Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supporting Information

Iridium-Catalysed Conjugated Alkynylation of α,β–Unsaturated Amide through Alkene Isomerization

Yun Chen, [a,c] Zi-Xuan Wang, [c] Qian Li,* [b] Li-Jin Xu* [a] and Bi-Jie Li* [c]

[a]Department of Chemistry, Renmin University of China, Beijing, 100872, China .

[b]The Affiliated High School of Peking University, Beijing, 100080, China..

[c]Center of Basic Molecular Science (CBMS), Department of Chemistry, Tsinghua University, Beijing, 100084, China.

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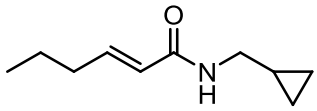
Materials and Methods

Unless otherwise noted, all reactions were assembled on a Schlenk vacuum line or in a glovebox using oven-dried glassware and were stirred with Teflon-coated magnetic stirring bars. All the ligands were purchased from Strem Chemicals and were used as received. $[Ir(cod)_2OTf]$[1] was prepared according to literature methods. Triisopropylsilylacetylene was purchased from Alfa Aesar. Dppb (1,4-bis(diphenylphosphino)butane) and DIOP were purchased from Aldrich and were used as received. Tetrahydrofuran (THF), 1,4-dioxane, toluene, 1,2-dichloroethane (DCE) were degassed by purging with nitrogen and then dried with a solvent purification system containing activated alumina. All other solvents and reagents were used as received. The α, β-unsaturated amides were prepared according to literature methods.[2] All work-up and purification procedures were carried out with reagent grade solvents in air. Reaction temperatures above 23 ℃ refer to temperatures of an aluminum heating block or a silicon oil bath, which were controlled by an electronic temperature modulator from IKA. NMR spectra were acquired on NMR spectrometer with 400 MHz for ^{1}H NMR and 101 MHz for ^{13}C NMR at the NMR facility at Center of Basic Molecular Science (CBMS). Chemical shifts (δ) are reported in ppm relative to the residual solvent signal (δ = 7.26 for ^{1}H NMR and δ = 77.16 for ^{13}C NMR). Data for ^{1}H NMR spectra are reported as follows: chemical shift (multiplicity, coupling constants, number of hydrogens). Abbreviations are as follows: s (singlet), d (doublet), t (triplet), q (quartet), m (multiplet), br (broad). Infrared (IR) spectra were recorded on a Bruker FT–IR alpha (ATR mode) spectrophotometer. High-resolution mass spectral data was performed on a Thermo Scientific Q Exactive (positive mode) at the Mass Spectrometry Facility, CBMS.

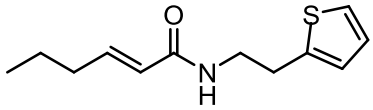
General Procedure for the Catalytic Alkynylation

In an N_2-filled glovebox, the α, β-unsaturated amide (0.20 mmol, 1.0 equiv), $Ir(cod)_2OTf$ (0.020 mmol, 10 mol%) and dppb (0.024 mmol, 12 mol%) were weighed into a one-dram screw-capped vial. Subsequently, 1,4-dioxane (0.40 mL) and alkyne (0.60 mmol, 3.0 equiv) were added via syringe. The vial was capped with a Teflon-lined screw cap, and the resulting solution was then removed from the glovebox, placed in a pre-heated aluminum block at 70 ℃ for 12 h. The reaction mixture was concentrated and purified directly by column chromatography on silica gel with EtOAc/hexanes mixture as eluent.

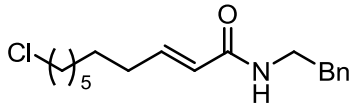
Characterization of Substrates



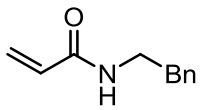
Enamide 1d: **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 6.81 (ddd, *J* = 15.3, 6.7, 2.4 Hz, 1H), 5.92 (s, 1H), 5.78 (dd, *J* = 15.3, 2.0 Hz, 1H), 3.23 – 3.10 (m, 2H), 2.12 (q, *J* = 7.0 Hz, 2H), 1.52 – 1.37 (m, 2H), 1.01-0.85 (m, 4H), 0.53 – 0.43 (m, 2H), 0.19 (t, *J* = 5.0 Hz, 2H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 166.17, 144.36, 123.92, 44.37, 34.11, 21.58, 13.74, 10.80, 3.46. **ESI-HR** calcd for $C_{10}H_{17}NNaO^+$ ($[M+Na]^+$) 190.1202, found 190.1199. **IR** ν (cm^{-1}) 3275, 3075, 1660, 1526, 977. **M. P.** 36-38 °C.



Enamide 1k: **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.15 (dd, *J* = 5.2, 1.3 Hz, 1H), 6.94 (dd, *J* = 5.2, 3.4 Hz, 1H), 6.86 – 6.77 (m, 2H), 5.84 – 5.69 (m, 2H), 3.58 (q, *J* = 6.5 Hz, 2H), 3.05 (t, *J* = 6.7 Hz, 2H), 2.13 (qd, *J* = 7.2, 1.5 Hz, 2H), 1.51 – 1.40 (m, 2H), 0.91 (t, *J* = 7.42 Hz, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 166.18, 144.93, 141.51, 127.15, 125.45, 124.02, 123.67, 40.91, 34.16, 30.06, 21.59, 13.81. **ESI-HR** calcd for $C_{12}H_{17}NNaOS^+$ ($[M+Na]^+$) 246.0923, found 246.0915. **IR** ν (cm^{-1}) 3275, 2866, 1667, 1627, 975, 686. **M. P.** 73-75 °C.

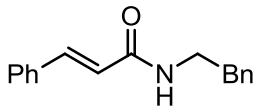


Enamide 1n: **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.36 – 7.28 (m, 2H), 7.26 – 7.17 (m, 3H), 6.87 – 6.75 (m, 1H), 5.68 (d, *J* = 15.2 Hz, 1H), 5.41 (s, 1H), 3.63-3.49 (m, 4H), 2.85 (td, *J* = 6.9, 1.9 Hz, 2H), 2.15 (q, *J* = 7.3 Hz, 2H), 1.82 – 1.69 (m, 2H), 1.48-1.36 (m, 4H), 1.31 (dq, *J* = 6.6, 3.1 Hz, 4H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 166.09, 144.94, 139.09, 128.93, 128.80, 126.66, 123.66, 45.26, 40.70, 35.84, 32.69, 32.07, 29.09, 28.79, 28.26, 26.89. **ESI-HR** calcd for $C_{18}H_{26}ClNNaO^+$ ($[M+Na]^+$) 330.1595, found 330.1588. **IR** ν (cm^{-1}) 3280, 2926, 1668, 1626, 757. **M. P.** 76-78 °C.



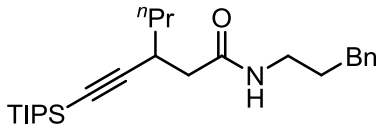
Enamide 1r: **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.31 (dd, *J* = 8.2, 6.7 Hz, 2H), 7.28 – 7.22 (m, 1H), 7.20 (d, *J* = 7.6 Hz, 2H), 6.25 (dd, *J* = 17.0, 1.5 Hz, 1H), 6.05 (ddd, *J* = 17.0, 10.3, 4.0 Hz, 1H), 5.94 – 5.70 (m, 1H), 5.61 (dt, *J* = 10.3, 1.5 Hz, 1H), 3.64-3.53 (m, 2H), 2.85 (t, *J* = 7.0 Hz,

2H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 165.63, 138.91, 130.96, 128.86, 128.76, 126.65, 126.44, 40.79, 35.69. **ESI-HR** calcd for $C_{11}H_{13}NNaO^+$ ($[M+Na]^+$) 198.0889, found 198.0884. **IR** ν (cm^{-1}) 3278, 3062, 1660, 1624, 805. **M. P.** 60-62 °C.

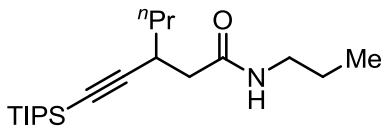


Enamide 1s: ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.62 (d, *J* = 15.6 Hz, 1H), 7.48 (dd, *J* = 6.7, 2.9 Hz, 2H), 7.36 (dd, *J* = 5.4, 3.5 Hz, 3H), 7.32 (d, *J* = 7.4 Hz, 2H), 7.27 – 7.20 (m, 3H), 6.33 (d, *J* = 15.6 Hz, 1H), 5.72 (s, 1H), 3.66 (d, *J* = 6.5 Hz, 2H), 2.90 (t, *J* = 6.9 Hz, 2H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 165.97, 141.17, 139.00, 134.93, 129.78, 128.94, 128.92, 128.82, 127.91, 126.69, 120.73, 40.94, 35.80. **ESI-HR** calcd for $C_{17}H_{17}NNaO^+$ ($[M+Na]^+$) 274.1202, found 274.1195. **IR** ν (cm^{-1}) 3293, 3048, 1651, 1538, 974. **M. P.** 120-122 °C.

Characterization of Products

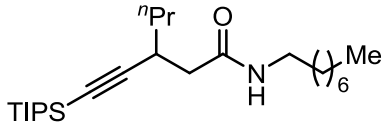


Amide 3a: ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.30 (t, *J* = 7.4 Hz, 2H), 7.23 (d, *J* = 7.1 Hz, 1H), 7.19 (d, *J* = 7.7 Hz, 2H), 5.98 (s, 1H), 3.50 (ddq, *J* = 33.8, 13.6, 6.8 Hz, 2H), 2.83 (dt, *J* = 14.3, 6.9 Hz, 3H), 2.31 (t, *J* = 6.0 Hz, 2H), 1.59 – 1.50 (m, 1H), 1.44 (q, *J* = 7.7, 6.8 Hz, 3H), 1.11-0.95 (m, 21H), 0.91 (t, *J* = 6.4 Hz, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 171.01, 139.00, 128.83, 128.71, 126.59, 111.17, 82.56, 42.87, 40.88, 37.09, 35.96, 29.63, 20.46, 18.74, 13.85, 11.31. **ESI-HR** calcd for $C_{25}H_{41}NNaOSi^+$ ($[M+Na]^+$) 422.2850, found 422.2842. **IR** ν (cm^{-1}) 2939, 2864. 1650, 1262, 883. **M. P.** 50-52 °C.

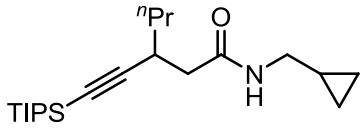


Amide 3b: ^{1}H NMR (400 MHz, Chloroform-*d*) δ 6.04 (s, 1H), 3.20 (dp, *J* = 19.4, 6.6 Hz, 2H), 2.85 (q, *J* = 6.9 Hz, 1H), 2.41 – 2.26 (m, 2H), 1.59 – 1.51 (m, 2H), 1.51 – 1.45 (m, 2H), 1.43 (d, *J* = 6.4 Hz, 2H), 1.22 – 1.13 (m, 1H), 1.11-0.98 (m, 21H), 0.90 (t, *J* = 7.1 Hz, 5H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 171.04, 111.31, 82.57, 42.91, 41.40, 37.21, 29.70, 23.00, 20.45, 18.72, 13.84,

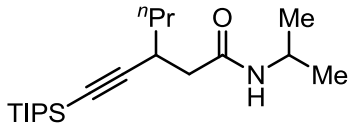
11.55, 11.32. **ESI-HR** calcd for $C_{20}H_{39}NNaOSi^+$ ([M+Na]$^+$) 360.2693, found 360.2682. **IR** ν (cm^{-1}) 3285, 2165, 1643, 883.



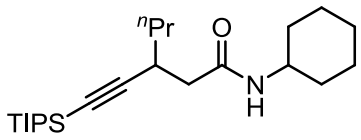
Amide 3c: ^{1}**H NMR** (400 MHz, Chloroform-*d*) δ 5.98 (s, 1H), 5.58 (s, 1H), 3.23 (q, *J* = 6.7 Hz, 2H), 3.05 (d, *J* = 7.8 Hz, 2H), 2.16 (q, *J* = 7.5 Hz, 2H), 1.48 (t, *J* = 7.1 Hz, 2H), 1.26 (dd, *J* = 8.4, 3.9 Hz, 12H), 1.12 (d, *J* = 7.5 Hz, 3H), 1.11-0.98 (m, 21H), 0.87 (t, *J* = 6.6 Hz, 3H). ^{13}**C NMR** (101 MHz, $CDCl_3$) δ 169.88, 129.89, 128.67, 107.98, 89.88, 39.88, 36.22, 31.92, 29.73, 29.38, 29.34, 27.03, 24.39, 22.77, 18.78, 14.22, 13.02, 11.44. **ESI-HR** calcd for $C_{25}H_{49}NNaOSi^+$ ([M+Na]$^+$) 430.3476, found 430.3367. **IR** ν (cm^{-1}) 3280, 2140, 1644, 882.



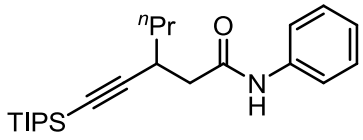
Amide 3d: ^{1}**H NMR** (400 MHz, Chloroform-*d*) δ 6.00 (s, 1H), 3.21 – 3.05 (m, 2H), 2.87 (ddt, *J* = 11.2, 7.7, 3.8 Hz, 1H), 2.40 – 2.30 (m, 2H), 1.57 – 1.40 (m, 4H), 1.11-0.98 (m, 21H), 0.92 (dd, *J* = 7.9, 5.1 Hz, 4H), 0.53 – 0.45 (m, 2H), 0.19 (q, *J* = 5.1 Hz, 2H). ^{13}**C NMR** (101 MHz, $CDCl_3$) δ 170.99, 111.28, 82.51, 44.54, 43.00, 37.26, 29.70, 20.49, 18.77, 13.90, 11.35, 10.82, 3.56. **ESI-HR** calcd for $C_{21}H_{39}NNaOSi^+$ ([M+Na]$^+$) 372.2693, found 372.2680. **IR** ν (cm^{-1}) 3286, 2166, 1644, 883.



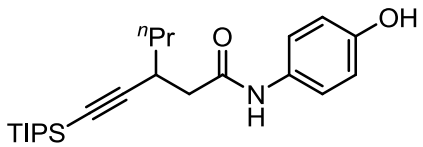
Amide 3e: ^{1}**H NMR** (400 MHz, Chloroform-*d*) δ 5.68 (s, 1H), 3.99 (hept, *J* = 6.7 Hz, 1H), 2.74 (dd, *J* = 9.4, 4.5 Hz, 1H), 2.26 – 2.14 (m, 2H), 1.50 – 1.40 (m, 1H), 1.40 – 1.28 (m, *J* = 5.2 Hz, 3H), 1.03 (d, *J* = 6.5 Hz, 6H), 1.11-0.95 (m, 21H), 0.81 (t, *J* = 6.5 Hz, 3H). ^{13}**C NMR** (101 MHz, $CDCl_3$) δ 170.16, 111.41, 82.46, 43.01, 41.51, 37.29, 29.65, 22.88, 20.44, 18.78, 13.86, 11.37.**ESI-HR** calcd for $C_{20}H_{39}NNaOSi^+$ ([M+Na]$^+$) 360.2693, found 360.2681. **IR** ν (cm^{-1}) 3281, 2161, 1665, 885.



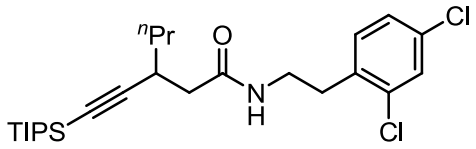
Amide 3f: **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 5.74 (s, 1H), 3.85 – 3.70 (m, 1H), 2.85 (dt, *J* = 8.1, 3.4 Hz, 1H), 2.39 – 2.24 (m, 2H), 1.97 – 1.87 (m, 2H), 1.70 (dt, *J* = 13.5, 3.8 Hz, 2H), 1.65 – 1.55 (m, 2H), 1.55 – 1.48 (m, 1H), 1.45 (q, *J* = 6.2, 5.0 Hz, 2H), 1.43 – 1.32 (m, 2H), 1.31 – 1.22 (m, 1H), 1.22 – 1.12 (m, 2H), 1.11-1.02 (m, 21H), 0.91 (t, *J* = 6.3 Hz, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 170.11, 111.41, 82.44, 48.44, 43.06, 37.25, 33.35, 29.68, 25.74, 25.10, 20.47, 18.81, 13.90, 11.37. **ESI-HR** calcd for $C_{23}H_{43}NNaOSi^+$ ($[M+Na]^+$) 400.3006, found 400.2993. **IR** ν (cm^{-1}) 3281, 2934, 1642, 885. **M. P.** 105-107 °C.



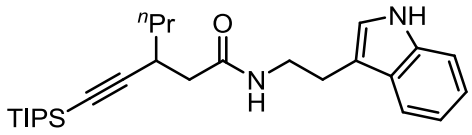
Amide 3g: **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.59 (s, 1H), 7.50 (d, *J* = 8.0 Hz, 2H), 7.31 (t, *J* = 7.9 Hz, 2H), 7.10 (t, *J* = 7.4 Hz, 1H), 2.97 (q, *J* = 6.6 Hz, 1H), 2.56 – 2.48 (m, 2H), 1.56 (d, *J* = 4.9 Hz, 2H), 1.52 (d, *J* = 4.4 Hz, 2H), 1.11-0.98 (m, 21H), 0.97 – 0.92 (m, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 170.23, 111.74, 81.07, 42.41, 40.66, 38.76, 37.44, 29.60, 20.65, 18.76, 14.73, 13.94, 13.32, 11.40. **ESI-HR** calcd for $C_{23}H_{37}NNaOSi^+$ ($[M+Na]^+$) 394.2537, found 394.2530. **IR** ν (cm^{-1}) 3286, 2834, 1642, 885.



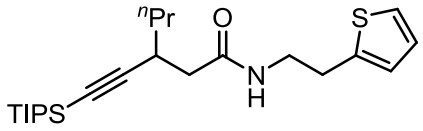
Amide 3h: **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.32 (d, *J* = 16.0 Hz, 1H), 7.05 – 6.94 (m, 2H), 6.85 – 6.76 (m, 2H), 6.15 (s, 1H), 3.48 (dp, *J* = 35.2, 6.8 Hz, 2H), 2.84 (p, *J* = 6.8 Hz, 1H), 2.73 (t, *J* = 7.2 Hz, 2H), 2.38 – 2.29 (m, 2H), 1.53 (q, *J* = 7.5 Hz, 1H), 1.43 (q, *J* = 9.9, 6.8 Hz, 3H), 1.11-0.98 (m, 21H), 0.94 – 0.85 (m, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 171.78, 155.31, 129.89, 129.77, 115.75, 110.93, 82.93, 42.74, 41.29, 37.06, 34.99, 29.65, 20.43, 18.75, 13.81, 11.32. **ESI-HR** calcd for $C_{25}H_{41}NNaO_2Si^+$ ($[M+Na]^+$) 438.2799, found 438.2789. **IR** ν (cm^{-1}) 2865, 1647, 1514, 1256, 885.



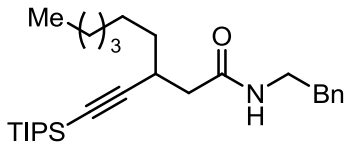
Amide 3i: **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.36 (d, *J* = 1.7 Hz, 1H), 7.17 (d, *J* = 2.4 Hz, 2H), 6.12 (s, 1H), 3.49 (dp, *J* = 23.5, 6.7 Hz, 2H), 2.92 (t, *J* = 7.1 Hz, 2H), 2.88 – 2.77 (m, 1H), 2.32 (dd, *J* = 7.0, 2.5 Hz, 2H), 1.54 (tt, *J* = 9.8, 4.4 Hz, 1H), 1.49 – 1.35 (m, 3H), 1.11-0.98 (m, 21H), 0.91 (t, *J* = 6.6 Hz, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 171.22, 135.37, 134.90, 133.16, 131.86, 129.50, 127.34, 111.18, 82.91, 42.81, 39.19, 37.19, 33.17, 29.62, 20.46, 18.73, 13.83, 11.34. **ESI-HR** calcd for $C_{25}H_{39}Cl_2NNaOSi^+$ ($[M+Na]^+$) 490.2070, found 490.2061. **IR** ν (cm^{-1}) 2942, 2865, 1652, 1264, 885. **M. P.** 61-63 °C.



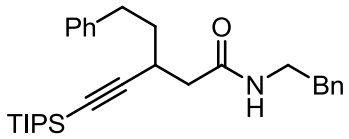
Amide 3j: **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 8.33 (s, 1H), 7.61 (d, *J* = 7.8 Hz, 1H), 7.37 (d, *J* = 8.1 Hz, 1H), 7.20 (t, *J* = 7.5 Hz, 1H), 7.12 (t, *J* = 7.4 Hz, 1H), 7.02 (d, *J* = 2.3 Hz, 1H), 6.02 (t, *J* = 5.6 Hz, 1H), 3.61 (dp, *J* = 28.0, 6.5 Hz, 2H), 2.98 (t, *J* = 7.1 Hz, 2H), 2.94 – 2.82 (m, 1H), 2.32 (h, *J* = 8.0 Hz, 2H), 1.55 (dddd, *J* = 13.0, 10.2, 7.3, 3.5 Hz, 1H), 1.45 (dt, *J* = 16.2, 5.3 Hz, 3H), 1.04 (d, *J* = 5.3 Hz, 21H), 0.92 (t, *J* = 6.6 Hz, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 171.10, 136.54, 127.48, 122.22, 122.06, 119.52, 118.78, 113.08, 111.38, 111.16, 82.49, 42.96, 40.07, 37.12, 29.65, 25.59, 20.47, 18.72, 13.86, 11.32. **ESI-HR** calcd for $C_{27}H_{42}N_2NaOSi^+$ ($[M+Na]^+$) 461.2959, found 461.2951. **IR** ν (cm^{-1}) 3307, 2865, 1648, 1460, 884. **M. P.** 100-102 °C.



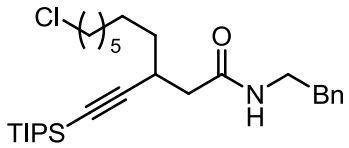
Amide 3k: **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.15 (d, *J* = 5.1 Hz, 1H), 6.94 (dd, *J* = 5.2, 3.5 Hz, 1H), 6.83 (d, *J* = 3.4 Hz, 1H), 6.06 (s, 1H), 3.52 (ddq, *J* = 33.1, 13.3, 6.7 Hz, 2H), 3.03 (t, *J* = 6.9 Hz, 2H), 2.92 – 2.81 (m, 1H), 2.39 – 2.26 (m, 2H), 1.54 (ddt, *J* = 13.1, 7.5, 3.2 Hz, 1H), 1.44 (pd, *J* = 10.5, 10.0, 4.0 Hz, 3H), 1.11-0.98 (m, 21H), 0.92 (t, *J* = 6.6 Hz, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 171.09, 141.42, 127.14, 125.39, 124.00, 111.12, 82.64, 42.88, 41.09, 37.10, 30.14, 29.64, 20.48, 18.75, 13.87, 11.32. **ESI-HR** calcd for $C_{23}H_{39}NNaOSSi^+$ ($[M+Na]^+$) 428.2414, found 428.3312. **IR** ν (cm^{-1}) 3283, 2166, 1646, 1545, 883. **M. P.** 56-58 °C.



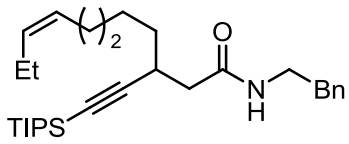
Amide 3l: **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.30 (dt, *J* = 7.7, 4.1 Hz, 2H), 7.26 – 7.21 (m, 1H), 7.19 (d, *J* = 7.6 Hz, 2H), 5.98 (s, 1H), 3.63 – 3.41 (m, 2H), 2.83 (qd, *J* = 8.9, 7.3, 4.2 Hz, 3H), 2.39 – 2.22 (m, 2H), 1.56 – 1.46 (m, 2H), 1.45 – 1.37 (m, 3H), 1.34 – 1.20 (m, 6H), 1.09 – 0.94 (m, 21H), 0.88 (td, *J* = 6.8, 2.2 Hz, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 171.02, 139.02, 128.83, 128.71, 126.59, 111.26, 82.61, 42.90, 40.88, 35.97, 34.99, 31.86, 29.89, 28.97, 27.19, 22.66, 18.75, 14.18, 11.33. **ESI-HR** calcd for $C_{28}H_{47}NNaOSi^+$ ($[M+Na]^+$) 464.3319, found 464.3311. **IR** ν (cm^{-1}) 3283, 2165, 1645, 882. **M. P.** 64-66 °C.



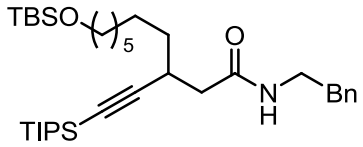
Amide 3m: **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.32 – 7.28 (m, 2H), 7.26 (d, *J* = 3.2 Hz, 2H), 7.22 (d, *J* = 7.5 Hz, 1H), 7.20 (q, *J* = 2.7, 1.9 Hz, 2H), 7.18 (t, *J* = 1.8 Hz, 2H), 7.17 (s, 1H), 5.89 (s, 1H), 3.51 (dddd, *J* = 20.5, 19.2, 13.4, 7.0 Hz, 2H), 2.89 (dtd, *J* = 13.6, 9.2, 8.7, 5.0 Hz, 2H), 2.81 (t, *J* = 7.2 Hz, 2H), 2.78 – 2.69 (m, 1H), 2.34 (qd, *J* = 14.3, 7.0 Hz, 2H), 1.82 (dddd, *J* = 14.2, 9.6, 7.1, 4.6 Hz, 1H), 1.76 – 1.66 (m, 1H), 1.16 – 0.97 (m, 21H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 170.71, 141.71, 138.93, 128.81, 128.72, 128.61, 128.54, 126.60, 126.07, 110.65, 83.40, 42.80, 40.88, 36.94, 35.92, 33.65, 29.55, 18.80, 11.34. **ESI-HR** calcd for $C_{30}H_{43}NNaOSi^+$ ($[M+Na]^+$) 484.3006, found 484.2999. **IR** ν (cm^{-1}) 3286, 2162, 1666, 883.



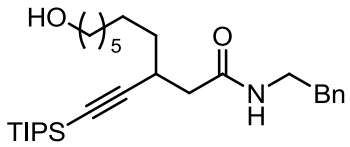
Amide 3n: **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.30 (t, *J* = 7.4 Hz, 2H), 7.23 (d, *J* = 7.1 Hz, 1H), 7.18 (d, *J* = 7.6 Hz, 2H), 5.99 (s, 1H), 3.51 (tq, *J* = 13.5, 6.9 Hz, 4H), 2.82 (q, *J* = 7.6 Hz, 3H), 2.39 – 2.23 (m, 2H), 1.75 (p, *J* = 6.9 Hz, 2H), 1.57 – 1.46 (m, 2H), 1.46 – 1.36 (m, 4H), 1.29 (qd, *J* = 10.5, 9.7, 5.7 Hz, 4H), 1.11-0.98 (m, 21H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 170.92, 138.96, 128.79, 128.68, 126.56, 111.09, 82.60, 45.18, 42.82, 40.85, 35.92, 34.84, 32.70, 29.81, 29.08, 28.87, 27.10, 26.86, 18.72, 11.29. **ESI-HR** calcd for $C_{29}H_{48}ClNNaOSi^+$ ($[M+Na]^+$) 512.3086, found 512.3076. **IR** ν (cm^{-1}) 3287, 2164, 1648, 882.



Amide 3o: **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.36 – 7.30 (m, 2H), 7.24 (dd, *J* = 17.6, 7.0 Hz, 3H), 5.98 (s, 1H), 5.37 (dtq, *J* = 17.7, 11.0, 6.6 Hz, 2H), 3.65 – 3.42 (m, 2H), 2.91 – 2.80 (m, 3H), 2.40 – 2.28 (m, 2H), 2.05 (q, *J* = 7.1 Hz, 4H), 1.59 – 1.33 (m, 6H), 1.11-0.98 (m, 21H), 0.98 (td, *J* = 7.5, 2.1 Hz, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 170.97, 139.01, 131.91, 129.04, 128.83, 128.72, 126.60, 111.15, 82.71, 42.89, 40.88, 35.98, 34.91, 29.88, 29.48, 27.14, 26.94, 20.64, 18.76, 14.50, 11.34. **ESI-HR** calcd for $C_{30}H_{49}NNaOSi^+$ ($[M+Na]^+$) 490.3476, found 490.3470. **IR** ν (cm^{-1}) 3283, 2166, 1646, 1547, 883.



Amide 3p: **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.30 (t, *J* = 7.7 Hz, 2H), 7.24 – 7.17 (m, 3H), 5.94 (s,1H), 3.57 (dt, *J* = 13.7, 6.7 Hz, 3H), 3.48 (td, *J* = 13.7, 6.9 Hz, 1H), 2.81 (t, *J* = 7.2 Hz, 3H), 2.36 – 2.25 (m, 2H), 1.51 (dd, *J* = 12.2, 6.1 Hz, 4H), 1.41 (dd, *J* = 13.5, 6.0 Hz, 2H), 1.30 (d, *J* = 9.6 Hz, 6H), 1.11-0.98 (m, 21H), 0.89 (s, 9H), 0.04 (s, 6H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 171.03, 139.01, 128.85, 128.73, 126.61, 111.22, 82.67, 63.43, 42.91, 40.89, 35.98, 35.00, 33.01, 29.90, 29.52, 29.36, 27.26, 26.14, 25.87, 18.77, 18.19, 11.33, -5.11. **ESI-HR** calcd for $C_{35}H_{63}NNaO_2Si^+$ ($[M+Na]^+$) 608.4290, found 608.4279. **IR** ν (cm^{-1}) 2933, 2860, 1651, 883.



Amide 3q: **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.29 (t, *J* = 7.4 Hz, 2H), 7.20 (dd, *J* = 16.5, 7.4 Hz, 3H), 6.04 (m, 1H), 3.60 (t, *J* = 6.7 Hz, 2H), 3.48 (ddt, *J* = 33.6, 13.4, 6.8 Hz, 2H), 2.81 (q, *J* = 7.3 Hz, 3H), 2.36 – 2.24 (m, 2H), 1.54 (p, *J* = 6.6 Hz, 3H), 1.49 – 1.39 (m, 3H), 1.38 – 1.22 (m, 7H), 1.11-0.98 (m, 21H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 171.04, 138.97, 128.79, 128.67, 126.55, 111.16, 82.56, 62.99, 42.77, 40.86, 35.90, 34.85, 32.85, 29.80, 29.37, 29.19, 27.11, 25.73, 18.72, 11.30. **ESI-HR** calcd for $C_{29}H_{49}NNaO_2Si^+$ ($[M+Na]^+$) 494.3425, found 494.3415. **IR** ν (cm^{-1}) 2933, 2860, 1651, 883.

