Supporting Information

Synthesis of 3-trifluoromethylated 1,3-butadienes via a Pd(0)-catalyzed fluorinated Heck reaction

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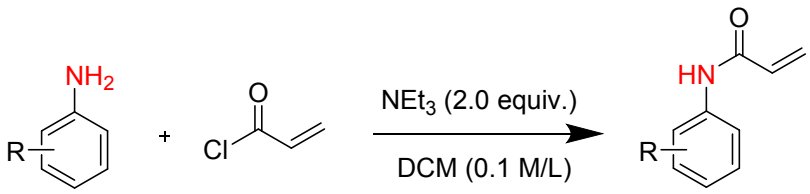
1 General information

All reactions were carried out under an atmosphere of nitrogen. Chemicals were purchased from Sigma-Aldrich, TCI and Alfa Aesar. Anilines and 2-Bromo-3,3,3-Trifluoropropane were used without any purification. Other chemicals were used as received. Multiplets of NMR were assigned as s (singlet), d (doublet), t (triplet), dd (doublet of doublet), dt (doublet of triplet), td (triplet of doublet), m (multiplet), and br. s (broad singlet).

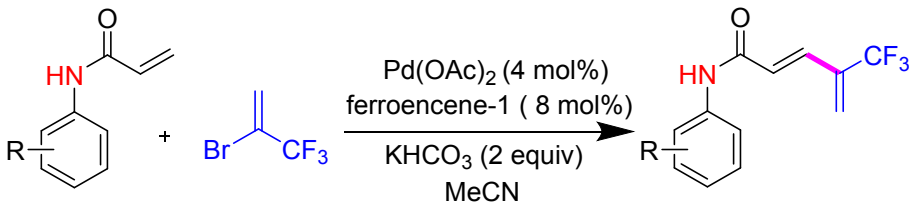
2 General methods

NMR data were recorded on Bruker Avance 300 or Bruker ARX 400 spectrometers at room temperature. ^{1}H NMR, ^{13}C NMR and ^{19}F NMR spectra were referenced to signals of deutero solvents and residual protiated solvents, respectively. High resolution mass spectra (HRMS) were recorded on Agilent 6210. The data are given as mass units per charge (m/z).

3 General procedures



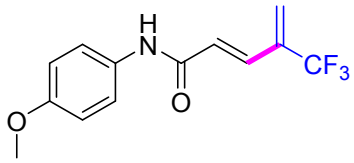
Acryloyl chloride (12.0 mmol) was slowly added to a solution of aniline (10.0 mmol), NEt_3 (20.0 mmol) in dry DCM (100 mL) at 0 ^{o}C. After stirring at room temperature for 30 minutes, the solvent removed under vacuum and purification of the residue mixture by silica gel column chromatography afforded the desired the acrylamide as white solid (all of the yields > 95%)



The reaction was carried out in an autoclave containing a 25.0 mL glass reaction tube. $Pd(OAc)_2$ (0.04 mmol), ligand (0.08 mmol), acrylamide (1.0 mmol), 2-bromo-3,3,3-trifluoropropane (2.0 mmol), $KHCO_3$ (2.0 mmol), MeCN (4.0 mL) were added to the tube. The tube was placed in the autoclave. Once sealed, the autoclave was purged three times with nitrogen, then heated in an oil bath at 80 °C for 5 h. After the reaction, the autoclave was then cooled to room temperature and the crude product was purified by column chromatography on silica gel using a mixture of ethyl acetate and petroleum ether as eluent to give the following compounds.

4 Characterization data of the 3-trifluoromethylated 1,3-butadienes

(*E*)-N-(4-methoxyphenyl)-4-(trifluoromethyl)penta-2,4-dienamide **(3a)**



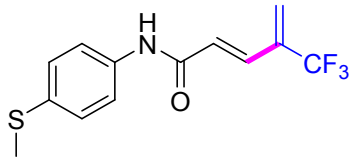
^{1}H NMR (300 MHz, $CDCl_3$) δ 7.51 (d, 1 H, J = 9.0 Hz), 7.46 (s, 1 H), 7.35 (d, 1 H, J = 15.0 Hz), 6.89 (d, 2 H, J = 9.0 Hz), 6.32 (dd, 1 H, J = 15.0, 3.0 Hz), 6.06 (d, 1 H, J = 3.0 Hz), 5.89 (d, 1 H, J = 3.0 Hz).

^{13}C NMR (75 MHz, $CDCl_3$) δ 163.4, 156.4, 135.2, 134.8, 134.6, 130.7, 126.4 (q, J = 5.3 Hz), 121.8, 114.3, 54.7

^{19}F NMR (282 MHz, $CDCl_3$) δ -65.8 (s, 3 F).

HRMS (EI) $[M+H]_+$ calcd for C13H13F3NO2, 272.0898; found, 272.0892.

(E)-N-(4-(methylthio)phenyl)-4-(trifluoromethyl)penta-2,4-dienamide **(3b)**



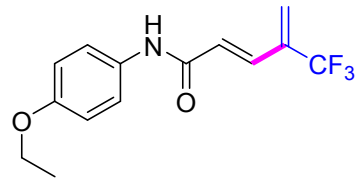
^{1}H NMR (300 MHz, $CDCl_3$) δ 8.03 (s, 1 H), 7.53 (d, 2 H, J = 9.0 Hz), 7.31 (d, 1 H, J = 15.0 Hz), 6.37 (dd, 1 H, J = 15.0, 3.0 Hz), 7.21 (d, 2 H, J = 9.0 Hz), 6.05 (d, 1 H, J = 3.0 Hz), 5.84 (d, 1 H, J = 3.0 Hz).

^{13}C NMR (75 MHz, $CDCl_3$) δ 162.6, 135.2, 134.9 (q, J = 30.8 Hz), 135.2, 134.8, 134.4, 127.7, 126.6 (q, J = 5.3 Hz), 122.5 (q, J = 273.0 Hz), 120.9, 16.4.

^{19}F NMR (282 MHz, $CDCl_3$) δ -66.0 (s, 3 F).

HRMS (EI) $[M+H]_+$ calcd for C13H13F3NOS, 288.0670; found, 288.0664.

(E)-N-(4-ethoxyphenyl)-4-(trifluoromethyl)penta-2,4-dienamide **(3c)**



^{1}H NMR (300 MHz, $CDCl_3$) δ 7.50 (d, 2 H, J = 9.0 Hz), 7.39 (s, 1 H), 7.35 (d, 1 H, J = 15.0 Hz), 6.89 (d, 2 H, J = 9.0 Hz), 6.30 (dd, 1 H, J = 18.0, 3.0 Hz), 6.07 (d, 1 H, J = 3.0 Hz), 5.89 (d, 1 H, J = 3.0 Hz), 4.04 (q, 2 H, J = 6.0 Hz), 1.43 (q, 3 H, J = 6.0 Hz).

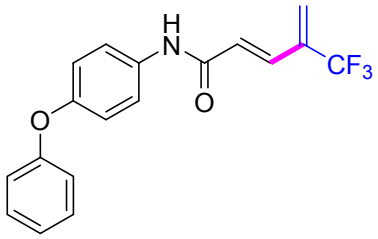
^{13}C NMR (75 MHz, $CDCl_3$) δ 162.6, 156.1, 135.0 (q, J = 30.8 Hz), 134.6, 130.6,

126.4 (q, J = 6.0 Hz), 122.5 (q, J = 275.5Hz), 121.8, 114.9, 67.7, 18.6.

^{19}F NMR (282 MHz, $CDCl_3$) δ -65.8 (s, 3 F).

HRMS (EI) $[M+H]_+$ calcd for C14H15F3NO2, 286.1055; found, 286.1050

(E)-N-(4-phenoxyphenyl)-4-(trifluoromethyl)penta-2,4-dienamide **(3d)**



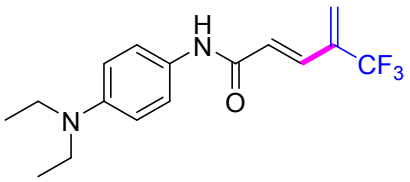
^{1}H NMR (300 MHz, $CDCl_3$) δ 7.58 (d, 2 H, J = 9.0 Hz), 7.51 (s, 1 H), 7.39-7.33 (m, 3 H), 7.12 (t, 1 H, J = 9.0 Hz), 7.03-7.00 (m, 4 H), 6.30 (dd, 1 H, J = 18.0, 3.0 Hz), 6.09 (d, 1 H, J = 3.0 Hz), 5.91 (d, 1 H, J = 3.0 Hz).

^{13}C NMR (75 MHz, $CDCl_3$) δ 161.3, 158.5, 154.6, 135.1, 135.0, 134.7, 133.0, 129.8, 126.7 (q, J = 5.3 Hz), 124.8, 123., 121.8, 119.5, 118.7.

^{19}F NMR (282 MHz, $CDCl_3$) δ -65.9 (s, 3 F).

HRMS (EI) $[M+H]_+$ calcd for C18H15F3NO2, 334.1055; found, 334.1050

(E)-N-(4-(diethylamino)phenyl)-4-(trifluoromethyl)penta-2,4-dienamide **(3e)**



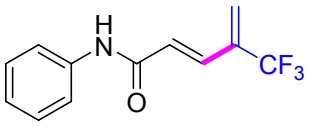
^{1}H NMR (300 MHz, $CDCl_3$) δ 7.43 (d, 3 H, J = 9.0 Hz), 7.32 (d, 1 H, J = 15.0 Hz), 6.66 (d, 2 H, J = 9.0 Hz), 6.32 (dd, 1 H, J = 15.0, 3.0 Hz), 6.03 (d, 1 H, J = 3.0 Hz), 5.85 (d, 1 H, J = 3.0 Hz), 3.35 (q, 4 H, J = 6.0 Hz), 1.16 (t, 6 H, J = 6.0 Hz).

^{13}C NMR (75 MHz, $CDCl_3$) δ 161.9, 147.7, 135.0 (q, J = 30.0 Hz), 133.9, 127.1, 125.9 (q. J = 5.3 Hz), 122.8 (q, J = 300.0 Hz), 113.3, 47.7, 13.7.

^{19}F NMR (282 MHz, $CDCl_3$) δ -65.7 (s, 3 F).

HRMS (EI) $[M+H]^+$ calcd for C16H20F3N2O, 313.1528; found, 313.1522

(E)-N-phenyl-4-(trifluoromethyl)penta-2,4-dienamide **(3f)**



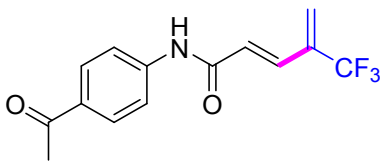
^{1}H NMR (300 MHz, d_4-MeOD) δ 7.66 (d, 2 H, J = 9.0 Hz), 7.37-7.29 (m, 3 H), 7.13 (tt, 1 H, J = 9.0, 3.0 Hz), 6.59 (dd, 1 H, J = 15.0, 3.0 Hz), 6.13 (d, 1 H, J = 3.0 Hz), 6.09 (d, 1 H, J = 3.0 Hz).

^{13}C NMR (400 MHz NMR, 100 MHz, d_4-MeOD) δ 162.9, 137.5, 134.9 (q, J = 31.0 Hz), 133.5, 128.5, 125.8 (q, J = 5.0 Hz), 124.2, 122.0, 121.0.

^{19}F NMR (282 MHz, d_4-MeOD) δ -67.4 (s, 3 F).

HRMS (EI) $[M+H]^+$ calcd for C12H11F3NO, 242.0793; found, 242.0790.

(E)-N-(4-acetylphenyl)-4-(trifluoromethyl)penta-2,4-dienamide **(3g)**



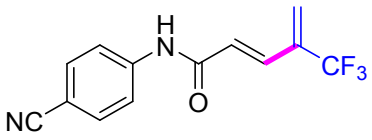
^{1}H NMR (300 MHz, $CDCl_3$) δ 7.99 (d, 2 H, J = 9.0 Hz), 7.76 (d, 2 H, J = 3.0 Hz), 7.76 (s, 1 H), 7.40 (d, 1 H, J = 18.0 Hz), 6.36 (dd, 1 H, J = 18.0, 3.0 Hz), 6.12 (d, 1 H, J = 3.0 Hz), 5.94 (d, 1 H, J = 3.0 Hz), 2.62 (s, 3 H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 197.1, 160.0, 142.1, 134.8 (q, J = 30.8 Hz), 133.3, 129.3, 127.3 (q, J = 5.3 Hz), 124.5, 117.7, 23.4.

^{19}F NMR (282 MHz, $CDCl_3$) δ -65.7 (s, 3 F).

HRMS (EI) $[M+H]_+$ calcd for C14H13F3NO2, 284.0898; found, 284.0890.

(E)-N-(4-cyanophenyl)-4-(trifluoromethyl)penta-2,4-dienamide **(3h)**



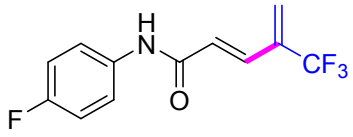
^{1}H NMR (300 MHz, $CDCl_3$) δ 7.78 (d, 2 H, J = 9.0 Hz), 7.66 (d, 2 H, J = 6.0 Hz), 7.38 (d, 1 H, J = 18.0 Hz), 6.35 (dd, 1 H, J = 15.0, 3.0 Hz), 6.13 (d, 1 H, J = 3.0 Hz), 5.95 (d, 1 H, J = 3.0 Hz).

^{13}C NMR (75 MHz, $CDCl_3$) δ 163.2, 140.5, 136.2, 134.7 (q, J = 31.5 Hz), 133.4, 127.6 (q, J = 5.3 Hz), 124.2, 120.6, 118.8, 108.3.

^{19}F NMR (282 MHz, $CDCl_3$) δ -65.7 (s, 3 F).

HRMS (EI) $[M+H]_+$ calcd for C13H10F3N2O, 267.0745; found, 267.0741.

(E)-N-(4-fluorophenyl)-4-(trifluoromethyl)penta-2,4-dienamide **(3i)**



^{1}H NMR (300 MHz, d_4-MeOD) δ 9.62 (s, 1 H), 7.80 (dd, 2 H, J = 9.0, 3.0 Hz), 7.36 (d, 1 H, J = 15.0 Hz), 6.55 (dq, 1 H, J = 15.0, 3.0 Hz), 6.20 (d, 1 H, J = 3.0 Hz), 6.18 (d, 1 H, J = 3.0 Hz).

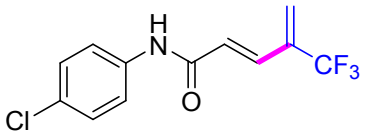
^{13}C NMR (75 MHz, d_4-MeOD) δ 162.4, 161.0, 157.4, 135.5 (q, J = 30.0 Hz),

133.4, 126.6 (q, J = 5.3 Hz), 125.8, 121.1 (q, J = 7.5 Hz), 124:8, 115.2 (q, J = 22.5 Hz).

^{19}F NMR (282 MHz, *d*$_4$-MeOD) δ -66.5 (s, 3 F), -120.3 (s, 1 F).

HRMS (EI) $[M+H]_+$ calcd for C12H10F4NO, 260.0699; found, 260.0686

(E)-N-(4-chlorophenyl)-4-(trifluoromethyl)penta-2,4-dienamide **(3j)**



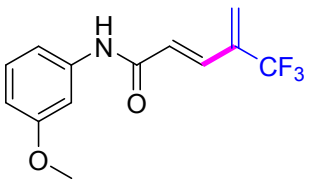
H NMR (300 MHz, CDCl$_3$) δ 7.57 (d, 2 H, J = 9.0 Hz), 7.40 (s, 1 H), 7.33 (d, 2 H, J = 9.0 Hz), 6.30 (dd, 1 H, J = 15.0, 3.0 Hz), 6.11 (d, 1 H, J = 3.0 Hz), 5.93 (d, 1 H, J = 3.0 Hz).

C NMR (75 MHz, CDCl$_3$) δ 136.2, 135.4, 134.9, 129.2, 127.0 (q, J = 5.3 Hz), 124.5, 121.2.

F NMR (282 MHz, CDCl$_3$) δ -65.8 (s, 3 F).

HRMS (EI) $[M+H]_+$ calcd for C12H10ClF3NO, 276.0403; found, 276.0401

(E)-N-(3-methoxyphenyl)-4-(trifluoromethyl)penta-2,4-dienamide **(3k)**



^{1}H NMR (300 MHz, CDCl$_3$) δ 7.80 (s, 1 H), 7.37 (d, 1 H, J = 6.0 Hz), 7.31-7.21 (m, 2 H), 7.08 (d, 1 H, J = 6.0 Hz), 7.21 (dd, 1 H, J = 9.0, 3.0 Hz), 6.35 (dd, 1 H, J = 15.0, 3.0 Hz), 6.05 (d, 1 H, J = 3.0 Hz), 5.86 (d, 1 H, J = 3.0 Hz), 3.82 (s, 3 H).

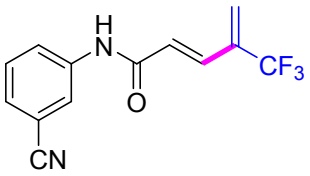
^{13}C NMR (75 MHz, CDCl$_3$) δ 163.0, 160.2, 138.9, 135.0, 134.9 (q, J = 30.8 Hz),

129.8, 126.7 (q, J = 5.3 Hz), 125.0, 122.5 (q, J = 273.0 Hz), 112.3, 110.7, 105.7, 60.0.

^{19}F NMR (282 MHz, $CDCl_3$) δ -65.9 (s, 3 F).

HRMS (EI) $[M+H]_+$ calcd for C13H13F3NO2, 272.0898; found, 272.0894.

(E)-N-(3-cyanophenyl)-4-(trifluoromethyl)penta-2,4-dienamide **(3l)**



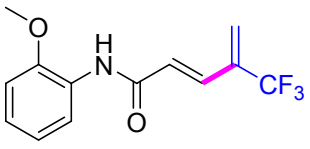
^{1}H NMR (300 MHz, *d6*-acetone) δ 8.18-8.17 (m, 1 H), 7.89-7.85 (m, 1 H), 7.53 (td, 1 H, J = 9.0, 3.0 Hz), 7.49-7.46 (m, 1 H), 7.37 (d, 1 H, J = 18.0 Hz), 6.57 (dq, 1 H, J = 15.0, 3.0 Hz), 6.17 (d, 1 H, J = 3.0 Hz), 6.13 (d, 1 H, J = 3.0 Hz).

^{13}C NMR (400 MHz NMR, 100 MHz, *d6*-acetone) δ 164.8, 138.8, 134.9 (q, J = 37.5 Hz), 134.4, 130.2, 128.4, 127.3, 126.5 (q, J = 7.5 Hz), 124.7, 124.8 (q, J = 188.8 Hz), 122.6, 121.4, 118.1, 112.4.

^{19}F NMR (282 MHz, *d6*-acetone) δ -67.3 (s, 3 F).

HRMS (EI) $[M+H]_+$ calcd for C13H10F3N2O, 267.0745; found, 267.0741

(E)-N-(2-methoxyphenyl)-4-(trifluoromethyl)penta-2,4-dienamide **(3m)**



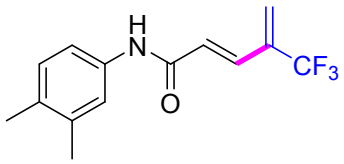
^{1}H NMR (300 MHz, *d6*-acetone) δ 9.05 (s, 1 H), 8.46 (d, 1 H, J = 33.0 Hz), 7.38-7.31 (m, 1 H), 7.12-6.92 (m, 3 H), 6.83 (dd, 1 H, J = 18.0, 3.0 Hz), 6.21 (d, 1 H, J = 3.0 Hz), 6.15 (d, 1 H, J = 3.0 Hz).

^{13}C NMR (400 MHz NMR, 100 MHz, *d6*-acetone) δ 161.0, 147.8, 134.8 (q, J = 37.5 Hz), 133.1, 128.1, 126.4, 126.1 (q, J = 6.3 Hz), 124.1, 122.9 (q, J = 340.0 Hz), 120.5, 120.4, 54.4.

^{19}F NMR (282 MHz, *d6*-acetone) δ -66.5 (s, 3 F).

HRMS (EI) $[M+H]_+$ calcd for C13H13F3NO2, 272.0898; found, 272.0892

(E)-N-(3,4-dimethylphenyl)-4-(trifluoromethyl)penta-2,4-dienamide **(3n)**



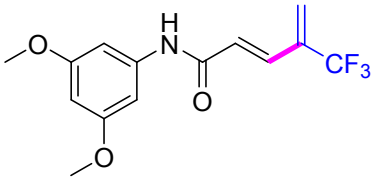
^{1}H NMR (300 MHz, $CDCl_3$) δ 7.87 (s, 1 H), 7.36-7.28 (m, 3 H), 7.08 (d, 1 H, J = 9.0 Hz), 6.37 (dd, 1 H, J = 15.0, 3.0 Hz), 6.03 (d, 1 H, J = 3.0 Hz), 5.83 (d, 1 H, J = 3.0 Hz), 2.22 (s, 6 H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 162.3, 137.3, 135.2, 134.8, 134.4, 133.2, 130.1, 126.2 (q, J = 52.5 MHz, 125.3, 122.2 (q, J = 309.8 MHz), 121.2, 117.8, 19.8, 18.6.

^{19}F NMR (282 MHz, $CDCl_3$) δ -66.5 (s, 3 F).

HRMS (EI) $[M+H]_+$ calcd for C14H15F3NO, 270.1106; found, 270.1102

(E)-N-(3,5-dimethoxyphenyl)-4-(trifluoromethyl)penta-2,4-dienamide **(3o)**



^{1}H NMR (300 MHz, $CDCl_3$) δ 7.36 (t, 2 H, J = 9.0 Hz), 6.86 (s, 2 H), 6.29 (d, 2 H, J = 3.0 Hz), 6.08 (d, 1 H, J = 3.0 Hz), 5.92 (d, 1 H, J = 3.0 Hz), 3.82 (s, 6 H).

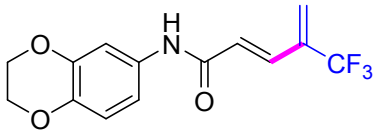
^{13}C NMR (75 MHz, $CDCl_3$) δ 160.2, 138.9, 135.2, 134.7, 126.8 (q, J = 5.3 Hz), 123.5, 99.9, 97.7, 56.3,

^{19}F NMR (282 MHz, $CDCl_3$) δ -65.9 (s, 3 F).

HRMS (EI) $[M+H]_+$ calcd for C14H15F3NO3, 302.1004; found, 302.1012.

(E)-N-(2,3-dihydrobenzo[b][1,4]dioxin-6-yl)-4-(trifluoromethyl)penta-2,4-dienamide

(3p)



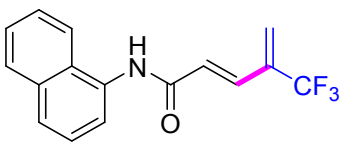
^{1}H NMR (300 MHz, $CDCl_3$) δ 7.52 (s, 1 H), 7.33 (d, 1 H, J = 12.0 Hz), 7.23 (d, 1 H, J = 3.0 Hz), 6.98 (dd, 1 H, J = 9.0. 3.0 Hz), 6.82 (d, 1 H, J = 9.0 Hz), 6.30 (dd, 1 H, J = 15.0. 3.0 Hz), 6.06 (d, 1 H, J = 3.0 Hz), 5.87 (d, 1 H, J = 3.0 Hz), 4.25 (s, 4 H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 165.6, 144.6, 141.2, 135.4 (q, J = 36.8 Hz), 134.7, 131.3, 126.4 (q, J = 5.3 Hz), 125.0, 122.5 (q, J = 272.3 Hz), 117.3. 113.1, 109.9, 58.8.

^{19}F NMR (282 MHz, $CDCl_3$) δ -65.9 (s, 3 F).

HRMS (EI) $[M+H]_+$ calcd for C14H13F3NO3, 300.0848; found, 300.0838

(E)-N-(naphthalen-1-yl)-4-(trifluoromethyl)penta-2,4-dienamide **(3p)**



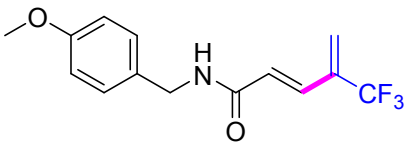
^{1}H NMR (300 MHz, d_4-MeOD) δ 8.02-7.98 (m, 1 H), 7.94-7.92 (m, 1 H), 7.81 (d, 1 H, J = 12.0 Hz), 7.72 (d, 1 H, J = 6.0 Hz), 7.57-7.49 (m, 1 H), 6.83 (dd, 1 H, J = 15.0, 3.0 Hz), 6.17 (d, 1 H, J = 3.0 Hz), 6.13 (d, 1 H, J = 3.0 Hz).

^{13}C NMR (75 MHz, d_4-MeOD) δ 165.0, 135.1 (q, J = 30.0 Hz), 134.3, 134.0, 132.5, 128.4, 128.0, 126.4, 125.9 (q, J = 3.8 Hz), 125.8, 125.1, 125.0, 122.3, 121.9.

^{19}F NMR (282 MHz, d_4-MeOD) δ -67.4 (s, 3 F).

HRMS (EI) $[M+H]_+$ calcd for C16H13F3NO, 292.0949; found, 292.0941

(E)-N-(4-methoxybenzyl)-4-(trifluoromethyl)penta-2,4-dienamide **(4a)**



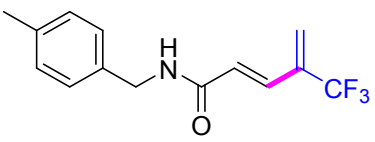
H NMR (300 MHz, $CDCl_3$) δ 7.22 (d, 2 H, J = 12.0 Hz), 6.87 (d, 2 H, J = 9.0 Hz), 6.21 (d, 1 H, J = 3.0 Hz), 6.16 (d, 1 H, J = 3.0 Hz), 6.01 (d, 1 H, J = 3.0 Hz), 5.83 (d, 1 H, J = 3.0 Hz), 4.45 (d, 2 H, J = 6.0 Hz), 3.80 (s, 3 H).

C NMR (75 MHz, $CDCl_3$) δ 164.6, 159.2, 135.0 (q, J = 22.5 Hz), 134.0, 129.9, 129.3, 126.0 (q, J = 5.3 Hz), 124.6, 122.5 (q, J = 273.0 Hz), 114.1, 55.3, 43.4.

F NMR (282 MHz, $CDCl_3$) δ -65.6 (s, 3 F).

HRMS (EI) $[M+H]_+$ calcd for C14H15F3NO2, 286.1055; found, 286.1049

(E)-N-(4-methylbenzyl)-4-(trifluoromethyl)penta-2,4-dienamide **(4b)**



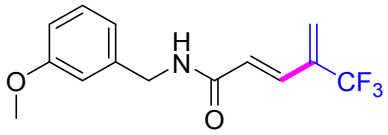
^{1}H NMR (300 MHz, $CDCl_3$) δ 7.27 (s, 1 H), 7.22-7.12 (m, 4 H), 6.40 (s, 1 H), 6.22 (dq, 1 H, J = 15.0, 3.0 Hz), 6.01 (d, 1 H, J = 3.0 Hz), 5.81 (d, 1 H, J = 3.0 Hz), 4.46 (d, 2 H, J= 6.0 Hz), 2.34 (s, 3 H).

^{13}C NMR (400 MHz NMR, 100 MHz, $CDCl_3$) δ 164.8, 137.4, 134.8, 135.0 (q, J = 31.0 Hz), 134.8, 133.9, 129.5, 127.9, 125.9 (q, J = 5.0 Hz), 124.7, 122.5 (q, J = 273.0 Hz).

^{19}F NMR (282 MHz, $CDCl_3$) δ -66.1 (s, 3 F).

HRMS (EI) $[M+H]_+$ calcd for C14H15F3NO, 270.1106; found, 270.1102

(E)-N-(3-methoxybenzyl)-4-(trifluoromethyl)penta-2,4-dienamide **(4c)**



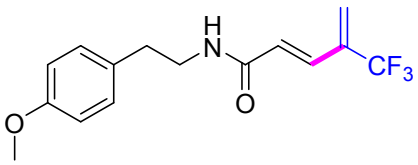
^{1}H NMR (300 MHz, $CDCl_3$) δ 7.31-7.25 (m, 2 H), 6.90 (d, 1 H, J = 6.0 Hz), 6.86-6.83 (m, 2 H), 6.04 (d, 1 H, J = 3.0 Hz), 5.85 (d, 1 H, J = 3.0 Hz), 4.52 (d, 2 H, J = 3.0 Hz), 3.82 (s, 3 H).

^{13}C NMR (400 MHz NMR, 100 MHz, $CDCl_3$) δ 164.2, 160.9, 138.6, 134.2, 135.9 (q, J = 30.0 Hz), 129.9, 126.2 (q, J = 5.0 Hz), 124.4, 122.5 (q, J = 273.0 Hz), 120.2, 114.4, 113.0.

^{19}F NMR (282 MHz, $CDCl_3$) δ -66.0 (s, 3 F).

HRMS (EI) $[M+H]_+$ calcd for C14H15F3NO2, 286.1055; found, 286.1050

(E)-N-(4-methoxyphenethyl)-4-(trifluoromethyl)penta-2,4-dienamide **(4d)**



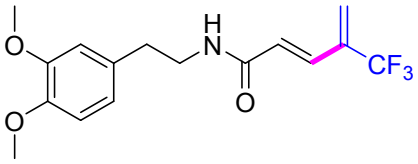
^{1}H NMR (300 MHz, $CDCl_3$) δ 7.24 (d, 2 H, J = 15.0 Hz), 7.15 (d, 2 H, J = 9.0 Hz), 6.88 (d, 2 H, J = 9.0 Hz), 6.09 (dq, 1 H, J = 15.0, 3.0 Hz), 6.03 (d, 1 H, J = 3.0 Hz), 5.85 (d, 1H, J = 3.0 Hz), 5.71 (s, 1 H), 3.80 (s, 3 H), 3.62 (q, 2 H, J = 6.0 Hz), 2.83 (t, 2 H, J = 6.0 Hz).

^{13}C NMR (75 MHz, $CDCl_3$) δ 164.6, 159.2, 135.0 (q, J = 22.5 Hz), 134.0, 129.9, 129.3, 126.0 (q, J = 5.3 Hz), 124.6, 122.5 (q, J = 273.0 Hz), 114.1, 55.3, 43.4.

^{19}F NMR (282 MHz, $CDCl_3$) δ -65.6 (s, 3 F).

HRMS (EI) $[M+H]_+$ calcd for C15H17F3N2O, 300.1211; found, 300.1212

(E)-N-(3,4-dimethoxyphenethyl)-4-(trifluoromethyl)penta-2,4-dienamide **(4e)**



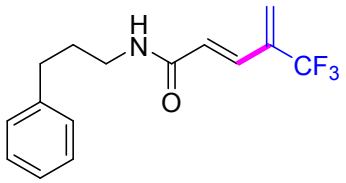
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.15 (d, 1 H, J = 12.0 Hz), 6.74 (d, 1 H, J = 8.0 Hz), 6.68 (d, 1 H, J = 8.0 Hz), 6.65 (s, 1 H), 6.02 (d, 1 H, J = 12.0 Hz), 5.92 (s, 1 H), 5.84 (s, 1 H), 5.75 (s, 1 H), 3.79 (s, 3 H), 3.78 (s, 3 H), 3.52 (q, 2 H, J = 4.0 Hz), 2.74 (t, 2 H, J = 4.0 Hz).

^{13}C NMR (100 MHz, $CDCl_3$) δ 163.8, 148.1, 146.8, 133.9 (q, J = 20.4 Hz), 130.2, 124.9, 123.7, 121.5 (q, J = 233.1 Hz), 117.6, 110.9, 110.5, 54.9, 54.8, 40.0, 34.1.

^{19}F NMR (470 MHz, $CDCl_3$) δ -65.9 (s, 3 F).

HRMS (EI) $[M+H]_+$ calcd for C16H19F3NO3, 330.1317; found, 330.1310

(E)-N-(3-phenylpropyl)-4-(trifluoromethyl)penta-2,4-dienamide **(4f)**



^{1}H NMR (300 MHz, *d*$_4$-MeOD) δ 7.29-7.16 (m, 6 H), 6.40 (dq, 1 H, J = 15.0, 3.0 Hz), 6.07 (d, 1 H, J = 3.0 Hz), 6.01 (d, 1 H, J = 3.0 Hz), 3.31 (t, 2 H, J = 9.0 Hz), 2.67 (t, 2 H, J = 9.0 Hz), 1.85 (m, 2 H).

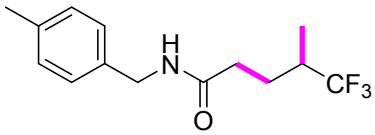
^{13}C NMR (75 MHz, *d*$_4$-MeOD) δ 166.9, 141.5, 135.0 (q, J = 30.0 Hz), 132.5, 128.6,

125.5, 125.3 (q, J = 5.3 Hz), 125.0, 122.7 (q, J = 271.5 Hz), 40.4, 33.0, 29.9.

^{19}F NMR (282 MHz, *d*$_4$-MeOD) δ -67.6 (s, 3 F)

HRMS (EI) $[M+H]_+$ calcd for C15H17F3NO, 284.1262; found, 284.1260

5,5,5-trifluoro-4-methyl-N-(4-methylbenzyl)pentanamide **(5a)**



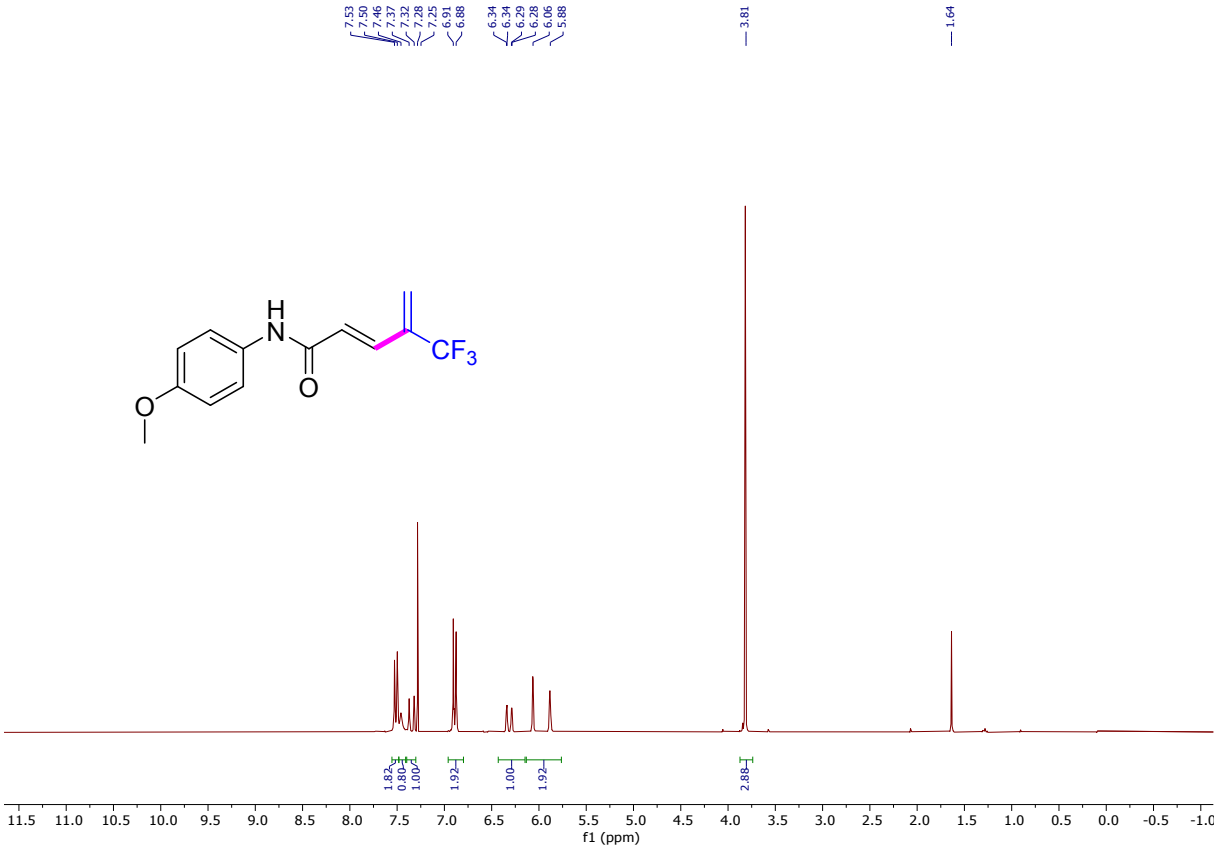
^{1}H NMR (300 MHz, CDCl$_3$) δ 7.2 (s, 1 H), 5.91 (s, 1 H), 4.40 (d, 2 H, J = 6.0 Hz), 2.37 (s, 3 H), 2.36-2.23 (m, 2 H), 2.09-1.97 (m, 1 H), 1.82-1.69 (m, 2 H), 1.16 (s, 3 H), 1.12 (s, 3 H).

