

Supporting Information for

Defluorinative [4 + 1] Annulation of Perfluoroalkyl *N*-Mesylhydrazones with Primary Amines Provides 5-Fluoroalkyl 1,2,3-Triazoles

Yongquan Ning^{†a}, Hongwei Wang^{†a}, Paramasivam Sivaguru^{†a}, Shuang Li,^a Giuseppe Zanoni,^b Steven P. Nolan,^c and Xihe Bi^{*a,d}

^a Department of Chemistry, Northeast Normal University, Changchun 130024, China. ^b

Department of Chemistry, University of Pavia, Viale Taramelli 12, 27100 Pavia, Italy. ^c

Department of Chemistry and Sustainable Chemistry, Ghent University, 281 Krijgslaan S-3, 9000,

Ghent Belgium. ^d State Key Laboratory of Elemento-Organic Chemistry, Nankai University, Tianjin 300071, China.

E-mail: bixh507@nenu.edu.cn

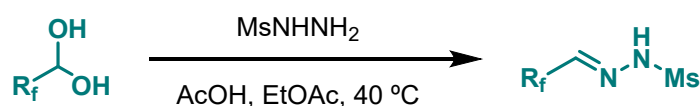
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I. General information

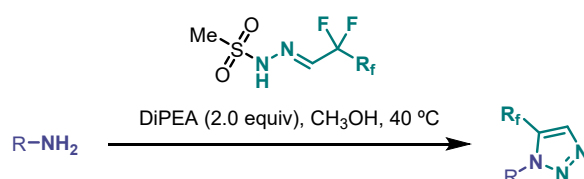
All reagents were purchased from commercial sources and used without purification unless otherwise mentioned. The products were purified by column chromatography over silica gel (300-400). NMR spectra were recorded on a Bruker Advance 600 (^1H : 600 MHz, ^{13}C : 150 MHz) and Bruker Advance 500 (^1H : 500 MHz, ^{13}C : 125 MHz, ^{19}F : 471 MHz) at ambient temperature. Data were reported as chemical shifts in ppm relative to TMS (0.00 ppm) for ^1H and CDCl_3 (77.0 ppm) for ^{13}C . The following abbreviations were used to explain the multiplicities: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, br = broad. Mass spectra were recorded on BRUKER AutoflexIII Smartbeam MS-spectrometer. High-resolution mass spectra (HRMS) were recorded on Bruker microTof by using ESI method.

II. General procedures for the synthesis of perfluoroalkyl *N*-sulfonylhydrazones



A 250 mL bottom flask was charged with pentafluoropropionaldehyde hydrate (75.0 mmol), methanesulfonylhydrazide (MsNHNH_2) (50.0 mmol) and ethyl acetate (200.0 mL). Then acetic acid (5.5 mmol) was added dropwise under N_2 atmosphere and the mixture was stirred at 40 °C for 4-5 h. The progress of the reaction was monitored by TLC (PE:EA = 5:1 to 4:1). After completion, the reaction mixture was concentrated under reduced pressure and the obtained crude solid was purified by column chromatography using PE/EA (5:1 to 4:1) as eluent to afford the product **1a** as a white solid. The same procedure was followed for the preparation other pentafluoroalkyl *N*-sulfonylhydrazones **1b-1f** using corresponding *p*-toluenesulfonyl hydrazide (TsNHNH_2) and 2-(trifluoromethyl)benzenesulfonylhydrazide (TfsNHNH_2)^[1]

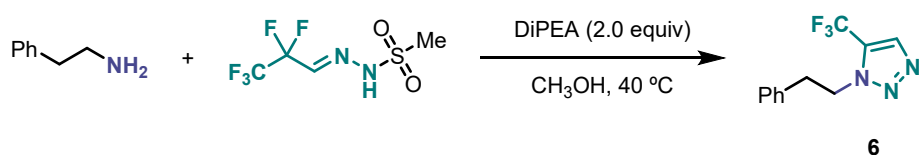
III. General procedures for synthesis of 5-fluoroalkyl 1,2,3-triazoles (with **2** as an example):



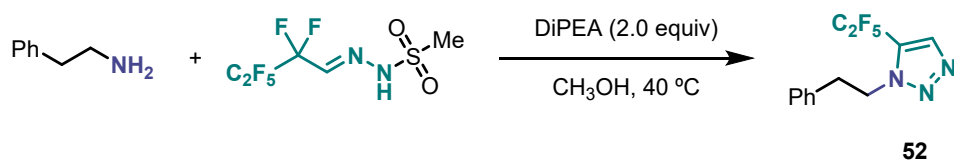
In a 15 mL of Schlenk tube equipped with Teflon coated magnetic stirring bar, perfluoroalkyl *N*-

sulfonylhydrazone (**1**, 0.30 mmol, 1.0 equiv) in CH₃OH (2 mL) was charged under air, then amine (0.60 mmol, 2.0 equiv) and DiPEA (0.60 mmol, 2 equiv) were added in one portion and the reaction was allowed to stirred at 40 °C until the complete consumption of **1** as evidenced by TLC. After completion, water was added to the mixture and was extracted with EtOAc (3x5 mL). The combined organic layer was dried with anhydrous MgSO₄, filtered, and evaporated under reduced pressure to give the crude mixture, which was purified by flash column chromatography to afford the pure 5-fluoroalkyl 1,2,3-triazole products.

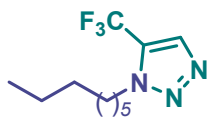
IV. General procedures for scale experiments of **6** and **52**.



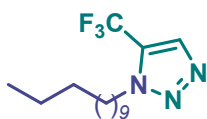
In a 50 mL of Schlenk tube equipped with Teflon coated magnetic stirring bar, perfluoroalkyl *N*-sulfonylhydrazone (**1a**, 10 mmol, 1.0 equiv) in CH₃OH (15 mL) was charged under air, then amine (20 mmol, 2.0 equiv) and DiPEA (20 mmol, 2 equiv) were added in one portion and the reaction was allowed to stirred at 40 °C until the complete consumption of **1a** as evidenced by TLC. After completion, water was added to the mixture and was extracted with EtOAc (3x15 mL). The combined organic layer was dried with anhydrous MgSO₄, filtered, and evaporated under reduced pressure to give the crude mixture, which was purified by flash column chromatography to afford the pure 5-CF₃ 1,2,3-triazole products in 82% yield.



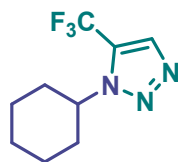
In a 50 mL of Schlenk tube equipped with Teflon coated magnetic stirring bar, perfluoroalkyl *N*-sulfonylhydrazone (**1d**, 10 mmol, 1.0 equiv) in CH₃OH (15 mL) was charged under air, then amine (20 mmol, 2.0 equiv) and DiPEA (20 mmol, 2 equiv) were added in one portion and the reaction was allowed to stirred at 40 °C until the complete consumption of **1d** as evidenced by TLC. After completion, water was added to the mixture and was extracted with EtOAc (3x15 mL). The combined organic layer was dried with anhydrous MgSO₄, filtered, and evaporated under



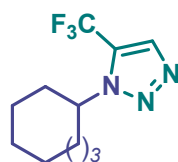
(2) Colorless oil. **¹H NMR** (600 MHz, CDCl₃) δ 7.96 (s, 1H), 4.45 (t, *J* = 7.2 Hz, 2H), 2.00-1.94 (m, 2H), 1.40-1.32 (m, 4H), 1.31-1.22 (m, 6H), 0.88 (t, *J* = 7.2 Hz, 3H). **¹³C NMR** (150 MHz, CDCl₃) δ 134.1, 127.6 (q, *J* = 42.0 Hz), 120.0 (q, *J* = 265.5 Hz), 50.1, 31.6, 30.0, 29.0, 28.8, 26.4, 22.6, 14.0. **¹⁹F NMR** (471 MHz, CDCl₃) δ -59.15 (s). **HRMS** (ESI) *m/z* calcd. for C₁₁H₁₈F₃N₃Na [M+Na]⁺ 272.1345, found 272.1345.



(3) Colorless oil. **¹H NMR** (600 MHz, CDCl₃) δ 7.96 (s, 1H), 4.45 (t, *J* = 7.2 Hz, 2H), 2.02-1.93 (m, 2H), 1.42-1.21 (m, 18H), 0.88 (t, *J* = 7.2 Hz, 3H). **¹³C NMR** (150 MHz, CDCl₃) δ 134.1, 127.6 (q, *J* = 40.5 Hz), 120.0 (q, *J* = 265.5 Hz), 50.1, 31.9, 29.9, 29.5, 29.4, 29.3, 28.9, 26.4, 22.6, 14.0. **¹⁹F NMR** (471 MHz, CDCl₃) δ -59.18 (s). **HRMS** (ESI) *m/z* calcd. for C₁₅H₂₆F₃N₃Na [M+Na]⁺ 328.1971, found 328.1978.

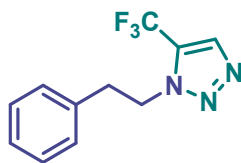


(4) Yellow oil. **¹H NMR** (600 MHz, CDCl₃) δ 7.92 (s, 1H), 4.38-4.31 (m, 1H), 2.13-2.07 (m, 4H), 2.00-1.94 (m, 2H), 1.80-1.74 (m, 1H), 1.48-1.39 (m, 2H), 1.38-1.32 (m, 1H). **¹³C NMR** (150 MHz, CDCl₃) δ 133.5, 127.1 (q, *J* = 40.5 Hz), 120.1 (q, *J* = 267.0 Hz), 60.7, 33.3, 25.4, 24.9. **¹⁹F NMR** (471 MHz, CDCl₃) δ -59.17 (s). **HRMS** (ESI) *m/z* calcd. for C₉H₁₂F₃N₃ [M+H]⁺ 220.1070, found 220.1062.

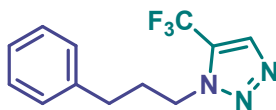


(5) Yellow oil; **¹H NMR** (600 MHz, CDCl₃) δ 7.89 (s, 1H), 4.67-4.62 (m, 1H), 2.35-2.29 (m, 2H), 2.03-1.97 (m, 2H), 1.91-1.84 (m, 2H), 1.68-1.58 (m, 8H). **¹³C NMR** (150 MHz, CDCl₃) δ 133.4,

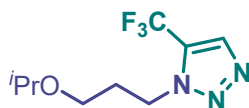
126.6 (q, $J = 40.5$ Hz), 120.1 (q, $J = 267.0$ Hz), 61.6, 33.3, 26.5, 25.9, 24.2. ^{19}F NMR (471 MHz, CDCl_3) δ -59.07 (s). HRMS (ESI) m/z calcd. for $\text{C}_{11}\text{H}_{18}\text{F}_3\text{N}_3[\text{M}+\text{H}]^+$ 248.2732, found 248.2735.



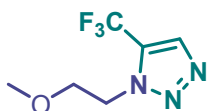
(6) Colorless oil; ^1H NMR (600 MHz, CDCl_3) δ 7.95 (q, $J = 0.6$ Hz, 1H), 7.33-7.29 (m, 2H), 7.28-7.25 (m, 1H), 7.18-7.15 (m, 2H), 4.68-4.64 (m, 2H), 3.29-3.26 (m, 2H). ^{13}C NMR (150 MHz, CDCl_3) δ 136.2, 134.1 (q, $J = 3.0$ Hz), 128.9, 128.7, 127.8 (q, $J = 42.0$ Hz), 127.3, 119.9 (q, $J = 267.0$ Hz), 51.2, 36.5. ^{19}F NMR (471 MHz, CDCl_3) δ -59.09 (s). HRMS (ESI) m/z calcd. for $\text{C}_{11}\text{H}_{10}\text{F}_3\text{N}_3\text{Na} [\text{M}+\text{Na}]^+$ 264.0719, found 264.0716.



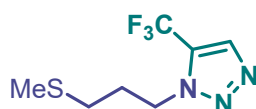
(7) Colorless oil; ^1H NMR (600 MHz, CDCl_3) δ 7.97 (s, 1H), 7.31 (t, $J = 7.2$ Hz, 2H), 7.24-7.18 (m, 3H), 4.47 (t, $J = 7.8$ Hz, 2H), 2.72 (t, $J = 7.2$ Hz, 2H), 2.34-2.28 (m, 2H). ^{13}C NMR (150 MHz, CDCl_3) δ 139.8, 134.2 (q, $J = 1.5$ Hz), 128.6, 128.3, 127.7 (q, $J = 42.0$ Hz), 126.4, 119.9 (q, $J = 267.0$ Hz), 49.4, 32.5, 31.3. ^{19}F NMR (471 MHz, CDCl_3) δ -59.14 (s). HRMS (ESI) m/z calcd. for $\text{C}_{12}\text{H}_{12}\text{F}_3\text{N}_3\text{Na} [\text{M}+\text{Na}]^+$ 278.0876, found 278.0874.



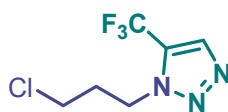
(8) White solid; mp: 57-58 °C; ^1H NMR (600 MHz, CDCl_3) δ 7.94 (s, 1H), 4.56 (t, $J = 7.2$ Hz, 2H), 3.55-3.50 (m, 1H), 3.45 (t, $J = 5.4$ Hz, 2H), 2.23-2.18 (m, 2H), 1.11 (d, $J = 6.6$ Hz, 6H). ^{13}C NMR (150 MHz, CDCl_3) δ 134.1, 127.8 (q, $J = 40.5$ Hz), 119.9 (q, $J = 265.5$ Hz), 71.7, 64.0, 47.4, 30.3, 21.9. ^{19}F NMR (471 MHz, CDCl_3) δ -59.23 (s). HRMS (ESI) m/z calcd. for $\text{C}_9\text{H}_{14}\text{F}_3\text{N}_3\text{ONa} [\text{M}+\text{Na}]^+$ 260.0981, found 260.0976.



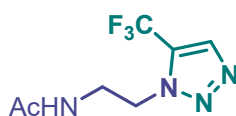
(9) Colorless oil; $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 7.97 (s, 1H), 4.63 (t, $J = 5.5$ Hz, 2H), 3.88 (t, $J = 5.5$ Hz, 2H), 3.34 (s, 3H). $^{13}\text{C NMR}$ (125 MHz, CDCl_3) δ 134.2, 128.3 (q, $J = 41.6$ Hz), 119.8 (q, $J = 268.4$ Hz), 69.9, 59.0, 49.5. $^{19}\text{F NMR}$ (471 MHz, CDCl_3) δ -58.77 (s). **HRMS** (ESI) m/z calcd. for $\text{C}_6\text{H}_9\text{F}_3\text{N}_3\text{O}$ $[\text{M}+\text{H}]^+$ 196.0692, found 196.0698.



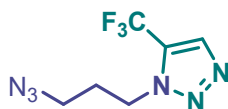
(10) Colorless oil; $^1\text{H NMR}$ (600 MHz, CDCl_3) δ 7.96 (s, 1H), 4.58 (t, $J = 7.2$ Hz, 2H), 2.57 (t, $J = 7.2$ Hz, 2H), 2.28-2.23 (m, 2H), 2.10 (s, 3H). $^{13}\text{C NMR}$ (150 MHz, CDCl_3) δ 134.2, 127.8 (q, $J = 40.5$ Hz), 119.9 (q, $J = 265.5$ Hz), 48.6, 30.7, 28.8, 15.2. $^{19}\text{F NMR}$ (471 MHz, CDCl_3) δ -59.16 (s). **HRMS** (ESI) m/z calcd. for $\text{C}_7\text{H}_{10}\text{F}_3\text{N}_3\text{SNa}$ $[\text{M}+\text{Na}]^+$ 248.2226, found 248.2230.



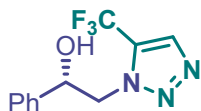
(11) Colorless oil; $^1\text{H NMR}$ (600 MHz, CDCl_3) δ 7.99 (s, 1H), 4.66 (t, $J = 7.2$ Hz, 2H), 3.64 (t, $J = 6.0$ Hz, 2H), 2.51-2.44 (m, 2H). $^{13}\text{C NMR}$ (150 MHz, CDCl_3) δ 134.3, 128.0 (q, $J = 40.5$ Hz), 119.8 (q, $J = 267.0$ Hz), 47.1, 40.9, 32.3. $^{19}\text{F NMR}$ (471 MHz, CDCl_3) δ -59.18 (s). **HRMS** (ESI) m/z calcd. for $\text{C}_6\text{H}_8\text{ClF}_3\text{N}_3$ $[\text{M}+\text{H}]^+$ 214.0359, found 214.0359.



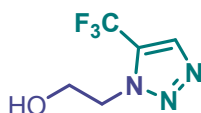
(12) Colorless oil. $^1\text{H NMR}$ (600 MHz, CDCl_3) δ 7.98 (s, 1H), 6.30 (s, 1H), 4.59 (t, $J = 4.8$ Hz, 2H), 3.90-3.85 (m, 2H), 1.98 (s, 3H). $^{13}\text{C NMR}$ (150 MHz, CDCl_3) δ 170.7, 134.2, 128.5 (q, $J = 40.5$ Hz), 119.7 (q, $J = 267.0$ Hz), 49.5, 38.7, 22.9. $^{19}\text{F NMR}$ (471 MHz, CDCl_3) δ -59.12 (s). **HRMS** (ESI) m/z calcd. for $\text{C}_7\text{H}_9\text{F}_3\text{N}_4\text{ONa}$ $[\text{M}+\text{Na}]^+$ 245.0621, found 245.0625.



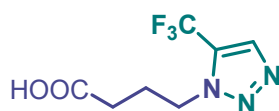
(13) Colorless oil. **¹H NMR** (600 MHz, CDCl₃) δ 7.99 (s, 1H), 4.57 (t, *J* = 6.6 Hz, 2H), 3.46 (t, *J* = 6.6 Hz, 2H), 2.27-2.21 (m, 2H). **¹³C NMR** (150 MHz, CDCl₃) δ 134.3, 127.9 (q, *J* = 42.0 Hz), 119.9 (q, *J* = 267.0 Hz), 48.1, 47.1, 29.1. **¹⁹F NMR** (471 MHz, CDCl₃) δ -59.19 (s). **HRMS** (ESI) *m/z* calcd. for C₆H₈F₃N₆ [M+H]⁺ 221.0767, found 221.0763.



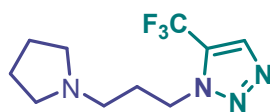
(14) Colorless oil; **¹H NMR** (600 MHz, CDCl₃) δ 7.96 (s, 1H), 7.44-7.39 (m, 4H), 7.38-7.33 (m, 1H), 5.40-5.32 (m, 1H), 4.64-4.55 (m, 2H), 3.30 (d, *J* = 3.0 Hz, 1H). **¹³C NMR** (150 MHz, CDCl₃) δ 139.5, 134.0, 128.9, 128.7, 128.6 (q, *J* = 40.5 Hz), 125.8, 119.7 (q, *J* = 267.0 Hz), 72.4, 56.8. **¹⁹F NMR** (471 MHz, CDCl₃) δ -58.62 (s). **HRMS** (ESI) *m/z* calcd. for C₁₁H₁₀F₃N₃ONa [M+Na]⁺ 280.0668, found 280.0675.



(15) Colorless oil; **¹H NMR** (600 MHz, CDCl₃) δ 7.96 (s, 1H), 4.59 (t, *J* = 5.4 Hz, 2H), 4.18 (t, *J* = 5.4 Hz, 2H), 3.30 (s, 1H). **¹³C NMR** (150 MHz, CDCl₃) δ 134.1, 128.5 (q, *J* = 42.0 Hz), 119.7 (q, *J* = 267.0 Hz), 60.3, 52.2. **¹⁹F NMR** (471 MHz, CDCl₃) δ -59.03 (s). **HRMS** (ESI) *m/z* calcd. for C₅H₆F₃N₃ONa [M+Na]⁺ 204.0355, found 204.0364.

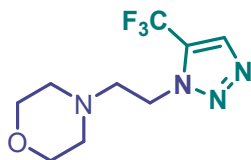


(16) White solid; mp: 66-67 °C; **¹H NMR** (600 MHz, CDCl₃) δ 8.00 (s, 1H), 4.59 (t, *J* = 7.2 Hz, 2H), 2.50 (t, *J* = 7.2 Hz, 2H), 2.35-2.28 (m, 2H). **¹³C NMR** (150 MHz, CDCl₃) δ 177.3, 134.2, 127.9 (q, *J* = 40.5 Hz), 119.8 (q, *J* = 267.0 Hz), 48.9, 30.3, 24.6. **¹⁹F NMR** (471 MHz, CDCl₃) δ -59.24 (s). **HRMS** (ESI) *m/z* calcd. for C₇H₈F₃N₃O₂Na [M+Na]⁺ 246.0461, found 246.0453.

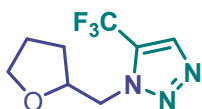


(17) Yellow oil; **¹H NMR** (600 MHz, CDCl₃) δ 7.96 (s, 1H), 4.56 (t, *J* = 7.2 Hz, 2H), 2.57 (t, *J* =

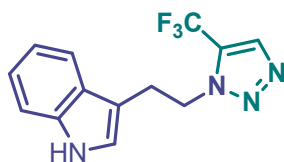
7.2 Hz, 2H), 2.54-2.48 (m, 4H), 2.22-2.14 (m, 2H), 1.81-1.75 (m, 4H). ^{13}C NMR (150 MHz, CDCl_3) δ 134.1, 127.7 (q, $J = 40.5$ Hz), 119.9 (q, $J = 267.0$ Hz), 54.0, 52.9, 48.5, 29.2, 23.5. ^{19}F NMR (471 MHz, CDCl_3) δ -59.17 (s). HRMS (ESI) m/z calcd. for $\text{C}_{10}\text{H}_{16}\text{F}_3\text{N}_4\text{Na}$ $[\text{M}+\text{H}]^+$ 249.1330, found 249.1322.



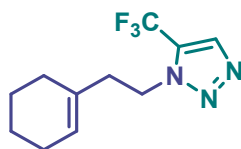
(18) Yellow oil; ^1H NMR (600 MHz, CDCl_3) δ 7.97 (s, 1H), 4.58 (t, $J = 6.6$ Hz, 2H), 3.69-3.63 (m, 4H), 2.93 (t, $J = 6.6$ Hz, 2H), 2.54-2.49 (m, 4H). ^{13}C NMR (150 MHz, CDCl_3) δ 134.1, 128.0 (q, $J = 42.0$ Hz), 119.9 (q, $J = 265.5$ Hz), 66.7, 57.4, 53.4, 47.2. ^{19}F NMR (471 MHz, CDCl_3) δ -58.90 (s). HRMS (ESI) m/z calcd. for $\text{C}_9\text{H}_{13}\text{F}_3\text{N}_4\text{ONa}$ $[\text{M}+\text{Na}]^+$ 251.1114, found 251.1123.



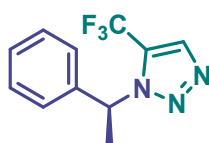
(19) Yellow oil; ^1H NMR (600 MHz, CDCl_3) δ 7.98 (s, 1H), 4.55-4.47 (m, 2H), 4.47-4.39 (m, 1H), 3.91-3.86 (m, 1H), 3.81-3.77 (m, 1H), 2.14-2.05 (m, 1H), 1.98-1.87 (m, 2H), 1.80-1.74 (m, 1H). ^{13}C NMR (150 MHz, CDCl_3) δ 134.1, 128.4 (q, $J = 42.0$ Hz), 119.9 (q, $J = 267.0$ Hz), 76.6, 68.4, 53.5, 29.2, 25.4. ^{19}F NMR (471 MHz, CDCl_3) δ -58.50 (s). HRMS (ESI) m/z calcd. for $\text{C}_8\text{H}_{10}\text{F}_3\text{N}_3\text{ONa}$ $[\text{M}+\text{Na}]^+$ 244.0668, found 244.0661.



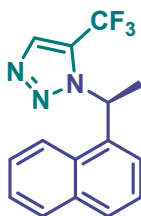
(20) White solid; mp: 84-85 °C; ^1H NMR (600 MHz, CDCl_3) δ 8.16 (s, 1H), 7.97 (s, 1H), 7.58 (d, $J = 7.8$ Hz, 1H), 7.37 (d, $J = 7.8$ Hz, 1H), 7.22 (t, $J = 7.2$ Hz, 1H), 7.16 (t, $J = 7.8$ Hz, 1H), 7.01 (d, $J = 1.8$ Hz, 1H), 4.73 (t, $J = 7.8$ Hz, 2H), 3.44 (t, $J = 7.8$ Hz, 2H). ^{13}C NMR (150 MHz, CDCl_3) δ 136.3, 134.1, 127.8 (q, $J = 40.5$ Hz), 126.9, 122.5, 122.4, 119.9 (q, $J = 267.0$ Hz), 119.8, 118.1, 111.4, 110.6, 50.6, 26.5. ^{19}F NMR (471 MHz, CDCl_3) δ -59.06 (s). HRMS (ESI) m/z calcd. for $\text{C}_{13}\text{H}_{11}\text{F}_3\text{N}_4\text{Na}$ $[\text{M}+\text{Na}]^+$ 303.0828, found 303.0834.



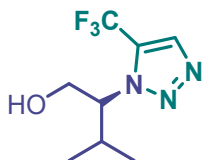
(21) Yellow oil; $^1\text{H NMR}$ (600 MHz, CDCl_3) δ 7.95 (s, 1H), 5.43-5.40 (m, 1H), 4.53 (t, $J = 7.8$ Hz, 2H), 2.57 (t, $J = 7.8$ Hz, 2H), 2.02-1.92 (m, 4H), 1.67-1.61 (m, 2H), 1.58-1.50 (m, 2H). $^{13}\text{C NMR}$ (150 MHz, CDCl_3) δ 134.0 (q, $J = 1.5$ Hz), 132.4, 127.5 (q, $J = 42.0$ Hz), 125.0, 119.9 (q, $J = 267.0$ Hz), 48.8, 38.4, 27.9, 25.1, 22.6, 21.9. $^{19}\text{F NMR}$ (471 MHz, CDCl_3) δ -59.09 (s). **HRMS** (ESI) m/z calcd. for $\text{C}_{11}\text{H}_{14}\text{F}_3\text{N}_3\text{Na}$ $[\text{M}+\text{Na}]^+$ 268.1032, found 268.1032.



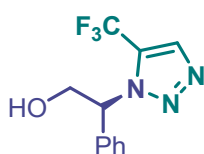
(22) Yellow oil; $^1\text{H NMR}$ (600 MHz, CDCl_3) δ 7.97 (s, 1H), 7.37-7.29 (m, 5H), 5.75 (q, $J = 7.2$ Hz, 1H), 2.09 (d, $J = 7.2$ Hz, 3H). $^{13}\text{C NMR}$ (150 MHz, CDCl_3) δ 139.3, 134.2, 128.9, 128.6, 127.5 (q, $J = 42.0$ Hz), 126.4, 119.9 (q, $J = 267.0$ Hz), 60.8, 22.5. $^{19}\text{F NMR}$ (471 MHz, CDCl_3) δ -58.67 (s). **HRMS** (ESI) m/z calcd. for $\text{C}_{11}\text{H}_{10}\text{F}_3\text{N}_3\text{Na}$ $[\text{M}+\text{Na}]^+$ 264.0719, found 264.0721.



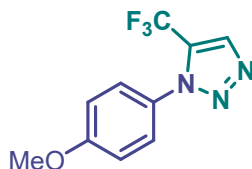
(23) Yellow oil; $^1\text{H NMR}$ (600 MHz, CDCl_3) δ 8.03 (s, 1H), 7.99 (d, $J = 8.4$ Hz, 1H), 7.89 (d, $J = 8.4$ Hz, 1H), 7.81 (d, $J = 7.8$ Hz, 1H), 7.57 (t, $J = 7.8$ Hz, 1H), 7.51 (t, $J = 7.8$ Hz, 1H), 7.39 (t, $J = 7.2$ Hz, 1H), 7.18 (d, $J = 7.2$ Hz, 1H), 6.65 (q, $J = 7.2$ Hz, 1H), 2.20 (d, $J = 6.6$ Hz, 3H). $^{13}\text{C NMR}$ (150 MHz, CDCl_3) δ 135.3, 134.8 (q, $J = 1.5$ Hz), 133.7, 129.6, 129.2, 129.1, 127.7 (q, $J = 40.5$ Hz), 127.0, 125.9, 125.4, 123.6, 121.4, 119.8 (q, $J = 267.0$ Hz), 57.1, 21.9. $^{19}\text{F NMR}$ (471 MHz, CDCl_3) δ -59.12 (s). **HRMS** (ESI) m/z calcd. for $\text{C}_{15}\text{H}_{12}\text{F}_3\text{N}_3\text{Na}$ $[\text{M}+\text{Na}]^+$ 314.0876, found 314.0870.



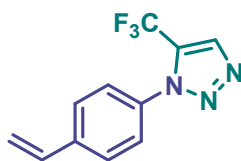
(24) Colorless oil; $^1\text{H NMR}$ (600 MHz, CDCl_3) δ 7.88 (s, 1H), 4.33-4.22 (m, 2H), 4.09-4.02 (m, 1H), 3.15 (t, $J = 5.4$ Hz, 1H), 2.56-2.46 (m, 1H), 1.11 (d, $J = 6.6$ Hz, 3H), 0.74 (d, $J = 7.2$ Hz, 3H). $^{13}\text{C NMR}$ (150 MHz, CDCl_3) δ 133.2, 129.5 (q, $J = 40.5$ Hz), 119.7 (q, $J = 267.0$ Hz), 69.8, 63.0, 30.4, 19.4, 19.2. $^{19}\text{F NMR}$ (471 MHz, CDCl_3) δ -57.92 (s). **HRMS** (ESI) m/z calcd. for $\text{C}_8\text{H}_{12}\text{F}_3\text{N}_3\text{ONa}$ $[\text{M}+\text{Na}]^+$ 246.0825, found 246.0813.



(25) Colorless oil; $^1\text{H NMR}$ (600 MHz, CDCl_3) δ 7.93 (s, 1H), 7.38-7.33 (m, 3H), 7.32-7.26 (m, 2H), 5.76-5.68 (m, 1H), 4.83-4.74 (m, 1H), 4.22-4.16 (m, 1H), 3.67 (br, 1H). $^{13}\text{C NMR}$ (150 MHz, CDCl_3) δ 134.9, 134.1, 129.1, 129.0, 128.8 (q, $J = 40.5$ Hz), 127.0, 119.6 (q, $J = 267.0$ Hz), 67.5, 64.9. $^{19}\text{F NMR}$ (471 MHz, CDCl_3) δ -58.70 (s). **HRMS** (ESI) m/z calcd. for $\text{C}_{11}\text{H}_{10}\text{F}_3\text{N}_3\text{ONa}$ $[\text{M}+\text{Na}]^+$ 280.0668, found 280.0664.

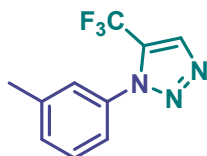


(26) Colorless oil; $^1\text{H NMR}$ (600 MHz, CDCl_3) δ 8.09 (s, 1H), 7.41 (d, $J = 9.0$ Hz, 2H), 7.03 (d, $J = 9.0$ Hz, 2H), 3.88 (s, 3H). $^{13}\text{C NMR}$ (150 MHz, CDCl_3) δ 161.2, 134.4, 128.9 (q, $J = 40.5$ Hz), 128.0, 126.8, 119.6 (q, $J = 267.0$ Hz), 114.6, 55.6. $^{19}\text{F NMR}$ (471 MHz, CDCl_3) δ -57.72 (s). **HRMS** (ESI) m/z calcd. for $\text{C}_{10}\text{H}_8\text{F}_3\text{N}_3\text{ONa}$ $[\text{M}+\text{Na}]^+$ 266.0512, found 266.0515.

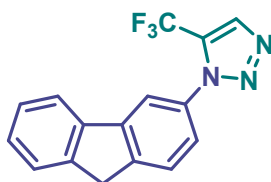


(27) Colorless oil; $^1\text{H NMR}$ (600 MHz, CDCl_3) δ 8.12 (s, 1H), 7.58 (d, $J = 8.4$ Hz, 2H), 7.48 (d, J

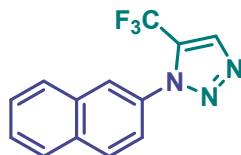
= 8.4 Hz, 2H), 6.78 (dd, $J=17.4, 10.8$ Hz, 1H), 5.88 (d, $J = 17.4$ Hz, 1H), 5.43 (d, $J = 10.8$ Hz, 1H). ^{13}C NMR (150 MHz, CDCl_3) δ 140.1, 135.2, 134.7, 134.4, 128.8 (q, $J = 42.0$ Hz), 127.1, 125.5, 119.6 (q, $J = 267.0$ Hz), 116.7. ^{19}F NMR (471 MHz, CDCl_3) δ -57.46 (s). HRMS (ESI) m/z calcd. for $\text{C}_{11}\text{H}_8\text{F}_3\text{N}_3\text{Na}$ $[\text{M}+\text{Na}]^+$ 262.0567, found 262.0563.



(28) Colorless oil; ^1H NMR (600 MHz, CDCl_3) δ 8.11 (s, 1H), 7.44 (t, $J = 7.2$ Hz, 1H), 7.40 (d, $J = 7.8$ Hz, 1H), 7.33 (s, 1H), 7.30 (d, $J = 7.8$ Hz, 1H), 2.45 (s, 3H). ^{13}C NMR (150 MHz, CDCl_3) δ 139.8, 135.2, 134.6, 131.5, 129.2, 128.8 (q, $J = 40.5$ Hz), 126.0, 122.3, 119.6 (q, $J = 267.0$ Hz), 21.2. ^{19}F NMR (471 MHz, CDCl_3) δ -57.52 (s). HRMS (ESI) m/z calcd. for $\text{C}_{10}\text{H}_9\text{F}_3\text{N}_3$ $[\text{M}+\text{H}]^+$ 228.0749, found 228.0755.

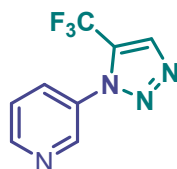


(29) Colorless oil; ^1H NMR (600 MHz, CDCl_3) δ 8.14 (s, 1H), 7.89 (d, $J = 8.4$ Hz, 1H), 7.82 (d, $J = 7.2$ Hz, 1H), 7.65 (s, 1H), 7.57 (d, $J = 7.2$ Hz, 1H), 7.50 (d, $J = 7.8$ Hz, 1H), 7.42 (t, $J = 7.8$ Hz, 1H), 7.40-7.35 (m, 1H), 3.96 (s, 2H). ^{13}C NMR (150 MHz, CDCl_3) δ 144.3, 144.2, 143.6, 139.9, 134.6 (q, $J = 1.5$ Hz), 133.4, 128.9 (q, $J = 42.0$ Hz), 127.9, 127.1, 125.2, 124.2, 122.2, 120.5, 120.3, 119.6 (q, $J = 267.0$ Hz), 36.9. ^{19}F NMR (471 MHz, CDCl_3) δ -57.43 (s). HRMS (ESI) m/z calcd. for $\text{C}_{10}\text{H}_8\text{F}_3\text{N}_3$. HRMS (ESI) m/z calcd. for $\text{C}_{16}\text{H}_{10}\text{F}_3\text{N}_3\text{Na}$ $[\text{M}+\text{Na}]^+$ 324.0719, found 324.0717.

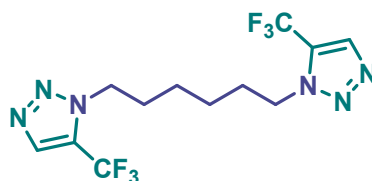


(30) Colorless oil; ^1H NMR (600 MHz, CDCl_3) δ 8.17 (s, 1H), 8.03-8.00 (m, 2H), 7.97-7.92 (m, 2H), 7.65-7.59 (m, 2H), 7.59-7.56 (m, 1H). ^{13}C NMR (150 MHz, CDCl_3) δ 134.7, 133.7, 132.7,

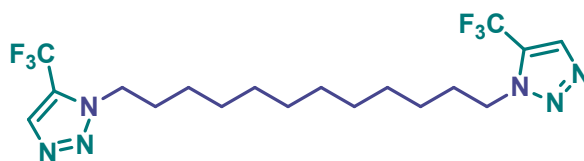
132.6, 129.7, 129.0 (q, $J = 40.5$ Hz), 128.5, 128.0, 127.9, 127.6, 124.7, 122.4, 119.7 (q, $J = 267.0$ Hz). ^{19}F NMR (471 MHz, CDCl_3) δ -57.37 (s). HRMS (ESI) m/z calcd. for $\text{C}_{13}\text{H}_8\text{F}_3\text{N}_3\text{Na}$ $[\text{M}+\text{Na}]^+$ 286.0563, found 286.0558.



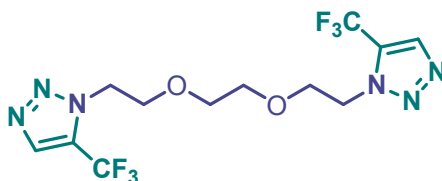
(31) Colorless oil; ^1H NMR (600 MHz, CDCl_3) δ 8.87 (d, $J = 4.2$ Hz, 1H), 8.84 (d, $J = 1.8$ Hz, 1H), 8.18 (s, 1H), 7.90 (d, $J = 8.4$ Hz, 1H), 7.57 (dd, $J = 8.4, 4.2$ Hz, 1H). ^{13}C NMR (150 MHz, CDCl_3) δ 151.8, 146.0, 134.9, 132.8, 132.2, 129.1 (q, $J = 42.0$ Hz), 124.0, 119.4 (q, $J = 267.0$ Hz). ^{19}F NMR (471 MHz, CDCl_3) δ -60.54 (s). HRMS (ESI) m/z calcd. for $\text{C}_8\text{H}_6\text{F}_3\text{N}_4$. $[\text{M}+\text{H}]^+$ 215.0543, found 215.0545.



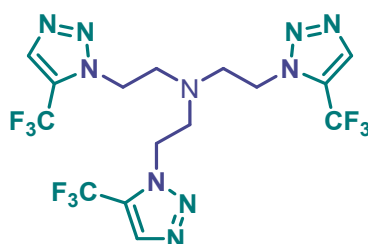
(32) White solid; mp: 78-79 °C; ^1H NMR (600 MHz, CDCl_3) δ 7.96 (s, 2H), 4.47-4.43 (m, 4H), 1.99-1.96 (m, 4H), 1.43-1.30 (m, 4H). ^{13}C NMR (150 MHz, CDCl_3) δ 134.2, 127.7 (q, $J = 42.0$ Hz), 119.9 (q, $J = 265.5$ Hz), 49.7, 29.5, 25.7. ^{19}F NMR (471 MHz, CDCl_3) δ -59.12 (s). HRMS (ESI) m/z calcd. for $\text{C}_{12}\text{H}_{14}\text{F}_6\text{N}_6$ $[\text{M}+\text{Na}]^+$ 379.1082, found 379.1080.



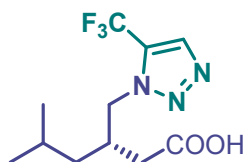
(33) Colorless oil; ^1H NMR (600 MHz, CDCl_3) δ 7.95 (s, 2H), 4.48-4.41 (m, 4H), 1.98-1.92 (m, 4H), 1.37-1.22 (m, 16H). ^{13}C NMR (150 MHz, CDCl_3) δ 134.1, 127.6 (q, $J = 42.0$ Hz), 120.0 (q, $J = 267.0$ Hz), 50.1, 29.9, 29.3, 29.2, 28.8, 26.3. ^{19}F NMR (471 MHz, CDCl_3) δ -59.14 (s). HRMS (ESI) m/z calcd. for $\text{C}_{18}\text{H}_{27}\text{F}_6\text{N}_6$ $[\text{M}+\text{H}]^+$ 441.2201, found 441.2201.



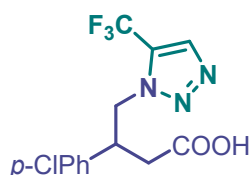
(34) Colorless oil; $^1\text{H NMR}$ (600 MHz, CDCl_3) δ 7.95 (s, 2H), 4.60 (t, $J = 6.0$ Hz, 4H), 3.92 (t, $J = 6.0$ Hz), 4H, 3.52 (s, 4H). $^{13}\text{C NMR}$ (150 MHz, CDCl_3) δ 134.1, 128.3 (q, $J = 40.5$ Hz), 119.8 (q, $J = 267.0$ Hz), 70.6, 68.7, 49.6. $^{19}\text{F NMR}$ (471 MHz, CDCl_3) δ -58.74 (s). **HRMS** (ESI) m/z calcd. for $\text{C}_{12}\text{H}_{15}\text{F}_6\text{N}_6\text{O}_2$ $[\text{M}+\text{H}]^+$ 389.1164, found 389.1161.



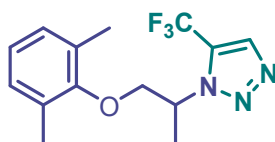
(35) Colorless liquid. $^1\text{H NMR}$ (600 MHz, CDCl_3) δ 7.97 (s, 3H), 4.41 (t, $J = 7.0$ Hz, 6H), 3.18 (t, $J = 7.0$ Hz, 6H). $^{13}\text{C NMR}$ (150 MHz, CDCl_3) δ 134.3, 127.9 (q, $J = 40.5$ Hz), 119.8 (q, $J = 267.0$ Hz), 53.3, 47.7. $^{19}\text{F NMR}$ (471 MHz, CDCl_3) δ -59.05 (s). **HRMS** (ESI) m/z calcd. for $\text{C}_{15}\text{H}_{16}\text{F}_9\text{N}_{10}$ $[\text{M}+\text{H}]^+$ 507.1414, found 507.1416.



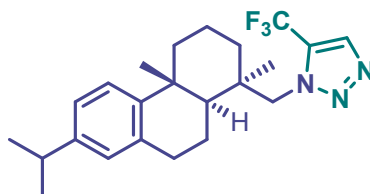
(36) Colorless oil; $^1\text{H NMR}$ (600 MHz, CDCl_3) δ 9.75 (br, 1H), 7.98 (s, 1H), 4.52-4.39 (m, 2H), 2.67-2.59 (m, 1H), 2.45-2.36 (m, 2H), 1.65-1.58 (m, 1H), 1.35-1.29 (m, 1H), 1.22-1.16 (m, 1H), 0.90 (d $J = 6.6$ Hz, 3H), 0.85 (d $J = 6.6$ Hz, 3H). $^{13}\text{C NMR}$ (150 MHz, CDCl_3) δ 177.0, 134.3, 128.2 (q, $J = 42.0$ Hz), 119.7 (q, $J = 265.5$ Hz), 53.5, 41.0, 36.2, 33.4, 25.1, 22.5, 22.1. $^{19}\text{F NMR}$ (471 MHz, CDCl_3) δ -58.87 (s). **HRMS** (ESI) m/z calcd. for $\text{C}_{11}\text{H}_{17}\text{F}_3\text{N}_3\text{O}_2$ $[\text{M}+\text{H}]^+$ 280.1279, found 280.1273.



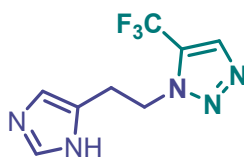
(37) Colorless oil; $^1\text{H NMR}$ (600 MHz, CDCl_3) δ 7.91 (s, 1H), 7.27 (d, $J = 8.4$ Hz, 2H), 7.09 (d, $J = 8.4$ Hz, 2H), 4.72-4.68 (m, 1H), 4.59-4.54 (m, 1H), 3.91-3.85 (m, 1H), 2.87-2.77 (m, 2H). $^{13}\text{C NMR}$ (150 MHz, CDCl_3) δ 175.2, 137.0, 134.2, 133.9, 129.2, 128.7, 128.2 (q, $J = 42.0$ Hz), 119.7 (q, $J = 267.0$ Hz), 54.2, 41.2, 37.2. $^{19}\text{F NMR}$ (471 MHz, CDCl_3) δ -58.74 (s). **HRMS** (ESI) m/z calcd. for $\text{C}_{13}\text{H}_{12}\text{ClF}_3\text{N}_3\text{O}_2$ $[\text{M}+\text{H}]^+$ 334.0565, found 334.0570.



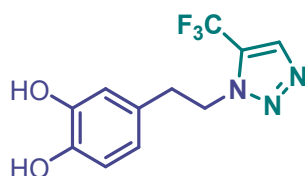
(38) Colorless oil; $^1\text{H NMR}$ (600 MHz, CDCl_3) δ 8.00 (s, 1H), 6.96 (d, $J = 7.2$ Hz, 2H), 6.92-6.88 (m, 1H), 5.12-5.04 (m, 1H), 4.31 (t, $J = 9.0$ Hz, 1H), 4.09 (dd, $J = 9.6, 4.8$ Hz, 1H), 2.09 (s, 6H), 1.77 (d, $J = 7.2$ Hz, 3H). $^{13}\text{C NMR}$ (150 MHz, CDCl_3) δ 154.4, 133.6 (q, $J = 1.5$ Hz), 130.6, 128.9, 128.4 (q, $J = 40.5$ Hz), 124.3, 119.9 (q, $J = 267.0$ Hz), 73.4, 57.1, 17.8, 15.7. $^{19}\text{F NMR}$ (471 MHz, CDCl_3) δ -58.57 (s). **HRMS** (ESI) m/z calcd. for $\text{C}_{14}\text{H}_{17}\text{F}_3\text{N}_3\text{O}$ $[\text{M}+\text{H}]^+$ 300.1328, found 300.1324.



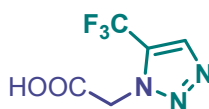
(39) Yellow solid; mp: 102-103 $^\circ\text{C}$; $^1\text{H NMR}$ (600 MHz, CDCl_3) δ 7.96 (s, 1H), 7.17 (d, $J = 8.4$ Hz, 1H), 7.03-6.99 (m, 1H), 6.94 (s, 1H), 4.34 (q, $J = 14.4$ Hz, 1H), 3.10-3.03 (m, 1H), 3.01-2.96 (m, 1H), 2.88-2.82 (m, 1H), 2.33-2.26 (m, 1H), 2.05-2.01 (m, 1H), 1.93-1.88 (m, 1H), 1.80-1.63 (m, 3H), 1.51-1.44 (m, 1H), 1.35 (td, $J = 12.6, 4.2$ Hz, 1H), 1.28 (s, 3H), 1.27-1.20 (m, 7H), 1.13 (s, 3H). $^{13}\text{C NMR}$ (150 MHz, CDCl_3) δ 146.7, 145.8, 134.5, 133.8 (q, $J = 1.5$ Hz), 129.2 (q, $J = 40.5$ Hz), 126.9, 124.0, 123.9, 119.9 (q, $J = 265.5$ Hz), 60.0, 45.8, 38.9, 38.0, 37.7, 36.1, 33.4, 29.8, 25.5, 23.94, 23.90, 19.3, 18.4, 18.3. $^{19}\text{F NMR}$ (471 MHz, CDCl_3) δ -57.25 (s). **HRMS** (ESI) m/z calcd. for $\text{C}_{23}\text{H}_{31}\text{F}_3\text{N}_3$ $[\text{M}+\text{H}]^+$ 406.2474, found 406.2470.



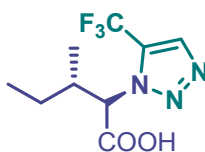
(40) White solid; mp: 55-56 °C; $^1\text{H NMR}$ (600 MHz, CDCl_3) δ 7.92 (s, 1H), 7.56 (s, 1H), 6.74 (s, 1H), 4.76-4.69 (m, 3H), 3.27 (t, $J = 7.2$ Hz, 2H). $^{13}\text{C NMR}$ (150 MHz, CDCl_3) δ 135.2, 134.3, 134.0 (q, $J = 1.5$ Hz), 127.9 (q, $J = 42.0$ Hz), 119.8 (q, $J = 267.0$ Hz), 115.2, 49.9, 28.2. $^{19}\text{F NMR}$ (471 MHz, CDCl_3) δ -58.21 (s). **HRMS** (ESI) m/z calcd. for $\text{C}_8\text{H}_9\text{F}_3\text{N}_5$ $[\text{M}+\text{H}]^+$ 232.0816, found 232.0810.



(41) Colorless oil; $^1\text{H NMR}$ (500 MHz, DMSO) δ 8.78 (s, 1H), 8.74 (s, 1H), 8.39 (s, 1H), 6.60 (d, $J = 8.0$ Hz, 1H), 6.51 (s, 1H), 6.35 (d, $J = 8.0$ Hz, 1H), 4.62 (t, $J = 7.3$ Hz, 2H), 3.01 (t, $J = 7.5$ Hz, 2H). $^{13}\text{C NMR}$ (125 MHz, DMSO) δ 145.7, 144.6, 135.1, 127.9, 127.2 (q, $J = 40.0$ Hz), 120.4 (q, $J = 267.0$ Hz), 119.8, 116.5, 116.1, 51.7, 35.4. $^{19}\text{F NMR}$ (471 MHz, MeOD) δ -56.46 (s). **HRMS** (ESI) m/z calcd. for $\text{C}_{11}\text{H}_{11}\text{F}_3\text{N}_3\text{O}_2$ $[\text{M}+\text{H}]^+$ 274.0806, found 274.0803.



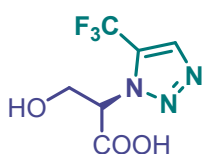
(42) Colorless oil; $^1\text{H NMR}$ (600 MHz, MeOD) δ 8.24 (s, 1H), 5.42 (s, 2H). $^{13}\text{C NMR}$ (150 MHz, MeOD) δ 169.0, 135.7, 130.0 (q, $J = 42.0$ Hz), 121.4 (q, $J = 265.5$ Hz), 51.8. $^{19}\text{F NMR}$ (471 MHz, MeOD) δ -60.70 (s). **HRMS** (ESI) m/z calcd. for $\text{C}_5\text{H}_5\text{F}_3\text{N}_3\text{O}_2$ $[\text{M}+\text{H}]^+$ 196.0343, found 196.0334.



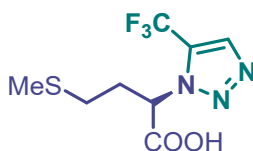
(43) White solid; mp: 142-143 °C; $^1\text{H NMR}$ (600 MHz, MeOD) δ 8.23 (s, 1H), 5.06 (d, $J = 7.8$ Hz, 1H), 2.76-2.66 (m, 1H), 1.46-1.33 (m, 2H), 1.14 (d, $J = 6.6$ Hz, 3H), 0.93 (t, $J = 7.8$ Hz, 3H). $^{13}\text{C NMR}$ (150 MHz, MeOD) δ 170.1, 135.0 (q, $J = 2.0$ Hz), 130.4 (q, $J = 40.5$ Hz), 121.4 (q, $J = 265.5$ Hz), 68.7, 38.3, 27.2, 16.3, 11.7. $^{19}\text{F NMR}$ (471 MHz, MeOD) δ -56.27 (s). **HRMS** (ESI) m/z calcd. for $[\text{M}+\text{H}]^+$ $\text{C}_9\text{H}_{13}\text{F}_3\text{N}_3\text{O}_2$ $[\text{M}+\text{H}]^+$ 252.0961, found 252.0960.



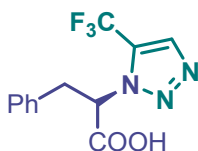
(44) White solid; mp: 65-66 °C; $^1\text{H NMR}$ (600 MHz, MeOD) δ 8.19 (s, 1H), 4.83-4.80 (m, 1H), 2.97-2.89 (m, 1H), 1.13 (d, $J = 6.6$ Hz, 3H), 0.99 (d, $J = 6.6$ Hz, 3H). $^{13}\text{C NMR}$ (150 MHz, CDCl_3) δ 170.2, 133.4, 129.3 (q, $J = 40.5$ Hz), 119.5 (q, $J = 267.0$ Hz), 68.1, 30.8, 19.3, 19.1. $^{19}\text{F NMR}$ (471 MHz, CDCl_3) δ -58.70 (s). **HRMS** (ESI) m/z calcd. for $\text{C}_8\text{H}_{11}\text{F}_3\text{N}_3\text{O}_2$ $[\text{M}+\text{H}]^+$ 238.0810, found 238.0803.



(45) White solid; mp: 128-129 °C; $^1\text{H NMR}$ (600 MHz, DMSO) δ 8.46 (s, 1H), 5.41 (dd, $J = 8.4$, 5.4 Hz, 1H), 4.30-4.22 (m, 2H). $^{13}\text{C NMR}$ (150 MHz, DMSO) δ 167.9, 134.9, 128.7 (q, $J = 40.5$ Hz), 120.3 (q, $J = 267.0$ Hz), 65.4, 60.7. $^{19}\text{F NMR}$ (471 MHz, DMSO) δ -57.49 (s). **HRMS** (ESI) m/z calcd. for $\text{C}_6\text{H}_7\text{F}_3\text{N}_3\text{O}_3$ $[\text{M}+\text{H}]^+$ 226.0450, found 226.0440.

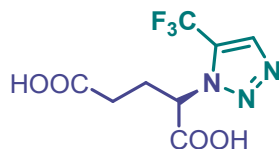


(46) White solid; mp: 85-86 °C; $^1\text{H NMR}$ (600 MHz, MeOD) δ 8.25 (s, 1H), 5.65-5.60 (m, 1H), 2.89-2.81 (m, 1H), 2.75-2.68 (m, 1H), 2.62-2.56 (m, 1H), 2.48-2.42 (m, 1H), 2.08 (s, 3H). $^{13}\text{C NMR}$ (150 MHz, MeOD) δ 170.9, 135.5, 130.4 (q, $J = 42.0$ Hz), 121.4 (q, $J = 267.0$ Hz), 62.6, 31.2, 31.1, 15.0. $^{19}\text{F NMR}$ (471 MHz, MeOD) δ -60.25 (s). **HRMS** (ESI) m/z calcd. for $\text{C}_8\text{H}_{11}\text{F}_3\text{N}_3\text{O}_2\text{S}$ $[\text{M}+\text{H}]^+$ 270.0531, found 270.0524.

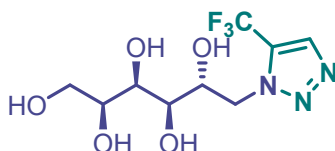


(47) White solid; mp: 130-131 °C; $^1\text{H NMR}$ (600 MHz, MeOD) δ 8.07 (s, 1H), 7.20-7.12 (m, 3H), 7.09 (d, $J = 7.2$ Hz, 2H), δ 5.58 (dd, $J = 11.4$, 4.8 Hz, 1H), 3.82-3.71 (m, 2H). $^{13}\text{C NMR}$ (150

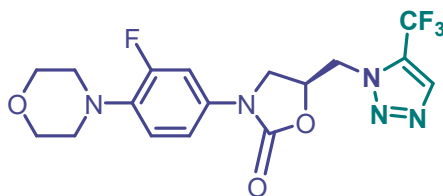
MHz, MeOD) δ 170.1, 137.2, 134.9 (q, $J = 1.5$ Hz), 130.5 (q, $J = 40.5$ Hz), 130.1, 129.7, 128.3, 121.1 (q, $J = 265.5$ Hz), 65.7, 38.2. **^{19}F NMR** (471 MHz, MeOD) δ -60.24 (s). **HRMS** (ESI) m/z calcd. for $\text{C}_{12}\text{H}_{11}\text{F}_3\text{N}_3\text{O}_2[\text{M}+\text{H}]^+$ 286.0811, found 286.0803.



(48) White solid; mp: 51-52 °C; **^1H NMR** (600 MHz, DMSO) δ 8.27 (s, 1H), 4.85 (dd, $J = 10.0$, 4.5 Hz, 1H), 2.66-2.55 (m, 1H), 2.46-2.35 (m, 1H), 2.10-1.94 (m, 2H). **^{13}C NMR** (150 MHz, MeOD) δ 175.7, 170.9, 135.4, 130.4 (q, $J = 40.5$ Hz), 121.3 (q, $J = 267.0$ Hz), 63.3, 30.8, 27.5. **^{19}F NMR** (471 MHz, MeOD) δ -60.20 (s). **HRMS** (ESI) m/z calcd. for $\text{C}_8\text{H}_8\text{F}_3\text{N}_3\text{O}_4\text{Na} [\text{M}+\text{Na}]^+$ 290.1540, found 290.1542.

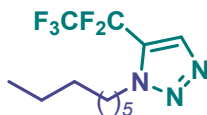


(49) White solid; mp: 154-155 °C; **^1H NMR** (600 MHz, DMSO) δ 8.38 (s, 1H), 5.11 (d, $J = 5.4$ Hz, 1H), 4.75 (d, $J = 6.6$ Hz, 1H), 4.72-4.67 (m, 1H), 4.54-4.47 (m, 2H), 4.43 (d, $J = 7.2$ Hz, 1H), 4.39 (t, $J = 5.4$ Hz, 1H), 4.14-4.09 (m, 1H), 3.81-3.74 (m, 1H), 3.63-3.54 (m, 2H), 3.52-3.46 (m, 1H), 3.45-3.39 (m, 1H). **^{13}C NMR** (150 MHz, DMSO) δ 134.9, 128.1 (q, $J = 40.5$ Hz), 120.4 (q, $J = 267.0$ Hz), 72.3, 72.0, 70.7, 70.5, 63.8, 53.3. **^{19}F NMR** (471 MHz, DMSO) δ -57.06 (s). **HRMS** (ESI) m/z calcd. for $\text{C}_9\text{H}_{15}\text{F}_3\text{N}_3\text{O}_5 [\text{M}+\text{H}]^+$ 302.0971, found 302.0964.

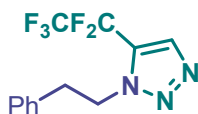


(50) White solid; mp: 148-149 °C; **^1H NMR** (600 MHz, CDCl_3) δ 8.02 (s, 1H), 7.37 (dd, $J = 14.4$, 2.4 Hz, 1H), 7.06 (dd, $J = 9.0$, 1.8 Hz, 1H), 6.90 (t, $J = 9.0$ Hz, 1H), 5.21-5.15 (m, 1H), 4.83-4.72 (m, 2H), 4.20 (t, $J = 9.0$ Hz, 1H), 4.02 (dd, $J = 9.0$, 6.0 Hz, 1H), 3.87-3.81 (m, 4H), 3.07-3.00 (m, 4H). **^{13}C NMR** (150 MHz, CDCl_3) δ 155.4 (d, $J = 246.0$ Hz), 153.1, 136.8 (d, $J = 9.0$ Hz), 134.4,

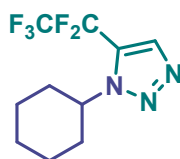
132.3 (d, $J = 10.5$ Hz), 128.8 (q, $J = 42.0$ Hz), 119.5 (q, $J = 267.0$ Hz), 118.8 (d, $J = 4.5$ Hz), 114.1 (d, $J = 3.0$ Hz), 107.6 (d, $J = 26.0$ Hz), 69.5, 66.9, 51.5, 50.9 (d, $J = 3.0$ Hz), 48.3. **^{19}F NMR** (471 MHz, CDCl_3) δ -58.54 (s), (-119.88)-(-120.05) (m). **HRMS** (ESI) m/z calcd. for $\text{C}_{17}\text{H}_{18}\text{F}_4\text{N}_5\text{O}_3$ $[\text{M}+\text{H}]^+$ 416.1341, found 416.1346.



(51) Colorless oil; **^1H NMR** (600 MHz, CDCl_3) δ 7.93 (s, 1H), 4.47 (t, $J = 7.2$ Hz, 2H), 2.01-1.94 (m, 2H), 1.41-1.15 (m, 10H), 0.87 (t, $J = 7.2$ Hz, 3H). **^{13}C NMR** (150 MHz, CDCl_3) δ 135.2, 125.4 (t, $J = 30.0$ Hz), 118.3 (qt, $J = 284.0$ Hz, 36.0 Hz), 117.3 (tq, $J = 250.5$ Hz, 40.5 Hz), 50.7, 31.7, 30.2, 29.0, 28.9, 26.4, 22.6, 14.0. **^{19}F NMR** (471 MHz, CDCl_3) δ (-83.72)-(-84.50) (m), (-109.45)-(-109.50) (m). **HRMS** (ESI) m/z calcd. for $\text{C}_{12}\text{H}_{18}\text{F}_5\text{N}_3\text{Na}$ $[\text{M}+\text{Na}]^+$ 322.1313, found 322.1308.

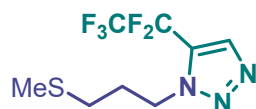


(52) Colorless oil; **^1H NMR** (600 MHz, CDCl_3) δ 7.94 (s, 1H), 7.34-7.29 (m, 2H), 7.28-7.25 (m, 1H), 7.19-7.16 (m, 2H), 4.70-4.66 (m, 2H), 3.31-3.27 (m, 2H). **^{13}C NMR** (150 MHz, CDCl_3) δ 136.2, 135.2, 128.9, 128.7, 127.3, 125.6 (t, $J = 28.5$ Hz), 118.2 (qt, $J = 285.0$, 37.5 Hz), 110.0 (tq, $J = 250.5$, 40.5 Hz), 51.7, 36.7. **^{19}F NMR** (471 MHz, CDCl_3) δ (-83.73)-(-84.39) (m), -109.53 (s). **HRMS** (ESI) m/z calcd. for $\text{C}_{12}\text{H}_{10}\text{F}_5\text{N}_3\text{Na}$ $[\text{M}+\text{Na}]^+$ 314.0687, found 314.0665.

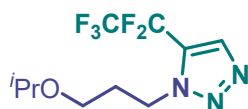


(53) White solid; mp: 41-42 °C; **^1H NMR** (600 MHz, CDCl_3) δ 7.93 (s, 1H), 4.42-4.39 (m, 1H), 2.16-2.06 (m, 4H), 2.01-1.95 (m, 2H), 1.81-1.75 (m, 1H), 1.51-1.40 (m, 2H), 1.39-1.29 (m, 1H). **^{13}C NMR** (150 MHz, CDCl_3) δ 134.6, 124.9 (t, $J = 28.5$ Hz), 118.3 (qt, $J = 283.5$, 36.0 Hz), 110.1 (tq, $J = 250.5$, 42.0 Hz), 61.2, 33.5, 25.5, 24.9. **^{19}F NMR** (471 MHz, CDCl_3) δ (-83.75)-(-84.34) (m), (-109.15)-(-109.86) (m). **HRMS** (ESI) m/z calcd. for $\text{C}_{10}\text{H}_{12}\text{F}_5\text{N}_3\text{Na}$ $[\text{M}+\text{Na}]^+$ 292.0844,

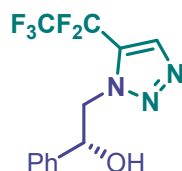
found 292.0838.



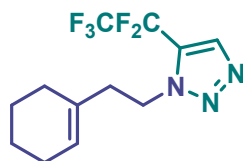
(54) Colorless oil; $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 7.95 (s, 1H), 4.61 (t, $J = 7.0$ Hz, 2H), 2.59 (t, $J = 7.0$ Hz, 2H), 2.31-2.26 (m, 2H), 2.11 (s, 3H). $^{13}\text{C NMR}$ (125 MHz, CDCl_3) δ 135.3, 125.6 (t, $J = 29.0$ Hz), 118.2 (qt, $J = 286.0, 36.5$ Hz), 110.0 (tq, $J = 253.3, 41.6$ Hz), 49.3, 30.8, 29.0, 15.2. $^{19}\text{F NMR}$ (471 MHz, CDCl_3) δ (-83.81)-(-84.13) (m), (-109.34)-(-109.55) (m). **HRMS** (ESI) m/z calcd. for $\text{C}_8\text{H}_{11}\text{F}_5\text{N}_3\text{S}$ $[\text{M}+\text{H}]^+$ 276.0604, found 276.0594.



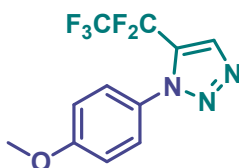
(55) Colorless oil; $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 7.94 (s, 1H), 4.59 (t, $J = 7.0$ Hz, 2H), 3.58-3.49 (m, 1H), 3.47 (t, $J = 6.0$ Hz, 2H), 2.27-2.18 (m, 2H), 1.12 (d, $J = 6.0$ Hz, 3H). $^{13}\text{C NMR}$ (125 MHz, CDCl_3) δ 135.3, 125.7 (t, $J = 29.0$ Hz), 118.3 (qt, $J = 287.3, 36.5$ Hz), 110.0 (tq, $J = 253.3, 41.6$ Hz), 71.7, 64.1, 48.0, 30.5, 21.9. $^{19}\text{F NMR}$ (471 MHz, CDCl_3) δ (-83.43)-(-84.57) (m), -109.54 (s). **HRMS** (ESI) m/z calcd. for $\text{C}_{10}\text{H}_{14}\text{F}_5\text{N}_3\text{ONa}$ $[\text{M}+\text{Na}]^+$ 310.0949, found 310.0939.



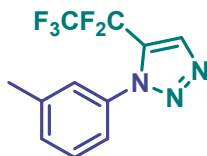
(56) Colorless oil; $^1\text{H NMR}$ (600 MHz, CDCl_3) δ 7.97 (s, 1H), 7.45-7.38 (m, 4H), 7.38-7.34 (m, 1H), 5.37 (dd, $J = 9.0, 3.0$ Hz, 1H), 4.68-4.57 (m, 2H), 3.22 (s, 1H). $^{13}\text{C NMR}$ (150 MHz, CDCl_3) δ 139.4, 135.3, 128.9, 128.7, 126.5 (t, $J = 30.0$ Hz), 125.9, 118.2 (qt, $J = 284.0, 36.5$ Hz), 109.9 (tq, $J = 252.0, 40.5$ Hz), 72.6, 57.3. $^{19}\text{F NMR}$ (471 MHz, CDCl_3) δ (-85.47)-(-85.89) (m), -109.95 (s). **HRMS** (ESI) m/z calcd. for $\text{C}_{12}\text{H}_{10}\text{F}_5\text{N}_3\text{ONa}$ $[\text{M}+\text{Na}]^+$ 330.0636, found 330.0611.



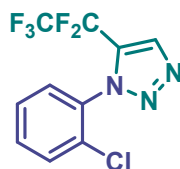
(57) Colorless oil; $^1\text{H NMR}$ (600 MHz, CDCl_3) δ 7.91 (s, 1H), 5.42-5.39 (m, 1H), 4.53 (t, $J = 7.2$ Hz, 2H), 2.56 (t, $J = 7.2$ Hz, 2H), 2.00-1.90 (m, 4H), 1.66-1.60 (m, 2H), 1.56-1.50 (m, 2H). $^{13}\text{C NMR}$ (150 MHz, CDCl_3) δ 135.2, 132.5, 125.4 (t, $J = 28.5$ Hz), 125.0, 118.3 (qt, $J = 284.0$, 36.5 Hz), 110.1 (tq, $J = 252.0$, 41.0 Hz), 49.5, 38.7, 28.0, 25.1, 22.6, 22.0. $^{19}\text{F NMR}$ (471 MHz, CDCl_3) δ (-83.87)-(-84.24) (m), (-109.32)-(-109.52) (m). **HRMS** (ESI) m/z calcd. for $\text{C}_{12}\text{H}_{14}\text{F}_5\text{N}_3$ Na $[\text{M}+\text{Na}]^+$ 318.1000, found 318.0999.



(58) Colorless oil; $^1\text{H NMR}$ (600 MHz, CDCl_3) δ 8.07 (s, 1H), 7.36 (d, $J = 9.0$ Hz, 2H), 7.03-6.99 (m, 2H), 3.87 (s, 3H). $^{13}\text{C NMR}$ (150 MHz, CDCl_3) δ 161.2, 135.4, 128.4, 127.5, 127.1 (t, $J = 30.0$ Hz), 118.2 (qt, $J = 285.0$, 36.0 Hz), 114.3, 109.6 (tq, $J = 252.0$, 40.5 Hz), 55.6. $^{19}\text{F NMR}$ (471 MHz, CDCl_3) δ (-83.48)-(-84.02) (m), -107.28 (s). **HRMS** (ESI) m/z calcd. for $\text{C}_{11}\text{H}_8\text{F}_5\text{N}_3\text{ONa}$ $[\text{M}+\text{Na}]^+$ 316.0480, found 316.0472.

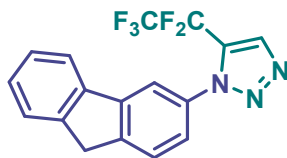


(59) Colorless oil; $^1\text{H NMR}$ (600 MHz, CDCl_3) δ 8.08 (s, 1H), 7.43-7.37 (m, 2H), 7.29-7.24 (m, 2H), 2.44 (s, 3H). $^{13}\text{C NMR}$ (150 MHz, CDCl_3) δ 139.6, 135.6, 135.4, 131.6, 129.0, 126.9 (t, $J = 30.0$ Hz), 126.7, 123.2, 118.2 (qt, $J = 283.5$, 36.0 Hz), 109.5 (tq, $J = 252.0$, 40.5 Hz), 21.1. $^{19}\text{F NMR}$ (471 MHz, CDCl_3) δ (-83.44)-(-84.03) (m), (-106.90)-(-107.10) (m). **HRMS** (ESI) m/z calcd. for $\text{C}_{11}\text{H}_8\text{F}_5\text{N}_3\text{Na}$ $[\text{M}+\text{Na}]^+$ 300.0531, found 300.0524.

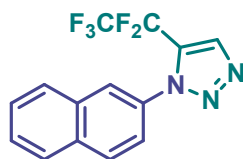


(60) Colorless oil; $^1\text{H NMR}$ (600 MHz, CDCl_3) δ 8.14 (s, 1H), 7.61 (d, $J = 7.8$ Hz, 1H), 7.57 (td, $J = 7.2$, 2.4 Hz, 1H), 7.49-7.43 (m, 2H). $^{13}\text{C NMR}$ (150 MHz, CDCl_3) δ 135.1, 133.3, 132.6, 132.5,

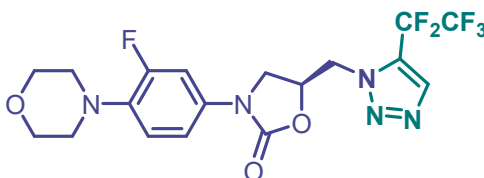
130.5, 129.0, 127.8 (t, $J = 28.5$ Hz), 127.4, 118.1 (qt, $J = 283.5, 36.0$ Hz), 109.4 (tq, $J = 252.0, 40.5$ Hz). ^{19}F NMR (471 MHz, CDCl_3) δ (-83.85)-(-84.40) (m), (-108.32)-(-110.83) (m). HRMS (ESI) m/z calcd. for $\text{C}_{10}\text{H}_6\text{ClF}_5\text{N}_3$ $[\text{M}+\text{H}]^+$ 298.0177, found 298.0170.



(61) White solid; mp: 120-121 °C; ^1H NMR (600 MHz, CDCl_3) δ 8.13 (s, 1H), 7.88 (d, $J = 7.8$ Hz, 1H), 7.83 (d, $J = 7.8$ Hz, 1H), 7.61 (s, 1H), 7.58 (d, $J = 7.2$ Hz, 1H), 7.46 (d, $J = 7.8$ Hz, 1H), 7.42 (t, $J = 7.2$ Hz, 1H), 7.38 (td, $J = 7.8, 1.2$ Hz, 1H), 3.96 (s, 2H). ^{13}C NMR (150 MHz, CDCl_3) δ 144.3, 144.0, 143.7, 139.9, 135.5, 133.8, 127.9, 127.1, 127.0 (t, $J = 28.5$ Hz), 125.2, 125.0, 122.9, 120.6, 120.1, 118.2 (qt, $J = 285.0, 36.0$ Hz), 109.6 (tq, $J = 252.0, 40.5$ Hz), 36.8. ^{19}F NMR (471 MHz, CDCl_3) δ (-83.42)-(-83.86) (m), -106.93 (s). HRMS (ESI) m/z calcd. for $\text{C}_{17}\text{H}_{11}\text{F}_5\text{N}_3$ $[\text{M}+\text{H}]^+$ 352.0874, found 352.0873.

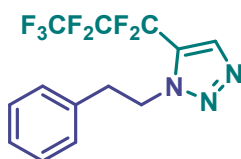


(62) White solid; mp: 62-63 °C; ^1H NMR (600 MHz, CDCl_3) δ 8.16 (s, 1H), 8.02-7.98 (m, 2H), 7.97-7.91 (m, 2H), 7.66-7.59 (m, 2H), 7.54-7.50 (m, 1H). ^{13}C NMR (150 MHz, CDCl_3) δ 135.6, 133.8, 133.0, 132.5, 129.4, 128.5, 128.0, 127.9, 127.6, 127.2 (t, $J = 28.5$ Hz), 125.6, 123.1, 118.2 (qt, $J = 285.0, 36.0$ Hz), 109.6 (tq, $J = 252.0, 40.5$ Hz). ^{19}F NMR (471 MHz, CDCl_3) δ (-83.47)-(-83.84) (m), -106.88 (s). HRMS (ESI) m/z calcd. for $\text{C}_{14}\text{H}_8\text{F}_5\text{N}_3\text{Na}$ $[\text{M}+\text{Na}]^+$ 336.0531, found 336.0546.

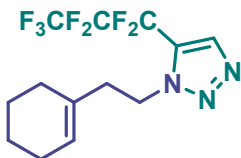


(63) White solid; mp: 152-153 °C; ^1H NMR (600 MHz, CDCl_3) δ 8.01 (s, 1H), 7.39 (dd, $J = 14.4, 2.4$ Hz, 1H), 7.08 (dd, $J = 8.4, 1.8$ Hz, 1H), 6.91 (t, $J = 9.0$ Hz, 1H), 5.24-5.19 (m, 1H), 4.85-4.74

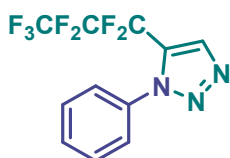
(m, 2H), 4.22 (t, $J = 9.0$ Hz, 1H), 4.01 (dd, $J = 9.0, 6.0$ Hz, 1H), 3.84 (t, $J = 4.8$ Hz, 4H), 3.03 (t, $J = 4.8$ Hz, 4H). ^{13}C NMR (150 MHz, CDCl_3) δ 155.5 (d, $J = 246.0$ Hz), 153.1, 136.8 (d, $J = 9.0$ Hz), 135.6, 132.4 (d, $J = 10.5$ Hz), 126.7 (t, $J = 28.5$ Hz), 118.8 (d, $J = 4.5$ Hz), 118.0 (qt, $J = 285.0, 36.0$ Hz), 114.1 (d, $J = 3.0$ Hz), 109.8 (tq, $J = 252.0, 42.0$ Hz), 107.6 (d, $J = 26.0$ Hz), 69.6, 66.9, 52.1, 50.9 (d, $J = 3.0$ Hz), 48.6. ^{19}F NMR (471 MHz, CDCl_3) δ (-83.81)-(-84.03) (m), -109.29 (s), (-119.89)-(-120.04) (m). HRMS (ESI) m/z calcd. for $\text{C}_{18}\text{H}_{17}\text{F}_6\text{N}_5\text{O}_3$ $[\text{M}+\text{H}]^+$ 466.1313, found 466.1314.



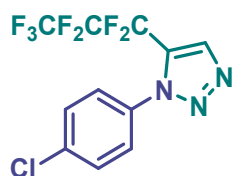
(64) Colorless oil; ^1H NMR (600 MHz, CDCl_3) δ 7.95 (s, 1H), 7.32 (t, $J = 7.2$ Hz, 2H), 7.27 (t, $J = 7.2$ Hz, 1H), 7.18 (d, $J = 7.2$ Hz, 2H), 4.66 (t, $J = 8.0$ Hz, 2H), 2.96 (t, $J = 8.0$ Hz, 2H). ^{13}C NMR (150 MHz, CDCl_3) δ 136.2, 135.6, 128.9, 128.7, 127.3, 125.7 (t, $J = 31.5$ Hz), 117.5 (qt, $J = 287.0, 33.6$ Hz), 112.3 (tt, $J = 253.0, 33.0$ Hz), 110.1-105.9 (m), 51.8, 36.7. ^{19}F NMR (471 MHz, CDCl_3) δ (-79.57)-(-80.20) (m), (-106.98)-(-107.38) (m), (-125.50)-(-125.79) (m). HRMS (ESI) m/z calcd. for $\text{C}_{13}\text{H}_{11}\text{F}_7\text{N}_3$ $[\text{M}+\text{H}]^+$ 342.0839, found 342.0841.



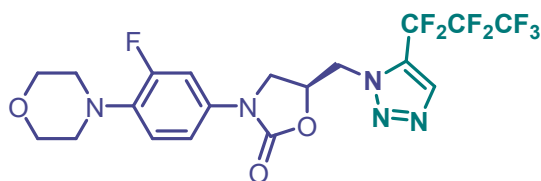
(65) Colorless oil; ^1H NMR (600 MHz, CDCl_3) δ 7.90 (s, 1H), 5.38 (s, 1H), 4.49 (t, $J = 7.2$ Hz, 2H), 2.54 (t, $J = 7.8$ Hz, 2H), 1.99-1.87 (m, 4H), 1.64-1.57 (m, 2H), 1.54-1.47 (m, 2H). ^{13}C NMR (150 MHz, CDCl_3) δ 135.5, 132.5, 125.5 (t, $J = 30.0$ Hz), 124.9, 117.5 (qt, $J = 288.0, 33.5$ Hz), 112.4 (tt, $J = 255.0, 32.5$ Hz), 110.6-105.9 (m), 49.5, 38.7, 28.0, 25.1, 22.6, 21.9. ^{19}F NMR (471 MHz, CDCl_3) δ (-79.03)-(-80.71) (m), (-106.33)-(-108.24) (m), (-124.80)-(-126.64) (m). HRMS (ESI) m/z calcd. for $\text{C}_{13}\text{H}_{15}\text{F}_7\text{N}_3$. $[\text{M}+\text{H}]^+$ 346.1158, found 346.1154.



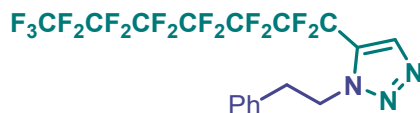
(66) Colorless oil; $^1\text{H NMR}$ (600 MHz, CDCl_3) δ 8.10 (s, 1H), 7.58-7.54 (m, 1H), 7.53-7.49 (m, 2H), 7.43 (d, $J = 7.8$ Hz, 2H). $^{13}\text{C NMR}$ (150 MHz, CDCl_3) δ 135.8, 135.8, 130.8, 129.1, 127.1 (t, $J = 30.0$ Hz), 126.3, 117.3 (qt, $J = 287.0, 33.0$ Hz), 111.9 (tt, $J = 255.0, 33.0$ Hz), 110.4-105.7 (m). $^{19}\text{F NMR}$ (471 MHz, CDCl_3) δ (-80.01)-(-80.36) (m), (-104.47)-(-104.77) (m), (-125.04)-(-125.43) (m). **HRMS** (ESI) m/z calcd. for $\text{C}_{11}\text{H}_6\text{F}_7\text{N}_3\text{Na}$ $[\text{M}+\text{Na}]^+$ 336.1686, found 336.1690.



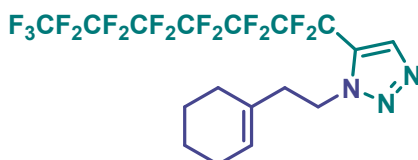
(67) White solid; mp: 44-45 °C; $^1\text{H NMR}$ (600 MHz, CDCl_3) δ 8.11 (s, 1H), 7.54-7.50 (m, 2H), 7.39 (d, $J = 8.4$ Hz, 2H). $^{13}\text{C NMR}$ (150 MHz, CDCl_3) δ 137.2, 135.9, 134.2, 129.5, 127.6, 127.2 (t, $J = 30.0$ Hz), 117.3 (qt, $J = 286.5, 33.0$ Hz), 111.9 (tt, $J = 253.5, 33.0$ Hz), 110.4-105.8 (m). $^{19}\text{F NMR}$ (471 MHz, CDCl_3) δ (-80.04)-(-80.16) (m), (-104.34)-(-104.80) (m), (-124.96)-(-125.33) (m). **HRMS** (ESI) m/z calcd. for $\text{C}_{11}\text{H}_6\text{ClF}_7\text{N}_3$ $[\text{M}+\text{H}]^+$ 348.0147, found 348.0138.



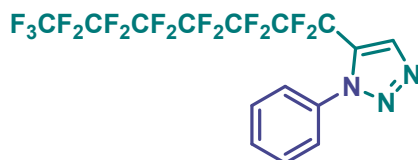
(68) White solid; mp: 158-159 °C; $^1\text{H NMR}$ (600 MHz, CDCl_3) δ 8.01 (s, 1H), 7.38 (dd, $J = 14.4, 2.4$ Hz, 1H), 7.07 (dd, $J = 8.4, 1.8$ Hz, 1H), 6.90 (t, $J = 9.0$ Hz, 1H), 5.24-5.18 (m, 1H), 4.83-4.71 (m, 2H), 4.22 (t, $J = 9.0$ Hz, 1H), 4.04-3.99 (m, 1H), 3.84 (t, $J = 4.8$ Hz, 4H), 3.03 (t, $J = 4.8$ Hz, 4H). $^{13}\text{C NMR}$ (150 MHz, CDCl_3) δ 155.4 (d, $J = 246.0$ Hz), 154.6, 153.2, 136.8 (d, $J = 9.0$ Hz), 136.0, 132.4 (d, $J = 10.5$ Hz), 126.8 (t, $J = 30.0$ Hz), 118.8 (d, $J = 4.5$ Hz), 117.3 (qt, $J = 286.5, 33.0$ Hz), 114.1 (d, $J = 9.0$ Hz), 112.1 (tt, $J = 253.5, 33.0$ Hz), 110.5-105.9 (m), 107.6 (d, $J = 26.0$ Hz), 69.6, 66.8, 52.2, 50.9 (d, $J = 3.0$ Hz), 48.7. $^{19}\text{F NMR}$ (471 MHz, CDCl_3) δ -79.72 (t, $J = 10.8$ Hz), -107.04 (q, $J = 10.4$ Hz), (-119.87)-(-120.14) (m), (-125.26)-(-125.73) (m). **HRMS** (ESI) m/z calcd. for $\text{C}_{19}\text{H}_{18}\text{F}_8\text{N}_5\text{O}_3$ $[\text{M}+\text{H}]^+$ 516.1279, found 516.1282.



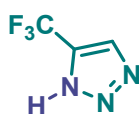
(69) White solid; mp: 40-41 °C; ¹H NMR (600 MHz, CDCl₃) δ 7.95 (s, 1H), 7.34-7.30 (m, 2H), 7.29-7.25 (m, 1H), 7.19-7.16 (m, 2H), 4.68-4.64 (m, 2H), 3.32-3.28 (m, 2H). ¹³C NMR (150 MHz, CDCl₃) δ 136.3, 135.7, 128.9, 128.7, 127.3, 126.0 (t, *J* = 30.0 Hz), 117.1 (qt, *J* = 288.0, 33.0 Hz), 114.5-105.9 (m), 51.8, 36.8. ¹⁹F NMR (471 MHz, CDCl₃) δ -80.91 (t, *J* = 11.8 Hz), -106.48 (t, *J* = 15.5 Hz), (-121.86)-(-122.16) (m), (-122.61)-(-122.91) (m), (-126.03)-(-126.41) (m). HRMS (ESI) *m/z* calcd. for C₁₇H₁₁F₁₅N₃·[M+H]⁺ 542.0710, found 542.0713.



(70) White solid; mp: 38-39 °C; ¹H NMR (600 MHz, CDCl₃) δ 7.92 (s, 1H), 5.43-5.39 (m, 1H), 4.51 (t, *J* = 7.8 Hz, 2H), 2.57 (t, *J* = 7.8 Hz, 2H), 2.00-1.90 (m, 4H), 1.66-1.60 (m, 2H), 1.56-1.50 (m, 2H). ¹³C NMR (150 MHz, CDCl₃) δ 135.6, 132.6, 125.8 (t, *J* = 30.0 Hz), 125.0, 117.1 (qt, *J* = 286.5, 33.0 Hz), 114.4-106.2 (m), 49.6, 38.8, 28.0, 25.1, 22.7, 22.0. ¹⁹F NMR (471 MHz, CDCl₃) δ -80.88 (t, *J* = 10.0 Hz), (-106.11)-(-106.57) (m), (-120.87)-(-121.50) (m), -122.00 (s), (-121.86)-(-121.14) (m), (-122.58)-(-122.90) (m), (-125.90)-(-126.47) (m). HRMS (ESI) *m/z* calcd. for C₁₇H₁₅F₁₅N₃·[M+H]⁺ 546.1031, found 546.1026.

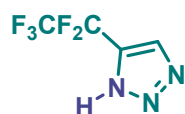


(71) Colorless oil; ¹H NMR (600 MHz, CDCl₃) δ 8.12 (s, 1H), 7.62-7.58 (m, 1H), 7.57-7.53 (m, 2H), 7.45 (d, *J* = 7.8 Hz, 2H). ¹³C NMR (150 MHz, CDCl₃) δ 136.0, 135.8 130.9, 129.2, 127.5 (t, *J* = 31.5 Hz), 126.4, 119.0-103.2 (m). ¹⁹F NMR (471 MHz, CDCl₃) δ -80.77 (t, *J* = 11.3 Hz), -103.74 (t, *J* = 16.0 Hz), (-120.56)-(-120.87) (m), (-121.13)-(-121.56) (m), (-121.83)-(-121.14) (m), (-122.55)-(-122.92) (m), (-125.78)-(-126.52) (m). HRMS (ESI) *m/z* calcd. for C₁₅H₇F₁₅N₃·[M+H]⁺ 514.0409, found 514.0400.

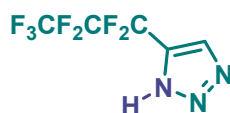


(72) White solid; mp: 37-38 °C; ¹H NMR (600 MHz, MeOD) δ 8.28 (s, 1H). ¹³C NMR (150 MHz,

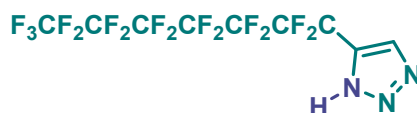
MeOD) δ 137.8 (q, $J = 46.5$ Hz), 127.2, 121.2 (q, $J = 266.5$ Hz). ^{19}F NMR δ (471 MHz, MeOD) δ -62.4 (s). **HRMS** (ESI) m/z calcd. for $\text{C}_3\text{H}_3\text{F}_3\text{N}_3$ $[\text{M}+\text{H}]^+$ 138.0276, found 138.0279.



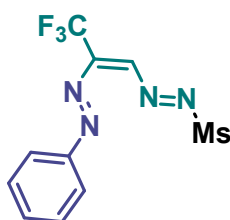
(73) White solid; mp: 33-34 °C; ^1H NMR (600 MHz, MeOD) δ 8.32 (s, 1H). ^{13}C NMR (150 MHz, MeOD) δ 136.3 (t, $J = 28.0$ Hz), 128.5, 118.7 (qt, $J = 285.0, 38.0$ Hz), 110.6 (tq, $J = 249.0, 39.5$ Hz). ^{19}F NMR δ (471 MHz, MeOD) δ -86.5 (s), -113.4 (s). **HRMS** (ESI) m/z calcd. for $\text{C}_4\text{H}_3\text{F}_4\text{N}_3$ $[\text{M}+\text{H}]^+$ 188.0254, found 188.0247.



(74) White solid; mp: 41-42 °C; ^1H NMR (600 MHz, MeOD) δ 8.29 (s, 1H). ^{13}C NMR (150 MHz, MeOD) δ 136.3 (t, $J = 29.5$ Hz), 128.7, 117.8 (qt, $J = 286.0, 33.0$ Hz), 112.5 (tt, $J = 251.0, 32.0$ Hz), 112.0-105.6 (m). ^{19}F NMR δ (471 MHz, MeOD) δ (-81.84)-(-81.94) (m), (-110.92)-(-110.04) (m), (-128.51)-(-128.57) (m). **HRMS** (ESI) m/z calcd. for $\text{C}_5\text{H}_3\text{F}_7\text{N}_3$ $[\text{M}+\text{H}]^+$ 238.0223, found 238.0215.



(75) White solid; mp: 73-74 °C; ^1H NMR (600 MHz, MeOD) δ 8.31 (s, 1H). ^{13}C NMR (150 MHz, MeOD) δ 136.5 (t, $J = 30.0$ Hz), 128.8, 121.0-105.1 (m). ^{19}F NMR δ (471 MHz, MeOD) δ (-82.49) - (-82.58) (m), (-122.36) - (-122.65) (m), (-123.00) - (-123.30) (m), (-123.69) - (-124.00) (m), (-127.33) - (-127.55) (m). **HRMS** (ESI) m/z calcd. for $\text{C}_9\text{H}_3\text{F}_{15}\text{N}_3$ $[\text{M}+\text{H}]^+$ 438.0096, found 438.0087.

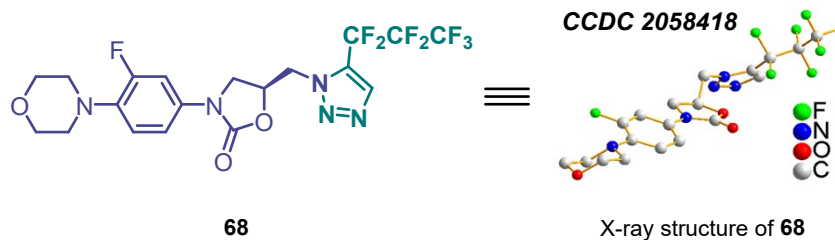


(77) Yellow solid; mp: 124-125 °C; ¹H NMR (600 MHz, MeOD) 7.78 (s, 1H), 7.33 (t, *J* = 7.8 Hz, 2H), 7.23 (d, *J* = 7.8 Hz, 2H), 7.04 (t, *J* = 7.2 Hz, 1H), 3.11 (s, 3H). ¹³C NMR (150 MHz, MeOD) δ 142.3, 136.9, 129.2, 123.5, 122.1 (q, *J* = 270.0 Hz), 121.0 (q, *J* = 33.5 Hz), 114.2, 38.0. ¹⁹F NMR (471 MHz, MeOD) δ -66.47 (s). HRMS (ESI) *m/z* calcd. for C₉H₁₀F₃N₄O₂SNa [M+Na]⁺ 329.2530, found 329.2533.

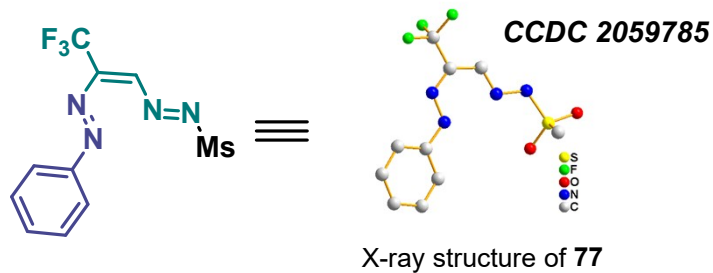
References

- [1] a) X. Zhang, Z. Liu, X. Yang, Y. Dong, M. Virelli, G. Zanoni, E. A. Anderson, X. Bi, *Nat. Commun.* **2019**, *10*, 284–292; b) Y. Ning, Y. Gai, X. Zhang, Y. Dong, P. Sivaguru, Y. Wang, B. R. P. Reddy, G. Zanoni, X. Bi, *Angew. Chem. Int. Ed.* **2020**, *59*, 6473–6481; *Angew. Chem.* **2020**, *132*, 6535–6543.

