Supporting Information for

Straightforward access to Fluoroalkyl Tetrazoles from Fluoroalkyl *N*-sulfonylhydrazones

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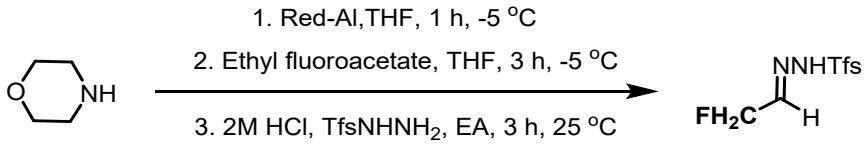
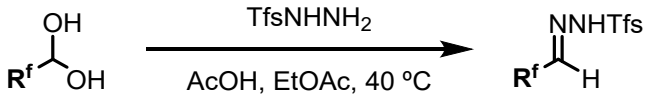
I. General information

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 Brüker Advance 600 (^{1}H: 600 MHz, ^{13}C: 150 MHz) and Brüker Advance 500 (^{1}H: 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 ^{1}H 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 Bruck microTof by using ESI method.

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

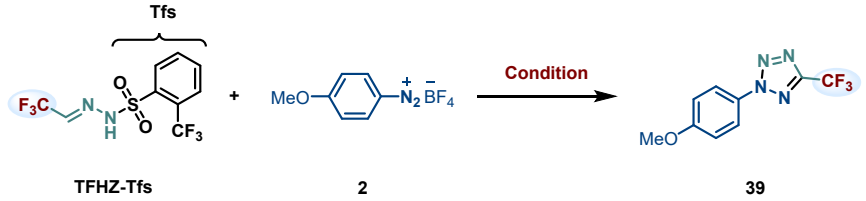


In a -5 ℃ low temperature bath, a 100 mL bottom flask was placed as the reaction vessel and nitrogen was replaced three times, morpholine (14 mmol) and THF (10 mL) were added to the bottom flask, Red-Al (12 mmol, 4.4 mL) was slowly dropwise into the mixture, the reaction stired at -5 ℃ for 1 hour. Add ethyl fluoroacetate and THF to the reaction system and continue to stir at -5 ℃ for 3 h. After that, quench the reaction system with 2M HCl (60 mL) until the solid disappears completely, add 2-(trifluoromethyl)benzenesulfonohydrazide ($TfsNHNH_2$) (5 mmol) and EA, the mixture was moved to 25 ℃ and stir for 3 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 recrystallization with ethyl ether and petroleum ether to obtain the product as a white solid.



A 250 mL bottom flask was charged with fluoropropionaldehyde hydrate (75.0 mmol), 2-(trifluoromethyl)benzenesulfonohydrazide ($TfsNHNH_2$) (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 ℃ 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 as a white solid.

III. Optimization of the reaction conditions for CF_3-substituted tetrazole 39.

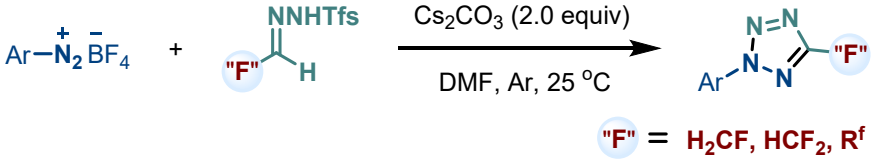


TFHZ-Tfs 2 39

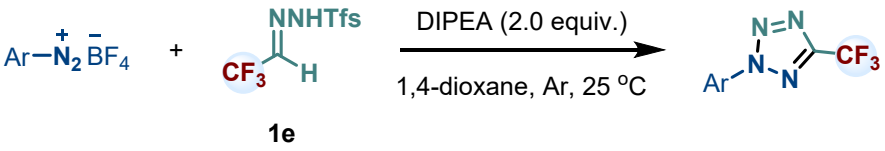
Entry	Base	Solvent	*T* (°C)	Yield (%)[b]
1	NaH	1,4-dioxane	25	90
2	Cs_2CO_3	1,4-dioxane	25	85
3	DBU	1,4-dioxane	25	92
4	Et_3N	1,4-dioxane	25	95
5	DIPEA	1,4-dioxane	25	98
6	DIPEA	DMF	25	66
7	DIPEA	THF	25	95
8	DIPEA	DCM	25	97
9	DIPEA	Toluene	25	67

[a] Reaction conditions: TFHZ-Tfs (0.6 mmol), aryl diazonium salts (0.3 mmol), and base (0.6mmol) in solvent (2 mL) at 25 °C under Ar for 2 h. [b] Isolated yield.

IV. General procedures for synthesis fluoroalkyl tetrazoles.



In a 15 mL of Schlenk tube equipped with Teflon coated magnetic stirring bar, aryl diazonium salts (1.0 equiv) in DMF (2 mL) was charged under Ar, then fluoroalkyl *N*-benzenesulfonylhydrazone (2.0 equiv.) and Cs_2CO_3 (2 equiv.) were added in one portion and the reaction was allowed to stirred at 25 °C for 2 h. After completion, water was added to the mixture and was extracted with EtOAc (3×5 mL). The combined organic layer was dried with anhydrous $MgSO_4$, filtered, and evaporated under reduced pressure to give the crude mixture, which was purified by flash column chromatography to afford the pure fluoroalkyl tetrazoles.

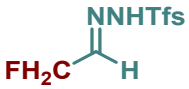


In a 15 mL of Schlenk tube equipped with Teflon coated magnetic stirring bar, aryl diazonium salts (1.0 equiv) in 1,4-dioxane (2 mL) was charged under Ar, then Trifluoroacetaldehyde *N*-Triftosylhydrazone (2.0 equiv) and DIPEA (2 equiv) were added in one portion and the reaction was allowed to stirred at 25 °C for 2 h. After completion, water was added to the mixture and was extracted with EtOAc (3×5 mL). The combined organic layer was dried with anhydrous $MgSO_4$, filtered, and evaporated under reduced pressure to give the crude mixture, which was purified by flash column chromatography to afford the pure 2-aryl-5-fluoroalkyl-tetrazoles.

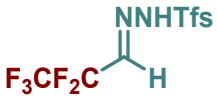
In a 15 mL of Schlenk tube equipped with Teflon coated magnetic stirring bar, was added arylamines (0.3 mmol), HBF_4 (50% in water, 0.6 mmol, 2.0 equiv.), *t*-BuONO (90% tech., 0.33 mmol, 1.1 equiv.), 1,4-dioxane (2.0 mL). Then the reaction was allowed to stir at 0 °C for 15 minutes before the organic base DIPEA (3.0 equiv.) and

fluoroalkyl *N*-benzenesulfonylhydrazone (2.0 equiv.) was added, the mixture was allowed to stir at 25 °C for additional 2 hours. After completion, water was added to the mixture and was extracted with EtOAc (3×5 mL). The combined organic layer was dried with anhydrous $MgSO_4$, filtered, and evaporated under reduced pressure to give the crude mixture, which was purified by flash column chromatography to afford the pure 2-aryl-5-fluoroalkyl-tetrazoles.

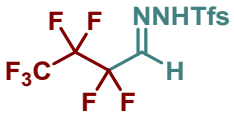
IV. Characterization data of prepared compounds



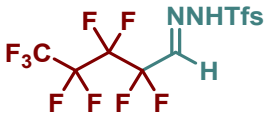
(**1a**) **^{1}H NMR** (500 MHz, DMSO) δ 12.22 (s, 1H), 8.06-7.88 (m, 4H), 7.52 (s, 1H), 4.93 (d, *J* = 47.0, 2H). **^{13}C NMR** (125 MHz, DMSO) δ 144.8 (d, *J* = 21.3 Hz), 138.3, 134.1, 133.9, 131.6, 129.1 (q, *J* = 6.3 Hz), 126.9 (q, *J* = 32.5 Hz), 82.3 (d, *J* = 160.0 Hz). **^{19}F NMR** (471 MHz, DMSO) δ -56.36 (s), (-221.38)-(-221.60) (m).



(**1f**) **^{1}H NMR** (500 MHz, DMSO) δ 13.08 (s, 1H), 8.13-8.10 (m, 1H), 8.04-7.99 (m, 1H), 7.94-7.89 (m, 2H), 7.56-7.53 (m, 1H). **^{13}C NMR** (150 MHz, DMSO) δ 137.3, 134.7, 134.0, 132.7 (t, *J* = 30.0 Hz), 132.3, 129.1 (q, *J* = 6.0 Hz), 127.1 (q, *J* = 34.5 Hz), 119.5 (qt, *J* = 285.0, 45.0 Hz), 110.3 (tq, *J* = 249.0, 39.0 Hz). **^{19}F NMR** (471 MHz, DMSO) δ -56.65 (s), -83.02 (s), -115.71 (s).



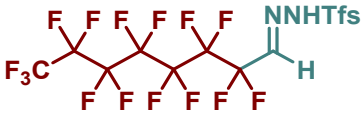
(**1g**) **^{1}H NMR** (500 MHz, $CDCl_3$) δ 9.14 (m, 1H), 8.35-8.32 (m, 1H), 7.92-7.90 (m, 1H), 7.80-7.77 (m, 2H), 7.21-7.18 (m, 1H). **^{13}C NMR** (125 MHz, DMSO) δ 135.6, 134.2, 133.4, 133.0 (t, *J* = 28.8 Hz), 132.7, 128.5 (q, *J* = 6.3 Hz), 127.9 (q, *J* = 32.5 Hz), 119.3-107.9 (m). **^{19}F NMR** (471 MHz, DMSO) δ -53.34 (s), (-80.63)-(-80.66) (m), (-115.95)-(-115.99) (m), -127.65 (s).



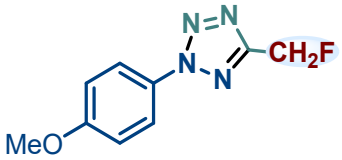
(**1j**) **^{1}H NMR** (500 MHz, $CDCl_3$) δ 9.14 (s, 1H), 8.36-8.34 (m, 1H), 7.92-7.90 (m, 1H), 7.80-7.78 (m, 2H), 7.19-7.16 (m, 1H). **^{13}C NMR** (125 MHz, DMSO) δ 137.5, 134.6, 133.7, 132.7 (t, *J* = 26.3 Hz), 132.6, 129.0 (q, *J* = 6.3 Hz), 127.5 (q, *J* = 33.8 Hz), 120.9-110.1 (m). **^{19}F NMR** (471 MHz, DMSO) δ -(-58.31)-(-58.43) (m), (-81.01)-(-81.11) (m), (-115.03)-(-115.08) (m), (-124.14)-(-124.25) (m), (-125.79)-(-125.88) (m).

(**1i**) **^{1}H NMR** (500 MHz, DMSO) δ 13.14 (s, 1H), 8.13-8.12 (m, 1H), 8.03-7.98 (m, 1H), 7.94-7.88 (m, 2H), 7.56-7.52 (m, 1H). **^{13}C NMR** (125 MHz, DMSO) δ 137.1, 134.7, 134.0, 133.8, 132.6 (t, *J* = 27.5 Hz), 132.4, 129.1-110.1 (m). **^{19}F NMR** (471 MHz, DMSO) δ -56.89 (s), -80.70 (s), -113.93 (s), -122.39 (s), -123.65 (s), 126.34 (s).

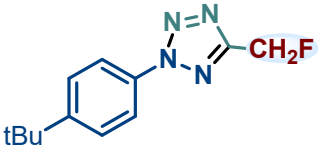
(**1j**) **^{1}H NMR** (500 MHz, DMSO) δ 8.12-8.11 (m, 1H), 7.96-7.95 (m, 1H), 7.89-7.83 (m, 2H), 7.52-7.50 (m, 1H). **^{13}C NMR** (125 MHz, DMSO) δ 137.2, 134.5, 133.9, 133.7, 132.6 (t, *J* = 27.5 Hz), 132.4, 128.9-108.6 (m). **^{19}F NMR** (471 MHz, DMSO) δ -57.13 (s), -81.24 (s), (-104.36)-(-126.68) (m).



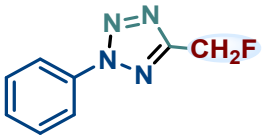
(**1k**) **^{1}H NMR** (500 MHz, DMSO) δ 8.12-8.10 (m, 1H), 7.93-7.91 (m, 1H), 7.85-7.81 (m, 2H), 7.50-7.47 (m, 1H). **^{13}C NMR** (125 MHz, DMSO) δ 137.2, 134.3, 134.0, 133.5, 132.6 (t, *J* = 27.5 Hz), 132.4, 128.8-108.9 (m). **^{19}F NMR** (471 MHz, DMSO) δ -57.30 (s), -81.75 (s), (-104.95)-(-126.26) (m).



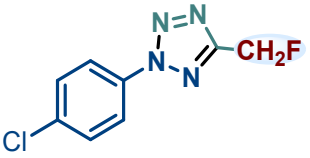
(**3**) White solid, m.p. 61–62 °C; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.05-8.02 (m, 2H), 7.05-7.02 (m, 2H), 5.73 (d, *J* = 47.5 Hz, 2H), 3.88 (s, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 161.4 (d, *J* = 20.0 Hz), 160.8, 130.1, 121.5, 114.7, 75.2 (d, *J* = 167.5 Hz), 55.6. **^{19}F NMR** (471 MHz, $CDCl_3$) δ -216.73 (t, *J* = 48.0 Hz). HRMS (ESI) m/z calcd. for $C_9H_9FN_4ONa$ $[M+Na]^+$ 231.0760, found 231.0768.



(4) White solid, m.p. 53–54 °C; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.05-8.03 (m, 2H), 7.58-7.58 (m, 2H), 5.75 (d, *J* = 47.5 Hz, 2H), 1.37 (s, 9H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 161.6 (d, *J* = 20.0 Hz), 153.6, 134.2, 126.6, 119.7, 75.2 (d, *J* = 167.5 Hz), 34.9, 31.2. **^{19}F NMR** (471 MHz, $CDCl_3$) δ -216.87 (t, *J* = 47.6 Hz). HRMS (ESI) m/z calcd. for $C_{12}H_{15}FN_4Na$ $[M+Na]^+$ 257.1289, found 257.1287.

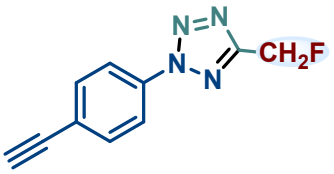


(**5**) Colorless oil; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.14-8.13 (m, 2H), 7.58-7.50 (m, 3H), 5.76 (d, *J* = 47.5 Hz, 2H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 161.7 (d, *J* = 20.0 Hz), 136.6, 130.1, 129.7, 120.0, 75.2 (d, *J* = 167.5 Hz). **^{19}F NMR** (471 MHz, $CDCl_3$) δ -217.15 (t, *J* = 48.5 Hz). HRMS (ESI) m/z calcd. for $C_8H_7FN_4Na$ $[M+Na]^+$ 201.0548, found 201.0542.

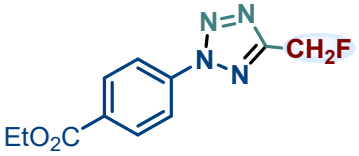


(6) White solid, m.p. 58–60 °C; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.11-8.09 (m, 2H), 7.56-7.54 (m, 2H), 5.75 (d, *J* = 47.5 Hz, 2H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 161.9 (d, *J* = 24.5 Hz), 136.1, 135.0, 130.0, 121.2, 75.1 (d, *J* = 201.8 Hz). **^{19}F NMR** (565 MHz, $CDCl_3$) δ -217.52 (t, *J* = 46.9

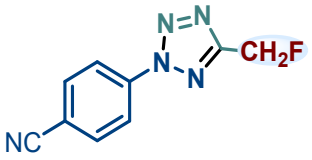
Hz). HRMS (ESI) m/z calcd. for $C_8H_6ClFN_4Na$ $[M+Na]^+$ 235.0799, found 235.0792.



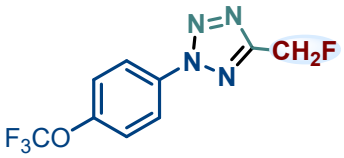
(7) White solid, m.p. 71–73 °C; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.13-8.11 (m, 2H), 7.69-7.67 (m, 2H), 5.76 (d, *J* = 47.5 Hz, 2H), 3.23 (s, 1H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 161.9 (d, *J* = 21.3 Hz), 136.2, 133.5, 124.2, 119.8, 82.0, 79.8, 75.1 (d, *J* = 168.8 Hz). **^{19}F NMR** (471 MHz, $CDCl_3$) δ -217.54 (t, *J* = 47.6 Hz). HRMS (ESI) m/z calcd. for $C_{10}H_7FN_4Na$ $[M+Na]^+$ 225.0548, found 225.0549.



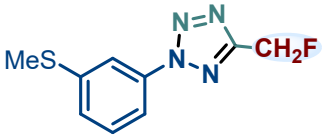
(8) White solid, m.p. 125–126 °C; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.26-8.22 (m, 4H), 5.77 (d, *J* = 47.0 Hz, 2H), 4.43 (q, *J* = 7.0 Hz, 2H), 1.43 (t, *J* = 7.5 Hz, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 165.2, 162.0 (d, *J* = 19.5 Hz), 139.3, 131.9, 131.2, 119.7, 75.0 (d, *J* = 169.5 Hz), 61.6, 14.3. **^{19}F NMR** (471 MHz, $CDCl_3$) δ -217.83 (t, *J* = 47.6 Hz). HRMS (ESI) m/z calcd. for $C_{11}H_{11}FN_4O_2Na$ $[M+Na]^+$ 273.0951, found 273.0955.



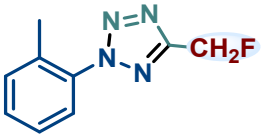
(9) Yellow oil; **^{1}H NMR** (600 MHz, $CDCl_3$) δ 8.33-8.31 (m, 2H), 7.91-7.89 (m, 2H), 5.77 (d, *J* = 47.4 Hz, 2H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 162.3 (d, *J* = 19.5 Hz), 139.0, 133.9, 120.4, 117.4, 114.0, 74.9 (d, *J* = 169.5 Hz). **^{19}F NMR** (565 MHz, $CDCl_3$) δ -218.34 (t, *J* = 47.5 Hz). HRMS (ESI) m/z calcd. for $C_9H_6FN_5Na$ $[M+Na]^+$ 226.0514, found 226.0518.



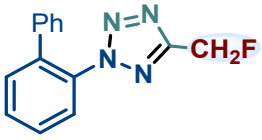
(10) Colorless oil; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.22-8.19 (m, 2H), 7.44-7.42 (m, 2H), 5.76 (d, *J* = 47.0 Hz, 2H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 162.0 (d, *J* = 21.0 Hz), 150.1, 134.8, 122.2, 121.6, 121.2 (q, *J* = 256.5 Hz), 75.0 (d, *J* = 168.0 Hz). **^{19}F NMR** (565 MHz, $CDCl_3$) δ -57.95 (s), -217.68 (t, *J* = 46.9 Hz). HRMS (ESI) m/z calcd. for $C_9H_6F_4N_4ONa$ $[M+Na]^+$ 285.0513, found 285.0516.



(11) Yellow solid, m.p. 75–76 °C; **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.98 (s, 1H), 7.88-7.87 (m, 1H), 7.47-7.44 (m, 1H), 7.37-7.35 (m, 1H), 5.75 (d, *J* = 47.5 Hz, 2H), 2.57 (s, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 161.7 (d, *J* = 19.5 Hz), 141.6, 137.0, 129.9, 127.5, 116.9, 116.1, 75.0 (d, *J* = 168.0 Hz), 15.4. **^{19}F NMR** (565 MHz, $CDCl_3$) δ -217.26 (t, *J* = 47.5 Hz). HRMS (ESI) m/z calcd. for $C_9H_9FN_4SNa$ $[M+Na]^+$ 247.0432, found 247.0430.

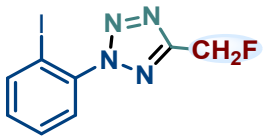


(12) Colorless oil; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.60-7.59 (m, 1H), 7.48-7.45 (m, 1H), 7.42-7.37 (m, 2H), 5.77 (d, *J* = 47.5 Hz, 2H), 2.37 (s, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ161.4 (d, *J* = 20.0 Hz), 136.1, 133.0, 131.9, 130.6, 126.9, 125.2, 75.2 (d, *J* = 167.5 Hz), 18.6. **^{19}F NMR** (471 MHz, $CDCl_3$) δ -217.27 (t, *J* = 48.5 Hz). HRMS (ESI) m/z calcd. for $C_9H_9FN_4Na$ $[M+Na]^+$ 215.0733, found 215.0739.

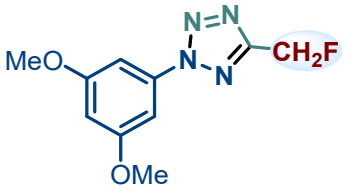


(13) White solid, m.p. 63–65 °C; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.68-7.54 (m, 4H), 7.28-7.24 (m, 3H), 7.06-7.04 (m, 2H), 5.60 (d, *J* = 47.0 Hz, 2H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 161.3 (d, *J* =

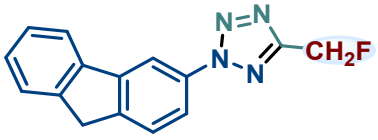
21.3 Hz), 138.4, 137.1, 134.8, 131.4, 131.2, 128.5, 128.3, 128.2, 127.9, 126.4, 74.9 (d, J = 167.5 Hz). **^{19}F NMR** (471 MHz, $CDCl_3$) δ -216.77 (t, J = 47.1 Hz). HRMS (ESI) m/z calcd. for $C_{14}H_{11}FN_4Na$ $[M+Na]^+$ 277.0955, found 277.0952.



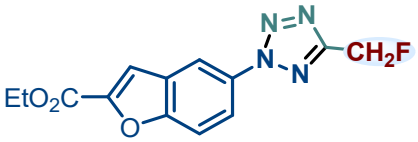
(14) Yellow oil; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.07-8.06 (m, 1H), 7.58-7.51 (m, 2H), 7.34-7.31 (m, 1H), 5.80 (d, J = 47.0 Hz, 2H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 161.7 (d, J = 20.0 Hz), 140.7, 139.9, 132.4, 129.2, 127.6, 92.5, 75.1 (d, J = 168.8 Hz). **^{19}F NMR** (471 MHz, $CDCl_3$) δ -217.33 (t, J = 47.1 Hz). HRMS (ESI) m/z calcd. for $C_8H_6FIN_4Na$ $[M+Na]^+$ 326.9602, found 326.9607.



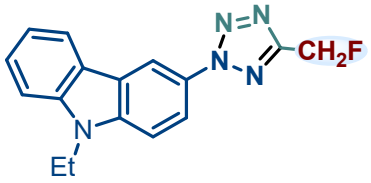
(15) White solid, m.p. 106–108 °C; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.30-7.29 (m, 2H), 6.57-6.56 (m, 1H), 5.74 (d, J = 47.5 Hz, 2H), 3.87 (s, 6H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 161.6 (d, J = 21.3 Hz), 161.5, 137.9, 102.4, 98.3, 75.2 (d, J = 167.5 Hz), 55.8. **^{19}F NMR** (471 MHz, $CDCl_3$) δ -217.22 (t, J = 48.0 Hz). HRMS (ESI) m/z calcd. for $C_{10}H_{11}FN_4O_2Na$ $[M+Na]^+$ 261.0853, found 261.0850.



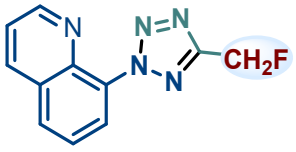
(16) Yellow solid, m.p. 123–125 °C; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.27 (s, 1H), 8.14 (dd, J = 8.5 Hz, J = 2.0 Hz, 1H), 7.89 (d, J = 8.0 Hz, 1H), 7.82 (d, J = 7.5 Hz, 1H), 7.58 (d, J = 7.5 Hz, 1H), 7.44-7.35 (m, 2H), 5.76 (d, J = 47.5 Hz, 2H), 3.98 (s, 2H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 161.6 (d, J = 19.5 Hz), 144.6, 143.7, 140.1, 135.1, 127.8, 127.2, 125.2, 120.6, 120.4, 119.0, 116.8, 75.1 (d, J = 168.0 Hz), 37.0. **^{19}F NMR** (565 MHz, $CDCl_3$) δ -217.00 (t, J = 48.0 Hz). HRMS (ESI) m/z calcd. for $C_{15}H_{11}FN_4Na$ $[M+Na]^+$ 289.0977, found 289.9073.



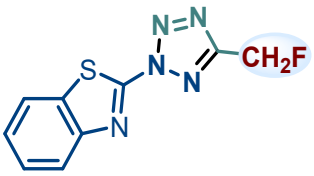
(17) White solid, m.p. 133–134 °C; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.46 (d, *J* = 2.0 Hz, 1H), 8.26 (dd, *J* = 9.0 Hz, *J* = 2.5 Hz, 1H), 7.77 (d, *J* = 9.0 Hz, 1H), 7.62 (s, 1H), 5.77 (d, *J* = 47.5 Hz, 2H), 4.48 (q, *J* = 7.0 Hz, 2H), 1.45 (t, *J* = 7.0 Hz, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 161.8 (d, *J* = 20.0 Hz), 158.9, 155.6, 148.0, 133.1, 127.7, 119.8, 114.5, 113.6, 75.2 (d, *J* = 168.8 Hz), 62.0, 14.3. **^{19}F NMR** (471 MHz, $CDCl_3$) δ -216.82 (t, *J* = 47.1 Hz). HRMS (ESI) m/z calcd. for $C_{13}H_{11}FN_4O_3Na$ $[M+Na]^+$ 313.0832, found 313.0835.



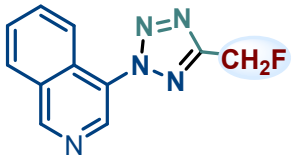
(18) Yellow solid, m.p. 164–165 °C; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.81 (d, *J* = 2.0 Hz, 1H), 8.23 (dd, *J* = 8.5 Hz, *J* = 2.0 Hz, 1H), 8.17 (d, *J* = 7.5 Hz, 1H), 7.57-7.46 (m, 3H), 7.32 (t, *J* = 7.5 Hz, 2H), 5.80 (d, *J* = 47.5 Hz, 2H), 4.34 (q, *J* = 7.5 Hz, 2H), 1.50 (t, *J* = 7.5 Hz, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 161.4 (d, *J* = 21.0 Hz), 140.8, 140.2, 129.1, 126.9, 123.2, 122.6, 120.9, 119.8, 117.8, 112.6, 109.0, 108.9, 75.3 (d, *J* = 201 Hz), 37.9, 13.8. **^{19}F NMR** (565 MHz, $CDCl_3$) δ -216.36 (t, *J* = 58.2 Hz). HRMS (ESI) m/z calcd. for $C_{16}H_{14}FN_5Na$ $[M+Na]^+$ 318.0744, found 318.0740.



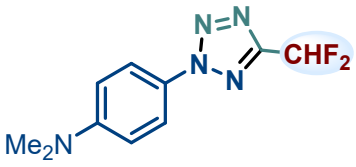
(19) Yellow solid, m.p. 153–155 °C; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.98 (t, *J* = 2.5 Hz, 1H), 8.32 (dd, *J* = 8.5 Hz, *J* = 1.5 Hz, 1H), 8.11 (d, *J* = 8.0 Hz, 1H), 8.00 (d, *J* = 7.5 Hz, 1H), 7.74 (t, *J* = 8.5 Hz, 1H), 7.57 (dd, *J* = 8.5 Hz, *J* = 4.5 Hz, 1H), 5.86 (d, *J* = 47.5 Hz, 2H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 161.7 (d, *J* = 17.5 Hz), 152.3, 142.2, 136.2, 134.0, 131.5, 129.1, 127.3, 125.7, 122.6, 75.2 (d, *J* = 140.0 Hz). **^{19}F NMR** (471 MHz, $CDCl_3$) δ -216.88 (t, *J* = 39.6 Hz). HRMS (ESI) m/z calcd. for $C_{11}H_8FN_5Na$ $[M+Na]^+$ 252.0316, found 252.0315.



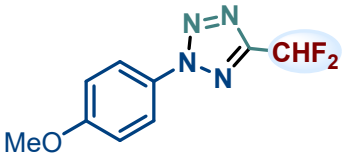
(20) Yellow solid, m.p. 153–155 °C; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 9.16 (s, 1H), 8.90 (d, *J* = 1.5 Hz, 1H), 8.29 (dd, *J* = 8.5 Hz, *J* = 2.0 Hz, 1H), 8.15 (d, *J* = 8.5 Hz, 1H), 5.79 (d, *J* = 47.5 Hz, 2H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 161.9 (d, *J* = 20.0 Hz), 156.8, 153.6, 135.4, 135.2, 123.2, 117.5, 115.1, 75.1 (d, *J* = 167.5 Hz). **^{19}F NMR** (471 MHz, $CDCl_3$) δ -217.32 (t, *J* = 48.5 Hz). HRMS (ESI) m/z calcd. for $C_9H_6FN_5SNa$ $[M+Na]^+$ 258.0316, found 258.0315.



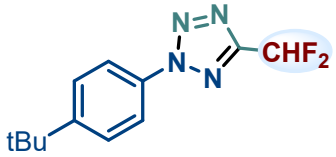
(21) Yellow solid, m.p. 132–134 °C; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 9.70 (d, *J* = 2.4 Hz, 1H), 8.88 (d, *J* = 2.2 Hz, 1H), 8.21 (d, *J* = 8.5 Hz, 1H), 7.98 (d, *J* = 8.1 Hz, 1H), 7.87 – 7.82 (m, 1H), 7.69 (t, *J* = 7.5 Hz, 1H), 5.77 (d, *J* = 47.5 Hz, 2H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 162.2 (d, *J* = 20.0 Hz), 148.4, 142.1, 131.2, 123.0, 129.8, 128.5, 128.5, 127.0, 126.2, 74.5. (d, *J* = 168.8 Hz). **^{19}F NMR** (471 MHz, $CDCl_3$) δ -217.89 (t, *J* = 47.5Hz). HRMS (ESI) m/z calcd. for $C_{11}H_8FN_5Na$ $[M+Na]^+$ 252.0661, found 252.0663.



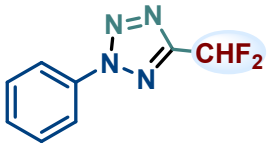
(22) Yellow solid, m.p. 92–94 °C; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.97-7.94 (m, 2H), 7.01 (t, *J* = 53.0 Hz, 1H), 6.78-6.75 (m, 2H), 3.06 (s, 6H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 159.5 (t, *J* = 28.5 Hz), 151.5, 125.9, 121.3, 111.8, 107.9 (t, *J* = 237.0 Hz), 40.3. **^{19}F NMR** (471 MHz, $CDCl_3$) δ -116.76 (d, *J* = 44.3 Hz). HRMS (ESI) m/z calcd. for $C_{10}H_{11}F_2N_5Na$ $[M+Na]^+$ 262.0971, found 262.0976.



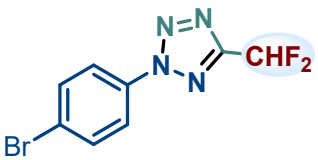
(23) White solid, m.p. 46–47 °C; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.07-8.04 (m, 2H), 7.07-7.04 (m, 2H), 7.02 (t, *J* = 53.0 Hz, 1H), 3.90 (s, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 161.1, 159.9 (t, *J* = 27.5 Hz), 129.8, 121.7, 114.8, 107.8 (t, *J* = 237.5 Hz), 55.7. **^{19}F NMR** (471 MHz, $CDCl_3$) δ -116.97 (d, *J* = 51.8 Hz). HRMS (ESI) m/z calcd. for $C_9H_8F_2N_4ONa$ $[M+Na]^+$ 249.0645, found 249.0651.



(24) White solid, m.p. 66–67 °C; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.07-8.04 (m, 2H), 7.60-7.58 (m, 2H), 7.03 (t, *J* = 53.0 Hz, 1H), 1.38 (s, 9H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 160.1 (t, *J* = 27.0 Hz), 154.2, 134.0, 126.7, 119.8, 107.8 (t, *J* = 237.0 Hz), 35.0, 31.2. **^{19}F NMR** (565 MHz, $CDCl_3$) δ -117.02 (d, *J* = 53.1 Hz). HRMS (ESI) m/z calcd. for $C_{12}H_{14}F_2N_4Na$ $[M+Na]^+$ 275.1174, found 275.1172.

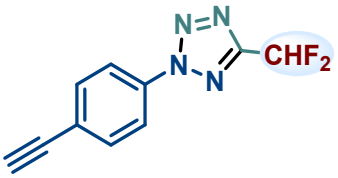


(25) Colorless oil; **^{1}H NMR** (600 MHz, $CDCl_3$) δ 8.15-8.13 (m, 2H), 7.59-7.53 (m, 3H), 7.04 (t, *J* = 52.8 Hz, 1H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 160.2 (t, *J* = 28.8 Hz), 136.3, 130.5, 129.8, 120.1, 107.7 (t, *J* = 237.5 Hz). **^{19}F NMR** (471 MHz, $CDCl_3$) δ -117.11 (d, *J* = 53.2 Hz). HRMS (ESI) m/z calcd. for $C_8H_6F_2N_4Na$ $[M+Na]^+$ 219.0573, found 219.0571.

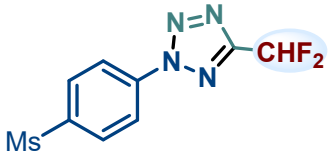


(26) Yellow solid, m.p. 53–55 °C; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.07-8.04 (m, 2H), 7.75-7.72 (m, 2H), 7.04 (t, *J* = 52.5 Hz, 1H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 160.4 (t, *J* = 27.5 Hz), 135.2, 133.1,

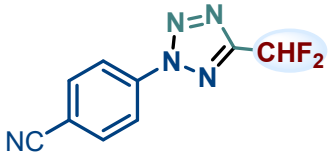
124.7, 121.5, 107.6 (t, J = 238.8 Hz). **^{19}F NMR** (471 MHz, $CDCl_3$) δ -117.18 (d, J = 52.8 Hz). HRMS (ESI) m/z calcd. for $C_8H_5BrF_2N_4Na$ $[M+Na]^+$ 296.9646, found 296.9651.



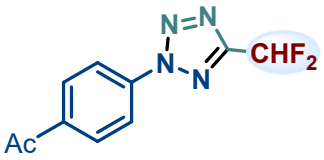
(27) White solid, m.p. 83–84 °C; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.14-8.13 (m, 2H), 7.70-7.68 (m, 2H), 7.04 (t, J = 53.0 Hz, 1H), 3.25 (s, 1H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 160.3 (t, J = 28.5 Hz), 136.0, 133.6, 124.7, 120.0, 107.6 (t, J = 238.5 Hz), 81.9, 80.1. **^{19}F NMR** (565 MHz, $CDCl_3$) δ -117.19 (d, J = 52.5 Hz). HRMS (ESI) m/z calcd. For $C_{10}H_6F_2N_4Na$ $[M+Na]^+$ 243.0573, found 243.0575.



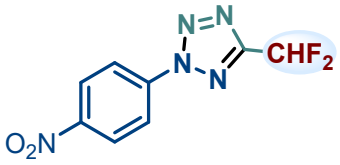
(28) Yellow solid, m.p. 135–136 °C **^{1}H NMR** (500 MHz, DMSO) δ 8.42-8.40 (m, 2H), 8.26-8.24 (m, 2H), 7.65 (t, J = 52.0 Hz, 1H), 3.35 (s, 3H). **^{13}C NMR** (150 MHz, DMSO) δ 164.7 (t, J = 27.0 Hz), 146.9, 143.4, 133.8, 125.7, 112.6 (t, J = 235.5 Hz), 47.8. **^{19}F NMR** (565 MHz, DMSO) δ -118.21 (d, J = 52.5 Hz). HRMS (ESI) m/z calcd. for $C_9H_8F_2N_4O_2SNa$ $[M+Na]^+$ 297.0315, found 297.0318.



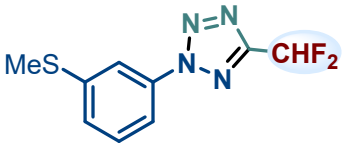
(29) Yellow oil; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.35-8.33 (m, 2H), 7.93-7.91 (m, 2H), 7.05 (t, J = 53.0 Hz, 1H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 160.7 (t, J = 28.8 Hz), 138.8, 134.0, 120.7, 117.3, 114.5, 107.4 (t, J = 238.8 Hz). **^{19}F NMR** (471 MHz, $CDCl_3$) δ -117.37 (d, J = 52.8 Hz). HRMS (ESI) m/z calcd. for $C_9H_5F_2N_5Na$ $[M+Na]^+$ 244.0537, found 244.0541.



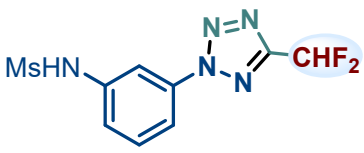
(30) White solid, m.p. 106–107 °C; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.28-8.26 (m, 2H), 8.18-8.16 (m, 2H), 7.04 (t, *J* = 53.0 Hz, 1H), 2.67 (s, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 196.3, 160.5 (t, *J* = 27.5 Hz), 139.0, 138.3, 130.0, 120.1, 107.5 (t, *J* = 238.8 Hz), 26.7. **^{19}F NMR** (471 MHz, $CDCl_3$) δ -117.29 (d, *J* = 52.8 Hz). HRMS (ESI) m/z calcd. for $C_{10}H_8F_2N_4ONa$ $[M+Na]^+$ 261.0655, found 261.0658.



(31) White solid, m.p. 77–79 °C; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.50-8.47 (m, 2H), 8.42-8.39 (m, 2H), 7.06 (t, *J* = 53.0 Hz, 1H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 160.9 (t, *J* = 28.8 Hz), 148.5, 140.0, 125.6, 120.8, 107.4 (t, *J* = 238.8 Hz). **^{19}F NMR** (471 MHz, $CDCl_3$) δ -117.44 (d, *J* = 52.3 Hz). HRMS (ESI) m/z calcd. for $C_8H_5F_2N_5O_2Na$ $[M+Na]^+$ 264.0435, found 264.0433.

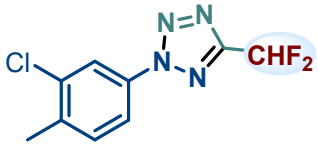


(32) Yellow solid, m.p. 53–54 °C; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.99 (s, 1H), 7.90 (dd, *J* = 8.0 Hz, *J* = 1.0 Hz, 1H), 7.47 (t, *J* = 8.0 Hz, 1H), 7.39 (d, *J* = 8.0 Hz, 1H), 7.03 (t, *J* = 53.0 Hz, 1H), 2.57 (s, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 160.2 (t, *J* = 28.5 Hz), 141.9, 136.8, 130.0, 128.0, 117.1, 116.3, 107.7 (t, *J* = 237.0 Hz), 15.4. **^{19}F NMR** (565 MHz, $CDCl_3$) δ -117.12 (d, *J* = 54.2 Hz). HRMS (ESI) m/z calcd. for $C_9H_8F_2N_4SNa$ $[M+Na]^+$ 265.0417, found 265.0411.

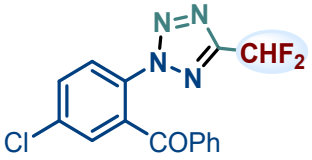


(33) Yellow solid, m.p. 149–151 °C; **^{1}H NMR** (500 MHz, DMSO) δ 10.30 (s, 1H), 8.00 (s, 1H),

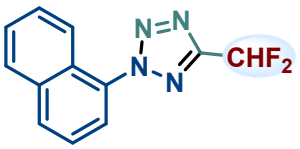
7.85 (dd, J = 8.0 Hz, J = 1.0 Hz, 1H), 7.65 (t, J = 8.0 Hz, 1H), 7.61 (t, J = 52.5 Hz, 1H), 7.45 (dd, J = 8.0 Hz, J = 1.5 Hz, 1H), 3.11 (s, 3H). **^{13}C NMR** (125 MHz, DMSO) δ 164.4 (t, J = 28.8 Hz), 144.6, 141.0, 135.8, 125.4, 119.5, 114.8, 112.7 (t, J = 236.3 Hz). **^{19}F NMR** (471 MHz, DMSO) δ -113.24 (d, J = 51.3 Hz). HRMS (ESI) m/z calcd. for $C_9H_9F_2N_5O_2SNa$ $[M+Na]^+$ 312.0473, found 312.0477.



(34) White solid, m.p. 83–85 °C; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.15 (s, 1H), 7.95 (dd, J = 8.0 Hz, J = 1.5 Hz, 1H), 7.44 (d, J = 8.5 Hz, 1H), 7.02 (t, J = 52.5 Hz, 1H), 2.45 (s, 1H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 160.2 (t, J = 27.5 Hz), 139.1, 135.6, 134.9, 131.9, 120.7, 118.1, 107.6 (t, J = 237.5 Hz), 19.9. **^{19}F NMR** (471 MHz, $CDCl_3$) δ -117.19 (d, J = 53.2 Hz). HRMS (ESI) m/z calcd. for $C_9H_7ClF_2N_4Na$ $[M+Na]^+$ 267.0349, found 267.0352.

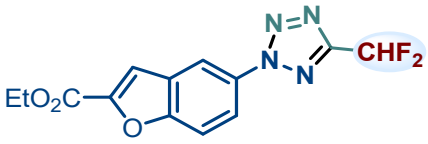


(35) White solid, m.p. 95–97 °C; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.96 (d, J = 8.5 Hz, 1H), 7.74 (dd, J = 8.5 Hz, J = 2.5 Hz, 1H), 7.68-7.64 (m, 3H), 7.53 (t, J =7.5 Hz, 1H), 7.37 (t, J =7.5 Hz, 2H), 6.77 (t, J = 52.5 Hz, 1H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 192.0, 160.2 (t, J = 28.8 Hz), 137.3, 135.6, 135.1, 133.9, 132.4, 131.7, 130.2, 129.1, 128.7, 125.1 , 107.1 (t, J = 238.8 Hz). **^{19}F NMR** (471 MHz, $CDCl_3$) δ -117.53 (d, J = 53.2 Hz). HRMS (ESI) m/z calcd. for $C_{15}H_9ClF_2N_4ONa$ $[M+Na]^+$ 357.0742, found 357.0742.

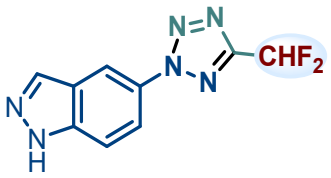


(36) White solid, m.p. 46–47 °C; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.11 (d, J = 8.0 Hz, 1H), 8.01-7.94 (m, 2H), 7.87 (d, J = 7.5 Hz, 1H), 7.64-7.61 (m, 3H), 7.14 (t, J = 53.0 Hz, 1H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 160.2 (t, J = 28.8 Hz), 134.2, 132.9, 131.9, 128.5, 127.3, 126.8, 124.8, 123.6,

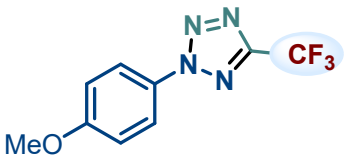
122.2, 107.8 (t, J = 237.5 Hz). **^{19}F NMR** (471 MHz, $CDCl_3$) δ -116.88 (d, J = 52.8 Hz). HRMS (ESI) m/z calcd. for $C_{12}H_8F_2N_4Na$ $[M+Na]^+$ 269.0239, found 269.0236.



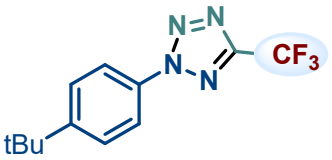
(37) White solid, m.p. 104–105 °C; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.48 (s, 1H), 8.27 (dd, J = 9.0 Hz, J = 1.5 Hz, 1H), 7.79 (d, J = 9.0 Hz, 1H), 7.62 (s, 1H), 7.05 (t, J = 53.0 Hz, 1H), 4.48 (q, J = 7.0 Hz, 2H), 1.45 (t, J = 7.0 Hz, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 160.3 (t, J = 28.5 Hz), 158.8, 155.8, 148.1, 132.8, 127.8, 119.8, 114.8, 113.8, 113.6, 107.6 (t, J = 238.5 Hz), 62.0, 14.3. **^{19}F NMR** (565 MHz, $CDCl_3$) δ -117.12 (d, J = 53.1 Hz). HRMS (ESI) m/z calcd. for $C_{13}H_{10}F_2N_4O_3Na$ $[M+Na]^+$ 331.0535, found 331.0533.



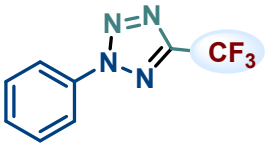
(38) White solid, m.p. 124–125 °C; **^{1}H NMR** (600 MHz, DMSO) δ 13.54 (s, 1H), 8.56 (s, 1H), 8.32 (s, 1H), 8.08 (dd, J = 9.0 Hz, J = 1.8 Hz, 1H), 7.84 (d, J = 9.0 Hz, 1H), 7.61 (t, J = 52.2 Hz, 1H). **^{13}C NMR** (150 MHz, DMSO) δ 164.4 (t, J = 27.0 Hz), 144.5, 139.6, 133.9, 127.0, 123.4, 117.9, 116.3, 112.8 (t, J = 235.5 Hz). **^{19}F NMR** (565 MHz, DMSO) δ -117.78 (d, J = 53.1 Hz). HRMS (ESI) m/z calcd. for $C_9H_6F_2N_6Na$ $[M+Na]^+$ 259.0648, found 259.0651.



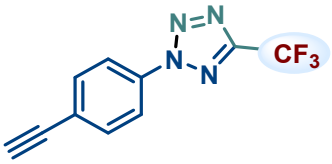
(39)[2] Yellow solid, m.p. 49–50 °C; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.08-8.06 (m, 2H), 7.08-7.06 (m, 2H), 3.90 (s, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 161.0, 157.1 (q, J = 40.5 Hz), 121.8, 119.4 (d, J = 268.5 Hz), 114.9, 55.7. **^{19}F NMR** (471 MHz, $CDCl_3$) δ -63.56 (s). HRMS (ESI) m/z calcd. for $C_9H_8F_3N_4O$ $[M+H]^+$ 245.0645, found 245.0643.



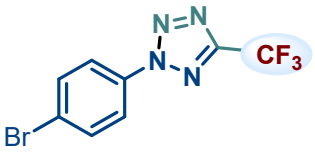
(40)[2] Yellow solid, m.p. 44–45 °C; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.08-8.05 (m, 2H), 7.62-7.59 (m, 2H), 1.39 (s, 9H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 157.3 (q, J = 40.6 Hz), 154.6, 133.8, 126.8, 119.9, 119.6 (q, J = 273.8 Hz), 35.0, 31.1. **^{19}F NMR** (471 MHz, $CDCl_3$) δ -63.58 (s). HRMS (ESI) m/z calcd. for $C_{12}H_{13}F_3N_4$ $[M]^+$ 270.1087, found 270.1093.



(41)[2] Yellow oil; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.17-8.15 (m, 2H), 7.63-7.56 (m, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 157.4 (q, J = 33.8 Hz), 136.2, 130.9, 130.0, 120.2, 119.4 (q, J = 223.8 Hz). **^{19}F NMR** (565 MHz, $CDCl_3$) δ -63.65 (s). HRMS (ESI) m/z calcd. for $C_8H_6F_3N_4$ $[M+H]^+$ 215.0539, found 215.0541.

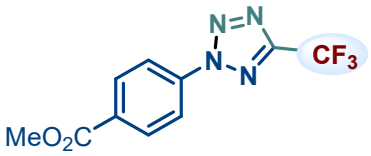


(42) White solid, m.p. 63–65 °C; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.16-8.14 (m, 2H), 7.72-7.69 (m, 2H), 3.27 (s, 1H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 157.4 (q, J = 41.3 Hz), 135.7, 133.7, 125.1, 120.1, 118.3 (q, J = 270.0 Hz), 81.8, 80.4. **^{19}F NMR** (471 MHz, $CDCl_3$) δ -63.64 (s). HRMS (ESI) m/z calcd. for $C_{10}H_5F_3N_4Na$ $[M+Na]^+$ 261.0573, found 261.0572.

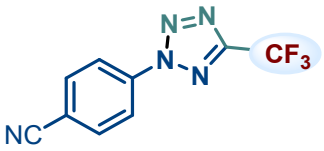


(43)[2] Yellow solid, m.p. 36–37 °C; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.15-8.12 (m, 2H), 7.61-7.58 (m, 2H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 157.4 (q, J = 35.0 Hz), 135.1, 133.2, 125.1, 121.6, 119.2 (q, J = 223.8 Hz). **^{19}F NMR** (565 MHz, $CDCl_3$) δ -63.62 (s). HRMS (ESI) m/z calcd. for

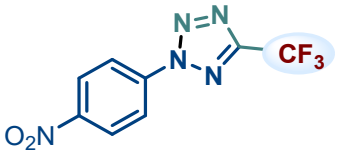
$C_8H_4BrF_3N_4$ $[M]^+$ 291.9566, found 291.9569.



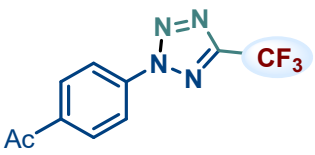
(44)[2] White solid, m.p. 52–54 °C; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.30-8.26 (m, 4H), 4.00 (s, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 165.4, 157.6 (q, J = 41.3 Hz), 138.8,132.4, 131.4, 120.0, 119.3 (q, J = 268.8 Hz), 52.6. **^{19}F NMR** (471 MHz, $CDCl_3$) δ -63.70 (s). HRMS (ESI) m/z calcd. for $C_{10}H_7F_3N_4O_2$ $[M]^+$ 272.0516, found 272.0518.



(45)[2] Yellow oil; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.36-8.35 (m, 2H), 7.96-7.94 (m, 2H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 157.9 (q, J = 40.5 Hz), 138.5, 134.1, 120.8, 119.0 (q, J = 268.5 Hz), 117.1, 114.8. **^{19}F NMR** (565 MHz, $CDCl_3$) δ -63.71 (s). HRMS (ESI) m/z calcd. for $C_9H_4F_3N_3$ $[M\text{-}N_2]^+$ 211.0352, found 211.0354.

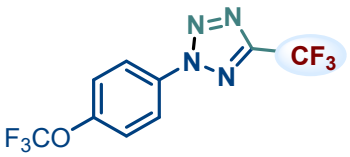


(46)[2] White solid, m.p. 53–55 °C; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.52-8.49 (m, 2H), 8.45-8.42 (m, 2H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 158.1 (q, J = 41.3 Hz), 148.8, 139.8, 125.6, 121.0, 119.2 (q, J = 268.8 Hz). **^{19}F NMR** (471 MHz, $CDCl_3$) δ -63.71 (s). HRMS (ESI) m/z calcd. for $C_8H_4F_3N_3O_2$ $[M\text{-}N_2]^+$ 231.0251, found 231.0250.

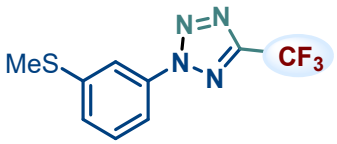


(47)[2] White solid, m.p. 146–148 °C; **^{1}H NMR** (500 MHz, DMSO) δ 8.30-8.24 (m, 4H), 2.68 (s,

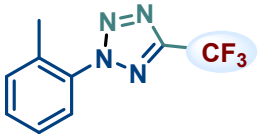
3H). **^{13}C NMR** (150 MHz, DMSO) δ 197.4, 156.7 (q, *J* = 33.8 Hz), 138.9, 138.8, 130.7, 121.3, 119.8 (q, *J* = 223.8 Hz), 27.4. **^{19}F NMR** (565 MHz, DMSO) δ -62.73 (s). HRMS (ESI) m/z calcd. for $C_{10}H_7F_3N_4O$ $[M]^+$ 256.0567, found 256.0568.



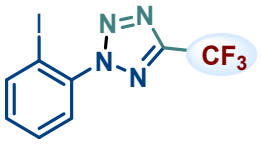
(48)[3] Red oil; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.26-8.23 (m, 2H), 7.47 (d, *J* = 8.5 Hz, 2H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 157.6 (q, *J* = 42.0 Hz), 150.7, 134.3, 122.3, 121.9, 121.2 (q, *J* = 213.8Hz), 119.2 (q, *J* = 268.5 Hz). **^{19}F NMR** (565 MHz, $CDCl_3$) δ -58.00 (s), -63.71 (s). HRMS (ESI) m/z calcd. for $C_{12}H_{13}F_3N_4O$ $[M+H]^+$ 299.0362, found 299.0366.



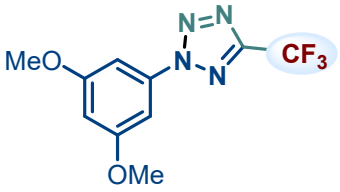
(49) Yellow solid, m.p. 60–62 °C; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.00 (s, 1H), 7.90 (d, *J* = 7.5 Hz, 1H), 7.51 (t, *J* = 8.0 Hz, 1H), 7.72 (d, *J* = 8.0 Hz, 1H), 2.60 (s, 3H) . **^{13}C NMR** (150 MHz, $CDCl_3$) δ 157.3 (q, *J* = 40.5 Hz), 142.1, 136.6, 130.0, 128.2, 119.3 (q, *J* = 270.0 Hz), 117.1, 116.3, 15.4. **^{19}F NMR** (565 MHz, $CDCl_3$) δ -63.60 (s). HRMS (ESI) m/z calcd. for $C_9H_7F_3N_4SNa$ $[M+Na]^+$ 283.0357, found 283.0359.



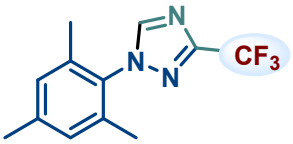
(50)[2] Yellow oil; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.63 (d, *J* = 8.0 Hz, 1H), 7.53 (t, *J* = 7.5 Hz, 1H), 7.45-7.40 (m, 2H), 2.39 (s, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 157.2 (q, *J* = 40.0 Hz), 135.7, 133.1, 132.1, 131.2, 127.1, 125.3, 119.6 (q, *J* = 268.8 Hz), 18.6. **^{19}F NMR** (565 MHz, $CDCl_3$) δ -63.48 (s). HRMS (ESI) m/z calcd. for $C_9H_8F_3N_4$ $[M+H]^+$ 229.0696, found 229.0702.



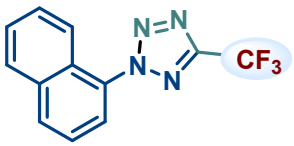
(51)[2] Red solid, m.p. 39–41 °C; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.08-8.07 (m, 1H), 7.61-7.54 (m, 2H), 7.38-7.35 (m, 1H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 157.5 (q, *J* = 37.5 Hz), 140.8, 139.3, 132.9, 129.3, 127.6, 118.4 (q, *J* = 268.8 Hz), 92.3. **^{19}F NMR** (565 MHz, $CDCl_3$) δ -63.42 (s). HRMS (ESI) m/z calcd. for $C_8H_4IF_3N_4$ $[M]^+$ 339.9428, found 339.9435.



(52)[3] White solid, m.p. 87–89 °C; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.27 (d, *J* = 2.0 Hz, 2H), 6.58 (t, *J* = 2.5 Hz, 1H), 3.87 (s, 6H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 161.6, 157.0 (q, *J* = 40.5 Hz), 137.4, 119.3 (q, *J* = 268.5 Hz), 102.9, 98.4, 55.8. **^{19}F NMR** (565 MHz, $CDCl_3$) δ -63.67 (s). HRMS (ESI) m/z calcd. for $C_{10}H_{10}F_3N_4O_2$ $[M+H]^+$ 275.0750, found 275.0750.

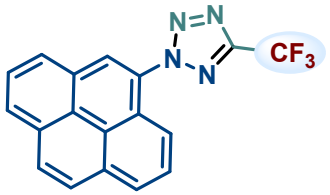


(53)[3] Red oil; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.03 (s, 2H), 2.37 (s, 3H), 1.94 (s, 9H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 157.3 (q, *J* = 40.0 Hz), 141.8, 134.8, 133.0, 129.4, 119.6 (q, *J* = 268.8 Hz), 21.2, 17.2. **^{19}F NMR** (471 MHz, $CDCl_3$) δ -63.47 (s). HRMS (ESI) m/z calcd. for $C_{11}H_{12}F_3N_4$ $[M+H]^+$ 257.1008, found 257.1009.

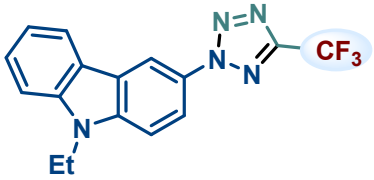


(54)[2] White solid, m.p. 44–45 °C; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.11 (d, *J* = 8.5 Hz, 1H), 8.00-7.99 (m, 1H), 7.94-7.92 (m, 1H), 7.86 (d, *J* = 7.5 Hz, 1H), 7.64-7.61 (m, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 157.3 (q, *J* = 41.3 Hz), 134.2, 132.6, 132.2, 128.7, 128.5, 127.4, 126.6, 124.7,

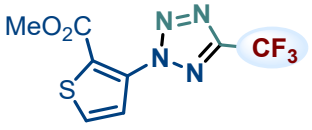
123.7, 122.1, 119.6 (q, J = 268.8 Hz). **^{19}F NMR** (471 MHz, $CDCl_3$) δ -63.34 (s). HRMS (ESI) m/z calcd. for $C_{12}H_7F_3N_4$ $[M]^+$ 264.0618, found 264.0618.



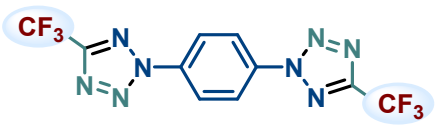
(55) Yellow solid, m.p. 84–86 °C; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.25 (d, J = 8.0 Hz, 2H), 8.21 (t, J = 6.5 Hz, 2H), 8.15-8.13 (m, 3H), 8.07-8.03 (m, 2H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 157.4 (q, J = 41.3 Hz), 133.2, 130.9, 130.5, 130.3, 129.7, 129.0, 126.9, 126.7, 126.5, 124.9, 124.8, 124.6, 123.8, 122.6, 120.5, 118.8 (q, J = 268.8 Hz). **^{19}F NMR** (471 MHz, $CDCl_3$) δ -63.23 (s). HRMS (ESI) m/z calcd. for $C_{18}H_9F_3N_4Na$ $[M+Na]^+$ 361.0735, found 361.0733.



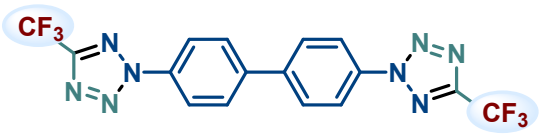
(56) Yellow solid, m.p. 135–137 °C; **^{1}H NMR** (600 MHz, $CDCl_3$) δ 8.75-8.73 (m, 1H), 8.19-8.11 (m, 2H), 7.56-7.53 (m, 1H), 7.48-7.43 (m, 2H), 7.32-7.29 (m, 1H), 4.40-4.36 (m, 2H), 1.49-1.46 (m, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 157.0 (q, J = 40.5 Hz), 140.8, 140.5, 128.4, 127.1, 123.2, 122.4, 120.9, 119.9, 119.6 (q, J = 223.8 Hz), 112.6, 109.1, 109.0, 37.8, 13.7. **^{19}F NMR** (565 MHz, $CDCl_3$) δ -63.41 (s). HRMS (ESI) m/z calcd. for $C_{16}H_{12}F_3N_5Na$ $[M+Na]^+$ 354.0341, found 351.0342.



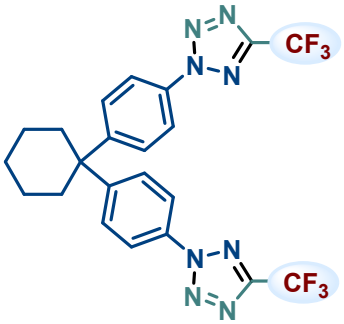
(57)[2] Yellow oil; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.75 (d, J = 5.0 Hz, 1H), 7.39 (d, J = 5.5 Hz, 1H), 3.79 (s, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 159.4, 157.0 (q, J = 40.5 Hz), 135.1, 131.2, 128.8, 126.0, 119.2 (q, J = 268.5 Hz), 52.8. **^{19}F NMR** (565 MHz, $CDCl_3$) δ -63.52 (s). HRMS (ESI) m/z calcd. for $C_8H_6F_3N_4O_2S$ $[M+H]^+$ 279.0158, found 279.0163.



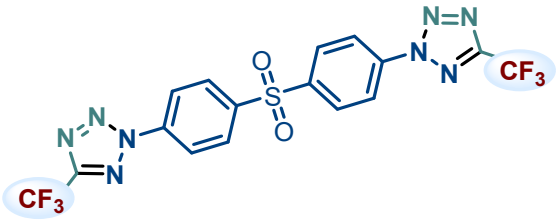
(58) White solid, m.p. 71–73 °C; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.49 (s, 4H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 158.0 (q, J = 42.0 Hz), 137.3, 121.9, 119.1 (q, J = 268.5 Hz). **^{19}F NMR** (565 MHz, $CDCl_3$) δ -63.70 (s). HRMS (ESI) m/z calcd. for $C_{10}H_4F_6N_8Na$ $[M+Na]^+$ 373.0252, found 373.0251.



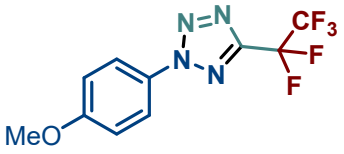
(59) White solid, m.p. 94–96 °C; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.33 (d, J = 9.0 Hz, 4H), 7.89 (d, J = 9.0 Hz, 4H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 157.6 (q, J = 40.0 Hz), 141.8, 136.0, 128.7, 120.9, 119.5 (q, J = 268.8 Hz). **^{19}F NMR** (471 MHz, $CDCl_3$) δ -63.56 (s). HRMS (ESI) m/z calcd. for $C_{16}H_8F_6N_8Na$ $[M+Na]^+$ 449.0766, found 449.0771.



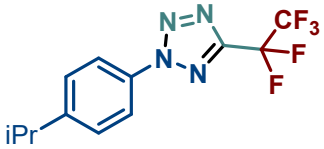
(60) White solid, m.p. 111–113 °C; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.10 (d, J = 9.0 Hz, 4H), 7.54 (d, J = 9.0 Hz, 4H), 2.40-2.38 (m, 4H), 1.66-1.57 (m, 6H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 157.4 (q, J = 40.0 Hz), 151.0, 134.1, 128.7, 120.4, 119.5 (q, J = 268.8 Hz), 46.6, 37.0, 26.0, 22.7. **^{19}F NMR** (565 MHz, $CDCl_3$) δ -63.58 (s). HRMS (ESI) m/z calcd. for $C_{22}H_{18}F_6N_8Na$ $[M+Na]^+$ 531.1578, found 531.1577.



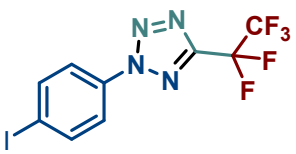
(61) Yellow solid; mp: 138-139 °C; **^{1}H NMR** (600 MHz, DMSO) δ 8.44-8.42 (m, 4H), 8.39-8.36 (m, 4H). **^{13}C NMR** (125 MHz, DMSO) δ 156.7 (q, J = 40.0 Hz), 142.6, 139.6, 130.5, 122.7, 119.1 (q, J = 267.5 Hz). **^{19}F NMR** (565 MHz, DMSO) δ -62.81 (s). HRMS (ESI) m/z calcd. for $C_{16}H_8F_6N_8O_2SNa$ $[M+Na]^+$ 513.0383, found 513.0388.



(62) Colorless oil; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.08-8.06 (m, 2H), 7.08-7.05 (m, 2H), 3.90 (s, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 161.5, 156.2 (t, J = 28.8 Hz), 129.6, 121.8, 119.3 (qt, J = 285.0, 36.3 Hz), 108.8 (tq, J = 252.0, 40.5 Hz), 55.7. **^{19}F NMR** (471 MHz, $CDCl_3$) δ -83.99 (s), -114.68 (s). HRMS (ESI) m/z calcd. for $C_{10}H_7F_5N_4ONa$ $[M+Na]^+$ 317.0118, found 317.0119.

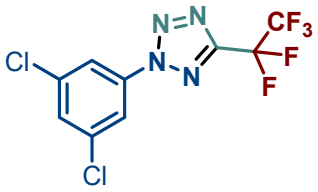


(63) Yelow oil; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.07-8.05 (m, 2H), 7.45-7.43 (m, 2H), 3.05-2.99 (m, 1H), 7.75 (d, J = 7.0 Hz, 6H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 156.4 (t, J = 28.8 Hz), 152.4, 134.1, 127.9, 120.3, 119.4 (qt, J = 285.0, 35.0 Hz), 108.8 (tq, J = 253.8, 40.0 Hz), 34.0, 23.7. **^{19}F NMR** (471 MHz, $CDCl_3$) δ -84.05 (s), -114.75 (s). HRMS (ESI) m/z calcd. for $C_{12}H_{11}F_5N_4Na$ $[M+Na]^+$ 329.0934, found 329.0932.

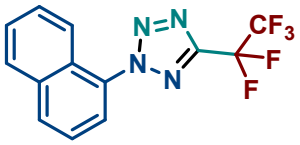


(64) Red oil; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.97-7.92 (m, 4H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ

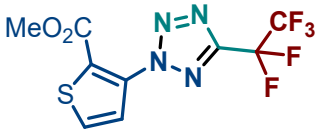
156.7 (t, J = 28.5 Hz), 139.2, 135.7, 121.7, 119.1 (qt, J = 285.0, 36.0 Hz), 108.6 (tq, J = 253.5, 40.5 Hz), 96.7. **^{19}F NMR** (565 MHz, $CDCl_3$) δ -83.91 (s), -114.72 (s). HRMS (ESI) m/z calcd. for $C_9H_4F_5IN_4Na$ $[M+Na]^+$ 412.9433, found 412.9436.



(65) White solid, m.p. 56–57 °C; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.69 (d, J = 2.5 Hz, 1H), 7.65 (d, J = 8.5 Hz, 1H), 7.52 (dd, J = 8.5 Hz, J = 2.0 Hz, 1H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 156.7 (t, J = 30.0 Hz), 138.6, 132.7, 131.3, 130.1, 128.3, 128.3, 119.3 (qt, J = 283.8, 35.0 Hz), 108.6 (tq, J = 253.8, 41.3 Hz). **^{19}F NMR** (471 MHz, $CDCl_3$) δ -84.02 (s), -114.70 (s). HRMS (ESI) m/z calcd. for $C_9H_3Cl_2F_5N_4Na$ $[M+Na]^+$ 354.9642, found 354.9646.

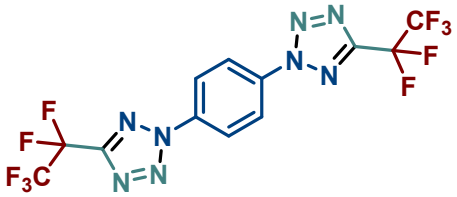


(66) White solid, m.p. 41–42 °C; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.13 (d, J = 8.5 Hz, 1H), 8.02-7.99 (m, 1H), 7.95-7.90 (m, 1H), 7.90 (dd, J = 7.5 Hz, J = 1.5 Hz, 1H), 7.67-7.63 (m, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 156.6 (t, J = 30.0 Hz), 134.2, 132.5, 132.2, 128.7, 128.5, 127.4, 126.6, 124.7, 123.7, 122.0, 119.4 (qt, J = 285.0, 35.0 Hz), 108.8 (tq, J = 253.8, 40.0 Hz). **^{19}F NMR** (565 MHz, $CDCl_3$) δ -83.83 (s), -114.43 (s). HRMS (ESI) m/z calcd. for $C_{13}H_7F_5N_4Na$ $[M+Na]^+$ 337.0297, found 337.0293.

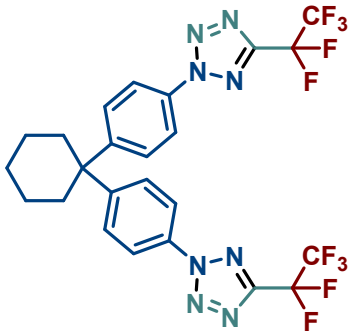


(67) Yellow oil; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.74 (d, J = 5.5 Hz, 1H), 7.40 (d, J = 5.5 Hz, 1H), 3.77 (s, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 159.5, 156.3 (t, J = 28.5 Hz), 135.0, 131.2, 129.2, 126.0, 119.1 (qt, J = 283.5, 36.0 Hz), 108.6 (tq, J = 255.0, 40.5 Hz). **^{19}F NMR** (565 MHz, $CDCl_3$) δ -88.79 (s), -119.52 (s). HRMS (ESI) m/z calcd. for $C_9H_5F_5N_4O_2SNa$ $[M+Na]^+$ 351.0071, found

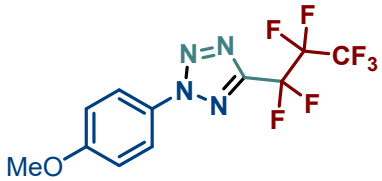
351.0072.



(68) White solid; mp: 53-54 °C; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.50 (s, 4H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 157.1 (t, J = 30.0 Hz), 137.3, 121.9, 119.2 (qt, J = 285.0, 35.0 Hz), 108.6 (tq, J = 253.8, 41.3 Hz). **^{19}F NMR** (565 MHz, $CDCl_3$) δ -83.86 (s), -114.76 (s). HRMS (ESI) m/z calcd. for $C_{12}H_4F_{10}N_8Na$ $[M+Na]^+$ 473.0392, found 473.0390.

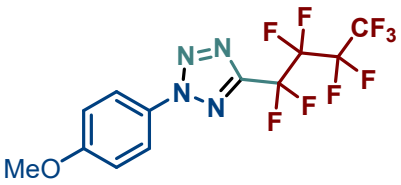


(69) White solid, m.p. 92–93 °C; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.13 (d, *J* = 9.0 Hz, 4H), 7.58 (d, *J* = 9.0 Hz, 4H), 2.43-2.41 (m, 4H), 1.68-1.58 (m, 6H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 156.5 (t, J = 28.5 Hz), 151.1, 134.0, 128.7, 120.4, 119.1 (qt, J = 285.0, 34.5 Hz), 108.7 (tq, J = 253.5, 40.5 Hz), 46.6, 36.9, 25.9, 22.7. **^{19}F NMR** (565 MHz, $CDCl_3$) δ -84.09 (s), -114.82 (s). HRMS (ESI) m/z calcd. for $C_{24}H_{18}F_{10}N_8Na$ $[M+Na]^+$ 631.1488, found 631.1485.

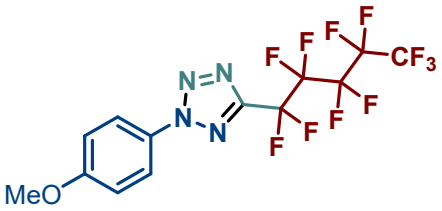


(70) Colorless oil; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.08-8.05 (m, 2H), 7.07-7.04 (m, 2H), 3.89 (s, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 161.5, 156.3 (t, *J* = 28.5 Hz), 129.6, 121.8, 118.6 (qt, *J* = 286.5, 33.0 Hz), 114.9, 110.6 (tt, *J* = 256.5, 31.5 Hz), 110.2-106.2 (m), 55.7. **^{19}F NMR** (565 MHz, $CDCl_3$) δ -80.16 (t, *J* = 7.9 Hz), (-112.53)-(-112.58) (m), -126.66 (s). HRMS (ESI) m/z calcd. for

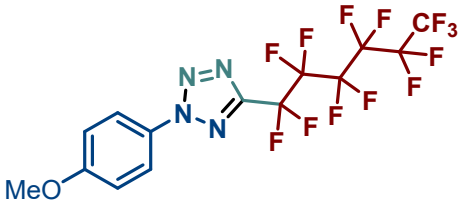
$C_{11}H_7F_7N_4ONa$ $[M+Na]^+$ 367.0546, found 367.0549.



(71) Colorless oil; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.10-8.07 (m, 2H), 7.09-7.05 (m, 2H), 3.90 (s, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 161.6, 156.5 (t, *J* = 28.5 Hz), 129.6, 121.8, 118.3 (qt, *J* = 286.5, 33.0 Hz), 114.9, 110.2 (tt, *J* = 256.5, 33.0 Hz), 109.8-106.6 (m), 55.6. **^{19}F NMR** (565 MHz, $CDCl_3$) δ (-80.97)-(-81.01) (m), (-111.80)-(-111.84) (m), (-123.07)-(-113.12) (m), (-125.65)-(-125.68) (m). HRMS (ESI) m/z calcd. for $C_{12}H_7F_9N_4ONa$ $[M+Na]^+$ 417.0489, found 417.0488.

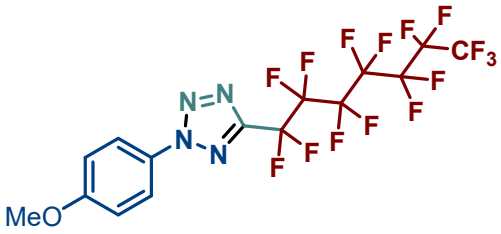


(72) Colorless oil; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.07-8.05 (m, 2H), 7.06-7.04 (m, 2H), 3.88 (s, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 161.6, 156.5 (t, *J* = 28.8 Hz), 129.6, 121.8, 118.4 (qt, *J* = 286.3, 32.5 Hz), 114.1-108.3 (m), 55.6. **^{19}F NMR** (471 MHz, $CDCl_3$) δ (-81.09)-(-81.13) (m), (-111.81)-(-111.87) (m), (-122.45)-(-122.58) (m), (-126.37)-(-126.45) (m). HRMS (ESI) m/z calcd. for $C_{13}H_7F_{11}N_4ONa$ $[M+Na]^+$ 467.0355, found 467.0353.

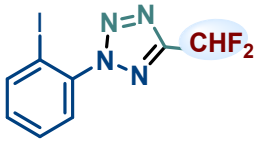


(73) Colorless oil; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.09-8.07 (m, 2H), 7.07-7.06 (m, 2H), 3.90 (s, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 161.6, 156.6 (t, *J* = 28.5 Hz), 129.7, 121.8, 118.2 (qt, *J* = 286.5, 33.0 Hz), 113.2-108.0 (m), 55.6. **^{19}F NMR** (565 MHz, $CDCl_3$) δ (-81.01)-(-81.05) (m), (-111.70)-(-111.75) (m), (-121.58)-(-121.62) (m), (-122.27)-(-122.31) (m), (-122.87)-(-122.90) (m), (-126.23)-(-126.29) (m). HRMS (ESI) m/z calcd. for $C_{14}H_7F_{13}N_4ONa$ $[M+Na]^+$ 517.0438, found

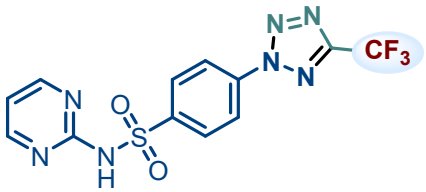
517.0441.



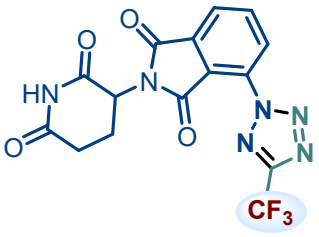
(74) Colorless oil; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.08-8.04 (m, 2H), 7.06-7.03 (m, 2H), 3.88 (s, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 161.6, 156.6 (t, *J* = 28.8 Hz), 129.7, 121.8, 118.3 (qt, *J* = 286.3, 32.5 Hz), 113.8-108.1 (m), 55.6. **^{19}F NMR** (471 MHz, $CDCl_3$) δ (-81.18)-(-81.22) (m), (-111.80)-(-111.85) (m), (-121.47)-(-121.59) (m), (-122.15)-(-122.37) (m), (-122.89)-(-122.98) (m), (-126.37)-(-126.45) (m). HRMS (ESI) m/z calcd. for $C_{15}H_7F_{15}N_4ONa$ $[M+Na]^+$ 567.0395, found 567.0391.



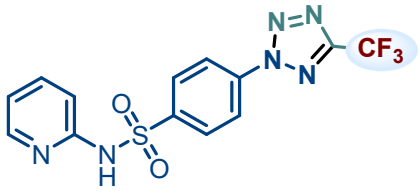
(75) Red oil; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.08 (dd, *J* = 8.0 Hz, 1.5 Hz, 1H), 7.60-7.53 (m, 2H), 7.37 (td, *J* = 7.0 Hz, 1.5 Hz, 1H), 7.08 (t, *J* = 53.0 Hz, 1H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 160.2 (t, *J* = 27.5 Hz), 140.8, 139.6, 132.7, 129.2, 127.6, 107.5 (t, *J* = 237.5 Hz), 92.4. **^{19}F NMR** (471 MHz, $CDCl_3$) δ -117.05 (d, *J* = 53.2 Hz). HRMS (ESI) m/z calcd. for $C_8H_5F_2IN_4Na$ $[M+Na]^+$ 344.9545, found 344.9546.