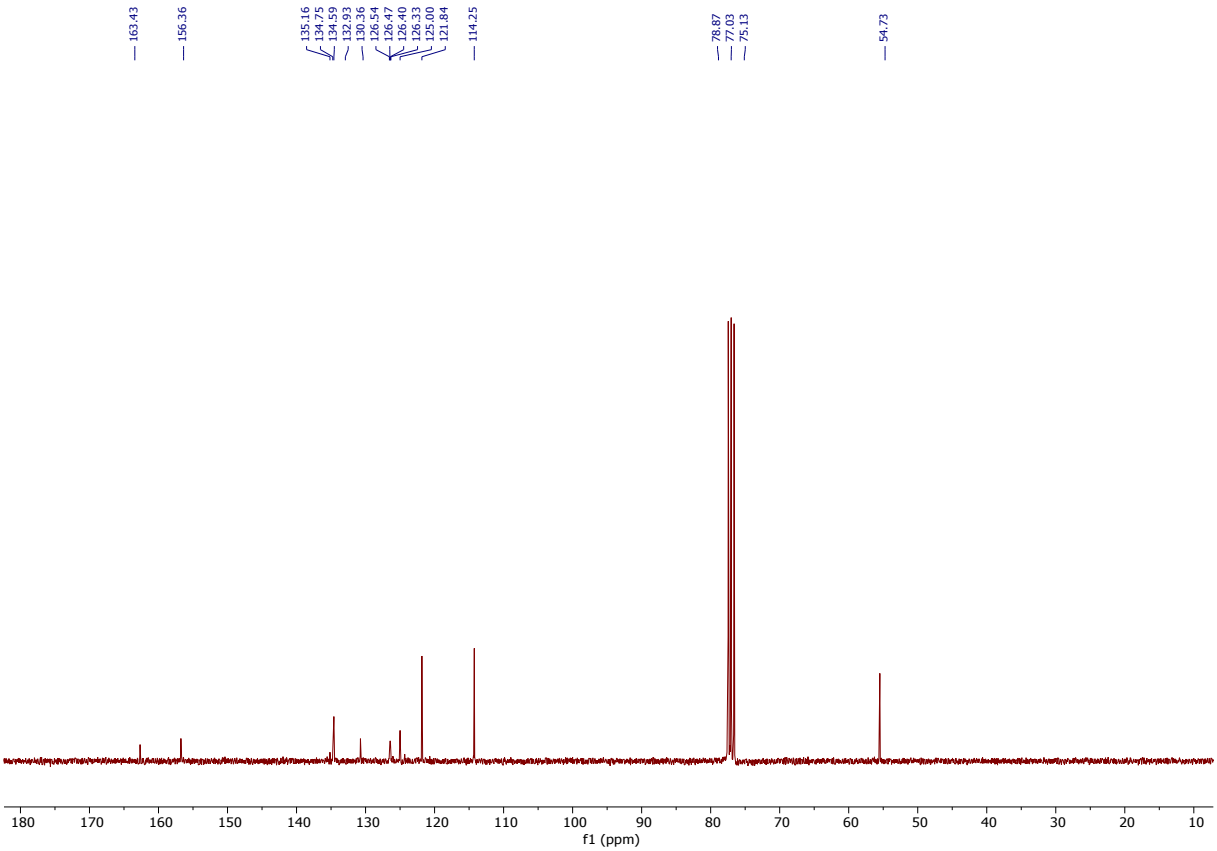
^{13}C NMR (75 MHz, CDCl$_3$) δ 171.5, 137.4, 135.1, 129.4,127.8, 128.3 (q, J = 278.3 Hz), 43.5, 33.3, 25.5 (q, J = 2.3 Hz), 21.0.

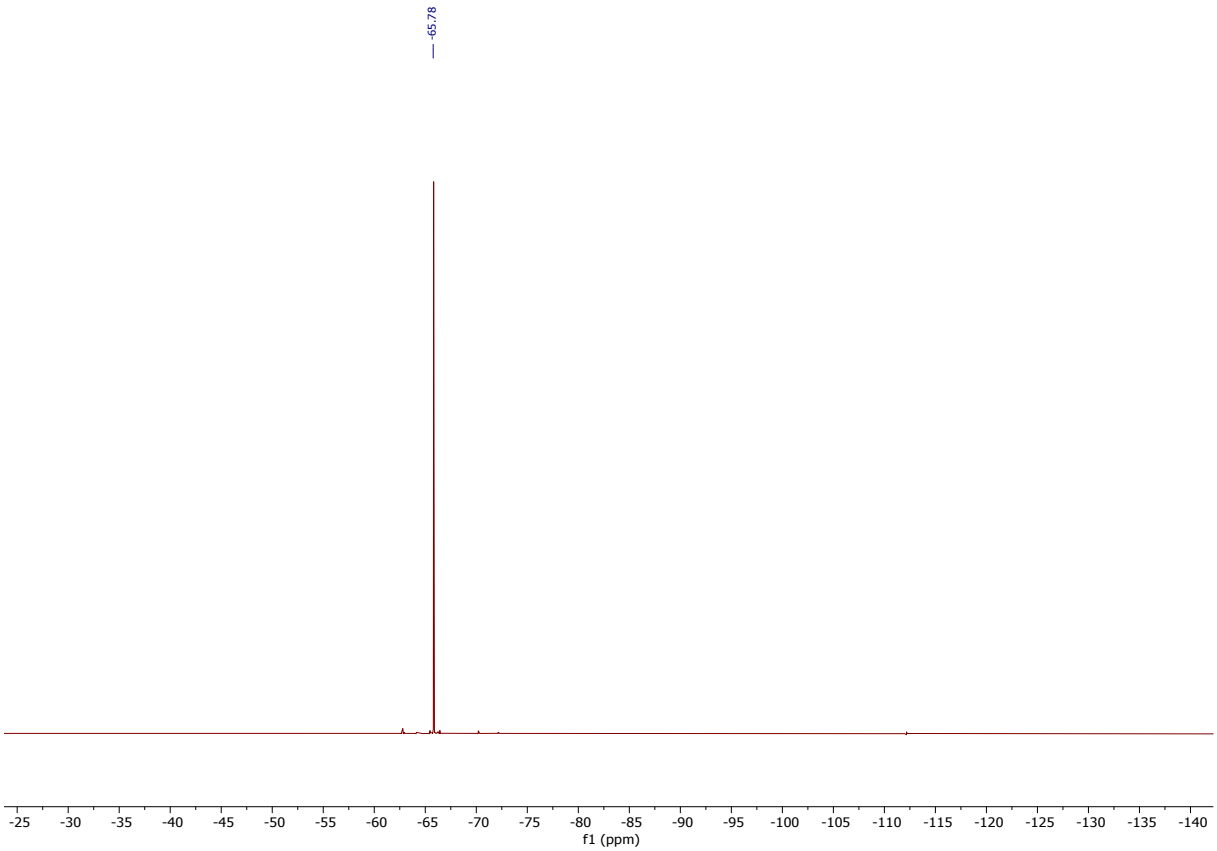
^{19}F NMR (282 MHz, $CDCl_3$) δ -72.7 (s, 3 F).

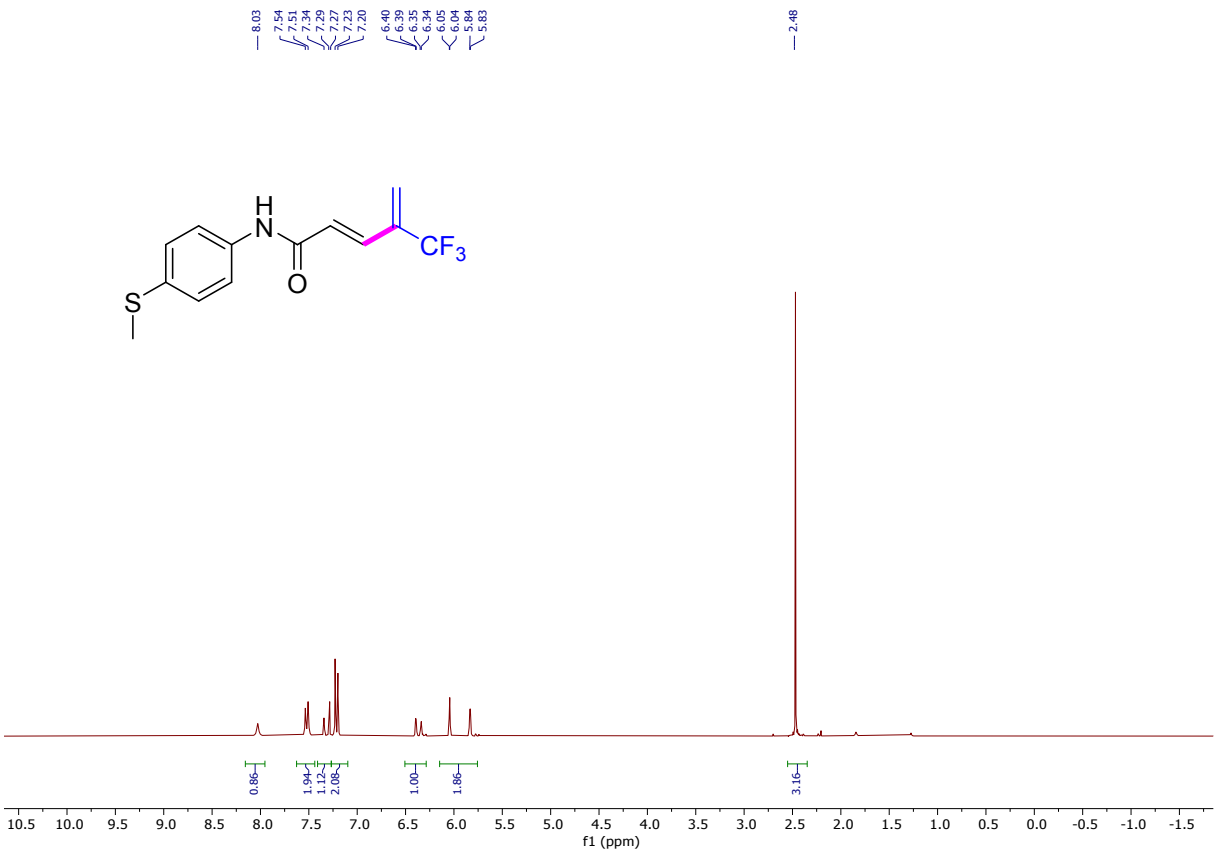
HRMS (EI) $[M+H]_+$ calcd for C14H19F3NO, 274.1419; found, 274.1412

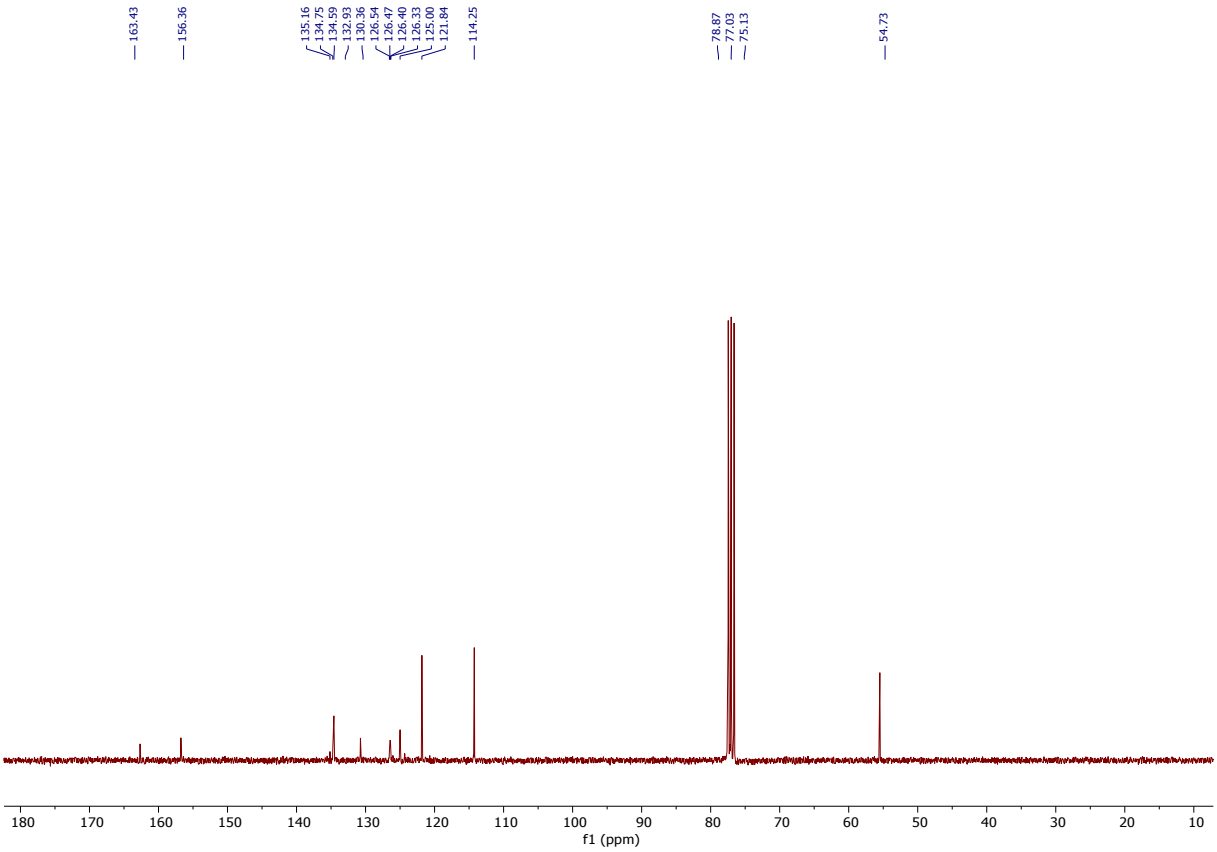
5 Copies of the NMR spectra of products

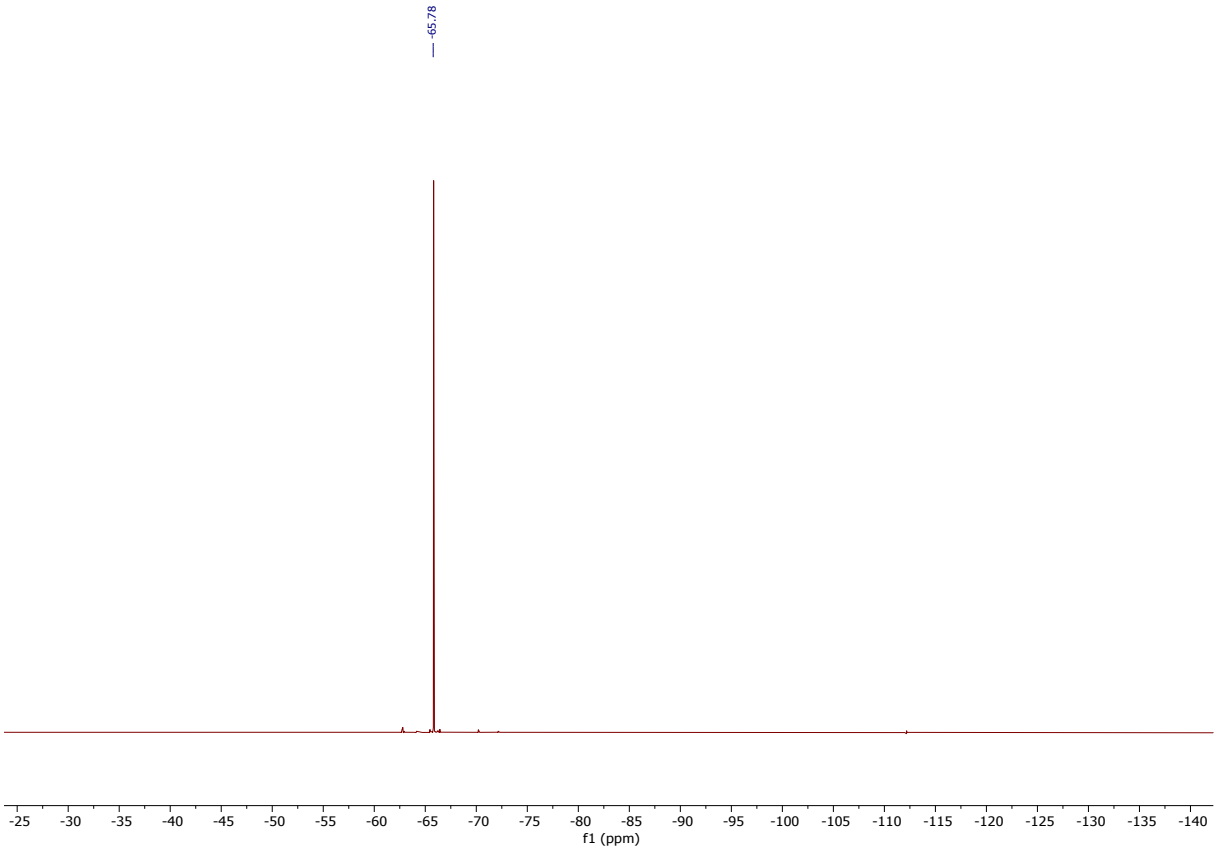


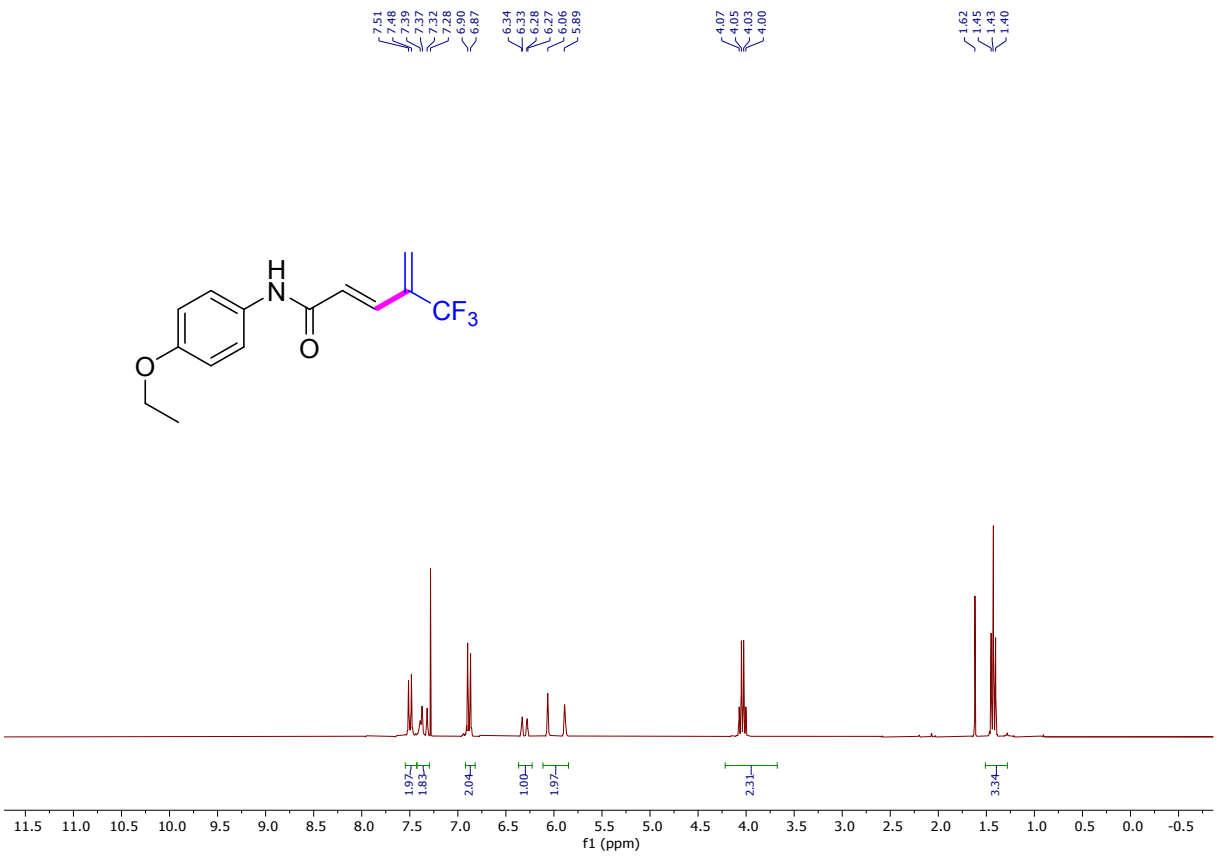



-65.78
-25 -30 -35 -40 -45 -50 -55 -60 -65 -70 -75 -80 -85 -90 -95 -100 -105 -110 -115 -120 -125 -130 -135 -140
f1 (ppm)


8.03
7.54
7.51
7.34
7.29
7.27
7.23
7.20
6.40
6.39
6.35
6.34
6.05
6.04
5.84
5.83
2.48
H
N
O
CF3
S
0.86
1.94
1.12
2.08
1.00
1.86
3.16
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)


163.43
156.36
135.16
134.75
134.59
132.93
130.36
126.54
126.47
126.40
126.33
125.00
121.84
114.25
78.87
77.03
75.13
54.73
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)


-65.78
-25 -30 -35 -40 -45 -50 -55 -60 -65 -70 -75 -80 -85 -90 -95 -100 -105 -110 -115 -120 -125 -130 -135 -140
f1 (ppm)


7.51
7.48
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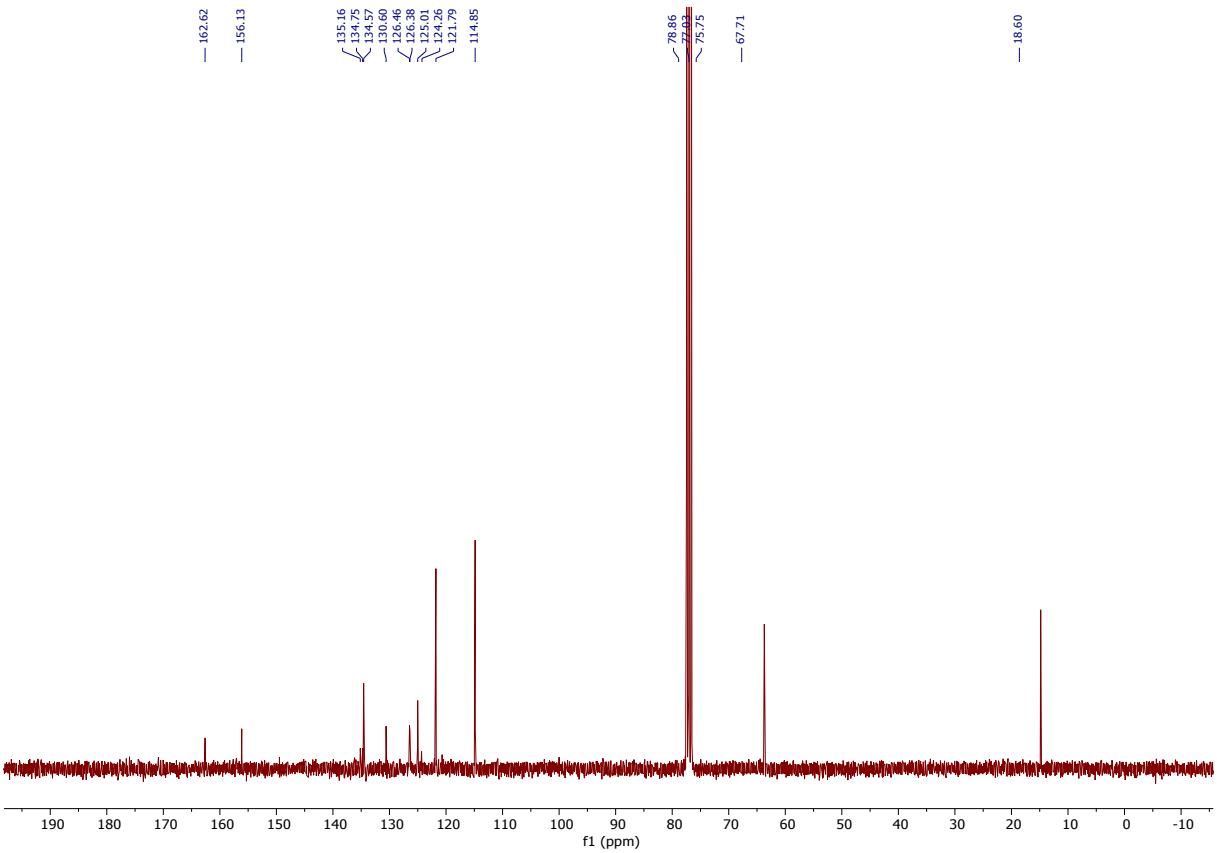
7.37
7.32
7.28
6.90
6.87
6.34
6.33
6.28
6.27
6.06
5.89
4.07
4.05
4.03
4.00
1.62
1.45
1.43
1.40
H
N
O
O
CF3
1.97
1.83
2.04
1.00
1.97
2.31
3.34
f1 (ppm)


162.62
156.13
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130.60
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126.38
125.01
124.26
121.79
114.85
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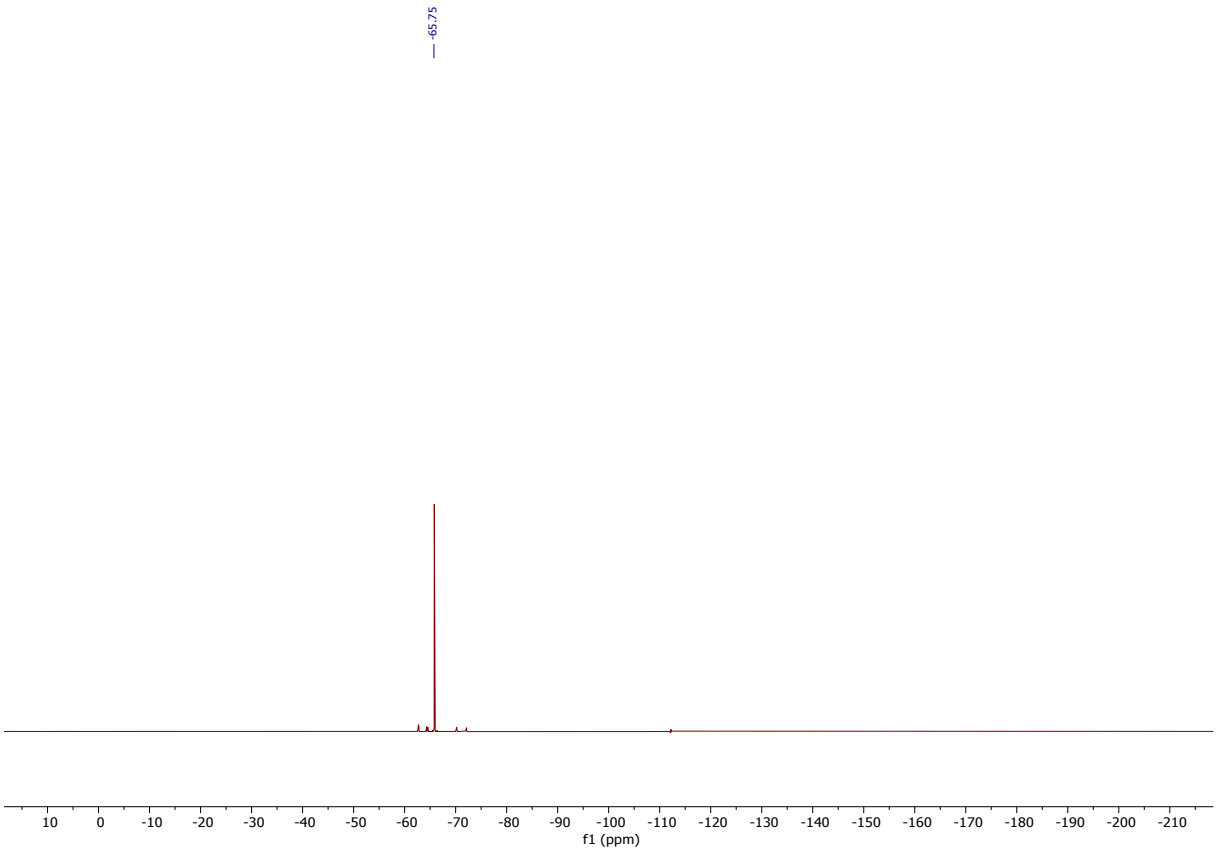
75.75
67.71
18.60
f1 (ppm)


-65.75
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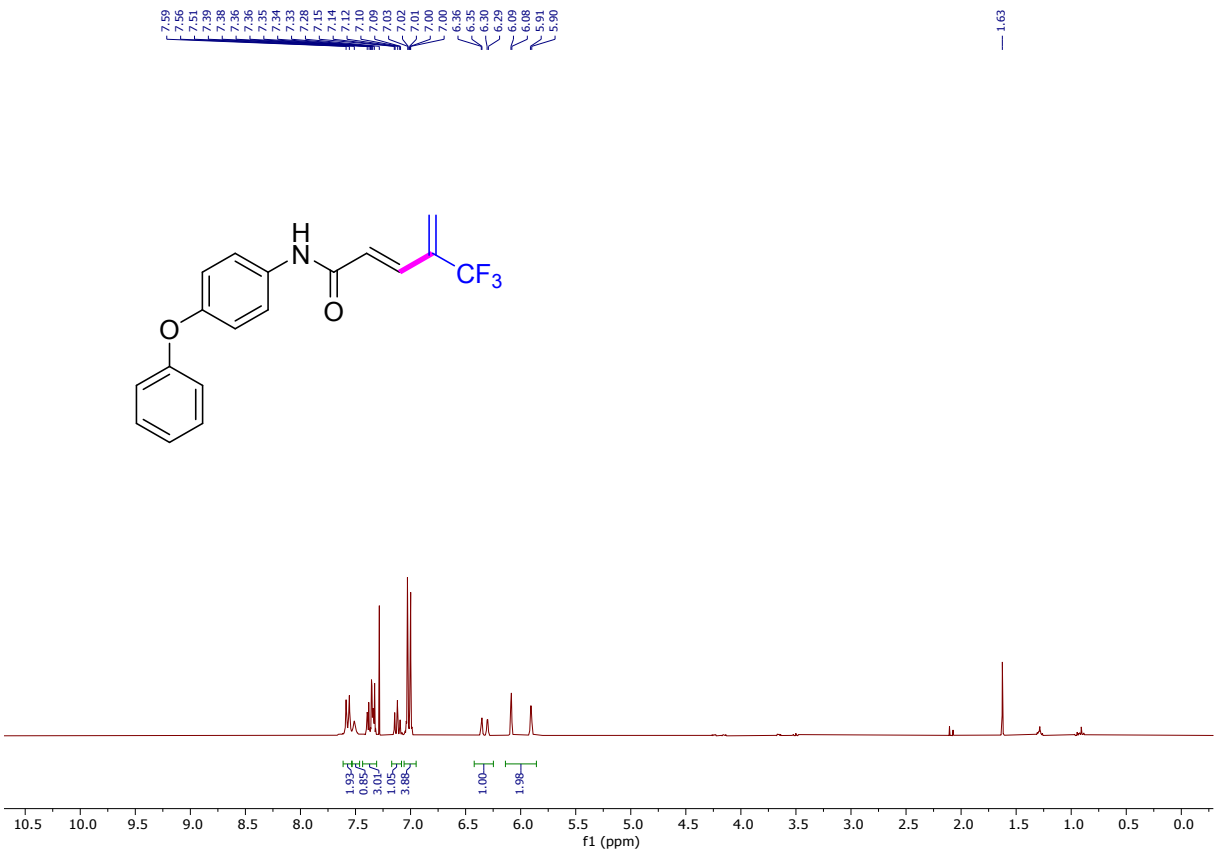
f1 (ppm)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7.56
7.51
7.39
7.38
7.36
7.36
7.35
7.34
7.33
7.28
7.15
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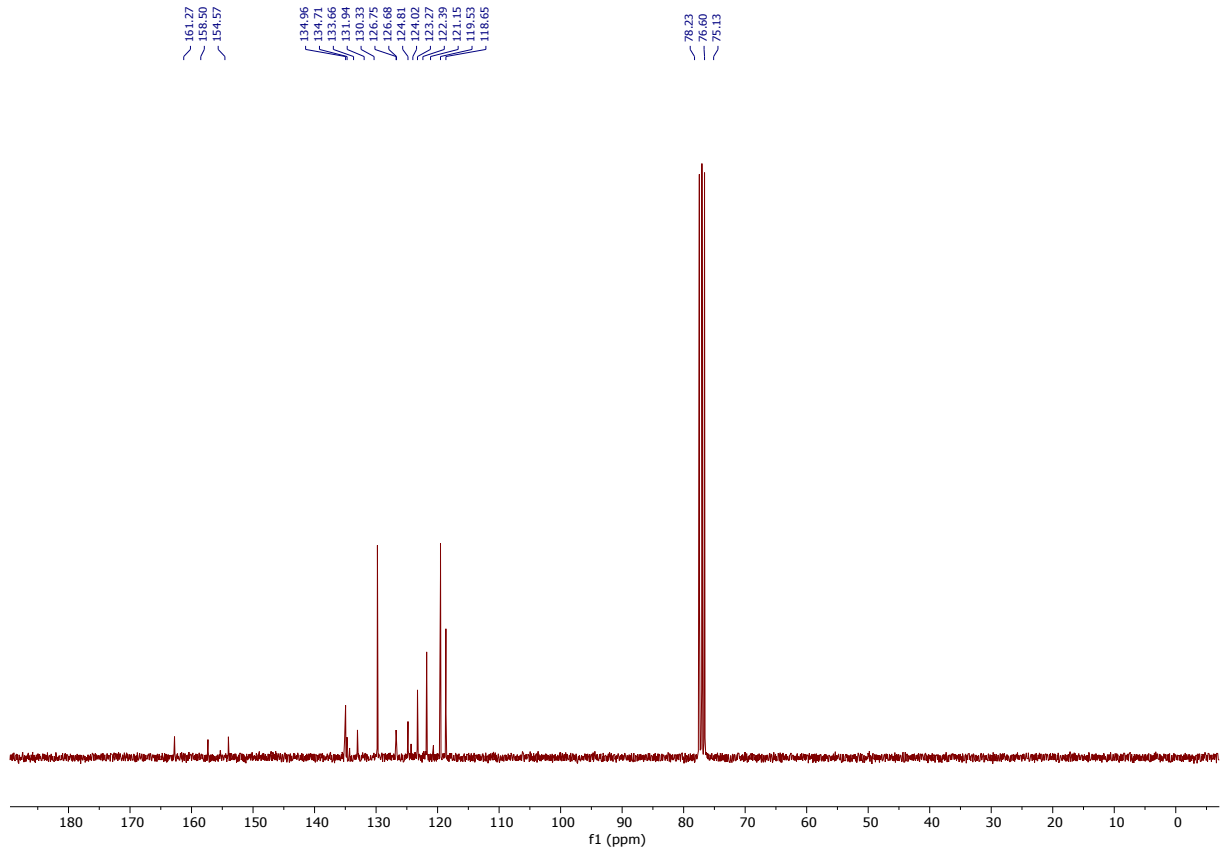
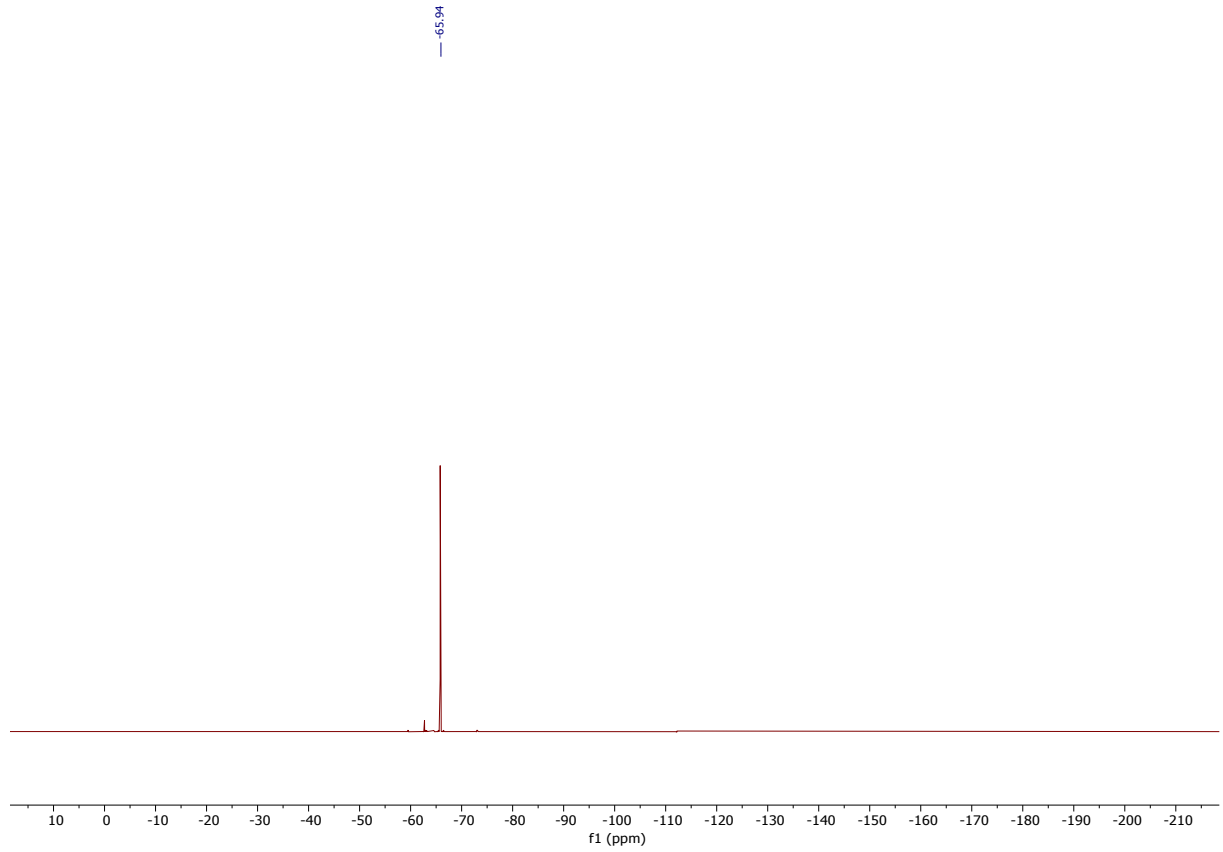
7.12
7.10
7.09
7.03
7.02
7.01
7.00
7.00
6.36
6.35
6.30
6.29
6.09
6.08
5.91
5.90
1.63
H
N
O
O
CF3
1.93
0.85
3.01
1.05
3.88
1.00
1.98
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