VI. X-ray single crystal data of 68 and 77

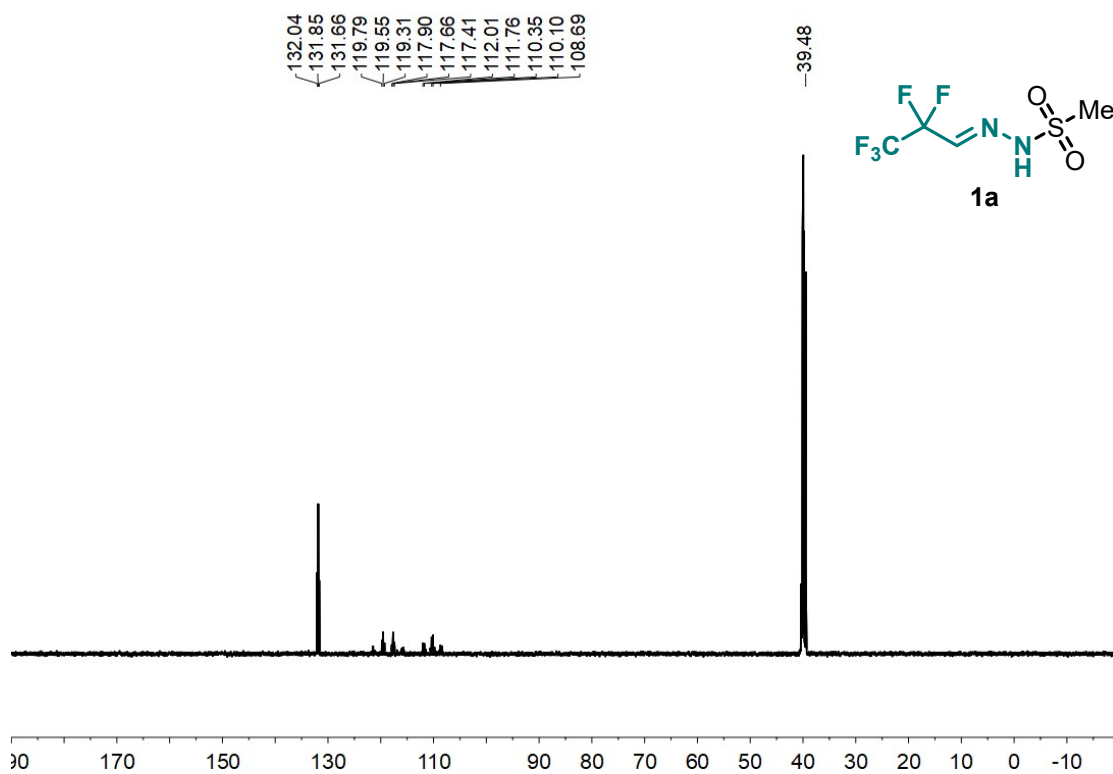
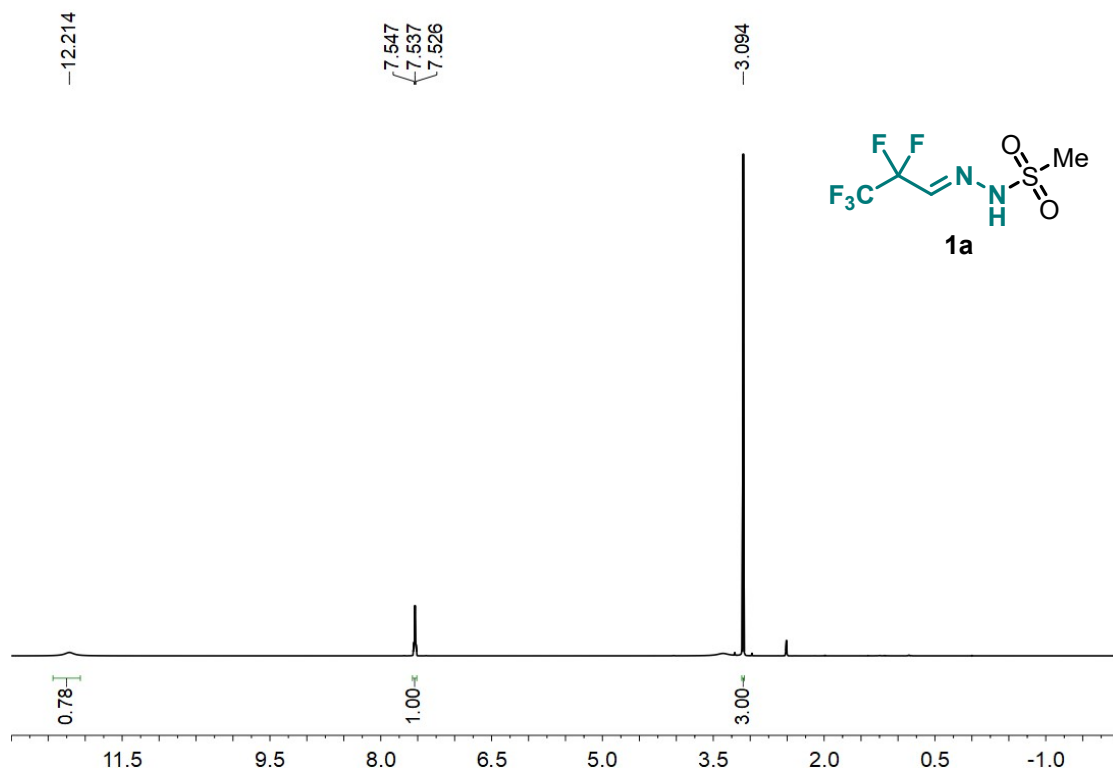


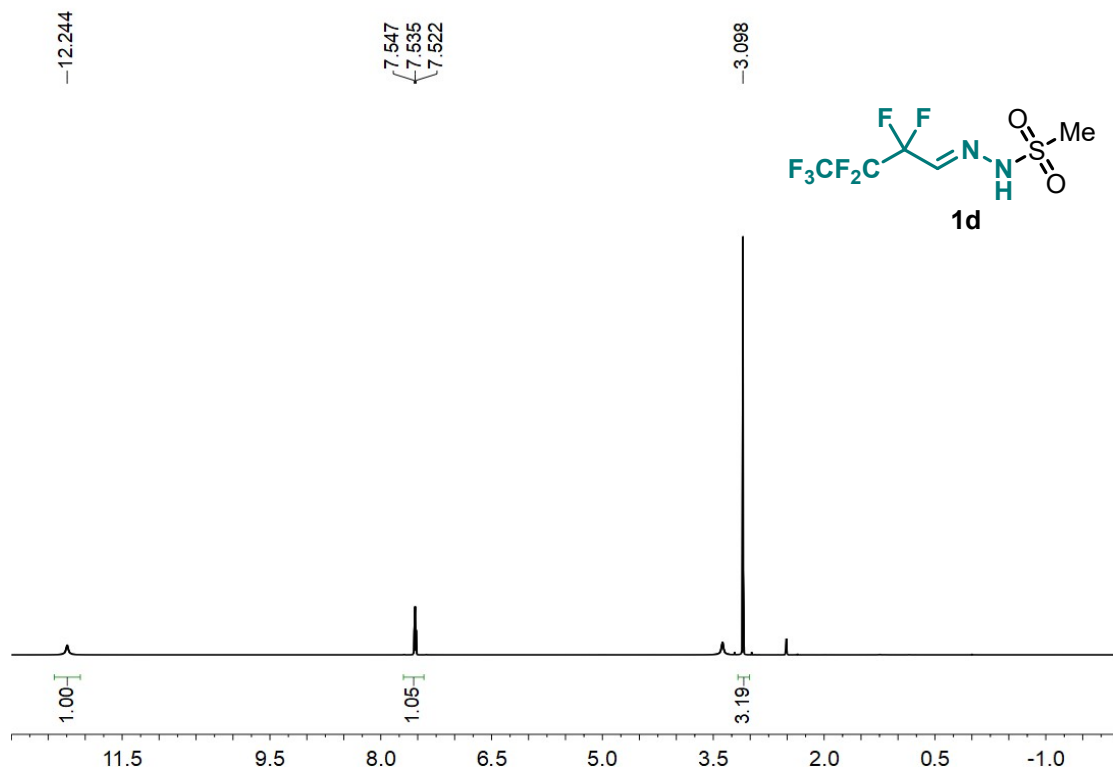
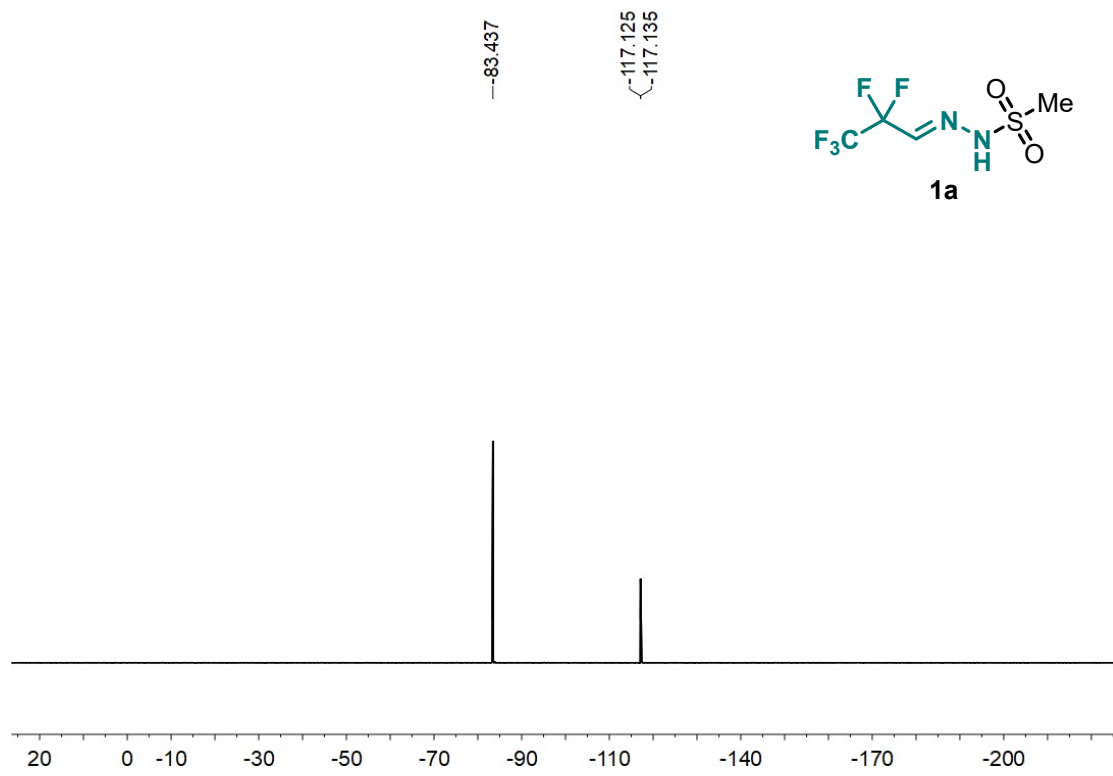
Empirical formula	C ₁₉ H ₁₇ F ₈ N ₅ O ₃
Temperature	298.15K
Wavelength	0.71073 Å
Unit cell dimensions	a = 11.1446(13) Å alpha = 90 deg. b = 6.5924(9) Å beta = 93.968(10) deg. c = 29.135(4) Å gamma = 90 deg.
Volume	2135.4(5) Å ³
Z	4
Calculated density	1.603 Mg/m ³
Absorption coefficient	0.157 mm ⁻¹
F(000)	1048.0
Crystal size	0.2 × 0.19 × 0.18
Theta range for data collection	7.168 to 58.424 deg
Reflections collected / unique	4871 / 3460 [R _{int} = 0.0230, R _{sigma} = 0.0502]
Data / restraints / parameters	3460 / 1 / 316
Goodness-of-fit on F ²	1.015
Final R indices [I > 2sigma(I)]	R ₁ = 0.0646, wR ₂ = 0.1551
R indices (all data)	R ₁ = 0.0970, wR ₂ = 0.1818

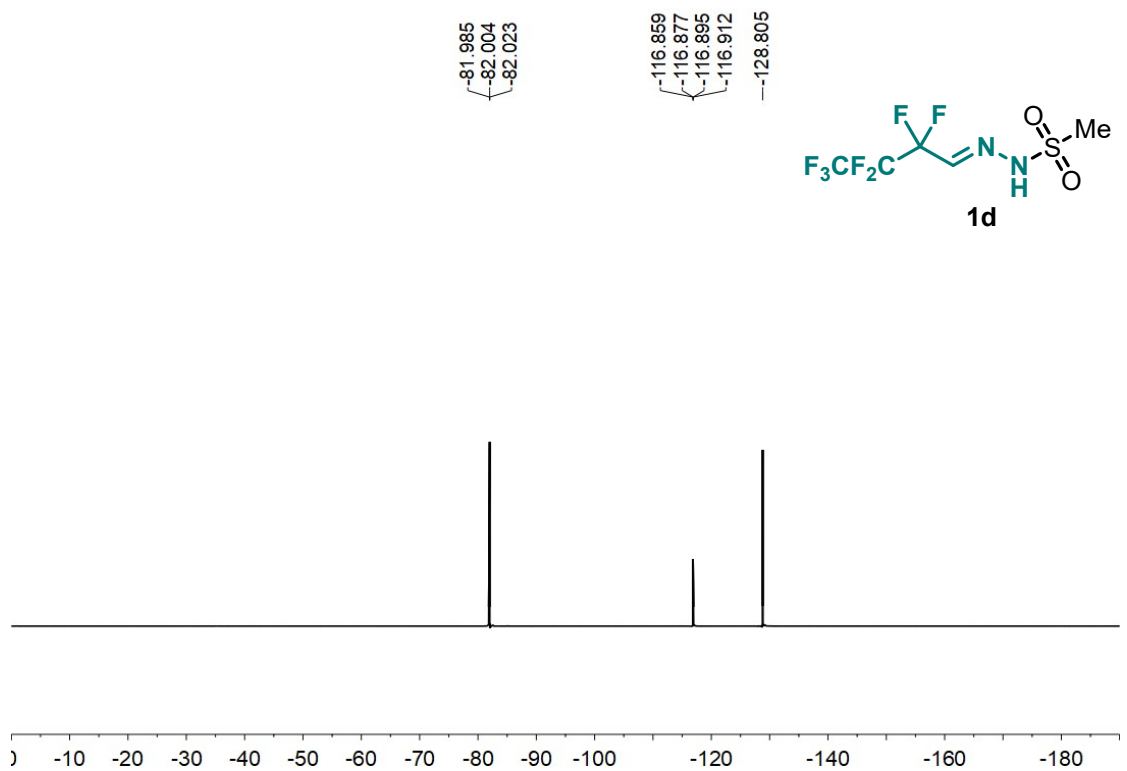
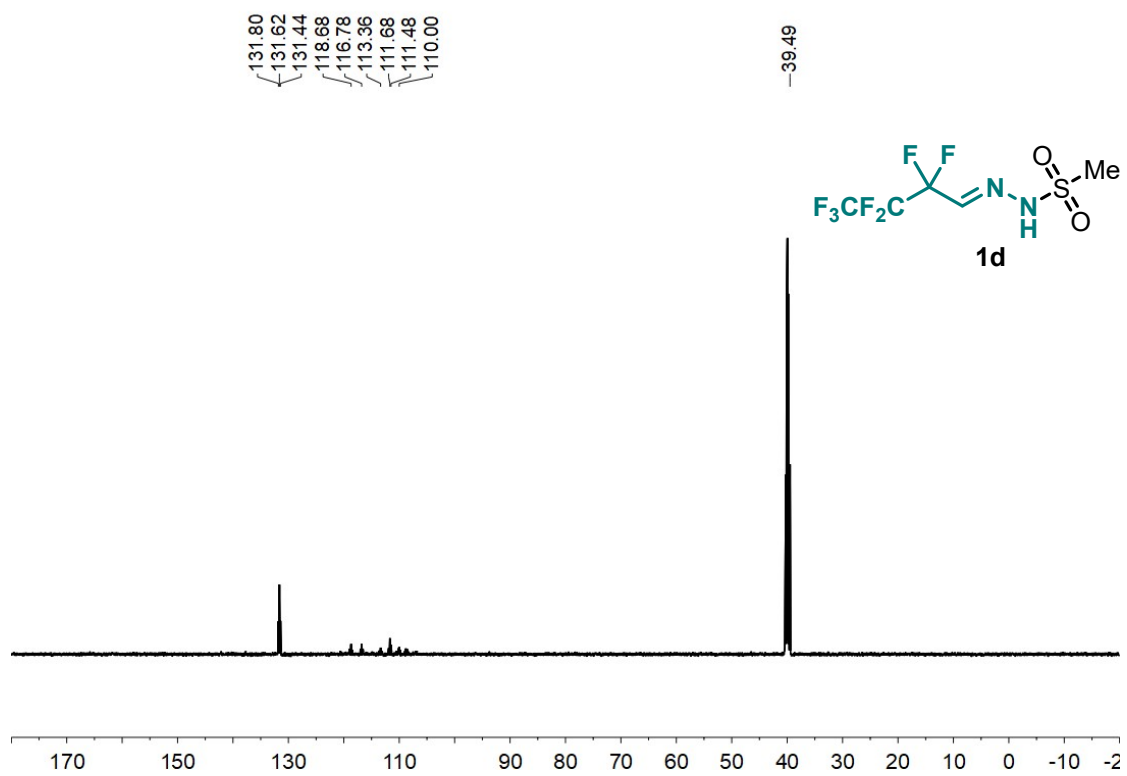


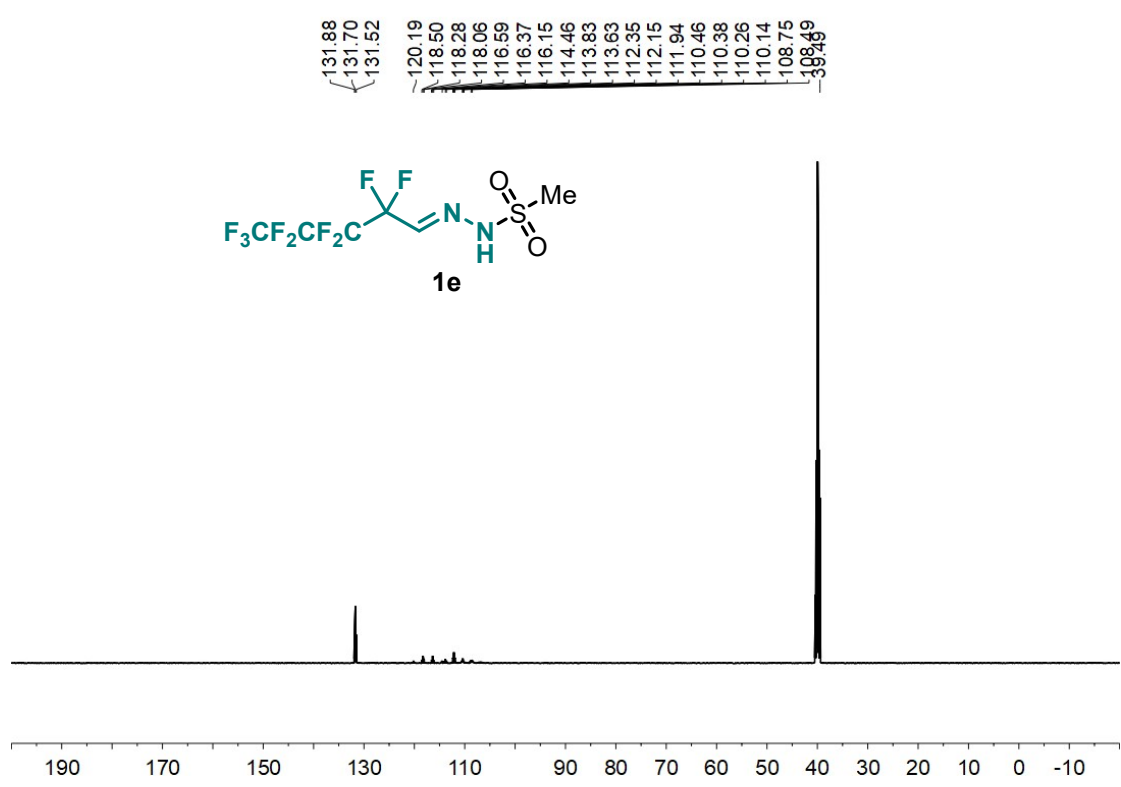
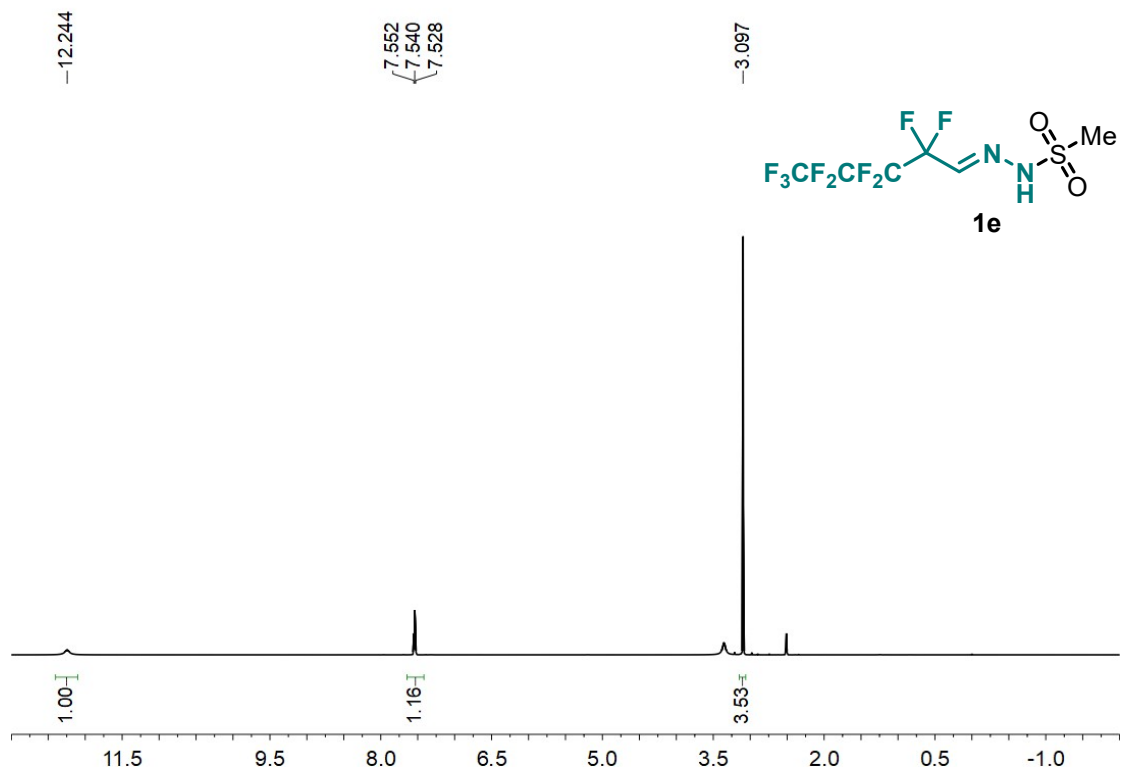
Empirical formula	C ₁₀ H ₉ F ₃ N ₄ O ₂ S
Temperature	298.15K
Wavelength	0.71073 Å
Unit cell dimensions	a = 5.2381(9) Å alpha = 90 deg. b = 9.2372(19) Å beta = 90 deg. c = 28.525(5) Å gamma = 90 deg.
Volume	1380.2(4) Å ³
Z	4
Calculated density	1.47 Mg/m ³
Absorption coefficient	0.275 mm ⁻¹
F(000)	624.0
Crystal size	0.2 × 0.19 × 0.18
Theta range for data collection	7.218 to 58.622 deg
Reflections collected / unique	4410 / 2801 [R _{int} = 0.0411, R _{sigma} = 0.0929]
Data / restraints / parameters	2801/0/182
Goodness-of-fit on F ²	1.003
Final R indices [I > 2σ(I)]	R ₁ = 0.0662, wR ₂ = 0.1236
R indices (all data)	R ₁ = 0.1326, wR ₂ = 0.1555

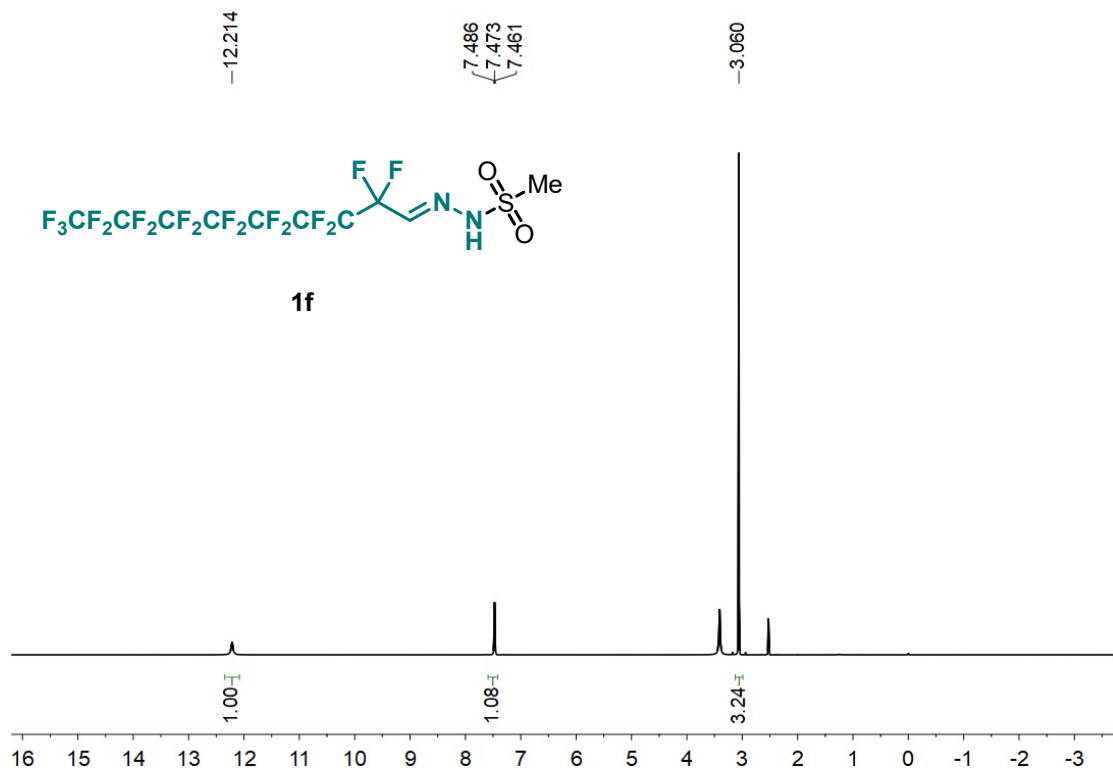
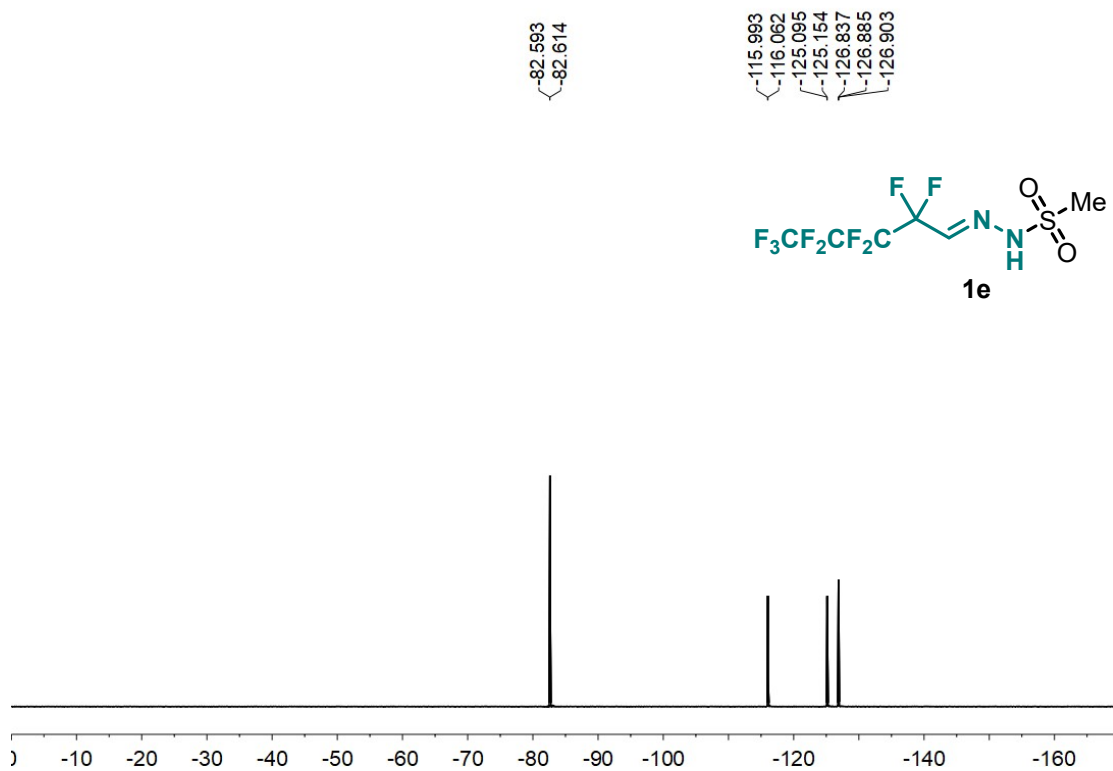
VII. Copies of NMR spectra

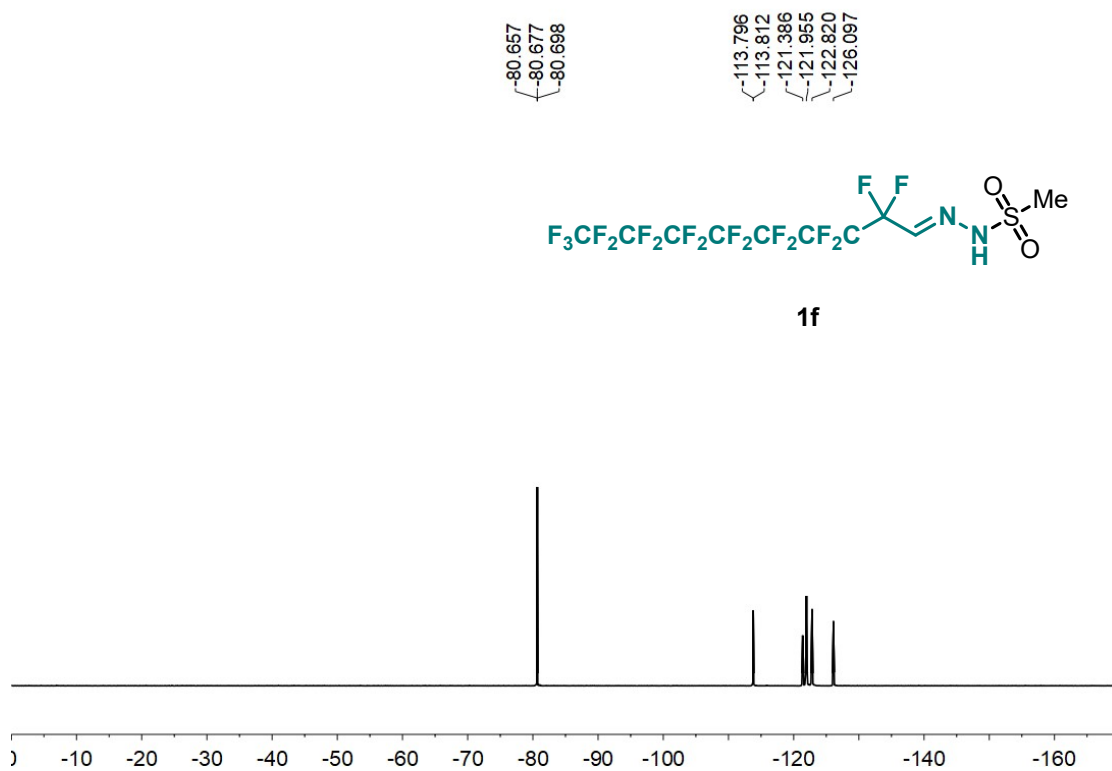
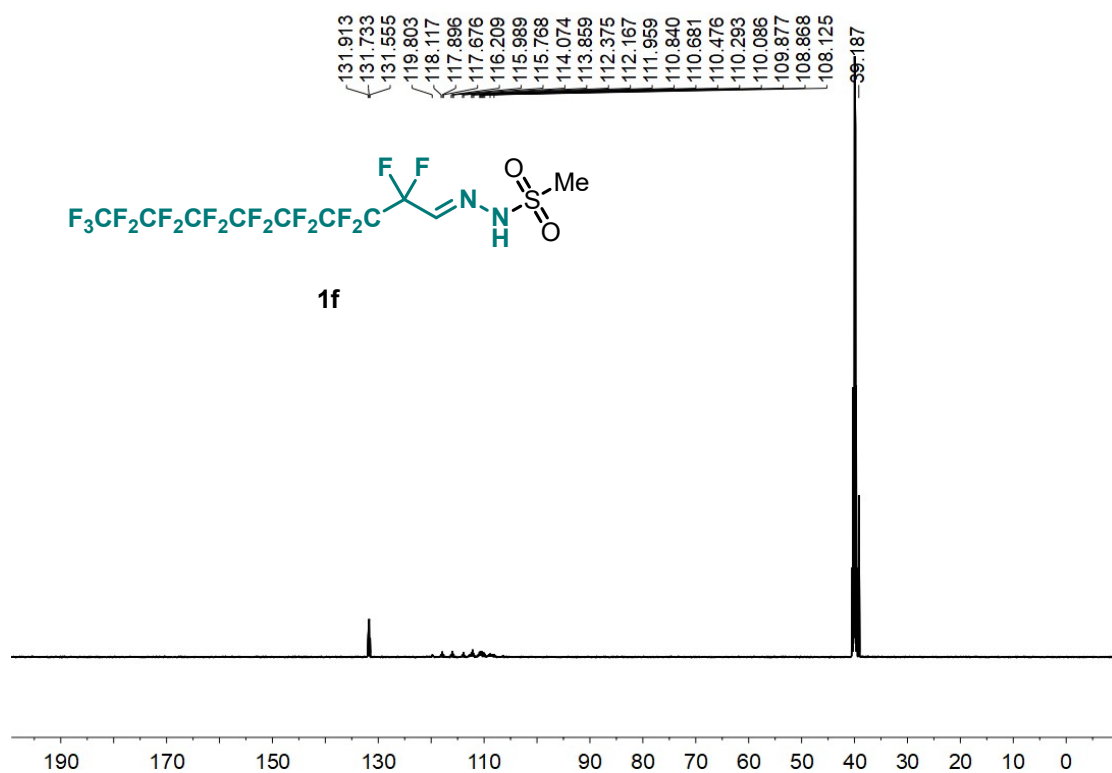


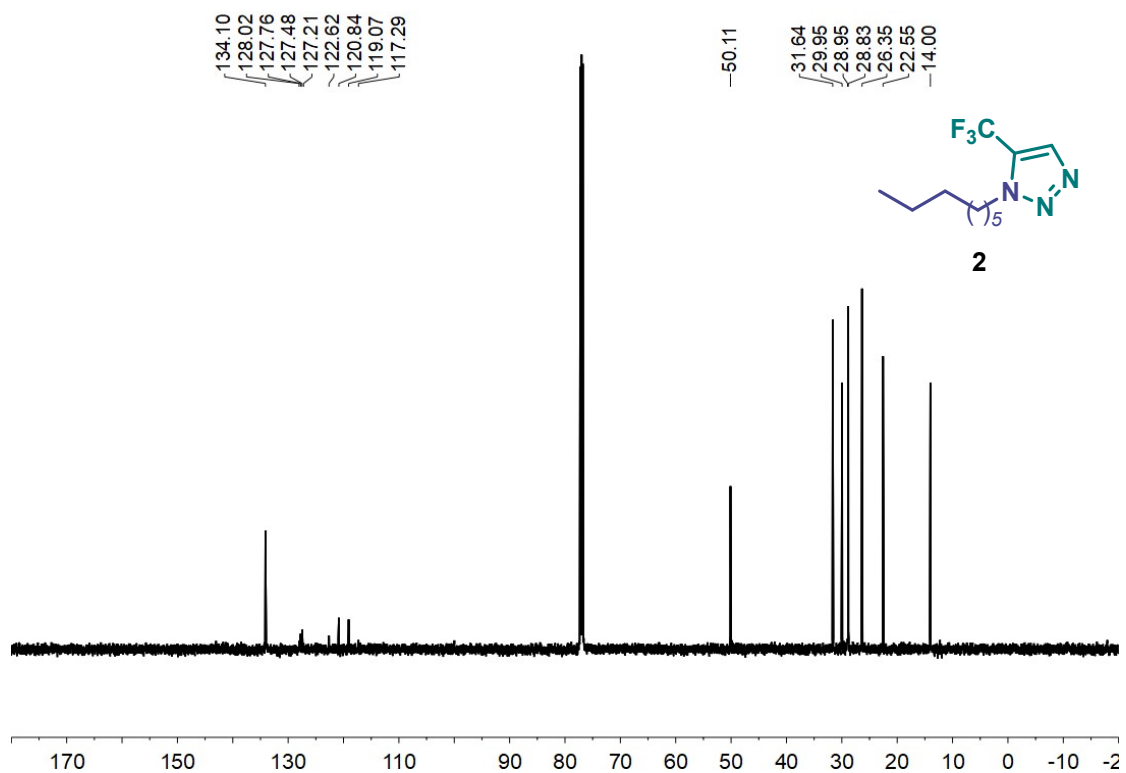
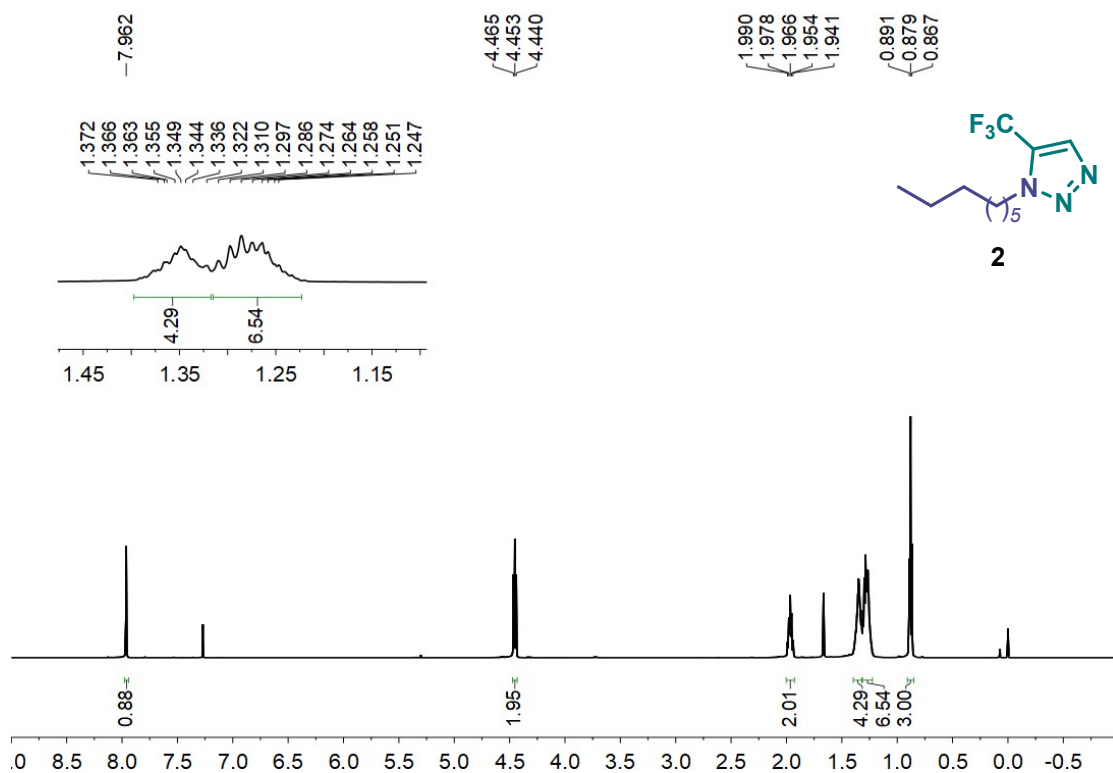


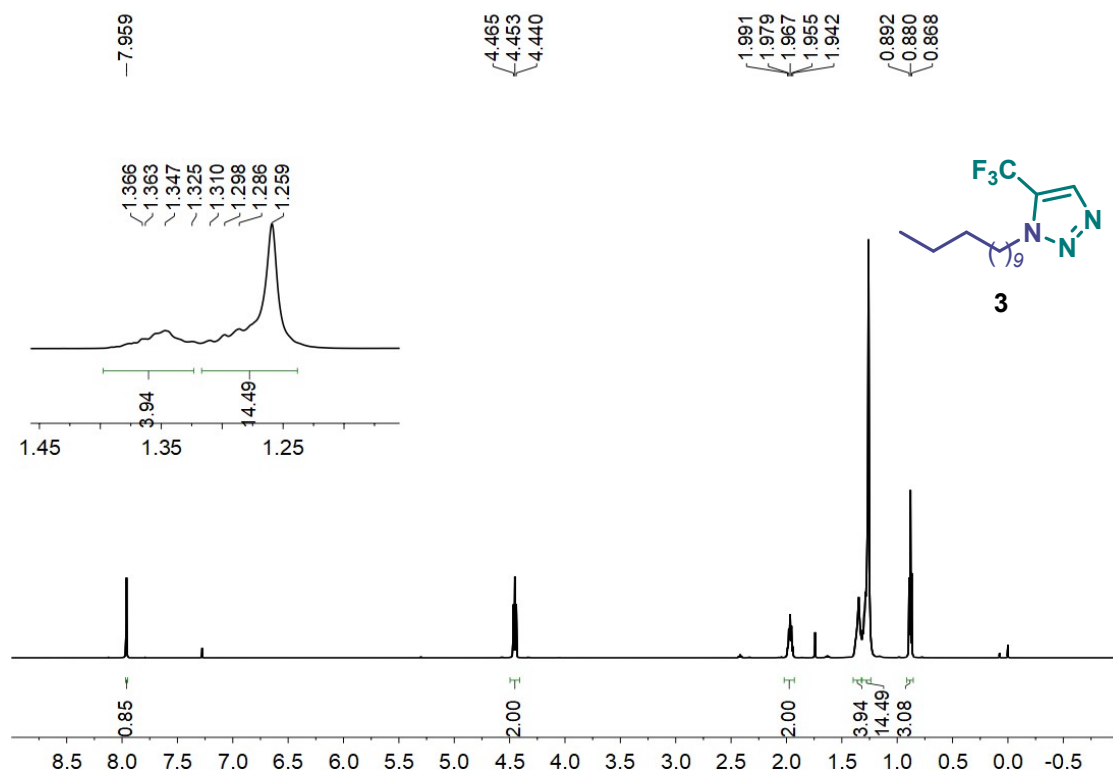
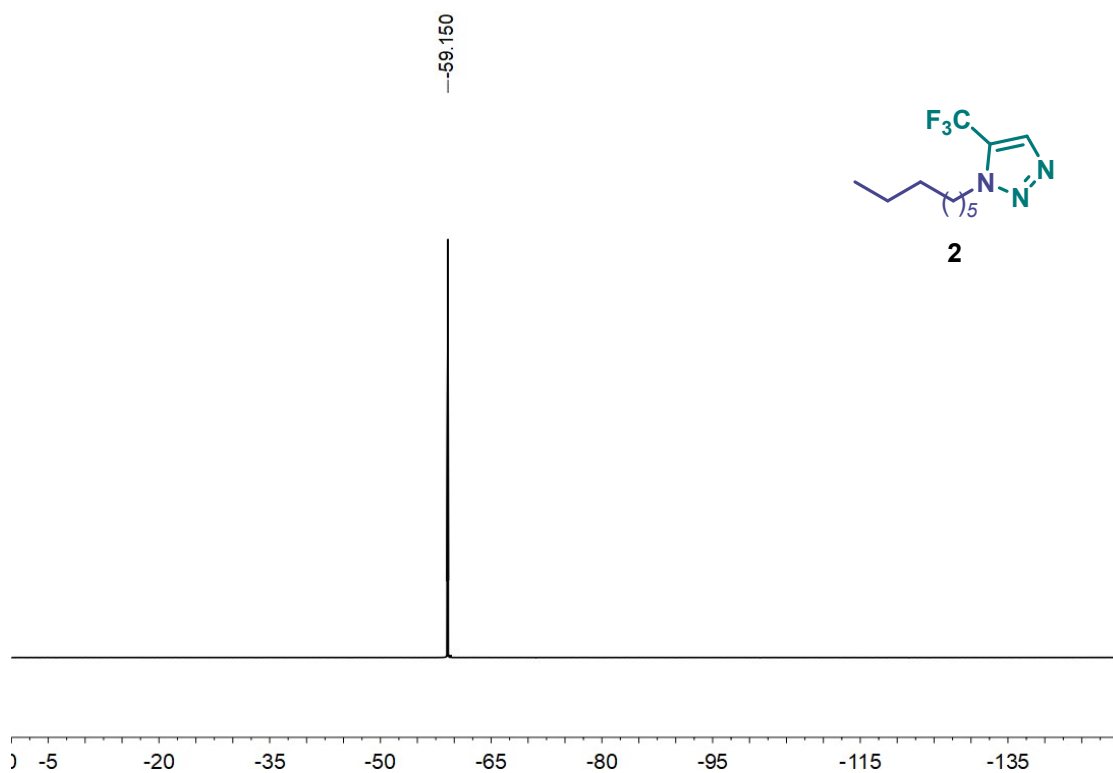


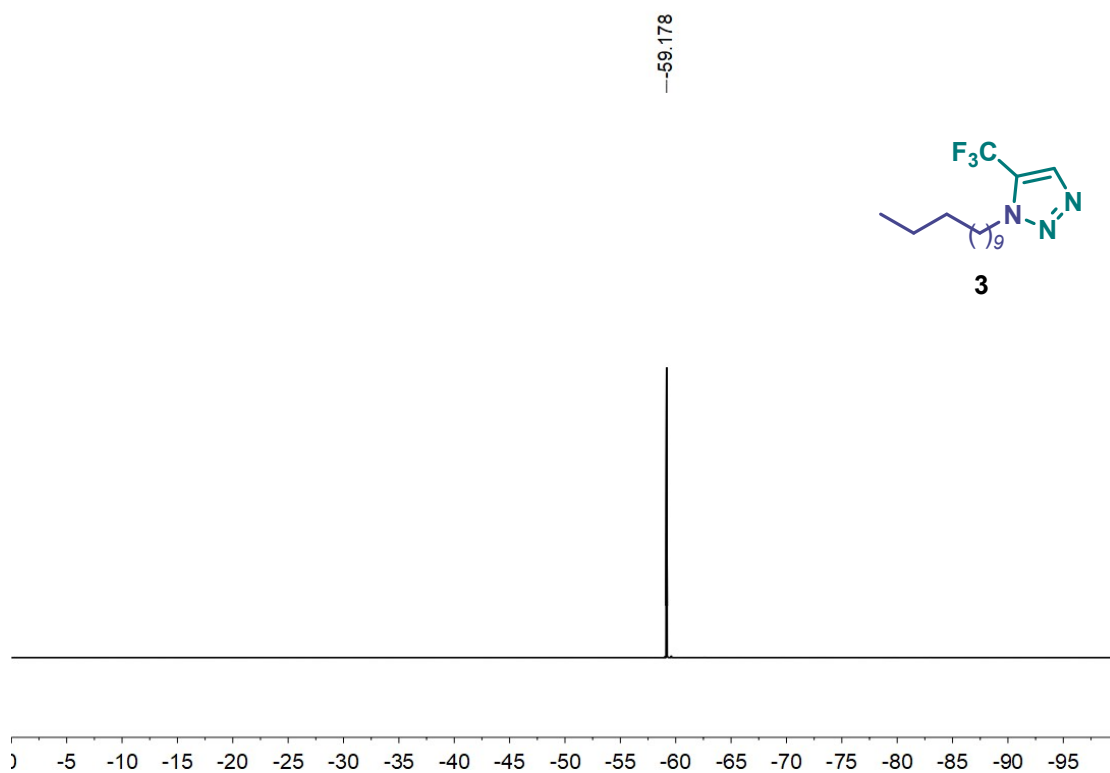
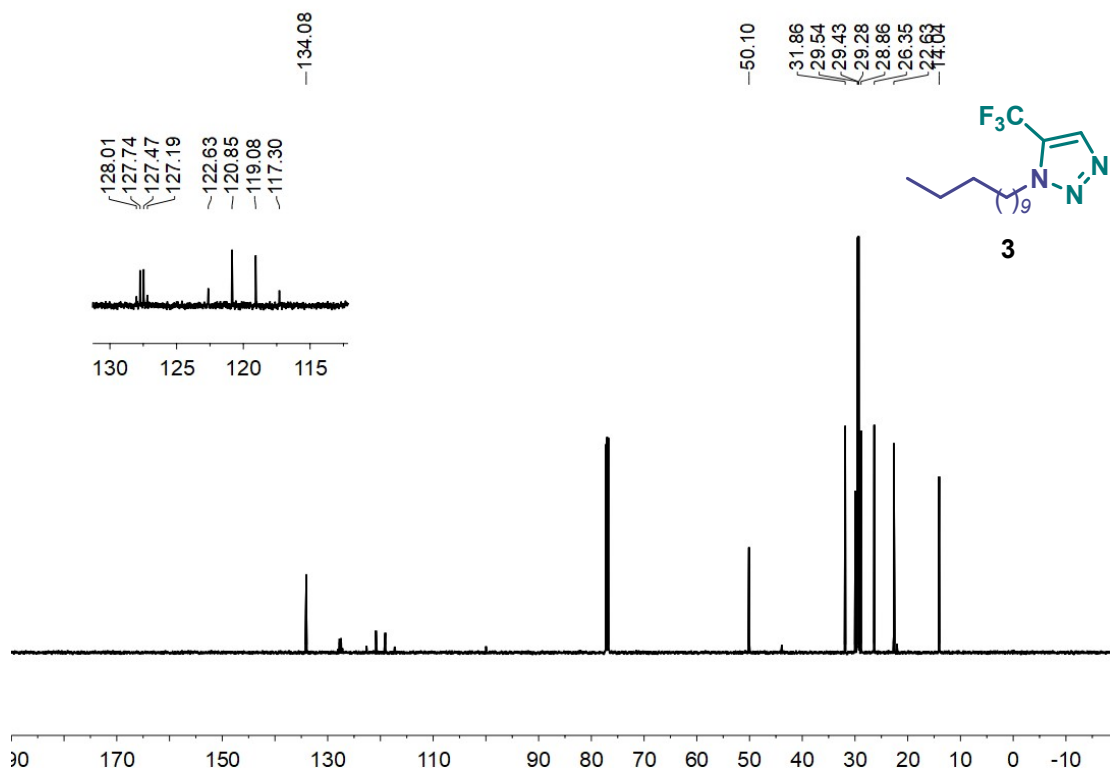


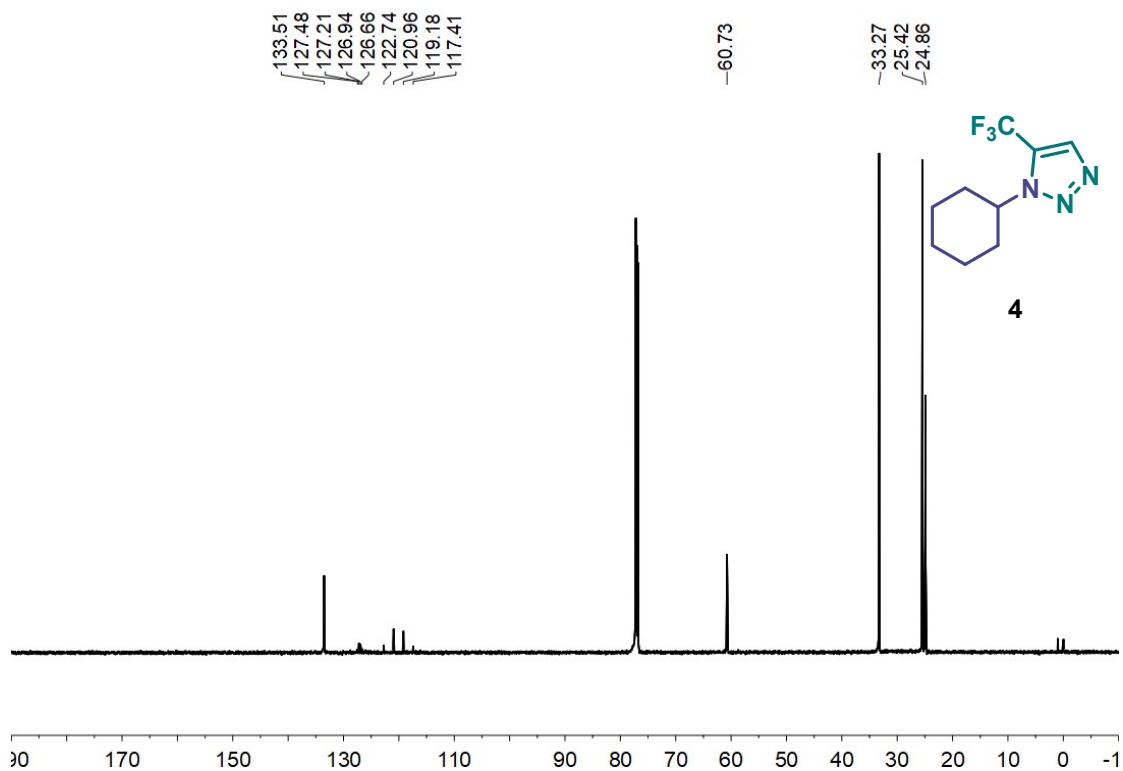
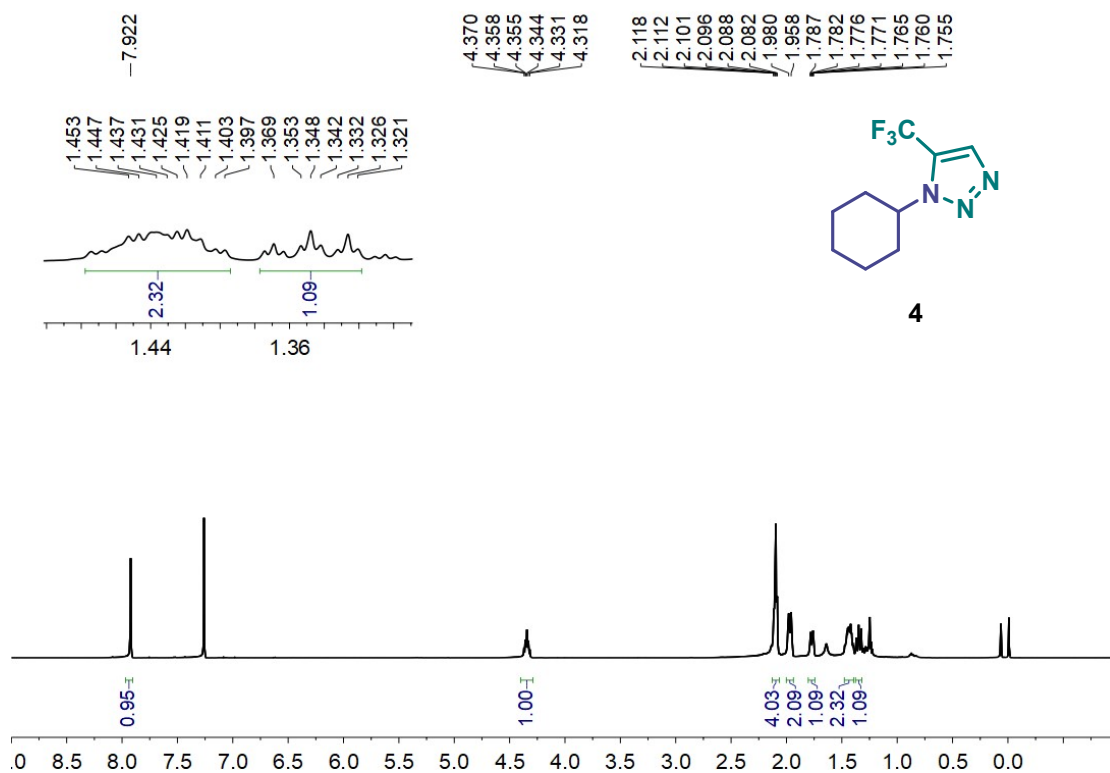


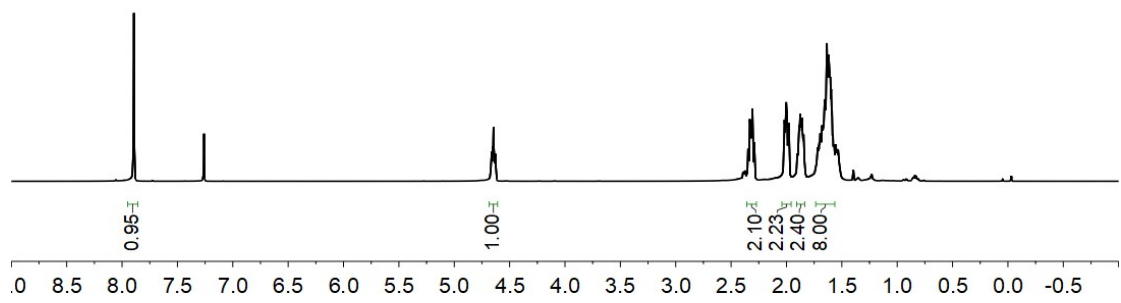
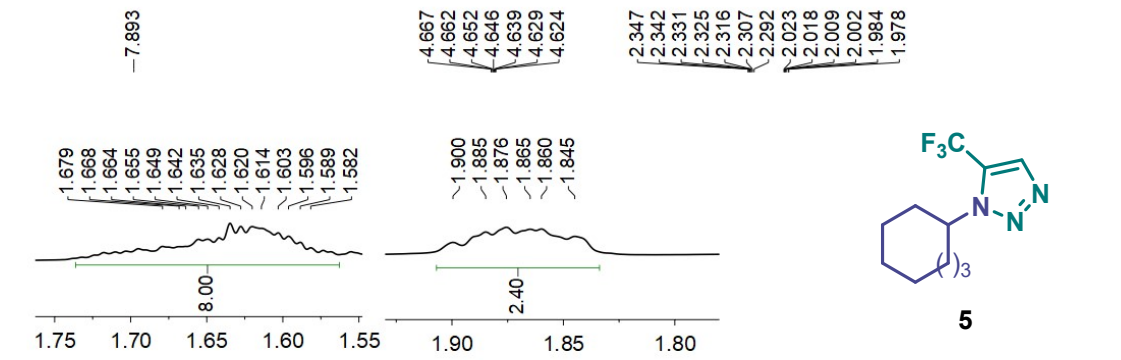
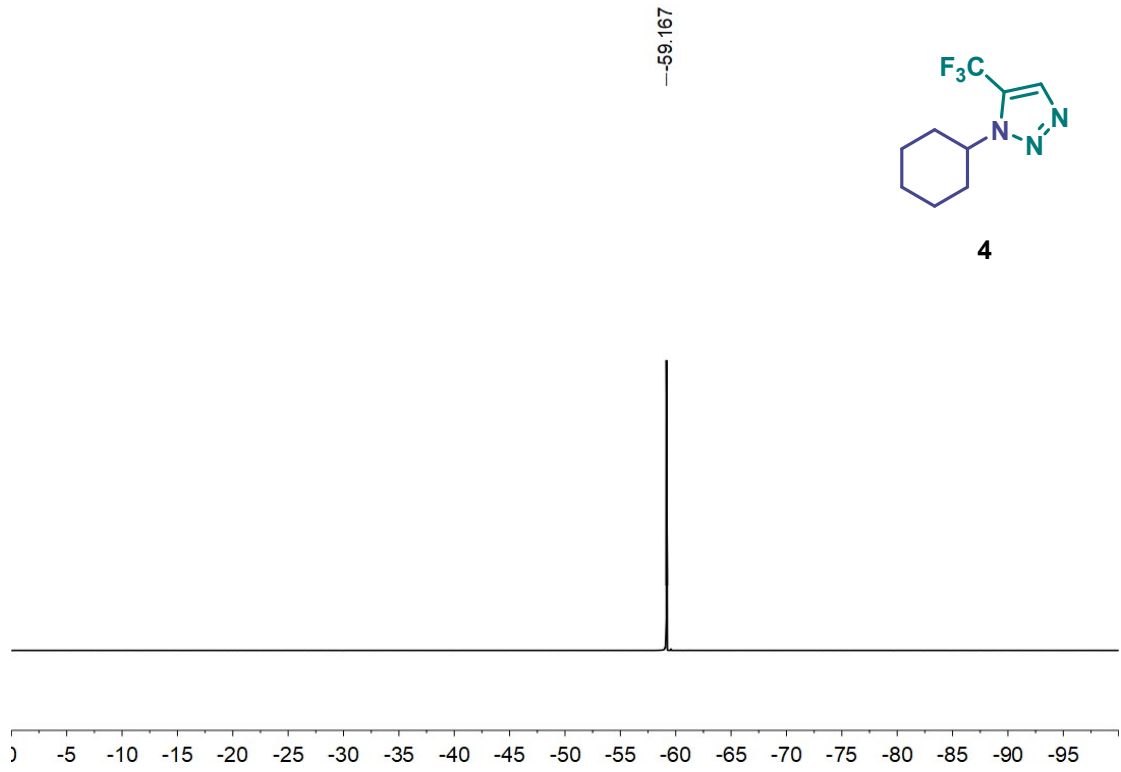


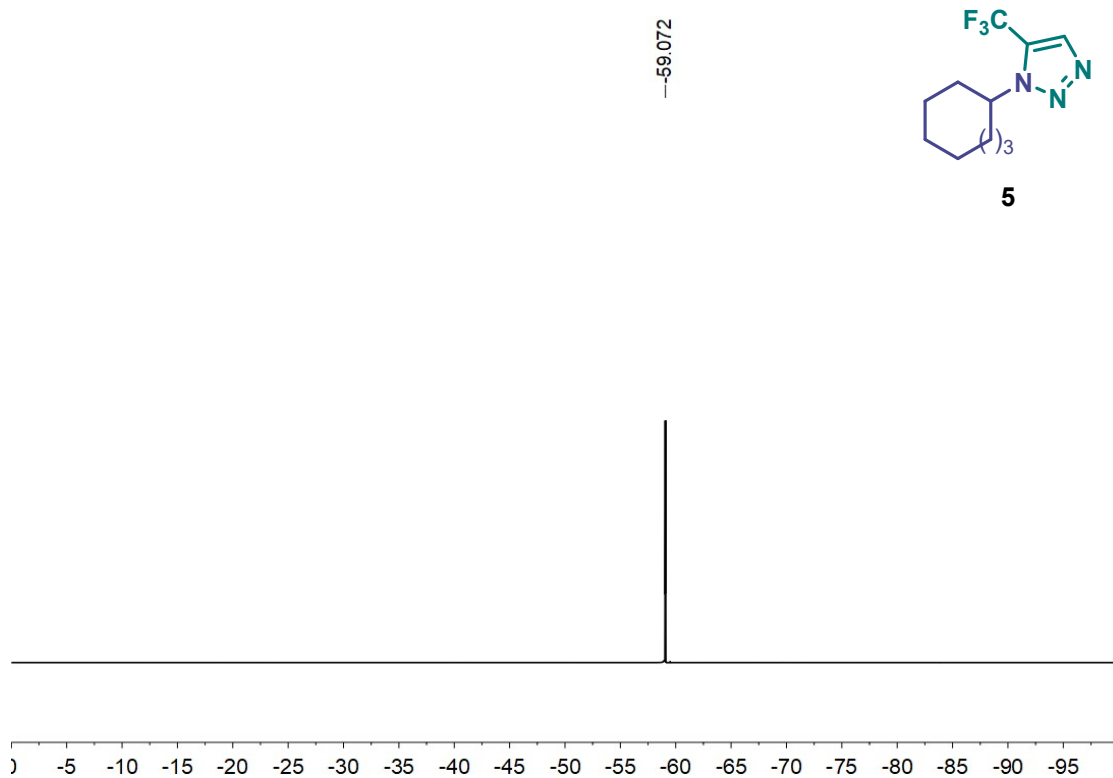
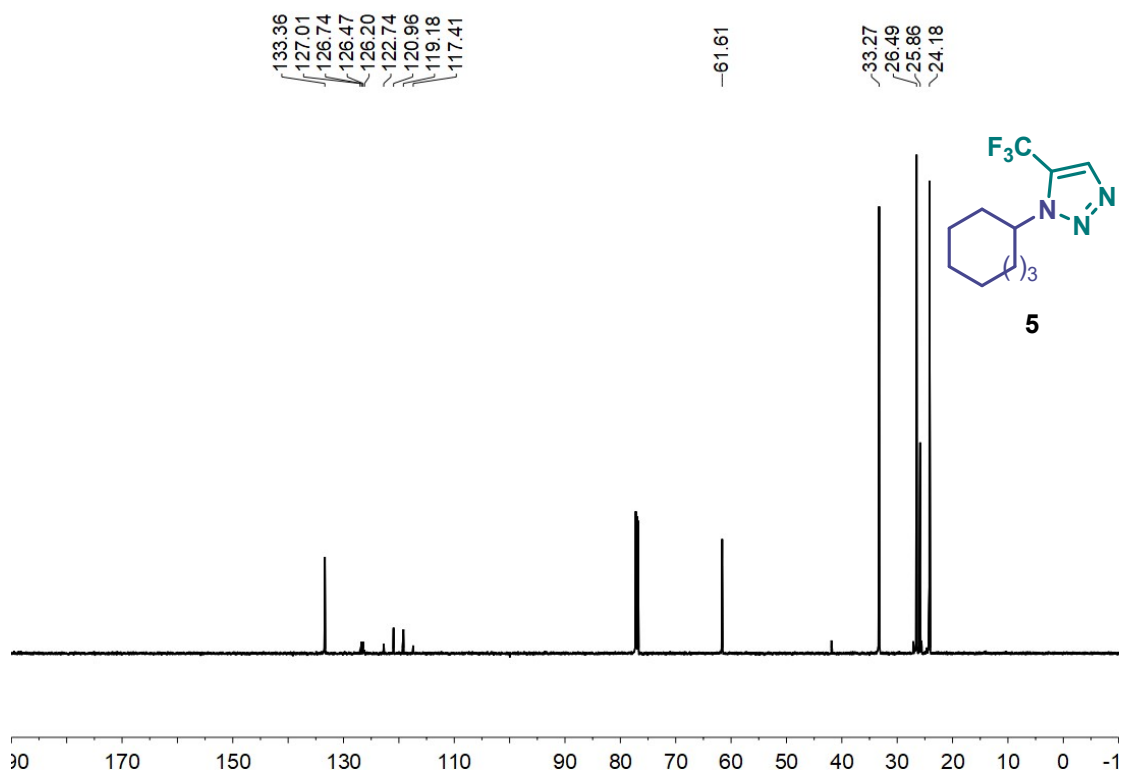


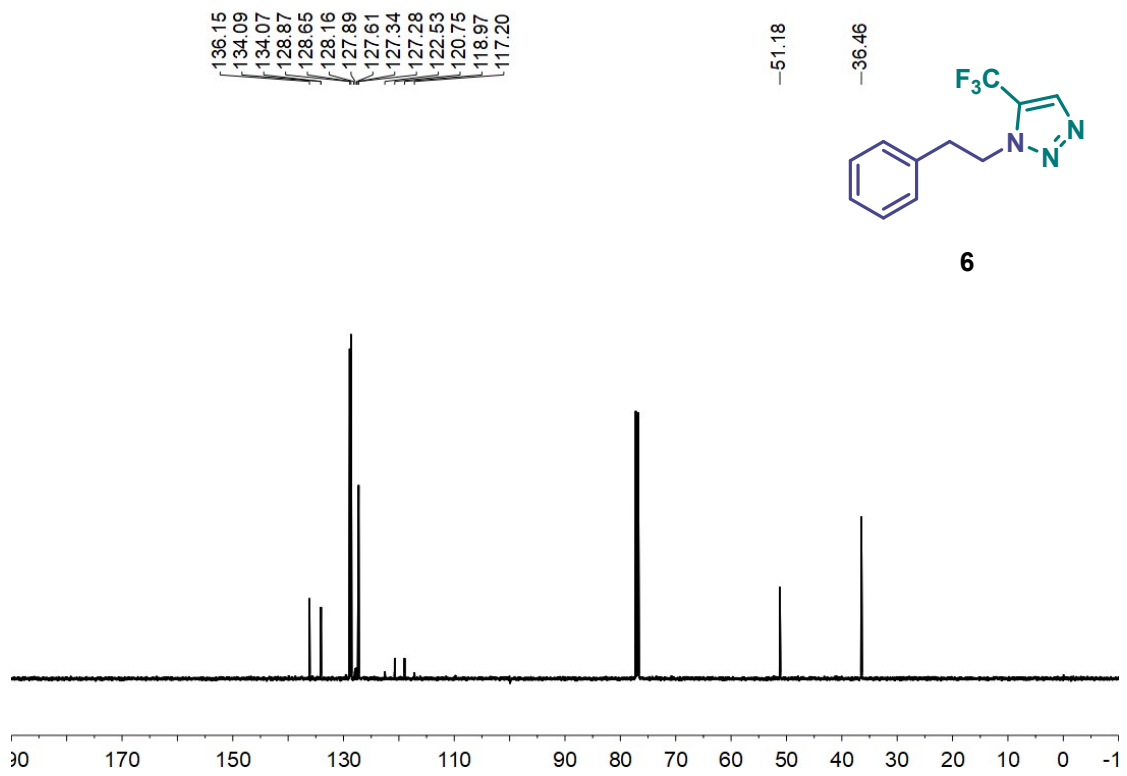
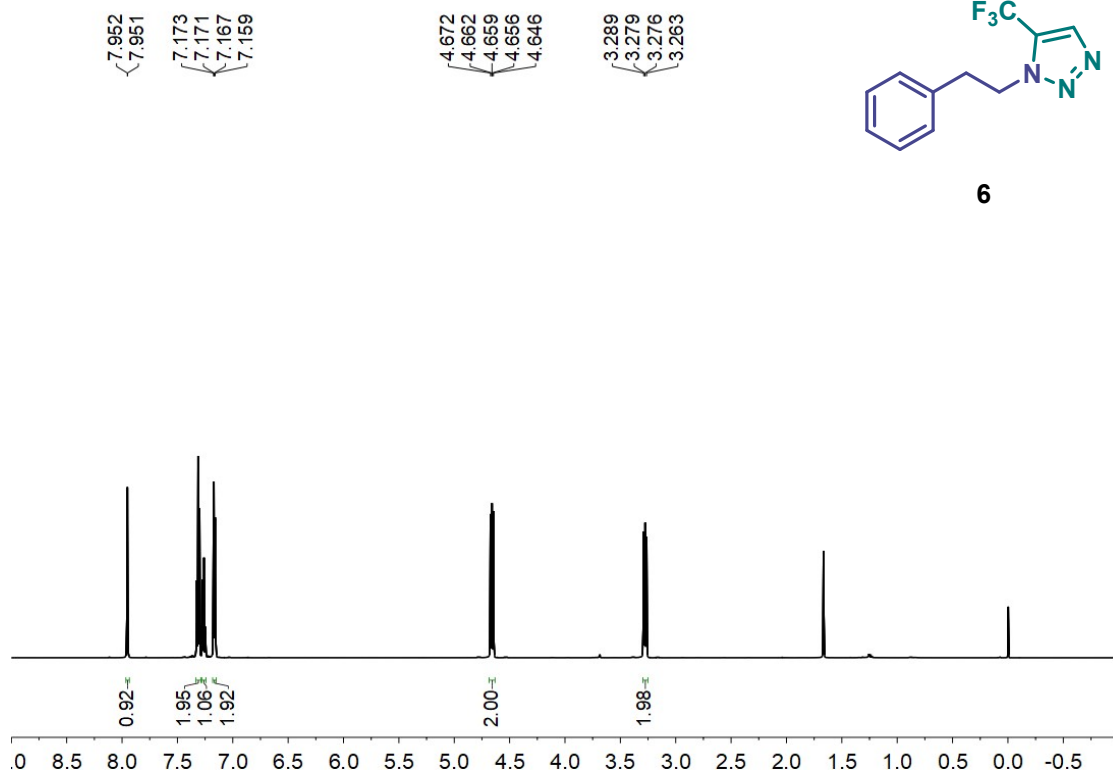


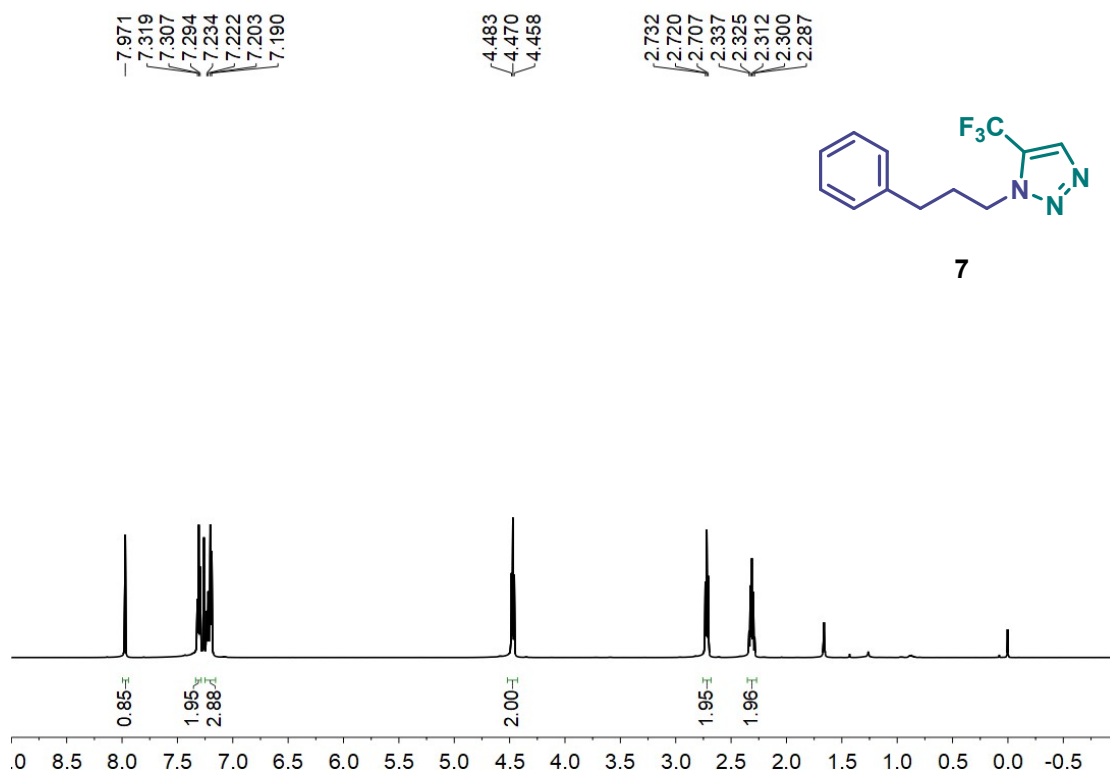
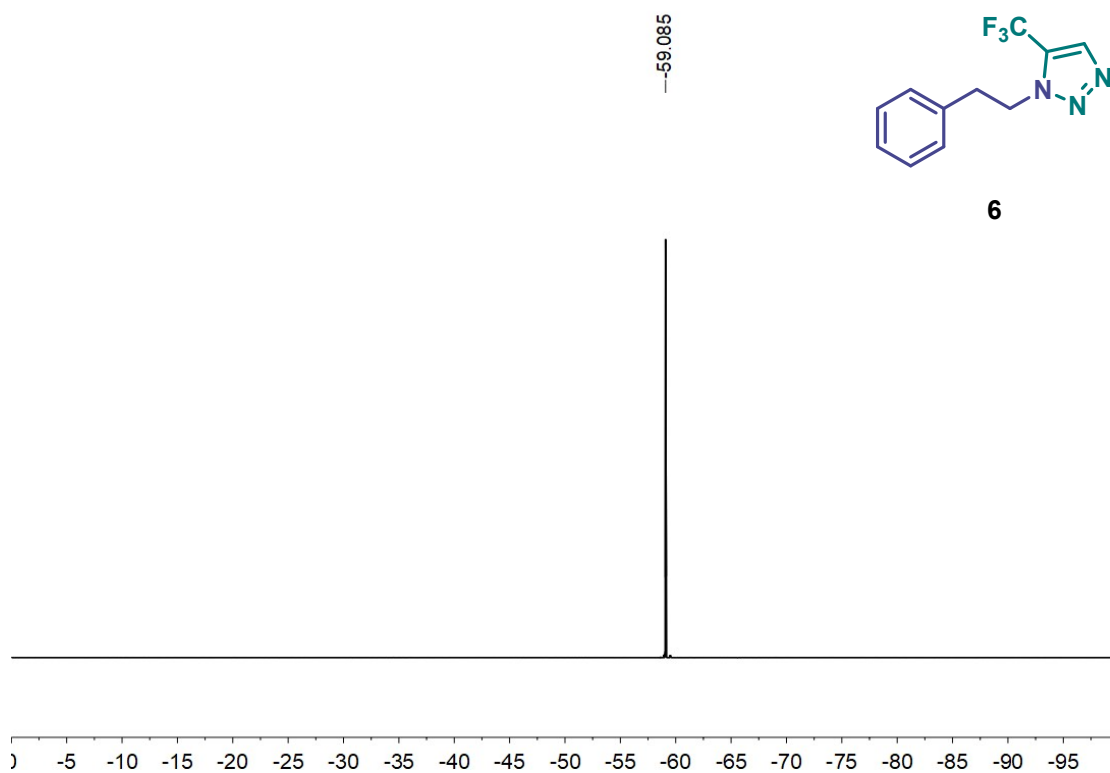


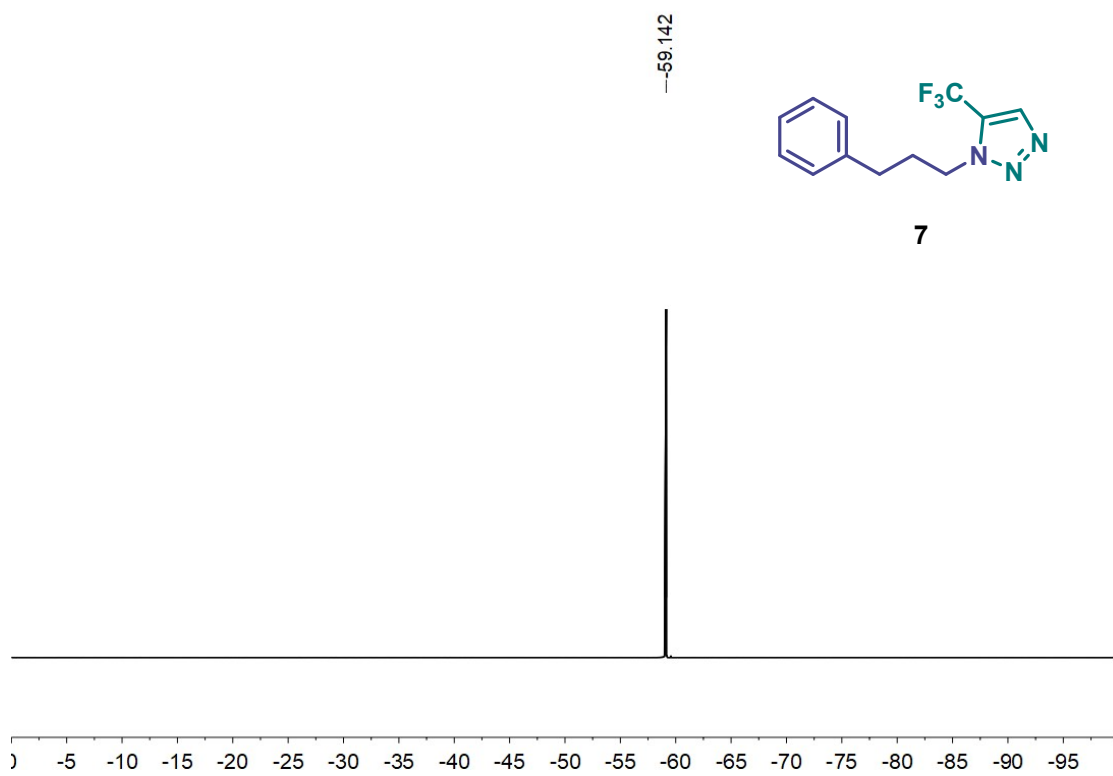
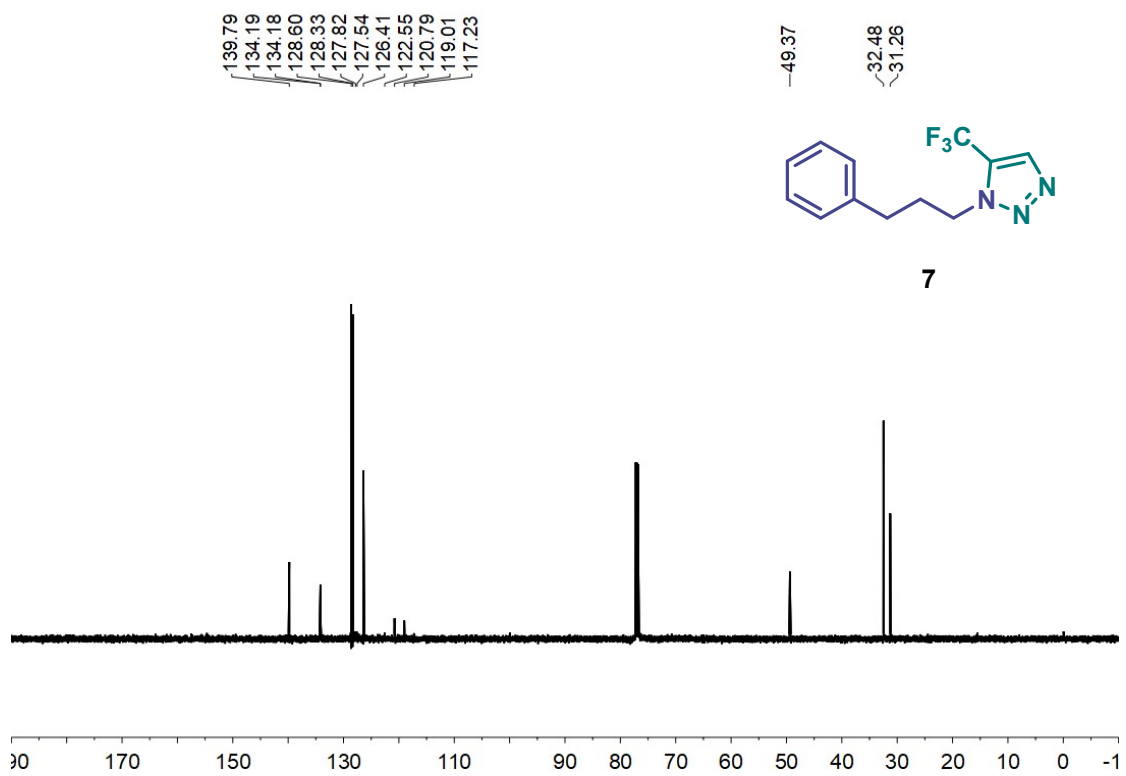


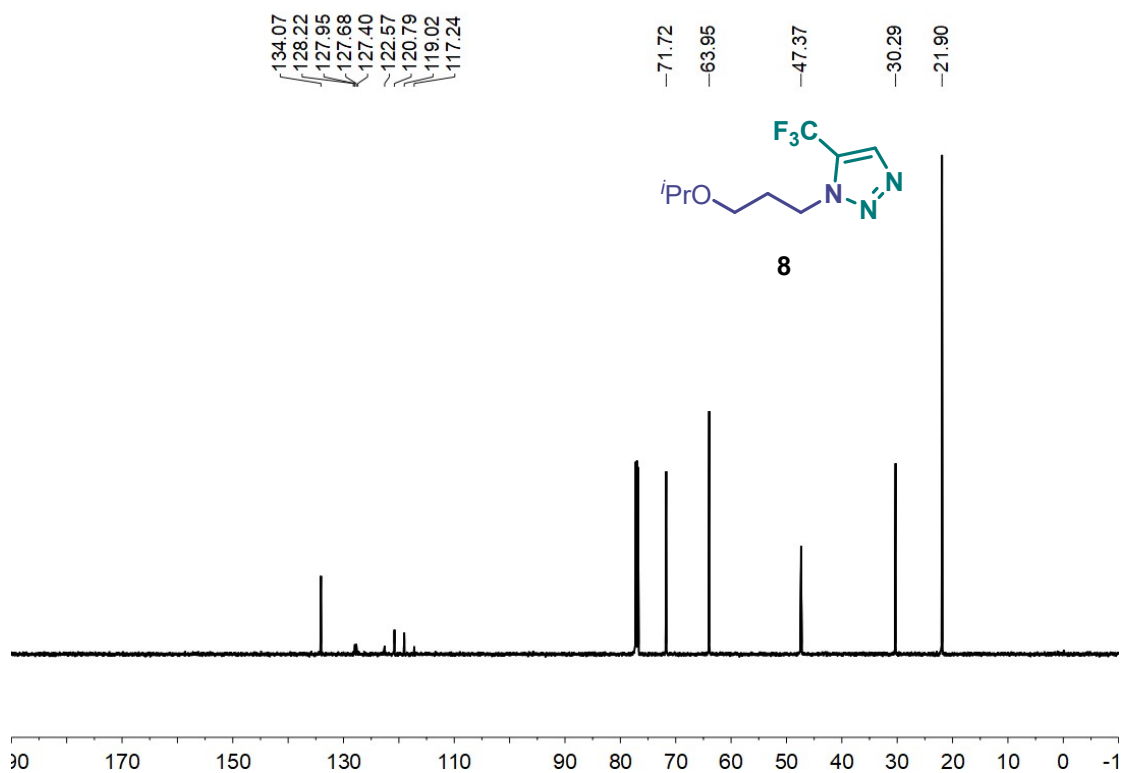
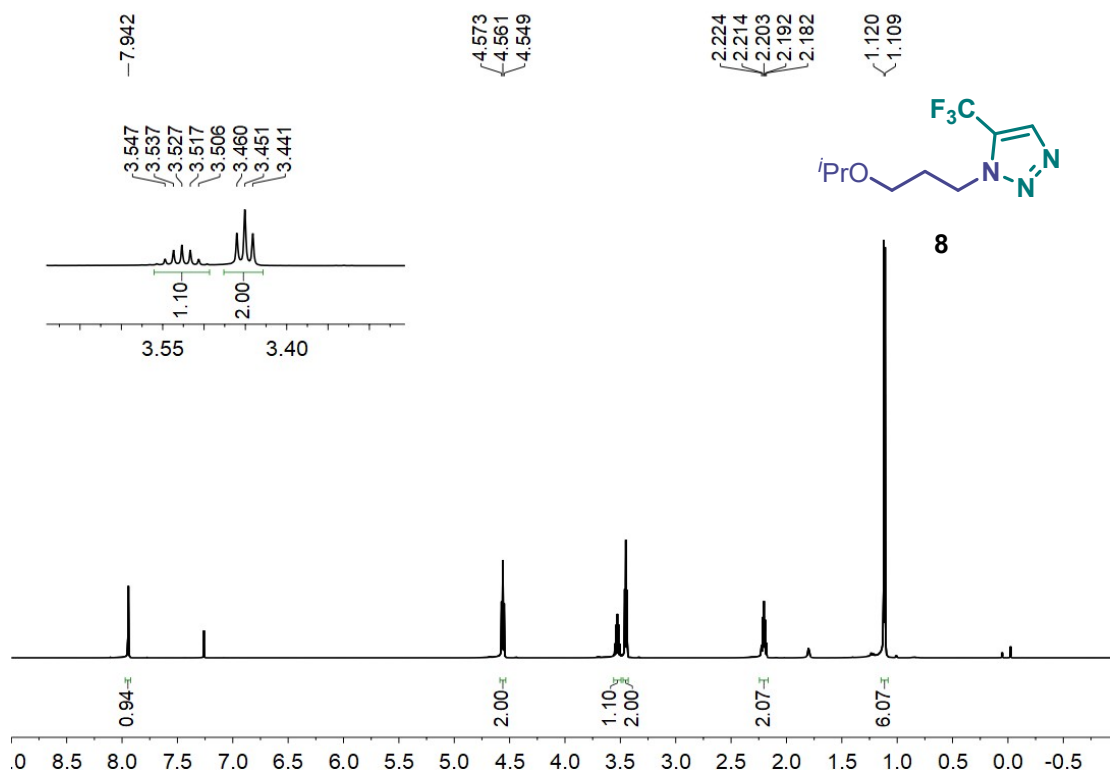


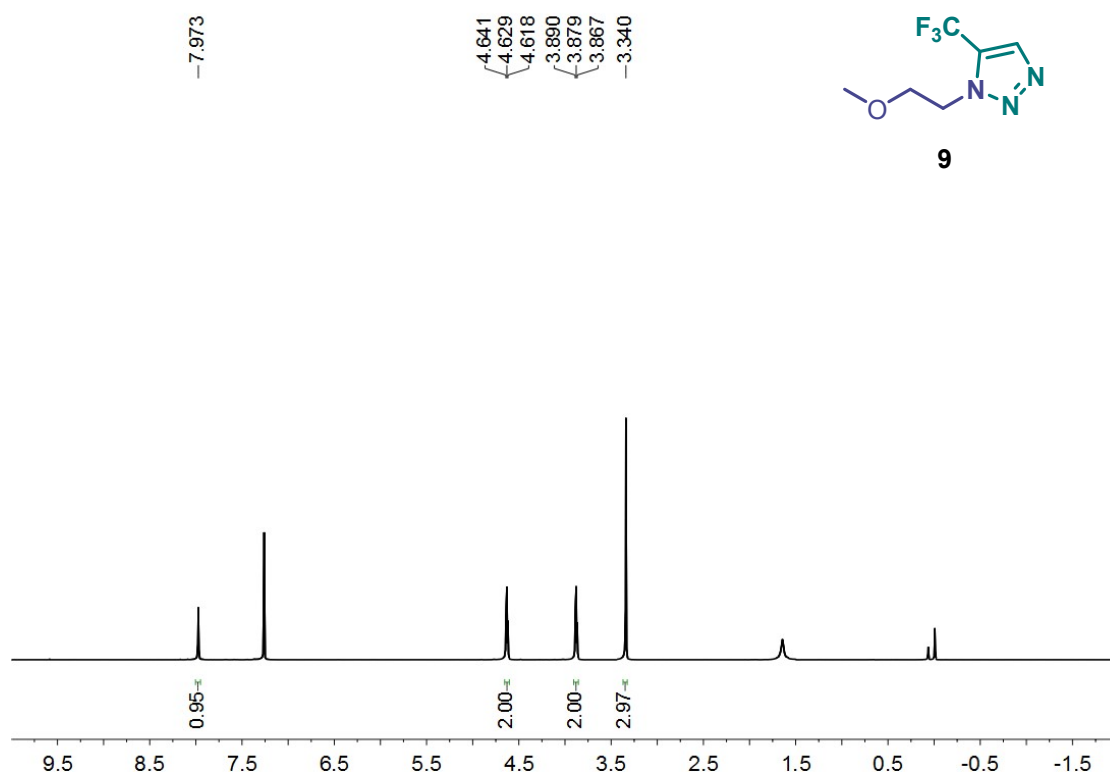
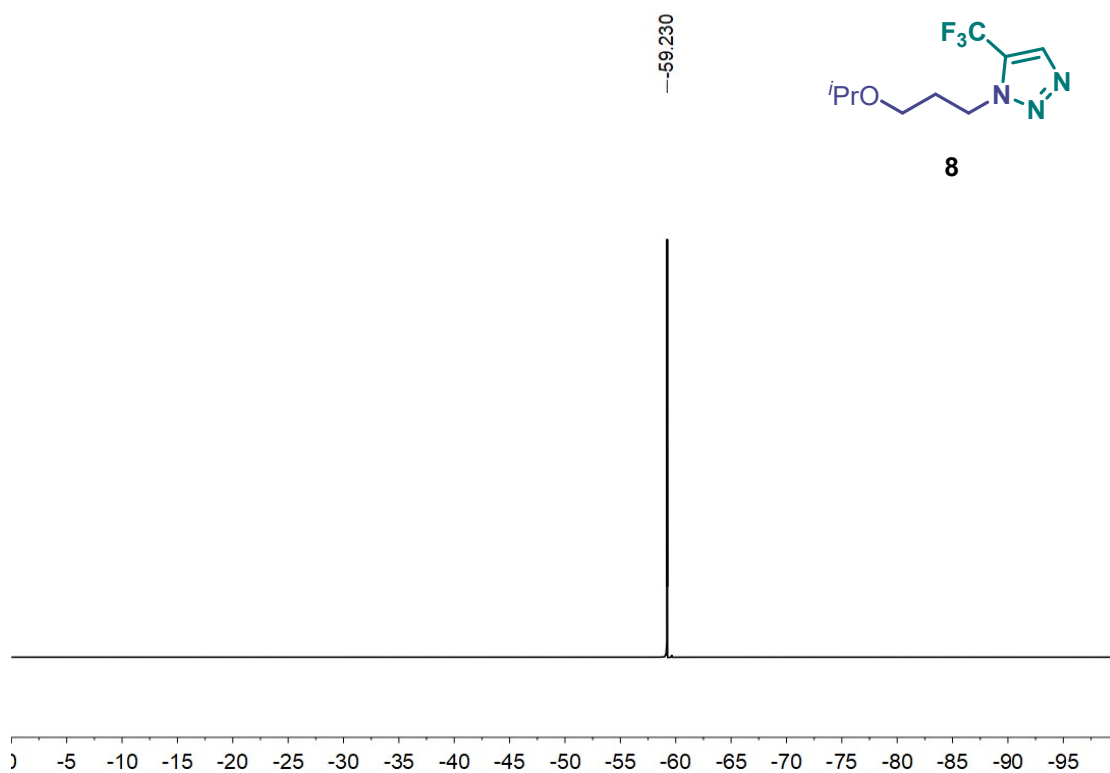


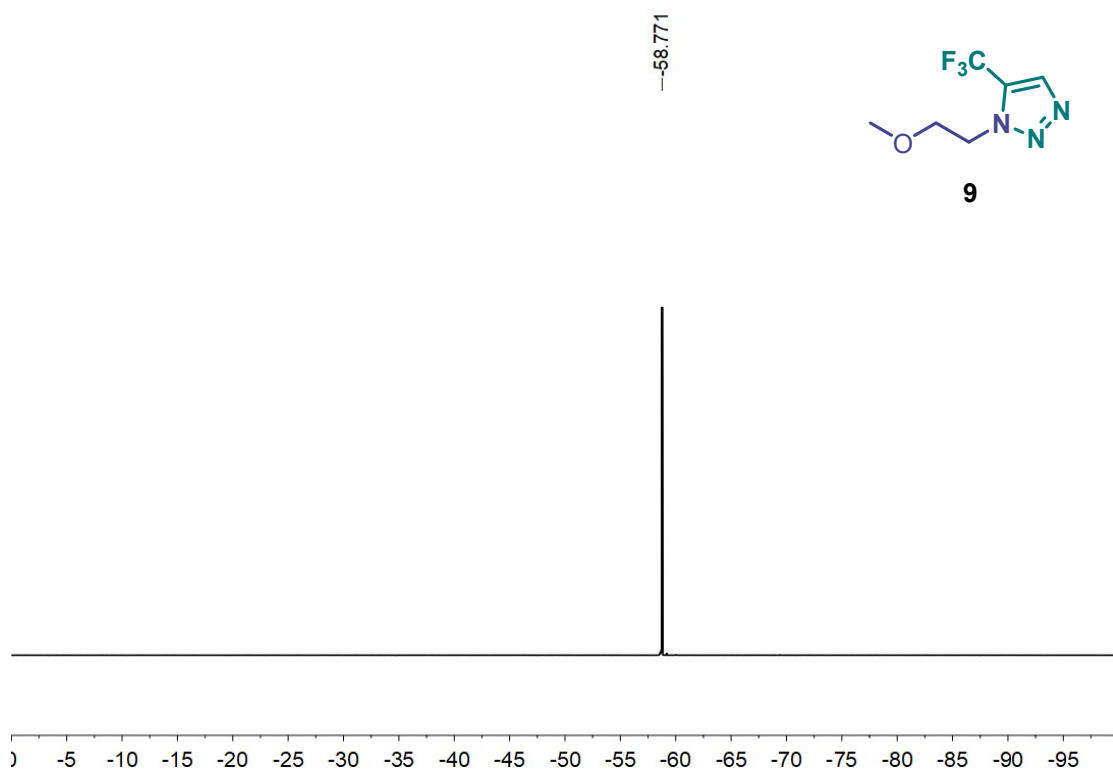
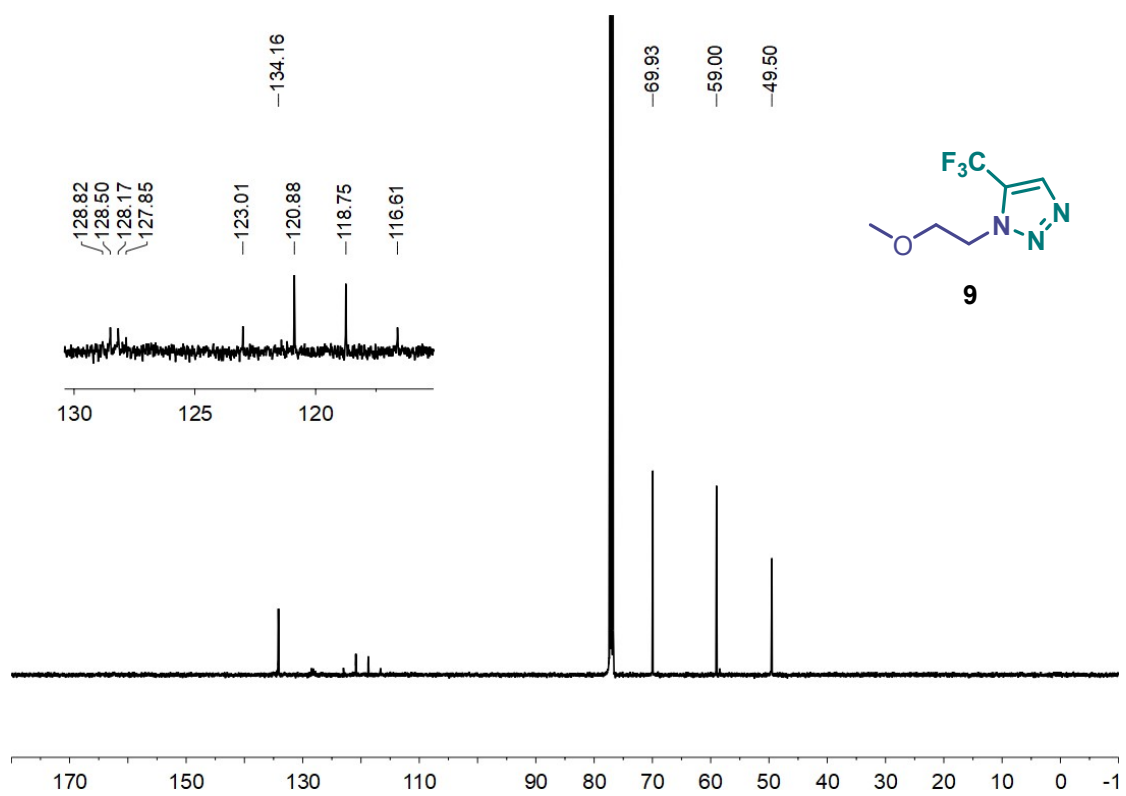