(76) Yellow solid; mp: 147-149 °C; **^{1}H NMR** (600 MHz, DMSO) δ 12.29 (s, 1H), 8.53 (d, *J* = 5.0 Hz, 2H), 8.37 (d, *J* = 8.5 Hz, 2H), 8.29 (d, *J* = 8.5 Hz, 2H), 7.06 (d, *J* = 5.0 Hz, 1H). **^{13}C NMR** (125 MHz, DMSO) δ 158.9, 157.4, 156.7 (q, *J* = 40.0 Hz), 143.3, 138.6, 130.2, 121.6, 119.9 (q, *J* = 267.5 Hz), 116.0. **^{19}F NMR** (565 MHz, DMSO) δ -62.80 (s). HRMS (ESI) m/z calcd. for $C_{12}H_8F_3N_7O_2SNa$ $[M+Na]^+$ 394.0483, found 394.0484.



(77) White solid; mp: 125-126 °C; **^{1}H NMR** (500 MHz, DMSO) δ 11.15 (s, 1H), 8.32 (t, *J* = 8.5 Hz, 2H), 8.23 (t, *J* = 7.5 Hz, 1H), 5.18 (dd, *J* = 13.0 Hz, *J* = 5.5 Hz, 1H), 2.90-2.83 (m, 1H), 2.62-2.58 (m, 1H), 2.53-2.44 (m, 2H), 2.09-2.05 (m, 1H). **^{13}C NMR** (150 MHz, DMSO) δ 173.2, 170.0, 166.0, 163.9, 156.6 (q, *J* = 40.5 Hz), 137.4, 133.6, 132.5, 130.9, 127.4, 125.7, 119.8 (q, *J* = 268.5 Hz), 49.9, 31.4, 22.2. **^{19}F NMR** (565 MHz, DMSO) δ -62.69 (s). HRMS (ESI) m/z calcd. for $C_{15}H_9F_3N_6O_4Na$ $[M+Na]^+$ 417.0736, found 417.0735.



(78) White solid; mp: 136-137 °C; **^{1}H NMR** (600 MHz, DMSO) δ 12.76 (s, 1H), 8.32 (d, *J* = 9.0 Hz, 2H), 8.18 (d, *J* = 9.0 Hz, 2H), 7.97 (d, *J* = 4.8 Hz, 1H), 7.82-7.79 (m, 1H), 7.28 (d, *J* = 9.0 Hz, 1H), 6.87 (d, *J* = 6.6 Hz, 1H). **^{13}C NMR** (150 MHz, DMSO) δ 156.6 (q, *J* = 40.0 Hz), 154.5, 145.6, 142.4, 138.0, 129.4, 129.0, 127.0, 121.8, 119.8 (q, *J* = 268.0 Hz), 115.4. **^{19}F NMR** (565 MHz, DMSO) δ -62.81 (s). HRMS (ESI) m/z calcd. for $C_{13}H_9F_3N_6O_2SNa$ $[M+Na]^+$ 393.0710, found 393.0711.

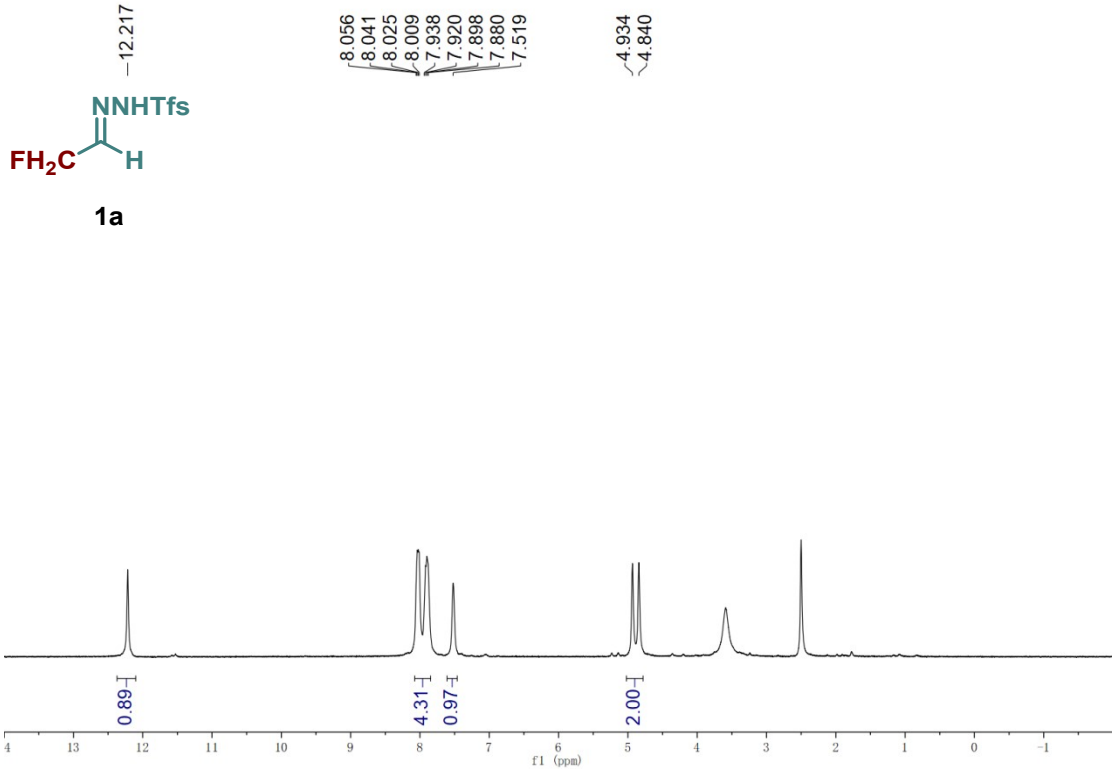
V. References

[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. Int. Ed*. **2020**, *132*, 6535-6543; c) Y. Ning, H. Wang, P. Sivaguru, S. Li, G. Zanoni, S. P. Nolan, X. Bi, *Green Chem.* **2021**, *23*, 7976-7981.

[2] Z Chen, S Q Fan, Y Zheng, J A Ma, *Chem. Commun.* **2015**, *51*, 16545-16548.

[3] X Lin, B Luo, W He, Q Lu, L Li, H Zheng, W Wu, and Z Weng, *Tetrahedron Lett.* **2022**, *95*, 153717.

VI. Copies of NMR spectra



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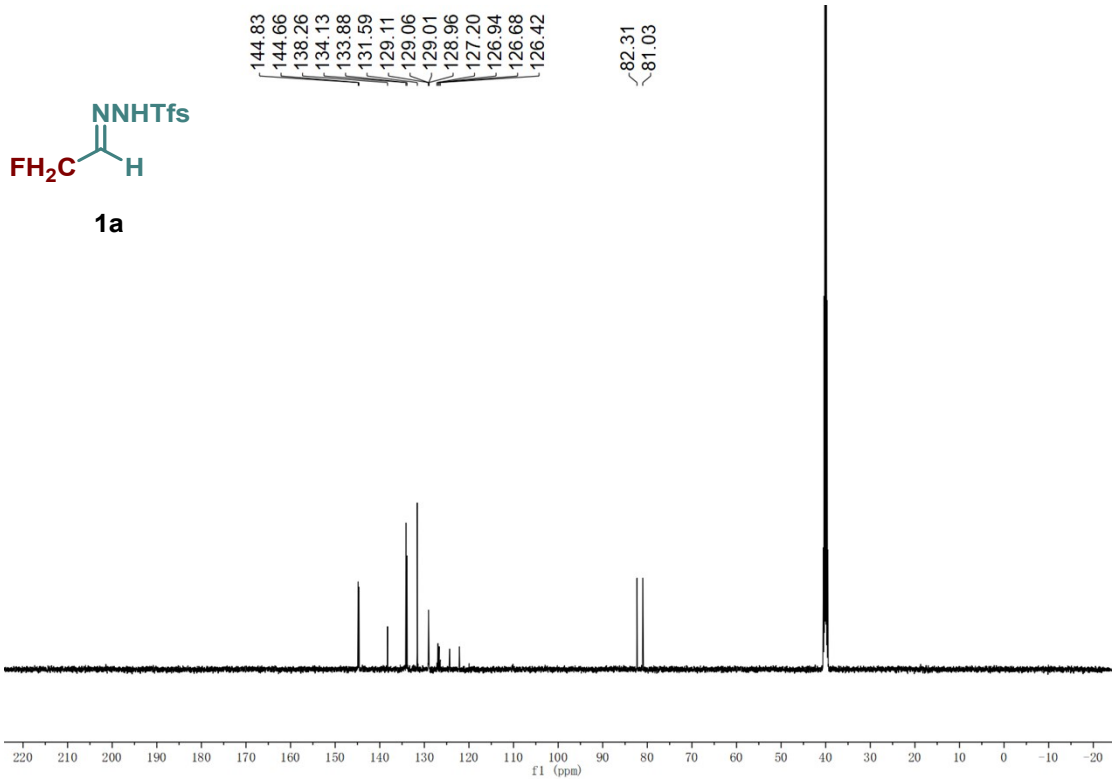

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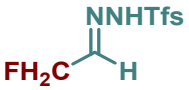
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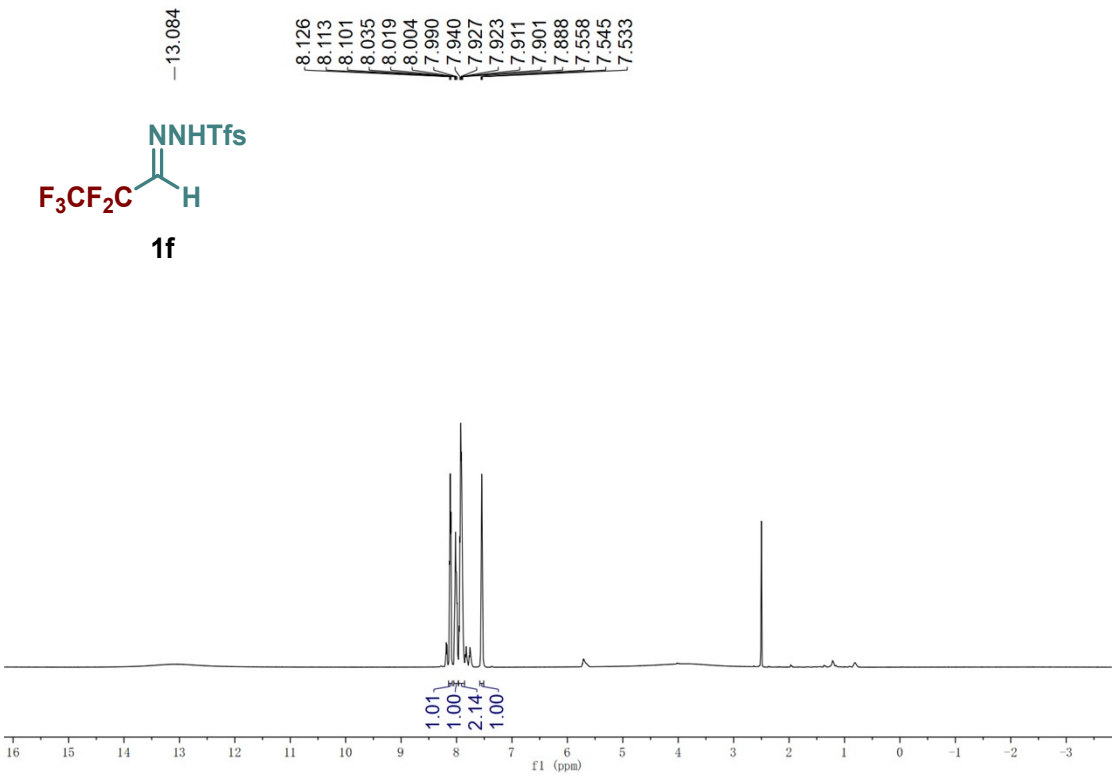
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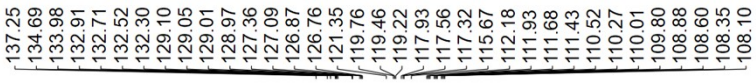
1.00
f1 (ppm)

NNHTfs
F3CF2C
H

1f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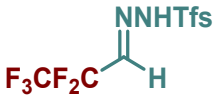
108.10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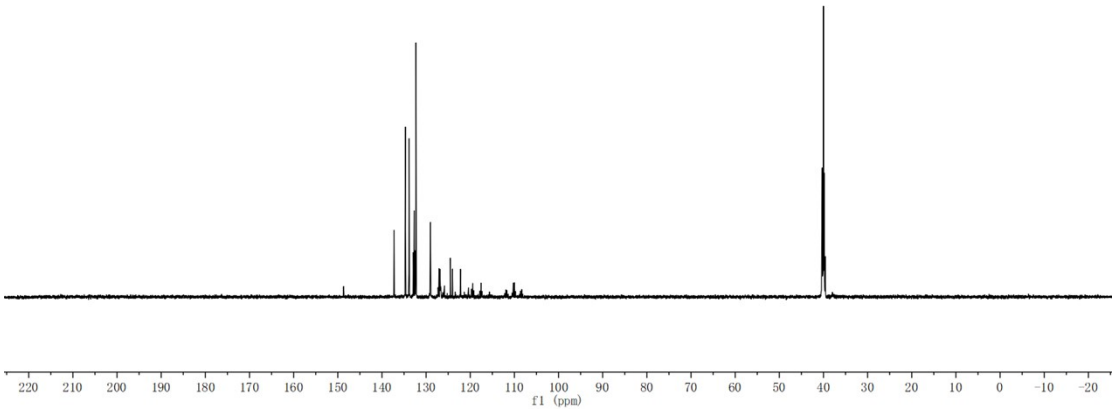
H

1f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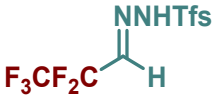
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F3CF2C
H

1f

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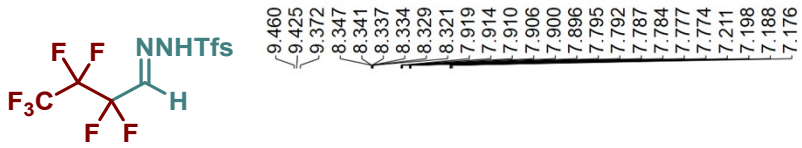
f1 (ppm)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H
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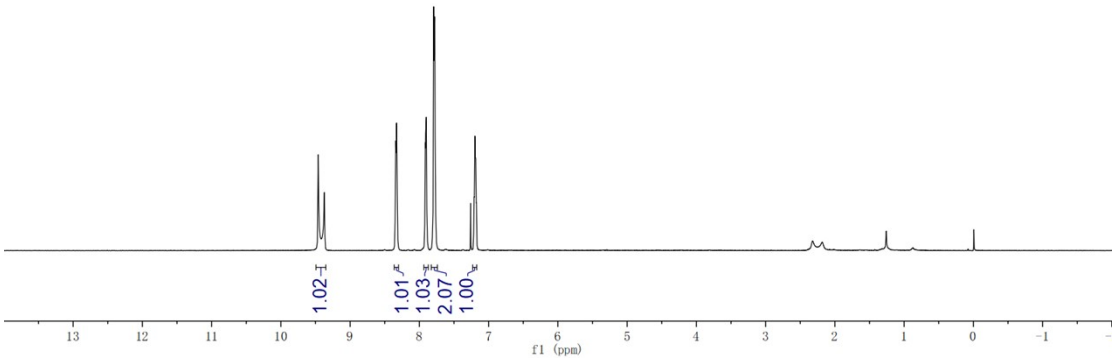
1g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f1 (ppm)


F F
NNHTfs
F3C
H
F F
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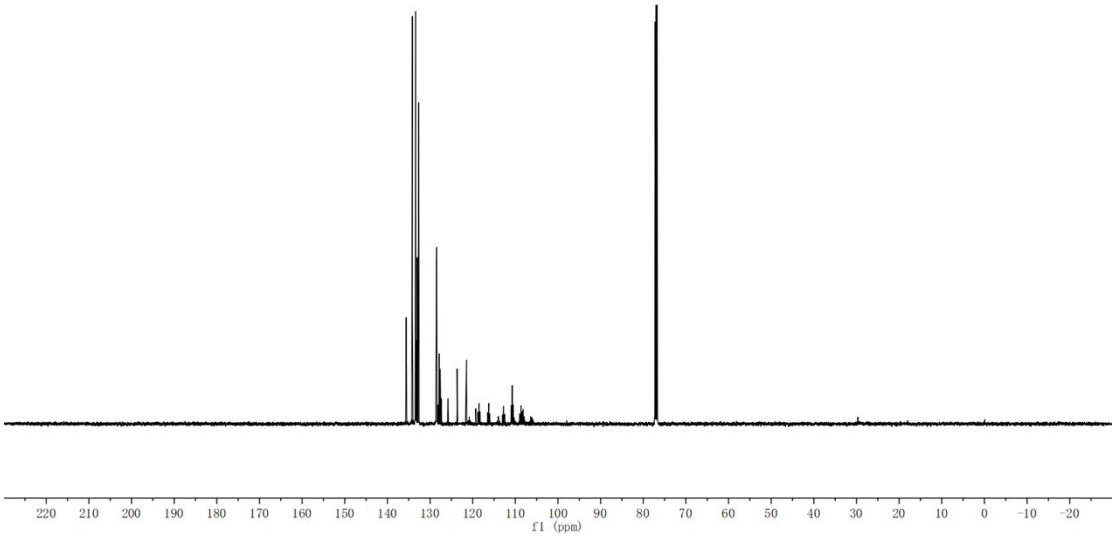
1g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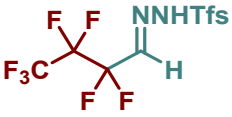
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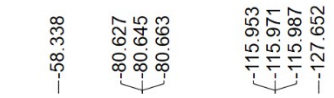
F3C
H
F F

1g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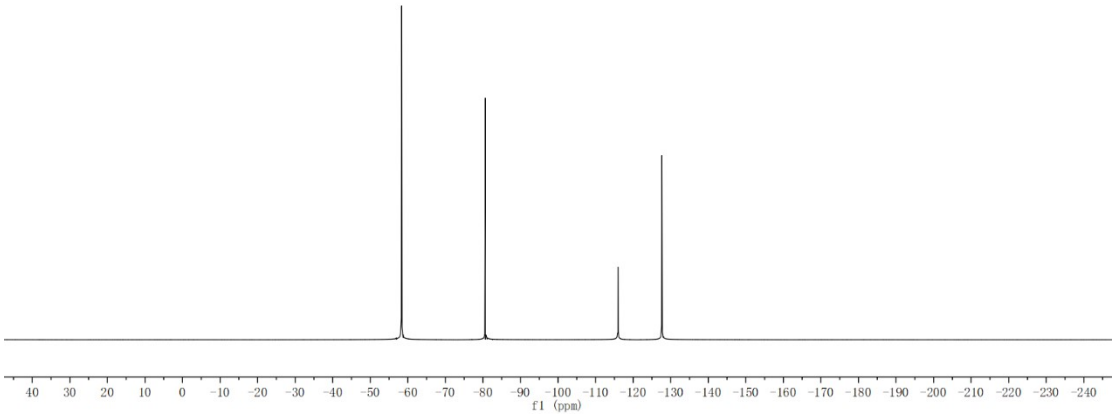
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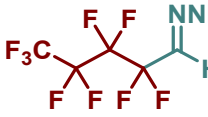
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F3C
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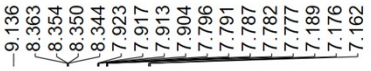
F F F F

1h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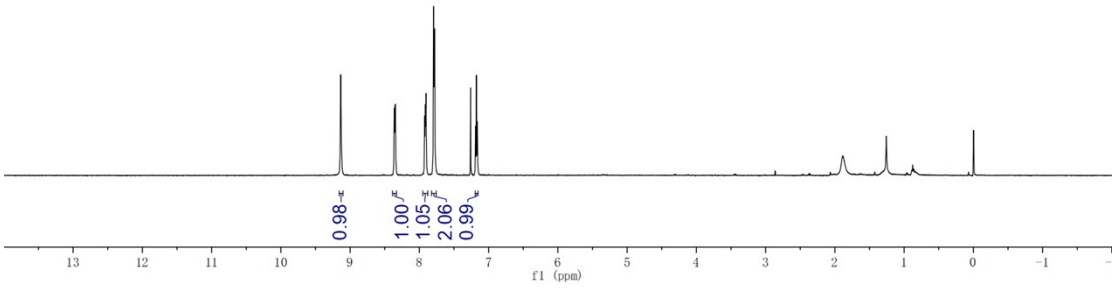
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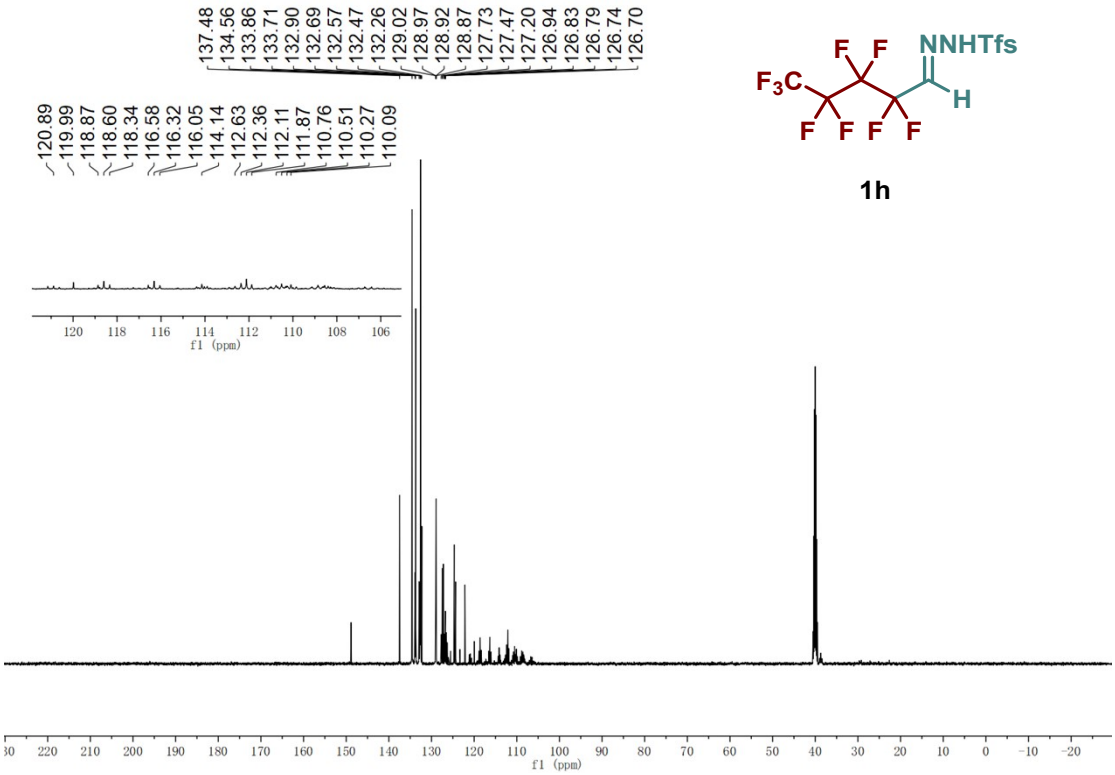
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f1 (ppm)
f1 (ppm)

F F
NNHTfs
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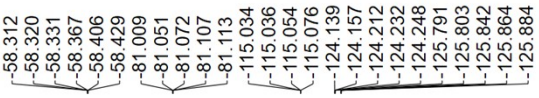
H
F F F F

1h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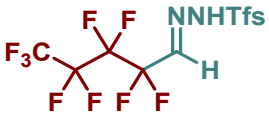
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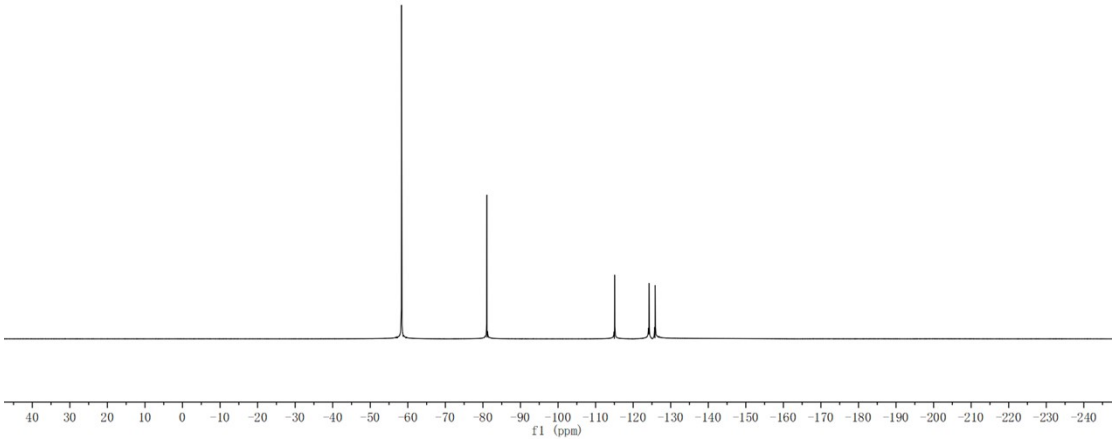
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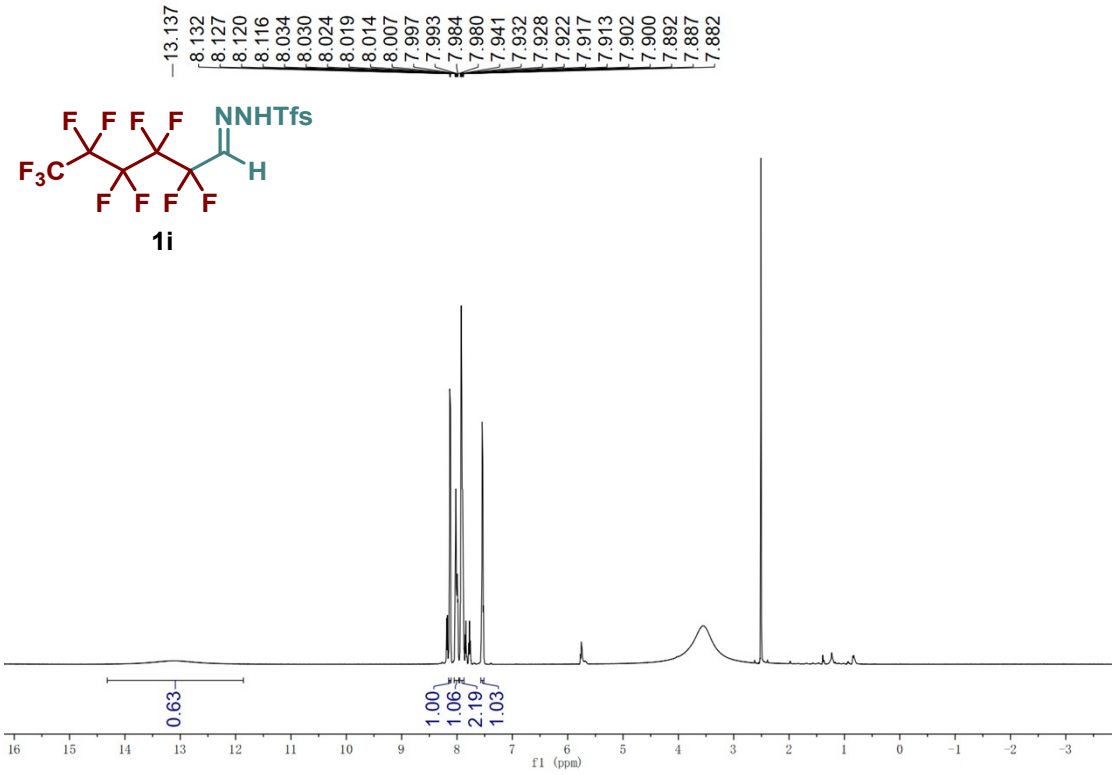
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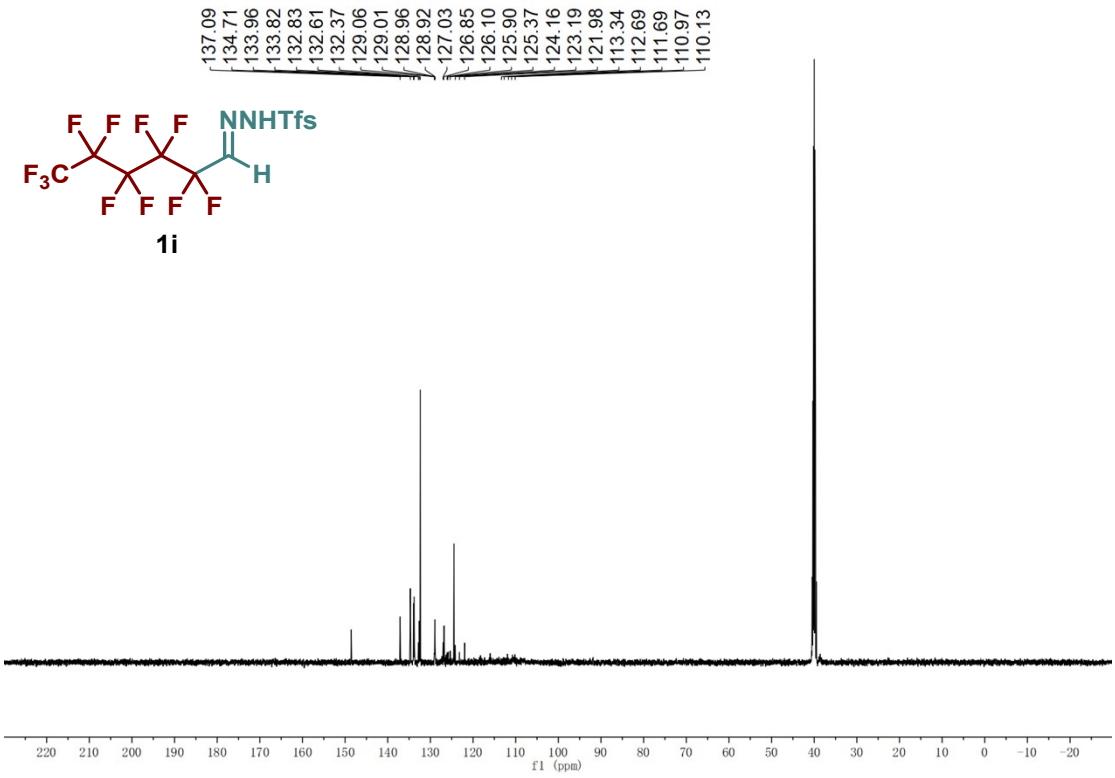
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113.34
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111.69
110.97
110.13
F F F F
NNHTfs
F3C
H
F F F F
1i
f1 (ppm)


F F F F
NNHTfs
F3C
H
F F F F

1i

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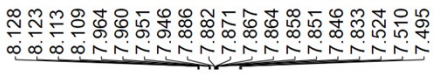
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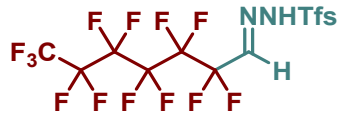
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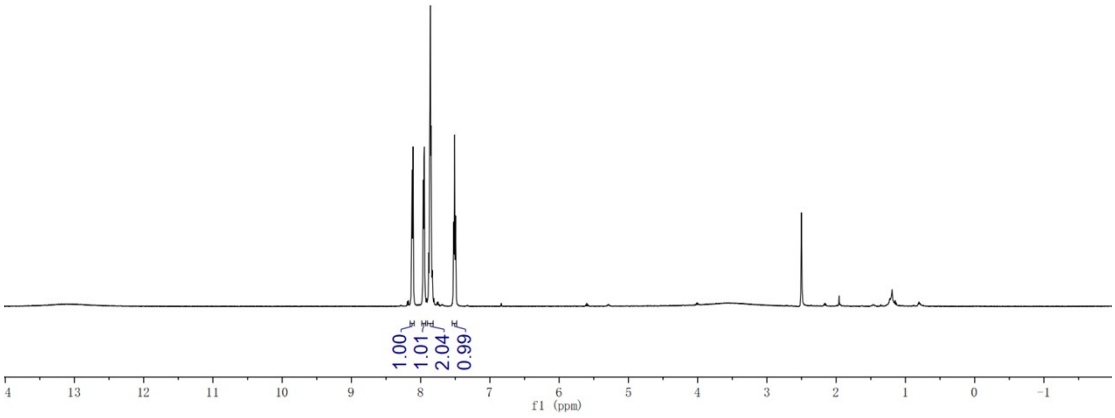
F F F F F F

1j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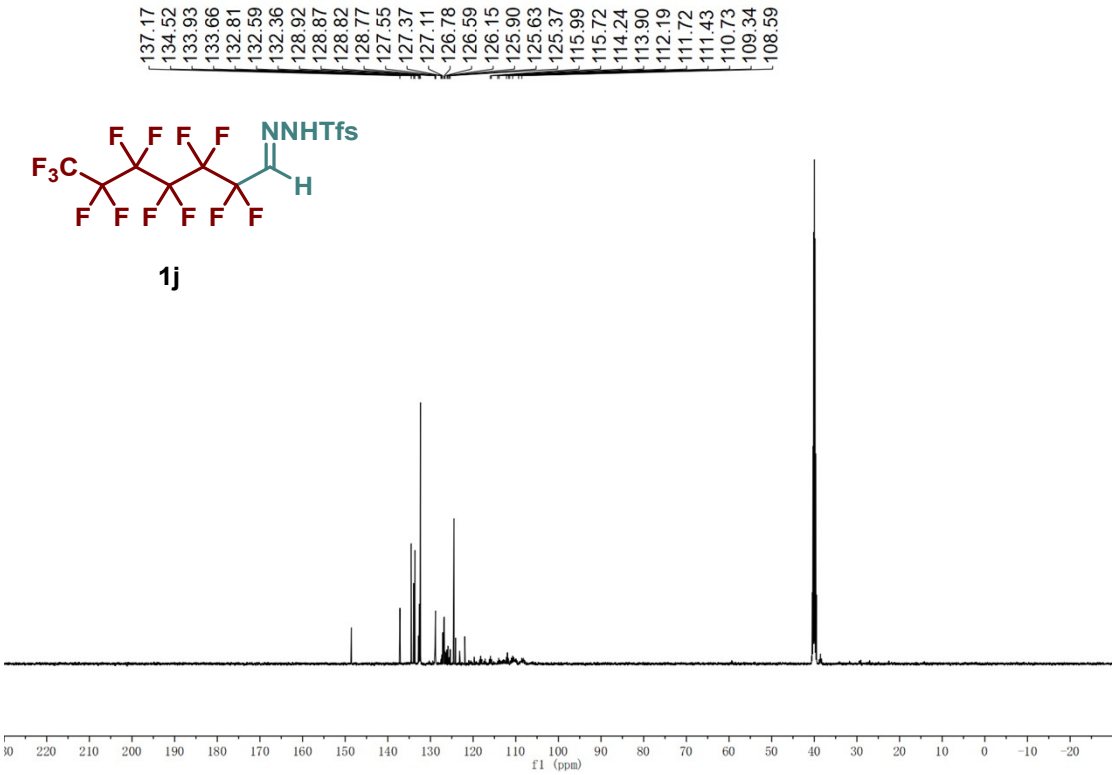
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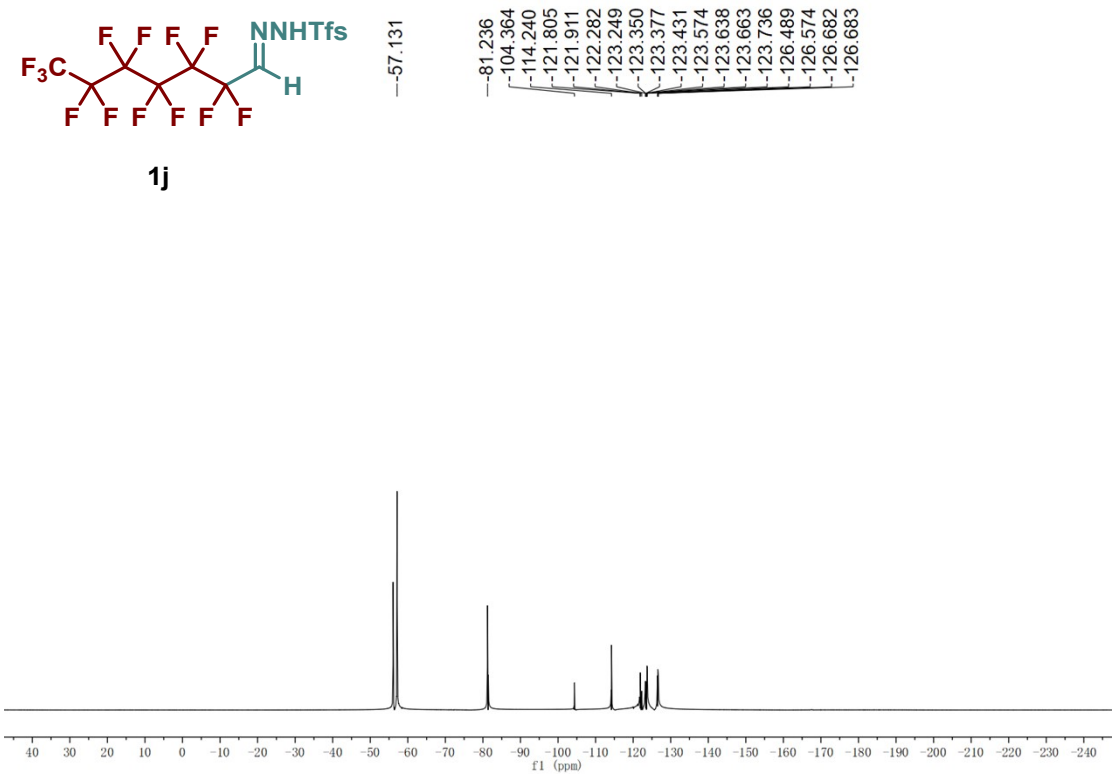
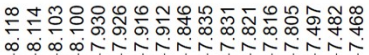
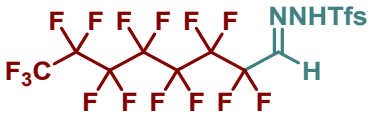
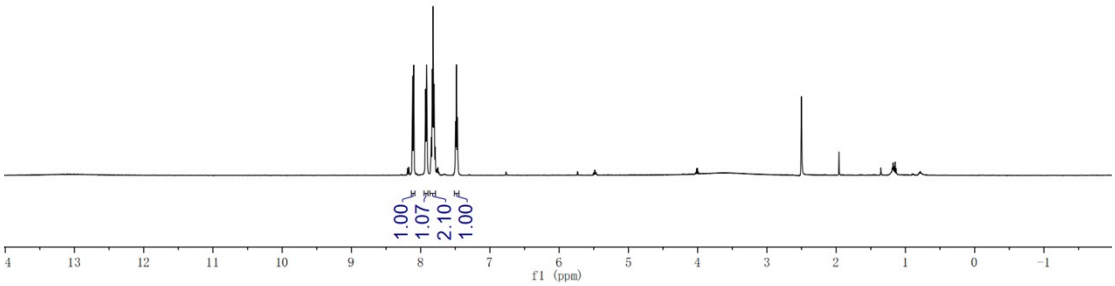
112.19
111.72
111.43
110.73
109.34
108.59
F F F F NNHTfs
F3C
F F F F F F H
1j
f1 (ppm)

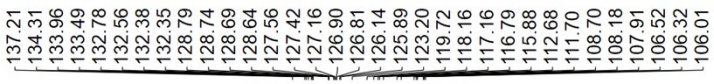

F F F F NNHTfs
F3C
F F F F F F H
1j
-57.131
-81.236
-104.364
-114.240
-121.805
-121.911
-122.282
-123.249
-123.350
-123.377
-123.431
-123.574
-123.638
-123.663
-123.736
-126.489
-126.574
-126.682
-126.683
f1 (ppm)

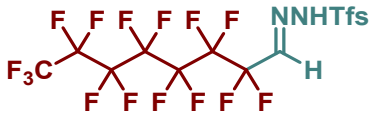

8.118
8.114
8.103
8.100
7.930
7.926
7.916
7.912
7.846
7.835
7.831
7.821
7.816
7.805
7.497
7.482
7.468


F F F F F F
NNHTfs
F3C
H
F F F F F F

1k

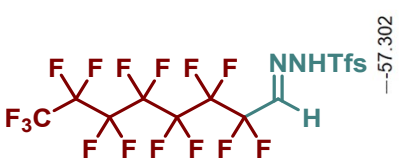

1.00
1.07
2.10
1.00
4 13 12 11 10 9 8 7 6 5 4 3 2 1 0 −1
f1 (ppm)

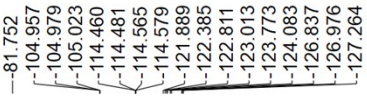

137.21
134.31
133.96
133.49
132.78
132.56
132.38
132.35
128.79
128.74
128.69
128.64
127.56
127.42
127.16
126.90
126.81
126.14
125.89
123.20
119.72
118.16
117.16
116.79
115.88
112.68
111.70
108.70
108.18
107.91
106.52
106.32
106.01


F F F F F F
NNHTfs
F3C
H
F F F F F F

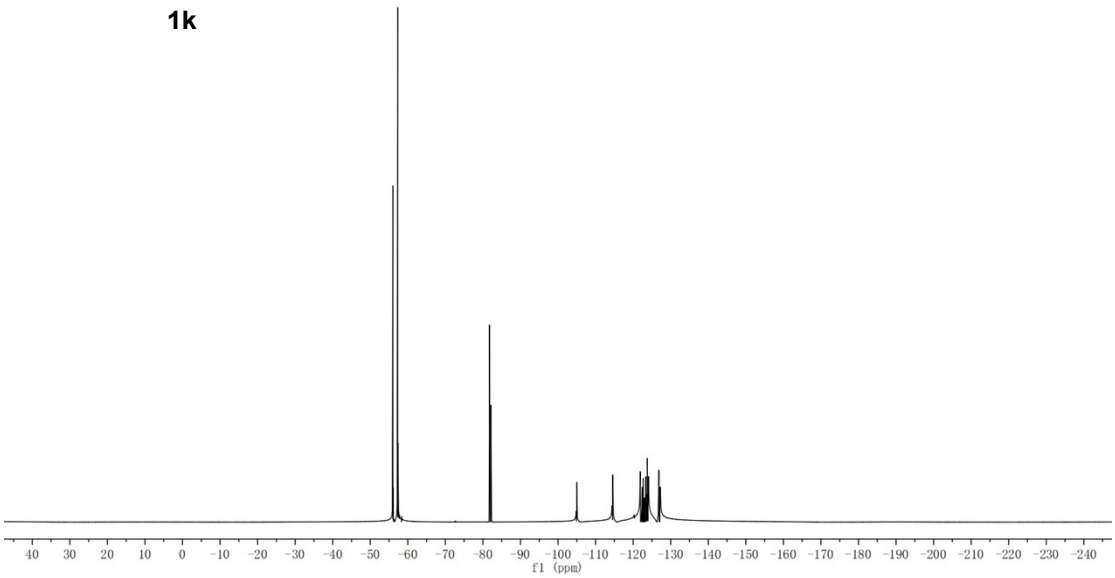
1k

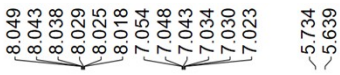
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10 −20 −30
f1 (ppm)

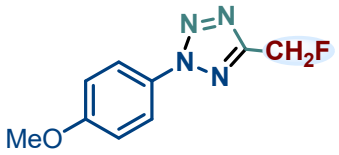

F F F F F F
NNHTfs
F3C
H
F F F F F F


81.752
104.957
104.979
105.023
114.460
114.481
114.565
114.579
121.889
122.385
122.811
123.013
123.773
124.083
126.837
126.976
127.264
57.302

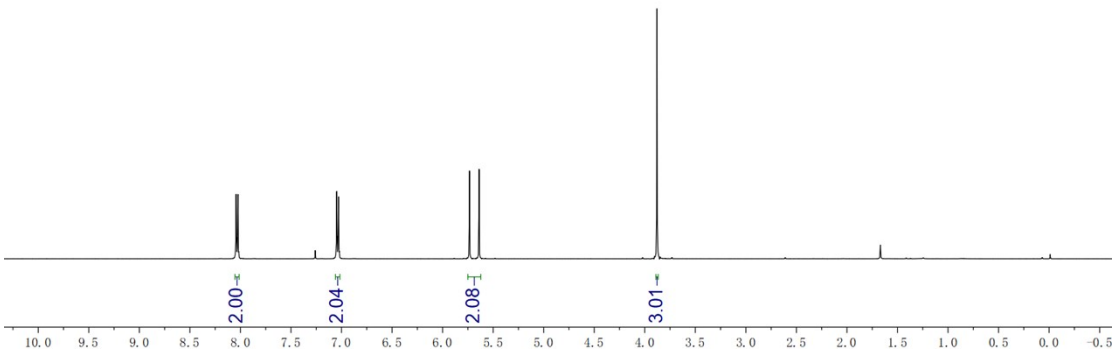
1k

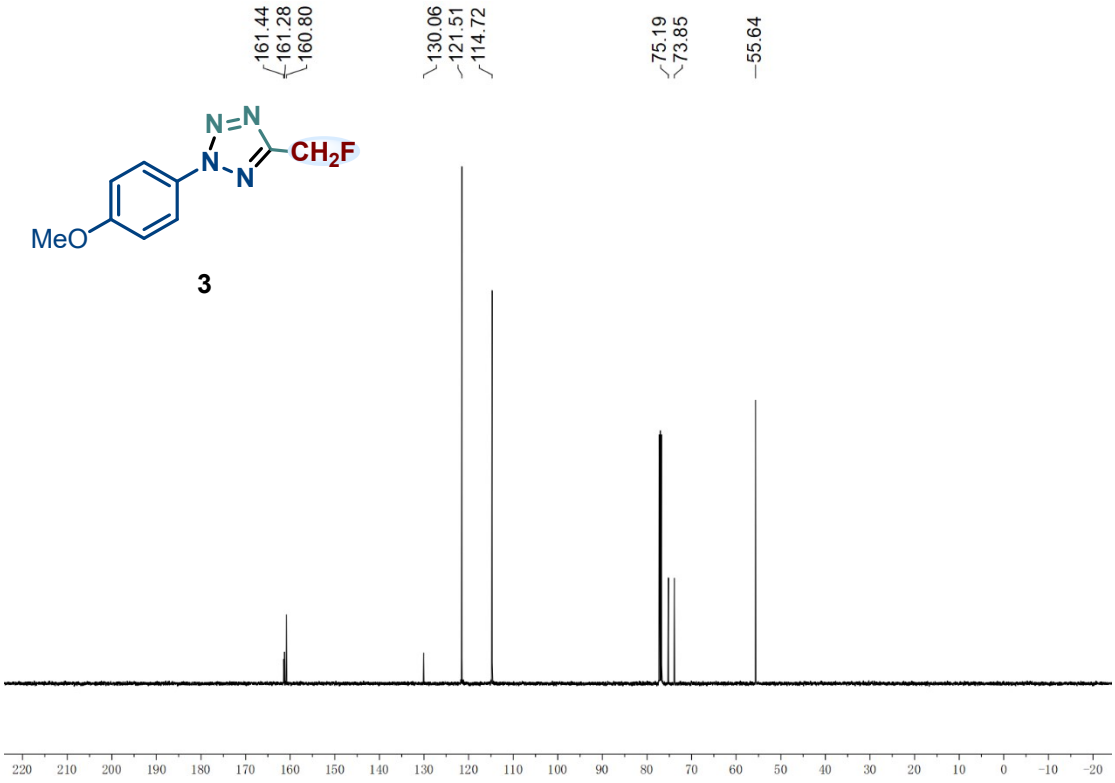

40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -220 -230 -240
f1 (ppm)


8.049
8.043
8.038
8.029
8.025
8.018
7.054
7.048
7.043
7.034
7.030
7.023
5.734
5.639
3.879

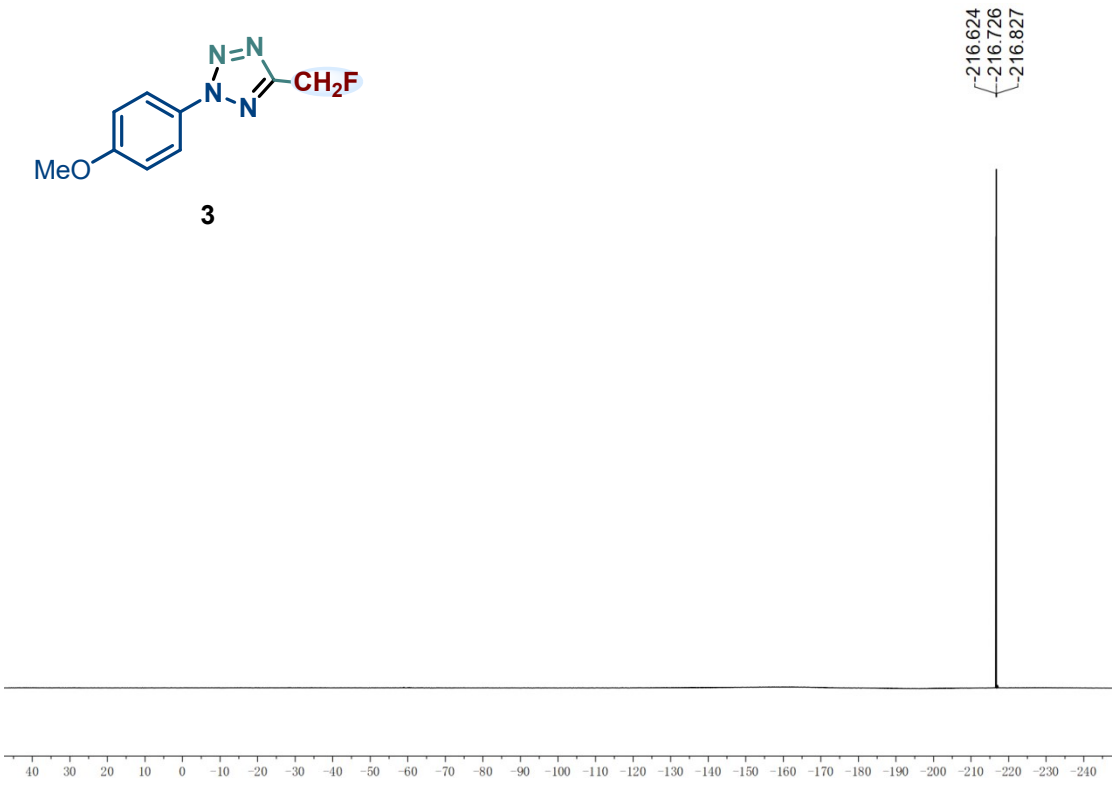

N=N
N
N
CH2F
MeO

3

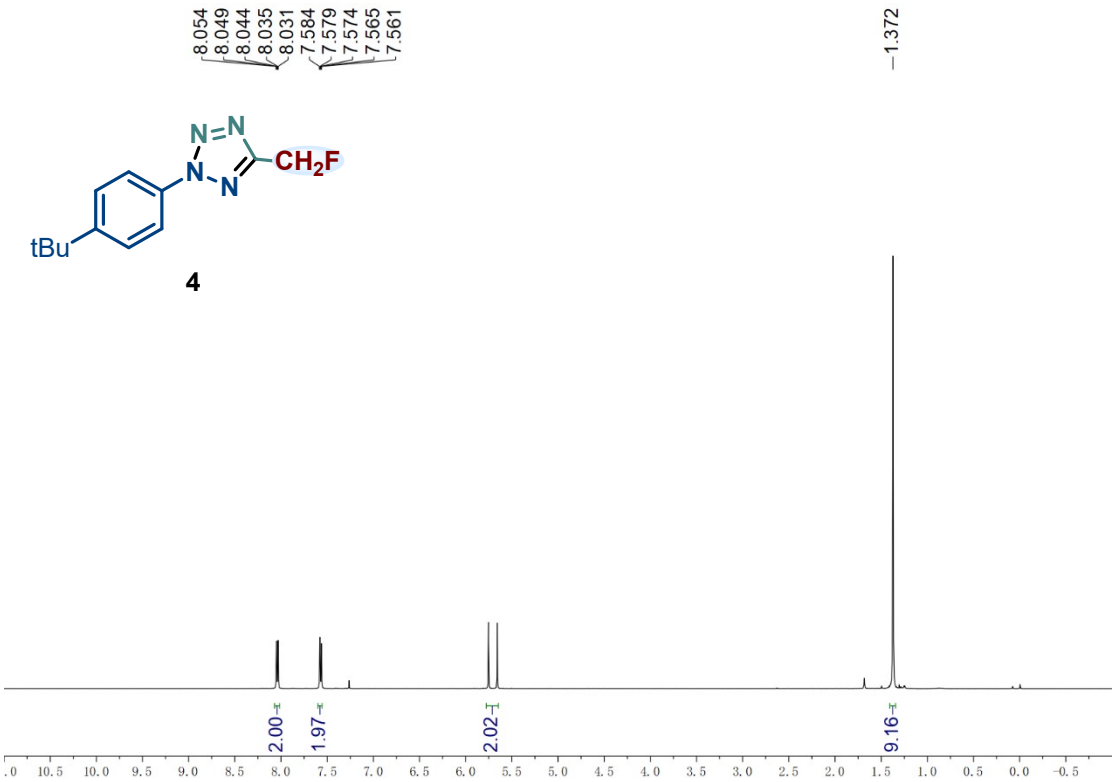

2.00
2.04
2.08
3.01
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5

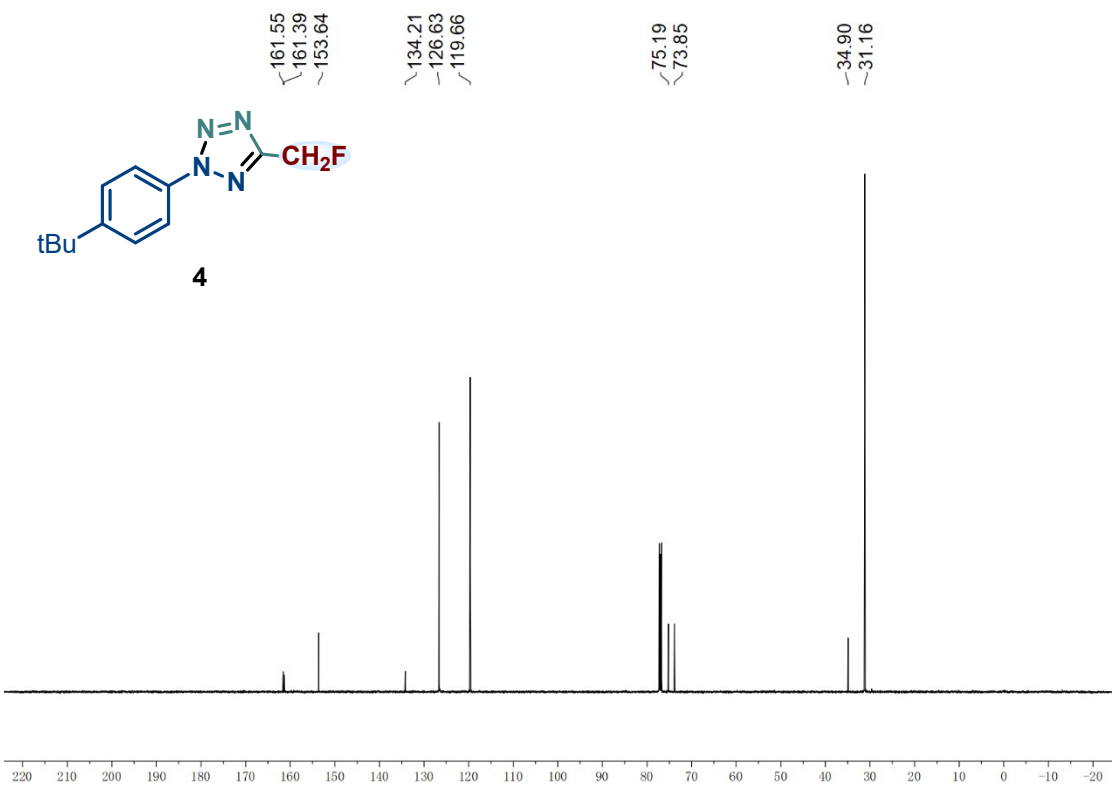

161.44
161.28
160.80
130.06
121.51
114.72
75.19
73.85
55.64
N=N
N
N
CH2F
MeO
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20

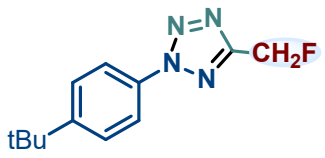
3


216.624
216.726
216.827
N=N
N
N
CH2F
MeO
40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -220 -230 -240

3

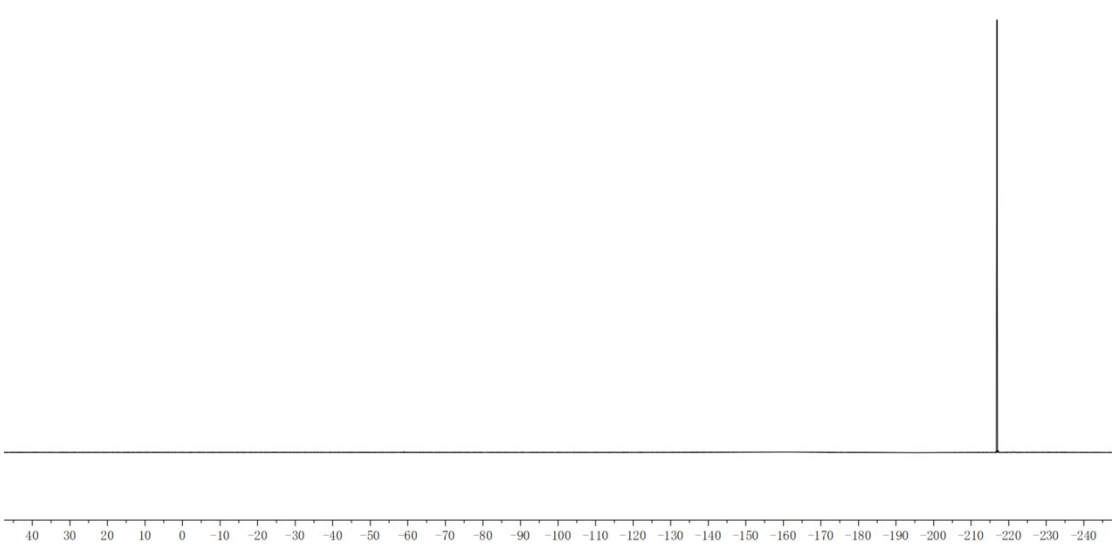

8.054
8.049
8.044
8.035
8.031
7.584
7.579
7.574
7.565
7.561
1.372
N=N
N
N
N
CH2F
tBu
4
2.00
1.97
2.02
9.16

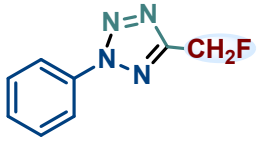

161.55
161.39
153.64
134.21
126.63
119.66
75.19
73.85
34.90
31.16
N=N
N
N
N
CH2F
tBu
4


N=N
N
N
CH2F
tBu

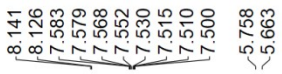
4

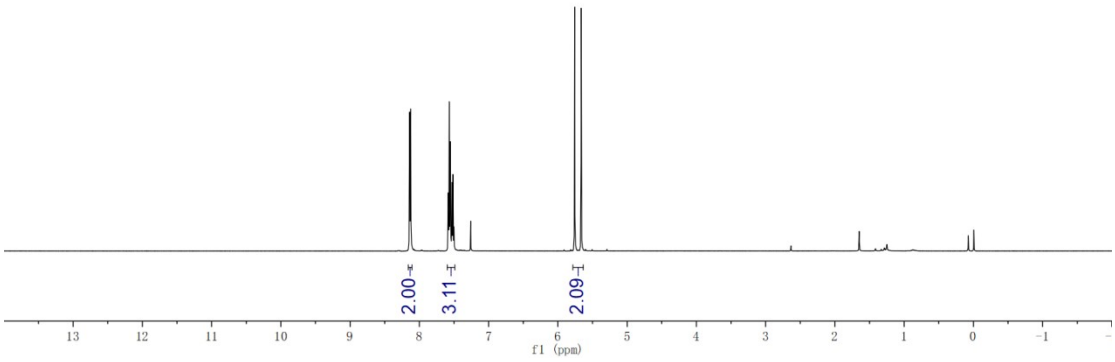

-216.773
-216.874
-216.972

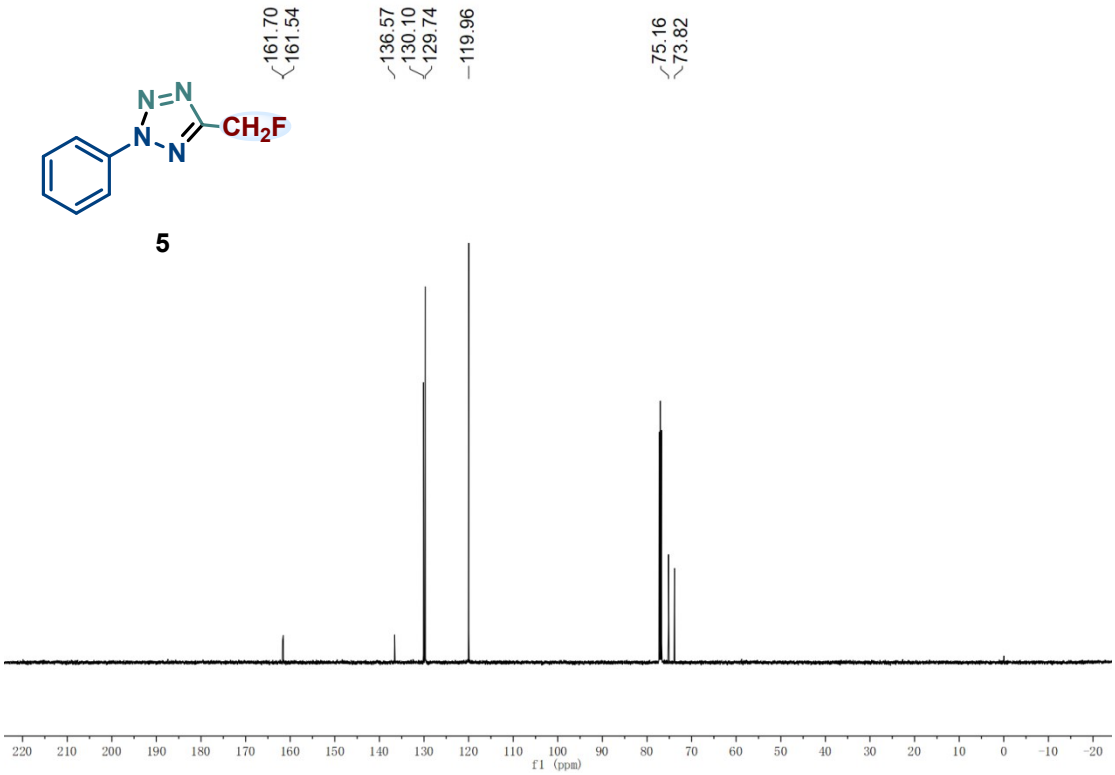

40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -220 -230 -240

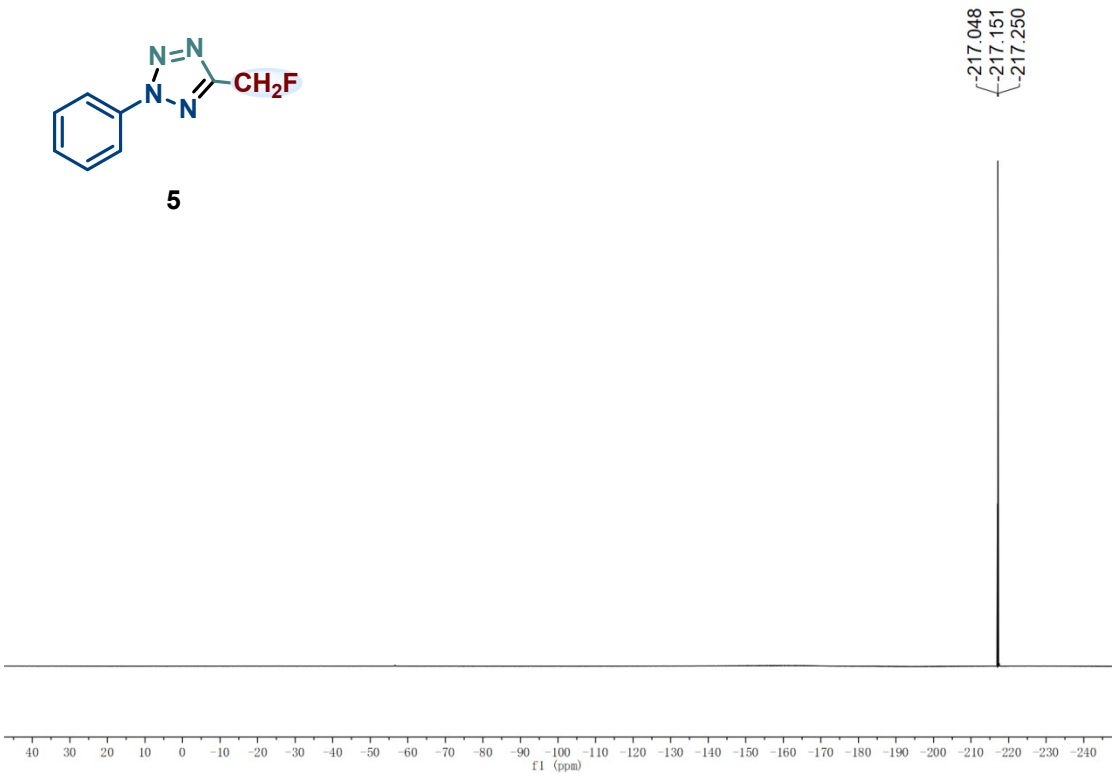

N=N
N
N
CH2F

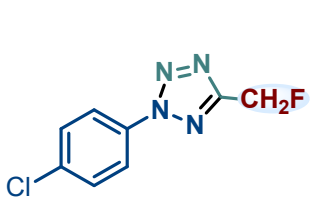
5


8.141
8.126
7.583
7.579
7.568
7.552
7.530
7.515
7.510
7.500
5.758
5.663

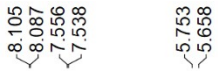

2.00
3.11
2.09
13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)

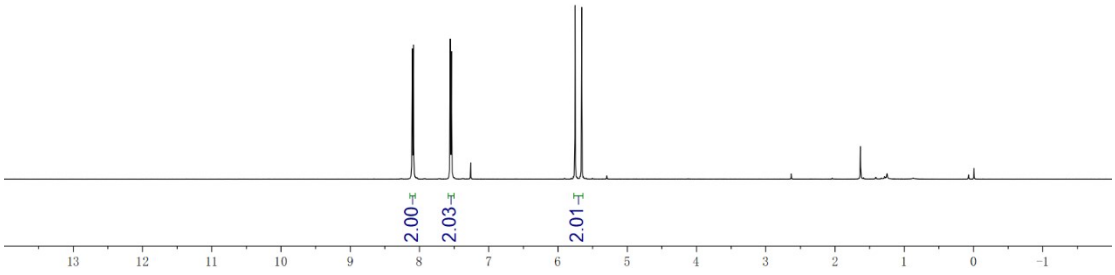

161.70
161.54
136.57
130.10
129.74
119.96
75.16
73.82
N=N
N
N
CH2F
5
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)

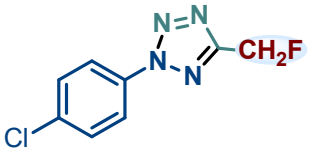

-217.048
-217.151
-217.250
N=N
N
N
CH2F
5
40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -220 -230 -240
f1 (ppm)


N=N
N
N
CH2F
Cl

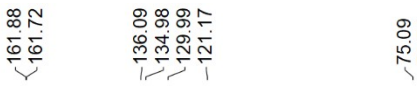
6


8.105
8.087
7.556
7.538
5.753
5.658

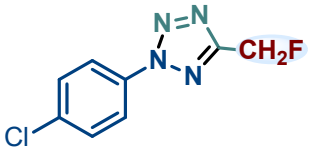

2.00
2.03
2.01
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1


N=N
N
N
CH2F
Cl

6

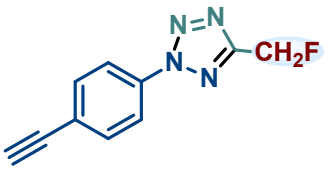

161.88
161.72
136.09
134.98
129.99
121.17
75.09
73.74

220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
-20


N=N
N
N
CH2F
Cl

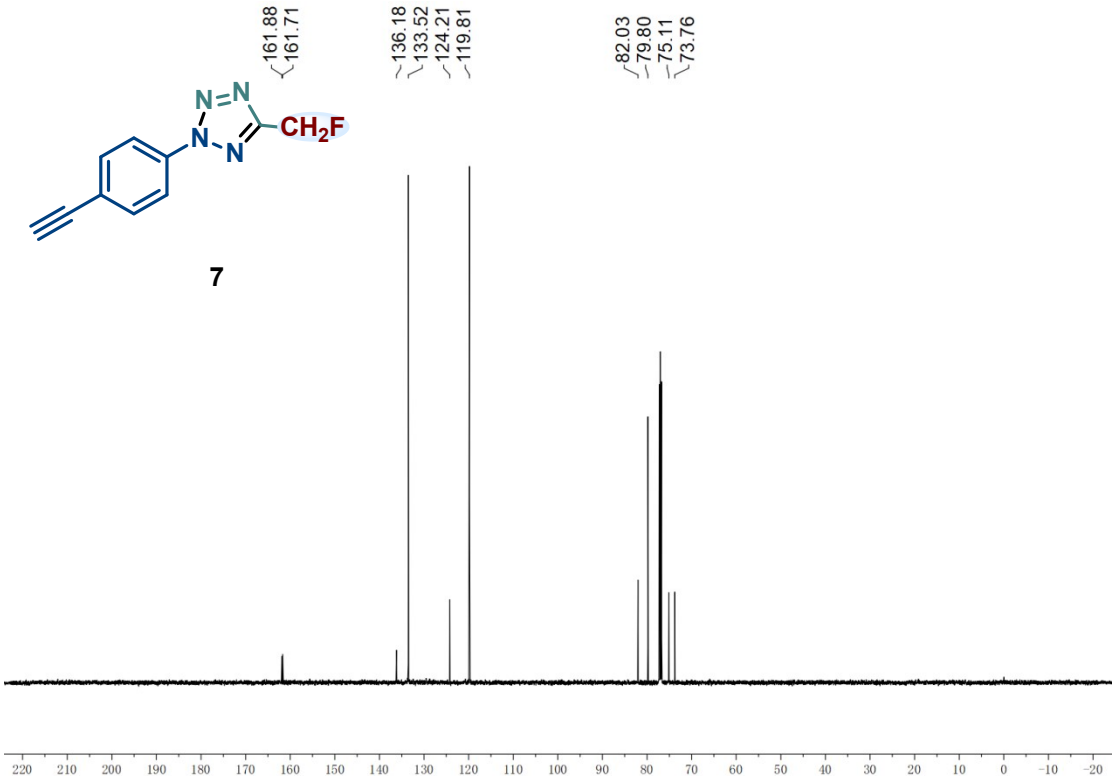
6

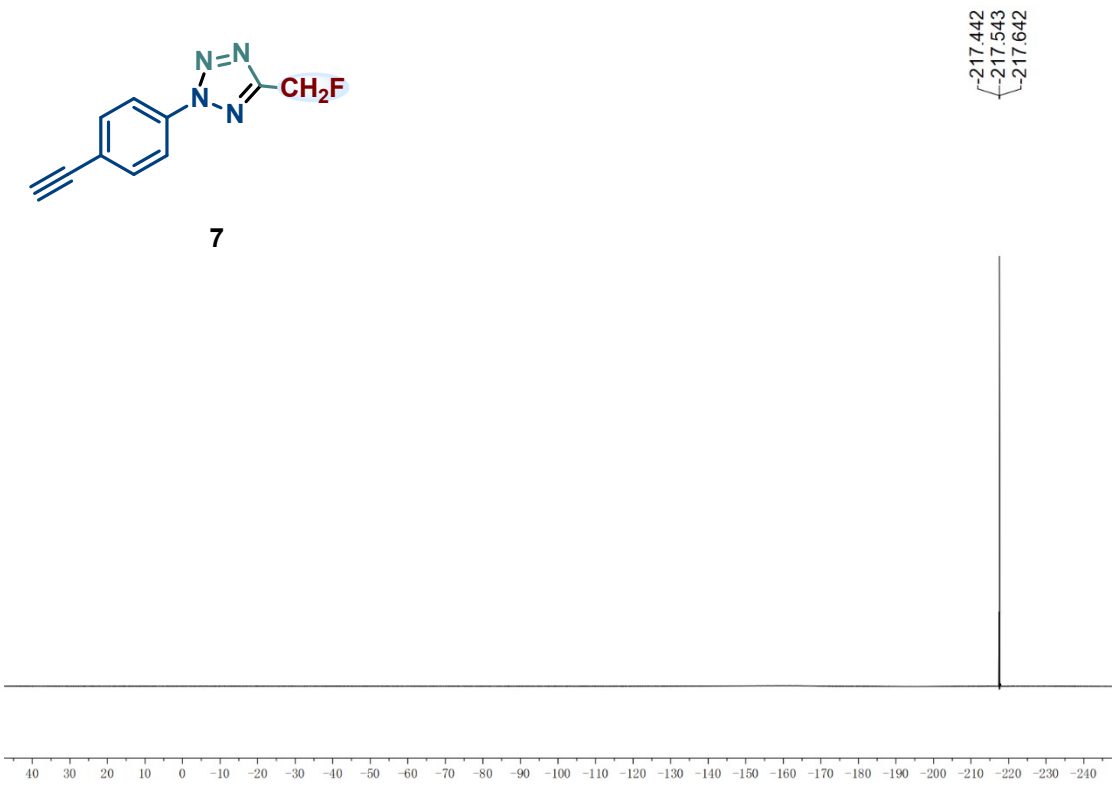
-217.435
-217.518
-217.604
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -220

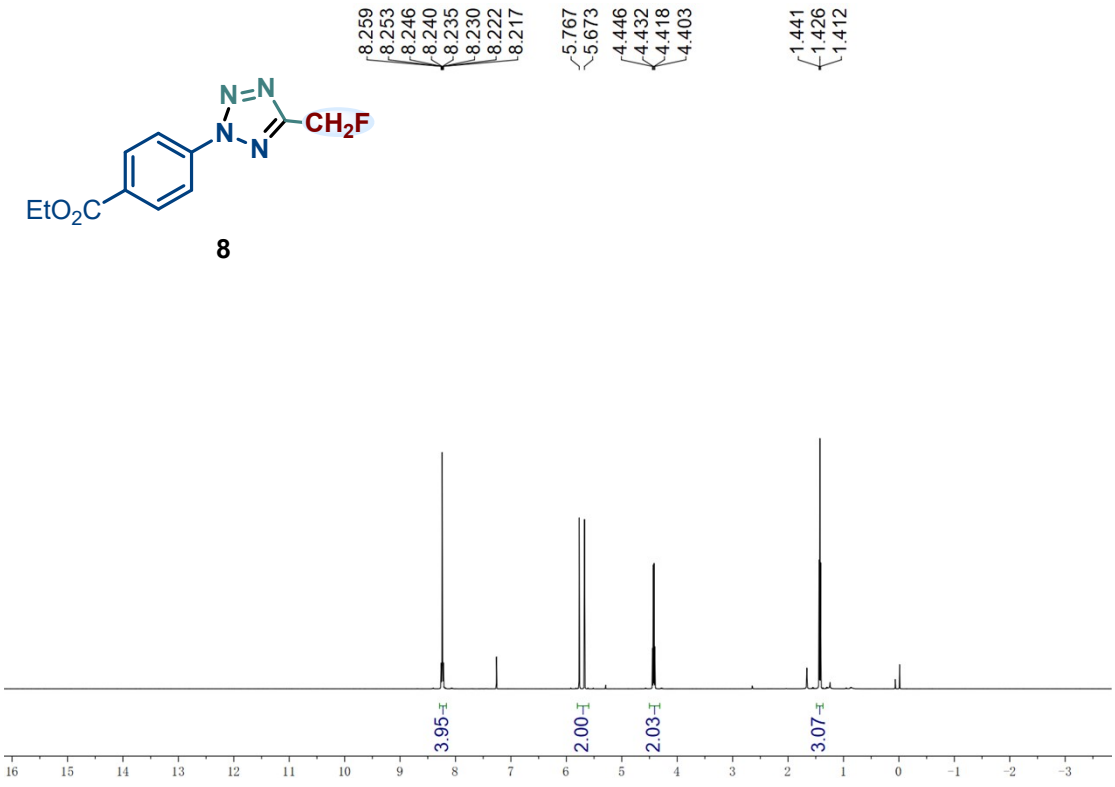

N=N
N
N
CH2F

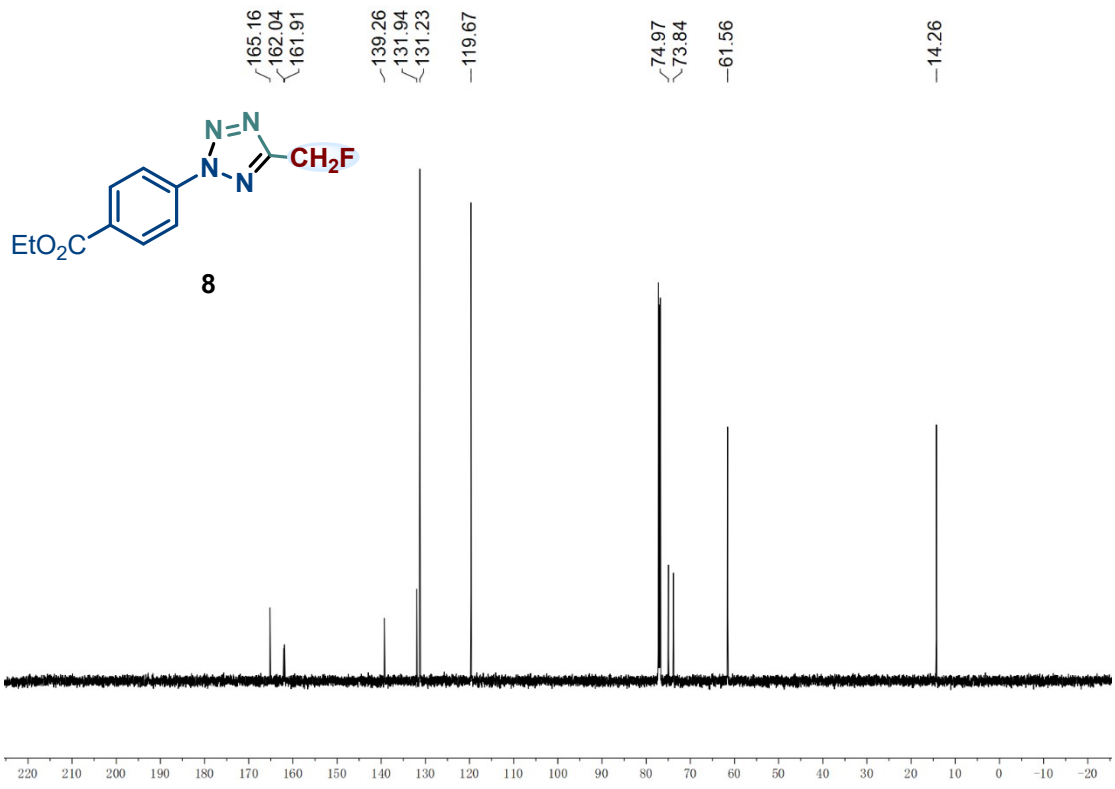
7

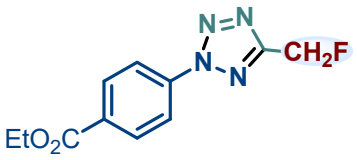
8.129
8.112
7.687
7.670
5.758
5.663
3.233
1.97
1.98
2.00
0.95
13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1