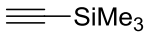
DFT Computational Studies

General Information for Computation

All calculations were performed with the Gaussian 09 program.[3] Density functional theory calculations using the M06 functional.[4] Geometry optimizations were conducted with the Gaussian 09 software package, B3LYP functional (with gd3 dispersion correction), and LANL2DZ basis set for Rh and 6-31g(d,p) basis set for all other atoms. The keyword "5D" in

Gaussian 09 program was used to specify that five (instead of six) *d*-type STO orbitals were used as basis sets in all elements of the calculations. Frequency calculations at the same level had been performed to confirm each stationary point to be either a minimum or a transition structure. Single-point energy calculations were conducted with the M06 functional and SDD basis set for Rh and the 6-31++g(d,p) basis set for all other atoms, along with the SMD 1,4-dioxane solvent correction. Thermal corrections were applied to the optimized geometries to provide Gibbs free energies.

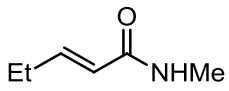
Coordinates and Energies of Stationary Point



2

G_{sol} = -485.903138033 Hatree

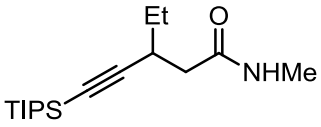
C	2.76117	0.00042	0.00024
H	3.82813	0.00053	0.0002
C	1.54559	0.00029	0.00031
Si	-0.30018	-0.00011	-0.00007
C	-0.8999	-1.7642	-0.30589
H	-0.54551	-2.44484	0.47475
H	-1.99503	-1.80516	-0.3148
H	-0.54251	-2.14425	-1.26822
C	-0.90059	1.14679	-1.37454
H	-1.99573	1.17173	-1.40702
H	-0.5465	2.17101	-1.2201
H	-0.54377	0.81388	-2.35438
C	-0.9011	0.61701	1.68009
H	-1.99624	0.62793	1.71953
H	-0.54295	-0.02531	2.4909
H	-0.54848	1.6341	1.87878



1

G_{sol} = -365.084272275 Hatree

C	1.28125	0.59104	0.42105
C	0.36632	-0.2135	-0.21052
H	0.66515	-1.00026	-0.89994
C	-1.07547	0.11829	-0.14268
O	-1.20527	1.29414	-0.57373
N	-2.03727	-0.70065	0.21844
H	-1.76552	-1.62075	0.54555
C	-3.47	-0.36603	0.17088
H	-3.58143	0.66708	-0.15672
H	-3.97677	-1.02768	-0.53469
H	-3.90341	-0.48411	1.1656
H	0.90343	1.44634	0.9794
C	2.74615	0.38575	0.42793
H	3.17692	1.33392	0.05697
H	3.06297	0.37873	1.48449
C	3.30654	-0.81352	-0.33365
H	2.93318	-1.75982	0.06937
H	3.06509	-0.76552	-1.40007
H	4.39473	-0.82859	-0.24723

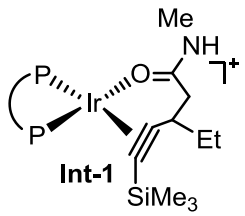


3

G_{sol} = -851.034212866 Hatree

C	-0.92286	0.32522	-0.72924
C	0.50526	0.12058	-0.46867
H	-1.64749	-0.30596	1.23854
C	-1.77315	-0.58669	0.18733
H	-1.40703	-1.61596	0.09242
C	-3.24466	-0.58801	-0.22469
O	-3.59071	-0.52157	-1.39991
N	-4.13367	-0.69384	0.80799
H	-3.77467	-0.74818	1.74877
C	-5.56817	-0.78084	0.59961
H	-5.74447	-0.69598	-0.47314
H	-5.96748	-1.73857	0.95286
H	-6.09347	0.03097	1.11482
C	1.69202	-0.04134	-0.23946
Si	3.48366	-0.29546	0.07984
C	3.85106	-2.14981	0.07707
H	3.59774	-2.60242	-0.88716
H	4.91456	-2.33655	0.2657

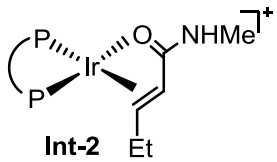
H	3.2775	-2.67049	0.85092
C	4.48024	0.56186	-1.27806
H	4.2379	0.15493	-2.26516
H	4.2762	1.63732	-1.30165
H	5.5559	0.42808	-1.11487
C	3.92114	0.44549	1.76357
H	4.98771	0.31642	1.98106
H	3.70137	1.51774	1.79438
H	3.35525	-0.03436	2.56885
H	-1.14048	0.00322	-1.75564
C	-1.31253	1.82605	-0.64092
H	-0.71185	2.36691	-1.3807
H	-2.35606	1.91516	-0.96173
C	-1.1206	2.47004	0.73531
H	-1.78183	2.03092	1.4904
H	-0.08902	2.35715	1.0837
H	-1.3468	3.54021	0.69225



G_{sol} = -2721.30215705 Hatree

Ir	0.06781	-0.3662	-0.05699
C	-0.97484	-3.16273	1.09081
C	-1.2495	-2.01716	0.18426
H	0.73898	-4.48023	1.43509
C	4.18952	-1.3398	0.90283
C	4.08649	-0.11856	-1.17783
C	5.27887	-2.06907	0.41909
H	3.83058	-1.54576	1.90608
C	5.17447	-0.84562	-1.65911
H	3.6382	0.64546	-1.80565
C	5.77521	-1.82366	-0.86164
H	5.74518	-2.81992	1.05044
H	5.5595	-0.64115	-2.65377
H	6.62958	-2.38186	-1.23258
C	2.59418	2.33063	0.23561
C	3.60775	3.0074	0.93687
C	1.99576	2.95943	-0.86366
C	3.99411	4.2907	0.5543
H	4.10789	2.53527	1.77662
C	2.38699	4.24389	-1.24886
H	1.21945	2.44611	-1.41776
C	3.38262	4.91276	-0.53797
H	4.77523	4.80415	1.10677
H	1.90715	4.71804	-2.09955
H	3.68556	5.91287	-0.83273
C	-1.65053	2.63433	-0.54992
C	-1.28804	2.46478	-1.89289
C	-2.295	3.82293	-0.16673
C	-1.55042	3.46329	-2.8341
H	-0.80135	1.54141	-2.19317
C	-2.55266	4.82159	-1.10508
H	-2.61079	3.97255	0.86102
C	-2.17936	4.64471	-2.44004
H	-1.26812	3.31505	-3.8723
H	-3.04908	5.73616	-0.79496
H	-2.38442	5.42281	-3.16919
C	-2.9961	0.79383	1.19984
C	-3.26324	0.37243	2.51127
C	-4.05124	0.81793	0.27504
C	-4.55158	-0.01372	2.88715
H	-2.4751	0.34847	3.25508
C	-5.33809	0.4296	0.6505
H	-3.87521	1.16121	-0.73848
C	-5.5921	0.01114	1.95772
H	-4.74162	-0.32518	3.91012
H	-6.14392	0.46672	-0.07668
H	-6.5945	-0.28463	2.25192
C	2.30006	0.5458	2.54048
H	3.36707	0.64879	2.76511
H	2.01377	-0.47122	2.82885
C	-0.66388	2.27209	2.1337
H	0.05969	2.98322	1.72244
H	-1.5018	2.86781	2.50699
C	-0.03031	1.45903	3.29078
H	-0.44907	1.83296	4.23095
H	-0.31458	0.40239	3.22719
C	1.50247	1.54871	3.38992
H	1.79164	1.35917	4.43062
H	1.8286	2.57157	3.1703
C	3.58366	-0.35269	0.11157
C	0.55783	-3.45731	1.09355
H	1.03684	-2.77817	1.80727
C	1.23294	-3.20544	-0.24139

O	1.27223	-2.06677	-0.7713
N	1.82547	-4.23983	-0.85089
H	1.80157	-5.14038	-0.39707
C	2.53002	-4.11043	-2.12527
H	1.8439	-3.77332	-2.90649
H	3.34662	-3.38958	-2.0386
H	2.93299	-5.08628	-2.39713
P	2.11115	0.6113	0.68582
P	-1.2943	1.2999	0.67519
C	-1.64859	-1.52392	-0.91003
Si	-2.56337	-1.80533	-2.52106
C	-1.49982	-3.01054	-3.51975
H	-1.36194	-3.96002	-2.99201
H	-1.96968	-3.23133	-4.48489
H	-0.51082	-2.58394	-3.71804
C	-4.22488	-2.58699	-2.08202
H	-4.08906	-3.52136	-1.52741
H	-4.82901	-1.91722	-1.4624
H	-4.79617	-2.81835	-2.98812
C	-2.81437	-0.24095	-3.53906
H	-3.39991	-0.48857	-4.43204
H	-3.35209	0.54307	-2.99951
H	-1.86161	0.17542	-3.87977
H	-1.48231	-4.03145	0.64589
C	-1.52189	-2.97298	2.52182
H	-1.00904	-2.11825	2.98068
H	-2.57708	-2.69225	2.44238
C	-1.38443	-4.21373	3.41037
H	-1.87868	-5.08237	2.96091
H	-0.33848	-4.48091	3.59464
H	-1.84946	-4.0405	4.38508

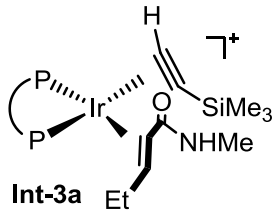


Int-2 Et

G_{sol} = -2235.3437014 Hatree

Ir	-0.09532	-0.66642	0.24083
P	-1.64499	0.63568	-0.76883
P	1.75961	0.48322	-0.63994
C	-3.37275	0.20458	-0.26824
C	-4.34614	-0.27194	-1.15859
C	-3.71699	0.3679	1.08514
C	-5.63355	-0.57643	-0.70643
H	-4.11689	-0.41618	-2.20882
C	-5.00152	0.06552	1.53333
H	-2.9806	0.74864	1.78737
C	-5.96413	-0.40855	0.6374
H	-6.37576	-0.9416	-1.40981
H	-5.25491	0.209	2.57956
H	-6.96604	-0.64006	0.98558
C	-1.55859	2.40474	-0.25463
C	-2.32782	3.38502	-0.90503
C	-0.76675	2.77902	0.84031
C	-2.2874	4.71154	-0.47824
H	-2.97133	3.11814	-1.73827
C	-0.73031	4.1081	1.26919
H	-0.17842	2.02753	1.35965
C	-1.48677	5.07572	0.60804
H	-2.88395	5.46025	-0.99054
H	-0.1104	4.3827	2.11711
H	-1.4588	6.10939	0.93912
C	2.66857	1.43599	0.64672
C	2.98337	0.78161	1.85183
C	3.05146	2.77547	0.478
C	3.67469	1.45447	2.85812
H	2.68773	-0.25315	1.99622
C	3.73959	3.44563	1.49262
H	2.8234	3.30846	-0.4382
C	4.05326	2.78789	2.68185
H	3.91963	0.93754	3.78127
H	4.03269	4.48107	1.34775
H	4.59123	3.31018	3.46716
C	2.99052	-0.7238	-1.28542
C	4.36519	-0.44055	-1.25245
C	2.55154	-1.91889	-1.87578
C	5.28002	-1.33852	-1.80238
H	4.72405	0.47463	-0.79225
C	3.46988	-2.81255	-2.42874
H	1.49001	-2.1454	-1.89559
C	4.83492	-2.52432	-2.39084
H	6.34147	-1.11248	-1.76796
H	3.11966	-3.73411	-2.88406
H	5.55035	-3.22185	-2.81569
C	-1.71407	0.67097	-2.62951
H	-2.70423	1.04561	-2.90939
H	-1.67376	-0.3776	-2.94515
C	1.55648	1.66992	-2.0513

H	1.03975	2.55642	-1.67044
H	2.56747	1.98145	-2.33311
C	0.81639	1.10465	-3.28667
H	1.32163	1.50369	-4.17227
H	0.93156	0.01635	-3.35278
C	-0.66735	1.49424	-3.40453
H	-0.95	1.40541	-4.46024
H	-0.78111	2.55554	-3.1558
C	-0.91139	-2.65211	-0.08379
H	0.02396	-3.19659	-0.22913
C	-1.21954	-2.26936	1.25957
H	-2.2425	-2.17056	1.6093
C	-0.09222	-2.34614	2.20165
C	-1.96896	-3.01868	-1.09327
H	-2.87863	-2.43733	-0.92665
H	-1.60043	-2.77149	-2.09662
C	-2.29872	-4.52302	-1.03987
H	-1.40986	-5.13519	-1.22417
H	-2.7041	-4.80347	-0.06263
H	-3.04379	-4.77751	-1.79919
O	1.02076	-1.94472	1.71871
N	-0.23201	-2.72791	3.4736
H	-1.12448	-3.11864	3.74167
C	0.85215	-2.73324	4.4519
H	1.63637	-2.06286	4.1026
H	0.47679	-2.38412	5.41634
H	1.27187	-3.73709	4.57076

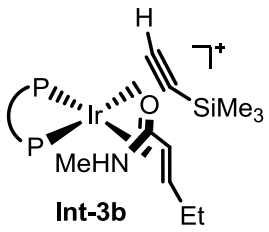


Int-3a

G_{sol} = -2721.26613623 Hatree

Ir	-0.05523	-0.39511	0.02519
P	-1.97816	0.82966	-0.7327
P	1.36738	1.51515	-0.20792
C	-3.50909	-0.09748	-1.22318
C	-3.68783	-0.54579	-2.54355
C	-4.50975	-0.37363	-0.27714
C	-4.83962	-1.24414	-2.90819
H	-2.93127	-0.35546	-3.29884
C	-5.65807	-1.07903	-0.6438
H	-4.40656	-0.02114	0.74427
C	-5.82711	-1.51393	-1.95861
H	-4.96473	-1.57457	-3.93494
H	-6.42423	-1.2774	0.09957
H	-6.72399	-2.0551	-2.24373
C	-2.62033	1.93254	0.59267
C	-3.58802	2.91239	0.30255
C	-2.20419	1.75293	1.92121
C	-4.0957	3.72377	1.31554
H	-3.96255	3.03577	-0.70924
C	-2.72533	2.56463	2.93392
H	-1.52004	0.9486	2.17599
C	-3.65885	3.55597	2.63284
H	-4.83772	4.4801	1.07834
H	-2.40836	2.40545	3.96013
H	-4.05922	4.18611	3.42133
C	2.3907	1.79588	1.30067
C	3.75402	1.47813	1.3721
C	1.75619	2.32871	2.4364
C	4.471	1.702	2.54957
H	4.26253	1.05684	0.51319
C	2.47536	2.54786	3.61116
H	0.69744	2.57023	2.41512
C	3.83559	2.23688	3.67025
H	5.52821	1.45664	2.58765
H	1.97247	2.96375	4.47899
H	4.3952	2.41037	4.58424
C	2.51655	1.36189	-1.63276
C	3.58158	2.25981	-1.82176
C	2.26018	0.39363	-2.61558
C	4.38211	2.17315	-2.96064
H	3.79411	3.024	-1.08038
C	3.05865	0.31399	-3.75894
C	4.12275	1.20058	-3.93023
H	5.20644	2.86729	-3.09277
H	2.85004	-0.43925	-4.51288
H	4.74635	1.13808	-4.81681
C	-1.74166	1.90001	-2.26652
H	-2.71407	1.89534	-2.76595
H	-1.05235	1.35164	-2.91875
C	0.69557	3.24652	-0.4474
H	-0.08261	3.41323	0.30395
H	1.53364	3.89461	-0.17283
C	0.19451	3.62735	-1.85151

H	0.35488	4.70591	-1.96406
H	0.81506	3.15644	-2.62198
C	-1.28474	3.36467	-2.13644
H	-1.52015	3.83728	-3.09796
H	-1.89442	3.88491	-1.39176
C	-0.76302	-2.56536	-0.15636
H	0.10848	-3.13845	0.15093
C	-1.49365	-1.95136	0.86333
H	-2.50356	-1.61374	0.65233
C	-1.27238	-2.15401	2.34667
C	-1.28768	-2.94827	-1.51785
H	-2.15597	-2.3448	-1.78193
H	-0.51505	-2.76136	-2.273
C	-1.6734	-4.44081	-1.55613
H	-0.81976	-5.08515	-1.31758
H	-2.47356	-4.6603	-0.84164
H	-2.02852	-4.71821	-2.55298
O	-1.4043	-1.23414	3.1552
N	-0.96828	-3.42831	2.71666
H	-0.96407	-4.14269	2.00474
C	-0.80846	-3.82775	4.10757
H	-0.90217	-2.93164	4.72061
H	-1.58222	-4.54417	4.402
H	0.17456	-4.28012	4.27308
C	1.30787	-1.05212	1.57934
H	1.10813	-0.79724	2.60408
C	1.9052	-1.57599	0.61054
Si	3.19387	-2.67507	-0.20698
C	3.54464	-4.04071	1.04937
H	2.65263	-4.64046	1.25693
H	4.31978	-4.71603	0.66971
H	3.89906	-3.6259	1.9983
C	2.52982	-3.41626	-1.80841
H	3.29907	-4.05605	-2.25559
H	1.64586	-4.03937	-1.64246
C	4.76464	-1.68849	-0.5398
H	5.53106	-2.35693	-0.94899
H	4.60445	-0.88428	-1.26283
H	5.16457	-1.25516	0.38197
H	1.43234	-0.29652	-2.47193
H	2.27521	-2.64658	-2.54234

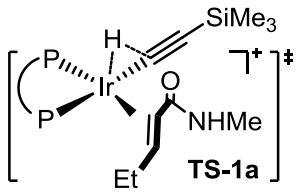


Int-3b

G_{sol} = -2721.26731345 Hatree

Ir	0.04045	-0.34796	0.38734
P	-1.73565	0.33519	-1.06562
P	1.48958	1.33866	-0.47669
C	-3.00823	-0.9575	-1.4435
C	-2.63869	-2.04471	-2.25554
C	-4.30708	-0.91965	-0.91467
C	-3.55045	-3.0603	-2.54136
H	-1.63308	-2.10679	-2.6627
C	-5.21769	-1.94101	-1.20093
H	-4.61534	-0.08955	-0.2887
C	-4.84365	-3.01109	-2.01389
H	-3.25194	-3.88879	-3.17663
H	-6.22284	-1.89311	-0.79243
H	-5.55414	-3.80061	-2.23836
C	-2.71143	1.79038	-0.51012
C	-3.75485	2.29968	-1.30561
C	-2.40603	2.42614	0.70252
C	-4.47019	3.42424	-0.89708
H	-4.01748	1.81531	-2.24164
C	-3.12714	3.55309	1.10848
H	-1.62578	2.02868	1.34397
C	-4.15478	4.05506	0.31009
H	-5.2727	3.80764	-1.51988
H	-2.88627	4.02909	2.05416
H	-4.71287	4.93115	0.62635
C	2.4103	2.1299	0.91111
C	3.73791	1.80083	1.2238
C	1.73095	3.05726	1.71987
C	4.37711	2.40314	2.30947
H	4.27816	1.07767	0.62381
C	2.37187	3.65276	2.80591
H	0.69683	3.31522	1.514
C	3.69778	3.32922	3.10177
H	5.40754	2.14499	2.53475
H	1.83409	4.36807	3.42052
H	4.19666	3.79461	3.94624
C	2.74691	0.77194	-1.69104

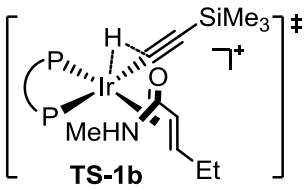
C	3.84007	1.57958	-2.05036
C	2.54382	-0.43812	-2.37051
C	4.71678	1.17215	-3.05574
H	4.01332	2.52441	-1.54453
C	3.41804	-0.83993	-3.38332
H	1.70027	-1.06476	-2.09417
C	4.50727	-0.03717	-3.72436
H	5.56154	1.80104	-3.31978
H	3.25004	-1.77911	-3.90199
H	5.18973	-0.34925	-4.50896
C	-1.21282	0.75899	-2.83155
H	-2.04295	0.41521	-3.45517
H	-0.35745	0.11777	-3.06812
C	0.8025	2.86548	-1.32412
H	-0.07205	3.20102	-0.75789
H	1.57967	3.62209	-1.17765
C	0.47668	2.76662	-2.82505
H	0.54028	3.78384	-3.22936
H	1.25485	2.1955	-3.34241
C	-0.90417	2.22267	-3.19655
H	-0.99757	2.29329	-4.28714
H	-1.67894	2.87992	-2.78977
C	-1.33018	-2.16508	1.01518
H	-2.24933	-2.01328	0.46149
C	-1.08209	-1.34622	2.10826
H	-0.3139	-1.65585	2.81098
C	-1.98725	-0.30869	2.71992
C	-0.72883	-3.53489	0.82393
H	-0.47678	-3.67801	-0.23239
H	0.19709	-3.62653	1.3972
C	-1.71963	-4.63308	1.25652
H	-1.97058	-4.54479	2.31851
H	-2.64983	-4.57601	0.68114
H	-1.28787	-5.62528	1.09378
O	-1.51494	0.63587	3.35326
N	-3.32553	-0.51236	2.56249
H	-3.62942	-1.36498	2.11723
C	-4.32365	0.3433	3.18808
H	-3.79713	1.05103	3.82835
H	-4.89833	0.90088	2.4408
H	-5.01132	-0.25148	3.7964
C	1.5594	-0.55149	1.95332
H	1.51565	0.07587	2.82432
C	1.96191	-1.4526	1.18339
Si	3.15998	-2.8299	0.70417
C	3.2859	-3.92914	2.23415
H	2.33363	-4.41187	2.47562
H	4.02566	-4.72036	2.06648
H	3.60414	-3.35604	3.11068
C	2.59447	-3.84359	-0.77958
H	1.67896	-4.40411	-0.57665
H	2.43434	-3.23071	-1.66967
H	3.37784	-4.57164	-1.0206
C	4.82551	-2.01861	0.34947
H	5.58506	-2.79101	0.18228
H	4.79094	-1.38651	-0.5424
H	5.15634	-1.40743	1.19512



G_{sol} = -2721.23458956 Hatree

Ir	0.12657	0.37417	-0.22461
C	-1.75015	1.09255	0.00417
H	-0.8773	0.71549	1.03056
C	3.76015	0.57219	-0.93514
C	4.06642	0.88124	-2.27159
C	4.51646	1.16527	0.08969
C	5.11461	1.7519	-2.57492
H	3.49811	0.44512	-3.0875
C	5.56178	2.03737	-0.2197
H	4.28634	0.95898	1.12986
C	5.86596	2.3296	-1.55005
H	5.34475	1.97338	-3.6127
H	6.13824	2.48493	0.58398
H	6.6831	3.00371	-1.78756
C	2.98718	-1.40328	1.00565
C	4.12616	-2.22716	0.9596
C	2.37288	-1.15257	2.24145
C	4.61544	-2.81704	2.12374
H	4.64484	-2.39853	0.02117
C	2.87331	-1.73904	3.4071
H	1.53011	-0.47184	2.29494
C	3.98585	-2.57824	3.3486
H	5.49234	-3.45537	2.07609
H	2.3996	-1.52573	4.36036

H	4.37236	-3.03425	4.25494
C	-1.98211	-1.98735	1.23694
C	-3.38148	-1.91924	1.19329
C	-1.34613	-2.23328	2.46597
C	-4.13079	-2.11027	2.35616
H	-3.88929	-1.71971	0.25702
C	-2.09971	-2.4203	3.62456
H	-0.26302	-2.27978	2.52819
C	-3.49395	-2.36109	3.57186
H	-5.21476	-2.06638	2.3077
H	-1.59716	-2.6159	4.56699
H	-4.07971	-2.51144	4.47353
C	-2.04675	-1.97617	-1.71355
C	-2.79425	-3.1592	-1.85801
C	-2.10954	-1.00353	-2.7219
C	-3.58921	-3.35699	-2.98573
H	-2.7701	-3.92487	-1.08826
C	-2.90335	-1.20749	-3.85257
C	-3.64324	-2.38245	-3.98593
H	-4.16584	-4.27165	-3.08355
H	-2.94346	-0.44667	-4.62618
H	-4.26137	-2.54027	-4.86448
C	2.55205	-1.82718	-1.91335
H	3.5981	-1.75396	-2.2244
H	1.95254	-1.44034	-2.74566
C	0.05565	-3.32216	-0.252
H	0.7739	-3.25444	0.57088
H	-0.6625	-4.09664	0.03436
C	0.75657	-3.71468	-1.5683
H	0.71477	-4.80711	-1.64073
H	0.19482	-3.34371	-2.43324
C	2.2286	-3.31312	-1.68275
H	2.64814	-3.84491	-2.5454
H	2.77494	-3.68365	-0.80936
C	0.42749	2.66386	-0.69249
H	-0.55422	3.09088	-0.50976
C	1.23483	2.32809	0.38566
H	2.29062	2.18111	0.20049
C	1.00496	2.55821	1.8605
C	0.92226	2.86454	-2.10202
H	1.88518	2.36802	-2.24545
H	0.20705	2.41408	-2.80177
C	1.05984	4.36653	-2.42621
H	0.10541	4.88982	-2.30878
H	1.79304	4.84491	-1.7702
H	1.38962	4.50011	-3.46041
O	1.91803	2.28468	2.6389
N	-0.18918	3.07591	2.25689
H	-0.9295	3.18565	1.57965
C	-0.49996	3.31883	3.65786
H	0.42492	3.22087	4.22566
H	-0.90109	4.32777	3.79061
H	-1.22999	2.59503	4.0387
P	2.37121	-0.58027	-0.5181
P	-0.94411	-1.74955	-0.26443
C	-2.87912	1.58493	0.10946
Si	-4.57485	2.33511	0.17916
C	-4.69619	3.33605	1.77581
H	-3.96709	4.15292	1.7985
H	-5.69225	3.78336	1.86793
H	-4.53182	2.70855	2.65772
C	-4.77189	3.45253	-1.3288
H	-5.76203	3.92191	-1.32763
H	-4.02528	4.25323	-1.33747
C	-5.8596	0.955	0.16214
H	-6.87137	1.37424	0.19527
H	-5.78148	0.3461	-0.74438
H	-5.74301	0.29586	1.02784
H	-1.54717	-0.08233	-2.61252
H	-4.67267	2.88808	-2.26148

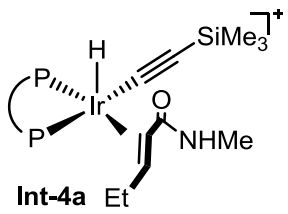


TS-1b

G_{sol} = -2721.23530754 Hatree

Ir	-0.014	0.35924	0.04286
C	1.78002	1.2318	-0.1524
H	0.94956	0.67637	-1.22674
C	-3.41954	0.35207	1.36583
C	-3.20227	0.72673	2.70431
C	-4.55801	0.83506	0.70438
C	-4.10739	1.55675	3.36543
H	-2.323	0.37597	3.23825
C	-5.46303	1.66671	1.37042
H	-4.74773	0.554	-0.32539
C	-5.24099	2.02942	2.69905

H	-3.92926	1.83073	4.40088
H	-6.34673	2.02329	0.84944
H	-5.94735	2.6725	3.21478
C	-3.03572	-1.4204	-0.93016
C	-4.23318	-2.14402	-0.77337
C	-2.49956	-1.25119	-2.21495
C	-4.87308	-2.69265	-1.88315
H	-4.67337	-2.27454	0.21103
C	-3.14796	-1.80153	-3.32449
H	-1.5961	-0.66663	-2.35296
C	-4.32894	-2.52467	-3.16038
H	-5.79543	-3.2502	-1.75181
H	-2.72779	-1.65607	-4.31492
H	-4.82973	-2.95376	-4.02299
C	2.43274	-1.7461	-1.20599
C	3.80837	-1.84316	-0.96208
C	1.96801	-1.71805	-2.53164
C	4.70496	-1.92116	-2.03086
H	4.1862	-1.85121	0.05396
C	2.86705	-1.79673	-3.59421
H	0.90591	-1.62251	-2.74008
C	4.23791	-1.89942	-3.34547
H	5.76964	-1.99857	-1.83181
H	2.49709	-1.77361	-4.61461
H	4.93763	-1.9608	-4.17333
C	2.08665	-1.88276	1.73227
C	2.77153	-3.07764	2.02041
C	2.08109	-0.85382	2.68631
C	3.43662	-3.23385	3.23565
H	2.79525	-3.88687	1.29678
C	2.74516	-1.01602	3.90386
H	1.57276	0.07868	2.46332
C	3.42239	-2.20392	4.17999
H	3.96493	-4.15888	3.44499
H	2.736	-0.21161	4.63308
H	3.93966	-2.32873	5.12639
C	-2.11076	-2.13021	1.78288
H	-3.08193	-2.0959	2.28479
H	-1.36359	-1.85162	2.53446
C	0.32409	-3.31183	-0.1301
H	-0.34737	-3.16933	-0.98382
H	1.12145	-3.97493	-0.48056
C	-0.40886	-3.98058	1.04696
H	-0.41269	-5.0576	0.84185
H	0.16741	-3.85848	1.97046
C	-1.86181	-3.5657	1.28693
H	-2.26299	-4.23165	2.06032
H	-2.45656	-3.76204	0.38895
C	-1.0347	2.46218	0.50543
H	-2.04977	2.21199	0.79897
C	-0.72286	2.42898	-0.84208
H	0.2159	2.86591	-1.17159
C	-1.65234	2.15687	-1.99863
C	-0.23619	3.18713	1.56188
H	-0.17845	2.56393	2.46316
H	0.78741	3.34576	1.21625
C	-0.90381	4.52837	1.92353
H	-0.9469	5.19483	1.05621
H	-1.92491	4.38201	2.29182
H	-0.33478	5.03429	2.70882
O	-1.2261	1.6522	-3.03501
N	-2.95099	2.53387	-1.82534
H	-3.18811	3.07377	-1.00659
C	-3.927	2.45081	-2.90319
H	-3.55552	1.73796	-3.63844
H	-4.88989	2.10778	-2.5146
H	-4.06808	3.42028	-3.394
P	-2.16831	-0.72461	0.52935
P	1.18756	-1.67463	0.14822
C	2.87191	1.79304	-0.28123
Si	4.51595	2.6289	-0.45329
C	4.33112	4.42743	0.08906
H	4.01233	4.50104	1.13405
H	5.2862	4.95648	-0.00393
H	3.59738	4.95772	-0.52673
C	5.762	1.73126	0.64457
H	5.46465	1.76068	1.69777
H	5.86404	0.68128	0.35258
H	6.75	2.19833	0.56405
C	5.02013	2.52443	-2.26891
H	5.99702	2.99673	-2.4225
H	5.09131	1.48427	-2.60194
H	4.29743	3.03503	-2.91337

