Supporting Information

Computation-Guided Development of Au-Catalyzed Cycloisomerizations Proceeding via 1,2-Si- or 1,2-H Migrations: Regiodivergent Synthesis of Silylfurans

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Content

General Information

NMR spectra were recorded on Bruker Avance DRX-500 (500 MHz) and DPX-400 (400 MHz) instruments. GC/MS analyses were performed on a Hewlett Packard Model 6890 GC interfaced to a Hewlett Packard Model 5973 mass selective detector (15 m × 0.25 mm capillary column, HP-5MS). Column chromatography was carried out employing Merck silica gel (Kieselgel 60, 63-200 μm), ICN silica gel (ICN SiliTech, 63-200 μm), and SiliCycle silica gel (40-63 μm). Analytical thin-layer chromatography (TLC) was performed on 0.2 mm precoated Silica gel plates (60 F_{254}).

All manipulations with transition metal catalysts were conducted under inert atmosphere using a combination of glovebox and standard Schlenk techniques. Anhydrous toluene, tetrahydrofuran, ether, 1,2-dichloroethane and dichloromethane purchased from Aldrich were additionally purified on PureSolv PS-400-4 by Innovative Technology, Inc. purification system and stored over calcium hydride. All other reagents were purchased from various commercial sources and used without additional purification. Silyl ketenes and phosphoranes were synthesized via known literature procedures.

Synthesis of Starting Materials

Procedure A:

Allenyl- (**4**) or homopropargyl (**6**) ketones were synthesized via Wittig olefination of the corresponding silyl ketenes with stabilized phosphoranes. Accordingly, to a stirred 0.1 M solution of silyl ketene in anhydrous DCM, DCM-Hexanes, or DCE was added in one portion phosphorane (1.1 eq). The mixture was stirred at -40 ^{o}C – +75 ^{o}C and monitored by GC and TLC for complete consumption of the silyl ketene. Hexanes were then added and the solution was filtered through silica gel. The filtrate was concentrated under reduced pressure and the residual oil purified by flash column chromatography.

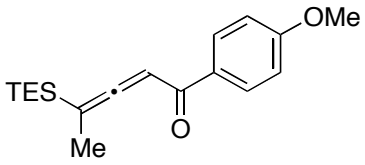
Procedure B:

Trimethylsilyl propargyl bromide (2 eq) was added to a mixture of the indium powder (2 eq) and indium tribromide (0.1 eq) in anhydrous THF (1 M) at room temperature with stirring under an atmosphere of dry argon. After 15 min, aryl aldehyde (1 eq) was added at room temperature. The mixture was refluxed overnight, and finally quenched with 1 M HCl solution. The aqueous layer was extracted with ethyl acetate. The combined organic extracts were washed with brine, dried over anhydrous magnesium sulfate, concentrated under vacuum, and filtered through flash silica gel to provide crude homopropargyl alcohol which was further oxidized with DMP. Accordingly, Dess-Martin periodinane (15 wt% solution in DCM, 2.6 mL, 1.2 equiv.) was added to the solution of propargyl alcohol in anhydrous DCM (0.3 M) and the mixture was stirred at room temperature for 1 h

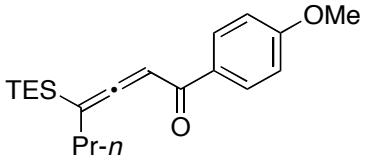
(monitored by TLC). Hexanes were then added and the solution was filtered through silica gel. The filtrate was concentrated under reduced pressure and the residual oil purified by flash column chromatography.

Procedure C:

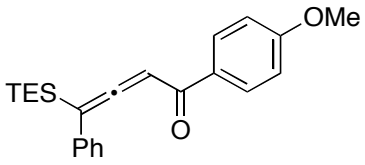
To a stirred 0.125 M solution of silyl acetylene (1 eq) at -78 ^{o}C was added dropwise *n*-BuLi (1.1 eq). After stirring for 30 min, BF_3-Et_2O (1.5 eq) was added followed by epoxide (1.3 eq), and the mixture was stirred for 1 h at -78 ^{o}C. The reaction mixture was quenched with aqueous NH_4Cl and extracted with ethyl acetate. The combined organic phases were washed with brine, dried over Na_2SO_4, and concentrated. The residue was purified by column chromatography (5-10% EtOAc in hexane) to give homopropargyl alcohol which was further oxidized with DMP. Accordingly, Dess-Martin periodinane (15 wt% solution in DCM, 2.6 mL, 1.2 equiv.) was added to the solution of propargyl alcohol in anhydrous DCM (0.3 M) and the mixture was stirred at room temperature for 1 h (monitored by TLC). Hexanes were then added and the solution was filtered through silica gel. The filtrate was concentrated under reduced pressure and the residual oil purified by flash column chromatography.



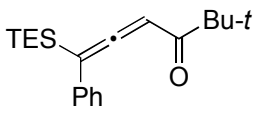
4a: (A, DCE, 40 ^{o}C, 3 days, 71%): ^{1}H NMR (500 MHz, $CDCl_3$) δ ppm 7.81 - 7.89 (m, 2 H), 6.83 - 6.97 (m, 2 H), 6.02 (q, *J*=2.81 Hz, 1 H), 3.85 (s, 3 H), 1.86 (d, *J*=2.81 Hz, 3 H), 0.87 (t, *J*=7.89 Hz, 9 H), 0.61 (td, *J*=7.89, 1.60 Hz, 6 H); ^{13}C NMR (126 MHz, $CDCl_3$) δ ppm 210.3, 192.0, 162.8, 131.3, 130.5, 113.3, 91.4, 87.7, 55.4, 14.6, 7.0, 2.8



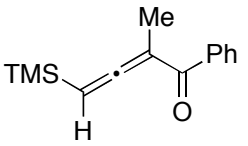
4b: (A, DCE, 75 ^{o}C, 3 days, 30%): ^{1}H NMR (500 MHz, $CDCl_3$) δ ppm 7.85 - 7.92 (m, 2 H), 6.83 - 6.93 (m, 2 H), 6.17 (t, *J*=3.12 Hz, 1 H), 3.85 (s, 3 H), 1.98 - 2.20 (m, 2 H), 1.52 - 1.64 (m, 2 H), 0.96 (t, *J*=7.34 Hz, 3 H), 0.91 (t, *J*=7.89 Hz, 9 H), 0.59 - 0.68 (m, 6 H); ^{13}C NMR (126 MHz, $CDCl_3$) δ ppm 209.6, 191.1, 162.8, 131.5, 130.4, 113.4, 96.7, 88.7, 55.4, 31.1, 22.5, 14.0, 7.1, 3.1



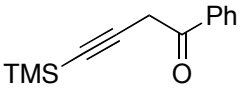
4c: (A, DCE, rt, 4 days, 74%): ^{1}H NMR (500 MHz, $CDCl_3$) δ ppm 7.82 - 7.88 (m, 2 H), 7.23 - 7.39 (m, 5 H), 6.82 - 6.89 (m, 2 H), 6.36 (s, 1 H), 3.84 (s, 3 H), 0.89 (t, *J*=7.82 Hz, 9 H), 0.70 - 0.77 (m, 6 H); ^{13}C NMR (126 MHz, $CDCl_3$) δ ppm 213.3, 190.8, 163.1, 135.0, 131.0, 130.7, 128.8, 127.9, 127.1, 113.4, 100.8, 89.3, 55.4, 7.1, 3.7



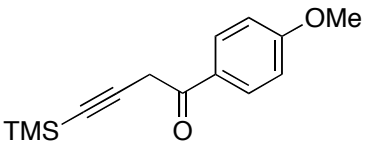
4d: (A, DCE, rt, 24 h, 79%): ^{1}H NMR (500 MHz, $CDCl_3$) δ ppm 7.25 - 7.34 (m, 4 H), 7.19 - 7.25 (m, 1 H), 6.14 (s, 1 H), 1.20 (s, 9 H), 0.93 - 1.00 (m, 9 H), 0.71 - 0.79 (m, 6 H); ^{13}C NMR (126 MHz, $CDCl_3$) δ ppm 212.1, 204.9, 135.1, 128.7, 128.0, 126.9, 100.8, 86.5, 44.0, 26.6, 7.2, 3.8



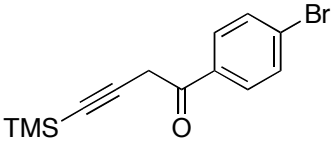
4e: (A, DCM, -40 °C - rt, 10 h, 99%): ^{1}H NMR (500 MHz, $CDCl_3$) δ ppm 7.63 - 7.68 (m, 2 H), 7.42 - 7.46 (m, 1 H), 7.31 - 7.37 (m, 2 H), 5.24 (q, *J*=3.30 Hz, 1 H), 1.95 (d, *J*=3.30 Hz, 3 H), 0.02 (s, 9 H); ^{13}C NMR (126 MHz, $CDCl_3$) δ ppm 217.0, 196.5, 139.2, 131.1, 128.4, 127.5, 97.2, 86.0, 13.9, -1.1



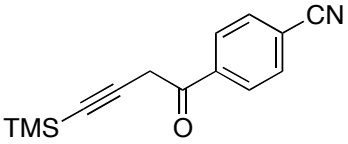
6f: (A, DCM, -40 °C - rt, 10 h, 60%): ^{1}H NMR (500 MHz, $CDCl_3$) δ ppm 7.97 - 8.03 (m, 2 H), 7.57 (dt, *J*=7.47, 1.49 Hz, 1 H), 7.44 - 7.49 (m, 2 H), 3.88 (s, 2 H), 0.15 (s, 9 H); ^{13}C NMR (126 MHz, $CDCl_3$) δ ppm 192.9, 135.4, 133.5, 128.7, 128.6, 98.4, 90.4, 32.0, -0.15



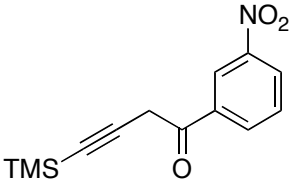
6g: (A, DCM, rt, 10 h, 72%): ^{1}H NMR (500 MHz, $CDCl_3$) δ ppm 7.95 - 8.02 (m, 2 H), 6.90 - 6.98 (m, 2 H), 3.87 (s, 3 H), 3.83 (s, 2 H), 0.15 (s, 9 H); ^{13}C NMR (126 MHz, $CDCl_3$) δ ppm 191.4, 163.8, 131.1, 128.5, 113.7, 98.9, 90.1, 55.5, 31.8, -0.1



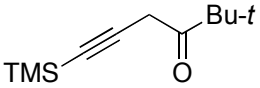
6h: (A, DCE, rt, 24 h, 35%): ^{1}H NMR (500 MHz, $CDCl_3$) δ ppm 7.84 - 7.92 (m, 2 H), 7.58 - 7.65 (m, 2 H), 3.84 (s, 2 H), 0.15 (s, 9 H); ^{13}C NMR (126 MHz, $CDCl_3$) δ ppm 191.9, 134.1, 131.9, 130.3, 128.8, 97.9, 90.9, 32.1, -0.2



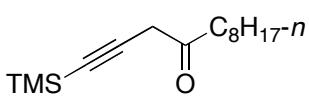
6i: (B, 12%): ^{1}H NMR (500 MHz, $CDCl_3$) δ ppm 8.04 - 8.21 (m, 2 H), 7.72 - 7.83 (m, 2 H), 3.87 (s, 2 H), 0.13 (s, 9 H); ^{13}C NMR (126 MHz, $CDCl_3$) δ ppm 191.7, 138.2, 132.4, 129.2, 117.8, 116.8, 97.2, 91.6, 32.4, -0.2



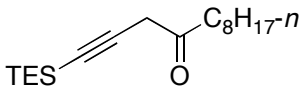
6j: (B, 43%): ^{1}H NMR (500 MHz, $CDCl_3$) δ ppm 8.88 - 8.92 (m, 1 H), 8.45 (ddd, *J*=8.21, 2.34, 1.01 Hz, 1 H), 8.34 - 8.37 (m, 1 H), 7.66 - 7.74 (m, 1 H), 3.91 (s, 2 H), 0.13 (s, 9 H); ^{13}C NMR (126 MHz, $CDCl_3$) δ ppm 190.9, 148.4, 136.5, 134.3, 129.9, 127.8, 123.8, 97.2, 91.9, 32.5, -0.3



6k: (A, DCM-Hexanes, -40 °C - rt, 6 h, 48%): ^{1}H NMR (500 MHz, $CDCl_3$) δ ppm 3.46 (s, 2 H), 1.18 (s, 9 H), 0.16 (s, 9 H); ^{13}C NMR (126 MHz, $CDCl_3$) δ ppm 208.3, 98.7, 89.2, 44.6, 30.0, 26.6, -0.1



6l: (C, 67%): ^{1}H NMR (500 MHz, $CDCl_3$) δ ppm 3.26 (s, 2 H), 2.61 (t, *J*=7.34 Hz, 2 H), 1.52 - 1.67 (m, 2 H), 1.26 (s, 10 H), 0.87 (s, 3 H), 0.17 (s, 9 H); ^{13}C NMR (126 MHz, $CDCl_3$) δ ppm 204.5, 98.7, 89.5, 41.2, 35.3, 31.8, 29.3, 29.1, 23.7, 22.6, 14.1, -0.1



6m: (C, 70%): ^{1}H NMR (500 MHz, $CDCl_3$) δ ppm 3.27 (s, 2 H), 2.64 (t, *J*=7.43 Hz, 2 H), 1.55 - 1.63 (m, 2 H), 1.18 - 1.33 (m, 10 H), 0.99 (t, *J*=7.98 Hz, 9 H), 0.83 - 0.90 (m, 3 H), 0.60 (q, *J*=7.89 Hz, 6 H); ^{13}C NMR (126 MHz, $CDCl_3$) δ ppm 204.7, 99.8, 86.9, 41.1, 35.4, 31.8, 29.3, 29.1, 23.7, 22.6, 14.1, 7.4, 4.4

6n: (C, 68%): ^{1}H NMR (500 MHz, $CDCl_3$) δ ppm 7.60 - 7.67 (m, 2 H), 7.35 - 7.43 (m, 3 H), 3.33 (s, 2 H), 2.65 (t, *J*=7.43 Hz, 2 H), 1.54 - 1.66 (m, 2 H), 1.26 - 1.39 (m, 2 H), 0.91 (t, *J*=7.34 Hz, 3 H), 0.43 (s, 6 H); ^{13}C NMR (126 MHz, $CDCl_3$) δ ppm 204.3, 136.8, 133.6, 129.5, 127.9, 100.6, 87.7, 41.1, 35.4, 25.7, 22.2, 13.8, -0.9

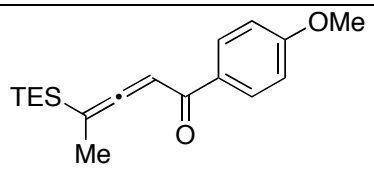
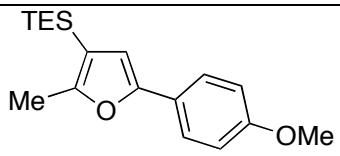
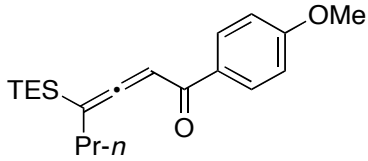
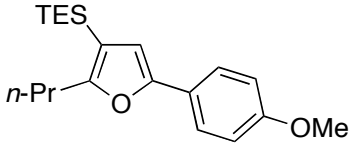
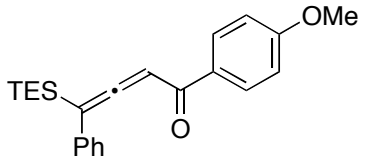
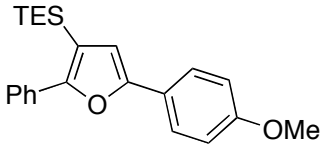
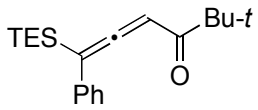
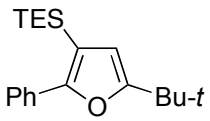
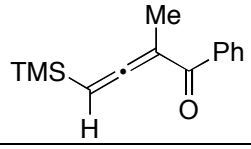
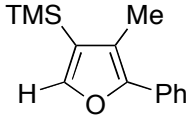
Optimization of Reaction Conditions

To a foiled 1–5 ml Wheaton V-vial charged with catalyst and appropriate amount of rigorously dried solvent was added homopropargyl- (**6**) or allenyl (**4**) ketone (0.1 – 0.5 mmol) under N_2 or argon atmosphere and the reaction mixture was stirred at room temperature until judged complete by TLC and GC/MS analysis. The reaction mixture was filtered through a layer of flash Silica, the solvents were removed in vacuo, and the residue was analyzed by ^{1}H NMR.

Synthesis of Furans

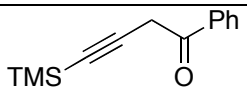
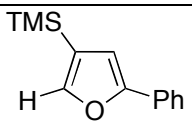
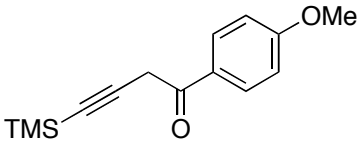
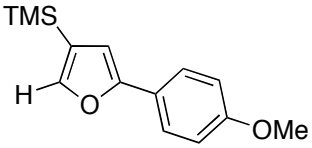
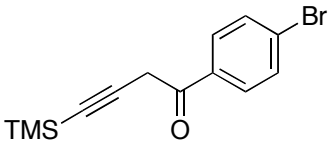
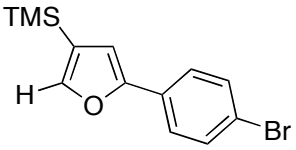
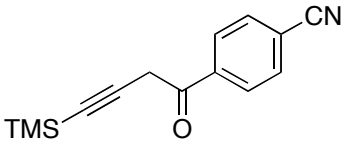
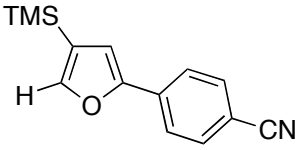
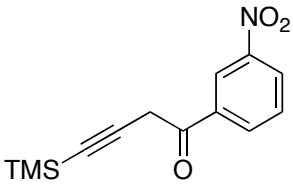
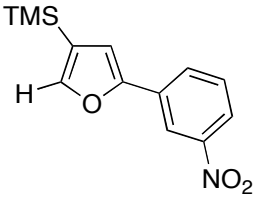
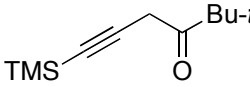
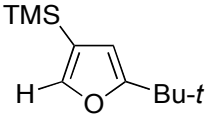
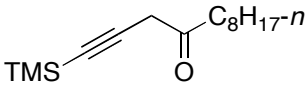
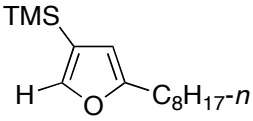
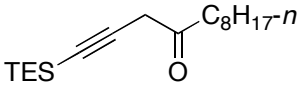
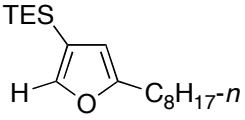
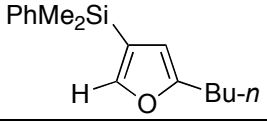
To a foiled 3–10 ml Wheaton V-vial charged with 5 mol % of $AuCl_3$ and the 1 ml of anhydrous toluene (0.5 M) in case of **4** or 5 mol % of 1:1 mixture of $Au(PPh_3)Cl$ and $AgSbF_6$ and the 10 ml of anhydrous 1,2-dichloroethane (0.05 M) in the case of **6** and stirred for 5 min was then added dry allenyl- (**4, Table S1**) or homopropargyl (**6, Table S2**) ketone (0.5 mmol), respectively, under argon atmosphere and the reaction mixture was stirred at room temperature until judged complete. The reaction mixture was then filtered through a layer of flash Silica, the solvents were removed in vacuo, and the residue was purified by column chromatography (Hexanes; Hexanes-Et_2O (20:1 – 10:1); Pentane; Pentane-Et_2O (20:1 – 10:1)).

Table S1: Synthesis of Furans from Allenyl Ketones 4

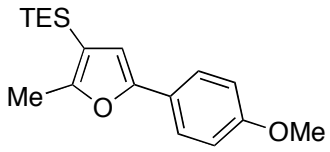
Entry	Substrate	Product	Time, h	Yield, %[a]
1			1	**2a**, 90
2			1	**2b**, 80
3			1	**2c**, 82
4			1	**2d**, 87
5			1.5	**2e**, 82 (77)[b]

[a] Isolated yield of product for reactions performed on 0.5 mmol scale. [b] Isolated yield of **2e** for reaction performed with 1 mol % of catalyst.

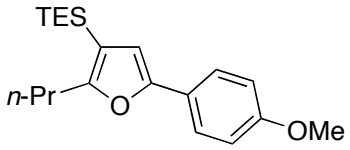
Table S2: Synthesis of Furans from Homopropargyl Ketones 6

Entry	Substrate	Product	Time, h	**2:3**	Yield, %[a,b]
1			1	1:0	**2f**, 79
2			5	1:0	**2g**, 91
3			24	14:1	**2h**, 91
4			30	10:1	**2i**, 48
5			30	8:1	**2j**, 65
6			10	1:0	**2k**, 71[c]
7			15	1:0	**2l**, 68
8			20	1:0	**2m**, 77
9			30	1:0	**2n**, 67

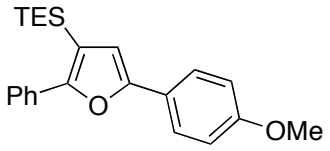
[a] Isolated yield of product for reactions performed on 0.5 mmol scale. [b] **2f** and **2l** contained 8 and 6% of the corresponding desilylated furan, respectively. [c] GC Yield, **2k** is a volatile compound.



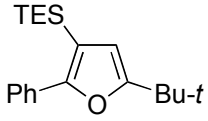
2a: ^{1}H NMR (500 MHz, $CDCl_3$) δ ppm 7.55 - 7.59 (m, 2 H), 6.88 - 6.92 (m, 2 H), 6.39 (s, 1 H), 3.83 (s, 3 H), 2.40 (s, 3 H), 0.99 (t, *J*=7.89 Hz, 9 H), 0.73 - 0.80 (m, 6 H); ^{13}C NMR (126 MHz, $CDCl_3$) δ ppm 158.5, 156.3, 152.1, 124.8, 124.3, 114.0, 111.4, 109.3, 55.3, 14.7, 7.4, 4.0; HRMS (EI) calcd. for $C_{18}H_{26}O_2Si$ [M+]: 302.17021. Found: 302.17030.



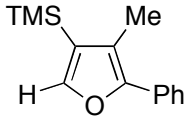
2b: ^{1}H NMR (500 MHz, $CDCl_3$) δ ppm 7.52 - 7.62 (m, 2 H), 6.85 - 6.95 (m, 2 H), 6.38 (s, 1 H), 3.83 (s, 3 H), 2.60 - 2.71 (m, 2 H), 1.70 - 1.79 (m, 2 H), 0.94 - 1.03 (m, 12 H), 0.76 (q, *J*=7.89 Hz, 6 H); ^{13}C NMR (126 MHz, $CDCl_3$) δ ppm 160.6, 158.5, 152.1, 124.8, 124.4, 114.0, 111.2, 109.0, 55.3, 31.2, 22.7, 14.0, 7.4, 4.1; HRMS (EI) calcd. for $C_{20}H_{30}O_2Si$ [M+]: 330.20151. Found: 330.20229.



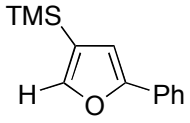
2c: ^{1}H NMR (500 MHz, $CDCl_3$) δ ppm 7.64 - 7.71 (m, 4 H), 7.39 - 7.46 (m, 2 H), 7.31 - 7.38 (m, 1 H), 6.90 - 6.99 (m, 2 H), 6.61 (s, 1 H), 3.85 (s, 3 H), 0.95 (t, *J*=7.84 Hz, 9 H), 0.78 - 0.84 (m, 6 H); ^{13}C NMR (126 MHz, $CDCl_3$) δ ppm 159.0, 157.9, 153.2, 133.0, 128.1, 127.7, 127.3, 125.3, 123.9, 114.2, 113.6, 111.4, 55.3, 7.5, 4.2; HRMS (EI) calcd. for $C_{23}H_{28}O_2Si$ [M+]: 364.18586. Found: 364.18584.



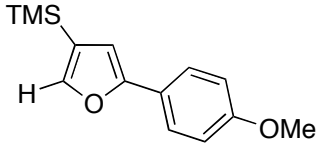
2d: ^{1}H NMR (500 MHz, $CDCl_3$) δ ppm 7.53 - 7.63 (m, 2 H), 7.35 - 7.43 (m, 2 H), 7.27 - 7.33 (m, 1 H), 5.99 (s, 1 H), 1.34 (s, 9 H), 0.89 - 0.98 (m, 9 H), 0.73 - 0.80 (m, 6 H); ^{13}C NMR (126 MHz, $CDCl_3$) δ ppm 163.3, 156.9, 133.5, 128.0, 127.3, 127.1, 111.6, 109.4, 32.6, 29.2, 7.6, 4.3; HRMS (EI) calcd. for $C_{20}H_{30}OSi$ [M+]: 314.20659. Found: 314.20694.



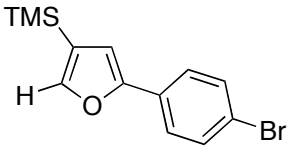
2e: ^{1}H NMR (500 MHz, $CDCl_3$) δ ppm 7.61 - 7.64 (m, 2 H), 7.40 - 7.45 (m, 2 H), 7.30 (s, 1 H), 7.27 - 7.30 (m, 1 H), 2.33 (s, 3 H), 0.31 (s, 9 H); ^{13}C NMR (126 MHz, $CDCl_3$) δ ppm 149.9, 146.3, 131.8, 128.4, 126.7, 125.9, 122.4, 119.8, 12.3, -0.6; HRMS (EI) calcd. for $C_{14}H_{18}OSi$ [M+]: 230.11269. Found: 230.11235.



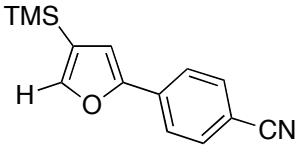
2f: (contained ca. 8% of the desilylated furan) ^{1}H NMR (500 MHz, $CDCl_3$) δ ppm 7.65 - 7.73 (m, 2 H), 7.34 - 7.43 (m, 3 H), 7.22 - 7.30 (m, 1 H), 6.66 (d, *J*=0.92 Hz, 1 H), 0.27 (s, 9 H); ^{13}C NMR (126 MHz, $CDCl_3$) δ ppm 154.7, 146.6, 130.9, 128.6, 127.2, 123.9, 121.0, 108.7, -0.7; HRMS (EI) calcd. for $C_{13}H_{16}OSi$ [M+]: 216.09704. Found: 216.09793.



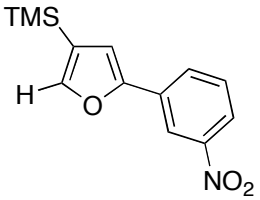
2g: ^{1}H NMR (500 MHz, $CDCl_3$) δ ppm 7.61 (s, 2 H), 7.33 (d, *J*=0.73 Hz, 1 H), 6.92 (s, 2 H), 6.51 (d, *J*=0.92 Hz, 1 H), 3.84 (s, 3 H), 0.26 (s, 9 H); ^{13}C NMR (126 MHz, $CDCl_3$) δ ppm 158.9, 154.7, 145.9, 125.3, 124.0, 120.9, 114.1, 107.0, 55.3, -0.7; HRMS (EI) calcd. for $C_{14}H_{18}O_2Si$ [M+]: 246.10761. Found: 246.10680.



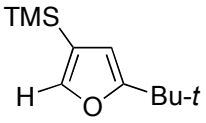
2h: (14 : 1 mixture with **3h**) ^{1}H NMR (500 MHz, $CDCl_3$) δ ppm 7.45 - 7.61 (m, 4 H), 7.36 (d, *J*=0.73 Hz, 1 H), 6.64 (d, *J*=0.73 Hz, 1 H), 0.25 (s, 9 H); ^{13}C NMR (126 MHz, $CDCl_3$) δ ppm 153.6, 146.9, 131.8, 129.8, 125.4, 121.3, 120.9, 109.3, -0.7; HRMS (EI) calcd. for $C_{13}H_{15}BrOSi$ [M+]: 294.00755. Found: 294.00712.



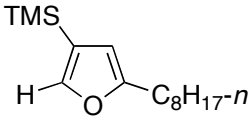
2i: (10 : 1 mixture with **3i**) ^{1}H NMR (500 MHz, $CDCl_3$) δ ppm 7.74 (s, 2 H), 7.61 - 7.68 (m, 2 H), 7.42 (d, *J*=0.73 Hz, 1 H), 6.80 (d, *J*=0.73 Hz, 1 H), 0.26 (s, 9 H); ^{13}C NMR (126 MHz, $CDCl_3$) δ ppm 152.7, 148.1, 134.6, 132.6, 124.0, 121.9, 119.0, 112.0, 110.1, -0.8; HRMS (EI) calcd. for $C_{14}H_{15}NOSi$ [M+]: 241.09229. Found: 241.09316.