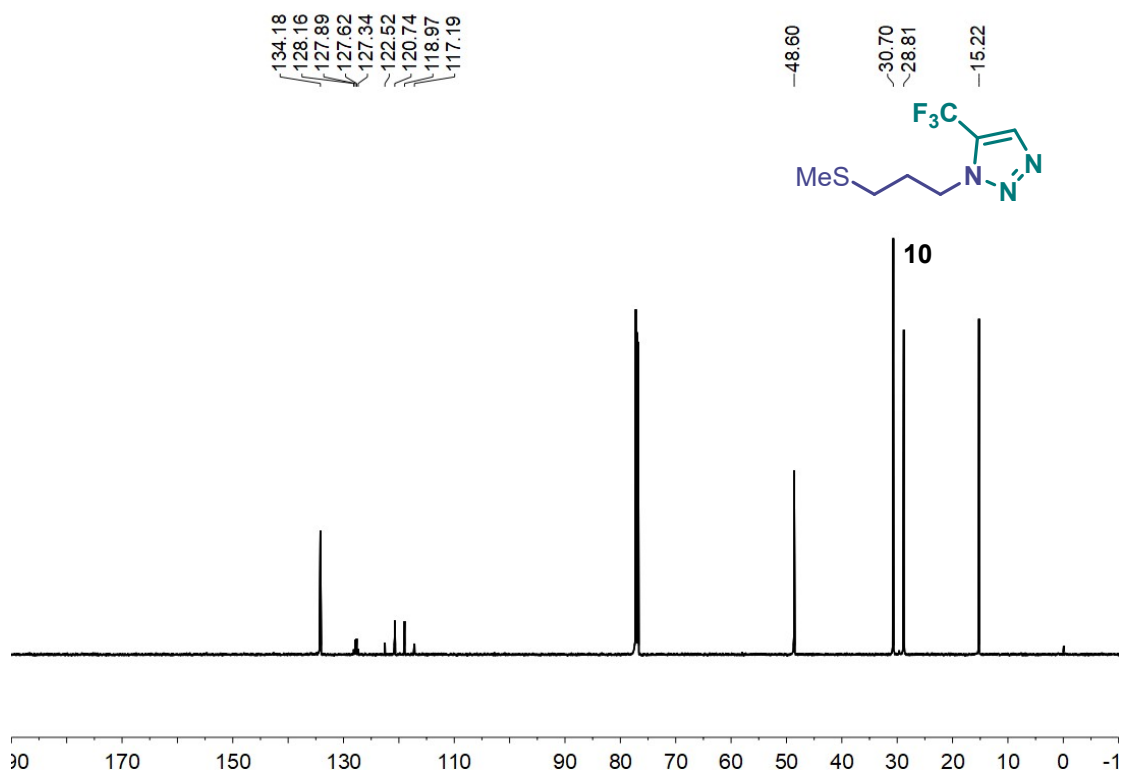
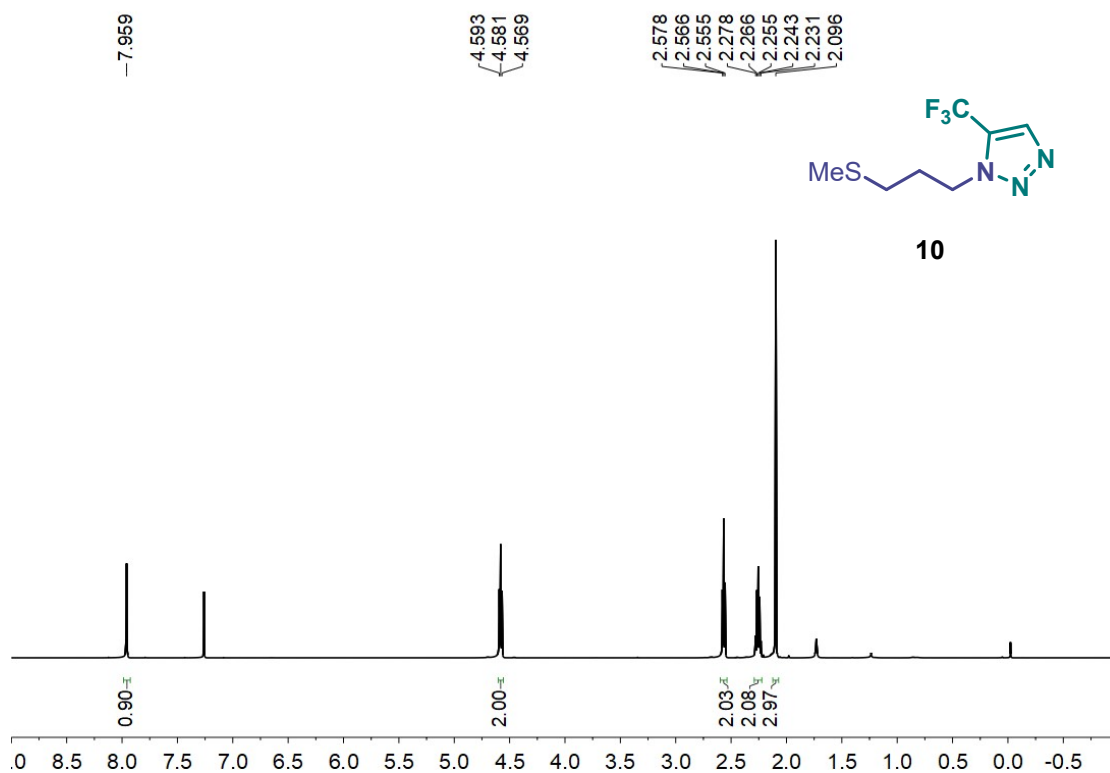


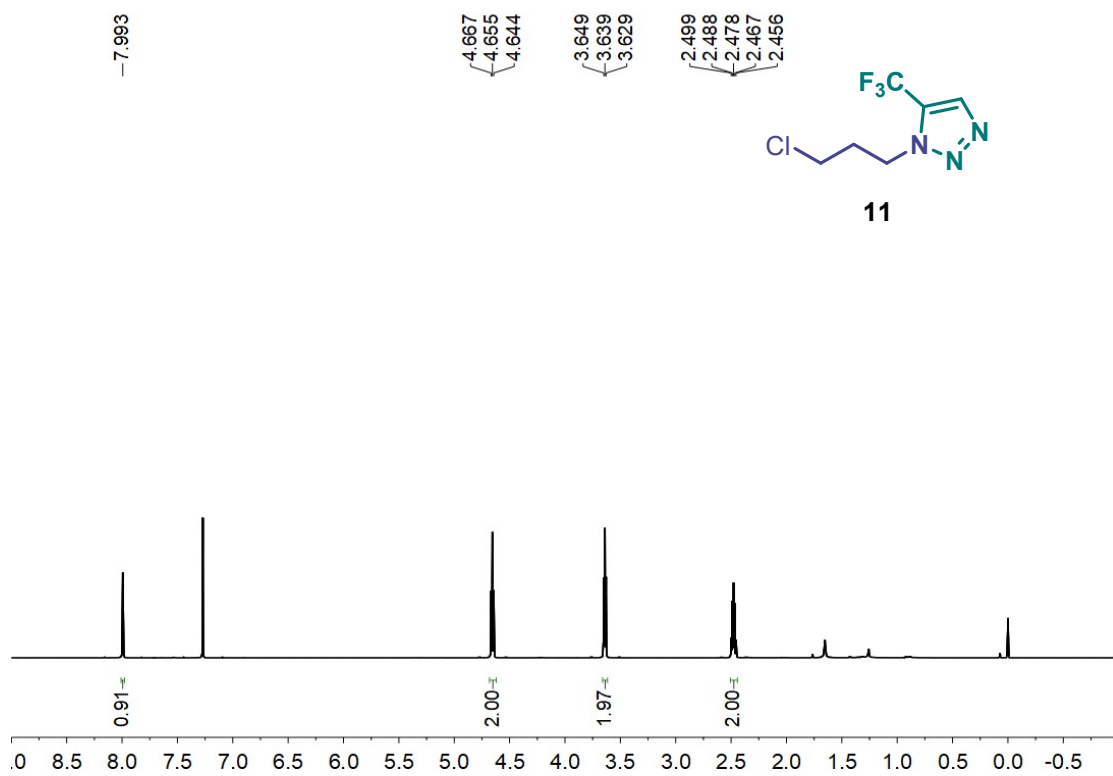
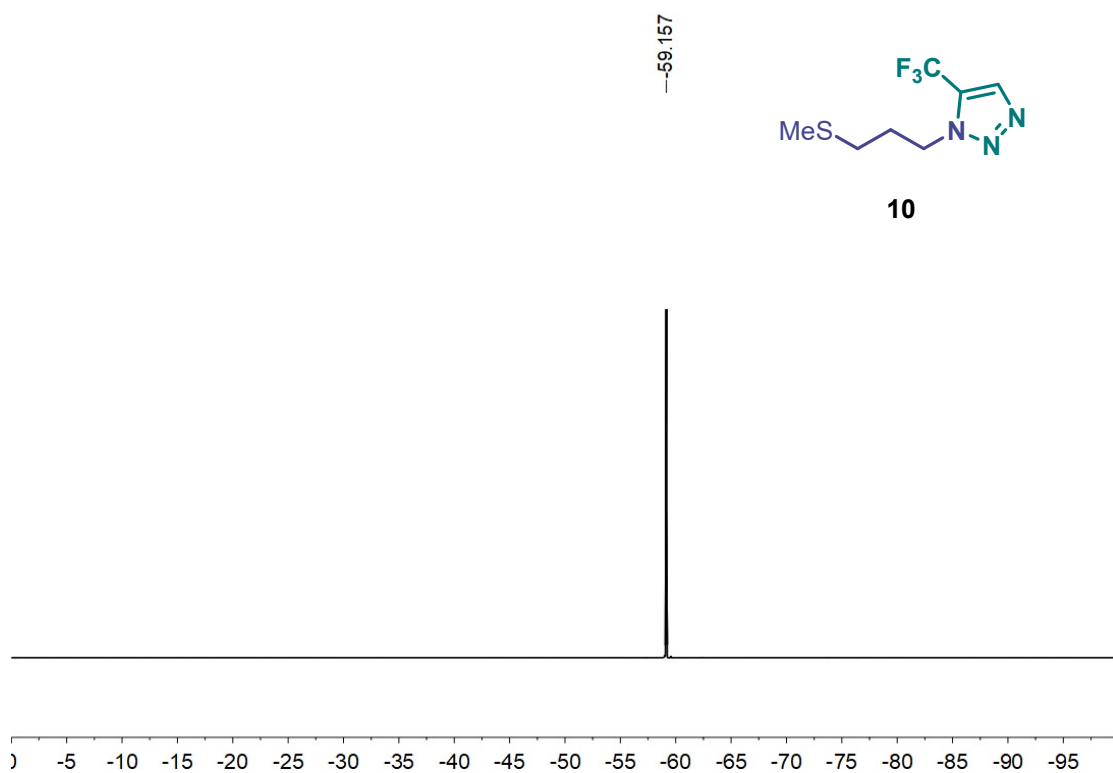


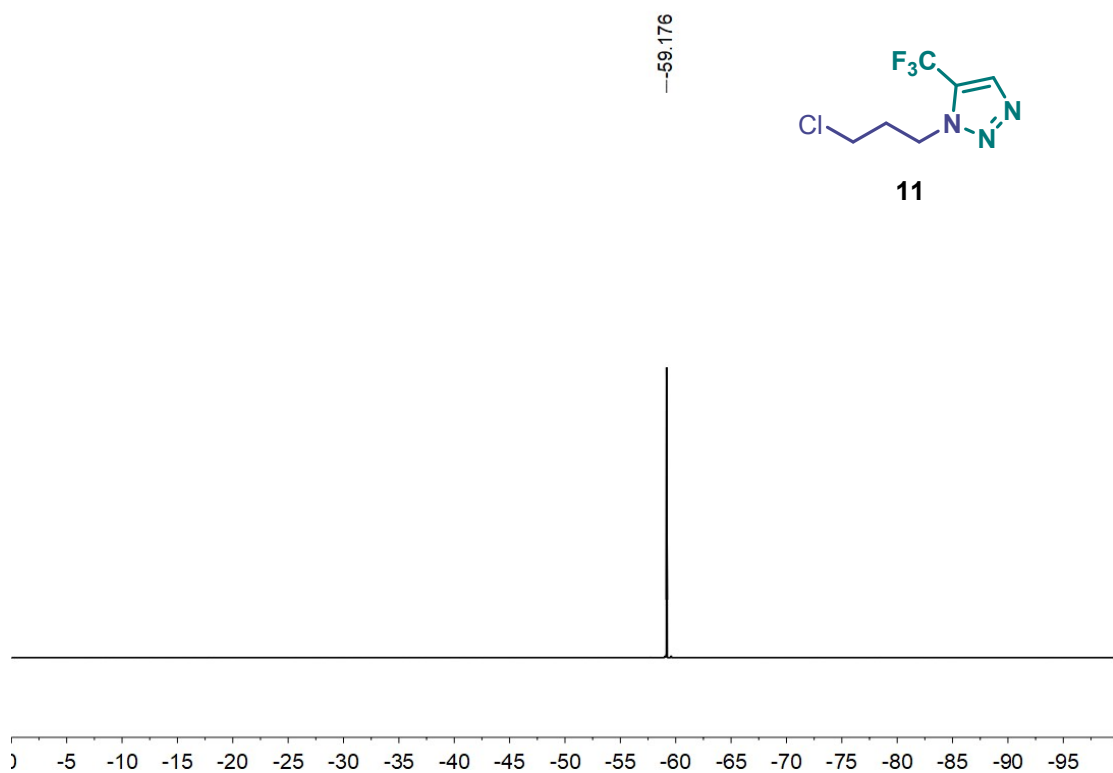
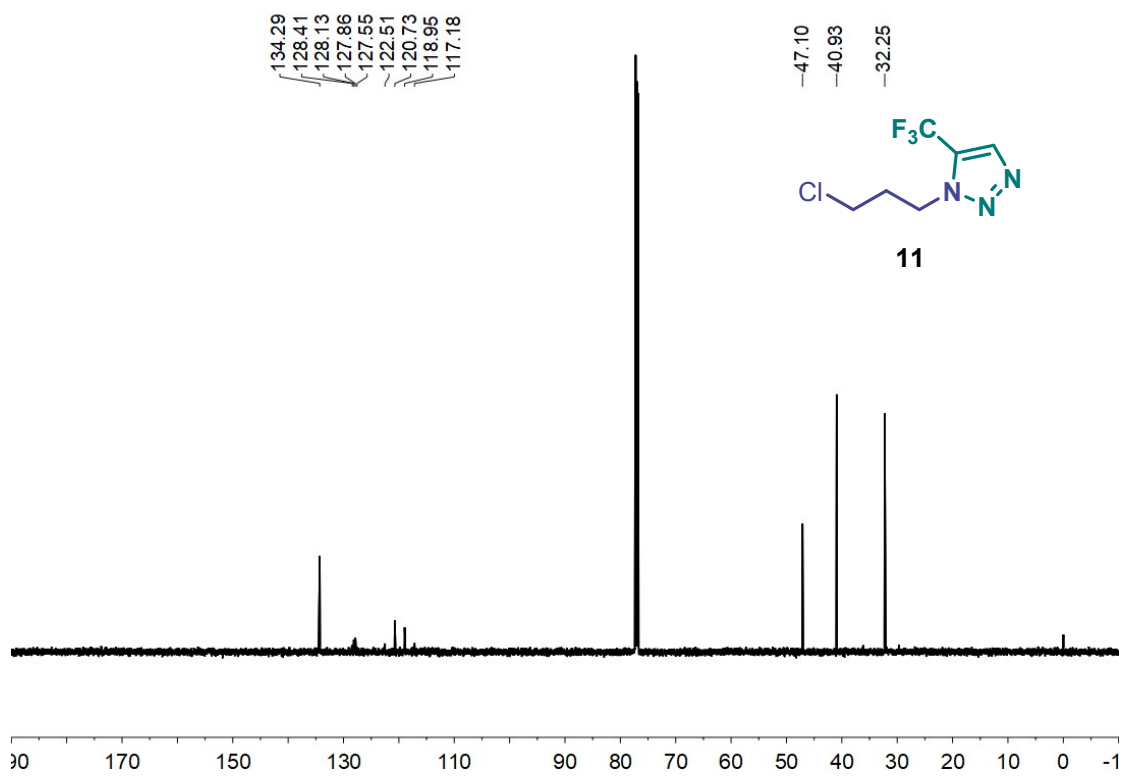


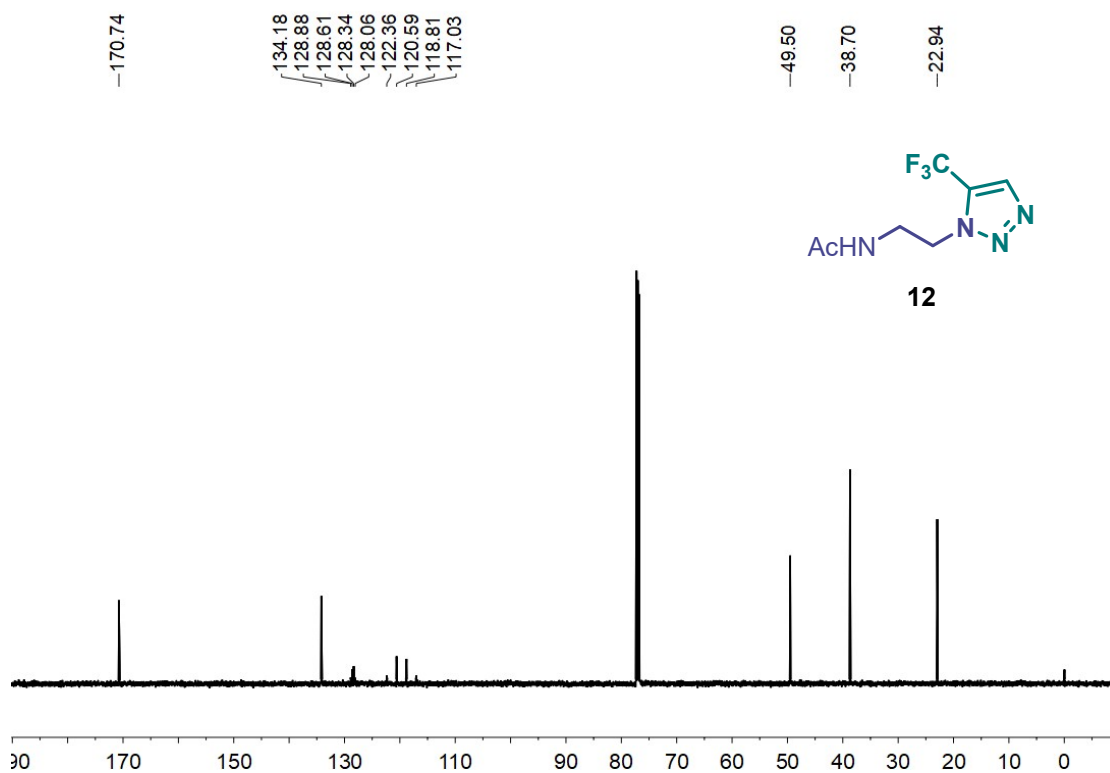
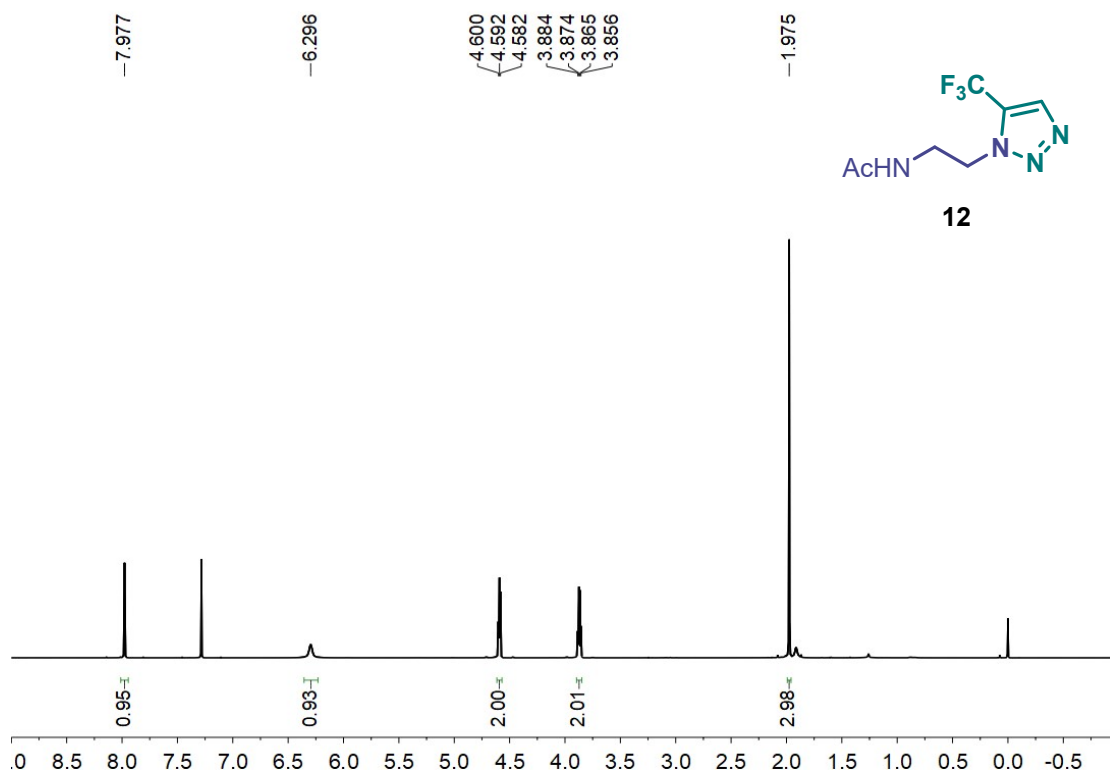


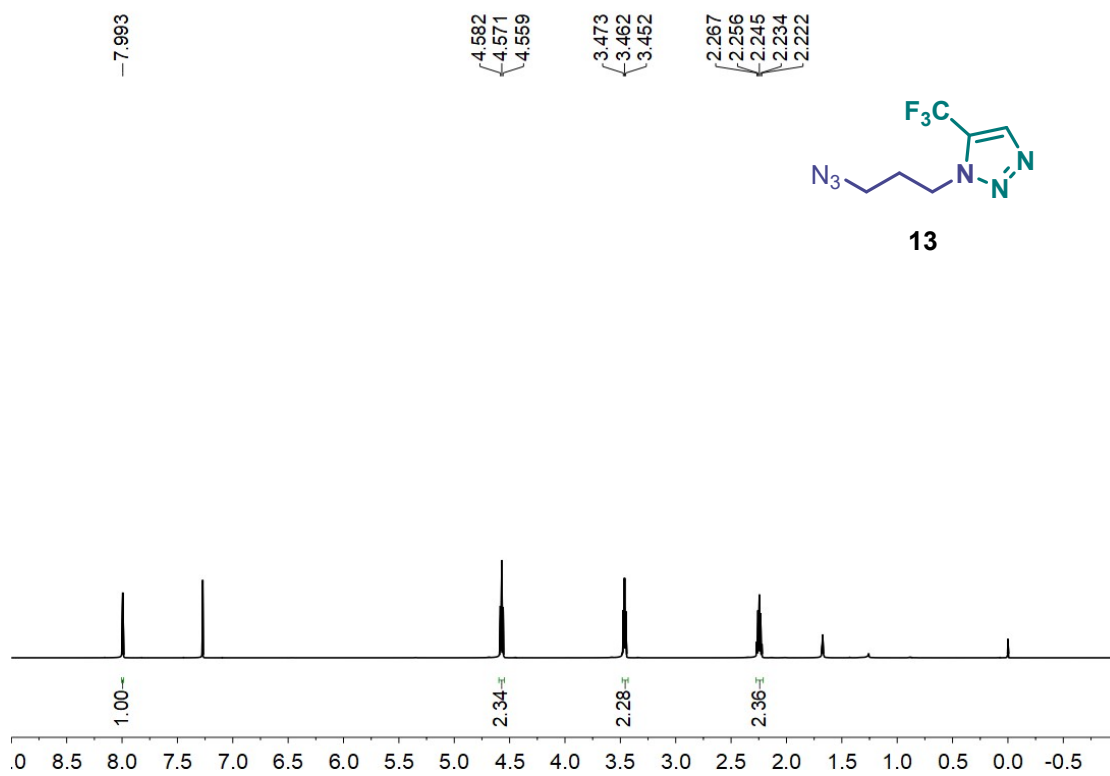
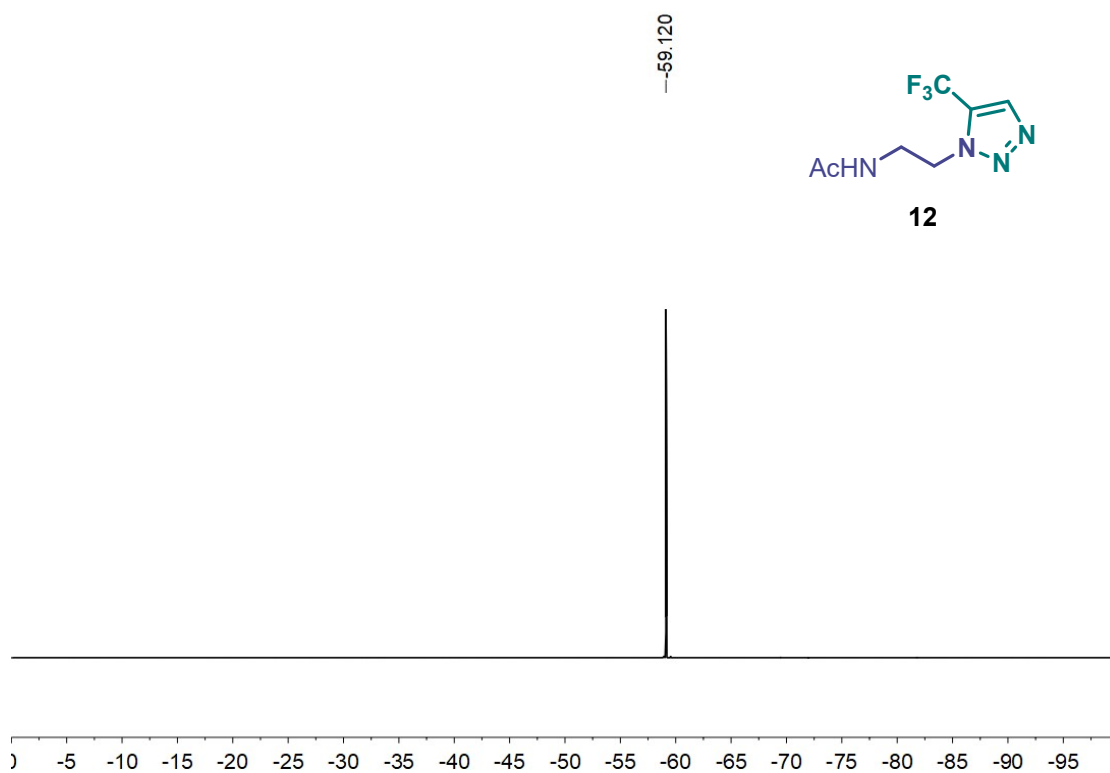


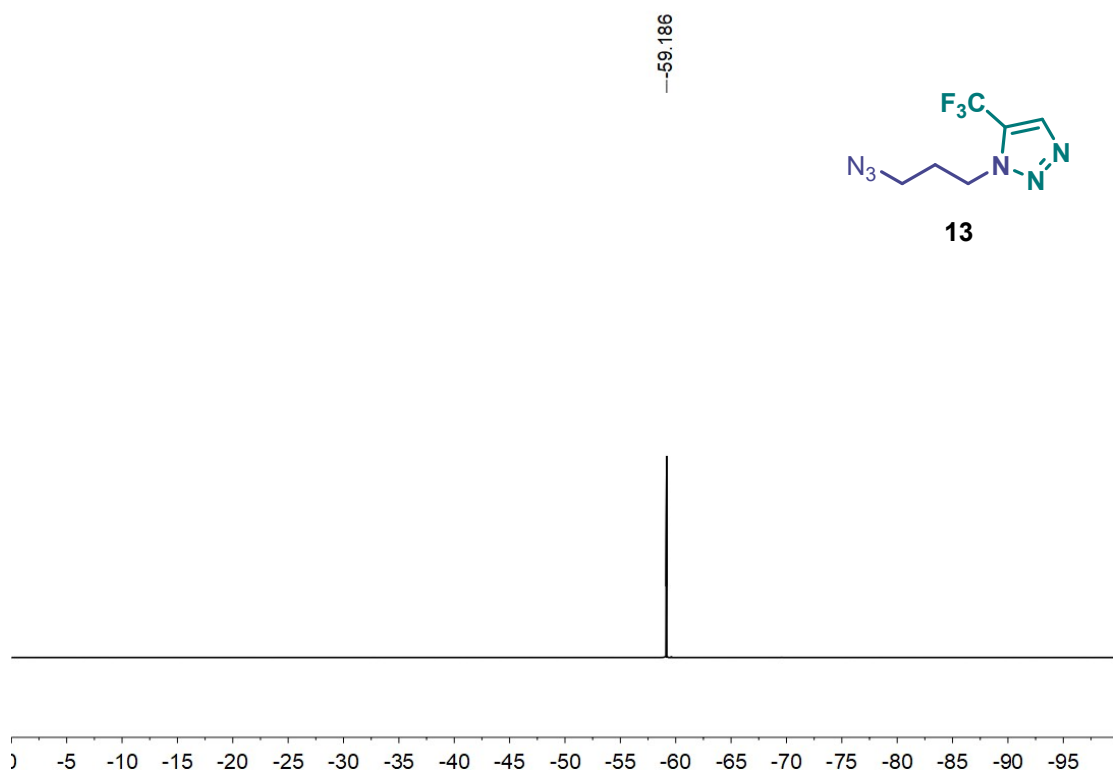
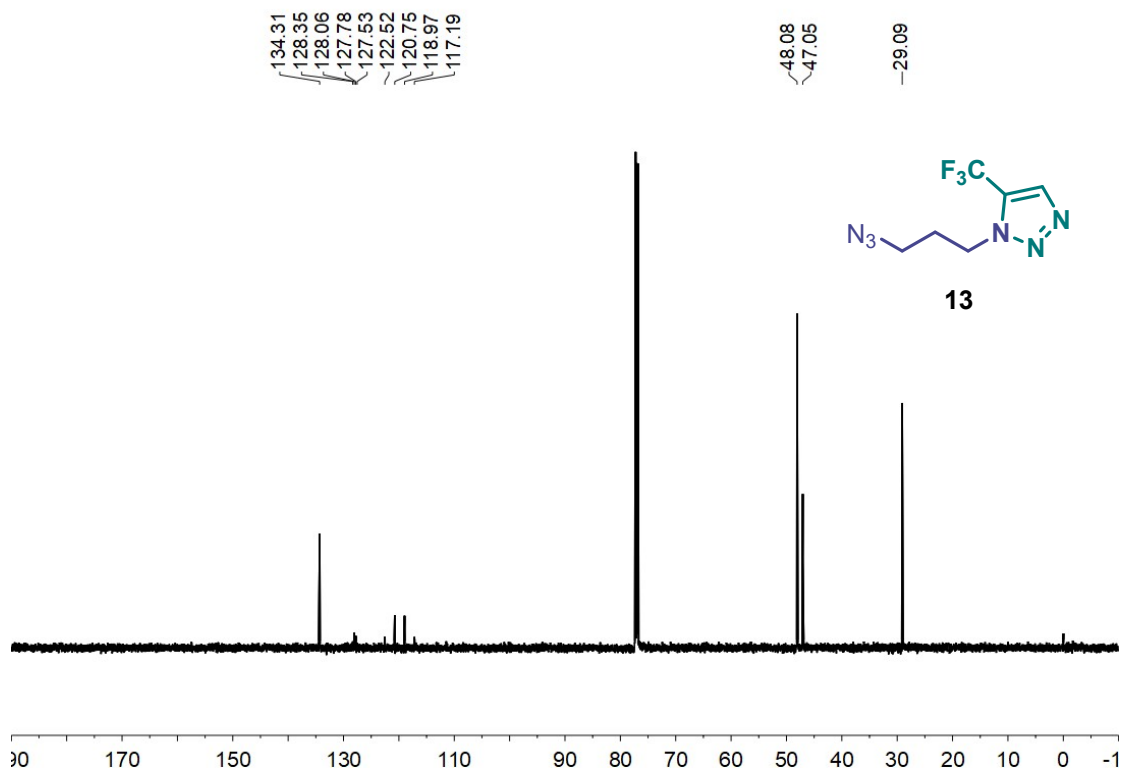


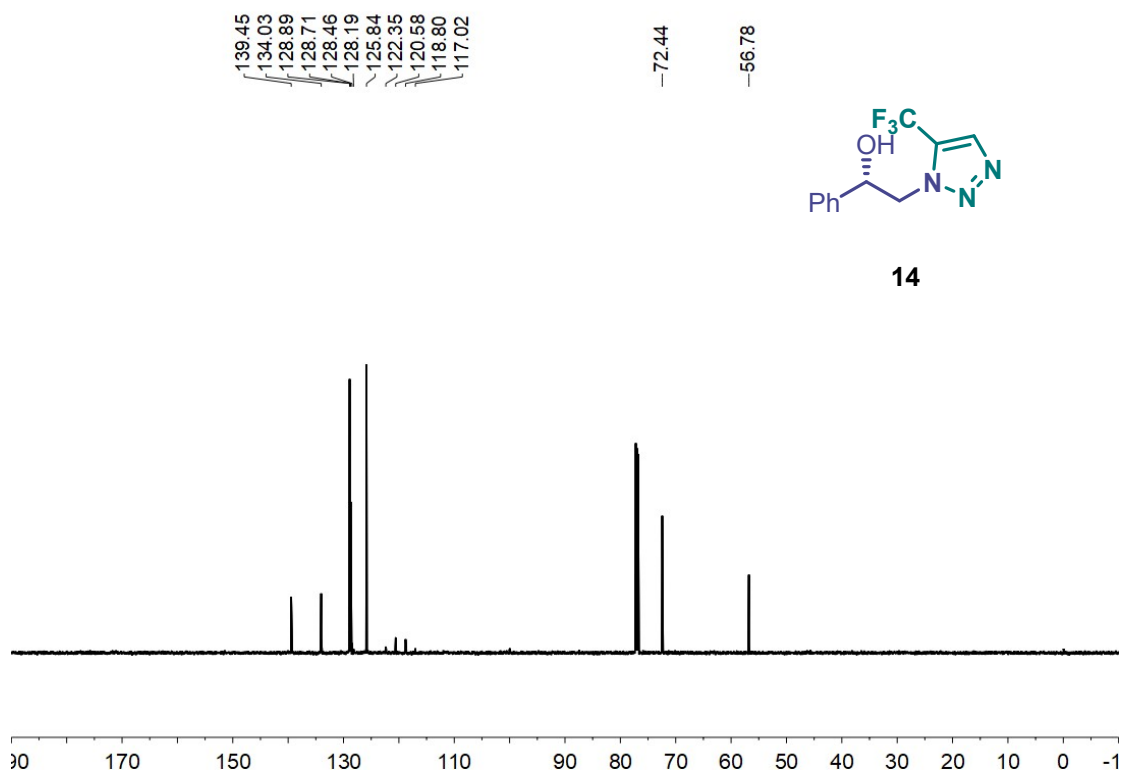
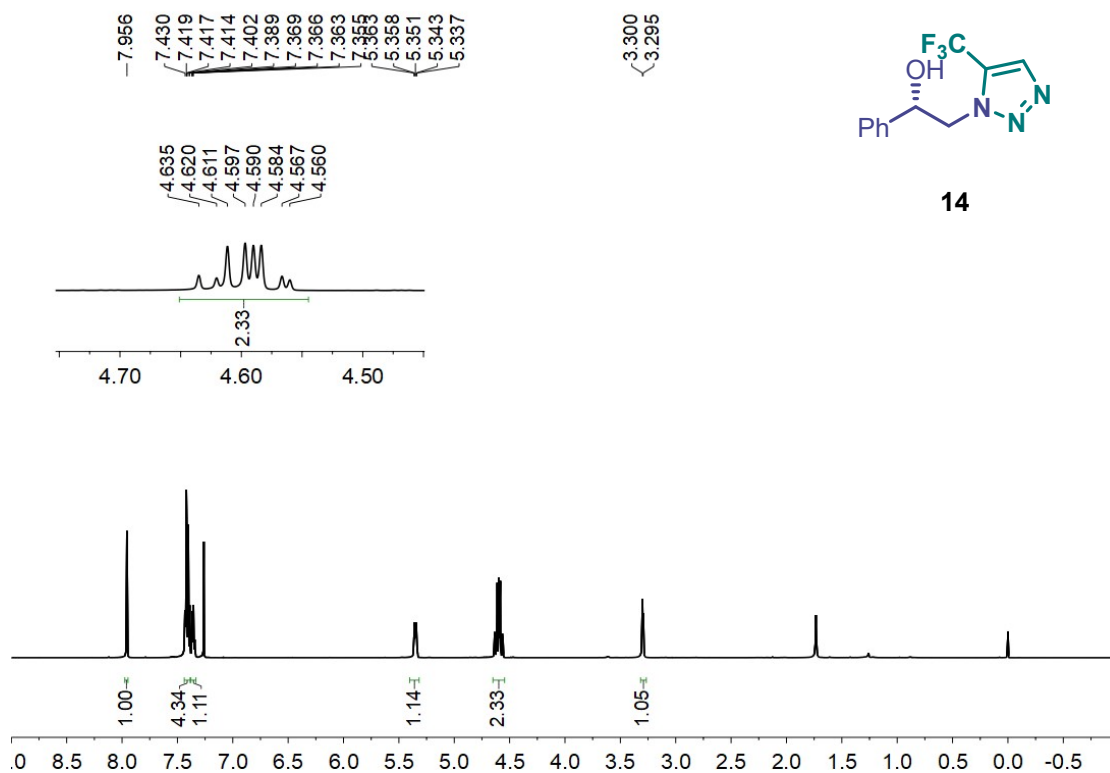


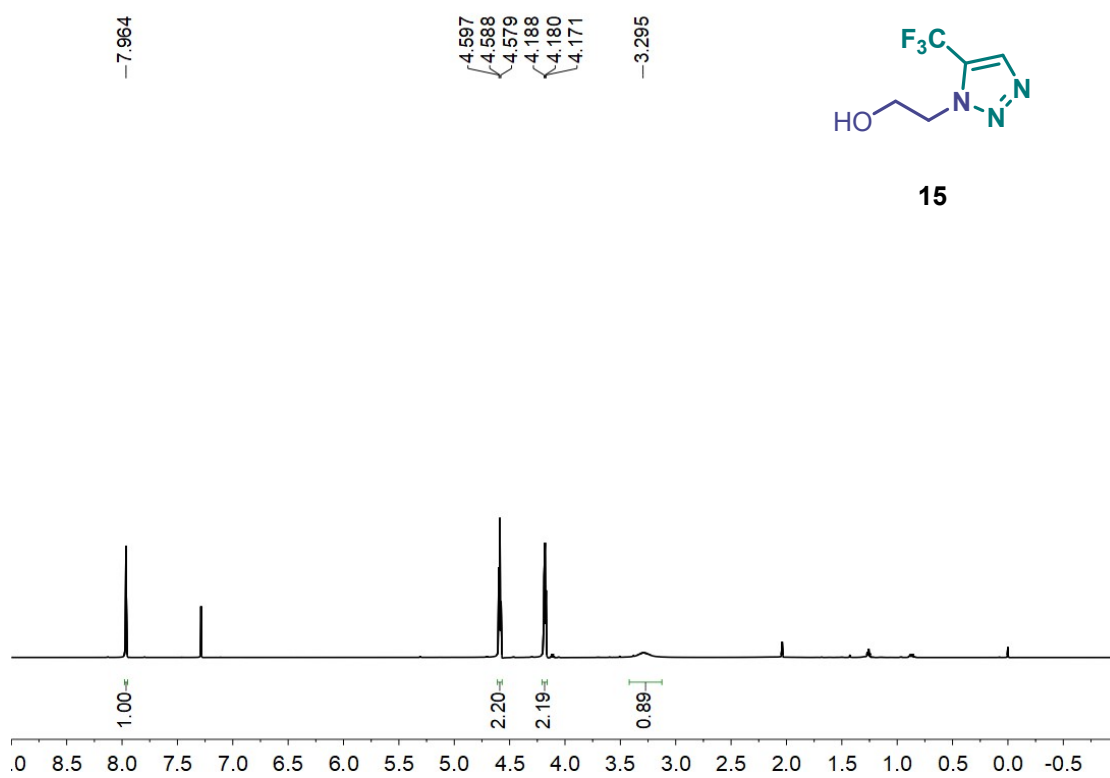
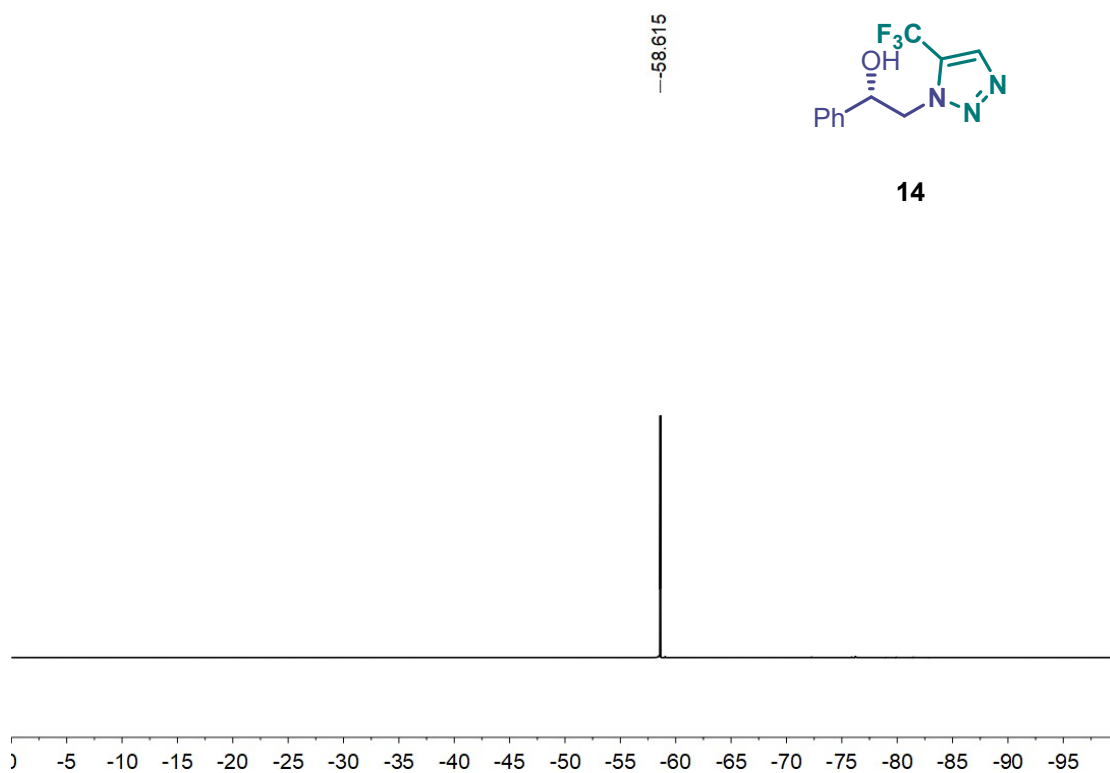


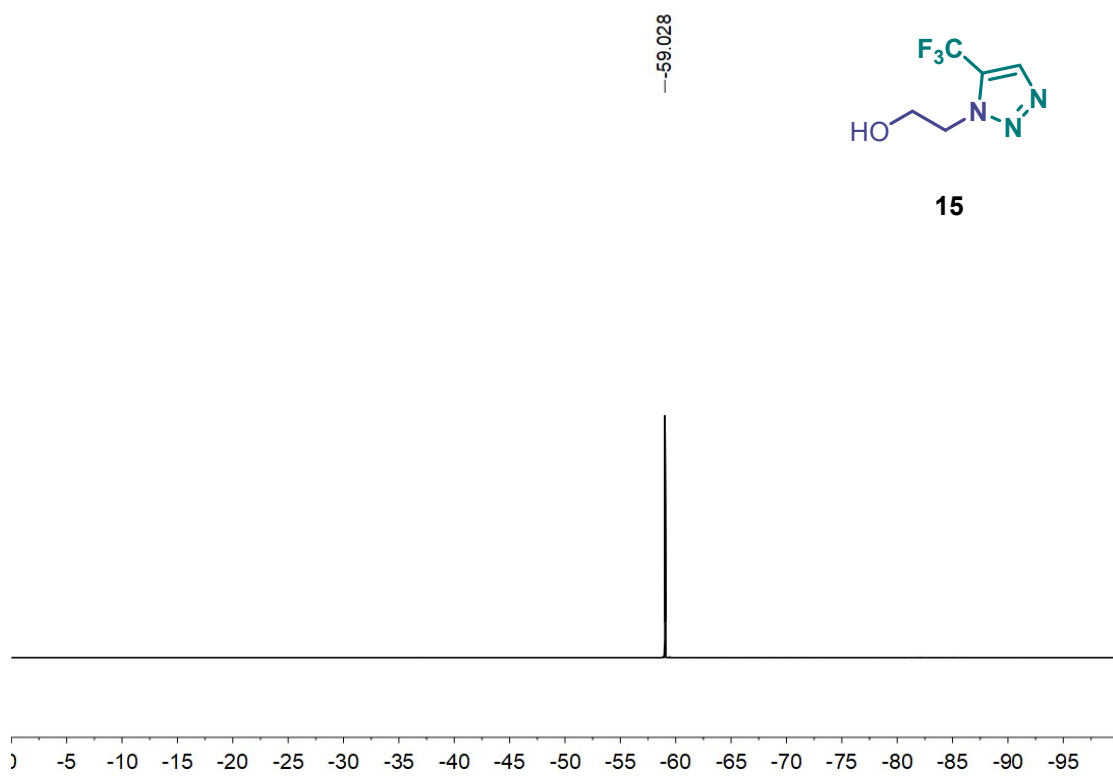
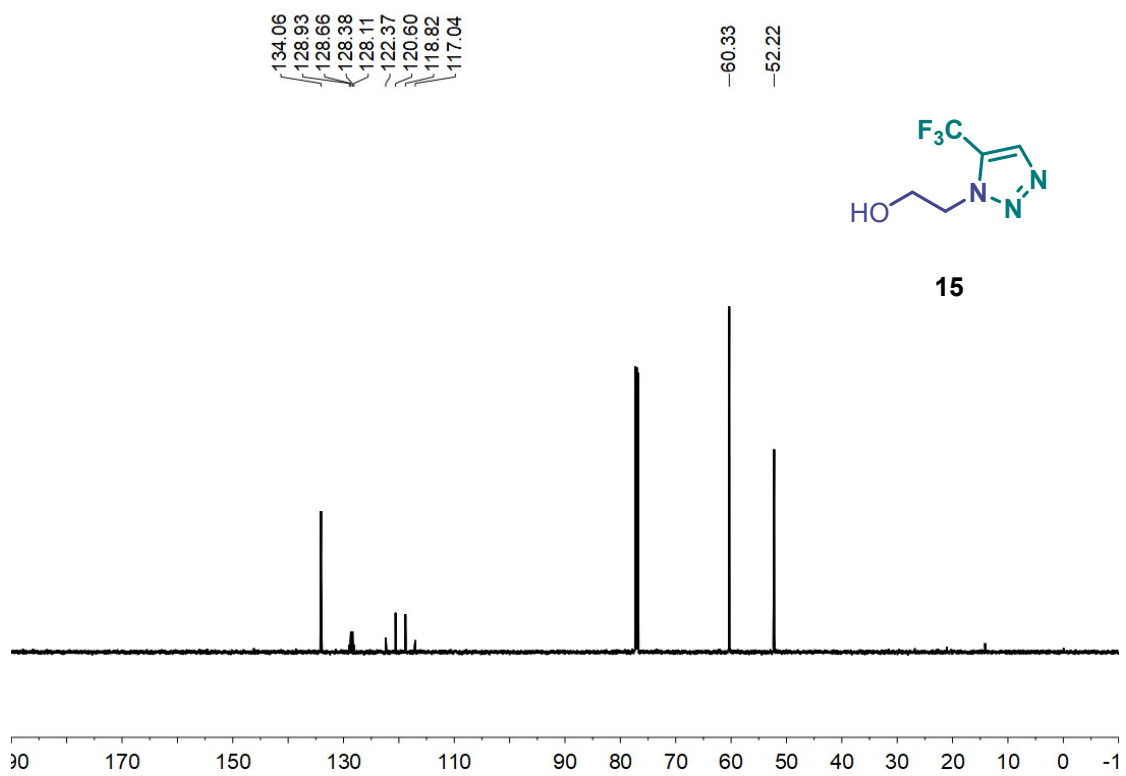


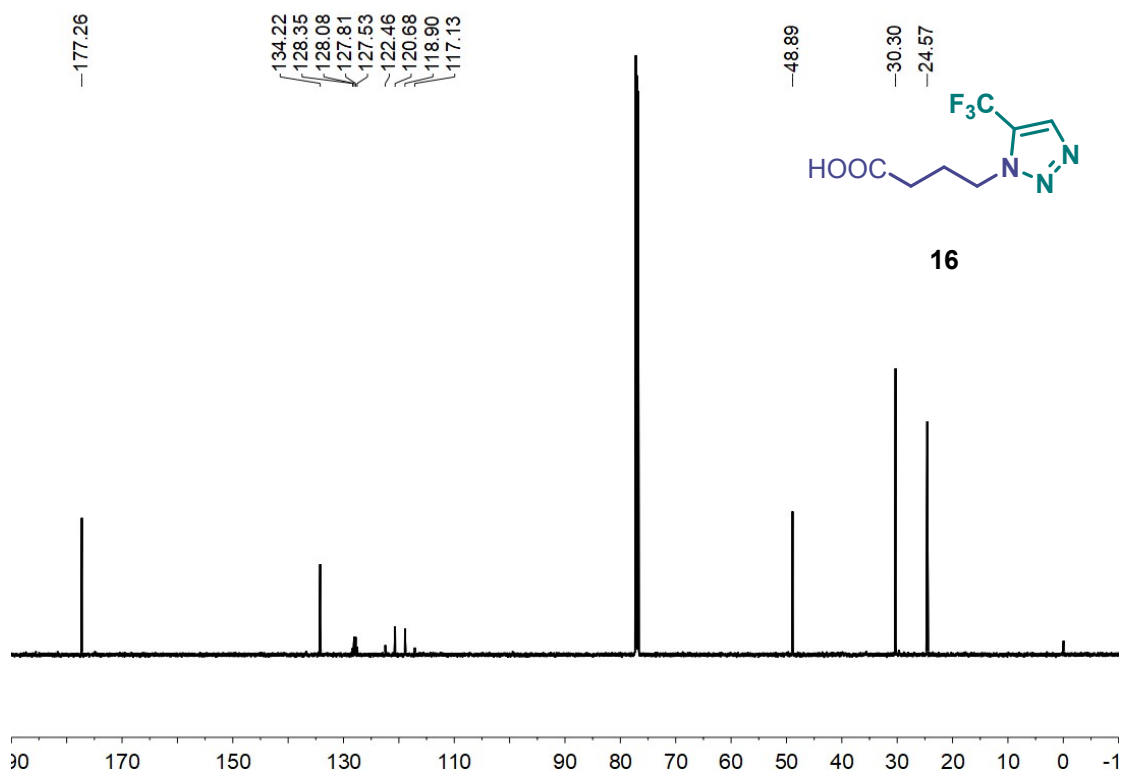
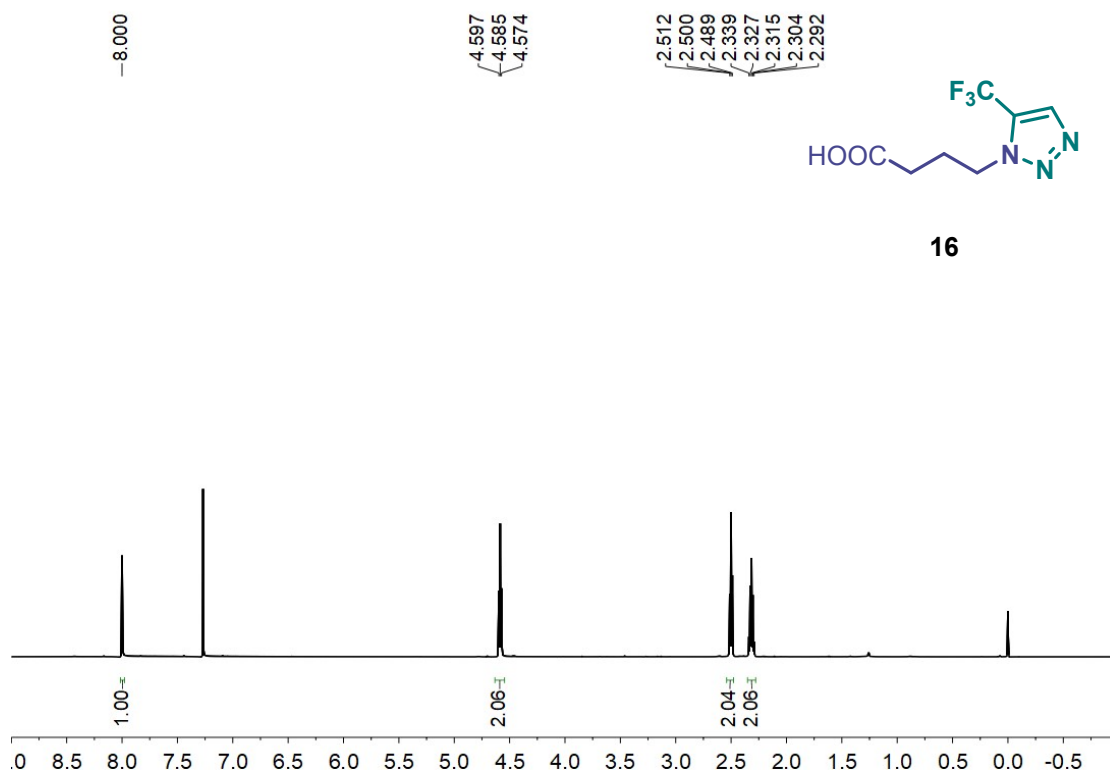


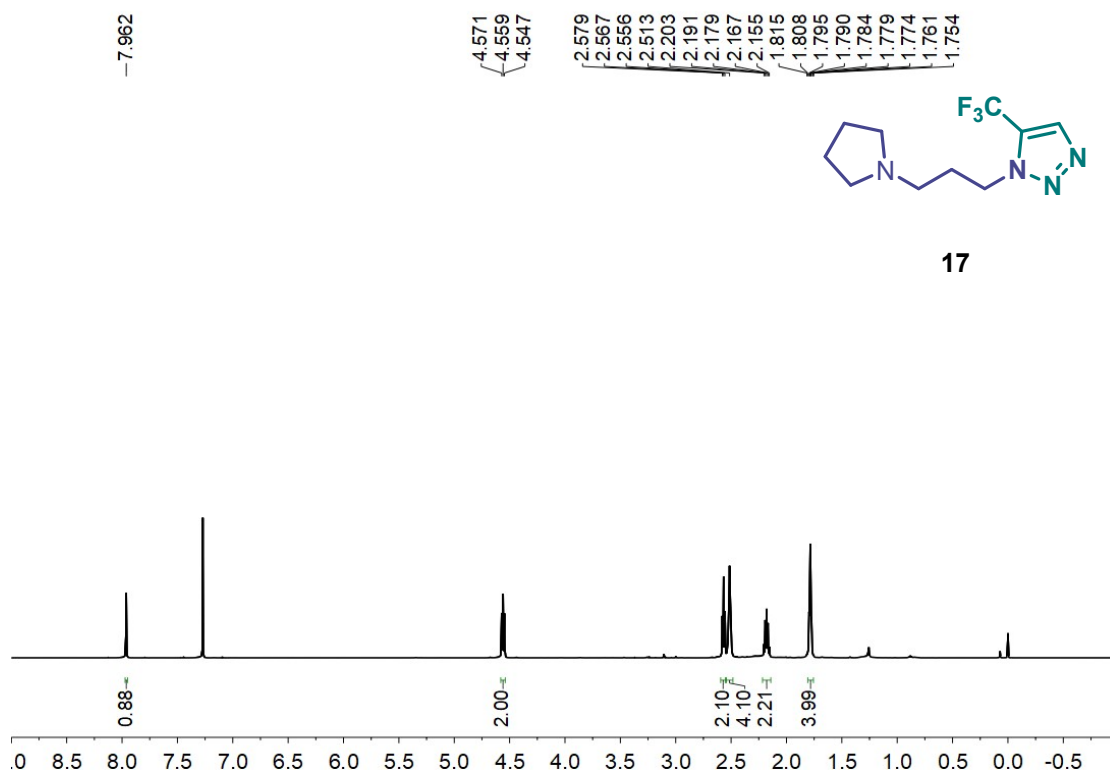
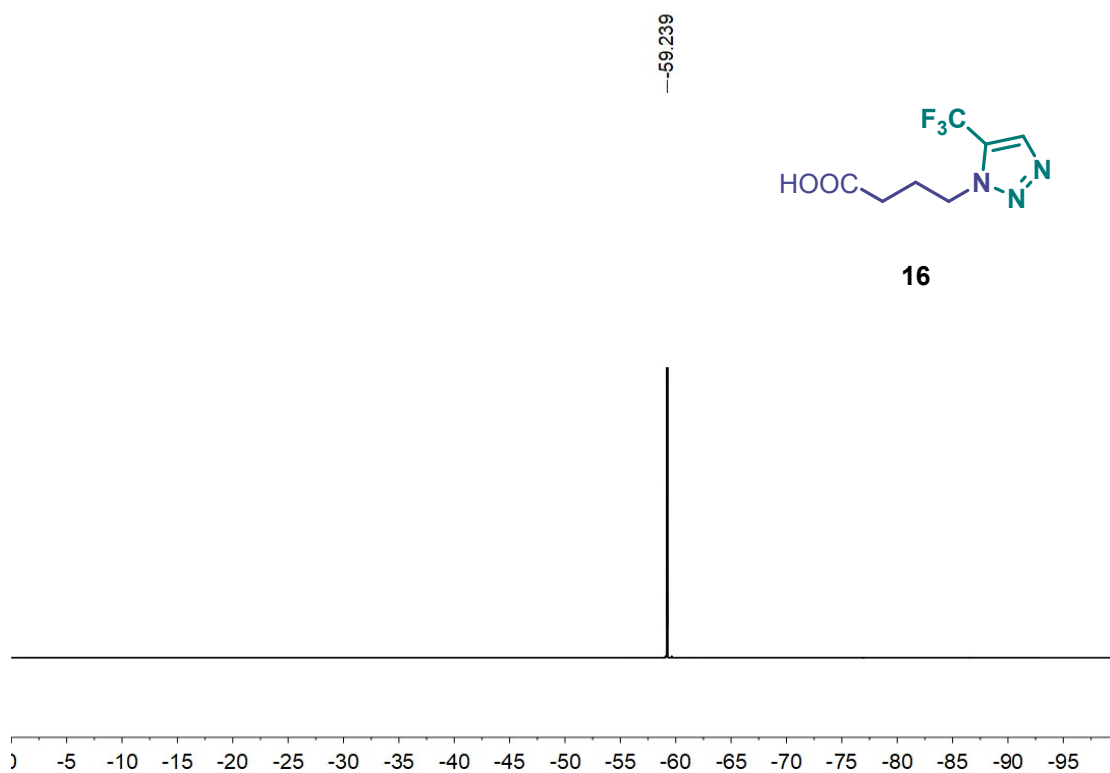


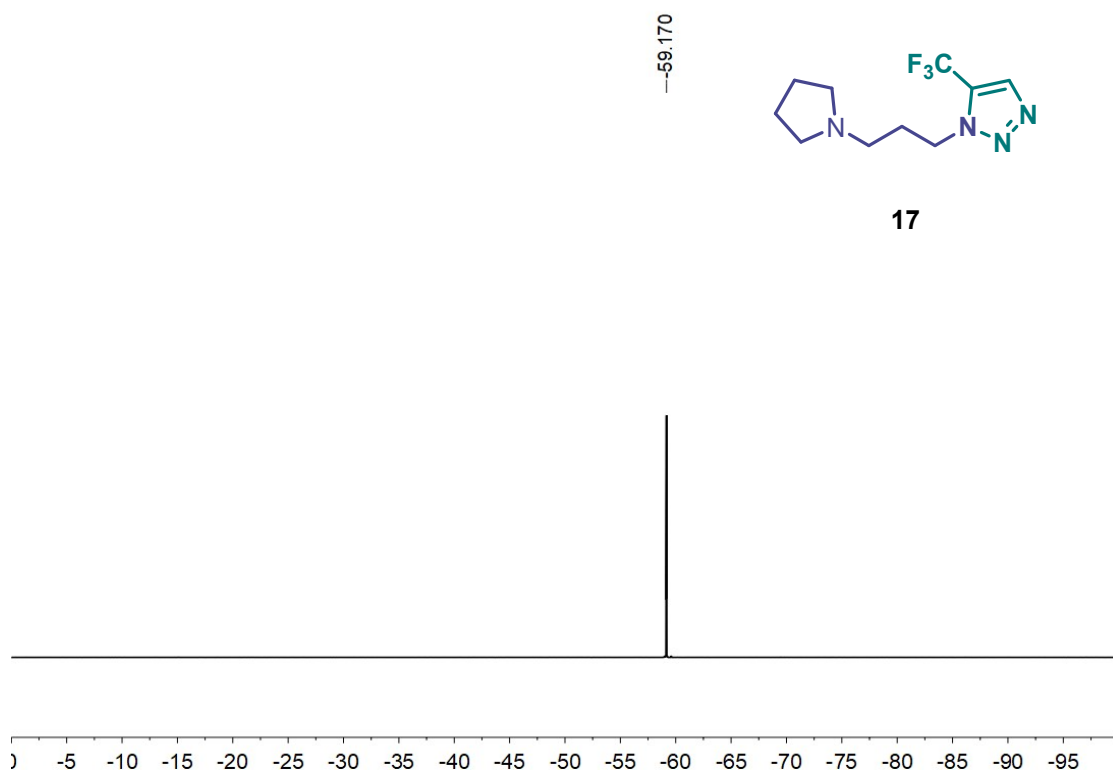
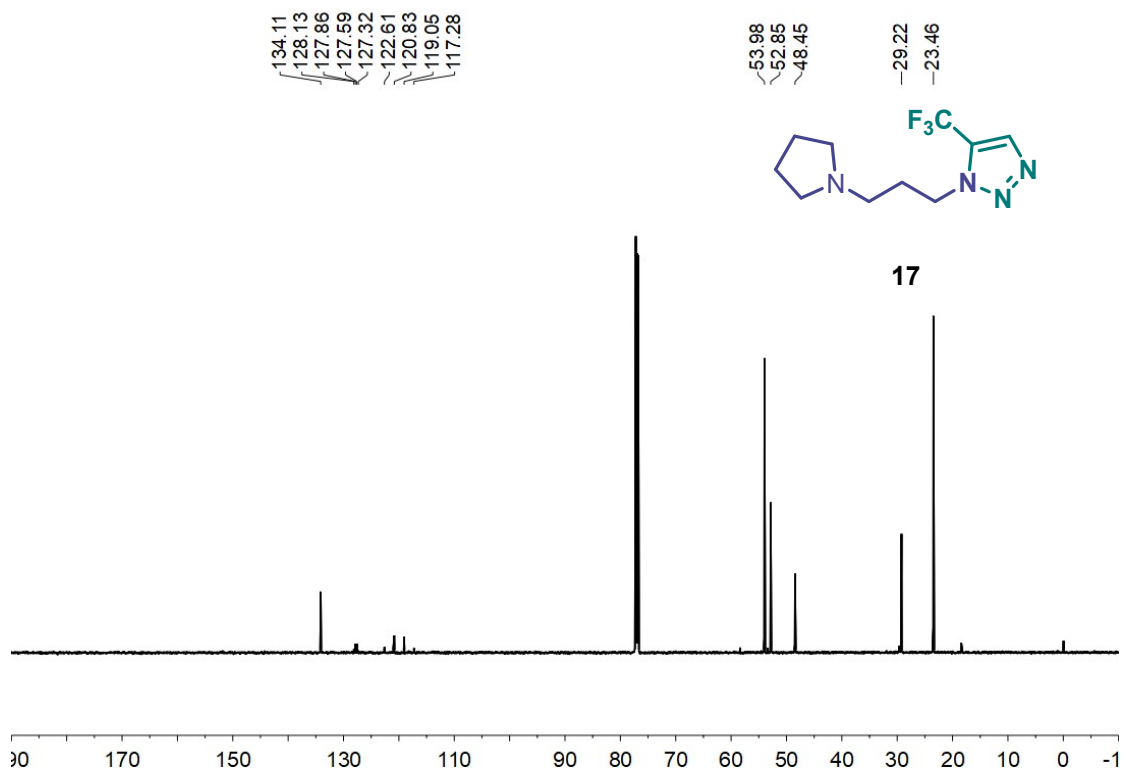


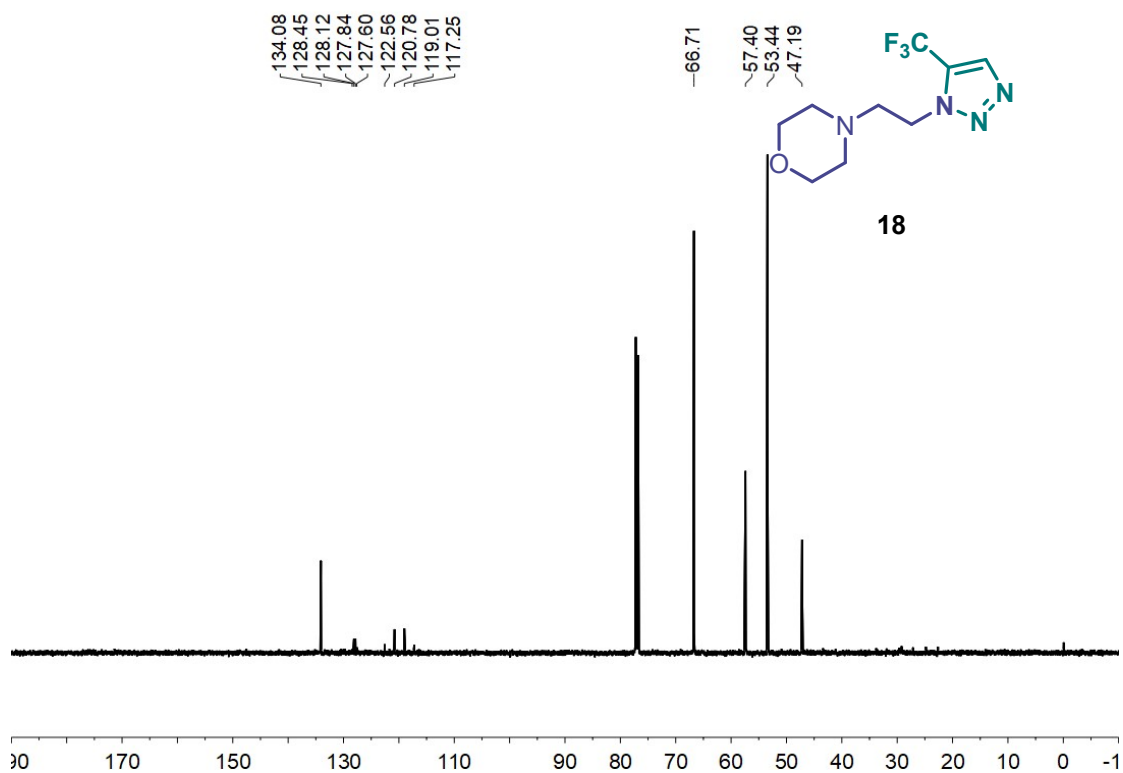
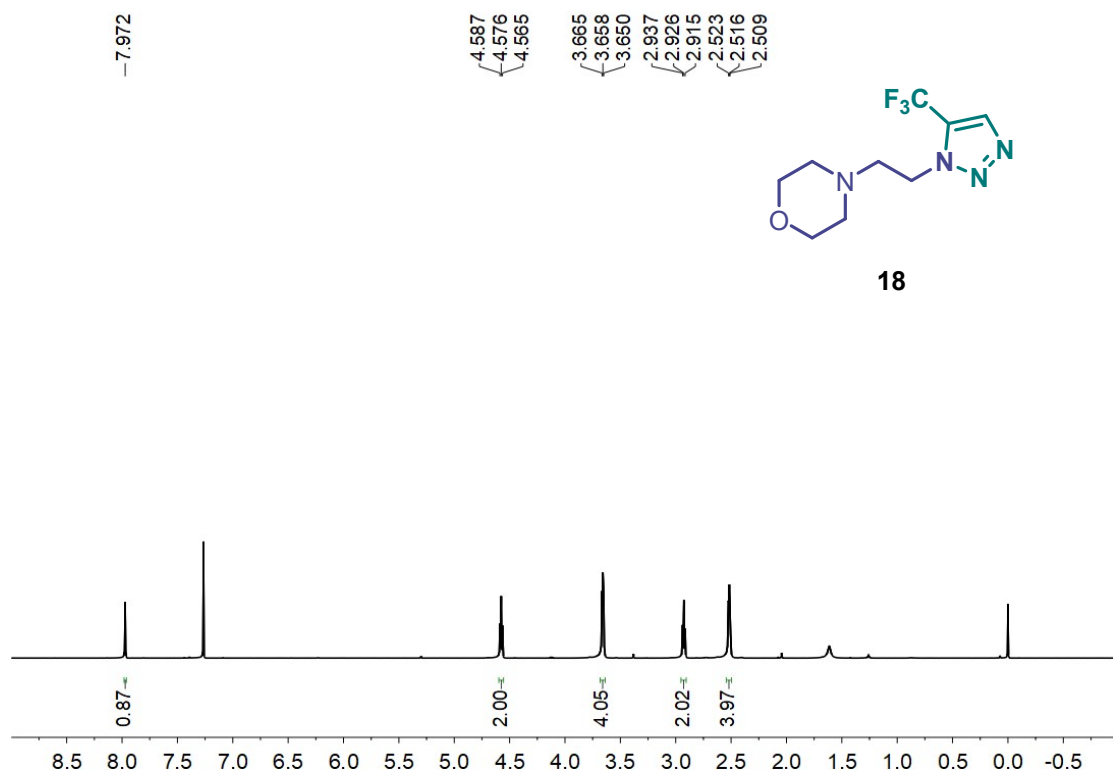


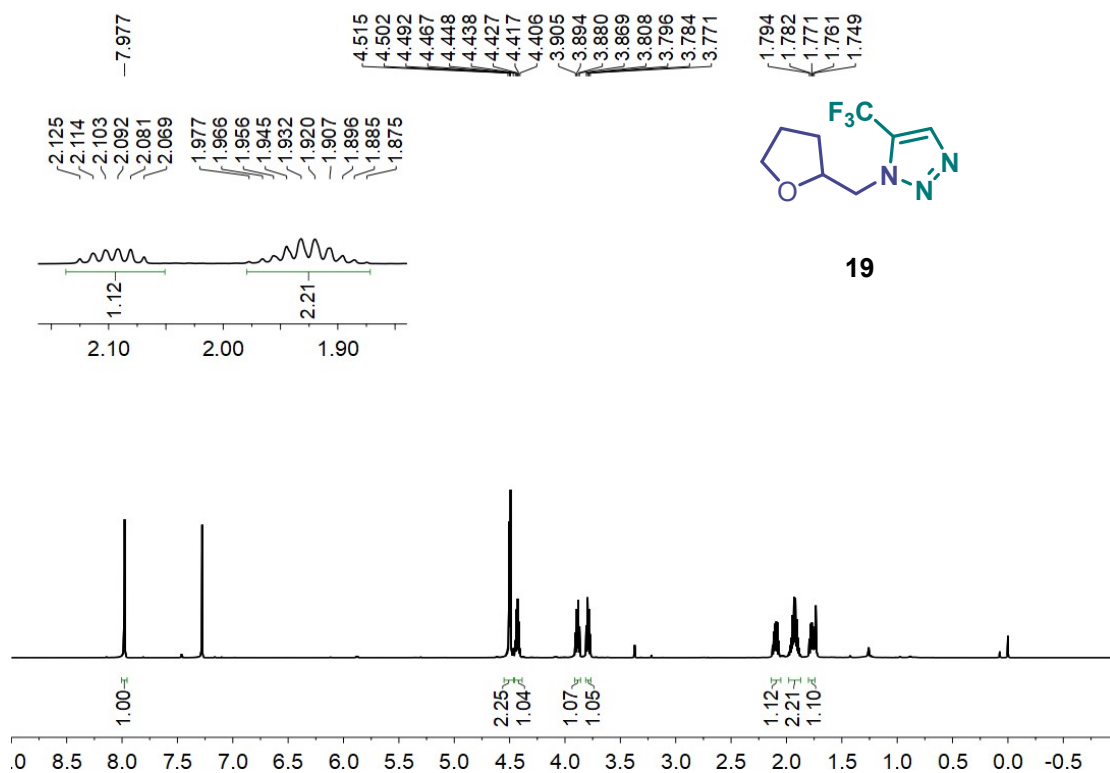
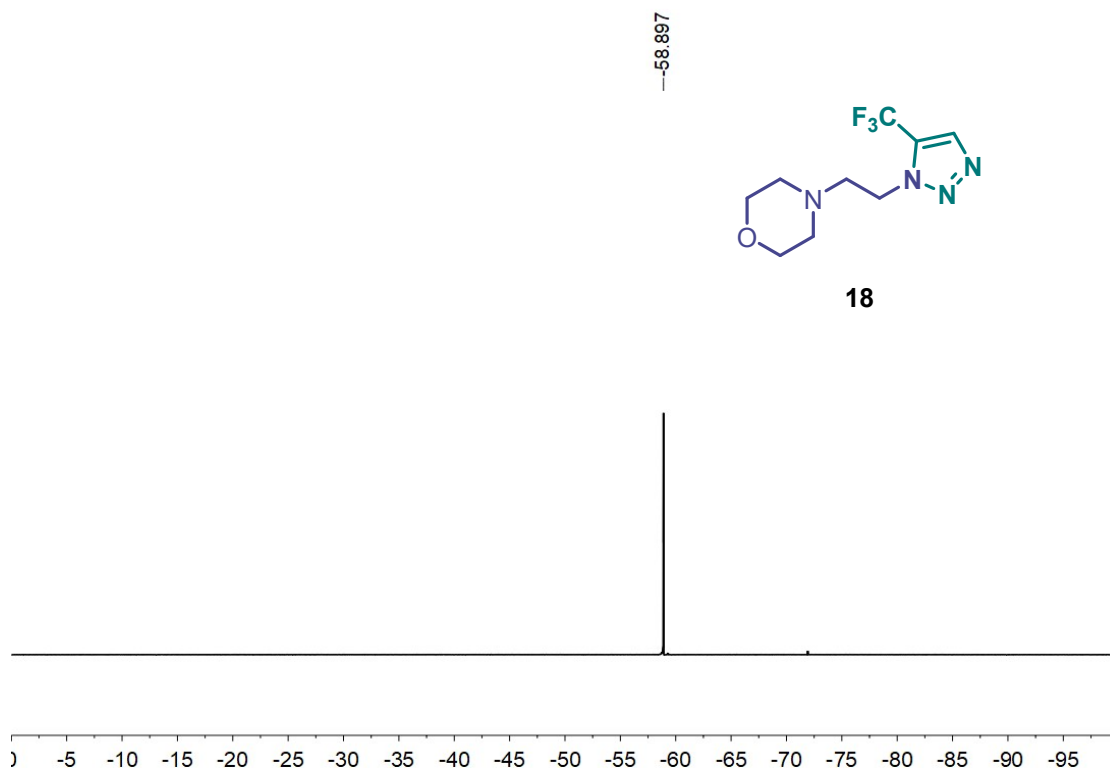


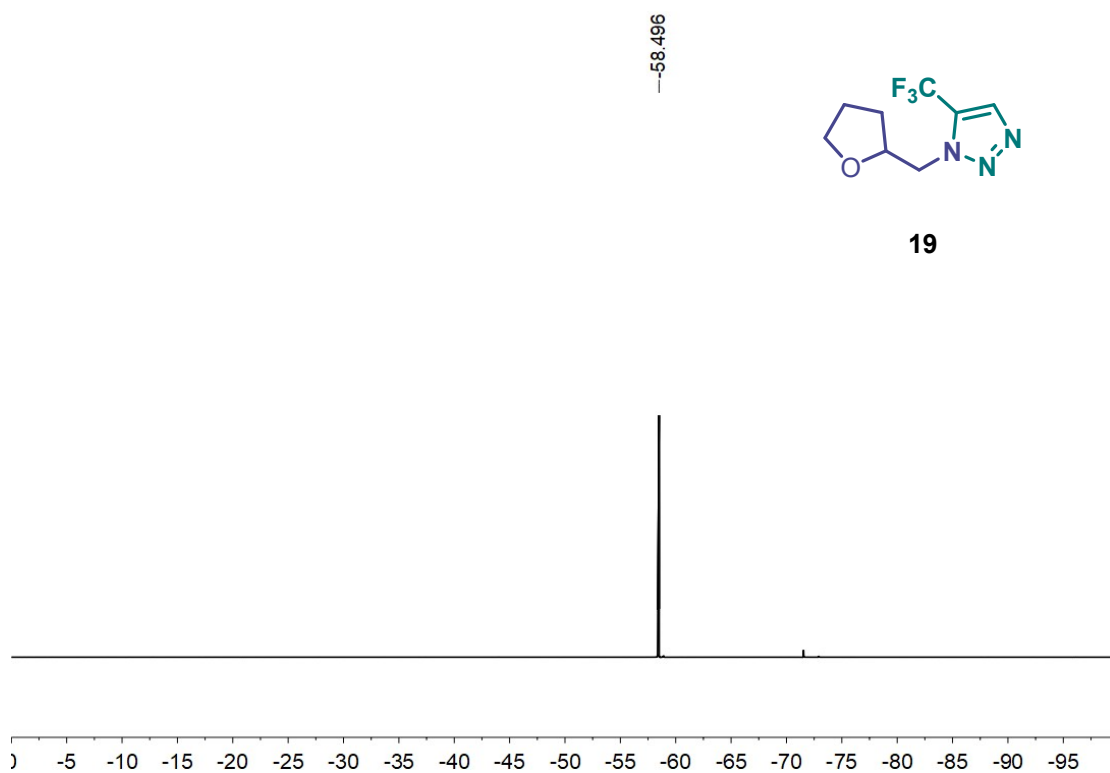
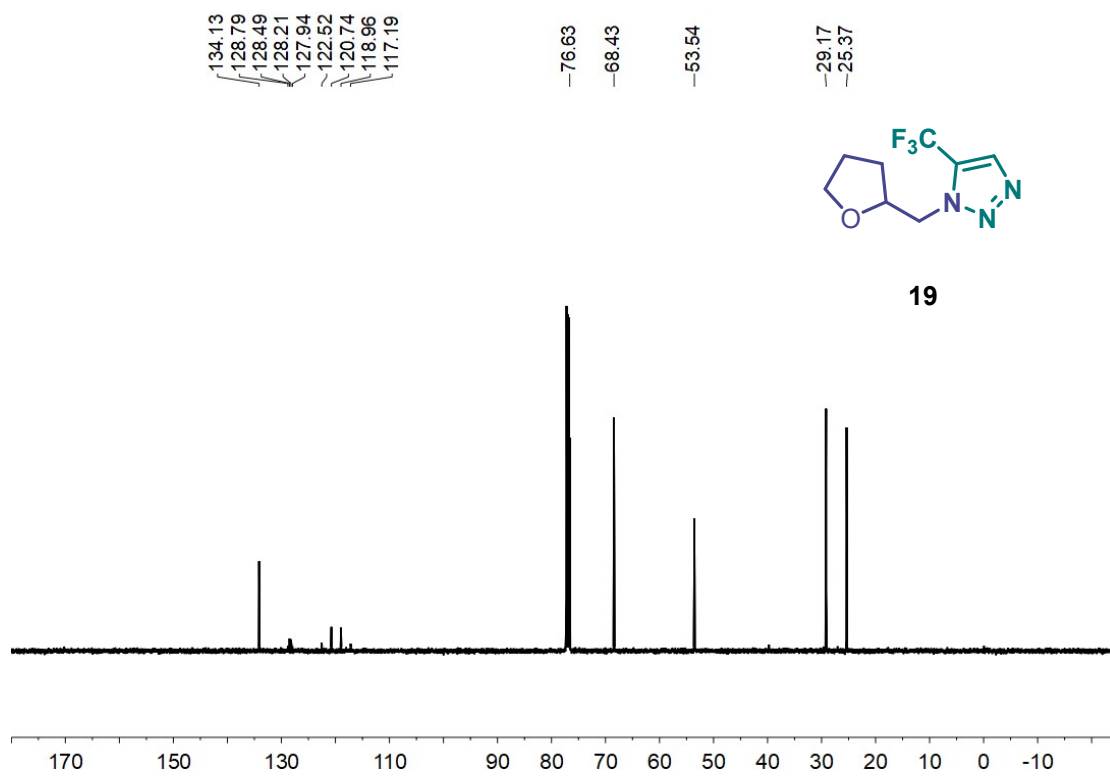


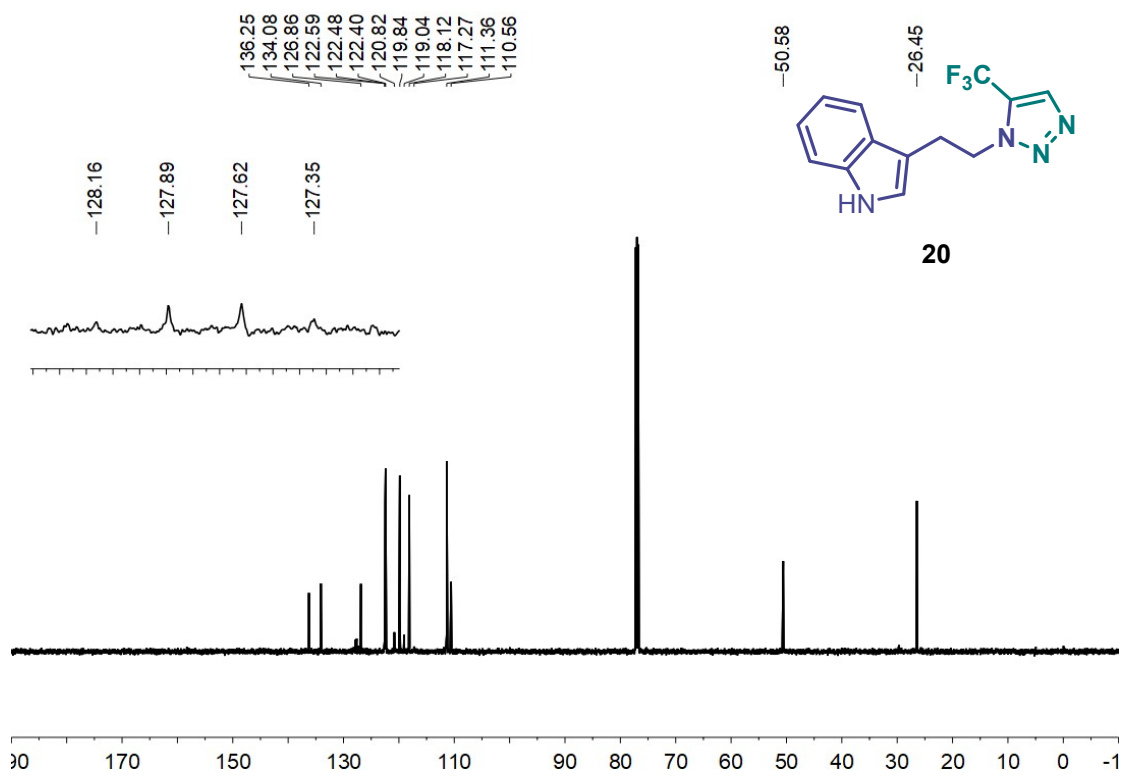
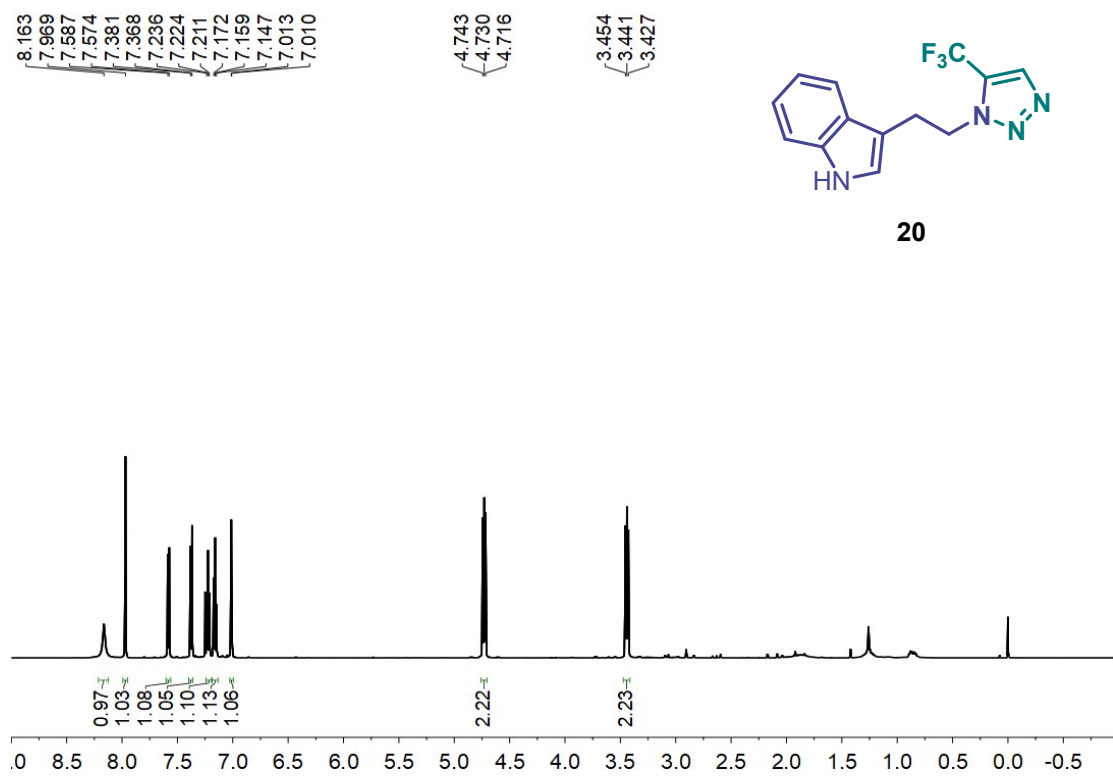


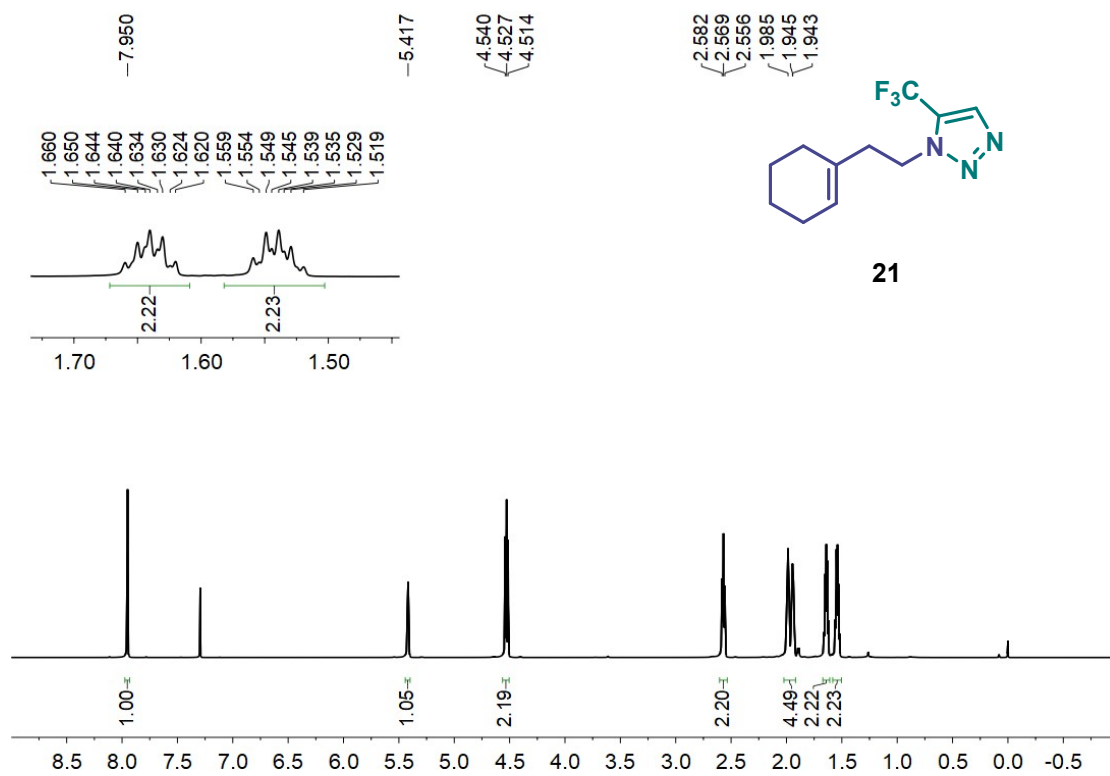
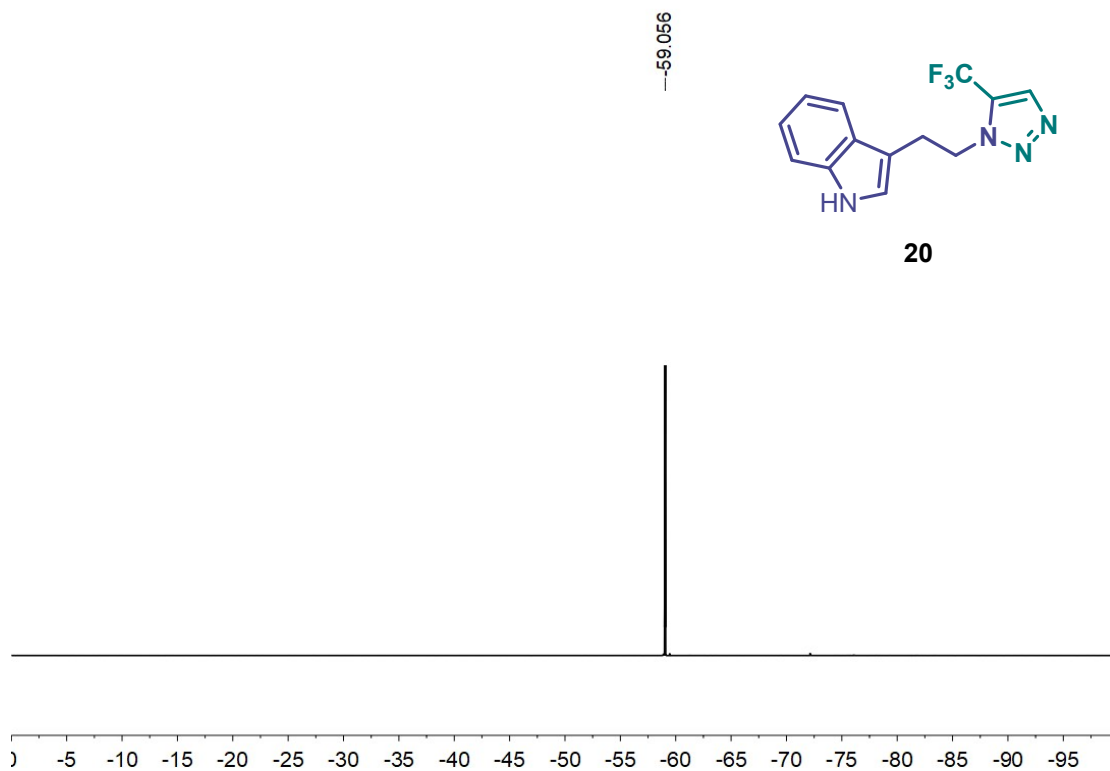


