

Supporting Information

Electrophilic Halogenation of Hydrazones of CF₃-ynones. Regioselective Synthesis of 4-halo-substituted 3-CF₃-pyrazoles

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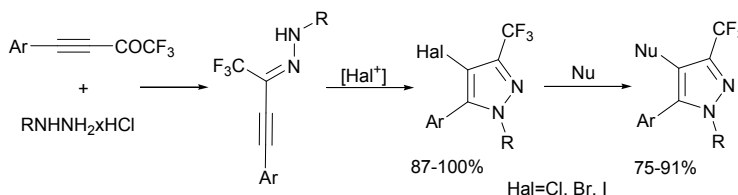


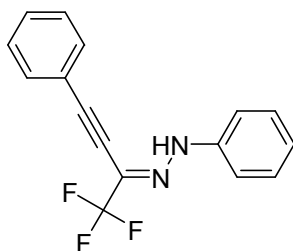
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General remarks. NMR spectra were recorded at 600.1 and 400.1 (^1H), 150.9 and 100.6 (^{13}C), 376.3 and 282.4 (^{19}F) MHz respectively from solutions in CDCl_3 , CD_3CN and $\text{DMSO-}d_6$. Chemical shifts (δ) in ppm are reported with the use of the residual CDCl_3 (7.25 for ^1H and 77.0 for ^{13}C), CD_3CN (1.94 for ^1H and 1.3, 118.2 for ^{13}C), $\text{DMSO-}d_6$ (2.49 for ^1H and 39.5 for ^{13}C) as internal references. The coupling constants (J) are given in Hertz (Hz). The ^{19}F chemical shifts were referenced to C_6F_6 (-162.9 ppm) respectively. The silica gel used for flash chromatography was 230–400 mesh. HRMS spectra were measured at MicroTof Bruker Daltonics and Orbitrap Elite instrument. All reagents were of reagent grade and were either used as such or distilled prior to use. All solvents were dried by standard procedures and freshly distilled prior to use. CF_3 -ynones **1** were obtained according to the literature procedure¹.

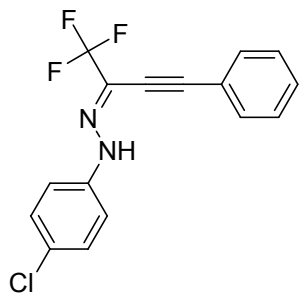
Synthesis of hydrazones **3 by the reaction of ketones **1** with hydrazines **2** in (general procedure):** A 20 mL screw neck vial was charged with corresponding ketone **1** (5 mmol), EtOH (10 mL), hydrochloride of arylhydrazine **2** (5.25 mmol, 1.05 equiv) and heated at 60-65 °C for 4-8 h at stirring (TLC control). Next, 1-1.5 mL of water was added to precipitate most amount of the product.* Precipitate formed was filtered off and washed with cold with diluted EtOH (1:1, 2-3 mL). The precipitate was dried in vacuo to give pure hydrazone **3**, which can be further purified by crystallization from the mixtures of EtOH and water.

*In case of hydrazones **3f** and **3k** after addition of water to the reaction mixture these compounds are formed as oils. Upper water layer was decanted, organic phase was dissolved in CH_2Cl_2 and dried over Na_2SO_4 . Evaporation of volatiles in vacuo afforded **3f** and **3k** as oils. Due to instability of **3k**, we did not succeed to obtain this compound in pure form. The purity of **3k** is about 85-90% accordingly NMR spectra.

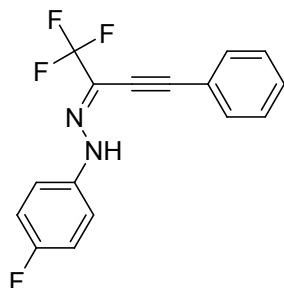


2-(1,1,1-trifluoro-4-phenylbut-3-yn-2-ylidene)-1-phenylhydrazine (3a). Pale yellow-green needles, m.p. 99-101 °C (Lit. data¹: 99-101 °C) (1.200 g, 83% yield); ^1H NMR (400.1 MHz, $\text{DMSO-}d_6$) δ 7.01 (td, $J_{\text{HH}} = 6.6$ Hz, $J_{\text{HF}} = 2.0$ Hz, 1H), 7.30-7.38 (m, 4H), 7.47-7.54 (m, 3H), 7.70-7.74 (m, 2H), 10.86 (br s, 1H, NH); ^{13}C NMR (100.6 MHz, $\text{DMSO-}d_6$) δ 75.6, 104.2, 112.1 (q, $J_{\text{CF}} = 38.0$ Hz, C- CF_3), 114.6, 120.5, 121.1 (q, $J_{\text{CF}} = 270.9$ Hz, CF_3), 122.5, 128.8, 129.2, 130.2, 132.0, 142.8; ^{19}F NMR (376.3 MHz, $\text{DMSO-}d_6$) δ -64.9; The NMR data are in agreement with those in the literature.¹

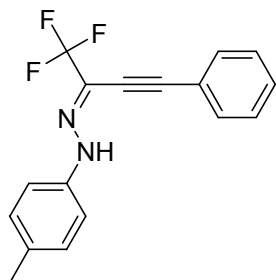
¹ V. M. Muzalevskiy, A. Yu. Rulev, A. R. Romanov, E. V. Kondrashov, I. A. Ushakov, V. A. Chertkov, V. G.



1-(4-Chlorophenyl)-2-(1,1,1-trifluoro-4-phenylbut-3-yn-2-ylidene)hydrazine (3b). Pale yellow crystals, m.p. 96-97 °C (1.116 g, 69% yield); $^1\text{H NMR}$ (400.1 MHz, CDCl_3): δ 7.13 (d, $J_{\text{HH}} = 8.8$ Hz, 2H, 4-ClC₆H₄), 7.29 (d, $J_{\text{HH}} = 8.8$ Hz, 2H, 4-ClC₆H₄), 7.40-7.49 (m, 3H, Ph), 7.57-7.59 (m, 2H, Ph), 8.67 (s, 1H, NH); $^{13}\text{C NMR}$ (100.6 MHz, CDCl_3): δ 74.4, 106.1, 115.4, 115.7 (q, $J_{\text{CF}} = 39.8$ Hz, C-CF₃), 120.3, 120.4 (q, $J_{\text{CF}} = 270.9$ Hz, CF₃), 127.8, 128.7, 129.4, 130.4, 132.0, 140.6 (Ar); $^{19}\text{F NMR}$ (376.5 MHz, CDCl_3): δ -67.4; HRMS (ESI): m/z calcd for C₁₆H₉ClF₃N₂⁻ [M-H⁺]: 321.0412; found: 321.0407.

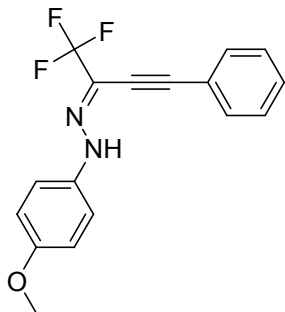


2-(1,1,1-Trifluoro-4-phenylbut-3-yn-2-ylidene)-1-(4-fluorophenyl)hydrazine (3c). Yellow powder, m.p. 82-84 °C (1.160 g, 76% yield); $^1\text{H NMR}$ (400.1 MHz, CDCl_3): δ 7.01-7.05 (m, 2H, 4-FC₆H₄), 7.13-7.16 (m, 2H, 4-FC₆H₄), 7.40-7.48 (m, 3H, Ph), 7.57-7.59 (m, 2H, Ph), 8.67 (s, 1H, NH); $^{13}\text{C NMR}$ (100.6 MHz, CDCl_3): δ 74.5, 105.9, 115.0 (q, $J_{\text{CF}} = 37.2$ Hz, C-CF₃), 115.4 (d, $^3J_{\text{CF}} = 7.7$ Hz), 116.1 (d, $^2J_{\text{CF}} = 22.9$ Hz), 120.4, 120.5 (q, $J_{\text{CF}} = 271.3$ Hz, CF₃), 128.7, 130.3, 132.0, 138.2, 158.8 (d, $^1J_{\text{CF}} = 241.4$ Hz, C-F); $^{19}\text{F NMR}$ (376.5 MHz, CDCl_3): δ -67.3 (3F, CF₃), -121.9 (1F, 4-FC₆H₄); HRMS (ESI): m/z calcd for C₁₆H₉F₄N₂⁻ [M-H⁺]: 305.0707; found: 305.0705.

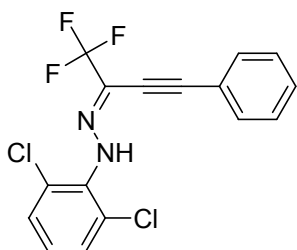


2-(1,1,1-Trifluoro-4-phenylbut-3-yn-2-ylidene)-1-p-tolylhydrazine (3d). Yellow powder, m.p. 115-116 °C (1.212 g, 80% yield); $^1\text{H NMR}$ (400.1 MHz, CDCl_3) δ 2.32 (s, 3H, Me), 7.10 (d, $J_{\text{HH}} = 8.6$ Hz, 2H, 4-MeC₆H₄), 7.14 (d, $J_{\text{HH}} = 8.6$

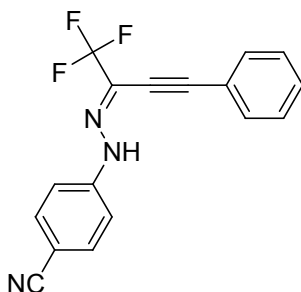
Hz, 2H, 4-MeC₆H₄), 7.40-7.48 (m, 3H), 7.58-7.60 (m, 2H), 8.69 (s, 1H, NH); ¹³C NMR (100.6 MHz, CDCl₃) δ 20.7, 74.7, 105.7, 114.1 (q, *J*_{CF} = 39.8 Hz, C-CF₃), 114.2, 120.6, 120.7 (q, *J*_{CF} = 271.3 Hz, CF₃), 128.7, 129.9, 130.1, 131.9, 132.5, 139.6; ¹⁹F NMR (376.3 MHz, CDCl₃) δ -67.1; HRMS (ESI): *m/z* calcd for C₁₇H₁₂F₃N₂⁻ [M-H⁺]: 301.0958; found: 301.0958.



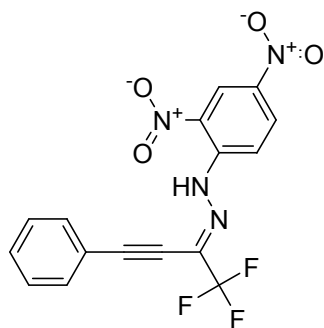
2-(1,1,1-Trifluoro-4-phenylbut-3-yn-2-ylidene)-1-(4-methoxyphenyl)hydrazine (3e). Yellow powder, m.p. 81-83 °C (0.956 g, 60% yield); ¹H NMR (400.1 MHz, CDCl₃): δ 3.79 (s, 3H, OCH₃), 6.88 (d, *J*_{HH} = 8.9 Hz, 2H, 4-MeOC₆H₄), 7.13 (d, *J*_{HH} = 8.9 Hz, 2H, 4-MeOC₆H₄), 7.39-7.47 (m, 3H, Ph), 7.56-7.59 (m, 2H, Ph), 8.66 (s, 1H, NH); ¹³C NMR (100.6 MHz, CDCl₃): δ 55.5 (OCH₃), 74.8, 105.7, 113.7 (q, *J*_{CF} = 39.1 Hz, C-CF₃), 114.7, 115.4, 120.7, 120.8 (q, *J*_{CF} = 270.9 Hz, CF₃), 128.7, 130.0, 131.9, 135.8 155.7 (Ar); ¹⁹F NMR (376.5 MHz, CDCl₃): δ -67.0; HRMS (ESI): *m/z* calcd for C₁₇H₁₂F₃N₂O⁻ [M-H⁺]: 317.0907; found: 317.0907.



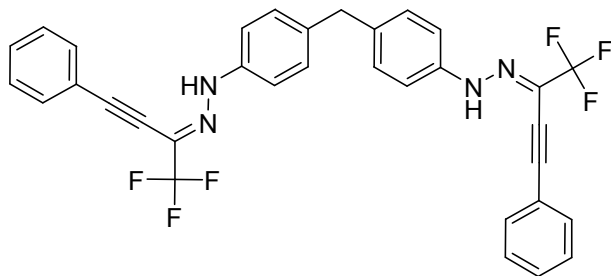
1-(2,6-diChlorophenyl)-2-(1,1,1-trifluoro-4-phenylbut-3-yn-2-ylidene)hydrazine (3f). Brown oil, (1.528 g, 86% yield); ¹H NMR (400.1 MHz, CDCl₃) δ 7.01 (t, *J*_{HH} = 8.1 Hz, 2H, 2,6-diClC₆H₃), 7.34 (d, *J*_{HH} = 8.1 Hz, 2H, 2,6-diClC₆H₃), 7.39-7.48 (m, 3H, Ph), 7.58-7.61 (m, 2H, Ph), 8.91 (s, 1H, NH); ¹³C NMR (100.6 MHz, CDCl₃) δ 74.1, 106.5, 118.4 (q, *J*_{CF} = 39.4 Hz, C-CF₃), 120.1 (q, *J*_{CF} = 271.7 Hz, CF₃), 120.2, 125.2, 126.5, 128.7, 129.3, 130.4, 132.0, 135.5; ¹⁹F NMR (376.3 MHz, CDCl₃) δ -67.9; HRMS (ESI): *m/z* calcd for C₁₆H₁₀Cl₂F₃N₂⁺ [M+H⁺]: 357.0168; found: 357.0172.



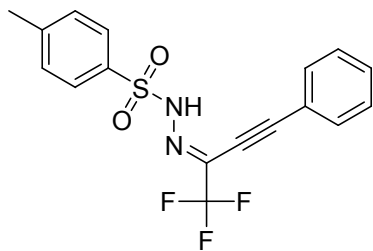
4-(2-(1,1,1-Trifluoro-4-phenylbut-3-yn-2-ylidene)hydrazinyl)benzonitrile (3g). Pale yellow powder, m.p. 149-151 °C (1.341 g, 86% yield); $^1\text{H NMR}$ (400.1 MHz, CDCl_3) δ 7.25 (d, $J_{\text{HH}} = 8.8$ Hz, 2H, 4- CNC_6H_4), 7.41-7.51 (m, 3H, Ph), 7.58-7.61 (m, 4H, Ph, 4- CNC_6H_4), 8.81 (s, 1H, NH); $^{13}\text{C NMR}$ (100.6 MHz, CDCl_3) δ 74.1, 105.2, 106.6, 114.4, 118.3 (q, $J_{\text{CF}} = 39.8$ Hz, C- CF_3), 119.1, 119.9, 120.1 (q, $J_{\text{CF}} = 272.0$ Hz, CF_3), 128.8, 130.6, 132.1, 133.7, 145.3; $^{19}\text{F NMR}$ (376.3 MHz, CDCl_3) δ -67.8; HRMS (ESI): m/z calcd for $\text{C}_{17}\text{H}_9\text{F}_3\text{N}_3$ $[\text{M}-\text{H}^+]$: 312.0754; found: 312.0754.



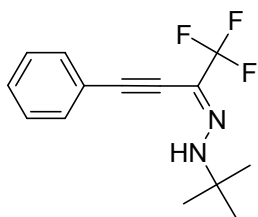
(2-(1,1,1-Trifluoro-4-phenylbut-3-yn-2-ylidene)-1-(2,4-dinitrophenyl)hydrazine (3h). Obtained by slightly modified general procedure: 2,4-dinitrophenylhydrazine was dissolved in 5M HCl in MeOH, CF_3 -ynone was added and heated at 60-65 °C for 4 h. Next, the product was isolated in usual manner. Yellow-orange powder, m.p. 183-185 °C (Lit. data¹: 183-185 °C) (1.723 g, 91%); $^1\text{H NMR}$ (400.1 MHz, CDCl_3) δ 7.44-7.54 (m, 3H, Ph), 7.72-7.75 (m, 2H, Ph), 8.06 (d, $J_{\text{HH}} = 9.4$ Hz, 1H, 2,4- $\text{diNO}_2\text{C}_6\text{H}_3$), 8.43 (dd, $J_{\text{HH}} = 9.4$ Hz, $J_{\text{HH}} = 2.4$ Hz, 1H, 2,4- $(\text{NO}_2)_2\text{C}_6\text{H}_4$), 9.16 (d, $J_{\text{HH}} = 2.4$ Hz, 1H, 2,4- $(\text{NO}_2)_2\text{C}_6\text{H}_4$), 12.11 (br s, 1H, NH); $^{13}\text{C NMR}$ (100.6 MHz, CDCl_3) δ 74.8, 109.4, 117.7, 119.2, 119.3 (q, $J_{\text{CF}} = 272.8$ Hz, CF_3), 123.0, 125.6 (q, $J_{\text{CF}} = 39.4$ Hz, C- CF_3), 129.0, 130.3, 131.4, 132.7, 140.5, 143.1; $^{19}\text{F NMR}$ (376.3 MHz, CDCl_3) δ -68.4; The NMR data are in agreement with those in the literature.¹



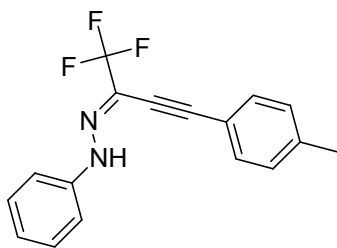
Bis-(4-(3-(Trifluoromethyl)-4-iodo-5-phenyl-1H-pyrazol-1-yl)phenyl)methane (3i). Yellow powder, m.p. 177-179 °C (0.813 g, 55% yield); $^1\text{H NMR}$ (400.1 MHz, CDCl_3) δ 3.91 (s, 2H, CH_2), 7.13 (s, 8H), 7.40-7.48 (m, 6H, Ph), 7.57-7.59 (m, 4H, Ph), 8.70 (s, 2H, NH); $^{13}\text{C NMR}$ (100.6 MHz, CDCl_3) δ 40.5, 74.7, 105.7, 114.4, 114.5 (q, $J_{\text{CF}} = 37.2$ Hz, C- CF_3), 120.6 (q, $J_{\text{CF}} = 271.3$ Hz, CF_3), 120.7, 128.7, 129.8, 130.2, 131.9, 135.9, 140.2; $^{19}\text{F NMR}$ (376.3 MHz, CDCl_3) δ -67.2; HRMS (ESI): m/z calcd for $\text{C}_{33}\text{H}_{21}\text{F}_6\text{N}_4$ $[\text{M}-\text{H}^+]$: 587.1676; found: 587.1674.



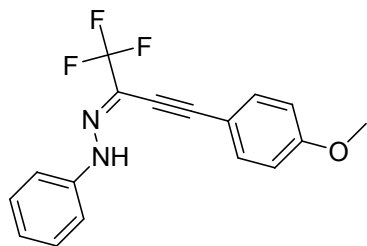
2-(1,1,1-Trifluoro-4-phenylbut-3-yn-2-ylidene)-1-tosylhydrazine (3j). White powder, m.p. 131-133 °C (decomp.) (1.102 g, 60% yield); ^1H NMR (400.1 MHz, CDCl_3) δ 2.44 (s, 3H, Me), 7.34 (d, $J_{\text{HH}} = 8.2$ Hz, 2H, Tos), 7.38-7.42 (m, 2H, Ph), 7.46-7.50 (m, 1H, Ph), 7.54-7.56 (m, 2H, Ph), 7.85 (d, $J_{\text{HH}} = 8.2$ Hz, 2H, Tos), 8.81 (s, 1H, NH); ^{13}C NMR (100.6 MHz, CDCl_3) δ 21.6, 73.3, 106.9, 118.9 (q, $J_{\text{CF}} = 274.2$ Hz, CF_3), 119.1, 124.7 (q, $J_{\text{CF}} = 40.2$ Hz, C- CF_3), 128.0, 128.7, 129.9, 131.1, 132.4, 134.4, 145.1; ^{19}F NMR (376.3 MHz, CDCl_3) δ -69.2; HRMS (ESI): m/z calcd for $\text{C}_{17}\text{H}_{12}\text{F}_3\text{N}_2\text{O}_2\text{S}^-$ [$\text{M}-\text{H}^+$]: 365.0577; found: 365.0577.



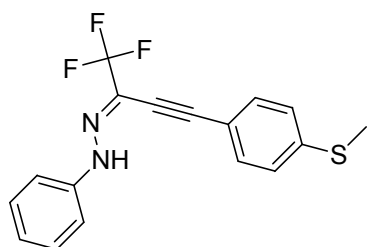
1-tert-Butyl-2-(1,1,1-trifluoro-4-phenylbut-3-yn-2-ylidene)hydrazine (3k). Colorless oil (0.760 g, 57% yield). ^1H NMR (400 MHz, CDCl_3): δ 1.34 (s, 9H), 6.89 (s, 1H, NH), 7.38-7.44 (m, 3H, Ph), 7.54-7.56 (m, 2H, Ph); ^{13}C NMR (100.6 MHz, CDCl_3): δ 28.7 (CH_3), 55.2 ($\text{C}(\text{CH}_3)_3$), 75.2, 103.9, 111.7 (q, $J_{\text{CF}} = 39.5$ Hz, C- CF_3), 121.0 (q, $J_{\text{CF}} = 270.5$ Hz, CF_3), 121.1, 128.6, 129.6, 131.7. ^{19}F NMR (376.5 MHz, CDCl_3): δ -67.0. HRMS (ESI): m/z calcd for $\text{C}_{14}\text{H}_{16}\text{F}_3\text{N}_2^+$ [$\text{M}+\text{H}^+$]: 269.1260; found: 269.1260.



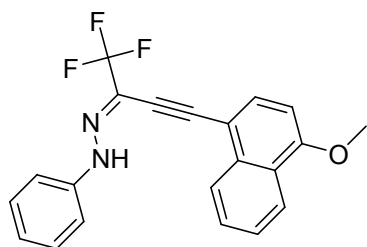
2-(1,1,1-Trifluoro-4-p-tolylbut-3-yn-2-ylidene)-1-phenylhydrazine (3l). Yellow powder, m.p. 101-102 °C (1.265 g, 84% yield); ^1H NMR (400.1 MHz, CDCl_3) δ 2.40 (s, 3H, Me), 7.01 (t, $J_{\text{HH}} = 7.2$ Hz, 1H, Ph), 7.17-7.25 (m, 4H, Ph, 4-MeC $_6$ H $_4$), 7.32 (t, $J_{\text{HH}} = 7.7$ Hz, 2H, Ph), 7.47 (d, $J_{\text{HH}} = 7.9$ Hz, 2H, 4-MeC $_6$ H $_4$), 8.70 (s, 1H, NH); ^{13}C NMR (100.6 MHz, CDCl_3) δ 21.6, 74.2, 106.2, 114.2, 115.1 (q, $J_{\text{CF}} = 39.8$ Hz, C- CF_3), 117.4, 120.6 (q, $J_{\text{CF}} = 271.3$ Hz, CF_3), 122.8, 129.4, 129.5, 131.9, 140.8, 142.0; ^{19}F NMR (376.3 MHz, CDCl_3) δ -67.3. HRMS (ESI): m/z calcd for $\text{C}_{17}\text{H}_{12}\text{F}_3\text{N}_2$ [$\text{M}-\text{H}^+$]: 301.0958; found: 301.0957.



2-(1,1,1-Trifluoro-4-(4-methoxyphenyl)but-3-yn-2-ylidene)-1-phenylhydrazine (3m). Pale yellow needles, m.p. 100-102 °C (1.386 g, 87%); $^1\text{H NMR}$ (400.1 MHz, CDCl_3) δ 3.86 (s, 3H, MeO), 6.93 (d, $J_{\text{HH}} = 8.9$ Hz, 2H, 4-MeOC₆H₄), 7.01 (t, $J_{\text{HH}} = 7.3$ Hz, 1H, Ph), 7.18 (d, $J_{\text{HH}} = 7.6$ Hz, 2H, Ph), 7.32 (dd, $J_{\text{HH}} = 8.4$ Hz, $J_{\text{HH}} = 7.5$ Hz, 2H, Ph), 7.52 (d, $J_{\text{HH}} = 8.9$ Hz, 2H, 4-MeOC₆H₄), 8.67 (s, 1H, NH); $^{13}\text{C NMR}$ (100.6 MHz, CDCl_3) δ 55.3, 73.7, 106.2, 112.4, 114.1, 114.3, 115.3 (q, $J_{\text{CF}} = 39.4$ Hz, C-CF₃), 120.6 (q, $J_{\text{CF}} = 271.3$ Hz, CF₃), 122.7, 129.4, 133.6, 142.0, 161.1; $^{19}\text{F NMR}$ (376.3 MHz, CDCl_3) δ -67.4. HRMS (ESI): m/z calcd for C₁₇H₁₄F₃N₂O⁺ [M+H⁺]: 319.1053; found: 319.1051.

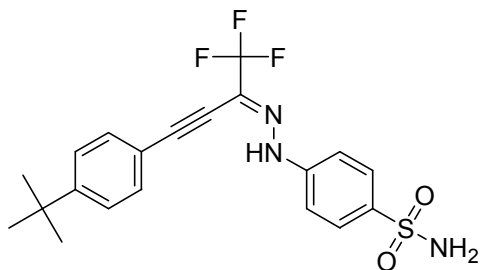


2-(1,1,1-Trifluoro-4-(4-(methylthio)phenyl)but-3-yn-2-ylidene)-1-phenylhydrazine (3n). Yellow crystals, m.p. 90-92 °C (1.441 g, 86%); $^1\text{H NMR}$ (400.1 MHz, CDCl_3) δ 2.51 (s, 3H, MeS), 7.02 (t, $J_{\text{HH}} = 7.4$ Hz, 1H, Ph), 7.18 (d, $J_{\text{HH}} = 7.7$ Hz, 2H, Ph), 7.24 (d, $J_{\text{HH}} = 8.4$ Hz, 2H, 4-MeSC₆H₄), 7.32 (t, $J_{\text{HH}} = 7.9$ Hz, 2H, Ph), 7.47 (d, $J_{\text{HH}} = 8.4$ Hz, 2H, 4-MeSC₆H₄), 8.68 (s, 1H, NH); $^{13}\text{C NMR}$ (100.6 MHz, CDCl_3) δ 14.9, 74.8, 105.8, 114.1, 115.0 (q, $J_{\text{CF}} = 39.1$ Hz, C-CF₃), 116.2, 120.6 (q, $J_{\text{CF}} = 271.3$ Hz, CF₃), 122.8, 125.5, 129.4, 132.1, 141.9, 142.4; $^{19}\text{F NMR}$ (376.3 MHz, CDCl_3) δ -67.3; HRMS (ESI): m/z calcd for C₁₇H₁₂F₃N₂S⁻ [M-H⁺]: 333.0679; found: 333.0677.



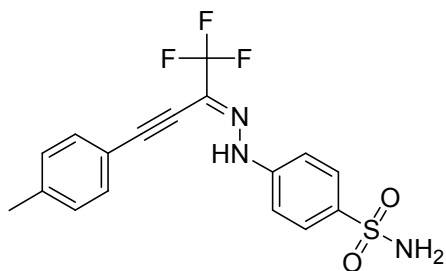
2-(1,1,1-Trifluoro-4-(1-methoxynaphthalen-4-yl)but-3-yn-2-ylidene)-1-phenylhydrazine (3o). Yellow needles, m.p. 99-101 °C (1.270 g, 69% yield); $^1\text{H NMR}$ (400.1 MHz, CDCl_3) δ 4.07 (s, 3H, MeO), 6.85 (d, $J_{\text{HH}} = 8.1$ Hz, 1H), 7.02 (t, $J_{\text{HH}} = 7.3$ Hz, 1H, Ph), 7.19 (d, $J_{\text{HH}} = 7.6$ Hz, 2H, Ph), 7.33 (t, $J_{\text{HH}} = 7.9$ Hz, 2H, Ph), 7.55-7.59 (m, 1H), 7.64-7.69 (m, 1H), 7.78 (d, $J_{\text{HH}} = 8.0$ Hz, 1H), 8.21 (d, $J_{\text{HH}} = 8.3$ Hz, 1H), 8.33 (d, $J_{\text{HH}} = 8.3$ Hz, 1H), 8.82 (s, 1H, NH); $^{13}\text{C NMR}$ (100.6

MHz, CDCl₃) δ 55.8, 78.2, 103.6, 105.0, 110.0, 114.1, 115.7 (q, J_{CF} = 39.1 Hz, C-CF₃), 120.7 (q, J_{CF} = 270.9 Hz, CF₃), 122.69, 122.72, 125.1, 125.3, 126.2, 128.2, 129.4, 132.8, 133.7, 142.1, 157.7; ¹⁹F NMR (376.3 MHz, CDCl₃) δ -67.2; HRMS (ESI): m/z calcd for C₂₁H₁₄F₃N₂O- [M-H⁺]: 367.1064; found: 367.1061.



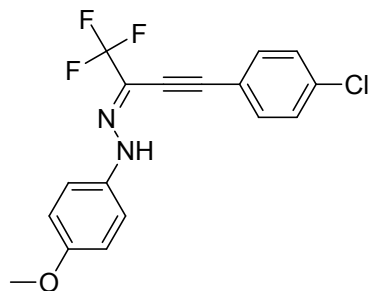
4-{2-[3-(4-*tert*-Butylphenyl)-1-(trifluoromethyl)prop-2-yn-1-ylidene]hydrazino}benzenesulfonamide (3p).

Pale brown powder, m.p. 160-162 °C (2.010 g, 95% yield); ¹H NMR (400.1 MHz, CDCl₃) δ 1.35 (s, 9H, *t*-Bu), 5.38 (s, 2H, NH₂), 7.22 (d, J_{HH} = 8.5 Hz, 2H), 7.43 (d, J_{HH} = 8.2 Hz, 2H), 7.54 (d, J_{HH} = 8.2 Hz, 2H), 7.81 (d, J_{HH} = 8.5 Hz, 2H), 8.95 (s, 1H, NH); ¹³C NMR (100.6 MHz, CDCl₃) δ 30.9 (C-(C(CH₃)₃), 35.0 (C-(C(CH₃)₃), 73.8, 107.0, 114.0, 116.9, 118.0 (q, J_{CF} = 39.4 Hz, C-CF₃), 120.2 (q, J_{CF} = 272.0 Hz, CF₃), 125.7, 128.1, 131.9, 134.9, 145.4, 154.2; ¹⁹F NMR (376.3 MHz, CDCl₃) δ -67.6; HRMS (ESI): m/z calcd for C₂₀H₂₀F₃N₃O₂SNa⁺ [M+Na⁺]: 446.1121; found: 446.1112.



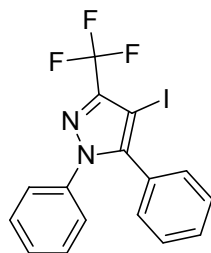
4-{2-[3-(4-Methylphenyl)-1-(trifluoromethyl)prop-2-yn-1-ylidene]hydrazino}benzenesulfonamide 3q. Barely

greenish powder, (1.750 g, 93% yield); m.p. 188-190 °C. ¹H NMR (400.1 MHz, DMSO-*d*₆) δ 2.36 (s, 3H, Me), 7.23 (s, 2H, NH₂), 7.31 (d, J_{HH} = 8.0 Hz, 2H, 4-MeC₆H₄), 7.47 (d, J_{HH} = 8.8 Hz, 2H, 4-(SO₂NH₂)C₆H₄), 7.62 (d, J_{HH} = 8.0 Hz, 2H, 4-MeC₆H₄), 7.81 (d, J_{HH} = 8.8 Hz, 2H, 4-(SO₂NH₂)C₆H₄), 11.09 (s, 1H, NH); ¹³C NMR (100.6 MHz, DMSO-*d*₆) δ 21.2, 75.0, 105.1, 114.1, 114.7 (q, J_{CF} = 38.3 Hz, C-CF₃), 117.1, 120.7 (q, J_{CF} = 271.6 Hz, CF₃), 127.3, 129.4, 132.1, 137.5, 140.7, 145.4; ¹⁹F NMR (376.3 MHz, DMSO-*d*₆) δ -65.4; HRMS (ESI): m/z calcd for C₁₇H₁₄F₃N₃O₂SNa⁺ [M+Na⁺]: 404.0651; found: 404.0637.

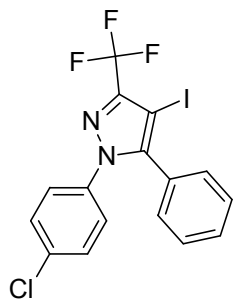


2-(4-(4-Chlorophenyl)-1,1,1-trifluorobut-3-yn-2-ylidene)-1-(4-methoxyphenyl)hydrazine (3r). Yellow powder, m.p. 101-103 °C (1.378 g, 78% yield); ^1H NMR (400.1 MHz, CDCl_3) δ 3.79 (s, 3H, MeO), 6.88 (d, $J_{\text{HH}} = 9.0$ Hz, 2H, 4-MeOC $_6\text{H}_4$), 7.13 (d, $J_{\text{HH}} = 9.0$ Hz, 2H, 4-MeOC $_6\text{H}_4$), 7.39 (d, $J_{\text{HH}} = 8.5$ Hz, 2H, 4-ClC $_6\text{H}_4$), 7.50 (d, $J_{\text{HH}} = 8.5$ Hz, 2H, 4-ClC $_6\text{H}_4$), 8.63 (s, 1H, NH); ^{13}C NMR (100.6 MHz, CDCl_3) δ 55.5, 75.7, 104.4, 113.3 (q, $J_{\text{CF}} = 39.4$ Hz, C-CF $_3$), 114.7, 115.5, 119.1, 120.7 (q, $J_{\text{CF}} = 270.5$ Hz, CF $_3$), 129.1, 133.0, 135.6, 136.3, 155.8; ^{19}F NMR (376.3 MHz, CDCl_3) δ -66.9; HRMS (ESI): m/z calcd for C $_{17}\text{H}_{12}\text{ClF}_3\text{N}_2\text{O}^+$ [M+H $^+$]: 353.0663; found: 353.0661; calcd for C $_{17}\text{H}_{11}\text{ClF}_3\text{N}_2\text{O}$ [M]: 352.0585; found: 352.0580.

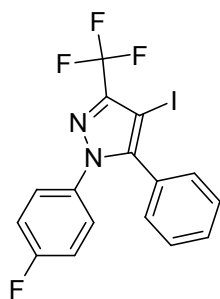
Synthesis of iodopyrazoles 4 (general procedure): A 8 mL screw neck vial was charged with MeCN (6 mL) corresponding hydrazone **3** (1.5 mmol), I $_2$ (0.800 g, 3.15 mmol, 2.1 equiv), NaHCO $_3$ (0.265 g, 3.15 mmol, 2.1 equiv) and maintained at stirring for 1 day at room temperature. The reaction mixture was poured into water (50 mL) and few milliliters of sat. solution of Na $_2\text{SO}_3$ was added until brown color of iodine disappeared. Solution obtained was extracted with dichloromethane (3x20 mL), the combined organic phase was washed with water (20 mL) and dried over anhydrous sodium sulfate. Evaporation of the volatiles *in vacuo* gave pure iodopyrazoles **4**.



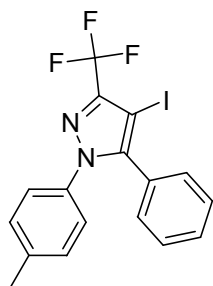
3-(Trifluoromethyl)-4-iodo-1,5-diphenyl-1H-pyrazole (4a). Pale brown powder, m.p. 134-135 °C (0.604 g, 97% yield). ^1H NMR (400 MHz, CDCl_3) δ 7.22-7.33 (m, 7H, Ph), 7.38-7.45 (m, 3H, Ph); ^{13}C NMR (100.6 MHz, CDCl_3) δ 59.5 (C-I), 120.8 (q, $J = 270.5$ Hz, CF $_3$), 124.9, 128.5, 128.6, 129.0, 129.6, 130.3, 138.9, 144.3 (q, $J = 36.9$ Hz, C-CF $_3$), 146.6 (C 5); ^{19}F NMR (376.5 MHz, CDCl_3) δ -63.3. HRMS (ESI): m/z calcd for C $_{16}\text{H}_{11}\text{F}_3\text{IN}_2^+$ [M+H $^+$]: 414.9914; found: 414.9922.



1-(4-Chlorophenyl)-3-(trifluoromethyl)-4-iodo-5-phenyl-1H-pyrazole (4b). Pale brown powder, m.p. 104-106 °C (0.672 g, 100% yield); ^1H NMR (400.1 MHz, CDCl_3): δ 7.16 (d, $J_{\text{HH}} = 8.7$ Hz, 2H, 4-ClC₆H₄), 7.25-7.30 (m, 4H, Ar), 7.40-7.47 (m, 3H, Ar); ^{13}C NMR (100.6 MHz, CDCl_3): δ 59.9 (C-I), 120.7 (q, $J_{\text{CF}} = 270.2$ Hz, CF₃), 126.0, 128.3, 128.8, 129.2, 129.8, 130.3, 134.4, 137.5, 144.7 (q, $J_{\text{CF}} = 36.5$ Hz, C-CF₃), 146.6 (Ar); ^{19}F NMR (376.5 MHz, CDCl_3): δ -63.4; HRMS (ESI): m/z calcd for C₁₆H₁₀ClF₃IN₂⁺ [M+H⁺]: 448.9524; found: 448.9533.

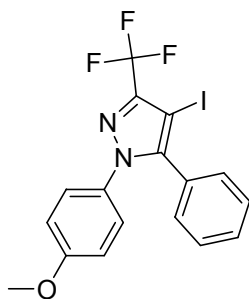


3-(Trifluoromethyl)-1-(4-fluorophenyl)-4-iodo-5-phenyl-1H-pyrazole (4c). Pale yellow powder, m.p. 116-118 °C (0.630 g, 97% yield); ^1H NMR (400.1 MHz, CDCl_3): δ 6.98-7.04 (m, 2H, 4-FC₆H₄), 7.18-7.23 (m, 2H, 4-FC₆H₄), 7.25-7.28 (m, 2H, Ph), 7.39-7.46 (m, 3H, Ph); ^{13}C NMR (100.6 MHz, CDCl_3): δ 59.5 (C-I), 116.0 (d, $^2J_{\text{CF}} = 23.2$ Hz), 120.7 (q, $J_{\text{CF}} = 270.5$ Hz, CF₃), 126.9 (d, $^3J_{\text{CF}} = 8.8$ Hz), 128.3, 128.8, 129.8, 130.3, 135.1 (d, $^4J_{\text{CF}} = 3.3$ Hz), 144.5 (q, $J_{\text{CF}} = 36.5$ Hz, C-CF₃), 146.7, 162.1 (d, $^1J_{\text{CF}} = 249.5$ Hz, C-F); ^{19}F NMR (376.5 MHz, CDCl_3): δ -63.6 (3F, CF₃), -113.1 (1F, 4-FC₆H₄); HRMS (ESI): m/z calcd for C₁₆H₁₀F₄IN₂⁺ [M+H⁺]: 432.9819; found: 432.9820.

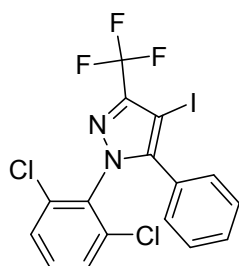


3-(Trifluoromethyl)-4-iodo-5-phenyl-1-p-tolyl-1H-pyrazole (4d). Pale brown powder, m.p. 100-102 °C (0.639 g, 100% yield); ^1H NMR (400.1 MHz, CDCl_3) δ 2.32 (s, 3H, Me), 7.09 (s, 4H), 7.24-7.27 (m, 2H), 7.37-7.41 (m, 3H); ^{13}C NMR (100.6 MHz, CDCl_3) δ 21.0, 59.2 (C-I), 120.7 (q, J_{CF}

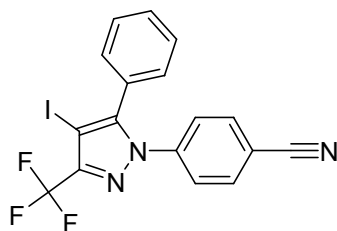
= 270.2 Hz, CF₃), 124.8, 128.6, 129.5, 130.3, 136.6, 138.6, 144.1 (q, J_{CF} = 36.9 Hz, C-CF₃), 146.5; ¹⁹F NMR (376.3 MHz, CDCl₃) δ -63.2; HRMS (ESI): m/z calcd for C₁₇H₁₃F₃IN₂⁺ [M+H⁺]: 429.007; found: 429.0064.



3-(Trifluoromethyl)-4-iodo-1-(4-methoxyphenyl)-5-phenyl-1H-pyrazole (4e). Brown powder, m.p. 109-110 °C (0.664 g, 100% yield); ¹H NMR (400.1 MHz, CDCl₃): δ 3.78 (s, 3H, OCH₃), 6.81 (d, J_{HH} = 9.0 Hz, 2H, 4-MeOC₆H₄), 7.13 (d, J_{HH} = 9.0 Hz, 2H, 4-MeOC₆H₄), 7.25-7.28 (m, 2H, Ph), 7.38-7.41 (m, 3H, Ph); ¹³C NMR (100.6 MHz, CDCl₃): δ 55.4 (OCH₃), 58.9 (C-I), 114.1, 120.8 (q, J_{CF} = 270.5 Hz, CF₃), 126.4, 128.6, 129.5, 130.3, 132.1, 144.0 (q, J_{CF} = 36.5 Hz, C-CF₃), 146.6, 159.4 (Ar); ¹⁹F NMR (376.5 MHz, CDCl₃): δ -63.2; HRMS (ESI): m/z calcd for C₁₇H₁₃F₃IN₂O⁺ [M+H⁺]: 445.0019; found: 445.0022.



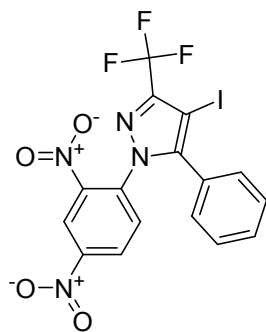
1-(2,6-dichlorophenyl)-3-(trifluoromethyl)-4-iodo-5-phenyl-1H-pyrazole (4f). Pale brown powder, m.p. 138-139 °C (0.723 g, 100% yield); ¹H NMR (400.1 MHz, CDCl₃) δ 7.27-7.40 (m, 8H, Ph); ¹³C NMR (100.6 MHz, CDCl₃) δ 58.1 (C-I), 120.6 (q, J_{CF} = 270.5 Hz, CF₃), 127.5, 128.5, 128.6, 129.5, 130.0, 131.6, 134.8, 145.6 (q, J_{CF} = 37.2 Hz, C-CF₃), 149.1; ¹⁹F NMR (376.3 MHz, CDCl₃) δ -63.6; HRMS (ESI): m/z calcd for C₁₆H₉Cl₂F₃IN₂⁺ [M+H⁺]: 482.9134; found: 482.9137.



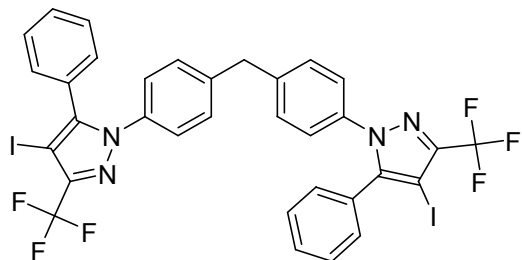
4-(3-(Trifluoromethyl)-4-iodo-5-phenyl-1H-pyrazol-1-yl)benzonitrile (4g). Pale brown powder, m.p. 137-138 °C (0.657 g, 100% yield); ¹H NMR (400.1 MHz, CDCl₃) δ 7.26-7.29 (m, 2H, Ph), 7.36 (d, J_{HH} = 8.7 Hz, 2H, 4-CNC₆H₄), 7.44-7.52 (m, 3H, Ph), 7.60 (d, J_{HH} = 8.7 Hz, 2H, 4-CNC₆H₄); ¹³C NMR (100.6 MHz, CDCl₃) δ 61.2 (C-I), 112.0, 117.6,

120.5 (q, $J_{CF} = 270.5$ Hz, CF_3), 124.9, 128.0, 129.1, 130.1, 130.2, 133.0, 142.0, 145.5 (q, $J_{CF} = 37.2$ Hz, C- CF_3), 146.8;

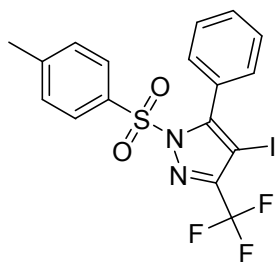
^{19}F NMR (376.3 MHz, $CDCl_3$) δ -63.6; HRMS (ESI): m/z calcd for $C_{17}H_{10}F_3IN_3^+$ [$M+H^+$]: 439.9866; found: 439.9867.



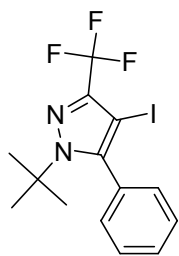
3-(Trifluoromethyl)-4-iodo-1-(2,4-dinitrophenyl)-5-phenyl-1H-pyrazole (4h). Pale yellow-green powder, m.p. 78-80 °C, (0.712 g, 94% yield); 1H NMR (400.1 MHz, $CDCl_3$) δ 7.26-7.28 (m, 2H, Ph), 7.40-7.49 (m, 3H, Ph), 7.54 (d, $J_{HH} = 8.7$ Hz, 1H, 2,4- $diNO_2C_6H_4$), 8.44 (dd, $J_{HH}=8.7$, $J_{HH}=2.1$ Hz, 1H, 2,4- $(NO_2)_2C_6H_4$), 8.76 (d, $J_{HH}=2.1$ Hz, 1H, 2,4- $(NO_2)_2C_6H_4$); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 60.6 (C-I), 120.1 (q, $J_{CF} = 270.5$ Hz, CF_3), 121.1, 126.5, 127.7, 129.2, 130.1, 130.5, 130.6, 136.8, 144.8 (q, $J_{CF} = 37.6$ Hz, C- CF_3), 147.3, 148.2; ^{19}F NMR (376.3 MHz, $CDCl_3$) δ -63.9; HRMS (ESI): m/z calcd for $C_{16}H_9F_3IN_4O_4^+$ [$M+H^+$]: 504.9615; found: 504.9612.



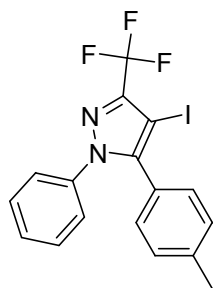
bis(4-(3-(Trifluoromethyl)-4-iodo-5-phenyl-1H-pyrazol-1-yl)phenyl)methane (4i). Pale brown powder, m.p. 97-99 °C (0.620 g, 98% yield); 1H NMR (400.1 MHz, $CDCl_3$) δ 3.93 (s, 2H, CH_2), 7.06 (d, $J_{HH} = 8.5$ Hz, 4H), 7.13 (d, $J_{HH} = 8.5$ Hz, 4H), 7.24-7.28 (m, 4H, Ph), 7.37-7.45 (m, 6H, Ph); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 40.7, 59.5 (C-I), 120.7 (q, $J_{CF} = 270.2$ Hz, CF_3), 125.0, 128.5, 128.7, 129.4, 129.7, 130.3, 137.4, 140.8, 144.3 (q, $J_{CF} = 36.9$ Hz, C- CF_3), 146.5; ^{19}F NMR (376.3 MHz, $CDCl_3$) δ -63.3; HRMS (ESI): m/z calcd for $C_{33}H_{21}F_6I_2N_4^+$ [$M+H^+$]: 840.9754; found: 840.9774.



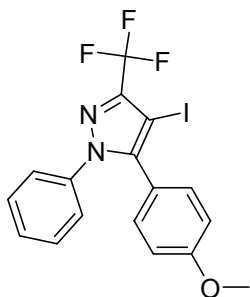
3-(Trifluoromethyl)-4-iodo-5-phenyl-1-tosyl-1H-pyrazole (4j). White powder, m.p. 121-123 °C (0.717 g, 97% yield); ¹H NMR (400.1 MHz, CDCl₃) δ 2.42 (s, 3H, Me), 7.21-7.24 (m, 2H, Ph), 7.27 (d, *J*_{HH} = 8.3 Hz, 2H, Tos), 7.47-7.51 (m, 2H, Ph), 7.54-7.56 (m, 1H, Ph), 7.58 (d, *J*_{HH} = 8.3 Hz, 2H, Tos); ¹³C NMR (100.6 MHz, CDCl₃) δ 21.8, 64.2 (C-I), 119.8 (q, *J*_{CF} = 271.3 Hz, CF₃), 127.7, 128.2, 128.6, 130.1, 130.4, 130.6, 133.2, 144.8 (q, *J*_{CF} = 37.6 Hz, C-CF₃), 146.9, 149.6; ¹⁹F NMR (376.3 MHz, CDCl₃) δ -64.2; HRMS (ESI): m/z calcd for C₁₇H₁₃F₃IN₂O₂S⁺ [M+H⁺]: 492.9689; found: 492.9697.



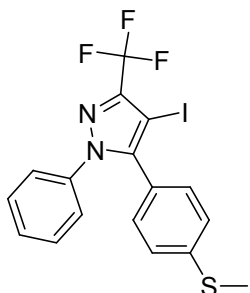
1-tert-Butyl-3-(trifluoromethyl)-4-iodo-5-phenyl-1H-pyrazole (4k). White powder, m.p. 89-91 °C (0.515 g, 87% yield). ¹H NMR (400 MHz, CDCl₃): δ 1.47 (s, 9H), 7.27-7.29 (m, 2H, Ph), 7.50-7.52 (m, 3H, Ph); ¹³C NMR (100.6 MHz, CDCl₃): δ 30.6 (CH₃), 61.8 (C-I), 63.8 (C(CH₃)₃), 121.1 (q, *J*_{CF} = 269.8 Hz, CF₃), 128.5, 129.6, 131.0, 132.0, 140.6 (q, *J*_{CF} = 39.5 Hz, C-CF₃), 146.9. ¹⁹F NMR (376.5 MHz, CDCl₃): δ -62.9. HRMS (ESI): m/z calcd for C₁₄H₁₅F₃IN₂⁺ [M+H⁺]: 395.0227; found: 395.0226.



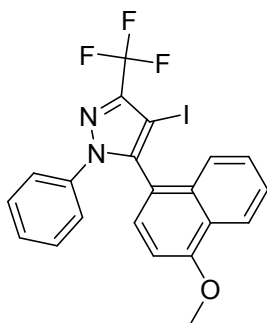
3-(Trifluoromethyl)-4-iodo-1-phenyl-5-p-tolyl-1H-pyrazole (4l). Pale yellow-brown powder, m.p. 122-123 °C (0.630 g, 98% yield); ¹H NMR (400.1 MHz, CDCl₃) δ 2.38 (s, 3H, Me), 7.14 (d, *J*_{HH} = 8.2 Hz, 2H, 4-MeC₆H₄), 7.19 (d, *J*_{HH} = 8.2 Hz, 2H, 4-MeC₆H₄), 7.20-7.23 (m, 2H, Ph), 7.29-7.31 (m, 3H, Ph); ¹³C NMR (100.6 MHz, CDCl₃) δ 21.4, 59.4 (C-I), 120.8 (q, *J*_{CF} = 270.5 Hz, CF₃), 125.0, 125.5, 128.4, 129.0, 129.4, 130.1, 139.1, 139.7, 144.3 (q, *J*_{CF} = 36.9 Hz, C-CF₃), 146.7; ¹⁹F NMR (376.3 MHz, CDCl₃) δ -63.3; HRMS (ESI): m/z calcd for C₁₇H₁₃F₃IN₂⁺ [M+H⁺]: 429.0070; found: 429.0070.



3-(Trifluoromethyl)-4-iodo-5-(4-methoxyphenyl)-1-phenyl-1H-pyrazole (4m). Pale yellow-brown powder, m.p. 143-145 °C (0.441 g, 99%); ¹H NMR (400.1 MHz, CDCl₃) δ 3.82 (s, 3H, MeO), 6.89 (d, *J*_{HH} = 8.8 Hz, 2H, 4-MeOC₆H₄), 7.18 (d, *J*_{HH} = 8.8 Hz, 2H, 4-MeOC₆H₄), 7.19-7.22 (m, 2H, Ph), 7.29-7.32 (m, 3H, Ph); ¹³C NMR (100.6 MHz, CDCl₃) δ 55.2, 59.5 (C-I), 114.1, 120.5, 120.8 (q, *J*_{CF} = 270.5 Hz, CF₃), 124.9, 128.4, 129.0, 131.6, 139.1, 144.2 (q, *J*_{CF} = 36.9 Hz, C-CF₃), 146.5, 160.3; ¹⁹F NMR (376.3 MHz, CDCl₃) δ -63.3. HRMS (ESI): m/z calcd for C₁₇H₁₃F₃IN₂O⁺ [M+H⁺]: 445.0019; found: 445.0020.

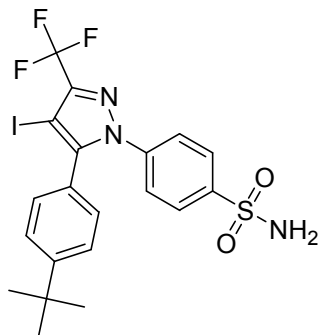


3-(Trifluoromethyl)-4-iodo-5-(4-(methylthio)phenyl)-1-phenyl-1H-pyrazole (4n). Brown powder, m.p. 92-94 °C (0.688 g, 100% yield); ¹H NMR (400.1 MHz, CDCl₃) δ 2.48 (s, 3H, MeS), 7.15 (d, *J*_{HH} = 8.5 Hz, 2H, 4-MeSC₆H₄), 7.20-7.23 (m, 4H, Ph), 7.30-7.33 (m, 3H, Ph); ¹³C NMR (100.6 MHz, CDCl₃) δ 14.9, 59.5 (C-I), 120.8 (q, *J*_{CF} = 270.2 Hz, CF₃), 124.5, 125.0, 125.5, 128.5, 129.1, 130.5, 139.0, 141.1, 144.4 (q, *J*_{CF} = 36.9 Hz, C-CF₃), 146.1; ¹⁹F NMR (376.3 MHz, CDCl₃) δ -63.3; HRMS (ESI): m/z calcd C₁₇H₁₃F₃IN₂S⁺ [M+H⁺]: 460.9791; found: 460.9795.

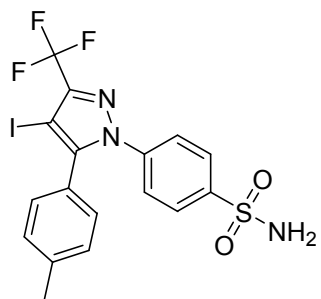


3-(Trifluoromethyl)-4-iodo-5-(1-methoxynaphthalen-4-yl)-1-phenyl-1H-pyrazole (4o). Pale brown powder, m.p. 159-161 °C (0.705 g, 95% yield); ¹H NMR (400.1 MHz, CDCl₃) δ 4.04 (s, 3H, MeO), 6.82 (d, *J*_{HH} = 8.0 Hz, 1H), 7.14-

7.21 (m, 5H), 7.26 (d, $J_{HH} = 8.0$ Hz, 1H), 7.42-7.45 (m, 1H), 7.47-7.54 (m, 2H), 8.32-8.35 (m, 1H); ^{13}C NMR (100.6 MHz, CDCl_3) δ 55.6, 62.5 (C-I), 103.2, 118.3, 120.9 (q, $J_{CF} = 270.2$ Hz, CF_3), 122.6, 123.9, 124.7, 125.5, 125.8, 127.7, 128.2, 128.8, 130.2, 132.3, 139.2, 144.2 (q, $J_{CF} = 37.2$ Hz, C- CF_3), 146.4, 157.0; ^{19}F NMR (376.3 MHz, CDCl_3) δ -63.1; HRMS (ESI): m/z calcd for $\text{C}_{21}\text{H}_{15}\text{F}_3\text{IN}_2\text{O}^+$ [$\text{M}+\text{H}^+$]: 495.0176; found: 495.0177.

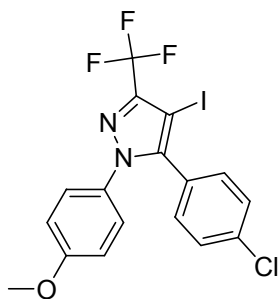


4-[5-(4-*tert*-Butylphenyl)-4-iodo-3-(trifluoromethyl)-1H-pyrazol-1-yl]benzenesulfonamide (4p). Pale yellow-brown powder, m.p. 185-187 °C (0.821 g, 100% yield); ^1H NMR (400.1 MHz, CDCl_3) δ 1.33 (s, 9H, *t*-Bu), 5.22 (s, 2H, NH_2), 7.17 (d, $J_{HH} = 8.5$ Hz, 2H, 4-*t*- BuC_6H_4), 7.34 (d, $J_{HH} = 8.7$ Hz, 2H, 4-(SO_2NH_2) C_6H_4), 7.43 (d, $J_{HH} = 8.5$ Hz, 2H, 4-*t*- BuC_6H_4), 7.81 (d, $J_{HH} = 8.7$ Hz, 2H, 4-(SO_2NH_2) C_6H_4); ^{13}C NMR (100.6 MHz, CDCl_3) δ 31.1 (C-(CH_3) $_3$), 34.9 (C-(CH_3) $_3$), 60.9 (C-I), 120.6 (q, $J_{CF} = 270.2$ Hz, CF_3), 124.9, 125.0, 126.0, 127.4, 129.8, 141.4, 142.2, 145.2 (q, $J_{CF} = 36.8$ Hz, C- CF_3), 147.0, 153.5; ^{19}F NMR (376.3 MHz, CDCl_3) δ -63.4; HRMS (ESI): m/z calcd for $\text{C}_{20}\text{H}_{20}\text{F}_3\text{IN}_3\text{O}_2\text{S}^+$ [$\text{M}+\text{H}^+$]: 550.0268; found: 550.0255.



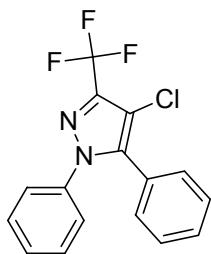
4-[5-(4-Methylphenyl)-4-iodo-3-(trifluoromethyl)-1H-pyrazol-1-yl]benzenesulfonamide (4q). Pale yellow-brown powder, m.p. 186-188 °C (0.759 g, 100% yield); ^1H NMR (400.1 MHz, CDCl_3) δ 2.41 (s, 3H, Me), 4.81 (s, 2H, NH_2), 7.13 (d, $J_{HH} = 8.1$ Hz, 2H, 4-Me C_6H_4), 7.23 (d, $J_{HH} = 8.1$ Hz, 2H, 4-Me C_6H_4), 7.37 (d, $J_{HH} = 8.8$ Hz, 2H, 4-(SO_2NH_2) C_6H_4), 7.85 (d, $J_{HH} = 8.8$ Hz, 2H, 4-(SO_2NH_2) C_6H_4); ^1H NMR (400.1 MHz, $\text{DMSO}-d_6$) δ 2.34 (s, 3H, Me), 7.23 (d, $J_{HH} = 8.3$ Hz, 2H, 4-Me C_6H_4), 7.27 (d, $J_{HH} = 8.3$ Hz, 2H, 4-Me C_6H_4), 7.47 (s, 2H, NH_2), 7.48 (d, $J_{HH} = 8.7$ Hz, 2H, 4-(SO_2NH_2) C_6H_4), 7.82 (d, $J_{HH} = 8.7$ Hz, 2H, 4-(SO_2NH_2) C_6H_4); ^{13}C NMR (100.6 MHz, $\text{DMSO}-d_6$) δ 20.8, 62.8 (C-I), 120.9 (q, $J_{CF} = 270.2$ Hz, CF_3), 125.1, 125.8, 126.6, 129.3, 130.2, 139.6, 140.9, 143.2 (q, $J_{CF} = 35.8$ Hz, C- CF_3), 144.0,

147.5; ^{19}F NMR (376.3 MHz, CDCl_3) δ -63.6; ^{19}F NMR (376.3 MHz, $\text{DMSO-}d_6$) δ -63.7; HRMS (ESI): m/z calcd for $\text{C}_{17}\text{H}_{14}\text{F}_3\text{IN}_3\text{O}_2\text{S}^+$ $[\text{M}+\text{H}^+]$: 507.9798; found: 507.9796.

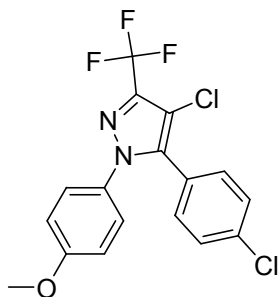


5-(4-Chlorophenyl)-3-(trifluoromethyl)-4-iodo-1-(4-methoxyphenyl)-1H-pyrazole (4r). Pale brown powder, m.p. 107-108 °C (0.717 g, 100% yield); ^1H NMR (400.1 MHz, CDCl_3) δ 3.77 (s, 3H, MeO), 6.81 (d, $J_{\text{HH}} = 9.0$ Hz, 2H, 4-MeOC $_6\text{H}_4$), 7.11 (d, $J_{\text{HH}} = 9.0$ Hz, 2H, 4-MeOC $_6\text{H}_4$), 7.19 (d, $J_{\text{HH}} = 8.5$ Hz, 2H, 4-ClC $_6\text{H}_4$), 7.35 (d, $J_{\text{HH}} = 8.5$ Hz, 2H, 4-ClC $_6\text{H}_4$); ^{13}C NMR (100.6 MHz, CDCl_3) δ 55.4, 59.1 (C-I), 114.2, 120.7 (q, $J_{\text{CF}} = 270.5$ Hz, CF $_3$), 126.4, 126.9, 128.9, 131.6, 131.8, 135.7, 144.1 (q, $J_{\text{CF}} = 36.9$ Hz, C-CF $_3$), 145.4, 159.6; ^{19}F NMR (376.3 MHz, CDCl_3) δ -63.2; HRMS (ESI): m/z calcd for $\text{C}_{17}\text{H}_{12}\text{ClF}_3\text{IN}_2\text{O}^+$ $[\text{M}+\text{H}^+]$: 478.9629; found: 478.9626.

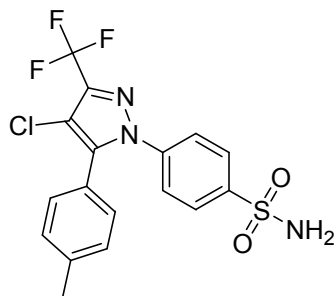
Synthesis of chloropyrazoles 5 (general procedure): A 8 mL screw neck vial was charged with corresponding hydrazone **3** (0.5 mmol), NCS (0.134 g, 1 mmol, 2 equiv), CuCl (0.0025 g, 0.025 mmol, 5 mol%), MeCN (2 mL) and heated for 2-4 h at 80 °C. The reaction mixture was poured into water (50 mL) and extracted with dichloromethane (3x20 mL). The combined organic phase was washed with water (20 mL) and dried over anhydrous sodium sulfate. Volatiles were evaporated in vacuo, the residue was purified by column chromatography on silica gel using mixture of hexane with CH_2Cl_2 (2:1) for **5a,b** or CH_2Cl_2 with MeOH (30:1) for **5c**.