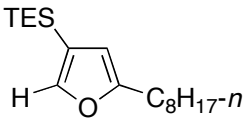
2j: (8 : 1 mixture with **3j**) ^{1}H NMR (500 MHz, $CDCl_3$) δ ppm 8.49 (t, *J*=1.93 Hz, 1 H), 8.08 (ddd, *J*=8.21, 2.25, 0.92 Hz, 1 H), 7.96 (ddd, *J*=7.84, 1.60, 1.01 Hz, 1 H), 7.54 (t, *J*=8.07 Hz, 1 H), 7.42 (d, *J*=0.73 Hz, 1 H), 6.80 (d, *J*=0.73 Hz, 1 H), 0.27 (s, 9 H); ^{13}C NMR (126 MHz, $CDCl_3$) δ ppm 152.2, 148.7, 147.7, 132.4, 129.7, 129.3, 121.7, 121.6, 118.6, 111.1, -0.8; HRMS (EI) calcd. for $C_{13}H_{15}NO_3Si$ [M+]: 261.08212. Found: 261.08224.



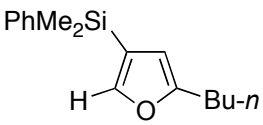
2k: ^{1}H NMR (500 MHz, $CDCl_3$) δ ppm 7.20 (d, *J*=0.92 Hz, 1 H), 5.92 (d, *J*=0.92 Hz, 1 H), 1.29 (s, 9 H), 0.20 (s, 9 H); ^{13}C NMR (126 MHz, $CDCl_3$) δ ppm 164.8, 145.2, 118.8, 105.2, 32.5, 29.1, -0.6; HRMS (EI) calcd. for $C_{11}H_{20}OSi$ [M+]: 196.12834. Found: 196.12911.



2l: (contained ca. 6% of the desilylated furan) ^{1}H NMR (500 MHz, $CDCl_3$) δ ppm 7.20 (d, *J*=0.92 Hz, 1 H), 5.92 - 5.98 (m, 1 H), 2.57 - 2.65 (m, 2 H), 1.59 - 1.71 (m, 2 H), 1.22 - 1.40 (m, 10 H), 0.89 (t, *J*=6.90 Hz, 3 H), 0.20 (s, 9 H); ^{13}C NMR (126 MHz, $CDCl_3$) δ ppm 157.2, 145.3, 119.3, 108.0, 31.9, 29.3, 29.3, 29.2, 28.1, 27.9, 22.7, 14.1, -0.7; HRMS (EI) calcd. for $C_{15}H_{28}OSi$ [M+]: 252.19094. Found: 252.19014.



2m: ^{1}H NMR (500 MHz, $CDCl_3$) δ ppm 7.20 (d, *J*=0.92 Hz, 1 H), 5.83 - 6.01 (m, 1 H), 2.61 (t, *J*=7.34 Hz, 2 H), 1.59 - 1.68 (m, 2 H), 1.22 - 1.38 (m, 10 H), 0.97 (t, *J*=7.89 Hz, 9 H), 0.85 - 0.91 (m, 3 H), 0.69 (q, *J*=8.13 Hz, 6 H); ^{13}C NMR (126 MHz, $CDCl_3$) δ ppm 156.9, 145.8, 115.6, 108.5, 31.9, 29.3, 29.3, 29.2, 28.0, 27.9, 22.7, 14.1, 7.4, 3.9; HRMS (EI) calcd. for $C_{18}H_{34}OSi$ [M+]: 294.23789. Found: 294.23822.



2n: ^{1}H NMR (500 MHz, $CDCl_3$) δ ppm 7.53 - 7.60 (m, 2 H), 7.33 - 7.42 (m, 3 H), 7.24 (d, *J*=0.92 Hz, 1 H), 6.00 (dt, *J*=0.92, 0.73 Hz, 1 H), 2.64 (dt, *J*=7.68, 0.73 Hz, 2 H), 1.59 - 1.69 (m, 2 H), 1.32 - 1.44 (m, 2 H), 0.95 (t, *J*=7.43 Hz, 3

H), 0.48 (s, 6 H); ^{13}C NMR (126 MHz, $CDCl_3$) δ ppm 157.4, 146.4, 138.6, 133.9, 129.1, 127.8, 117.3, 108.4, 30.2, 27.6, 22.4, 13.9, -1.9; HRMS (EI) calcd. for $C_{16}H_{22}OSi$ [M+]: 258.14399. Found: 258.14410.

Computational Section

1. Computation Details

All DFT calculations were performed with the Gaussian 03 program package.[1] The geometry optimizations of all minima and transition states along the potential energy surface were performed at the B3LYP levels of theory.[2] This method was proven to be appropriate for the investigation of gold-based systems,[3] and has been successfully applied to the mechanistic studies of various catalytic reactions.[4] The 6-31G* basis set was used for C, H, O, P, Si, S, F, and Cl atoms,[5] while LANL2DZ basis set[6] was used for Au. The vibrational frequencies were computed at the same level of theory as

[1] Gaussian 03, Revision C.02, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, Jr., J. A.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; and Pople, J. A.; Gaussian, Inc., Wallingford CT, 2004.

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that for the geometry optimization to check whether the optimized geometrical structure is at an energy minimum or a transition state and to evaluate the zero-point vibration energy (ZPVE). Intrinsic reaction coordinate (IRC)[7] calculations were used to confirm that the transition states found connected the related reactants and products. Solvent effects were computed by the conductor-like polarizable continuum model (CPCM) with UAKS radii[8] at the B3LYP/6-31G*(LANL2DZ) level using the gas phase optimized structures. The dielectric constant in the CPCM calculations was set to $\varepsilon = 2.379$ and 8.93 for the simulation of toluene and dichloroethane (DCE) solvent, respectively. The ΔE_0 values are the ZPVE corrected relative electronic energy in the gas phase. The ΔH_{298} values are gas phase relative enthalpies. Solvation free energies (ΔG_{Tol} and ΔG_{DCE}) in toluene and DCE were calculated by adding the solvation energies to the computed gas phase relative free energies (ΔG_{298}).

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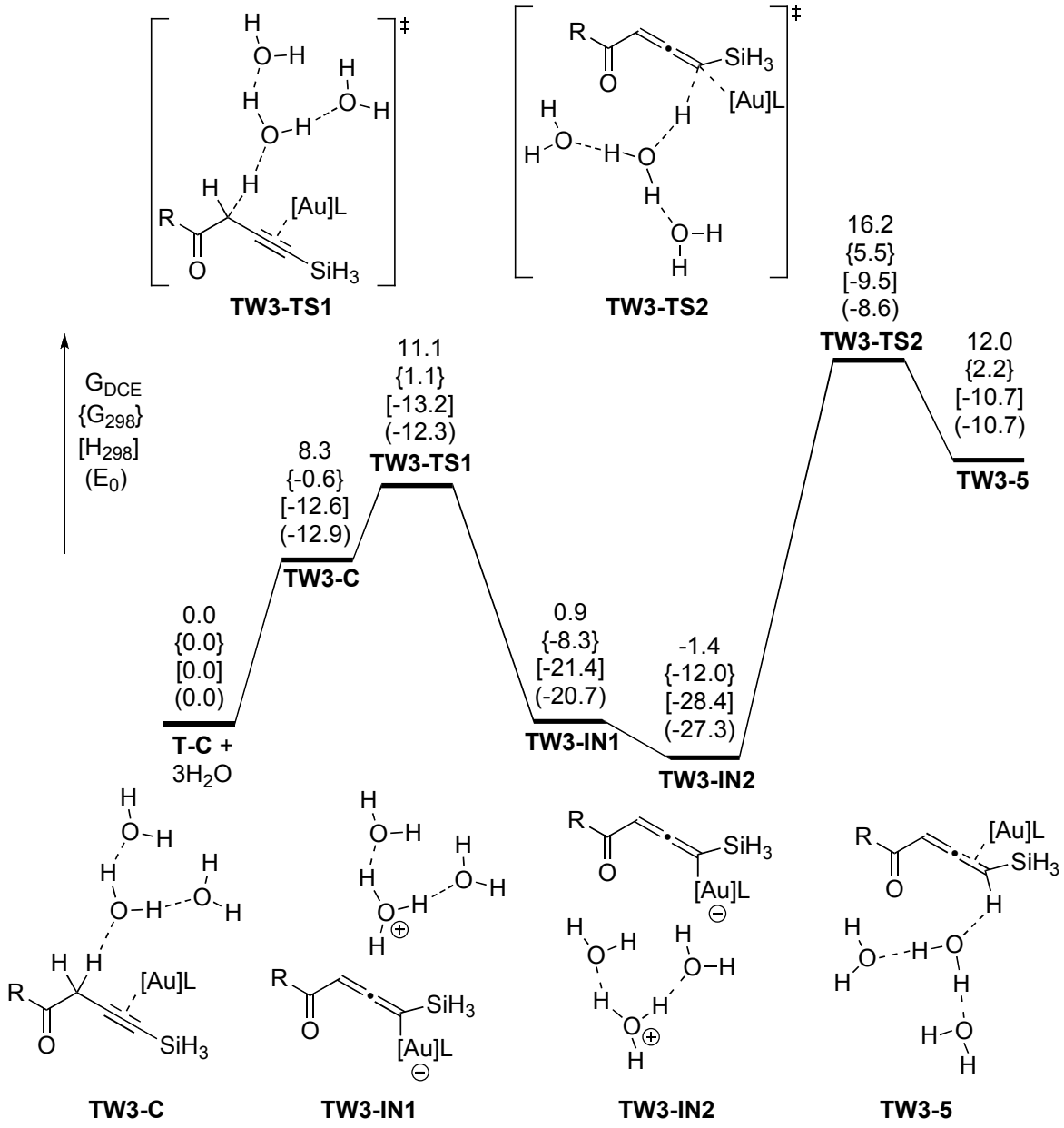
2. The Possibility of $(H_2O)_3$-Catalyzed Allenization in $Au(PH_3)OTf$-Catalyzed Reactions

The relative energies in **Scheme S1** show this process requires activation energy of 17.6 kcal/mol, about 6.7 kcal/mol higher than that of the cyclization transition state **T-TS1** (**Scheme 6**).

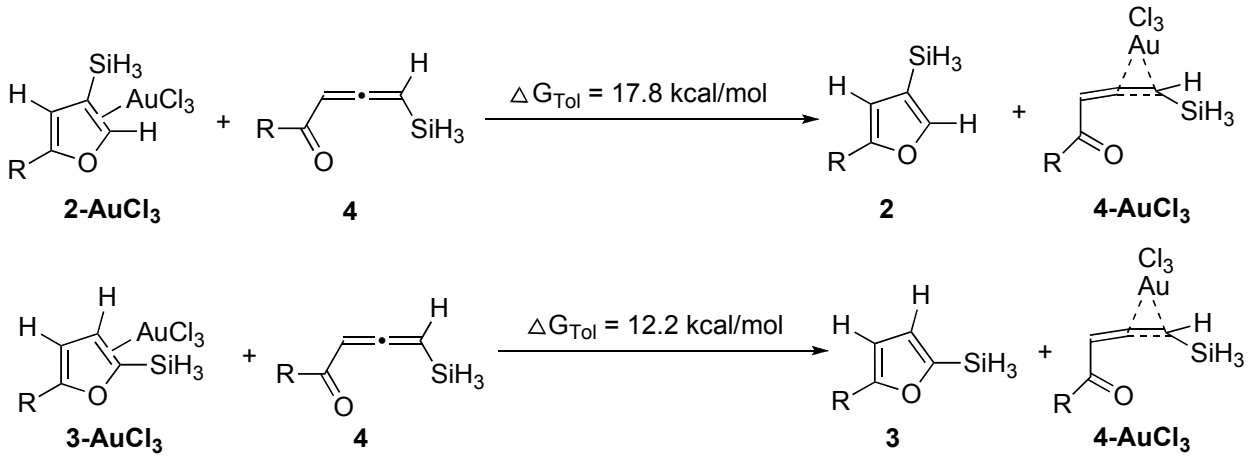
Scheme S1. Potential energy surface for a possible $(H_2O)_3$-catalyzed allenization in $Au(PH_3)OTf$-catalyzed reactions (in kcal/mol, the energies in toluene are similar)



3. Energetics for the Generation of Products 2 and 3 from Complexes 2-$AuCl_3$ and 3-$AuCl_3$, respectively (R = H)

Scheme 2 shows that the product complexes **2-$AuCl_3$** and **3-$AuCl_3$** could be formed after the 1,2-Si- and 1,2-H migrations, respectively. To complete the catalytic cycle, a ligand exchange reaction as illustrated in **Scheme S2** may proceed to generate the final products and the active complex of allene and $AuCl_3$. The free energy values indicate the generations of **2** and **3** from the reactions of allene **4** with **2-$AuCl_3$** and **3-$AuCl_3$** are endergonic by 17.8 and 12.2 kcal/mol, respectively.

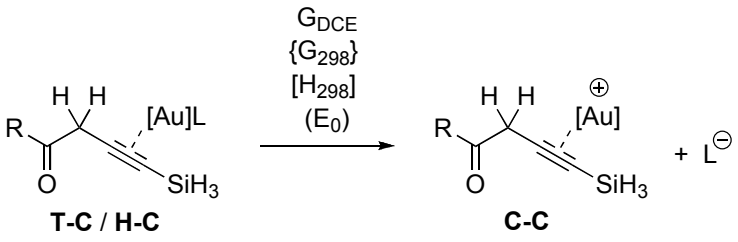
Scheme S2. Generation of products **2** and **3** from complexes **2-$AuCl_3$** and **3-$AuCl_3$**



4. Energetics for the Dissociation of the OTf and SbF_6 Ligands from the Reactant Complexes

The energies in **Scheme S3** indicate that only the dissociation of OTf ligand from the reactant complex **T-C** is possible in DCE solution. In other cases, the dissociation energies are much higher.

Scheme S3. Energies for the formation of cationic intermediate **C-C**

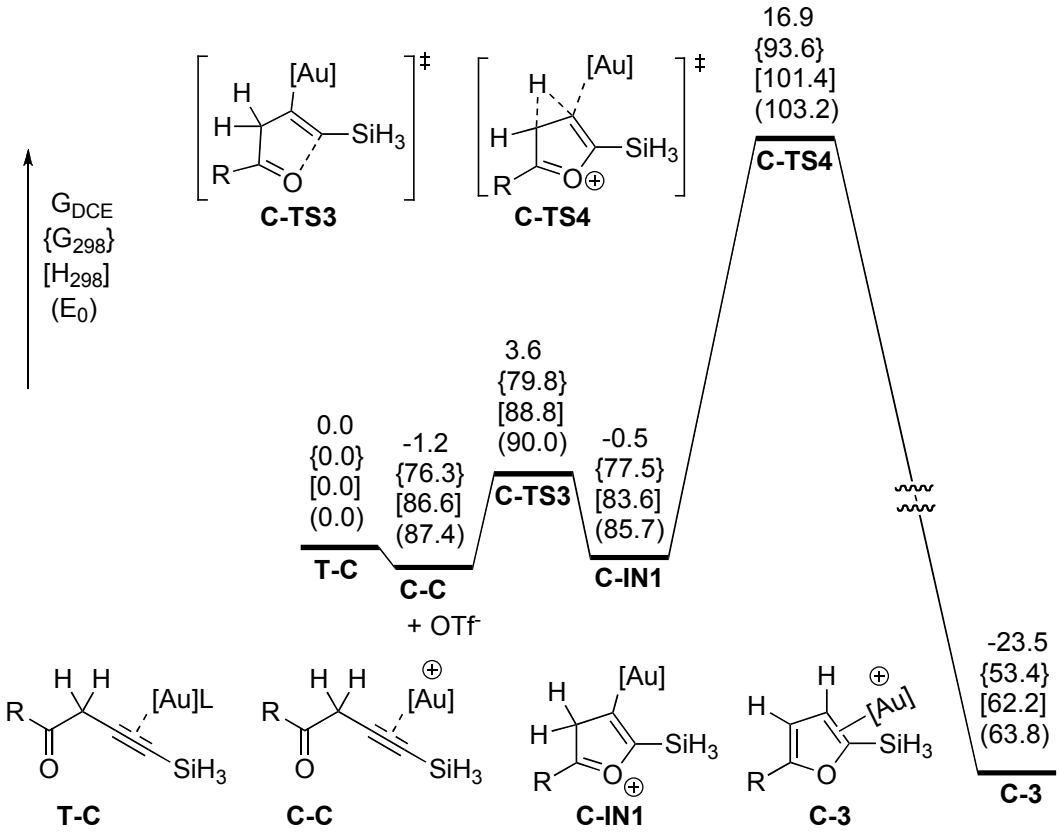


	In DCE	In Toluene
L = OTf	-1.2 {76.3} [86.6] (87.4)	25.1 {76.3} [86.6] (87.4)
L = SbF_6	10.8 {86.9} [97.8] (98.7)	39.8 {86.9} [97.8] (98.7)

5. The Possible Reaction via Cationic Intermediate C-C

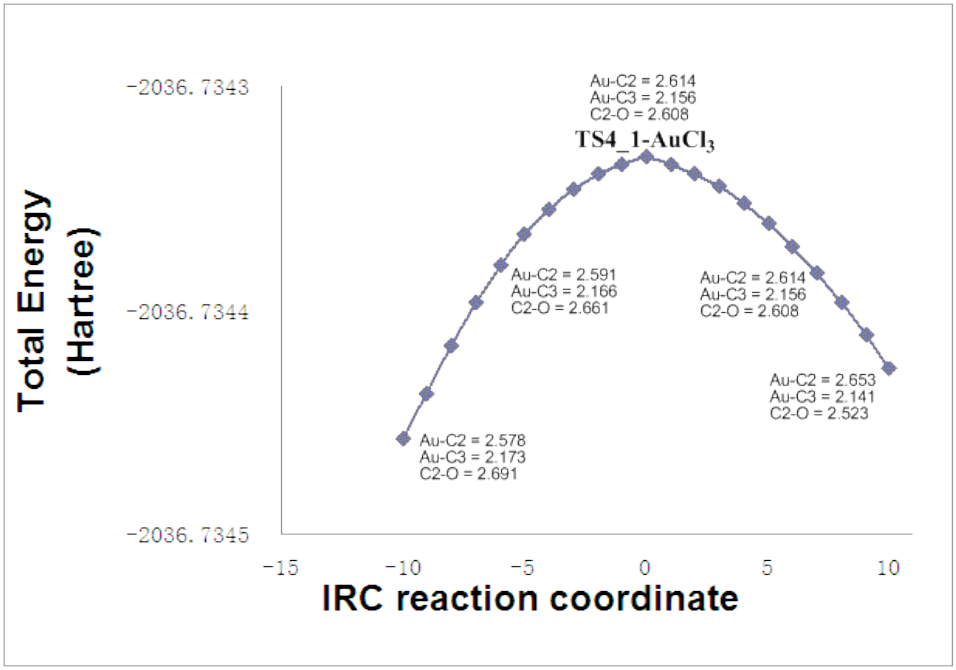
As **Scheme S3** shows, the formation of cationic intermediate **C-C** is possible in DCE when L = OTf, in **Scheme S4** we have calculated the following reaction without the influence of any ligand. Although the cyclization (**C-TS3**) is quite easy, this process is reversible, and the following 1,2-H migration (**C-TS4**) requires an activation energy of 17.4 kcal/mol. Actually, according to **Scheme 6**, the **C-IN1** intermediate would interact with the OTf ligand strongly to give the more energetically favorable **T-IN1** and HOTf .

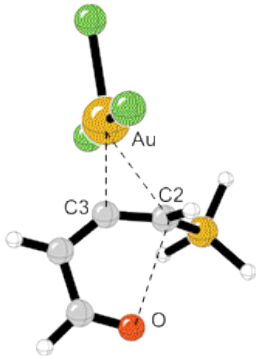
Scheme S4. Potential energy surface for the reaction via cationic intermediate **C-C**



6. IRC Plots for Selected Transition States

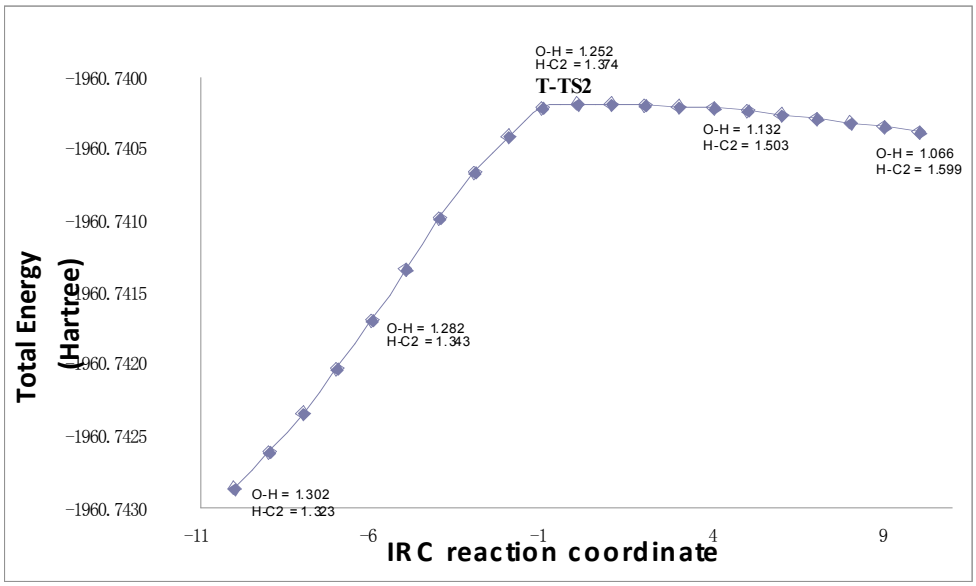
IRC analysis of TS4_1-$AuCl_3$

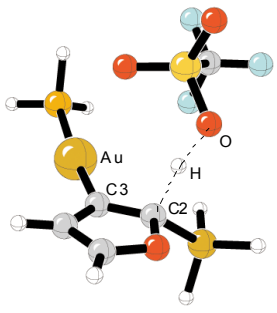




TS4_1-$AuCl_3$

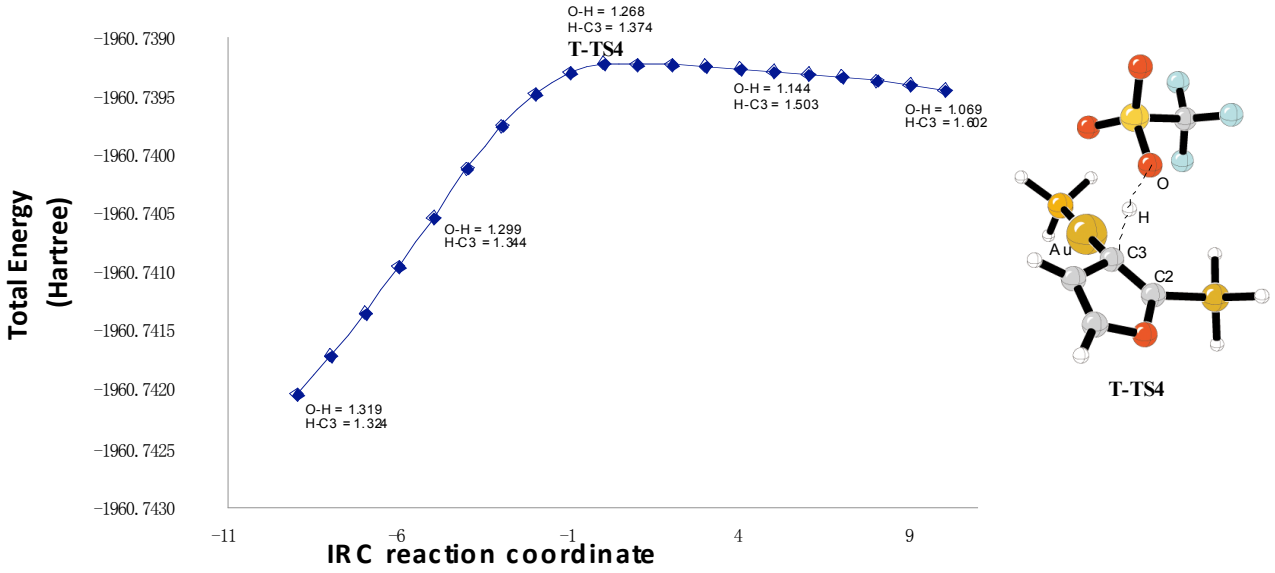
IRC analysis of T-TS2



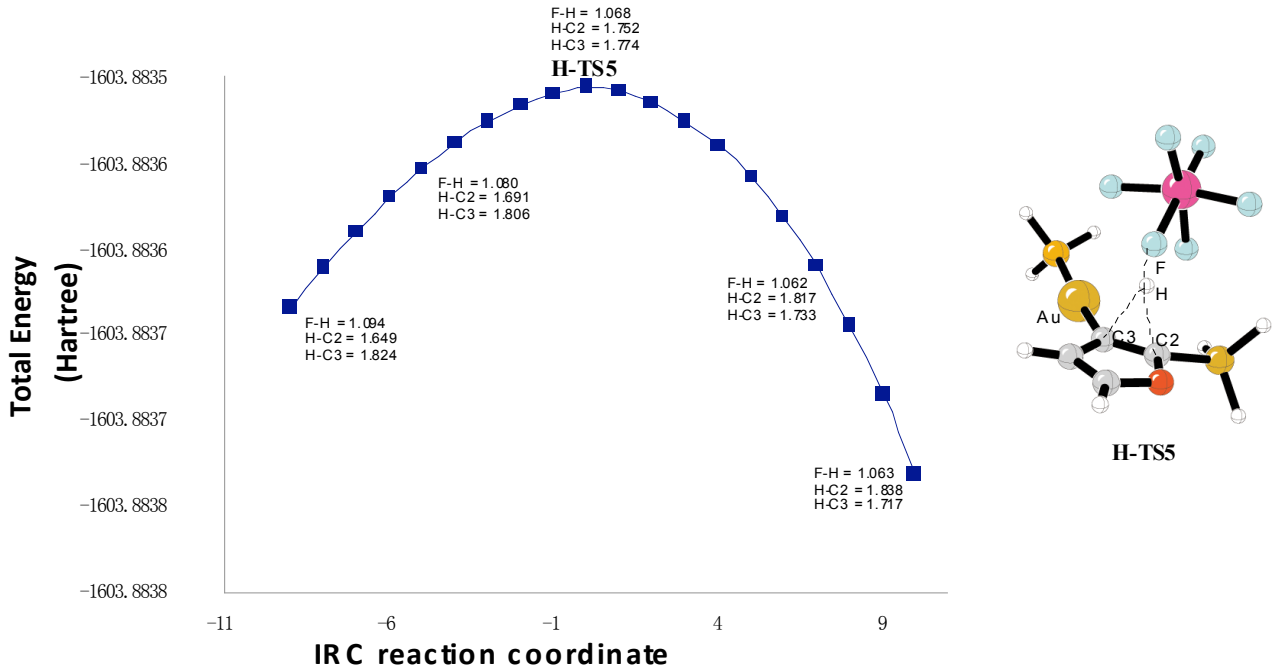


T-TS2

IRC analysis of T-TS4



IRC analysis of TS2-SbF_6



7. Tables of Computed Energy Values

Table S1. Gas phase free energies (in Hartree) for the species given in Scheme 2, calculated at B3LYP/6-31G* (LANL2DZ for Au and Sb) level

R \ Species	1'	1,2-R TS	12-Si TS
Me	−2076.021117	−2075.969677	−2076.006245
Ph	−2267.699090	−2267.658300	−2267.687319
H	−2036.730955	−2036.694135	−2036.711765

Table S2. Energies (in Hartree) for the species given in the Schemes 4, 6, 7, and 8 and the Supporting Information, calculated at B3LYP/6-31G* (LANL2DZ for Au and Sb) level

