Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Copper-Catalyzed Regio- and Stereoselective Fluorocarboalkynylation of Alkynes

(Supporting Information)

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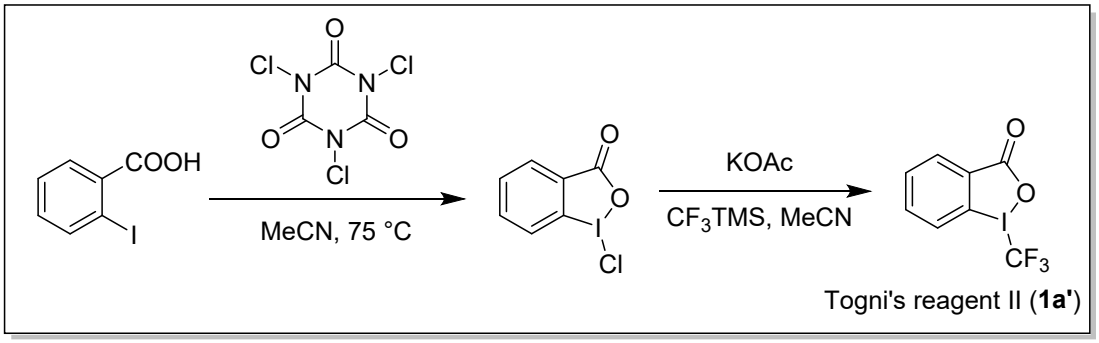
1. General Information.

Unless otherwise noted, all reactions were performed under an argon atmosphere using flame-dried glassware. All new compounds were fully characterized. NMR-spectra were recorded on Bruker AV-300, ARX-400 MHz or a ARX-600 Associated. ^{1}H NMR spectra data were reported as δ values in ppm relative to chloroform (δ 7.26) if collected in $CDCl_3$. ^{13}C NMR spectra data were reported as δ values in ppm relative to chloroform (δ 77.00). ^{1}H NMR coupling constants were reported in Hz, and multiplicity was indicated as follows: s (singlet); d (doublet); t (triplet); q (quartet); quint (quintet); m (multiplet); dd (doublet of doublets); ddd (doublet of doublet of doublets); dddd (doublet of doublet of doublet of doublets); dt (doublet of triplets); td (triplet of doublets); ddt (doublet of doublet of triplets); dq (doublet of quartets); app (apparent); br (broad). Mass spectra were conducted at Micromass Q-Tof instrument (ESI) and Agilent Technologies 5973N (EI). All reactions were carried out in flame-dried 25-mL Schlenk tubes with Teflon screw caps under argon. Unless otherwise noted, materials obtained from commercial suppliers were used without further purification.

2. Preparation of Starting Materials.

2.1 Prearation of 1-(Trifluoromethyl)-λ^3-benzo[*d*][1,2]iodaoxol-3(1*H*)-one (Togni's reagent II).

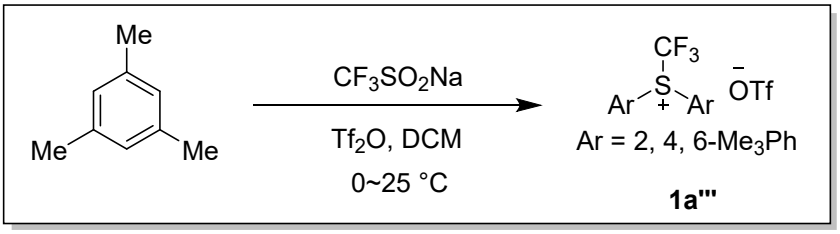


Togni's reagent II (**1a'**) was prepared according to the reported procedure.[1] A suspension of 2- iodobenzoic acid (15.0 g, 60 mmol, 1.0 equiv) in MeCN (100 mL) was

heated to 75 °C. A solution of trichloroisocyanuric acid (4.7 g, 20.4 mmol) in MeCN (25 mL) was added in one portion and the reaction mixture was heated at 75 °C for 10 min. The reaction mixture was diluted with MeCN (75 mL) and vacuum-filtered over an oven-preheated, sinteredglass funnel and the filter cake was rinsed with additional hot MeCN (75 mL). The filtrate was concentrated in vacuo to near dryness and the resulting yellow solid was collected by filtration and washed with cold MeCN. The mother liquor from filtration was partially concentrated in vacuo, giving a second crop of crystals. The combined crops were dried under vacuum overnight to afford the title compound as a slightly yellow crystalline solid.

The obtained yellow crystalline solid (11.3 g, 40 mmol, 1.0 equiv), absolute dry KOAc (7.9 g, 80 mmol, 2.0 equiv) and MeCN (115 mL) were added and the the reaction mixture was stirred at 75 °C for 2 h. The reaction mixture was cooled to rt, then CF_3TMS (6.5 mL, 44 mmol, 1.1 equiv) was one portion and the reaction mixture was stirred at rt for 15 h. MeCN (80 mL) was then added and the brown reaction mixture was heated to 75 °C and the hot reaction mixture was filtered through a pad of Celite, concentrated to about 40 mL end volume, and cooled to –20 °C. The crystals were filtered off, washed with cold (–20 °C) MeCN (40 mL) and dried under vacuum. The mother liquor was again concentrated to approximately 10 mL end volume and cooled to – 20 °C. The crystals were filtered off and washed with a cold (–20 °C) MeCN (10 mL). Both crystalline fractions were dried under a high vacuum to afford the title compound as a white crystalline solid.

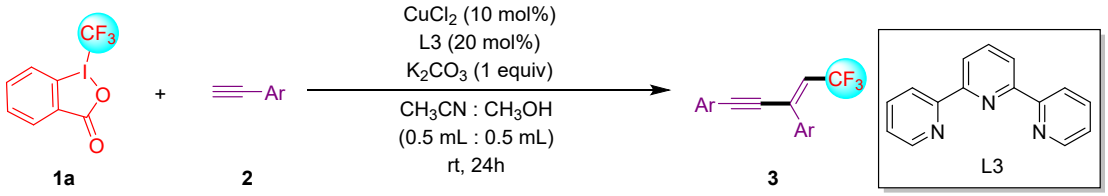
2.2 Prearation of 1a’’’.



CF_3 reagent **1a’’’** was prepared according to the reported procedure.[2] Mesitylene (7 mL, 50 mmol, 5.0 equiv) was added into a suspension of sodium trifluoromethylsulfinate (1.56 g, 10 mmol) in DCM (10 mL) at 0 °C. Tf_2O (3.4 mL, 20 mmol, 2.0 equiv) was added dropwise over the course of 15 minutes. The reaction

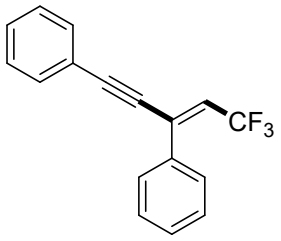
mixture was allowed to warm up to room temperature on its own and stirred at this temperature for 24 hours. The final mixture was quenched with saturated aqueous sodium bicarbonate at 0 °C. Dichloromethane (35 mL) was added and the organic layer was separated. Concentration of the organic solution yielded a brown oil. Dichloromethane (1.5 mL) was added followed by diethyl ether (35 mL) to crash out the product as a white precipitate. This mixture was sonicated for 30 minutes and filtered to yield the product. The product was furthered purified by recrystallization via layering technique (diethyl ether over DCM at room temperature) to yield pure **1a'''** as a white solid.

3. General Procedures for the Synthesis of Trifluoromethyl 1, 3-enynes.



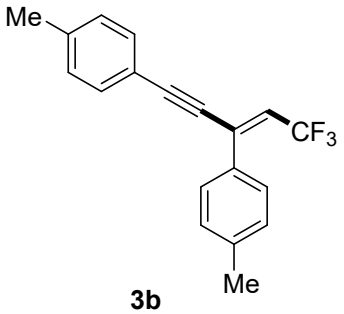
Flame-dried 10 mL Schlenk tube filled with argon, Togni's reagent II (**1a**) (0.2 mmol, 1.0 equiv), alkynes **2** (0.6 mmol, 3.0 equiv), $CuCl_2$ (0.02 mmol, 10 mol%), 2,2':6',2"-terpyridine (0.04 mmol, 20 mol%), K_2CO_3 (0.2 mmol, 1.0 equiv), absolute dry CH_3CN (0.5 mL) and absolute dry CH_3OH (0.5 mL) were added under N_2. The formed mixture was stirred at room temperature under N_2 for 24 h as monitored by TLC. The solvent was removed under vaccum directly. The crude product was purified by flash column chromatography on silica gel (eluent: PE/EA) to afford the product **3**.

4. Characterization Data of the Products 3.



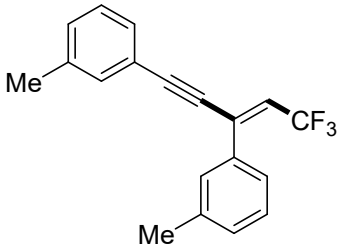
3a

(*E*)-(5,5,5-Trifluoropent-3-en-1-yne-1,3-diyl)dibenzene (3a): colorless oil, 39.5 mg (73% yield). **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.55 – 7.46 (m, 4H), 7.42 (dt, *J* = 4.4, 2.7 Hz, 3H), 7.36 (td, *J* = 5.4, 2.6 Hz, 3H), 6.22 (q, *J* = 8.7 Hz, 1H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 135.4, 135.0 (q, *J* = 6.3 Hz), 132.5, 131.8, 129.3, 129.2, 128.4, 128.2, 122.5 (q, *J* = 34.8 Hz), 122.4 (q, *J* = 270.7 Hz), 121.9, 94.5, 88.6; **^{19}F NMR (376 MHz, $CDCl_3$)** δ -56.1; **ATR-FTIR (cm $^{-1}$):** 3062, 2922, 2206, 1622, 1271, 1184, 1127, 759; **HRMS m/z (ESI)** calcd for $C_{17}H_{12}F_3$ $(M + H)^+$ 273.0886, found 273.0889.



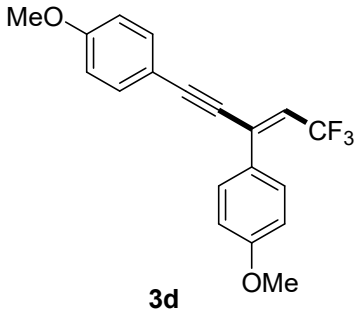
3b

(*E*)-4,4'-(5,5,5-Trifluoropent-3-en-1-yne-1,3-diyl)bis(methylbenzene) (3b): colorless oil, 42.7 mg (71% yield). **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.40 (d, *J* = 8.0 Hz, 2H), 7.34 (d, *J* = 8.2 Hz, 2H), 7.19 (d, *J* = 8.0 Hz, 2H), 7.13 (d, *J* = 7.9 Hz, 2H), 6.14 (q, *J* = 8.8 Hz, 1H), 2.37 (s, 3H), 2.35 (s, 3H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 139.7, 139.4, 135.3 (q, *J* = 6.3 Hz), 132.8, 131.9, 129.3, 129.1, 128.4 (q, *J* = 2.2 Hz), 122.7 (q, *J* = 270.3 Hz), 121.7 (q, *J* = 34.6 Hz), 119.1, 94.6, 88.5, 21.7, 21.5; **^{19}F NMR (376 MHz, $CDCl_3$)** δ -55.9; **ATR-FTIR (cm $^{-1}$):** ν = 3013, 2893, 2152, 1618, 1490, 1300, 1170, 1129, 900, 538; **HRMS m/z (ESI)** calcd for $C_{19}H_{16}F_3$ $(M + H)^+$ 301.1199, found 301.1196.



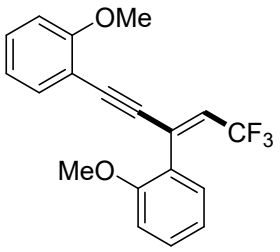
3c

(*E*)-3,3'-(5,5,5-Trifluoropent-3-en-1-yne-1,3-diyl)bis(methylbenzene) (3c): colorless oil, 41.9 mg (71% yield). **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.28-7.16 (m, 8H), 6.17 (q, *J* = 8.6 Hz, 1H), 2.38 (s, 3H), 2.32 (s, 3H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 138.2, 137.9, 135.4, 135.2 (q, *J* = 6.0 Hz), 132.4, 130.2, 129.9, 128.9, 128.8, 128.3, 128.1, 125.3, 122.5 (q, *J* = 270.5 Hz), 122.2 (q, *J* = 34.6 Hz), 121.8, 94.6, 88.4, 21.4, 21.2; **^{19}F NMR (376 MHz, $CDCl_3$)** δ -56.0; **ATR-FTIR (cm $^{-1}$):** 3033, 2923, 2204, 1613, 1510, 1266, 1180, 1110, 817, 524; **HRMS m/z (ESI)** calcd for $C_{19}H_{16}F_3$ $(M + H)^+$ 301.1199, found 301.1205.



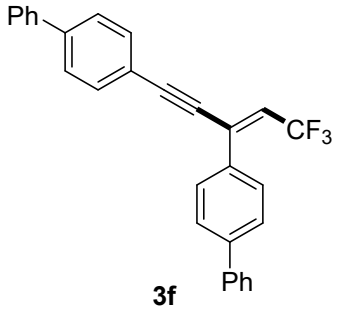
3d

(*E*)-4,4'-(5,5,5-Trifluoropent-3-en-1-yne-1,3-diyl)bis(methoxybenzene) (3d): colorless oil, 46.3 mg (70% yield). **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.48 (d, *J* = 8.7 Hz, 2H), 7.41 (d, *J* = 8.8 Hz, 2H), 6.92 (d, *J* = 8.8 Hz, 2H), 6.87 (d, *J* = 8.8 Hz, 2H), 6.10 (q, *J* = 8.9 Hz, 1H), 3.84 (s, 3H), 3.82 (s, 3H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 160.3, 134.7, 133.4, 129.9, 127.8, 122.7 (q, *J* = 268.9 Hz), 120.5 (q, *J* = 34.5 Hz), 114.1, 113.6, 94.2, 88.0, 55.32, 55.28; **^{19}F NMR (376 MHz, $CDCl_3$)** δ -55.9; **ATR-FTIR (cm $^{-1}$):** 2939, 2779, 2243, 1630, 1492, 1284, 1168, 1101, 1020, 760; **HRMS m/z (ESI)** calcd for $C_{19}H_{15}F_3NaO_2$ $(M + Na)^+$ 355.0916, found 355.0920.



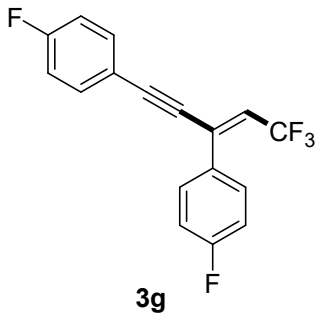
3e

(*E*)-2,2'-(5,5,5-Trifluoropent-3-en-1-yne-1,3-diyl)bis(methoxybenzene) (3e): colorless oil, 53.9 mg (81% yield). **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.38 – 7.22 (m, 4H), 7.00 – 6.79 (m, 4H), 6.25 (q, *J* = 8.4 Hz, 1H), 3.83 (s, 3H), 3.80 (s, 3H).; **^{13}C NMR (101 MHz, $CDCl_3$)** δ 160.2, 156.3, 133.7, 131.3 (q, *J* = 6.2 Hz), 130.6, 130.1, 129.5, 124.6, 123.75 (q, *J* = 33.9 Hz), 122.4 (q, *J* = 270.5 Hz), 120.3, 120.2, 111.5, 111.0, 110.7, 92.2, 90.0, 55.7, 55.6; **^{19}F NMR (376 MHz, $CDCl_3$)** δ -59.0; **ATR-FTIR (cm $^{-1}$):** 2939, 2840, 2203, 1627, 1492, 1274, 1179, 1104, 1022, 751; **HRMS m/z (ESI)** calcd for $C_{19}H_{16}F_3O_2$ $(M + H)^+$ 333.1097, found 333.1095.



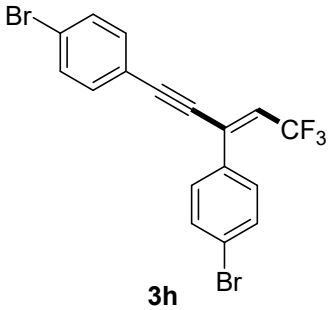
3f

(*E*)-4,4''-(5,5,5-trifluoropent-3-en-1-yne-1,3-diyl)di-1,1'-biphenyl (3f): colorless oil, 71.8 mg (85% yield). **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.69 – 6.60 (m, 12H), 7.50 – 7.48 (m, 4H), 7.43 – 7.32 (m, 2H), 6.31 (q, *J* = 8.4 Hz, 1H); **^{13}C NMR (126 MHz, $CDCl_3$)** δ 142.1, 142.0, 140.3, 140.0, 134.7 (q, *J* = 6.3 Hz), 134.2, 132.9, 132.3, 128.9, 128.8, 127.9, 127.7, 127.12, 127.09, 127.0, 126.9, 122.5 (q, *J* = 270.6 Hz), 122.3 (q, *J* = 34.6 Hz), 120.7, 94.5, 89.3; **^{19}F NMR (471 MHz, $CDCl_3$)** δ -55.8; **ATR-FTIR (cm $^{-1}$):** 2921, 2855, 2209, 1609, 1439, 1256, 1178, 1130, 1026, , 820; **HRMS m/z (ESI)** calcd for $C_{29}H_{19}F_3Na$ $(M + Na)^+$ 447.1331, found 447.1335.



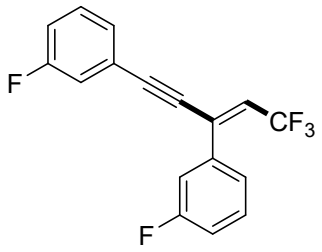
3g

(*E*)-4,4'-(5,5,5-trifluoropent-3-en-1-yne-1,3-diyl)bis(fluorobenzene) (3g): colorless oil, 38.2 mg (62% yield). **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.55 – 7.38 (m, 4H), 7.18 – 6.94 (m, 4H), 6.20 (q, *J* = 8.6 Hz, 1H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 163.2 (d, *J* = 249.4 Hz), 163.1 (d, *J* = 251.6 Hz), 133.9 (d, *J* = 8.6 Hz), 131.2 (d, *J* = 3.0 Hz), 130.2 (d, *J* = 8.8 Hz), 122.7 (q, *J* = 34.7 Hz), 122.3 (q, *J* = 270.6 Hz), 117.9 (d, *J* = 3.2 Hz), 115.9 (d, *J* = 22.2 Hz), 115.4 (d, *J* = 21.8 Hz), 93.6, 88.1; **^{19}F NMR (376 MHz, $CDCl_3$)** δ -56.2, -108.8, -111.6; **ATR-FTIR (cm $^{-1}$):** 2358, 2199, 1576, 1479, 1444, 1268, 1200, 1134, 952, 880; **HRMS m/z (ESI)** calcd for $C_{17}H_{10}F_5$ $(M + H)^+$ 309.0697, found 309.0695.



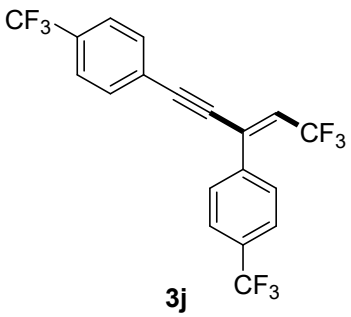
3h

(*E*)-4,4'-(5,5,5-trifluoropent-3-en-1-yne-1,3-diyl)bis(bromobenzene) (3h): yellow oil, 57.0 mg (66% yield). **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.54 (d, *J* = 8.6 Hz, 2H), 7.49 (d, *J* = 8.5 Hz, 2H), 7.35 (d, *J* = 8.5 Hz, 2H), 7.31 (d, *J* = 8.5 Hz, 2H), 6.20 (q, *J* = 8.6 Hz, 1H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 134.0, 133.6 (q, *J* = 6.4 Hz), 133.2, 131.8, 131.5, 129.8, 124.1, 123.3 (q, *J* = 34.8 Hz), 122.3 (q, *J* = 268.5 Hz), 120.6, 93.7, 89.0; **^{19}F NMR (376 MHz, $CDCl_3$)** δ -56.2; **ATR-FTIR (cm $^{-1}$):** 2923, 2207, 1586, 1484, 1357, 1266, 1123, 1008, 823; **HRMS m/z (ESI)** calcd for $C_{17}H_{10}Br_2F_3$ $(M + H)^+$ 428.9096, found 428.9099.



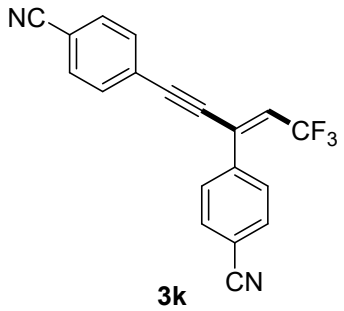
3i

(*E*)-3,3'-(5,5,5-trifluoropent-3-en-1-yne-1,3-diyl)bis(fluorobenzene) (3i): colorless oil, 34.3 mg (56% yield). **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.41 – 7.29 (m, 2H), 7.26 – 7.05 (m, 6H), 6.24 (q, *J* = 8.5 Hz, 1H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 162.4 (d, *J* = 247.0 Hz), 162.3 (d, *J* = 247.5 Hz), 136.9 (d, *J* = 7.6 Hz), 133.3 (q, *J* = 5.9 Hz), 130.1 (d, *J* = 8.6 Hz), 129.9 (d, *J* = 8.3 Hz), 127.8 (d, *J* = 3.1 Hz), 124.0, 123.9 (q, *J* = 34.5 Hz), 122.0 (q, *J* = 270.5 Hz), 118.6 (d, *J* = 22.9 Hz), 116.8 (d, *J* = 21.2 Hz), 116.3 (d, *J* = 20.9 Hz), 115.4 (d, *J* = 23.1 Hz), 93.4, 88.5; **^{19}F NMR (376 MHz, $CDCl_3$)** δ -56.4, -112.3, -112.5; **ATR-FTIR (cm $^{-1}$):** 2348, 2207, 1582, 1486, 1436, 1269, 1199, 1120, 943, 787; **HRMS m/z (ESI)** calcd for $C_{17}H_{10}F_5$ $(M + H)^+$ 309.0697, found 309.0690.



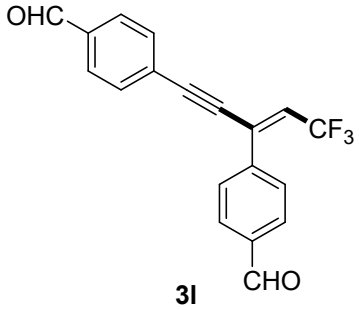
3j

(*E*)-4,4'-(5,5,5-trifluoropent-3-en-1-yne-1,3-diyl)bis((trifluoromethyl)benzene) (3j): colorless oil, 53.2 mg (65% yield). **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.41 – 7.29 (m, 2H), 7.26 – 7.05 (m, 6H), 6.24 (q, *J* = 8.5 Hz, 1H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 138.5, 133.2 (q, *J* = 6.1 Hz), 132.8, 132.1, 131.4 (q, *J* = 32.8 Hz), 131.2 (q, *J* = 32.9 Hz), 128.6 (q, *J* = 2.2 Hz), δ 125.51, 125.47, 125.43, 125.39, 125.36, 124.9 (q, *J* = 35.0 Hz), 121.9 (q, *J* = 271.0 Hz), 93.6, 89.5; **^{19}F NMR (376 MHz, $CDCl_3$)** δ -56.5, -62.9, -63.1; **ATR-FTIR (cm $^{-1}$):** 2957, 2207, 1498, 1436, 1256, 1123, 1045, 943, 871, 787; **HRMS m/z (ESI)** calcd for $C_{19}H_{10}F_9$ $(M + H)^+$ 409.0633, found 409.0639.



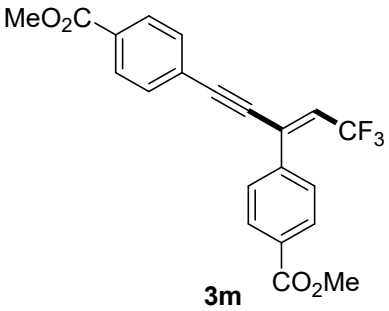
3k

(*E*)-4,4'-(5,5,5-trifluoropent-3-en-1-yne-1,3-diyl)dibenzonitrile (3k): yellow oil, 43.1 mg (67% yield). **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.74 – 7.70 (m, 2H), 7.66 – 7.63 (m, 2H), 7.58 – 7.52 (m, 4H), 6.36 (q, *J* = 8.3 Hz, 1H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 139.2, 132.3, 132.22, 132.17, 128.9 (d, *J* = 2.0 Hz), 126.0, 125.6 (d, *J* = 35.2 Hz), 121.7 (d, *J* = 271.1 Hz), 118.1, 118.0, 113.3, 113.1, 93.4, 90.6; **^{19}F NMR (376 MHz, $CDCl_3$)** δ -56.5; **ATR-FTIR (cm $^{-1}$):** 3068, 2924, 2229, 1622, 1502, 1266, 1122, 838; **HRMS m/z (ESI)** calcd for $C_{19}H_{10}F_3N_2$ $(M + H)^+$ 409.0633, found 409.0639.



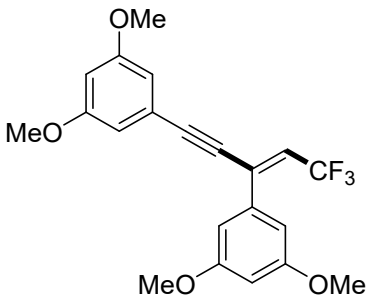
3l

(*E*)-4,4'-(5,5,5-Trifluoropent-3-en-1-yne-1,3-diyl)dibenzaldehyde (3l): yellow oil, 28.3 mg (43% yield). **^{1}H NMR (400 MHz, $CDCl_3$)** δ 10.06 (s, 1H), 10.02 (s, 1H), 7.94 (d, *J* = 8.3 Hz, 2H), 7.86 (d, *J* = 8.4 Hz, 2H), 7.62 (dd, *J* = 12.2, 8.2 Hz, 4H), 6.35 (q, *J* = 8.4 Hz, 1H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 191.5, 191.2, 140.7, 136.7, 136.4, 133.2 (q, *J* = 5.9 Hz), 132.4, 129.7, 129.6, 128.9, 127.5, 125.0 (q, *J* = 35.0 Hz), 121.9 (q, *J* = 270.8 Hz), 94.1, 90.7; **^{19}F NMR (376 MHz, $CDCl_3$)** δ -56.4; **ATR-FTIR (cm $^{-1}$):** 2923, 2207, 1683, 1606, 1357, 1259, 1183, 1110, 1023, 833; **HRMS m/z (ESI)** calcd for $C_{19}H_{12}F_3O_2$ $(M + H)^+$ 329.0784, found 329.0788.



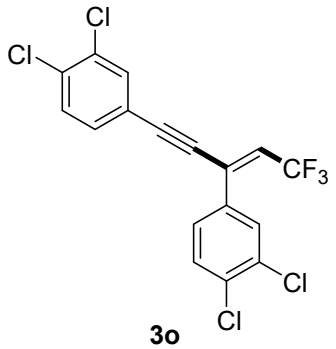
3m

Dimethyl 4,4'-(5,5,5-trifluoropent-3-en-1-yne-1,3-diyl)(*E*)-dibenzoate (3m): yellow oil, 54.2 mg (70% yield). **^{1}H NMR (400 MHz, $CDCl_3$)** ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.08 (d, *J* = 8.4 Hz, 2H), 8.00 (d, *J* = 8.4 Hz, 2H), 7.52 (dd, *J* = 12.7, 8.3 Hz, 4H), 6.30 (q, *J* = 8.4 Hz, 1H), 3.93 (s, 3H), 3.91 (s, 3H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 166.4, 166.2, 139.4, 133.6 (q, *J* = 6.0 Hz), 132.4, 131.7, 130.8, 130.6, 129.5, 128.2 (q, *J* = 1.8 Hz), 126.1 (q, *J* = 7.9 Hz), 124.3 (q, *J* = 35.0 Hz), 122.0 (q, *J* = 270.9 Hz), 94.1, 90.1, 52.3, 52.2; **^{19}F NMR (376 MHz, $CDCl_3$)** δ -56.4; **ATR-FTIR (cm $^{-1}$):** 2954, 2208, 1716, 1615, 1436, 1270, 1184, 1113, 966, 864; **HRMS m/z (ESI)** calcd for $C_{21}H_{16}F_3O_4$ $(M + H)^+$ 389.0995, found 389.1001.



3n

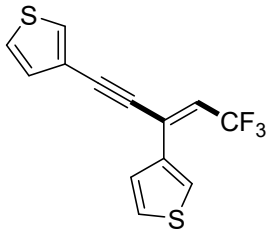
(*E*)-5,5'-(5,5,5-Trifluoropent-3-en-1-yne-1,3-diyl)bis(1,3-dimethoxybenzene) (3n): yellow oil, 55.5 mg (71% yield). **^{1}H NMR (400 MHz, $CDCl_3$)** δ 6.64 (d, *J* = 2.3 Hz, 2H), 6.61 (d, *J* = 2.3 Hz, 2H), 6.50 (t, *J* = 2.3 Hz, 1H), 6.49 (t, *J* = 2.3 Hz, 1H), 6.20 (q, *J* = 8.5 Hz, 1H), 3.81 (s, 6H), 3.78 (s, 6H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 160.54, 160.45, 137.0, 134.8 (q, *J* = 6.1 Hz), 122.7 (q, *J* = 34.7 Hz), 120.2 (q, *J* = 270.6 Hz), 110.2, 109.6, 106.3, 102.7, 101.2, 94.5, 87.7, 55.4, 55.38; **^{19}F NMR (376 MHz, $CDCl_3$)** δ -56.1; **ATR-FTIR (cm $^{-1}$):** 3008, 2940, 2843, 2205, 1588, 1457, 1276, 1200, 1116, 832; **HRMS m/z (ESI)** calcd for $C_{21}H_{19}F_3NaO_4$ $(M + Na)^+$ 415.1128, found 415.1129.



3o

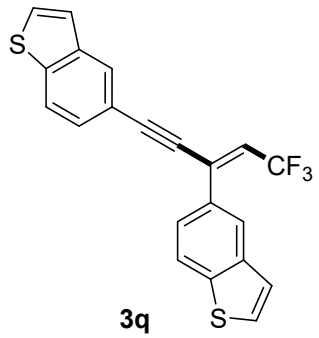
(*E*)-4,4'-(5,5,5-trifluoropent-3-en-1-yne-1,3-diyl)bis(1,2-dichlorobenzene) (3o): yellow oil, 47.2 mg (58% yield). **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.55 (s, 2H), 7.49 (d, *J* = 8.3 Hz, 1H), 7.43 (d, *J* = 8.3 Hz, 1H), 7.33 – 7.24 (m, 2H), 6.26 (q, *J* = 8.4 Hz, 1H);

^{13}C NMR (101 MHz, $CDCl_3$) 134.6, 134.2, 133.8, 133.4, 132.9, 132.7, 132.0 (q, *J* = 6.1 Hz), 130.9, 130.6, 130.4, 130.0, 127.5, 124.6 (q, *J* = 35.1 Hz), 121.9 (d, *J* = 270.9 Hz), 121.3, 92.7, 89.0; **^{19}F NMR (376 MHz, $CDCl_3$)** δ -56.5; **ATR-FTIR (cm $^{-1}$):** 2933, 2207, 1582, 1484, 1366, 1269, 1199, 1110, 943, 871, 787; **HRMS m/z (ESI)** calcd for $C_{17}H_8Cl_4F_3$ $(M + H)^+$ 408.9327, found 408.9330.



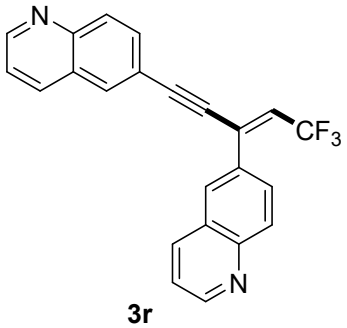
3p

(*E*)-3,3'-(5,5,5-Trifluoropent-3-en-1-yne-1,3-diyl)dithiophene (3p): yellow oil, 25.1 mg (44% yield). **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.65 (t, *J* = 2.3 Hz, 1H), 7.56 (dd, *J* = 3.0, 1.2 Hz, 1H), 7.36-7.30 (m, 3H), 7.16 (dd, *J* = 5.0, 1.2 Hz, 1H), 6.12 (q, *J* = 9.0 Hz, 1H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 135.0, 130.3, 129.7, 129.0 (q, *J* = 6.5 Hz), 127.9, 127.2, 125.8, 125.6, 122.5 (q, *J* = 270.3 Hz), 120.8 (q, *J* = 35.4 Hz), 88.3, 88.0; **^{19}F NMR (376 MHz, $CDCl_3$)** δ -56.5; **ATR-FTIR (cm $^{-1}$):** 3110, 2924, 2205, 1611, 1417, 1263, 1113, 782; **HRMS m/z (ESI)** calcd for $C_{13}H_8F_3S_2$ $(M + H)^+$ 285.0014, found 285.0016.



3q

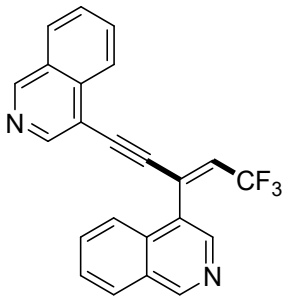
(*E*)-5,5'-(5,5,5-trifluoropent-3-en-1-yne-1,3-diyl)bis(benzo[*b*]thiophene) (3q): yellow oil, 51.7 mg (67% yield). **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.98 (dd, *J* = 16.8, 1.6 Hz, 2H), 7.93 (d, *J* = 8.4 Hz, 1H), 7.84 (d, *J* = 8.4 Hz, 1H), 7.54-7.48 (m, 3H), 7.44-7.39 (m, 2H), 7.31 (d, *J* = 5.6 Hz, 1H), 6.31 (q, *J* = 8.7 Hz, 1H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 140.6, 140.5, 139.5, 139.4, 135.2 (q, *J* = 6.3 Hz), 131.7, 127.7, 127.4, 127.3, 127.2, 124.2 (q, *J* = 1.7 Hz), 124.1, 123.6, 123.4 (q, *J* = 2.2 Hz), 122.6, 122.30, 122.25 (q, *J* = 34.6 Hz), 120.3 (d, *J* = 270.5 Hz), 117.7, 95.1, 88.4; **^{19}F NMR (376 MHz, $CDCl_3$)** δ -55.8; **ATR-FTIR (cm $^{-1}$):** 3074, 2924, 2199, 1617, 1264, 1112, 1027, 813; **HRMS m/z (ESI)** calcd for $C_{21}H_{12}F_3S_2$ $(M + H)^+$ 385.0327, found 385.0325.



3r

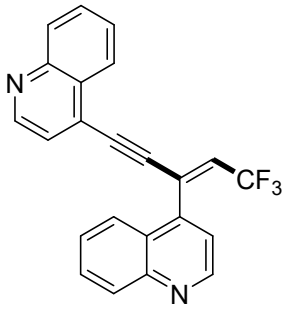
(*E*)-6,6'-(5,5,5-Trifluoropent-3-en-1-yne-1,3-diyl)diquinoline (3r): yellow oil, 49.8 mg (67% yield). **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.93 (dd, *J* = 21.8, 4.4 Hz, 2H), 8.19 (d, *J* = 8.3 Hz, 1H), 8.17 (d, *J* = 8.8 Hz, 1H), 8.11-8.01 (m, 2H), 7.95 (d, *J* = 2.1 Hz, 2H), 7.85 (dd, *J* = 8.8, 2.0 Hz, 1H), 7.71 (dd, *J* = 8.7, 1.8 Hz, 1H), 7.42 (ddd, *J* = 17.0, 8.3, 4.2 Hz, 2H), 6.38 (q, *J* = 8.5 Hz, 1H); **^{13}C NMR (126 MHz, $CDCl_3$)** δ 151.5, 151.4, 148.1, 148.0, 136.5, 135.8, 134.0 (q, *J* = 6.1 Hz), 133.3, 132.0, 131.7, 129.8, 129.6, 129.2 (q, *J* = 1.9 Hz), 127.8, 127.67, 127.66, 123.8 (q, *J* = 34.8 Hz), 122.2 (q, *J* = 270.8

Hz), 121.9, 121.7, 119.9, 94.7, 89.1; **^{19}F NMR (471 MHz, $CDCl_3$)** δ -56.1; **ATR-FTIR (cm $^{-1}$):** 3110, 2933, 2203, 1626, 1567, 1499, 1346, 1277, 1120, 760; **HRMS m/z (ESI)** calcd for $C_{23}H_{13}F_3N_2Na$ $(M + Na)^+$ 397.0923, found 397.0925.



3s

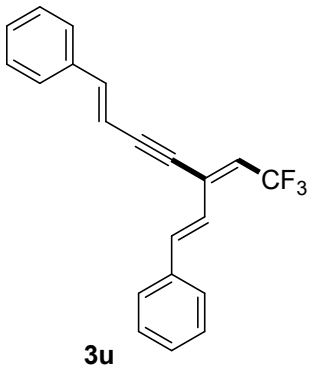
(*E*)-4,4'-(5,5,5-Trifluoropent-3-en-1-yne-1,3-diyl)diisoquinoline (3s): yellow oil, 46.9 mg (63% yield). **^{1}H NMR (400 MHz, $CDCl_3$)** δ 9.33 (d, *J* = 0.9 Hz, 1H), 9.18 (d, *J* = 0.8 Hz, 1H), 8.62 (s, 1H), 8.57 (s, 1H), 8.13-8.04 (m, 2H), 7.97-7.93 (m, 1H), 7.88 (dd, *J* = 8.2, 1.2 Hz, 1H), 7.80 (ddd, *J* = 8.4, 6.9, 1.3 Hz, 1H), 7.69-7.58 (m, 3H), 6.71 (q, *J* = 7.9 Hz, 1H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 153.8, 153.1, 147.1, 141.7, 135.2, 133.1, 131.5, 131.2, 130.1 (q, *J* = 6.0 Hz), 128.2, 128.13, 128.10, 128.0, 127.8, 127.6, 127.3 (q, *J* = 34.4 Hz), 126.5, 124.5, 124.0, 121.9 (q, *J* = 271.1 Hz), 114.3, 94.3, 91.4; **^{19}F NMR (376 MHz, $CDCl_3$)** δ -57.4; **ATR-FTIR (cm $^{-1}$):** 3064, 2924, 2205, 1628, 1577, 1504, 1351, 1283, 1120, 764; **HRMS m/z (ESI)** calcd for $C_{23}H_{13}F_3N_2Na$ $(M + Na)^+$ 397.0923, found 397.0931.