4-Chloro-3-(trifluoromethyl)-1,5-diphenyl-1H-pyrazole (5a). Yellow powder, m.p. 91-93 °C (0.137 g, 85% yield). ^1H NMR (400 MHz, CDCl_3) δ 7.25-7.31 (m, 4H, Ph), 7.33-7.37 (m, 3H, Ph), 7.37-7.43 (m, 3H, Ph); ^{13}C NMR (100.6 MHz, CDCl_3) δ 108.7 (C-Cl), 120.6 (q, $J = 269.8$ Hz, CF $_3$), 125.0, 126.7, 128.6, 128.7, 129.1, 129.6, 129.8, 138.9, 139.6 (q, $J = 37.6$ Hz, C-CF $_3$), 141.3; ^{19}F NMR (376.5 MHz, CDCl_3) δ -63.6. HRMS (ESI): m/z calcd for $\text{C}_{16}\text{H}_{11}^{35}\text{ClF}_3\text{N}_2^+$ $[\text{M}+\text{H}^+]$: 323.0557; found: 325.0558; calcd for $\text{C}_{16}\text{H}_{11}^{37}\text{ClF}_3\text{N}_2^+$ $[\text{M}+\text{H}^+]$: 325.0528; found: 325.0527.

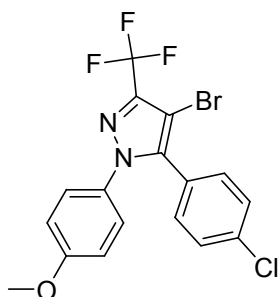


4-Chloro-5-(4-chlorophenyl)-3-(trifluoromethyl)-1-(4-methoxyphenyl)-1H-pyrazole (5b). Pale yellow powder, m.p. 87-89 °C (0.186 g, 96% yield); ^1H NMR (400.1 MHz, CDCl_3) δ 3.78 (s, 3H, MeO), 6.84 (d, $J_{\text{HH}} = 9.0$ Hz, 2H, 4-MeOC $_6$ H $_4$), 7.14 (d, $J_{\text{HH}} = 9.0$ Hz, 2H, 4-MeOC $_6$ H $_4$), 7.21 (d, $J_{\text{HH}} = 8.6$ Hz, 2H, 4-ClC $_6$ H $_4$), 7.35 (d, $J_{\text{HH}} = 8.6$ Hz, 2H, 4-ClC $_6$ H $_4$); ^{13}C NMR (100.6 MHz, CDCl_3) δ 55.4, 108.4 (C-Cl), 114.3, 120.5 (q, $J_{\text{CF}} = 270.5$ Hz, CF $_3$), 125.2, 126.4, 129.0, 131.1, 131.7, 135.7, 139.3 (q, $J_{\text{CF}} = 37.2$ Hz, C-CF $_3$), 140.1, 159.7; ^{19}F NMR (376.3 MHz, CDCl_3) δ -63.5; HRMS (ESI): m/z calcd for C $_{17}$ H $_{12}$ Cl $_2$ F $_3$ N $_2$ O $^+$ [M+H $^+$]: 387.0273; found: 387.0265.



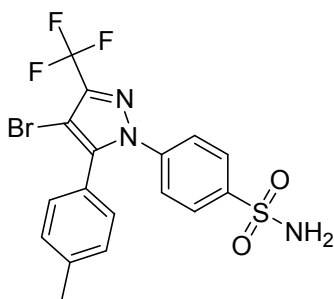
4-[4-Chloro-5-(4-methylphenyl)-3-(trifluoromethyl)-1H-pyrazol-1-yl]benzenesulfonamide (5c)

Pale yellow crystals, m.p. 169-171 °C (0.181 g, 87% yield); ^1H NMR (600.1 MHz, CDCl_3) δ 2.39 (s, 3H, Me), 5.16 (s, 2H, NH $_2$), 7.15 (d, $J_{\text{HH}} = 7.7$ Hz, 2H, 4-MeC $_6$ H $_4$), 7.23 (d, $J_{\text{HH}} = 7.7$ Hz, 2H, 4-MeC $_6$ H $_4$), 7.39 (d, $J_{\text{HH}} = 8.8$ Hz, 2H, 4-(SO $_2$ NH $_2$)C $_6$ H $_4$), 7.85 (d, $J_{\text{HH}} = 8.8$ Hz, 2H, 4-(SO $_2$ NH $_2$)C $_6$ H $_4$); ^{13}C NMR (150.9 MHz, CDCl_3) δ 21.4, 109.7 (C-Cl), 120.3 (q, $J_{\text{CF}} = 270.9$ Hz, CF $_3$), 123.2, 125.1, 127.5, 129.6, 129.9, 140.5, 140.6 (q, $J_{\text{CF}} = 37.6$ Hz, C-CF $_3$), 141.5, 141.9, 142.1; ^{19}F NMR (376.3 MHz, CDCl_3) δ -63.9; HRMS (ESI): m/z calcd for C $_{17}$ H $_{14}$ ClF $_3$ N $_3$ O $_2$ S $^+$ [M+H $^+$]: 416.0442; found: 416.0440.

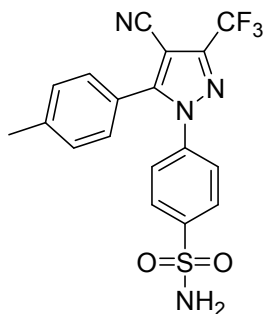


4-Bromo-5-(4-chlorophenyl)-3-(trifluoromethyl)-1-(4-methoxyphenyl)-1H-pyrazole (6a). A 8 mL screw neck vial was charged with hydrazone **3r** (1 mmol), MeCN (4 mL), NaHCO₃ (0.126 g, 1.5 mmol), Br₂ (1.5 mL of 1M solution in MeCN, 1.5 mmol) and stirred at room temperature overnight. The reaction mixture was poured into water (50 mL) and extracted with dichloromethane (3x20 mL). The combined organic phase was washed with water (20 mL) and dried over anhydrous sodium sulfate. Volatiles were evaporated in vacuo, the residue was purified by column chromatography on silica gel using mixture of hexane with CH₂Cl₂ (2:1).

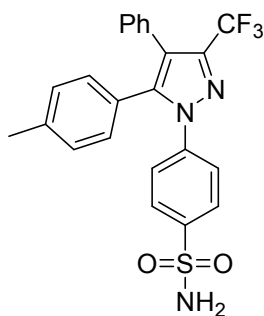
Pale brown powder, m.p. 104-106 °C (0.374 g, 87% yield); ¹H NMR (400.1 MHz, CDCl₃) δ 3.78 (s, 3H, MeO), 6.83 (d, *J*_{HH} = 9.0 Hz, 2H, 4-MeOC₆H₄), 7.13 (d, *J*_{HH} = 9.0 Hz, 2H, 4-MeOC₆H₄), 7.21 (d, *J*_{HH} = 8.6 Hz, 2H, 4-ClC₆H₄), 7.35 (d, *J*_{HH} = 8.6 Hz, 2H, 4-ClC₆H₄); ¹³C NMR (100.6 MHz, CDCl₃) δ 55.4, 93.0 (C-Br), 114.3, 120.6 (q, *J*_{CF} = 269.8 Hz, CF₃), 125.8, 126.4, 129.0, 131.3, 131.7, 135.7, 140.9 (q, *J*_{CF} = 37.2 Hz, C-CF₃), 141.9, 159.7; ¹⁹F NMR (376.3 MHz, CDCl₃) δ -63.5; HRMS (ESI): m/z calcd for C₁₇H₁₂⁷⁹BrClF₃N₂O⁺ [M+H⁺]: 430.9768; found: 430.9753; calcd for C₁₇H₁₂⁸¹BrClF₃N₂O⁺ [M+H⁺]: 432.9747; found: 432.9749.



4-[4-Bromo-5-(4-methylphenyl)-3-(trifluoromethyl)-1H-pyrazol-1-yl]benzenesulfonamide (6b). A 8 mL screw neck vial was charged with corresponding hydrazone **3p** (0.5 mmol), NBS (0.134 g, 1 mmol, 2 equiv), MeCN (2 mL) and heated for 2 h at 80 °C. The reaction mixture was poured into water (50 mL) and extracted with dichloromethane (3x20 mL). The combined organic phase was washed with water (20 mL) and dried over anhydrous sodium sulfate. Volatiles were evaporated in vacuo, the residue was purified by column chromatography on silica gel using mixture of CH₂Cl₂ with MeOH (30:1). Pale yellow-green powder, m.p. 155-157 °C (0.209 g, 91% yield); ¹H NMR (600.1 MHz, CDCl₃) δ 2.40 (s, 3H, Me), 5.28 (s, 2H, NH₂), 7.16 (d, *J*_{HH} = 8.0 Hz, 2H, 4-MeC₆H₄), 7.24 (d, *J*_{HH} = 8.0 Hz, 2H, 4-MeC₆H₄), 7.38 (d, *J*_{HH} = 8.8 Hz, 2H, 4-(SO₂NH₂)C₆H₄), 7.85 (d, *J*_{HH} = 8.8 Hz, 2H, 4-(SO₂NH₂)C₆H₄); ¹³C NMR (150.9 MHz, CDCl₃) δ 21.4, 94.4 (C-Br), 120.4 (q, *J*_{CF} = 269.8 Hz, CF₃), 123.8, 125.0, 127.4, 129.76, 129.84, 140.5, 141.5, 142.1 (q, *J*_{CF} = 37.6 Hz, C-CF₃), 142.1, 143.7; ¹⁹F NMR (376.3 MHz, CDCl₃) δ -63.9; HRMS (ESI): m/z calcd for C₁₇H₁₄⁷⁹BrF₃N₃O₂S⁺ [M+H⁺]: 459.9937; found: 459.9935; calcd for C₁₇H₁₄⁸⁴BrF₃N₃O₂S⁺ [M+H⁺]: 461.9917; found: 461.9917.

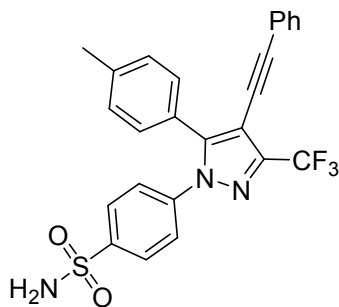


4-[4-Cyano-5-(4-methylphenyl)-3-(trifluoromethyl)-1H-pyrazol-1-yl]benzenesulfonamide (7). A 25 mL one necked round-bottomed flask was charged with iodopyrazole **4q** (0.177 g, 0.35 mmol), CuCN (0.038 g, 0.42 mmol), dry DMF (2 mL), flushed with argon and heated with reflux condenser at 150-155 °C (oil bath) for 8 h. The cooled reaction mixture was dispersed between CH₂Cl₂ and water (both 50 mL) and filtered through celite. Organic layer was separated, the water layer was extracted with CH₂Cl₂ (3x20 mL), combined extract was washed with 0.1 M HCl (50 mL) and dried over Na₂SO₄. Volatiles were evaporated in vacuo, the residue was purified by column chromatography on silica gel using mixture of CH₂Cl₂ and MeOH (30:1). Evaporation of the solvents gave compound **7** as white powder, 0.129 g, 91% yield; m.p. 174-176 °C. ¹H NMR (600.1 MHz, CDCl₃) δ 2.38 (s, 3H, Me), 5.32 (s, 2H, NH₂), 7.20 (d, *J*_{HH} = 8.4 Hz, 2H, 4-MeC₆H₄), 7.24 (d, *J*_{HH} = 8.4 Hz, 2H, 4-MeC₆H₄), 7.42 (d, *J*_{HH} = 8.9 Hz, 2H, 4-(SO₂NH₂)C₆H₄), 7.90 (d, *J*_{HH} = 8.9 Hz, 2H, 4-(SO₂NH₂)C₆H₄); ¹³C NMR (150.9 MHz, CDCl₃) δ 21.4, 92.7, 110.8, 119.5 (q, *J*_{CF} = 270.9 Hz, CF₃), 121.9, 125.6, 127.7, 129.0, 130.3, 141.0, 142.0, 142.7, 144.9 (q, *J*_{CF} = 39.4 Hz, C-CF₃), 150.4; ¹⁹F NMR (376.3 MHz, CDCl₃) δ -63.7; HRMS (ESI): m/z calcd for C₁₈H₁₄F₃N₄O₂S⁺ [M+H⁺]: 407.0784; found: 407.0777.

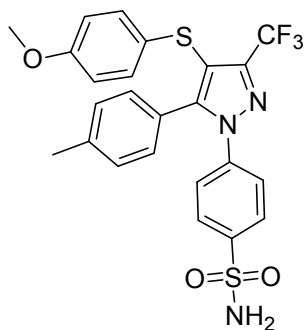


4-[5-(4-Methylphenyl)-4-phenyl-3-(trifluoromethyl)-1H-pyrazol-1-yl]benzenesulfonamide (8). A 12 mL screw neck vial was flushed with argon and charged with iodopyrazole **4q** (0.177 g, 0.35 mmol), PhB(OH)₂ (0.051 g, 0.42 mmol), K₂CO₃ (0.097 g, 0.7 mmol), DMF (4 mL), water (0.5 mL), Pd(PPh₃)₄ (0.020 g, 0.0175 mmol, 5 mol%). The vial was repeatedly flushed with argon, close tightly and heated at 110 °C for 14 h. The cooled reaction mixture was dispersed between CH₂Cl₂ and water (both 50 mL) and filtered through celite. Organic layer was separated, the water layer was extracted with CH₂Cl₂ (3x20 mL), combined extract was washed with 0.1 M HCl (50 mL) and dried over Na₂SO₄. Volatiles were evaporated in vacuo, the residue was

purified by column chromatography on silica gel using mixture of CH₂Cl₂ and MeOH (30:1). Evaporation of the solvents gave compound **8** as white powder, 0.132 g, 83% yield; m.p. 95-97 °C. ¹H NMR (600.1 MHz, CDCl₃) δ 2.27 (s, 3H, Me), 5.50 (s, 2H, NH₂), 6.89 (d, *J*_{HH} = 8.1 Hz, 2H, 4-MeC₆H₄), 7.02 (d, *J*_{HH} = 8.1 Hz, 2H, 4-MeC₆H₄), 7.19-7.20 (m, 2H, Ph), 7.28-7.29 (m, 3H, Ph), 7.41 (d, *J*_{HH} = 8.6 Hz, 2H, 4-(SO₂NH₂)C₆H₄), 7.84 (d, *J*_{HH} = 8.6 Hz, 2H, 4-(SO₂NH₂)C₆H₄); ¹³C NMR (150.6 MHz, CDCl₃) δ 21.2, 121.3 (q, *J*_{CF} = 270.9 Hz, CF₃), 121.7, 124.8, 125.4, 127.3, 127.7, 128.1, 129.6, 129.8, 130.0, 130.1, 139.4, 141.2, 141.6 (q, *J*_{CF} = 36.5 Hz, C-CF₃), 142.3, 142.9; ¹⁹F NMR (376.3 MHz, CDCl₃) δ -60.9; HRMS (ESI): m/z calcd for C₂₃H₁₉F₃N₃O₂S⁺ [M+H⁺]: 458.1145; found: 458.1145.



4-[5-(4-Methylphenyl)-4-(phenylethynyl)-3-(trifluoromethyl)-1H-pyrazol-1-yl]benzenesulfonamide (9). A 12 mL screw neck vial was flushed with argon and charged with iodopyrazole **4q** (0.177 g, 0.35 mmol), phenylacetylene (0.042 g, 0.42 mmol), Et₃N (0.071 g, 0.7 mmol), MeCN (2.5 mL), Pd(PPh₃)₂Cl₂ (0.012 g, 0.0175 mmol, 5 mol%), CuI (0.0067 g, 0.035 mmol, 10 mol%). The vial was repeatedly flushed with argon, close tightly and heated at 80 °C for 14 h. The cooled reaction mixture was dispersed between CH₂Cl₂ and water (both 50 mL) and filtered through celite. Organic layer was separated, the water layer was extracted with CH₂Cl₂ (3x20 mL), combined extract was washed with 0.1 M HCl (50 mL) and dried over Na₂SO₄. Volatiles were evaporated in vacuo, the residue was purified by column chromatography on silica gel using mixture of CH₂Cl₂ and MeOH (30:1). Evaporation of the solvents gave compound **9** as white powder, 0.126 g, 75% yield; m.p. 233-235 °C. ¹H NMR (600.1 MHz, CD₃CN) δ 2.37 (s, 3H, Me), 5.67 (br s, 2H, NH₂), 7.27-7.29 (m, 2H, 4-MeC₆H₄), 7.34 (d, *J*_{HH} = 8.1 Hz, 2H, 4-MeC₆H₄), 7.37-7.40 (m, 3H, Ph), 7.41-7.44 (m, 2H, Ph), 7.49 (d, *J*_{HH} = 8.9 Hz, 2H, 4-(SO₂NH₂)C₆H₄), 7.88 (d, *J*_{HH} = 8.9 Hz, 2H, 4-(SO₂NH₂)C₆H₄); ¹³C NMR (150.9 MHz, CD₃CN) δ 21.4, 78.5, 95.1, 103.6, 122.1 (q, *J*_{CF} = 269.6 Hz, CF₃), 123.2, 125.3, 126.9, 128.1, 129.6, 129.9, 130.4, 130.5, 132.1, 141.4, 142.6, 144.0 (q, *J*_{CF} = 36.7 Hz, C-CF₃), 144.3, 148.2; ¹⁹F NMR (376.3 MHz, CDCl₃) δ -61.5; HRMS (ESI): m/z calcd for C₂₅H₁₉F₃N₃O₂S⁺ [M+H⁺]: 482.1145; found: 482.1147.

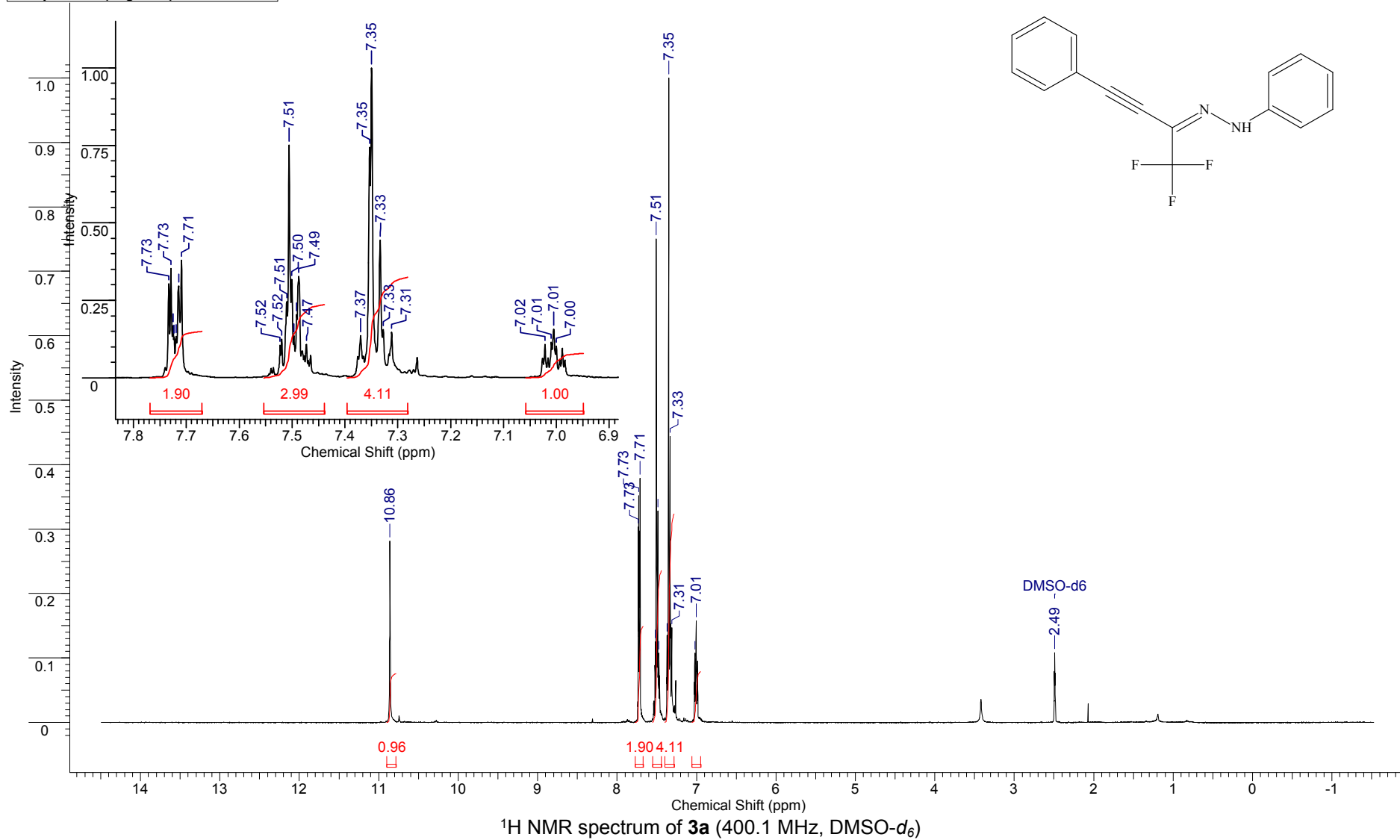


4-[4-[(4-Methoxyphenyl)thio]-5-(4-methylphenyl)-3-(trifluoromethyl)-1H-pyrazol-1-yl]benzenesulfonamide (10).

A 12 mL screw neck vial was flushed with argon and charged with iodopyrazole **4q** (0.177 g, 0.35 mmol), 4-methoxybenzenethiol (0.074 g, 0.53 mmol), *i*-PrNEt₂ (0.141 g, 1.23 mmol), dioxane (4 mL), Pd(dba)₂ (0.010 g, 0.0175 mmol, 5 mol%), Xantphos (0.020 g, 0.035 mmol, 10 mol%). The vial was repeatedly flushed with argon, close tightly and heated at 100 °C for 6 h. The cooled reaction mixture was dispersed between CH₂Cl₂ and water (both 50 mL) and filtered through celite. Organic layer was separated, the water layer was extracted with CH₂Cl₂ (3x20 mL), combined extract was washed with 0.1 M HCl (50 mL) and dried over Na₂SO₄. Volatiles were evaporated in vacuo, the residue was purified by column chromatography on silica gel using mixture of CH₂Cl₂ and MeOH (30:1). Evaporation of the solvents gave compound **10** as white powder, 0.153 g, 84% yield; m.p. 137-139 °C. ¹H NMR (600.1 MHz, CDCl₃) δ 2.37 (s, 3H, Me), 3.73 (s, 3H, Me), 5.00 (br s, 2H, NH₂), 6.71 (d, *J*_{HH} = 8.9 Hz, 2H, 4-MeOC₆H₄), 7.01 (d, *J*_{HH} = 8.9 Hz, 2H, 4-MeOC₆H₄), 7.04 (d, *J*_{HH} = 8.0 Hz, 2H, 4-MeC₆H₄), 7.15 (d, *J*_{HH} = 8.0 Hz, 2H, 4-MeC₆H₄), 7.39 (d, *J*_{HH} = 9.0 Hz, 2H, 4-(SO₂NH₂)C₆H₄), 7.83 (d, *J*_{HH} = 9.0 Hz, 2H, 4-(SO₂NH₂)C₆H₄); ¹³C NMR (150.9 MHz, CDCl₃) δ 21.4, 55.3, 111.1, 114.6, 120.8 (q, *J*_{CF} = 269.6 Hz, CF₃), 124.4, 125.2, 126.9, 127.4, 129.6, 130.1, 131.2, 140.2, 141.3, 142.3, 146.0 (q, *J*_{CF} = 36.1 Hz, C-CF₃), 148.9, 158.9; ¹⁹F NMR (376.3 MHz, CDCl₃) δ -62.8; HRMS (ESI): *m/z* calcd for C₂₄H₂₁F₃N₃O₃S₂⁺ [M+H⁺]: 520.0971; found: 520.0971.

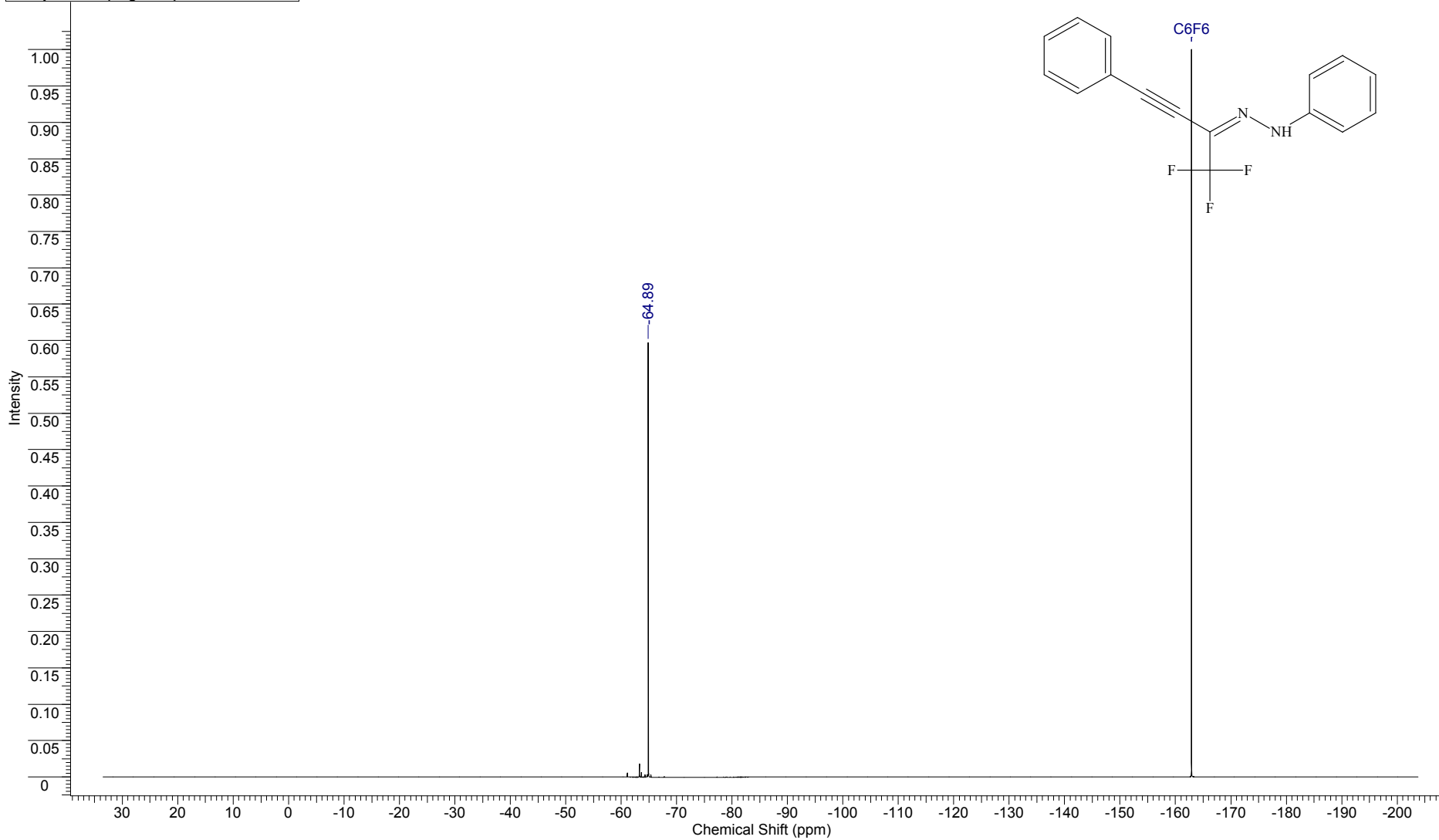
FW	288.2672	Formula	C ₁₆ H ₁₁ F ₃ N ₂
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Acquisition Time (sec)	2.5559	Comment	Imported from UXMNR.		Date	17 Jun 2014 13:55:42	
File Name	C:\BM_DATA\SPEC_BM\BM-504.H_001001r	Frequency (MHz)	400.13	Nucleus	1H	Number of Transients	4
Original Points Count	16384	Points Count	65536	Pulse Sequence	zg30	Solvent	DMSO-D6
Temperature (degree C)	27.000					Sweep Width (Hz)	6410.26



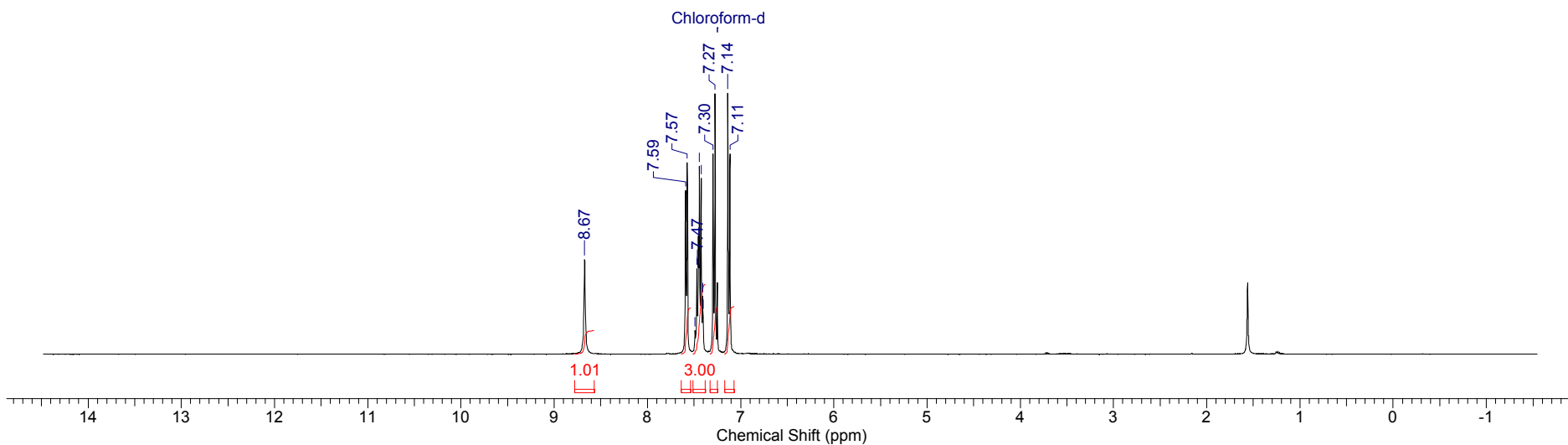
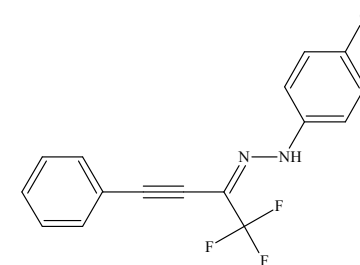
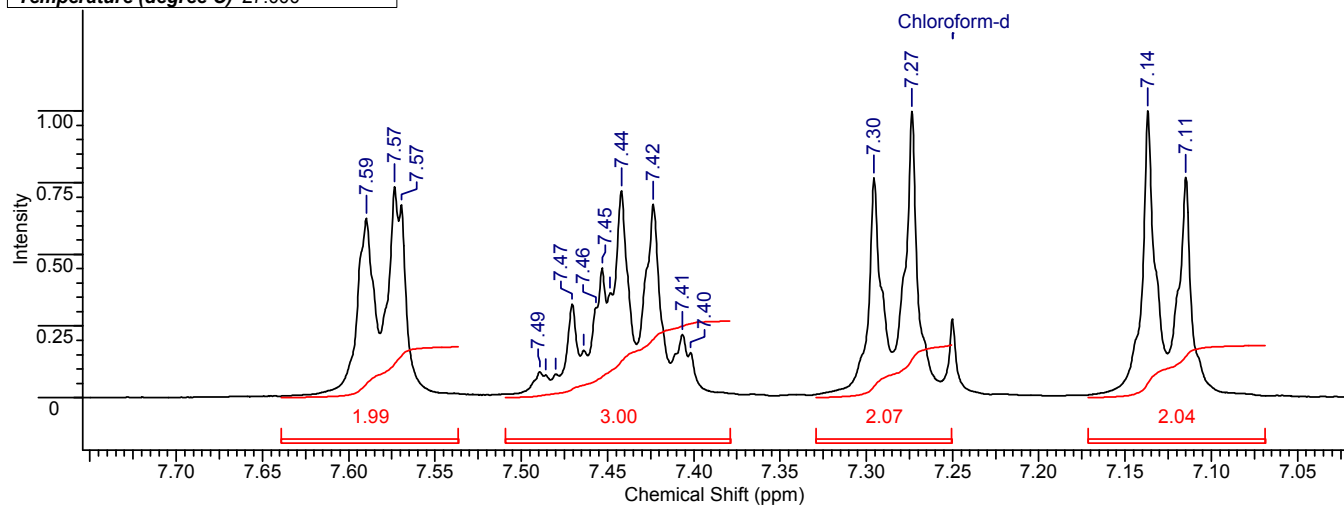
FW 288.2672 Formula C₁₆H₁₁F₃N₂

Acquisition Time (sec)	2.0000	Date	Jun 17 2014	File Name	C:\BM_DATA\SPECTRA\19F\2014.06.17\BM-504_20140617_01\FLUORINE_01		
Frequency (MHz)	376.31	Nucleus	19F	Number of Transients	16	Original Points Count	178571
Points Count	262144	Pulse Sequence	s2pul	Solvent	DMSO-D6	Sweep Width (Hz)	89285.71
Temperature (degree C)	50.000						



FW 322.7120 **Formula** C₁₆H₁₀ClF₃N₂

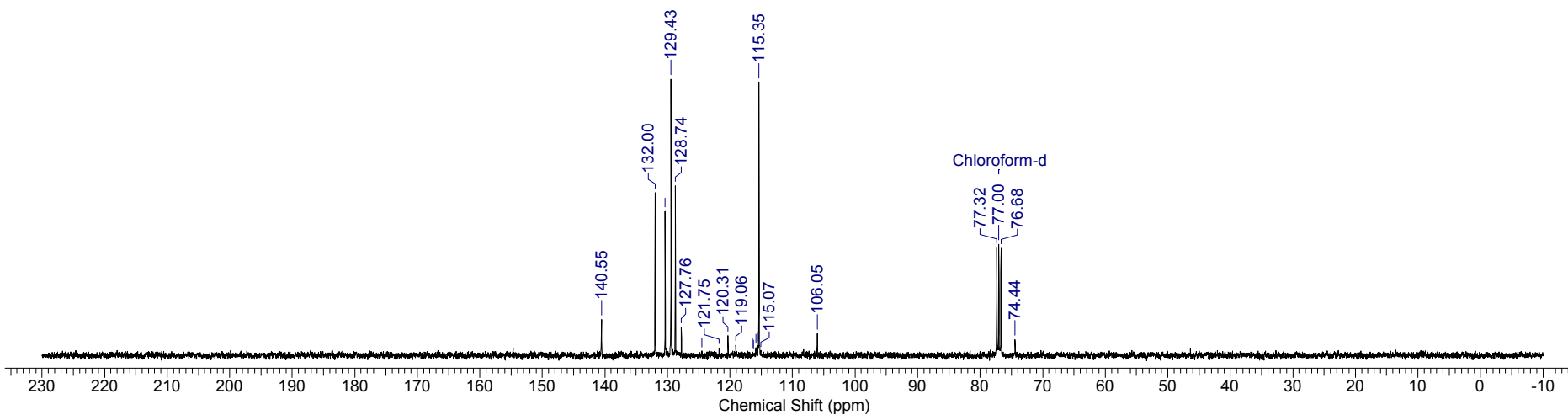
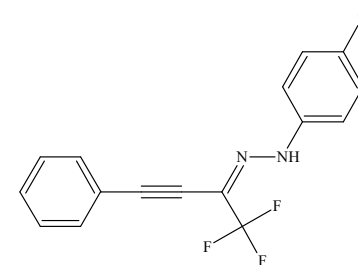
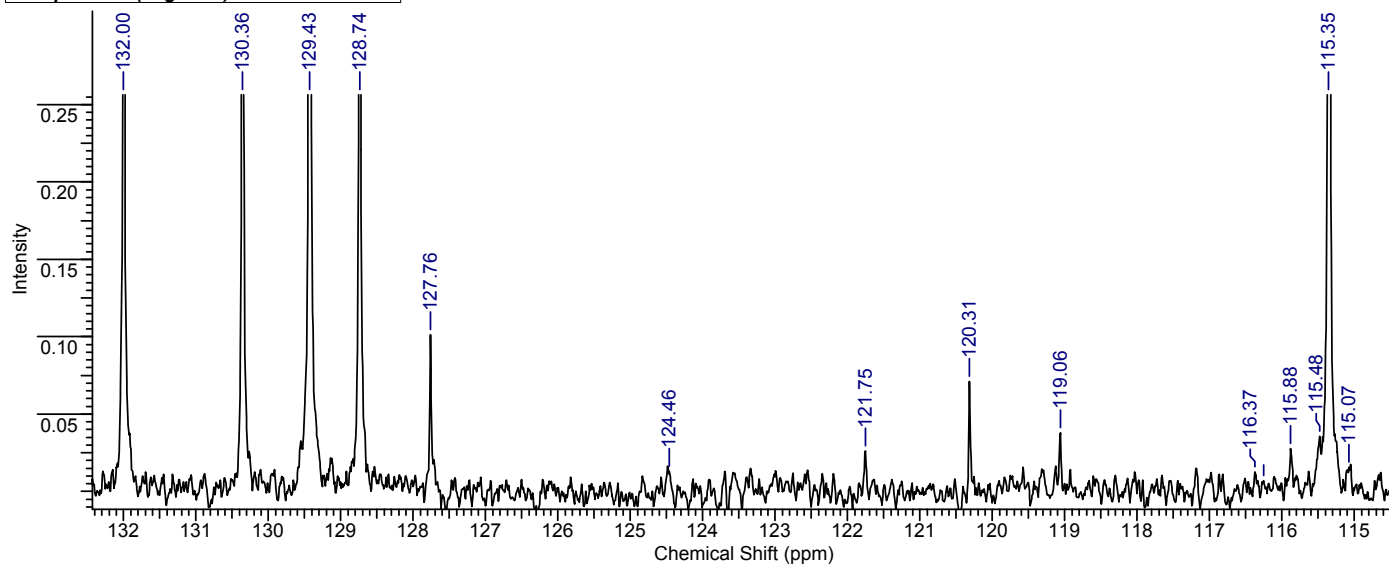
Acquisition Time (sec)	2.5559	Comment	Imported from UXMNR.	Date	25 Mar 2017 13:27:26
File Name	C:\BM_DATA\DOCS\SPEC_BM_H,C_I-IV.2017\BM-1020-1.H_001001r			Frequency (MHz)	400.13
Nucleus	1H	Number of Transients	4	Original Points Count	16384
Pulse Sequence	zg30	Solvent	CHLOROFORM-D	Points Count	65536
Temperature (degree C)	27.000			Sweep Width (Hz)	6410.26



¹H NMR spectrum of **3b** (400.1 MHz, CDCl₃)

FW 322.7120 **Formula** C₁₆H₁₀ClF₃N₂

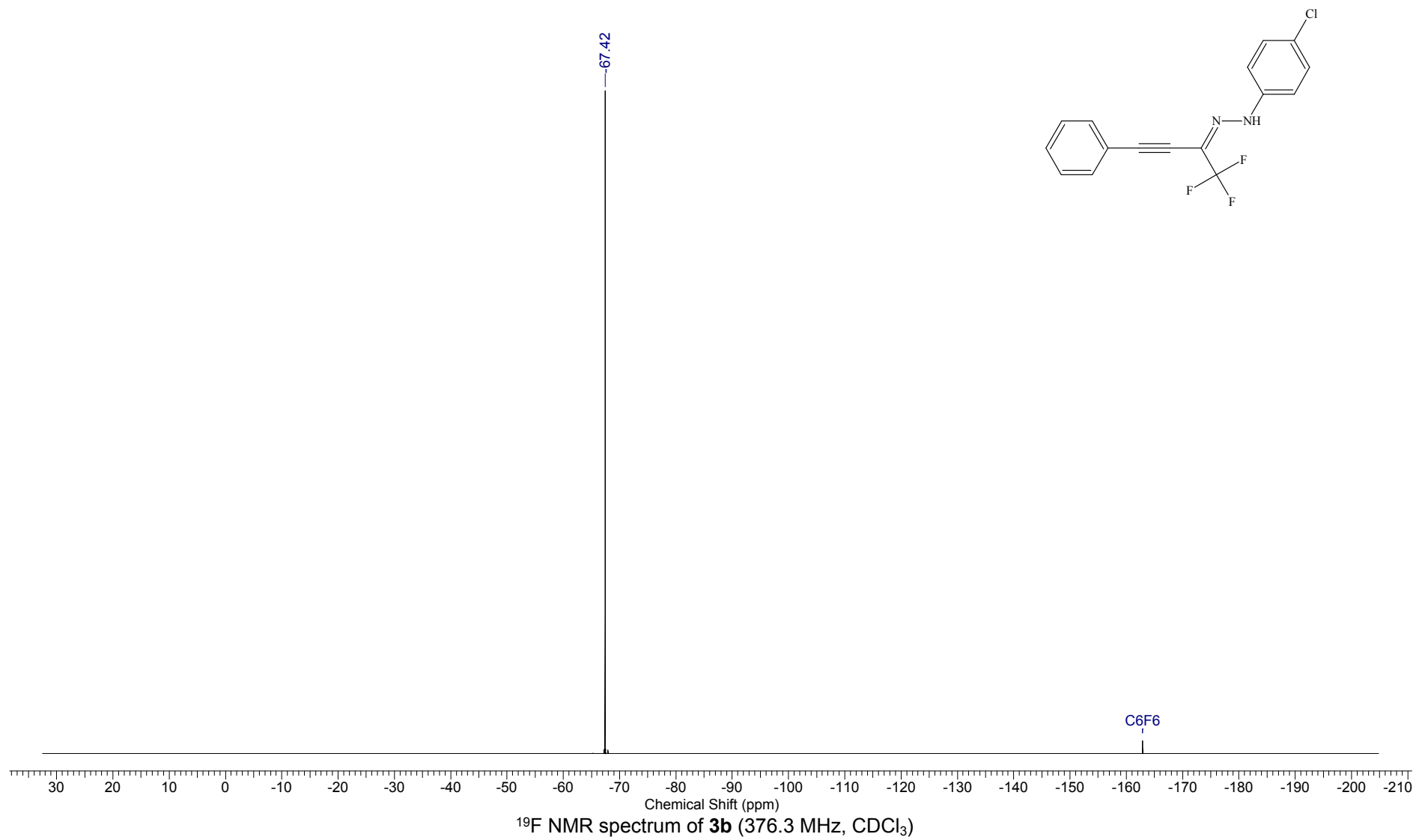
Acquisition Time (sec)	0.4999	Comment	Imported from UXMNR.	Date	25 Mar 2017 13:37:52
File Name	C:\BM_DATA\DOCS\SPEC_BM_H,C_I-IV.2017\BM-1020-1.C_002001r			Frequency (MHz)	100.61
Nucleus	13C	Number of Transients	367	Original Points Count	12076
Pulse Sequence	zgpg30	Solvent	CHLOROFORM-D	Points Count	65536
Temperature (degree C)	27.000			Sweep Width (Hz)	24154.59



¹³C NMR spectrum of **3b** (100.6 MHz, CDCl₃)

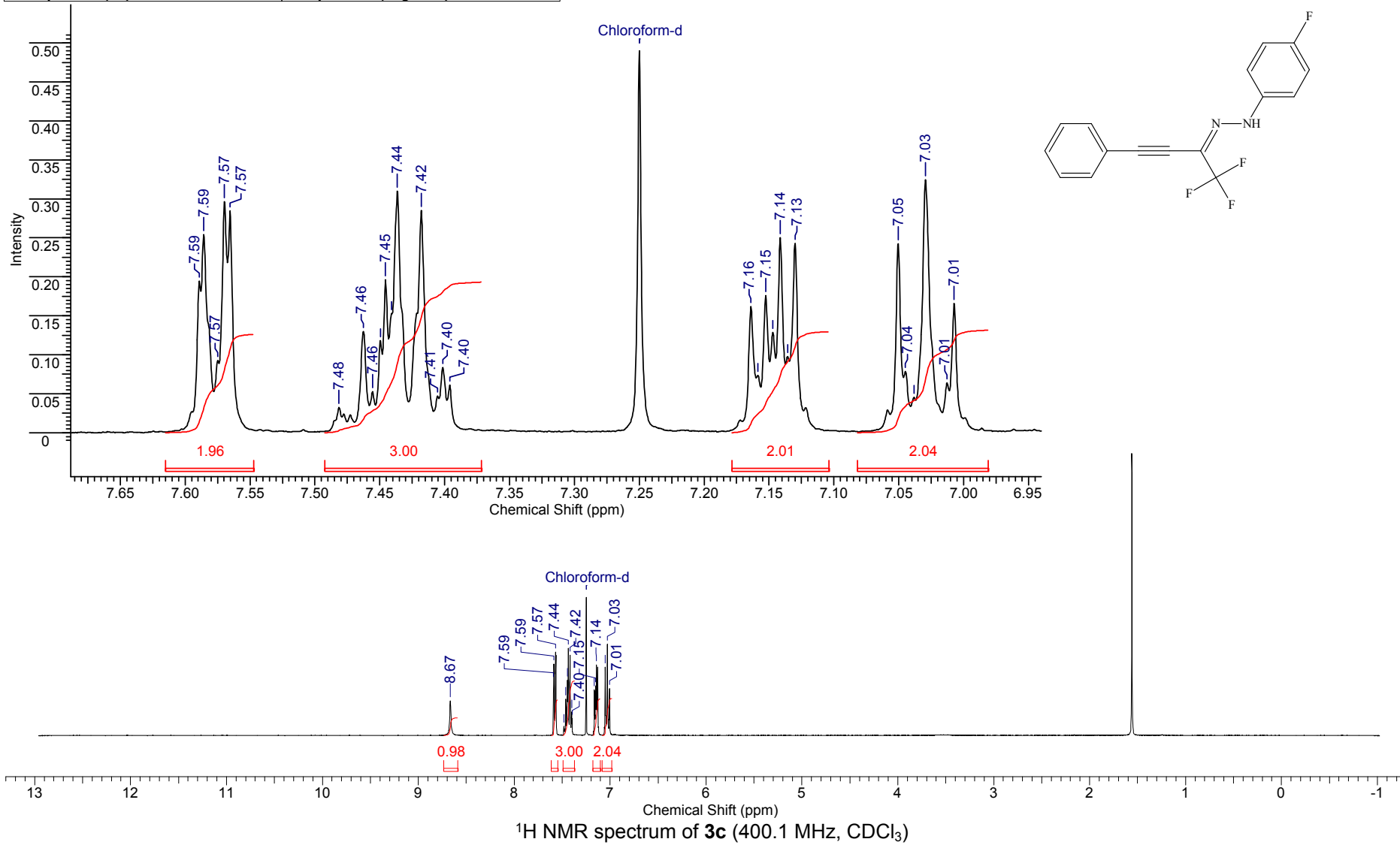
FW	322.7120	Formula	C ₁₆ H ₁₀ ClF ₃ N ₂
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Acquisition Time (sec)	0.7340	Date	Apr 3 2017	File Name	C:\BM_DATA\DOCS\SPEC_F_I-XII.2017\BM-1020-1_20170403_01\FLUORINE_01		
Frequency (MHz)	376.31	Nucleus	¹⁹ F	Number of Transients	10	Original Points Count	65536
Points Count	65536	Pulse Sequence	s2pul	Solvent	CHLOROFORM-D		
Sweep Width (Hz)	89285.71	Temperature (degree C)	25.000				



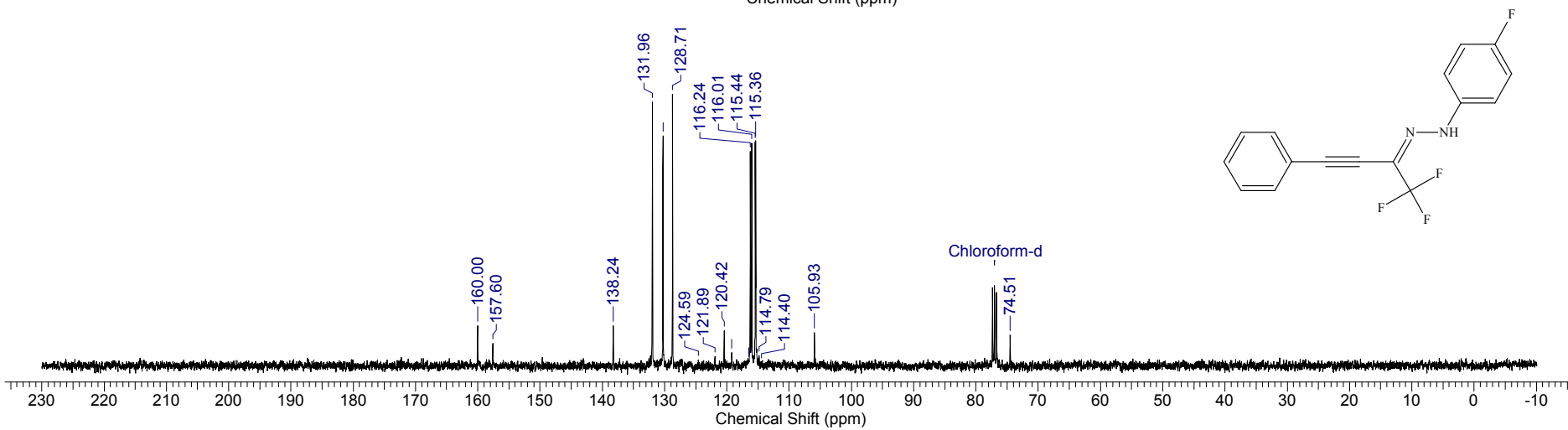
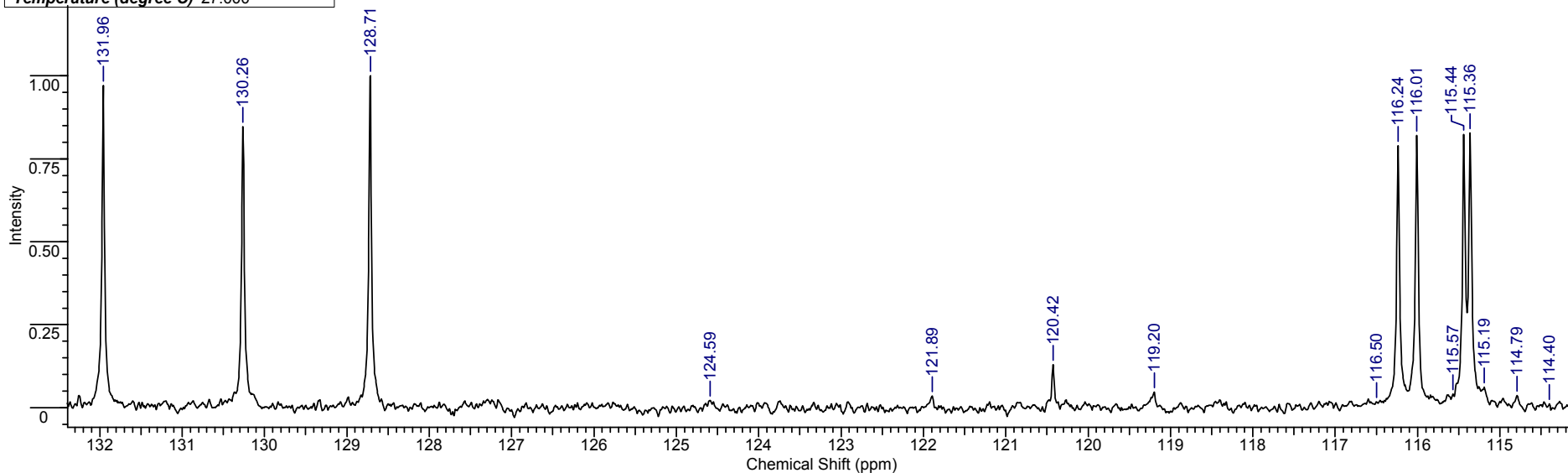
FW 306.2577 Formula $C_{16}H_{10}F_4N_2$

Acquisition Time (sec)	2.9295	Comment	Imported from UXMNR.		Date	26 Apr 2017 23:22:04	
File Name	C:\BM_DATA\BM-1044-d\BM-1044-d_001001r	Frequency (MHz)	400.13	Nucleus	1H	Number of Transients	8
Original Points Count	16384	Points Count	65536	Pulse Sequence	zg30	Solvent	CHLOROFORM-D
Sweep Width (Hz)	5592.84	Temperature (degree C)	27.000				



FW	306.2577	Formula	C ₁₆ H ₁₀ F ₄ N ₂
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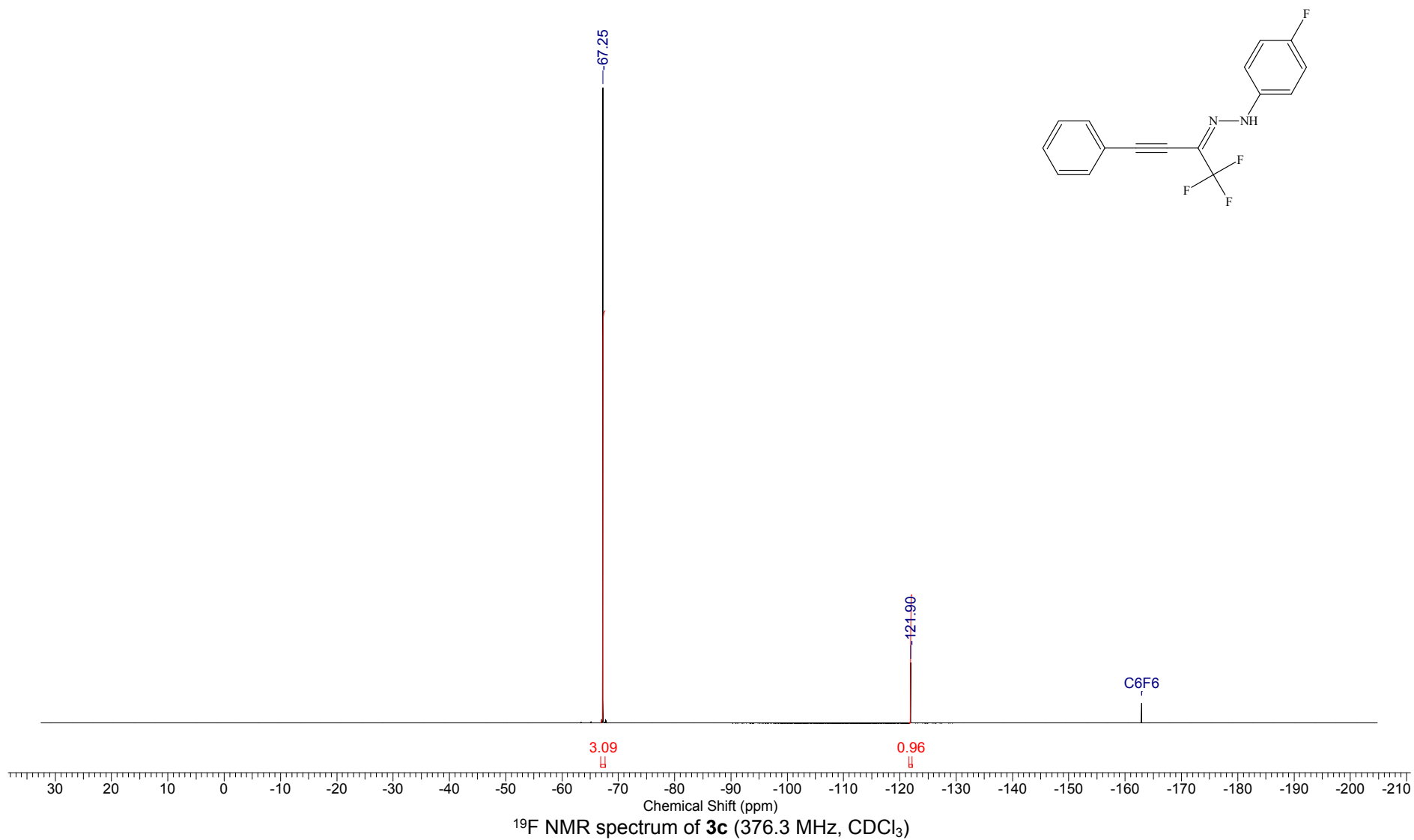
Acquisition Time (sec)	0.4999	Comment	Imported from UXMNR.		Date	25 Apr 2017 15:58:36	
File Name	C:\BM_DATA\DOCS\SPEC_BM_H,C_I-IV.2017\BM-1044.C_002001r			Frequency (MHz)	100.61		
Nucleus	13C	Number of Transients	182	Original Points Count	12076	Points Count	65536
Pulse Sequence	zpgg30	Solvent	CHLOROFORM-D		Sweep Width (Hz)	24154.59	
Temperature (degree C)	27.000						



¹³C NMR spectrum of **3c** (100.6 MHz, CDCl₃)

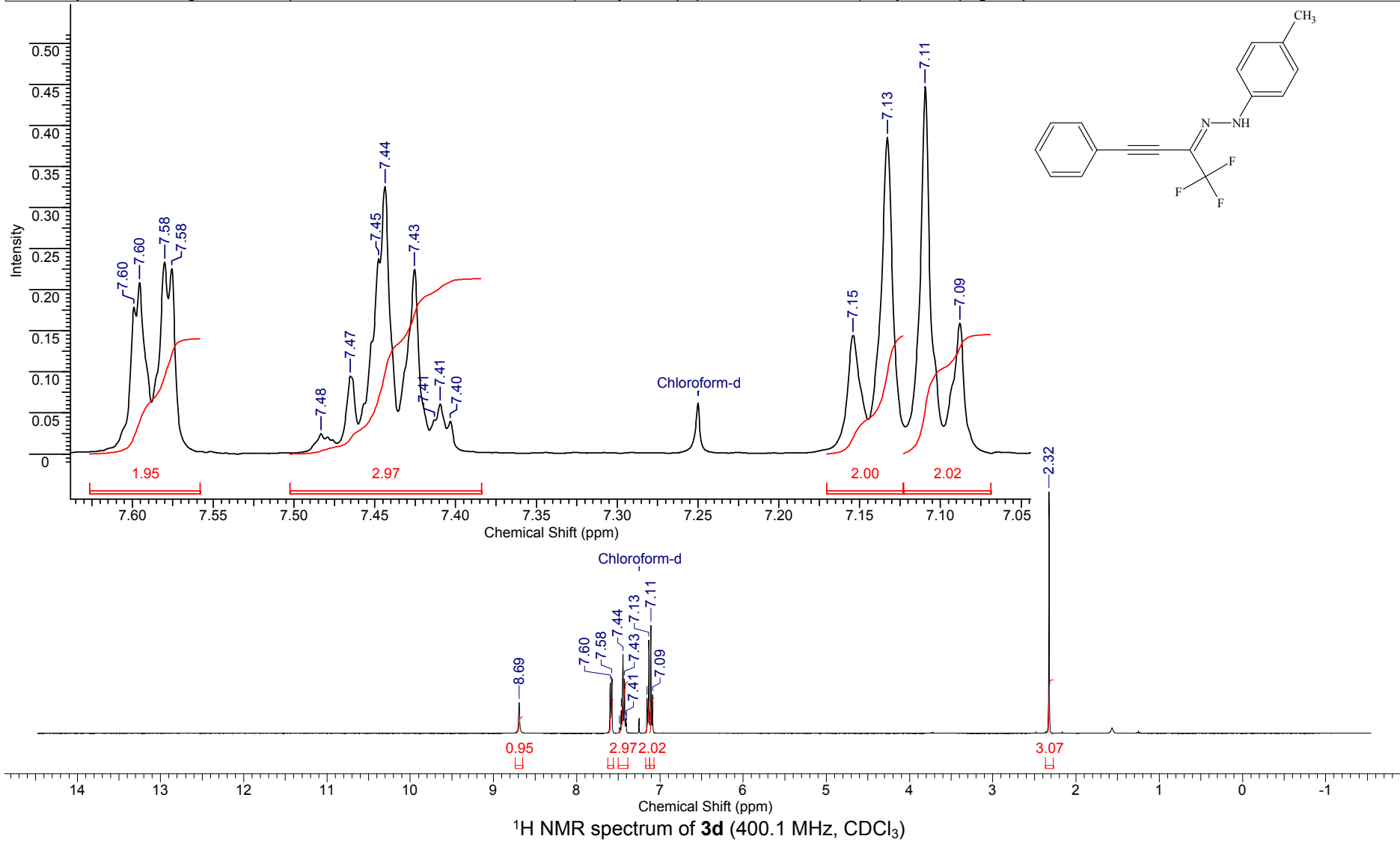
FW	306.2577	Formula	C ₁₆ H ₁₀ F ₄ N ₂
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Acquisition Time (sec)	1.5000	Date	Apr 26 2017	File Name	C:\BM_DATA\DOCS\SPEC_F_I-XII.2017\BM-1044_20170426_01\FLUORINE_01		
Frequency (MHz)	376.31	Nucleus	19F	Number of Transients	16	Original Points Count	133929
Points Count	262144	Pulse Sequence	s2pul	Solvent	CHLOROFORM-D		
Sweep Width (Hz)	89285.71	Temperature (degree C)	25.000				