Species	E_0[a]	H_{298}[b]	G_{298}[c]	E[d]	G_{DCE}[e]	G_{Tol}[e]
4-$AuCl_3$	-2036.651647	-2036.635544	-2036.697592	-2036.7378168	-2036.727995	-2036.727250
TS4_1- $AuCl_3$	-2036.648233	-2036.633113	-2036.692464	-2036.7343317	-2036.727995	-2036.724981
1-$AuCl_3$	-2036.687021	-2036.672621	-2036.730816	-2036.777346	-2036.779301	-2036.772992
TS1_2- $AuCl_3$	-2036.669935	-2036.656278	-2036.712116	-2036.7601858	-2036.762127	-2036.756877
TS1_3- $AuCl_3$	-2036.650983	-2036.636798	-2036.694294	-2036.7370094	-2036.736414	-2036.731634
2- $AuCl_3$	-2036.698674	-2036.684262	-2036.741588	-2036.7893276	-2036.787867	-2036.783001
3- $AuCl_3$	-2036.696242	-2036.681788	-2036.739299	-2036.7866962	-2036.784013	-2036.780207
T-C	-1960.592005	-1960.568779	-1960.650726	-1960.731171	-1960.726307	-1960.722515
T-TS1	-1960.575384	-1960.553734	-1960.629608	-1960.715055	-1960.713901	-1960.70894
T-IN2	-1960.613547	-1960.59175	-1960.66957	-1960.755452	-1960.741562	-1960.740994
T-IN1	-998.645426	-998.633142	-998.686647	-998.7477219	-998.741234	-998.73994
T-TS2	-1960.602815	-1960.581743	-1960.656818	-1960.740175	-1960.731587	-1960.728895
T-1	-1960.610465	-1960.589768	-1960.662967	-1960.754431	-1960.751626	-1960.747924
T-TS4	-1960.602385	-1960.581154	-1960.656988	-1960.73922	-1960.730221	-1960.727881
T-3	-1960.625137	-1960.603973	-1960.678305	-1960.768818	-1960.766863	-1960.762807
T-TS3	-1960.594036	-1960.573924	-1960.64455	-1960.73788	-1960.736427	-1960.732741
T-2	-1960.624155	-1960.6031	-1960.676783	-1960.768172	-1960.766195	-1960.762611
T-TS5	-1960.5831	-1960.56084	-1960.638545	-1960.717856	-1960.708192	-1960.705962
T-IN3	-1960.589205	-1960.566198	-1960.646477	-1960.728217	-1960.715282	-1960.713961
T-TS6	-1960.569209	-1960.546633	-1960.625735	-1960.703006	-1960.697042	-1960.69338
T-5	-1960.587766	-1960.564979	-1960.644047	-1960.726781	-1960.721512	-1960.717818
T-TS7	-1960.579081	-1960.557628	-1960.632508	-1960.718943	-1960.714167	-1960.711113
C-1	-999.010531	-998.999085	-999.049265	-999.1251372	-999.167962	-999.148291
C-TS1	-998.993402	-998.981564	-999.033267	-999.107629	-999.150271	-999.131275
C-TS2	-998.973819	-998.961638	-999.014657	-999.0842541	-999.126155	-999.107289
C-2	-999.018656	-999.006099	-999.059616	-999.1334958	-999.175586	-999.157005
C-3	-999.01965	-999.006988	-999.06241	-999.1340098	-999.177157	-999.157333
TW3-C	-2189.805909	-2189.77469	-2189.87339	-2190.021145	-2190.007166	-2190.004258
TW3-TS1	-2189.804993	-2189.775611	-2189.87072	-2190.019036	-2190.003402	-2190.001942
TW3-IN1	-2189.818303	-2189.788703	-2189.885661	-2190.033224	-2190.018833	-2190.016385
TW3-IN2	-2189.828842	-2189.799756	-2189.891665	-2190.04529	-2190.028594	-2190.027057
TW3-TS2	-2189.799129	-2189.769659	-2189.863805	-2190.011256	-2189.994392	-2189.992795
TW3-5	-2189.802478	-2189.771561	-2189.868995	-2190.017518	-2190.002103	-2189.999922
H-C	-1603.777519	-1603.753236	-1603.835949	-1603.903525	-1603.893844	-1603.890779
H-TS1	-1603.760151	-1603.737394	-1603.815245	-1603.886371	-1603.880147	-1603.876103
H-IN1	-1603.764873	-1603.742352	-1603.819036	-1603.892203	-1603.88745	-1603.882801
H-TS2	-1603.753363	-1603.731028	-1603.807844	-1603.878989	-1603.861978	-1603.861438
$(H_2O)_3$	-229.193356	-229.18576	-229.221766	-229.2675348	-229.272668	-229.270119
H-5	-1603.768971	-1603.745185	-1603.825259	-1603.894822	-1603.887407	-1603.882775
H-TS3	-1603.759284	-1603.736529	-1603.814438	-1603.885197	-1603.880147	-1603.876103

H-1	-1603.791793	-1603.769821	-1603.844684	-1603.921764	-1603.91493	-1603.911027
H-3	-1603.806078	-1603.783674	-1603.860573	-1603.935871	-1603.928631	-1603.925113
H-TS5	-1603.758582	-1603.736623	-1603.81191	-1603.883506	-1603.866888	-1603.865809
H-3	-1603.806078	-1603.783674	-1603.860573	-1603.935871	-1603.928631	-1603.925113
H-TS4	-1603.776425	-1603.754916	-1603.828688	-1603.906004	-1603.895512	-1603.898728
H-2	-1603.805398	-1603.783133	-1603.858901	-1603.935546	-1603.928581	-1603.925189
HW-C1	-1832.988653	-1832.956281	-1833.055621	-1833.190323	-1833.171281	-1833.167984
HW-TS1	-1832.974012	-1832.942683	-1833.039697	-1833.175407	-1833.15784	-1833.155153
HW-IN1	-1833.020018	-1832.990553	-1833.083643	-1833.225438	-1833.204016	-1833.203429
HW-TS4	-1832.983416	-1832.952622	-1833.048289	-1833.182739	-1833.164773	-1833.163002
HW-IN2	-1832.993827	-1832.96299	-1833.058958	-1833.196231	-1833.178325	-1833.17672
HW-TS5	-1832.973800	-1832.943768	-1833.037595	-1833.171485	-1833.155395	-1833.152101
HW-5	-1832.978571	-1832.946408	-1833.045494	-1833.179646	-1833.163723	-1833.160121
HW-TS2	-1833.009008	-1832.979838	-1833.071077	-1833.2108229	-1833.191849	-1833.190098
HW-TS3	-1833.007657	-1832.978338	-1833.070343	-1833.2090997	-1833.189439	-1833.188197

[a] Sum of electronic and zero-point energies [b] Sum of electronic and thermal enthalpies

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

[e] Total free energies in DCE and Toluene solutions, respectively

8. Cartesian Coordinates for All Species

4- $AuCl_3$

6	-2.239602	-0.744975	0.073195
6	-0.995740	-0.325181	0.036425
1	-0.737004	0.726189	-0.040708
6	-3.368940	-1.466395	0.185111
6	0.104771	-1.342106	0.113793
8	-0.074145	-2.528507	0.276535
14	-3.975289	-2.264929	1.827220
1	-5.361982	-1.828260	2.093990
1	-3.945899	-3.715656	1.512652
1	-3.038055	-1.931548	2.914695
79	-4.038755	0.812169	-0.037550
1	-3.799653	-1.835880	-0.749829
17	-3.697626	1.228213	2.281042
17	-5.215941	2.831001	-0.262157
17	-4.311380	0.353589	-2.358434
1	1.119647	-0.910679	0.016943

1-$AuCl_3$

6	-3.600534	0.736501	0.713992
6	-2.865689	1.883115	0.988565
6	-1.999619	1.561584	2.030679
6	-2.193947	0.148158	2.329210
1	-2.453825	-0.062878	3.372298
79	-0.691890	2.768531	3.006843
1	-2.953331	2.835263	0.485805
1	-4.378022	0.560946	-0.021955
8	-3.285871	-0.292464	1.468145
14	-0.638851	-0.963621	1.888186
1	0.495737	-0.490708	2.701979
1	-1.037404	-2.349716	2.222252
1	-0.414895	-0.800619	0.434396
17	0.828162	4.199276	4.145157
17	-0.200944	3.815131	0.921809
17	-1.223762	1.634498	5.051170

TS4_1- $AuCl_3$

6	-2.334949	-0.423478	0.056743
6	-1.026892	-0.186632	0.058876
1	-0.552194	0.784842	0.009887
6	-3.154508	-1.510986	0.164221
6	-0.241837	-1.439440	0.168538
8	-0.760841	-2.543168	0.242765
14	-3.693493	-2.331325	1.816010
1	-5.091648	-1.925863	2.080867
1	-3.627986	-3.783943	1.528454
1	-2.764559	-1.923792	2.885867
79	-3.988064	0.953680	-0.088397
1	-3.560476	-1.902626	-0.773568
17	-3.742836	1.353066	2.247203
17	-5.522155	2.735728	-0.296350
17	-4.158154	0.444109	-2.410705
1	0.856304	-1.334245	0.199446

TS1_2- $AuCl_3$

6	-3.544712	0.762882	0.738309
6	-2.719629	1.840874	0.770440
6	-1.955195	1.750481	1.997571
6	-2.388337	0.546792	2.581867
1	-2.237337	0.146948	3.575221
79	-0.926682	3.279675	2.967998
1	-2.653732	2.641090	0.049406
1	-4.284375	0.413407	0.032885
8	-3.357607	-0.036927	1.829055
14	-0.371285	0.194610	1.585484
1	0.104890	-0.750609	2.610803
1	-0.966910	-0.497072	0.420172
1	0.660962	1.165326	1.183649
17	0.172427	5.030168	4.135662
17	-1.708146	4.852296	1.367121
17	-0.095448	1.660258	4.531148

TS1_3- $AuCl_3$

6	-3.593683	0.960887	0.421902
6	-3.131269	2.061147	1.054576
6	-1.967661	1.643539	1.815532
6	-1.833432	0.244999	1.559148
1	-2.335206	0.806821	2.716367
79	-0.648821	2.815651	2.874239
1	-3.517042	3.067630	0.998967
1	-4.425170	0.776342	-0.242673
8	-2.842125	-0.143318	0.729732
14	-0.513681	-1.079123	2.017969
1	0.733075	-0.379739	2.369453
1	-1.052272	-1.914582	3.110954
1	-0.381762	-1.865929	0.769602
17	0.870746	4.168272	4.093936
17	-0.478125	4.209473	0.958083
17	-0.955699	1.296307	4.713655

3-$AuCl_3$

6	-2.966408	1.397833	0.170259
6	-3.660214	1.606233	1.347392
6	-2.827353	1.116848	2.359901
6	-1.620048	0.641092	1.764462
1	-3.020172	1.094028	3.424815
79	-0.422349	2.433148	2.576965
1	-4.624571	2.081616	1.450774
1	-3.207767	1.626514	-0.858841
8	-1.797135	0.804426	0.376403
14	-0.631570	-0.970289	2.150822
1	0.821011	-0.714879	2.115303
1	-1.100340	-1.526089	3.433906
1	-1.013318	-1.879797	1.039052
17	0.999909	4.144588	3.387412
17	-0.793326	3.691747	0.599616
17	-0.206864	1.221413	4.619905

2-$AuCl_3$

6	-3.690103	1.401739	1.038910
6	-2.457029	1.120228	0.464643
6	-1.562662	0.882227	1.517053
6	-2.315588	1.101258	2.718498
1	-2.220608	0.551133	3.647586
79	-1.441130	3.070900	3.364351
1	-2.242666	1.114390	-0.594819
1	-4.645722	1.657186	0.601295
8	-3.654111	1.319488	2.357567
14	0.262594	0.368874	1.349655
1	0.543379	-0.719738	2.310441
1	0.390659	-0.122598	-0.045794
1	1.141703	1.536652	1.564747
17	-0.554941	5.095583	4.227058
17	-2.776144	4.275184	1.812670
17	-0.081089	1.756089	4.811389

T-1

6	-2.872049	0.786162	-0.149981
6	-1.984275	1.711243	0.382798
6	-1.841852	1.416641	1.746303
6	-2.622292	0.212985	1.975282
1	-3.331308	0.208148	2.806231
79	-0.839708	2.329185	3.261140
1	-1.518399	2.516602	-0.167841
1	-3.246536	0.669614	-1.161422
8	-3.316777	-0.080691	0.728145
14	-1.444357	-1.342713	2.344582
1	-0.266291	-1.017158	3.158938
1	-2.300835	-2.443245	2.827082
1	-0.992354	-1.665331	0.956600
15	0.181468	3.220713	5.214184
1	0.513749	4.593358	5.269710
1	-0.597003	3.071753	6.371800
1	1.403564	2.646759	5.594548
16	-1.610604	0.076158	5.907178
8	-2.303659	1.049956	6.767518
8	-2.386955	-0.373185	4.709059
8	-0.188819	0.406889	5.603841
6	-1.482348	-1.484235	6.907525
9	-0.776532	-1.269596	8.025397
9	-0.866111	-2.440432	6.192058
9	-2.699234	-1.927011	7.247016

T-2

6	-3.517814	1.927361	0.468586
6	-2.196818	1.637120	0.406258
6	-1.889244	0.767410	1.540726
6	-3.121720	0.635881	2.193865
1	-3.420251	0.025756	3.034954
79	-1.477137	2.120203	3.438288
1	-1.501153	1.966017	-0.352828
1	-4.183059	2.528774	-0.131918
8	-4.092992	1.324267	1.557753
14	-0.404528	-0.431477	1.622501
1	0.710918	0.082271	2.445111
1	-0.858245	-1.763778	2.067449
1	0.062883	-0.502953	0.209642
15	-0.835445	3.552642	5.139322
1	-0.569580	4.894935	4.790537
1	-1.763998	3.716532	6.174393
1	0.341935	3.200529	5.809763
16	-1.135290	-0.202157	5.975445
6	0.703678	-0.441524	5.833986
9	1.281026	-0.475564	7.038942
9	0.998296	-1.573901	5.182377
9	1.249318	0.588735	5.139980
8	-1.239136	1.174983	6.531802
8	-1.610357	-1.293160	6.826643
8	-1.562948	-0.280871	4.535671

T-3

6	-3.085842	1.327816	0.268980
6	-3.910918	1.141761	1.345282
6	-3.156231	0.387147	2.281731
6	-1.877208	0.169759	1.735042
1	-3.470486	0.014196	3.249061
79	-1.018008	1.615597	3.289418
1	-4.923529	1.501990	1.455645
1	-3.220294	1.846970	-0.670015
8	-1.879338	0.772675	0.460709
14	-0.732236	-1.350032	1.879032
1	-0.970125	-1.978905	3.189456
1	-1.108660	-2.264062	0.767532
1	0.676948	-0.930284	1.699729
15	0.111722	3.143674	4.630918
1	0.723014	4.219364	3.948343
1	-0.653945	3.827805	5.582562
1	1.189653	2.646961	5.372958
16	-1.391856	0.109005	6.406465
6	0.105675	-0.969584	6.171719
9	0.877687	-0.977088	7.262855
9	-0.242416	-2.230578	5.882132
9	0.856738	-0.504577	5.137681
8	-0.787664	1.457636	6.593005
8	-2.098046	-0.457053	7.556386
8	-2.083573	-0.040939	5.084426

T-5

6	-3.169840	0.004719	-0.097976
6	-2.082801	0.084892	0.733278
14	-0.344582	-0.537337	0.255962
1	-0.383511	-0.951178	-1.167861
1	0.653329	0.535571	0.458037
1	-0.042234	-1.693249	1.134320
6	-4.120315	-0.688350	-0.715378
1	-2.262990	0.255834	1.798237
1	-4.825493	-0.230935	-1.401620
6	-4.225731	-2.150590	-0.464827
1	-5.084939	-2.639502	-0.968779
8	-3.452984	-2.793348	0.217649
79	-2.573973	2.056424	-0.164495
15	-3.529074	4.030612	-1.279507
1	-4.616716	4.018278	-2.180033
1	-3.963248	5.017382	-0.376607
1	-2.595933	4.768916	-2.029128
6	0.881912	4.037125	2.040432
9	1.286223	4.100625	3.312663
9	1.460131	2.975353	1.458330
9	1.277019	5.143391	1.401678
16	-0.969768	3.877290	1.975190
8	-1.197946	3.812566	0.460086
8	-1.503943	5.099908	2.578940
8	-1.265425	2.584798	2.624160

T-C

6	-2.975853	0.024218	0.065456
6	-1.768552	0.255162	-0.162384
14	0.068152	0.130735	-0.349743
1	0.437580	-1.303493	-0.309250
1	0.456684	0.729840	-1.648506
1	0.709424	0.872867	0.760445
6	-4.185643	-0.696060	0.475381
1	-4.866858	-0.028727	1.029578
1	-4.761095	-1.019628	-0.405033
6	-3.862404	-1.923988	1.321416
1	-4.768203	-2.478953	1.643587
8	-2.753702	-2.285287	1.633099
79	-2.900283	2.177918	-0.449314
15	-2.662275	4.493379	-1.055803
1	-3.532788	4.907801	-2.077994
1	-3.004191	5.398432	-0.037293
1	-1.450836	5.057938	-1.508101
16	-6.023677	2.974199	0.897522
6	-5.140611	4.062288	2.122563
9	-5.786555	4.104833	3.287166
9	-3.888602	3.600087	2.347151
9	-5.025308	5.317215	1.646868
8	-5.934661	1.629764	1.504391
8	-7.347698	3.574418	0.743907
8	-5.142924	3.129834	-0.329089

T-IN1

6	-3.027647	-0.032132	-0.466979
6	-2.176673	-0.480663	0.521968
14	-0.768903	0.289659	1.460626
1	0.506151	-0.456571	1.264005
1	-0.587035	1.681880	0.971508
1	-1.031036	0.329100	2.927324
6	-3.900035	-1.144259	-0.755639
1	-4.701891	-1.170507	-1.480861
6	-3.525602	-2.166793	0.060573
1	-3.880905	-3.177735	0.200400
8	-2.483726	-1.795818	0.846800
79	-3.041096	1.802201	-1.324207
15	-3.050137	3.967809	-2.334566
1	-3.992750	4.926571	-1.904555
1	-1.884472	4.757193	-2.236329
1	-3.261584	4.072936	-3.726265

T-IN2

6	-3.007472	-0.018142	-0.471157
6	-2.186863	-0.466346	0.548913
14	-0.756272	0.276790	1.488731
1	0.485036	-0.519088	1.285325
1	-0.538830	1.656767	0.987099
1	-1.030641	0.321902	2.950676
6	-3.883088	-1.130026	-0.770221
1	-4.375187	1.099077	0.808384
1	-4.667664	-1.155246	-1.513877
6	-3.537114	-2.146224	0.065030
1	-3.904451	-3.151824	0.209620
8	-2.513006	-1.771710	0.874274
79	-2.948916	1.790622	-1.404163
15	-3.042556	3.964513	-2.372619
1	-4.315173	4.416054	-2.773003
1	-2.664569	5.042506	-1.548435
1	-2.305636	4.293010	-3.530778
16	-5.358171	2.890254	1.615927
6	-4.028504	3.347725	2.840344
9	-4.214207	2.702874	3.986020
9	-2.832126	3.024336	2.332357
9	-4.075742	4.663000	3.048866
8	-5.079886	1.316295	1.479599
8	-6.635969	3.045678	2.280270
8	-5.031106	3.597545	0.380405

T-IN3

6	-2.742943	-0.060220	0.037217
6	-1.731600	0.622090	-0.369166
14	-0.037831	-0.139668	-0.611264
1	-0.057582	-1.592039	-0.289770
1	0.389462	0.035663	-2.025155
1	0.950778	0.544051	0.262435
6	-3.789417	-0.763190	0.504967
1	-5.165788	0.791329	0.470503
1	-4.412711	-1.334733	-0.183240
6	-3.999402	-0.973676	1.950455
1	-4.821610	-1.687154	2.177988
8	-3.373039	-0.439391	2.848872
79	-2.037926	2.642918	-0.694352
15	-2.536002	4.926444	-1.032975
1	-3.438886	5.229067	-2.068754
1	-3.155796	5.596062	0.038525
1	-1.504592	5.840723	-1.330602
16	-6.062474	2.797385	0.611307
6	-5.175781	3.198086	2.205224
9	-5.926047	2.866861	3.246334
9	-4.020573	2.533191	2.244220
9	-4.931988	4.513604	2.223429
8	-6.058251	1.194786	0.670391
8	-7.439006	3.229429	0.737773
8	-5.193321	3.281861	-0.460923

T-TS1

6	-2.665438	0.154358	-0.086971
6	-1.558259	-0.385190	0.291858
14	0.260670	-0.608070	0.603019
1	0.705562	-1.868310	-0.036358
1	0.938881	0.559601	-0.006617
1	0.501787	-0.659493	2.063165
6	-3.948186	-0.555065	0.229534
1	-4.612453	0.075264	0.870449
1	-4.565412	-0.775984	-0.652787
6	-3.536794	-1.803706	0.926833
1	-4.279149	-2.532666	1.274445
8	-2.343055	-2.020550	1.132829
79	-2.712253	2.079446	-0.843716
15	-3.114720	4.293381	-1.541724
1	-4.240416	4.446855	-2.365004
1	-3.403961	5.182064	-0.495381
1	-2.154810	5.032175	-2.266615
16	-5.871143	2.796706	1.168881
6	-4.664044	3.755615	2.212165
9	-5.013948	3.755792	3.500343
9	-3.420026	3.226020	2.117704
9	-4.582269	5.035889	1.793233
8	-5.692473	1.403734	1.662568
8	-7.166885	3.422661	1.442495
8	-5.330215	3.012193	-0.210952

T-TS2

6	-3.618666	0.741898	0.842574
6	-2.905111	1.823393	1.306731
6	-1.773726	1.309924	1.986911
6	-1.878482	-0.102364	1.923816
1	-2.067686	-0.487024	3.255496
79	-0.433768	2.234835	3.205784
1	-3.186998	2.860743	1.192767
1	-4.550258	0.675271	0.294295
8	-3.051592	-0.415225	1.163498
14	-0.454645	-1.296267	1.530453
1	0.660046	-1.007267	2.460948
1	-0.939217	-2.686749	1.702287
1	-0.004870	-1.106696	0.125281
15	0.967937	3.030722	4.951827
1	1.772378	4.182169	4.811434
1	0.299937	3.340844	6.149171
1	1.927179	2.118897	5.426787
16	-1.953700	0.044237	5.578516
8	-2.885870	1.171479	5.489866
8	-2.101722	-0.952089	4.400638
8	-0.545725	0.338964	5.898455
6	-2.558616	-1.048401	6.959633
9	-2.484779	-0.363863	8.106578
9	-1.801899	-2.143500	7.055446
9	-3.826286	-1.404828	6.745117

T-TS3

6	-3.335954	1.136845	0.018469
6	-2.338247	1.890632	0.540637
6	-2.154167	1.476475	1.923039
6	-3.092346	0.445359	2.079401
1	-3.426939	-0.079466	2.964089
79	-1.275404	2.531883	3.480504
1	-1.779092	2.659693	0.027877
1	-3.808941	1.088136	-0.951518
8	-3.801868	0.236487	0.936214
14	-0.973318	-0.456547	1.963088
1	0.316522	-0.033713	2.524306
1	-1.462187	-1.768599	2.421968
1	-0.874127	-0.510221	0.479799
15	-0.404725	3.679396	5.333955
1	0.044304	5.006950	5.154731
1	-1.275911	3.846616	6.419663
1	0.719526	3.106699	5.945249
16	-1.186669	-0.191364	5.857102
6	0.625867	-0.561955	5.655581
9	1.227340	-0.675439	6.842871
9	0.814083	-1.698772	4.967258
9	1.235421	0.437122	4.972469
8	-1.177949	1.175986	6.434811
8	-1.707284	-1.264989	6.704393
8	-1.673733	-0.226380	4.432520

T-TS4

6	-3.684401	0.849752	0.751151
6	-3.444584	1.414758	1.956585
6	-2.209105	0.833968	2.470128
6	-1.803307	-0.055963	1.469892
1	-2.322504	0.196354	3.682051
79	-0.775106	2.047649	3.443603
1	-4.067122	2.142059	2.459031
1	-4.465108	0.945239	0.011653
8	-2.693566	-0.051408	0.443467
14	-0.373891	-1.275154	1.352277
1	0.428437	-1.154747	2.589716
1	-0.905351	-2.653558	1.203214
1	0.461981	-0.953198	0.166062
15	0.718864	3.400603	4.628324
1	1.622314	4.253196	3.962048
1	0.137905	4.313971	5.528229
1	1.606479	2.733354	5.493427
16	-2.148874	-0.113129	6.075298
6	-0.505856	-0.972526	6.230426
9	0.030819	-0.713563	7.427174
9	-0.637909	-2.291306	6.085350
9	0.344267	-0.522403	5.281966
8	-1.809807	1.322354	6.122257
8	-2.991219	-0.678944	7.120211
8	-2.585935	-0.558569	4.666410

T-TS5

6	-2.803448	0.017572	0.036074
6	-1.726508	0.562382	-0.341898
14	-0.015167	-0.146517	-0.603914
1	-0.023643	-1.610071	-0.353996
1	0.404722	0.117895	-2.002337
1	0.926493	0.521684	0.326138
6	-3.996759	-0.509519	0.501462
1	-4.909494	0.510804	0.567512
1	-4.544248	-1.144696	-0.202632
6	-4.032172	-0.981754	1.929571
1	-4.928842	-1.593855	2.161098
8	-3.208485	-0.717623	2.776755
79	-2.088409	2.619729	-0.634077
15	-2.650232	4.871690	-0.942859
1	-3.551594	5.133021	-1.987364
1	-3.301271	5.475745	0.144476
1	-1.643237	5.819613	-1.215345
16	-5.975252	2.721293	0.561735
6	-5.114156	3.270829	2.116604
9	-5.840456	2.993190	3.194796
9	-3.924142	2.652227	2.218689
9	-4.896093	4.596421	2.064451
8	-5.958609	1.191811	0.732177
8	-7.325889	3.262023	0.625747
8	-5.077612	3.175557	-0.520070

T-TS6

6	-2.903323	-0.046161	0.106908
6	-1.745838	0.574309	0.067599
14	-0.256340	-0.273482	-0.752567
1	-0.677284	-1.566928	-1.351355
1	0.292734	0.601654	-1.819817
1	0.783759	-0.503764	0.277382
6	-4.041152	-0.711868	0.233841
1	-1.418632	1.221564	1.224358
1	-4.844285	-0.570524	-0.484737
6	-4.249125	-1.673915	1.339113
1	-5.263129	-2.126906	1.338945
8	-3.423629	-1.977488	2.177491
79	-2.363669	2.507300	-0.722156
15	-2.843474	4.671047	-1.422341
1	-3.506281	4.926289	-2.638907
1	-3.632566	5.416538	-0.528903
1	-1.726871	5.515668	-1.554091
16	-0.674914	3.159760	2.445117
6	1.013266	3.224983	1.667016
9	1.887519	2.493984	2.354320
9	0.944444	2.739191	0.405852
9	1.443018	4.487892	1.604650
8	-1.000305	1.660492	2.335615
8	-0.511186	3.594414	3.823893
8	-1.510424	3.974236	1.534368

T-TS7

6	-3.213157	-0.105381	-0.135574
6	-2.235756	0.007645	0.814785
14	-0.344486	-0.149418	0.475916
1	-0.209087	-1.326583	-0.422397
1	0.154346	1.050906	-0.218484
1	0.304181	-0.407539	1.777043
6	-3.892671	-1.160731	-0.605421
1	-2.519455	0.306715	1.826063
1	-4.634355	-1.144076	-1.394355
6	-3.531168	-2.416406	0.081728
1	-4.031698	-3.338776	-0.262181
8	-2.714367	-2.463979	0.991721
79	-3.223780	1.973233	-0.542155
15	-3.379603	4.289224	-1.024268
1	-4.576015	4.773602	-1.597940
1	-3.225459	5.111938	0.102065
1	-2.426833	4.781292	-1.926282
6	0.831569	3.993694	2.011376
9	0.938069	4.024143	3.344291
9	1.642166	3.032312	1.539048
9	1.236671	5.170737	1.518927
16	-0.924617	3.650511	1.508805
8	-0.861992	3.681582	0.012451
8	-1.731929	4.733323	2.099429
8	-1.177524	2.286064	2.053836

TW3-5

6	-2.190570	-0.259868	-0.146594
6	-1.015834	0.053332	-0.713105
14	0.645723	0.042893	0.209047
1	1.345935	-1.215128	-0.151028
1	1.450924	1.208496	-0.227340
1	0.403822	0.098449	1.671209
6	-3.222803	-0.925297	0.361515
1	-4.063462	-0.395992	0.800665
1	-0.998382	0.098783	-1.838550
6	-3.254285	-2.397352	0.319586
1	-4.068290	-2.851779	0.915884
8	-2.484629	-3.116429	-0.303592
79	-2.214050	1.995444	-0.268879
15	-2.244314	4.363933	-0.399200
1	-2.545551	4.923572	-1.650212
1	-3.173870	5.003109	0.433914
1	-1.066211	5.070432	-0.076374
16	-5.500263	2.399264	-0.421311
8	-6.039386	1.270606	-1.213069
8	-4.943219	3.523163	-1.222368
8	-3.753046	1.163744	-2.895938
1	-3.912632	2.112773	-3.025429
1	-4.570955	0.880172	-2.436337
1	-1.365038	-1.025659	-3.546309
8	-1.270724	-0.047652	-3.607428
1	-2.184248	0.301151	-3.556430
8	-4.601024	1.987571	0.707805
6	-6.969683	3.131299	0.449904
9	-6.576271	4.174896	1.193592
9	-7.869143	3.552628	-0.443054
9	-7.537055	2.221549	1.247212
1	-1.695306	-2.839251	-2.004848
8	-1.475408	-2.757380	-2.954823
1	-2.107400	-3.339023	-3.402026

TW3-C

6	−2.608338	−0.075944	0.154871
6	−1.482611	0.126338	−0.323449
14	0.277960	−0.162408	−0.820874
1	0.550474	−1.612038	−0.692591
1	0.462811	0.281673	−2.222815
1	1.162043	0.623859	0.071392
6	−3.859719	−0.492977	0.762894
1	−4.356152	0.340574	1.280900
1	−4.589953	−0.821128	−0.025301
6	−3.655328	−1.649206	1.734074
1	−4.594789	−1.953351	2.238910
8	−2.607139	−2.212681	1.942477
79	−2.362489	2.180574	−0.710515
15	−2.674780	4.465604	−1.058924
1	−3.386430	4.849234	−2.205046
1	−3.355963	5.112527	−0.015519
1	−1.494407	5.222814	−1.203215
16	−5.822200	3.521681	0.576110
8	−5.885446	2.168729	1.187637
8	−5.471340	3.498965	−0.885338
8	−4.707229	1.292383	−2.319952
1	−5.121379	2.029739	−1.810458
1	−4.739307	1.570034	−3.248229
1	−6.657067	−0.744481	−0.841516
8	−5.900293	−1.114396	−1.352033
1	−5.564427	−0.346862	−1.857267
8	−5.087205	4.542543	1.340155
6	−7.592025	4.091486	0.563232
9	−7.689664	5.293864	−0.009711
9	−8.071682	4.157591	1.805948
9	−8.346601	3.222644	−0.142150
1	−7.124055	0.861049	0.688824
8	−7.737916	0.214411	0.283427
1	−8.402965	0.771573	−0.147244