161.27
158.50
154.57
134.96
134.71
133.66
131.94
130.33
126.75
126.68
124.81
124.02
123.27
122.39
121.15
119.53
118.65
78.23
76.60
75.13
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


-65.94
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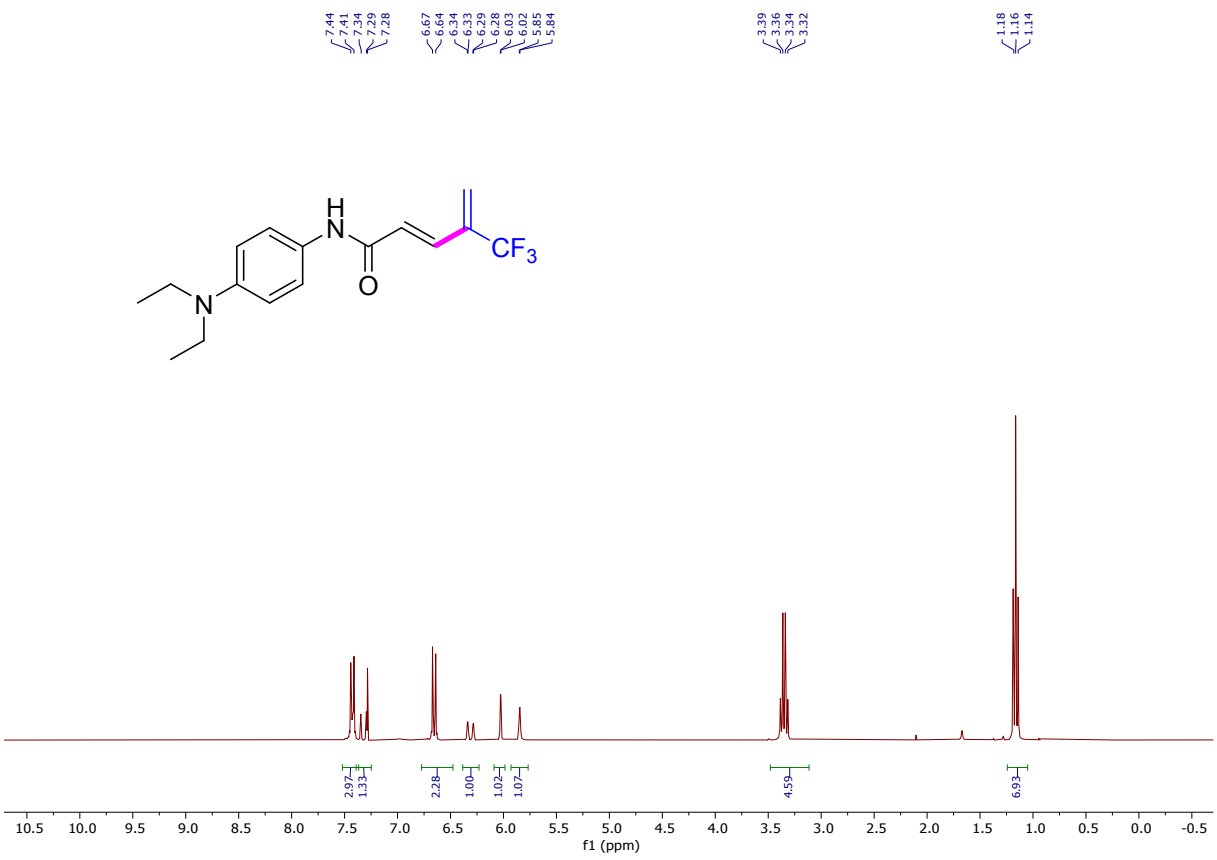
f1 (ppm)


7.44
7.41
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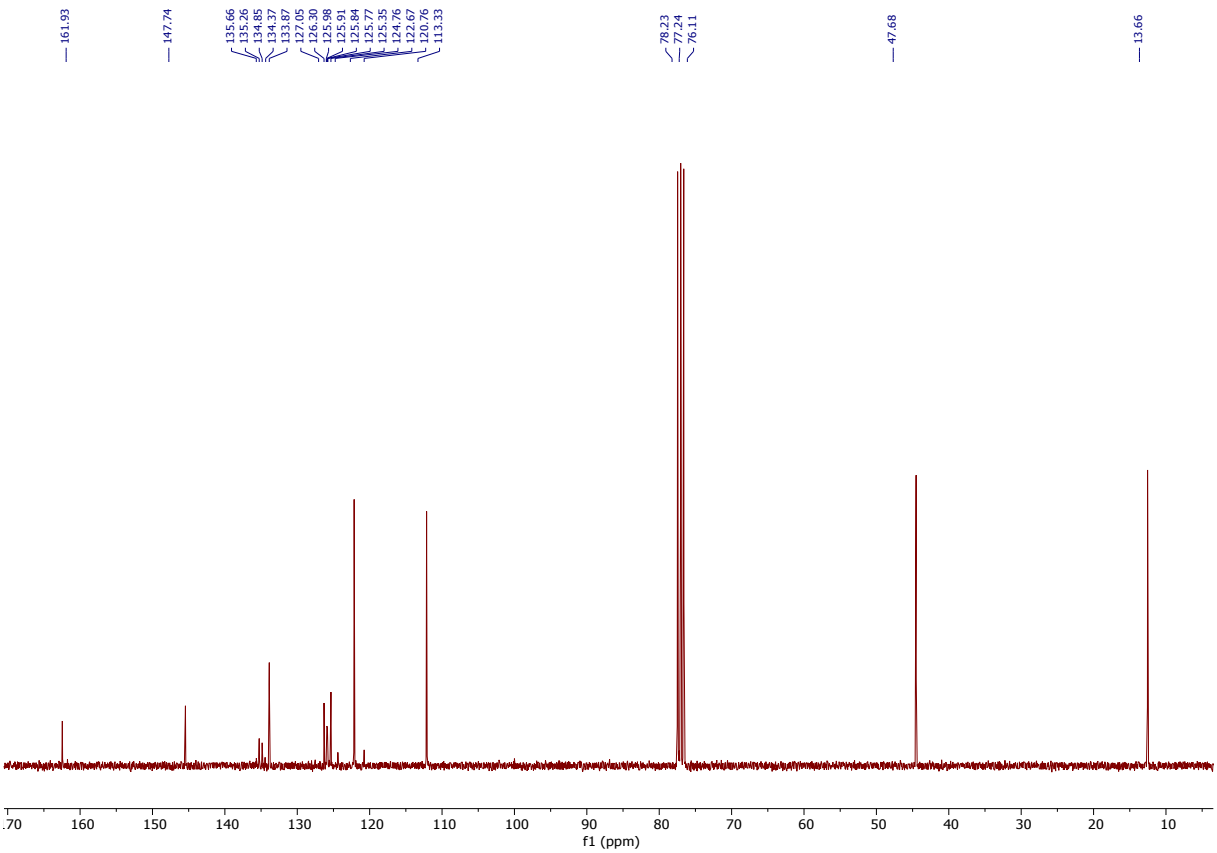
7.29
7.28
6.67
6.64
6.34
6.33
6.29
6.28
6.03
6.02
5.85
5.84
3.39
3.36
3.34
3.32
1.18
1.16
1.14
H
N
O
CF3
N
2.97
1.33
2.28
1.00
1.02
1.07
4.59
6.93
f1 (ppm)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135.66
135.26
134.85
134.37
133.87
127.05
126.30
125.98
125.91
125.84
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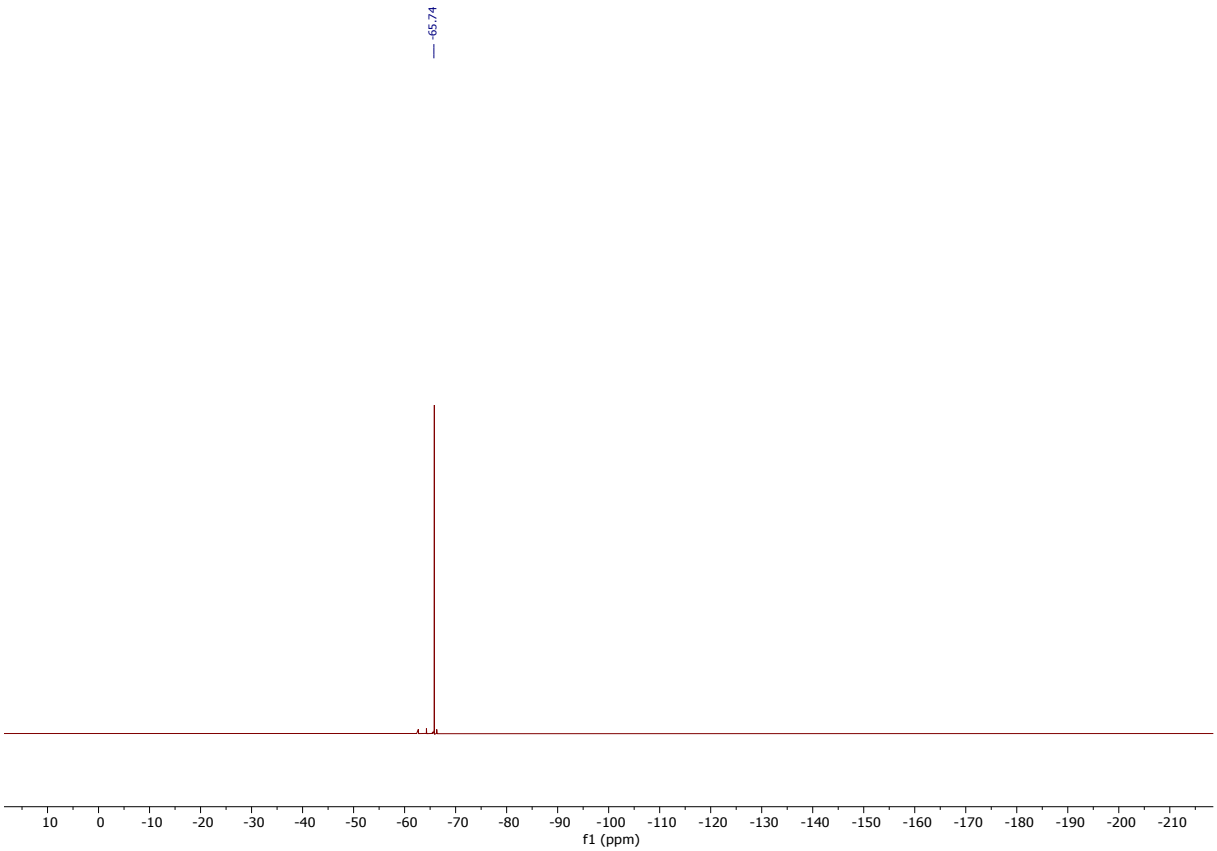
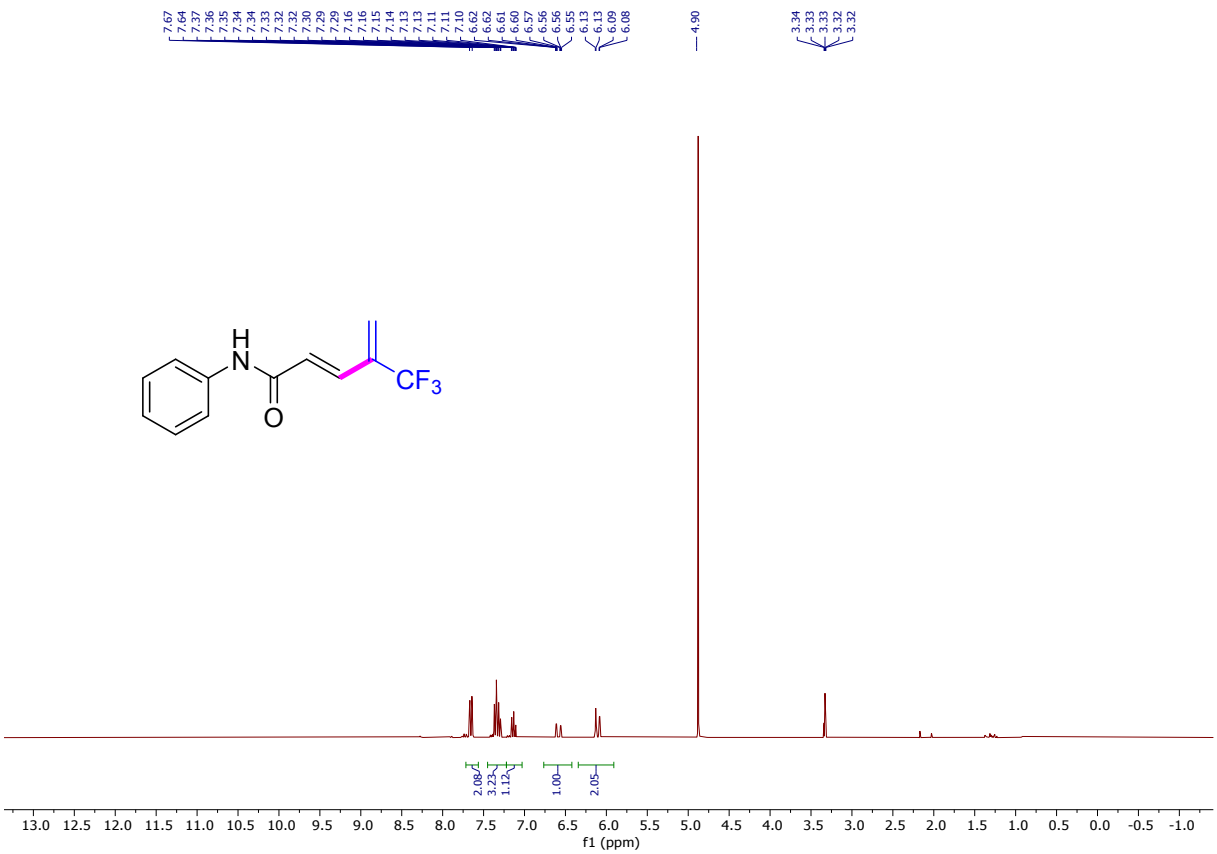
125.35
124.76
122.67
120.76
113.33
78.23
77.24
76.11
47.68
13.66
f1 (ppm)


-65.74
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)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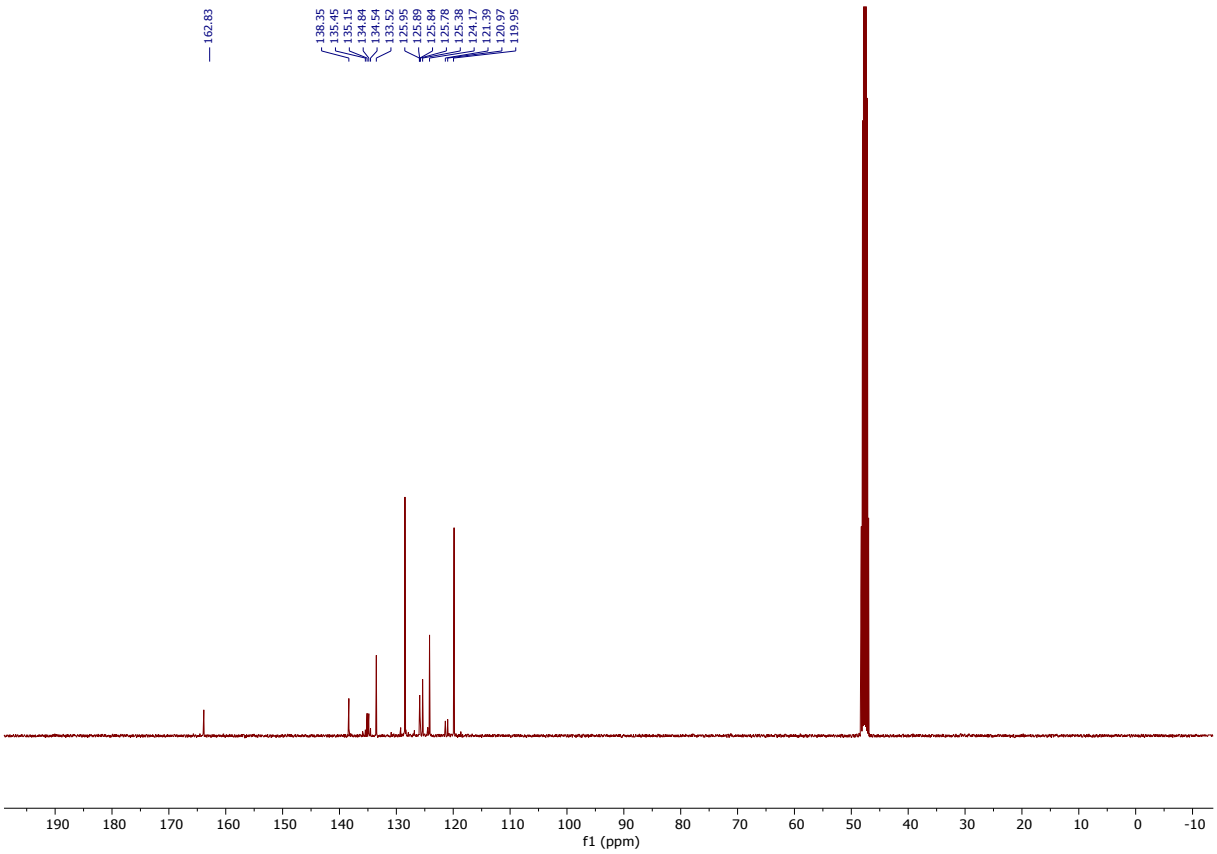
4.90
3.34 3.33 3.33 3.32 3.32
H
N
O
CF3
2.08 3.23 1.12 1.00 2.05
13.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)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138.35
135.45
135.15
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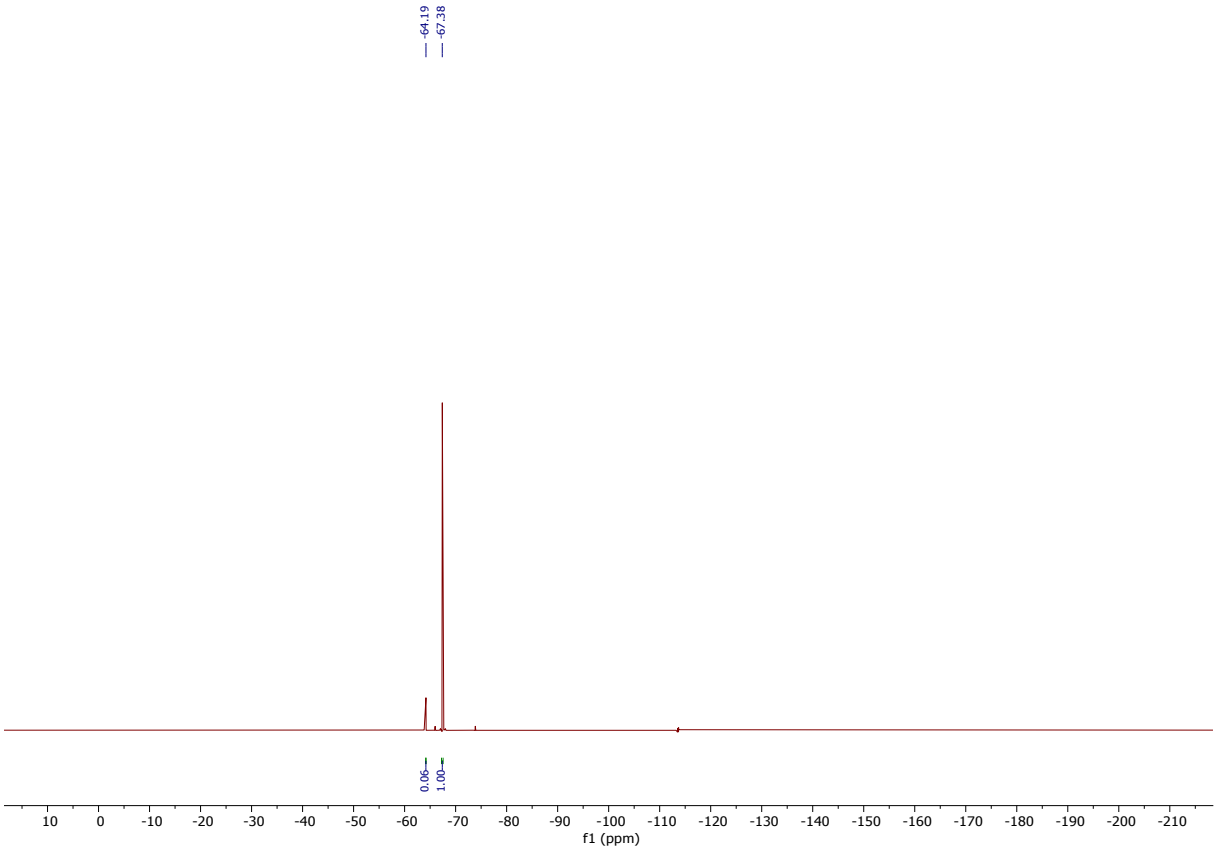
125.95
125.89
125.84
125.78
125.38
124.17
121.39
120.97
119.95
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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-67.38
0.06
1.00
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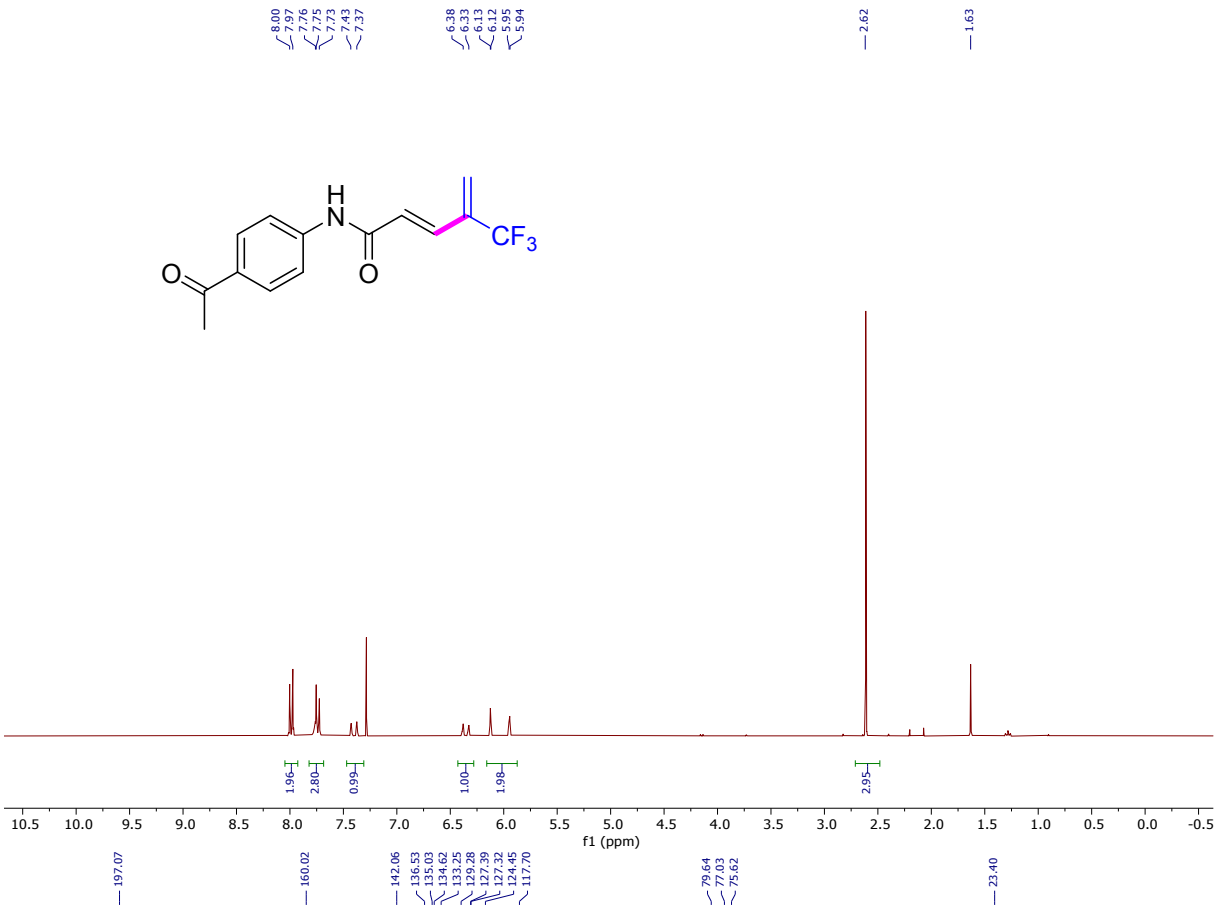
f1 (ppm)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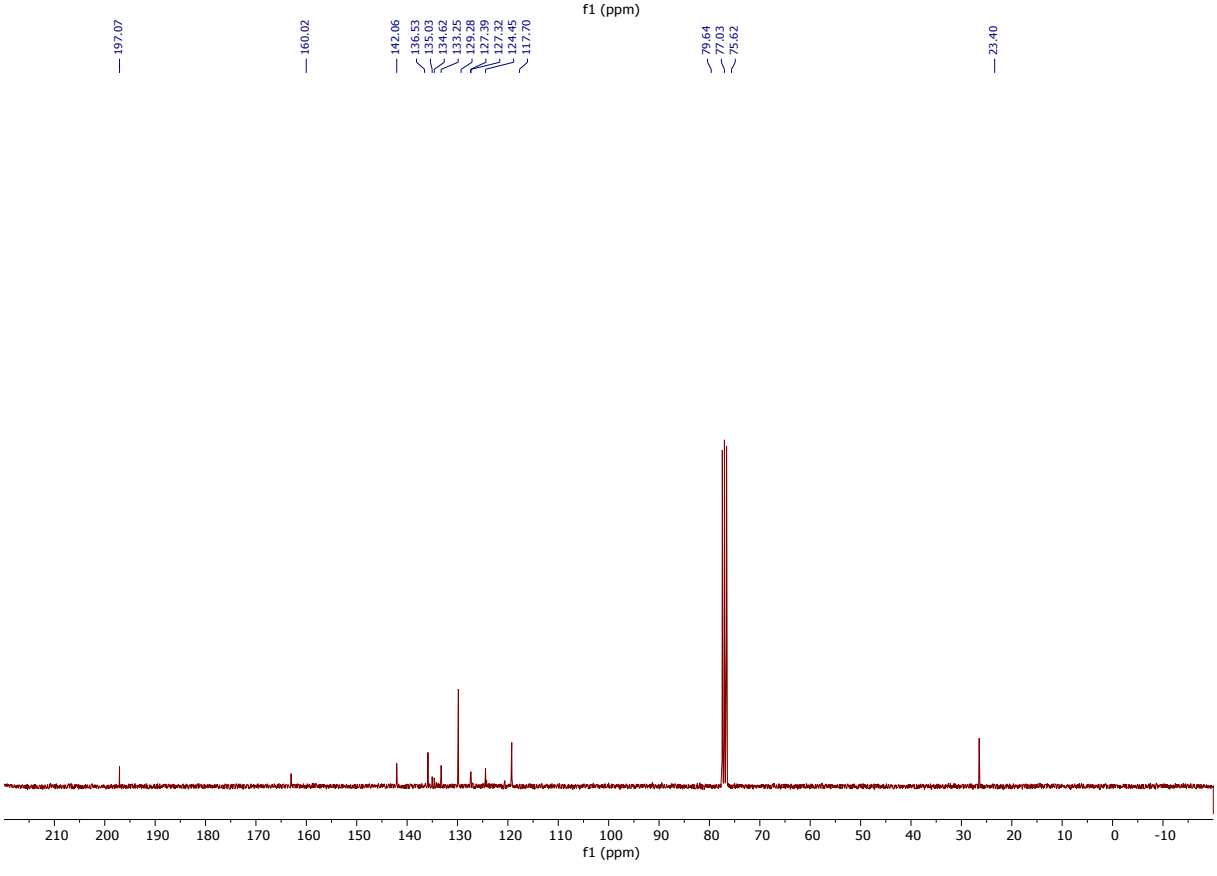
7.76
7.75
7.73
7.43
7.37
6.38
6.33
6.13
6.12
5.95
5.94
2.62
1.63
H
N
O
O
CF3
1.96
2.80
0.99
1.00
1.98
2.95
f1 (ppm)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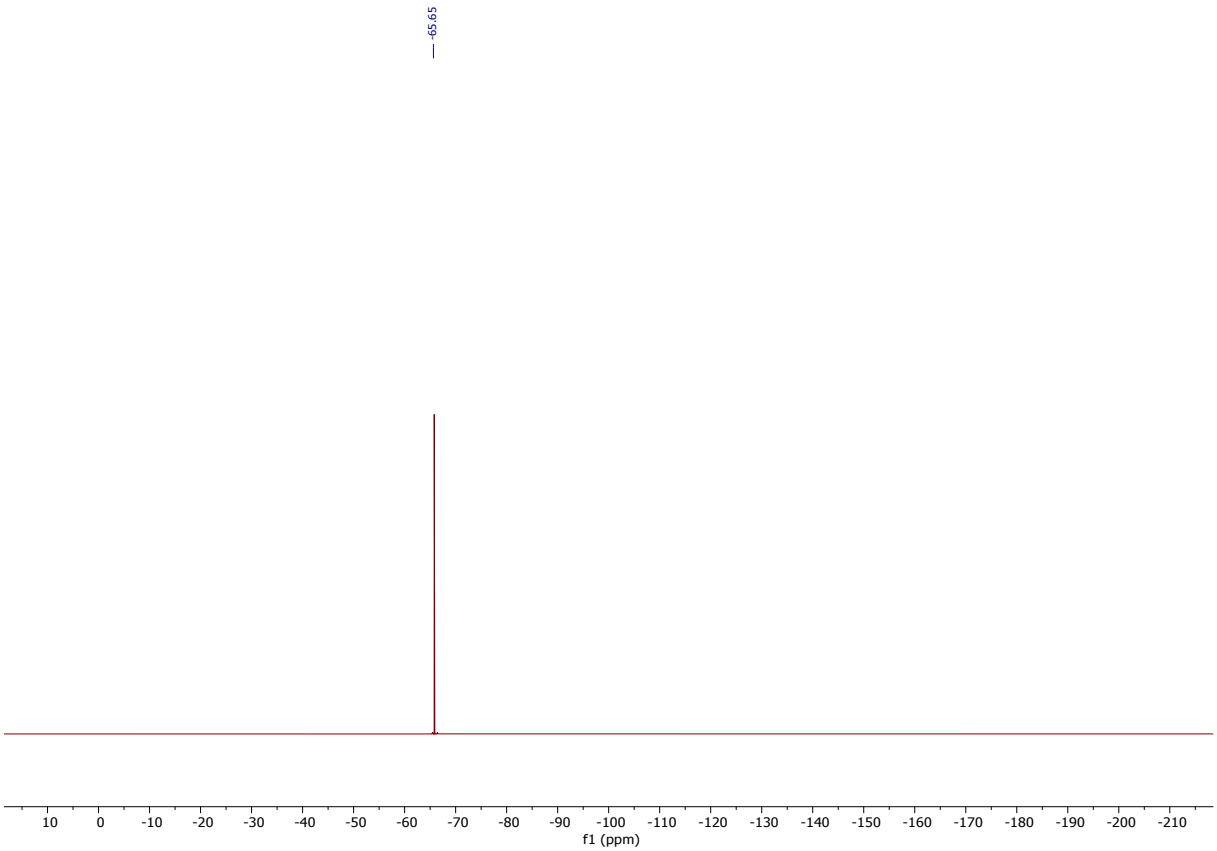
160.02
142.06
136.53
135.03
134.62
133.25
129.28
127.39
127.32
124.45
117.70
79.64
77.03
75.62
23.40
f1 (ppm)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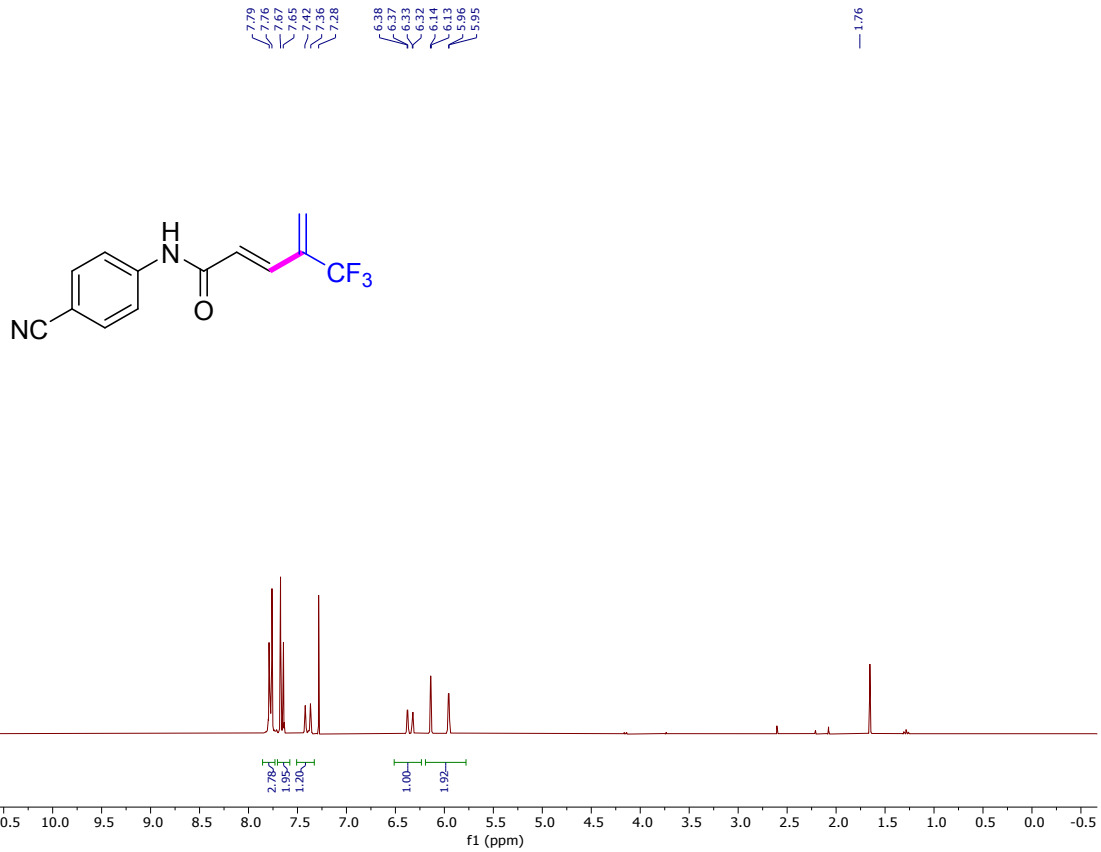
f1 (ppm)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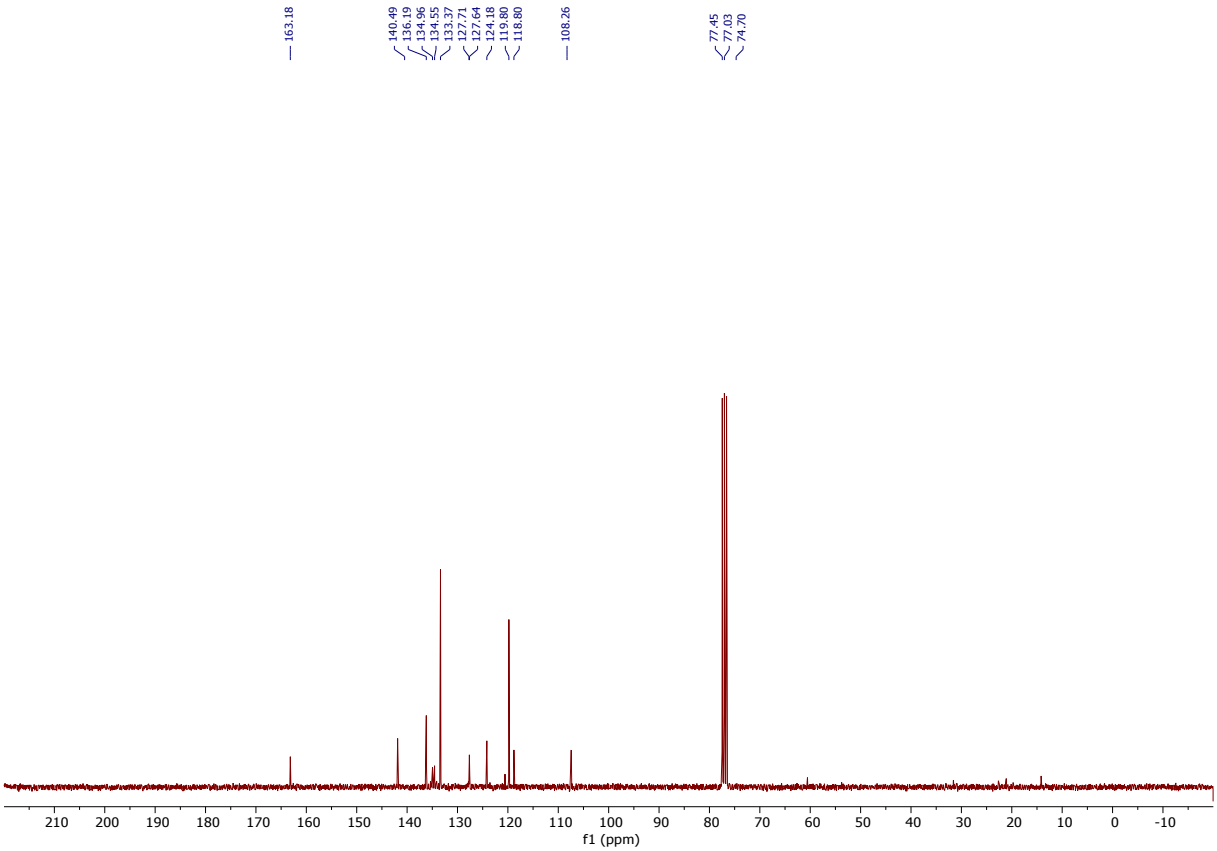
6.32
6.14
6.13
5.96
5.95
1.76
H
N
O
CF3
NC
2.78
1.95
1.20
1.00
1.92
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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140.49
136.19
134.96
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127.64
124.18
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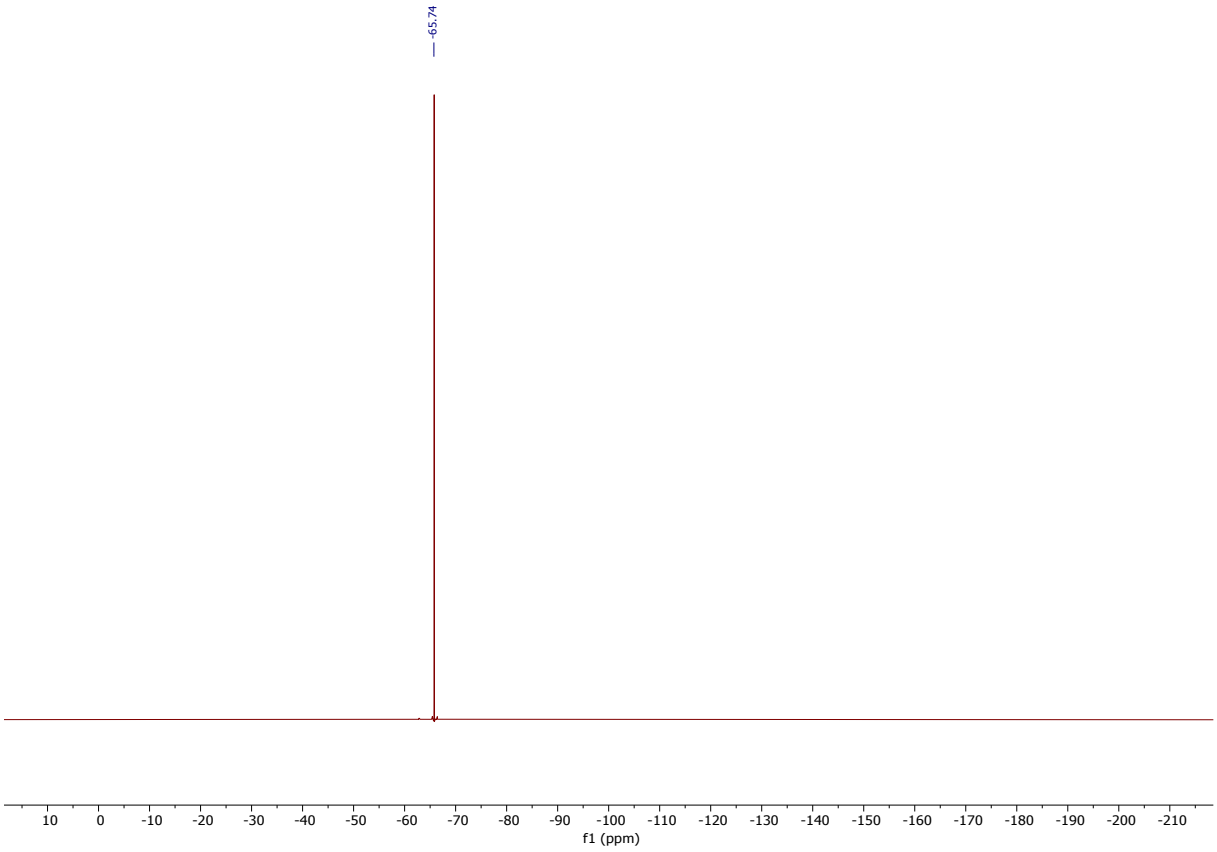
118.80
108.26
77.45
77.03
74.70
f1 (ppm)