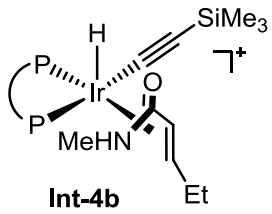


Int-4a

G_{sol} = -2721.2507635 Hatree

Ir	0.11263	0.36092	-0.20777
C	-1.75449	1.05308	0.00802
H	0.23423	0.00416	1.2769
C	3.70158	0.71756	-0.98982
C	3.89622	1.15027	-2.31297
C	4.50744	1.25912	0.02542
C	4.88176	2.09226	-2.61334
H	3.28975	0.75399	-3.12165
C	5.48813	2.20496	-0.27954
H	4.37232	0.94988	1.05675
C	5.68023	2.62112	-1.59757
H	5.02647	2.40809	-3.64211
H	6.10297	2.6115	0.51742
H	6.4476	3.35207	-1.83274
C	3.14509	-1.4425	0.81992
C	4.25087	-2.28572	0.60466
C	2.69081	-1.24757	2.1335
C	4.85837	-2.94448	1.6723
H	4.65453	-2.42138	-0.39372
C	3.30872	-1.90096	3.20289
H	1.88394	-0.55219	2.33574
C	4.38467	-2.75796	2.97348
H	5.70718	-3.59602	1.48876
H	2.95367	-1.72691	4.21388
H	4.86266	-3.26749	3.80446
C	-1.88213	-2.05776	1.20992
C	-3.27624	-1.93459	1.2812
C	-1.16503	-2.42627	2.3608
C	-3.94197	-2.19284	2.48082
H	-3.84408	-1.63682	0.40783
C	-1.83545	-2.67869	3.55742
H	-0.08273	-2.51667	2.33619
C	-3.22578	-2.56474	3.61913
H	-5.02333	-2.10356	2.52254
H	-1.27164	-2.96796	4.43907
H	-3.74744	-2.76595	4.54975
C	-2.13977	-1.88193	-1.73306
C	-2.92499	-3.04235	-1.85585
C	-2.22203	-0.89657	-2.72693
C	-3.77709	-3.20404	-2.94702
H	-2.88723	-3.81632	-1.09517
C	-3.07087	-1.06473	-3.82244
C	-3.84943	-2.21699	-3.93325
H	-4.38424	-4.10046	-3.02661
H	-3.1259	-0.2931	-4.58412
H	-4.51219	-2.3463	-4.78335
C	2.53059	-1.64579	-2.08115
H	3.56805	-1.549	-2.4144
H	1.91273	-1.18379	-2.86035
C	0.06162	-3.2746	-0.50043
H	0.80979	-3.27367	0.29839
H	-0.63824	-4.08095	-0.25916
C	0.71903	-3.53709	-1.87105
H	0.65832	-4.61496	-2.0564
H	0.14067	-3.07086	-2.67722
C	2.19412	-3.14327	-1.98161
H	2.58747	-3.59706	-2.89938
H	2.75344	-3.60153	-1.15957
C	0.37009	2.79785	-0.39372
H	-0.62039	3.15692	-0.13346
C	1.20037	2.35237	0.61131
H	2.25492	2.22593	0.40135
C	0.95213	2.42999	2.10173
C	0.8004	3.11064	-1.80291
H	1.79528	2.70607	-2.00251
H	0.0994	2.6451	-2.51002
C	0.79198	4.63521	-2.04399
H	-0.2006	5.06085	-1.86758
H	1.50208	5.13931	-1.3822
H	1.07384	4.85341	-3.07768
O	1.92759	2.36025	2.84856
N	-0.32241	2.60854	2.53419
H	-1.08565	2.42295	1.89315
C	-0.62808	2.68166	3.95584
H	0.21864	3.13355	4.47262
H	-1.51782	3.29751	4.10463
H	-0.80796	1.6895	4.38864
P	2.3856	-0.52133	-0.58171
P	-0.95694	-1.7264	-0.34163
C	-2.88562	1.53209	0.12541
Si	-4.58036	2.25879	0.25422

C	-4.69328	3.22062	1.87687
H	-3.96571	4.0386	1.91079
H	-5.68963	3.66134	1.9941
H	-4.51508	2.57149	2.74066
C	-4.84481	3.4153	-1.21556
H	-5.84123	3.86921	-1.17319
H	-4.11055	4.22754	-1.22332
C	-5.86046	0.87014	0.23193
H	-6.87504	1.28017	0.28805
H	-5.79268	0.27624	-0.68557
H	-5.72754	0.19683	1.08481
H	-1.64072	0.01516	-2.63897
H	-4.76408	2.87915	-2.16677

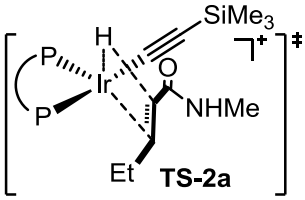


Int-4b

G_{sol} = -2721.24850962 Hatree

Ir	-0.02496	0.33214	0.05016
C	1.76222	1.19744	-0.12242
H	-0.26637	0.03615	-1.44121
C	-3.36389	0.38276	1.43308
C	-3.12387	0.73494	2.77291
C	-4.46557	0.94791	0.7723
C	-3.97156	1.62181	3.43748
H	-2.27573	0.31732	3.30834
C	-5.31161	1.83682	1.44046
H	-4.67198	0.68812	-0.26063
C	-5.0681	2.17575	2.77214
H	-3.77859	1.87504	4.47563
H	-6.16685	2.25707	0.91952
H	-5.73029	2.86205	3.29084
C	-3.19714	-1.49775	-0.76669
C	-4.38405	-2.1798	-0.43501
C	-2.80996	-1.42376	-2.11195
C	-5.15422	-2.78298	-1.42665
H	-4.71517	-2.23443	0.59799
C	-3.58729	-2.02933	-3.10423
H	-1.92762	-0.86388	-2.39834
C	-4.75403	-2.71214	-2.76469
H	-6.06599	-3.30692	-1.15633
H	-3.2778	-1.95812	-4.14249
H	-5.35496	-3.18331	-3.5366
C	2.38977	-1.70939	-1.34524
C	3.77622	-1.80844	-1.17212
C	1.85899	-1.67381	-2.64468
C	4.61754	-1.87773	-2.28495
H	4.2052	-1.8246	-0.17677
C	2.70294	-1.74376	-3.75164
H	0.78873	-1.57671	-2.80323
C	4.08451	-1.84632	-3.57388
H	5.69091	-1.95521	-2.14028
H	2.2813	-1.71266	-4.75155
H	4.74146	-1.89938	-4.43662
C	2.22211	-1.88727	1.60371
C	2.87842	-3.10804	1.84686
C	2.32241	-0.86212	2.55621
C	3.61458	-3.29408	3.01598
H	2.82554	-3.91544	1.12311
C	3.05503	-1.05437	3.72918
H	1.85932	0.10051	2.36886
C	3.70043	-2.26886	3.96133
H	4.11989	-4.23935	3.18833
H	3.12623	-0.25088	4.45587
H	4.27216	-2.41685	4.87232
C	-2.0339	-2.10468	1.8524
H	-2.97615	-2.07617	2.4073
H	-1.24925	-1.79753	2.55329
C	0.33227	-3.28187	-0.15348
H	-0.38668	-3.12534	-0.96514
H	1.09629	-3.95498	-0.55541
C	-0.33975	-3.94464	1.06508
H	-0.34075	-5.024	0.87307
H	0.27737	-3.80633	1.9593
C	-1.78568	-3.54582	1.37133
H	-2.13466	-4.20498	2.17524
H	-2.42288	-3.76831	0.50927
C	-1.08641	2.47484	0.41402
H	-2.13215	2.2688	0.62209
C	-0.67199	2.41376	-0.90034
H	0.30784	2.78972	-1.18188
C	-1.58309	2.15204	-2.08029
C	-0.32783	3.13286	1.54313
H	-0.341	2.47625	2.42363
H	0.71758	3.27716	1.2623

C	-0.98412	4.47393	1.92681
H	-0.96335	5.17699	1.0879
H	-2.02604	4.33556	2.23377
H	-0.44593	4.93197	2.76146
O	-1.3122	1.3087	-2.93648
N	-2.68083	2.94951	-2.13677
H	-2.77723	3.67781	-1.44448
C	-3.60341	2.93537	-3.26521
H	-3.40674	2.03446	-3.84531
H	-4.63686	2.92344	-2.90823
H	-3.45851	3.81008	-3.90801
P	-2.17617	-0.73913	0.56383
P	1.22958	-1.65823	0.07956
C	2.85047	1.77243	-0.19869
Si	4.49084	2.60769	-0.33275
C	4.31516	4.39678	0.2501
H	3.9831	4.44829	1.29249
H	5.27453	4.92193	0.18214
H	3.59247	4.94715	-0.36145
C	5.73459	1.69275	0.75706
H	5.42623	1.69424	1.80767
H	5.84631	0.65009	0.44242
H	6.721	2.16655	0.69897
C	5.03157	2.55416	-2.14141
H	6.01346	3.02476	-2.26579
H	5.10185	1.52342	-2.50295
H	4.32235	3.08577	-2.78403

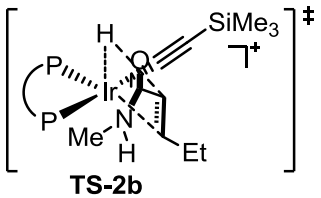


TS-2a

G_{sol} = -2721.22982602 Hatree

Ir	-0.17819	-0.44384	-0.12194
H	-0.82246	-1.23095	1.11871
C	-1.07564	-2.54288	0.25403
C	-0.35784	-2.45914	-0.98711
C	-4.51246	-1.40105	-1.29446
C	-4.20865	-0.98418	1.06807
C	-5.53832	-2.30282	-0.99903
H	-4.25723	-1.22829	-2.33463
C	-5.22998	-1.88671	1.35854
H	-3.70883	-0.46841	1.88292
C	-5.89716	-2.54935	0.32533
H	-6.05483	-2.80969	-1.80834
H	-5.50549	-2.07087	2.39218
H	-6.69172	-3.25277	0.55318
C	-2.90849	1.8643	0.47992
C	-4.0388	2.64252	0.17374
C	-2.18052	2.14946	1.64408
C	-4.4153	3.6957	1.00505
H	-4.63709	2.4213	-0.70511
C	-2.56355	3.20249	2.47924
H	-1.31397	1.54744	1.90156
C	-3.67693	3.97845	2.15818
H	-5.28849	4.29155	0.75748
H	-1.98974	3.4119	3.37655
H	-3.97528	4.79715	2.80586
C	1.38854	2.52804	1.0445
C	2.02336	1.78536	2.05585
C	1.14289	3.89645	1.25442
C	2.40724	2.40431	3.24512
H	2.21934	0.72994	1.90754
C	1.53114	4.5076	2.44795
H	0.65354	4.50068	0.5001
C	2.16301	3.76436	3.44534
H	2.89812	1.81951	4.01713
H	1.33881	5.56622	2.59319
H	2.46342	4.24242	4.37273
C	2.42913	1.586	-1.56069
C	3.45755	2.52898	-1.41528
C	2.52766	0.60638	-2.55966
C	4.56712	2.49009	-2.26091
H	3.40246	3.28613	-0.63938
C	3.63428	0.57721	-3.40849
C	4.65593	1.51737	-3.2588
H	5.36199	3.2192	-2.13739
H	3.70182	-0.18378	-4.17998
H	5.52012	1.48983	-3.91539
C	-2.74349	0.98445	-2.33772
H	-3.82921	0.99752	-2.47896
H	-2.35449	0.17823	-2.96903
C	-0.08236	2.98242	-1.44417
H	-0.88432	3.3136	-0.77863
H	0.5863	3.83589	-1.59163
C	-0.65474	2.52258	-2.80799
H	-0.41064	3.29503	-3.54355

H	-0.15442	1.61576	-3.16908
C	-2.18024	2.33037	-2.82771
H	-2.52005	2.43016	-3.86532
H	-2.65402	3.15196	-2.27893
C	-3.83562	-0.73027	-0.26363
H	0.64859	-2.87261	-0.9867
C	1.68112	-1.05357	0.29402
H	-2.15721	-2.49135	0.1848
C	-0.7057	-3.54877	1.35137
C	-1.03584	-2.52753	-2.32993
H	-2.045	-2.11323	-2.26907
H	-0.46752	-1.92525	-3.05076
C	-1.10547	-3.98706	-2.82857
H	-0.1059	-4.42199	-2.92432
H	-1.68309	-4.60955	-2.13919
H	-1.58559	-4.02643	-3.81044
O	-1.5549	-4.40031	1.58714
N	0.49584	-3.45192	1.95332
H	1.15861	-2.75476	1.62353
C	0.93243	-4.44123	2.92963
H	0.05051	-4.91529	3.36106
H	1.55351	-5.21813	2.46863
H	1.50768	-3.95047	3.71806
P	-2.43357	0.43429	-0.57732
P	0.91419	1.71096	-0.53459
C	2.83187	-1.44549	0.50947
Si	4.59904	-1.94133	0.74694
C	4.73219	-3.04351	2.27577
H	4.14522	-3.96134	2.16547
H	5.77422	-3.33822	2.44336
H	4.38729	-2.52699	3.17783
C	5.15776	-2.88119	-0.79252
H	6.206	-3.18634	-0.69891
H	4.5609	-3.78565	-0.9492
C	5.63088	-0.37644	0.97887
H	6.68855	-0.62845	1.11534
H	5.55163	0.28273	0.10858
H	5.30859	0.19024	1.85869
H	1.75172	-0.1459	-2.66251
H	5.06913	-2.25836	-1.68845

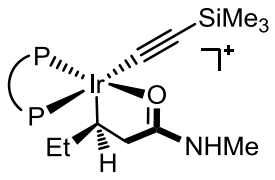


TS-2b

G_{sol} = -2721.22412048 Hatree

Ir	0.06202	0.32266	-0.05615
H	0.7282	1.11289	1.20197
C	0.9767	2.33187	0.41792
C	0.92937	2.07354	-1.00696
C	3.91754	0.5315	-2.11373
C	4.62331	0.35051	0.19223
C	5.0753	1.24973	-2.41555
H	3.21042	0.32307	-2.91187
C	5.78467	1.06217	-0.11612
H	4.45362	0.02024	1.20993
C	6.01507	1.51237	-1.41692
H	5.24709	1.59083	-3.43208
H	6.51369	1.25672	0.66492
H	6.92322	2.05855	-1.65357
C	2.65552	-1.9415	1.00694
C	3.64699	-2.93216	0.8913
C	2.07361	-1.70488	2.26186
C	4.02541	-3.68509	2.00188
H	4.13816	-3.11024	-0.06056
C	2.45897	-2.45737	3.37403
H	1.34408	-0.90919	2.37329
C	3.42821	-3.45215	3.24391
H	4.7903	-4.44883	1.89955
H	2.00884	-2.25637	4.34139
H	3.7271	-4.03764	4.10804
C	-2.48326	-1.8211	0.99817
C	-3.87635	-1.71797	0.89413
C	-1.90183	-2.12674	2.23938
C	-4.67708	-1.92308	2.0194
H	-4.33859	-1.47837	-0.05692
C	-2.70733	-2.32778	3.35944
H	-0.82323	-2.20645	2.34135
C	-4.09601	-2.22524	3.25194
H	-5.75648	-1.84707	1.92957
H	-2.25024	-2.5638	4.31555
H	-4.72195	-2.38296	4.12485
C	-2.46713	-1.42065	-1.9373

C	-3.10267	-2.55246	-2.48054
C	-2.68229	-0.1676	-2.53141
C	-3.92923	-2.42988	-3.59651
H	-2.96614	-3.53289	-2.03696
C	-3.51005	-0.05187	-3.64939
H	-2.2288	0.7176	-2.10272
C	-4.13099	-1.17997	-4.18585
H	-4.4145	-3.31137	-4.00395
H	-3.67045	0.92367	-4.09822
H	-4.77266	-1.0873	-5.05672
C	2.2062	-2.07318	-1.91906
H	3.26582	-2.15104	-2.17951
H	1.728	-1.52636	-2.74001
C	-0.65373	-3.29826	-0.60298
H	-0.01305	-3.4333	0.27475
H	-1.49715	-3.98035	-0.45686
C	0.10528	-3.65002	-1.89804
H	-0.10403	-4.70355	-2.11478
H	-0.29594	-3.09139	-2.75155
C	1.62757	-3.49562	-1.83893
H	2.04218	-4.03313	-2.70039
H	2.01297	-4.0121	-0.95334
C	3.67921	0.06839	-0.80614
H	1.88371	1.81854	-1.46317
C	-1.65031	1.26061	0.3681
H	0.17305	2.96124	0.80424
C	2.27981	2.52401	1.19828
C	0.0054	2.814	-1.94661
H	-0.22611	2.16254	-2.79859
H	-0.93783	3.04301	-1.44687
C	0.66928	4.10353	-2.47064
H	0.85493	4.8154	-1.6581
H	1.62114	3.89645	-2.97125
H	0.01414	4.59926	-3.19258
O	2.58228	1.78196	2.12928
N	2.98444	3.6178	0.82437
H	2.66337	4.15203	0.03042
C	4.17366	4.0731	1.53376
H	4.28706	3.45477	2.4239
H	5.06544	3.96907	0.90841
H	4.06175	5.1195	1.83186
P	2.15299	-0.9164	-0.43304
P	-1.39089	-1.59735	-0.46191
C	-2.66181	1.88505	0.6955
Si	-4.19256	2.77261	1.21779
C	-3.94547	4.62715	0.94733
H	-3.75928	4.85964	-0.10661
H	-4.83686	5.1847	1.25615
H	-3.09973	5.00624	1.53065
C	-5.64503	2.15799	0.17565
H	-5.47211	2.32125	-0.89314
H	-5.81744	1.08755	0.32758
H	-6.56601	2.68564	0.44807
C	-4.49715	2.41147	3.04609
H	-5.41097	2.90729	3.39274
H	-4.60763	1.3369	3.223
H	-3.66766	2.76864	3.66491

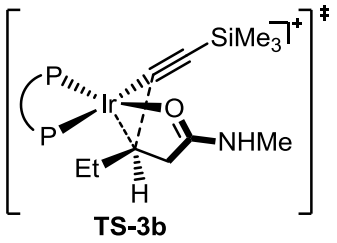


Int-5a

G_{sol} = -2721.27725898 Hatree

Ir	-0.15381	0.30976	0.02613
H	0.82982	3.20754	1.16982
C	-0.14699	2.83602	1.49802
C	-0.01059	1.34002	1.8687
C	-4.48825	0.72656	1.2983
C	-4.17384	0.92169	-1.08894
C	-5.55539	1.62542	1.23066
H	-4.22448	0.30548	2.26268
C	-5.24528	1.81201	-1.15567
H	-3.64995	0.65112	-1.99984
C	-5.93857	2.16842	0.00403
H	-6.09387	1.88769	2.13647
H	-5.54435	2.21994	-2.11685
H	-6.77779	2.85532	-0.05026
C	-2.64404	-1.84427	-1.30849
C	-3.8661	-2.51002	-1.50765
C	-1.64072	-1.97387	-2.27871
C	-4.06772	-3.29259	-2.64309
H	-4.6698	-2.40821	-0.7845
C	-1.84307	-2.75449	-3.41944
H	-0.68819	-1.46666	-2.14996
C	-3.05646	-3.41726	-3.60045
H	-5.01592	-3.80253	-2.78374

H	-1.05349	-2.84322	-4.1592
H	-3.2176	-4.02649	-4.48451
C	2.30825	-2.02332	-0.82321
C	2.17306	-1.50708	-2.11935
C	3.28874	-3.00017	-0.5802
C	2.98659	-1.97198	-3.15511
H	1.46578	-0.7104	-2.3194
C	4.10284	-3.45938	-1.61438
H	3.43474	-3.39308	0.42184
C	3.9498	-2.94964	-2.90576
H	2.87275	-1.55916	-4.15304
H	4.85987	-4.2103	-1.40981
H	4.58519	-3.30686	-3.71048
C	2.33276	-1.27461	1.97915
C	2.40843	-2.19374	3.03774
C	3.20648	-0.17234	1.97292
C	3.32851	-2.00879	4.07283
H	1.76547	-3.06509	3.06684
C	4.12433	0.00482	3.00713
H	3.17038	0.5401	1.15438
C	4.18616	-0.90964	4.06142
H	3.3738	-2.72936	4.88385
H	4.79719	0.85691	2.98502
H	4.90218	-0.76892	4.86542
C	-2.8587	-1.95109	1.58148
H	-3.93314	-2.12539	1.46157
H	-2.73481	-1.39197	2.51337
C	0.33051	-3.13037	0.87222
H	-0.1797	-3.35923	-0.0695
H	1.13102	-3.87169	0.95524
C	-0.64909	-3.26546	2.06482
H	-0.41251	-4.21039	2.5663
H	-0.47817	-2.48902	2.81888
C	-2.14302	-3.30472	1.69971
H	-2.66869	-3.85416	2.48961
H	-2.288	-3.88939	0.78393
C	-3.78528	0.36193	0.13896
C	1.46564	1.29903	-0.56261
H	-0.46019	3.4385	2.35968
C	-1.07706	3.03822	0.33213
O	-1.27463	2.09442	-0.48237
N	-1.6458	4.22949	0.13934
H	-1.4803	4.94636	0.83049
C	-2.48028	4.55245	-1.01671
H	-2.08604	4.04347	-1.89724
H	-3.51401	4.23298	-0.85808
H	-2.45242	5.6309	-1.17838
P	-2.35507	-0.80901	0.18978
P	1.18842	-1.50979	0.55333
C	2.40745	1.94771	-1.02489
Si	3.81399	2.85611	-1.79267
C	3.57694	4.71221	-1.5175
H	3.55011	4.95872	-0.45057
H	4.40114	5.27798	-1.96639
H	2.64504	5.0678	-1.96951
C	5.42875	2.29257	-0.98708
H	5.44168	2.51347	0.08574
H	5.58164	1.21545	-1.11002
H	6.28548	2.80484	-1.43937
C	3.84298	2.47131	-3.64248
H	4.67192	2.99124	-4.13579
H	3.96895	1.39817	-3.81977
H	2.91387	2.78571	-4.12909
H	1.00615	1.16291	2.21947
C	-0.99259	0.87421	2.93894
H	-2.02084	1.10926	2.63869
H	-0.92146	-0.21393	3.02505
C	-0.70515	1.47908	4.32732
H	-1.40501	1.08033	5.06813
H	0.30912	1.23494	4.65911
H	-0.80744	2.56879	4.33784

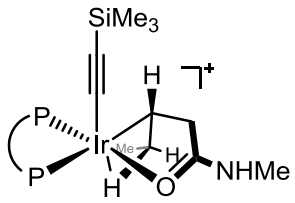


TS-3b

G_{sol} = -2721.22830837 Hatree

Ir	0.22418	0.38398	-0.38256
C	-1.21595	2.23348	-1.30139
C	-1.33063	1.4105	0.37168
H	-1.14492	4.07839	-0.16857
C	4.3697	1.10148	-1.08878
C	4.16674	0.54696	1.25443
C	5.45003	1.93615	-0.79692
H	4.04531	1.00801	-2.12006

C	5.24196	1.38811	1.54505
H	3.68685	-0.00055	2.05925
C	5.89089	2.07993	0.51985
H	5.9517	2.46582	-1.60162
H	5.58152	1.48932	2.57163
H	6.73814	2.7208	0.74498
C	2.59644	-2.13073	0.73719
C	3.66031	-3.03149	0.55194
C	1.7856	-2.26051	1.87229
C	3.88859	-4.05044	1.4754
H	4.32048	-2.93782	-0.30467
C	2.01886	-3.27952	2.79858
H	0.97095	-1.5628	2.0248
C	3.06661	-4.178	2.59878
H	4.71001	-4.74323	1.31974
H	1.37708	-3.37053	3.66952
H	3.24691	-4.97364	3.31528
C	-1.82198	-2.23372	0.81169
C	-1.66725	-1.64559	2.07437
C	-2.5812	-3.41132	0.69934
C	-2.24203	-2.23386	3.20433
H	-1.1134	-0.71763	2.16319
C	-3.15229	-3.99713	1.82806
H	-2.74818	-3.86903	-0.27123
C	-2.98082	-3.41118	3.0846
H	-2.11294	-1.76895	4.17762
H	-3.73581	-4.90708	1.72541
H	-3.42725	-3.86766	3.96296
C	-2.56179	-1.21852	-1.75851
C	-2.67149	-1.73964	-3.05736
C	-3.63674	-0.47414	-1.2402
C	-3.82068	-1.51556	-3.82064
H	-1.87248	-2.33068	-3.48878
C	-4.78203	-0.25334	-2.00393
H	-3.58045	-0.07374	-0.23406
C	-4.87696	-0.77062	-3.29838
H	-3.88792	-1.93126	-4.8216
H	-5.60672	0.31437	-1.58281
H	-5.77118	-0.6014	-3.89056
C	2.79904	-1.41763	-2.10983
H	3.88496	-1.56057	-2.09498
H	2.59725	-0.60542	-2.81634
C	-0.21573	-2.93362	-1.48287
H	0.43246	-3.35016	-0.70591
H	-0.97923	-3.69283	-1.67421
C	0.59256	-2.64182	-2.77386
H	0.30961	-3.38914	-3.52305
H	0.31871	-1.66835	-3.19769
C	2.11974	-2.70146	-2.60854
H	2.56506	-2.9195	-3.58661
H	2.38673	-3.54462	-1.96156
C	3.72422	0.3876	-0.06755
C	-0.53528	3.54675	-0.90479
H	-0.44877	4.19671	-1.78563
C	0.85127	3.35631	-0.31642
O	1.34715	2.22332	-0.10611
N	1.53538	4.46709	-0.01353
H	1.10671	5.35477	-0.23454
C	2.86258	4.47592	0.59591
H	3.04291	3.50659	1.05769
H	3.63927	4.65795	-0.15272
H	2.90508	5.25856	1.35673
P	2.30899	-0.74435	-0.43582
P	-1.06491	-1.47939	-0.69752
C	-2.0719	1.79069	1.29697
Si	-3.14264	2.343	2.69378
C	-3.41148	4.20844	2.52215
H	-3.90179	4.46271	1.57656
H	-4.05137	4.57473	3.33296
H	-2.46613	4.75904	2.57599
C	-4.79399	1.43254	2.59848
H	-5.32461	1.66046	1.66801
H	-4.65522	0.3478	2.65183
H	-5.44476	1.72662	3.42967
C	-2.27324	1.96698	4.32801
H	-2.87486	2.32075	5.17291
H	-2.11802	0.8913	4.45829
H	-1.29582	2.45688	4.38344
H	-2.29552	2.3517	-1.28358
C	-0.86533	1.77339	-2.7387
H	0.21471	1.80544	-2.90993
H	-1.18499	0.74315	-2.89421
C	-1.59326	2.65413	-3.77552
H	-2.67948	2.58811	-3.65412
H	-1.31005	3.71027	-3.71523
H	-1.35023	2.31107	-4.78569

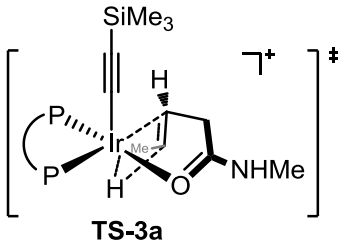


Int-6a

G_{sol} = -2721.26758737 Hatree

Ir	0.01694	-0.82298	0.31598
C	0.95012	-1.92243	1.83557
C	0.58552	-3.1957	1.0672
H	0.22201	-2.91445	0.00842
C	-3.58343	-2.27235	-0.49831
C	-4.43845	-0.03466	-0.8015
C	-4.8437	-2.70164	-0.08491
H	-2.76677	-2.98825	-0.52255
C	-5.69764	-0.46307	-0.3731
H	-4.29999	1.00164	-1.08723
C	-5.90609	-1.79564	-0.01943
H	-4.99652	-3.74256	0.18528
H	-6.51696	0.24814	-0.32748
H	-6.88862	-2.12918	0.30075
C	-1.97825	1.24247	-2.1826
C	-2.30707	1.45197	-3.53199
C	-1.93215	2.34685	-1.31242
C	-2.56823	2.73957	-4.00393
H	-2.37696	0.61846	-4.22219
C	-2.20851	3.63039	-1.78734
H	-1.67237	2.20326	-0.26765
C	-2.52106	3.82991	-3.13369
H	-2.81686	2.88736	-5.05051
H	-2.17616	4.47215	-1.10201
H	-2.73096	4.82928	-3.50277
C	2.53577	1.46892	-0.89801
C	1.6335	2.52011	-1.12129
C	3.90516	1.76016	-0.80181
C	2.08878	3.83194	-1.23839
H	0.57311	2.32158	-1.19994
C	4.35588	3.07807	-0.90648
H	4.63043	0.96989	-0.65311
C	3.45139	4.11667	-1.12367
H	1.37533	4.63085	-1.41713
H	5.41832	3.28642	-0.82475
H	3.8053	5.13953	-1.21046
C	3.38715	-1.28335	-0.55043
C	3.91125	-2.21479	-1.45927
C	4.02779	-1.11782	0.69182
C	5.03975	-2.97131	-1.13064
H	3.45298	-2.35946	-2.43072
C	5.15809	-1.86775	1.01378
H	3.65744	-0.38084	1.39832
C	5.66347	-2.80154	0.10495
H	5.43226	-3.68693	-1.84663
H	5.64702	-1.71941	1.97183
H	6.54271	-3.38643	0.3568
C	-1.56458	-1.59823	-2.93293
H	-2.5052	-1.50985	-3.48731
H	-1.58438	-2.59287	-2.47335
C	1.66759	-0.43999	-2.77424
H	1.06294	0.43222	-3.04371
H	2.65048	-0.26198	-3.22283
C	1.02192	-1.7334	-3.32627
H	1.66609	-2.11418	-4.12616
H	0.99321	-2.52924	-2.57113
C	-0.38458	-1.53016	-3.91552
H	-0.56628	-2.31807	-4.6564
H	-0.40431	-0.58732	-4.47371
C	-3.36742	-0.93543	-0.87246
C	0.05122	0.90988	1.20338
H	0.36946	-2.49625	3.88993
C	-1.27538	-1.57301	2.83833
O	-1.63455	-1.30412	1.65617
N	-2.1792	-1.74986	3.80223
H	-1.83215	-1.937	4.73257
C	-3.6185	-1.56178	3.62687
H	-3.86235	-1.67072	2.57097
H	-4.15318	-2.31809	4.20517
H	-3.92436	-0.56655	3.96449
P	-1.69045	-0.4279	-1.47366
P	1.90335	-0.26591	-0.94078
C	0.05061	1.93148	1.88915
Si	0.11239	3.47946	2.87444
C	-0.71351	3.18385	4.55154
H	-0.19743	2.40096	5.1178
H	-0.69709	4.09589	5.15885
H	-1.75964	2.88163	4.43417
C	1.91601	3.98405	3.12636
H	2.46882	3.21868	3.68132

H	2.42182	4.13123	2.16678
H	1.98504	4.92036	3.69177
C	-0.81244	4.85038	1.95281
H	-0.7824	5.79012	2.51571
H	-0.36287	5.03728	0.97163
H	-1.86531	4.58838	1.80138
H	2.02174	-1.81692	1.98108
C	0.19519	-1.70433	3.14695
H	-0.30858	-3.6703	1.48676
H	0.52043	-0.75693	3.59302
C	1.69971	-4.22862	0.86858
H	1.35938	-5.06666	0.25277
H	2.58041	-3.78905	0.39841
H	2.0009	-4.62751	1.8425