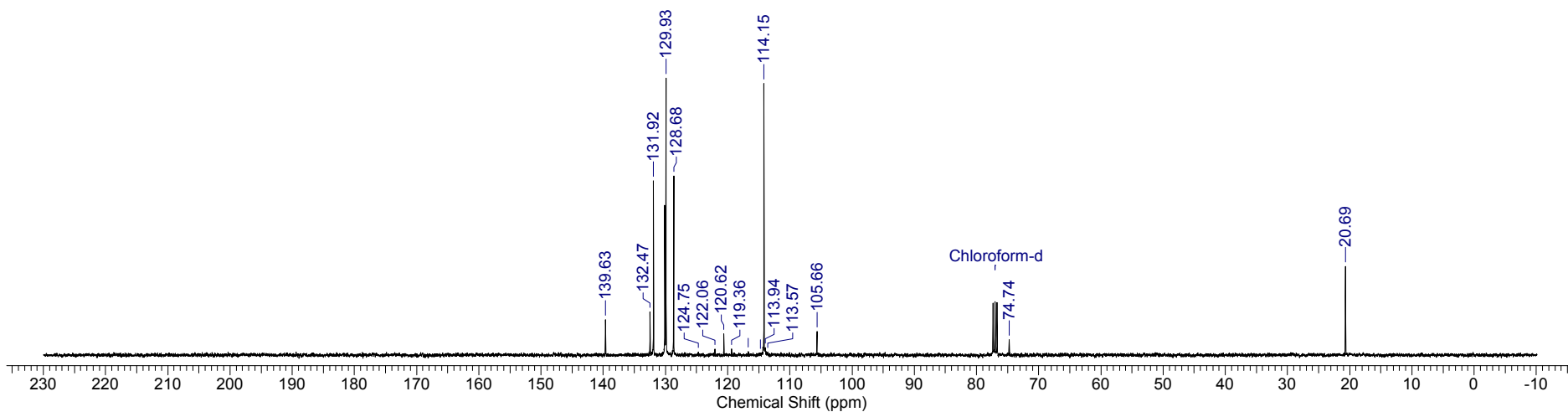
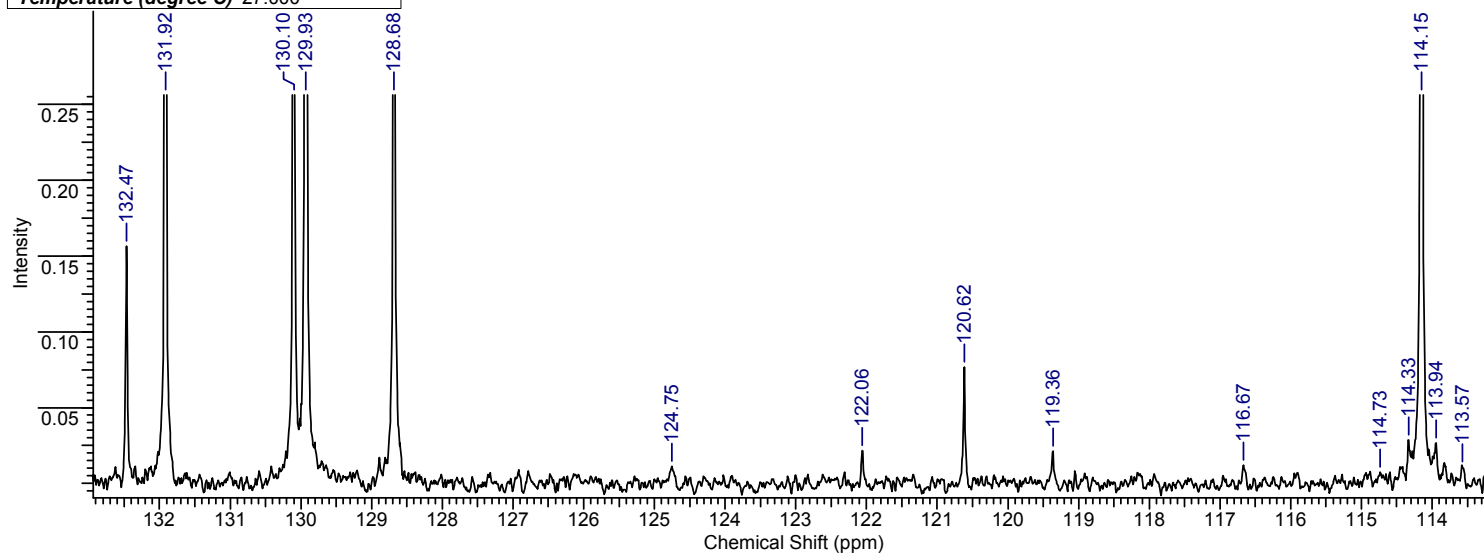
FW 302.2938 **Formula** C₁₇H₁₃F₃N₂

Acquisition Time (sec)	2.5559	Comment	Imported from UXNMR.		Date	25 Apr 2017 15:00:58	
File Name	C:\IBM_DATA\DOCS\SPEC_BM_H,C_I-IV.2017\BM-1043.H_001001r			Frequency (MHz)	400.13		
Nucleus	1H	Number of Transients	4	Original Points Count	16384	Points Count	65536
Pulse Sequence	zg30	Solvent	DMSO-D6	Sweep Width (Hz)	6410.26	Temperature (degree C)	27.000



FW	302.2938	Formula	C ₁₇ H ₁₃ F ₃ N ₂
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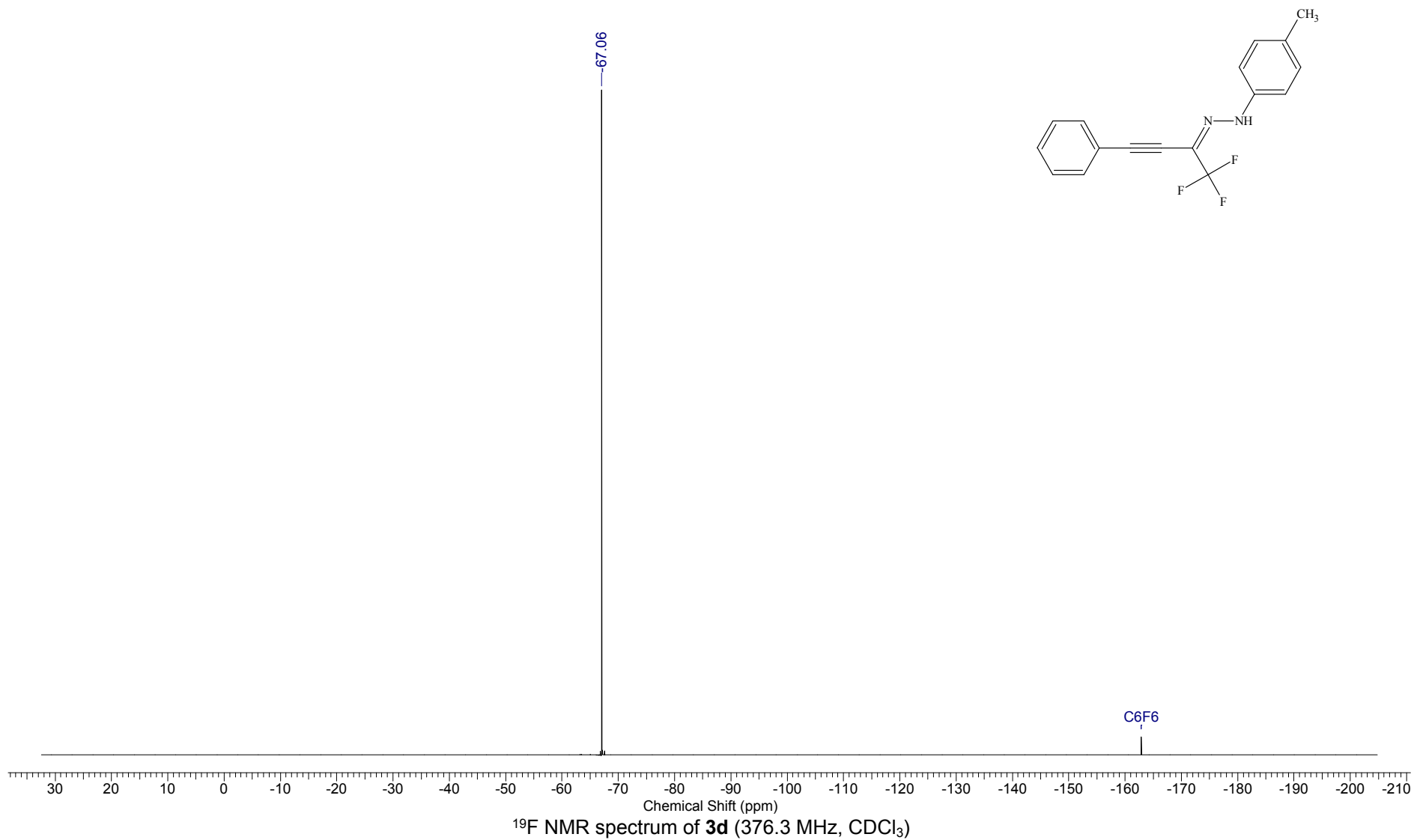
Acquisition Time (sec)	0.4999	Comment	Imported from UXMNR.	Date	25 Apr 2017 15:11:00
File Name	C:\BM_DATA\DOCS\SPEC_BM_H,C_I-IV.2017\BM-1043.C_002001r			Frequency (MHz)	100.61
Nucleus	13C	Number of Transients	350	Original Points Count	12076
Pulse Sequence	zgpg30	Solvent	CHLOROFORM-D	Points Count	65536
Temperature (degree C)	27.000			Sweep Width (Hz)	24154.59



¹³C NMR spectrum of **3d** (100.6 MHz, CDCl₃)

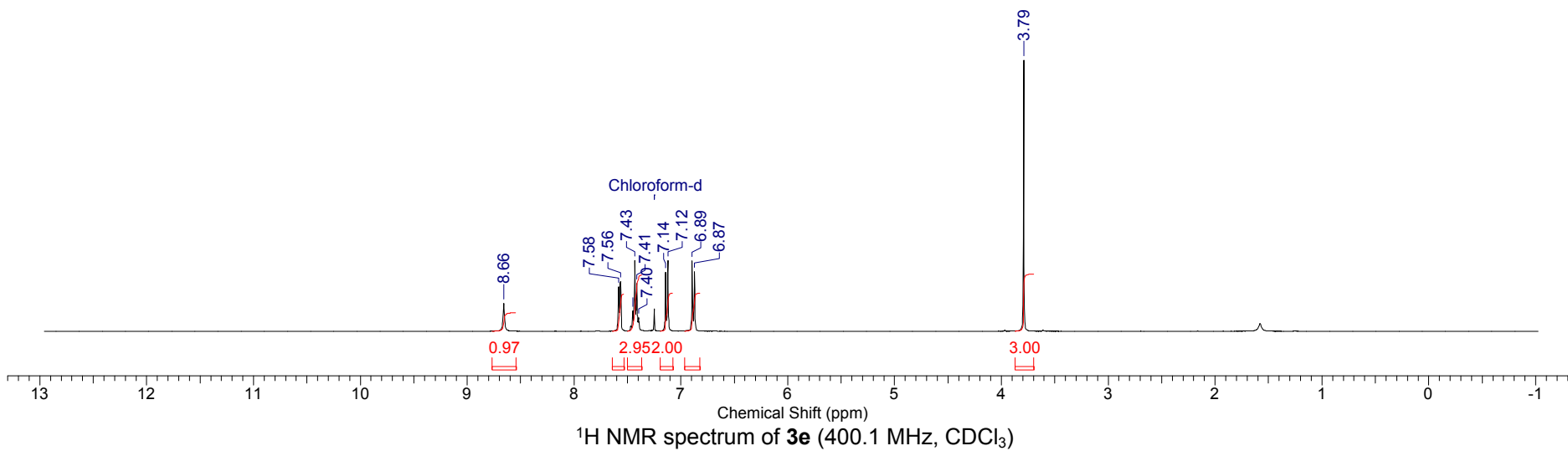
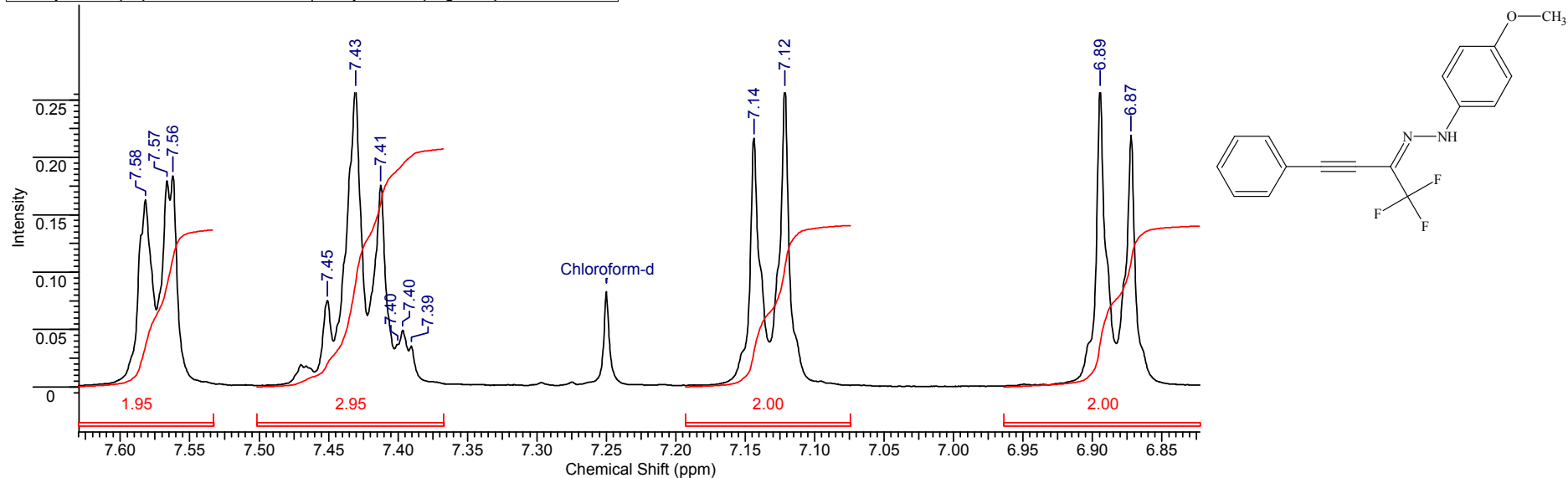
FW	302.2938	Formula	C ₁₇ H ₁₃ F ₃ N ₂
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Acquisition Time (sec)	1.5000	Date	Apr 26 2017	File Name	C:\BM_DATA\DOCS\SPEC_F_I-XII.2017\BM-1043_20170426_01\FLUORINE_01		
Frequency (MHz)	376.31	Nucleus	19F	Number of Transients	16	Original Points Count	133929
Points Count	262144	Pulse Sequence	s2pul	Solvent	CHLOROFORM-D		
Sweep Width (Hz)	89285.71	Temperature (degree C)	25.000				



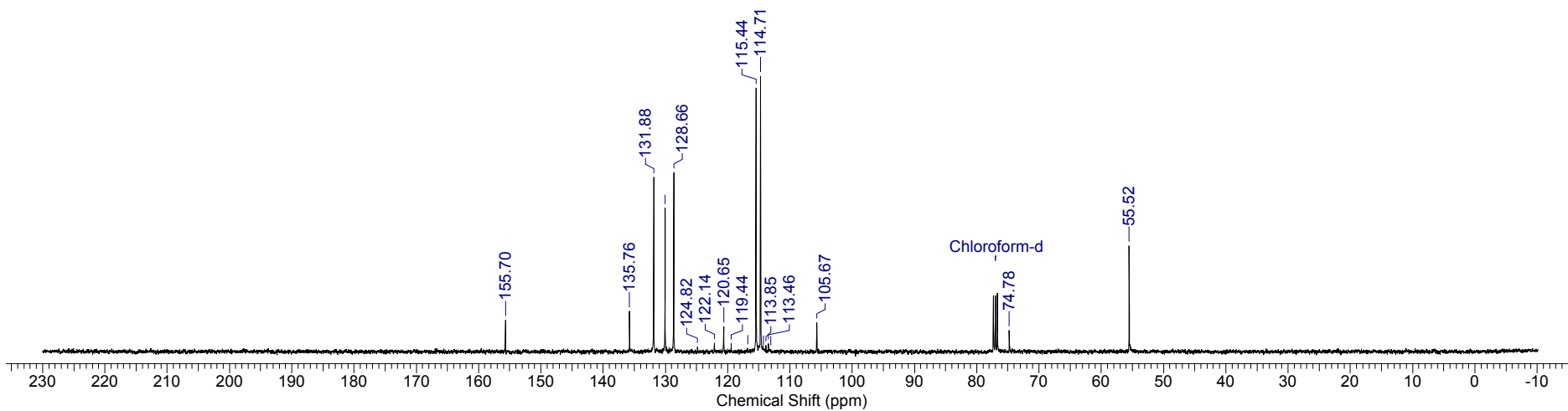
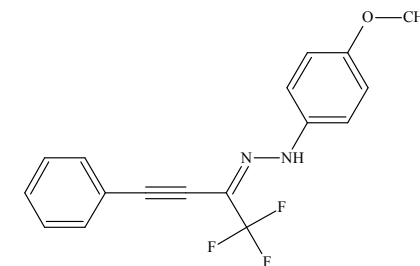
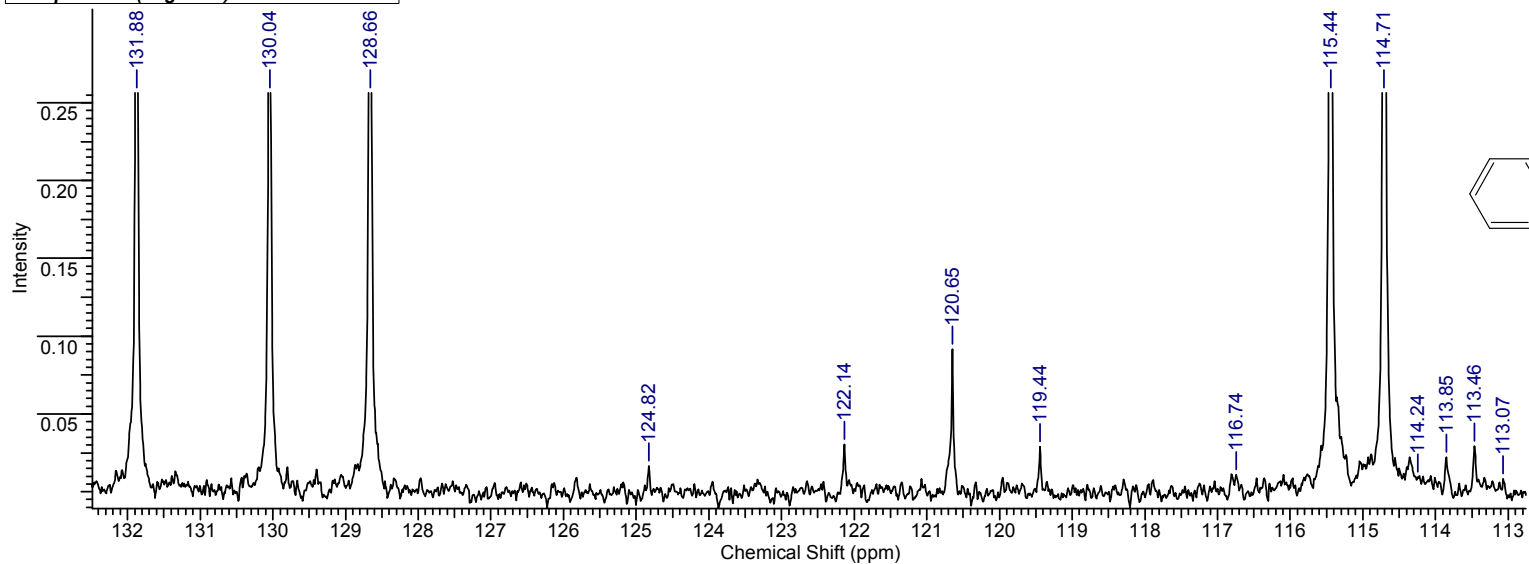
FW 318.2932 **Formula** C₁₇H₁₃F₃N₂O

Acquisition Time (sec)	2.9295	Comment	Imported from UXNMR.		Date	25 Apr 2017 22:28:06	
File Name	C:\BM_DATA\170425\BM-1042_001001r	Frequency (MHz)	400.13	Nucleus	1H	Number of Transients	8
Original Points Count	16384	Points Count	65536	Pulse Sequence	zg30	Solvent	CHLOROFORM-D
Sweep Width (Hz)	5592.84	Temperature (degree C)	27.000				



FW 318.2932 Formula C₁₇H₁₃F₃N₂O

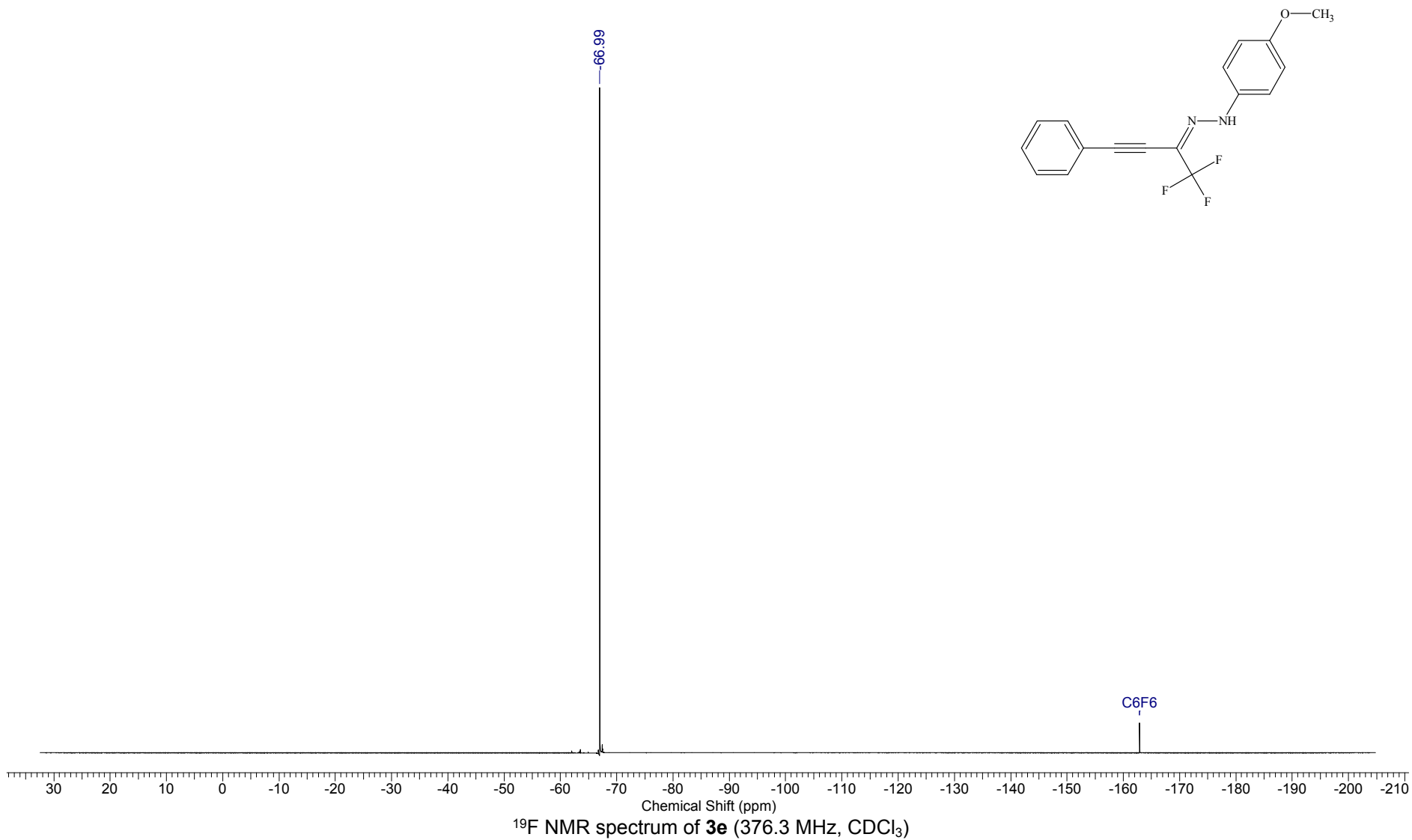
Acquisition Time (sec)	0.4999	Comment	Imported from UXMNR.	Date	26 Apr 2017 17:24:04
File Name	C:\BM_DATA\DOCS\SPEC_BM_H,C_I-IV.2017\BM-1042.C_002001r			Frequency (MHz)	100.61
Nucleus	13C	Number of Transients	256	Original Points Count	12076
Pulse Sequence	zgpg30	Solvent	CHLOROFORM-D	Points Count	65536
Temperature (degree C)	27.000			Sweep Width (Hz)	24154.59



¹³C NMR spectrum of **3e** (100.6 MHz, CDCl₃)

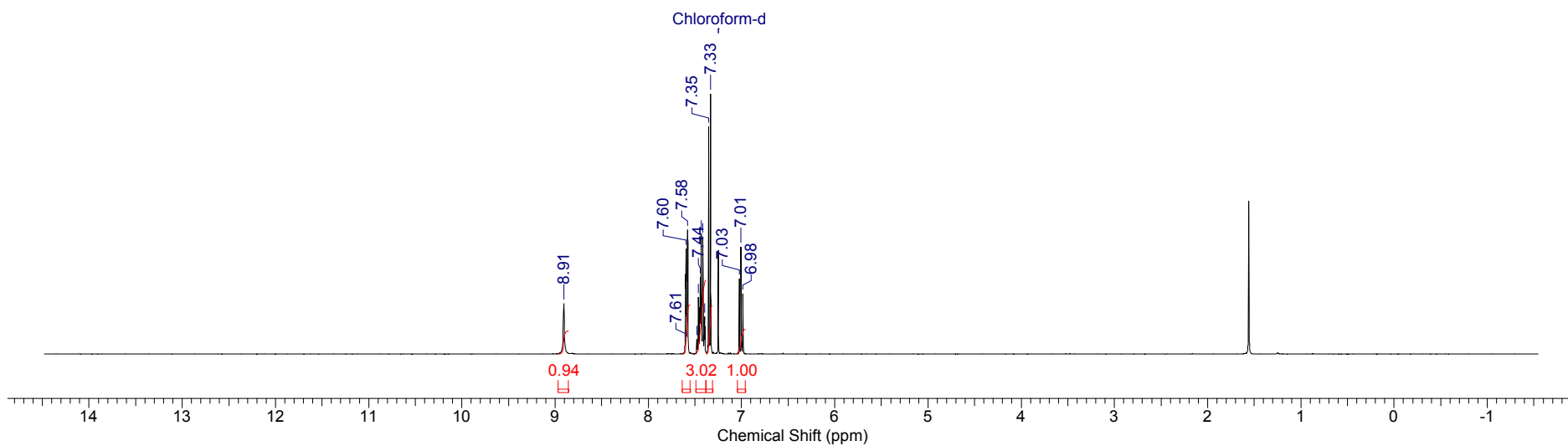
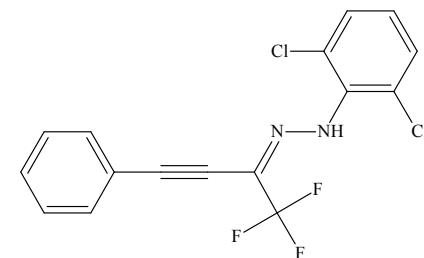
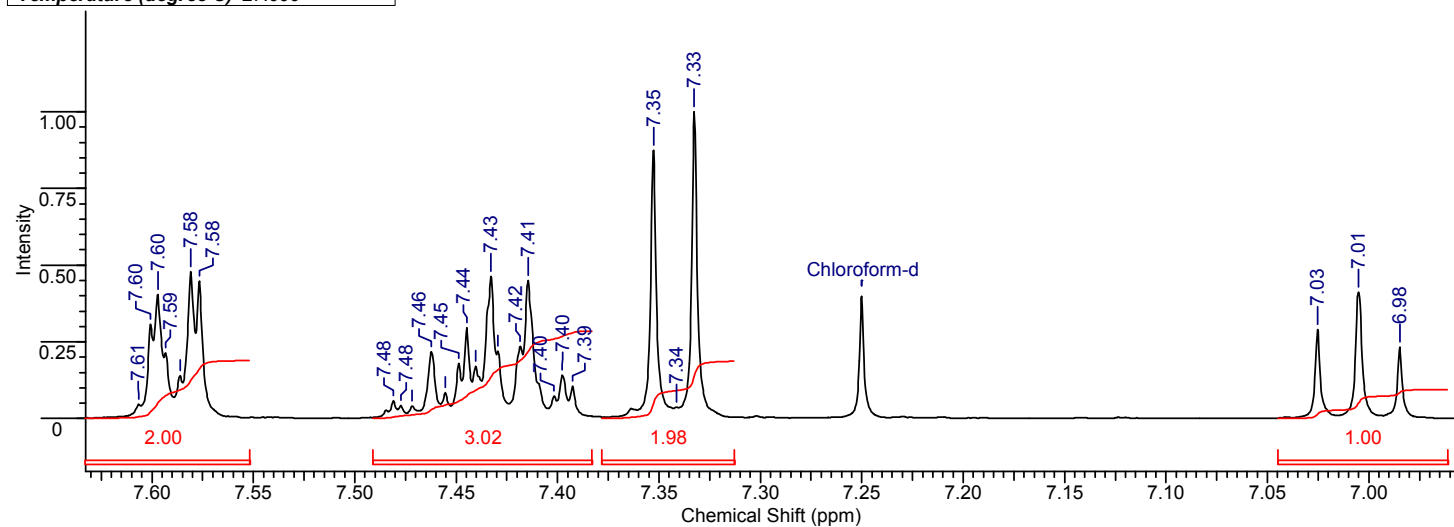
FW	318.2932	Formula	C ₁₇ H ₁₃ F ₃ N ₂ O
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Acquisition Time (sec)	1.5000	Date	Apr 26 2017	File Name	C:\BM_DATA\DOCS\SPEC_F_I-XII.2017\BM-1042_20170426_01\FLUORINE_01		
Frequency (MHz)	376.31	Nucleus	19F	Number of Transients	16	Original Points Count	133929
Points Count	262144	Pulse Sequence	s2pul	Solvent	CHLOROFORM-D		
Sweep Width (Hz)	89285.71	Temperature (degree C)	25.000				



FW 357.1567 Formula C₁₆H₉Cl₂F₃N₂

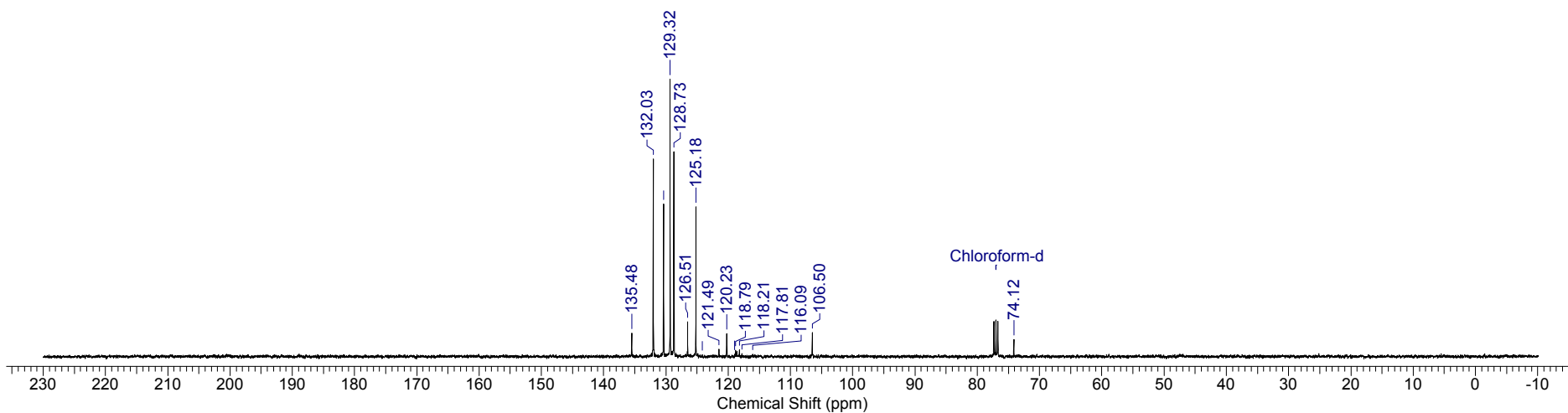
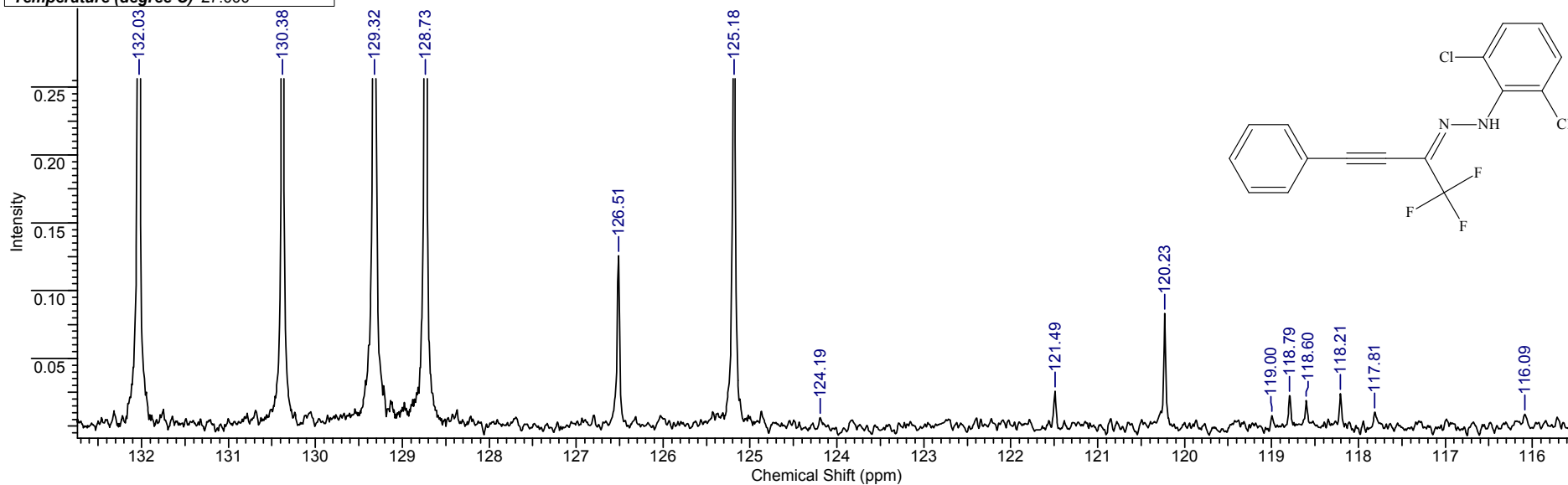
Acquisition Time (sec)	2.5559	Comment	Imported from UXMNR.	Date	29 Apr 2017 13:25:00
File Name	C:\BM_DATA\DOCS\SPEC_BM_H,C_I-IV.2017\BM-1048.H_001001r			Frequency (MHz)	400.13
Nucleus	1H	Number of Transients	4	Original Points Count	16384
Pulse Sequence	zg30	Solvent	CHLOROFORM-D	Points Count	65536
Temperature (degree C)	27.000			Sweep Width (Hz)	6410.26



¹H NMR spectrum of **3f** (400.1 MHz, CDCl₃)

FW 357.1567 **Formula** C₁₆H₉Cl₂F₃N₂

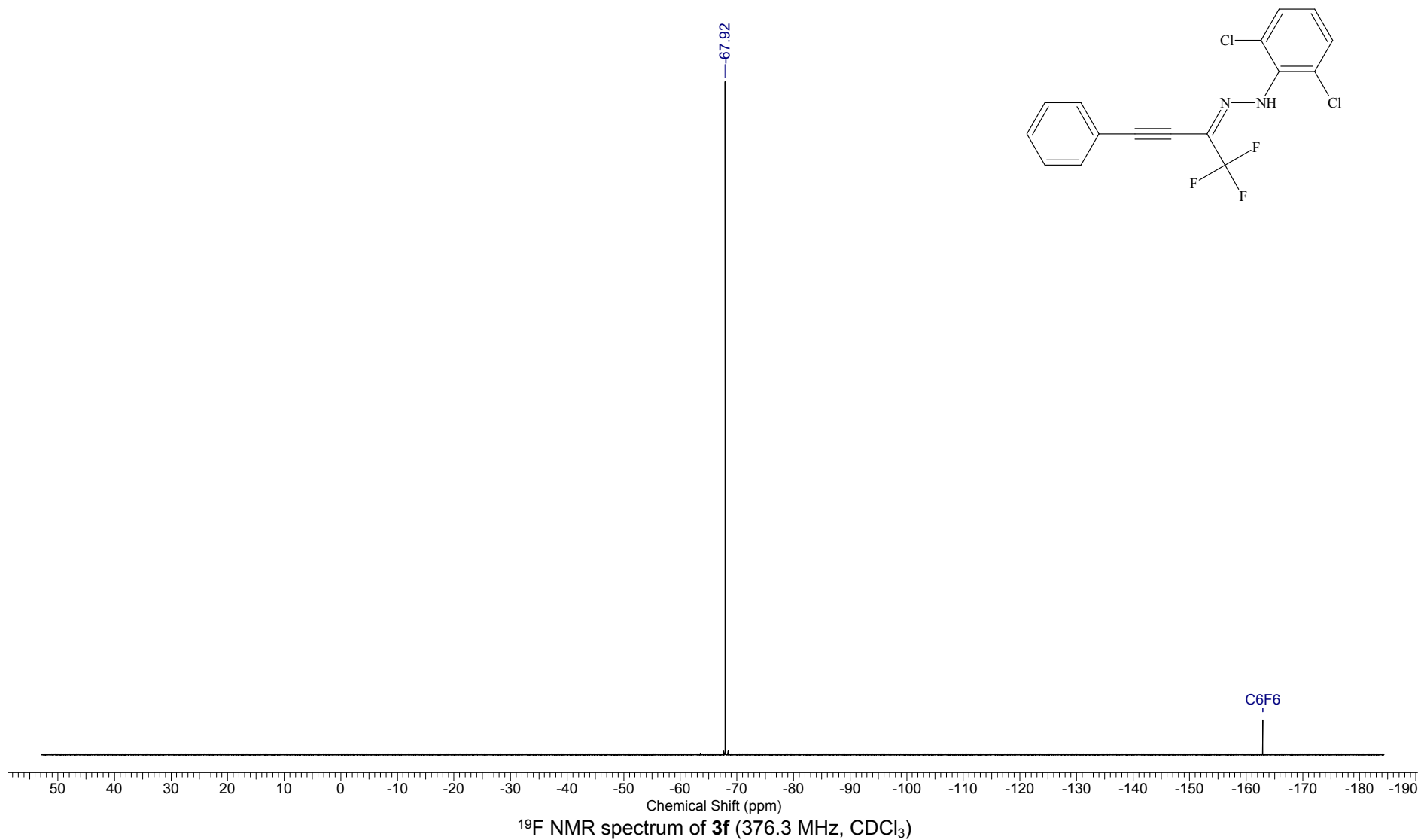
Acquisition Time (sec)	0.4999	Comment	Imported from UXMNR.	Date	29 Apr 2017 13:47:04
File Name	C:\BM_DATA\DOCS\SPEC_BM_H,C_I-IV.2017\BM-1048.C_002001r			Frequency (MHz)	100.61
Nucleus	¹³ C	Number of Transients	224	Original Points Count	12076
Pulse Sequence	zgpg30	Solvent	CHLOROFORM-D	Points Count	65536
Temperature (degree C)	27.000			Sweep Width (Hz)	24154.59



¹³C NMR spectrum of **3f** (100.6 MHz, CDCl₃)

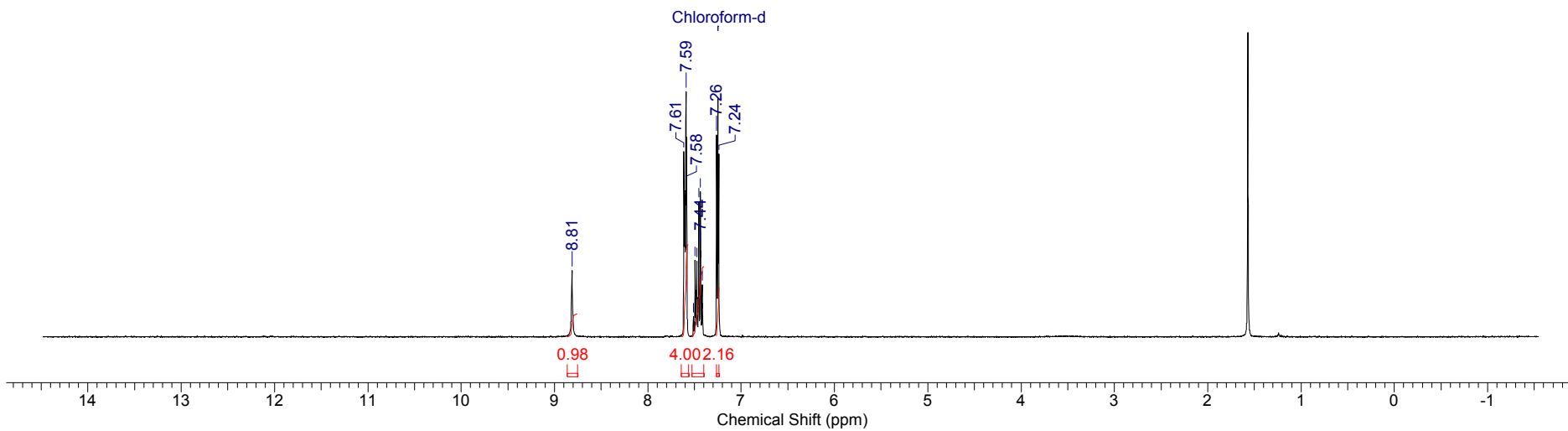
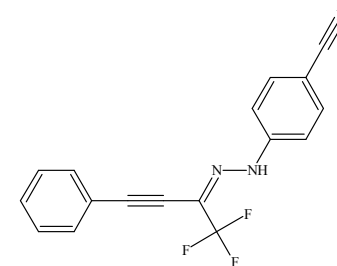
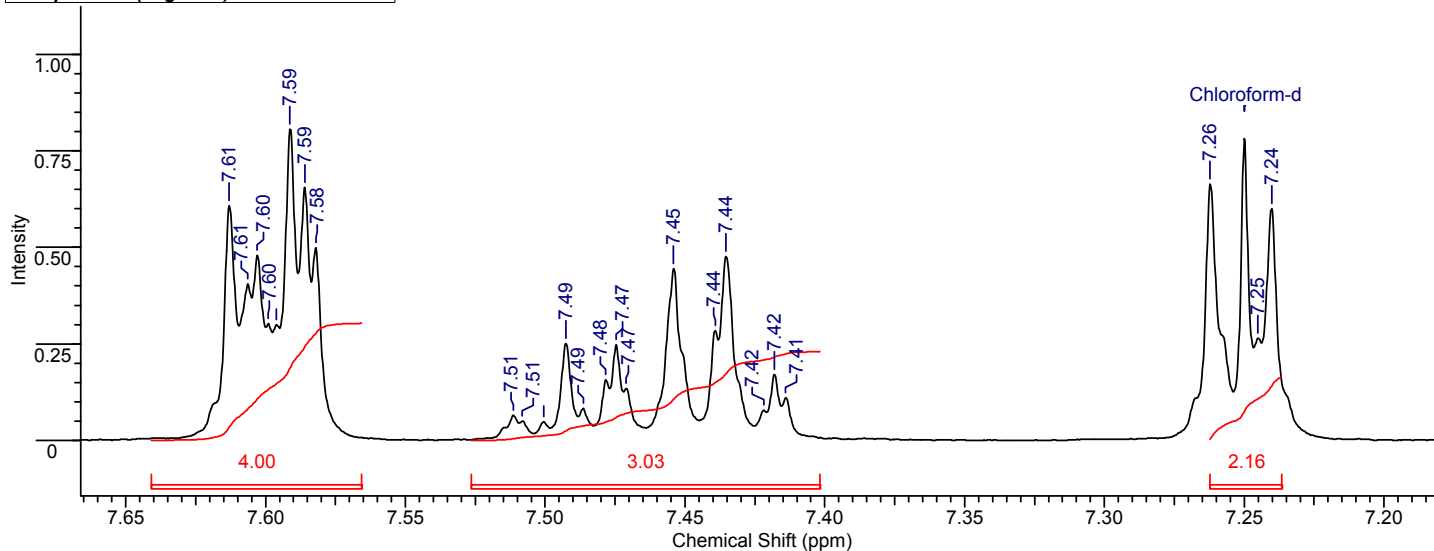
FW	357.1567	Formula	C ₁₆ H ₉ Cl ₂ F ₃ N ₂
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Acquisition Time (sec)	1.4680	Date	May 4 2017	File Name	C:\BM_DATA\DOCS\SPEC_F_I-XII.2017\BM-1048-F_20170504_01\FLUORINE_01		
Frequency (MHz)	376.32	Nucleus	19F	Number of Transients	8	Original Points Count	131073
Points Count	262144	Pulse Sequence	s2pul	Solvent	CHLOROFORM-D		
Sweep Width (Hz)	89285.71	Temperature (degree C)	22.000				



FW 313.2767 Formula C₁₇H₁₀F₃N₃

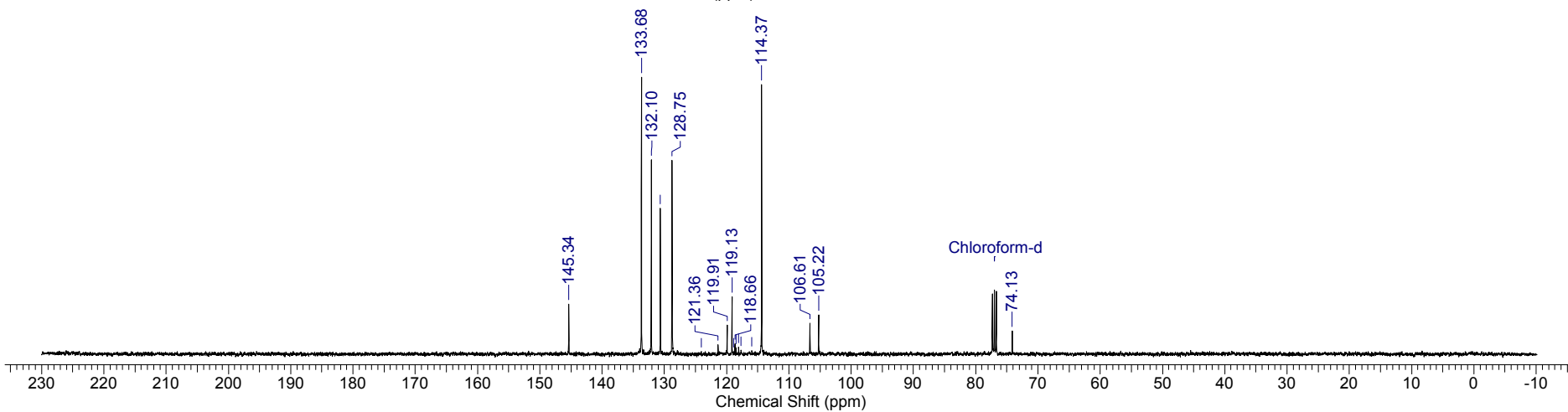
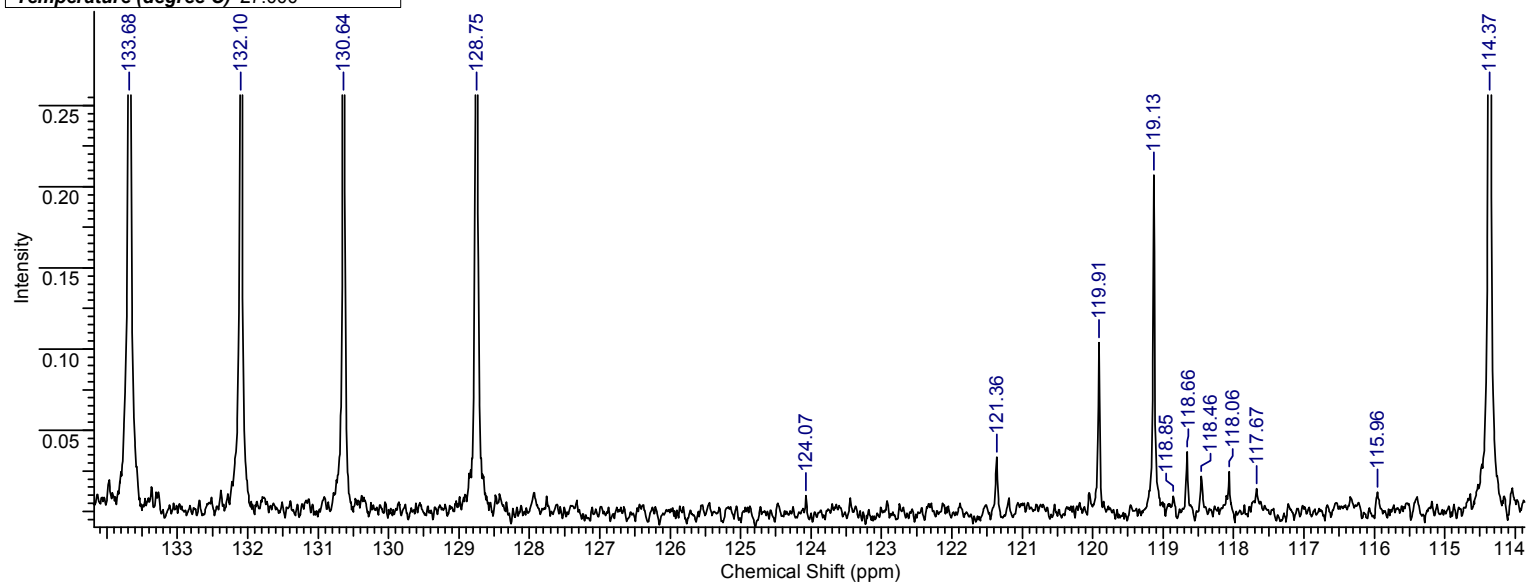
Acquisition Time (sec)	2.5559	Comment	Imported from UXMNR.	Date	02 May 2017 14:13:24
File Name	C:\BM_DATA\DOCS\SPEC_BM_H,C_V-XII.2017\BM-1056.H_001001r			Frequency (MHz)	400.13
Nucleus	1H	Number of Transients	4	Original Points Count	16384
Pulse Sequence	zg30	Solvent	CHLOROFORM-D	Points Count	65536
Temperature (degree C)	27.000			Sweep Width (Hz)	6410.26



¹H NMR spectrum of **3g** (400.1 MHz, CDCl₃)

FW	313.2767	Formula	C ₁₇ H ₁₀ F ₃ N ₃
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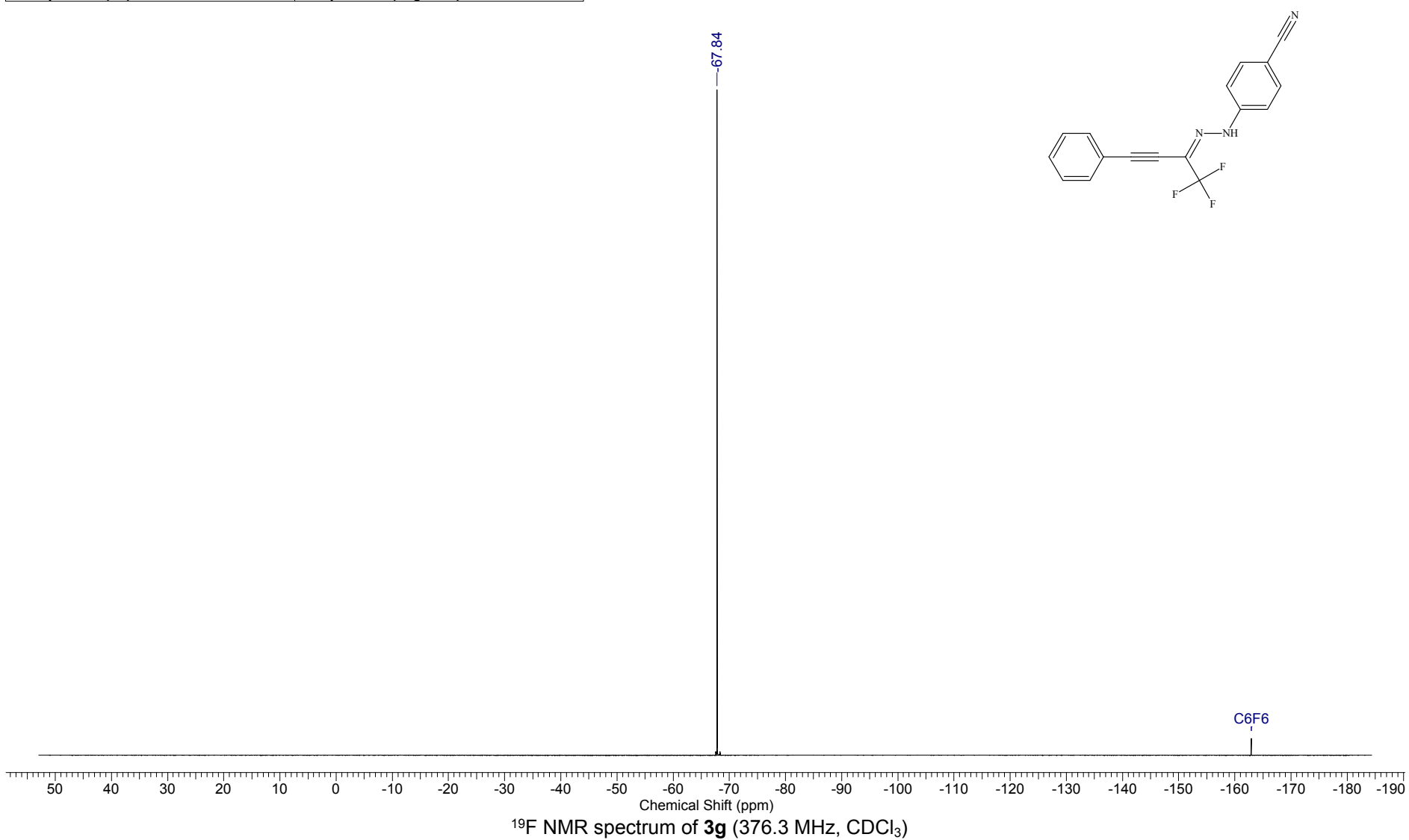
Acquisition Time (sec)	0.4999	Comment	Imported from UXMNR.		Date	02 May 2017 15:04:44	
File Name	C:\BM_DATA\DOCS\SPEC_BM_H,C_V-XII.2017\BM-1056.C_002001r			Frequency (MHz)	100.61		
Nucleus	13C	Number of Transients	256	Original Points Count	12076	Points Count	65536
Pulse Sequence	zpgpg30	Solvent	CHLOROFORM-D		Sweep Width (Hz)	24154.59	
Temperature (degree C)	27.000						



¹³C NMR spectrum of **3g** (100.6 MHz, CDCl₃)

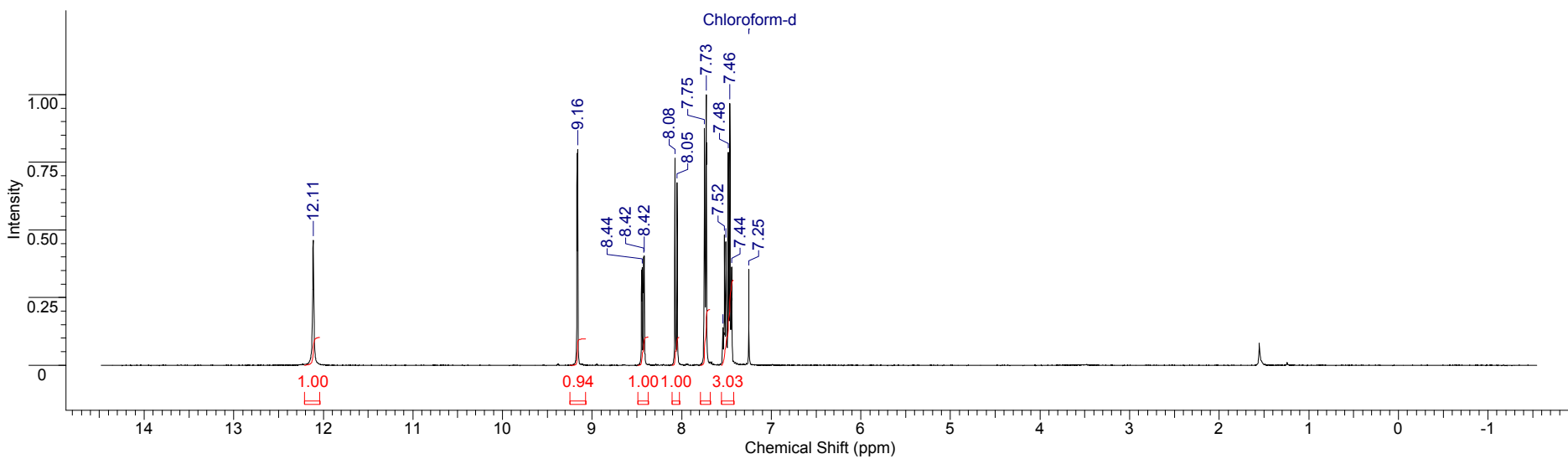
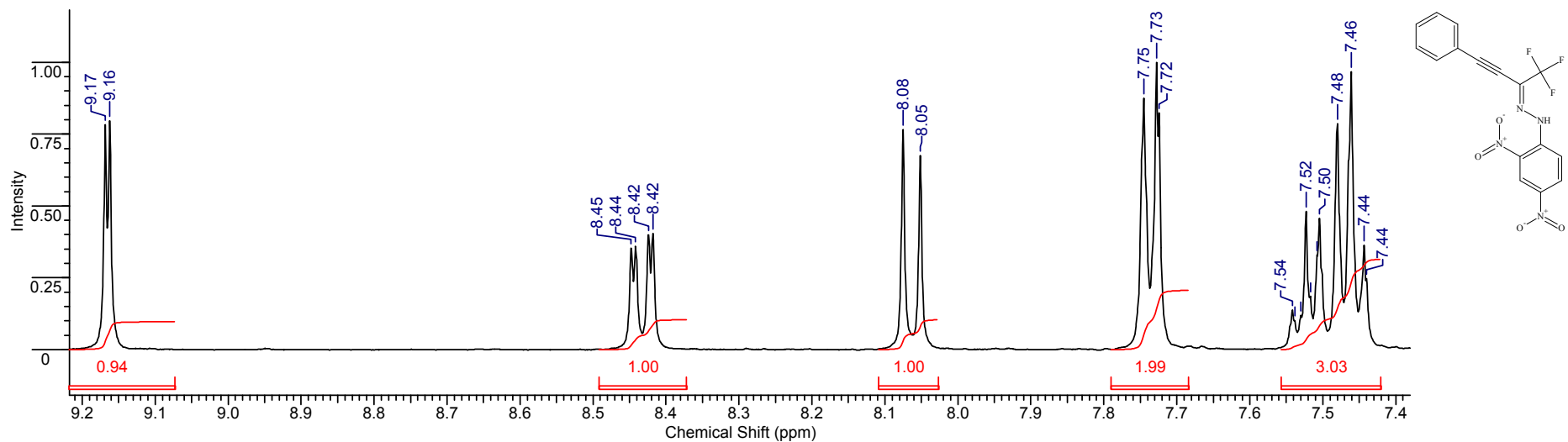
FW	313.2767	Formula	C ₁₇ H ₁₀ F ₃ N ₃
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Acquisition Time (sec)	1.4680	Date	May 4 2017	File Name	C:\BM_DATA\DOCS\SPEC_F_I-XII.2017\BM-1056_20170504_01\FLUORINE_01		
Frequency (MHz)	376.32	Nucleus	¹⁹ F	Number of Transients	8	Original Points Count	131073
Points Count	262144	Pulse Sequence	s2pul	Solvent	CHLOROFORM-D		
Sweep Width (Hz)	89285.71	Temperature (degree C)	22.000				



FW 378.2624 Formula C₁₆H₉F₃N₄O₄

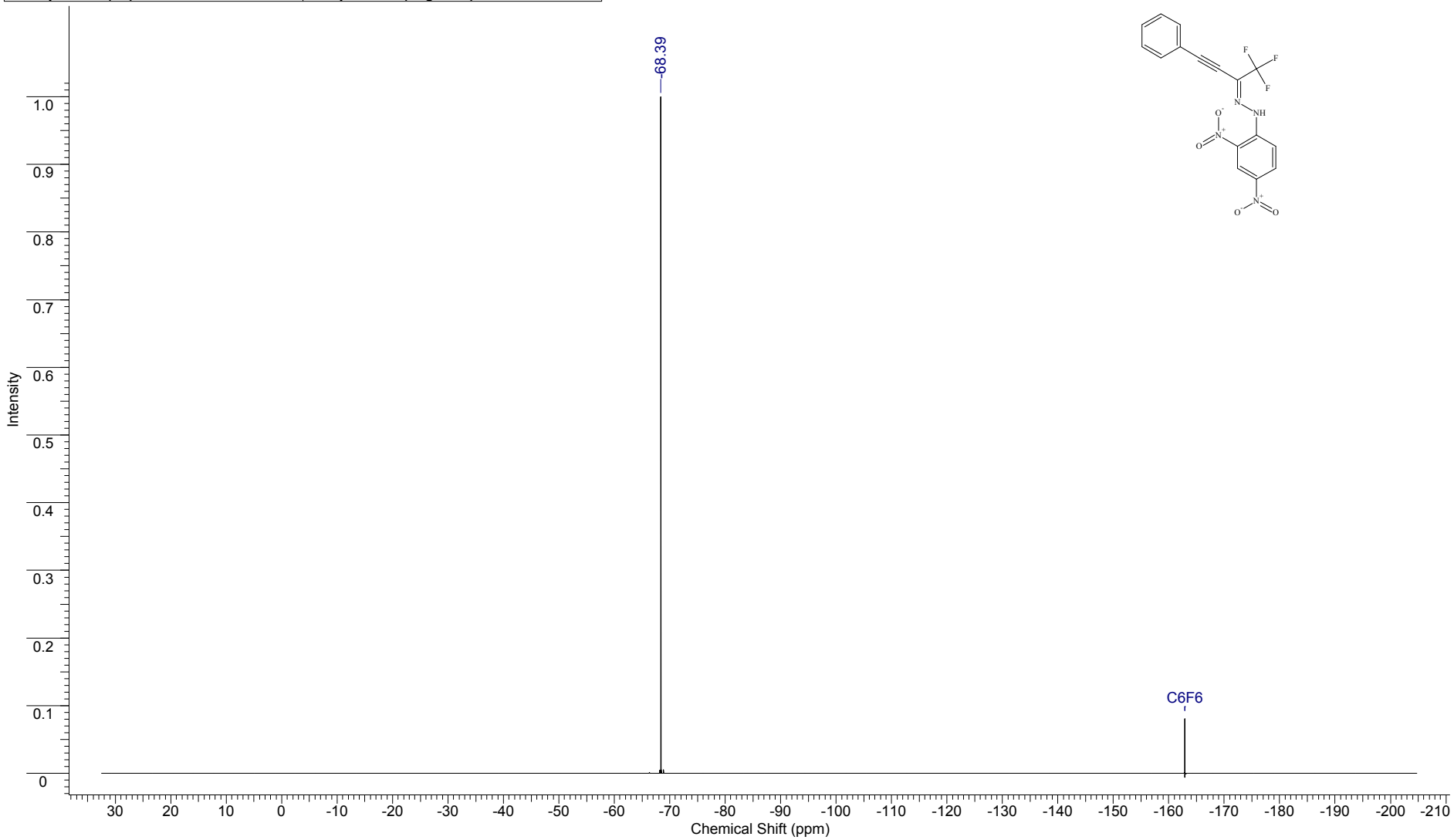
Acquisition Time (sec)	2.5559	Comment	Imported from UXNMR.		Date	06 Sep 2016 14:35:04
File Name	D:\BN\output\2016\09\řáf öýádü\BM-838-11.H_001001r	Frequency (MHz)	400.13	Nucleus	1H	
Number of Transients	4	Original Points Count	16384	Points Count	65536	
Solvent	CHLOROFORM-D	Sweep Width (Hz)	6410.26	Pulse Sequence	zg30	
		Temperature (degree C)	27.000			



¹H NMR spectrum of **3h** (400.1 MHz, CDCl₃)