-65.74
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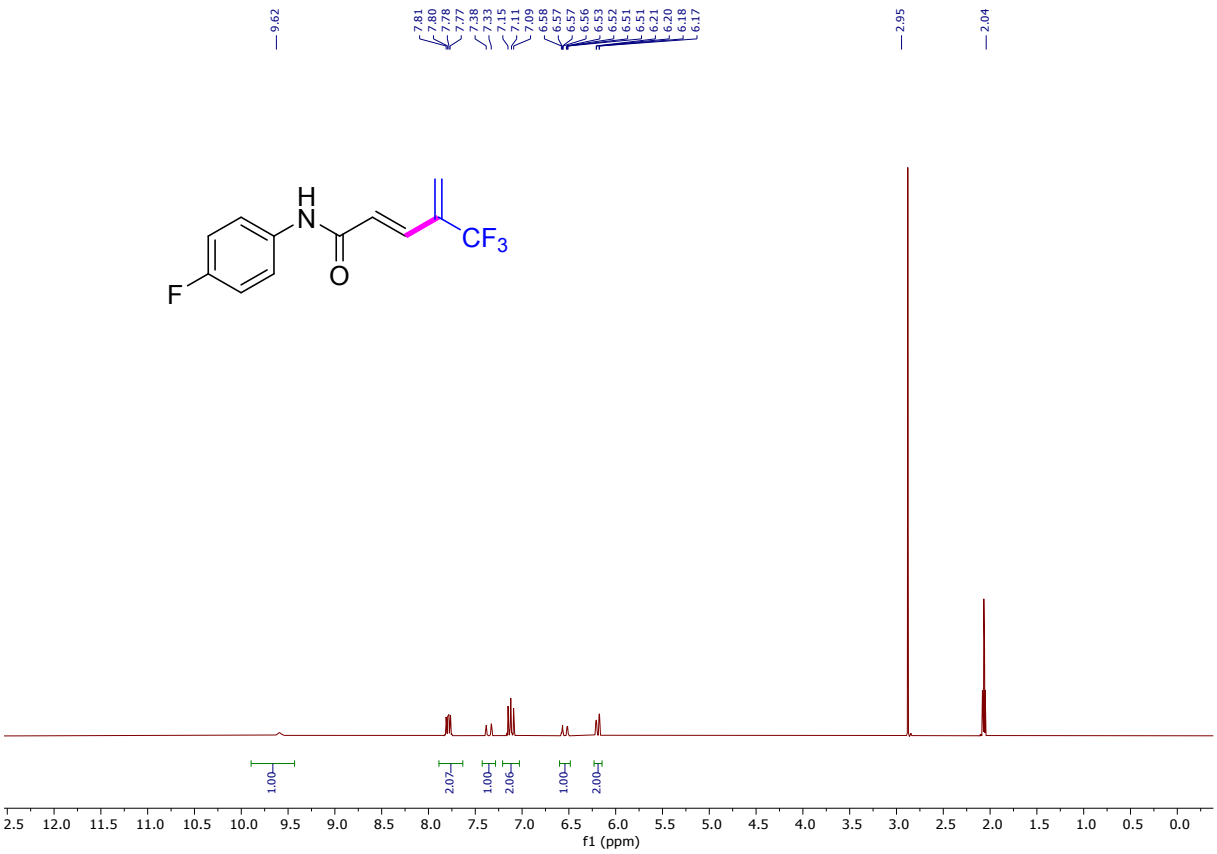
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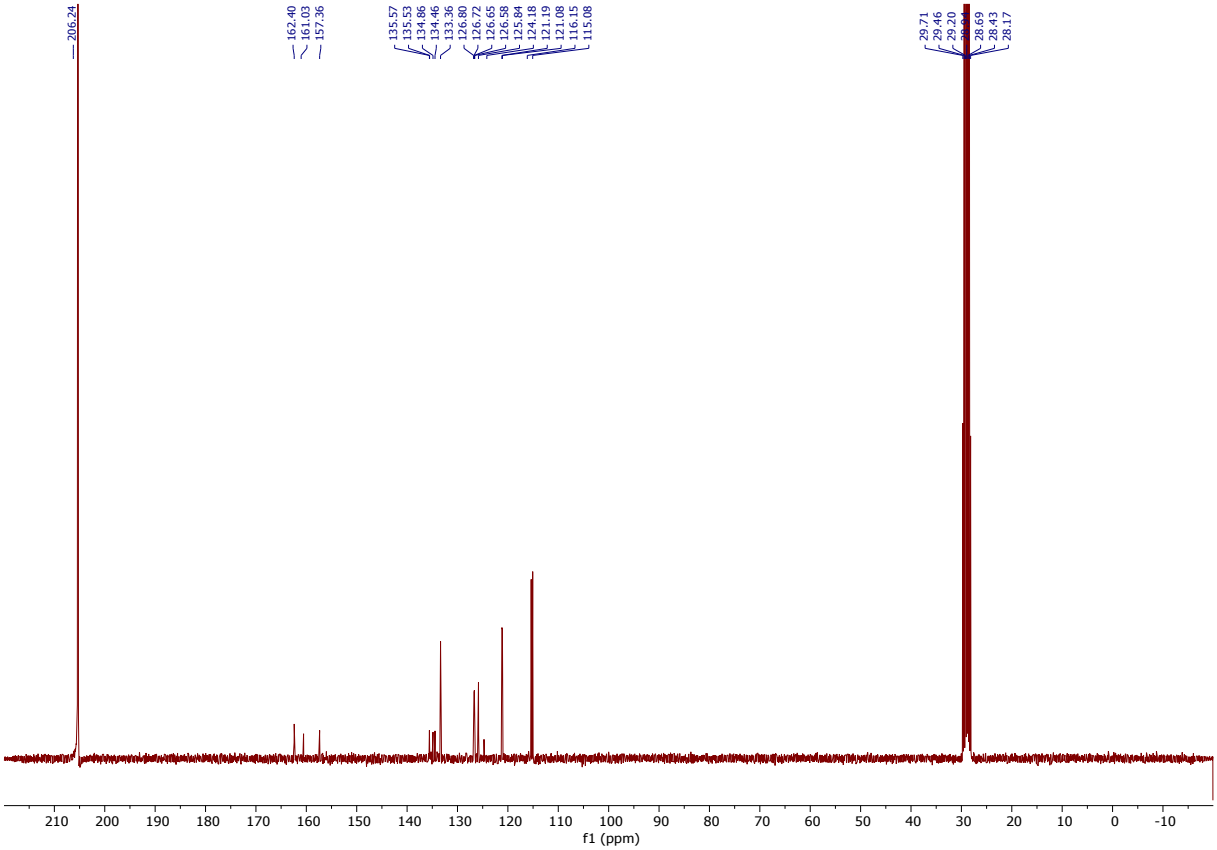
7.81
7.80
7.78
7.77
7.38
7.33
7.15
7.11
7.09
6.58
6.57
6.56
6.53
6.52
6.51
6.51
6.21
6.20
6.18
6.17
2.95
2.04
H
N
O
F
CF3
1.00
2.07
1.00
2.06
1.00
2.00
f1 (ppm)


206.24
162.40
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157.36
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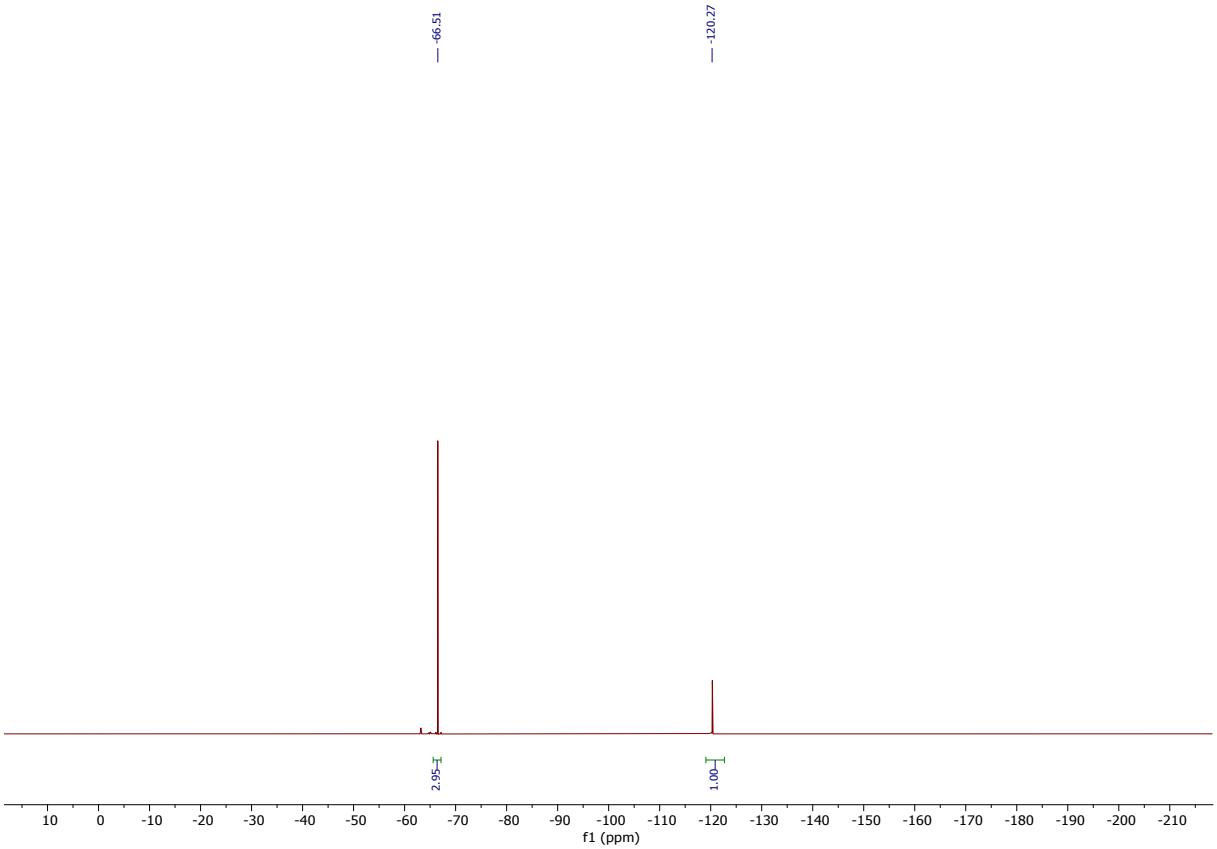
134.86
134.46
133.36
126.80
126.72
126.65
126.58
125.84
124.18
121.19
121.08
116.15
115.08
29.71
29.46
29.20
28.69
28.43
28.17
f1 (ppm)


-66.51
-120.27
2.95
1.00
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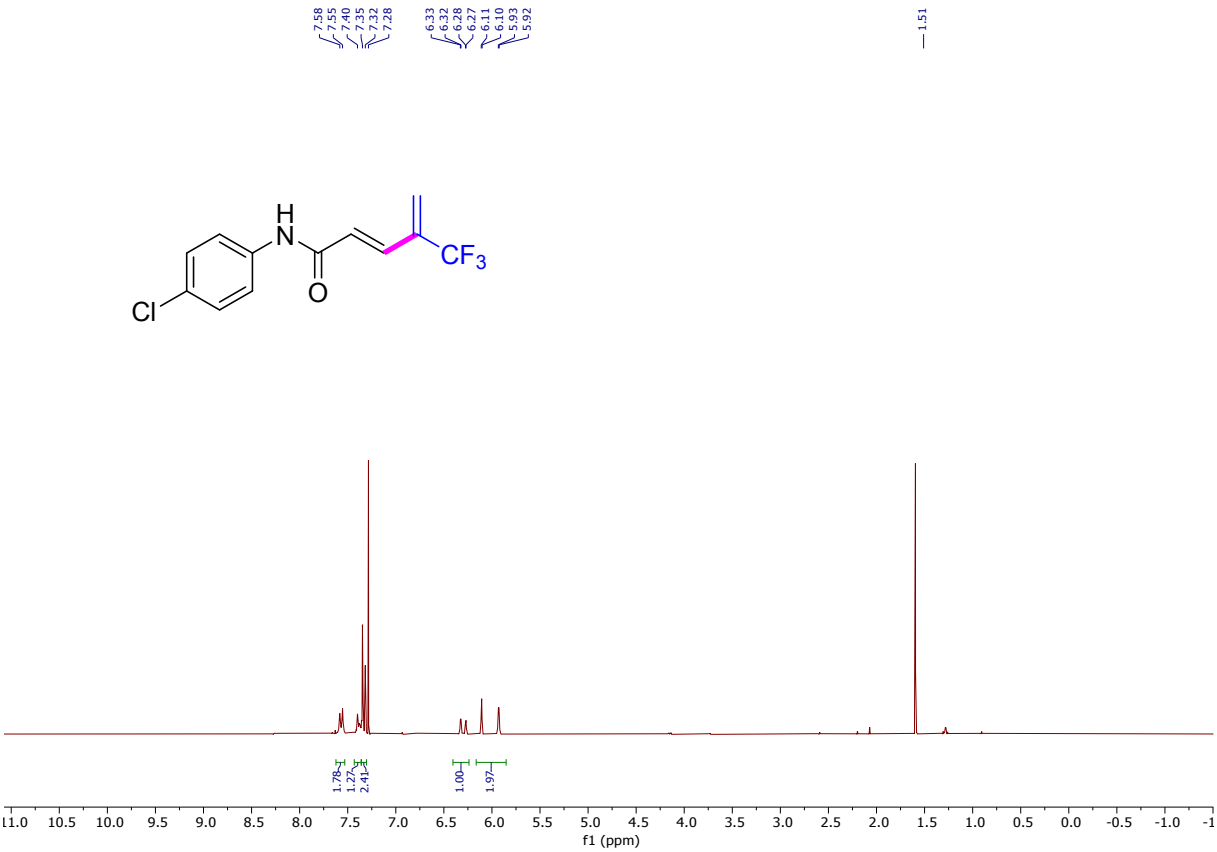
f1 (ppm)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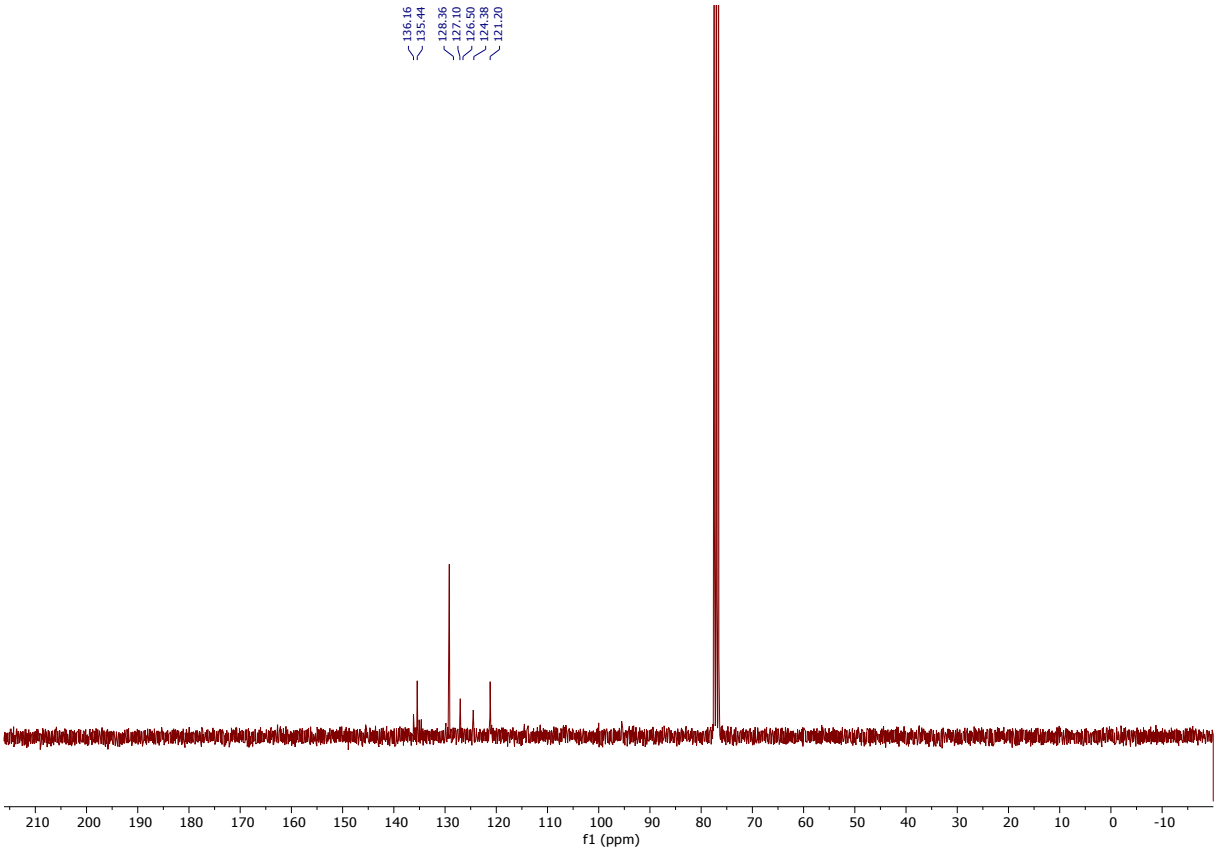
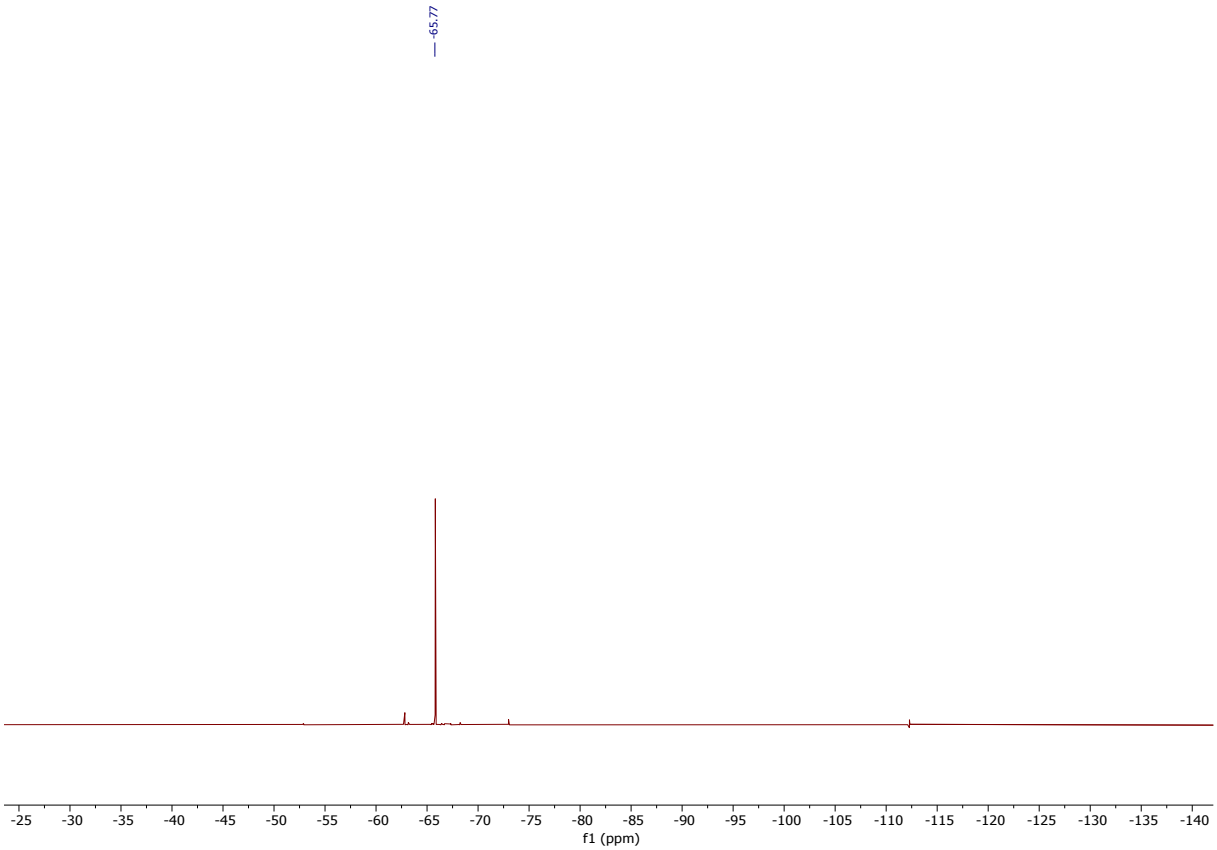
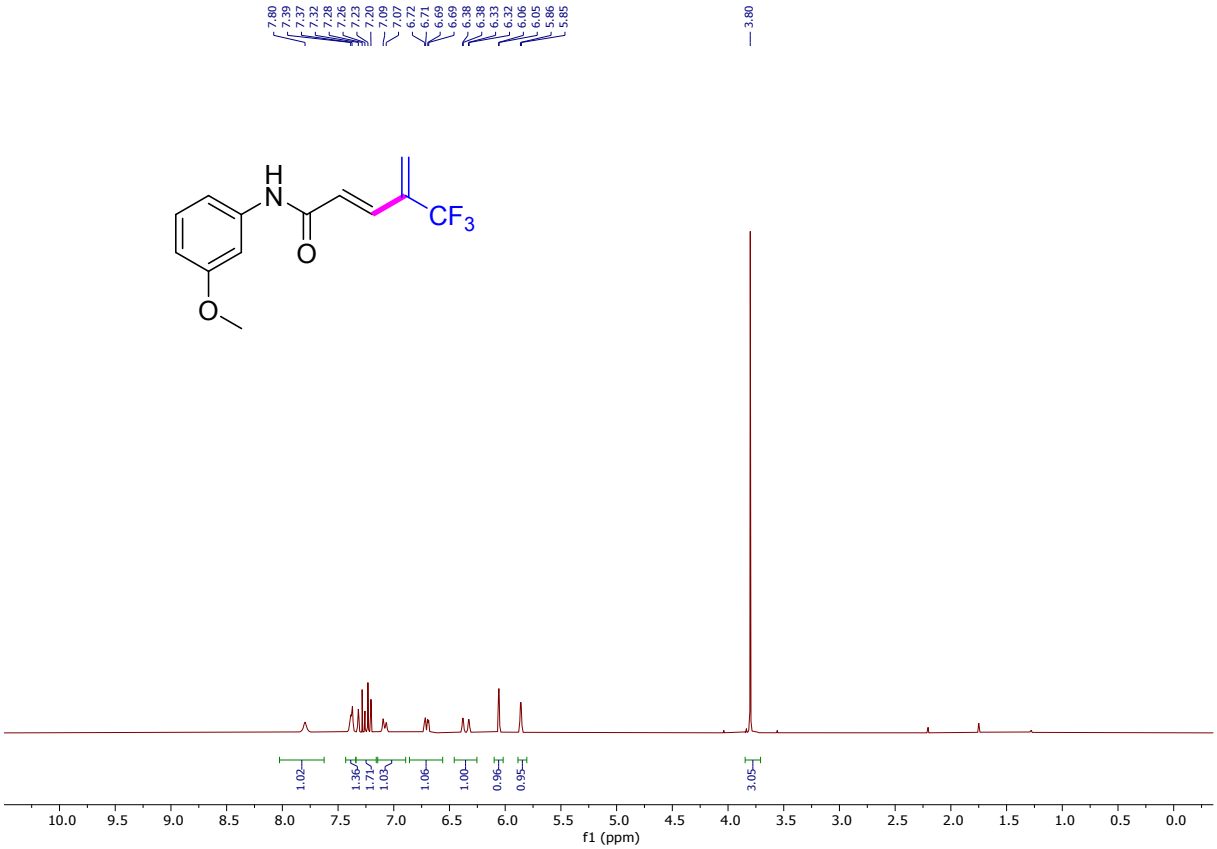
7.35
7.32
7.28
6.33
6.32
6.28
6.27
6.11
6.10
5.93
5.92
1.51
H
N
O
Cl
CF3
1.78
1.27
2.41
1.00
1.97
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1
f1 (ppm)


136.16
135.44
128.36
127.10
126.50
124.38
121.20
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