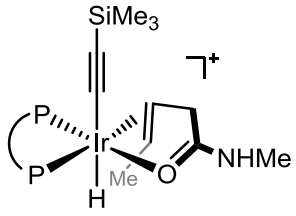


TS-3a

G_{sol} = -2721.25172135 Hatree

Ir	-0.01427	-0.86208	0.37113
C	0.86602	-1.71485	2.17586
C	0.46332	-2.8897	1.44322
H	-0.10565	-2.48986	-0.08946
C	-3.54943	-2.30235	-0.35021
C	-4.37037	-0.08183	-0.82704
C	-4.8219	-2.68714	0.06816
H	-2.73857	-3.02322	-0.30618
C	-5.64291	-0.46552	-0.39483
H	-4.21523	0.9304	-1.18151
C	-5.87436	-1.76714	0.04808
H	-4.99222	-3.70407	0.40971
H	-6.45408	0.25608	-0.41623
H	-6.86687	-2.06634	0.37147
C	-1.87426	1.06187	-2.2591
C	-2.12402	1.17637	-3.63691
C	-1.88724	2.22302	-1.46506
C	-2.37001	2.42547	-4.20965
H	-2.14191	0.29902	-4.27332
C	-2.14668	3.46755	-2.04184
H	-1.67515	2.15461	-0.40269
C	-2.38416	3.57203	-3.41423
H	-2.55723	2.49874	-5.27665
H	-2.15778	4.35428	-1.41521
H	-2.58154	4.54157	-3.86154
C	2.53146	1.28529	-1.02801
C	1.63842	2.29647	-1.41335
C	3.89448	1.59724	-0.91044
C	2.09397	3.58833	-1.667
H	0.5828	2.08329	-1.51167
C	4.34601	2.89716	-1.15216
H	4.6162	0.83728	-0.63883
C	3.44956	3.89582	-1.5293
H	1.38571	4.35398	-1.96915
H	5.40357	3.12135	-1.05105
H	3.80427	4.90381	-1.72224
C	3.38459	-1.38859	-0.33937
C	3.9575	-2.40367	-1.1203
C	3.97334	-1.07644	0.90037
C	5.08121	-3.10034	-0.66691
H	3.5366	-2.6661	-2.08439
C	5.09782	-1.76897	1.34745
H	3.56817	-0.26902	1.50343
C	5.65112	-2.78781	0.56692
H	5.51108	-3.88344	-1.28396
H	5.54629	-1.50825	2.30133
H	6.52606	-3.32745	0.91587
C	-1.52313	-1.83085	-2.80745
H	-2.44808	-1.72523	-3.38479
H	-1.61182	-2.78081	-2.27119
C	1.74158	-0.81935	-2.70364
H	1.20047	0.04486	-3.10279
H	2.75341	-0.73538	-3.11356
C	1.05749	-2.13196	-3.14496
H	1.69571	-2.61052	-3.89557
H	0.97951	-2.84408	-2.3153
C	-0.33048	-1.92058	-3.773
H	-0.54753	-2.77022	-4.43161
H	-0.29479	-1.0415	-4.42643
C	-3.31018	-0.99759	-0.8134
C	0.06421	1.02491	1.10868
H	0.15829	-1.85491	4.24723
C	-1.42005	-1.14364	2.95467
O	-1.72975	-1.09246	1.73361
N	-2.36007	-1.12828	3.90148

H	-2.05073	-1.14203	4.86324
C	-3.78639	-0.94664	3.63631
H	-4.00307	-1.28005	2.62226
H	-4.36158	-1.54267	4.34753
H	-4.07009	0.10596	3.73458
P	-1.62067	-0.56078	-1.43613
P	1.90211	-0.44848	-0.89199
C	0.09322	2.10623	1.69723
Si	0.1841	3.73868	2.52974
C	-0.63935	3.62076	4.23102
H	-0.13229	2.88977	4.87041
H	-0.60996	4.58663	4.74794
H	-1.68993	3.32277	4.14541
C	1.99546	4.24105	2.72982
H	2.53888	3.52673	3.35751
H	2.50125	4.28383	1.75983
H	2.08028	5.22795	3.19879
C	-0.72511	5.03277	1.48819
H	-0.67679	6.02065	1.96
H	-0.28014	5.11852	0.49108
H	-1.78312	4.77453	1.36837
H	1.93334	-1.56777	2.29601
C	0.03373	-1.2272	3.35395
H	-0.51898	-3.28908	1.69345
H	0.35052	-0.21032	3.61271
C	1.44474	-3.95468	1.01292
H	1.04008	-4.59038	0.221
H	2.39489	-3.53908	0.68372
H	1.64056	-4.593	1.88373

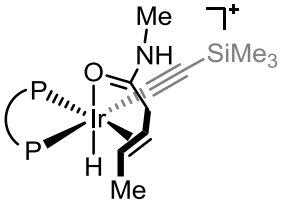


Int-7a

G_{sol} = -2721.25602189 Hatree

Ir	-0.00403	-0.91333	-0.35564
C	-0.85197	-1.45354	-2.42004
C	-0.67979	-2.68459	-1.77377
H	0.0601	-2.40568	0.33728
C	3.4393	-2.41133	0.50187
C	4.30066	-0.21994	1.04641
C	4.72533	-2.83876	0.17759
H	2.60763	-3.09993	0.39081
C	5.58745	-0.64746	0.70716
H	4.15653	0.79606	1.39422
C	5.80511	-1.95627	0.27926
H	4.88461	-3.86022	-0.15549
H	6.41934	0.04536	0.79091
H	6.80782	-2.29007	0.02958
C	1.74614	1.0105	2.30211
C	1.85527	1.13989	3.6965
C	1.90385	2.1527	1.49646
C	2.1035	2.38685	4.27328
H	1.76301	0.27601	4.34418
C	2.16548	3.3936	2.0786
H	1.80321	2.07267	0.41872
C	2.26112	3.51438	3.46693
H	2.18052	2.47221	5.35289
H	2.29129	4.26507	1.44332
H	2.4607	4.48175	3.91788
C	-2.5313	1.32443	1.01888
C	-1.61652	2.37072	1.19572
C	-3.90331	1.59367	1.17006
C	-2.06074	3.65786	1.49971
H	-0.55901	2.19012	1.08012
C	-4.34402	2.88446	1.46533
H	-4.63729	0.80418	1.0607
C	-3.42507	3.9212	1.62849
H	-1.3343	4.45379	1.6339
H	-5.40791	3.07448	1.57021
H	-3.76965	4.92464	1.85983
C	-3.44936	-1.26193	0.19193
C	-4.04333	-2.34519	0.85452
C	-4.02684	-0.79511	-1.00267
C	-5.18276	-2.9589	0.32723
H	-3.62599	-2.72231	1.7818
C	-5.16494	-1.40753	-1.52527
H	-3.60313	0.06783	-1.50839
C	-5.7424	-2.49535	-0.86349
H	-5.63256	-3.7965	0.85154
H	-5.60641	-1.03096	-2.44304
H	-6.62935	-2.97148	-1.26998
C	1.33611	-1.87875	2.86525
H	2.23433	-1.7581	3.48083
H	1.46134	-2.82558	2.33245

C	-1.89642	-0.85445	2.64766
H	-1.37438	-0.00693	3.10492
H	-2.93277	-0.76956	2.99064
C	-1.25827	-2.18195	3.10562
H	-1.93031	-2.64549	3.83605
H	-1.16787	-2.89387	2.2778
C	0.10806	-1.99181	3.78251
H	0.30421	-2.85987	4.42354
H	0.04873	-1.13269	4.46032
C	3.21385	-1.09898	0.95186
C	0.05787	0.99806	-1.14407
H	0.05802	-1.45326	-4.38815
C	1.56959	-1.11145	-2.88536
O	1.76662	-1.2413	-1.64842
N	2.58641	-1.11685	-3.75096
H	2.36103	-0.99191	-4.72801
C	3.99666	-1.17552	-3.37367
H	4.07055	-1.51321	-2.34131
H	4.51927	-1.87941	-4.02559
H	4.4629	-0.18937	-3.46282
P	1.50884	-0.61871	1.49265
P	-1.94739	-0.42367	0.84089
C	0.13229	2.08383	-1.72208
Si	0.19088	3.71065	-2.56937
C	0.97316	3.49399	-4.28146
H	0.38386	2.81572	-4.90865
H	1.03501	4.45408	-4.80611
H	1.98912	3.09085	-4.20867
C	-1.56221	4.39273	-2.75169
H	-2.18544	3.73045	-3.36197
H	-2.047	4.49904	-1.77589
H	-1.5516	5.37724	-3.23294
C	1.24267	4.91844	-1.55872
H	1.30882	5.89249	-2.05633
H	0.81024	5.0834	-0.56589
H	2.26365	4.54348	-1.42707
H	-1.86195	-1.08252	-2.55424
C	0.1669	-0.94313	-3.42149
H	0.28866	-3.16691	-1.88263
H	0.01217	0.1283	-3.58295
C	-1.78832	-3.64181	-1.43341
H	-1.60912	-4.17016	-0.4948
H	-2.76514	-3.16677	-1.39858
H	-1.8134	-4.39656	-2.23126

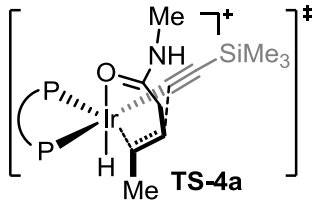


Int-8a

G_{sol} = -2721.27788013 Hatree

Ir	-0.07589	-0.70163	-0.42451
C	-1.23039	-2.83654	-0.68434
C	-0.08037	-3.04266	0.04209
C	1.83223	-1.25255	-0.06601
C	-4.42179	-1.56665	-1.83119
C	-4.26149	-1.23659	0.55648
C	-5.49933	-2.43532	-1.63458
H	-4.09065	-1.37348	-2.84578
C	-5.33437	-2.10542	0.74965
H	-3.79904	-0.7593	1.4154
C	-5.95723	-2.7081	-0.34657
H	-5.98055	-2.89339	-2.49343
H	-5.69247	-2.30296	1.75572
H	-6.79683	-3.37968	-0.19639
C	-2.9447	1.58813	0.12743
C	-4.06048	2.34183	-0.27962
C	-2.34985	1.86633	1.36591
C	-4.55241	3.36729	0.52558
H	-4.55858	2.12331	-1.21937
C	-2.8508	2.89235	2.17322
H	-1.50597	1.27693	1.70391
C	-3.94615	3.64629	1.75399
H	-5.41157	3.94446	0.19748
H	-2.37713	3.10126	3.12772
H	-4.33225	4.44432	2.38099
C	1.24672	2.15067	1.14213
C	1.92918	1.36853	2.09055
C	0.86504	3.45765	1.48847
C	2.22485	1.88849	3.35031
H	2.23645	0.36121	1.83245
C	1.16146	3.97114	2.75321
H	0.33751	4.09037	0.78462
C	1.84166	3.18919	3.68654
H	2.76484	1.27787	4.06833
H	0.86342	4.98514	3.00243
H	2.07702	3.59221	4.66709
C	2.50019	1.5304	-1.43225

C	2.77216	0.68661	-2.51856
C	3.41761	2.54212	-1.10719
C	3.93416	0.85938	-3.27145
H	2.0921	-0.12142	-2.75992
C	4.58406	2.70463	-1.8562
H	3.23289	3.20081	-0.26471
C	4.84354	1.86601	-2.9413
H	4.13212	0.19908	-4.11048
H	5.28852	3.48644	-1.58878
H	5.75062	1.99398	-3.52421
C	-2.50084	0.77225	-2.68236
H	-3.56396	0.74796	-2.94017
H	-2.00706	-0.0007	-3.28207
C	-0.05554	2.76148	-1.40795
H	-0.93733	3.01243	-0.8137
H	0.5982	3.6387	-1.39918
C	-0.45322	2.42188	-2.86622
H	-0.18489	3.28063	-3.48952
H	0.13416	1.584	-3.25772
C	-1.95149	2.15643	-3.0729
H	-2.17194	2.27212	-4.14089
H	-2.52768	2.93654	-2.56289
C	-3.79037	-0.9542	-0.7385
H	0.22079	-0.77684	-1.95149
H	-0.48926	-4.0903	1.88297
C	-0.50046	-1.97831	2.33028
O	-0.60088	-0.8448	1.81123
N	-0.78777	-2.16249	3.62621
H	-0.70453	-3.09248	4.00964
C	-1.1662	-1.06535	4.51404
H	-2.16243	-0.68621	4.26807
H	-1.1687	-1.43329	5.54027
H	-0.4495	-0.24574	4.42382
P	-2.33905	0.18898	-0.91513
P	0.90075	1.43918	-0.52136
C	2.98855	-1.60095	0.1702
Si	4.7505	-2.04856	0.45445
C	4.83772	-3.43587	1.7401
H	4.30577	-4.33123	1.40039
H	5.87787	-3.72352	1.93029
H	4.4022	-3.12614	2.69652
C	5.50772	-2.63626	-1.17363
H	4.98522	-3.51636	-1.5629
H	5.4568	-1.85163	-1.93533
H	6.56134	-2.9058	-1.03893
C	5.67812	-0.52912	1.0914
H	6.73559	-0.76068	1.26217
H	5.62605	0.2936	0.37099
H	5.26012	-0.17023	2.03803
H	0.78519	-3.42316	-0.48794
C	0.01386	-3.17324	1.55038
H	-2.16489	-2.68507	-0.15373
H	1.07376	-3.27191	1.81013
C	-1.33426	-3.24495	-2.13197
H	-1.93928	-2.55345	-2.72078
H	-0.34784	-3.32611	-2.5946
H	-1.82419	-4.22537	-2.19012

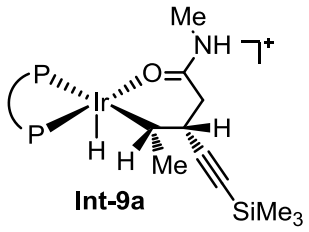


TS-4a

G_{sol} = -2721.24801063 Hatree

Ir	-0.18901	-0.66468	-0.30307
C	-0.76855	-2.75849	0.08593
C	0.45711	-2.88457	0.84902
C	1.64109	-1.53747	0.19475
C	-4.09772	-2.11383	-1.78021
C	-4.20001	-1.50137	0.55497
C	-5.06114	-3.10169	-1.55988
H	-3.70037	-1.98618	-2.78178
C	-5.15966	-2.48951	0.77262
H	-3.88597	-0.86952	1.38083
C	-5.59368	-3.29224	-0.28523
H	-5.39562	-3.71824	-2.38878
H	-5.57673	-2.6255	1.76617
H	-6.34546	-4.0572	-0.11683
C	-3.13767	1.426	-0.07011
C	-4.35696	1.95199	-0.53348
C	-2.54753	1.98361	1.07324
C	-4.96049	3.02426	0.1208
H	-4.84625	1.51925	-1.40118
C	-3.15838	3.05732	1.72887
H	-1.62037	1.57602	1.45968
C	-4.35975	3.58159	1.25315
H	-5.89981	3.42267	-0.25061

H	-2.68829	3.48363	2.61029
H	-4.83077	4.41715	1.76222
C	1.2162	2.38312	0.86156
C	2.015	1.75041	1.83076
C	0.74754	3.68091	1.11843
C	2.34381	2.4046	3.01724
H	2.38215	0.74566	1.64853
C	1.07264	4.33141	2.31234
H	0.13023	4.20141	0.39527
C	1.87183	3.69753	3.26297
H	2.97578	1.90871	3.7488
H	0.70563	5.33775	2.49117
H	2.13173	4.20818	4.18545
C	2.42633	1.42331	-1.59616
C	2.70064	0.40058	-2.51659
C	3.34436	2.47798	-1.45953
C	3.86002	0.4405	-3.29505
H	2.01382	-0.43202	-2.61524
C	4.50569	2.51103	-2.23191
H	3.15578	3.27617	-0.74817
C	4.76476	1.49382	-3.15404
H	4.05421	-0.35323	-4.01063
H	5.20612	3.33261	-2.11495
H	5.66663	1.52325	-3.75817
C	-2.51075	0.4222	-2.75911
H	-3.56481	0.30321	-3.03093
H	-1.95418	-0.36045	-3.28563
C	-0.13487	2.67883	-1.70442
H	-1.01326	2.97951	-1.12637
H	0.50167	3.56337	-1.80554
C	-0.5615	2.17674	-3.10608
H	-0.36568	2.98826	-3.81451
H	0.06723	1.34369	-3.44097
C	-2.04794	1.80784	-3.24744
H	-2.29833	1.84056	-4.31476
H	-2.65907	2.58625	-2.77577
C	-3.65874	-1.29848	-0.72617
H	0.04802	-0.97887	-1.81113
H	-0.13852	-3.46997	2.80481
C	-0.18414	-1.32563	2.77482
O	-0.51657	-0.43431	1.96784
N	-0.34658	-1.14082	4.09384
H	-0.06891	-1.87922	4.72362
C	-0.87312	0.10263	4.65313
H	-1.86319	0.31652	4.24274
H	-0.94982	-0.00873	5.73487
H	-0.21037	0.94062	4.41985
P	-2.36094	-0.00078	-0.94792
P	0.82127	1.45439	-0.68435
C	2.86926	-1.7061	0.28468
Si	4.6932	-2.03208	0.40442
C	4.95291	-3.14755	1.91099
H	4.41768	-4.09786	1.81342
H	6.01751	-3.38216	2.02306
H	4.62452	-2.6625	2.83633
C	5.26027	-2.90001	-1.16958
H	4.72923	-3.84524	-1.32125
H	5.08749	-2.2704	-2.04776
H	6.33207	-3.123	-1.12252
C	5.58537	-0.38742	0.63514
H	6.66453	-0.55661	0.72365
H	5.41811	0.27985	-0.21554
H	5.2536	0.12979	1.5411
H	1.10786	-3.70542	0.56441
C	0.43599	-2.65188	2.34779
H	-1.66886	-2.67149	0.69556
H	1.45138	-2.70495	2.75377
C	-0.90841	-3.67997	-1.11365
H	-1.73465	-3.37649	-1.75841
H	0.00512	-3.68075	-1.71717
H	-1.10521	-4.71439	-0.7991



Int-9a

G_{sol} = -2721.25967373 Hatree

Ir	-0.12275	0.36238	-0.13723
C	0.75995	2.21752	-0.77782
C	2.01041	2.07655	-1.70632
C	3.28685	1.86791	-1.00902
C	-2.20024	4.24898	1.0742
C	-2.65221	3.38029	-1.13385
C	-2.46662	5.5414	0.61572
H	-1.91434	4.11603	2.11184
C	-2.91456	4.67066	-1.59016

H	-2.75039	2.545	-1.82155
C	-2.82256	5.75573	-0.71509
H	-2.39393	6.37841	1.3034
H	-3.19855	4.82776	-2.62635
H	-3.03122	6.76067	-1.06883
C	-3.57325	0.63794	0.21645
C	-4.76402	0.95328	0.89411
C	-3.63689	-0.18884	-0.91349
C	-5.98202	0.42983	0.46349
H	-4.74919	1.62013	1.75083
C	-4.85927	-0.70601	-1.34968
H	-2.73038	-0.43869	-1.45662
C	-6.03167	-0.40215	-0.65847
H	-6.89333	0.67683	0.99955
H	-4.88942	-1.34805	-2.22444
H	-6.98224	-0.80563	-0.99375
C	-1.52145	-3.005	-0.60935
C	-0.9327	-3.06487	-1.88537
C	-2.65555	-3.79216	-0.35592
C	-1.46034	-3.89182	-2.87614
H	-0.05173	-2.46684	-2.09501
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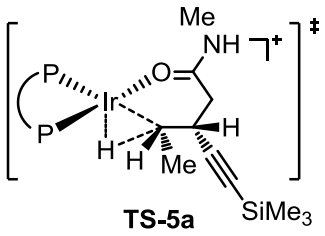

TS-5a

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H	4.19002	-2.58529	-1.4468
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H	6.6549	1.88084	2.76399	C	1.1379	3.49178	-0.1023
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References

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3 Full citation of Gaussian 09: Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. A., Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Keith, T.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, O.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J.; *Gaussian 09, revision B.01*; Gaussian Inc.: Wallingford, CT, 2010.

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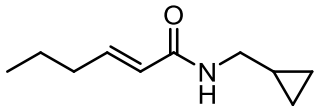
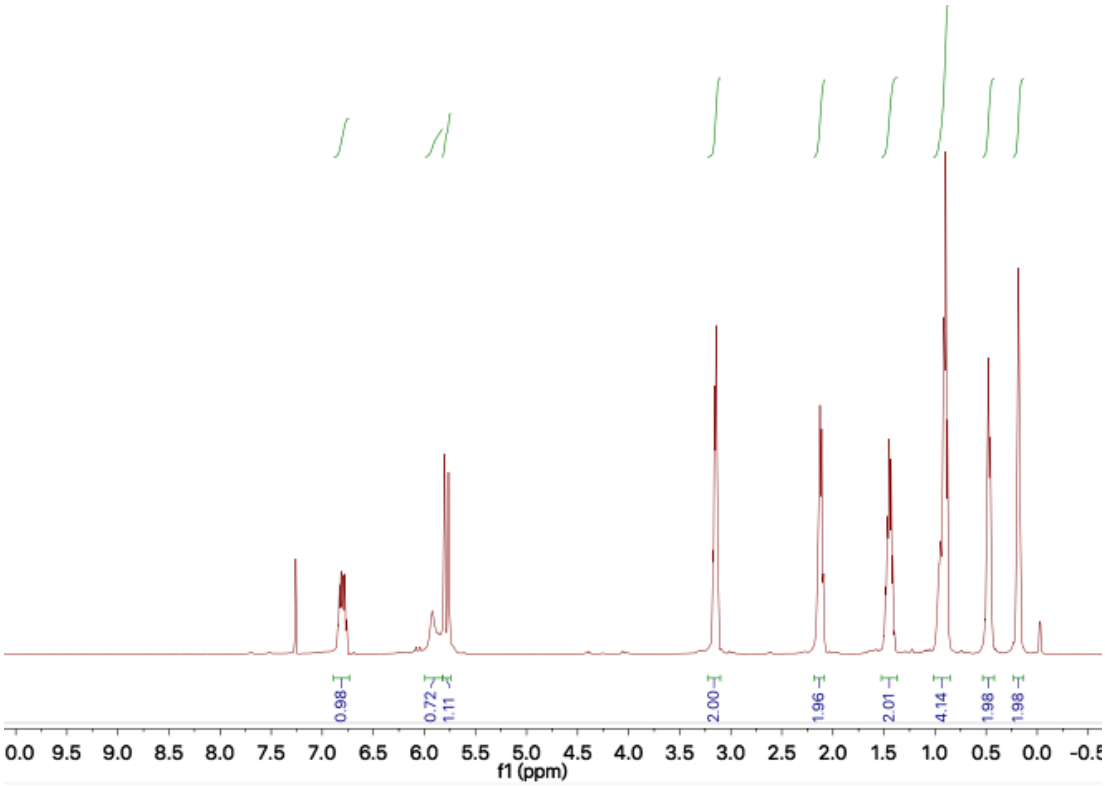
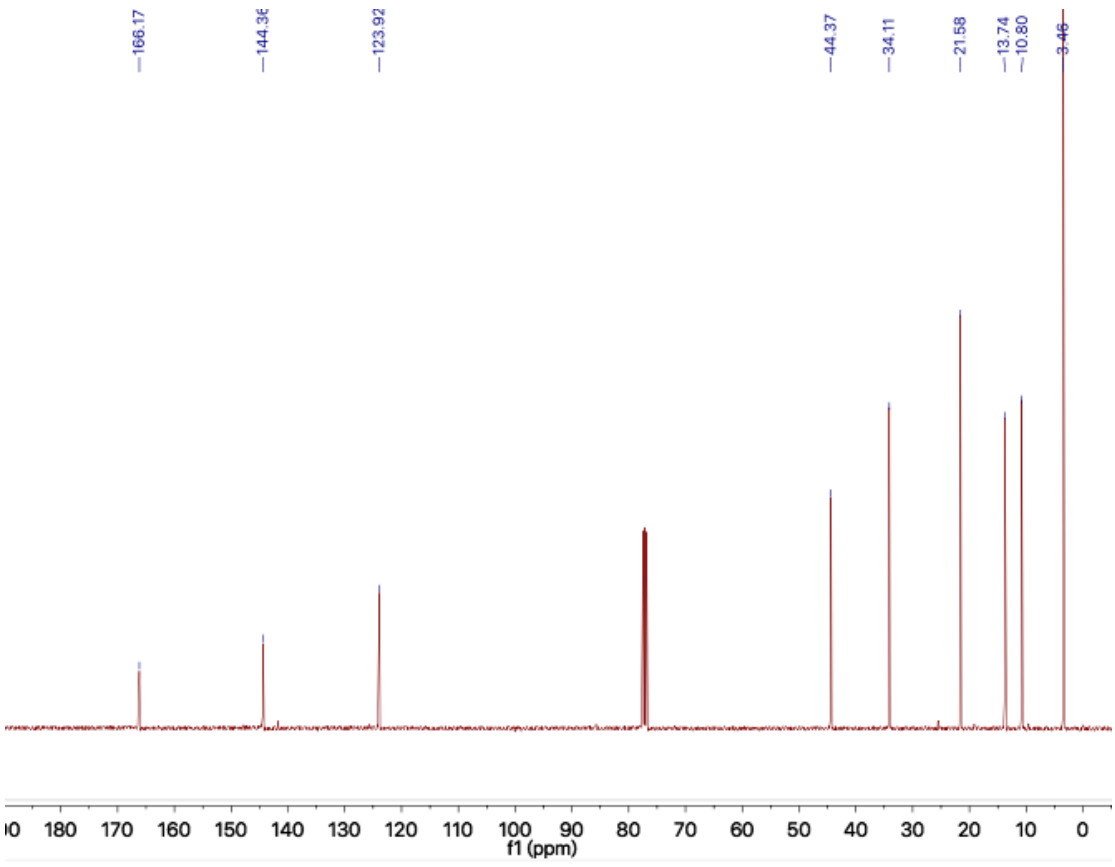
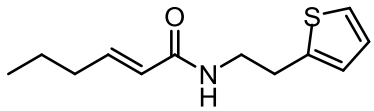
Copies of NMR Spectra