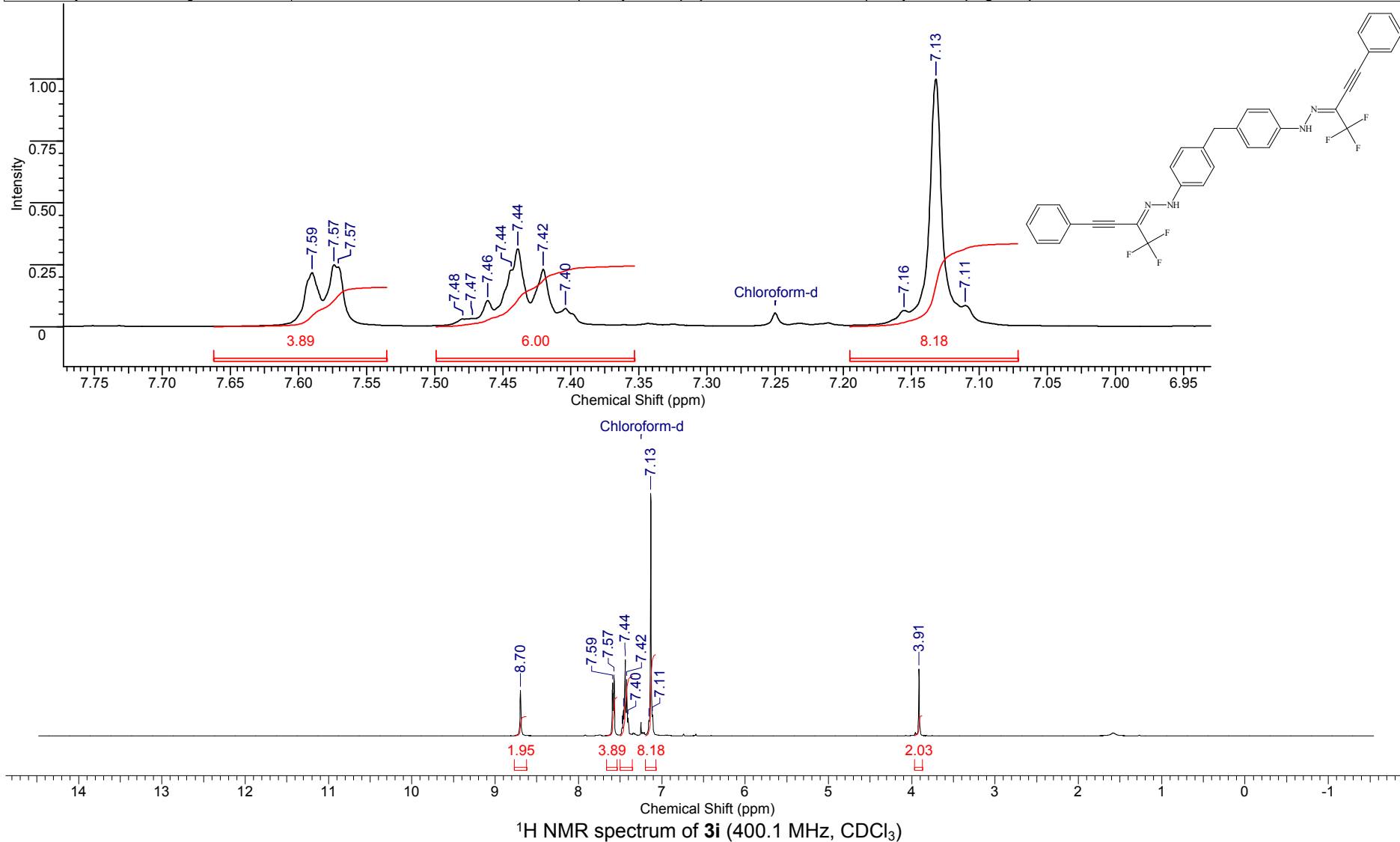
FW 378.2624 Formula $C_{16}H_9F_3N_4O_4$

Acquisition Time (sec)	0.7340	Date	Mar 23 2015	File Name	D:\BN\Docs (BN)\vasiliy\SPEC_BM_FBM733-2-F_20150323_01\FLUORINE_01	
Frequency (MHz)	376.31	Nucleus	^{19}F	Number of Transients	1000	Original Points Count 65536
Points Count	65536	Pulse Sequence	s2pul	Solvent	CHLOROFORM-D	
Sweep Width (Hz)	89285.71	Temperature (degree C)	26.000			



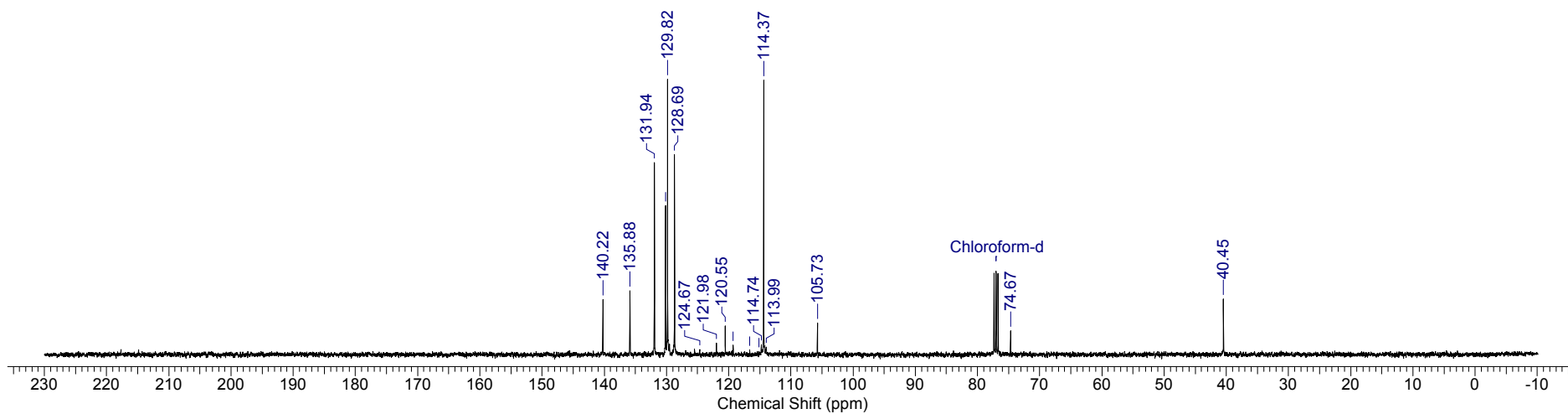
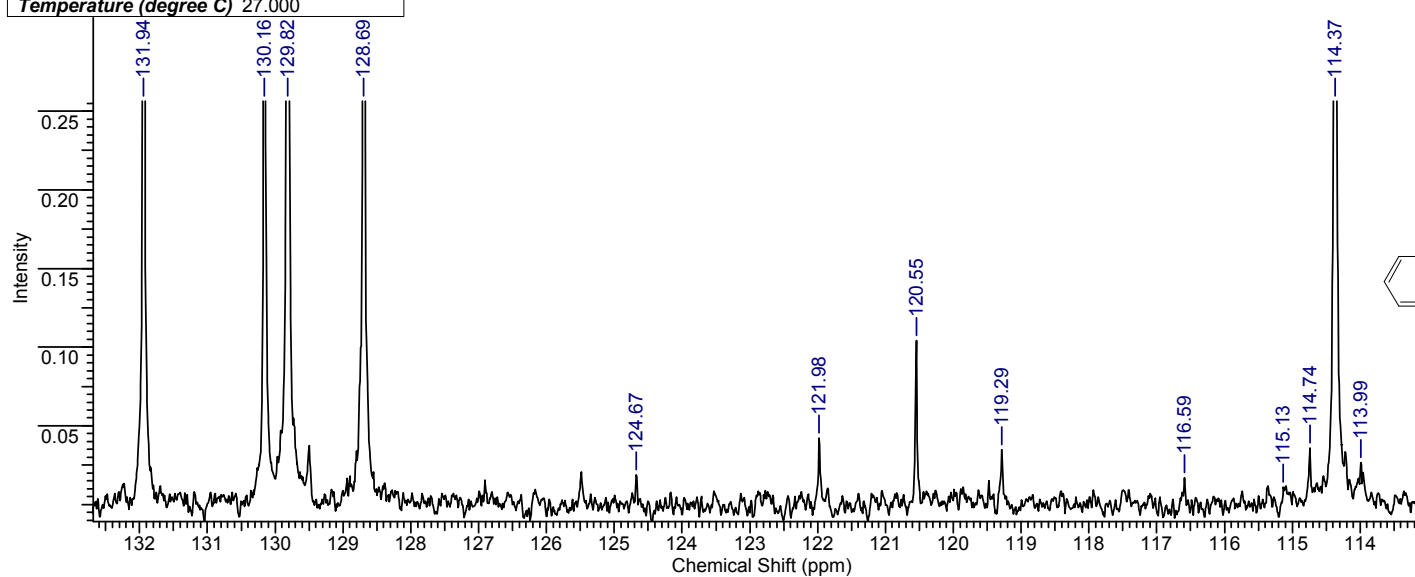
FW 588.5452 Formula C₃₃H₂₂F₆N₄

Acquisition Time (sec)	2.5559	Comment	Imported from UXNMR.		Date	02 May 2017 14:38:50	
File Name	C:\BM_DATA\DOCS\SPEC_BM_H,C_V-XII.2017\BM-1053-a.H_001001r				Frequency (MHz)	400.13	
Nucleus	1H	Number of Transients	4	Original Points Count	16384	Points Count	65536
Pulse Sequence	zg30	Solvent	DMSO-D6	Sweep Width (Hz)	6410.26	Temperature (degree C)	27.000



FW 588.5452 Formula C₃₃H₂₂F₆N₄

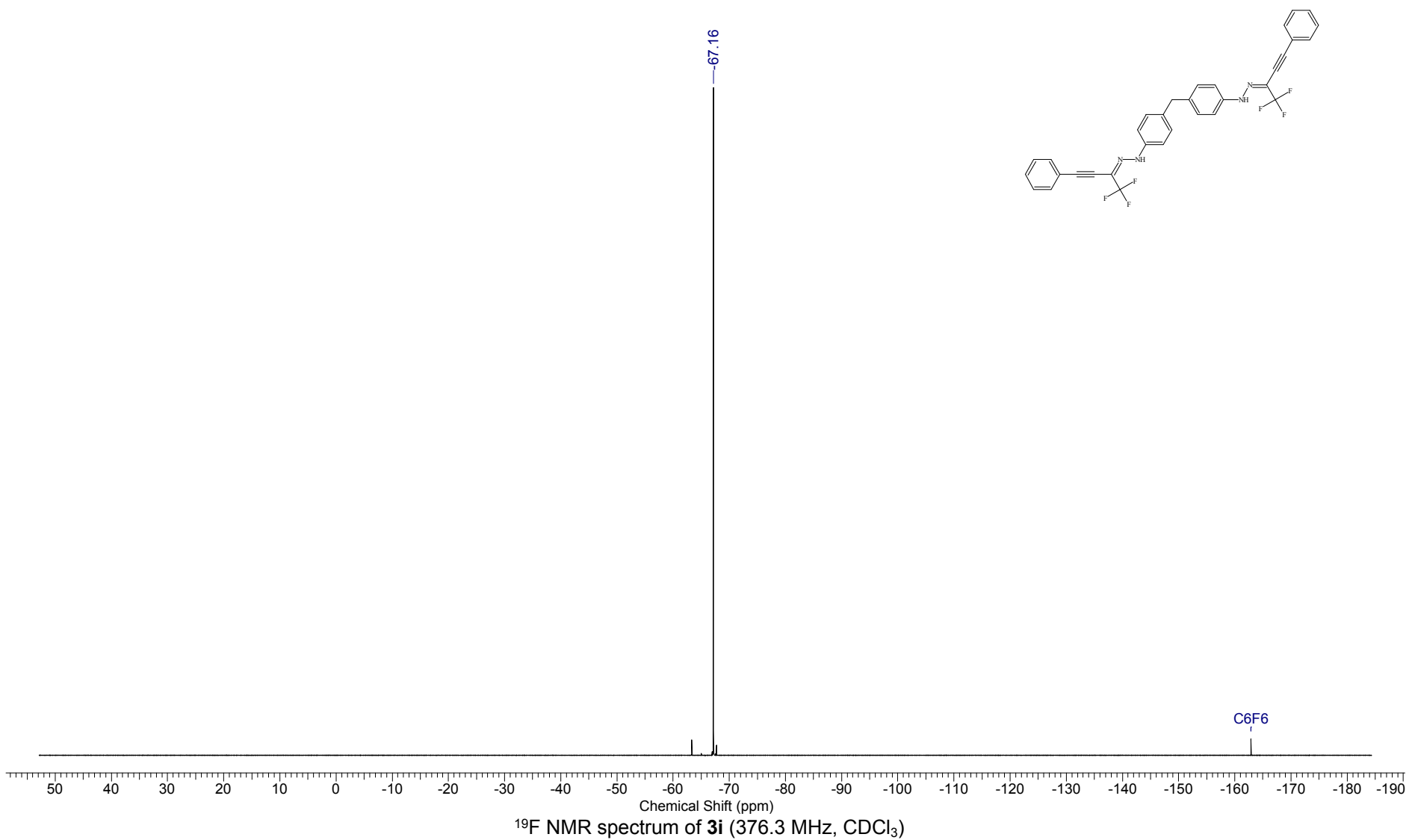
Acquisition Time (sec)	0.4999	Comment	Imported from UXNMR.	Date	02 May 2017 14:48:12
File Name	C:\BM_DATA\DOCS\SPEC_BM_H,C_V-XII.2017\BM-1053-a.C_002001r			Frequency (MHz)	100.61
Nucleus	13C	Number of Transients	316	Original Points Count	12076
Pulse Sequence	zgpg30	Solvent	CHLOROFORM-D	Points Count	65536
Temperature (degree C)	27.000			Sweep Width (Hz)	24154.59



¹³C NMR spectrum of **3i** (100.6 MHz, CDCl₃)

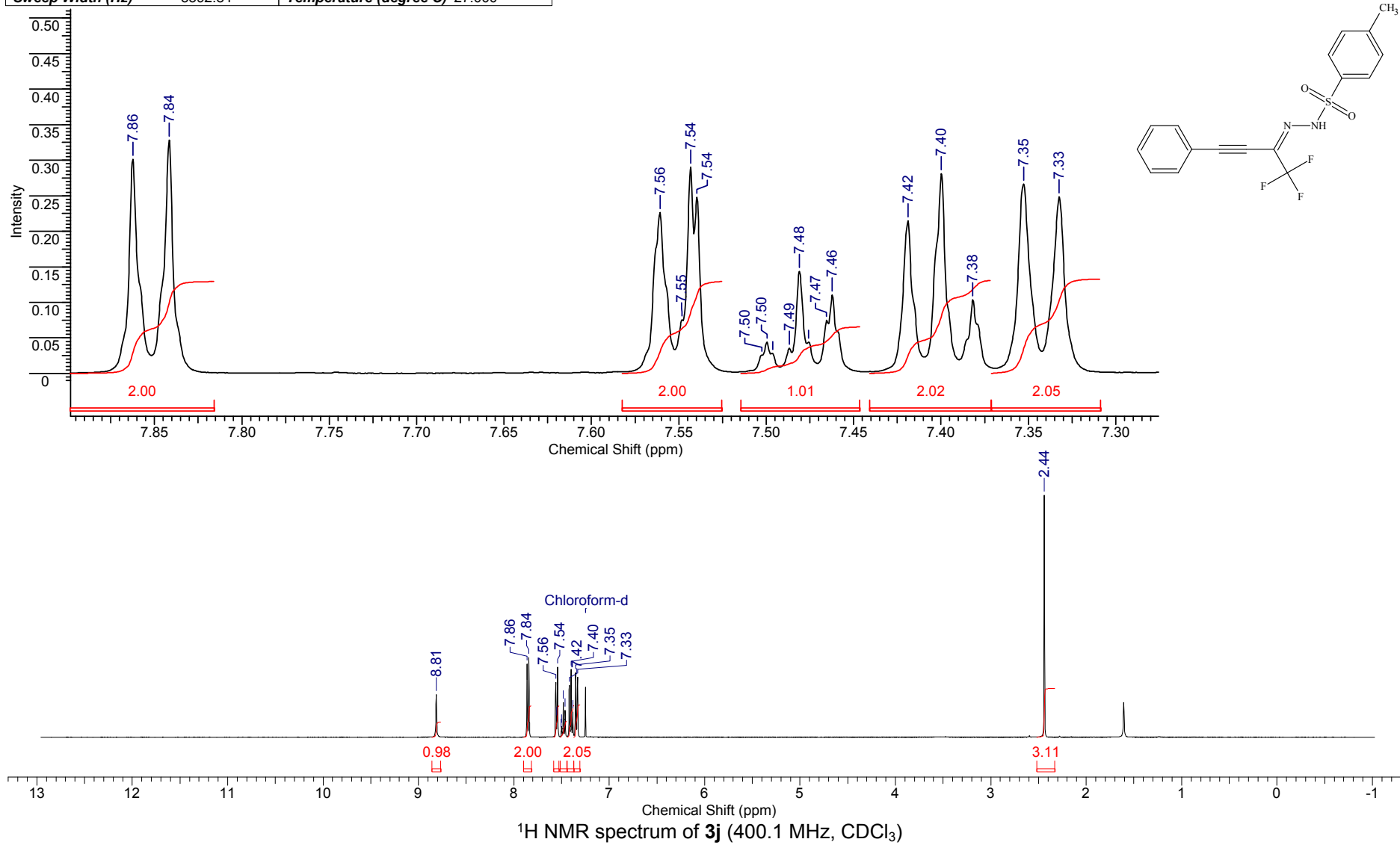
FW	588.5452	Formula	C ₃₃ H ₂₂ F ₆ N ₄
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Acquisition Time (sec)	1.4680	Date	May 4 2017	File Name	C:\BM_DATA\DOCS\SPEC_F_I-XII.2017\BM-1053a-F_20170504_01\FLUORINE_01		
Frequency (MHz)	376.32	Nucleus	¹⁹ F	Number of Transients	8	Original Points Count	131073
Points Count	262144	Pulse Sequence	s2pul	Solvent	CHLOROFORM-D		
Sweep Width (Hz)	89285.71	Temperature (degree C)	22.000				



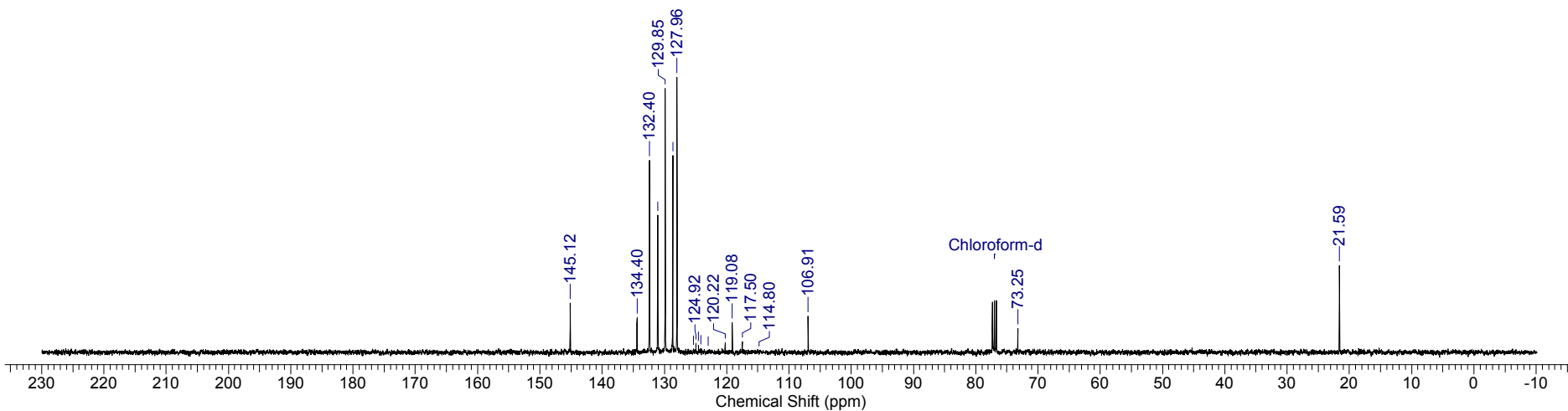
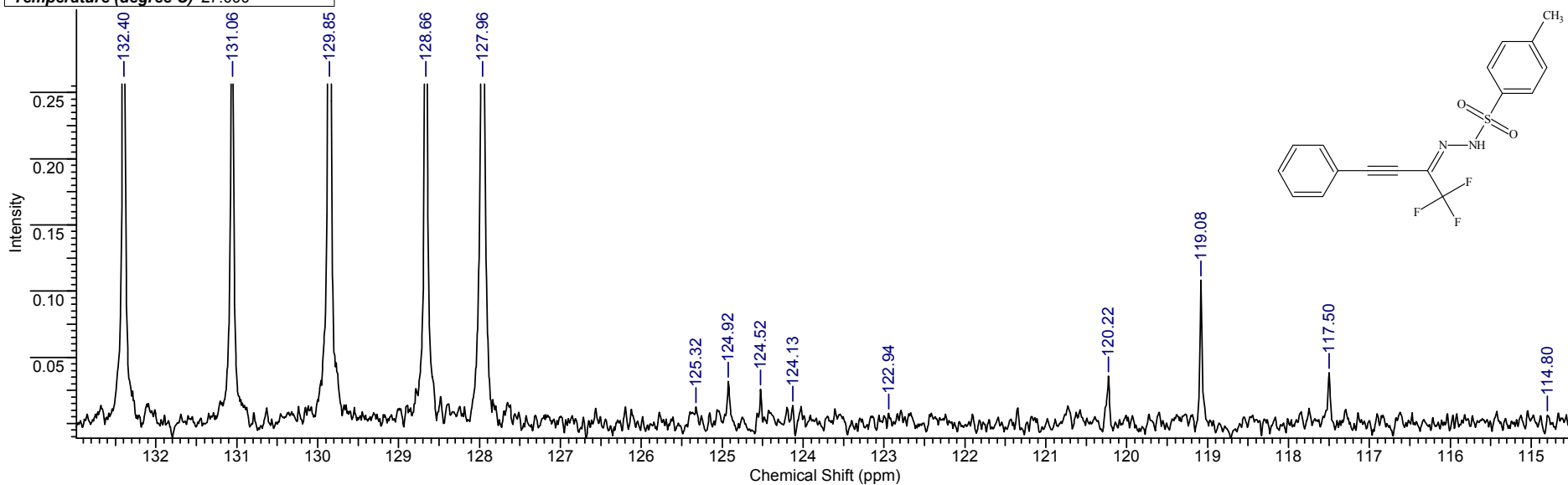
FW 366.3586 Formula C₁₇H₁₃F₃N₂O₂S

Acquisition Time (sec)	2.9295	Comment	Imported from UXNMR.		Date	25 Apr 2017 22:30:40	
File Name	C:\BM_DATA\170425\BM-1045_001001r	Frequency (MHz)	400.13	Nucleus	1H	Number of Transients	8
Original Points Count	16384	Points Count	65536	Pulse Sequence	zg30	Solvent	CHLOROFORM-D
Sweep Width (Hz)	5592.84	Temperature (degree C)	27.000				



FW 366.3586 Formula C₁₇H₁₃F₃N₂O₂S

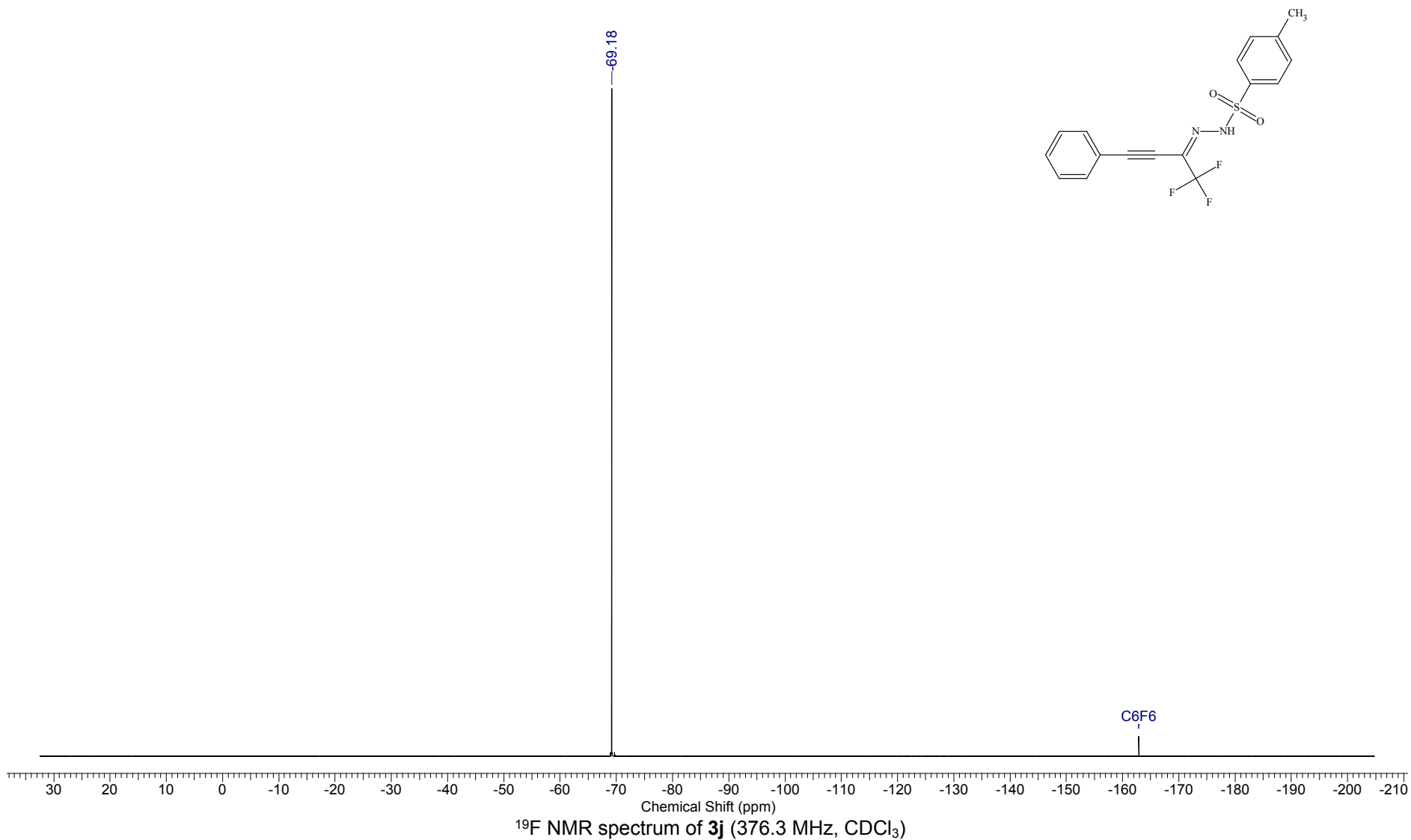
Acquisition Time (sec)	0.4999	Comment	Imported from UXMNR.	Date	26 Apr 2017 17:28:46
File Name	C:\BM_DATA\DOCS\SPEC_BM_H,C_I-IV.2017\BM-1045.C_002001r			Frequency (MHz)	100.61
Nucleus	13C	Number of Transients	128	Original Points Count	12076
Pulse Sequence	zpgg30	Solvent	CHLOROFORM-D	Points Count	65536
Temperature (degree C)	27.000			Sweep Width (Hz)	24154.59



¹³C NMR spectrum of **3j** (100.6 MHz, CDCl₃)

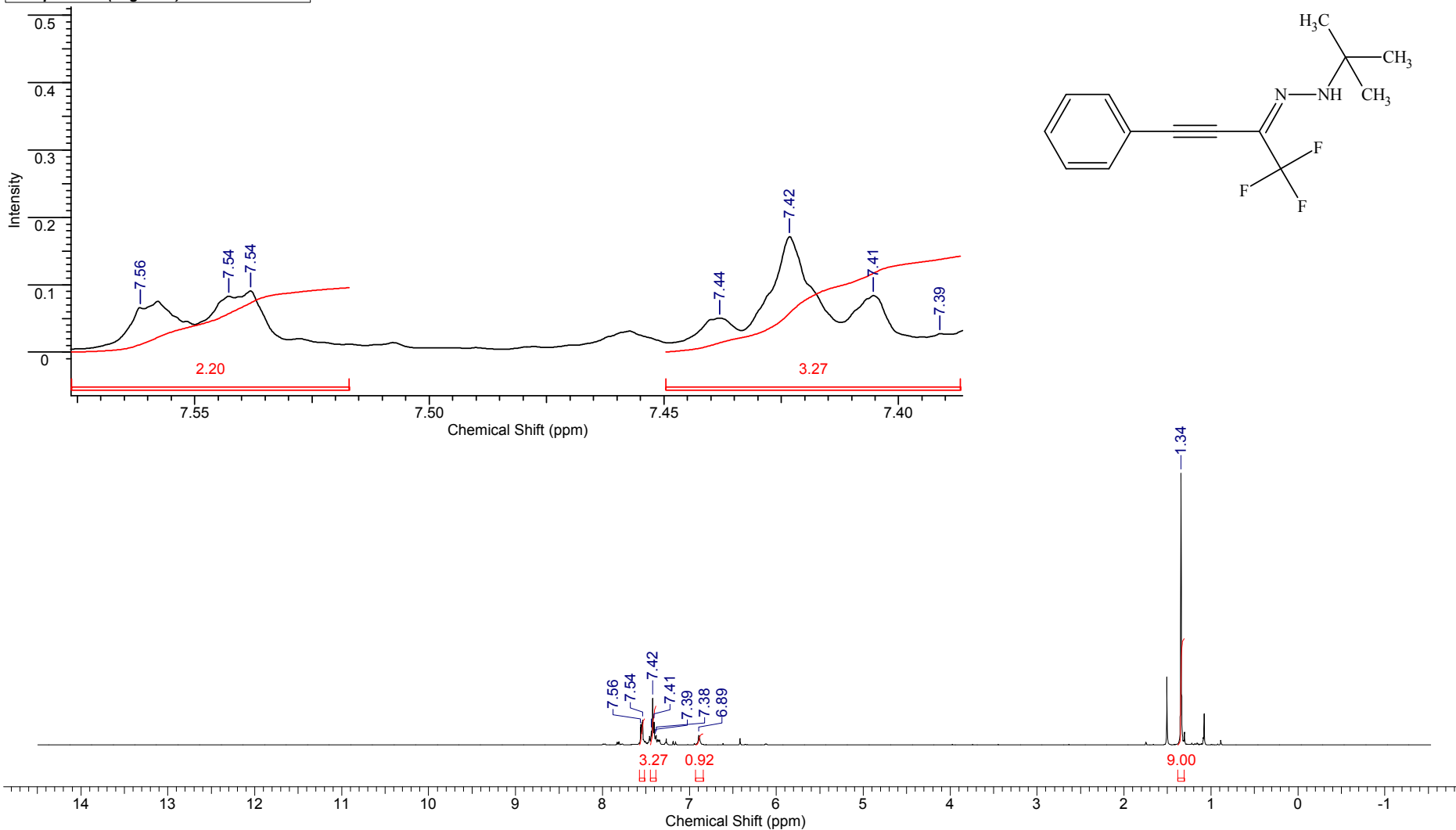
FW	366.3586	Formula	C ₁₇ H ₁₃ F ₃ N ₂ O ₂ S
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Acquisition Time (sec)	1.5000	Date	Jun 19 2017	File Name	C:\BM_DATA\DOCS\SPEC_F_I-XII.2017\BM-1045_20170619_01\FLUORINE_01		
Frequency (MHz)	376.31	Nucleus	19F	Number of Transients	16	Original Points Count	133929
Points Count	262144	Pulse Sequence	s2pul	Solvent	CHLOROFORM-D		
Sweep Width (Hz)	89285.71	Temperature (degree C)	25.000				



FW 268.2776 Formula C₁₄H₁₅F₃N₂

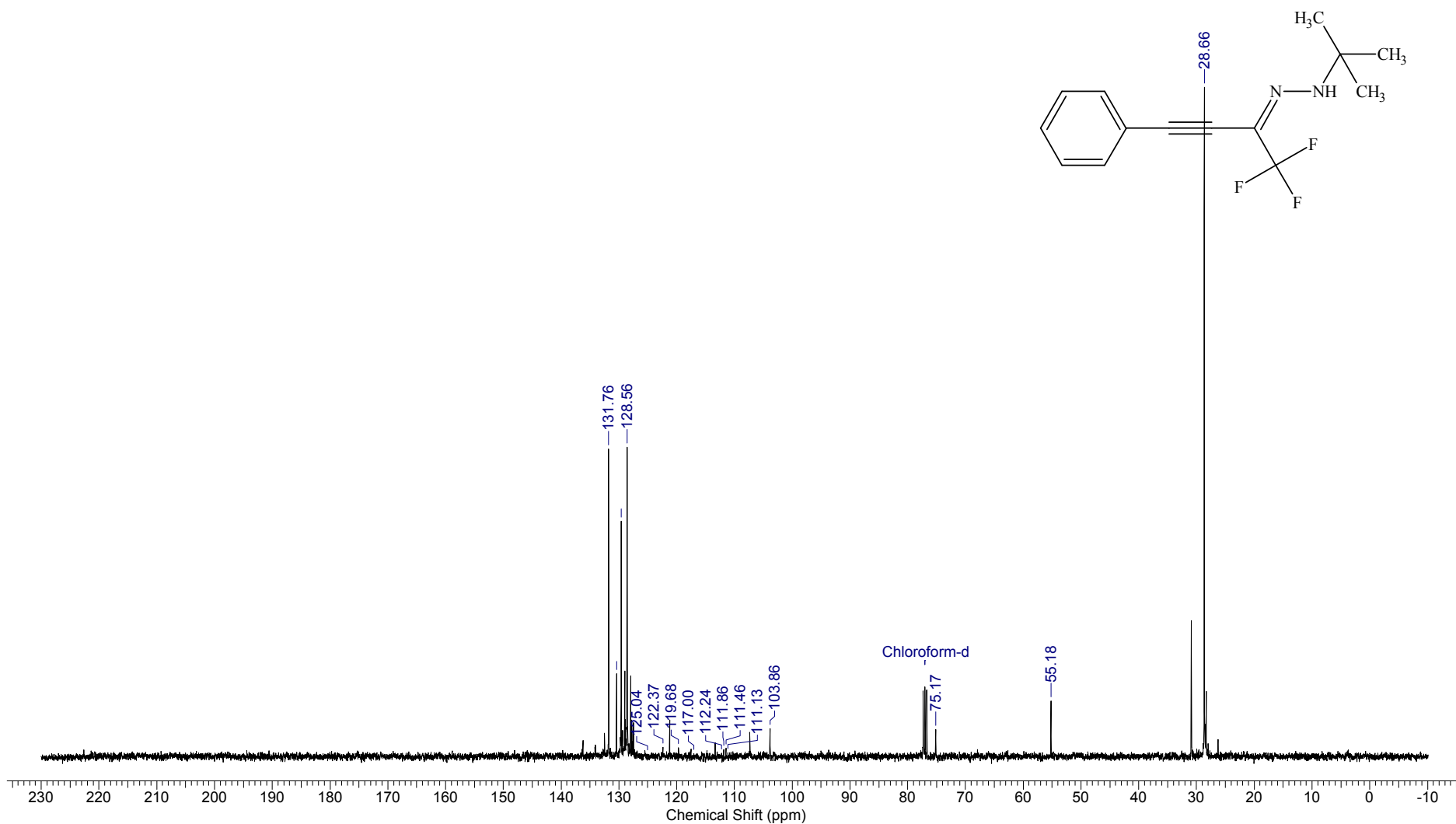
Acquisition Time (sec)	2.5559	Comment	Imported from UXNMR.	Date	03 Jun 2017 13:20:46
File Name	C:\IBM_DATA\DOCS\SPEC_BM_H,C_V-XII.2017\BM-1096-R.H_001001r			Frequency (MHz)	400.13
Nucleus	1H	Number of Transients	4	Original Points Count	16384
Pulse Sequence	zg30	Solvent	CHLOROFORM-D	Points Count	65536
Temperature (degree C)	27.000			Sweep Width (Hz)	6410.26



¹H NMR spectrum of **3k** (400.1 MHz, CDCl₃). Due to instability of **3k**, we did not succeed to obtain this compound in pure form. The purity of **3k** is about 85-90% accordingly NMR spectra.

FW	268.2776	Formula	C ₁₄ H ₁₅ F ₃ N ₂
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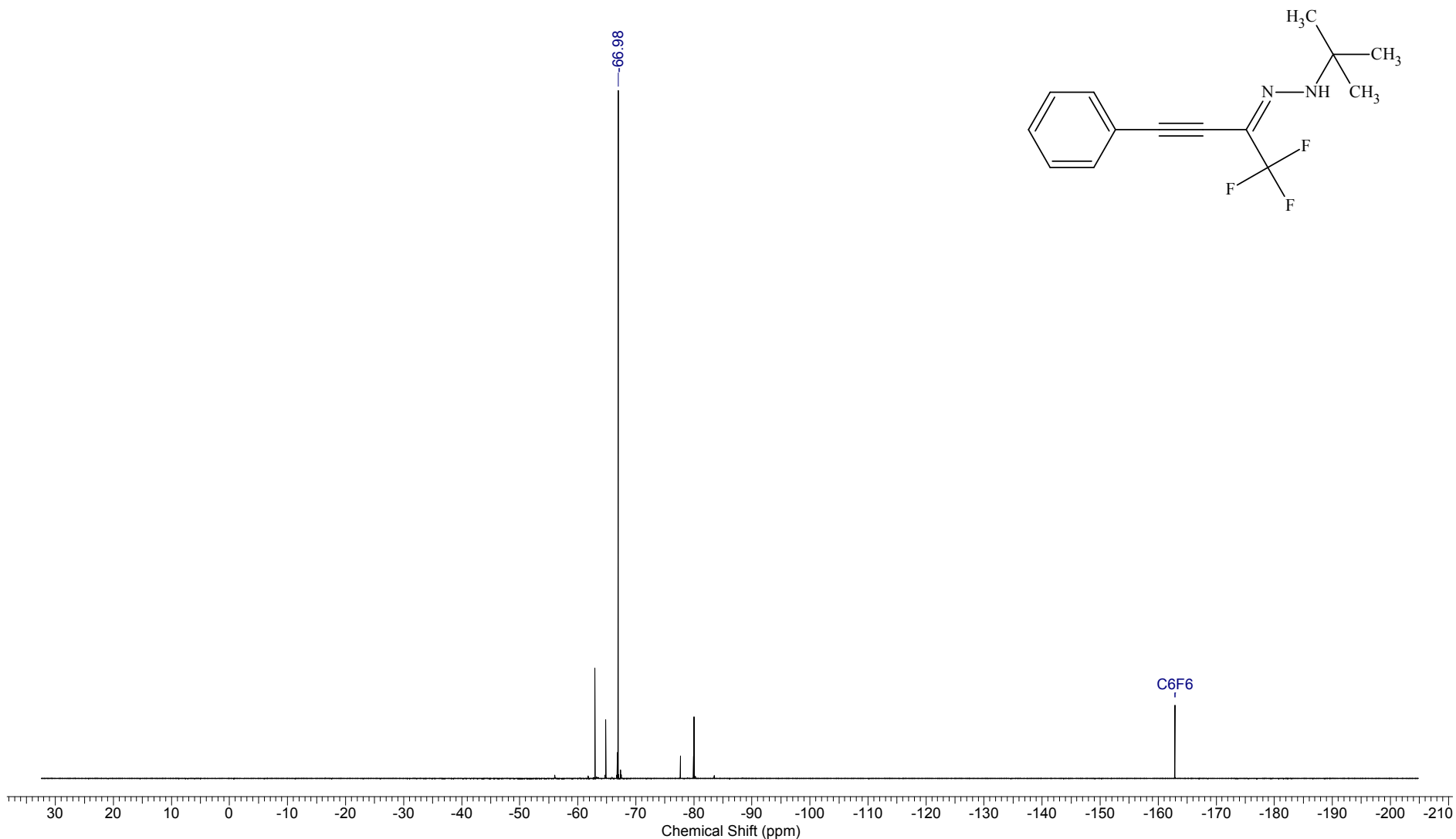
Acquisition Time (sec)	0.4999	Comment	Imported from UXMNR.	Date	03 Jun 2017 13:25:16
File Name	C:\BM_DATA\DOCS\SPEC_BM_H,C_V-XII.2017\BM-1096-R.C_002001r			Frequency (MHz)	100.61
Nucleus	13C	Number of Transients	77	Original Points Count	12076
Pulse Sequence	zgpg30	Solvent	CHLOROFORM-D	Points Count	65536
Temperature (degree C)	27.000			Sweep Width (Hz)	24154.59



¹³C NMR spectrum of **3k** (100.6 MHz, CDCl₃). Due to instability of **3k**, we did not succeed to obtain this compound in pure form. The purity of **3k** is about 85-90% accordingly NMR spectra.

FW	268.2776	Formula	C ₁₄ H ₁₅ F ₃ N ₂
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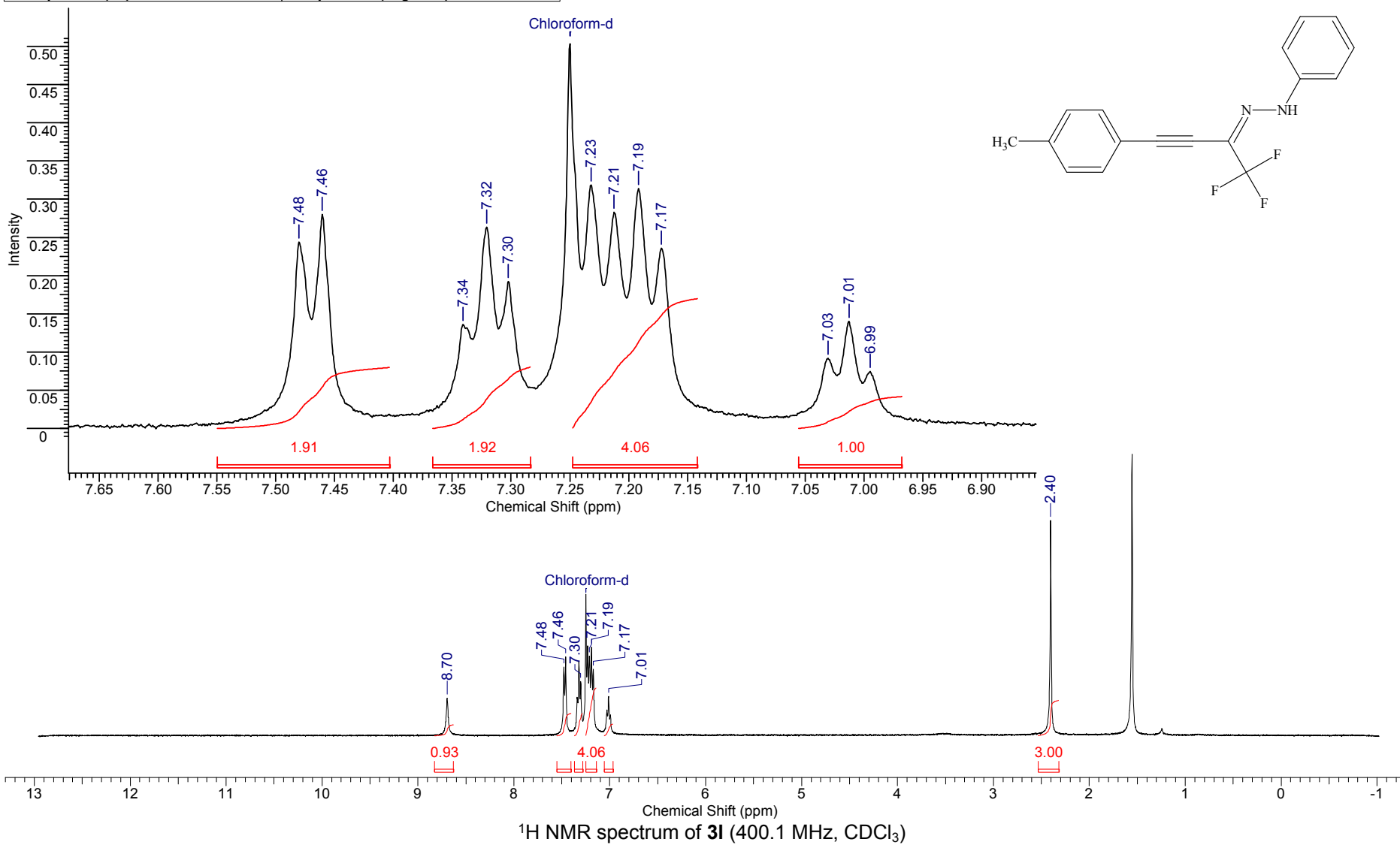
Acquisition Time (sec)	1.5000	Date	Jun 5 2017	File Name	C:\BM_DATA\DOCS\SPEC_F_I-XII.2017\BM-1096-R_20170605_01\FLUORINE_01		
Frequency (MHz)	376.31	Nucleus	¹⁹ F	Number of Transients	16	Original Points Count	133929
Points Count	262144	Pulse Sequence	s2pul	Solvent	CHLOROFORM-D		
Sweep Width (Hz)	89285.71	Temperature (degree C)	25.000				



¹⁹F NMR spectrum of **3k** (376.3 MHz, CDCl₃). Due to instability of **3k**, we did not succeed to obtain this compound in pure form. The purity of **3k** is about 85-90% accordingly NMR spectra.

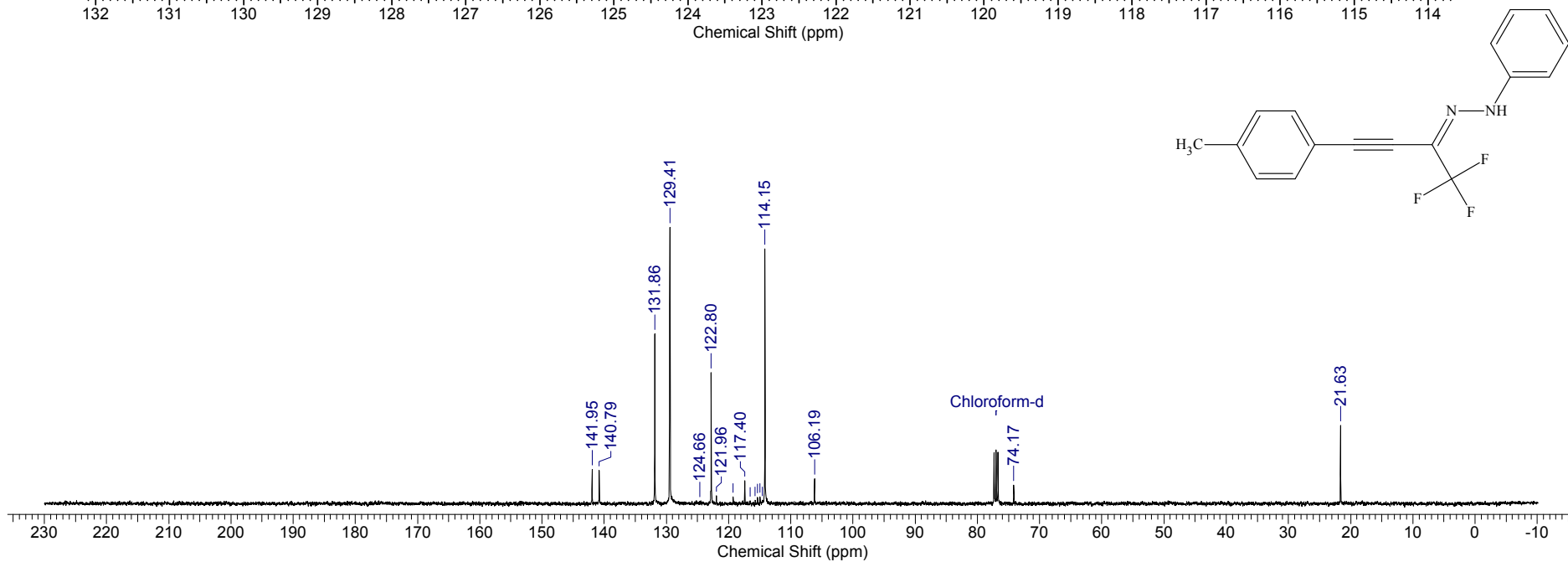
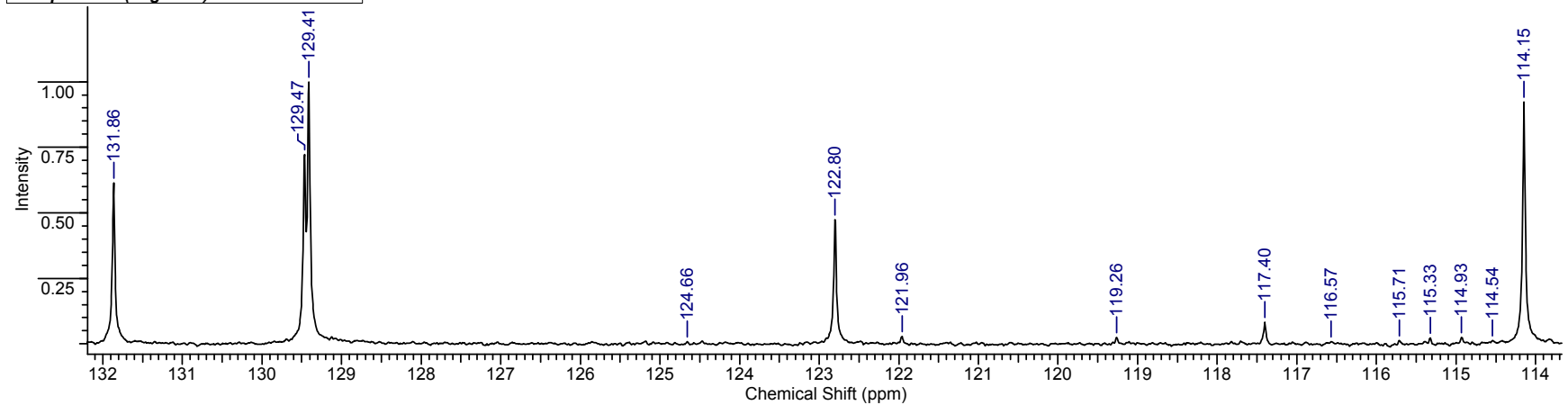
FW 302.2938 Formula C₁₇H₁₃F₃N₂

Acquisition Time (sec)	2.9295	Comment	Imported from UXNMR.		Date	27 Apr 2017 22:40:32	
File Name	C:\BM_DATA\BM-1051-d\BM-1051-d_001001r	Frequency (MHz)	400.13	Nucleus	1H	Number of Transients	8
Original Points Count	16384	Points Count	65536	Pulse Sequence	zg30	Solvent	CHLOROFORM-D
Sweep Width (Hz)	5592.84	Temperature (degree C)	27.000				



FW 302.2938 **Formula** C₁₇H₁₃F₃N₂

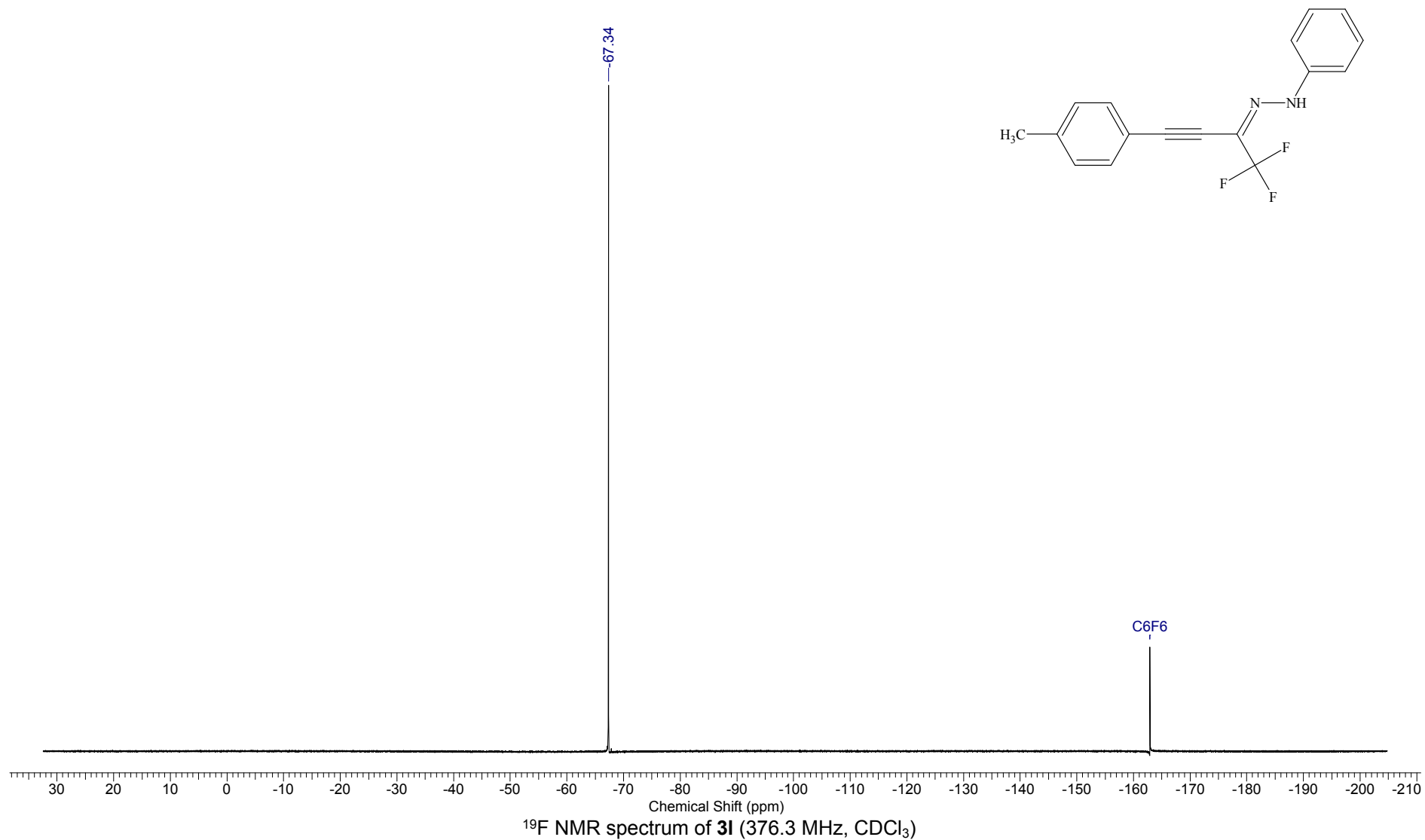
Acquisition Time (sec)	0.4999	Comment	Imported from UXMNR.	Date	28 Apr 2017 15:39:12
File Name	C:\BM_DATA\DOCS\SPEC_BM_H,C_I-IV.2017\BM-1051-d.C_002001r			Frequency (MHz)	100.61
Nucleus	13C	Number of Transients	397	Original Points Count	12076
Pulse Sequence	zgpg30	Solvent	CHLOROFORM-D	Points Count	65536
Temperature (degree C)	27.000			Sweep Width (Hz)	24154.59



¹³C NMR spectrum of **3I** (100.6 MHz, CDCl₃)

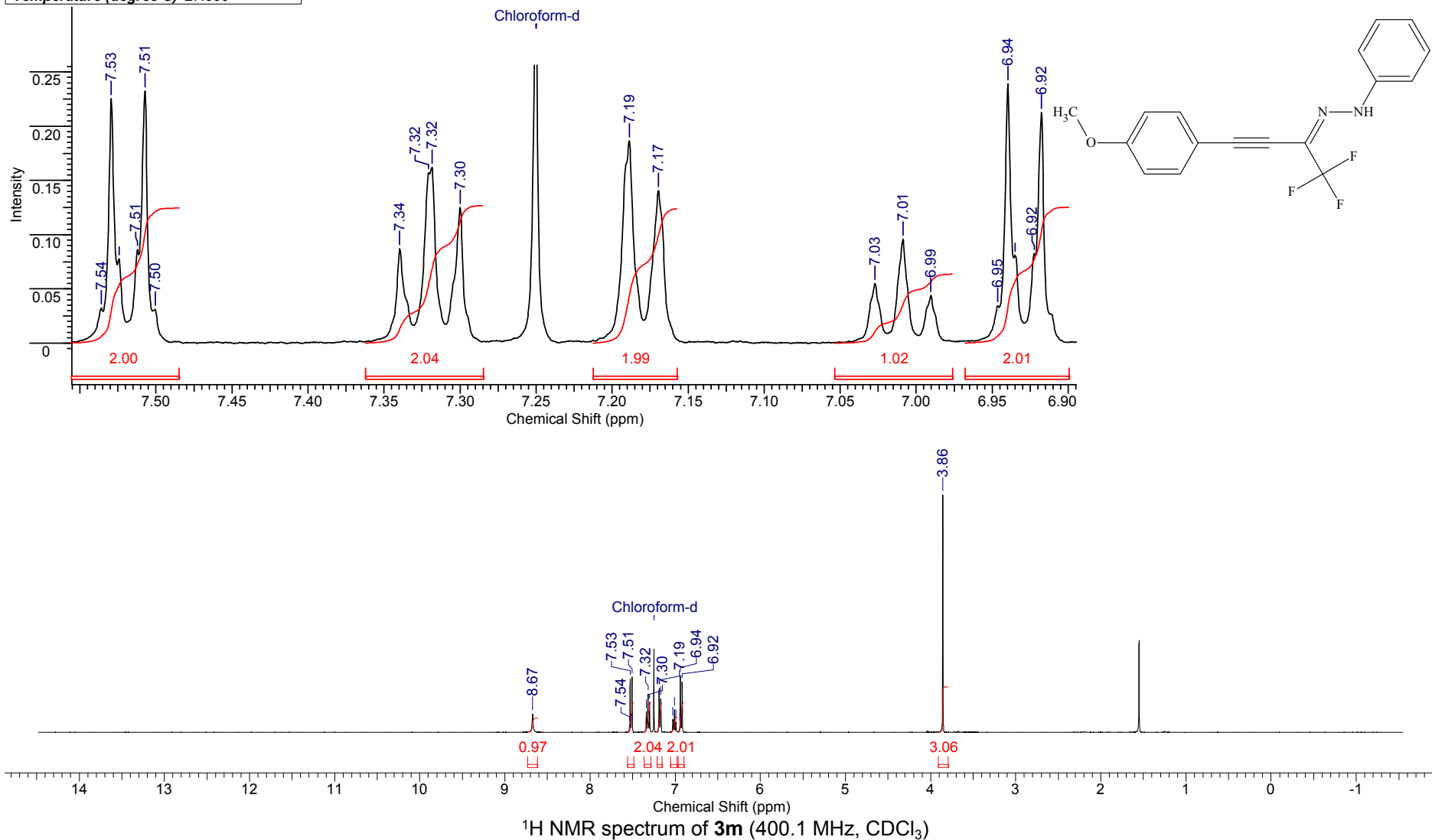
FW	302.2938	Formula	C ₁₇ H ₁₃ F ₃ N ₂
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Acquisition Time (sec)	1.0000	Date	Apr 28 2017	File Name	C:\BM_DATA\DOCS\SPEC_F_I-XII.2017\BM-1051_20170428_01\FLUORINE_01		
Frequency (MHz)	376.31	Nucleus	¹⁹ F	Number of Transients	16	Original Points Count	89286
Points Count	131072	Pulse Sequence	s2pul	Solvent	CHLOROFORM-D		
Sweep Width (Hz)	89285.71	Temperature (degree C)	25.000				



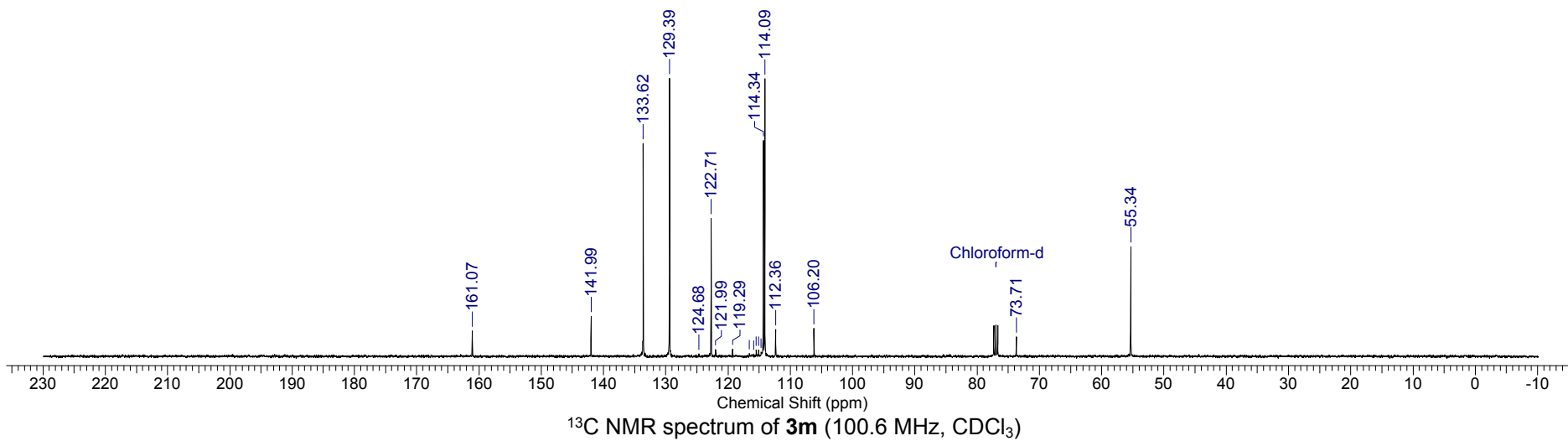
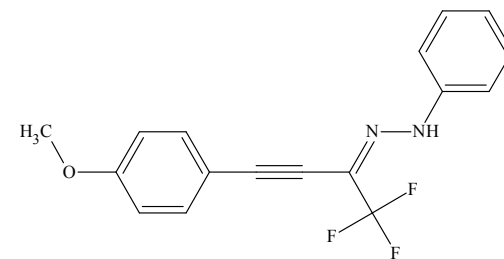
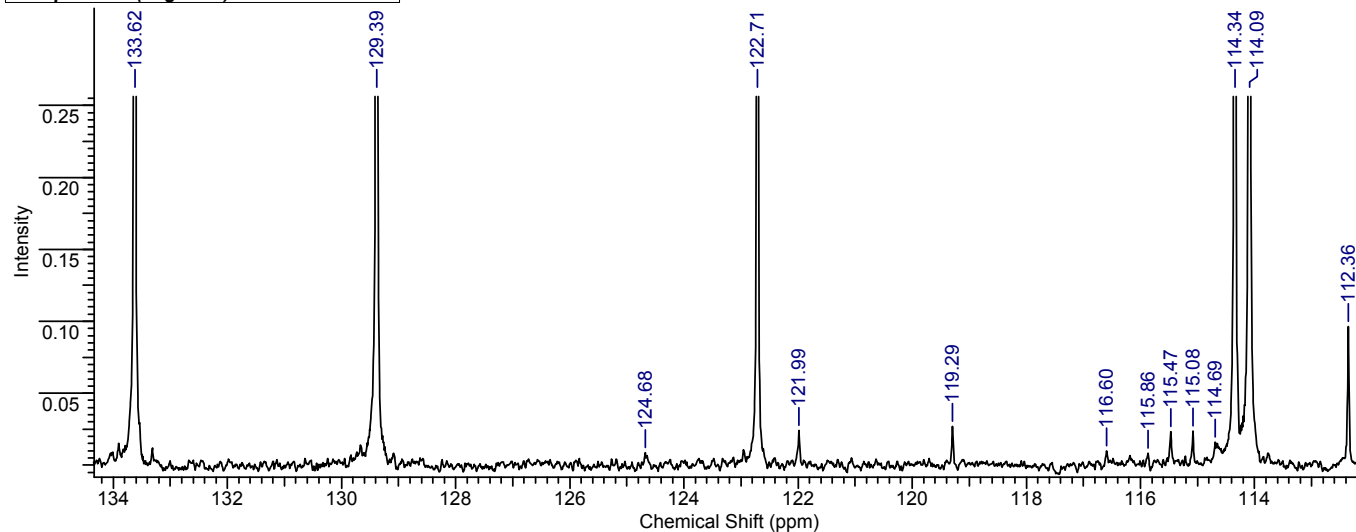
FW 318.2932 **Formula** C₁₇H₁₃F₃N₂O