161.88
161.71
136.18
133.52
124.21
119.81
82.03
79.80
75.11
73.76
N=N
N
N
CH2F
7
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20


-217.442
-217.543
-217.642
N=N
N
N
CH2F
7
40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -220 -230 -240

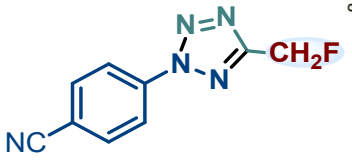

8.259
8.253
8.246
8.240
8.235
8.230
8.222
8.217
5.767
5.673
4.446
4.432
4.418
4.403
1.441
1.426
1.412
N=N
N
N
CH2F
EtO2C
8
3.95
2.00
2.03
3.07
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 −1 −2 −3


165.16
162.04
161.91
139.26
131.94
131.23
119.67
74.97
73.84
61.56
14.26
N=N
N
N
CH2F
EtO2C
8
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10 −20


N=N
N
N
N
CH2F
EtO2C

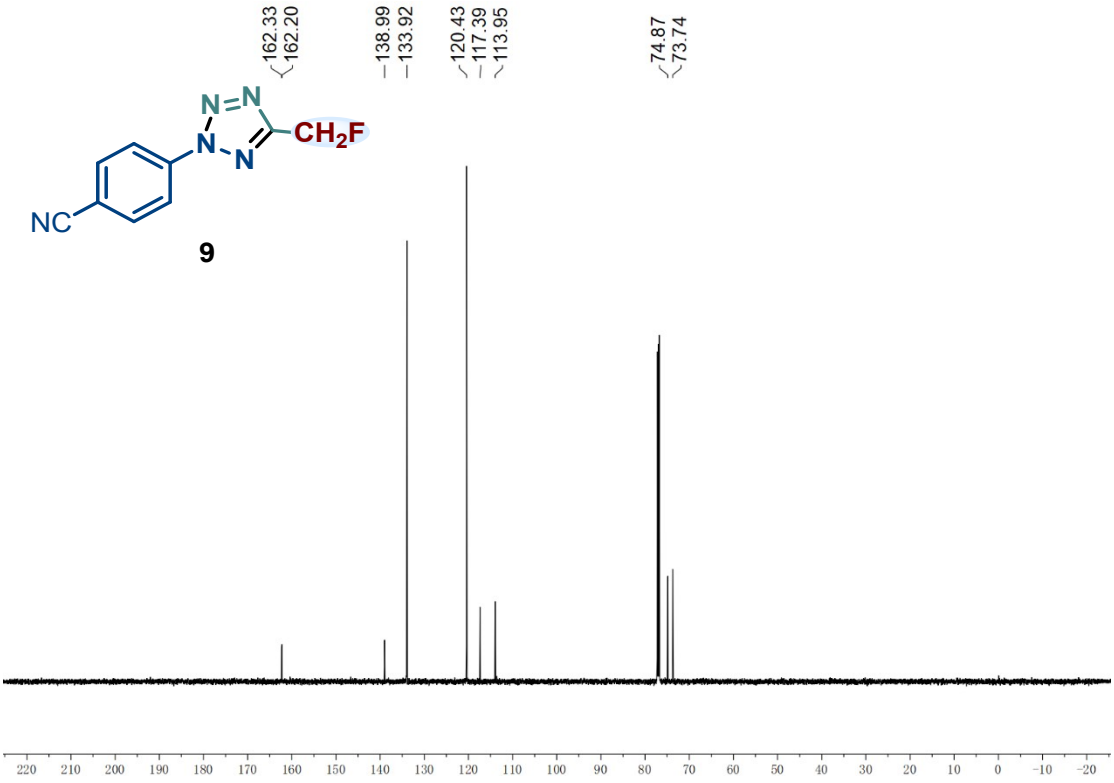
8

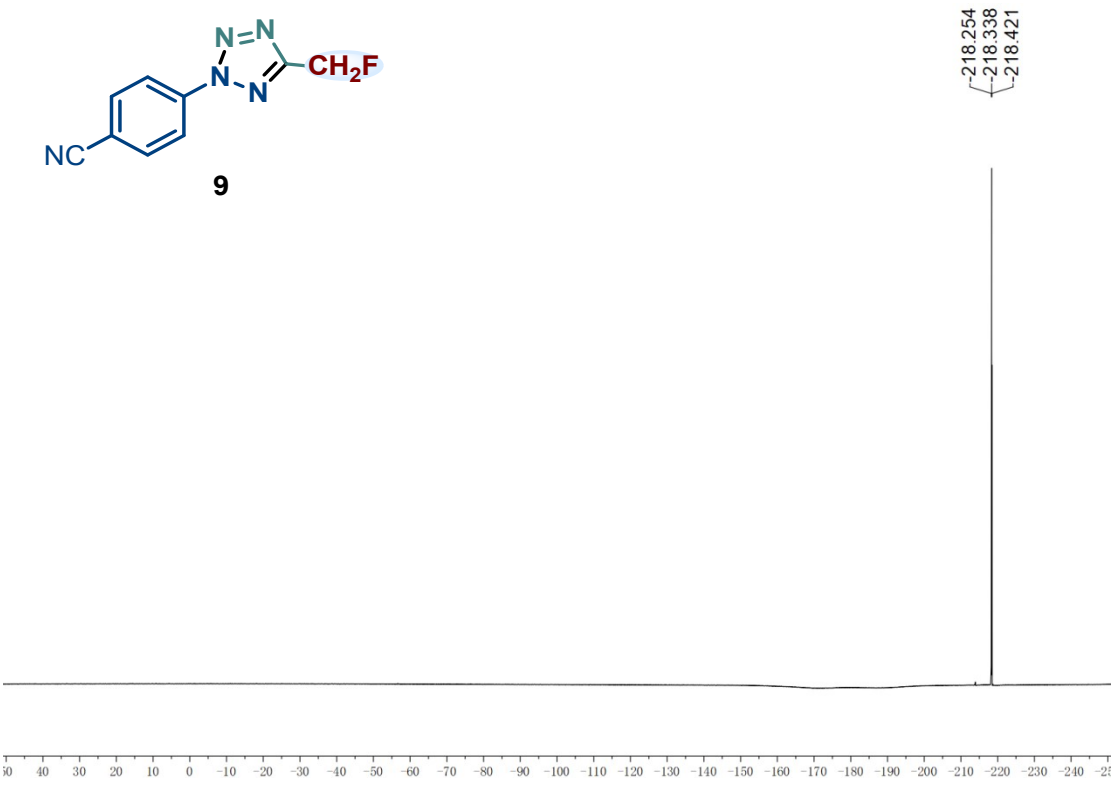
-217.728
-217.829
-217.932
70 50 30 10 -10 -30 -50 -70 -90 -110 -130 -150 -170 -190 -210 -230 -250 -270

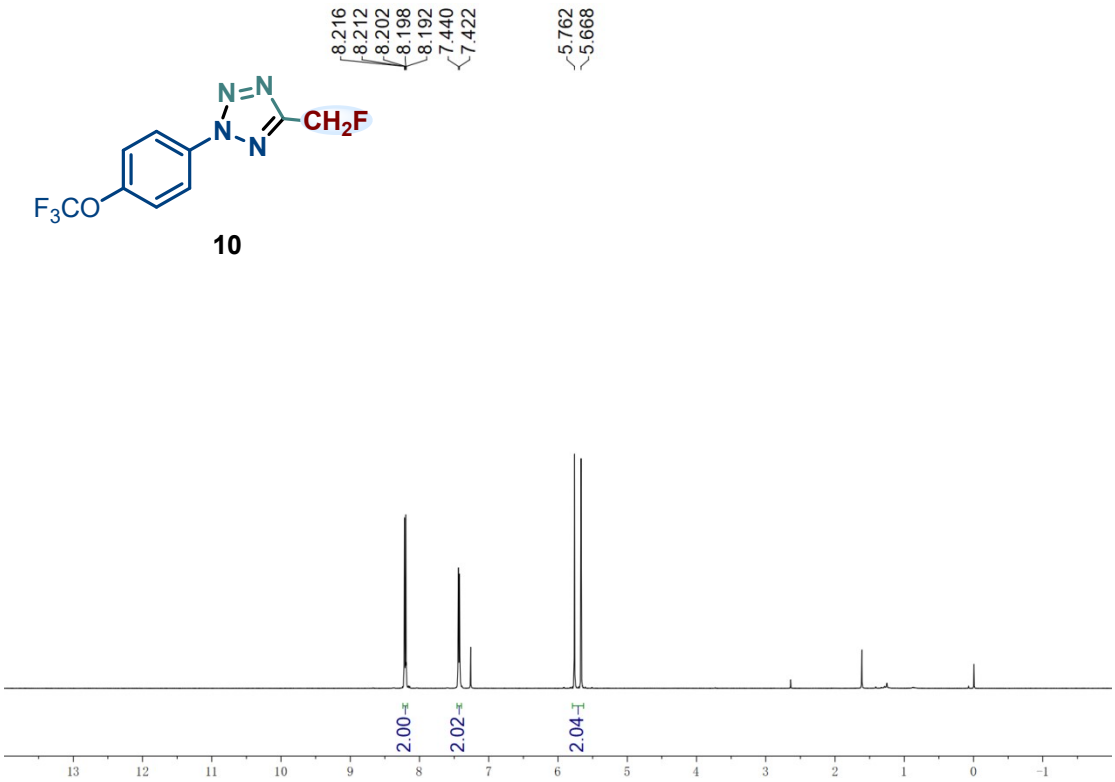

N=N
N
N
N
CH2F
NC

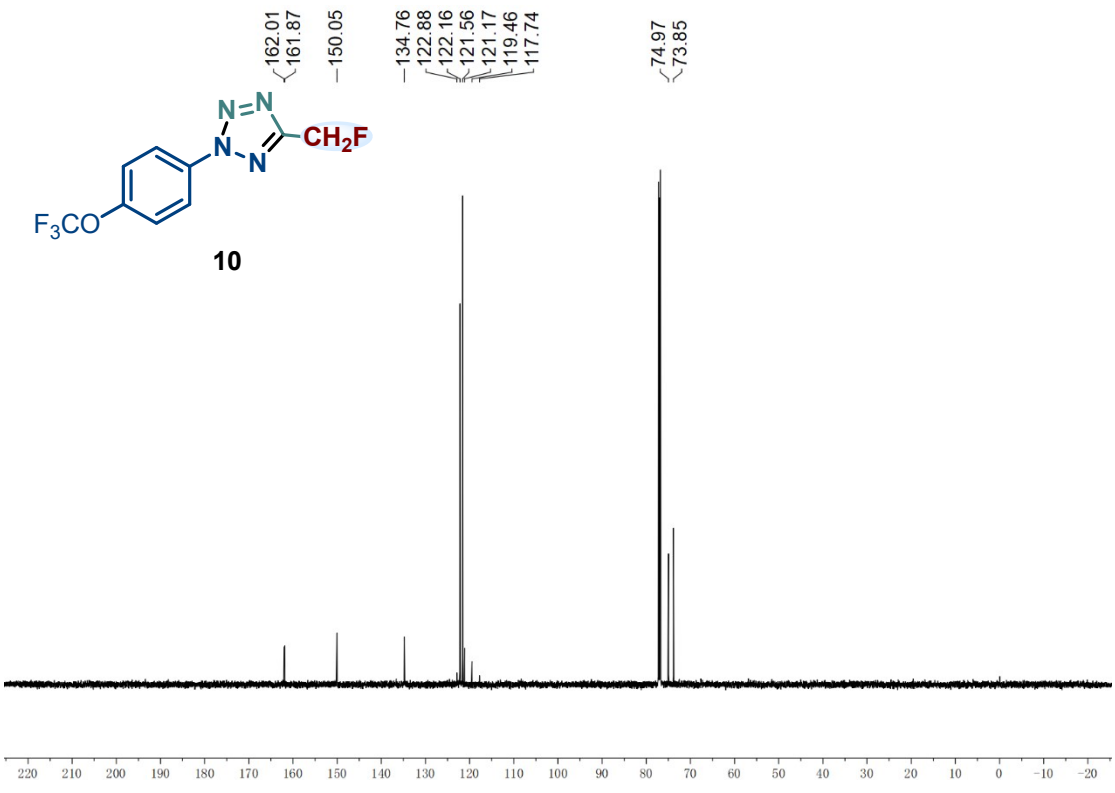
9

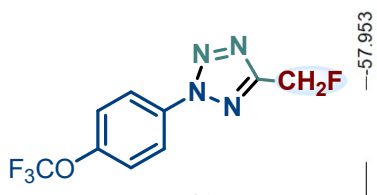
8.329
8.314
7.907
7.893
5.768
5.689
2.00
2.01
1.96
10.2 10.0 9.8 9.6 9.4 9.2 9.0 8.8 8.6 8.4 8.2 8.0 7.8 7.6 7.4 7.2 7.0 6.8 6.6 6.4 6.2 6.0 5.8 5.6 5.4 5.2 5.0 4.8 4.6


162.33
162.20
138.99
133.92
120.43
117.39
113.95
74.87
73.74
N=N
N
N
CH2F
NC
9
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20


218.254
218.338
218.421
N=N
N
N
CH2F
NC
9
50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -220 -230 -240

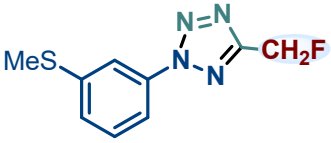

8.216
8.212
8.202
8.198
8.192
7.440
7.422
5.762
5.668
N=N
N
N
CH2F
F3CO
10
2.00
2.02
2.04
13
12
11
10
9
8
7
6
5
4
3
2
1
0
−1


162.01
161.87
150.05
134.76
122.88
122.16
121.56
121.17
119.46
117.74
74.97
73.85
N=N
N
N
CH2F
F3CO
10
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
−20


N=N
N
N
CH2F
F3CO

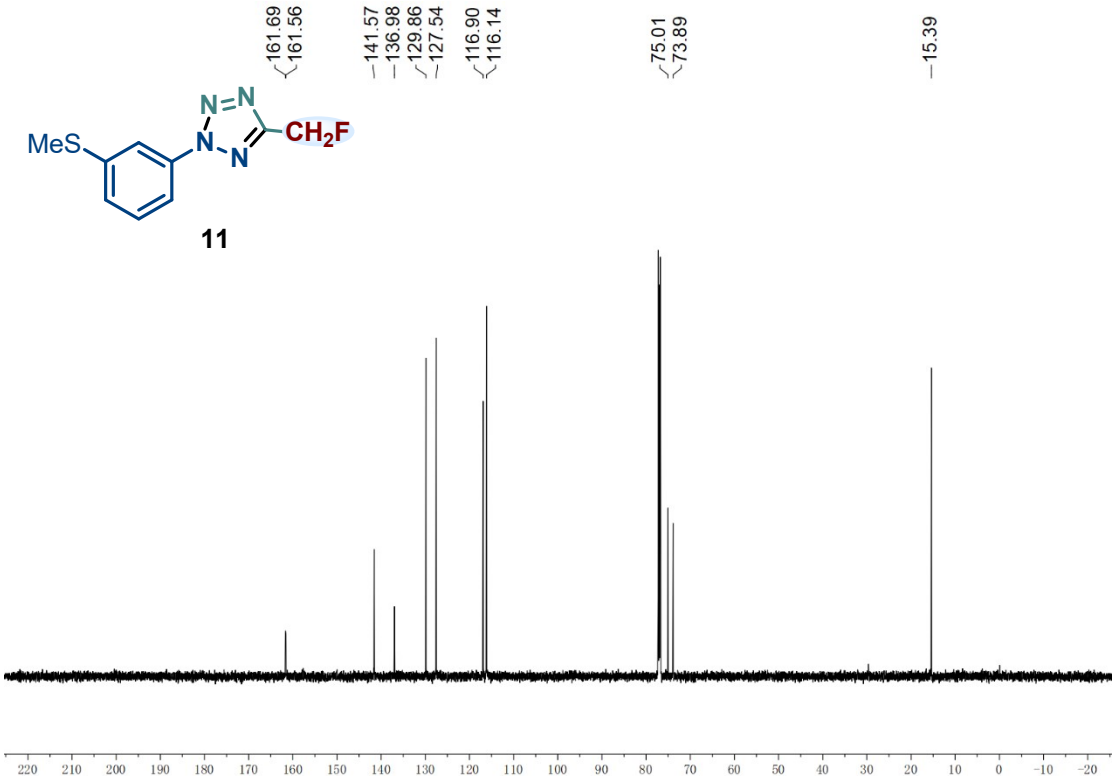
10

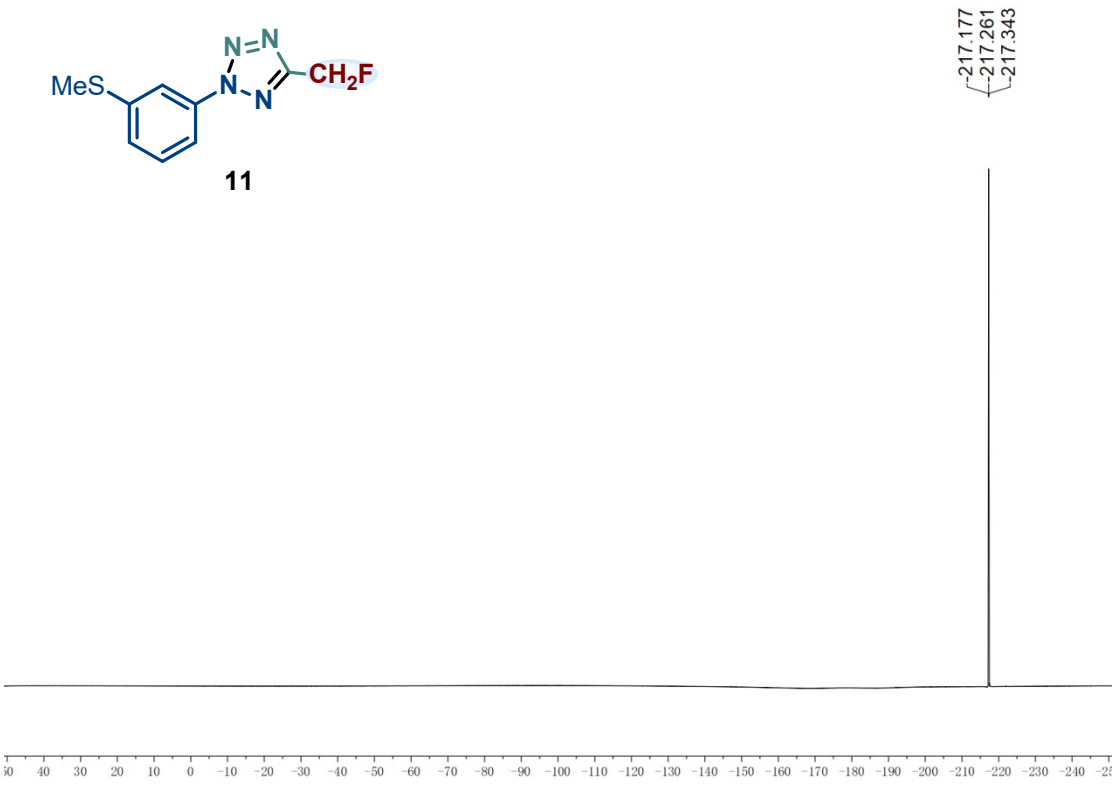
-57.953
-217.597
-217.680
-217.766
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -220

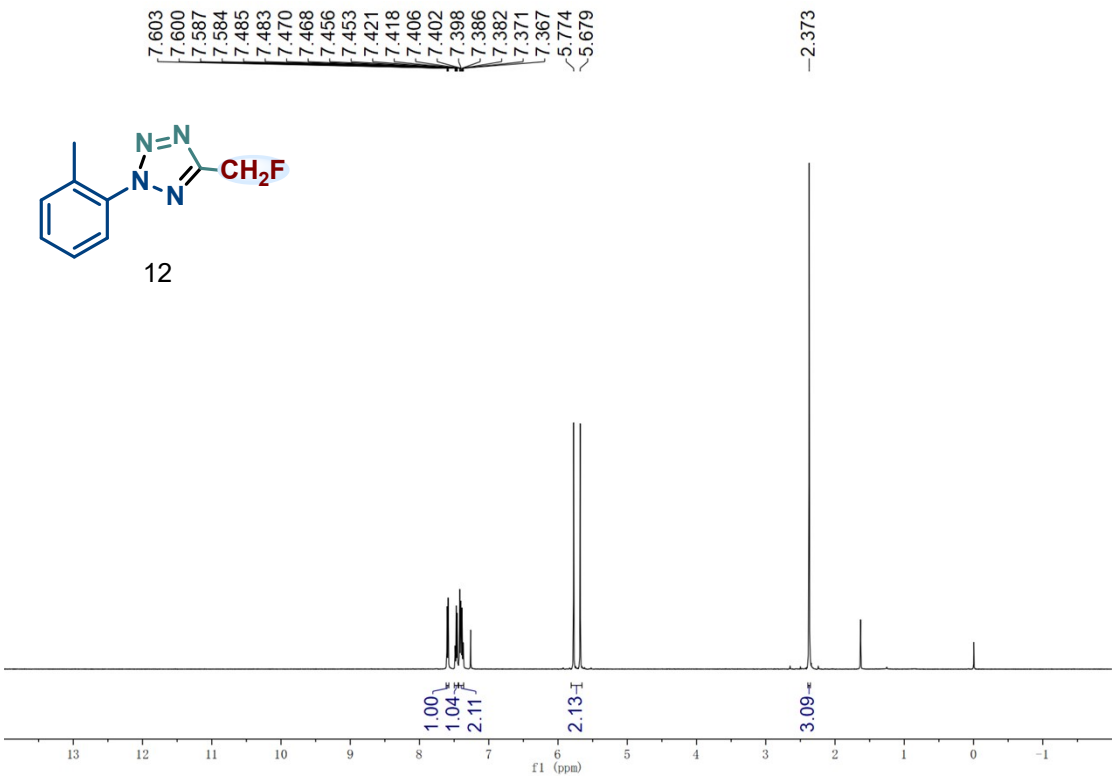

N=N
N
N
CH2F
MeS

11

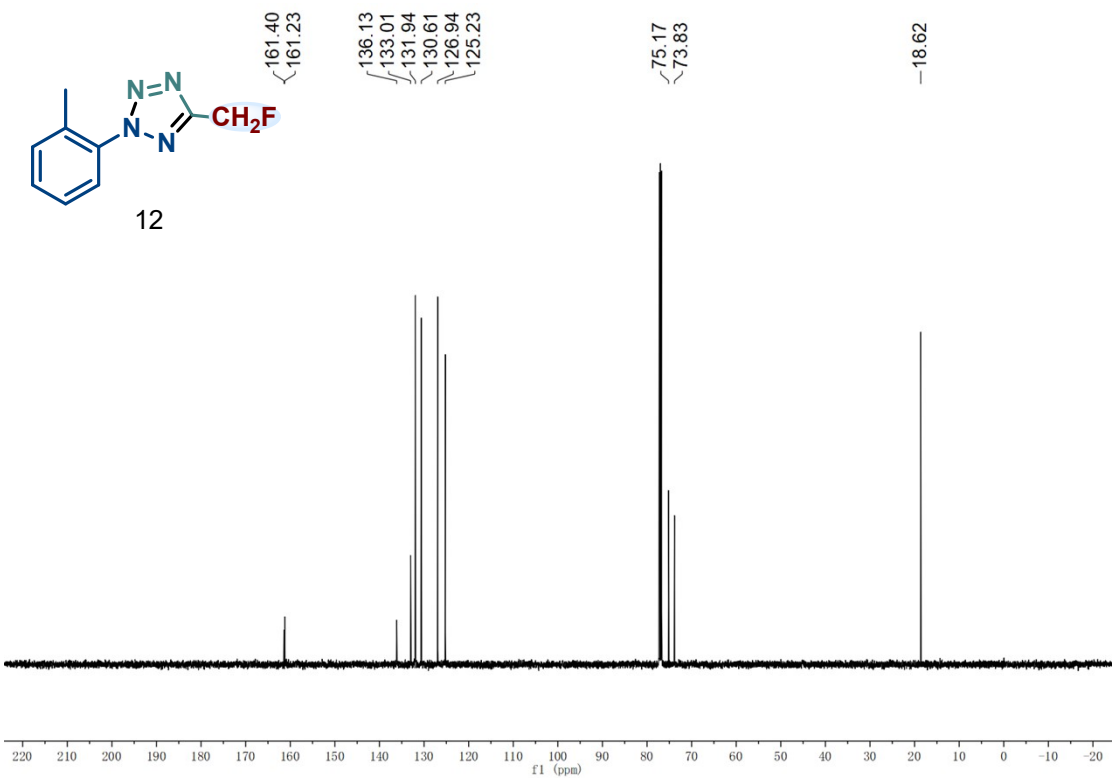
7.985
7.982
7.884
7.883
7.882
7.871
7.870
7.868
7.466
7.453
7.440
7.365
7.364
7.352
7.351
5.749
5.670
2.569
0.90
0.92
1.05
0.97
2.00
2.84
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3


161.69
161.56
141.57
136.98
129.86
127.54
116.90
116.14
75.01
73.89
15.39
MeS
CH2F
11

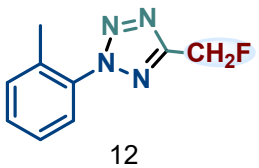

217.177
217.261
217.343
MeS
CH2F
11


7.603
7.600
7.587
7.584
7.485
7.483
7.470
7.468
7.456
7.453
7.421
7.418
7.406
7.402
7.398
7.386
7.382
7.371
7.367
5.774
5.679
2.373
N=N
N
N
CH2F
1.00
1.04
2.11
2.13
3.09
f1 (ppm)

12

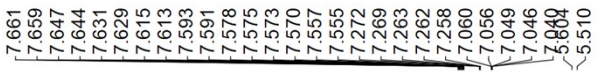

161.40
161.23
136.13
133.01
131.94
130.61
126.94
125.23
75.17
73.83
18.62
N=N
N
N
CH2F
f1 (ppm)

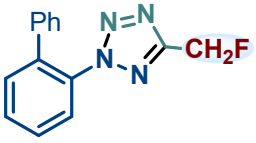
12



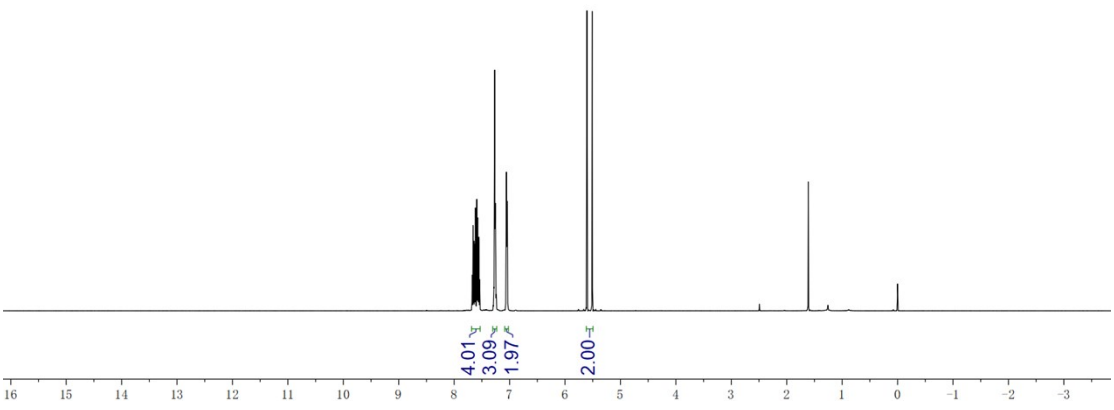
12

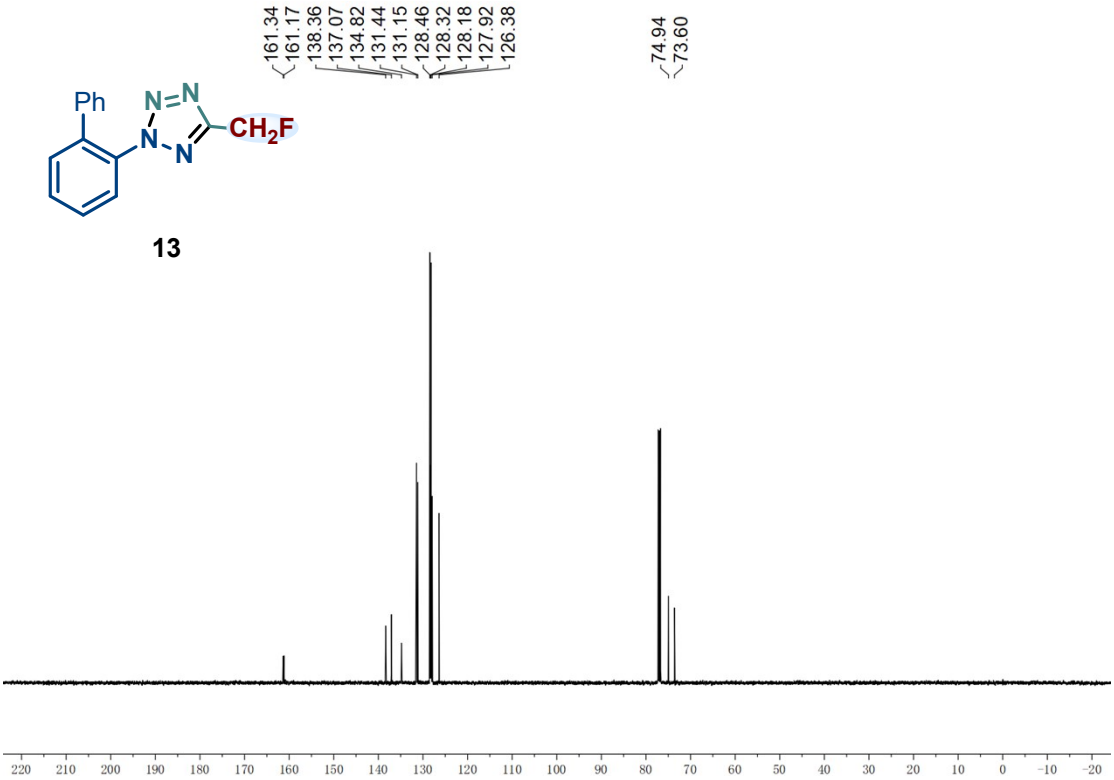
-217.165
-217.268
-217.364
f1 (ppm)

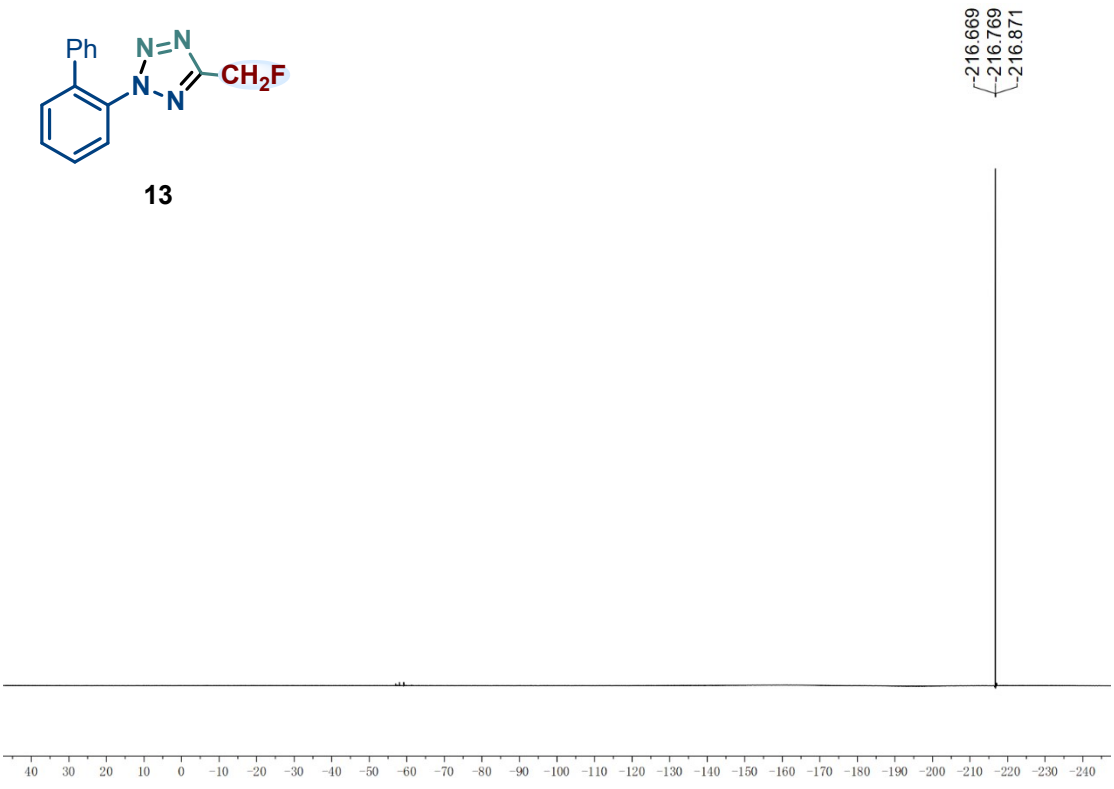

7.661
7.659
7.647
7.644
7.631
7.629
7.615
7.613
7.593
7.591
7.578
7.575
7.573
7.570
7.557
7.555
7.272
7.269
7.263
7.262
7.258
7.060
7.056
7.049
7.046
5.604
5.510

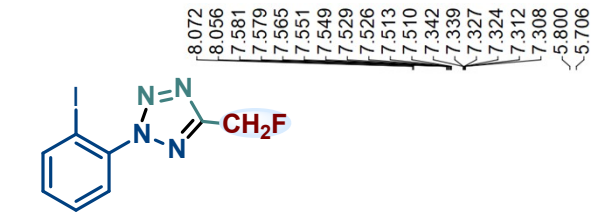


13

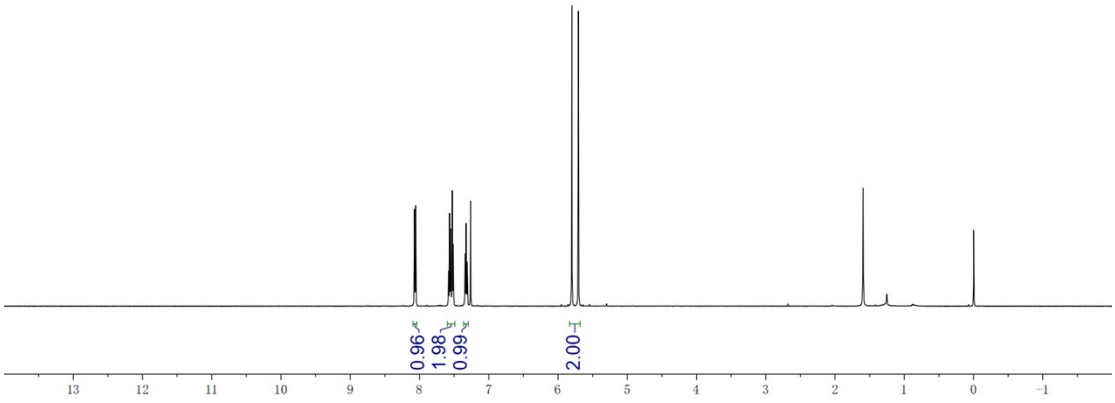

4.01
3.09
1.97
2.00

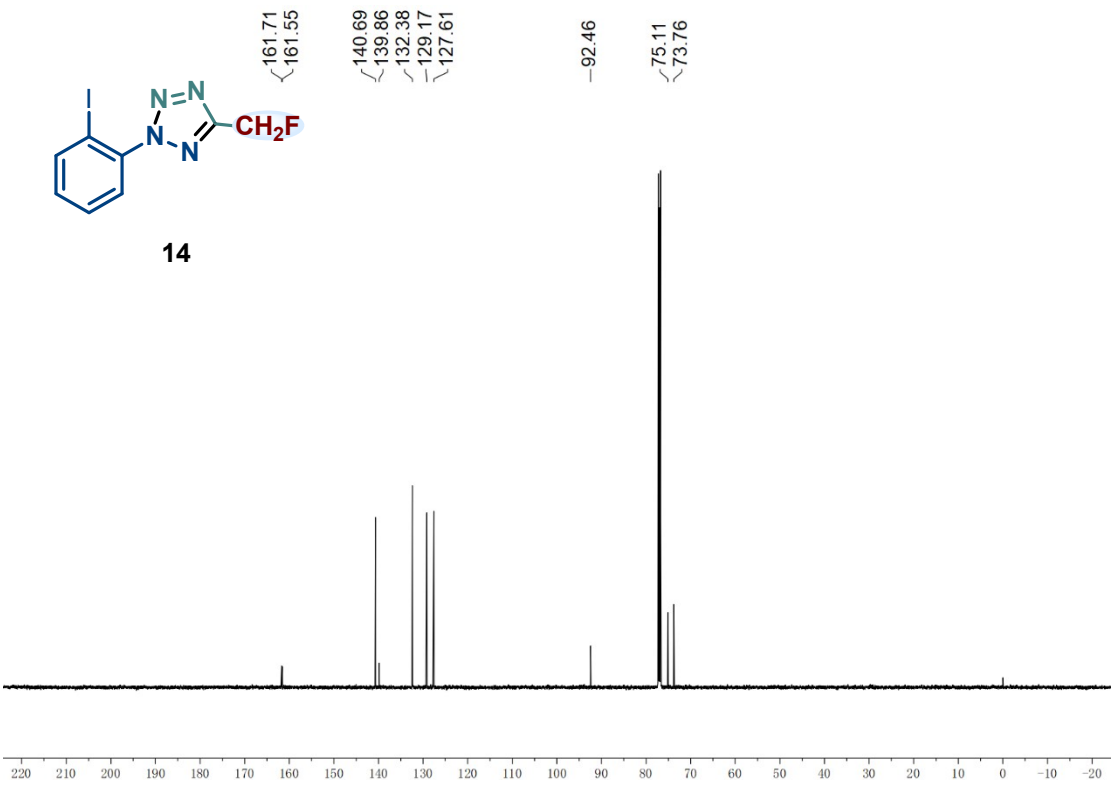

161.34
161.17
138.36
137.07
134.82
131.44
131.15
128.46
128.32
128.18
127.92
126.38
74.94
73.60
Ph
N=N
N
N
CH2F
13
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20


216.669
216.769
216.871
Ph
N=N
N
N
CH2F
13
40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -220 -230 -240

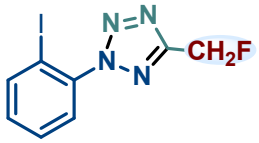

8.072
8.056
7.581
7.579
7.565
7.551
7.549
7.529
7.526
7.513
7.510
7.342
7.339
7.327
7.324
7.312
7.308
5.800
5.706
N=N
N
N
CH2F

14


0.96
1.98
0.99
2.00
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1

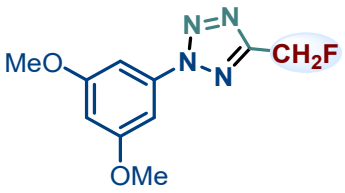

161.71
161.55
140.69
139.86
132.38
129.17
127.61
92.46
75.11
73.76
N=N
N
N
CH2F
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
-20

14



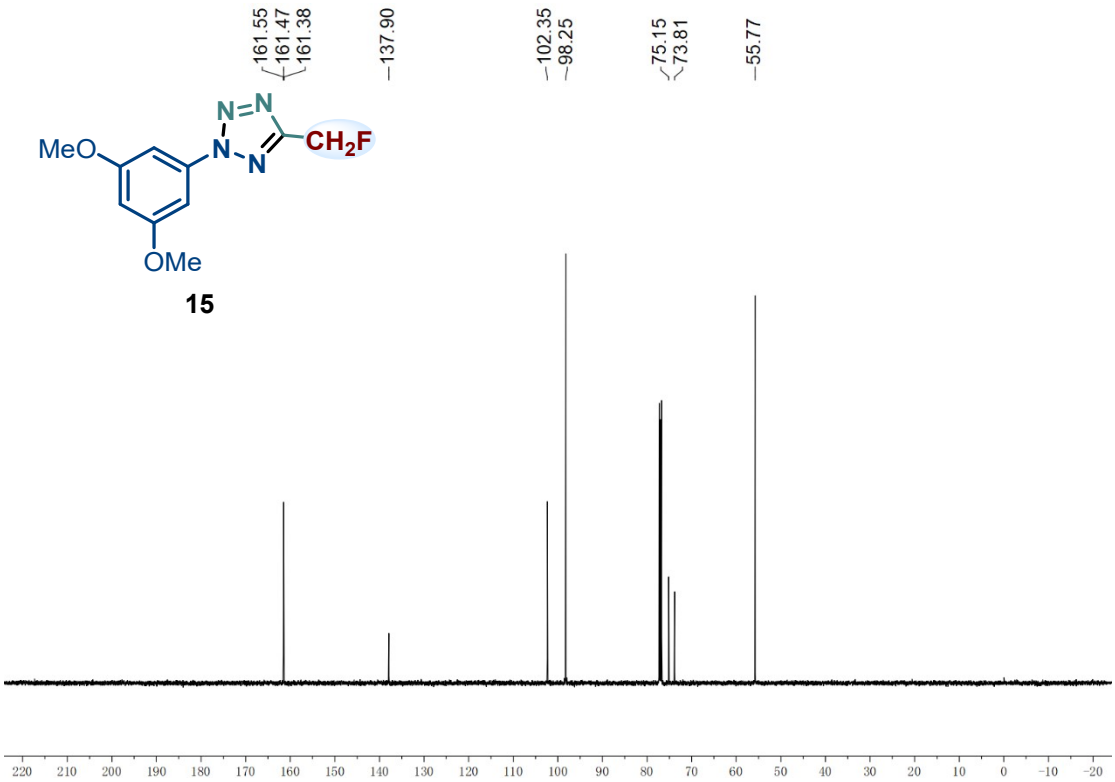
14

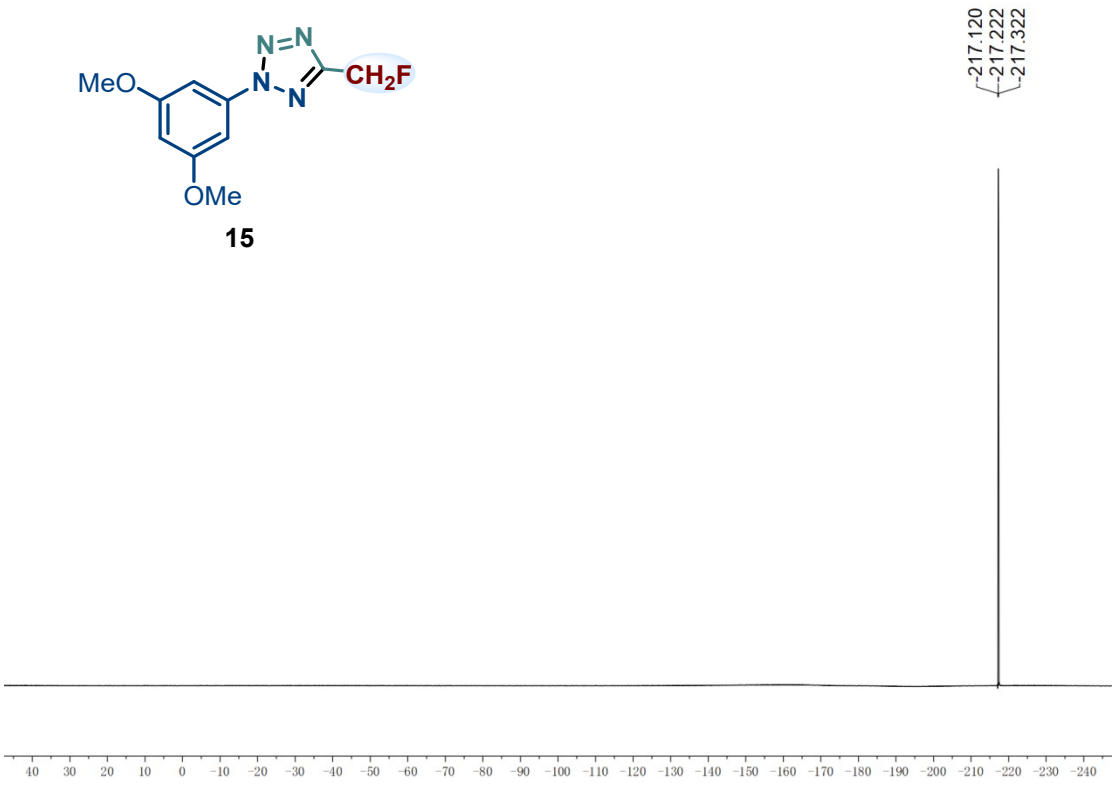
-217.227
-217.327
-217.426

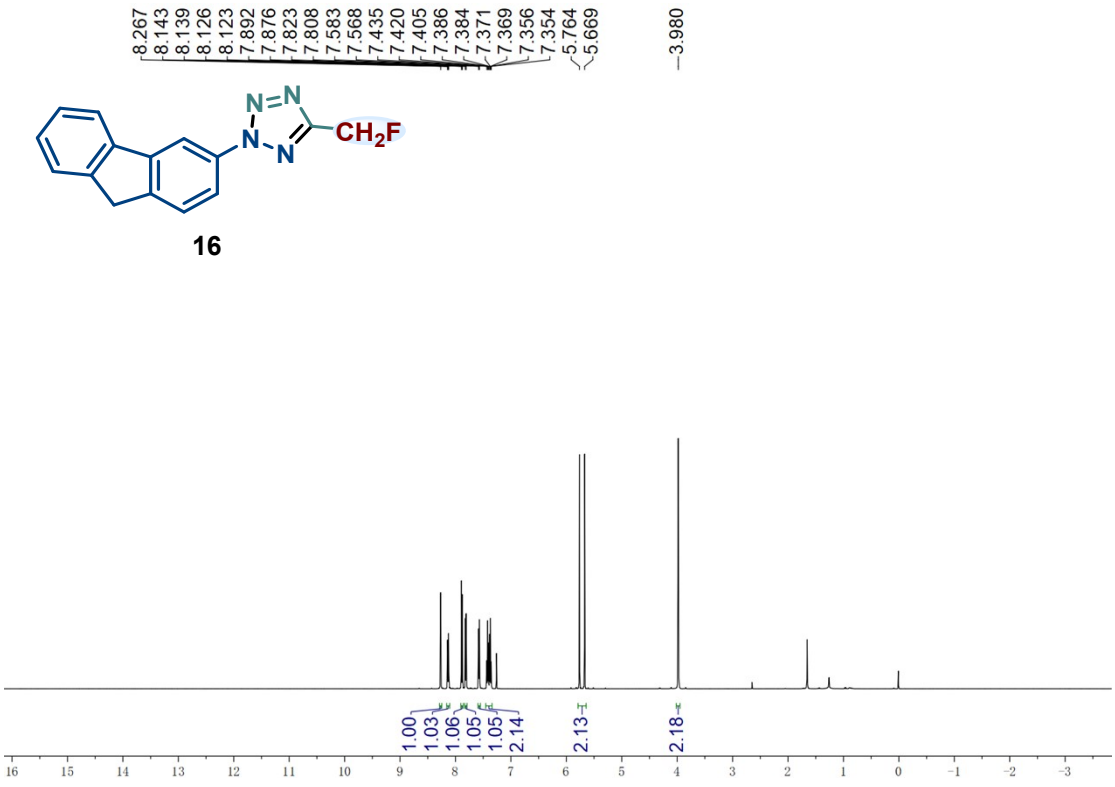


15

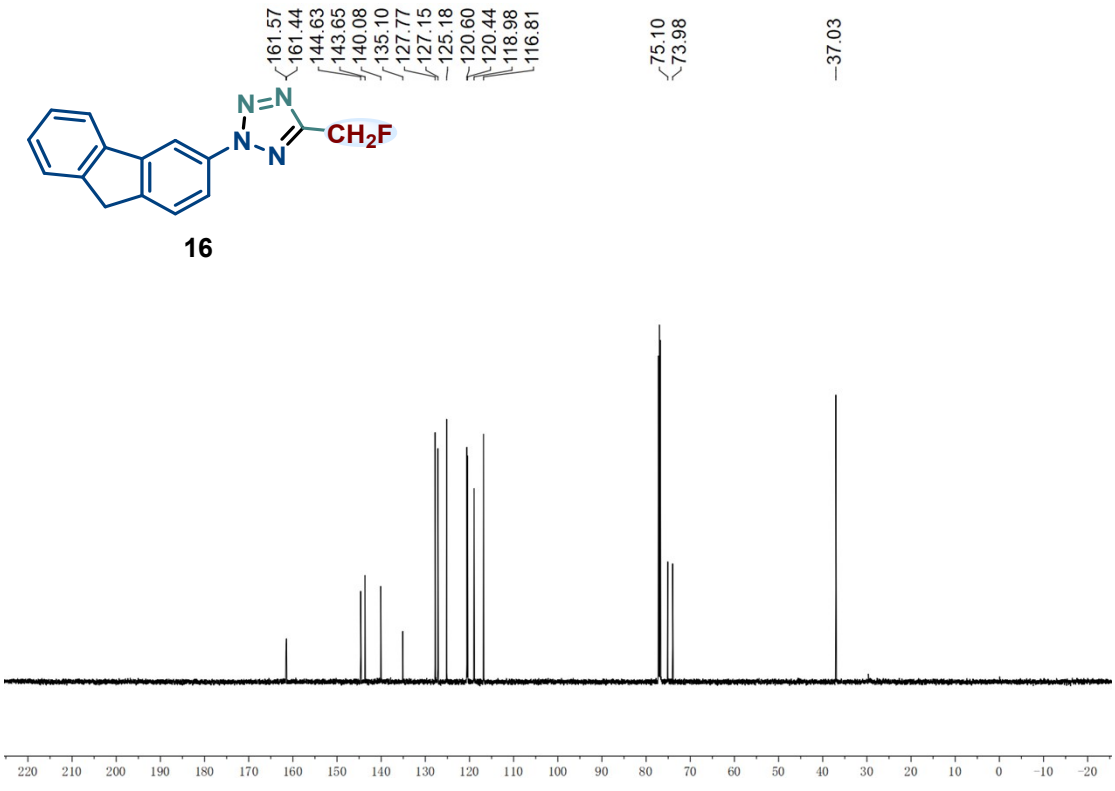
7.296
7.292
6.568
6.564
5.744
5.649
3.873
1.87
0.95
2.00
6.02


161.55
161.47
161.38
137.90
102.35
98.25
75.15
73.81
55.77
MeO
OMe
CH2F
15
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20

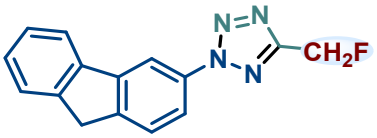

217.120
217.222
217.322
MeO
OMe
CH2F
15
40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -220 -230 -240


8.267
8.143
8.139
8.126
8.123
7.892
7.876
7.823
7.808
7.583
7.568
7.435
7.420
7.405
7.386
7.384
7.371
7.369
7.356
7.354
5.764
5.669
3.980
N=N
N
N
CH2F
1.00
1.03
1.06
1.05
1.05
2.14
2.13
2.18
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 −1 −2 −3

16

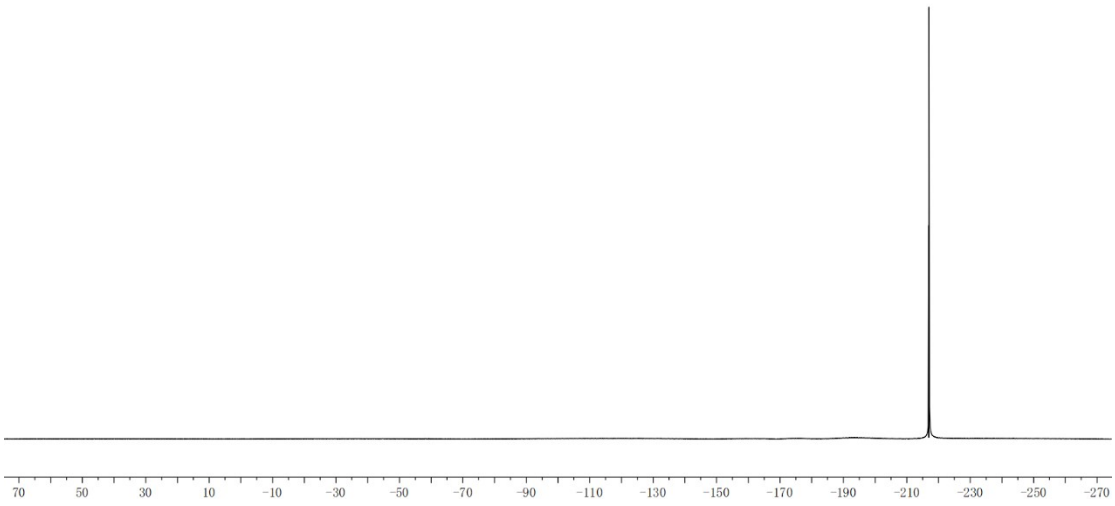

161.57
161.44
144.63
143.65
140.08
135.10
127.77
127.15
125.18
120.60
120.44
118.98
116.81
75.10
73.98
37.03
N=N
N
N
CH2F
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10 −20

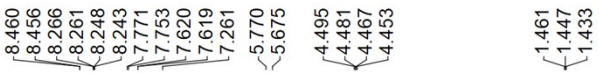
16

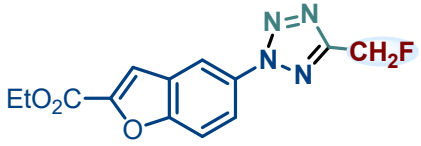

N=N
N
N
CH2F

16

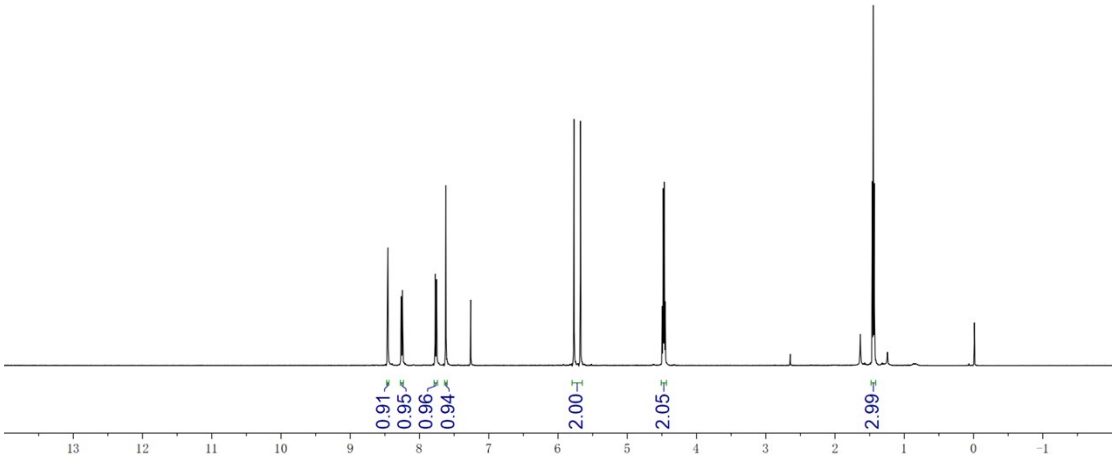

-216.917
-217.002
-217.087

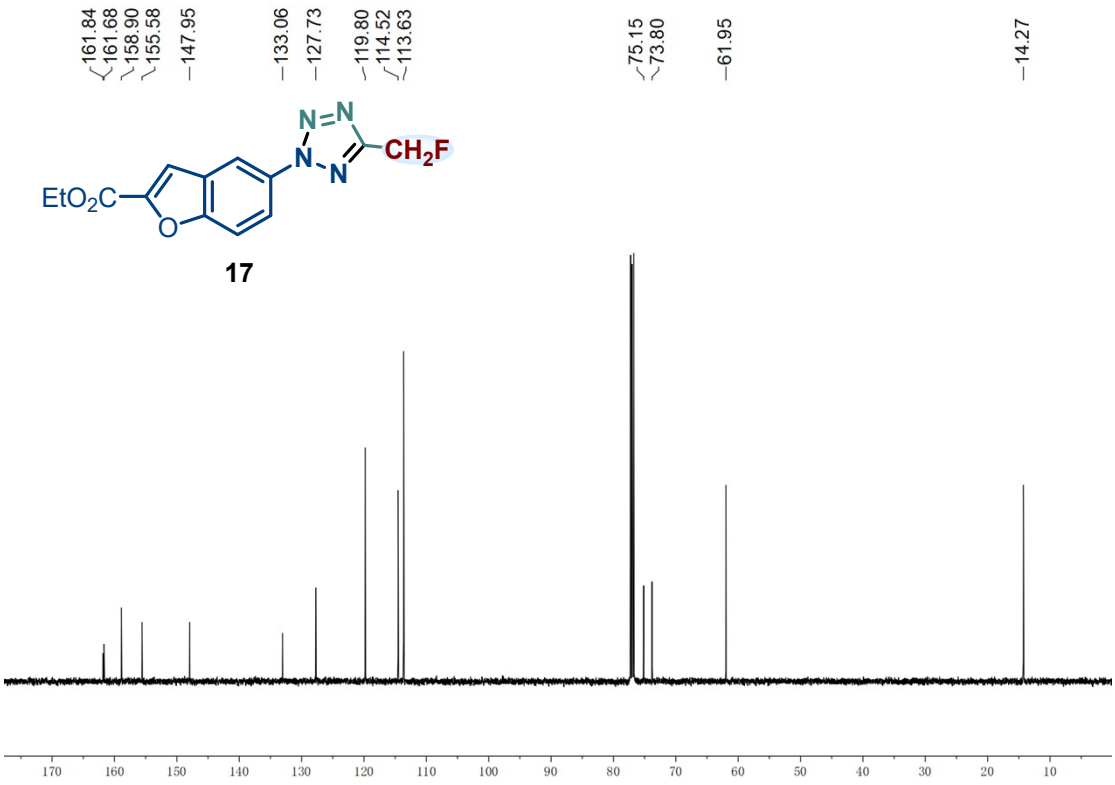

70
50
30
10
-10
-30
-50
-70
-90
-110
-130
-150
-170
-190
-210
-230
-250
-270

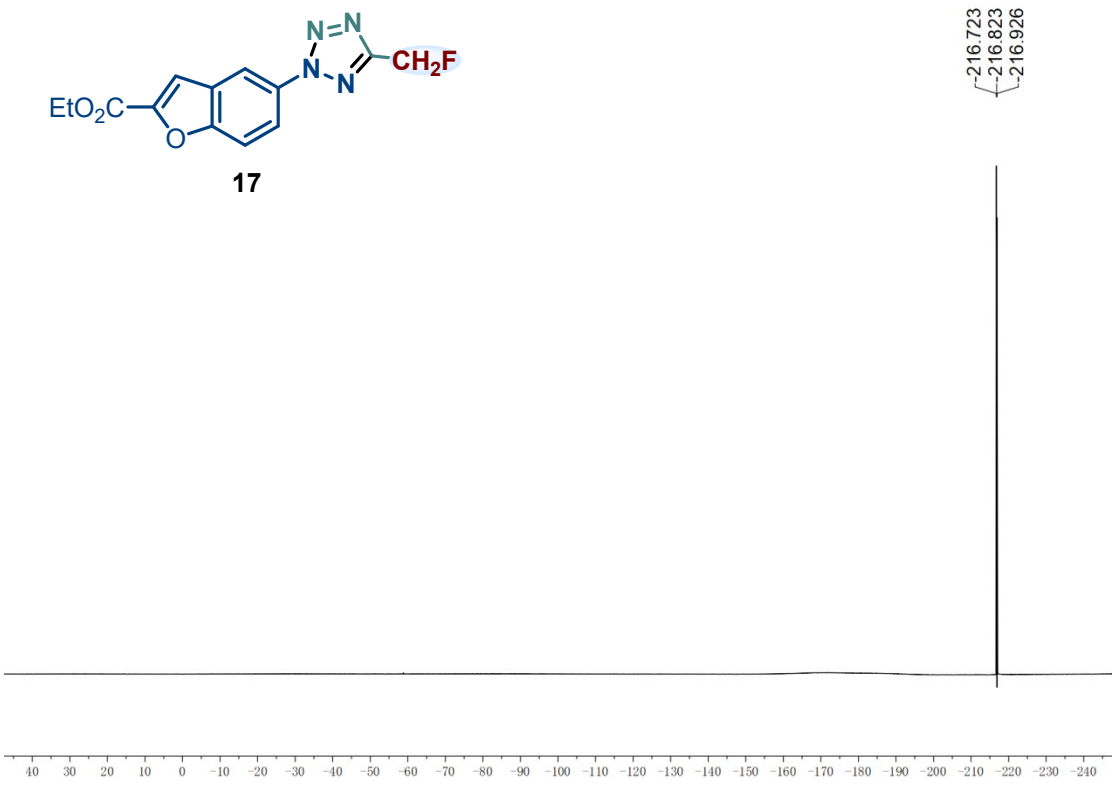

8.460
8.456
8.266
8.261
8.248
8.243
7.771
7.753
7.620
7.619
7.261
5.770
5.675
4.495
4.481
4.467
4.453
1.461
1.447
1.433

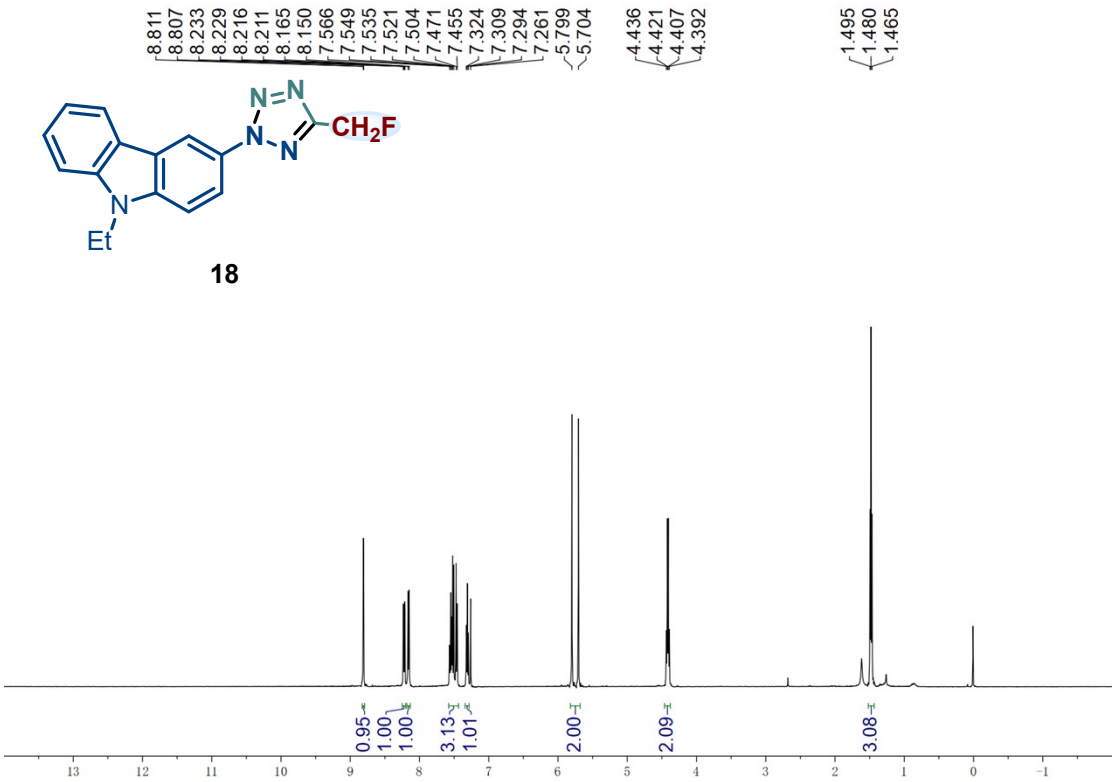

N=N
N
N
CH2F
EtO2C
O

17

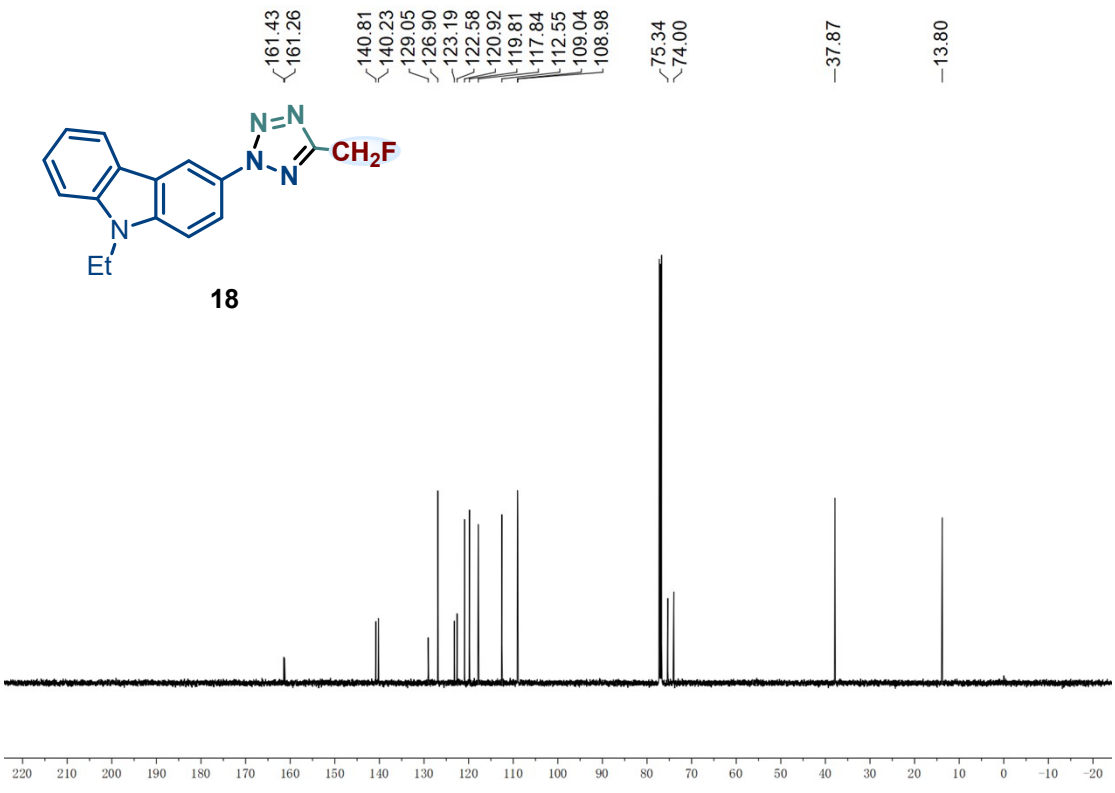

0.91
0.95
0.96
0.94
2.00
2.05
2.99
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1


161.84
161.68
158.90
155.58
147.95
133.06
127.73
119.80
114.52
113.63
75.15
73.80
61.95
14.27
N=N
N
N
CH2F
EtO2C
O
17
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10

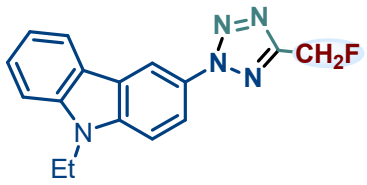

216.723
216.823
216.926
N=N
N
N
CH2F
EtO2C
O
17
40
30
20
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
-220
-230
-240


8.811
8.807
8.233
8.229
8.216
8.211
8.165
8.150
7.566
7.549
7.535
7.521
7.504
7.471
7.455
7.324
7.309
7.294
7.261
5.799
5.704
4.436
4.421
4.407
4.392
1.495
1.480
1.465
N=N
N
N
CH2F
N
Et
0.95
1.00
1.00
3.13
1.01
2.00
2.09
3.08
13
12
11
10
9
8
7
6
5
4
3
2
1
0
−1

18

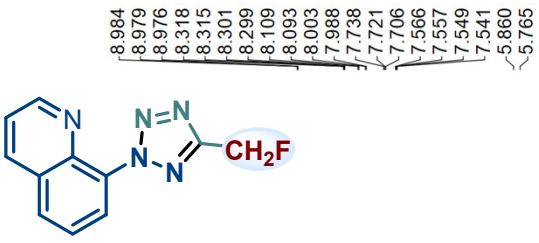

161.43
161.26
140.81
140.23
129.05
126.90
123.19
122.58
120.92
119.81
117.84
112.55
109.04
108.98
75.34
74.00
37.87
13.80
N=N
N
N
CH2F
N
Et
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
−20

18


N=N
N
N
CH2F
N
Et

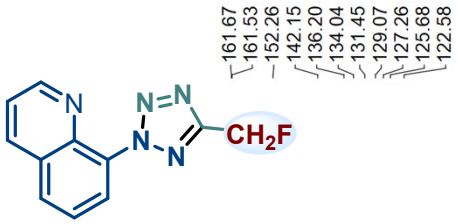
18

-216.359
-216.462
-216.561
40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -220 -230 -240

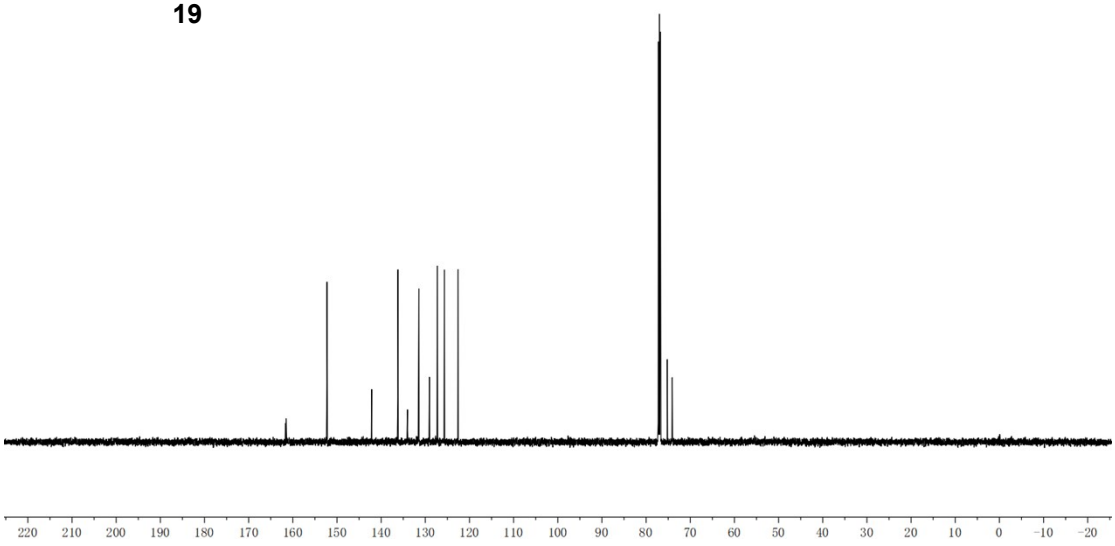

N=N
N
N
CH2F
N

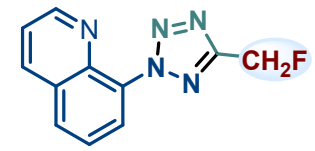
19

8.984
8.979
8.976
8.318
8.315
8.301
8.299
8.109
8.093
8.003
7.988
7.738
7.721
7.706
7.566
7.557
7.549
7.541
5.860
5.765
0.97
1.00
0.99
0.96
1.06
1.02
2.00
13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1


161.67
161.53
152.26
142.15
136.20
134.04
131.45
129.07
127.26
125.68
122.58
75.21
74.09
N
N=N
N
N
CH2F

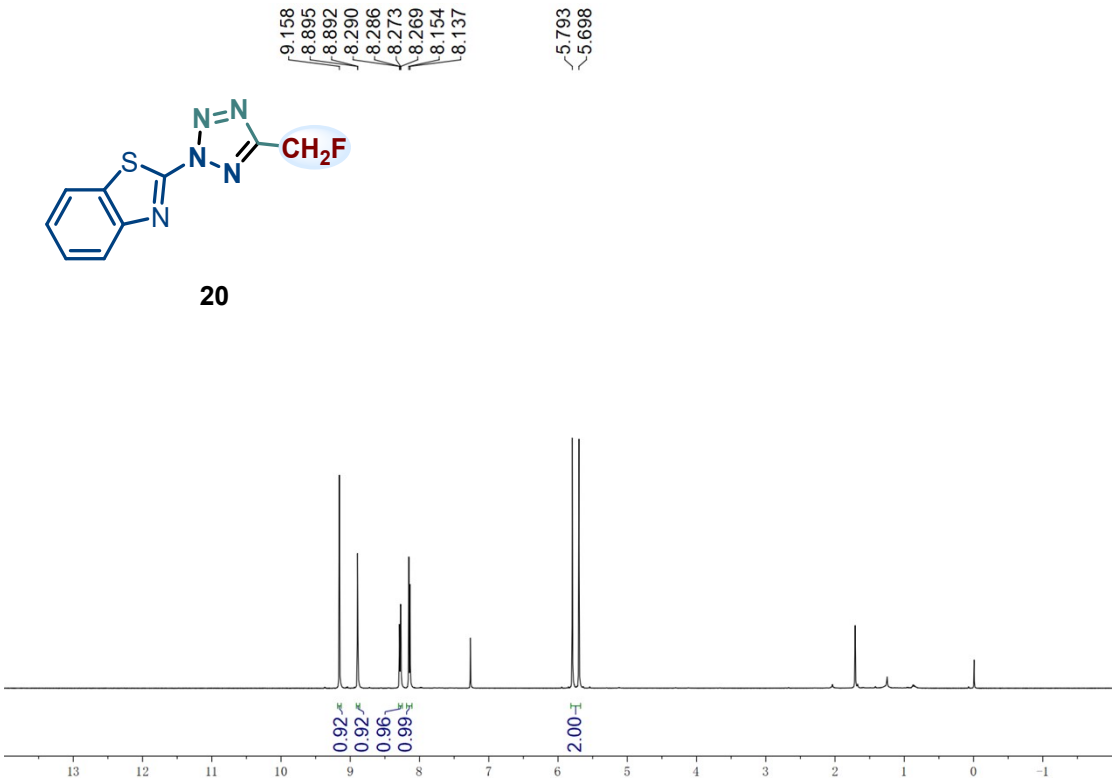
19


220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20

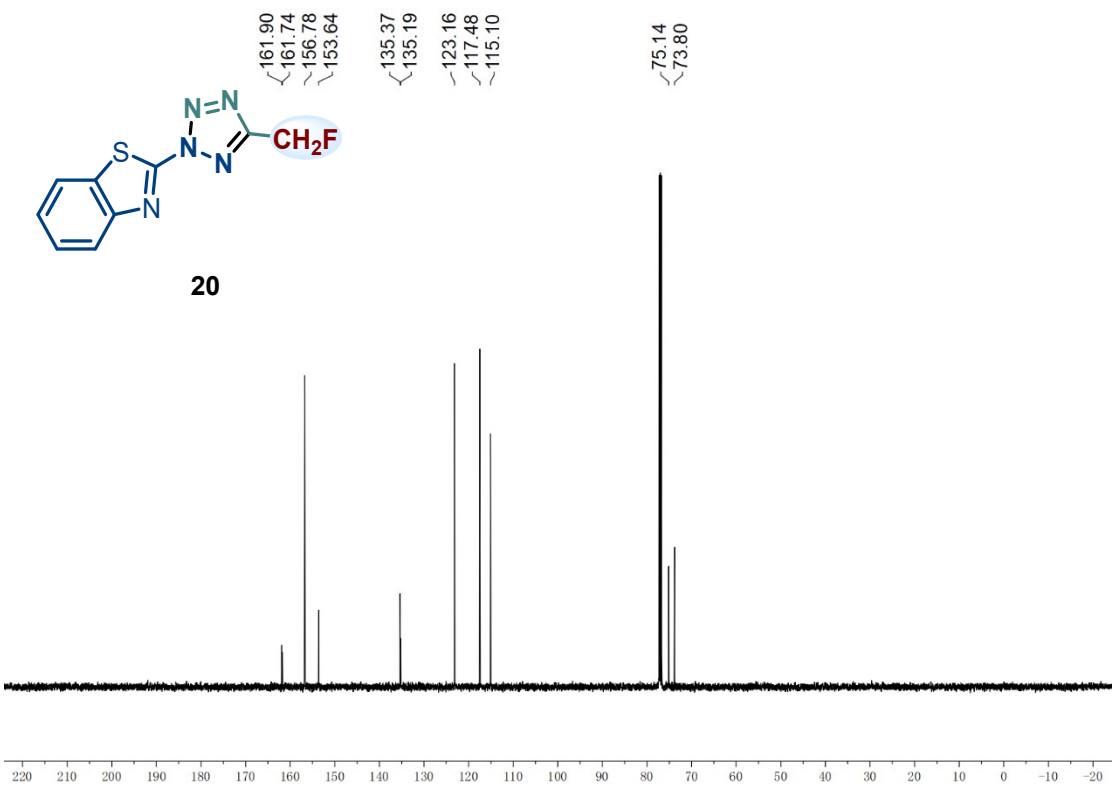

N
N=N
N
N
CH2F

19

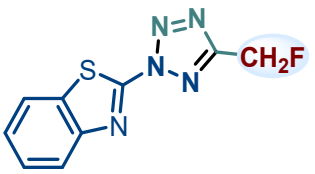
216.884
216.968
217.053
50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -220 -230 -240