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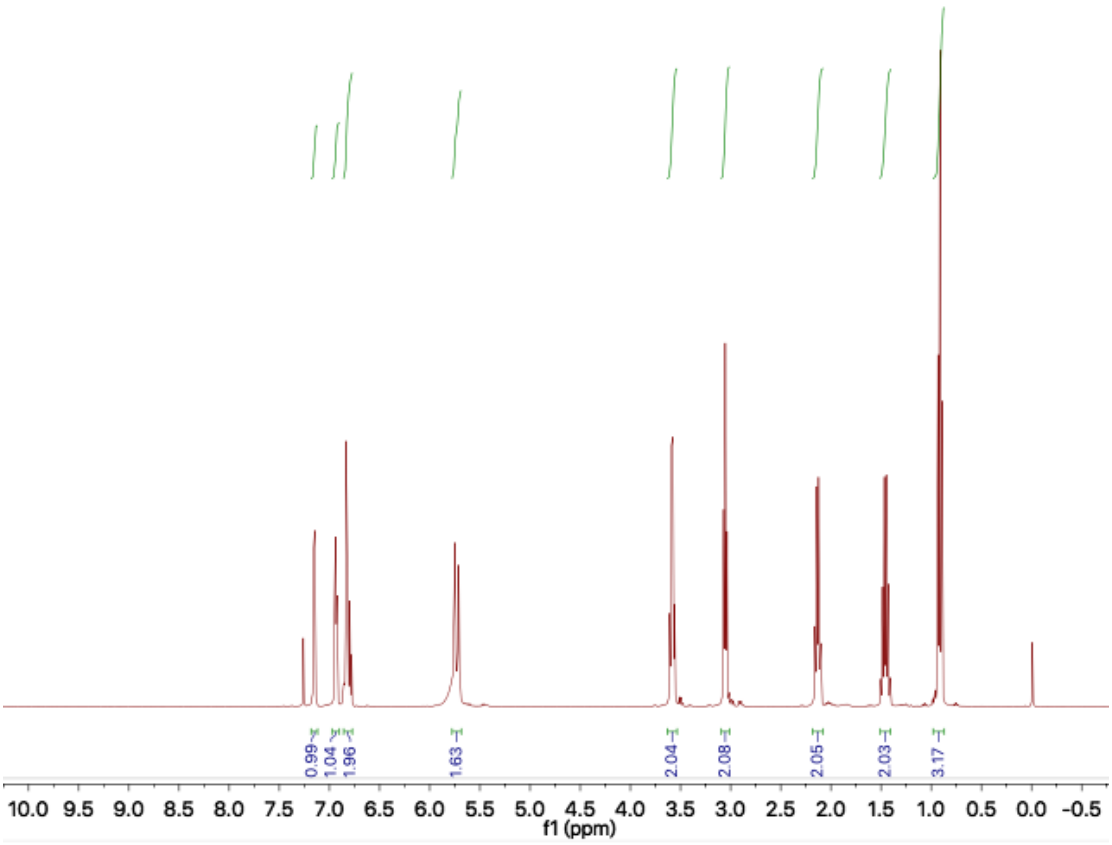
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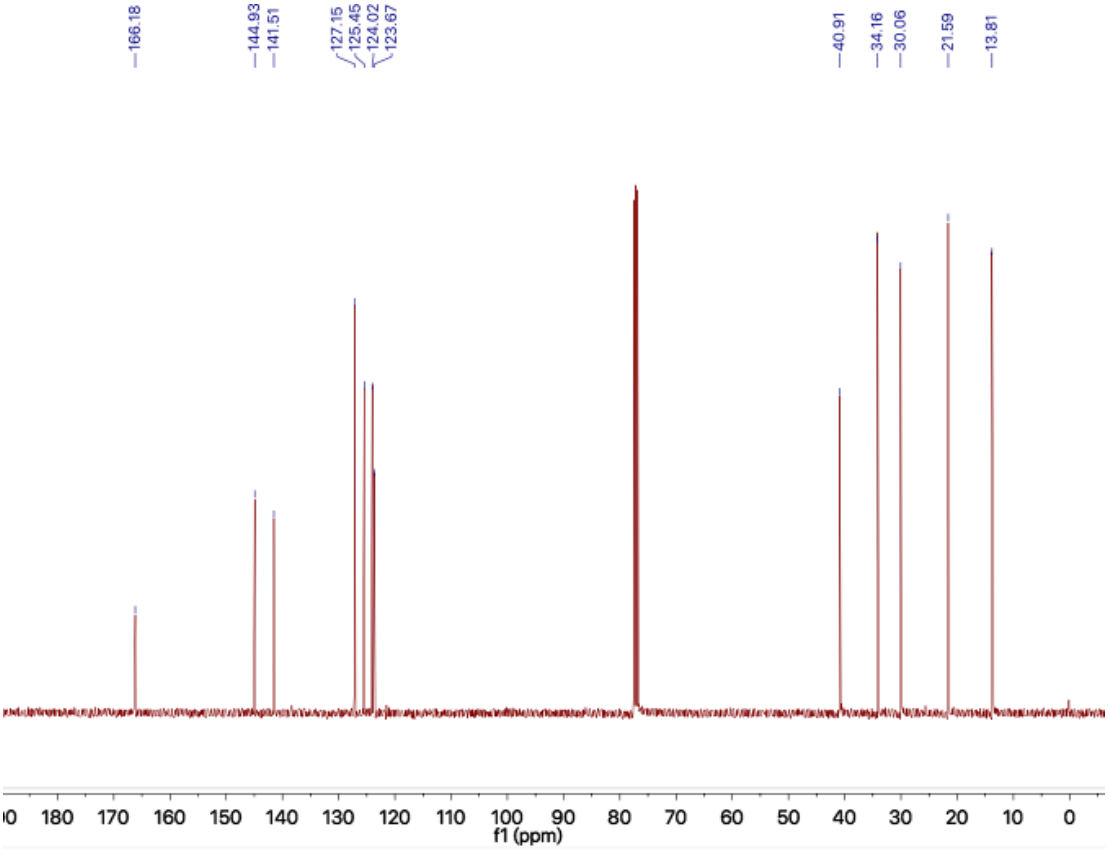
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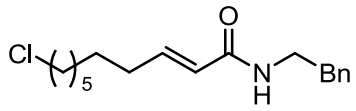
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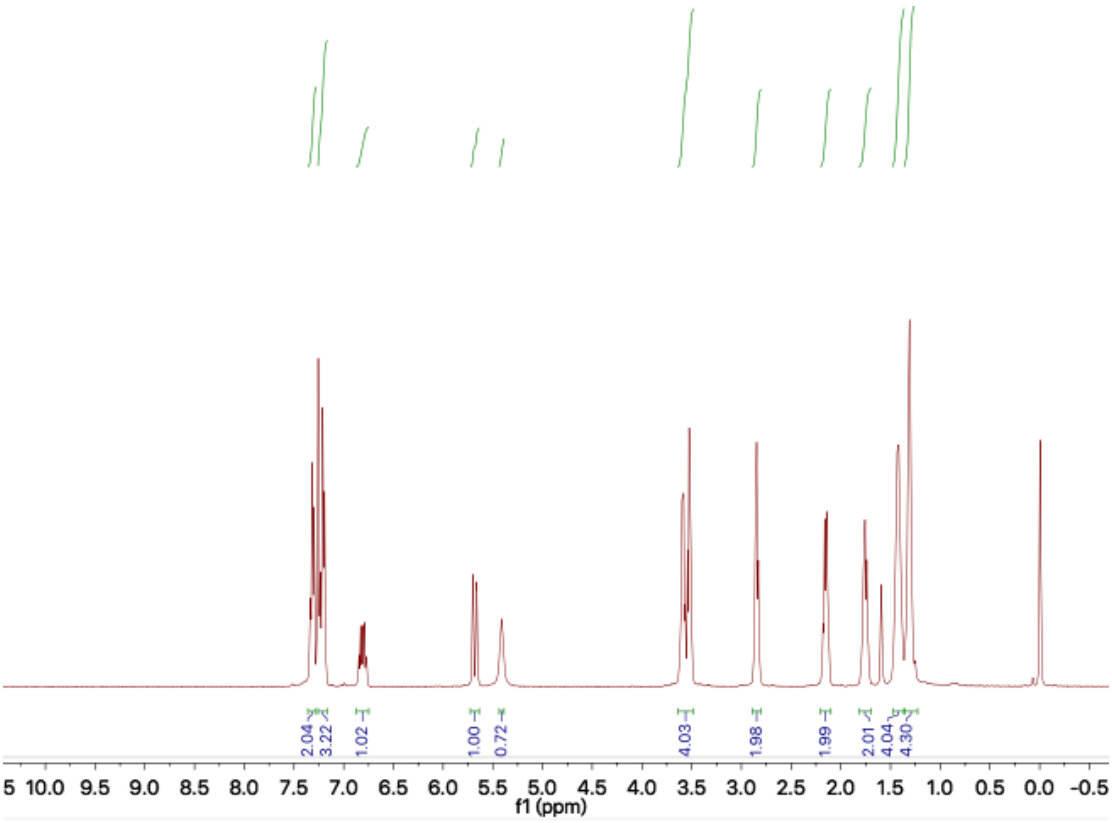
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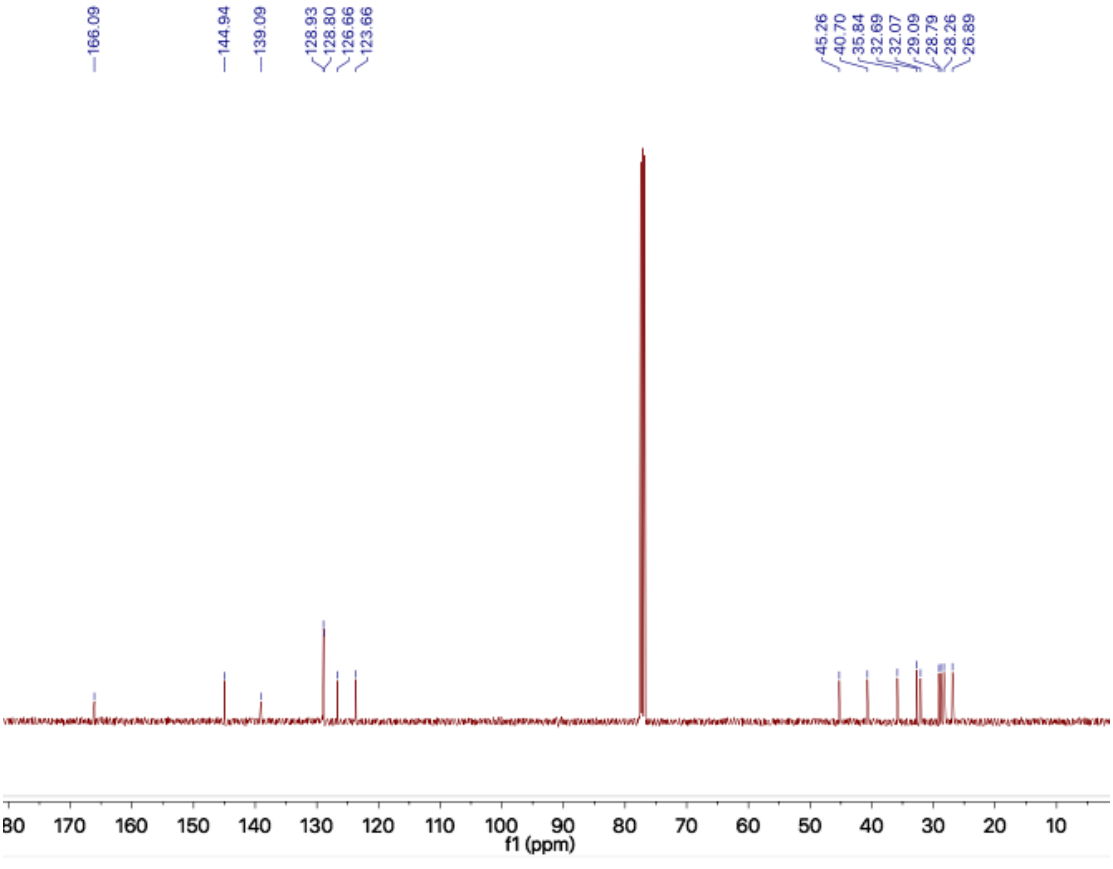
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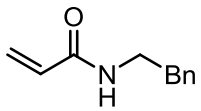
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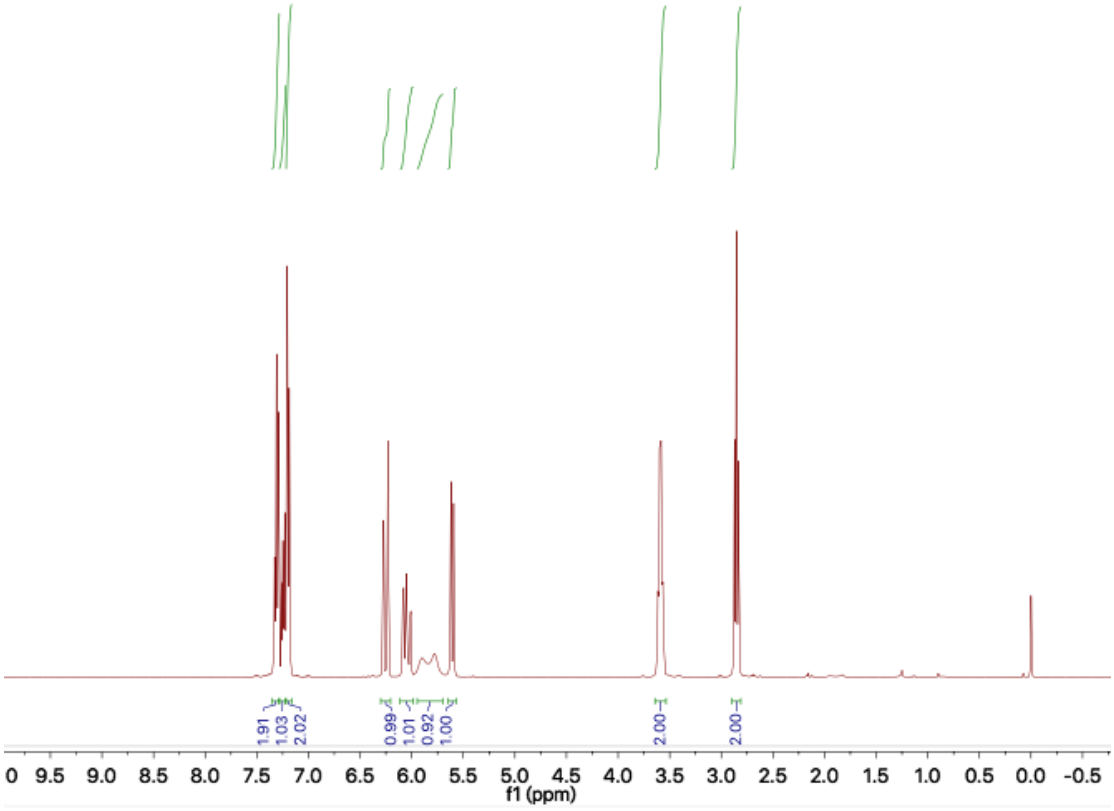
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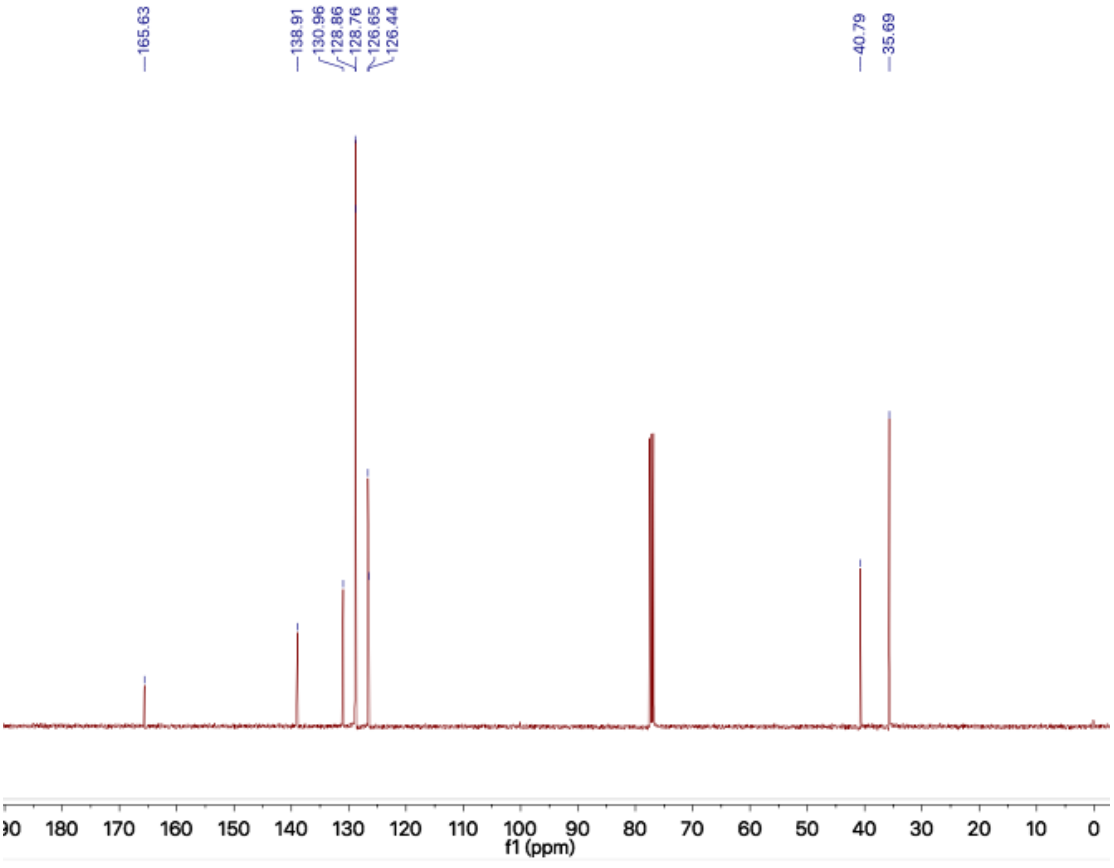
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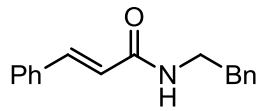
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Ph
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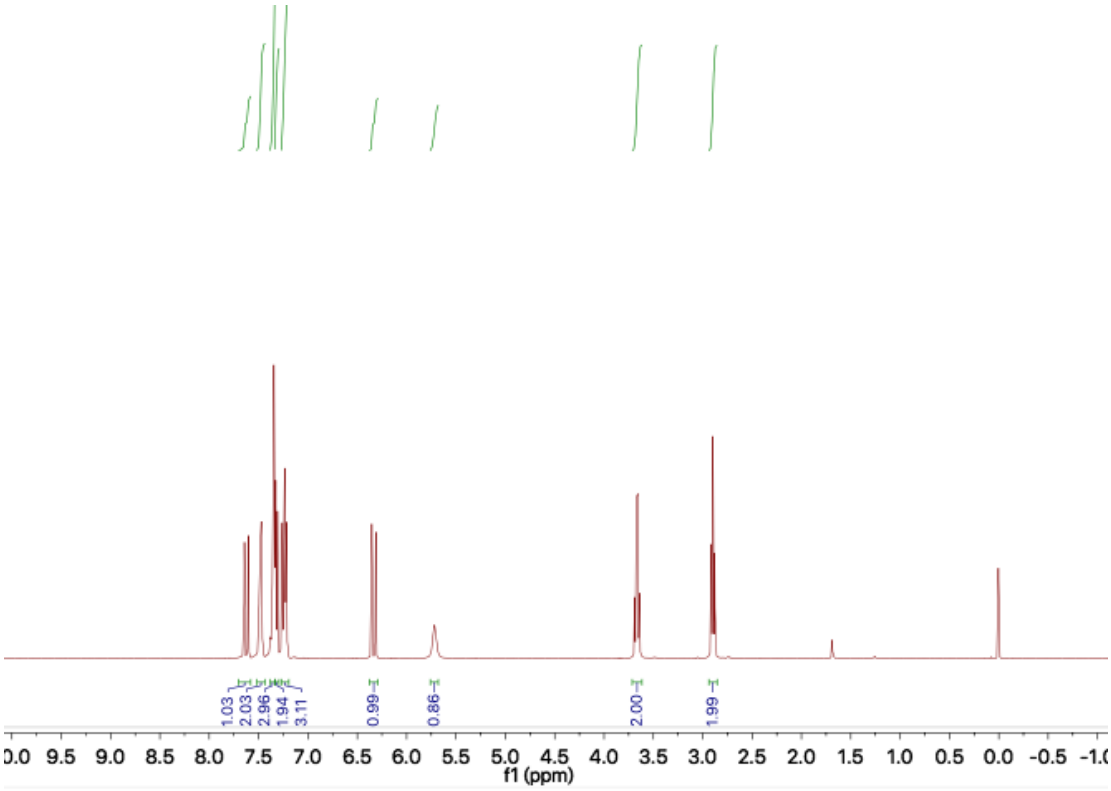
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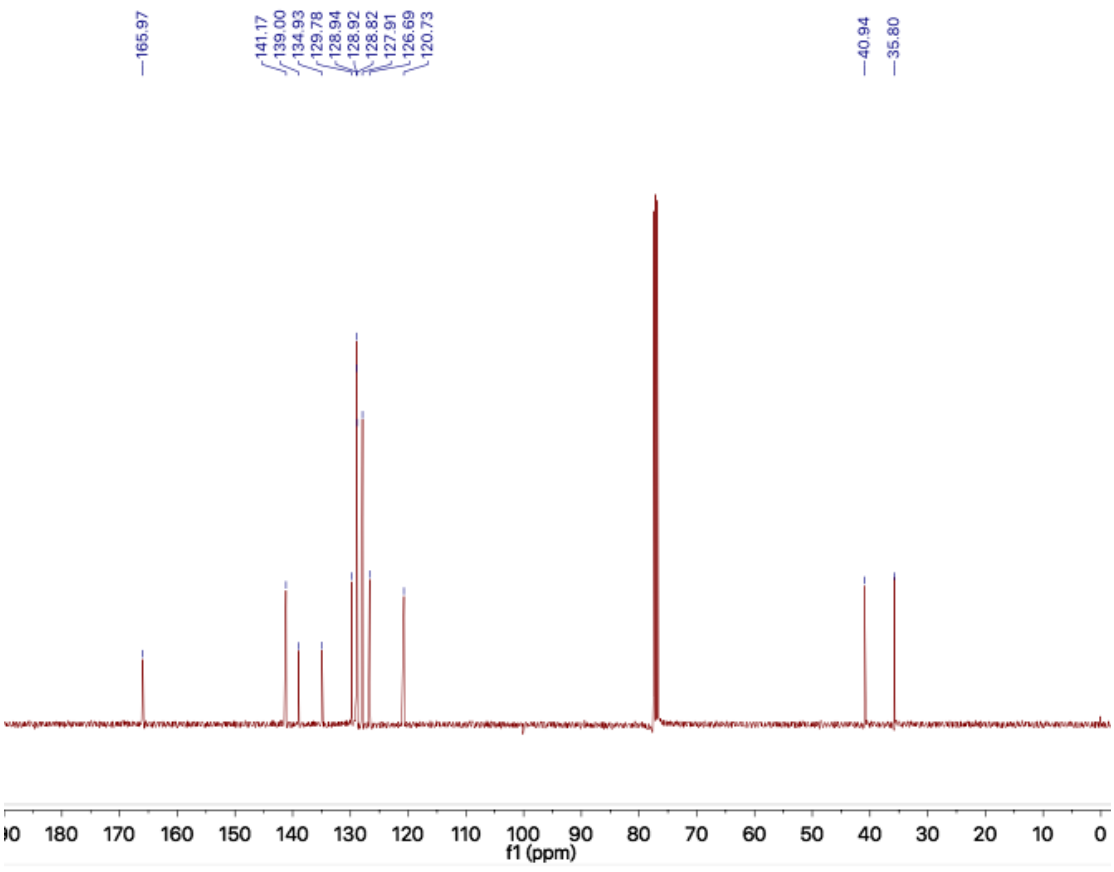
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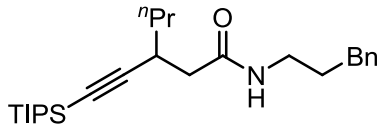
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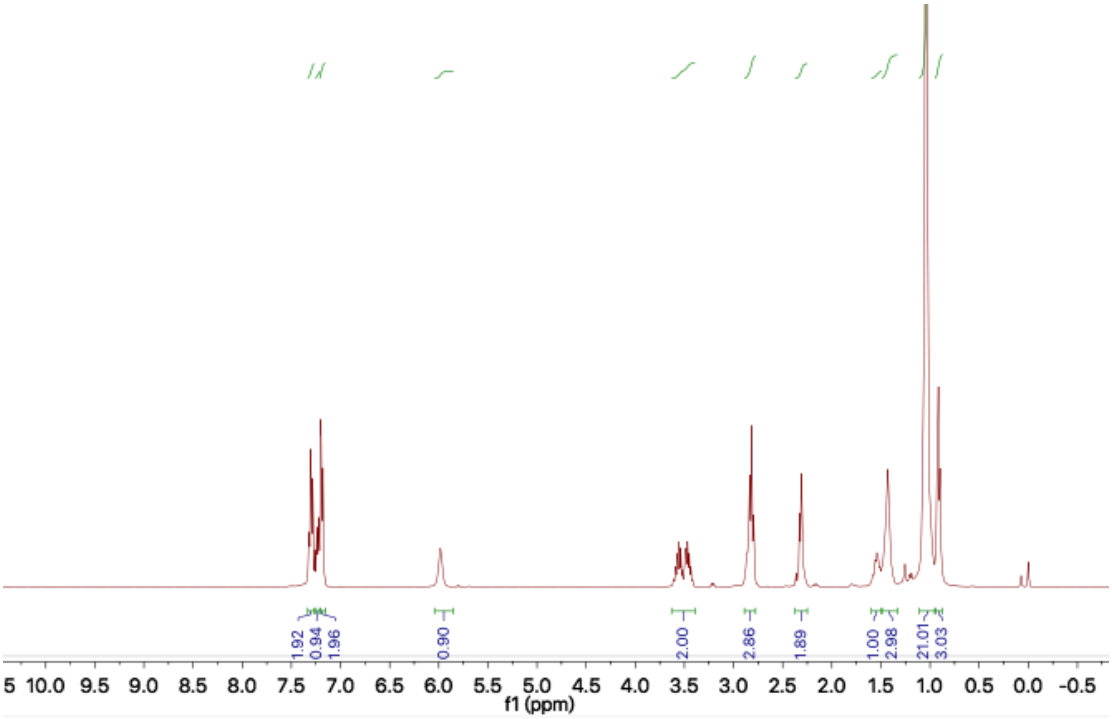
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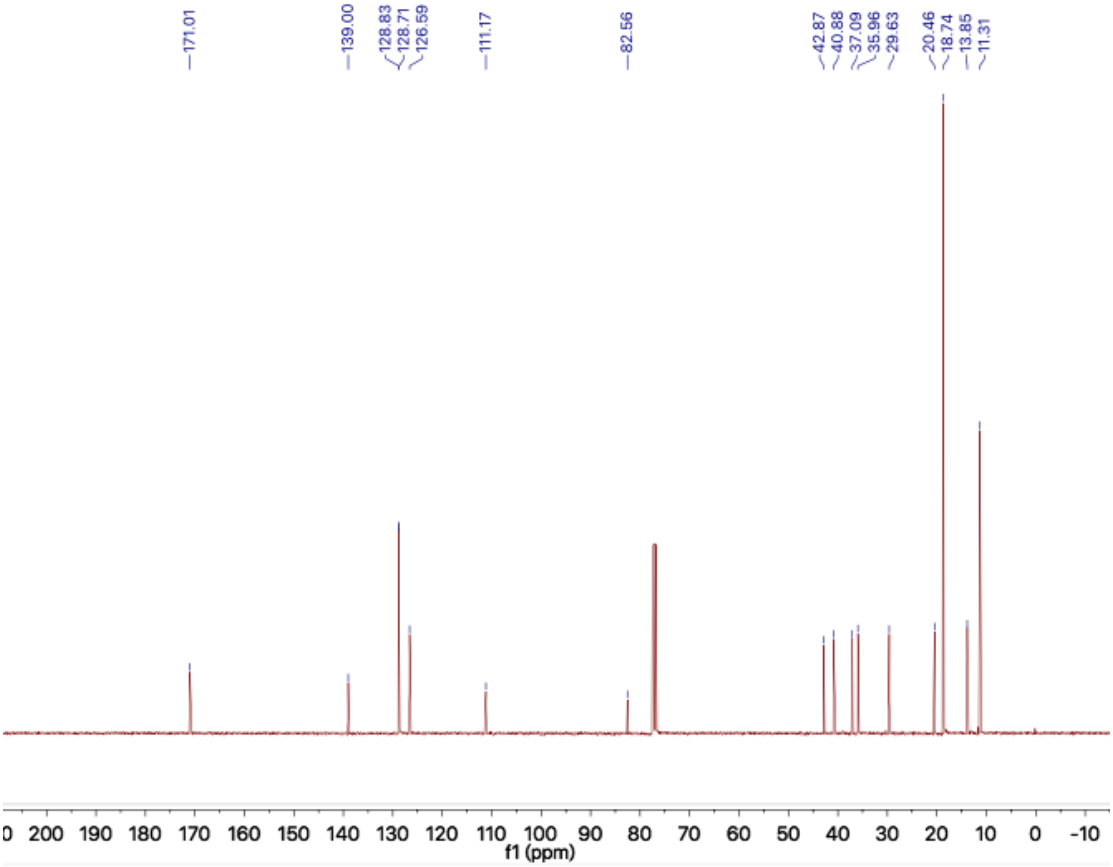
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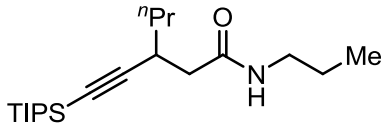
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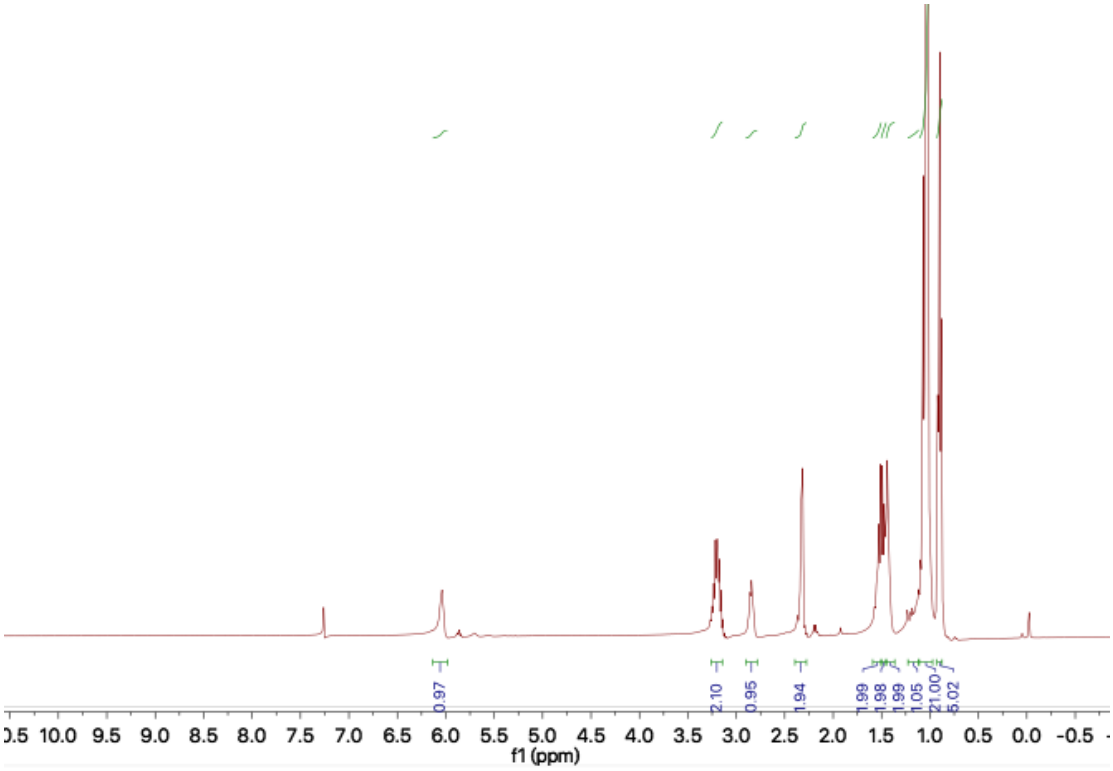
TIPS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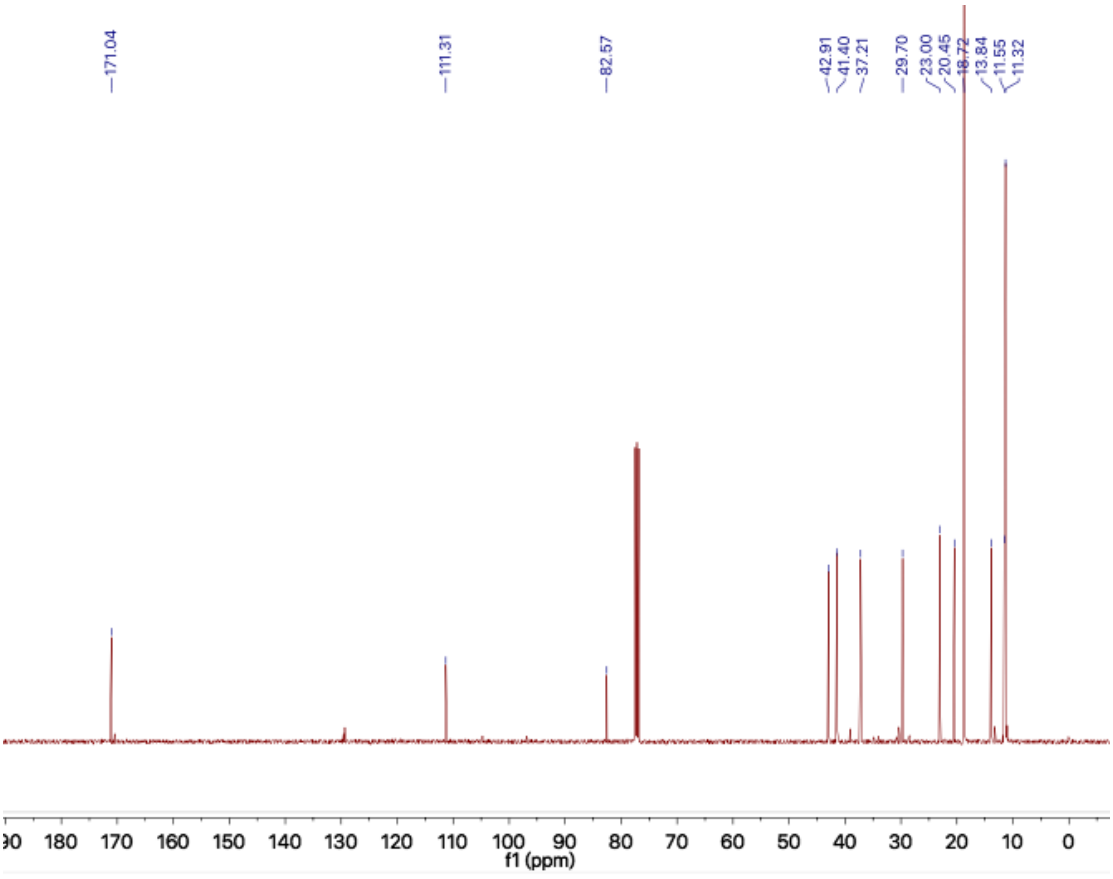
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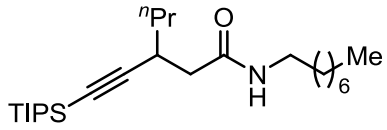
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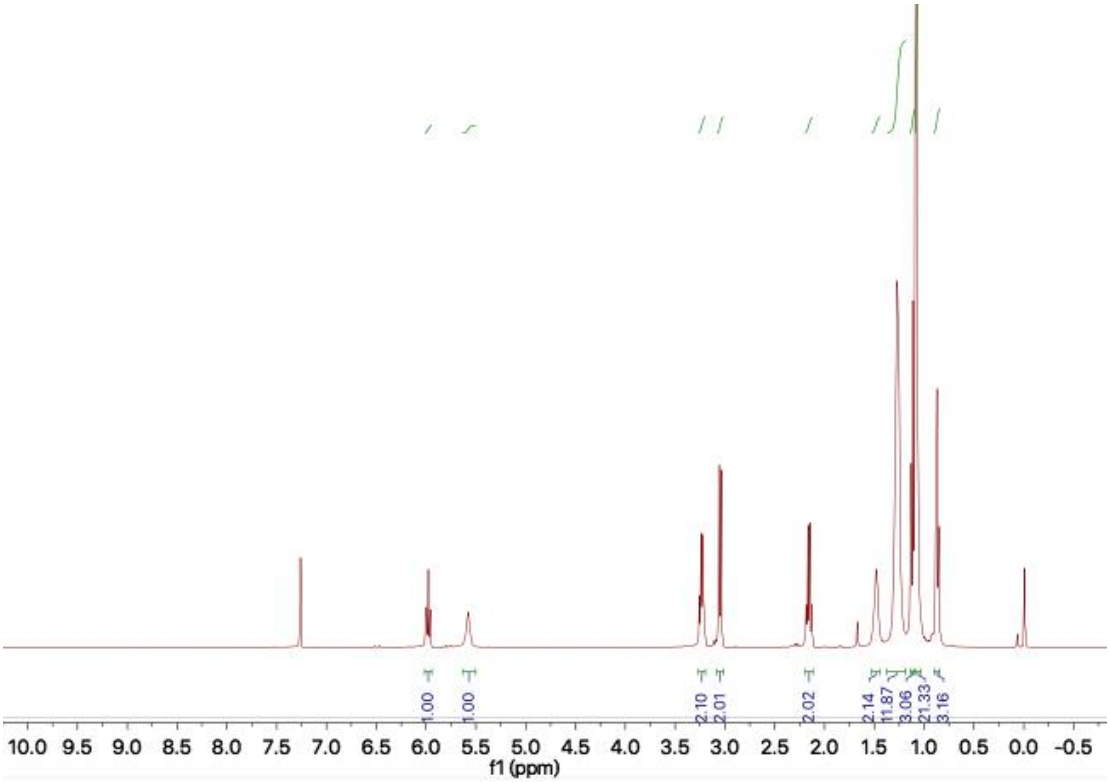
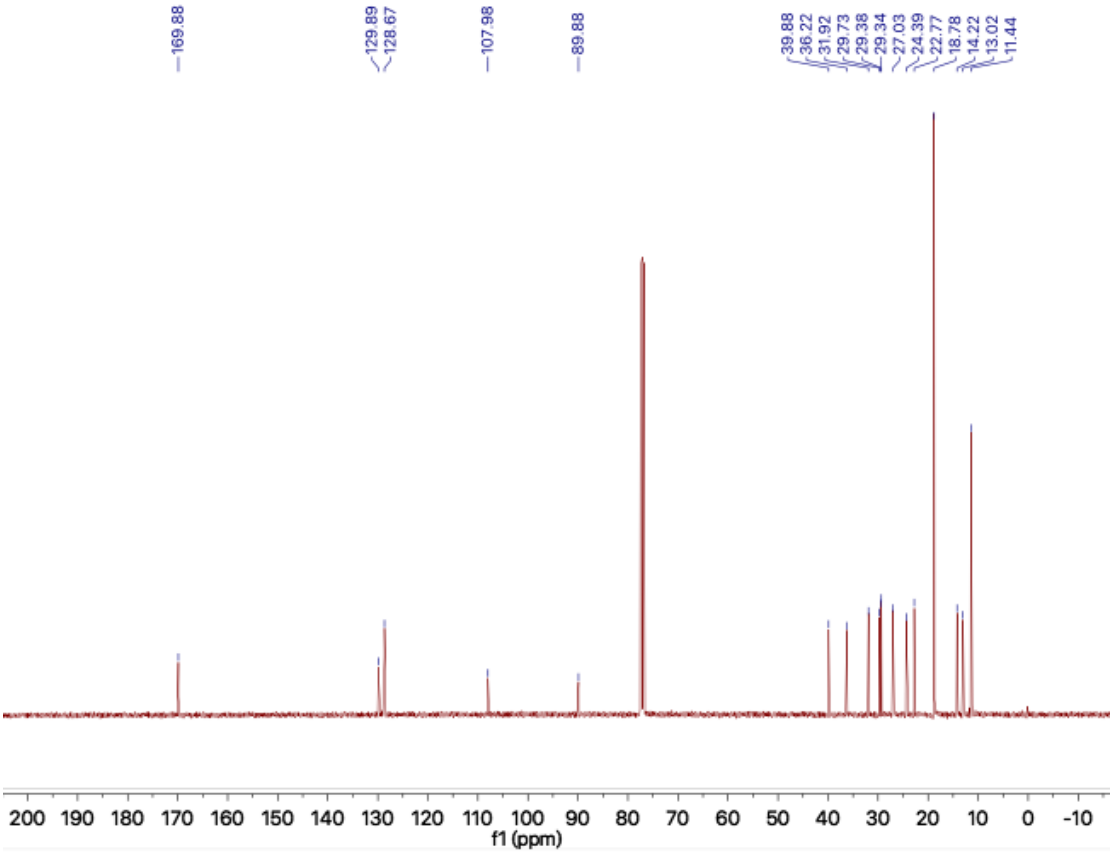
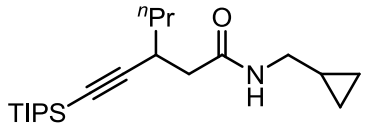
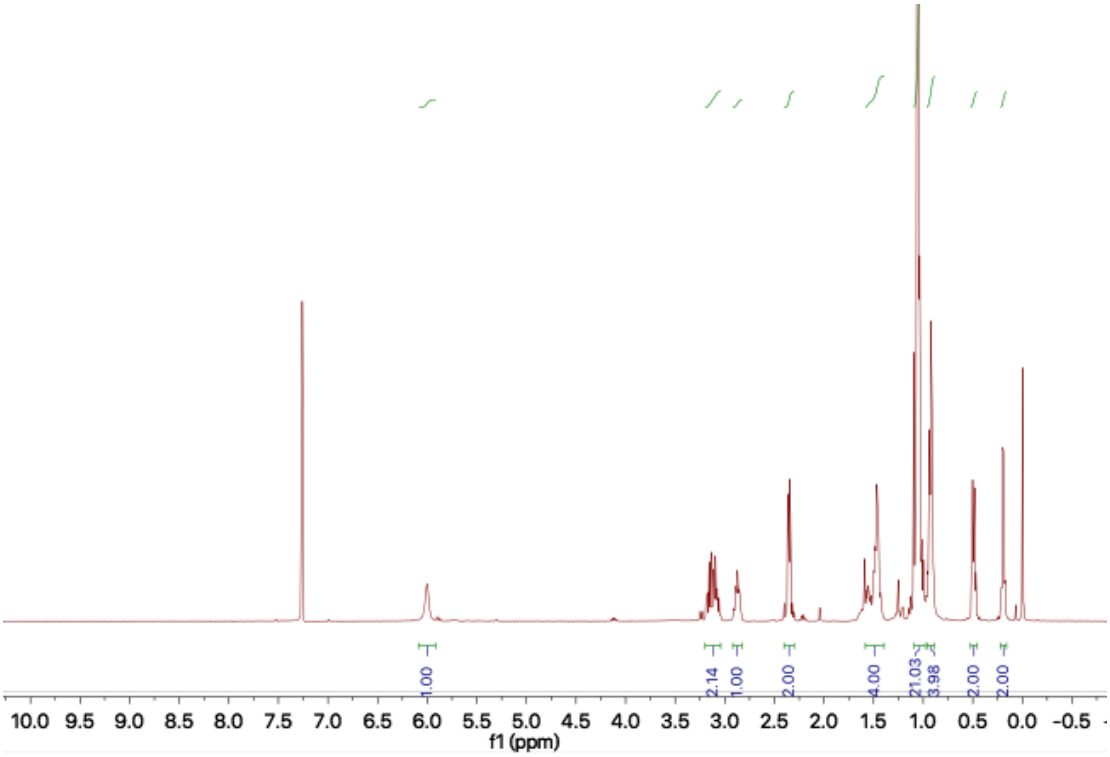
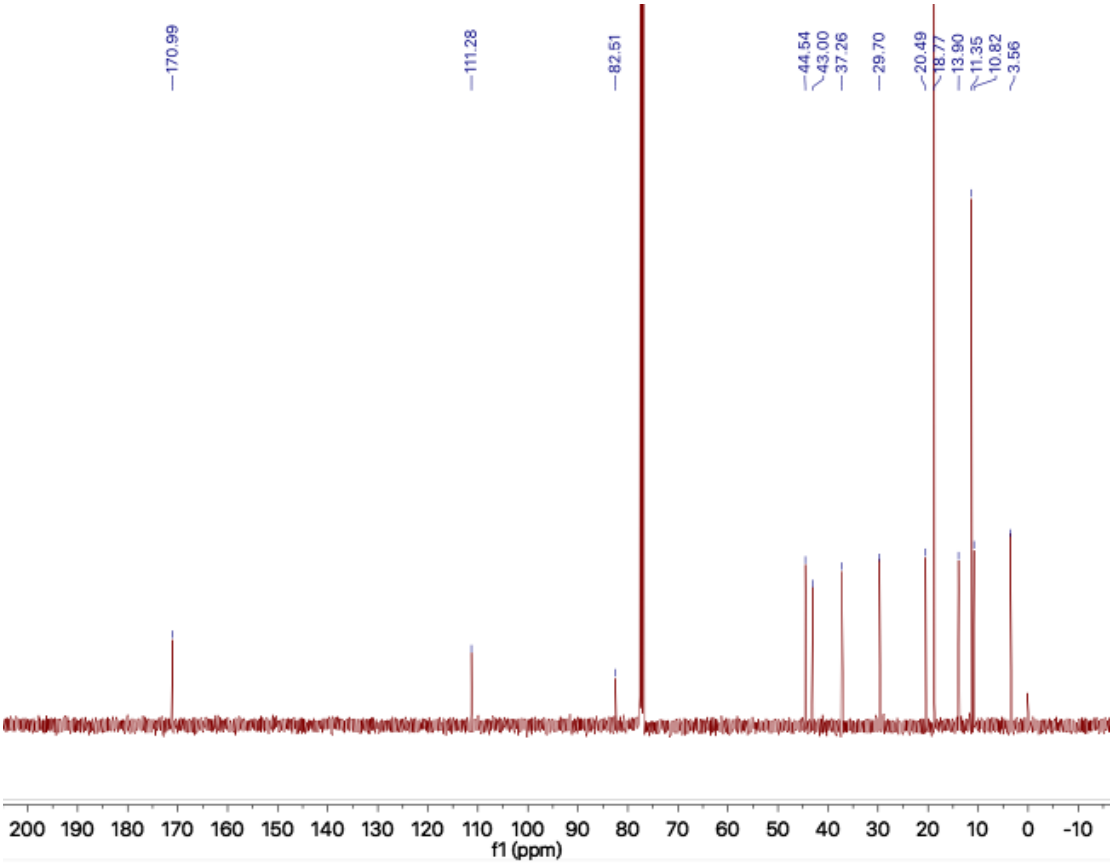
6
TIPS