Acquisition Time (sec)	2.5559	Comment	Imported from UXMNR.	Date	21 Mar 2017 14:28:22
File Name	C:\BM_DATA\DOCS\SPEC_BM_H,C I-IV.2017\BM-975.H_001001r			Frequency (MHz)	400.13
Nucleus	1H	Number of Transients	4	Original Points Count	16384
Pulse Sequence	zg30	Solvent	CHLOROFORM-D	Points Count	65536
Temperature (degree C)	27.000			Sweep Width (Hz)	6410.26



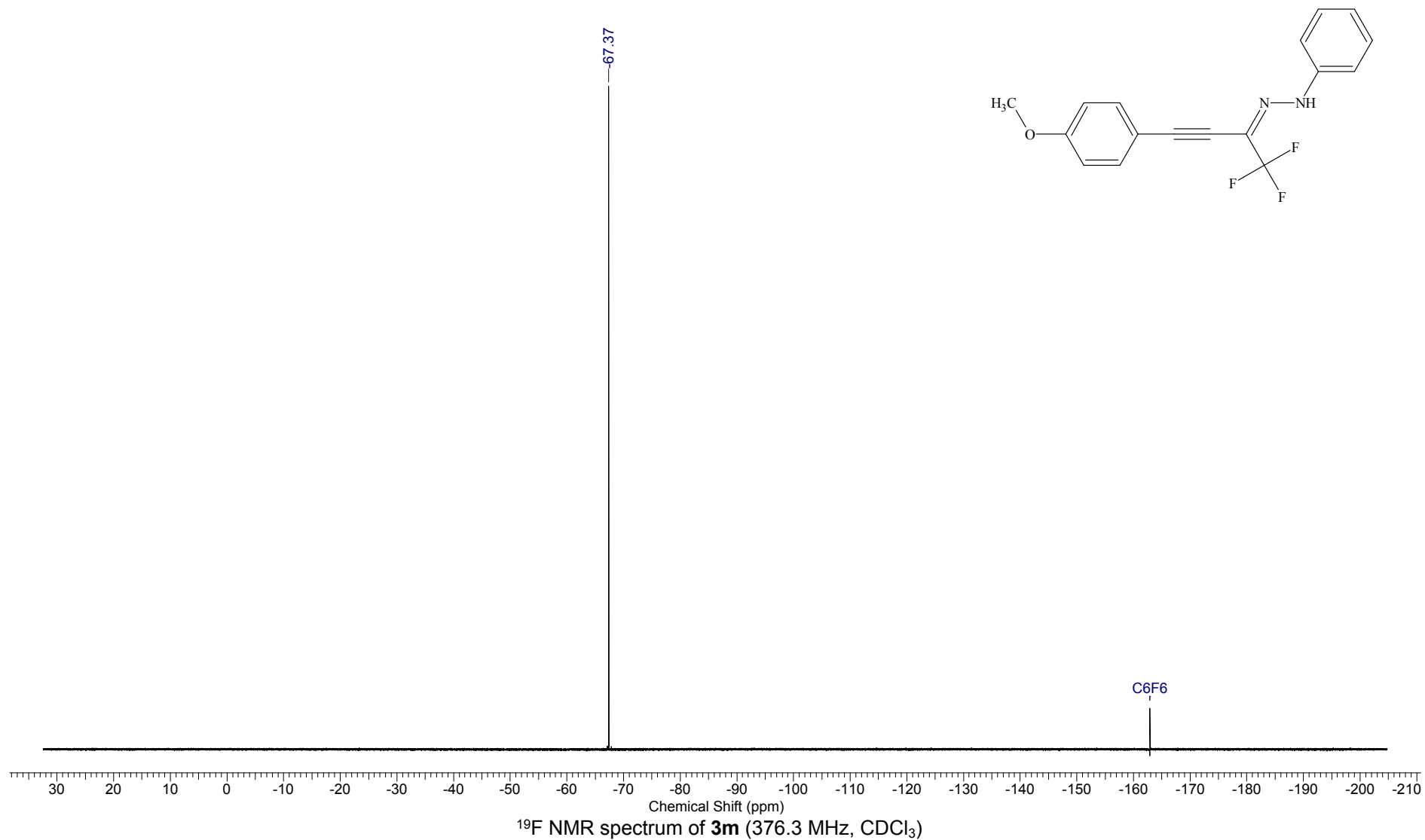
FW 318.2932 **Formula** C₁₇H₁₃F₃N₂O

Acquisition Time (sec)	0.4999	Comment	Imported from UXMNR.	Date	27 Apr 2017 11:30:26
File Name	C:\BM_DATA\DOCS\SPEC_BM_H,C_I-IV.2017\BM-975-c.c_002001r			Frequency (MHz)	100.61
Nucleus	13C	Number of Transients	282	Original Points Count	12076
Pulse Sequence	zgpg30	Solvent	CHLOROFORM-D	Points Count	65536
Temperature (degree C)	27.000			Sweep Width (Hz)	24154.59



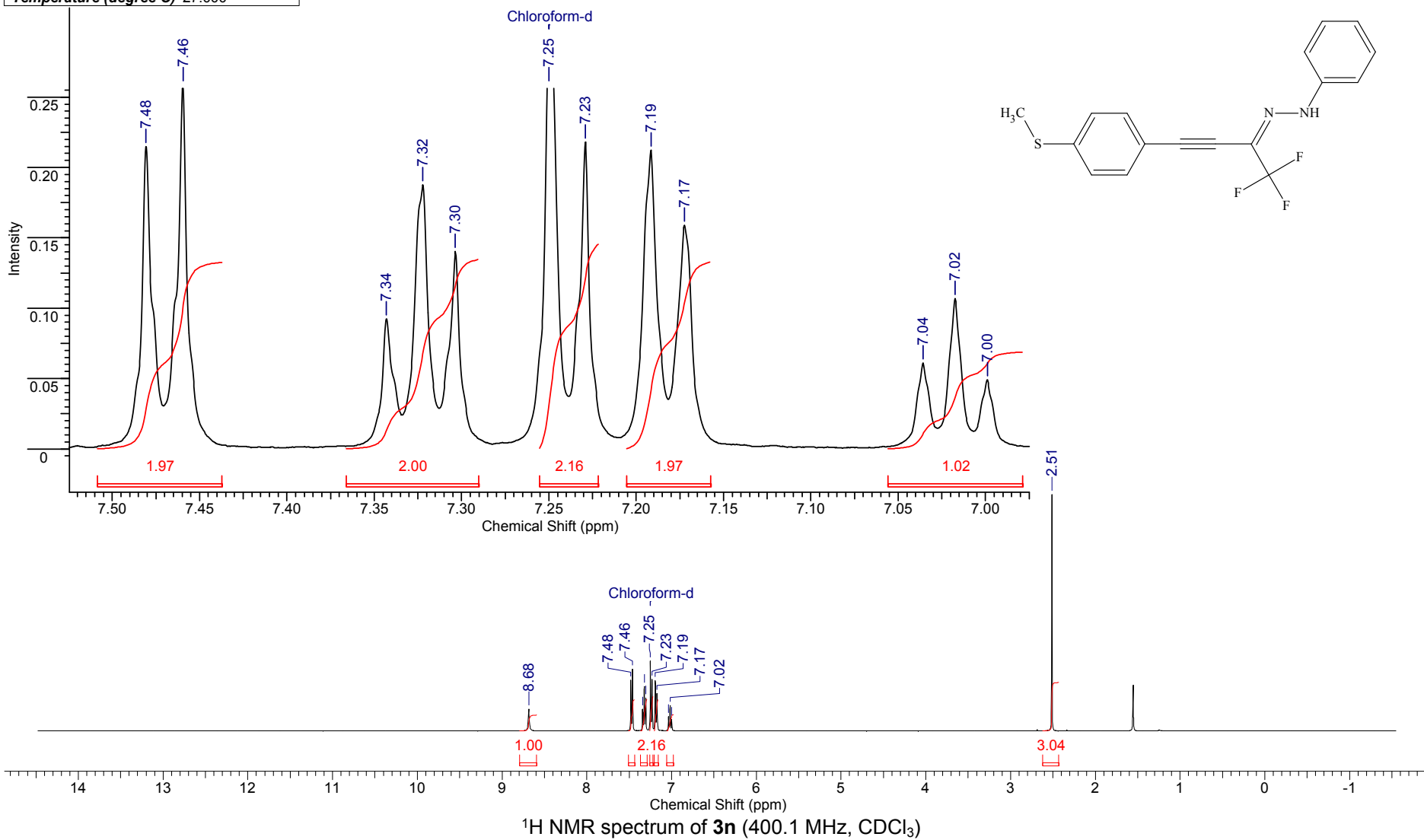
FW	318.2932	Formula	C ₁₇ H ₁₃ F ₃ N ₂ O
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Acquisition Time (sec)	1.0000	Date	Mar 17 2017	File Name	C:\BM_DATA\DOCS\SPEC_F_I-XII.2017\BM-975_20170317_01\FLUORINE_01		
Frequency (MHz)	376.31	Nucleus	¹⁹ F	Number of Transients	1	Original Points Count	89286
Points Count	131072	Pulse Sequence	s2pul	Solvent	CHLOROFORM-D		
Sweep Width (Hz)	89285.71	Temperature (degree C)	25.000				



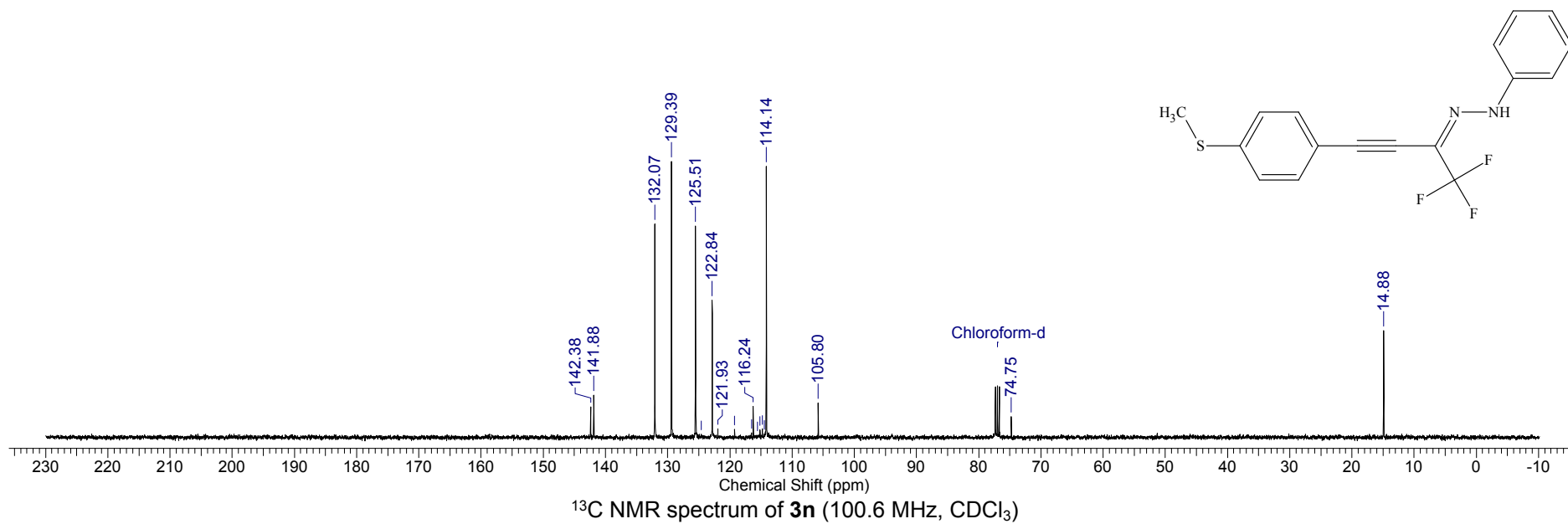
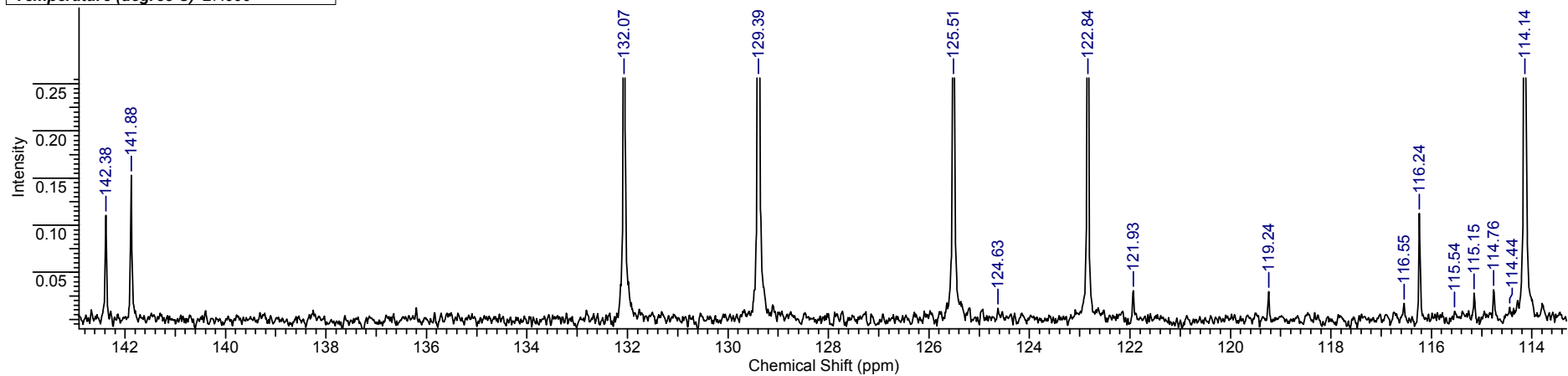
FW 334.3598 Formula C₁₇H₁₃F₃N₂S

Acquisition Time (sec)	2.5559	Comment	Imported from UXMNR.	Date	28 Apr 2017 15:18:18
File Name	C:\BM_DATA\DOCS\SPEC_BM_H,C_I-IV.2017\BM-1050.H_001001r			Frequency (MHz)	400.13
Nucleus	1H	Number of Transients	4	Original Points Count	16384
Pulse Sequence	zg30	Solvent	CHLOROFORM-D	Points Count	65536
Temperature (degree C)	27.000			Sweep Width (Hz)	6410.26



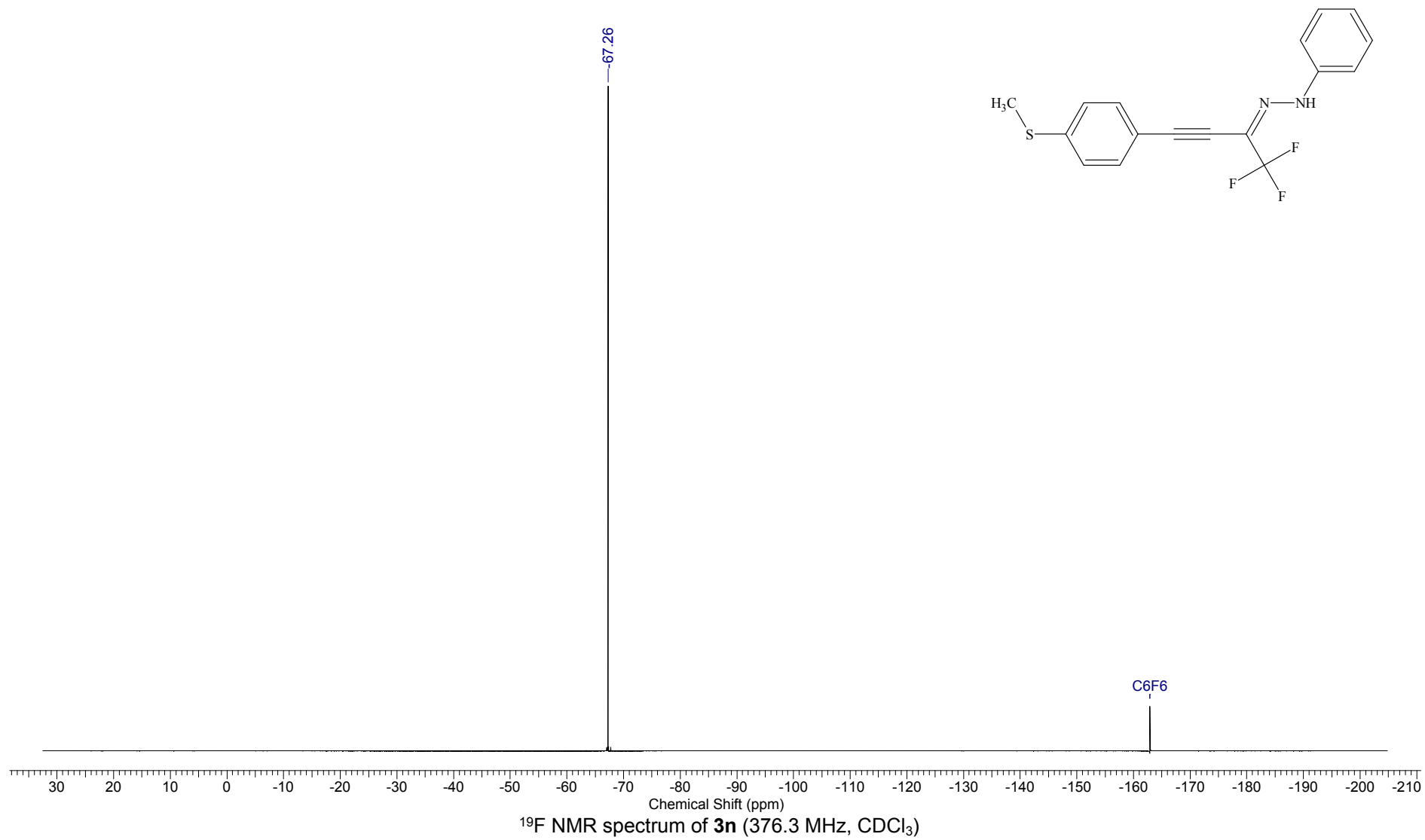
FW 334.3598 **Formula** C₁₇H₁₃F₃N₂S

Acquisition Time (sec)	0.4999	Comment	Imported from UXMNR.	Date	29 Apr 2017 13:37:50
File Name	C:\BM_DATA\DOCS\SPEC_BM_H,C_I-IV.2017\BM-1050.C_002001r			Frequency (MHz)	100.61
Nucleus	13C	Number of Transients	128	Original Points Count	12076
Pulse Sequence	zgpg30	Solvent	CHLOROFORM-D	Points Count	65536
Temperature (degree C)	27.000			Sweep Width (Hz)	24154.59



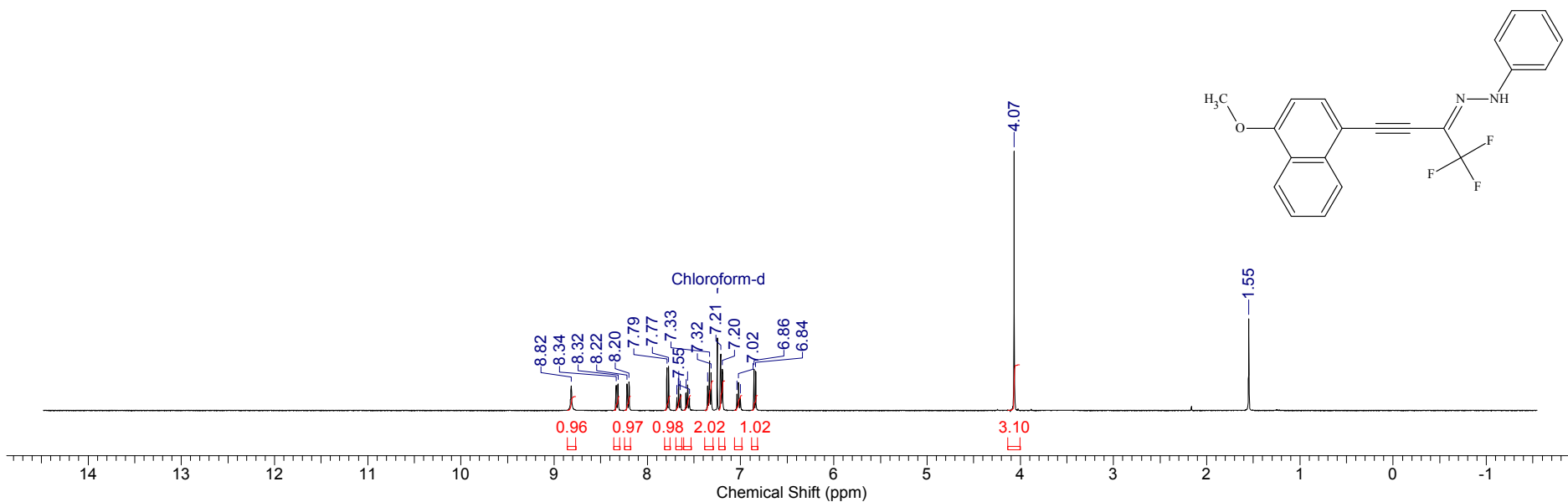
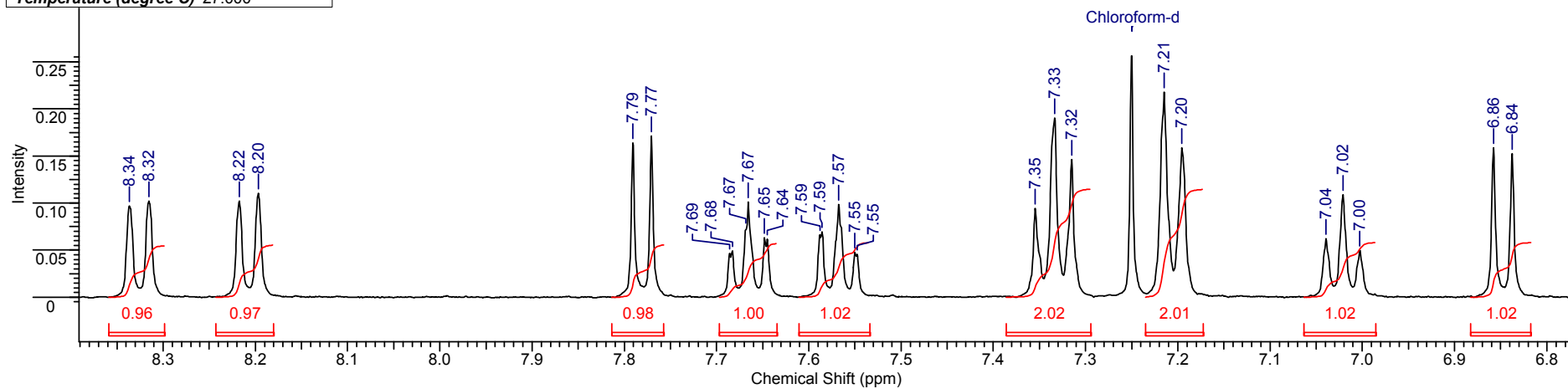
FW	334.3598	Formula	C ₁₇ H ₁₃ F ₃ N ₂ S
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Acquisition Time (sec)	1.0000	Comment	STANDARD FLUORINE PARAMETERS	Date	Apr 28 2017		
File Name	C:\BM_DATA\DOCS\SPEC_F_I-XII.2017\BM-1050_20170428_01\FLUORINE_01			Frequency (MHz)	376.31		
Nucleus	19F	Number of Transients	16	Original Points Count	89286	Points Count	131072
Pulse Sequence	s2pul	Solvent	CHLOROFORM-D	Sweep Width (Hz)	89285.71	Temperature (degree C)	25.000



FW 368.3519 Formula C₂₁H₁₈F₃N₂O

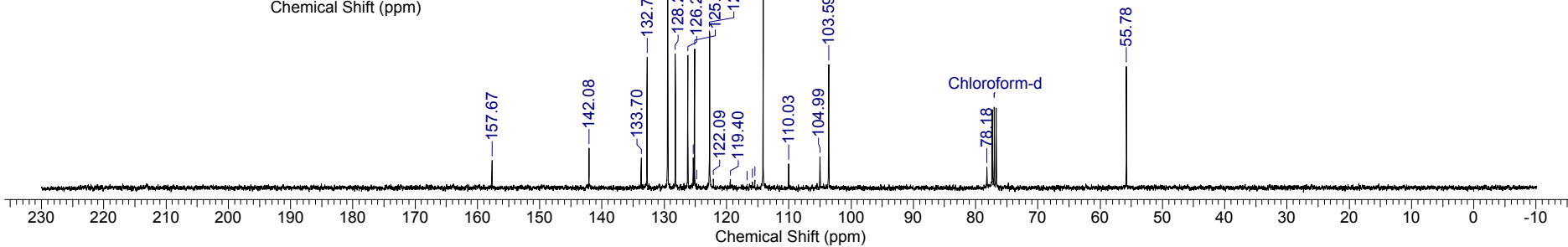
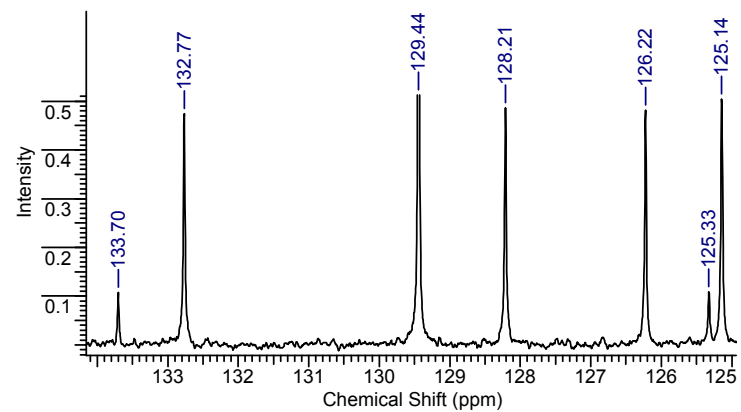
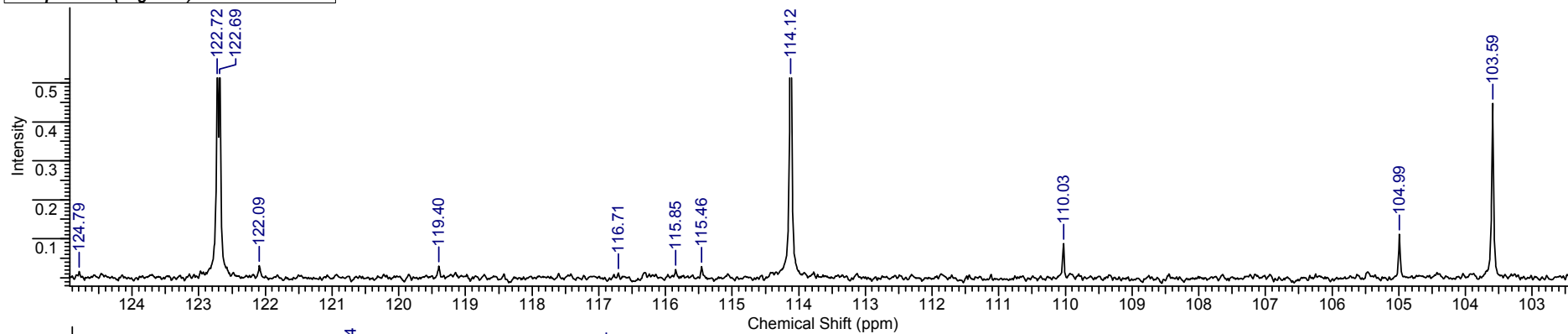
Acquisition Time (sec)	2.5559	Comment	Imported from UXMNR.	Date	21 Mar 2017 14:26:58
File Name	C:\BM_DATA\DOCS\SPEC_BM_H,C_I-IV.2017\BM-976-2a.H_001001r			Frequency (MHz)	400.13
Nucleus	1H	Number of Transients	4	Original Points Count	16384
Pulse Sequence	zg30	Solvent	CHLOROFORM-D	Points Count	65536
Temperature (degree C)	27.000			Sweep Width (Hz)	6410.26



¹H NMR spectrum of **3o** (400.1 MHz, CDCl₃)

FW 368.3519 Formula C₂₁H₁₈F₃N₂O

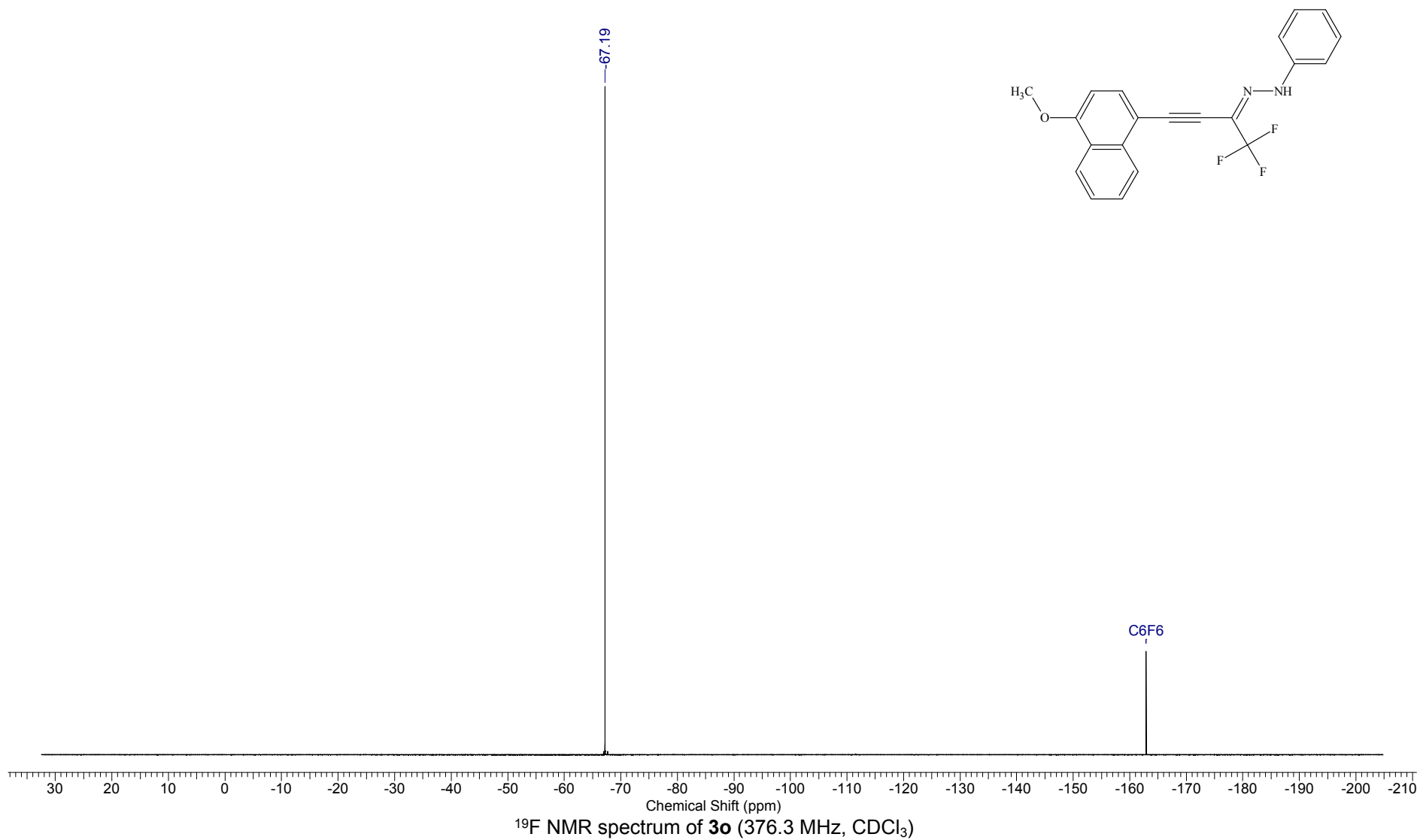
Acquisition Time (sec)	0.4999	Comment	Imported from UXMNR.	Date	23 Mar 2017 12:00:54
File Name	C:\BM_DATA\DOCS\SPEC_BM_H,C_I-IV.2017\BM-976-2a.C_002001r			Frequency (MHz)	100.61
Nucleus	13C	Number of Transients	418	Original Points Count	12076
Pulse Sequence	zgpg30	Solvent	CHLOROFORM-D	Points Count	65536
Temperature (degree C)	27.000			Sweep Width (Hz)	24154.59



¹³C NMR spectrum of **3o** (100.6 MHz, CDCl₃)

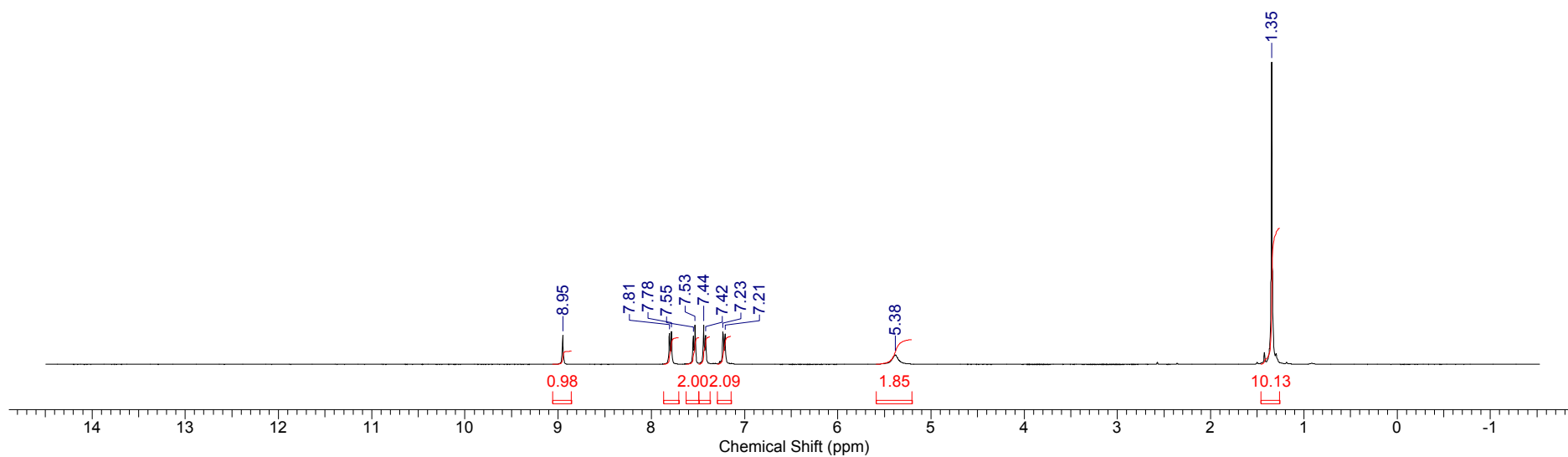
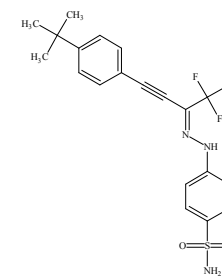
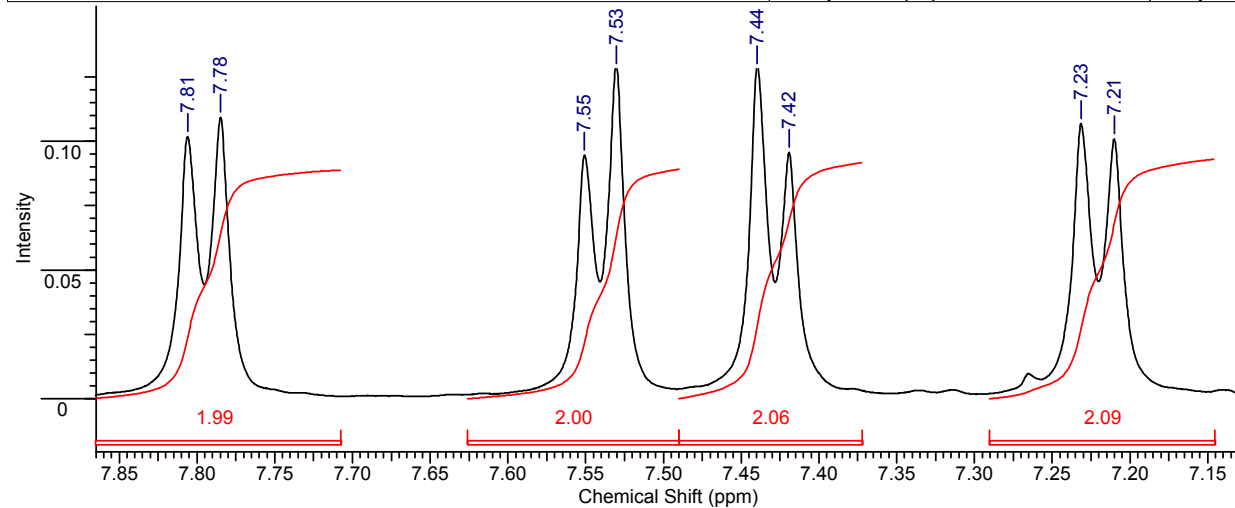
FW	368.3519	Formula	C ₂₁ H ₁₈ F ₃ N ₂ O
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Acquisition Time (sec)	1.5000	Date	Mar 20 2017	File Name	C:\BM_DATA\DOCS\SPEC_F_I-XII.2017\BM-976-2a_20170320_01\FLUORINE_01		
Frequency (MHz)	376.31	Nucleus	¹⁹ F	Number of Transients	16	Original Points Count	133929
Points Count	262144	Pulse Sequence	s2pul	Solvent	CHLOROFORM-D		
Sweep Width (Hz)	89285.71	Temperature (degree C)	25.000				



FW 423.4530 Formula C₂₀H₂₀F₃N₃O₂S

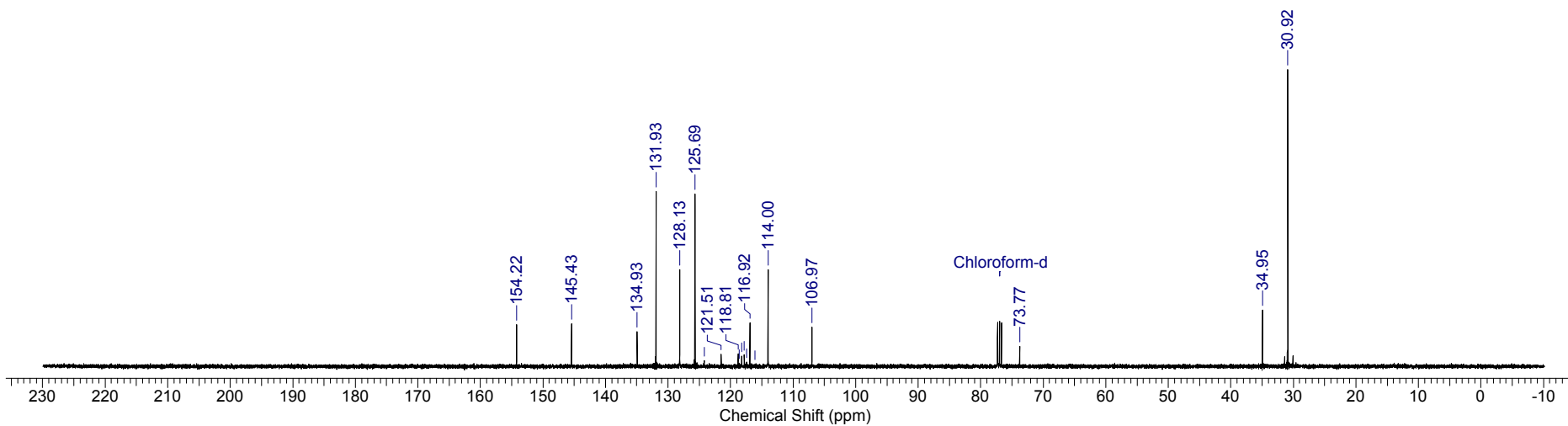
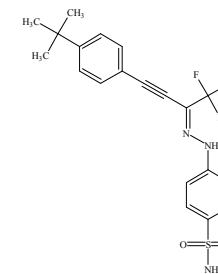
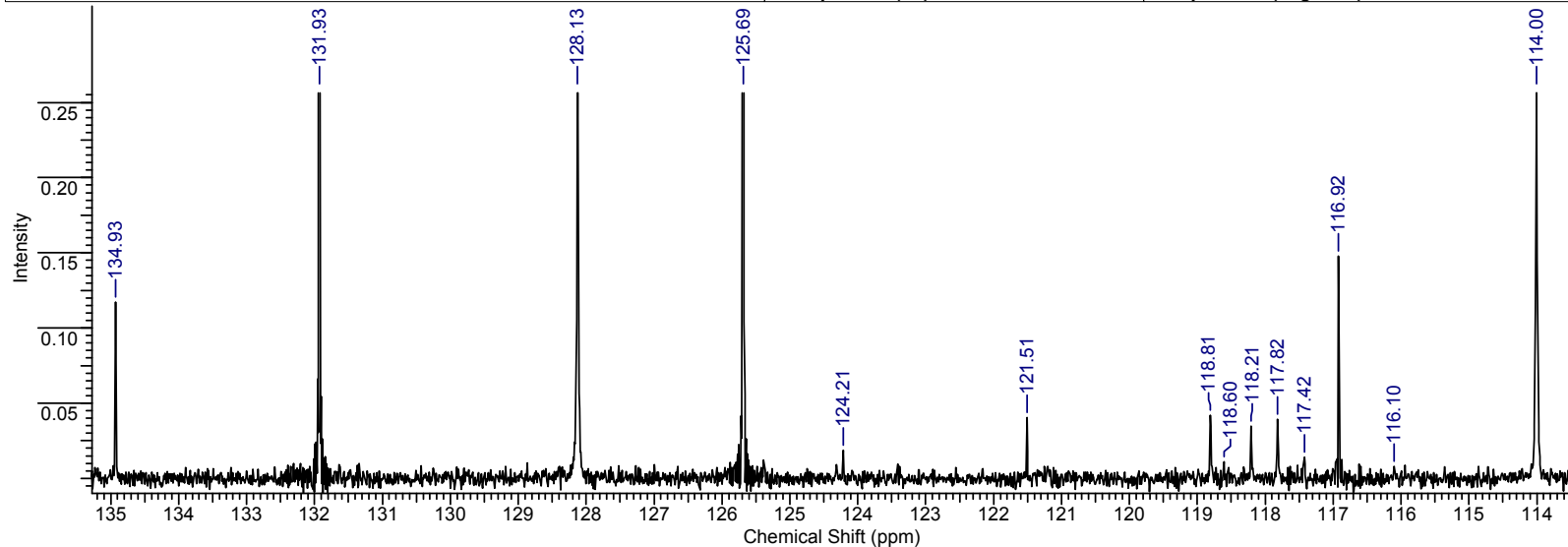
Acquisition Time (sec)	2.5559	Comment	Imported from UXNMR.	Date	29 Mar 2014 12:42:44
File Name	D:\BN\Docs (BN)\vasiliy\SPEC_BM_H.C\BM-448.H_001001r	Frequency (MHz)	400.13	Nucleus	¹ H
Number of Transients	4	Original Points Count	16384	Points Count	65536
Solvent	CHLOROFORM-D	Sweep Width (Hz)	6410.26	Pulse Sequence	zg30
				Temperature (degree C)	27.000



¹H NMR spectrum of **3p** (400.1 MHz, CDCl₃)

FW	423.4530	Formula	C ₂₀ H ₂₀ F ₃ N ₃ O ₂ S
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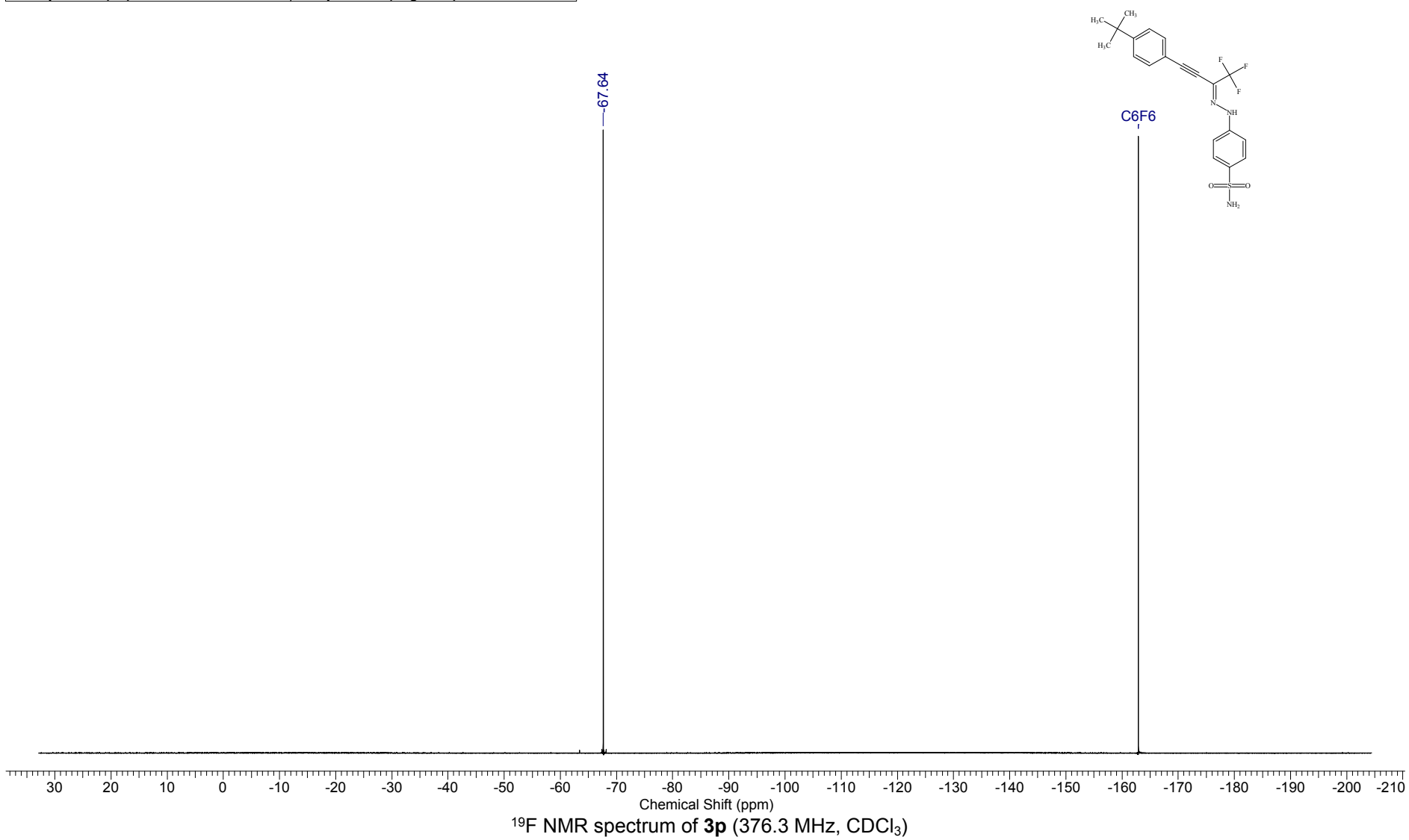
Acquisition Time (sec)	0.4999	Comment	Imported from UXMNR.		Date	29 Mar 2014 12:46:48	
File Name	D:\BN\Docs (BN)\vasiliy\SPEC_BM_H.C\BM-448.C_002001r		Frequency (MHz)	100.61	Nucleus	13C	
Number of Transients	80	Original Points Count	12076	Points Count	65536	Pulse Sequence	zgpg30
Solvent	CHLOROFORM-D		Sweep Width (Hz)	24154.59	Temperature (degree C)	27.000	



¹³C NMR spectrum of **3p** (100.6 MHz, CDCl₃)

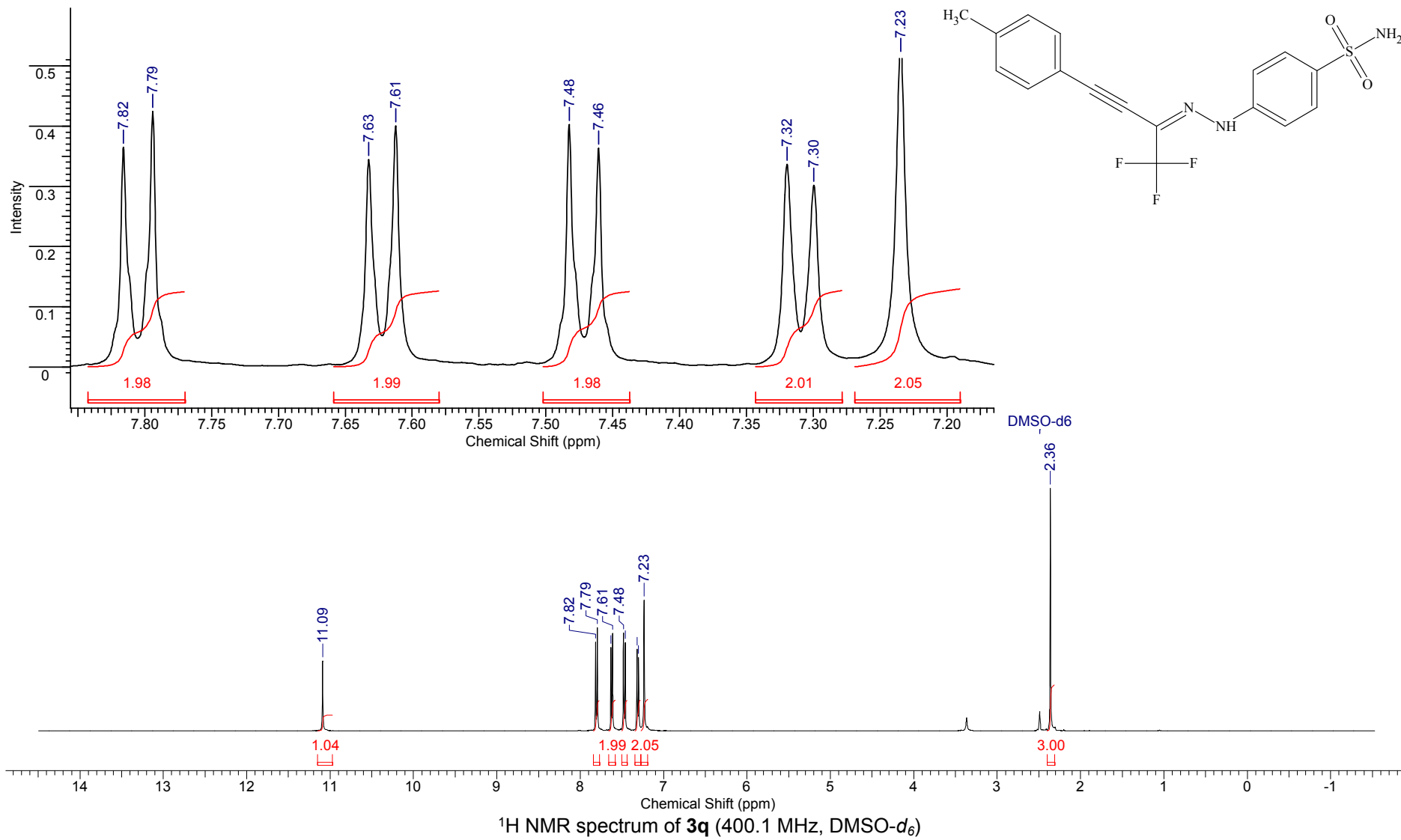
FW	423.4530	Formula	C ₂₀ H ₂₀ F ₃ N ₃ O ₂ S
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Acquisition Time (sec)	1.0000	Date	Feb 28 2014	File Name	D:\BN\Docs (BN)\vasiliy\SPEC_BM_F\BM-448_20140228_01\FLUORINE_01		
Frequency (MHz)	376.31	Nucleus	19F	Number of Transients	8	Original Points Count	89286
Points Count	131072	Pulse Sequence	s2pul	Solvent	CHLOROFORM-D		
Sweep Width (Hz)	89285.71	Temperature (degree C)	28.000				



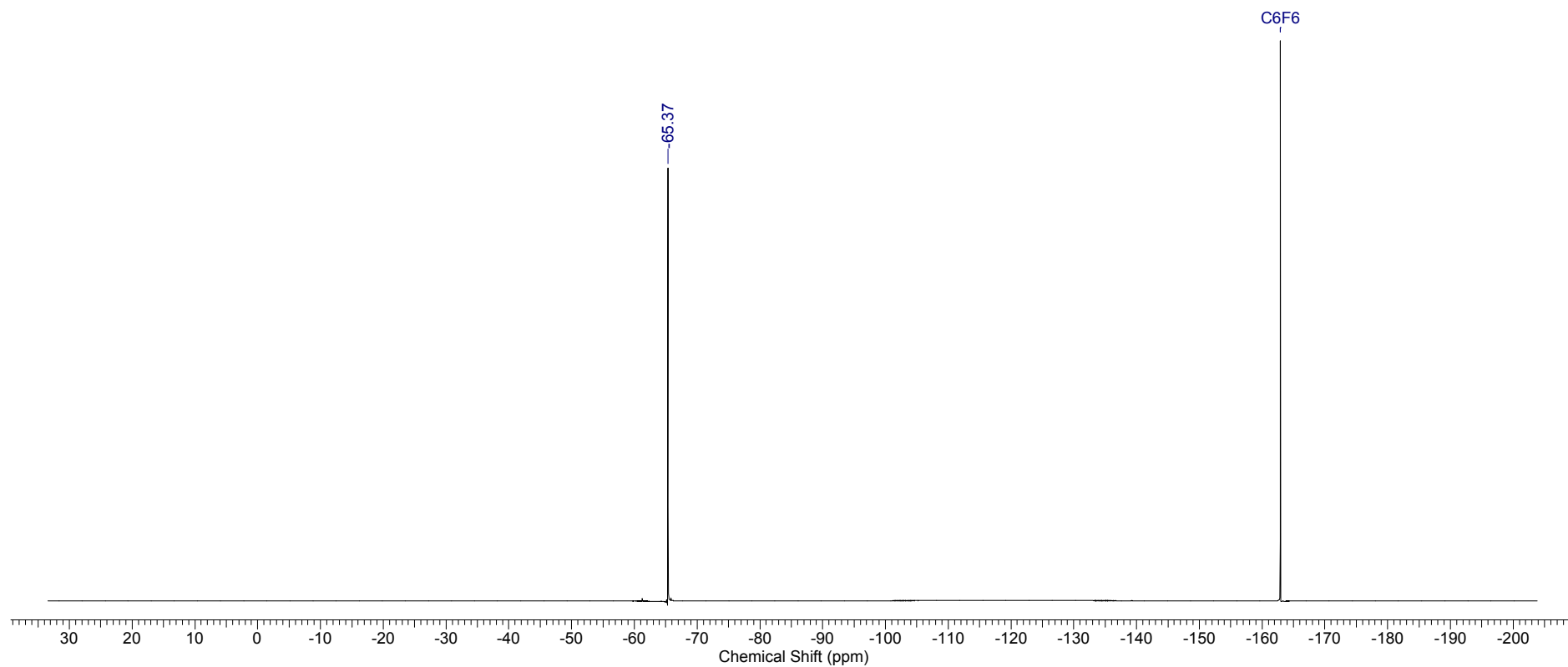
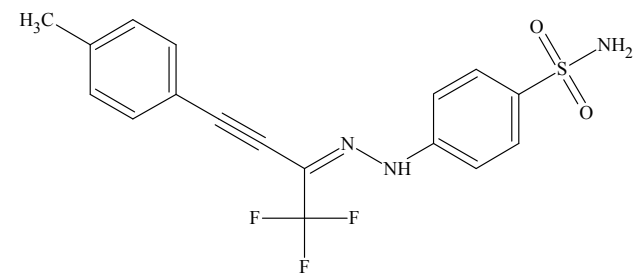
FW 381.3733 Formula C₁₇H₁₄F₃N₃O₂S

Acquisition Time (sec)	2.5559	Comment	Imported from UXNMR.		Date	03 Jun 2014 13:45:42	
File Name	C:\BM_DATA\SPEC_BMBM-496.H_001001r	Frequency (MHz)	400.13	Nucleus	1H	Number of Transients	8
Original Points Count	16384	Points Count	65536	Pulse Sequence	zg30	Solvent	DMSO-D6
Temperature (degree C)	27.000	Sweep Width (Hz)	6410.26				



FW	381.3733	Formula	C ₁₇ H ₁₄ F ₃ N ₃ O ₂ S
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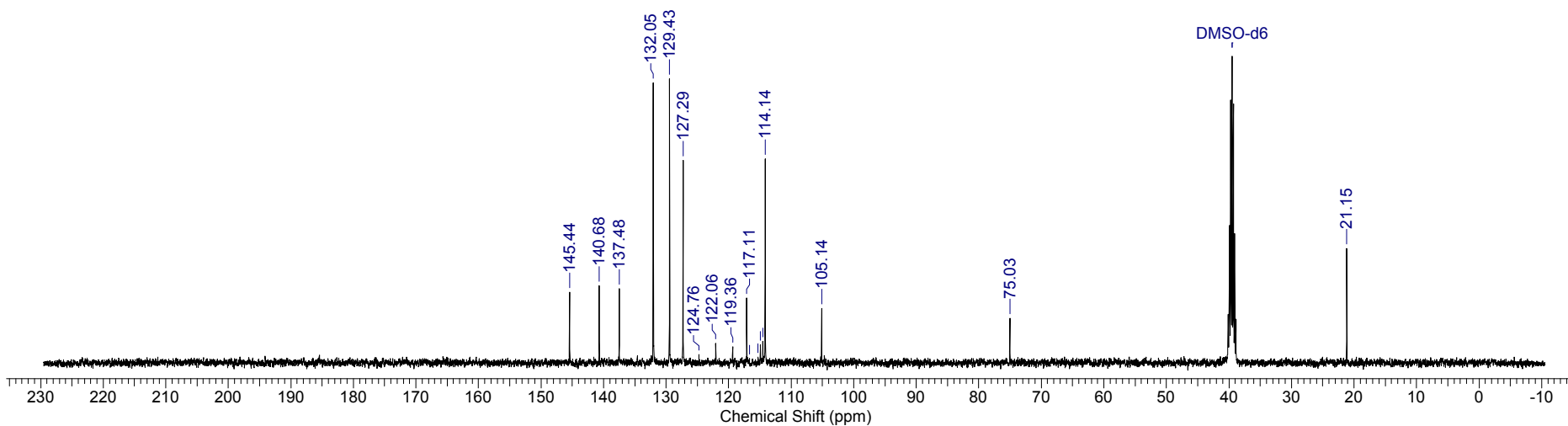
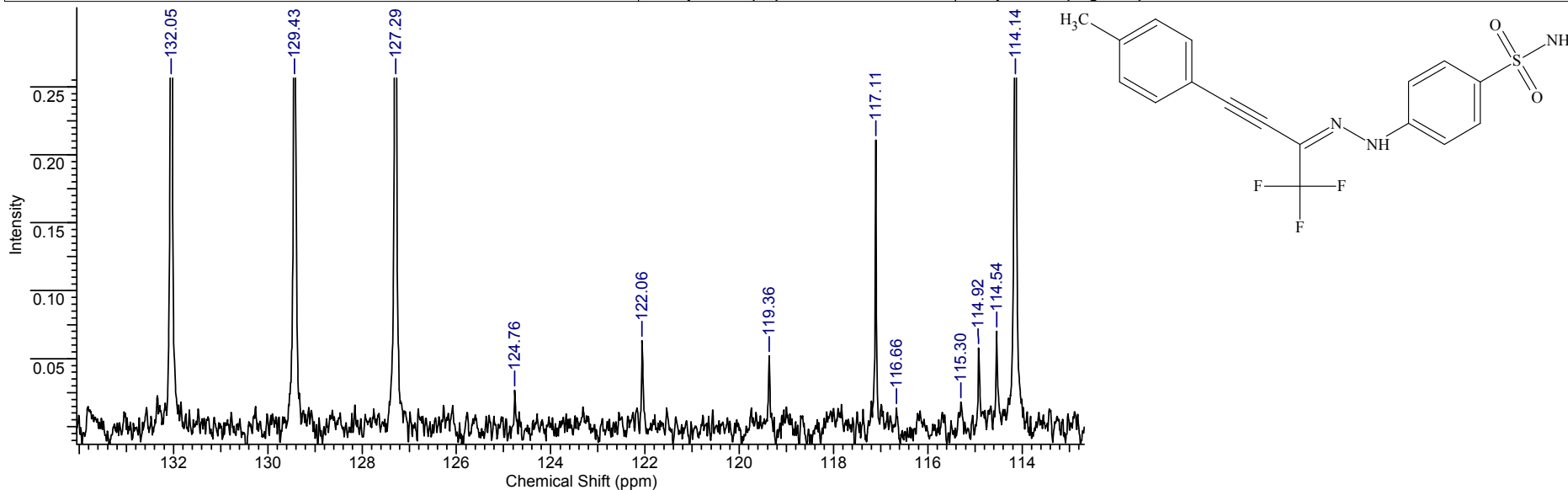
Acquisition Time (sec)	1.0000	Date	Jun 3 2014	File Name	C:\BM_DATA\SPECTRA\19F\2014.06.03\bm-496_20140603_01\FLUORINE_01		
Frequency (MHz)	376.31	Nucleus	19F	Number of Transients	32	Original Points Count	89286
Points Count	131072	Pulse Sequence	s2pul	Solvent	DMSO-D6	Sweep Width (Hz)	89285.71
Temperature (degree C)	28.000						



¹³C NMR spectrum of **3q** (100.6 MHz, DMSO-d₆)