3t

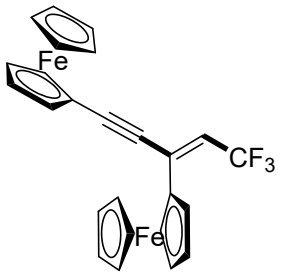
(*E*)-4,4'-(5,5,5-trifluoropent-3-en-1-yne-1,3-diyl)diquinoline (3t): yellow oil, 44.8 mg (60% yield). **^{1}H NMR (400 MHz, $CDCl_3$)** δ 9.01 (d, *J* = 4.4 Hz, 1H), 8.87 (d, *J* = 4.5 Hz, 1H), 8.23 (d, *J* = 8.5 Hz, 1H), 8.10 (dd, *J* = 8.0, 4.9 Hz, 2H), 7.92 – 7.87 (m, 1H), 7.81 (ddd, *J* = 8.4, 6.9, 1.3 Hz, 1H), 7.72 (ddd, *J* = 8.4, 7.0, 1.4 Hz, 1H), 7.66 (ddd,

J = 8.2, 6.9, 1.2 Hz, 1H), 7.51 (ddd, *J* = 8.2, 7.0, 1.1 Hz, 1H), 7.43 (d, *J* = 4.5 Hz, 2H), 6.73 (q, *J* = 7.8 Hz, 1H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 149.9, 149.5, 148.3, 148.0, 140.9, 130.2, 130.12, 130.08, 130.0, 127.9 (q, *J* = 34.7 Hz), 127.7, 127.5, 127.1, 125.3, 124.8, 124.4 (q, *J* = 276.8 Hz), 124.0, 120.2, 94.5, 92.1. **^{19}F NMR (376 MHz, $CDCl_3$)** δ -57.9; **ATR-FTIR (cm $^{-1}$):** 3078, 2945, 2203, 1632, 1589, 1500, 1347, 1300, 1134, 759; **HRMS m/z (ESI)** calcd for $C_{23}H_{13}F_3N_2Na$ $(M + Na)^+$ 397.0923, found 397.0925.



3u

((1*E*,5*E*,6*E*)-5-(2,2,2-trifluoroethylidene)hepta-1,6-dien-3-yne-1,7-diyl)dibenzene (3u): yellow oil, 23.4 mg (36% yield). **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.55 – 7.51 (m, 2H), 7.48 – 7.44 (m, 2H), 7.42 – 7.28 (m, 7H), 7.21 – 7.08 (m, 2H), 6.39 (d, *J* = 16.3 Hz, 1H), 5.96 (q, *J* = 9.0 Hz, 1H). **^{13}C NMR (126 MHz, $CDCl_3$)** δ 143.4, 139.0, 135.7 (q, *J* = 5.8 Hz), 131.9 (q, *J* = 5.9 Hz), 129.2, 128.84, 128.81, 127.6, 126.5, 123.1 (q, *J* = 270.8 Hz), 121.3, 120.6 (q, *J* = 34.5 Hz), 106.9, 93.9, 87.0; **^{19}F NMR (471 MHz, $CDCl_3$)** δ -55.7; **ATR-FTIR (cm $^{-1}$):** 3031, 2925, 2196, 1589, 1324, 1122, 958; **HRMS m/z (ESI)** calcd for $C_{21}H_{16}F_3$ $(M + H)^+$ 325.1199, found 325.1205.



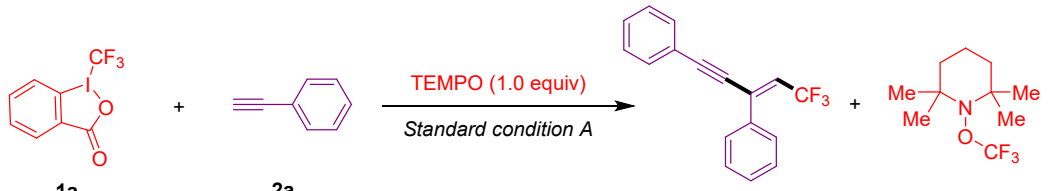
3v

(*E*)-(5,5,5-Trifluoropent-3-en-1-yne-1,3-diyl)diferrocene (3v): red oil, 55.9 mg (57% yield). **^{1}H NMR (400 MHz, $CDCl_3$)** δ 5.93 (q, *J* = 9.6 Hz, 1H), 4.73 (s, 2H), 4.55 (t, *J*

= 1.8 Hz, 2H), 4.43 – 4.37 (m, 2H), 4.33 – 4.31 (m, 2H), 4.29 (s, 5H), 4.26 (s, 5H); **^{13}C NMR (126 MHz, $CDCl_3$)** δ 123.3 (d, *J* = 269.8 Hz), 116.7 (q, *J* = 36.0 Hz), 71.7, 70.3, 70.2, 70.1 (q, *J* = 3.1 Hz), 70.0, 69.4, 67.6; **^{19}F NMR (471 MHz, $CDCl_3$)** δ -56.4; **ATR-FTIR (cm $^{-1}$):** 3094, 2923, 2853, 2206, 1605, 1470, 1263, 1141, 1100, 965, 818; **HRMS m/z (ESI)** calcd for $C_{25}H_{19}F_3Fe_2$ $(M + H)^+$ 489.0210, found 489.0215.

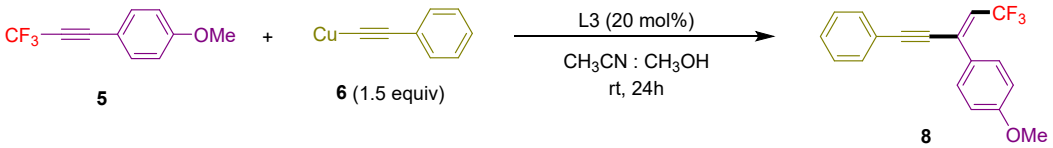
5. Mechanistic Experiments

a)



Flame-dried 10 mL Schlenk tube filled with argon, Togni's reagent II (**1a**) (0.2 mmol, 1.0 equiv), phenylacetylene (**2a**) (0.6 mmol, 3.0 equiv), $CuCl_2$ (0.02 mmol, 10 mol%), 2,2':6',2''-terpyridine (0.04 mmol, 20 mol%), K_2CO_3 (0.2 mmol, 1.0 equiv), TEMPO (0.3 mmol, 1.5 equiv), absolute dry CH_3CN (0.5 mL) and absolute dry CH_3OH (0.5 mL) were added under N_2. The formed mixture was stirred at room temperature under N_2 for 24 h. The reaction mixture was analyzed by GC-MS showing that no desired product **3a** was formed and CF_3-TEMPO adduct **4** was detected.

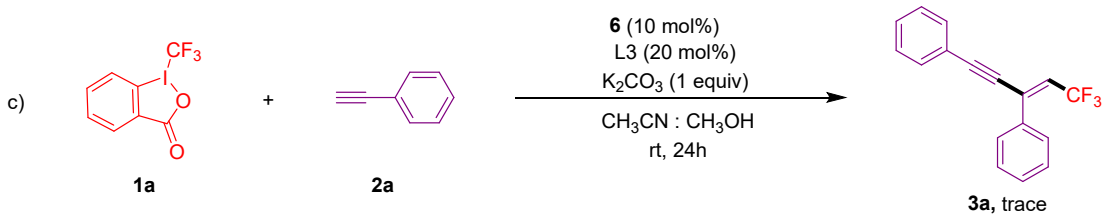
b)



With K_2CO_3 **8**, nd
Without K_2CO_3 **8**, nd

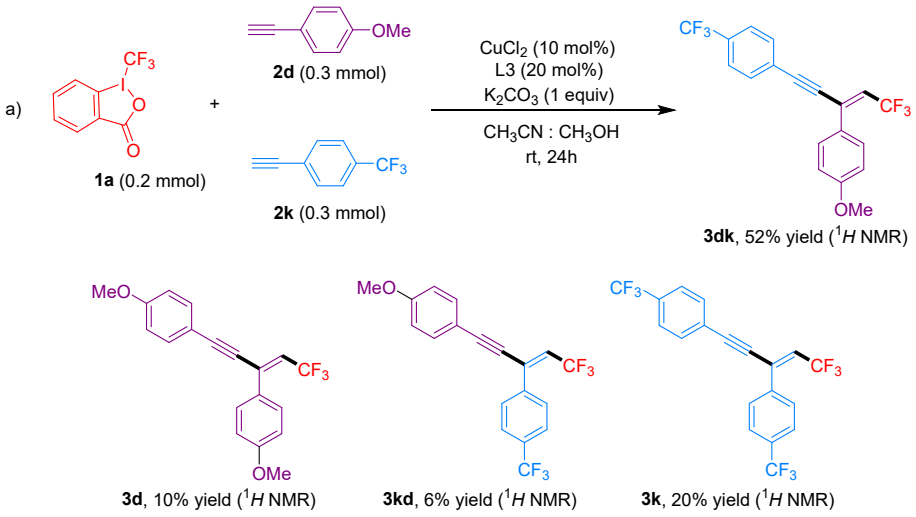
With K_2CO_3: Flame-dried 10 mL Schlenk tube filled with argon, 1-methoxy-4-(3,3,3-trifluoroprop-1-yn-1-yl)benzene (**5**)[4] (0.1 equiv, 1.0 equiv), copper acetylide **6**[5] (0.15 mmol, 1.5 equiv), 2,2':6',2''-terpyridine (0.02 mmol, 20 mol%), K_2CO_3 (0.1 mmol, 1.0 equiv), absolute dry CH_3CN (0.5 mL) and absolute dry CH_3OH (0.5 mL) were added under N_2. The formed mixture was stirred at room temperature under N_2 for 24 h. The reaction mixture was analyzed by GC-MS showing that no desired product **8** was detected.

Without K_2CO_3: Flame-dried 10 mL Schlenk tube filled with argon, 1-methoxy-4-(3,3,3-trifluoroprop-1-yn-1-yl)benzene (**5**) (0.1 equiv, 1.0 equiv), copper acetylide **6** (0.15 mmol, 1.5 equiv), 2,2':6',2"-terpyridine (0.02 mmol, 20 mol%), absolute dry CH_3CN (0.5 mL) and absolute dry CH_3OH (0.5 mL) were added under N_2. The formed mixture was stirred at room temperature under N_2 for 24 h. The reaction mixture was analyzed by GC-MS showing that no desired product **8** was detected.



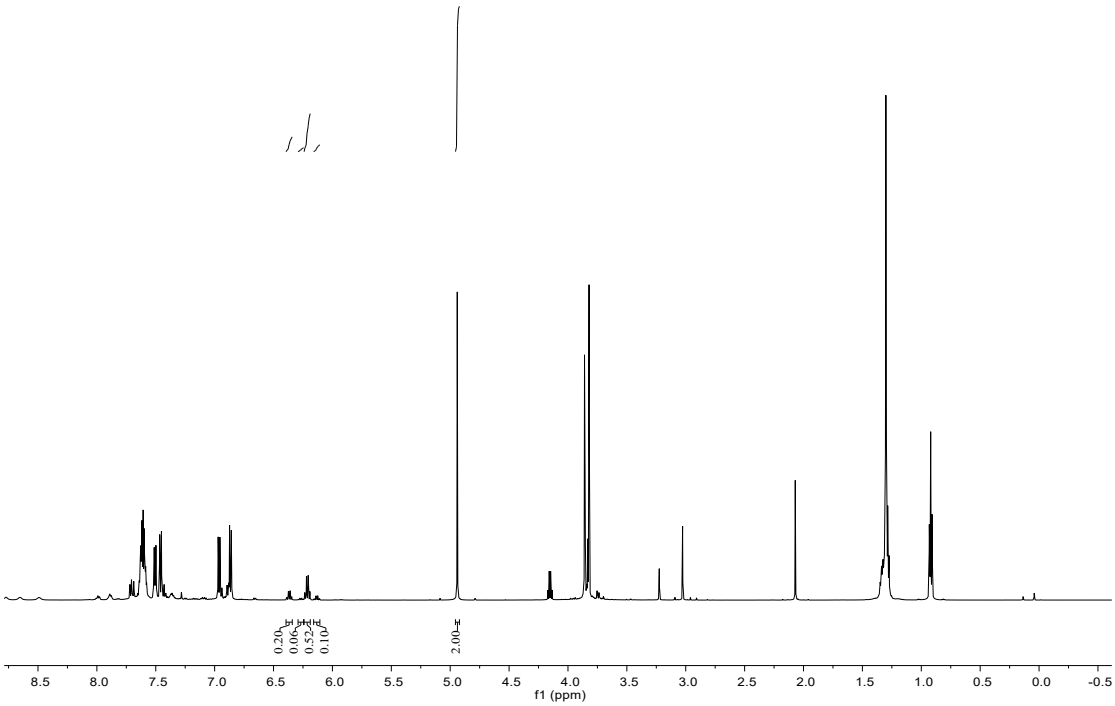
Flame-dried 10 mL Schlenk tube filled with argon, Togni's reagent II (**1a**) (0.2 mmol, 1.0 equiv), alkynes **2** (0.6 mmol, 3.0 equiv), copper acetylide **6** (0.02 mmol, 10 mol%), 2,2':6',2"-terpyridine (0.04 mmol, 20 mol%), K_2CO_3 (0.2 mmol, 1.0 equiv), absolute dry CH_3CN (0.5 mL) and absolute dry CH_3OH (0.5 mL) were added under N_2. The formed mixture was stirred at room temperature under N_2 for 24 h. The reaction mixture was analyzed by GC-MS showing that trace amount of desired product **3a** was detected.

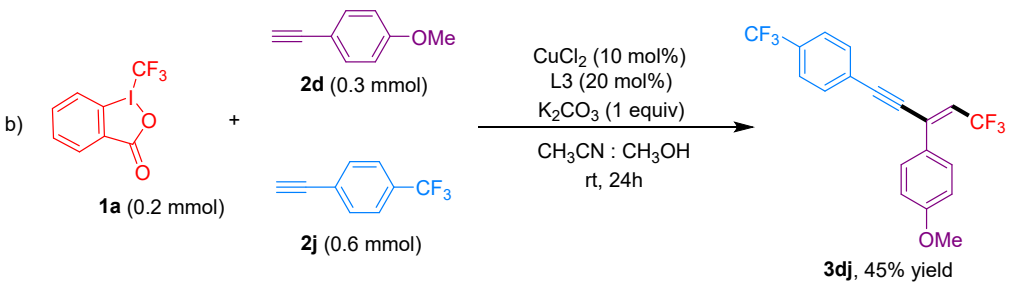
6. Crossover Experiments



Flame-dried 10 mL Schlenk tube filled with argon, Togni's reagent II (**1a**) (0.2 mmol, 1.0 equiv), alkyne **2d** (0.3 mmol, 1.5 equiv), alkyne **2j** (0.3 mmol, 1.5 equiv), $CuCl_2$ (0.02 mmol, 10 mol%), 2,2':6',2"-terpyridine (0.04 mmol, 20 mol%), K_2CO_3 (0.2

mmol, 1.0 equiv), absolute dry CH_3CN (0.5 mL) and absolute dry CH_3OH (0.5 mL) were added under N_2. The formed mixture was stirred at room temperature under N_2 for 24 h as monitored by TLC. The solvent was removed under vaccum directly. The crude product was analyzed by crude ^1H NMR using dibromomethane (0.2 mmol) as internal standard.





Flame-dried 10 mL Schlenk tube filled with argon, Togni's reagent II (**1a**) (0.2 mmol, 1.0 equiv), alkyne **2d** (0.3 mmol, 1.5 equiv), alkyne **2j** (0.6 mmol, 3.0 equiv), $CuCl_2$ (0.02 mmol, 10 mol%), 2,2':6',2"-terpyridine (0.04 mmol, 20 mol%), K_2CO_3 (0.2 mmol, 1.0 equiv), absolute dry CH_3CN (0.5 mL) and absolute dry CH_3OH (0.5 mL) were added under N_2. The formed mixture was stirred at room temperature under N_2 for 24 h as monitored by TLC. The solvent was removed under vaccum directly. The

crude product was purified by flash column chromatography on silica gel (eluent: PE/EA) to afford the product **3dj**.

(*E*)-1-Methoxy-4-(5,5,5-trifluoro-1-(4-(trifluoromethyl)phenyl)pent-3-en-1-yn-3-yl)benzene: colorless oil, 35.1 mg (48% yield). **^{1}H NMR (600 MHz, $CDCl_3$)** δ 7.60 (d, *J* = 8.2 Hz, 2H), 7.57 (d, *J* = 8.3 Hz, 2H), 7.47 (d, *J* = 8.5 Hz, 2H), 6.93 (d, *J* = 8.6 Hz, 2H), 6.18 (q, *J* = 8.7 Hz, 1H), 3.85 (s, 3H); **^{13}C NMR (126 MHz, $CDCl_3$)** δ 160.5, 134.3, 134.0 (q, *J* = 6.2 Hz), 133.5, 132.1, 130.8 (q, *J* = 32.8 Hz), 129.9 (d, *J* = 2.1 Hz), 127.0, 125.4 (q, *J* = 3.8 Hz), 122.4 (d, *J* = 270.6 Hz), 122.2 (q, *J* = 34.8 Hz), 113.7, 91.9, 90.8, 55.3; **^{19}F NMR (376 MHz, $CDCl_3$)** δ -56.3, -63.0; **ATR-FTIR (cm $^{-1}$):** 2962, 2215, 1630, 1498, 1274, 1170, 1106, 1025, 749; **HRMS m/z (ESI)** calcd for $C_{19}H_{13}F_6O$ $(M + H)^+$ 371.0865, found 371.0869.

7. Computational Details

The DFT calculations were performed using the Gaussian 09 package[6]. Geometry optimizations of all the intermediates and transition states were carried out in gas phase with B3LYP[7] functional and a mixed basis set of SDD[8] for Cu and I atom and 6-31G*[9] for all other atoms. Frequency computations were conducted at the same level theory to identify all the stationary points and to provide the thermal correction to free energies at 298.15 K and 1 atm pressure. In order to confirm the transition states, intrinsic reaction coordinate (IRC) calculations connected reactants and products were performed. Single-point solvation energies were calculated with M06[10] method and a mixed basis set of SDD (Cu and I) and 6-311+G(d,p)[11] for all other atoms with continuum model SMD[12] (solvent = methanol). All energies are reported here in kcal/mol. The calculated optimized structures are illustrated by CYLview.[13]

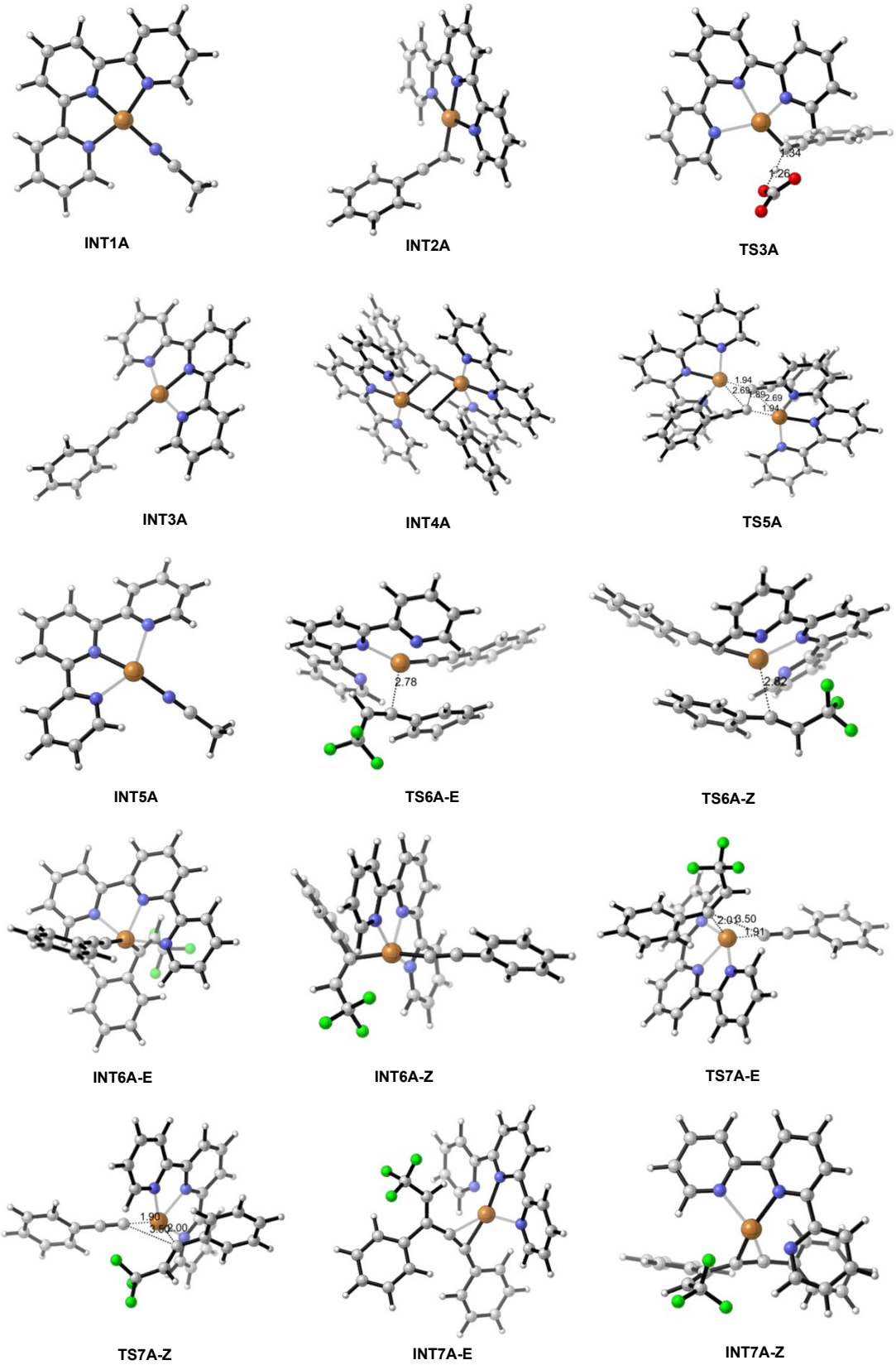


Fig. S2 The calculated optimized structures of the key intermediates and TS. Distances are in Å.

Cartesian coordinates of the optimized structures

INT1A

Charge = 2 Multiplicity = 2

G_{sol} = -1071.748811 Hartree

Zero-point correction = 0.279085 Hartree

Thermal correction to Energy = 0.298156 Hartree

Thermal correction to Enthalpy = 0.299100 Hartree

Thermal correction to Gibbs Free Energy = 0.229562 Hartree

C	1.187947	1.902853	0.004405	C	-2.343051	0.989245	-0.001270
C	-1.181473	1.906228	0.004011	C	-3.671797	1.403878	-0.004795
C	-1.209180	3.302207	0.014109	C	-2.995765	-1.255010	-0.007800
C	0.006163	3.991827	0.019073	C	-4.686936	0.443216	-0.009433
C	1.219524	3.298781	0.014555	H	-3.920688	2.458978	-0.004702
C	2.346952	0.982381	-0.001057	C	-4.345899	-0.907312	-0.010676
C	2.992849	-1.263990	-0.007396	H	-2.681674	-2.292176	-0.009584
C	4.344023	-0.920398	-0.010828	H	-5.727780	0.751316	-0.012372
C	4.689184	0.429128	-0.009817	H	-5.103350	-1.683381	-0.014247
C	3.676962	1.392887	-0.004967	N	-2.019253	-0.335676	-0.003091
H	-2.146244	3.846470	0.019005	N	0.002318	1.267713	-0.001101
H	0.007719	5.077322	0.027169	N	-0.003267	-2.656556	-0.009640
H	2.158076	3.840482	0.019562	C	-0.007949	-3.814080	0.007397
H	2.675467	-2.300233	-0.008800	C	-0.014077	-5.268201	0.032704
H	5.099070	-1.698799	-0.014463	H	-0.241939	-5.618897	1.045799
H	5.730970	0.734031	-0.013029	H	-0.772526	-5.647964	-0.661280
H	3.929065	2.447237	-0.005058	H	0.968507	-5.649023	-0.268443
N	2.019245	-0.341598	-0.002521	Cu	-0.000443	-0.671875	-0.005323

2a

Charge = 0 Multiplicity = 1

G_{sol} = -308.150671 Hartree

Zero-point correction = 0.109556 Hartree

Thermal correction to Energy = 0.116033 Hartree

Thermal correction to Enthalpy = 0.116977 Hartree

Thermal correction to Gibbs Free Energy = 0.079123 Hartree

C	-1.512820	-1.208866	-0.000012	H	0.428631	-2.150259	0.000021
C	-0.119887	-1.213400	0.000010	H	0.428696	2.150223	0.000022
C	0.594495	-0.000022	0.000030	H	-2.053255	2.151578	-0.000023
C	-0.119866	1.213390	0.000012	H	-3.300021	0.000036	-0.000041
C	-1.512785	1.208889	-0.000014	C	2.024444	-0.000014	0.000068
C	-2.213437	0.000013	-0.000023	C	3.234619	0.000002	0.000014
H	-2.053293	-2.151554	-0.000021	H	4.300666	0.000035	-0.000458

INT2A

Charge = 2 Multiplicity = 2

G_{sol} = -1247.200840 Hartree

Zero-point correction = 0.342735 Hartree

Thermal correction to Energy = 0.364929 Hartree

Thermal correction to Enthalpy = 0.365873 Hartree

Thermal correction to Gibbs Free Energy = 0.287671 Hartree

C	-2.611810	-1.182136	0.564997	H	-4.314576	-2.151482	1.494507
C	-2.611840	1.182070	0.564975	H	1.029089	-2.695411	-1.520048
C	-3.835900	1.213847	1.237429	H	0.434426	-5.115790	-1.315255
C	-4.440153	-0.000047	1.573714	H	-1.697253	-5.729500	-0.132753
C	-3.835878	-1.213936	1.237422	H	-3.140436	-3.916571	0.766338
C	-1.821625	-2.345958	0.098839	N	-0.657474	-2.028734	-0.535326
C	0.118400	-3.008403	-1.021823	C	-1.821687	2.345914	0.098813
C	-0.219113	-4.355887	-0.901034	C	-2.213751	3.672625	0.259649
C	-1.402345	-4.691095	-0.246814	C	0.118296	3.008413	-1.021888
C	-2.213676	-3.672680	0.259625	C	-1.402448	4.691066	-0.246798
H	-4.314601	2.151385	1.494535	H	-3.140489	3.916498	0.766409
H	-5.391196	-0.000065	2.096969	C	-0.219234	4.355894	-0.901057

H	1.028982	2.695459	-1.520142	C	5.350900	1.222786	1.158063
H	-1.697370	5.729464	-0.132701	H	3.783591	2.168711	0.026248
H	0.434283	5.115810	-1.315290	C	5.350898	-1.222803	1.157837
N	-0.657551	2.028726	-0.535398	H	3.783606	-2.168488	0.025804
N	-2.048246	-0.000025	0.265230	C	5.912212	-0.000048	1.558292
Cu	-0.309357	0.000002	-0.650997	H	5.804079	2.156808	1.473571
C	2.537380	0.000186	-0.906716	H	5.804060	-2.156888	1.473176
C	3.640518	0.000119	-0.059518	H	6.799183	-0.000103	2.185212
C	4.223704	1.232711	0.354188	C	1.497830	-0.000019	-1.614831
C	4.223706	-1.232552	0.353945	H	1.362560	-0.000081	-2.693064

MeCN

Charge = 0 Multiplicity = 1

G_{sol} = -132.679750 Hartree

Zero-point correction = 0.045643 Hartree

Thermal correction to Energy = 0.049235 Hartree

Thermal correction to Enthalpy = 0.050179 Hartree

Thermal correction to Gibbs Free Energy = 0.022666 Hartree

C	0.000000	0.000000	-1.181066	H	-0.889070	-0.513305	-1.561123
H	0.000000	1.026609	-1.561123	C	0.000000	0.000000	0.280614
H	0.889070	-0.513305	-1.561123	N	0.000000	0.000000	1.440869

CO_3^{2-}

Charge = -2 Multiplicity = 1

G_{sol} = -264.054151 Hartree

Zero-point correction = 0.013998 Hartree

Thermal correction to Energy = 0.017190 Hartree

Thermal correction to Enthalpy = 0.018134 Hartree

Thermal correction to Gibbs Free Energy = -0.011582 Hartree

C	0.000000	-0.000136	0.000000	O	-0.870773	-0.982985	0.000000

O	-0.415740	1.245631	0.000000	O	1.286514	-0.262545	0.000000

TS3A

Charge = 0 Multiplicity = 2

G_{sol} = -1511.243037 Hartree

Zero-point correction = 0.349663 Hartree

Thermal correction to Energy = 0.377381 Hartree

Thermal correction to Enthalpy = 0.378325 Hartree

Thermal correction to Gibbs Free Energy = 0.284100 Hartree

C	-2.153202	1.687288	-1.261851	C	-2.572526	-4.310646	-0.664059
C	-2.713837	-0.583064	-1.372934	H	-3.471876	-3.130443	-2.230578
C	-3.797425	-0.311779	-2.216331	C	-1.794836	-4.265962	0.492942
C	-4.031190	1.009918	-2.596669	H	-0.718633	-2.927062	1.832789
C	-3.218445	2.030229	-2.102237	H	-2.930572	-5.258662	-1.055308
C	-1.277098	2.661957	-0.559809	H	-1.540524	-5.169536	1.037553
C	0.127597	2.976079	1.264215	N	-1.634160	-1.880627	0.318860
C	0.296712	4.326588	0.955412	N	-1.898264	0.402628	-0.966230
C	-0.339979	4.841329	-0.173719	Cu	-0.379813	-0.011433	0.392061
C	-1.141246	3.999529	-0.943654	C	2.499763	-0.604016	0.021494
H	-4.463904	-1.103491	-2.540738	C	3.682642	-0.615349	-0.773355
H	-4.870977	1.249042	-3.242470	C	3.912146	-1.644598	-1.710819
H	-3.432483	3.067101	-2.337268	C	4.652612	0.399791	-0.632853
H	0.593694	2.514404	2.130405	C	5.070647	-1.652766	-2.482968
H	0.915157	4.953360	1.589714	H	3.170360	-2.430127	-1.818677
H	-0.216065	5.883566	-0.453635	C	5.810871	0.382670	-1.405303
H	-1.637986	4.373564	-1.833034	H	4.482176	1.190966	0.090812
N	-0.635182	2.162096	0.521432	C	6.023502	-0.640975	-2.333135
C	-2.403707	-1.916272	-0.792059	H	5.233973	-2.451703	-3.201514
C	-2.882934	-3.119989	-1.319155	H	6.550982	1.169271	-1.284083
C	-1.338486	-3.026917	0.945043	H	6.928336	-0.651368	-2.934996

C	1.477589	-0.588008	0.715038	C	0.388388	-0.382163	3.886473
H	1.060646	-0.922486	1.939087	O	0.663119	0.843798	3.714462
O	0.647809	-1.334071	3.060019	O	-0.202155	-0.601070	4.998705

INT3A

Charge = 1 Multiplicity = 2

G_{sol} = -1246.775497 Hartree

Zero-point correction = 0.332098 Hartree

Thermal correction to Energy = 0.354007 Hartree

Thermal correction to Enthalpy = 0.354951 Hartree

Thermal correction to Gibbs Free Energy = 0.277244 Hartree

C	-3.011378	1.180214	-0.000126	C	-2.530554	-3.682542	-0.000284
C	-3.012751	-1.178441	-0.000218	C	0.135811	-3.010051	-0.000108
C	-4.409837	-1.210148	-0.000307	C	-1.569538	-4.697054	-0.000268
C	-5.101760	0.001998	-0.000298	H	-3.586168	-3.930026	-0.000352
C	-4.408504	1.213354	-0.000207	C	-0.218002	-4.360833	-0.000180
C	-2.104150	2.356130	-0.000031	H	1.167022	-2.669984	-0.000036
C	0.138592	3.009669	0.000046	H	-1.879889	-5.737323	-0.000325
C	-0.214340	4.360680	0.000127	H	0.554519	-5.121928	-0.000165
C	-1.565647	4.697749	0.000121	N	-0.787330	-2.043227	-0.000123
C	-2.527305	3.683858	0.000039	N	-2.367400	0.000523	-0.000130
H	-4.950641	-2.149167	-0.000379	Cu	-0.371253	-0.000697	-0.000010
H	-6.187255	0.002563	-0.000364	C	1.515871	-0.001175	0.000089
H	-4.948355	2.152908	-0.000204	C	2.742242	-0.001210	0.000153
H	1.169584	2.668885	0.000039	C	4.173285	-0.001026	0.000242
H	0.558690	5.121260	0.000187	C	4.889178	-0.001055	1.213898
H	-1.875307	5.738220	0.000178	C	4.889328	-0.000854	-1.213325
H	-3.582731	3.932104	0.000032	C	6.282031	-0.000852	1.209286
N	-0.785132	2.043399	-0.000031	H	4.342605	-0.001167	2.152258
C	-2.106505	-2.355121	-0.000210	C	6.282180	-0.000654	-1.208542

H	4.342870	-0.000811	-2.151752	H	6.822952	-0.000519	-2.150816
C	6.982727	-0.000672	0.000415	H	8.068952	-0.000567	0.000482
H	6.822688	-0.000873	2.151627				

$^{-}$OCOOH

Charge = -1 Multiplicity = 1

G_{sol} = -264.529001 Hartree

Zero-point correction = 0.026267 Hartree

Thermal correction to Energy = 0.029785 Hartree

Thermal correction to Enthalpy = 0.030729 Hartree

Thermal correction to Gibbs Free Energy = 0.000490 Hartree

C	0.158035	-0.072913	0.000284	O	-1.004158	0.799073	-0.000013
O	-0.141684	-1.291655	-0.000064	H	-1.716907	0.139610	-0.000301
O	1.241929	0.529815	-0.000097				

INT4A

Charge = 2 Multiplicity = 3

G_{sol} = -2493.552649 Hartree

Zero-point correction = 0.664465 Hartree

Thermal correction to Energy = 0.709600 Hartree

Thermal correction to Enthalpy = 0.710544 Hartree

Thermal correction to Gibbs Free Energy = 0.580206 Hartree

C	-3.786330	1.181228	1.397235	C	-2.384882	4.689440	1.800995
C	-3.790189	-1.170441	1.395469	C	-3.327340	3.674949	1.624685
C	-5.186878	-1.201539	1.367532	H	-5.728413	-2.140013	1.372620
C	-5.879693	0.008865	1.343029	H	-6.964694	0.010678	1.319098
C	-5.182868	1.216976	1.369224	H	-5.721321	2.157224	1.375579
C	-2.887105	2.356510	1.502199	H	0.371289	2.696652	1.741032
C	-0.663080	3.023259	1.707414	H	-0.272089	5.119951	2.008715
C	-1.031257	4.361456	1.851212	H	-2.709698	5.719500	1.910969

H	-4.384933	3.911936	1.602126	C	5.879673	0.013916	-1.343259
N	-1.566419	2.053268	1.531693	C	5.187580	-1.196878	-1.368863
C	-2.894892	-2.348885	1.498379	C	2.896264	-2.345456	-1.500865
C	-3.339585	-3.666114	1.617779	C	0.674947	-3.021254	-1.705410
C	-0.673183	-3.023546	1.702425	C	1.048435	-4.358160	-1.847421
C	-2.400579	-4.684169	1.791901	C	2.403342	-4.680743	-1.796683
H	-4.397962	-3.899469	1.594384	C	3.341747	-3.662294	-1.621611
C	-1.045872	-4.360820	1.843073	H	5.720044	2.162212	-1.373818
H	0.362280	-2.700549	1.736954	H	6.964673	0.016354	-1.319291
H	-2.728845	-5.713397	1.899382	H	5.729669	-2.135026	-1.374734
H	-0.289274	-5.122232	1.998869	H	-0.360721	-2.698867	-1.739499
N	-1.573207	-2.050102	1.528832	H	0.292280	-5.119870	-2.003910
N	-3.139081	0.004320	1.384852	H	2.732215	-5.709666	-1.905219
Cu	-1.144273	0.001024	1.283899	H	4.400269	-3.895017	-1.598524
C	0.776061	-0.002121	1.444115	N	1.574399	-2.047446	-1.530919
C	1.962337	-0.006760	1.775244	C	2.885668	2.359936	-1.499993
C	3.331224	-0.012188	2.193452	C	3.325082	3.678774	-1.621104
C	4.011419	-1.228311	2.414935	C	0.661210	3.025568	-1.704158
C	4.019012	1.198222	2.422488	C	2.381991	4.692893	-1.796122
C	5.334356	-1.230123	2.850939	H	4.382538	3.916372	-1.598477
H	3.484637	-2.165805	2.261474	C	1.028558	4.364147	-1.846491
C	5.341960	1.188887	2.858349	H	-0.372964	2.698377	-1.738035
H	3.498179	2.139990	2.275016	H	2.706164	5.723275	-1.904969
C	6.004031	-0.023387	3.073049	H	0.268910	5.122368	-2.002995
H	5.841086	-2.173681	3.032612	N	1.565154	2.055917	-1.529622
H	5.854676	2.128069	3.045812	N	3.139078	0.007794	-1.385178
H	7.031483	-0.027666	3.424737	Cu	1.144321	0.003150	-1.284002
C	3.790874	-1.166570	-1.396846	C	-0.776079	-0.000941	-1.443642
C	3.785624	1.185105	-1.396365	C	-1.962379	-0.004732	-1.774704
C	5.182137	1.221646	-1.368340	C	-3.331225	-0.009377	-2.193047