9.158
8.895
8.892
8.290
8.286
8.273
8.269
8.154
8.137
5.793
5.698
N=N
N
N
S
N
CH2F
0.92
0.92
0.96
0.99
2.00
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1

20

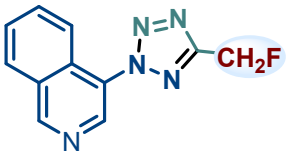

161.90
161.74
156.78
153.64
135.37
135.19
123.16
117.48
115.10
75.14
73.80
N=N
N
N
S
N
CH2F
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
-20

20



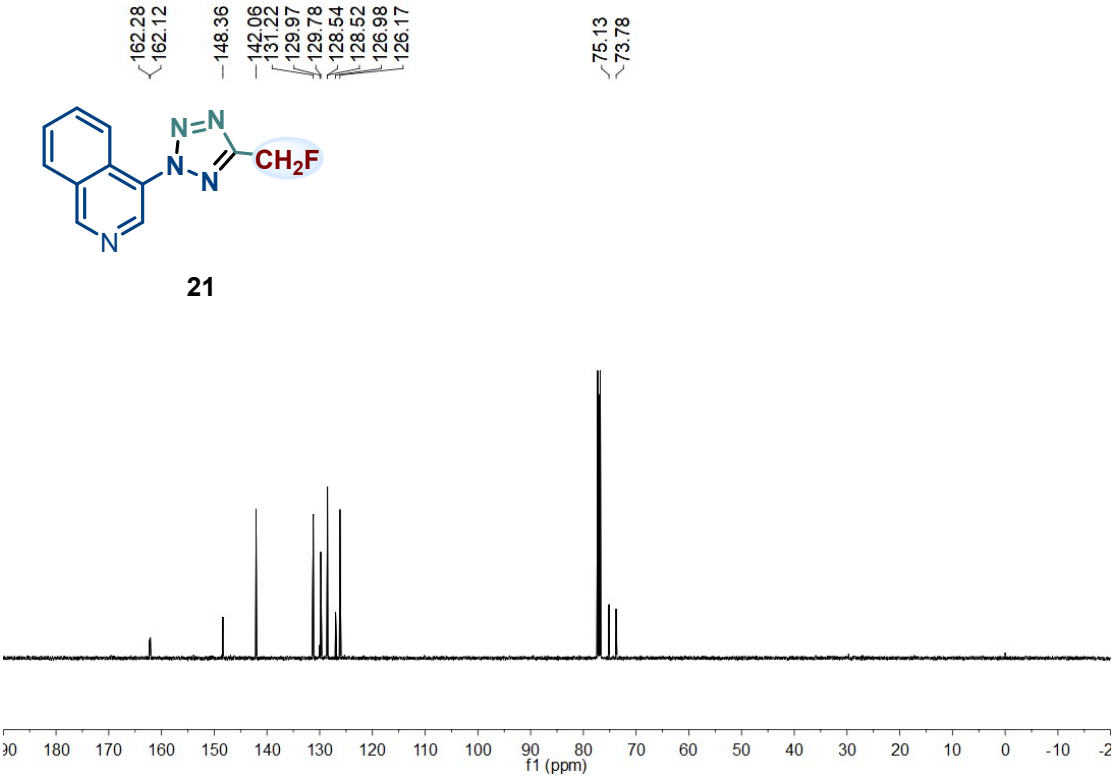
20

-217.219
-217.322
-217.421
40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -220 -230 -240

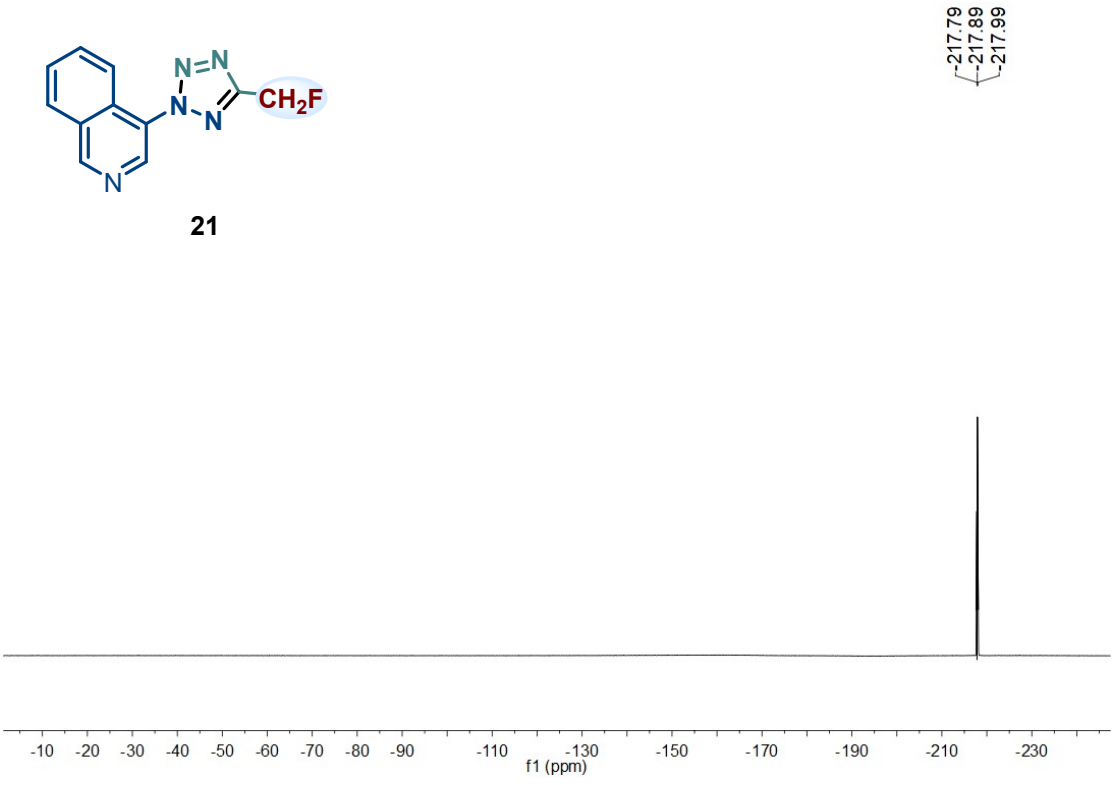


21

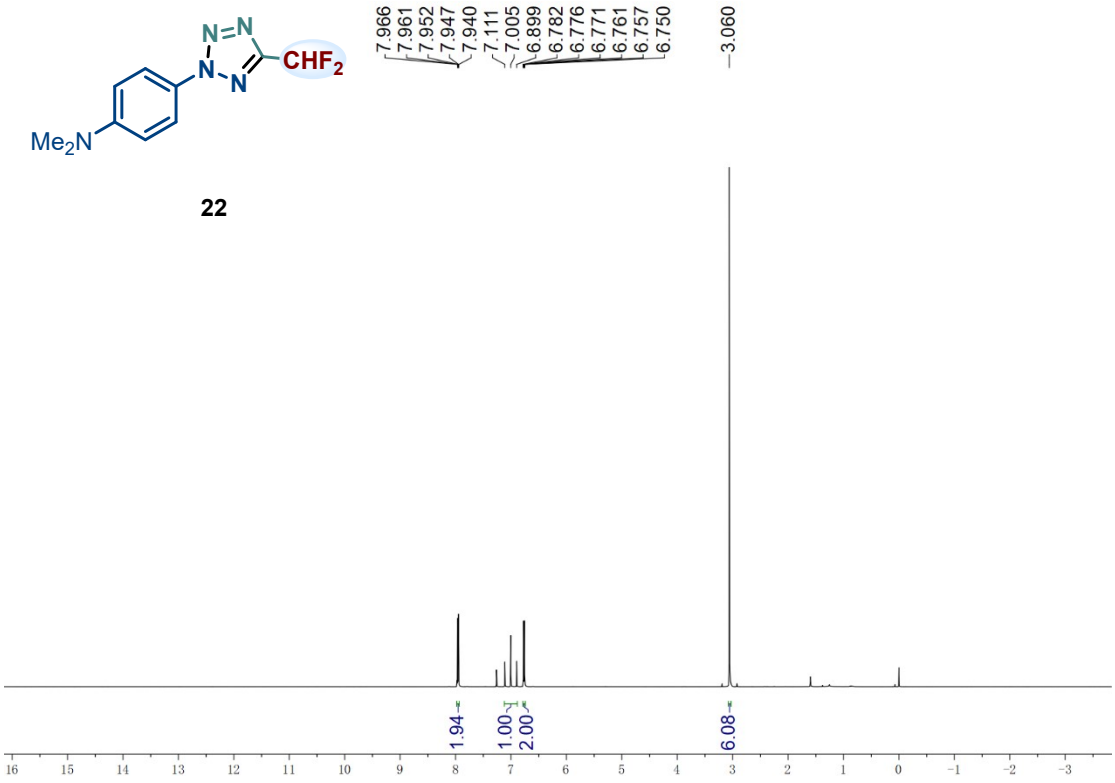
9.699
9.694
8.882
8.877
8.222
8.205
7.993
7.977
7.845
7.708
7.692
5.817
5.722
1.00
1.03
1.04
1.07
1.06
1.07
2.16
13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)


162.28
162.12
148.36
142.06
131.22
129.97
129.78
128.54
128.52
126.98
126.17
75.13
73.78
N=N
N
N
CH2F
N
f1 (ppm)

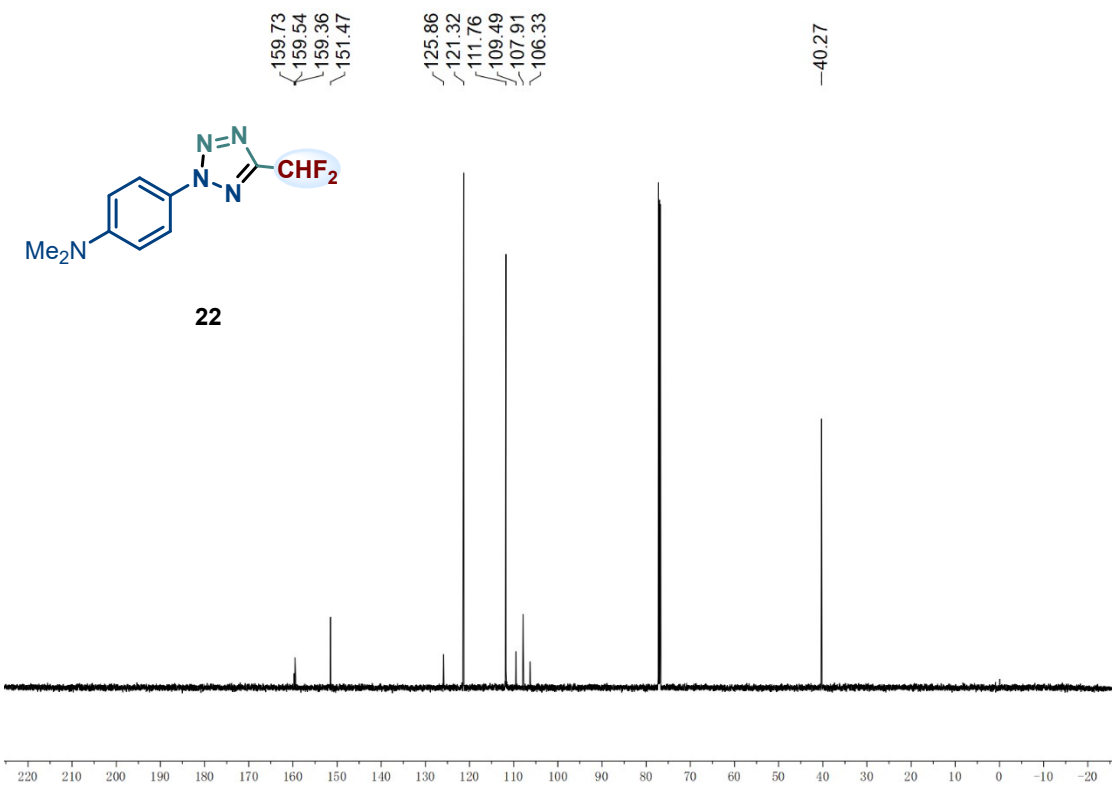
21


-217.79
-217.89
-217.99
N=N
N
N
CH2F
N
f1 (ppm)

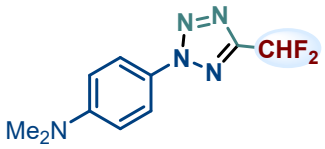
21


7.966
7.961
7.952
7.947
7.940
7.111
7.005
6.899
6.782
6.776
6.771
6.761
6.757
6.750
3.060
1.94
1.00
2.00
6.08

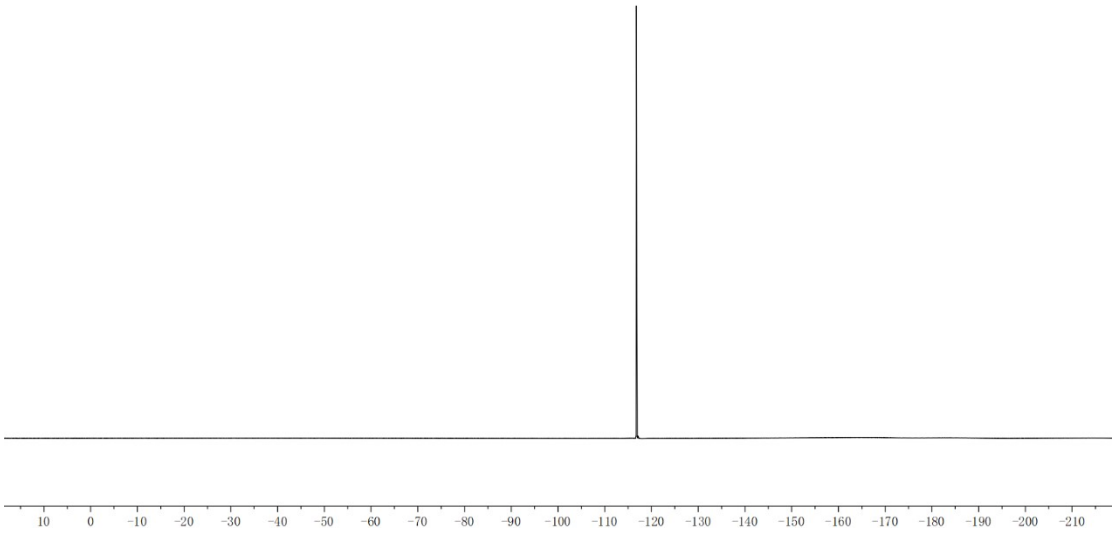
22

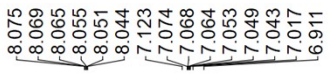

159.73
159.54
159.36
151.47
125.86
121.32
111.76
109.49
107.91
106.33
40.27

22

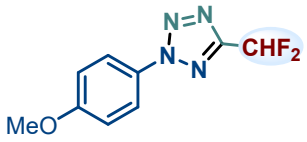

N=N
N
N
CHF2
Me2N

22

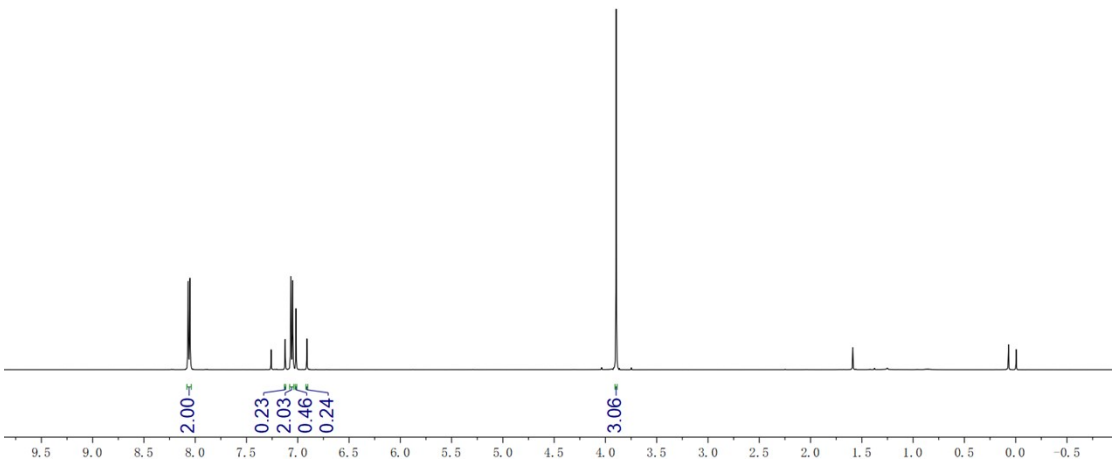

-116.764
-116.858
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210

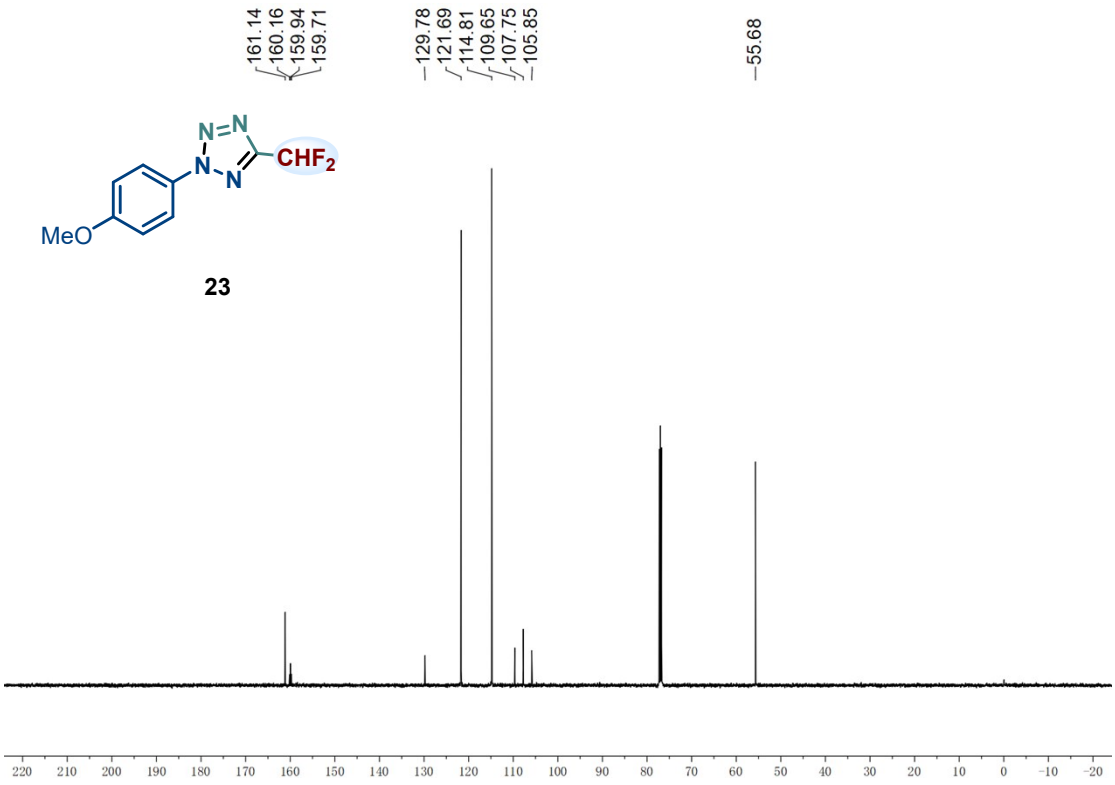

8.075
8.069
8.065
8.055
8.051
8.044
7.123
7.074
7.068
7.064
7.053
7.049
7.043
7.017
6.911

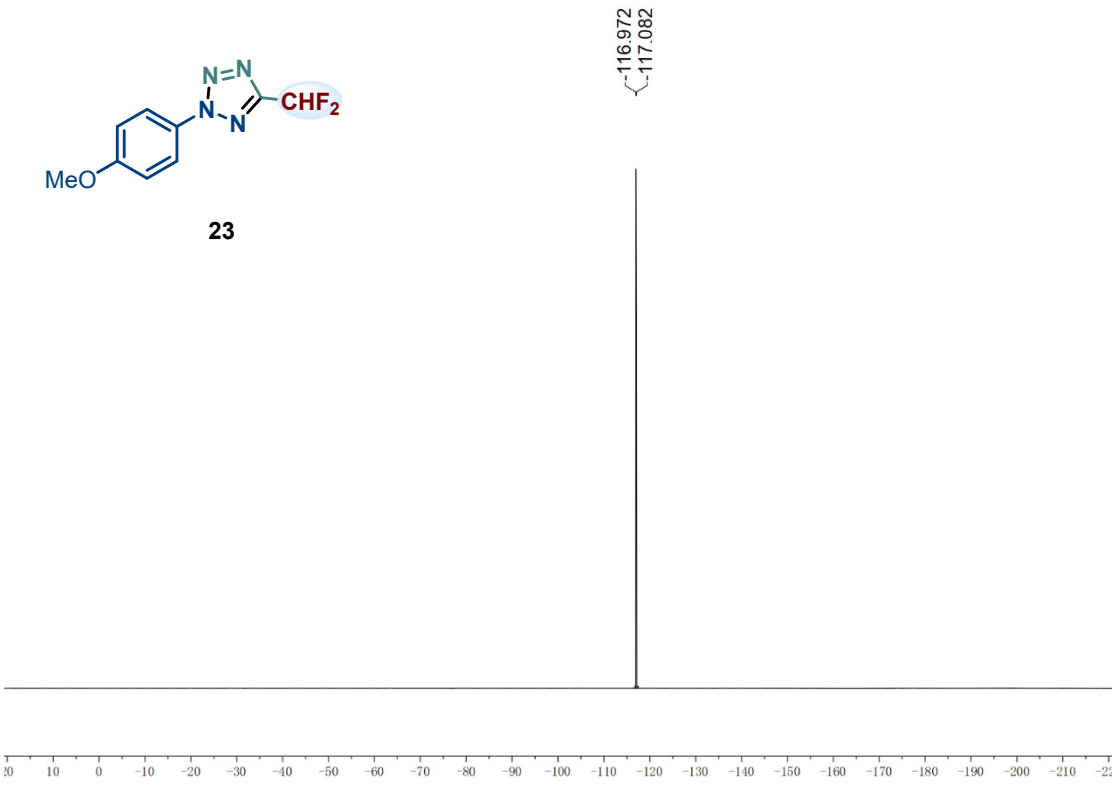

3.895

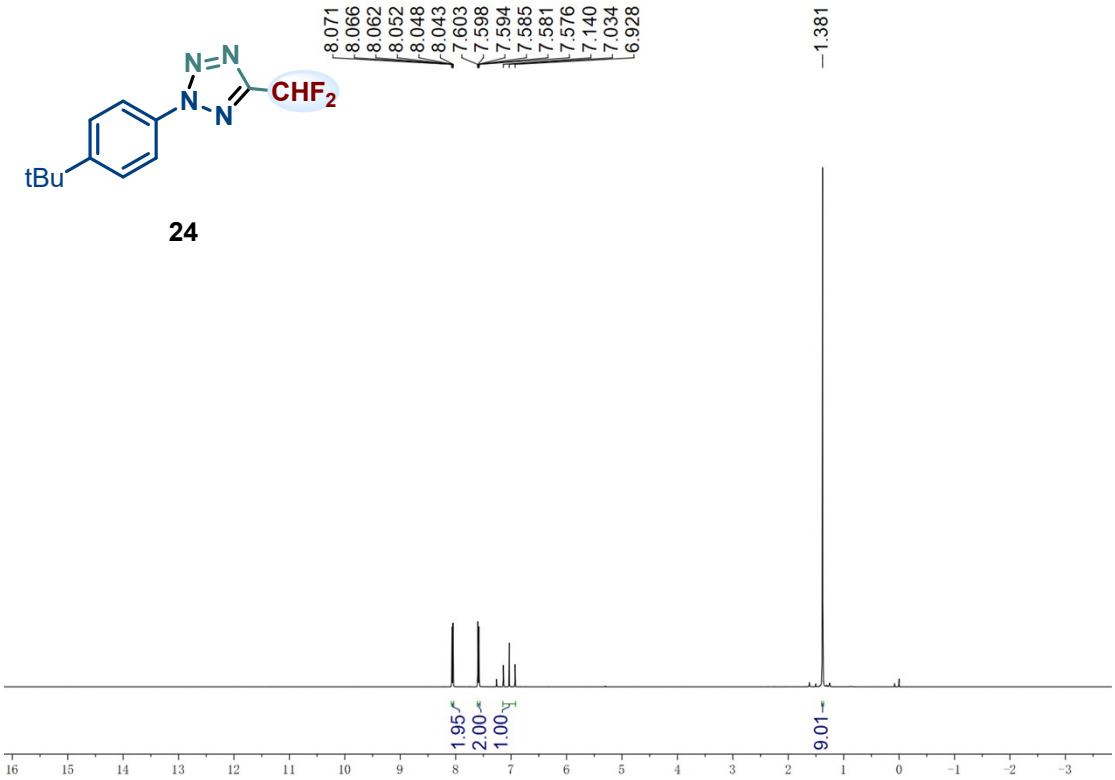

N=N
N
N
CHF2
MeO

23

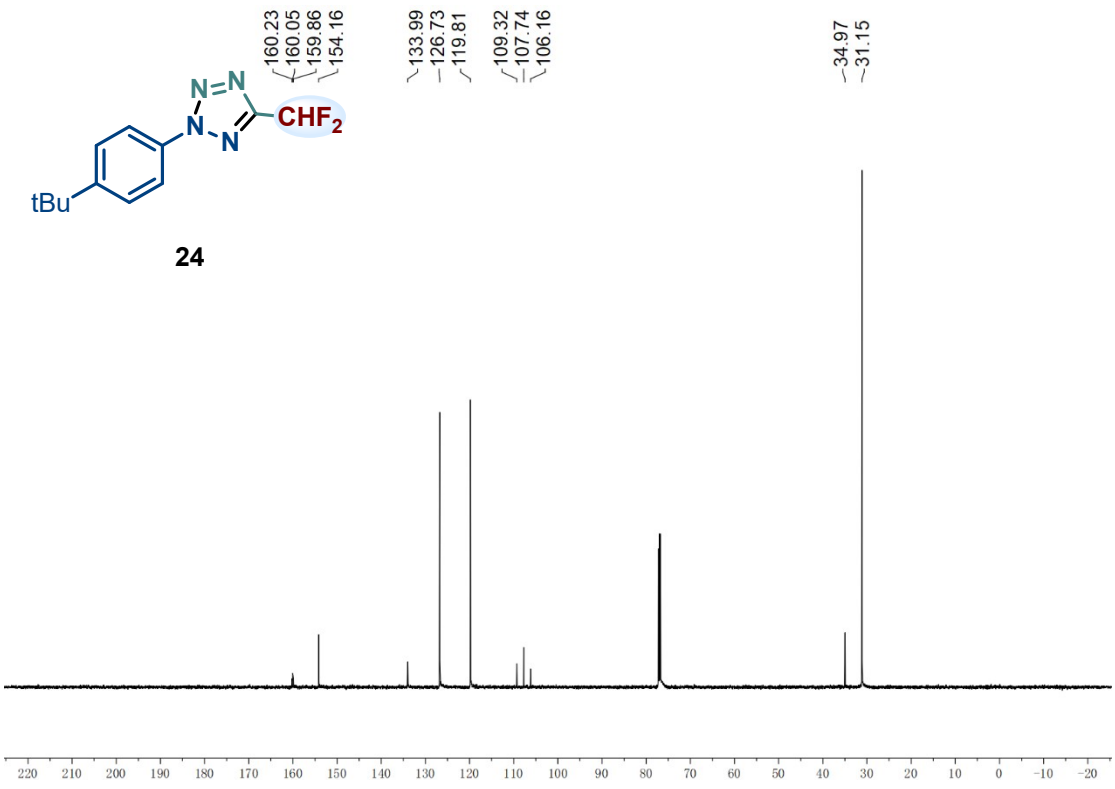

2.00
0.23
2.03
0.46
0.24
3.06
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5


161.14
160.16
159.94
159.71
129.78
121.69
114.81
109.65
107.75
105.85
55.68
N=N
N
N
CHF2
MeO
23
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20

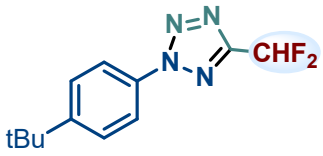

116.972
117.082
N=N
N
N
CHF2
MeO
23
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210


8.071
8.066
8.062
8.052
8.048
8.043
7.603
7.598
7.594
7.585
7.581
7.576
7.140
7.034
6.928
1.381
N=N
N
N
CHF2
tBu
1.95
2.00
1.00
9.01

24

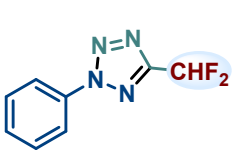

160.23
160.05
159.86
154.16
133.99
126.73
119.81
109.32
107.74
106.16
34.97
31.15
N=N
N
N
CHF2
tBu

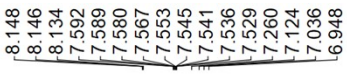
24


N=N
N
N
CHF2
tBu

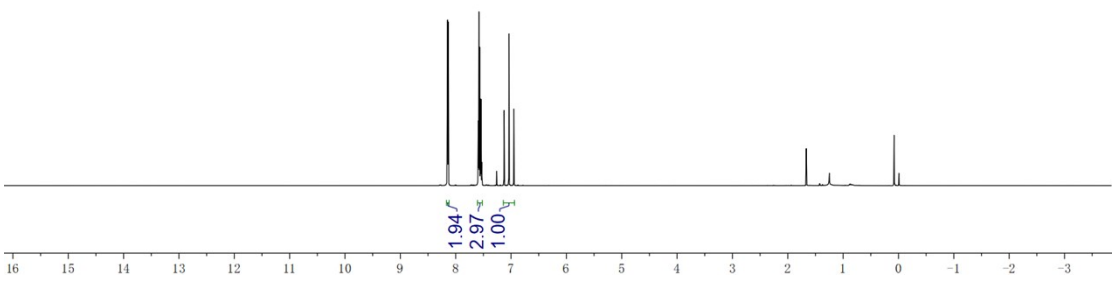
24

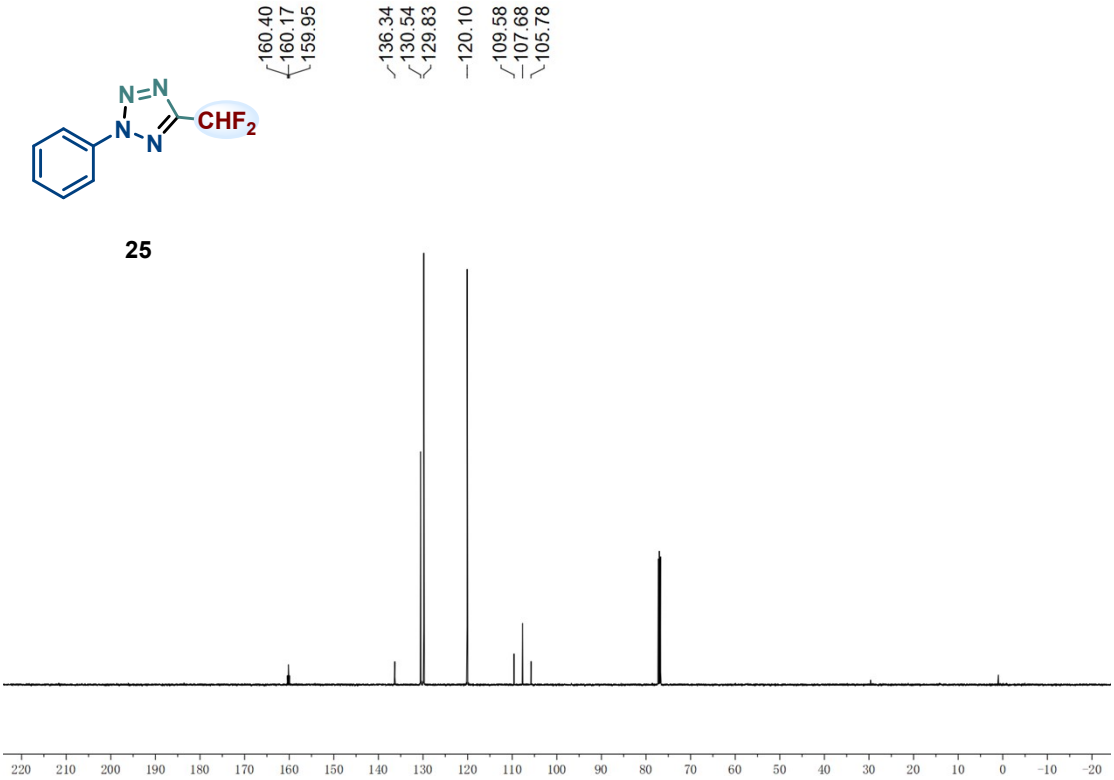
-117.023
-117.117
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210

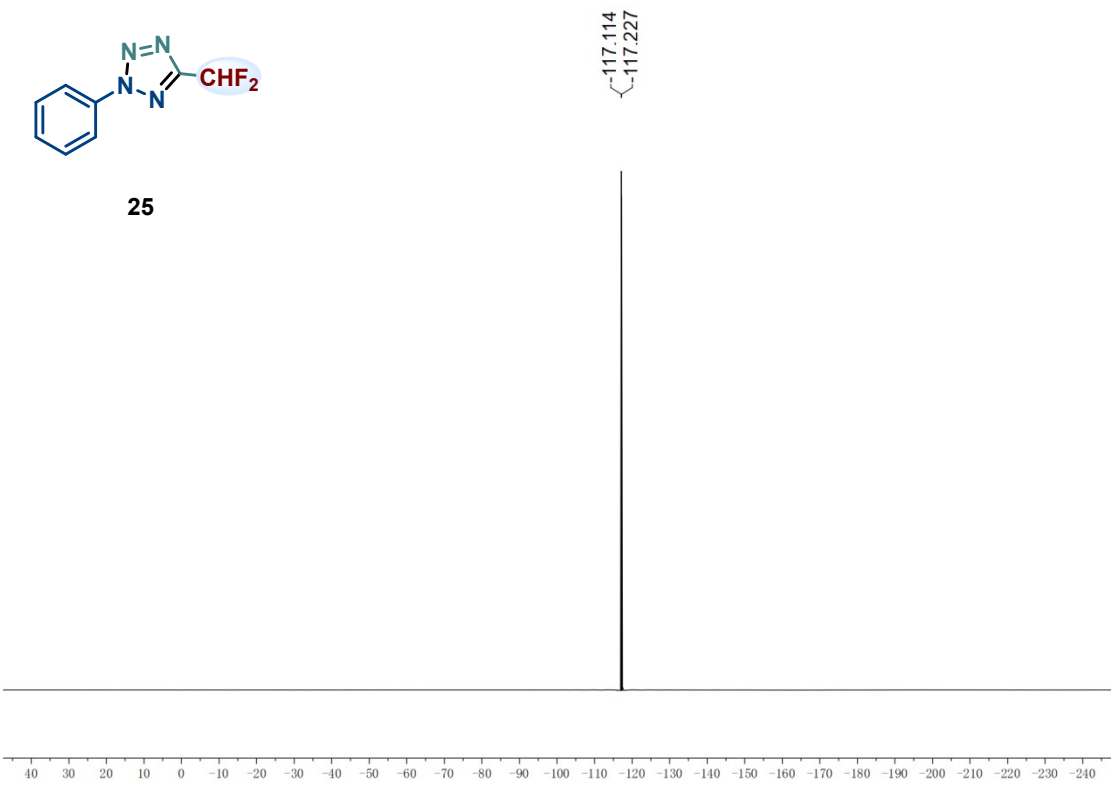

N=N
N
N
CHF2

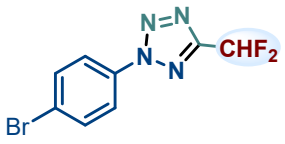

8.148
8.146
8.134
7.592
7.589
7.580
7.567
7.553
7.545
7.541
7.536
7.529
7.260
7.124
7.036
6.948

25

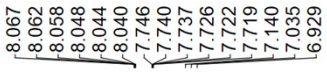

1.94
2.97
1.00
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3

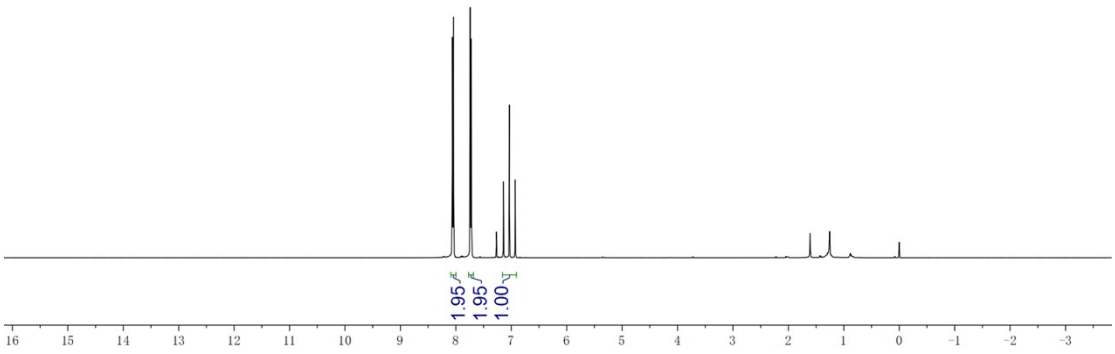

160.40
160.17
159.95
136.34
130.54
129.83
120.10
109.58
107.68
105.78
CHF2
25

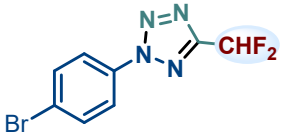

117.114
117.227
CHF2
25


N=N
N
N
CHF2
Br

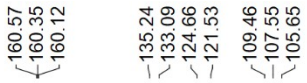
26


8.067
8.062
8.058
8.048
8.044
8.040
7.746
7.740
7.737
7.726
7.722
7.719
7.140
7.035
6.929

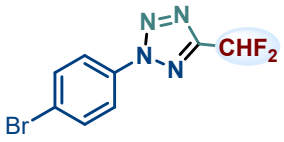

1.95
1.95
1.00
16
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
−1
−2
−3


N=N
N
N
CHF2
Br

26

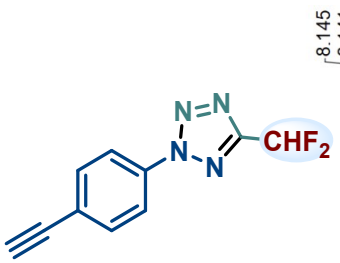

160.57
160.35
160.12
135.24
133.09
124.66
121.53
109.46
107.55
105.65

220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
−20


N=N
N
N
CHF2
Br

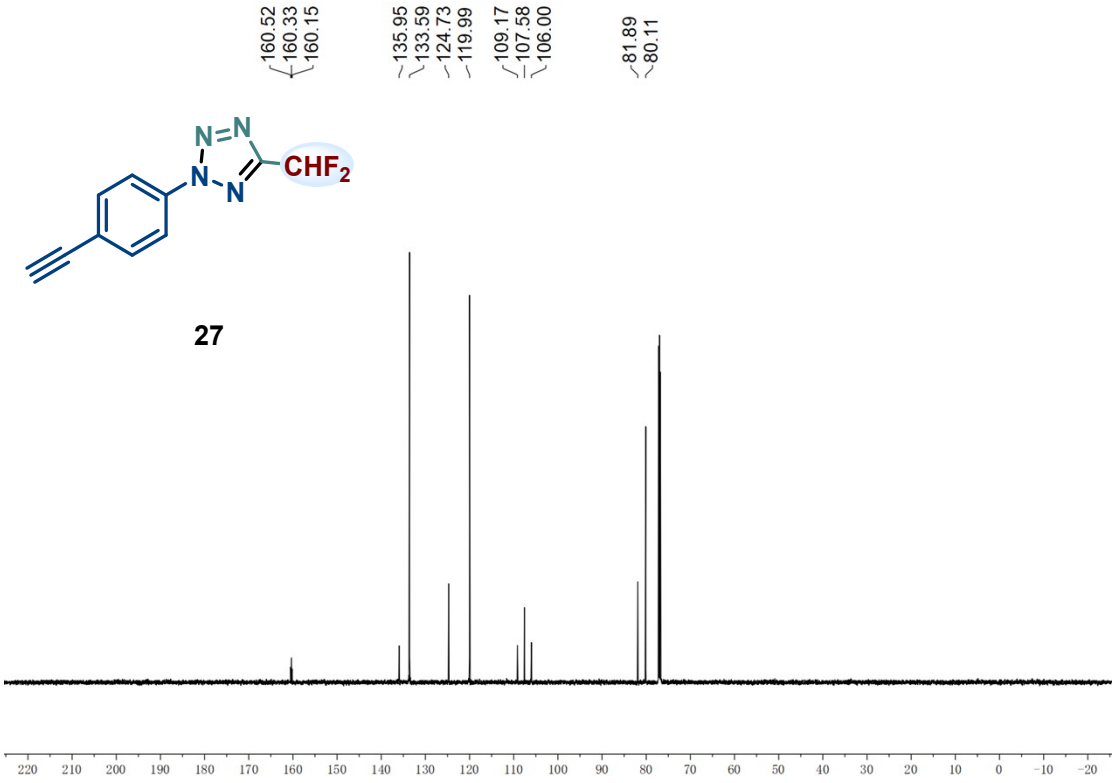
26

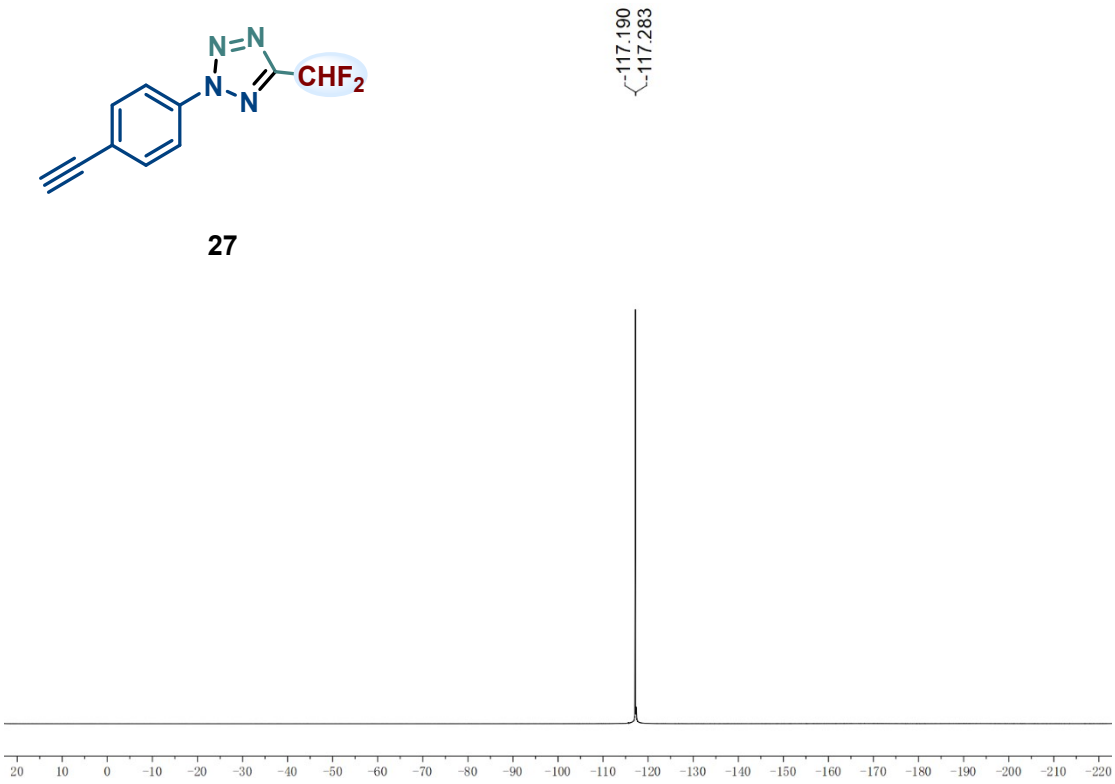
-117.180
-117.292
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210

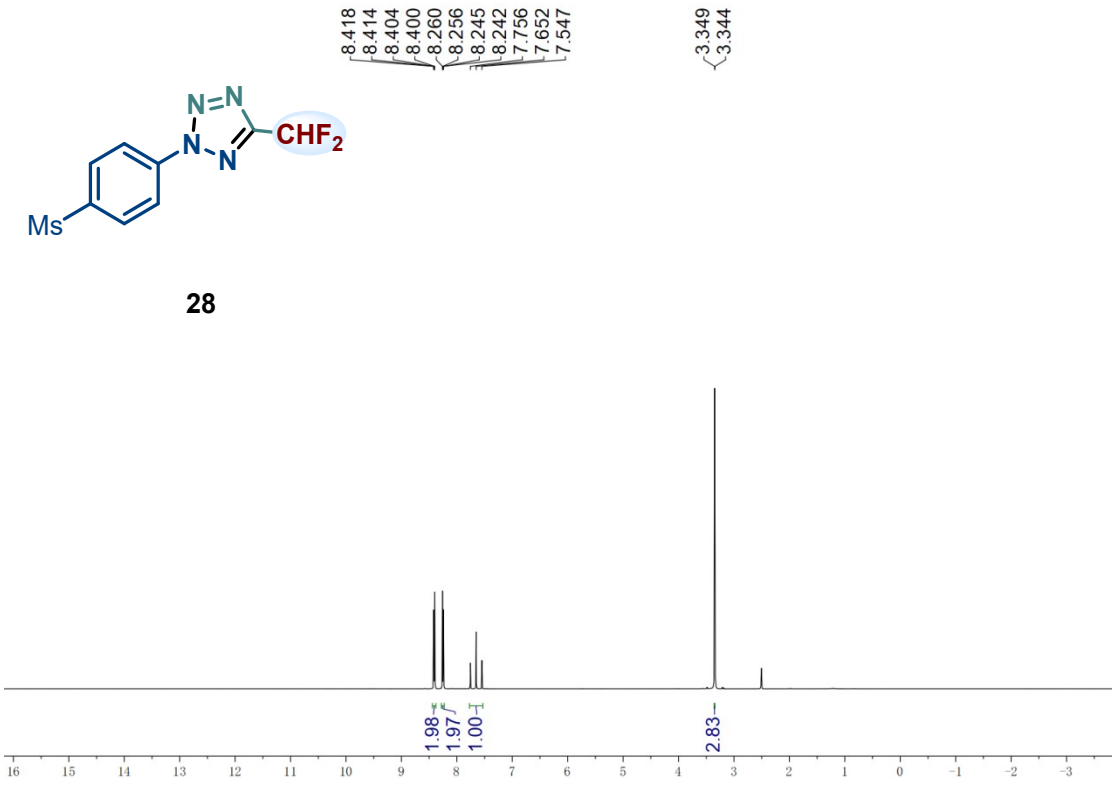

N=N
N
N
CHF2

27

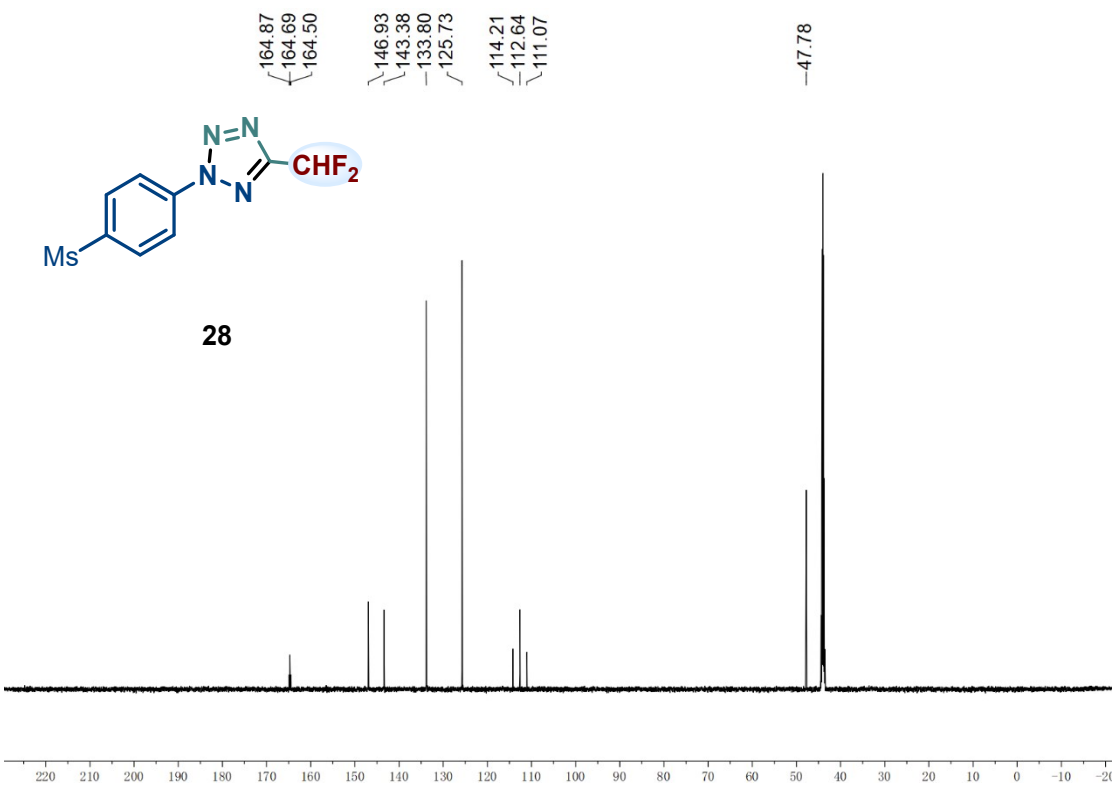
8.145
8.141
8.131
8.128
7.702
7.698
7.688
7.684
7.141
7.035
6.929
3.250
1.98
1.97
1.00
0.96
13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1


160.52
160.33
160.15
135.95
133.59
124.73
119.99
109.17
107.58
106.00
81.89
80.11
N=N
N
N
CHF2
27
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20

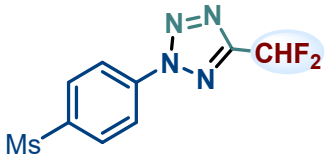

-117.190
-117.283
N=N
N
N
CHF2
27
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -220


8.418
8.414
8.404
8.400
8.260
8.256
8.245
8.242
7.756
7.652
7.547
3.349
3.344
N=N
N
N
CHF2
Ms
1.98
1.97
1.00
2.83

28

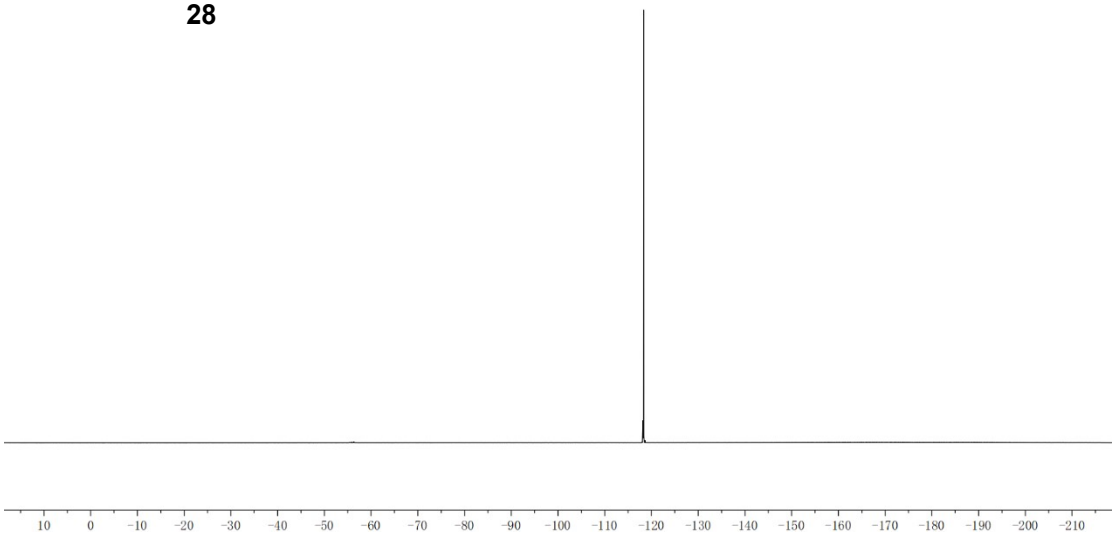

164.87
164.69
164.50
146.93
143.38
133.80
125.73
114.21
112.64
111.07
47.78
N=N
N
N
CHF2
Ms

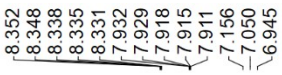
28

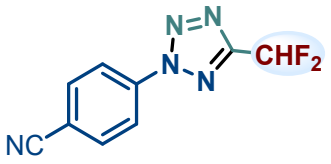

N=N
N
N
CHF2
Ms


-118.206
-118.299

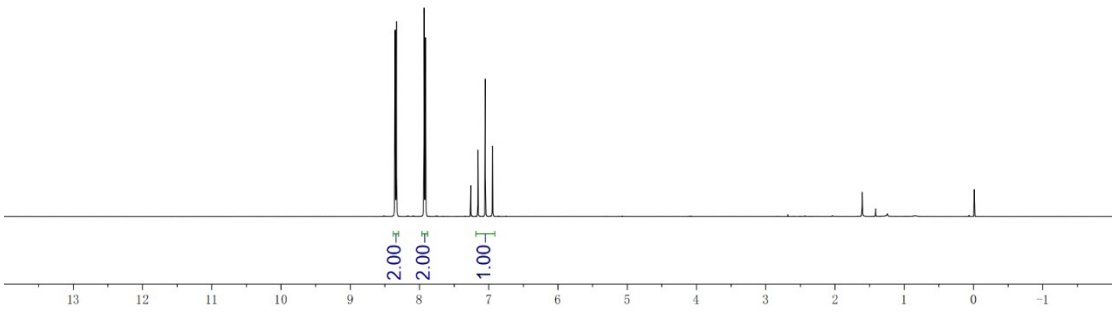
28

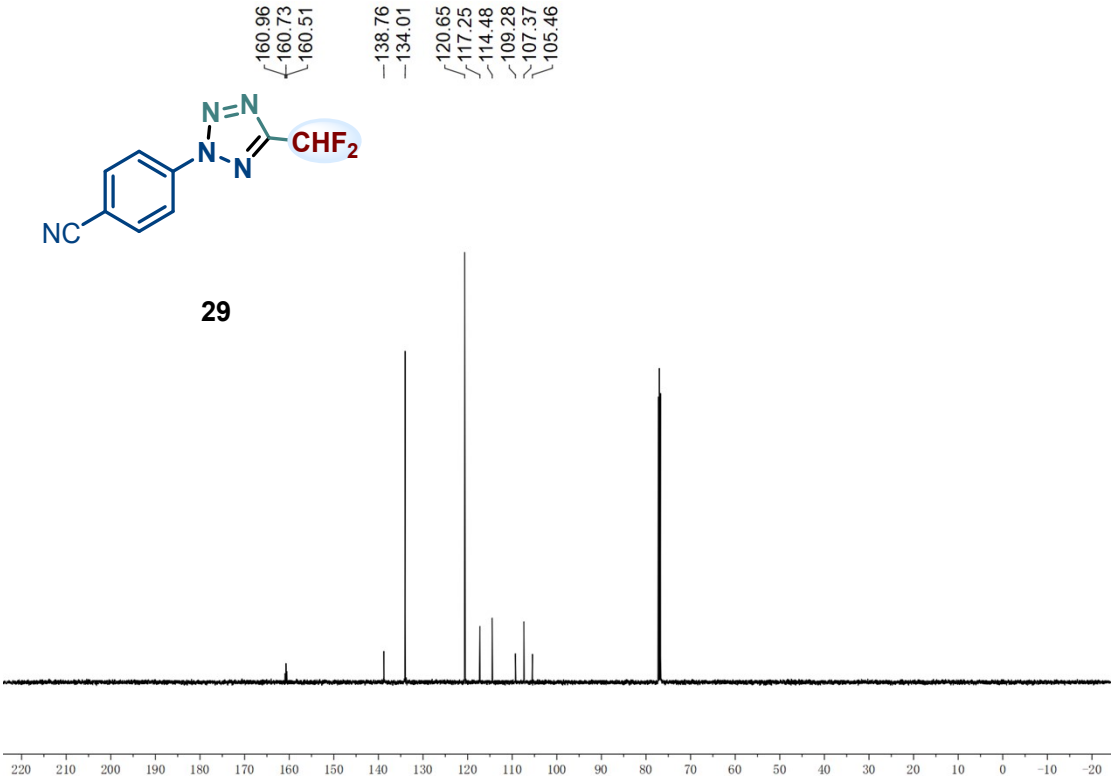

10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210


8.352
8.348
8.338
8.335
8.331
7.932
7.929
7.918
7.915
7.911
7.156
7.050
6.945

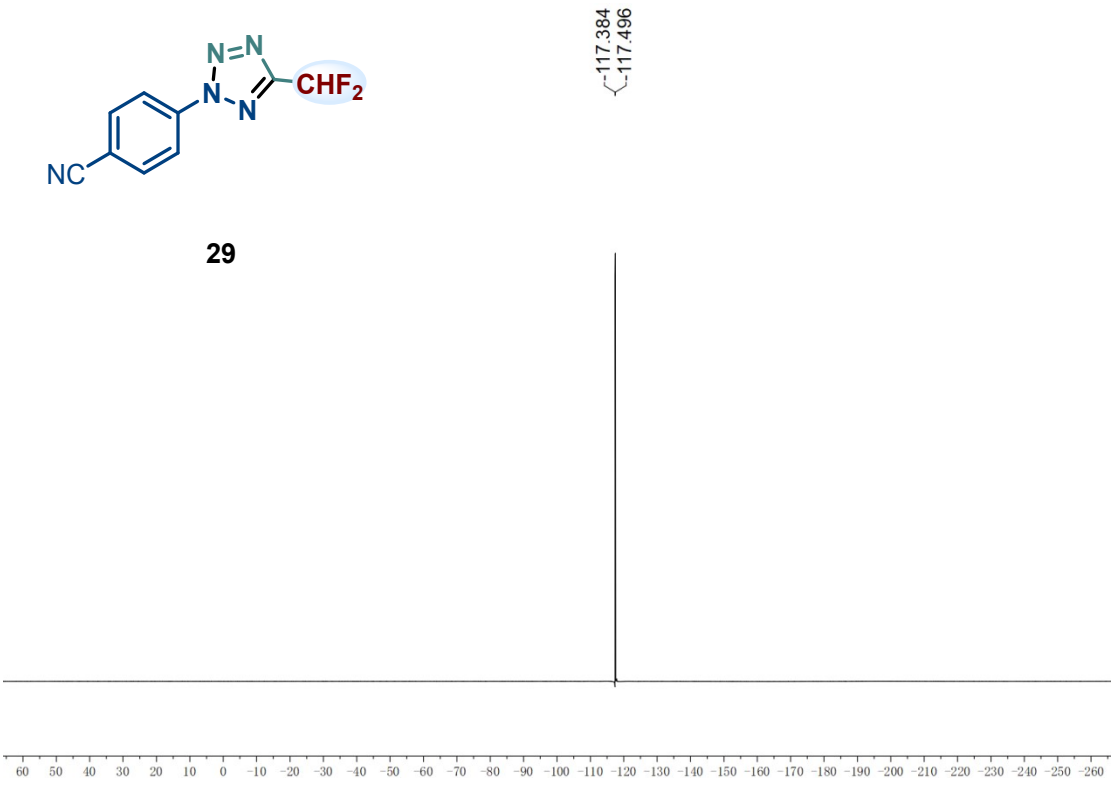

N=N
N
N
CHF2
NC

29

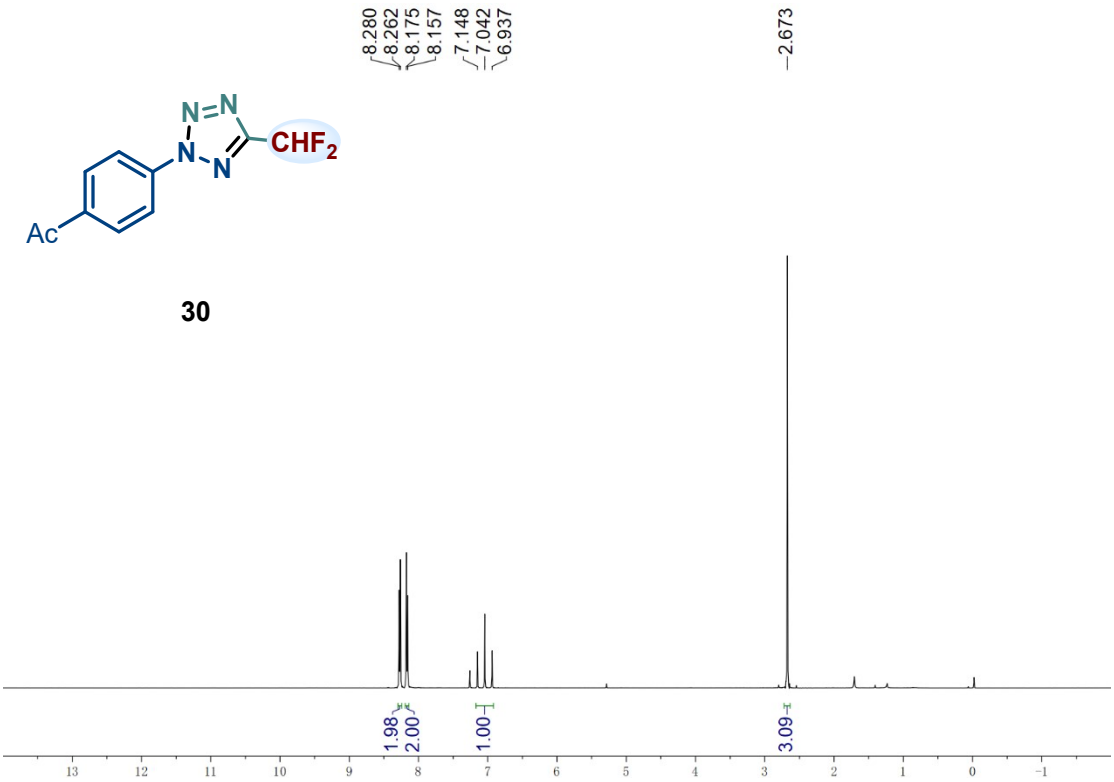

2.00
2.00
1.00
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1


160.96
160.73
160.51
138.76
134.01
120.65
117.25
114.48
109.28
107.37
105.46
N=N
N
N
CHF2
NC
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20

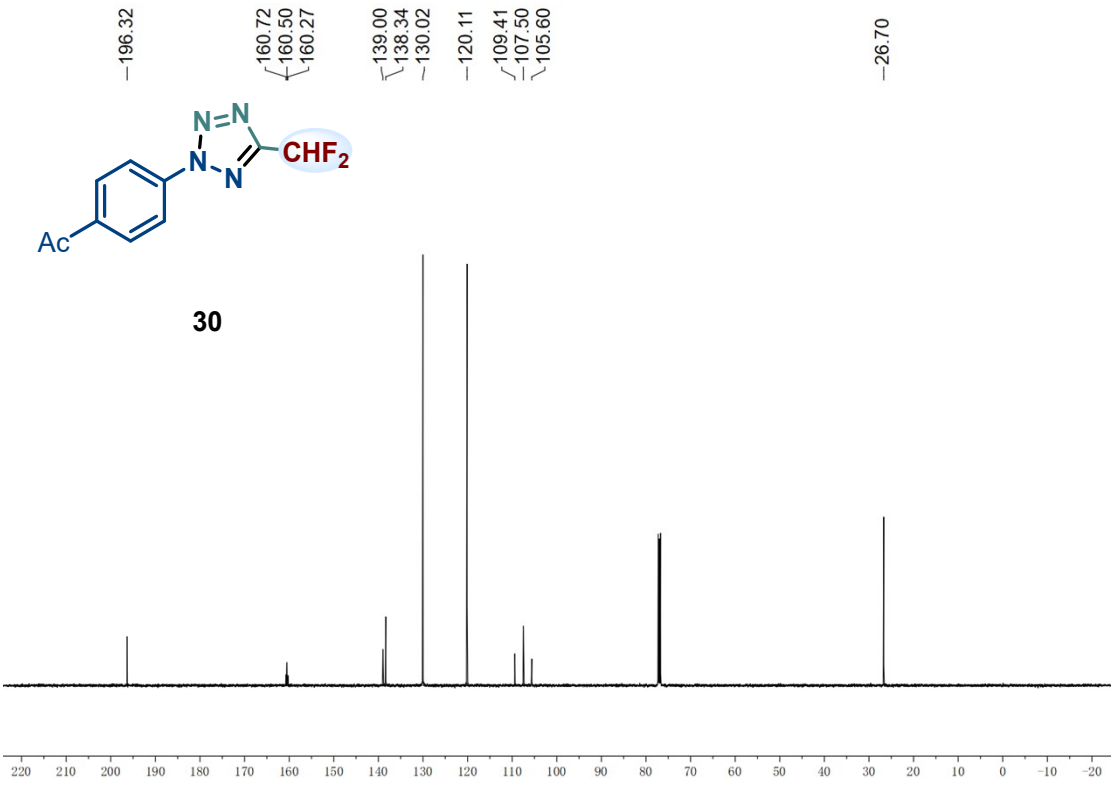
29


-117.384
-117.496
N=N
N
N
CHF2
NC
60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -220 -230 -240 -250 -260

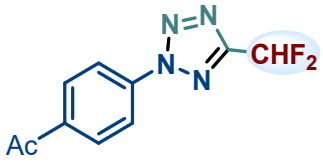
29


8.280
8.262
8.175
8.157
7.148
7.042
6.937
2.673
N=N
N
N
CHF2
Ac
1.98
2.00
1.00
3.09
13
12
11
10
9
8
7
6
5
4
3
2
1
0
−1

30

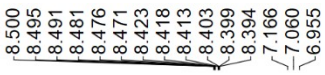

196.32
160.72
160.50
160.27
139.00
138.34
130.02
120.11
109.41
107.50
105.60
26.70
N=N
N
N
CHF2
Ac
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
−20

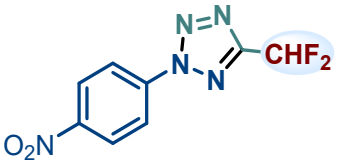
30


N=N
N
N
CHF2
Ac

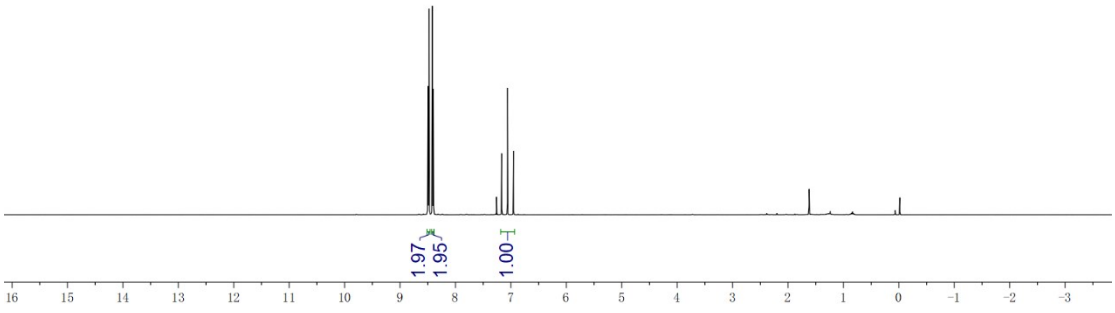
30

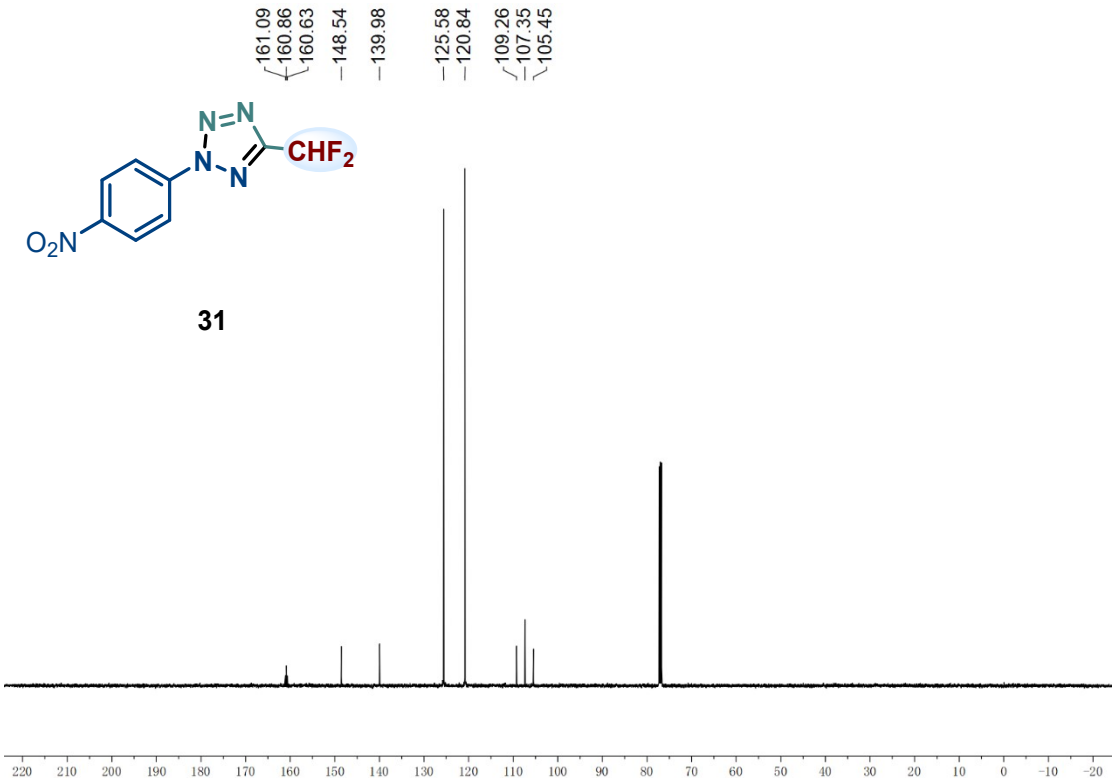
-117.290
-117.402
5 10 5 0 -5 -10 -15 -20 -25 -30 -35 -40 -45 -50 -55 -60 -65 -70 -75 -80 -85 -90 -95 -100 -105 -110 -115 -120 -125 -130


8.500
8.495
8.491
8.481
8.476
8.471
8.423
8.418
8.413
8.403
8.399
8.394
7.166
7.060
6.955

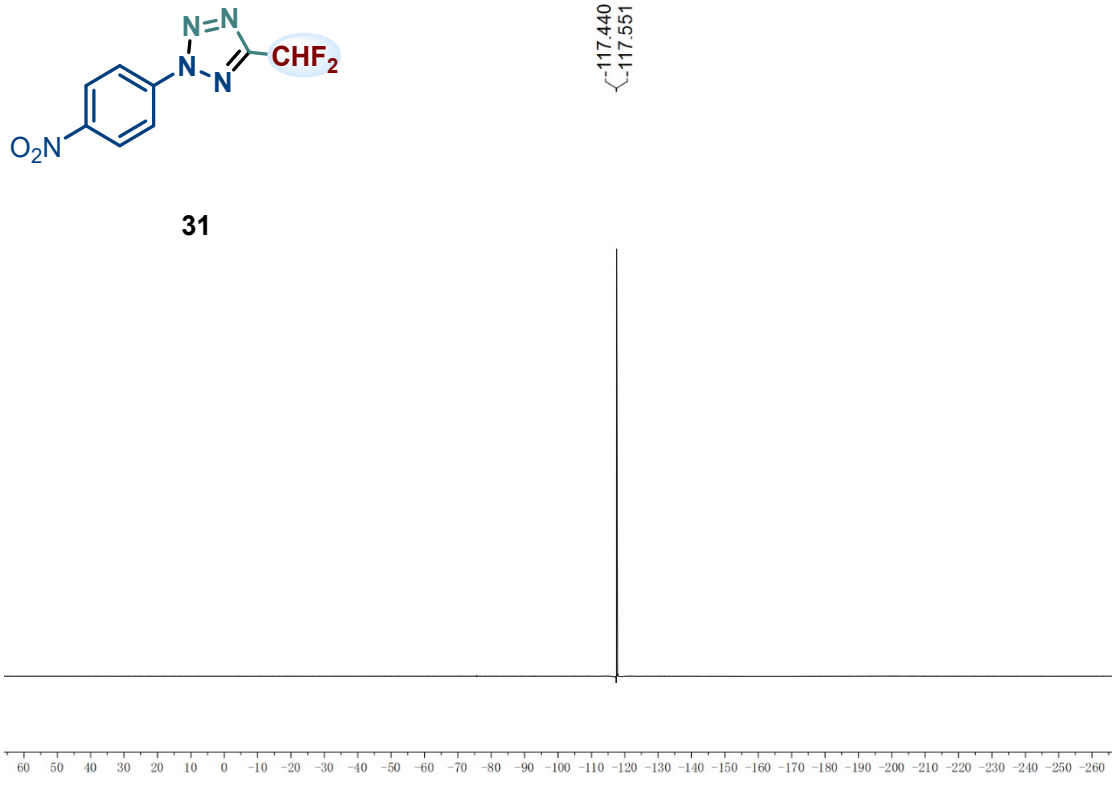

N=N
N
N
CHF2
O2N

31

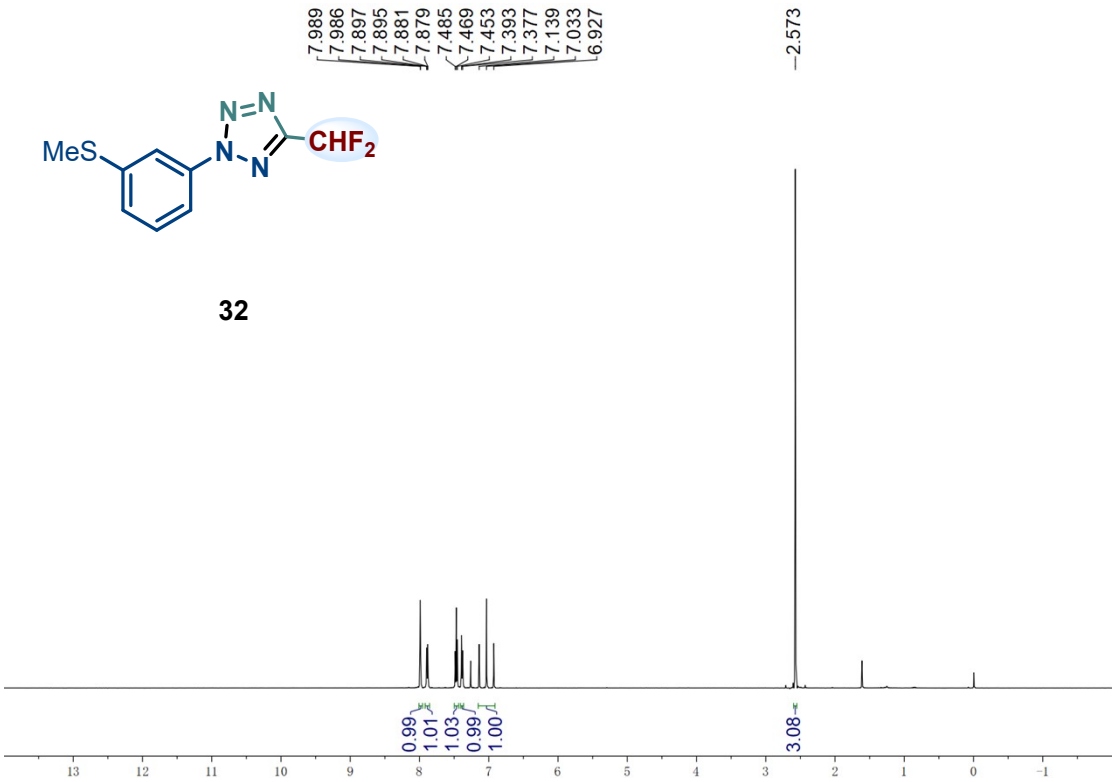

1.97
1.95
1.00
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3


161.09
160.86
160.63
148.54
139.98
125.58
120.84
109.26
107.35
105.45
N=N
N
N
CHF2
O2N
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20