FW 381.3733 **Formula** C₁₇H₁₄F₃N₃O₂S

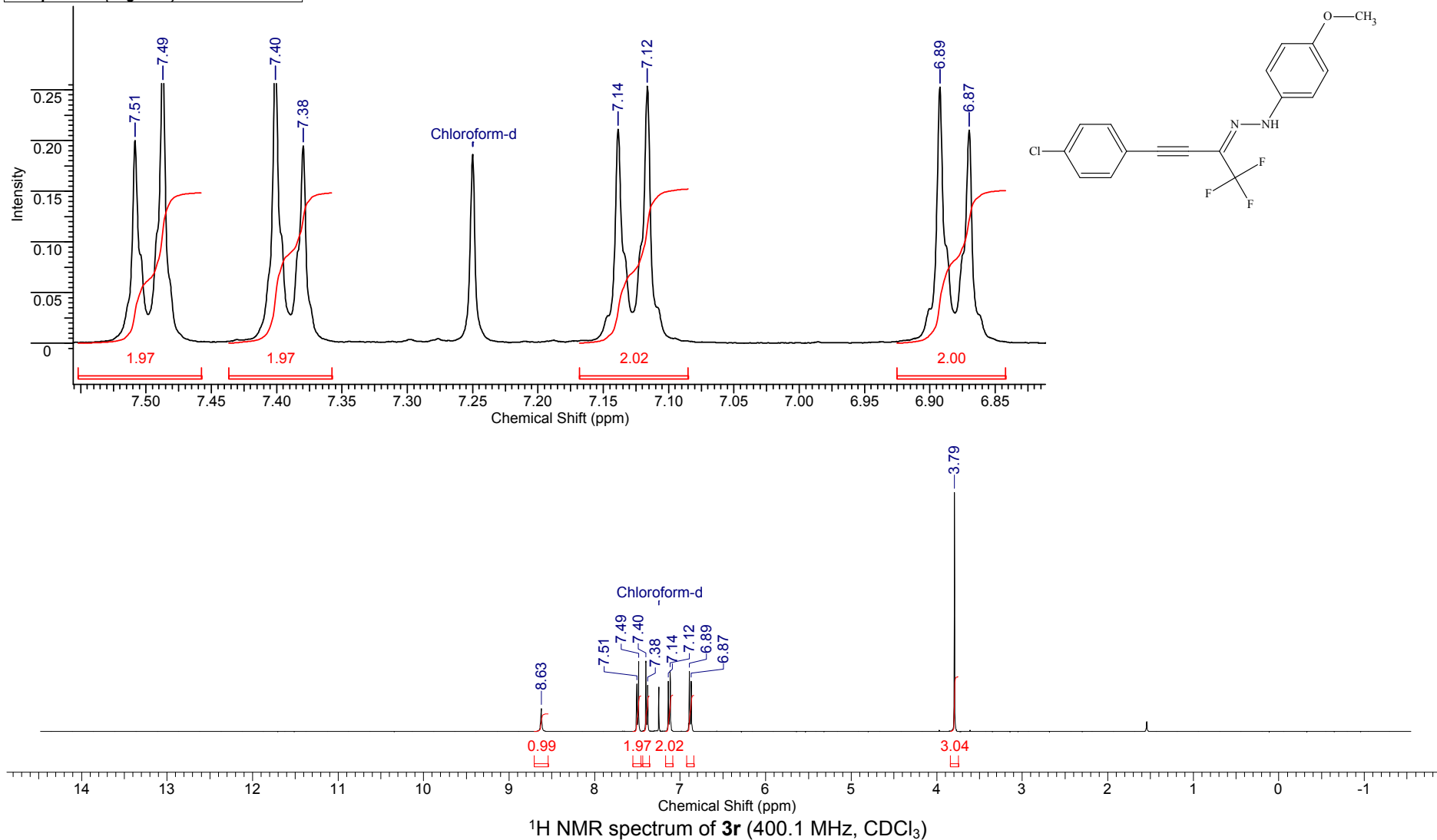
Acquisition Time (sec)	0.4999	Comment	Imported from UXNMR.	Date	03 Jun 2014 13:50:50
File Name	C:\BM_DATA\SPEC_BMBM-496.C_002001r	Frequency (MHz)	100.61	Nucleus	13C
Number of Transients	100	Original Points Count	12076	Points Count	65536
Solvent	DEUTERIUM OXIDE	Sweep Width (Hz)	24154.59	Pulse Sequence	zgpg30
				Temperature (degree C)	27.000



¹⁹F NMR spectrum of **3q** (376.3 MHz, DMSO-*d*₆)

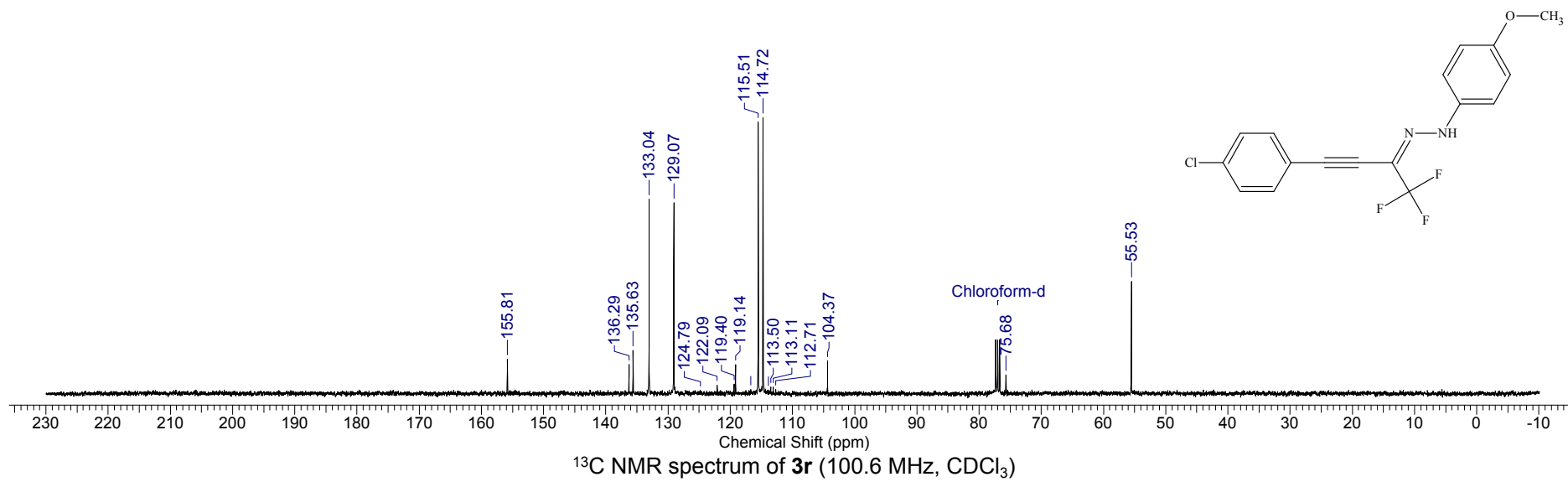
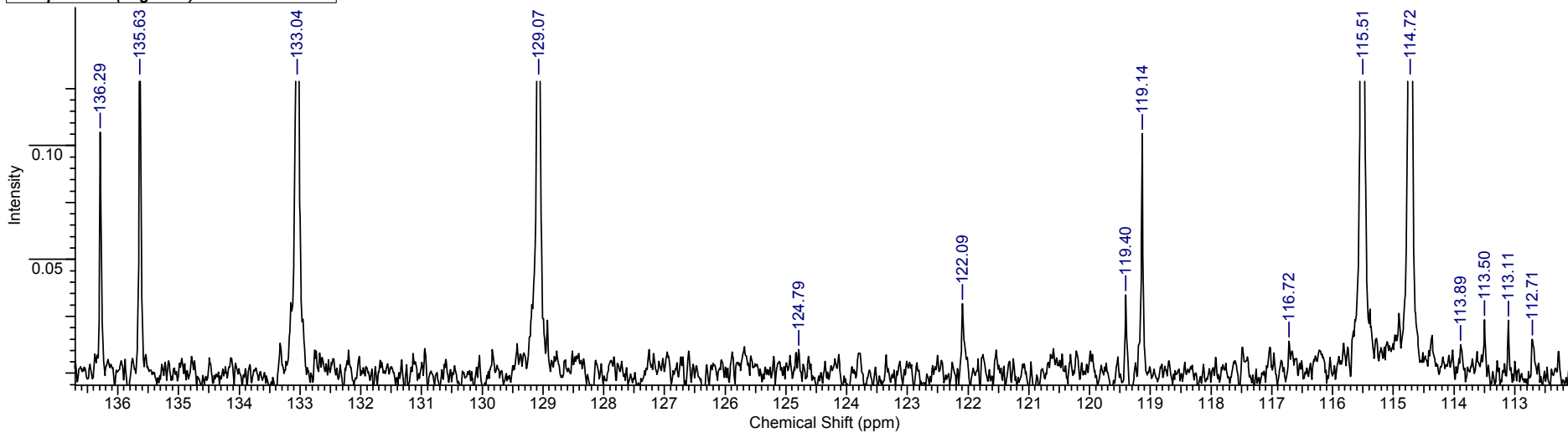
FW 352.7380 **Formula** C₁₇H₁₂ClF₃N₂O

Acquisition Time (sec)	2.5559	Comment	Imported from UXMNR.	Date	26 Jul 2017 17:33:04
File Name	C:\BM_DATA\DOCS\SPEC_BM_H,C_V-XII.2017\BM-1138.H_001001r			Frequency (MHz)	400.13
Nucleus	1H	Number of Transients	4	Original Points Count	16384
Pulse Sequence	zg30	Solvent	CHLOROFORM-D	Points Count	65536
Temperature (degree C)	27.000			Sweep Width (Hz)	6410.26



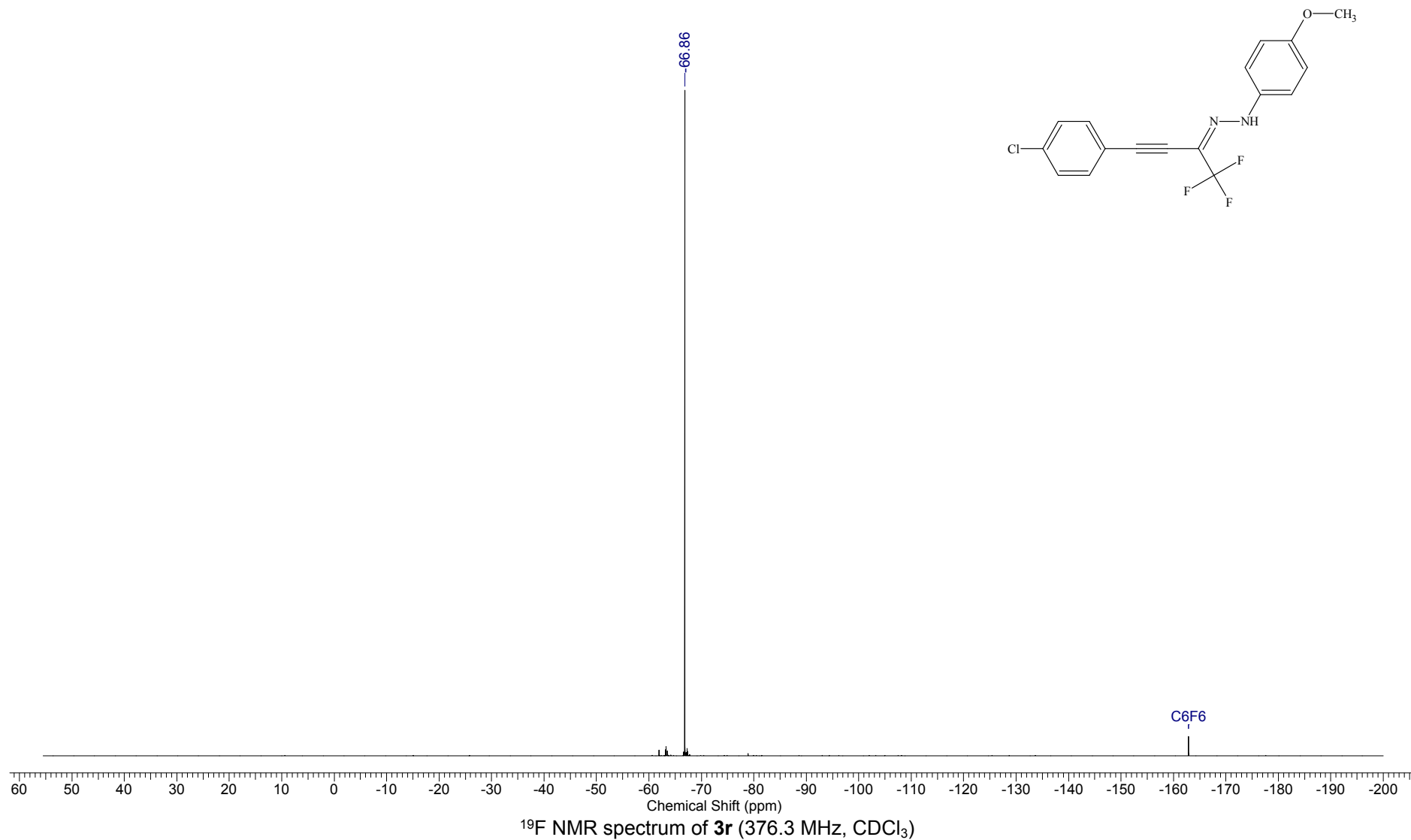
FW	352.7380	Formula	C ₁₇ H ₁₂ ClF ₃ N ₂ O
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Acquisition Time (sec)	0.4999	Comment	Imported from UXMNR.	Date	26 Jul 2017 17:52:32
File Name	C:\IBM_DATA\DOCS\SPEC_BM_H,C_V-XII.2017\BM-1138.C_002001r			Frequency (MHz)	100.61
Nucleus	13C	Number of Transients	177	Original Points Count	12076
Pulse Sequence	zgpg30	Solvent	CHLOROFORM-D	Points Count	65536
Temperature (degree C)	27.000			Sweep Width (Hz)	24154.59



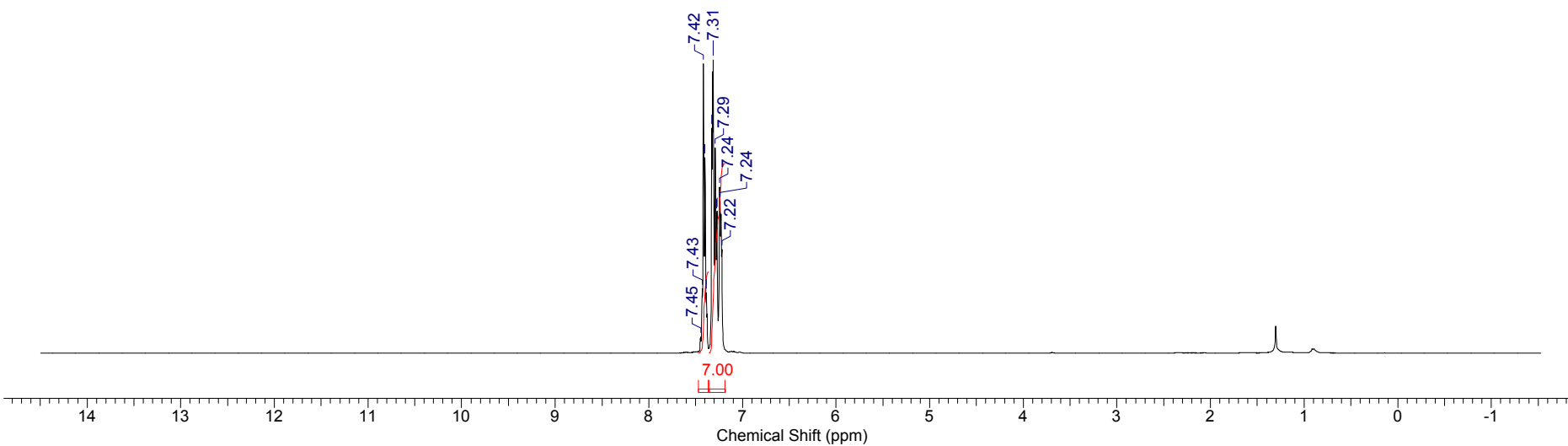
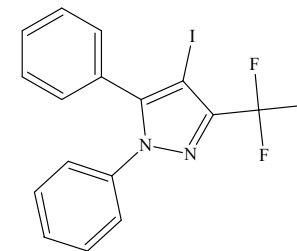
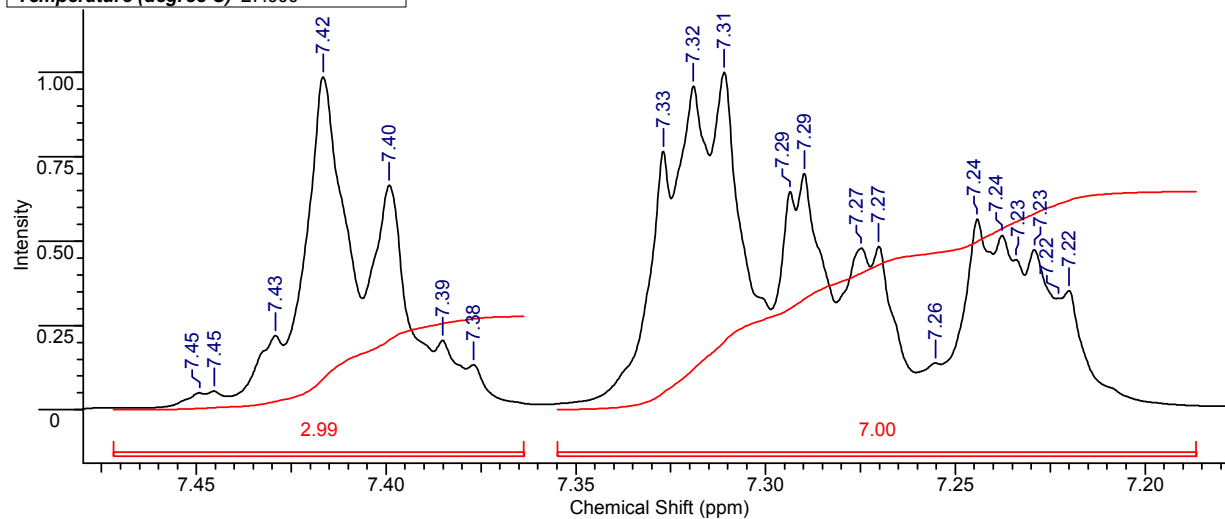
FW	352.7380	Formula	C ₁₇ H ₁₂ ClF ₃ N ₂ O
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Acquisition Time (sec)	2.4117	Date	Jan 22 2018	File Name	I:\SPEC_BM_F_2018.04.27\BM-1138-F_20180122_01\FLUORINE_01		
Frequency (MHz)	376.31	Nucleus	19F	Number of Transients	8	Original Points Count	231897
Points Count	262144	Pulse Sequence	s2pul	Solvent	CHLOROFORM-D		
Sweep Width (Hz)	96153.84	Temperature (degree C)	5.000				



FW	414.1638	Formula	C ₁₆ H ₁₀ F ₃ IN ₂
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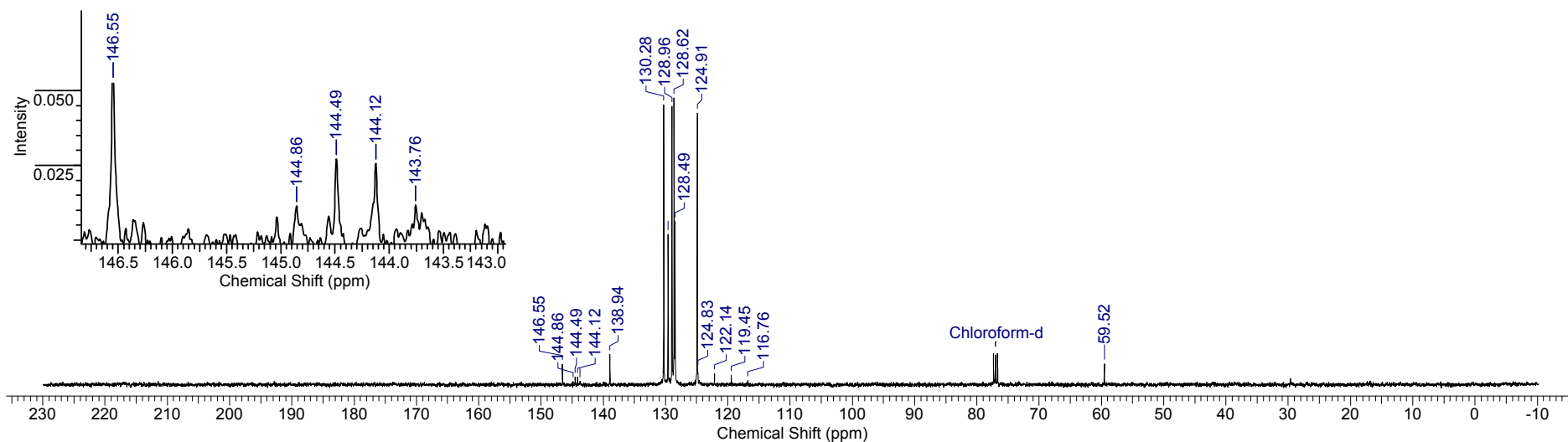
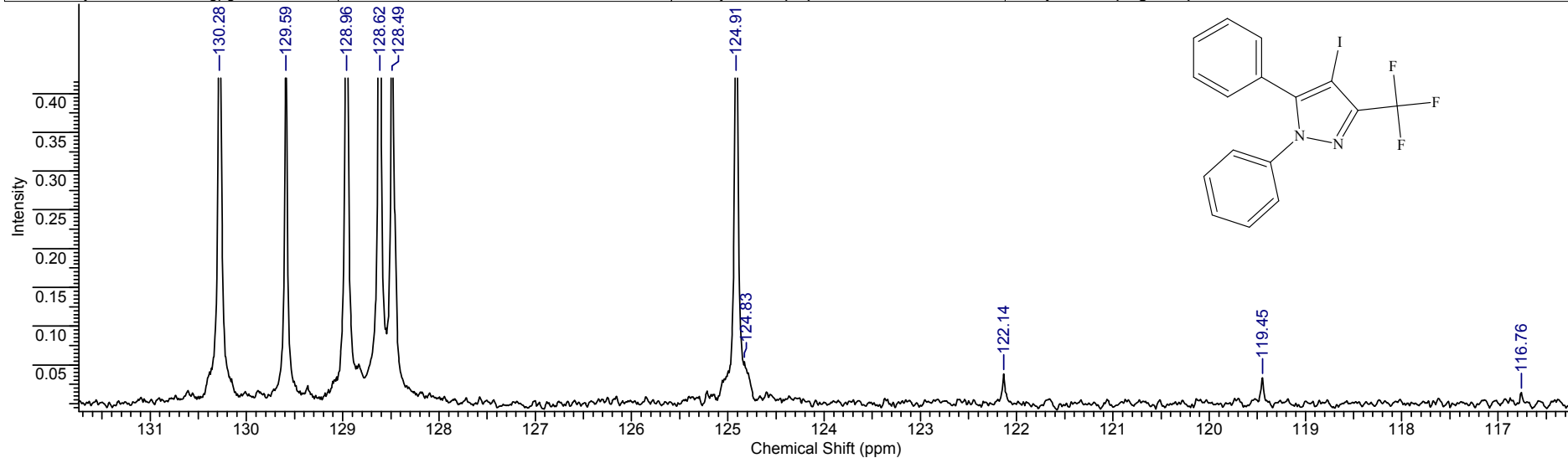
Acquisition Time (sec)	2.5559	Comment	Imported from UXNMR.	Date	10 Oct 2016 15:35:44
File Name	C:\IBM_DATA\DOCS\Manuscr_Ultra\Iodo_Pyrazoles\BM-943,946\BM-943.H_001001r			Frequency (MHz)	400.13
Nucleus	1H	Number of Transients	5	Original Points Count	16384
Pulse Sequence	zg30	Solvent	CHLOROFORM-D	Points Count	65536
Temperature (degree C)	27.000			Sweep Width (Hz)	6410.26



¹H NMR spectrum of **4a** (400.1 MHz, CDCl₃)

FW 414.1638 **Formula** C₁₆H₁₀F₃IN₂

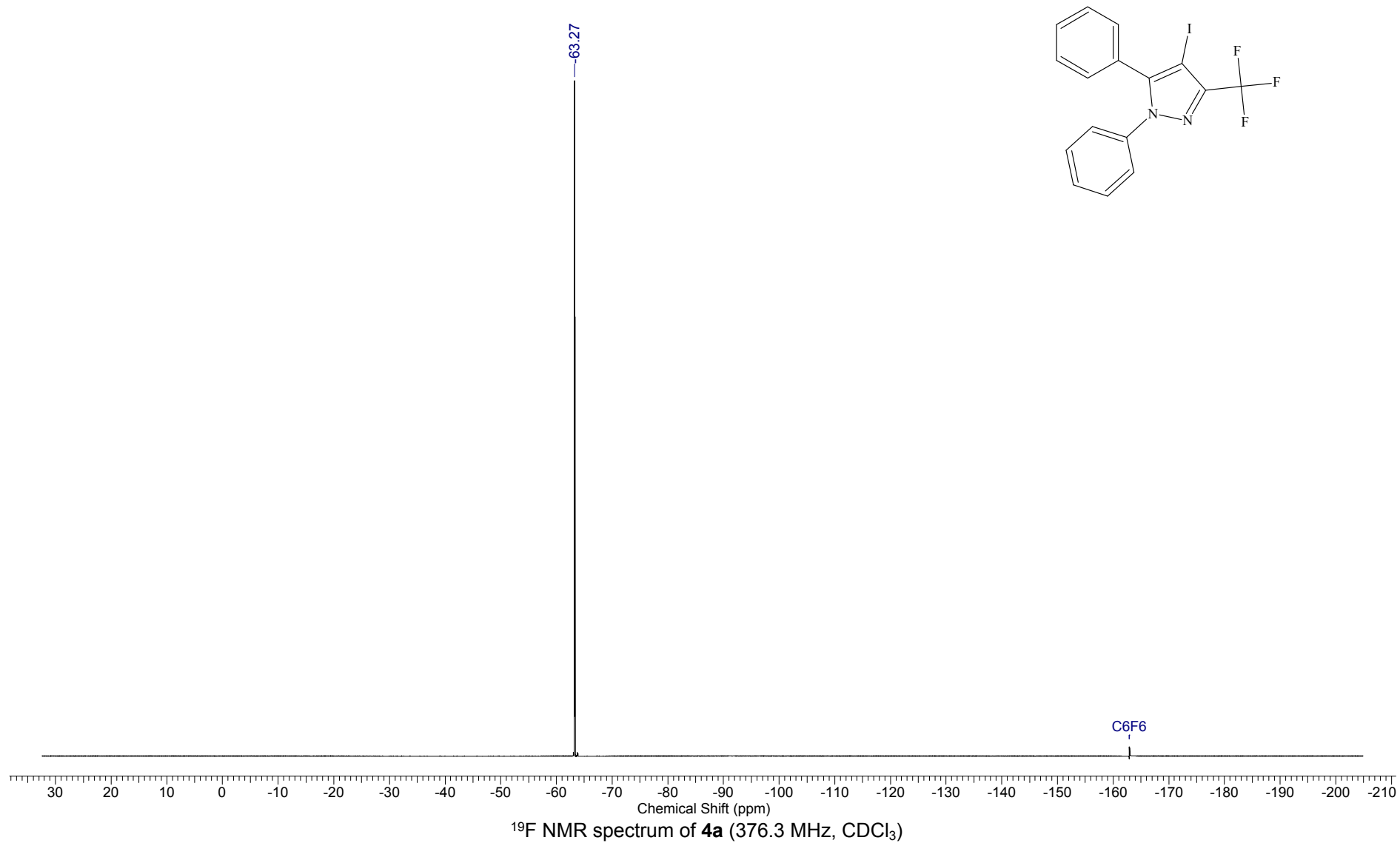
Acquisition Time (sec)	0.4999	Comment	Imported from UXNMR.		Date	10 Oct 2016 15:38:42	
File Name	C:\BM_DATA\DOCS\Manuscr_UltraIodo_Pyrazoles\BM-943,946\BM-943.C_002001r				Frequency (MHz)	100.61	
Nucleus	13C	Number of Transients	64	Original Points Count	12076	Points Count	65536
Pulse Sequence	zgpg30	Solvent	DMSO-D6	Sweep Width (Hz)	24154.59	Temperature (degree C)	27.000



¹³C NMR spectrum of **4a** (100.6 MHz, CDCl₃)

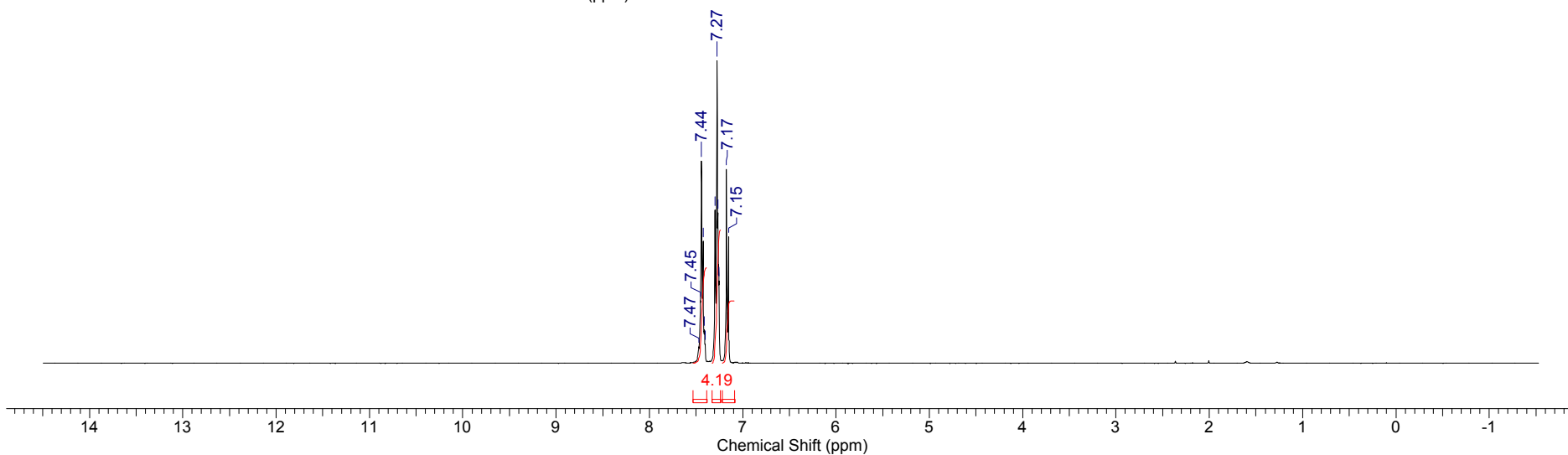
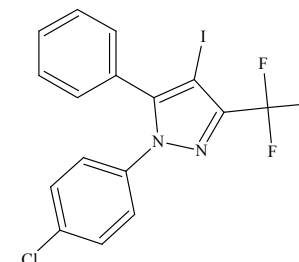
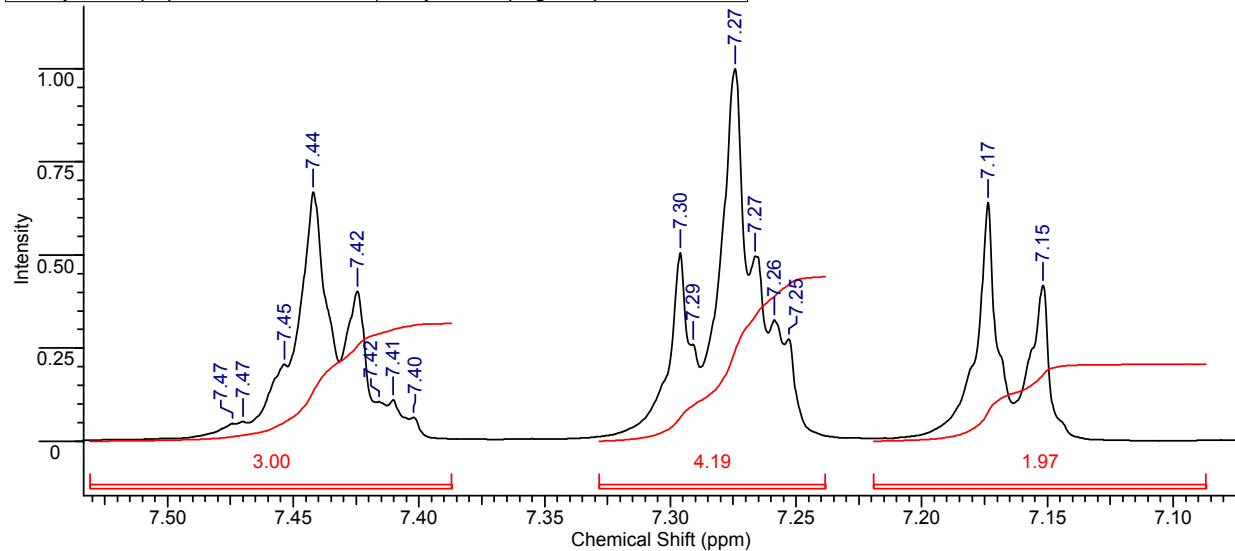
FW	414.1638	Formula	C ₁₆ H ₁₀ F ₃ IN ₂
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Acquisition Time (sec)	1.0000	Date	Oct 21 2016	File Name	C:\BM_DATA\BM-943,946F\BM-943_20161021_01\FLUORINE_01				
Frequency (MHz)	376.31	Nucleus	¹⁹ F	Number of Transients	16	Original Points Count	89286	Points Count	131072
Pulse Sequence	s2pul	Solvent	CHLOROFORM-D	Sweep Width (Hz)	89285.71		Temperature (degree C) 25.000		



FW	448.6085	Formula	C ₁₆ H ₉ ClF ₃ IN ₂
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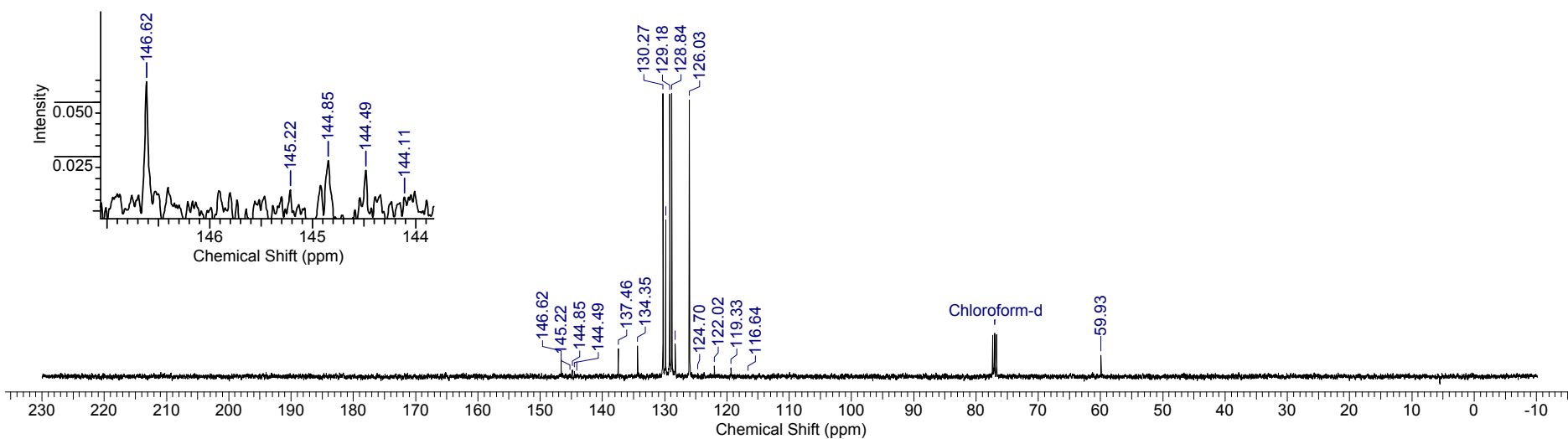
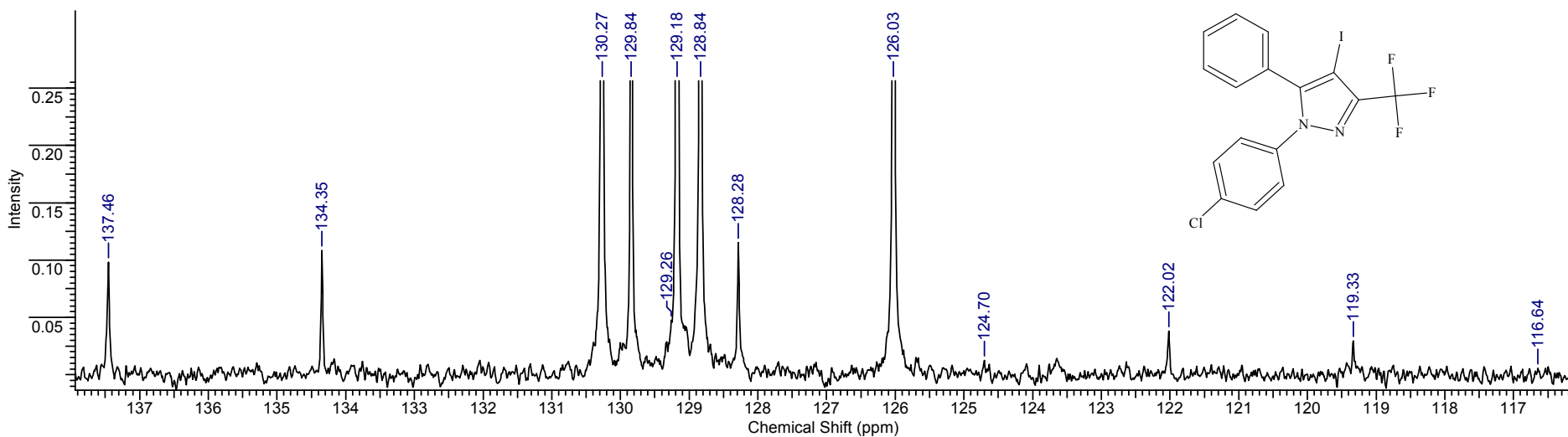
Acquisition Time (sec)	2.5559	Comment	Imported from UXMNR.		Date	30 May 2017 15:17:44	
File Name	D:\BN\output\2017\05.i à\BM-1089.H_001001r	Frequency (MHz)	400.13	Nucleus	1H	Number of Transients	4
Original Points Count	16384	Points Count	65536	Pulse Sequence	zg30	Solvent	CHLOROFORM-D
Sweep Width (Hz)	6410.26	Temperature (degree C)	27.000				



¹H NMR spectrum of **4b** (400.1 MHz, CDCl₃)

FW 448.6085 **Formula** C₁₆H₉ClF₃IN₂

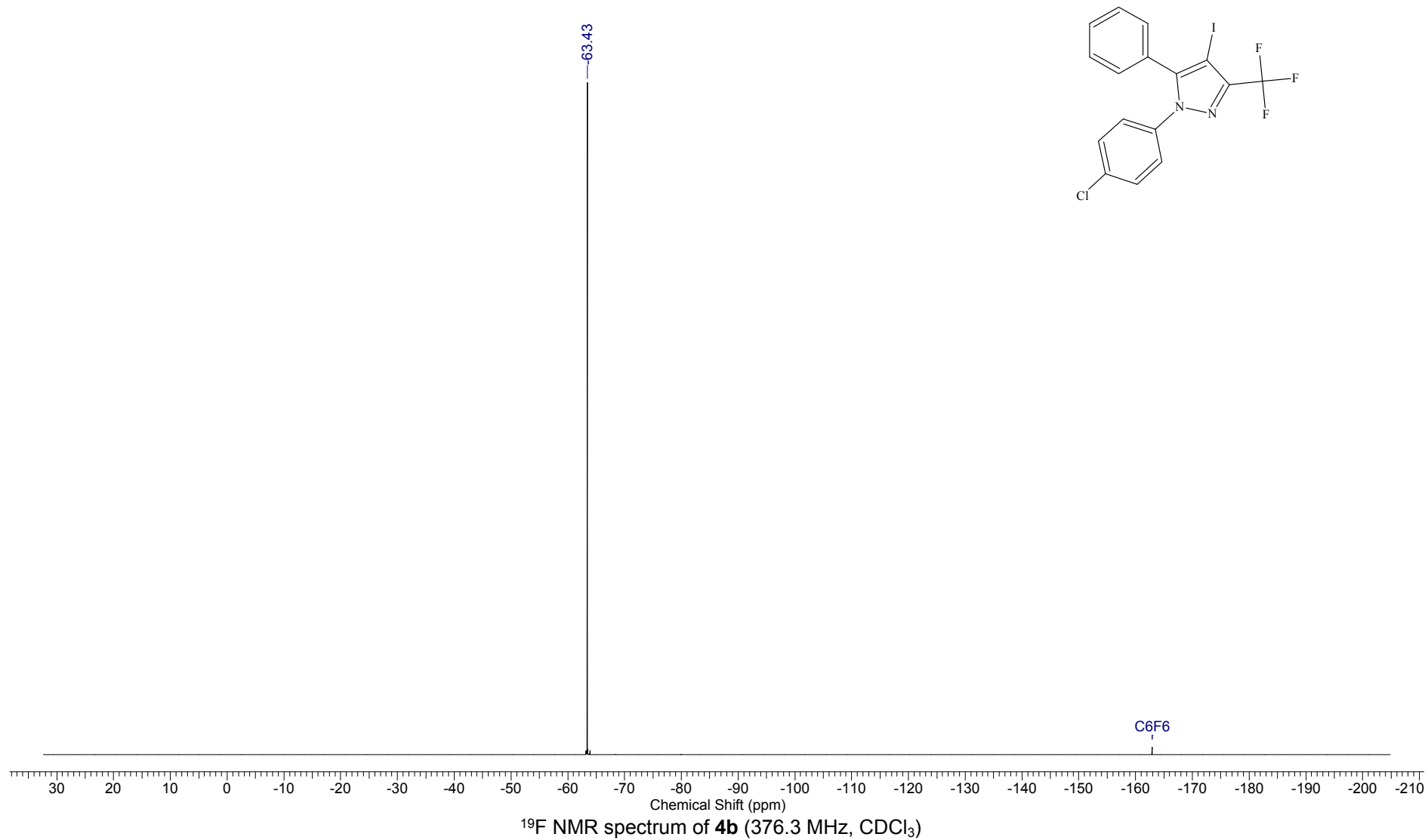
Acquisition Time (sec)	0.4999	Comment	Imported from UXNMR.	Date	30 May 2017 15:24:38
File Name	D:\BN\output\2017\05.i à à\BM-1089.C_002001r	Frequency (MHz)	100.61	Nucleus	13C
Number of Transients	124	Original Points Count	12076	Points Count	65536
Solvent	CHLOROFORM-D	Sweep Width (Hz)	24154.59	Pulse Sequence	zgpg30
				Temperature (degree C)	27.000



¹³C NMR spectrum of **4b** (100.6 MHz, CDCl₃)

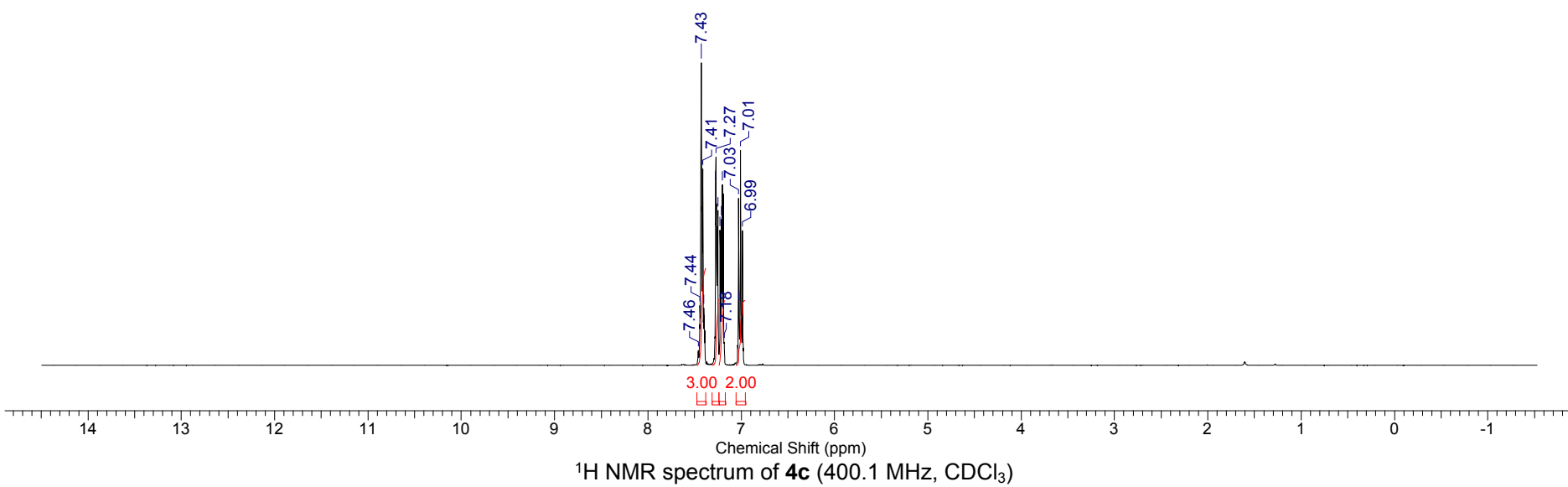
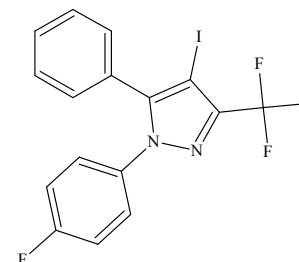
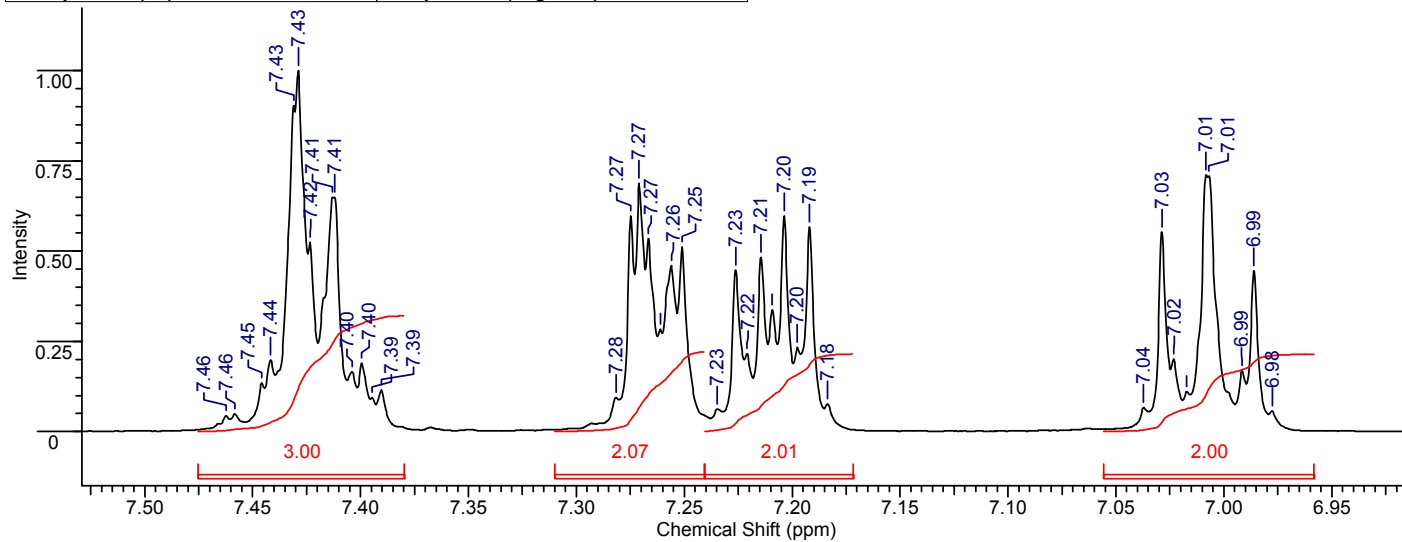
FW	448.6085	Formula	C ₁₆ H ₉ ClF ₃ I ₂ N ₂
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Acquisition Time (sec)	1.5000	Date	May 31 2017	File Name	D:\BN\Docs (BN)\vasily\SPEC_BM_F\2017.06.03_F\BM-1089_20170531_01\FLUORINE_01		
Frequency (MHz)	376.31	Nucleus	¹⁹ F	Number of Transients	16	Original Points Count	133929
Points Count	262144	Pulse Sequence	s2pul	Solvent	CHLOROFORM-D		
Sweep Width (Hz)	89285.71	Temperature (degree C)	25.000				



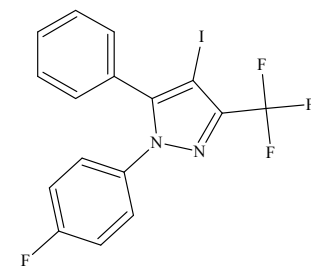
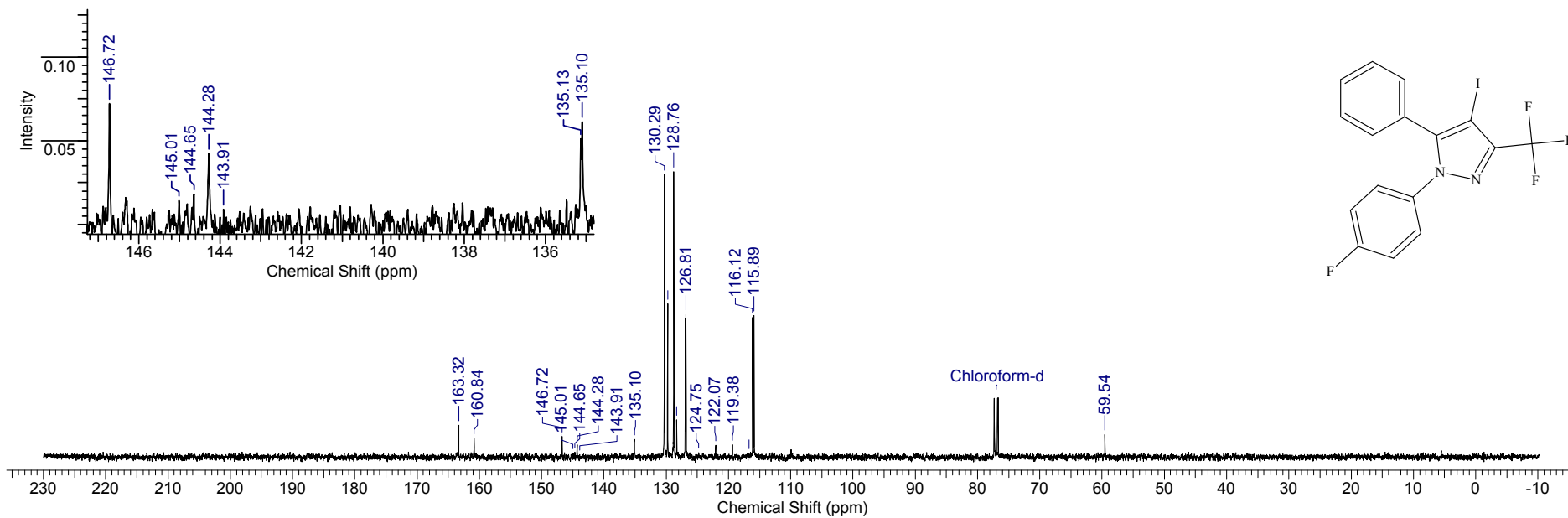
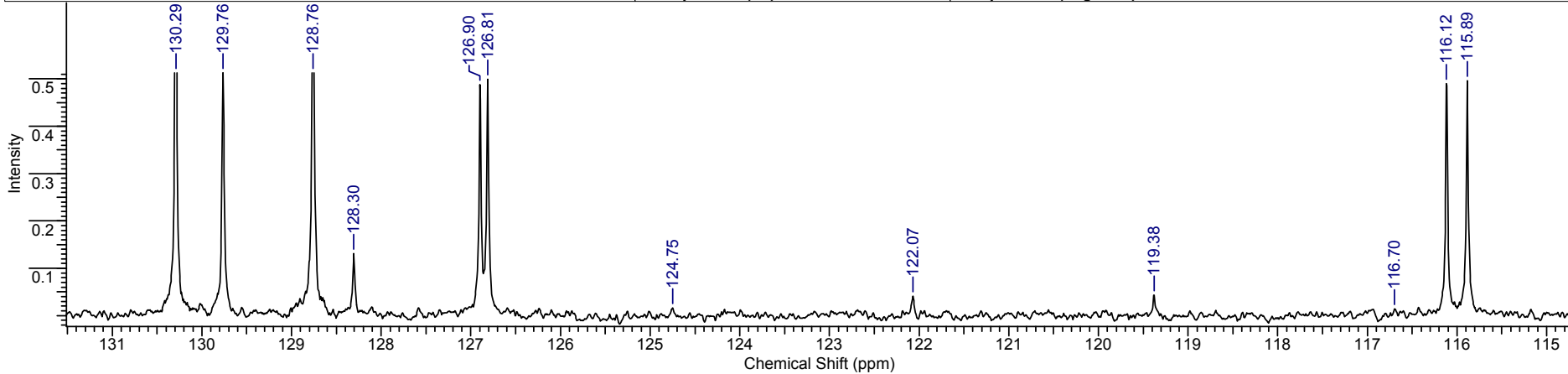
FW	432.1542	Formula	C ₁₆ H ₉ F ₄ IN ₂
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Acquisition Time (sec)	2.5559	Comment	Imported from UXMNR.		Date	31 May 2017 17:44:48		
File Name	D:\BN\output\2017\05.i àé\BM-1092.H_001001r		Frequency (MHz)	400.13	Nucleus	1H	Number of Transients	4
Original Points Count	16384	Points Count	65536	Pulse Sequence	zg30	Solvent	CHLOROFORM-D	
Sweep Width (Hz)	6410.26	Temperature (degree C)	27.000					



FW	432.1542	Formula C ₁₆ H ₉ F ₄ IN ₂
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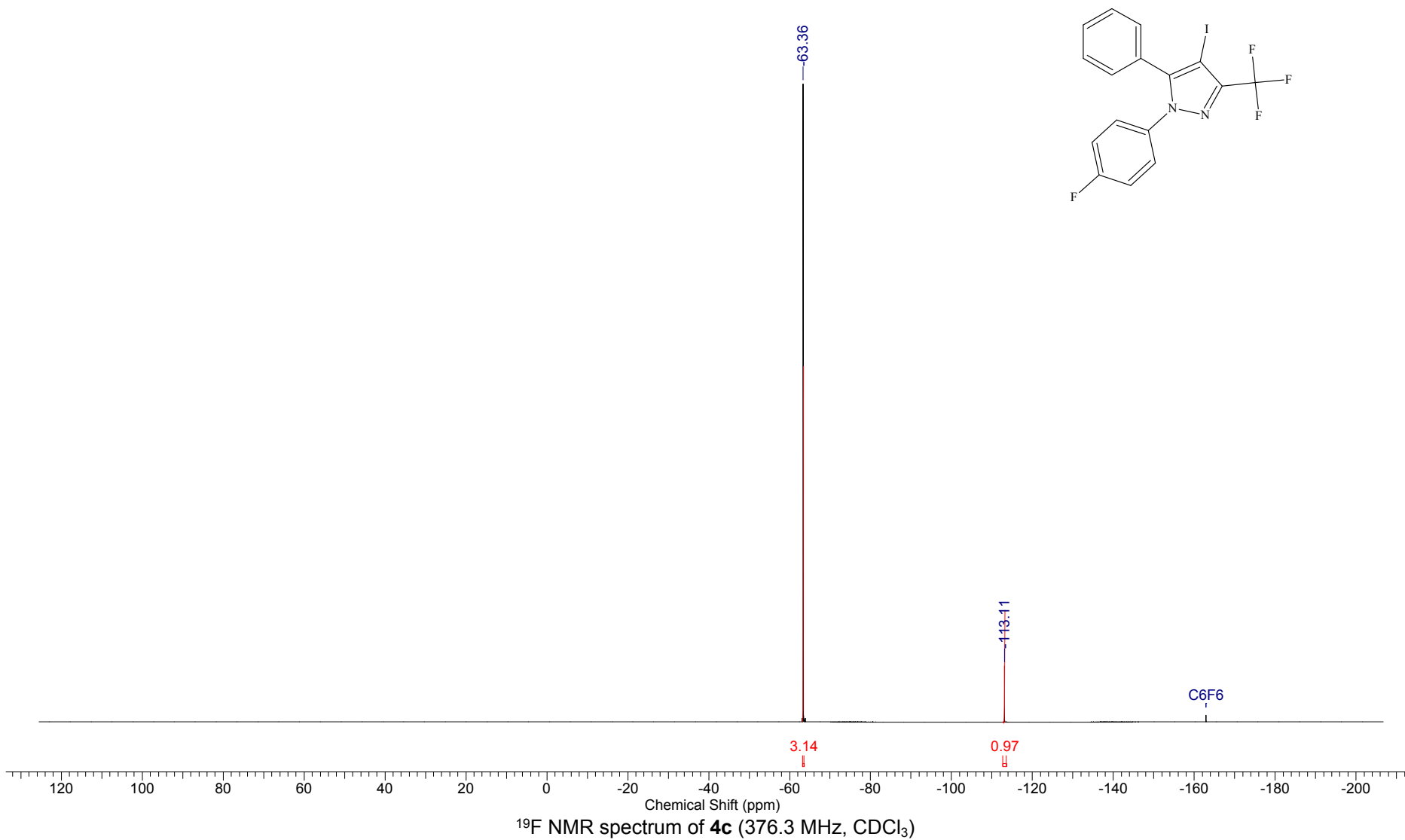
Acquisition Time (sec)	0.4999	Comment	Imported from UYNMR.	Date	31 May 2017 17:47:30
File Name	D:\BN\output\2017\05.i à\BM-1092.C_002001r	Frequency (MHz)	100.61	Nucleus	13C
Number of Transients	64	Original Points Count	12076	Points Count	65536
Solvent	CHLOROFORM-D	Sweep Width (Hz)	24154.59	Pulse Sequence	zgpg30
				Temperature (degree C)	27.000



¹³C NMR spectrum of **4c** (100.6 MHz, CDCl₃)

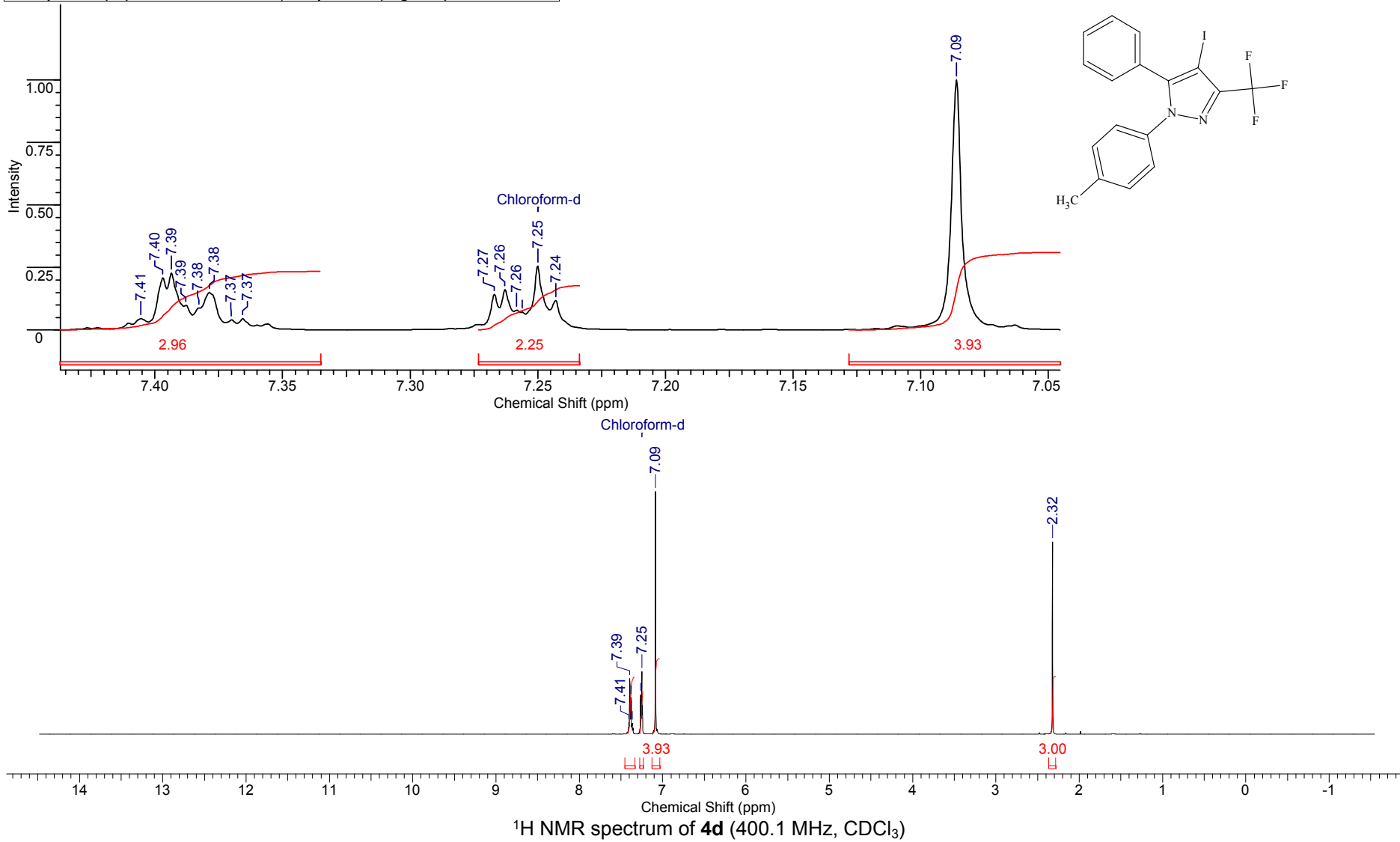
FW	432.1542	Formula	C ₁₆ H ₉ F ₄ IN ₂
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Acquisition Time (sec)	2.0000	Date	Jun 1 2017	File Name	D:\BN\output\F19\F_2017\2017.06.01\BM-1092-F_20170601_01\FLUORINE_01		
Frequency (MHz)	376.33	Nucleus	¹⁹ F	Number of Transients	8	Original Points Count	250000
Points Count	262144	Pulse Sequence	s2pul	Solvent	CHLOROFORM-D		
Sweep Width (Hz)	125000.00	Temperature (degree C)	22.000				