-65.77
-25 -30 -35 -40 -45 -50 -55 -60 -65 -70 -75 -80 -85 -90 -95 -100 -105 -110 -115 -120 -125 -130 -135 -140
f1 (ppm)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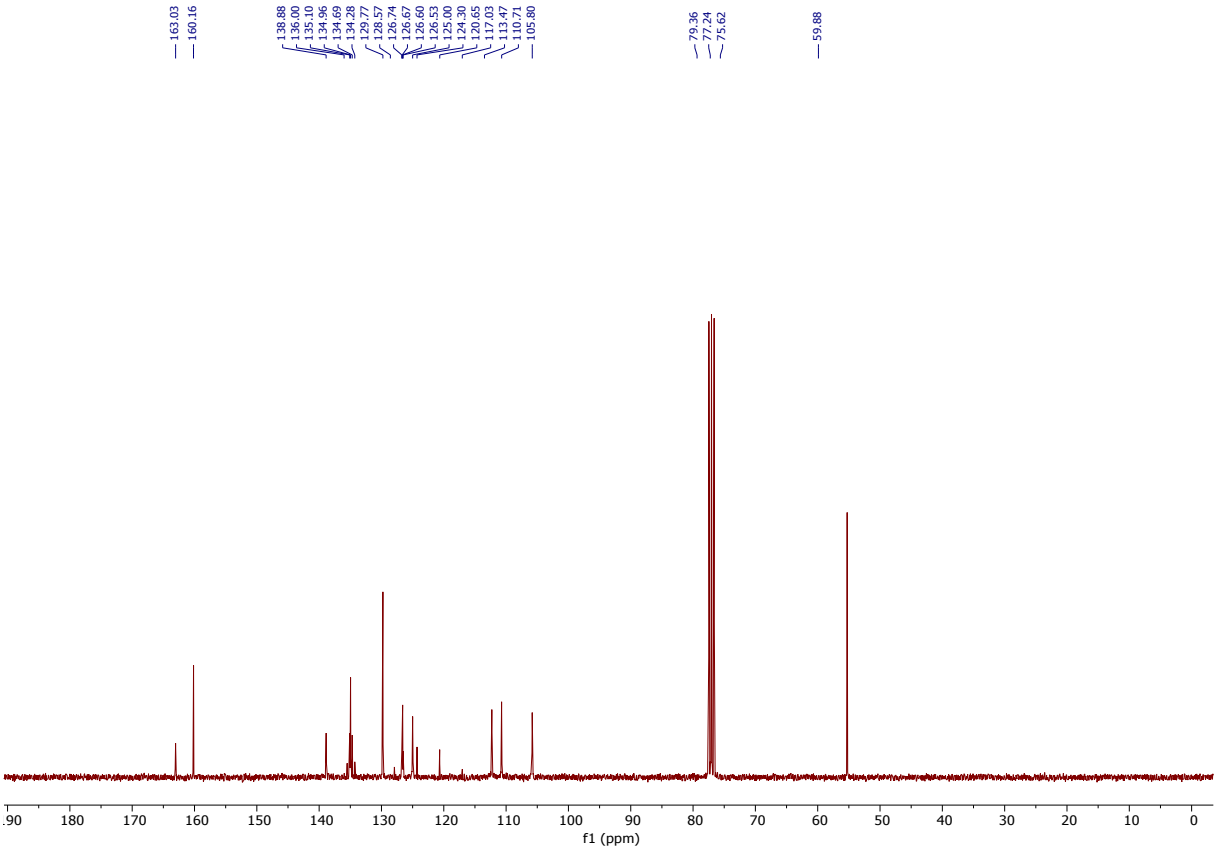
7.28
7.26
7.23
7.20
7.09
7.07
6.72
6.71
6.69
6.69
6.38
6.38
6.33
6.32
6.06
6.05
5.86
5.85
3.80
H
N
O
CF3
O
1.02
1.36
1.71
1.03
1.06
1.00
0.96
0.95
3.05
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


163.03
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134.96
134.69
134.28
129.77
128.57
126.74
126.67
126.60
126.53
125.00
124.30
120.65
117.03
113.47
110.71
105.80
79.36
77.24
75.62
59.88
190
180
170
160
150
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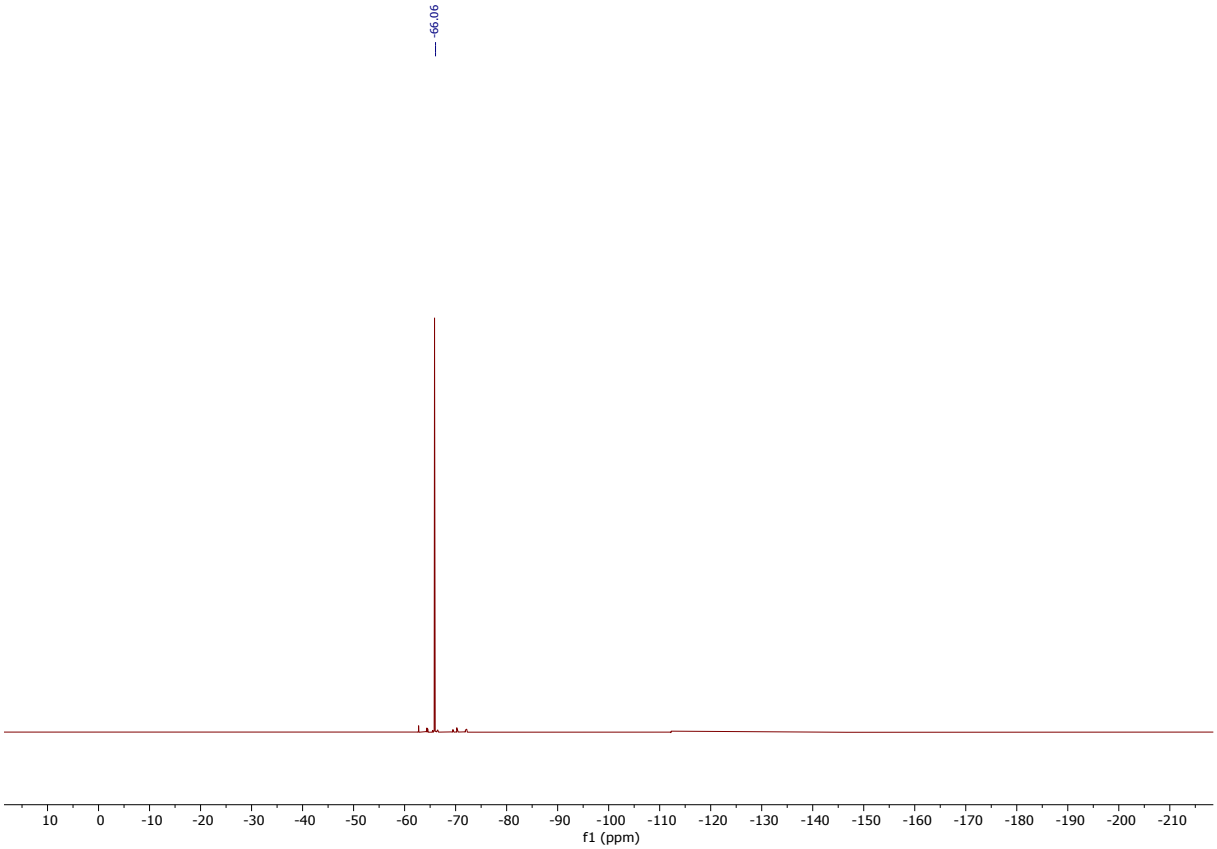
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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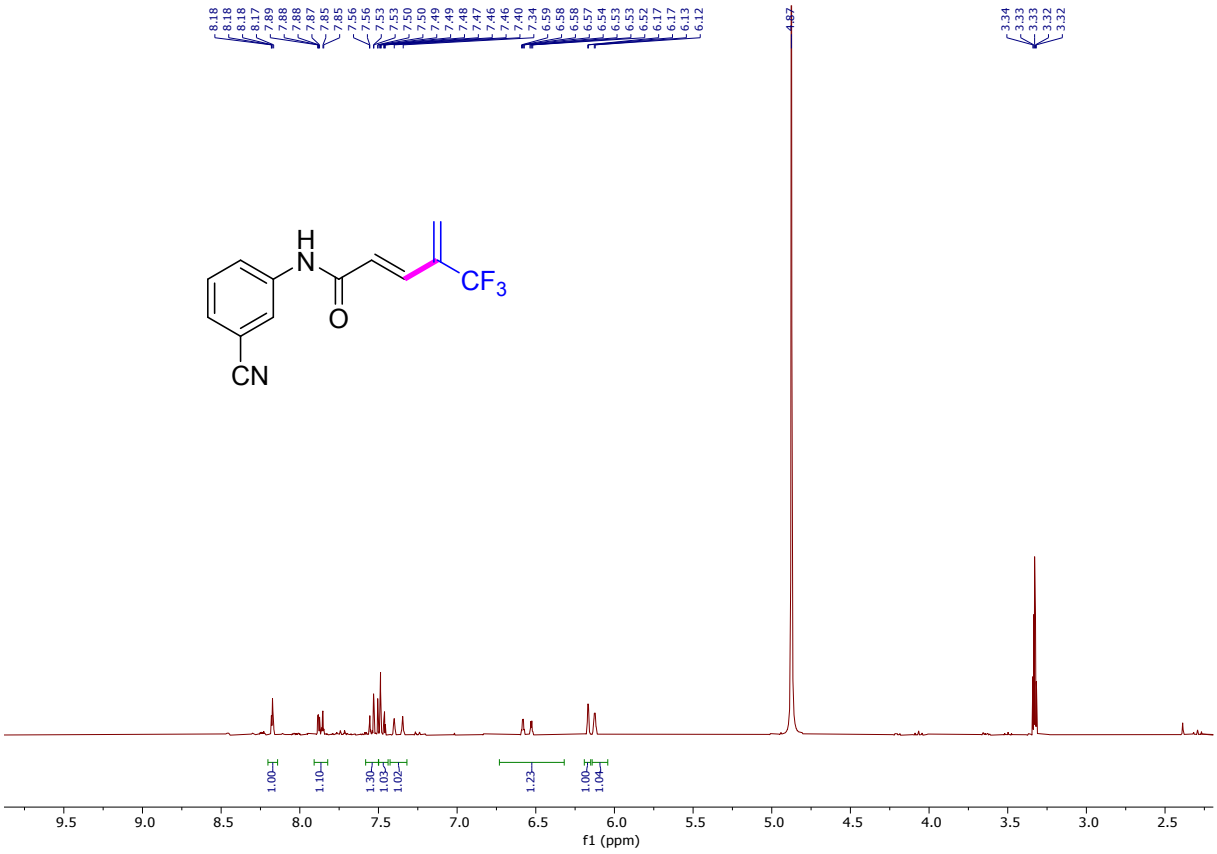
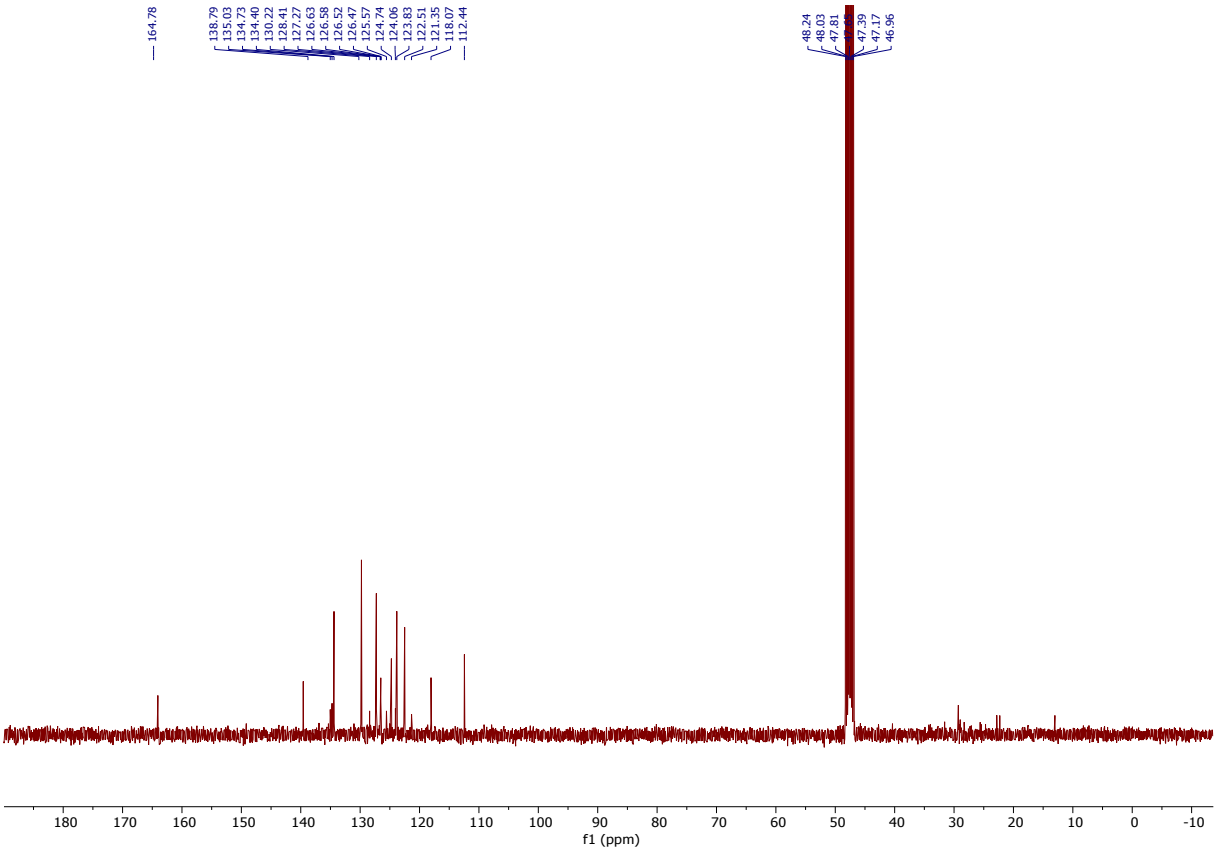
f1 (ppm)