TW3-IN1

6	−0.002266	−0.003263	0.003192
6	−0.002042	−0.000901	1.286644
14	1.642636	0.006705	2.196105
1	2.778376	−0.016034	1.235220
1	1.743268	1.220769	3.046776
1	1.732287	−1.189319	3.075751
6	0.023154	0.026496	−1.343152
1	0.122488	−0.905227	−1.901973
1	−1.961059	−0.059786	−1.499539
6	0.183809	1.284485	−2.097129
1	0.323759	1.126703	−3.190136
8	0.167445	2.408789	−1.629137
79	−1.711980	0.066508	2.456585
15	−3.545533	0.186257	3.952840
1	−4.254623	1.397180	3.997740
1	−4.590433	−0.747109	3.852792
1	−3.183949	0.056504	5.311076
16	−6.209212	−0.508228	1.304174
8	−6.003630	−1.267135	0.036666
8	−5.186778	0.577533	1.498594
8	−4.339907	1.606046	−0.809542
1	−4.630656	1.306093	0.099800
1	−5.167153	1.720686	−1.305625
1	−3.231736	−1.130589	−1.368855
8	−2.916177	−0.205190	−1.755691
1	−3.528070	0.585206	−1.359413
8	−6.479304	−1.296462	2.510993
6	−7.756446	0.449691	0.937002
9	−8.087406	1.214405	1.979937
9	−7.540423	1.249207	−0.128445
9	−8.767537	−0.371961	0.656494
1	−3.967264	−3.055306	−1.410752
8	−3.726754	−2.378482	−0.758074
1	−4.584943	−2.095245	−0.335526

TW3-IN2

6	−1.792539	−0.636701	0.615234
6	−0.801993	0.079671	0.229230
14	0.938807	−0.518135	−0.111091
1	1.041606	−1.993971	0.021658
1	1.359382	−0.096627	−1.471145
1	1.855926	0.118805	0.871805
6	−2.900979	−1.330107	0.946632
1	−3.178371	−1.470728	1.987805
1	−1.224661	1.286757	−2.801354
6	−3.836568	−1.712903	−0.062862
1	−4.808504	−2.083382	0.296262
8	−3.651284	−1.640832	−1.302566
79	−1.372372	2.071200	−0.058520
15	−2.179800	4.274455	−0.341116
1	−2.619354	4.665614	−1.617202
1	−3.296111	4.564609	0.458067
1	−1.308138	5.341904	−0.037993
16	−5.379849	2.177440	0.014489
8	−5.597227	0.725055	0.108882
8	−4.610017	2.555139	−1.250341
8	−4.143579	0.588644	−2.733817
1	−4.341514	1.422484	−2.106494
1	−4.188618	−0.238431	−2.173969
1	−1.379340	−0.210757	−3.218203
8	−1.690035	0.716311	−3.437587
1	−3.156713	0.669344	−3.063022
8	−4.884384	2.895914	1.196501
6	−7.053704	2.907069	−0.330645
9	−6.951845	4.232123	−0.498445
9	−7.570983	2.370394	−1.442020
9	−7.876580	2.662373	0.693383
1	−2.025405	−1.765225	−1.994554
8	−1.201096	−1.737756	−2.543837
1	−1.264421	−2.490752	−3.151423

TW3-TS1

6	−2.108484	−0.564174	0.359509
6	−1.345458	0.285644	−0.161537
14	0.460967	0.219015	−0.665067
1	1.041442	−1.080438	−0.249115
1	0.542774	0.378534	−2.135456
1	1.180135	1.332008	0.000025
6	−3.005281	−1.514099	0.874687
1	−2.880563	−1.713894	1.946514
1	−4.147893	−1.051212	0.836352
6	−3.141938	−2.788887	0.059180
1	−3.723728	−3.572324	0.585696
8	−2.705042	−2.955290	−1.054487
79	−2.371185	2.116368	−0.519864
15	−3.270055	4.245367	−0.887104
1	−3.896944	4.494438	−2.114282
1	−4.190346	4.685431	0.073988
1	−2.295484	5.265098	−0.863826
16	−6.728845	3.204833	−0.085621
8	−7.841252	2.244344	0.098107
8	−5.787562	2.859020	−1.196971
8	−6.588391	0.136911	−1.473173
1	−6.109754	0.973956	−1.641066
1	−7.433179	0.482149	−1.130446
1	−5.847447	−0.070048	1.516414
8	−5.575930	−0.772640	0.862071
1	−5.918681	−0.477600	−0.030138
8	−6.033894	3.620296	1.161515
6	−7.539587	4.764967	−0.684888
9	−6.598628	5.705869	−0.897469
9	−8.185512	4.543132	−1.832574
9	−8.404196	5.222419	0.222203
1	−7.395570	1.246249	2.098248
8	−6.524692	1.156786	2.525448
1	−6.130960	2.029357	2.320452

TW3-TS2

6	−1.946930	−0.276570	0.103158
6	−0.922100	0.162159	−0.592222
14	0.890626	−0.072601	−0.102605
1	1.355898	−1.364170	−0.667990
1	1.689461	1.034490	−0.682148
1	1.047927	−0.082956	1.374706
6	−3.010811	−0.807718	0.700027
1	−3.633552	−0.192124	1.343307
1	−1.171384	0.166695	−1.900817
6	−3.415987	−2.185850	0.436759
1	−4.264344	−2.530024	1.055773
8	−2.916248	−2.955583	−0.381103
79	−1.706645	2.225605	−0.273352
15	−2.343680	4.461001	−0.103052
1	−2.708970	5.111649	−1.289819
1	−3.437658	4.688912	0.740812
1	−1.389483	5.363813	0.413781
16	−5.263430	2.149817	−0.358129
8	−5.567461	0.854192	−1.013508
8	−4.576307	3.131128	−1.264305
8	−3.853537	1.138098	−3.218771
1	−3.896166	2.065572	−2.916646
1	−4.484005	0.725278	−2.589388
1	−1.601846	−0.969577	−3.225498
8	−1.448459	0.020883	−3.160116
1	−2.354763	0.458609	−3.253257
8	−4.652606	2.065534	0.988680
6	−6.920840	2.937038	−0.064089
9	−6.753141	4.134206	0.519682
9	−7.566561	3.111808	−1.221631
9	−7.664818	2.168504	0.737632
1	−2.124397	−2.732141	−1.995390
8	−1.868266	−2.604170	−2.937700
1	−2.595336	−2.994908	−3.445399

C-1

6	−3.698894	0.690463	0.874794
6	−2.983852	1.851778	1.170647
6	−1.999391	1.512841	2.098451
6	−2.113199	0.068261	2.300626
1	−2.274460	−0.260081	3.333291
79	−0.661267	2.741528	3.017819
1	−3.189060	2.826553	0.750063
1	−4.534293	0.529291	0.201044
8	−3.270468	−0.363335	1.519415
14	−0.579162	−0.954423	1.609492
1	0.581701	−0.557274	2.433433
1	−0.934948	−2.377283	1.784189
1	−0.431805	−0.569113	0.189967
15	0.874958	4.221230	4.097094
1	2.083613	4.482381	3.426612
1	0.418054	5.526620	4.352693
1	1.345073	3.843039	5.367615

C-2

6	−3.804495	1.396131	1.753542
6	−2.737542	1.720363	0.985583
6	−1.559972	1.070264	1.578824
6	−2.097548	0.398199	2.695213
1	−1.657544	−0.284651	3.409982
79	−0.728908	2.643557	2.977356
1	−2.751136	2.327240	0.090815
1	−4.857144	1.632837	1.722063
8	−3.413031	0.594559	2.801706
14	−0.004494	0.505207	0.610309
1	0.933680	−0.090705	1.589025
1	−0.450123	−0.489639	−0.390704
1	0.589933	1.689037	−0.050085
15	0.209898	4.378159	4.232785
1	1.533713	4.719999	3.908308
1	−0.445503	5.619208	4.161747
1	0.288737	4.160569	5.618755

C-3

6	-3.219530	1.514938	0.522452
6	-3.548500	1.750484	1.817216
6	-2.584337	1.011589	2.612446
6	-1.737396	0.345267	1.695742
1	-2.704726	0.732114	3.655458
79	-0.807654	2.442026	2.860365
1	-4.368397	2.351855	2.182938
1	-3.623678	1.844020	-0.423271
8	-2.131395	0.687150	0.441798
14	-0.430899	-1.032957	1.874792
1	-0.147840	-1.113218	3.325332
1	-1.028245	-2.280074	1.350416
1	0.765536	-0.632766	1.102813
15	0.786865	4.077316	3.363829
1	1.603868	4.490554	2.297828
1	0.284495	5.297884	3.846324
1	1.728735	3.730926	4.347238

C-TS1

6	-3.727478	0.797526	1.085158
6	-2.963231	1.926274	1.186449
6	-1.909198	1.645212	2.130639
6	-2.098292	0.281519	2.445237
1	-1.745559	-0.302879	3.287207
79	-0.675633	2.988476	3.089368
1	-3.133219	2.859502	0.668987
1	-4.614265	0.557718	0.514698
8	-3.234645	-0.204070	1.845468
14	-0.398825	0.232987	1.062828
1	0.607359	-0.314613	1.994452
1	-1.048795	-0.751771	0.172844
1	0.127735	1.375869	0.294720
15	0.640900	4.592384	4.247882
1	1.887426	4.924621	3.687722
1	0.066602	5.864921	4.416759
1	1.007231	4.276542	5.568374

C-TS2

6	-3.763409	0.920429	0.654216
6	-3.292666	1.987145	1.343463
6	-2.027565	1.590706	1.941752
6	-1.872306	0.214823	1.555150
1	-2.265616	0.629154	2.778924
79	-0.643727	2.805068	2.876557
1	-3.760149	2.957228	1.427202
1	-4.649112	0.749434	0.058513
8	-2.939607	-0.158026	0.794289
14	-0.431992	-1.047846	1.724452
1	0.347449	-0.596468	2.896711
1	-1.043063	-2.377464	1.917728
1	0.337588	-0.950191	0.466632
15	0.930221	4.262752	3.890698
1	1.965077	4.745093	3.069839
1	0.423413	5.458788	4.429274
1	1.657312	3.754298	4.981718

H-1

6	-3.382748	0.706692	0.186693
6	-2.627933	1.816436	0.547943
6	-2.022951	1.527359	1.777095
6	-2.389682	0.152817	2.092181
1	-2.854630	-0.022774	3.073335
79	-0.986881	2.637927	3.127116
1	-2.563735	2.736226	-0.016743
1	-4.004439	0.532291	-0.685271
8	-3.321606	-0.276147	1.049881
14	-0.861709	-1.089969	2.006738
1	0.403416	-0.448613	2.397739
1	-1.212240	-2.275717	2.812485
1	-0.804501	-1.447986	0.562691
15	0.030280	3.694234	4.996792
1	1.180925	4.497989	4.863121
1	-0.799835	4.561745	5.726704
1	0.423529	2.784148	5.991623
51	-1.918212	0.222428	6.123650
9	-2.301849	2.021581	5.667421
9	-0.433802	0.875568	7.049360
9	-0.807344	0.111939	4.576581

9	-1.498371	-1.540657	6.488232
9	-3.045988	0.349415	7.579632
9	-3.320177	-0.286871	4.973317

H-2

6	-3.728526	1.599381	0.614102
6	-2.397482	1.477035	0.407884
6	-1.835239	0.806141	1.585106
6	-2.958514	0.593684	2.405501
1	-3.076676	0.091508	3.359601
79	-1.305413	2.441592	3.111976
1	-1.849368	1.793731	-0.468298
1	-4.541838	2.025620	0.047359
8	-4.076069	1.067975	1.832737
14	-0.238922	-0.245229	1.570628
1	-0.505163	-1.557586	2.194160
1	0.068276	-0.422488	0.125181
1	0.914225	0.430128	2.206147
15	-0.698003	3.947825	4.768847
1	0.202817	4.994536	4.493354
1	-1.765503	4.646904	5.352820
1	-0.114266	3.297282	5.866856
51	-1.747117	0.236464	6.220858
9	-2.553025	1.855413	5.623639
9	-0.357350	1.308476	6.872054
9	-0.795961	0.165034	4.567471
9	-0.916423	-1.329197	6.737236
9	-2.713089	0.355948	7.789761
9	-3.119993	-0.666466	5.318391

H-3

6	-2.955525	1.444889	0.310607
6	-3.732944	1.352095	1.434980
6	-2.949234	0.654859	2.387474
6	-1.694742	0.375358	1.801026
1	-3.242213	0.358179	3.389219
79	-0.726683	1.881005	3.173079
1	-4.735641	1.732594	1.565137
1	-3.128097	1.897680	-0.656382
8	-1.751668	0.884209	0.483012
14	-0.599602	-1.187849	2.009264
1	0.723297	-0.877271	2.593797
1	-1.335278	-2.169740	2.830076
1	-0.408287	-1.698587	0.627266
15	0.246574	3.312694	4.726465
1	1.487295	3.923366	4.460029
1	-0.533108	4.422031	5.089054
1	0.460723	2.670882	5.955979
51	-2.209250	0.474857	6.414997
9	-2.286271	2.175996	5.561748
9	-0.567581	1.037814	7.116520
9	-1.237894	-0.182145	4.910204
9	-2.082443	-1.194833	7.193624
9	-3.166410	1.168424	7.834426
9	-3.755096	0.025041	5.456789

H-5

6	-2.189117	0.017695	0.761239
6	-0.977954	0.353187	0.278806
14	-0.435731	-0.039340	-1.509448
1	0.477348	-1.205978	-1.438085
1	-1.643890	-0.344309	-2.306778
1	0.291112	1.127161	-2.067000
6	-3.246179	-0.617099	1.219817
1	-0.201038	0.597883	1.009744
6	-3.139420	-2.092756	1.454554
1	-4.044738	-2.538670	1.909231
8	-2.169136	-2.765292	1.175685
79	-2.288575	2.262319	0.222801
15	-2.873869	4.501233	-0.246769
1	-3.544209	4.690461	-1.464037
1	-3.757495	5.048909	0.694969
1	-1.846723	5.459894	-0.340049
51	-5.845667	2.658014	1.643315
9	-5.473336	4.489499	1.784233
9	-7.508734	2.973001	0.907993
9	-5.072957	2.745903	-0.103117
9	-4.076334	2.334632	2.265616
9	-6.001210	0.806312	1.406409
9	-6.480399	2.571598	3.373797
1	-4.189017	-0.113943	1.424073

H-C

6	-2.811613	-0.010230	0.559459
6	-1.730821	0.291634	0.037009
14	-0.020132	0.266512	-0.674619
1	0.488318	-1.120434	-0.569489
1	-0.087758	0.697439	-2.090033
1	0.830445	1.199805	0.099533
6	-3.993292	-0.585324	1.193548
1	-4.225092	-0.058380	2.127638
1	-4.882130	-0.423181	0.570782
6	-3.832723	-2.076205	1.474177
1	-4.725732	-2.521111	1.958825
8	-2.854287	-2.731632	1.210033
79	-2.812740	2.319438	0.004907
15	-3.082769	4.594256	-0.426553
1	-4.141399	4.955858	-1.270126
1	-3.265422	5.429712	0.683322
1	-1.991685	5.215862	-1.066303
51	-6.188305	2.518120	1.470307
9	-6.735176	3.348122	3.026315
9	-7.816259	2.758623	0.632859
9	-5.530602	4.145999	0.775774
9	-4.456101	2.264201	2.219917
9	-5.508188	1.702398	-0.109928
9	-6.623112	0.814179	2.083311

H-IN1

6	-2.809407	0.274497	0.410025
6	-1.765139	-0.572367	0.463281
14	0.042071	-0.570968	-0.034459
1	0.298965	-1.673472	-0.995851
1	0.315158	0.743479	-0.654546
1	0.893121	-0.776908	1.165212
6	-3.987492	-0.426858	1.030993
1	-4.415756	0.137369	1.881343
1	-4.870822	-0.476208	0.369152
6	-3.457847	-1.725041	1.407134
1	-3.937751	-2.573534	1.886453
8	-2.225478	-1.843631	1.109908
79	-3.039493	2.186722	-0.280750
15	-3.513800	4.384661	-1.000651
1	-4.546661	4.529934	-1.940356
1	-3.914861	5.297050	-0.012150
1	-2.490213	5.124044	-1.630524
51	-6.709408	2.109282	0.940901
9	-7.496358	3.032711	2.336232
9	-7.052495	0.433337	1.691695
9	-8.273309	2.129118	-0.045160
9	-6.089115	3.693977	0.137145
9	-5.858909	1.168221	-0.471722
9	-5.080262	2.078243	1.917996

H-TS1

6	-2.841916	0.267019	0.372456
6	-1.698318	-0.334641	0.346520
14	0.119000	-0.553100	0.015276
1	0.311644	-1.709175	-0.891136
1	0.583550	0.701513	-0.620349
1	0.821704	-0.789124	1.298074
6	-3.994113	-0.490475	0.966383
1	-4.450274	0.041017	1.814323
1	-4.835976	-0.602717	0.268610
6	-3.421834	-1.801371	1.370321
1	-4.028860	-2.582505	1.841933
8	-2.224644	-2.015428	1.169387
79	-3.126665	2.209327	-0.311656
15	-3.605987	4.393601	-1.027488
1	-4.666176	4.534593	-1.935141
1	-3.957169	5.317618	-0.032171
1	-2.587755	5.102825	-1.698212
51	-6.680600	2.164117	0.973036
9	-7.430979	3.046313	2.414647
9	-6.962531	0.470225	1.707368
9	-8.280758	2.163305	0.046634
9	-6.136414	3.781795	0.173175
9	-5.856924	1.282303	-0.491461
9	-5.009438	2.162725	1.873515

H-TS2

6	-2.875159	-0.001964	0.024999
6	-1.778203	-0.383532	0.772234
14	-0.070841	0.334780	1.018170
1	0.976485	-0.619642	0.564919
1	0.015646	1.583616	0.222617
1	0.175395	0.639363	2.453396
6	-3.883438	-1.018476	0.291727
1	-4.291967	0.484352	1.267583
1	-4.868213	-1.084772	-0.150962
6	-3.320006	-1.922516	1.153934
1	-3.675697	-2.834078	1.612213
8	-2.057946	-1.562431	1.452321
79	-3.127353	1.663586	-1.120864
15	-3.573006	3.649636	-2.338081
1	-4.883978	3.809138	-2.826734
1	-3.430784	4.868074	-1.646868
1	-2.849313	3.959866	-3.508852
51	-6.521806	2.139298	1.105382
9	-6.372584	3.023749	2.709106
9	-7.366101	0.725605	1.927870
9	-8.026343	2.955046	0.453295
9	-5.339411	3.366539	0.354858
9	-6.198440	1.034045	-0.353502
9	-4.758014	1.164449	1.852798

H-TS3

6	-2.385934	-0.390543	0.193142
6	-1.061742	-0.192032	0.309690
1	-0.566063	0.763927	0.430259
6	-3.043850	-1.594355	0.070186
6	-0.358718	-1.478362	0.270351
8	-0.954182	-2.551492	0.139355
14	-3.699724	-2.613980	1.549330
1	-5.141770	-2.314666	1.726837
1	-3.527826	-4.042885	1.202166
1	-2.930227	-2.224118	2.750504
79	-3.960430	0.952656	0.164048
1	-3.306122	-1.924006	-0.939473
1	0.737235	-1.480676	0.367753
15	-5.621370	2.662439	0.211999
1	-6.040064	3.049034	1.495178
1	-5.156001	3.873021	-0.324424
1	-6.863881	2.489753	-0.430015
51	-1.877853	4.082878	0.356784
9	-2.362581	2.793154	-0.953288
9	-3.319788	5.110495	-0.252146
9	-3.132320	3.235449	1.524423
9	-0.598679	2.853181	0.955585
9	-1.470086	5.283969	1.699358
9	-0.702242	4.854172	-0.840753

H-TS4

6	-3.489650	0.913307	0.191872
6	-2.489820	1.779226	0.495369
6	-2.104255	1.531299	1.874619
6	-2.930587	0.460045	2.259212
1	-3.133522	0.029373	3.237012
79	-1.193078	2.800001	3.238855
1	-2.062418	2.522635	-0.161805
1	-4.078186	0.733812	-0.696139
8	-3.765090	0.091797	1.245499
14	-0.832908	-0.331612	1.889203
1	-1.069514	-1.527098	2.717600
1	-1.028536	-0.676568	0.459178
1	0.495599	0.266536	2.099389
15	-0.390221	4.093385	5.028155
1	0.571819	5.107147	4.845663
1	-1.372765	4.799828	5.742707
1	0.188951	3.317814	6.045701
51	-1.719053	0.269262	6.154120
9	-2.447733	1.963367	5.729945
9	-0.264106	1.181644	6.887287
9	-0.787206	0.307703	4.478803
9	-0.958427	-1.383642	6.475736
9	-2.668564	0.248476	7.736035
9	-3.130734	-0.498856	5.178519

H-TS5

6	-3.697699	0.752810	0.693905
6	-3.203515	1.867374	1.294761
6	-2.040646	1.462371	2.052914
6	-1.936289	0.085467	1.854217
1	-2.639885	0.486586	3.407807
79	-0.867473	2.631314	3.249519
1	-3.609294	2.866410	1.223721
1	-4.544140	0.572106	0.046609
8	-2.961220	-0.337808	1.011165
14	-0.626581	-1.230138	2.203249
1	0.578670	-0.575326	2.752261
1	-1.146251	-2.264583	3.127800
1	-0.305799	-1.870822	0.900018
15	0.358324	3.908442	4.823646
1	1.357019	4.817449	4.416341
1	-0.391512	4.744615	5.672299
1	1.080445	3.176885	5.785157
51	-2.165566	0.161199	6.157187
9	-2.015848	2.020374	6.108029
9	-1.261238	-0.007149	7.745007
9	-0.651495	0.098402	5.068110
9	-2.403807	-1.640253	5.856892
9	-3.866462	0.327178	6.836228
9	-3.168754	0.355605	4.325815

HW-1

6	-1.922390	0.310704	2.754793
6	-0.663952	0.724571	2.346339
1	-0.032557	0.200176	1.642769
1	-2.117226	3.201247	3.556188
6	-0.393283	1.940797	2.992839
6	-1.549712	2.231090	3.811830
79	1.254526	3.109424	2.779692
1	-2.499646	-0.567254	2.485837
8	-2.491151	1.132705	3.604336
14	-1.270243	2.418139	5.712458
1	-0.465237	3.643031	5.916853
1	-2.600849	2.529137	6.348787
1	-0.551139	1.220885	6.215814
15	3.240461	4.403818	2.533685
1	4.035487	4.161790	1.401841
1	3.089015	5.797355	2.477121
1	4.214925	4.290783	3.547705
8	-3.178093	4.482178	3.356605
1	-3.439956	4.417129	2.404828
1	-2.740526	5.368246	3.420967
1	-2.151733	7.182236	2.309731
8	-1.898189	6.931848	3.214514
1	-0.973249	6.655411	3.077995
51	0.135772	5.780312	0.147371
9	0.928377	7.425878	-0.120878
9	1.793706	4.901593	0.092033
9	0.416361	5.992856	2.016403
9	-0.174483	5.508127	-1.649606
9	-1.563239	6.572136	0.388379
9	-0.683989	4.116539	0.531347
1	-3.352588	5.328408	0.348168
8	-3.455112	4.395560	0.600220
1	-2.547762	4.061316	0.469123

HW-2

6	-1.404621	0.743948	1.749360
6	-0.398703	0.545781	2.628872
1	0.277937	-0.296839	2.656995
1	-1.943093	3.421804	3.448689
6	-0.399536	1.696855	3.545819
6	-1.471354	2.489238	3.090823
79	1.107061	3.132631	2.640660
1	-1.777831	0.198887	0.896252
8	-2.056437	1.922758	2.026901
14	0.187401	1.643862	5.350167
1	0.152777	3.007642	5.926554
1	-0.712946	0.742388	6.114179
1	1.564940	1.092995	5.398425
15	3.057515	4.261831	2.036714
1	3.718435	3.834793	0.876656
1	2.952906	5.646068	1.855399
1	4.097003	4.177353	2.984718
8	-3.075957	4.870039	3.669932
1	-3.517601	4.764397	2.797693
1	-2.635314	5.746523	3.592593
1	-2.145320	7.424095	2.129340
8	-1.739577	7.258885	2.995952
1	-0.883576	6.869901	2.741844
51	-0.092635	5.566156	-0.142408
9	0.712208	7.155000	-0.626636
9	1.544959	4.646757	-0.267925
9	0.364513	5.938375	1.669857
9	-0.566066	5.137703	-1.871004
9	-1.741544	6.427008	0.181277
9	-0.868210	3.962215	0.480168
1	-3.263355	5.278727	0.585493
8	-3.724481	4.499972	0.944289
1	-3.071808	3.794689	0.804710

HW-3

6	-1.020311	-0.578612	4.096942
6	-0.814406	0.129342	2.958831
1	-0.676568	-0.266076	1.962575
6	-0.838645	1.530525	3.336836
6	-1.069781	1.546085	4.725623
79	1.310105	2.049449	3.965003
1	-1.079652	-1.633280	4.320933
8	-1.168565	0.256647	5.171431
14	-1.501922	2.936304	5.938657
1	-1.193945	4.216009	5.268504
1	-2.942034	2.824982	6.279993
1	-0.689685	2.753133	7.166925
15	3.549432	2.357482	4.522000
1	4.464431	2.492372	3.471201
1	3.827128	3.476159	5.319756
1	4.096325	1.313707	5.292200
8	-1.197193	3.964571	1.744923
1	-0.667007	3.929623	0.915665
1	-0.840584	4.727240	2.252208
1	0.051241	6.750442	2.456213
8	-0.037435	6.109262	3.179477
1	0.874633	5.780931	3.285070
51	3.447092	5.146040	1.680815
9	4.109007	6.806962	2.134522
9	4.925803	4.281320	2.430142
9	2.590062	5.022396	3.385391
9	4.185967	5.131403	-0.007523
9	1.860646	5.918268	1.027080
9	2.684718	3.433725	1.362372
1	0.822514	4.817348	-0.406209
8	0.558558	3.882563	-0.444421
1	1.291684	3.456484	0.035731
1	-0.971534	2.408614	2.671000

HW-5

6	-2.281253	0.001657	0.492696
6	-1.040647	0.389591	0.181217
14	-0.140838	-0.083811	-1.428039
1	0.796682	-1.184667	-1.095534
1	-1.132348	-0.528975	-2.436268
1	0.613962	1.092235	-1.921170
6	-3.383620	-0.621460	0.875217
1	-0.439245	0.843355	1.020260
6	-3.287013	-1.970128	1.475484
1	-4.245532	-2.519872	1.518446
8	-2.265827	-2.475622	1.917728
79	-2.368852	2.254780	-0.122547
15	-2.993911	4.492758	-0.437169
1	-3.786468	4.777540	-1.560453
1	-3.746353	5.011702	0.623673
1	-1.950481	5.424898	-0.585033
51	-5.816891	2.604801	1.845019
9	-5.182515	4.346916	2.122054
9	-7.493892	3.183424	1.343998
9	-5.218765	2.775487	0.048442
9	-4.037059	2.047518	2.299880
9	-6.176074	0.811661	1.467284
9	-6.279470	2.419634	3.622782
8	0.205373	1.614568	2.510103
1	-0.452193	2.317044	2.701643
1	-2.716433	3.136406	2.754056
8	-1.857999	3.608853	2.758634
1	-1.896718	4.210775	3.517479
1	-4.365435	-0.159554	0.814208
1	-0.051065	0.844630	3.065629
1	-1.031253	-1.398551	2.972738
8	-0.670426	-0.794777	3.651644
1	-1.325196	-0.814819	4.364898

HW-C1

6	-2.365682	-0.528757	1.063113
6	-2.340872	-0.346516	-0.160577
14	-2.522601	-0.536201	-2.004694
1	-1.369635	-1.346829	-2.471396
1	-3.792306	-1.249018	-2.261605
1	-2.497107	0.795158	-2.641727
6	-2.494635	-0.876899	2.471287
1	-2.285879	-1.945643	2.615264
6	-1.661714	-0.058271	3.429544
1	-1.618713	-0.480672	4.452094
8	-1.122690	0.997772	3.170651
79	-2.128141	1.827709	0.512248
15	-1.952719	4.140707	0.622512
1	-2.566494	4.833385	-0.429378
1	-2.531013	4.732787	1.756114
1	-0.665810	4.711175	0.646077
51	-5.687414	2.847362	-0.787976
9	-7.086751	2.186437	0.283204
9	-6.519424	2.322054	-2.345800
9	-6.406050	4.545225	-0.825751
9	-4.790491	3.309100	0.839168
9	-4.131930	3.387754	-1.671942
9	-4.903331	1.117693	-0.639303
1	-5.548163	0.522748	3.260644
8	-5.307049	-0.425190	3.143638
1	-5.808304	-0.679350	2.334517
1	-5.926097	-0.209611	0.157868
8	-6.591681	-0.706241	0.668910
1	-7.340527	-0.088978	0.676735
1	-3.576970	-0.719696	2.779851
1	-5.529834	2.706867	2.460443
8	-6.155996	2.253805	3.053159
1	-6.930065	2.158373	2.474310