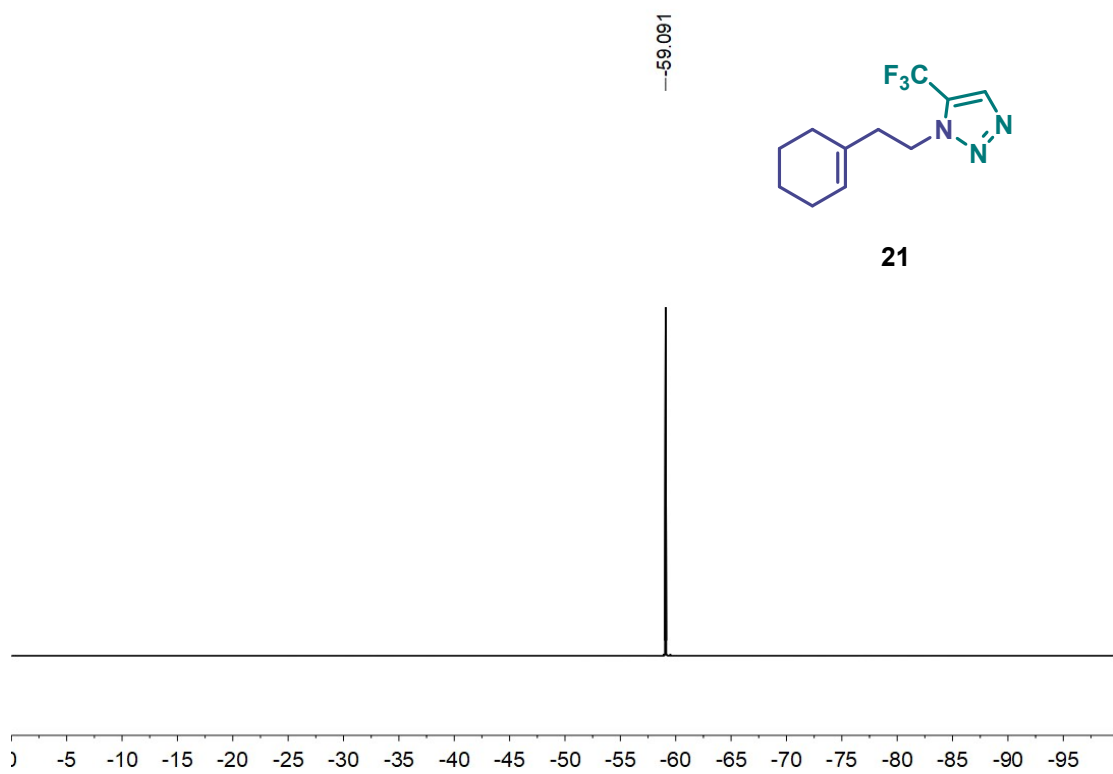
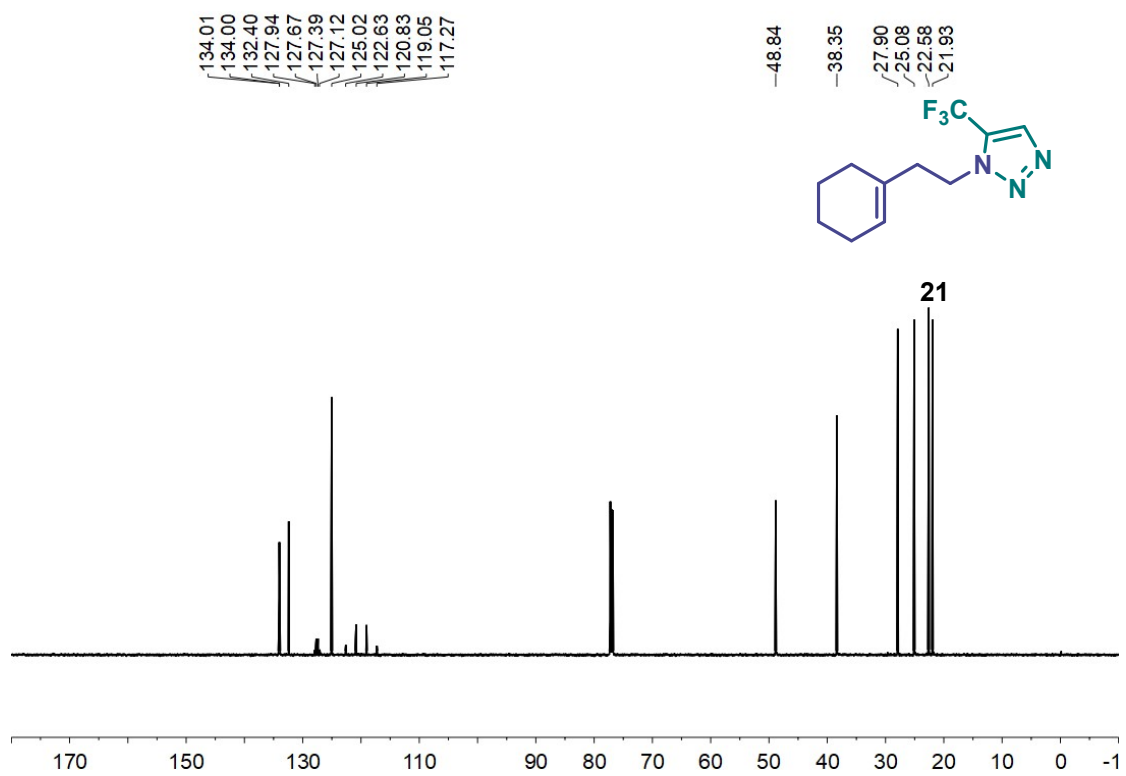


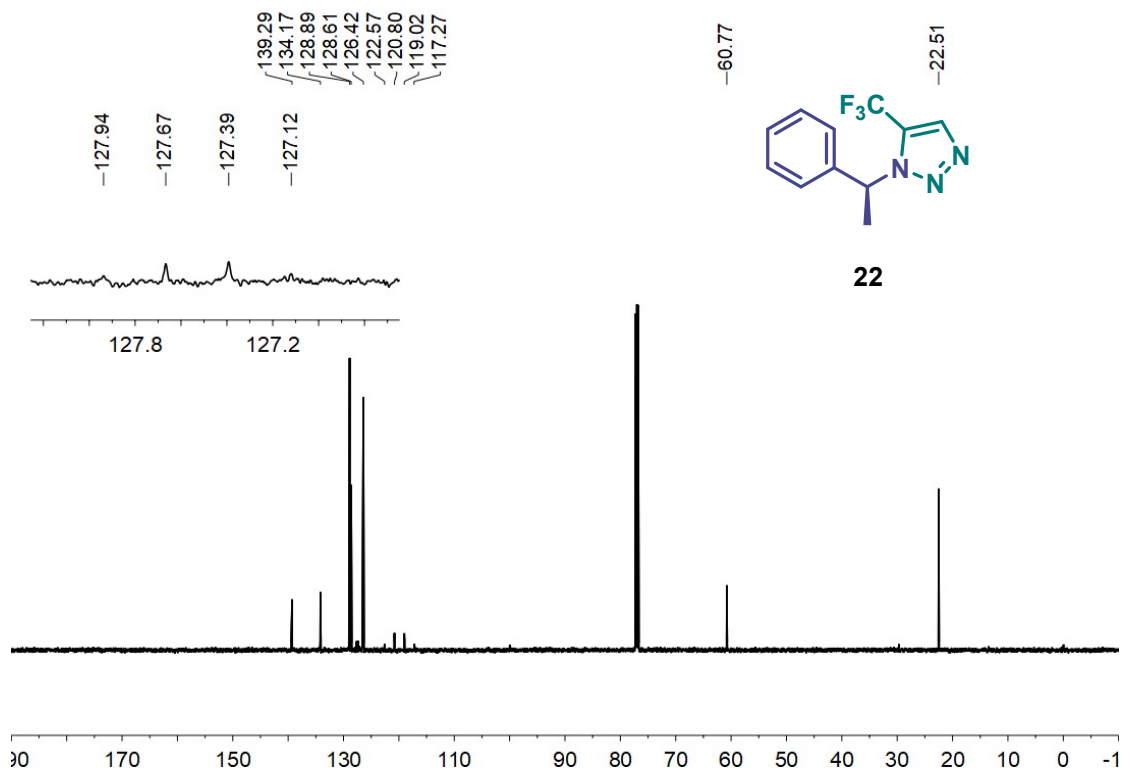
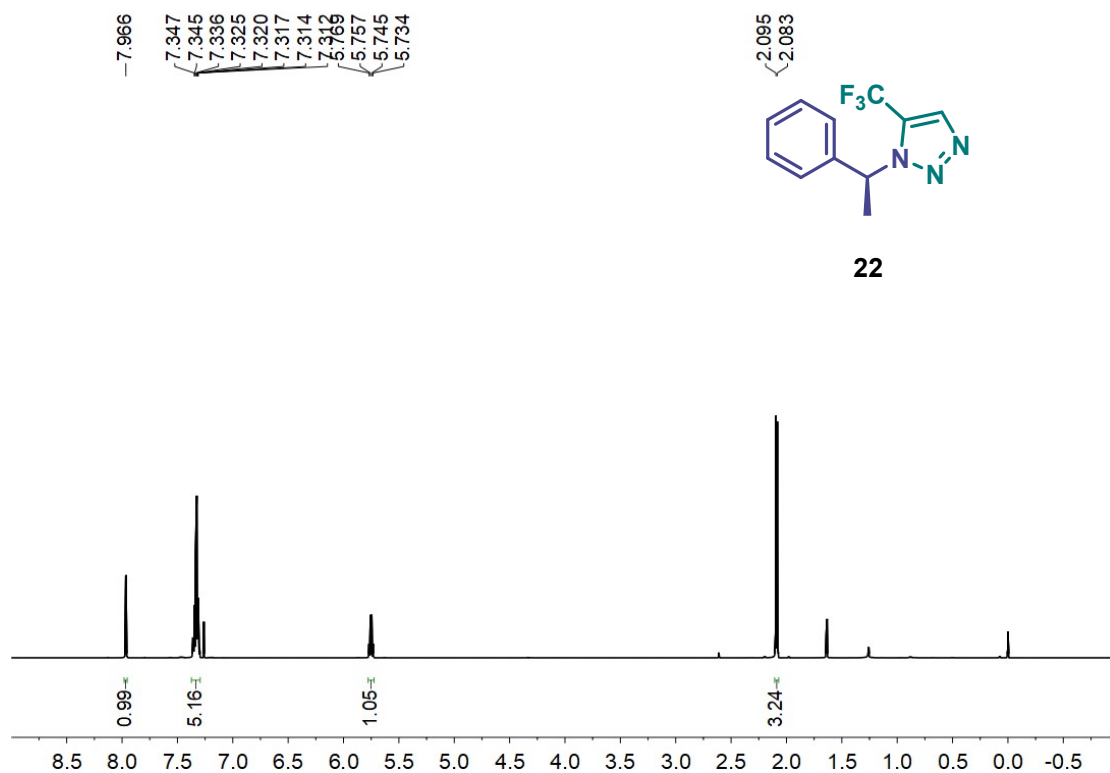


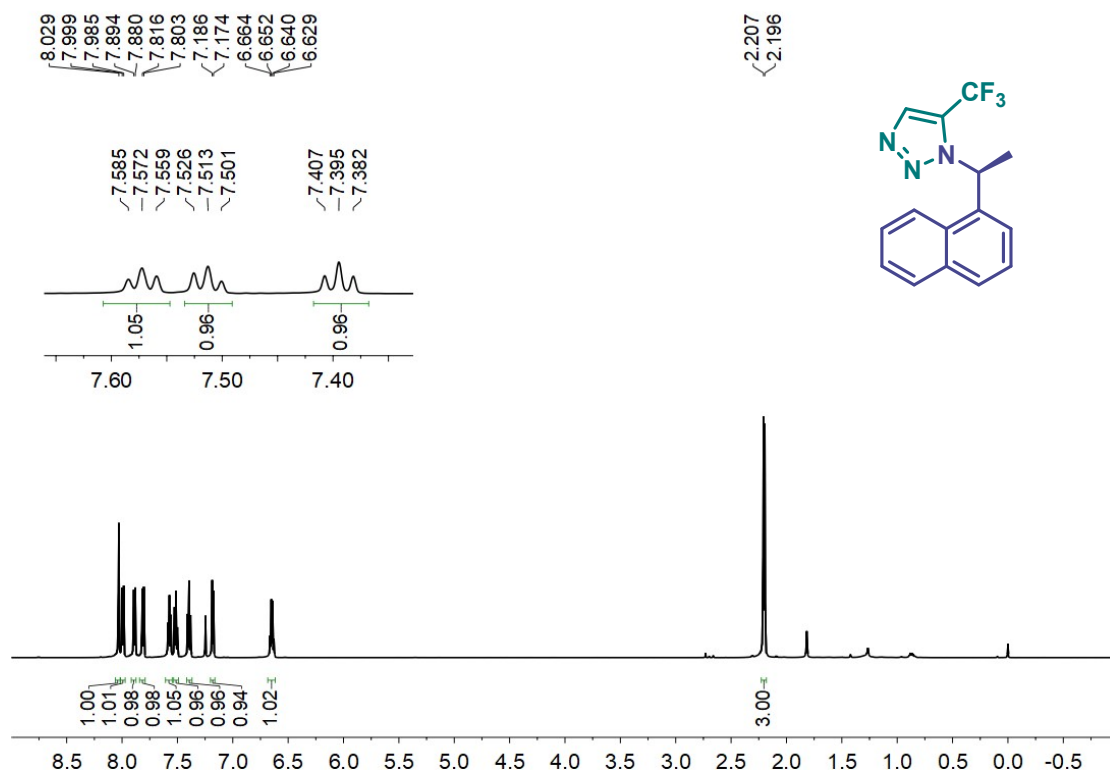
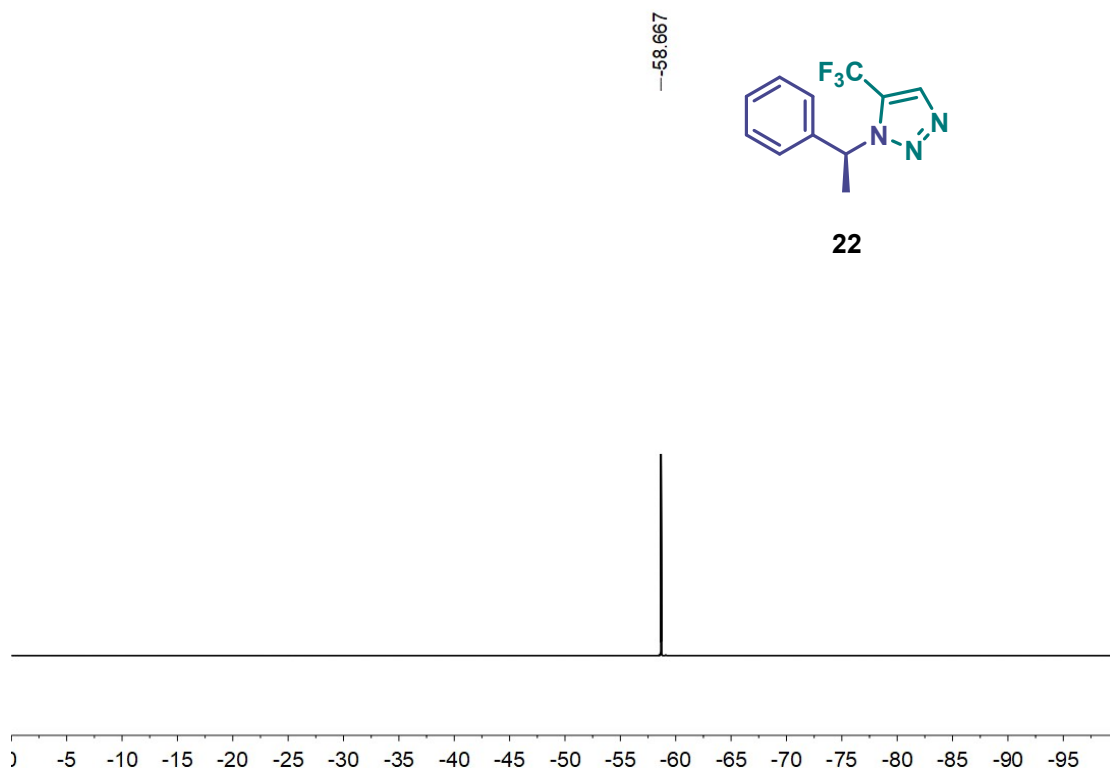


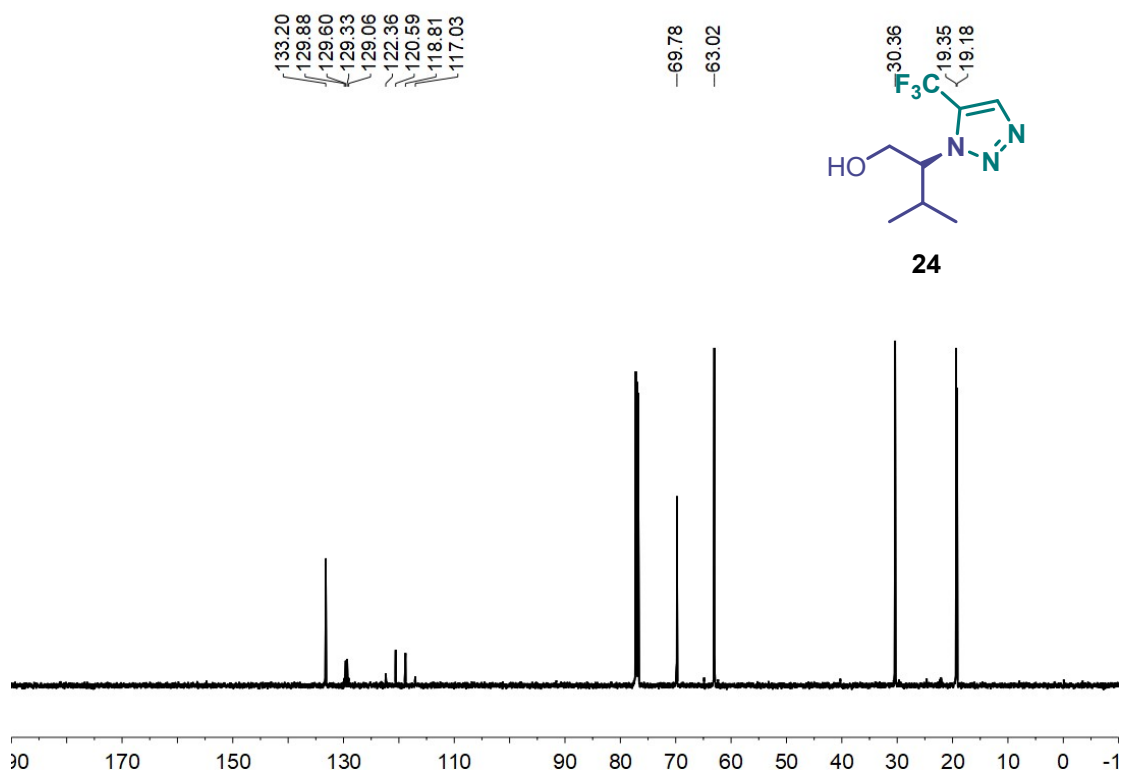
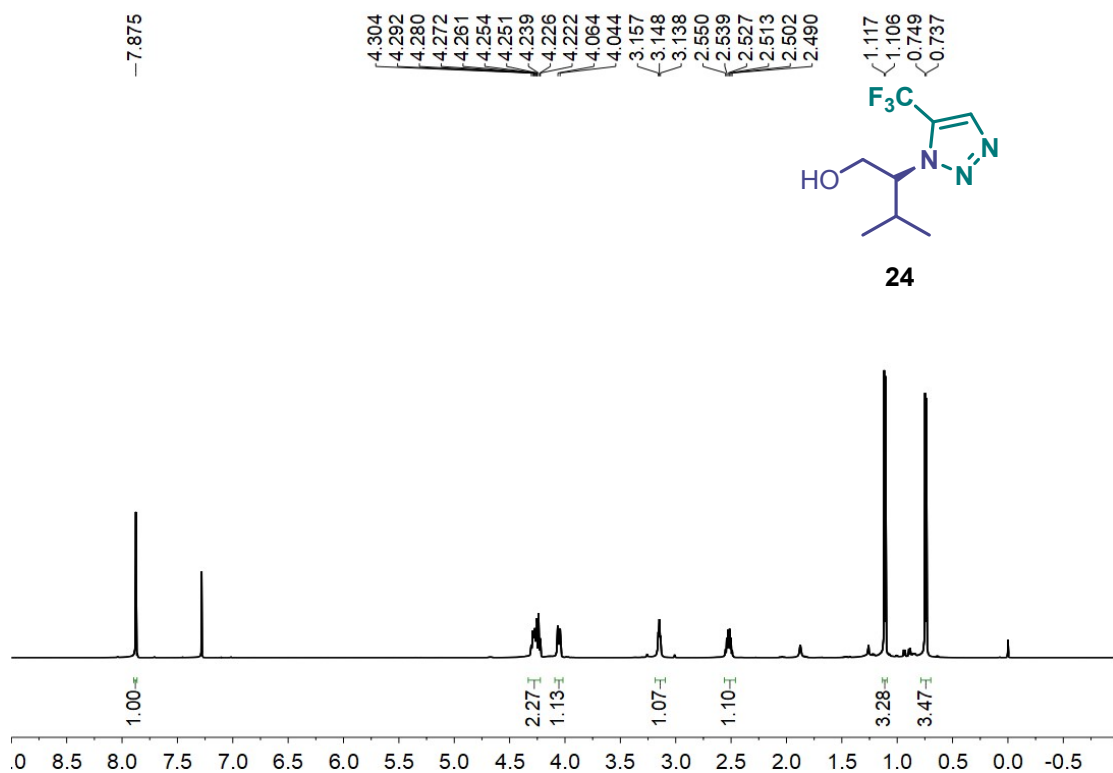


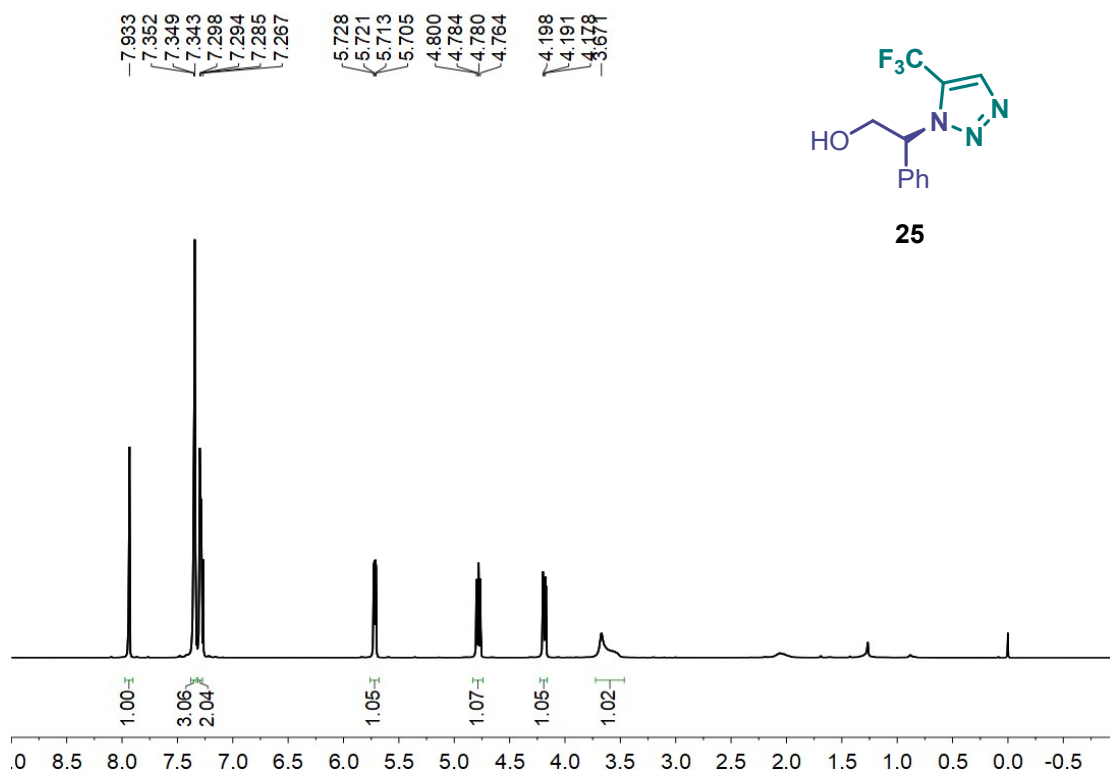
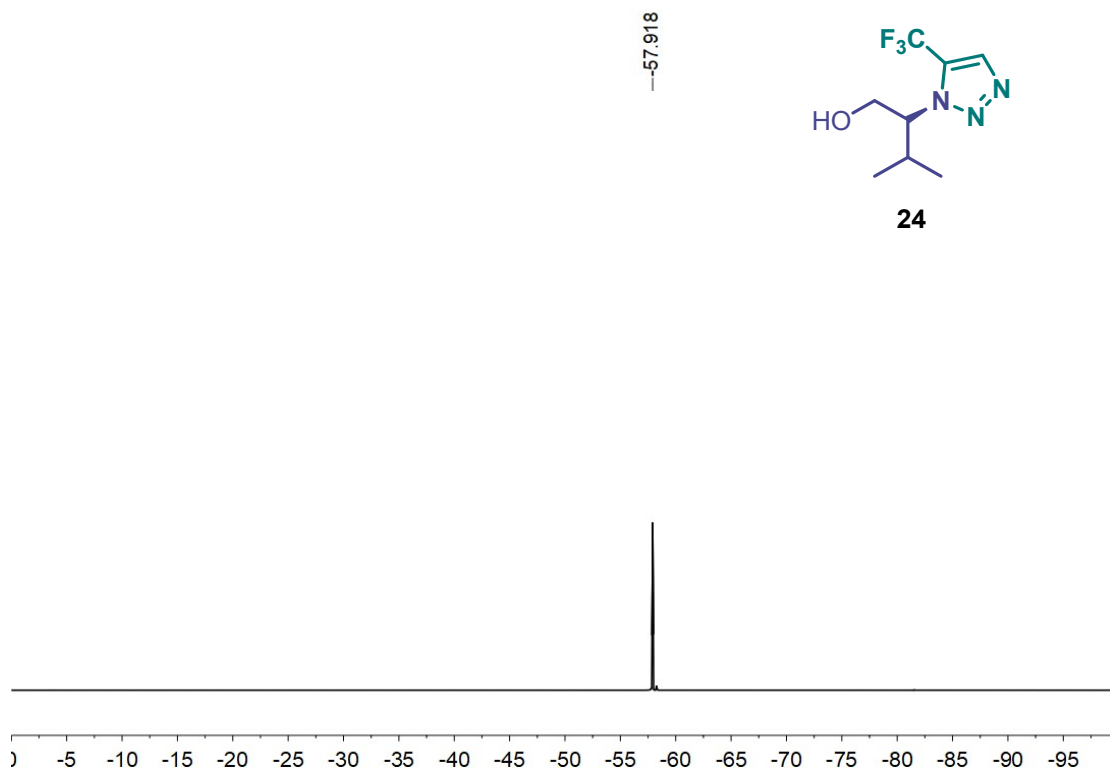






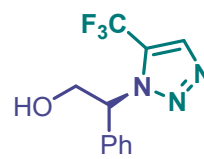




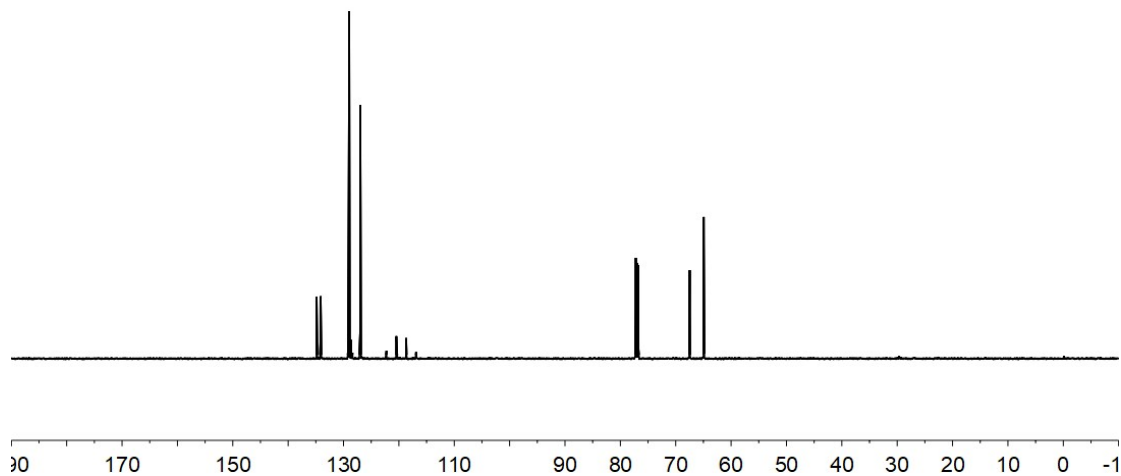


134.85
134.12
128.21
129.07
128.97
128.93
128.66
128.38
126.96
122.24
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118.68
116.90

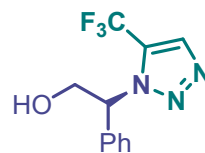
~67.47
~64.94



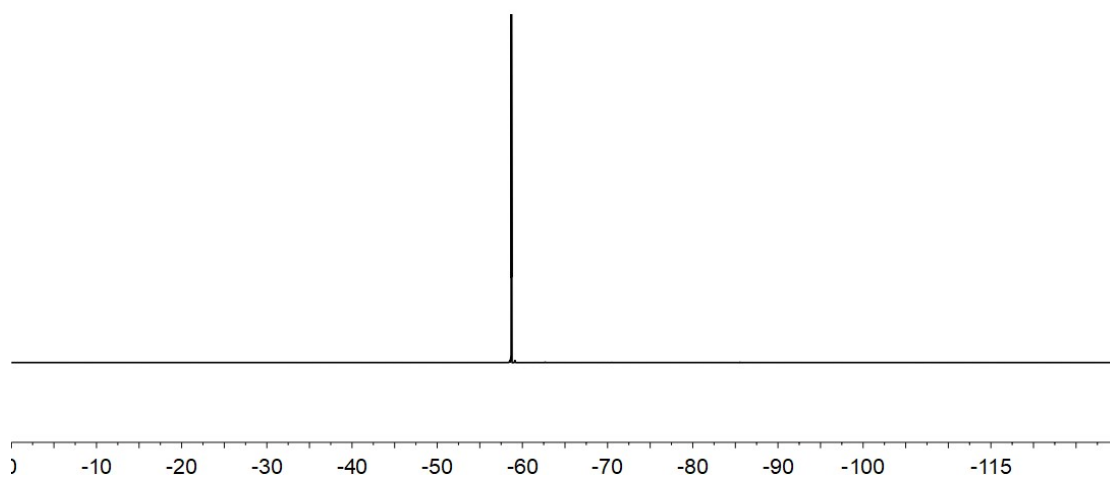
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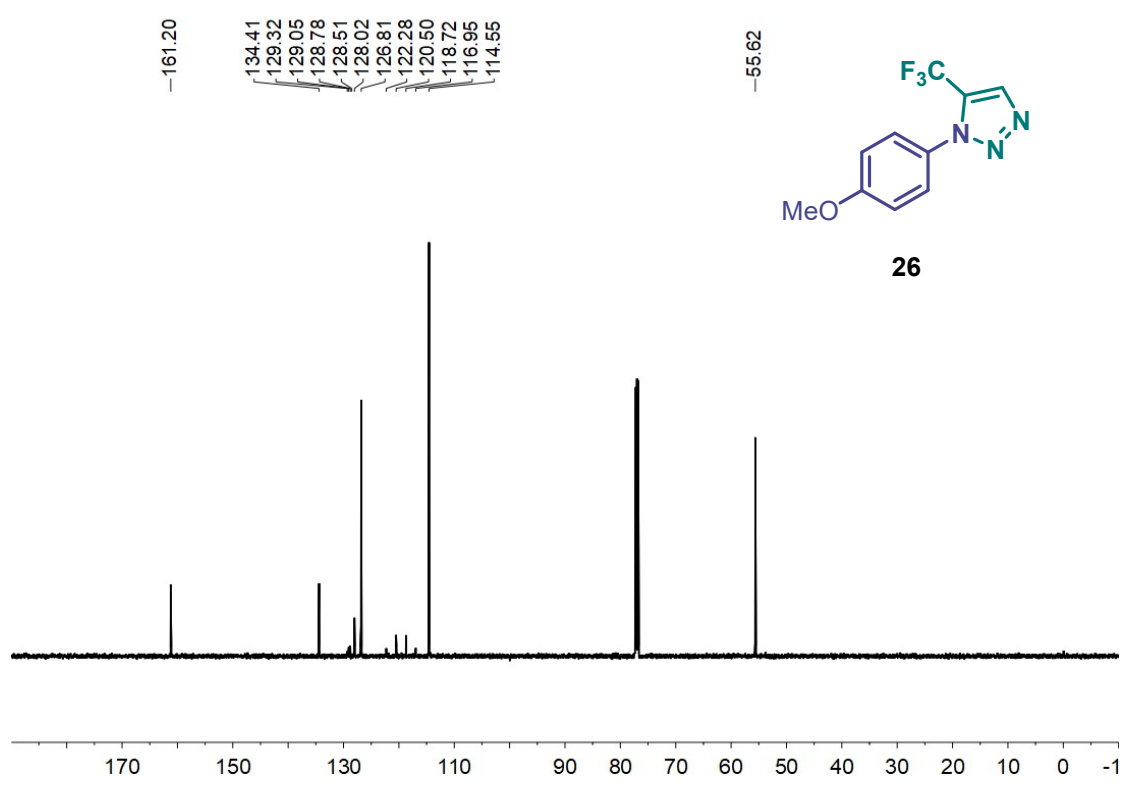
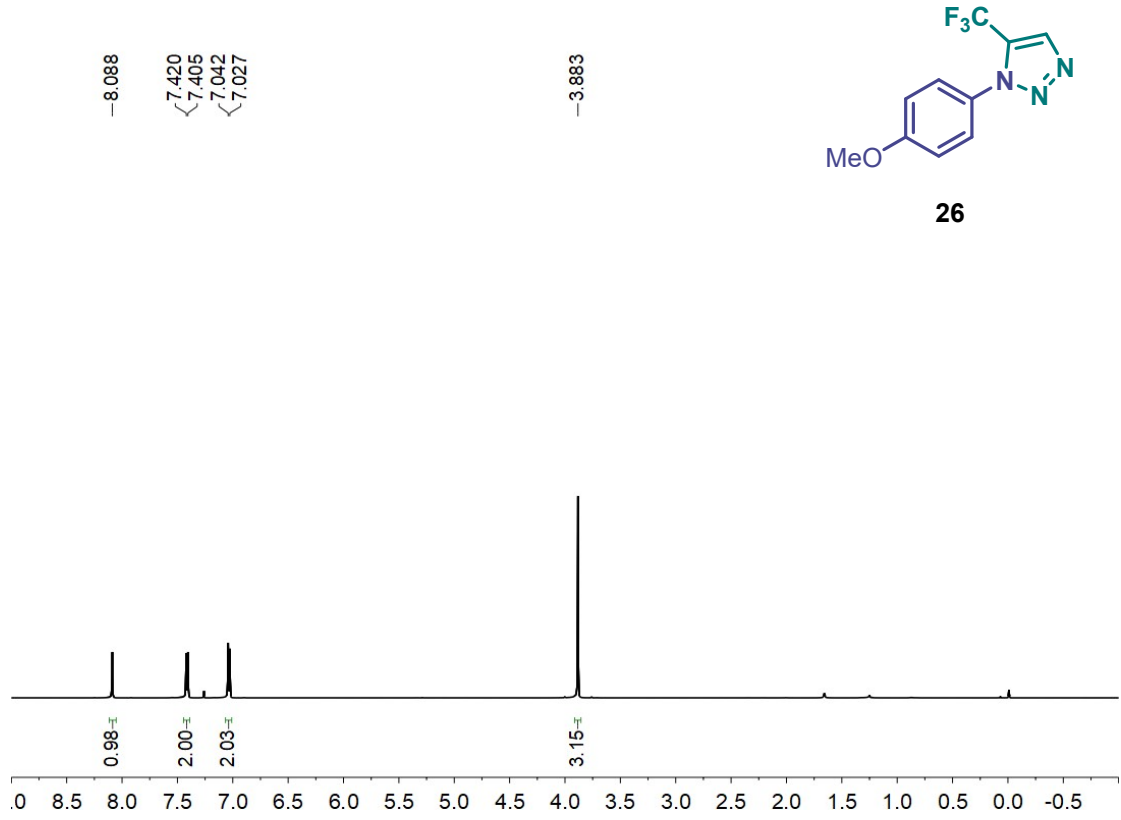


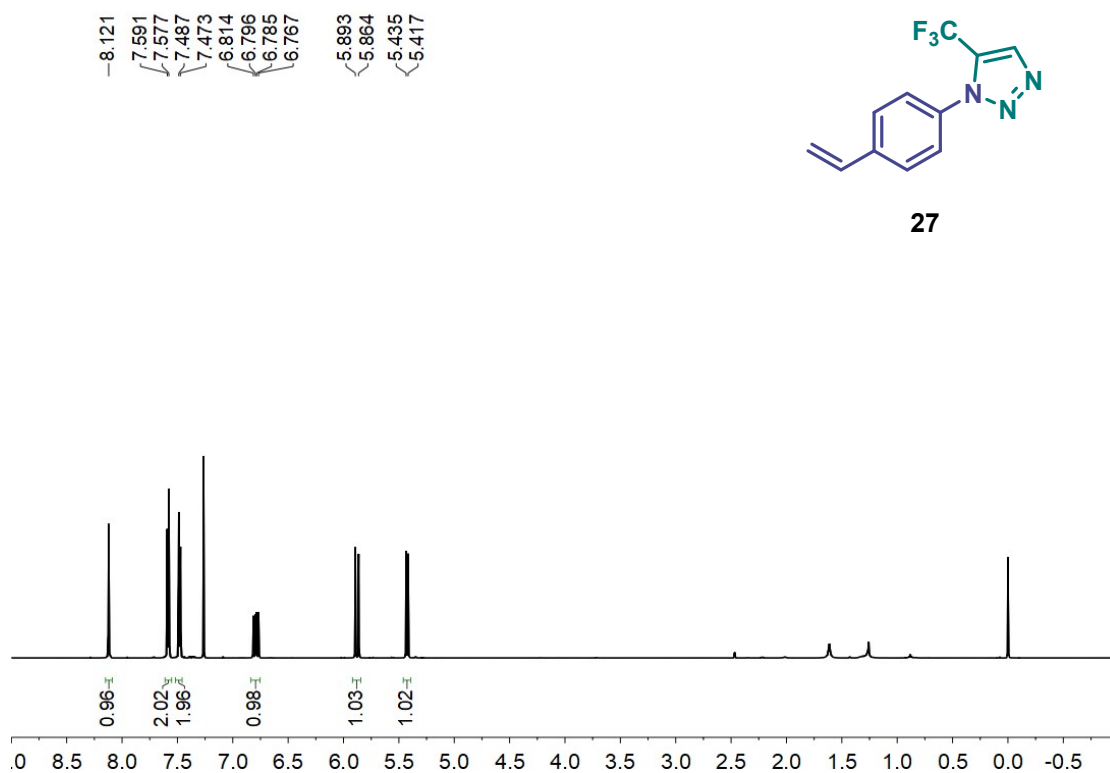
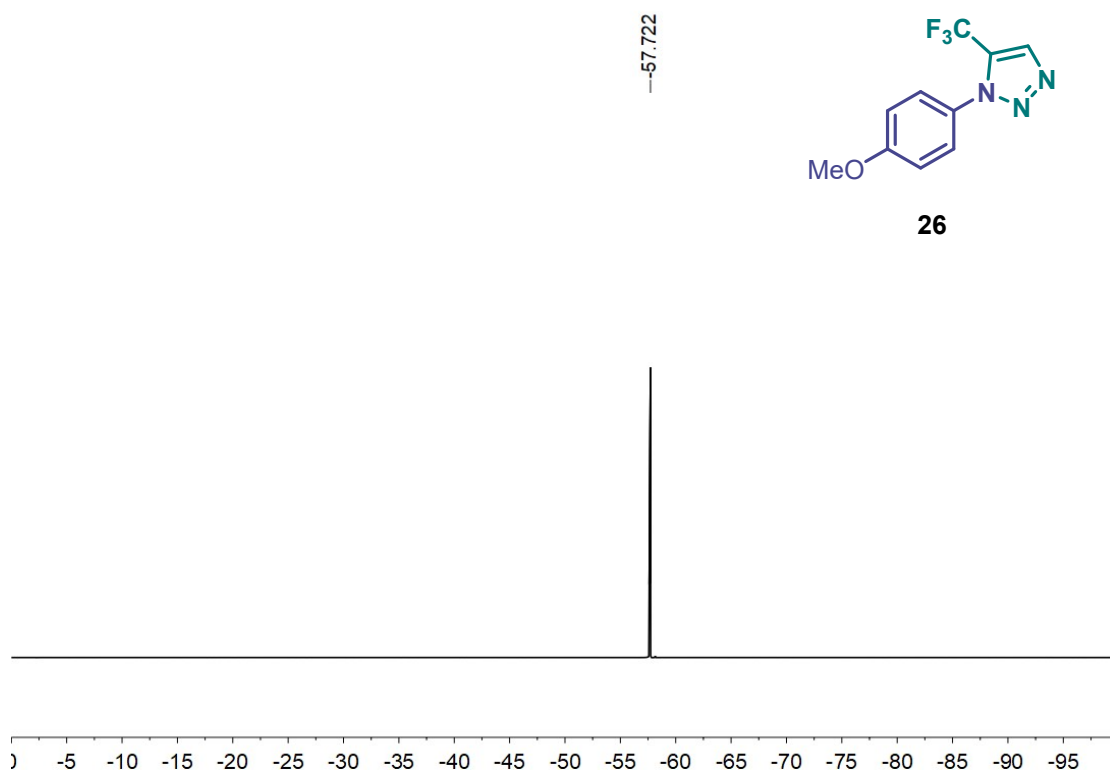
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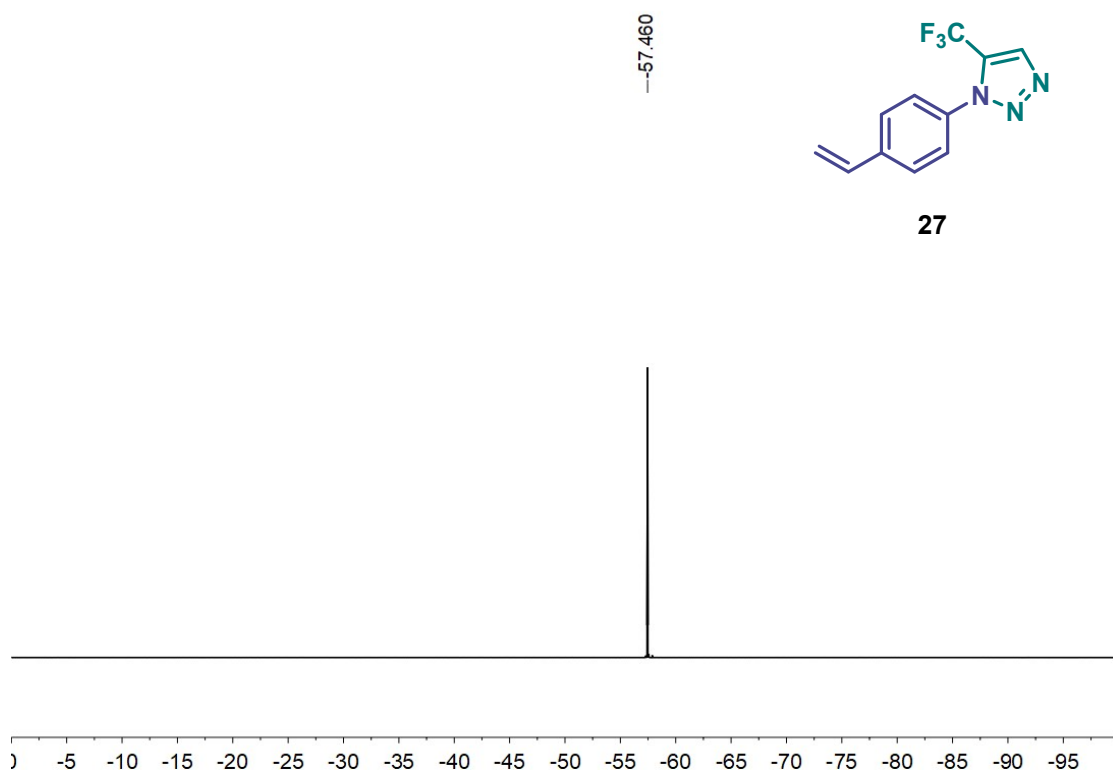
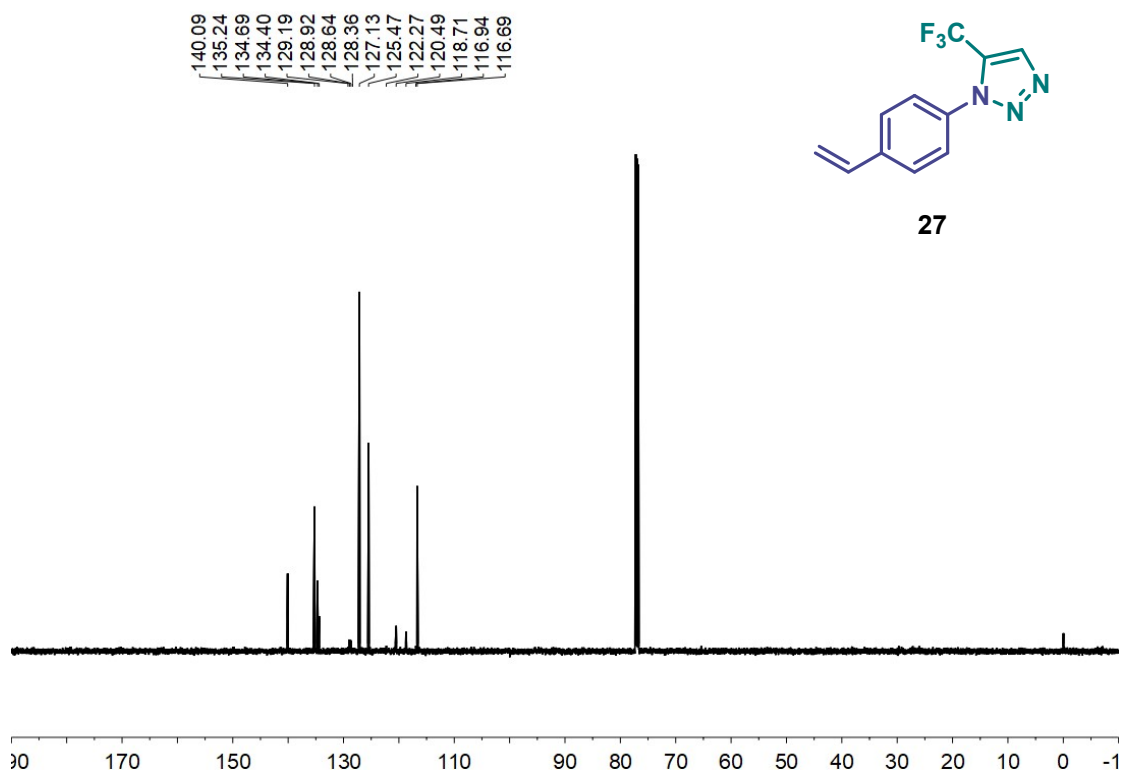


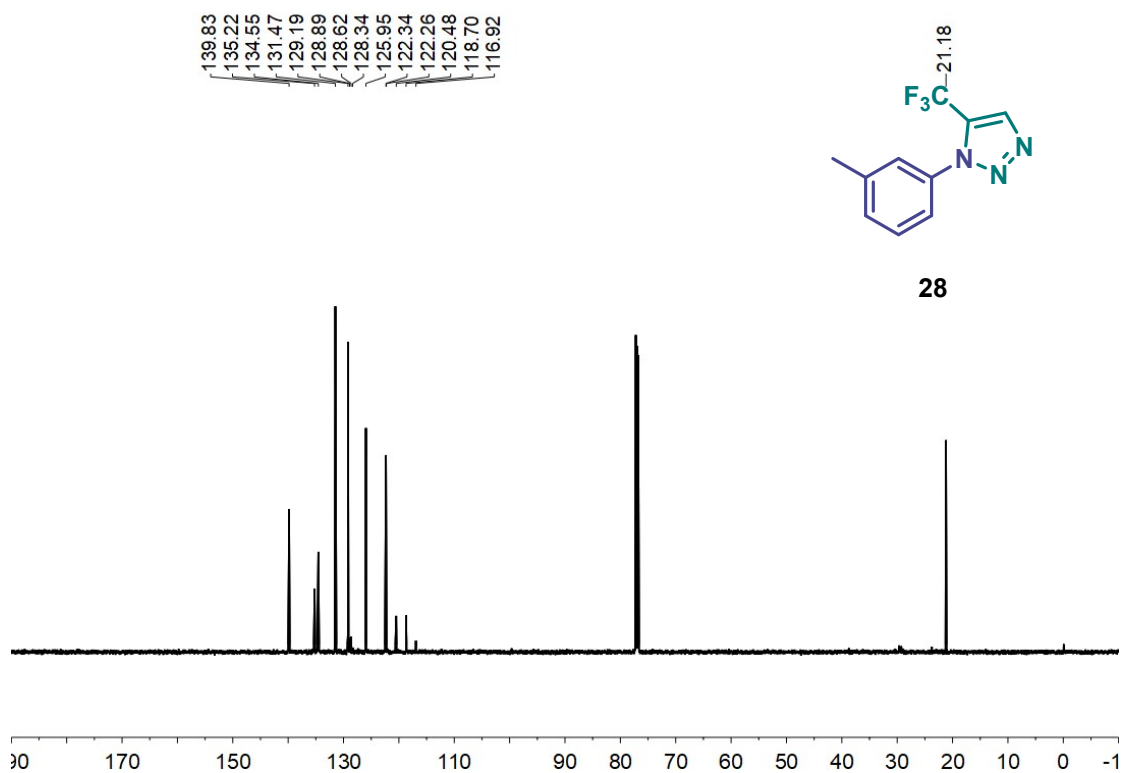
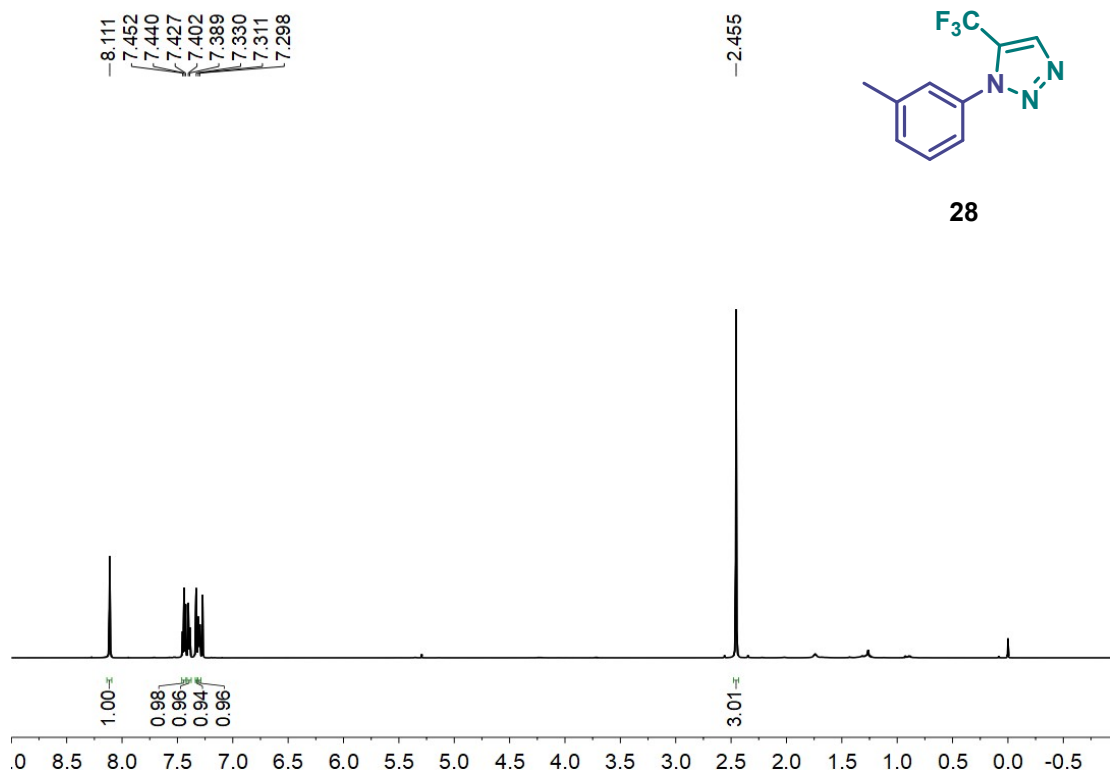
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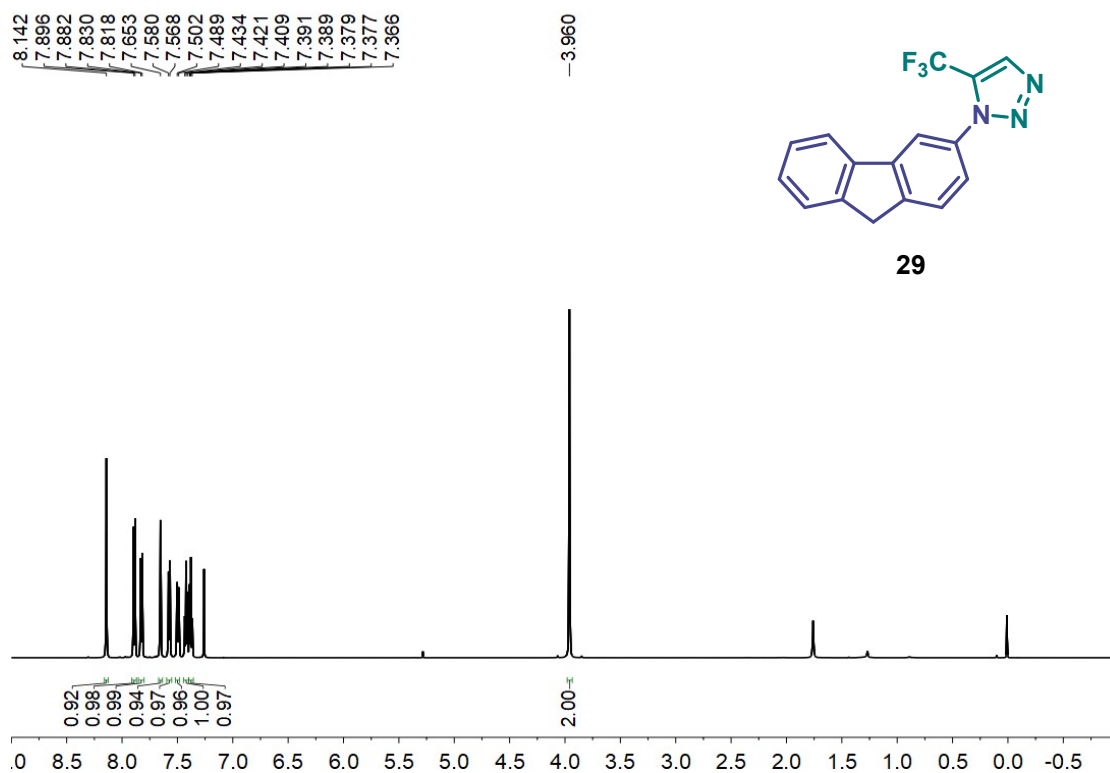
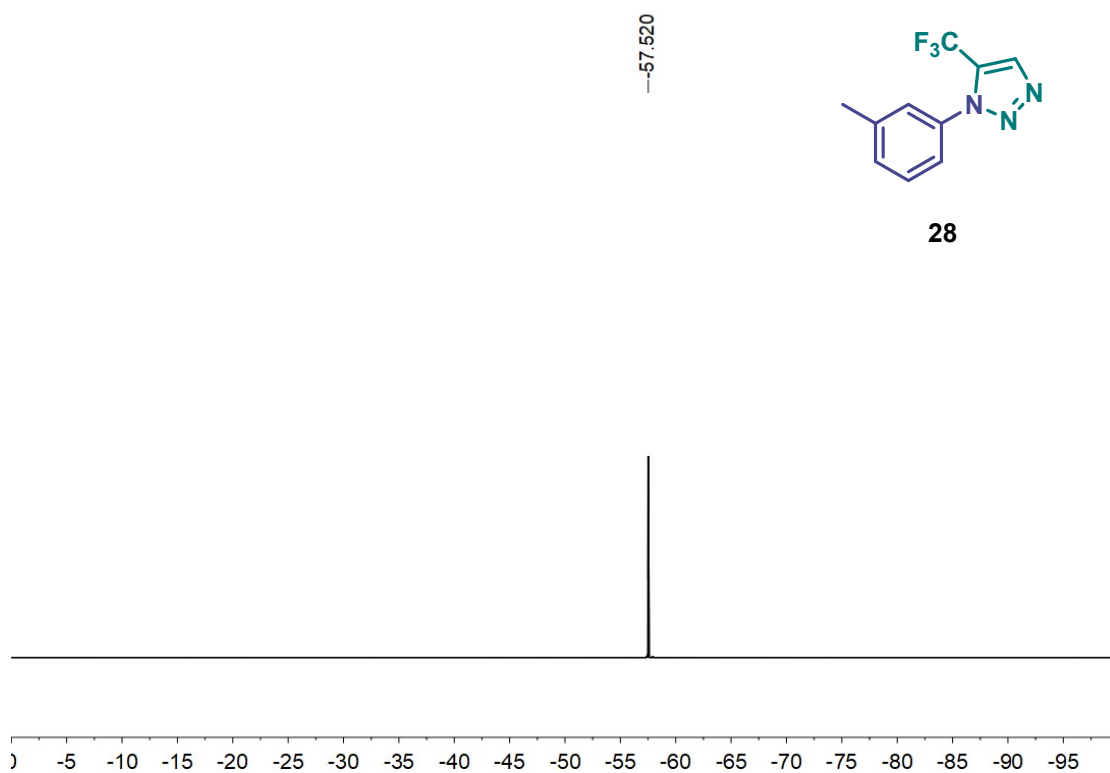


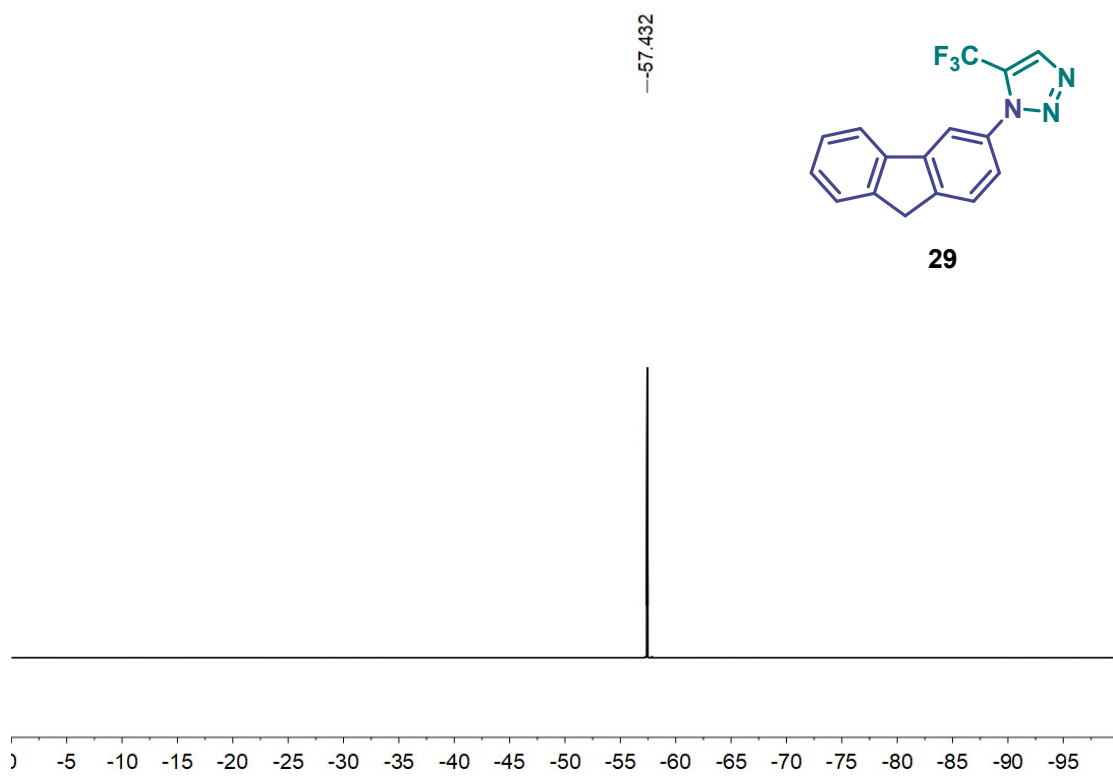
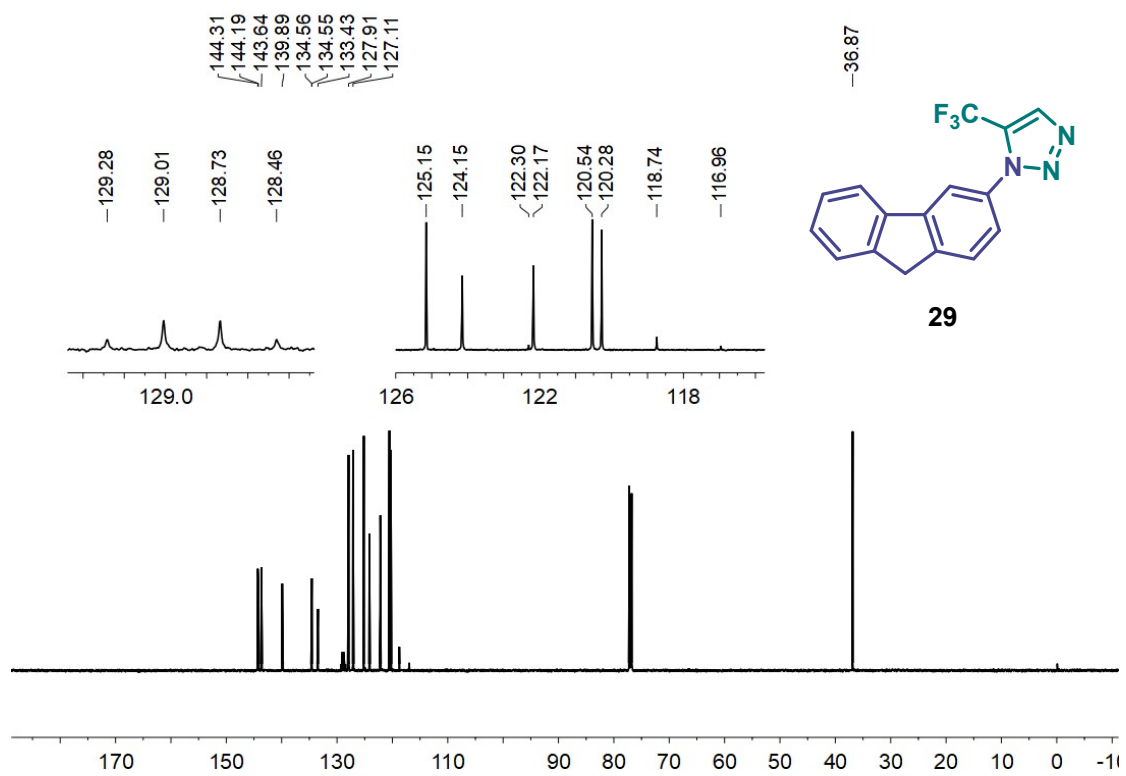




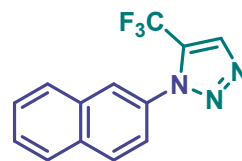




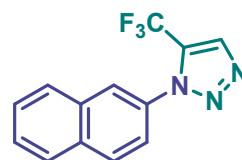
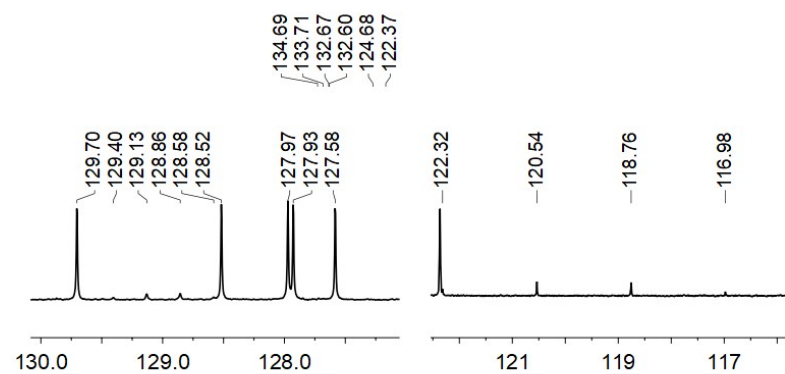
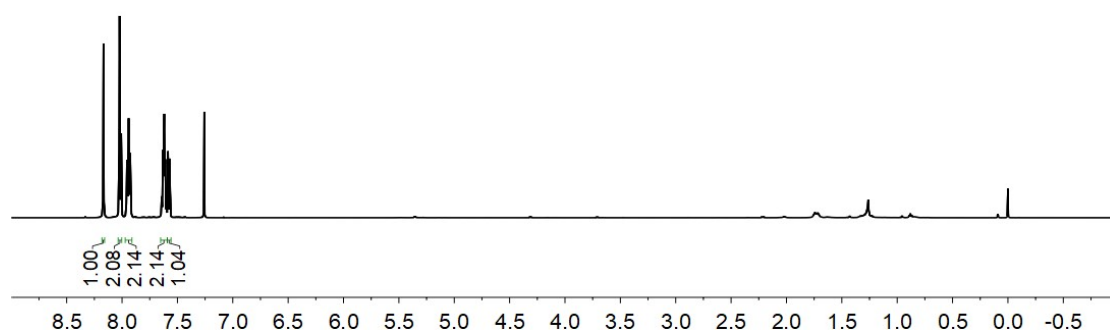




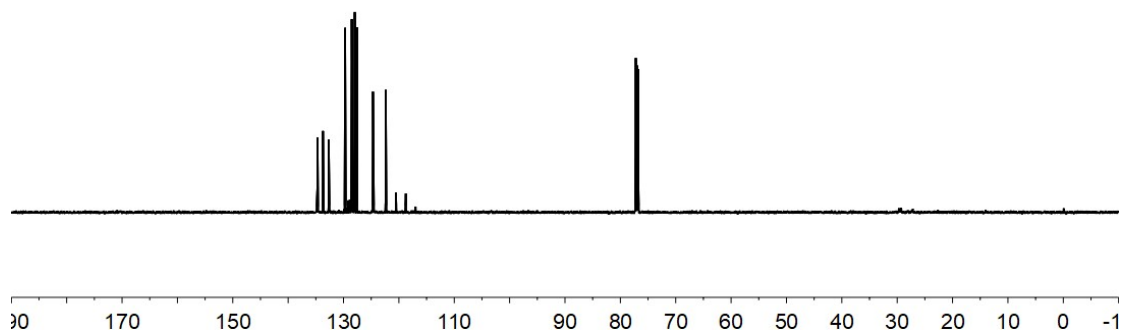
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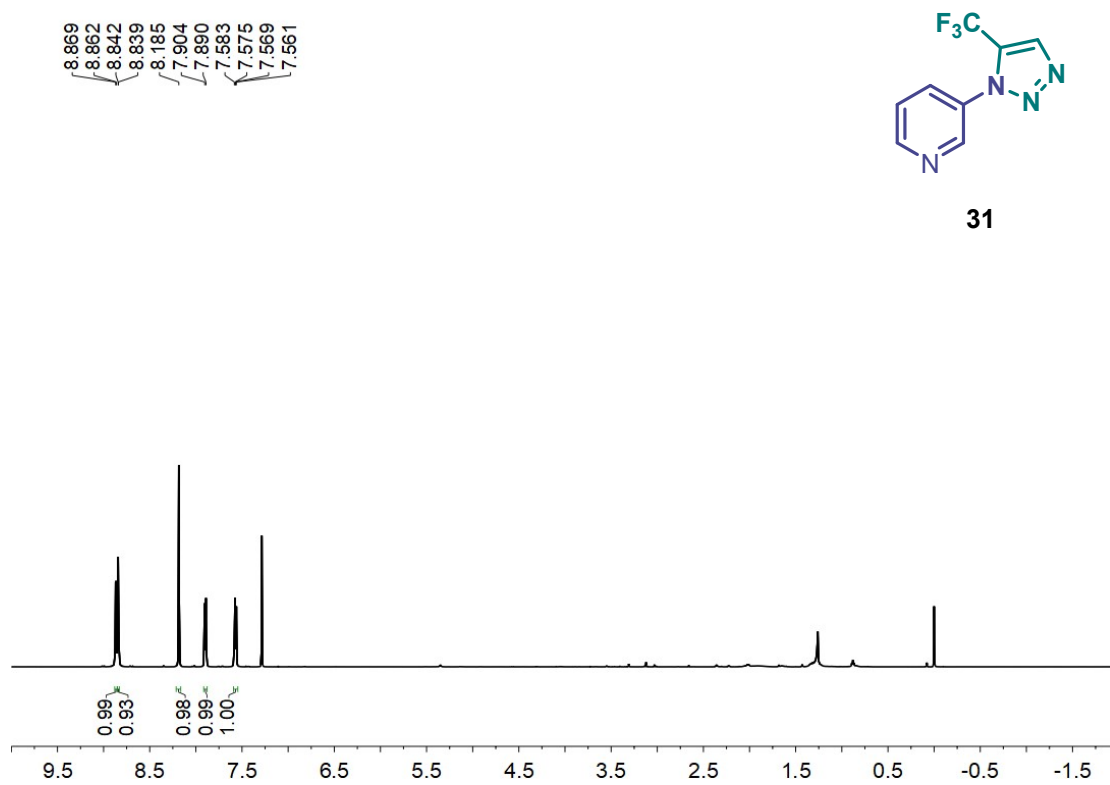
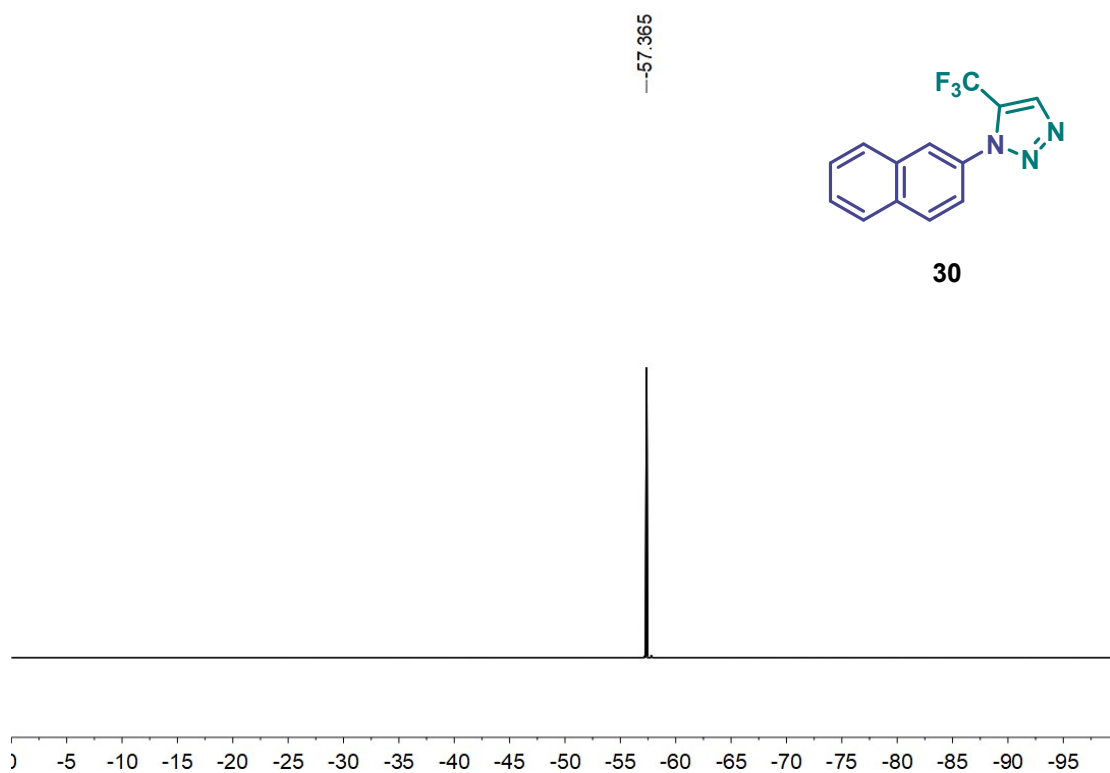


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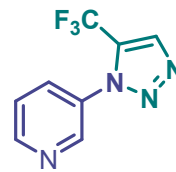


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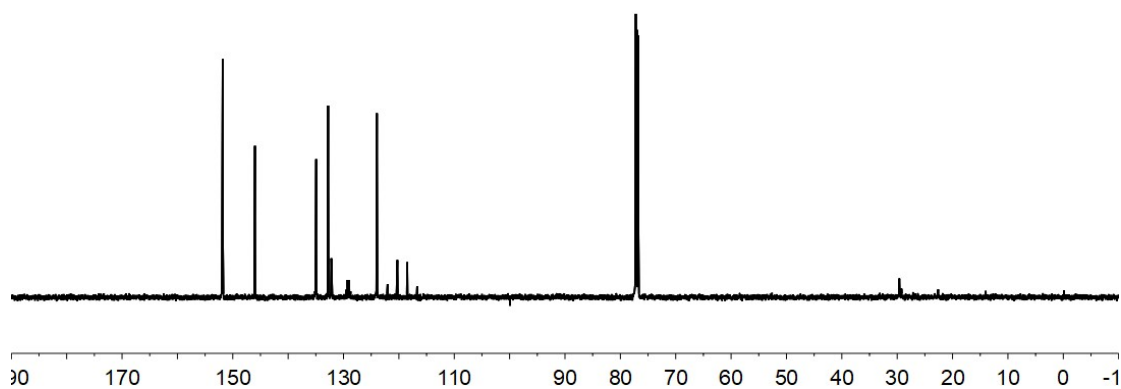




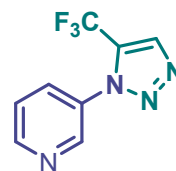
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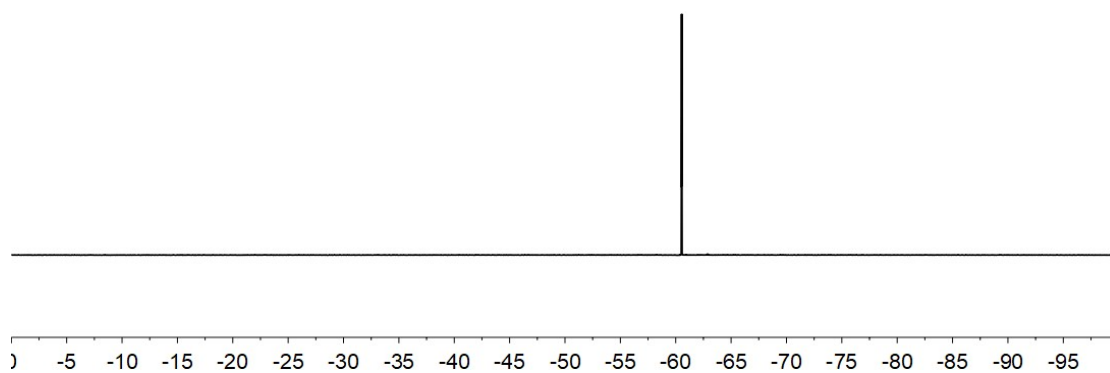
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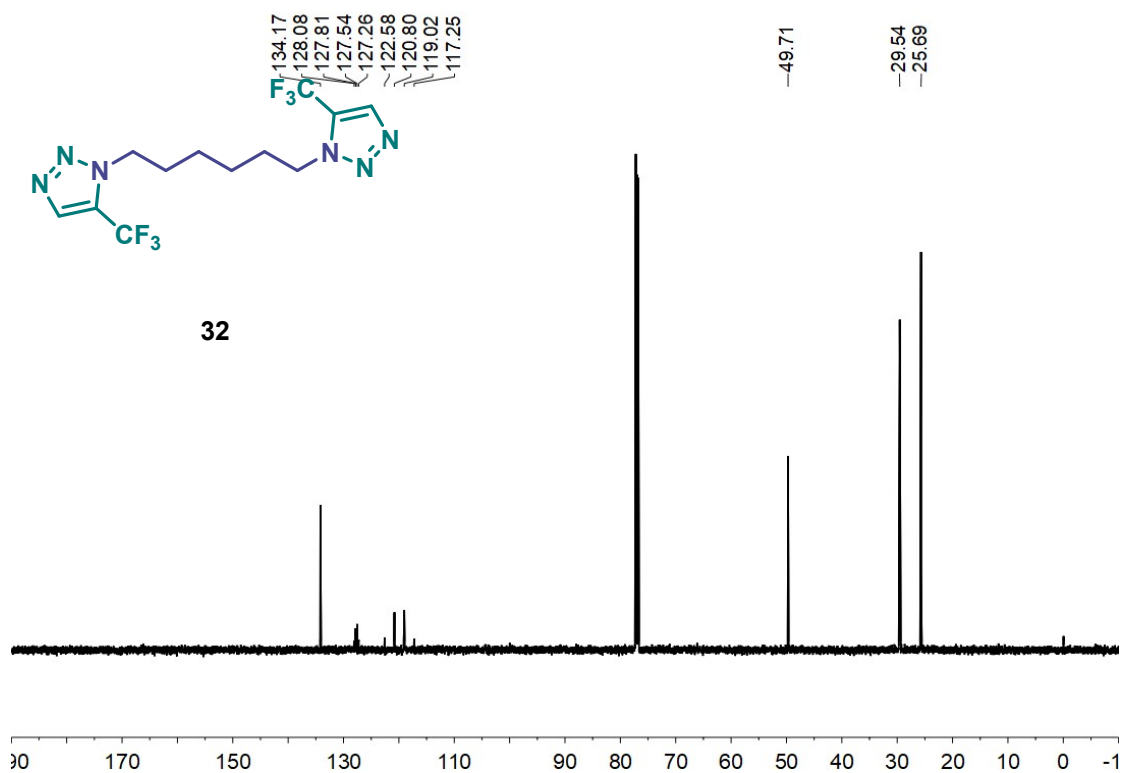
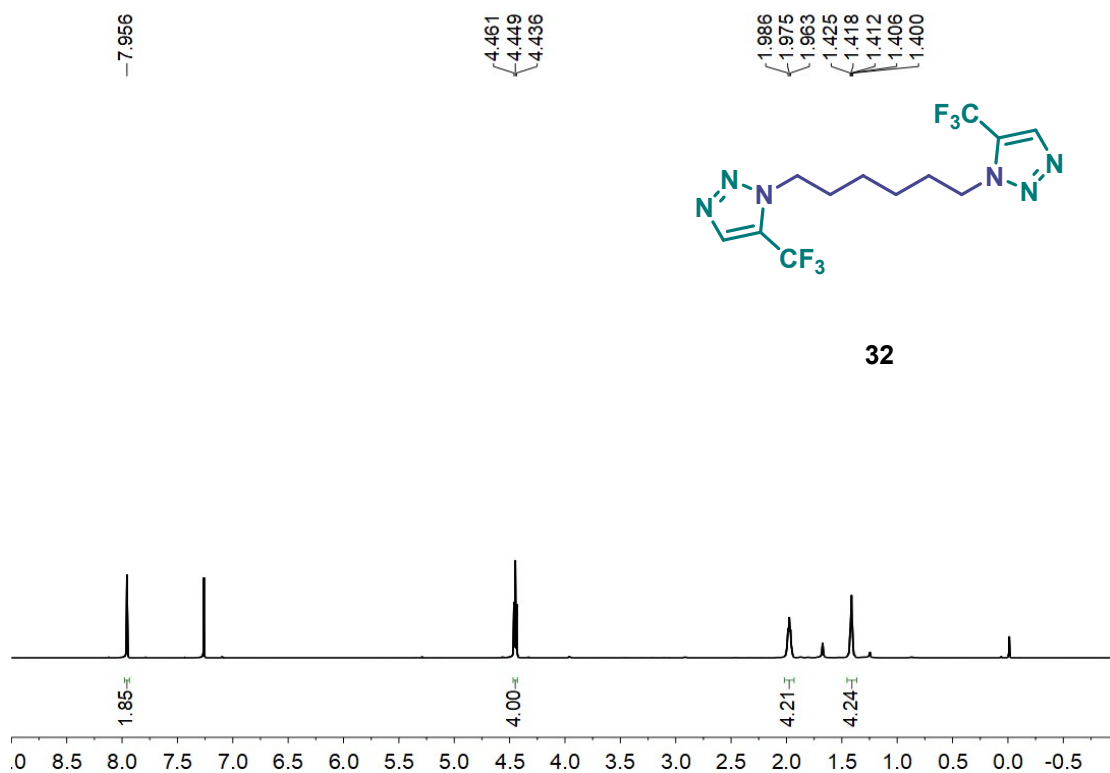


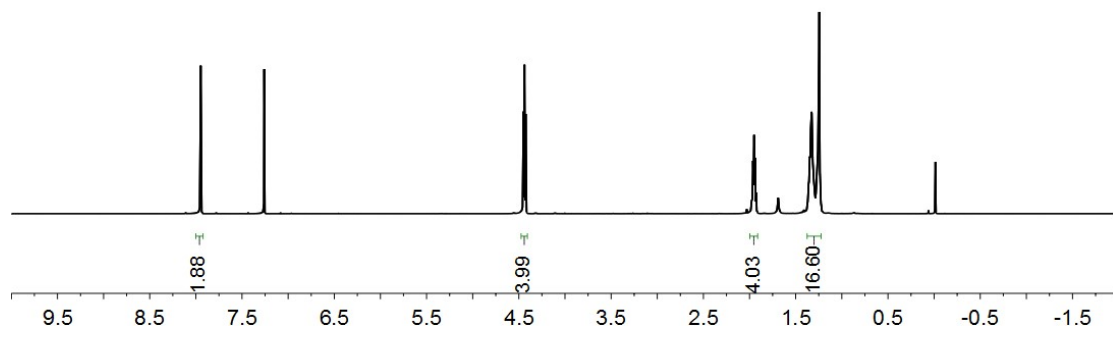
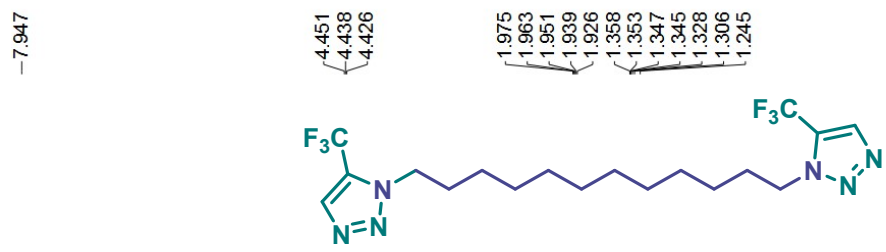
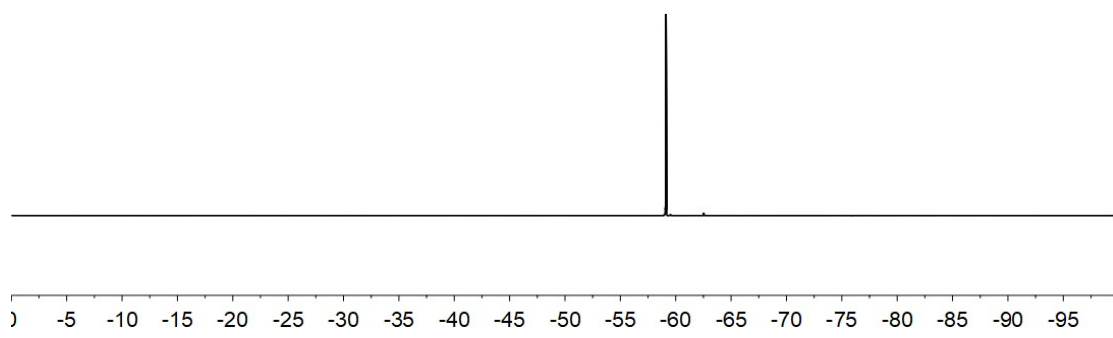
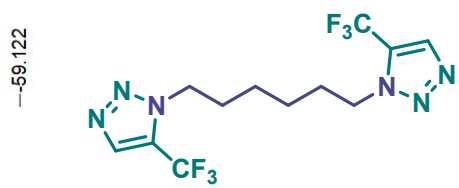
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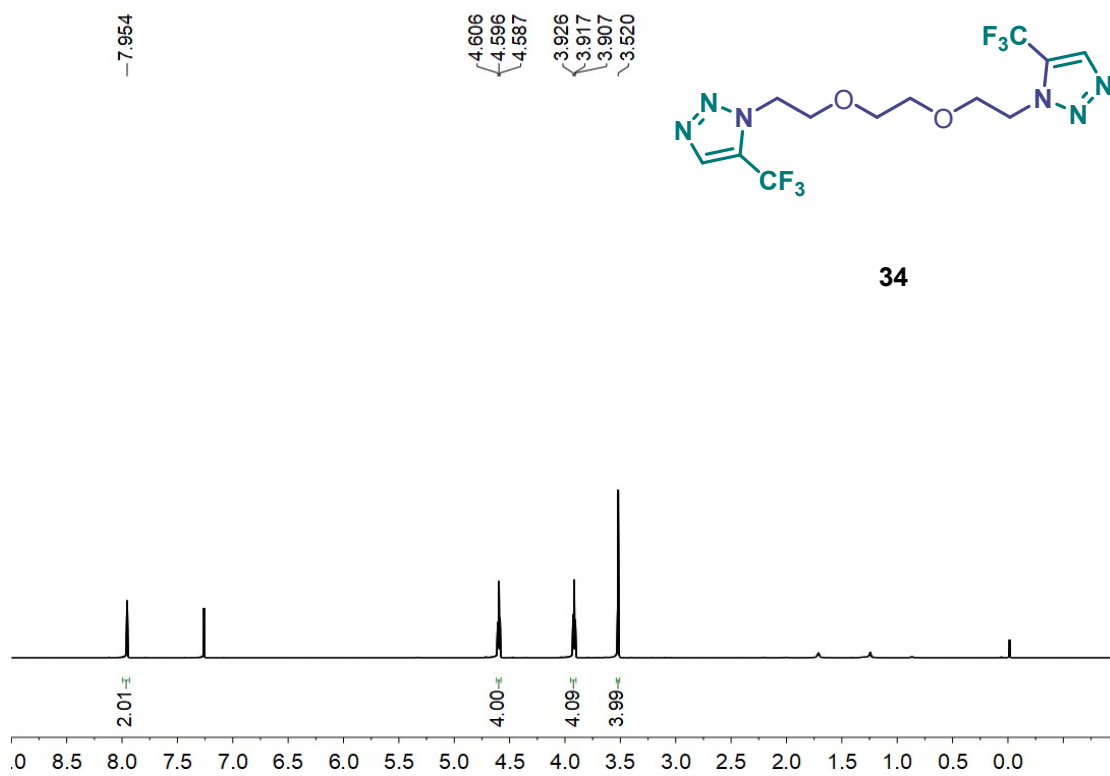
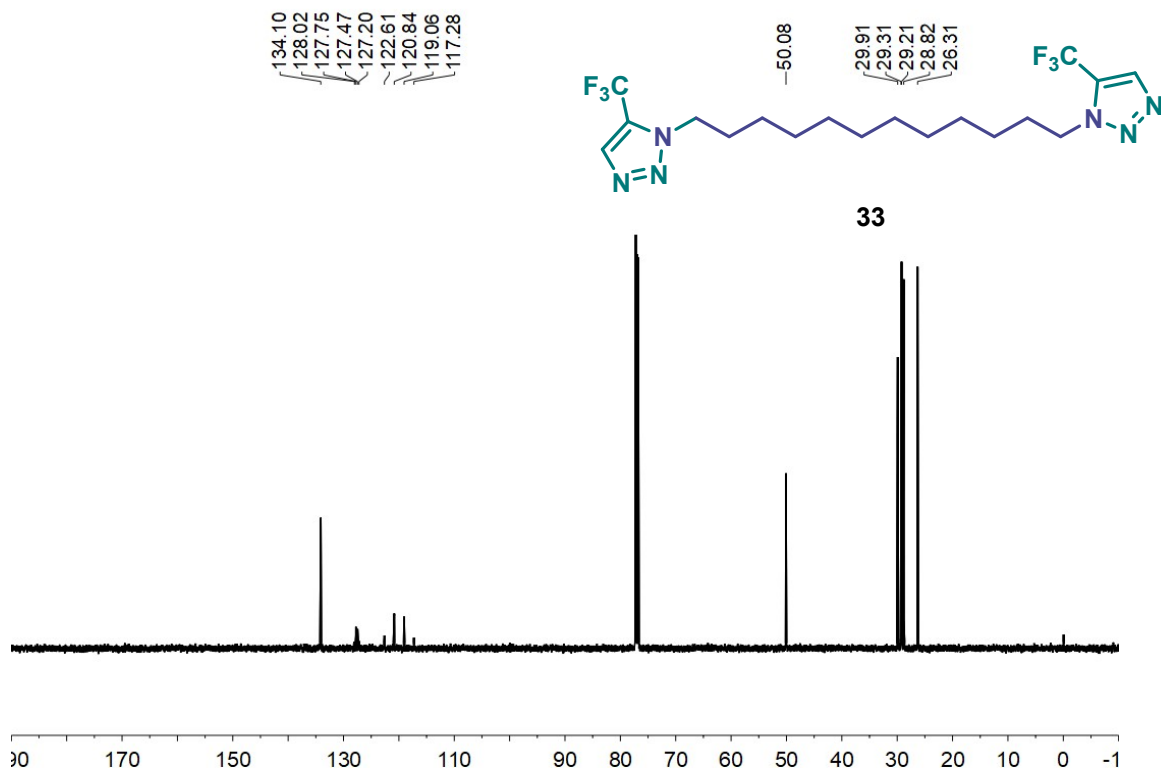