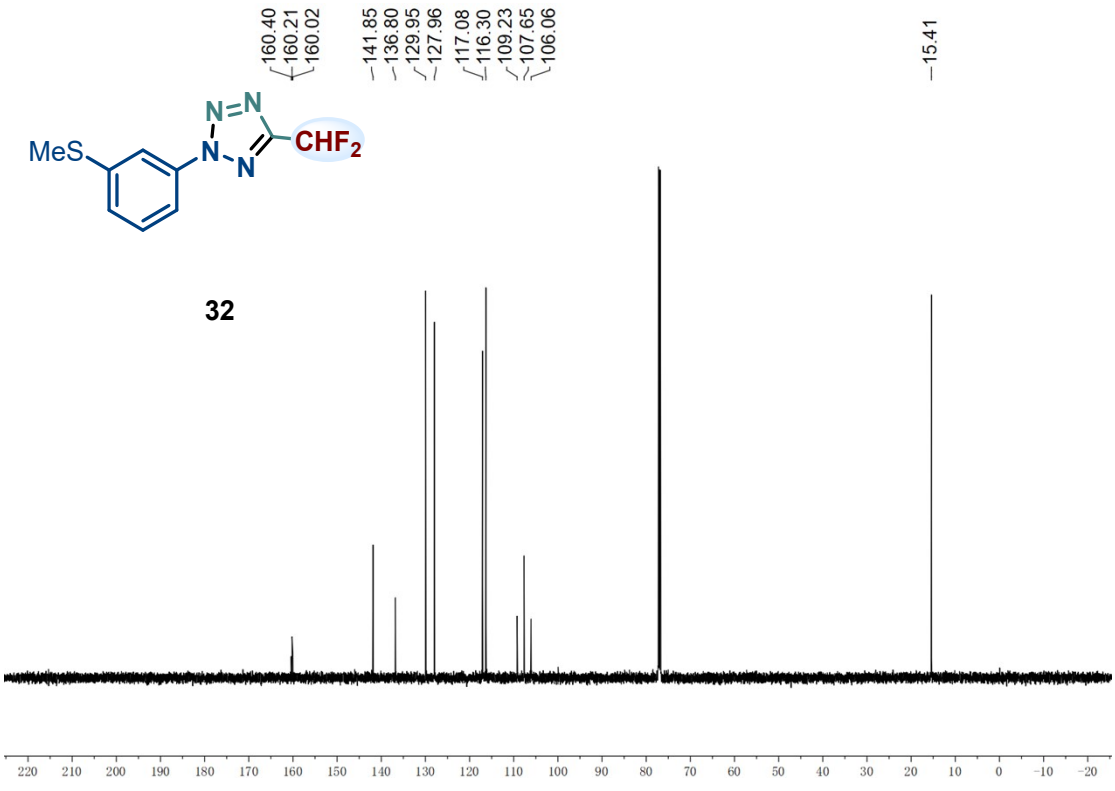
31


-117.440
-117.551
N=N
N
N
CHF2
O2N
60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -220 -230 -240 -250 -260

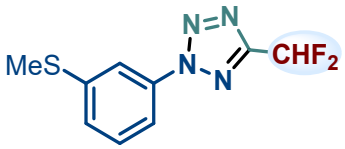
31


7.989
7.986
7.897
7.895
7.881
7.879
7.485
7.469
7.453
7.393
7.377
7.139
7.033
6.927
2.573
MeS
N=N
N
N
CHF2
0.99
1.01
1.03
0.99
1.00
3.08

32

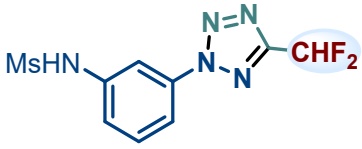

160.40
160.21
160.02
141.85
136.80
129.95
127.96
117.08
116.30
109.23
107.65
106.06
15.41
MeS
N=N
N
N
CHF2

32


MeS
N=N
N
N
CHF2

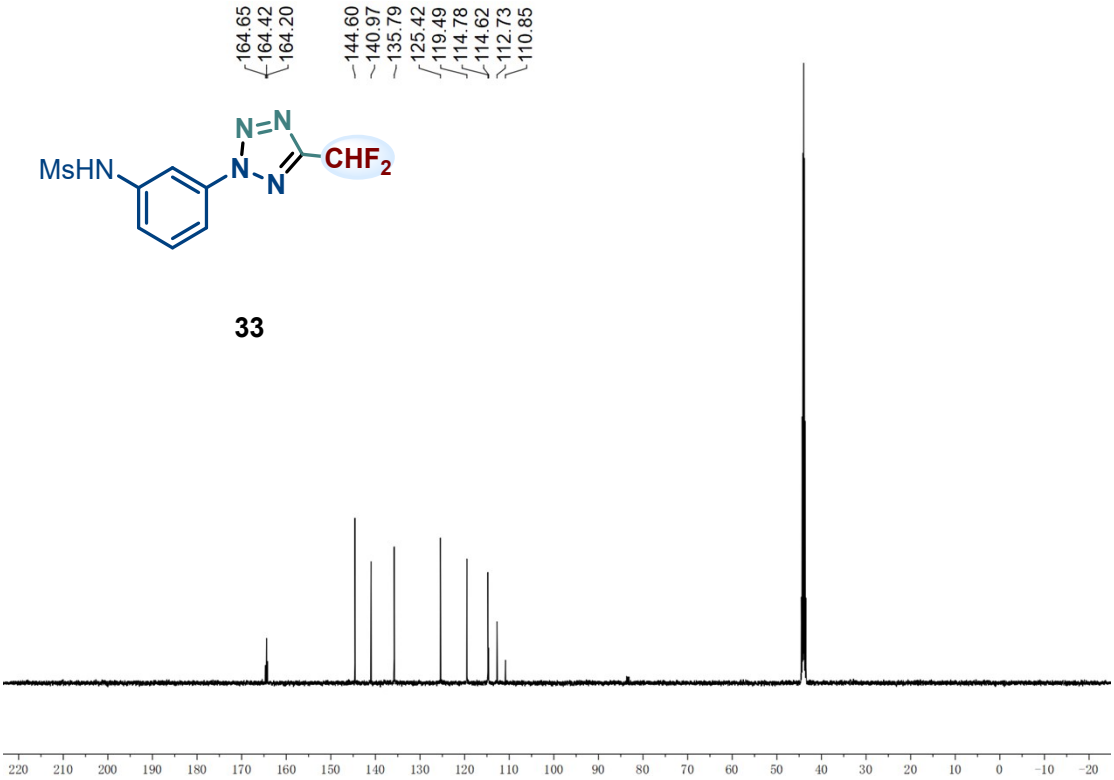
32

-117.120
-117.216
70
50
30
10
-10
-30
-50
-70
-90
-110
-130
-150
-170
-190
-210
-230
-250
-270

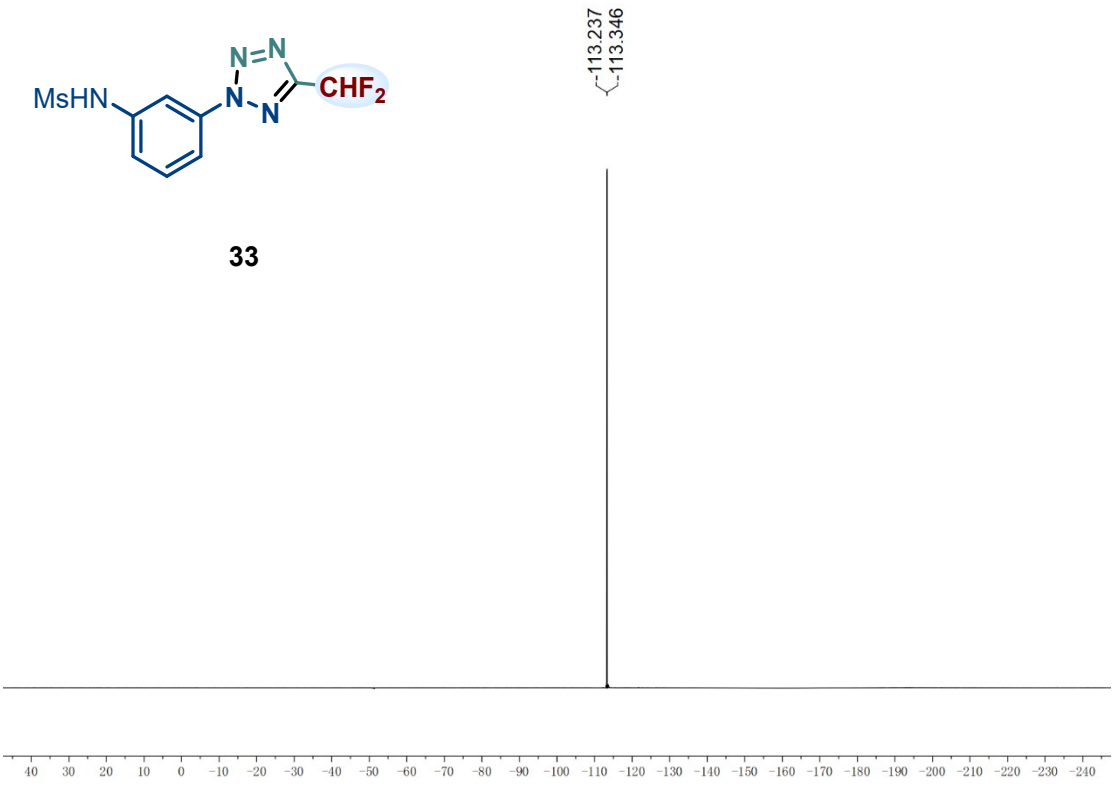

MsHN
N=N
N
N
CHF2

33

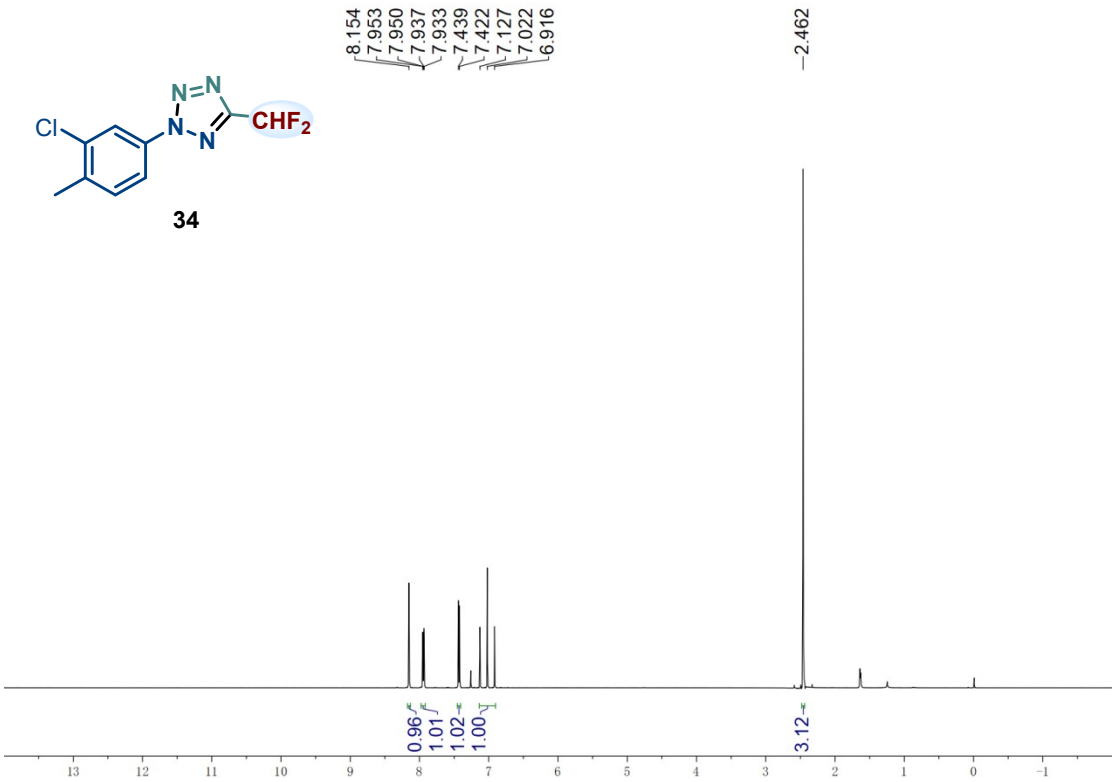
10.301
8.002
7.998
7.994
7.856
7.854
7.840
7.838
7.716
7.667
7.651
7.634
7.611
7.457
7.454
7.441
7.438
3.367
3.113
1.00
1.03
1.03
0.24
1.03
0.48
0.24
1.02
3.10
16
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
-3

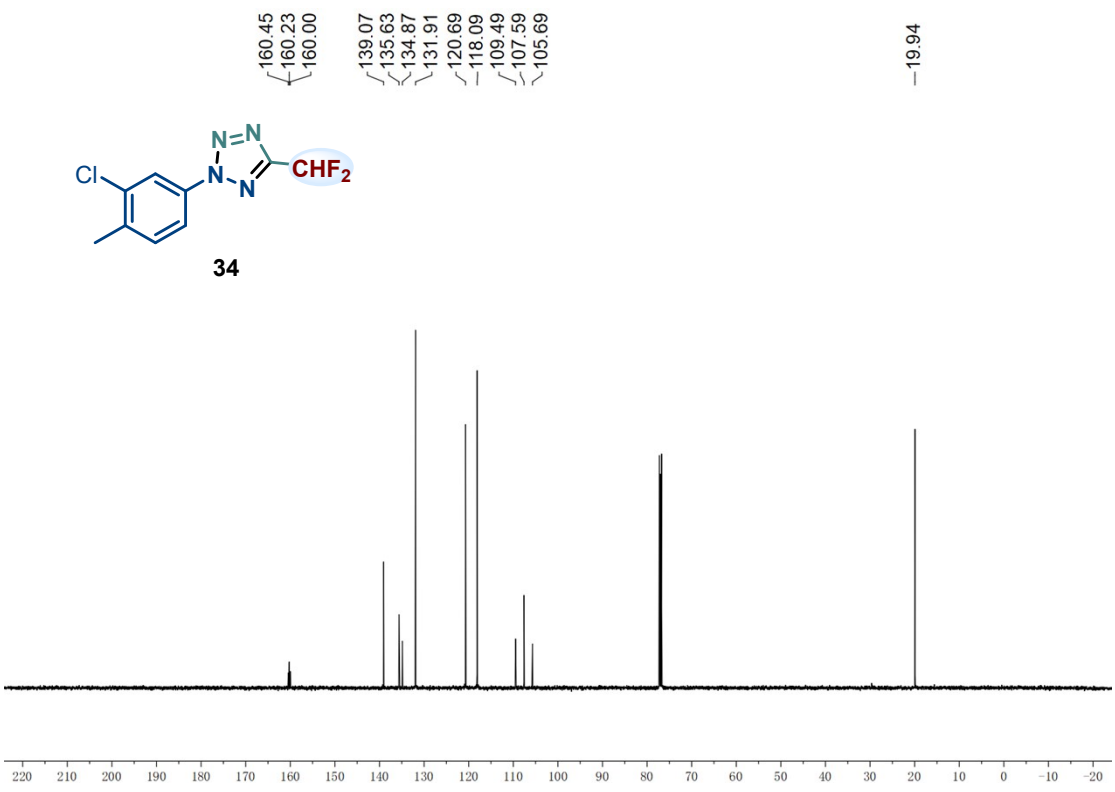

164.65
164.42
164.20
144.60
140.97
135.79
125.42
119.49
114.78
114.62
112.73
110.85
MsHN
N=N
N
N
CHF2
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20

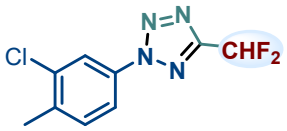
33


113.237
113.346
MsHN
N=N
N
N
CHF2
40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -220 -230 -240

33


8.154
7.953
7.950
7.937
7.933
7.439
7.422
7.127
7.022
6.916
2.462
Cl
N=N
N
N
CHF2
34
0.96
1.01
1.02
1.00
3.12
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1

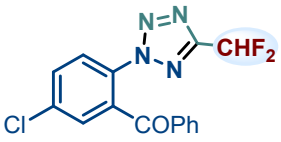

160.45
160.23
160.00
139.07
135.63
134.87
131.91
120.69
118.09
109.49
107.59
105.69
19.94
Cl
N=N
N
N
CHF2
34
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
-20


Cl
N=N
N
N
CHF2

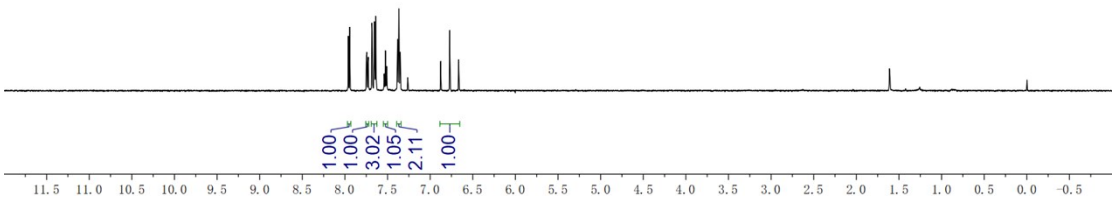
34

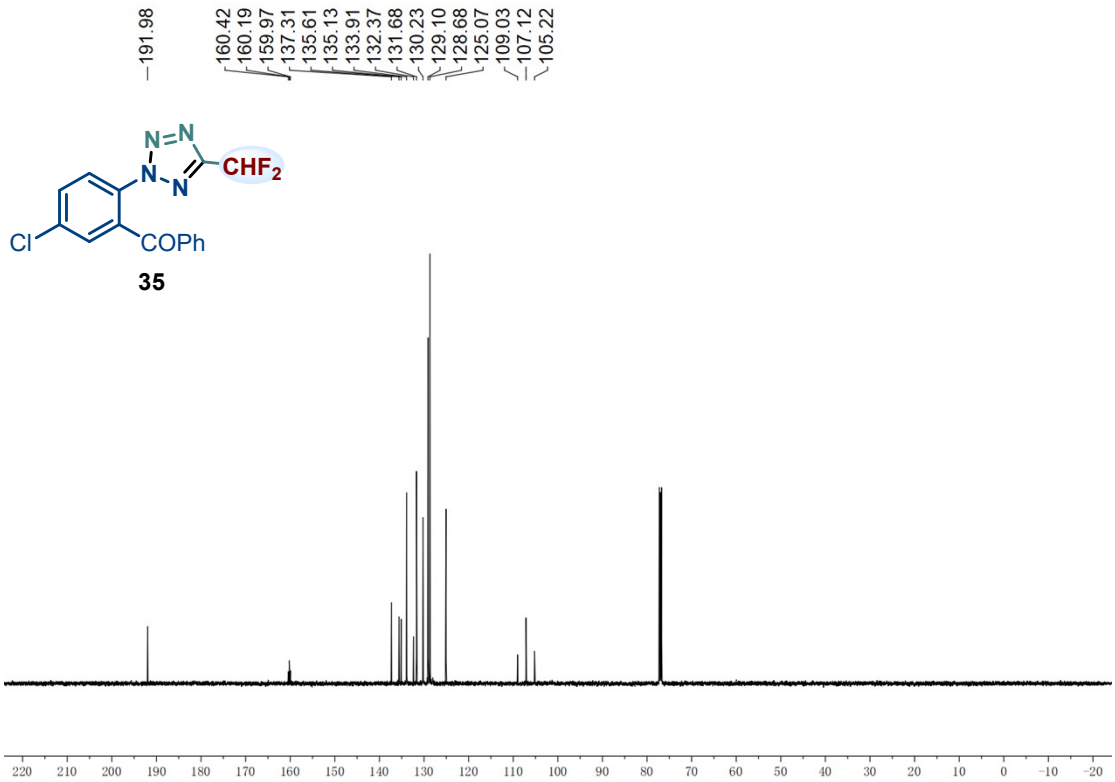
-117.186
-117.299
-94 -96 -98 -100 -102 -104 -106 -108 -110 -112 -114 -116 -118 -120 -122 -124 -126 -128 -130 -132 -134 -136 -138 -140 -142 -144 -146 -148

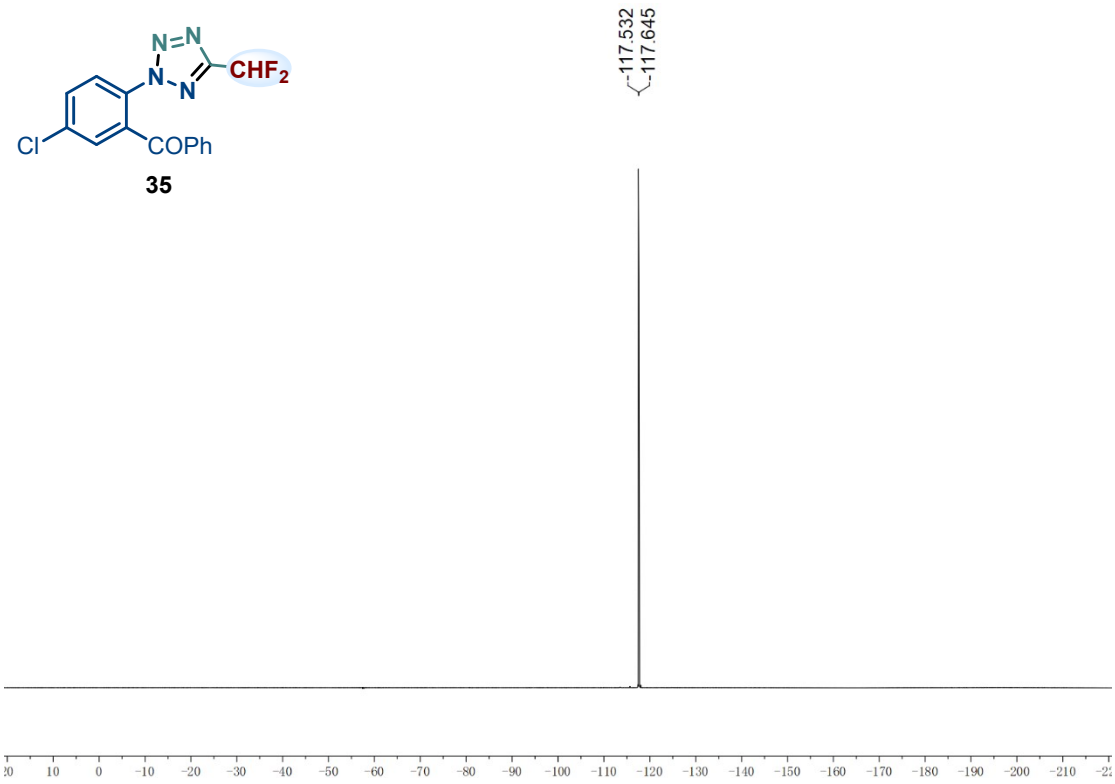

7.960
7.943
7.748
7.743
7.731
7.726
7.684
7.680
7.654
7.640
7.540
7.525
7.510
7.382
7.367
7.351
6.876
6.771
6.665

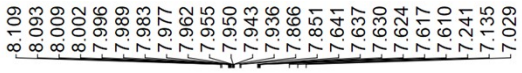

N=N
N
N
CHF2
Cl
COPh

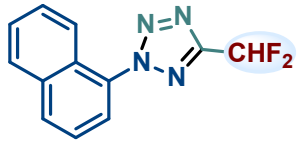
35


1.00
1.00
3.02
1.05
2.11
1.00
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5

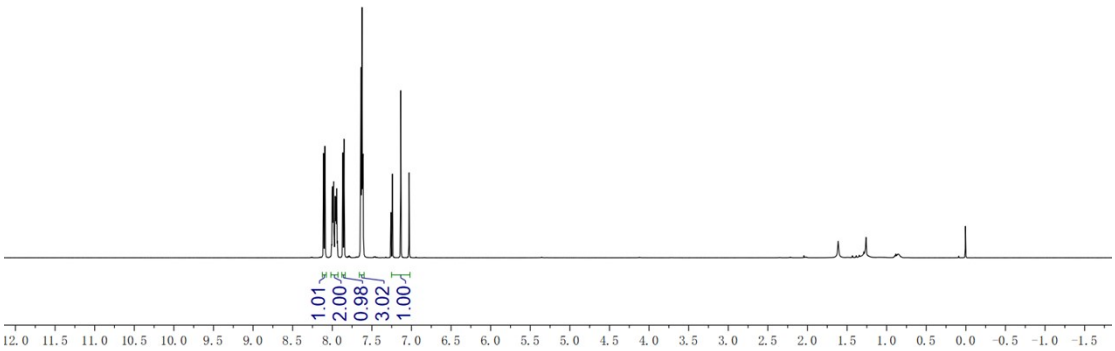

191.98
160.42
160.19
159.97
137.31
135.61
135.13
133.91
132.37
131.68
130.23
129.10
128.68
125.07
109.03
107.12
105.22
N=N
N
N
CHF2
Cl
COPh
35
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20

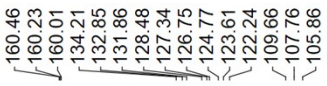

117.532
117.645
N=N
N
N
CHF2
Cl
COPh
35
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210

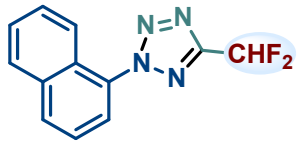

8.109
8.093
8.009
8.002
7.996
7.989
7.983
7.977
7.962
7.955
7.950
7.943
7.936
7.866
7.851
7.641
7.637
7.630
7.624
7.617
7.610
7.241
7.135
7.029


N=N
N
N
CHF2

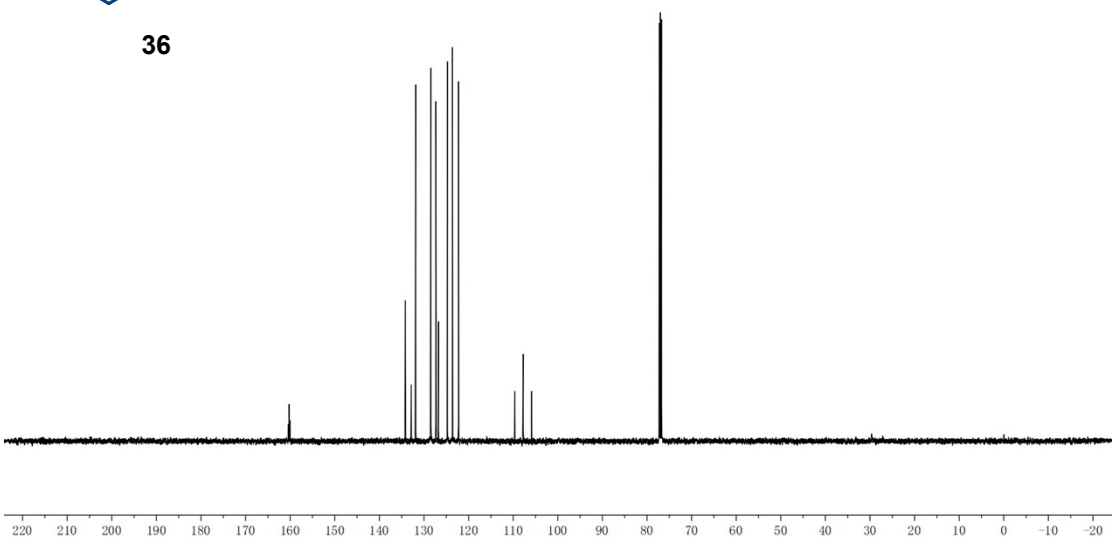
36

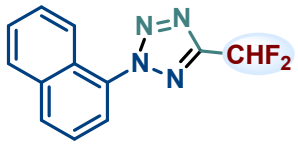

1.01
2.00
0.98
3.02
1.00
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5


160.46
160.23
160.01
134.21
132.85
131.86
128.48
127.34
126.75
124.77
123.61
122.24
109.66
107.76
105.86


N=N
N
N
CHF2

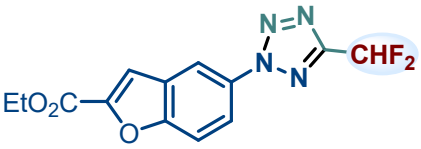
36


220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20



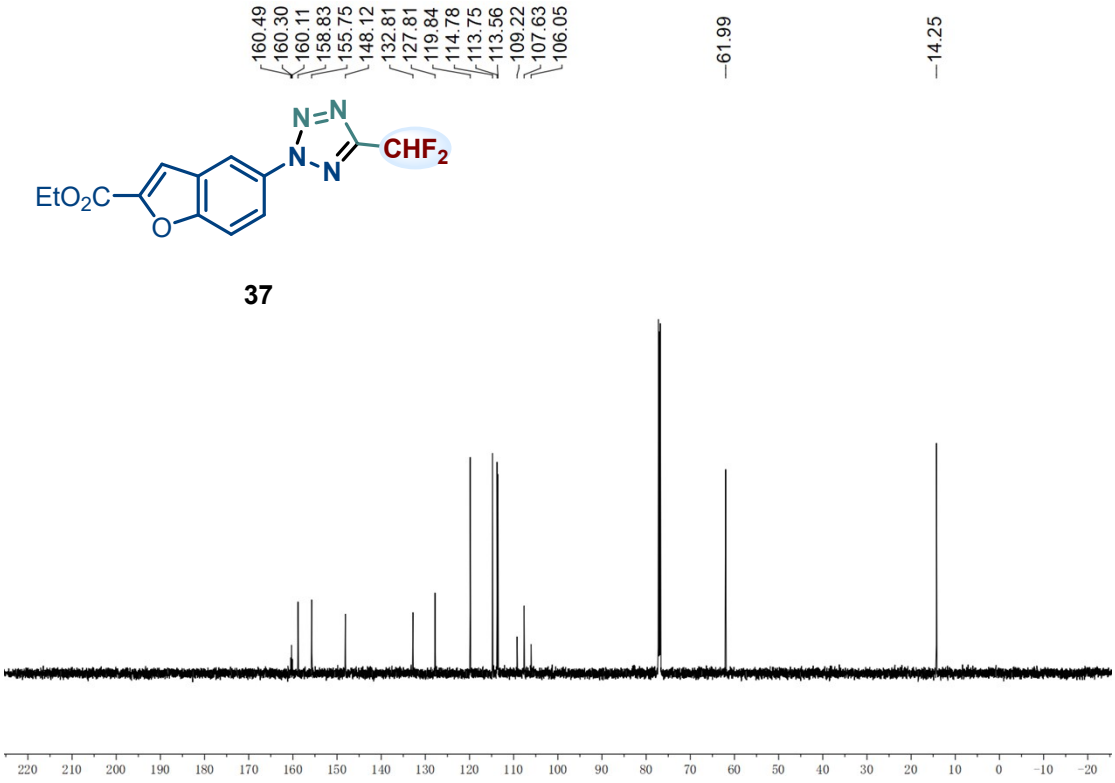
36

-116.876
-116.988

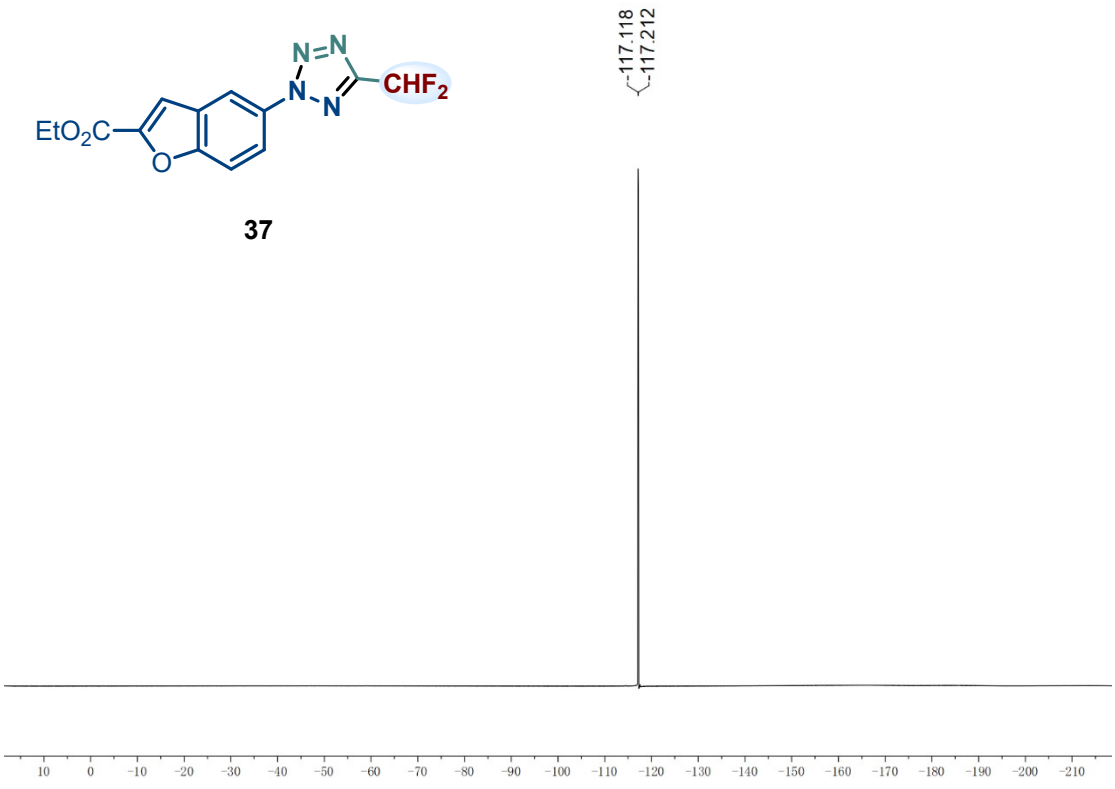


37

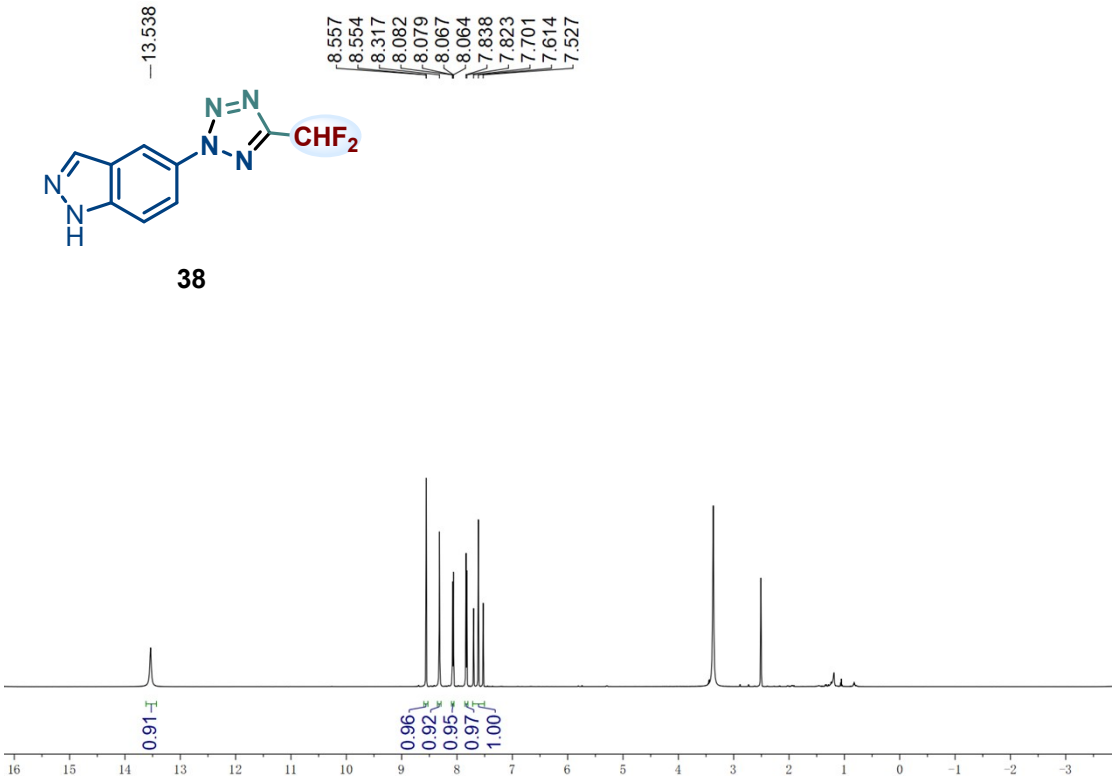
8.479
8.477
8.274
8.271
8.256
8.253
7.785
7.767
7.624
7.260
7.153
7.047
6.941
4.496
4.482
4.468
4.454
1.461
1.447
1.433
0.98
1.01
1.00
0.98
1.00
2.08
3.01

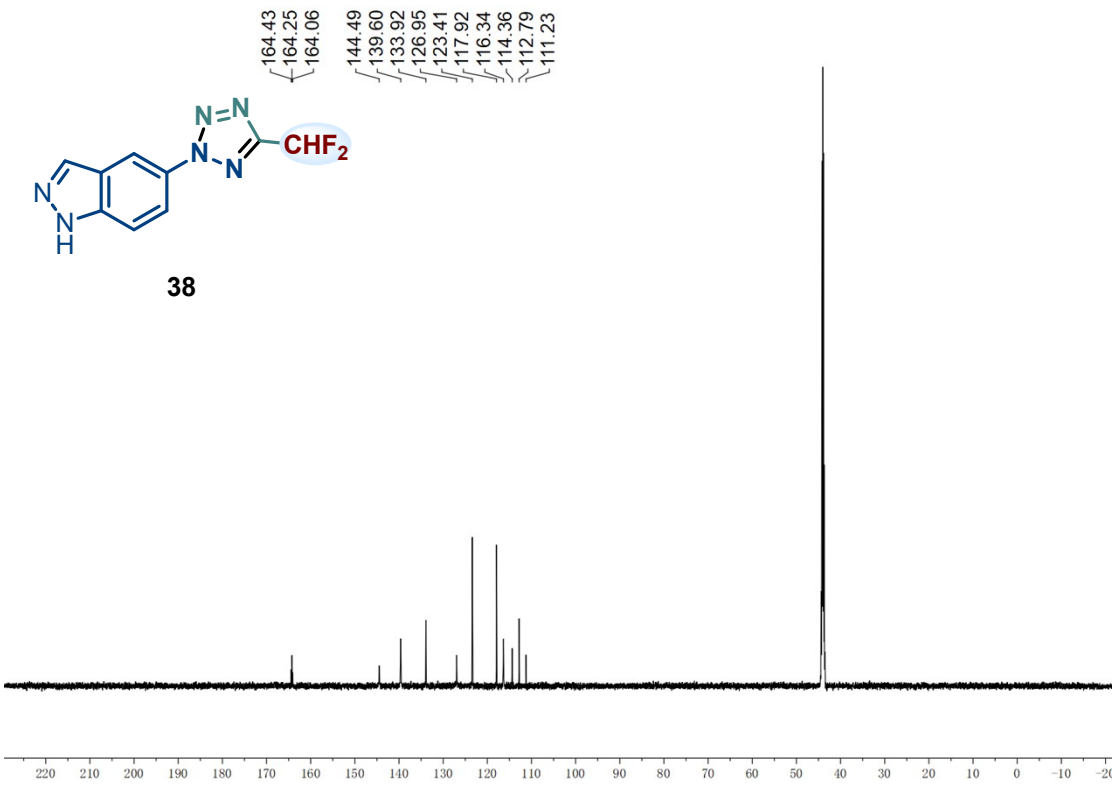

160.49
160.30
160.11
158.83
155.75
148.12
132.81
127.81
119.84
114.78
113.75
113.56
109.22
107.63
106.05
61.99
14.25
N=N
N
N
CHF2
EtO2C
O
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20

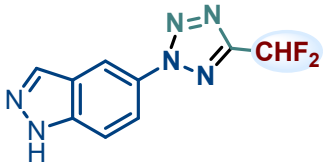
37


117.118
117.212
N=N
N
N
CHF2
EtO2C
O
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210

37

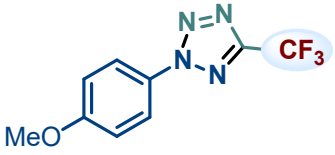

13.538
8.557
8.554
8.317
8.082
8.079
8.067
8.064
7.838
7.823
7.701
7.614
7.527
CHF2
38
0.91
0.96
0.92
0.95
0.97
1.00


164.43
164.25
164.06
144.49
139.60
133.92
126.95
123.41
117.92
116.34
114.36
112.79
111.23
CHF2
38


CHF2

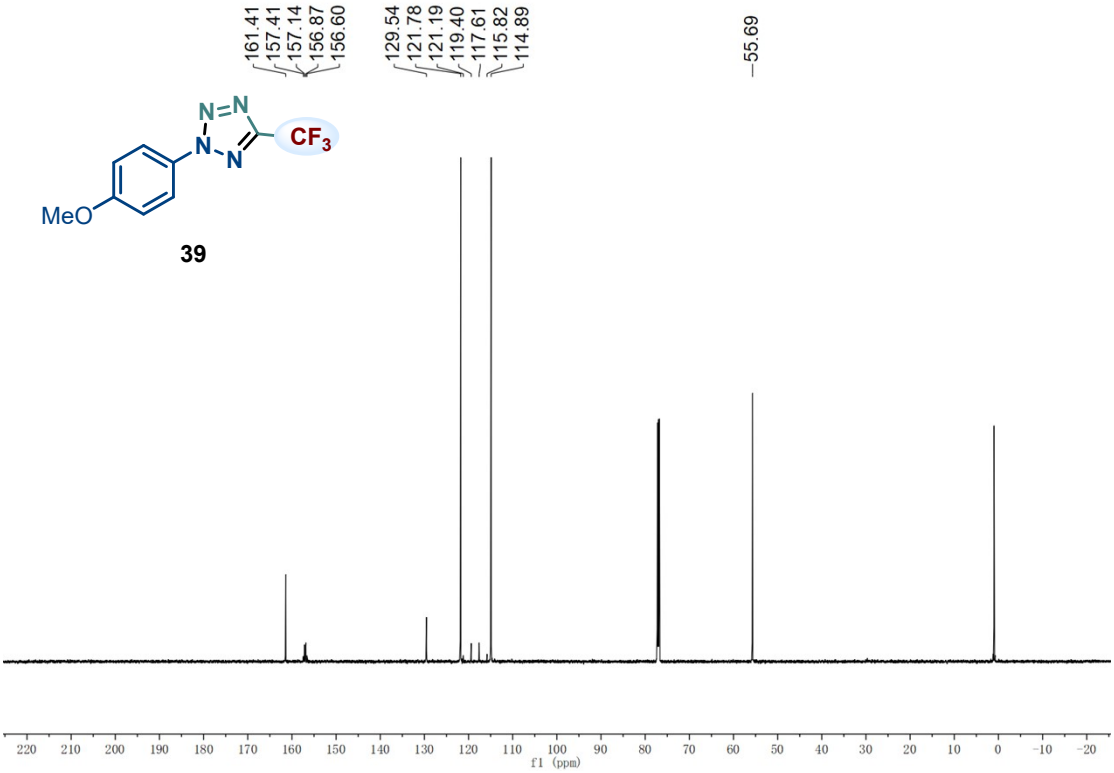
38

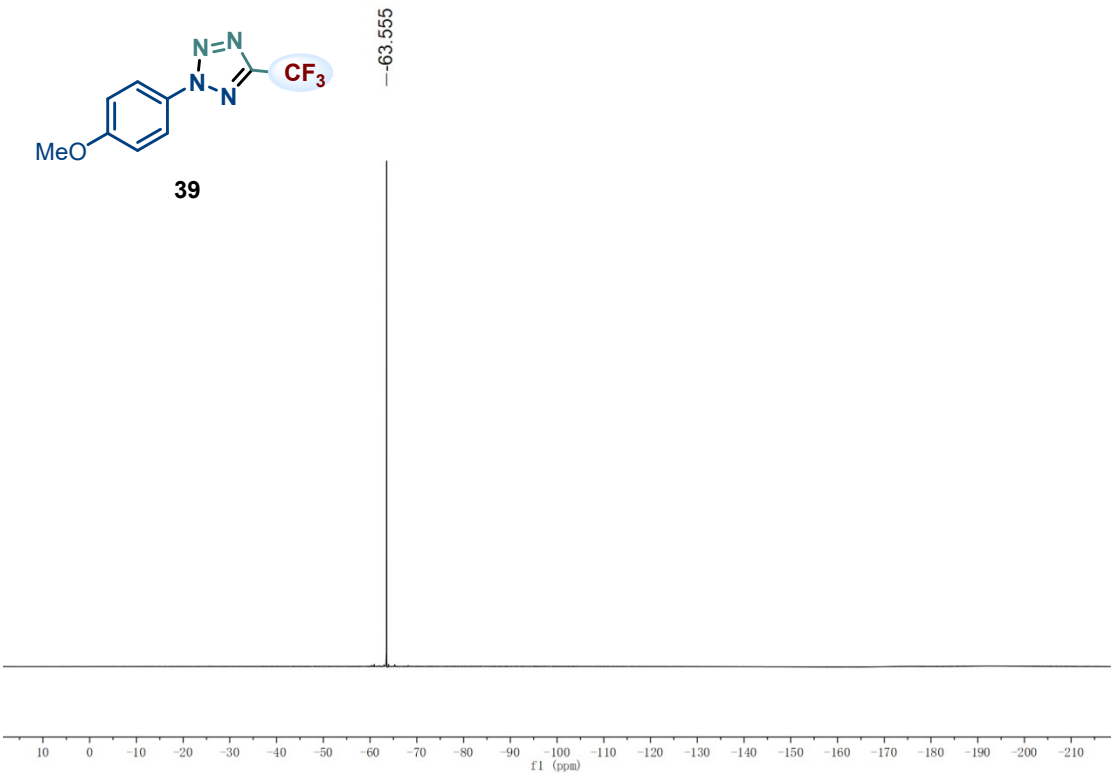
-117.783
-117.877
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210

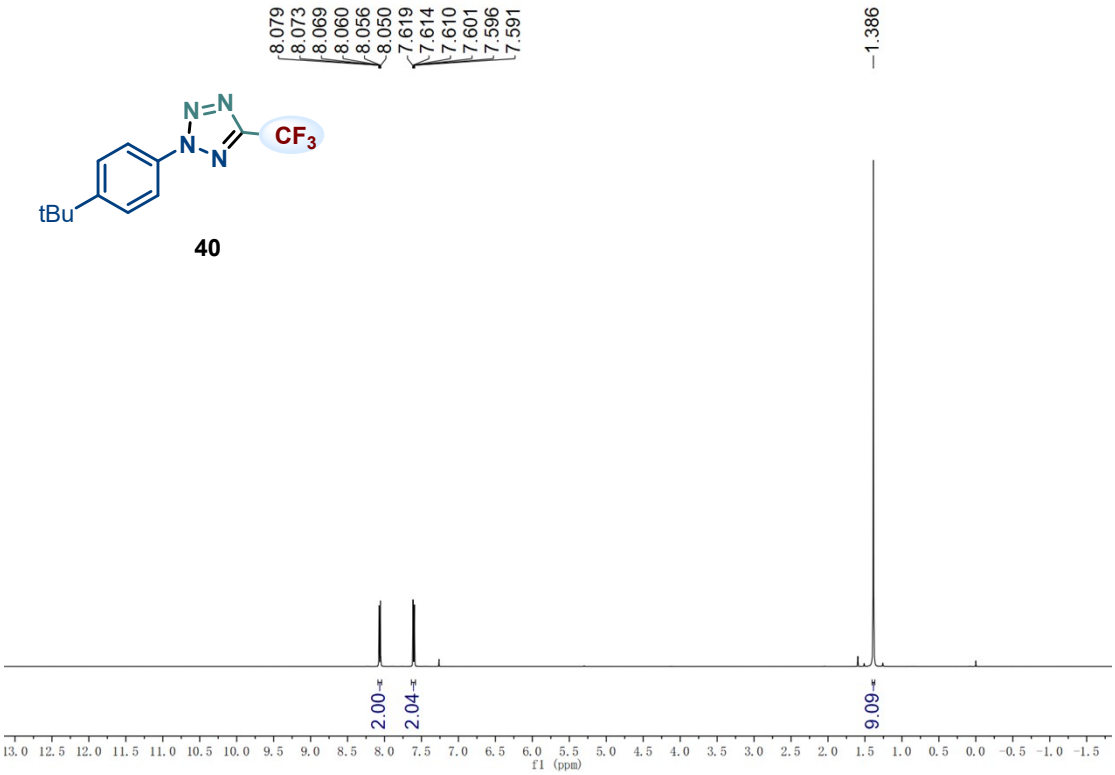

CF3
MeO

39

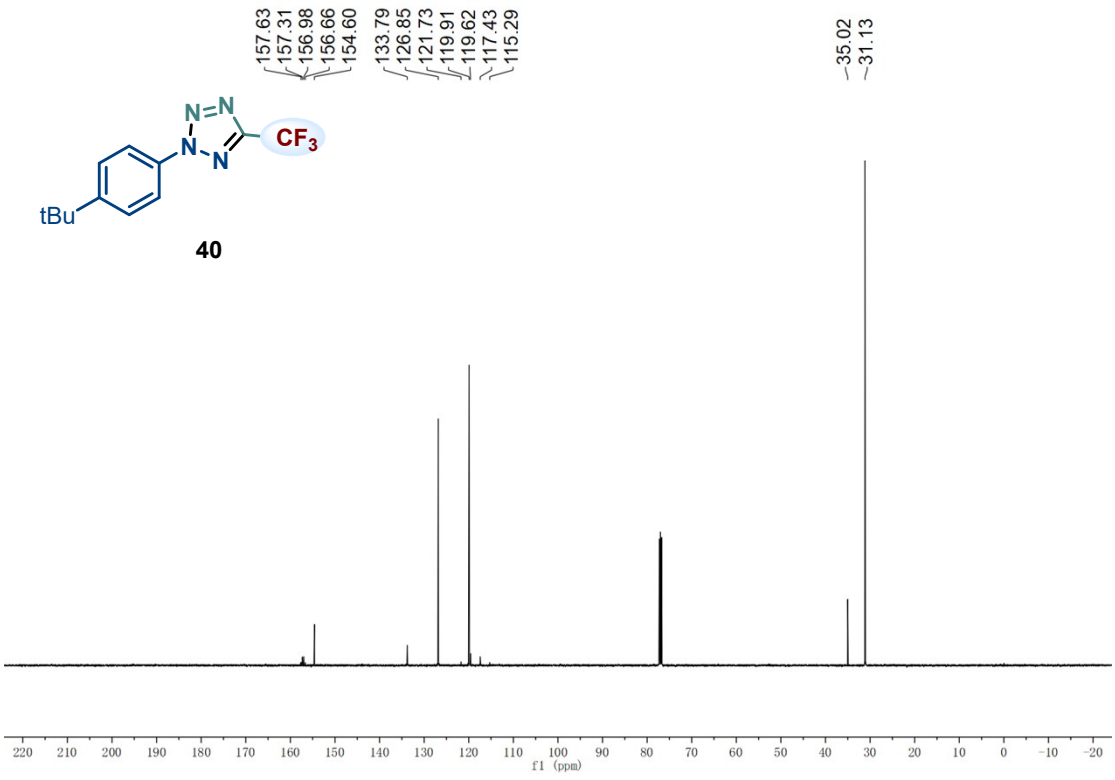
8.079
8.073
8.068
8.059
8.054
8.047
7.081
7.075
7.070
7.061
7.056
7.049
3.901
2.00
2.06
3.16
13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)


161.41
157.41
157.14
156.87
156.60
129.54
121.78
121.19
119.40
117.61
115.82
114.89
55.69
N=N
N
N
CF3
MeO
39
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)

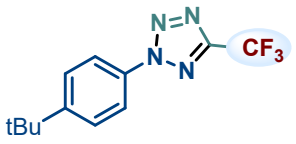

-63.555
N=N
N
N
CF3
MeO
39
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)


8.079
8.073
8.069
8.060
8.056
8.050
7.619
7.614
7.610
7.601
7.596
7.591
1.386
N=N
N
N
CF3
tBu
2.00
2.04
9.09
f1 (ppm)

40

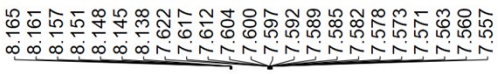

157.63
157.31
156.98
156.66
154.60
133.79
126.85
121.73
119.91
119.62
117.43
115.29
35.02
31.13
N=N
N
N
CF3
tBu
f1 (ppm)

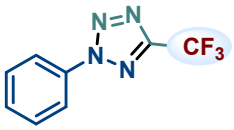
40


N=N
N
N
CF3
tBu

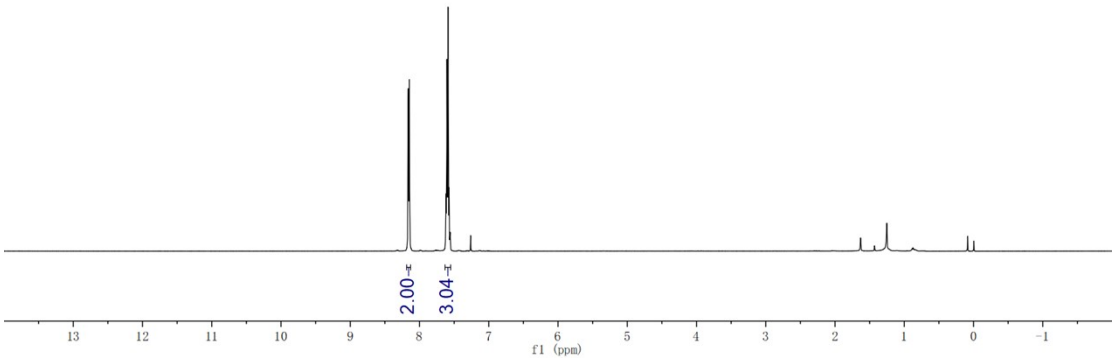
40

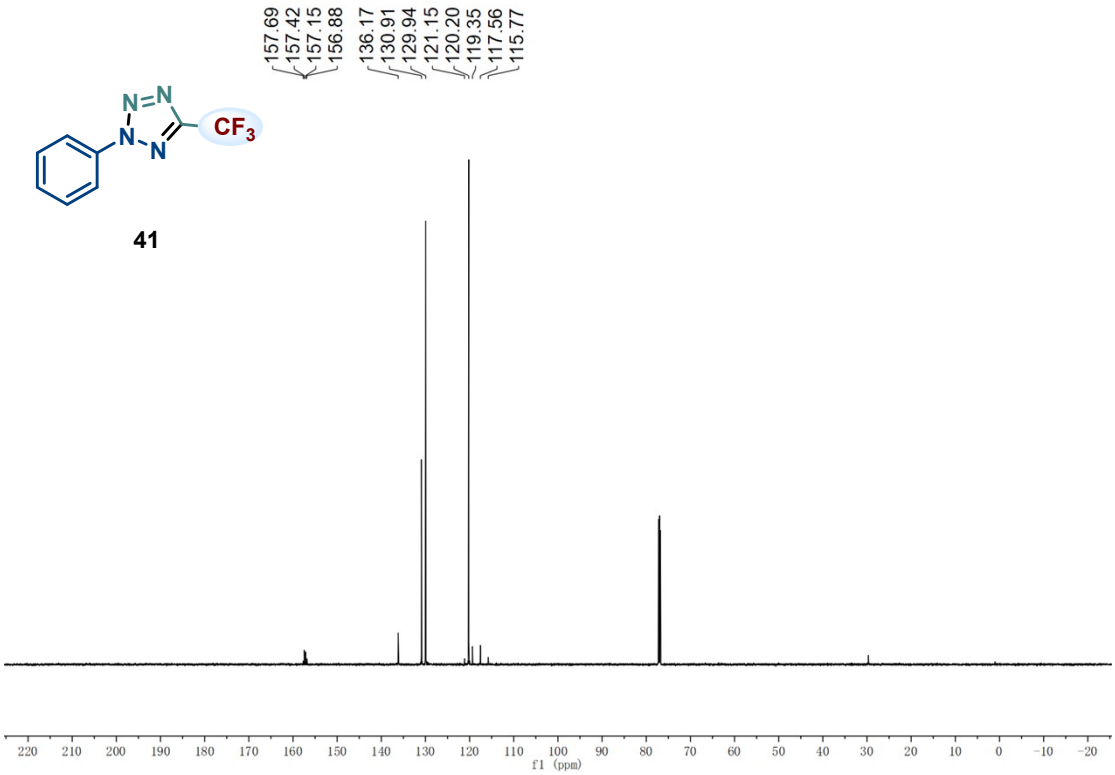
-63.574
f1 (ppm)

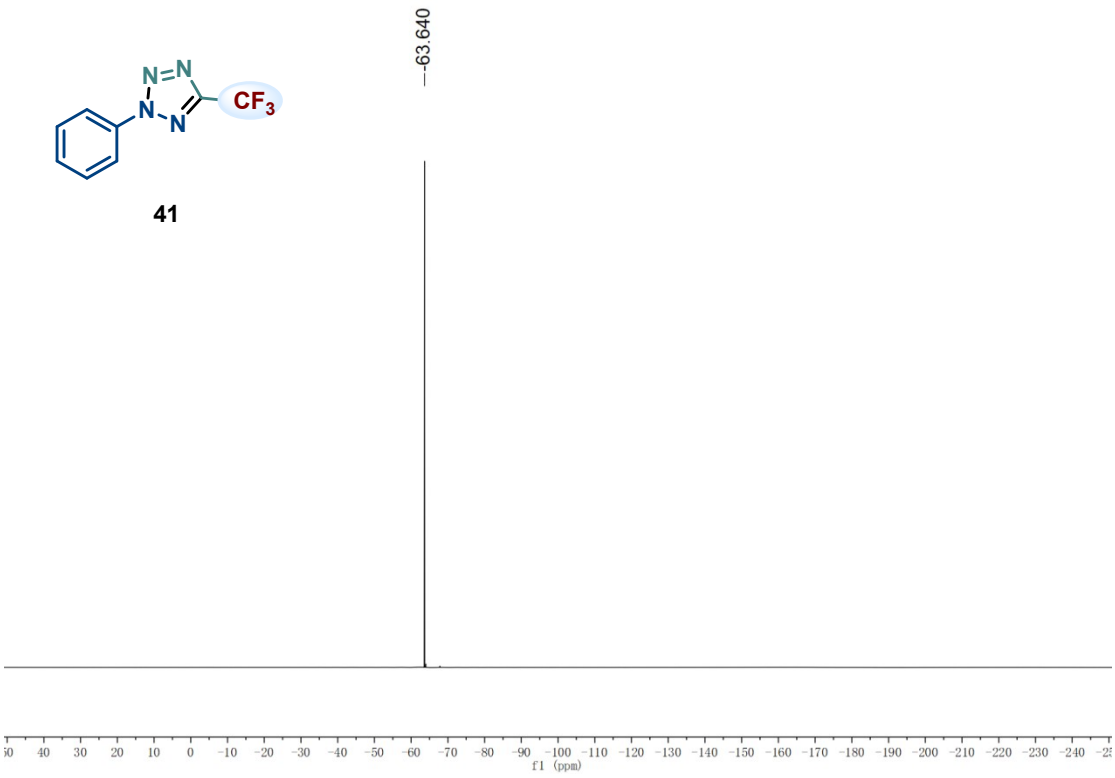

8.165
8.161
8.157
8.151
8.148
8.145
8.138
7.622
7.617
7.612
7.604
7.600
7.597
7.592
7.589
7.585
7.582
7.578
7.573
7.571
7.563
7.560
7.557

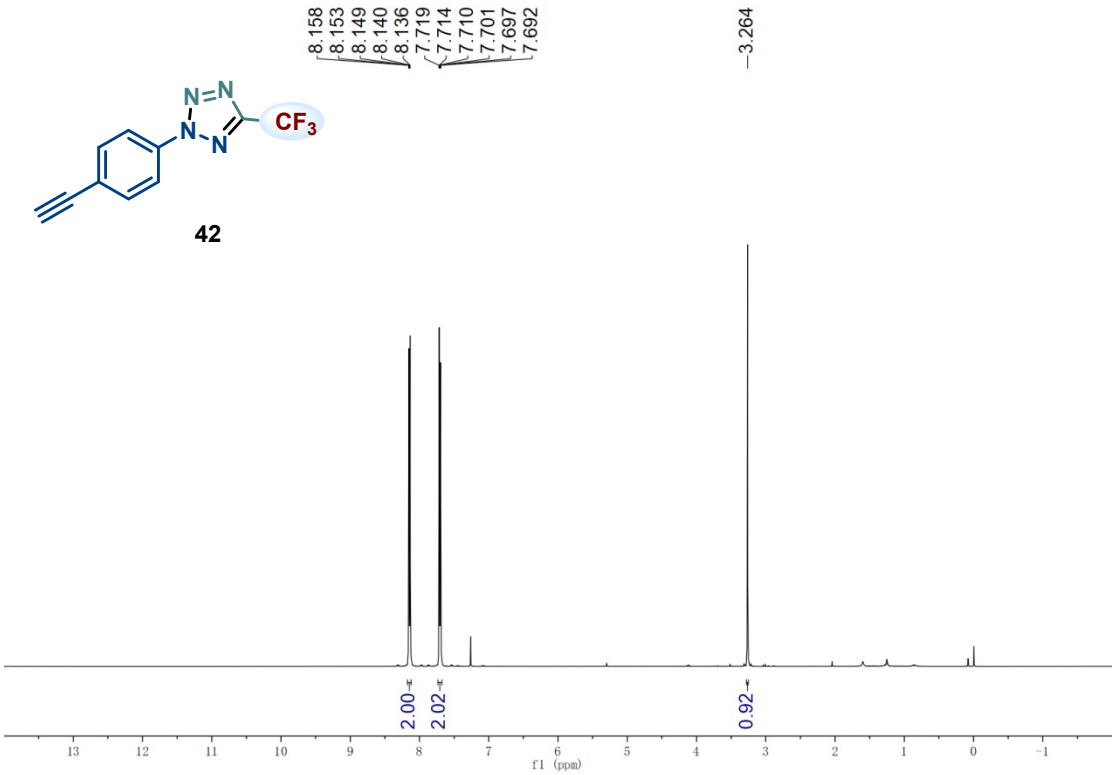

N=N
N
N
CF3

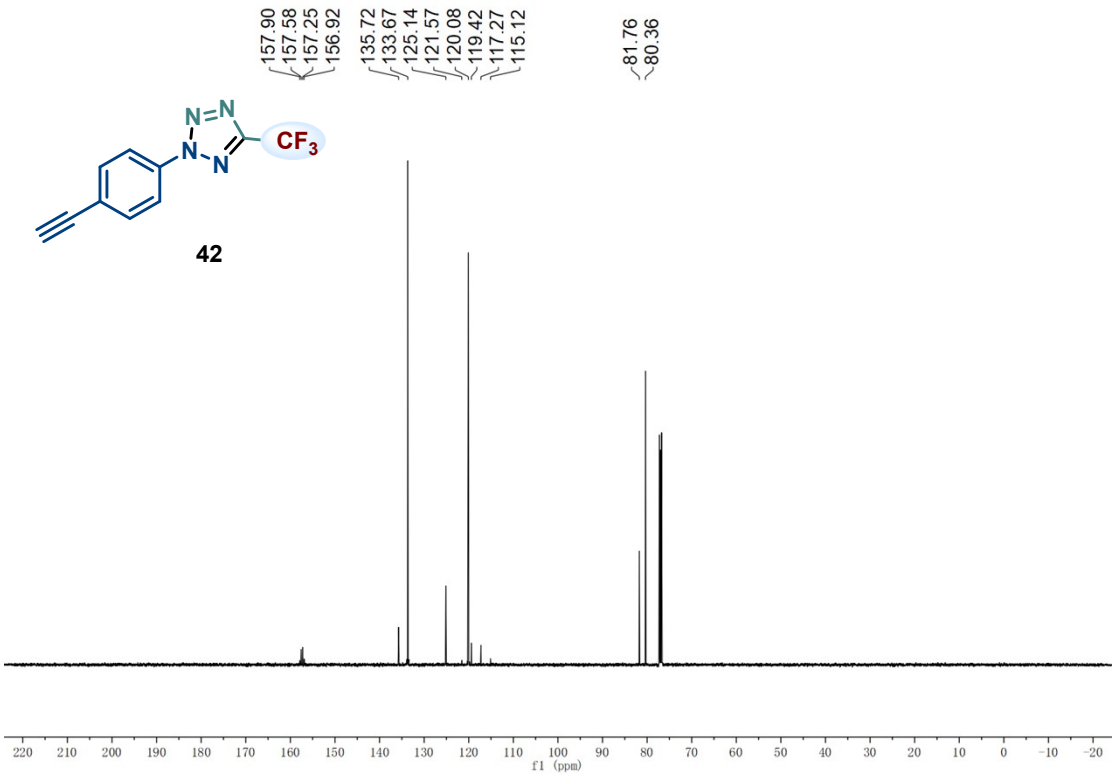
41

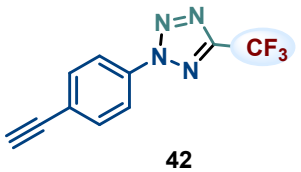

2.00
3.04
f1 (ppm)


157.69
157.42
157.15
156.88
136.17
130.91
129.94
121.15
120.20
119.35
117.56
115.77
CF3
41
f1 (ppm)


-63.640
CF3
41
f1 (ppm)

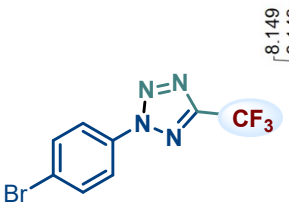

8.158
8.153
8.149
8.140
8.136
7.719
7.714
7.710
7.701
7.697
7.692
3.264
N=N
N
N
CF3
42
2.00
2.02
0.92
13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)


157.90
157.58
157.25
156.92
135.72
133.67
125.14
121.57
120.08
119.42
117.27
115.12
81.76
80.36
N=N
N
N
CF3
42
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)



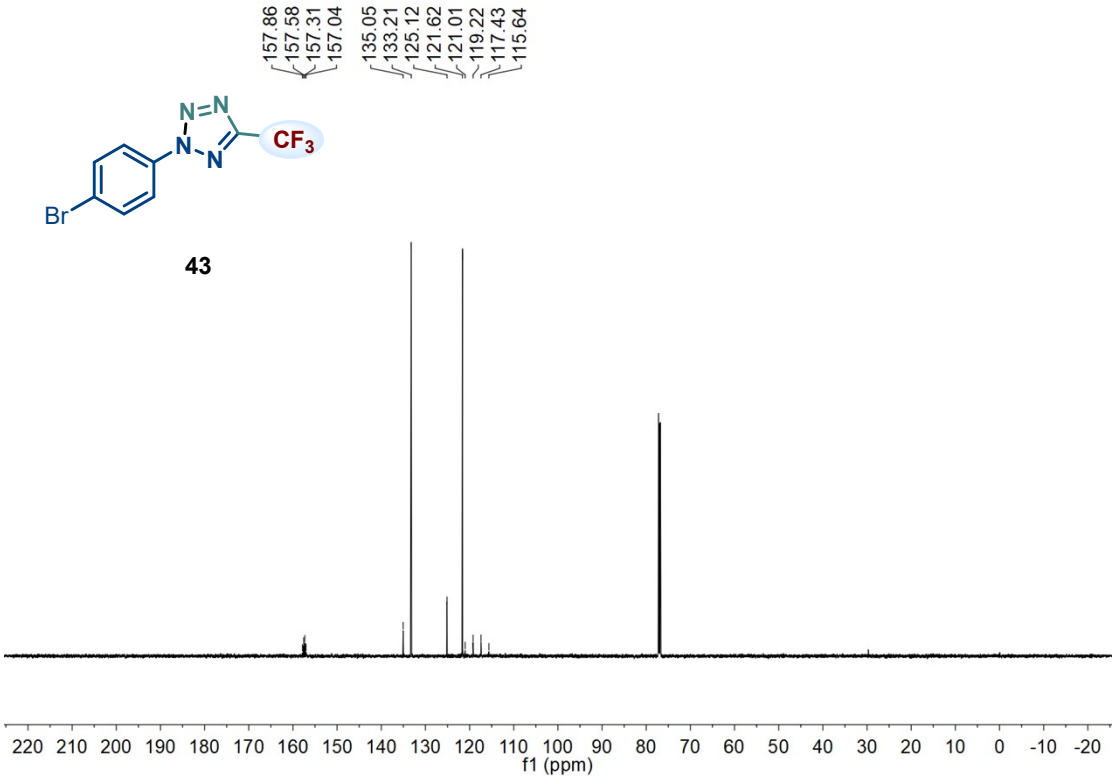
42

-63.634
f1 (ppm)

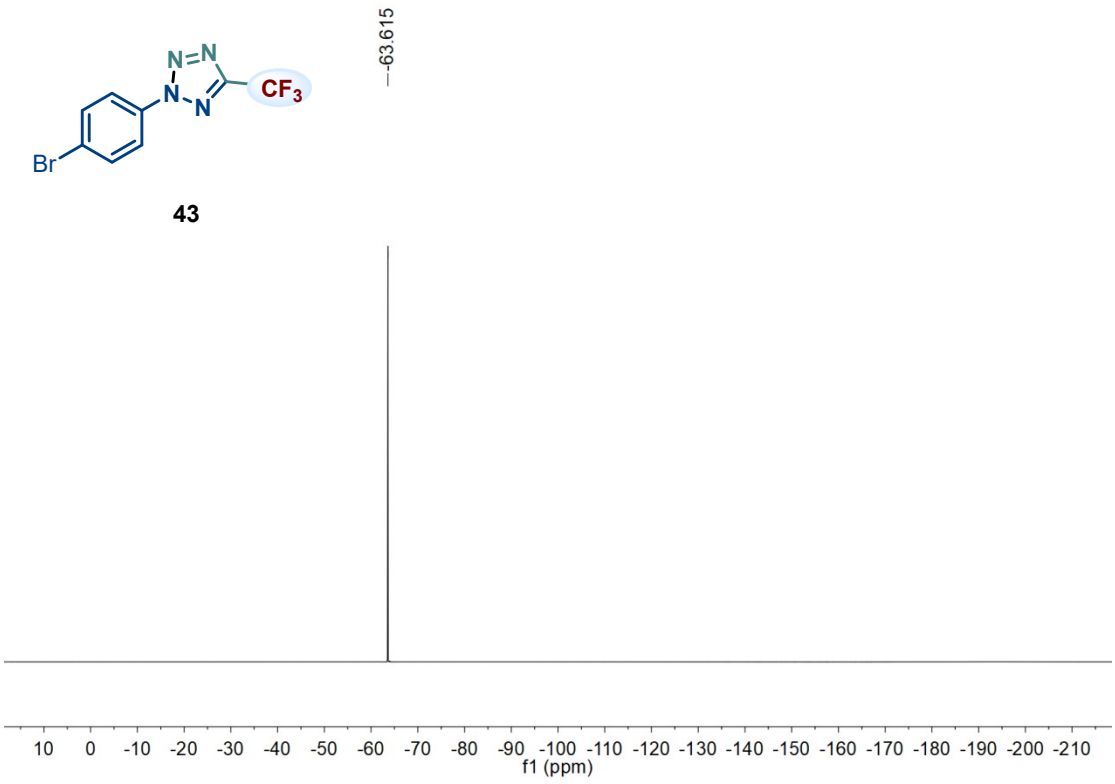


43

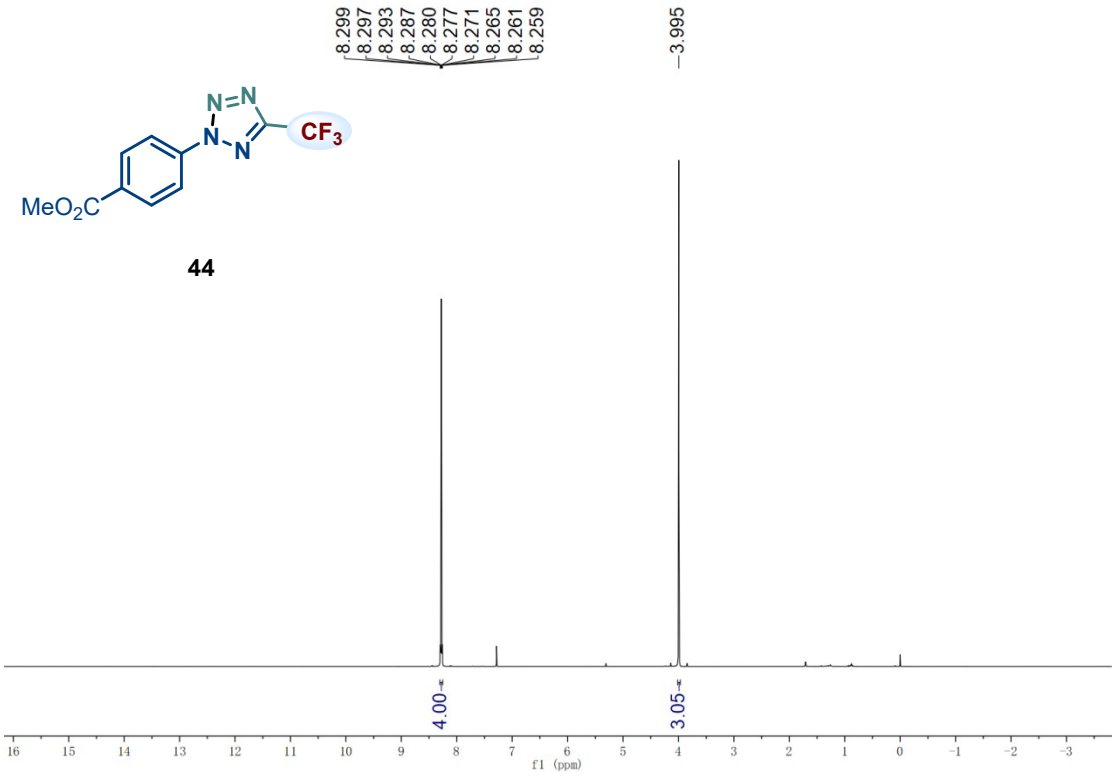
8.149
8.143
8.139
8.129
8.125
8.119
7.608
7.603
7.598
7.589
7.585
7.579
2.00
2.01
f1 (ppm)


157.86
157.58
157.31
157.04
135.05
133.21
125.12
121.62
121.01
119.22
117.43
115.64
N=N
N
N
CF3
Br
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)