HW-IN1

6	-2.305376	0.182931	3.175634
6	-1.349140	0.843168	2.467708
1	-1.076291	0.656396	1.438079
1	-2.163771	3.324459	3.136420
6	-0.764949	1.828833	3.353502
6	-1.444194	1.680505	4.552990
79	0.847129	3.019749	2.956476
1	-2.992246	-0.615817	2.935481
8	-2.387586	0.668952	4.439250
14	-1.277534	2.458302	6.244640
1	-0.428379	3.669029	6.110202
1	-2.613255	2.846087	6.771119
1	-0.648865	1.524337	7.216866
15	2.810150	4.302651	2.513046
1	3.044188	4.739813	1.199158
1	2.986634	5.506523	3.218968
1	4.039858	3.676817	2.806127
8	-2.750467	4.049866	2.776346
1	-2.754129	3.970013	1.720757
1	-2.308754	4.978854	3.007329
1	-1.953142	6.778193	2.315352
8	-1.706320	6.327503	3.147515
1	-0.737736	6.237308	3.024439
51	0.275758	6.350395	-0.066504
9	0.488707	8.177692	0.014932
9	2.069265	6.022615	-0.401223
9	0.642920	6.241453	1.802128
9	-0.212273	6.334508	-1.841675
9	-1.561995	6.544958	0.431272
9	-0.036111	4.479622	0.021522
1	-2.788316	4.962168	0.021441
8	-2.668979	4.020717	0.250144
1	-1.713869	3.896906	0.050000

HW-IN2

6	-2.472851	-0.497964	0.356941
6	-1.945760	0.447364	-0.331166
14	-0.450291	0.026174	-1.392197
1	-0.125558	-1.422831	-1.299733
1	-0.730254	0.366543	-2.812819
1	0.722253	0.821318	-0.943859
6	-2.944632	-1.524213	1.093090
1	-4.395986	-0.657621	2.112334
1	-3.659741	-2.220919	0.652808
6	-2.290194	-1.929507	2.352870
1	-2.665895	-2.896865	2.753970
8	-1.427079	-1.304542	2.943688
79	-2.525351	2.434912	-0.362576
15	-2.924466	4.755714	-0.577928
1	-3.641291	5.188523	-1.706637
1	-3.602431	5.431047	0.449043
1	-1.772847	5.560888	-0.697696
51	-6.362870	3.115592	0.979735
9	-7.484142	4.572925	1.076946
9	-7.651930	2.018245	0.171869
9	-5.662818	3.674703	-0.652154
9	-4.985852	3.973875	1.924064
9	-5.249563	1.597468	0.976927
9	-7.005499	2.498137	2.672677
1	-4.837205	0.474517	3.248251
8	-5.081559	-0.454564	2.816011
1	-6.018725	-0.357163	2.366326
1	-7.466654	0.326401	1.040778
8	-7.454146	-0.152790	1.894852
1	-7.799219	0.526090	2.503077
1	-5.538849	2.231997	3.721772
8	-4.659354	1.821401	3.861512
1	-4.082523	2.359856	3.290884

HW-TS1

6	-2.825915	0.313416	0.438611
6	-1.676068	-0.194320	0.197890
14	0.069716	-0.498833	-0.345304
1	0.096431	-1.658149	-1.266111
1	0.516711	0.730755	-1.043683
1	0.911558	-0.758438	0.844591
6	-3.867584	-0.439421	1.202093
1	-4.092186	0.037226	2.200806
1	-4.842236	-0.484519	0.701605
6	-3.277503	-1.784436	1.450319
1	-3.872408	-2.545163	1.975077
8	-2.126390	-2.047473	1.116427
79	-3.147744	2.218055	-0.347176
15	-3.652329	4.340200	-1.215981
1	-4.448808	4.381519	-2.371098
1	-4.344564	5.220679	-0.370325
1	-2.569640	5.151665	-1.610276
51	-6.976028	1.858783	-0.139367
9	-8.125927	2.568091	1.153271
9	-7.210827	0.138757	0.594024
9	-8.338028	1.646774	-1.361411
9	-6.524489	3.564326	-0.767456
9	-5.705211	1.113598	-1.294413
9	-5.604408	2.100041	1.163793
1	-4.282442	1.675916	3.752631
8	-4.572563	0.745372	3.850715
1	-5.553467	0.793038	3.765921
1	-7.686019	1.648286	2.968874
8	-7.360283	0.810425	3.339935
1	-7.368561	0.240589	2.550803
1	-4.761077	4.013688	3.647089
8	-4.196480	3.483302	3.063732
1	-4.794484	3.153864	2.366049

HW-TS2

6	-2.068718	0.237460	3.028542
6	-0.885284	0.656297	2.456498
1	-0.344652	0.135249	1.678685
1	-2.284936	3.189029	3.531831
6	-0.535998	1.881992	3.068200
6	-1.585929	2.182264	3.986508
79	1.116627	3.008390	2.685105
1	-2.684711	-0.634466	2.842923
8	-2.515074	1.075431	3.947559
14	-1.270590	2.740236	5.780331
1	-0.507109	4.009030	5.717300
1	-2.581438	2.952274	6.438052
1	-0.497642	1.709453	6.519309
15	3.170047	4.167863	2.321222
1	3.792424	4.059339	1.067801
1	3.210557	5.554539	2.531214
1	4.226649	3.753001	3.158956
8	-3.124229	4.129824	3.089387
1	-3.158276	4.042229	2.087583
1	-2.728181	5.039501	3.256591
1	-2.243663	6.924031	2.434571
8	-2.010697	6.555169	3.305281
1	-1.055633	6.387679	3.184797
51	0.213016	6.154027	0.216898
9	0.639440	7.942520	0.366721
9	2.002161	5.641462	0.071365
9	0.394467	5.987748	2.104003
9	-0.030642	6.239172	-1.607967
9	-1.620557	6.536828	0.521420
9	-0.270987	4.320785	0.189735
1	-3.037605	5.022373	0.203795
8	-3.002125	4.073024	0.415017
1	-2.056655	3.880273	0.255826

HW-TS3

6	-1.385091	-0.535068	3.516595
6	-1.110699	0.396249	2.574736
1	-1.013516	0.221842	1.511875
1	-1.785676	2.661881	2.793067
6	-1.000317	1.683545	3.255539
6	-1.223537	1.379240	4.604256
79	0.695161	2.907093	2.845812
1	-1.561490	-1.599975	3.500328
8	-1.458886	0.051963	4.757747
14	-1.321018	2.459195	6.144020
1	-1.219350	3.868710	5.699363
1	-2.608677	2.215822	6.840999
1	-0.202039	2.131578	7.064885
15	2.691571	4.077468	2.456915
1	3.041191	4.319503	1.120153
1	2.807851	5.357932	3.022205
1	3.857628	3.467990	2.961566
8	-2.717859	3.462411	2.335540
1	-2.726938	3.324552	1.338790
1	-2.406318	4.409221	2.467087
1	-2.021164	6.235665	1.494810
8	-1.836411	5.994858	2.421507
1	-0.861561	5.970777	2.412020
51	0.492313	5.609827	-0.590457
9	0.700305	7.423480	-0.838306
9	2.321541	5.277978	-0.687059
9	0.695652	5.854283	1.291206
9	0.204756	5.249072	-2.373818
9	-1.373642	5.831841	-0.320068
9	0.227291	3.769337	-0.191445
1	-2.641359	4.131586	-0.646021
8	-2.476405	3.228937	-0.323319
1	-1.501336	3.176668	-0.381474

HW-TS4

6	−2.592745	−0.402913	0.385020
6	−1.988242	0.436928	−0.330733
14	−0.497481	0.027024	−1.407805
1	−0.246065	−1.435285	−1.390377
1	−0.774253	0.468046	−2.796673
1	0.678940	0.755751	−0.877745
6	−3.189737	−1.339480	1.233734
1	−4.028051	−0.784713	1.991426
1	−3.837088	−2.065014	0.725088
6	−2.264240	−1.985692	2.247501
1	−2.732040	−2.847377	2.765634
8	−1.145811	−1.611954	2.512323
79	−2.552217	2.465410	−0.328494
15	−2.905896	4.773054	−0.531069
1	−3.567256	5.204034	−1.691553
1	−3.638605	5.404329	0.482845
1	−1.746278	5.572378	−0.580299
51	−6.318983	3.054571	0.903936
9	−7.445085	4.514849	0.881254
9	−7.525620	1.935806	0.016962
9	−5.530554	3.612529	−0.703380
9	−4.992527	3.987921	1.868502
9	−5.140365	1.589584	0.967414
9	−7.051081	2.493704	2.556794
1	−4.798679	0.426820	3.348395
8	−4.985821	−0.486202	2.991735
1	−5.872328	−0.423240	2.539218
1	−7.445726	0.207230	1.013658
8	−7.479702	−0.224188	1.886935
1	−7.793531	0.502469	2.451664
1	−5.632264	2.275442	3.951536
8	−4.687013	2.043218	3.978181
1	−4.327740	2.625517	3.286499

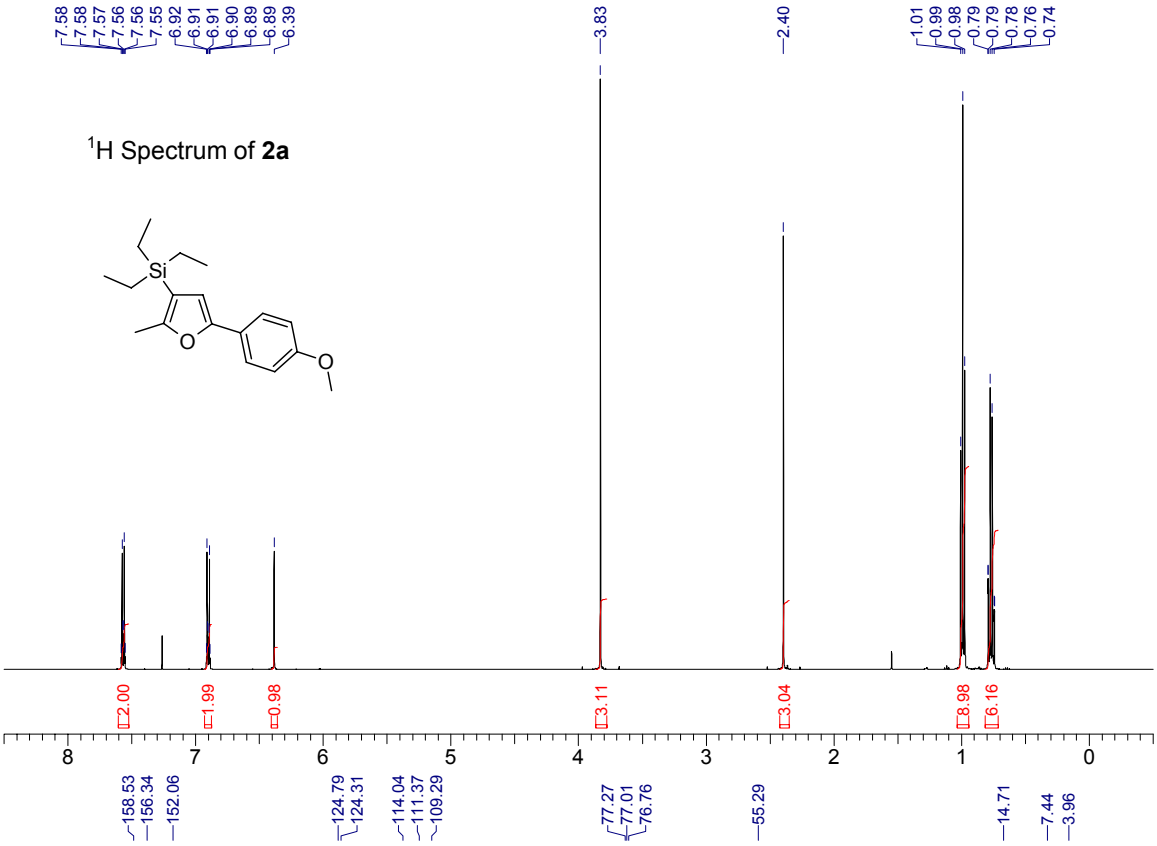
HW-TS5

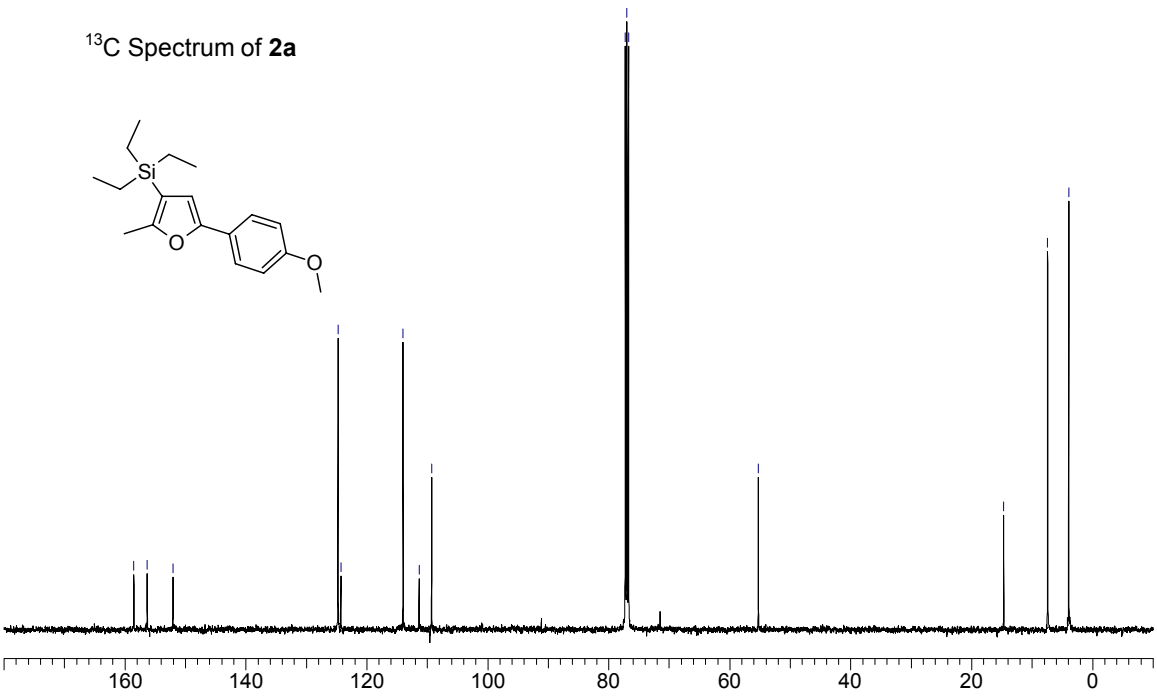
6	−2.384131	−0.004254	0.487785
6	−1.267000	0.609353	0.177152
14	−0.137259	0.082103	−1.249144
1	0.735897	−1.019930	−0.771048
1	−0.934934	−0.377545	−2.414806
1	0.704040	1.237895	−1.643619
6	−3.468080	−0.650792	0.904741
1	−0.624674	1.079316	1.262853
6	−3.367176	−1.804234	1.794435
1	−4.333715	−2.301239	1.993379
8	−2.344871	−2.245798	2.316509
79	−2.281023	2.550483	−0.171382
15	−3.141241	4.634811	−0.746228
1	−4.017474	4.637749	−1.841593
1	−3.890600	5.263024	0.258063
1	−2.225366	5.635427	−1.126772
51	−5.814207	2.752468	1.687328
9	−5.086574	4.462814	1.939380
9	−7.474270	3.420786	1.243104
9	−5.261456	2.893472	−0.121953
9	−4.048529	2.112336	2.095847
9	−6.272625	0.981646	1.334114
9	−6.220889	2.602529	3.482209
8	0.006529	1.391448	2.338200
1	−0.640382	1.972267	2.839664
1	−2.767936	2.595079	3.134996
8	−1.905800	2.809784	3.554589
1	−1.874131	3.776449	3.603949
1	−4.459436	−0.284652	0.649932
1	0.051601	0.510730	2.829198
1	−0.820353	−1.492731	2.900236
8	−0.089661	−1.037029	3.380696
1	−0.328095	−1.111672	4.317167

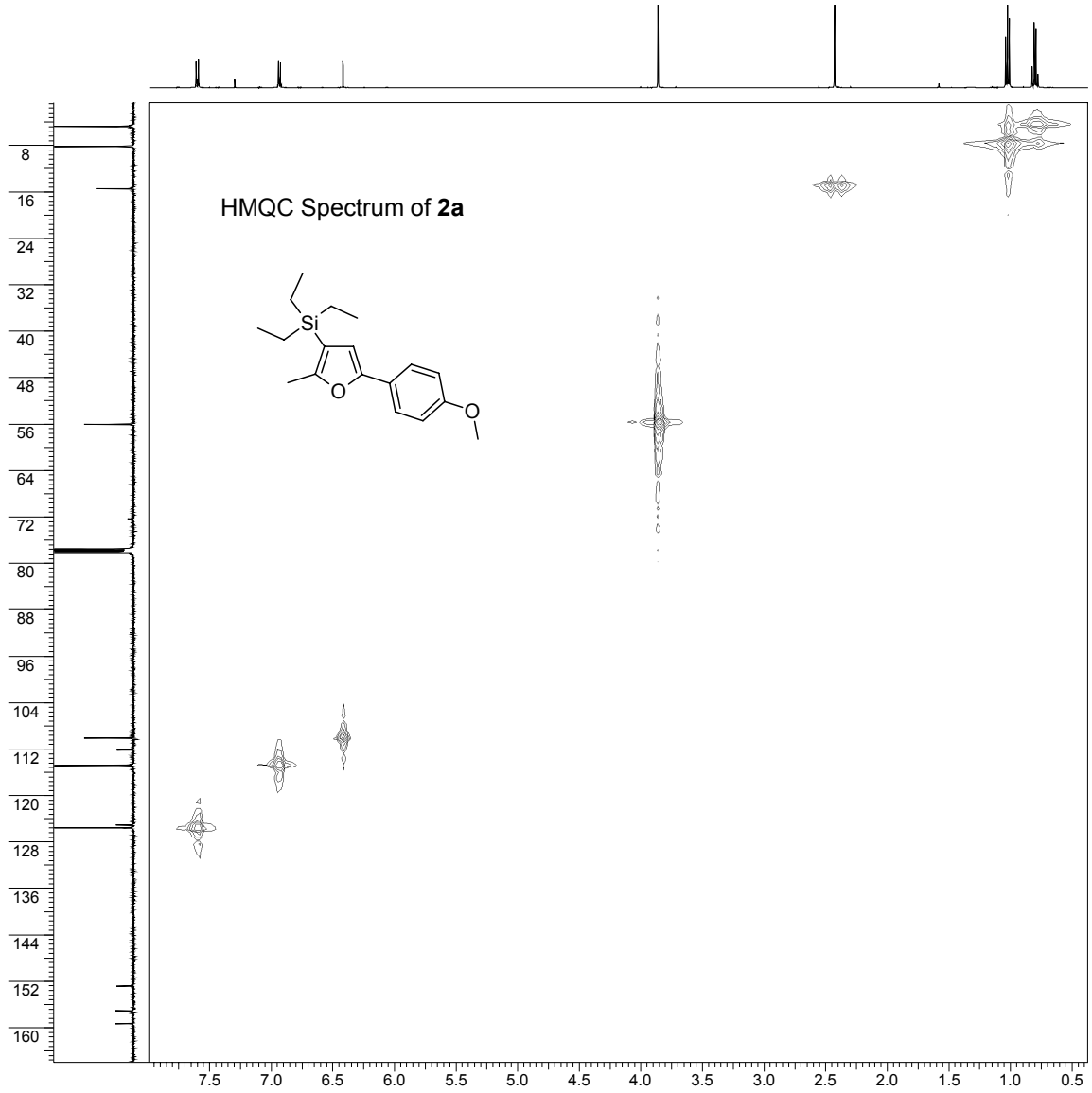
HW-TS6

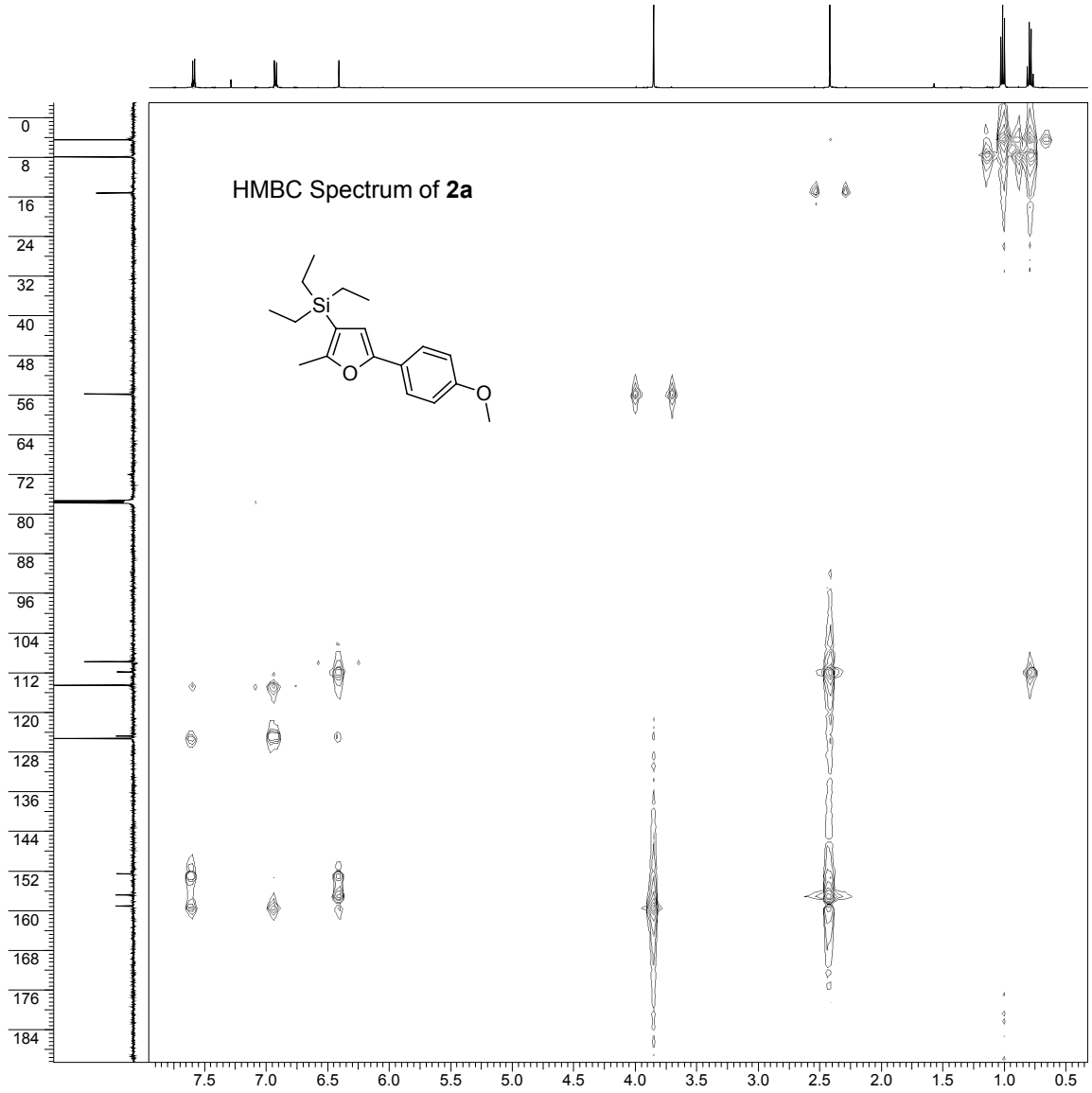
6	-1.594789	0.005009	2.609792
6	-0.274358	0.338741	2.598467
1	0.556426	-0.332511	2.435896
1	-2.045735	3.153300	3.012619
6	-0.199328	1.768701	2.809139
6	-1.537193	2.161667	3.010678
79	1.410314	3.000277	2.451278
1	-2.118526	-0.930532	2.470411
8	-2.377766	1.077487	2.863732
14	-0.680158	2.300389	4.976465
1	-0.624877	3.762196	5.155282
1	-1.840961	1.652220	5.632724
1	0.554169	1.640793	5.455499
15	3.301617	4.332536	1.940473
1	3.934589	4.090091	0.711088
1	3.095525	5.718567	1.889713
1	4.409504	4.260898	2.810679
8	-3.138432	4.540043	3.316093
1	-3.561321	4.642198	2.431916
1	-2.675376	5.399195	3.456755
1	-2.029063	7.312006	2.529204
8	-1.713512	6.949180	3.373749
1	-0.843341	6.595893	3.112941
51	-0.084148	5.760972	0.080796
9	0.874099	7.306907	-0.244623
9	1.456563	4.714945	-0.187485
9	0.416915	5.891729	1.911648
9	-0.617929	5.573532	-1.673856
9	-1.636331	6.749350	0.506876
9	-1.026806	4.190784	0.540086
1	-3.454836	5.740358	0.458240
8	-3.775066	4.834151	0.605604
1	-2.976499	4.315983	0.400133

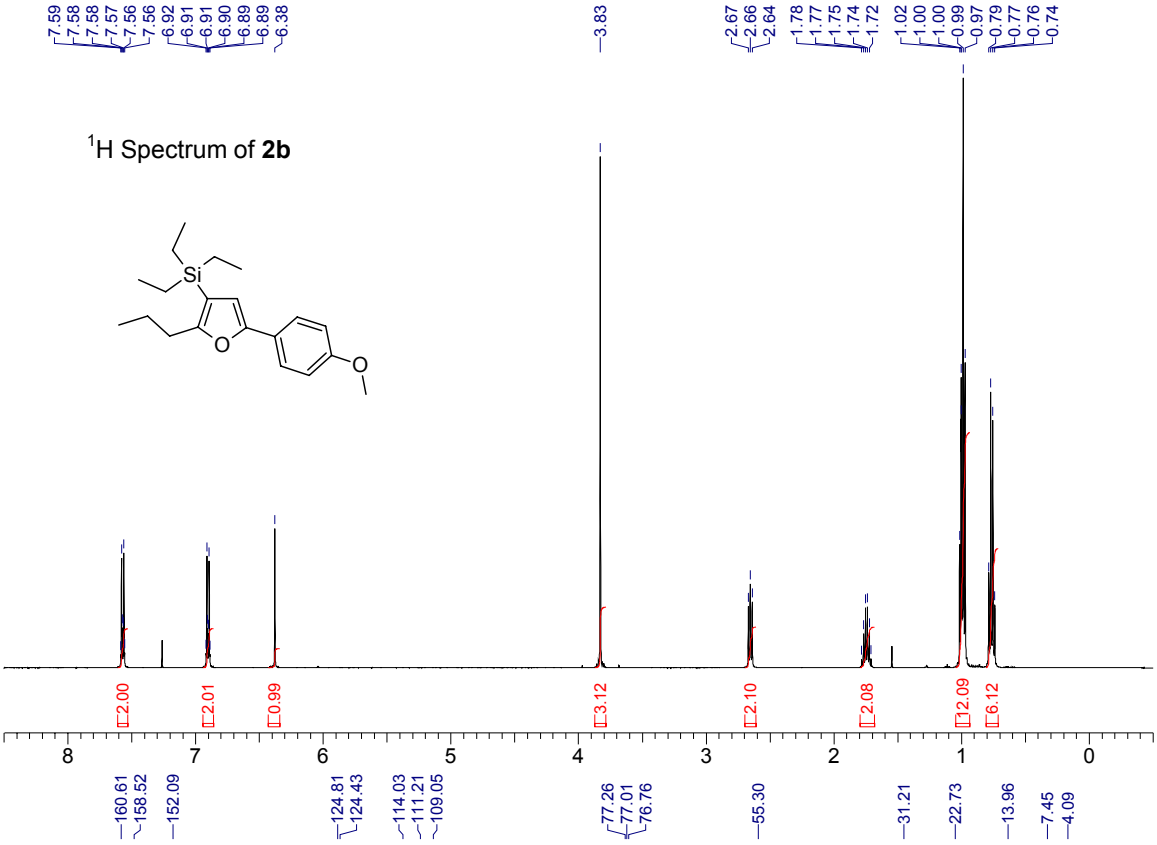
Spectral Charts



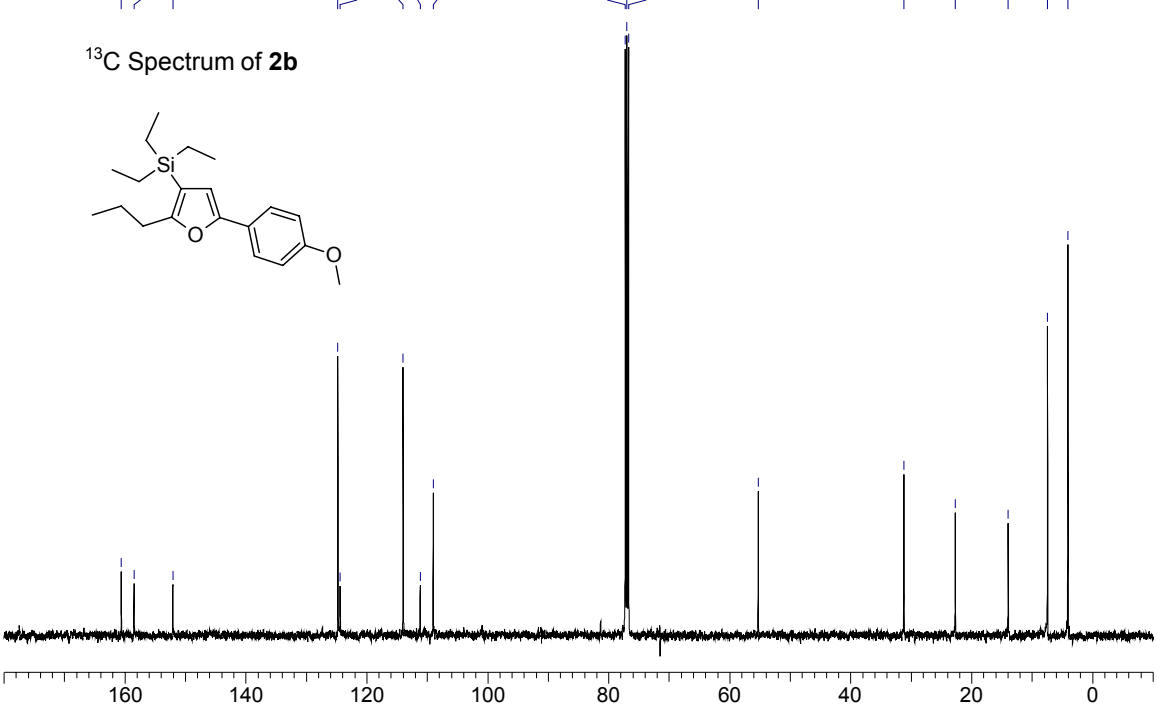



HMQC Spectrum of **2a**
Si
O
O
8
16
24
32
40
48
56
64
72
80
88
96
104
112
120
128
136
144
152
160
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5