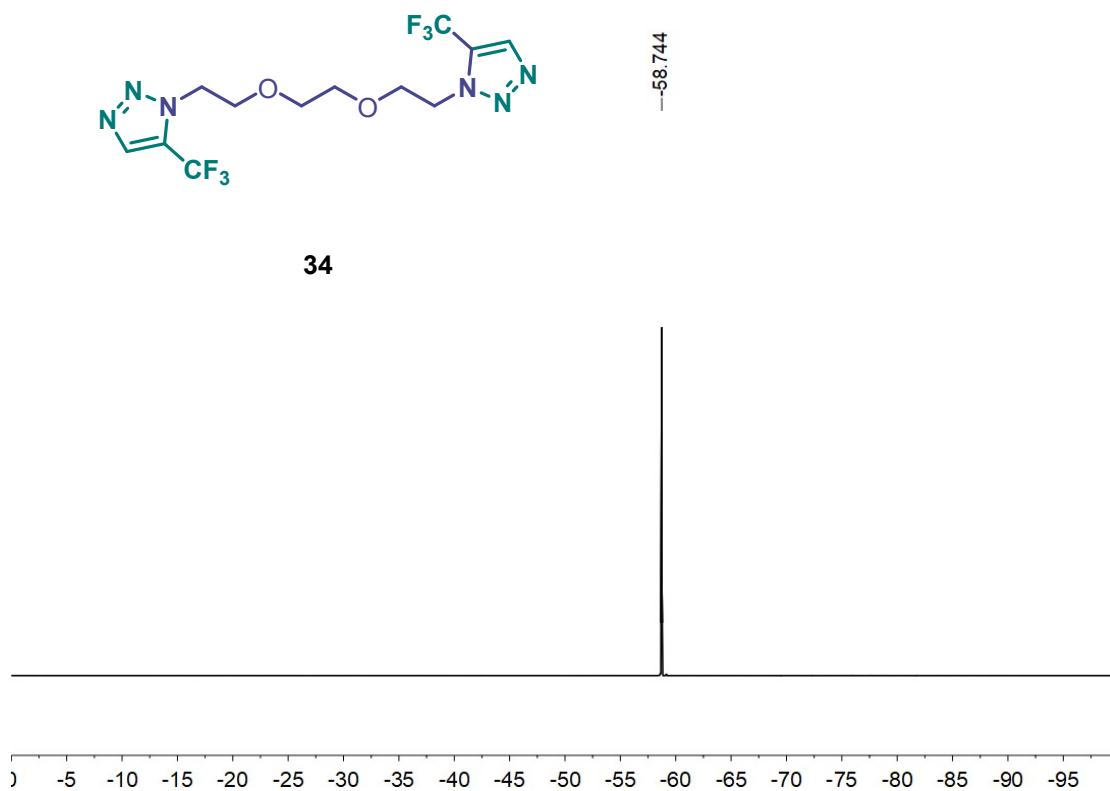
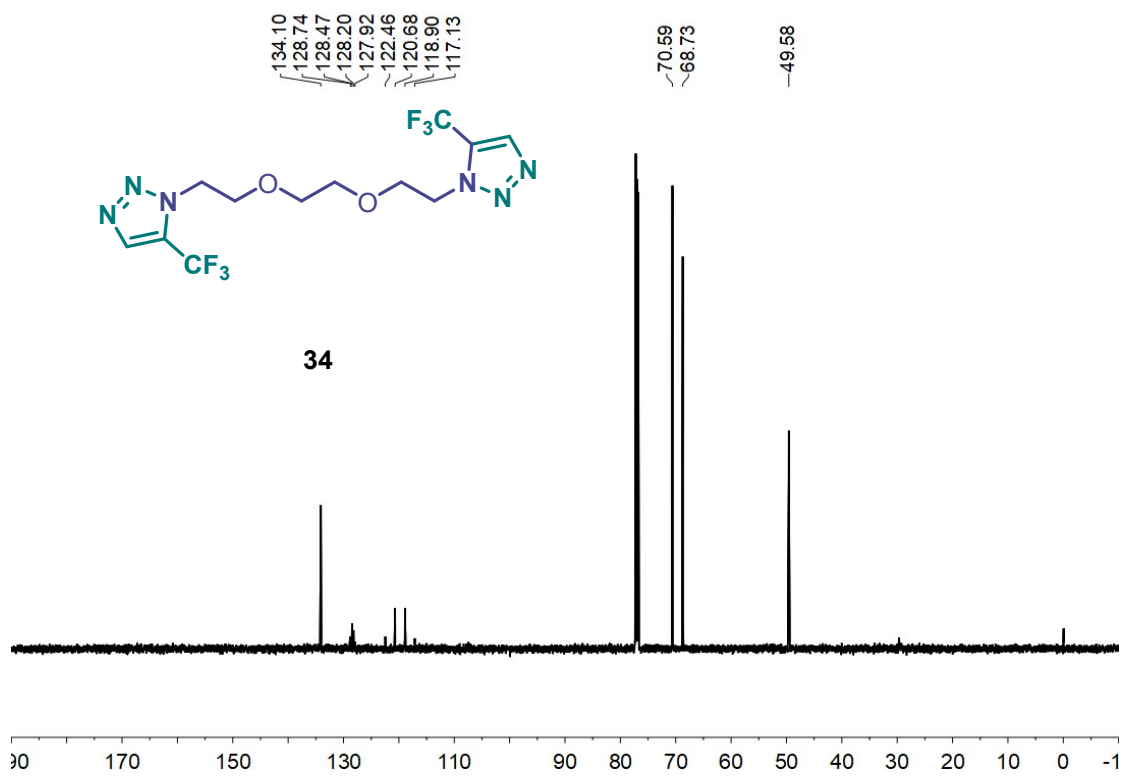
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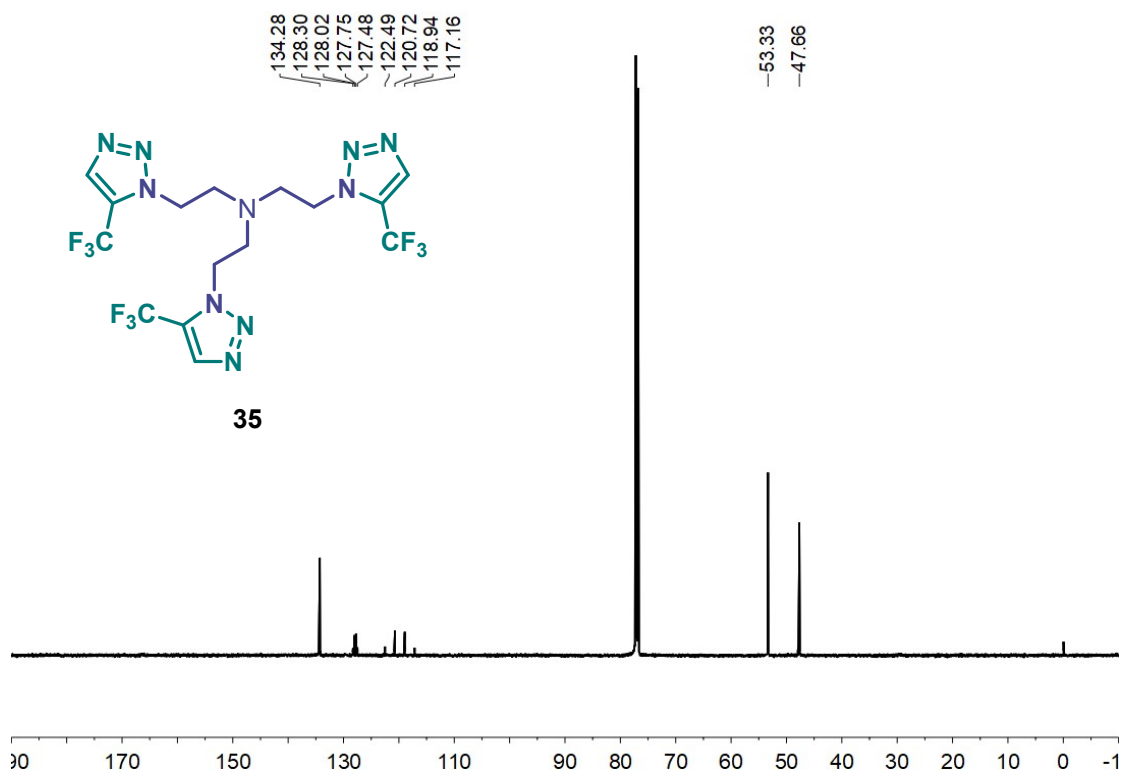
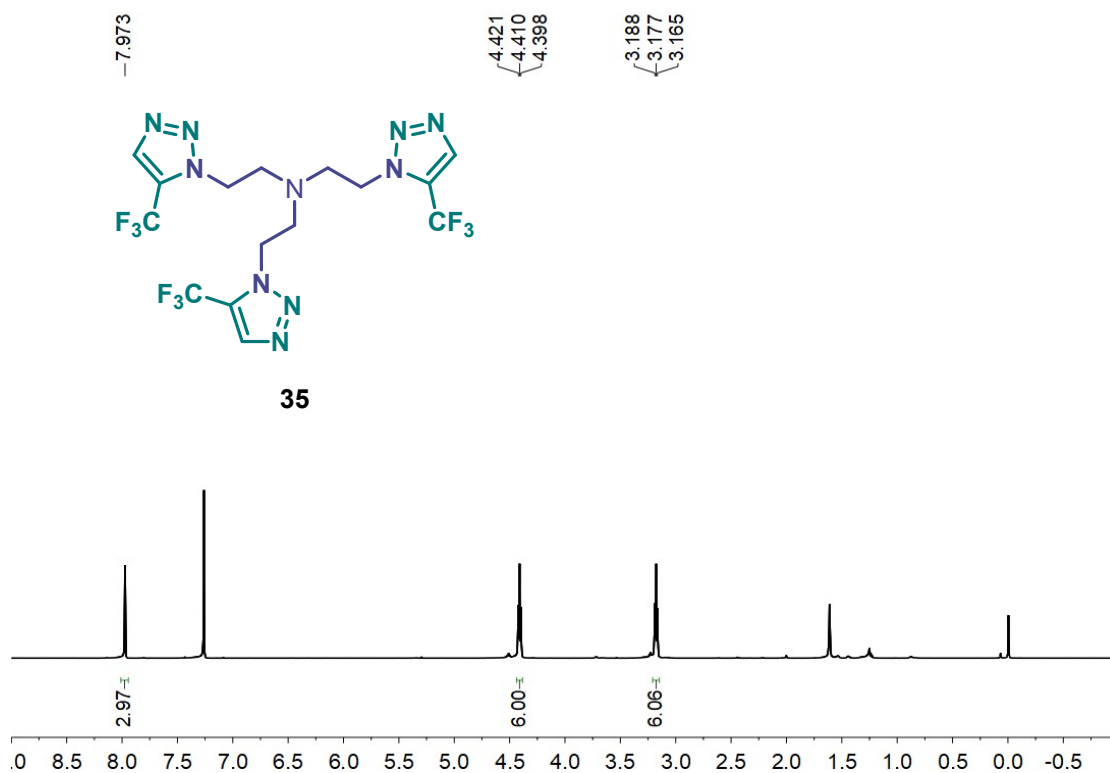


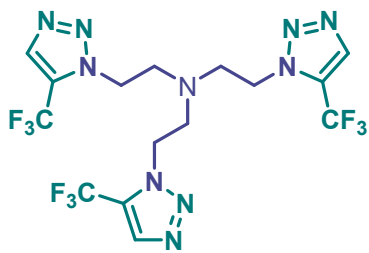






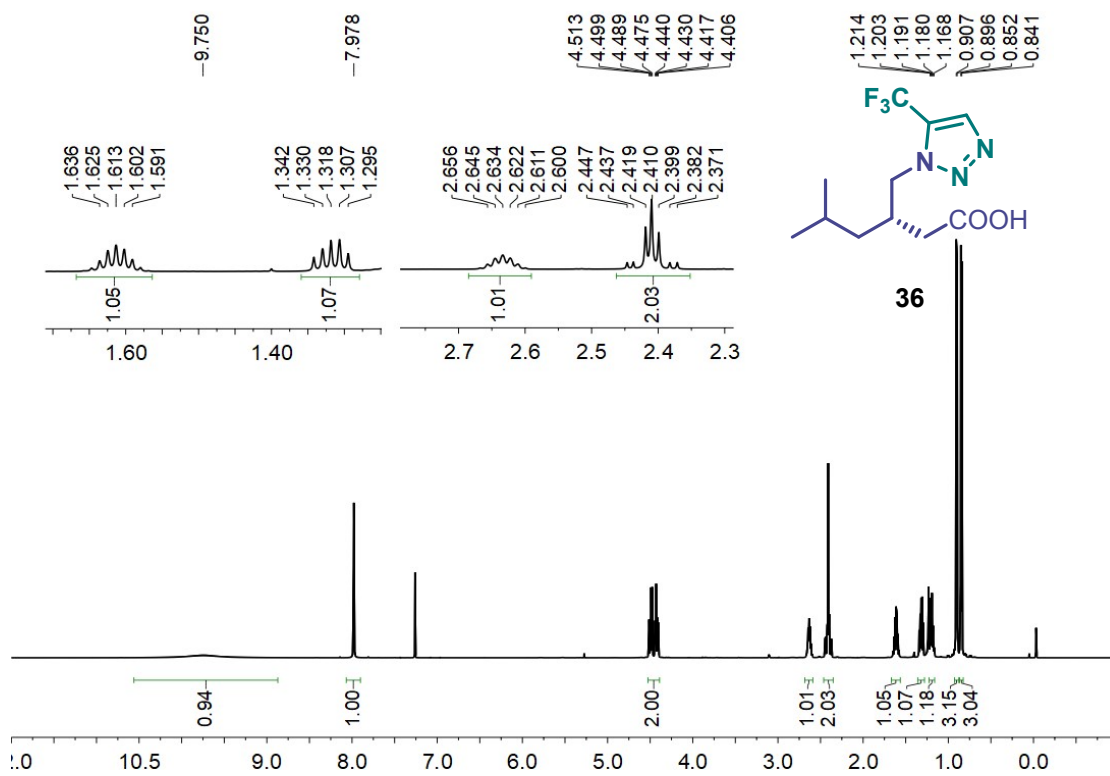
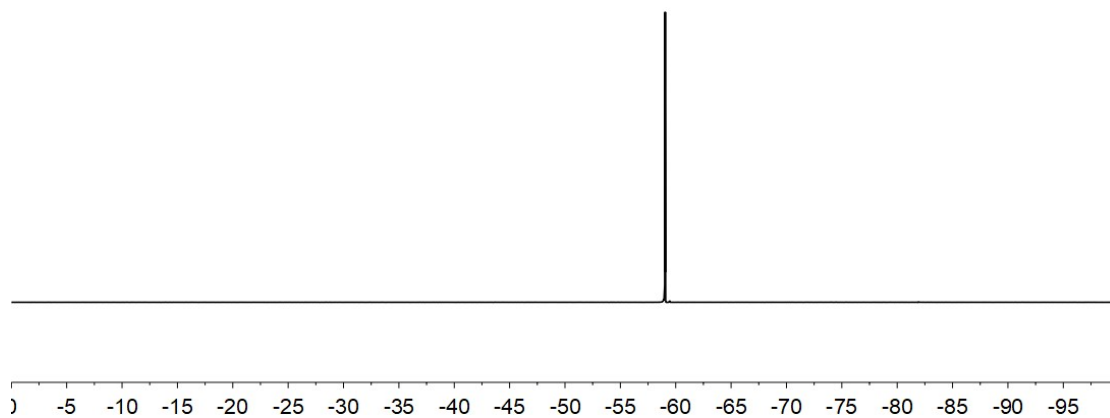


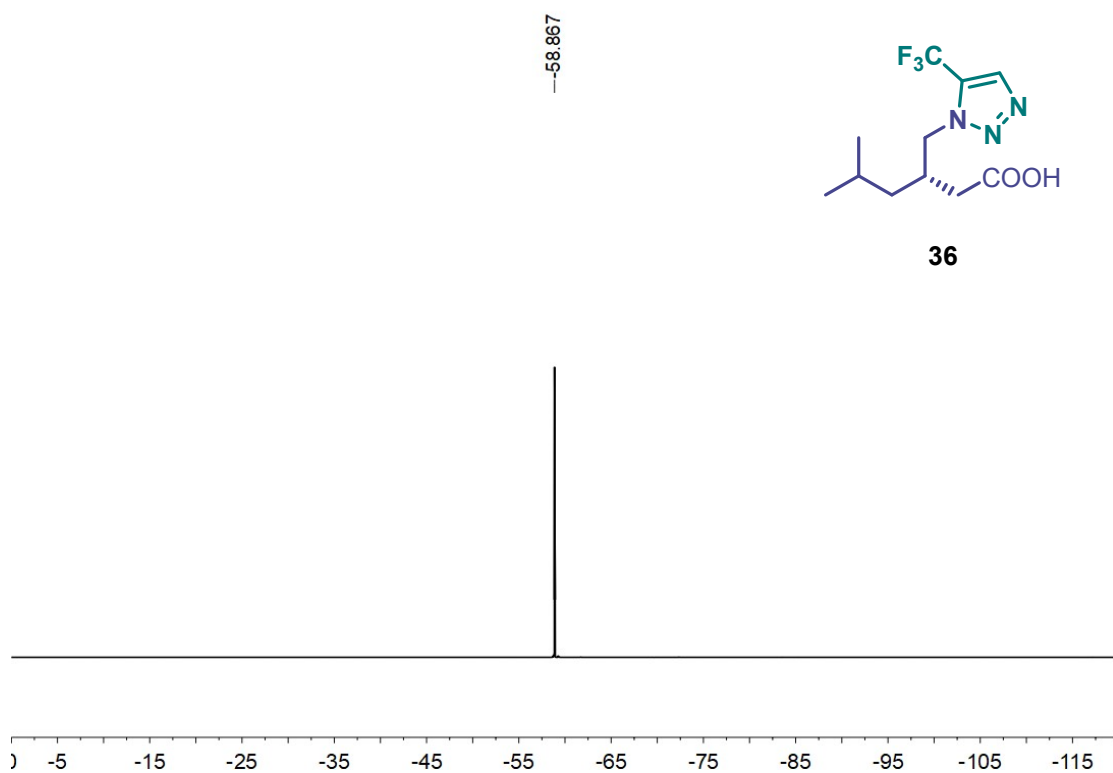
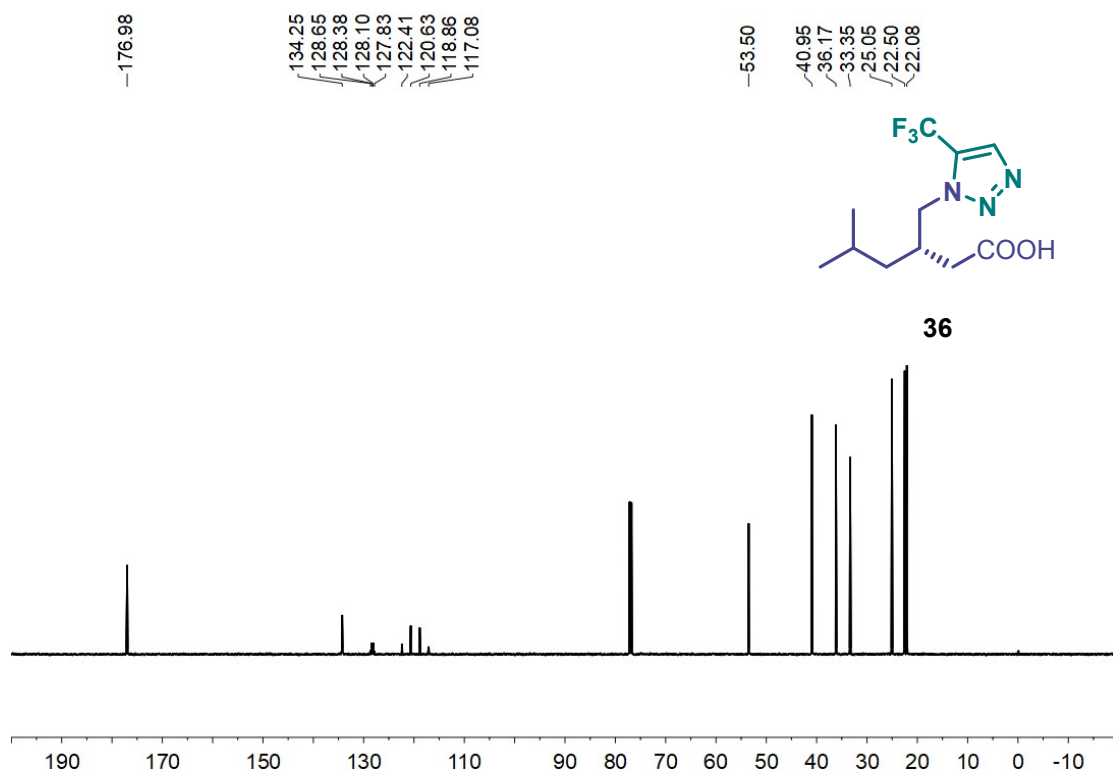


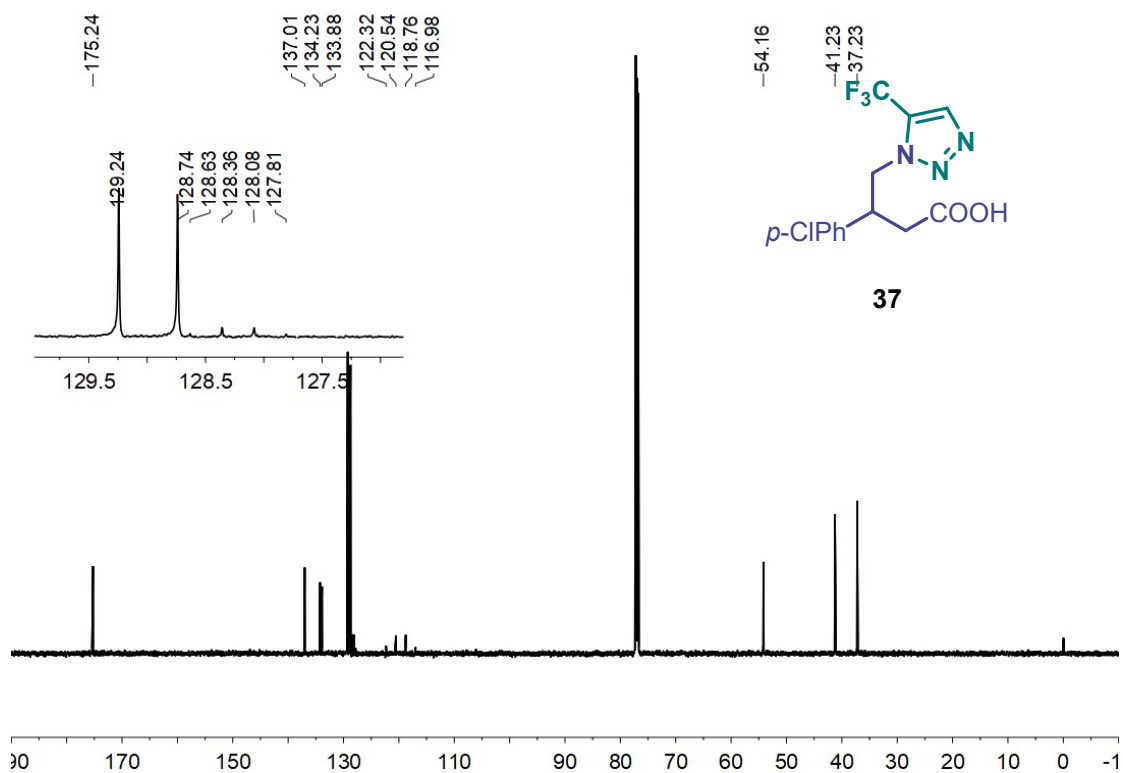
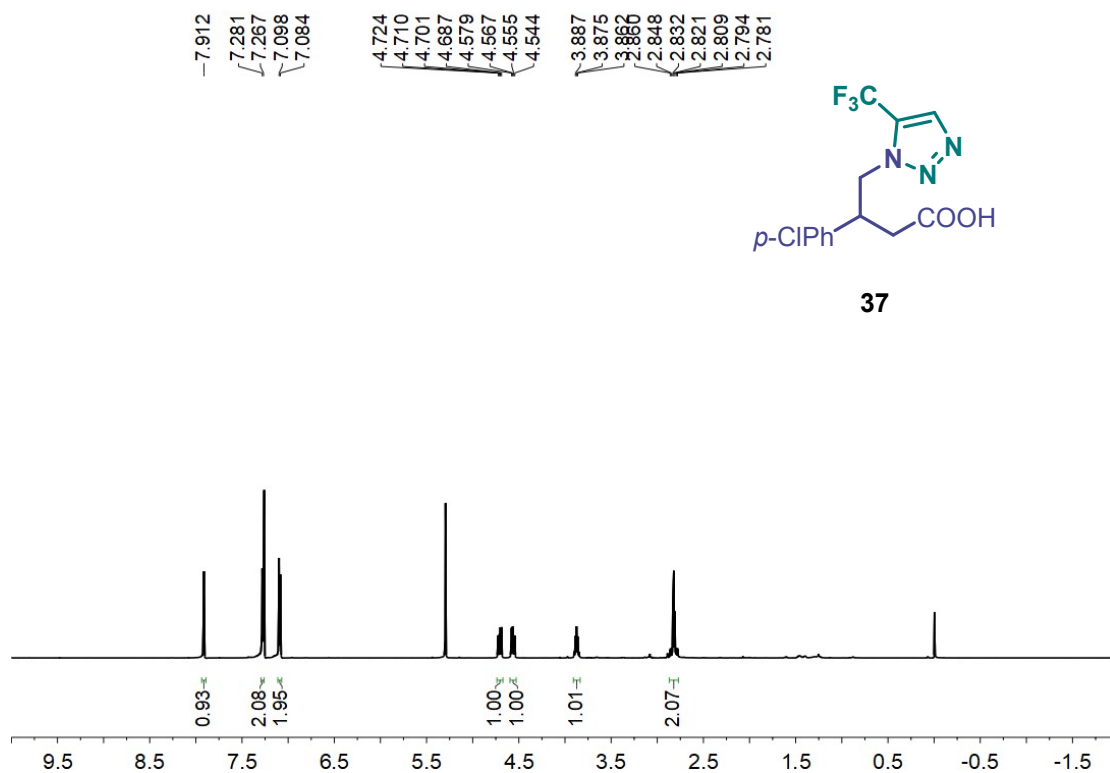


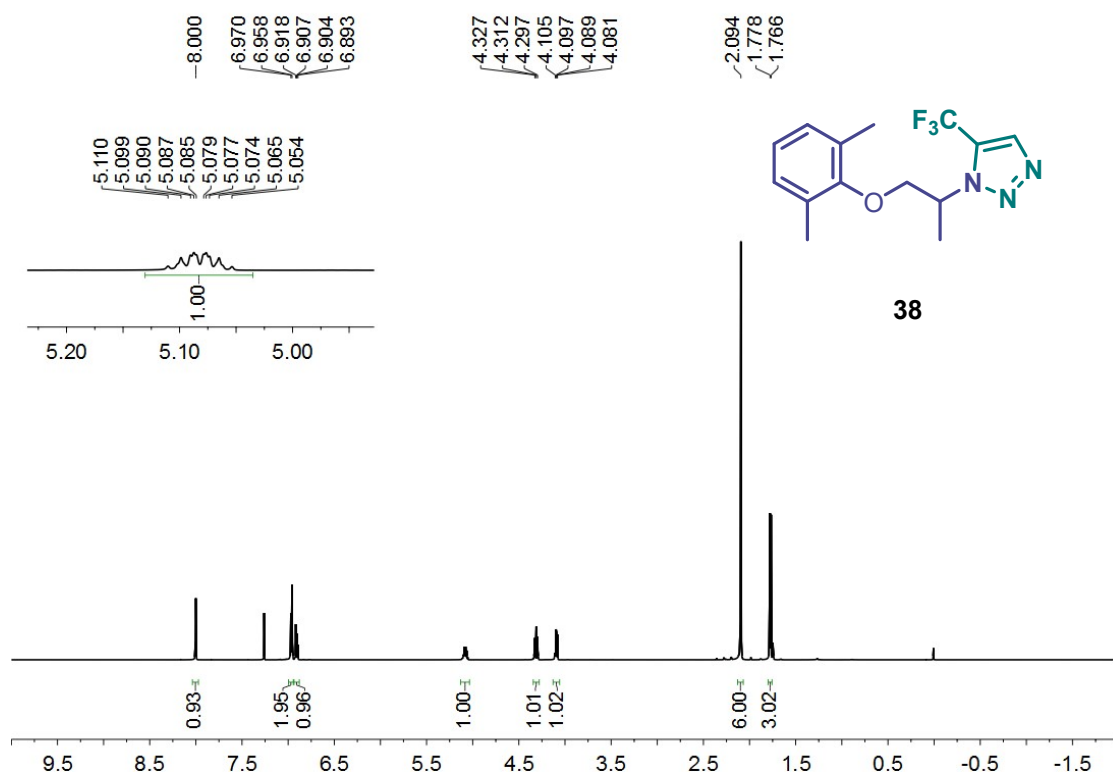
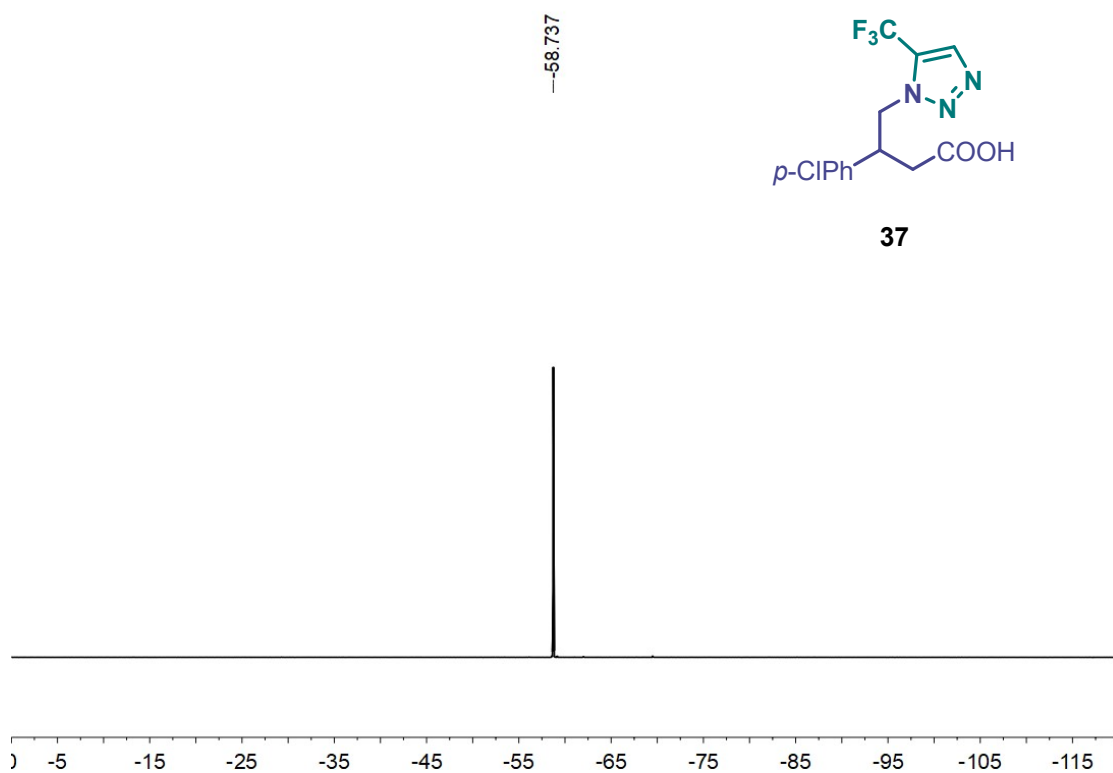
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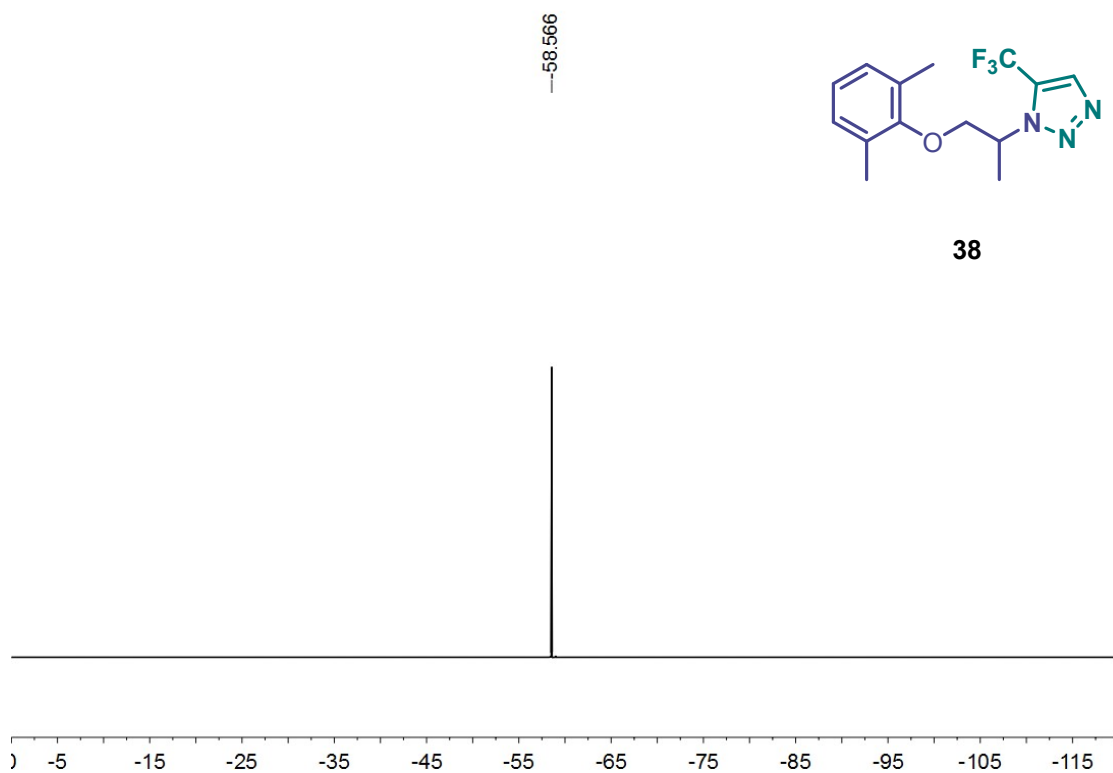
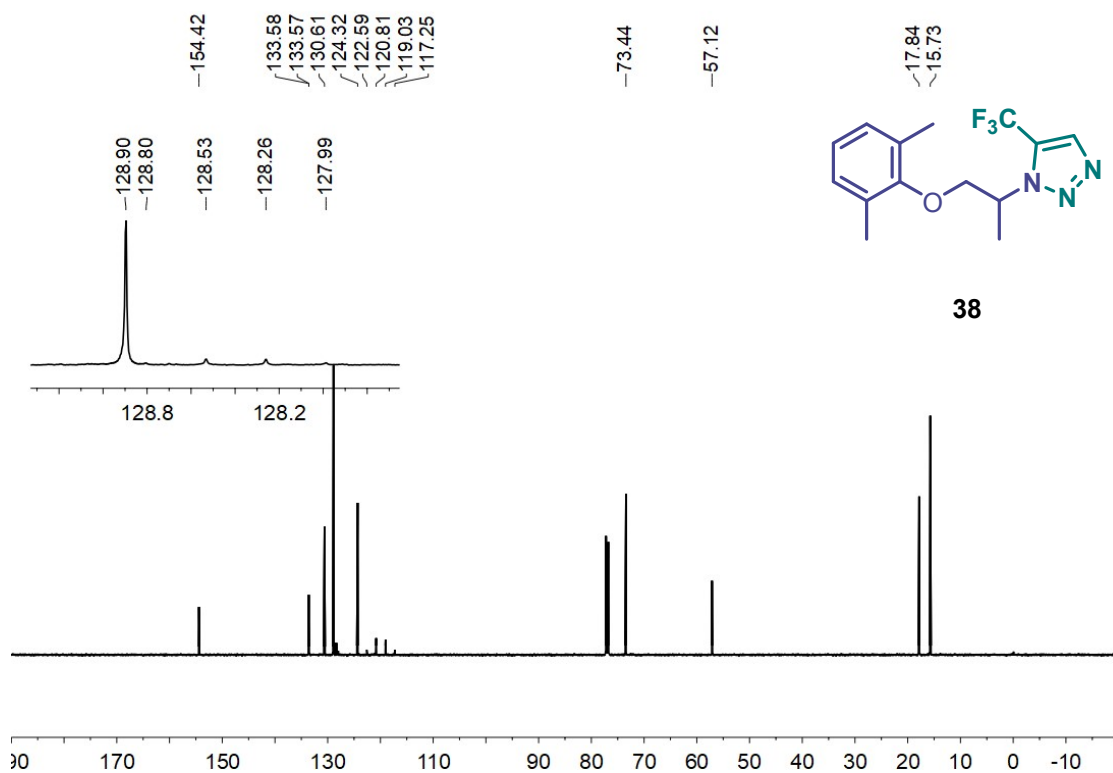
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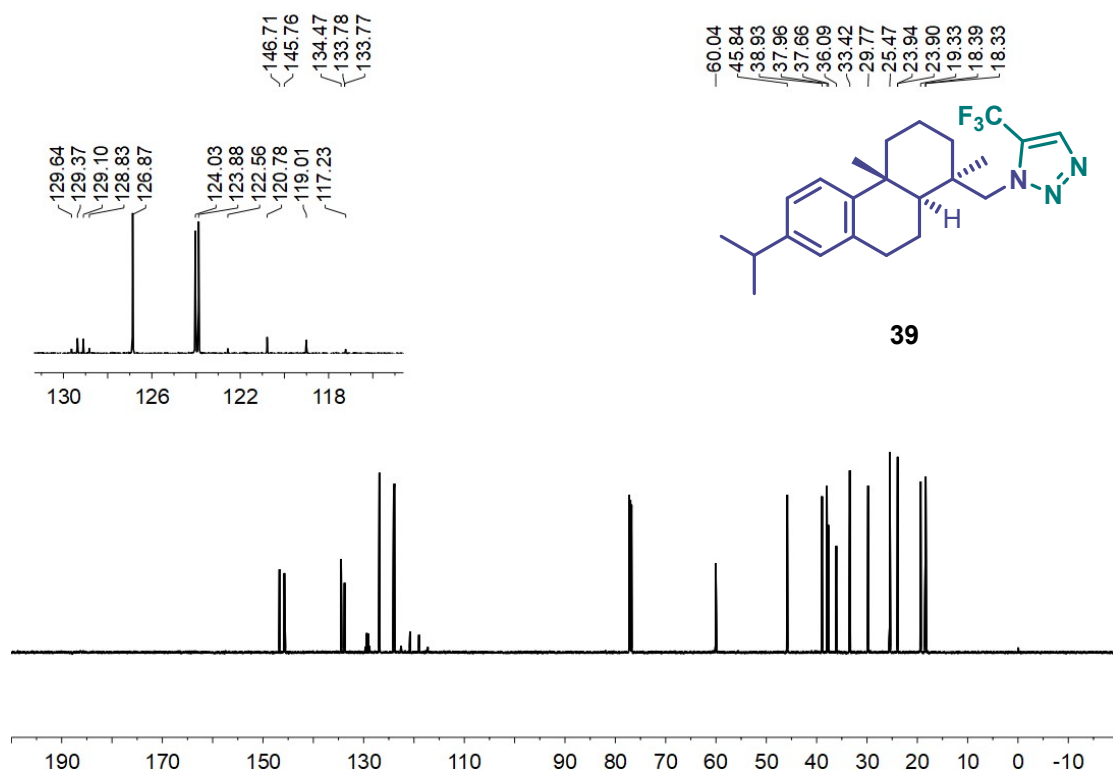
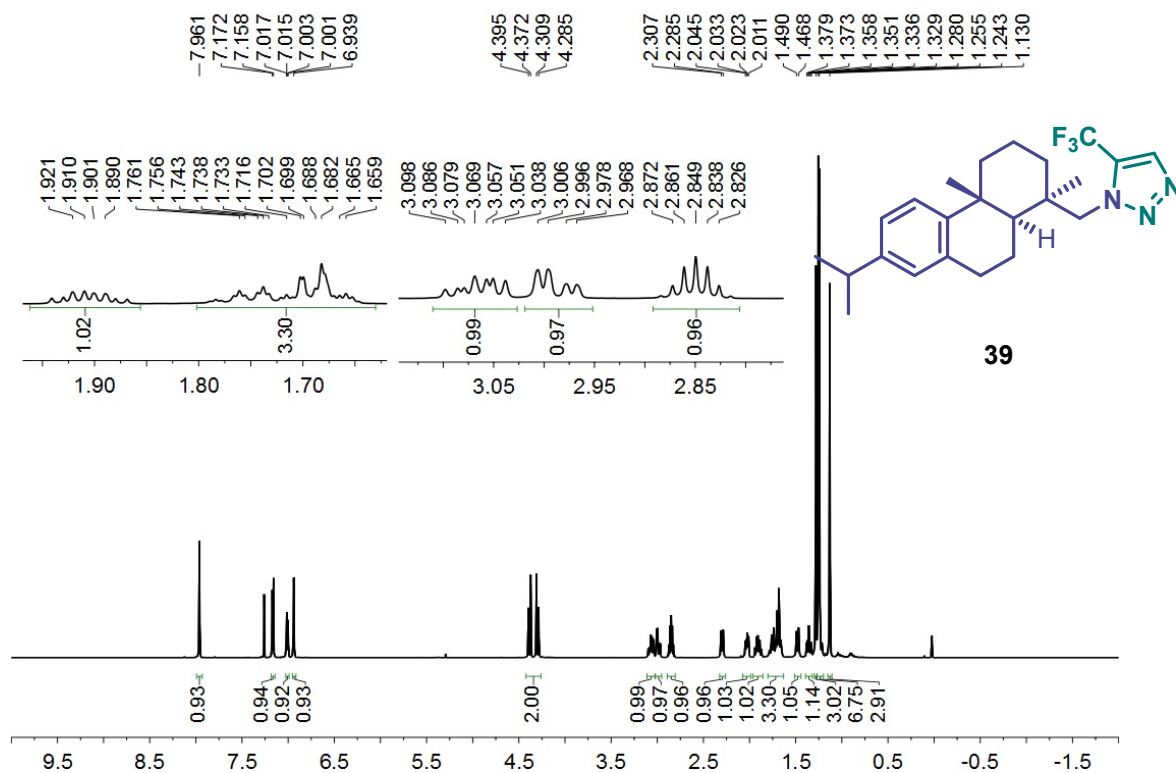


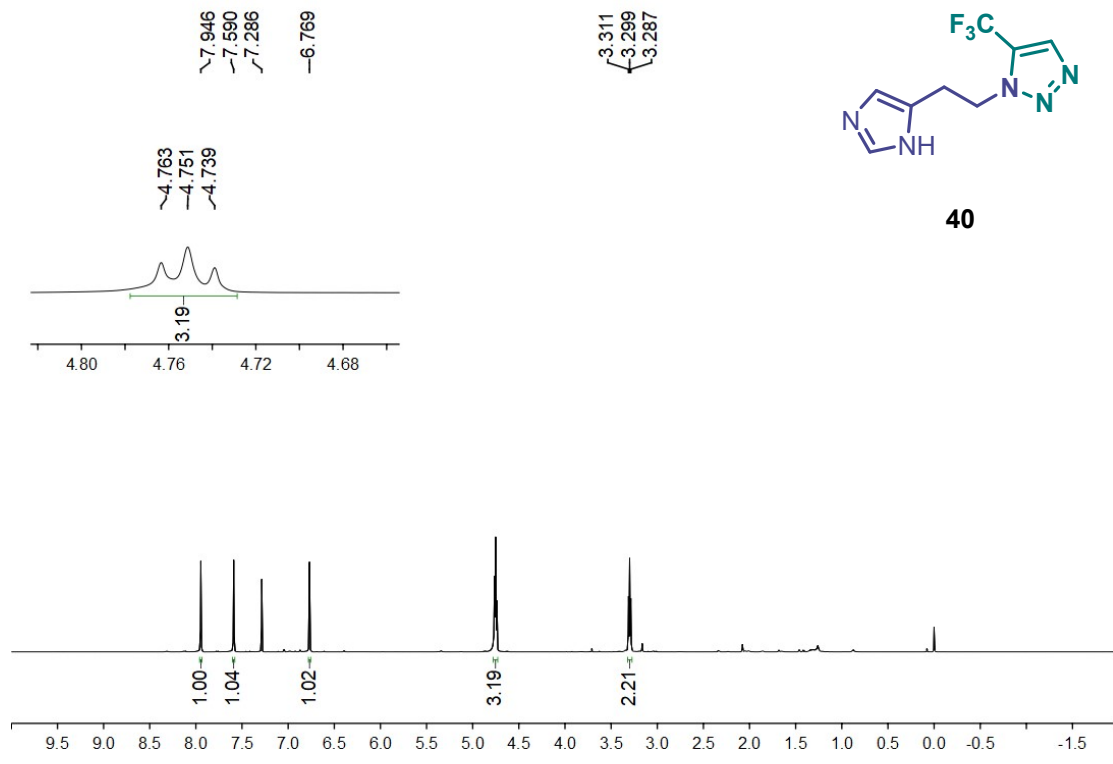
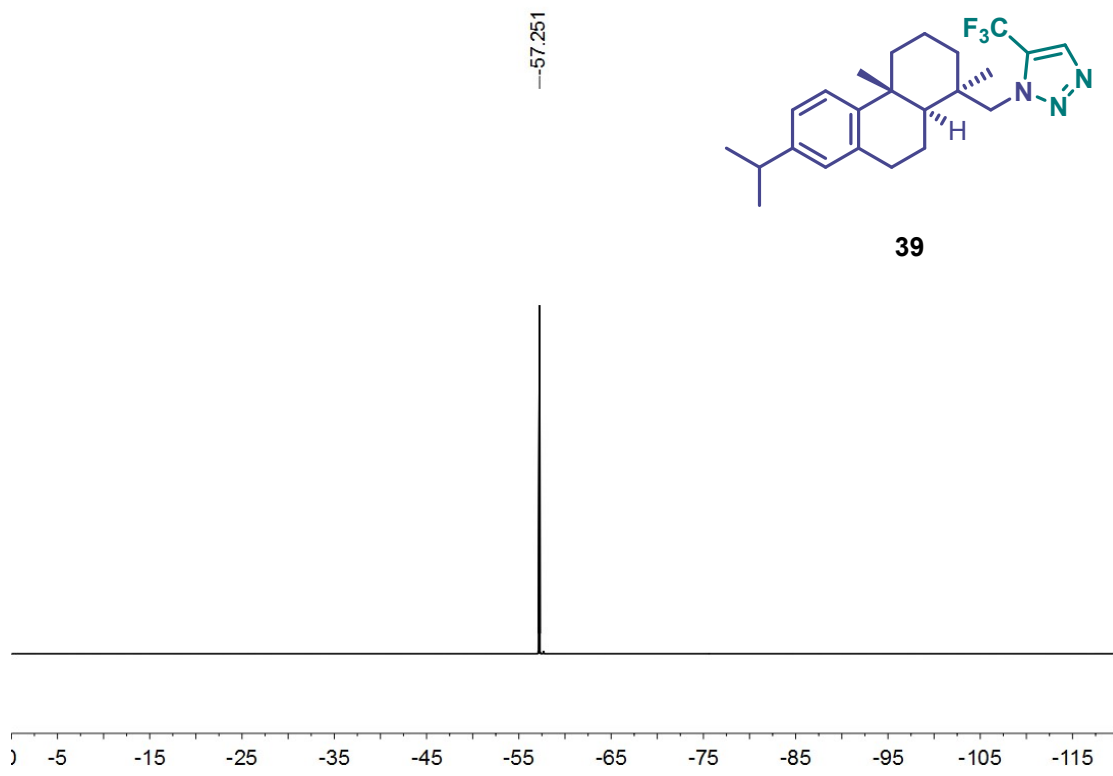


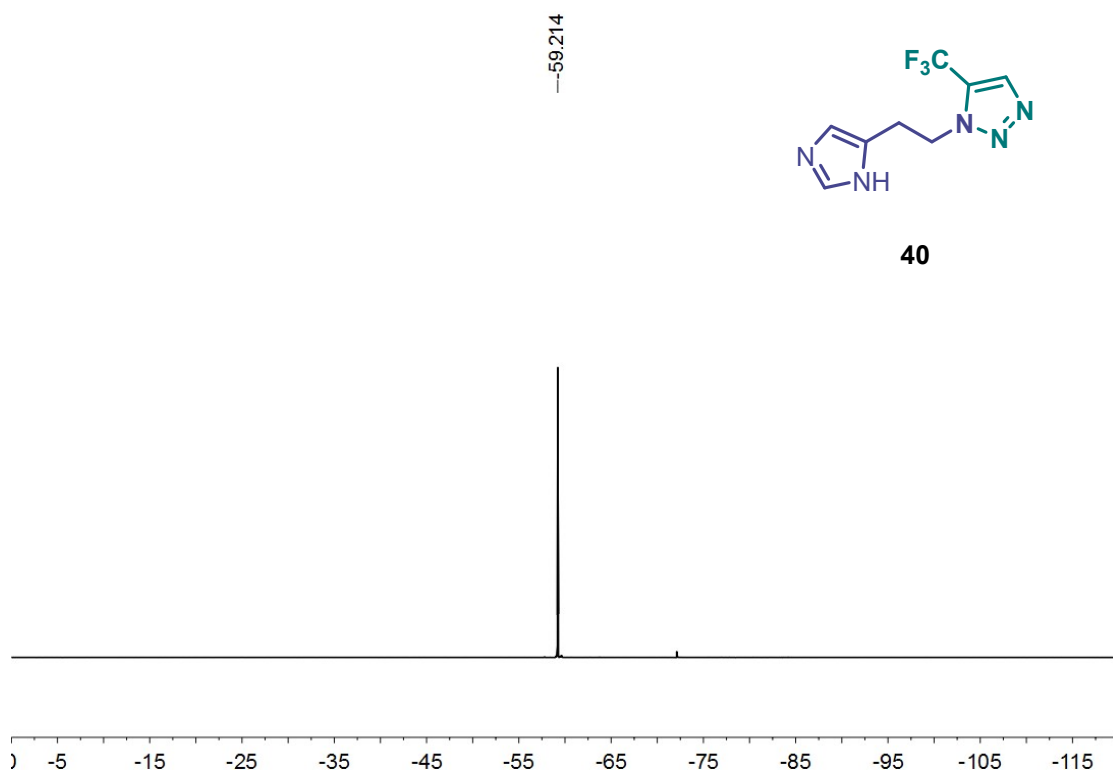
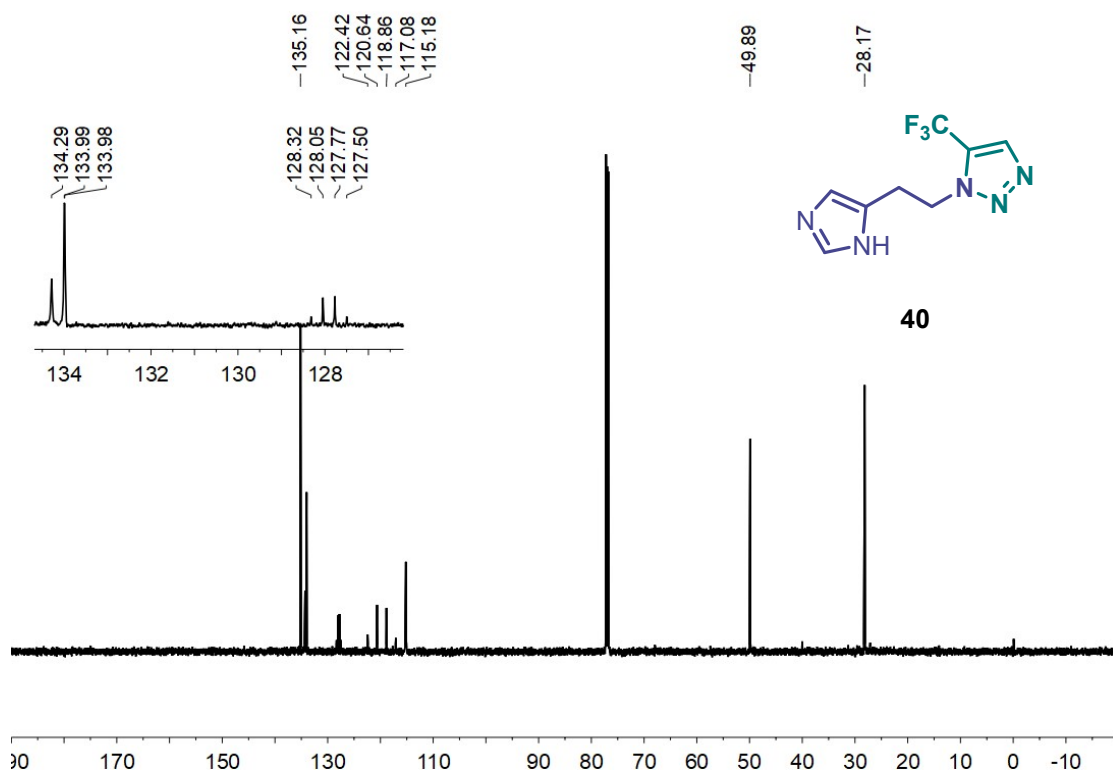


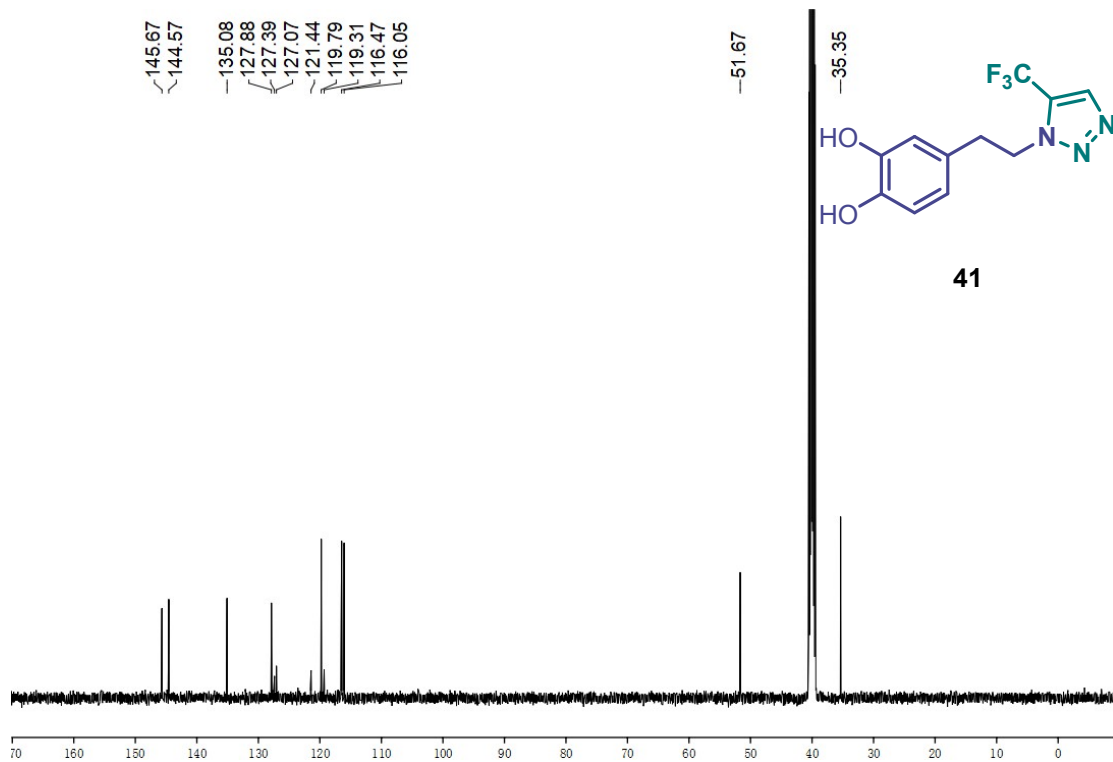
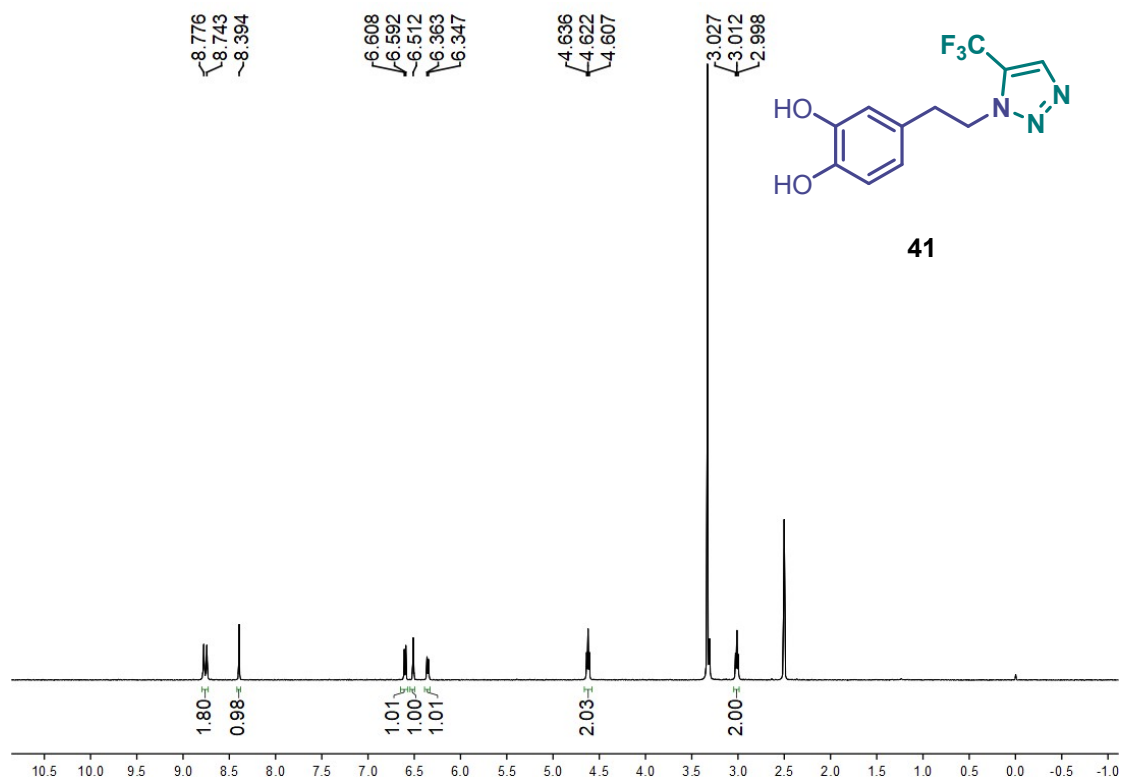


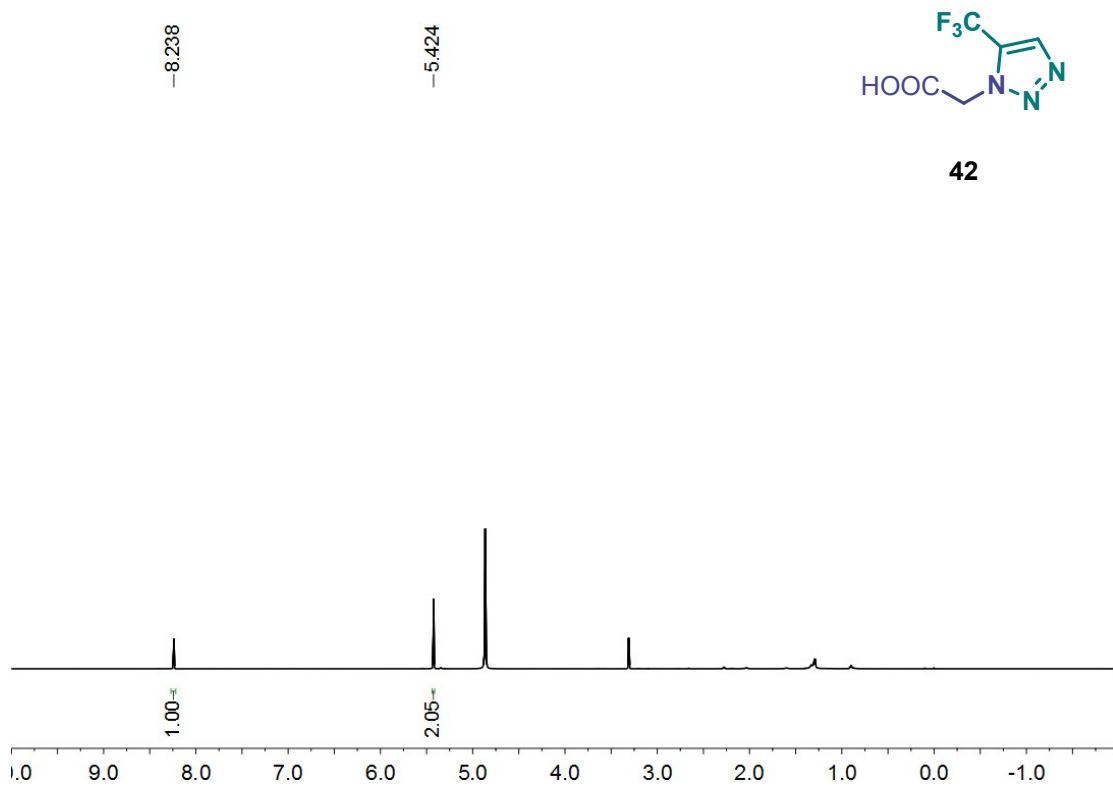
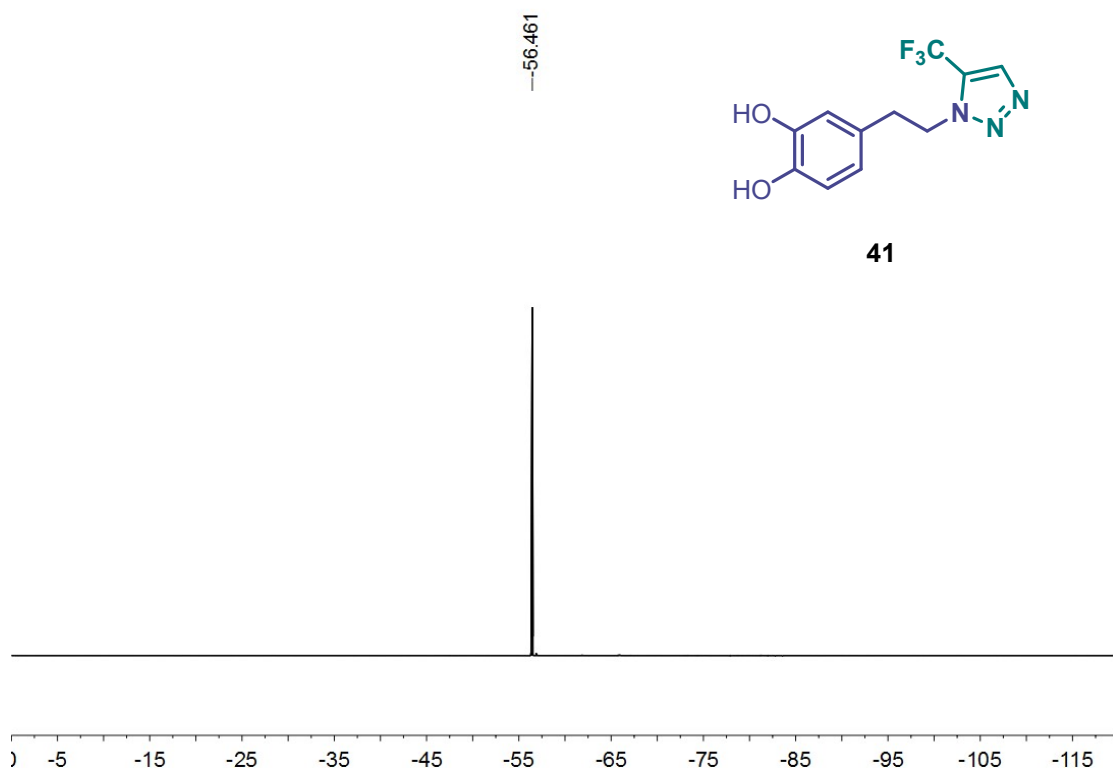


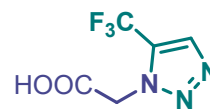
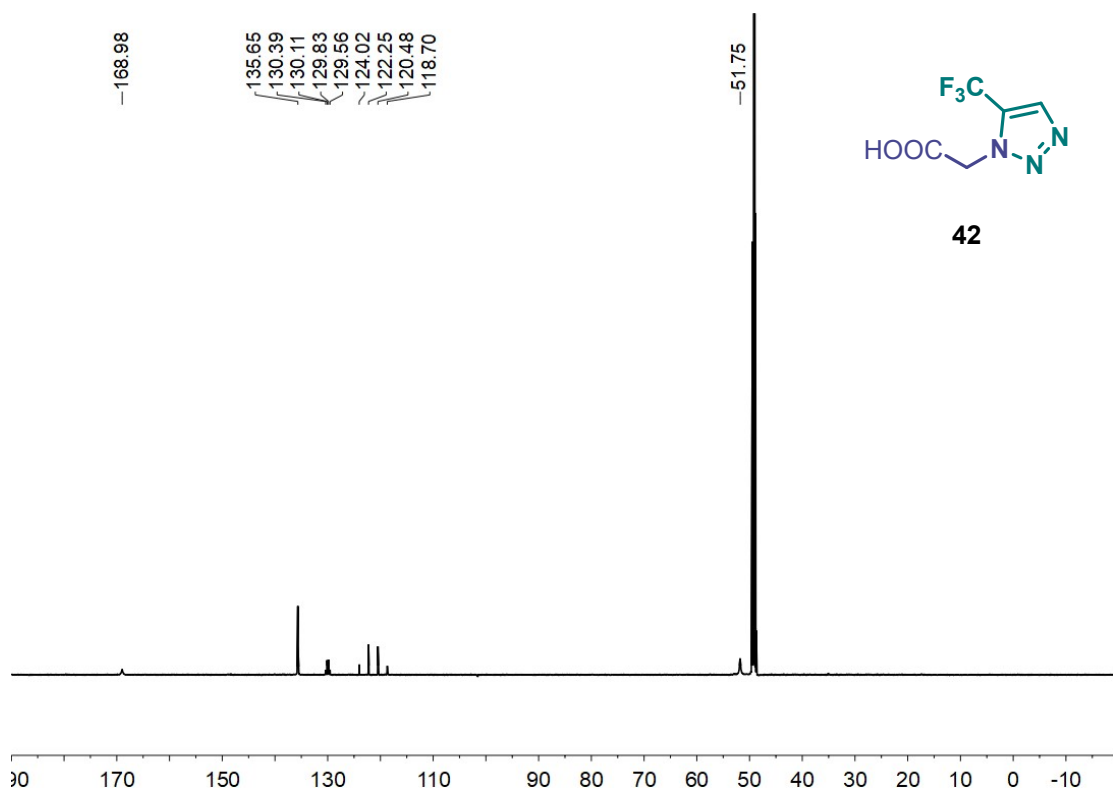




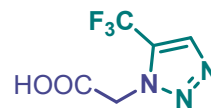
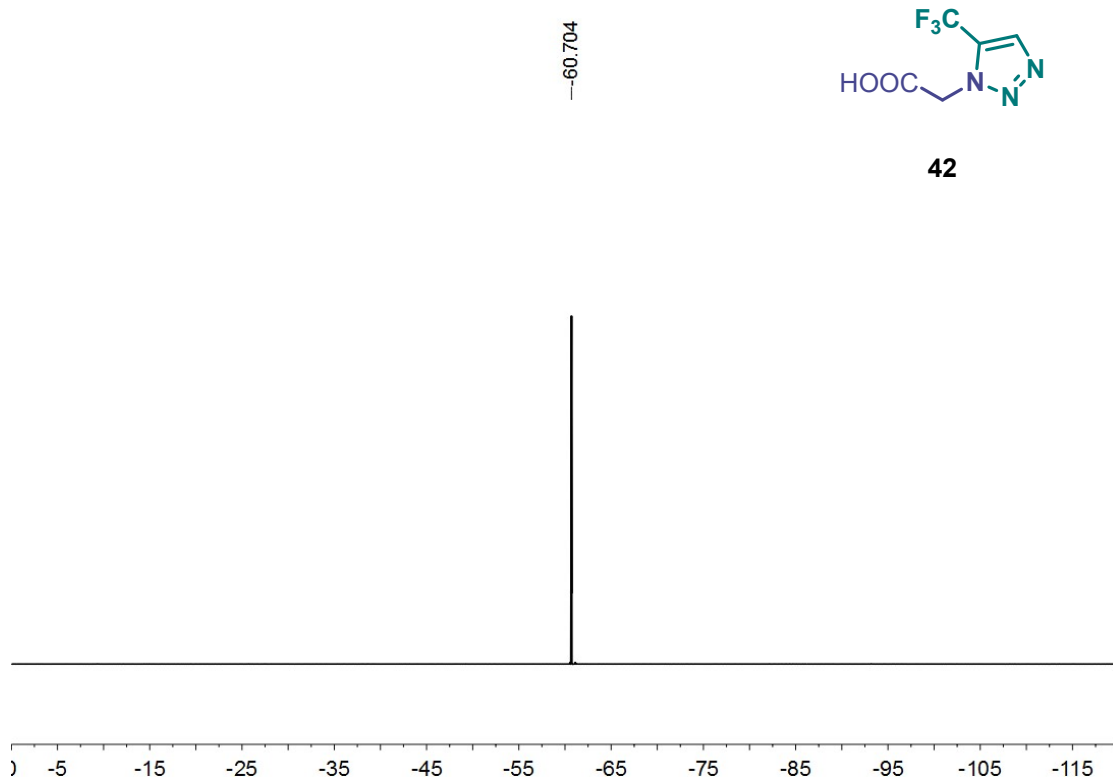




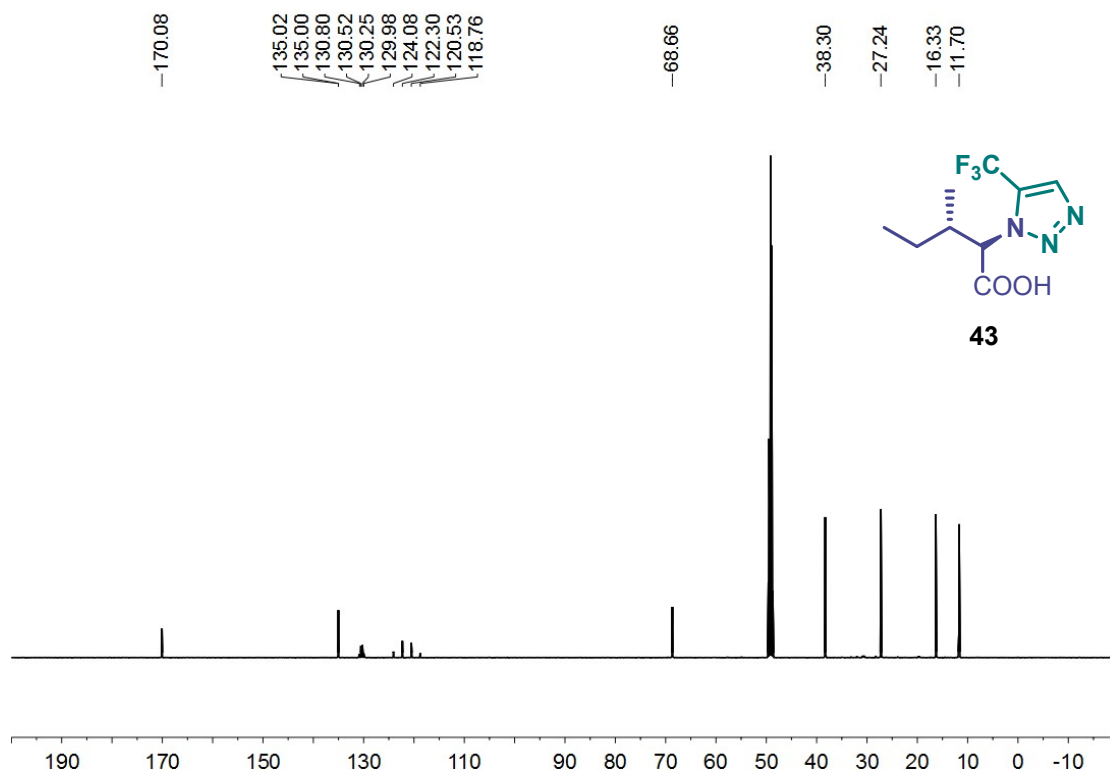
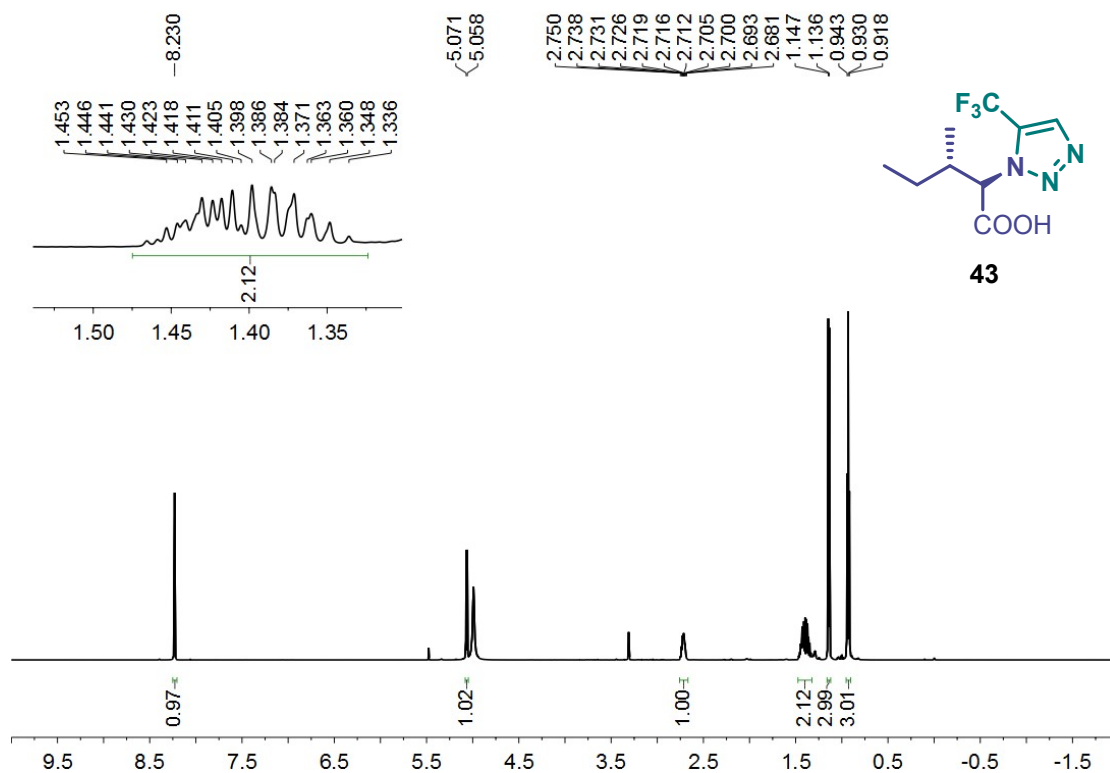


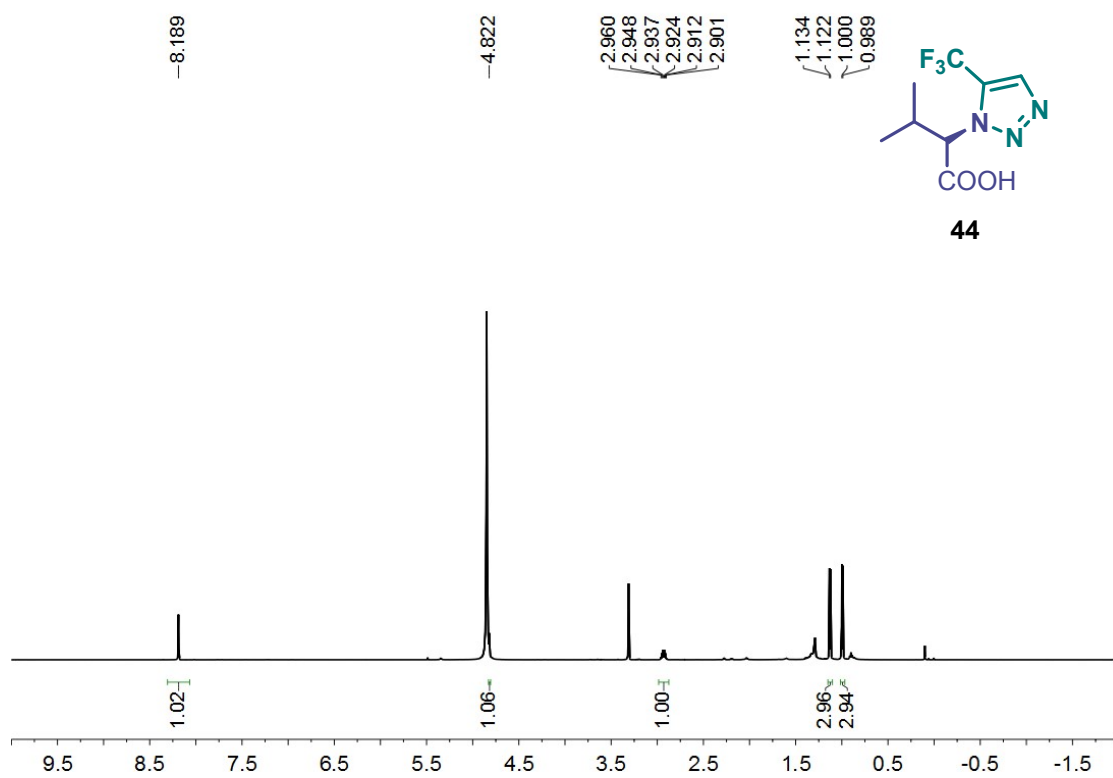
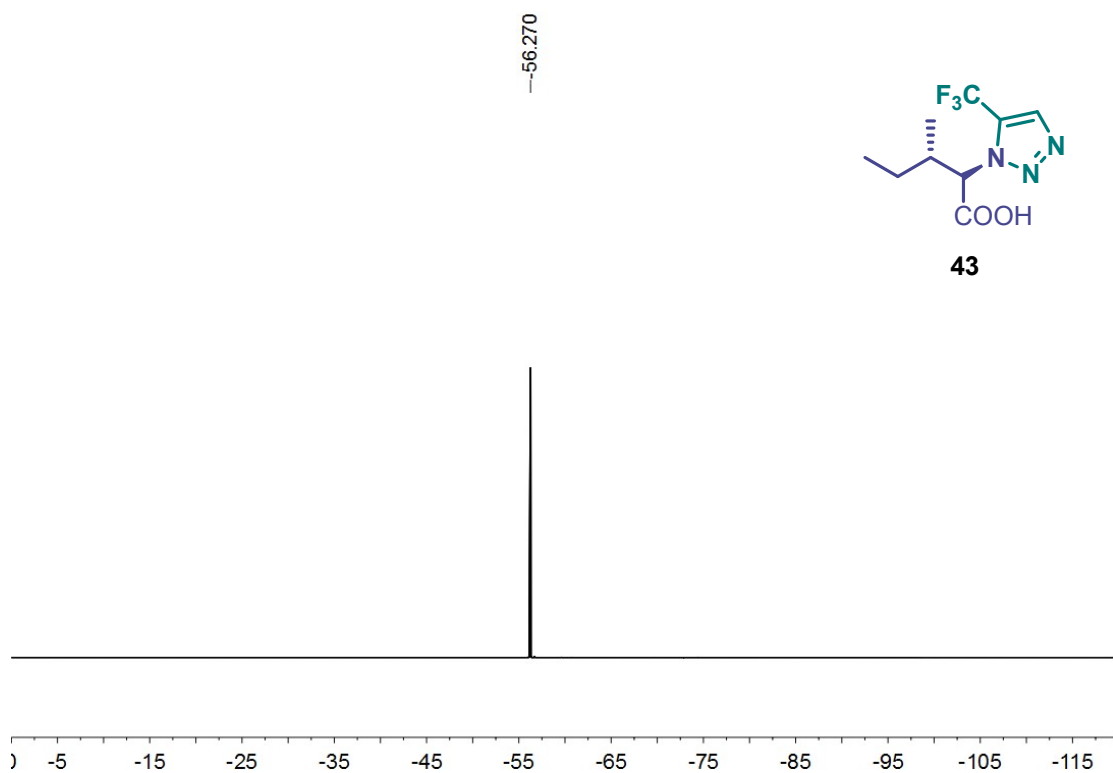


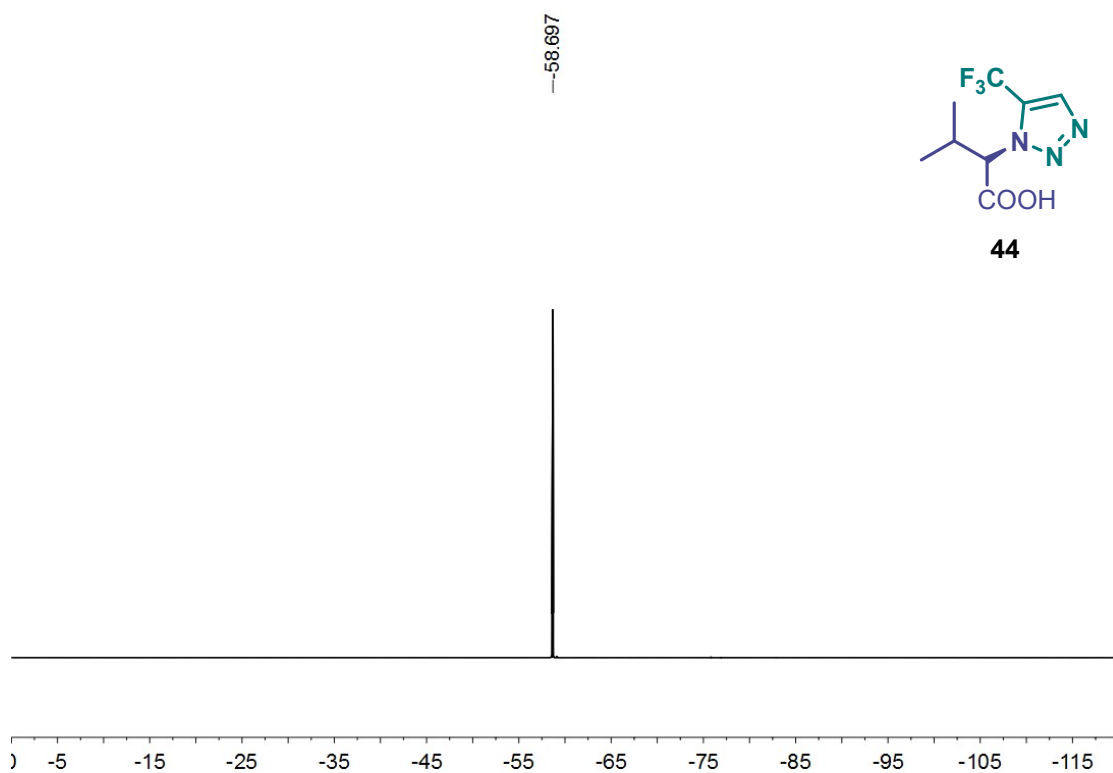
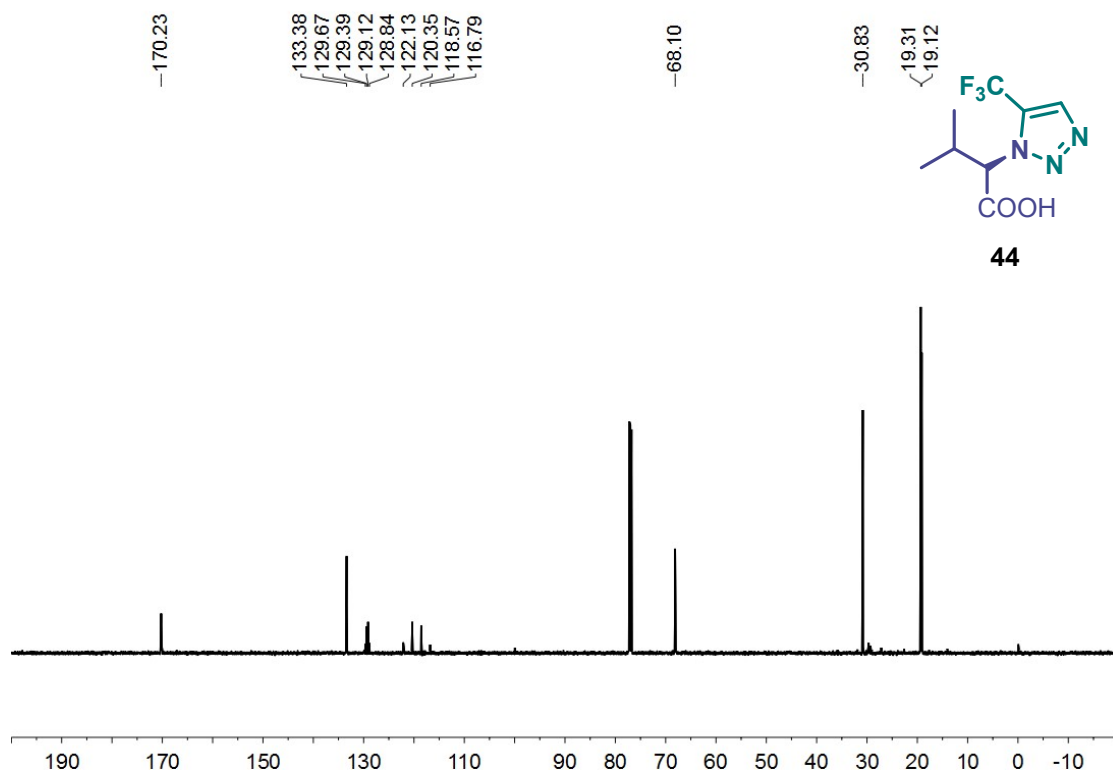
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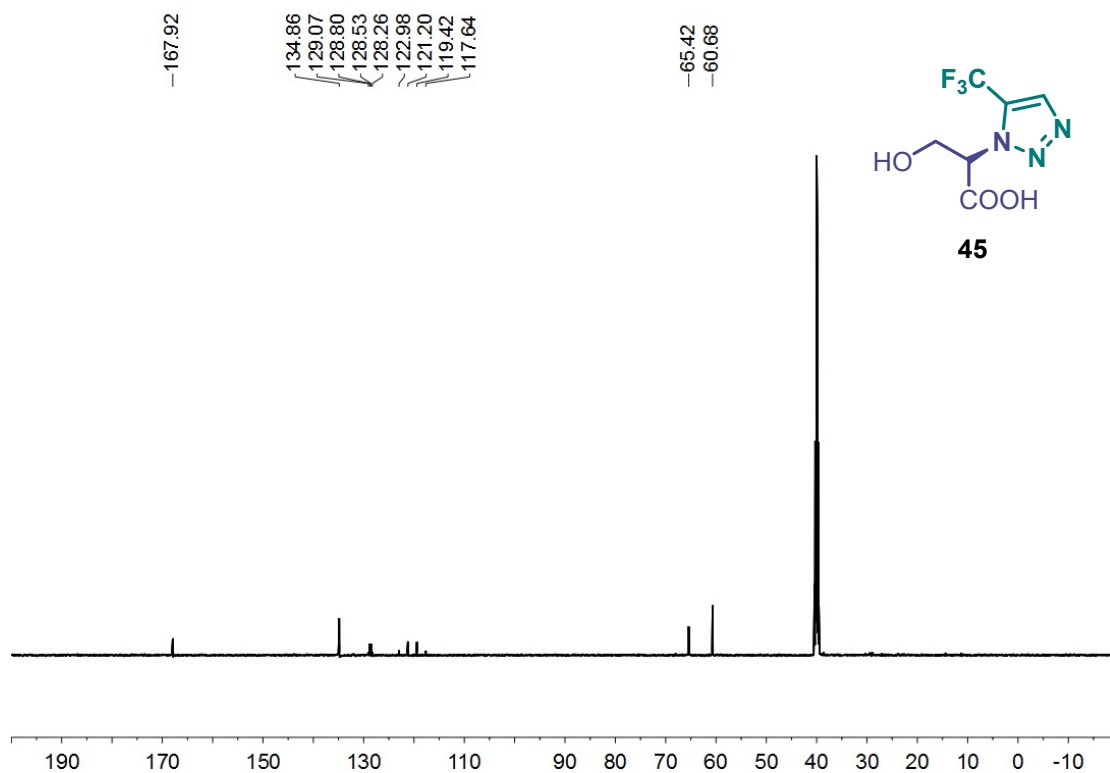
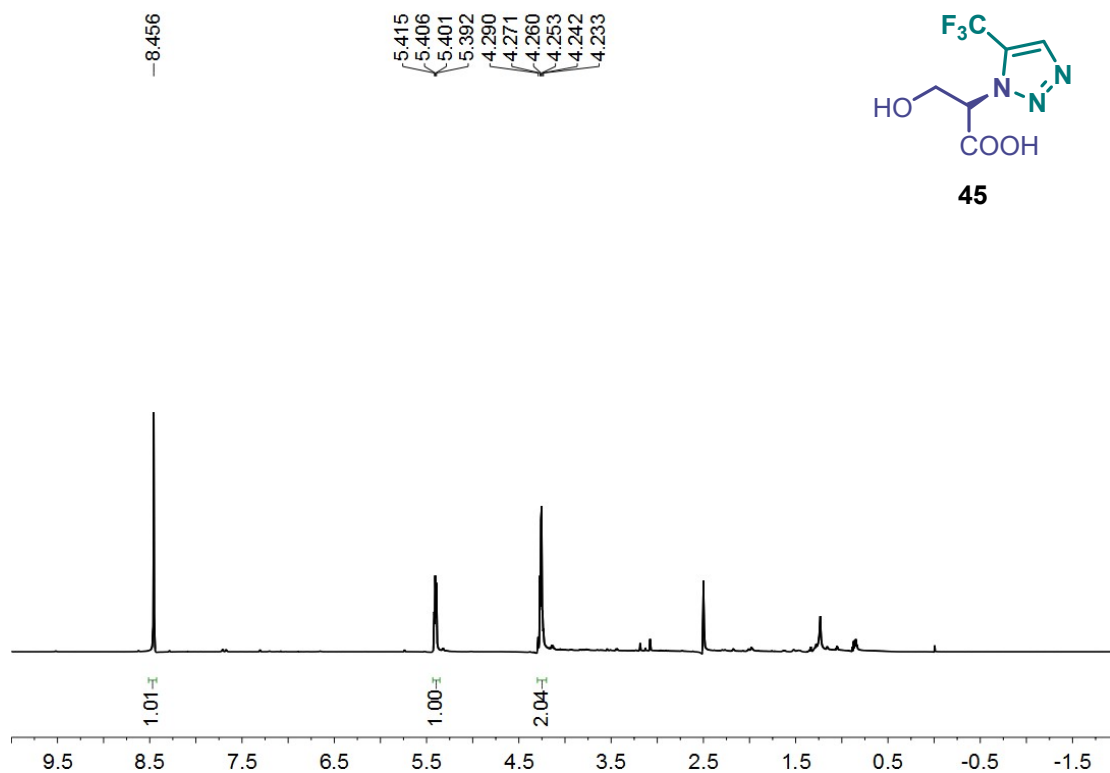


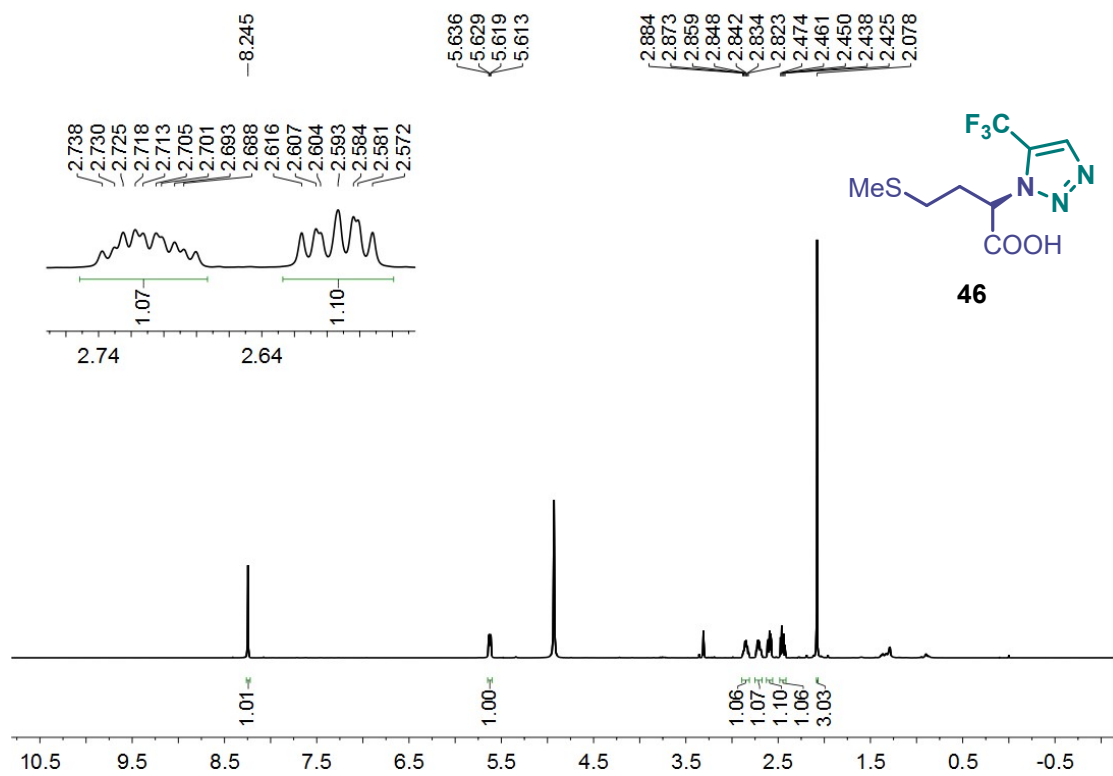
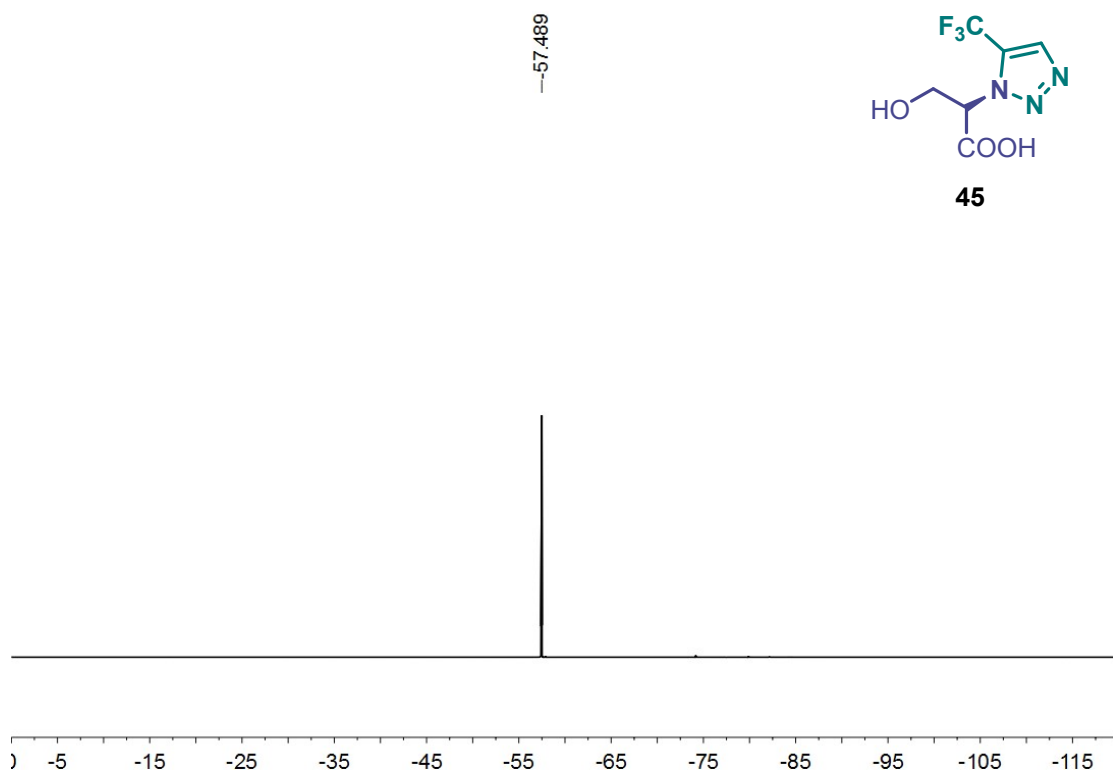
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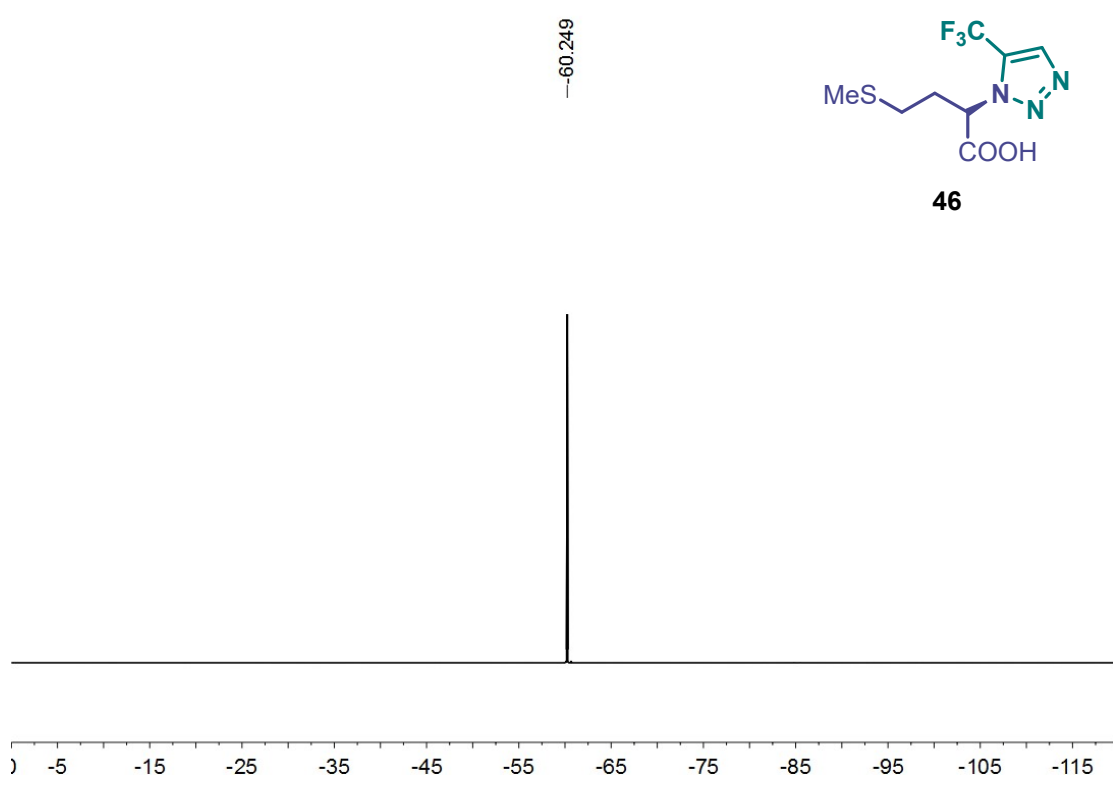
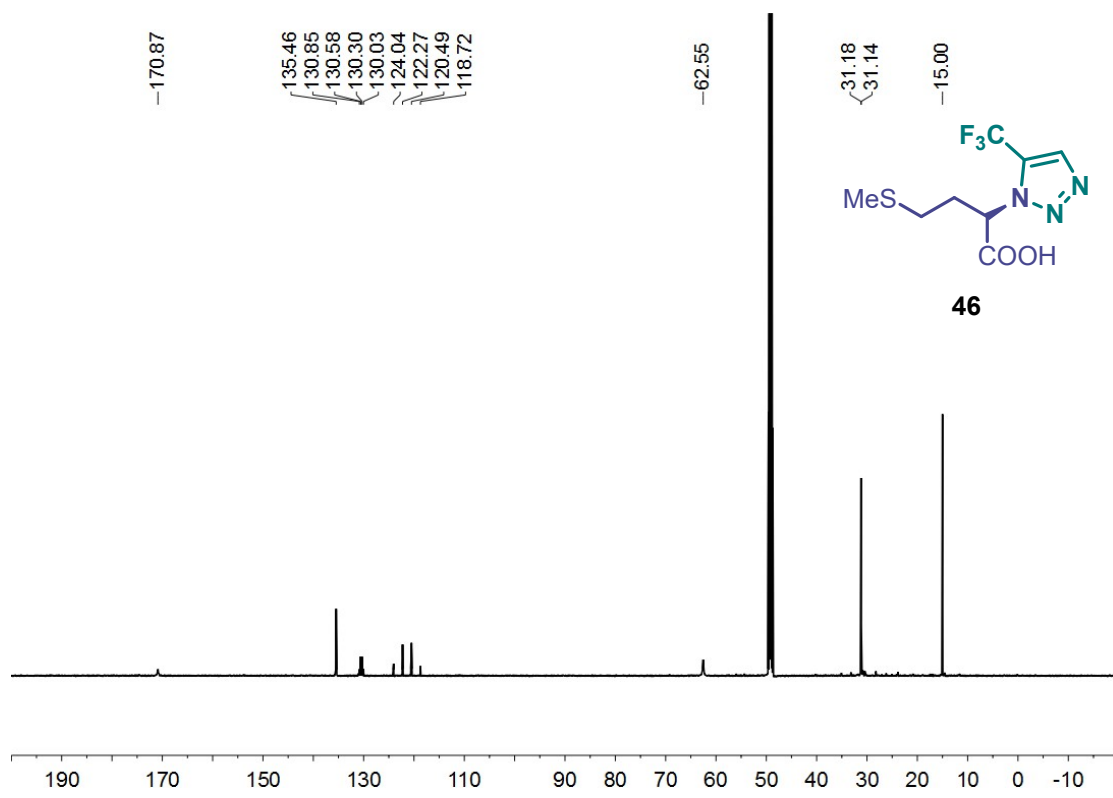