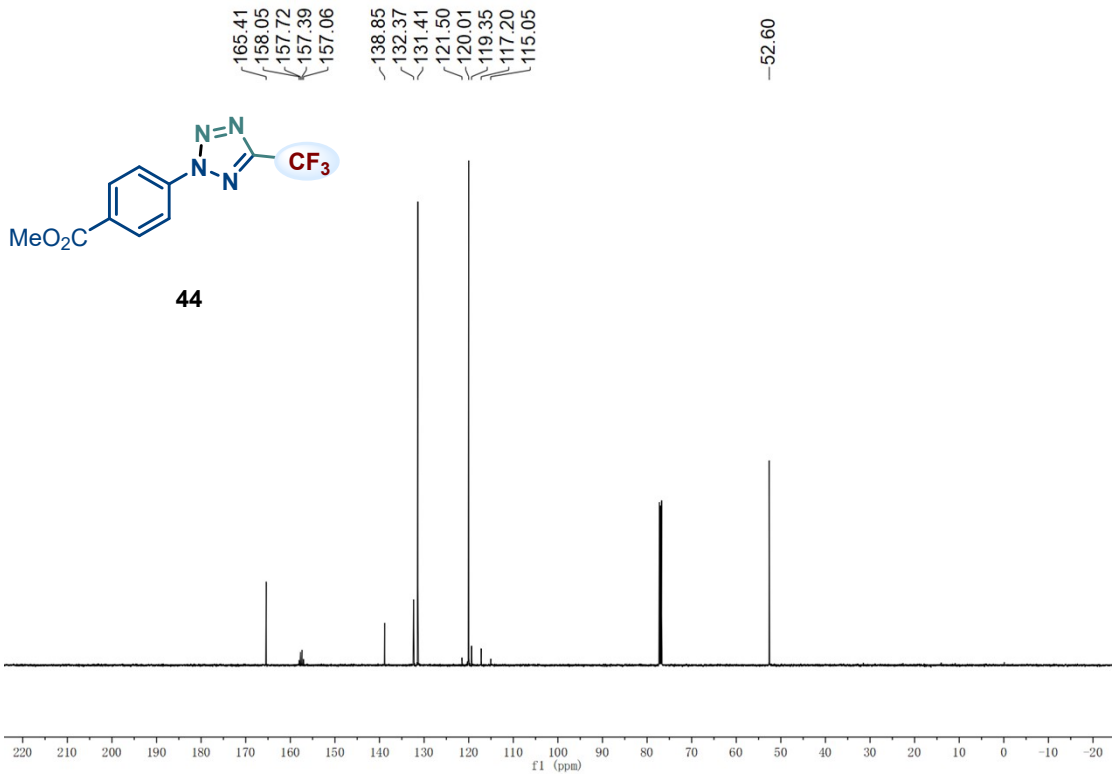
43


-63.615
N=N
N
N
CF3
Br
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)

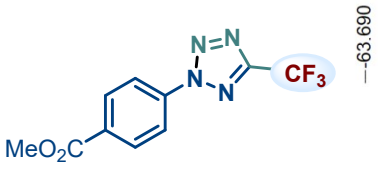
43


8.299
8.297
8.293
8.287
8.280
8.277
8.271
8.265
8.261
8.259
3.995
N=N
N
N
CF3
MeO2C
4.00
3.05
f1 (ppm)

44

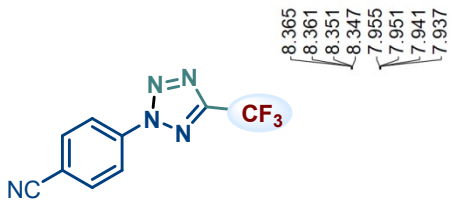

165.41
158.05
157.72
157.39
157.06
138.85
132.37
131.41
121.50
120.01
119.35
117.20
115.05
52.60
N=N
N
N
CF3
MeO2C
f1 (ppm)

44

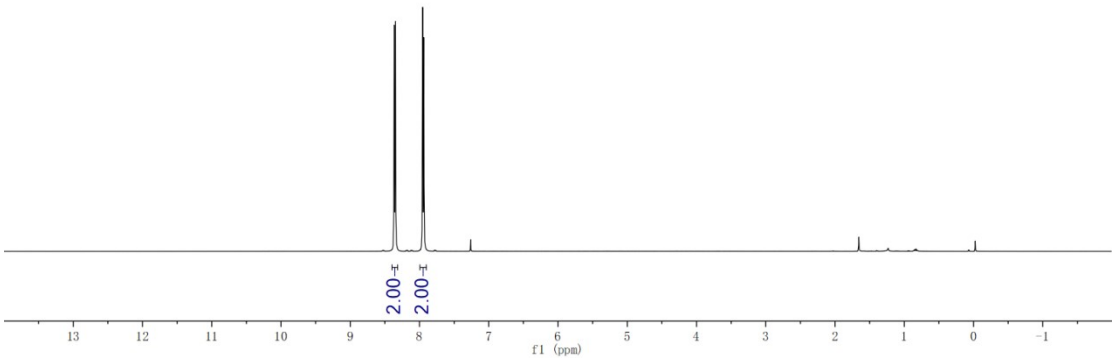

N=N
N
N
CF3
MeO2C

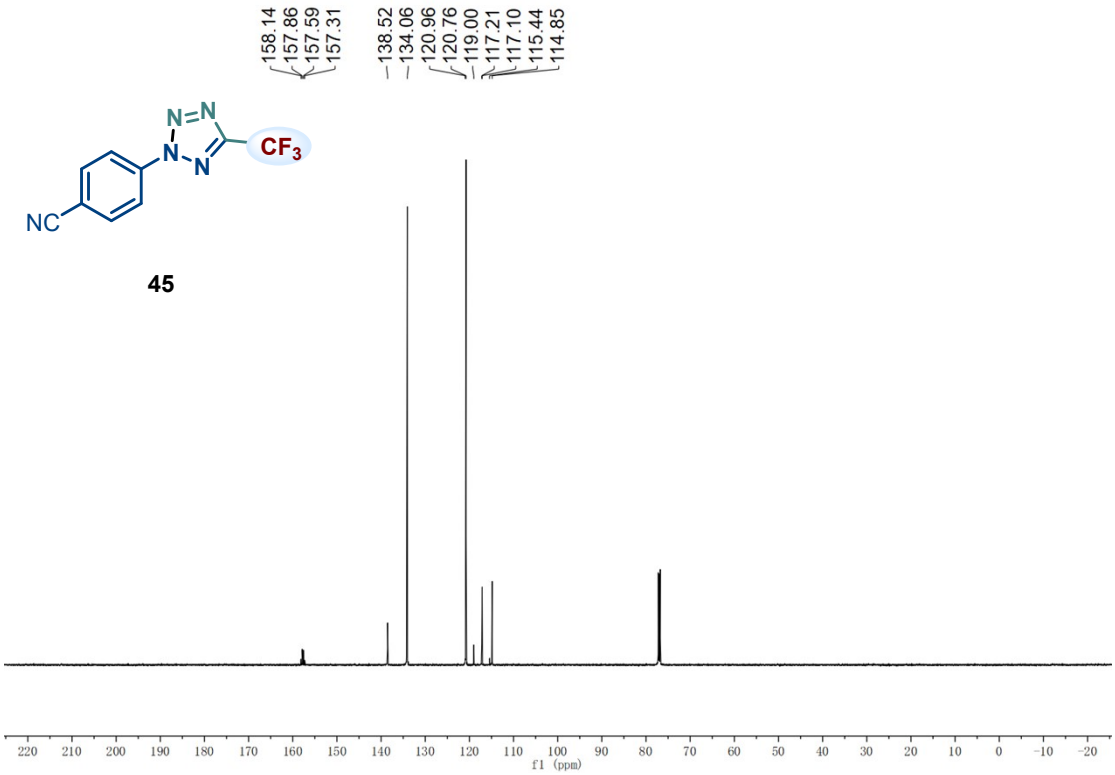
44

-63.690
f1 (ppm)

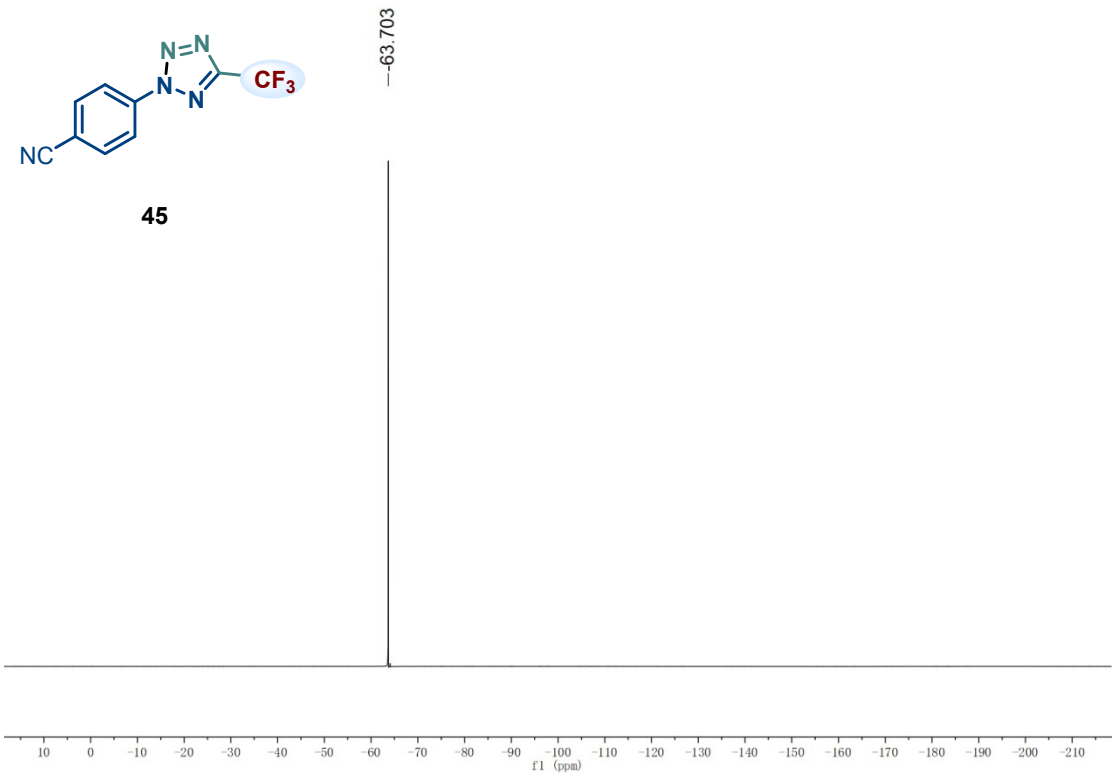

8.365
8.361
8.351
8.347
7.955
7.951
7.941
7.937
N=N
N
N
CF3
NC

45

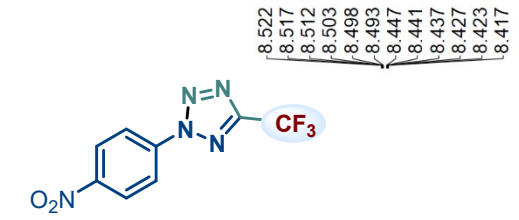

2.00
2.00
f1 (ppm)


158.14
157.86
157.59
157.31
138.52
134.06
120.96
120.76
119.00
117.21
117.10
115.44
114.85
N=N
N
N
CF3
NC
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)

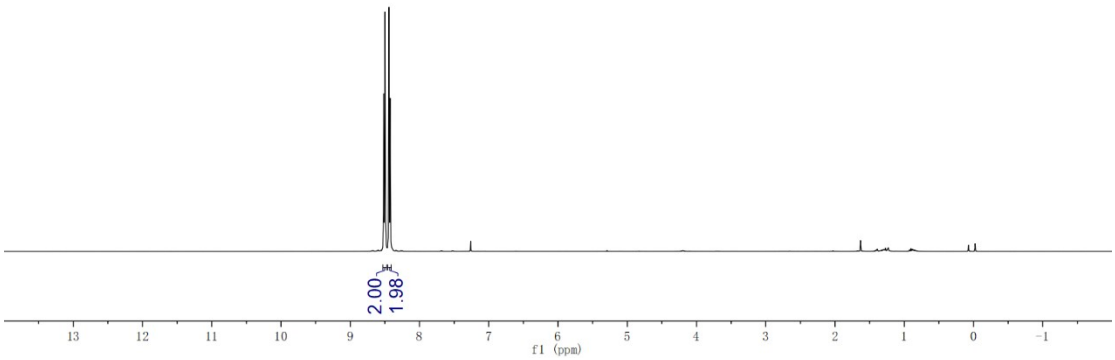
45

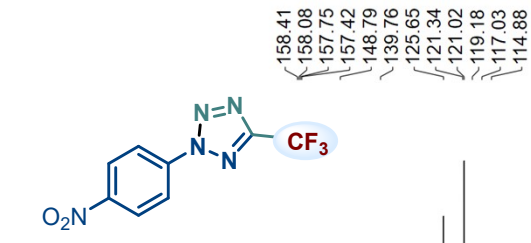

-63.703
N=N
N
N
CF3
NC
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)

45

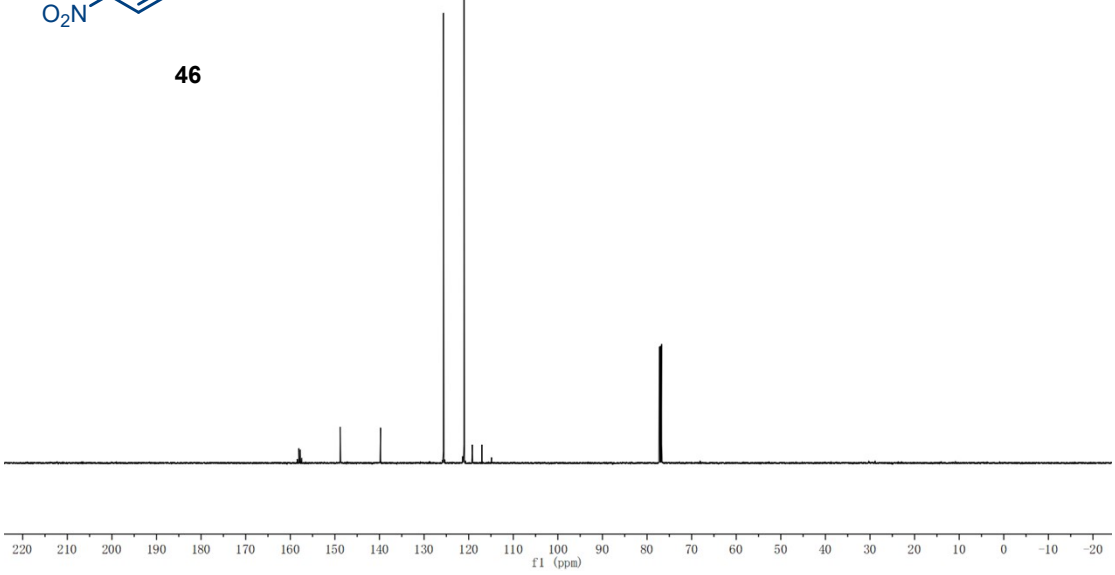

8.522
8.517
8.512
8.503
8.498
8.493
8.447
8.441
8.437
8.427
8.423
8.417
N=N
N
N
CF3
O2N

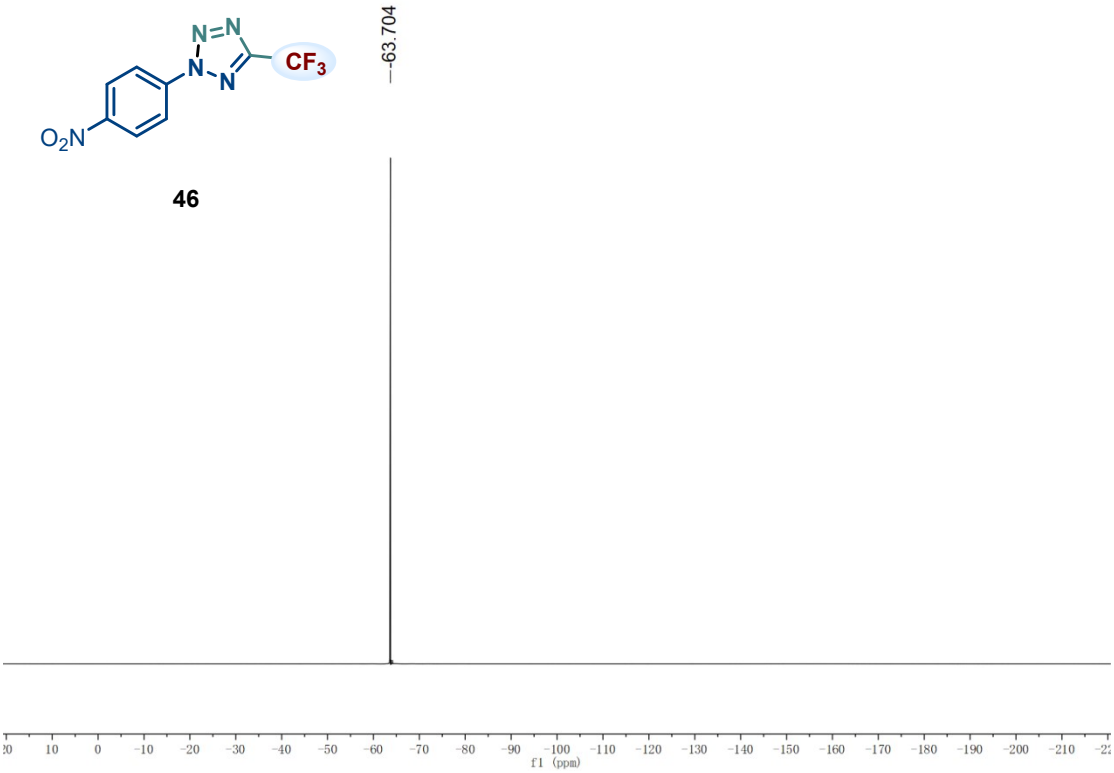
46


2.00
1.98
13
12
11
10
9
8
7
6
5
4
3
2
1
0
−1
f1 (ppm)

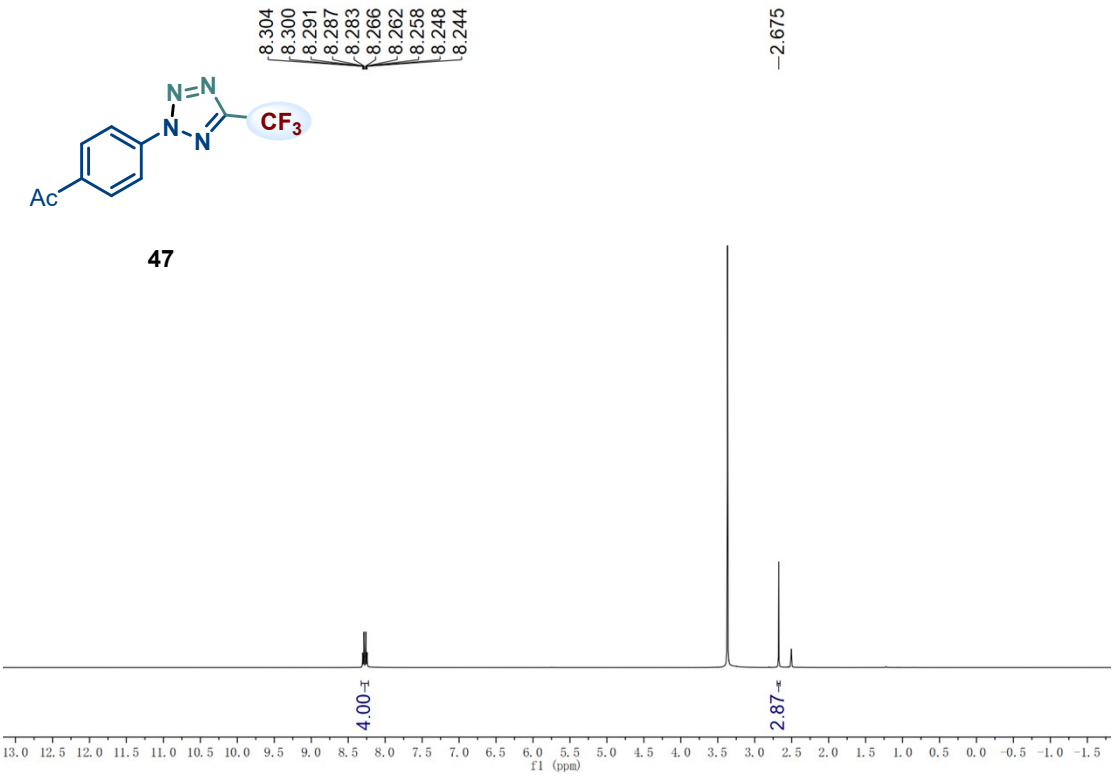

158.41
158.08
157.75
157.42
148.79
139.76
125.65
121.34
121.02
119.18
117.03
114.88
N=N
N
N
CF3
O2N

46

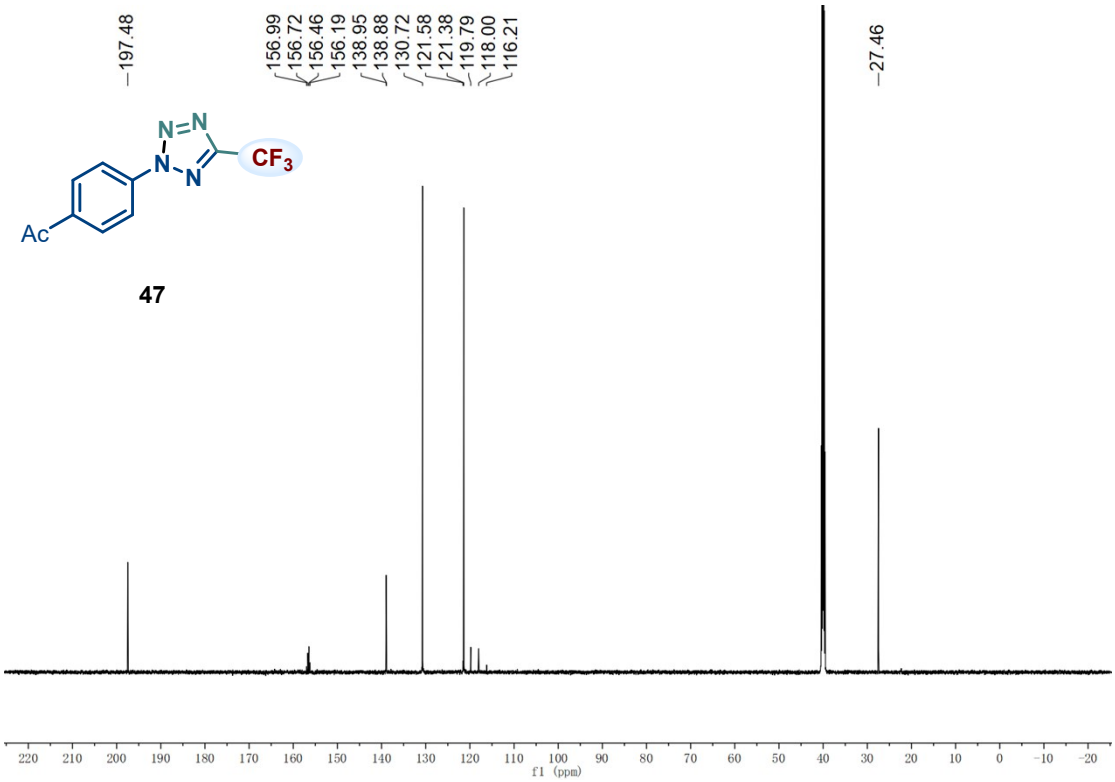

220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
−20
f1 (ppm)

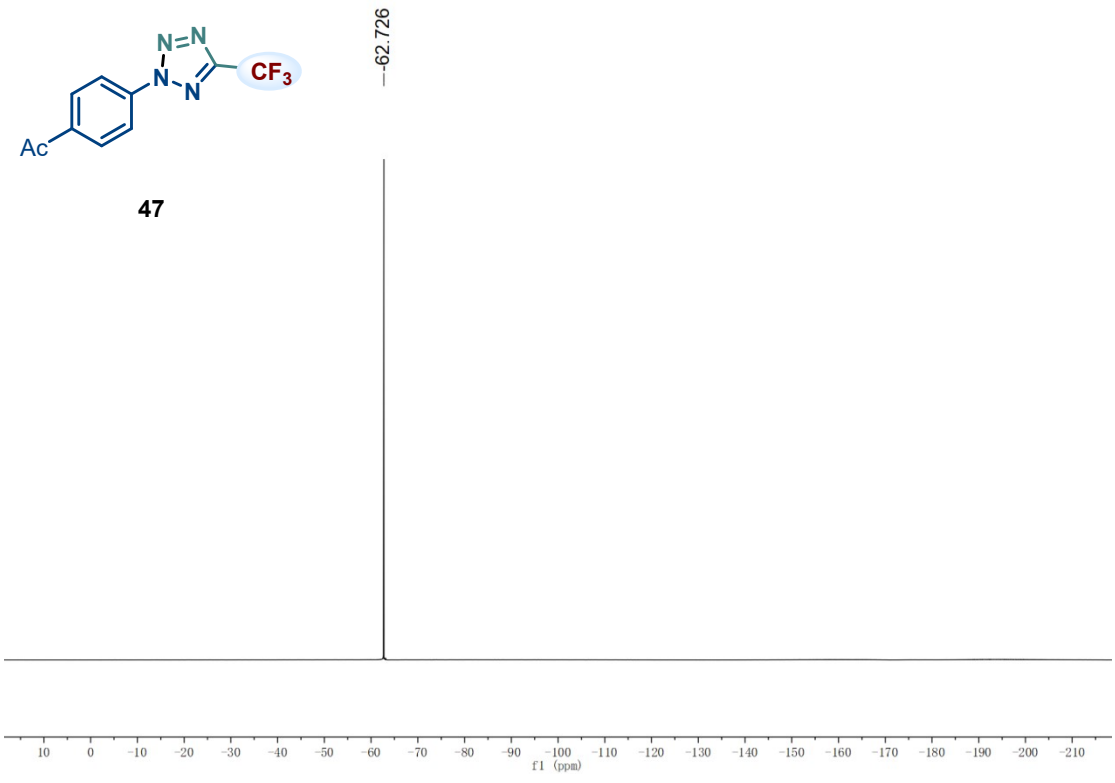

-63.704
f1 (ppm)

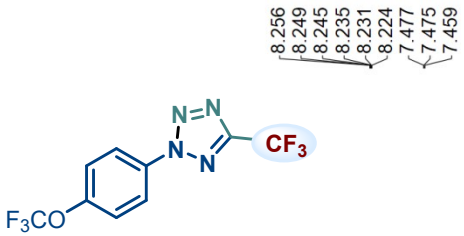
46


8.304
8.300
8.291
8.287
8.283
8.266
8.262
8.258
8.248
8.244
2.675
4.00
2.87
f1 (ppm)

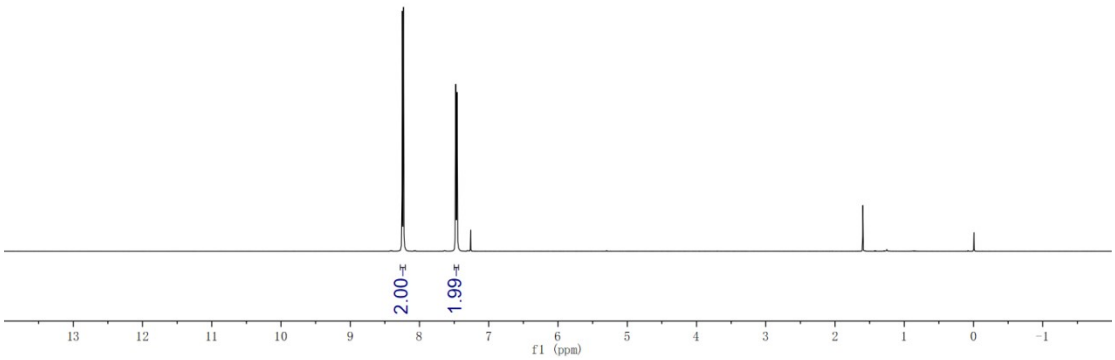
47

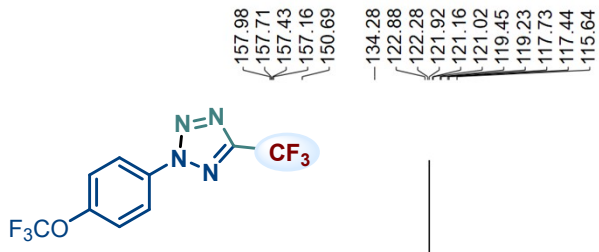

197.48
156.99
156.72
156.46
156.19
138.95
138.88
130.72
121.58
121.38
119.79
118.00
116.21
27.46
N=N
N
N
CF3
Ac
47
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)


62.726
N=N
N
N
CF3
Ac
47
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)

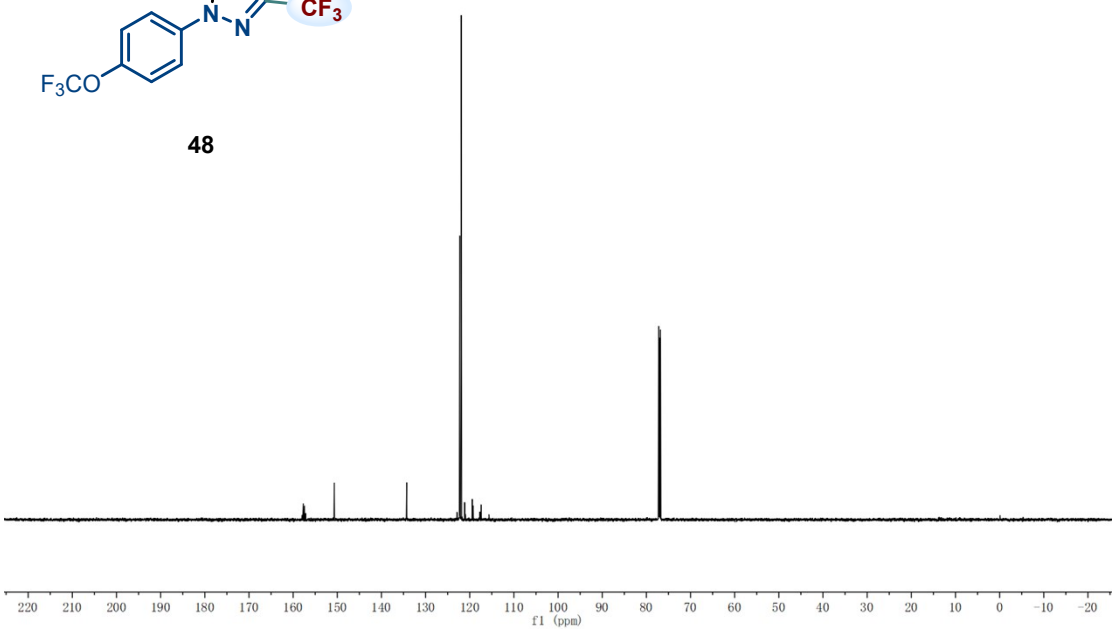

8.256
8.249
8.245
8.235
8.231
8.224
7.477
7.475
7.459
N=N
N
N
CF3
F3CO

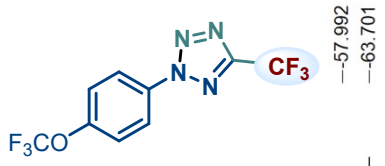
48


2.00
1.99
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
f1 (ppm)


157.98
157.71
157.43
157.16
150.69
134.28
122.88
122.28
121.92
121.16
121.02
119.45
119.23
117.73
117.44
115.64
N=N
N
N
CF3
F3CO

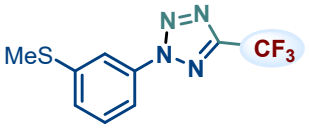
48


220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
-20
f1 (ppm)


N=N
N
N
CF3
F3CO

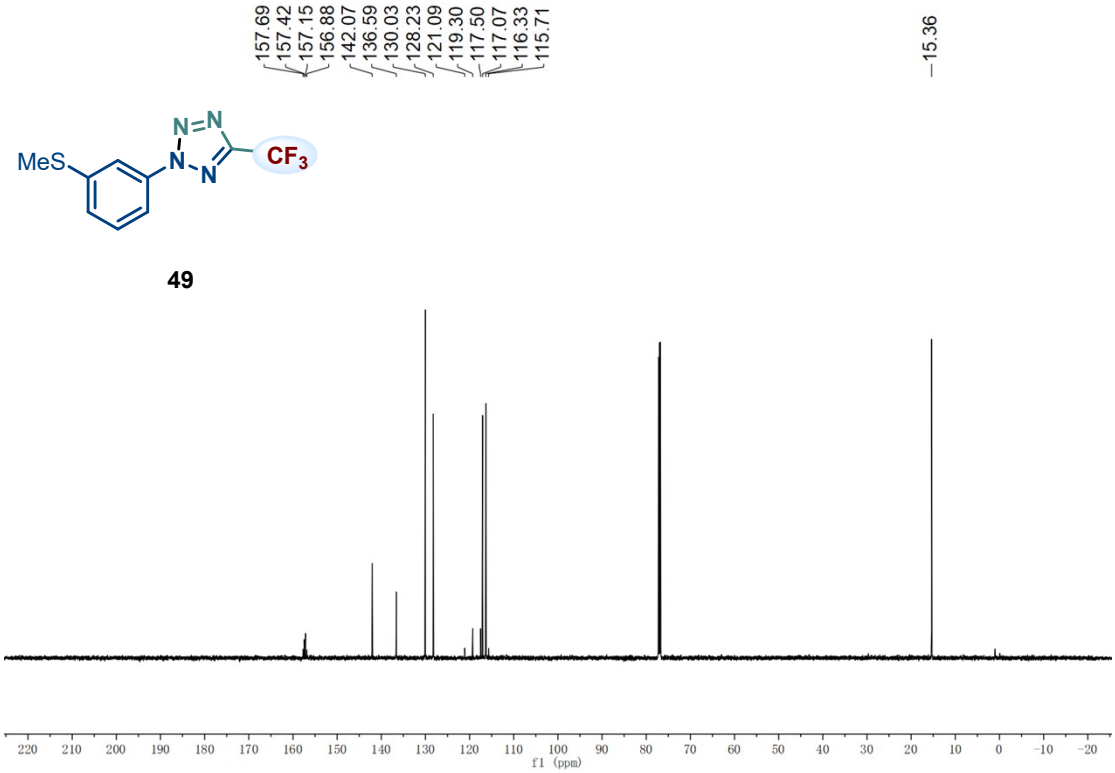
48

-57.992
-63.701
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)

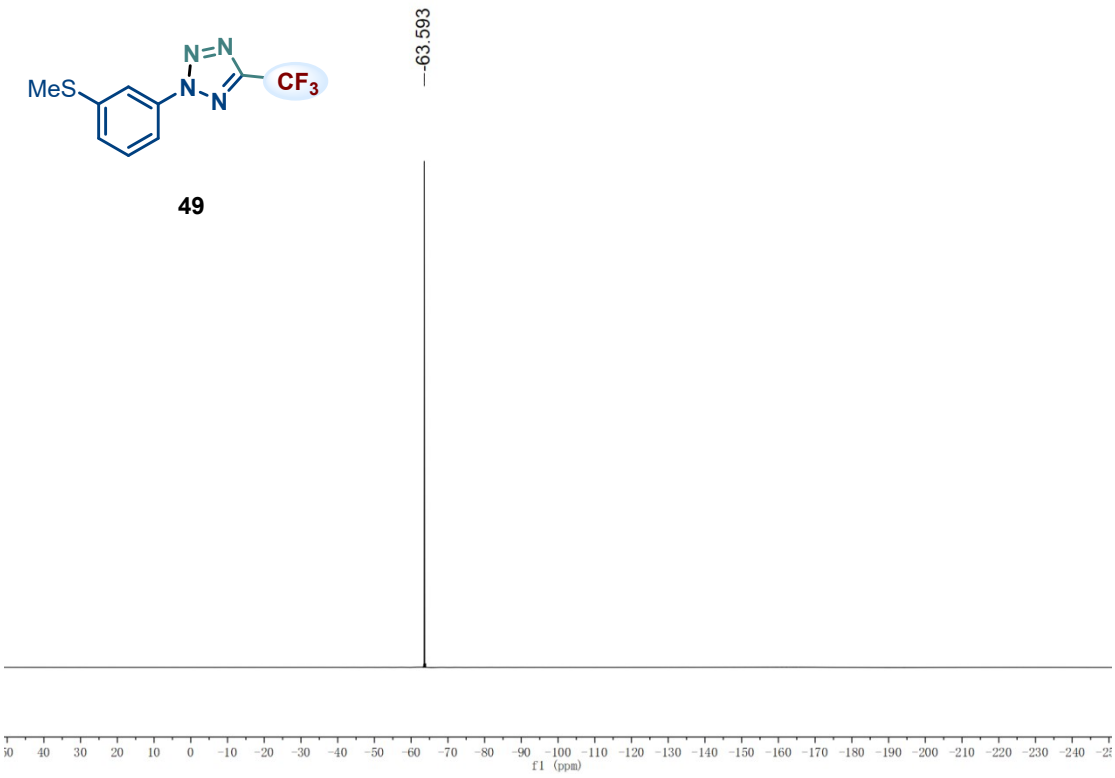

N=N
N
N
CF3
MeS

49

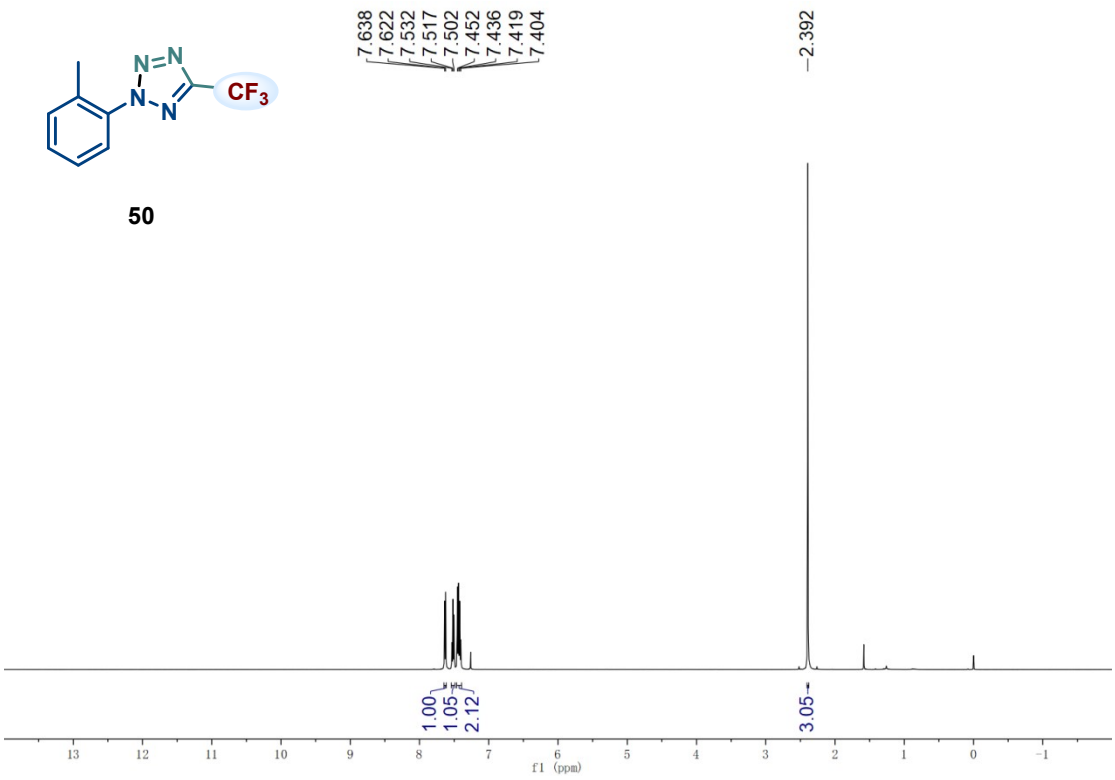
7.987
7.903
7.888
7.501
7.485
7.469
7.413
7.397
2.580
1.00
1.06
1.09
1.06
3.14
13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)


157.69
157.42
157.15
156.88
142.07
136.59
130.03
128.23
121.09
119.30
117.50
117.07
116.33
115.71
15.36
MeS
N=N
N
N
CF3
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)

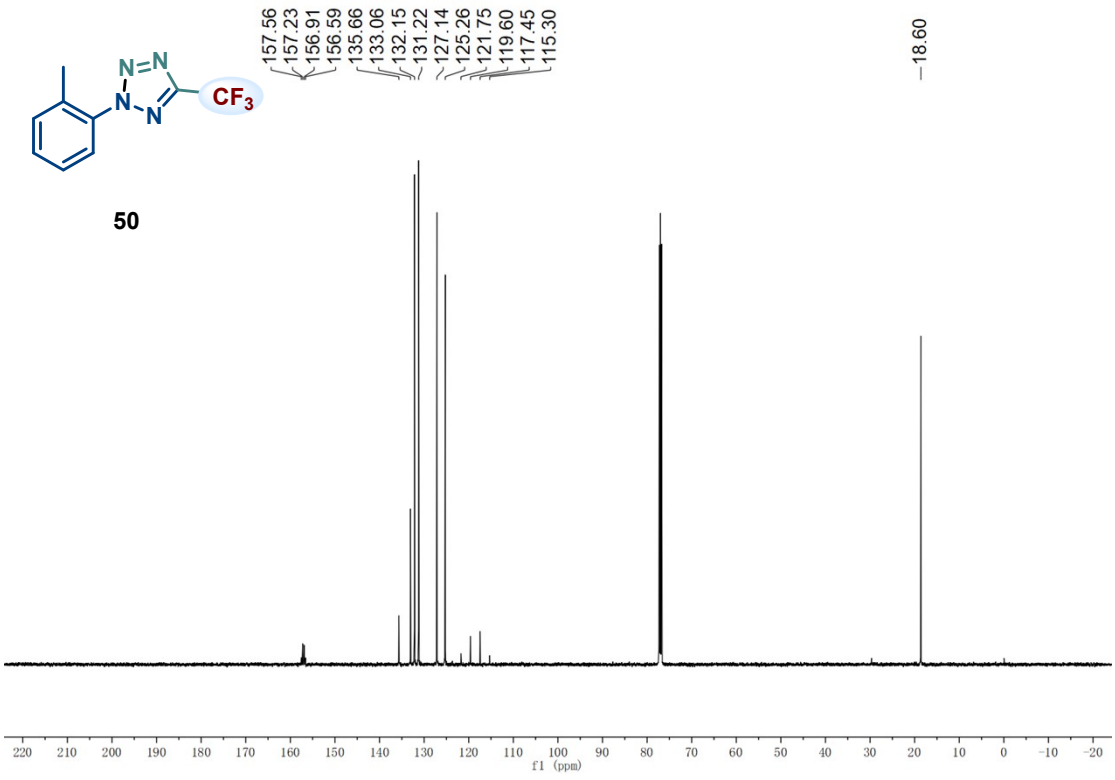
49


-63.593
MeS
N=N
N
N
CF3
60 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -220 -230 -240
f1 (ppm)

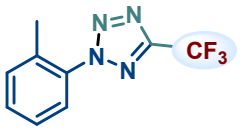
49


7.638
7.622
7.532
7.517
7.502
7.452
7.436
7.419
7.404
2.392
1.00
1.05
2.12
3.05
f1 (ppm)

50

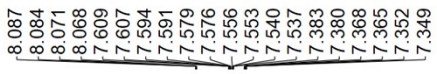

157.56
157.23
156.91
156.59
135.66
133.06
132.15
131.22
127.14
125.26
121.75
119.60
117.45
115.30
18.60
f1 (ppm)

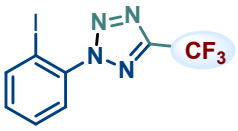
50



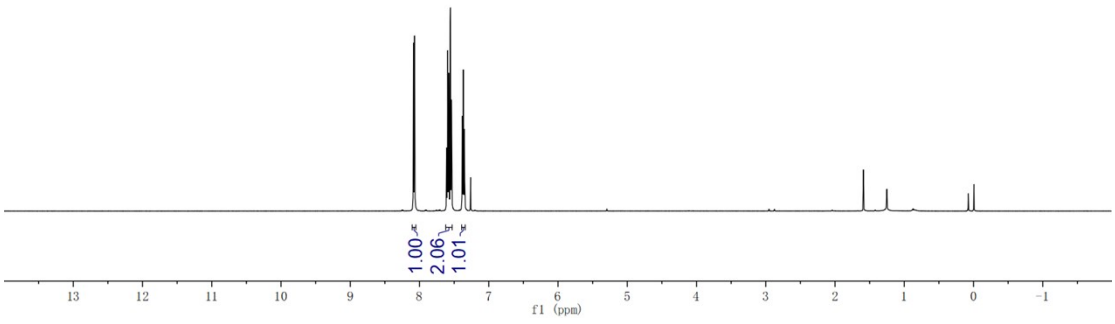
50

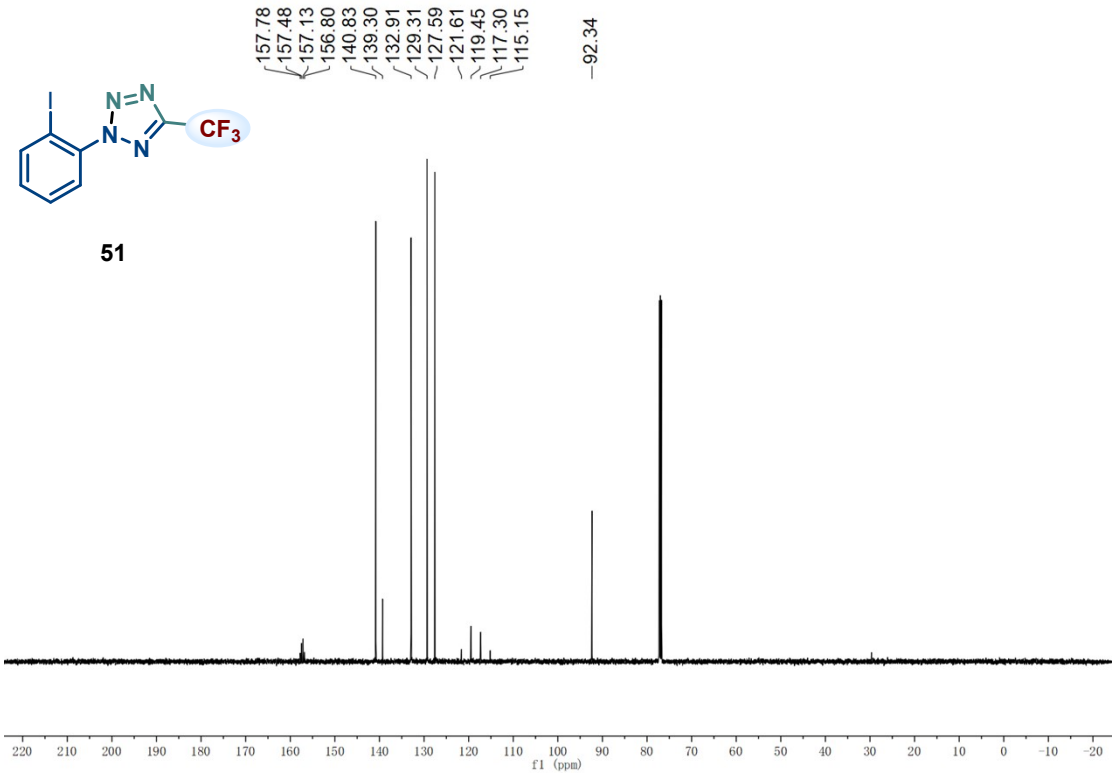
-63.468
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)

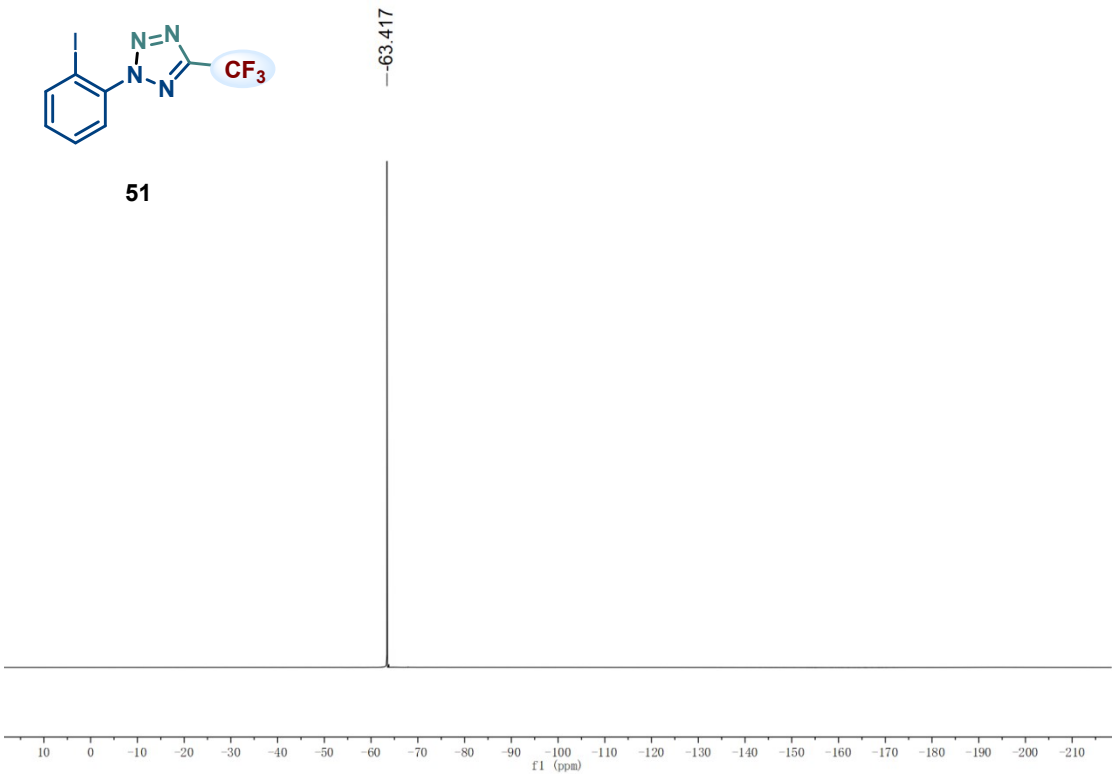

8.087
8.084
8.071
8.068
7.609
7.607
7.594
7.591
7.579
7.576
7.556
7.553
7.540
7.537
7.383
7.380
7.368
7.365
7.352
7.349

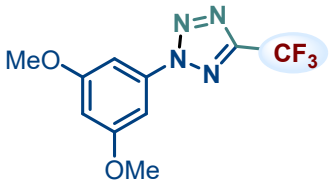


51


1.00
2.06
1.01
13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)

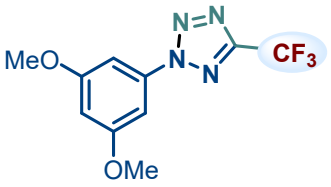

157.78
157.48
157.13
156.80
140.83
139.30
132.91
129.31
127.59
121.61
119.45
117.30
115.15
92.34
CF3
51
f1 (ppm)


63.417
CF3
51
f1 (ppm)


MeO
OMe
CF3

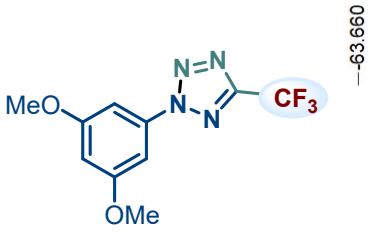
52

7.276
7.272
6.591
6.586
6.582
3.875
1.96
1.00
6.12
f1 (ppm)


MeO
OMe
CF3

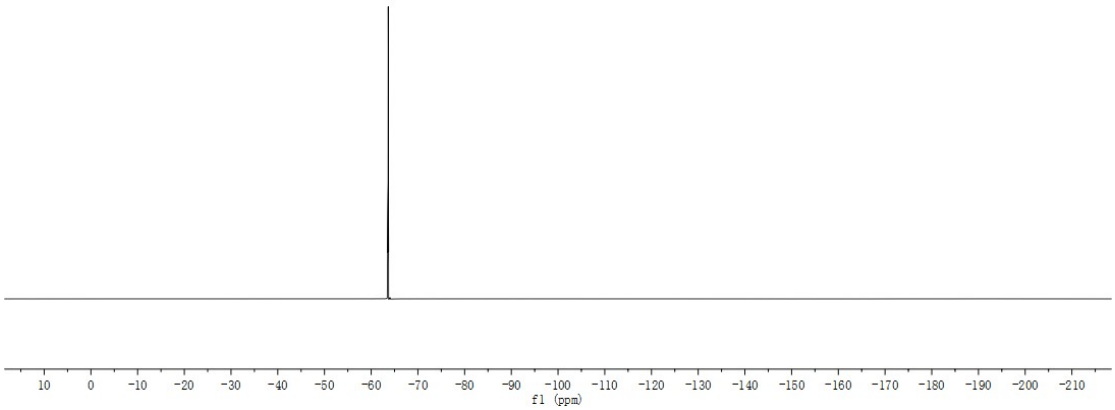
52

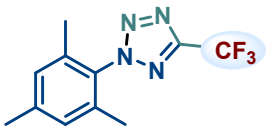
161.56
157.47
157.19
156.92
156.65
137.40
121.11
119.32
117.52
115.73
102.88
98.41
55.77
f1 (ppm)


MeO
OMe
N=N
N
N
CF3

52

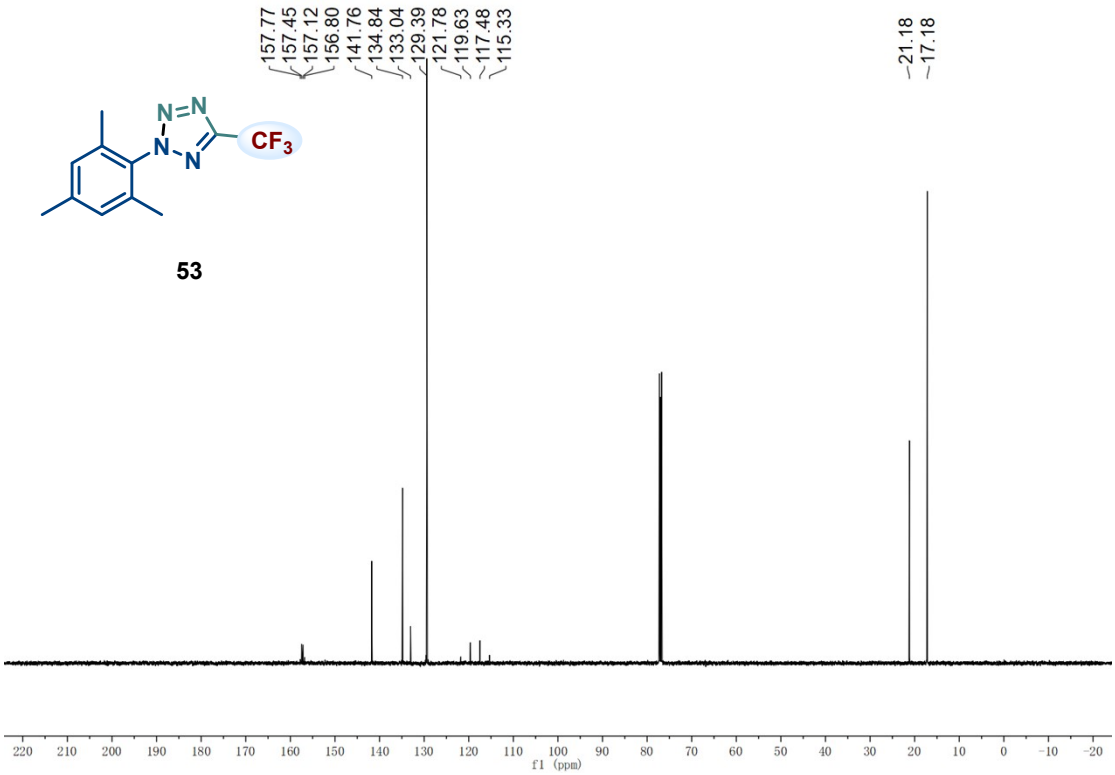
-63.660


10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)

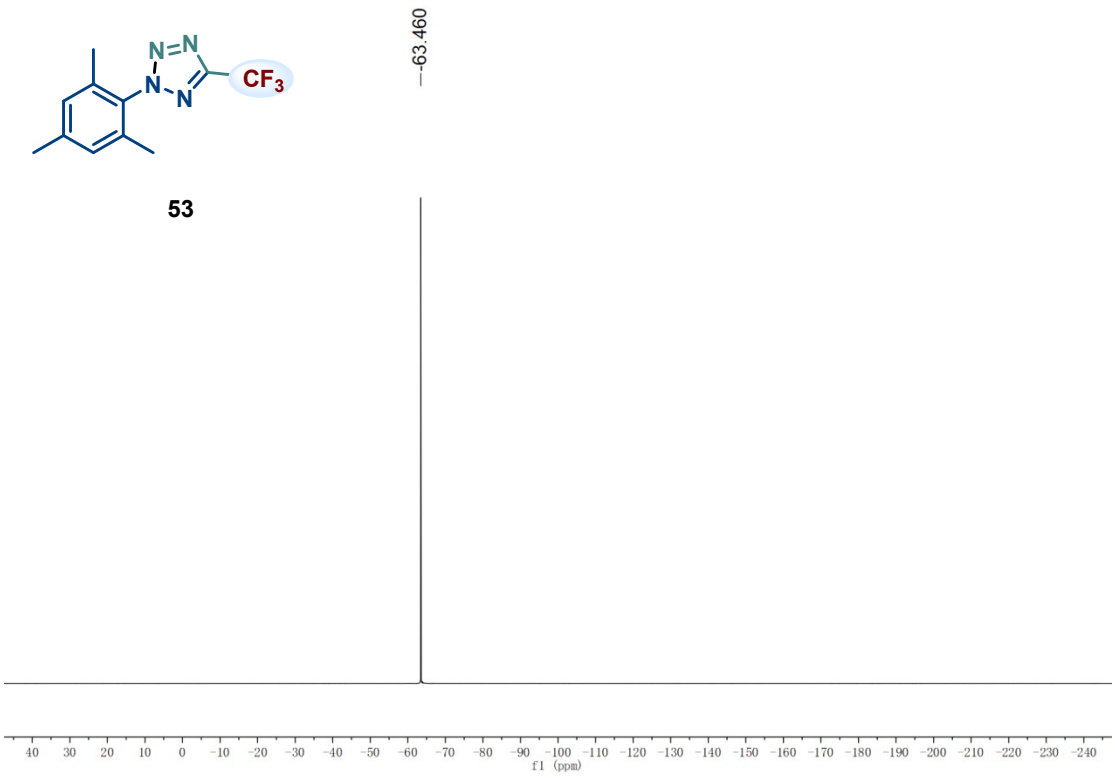

N=N
N
N
CF3

53

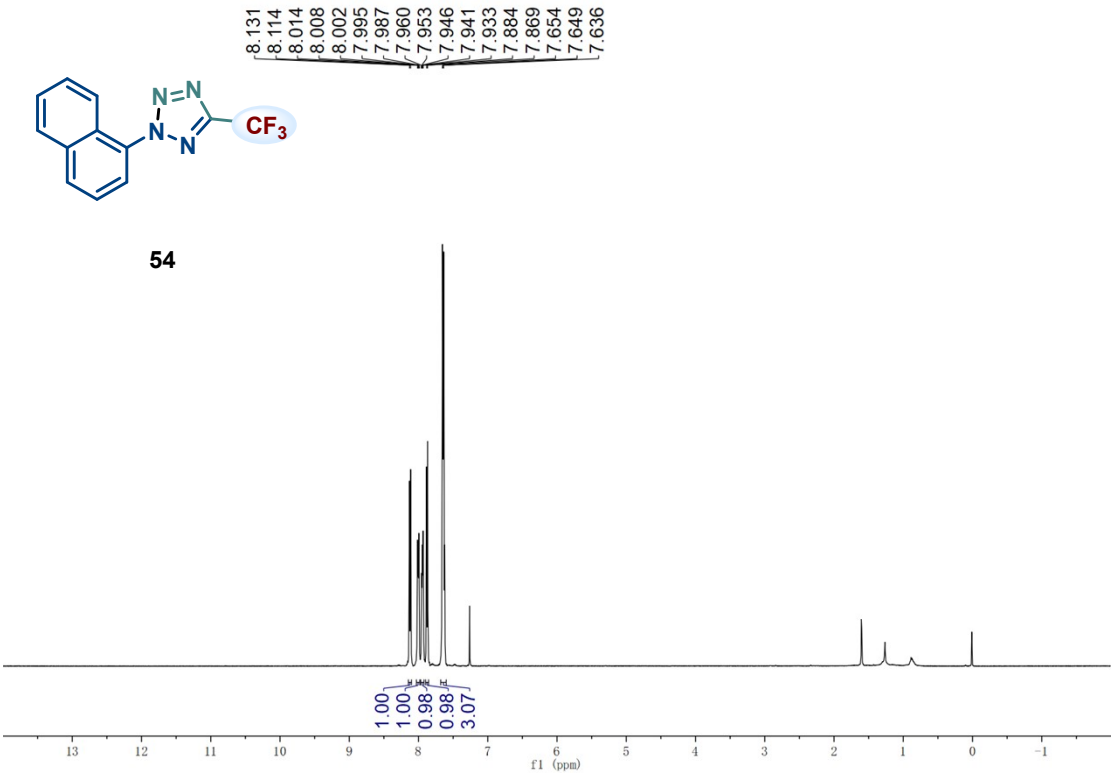
7.044
2.387
1.961
1.94
3.00
5.97
13.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5
f1 (ppm)

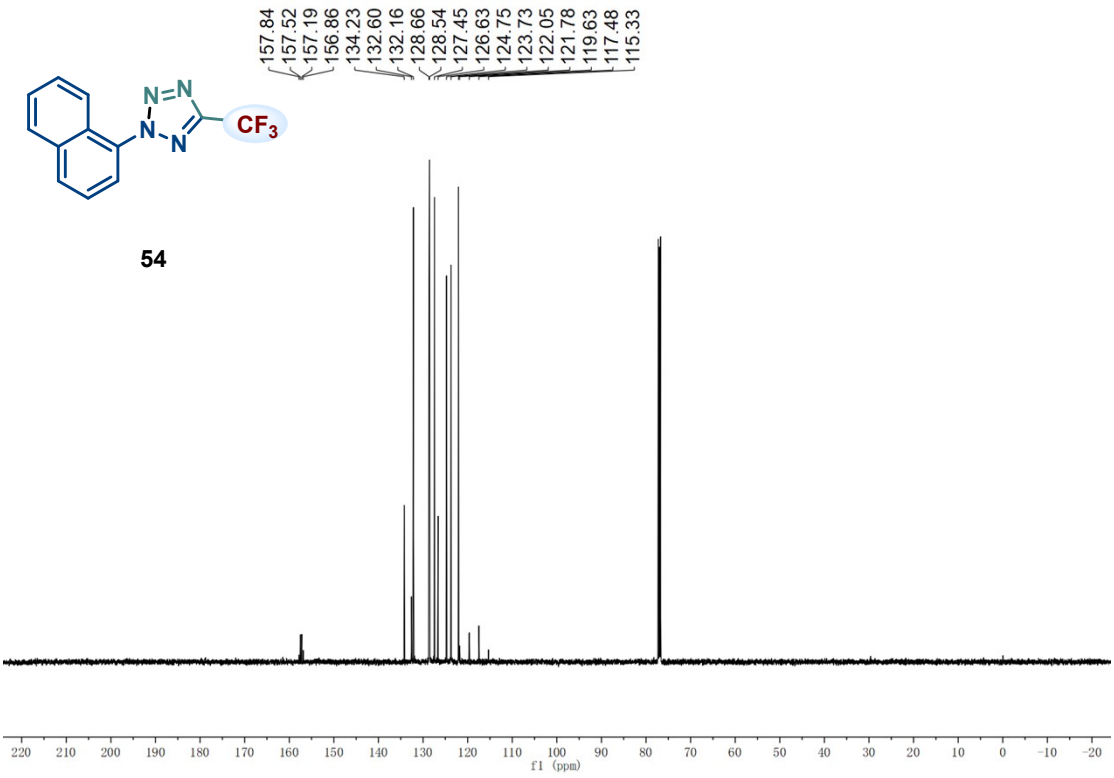

157.77
157.45
157.12
156.80
141.76
134.84
133.04
129.39
121.78
119.63
117.48
115.33
21.18
17.18
CF3
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)

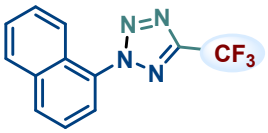
53


-63.460
CF3
40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -220 -230 -240
f1 (ppm)

53

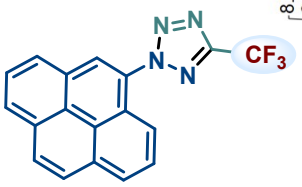

8.131
8.114
8.014
8.008
8.002
7.995
7.987
7.960
7.953
7.946
7.941
7.933
7.884
7.869
7.654
7.649
7.636
N=N
N
N
CF3
54
1.00
1.00
0.98
0.98
3.07
f1 (ppm)


157.84
157.52
157.19
156.86
134.23
132.60
132.16
128.66
128.54
127.45
126.63
124.75
123.73
122.05
121.78
119.63
117.48
115.33
N=N
N
N
CF3
54
f1 (ppm)



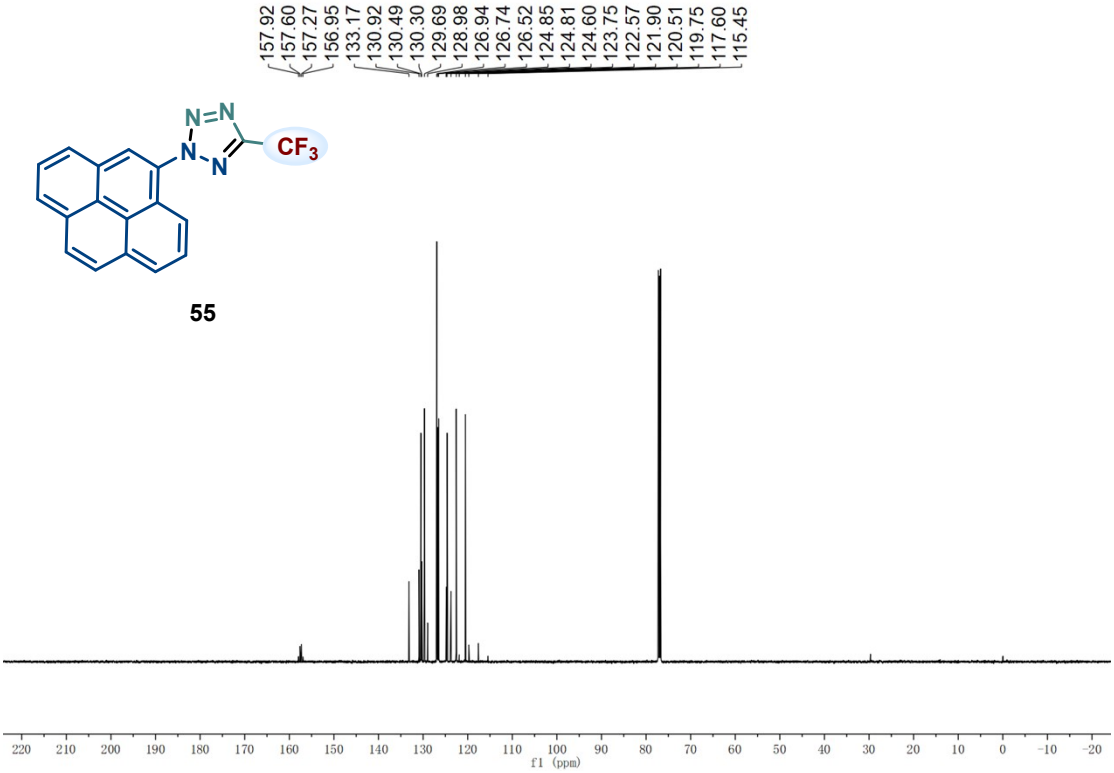
54

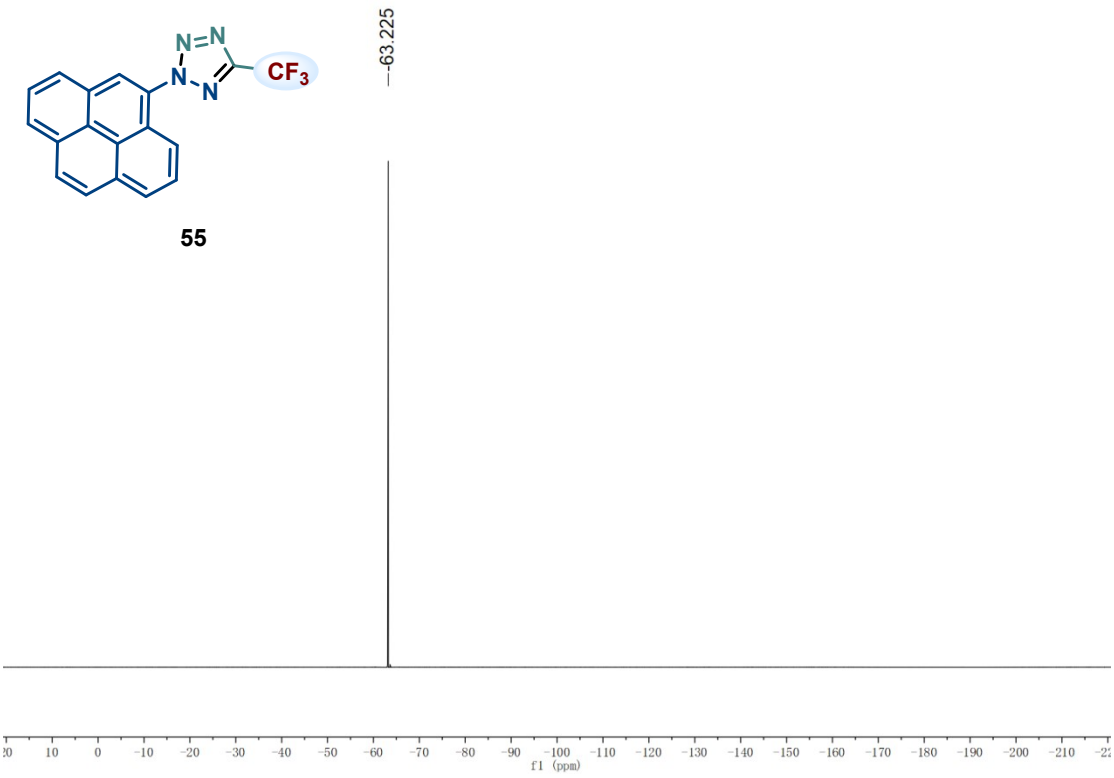
-63.334
40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -220 -230 -240
f1 (ppm)

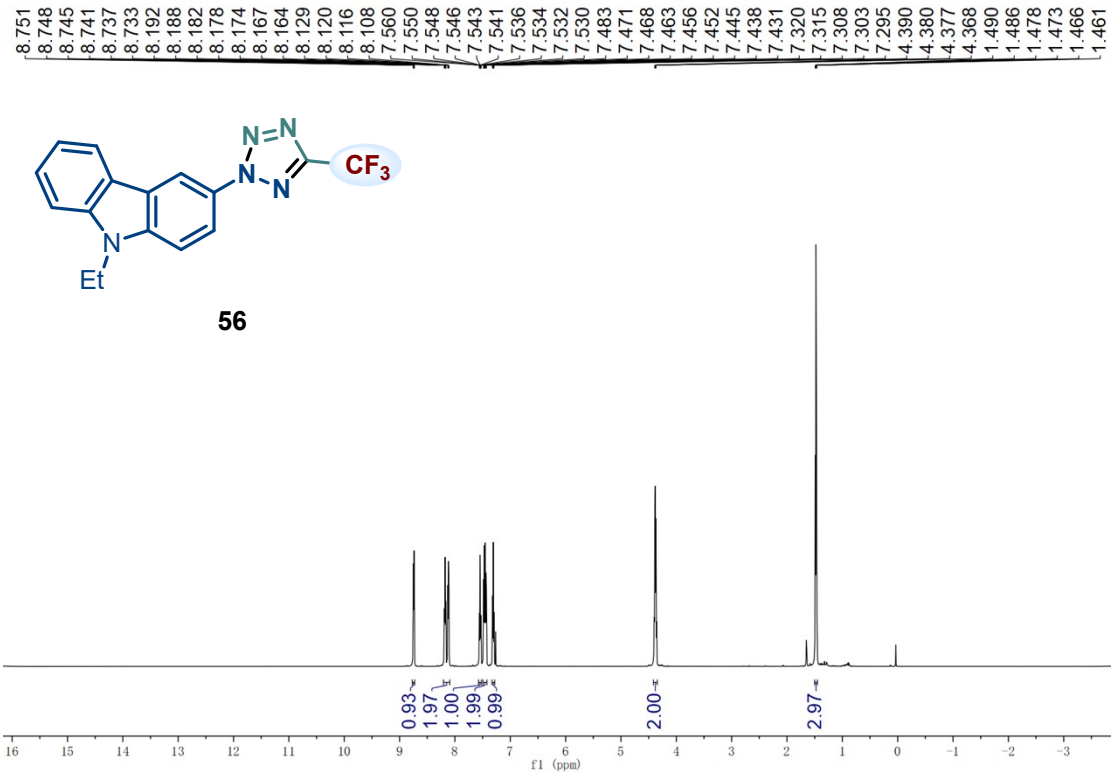


55

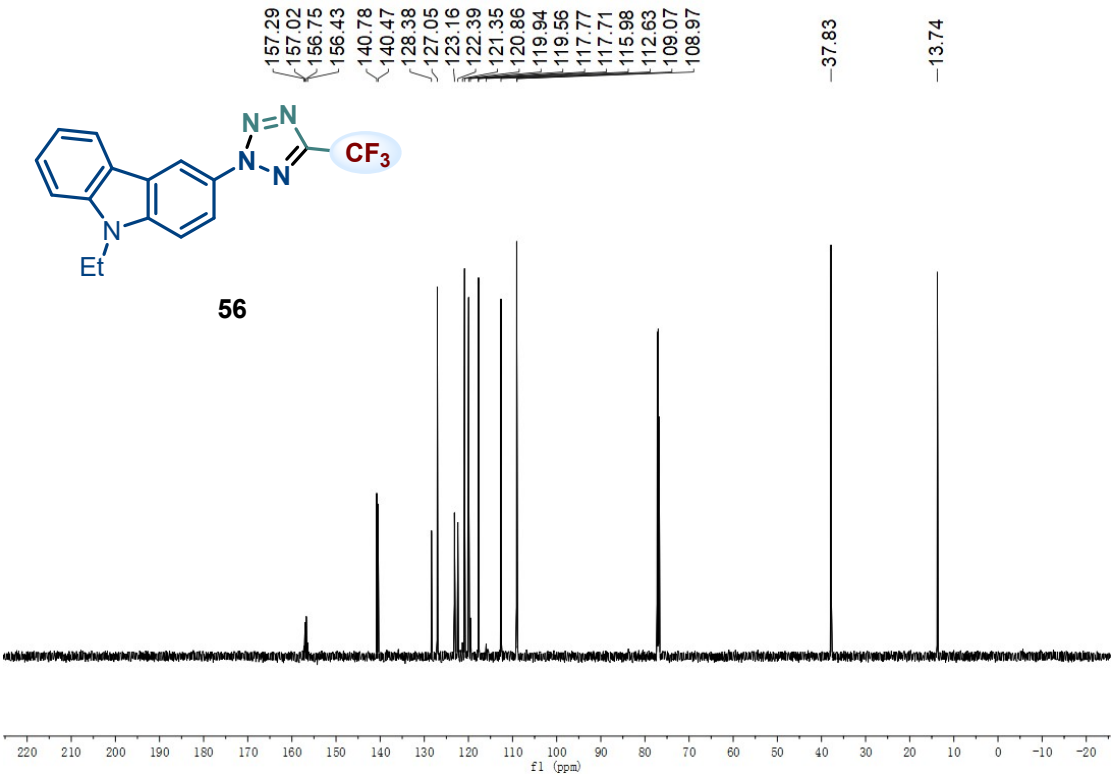
8.269
8.253
8.229
8.216
8.201
8.163
8.145
8.138
8.085
8.070
8.061
8.055
8.043
2.00
2.09
3.05
2.05
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3
f1 (ppm)


157.92
157.60
157.27
156.95
133.17
130.92
130.49
130.30
129.69
128.98
126.94
126.74
126.52
124.85
124.81
124.60
123.75
122.57
121.90
120.51
119.75
117.60
115.45
N=N
N
N
CF3
55
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)