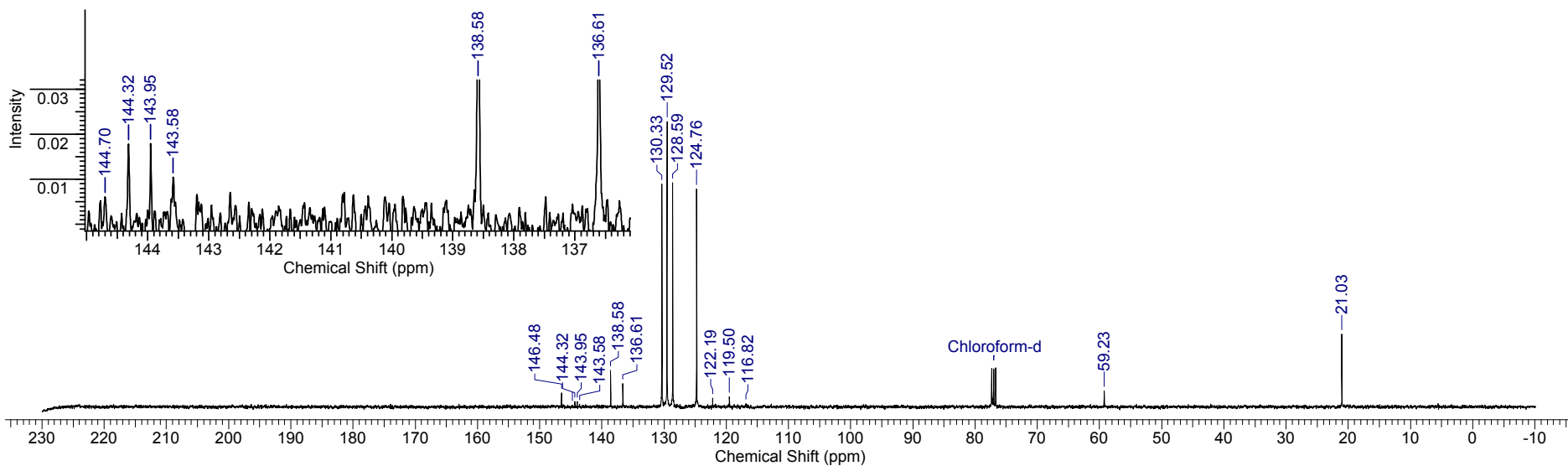
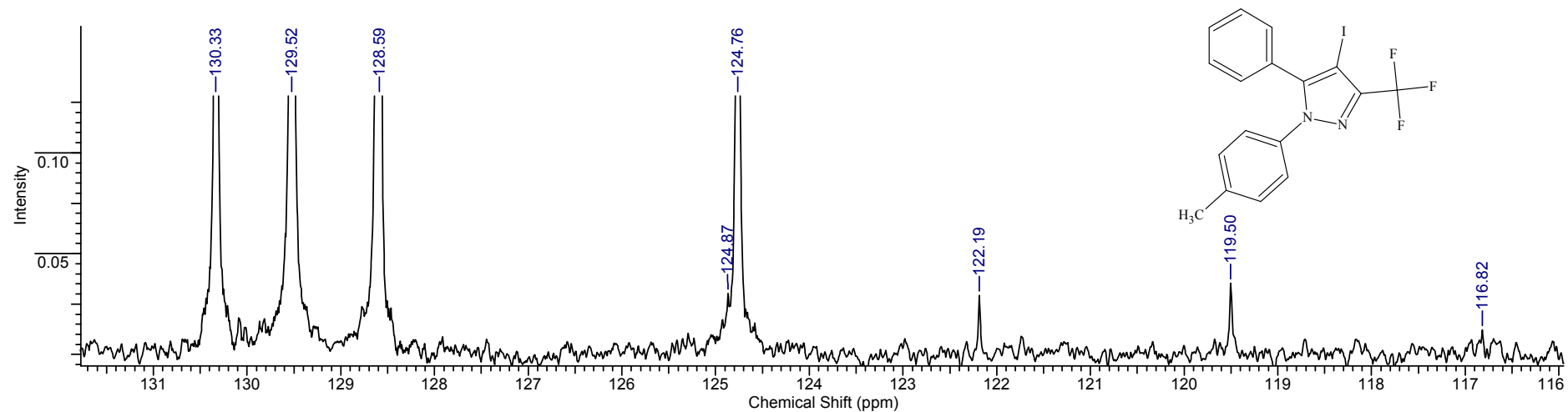
FW	428.1903	Formula	C ₁₇ H ₁₂ F ₃ IN ₂
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Acquisition Time (sec)	2.5559	Comment	Imported from UXMNR.		Date	30 May 2017 15:40:32	
File Name	D:\BN\output\2017\05.i à\BM-1091.H_001001r	Frequency (MHz)	400.13	Nucleus	1H	Number of Transients	4
Original Points Count	16384	Points Count	65536	Pulse Sequence	zg30	Solvent	CHLOROFORM-D
Sweep Width (Hz)	6410.26	Temperature (degree C)	27.000				



FW 428.1903 **Formula** C₁₇H₁₂F₃IN₂

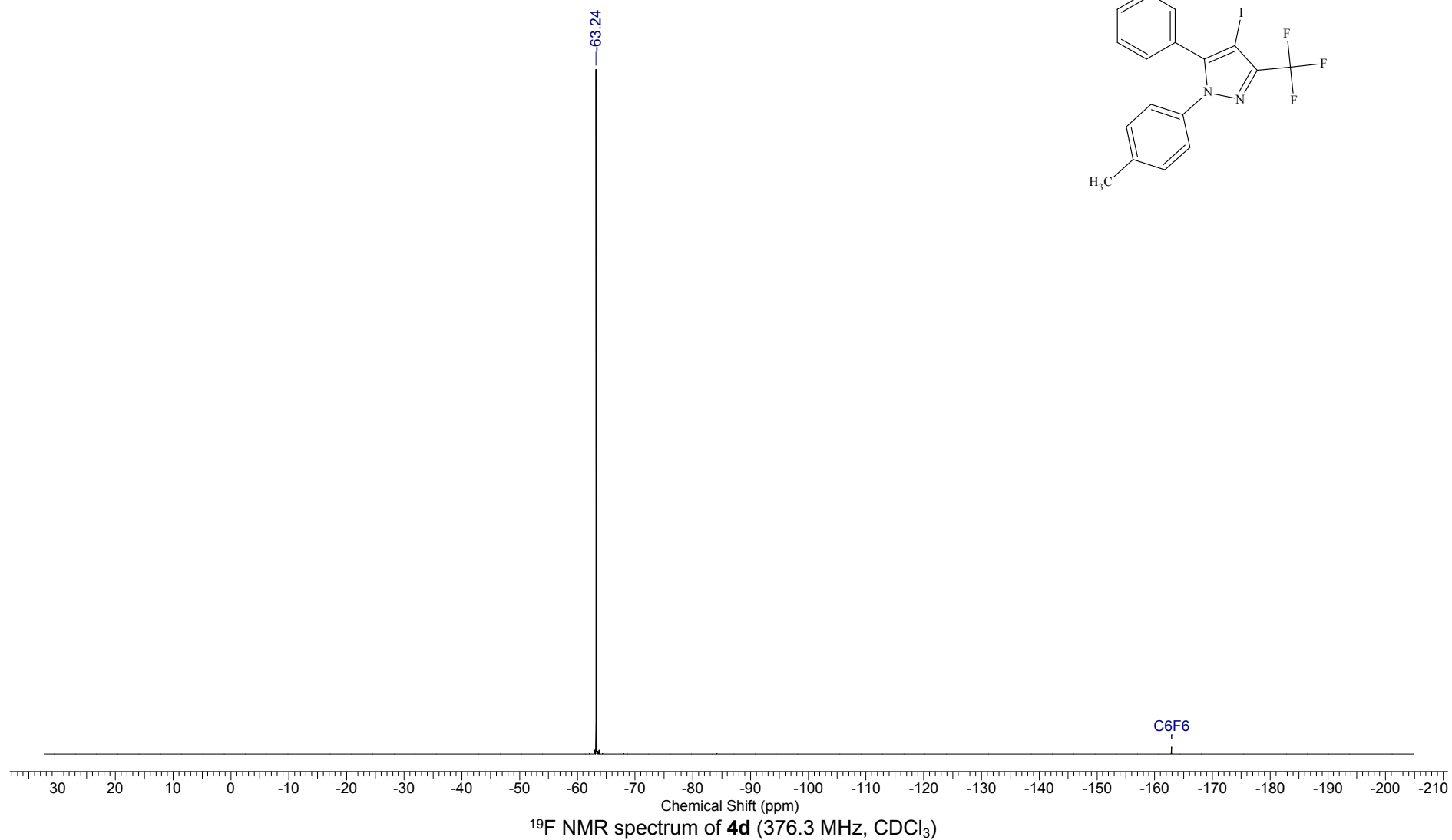
Acquisition Time (sec)	0.4999	Comment	Imported from UXMNR.	Date	30 May 2017 15:45:44
File Name	D:\BN\output\2017\05.i àé\BM-1091.C_002001r	Frequency (MHz)	100.61	Nucleus	13C
Number of Transients	166	Original Points Count	12076	Points Count	65536
Solvent	CHLOROFORM-D	Sweep Width (Hz)	24154.59	Pulse Sequence	zgpg30
				Temperature (degree C)	27.000



¹³C NMR spectrum of **4d** (100.6 MHz, CDCl₃)

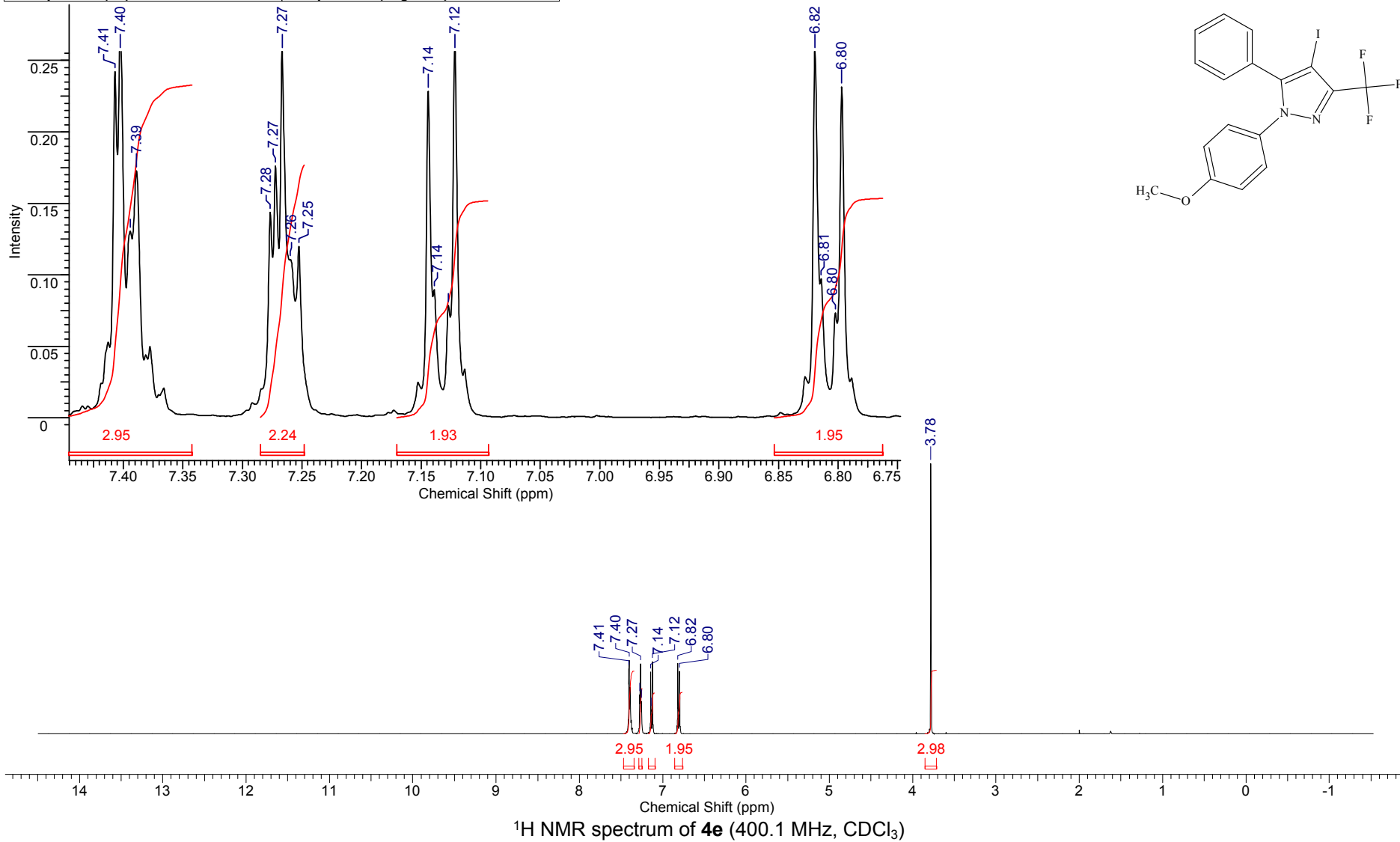
FW	428.1903	Formula	C ₁₇ H ₁₂ F ₃ IN ₂
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Acquisition Time (sec)	1.5000	Date	May 31 2017	File Name	D:\BN\Docs (BN)\vasily\SPEC_BM_F\2017.06.03_F\BM-1091_20170531_01\FLUORINE_01		
Frequency (MHz)	376.31	Nucleus	¹⁹ F	Number of Transients	16	Original Points Count	133929
Points Count	262144	Pulse Sequence	s2pul	Solvent	CHLOROFORM-D		
Sweep Width (Hz)	89285.71	Temperature (degree C)	25.000				



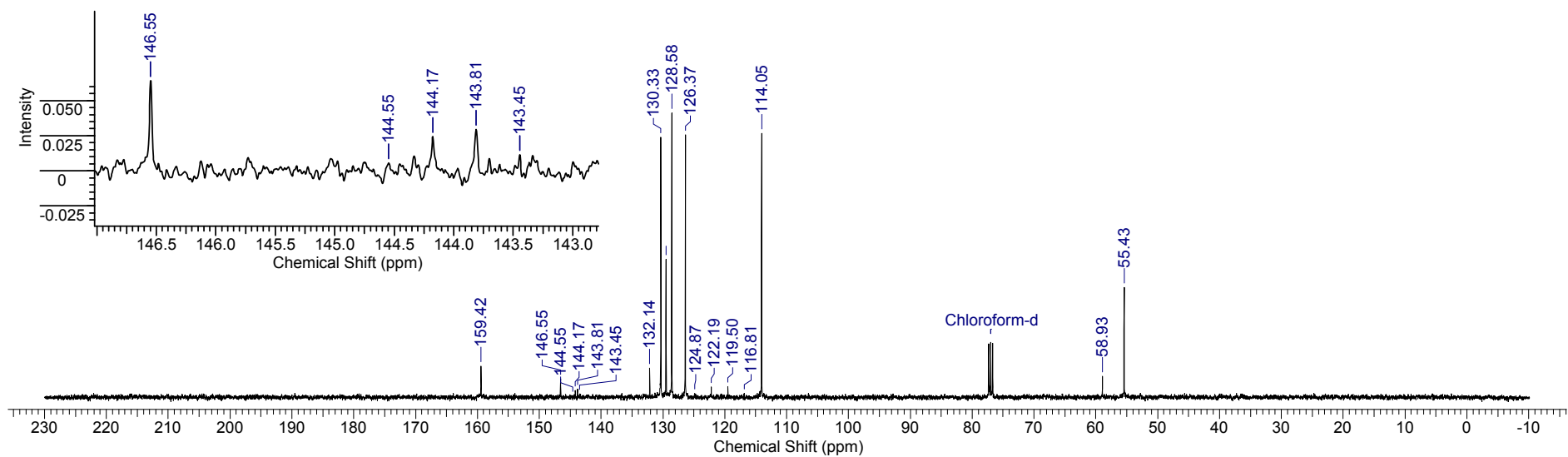
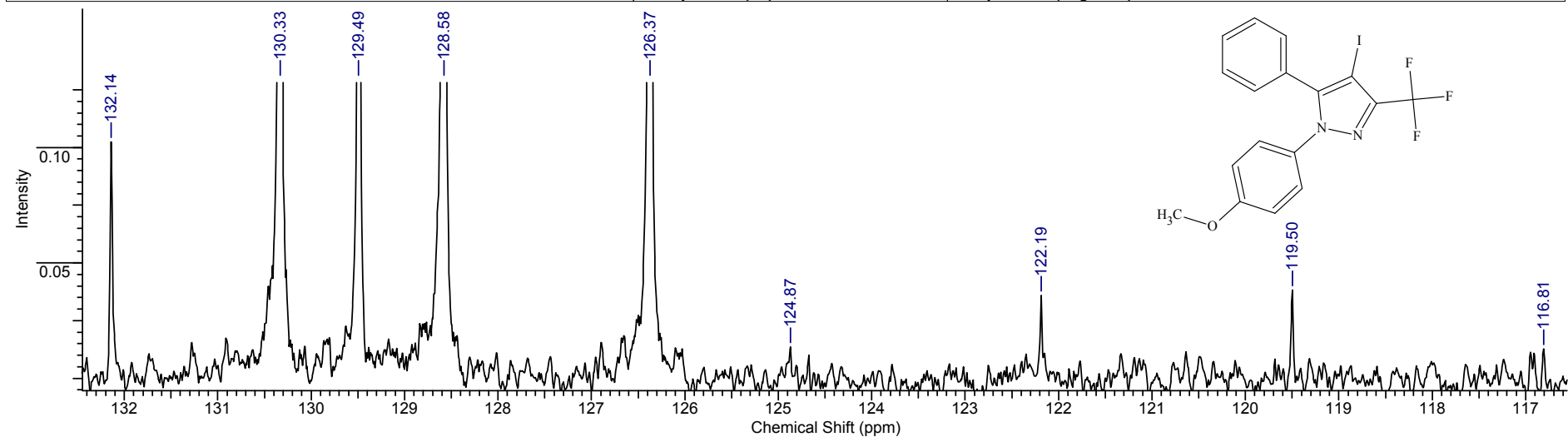
FW 444.1897 Formula C₁₇H₁₂F₃IN₂O

Acquisition Time (sec)	2.5559	Comment	Imported from UXMNR.		Date	30 May 2017 15:26:30	
File Name	D:\BN\output\2017\05.i à\BM-1090.H_001001r	Frequency (MHz)	400.13	Nucleus	1H	Number of Transients	4
Original Points Count	16384	Points Count	65536	Pulse Sequence	zg30	Solvent	CHLOROFORM-D
Sweep Width (Hz)	6410.26	Temperature (degree C)	27.000				



FW 444.1897 **Formula** C₁₇H₁₂F₃IN₂O

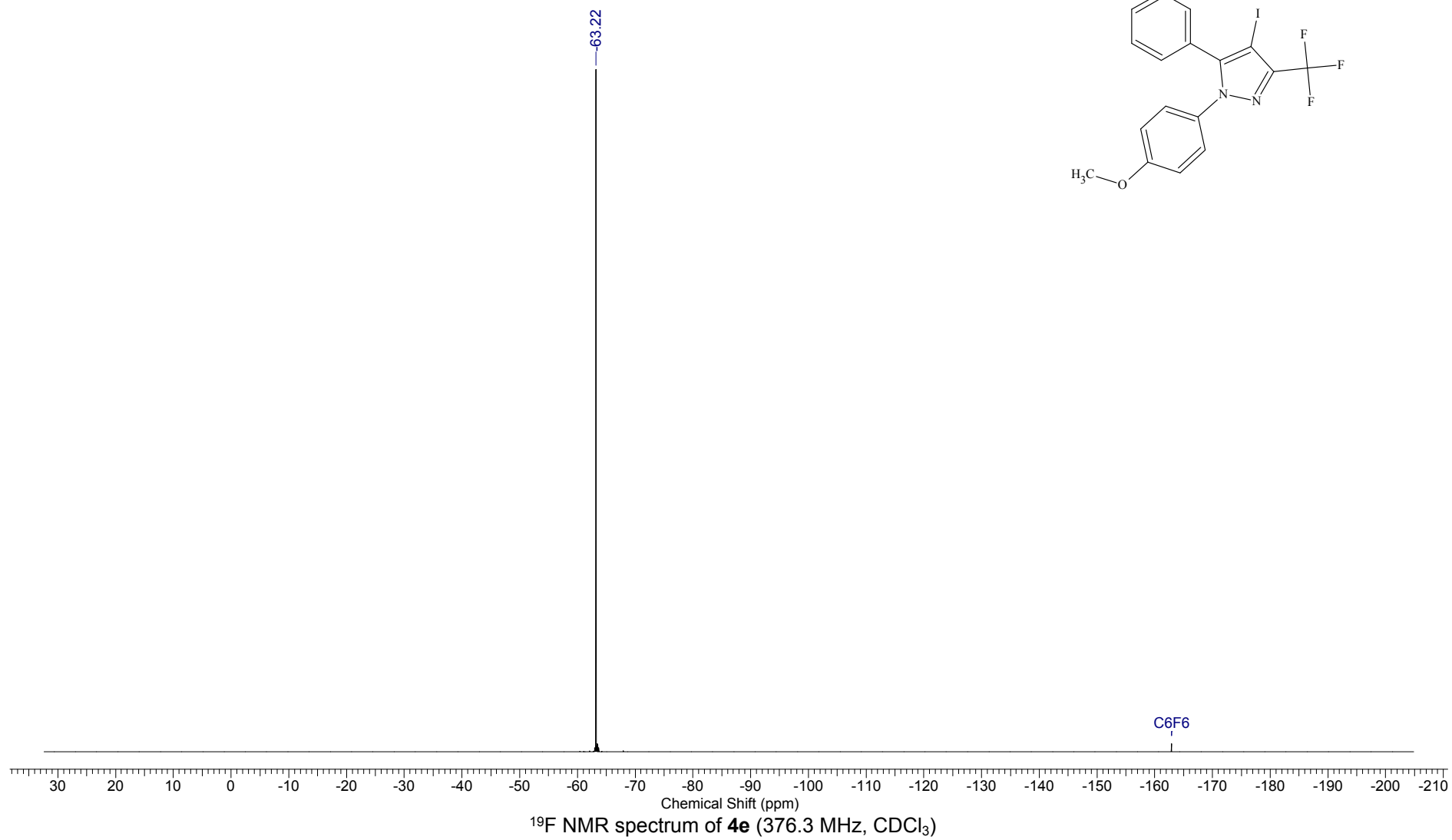
Acquisition Time (sec)	0.4999	Comment	Imported from UXNMR.		Date	30 May 2017 15:30:36
File Name	D:\BN\output\2017\05.i à\BM-1090.C_002001r	Frequency (MHz)	100.61	Nucleus	13C	
Number of Transients	125	Original Points Count	12076	Points Count	Pulse Sequence zgpg30	
Solvent	CHLOROFORM-D	Sweep Width (Hz)	24154.59	Temperature (degree C)	27.000	



¹³C NMR spectrum of **4e** (100.6 MHz, CDCl₃)

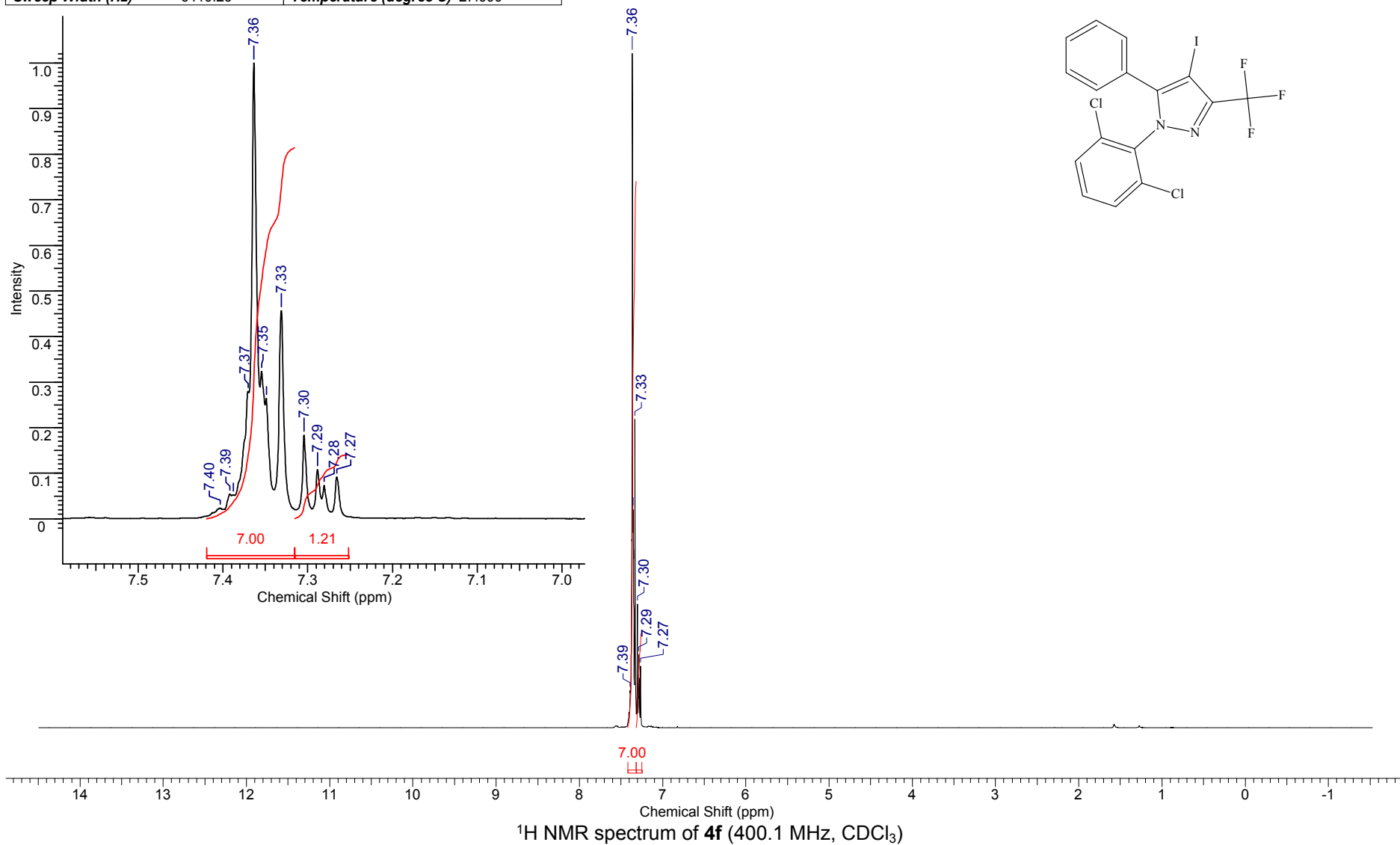
FW	444.1897	Formula	C ₁₇ H ₁₂ F ₃ IN ₂ O
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Acquisition Time (sec)	1.5000	Date	May 31 2017	File Name	D:\BN\Docs (BN)\vasily\SPEC_BM_F\2017.06.03_F\BM-1090_20170531_01\FLUORINE_01		
Frequency (MHz)	376.31	Nucleus	19F	Number of Transients	16	Original Points Count	133929
Points Count	262144	Pulse Sequence	s2pul	Solvent	CHLOROFORM-D		
Sweep Width (Hz)	89285.71	Temperature (degree C)	25.000				



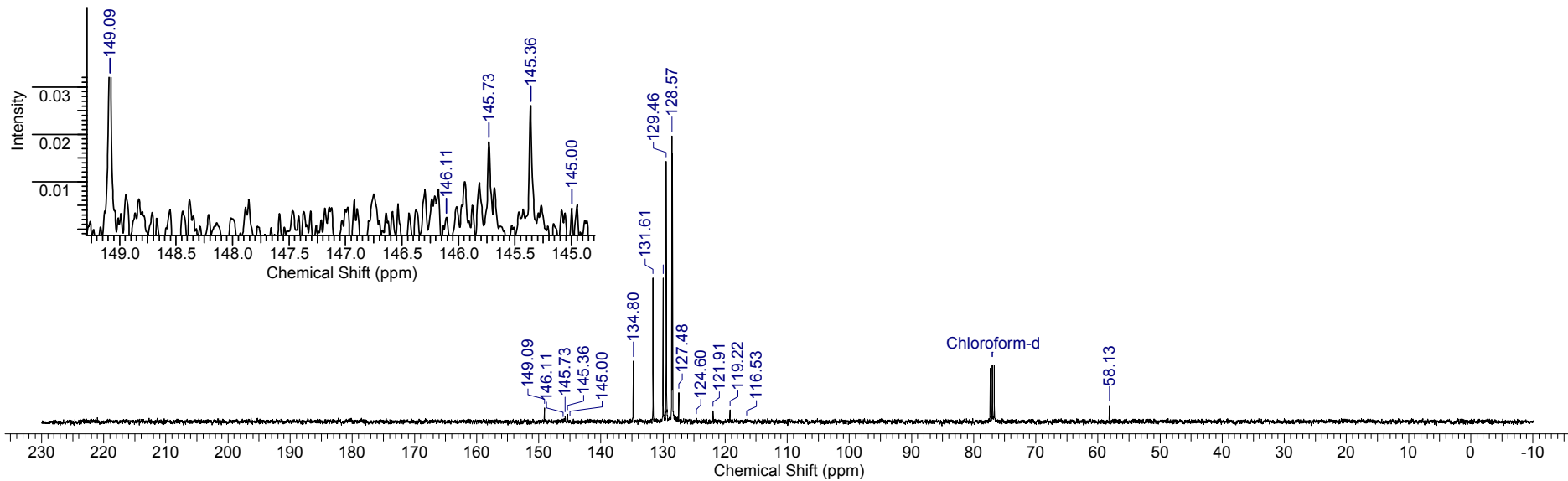
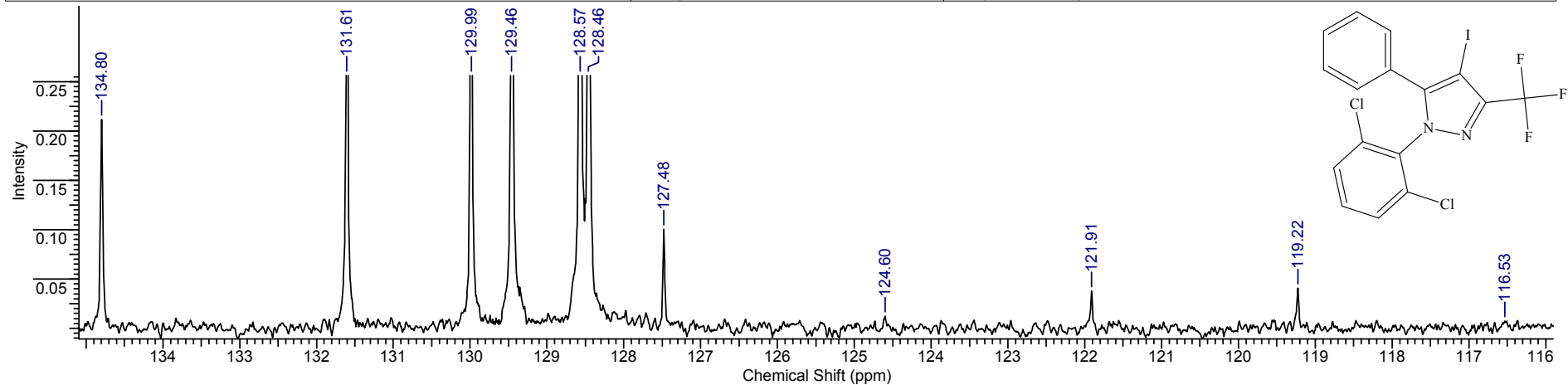
FW	483.0533	Formula	C ₁₆ H ₈ Cl ₂ F ₃ IN ₂
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Acquisition Time (sec)	2.5559	Comment	Imported from UXMNR.		Date	02 Jun 2017 15:15:44		
File Name	D:\BN\output\2017\06.epi\BM-1097.H_001001r		Frequency (MHz)	400.13	Nucleus	1H	Number of Transients	4
Original Points Count	16384	Points Count	65536	Pulse Sequence	zg30	Solvent	CHLOROFORM-D	
Sweep Width (Hz)	6410.26	Temperature (degree C)	27.000					



FW	483.0533	Formula	C ₁₆ H ₈ Cl ₂ F ₃ IN ₂
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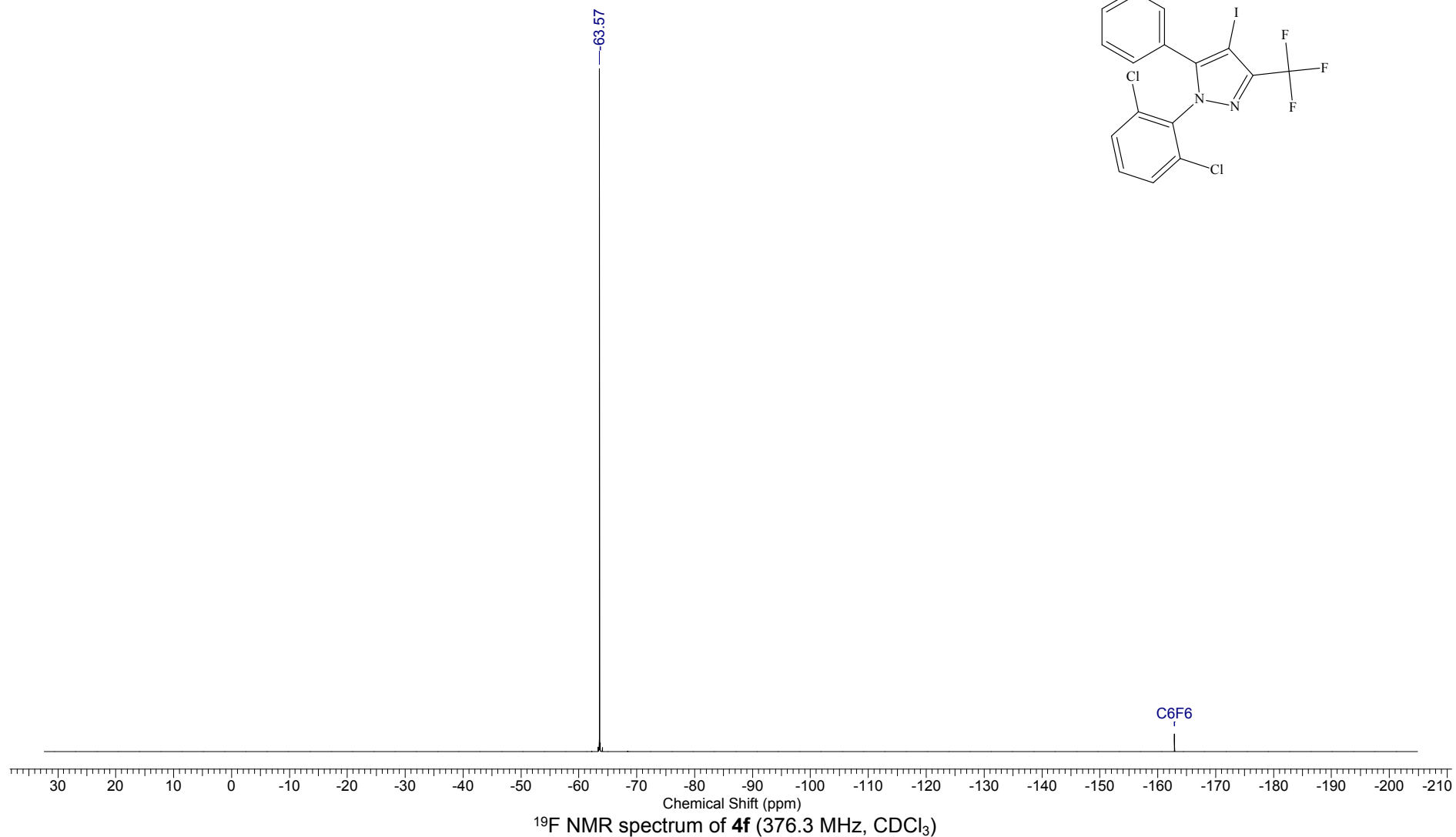
Acquisition Time (sec)	0.4999	Comment	Imported from UXMNR.	Date	02 Jun 2017 15:20:22
File Name	D:\BN\output\2017\06.epi\BM-1097.C_002001r	Frequency (MHz)	100.61	Nucleus	13C
Number of Transients	152	Original Points Count	12076	Points Count	65536
Solvent	CHLOROFORM-D	Sweep Width (Hz)	24154.59	Pulse Sequence	zgpg30
				Temperature (degree C)	27.000



¹³C NMR spectrum of **4f** (100.6 MHz, CDCl₃)

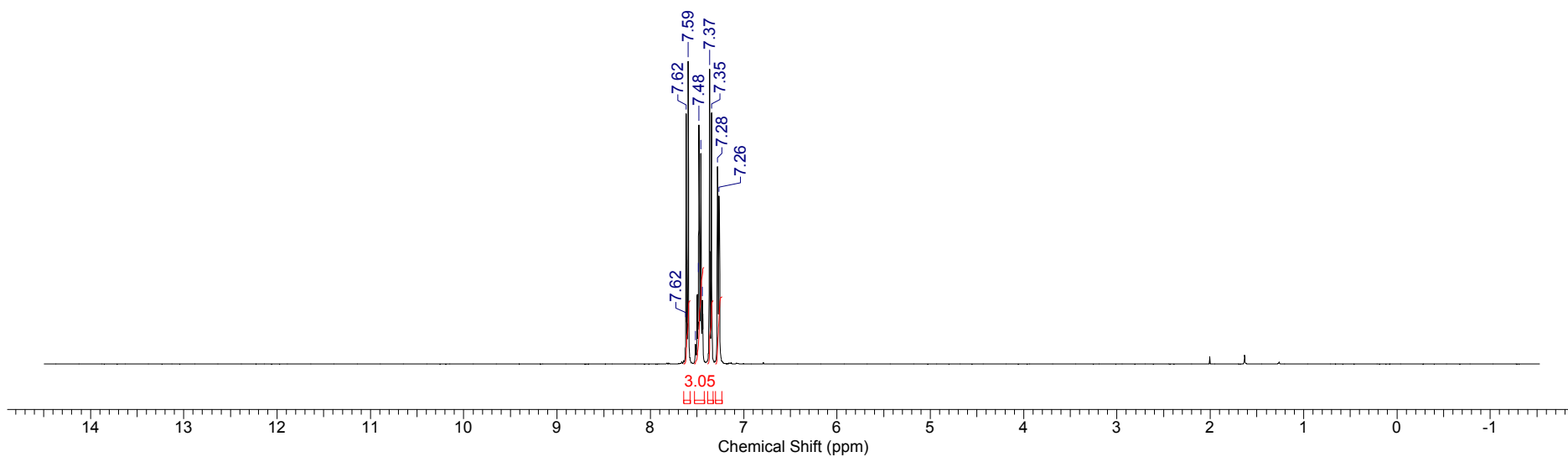
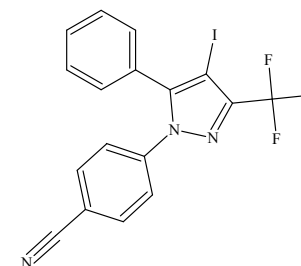
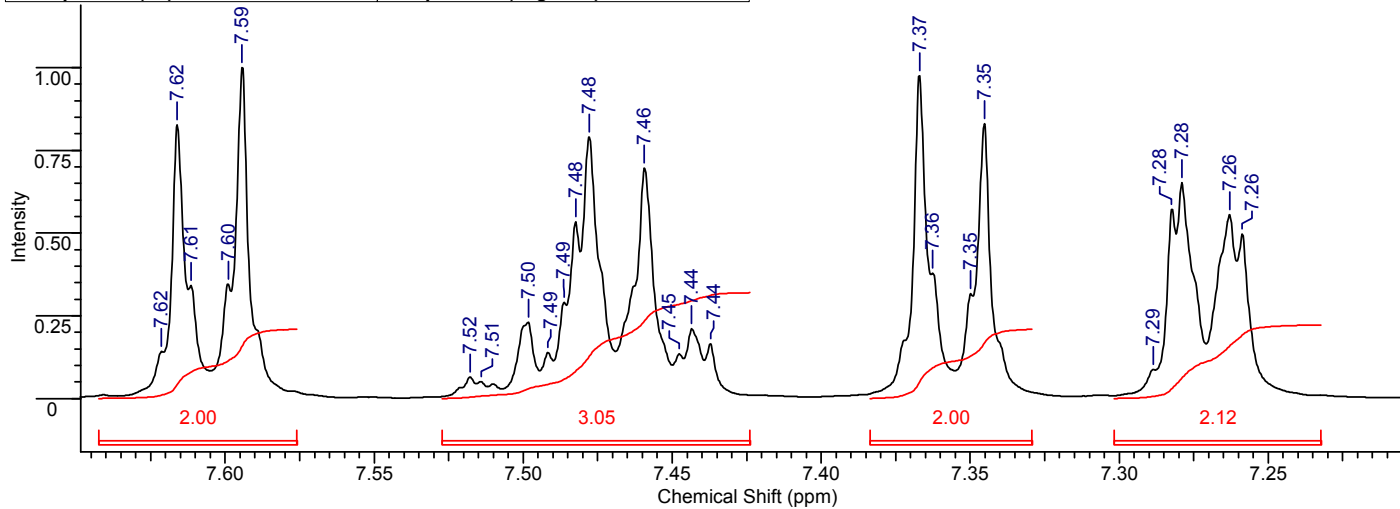
FW 483.0533	Formula C ₁₆ H ₈ Cl ₂ F ₃ IN ₂
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Acquisition Time (sec) 0.7340	Date Jun 7 2017	File Name D:\BN\output\F19\F_2017\2017.06.07\BM-1097_20170607_01\FLUORINE_01	
Frequency (MHz) 376.31	Nucleus 19F	Number of Transients 16	Original Points Count 65536
Points Count 65536	Pulse Sequence s2pul	Solvent CHLOROFORM-D	
Sweep Width (Hz) 89285.71	Temperature (degree C) 25.000		



FW	439.1733	Formula	C ₁₇ H ₉ F ₃ IN ₃
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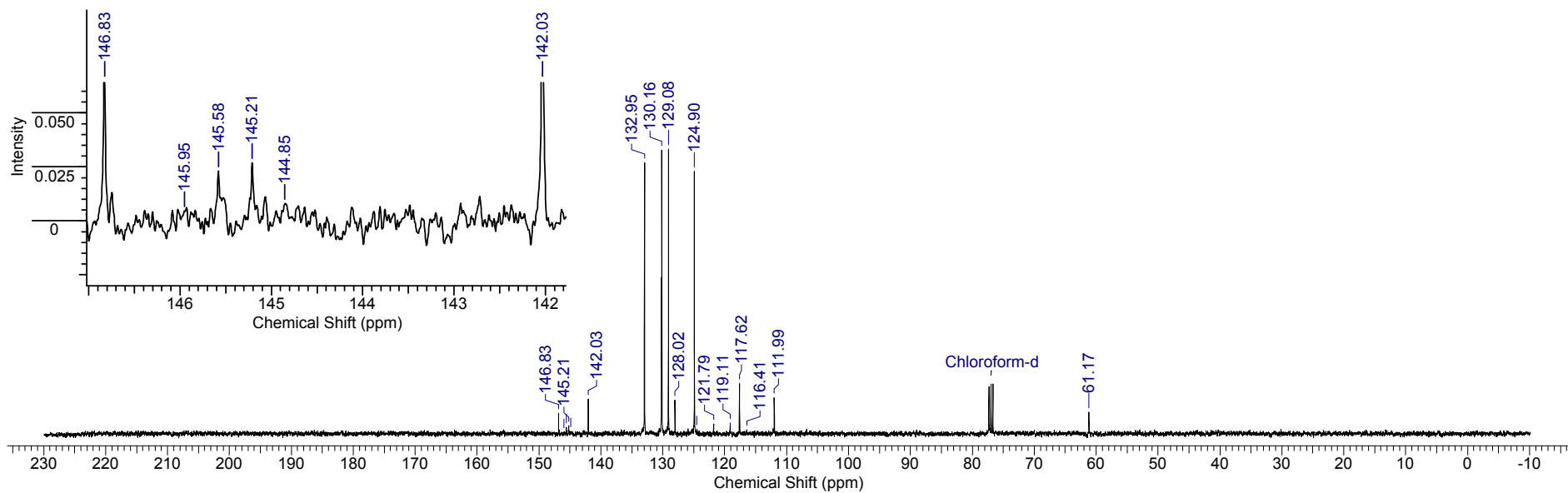
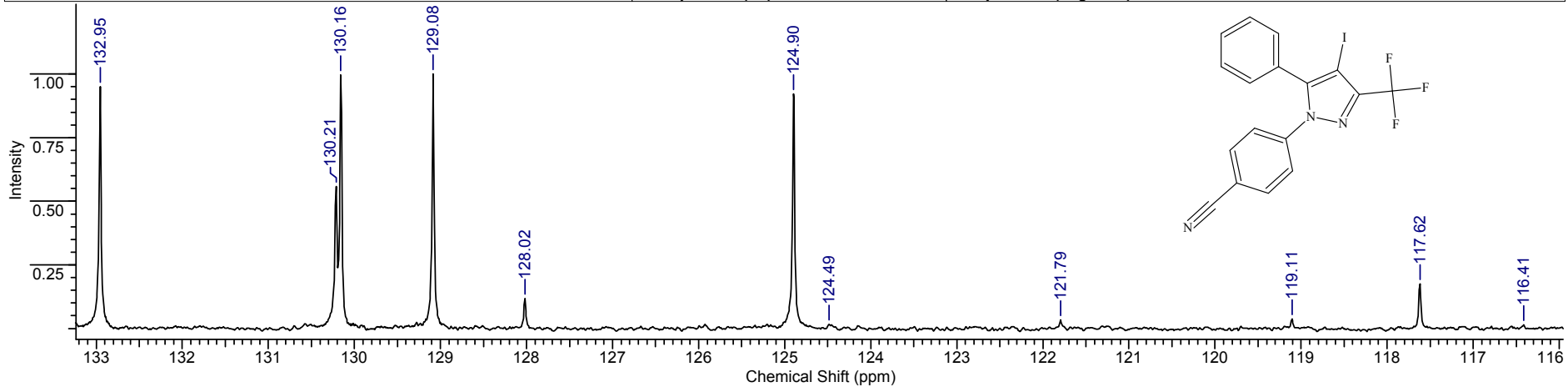
Acquisition Time (sec)	2.5559	Comment	Imported from UXNMR.		Date	03 Jun 2017 13:27:44			
File Name	D:\BN\output\2017\06.epi\BM-1100.H_001001r		Frequency (MHz)	400.13	Nucleus	1H	Number of Transients	4	
Original Points Count	16384	Points Count	65536	Pulse Sequence	zg30	Solvent	CHLOROFORM-D		
Sweep Width (Hz)	6410.26	Temperature (degree C)	27.000						



¹H NMR spectrum of **4g** (400.1 MHz, CDCl₃)

FW	439.1733	Formula	C ₁₇ H ₉ F ₃ IN ₃
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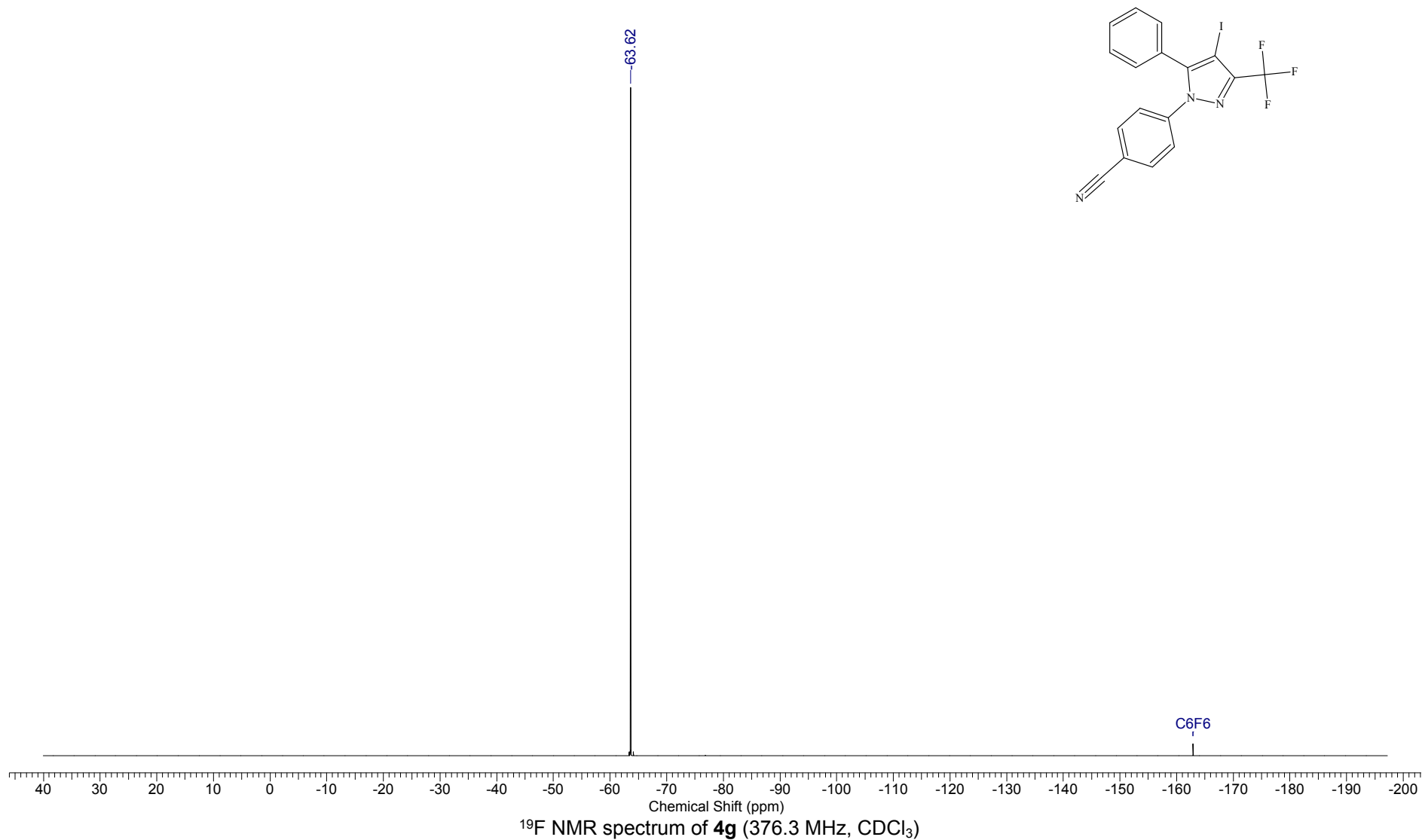
Acquisition Time (sec)	0.4999	Comment	Imported from UXMNR.	Date	03 Jun 2017 13:30:48
File Name	D:\BN\output\2017\06.epi\BM-1100.C_002001r	Frequency (MHz)	100.61	Nucleus	¹³ C
Number of Transients	88	Original Points Count	12076	Points Count	65536
Solvent	CHLOROFORM-D	Sweep Width (Hz)	24154.59	Pulse Sequence	zgpg30
				Temperature (degree C)	27.000



¹³C NMR spectrum of **4g** (100.6 MHz, CDCl₃)

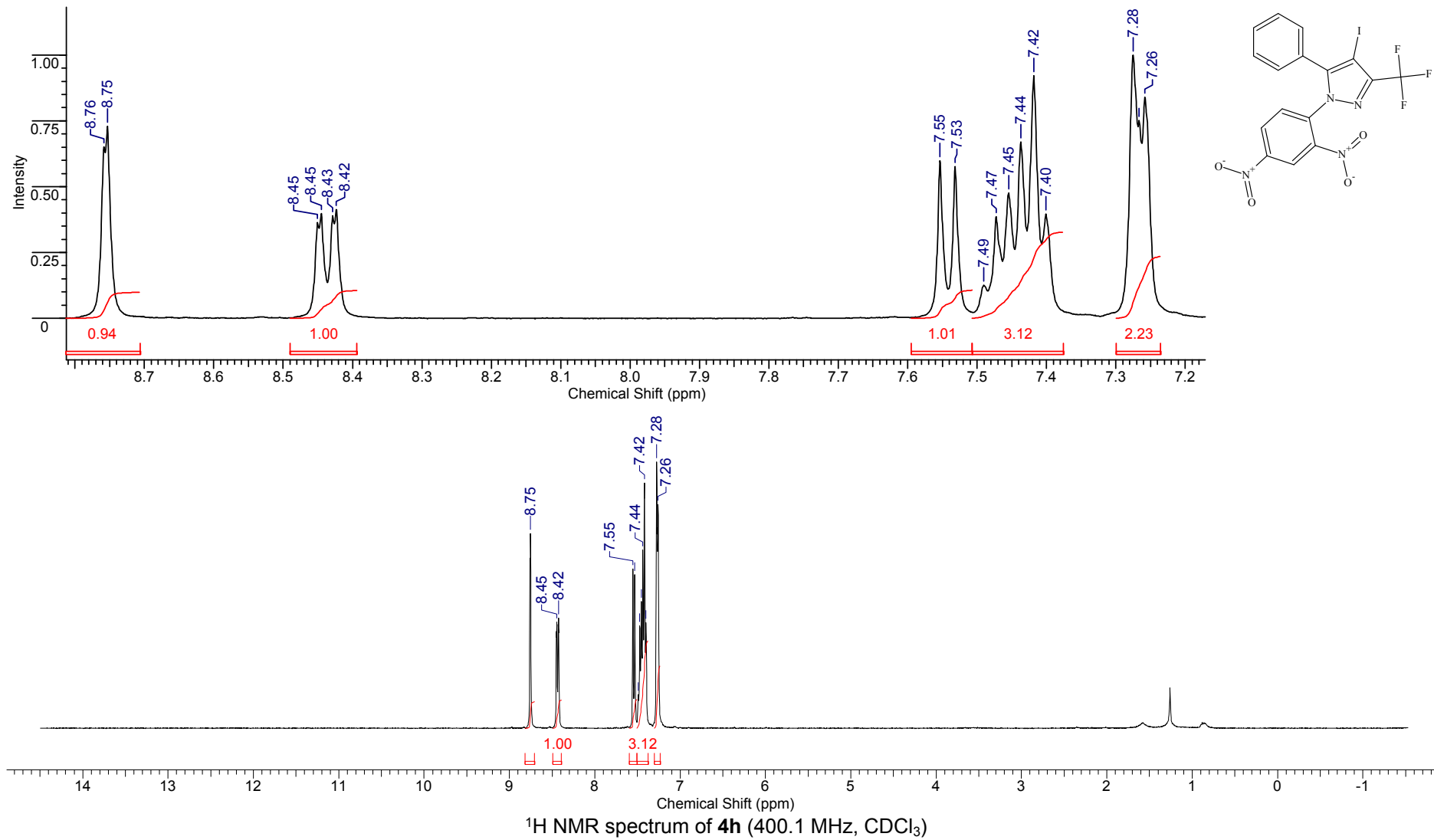
FW	439.1733	Formula	C ₁₇ H ₉ F ₃ IN ₃
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Acquisition Time (sec)	1.5729	Date	Jun 8 2017	File Name	D:\BN\output\F19\F_2017\2017.06.08\BM-1100-F_20170608_01\FLUORINE_01		
Frequency (MHz)	376.31	Nucleus	19F	Number of Transients	8	Original Points Count	140434
Points Count	262144	Pulse Sequence	s2pul	Solvent	CHLOROFORM-D		
Sweep Width (Hz)	89285.71	Temperature (degree C)	22.000				



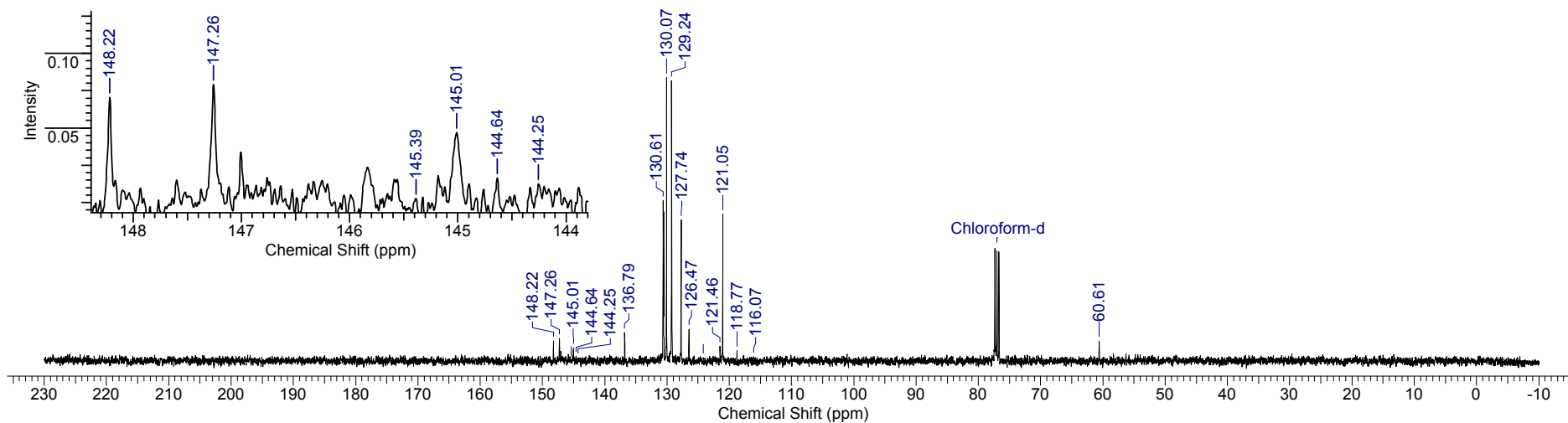
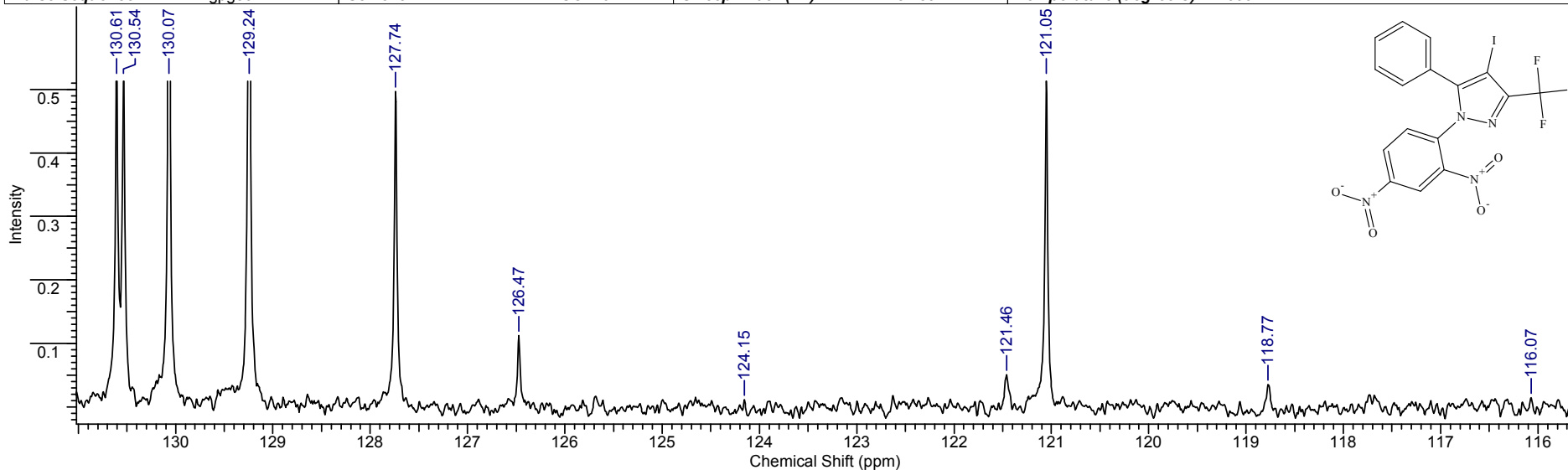
FW 504.1590 **Formula** C₁₆H₈F₃N₄O₄

Acquisition Time (sec)	2.5559	Comment	Imported from UXNMR.	Date	11 Oct 2016 14:34:06
File Name	C:\BM_DATA\DOCS\Manuscr_UltraIodo_Pyrazoles\BM-943,946\BM-946.H_001001r			Frequency (MHz)	400.13
Nucleus	1H	Number of Transients	4	Original Points Count	16384
Pulse Sequence	zg30	Solvent	CHLOROFORM-D	Points Count	65536
Temperature (degree C)	27.000			Sweep Width (Hz)	6410.26



FW 504.1590 **Formula** C₁₆H₈F₃I₂N₄O₄

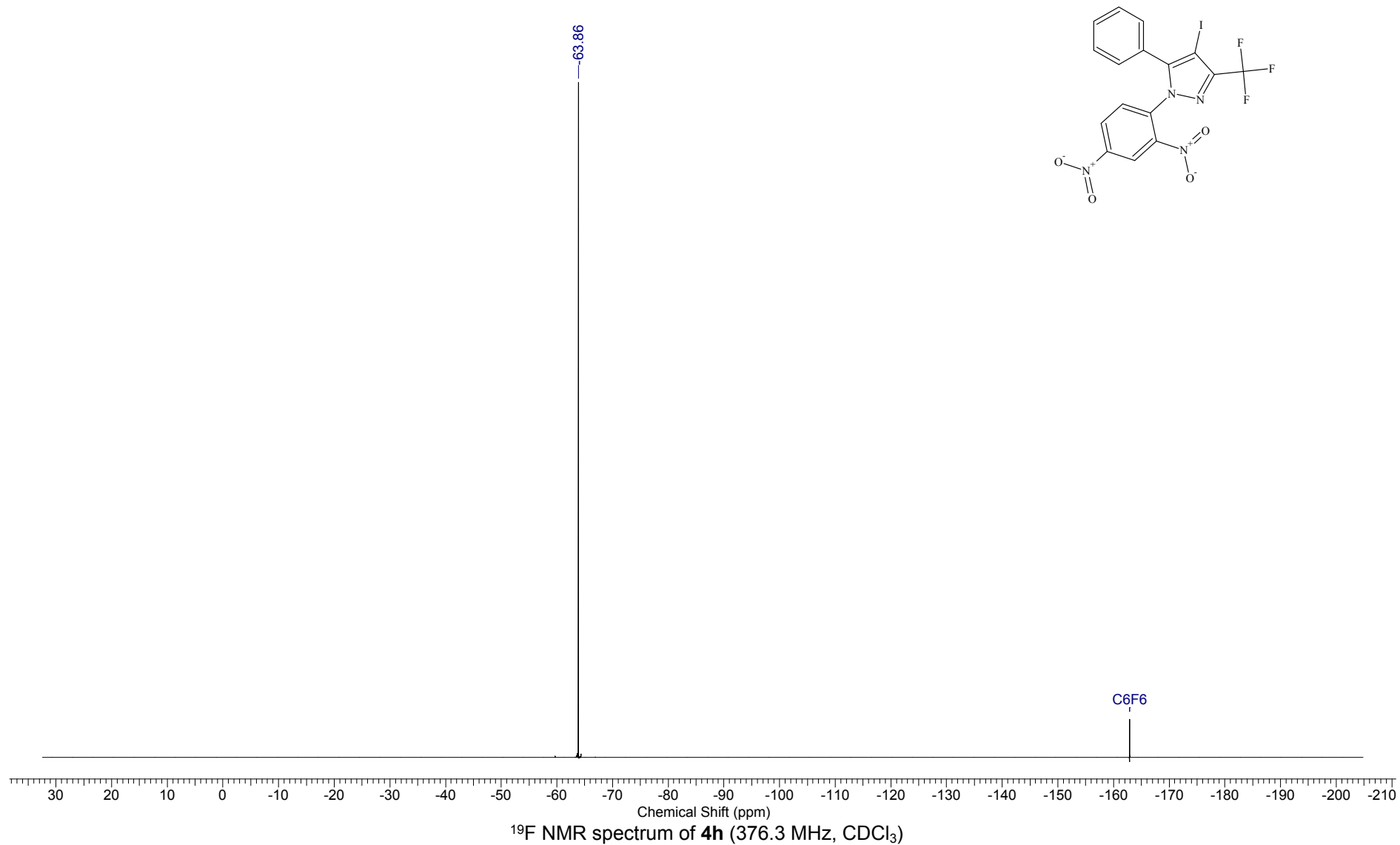
Acquisition Time (sec)	0.4999	Comment	Imported from UXNMR.		Date	11 Oct 2016 14:41:26	
File Name	C:\BM_DATA\DOCS\Manuscr_UltraIodo_Pyrazoles\BM-943,946\BM-946.C_002001r				Frequency (MHz)	100.61	
Nucleus	¹³ C	Number of Transients	256	Original Points Count	12076	Points Count	65536
Pulse Sequence	zgpg30	Solvent	DMSO-D6	Sweep Width (Hz)	24154.59	Temperature (degree C)	27.000