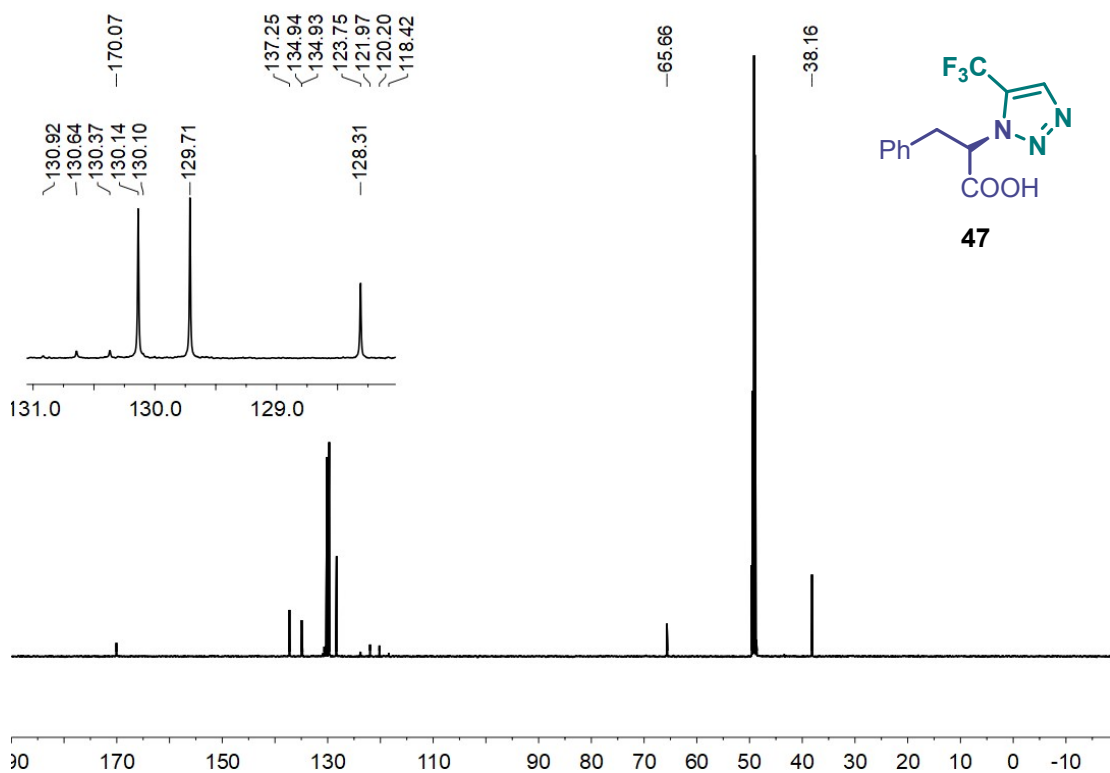
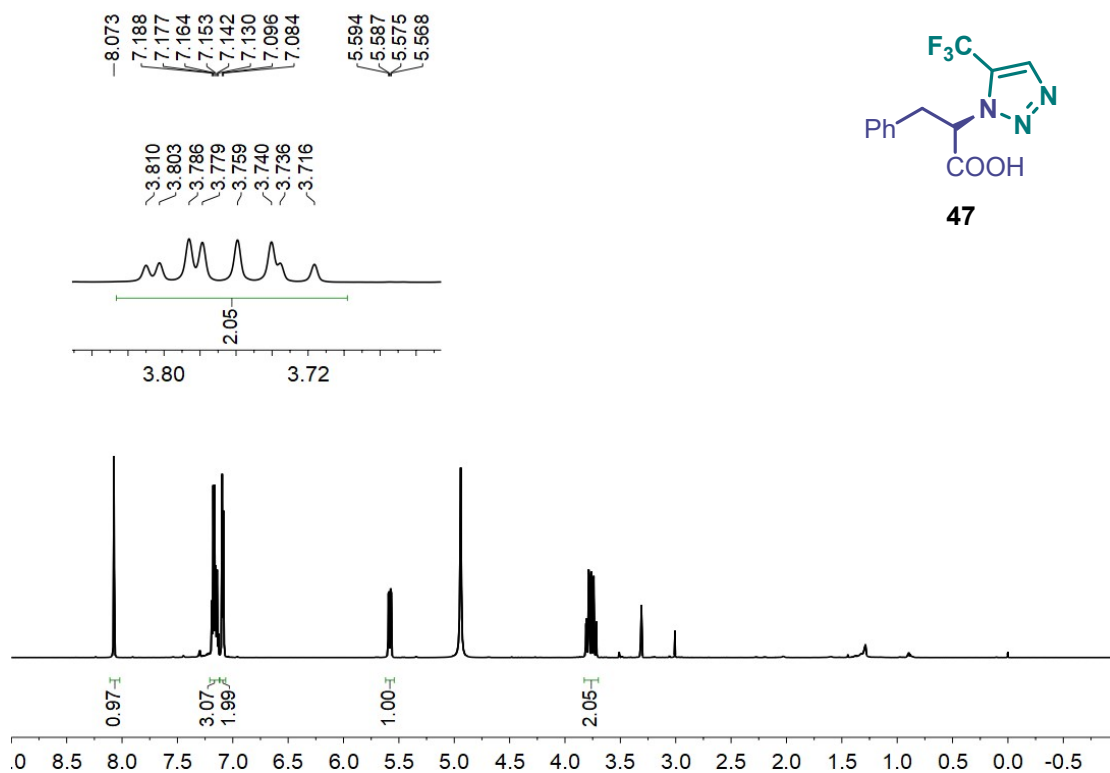


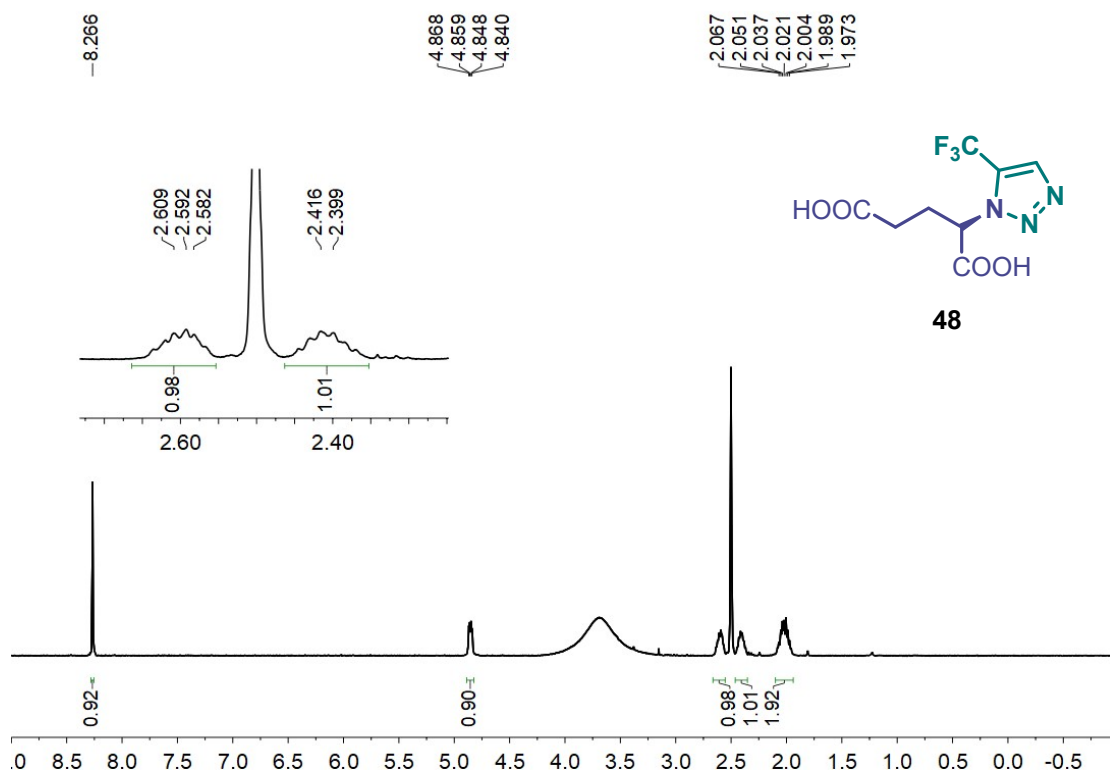
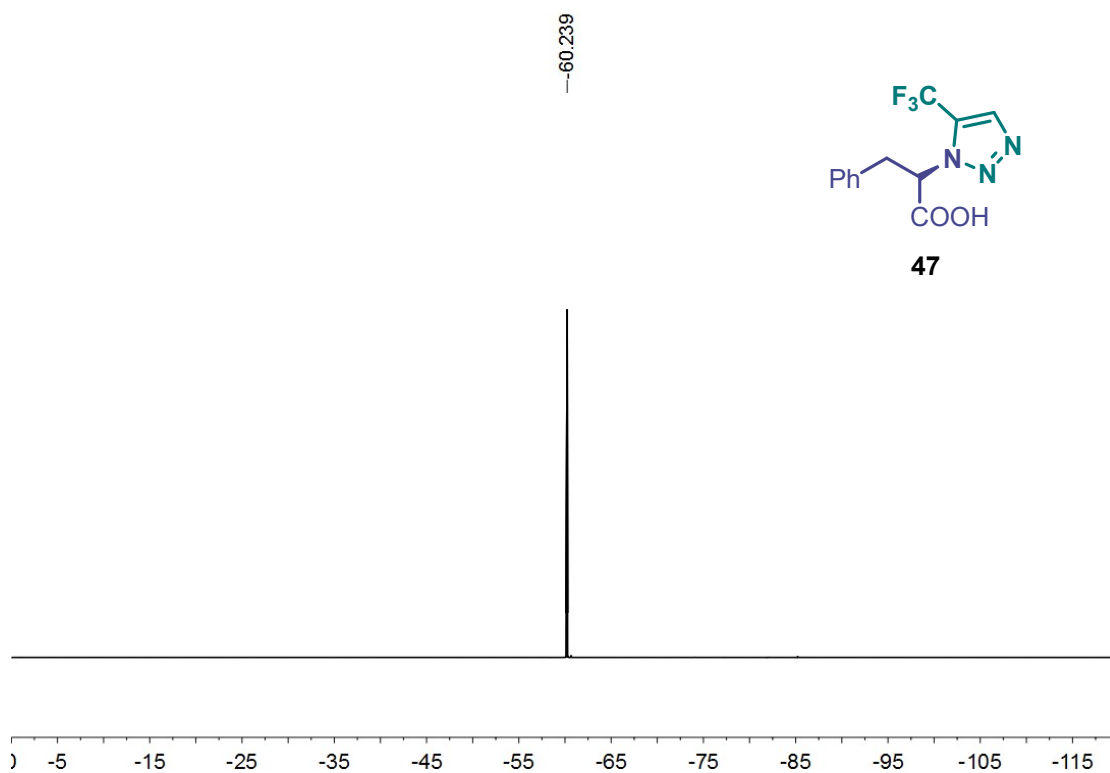


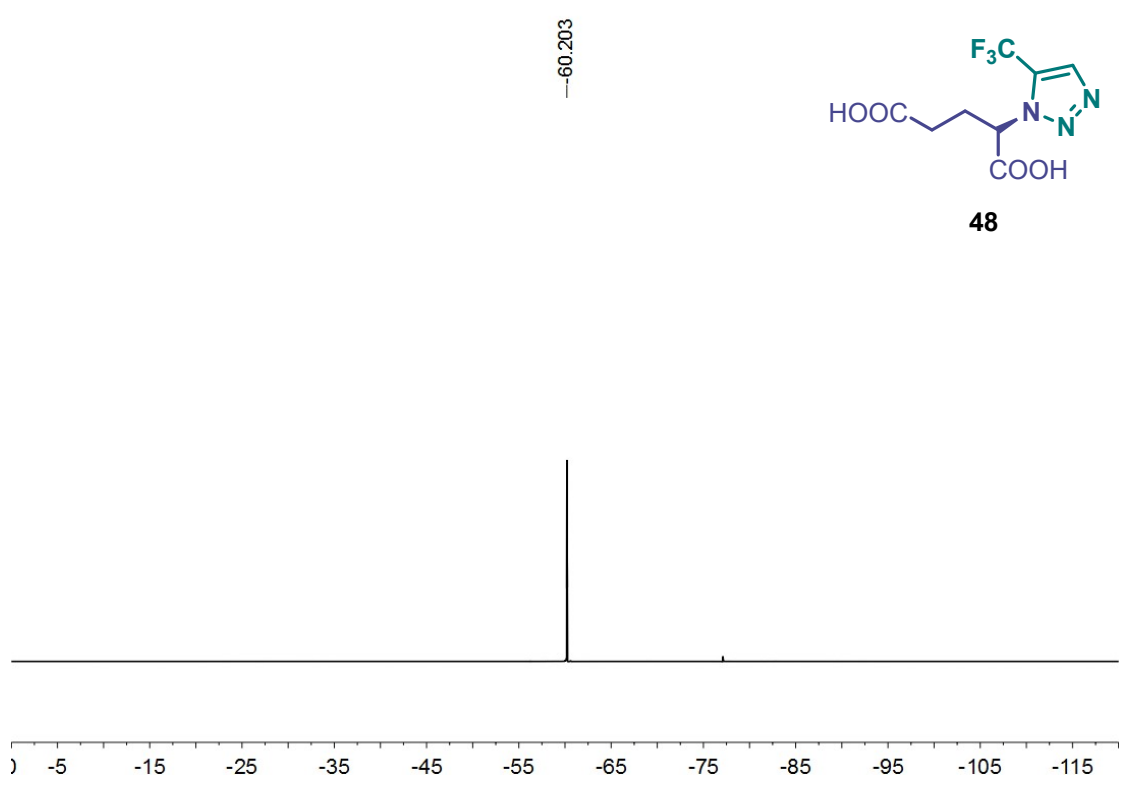
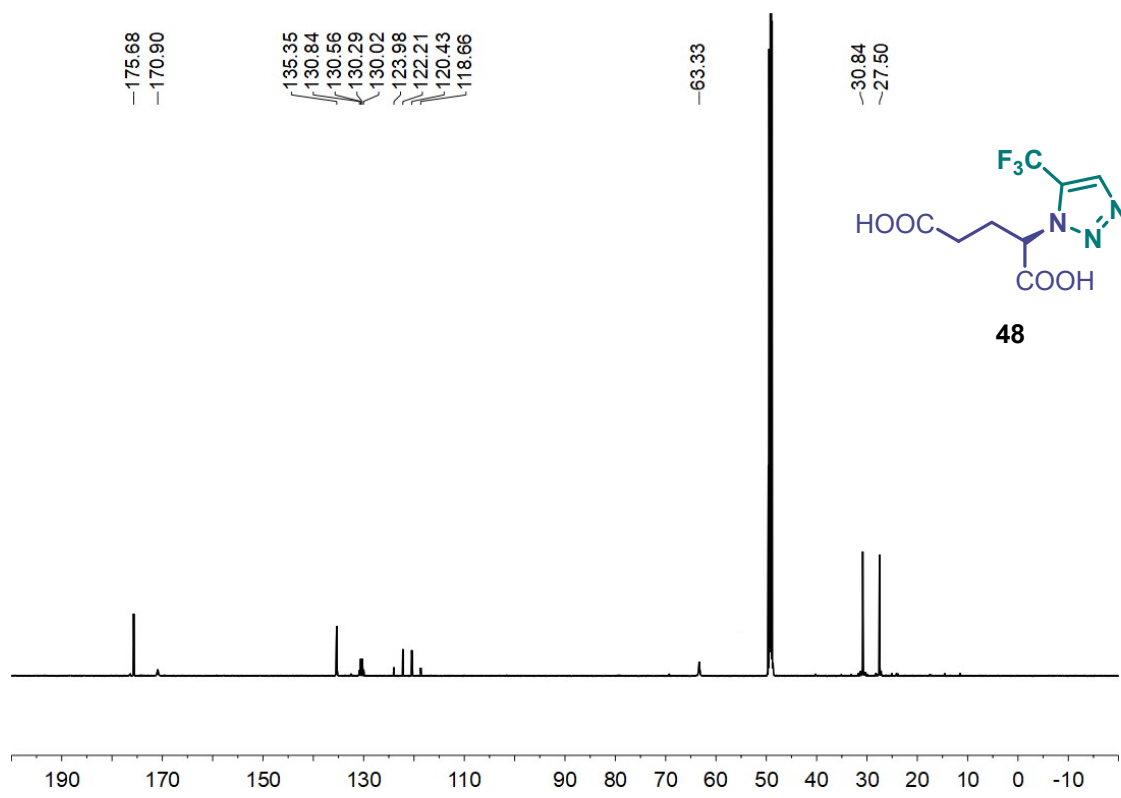


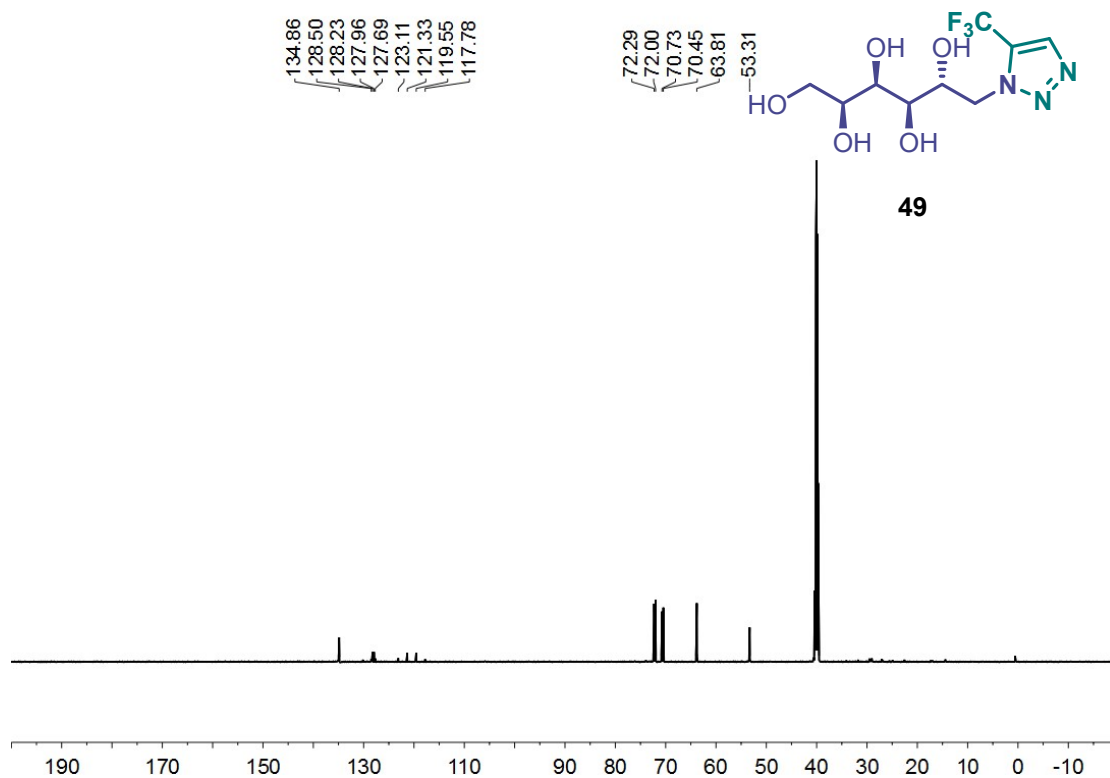
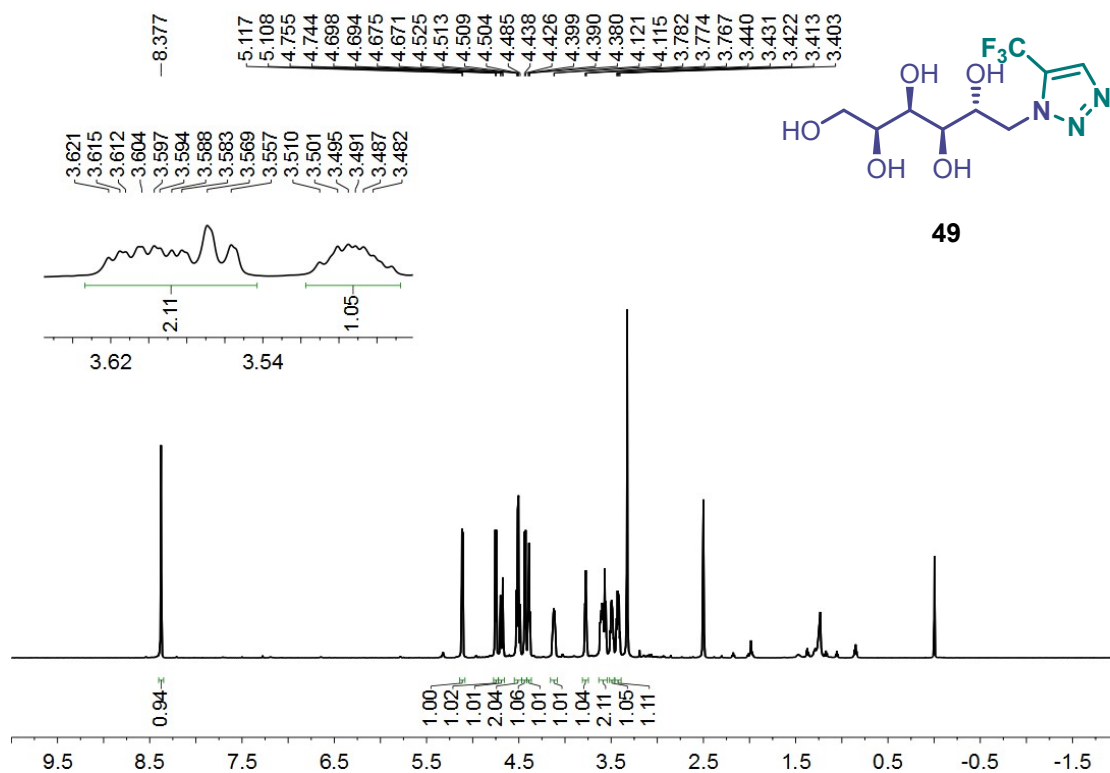


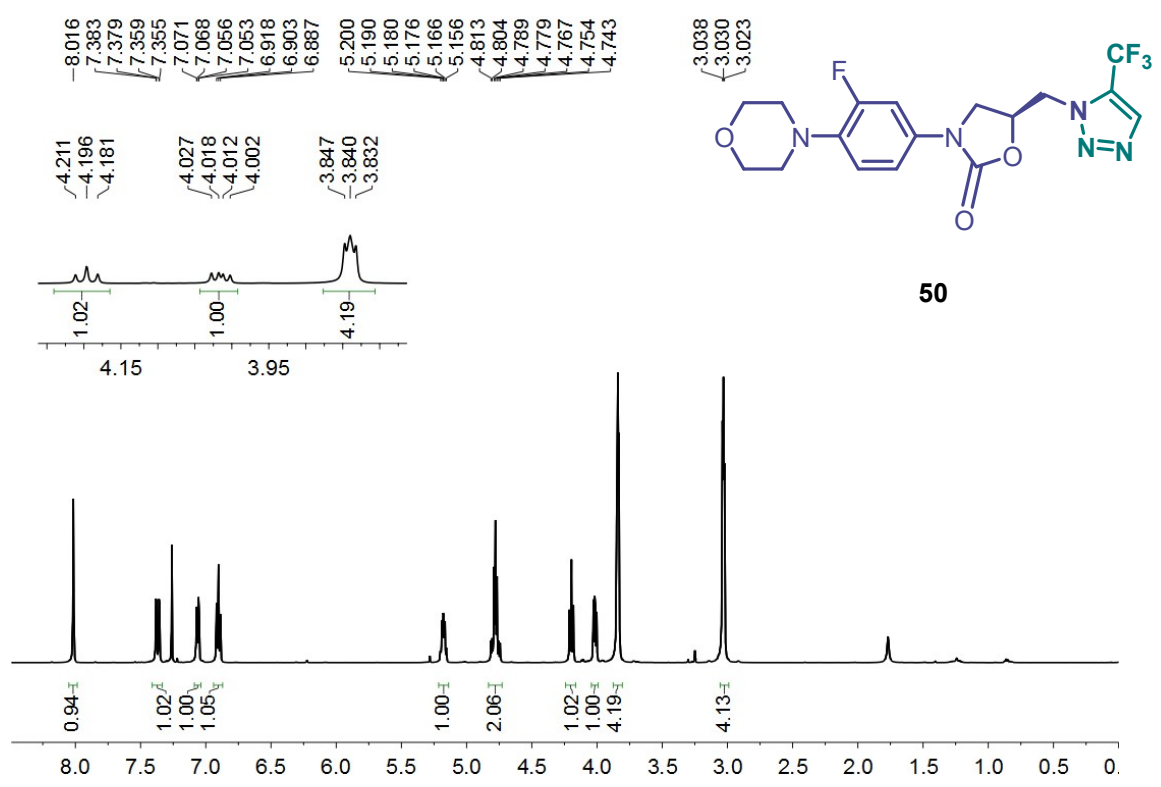
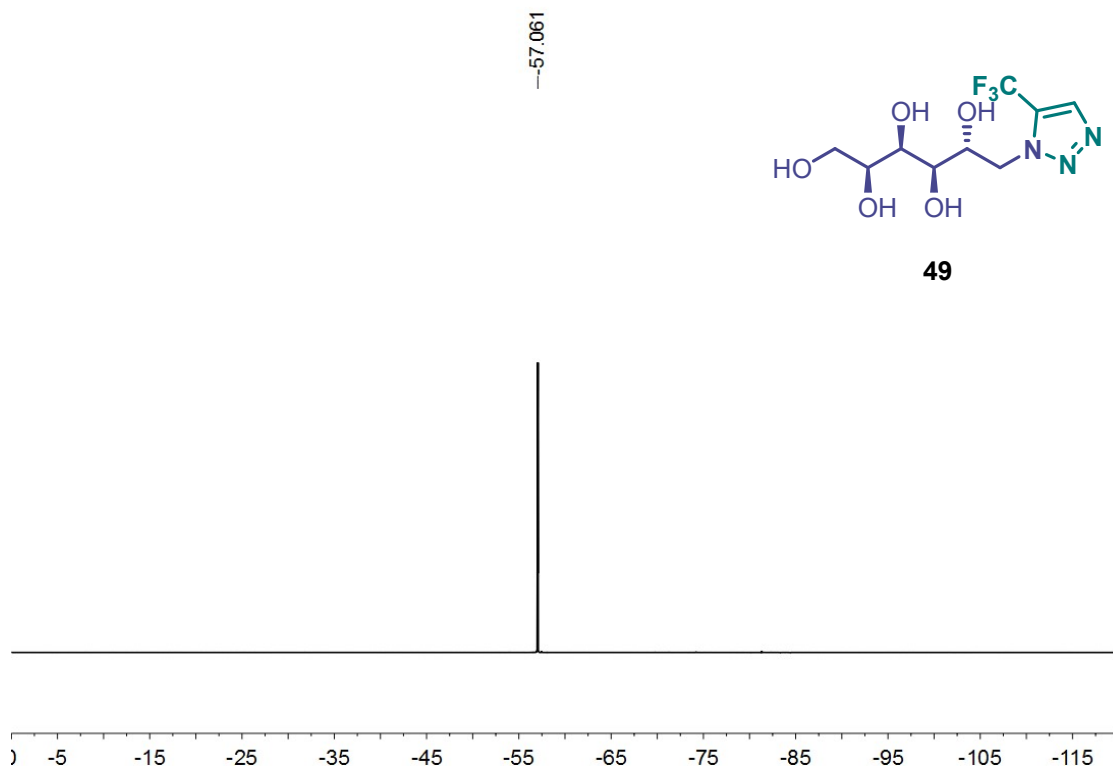


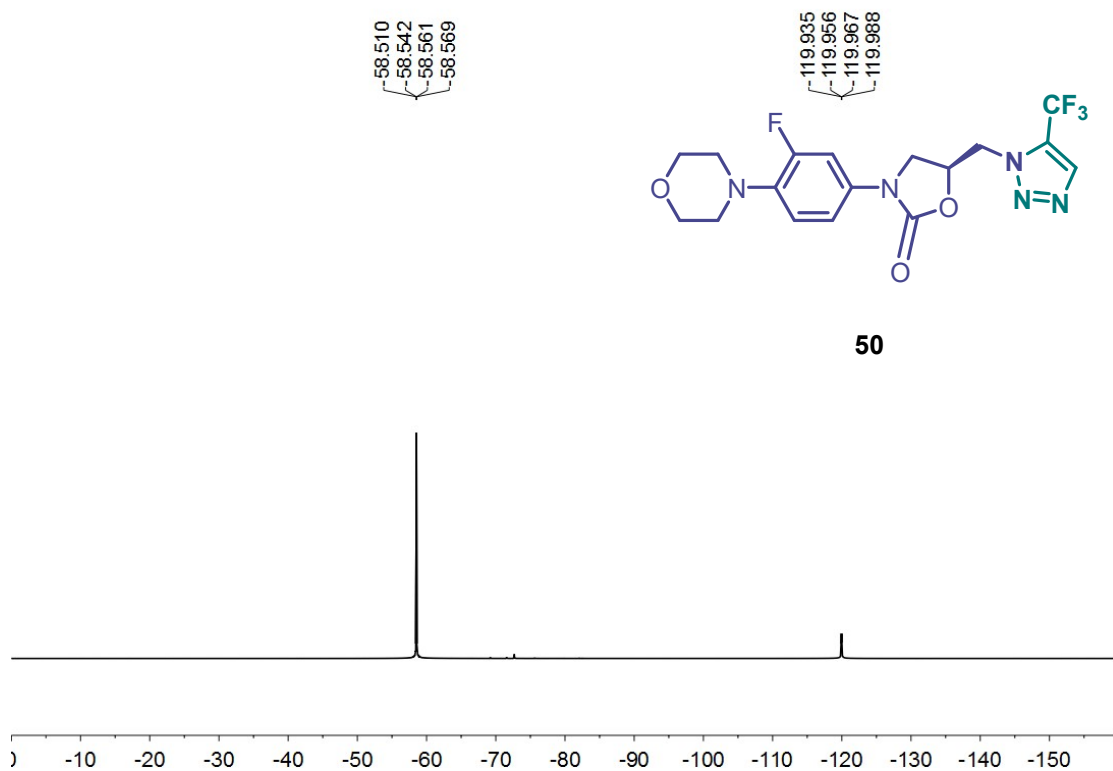
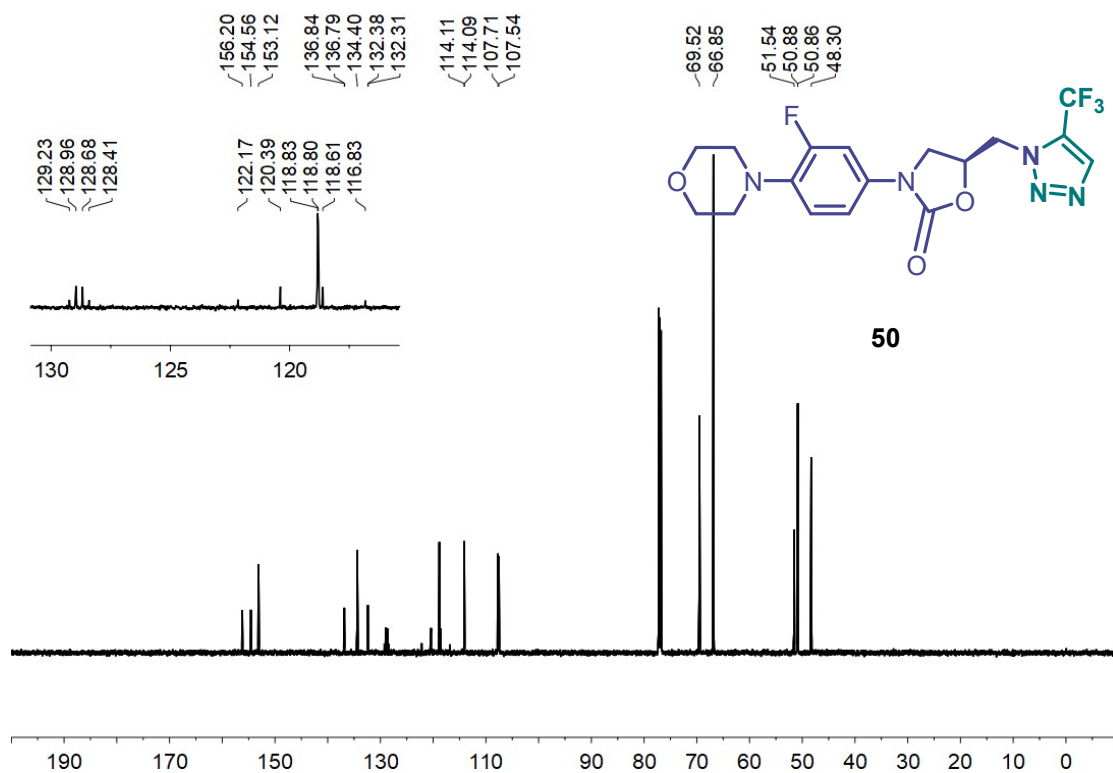


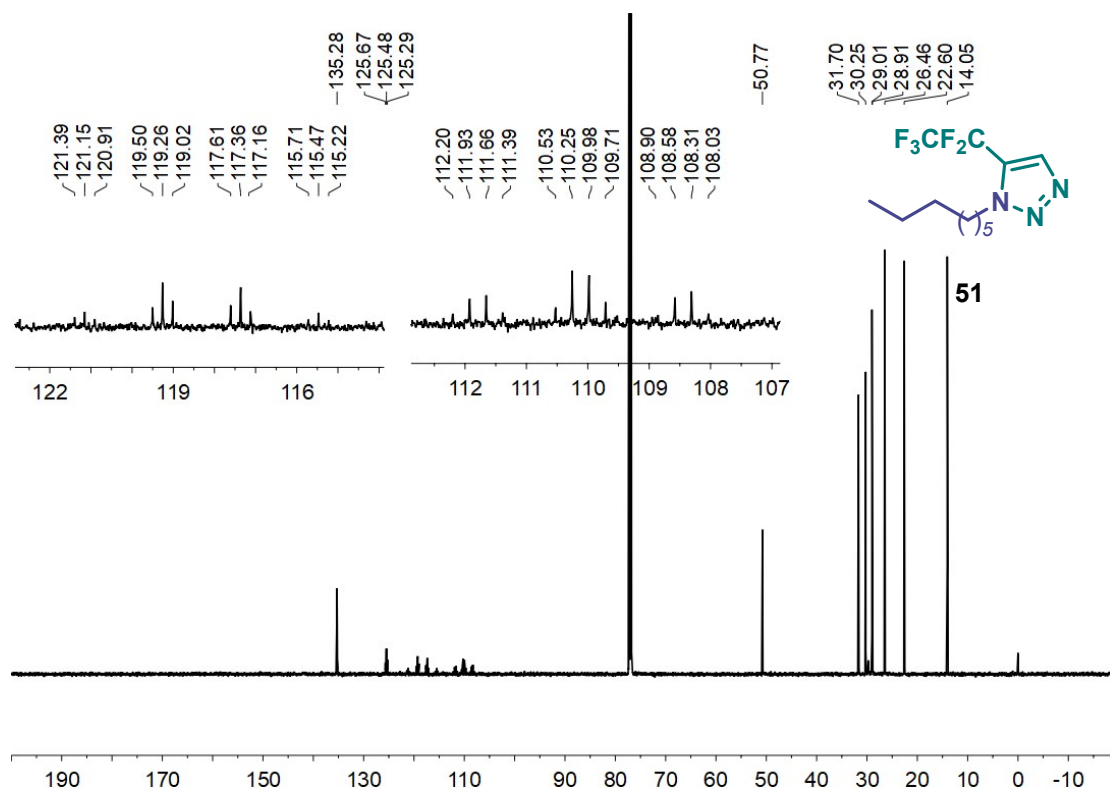
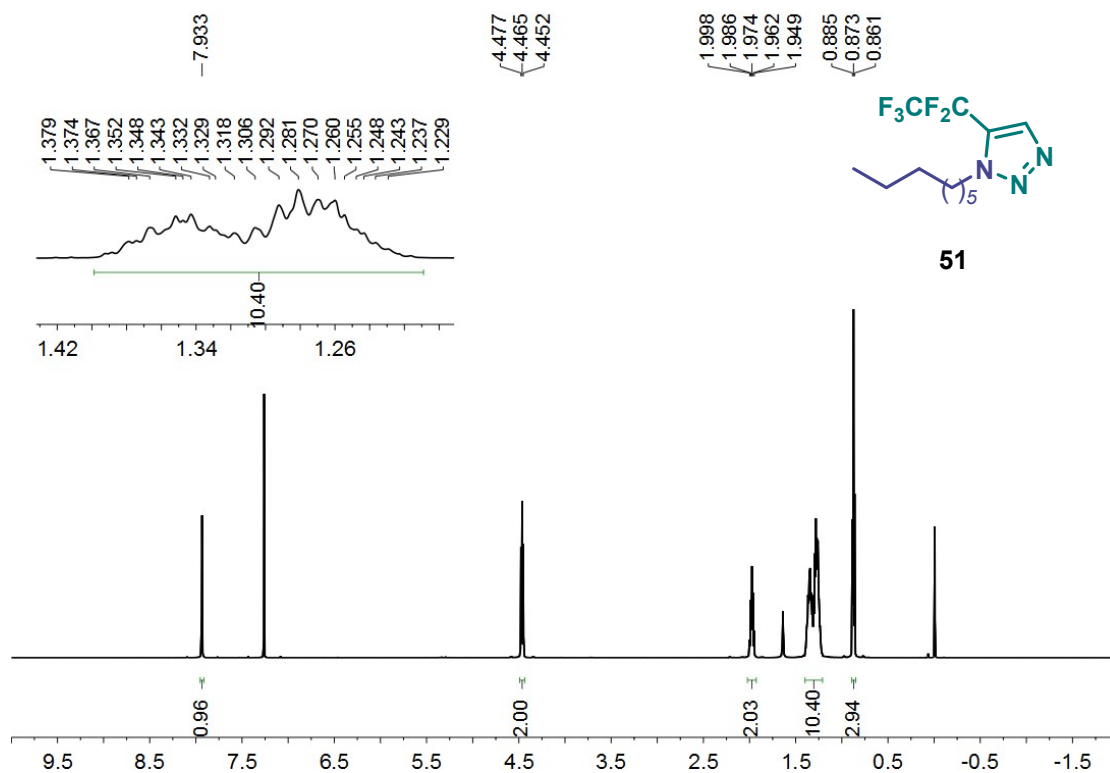


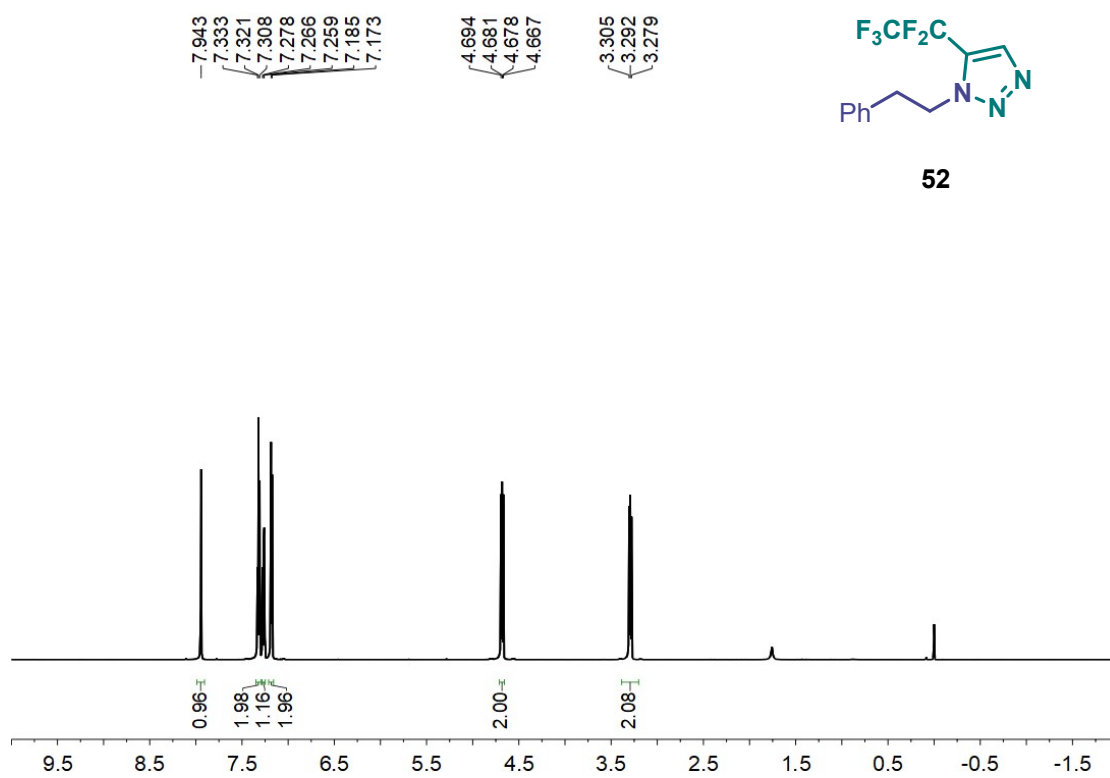
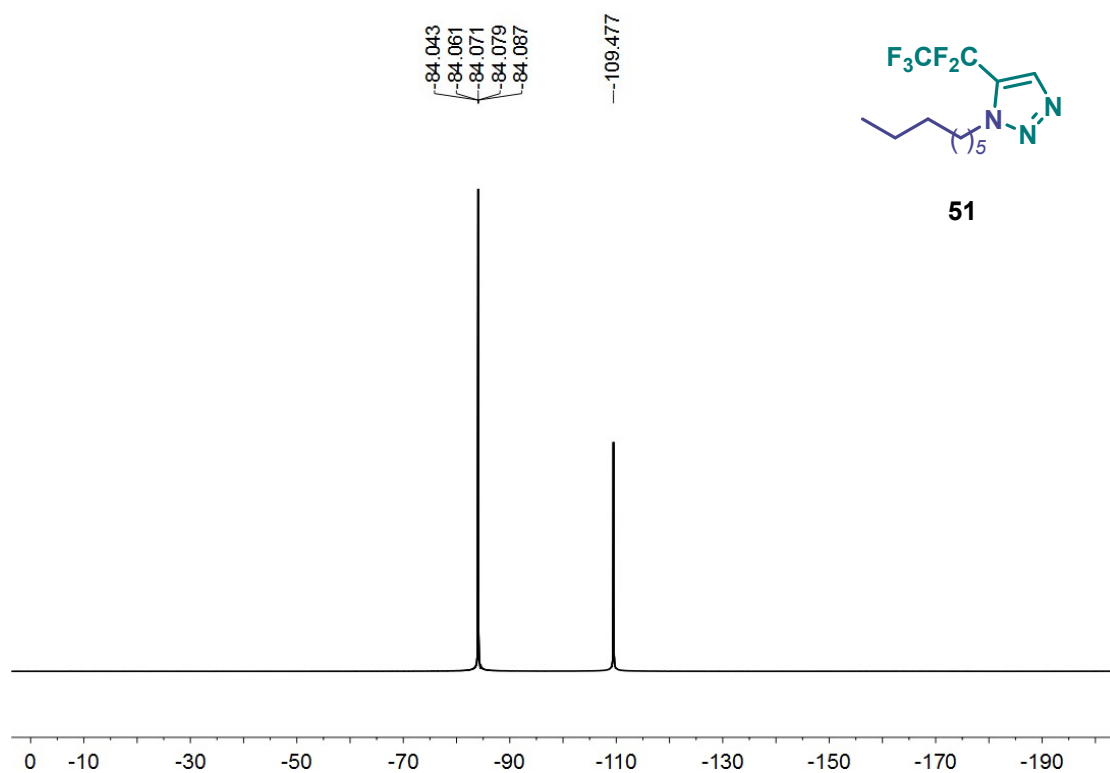


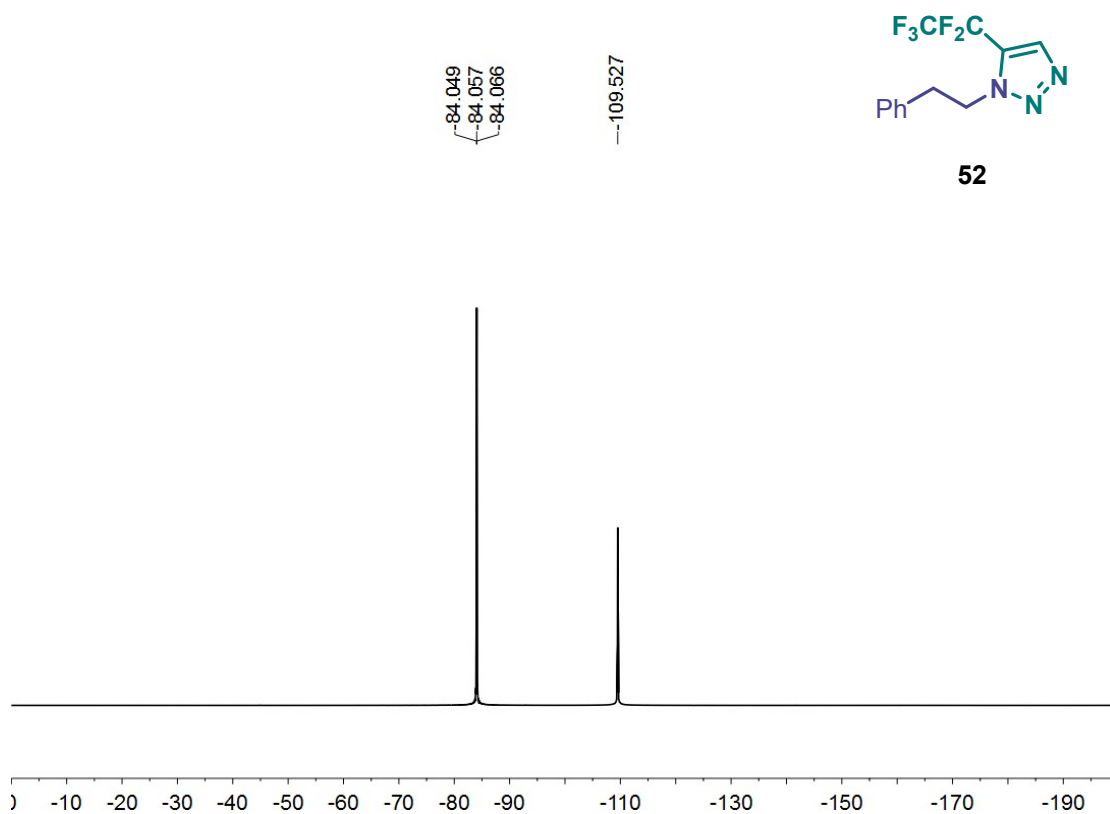
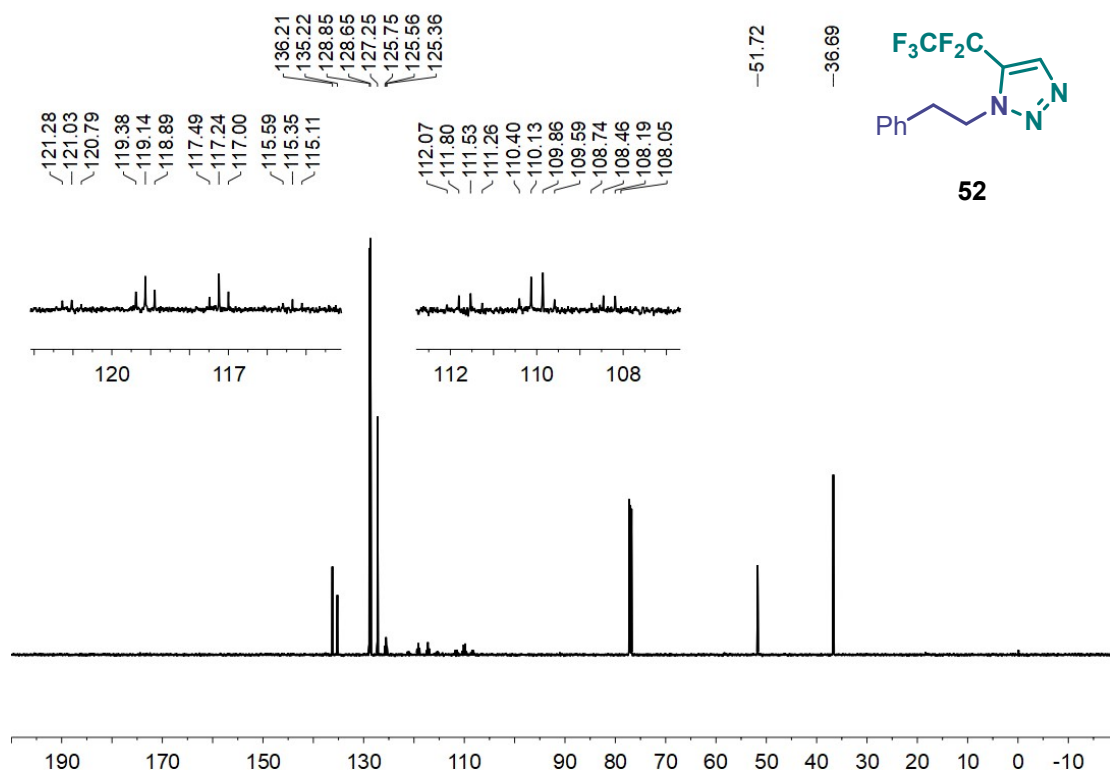


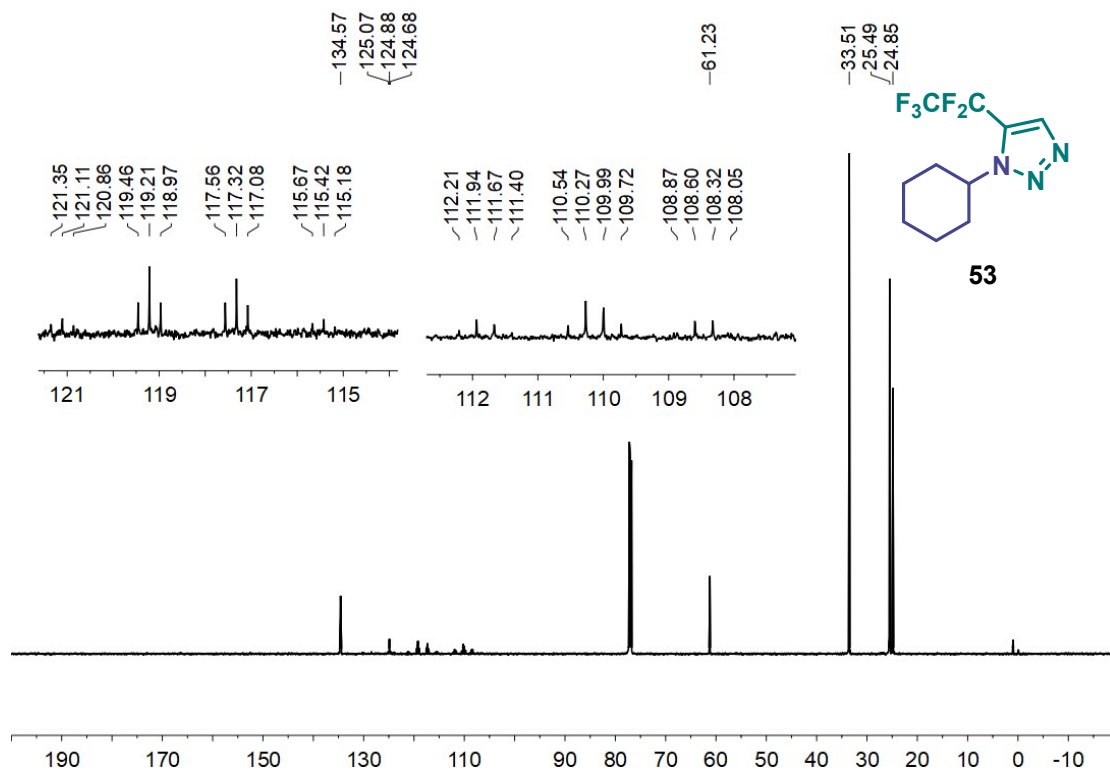
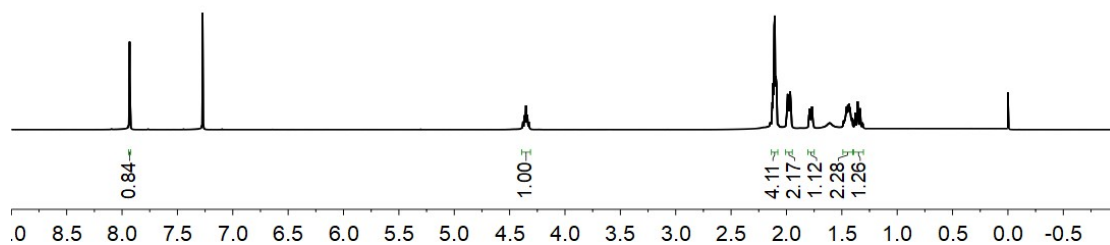
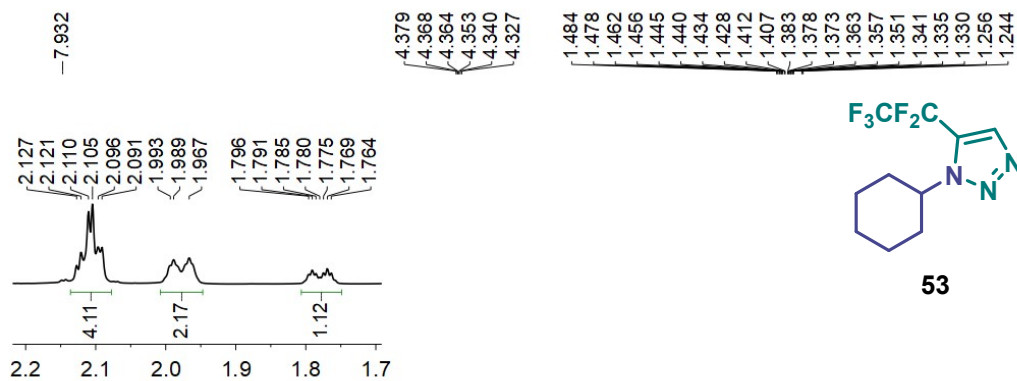


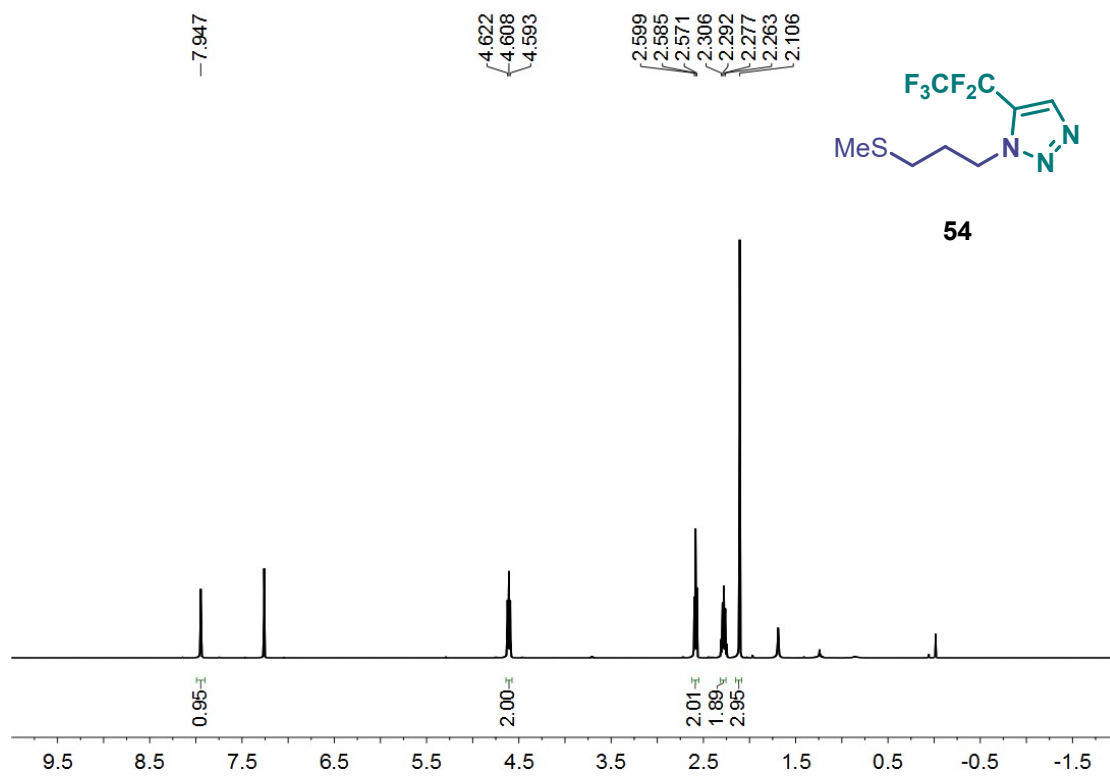
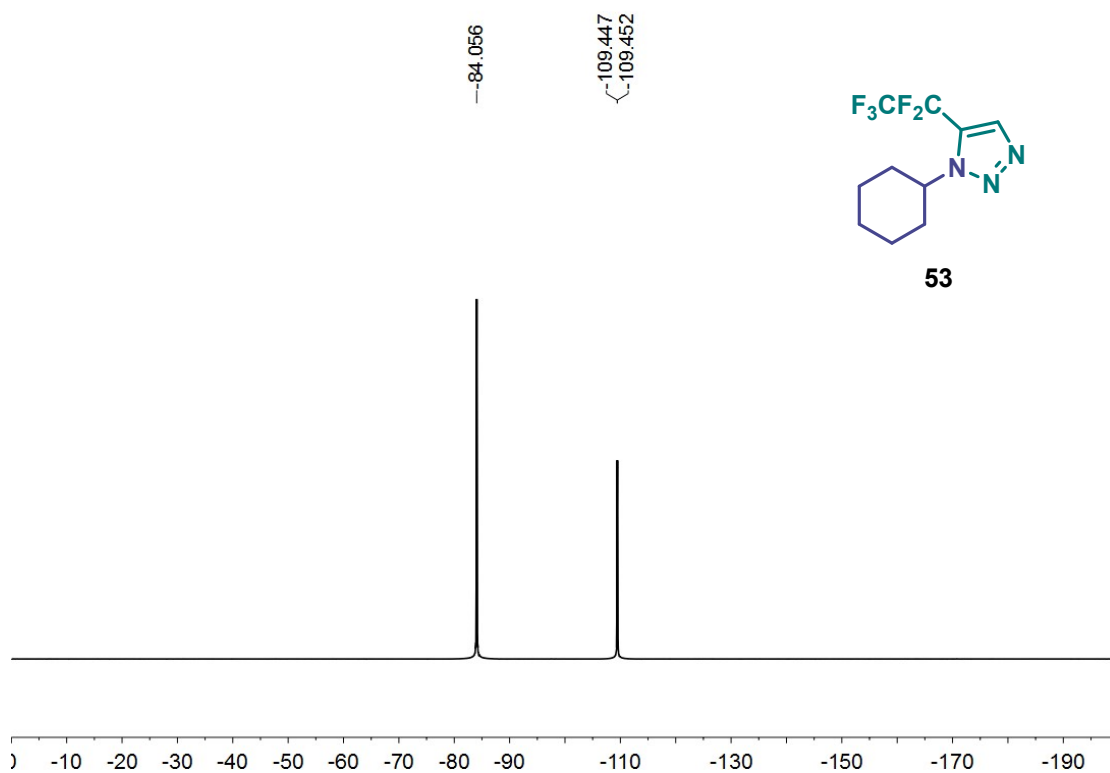


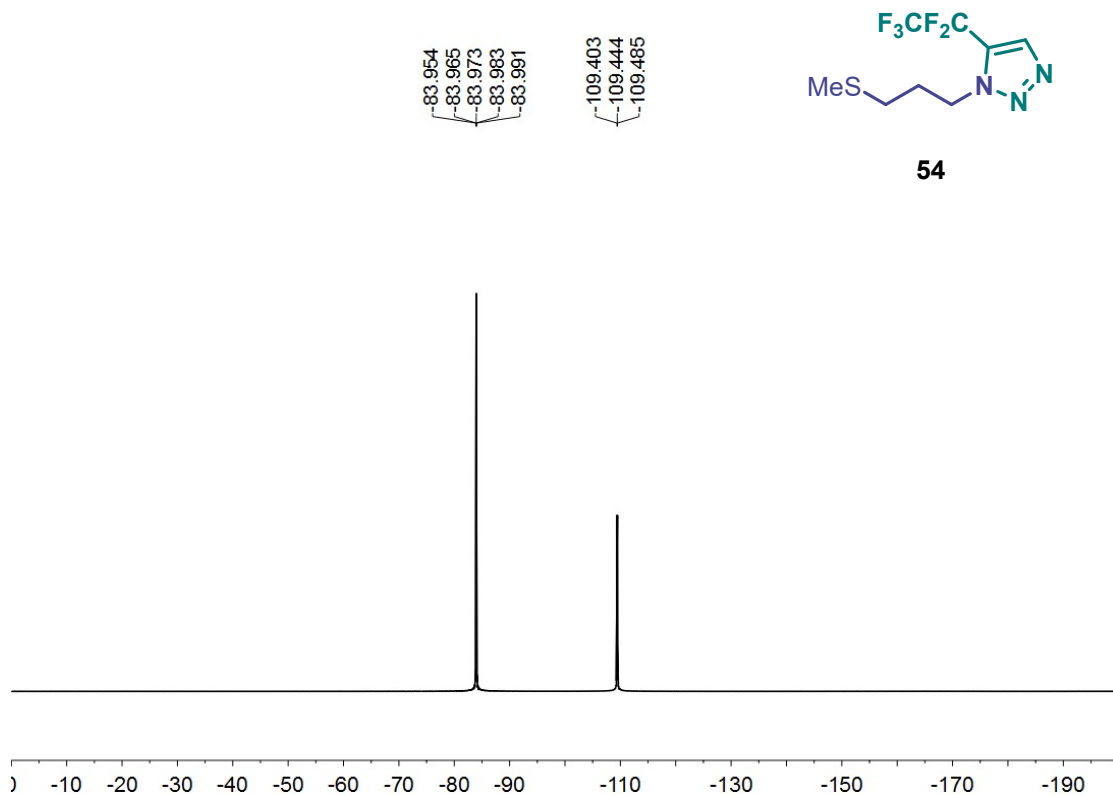
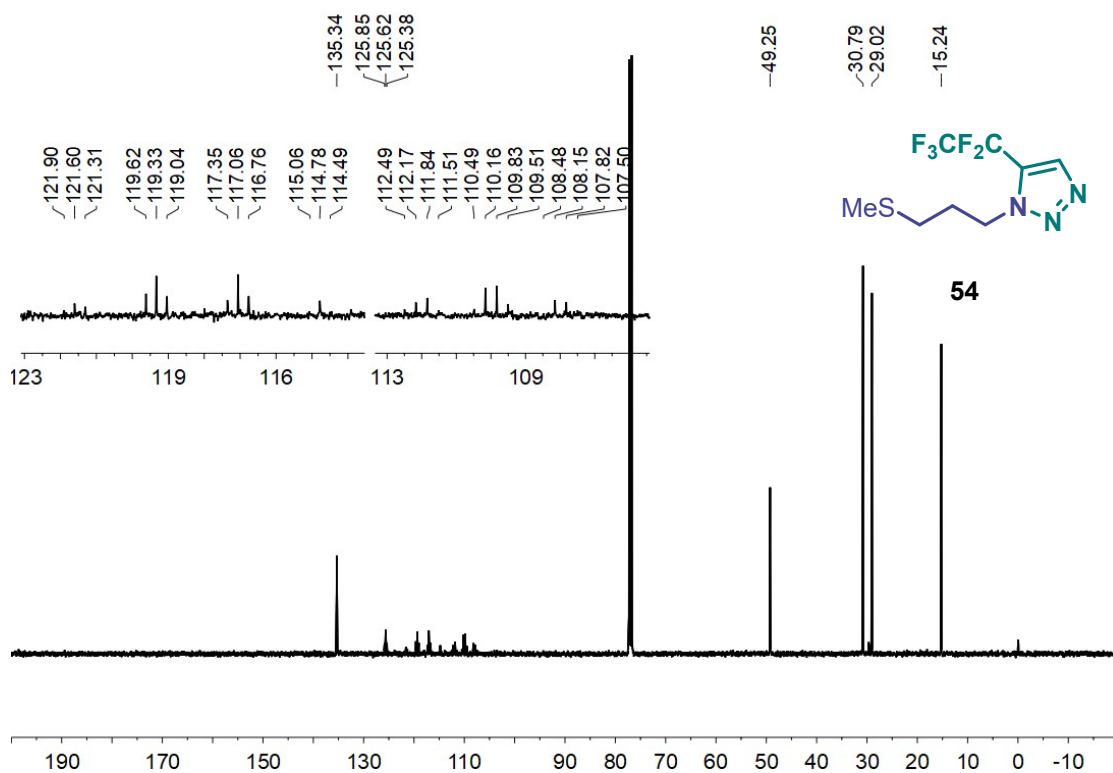


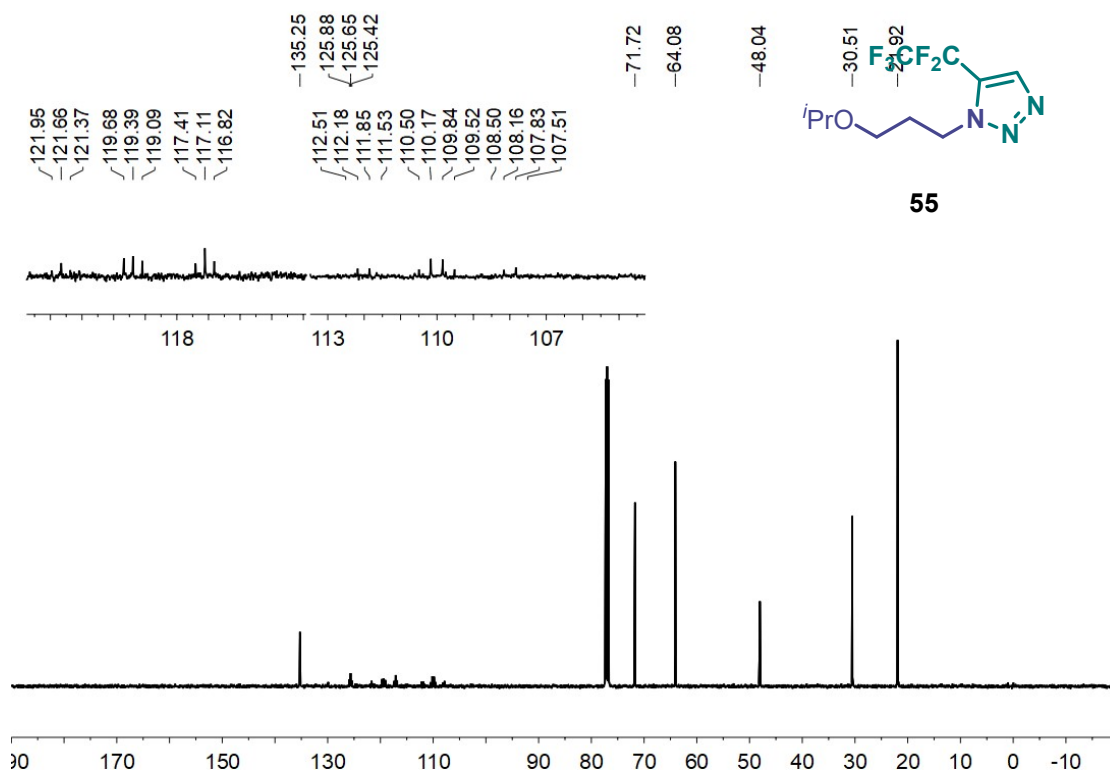
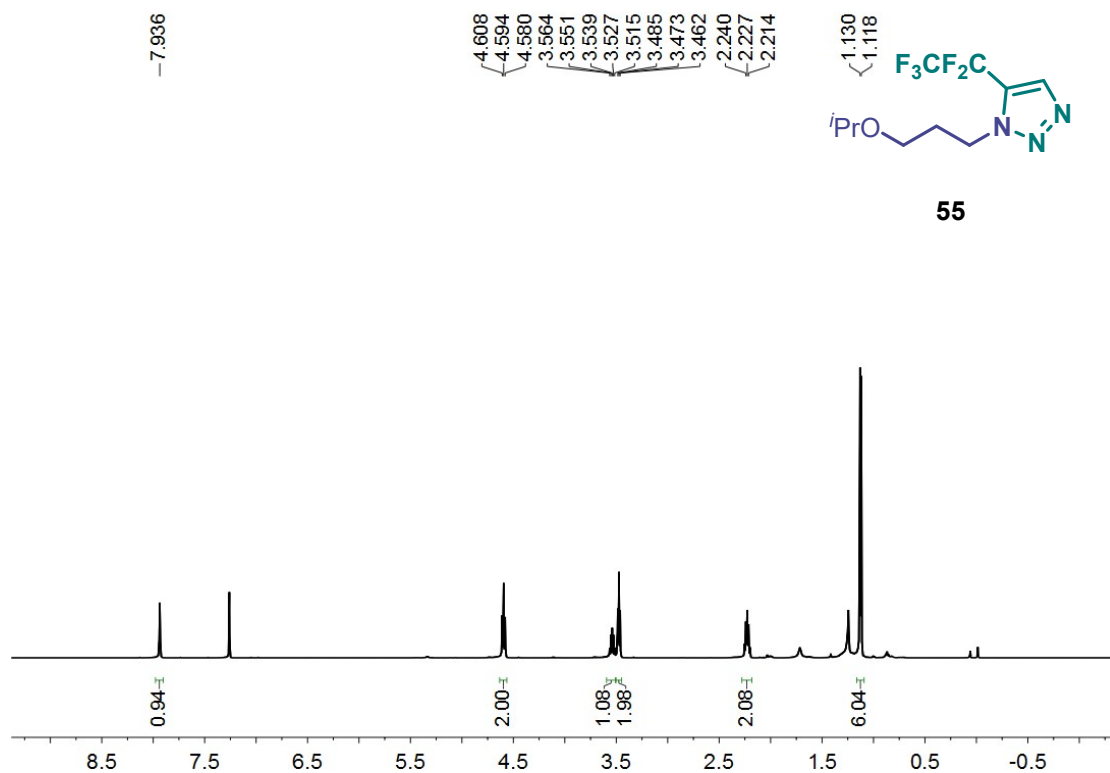


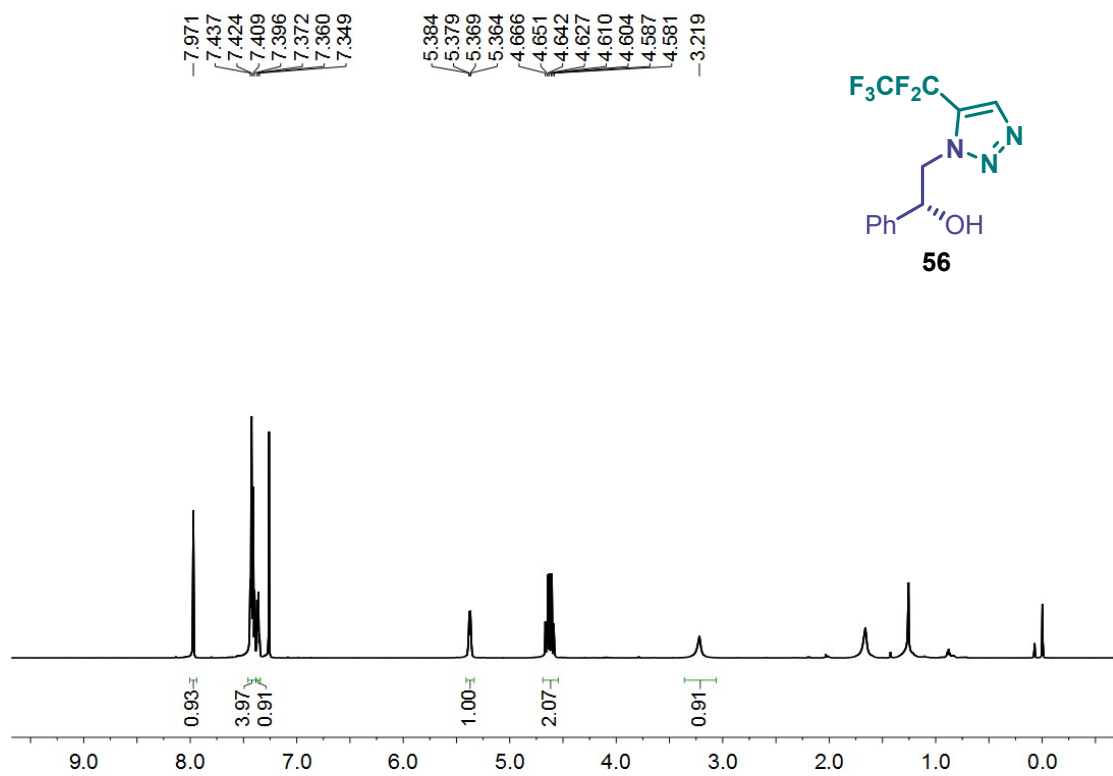
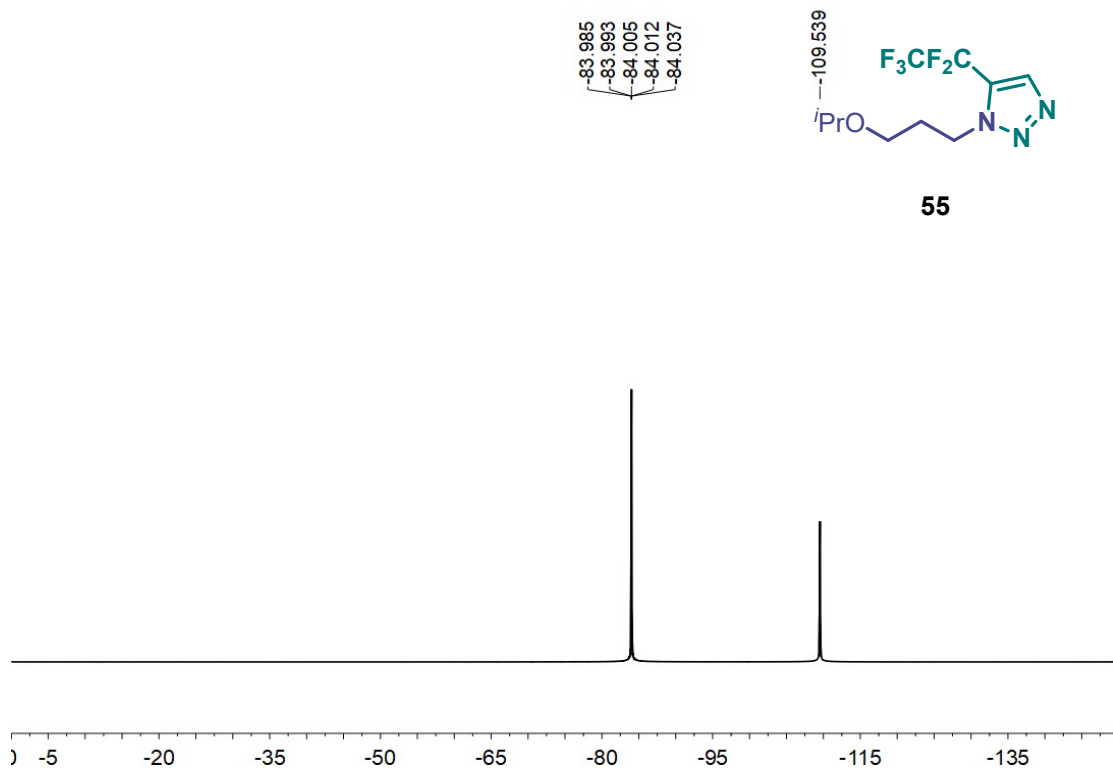


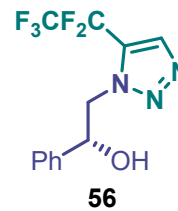
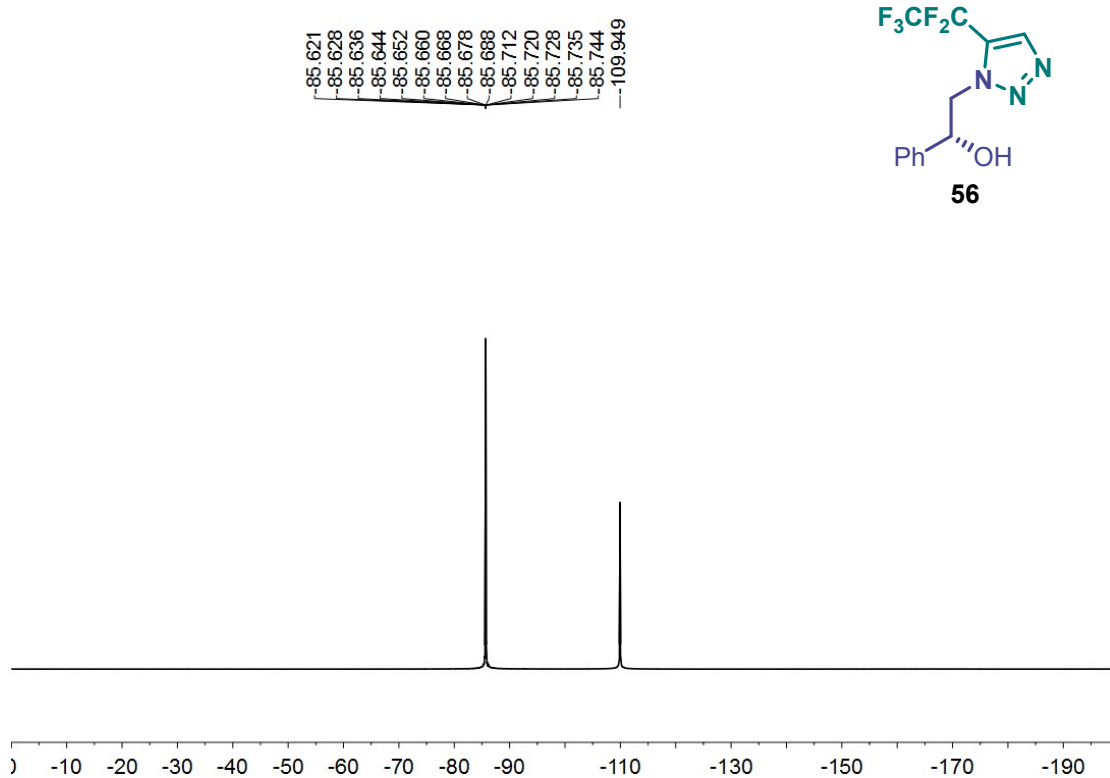
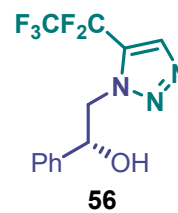
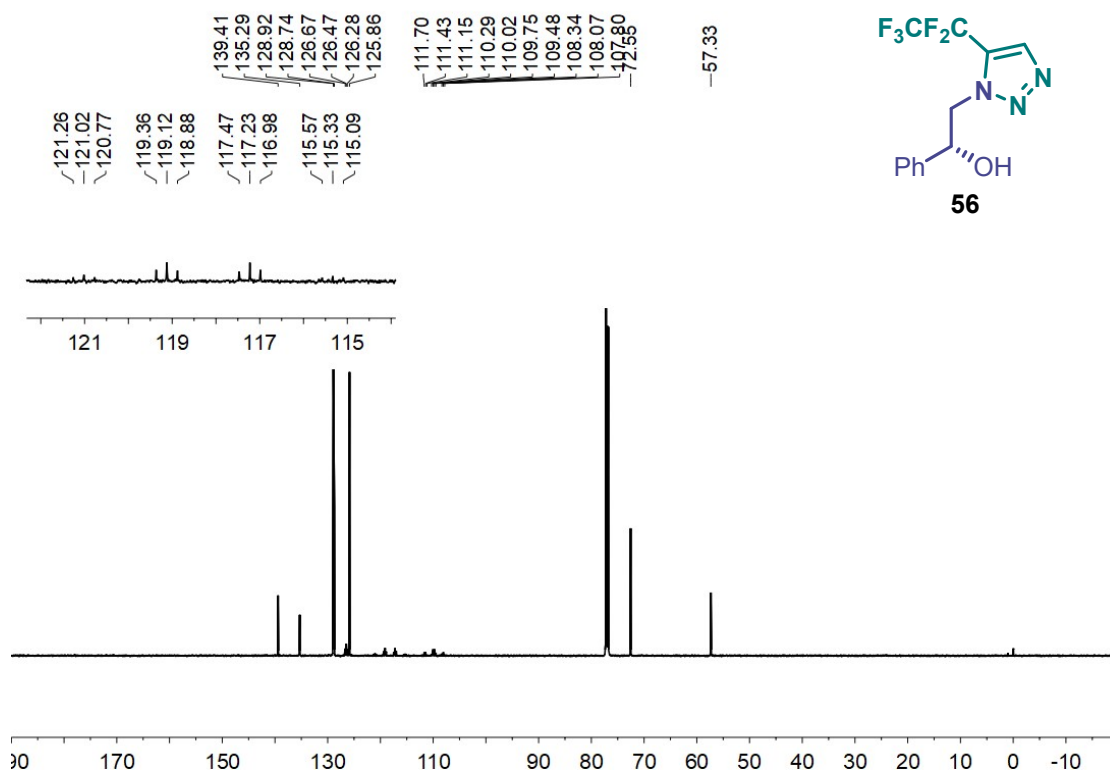


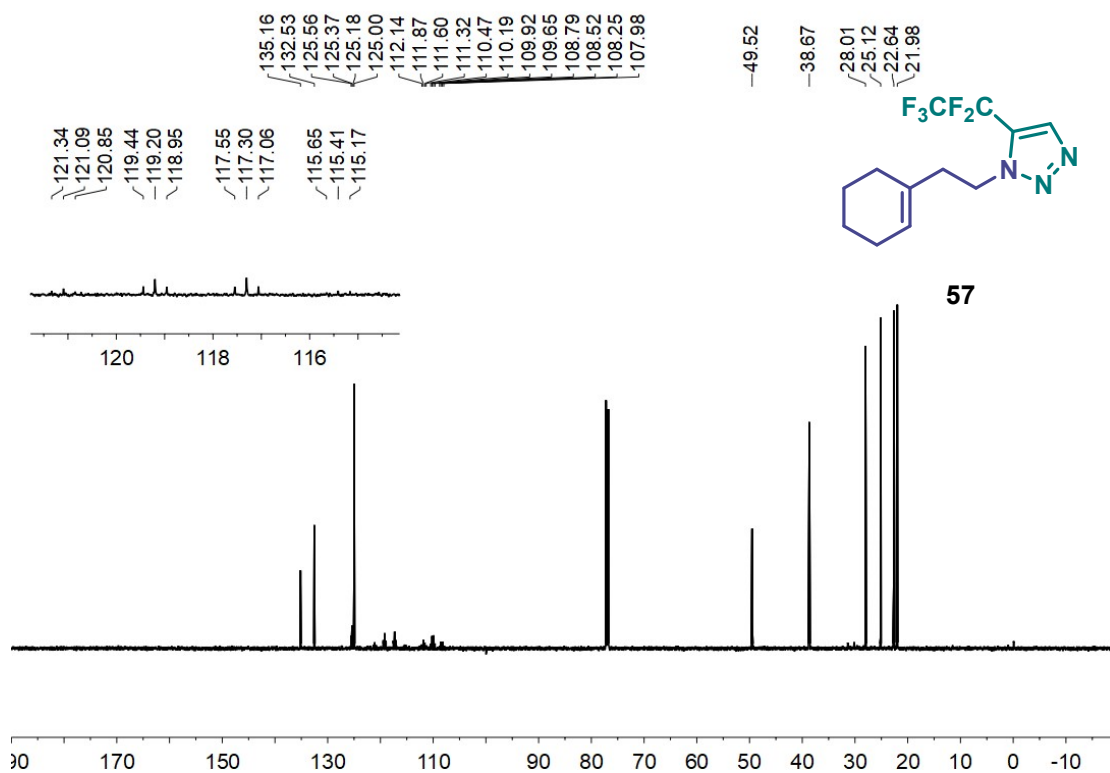
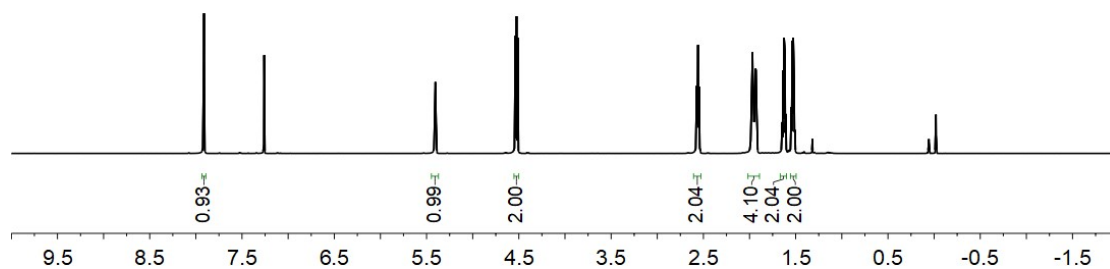
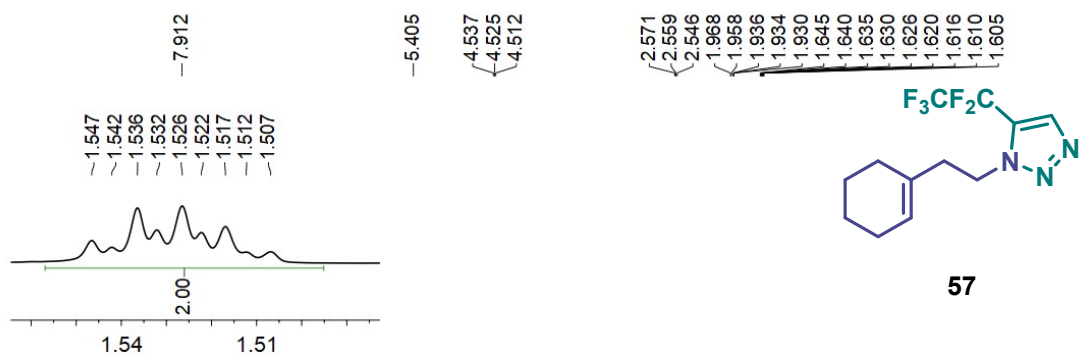


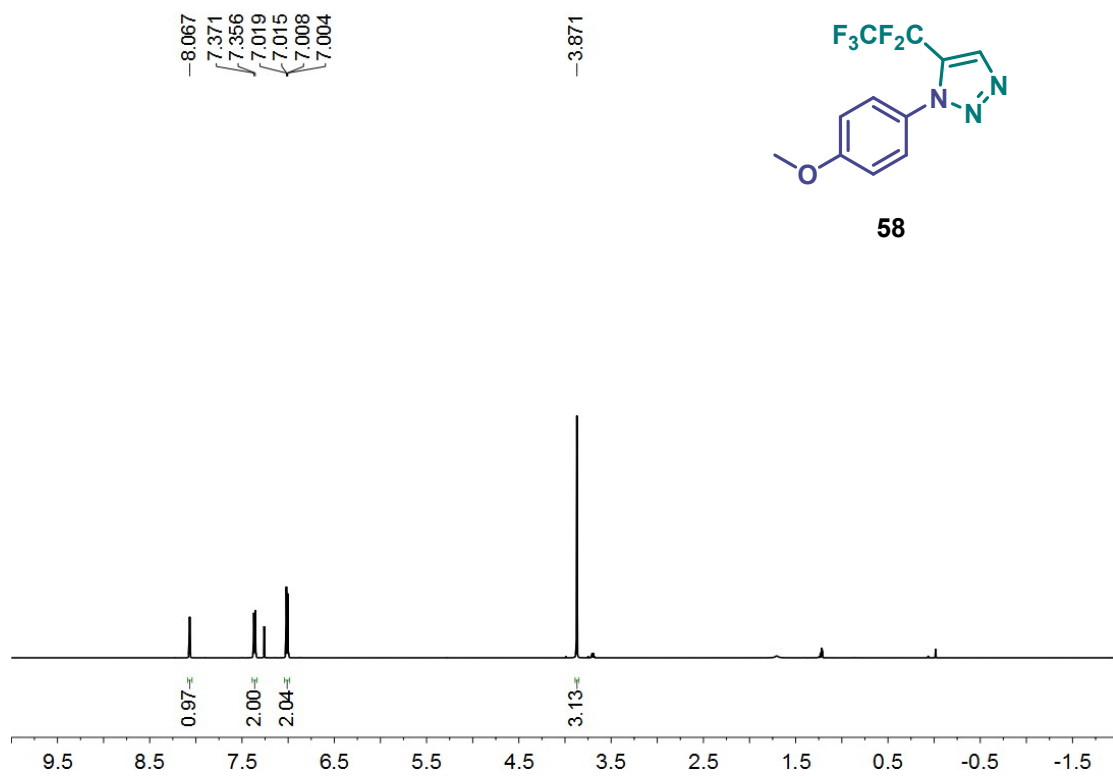
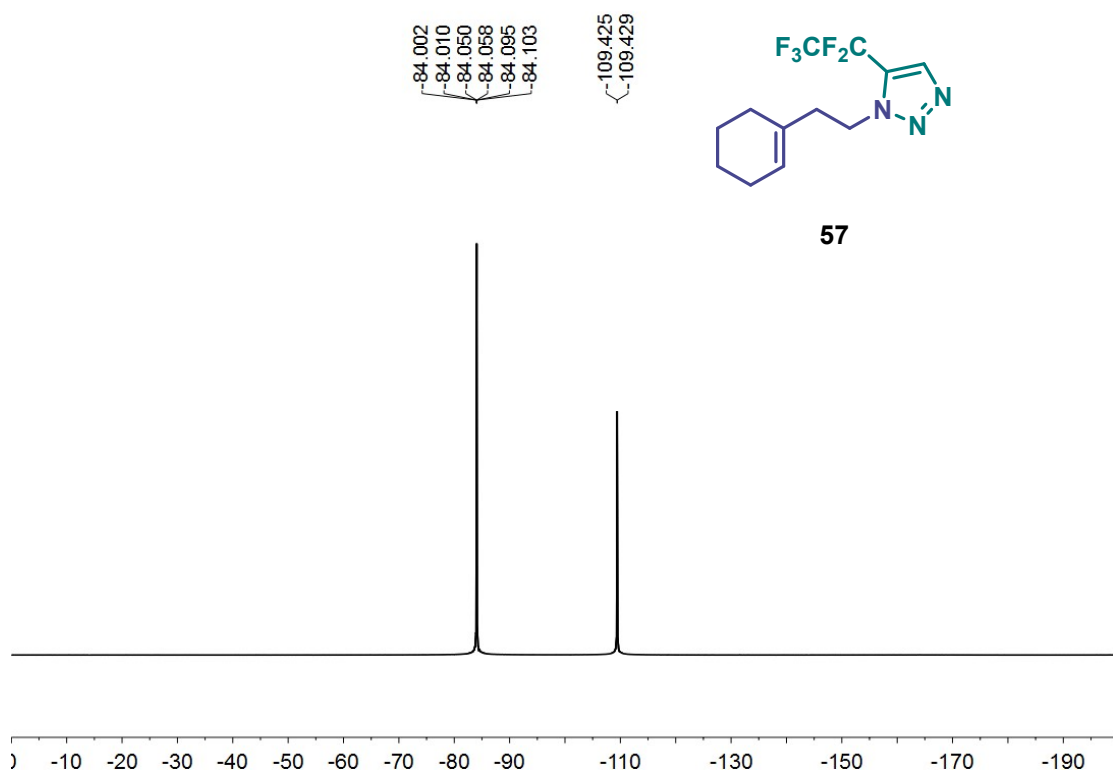