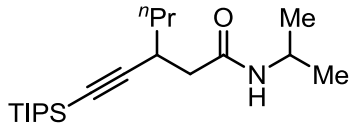

1.00
1.00
2.10
2.01
2.02
2.14
11.87
3.06
21.33
3.16
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

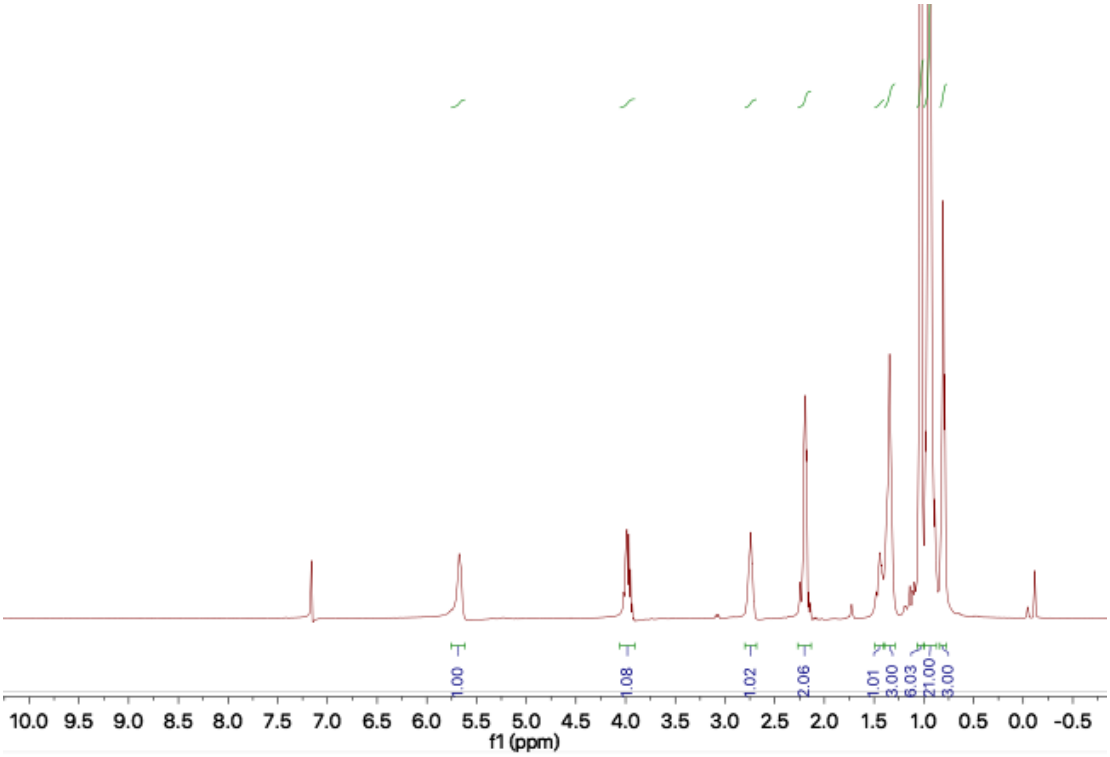

169.88
129.89
128.67
107.98
89.88
39.88
36.22
31.92
29.73
29.38
29.34
27.03
24.39
22.77
18.78
14.22
13.02
11.44
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

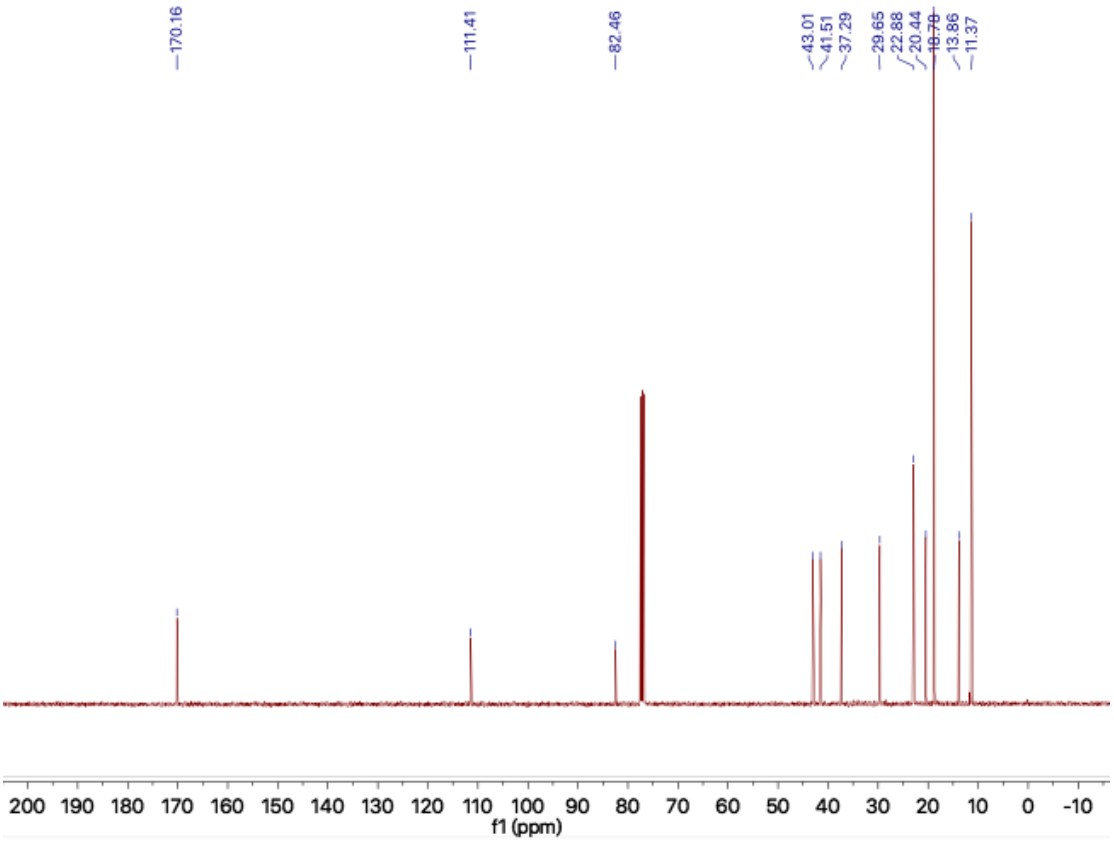

nPr
O
N
H
TIPS

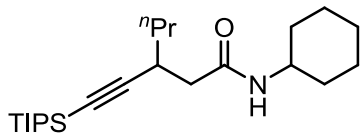

1.00
2.14
1.00
2.00
4.00
21.03
3.98
2.00
2.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

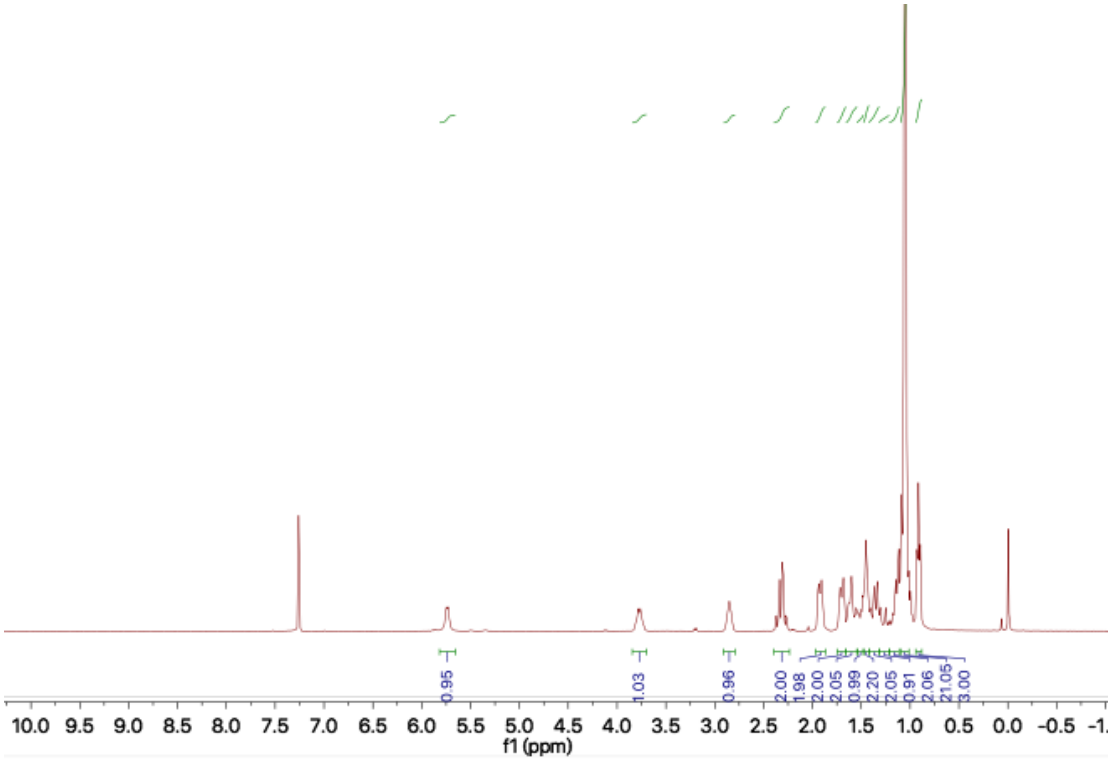

170.99
111.28
82.51
44.54
43.00
37.26
29.70
20.49
18.77
13.90
11.35
10.82
3.56
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

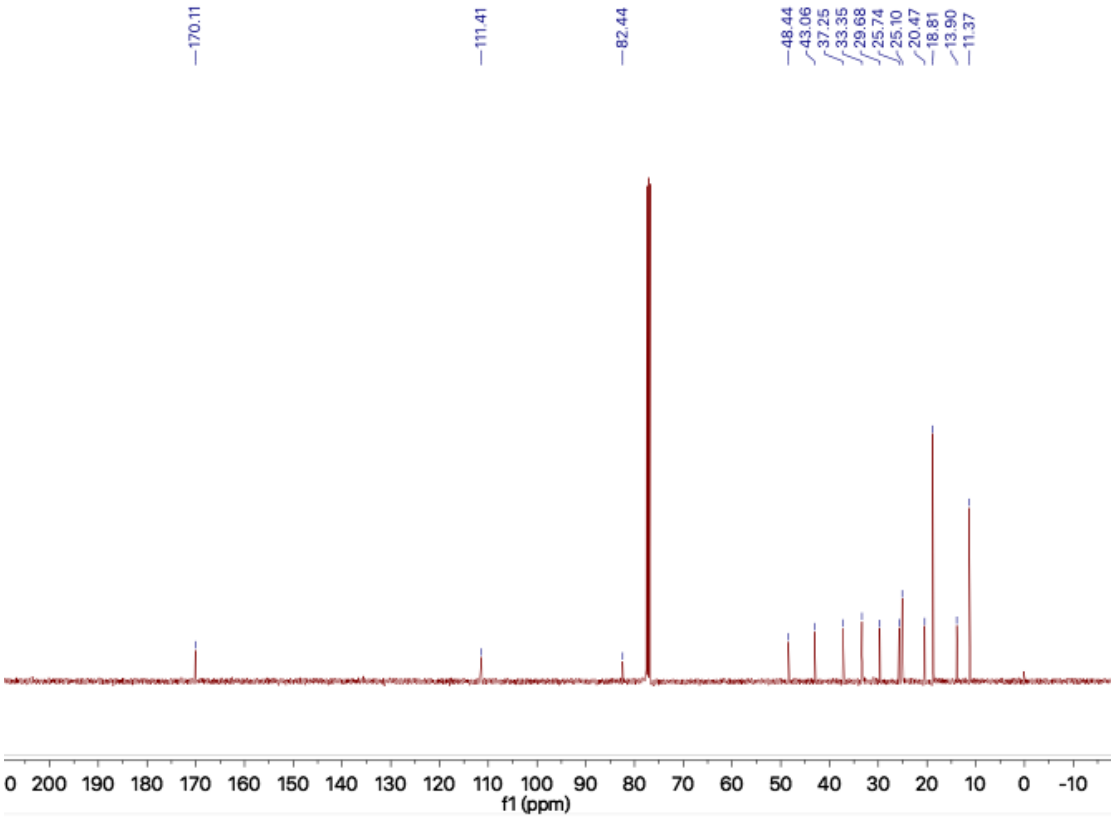

nPr
O
Me
N
H
Me
TIPS

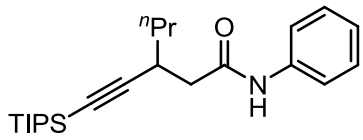

1.00
1.08
1.02
2.06
1.01
3.00
6.03
21.00
3.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

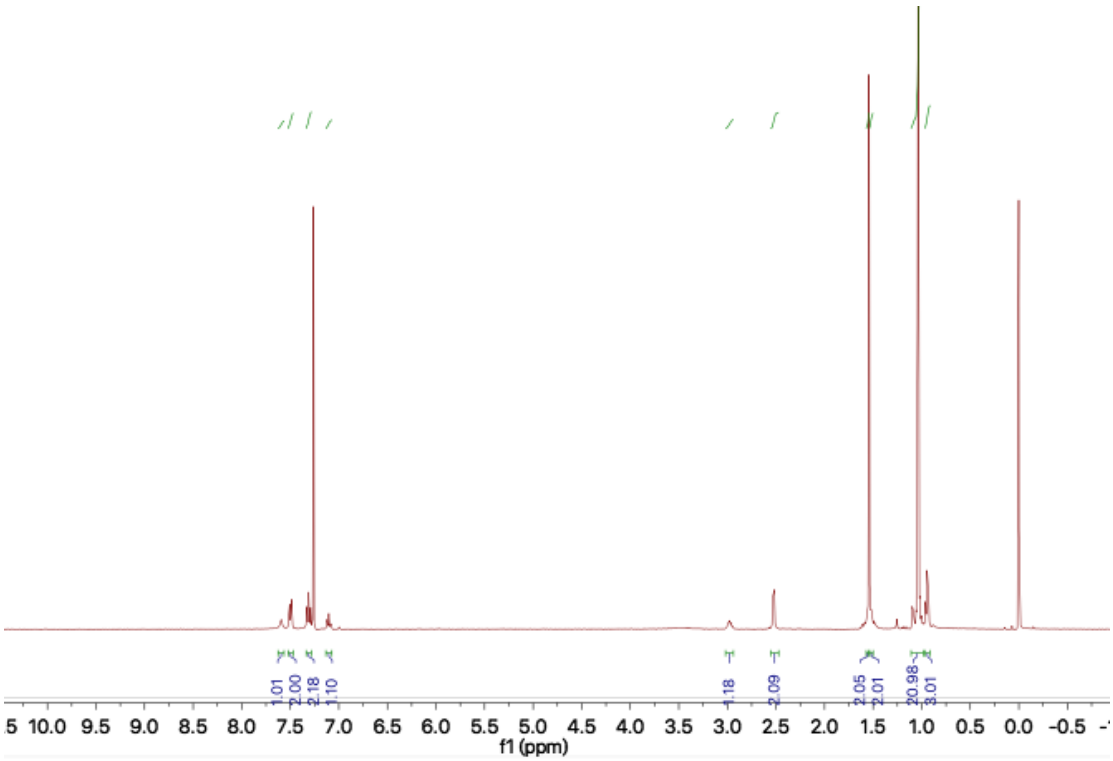

170.16
111.41
82.46
43.01
41.51
37.29
29.65
22.88
20.44
16.78
13.86
11.37
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

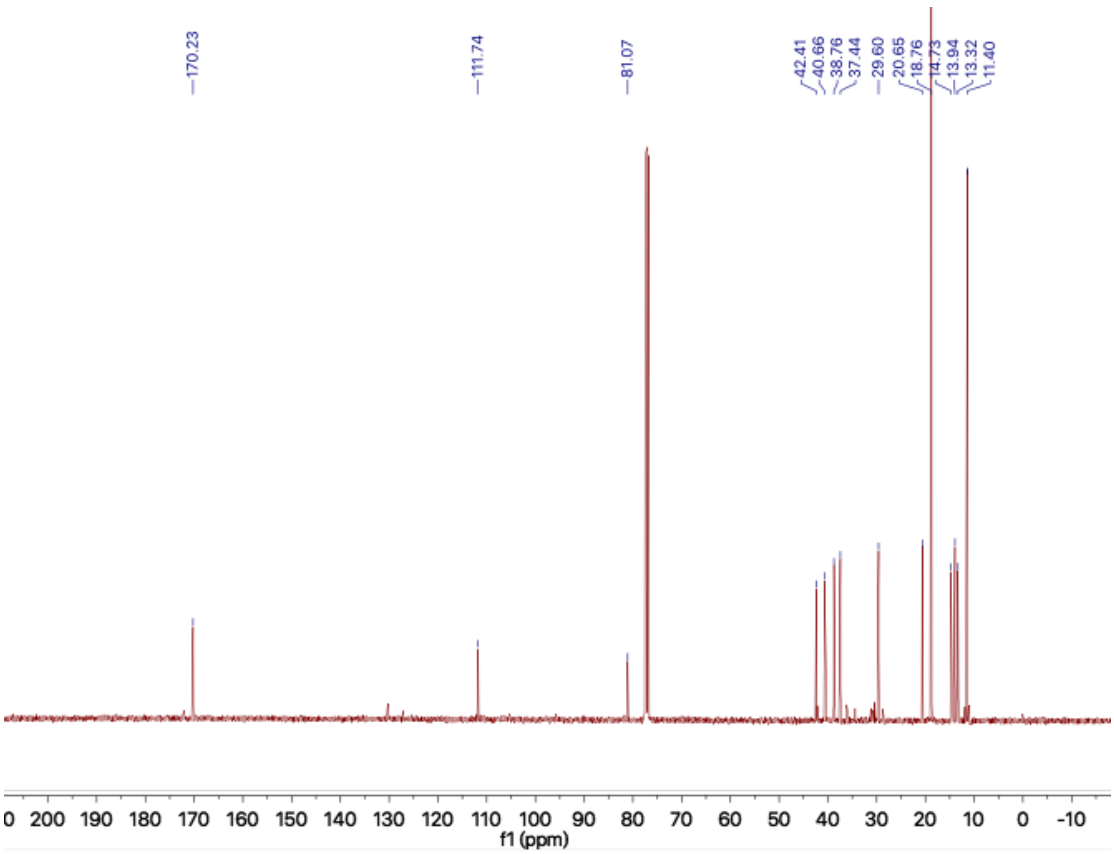

nPr
O
N
H
TIPS


0.95
1.03
0.96
2.00
1.98
2.00
2.05
0.99
2.20
2.05
0.91
2.06
21.05
3.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.
f1 (ppm)