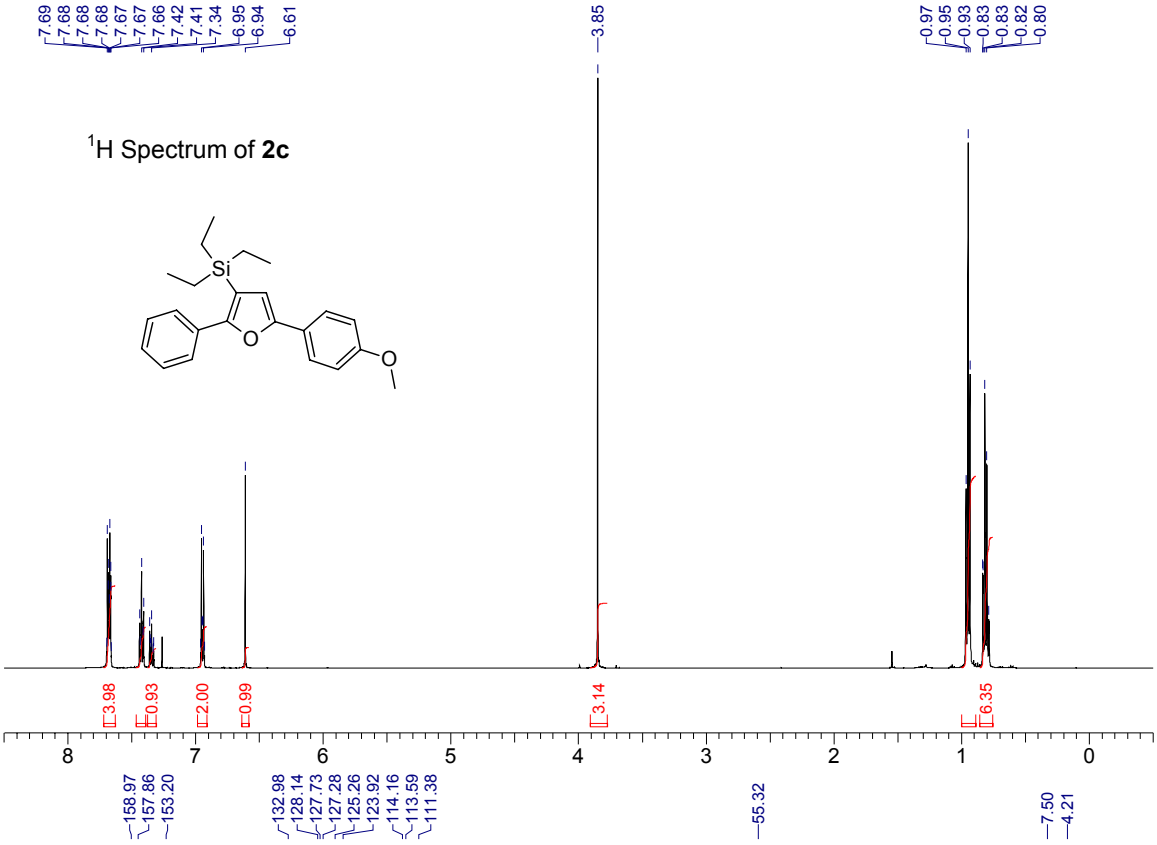

HMBC Spectrum of **2a**
Si
O
O
0
8
16
24
32
40
48
56
64
72
80
88
96
104
112
120
128
136
144
152
160
168
176
184
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5



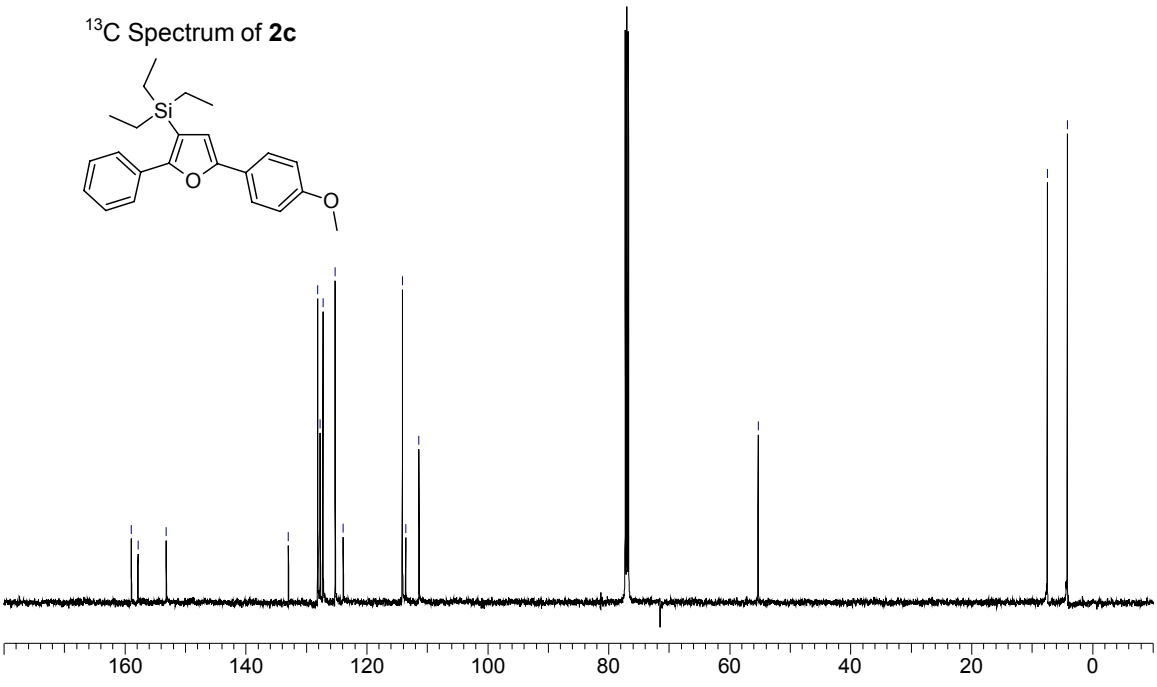
^{1}H Spectrum of **2b**



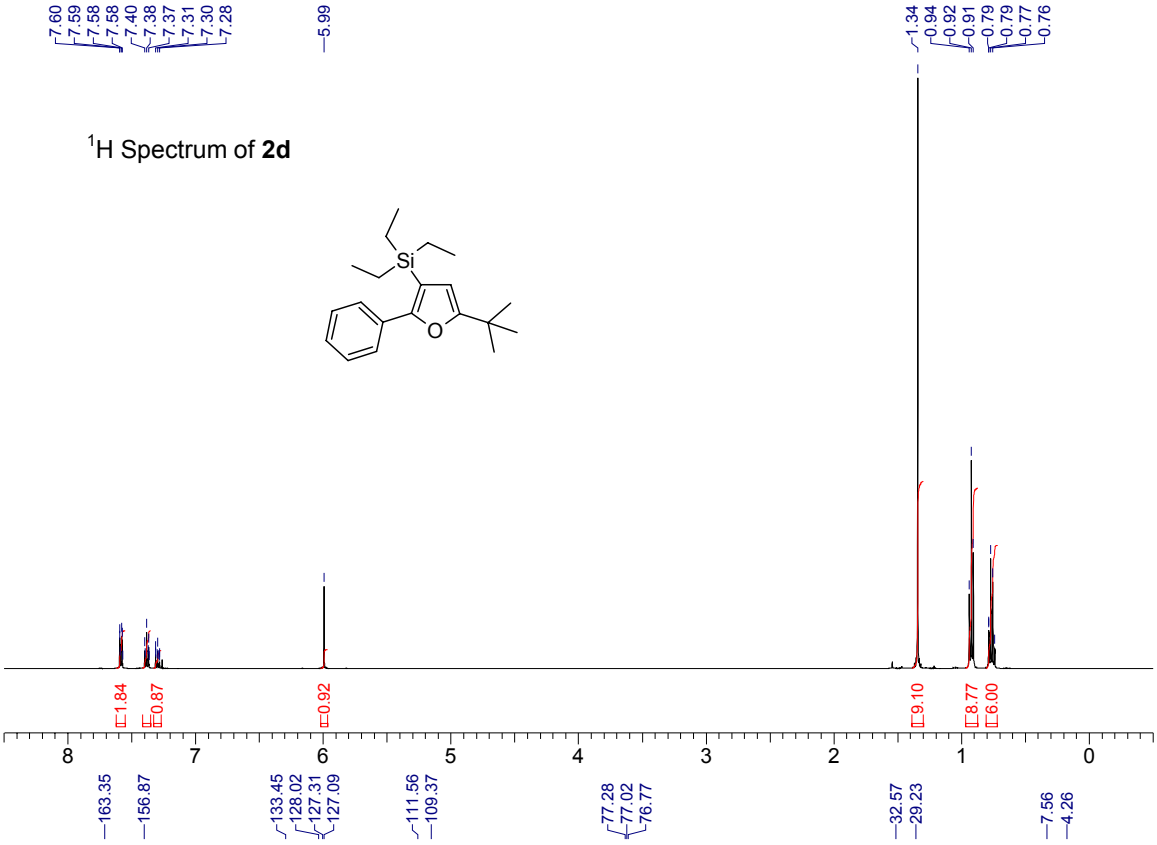
^{13}C Spectrum of **2b**

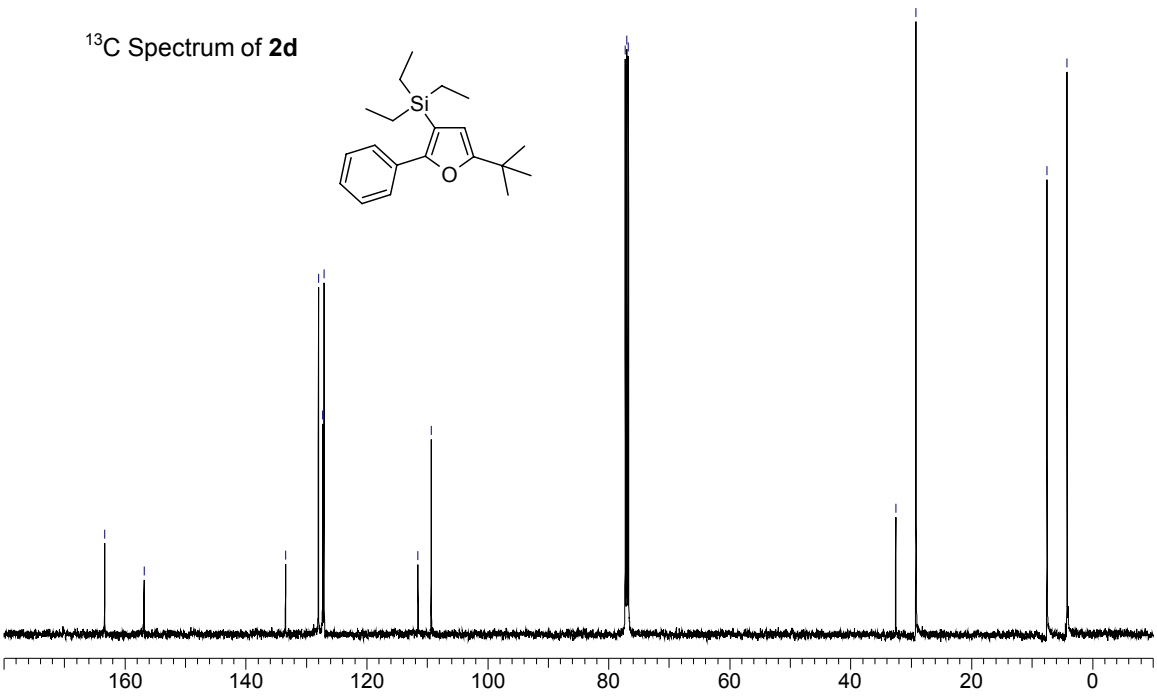


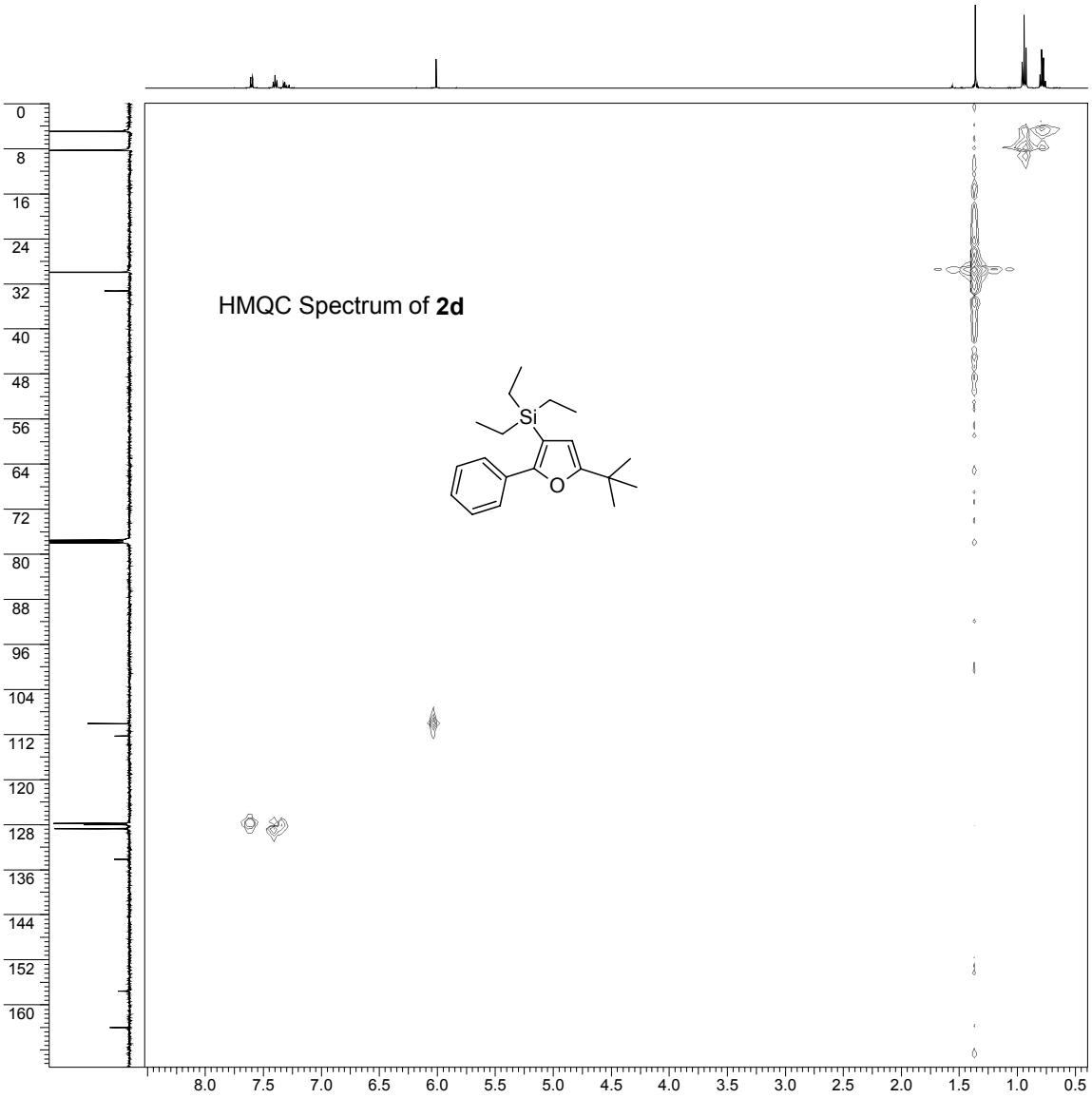
^{1}H Spectrum of **2c**

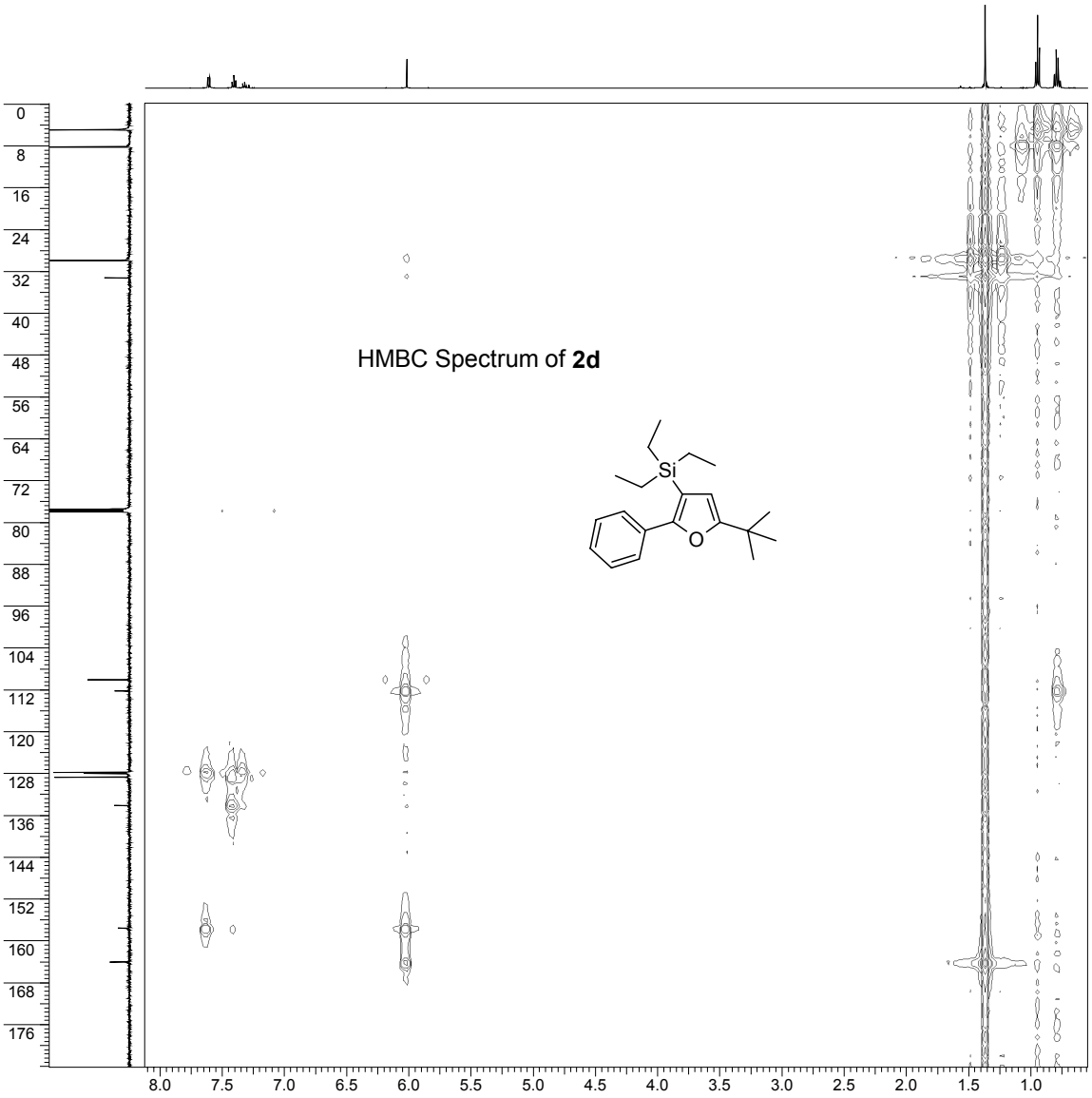


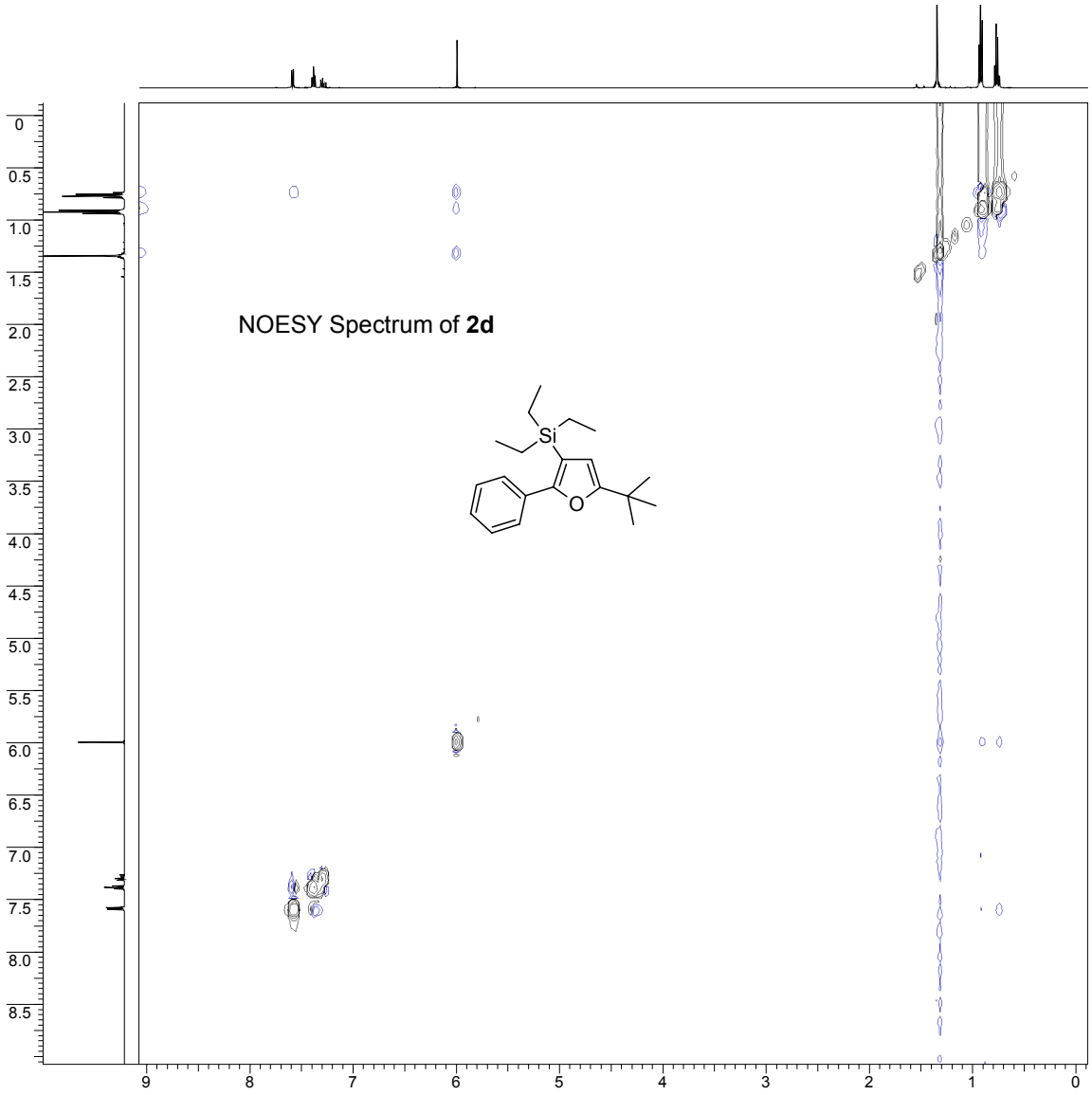
^{13}C Spectrum of **2c**

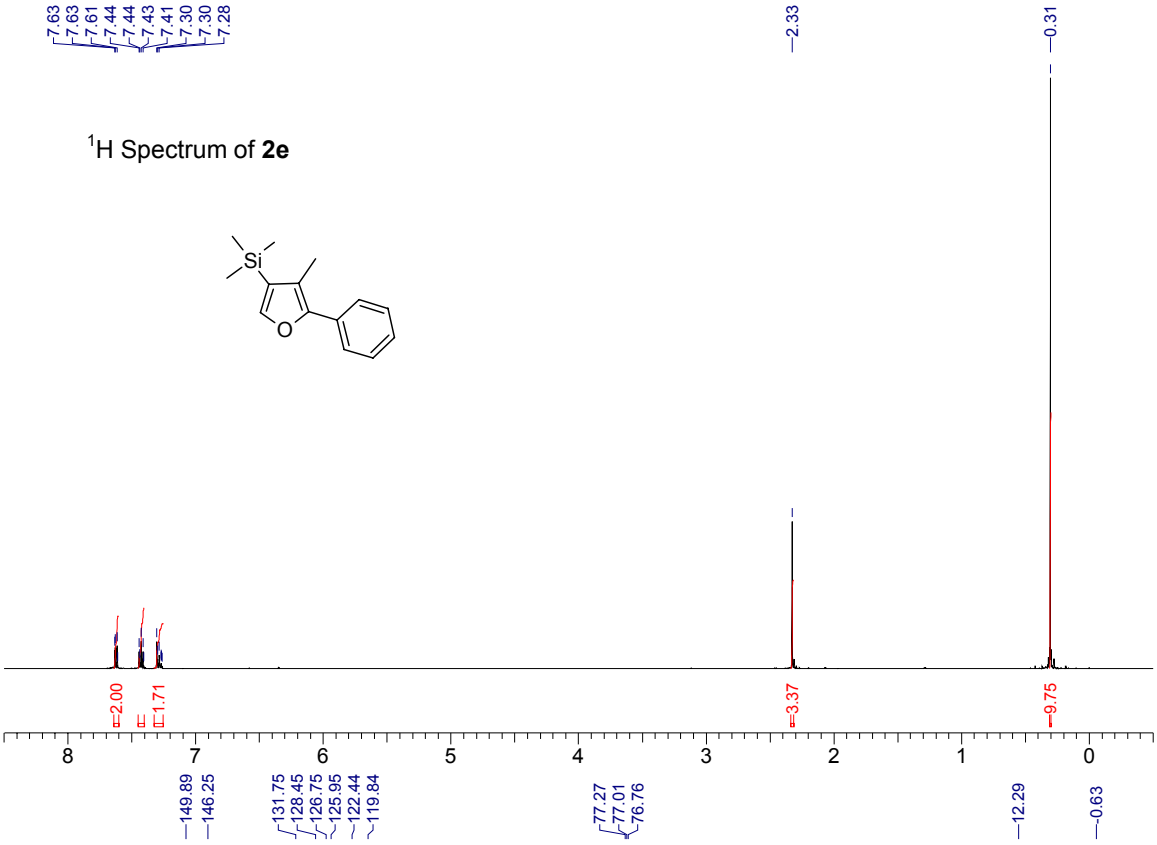

7.60
7.59
7.58
7.58
7.40
7.38
7.37
7.31
7.30
7.28
5.99
1.34
0.94
0.92
0.91
0.79
0.79
0.77
0.76
1H Spectrum of 2d
Si
O
1.84
0.87
0.92
9.10
8.77
6.00
8
7
6
5
4
3
2
1
0


163.35
156.87
133.45
128.02
127.31
127.09
111.56
109.37
77.28
77.02
76.77
32.57
29.23
7.56
4.26
13C Spectrum of 2d
Si
O
160
140
120
100
80
60
40
20
0

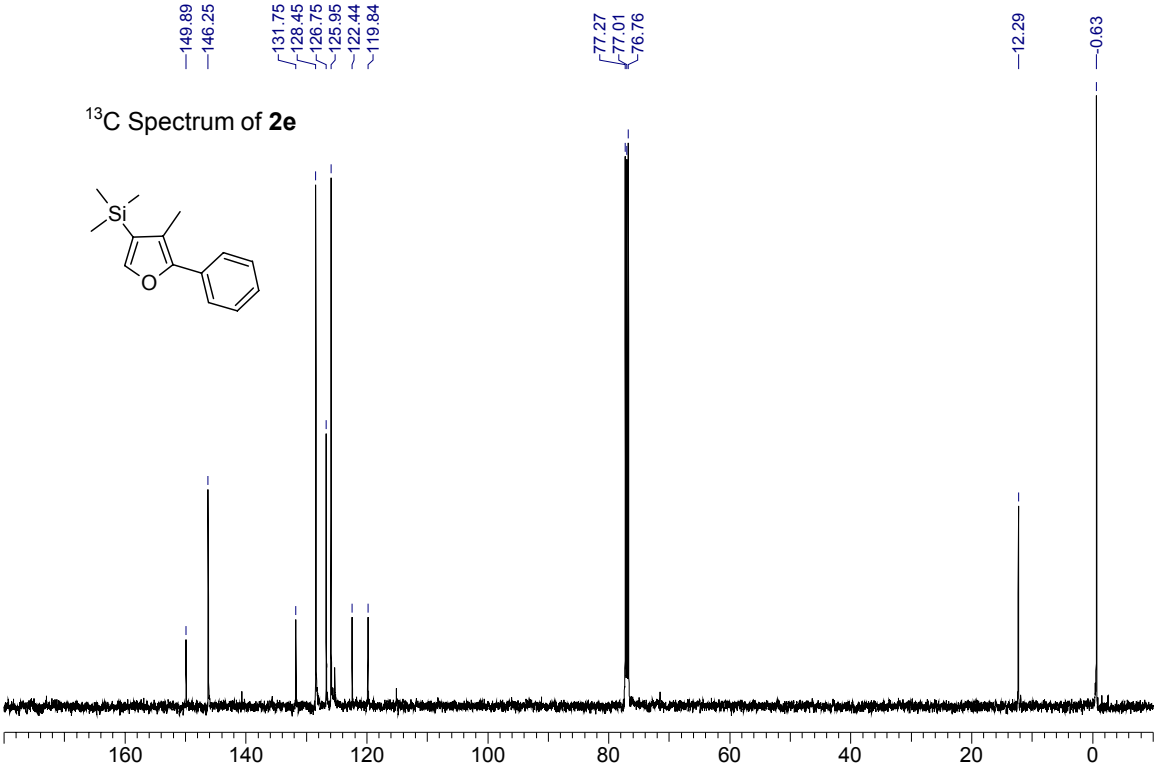

HMQC Spectrum of **2d**
Si
O
0
8
16
24
32
40
48
56
64
72
80
88
96
104
112
120
128
136
144
152
160
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5