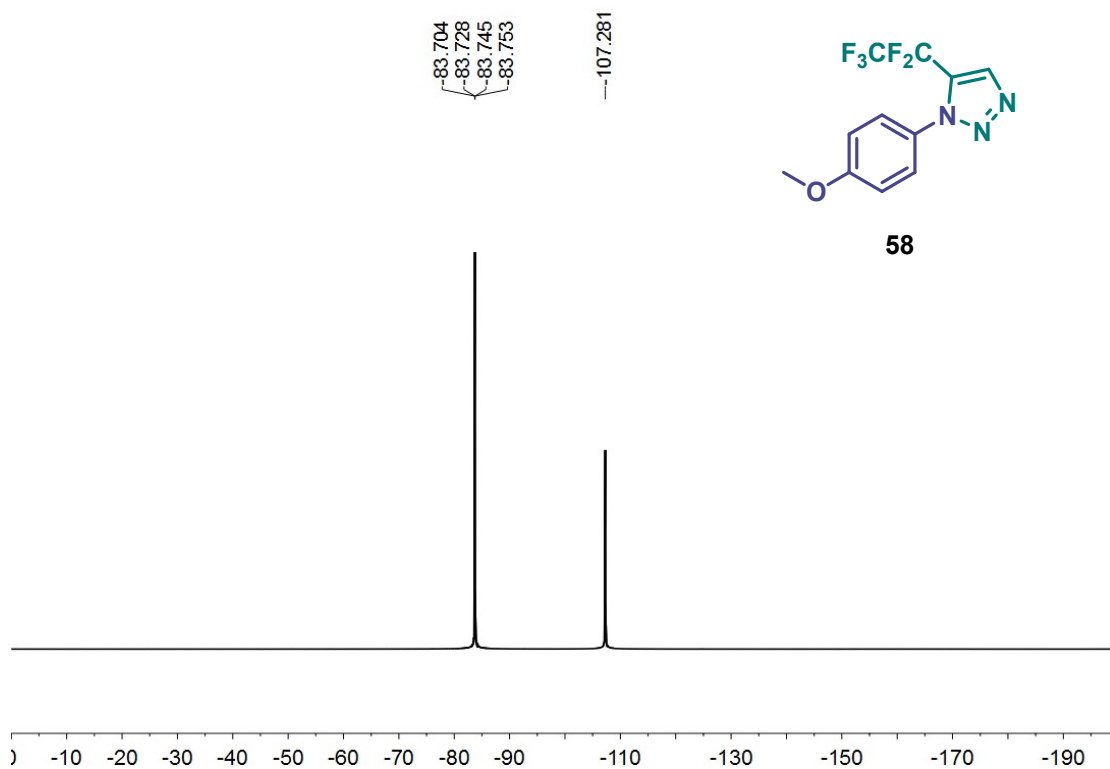
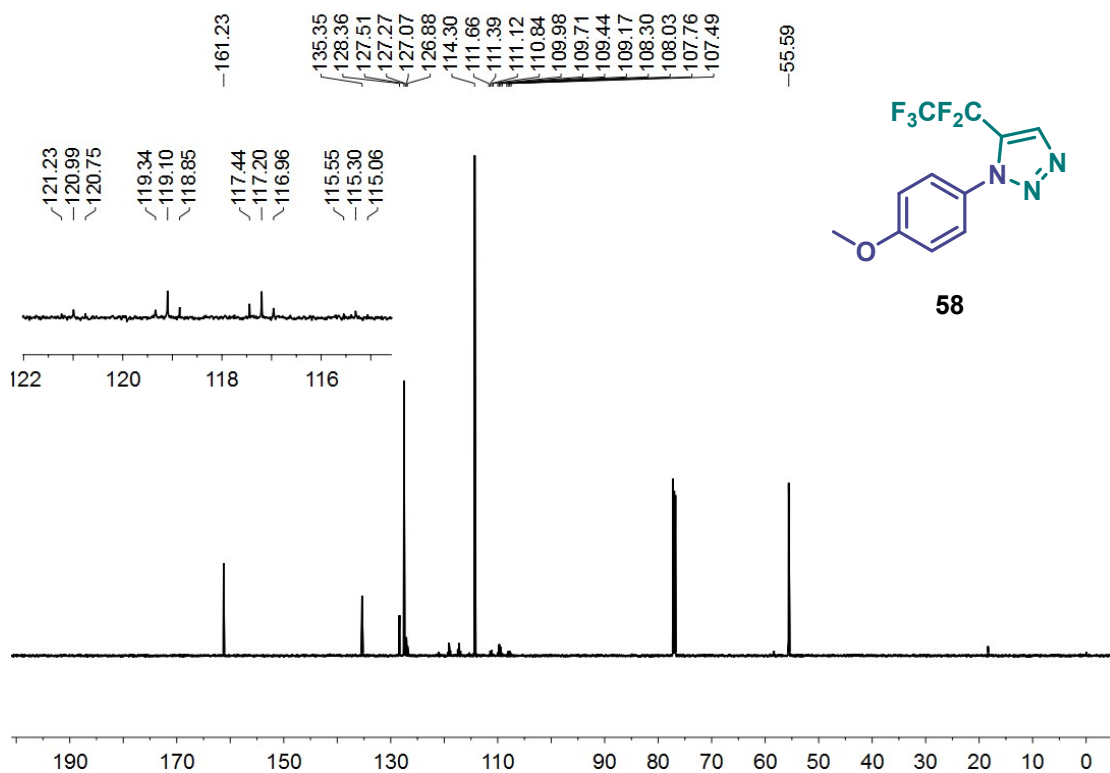


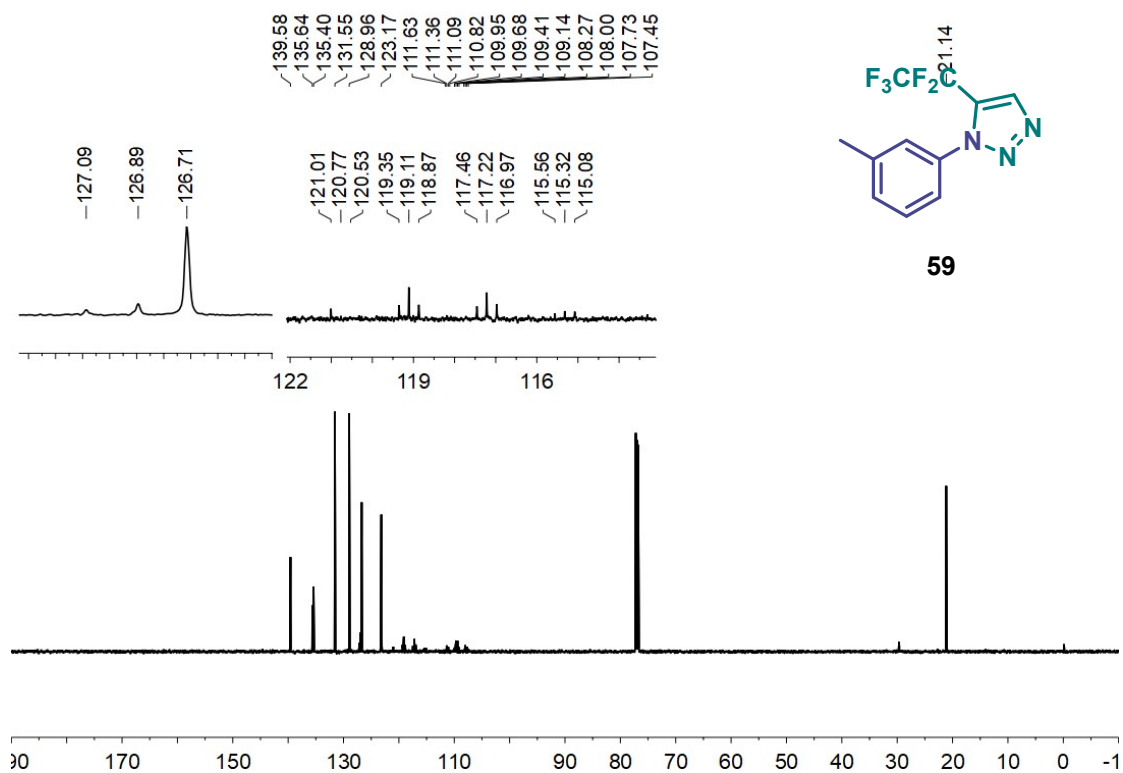
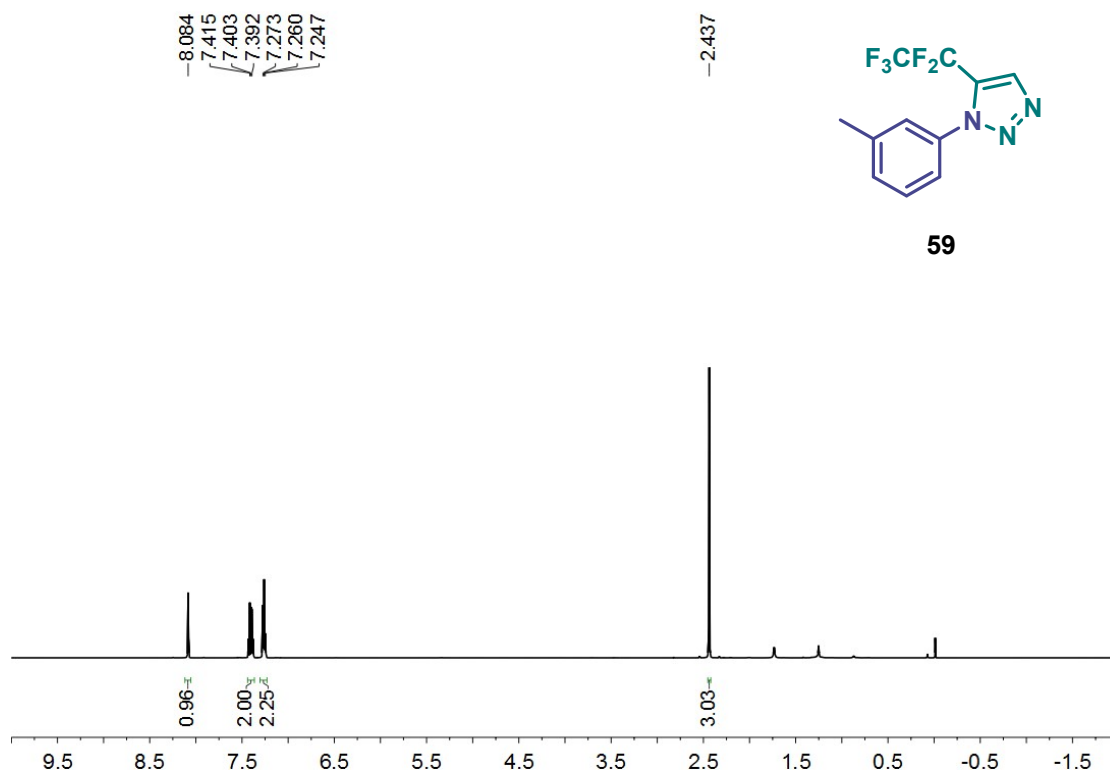


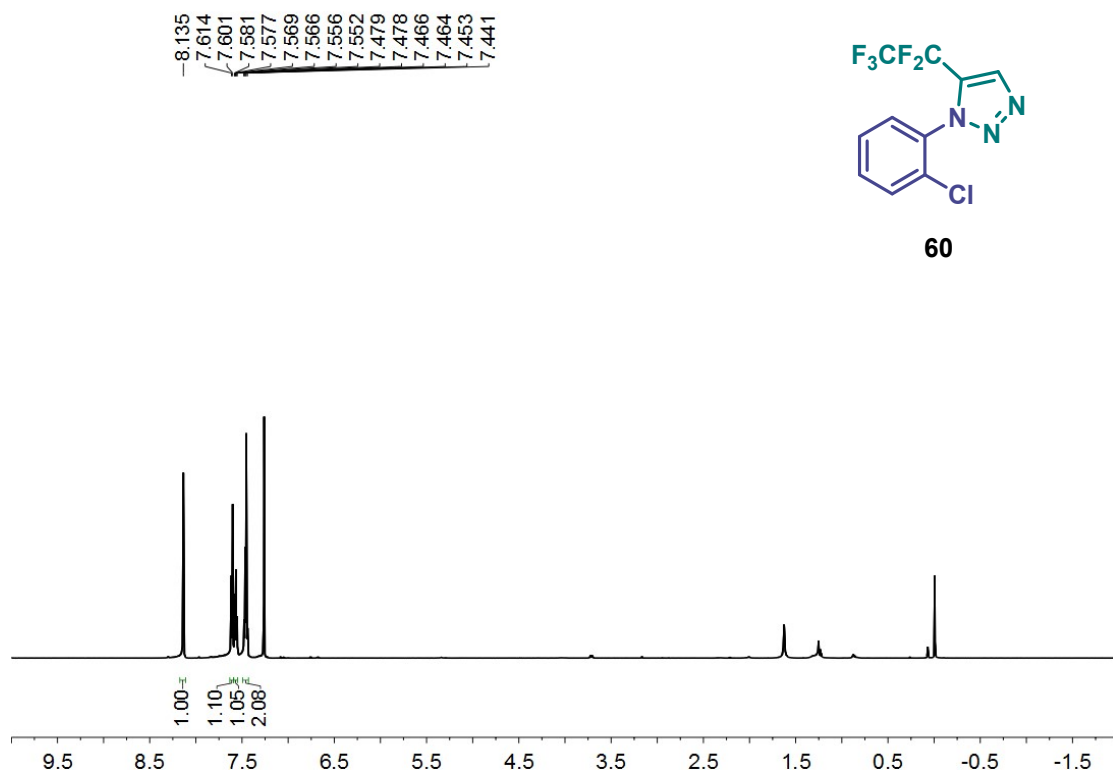
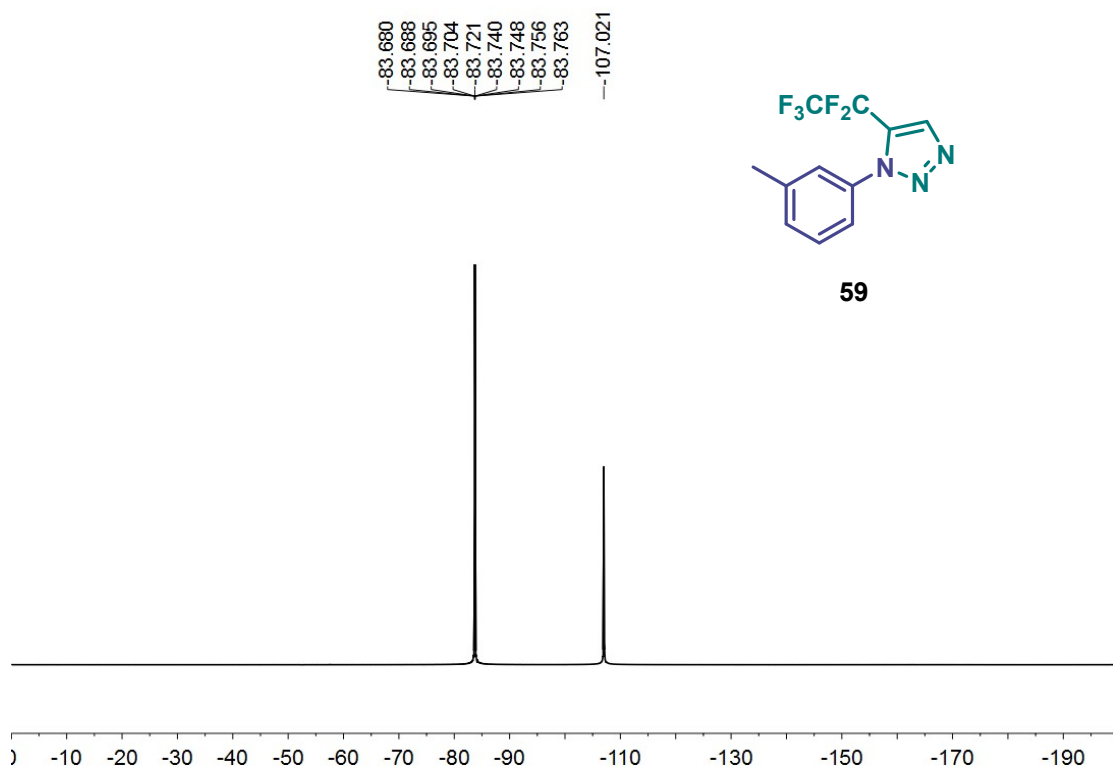


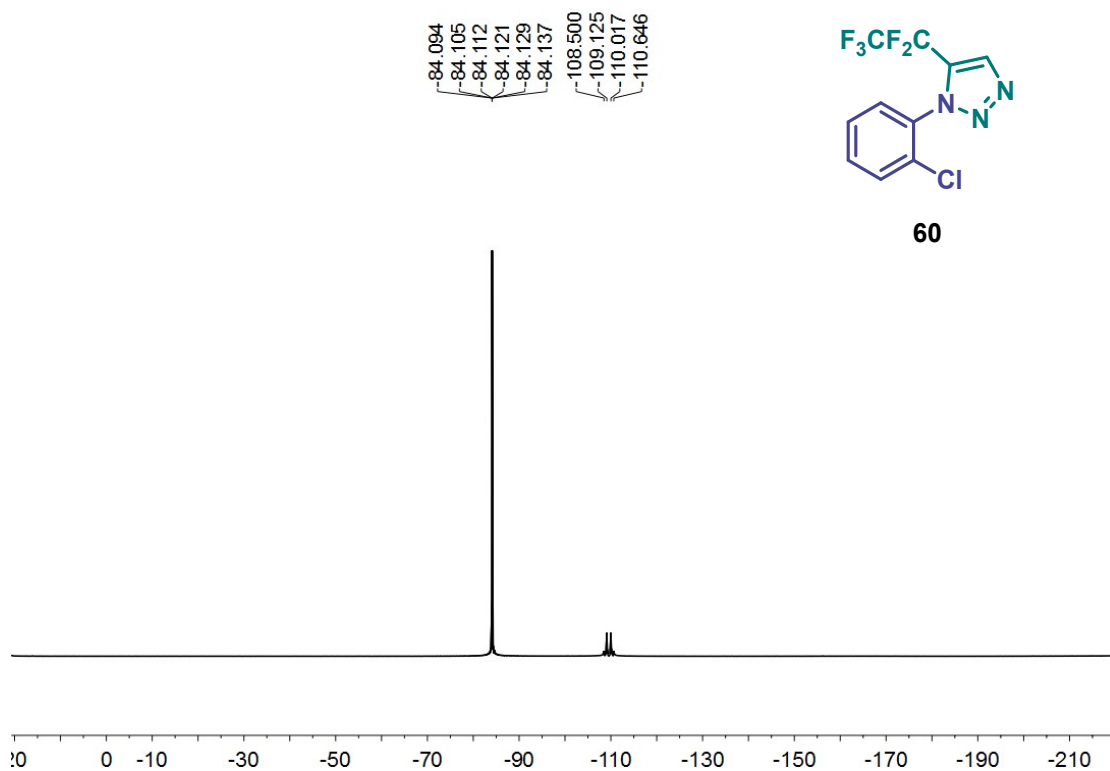
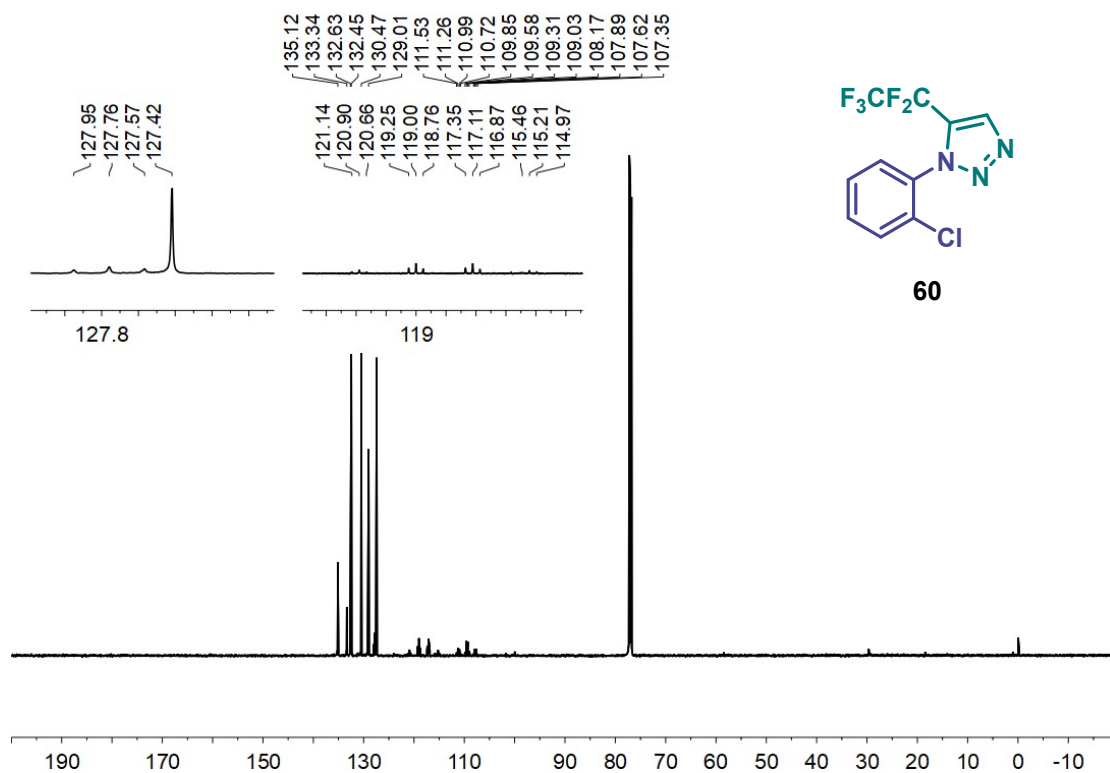


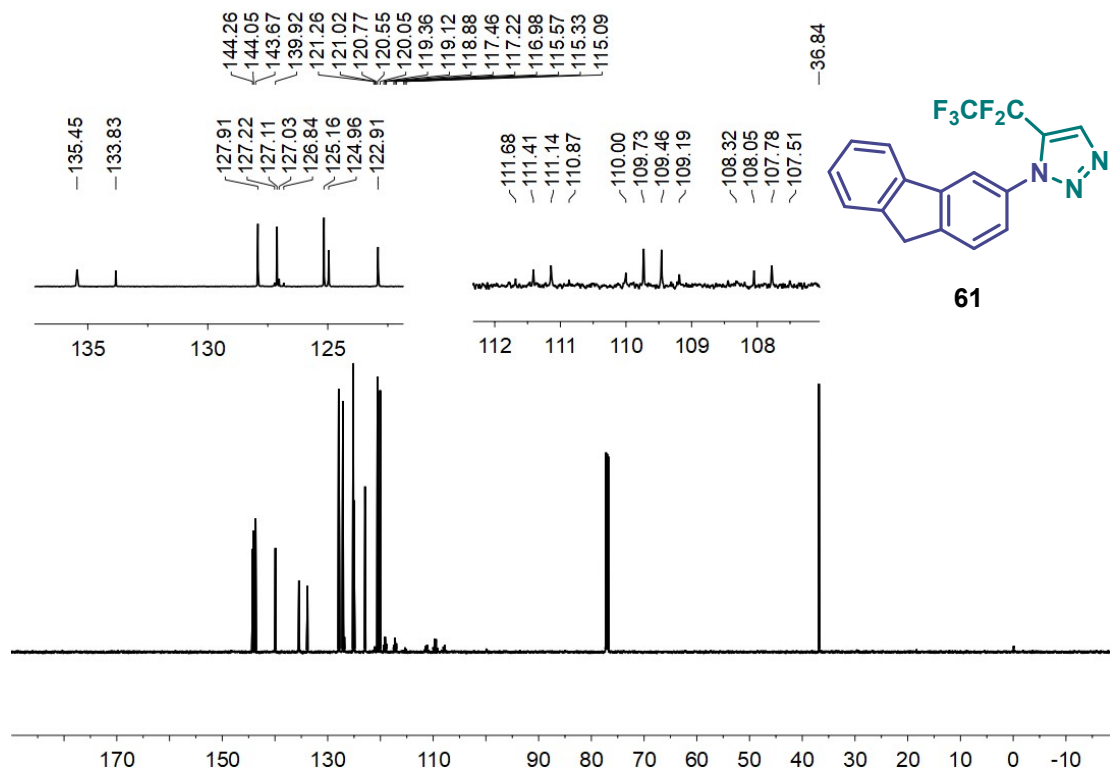
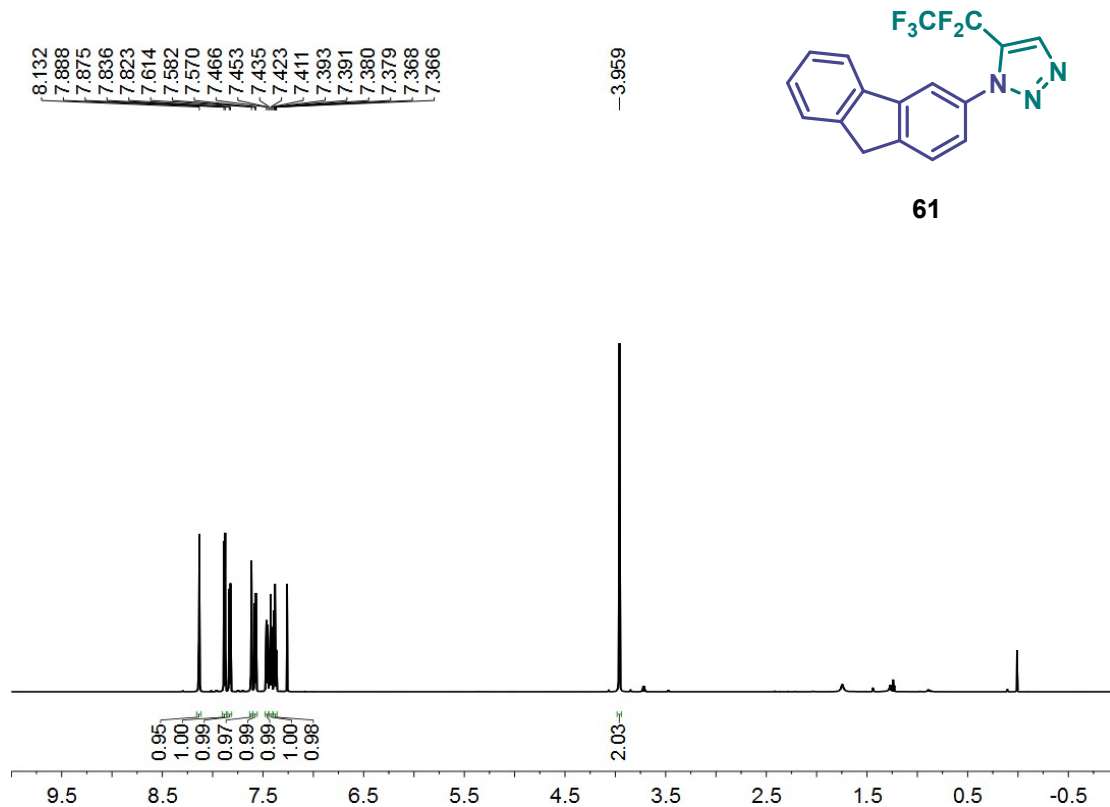


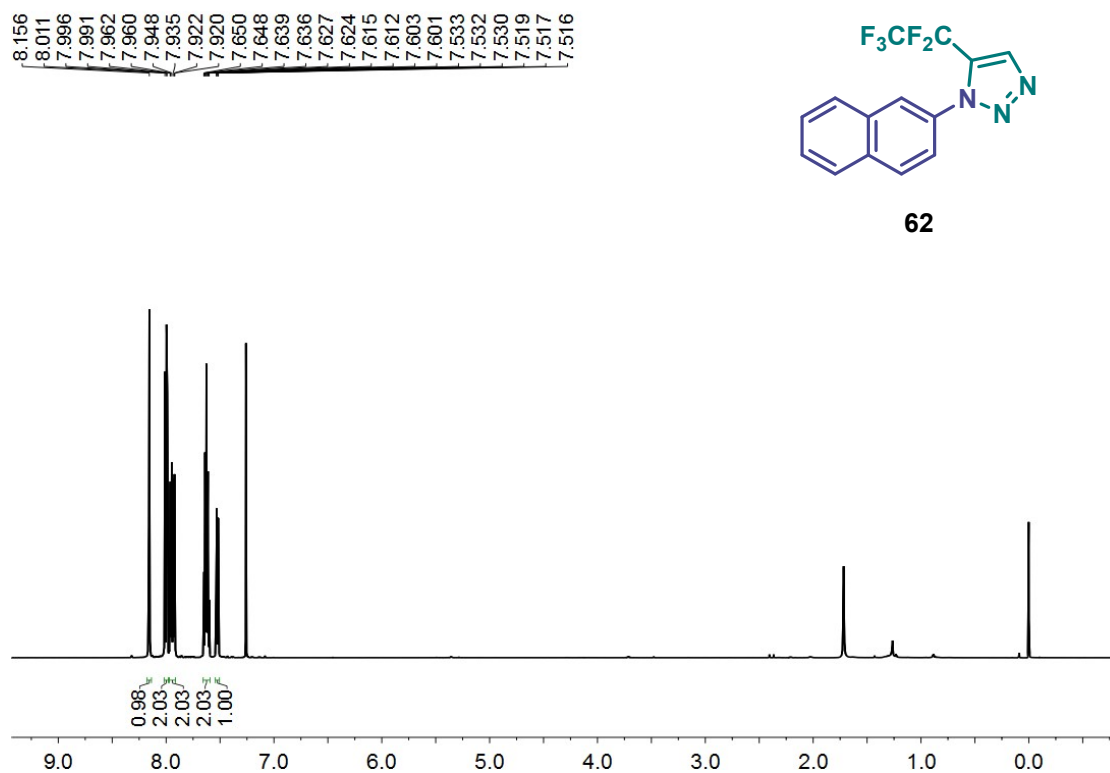
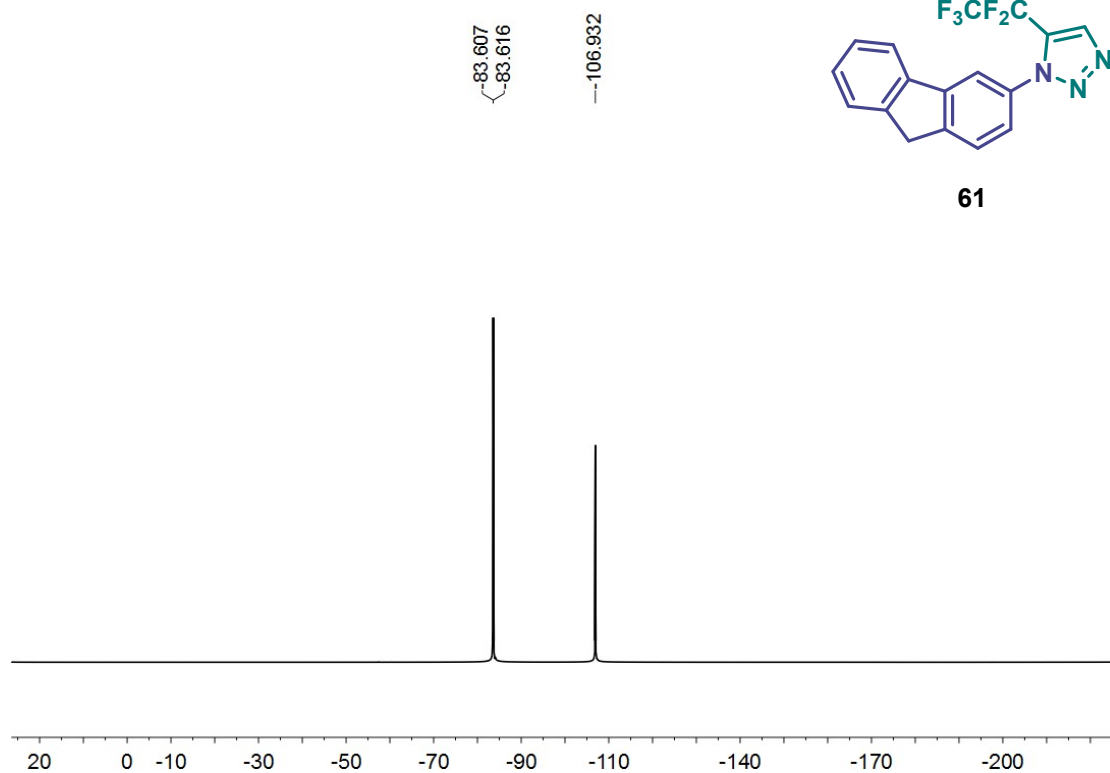


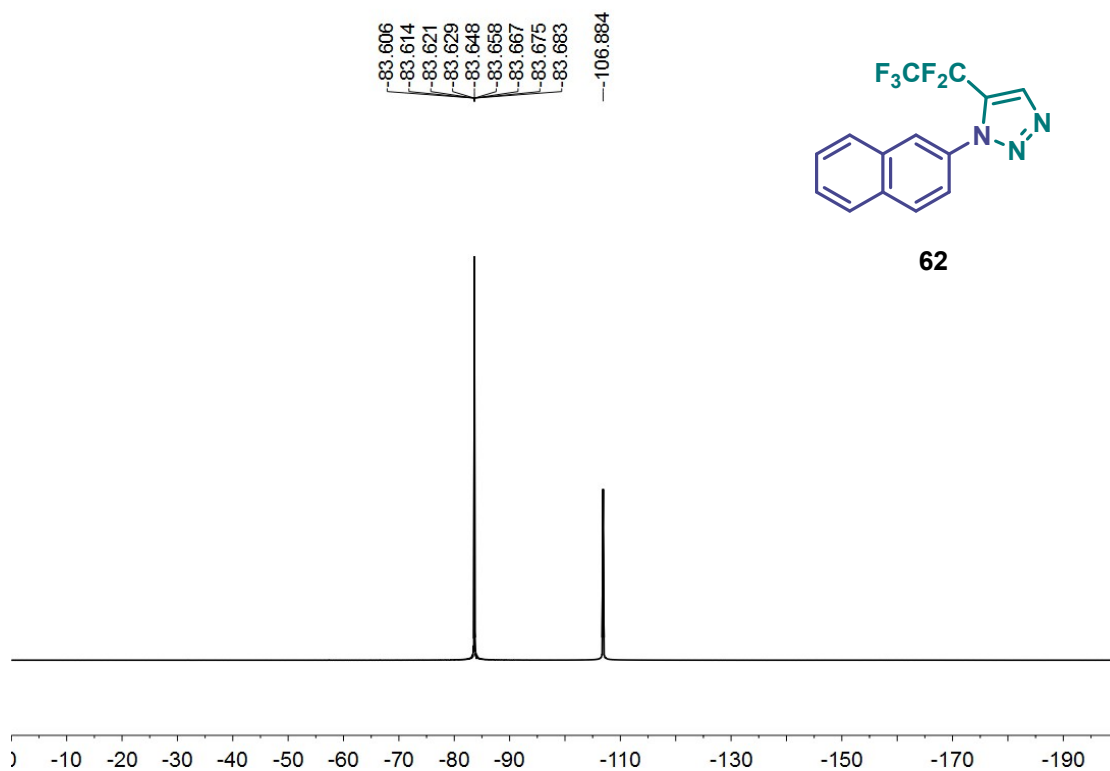
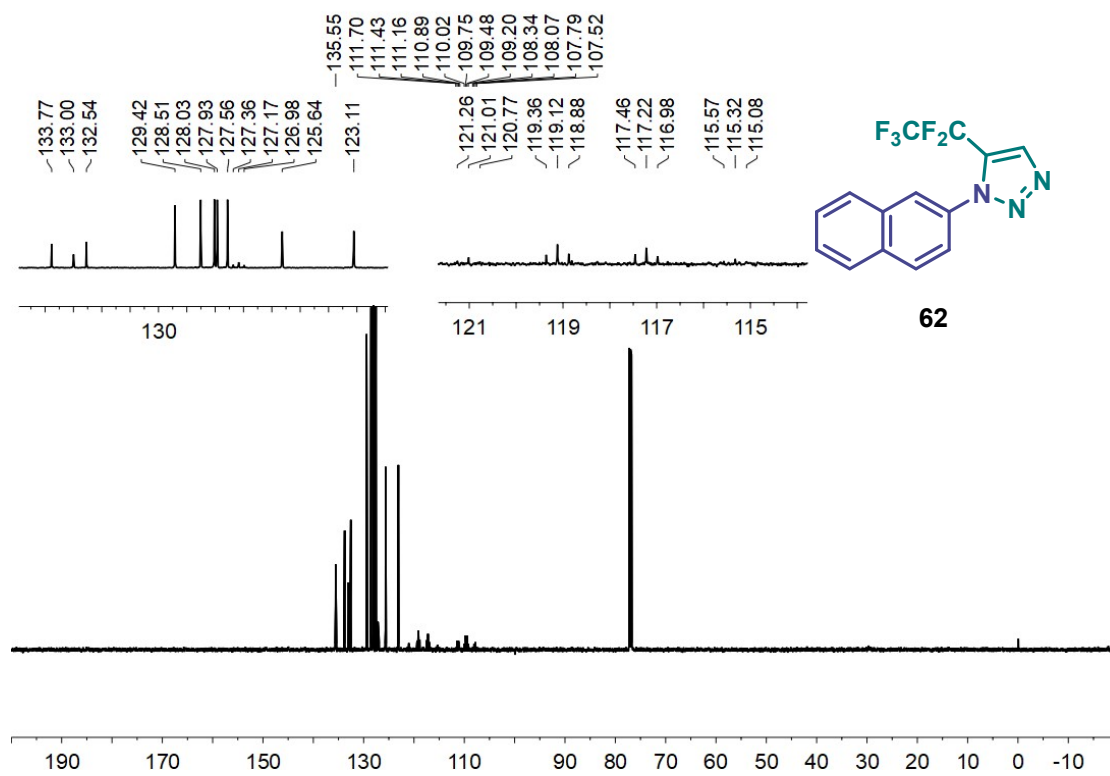


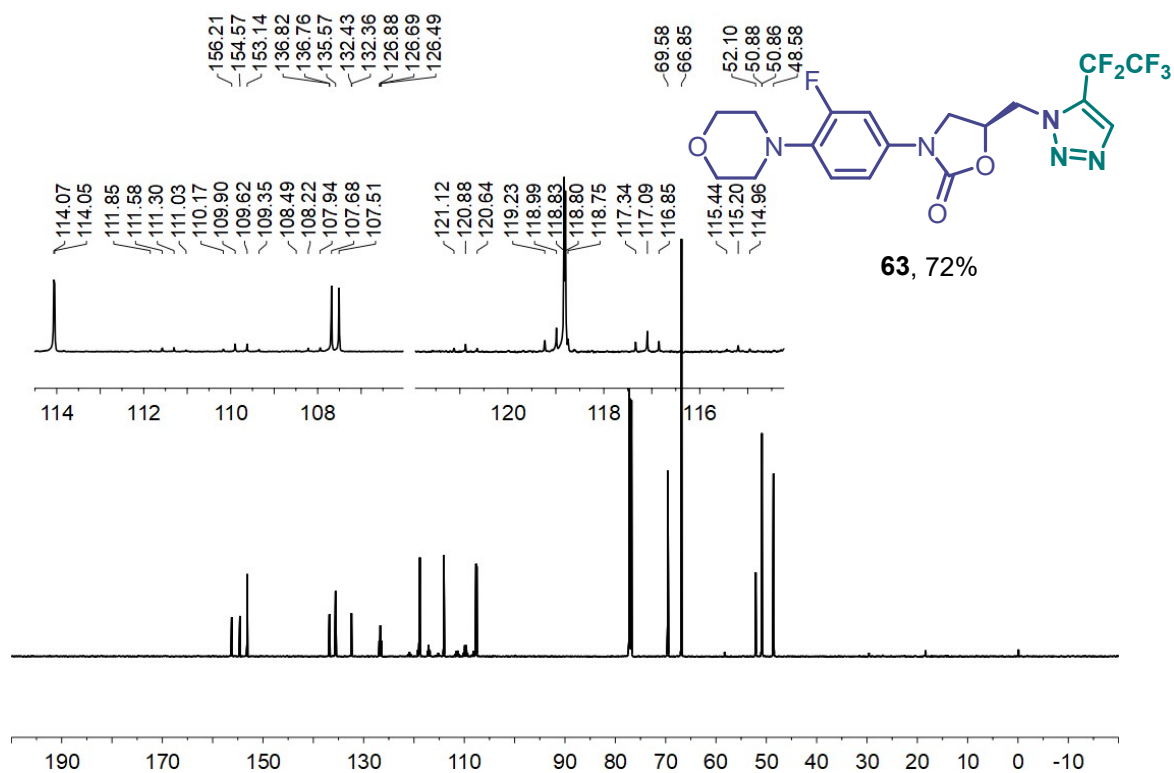
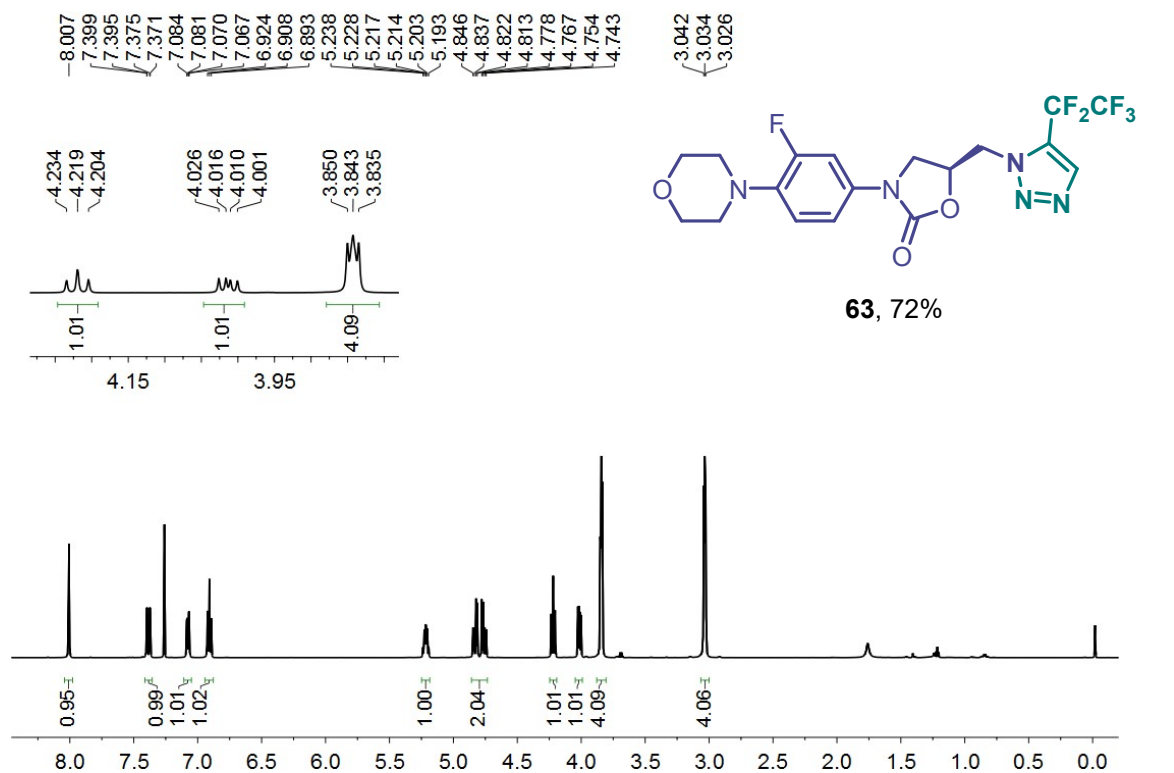


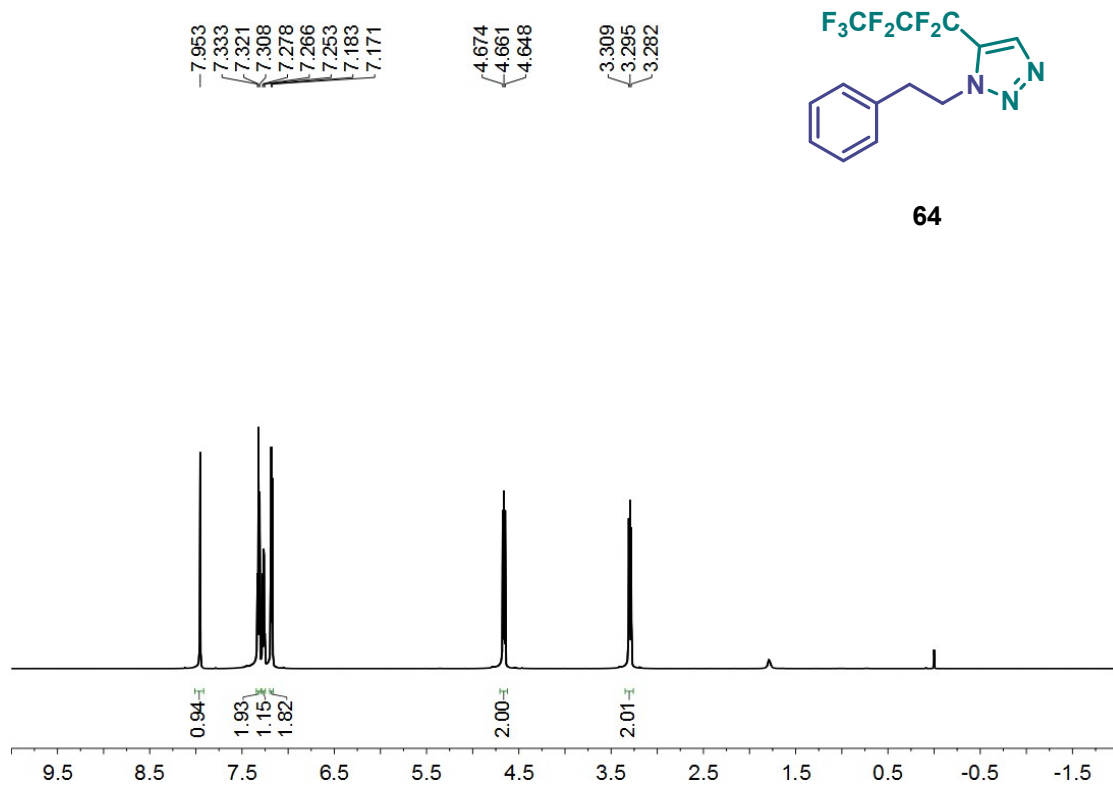
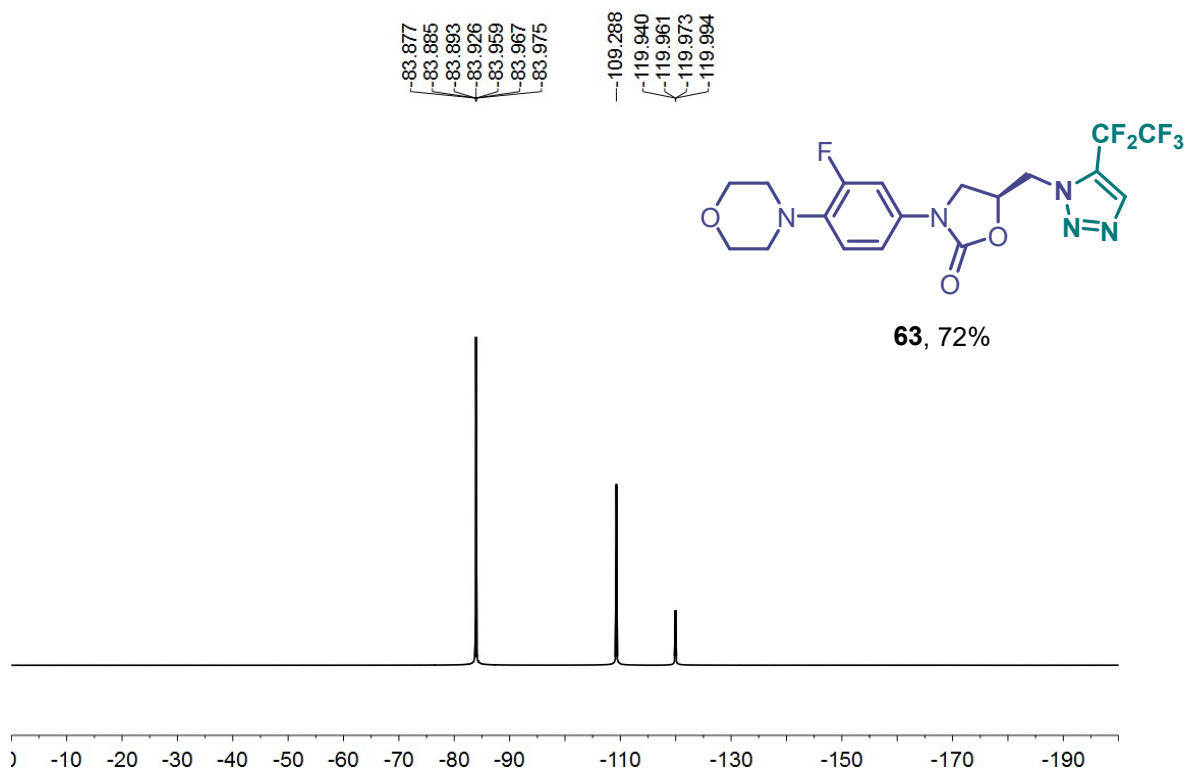


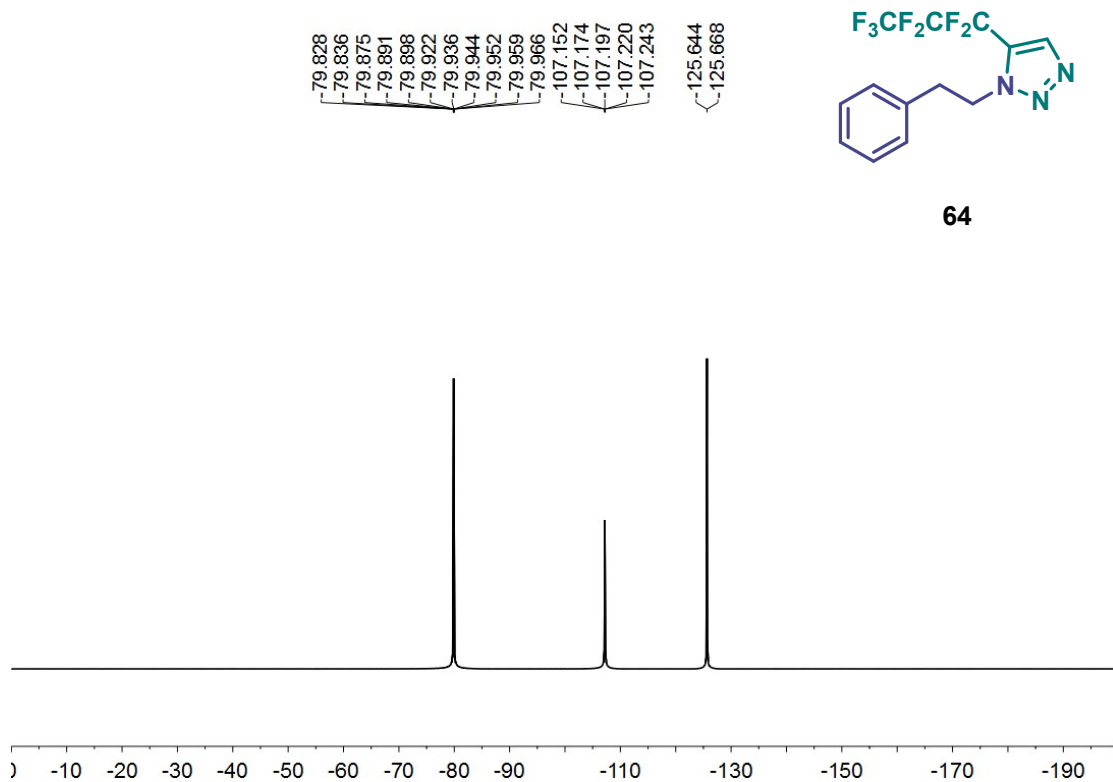
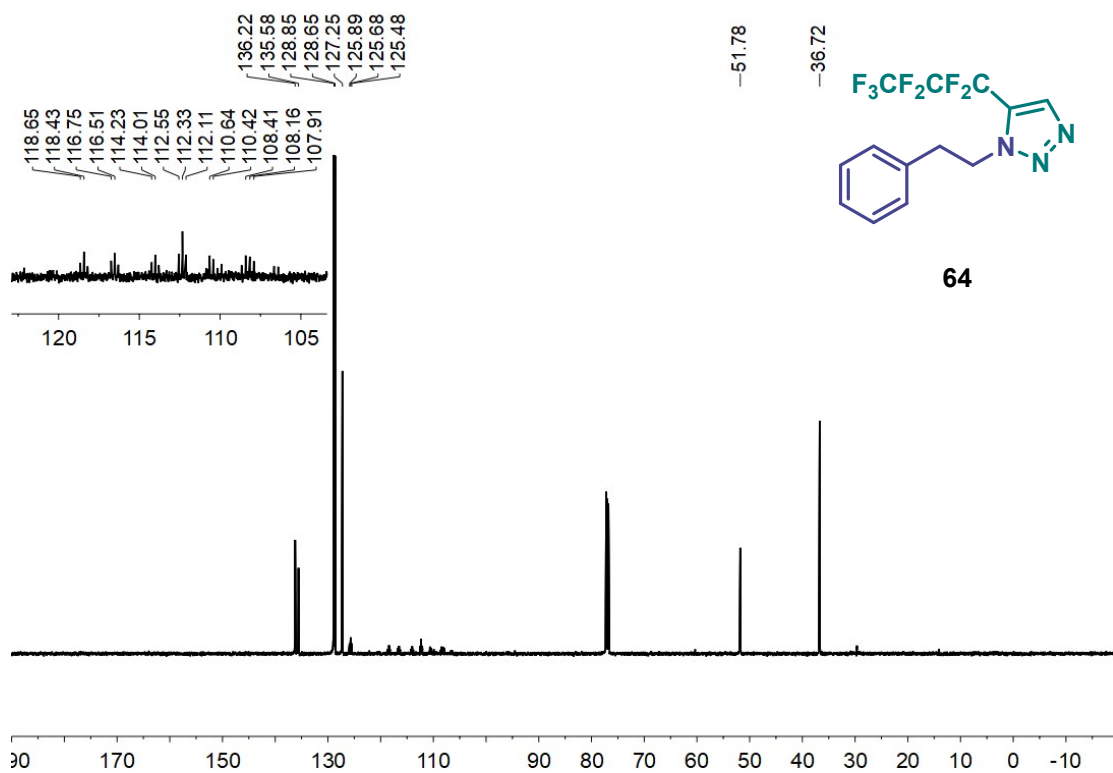


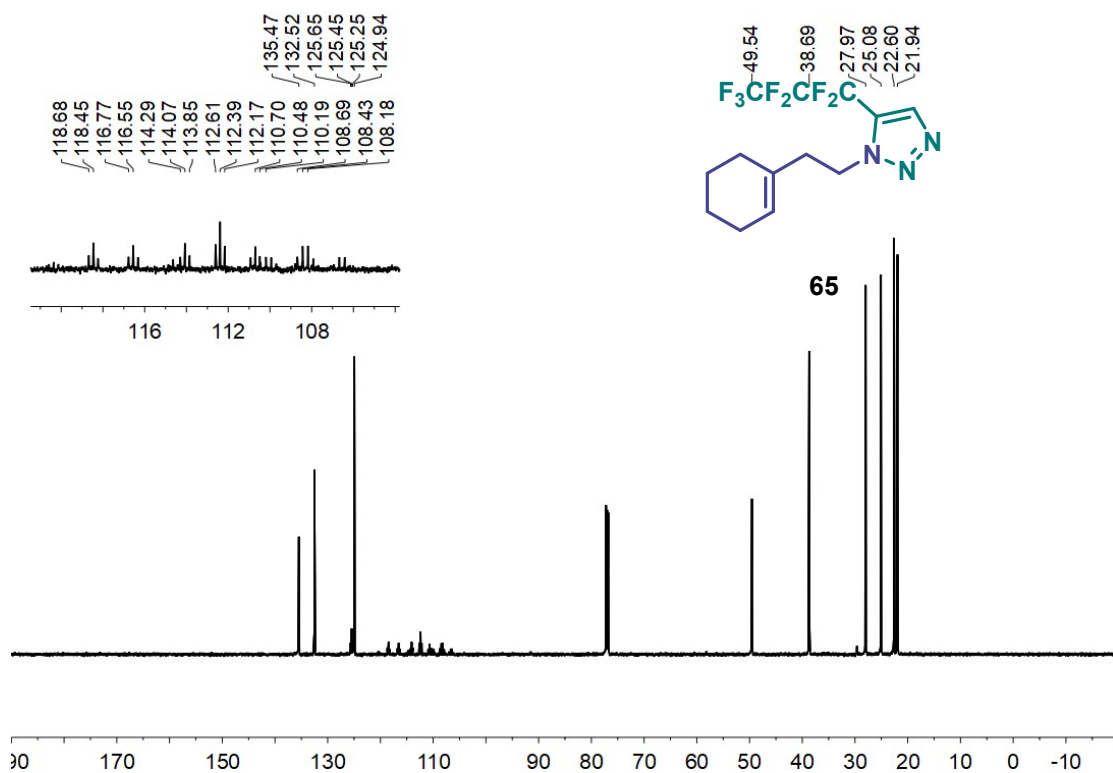
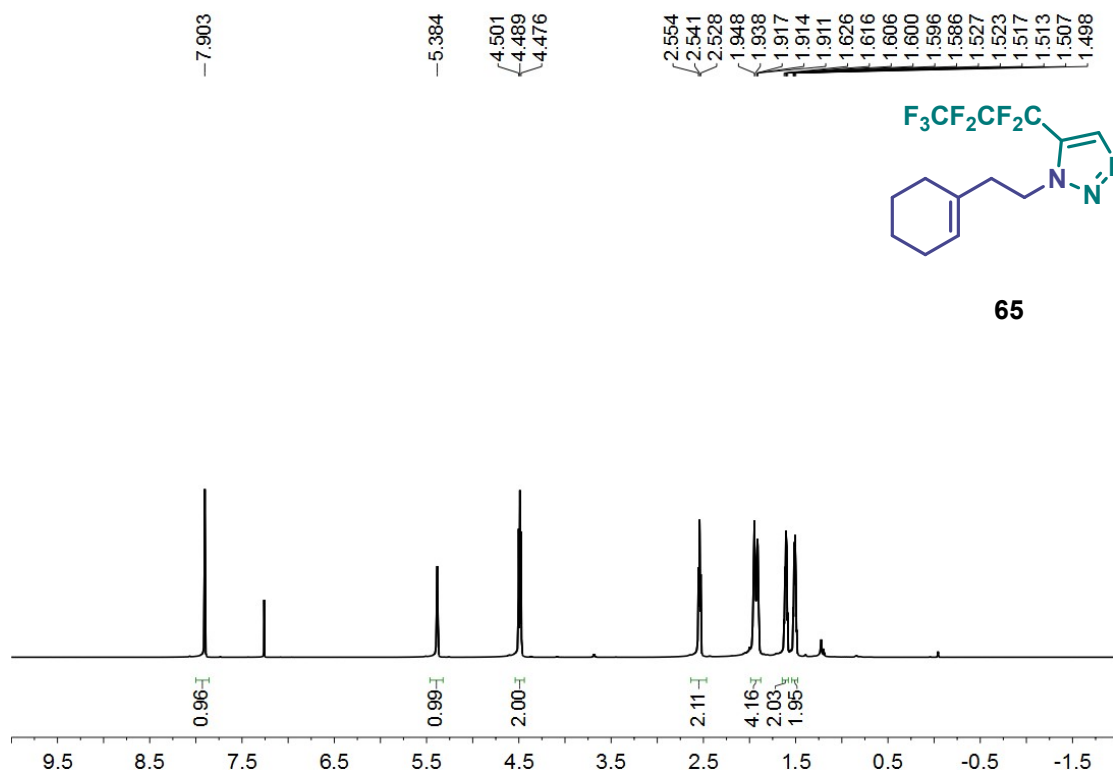


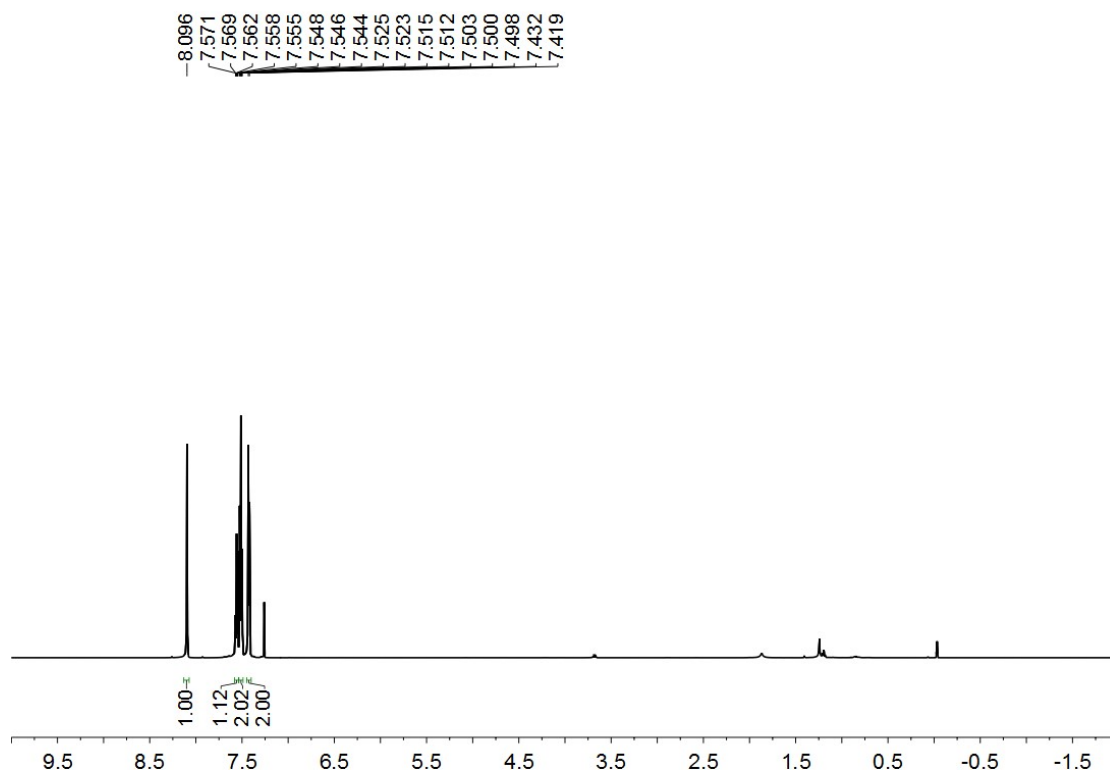
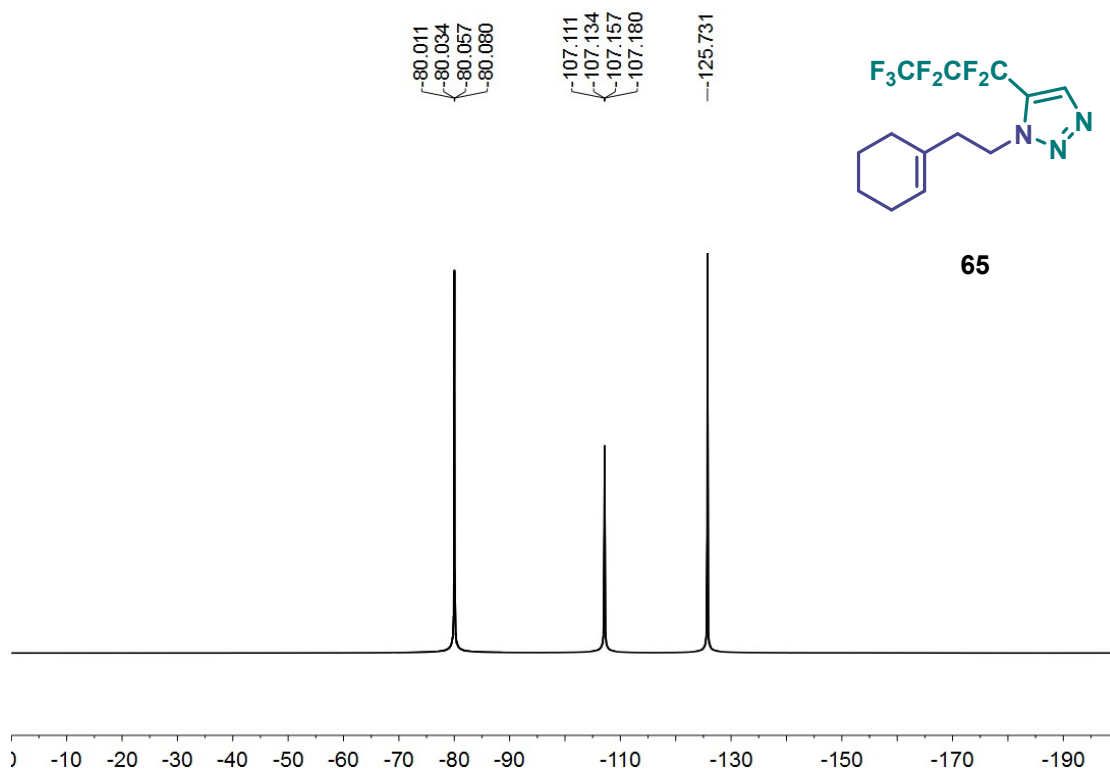


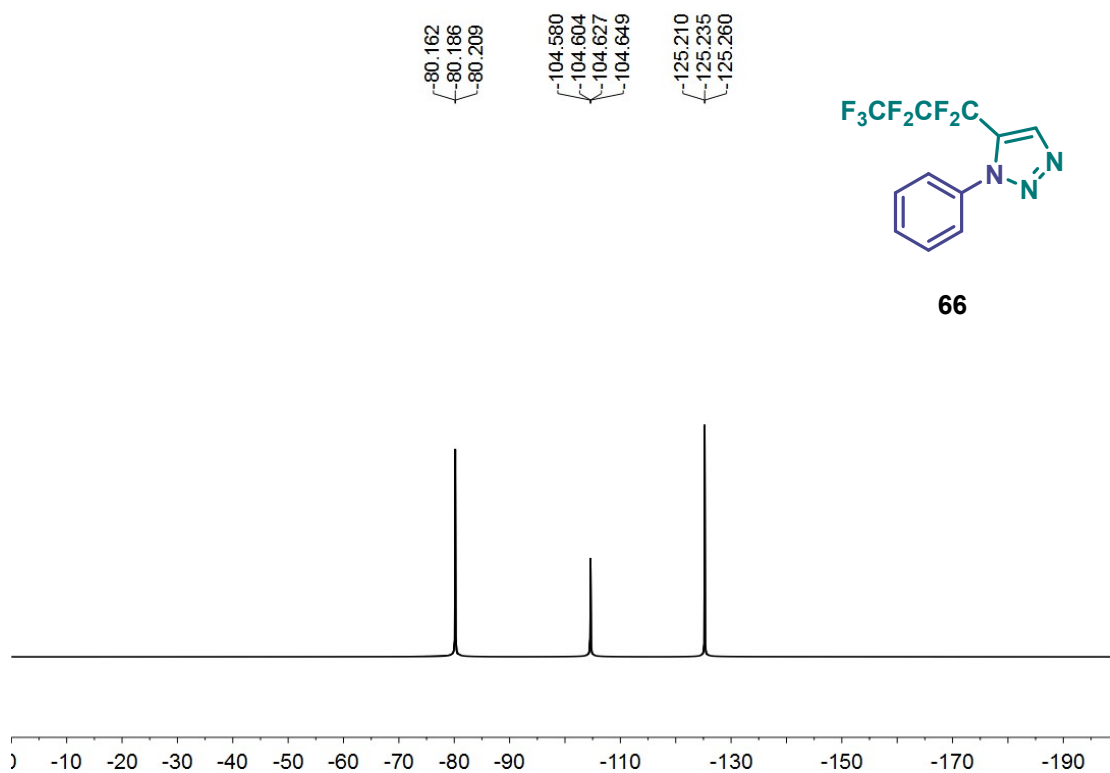
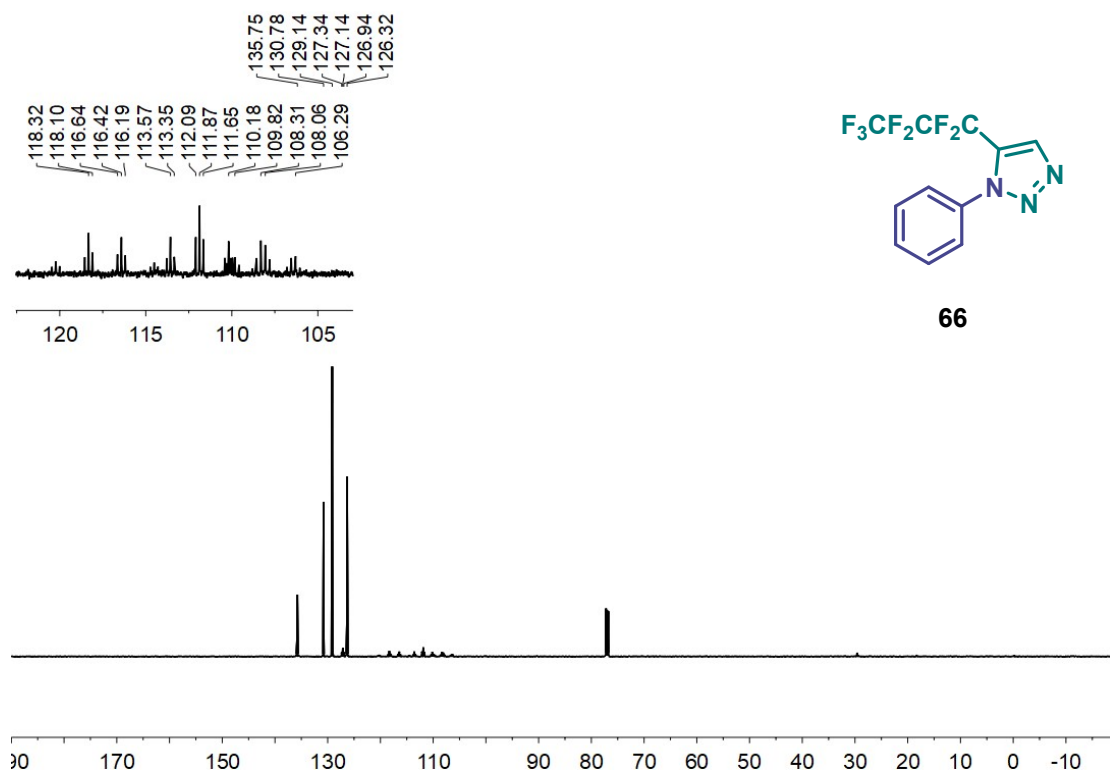


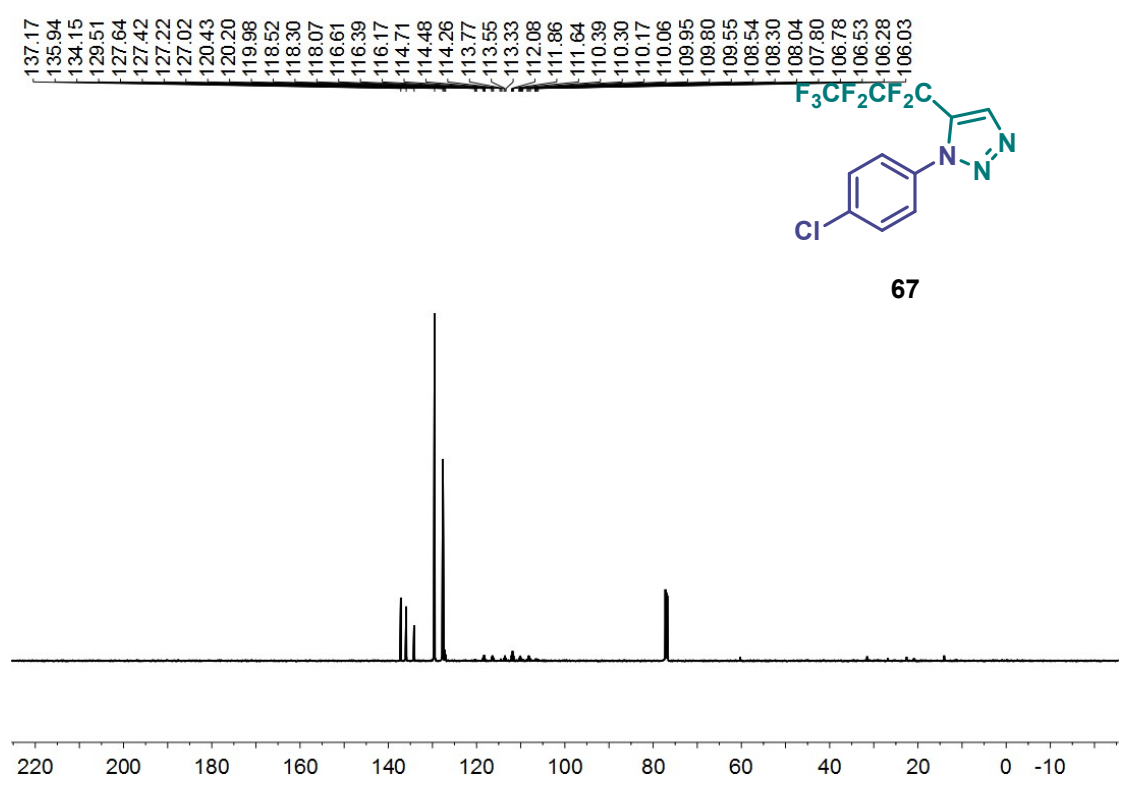
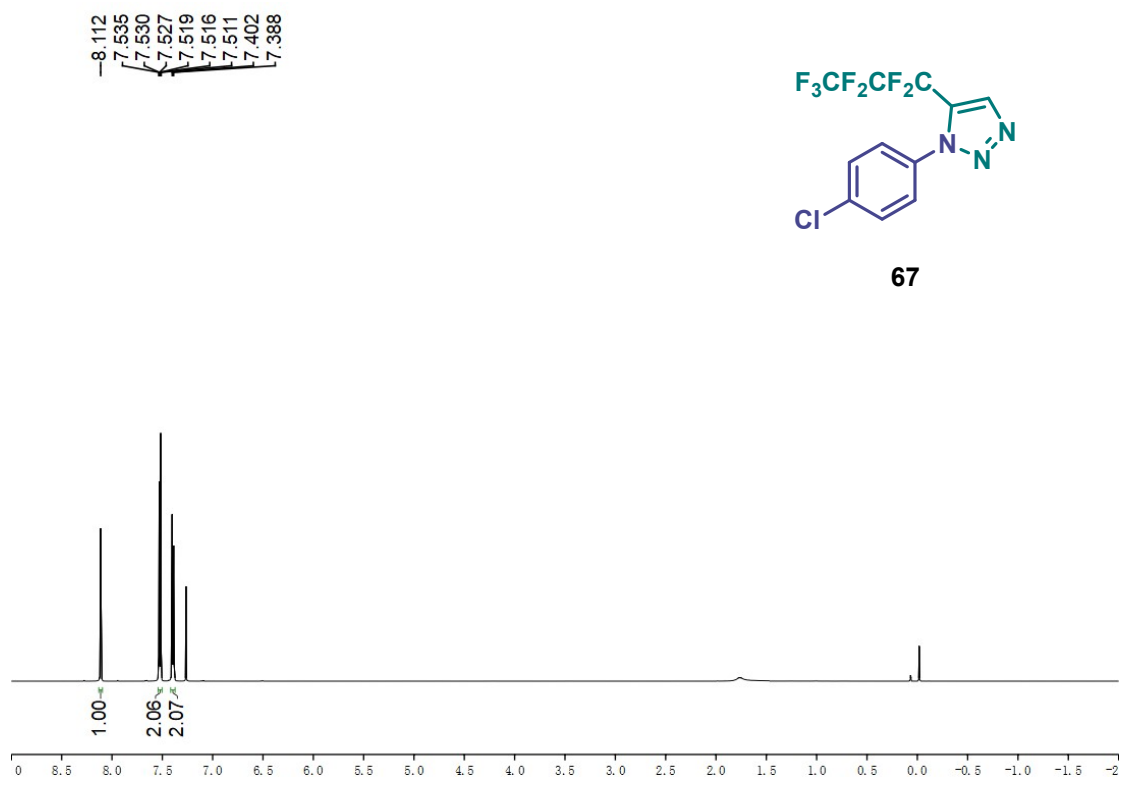


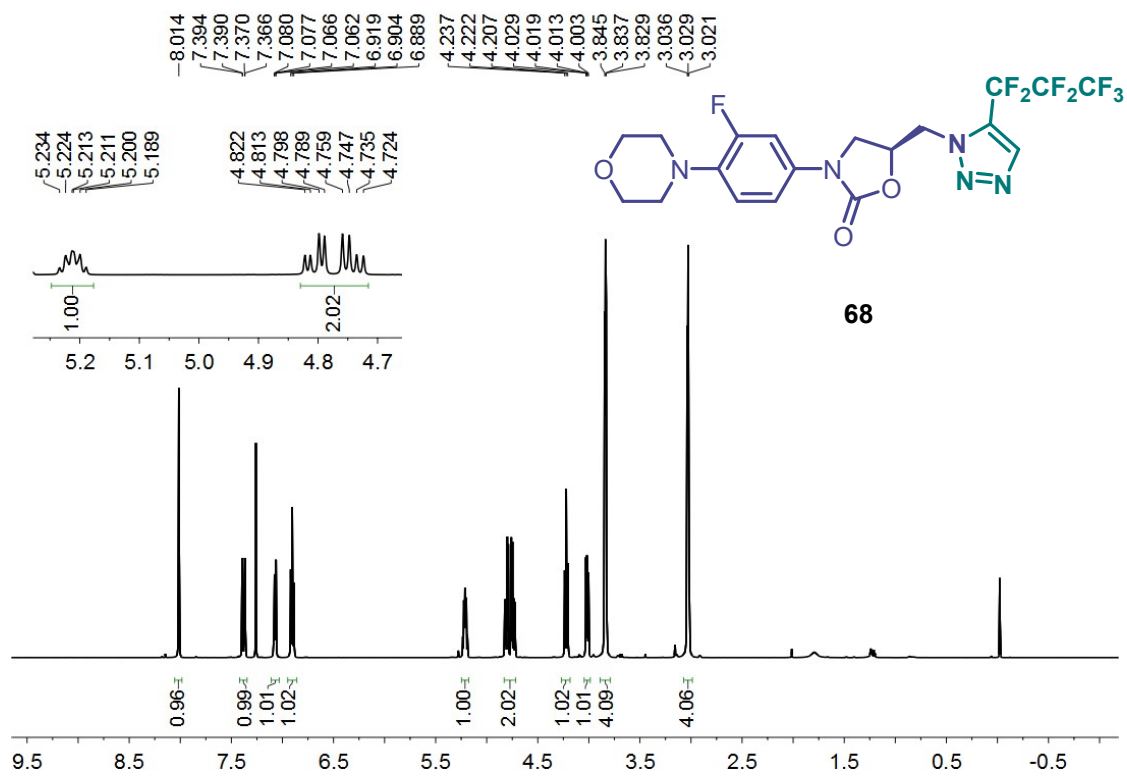
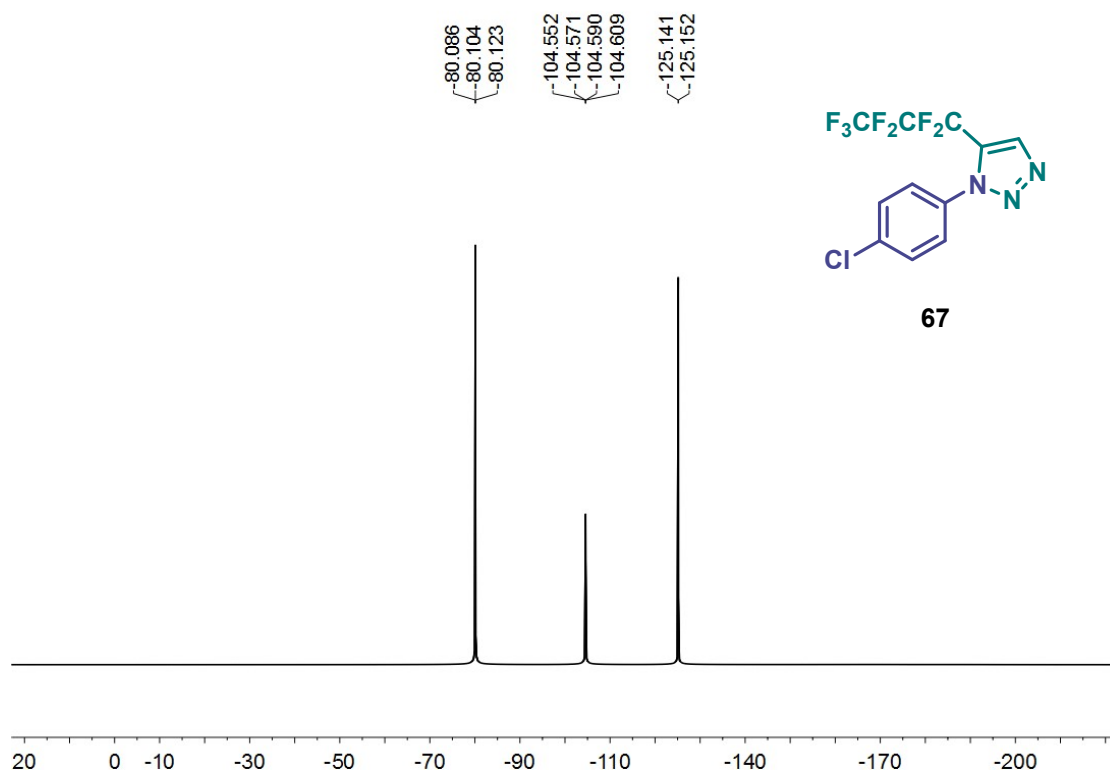


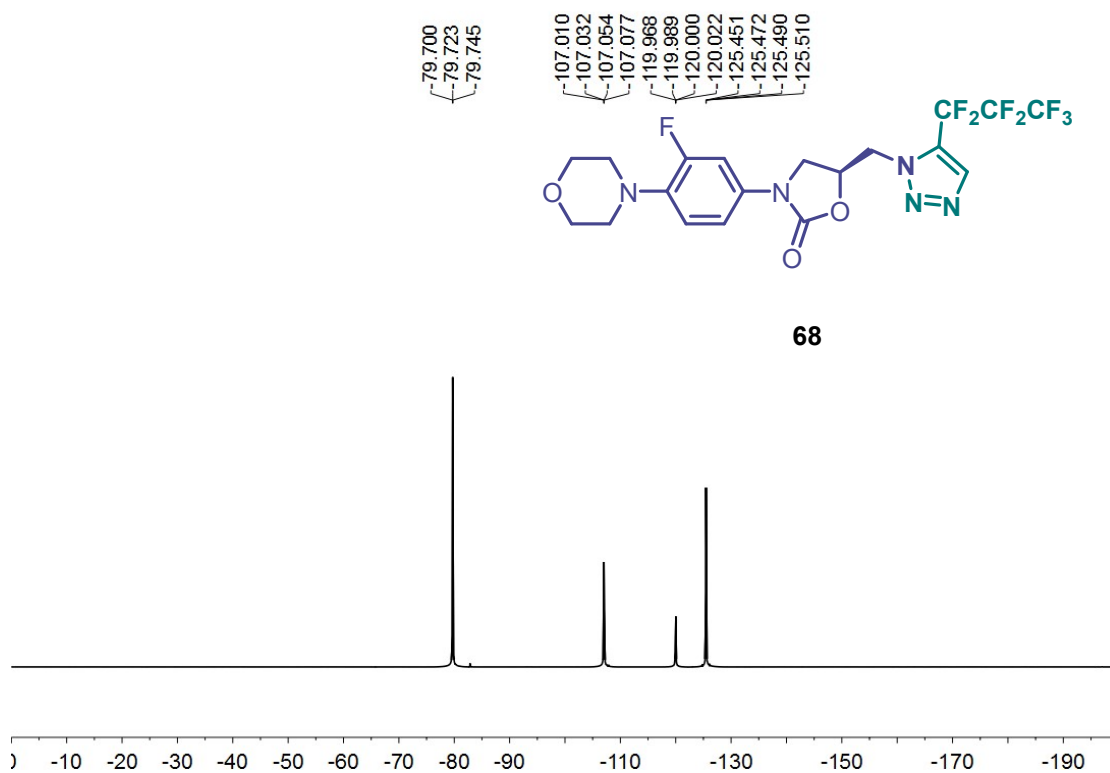
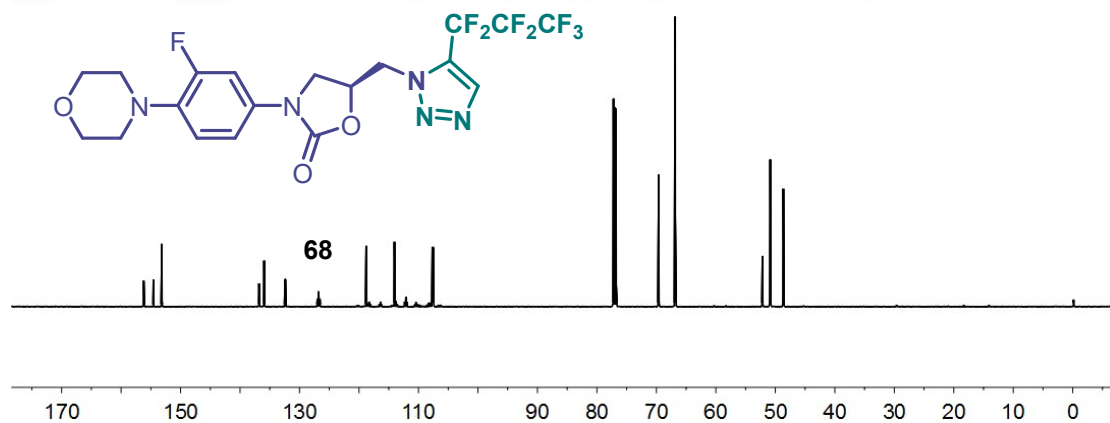
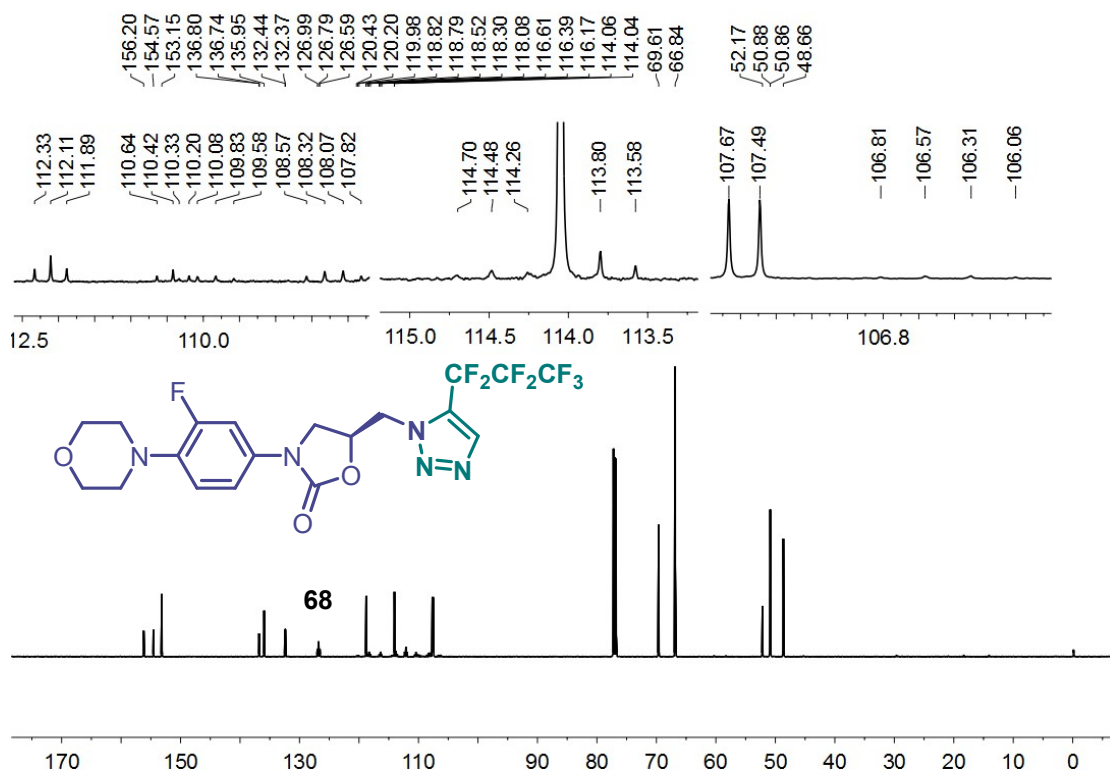


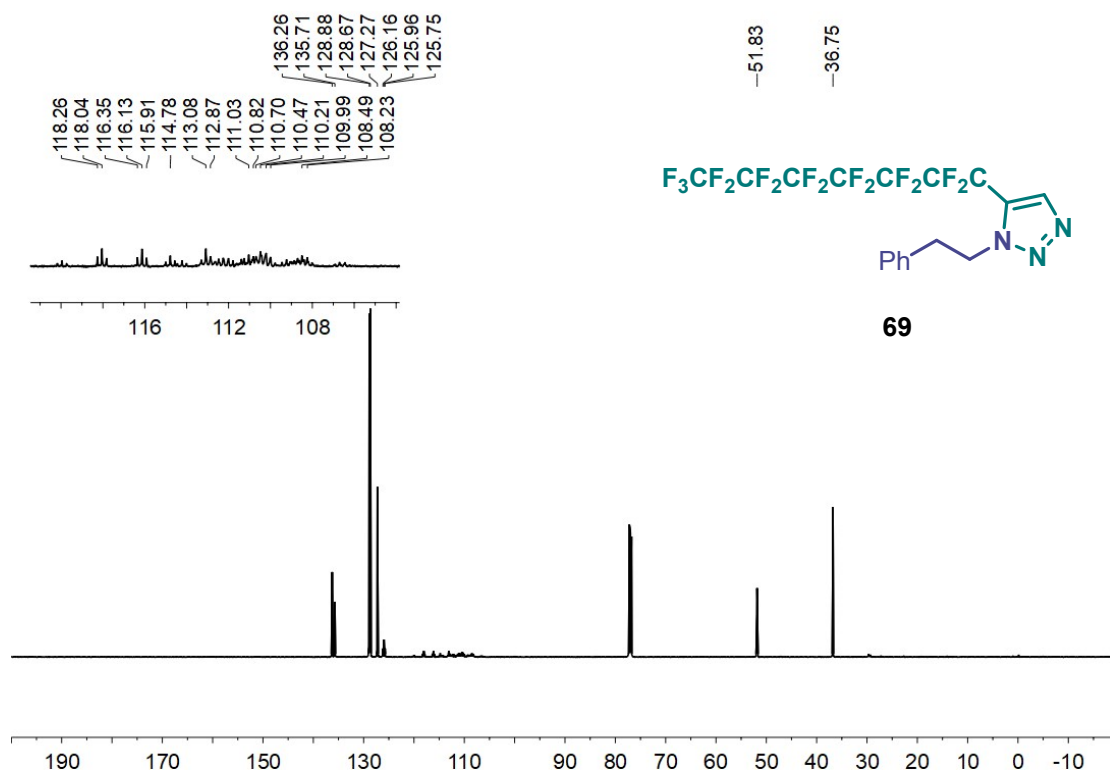
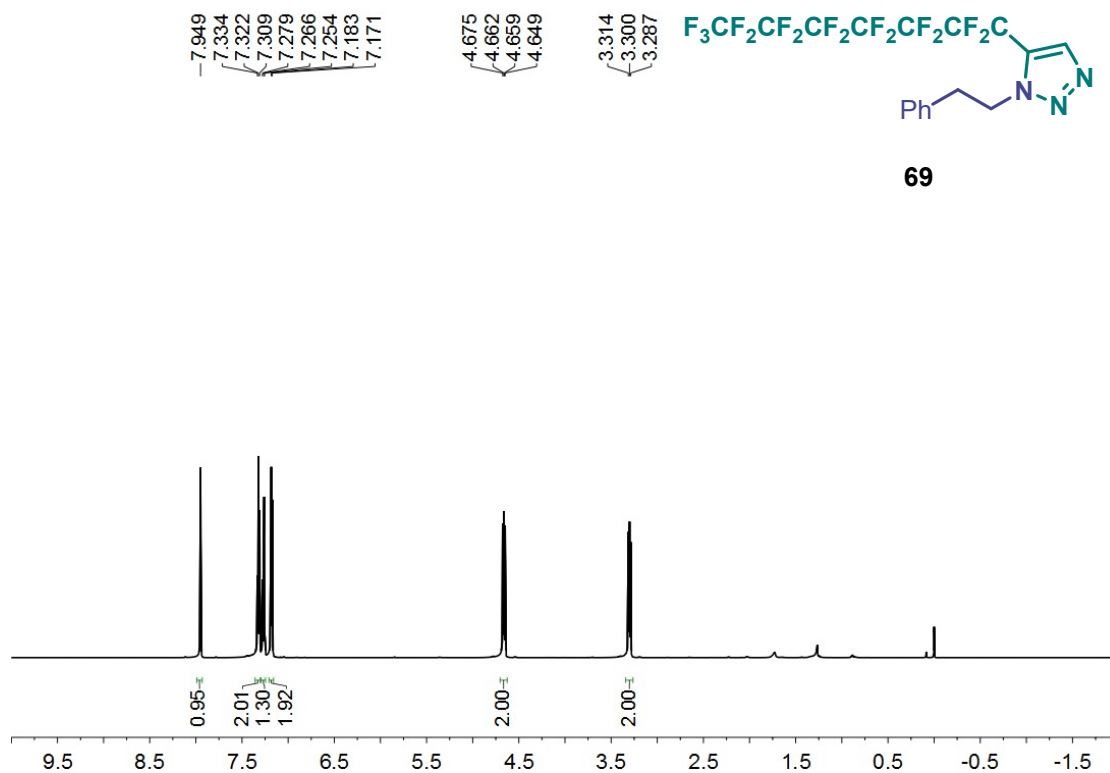