C	-4.018657	1.201489	-2.420788	H	-3.485207	-2.162876	-2.263628
C	-4.011691	-1.225054	-2.416093	C	-6.003855	-0.018808	-3.073193
C	-5.341513	1.193042	-2.856946	H	-5.853932	2.132583	-3.043414
H	-3.497599	2.142938	-2.272076	H	-5.841507	-2.169182	-3.035224
C	-5.334545	-1.225980	-2.852353	H	-7.031232	-0.022426	-3.425108

TS5A

Charge = 2 Multiplicity = 3

G_{sol} = -2493.512978 Hartree

Zero-point correction = 0.660716 Hartree

Thermal correction to Energy = 0.707139 Hartree

Thermal correction to Enthalpy = 0.708083 Hartree

Thermal correction to Gibbs Free Energy = 0.569140 Hartree

C	-4.622873	-0.997333	-0.847941	N	-2.493736	-2.049556	-1.172081
C	-4.493068	1.345672	-0.939662	C	-3.554230	2.480109	-1.152068
C	-5.881462	1.462008	-0.821881	C	-3.955586	3.816048	-1.224377
C	-6.639347	0.297524	-0.701188	C	-1.344855	3.068329	-1.577161
C	-6.015433	-0.949117	-0.727379	C	-3.000883	4.797228	-1.493570
C	-3.817333	-2.242179	-0.968398	H	-4.993678	4.094394	-1.083870
C	-1.693035	-3.105106	-1.350925	C	-1.672019	4.420590	-1.679852
C	-2.168431	-4.416533	-1.337320	H	-0.327708	2.711439	-1.707149
C	-3.528139	-4.626679	-1.114628	H	-3.296952	5.839367	-1.563459
C	-4.364890	-3.526511	-0.925891	H	-0.904021	5.152304	-1.906718
H	-6.369437	2.429208	-0.836111	N	-2.258741	2.126815	-1.320593
H	-7.718966	0.361105	-0.608450	N	-3.908351	0.137089	-0.918546
H	-6.607439	-1.854528	-0.668691	Cu	-1.883403	0.021804	-1.016310
H	-0.644329	-2.876218	-1.514551	C	0.051753	-0.087305	-0.945035
H	-1.489121	-5.245632	-1.504208	C	1.111298	-0.147385	-1.617291
H	-3.937826	-5.631806	-1.094051	C	2.249657	-0.229218	-2.453231
H	-5.425046	-3.675075	-0.756198	C	2.888299	0.943735	-2.928620

C	2.759182	-1.487747	-2.860727	N	2.258743	2.126769	1.320637
C	3.985238	0.854803	-3.778325	C	3.817328	-2.242221	0.968347
H	2.499077	1.914342	-2.635265	C	4.364883	-3.526551	0.925823
C	3.856805	-1.562519	-3.711248	C	1.693025	-3.105152	1.350836
H	2.271054	-2.393621	-2.513760	C	3.528131	-4.626722	1.114530
C	4.474551	-0.395292	-4.173906	H	5.425041	-3.675112	0.756138
H	4.456294	1.762119	-4.145374	C	2.168420	-4.416579	1.337211
H	4.227907	-2.533595	-4.026159	H	0.644317	-2.876266	1.514455
H	5.324965	-0.459095	-4.845878	H	3.937817	-5.631848	1.093938
C	4.493071	1.345630	0.939693	H	1.489107	-5.245680	1.504075
C	4.622871	-0.997372	0.847919	N	2.493730	-2.049599	1.172019
C	6.015429	-0.949156	0.727352	N	3.908351	0.137050	0.918552
C	6.639346	0.297485	0.701188	Cu	1.883403	0.021766	1.016310
C	5.881464	1.461967	0.821909	C	-0.051753	-0.087337	0.945037
C	3.554234	2.480064	1.152124	C	-1.111298	-0.147449	1.617293
C	1.344859	3.068280	1.577226	C	-2.249654	-0.229315	2.453232
C	1.672026	4.420537	1.679951	C	-2.759163	-1.487859	2.860702
C	3.000891	4.797177	1.493682	C	-2.888313	0.943620	2.928643
C	3.955593	3.816001	1.224468	C	-3.856784	-1.562662	3.711222
H	6.607433	-1.854568	0.668639	H	-2.271023	-2.393719	2.513718
H	7.718964	0.361066	0.608447	C	-3.985251	0.854657	3.778346
H	6.369440	2.429165	0.836158	H	-2.499105	1.914239	2.635307
H	0.327711	2.711390	1.707203	C	-4.474546	-0.395453	4.173904
H	0.904030	5.152248	1.906833	H	-4.227873	-2.533750	4.026114
H	3.296962	5.839313	1.563598	H	-4.456319	1.761959	4.145413
H	4.993687	4.094347	1.083971	H	-5.324959	-0.459281	4.845873

INT5A

Charge = 1 Multiplicity = 1

G_{sol} = -1071.920259 Hartree

Zero-point correction = 0.276553 Hartree

Thermal correction to Energy = 0.296731 Hartree

Thermal correction to Enthalpy = 0.297675 Hartree

Thermal correction to Gibbs Free Energy = 0.223992 Hartree

C	-1.169466	-1.824812	0.173174	C	2.380284	-0.977003	-0.000955
C	1.170262	-1.824381	0.173234	C	3.669298	-1.416704	0.318272
C	1.205741	-3.219113	0.279837	C	3.200787	1.057048	-0.740575
C	0.000779	-3.915662	0.349864	C	4.751698	-0.571662	0.080031
C	-1.204436	-3.219556	0.279764	H	3.827270	-2.393647	0.761544
C	-2.379796	-0.977875	-0.001028	C	4.517726	0.688600	-0.468132
C	-3.201026	1.055943	-0.740468	H	2.969454	2.031894	-1.161460
C	-4.517841	0.686971	-0.468145	H	5.760000	-0.893072	0.322387
C	-4.751369	-0.573444	0.079858	H	5.331705	1.373897	-0.679739
C	-3.668664	-1.418097	0.318079	N	2.154464	0.252818	-0.515541
H	2.147823	-3.754859	0.273612	N	0.000277	-1.162428	0.162193
H	0.000975	-4.998810	0.422205	N	-0.000542	2.724572	0.293824
H	-2.146320	-3.755650	0.273477	C	-0.001022	3.849349	0.569382
H	-2.970038	2.030938	-1.161195	C	-0.001863	5.263537	0.922572
H	-5.332065	1.371990	-0.679712	H	0.920724	5.516810	1.454450
H	-5.759566	-0.895262	0.322111	H	-0.070550	5.875768	0.017714
H	-3.826291	-2.395144	0.761244	H	-0.856588	5.486644	1.569048
N	-2.154413	0.252080	-0.515477	Cu	-0.000055	0.860358	-0.179975

1,4-diphenylbuta-1,3-diyne

Charge = 0 Multiplicity = 1

G_{sol} = -615.129484 Hartree

Zero-point correction = 0.202810 Hartree

Thermal correction to Energy = 0.215714 Hartree

Thermal correction to Enthalpy = 0.216658 Hartree

Thermal correction to Gibbs Free Energy = 0.159861 Hartree

C	-5.432715	-0.854626	-0.855685	C	0.680044	-0.000086	0.000155
C	-4.040492	-0.858531	-0.859598	C	1.901304	0.000037	0.000045
C	-3.324185	0.000029	0.000015	C	3.324188	0.000015	-0.000001
C	-4.040568	0.858580	0.859570	C	4.040519	0.859841	-0.858328
C	-5.432787	0.854612	0.855605	C	4.040534	-0.859804	0.858309
C	-6.133227	-0.000021	-0.000057	C	5.432738	0.855884	-0.854419
H	-5.973379	-1.520691	-1.522565	H	3.492189	1.522908	-1.520185
H	-3.492146	-1.520578	-1.522462	C	5.432758	-0.855877	0.854349
H	-3.492279	1.520655	1.522455	H	3.492223	-1.522845	1.520207
H	-5.973513	1.520655	1.522457	C	6.133222	-0.000007	-0.000050
H	-7.219734	-0.000042	-0.000080	H	5.973431	1.522934	-1.520291
C	-1.901295	-0.000007	0.000072	H	5.973458	-1.522926	1.520216
C	-0.680035	-0.000049	0.000071	H	7.219730	-0.000012	-0.000071

1a

Charge = 0 Multiplicity = 1

G_{sol} = -768.329427 Hartree

Zero-point correction = 0.106697 Hartree

Thermal correction to Energy = 0.119480 Hartree

Thermal correction to Enthalpy = 0.120425 Hartree

Thermal correction to Gibbs Free Energy = 0.065331 Hartree

C	-0.521174	1.992036	-0.000326	H	-1.417032	3.943012	-0.000335
C	-0.822956	0.640380	-0.000180	C	-2.361211	-1.392682	0.000083
C	-2.096181	0.108274	0.000025	O	-1.282428	-2.123129	-0.000307
C	-3.162357	1.017995	0.000138	I	0.703886	-0.946453	-0.000183
C	-2.919709	2.389289	0.000018	C	2.443654	0.555843	0.000229
C	-1.608537	2.873801	-0.000225	F	3.557984	-0.190088	0.000473
H	0.491476	2.371309	-0.000532	F	2.453990	1.342156	-1.085939
H	-4.165908	0.604462	0.000311	F	2.453473	1.342109	1.086430
H	-3.752156	3.086787	0.000094	O	-3.512637	-1.801971	0.000670

2-iodobenzoate

Charge = -1 Multiplicity = 1

G_{sol} = -430.941827 Hartree

Zero-point correction = 0.091170 Hartree

Thermal correction to Energy = 0.099890 Hartree

Thermal correction to Enthalpy = 0.100835 Hartree

Thermal correction to Gibbs Free Energy = 0.054504 Hartree

C	-0.664977	-1.964542	0.030984	H	-3.434842	0.713664	-0.033640
C	-0.368981	-0.598824	0.026537	H	-4.056404	-1.718718	0.068402
C	-1.344040	0.392143	0.021029	H	-2.234433	-3.438401	0.079883
C	-2.677562	-0.063107	0.018585	O	-0.111764	2.352094	0.614695
C	-3.011111	-1.413325	0.056305	I	1.782067	-0.149872	-0.049569
C	-1.997683	-2.376095	0.061545	C	-1.145548	1.956613	0.041314
H	0.134003	-2.699547	0.012815	O	-2.088042	2.584034	-0.494454

CF_3 radical

Charge = 0 Multiplicity = 2

G_{sol} = -337.552367 Hartree

Zero-point correction = 0.012167 Hartree

Thermal correction to Energy = 0.015619 Hartree

Thermal correction to Enthalpy = 0.016564 Hartree

Thermal correction to Gibbs Free Energy = -0.013521 Hartree

C	0.000000	0.000000	0.329152	F	-1.094981	-0.632187	-0.073145
F	0.000000	1.264375	-0.073145	F	1.094981	-0.632187	-0.073145

radical **A**

Charge = 0 Multiplicity = 2

G_{sol} = -645.758267 Hartree

Zero-point correction = 0.125025 Hartree

Thermal correction to Energy = 0.135386 Hartree

Thermal correction to Enthalpy = 0.136330 Hartree

Thermal correction to Gibbs Free Energy = 0.085709 Hartree

C	3.215444	1.212311	0.142919	H	3.739858	-2.156776	0.263818
C	1.866560	1.229846	-0.167539	H	4.958819	-0.004244	0.544405
C	1.145981	0.002086	-0.334196	C	-0.191285	0.004025	-0.643633
C	1.862877	-1.228029	-0.169082	C	-1.458732	0.001657	-0.943154
C	3.211795	-1.214937	0.141384	H	-1.825933	0.001149	-1.973047
C	3.900796	-0.002466	0.300070	C	-2.560854	-0.000116	0.085460
H	3.746349	2.152401	0.266530	F	-3.352138	-1.088136	-0.060364
H	1.335940	2.168971	-0.287282	F	-3.358352	1.083044	-0.062844
H	1.329425	-2.165388	-0.290008	F	-2.093949	0.002605	1.345676

TS6A-E

Charge = 1 Multiplicity = 1

G_{sol} = -1892.495563 Hartree

Zero-point correction = 0.456663 Hartree

Thermal correction to Energy = 0.490962 Hartree

Thermal correction to Enthalpy = 0.491906 Hartree

Thermal correction to Gibbs Free Energy = 0.383729 Hartree

C	-2.239187	1.168636	-1.917192	H	-3.990902	-2.146077	-2.722570
C	-2.239227	-1.168274	-1.917348	H	-5.136728	0.000320	-3.251290
C	-3.505259	-1.199934	-2.514763	H	-3.990828	2.146608	-2.722281
C	-4.145850	0.000274	-2.807770	H	0.981653	3.201783	0.395877
C	-3.505218	1.200420	-2.514602	H	0.669245	5.439105	-0.678951
C	-1.484785	2.408896	-1.597226	H	-1.101084	5.673953	-2.450231
C	0.210110	3.357630	-0.352805	H	-2.457102	3.682002	-3.057566
C	0.040086	4.601202	-0.960663	N	-0.537418	2.289255	-0.649351
C	-0.944429	4.728795	-1.939442	C	-1.484870	-2.408603	-1.597544
C	-1.714980	3.616092	-2.269839	C	-1.715112	-3.615704	-2.270311

C	0.209988	-3.357561	-0.353244	C	2.001640	0.000013	-0.309102
C	-0.944606	-4.728479	-1.940054	Cu	0.116494	0.000039	-0.444722
H	-2.457237	-3.681483	-3.058046	C	-1.456867	-0.000131	1.847081
C	0.039913	-4.601050	-0.961258	C	-0.195198	-0.000148	2.354298
H	0.981538	-3.201842	0.395457	C	0.505089	1.242854	2.562551
H	-1.101298	-5.673567	-2.450963	C	0.505104	-1.243167	2.562402
H	0.669038	-5.439013	-0.679651	C	1.866570	1.227995	2.724652
N	-0.537497	-2.289119	-0.649654	H	-0.055271	2.169878	2.519641
N	-1.634919	0.000150	-1.608969	C	1.866585	-1.228312	2.724502
C	3.245534	-0.000007	-0.288296	H	-0.055245	-2.170192	2.519381
C	4.666103	-0.000030	-0.331269	C	2.564073	-0.000152	2.684122
C	5.388343	1.215905	-0.354587	H	2.419563	2.155571	2.832422
C	5.388301	-1.215988	-0.354640	H	2.419589	-2.155895	2.832157
C	6.778330	1.211380	-0.399346	H	3.647645	-0.000149	2.738408
H	4.840266	2.153196	-0.344714	C	-2.736541	-0.000148	1.620151
C	6.778289	-1.211508	-0.399398	H	-3.158147	-0.000107	0.618788
H	4.840193	-2.153261	-0.344809	C	-3.756517	-0.000238	2.741598
C	7.477750	-0.000075	-0.420518	F	-4.542439	-1.087245	2.644543
H	7.321081	2.152076	-0.420782	F	-3.177088	-0.000250	3.950727
H	7.321008	-2.152222	-0.420874	F	-4.542552	1.086694	2.644617
H	8.563292	-0.000093	-0.456465				

TS6A-Z

Charge = 1 Multiplicity = 1

G_{sol} = -1892.489936 Hartree

Zero-point correction = 0.456456 Hartree

Thermal correction to Energy = 0.490649 Hartree

Thermal correction to Enthalpy = 0.491594 Hartree

Thermal correction to Gibbs Free Energy = 0.384409 Hartree

C	2.247457	-1.120816	-1.687828	C	2.224612	1.210452	-1.661157

C	3.420819	1.265068	-2.385927	C	-5.207642	1.198537	-0.842530
C	4.037327	0.074769	-2.758044	C	-6.556271	-1.233884	-1.148618
C	3.444465	-1.135565	-2.413244	H	-4.655517	-2.169230	-0.750165
C	1.534147	-2.365727	-1.298823	C	-6.566561	1.189632	-1.136657
C	-0.094178	-3.318313	0.030281	H	-4.673808	2.137138	-0.728801
C	0.076029	-4.573051	-0.552364	C	-7.245559	-0.024305	-1.289346
C	1.026269	-4.706079	-1.563165	H	-7.082609	-2.176079	-1.271871
C	1.758531	-3.586393	-1.949102	H	-7.100908	2.128481	-1.250624
H	3.877401	2.216645	-2.630354	H	-8.306958	-0.027675	-1.519908
H	4.976124	0.090192	-3.302997	C	-1.889030	-0.007213	-0.153435
H	3.919653	-2.072116	-2.679234	Cu	0.001286	-0.000596	0.012421
H	-0.845103	-3.160073	0.797965	C	1.282824	-0.033491	2.522631
H	-0.527885	-5.413892	-0.227588	C	-0.066218	-0.034914	2.743654
H	1.184081	-5.660228	-2.056644	C	-0.791465	-1.275706	2.833578
H	2.470767	-3.658736	-2.762906	C	-0.791577	1.203693	2.858042
N	0.622581	-2.243510	-0.315152	C	-2.165010	-1.261717	2.863515
C	1.487875	2.432321	-1.244053	H	-0.230637	-2.203341	2.845518
C	1.684001	3.669538	-1.871991	C	-2.165156	1.188738	2.888497
C	-0.152280	3.325458	0.110761	H	-0.230961	2.131063	2.887190
C	0.930899	4.766324	-1.461262	C	-2.857729	-0.035699	2.795813
H	2.390259	3.771836	-2.687821	H	-2.722375	-2.192282	2.900872
C	-0.011026	4.594378	-0.448563	H	-2.722720	2.118242	2.944899
H	-0.895587	3.137616	0.879256	H	-3.942273	-0.035416	2.760387
H	1.066407	5.732740	-1.937197	C	2.562256	-0.040424	2.769769
H	-0.630315	5.416256	-0.104721	H	2.896908	-0.052875	3.810433
N	0.584266	2.272197	-0.258569	C	3.684913	-0.034994	1.757519
N	1.669016	0.035114	-1.314189	F	3.643071	-1.120045	0.956979
C	-3.106480	-0.011093	-0.404468	F	3.641201	1.055795	0.965315
C	-4.496054	-0.015539	-0.695968	F	4.866892	-0.036511	2.391246
C	-5.197309	-1.234108	-0.854581				

INT6A-E

Charge = 1 Multiplicity = 1

G_{sol} =-1892.508173 Hartree

Zero-point correction = 0.459230 Hartree

Thermal correction to Energy = 0.493189 Hartree

Thermal correction to Enthalpy = 0.494133 Hartree

Thermal correction to Gibbs Free Energy = 0.386577 Hartree

C	-0.760983	1.523505	-2.312491	H	-0.585832	-3.318577	-3.790145
C	-0.767043	-0.792918	-2.653556	C	0.366568	-4.395263	-0.721819
C	-1.312564	-0.642559	-3.935019	H	0.557118	-3.050073	0.967175
C	-1.580769	0.648282	-4.391575	H	0.087868	-5.399765	-2.613997
C	-1.306434	1.751389	-3.582585	H	0.691322	-5.273579	-0.174398
C	-0.403789	2.584373	-1.329233	N	-0.113972	-2.049697	-0.702243
C	0.311331	3.045899	0.831668	N	-0.512721	0.278626	-1.898961
C	0.399352	4.412179	0.568915	C	3.141249	-0.049243	0.290409
C	0.062242	4.864585	-0.705332	C	4.562916	-0.054355	0.330435
C	-0.335495	3.939653	-1.668525	C	5.282710	1.146536	0.521092
H	-1.541135	-1.499657	-4.557636	C	5.283927	-1.259755	0.176463
H	-2.013946	0.794379	-5.376170	C	6.673127	1.138520	0.552092
H	-1.530261	2.752615	-3.931767	H	4.733810	2.075373	0.642367
H	0.585697	2.637541	1.799120	C	6.674349	-1.259307	0.208912
H	0.731765	5.094174	1.344129	H	4.735978	-2.185799	0.031785
H	0.122711	5.919634	-0.953675	C	7.373335	-0.062371	0.396800
H	-0.566623	4.267912	-2.675437	H	7.215365	2.068367	0.698438
N	-0.098313	2.162635	-0.083589	H	7.217597	-2.192290	0.088588
C	-0.417536	-2.093802	-2.016999	H	8.459227	-0.065557	0.422901
C	-0.356124	-3.294955	-2.731039	C	1.908005	-0.056038	0.334145
C	0.285865	-3.161427	-0.077834	Cu	0.018075	-0.025496	0.150117
C	0.032435	-4.460141	-2.073167	C	-1.857377	-0.110672	0.772165

C	-1.510453	-0.317911	2.155164	H	-0.896520	-2.832365	4.392093
C	-1.312583	0.786264	3.026898	H	-0.532257	-0.880795	5.883448
C	-1.343913	-1.631698	2.670076	C	-2.971772	-0.003167	0.070591
C	-0.969038	0.578274	4.355571	H	-2.972704	0.152074	-1.003627
H	-1.474618	1.789870	2.649641	C	-4.359716	-0.078459	0.654820
C	-1.000777	-1.824850	4.001037	F	-5.044921	-1.097159	0.093447
H	-1.529014	-2.479166	2.019232	F	-4.366530	-0.259062	1.985969
C	-0.802605	-0.723756	4.843593	F	-5.036926	1.058022	0.385902
H	-0.839913	1.427052	5.020196				

INT6A-Z

Charge = 1 Multiplicity = 1

G_{sol} = -1892.497331 Hartree

Zero-point correction = 0.459367 Hartree

Thermal correction to Energy = 0.492924 Hartree

Thermal correction to Enthalpy = 0.493868 Hartree

Thermal correction to Gibbs Free Energy = 0.389281 Hartree

C	-0.454488	1.356063	-1.990857	H	0.002384	2.557495	2.305228
C	-0.435686	-0.983675	-2.178375	H	-0.009756	5.021843	1.862048
C	-0.533098	-0.916154	-3.574301	H	-0.261616	5.805081	-0.516684
C	-0.593847	0.351383	-4.160769	H	-0.477329	4.110955	-2.321389
C	-0.552369	1.510097	-3.379823	N	-0.235813	2.040927	0.326090
C	-0.361642	2.437726	-0.966324	C	-0.328106	-2.213712	-1.339479
C	-0.109836	2.948999	1.300563	C	-0.314462	-3.502996	-1.877506
C	-0.114811	4.318628	1.043136	C	-0.100709	-3.082190	0.819581
C	-0.253590	4.746617	-0.275688	C	-0.187058	-4.602284	-1.030196
C	-0.376484	3.797089	-1.288553	H	-0.397393	-3.646144	-2.948922
H	-0.555505	-1.804443	-4.195301	C	-0.077706	-4.391505	0.342802
H	-0.666580	0.437339	-5.240502	H	-0.025690	-2.861981	1.878392
H	-0.589062	2.485600	-3.851253	H	-0.171825	-5.607627	-1.439498

H	0.024509	-5.216401	1.039415	C	-2.208323	-0.238573	2.509157
N	-0.224423	-2.029364	0.002158	H	-3.217419	-0.322292	2.915097
N	-0.412902	0.137174	-1.469967	C	-3.088293	-0.023732	0.207060
C	2.998227	-0.004046	0.192736	C	-3.617095	-1.196766	-0.369637
C	4.407060	0.010032	-0.010733	C	-3.635377	1.221260	-0.165814
C	5.124348	1.226691	0.008715	C	-4.667000	-1.123832	-1.282298
C	5.113172	-1.191740	-0.239293	H	-3.218848	-2.162440	-0.072996
C	6.499532	1.237227	-0.199880	C	-4.684987	1.286705	-1.079254
H	4.587284	2.152399	0.191238	H	-3.249577	2.129501	0.287491
C	6.488421	-1.172372	-0.447000	C	-5.201074	0.116495	-1.643768
H	4.567307	-2.130221	-0.247883	H	-5.079216	-2.036660	-1.702934
C	7.185619	0.040000	-0.428337	H	-5.110998	2.250843	-1.341973
H	7.040993	2.178757	-0.182074	H	-6.023086	0.169916	-2.351494
H	7.021216	-2.102862	-0.621022	C	-1.140350	-0.350272	3.550943
H	8.259924	0.051469	-0.588251	F	0.022931	0.257447	3.159481
C	1.800252	-0.026137	0.480480	F	-0.815866	-1.641038	3.814693
Cu	-0.102013	-0.030471	0.609331	F	-1.515751	0.212999	4.706425
C	-2.013772	-0.098740	1.195934				

TS7A-E

Charge = 1 Multiplicity = 1

G_{sol} = -1892.492336 Hartree

Zero-point correction = 0.457709 Hartree

Thermal correction to Energy = 0.491436 Hartree

Thermal correction to Enthalpy = 0.492380 Hartree

Thermal correction to Gibbs Free Energy = 0.385125 Hartree

C	-1.434139	-2.642333	0.049796	C	-2.309575	-3.630413	0.517042
C	-1.436101	-1.569104	2.126768	C	-0.895963	-2.588737	-1.338567
C	-2.311389	-2.522590	2.661288	C	0.257334	-1.319014	-2.904175
C	-2.745037	-3.561143	1.839185	C	0.182397	-2.330093	-3.861685

C	-0.458722	-3.519210	-3.517179	C	6.918351	0.427136	1.145315
C	-1.001528	-3.653767	-2.240529	H	4.979800	0.880998	1.971352
H	-2.663107	-2.454123	3.683984	C	7.614955	-0.143451	0.072863
H	-3.430393	-4.309400	2.225189	H	7.460774	-1.143940	-1.833743
H	-2.659933	-4.425150	-0.130981	H	7.464522	0.858812	1.978831
H	0.756687	-0.377166	-3.113131	H	8.701091	-0.152844	0.076728
H	0.620164	-2.185087	-4.843555	C	2.151270	-0.093396	0.051733
H	-0.529045	-4.336661	-4.228223	Cu	0.245537	-0.103607	0.056197
H	-1.480105	-4.581823	-1.949121	C	-0.972440	1.315127	-0.679976
N	-0.272016	-1.443530	-1.683614	C	-0.208357	2.277693	-1.173876
C	-0.900842	-0.404586	2.886628	H	0.875460	2.239754	-1.151276
C	-1.007461	-0.285377	4.277071	C	-2.384378	1.076722	-0.561412
C	0.246521	1.610486	2.757364	C	-3.096962	1.532987	0.574244
C	-0.468332	0.835376	4.906206	C	-3.090627	0.416216	-1.596118
H	-1.484003	-1.061461	4.865154	C	-4.472934	1.360896	0.651644
C	0.170110	1.806351	4.135943	H	-2.560022	2.042057	1.367071
H	0.744018	2.327390	2.110355	C	-4.466610	0.249833	-1.507369
H	-0.539458	0.942151	5.984303	H	-2.548875	0.068283	-2.468754
H	0.604857	2.692486	4.585928	C	-5.160953	0.717367	-0.384610
N	-0.279117	0.541186	2.152470	H	-5.016497	1.735954	1.513643
N	-1.023406	-1.654517	0.855529	H	-5.005302	-0.234849	-2.316112
C	3.393758	-0.101928	0.055159	H	-6.237167	0.586447	-0.320387
C	4.807033	-0.117915	0.062217	C	-0.743566	3.536792	-1.822958
C	5.527534	-0.692062	-1.014427	F	-0.298530	4.619044	-1.152786
C	5.529646	0.441985	1.144924	F	-2.084000	3.593359	-1.860018
C	6.916241	-0.702133	-1.004472	F	-0.286775	3.626190	-3.088506
H	4.976058	-1.122804	-1.844113				

TS7A-Z

Charge = 1 Multiplicity = 1

G_{sol} = -1892.482089 Hartree

Zero-point correction = 0.457723 Hartree

Thermal correction to Energy = 0.491164 Hartree

Thermal correction to Enthalpy = 0.492108 Hartree

Thermal correction to Gibbs Free Energy = 0.387714 Hartree

C	1.999047	-1.052637	-2.025189	H	0.886923	5.821349	-1.398645
C	1.946228	1.282972	-1.928267	H	-0.510618	5.266292	0.617317
C	2.942744	1.383506	-2.907188	N	0.548219	2.173361	-0.183154
C	3.465692	0.209545	-3.446339	N	1.504817	0.085547	-1.520665
C	2.997088	-1.027399	-3.007248	C	-3.072243	-0.005738	-0.505398
C	1.410190	-2.300372	-1.461575	C	-4.456487	0.003678	-0.758769
C	0.050418	-3.207749	0.191099	C	-5.170463	-1.213287	-0.913614
C	0.214739	-4.499923	-0.307507	C	-5.164301	1.230228	-0.855168
C	1.010854	-4.675948	-1.438338	C	-6.537463	-1.198044	-1.151175
C	1.612661	-3.564795	-2.026518	H	-4.628700	-2.150672	-0.839908
H	3.317979	2.346626	-3.232790	C	-6.531274	1.233376	-1.093100
H	4.245161	0.258364	-4.200477	H	-4.617780	2.160309	-0.737225
H	3.414269	-1.942378	-3.411155	C	-7.220426	0.022243	-1.241207
H	-0.569439	-3.006116	1.059815	H	-7.078827	-2.132208	-1.266619
H	-0.274155	-5.337790	0.178106	H	-7.067871	2.174718	-1.163958
H	1.155882	-5.663672	-1.865225	H	-8.290628	0.029410	-1.426802
H	2.212552	-3.682883	-2.921788	C	-1.842922	-0.014495	-0.297005
N	0.638192	-2.144119	-0.366366	Cu	0.021524	-0.020868	0.062230
C	1.303368	2.452818	-1.265041	C	0.932397	-0.074971	1.840886
C	1.441675	3.766241	-1.728722	C	0.221278	-0.140064	2.961605
C	-0.085749	3.159441	0.458913	H	0.760802	-0.160613	3.910442
C	0.792084	4.796979	-1.051433	C	2.377449	-0.042088	1.711975
H	2.028169	3.983570	-2.614220	C	3.075256	1.188140	1.713876
C	0.013450	4.493760	0.064645	C	3.117742	-1.245869	1.649725
H	-0.689540	2.859058	1.310576	C	4.464899	1.207772	1.678068

H	2.515259	2.115020	1.769914	H	6.270667	0.028451	1.595641
C	4.507168	-1.215843	1.613891	C	-1.271831	-0.189804	3.142127
H	2.589937	-2.193221	1.656690	F	-1.835480	-1.255839	2.527553
C	5.185116	0.008766	1.622959	F	-1.889855	0.920524	2.677451
H	4.991648	2.157210	1.704144	F	-1.559243	-0.287490	4.453553
H	5.066405	-2.146568	1.589982				

INT7A-E

Charge = 1 Multiplicity = 1

G_{sol} = -1892.610083 Hartree

Zero-point correction = 0.460794 Hartree

Thermal correction to Energy = 0.494375 Hartree

Thermal correction to Enthalpy = 0.495319 Hartree

Thermal correction to Gibbs Free Energy = 0.388611 Hartree

C	3.343649	-0.064154	-1.091082	H	4.030678	0.867868	-3.617911
C	2.973222	-1.419255	0.783428	N	1.959825	1.896949	-1.150072
C	4.164650	-2.116916	0.555313	C	2.110904	-1.618391	1.978845
C	4.941330	-1.773475	-0.549589	C	2.147193	-2.779511	2.757938
C	4.544945	-0.721884	-1.374339	C	0.510767	-0.673682	3.357222
C	2.865560	1.141713	-1.817430	C	1.329277	-2.862441	3.883959
C	1.517489	3.026508	-1.720233	H	2.784495	-3.612828	2.482784
C	1.946507	3.462291	-2.973178	C	0.498929	-1.787726	4.197231
C	2.864050	2.678294	-3.670358	H	-0.128945	0.182149	3.555542
C	3.330453	1.502054	-3.085677	H	1.338341	-3.755284	4.501535
H	4.498717	-2.885271	1.242747	H	-0.148201	-1.807741	5.067737
H	5.873555	-2.294998	-0.742920	N	1.294425	-0.582582	2.276336
H	5.176576	-0.401016	-2.194450	N	2.568366	-0.455449	-0.063439
H	0.797343	3.599834	-1.143701	C	-1.019364	1.410158	0.522486
H	1.564719	4.389720	-3.386535	C	-1.276599	2.724614	1.047686
H	3.210688	2.973444	-4.655912	C	-0.263250	3.508287	1.633142

C	-2.591766	3.231674	0.980142	C	-5.138666	0.271369	-1.637976
C	-0.559199	4.772943	2.136880	H	-3.114180	0.980901	-1.820118
H	0.749747	3.119128	1.697251	C	-5.426653	-1.807926	-0.440054
C	-2.875581	4.496236	1.486809	H	-3.629796	-2.726092	0.308506
H	-3.374233	2.625713	0.533901	C	-5.974362	-0.732286	-1.141620
C	-1.863294	5.269333	2.064297	H	-5.558060	1.105914	-2.192571
H	0.226974	5.369678	2.589766	H	-6.071844	-2.588866	-0.048474
H	-3.890101	4.879852	1.433044	H	-7.047191	-0.675522	-1.300945
H	-2.091619	6.254844	2.459099	C	-0.923160	-2.005909	-0.710010
C	-1.177126	0.274579	0.040101	H	0.125735	-1.943210	-0.443117
Cu	0.901890	0.660725	0.337245	C	-1.305383	-3.334283	-1.289670
C	-1.729202	-0.941365	-0.496354	F	-0.214354	-3.899074	-1.855283
C	-3.204059	-0.884029	-0.733574	F	-1.738268	-4.194201	-0.331044
C	-3.762494	0.202430	-1.426855	F	-2.262029	-3.262651	-2.228473
C	-4.049547	-1.887308	-0.236135				

INT7A-Z

Charge = 1 Multiplicity = 1

G_{sol} = -1892.613420 Hartree

Zero-point correction = 0.460724 Hartree

Thermal correction to Energy = 0.494325 Hartree

Thermal correction to Enthalpy = 0.495269 Hartree

Thermal correction to Gibbs Free Energy = 0.389129 Hartree

C	3.094246	1.351780	0.013319	C	3.707914	-2.336899	1.992100
C	1.442567	2.934495	-0.482140	C	4.781932	-1.798651	1.286303
C	2.404209	3.873077	-0.871371	C	4.604478	-0.599204	0.598770
C	3.748272	3.506683	-0.828622	H	2.122179	4.875685	-1.170016
C	4.106317	2.244136	-0.362372	H	4.515384	4.217711	-1.119400
C	3.353207	0.026053	0.639045	H	5.151289	1.976264	-0.260474
C	2.486601	-1.660993	1.959664	H	1.618840	-2.045098	2.486104

H	3.806150	-3.258694	2.556099	H	1.954014	-1.447592	-4.821108
H	5.744962	-2.299998	1.271262	H	2.872187	-4.565520	-1.999275
H	5.424808	-0.168674	0.035187	H	3.202573	-3.512059	-4.224998
N	2.306513	-0.512256	1.298732	C	-1.124392	-1.061595	0.025911
C	-0.011922	3.231970	-0.372925	Cu	0.270574	0.405792	0.400176
C	-0.595587	4.388955	-0.898149	C	-2.456285	-1.079766	0.596969
C	-2.043844	2.559388	0.521740	C	-2.645690	-1.159720	1.934589
C	-1.952767	4.624006	-0.685757	H	-3.642813	-1.264991	2.345011
H	-0.006162	5.094675	-1.472259	C	-3.605007	-1.022922	-0.351237
C	-2.692320	3.698653	0.047795	C	-3.490759	-1.541476	-1.651773
H	-2.578566	1.804735	1.089162	C	-4.834880	-0.468251	0.047947
H	-2.421655	5.517369	-1.086631	C	-4.583104	-1.530759	-2.517719
H	-3.748062	3.846959	0.247549	H	-2.551374	-1.973576	-1.980426
N	-0.741566	2.322674	0.316704	C	-5.922804	-0.453805	-0.821403
N	1.801492	1.696608	-0.100895	H	-4.937620	-0.029003	1.036016
C	-0.197263	-1.364518	-0.743061	C	-5.802125	-0.988968	-2.106399
C	0.743074	-1.923923	-1.668828	H	-4.481320	-1.949403	-3.514670
C	0.933808	-1.331409	-2.934094	H	-6.863755	-0.018765	-0.497360
C	1.453847	-3.094953	-1.336561	H	-6.650993	-0.977580	-2.783671
C	1.816460	-1.904139	-3.845397	C	-1.550761	-1.170382	2.952959
H	0.380739	-0.433142	-3.191824	F	-0.785712	-0.035912	2.908395
C	2.333771	-3.658261	-2.256900	F	-0.687760	-2.206269	2.786119
H	1.300451	-3.555407	-0.366075	F	-2.052876	-1.256248	4.191960
C	2.517827	-3.066134	-3.509627				