170.11
111.41
82.44
48.44
43.06
37.25
33.35
29.68
25.74
25.10
20.47
18.81
13.90
11.37
0 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


nPr
O
N
H
TIPS


1.01
2.00
2.18
1.10
1.18
2.09
2.05
2.01
20.98
3.01
f1 (ppm)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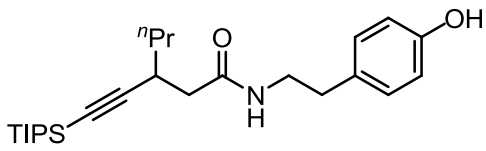
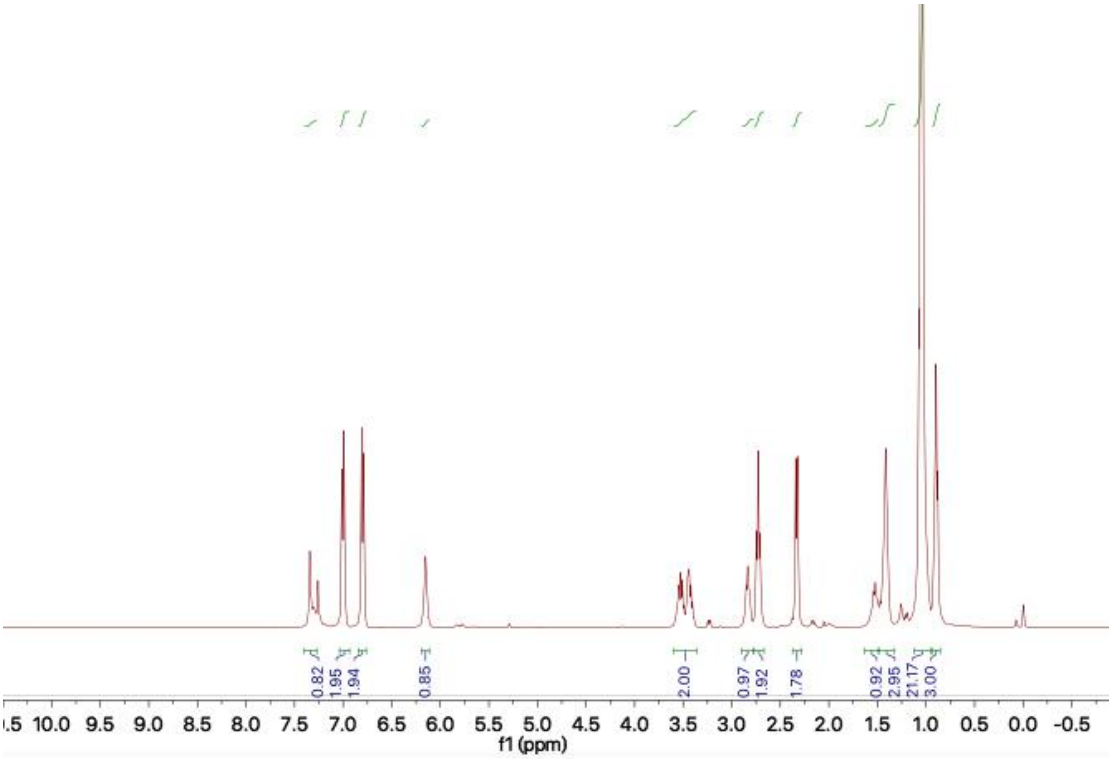
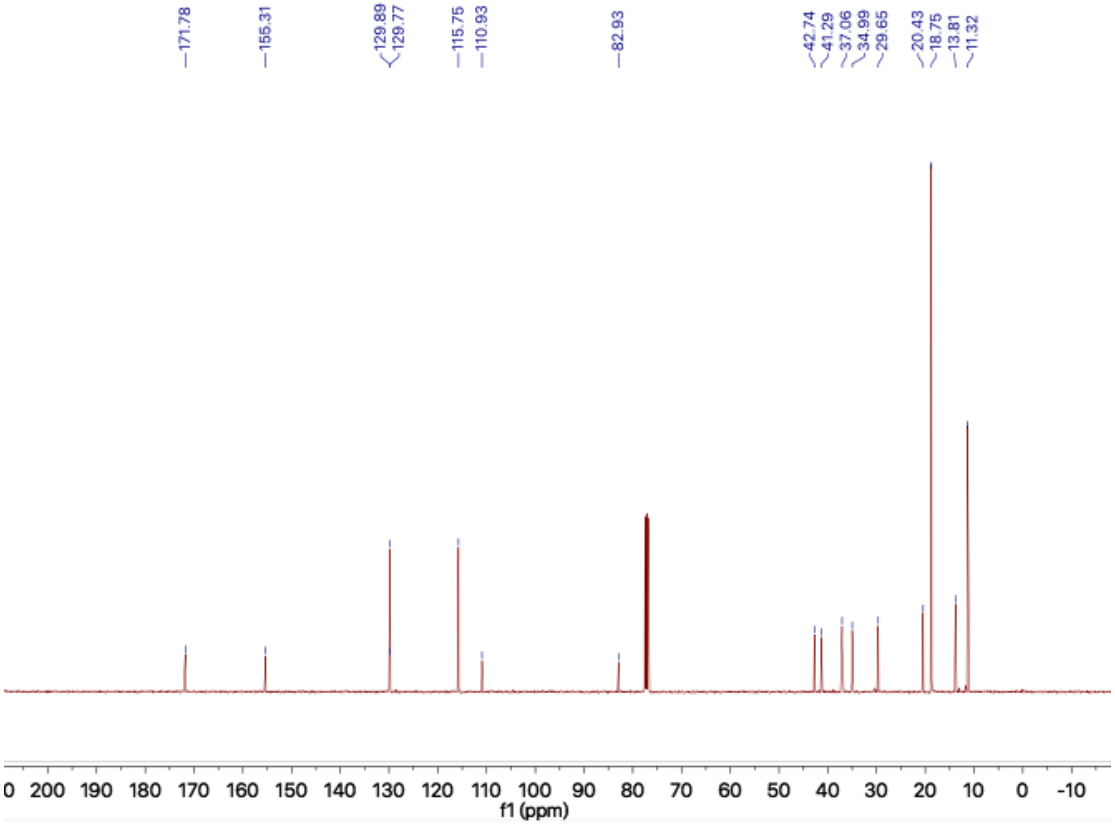
111.74
81.07
42.41
40.66
38.76
37.44
29.60
20.65
18.76
14.73
13.94
13.32
11.40
f1 (ppm)


nPr
O
OH
N
H
TIPS


0.82
1.95
1.94
0.85
2.00
0.97
1.92
1.78
0.92
2.95
21.17
3.00
f1 (ppm)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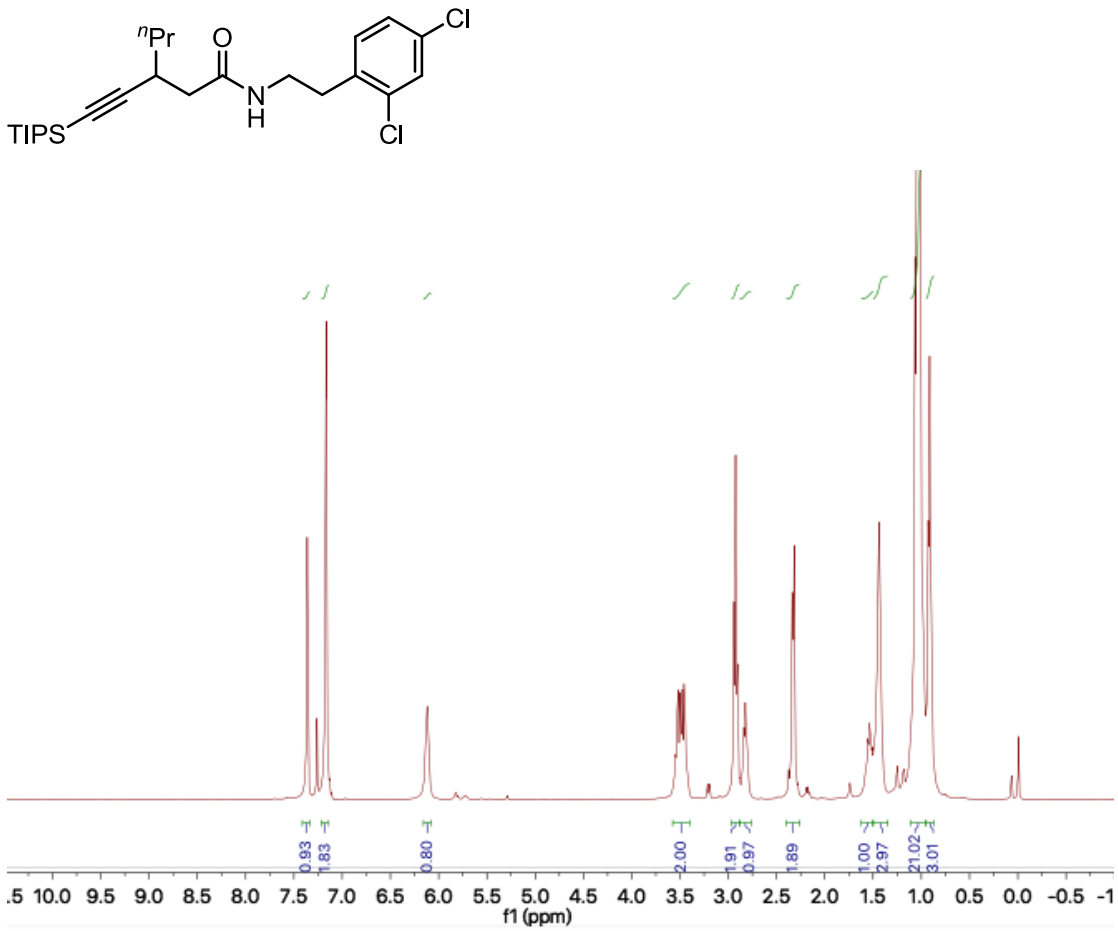
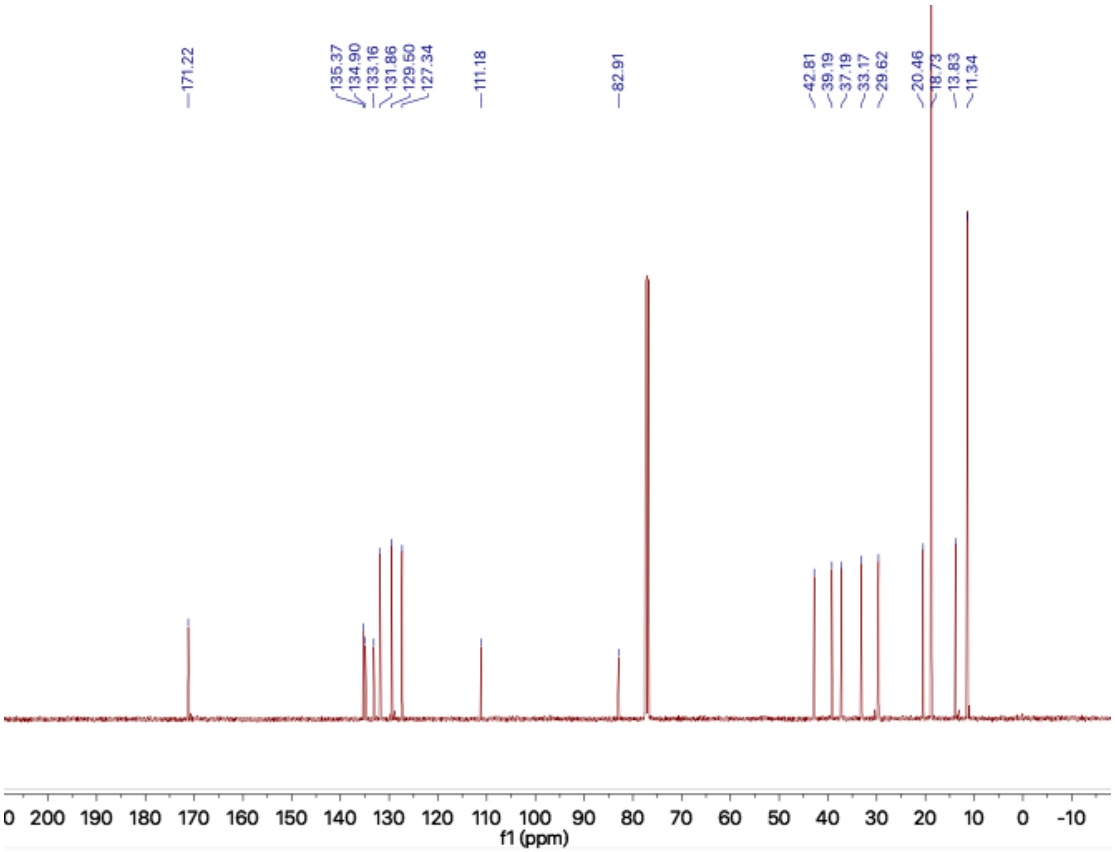
155.31
129.89
129.77
115.75
110.93
82.93
42.74
41.29
37.06
34.99
29.65
20.43
18.75
13.81
11.32
f1 (ppm)


nPr
O
N
H
Cl
Cl
TIPS
0.93
1.83
0.80
2.00
1.91
0.97
1.89
1.00
2.97
21.02
3.01
f1 (ppm)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135.37
134.90
133.16
131.86
129.50
127.34
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82.91
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39.19
37.19
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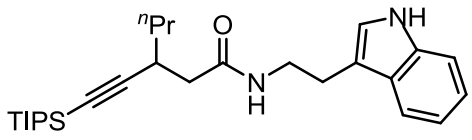
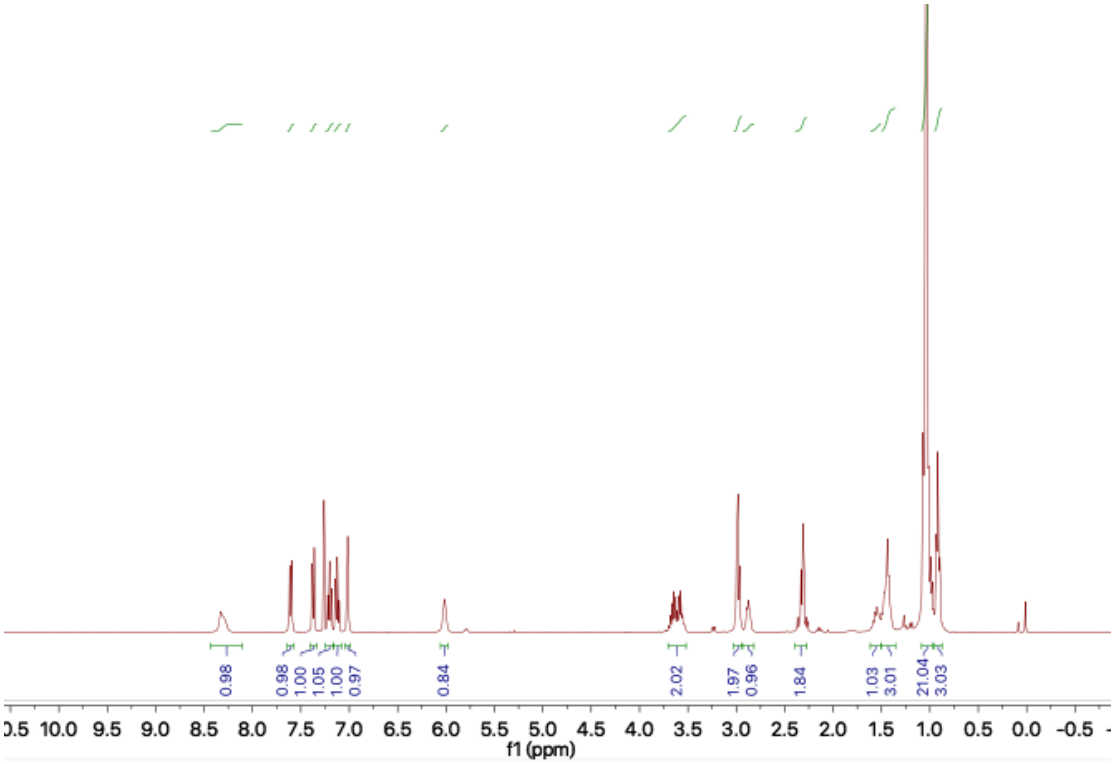
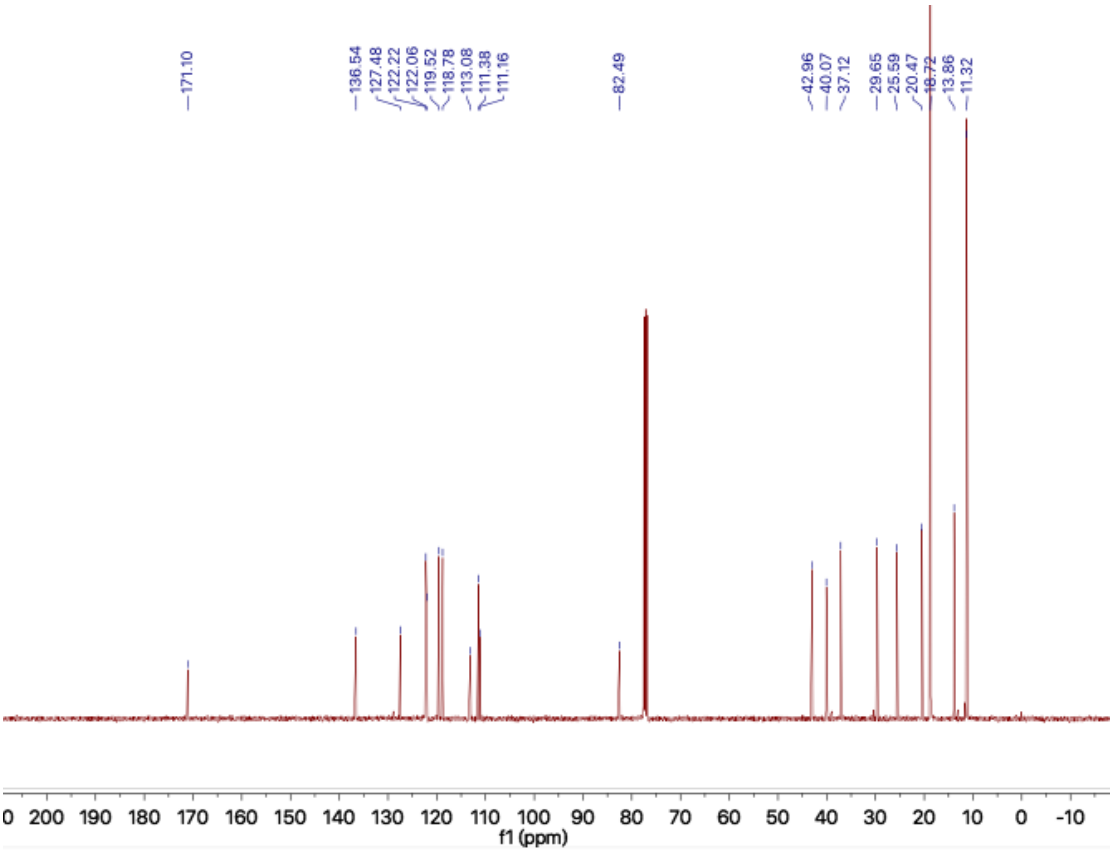
20.46
18.73
13.83
11.34
f1 (ppm)


nPr
O
NH
N
H
TIPS


0.98
0.98
1.00
1.05
1.00
0.97
0.84
2.02
1.97
0.96
1.84
1.03
3.01
21.04
3.03
f1 (ppm)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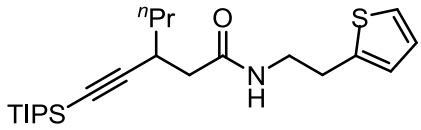
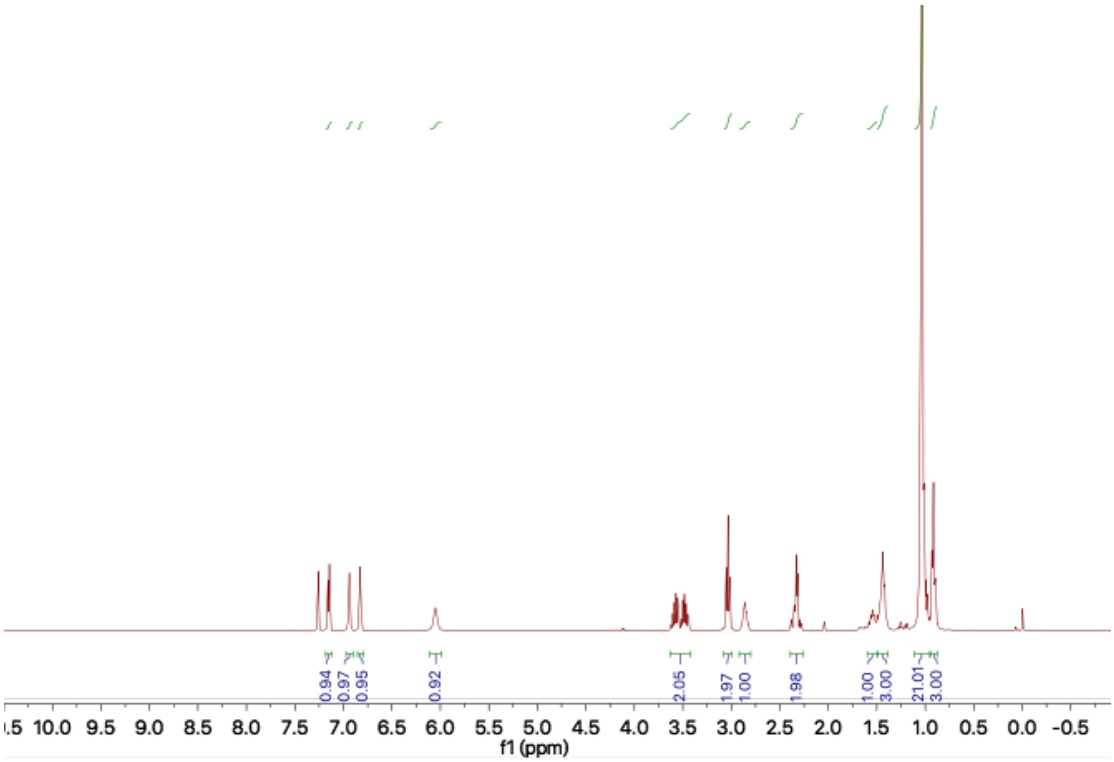
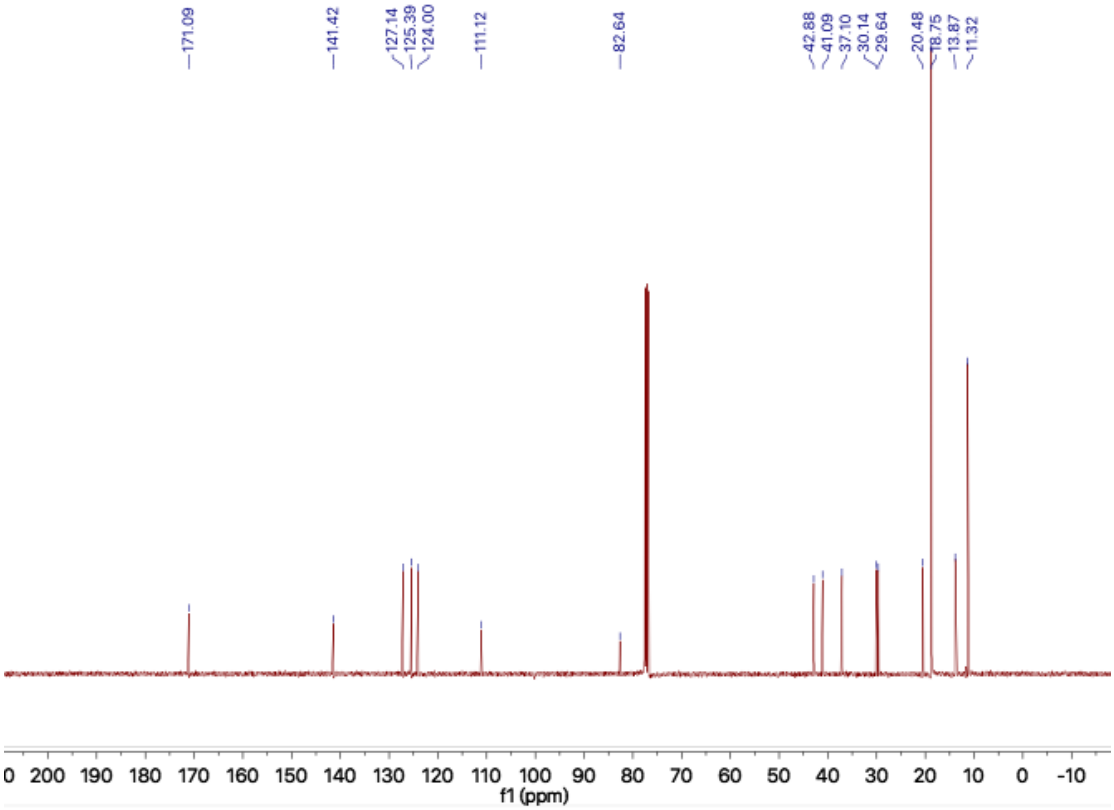
136.54
127.48
122.22
122.06
119.52
118.78
113.08
111.38
111.16
82.49
42.96
40.07
37.12
29.65
25.59
20.47
18.72
13.86
11.32
f1 (ppm)


nPr
O
S
N
H
TIPS


0.94
0.97
0.95
0.92
2.05
1.97
1.00
1.98
1.00
3.00
21.01
3.00
f1 (ppm)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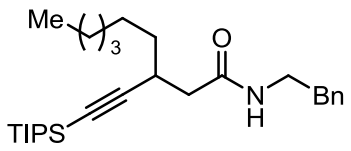
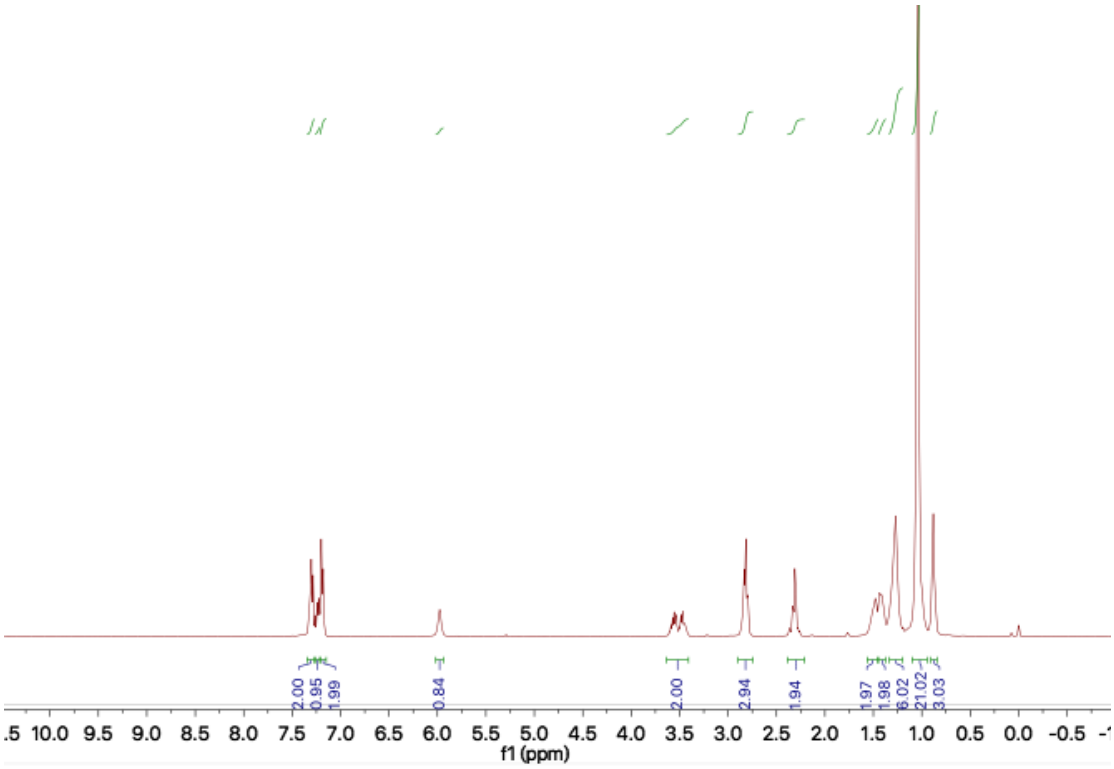
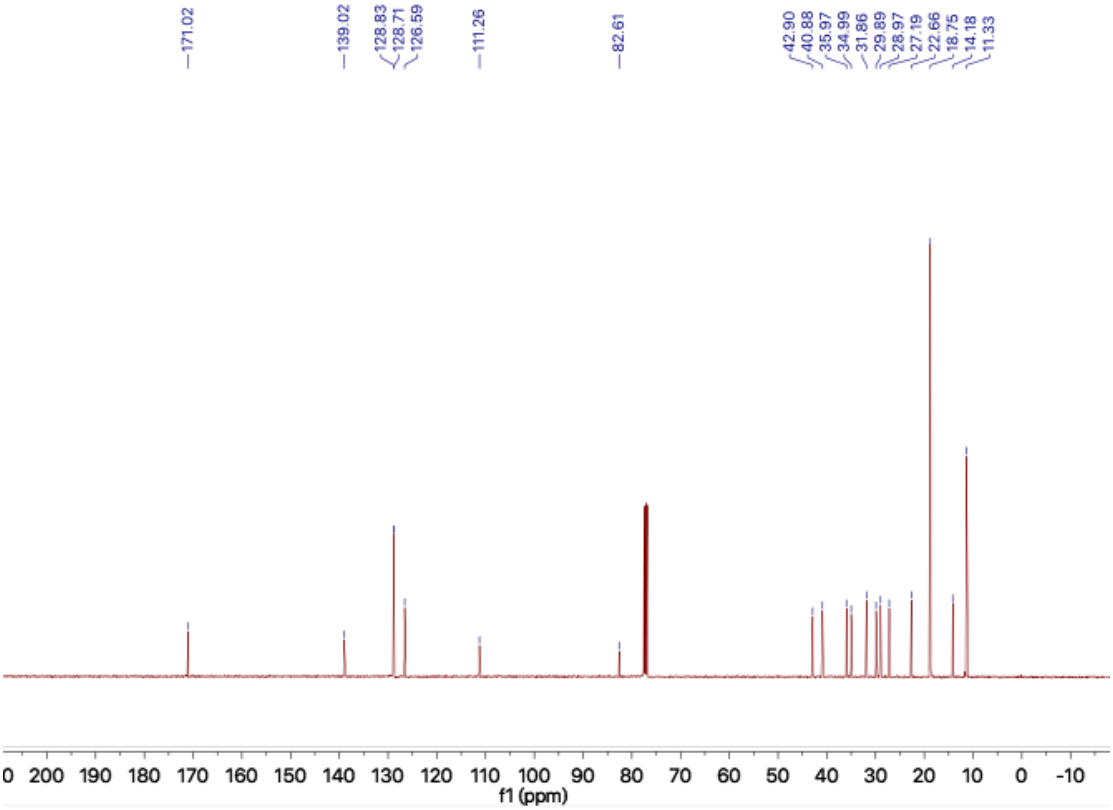
141.42
127.14
125.39
124.00
111.12
82.64
42.88
41.09
37.10
30.14
29.64
20.48
18.75
13.87
11.32
f1 (ppm)