8.18 8.18 8.18 8.17 7.89 7.88 7.88 7.87 7.85 7.85 7.56 7.56 7.53 7.53 7.50 7.50 7.49 7.49 7.48 7.47 7.46 7.46 7.40 7.34 6.59 6.58 6.58 6.57 6.54 6.53 6.52 6.17 6.17 6.13 6.12
4.87
3.34 3.33 3.33 3.32 3.32
H
N
O
CF3
CN
1.00 1.10 1.30 1.03 1.02 1.23 1.00 1.04
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
f1 (ppm)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124.74
124.06
123.83
122.51
121.35
118.07
112.44
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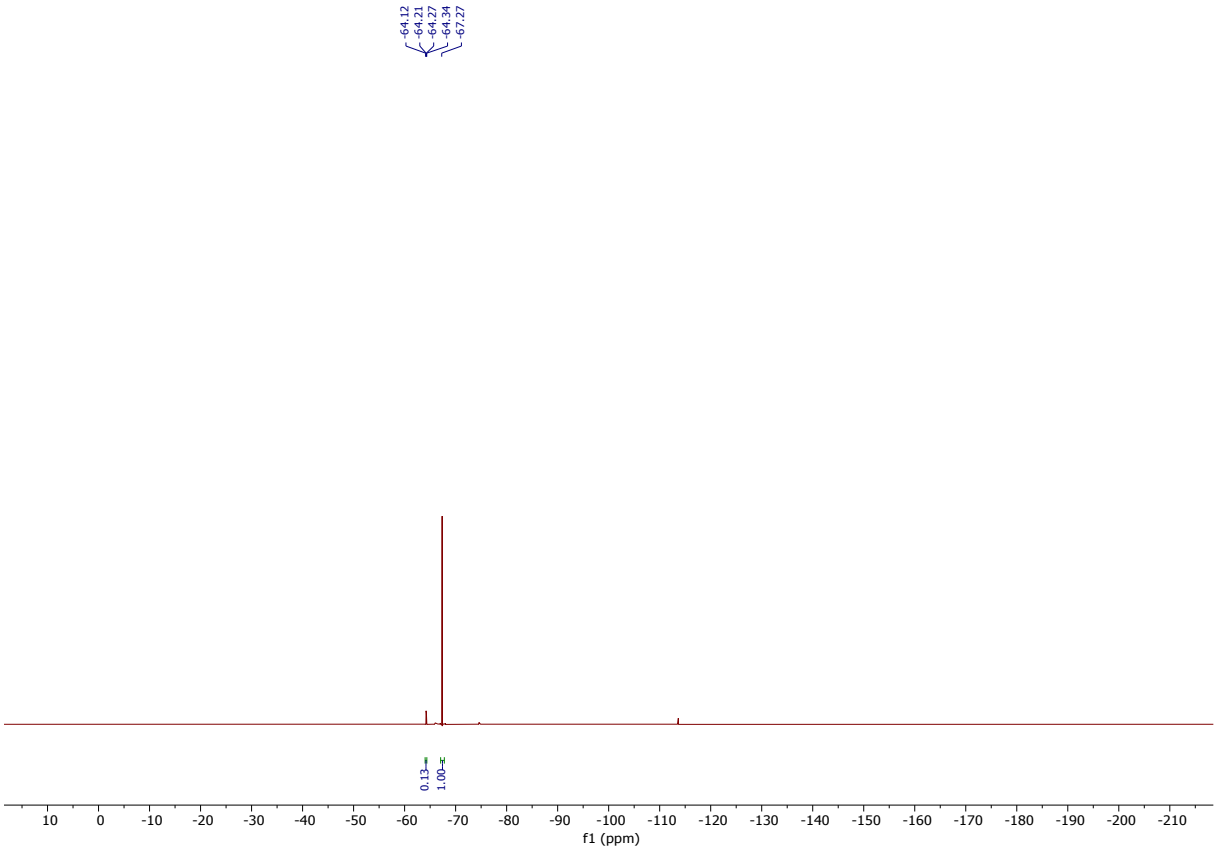
47.39
47.17
46.96
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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-64.27
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1.00
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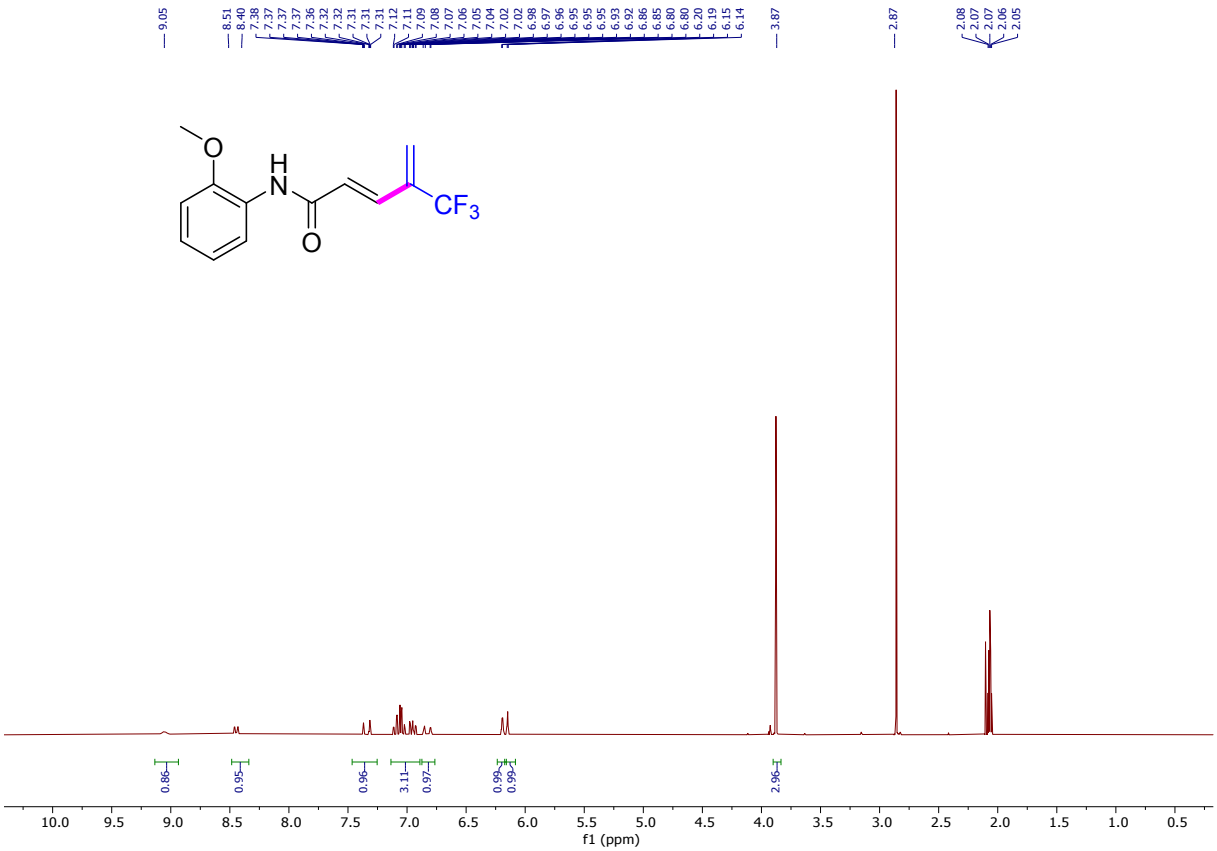
f1 (ppm)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7.08
7.07
7.06
7.05
7.04
7.02
7.02
6.98
6.97
6.96
6.95
6.95
6.93
6.92
6.86
6.85
6.80
6.80
6.20
6.19
6.15
6.14
3.87
2.87
2.08
2.07
2.07
2.06
2.05
O
H
N
O
CF3
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0.95
0.96
3.11
0.97
0.99
0.99
2.96
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
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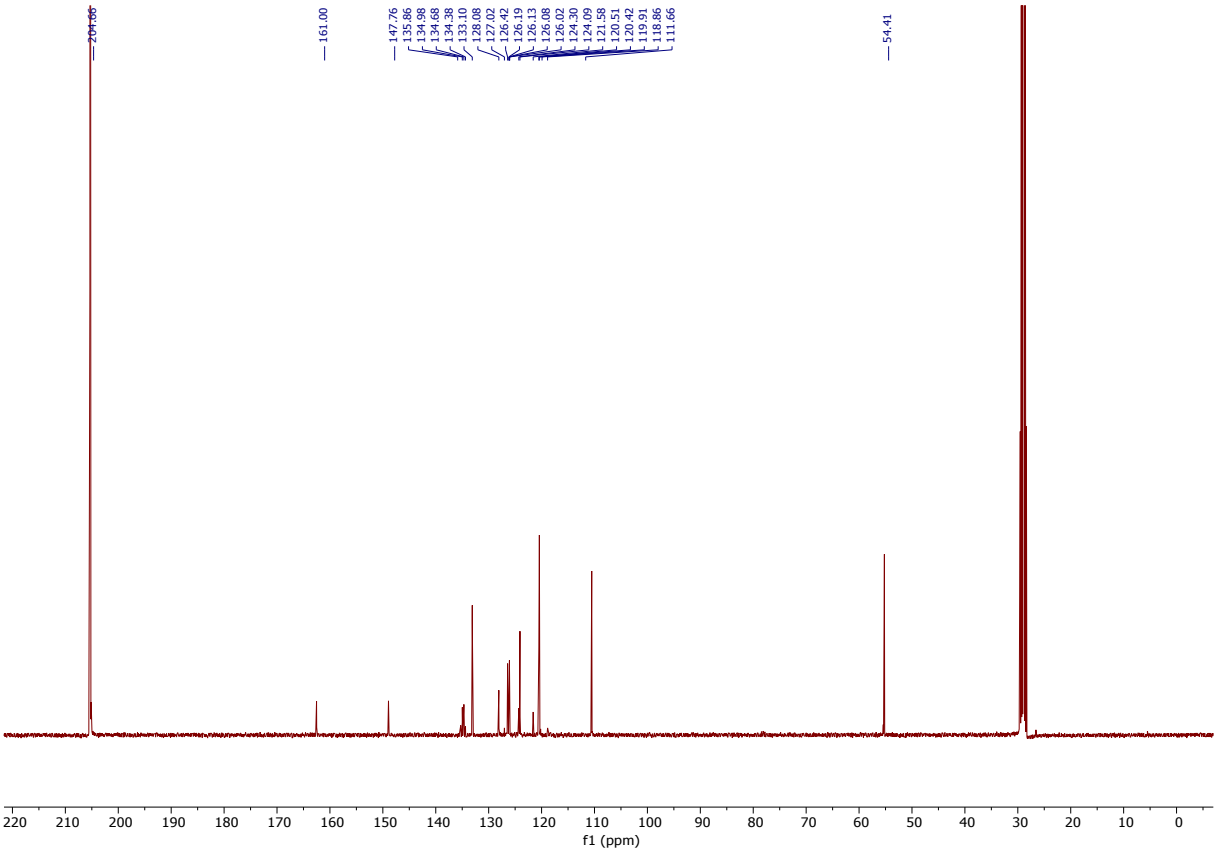
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)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120.42
119.91
118.86
111.66
54.41
220
210
200
190
180
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90
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70
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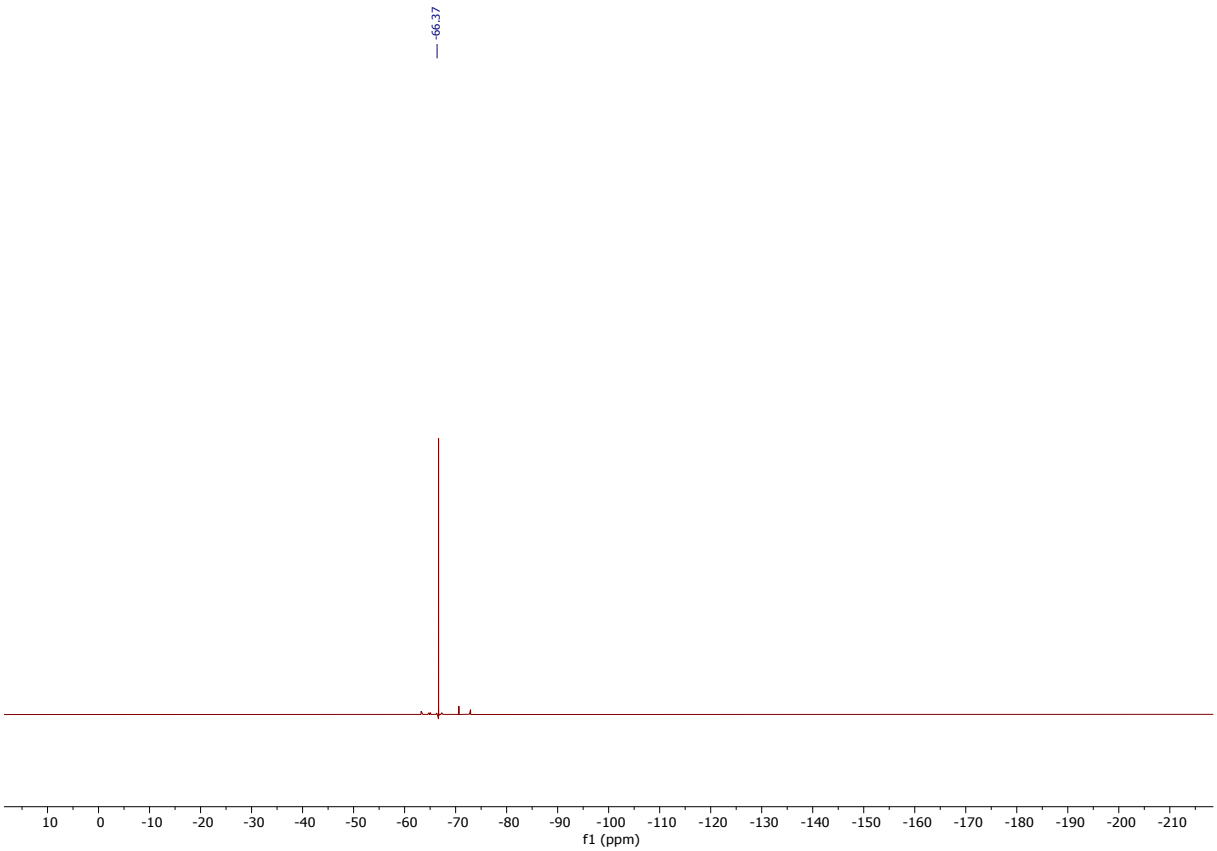
50
40
30
20
10
0
f1 (ppm)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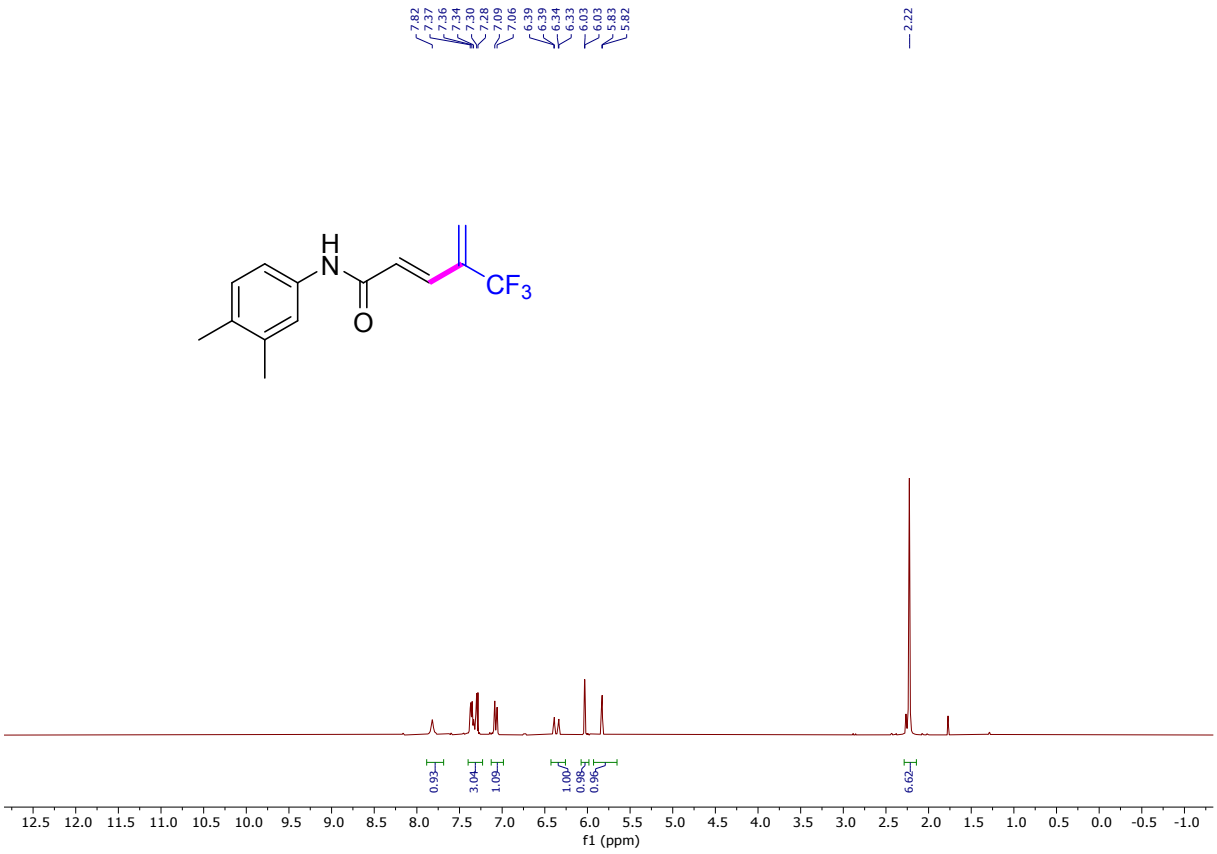
f1 (ppm)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6.34
6.33
6.03
6.03
5.83
5.82
2.22
H
N
O
CF3
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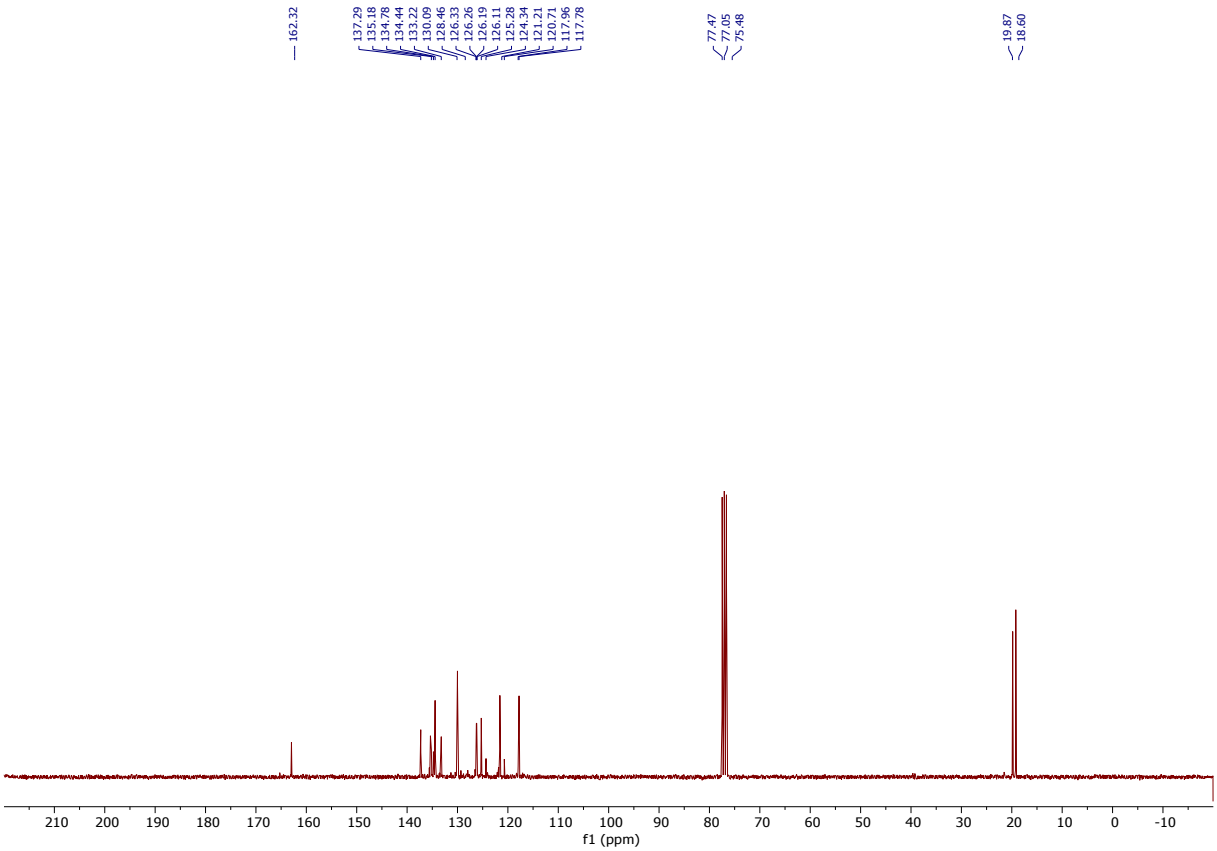
3.04
1.09
1.00
0.98
0.96
6.62
12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)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120.71
117.96
117.78
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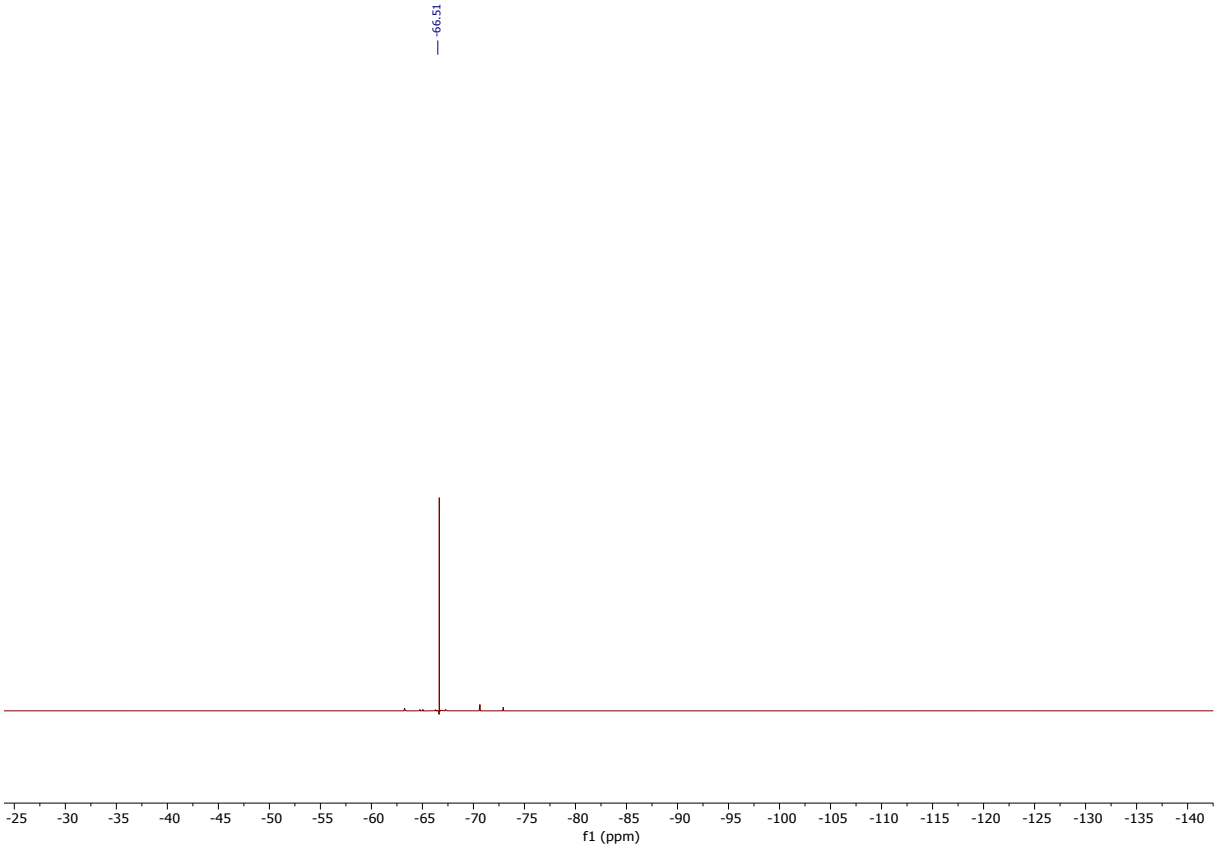
75.48
19.87
18.60
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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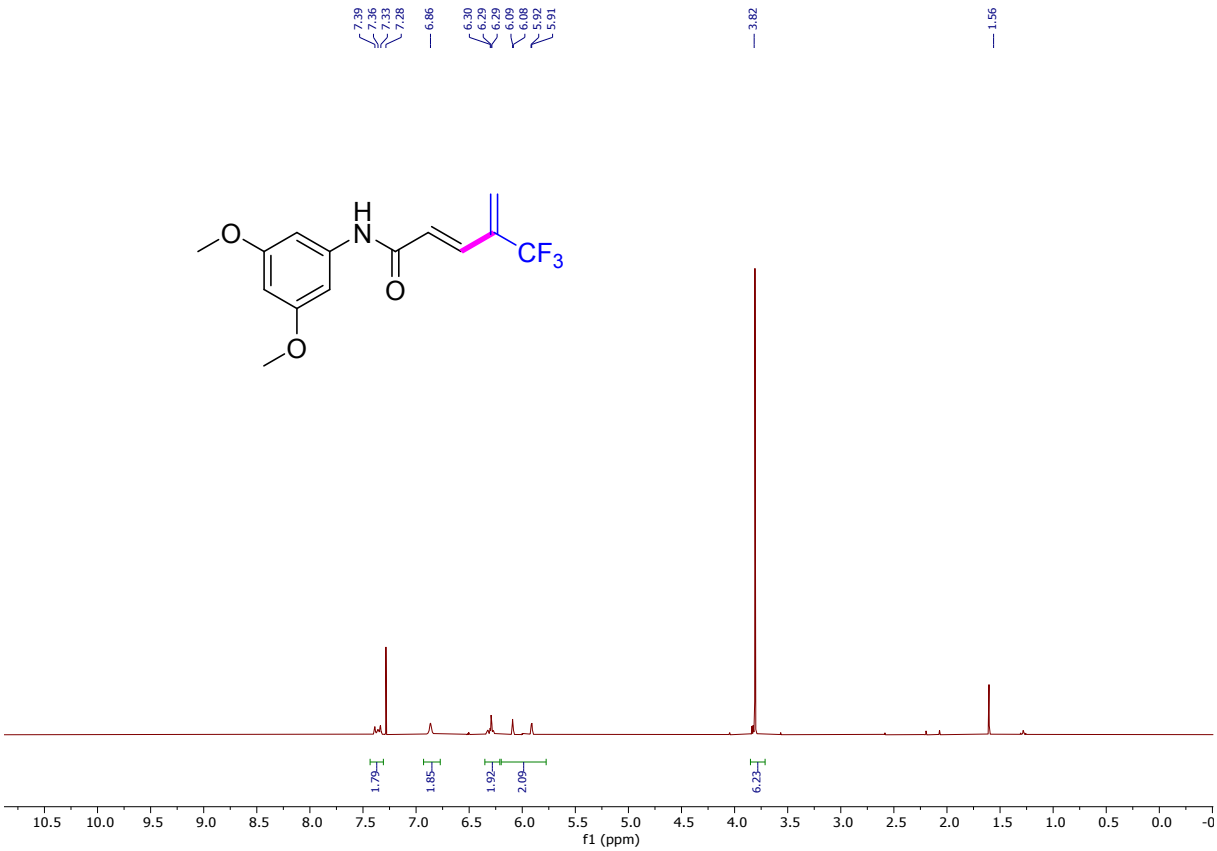
f1 (ppm)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5.91
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1.56
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O
O
O
CF3
1.79
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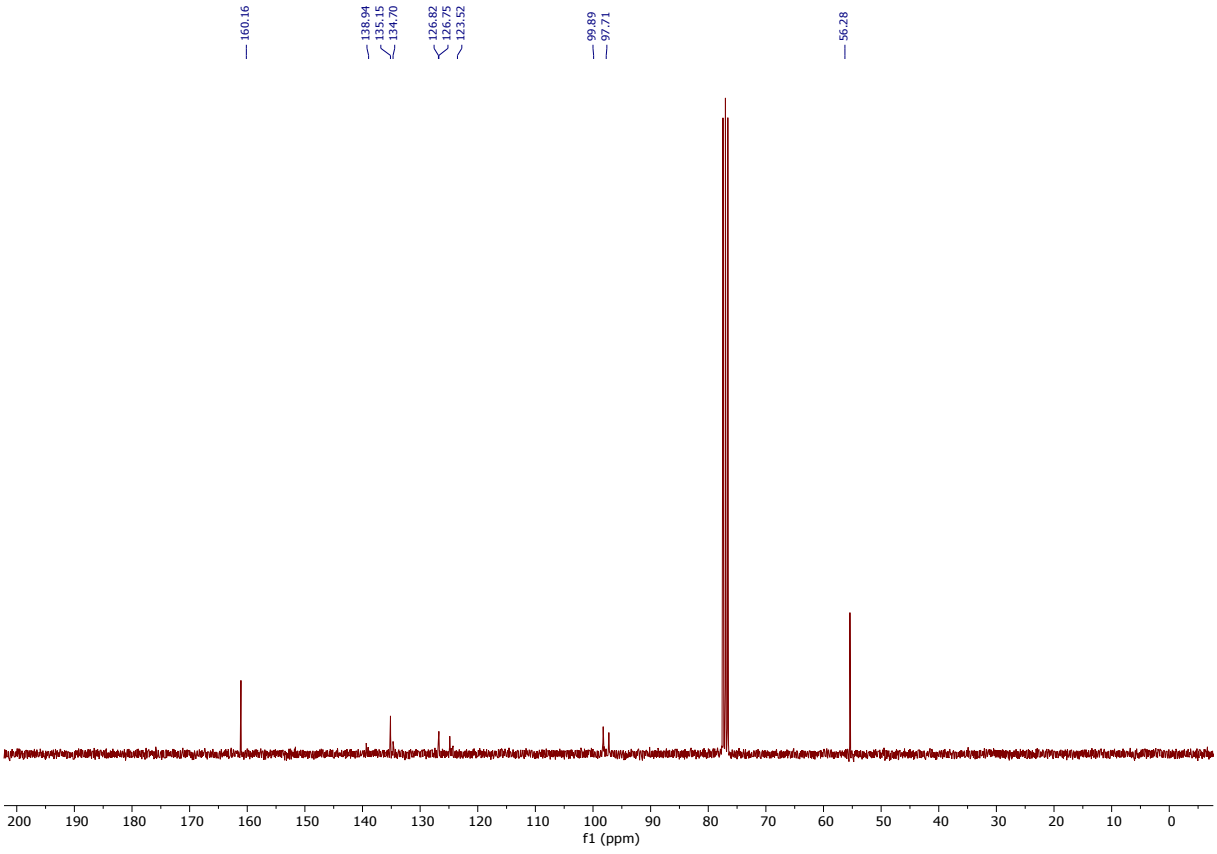
1.92
2.09
6.23
f1 (ppm)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99.89
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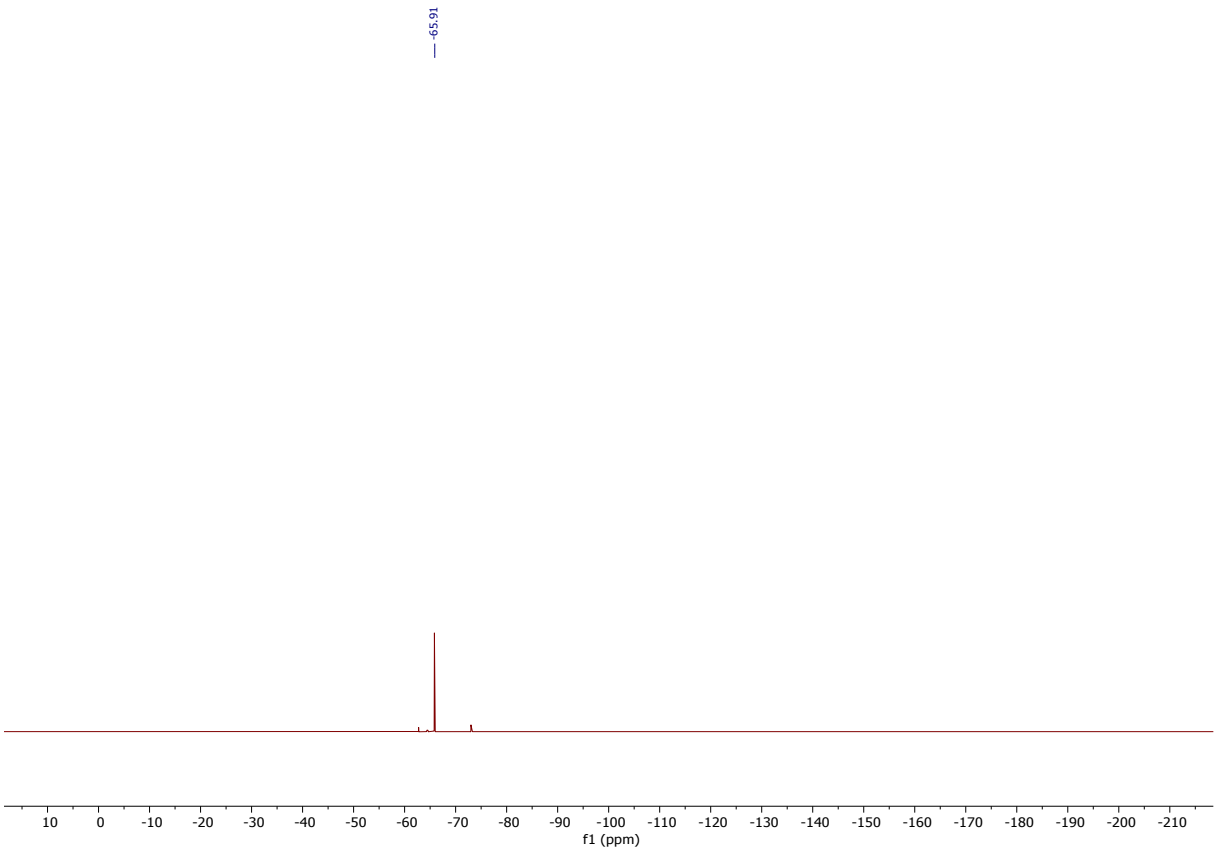
56.28
f1 (ppm)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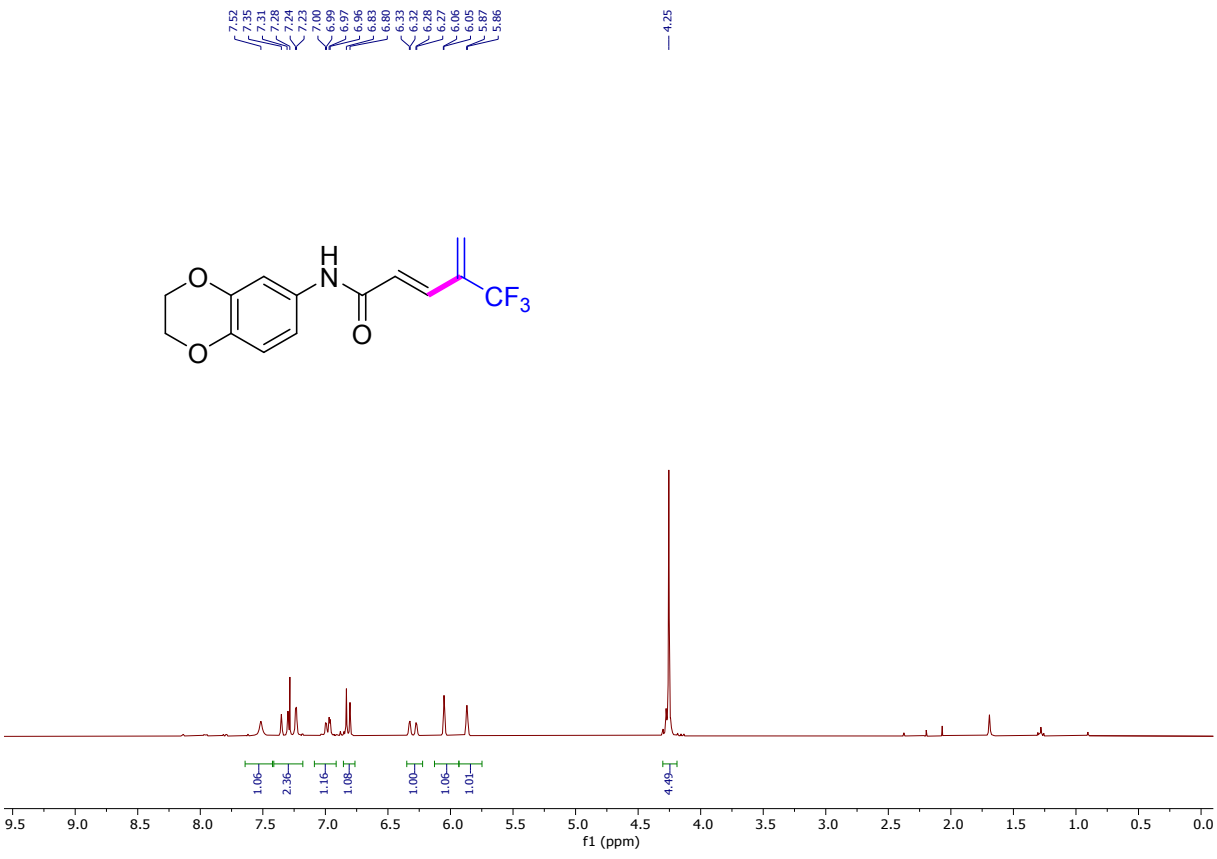
f1 (ppm)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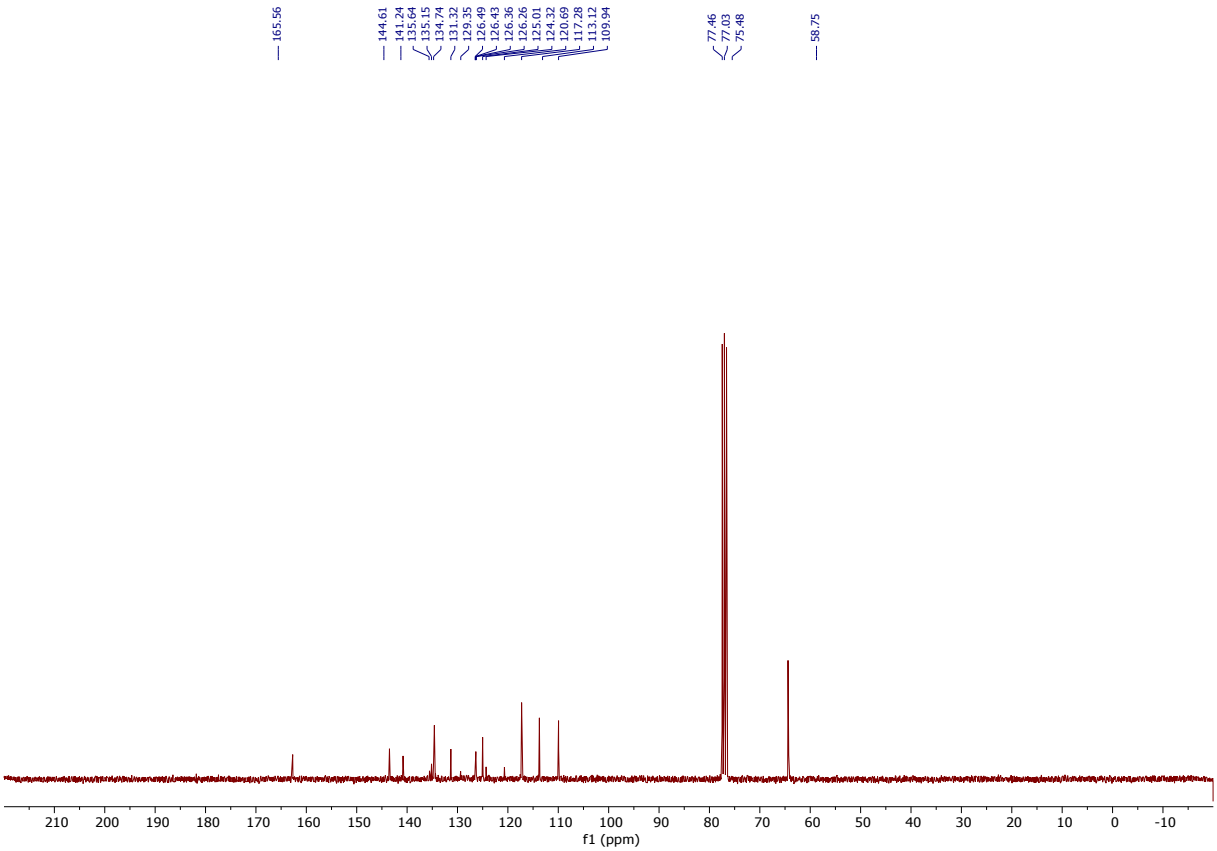
6.28
6.27
6.06
6.05
5.87
5.86
4.25
H
N
O
O
O
CF3
1.06
2.36
1.16
1.08
1.00
1.06
1.01
4.49
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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113.12
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77.03
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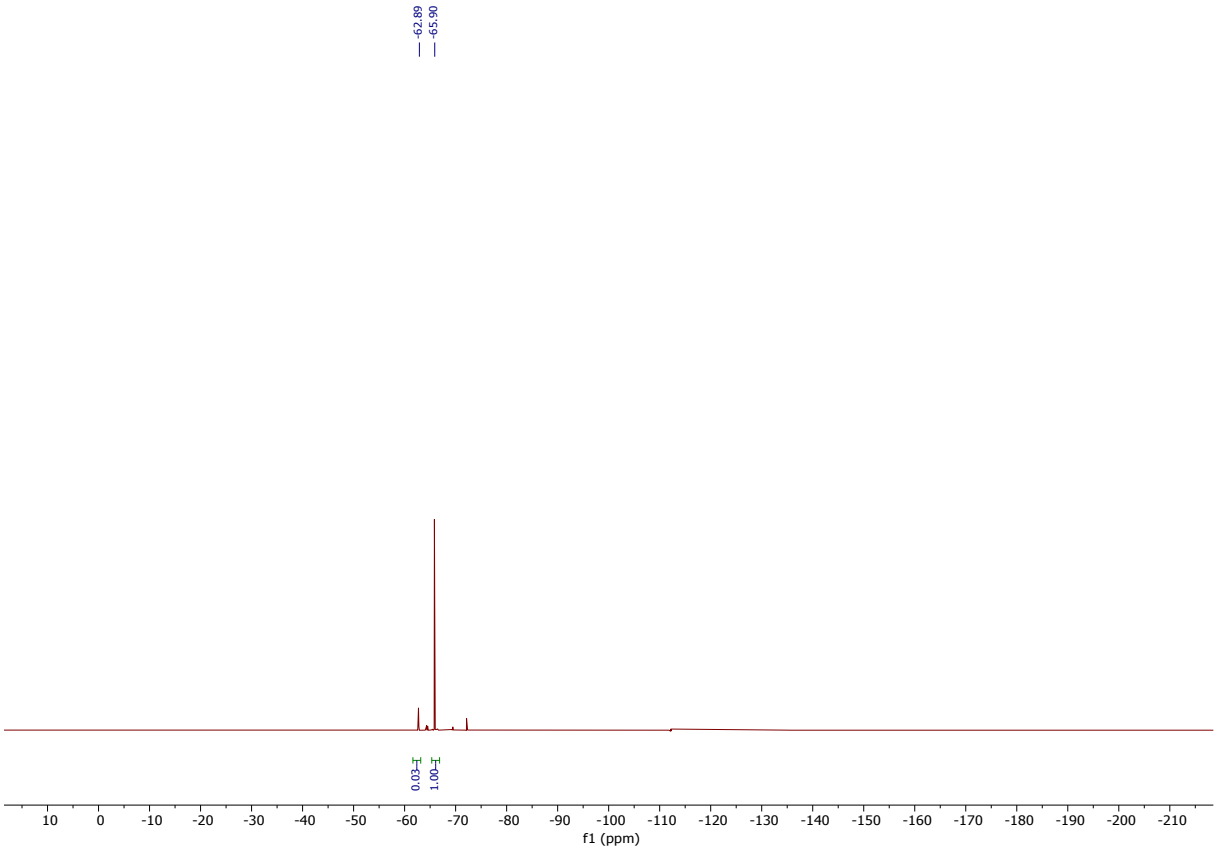
58.75
f1 (ppm)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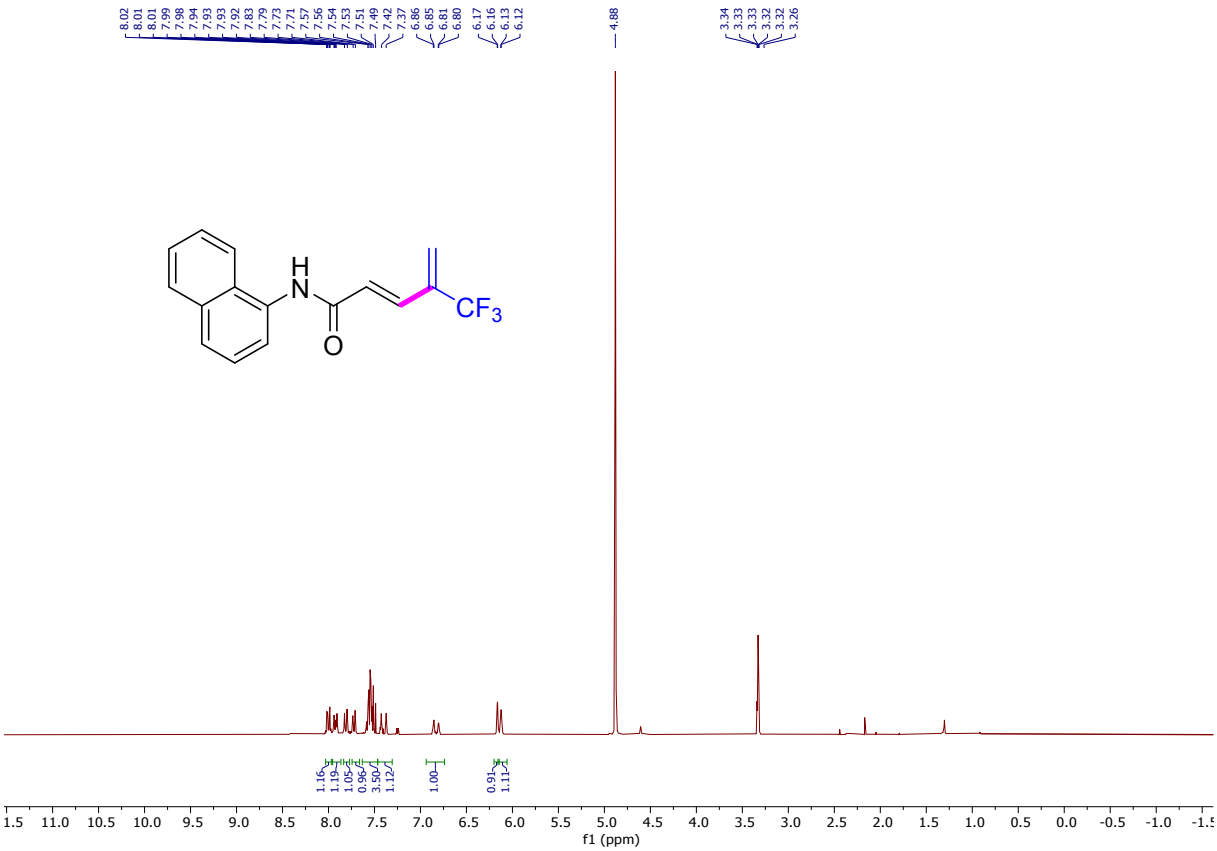
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7.79
7.73
7.71
7.57
7.56
7.54
7.53
7.51
7.49
7.42
7.37
6.86
6.85
6.81
6.80
6.17
6.16
6.13
6.12
4.88
3.34
3.33
3.33
3.32
3.32
3.26
H
N
O
CF3
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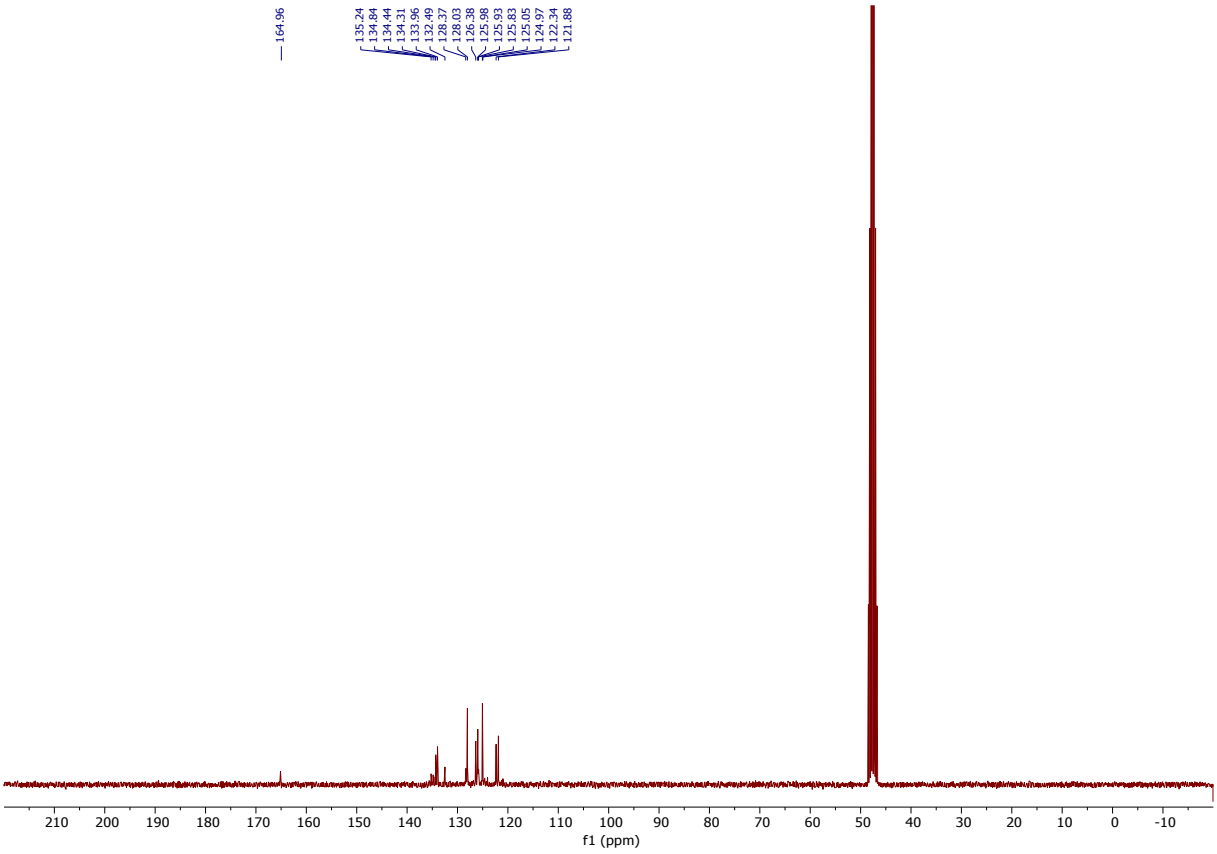
1.19
1.05
0.96
3.50
1.12
1.00
0.91
1.11
f1 (ppm)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134.44
134.31
133.96
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128.37
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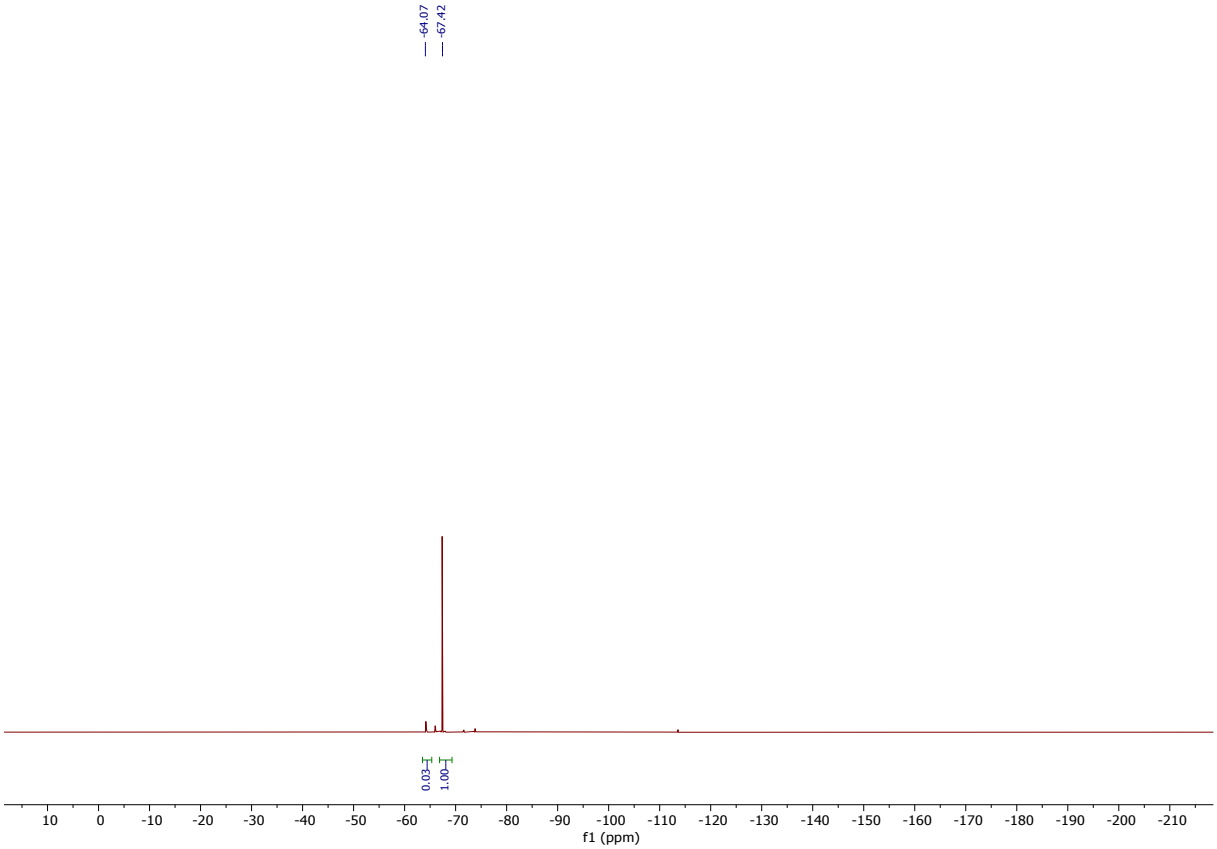
126.38
125.98
125.93
125.83
125.05
124.97
122.34
121.88
f1 (ppm)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-67.42
0.03
1.00
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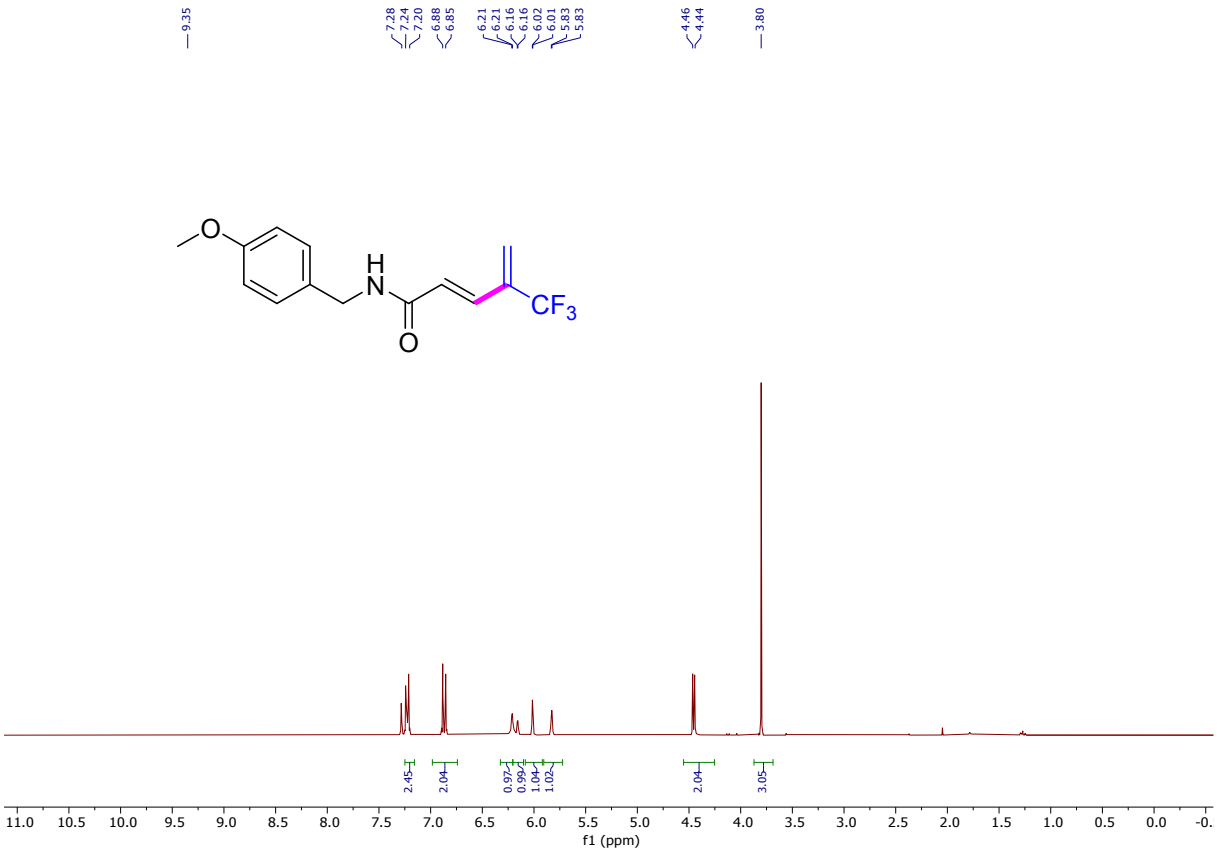
f1 (ppm)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7.28
7.24
7.20
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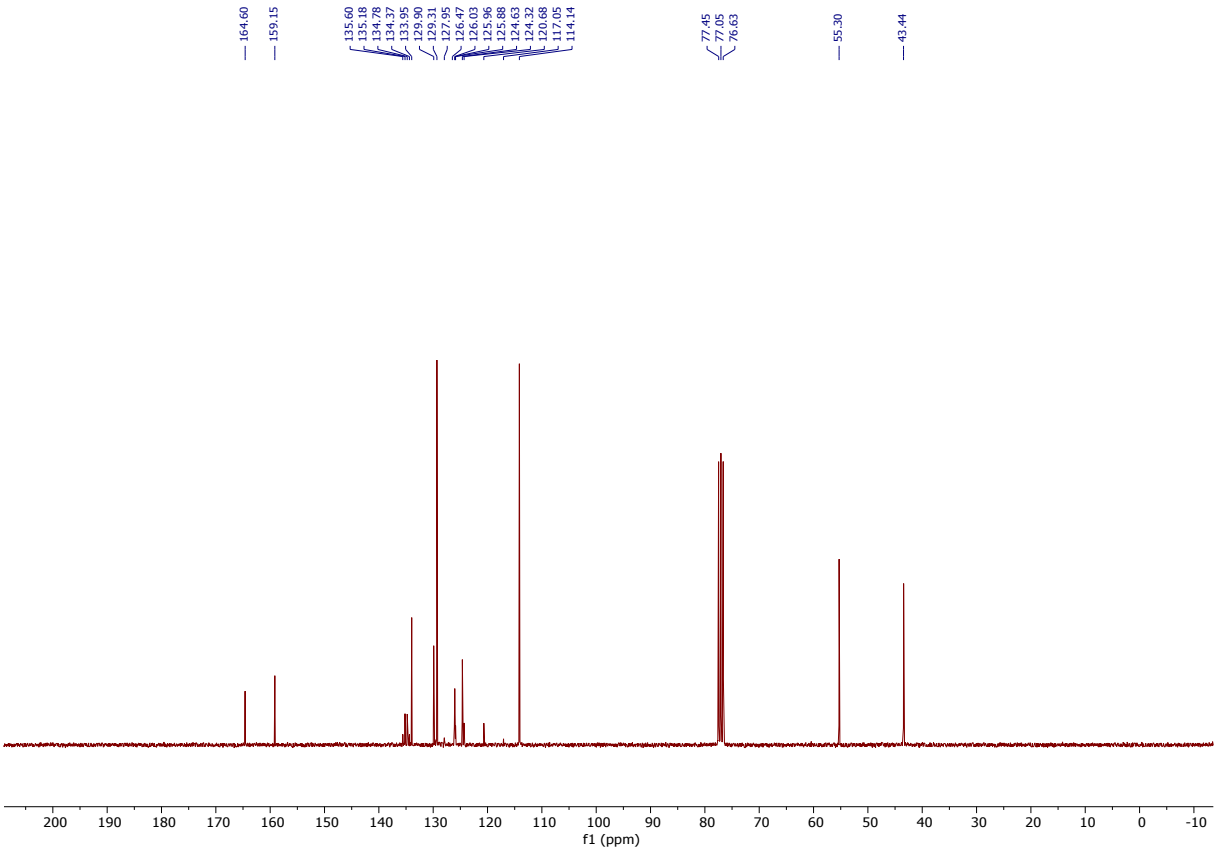
6.85
6.21
6.21
6.16
6.16
6.02
6.01
5.83
5.83
4.46
4.44
3.80
O
H
N
O
CF3
2.45
2.04
0.97
0.99
1.04
1.02
2.04
3.05
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.
f1 (ppm)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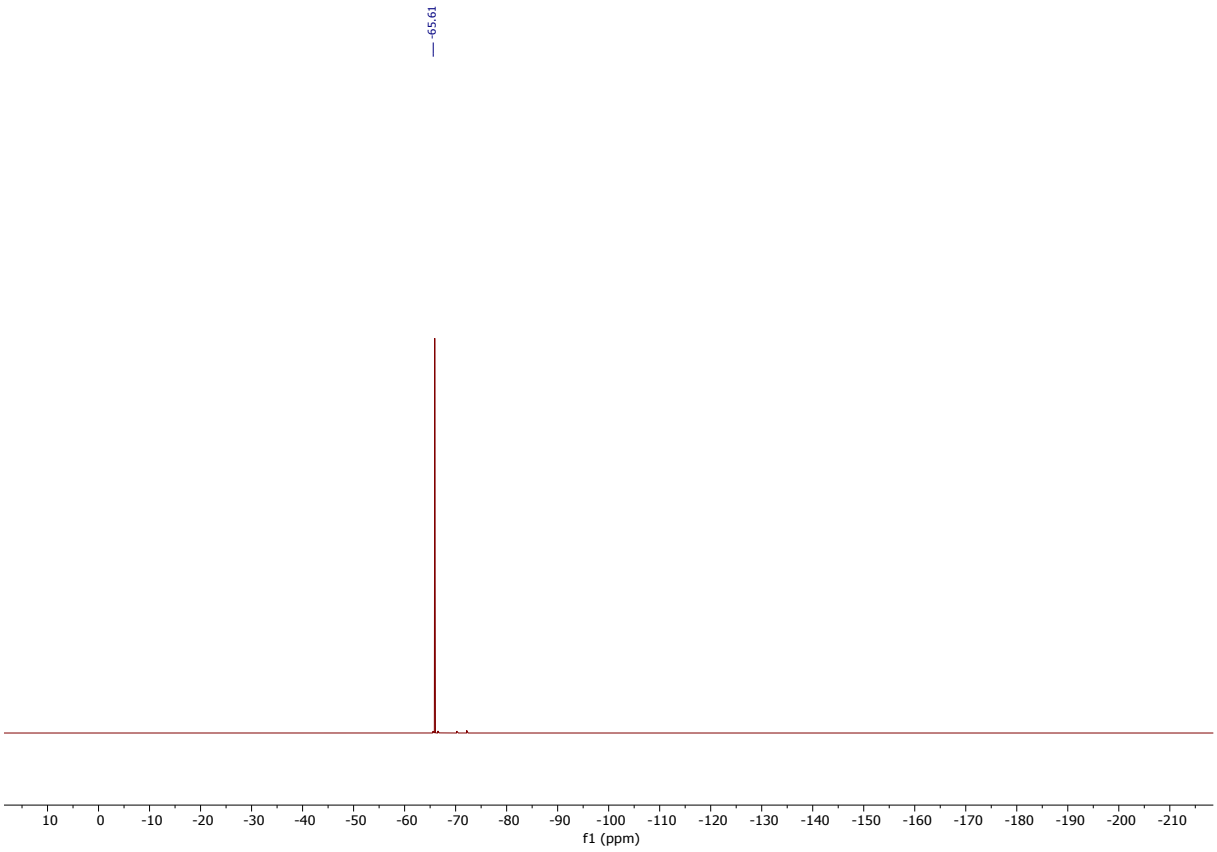
159.15
135.60
135.18
134.78
134.37
133.95
129.90
129.31
127.95
126.47
126.03
125.96
125.88
124.63
124.32
123.68
117.05
114.14
77.45
77.05
76.63
55.30
43.44
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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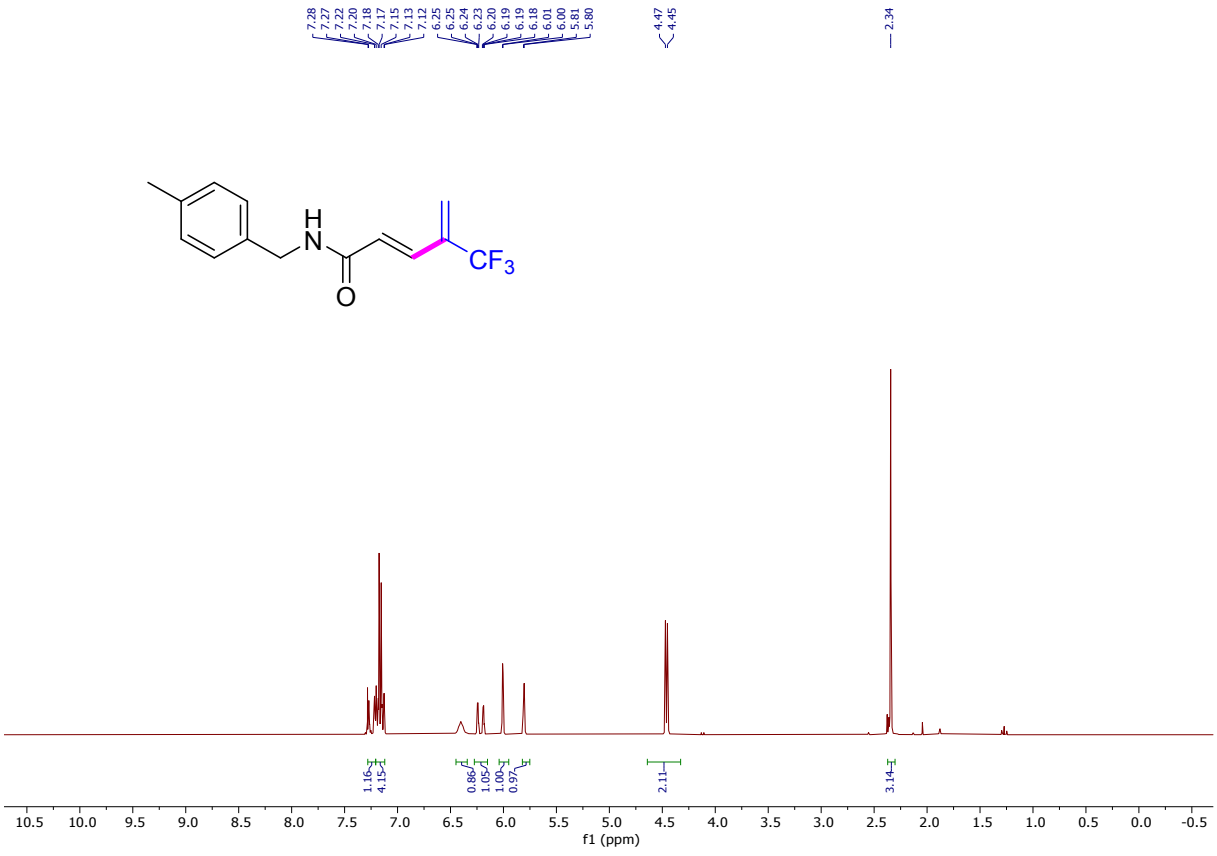
f1 (ppm)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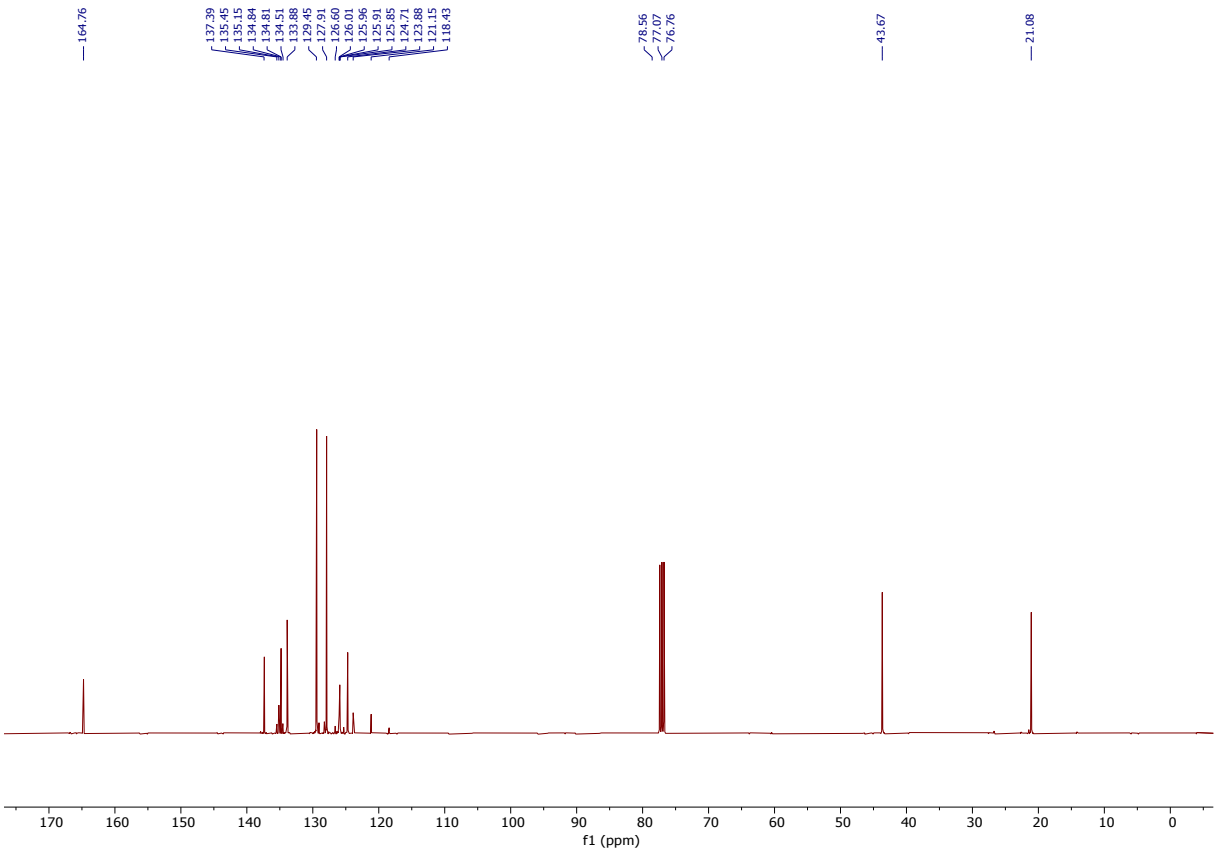
7.27
7.22
7.20
7.18
7.17
7.15
7.13
7.12
6.25
6.25
6.24
6.23
6.20
6.19
6.19
6.18
6.01
6.00
5.81
5.80
4.47
4.45
2.34
H
N
O
CF3
1.16
4.15
0.86
1.05
1.00
0.97
2.11
3.14
f1 (ppm)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137.39
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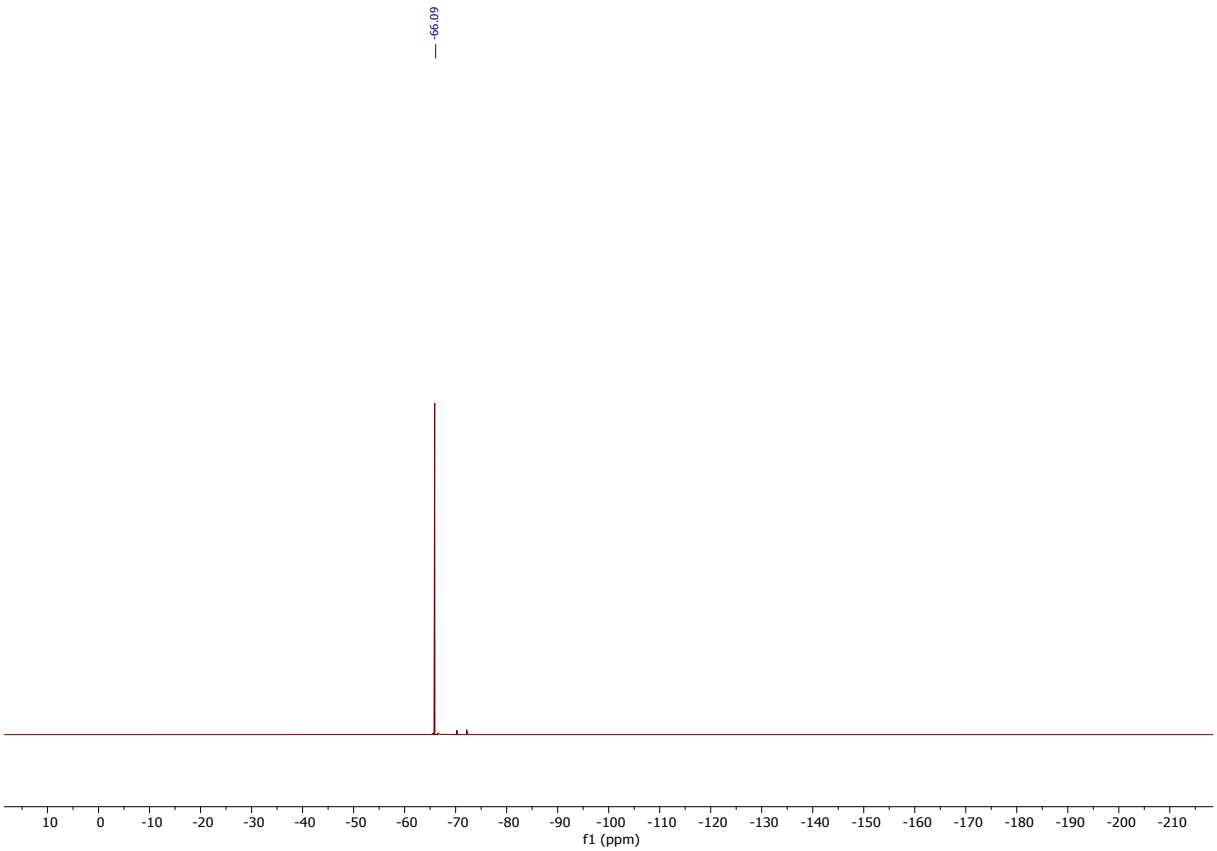
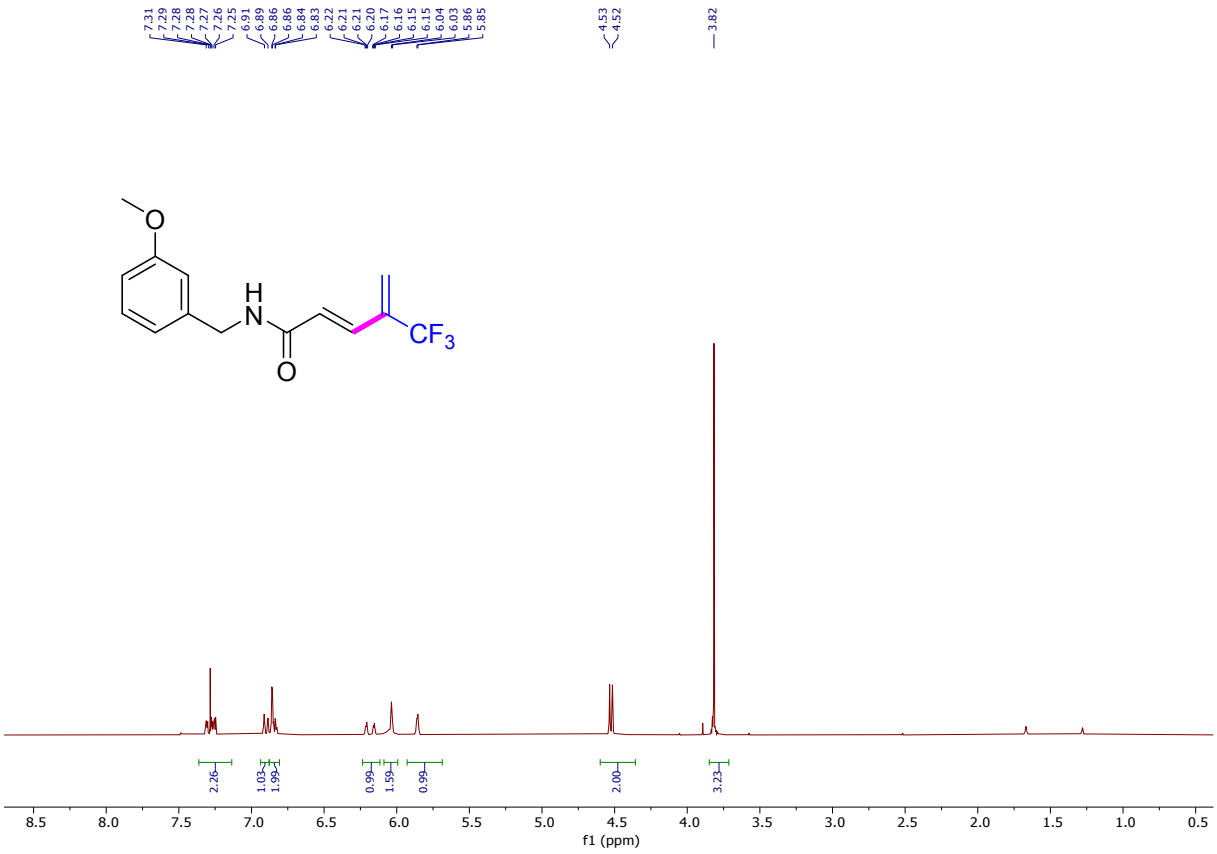
135.15
134.84
134.81
134.51
133.88
129.45
127.91
126.60
126.01
125.96
125.91
125.85
124.71
123.88
121.15
118.43
78.56
77.07
76.76
43.67
21.08
f1 (ppm)