E-**3aa**

Charge = 0 Multiplicity = 1

G_{sol} = -953.373189 Hartree

Zero-point correction = 0.230367 Hartree

Thermal correction to Energy = 0.247129 Hartree

Thermal correction to Enthalpy = 0.248073 Hartree

Thermal correction to Gibbs Free Energy = 0.182394 Hartree

C	-5.302347	1.112721	-0.192042	C	2.842378	-1.948288	0.087604
C	-3.912105	1.042144	-0.173398	F	3.452635	-1.951295	-1.131251
C	-3.265334	-0.204398	-0.049013	F	3.540487	-1.102906	0.871116
C	-4.046900	-1.373056	0.055233	F	3.001134	-3.192572	0.594200
C	-5.436583	-1.292434	0.034483	C	1.498113	0.914139	-0.000586
C	-6.068304	-0.051799	-0.088564	C	2.615098	1.155068	-0.815554
H	-5.790430	2.078603	-0.288769	C	1.002641	1.958278	0.797062
H	-3.312247	1.943174	-0.256066	C	3.231183	2.405728	-0.815510
H	-3.551323	-2.334103	0.151556	H	2.994258	0.367354	-1.456421
H	-6.029033	-2.199622	0.114989	C	1.628169	3.203442	0.804373
H	-7.153074	0.007271	-0.104078	H	0.127589	1.785076	1.416398
C	-1.842894	-0.280837	-0.030005	C	2.744484	3.431740	-0.003358
C	-0.628338	-0.353432	-0.019073	H	4.091253	2.578650	-1.456559
C	0.798184	-0.405933	-0.004431	H	1.240466	3.997023	1.437391
C	1.384162	-1.629014	-0.003635	H	3.227589	4.405097	-0.004799
H	0.757000	-2.511984	-0.061750				

***Z*-3aa**

Charge = 0 Multiplicity = 1

G_{sol} = -953.378799 Hartree

Zero-point correction = 0.230119 Hartree

Thermal correction to Energy = 0.247009 Hartree

Thermal correction to Enthalpy = 0.247953 Hartree

Thermal correction to Gibbs Free Energy = 0.181187 Hartree

C	4.395846	-2.351079	0.273300	C	4.887669	-0.015963	-0.135225
C	3.031823	-2.071240	0.265145	C	5.325941	-1.327010	0.073758
C	2.581690	-0.753121	0.055244	H	4.735133	-3.370290	0.436374
C	3.526589	0.274464	-0.145489	H	2.304802	-2.862239	0.421652

H	3.171184	1.287259	-0.308150	C	-2.389825	-0.677847	-0.013371
H	5.609144	0.781380	-0.290579	C	-2.135139	-1.955770	-0.536116
H	6.389342	-1.549966	0.081500	C	-3.664335	-0.408197	0.512576
C	1.193992	-0.435935	0.040353	C	-3.134495	-2.927392	-0.558165
C	0.032053	-0.078934	0.011625	H	-1.149566	-2.178704	-0.932976
C	-1.321574	0.362470	-0.024451	C	-4.661143	-1.381553	0.493595
C	-1.616500	1.684096	-0.083644	H	-3.867863	0.557418	0.965585
H	-2.643068	2.021425	-0.161907	C	-4.401875	-2.643810	-0.045985
C	-0.597518	2.780838	-0.046879	H	-2.921420	-3.907891	-0.975252
F	0.063803	2.839189	1.133222	H	-5.638425	-1.157485	0.912392
F	0.347108	2.665144	-1.010331	H	-5.179087	-3.403011	-0.057262
F	-1.203063	3.977668	-0.223891				

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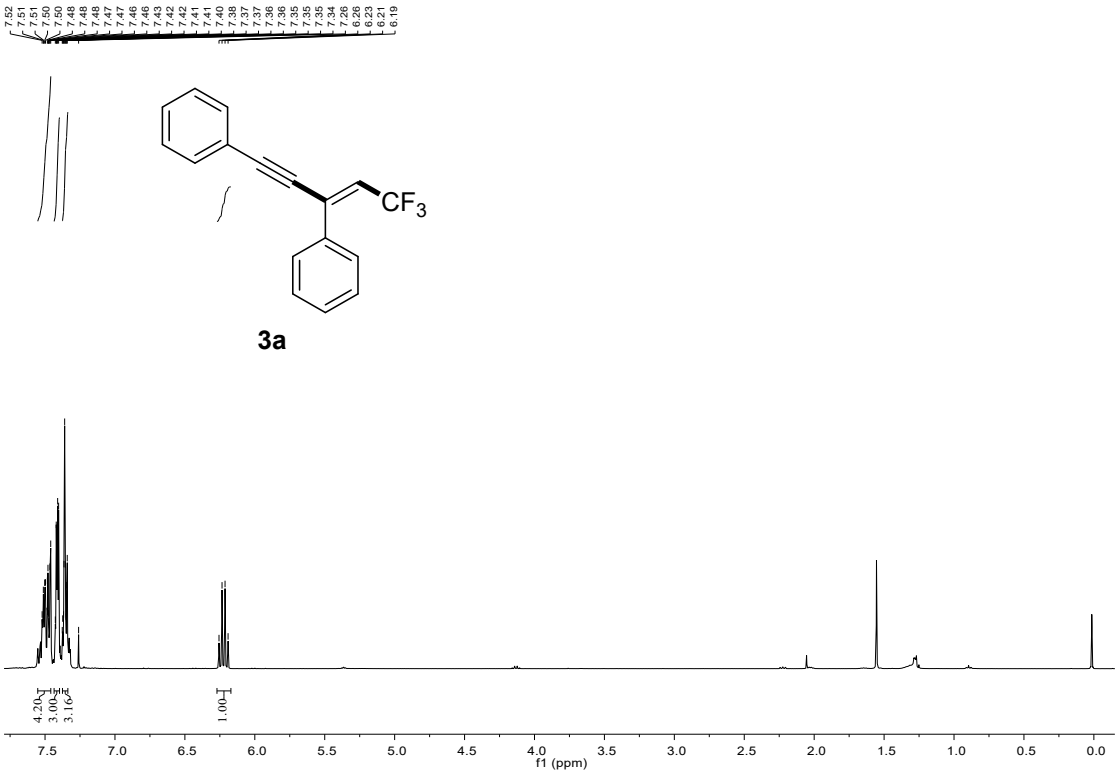
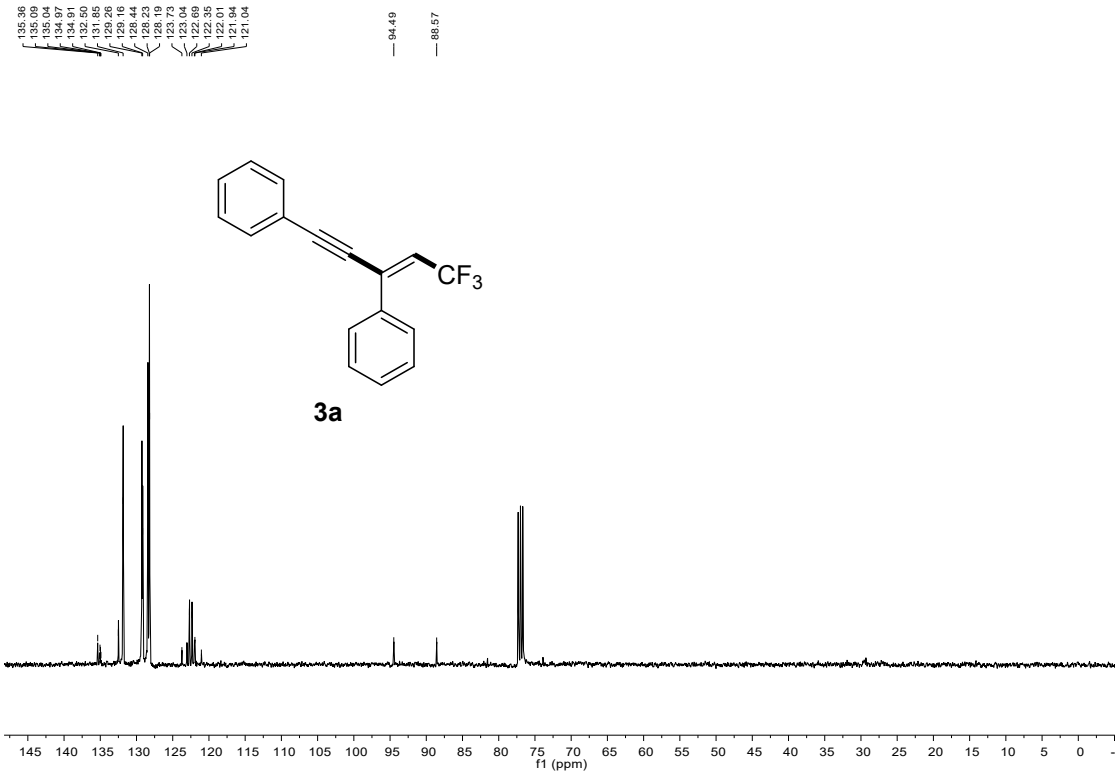
9. Copies of NMR Spectra

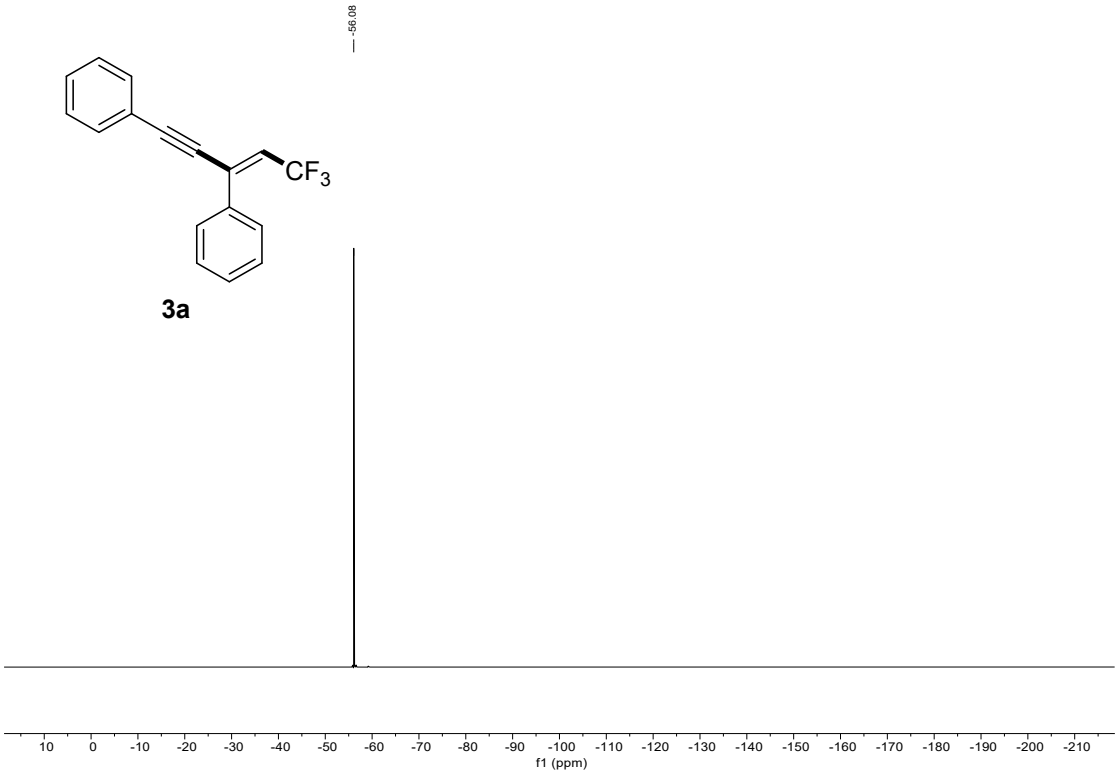
^{1}H NMR Spectrum of 3a



^{13}C NMR Spectrum of 3a



^{19}F NMR Spectrum of 3a



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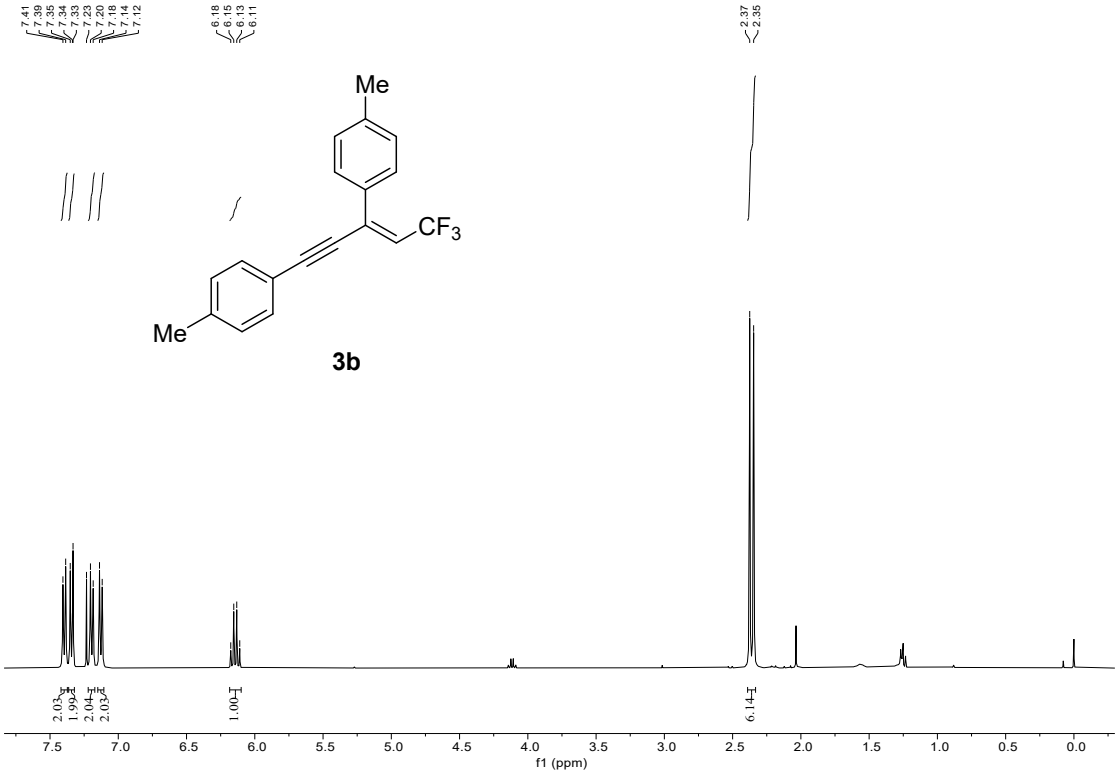

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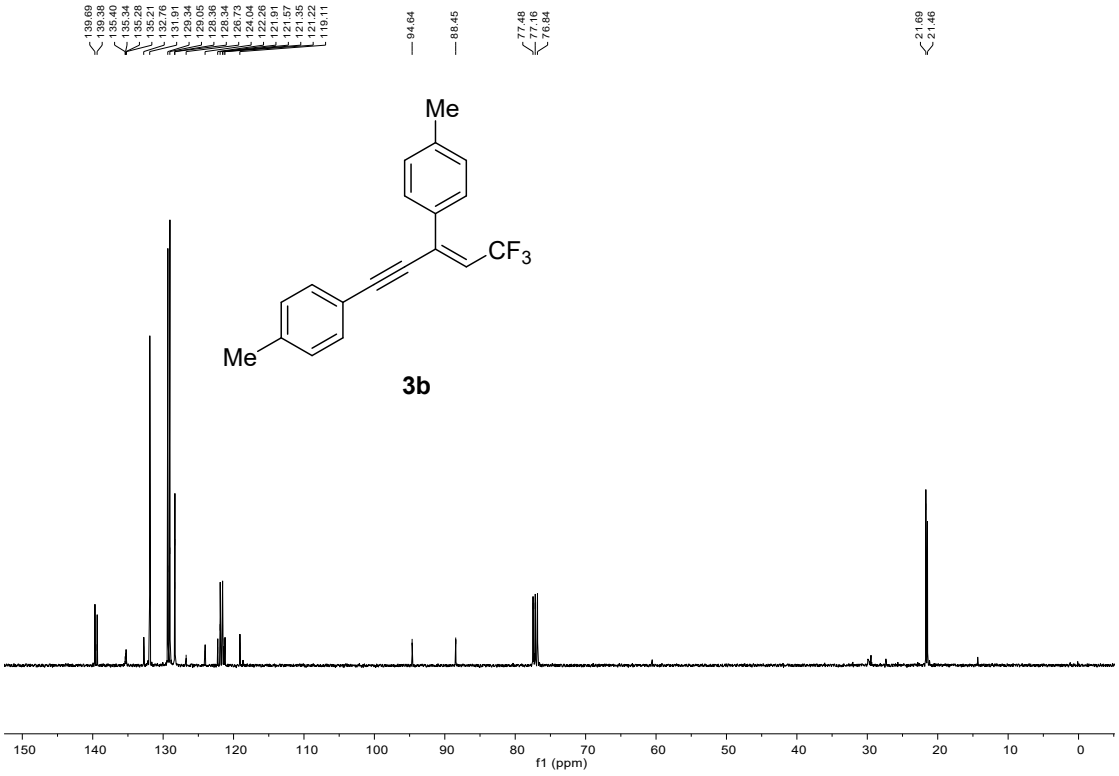

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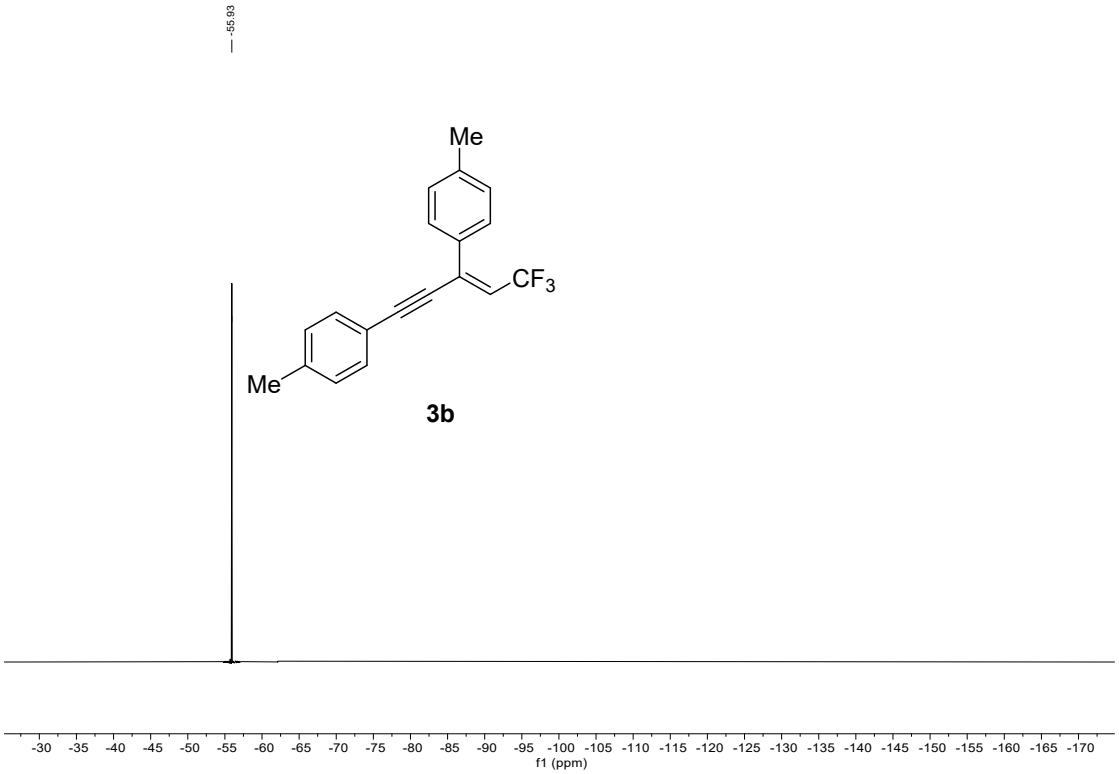

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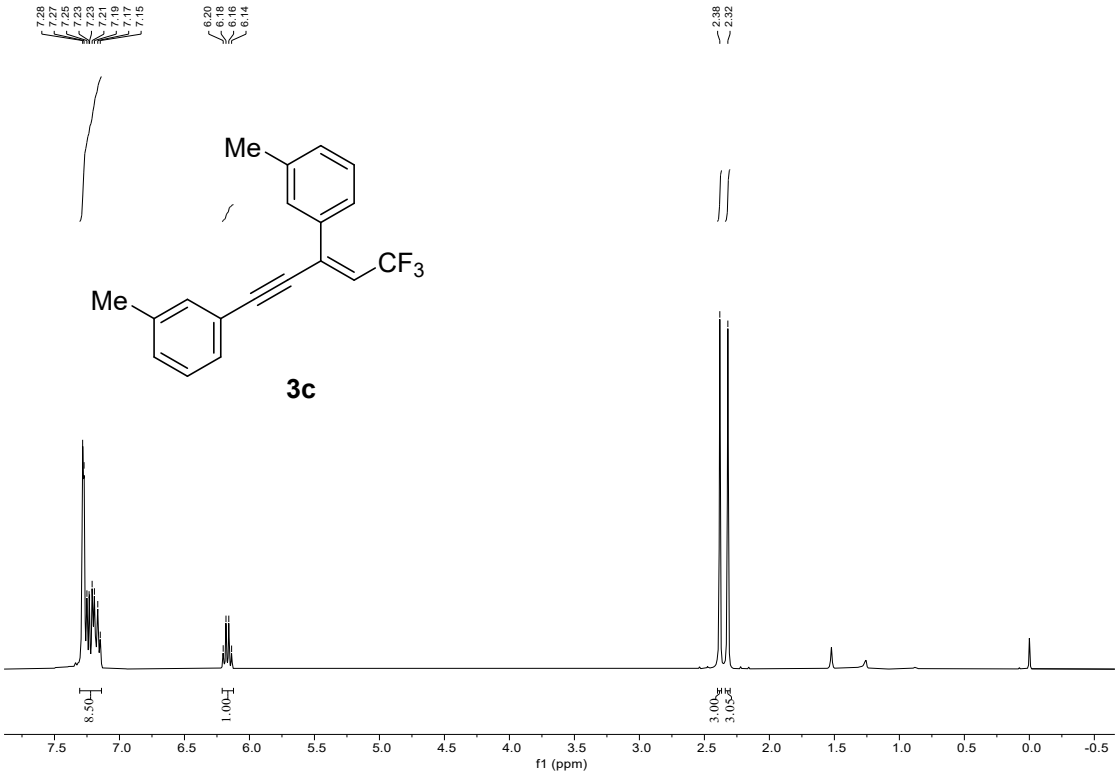

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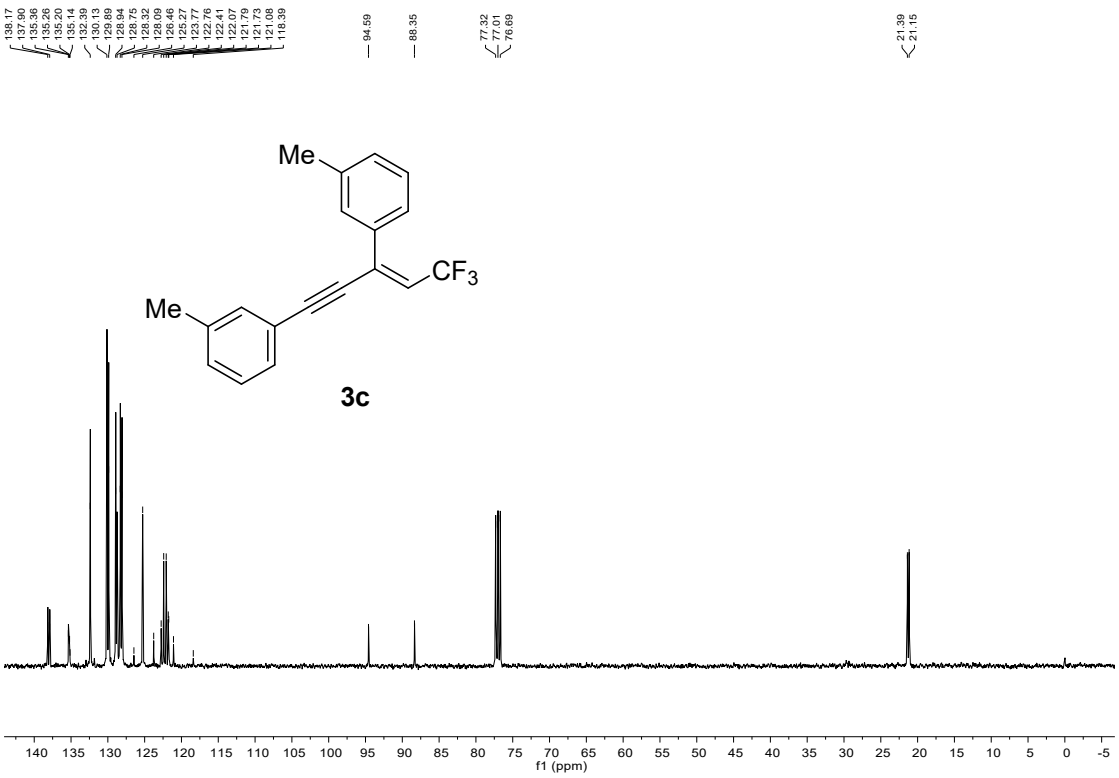
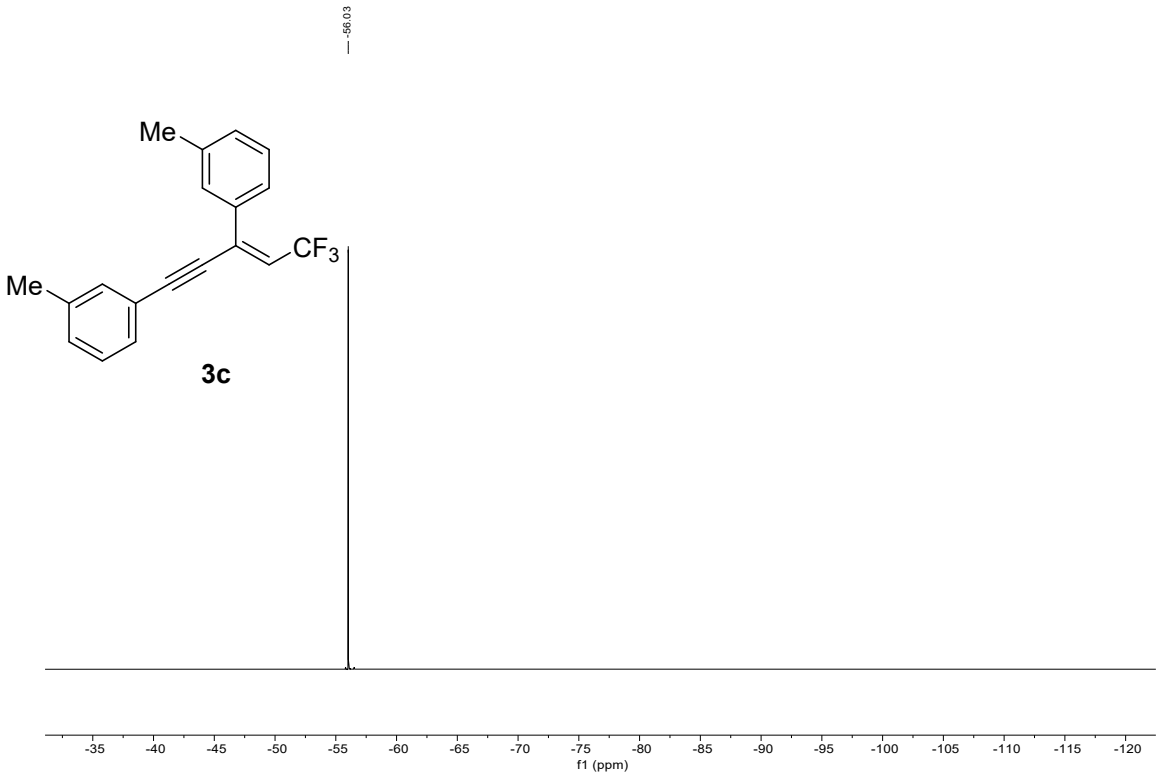


^{19}F NMR Spectrum of 3c



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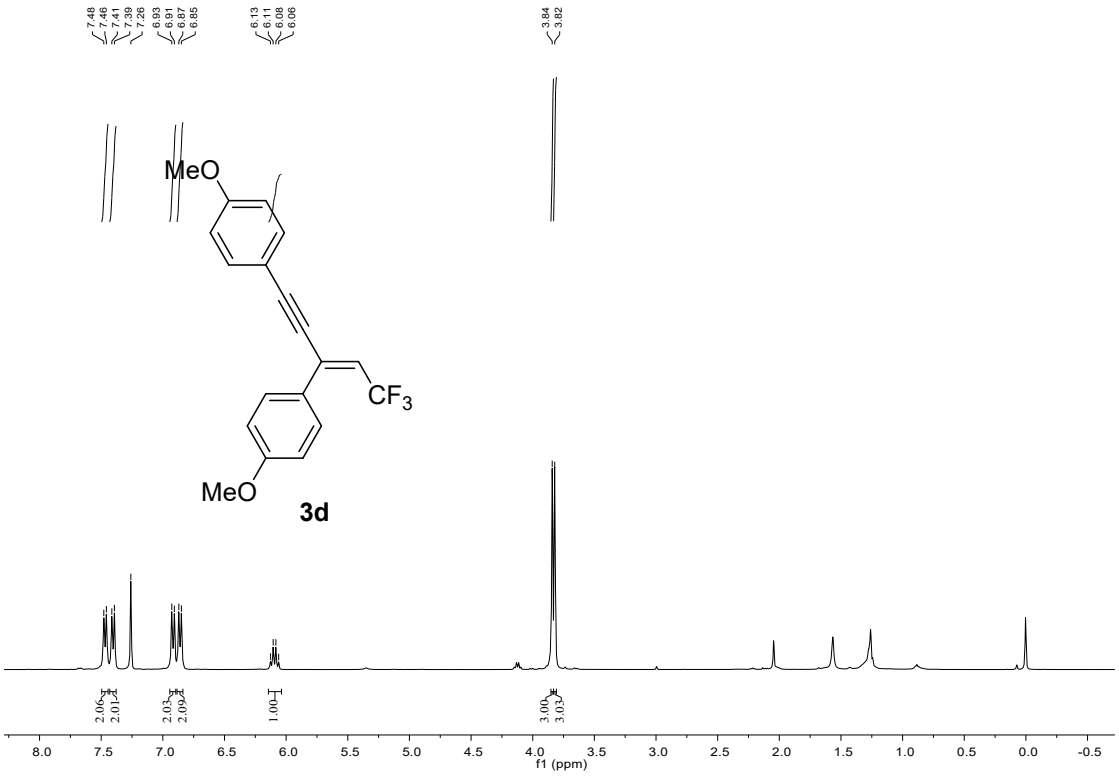

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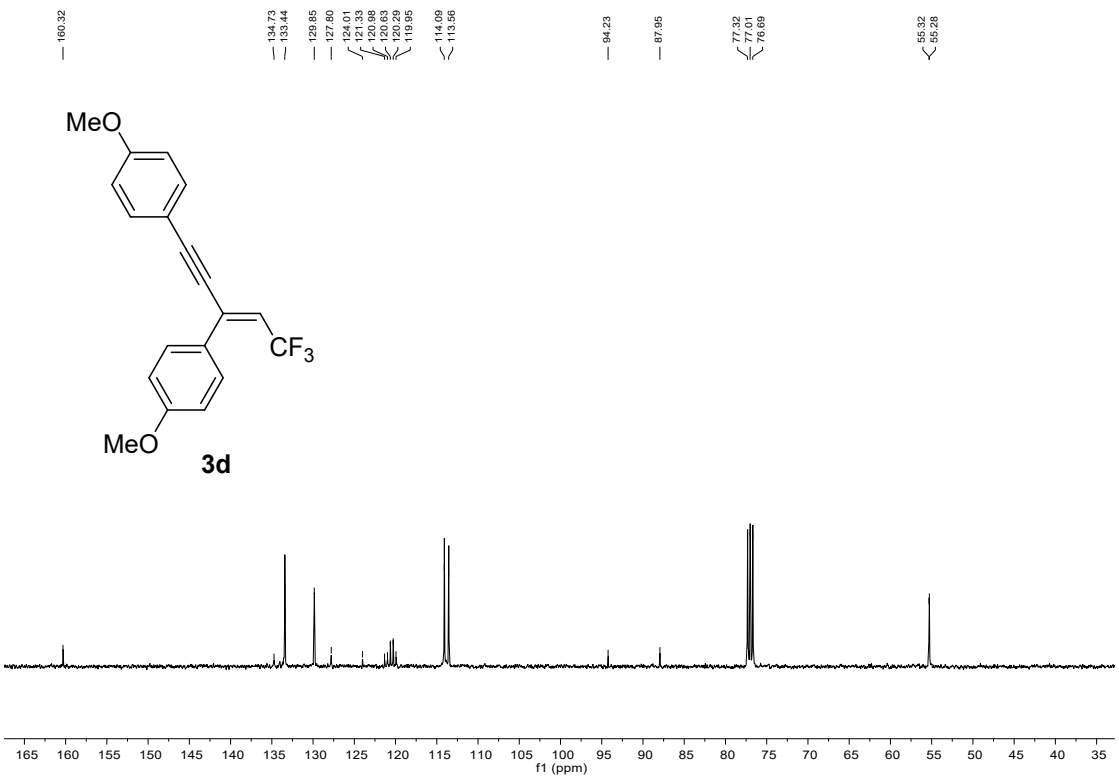
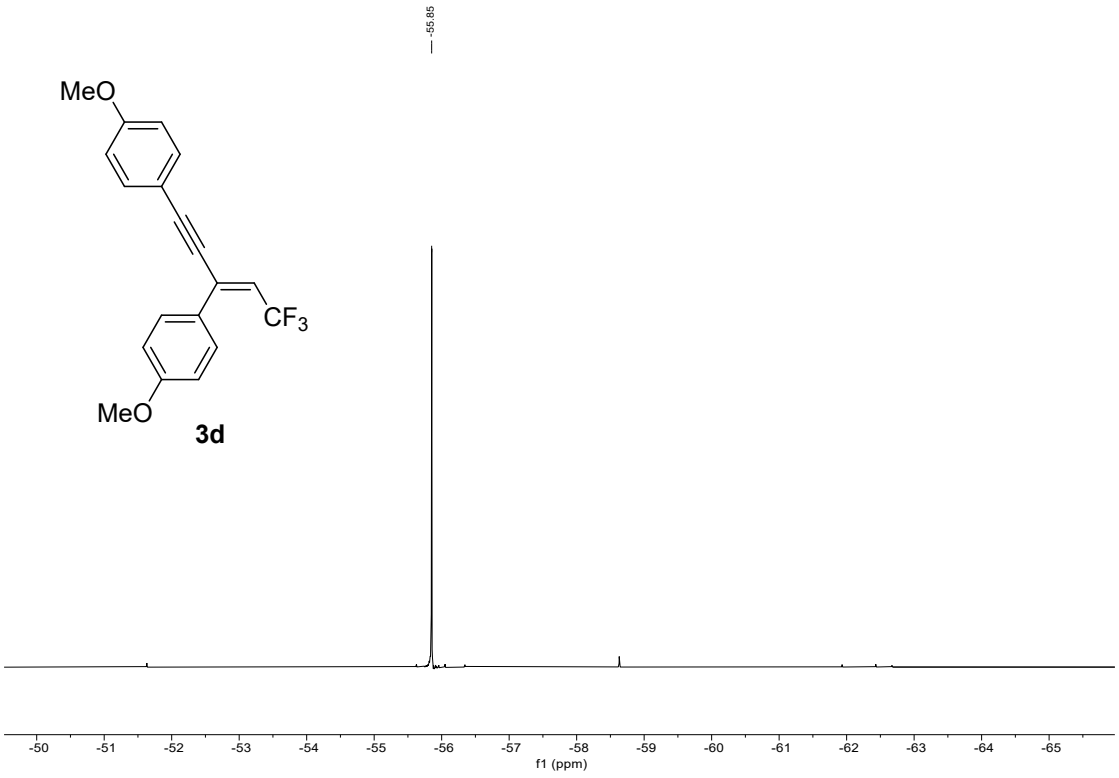


^{19}F NMR Spectrum of 3d



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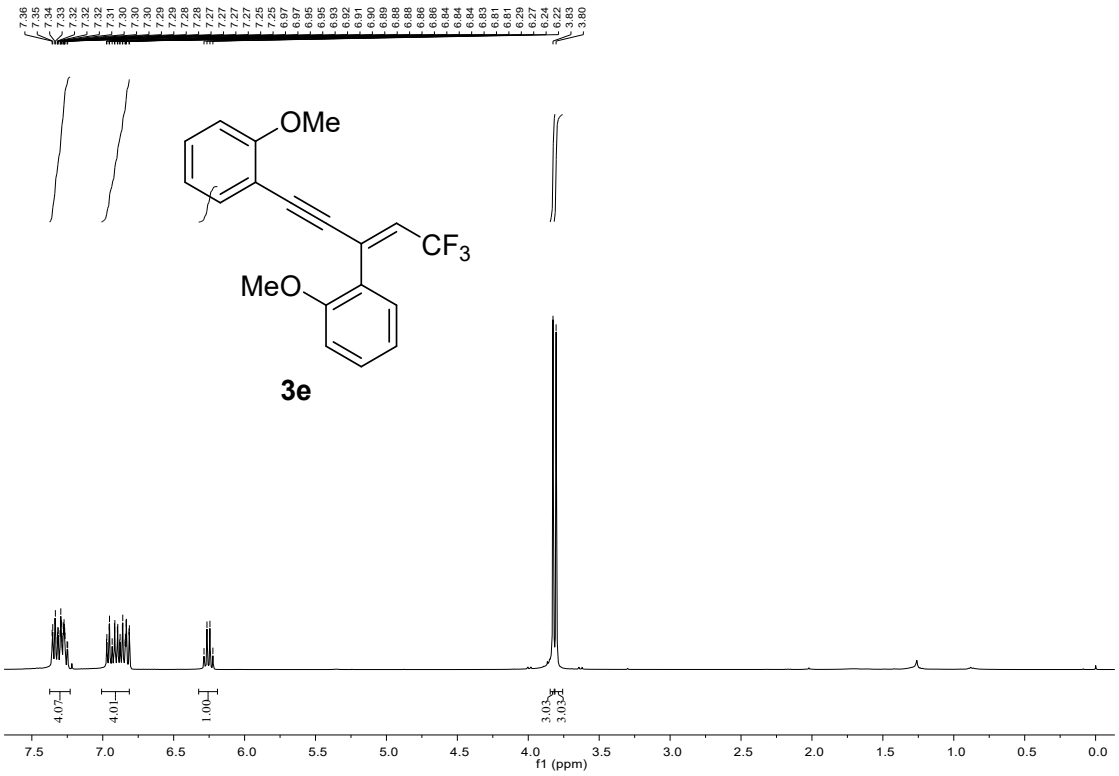