Me
3
O
N
H
Bn
TIPS


2.00
0.95
1.99
0.84
2.00
2.94
1.94
1.97
1.98
6.02
21.02
3.03
f1 (ppm)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139.02
128.83
128.71
126.59
111.26
82.61
42.90
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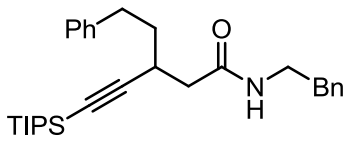
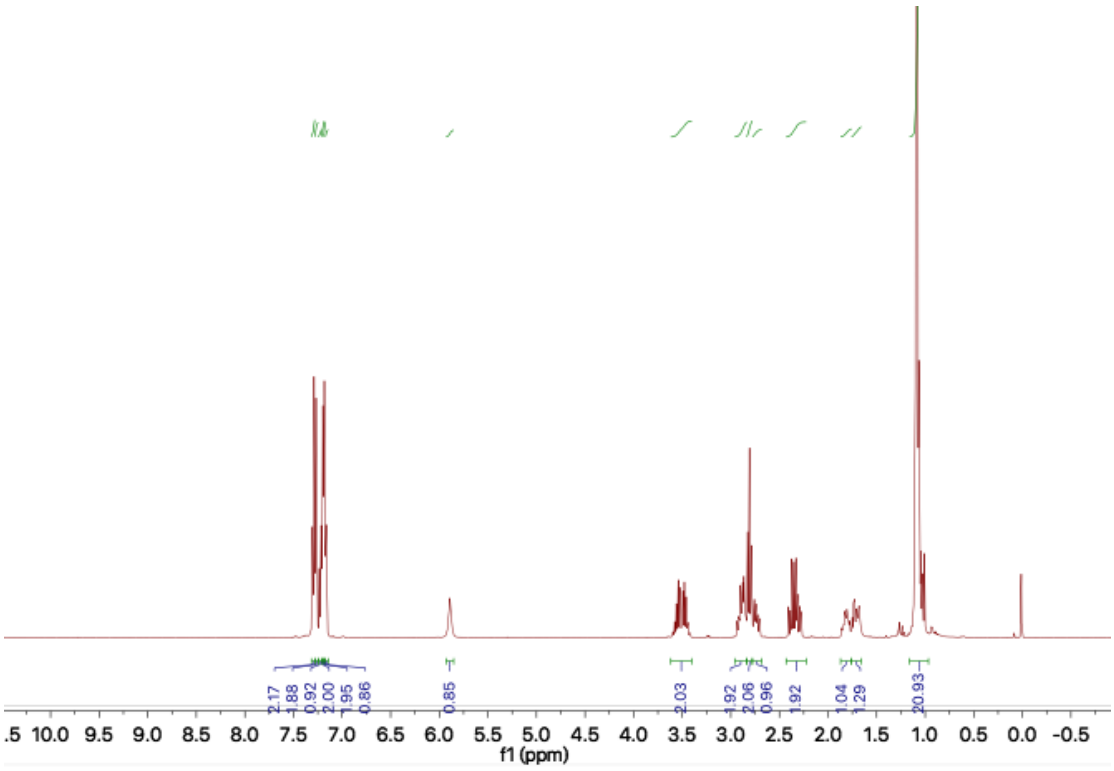
31.86
29.89
28.97
27.19
22.66
18.75
14.18
11.33
f1 (ppm)


Ph
O
N
H
Bn
TIPS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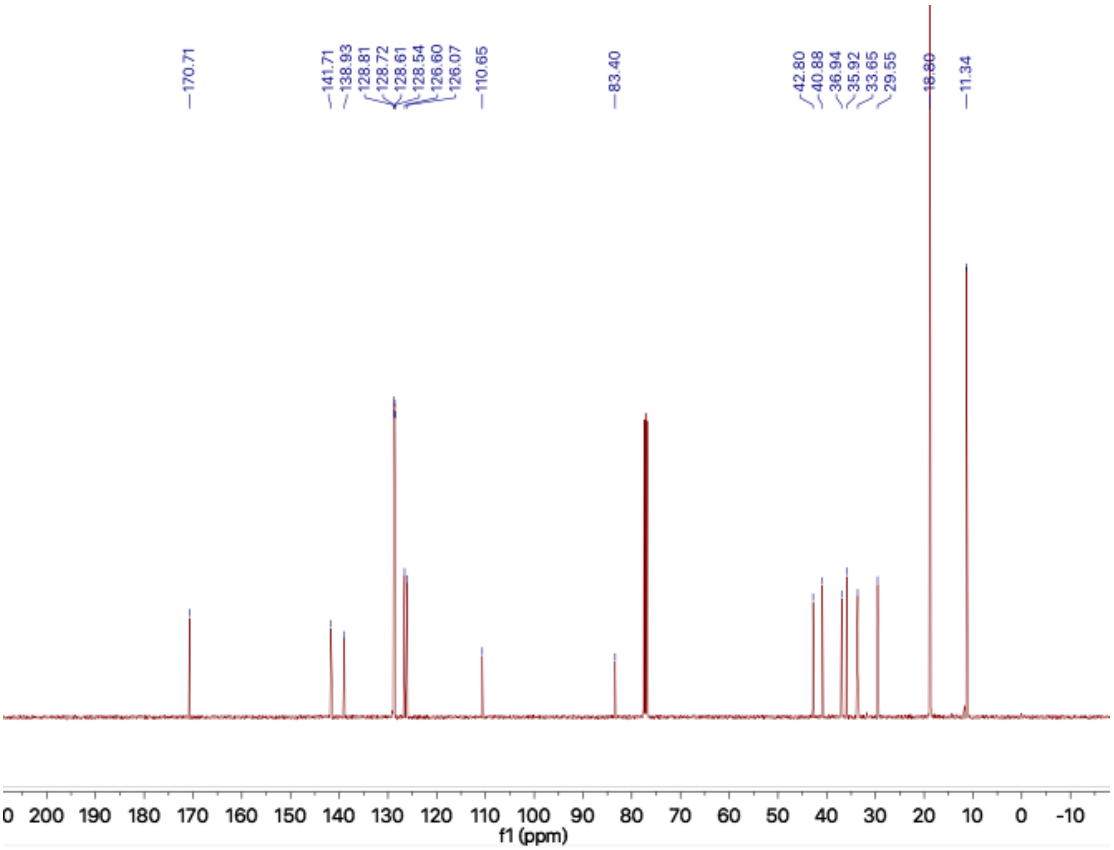
1.88
0.92
2.00
1.95
0.86
0.85
2.03
1.92
2.06
0.96
1.92
1.04
1.29
20.93
f1 (ppm)


170.71
141.71
138.93
128.81
128.72
128.61
128.54
126.60
126.07
110.65
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42.80
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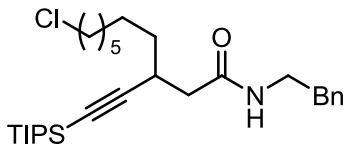
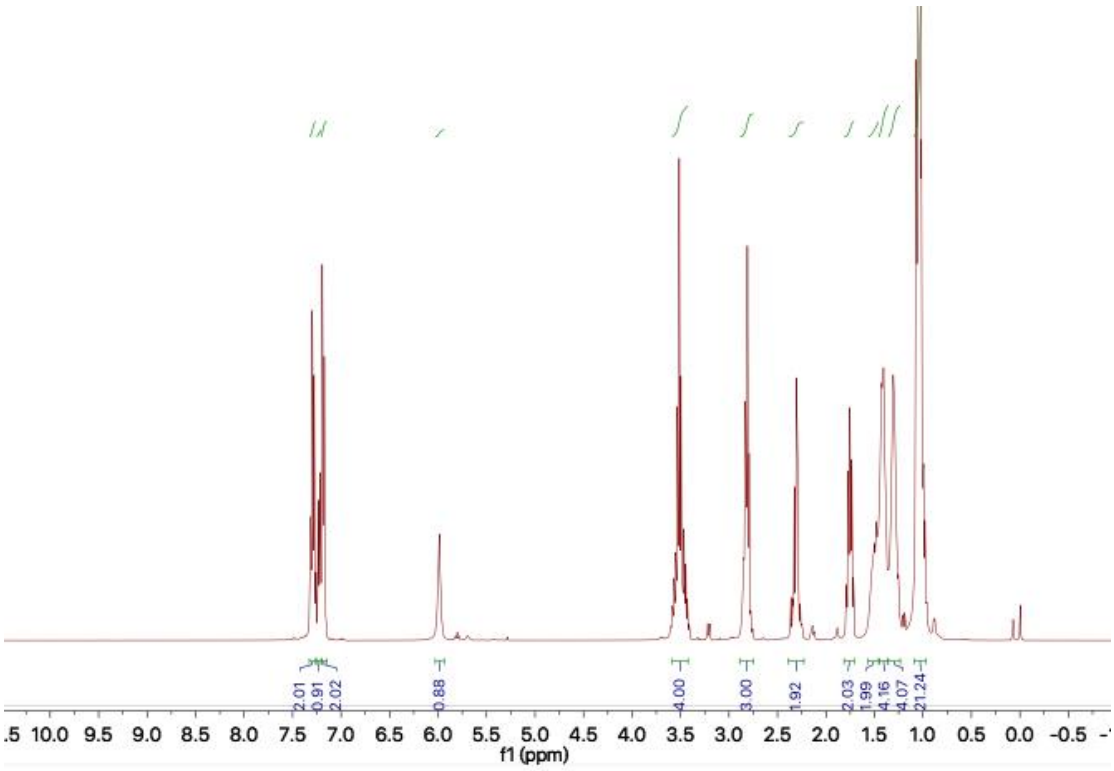
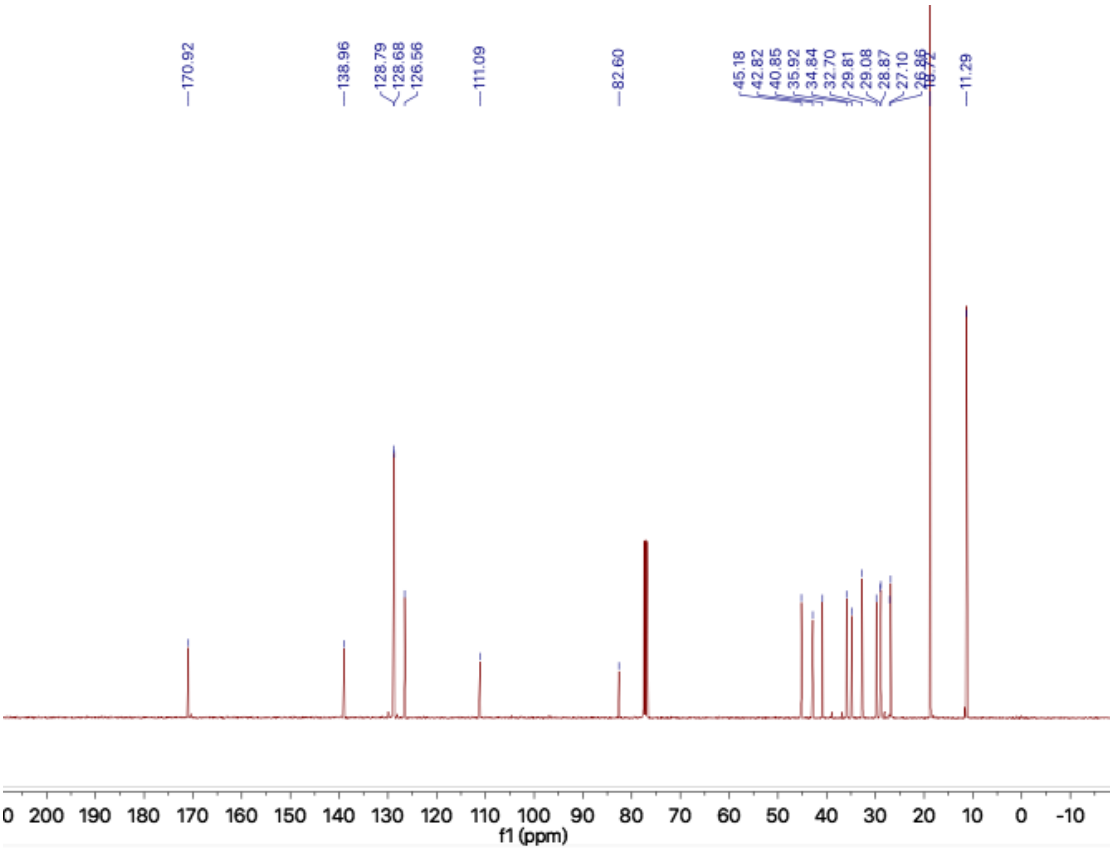
33.65
29.55
18.80
11.34
f1 (ppm)


Cl
5
O
N
H
Bn
TIPS


2.01
0.91
2.02
0.88
4.00
3.00
1.92
2.03
1.99
4.16
4.07
21.24
f1 (ppm)


170.92
138.96
128.79
128.68
126.56
111.09
82.60
45.18
42.82
40.85
35.92
34.84
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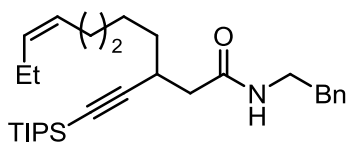
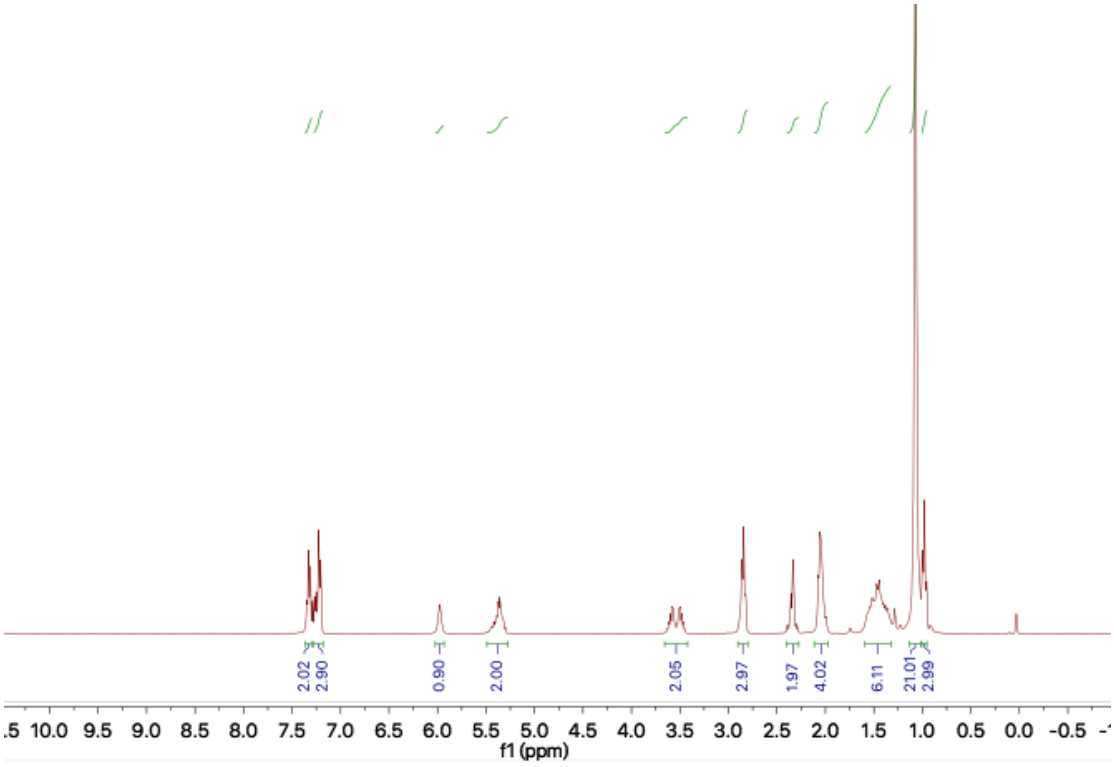
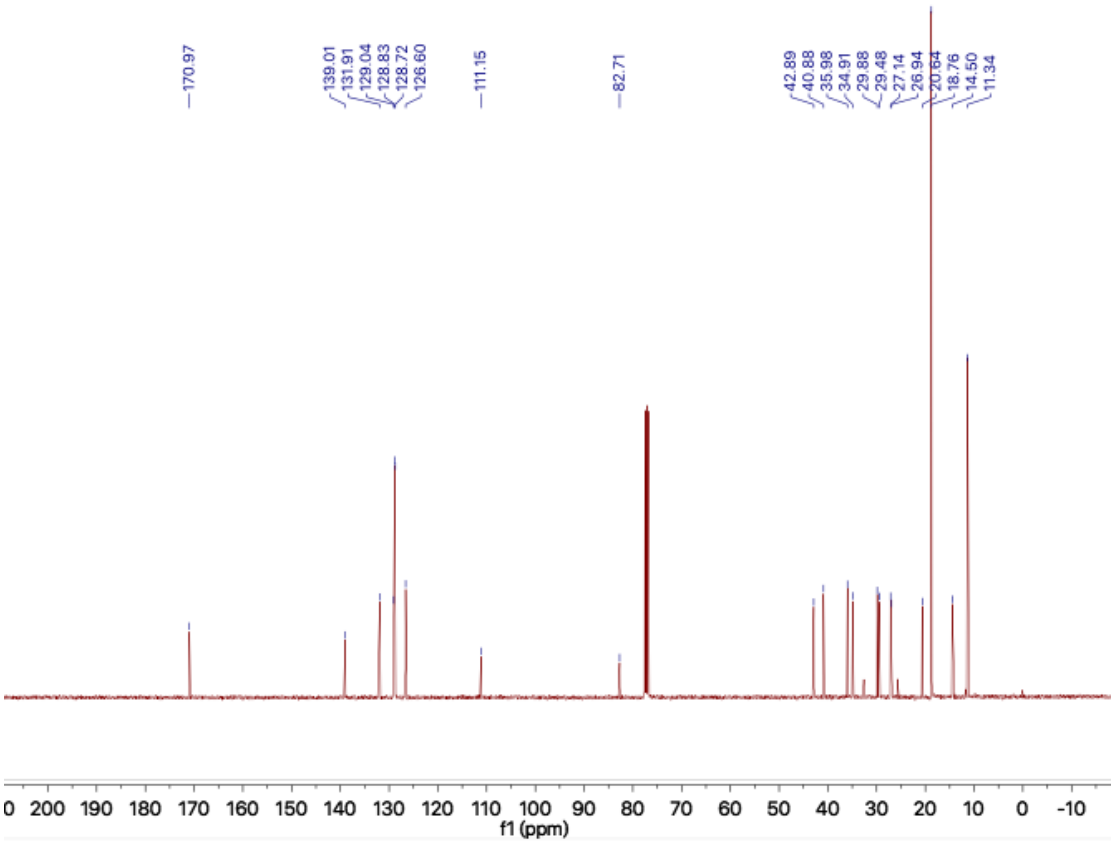
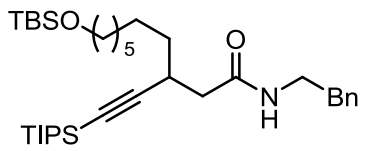
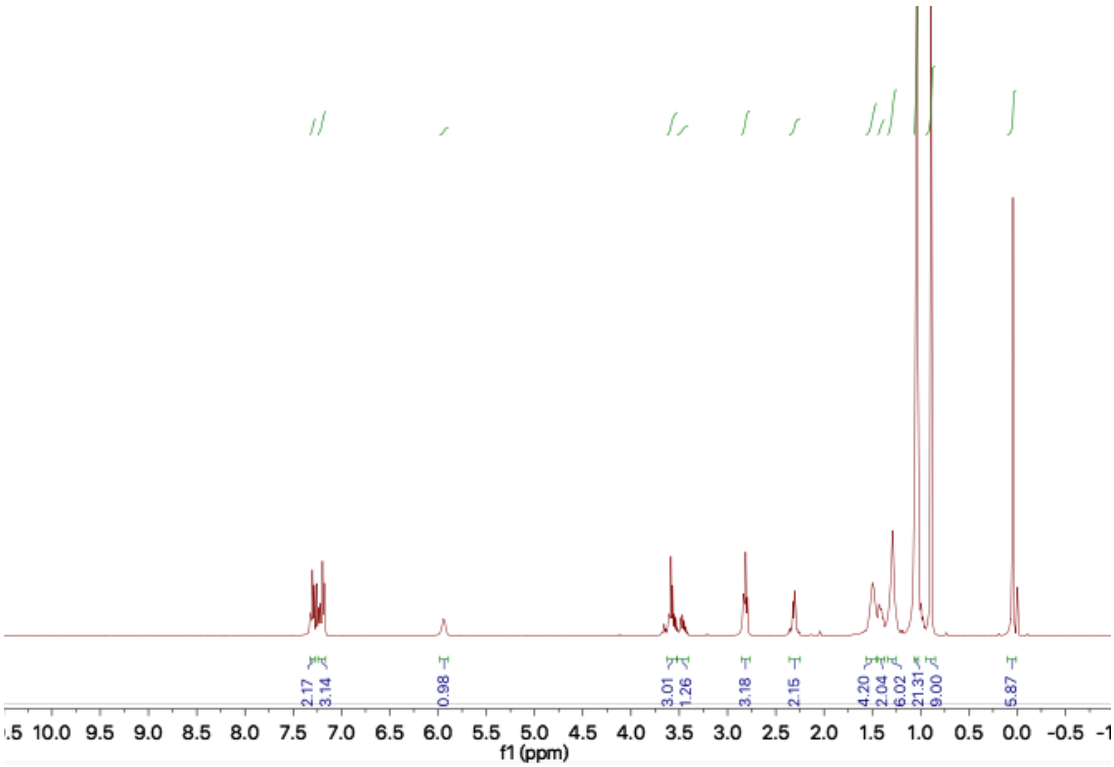
27.10
26.86
18.72
11.29
f1 (ppm)

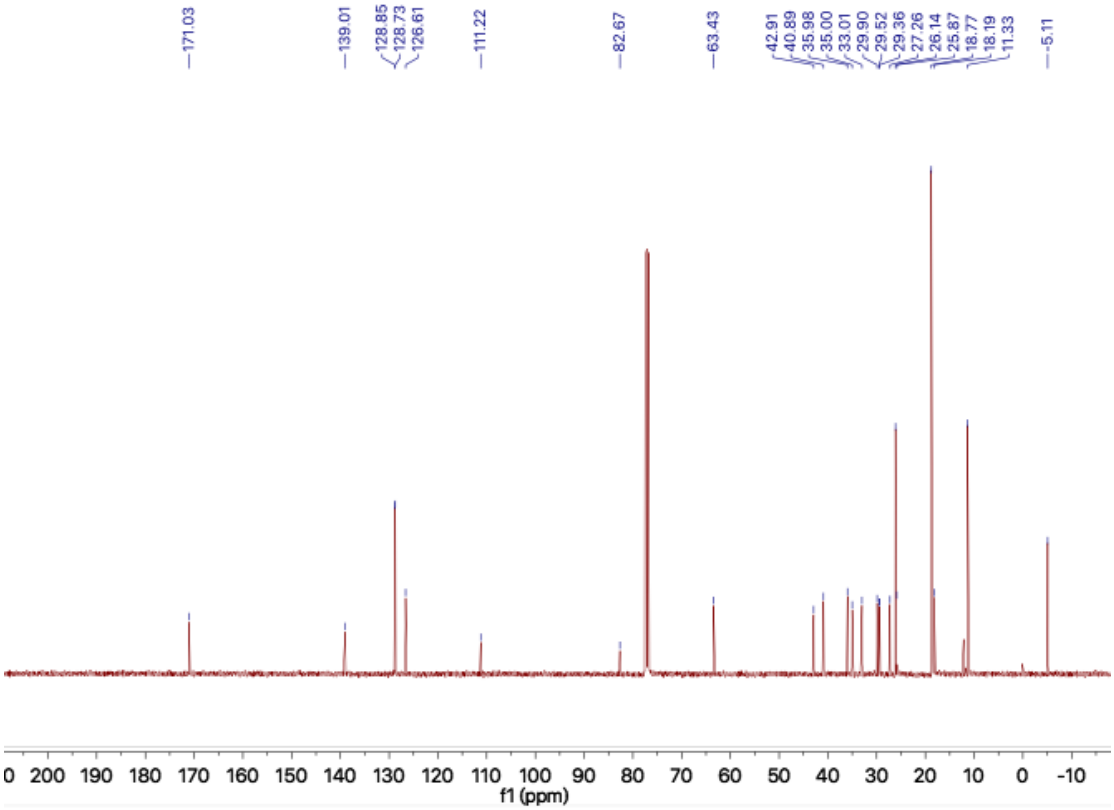

Et
2
O
N
H
Bn
TIPS

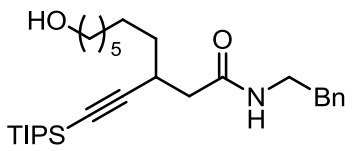

2.02
2.90
0.90
2.00
2.05
2.97
1.97
4.02
6.11
21.01
2.99
f1 (ppm)

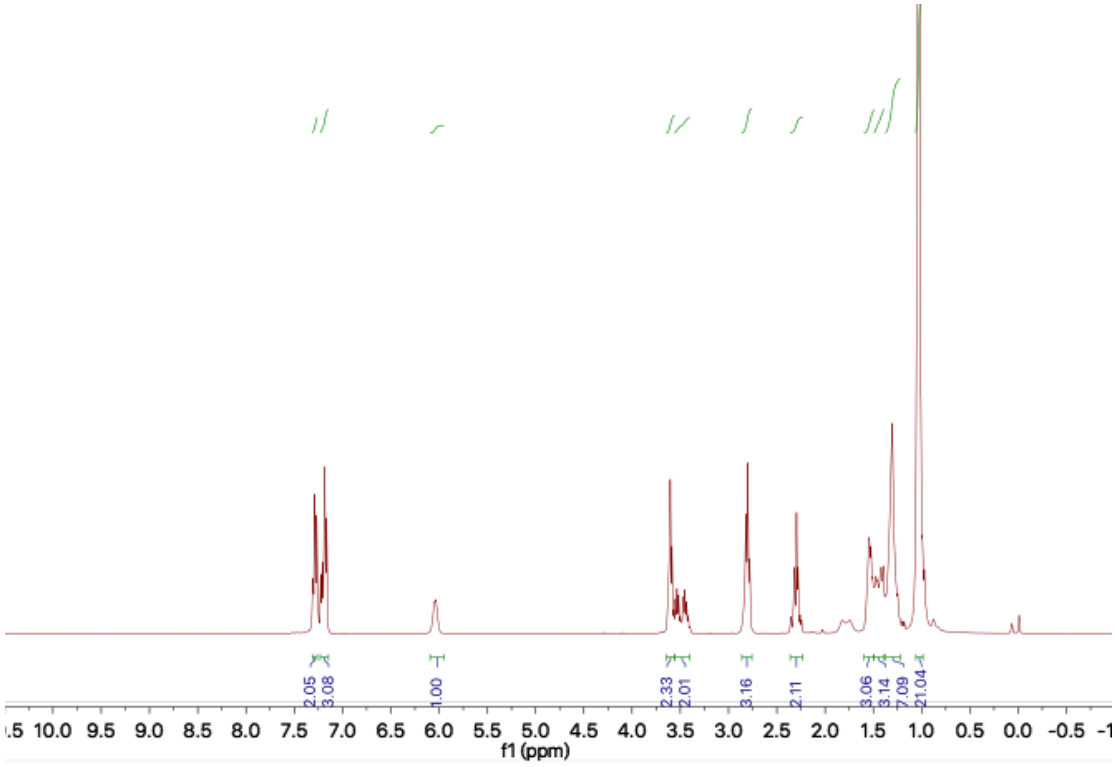

170.97
139.01
131.91
129.04
128.83
128.72
126.60
111.15
82.71
42.89
40.88
35.98
34.91
29.88
29.48
27.14
26.94
20.64
18.76
14.50
11.34
f1 (ppm)

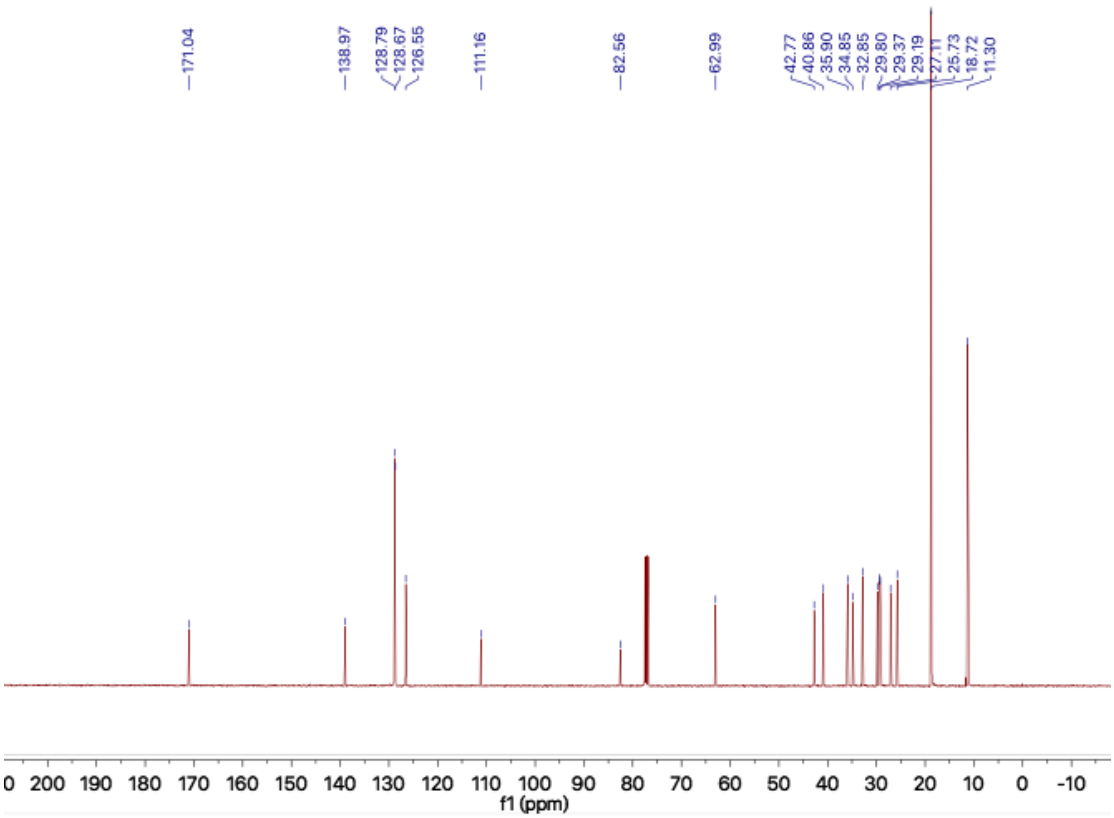

TBSO
5
O
N
H
Bn
TIPS


2.17
3.14
0.98
3.01
1.26
3.18
2.15
4.20
2.04
6.02
21.31
9.00
5.87
f1 (ppm)


171.03
139.01
128.85
128.73
126.61
111.22
82.67
63.43
42.91
40.89
35.98
35.00
33.01
29.90
29.52
29.36
27.26
26.14
25.87
18.77
18.19
11.33
-5.11
f1 (ppm)


HO
5
O
N
H
Bn
TIPS


2.05
3.08
1.00
2.33
2.01
3.16
2.11
3.06
3.14
7.09
21.04
f1 (ppm)


171.04
138.97
128.79
128.67
126.55
111.16
82.56
62.99
42.77
40.86
35.90
34.85
32.85
29.80
29.37
29.19
27.11
25.73
18.72
11.30
f1 (ppm)