HMBC Spectrum of **2d**
Si
O
0
8
16
24
32
40
48
56
64
72
80
88
96
104
112
120
128
136
144
152
160
168
176
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0

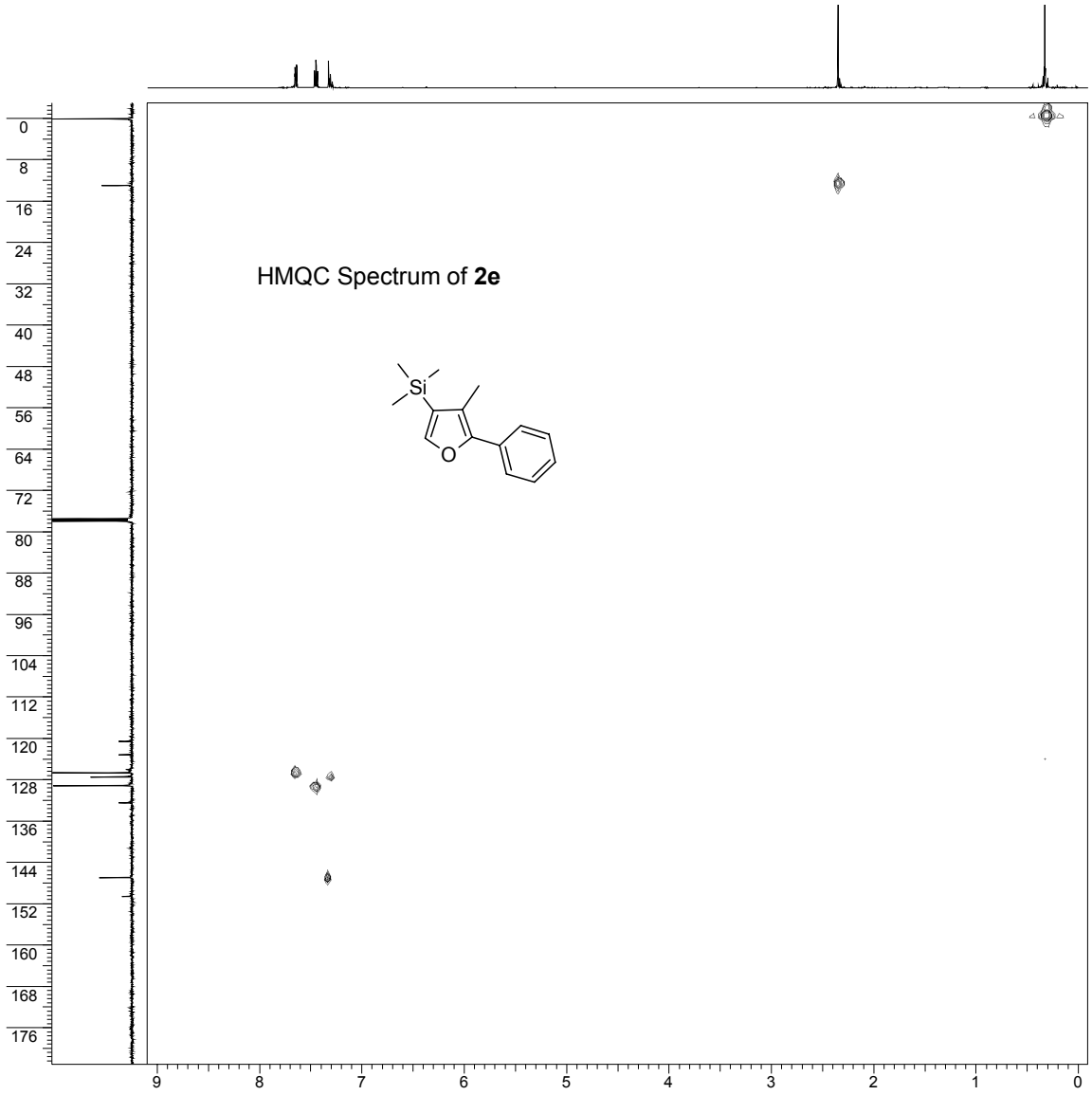

NOESY Spectrum of **2d**
Si
O
0
0.5
1.0
1.5
2.0
2.5
3.0
3.5
4.0
4.5
5.0
5.5
6.0
6.5
7.0
7.5
8.0
8.5
9
8
7
6
5
4
3
2
1
0

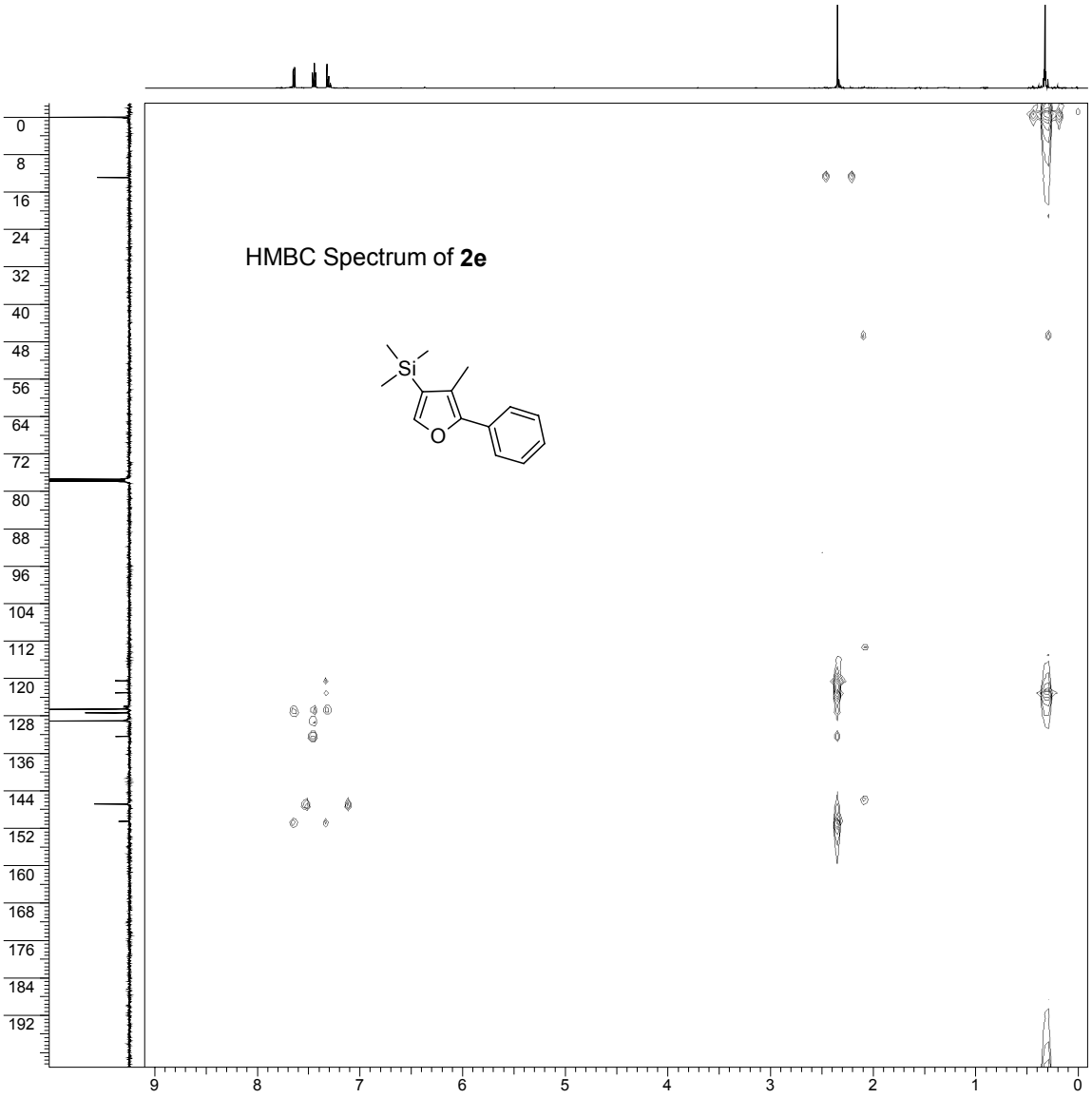


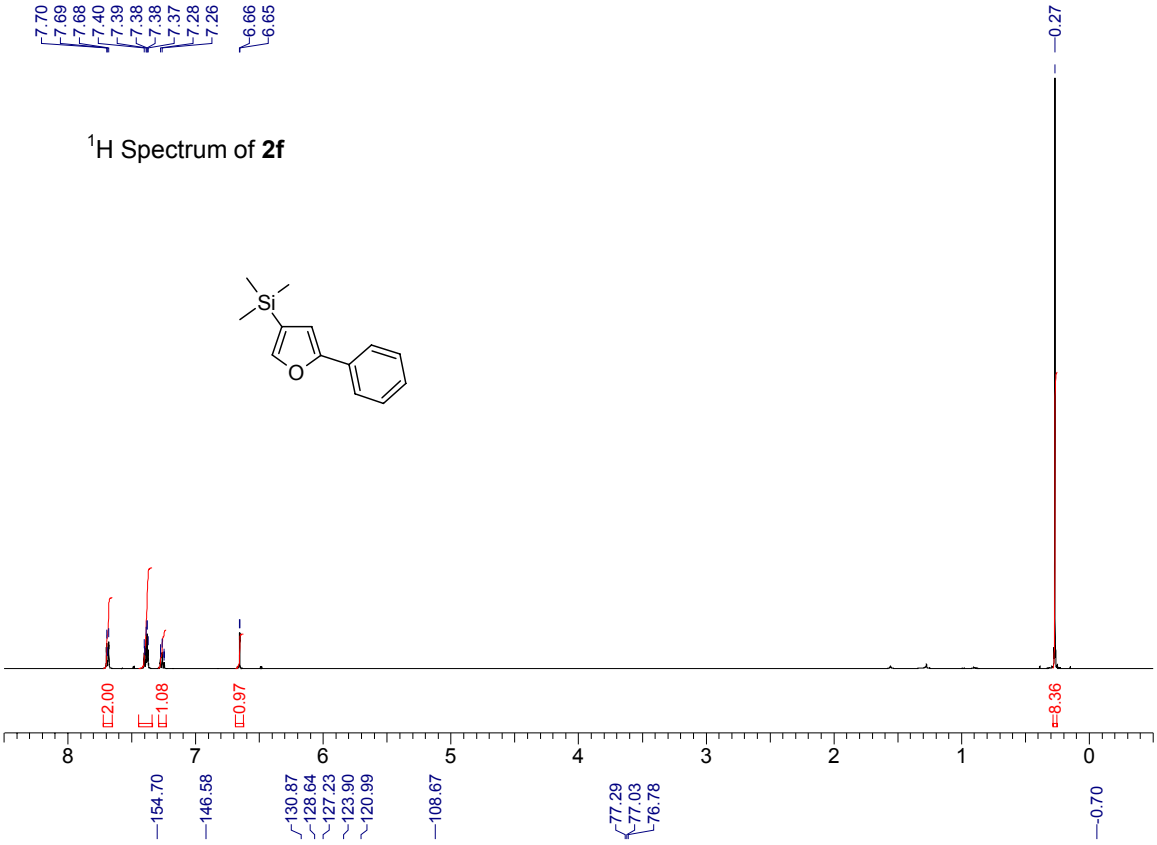
^{1}H Spectrum of **2e**



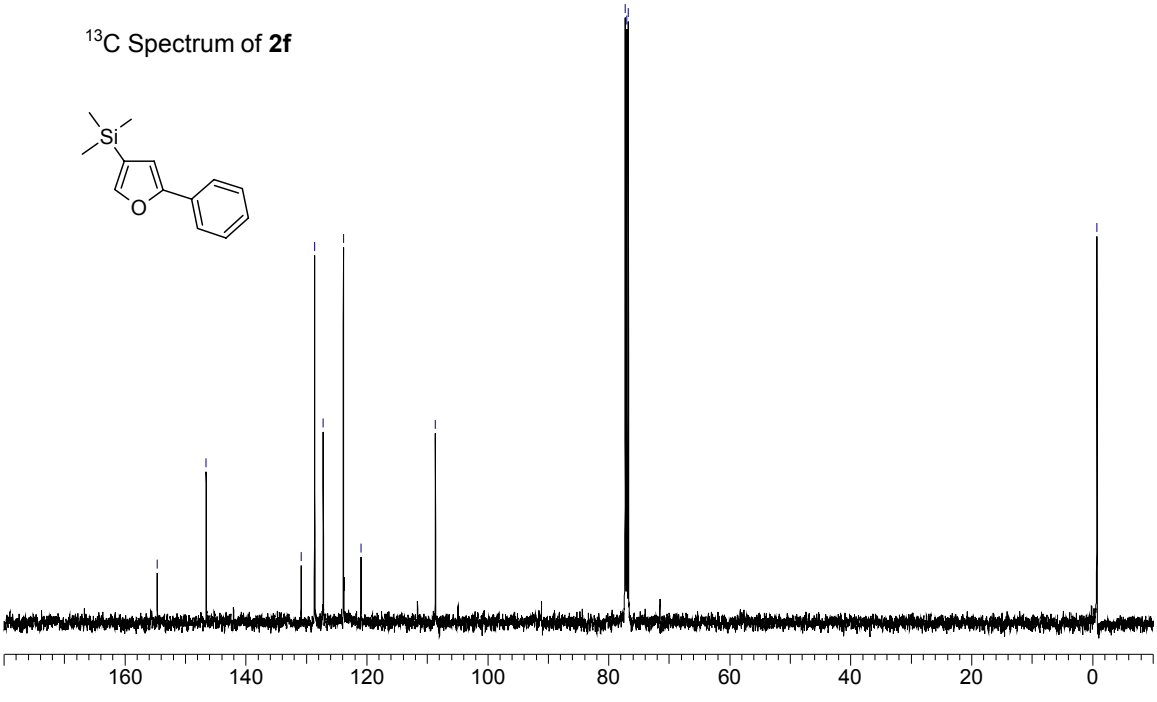
^{13}C Spectrum of **2e**


HMQC Spectrum of **2e**
Si
O
0
8
16
24
32
40
48
56
64
72
80
88
96
104
112
120
128
136
144
152
160
168
176
9
8
7
6
5
4
3
2
1
0

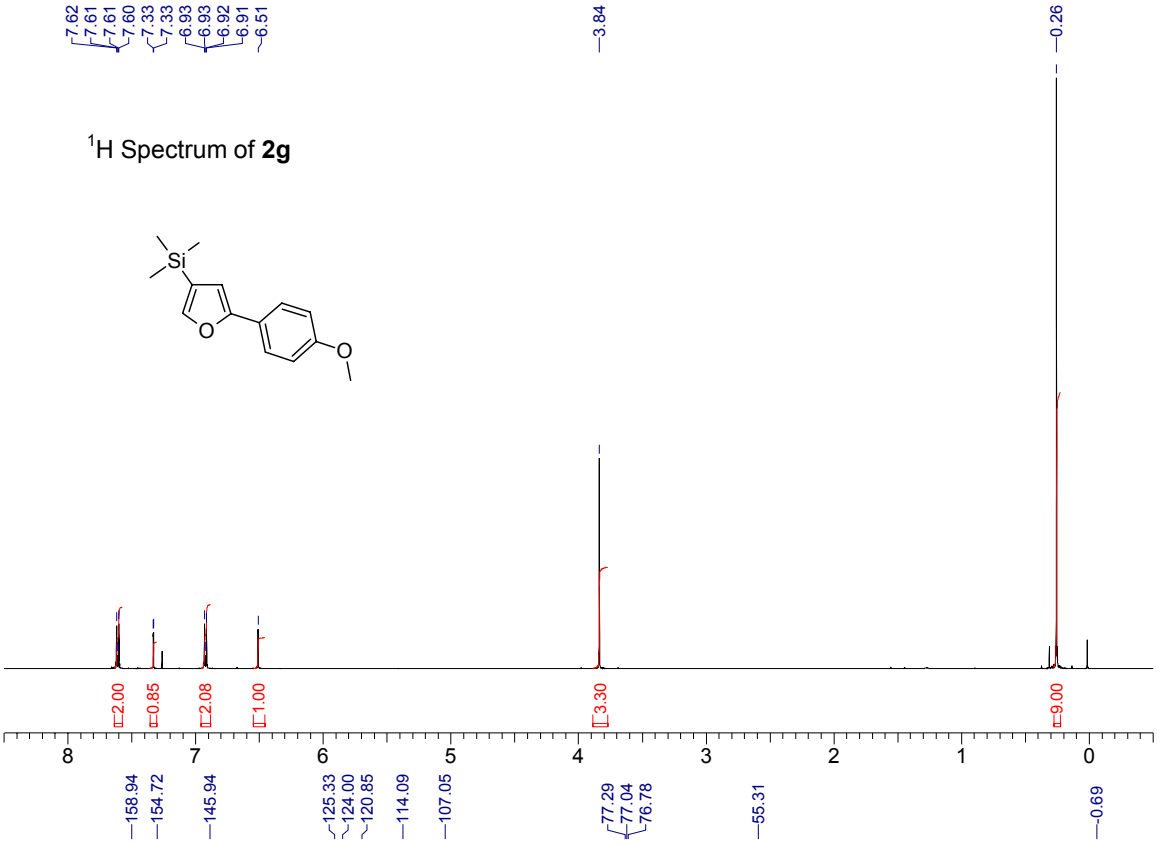

HMBC Spectrum of **2e**
Si
O
0
8
16
24
32
40
48
56
64
72
80
88
96
104
112
120
128
136
144
152
160
168
176
184
192
9
8
7
6
5
4
3
2
1
0