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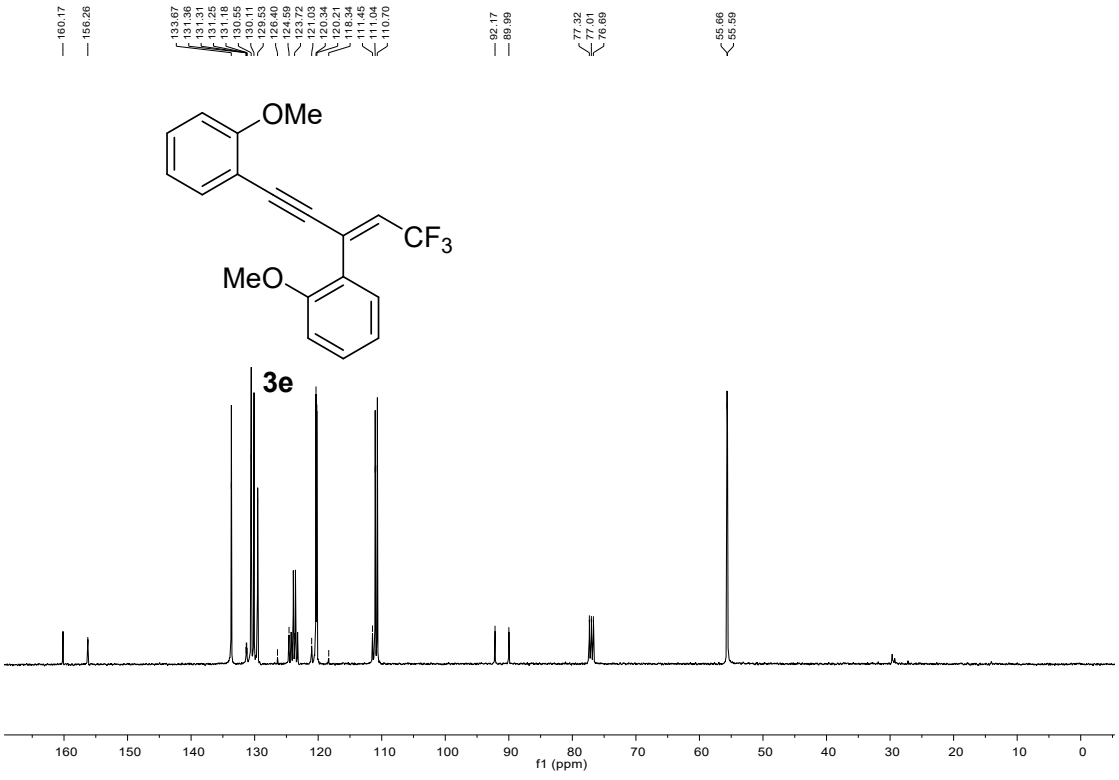
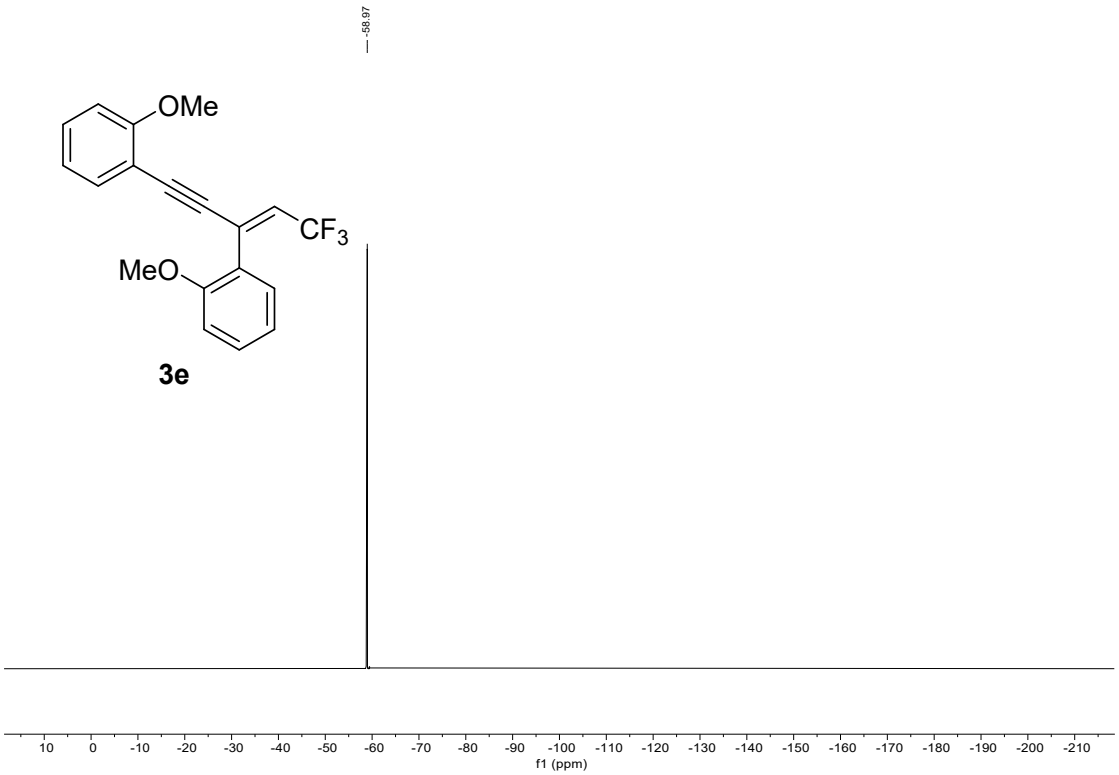
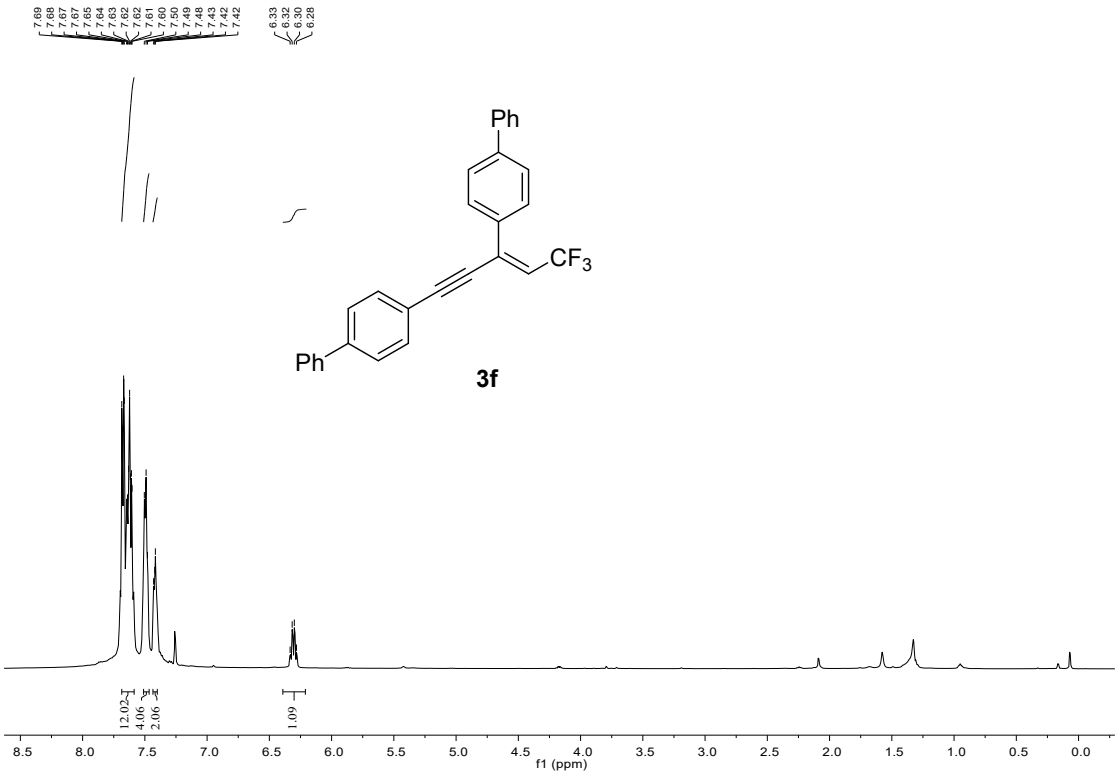


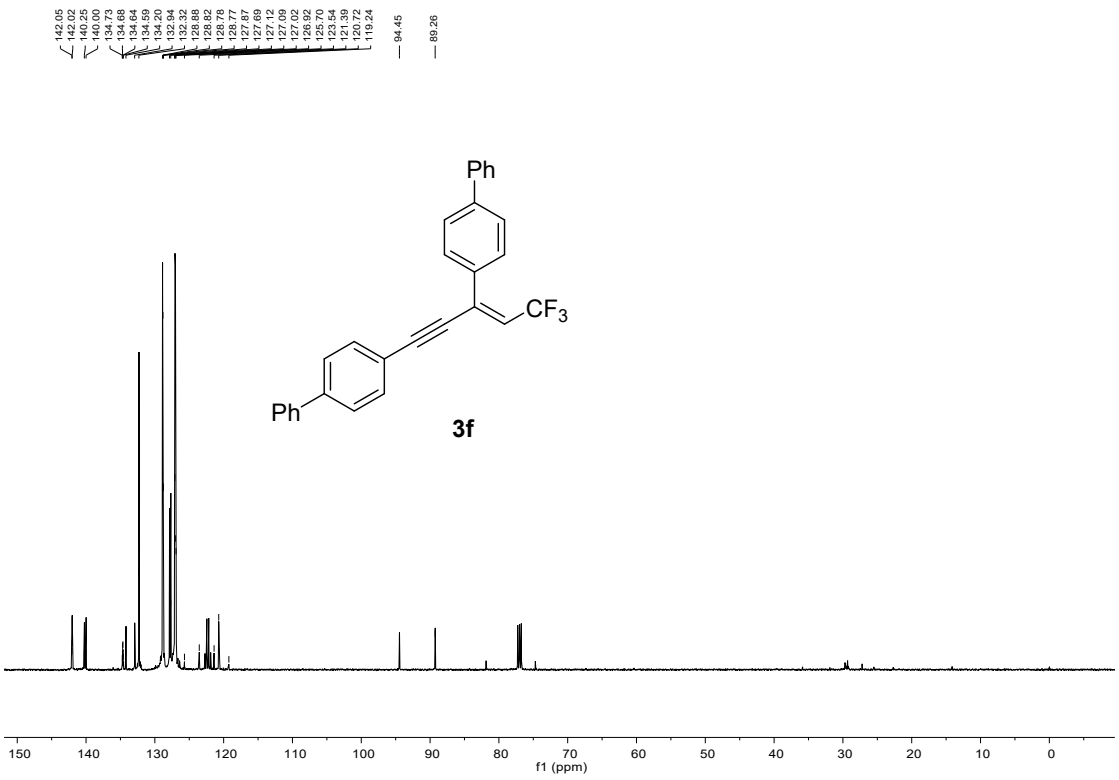
^{19}F NMR Spectrum of 3e



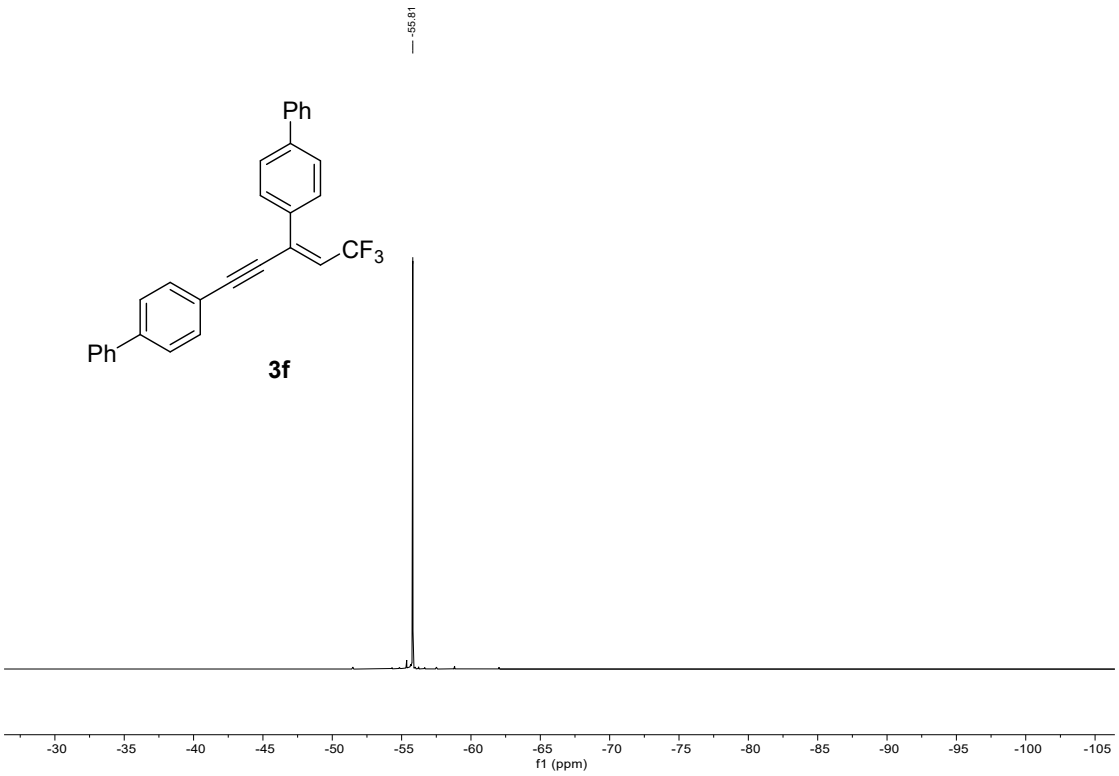
^{1}H NMR Spectrum of 3f



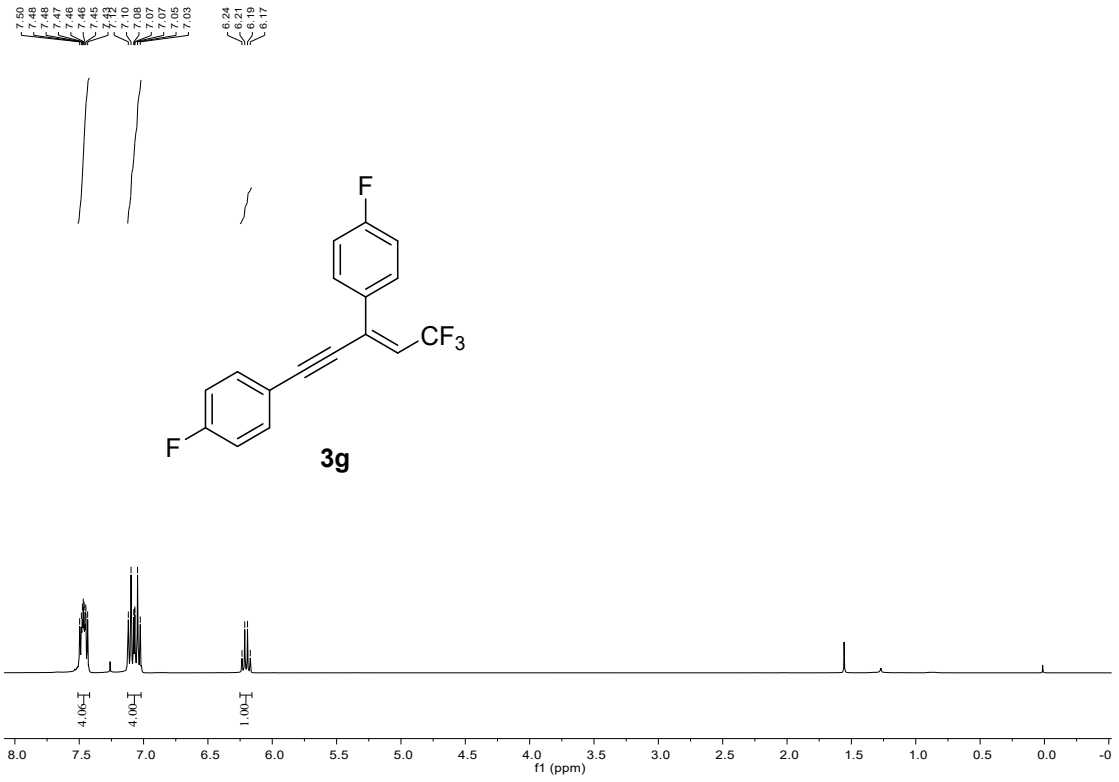
^{13}C NMR Spectrum of 3f



^{19}F NMR Spectrum of 3f



^{1}H NMR Spectrum of 3g



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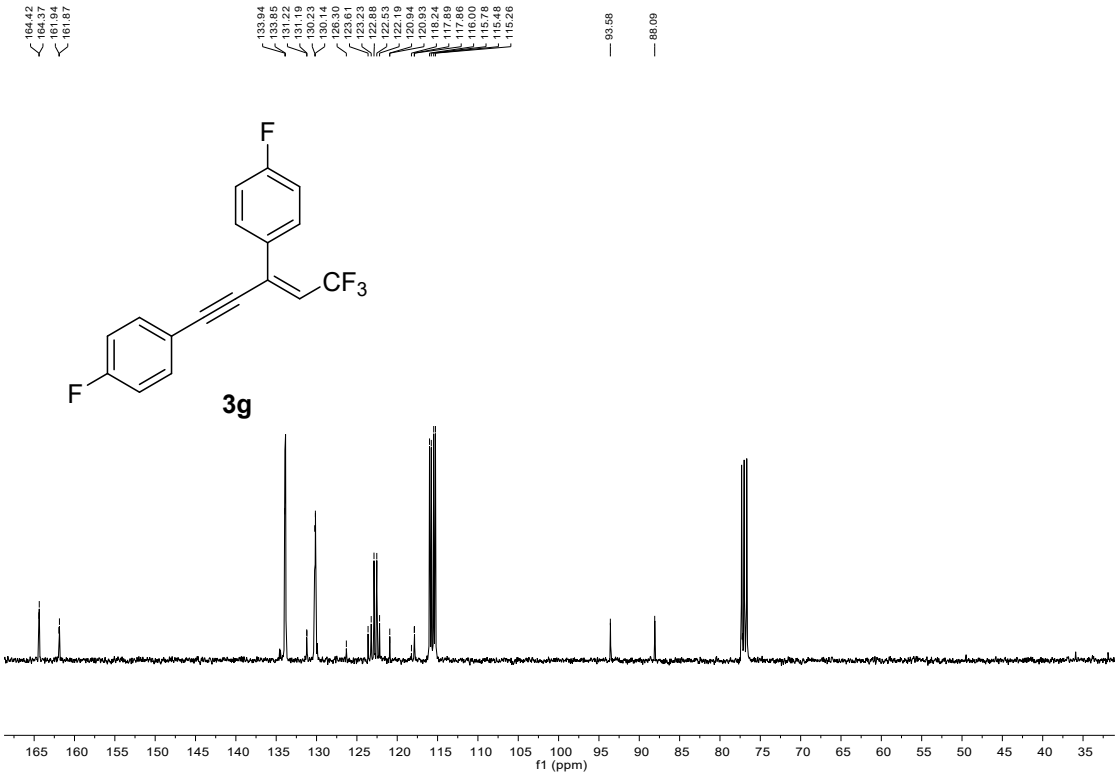

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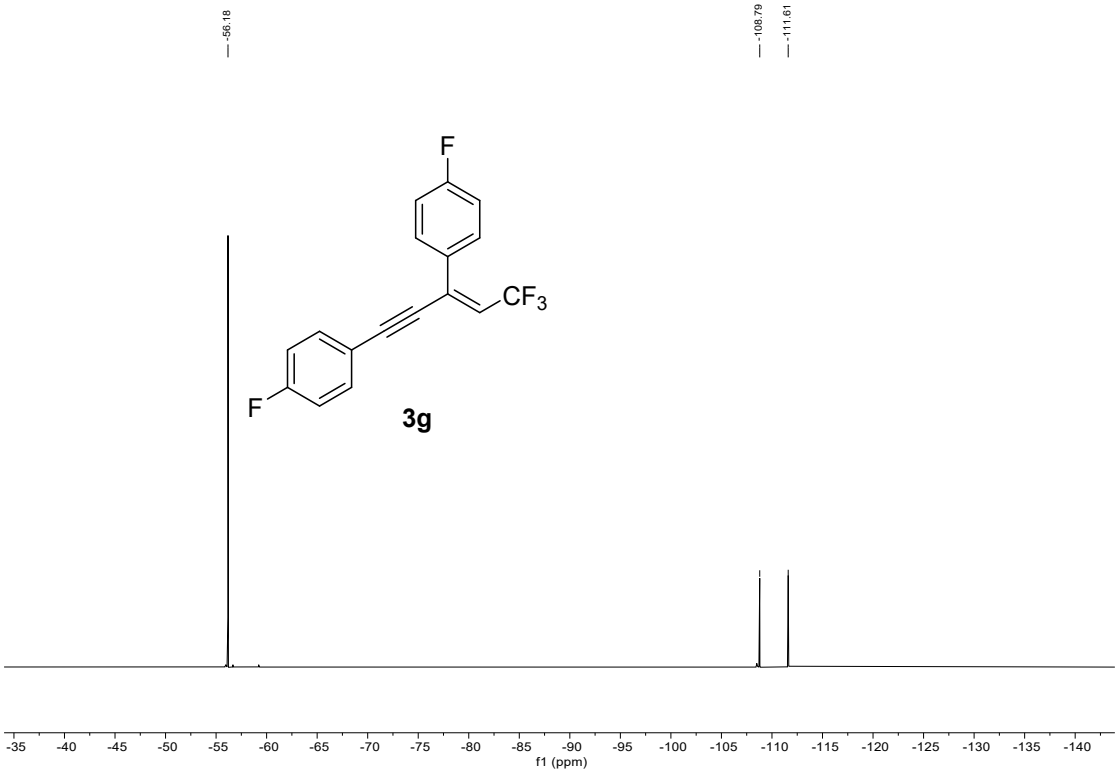

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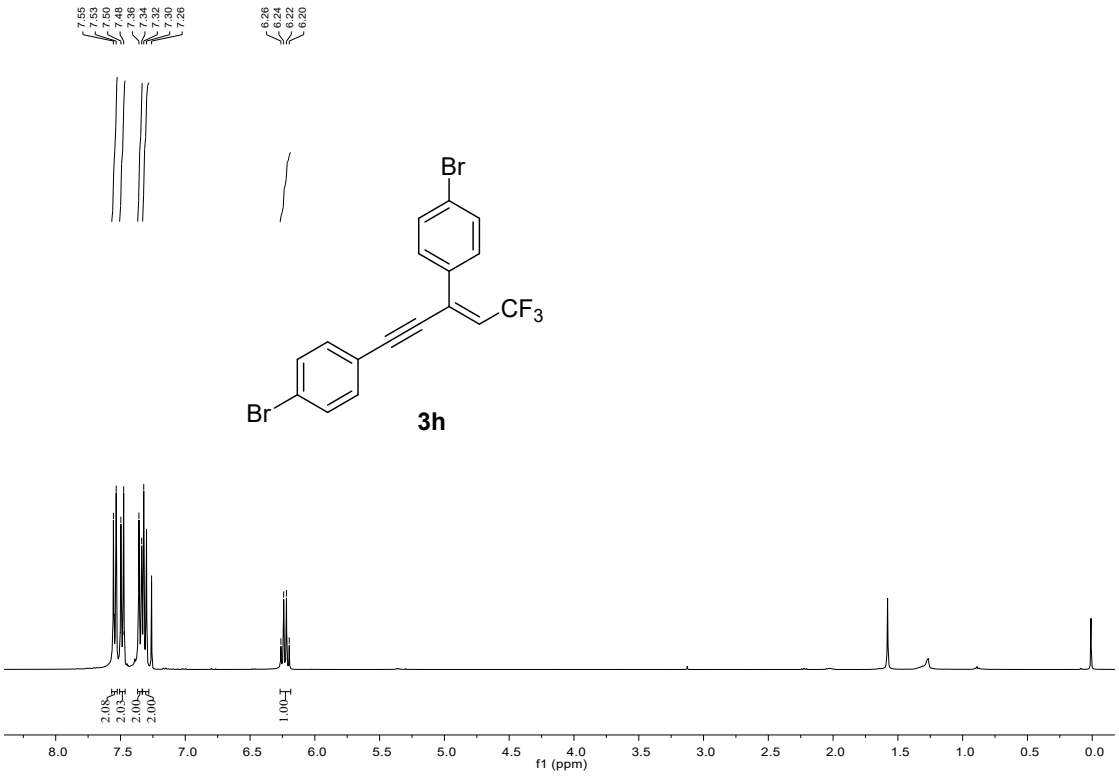

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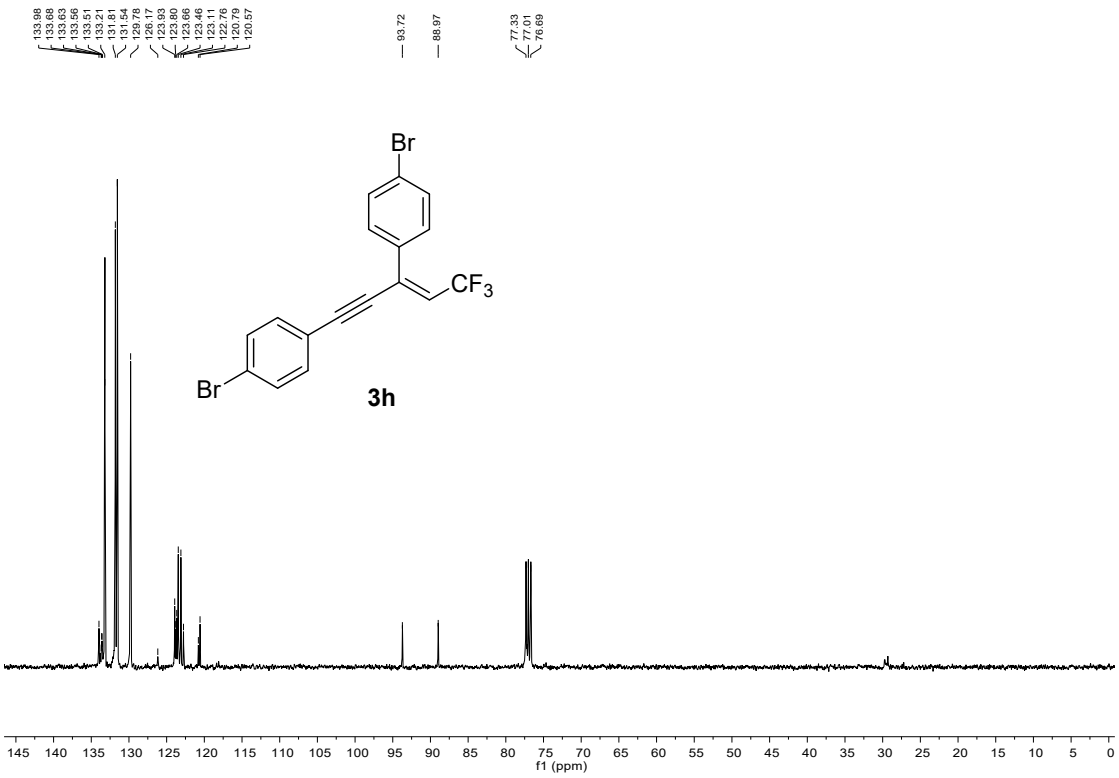

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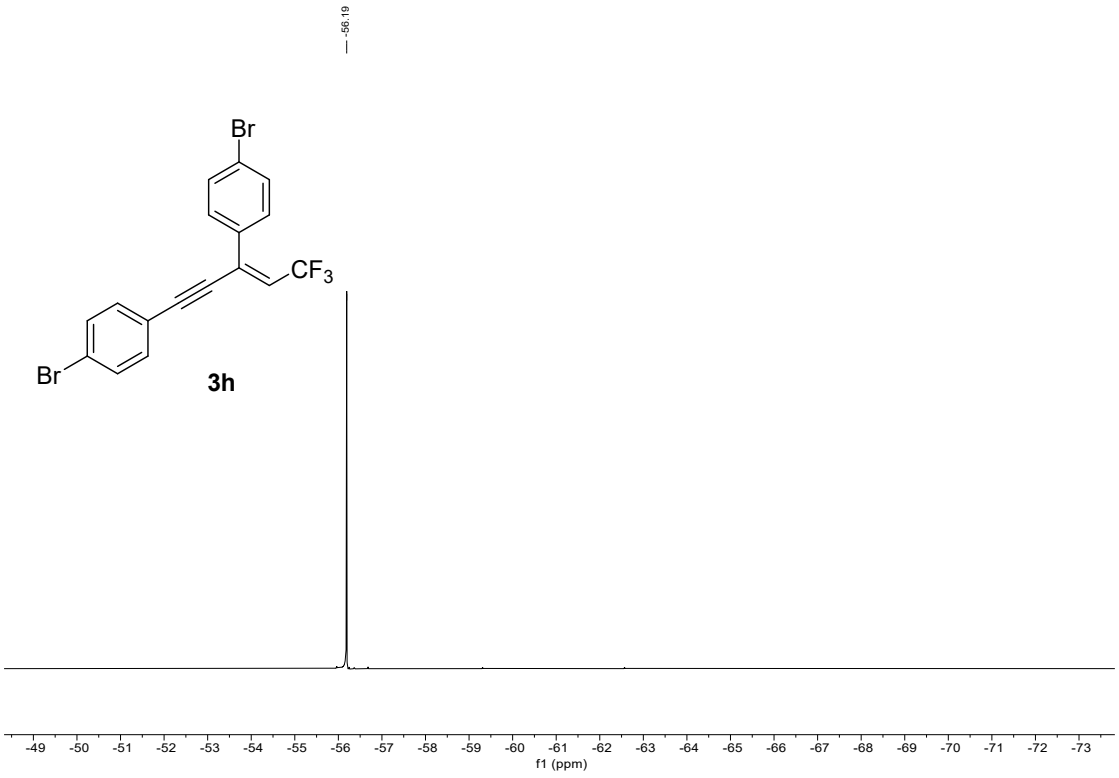
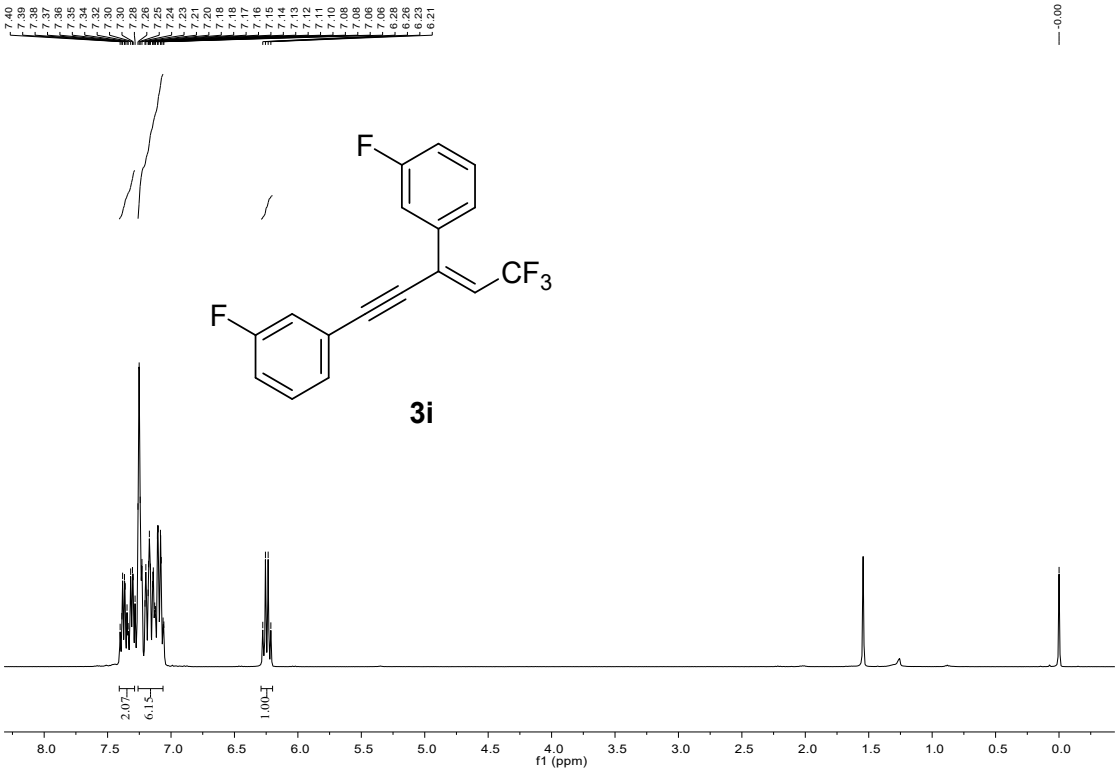
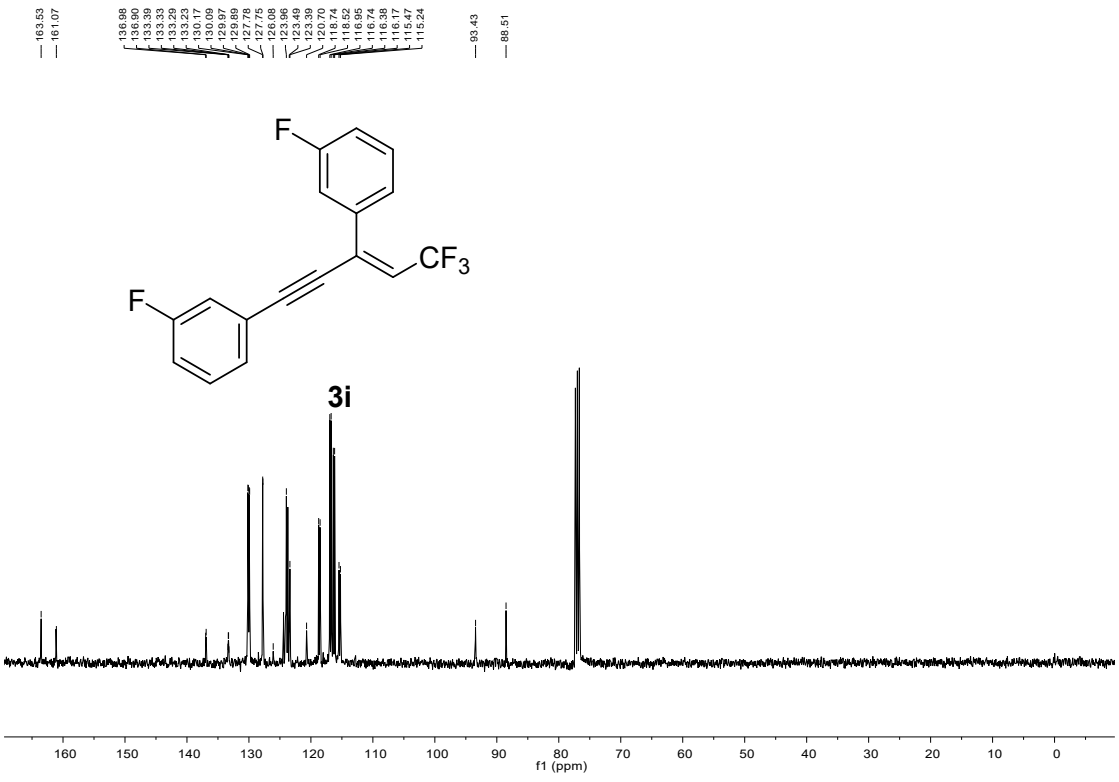