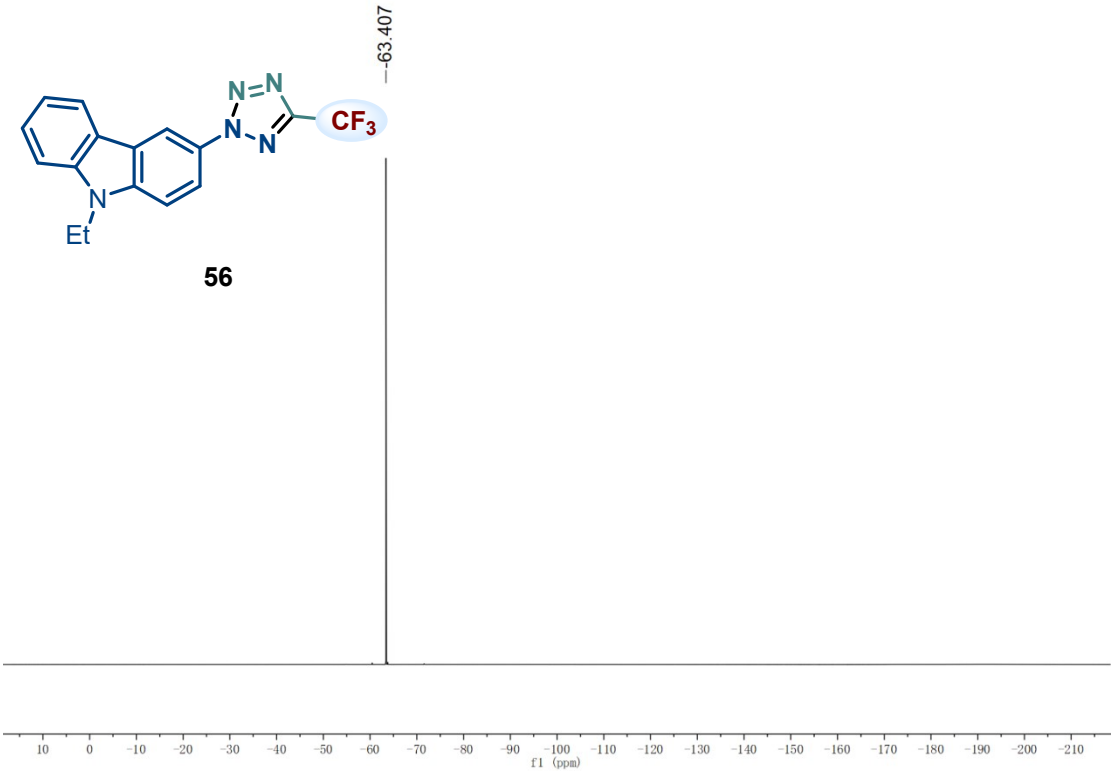

-63.225
N=N
N
N
CF3
55
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)


8.751
8.748
8.745
8.741
8.737
8.733
8.192
8.188
8.182
8.178
8.174
8.167
8.164
8.129
8.120
8.116
8.108
7.560
7.550
7.548
7.546
7.543
7.541
7.536
7.534
7.532
7.530
7.483
7.471
7.468
7.463
7.456
7.452
7.445
7.438
7.431
7.320
7.315
7.308
7.303
7.295
4.390
4.380
4.377
4.368
1.490
1.486
1.478
1.473
1.466
1.461
N=N
N
N
CF3
N
Et
0.93
1.97
1.00
1.99
0.99
2.00
2.97
f1 (ppm)

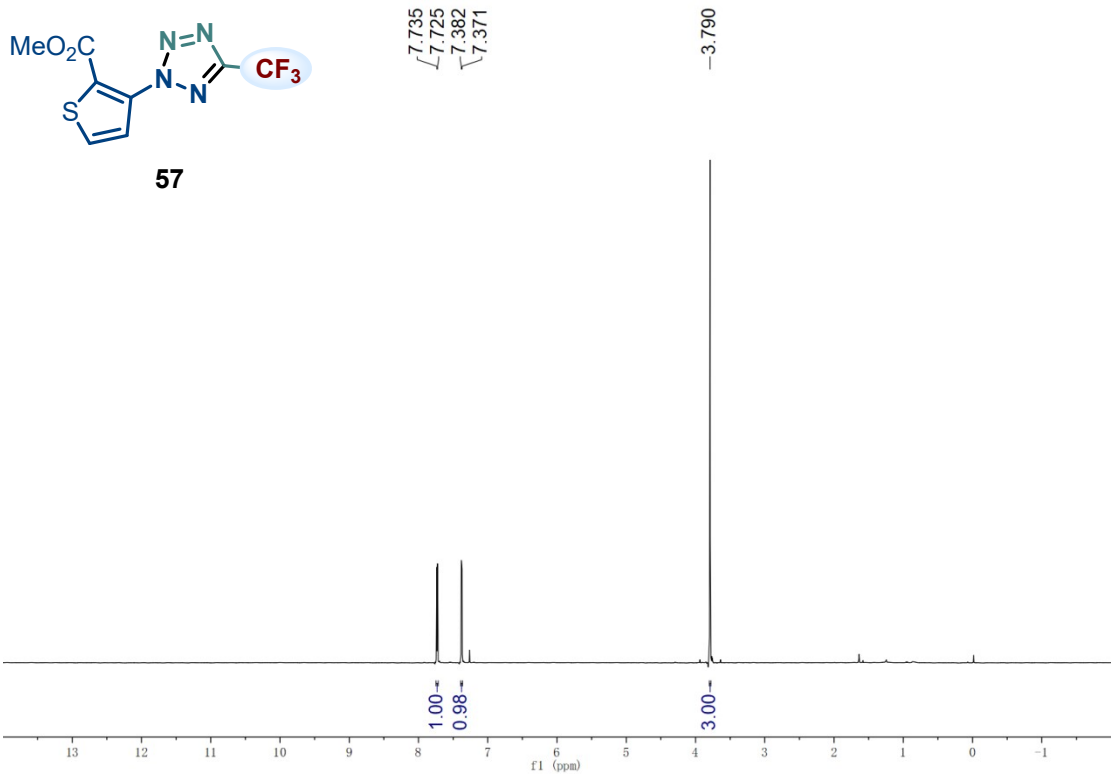
56


157.29
157.02
156.75
156.43
140.78
140.47
128.38
127.05
123.16
122.39
121.35
120.86
119.94
119.56
117.77
117.71
115.98
112.63
109.07
108.97
37.83
13.74
N=N
N
N
CF3
N
Et
f1 (ppm)

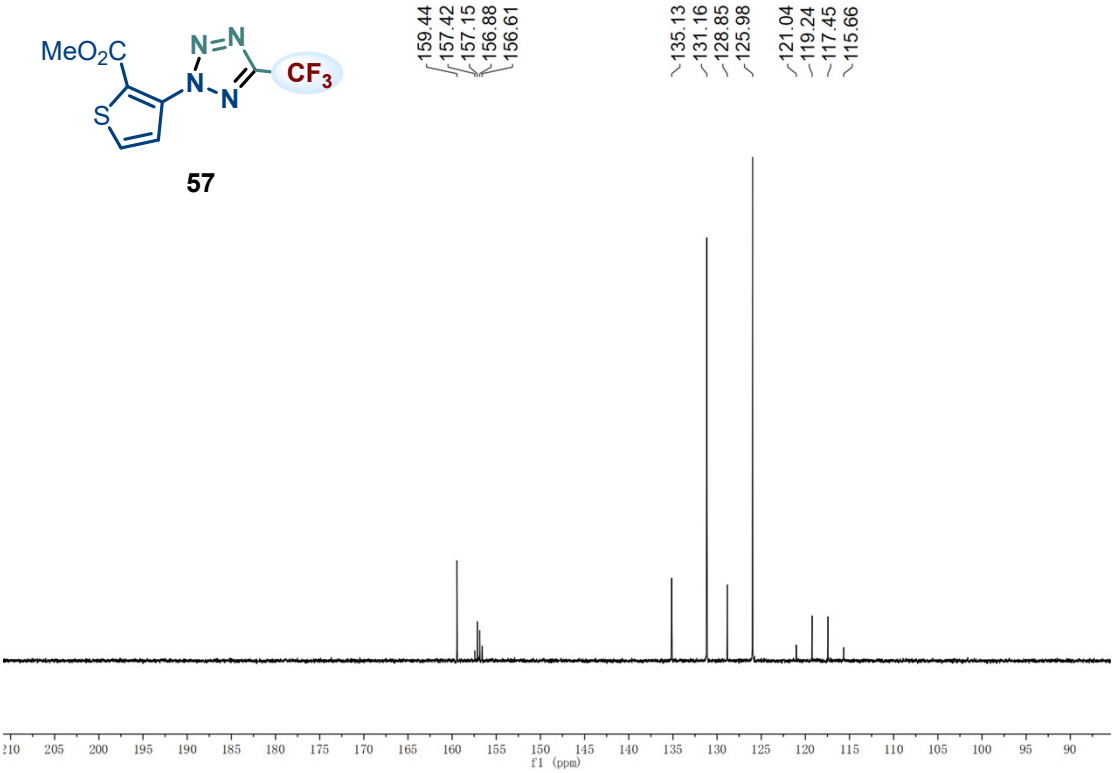
56


−63.407
N=N
N
N
CF3
N
Et
10 0 −10 −20 −30 −40 −50 −60 −70 −80 −90 −100 −110 −120 −130 −140 −150 −160 −170 −180 −190 −200 −210
f1 (ppm)

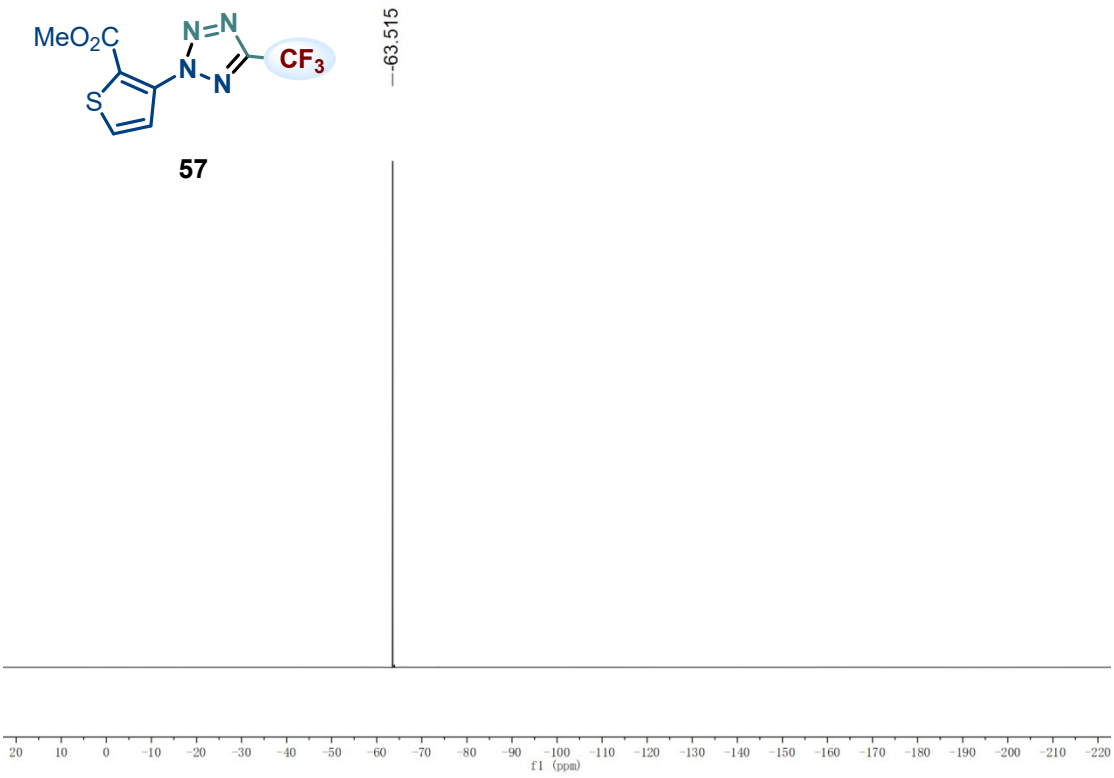
56


7.735
7.725
7.382
7.371
−3.790
MeO2C
N=N
N
N
CF3
S
1.00
0.98
3.00
13 12 11 10 9 8 7 6 5 4 3 2 1 0 −1
f1 (ppm)

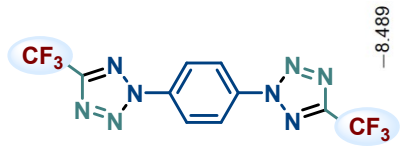
57


MeO2C
N=N
N
N
S
CF3
159.44
157.42
157.15
156.88
156.61
135.13
131.16
128.85
125.98
121.04
119.24
117.45
115.66
f1 (ppm)

57

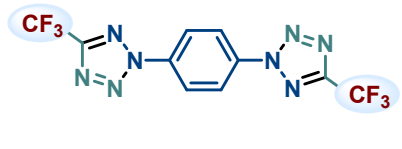

MeO2C
N=N
N
N
S
CF3
-63.515
f1 (ppm)

57



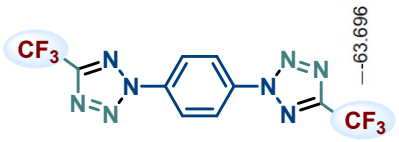
58

8.489
4.00



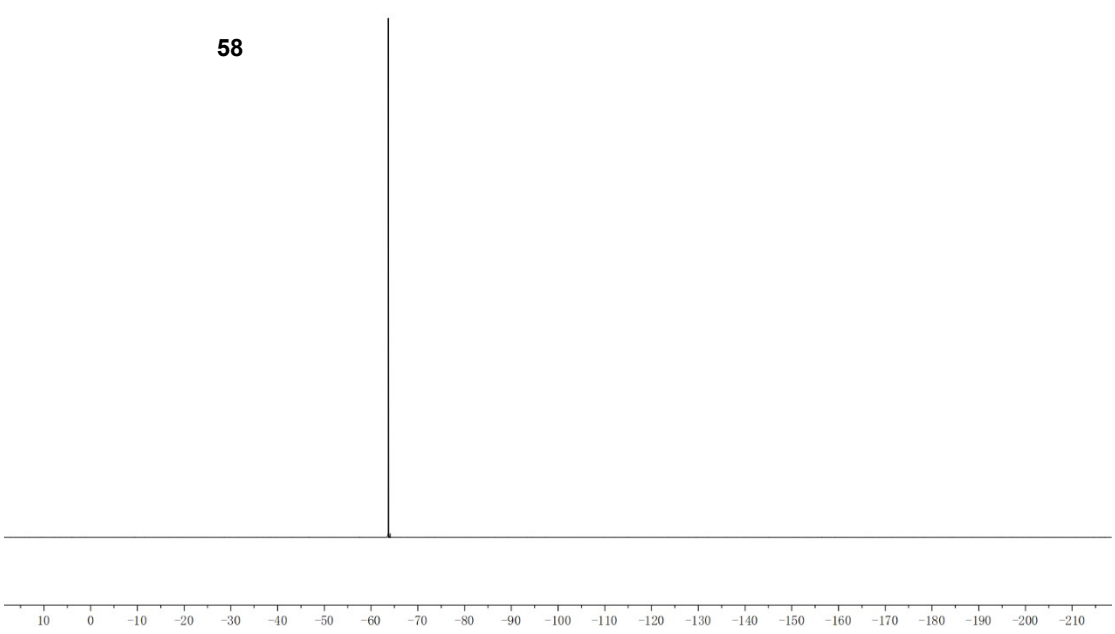
58

158.26
157.95
157.67
157.43
137.33
121.85
120.89
119.13
117.34
115.51

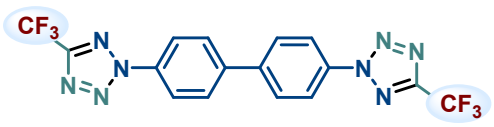

CF3
N
N
N
N
N
N
N
CF3

-63.696

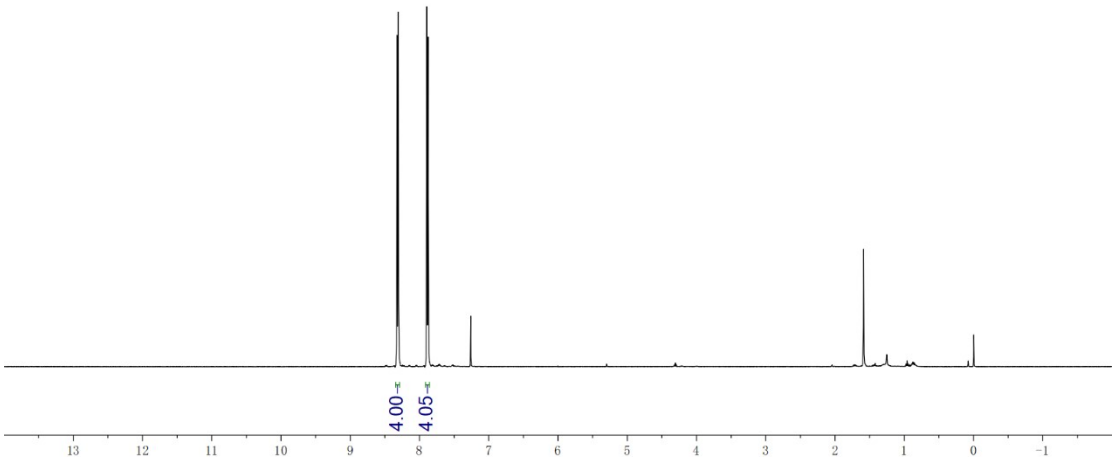
58

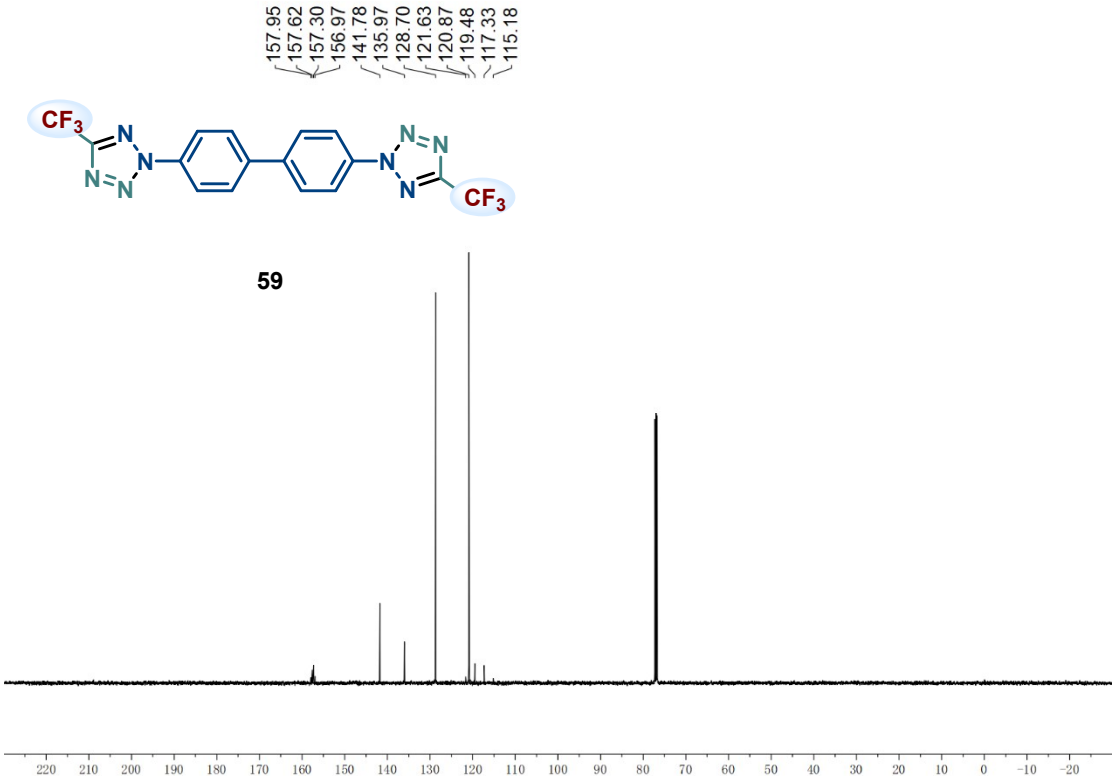

10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210

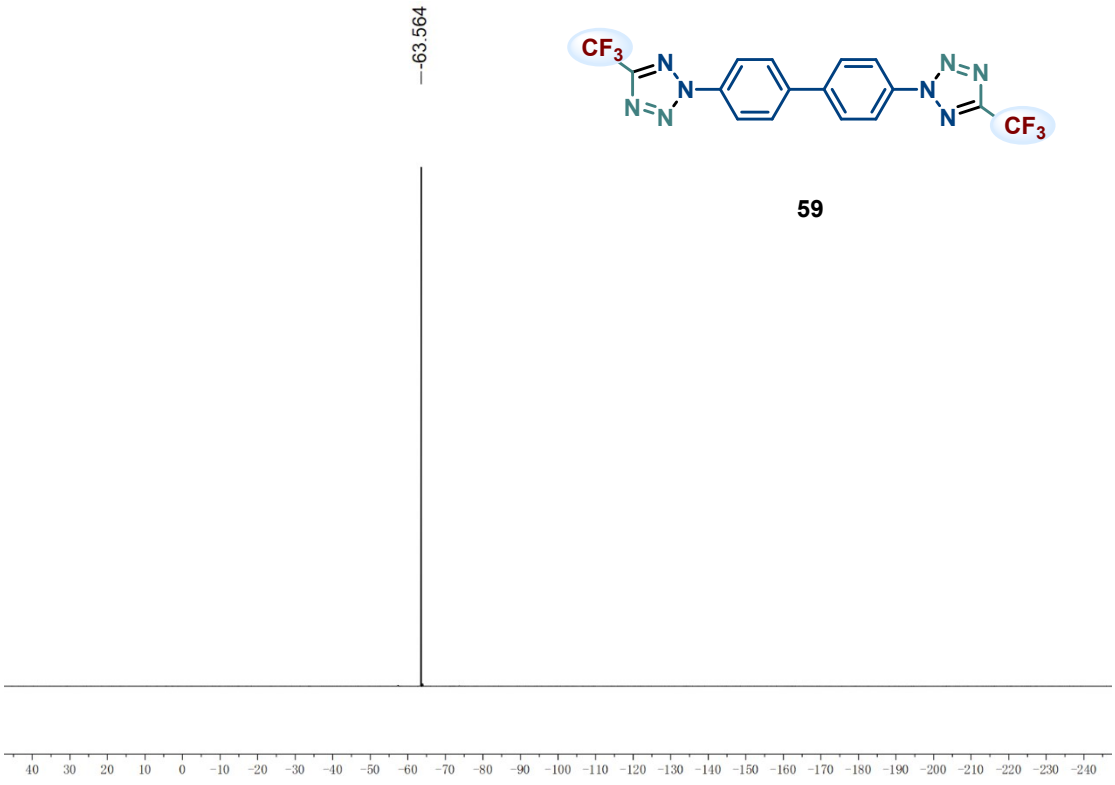

8.325
8.307
7.894
7.876

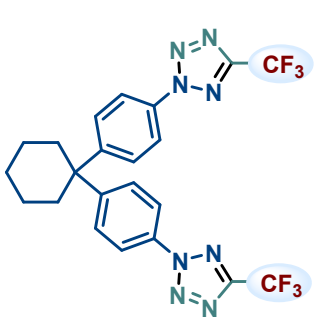

CF3
N
N
N
N
N
N
N
CF3

59


4.00
4.05
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1

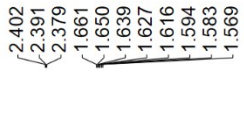

157.95
157.62
157.30
156.97
141.78
135.97
128.70
121.63
120.87
119.48
117.33
115.18
CF3
CF3
59
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20


-63.564
CF3
CF3
59
40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -220 -230 -240


CF3
CF3

60

8.098
8.080
7.539
7.521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2.379
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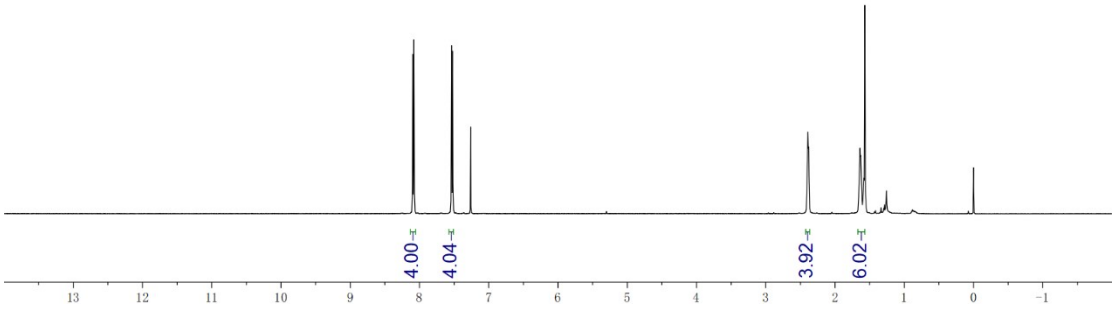
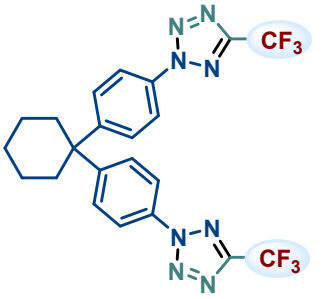
1.639
1.627
1.616
1.594
1.583
1.569


4.00
4.04
3.92
6.02


CF3
CF3

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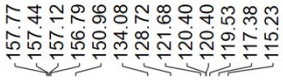
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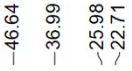
157.44
157.12
156.79
150.96
134.08
128.72
121.68
120.40
120.40
119.53
117.38
115.23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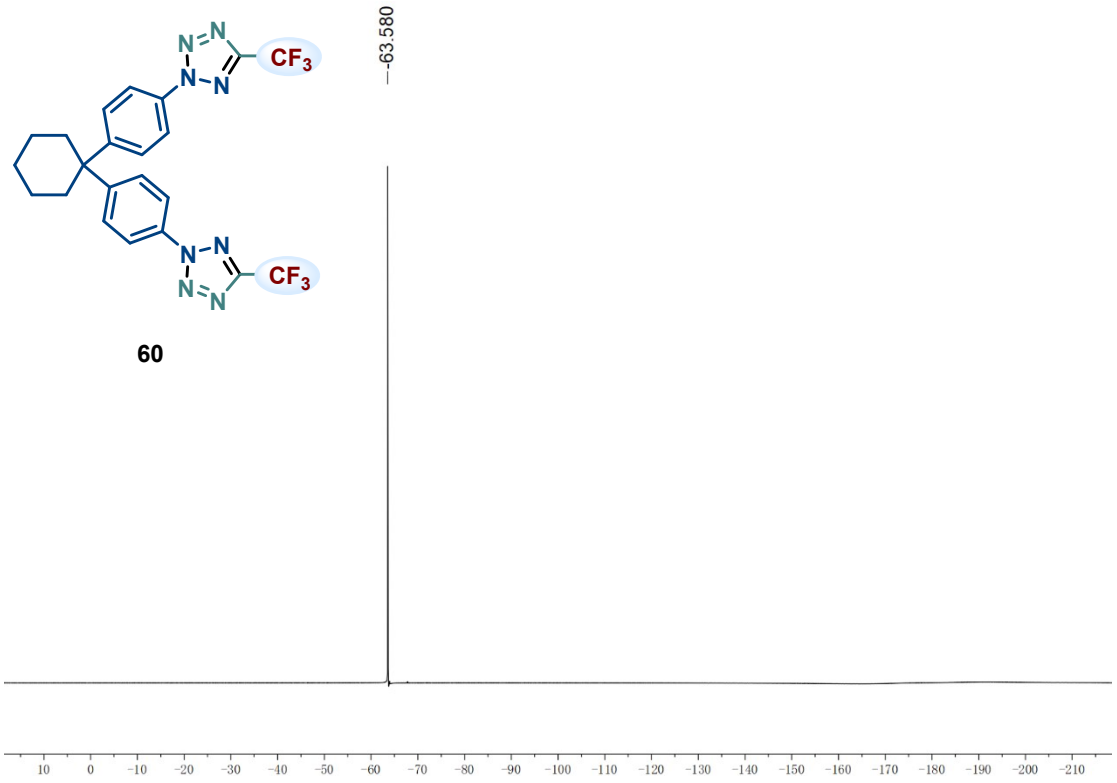
36.99
25.98
22.71


CF3
CF3
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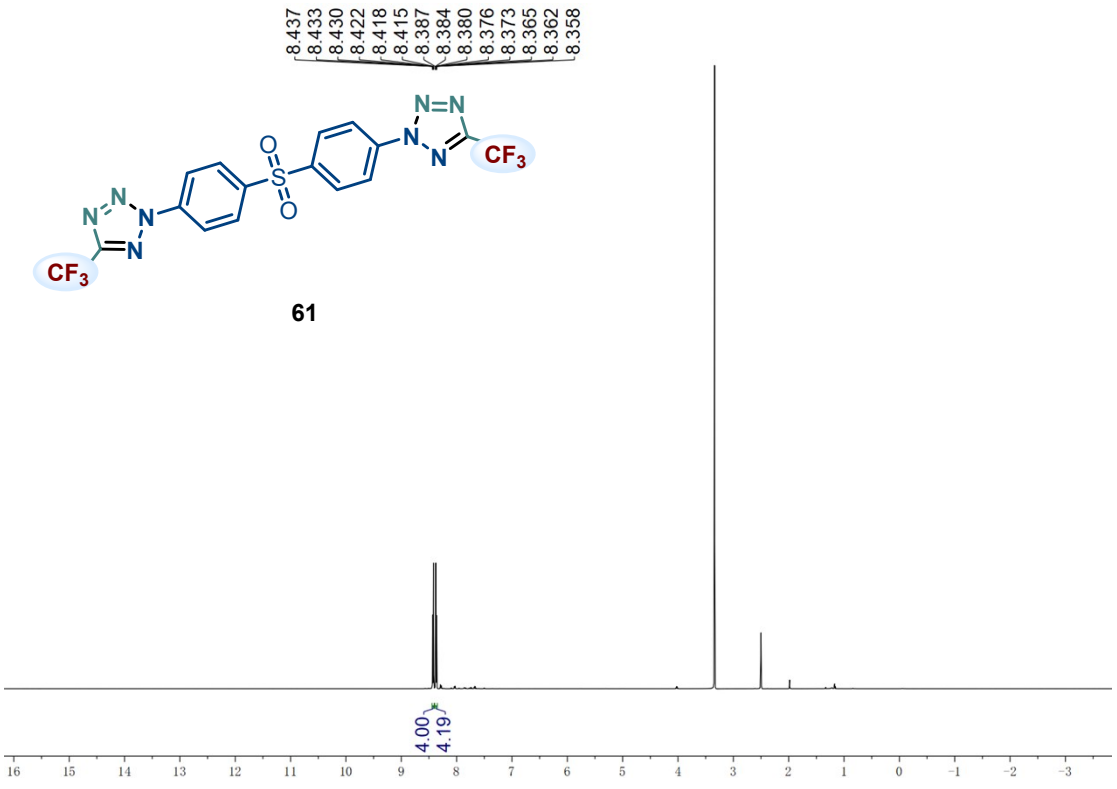
60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8.430
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8.418
8.415
8.387
8.384
8.380
8.376
8.373
8.365
8.362
8.358
CF3
CF3
4.00
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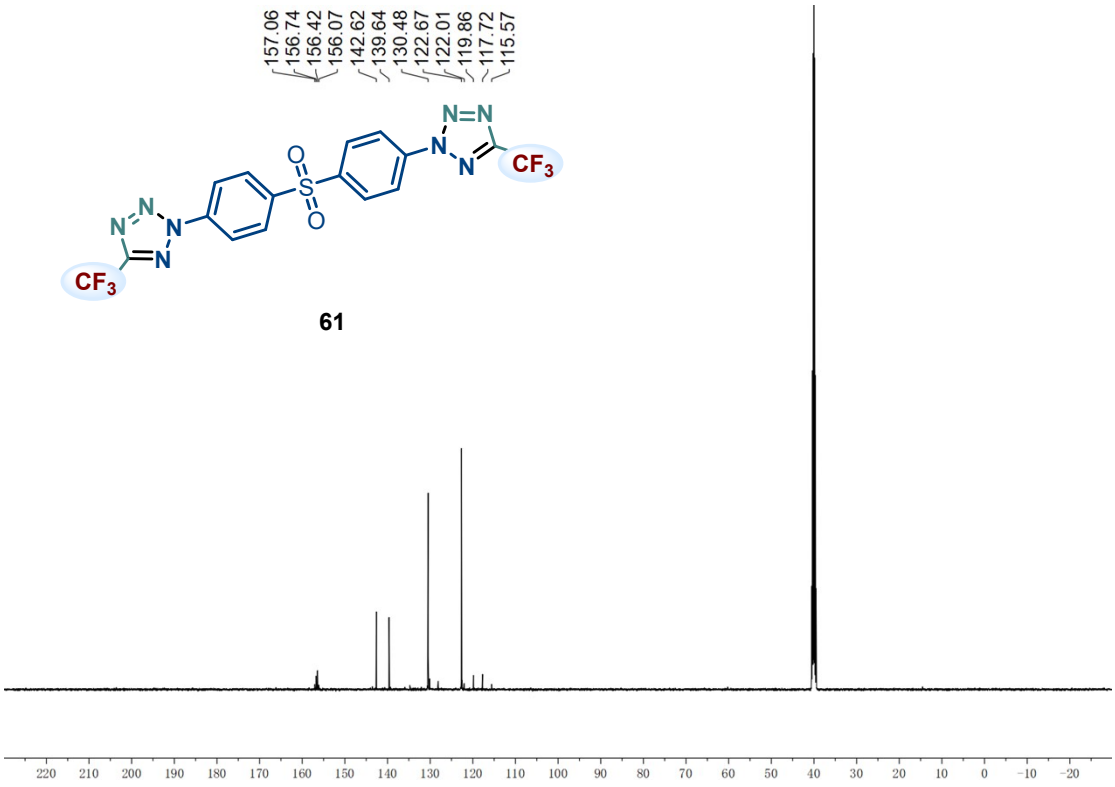
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3

61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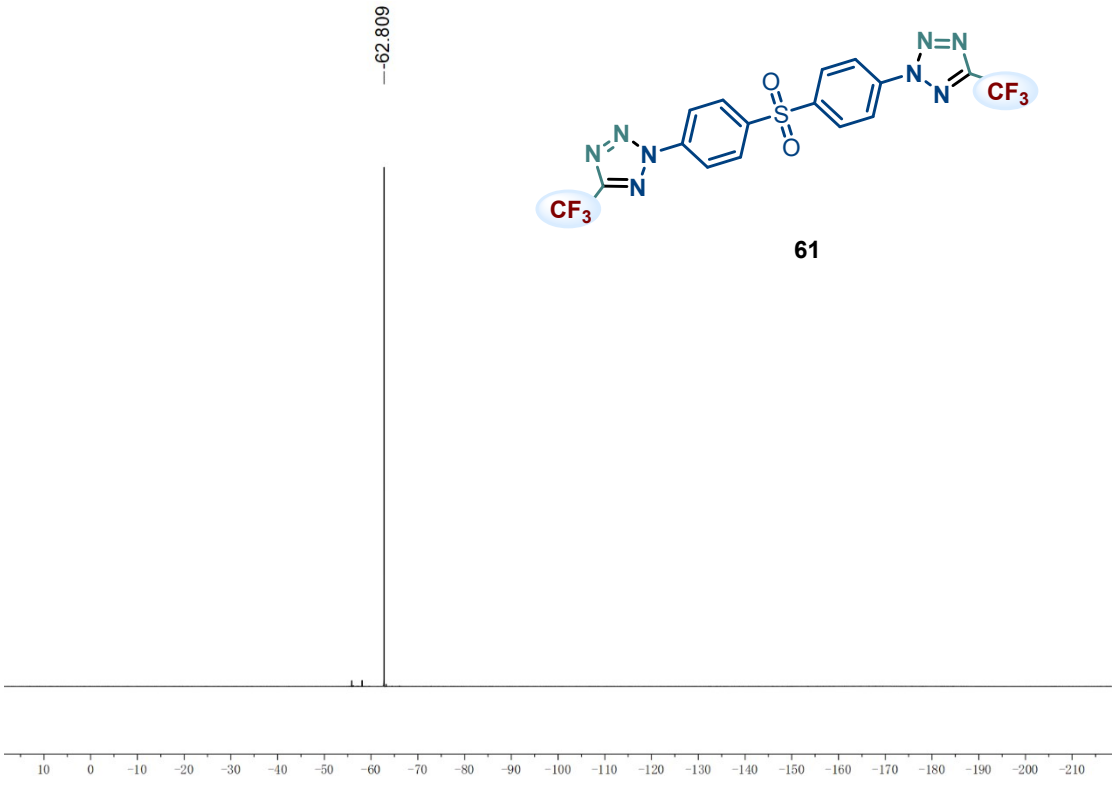
156.74
156.42
156.07
142.62
139.64
130.48
122.67
122.01
119.86
117.72
115.57
N=N
CF3
CF3
61
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20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CF3
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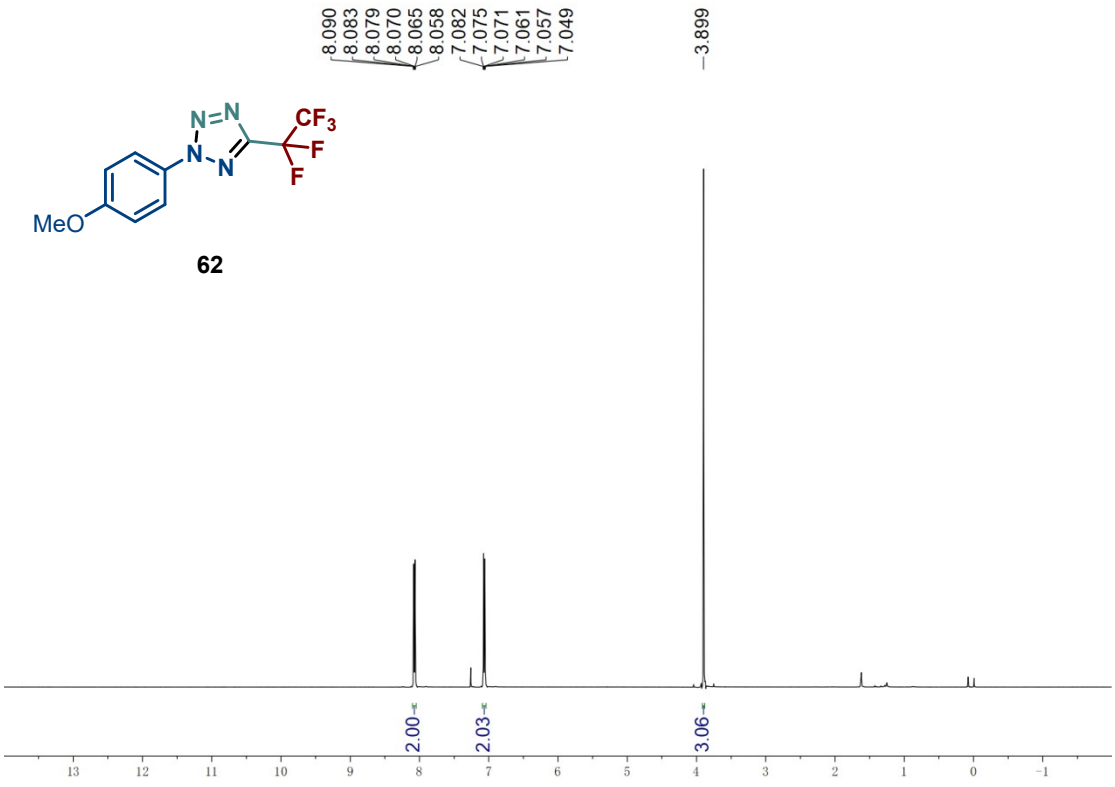
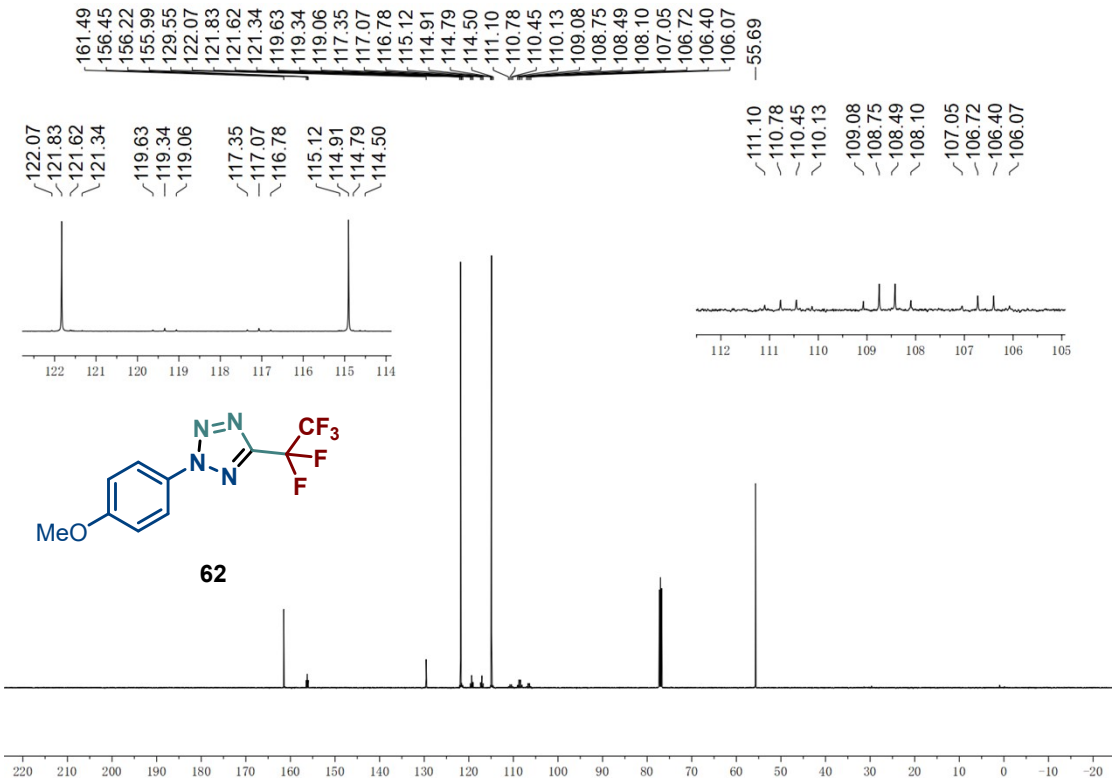

8.090
8.083
8.079
8.070
8.065
8.058
7.082
7.075
7.071
7.061
7.057
7.049
3.899
MeO
62
2.00
2.03
3.06


161.49
156.45
156.22
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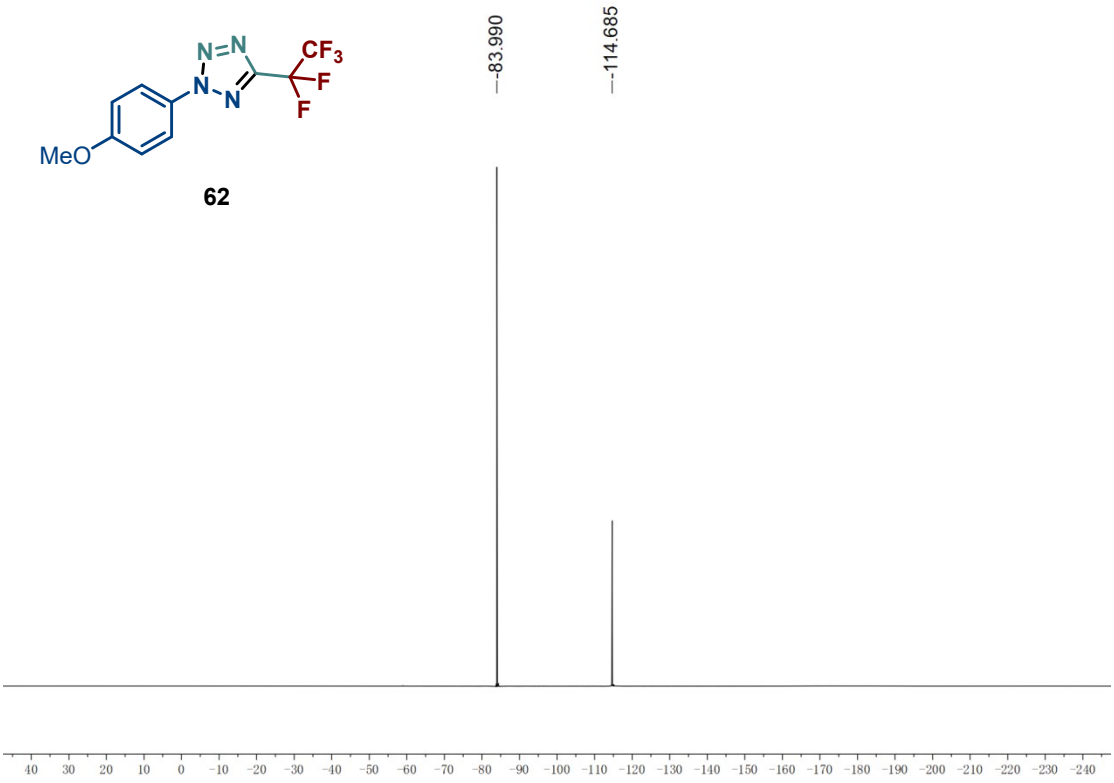
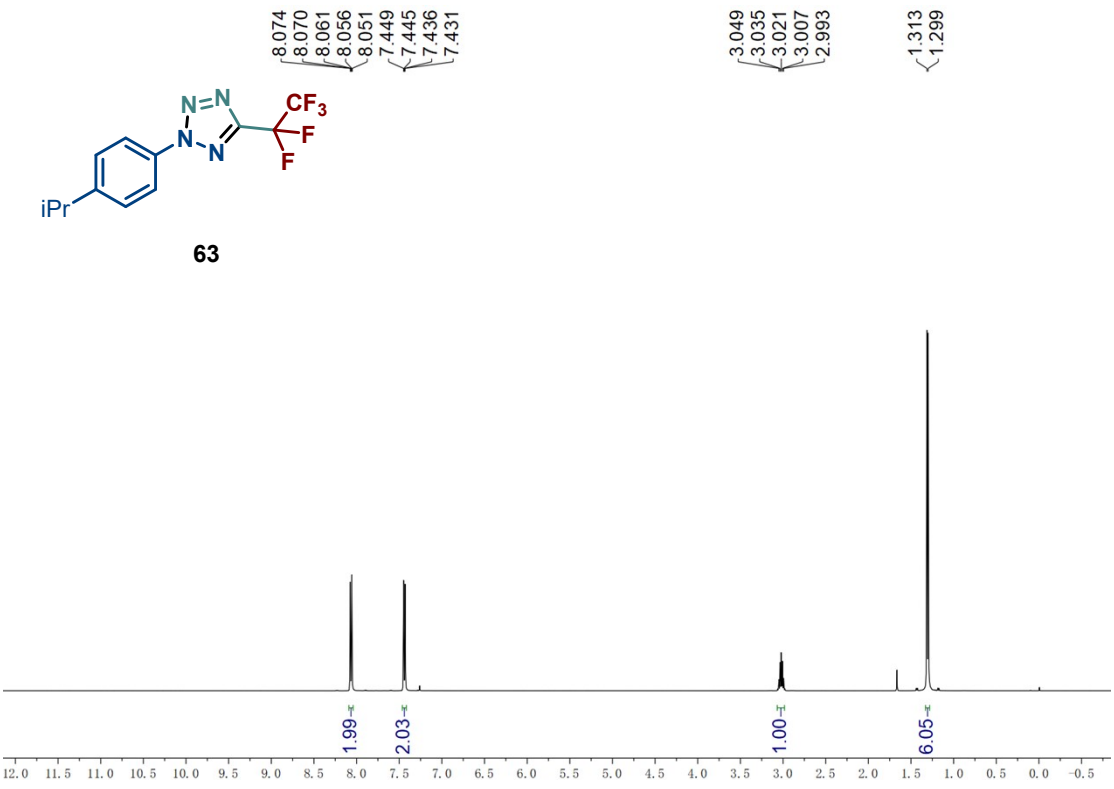
129.55
122.07
121.83
121.62
121.34
119.63
119.34
119.06
117.35
117.07
116.78
115.12
114.91
114.79
114.50
111.10
110.78
110.45
110.13
109.08
108.75
108.49
108.10
107.05
106.72
106.40
106.07
55.69
MeO
62


MeO
N=N
N
N
CF3
F
F
-83.990
-114.685
40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -220 -230 -240

62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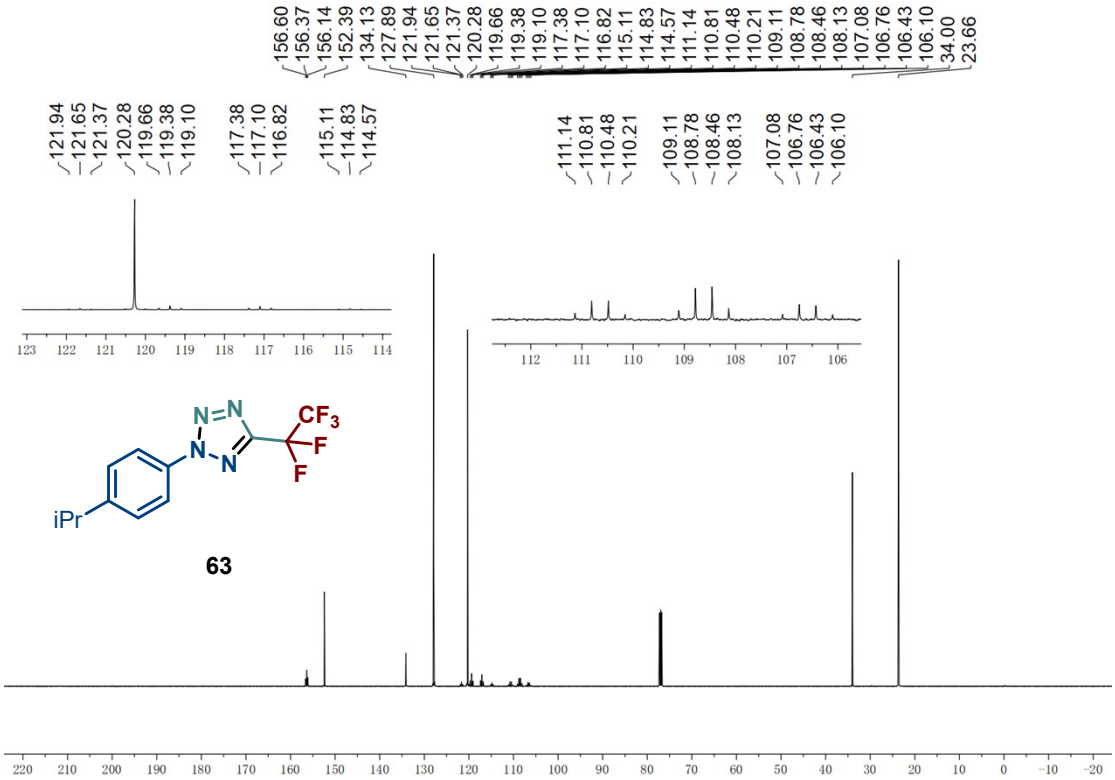
8.070
8.061
8.056
8.051
7.449
7.445
7.436
7.431
3.049
3.035
3.021
3.007
2.993
1.313
1.299
iPr
N=N
N
N
CF3
F
F
1.99
2.03
1.00
6.05
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5

63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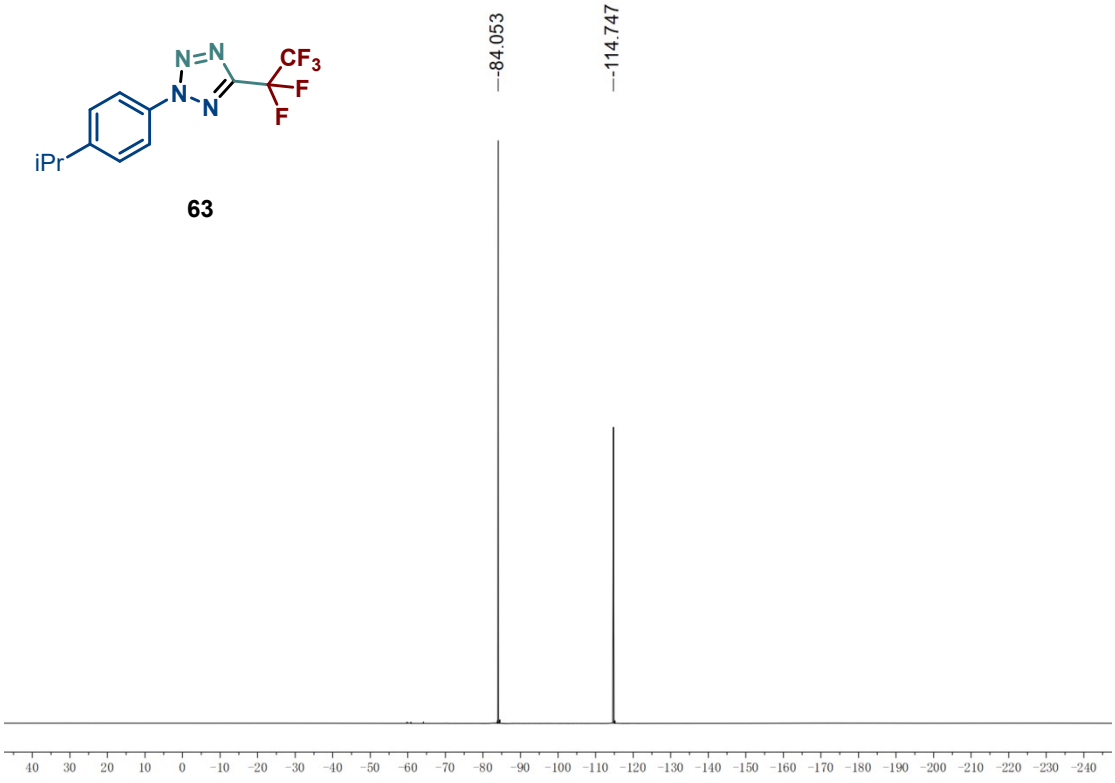
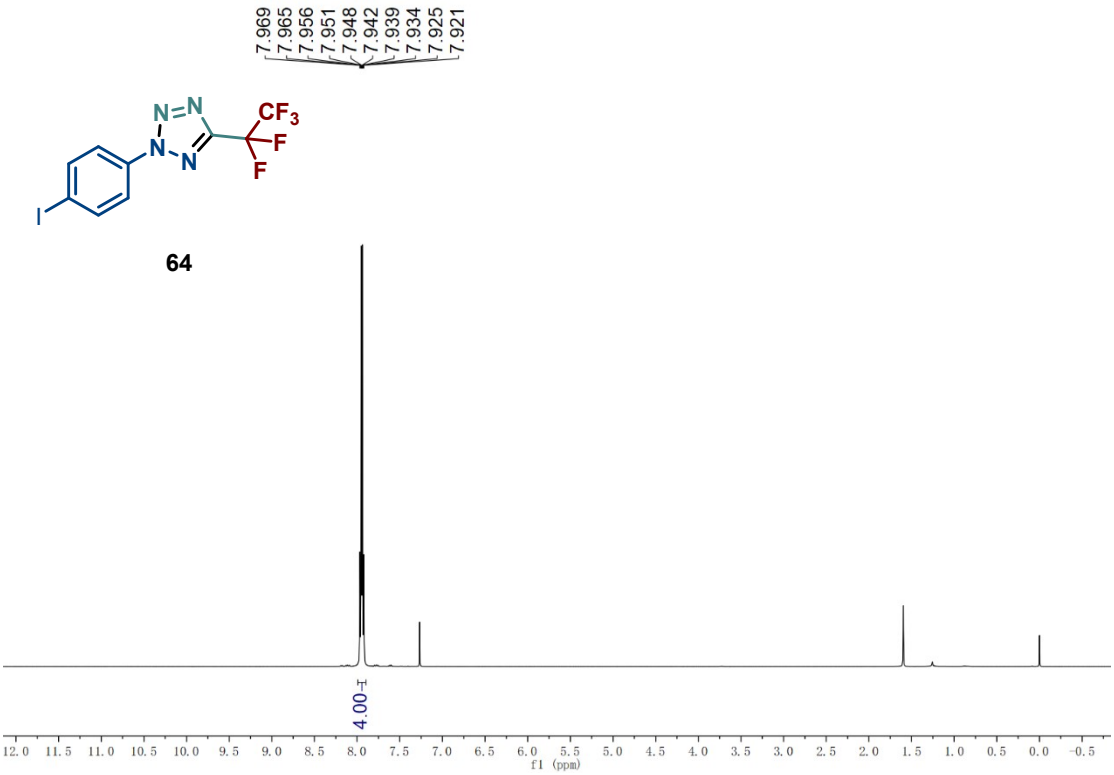
127.89
121.94
121.65
121.37
120.28
119.66
119.38
119.10
117.38
117.10
116.82
115.11
114.83
114.57
111.14
110.81
110.48
110.21
109.11
108.78
108.46
108.13
107.08
106.76
106.43
106.10
34.00
23.66
iPr
CF3
F
F
63


-84.053
-114.747
iPr
CF3
F
F
63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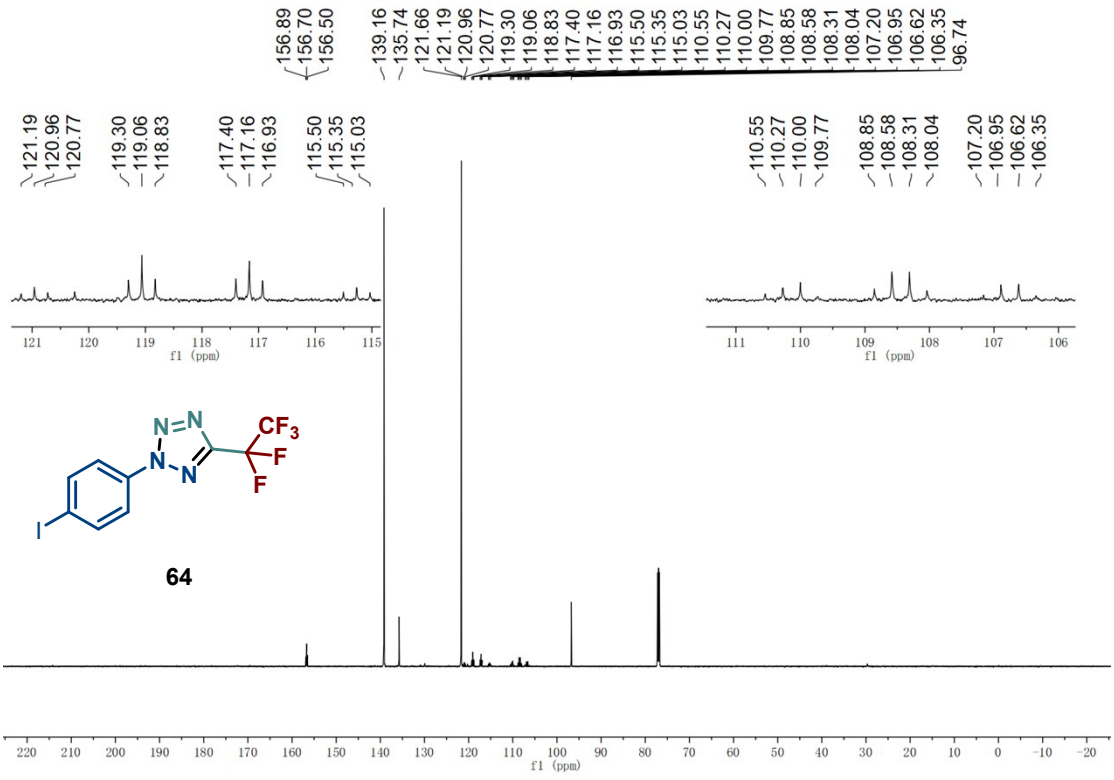
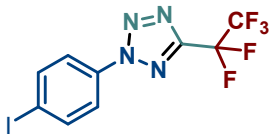
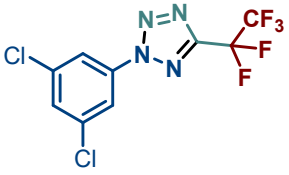
7.965
7.956
7.951
7.948
7.942
7.939
7.934
7.925
7.921
N=N
N
N
CF3
F
F
I
64
4.00
f1 (ppm)


156.89
156.70
156.50
139.16
135.74
121.66
121.19
120.96
120.77
119.30
119.06
118.83
117.40
117.16
116.93
115.50
115.35
115.03
110.55
110.27
110.00
109.77
108.85
108.58
108.31
108.04
107.20
106.95
106.62
106.35
96.74
f1 (ppm)
N=N
N
N
CF3
F
F
I
64



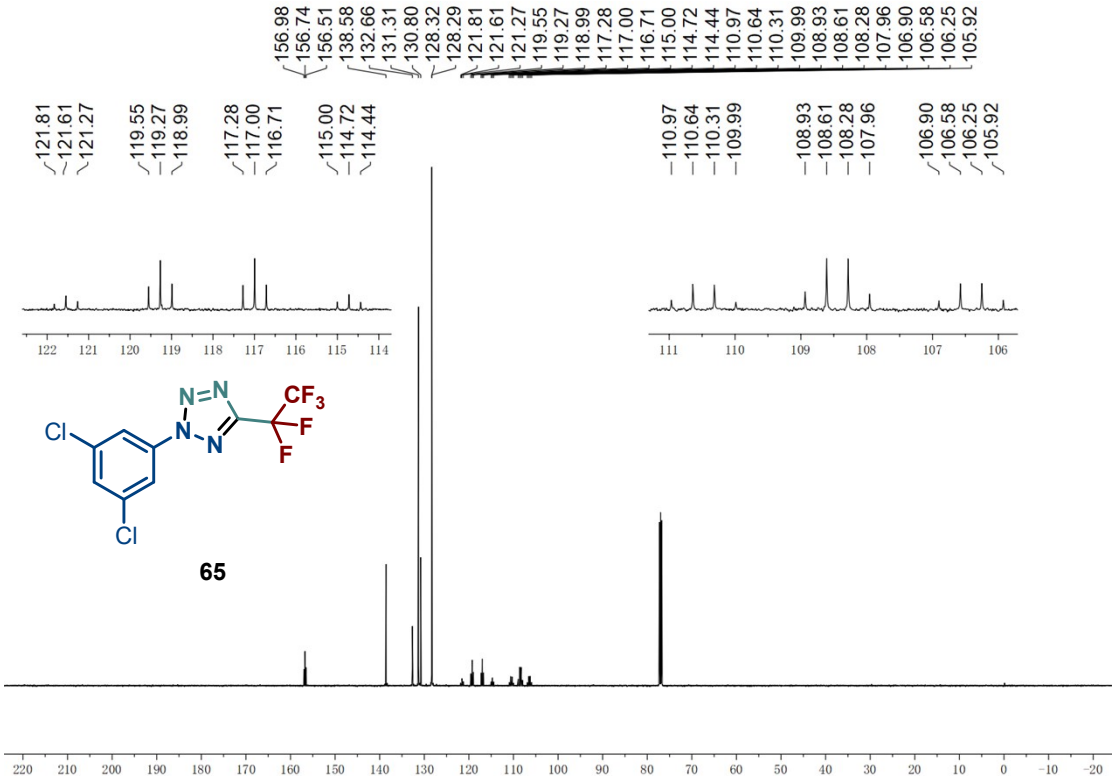
64

-83.907
-114.721
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)



65

7.688
7.683
7.648
7.631
7.521
7.517
7.504
7.499
1.00
1.05
1.05
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5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156.51
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128.32
128.29
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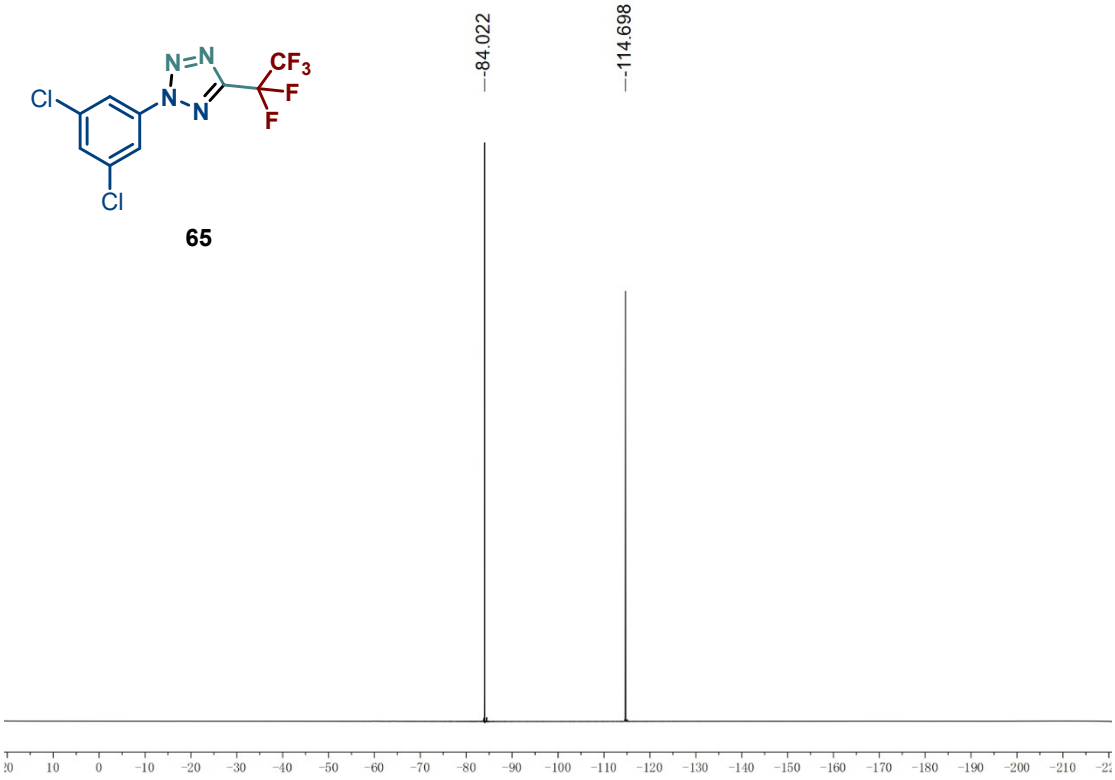
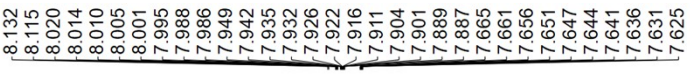
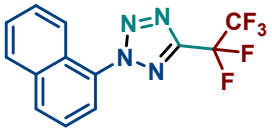
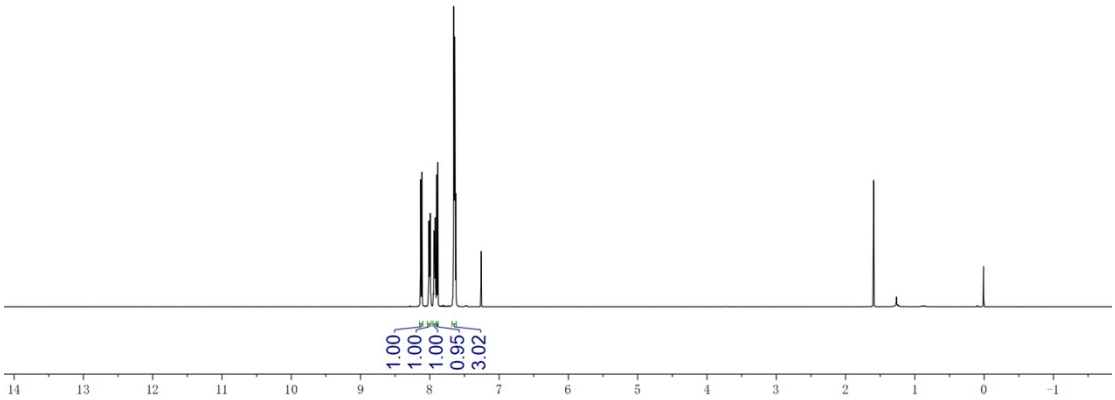
121.61
121.27
119.55
119.27
118.99
117.28
117.00
116.71
115.00
114.72
114.44
110.97
110.64
110.31
109.99
108.93
108.61
108.28
107.96
106.90
106.58
106.25
105.92
Cl
Cl
N=N
CF3
F
F
65

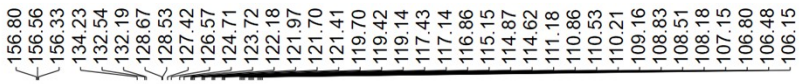

-84.022
-114.698
Cl
Cl
N=N
CF3
F
F
65


8.132
8.115
8.020
8.014
8.010
8.005
8.001
7.995
7.988
7.986
7.949
7.942
7.935
7.932
7.926
7.922
7.916
7.911
7.904
7.901
7.889
7.887
7.665
7.661
7.656
7.651
7.647
7.644
7.641
7.636
7.631
7.625


N=N
N
N
CF3
F
F

66


1.00
1.00
1.00
0.95
3.02
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
−1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132.19
128.67
128.53
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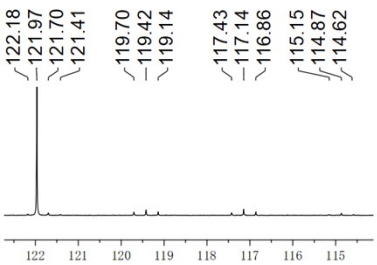
126.57
124.71
123.72
122.18
121.97
121.70
121.41
119.70
119.42
119.14
117.43
117.14
116.86
115.15
114.87
114.62
111.18
110.86
110.53
110.21
109.16
108.83
108.51
108.18
107.15
106.80
106.48
106.15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121.70
121.41
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119.42
119.14
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115.15
114.87
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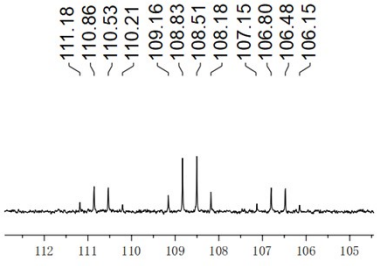
122
121
120
119
118
117
116
115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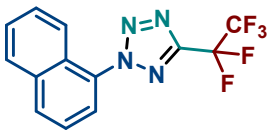
110.86
110.53
110.21
109.16
108.83
108.51
108.18
107.15
106.80
106.48
106.15
112
111
110
109
108
107
106
105


N=N
N
N
CF3
F
F

66

220
210
200
190
180
170
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150
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130
120
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90
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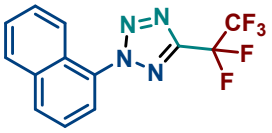
10
0
−10
−20



66

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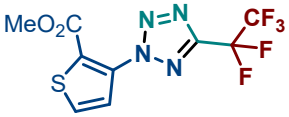
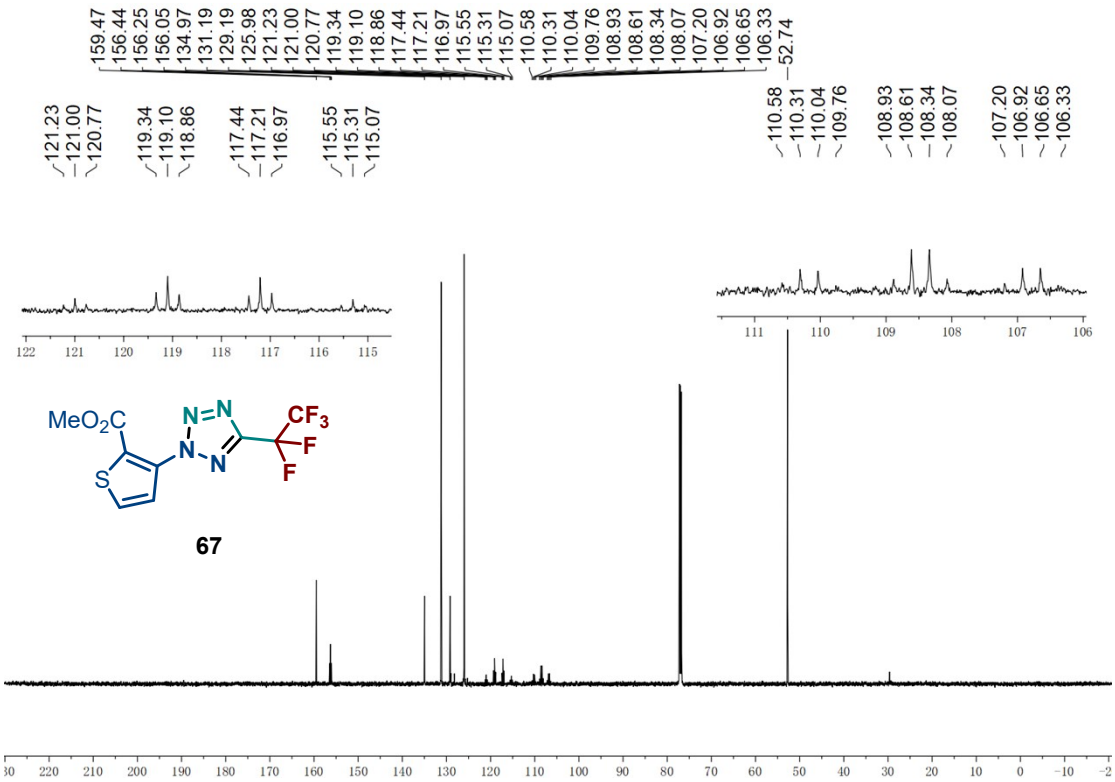


67

7.736
7.725
7.400
7.389
3.768
1.00
1.02
3.09
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5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156.05
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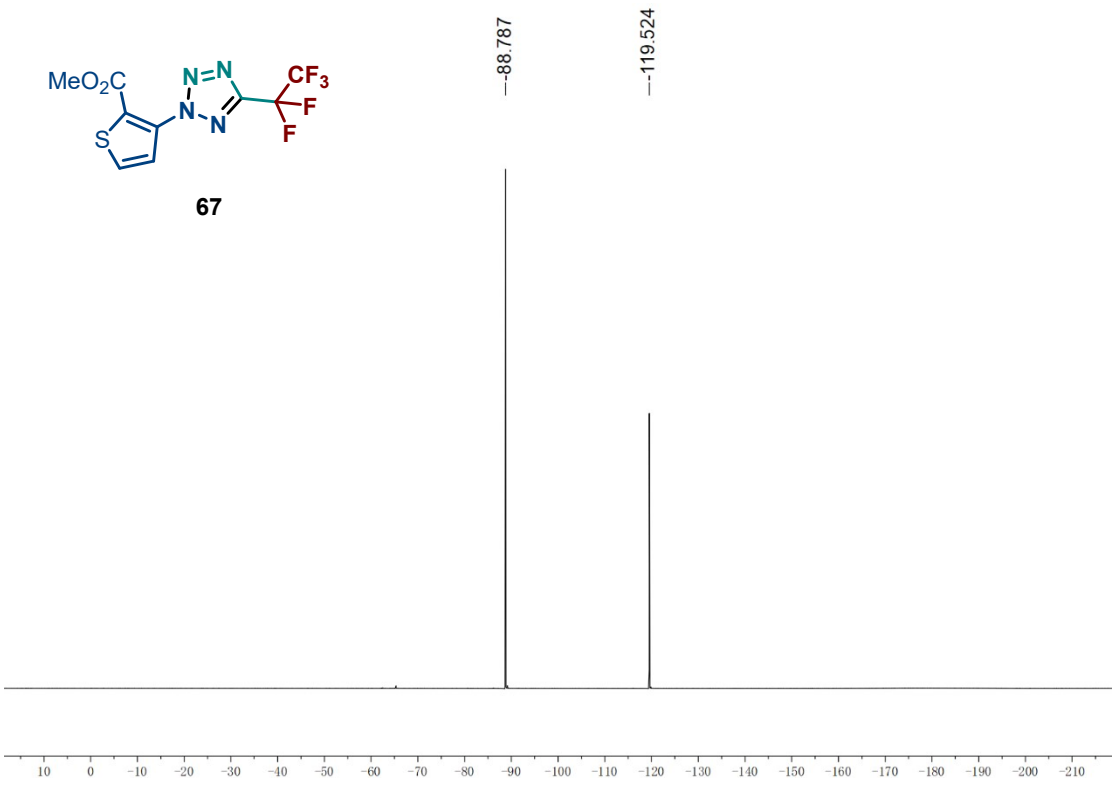
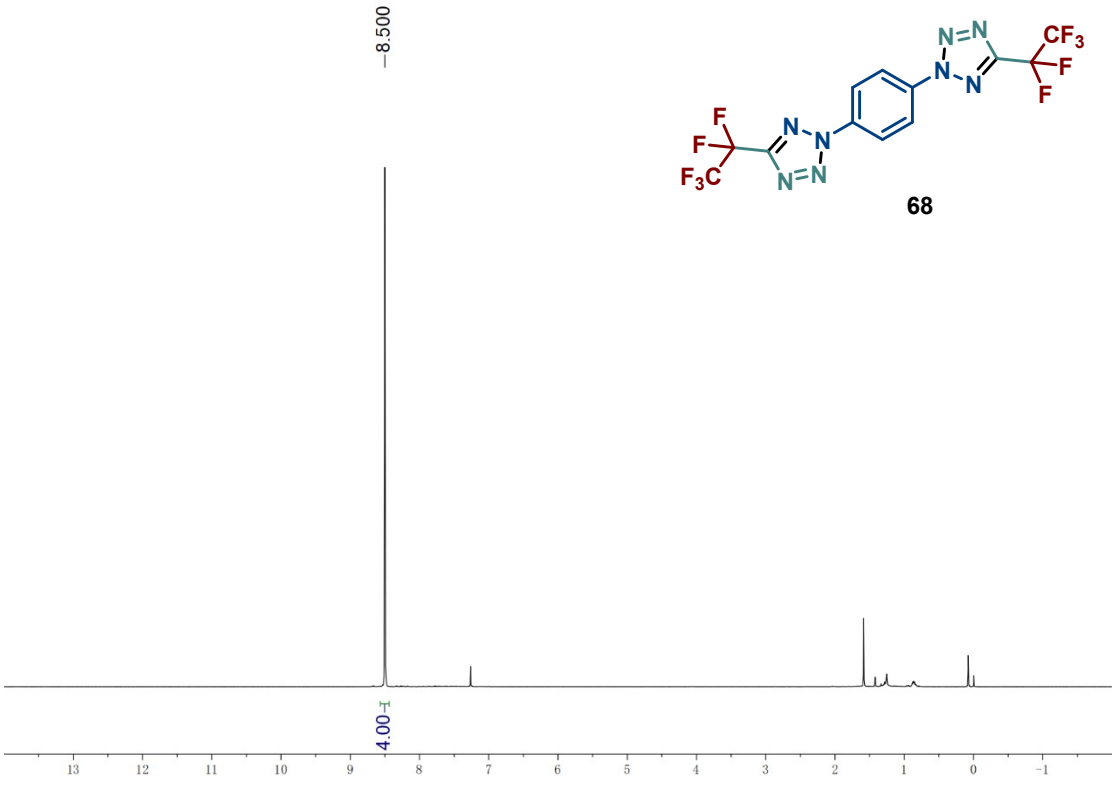
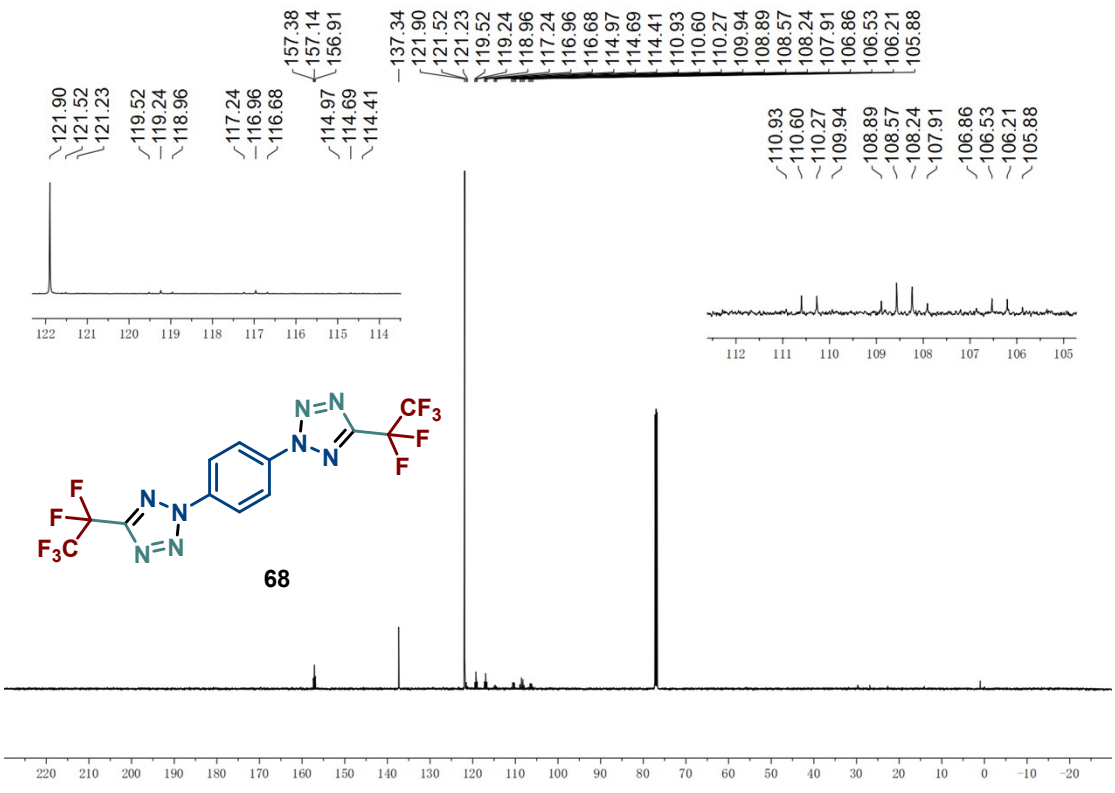
131.19
129.19
125.98
121.23
121.00
120.77
119.34
119.10
118.86
117.44
117.21
116.97
115.55
115.31
115.07
110.58
110.31
110.04
109.76
108.93
108.61
108.34
108.07
107.20
106.92
106.65
106.33
52.74
MeO2C
CF3
F
F
67