-66.09
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)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7.27
7.26
7.25
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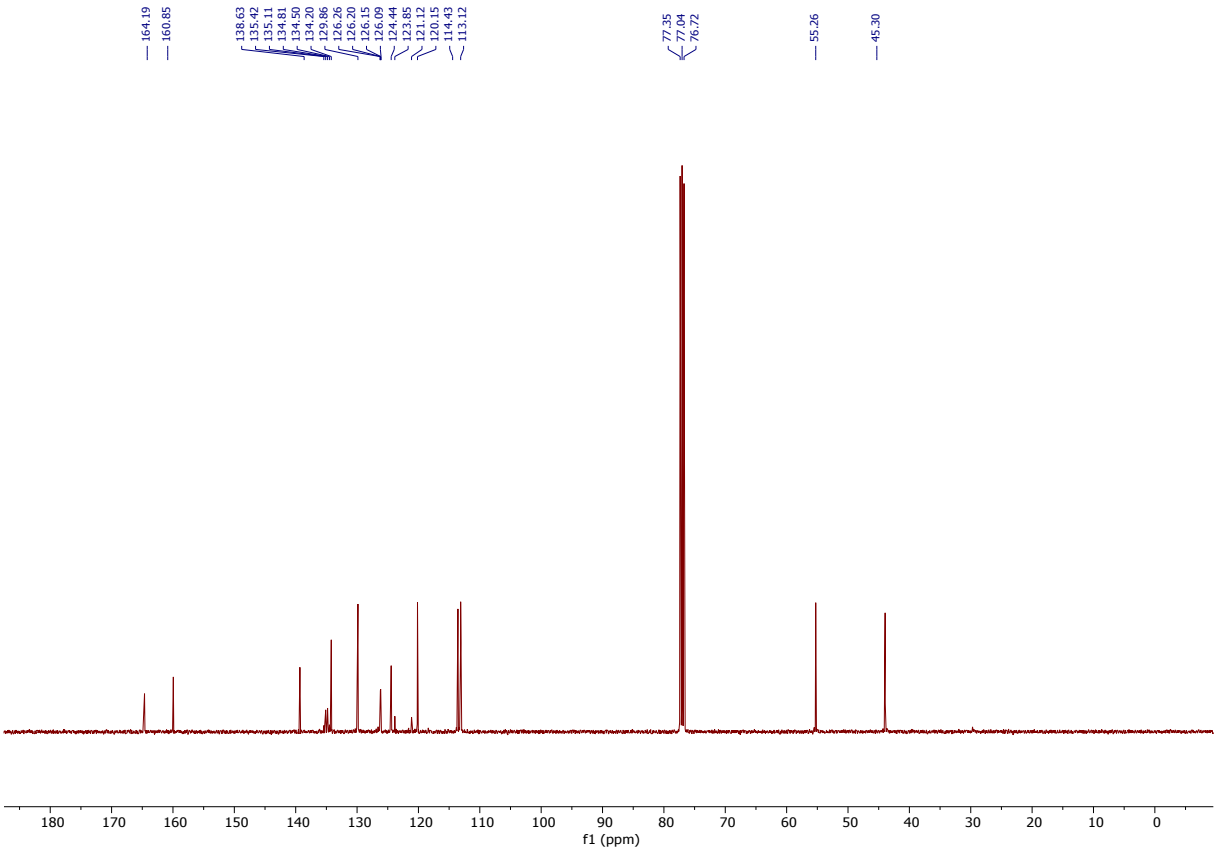
6.89
6.86
6.86
6.84
6.83
6.22
6.21
6.21
6.20
6.17
6.16
6.15
6.15
6.04
6.03
5.86
5.85
4.53
4.52
3.82
O
H
N
O
CF3
2.26
1.03
1.99
0.99
1.59
0.99
2.00
3.23
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)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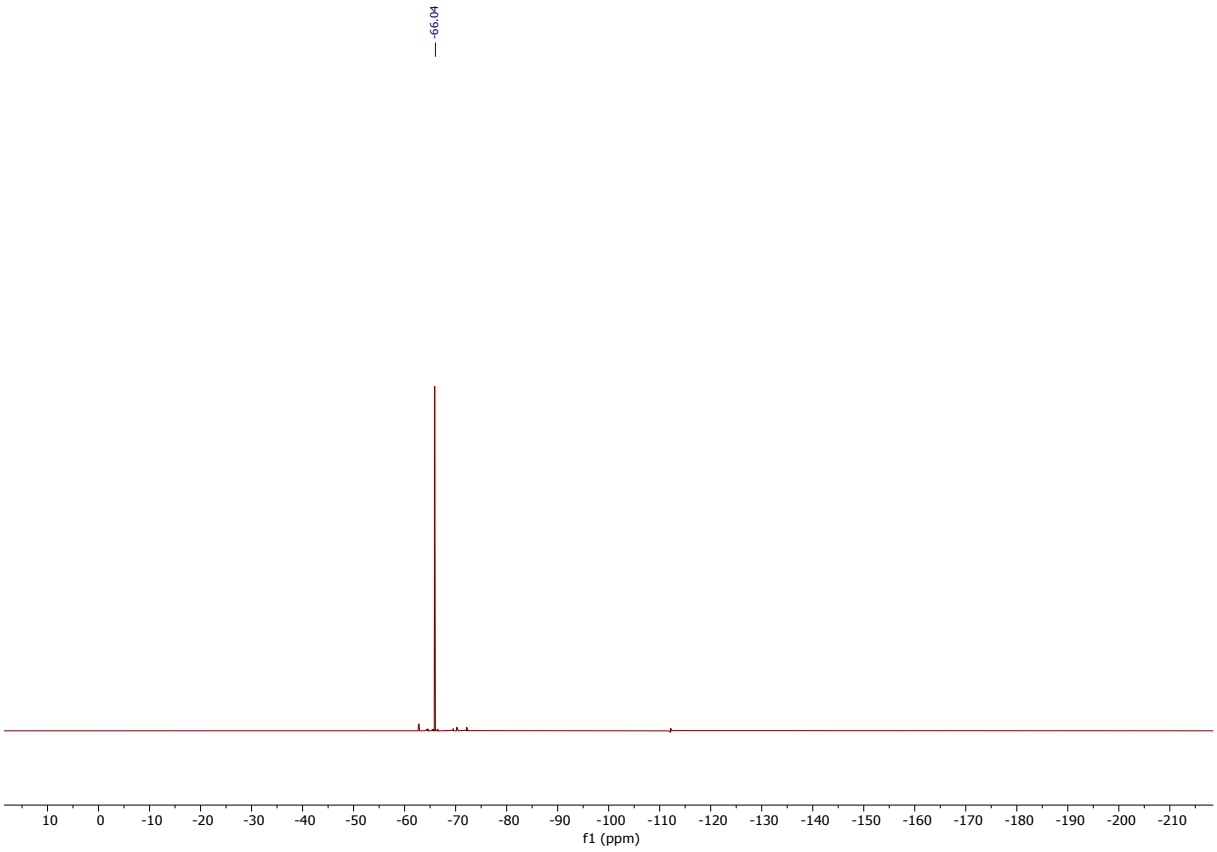
160.85
138.63
135.42
135.11
134.81
134.50
134.20
129.86
126.26
126.20
126.15
126.09
124.44
123.85
121.12
120.15
114.43
113.12
77.35
77.04
76.72
55.26
45.30
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