[1] H NMR Spectrum of 3i



[13]C NMR Spectrum of 3i



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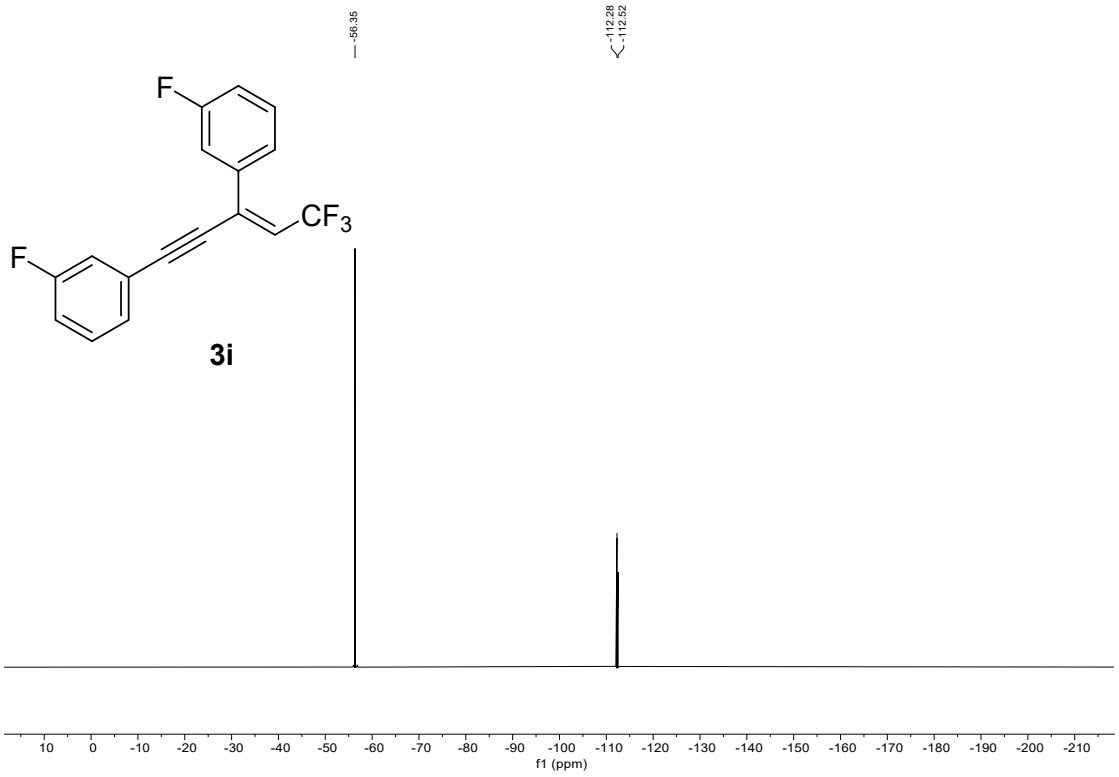
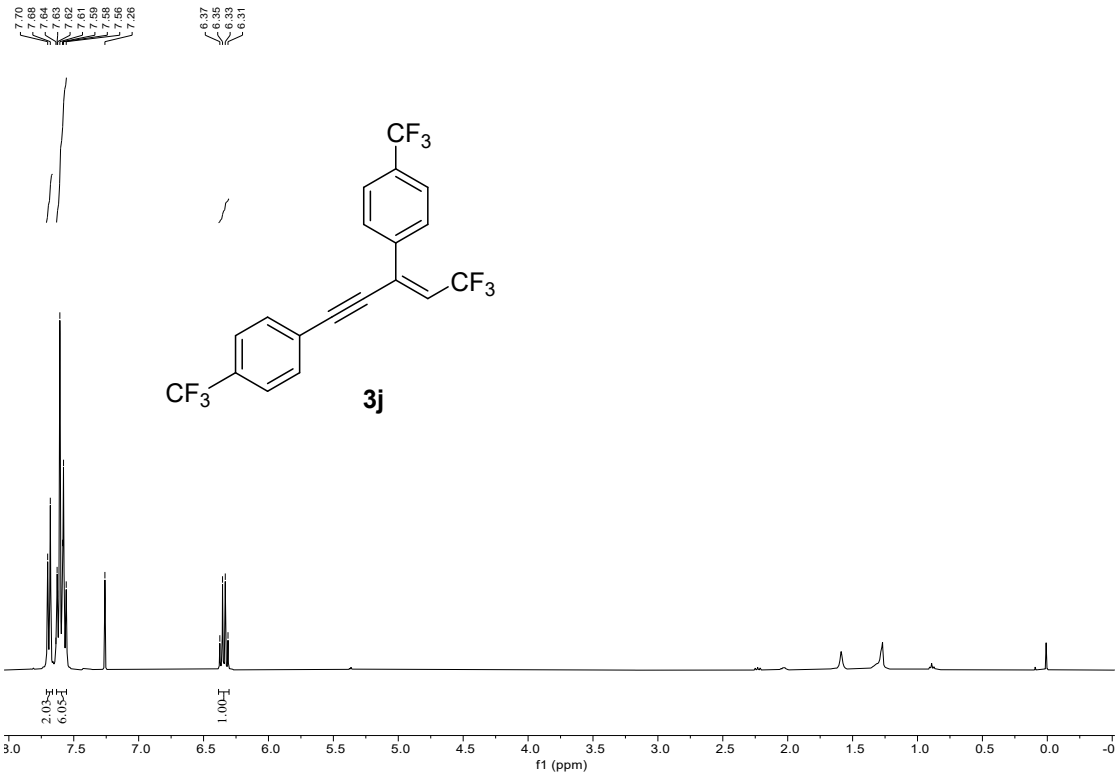


^{1}H NMR Spectrum of 3j



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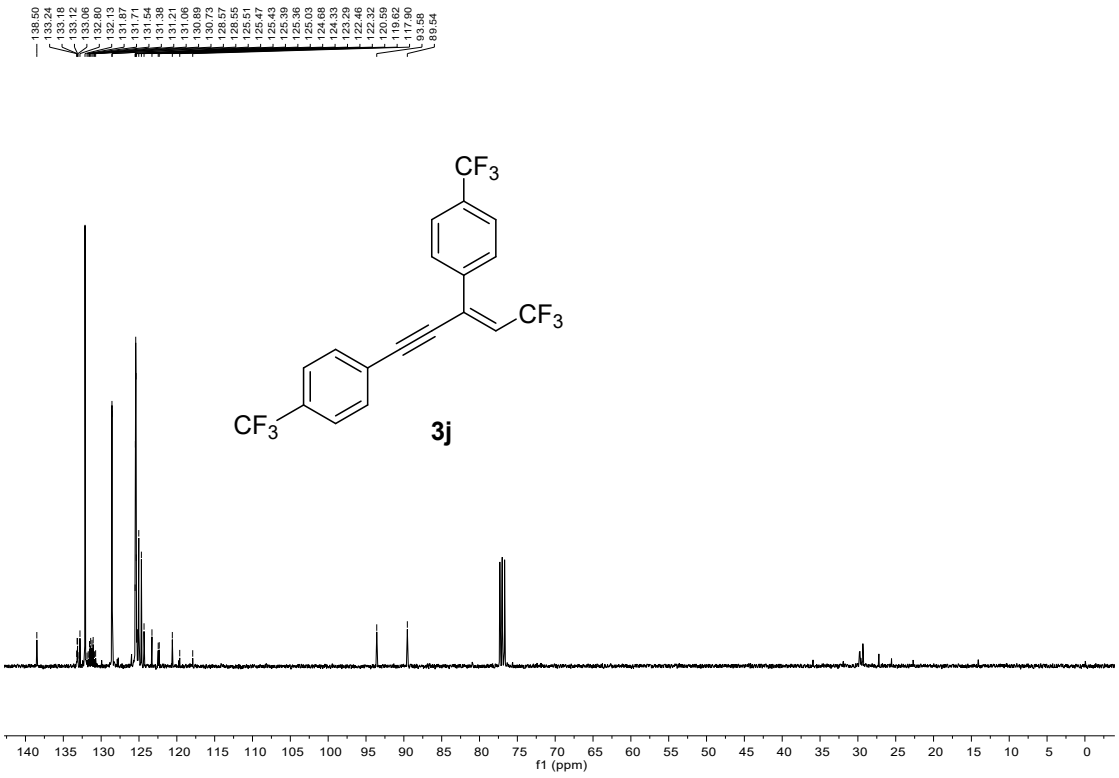
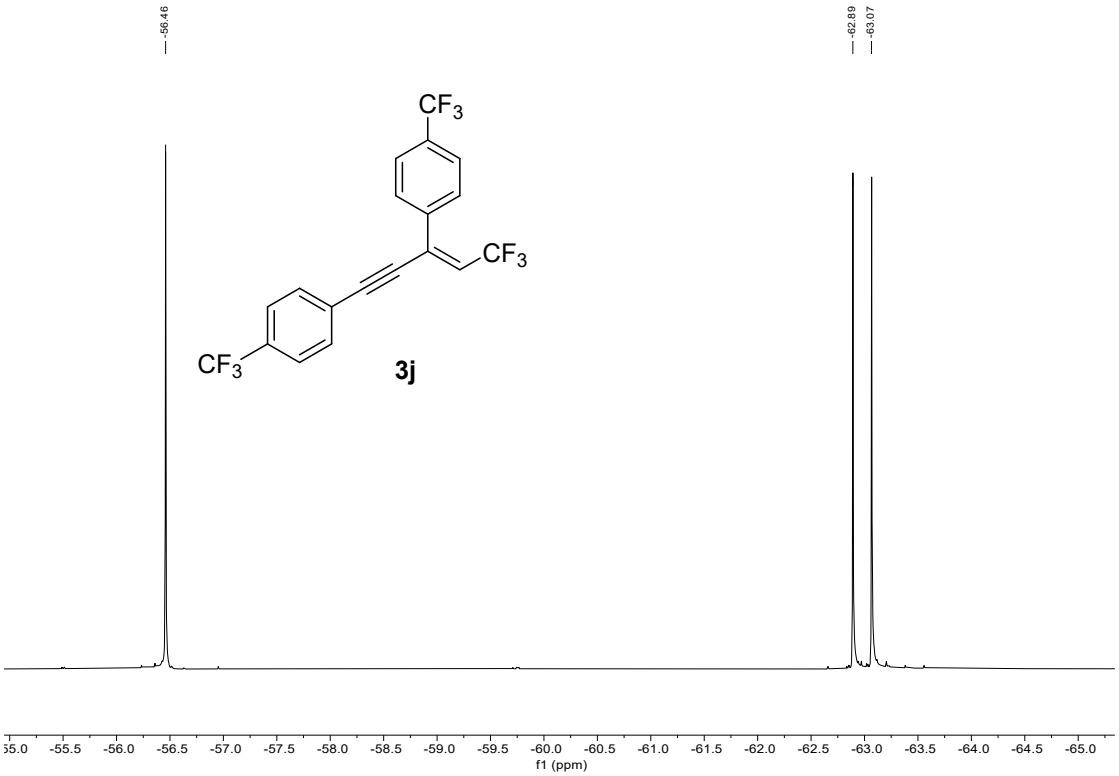


^{19}F NMR Spectrum of 3j



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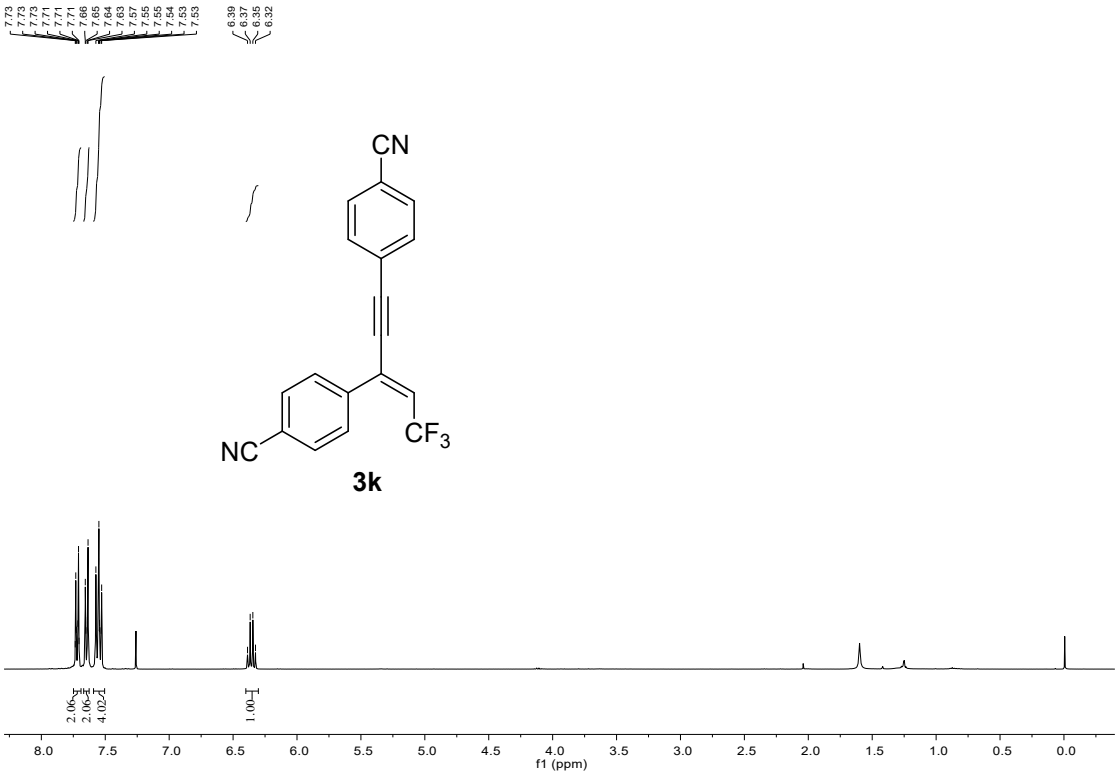
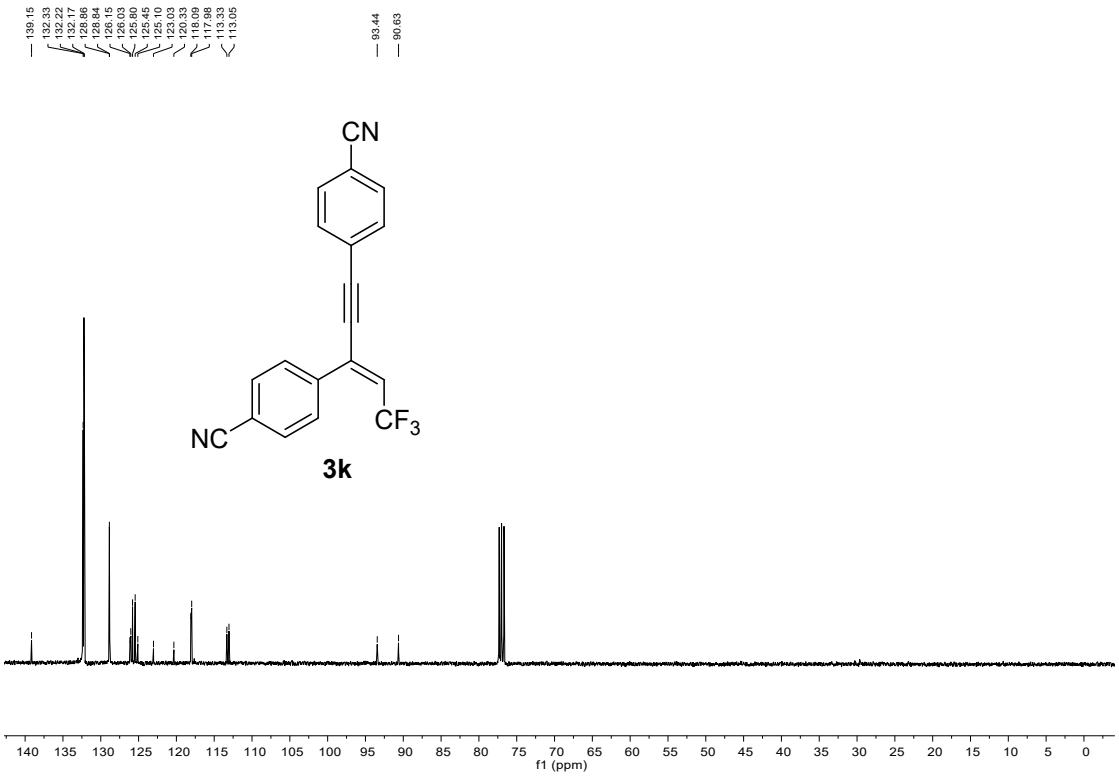


[13]C NMR Spectrum of 3k



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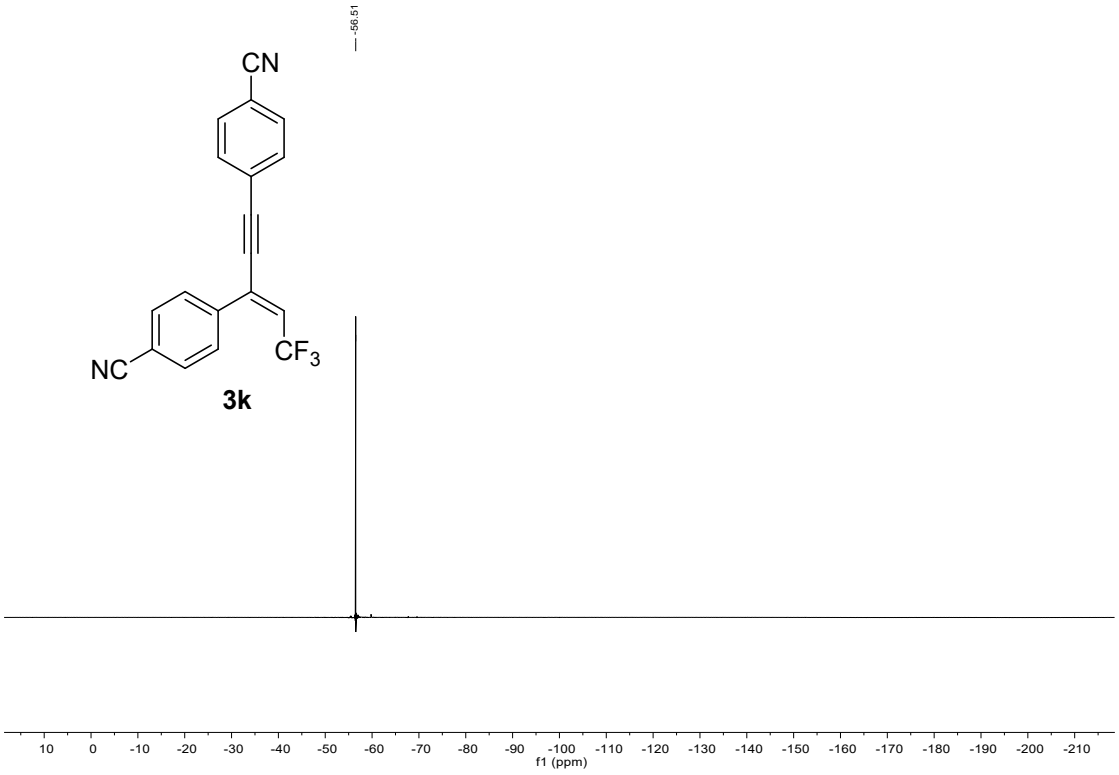

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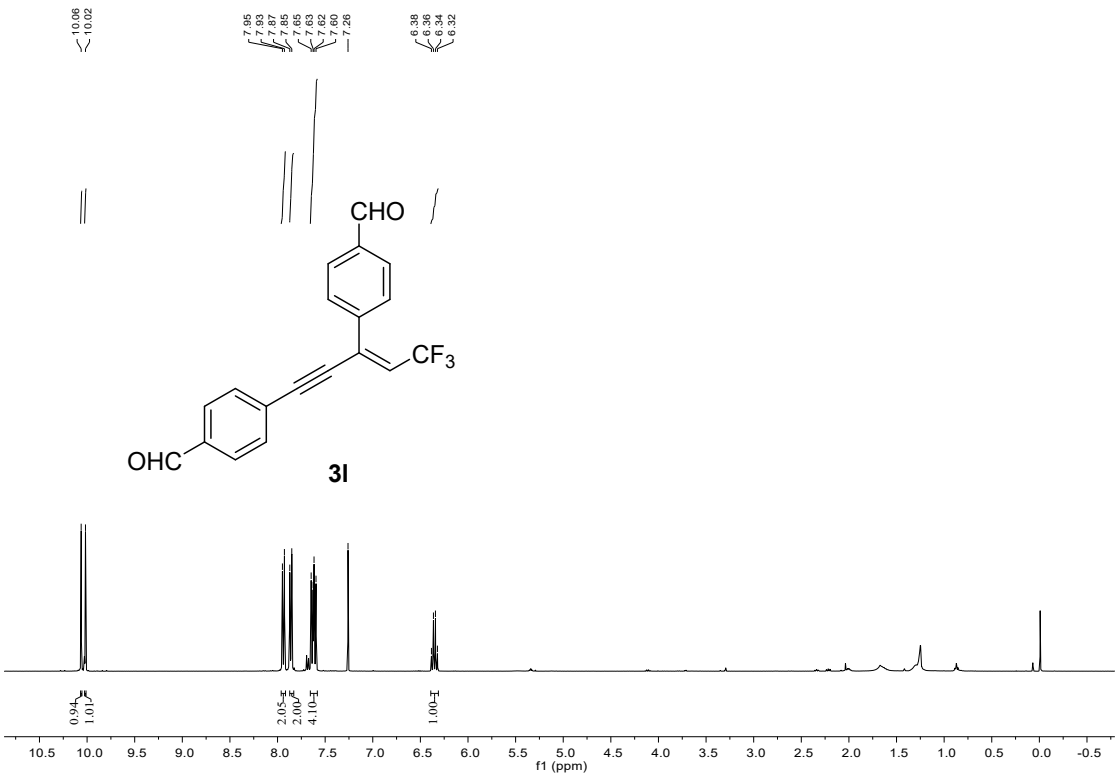

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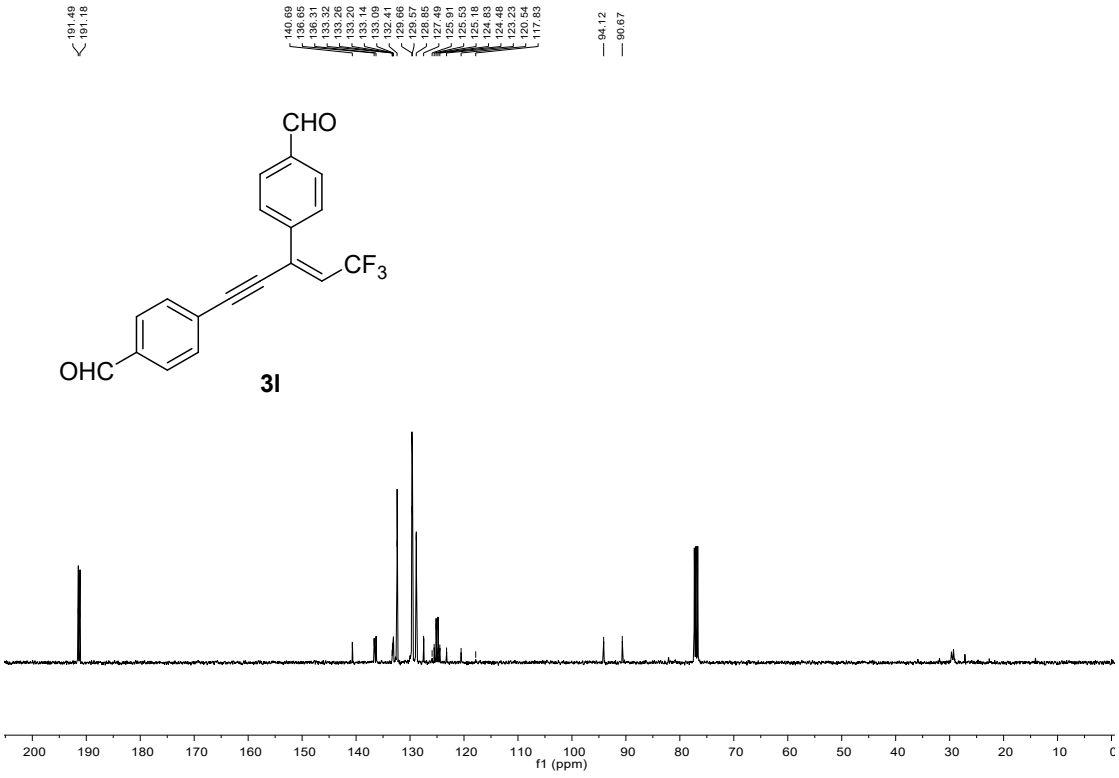

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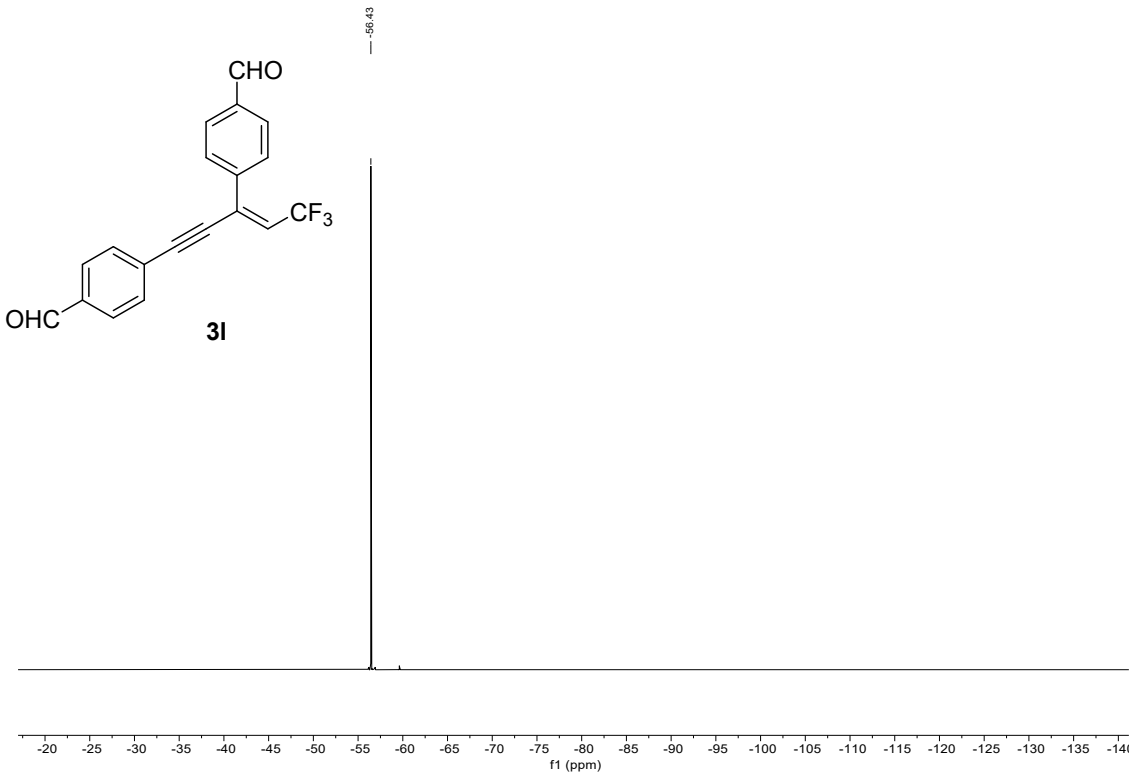

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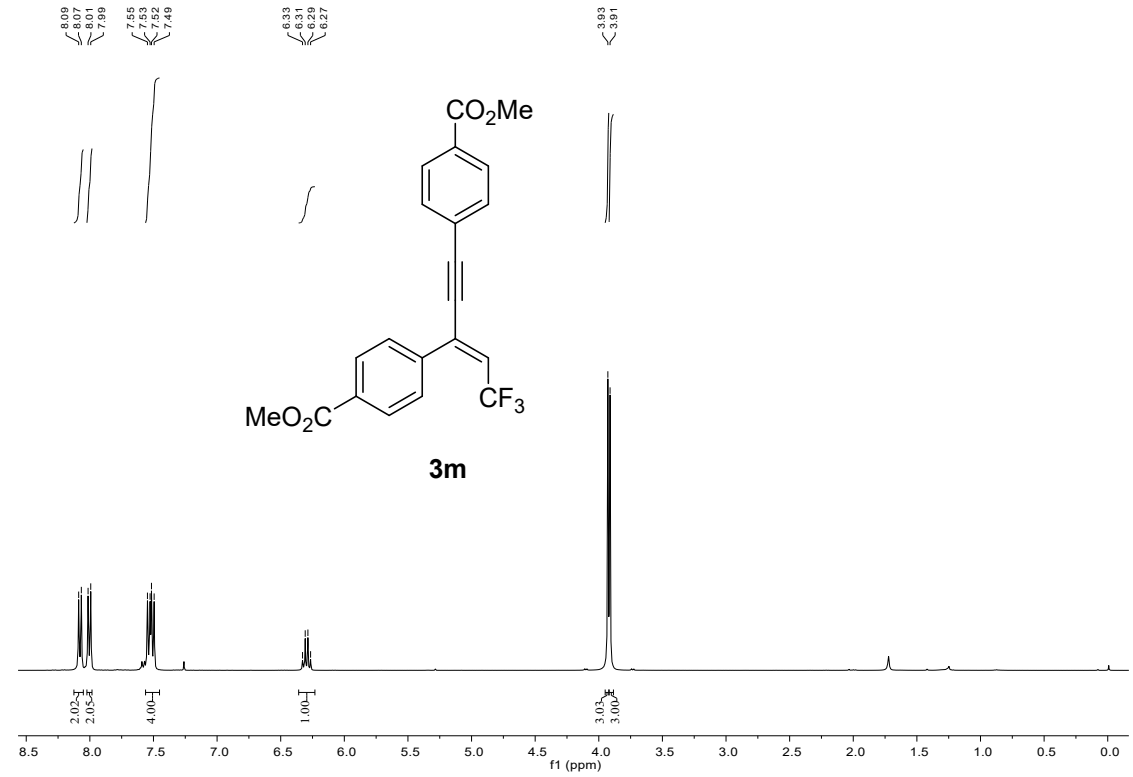
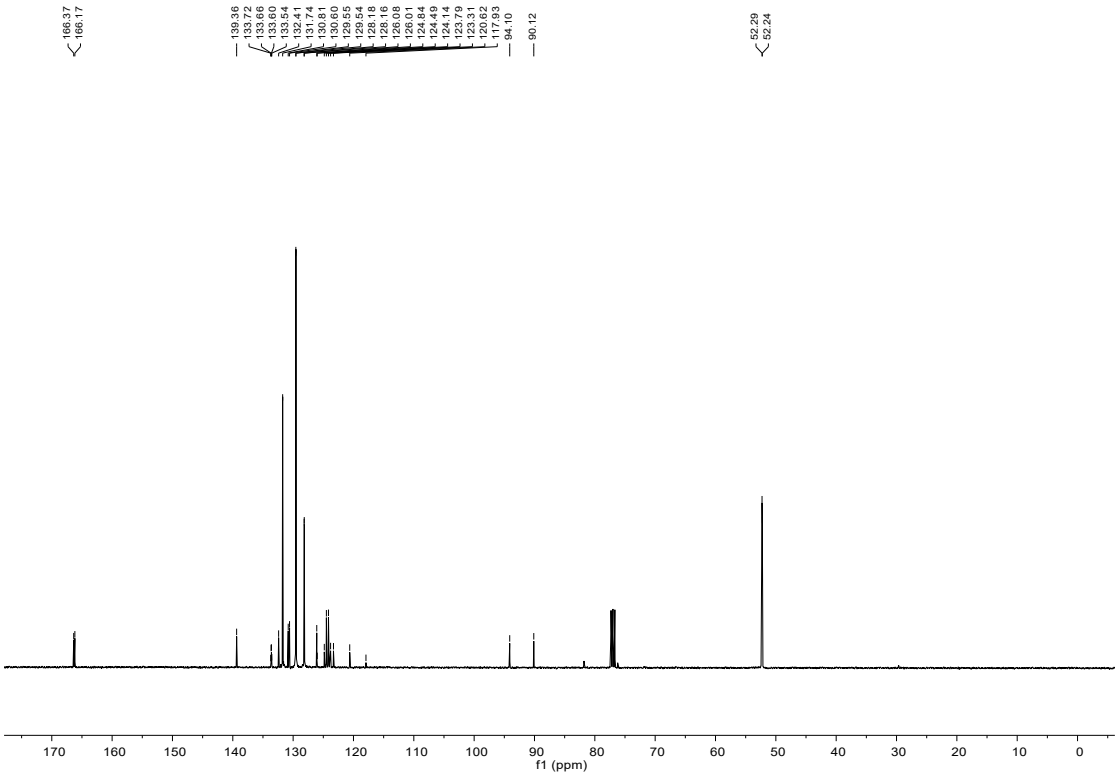
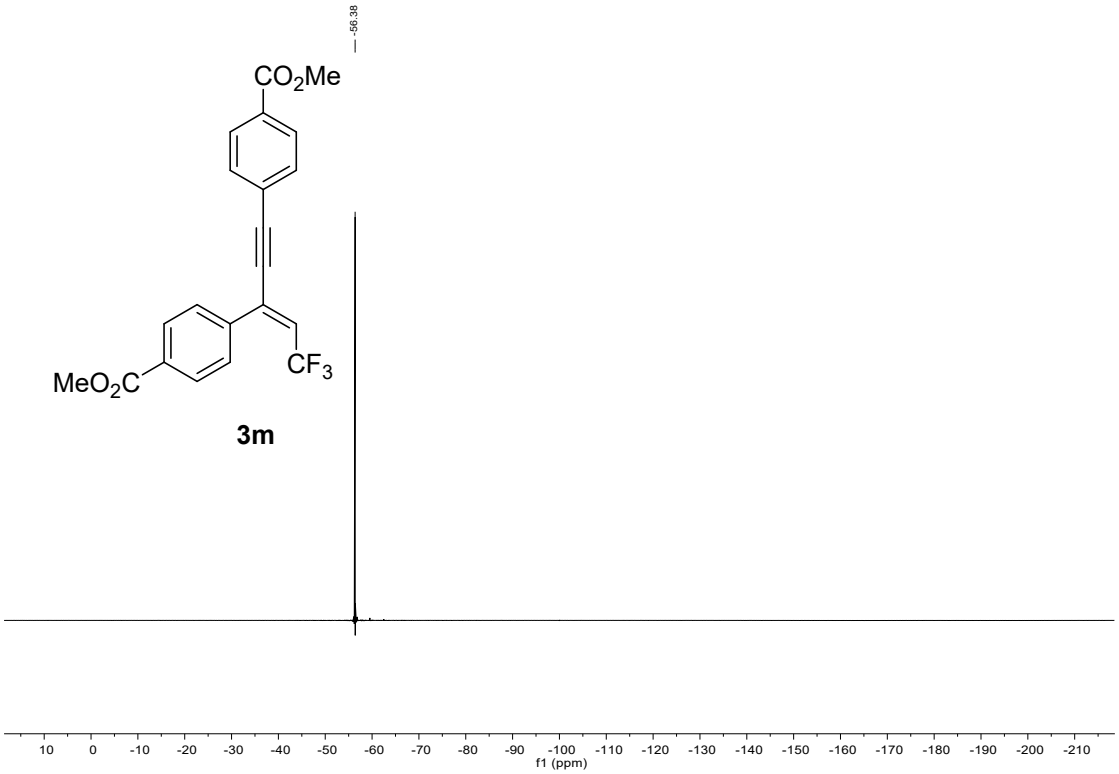