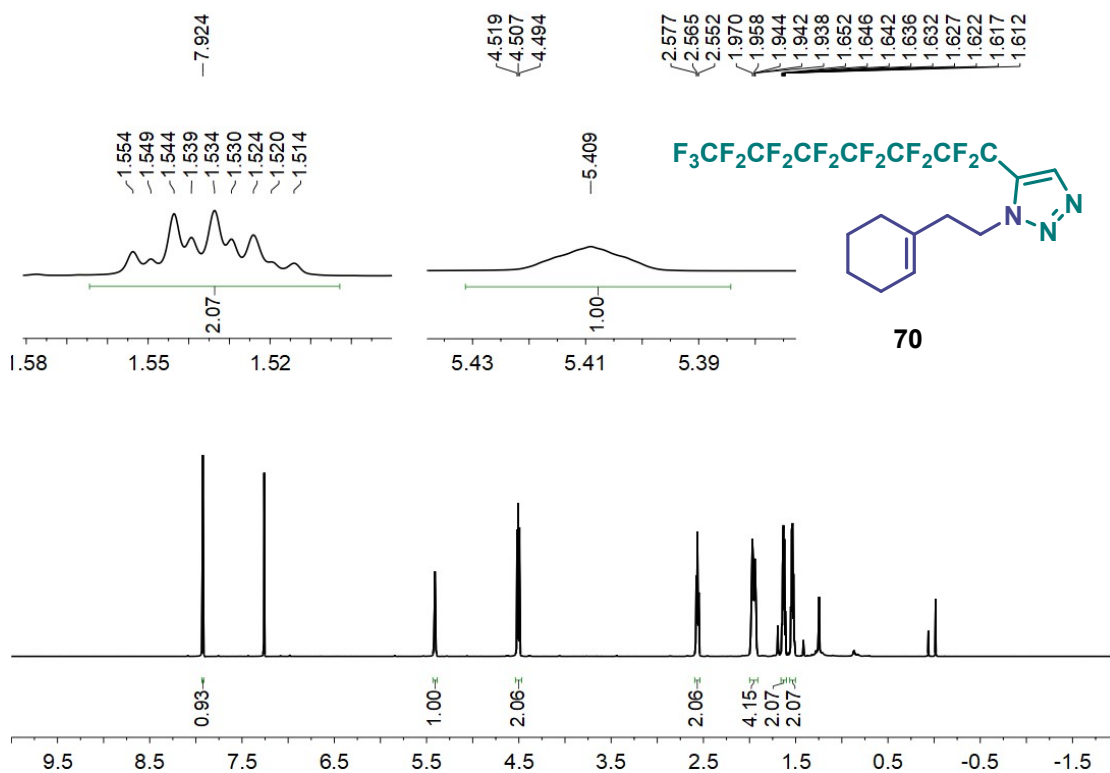
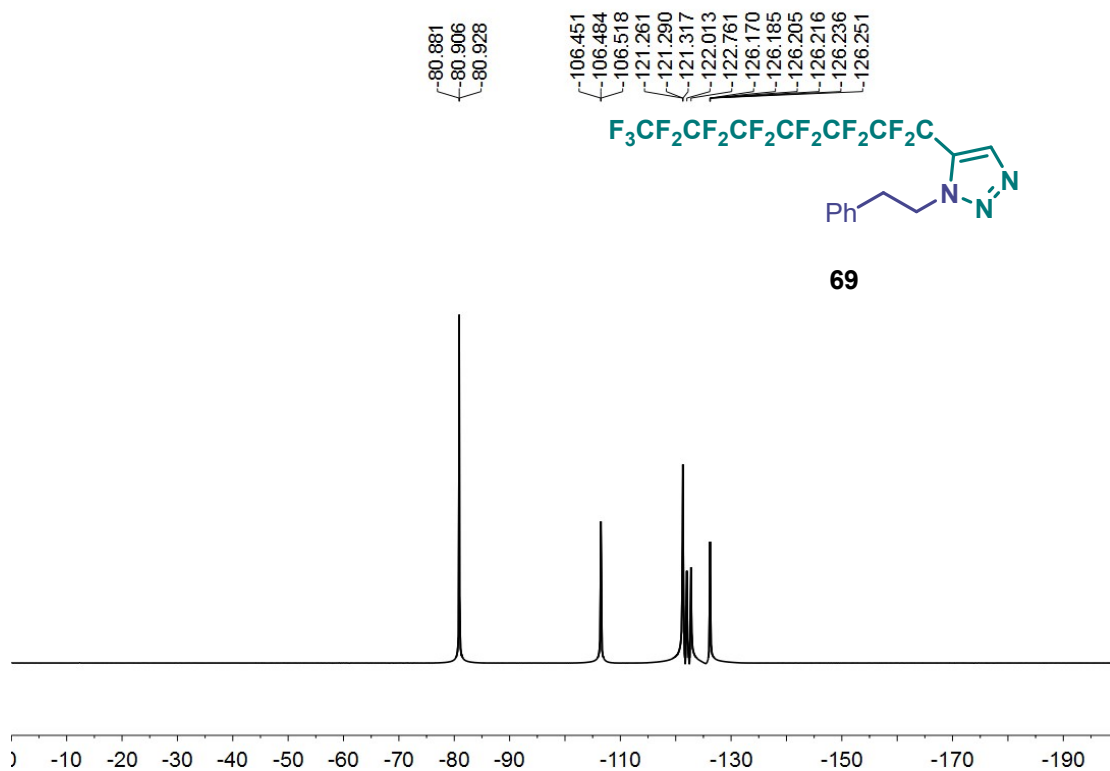


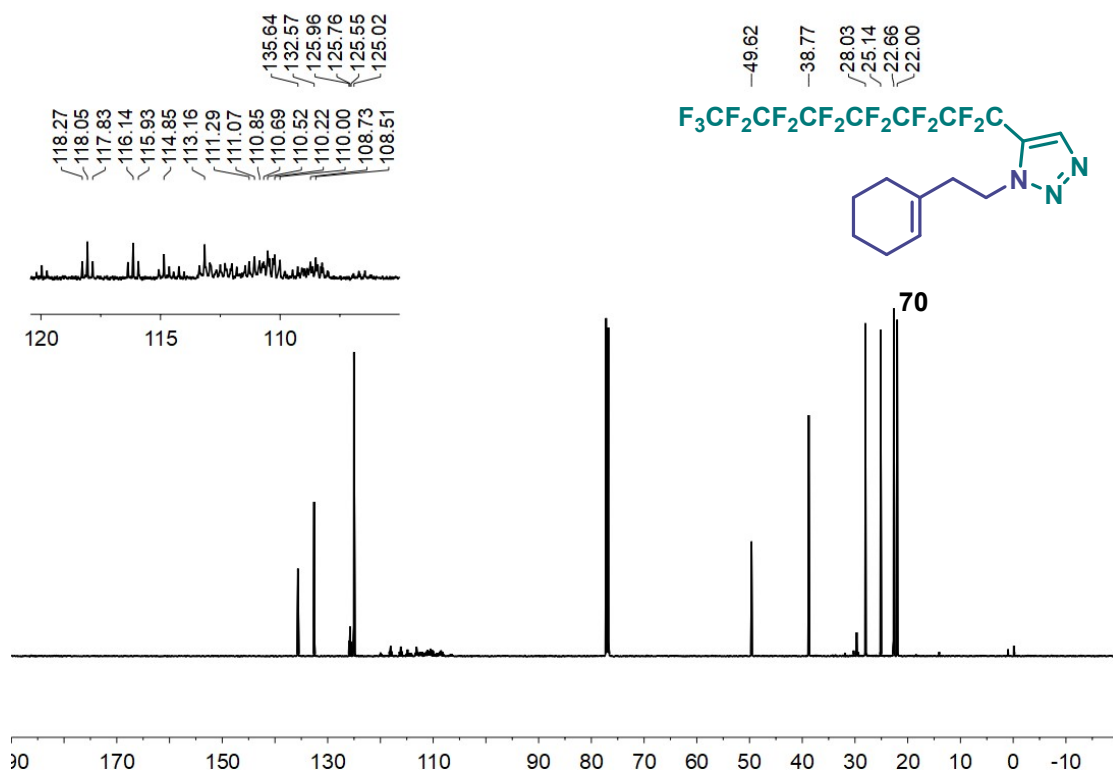




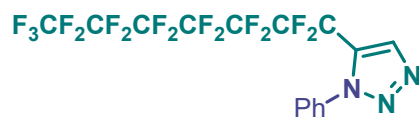




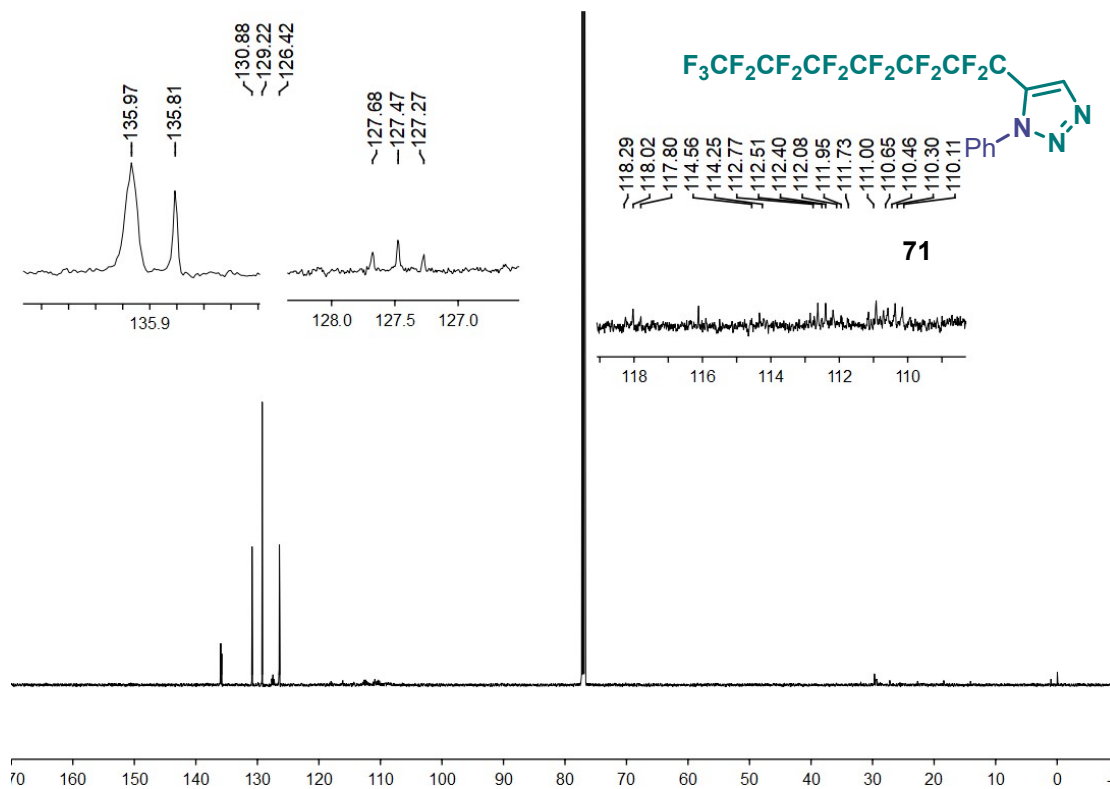
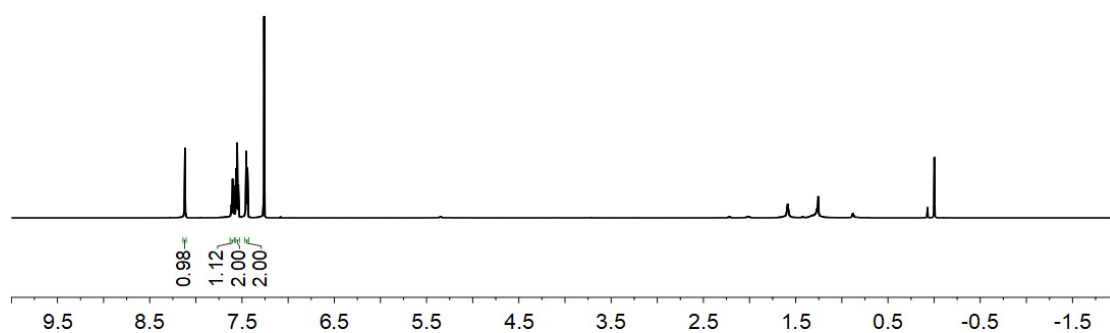




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7.614
7.601
7.598
7.589
7.565
7.552
7.540
7.454
7.441



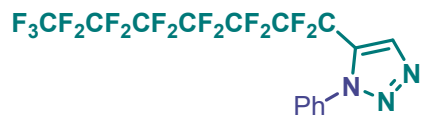
71



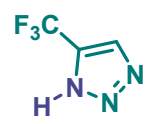
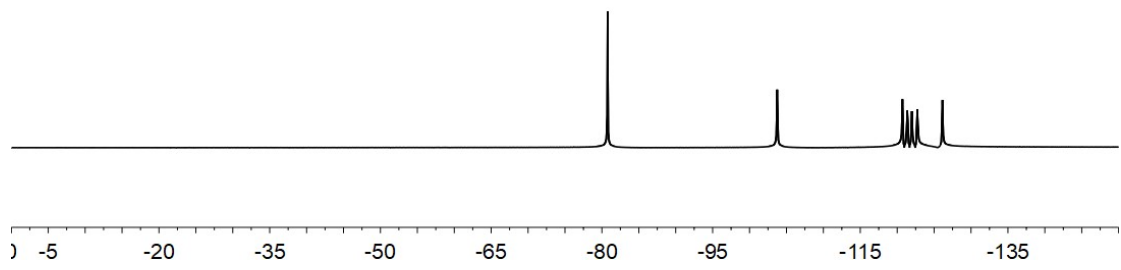
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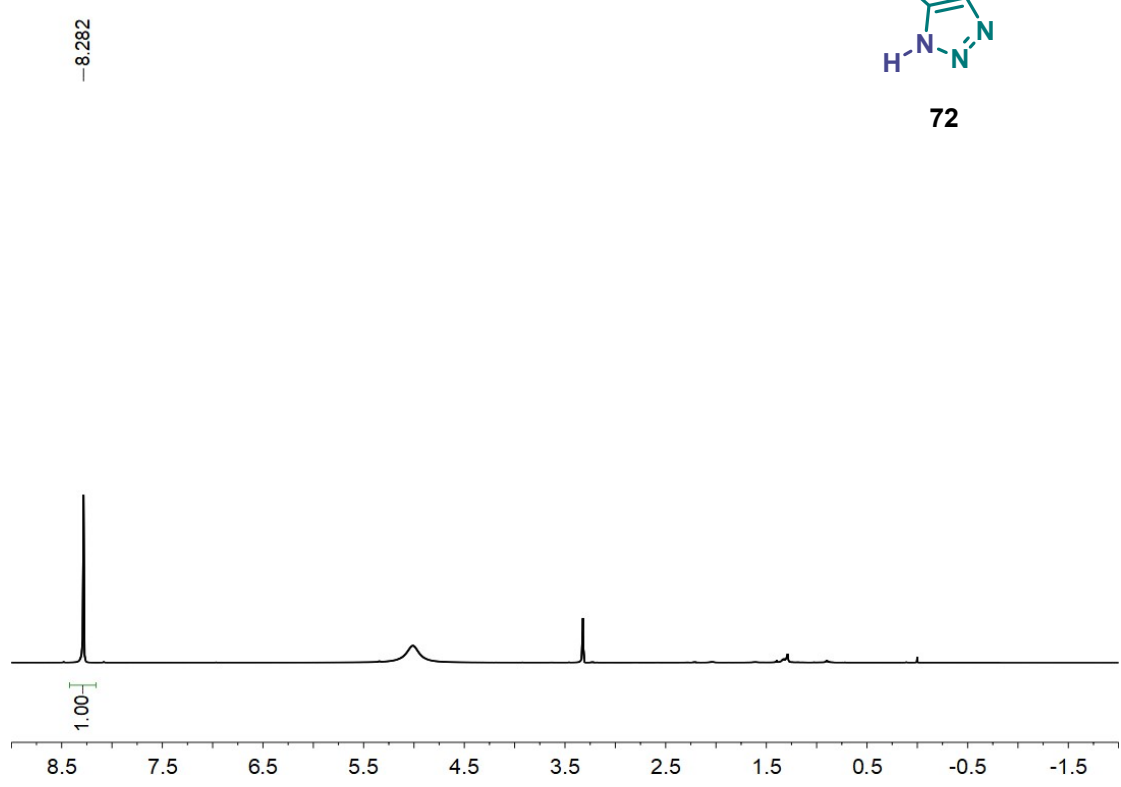
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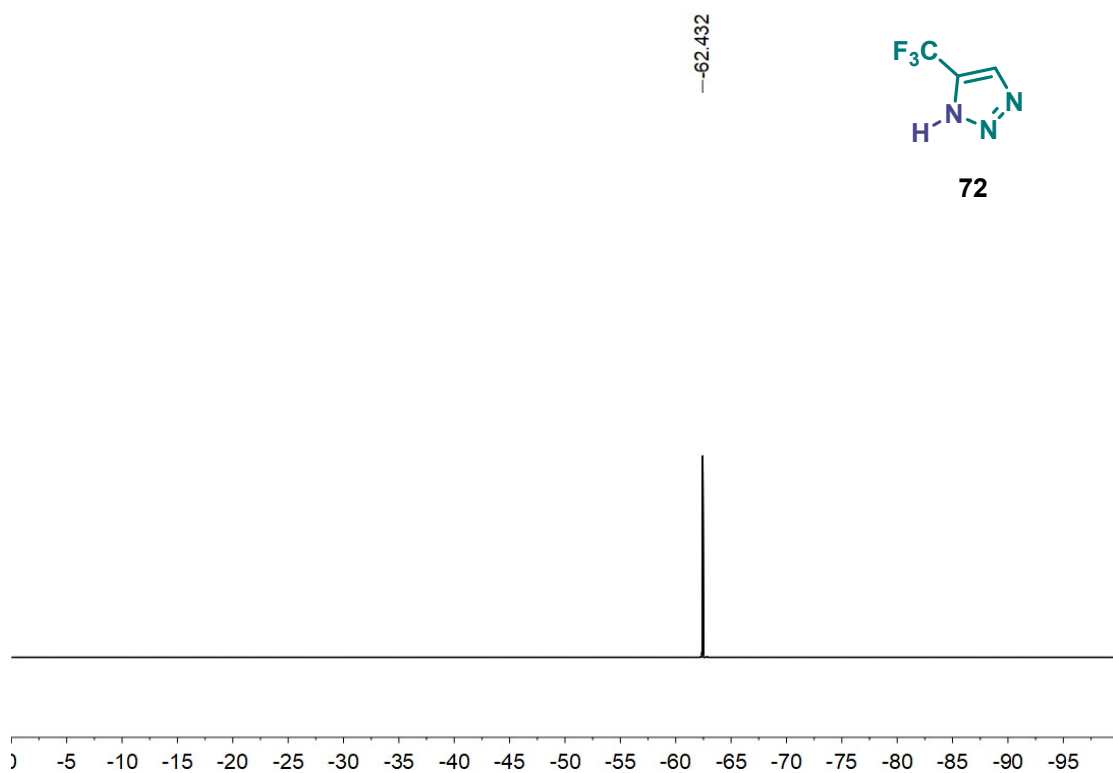
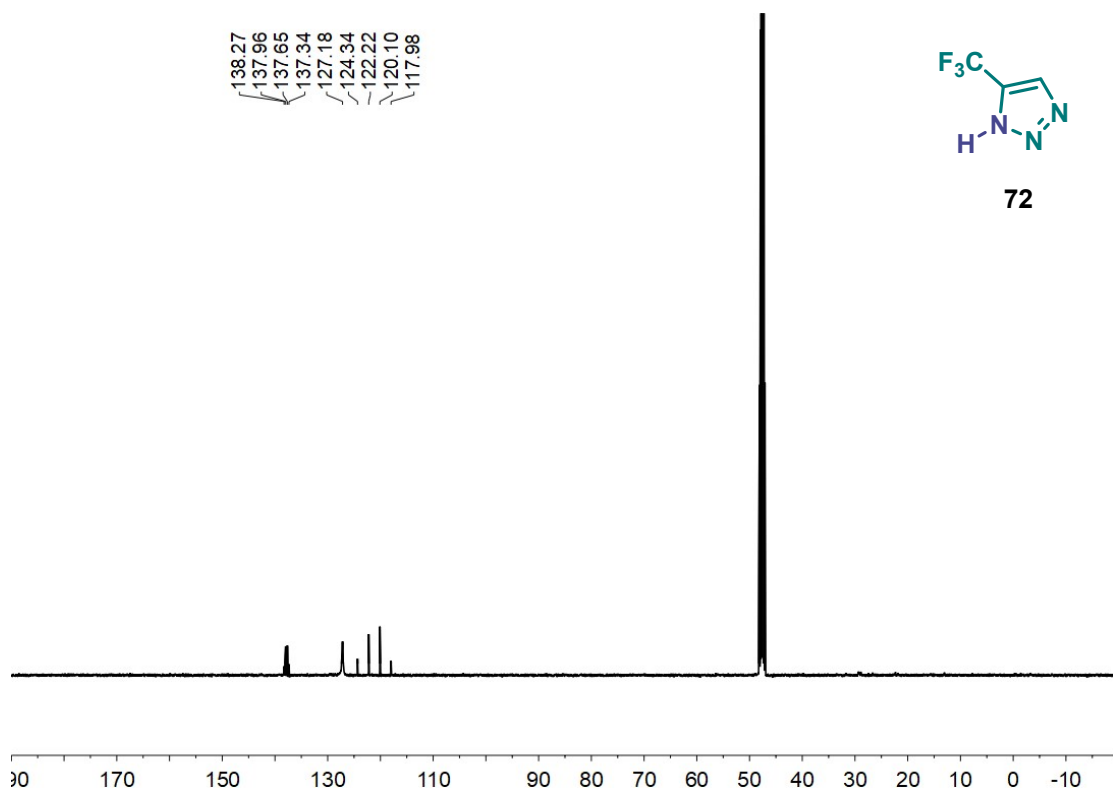


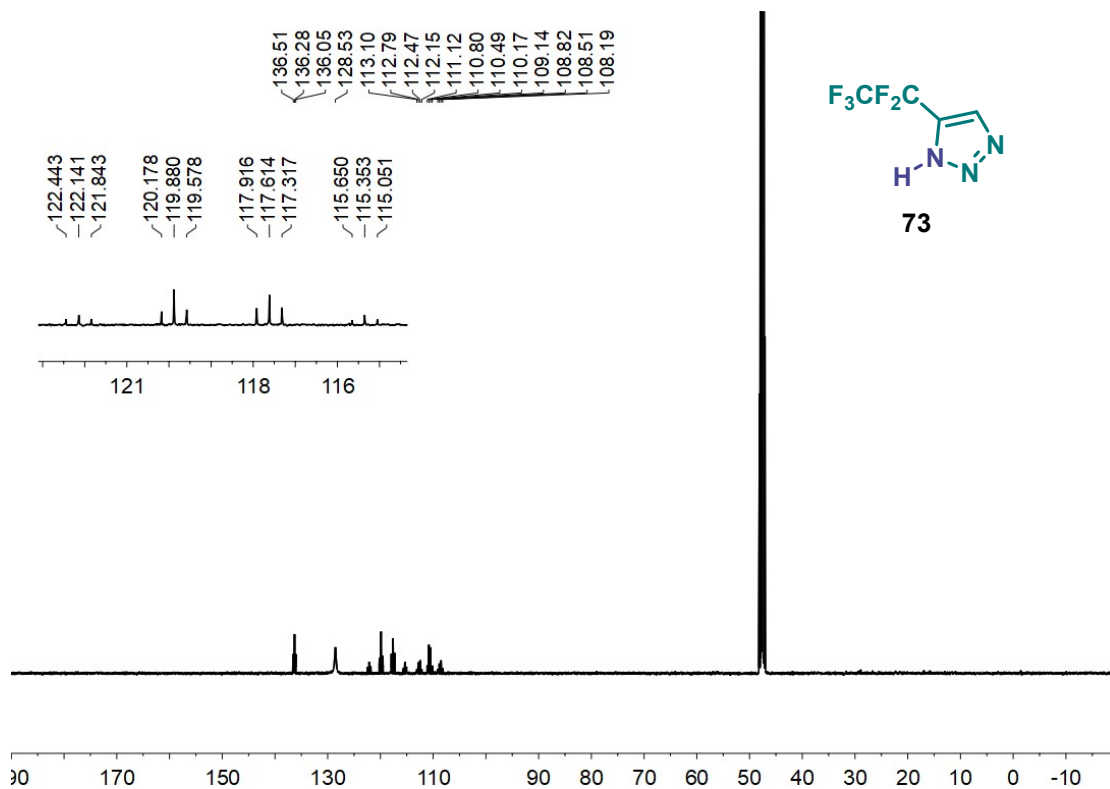
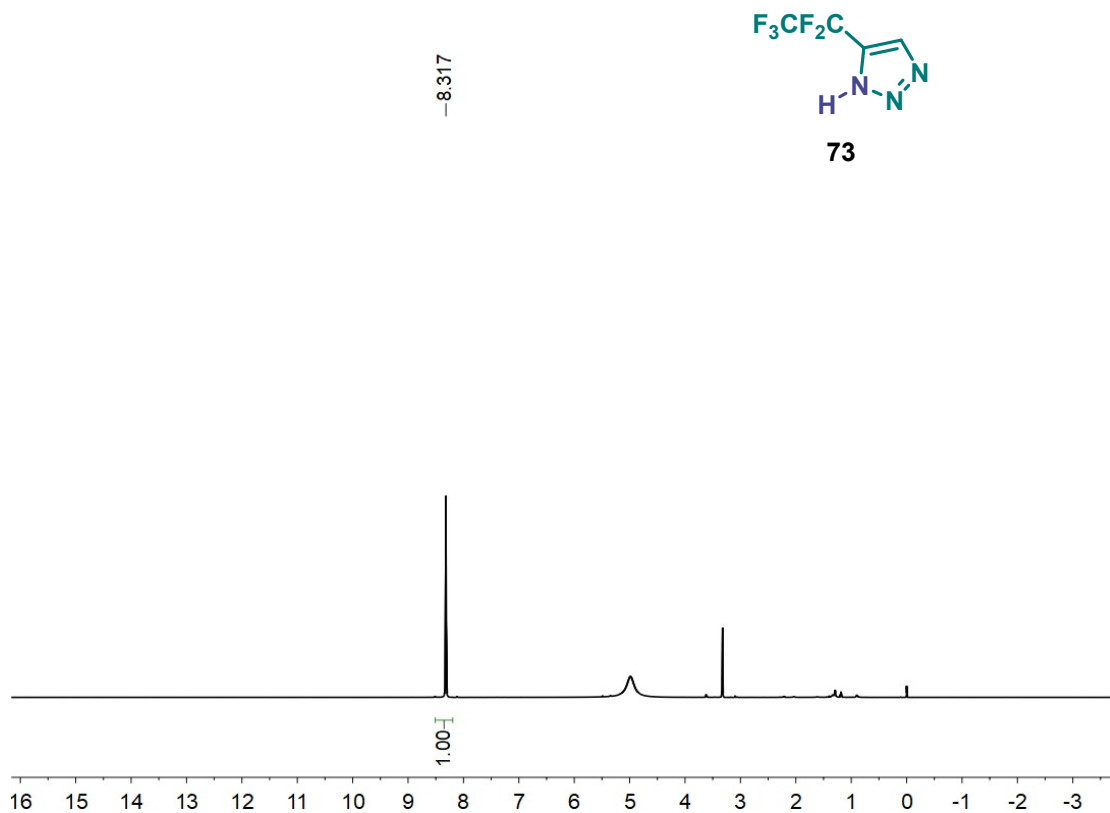
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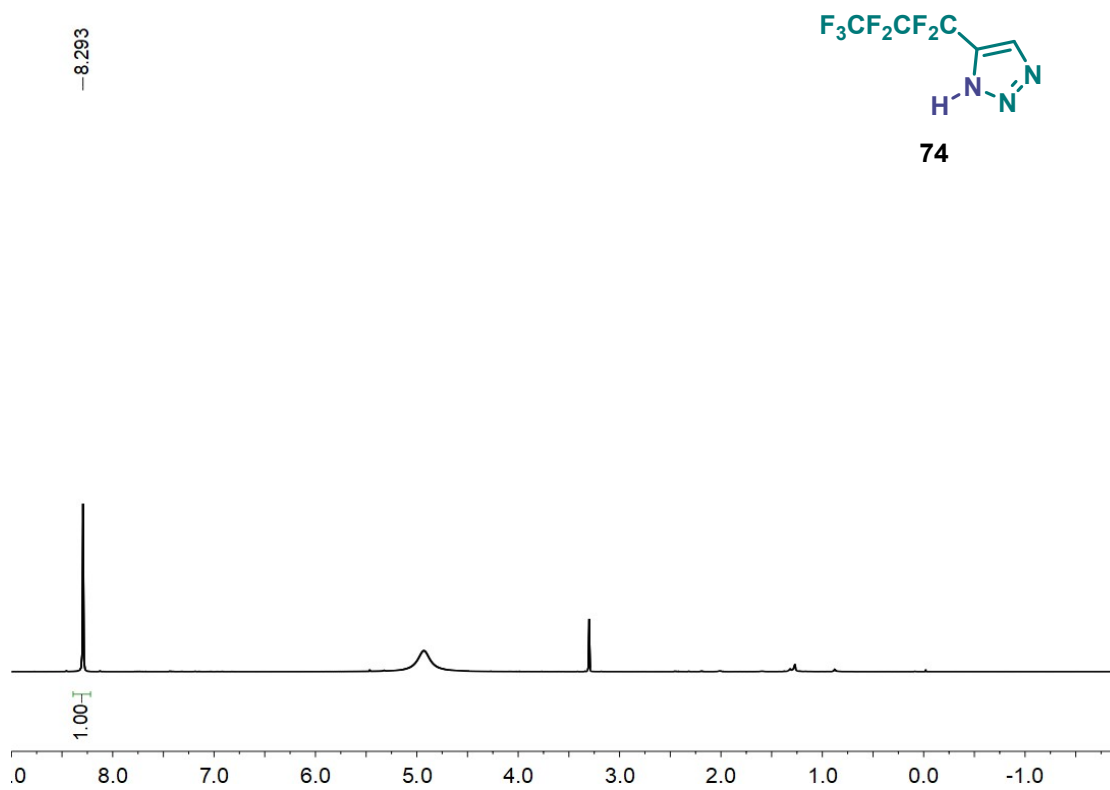
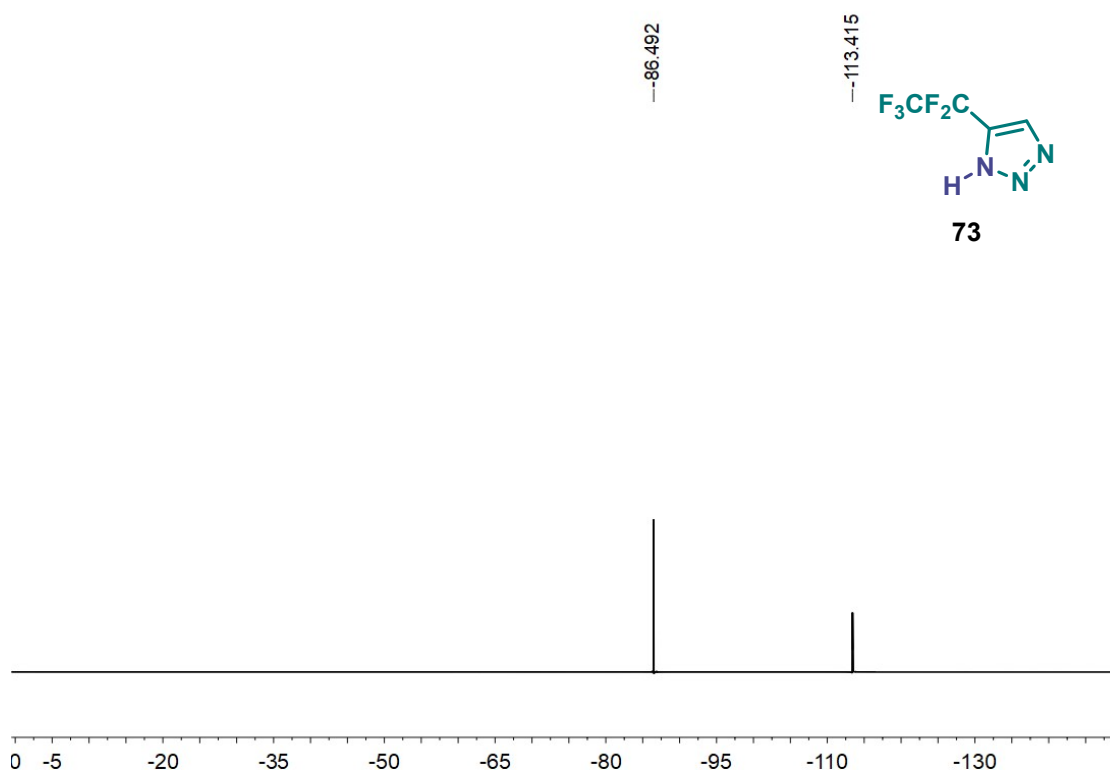


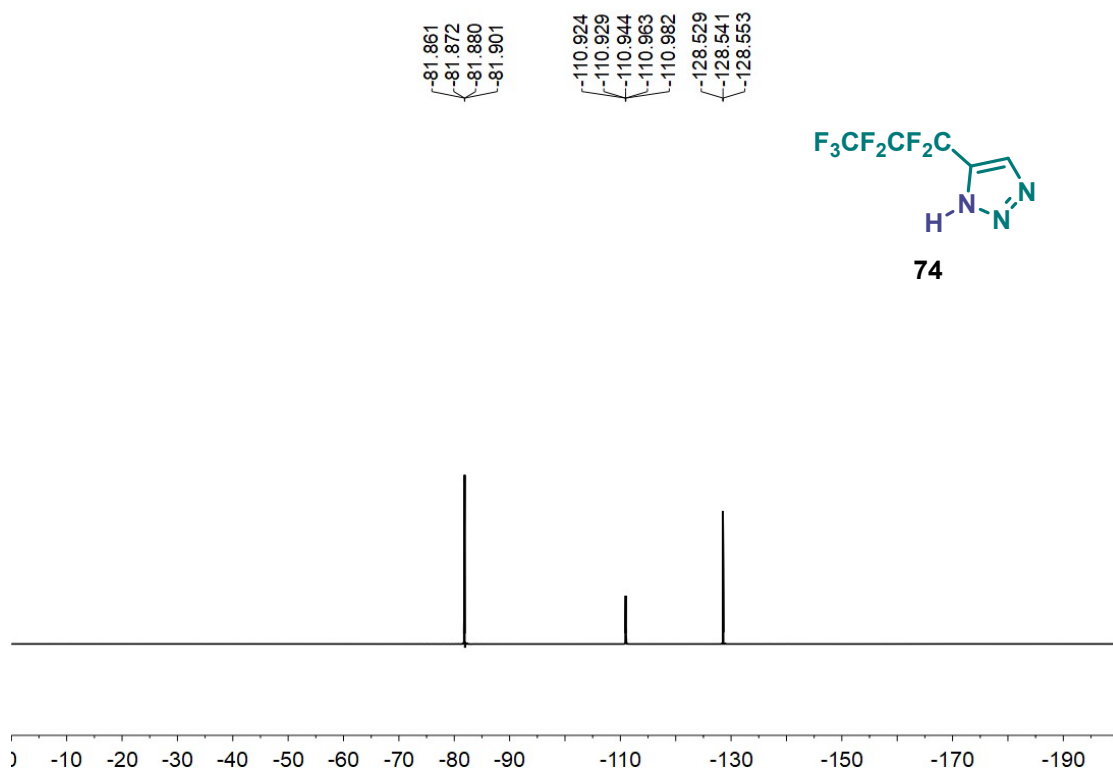
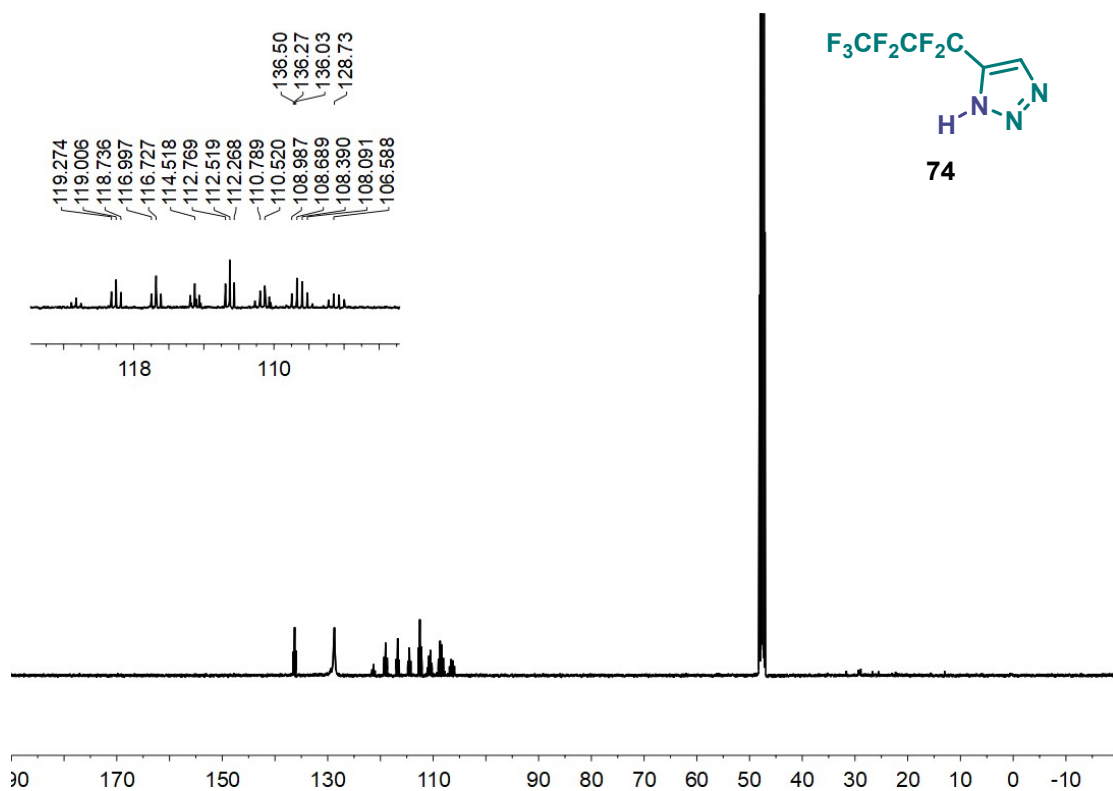
72



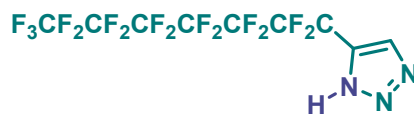




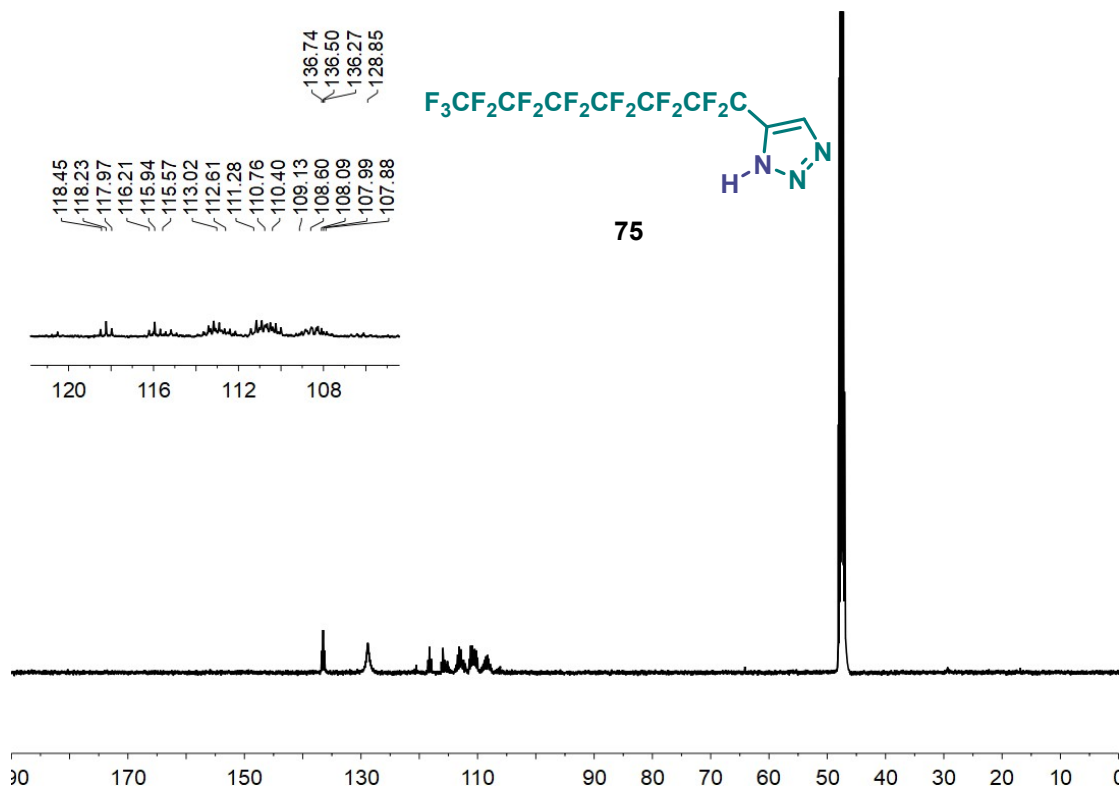
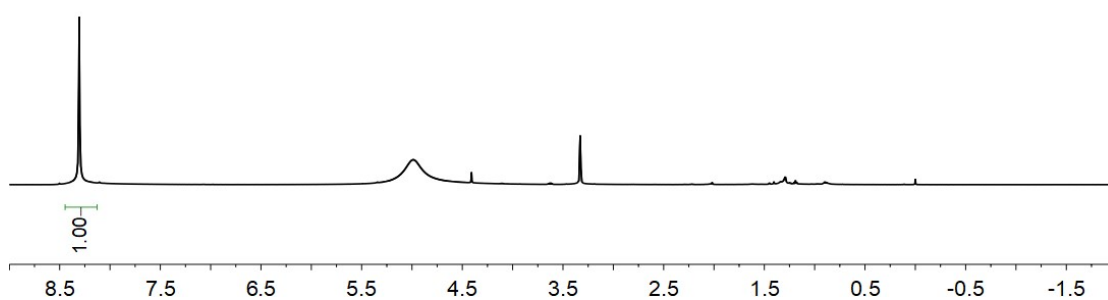


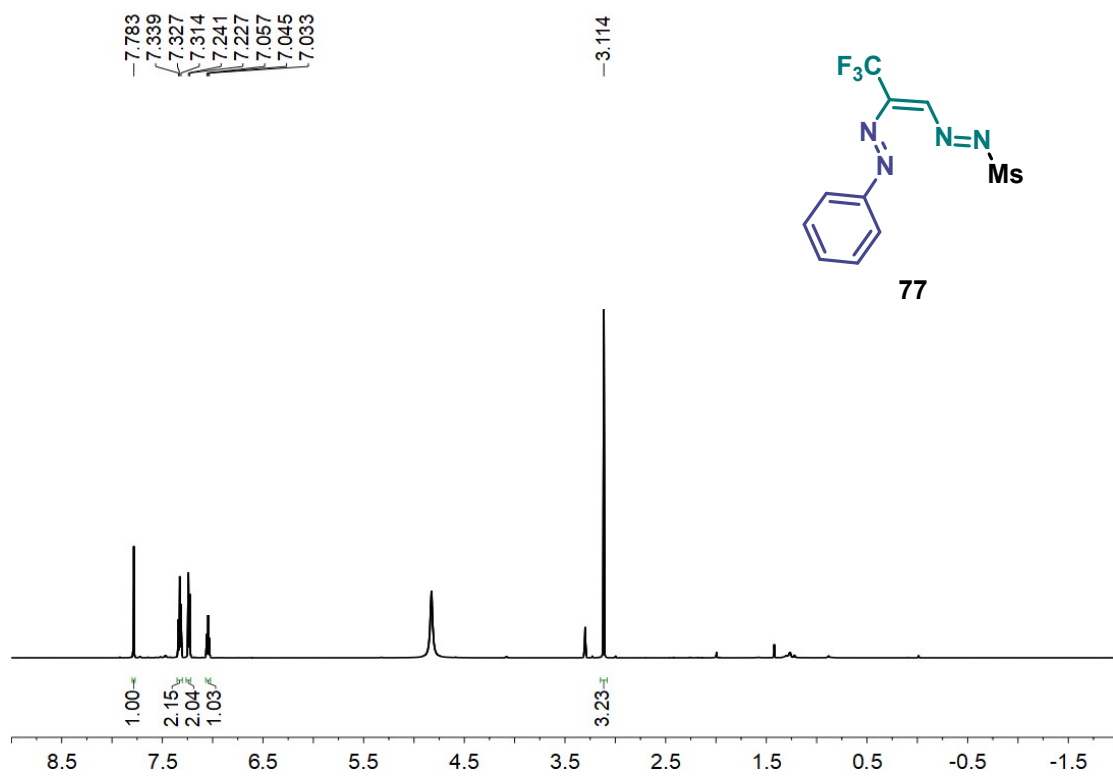
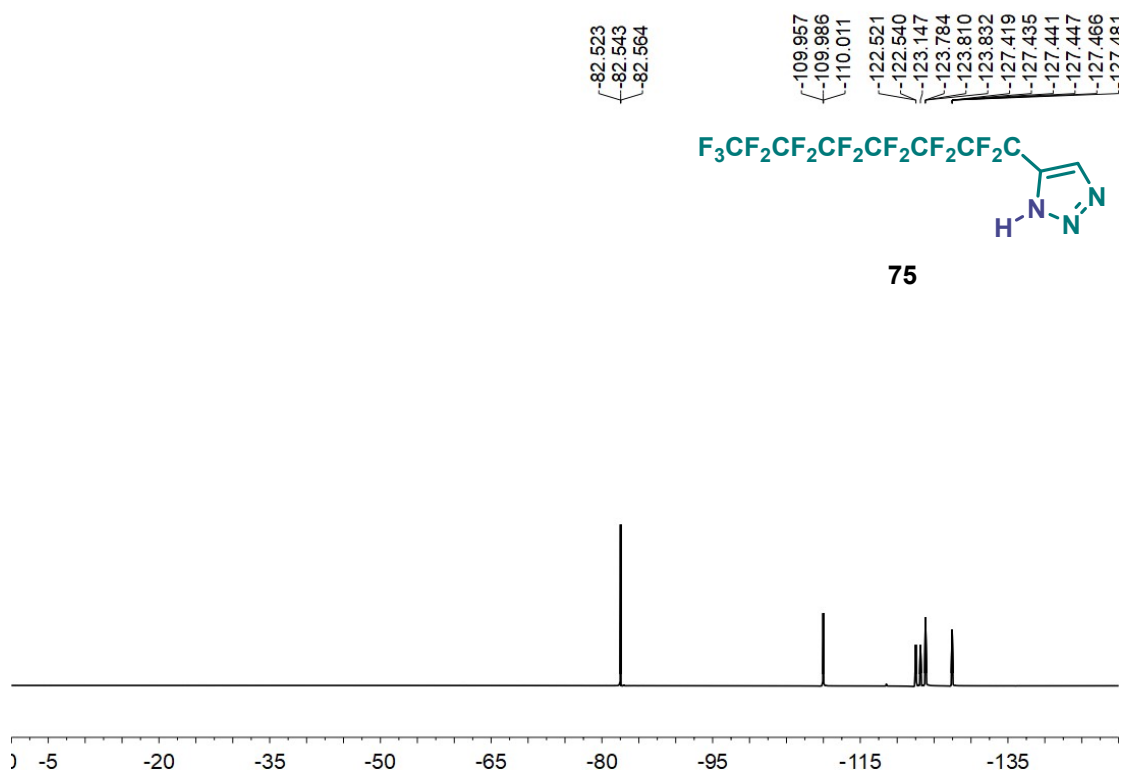


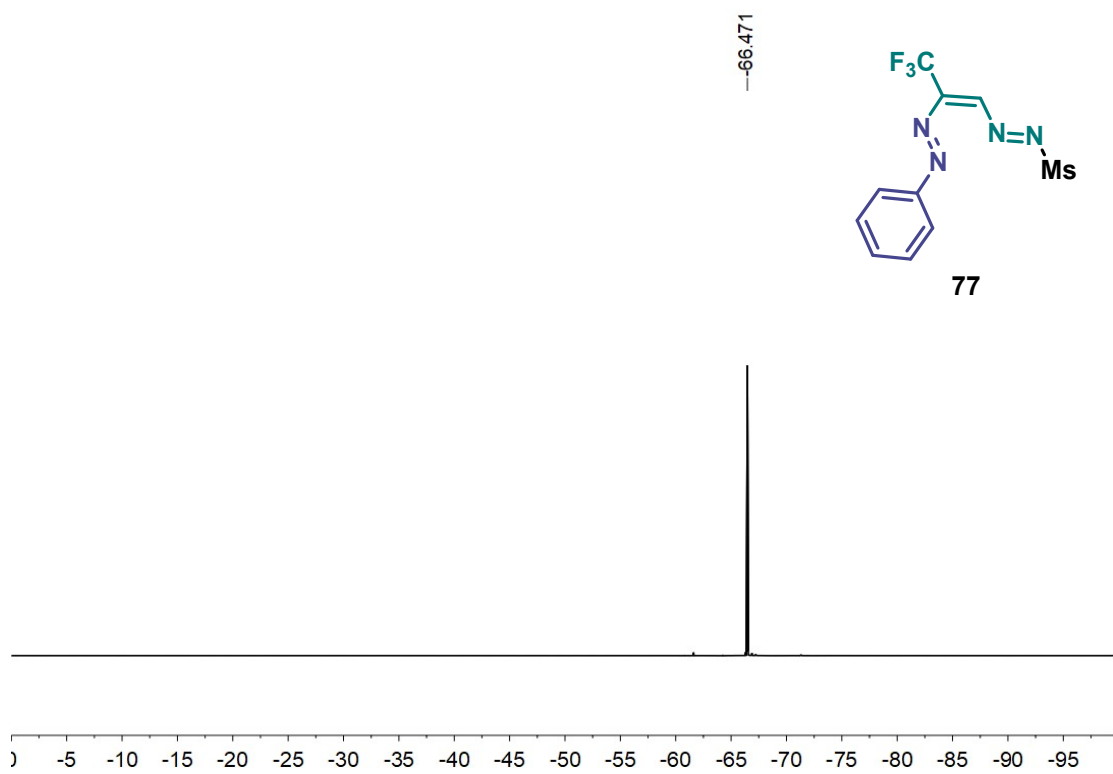
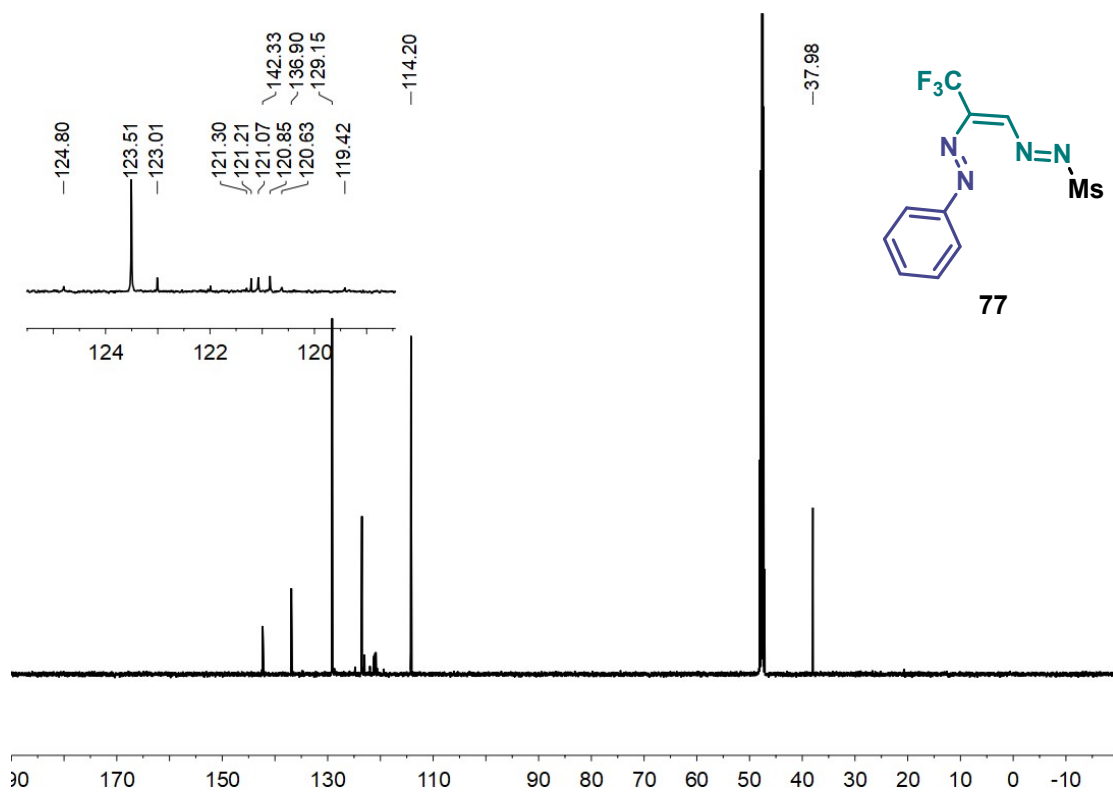
-8.306



75







VII. Computational details

All theoretical calculations of this work were performed based on density functional theory (DFT) methods with Gaussian 16 program.¹ All geometry optimizations were performed using the Becke's three-parameter hybrid exchange functional with Lee–Yang–Parr gradient-corrected correlation function²⁻⁴ (B3LYP) with the basis set 6-31G(d)⁵. The larger basis sets 6-311++g(d,p) was employed in the calculations to accurately describe the intermolecular interactions. The vibrational frequency analysis of reactants, products, intermediates and the transition states were given at the same level. All reactant, intermediate and product configurations having no imaginary frequency and each transition state has only one imaginary frequency, which has been confirmed by the intrinsic reaction coordinate⁶ (IRC). The SCRF calculations by using the SMD method⁷ are carried out to simulate the solvent effects and methanol is used as a solvent in our calculations.

Reference:

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Cartesian coordination and Gibbs free energies for all the calculated species were performed at the b3lyp/6-31g(d) //SMD_{Methanol} level in the solvent phase.

1a : (-1683.403164 a.u.)

S	0.91266700	2.79576800	0.02204300
O	2.37733500	2.66093300	-0.01453900
O	0.25400500	3.81414700	-0.80586200
N	-1.00503400	1.15683400	-0.45520500
N	0.34330500	1.27993900	-0.47233000
C	-1.51797900	0.01242800	-0.69445600
C	0.37036400	3.01723100	1.71499300
H	-0.71865200	2.94210000	1.74550800

H	0.83648500	2.25149100	2.33749000
H	0.69240200	4.01602500	2.02326000
H	0.98114200	0.45056700	-0.37087700
C	-3.01362200	-0.11547400	-0.67273900
F	-3.41841300	-0.86747800	-1.74304100
F	-3.63146800	1.09195800	-0.74112500
C	-3.55329400	-0.82617700	0.58941300
F	-4.87873300	-1.00835500	0.50691700
F	-2.96592200	-2.02804500	0.73104500
F	-3.28939000	-0.09098000	1.68055800
H	-0.95513700	-0.89415900	-0.90943300
N	2.36491600	-1.08992100	-0.18388200
C	3.41616800	-0.75646100	-1.20220200
H	4.21101600	-0.19047700	-0.70790900
H	3.89250700	-1.67824100	-1.56452500
C	2.90857900	-0.77353700	1.18860100
C	1.91465800	-2.50948200	-0.38428500
H	2.79187700	-3.16958100	-0.27225500
C	4.02231400	-1.71796200	1.67164200
H	4.46294600	-1.32408300	2.59571300
H	3.64084700	-2.72119600	1.89272400
H	4.82863000	-1.81313400	0.93563500
C	0.85730800	-2.98409500	0.62174700
H	0.48443300	-3.96406100	0.30206900
H	1.25739800	-3.11096200	1.62903800
H	-0.00083200	-2.30468100	0.67263100
C	1.37402800	-2.73894900	-1.80493800
H	0.50575300	-2.10435100	-2.01701900
H	2.12250500	-2.56323600	-2.58145200
H	1.05449500	-3.78318300	-1.89716800
C	2.93377600	0.07628400	-2.39296400
H	3.75308500	0.17492800	-3.11730300
H	2.08266100	-0.37335600	-2.91169400
H	2.64788100	1.08458400	-2.08063600
C	1.85059300	-0.58574200	2.29176400
H	0.93590400	-0.11842500	1.91447100
H	1.57059700	-1.51780900	2.78829000
H	2.26766400	0.07248900	3.06383800
H	3.35665400	0.21557500	1.05140800

TS1 : (-1683.400060 a.u.)

S	1.12033900	2.54584100	0.03750300
O	2.58378500	2.37227600	0.13733700
O	0.60648500	3.55009200	-0.91509600

N	-0.82896900	1.03964600	-0.37046700
N	0.52325800	1.02112200	-0.34769200
C	-1.48142200	-0.00928700	-0.70502500
C	0.46879500	2.96392200	1.65739000
H	-0.62157900	2.92741100	1.61586700
H	0.85617900	2.25229500	2.38841700
H	0.80781400	3.97767000	1.88822900
H	1.25334600	0.02686900	-0.29566400
C	-2.97861200	0.05076100	-0.67023300
F	-3.48964800	-0.58134900	-1.77551500
F	-3.44543000	1.32815300	-0.65860600
C	-3.59843200	-0.65847400	0.55456200
F	-4.93843800	-0.66304100	0.48626700
F	-3.17278000	-1.93376600	0.61607600
F	-3.23257600	-0.03367500	1.68527100
H	-1.04713900	-0.96080100	-0.99975900
N	2.22443400	-1.03292000	-0.16444900
C	3.33566200	-0.72281800	-1.14834900
H	4.10965600	-0.16909300	-0.61316000
H	3.79497400	-1.66634700	-1.46264600
C	2.77383700	-0.83212000	1.24695700
C	1.70035000	-2.43186000	-0.44027900
H	2.55511700	-3.11017300	-0.31435900
C	3.83120400	-1.86481300	1.65462200
H	4.28269100	-1.55156000	2.60330700
H	3.39709600	-2.85827100	1.81082300
H	4.63700000	-1.95023500	0.91803800
C	0.60346700	-2.89498400	0.52715700
H	0.17504700	-3.82670900	0.14150900
H	0.99214700	-3.11323400	1.52286500
H	-0.21250400	-2.17341100	0.62581000
C	1.22174400	-2.59285800	-1.89113000
H	0.42670000	-1.88736100	-2.15215500
H	2.03014400	-2.48077800	-2.61725700
H	0.82190200	-3.60549000	-2.01122200
C	2.93858400	0.10055800	-2.37604000
H	3.79243400	0.11629400	-3.06494700
H	2.08279400	-0.30856200	-2.91725400
H	2.71292100	1.13488400	-2.10880900
C	1.71028400	-0.67576500	2.34817100
H	0.81313300	-0.15772000	1.99973000
H	1.40444800	-1.62713400	2.78856700
H	2.14733800	-0.07571600	3.15511600
H	3.26678400	0.13936400	1.17098400

Int1: (-1683.401536 a.u.)

S	-3.39706800	-0.69455000	0.10144600
O	-3.07098500	-2.11516300	-0.17707900
O	-3.46895200	-0.35244900	1.53753500
N	-1.41794400	0.74473900	-0.07200400
N	-2.45839200	0.33256200	-0.79518400
C	-0.56261100	1.50801100	-0.66634000
C	-4.97916400	-0.38774200	-0.63531600
H	-5.28400100	0.64110800	-0.42110600
H	-4.90469500	-0.54527800	-1.71576700
H	-5.69226800	-1.09583500	-0.20010400
H	1.37519500	-0.80938100	-0.24018400
C	0.61491500	1.97516900	0.09505400
F	1.76176200	1.28966500	-0.27039600
F	0.48766200	1.80731900	1.42643400
C	0.95877200	3.45084900	-0.13529700
F	2.05246900	3.79352100	0.53915000
F	1.17271800	3.67924900	-1.42973400
F	-0.04566200	4.22050400	0.27338100
H	-0.64880000	1.81872600	-1.71375400
N	1.39643100	-1.83545900	-0.12572300
C	0.17007800	-2.34762500	-0.83979700
H	0.24161900	-3.44287900	-0.83868900
H	-0.69777600	-2.05709400	-0.24559400
C	2.66769300	-2.32965800	-0.84877800
C	1.35927400	-2.07672100	1.38817700
H	1.51805800	-3.15470900	1.51047600
C	3.24708800	-3.58643400	-0.23733100
H	4.01629700	-3.95783700	-0.92564100
H	3.72860300	-3.42031300	0.73320100
H	2.49490700	-4.37853700	-0.13325400
C	2.46469100	-1.28428900	2.06108700
H	2.38151100	-1.42323700	3.14514300
H	3.47238500	-1.59582800	1.77172700
H	2.35344800	-0.21047400	1.85299600
C	0.01486500	-1.68703100	1.97961700
H	-0.27757600	-0.66776100	1.68739300
H	-0.79701700	-2.37322400	1.71555500
H	0.11120100	-1.70910700	3.07170600
C	0.02062700	-1.76348100	-2.22624300
H	-0.99162200	-1.98709100	-2.58397800
H	0.12951400	-0.66860900	-2.20054000
H	0.72532800	-2.16543500	-2.96247400

C	3.66196400	-1.20183900	-1.03005800
H	3.20585300	-0.35812600	-1.56456700
H	4.08245300	-0.83413000	-0.08723600
H	4.49253700	-1.57109200	-1.64430800
H	2.30707300	-2.60064500	-1.84555800

TS2: (-1683.380134a.u.)

S	-3.59626400	-0.97004300	0.02156600
O	-3.17224100	-2.24552100	-0.56329400
O	-3.58605500	-0.82373400	1.47627600
N	-1.83753600	0.79133500	0.06618300
N	-2.57764500	0.23362700	-0.77478000
C	-0.93809400	1.68176100	-0.47342200
C	-5.16791500	-0.50089200	-0.63426800
H	-5.42796700	0.48928900	-0.24571100
H	-5.09859600	-0.48709600	-1.72650500
H	-5.90088300	-1.24585500	-0.30592500
H	1.74390200	-0.33731400	0.08441400
C	-0.04582700	2.24750200	0.35987800
F	1.82300000	0.81557700	0.39142300
F	-0.09189500	2.09783100	1.65725600
C	0.93037600	3.30824400	-0.09524600
F	1.94475400	3.44484700	0.74115000
F	1.38966200	3.04797800	-1.31442000
F	0.29141100	4.48617600	-0.14940400
H	-0.91520100	1.88042100	-1.54514600
N	1.67990400	-1.53397100	-0.19965900
C	0.62797200	-1.63128100	-1.25154600
H	0.57356200	-2.66782800	-1.61889200
H	-0.33047500	-1.40818100	-0.77834900
C	3.01838400	-1.95173800	-0.77502300
C	1.29097300	-2.20961900	1.09099900
H	1.28812600	-3.29611500	0.91424000
C	3.29987600	-3.43812600	-0.65592000
H	4.18928300	-3.67170300	-1.25555200
H	3.51068100	-3.75198200	0.37439000
H	2.47294800	-4.04774200	-1.04366600
C	2.28875800	-1.85622100	2.18398800
H	1.91688700	-2.22308400	3.14809000
H	3.27821400	-2.29752800	2.03204400
H	2.39547900	-0.76469900	2.24781300
C	-0.09998900	-1.78305300	1.54341900
H	-0.19656700	-0.68736000	1.53768900
H	-0.90776700	-2.21583600	0.94181200

H	-0.25574500	-2.12461900	2.57390900
C	0.83698800	-0.63370300	-2.37756300
H	-0.11174500	-0.48172500	-2.90808900
H	1.16031100	0.33282800	-1.96757300
H	1.57450700	-0.95602000	-3.12180700
C	4.16739100	-1.08455300	-0.28201200
H	3.87244000	-0.02918000	-0.27107200
H	4.51651200	-1.35520000	0.72093400
H	5.01689200	-1.20255800	-0.96710200
H	2.92299400	-1.73473800	-1.84481900

Int2: (-1614.146333a.u.)

S	4.23449500	-1.62779200	0.07696100
O	4.53134400	-2.15908600	1.42146300
O	3.37304400	-2.41253100	-0.82442300
N	2.43705200	0.12293300	-0.12715800
N	3.58234600	0.00831800	0.37658000
C	1.84142800	1.34919400	0.09828100
C	5.76111800	-1.20243300	-0.75147400
H	5.52110500	-0.74704100	-1.71513600
H	6.32040400	-0.51087700	-0.11763000
H	6.31998100	-2.13177800	-0.89418000
C	0.60864500	1.56482500	-0.40902900
F	-0.00611300	0.68480300	-1.18461200
C	-0.08478700	2.91274300	-0.36251400
F	-1.40334700	2.79700400	-0.56164900
F	0.13078300	3.52596600	0.81337600
F	0.40121900	3.71676000	-1.33468600
H	2.34273000	2.11329900	0.68628200
C	-4.40051600	-1.27770300	-0.00986600
C	-4.52472700	0.05184200	0.41957100
C	-3.43423000	0.72607800	0.95531700
C	-2.18621700	0.08844600	1.08021300
C	-2.07041000	-1.23874800	0.64509700
C	-3.16409900	-1.92180300	0.10591500
H	-5.48896900	0.54472400	0.32946100
H	-3.54511100	1.75697800	1.28289900
H	-1.11318000	-1.74797900	0.73036300
H	-3.03665800	-2.94980300	-0.21453500
O	-5.53954100	-1.85338700	-0.51964600
C	-5.46424000	-3.20911800	-0.95799600
H	-5.19177400	-3.88189400	-0.13522300
H	-6.46467800	-3.46246900	-1.31565700
H	-4.74526300	-3.32631900	-1.77843000

N	-1.06549100	0.79021000	1.55799500
H	-0.36360100	0.19484300	1.98928700
H	-1.29768900	1.56204100	2.17709800

TS3: (-1614.139411a.u.)

S	4.35691300	-1.45425200	0.08690200
O	4.92412300	-1.94995400	1.36162000
O	3.47786300	-2.36675400	-0.67650000
N	2.40663100	0.10870400	0.01254000
N	3.61296300	0.06554100	0.46059800
C	1.73547000	1.24318800	0.25162100
C	5.70965200	-0.93499000	-0.96767300
H	5.29612300	-0.52351600	-1.89152800
H	6.29856900	-0.18284400	-0.43820200
H	6.31932100	-1.81795300	-1.17987400
C	0.41292400	1.33220800	-0.19326900
F	-0.01280800	0.48940000	-1.14234300
C	-0.21789500	2.71129000	-0.34558600
F	-1.51952800	2.62954100	-0.65735600
F	-0.09119000	3.41792100	0.79304700
F	0.39450200	3.39865300	-1.32907800
H	2.16250400	2.06174200	0.82832800
C	-4.44946800	-1.16633900	0.06149700
C	-4.44165300	0.13763700	0.58522900
C	-3.25209900	0.72252800	0.99390900
C	-2.04938900	0.00794300	0.89171800
C	-2.05436700	-1.28711100	0.36686500
C	-3.24801700	-1.87942200	-0.04565500
H	-5.38142400	0.67544800	0.66778900
H	-3.25245200	1.73043100	1.39954500
H	-1.12299300	-1.84100100	0.28615700
H	-3.22855100	-2.88819800	-0.44087600
O	-5.67088200	-1.64885300	-0.30723200
C	-5.74400900	-2.97192700	-0.84554000
H	-5.39795200	-3.71613700	-0.11866100
H	-6.79958300	-3.14206300	-1.06600200
H	-5.15947800	-3.05787900	-1.76899300
N	-0.81421700	0.61101700	1.27114800
H	-0.14833800	-0.06872500	1.64156300
H	-0.92850900	1.35670700	1.96009700

Int3: (-1984.945729a.u.)

S	-0.43246900	3.95499500	-1.03882000
O	0.13239000	5.22514400	-1.55292600

O	-0.49928300	2.80845000	-1.98571500
N	0.36999000	2.31798200	0.63068200
N	0.42753800	3.61554000	0.36096800
C	0.98783800	1.86160900	1.67818600
C	-2.11622400	4.29396800	-0.50507000
H	-2.52405600	3.39575600	-0.03619900
H	-2.09594900	5.12073000	0.20869700
H	-2.70620300	4.56527500	-1.38502700
C	0.82798400	0.41311200	1.93036600
F	-0.36746300	0.10052700	2.60007900
C	1.92811500	-0.19275700	2.82520600
F	1.75294000	-1.51844700	2.97467500
F	3.15157500	0.02174800	2.32192500
F	1.86448600	0.37680800	4.03822800
H	1.54157700	2.47508400	2.38709000
C	4.04483100	-1.39000100	-1.74389400
C	3.47403500	-0.11087600	-1.85955500
C	2.37428100	0.24152900	-1.09059200
C	1.84715800	-0.69440900	-0.19928400
C	2.38761800	-1.97000700	-0.08220200
C	3.49229100	-2.32429900	-0.85641800
H	3.90284900	0.59433800	-2.56447700
H	1.92428700	1.22190500	-1.20104500
H	1.95616800	-2.69459500	0.60178600
H	3.90323900	-3.32192200	-0.76109200
O	5.11948000	-1.62772800	-2.53957000
C	5.75906900	-2.90694500	-2.46392200
H	5.07291600	-3.70982500	-2.75622500
H	6.58914700	-2.86098600	-3.17102800
H	6.14549300	-3.09556100	-1.45591300
N	0.66034400	-0.34177100	0.61450300
H	0.11175500	-1.18990900	0.81402400
H	0.04998400	0.29553200	0.06616600
N	-3.56562200	-1.75940400	-0.72216600
C	-4.13966100	-2.20370800	-2.01408100
H	-4.91438100	-2.97219600	-1.85676900
H	-4.65284100	-1.37014500	-2.49694700
C	-3.52968600	-2.92427900	0.20930500
C	-4.17533200	-0.48781300	-0.24831900
H	-5.27757500	-0.58106500	-0.21305100
C	-4.84393300	-3.21977100	0.95865900
H	-4.78149400	-4.20180800	1.44374800
H	-5.06598600	-2.48424600	1.73812900
H	-5.69666500	-3.24878300	0.26981100

C	-3.71018700	-0.04875200	1.14777900
H	-4.17284300	0.91767100	1.38103400
H	-3.99572000	-0.73920700	1.94352000
H	-2.62346000	0.08822500	1.18535500
C	-3.83287400	0.66147900	-1.21562000
H	-2.74855900	0.82723400	-1.24811200
H	-4.17381900	0.49005500	-2.24065500
H	-4.30994700	1.58625700	-0.87042300
C	-3.07577800	-2.74092400	-2.97238100
H	-3.53727200	-3.08590100	-3.90678300
H	-2.34533200	-1.96060100	-3.21786100
H	-2.52939900	-3.58826100	-2.53996700
C	-2.31021000	-2.92770400	1.14435600
H	-1.39249100	-2.80682300	0.55530600
H	-2.33624200	-2.14690100	1.90829400
H	-2.24620000	-3.89331900	1.66228400
H	-3.36777300	-3.78171900	-0.45405300
TS4: (-1984.910589a.u.)			
S	-2.03148100	-1.46681800	2.74069700
O	-3.47605900	-1.76784000	2.79456900
O	-1.19995300	-2.16770800	1.74457100
N	-1.41186400	0.60995700	1.46957500
N	-1.93382900	0.30419200	2.57259900
C	-1.34040000	1.96165300	1.22641600
C	-1.32086300	-1.65642900	4.37022100
H	-0.26614200	-1.37532700	4.32702200
H	-1.86982100	-1.01947500	5.06711800
H	-1.42729200	-2.70954700	4.64585500
C	-0.77409100	2.41659400	0.08047600
F	1.32413200	2.40803000	0.14421900
C	-0.80661900	3.90711100	-0.20556700
F	-0.10004500	4.22990400	-1.30438300
F	-2.08283200	4.30373500	-0.43026800
F	-0.34125000	4.61828300	0.82750200
H	-1.67868600	2.66618000	1.98331800
C	-2.82914500	-1.71601900	-2.30456800
C	-1.48059600	-1.91077900	-1.96170900
C	-0.70317400	-0.84023400	-1.54025400
C	-1.28309900	0.42396200	-1.46206800
C	-2.61194400	0.63917600	-1.80290900
C	-3.39642200	-0.43591700	-2.22203200
H	-1.05908800	-2.90866500	-2.03142300
H	0.33985700	-0.98489700	-1.27511000
H	-3.04015500	1.63522000	-1.73701300

H	-4.43368600	-0.26349000	-2.48231200
O	-3.50046300	-2.82923400	-2.70771900
C	-4.87493500	-2.69872800	-3.08521400
H	-4.98845700	-2.01939200	-3.93796000
H	-5.19633300	-3.70150000	-3.37257700
H	-5.48460900	-2.34575600	-2.24549900
N	-0.43693100	1.56783900	-1.07957500
H	-0.32624700	2.18989500	-1.89142000
H	0.57360200	1.37086500	-0.79039500
N	3.77145500	-1.22077000	-0.34427600
C	4.15780200	-2.60921800	-0.69066000
H	5.23638000	-2.67217700	-0.91201400
H	4.00000900	-3.25874000	0.17264200
C	4.57636500	-0.28003800	-1.17937900
C	3.74125400	-1.02157200	1.13271700
H	4.68508200	-1.38953000	1.57835200
C	5.99902400	0.02443200	-0.66657000
H	6.58088100	0.50690800	-1.46181400
H	6.01225000	0.69486800	0.19789000
H	6.52801900	-0.89496300	-0.38811900
C	3.55886200	0.43384100	1.58675500
H	3.50766300	0.44563300	2.68272500
H	4.38777900	1.08523100	1.30187400
H	2.63428400	0.87771200	1.20378000
C	2.58382900	-1.83103100	1.74745500
H	1.61926900	-1.44320200	1.39799600
H	2.61982100	-2.89858000	1.51055200
H	2.60993500	-1.74157300	2.84043800
C	3.36320200	-3.17093500	-1.87021300
H	3.71168700	-4.18131200	-2.12093400
H	2.29508000	-3.22854800	-1.62795100
H	3.47160000	-2.55118900	-2.76865500
C	3.80803000	0.98720400	-1.58288300
H	2.88909200	0.71108800	-2.11486000
H	3.51848700	1.62645900	-0.74707500
H	4.42179100	1.58488300	-2.26981900
H	4.71908400	-0.82626900	-2.11908800
Int4: (-1884.531692a.u.)			
S	4.73405400	-1.08626900	-0.02764100
O	5.93071300	-1.90158100	-0.31254300
O	4.49646100	0.12365700	-0.84406000
N	2.29673800	-1.59672800	-0.14546500
N	3.40927200	-2.22577000	-0.16054700
C	1.19805300	-2.37628000	-0.25621200

C	4.73518800	-0.61633200	1.70407200
H	3.80639300	-0.08412600	1.92125500
H	4.82099200	-1.51943700	2.31240800
H	5.59778500	0.03697100	1.86376700
C	-0.08682500	-1.84678400	-0.23498000
C	-1.22892800	-2.85998300	-0.30466400
F	-1.79828000	-3.00951400	0.91105000
F	-2.19140600	-2.44609000	-1.15442100
F	-0.82581100	-4.07117800	-0.71335600
H	1.31921500	-3.45008300	-0.36211400
C	1.99432300	2.82789100	0.16451800
C	1.46793600	2.23827300	1.32565800
C	0.65876700	1.11163600	1.23275000
C	0.36545900	0.56817200	-0.02197200
C	0.87297600	1.15871100	-1.17750200
C	1.69187100	2.28612400	-1.09213200
H	1.70551200	2.67524600	2.29104600
H	0.25997900	0.64959400	2.13085800
H	0.63820300	0.73411600	-2.14915100
H	2.08231700	2.72741900	-2.00141000
O	2.78172300	3.92301200	0.36323500
C	3.37443800	4.55045000	-0.77774100
H	2.60949800	4.93774500	-1.46090500
H	3.96369500	5.38069600	-0.38371000
H	4.03233100	3.85620500	-1.31333400
N	-0.49775900	-0.57971000	-0.11966500
H	-1.50956400	-0.37675600	-0.08540200
N	-3.51205500	0.79440700	0.23204100
C	-3.02482900	2.04142700	0.89395100
H	-3.85312500	2.54723100	1.42327900
H	-2.31283800	1.73668400	1.66291000
C	-4.22235500	1.11465200	-1.05108700
C	-4.31666800	0.02851800	1.24083200
H	-5.14080900	0.67360000	1.59514500
C	-5.64675400	1.67813200	-0.89301000
H	-5.99760800	2.05967000	-1.85971000
H	-6.36856900	0.92595800	-0.55755800
H	-5.67393800	2.51278800	-0.18245000
C	-4.95140600	-1.26140000	0.70270700
H	-5.45339700	-1.77309800	1.53209400
H	-5.70775800	-1.08238500	-0.06321700
H	-4.20042000	-1.94488900	0.29660100
C	-3.46972500	-0.33822300	2.47387400
H	-2.57626500	-0.90197100	2.18233800

H	-3.15601100	0.52883300	3.06062500
H	-4.06314900	-0.97507700	3.13960000
C	-2.31927200	3.07009800	0.00788300
H	-1.79435500	3.78045400	0.65806600
H	-1.57323300	2.60697200	-0.64636100
H	-3.00872300	3.65240100	-0.61199300
C	-4.15446700	-0.00629500	-2.10025900
H	-3.12399700	-0.35344700	-2.22507400
H	-4.78176500	-0.87132900	-1.87527100
H	-4.48821600	0.39600900	-3.06541800
H	-3.62879100	1.91653900	-1.49183600

TS5: (-1884.518213a.u.)

S	4.51184900	-1.27598300	-0.00120200
O	5.65226600	-2.19130900	-0.21919200
O	4.43696200	-0.05988500	-0.84669400
N	2.04760100	-1.56235300	-0.08197300
N	3.12593300	-2.27887700	-0.17980300
C	0.90701500	-2.24106200	-0.21437400
C	4.50992500	-0.75478300	1.71752600
H	3.61695500	-0.15309000	1.89947300
H	4.51639000	-1.64332200	2.35291200
H	5.41230900	-0.15939700	1.88259000
C	-0.38062200	-1.65611200	-0.13901600
C	-1.48334400	-2.69519700	-0.34433400
F	-2.66356000	-2.29014100	0.15009300
F	-1.65545400	-2.94048600	-1.66320500
F	-1.19391800	-3.87161500	0.24383700
H	0.95886500	-3.31435800	-0.38848200
C	2.13699300	2.67409800	0.15164500
C	1.55864300	2.19885000	1.33871500
C	0.61075500	1.18089800	1.29843300
C	0.22345200	0.63074500	0.07206800
C	0.78463200	1.11751400	-1.10941100
C	1.74096900	2.13373600	-1.07872200
H	1.86988800	2.63158700	2.28515900
H	0.17946000	0.80347800	2.22103200
H	0.48242000	0.69297500	-2.06271100
H	2.16689000	2.48929700	-2.00961900
O	3.06884300	3.66286000	0.29725200
C	3.77214700	4.10217500	-0.86765400
H	3.09407800	4.56700900	-1.59333700
H	4.49014400	4.84581700	-0.51600000
H	4.30753300	3.27055900	-1.34094000

N	-0.77478000	-0.40494200	0.02111200
H	-1.96814300	0.04436200	0.11035200
N	-3.16331200	0.82682700	0.24291800
C	-2.68197500	2.17960300	0.75244800
H	-3.53266700	2.69048000	1.21804600
H	-1.96754100	1.97186300	1.54826900
C	-3.78164100	0.99573900	-1.13442600
C	-4.08467300	0.29158300	1.34860900
H	-4.68272100	1.15387700	1.66836900
C	-5.07096300	1.83122300	-1.15074500
H	-5.30480000	2.09253100	-2.18932100
H	-5.93319100	1.29246700	-0.74779600
H	-4.96738800	2.76771800	-0.59379000
C	-5.10220500	-0.79900000	0.98631600
H	-5.68442400	-0.99364800	1.89495900
H	-5.81240000	-0.48854400	0.21933700
H	-4.65030000	-1.74244700	0.68337400
C	-3.25310700	-0.17410000	2.55376100
H	-2.66906400	-1.06728300	2.31310700
H	-2.57299900	0.59415800	2.93044000
H	-3.93397300	-0.43198600	3.37253500
C	-2.04232500	3.14285000	-0.24521900
H	-1.59782100	3.96076400	0.33457700
H	-1.24378400	2.68718300	-0.83395100
H	-2.77051600	3.58874700	-0.92905200
C	-3.92676800	-0.30501800	-1.93220700
H	-2.97446400	-0.83312100	-2.01417300
H	-4.67405700	-0.99263000	-1.53421800
H	-4.23642100	-0.03632900	-2.94945600
H	-3.02555600	1.56682100	-1.67617200

Int5: (-1884.552212a.u.)

S	0.74541800	0.73243500	0.88975800
O	2.20604500	0.57020800	1.15178400
O	0.37710500	1.72313800	-0.15785100
N	-1.12680500	-0.76999000	0.38289900
N	0.19546700	-0.81100900	0.57647900
C	-1.70024800	-1.90208200	0.07974300
C	-0.00819100	1.29186000	2.42541800
H	-1.09124000	1.32298400	2.28823100
H	0.25939000	0.59322700	3.22118700
H	0.37871800	2.29102900	2.64292800
C	-3.13834500	-2.00947800	-0.09690000
C	-3.59585200	-3.46301800	-0.23861400
F	-3.27058100	-4.18520200	0.86233000

F	-4.91734700	-3.59075400	-0.42359700
F	-2.98150700	-4.06174200	-1.28998300
H	-1.10584300	-2.81461500	-0.00988300
C	-3.73918600	3.06253200	-0.08244300
C	-4.35464500	2.38407800	0.97837800
C	-4.44924100	0.99565900	0.96485900
C	-3.89682700	0.24852600	-0.08895400
C	-3.29801900	0.93731700	-1.15289200
C	-3.21859200	2.33086200	-1.15735900
H	-4.76735400	2.95963400	1.80249600
H	-4.94315200	0.47754900	1.78245300
H	-2.88774100	0.37731600	-1.98844600
H	-2.74917100	2.82929500	-1.99799300
O	-3.70570700	4.43103500	0.01810900
C	-3.06612300	5.16460000	-1.02632400
H	-3.57121100	5.01513400	-1.98863900
H	-3.14002700	6.21581100	-0.73935400
H	-2.00924400	4.88652000	-1.12071300
N	-4.09399000	-1.14803700	-0.11702700
H	3.72522000	0.18368800	0.00886900
N	4.57179400	-0.09866700	-0.52056300
C	4.35980300	0.36425400	-1.95575400
H	5.33395600	0.31785900	-2.44759600
H	3.70355600	-0.35394300	-2.43886400
C	5.76539000	0.68830100	0.08538400
C	4.64132800	-1.63559300	-0.39736700
H	5.54134100	-1.92587200	-0.94432800
C	7.11142300	0.02306100	-0.19214300
H	7.89469300	0.73727800	0.08368500
H	7.27059700	-0.88504100	0.39537100
H	7.24496600	-0.21461500	-1.25250400
C	4.74583000	-2.06788900	1.06753800
H	4.71136700	-3.16147500	1.09954300
H	5.67520000	-1.76116000	1.54783700
H	3.90011000	-1.68806200	1.65093200
C	3.41433200	-2.29974500	-1.03476000
H	2.48025700	-1.89058200	-0.63337000
H	3.39578700	-2.23192700	-2.12465100
H	3.44596600	-3.36493400	-0.78465100
C	3.73158400	1.74905000	-2.05680000
H	3.58650700	1.97193100	-3.11974500
H	2.75122900	1.77770700	-1.57072500
H	4.35448300	2.54441900	-1.63696800
C	5.54591900	1.05125400	1.55413500

H	4.56469300	1.51033700	1.70816300
H	5.64601800	0.20287500	2.23382000
H	6.30665500	1.79020700	1.82933700
H	5.74563100	1.62533400	-0.47102000

TS6: (-1884.529322a.u.)

S	0.78919400	0.54603500	0.95234600
O	2.19393500	0.02827200	1.21062700
O	0.72731300	1.81465000	0.13178400
N	-1.44905400	-1.16647100	0.18733900
N	-0.26288200	-1.30589600	0.33034400
C	-2.46377800	-1.96869400	-0.11865500
C	0.15625700	1.00183300	2.59652600
H	-0.87497100	1.34810500	2.49082900
H	0.20151000	0.12211000	3.24309800
H	0.79175800	1.80281500	2.98693900
C	-3.82309000	-1.51301400	-0.14580700
C	-4.81608200	-2.67573200	-0.22964300
F	-4.82512200	-3.39080300	0.92337300
F	-6.07659200	-2.27896500	-0.46059000
F	-4.48290600	-3.54293000	-1.21871100
H	-2.25009700	-3.02234300	-0.28175400
C	-2.41691400	3.39112700	-0.11482400
C	-3.15629100	2.98677300	1.00569400
C	-3.77597000	1.74098900	1.02789900
C	-3.64998400	0.85266300	-0.05555000
C	-2.92396200	1.27808600	-1.17927200
C	-2.31714200	2.53488200	-1.21798100
H	-3.24261400	3.66443400	1.85085800
H	-4.36147200	1.44176800	1.89323000
H	-2.84143200	0.62064200	-2.04052700
H	-1.76568400	2.82763600	-2.10440300
O	-1.84326100	4.63530400	-0.03877300
C	-1.00317200	5.05205600	-1.11540500
H	-1.56467400	5.13759800	-2.05393000
H	-0.62397700	6.03644800	-0.83217300
H	-0.16188400	4.36194400	-1.25119200
N	-4.38201200	-0.35144500	-0.05154600
H	3.63983400	-0.30788800	0.04490100
N	4.46731400	-0.60838900	-0.51090500
C	4.25892000	-0.07164000	-1.92002500
H	5.19620700	-0.22813800	-2.45938000
H	3.49279200	-0.68462500	-2.38658400
C	5.70793500	0.07780000	0.11770800

C	4.45577100	-2.15090100	-0.46917500
H	5.33588700	-2.45921700	-1.03821700
C	7.01390200	-0.63555900	-0.22412300
H	7.83740100	0.01846300	0.08234500
H	7.13321700	-1.58583000	0.30337100
H	7.12059900	-0.81293500	-1.29924100
C	4.54698500	-2.66899700	0.96865000
H	4.44815700	-3.75878300	0.94052100
H	5.49778100	-2.44516300	1.45294300
H	3.73123200	-2.27326000	1.58299400
C	3.19351000	-2.71482700	-1.13446500
H	2.28422200	-2.26712000	-0.71794300
H	3.18398500	-2.59959400	-2.22049500
H	3.15925500	-3.78934100	-0.92901400
C	3.80722900	1.38357000	-1.96481600
H	3.60205800	1.63276200	-3.01203200
H	2.88330500	1.53308700	-1.39720500
H	4.56006200	2.08977100	-1.60305500
C	5.53111100	0.36001800	1.61046400
H	4.56551900	0.83313600	1.81294500
H	5.62230800	-0.53002300	2.23614100
H	6.31811600	1.06060100	1.91089500
H	5.72721200	1.04765000	-0.37798900

Int6: (-924.675622a.u.)

N	3.61092400	1.71986300	-0.41667400
N	3.80669400	2.81454200	-0.65494600
C	3.35774600	0.46691100	-0.14370100
C	1.98096700	0.06191200	0.03114700
C	1.82253400	-1.45462400	0.22315200
F	0.82124600	-1.75475700	1.06784800
F	1.57626300	-2.08333600	-0.95016800
F	2.94736300	-2.00492700	0.73076500
H	4.21674100	-0.18551000	-0.07633900
C	-3.16128800	0.43409700	0.11779300
C	-2.51350300	1.37763000	0.93156000
C	-1.13383300	1.51097300	0.88476500
C	-0.35072900	0.67754800	0.06071500
C	-1.01164900	-0.25085500	-0.75944500
C	-2.40270300	-0.37133800	-0.73931200
H	-3.11174400	2.00822400	1.58330500
H	-0.63765200	2.25585100	1.50062400
H	-0.44215100	-0.87176100	-1.44241200
H	-2.87753100	-1.09064300	-1.39690600

O	-4.52408400	0.39009400	0.22383300
C	-5.23489900	-0.54492200	-0.58989100
H	-4.93657500	-1.57615400	-0.36606600
H	-6.28977000	-0.41072800	-0.34197400
H	-5.08287100	-0.34140200	-1.65672700
N	1.03016900	0.92767400	0.02435100

TS7: (-924.662441a.u.)

N	3.27585800	1.99813500	-0.43340400
N	2.41540500	2.77559800	-0.50830800
C	3.38892500	0.69185700	-0.23625700
C	2.07769100	0.13456300	-0.03780600
C	2.03438200	-1.36671600	0.22064600
F	1.10417800	-1.68953800	1.13628900
F	1.75225500	-2.05270000	-0.91033800
F	3.22030000	-1.82096000	0.67198900
H	4.34432400	0.19790700	-0.20943000
C	-3.10676500	0.31174600	0.12344400
C	-2.48424400	1.35074100	0.83485100
C	-1.11119400	1.52602100	0.75710300
C	-0.31361200	0.65110200	-0.00706800
C	-0.94759900	-0.37183800	-0.73056600
C	-2.33073000	-0.54391900	-0.66832300
H	-3.09684000	2.01605300	1.43648200
H	-0.63197500	2.33699500	1.29770300
H	-0.36337700	-1.03128000	-1.36251900
H	-2.78767800	-1.34098000	-1.24354900
O	-4.46282800	0.22618900	0.25888500
C	-5.14957000	-0.81440900	-0.44098500
H	-4.80470500	-1.80449600	-0.12000400
H	-6.20420100	-0.69625200	-0.18442900
H	-5.02472300	-0.71402300	-1.52569100
N	1.05695100	0.92347600	-0.07705200

pro: (-924.708525a.u.)

N	2.82072000	2.25938000	-0.48238800
N	1.51172800	2.24989200	-0.44448800
C	3.27919900	1.00084700	-0.26528900
C	2.19688200	0.17048700	-0.07694900
C	2.17415600	-1.28830500	0.22779300
F	1.31589400	-1.58627400	1.22593300
F	1.81152700	-2.03858500	-0.84017500
F	3.40208300	-1.69669400	0.59970700

H	4.33251300	0.76184300	-0.24672700
C	-3.02618600	0.21462900	0.15059100
C	-2.42373900	1.23452600	0.90715500
C	-1.06200700	1.47494100	0.79931700
C	-0.29190700	0.69846700	-0.07448400
C	-0.88182300	-0.30592700	-0.83959400
C	-2.24883800	-0.55792500	-0.72310000
H	-3.03937700	1.82267200	1.58076800
H	-0.59212600	2.25392700	1.39064700
H	-0.28621500	-0.88938200	-1.53297300
H	-2.69234900	-1.34288000	-1.32372900
O	-4.36472200	0.05598800	0.33514500
C	-5.04102000	-0.96674400	-0.40436300
H	-4.64104900	-1.95868200	-0.16466600
H	-6.08590800	-0.91004000	-0.09417300
H	-4.96919000	-0.78792100	-1.48333100
N	1.10721500	0.98309200	-0.19921200