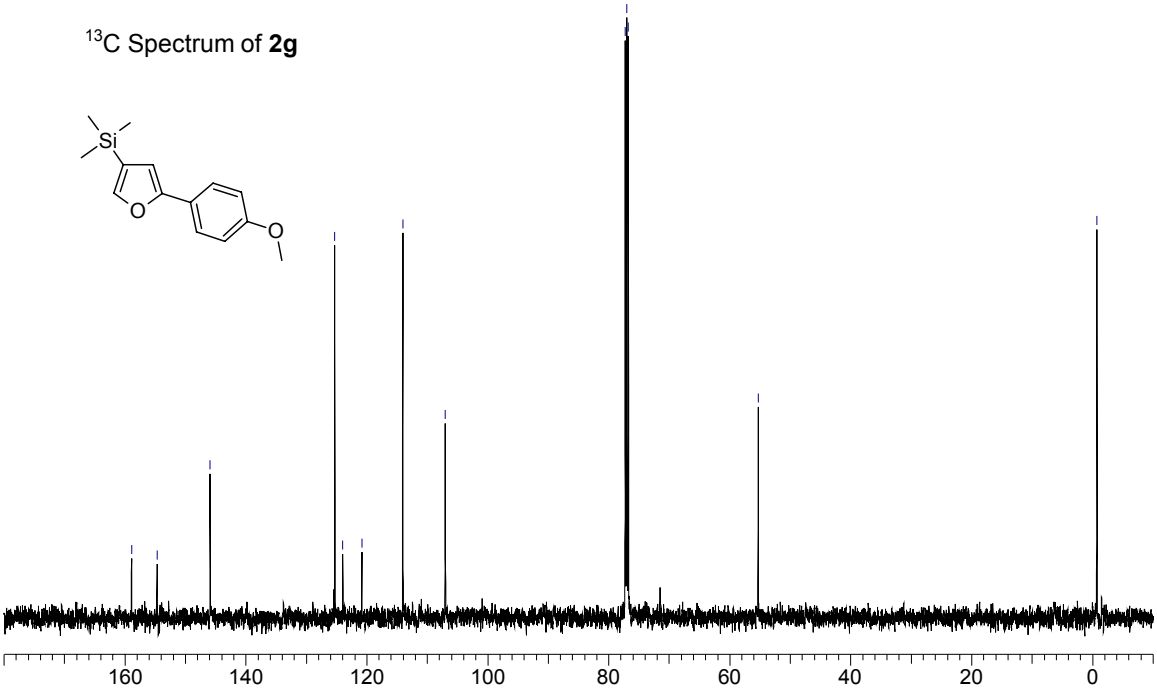
^{1}H Spectrum of **2f**



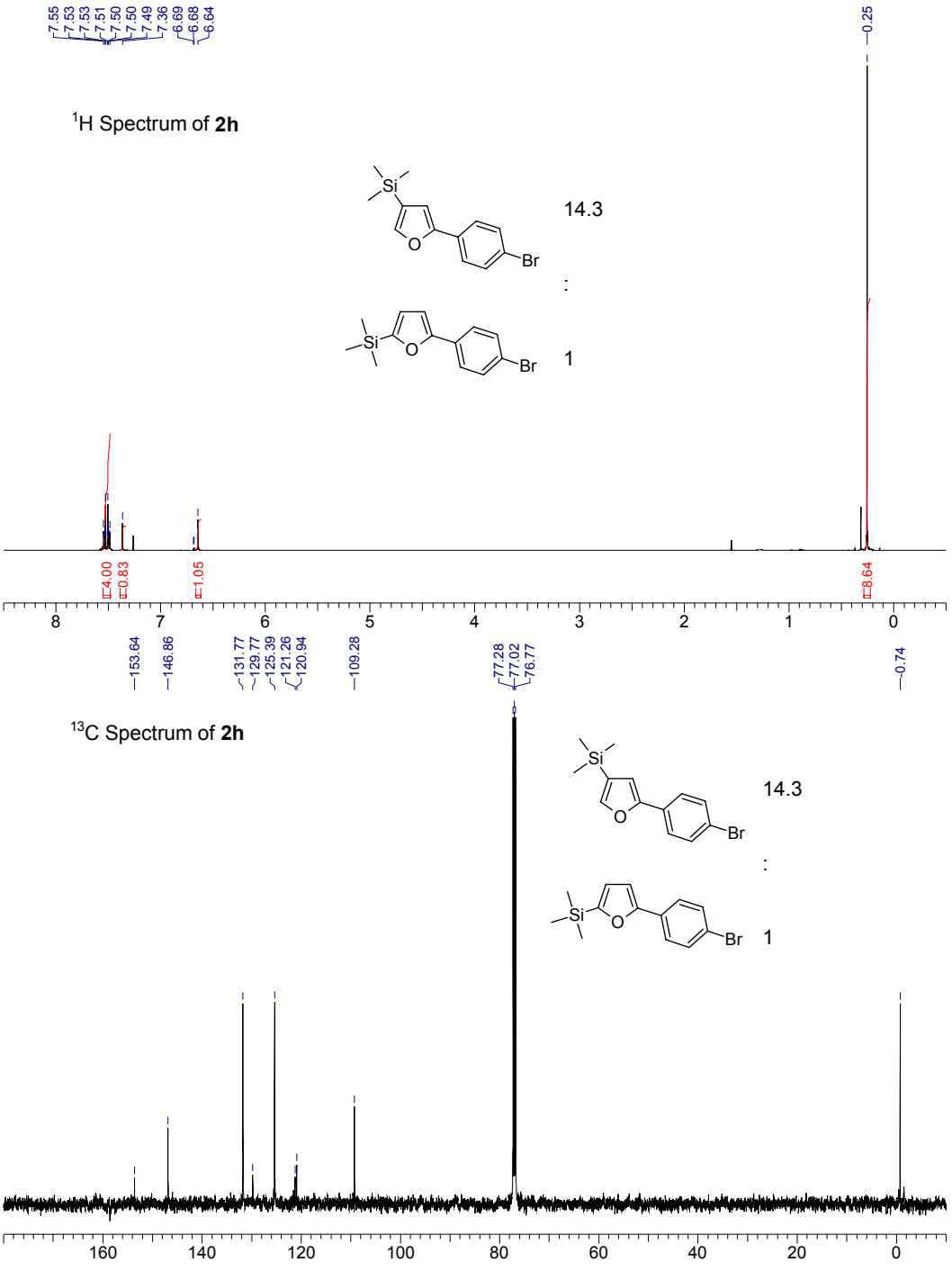
^{13}C Spectrum of **2f**

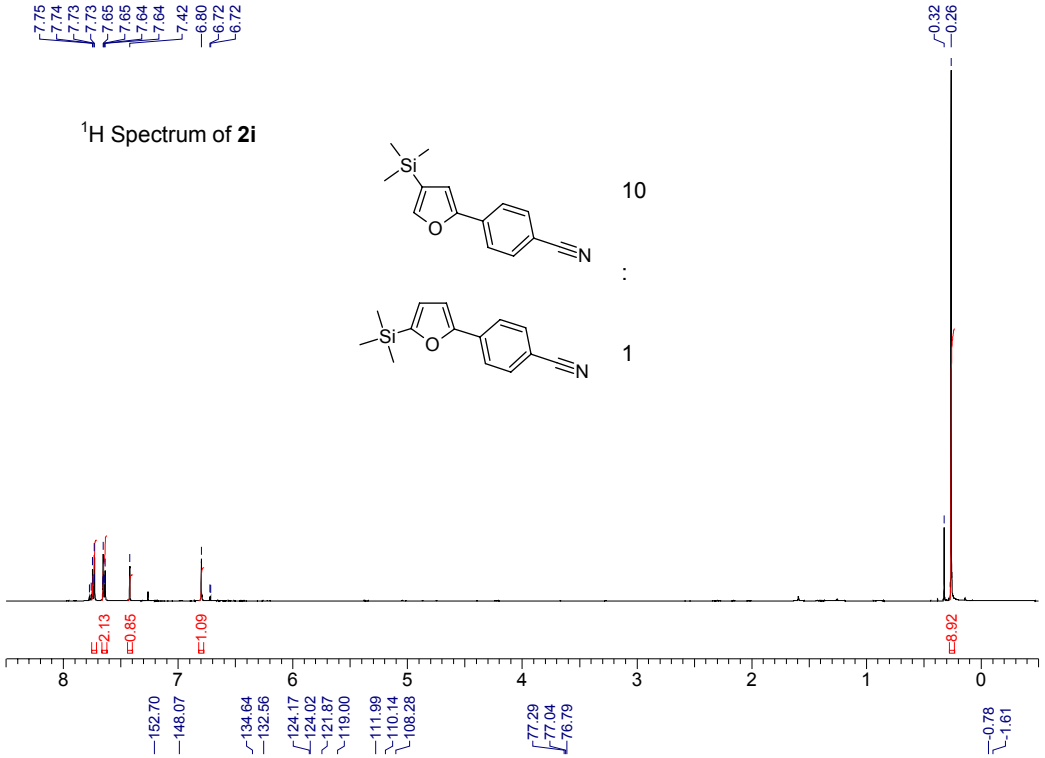


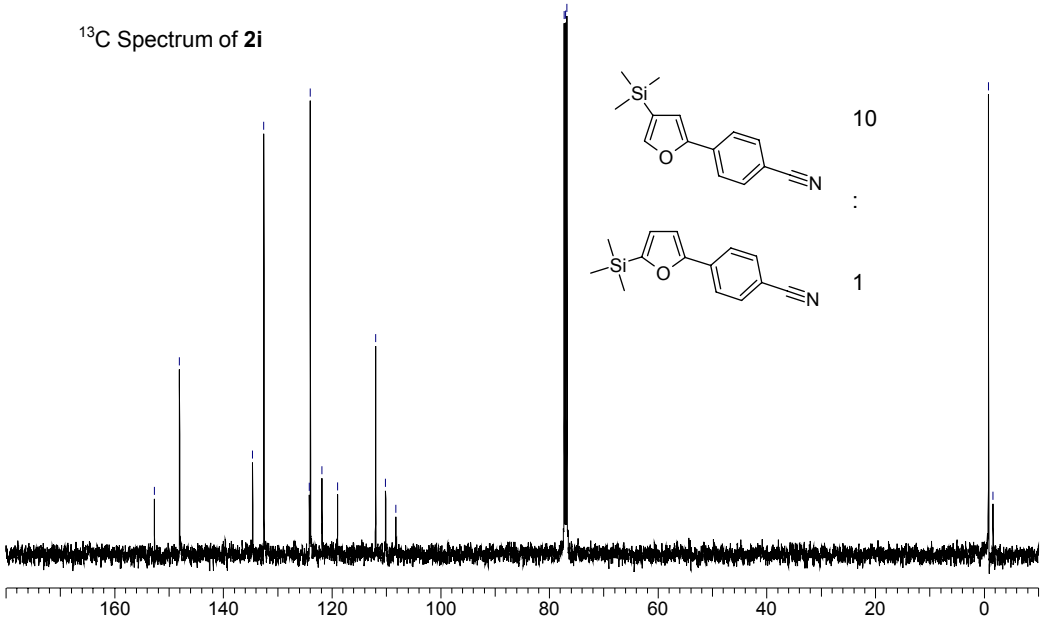
^{1}H Spectrum of **2g**

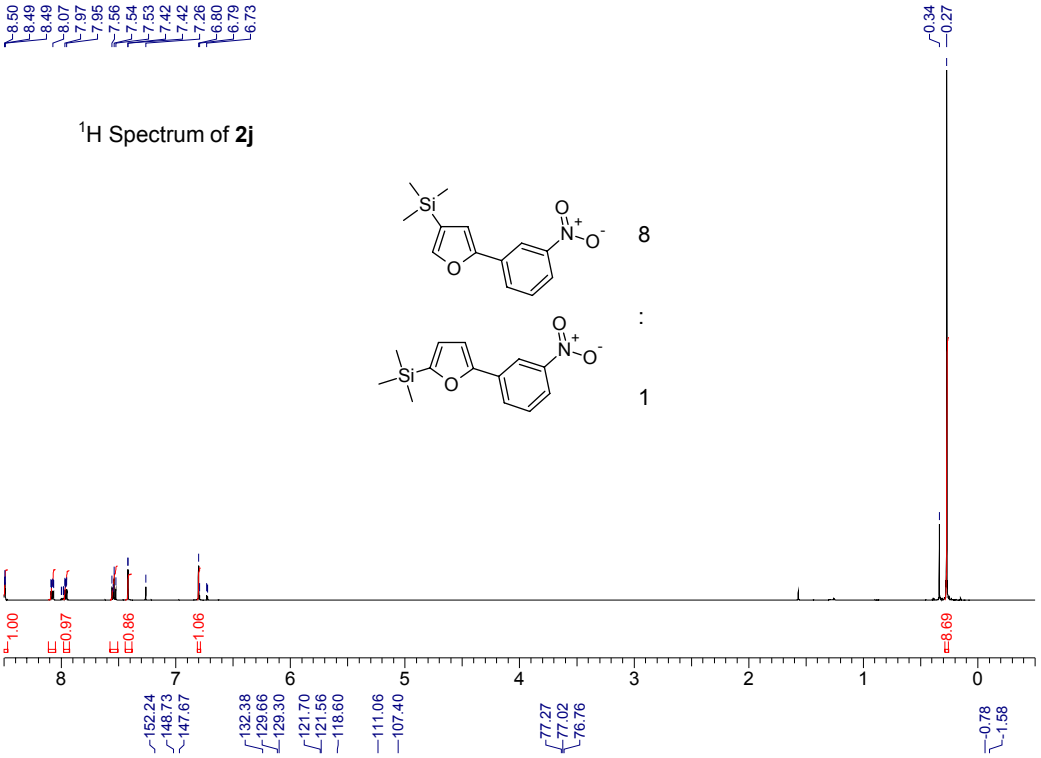


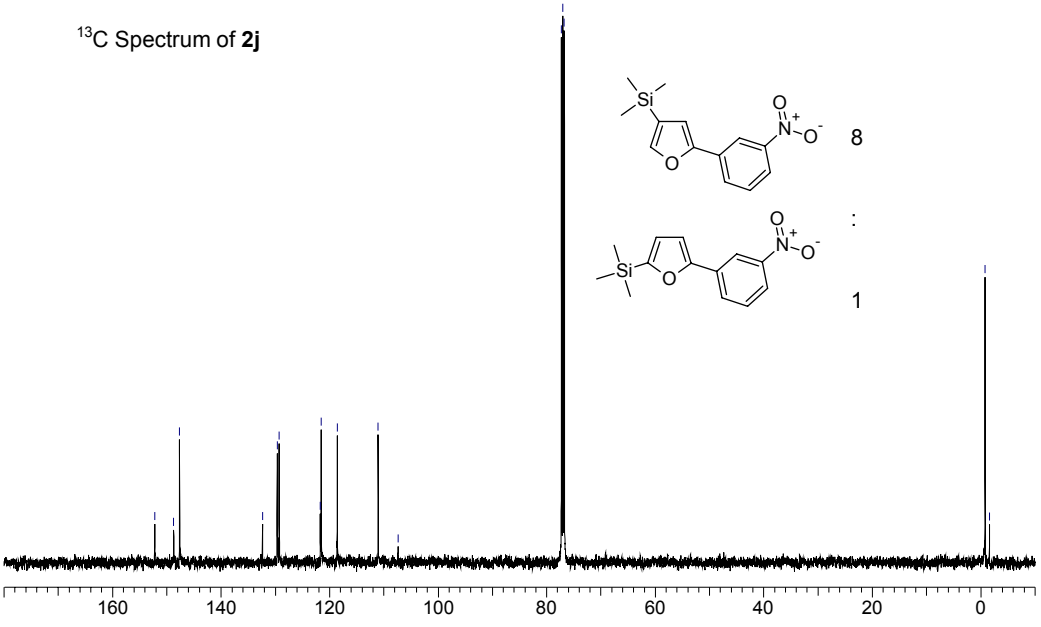
^{13}C Spectrum of **2g**

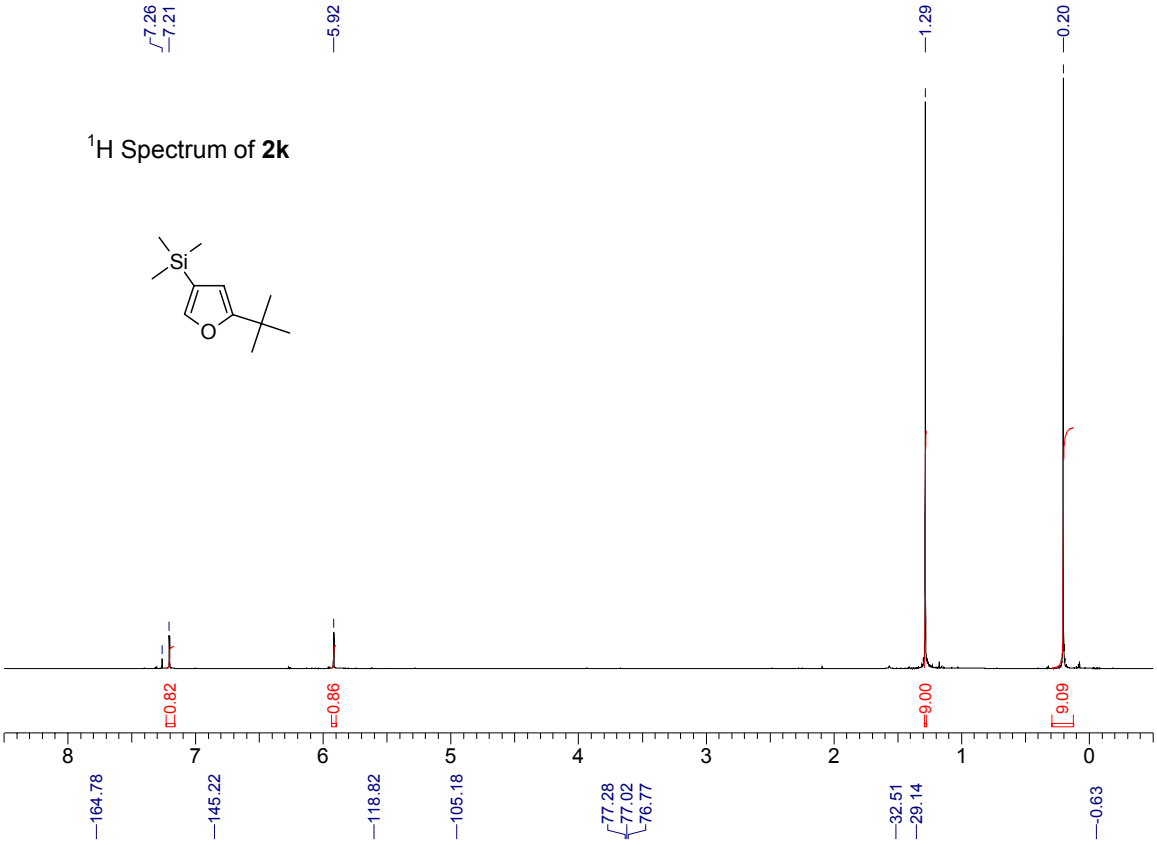

7.55
7.53
7.53
7.51
7.50
7.50
7.49
7.36
6.69
6.68
6.64
0.25
^{1}H Spectrum of **2h**
14.3
:
1
4.00
0.83
1.05
8.64
153.64
146.86
131.77
129.77
125.39
121.26
120.94
109.28
77.28
77.02
76.77
0.74
^{13}C Spectrum of **2h**
14.3
:
1


7.75
7.74
7.73
7.73
7.65
7.65
7.64
7.64
7.42
6.80
6.72
6.72
0.32
0.26
1H Spectrum of 2i
10
:
1
2.13
0.85
1.09
8.92
8
7
6
5
4
3
2
1
0

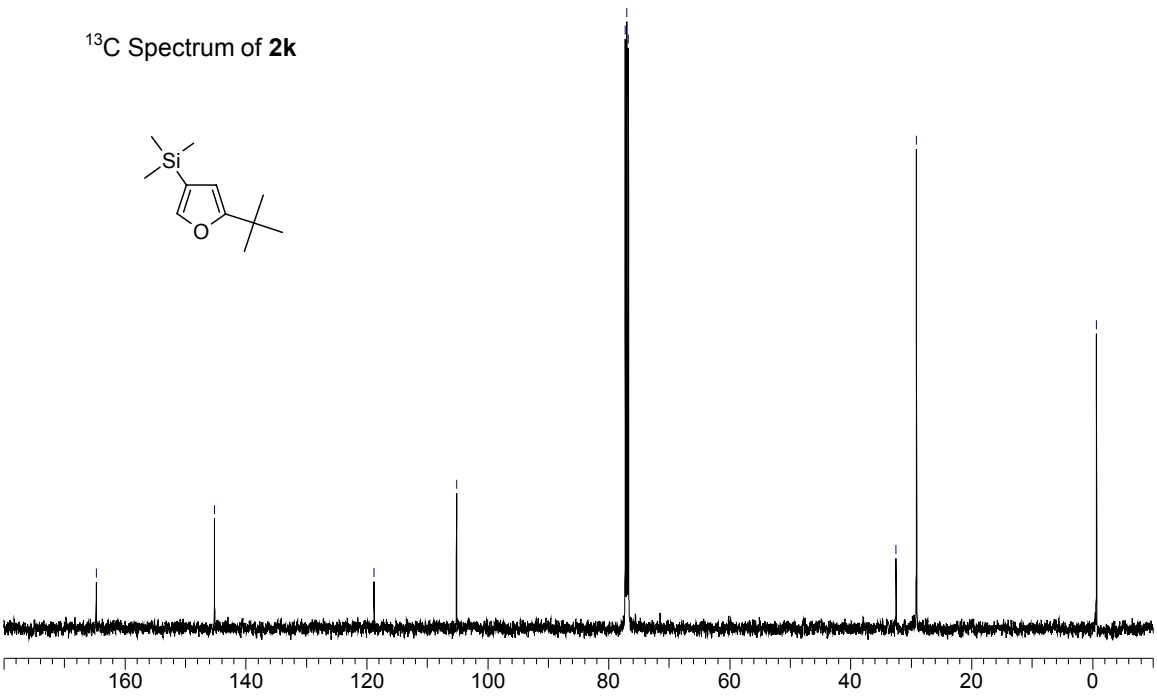

152.70
148.07
134.64
132.56
124.17
124.02
121.87
119.00
111.99
110.14
108.28
77.29
77.04
76.79
0.78
1.61
13C Spectrum of 2i
10
:
1
160
140
120
100
80
60
40
20
0


8.50
8.49
8.49
8.07
7.97
7.95
7.56
7.54
7.53
7.42
7.42
7.26
6.80
6.79
6.73
0.34
0.27
1H Spectrum of 2j
8
:
1
1.00
0.97
0.86
1.06
8.69
8
7
6
5
4
3
2
1
0


152.24
148.73
147.67
132.38
129.66
129.30
121.70
121.56
118.60
111.06
107.40
77.27
77.02
76.76
0.78
1.58
13C Spectrum of 2j
8
:
1
160
140
120
100
80
60
40
20
0

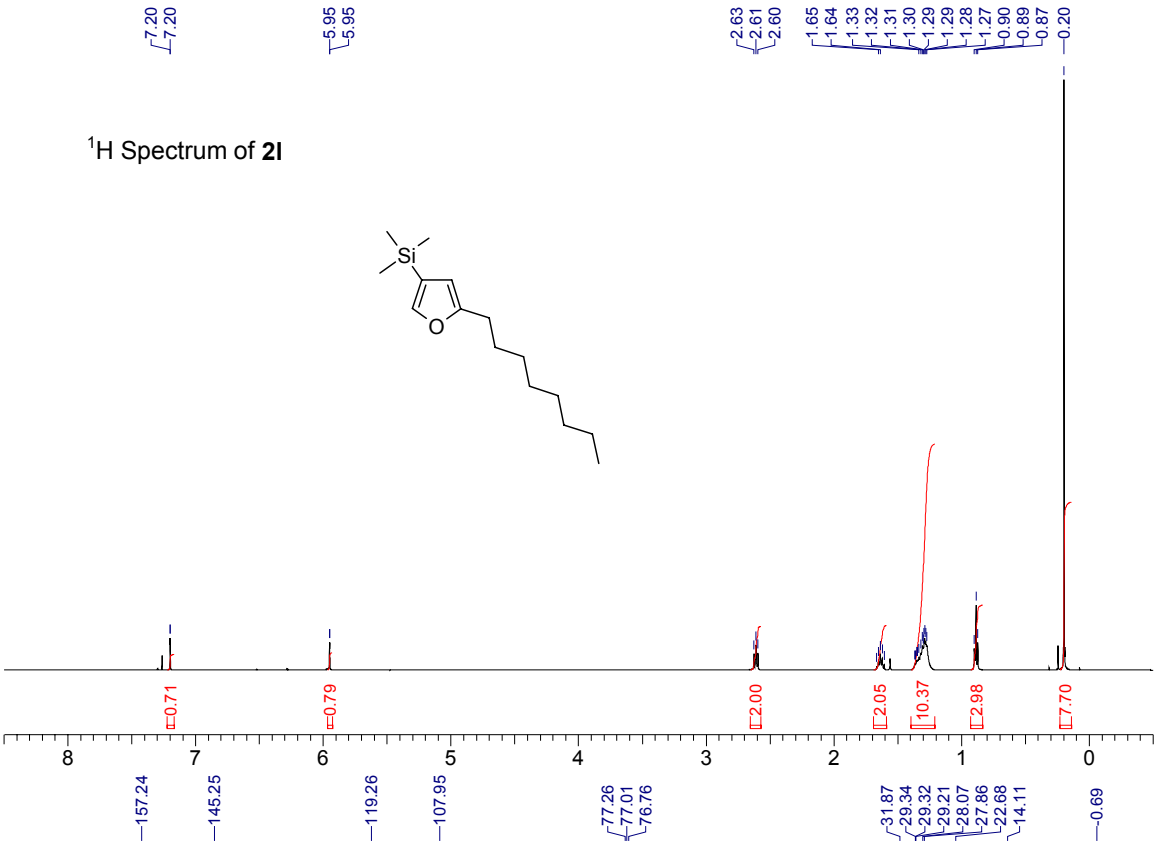


^{1}H Spectrum of **2k**

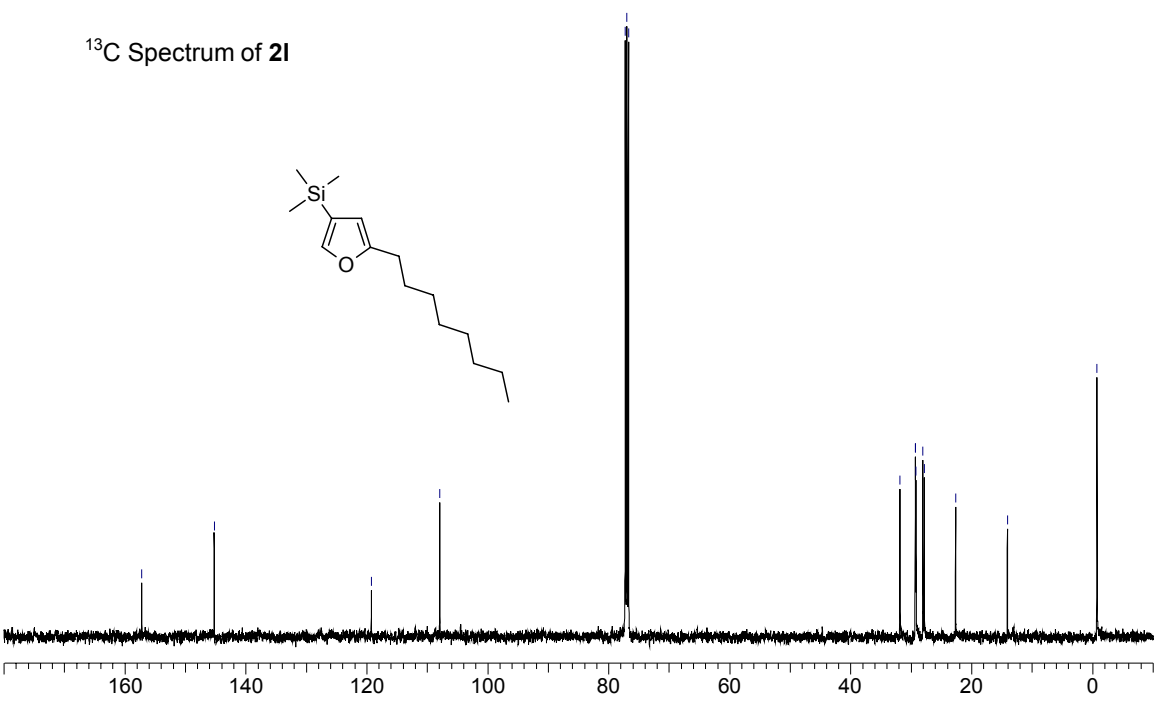


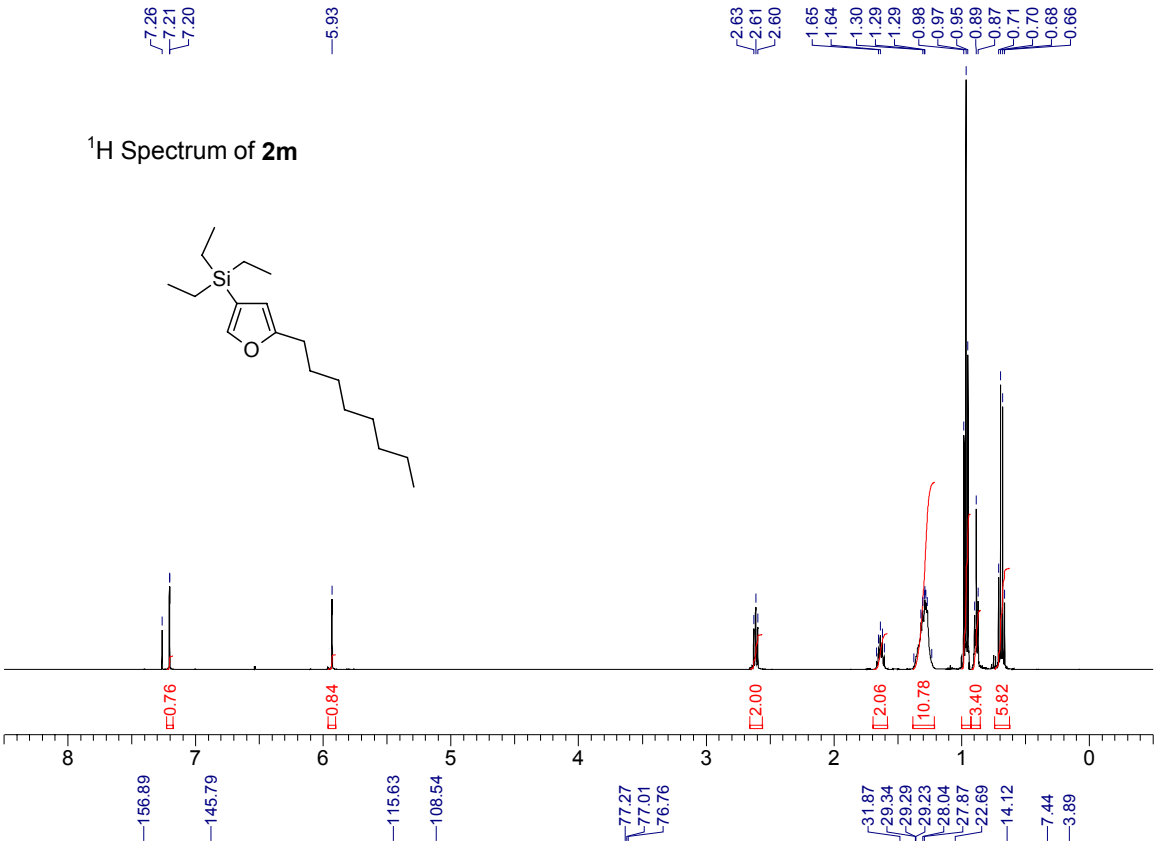
^{13}C Spectrum of **2k**

^{1}H Spectrum of **2l**

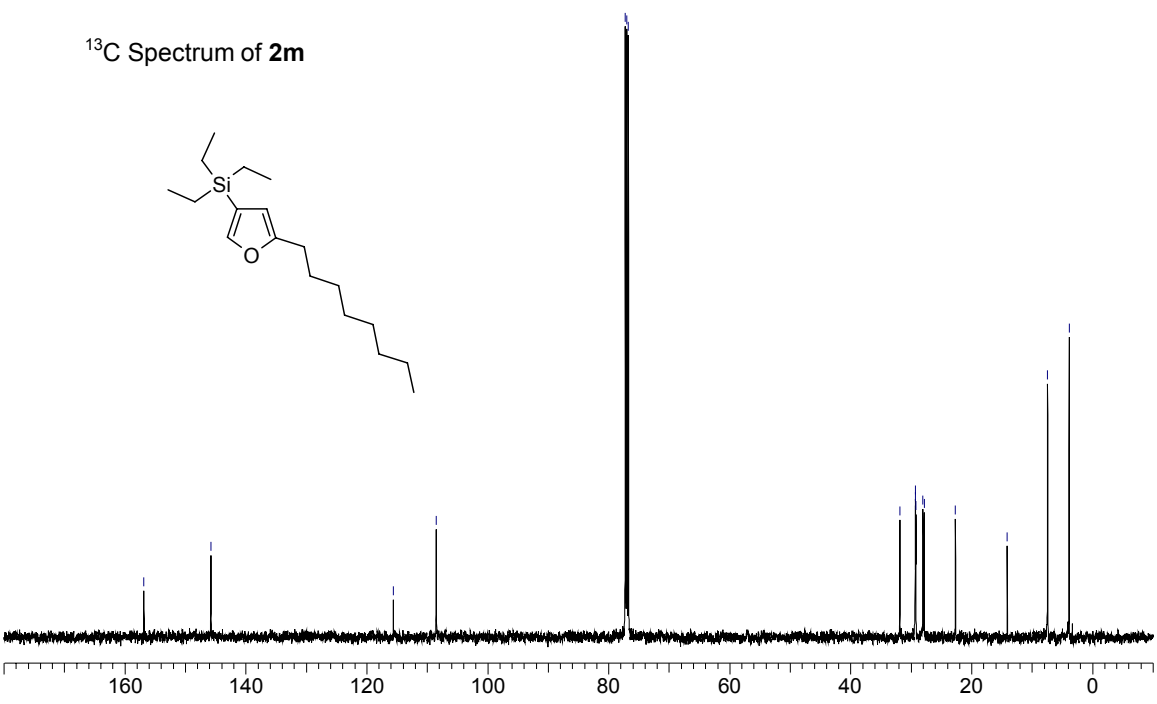


^{13}C Spectrum of **2l**

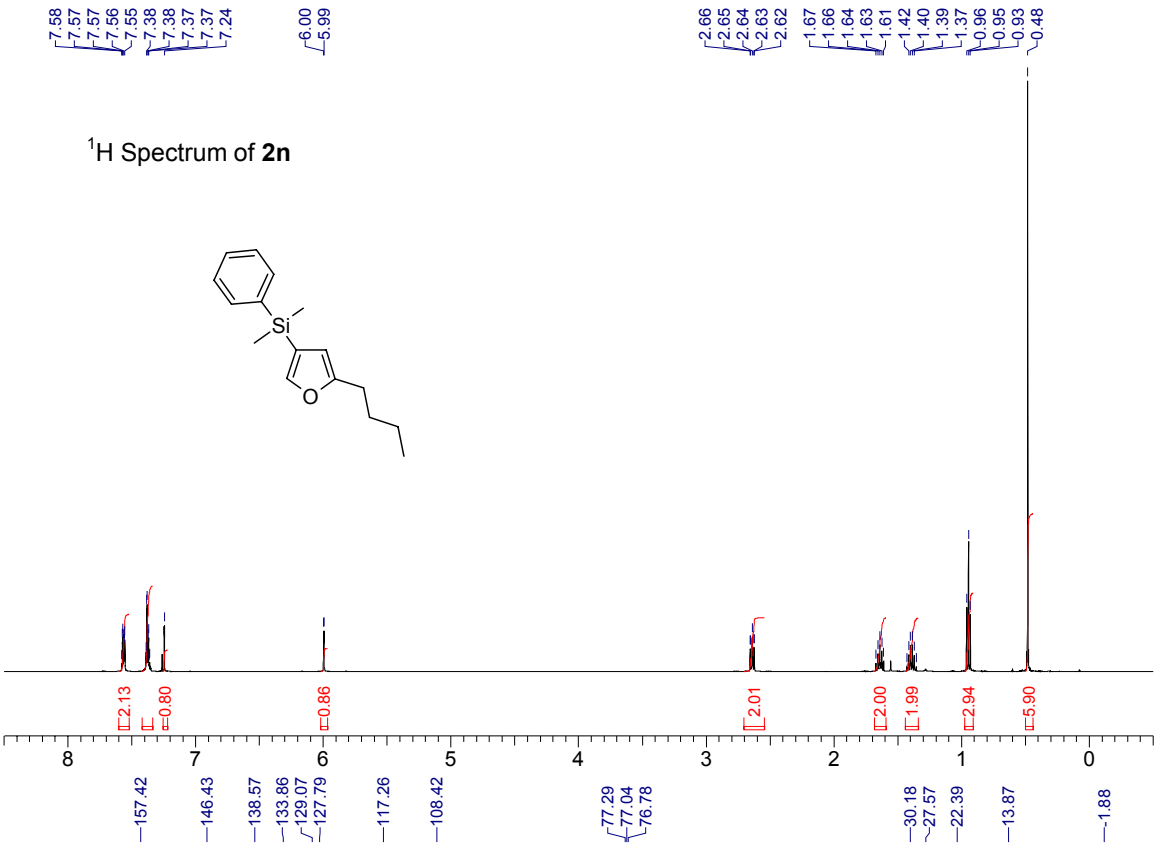




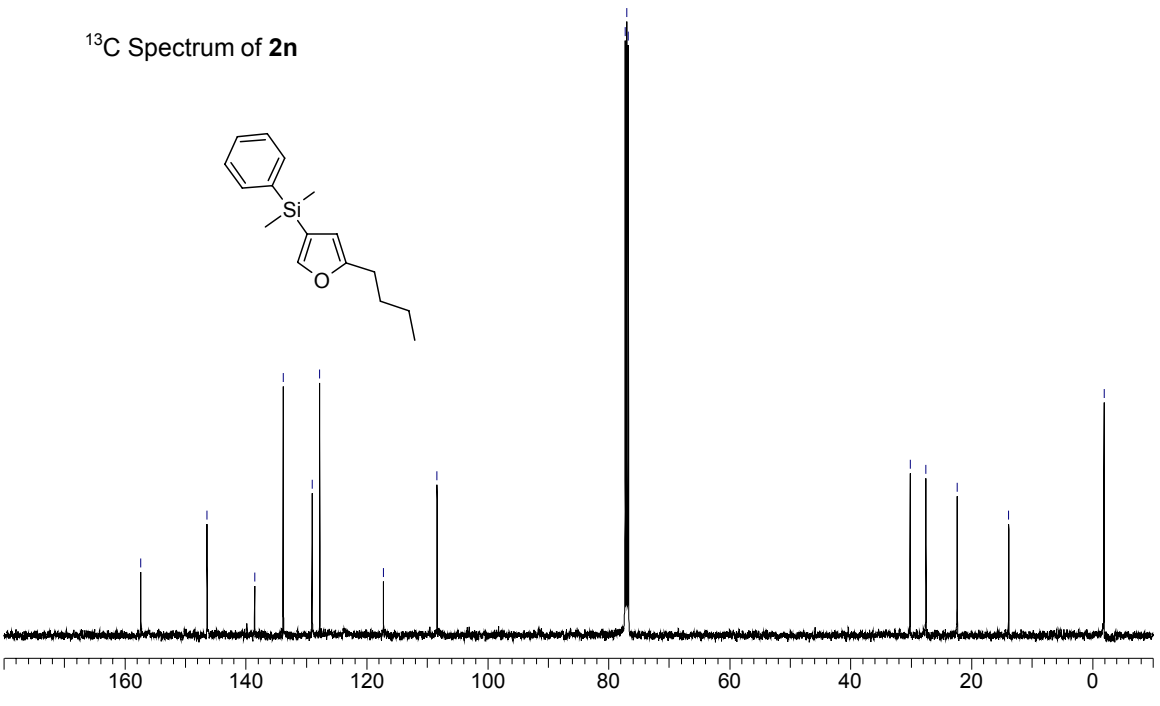
^{1}H Spectrum of **2m**



^{13}C Spectrum of **2m**



^{1}H Spectrum of **2n**



^{13}C Spectrum of **2n**