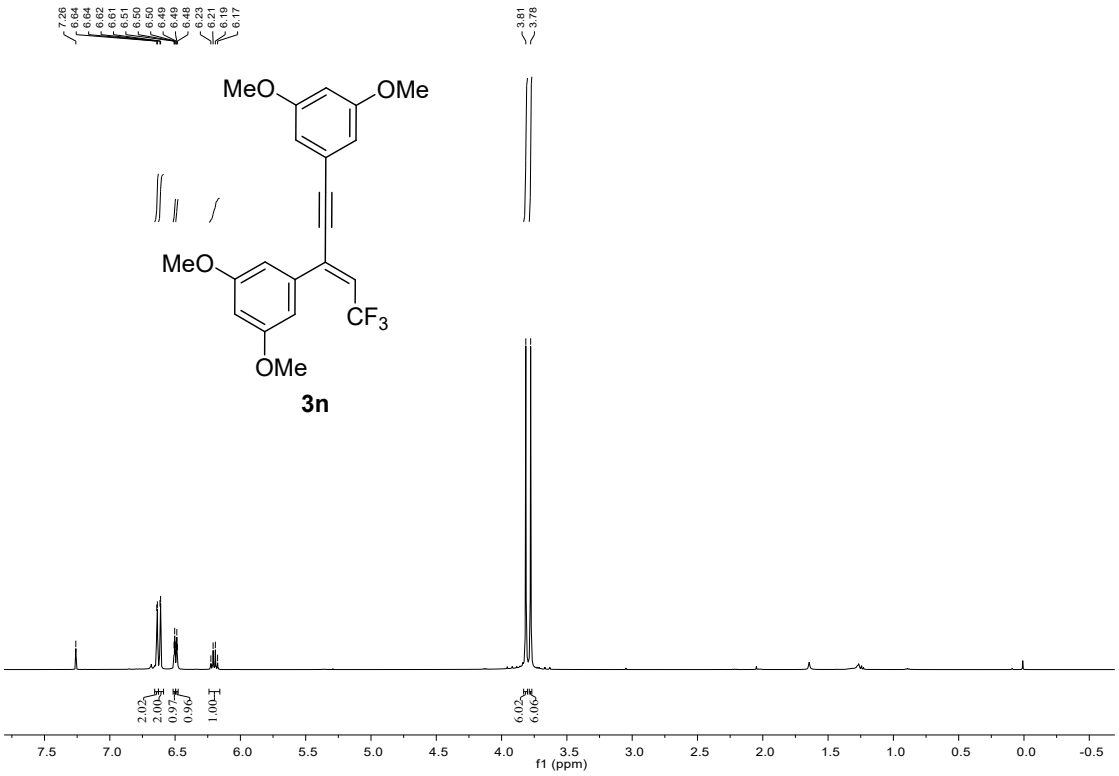
^{13}C NMR Spectrum of 3m



^{19}F NMR Spectrum of 3m



[1] H NMR Spectrum of 3n



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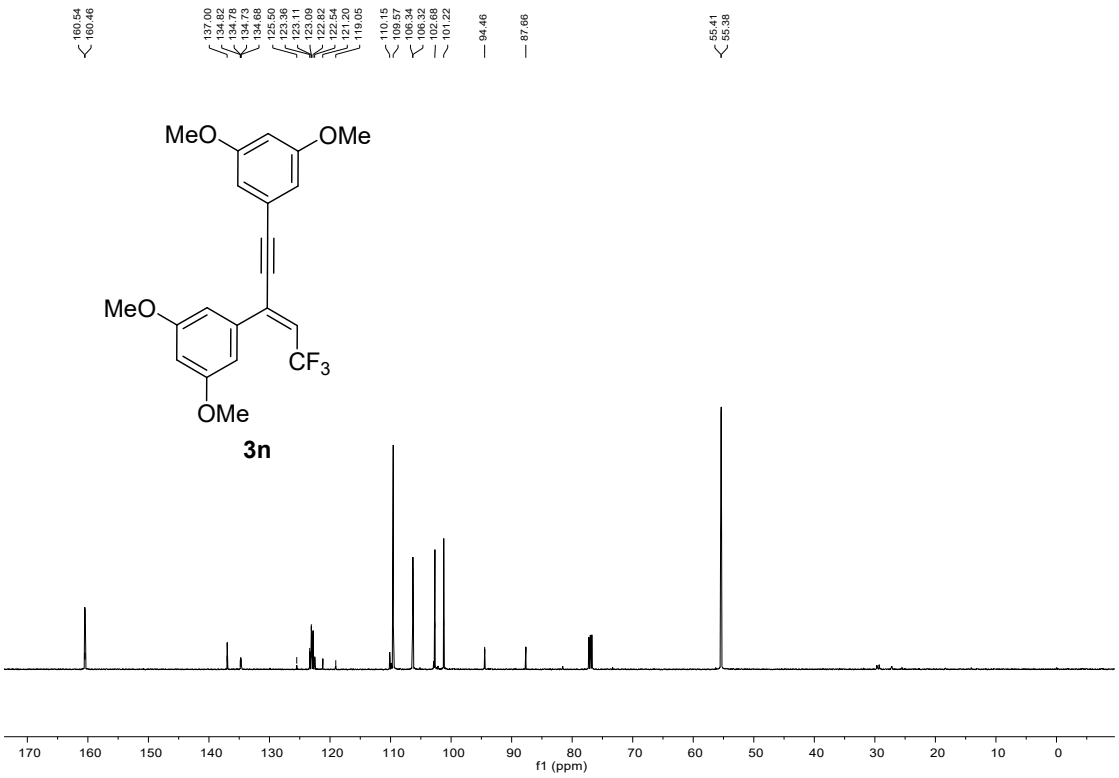
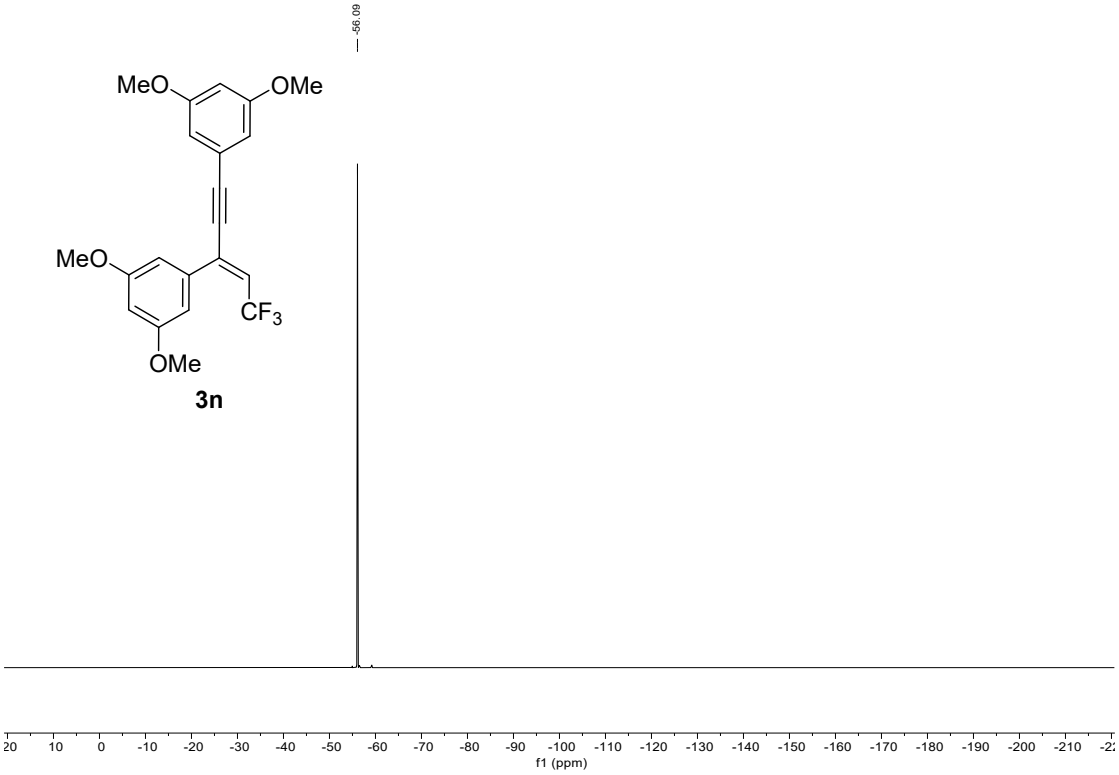
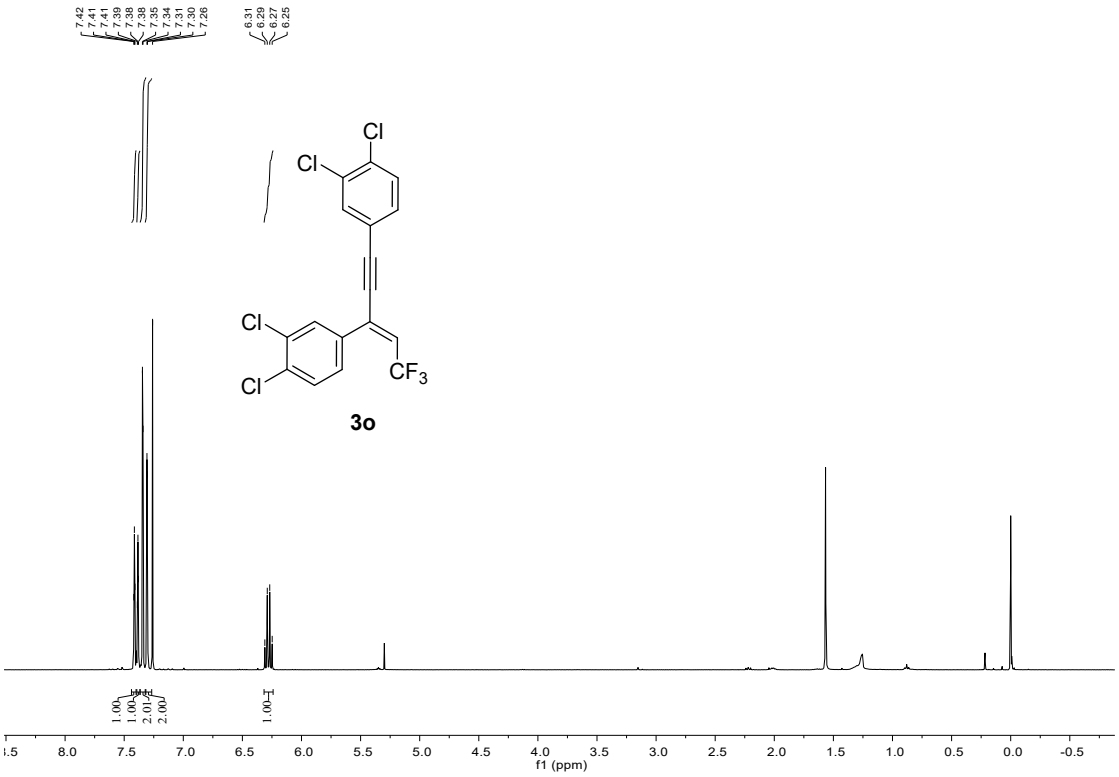