-66.04
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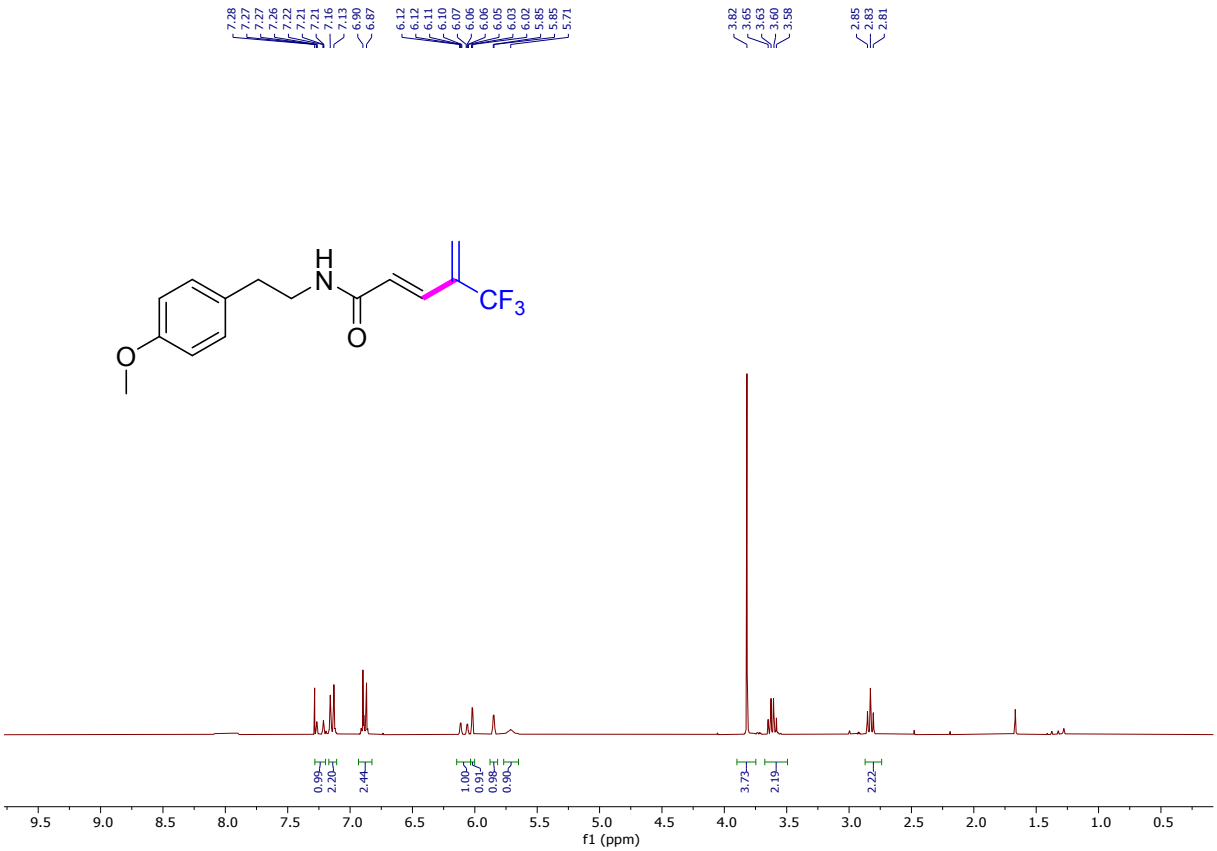
f1 (ppm)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7.27
7.27
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7.22
7.21
7.21
7.16
7.13
6.90
6.87
6.12
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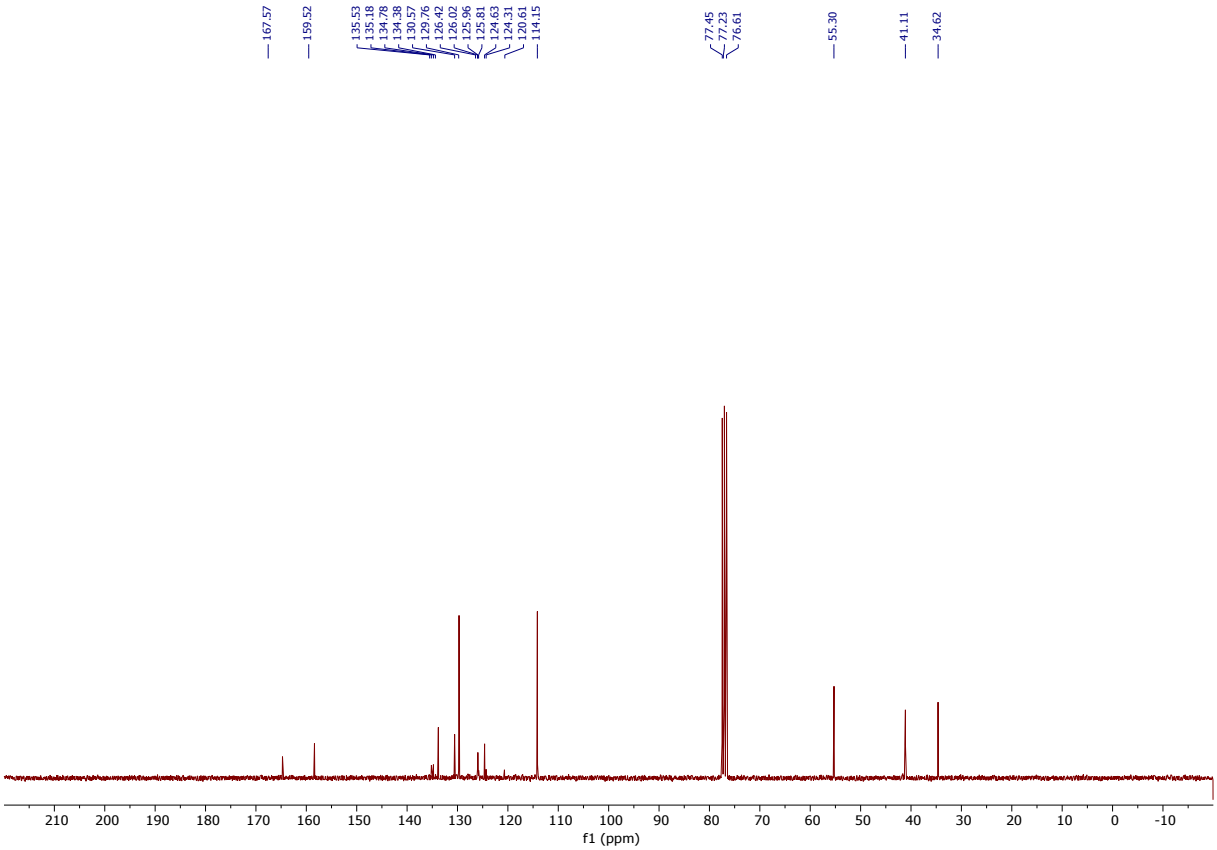
6.11
6.10
6.07
6.06
6.06
6.05
6.03
6.02
5.85
5.85
5.71
3.82
3.65
3.63
3.60
3.58
2.85
2.83
2.81
H
N
O
CF3
O
0.99
2.20
2.44
1.00
0.91
0.98
0.90
3.73
2.19
2.22
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)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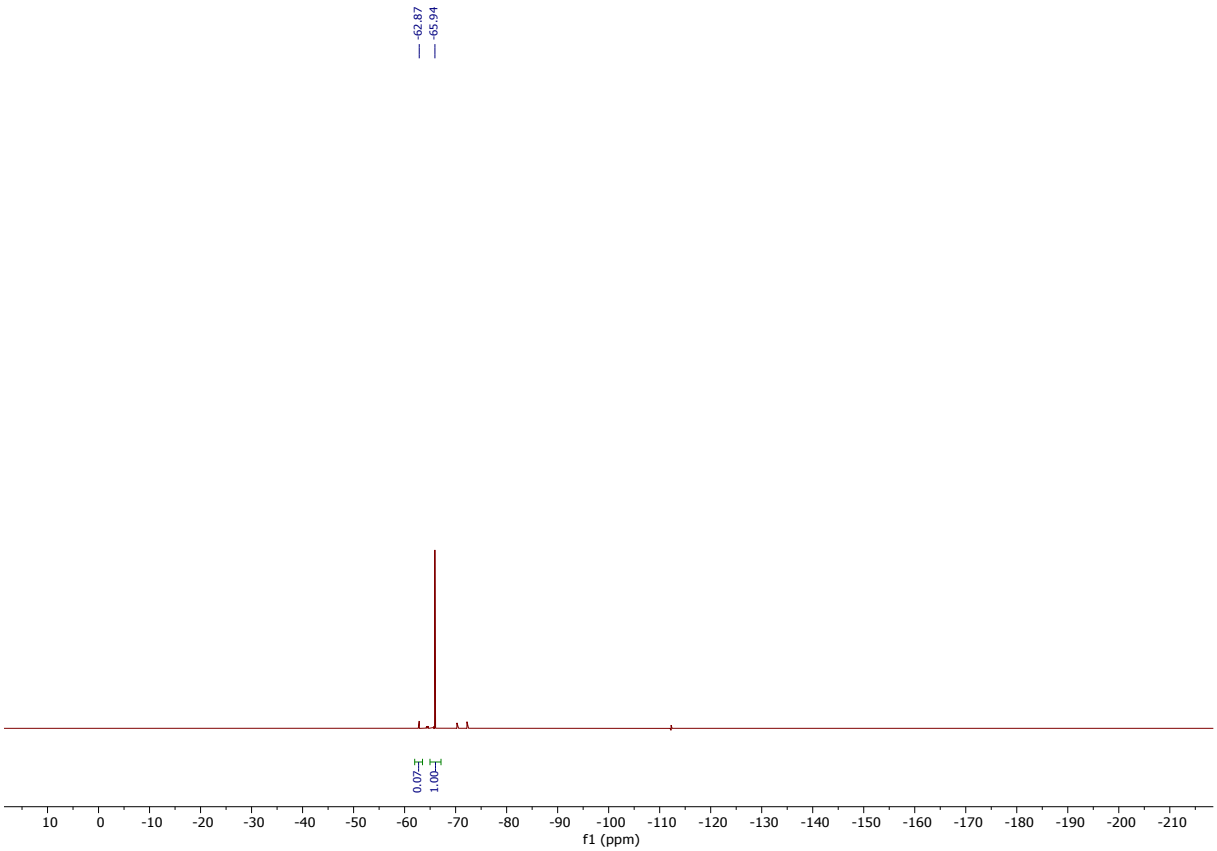
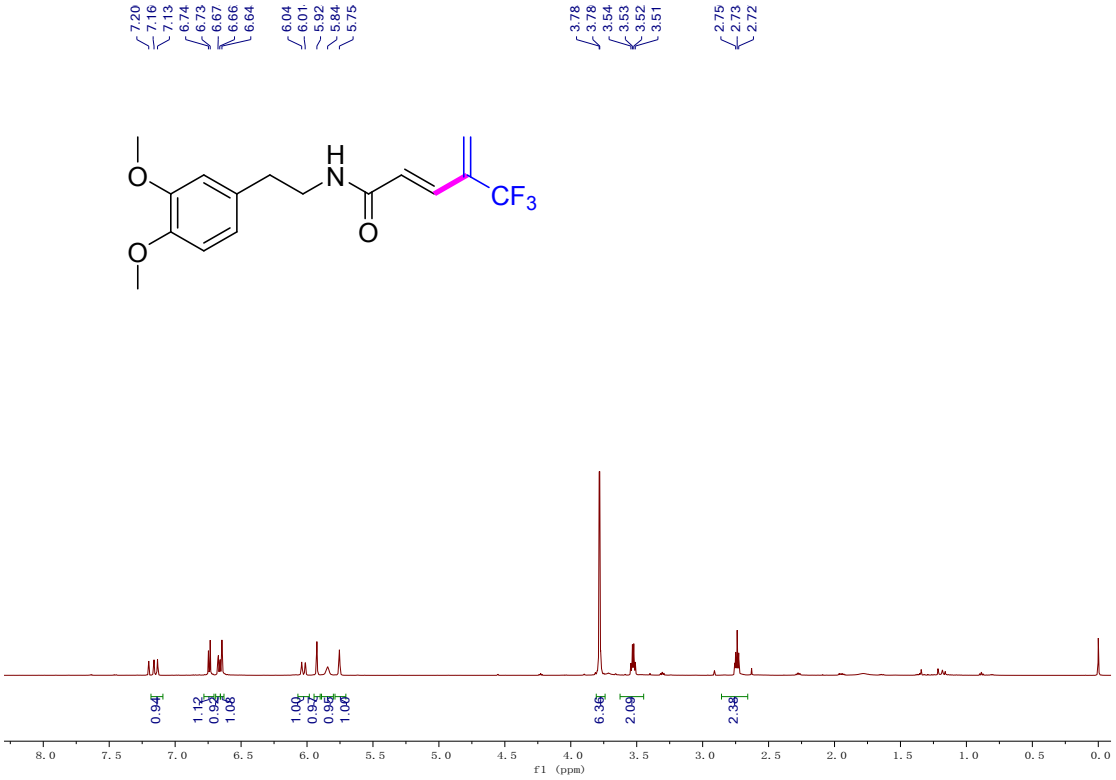
129.76
126.42
126.02
125.96
125.81
124.63
124.31
120.61
114.15
77.45
77.23
76.61
55.30
41.11
34.62
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


-62.87
-65.94
0.07
1.00
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)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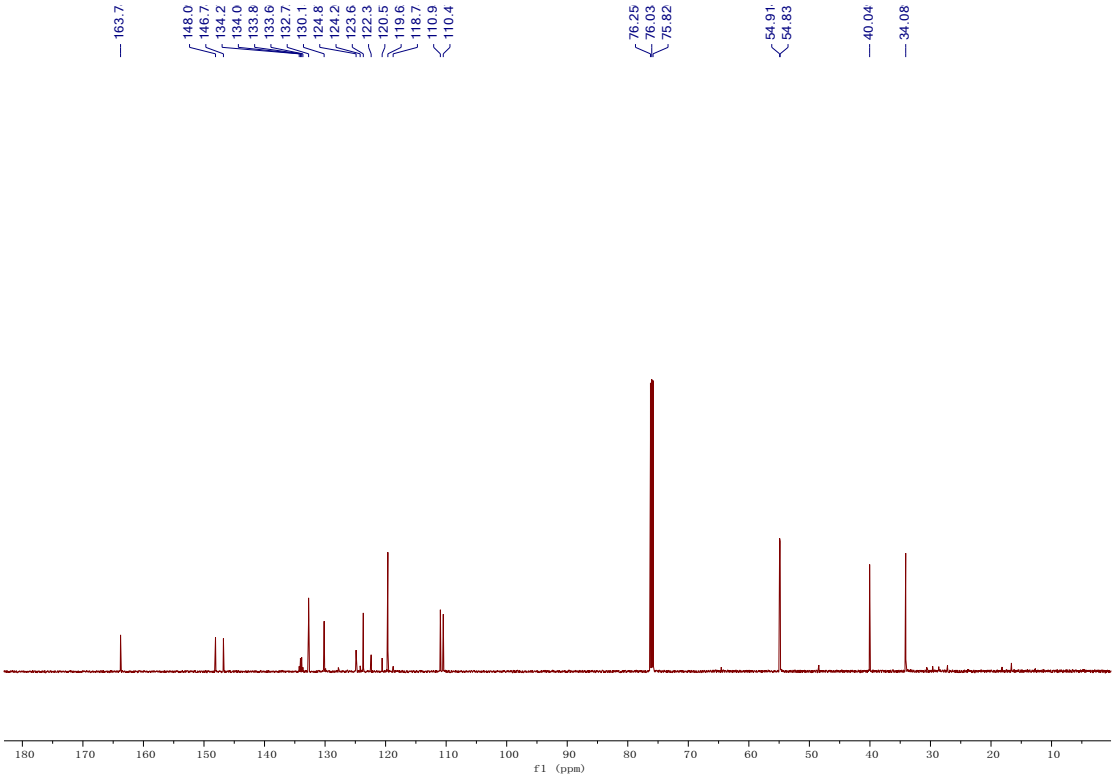
6.73
6.67
6.66
6.64
6.04
6.01
5.92
5.84
5.75
3.78
3.78
3.54
3.53
3.52
3.51
2.75
2.73
2.72
H
N
O
O
O
CF3
0.94
1.13
0.92
1.04
1.00
0.97
0.95
1.06
6.34
2.09
2.38
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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132.7
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124.8
124.2
123.6
122.3
120.5
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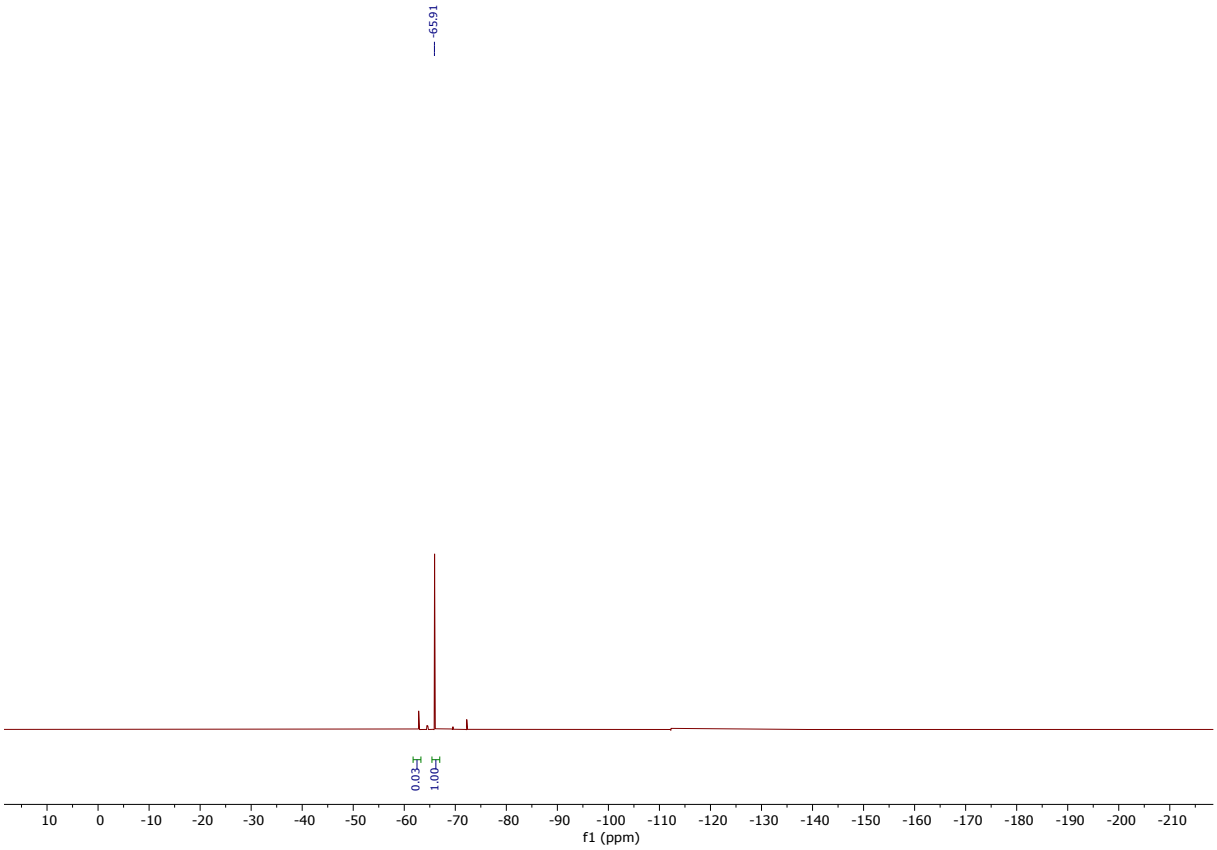
110.4
76.25
76.03
75.82
54.91
54.83
40.04
34.08
f1 (ppm)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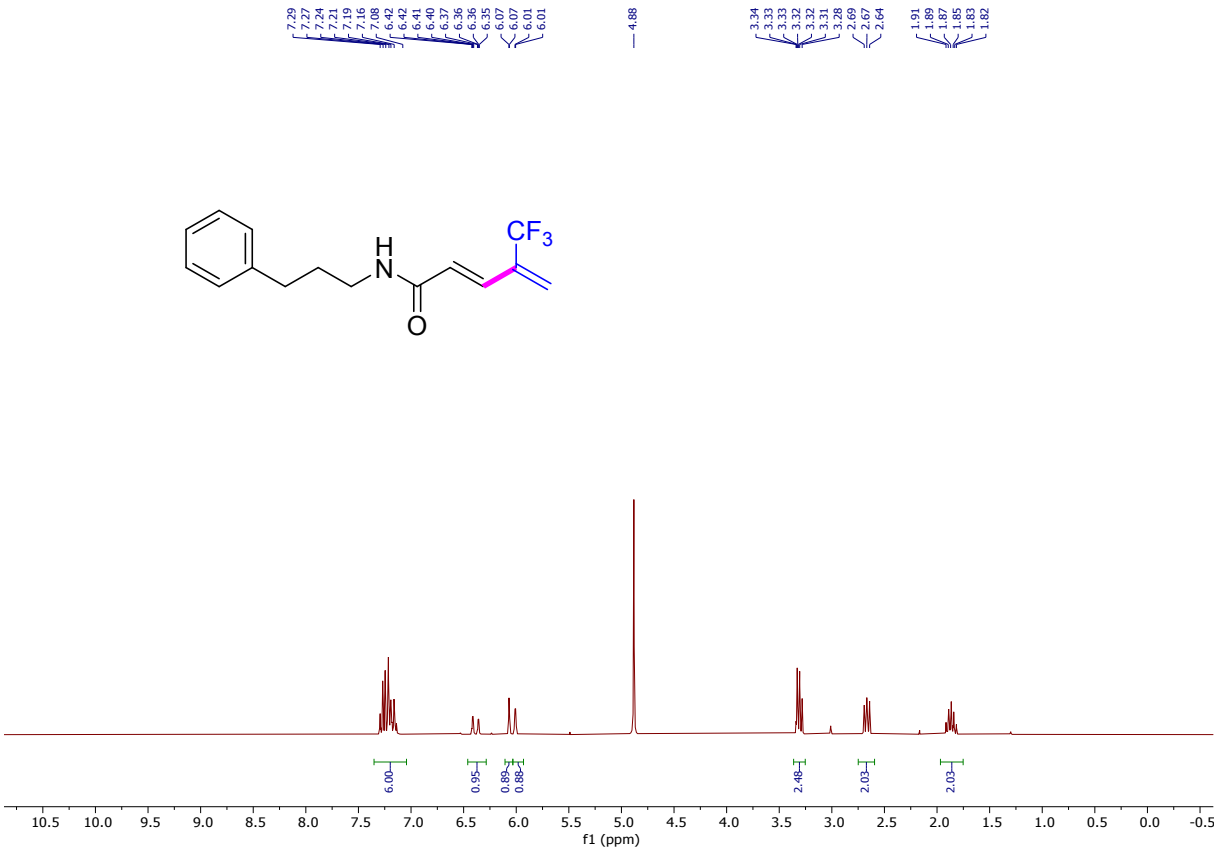
0.03
1.00
f1 (ppm)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6.40
6.37
6.36
6.36
6.35
6.07
6.01
6.01
4.88
3.34
3.33
3.33
3.32
3.32
3.31
3.28
2.69
2.67
2.64
1.91
1.89
1.87
1.85
1.83
1.82
CF3
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N
O
6.00
0.95
0.89
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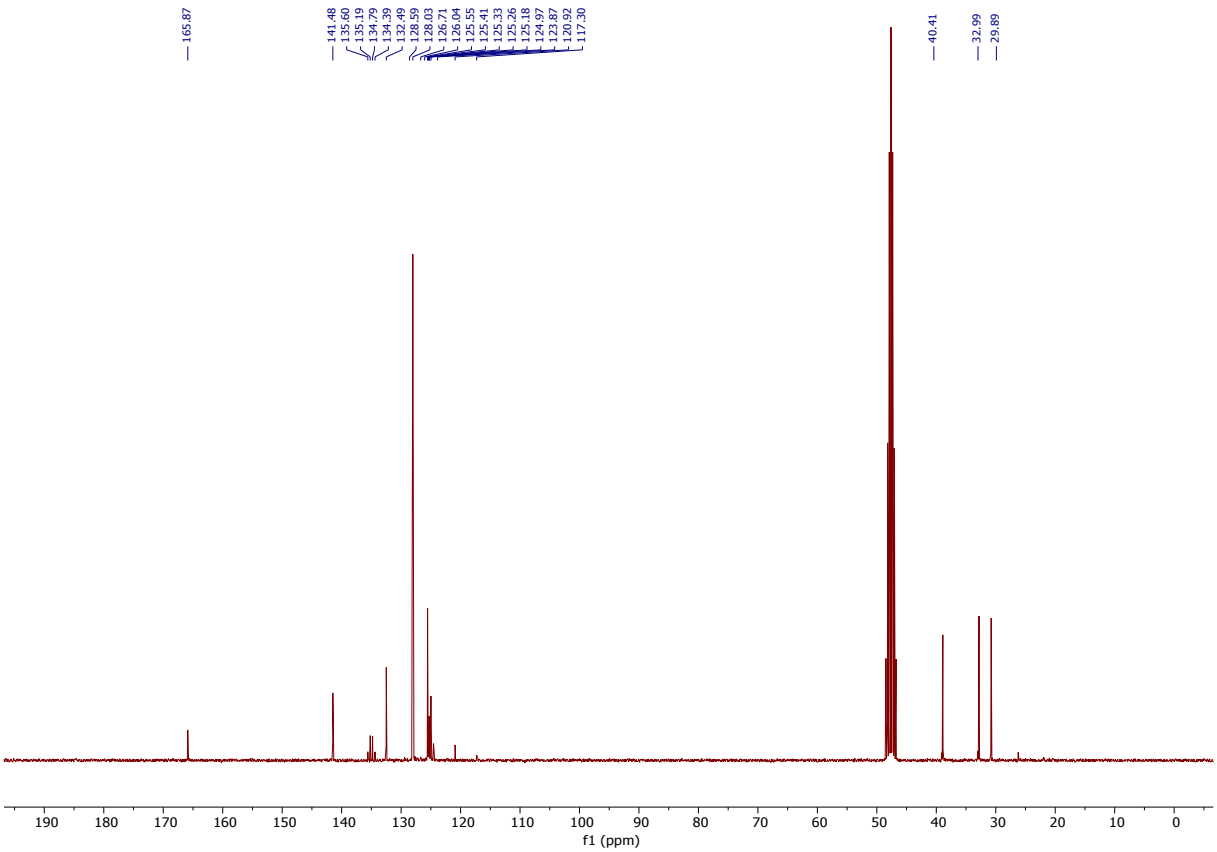
2.48
2.03
2.03
f1 (ppm)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128.03
126.71
126.04
125.55
125.41
125.33
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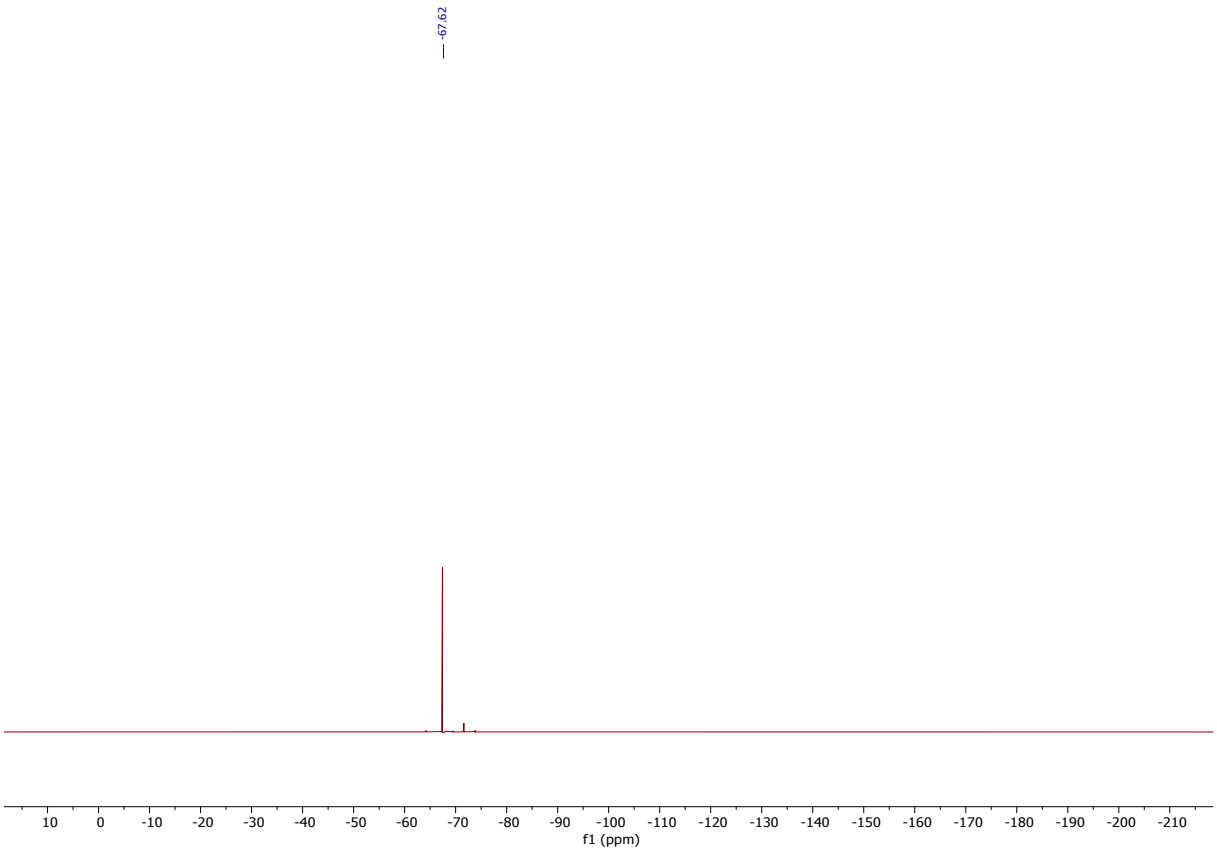
125.18
124.97
123.87
120.92
117.30
40.41
32.99
29.89
f1 (ppm)


-67.62
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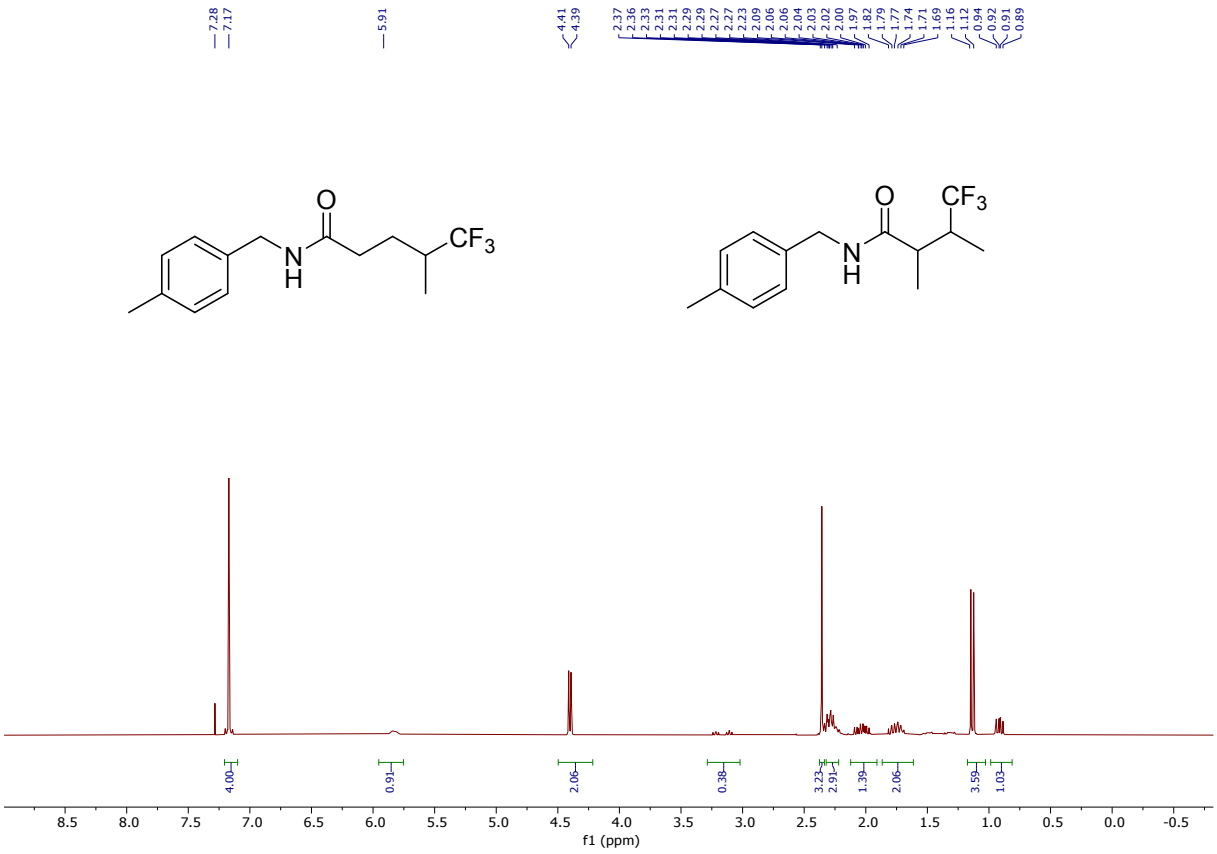
f1 (ppm)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4.41
4.39
2.37
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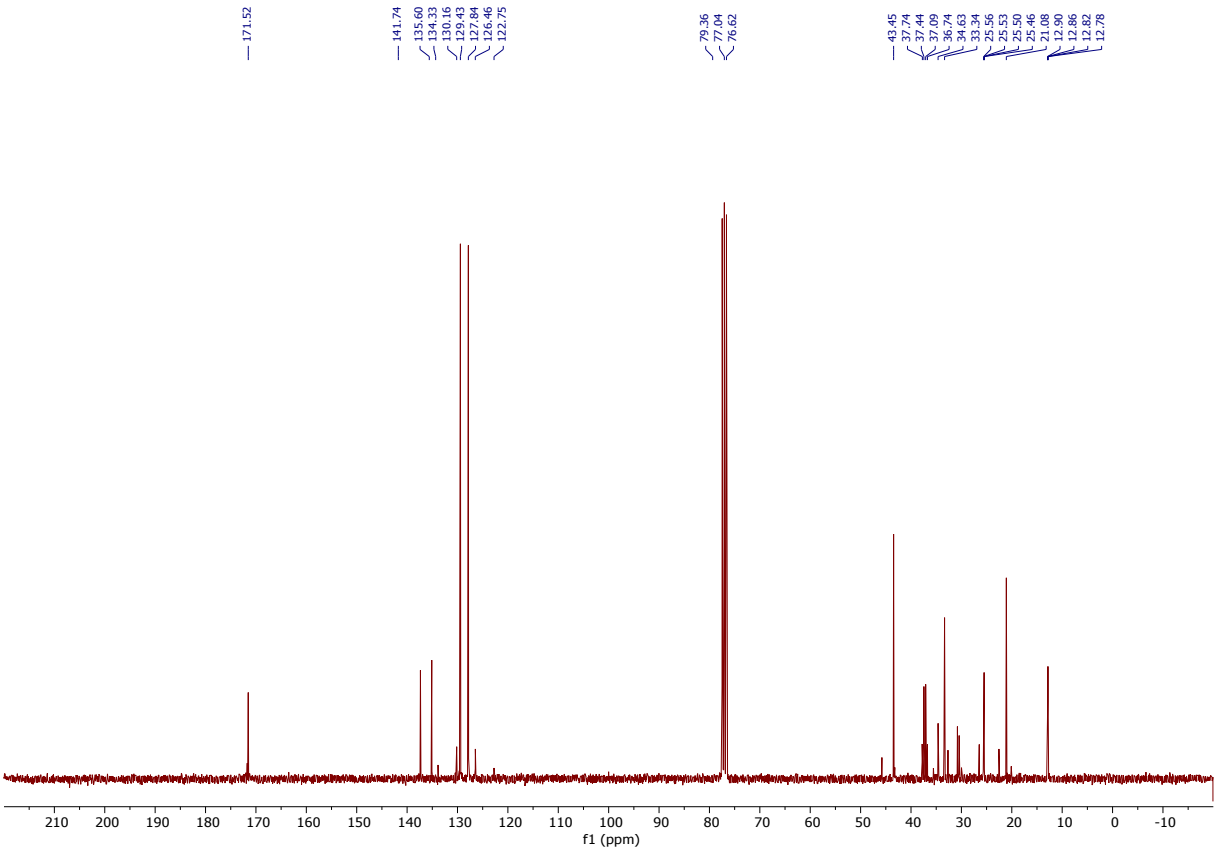
2.33
2.31
2.31
2.29
2.29
2.27
2.27
2.23
2.09
2.06
2.06
2.04
2.03
2.02
2.00
1.97
1.82
1.79
1.77
1.74
1.71
1.69
1.16
1.12
0.94
0.92
0.91
0.89
O
N
H
CF3
O
N
H
CF3
4.00
0.91
2.06
0.38
3.23
2.91
1.39
2.06
3.59
1.03
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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127.84
126.46
122.75
79.36
77.04
76.62
43.45
37.74
37.44
37.09
36.74
34.63
33.34
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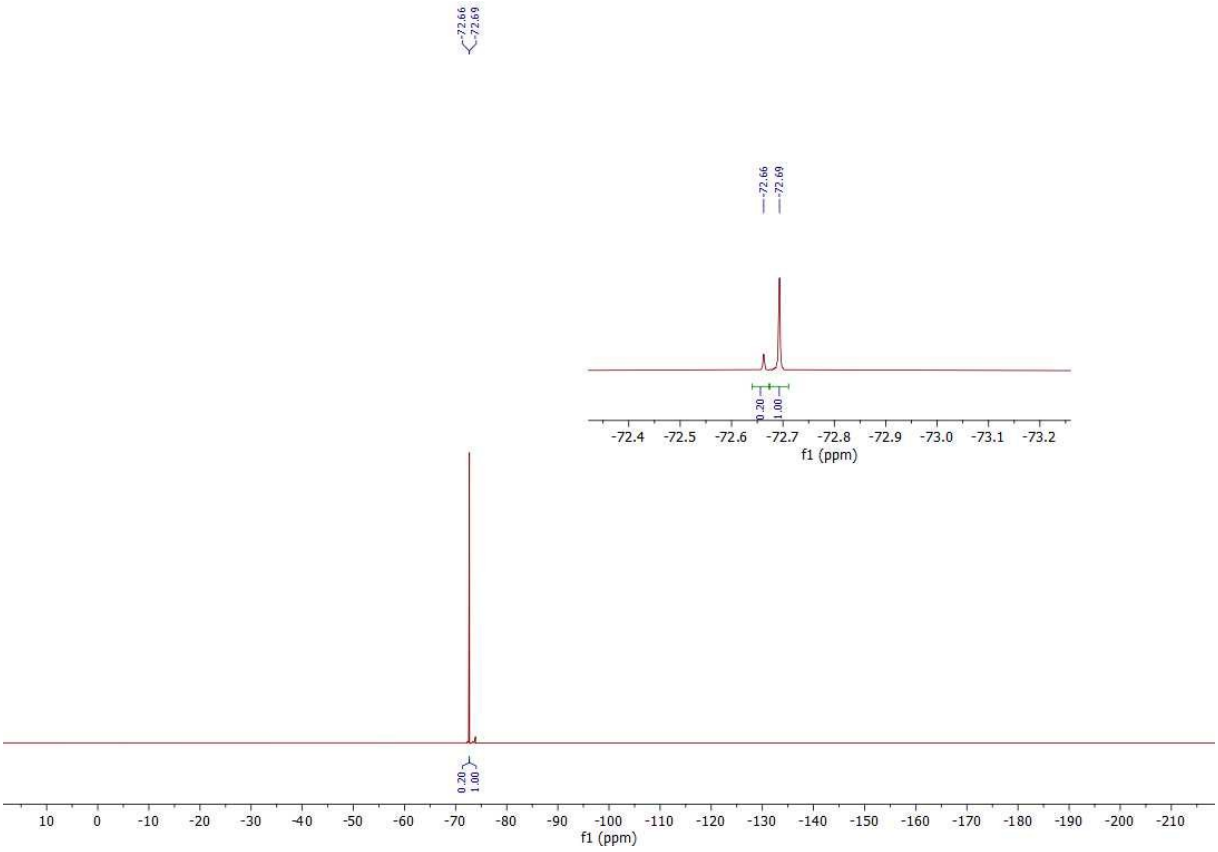
25.53
25.50
25.46
21.08
12.90
12.86
12.82
12.78
f1 (ppm)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-72.69
0.20
1.00
f1 (ppm)