MeO2C
CF3
F
F
67
-88.787
-119.524


8.500
4.00
68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121.52
121.23
119.52
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117.24
116.96
116.68
114.97
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114.41
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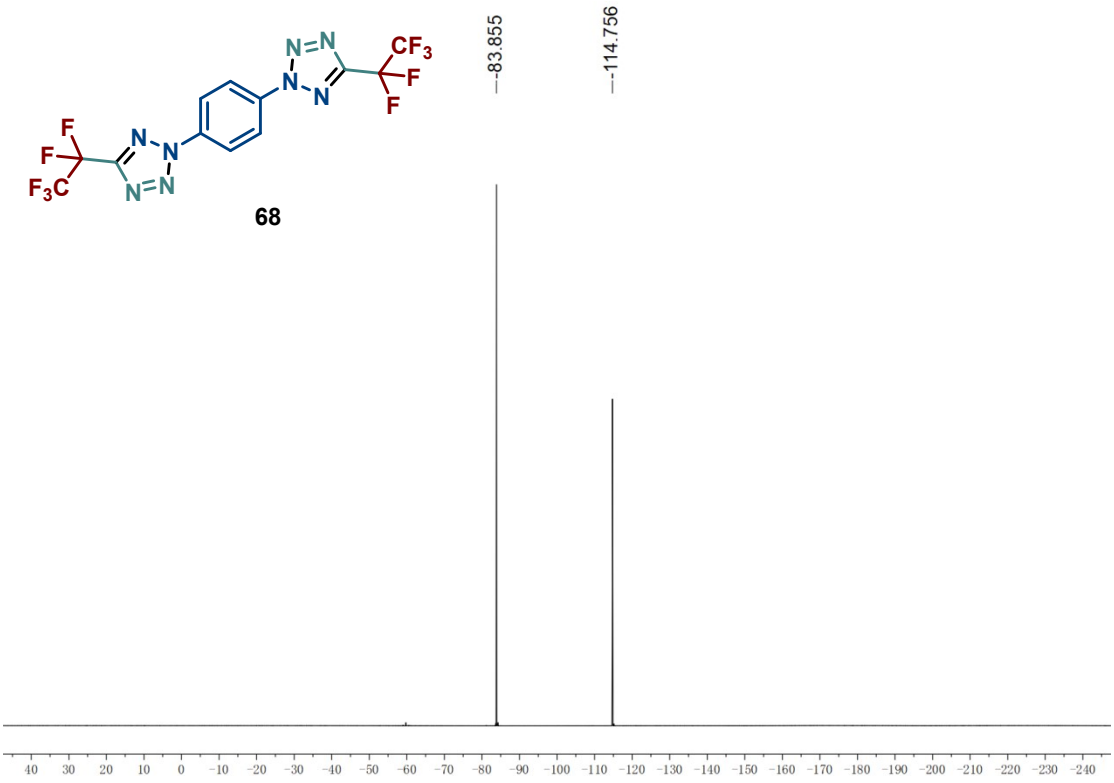
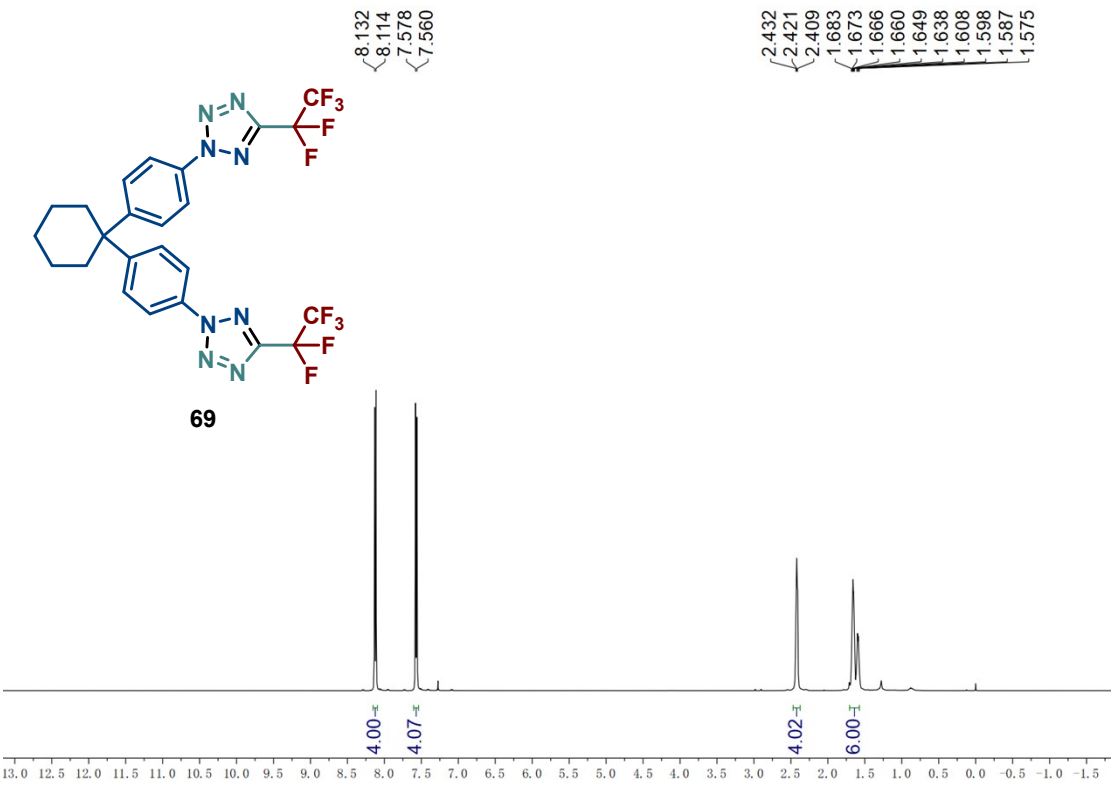
108.89
108.57
108.24
107.91
106.86
106.53
106.21
105.88
68


-83.855
-114.756

68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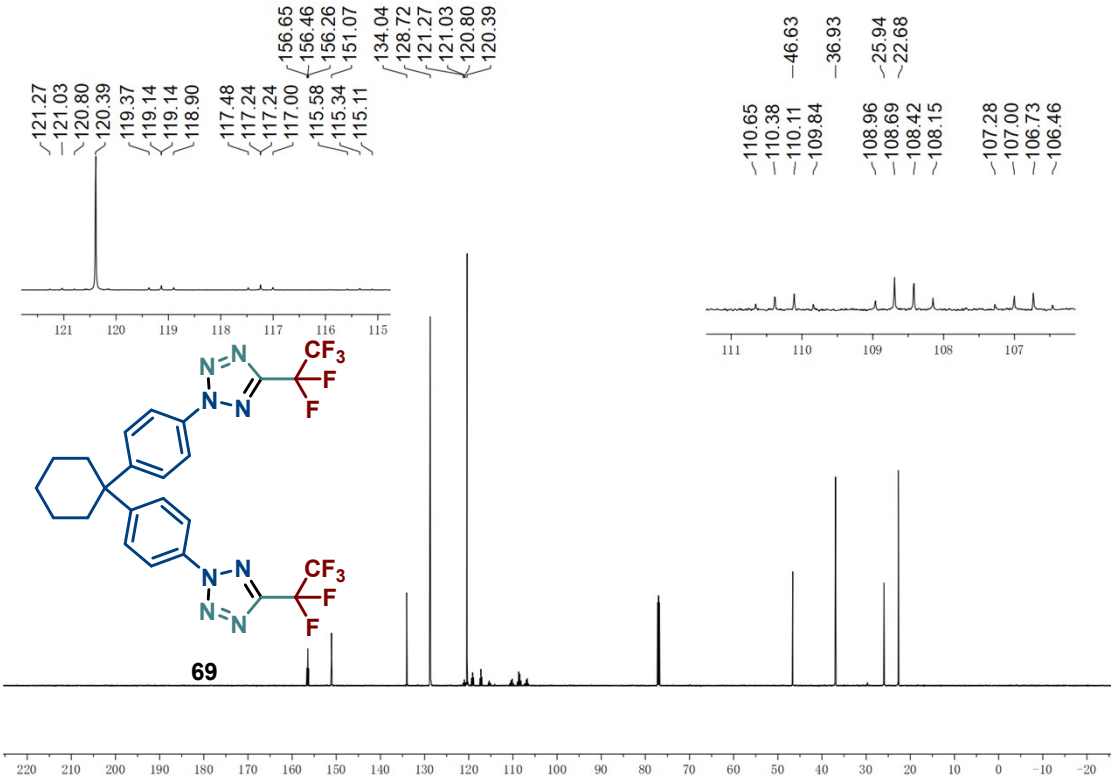
2.432
2.421
2.409
1.683
1.673
1.666
1.660
1.649
1.638
1.608
1.598
1.587
1.575
4.00
4.07
4.02
6.00

69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156.26
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121.03
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120.39
121.27
121.03
120.80
120.39
119.37
119.14
119.14
118.90
117.48
117.24
117.24
117.00
115.58
115.34
115.11
46.63
36.93
25.94
22.68
110.65
110.38
110.11
109.84
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108.15
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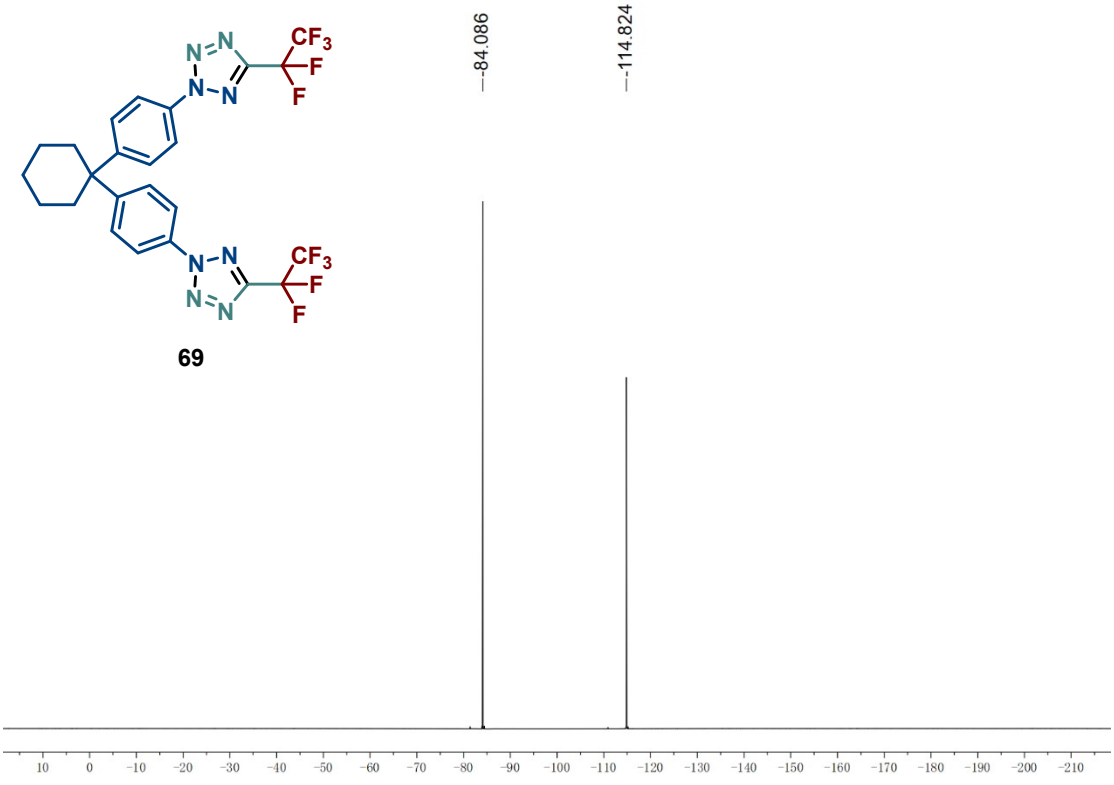
107.00
106.73
106.46
CF3
F
F
CF3
F
F
69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CF3
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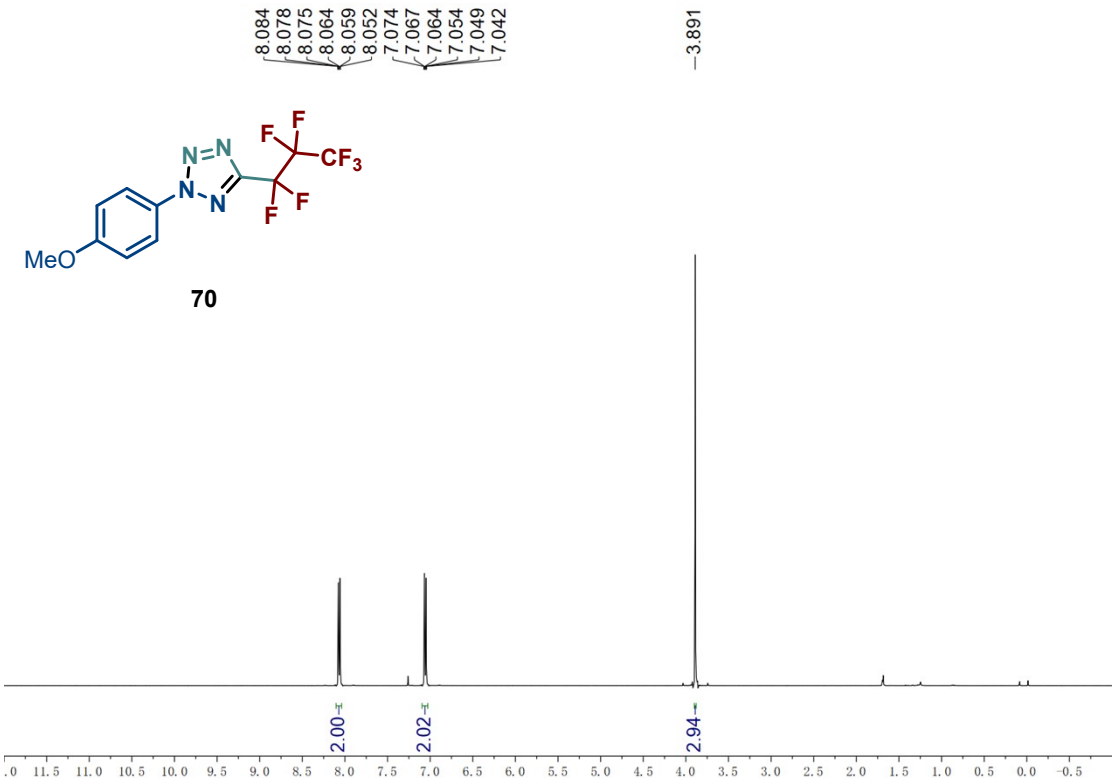
-114.824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8.078
8.075
8.064
8.059
8.052
7.074
7.067
7.064
7.054
7.049
7.042
3.891
F
F
CF3
F
F
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N
MeO
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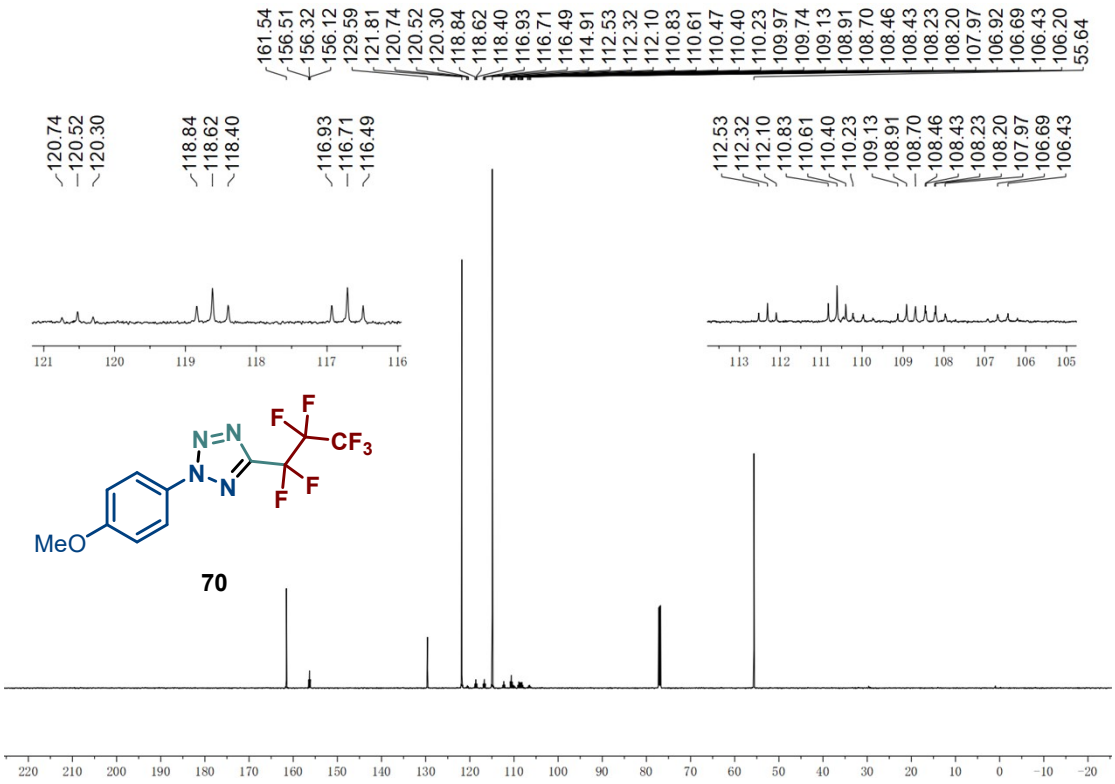
2.02
2.94

70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120.52
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118.62
118.40
116.93
116.71
116.49
114.91
112.53
112.32
112.10
110.83
110.61
110.47
110.40
110.23
109.97
109.74
109.13
108.91
108.70
108.46
108.43
108.23
108.20
107.97
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106.20
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F
CF3
F
F
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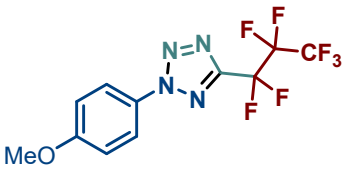
N
MeO

70


MeO
N=N
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N
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F
F
CF3

70

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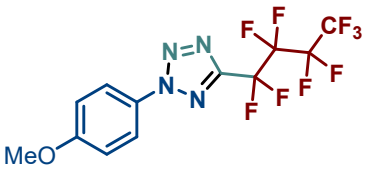
-112.540
-112.547
-112.564
-112.579
-126.657
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210


MeO
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N
N
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F
F
CF3

71

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8.090
8.086
8.076
8.072
8.065
7.086
7.079
7.075
7.065
7.061
7.054
3.901
2.00
2.05
2.96
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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2.5
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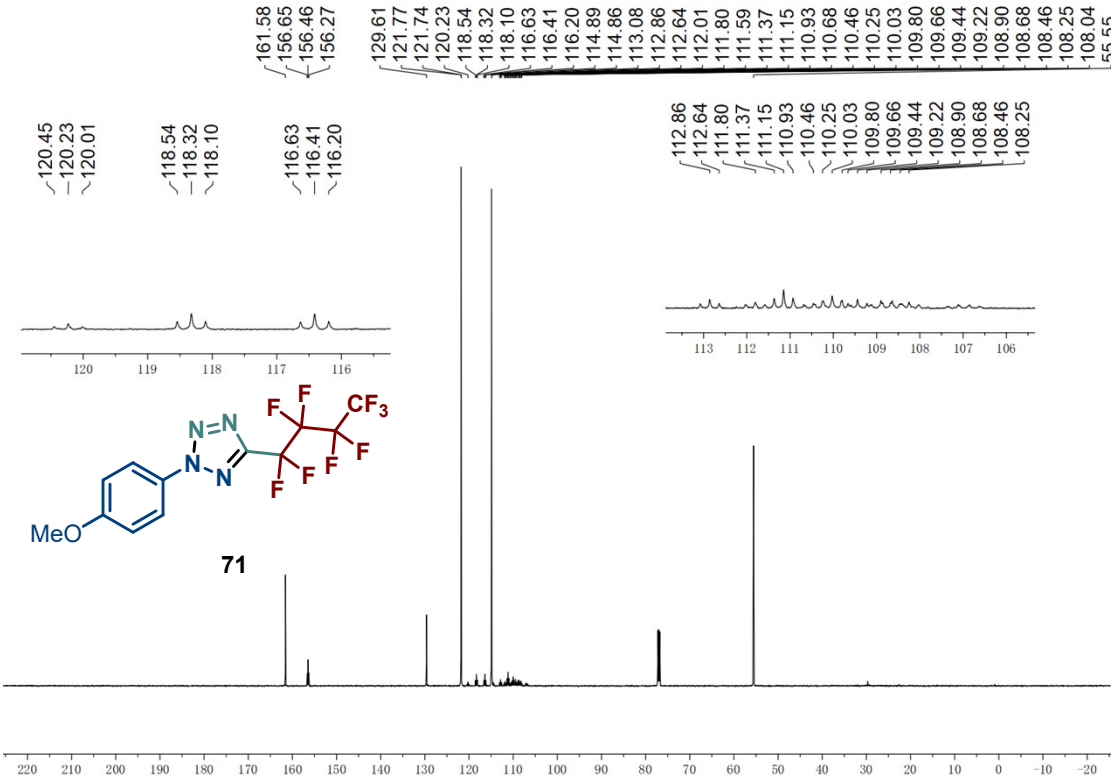
1.5
1.0
0.5
0.0
-0.5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116.20
114.89
114.86
113.08
112.86
112.64
112.01
111.80
111.59
111.37
111.15
110.93
110.68
110.46
110.25
110.03
109.80
109.66
109.44
109.22
108.90
108.68
108.46
108.25
108.04
120.45
120.23
120.01
118.54
118.32
118.10
116.63
116.41
116.20
112.86
112.64
111.80
111.37
111.15
110.93
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109.80
109.66
109.44
109.22
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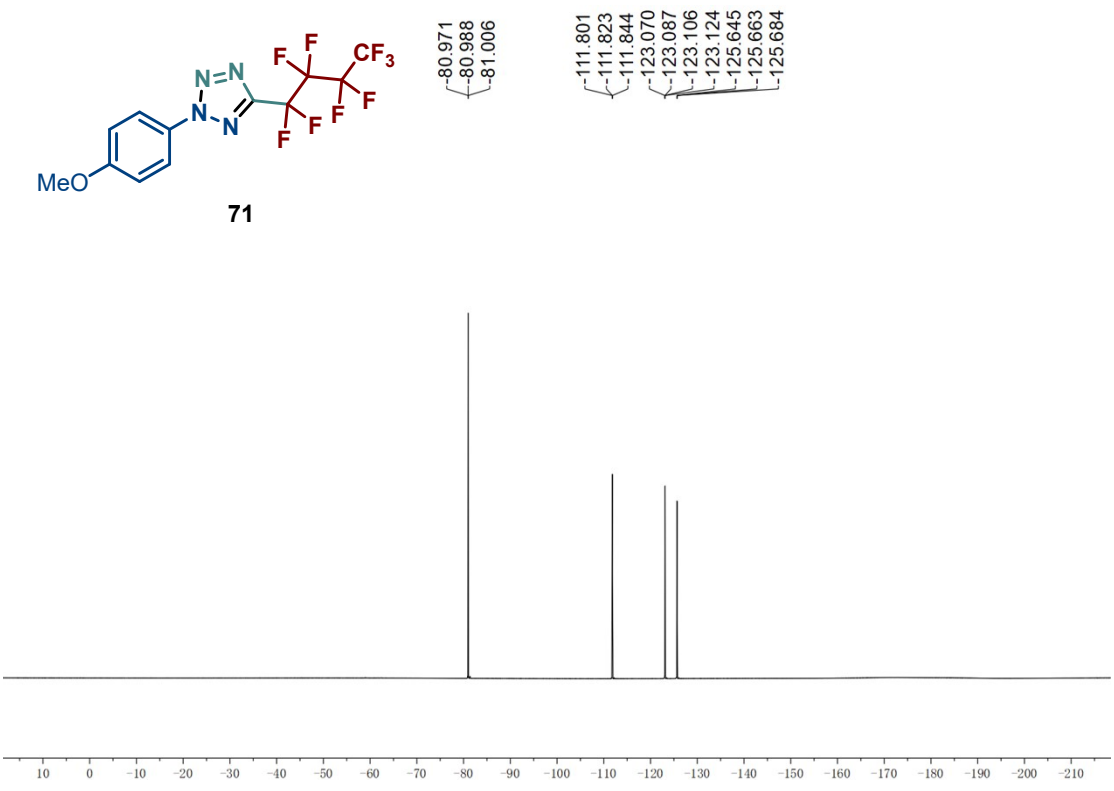
108.68
108.46
108.25
MeO
71


80.971
80.988
81.006
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123.087
123.106
123.124
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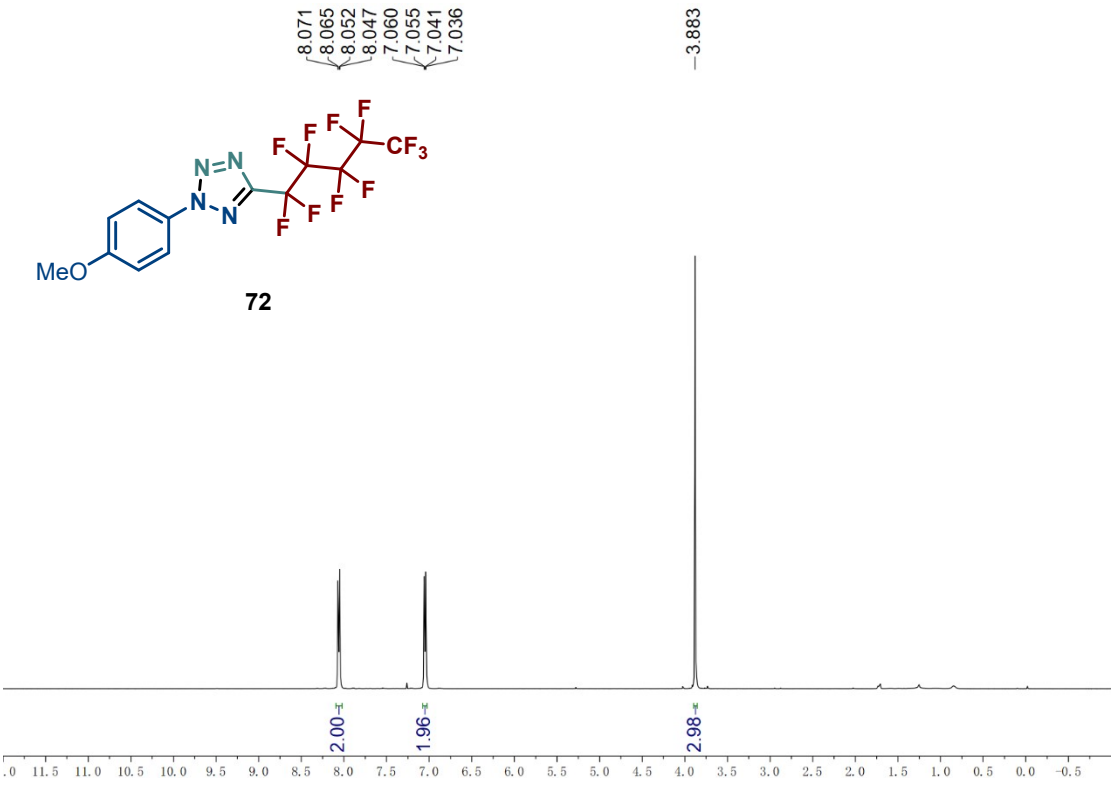
125.663
125.684
MeO
71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8.065
8.052
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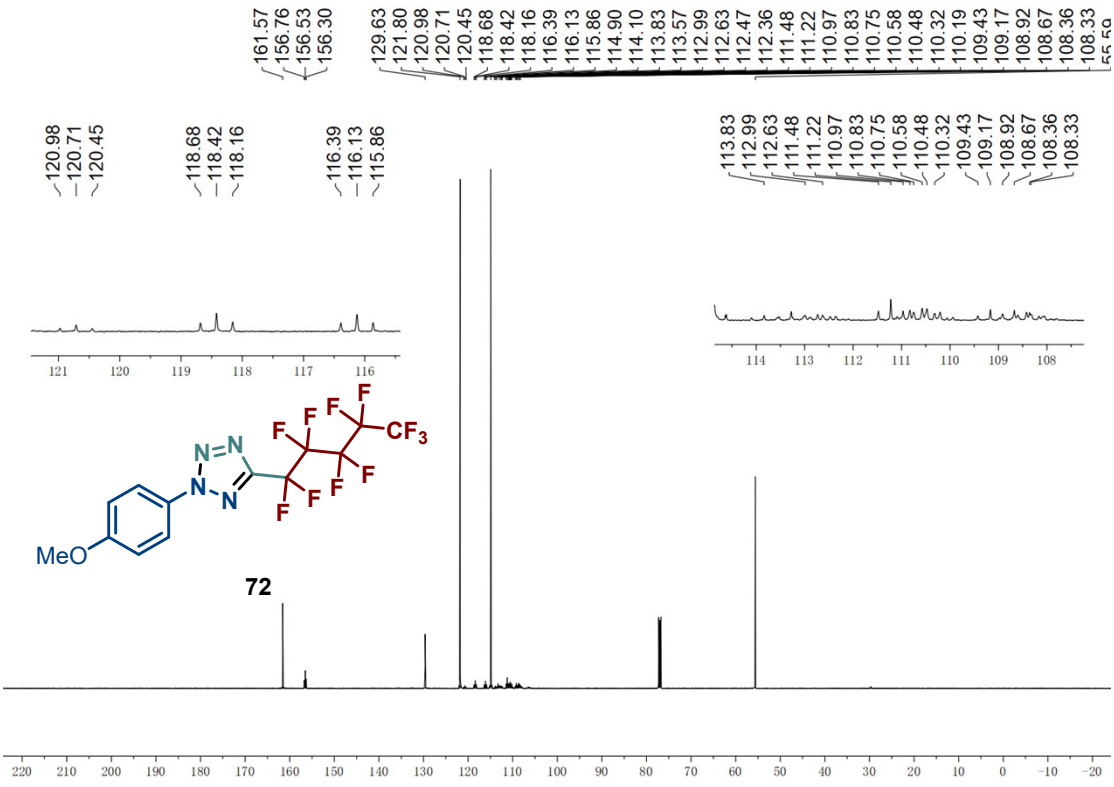
7.060
7.055
7.041
7.036
3.883
MeO
72
2.00
1.96
2.98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114.10
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113.57
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110.83
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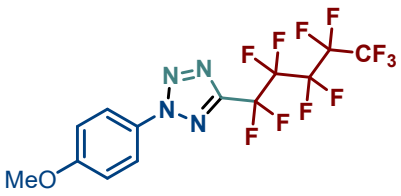
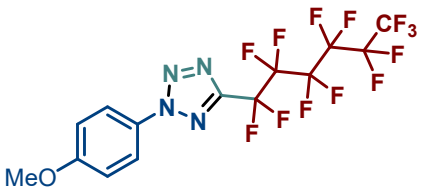
108.67
108.36
108.33
MeO
72


MeO
N=N
N
N
F
F
F
F
F
F
F
F
F
CF3

72

-81.087
-81.108
-81.130
-111.810
-111.838
-111.866
-122.449
-122.467
-122.474
-122.482
-122.498
-122.519
-122.536
-122.555
-122.581
-126.372
-126.383
-126.404
-126.420
-126.435
-126.449


MeO
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N
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F
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F
F
F
F
F
F
CF3

73

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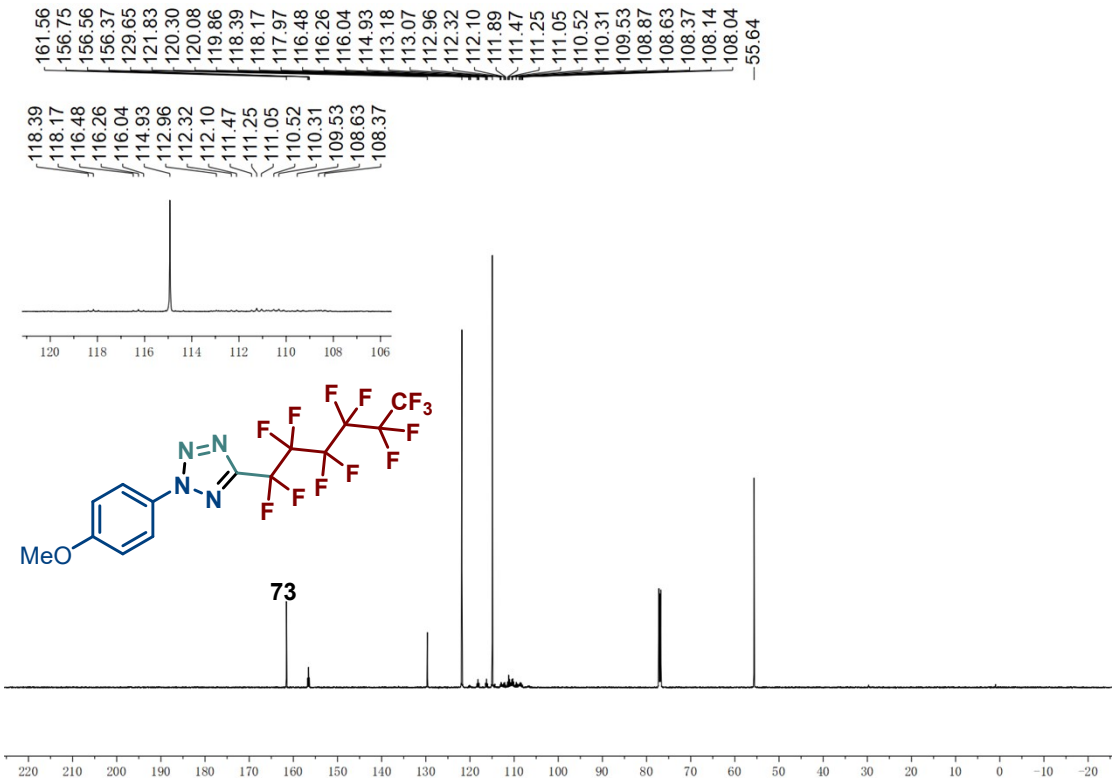
7.056
3.895
2.00
2.00
2.96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120.30
120.08
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118.39
118.17
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116.26
116.04
114.93
113.18
113.07
112.96
112.32
112.10
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111.47
111.25
111.05
110.52
110.31
109.53
108.87
108.63
108.37
108.14
108.04
55.64
118.39
118.17
116.48
116.26
116.04
114.93
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111.47
111.25
111.05
110.52
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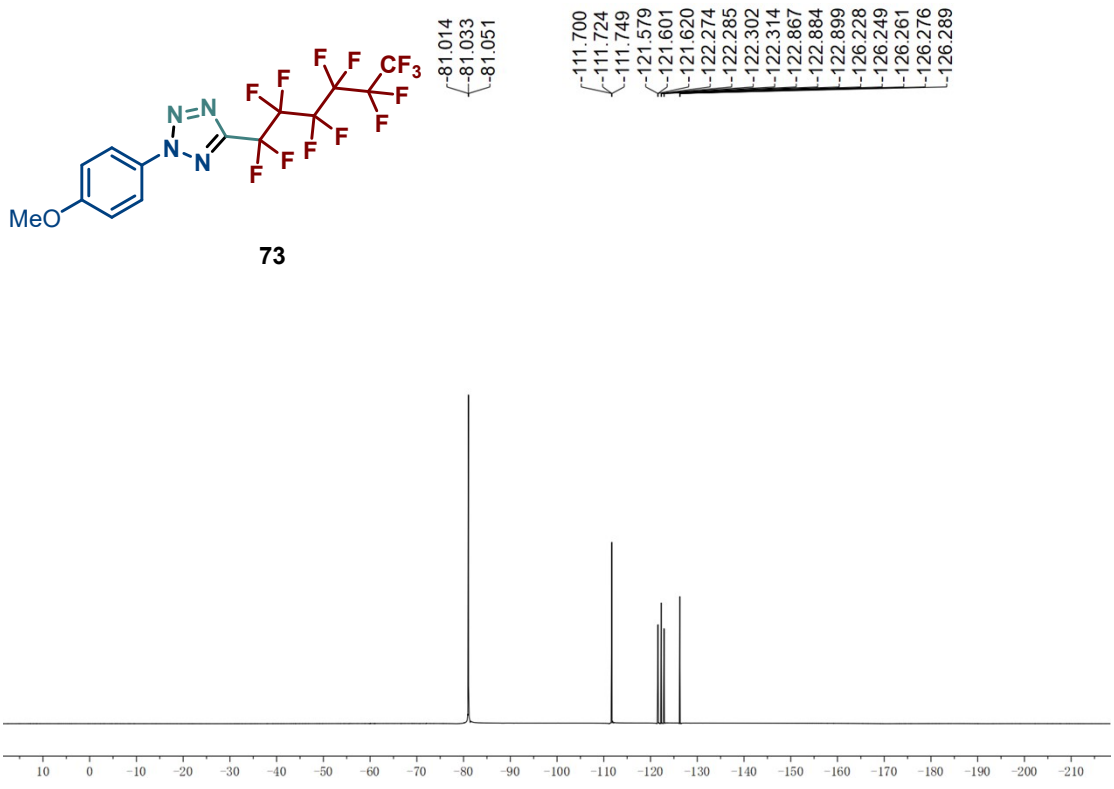
109.53
108.63
108.37
MeO
73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81.051
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111.749
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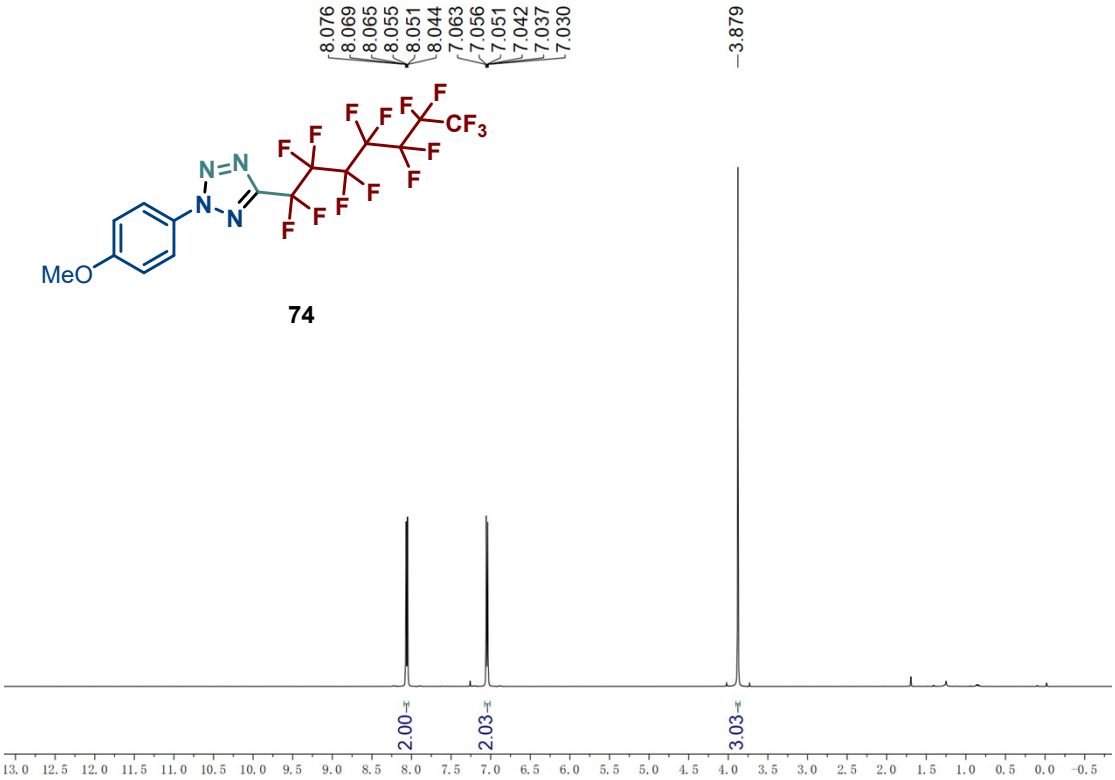
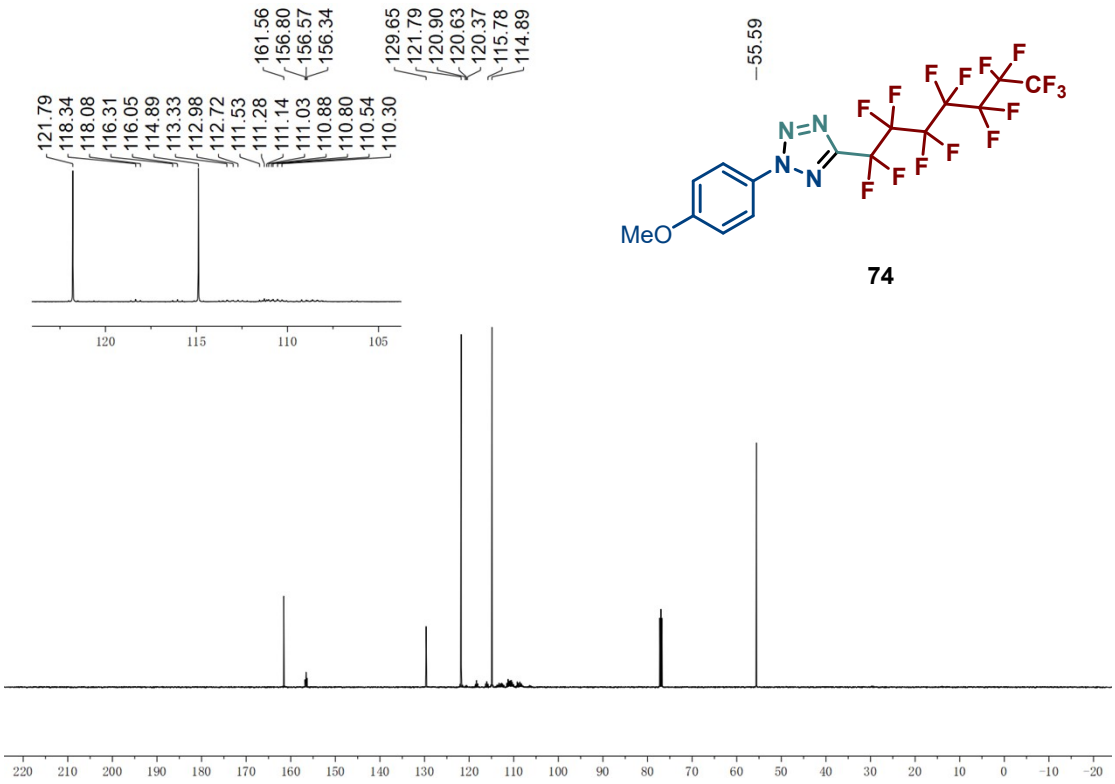
121.601
121.620
122.274
122.285
122.302
122.314
122.867
122.884
122.899
126.228
126.249
126.261
126.276
126.289
MeO
73


8.076
8.069
8.065
8.055
8.051
8.044
7.063
7.056
7.051
7.042
7.037
7.030
3.879
MeO
74
2.00
2.03
3.03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120.63
120.37
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114.89
121.79
118.34
118.08
116.31
116.05
114.89
113.33
112.98
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111.28
111.14
111.03
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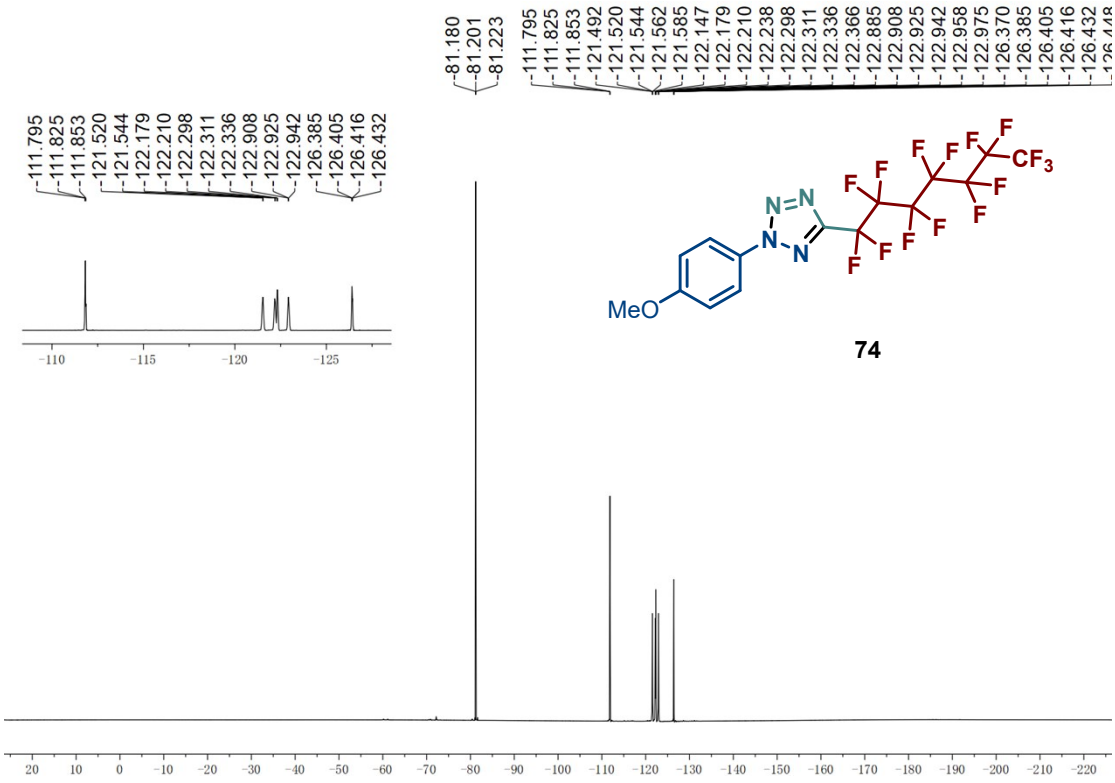
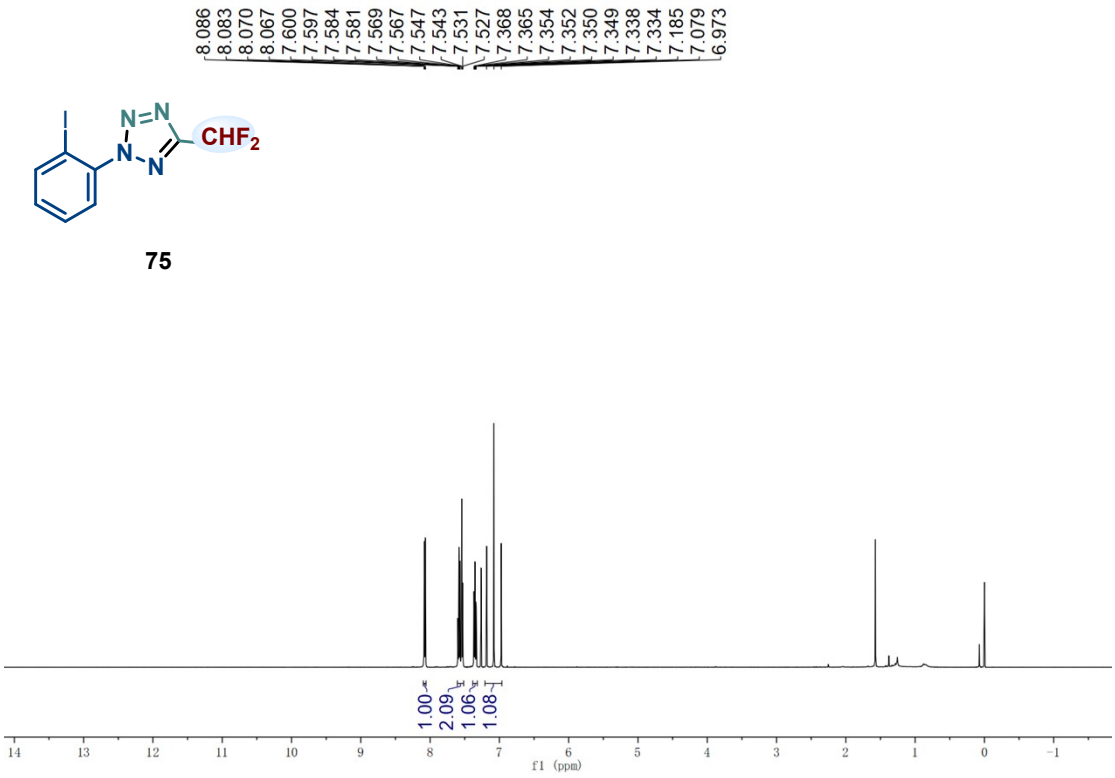
110.80
110.54
110.30
55.59
MeO
74


-81.180
-81.201
-81.223
-111.795
-111.825
-111.853
-121.492
-121.520
-121.544
-121.562
-121.585
-122.147
-122.179
-122.210
-122.238
-122.298
-122.311
-122.336
-122.366
-122.885
-122.908
-122.925
-122.942
-122.958
-122.975
-126.370
-126.385
-126.405
-126.416
-126.432
MeO
74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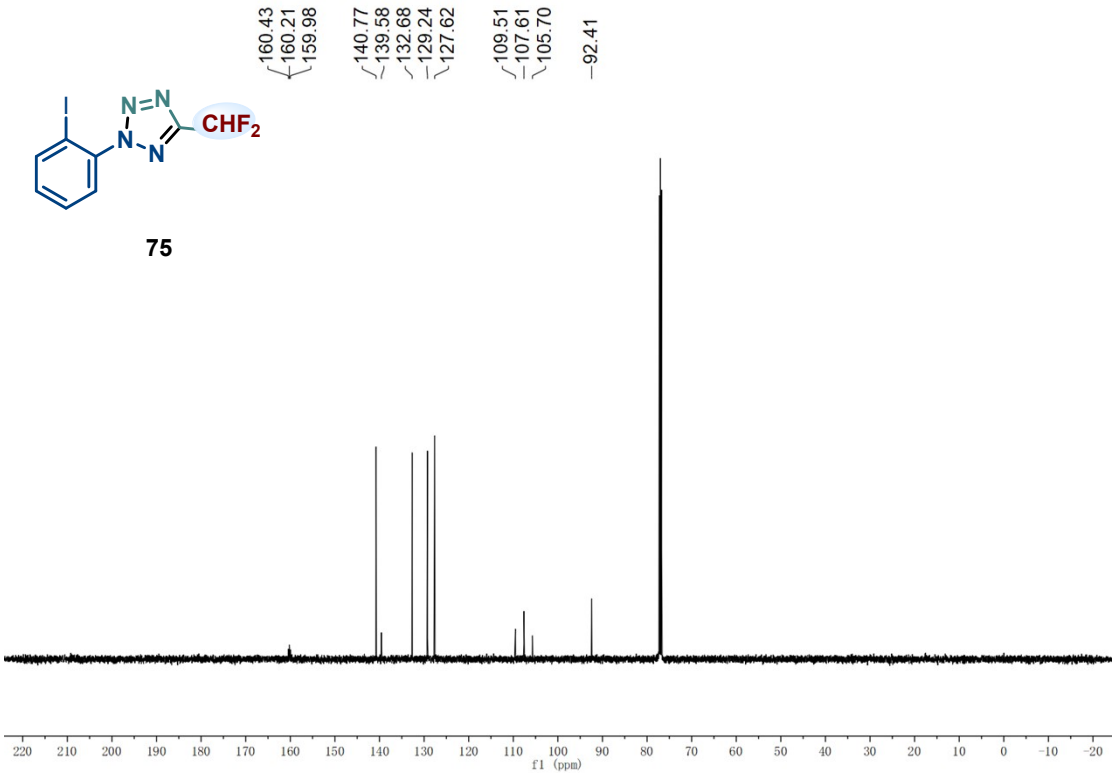
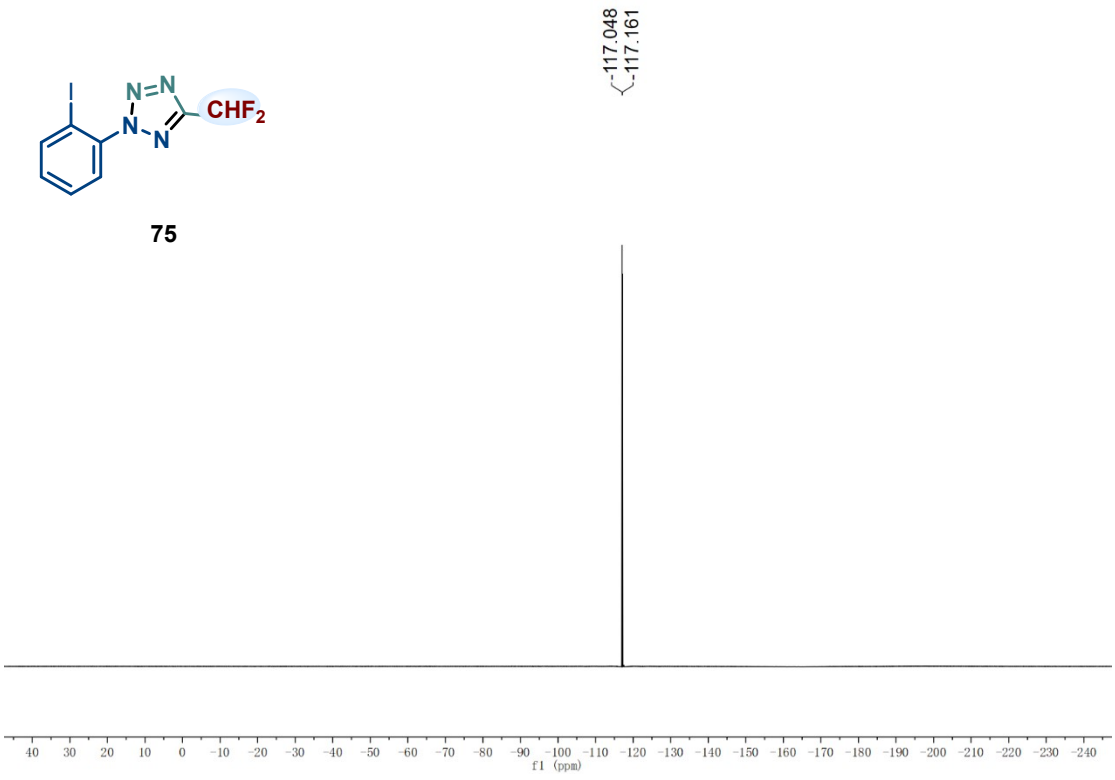
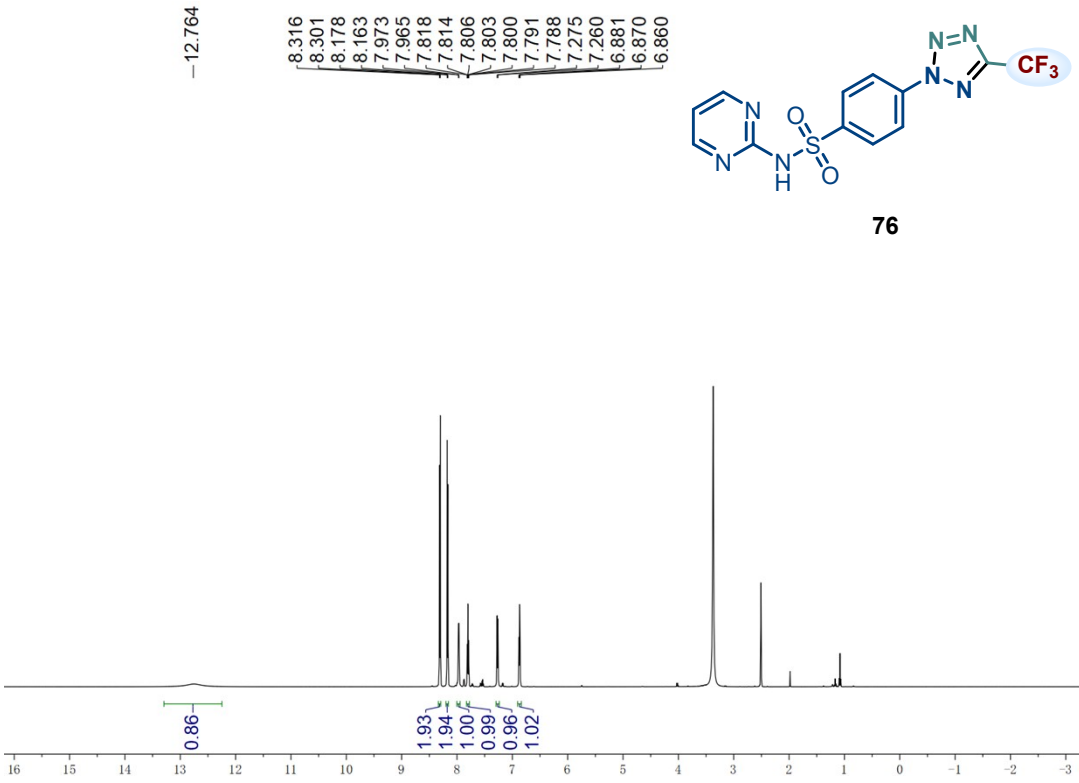
8.070
8.067
7.600
7.597
7.584
7.581
7.569
7.567
7.547
7.543
7.531
7.527
7.368
7.365
7.354
7.352
7.350
7.349
7.338
7.334
7.185
7.079
6.973
CHF2
75
1.00
2.09
1.06
1.08
f1 (ppm)


160.43
160.21
159.98
140.77
139.58
132.68
129.24
127.62
109.51
107.61
105.70
92.41
CHF2
75
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)


-117.048
-117.161
CHF2
75
40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -220 -230 -240
f1 (ppm)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8.178
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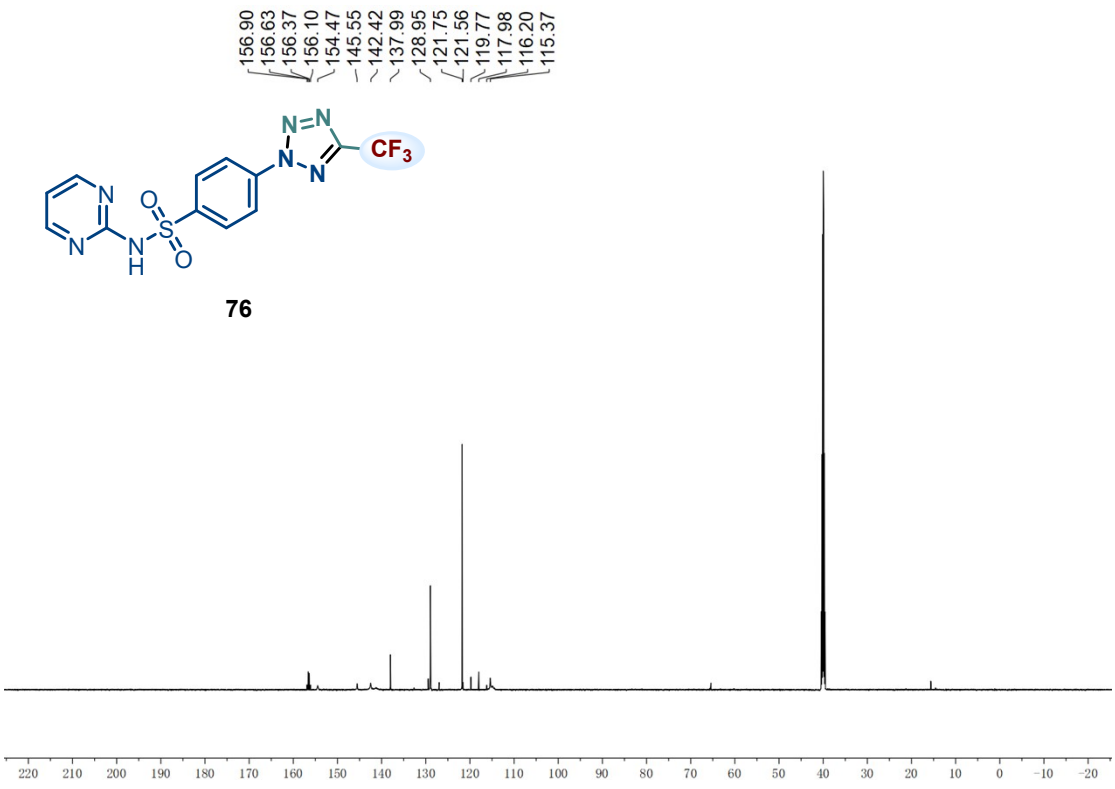
7.965
7.818
7.814
7.806
7.803
7.800
7.791
7.788
7.275
7.260
6.881
6.870
6.860
CF3
0.86
1.93
1.94
1.00
0.99
0.96
1.02

76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156.37
156.10
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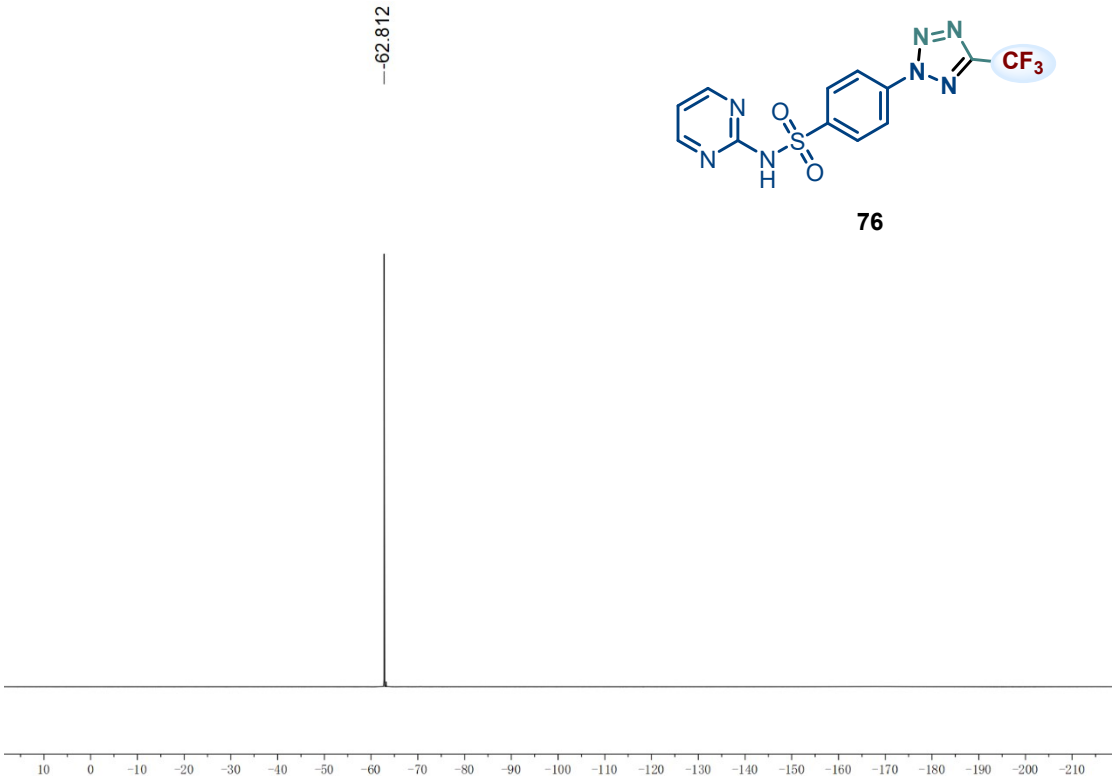
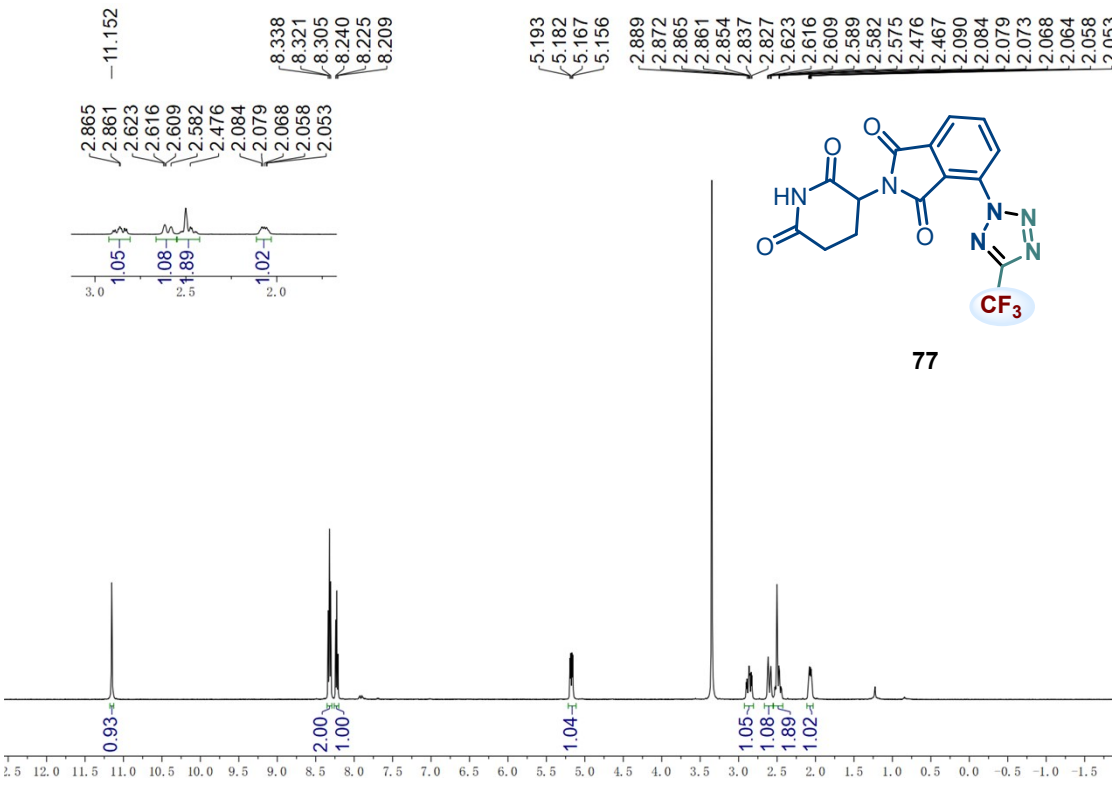
137.99
128.95
121.75
121.56
119.77
117.98
116.20
115.37
CF3

76


-62.812
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210

76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5.167
5.156
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2.872
2.865
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2.854
2.837
2.827
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2.616
2.609
2.589
2.582
2.575
2.476
2.467
2.090
2.084
2.079
2.073
2.068
2.064
2.058
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2.861
2.623
2.616
2.609
2.582
2.476
2.084
2.079
2.068
2.058
2.053
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1.08
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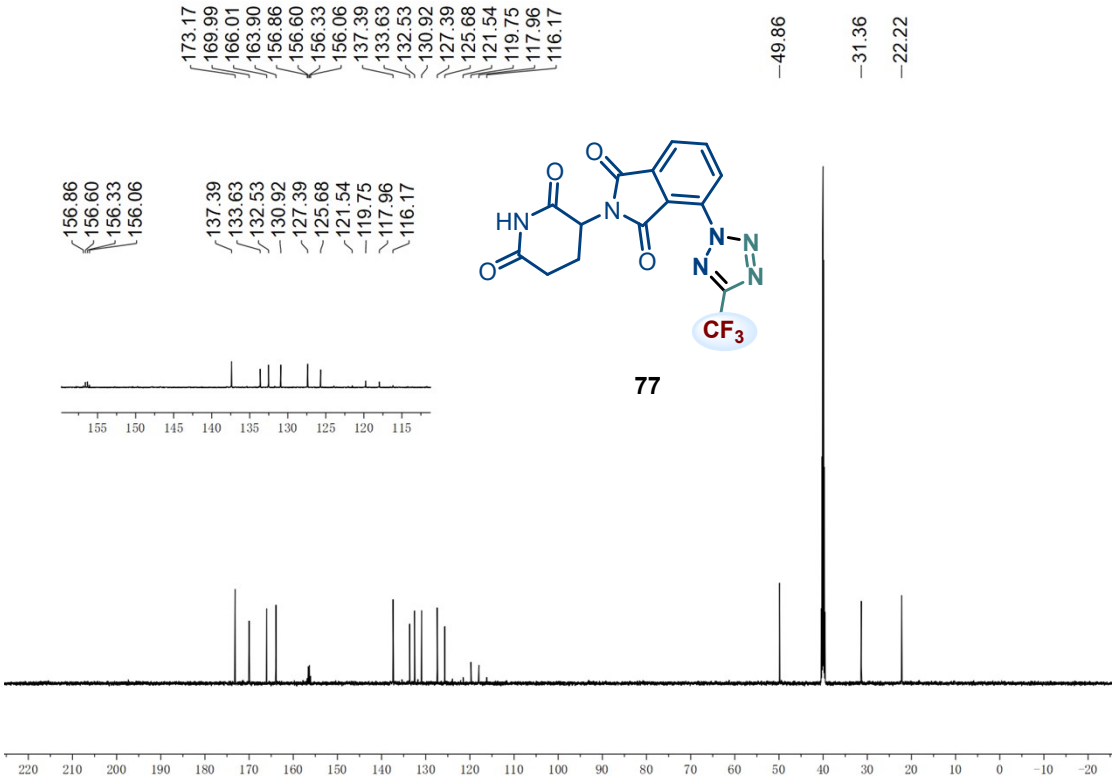
1.02
0.93
2.00
1.00
1.04
1.05
1.08
1.89
1.02

77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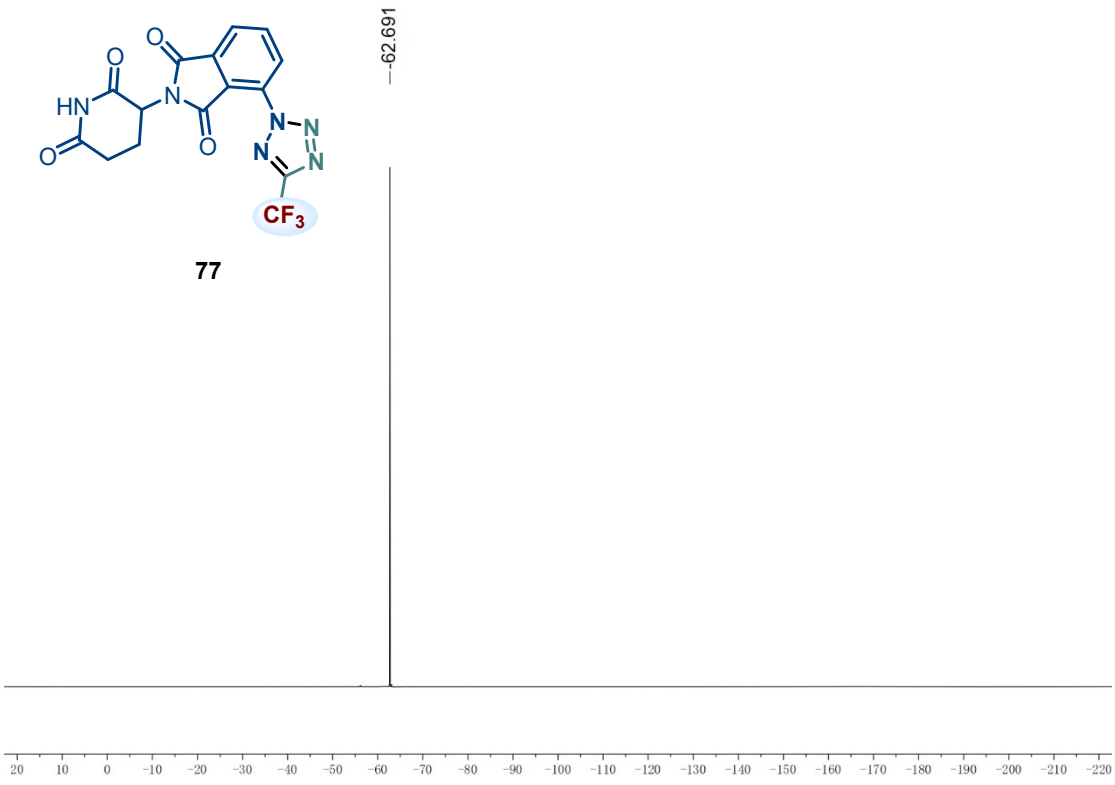
156.33
156.06
137.39
133.63
132.53
130.92
127.39
125.68
121.54
119.75
117.96
116.17
49.86
31.36
22.22
HN
O
N
N
N
N
CF3
77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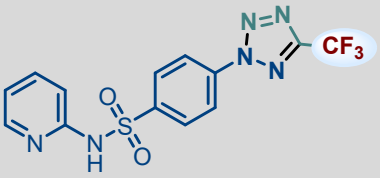
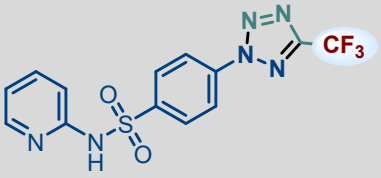
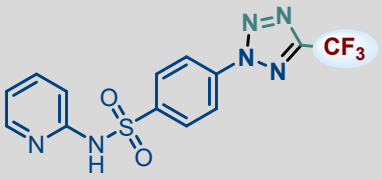
N
N
N
N
CF3
77



78



78



78