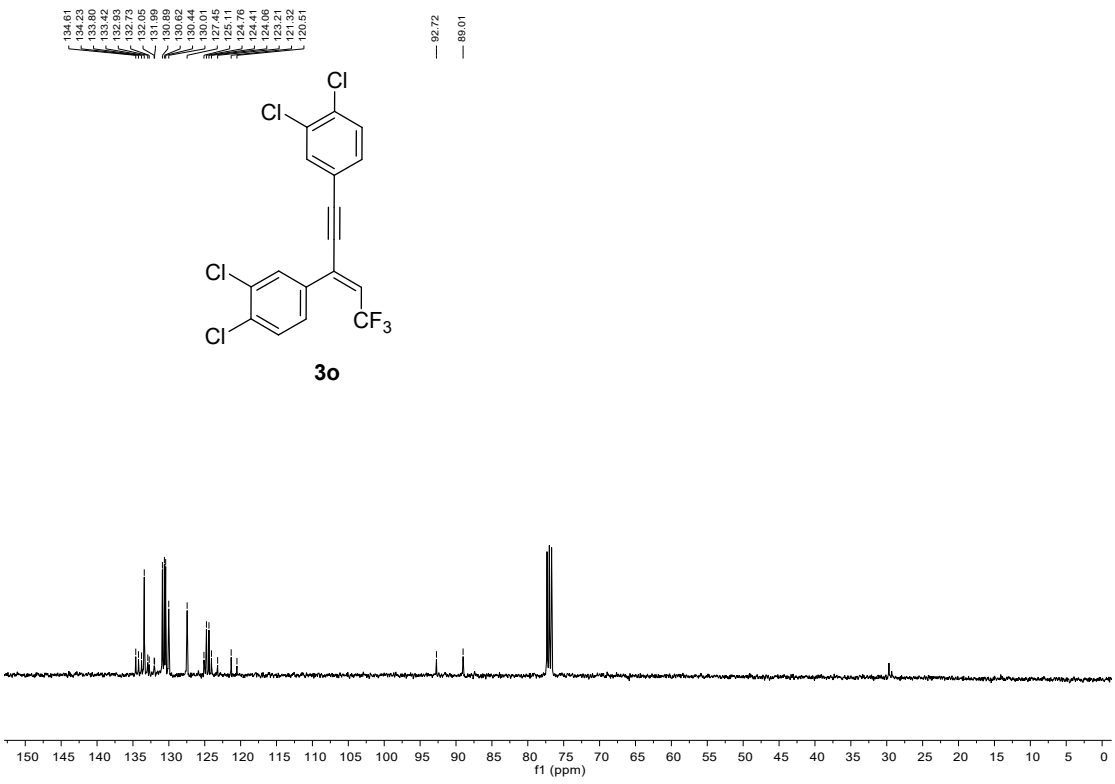
^{19}F NMR Spectrum of 3n



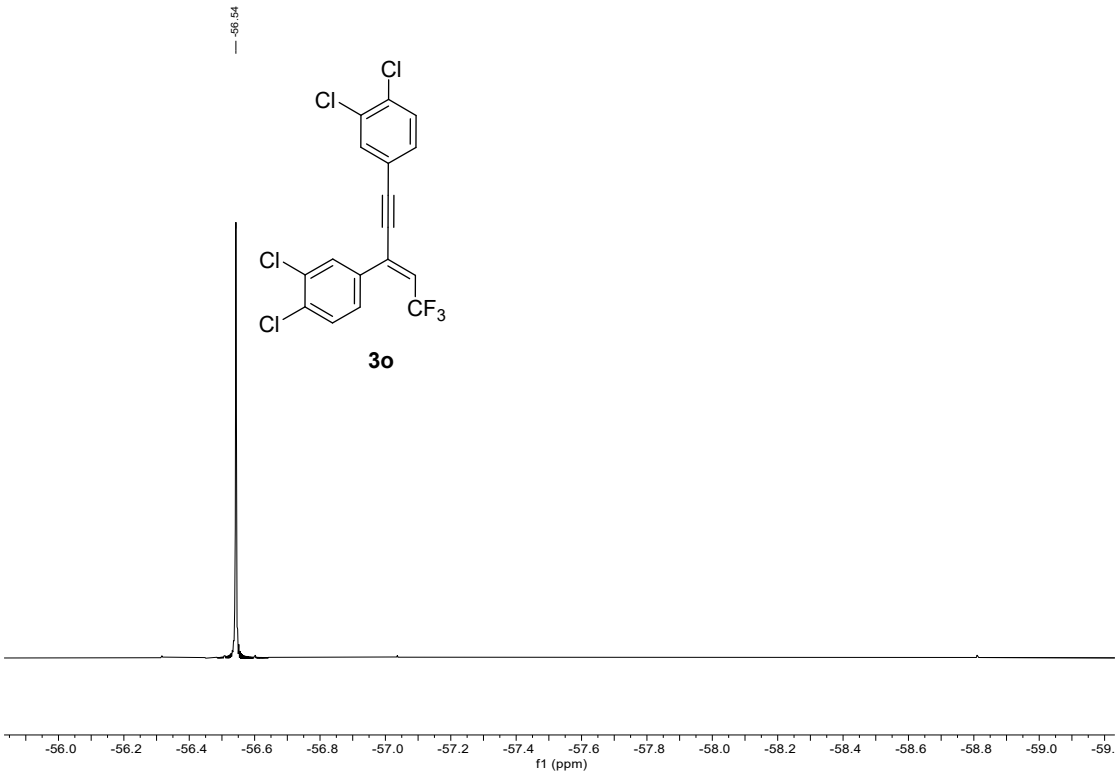
[1] H NMR Spectrum of 3o



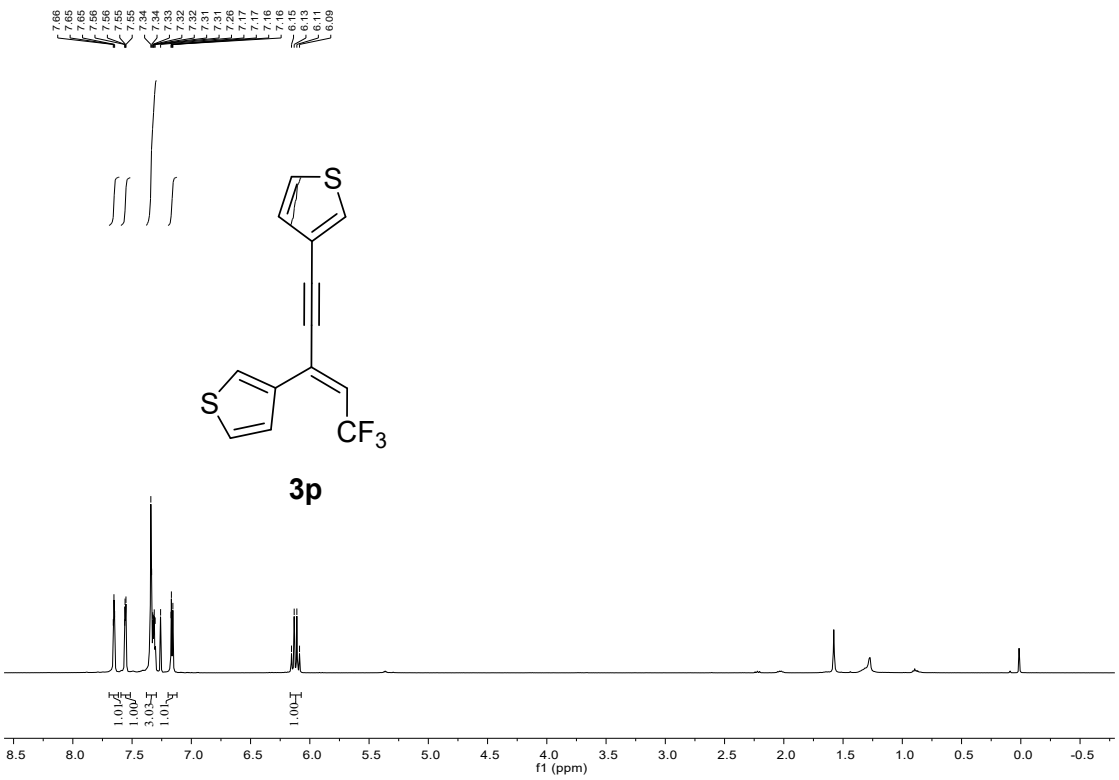
[13]C NMR Spectrum of 3o



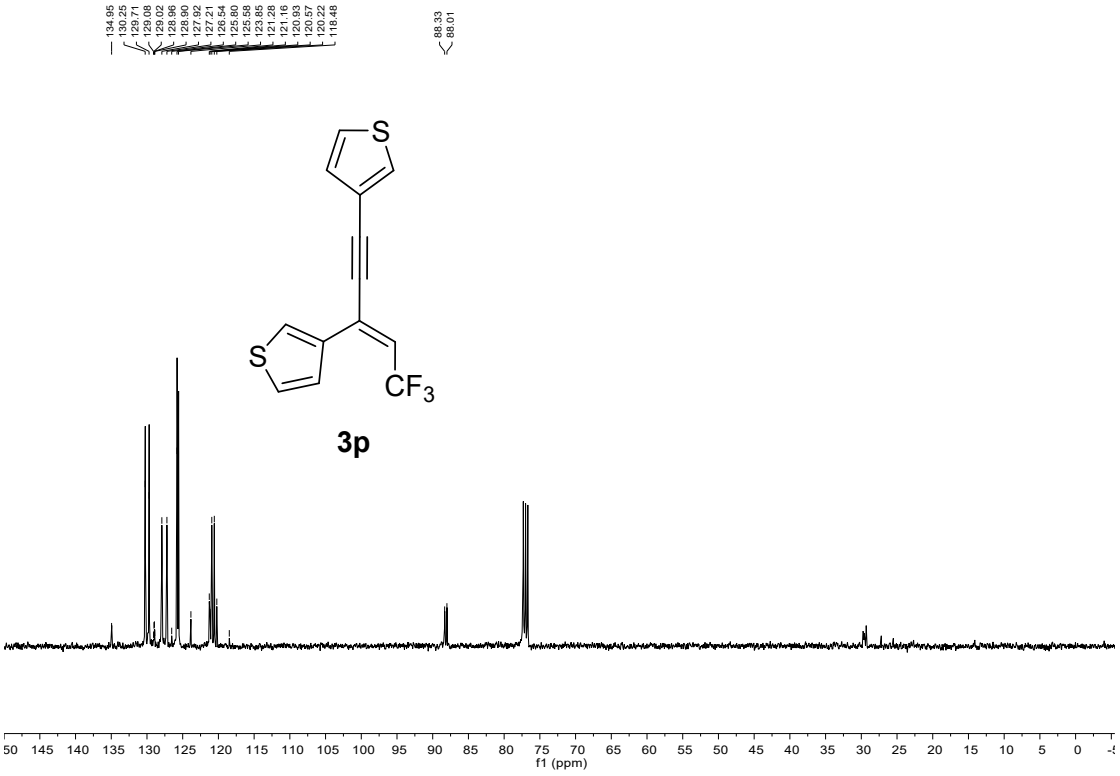
^{19}F NMR Spectrum of 3o



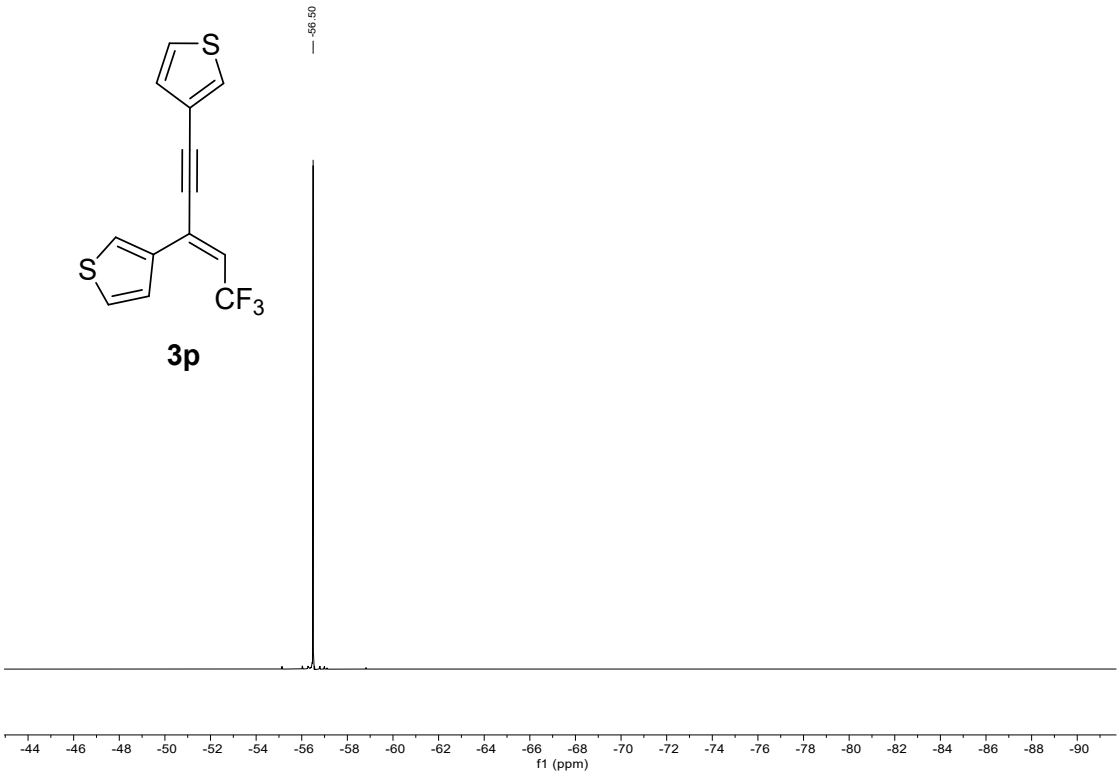
^{1}H NMR Spectrum of 3p



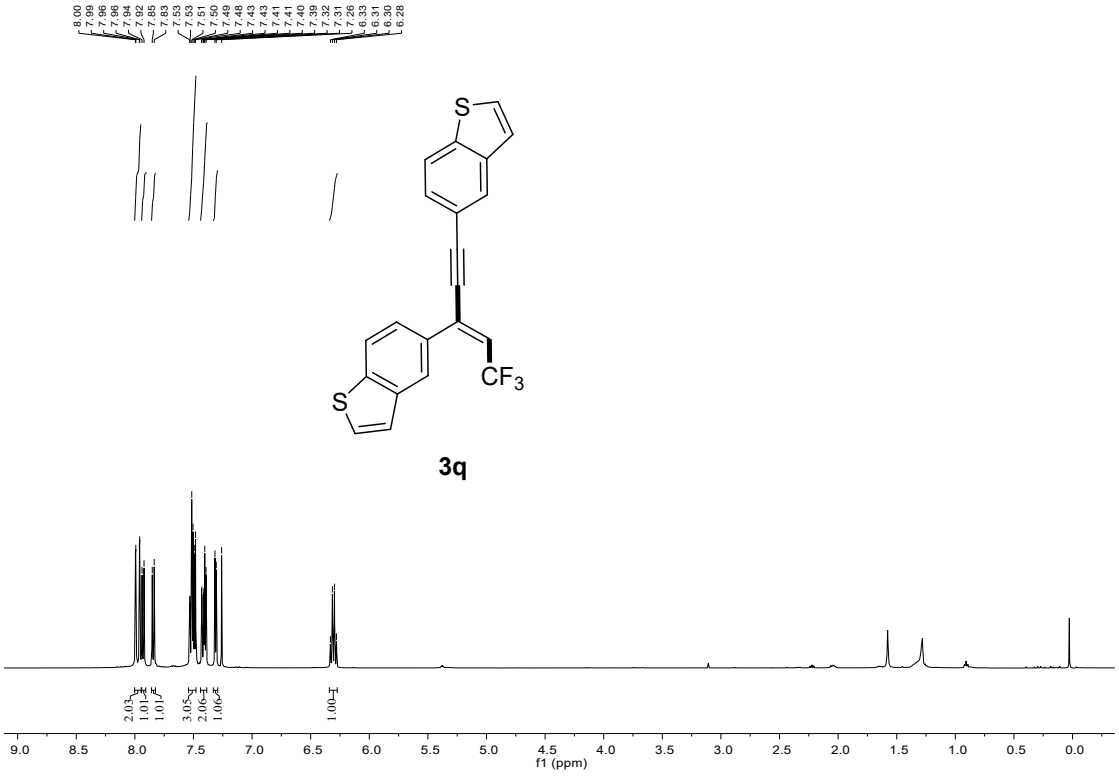
^{13}C NMR Spectrum of 3p



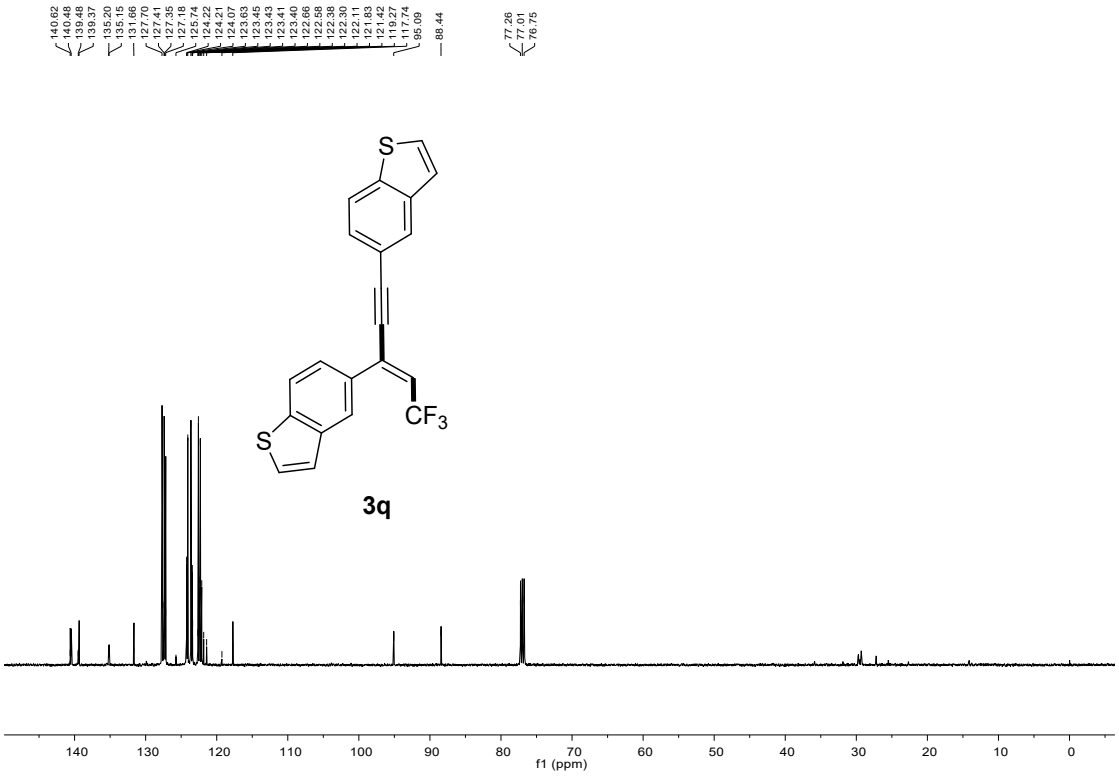
^{19}F NMR Spectrum of 3p



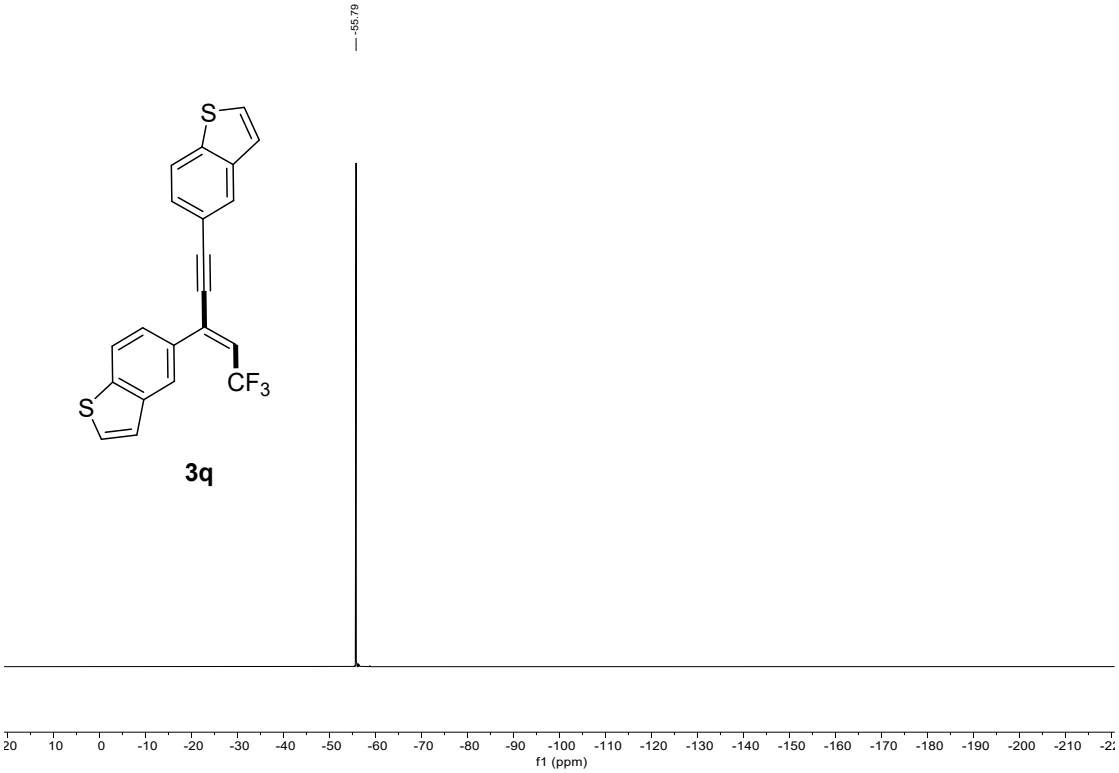
[1] H NMR Spectrum of 3q



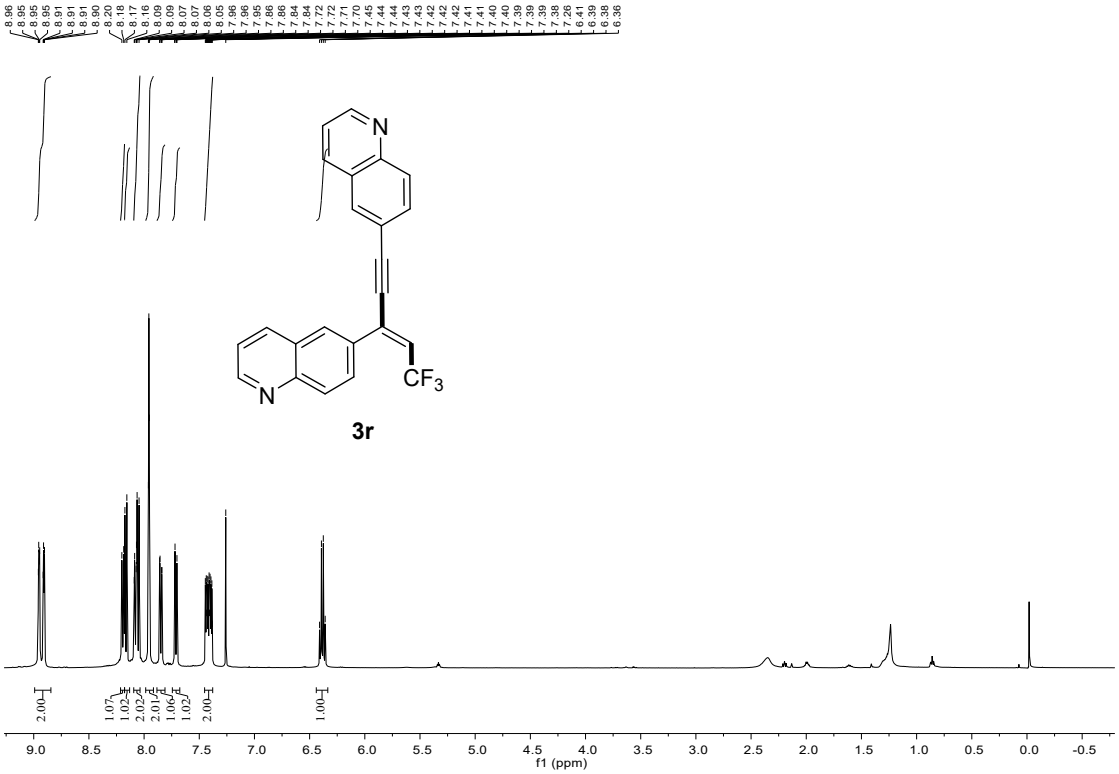
[13]C NMR Spectrum of 3q



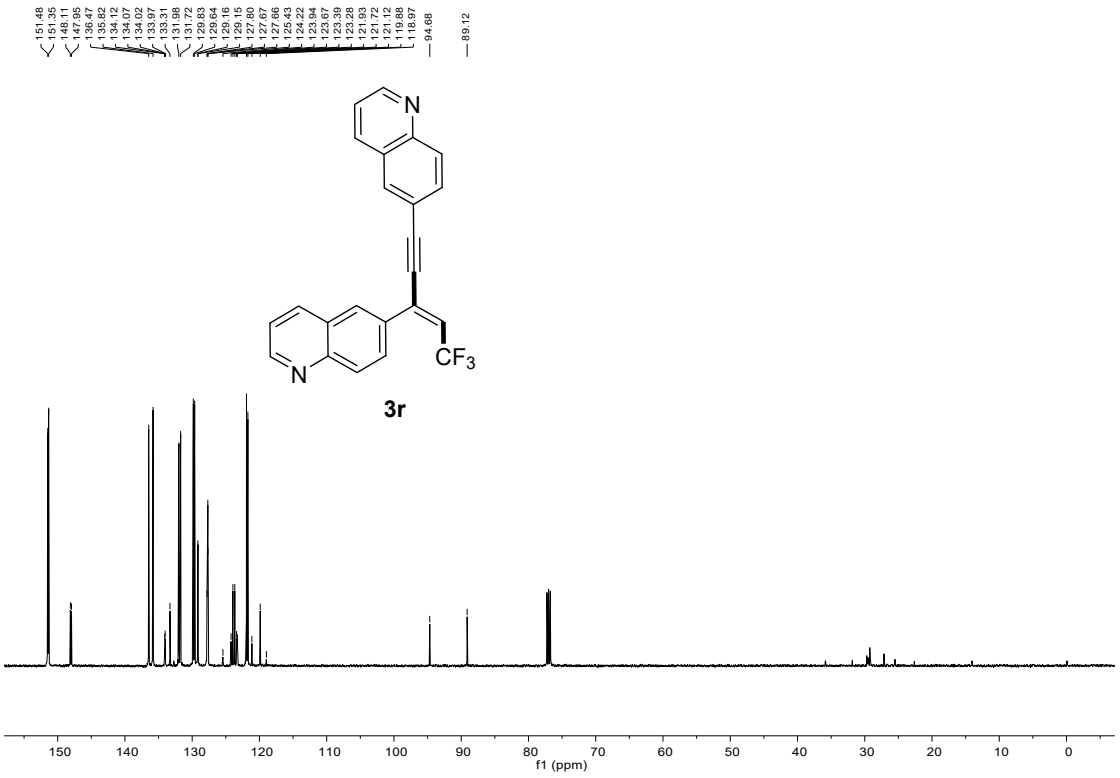
^{19}F NMR Spectrum of 3q



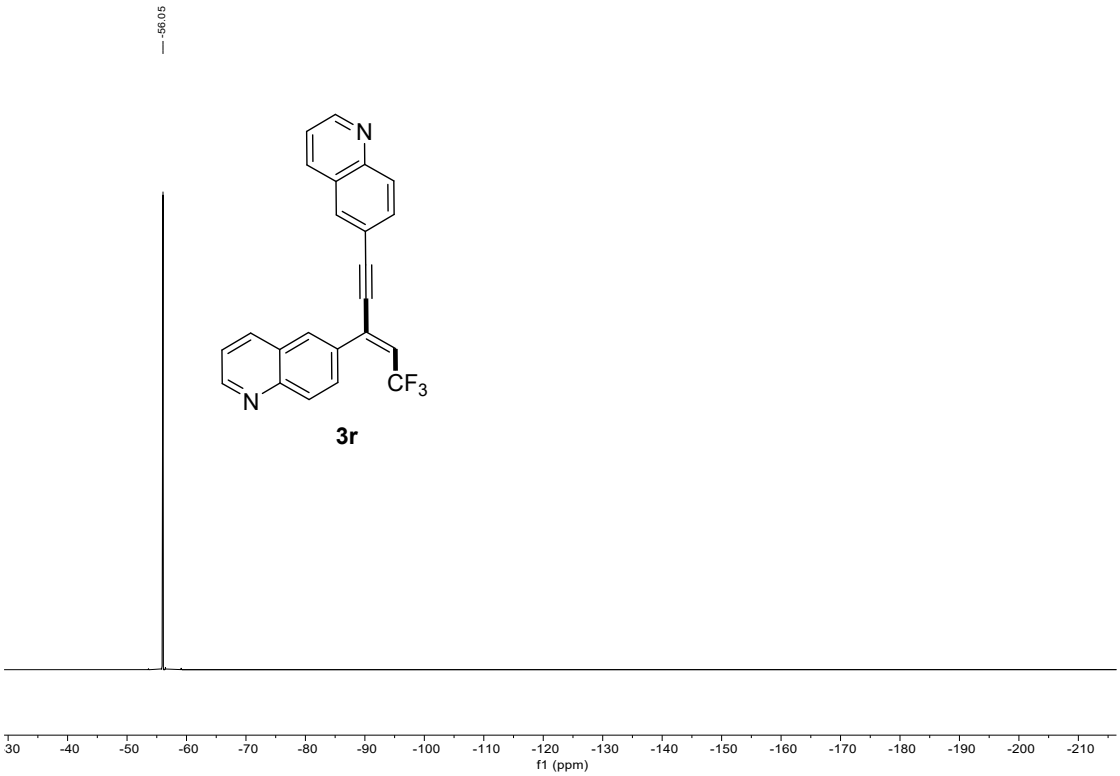
^{1}H NMR Spectrum of 3r



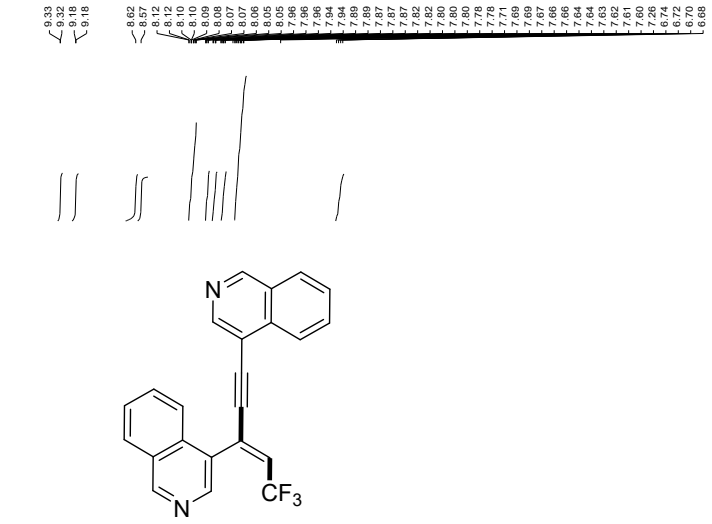
^{13}C NMR Spectrum of 3r



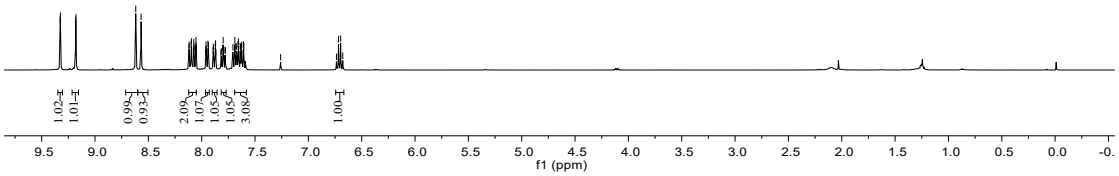
^{19}F NMR Spectrum of 3r



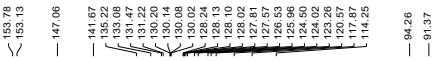
^{1}H NMR Spectrum of 3s

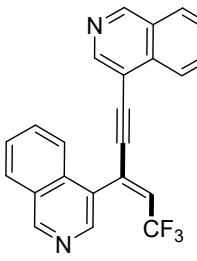


3s

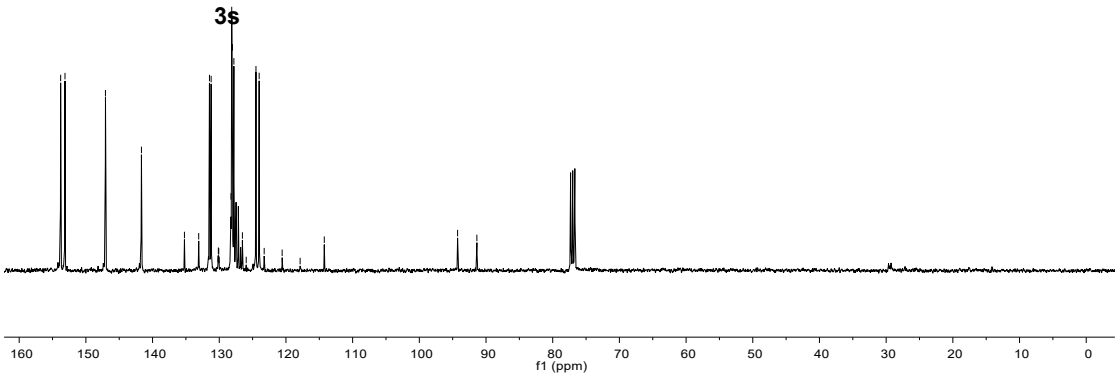


^{13}C NMR Spectrum of 3s

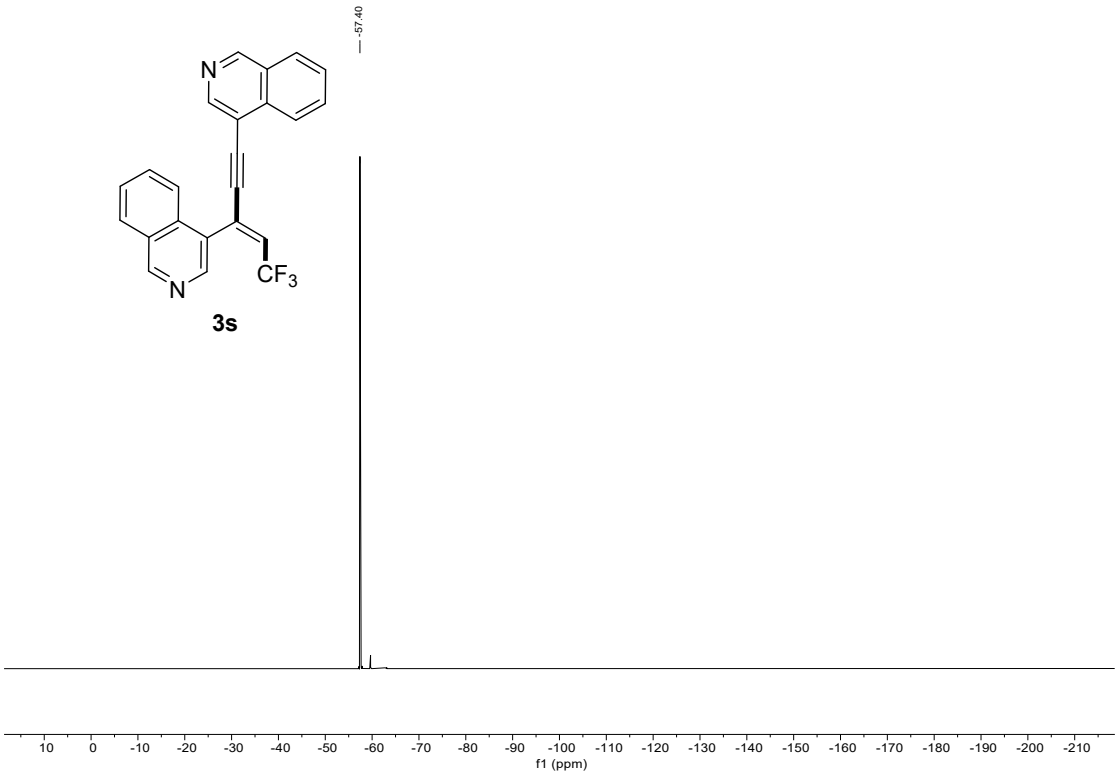




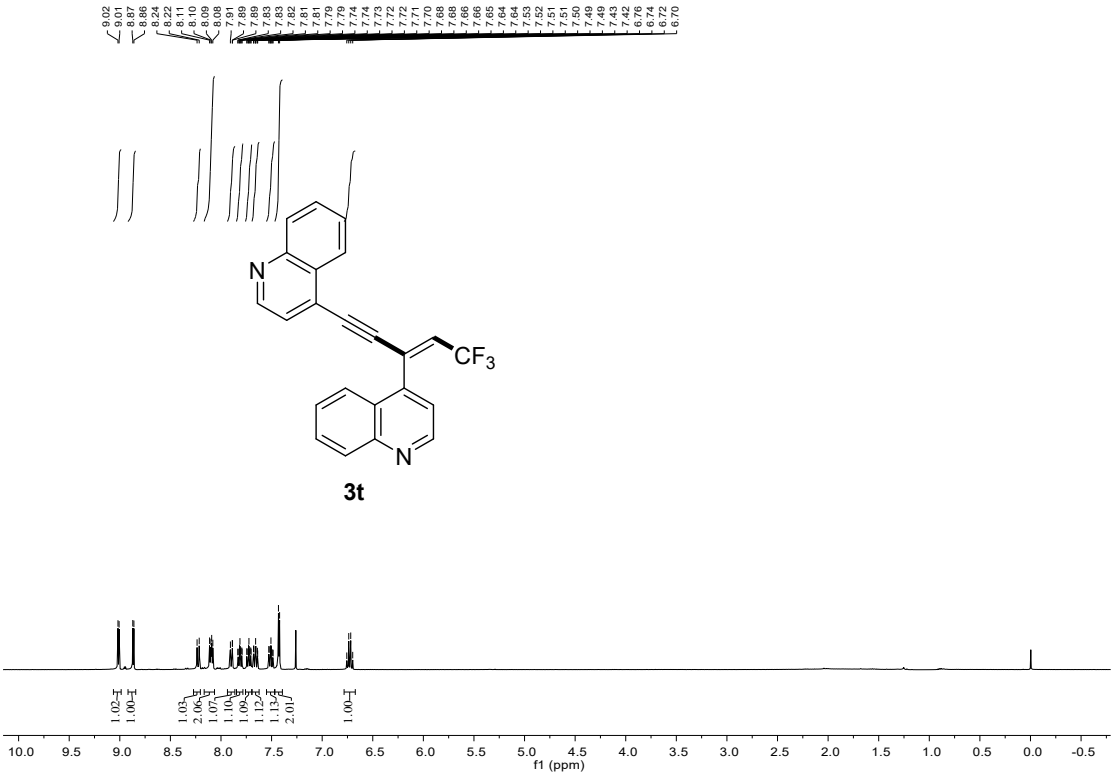
3s



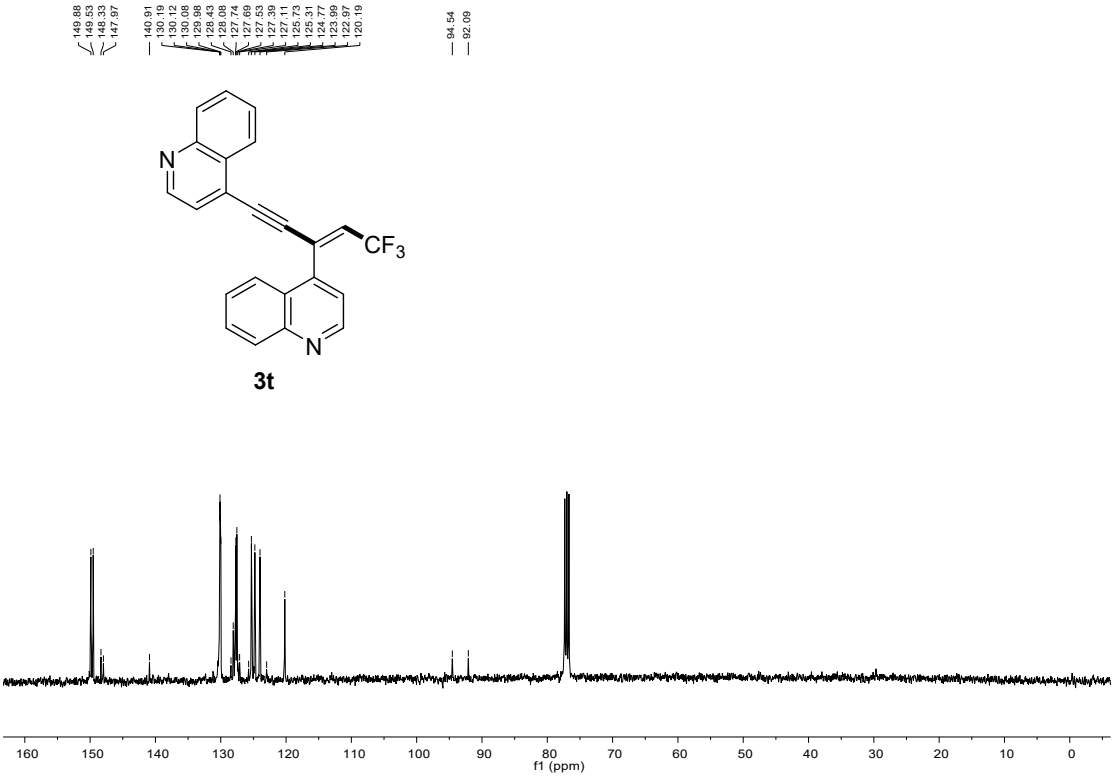
^{19}F NMR Spectrum of 3s



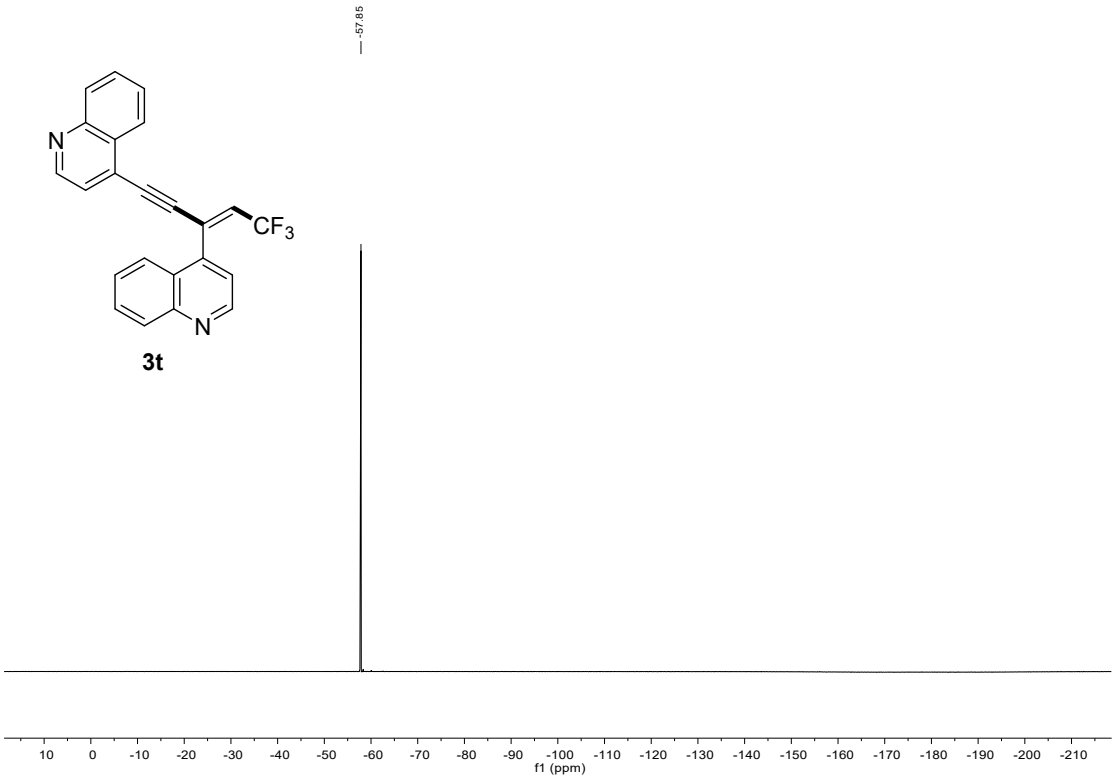
^{1}H NMR Spectrum of 3t



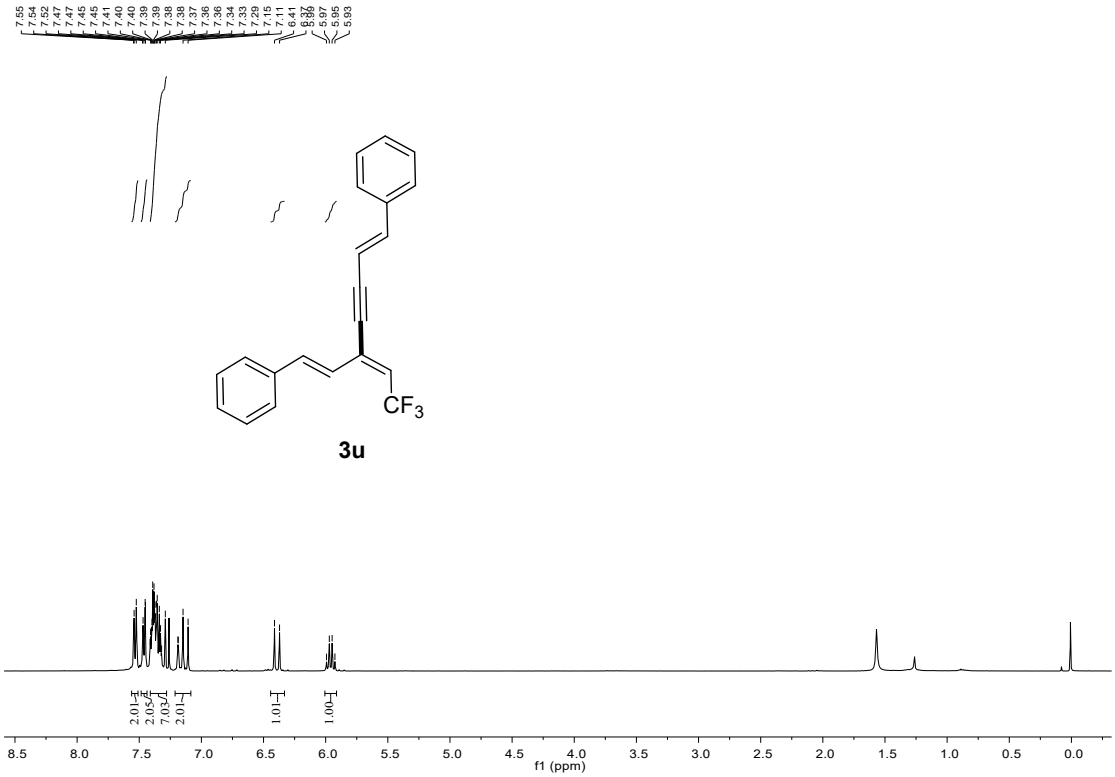
^{13}C NMR Spectrum of 3t



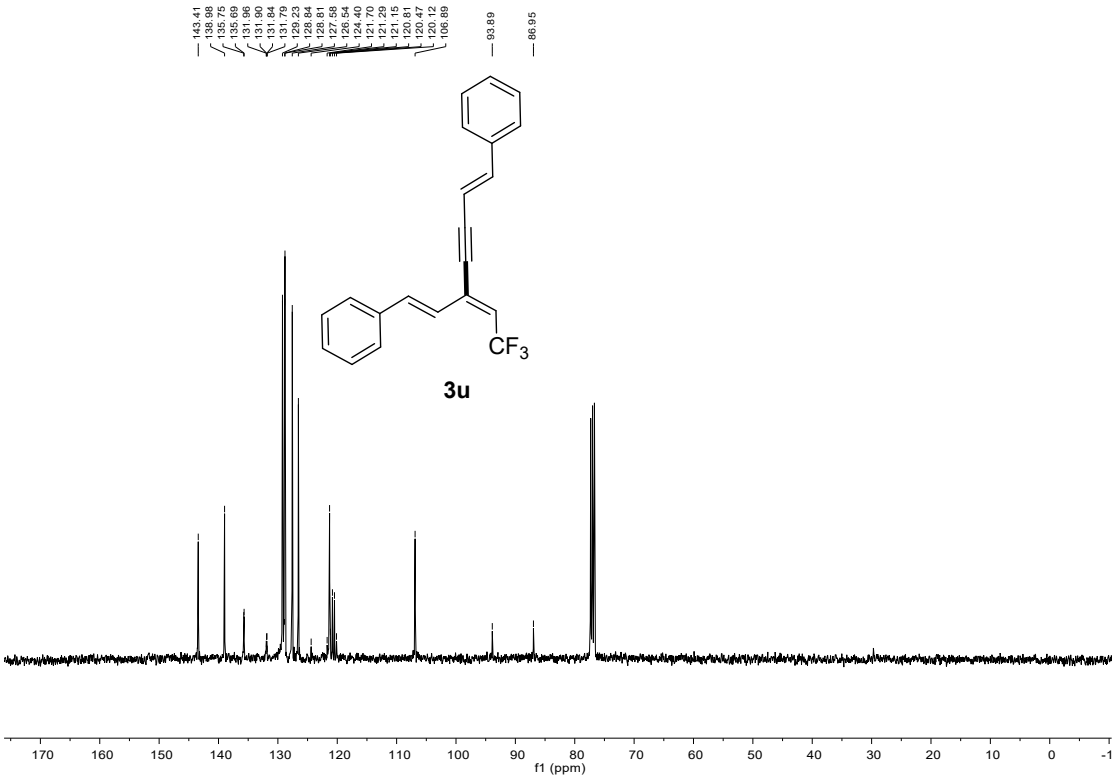
^{19}F NMR Spectrum of 3t



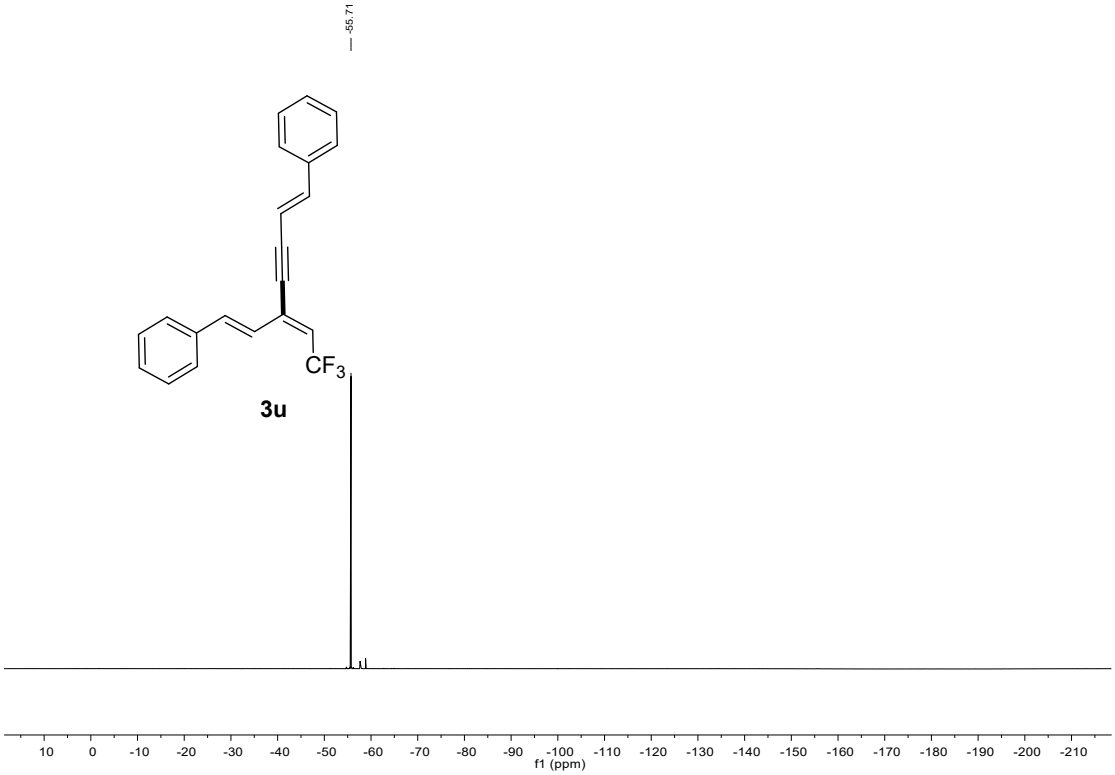
[1] H NMR Spectrum of 3u



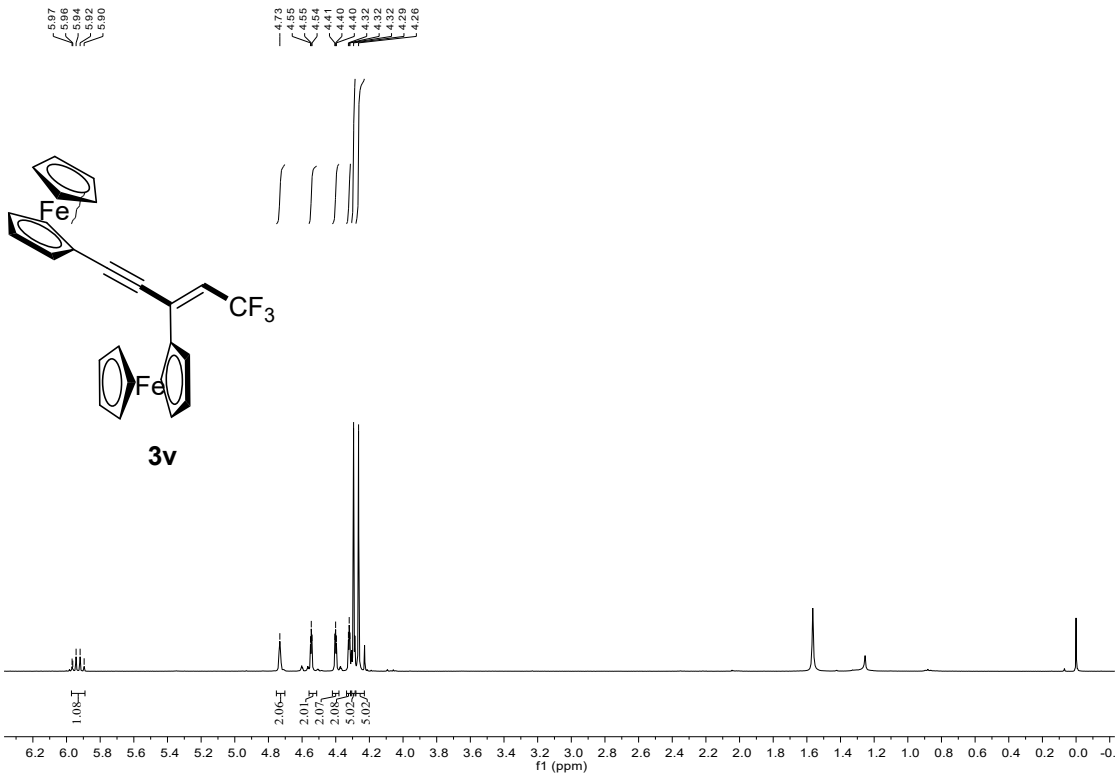
[13]C NMR Spectrum of 3u



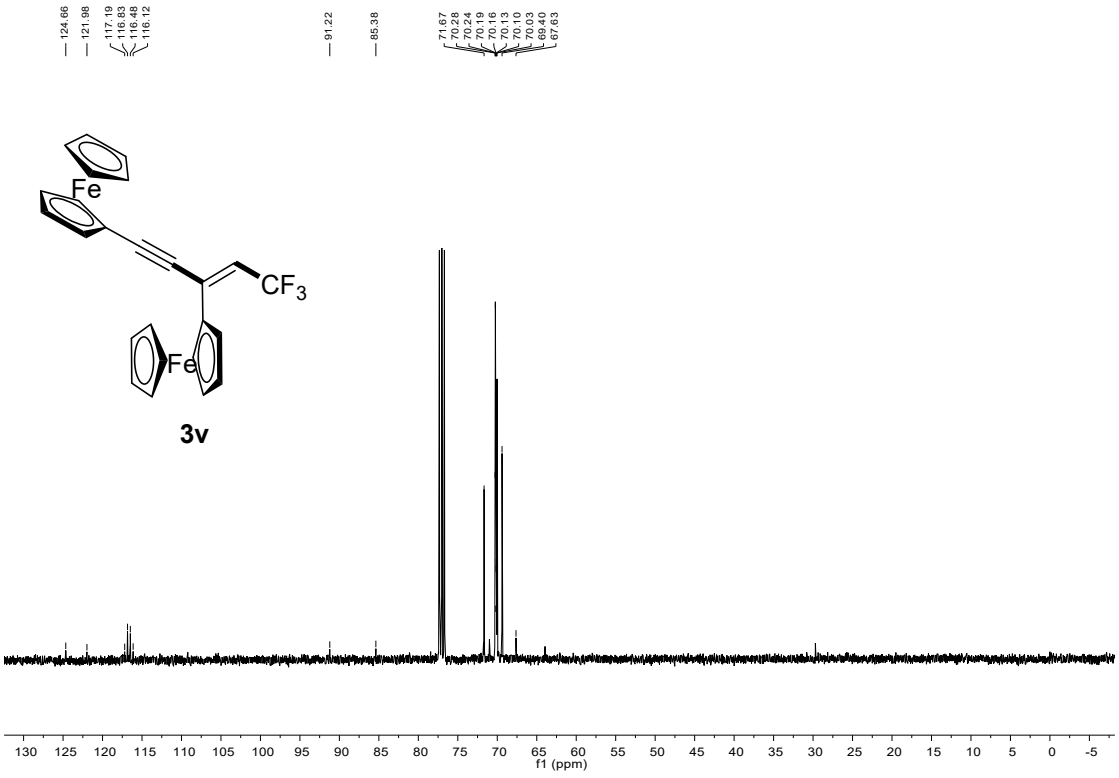
^{19}F NMR Spectrum of 3u



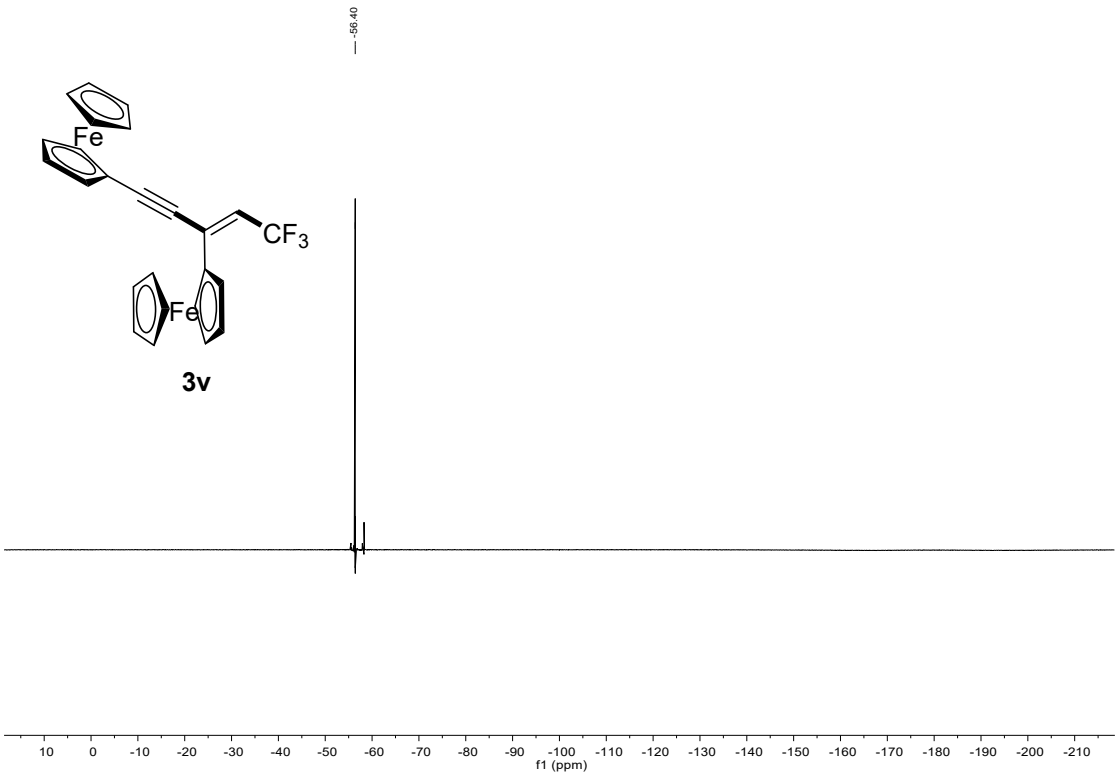
^{1}H NMR Spectrum of 3v



^{13}C NMR Spectrum of 3v

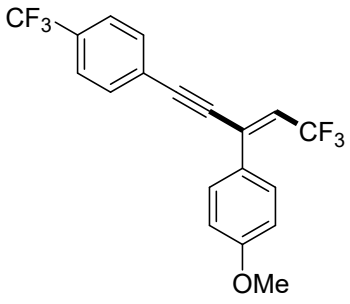


^{19}F NMR Spectrum of 3v

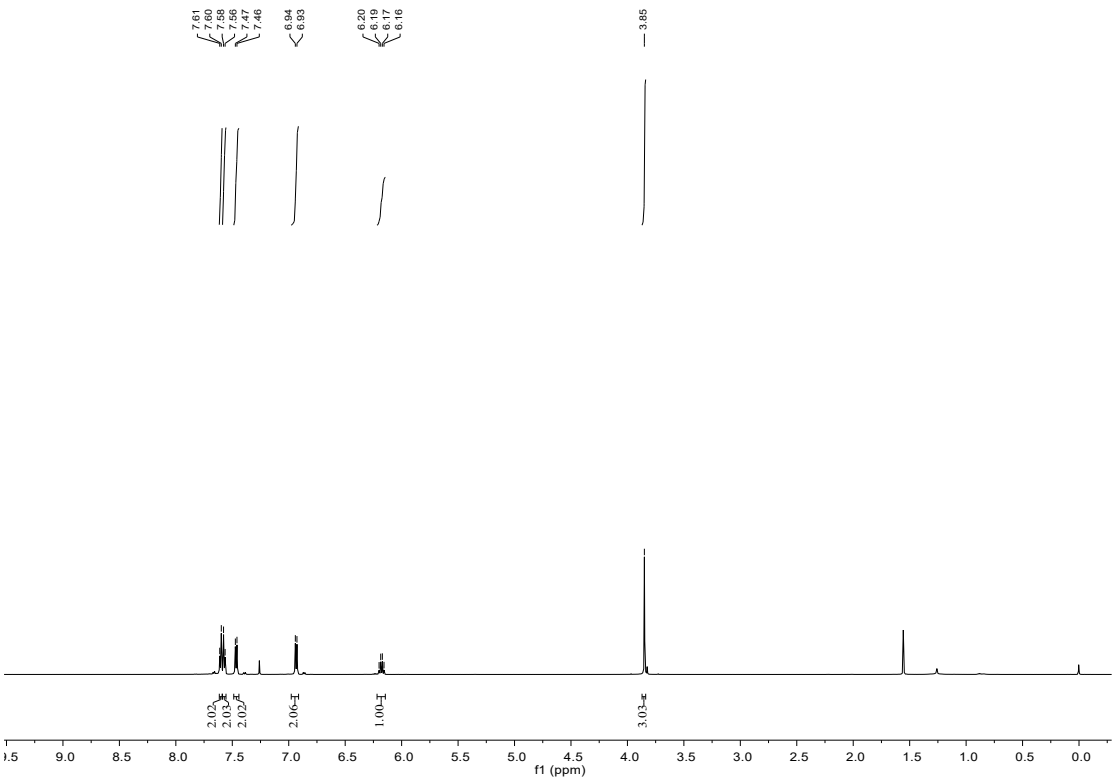


3v

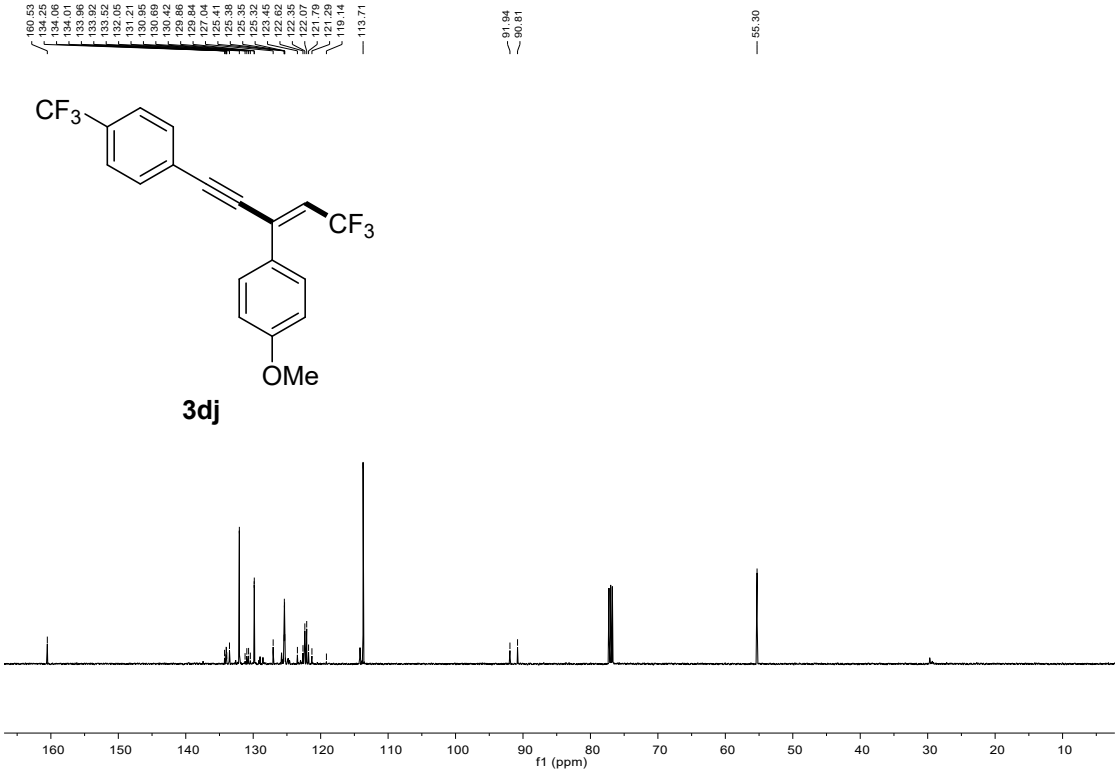
^{1}H NMR Spectrum of 3dj



3dj

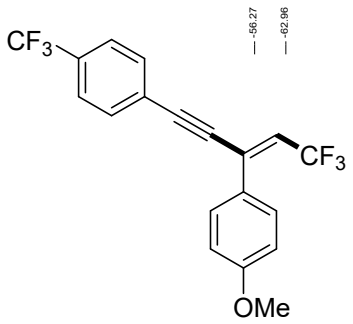


^{13}C NMR Spectrum of 3dj



3dj

^{19}F NMR Spectrum of 3dj



3dj