¹³C NMR spectrum of **4h** (100.6 MHz, CDCl₃)

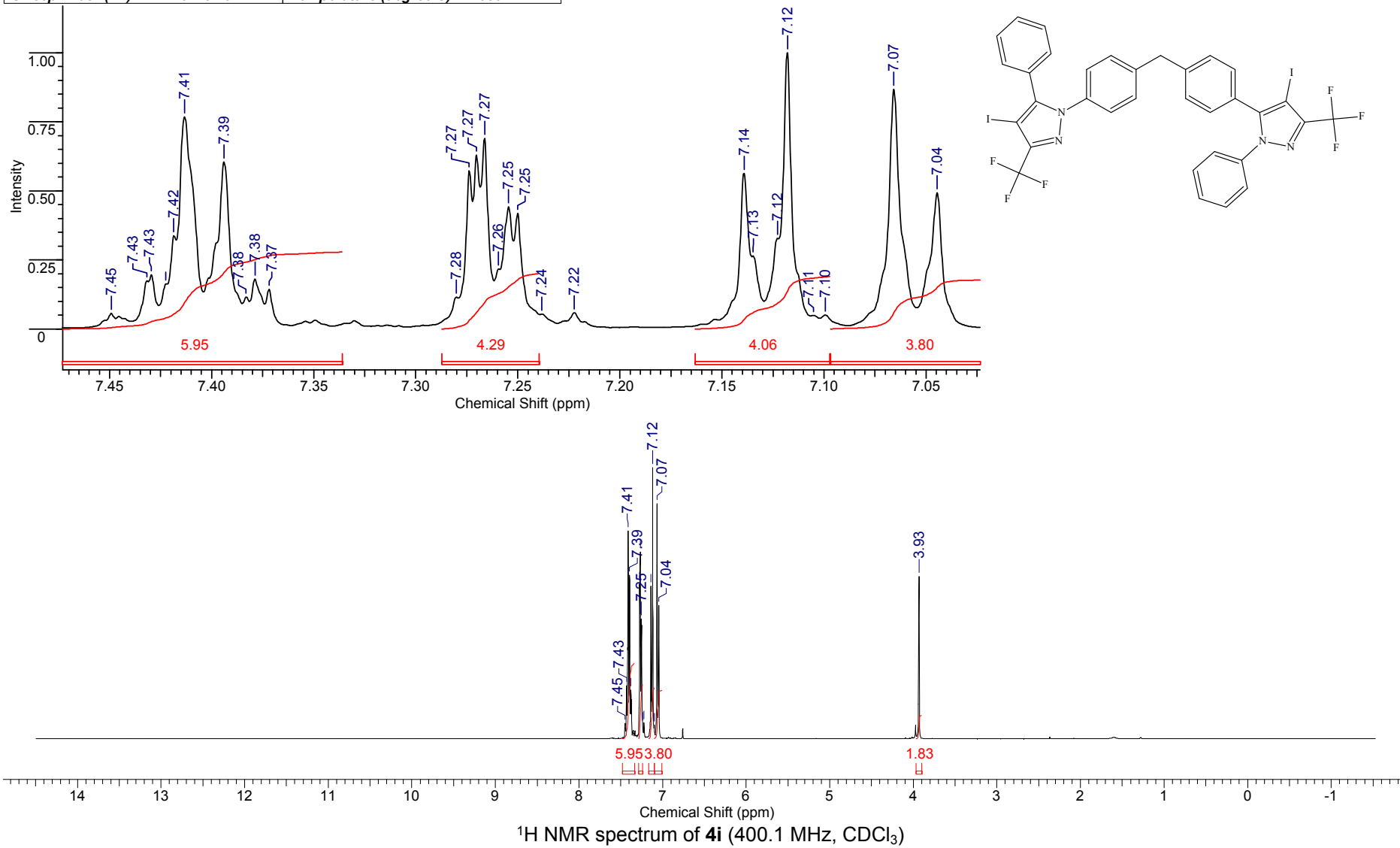
FW	504.1590	Formula	C ₁₆ H ₈ F ₃ I ₁ N ₄ O ₄
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Acquisition Time (sec)	1.0000	Date	Oct 21 2016	File Name	C:\BM_DATA\BM-943,946F\BM-946_20161021_01\FLUORINE_01				
Frequency (MHz)	376.31	Nucleus	¹⁹ F	Number of Transients	16	Original Points Count	89286	Points Count	131072
Pulse Sequence	s2pul	Solvent	CHLOROFORM-D	Sweep Width (Hz)	89285.71	Temperature (degree C)	25.000		



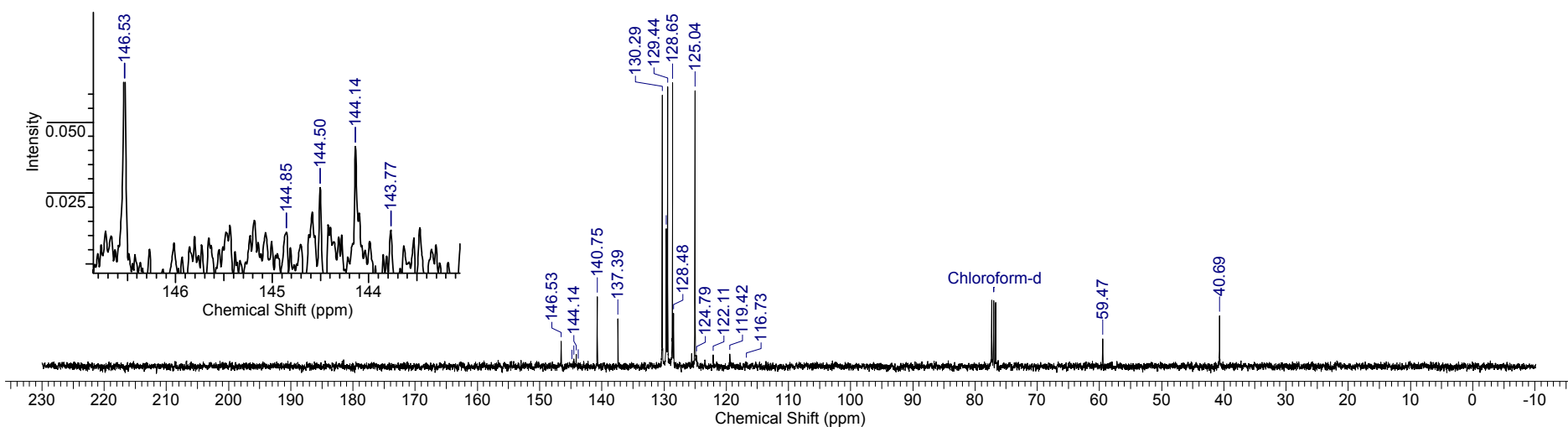
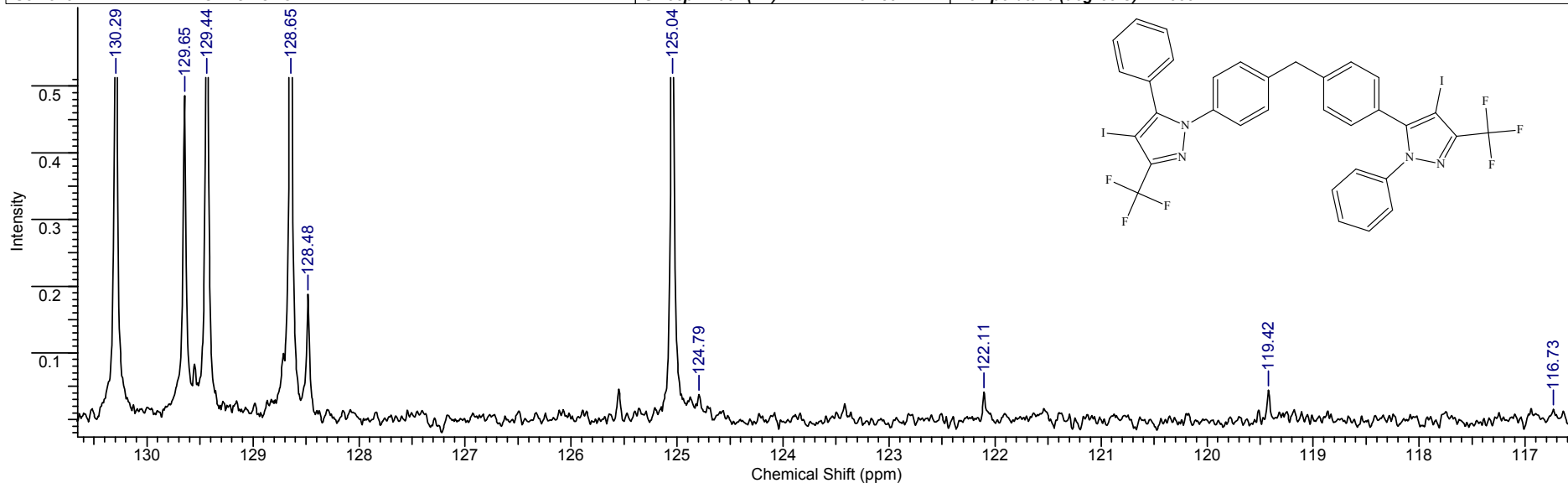
FW 840.3382 Formula $C_{33}H_{20}F_6I_2N_4$

Acquisition Time (sec)	2.5559	Comment	Imported from UXMNR.		Date	31 May 2017 17:39:46	
File Name	D:\BN\output\2017\05.i æ\BM-1094.H_001001r	Frequency (MHz)	400.13	Nucleus	1H	Number of Transients	4
Original Points Count	16384	Points Count	65536	Pulse Sequence	zg30	Solvent	CHLOROFORM-D
Sweep Width (Hz)	6410.26	Temperature (degree C)	27.000				



FW 840.3382 **Formula** C₃₃H₂₀F₆I₂N₄

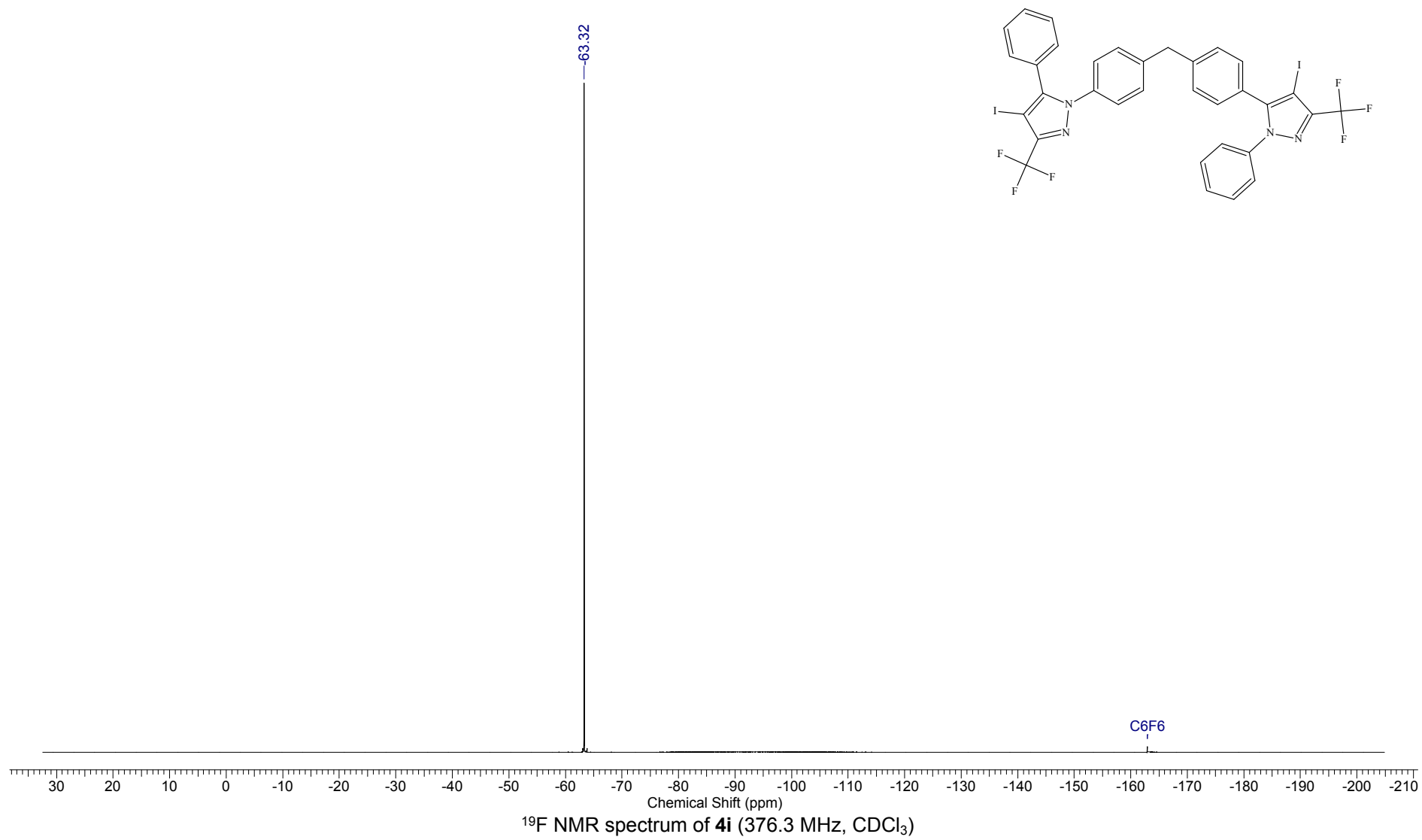
Acquisition Time (sec)	0.4999	Comment	Imported from UXMNR.		Date	31 May 2017 17:43:26
File Name	D:\BN\output\2017\05.i àé\BM-1094.C_002001r	Frequency (MHz)	100.61	Nucleus	13C	
Number of Transients	64	Original Points Count	12076	Points Count	65536	
Solvent	CHLOROFORM-D	Sweep Width (Hz)	24154.59	Pulse Sequence	zgpg30	
				Temperature (degree C)	27.000	



¹³C NMR spectrum of **4i** (100.6 MHz, CDCl₃)

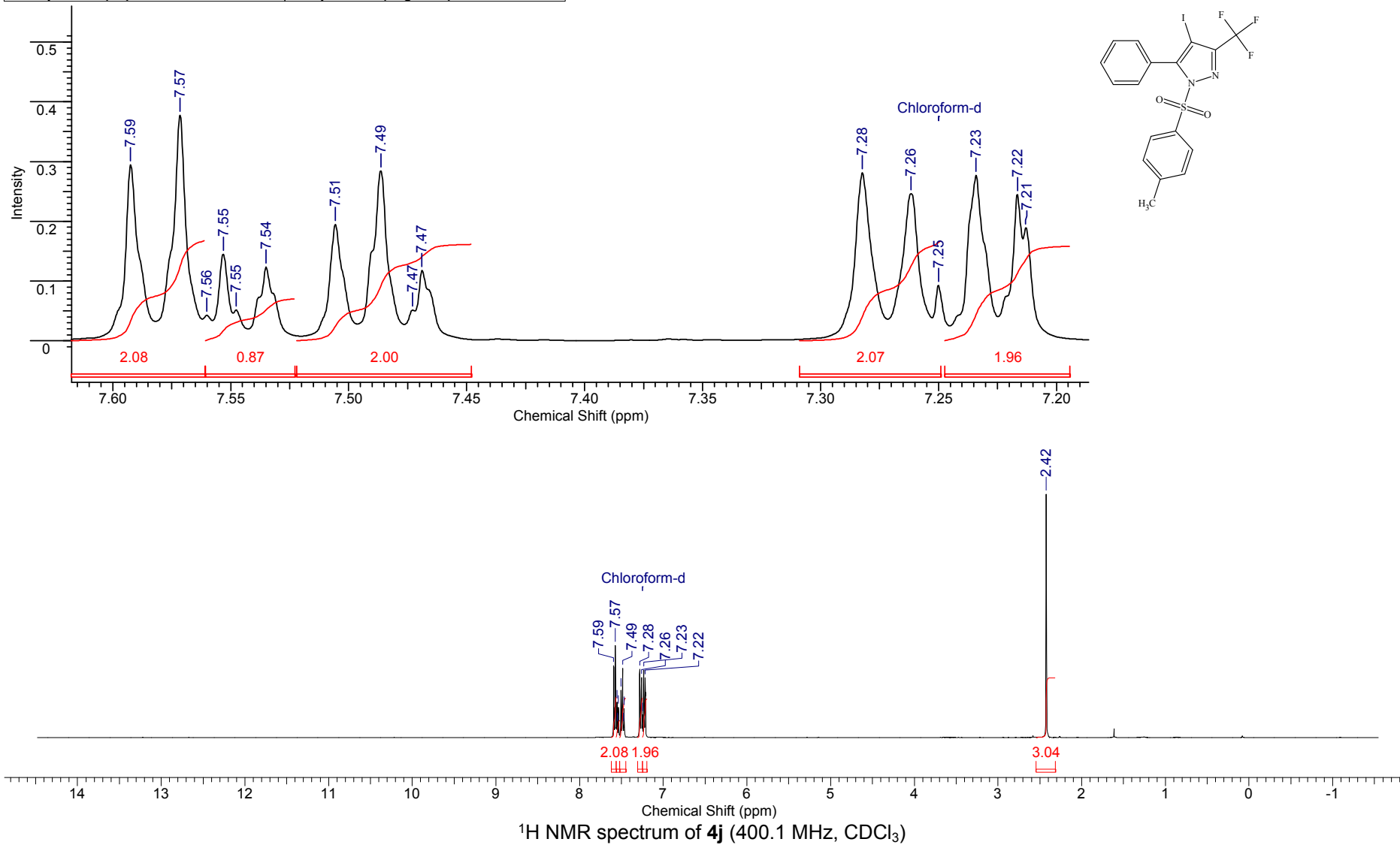
FW	840.3382	Formula	C ₃₃ H ₂₀ F ₆ I ₂ N ₄
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Acquisition Time (sec)	0.7340	Date	Jun 2 2017	File Name	D:\BN\output\F19\F_2017\2017.06.02\BM-1094_20170602_01\FLUORINE_01		
Frequency (MHz)	376.31	Nucleus	19F	Number of Transients	16	Original Points Count	65536
Points Count	65536	Pulse Sequence	s2pul	Solvent	CHLOROFORM-D		
Sweep Width (Hz)	89285.71	Temperature (degree C)	25.000				



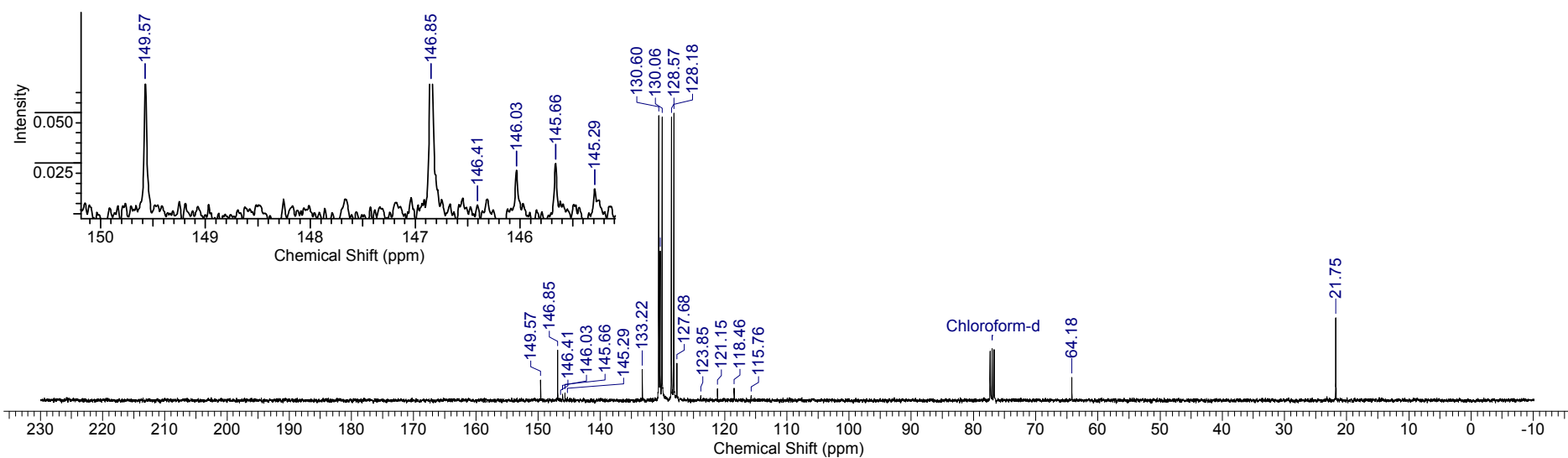
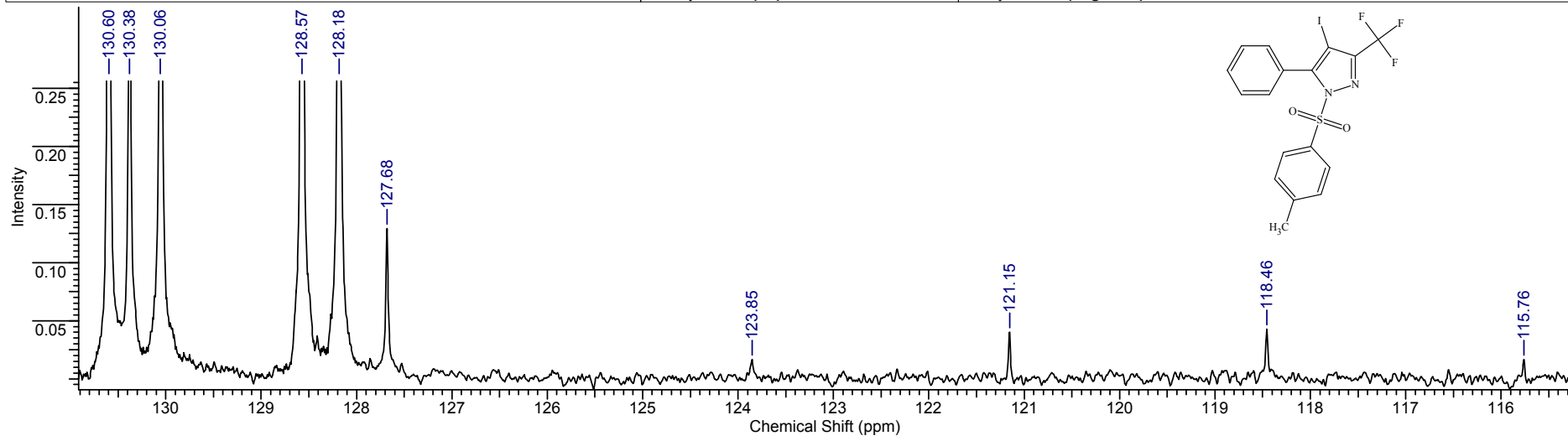
FW	492.2551	Formula	C ₁₇ H ₁₂ F ₃ IN ₂ O ₂ S
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Acquisition Time (sec)	2.5559	Comment	Imported from UXMNR.		Date	01 Jun 2017 11:20:26	
File Name	D:\BN\output\2017\06.epi\BM-1093-1.H_001001r	Frequency (MHz)	400.13	Nucleus	1H	Number of Transients	4
Original Points Count	16384	Points Count	65536	Pulse Sequence	zg30	Solvent	CHLOROFORM-D
Sweep Width (Hz)	6410.26	Temperature (degree C)	27.000				



FW	492.2551	Formula	C ₁₇ H ₁₂ F ₃ IN ₂ O ₂ S
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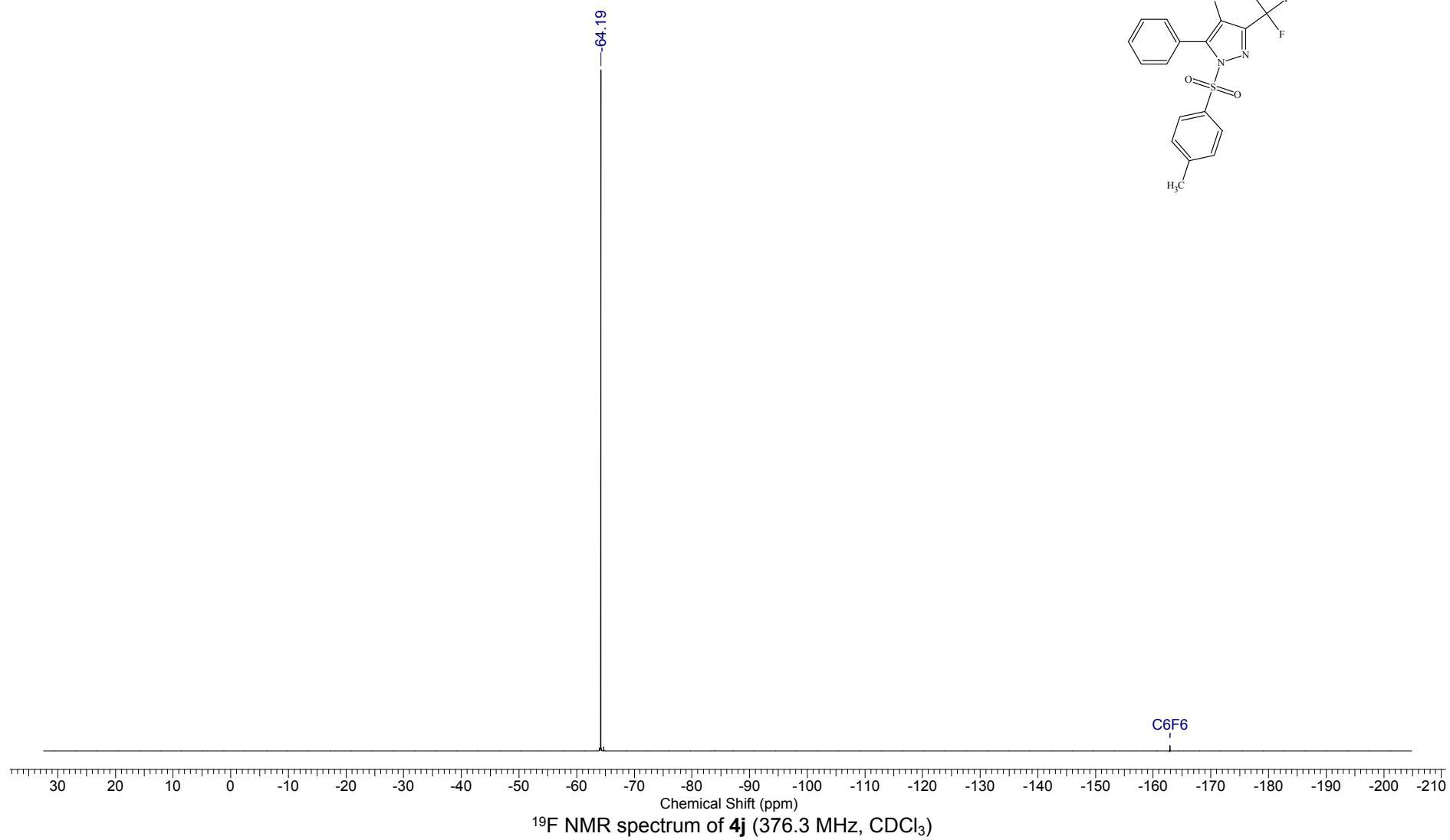
Acquisition Time (sec)	0.4999	Comment	Imported from UXNMR.	Date	01 Jun 2017 11:28:44
File Name	D:\BN\output\2017\06.ep f \BM-1093-1.C_002001r	Frequency (MHz)	100.61	Nucleus	¹³ C
Number of Transients	256	Original Points Count	12076	Points Count	65536
Solvent	CHLOROFORM-D	Sweep Width (Hz)	24154.59	Pulse Sequence	zpgg30
				Temperature (degree C)	27.000



¹³C NMR spectrum of **4j** (100.6 MHz, CDCl₃)

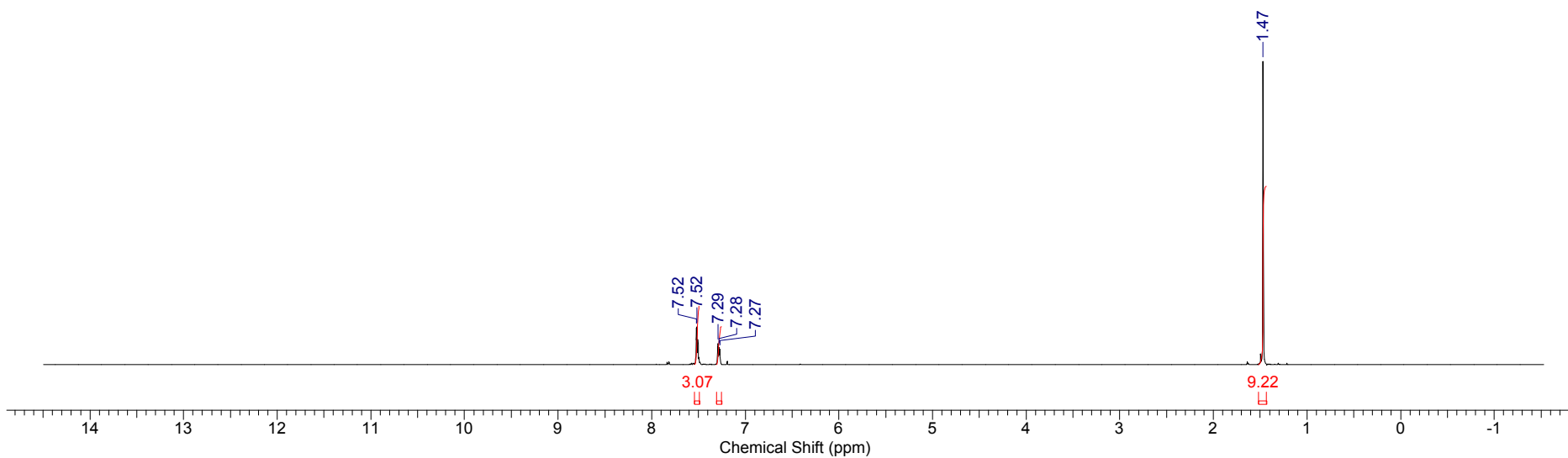
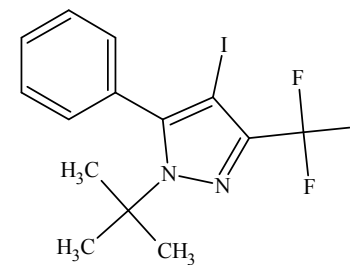
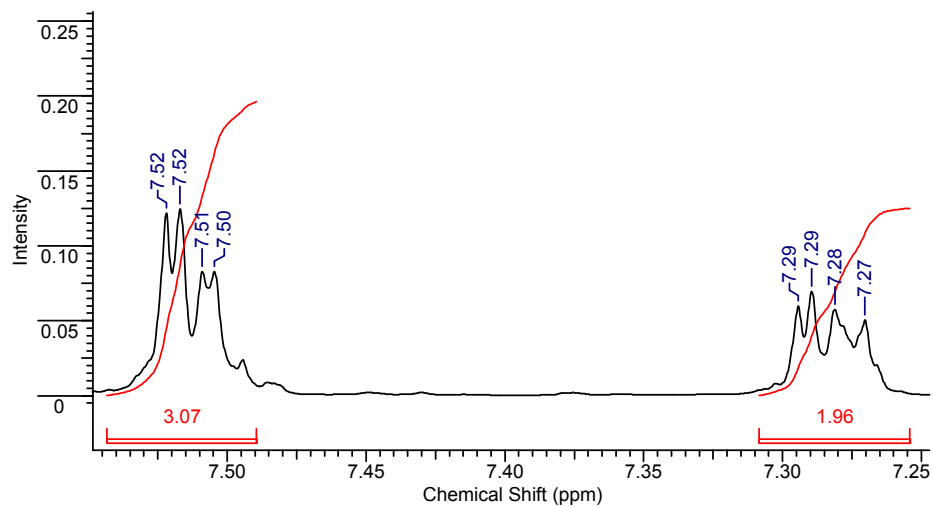
FW	492.2551	Formula	C ₁₇ H ₁₂ F ₃ IN ₂ O ₂ S
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Acquisition Time (sec)	0.7340	Date	Jun 2 2017	File Name	D:\BN\output\F19\F_2017\2017.06.02\BM-1093-1_20170602_01\FLUORINE_01		
Frequency (MHz)	376.31	Nucleus	¹⁹ F	Number of Transients	16	Original Points Count	65536
Points Count	65536	Pulse Sequence	s2pul	Solvent	CHLOROFORM-D		
Sweep Width (Hz)	89285.71	Temperature (degree C)	25.000				



FW	394.1741	Formula	C ₁₄ H ₁₄ F ₃ IN ₂
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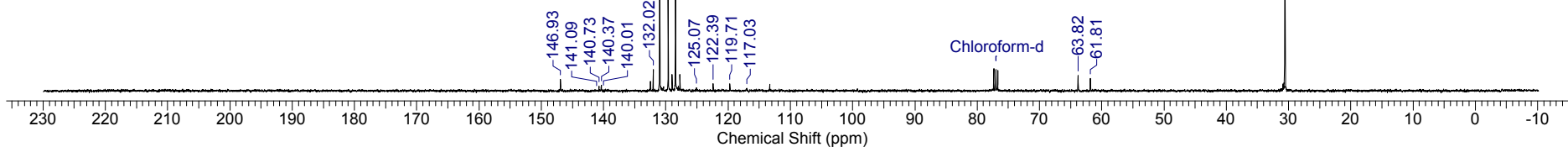
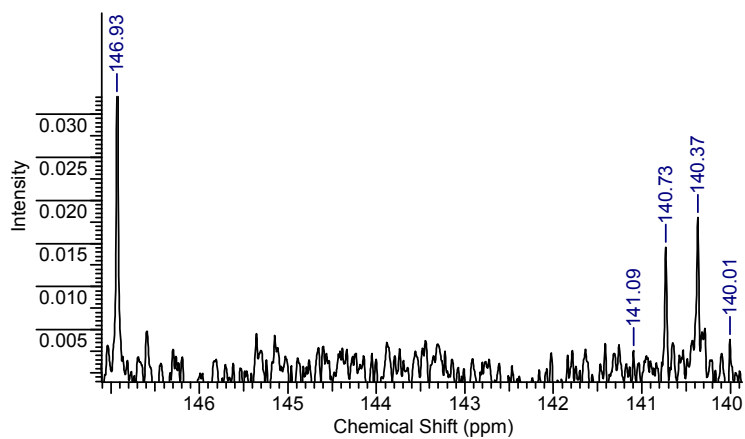
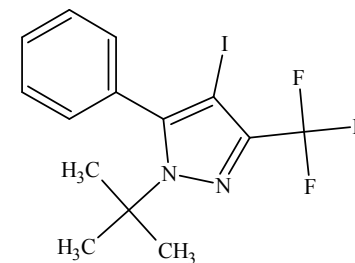
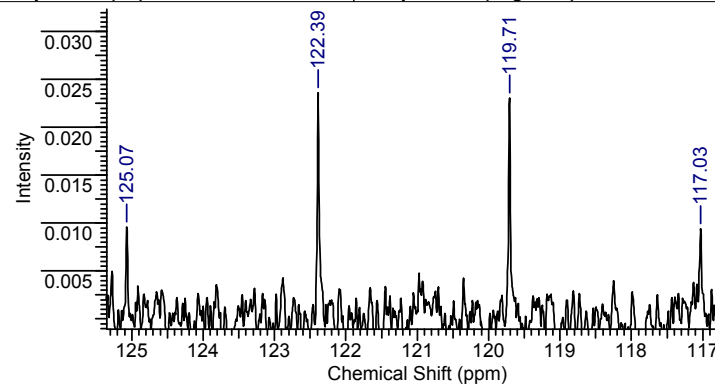
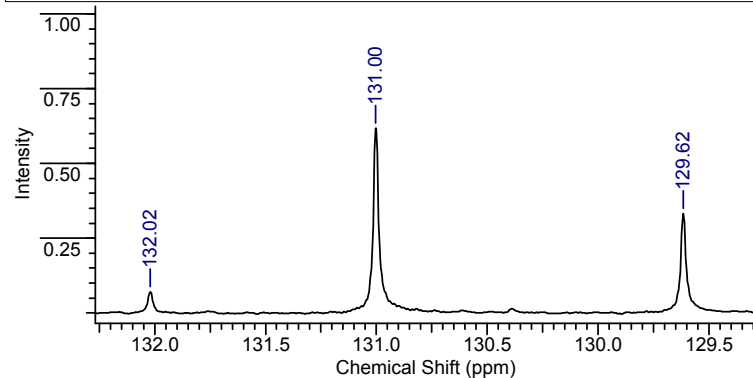
Acquisition Time (sec)	2.5559	Comment	Imported from UXMNR.		Date	06 Jun 2017 15:09:52	
File Name	D:\BN\output\2017\06.epi\BM-1106.H_001001r	Frequency (MHz)	400.13	Nucleus	1H	Number of Transients	4
Original Points Count	16384	Points Count	65536	Pulse Sequence	zg30	Solvent	CHLOROFORM-D
Sweep Width (Hz)	6410.26	Temperature (degree C)	27.000				



¹H NMR spectrum of **4k** (400.1 MHz, CDCl₃)

FW 394.1741 **Formula** C₁₄H₁₄F₃IN₂

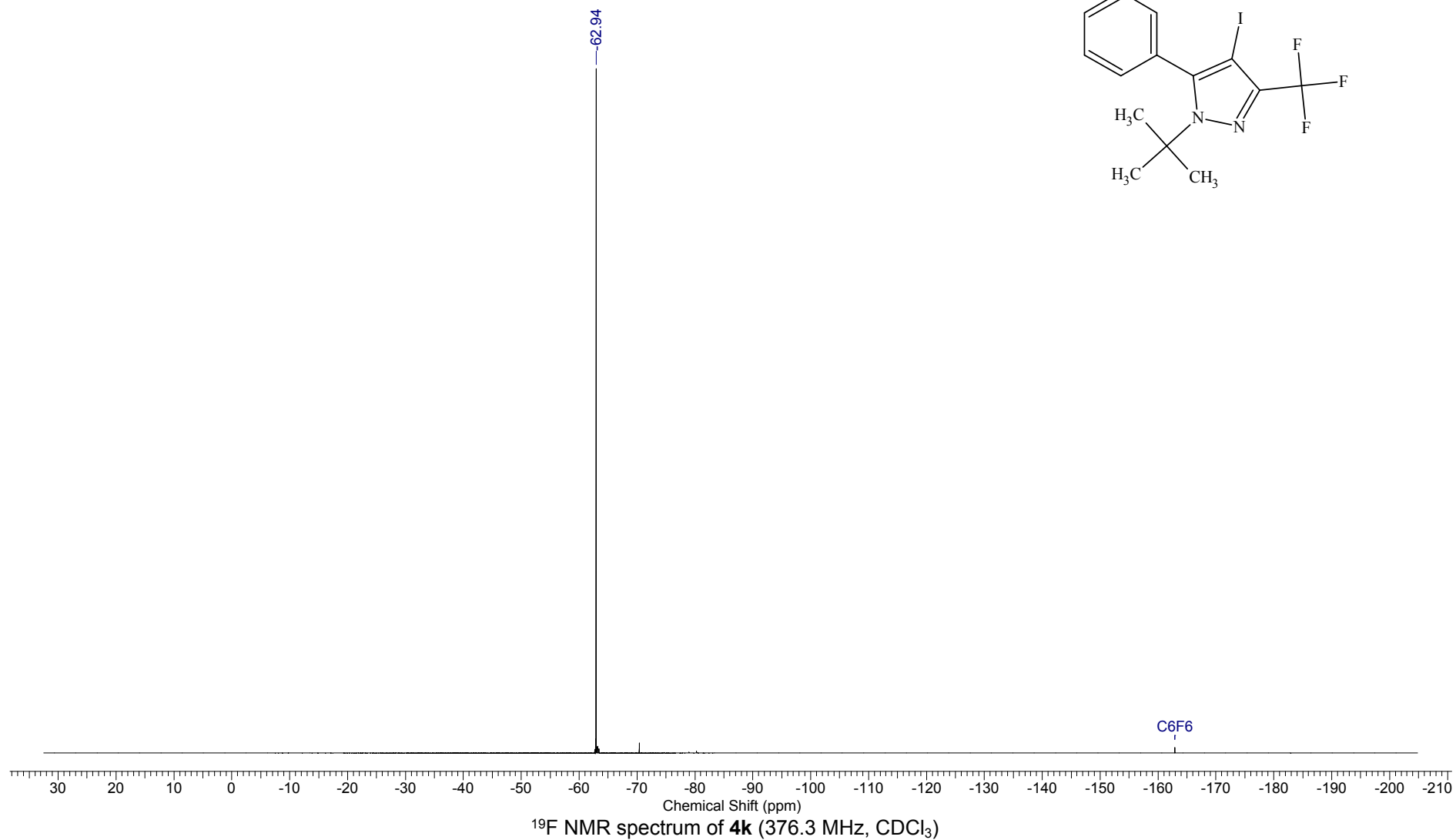
Acquisition Time (sec)	0.4999	Comment	Imported from UXMNR.	Date	06 Jun 2017 15:13:34
File Name	D:\BN\output\2017\06.ép í ú\BM-1106.C_002001r	Frequency (MHz)	100.61	Nucleus	13C
Number of Transients	74	Original Points Count	12076	Points Count	65536
Solvent	CHLOROFORM-D	Sweep Width (Hz)	24154.59	Pulse Sequence	zgpg30
		Temperature (degree C)	27.000		



¹³C NMR spectrum of **4k** (100.6 MHz, CDCl₃)

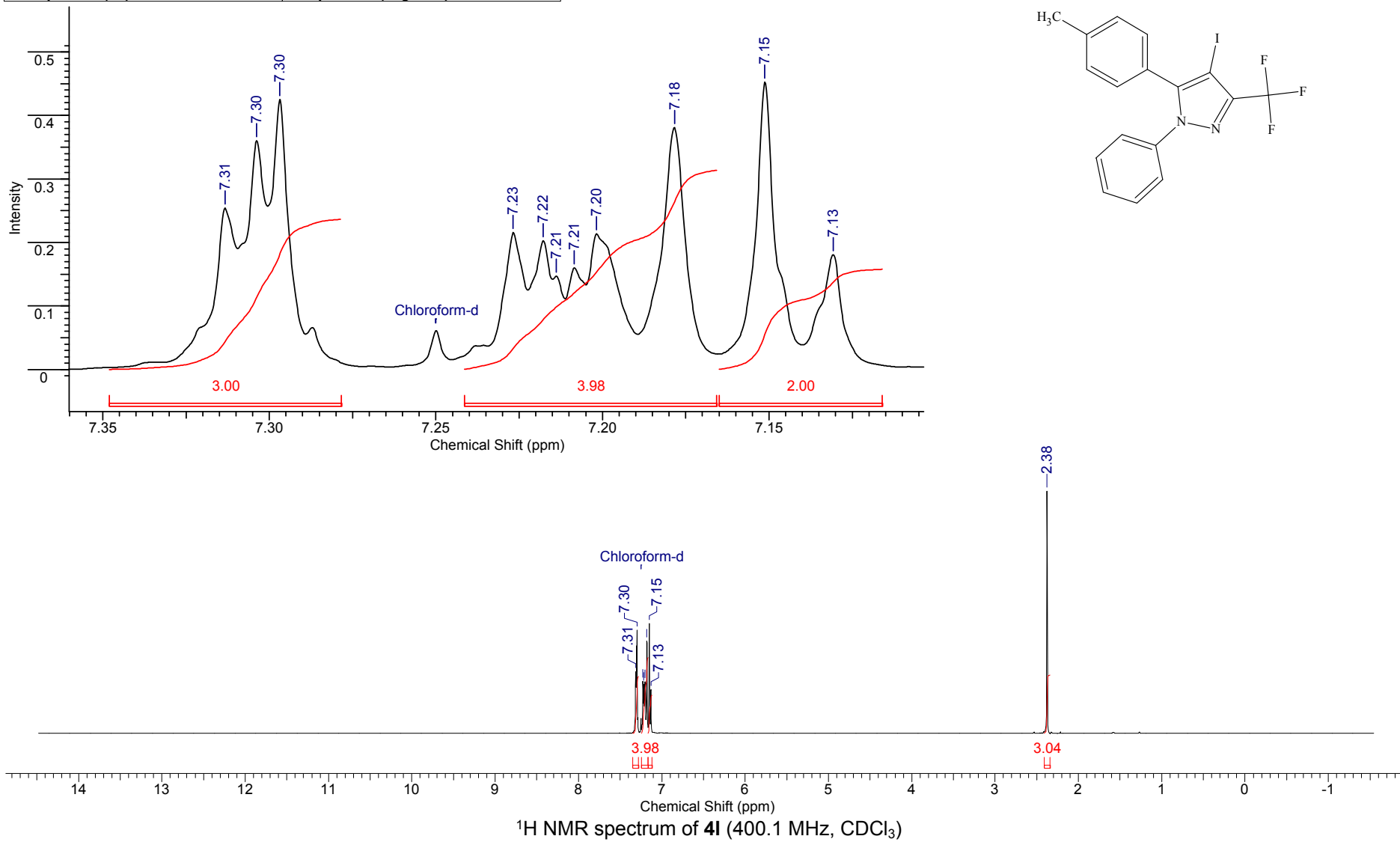
FW	394.1741	Formula	C ₁₄ H ₁₄ F ₃ IN ₂
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Acquisition Time (sec)	0.7340	Date	Jun 7 2017	File Name	D:\BN\output\F19\F_2017\2017.06.07\BM-1106_20170607_01\FLUORINE_01		
Frequency (MHz)	376.31	Nucleus	¹⁹ F	Number of Transients	16	Original Points Count	65536
Points Count	65536	Pulse Sequence	s2pul	Solvent	CHLOROFORM-D		
Sweep Width (Hz)	89285.71	Temperature (degree C)	25.000				



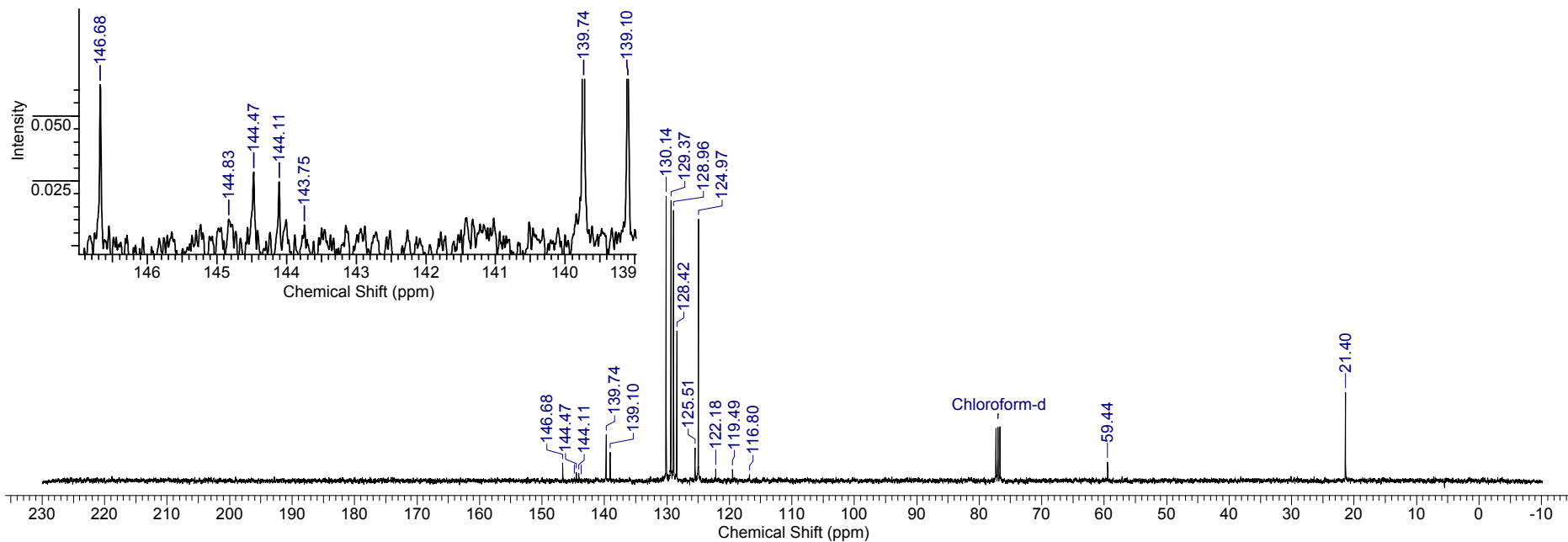
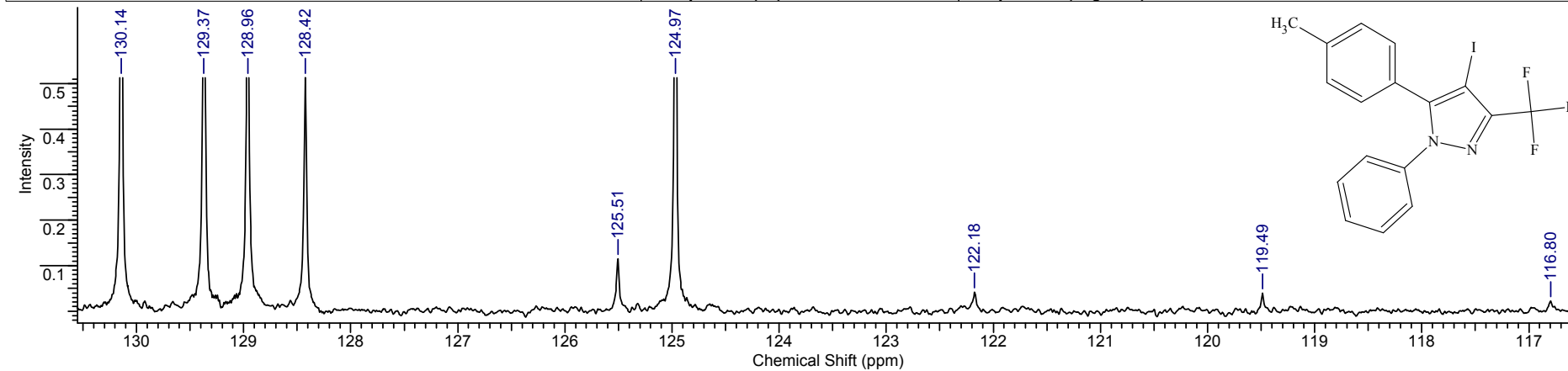
FW 428.1903 Formula C₁₇H₁₂F₃IN₂

Acquisition Time (sec)	2.5559	Comment	Imported from UXNMR.		Date	02 Jun 2017 15:27:22	
File Name	D:\BN\output\2017\06.epi\BM-1099.H_001001r	Frequency (MHz)	400.13	Nucleus	1H	Number of Transients	4
Original Points Count	16384	Points Count	65536	Pulse Sequence	zg30	Solvent	CHLOROFORM-D
Sweep Width (Hz)	6410.26	Temperature (degree C)	27.000				



FW 428.1903 **Formula** C₁₇H₁₂F₃IN₂

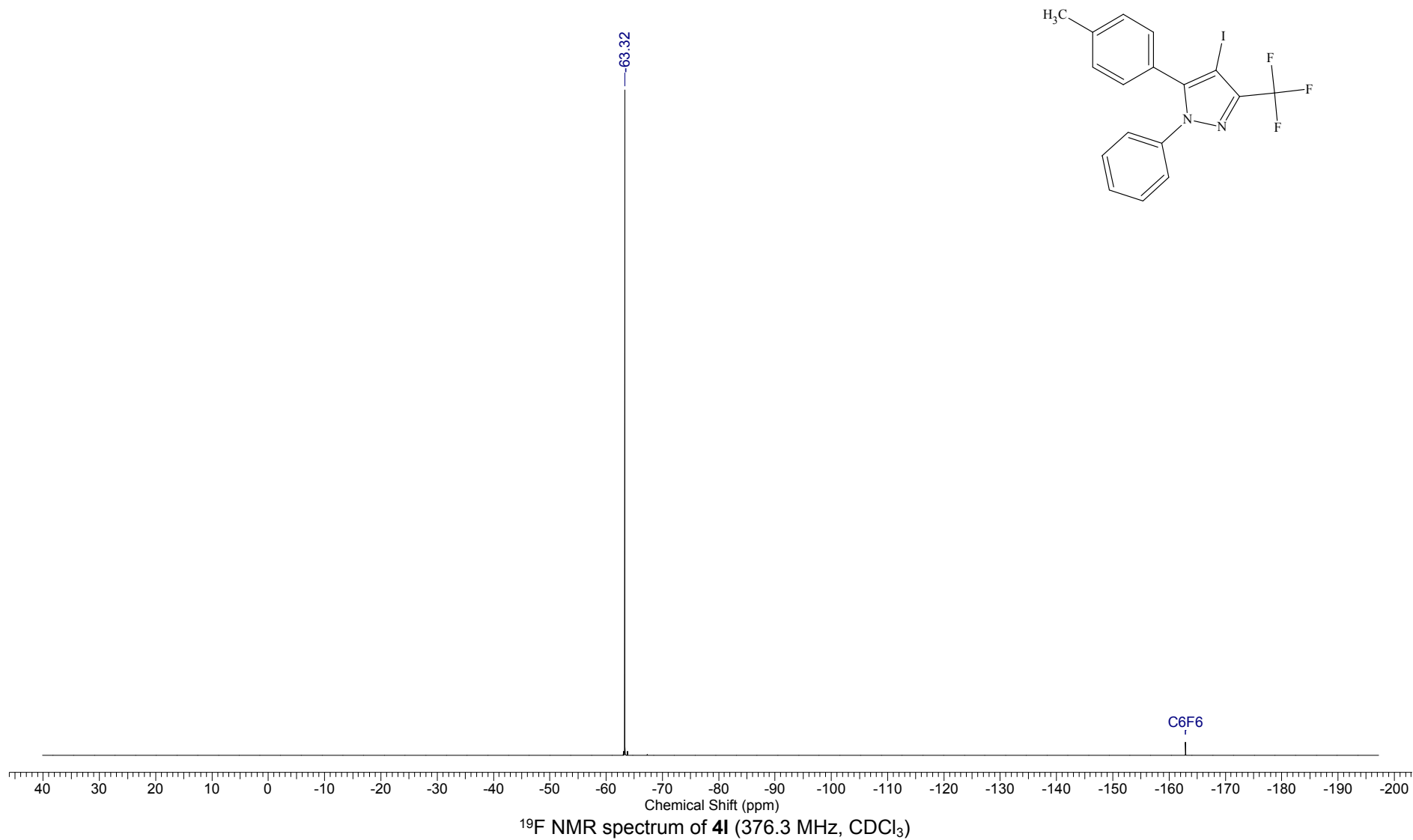
Acquisition Time (sec)	0.4999	Comment	Imported from UXMNR.	Date	02 Jun 2017 15:31:02
File Name	D:\BN\output\2017\06.epi\BM-1099.C_002001r	Frequency (MHz)	100.61	Nucleus	¹³ C
Number of Transients	116	Original Points Count	12076	Points Count	65536
Solvent	CHLOROFORM-D	Sweep Width (Hz)	24154.59	Pulse Sequence	zgpg30
		Temperature (degree C)	27.000		



¹³C NMR spectrum of **4I** (100.6 MHz, CDCl₃)

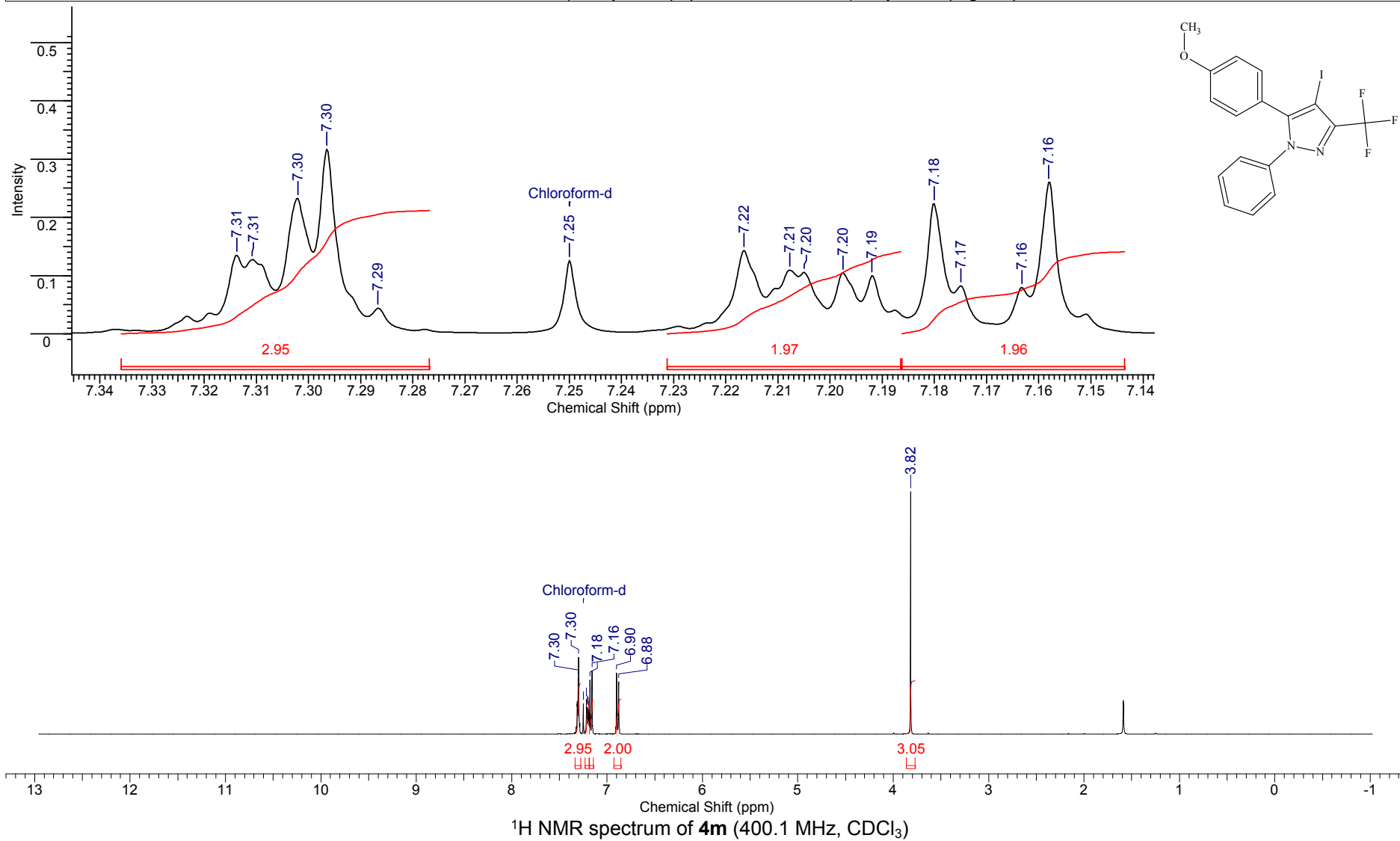
FW	428.1903	Formula	C ₁₇ H ₁₂ F ₃ IN ₂
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Acquisition Time (sec)	1.5729	Date	Jun 8 2017	File Name	D:\BN\output\F19\F_2017\2017.06.08\BM-1099-F_20170608_01\FLUORINE_01		
Frequency (MHz)	376.31	Nucleus	19F	Number of Transients	8	Original Points Count	140434
Points Count	262144	Pulse Sequence	s2pul	Solvent	CHLOROFORM-D		
Sweep Width (Hz)	89285.71	Temperature (degree C)	22.000				



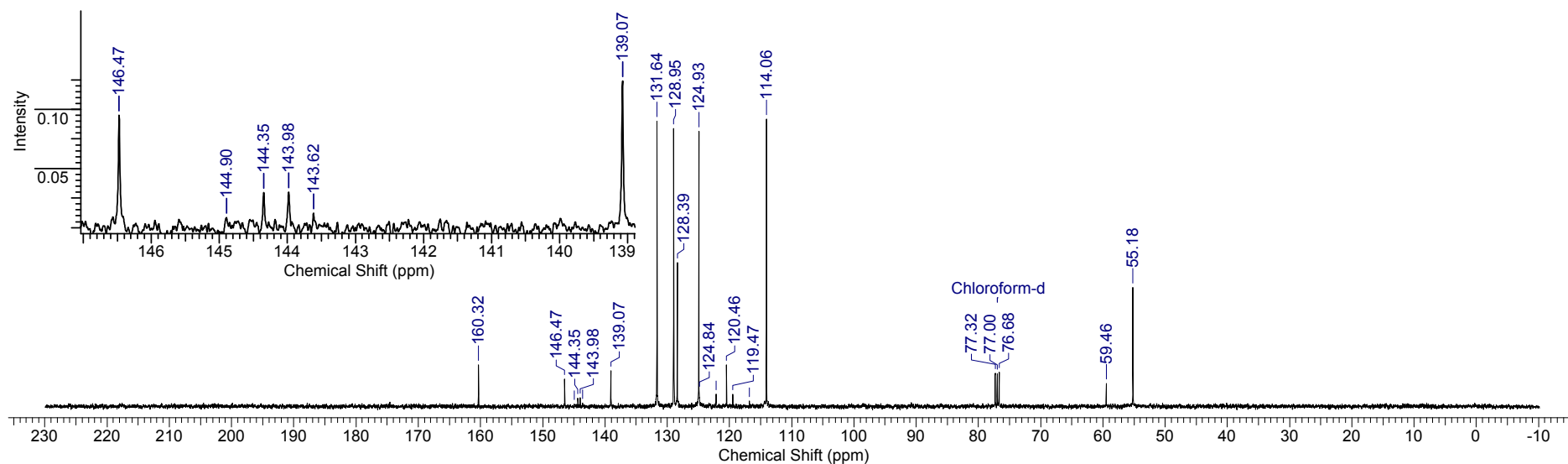
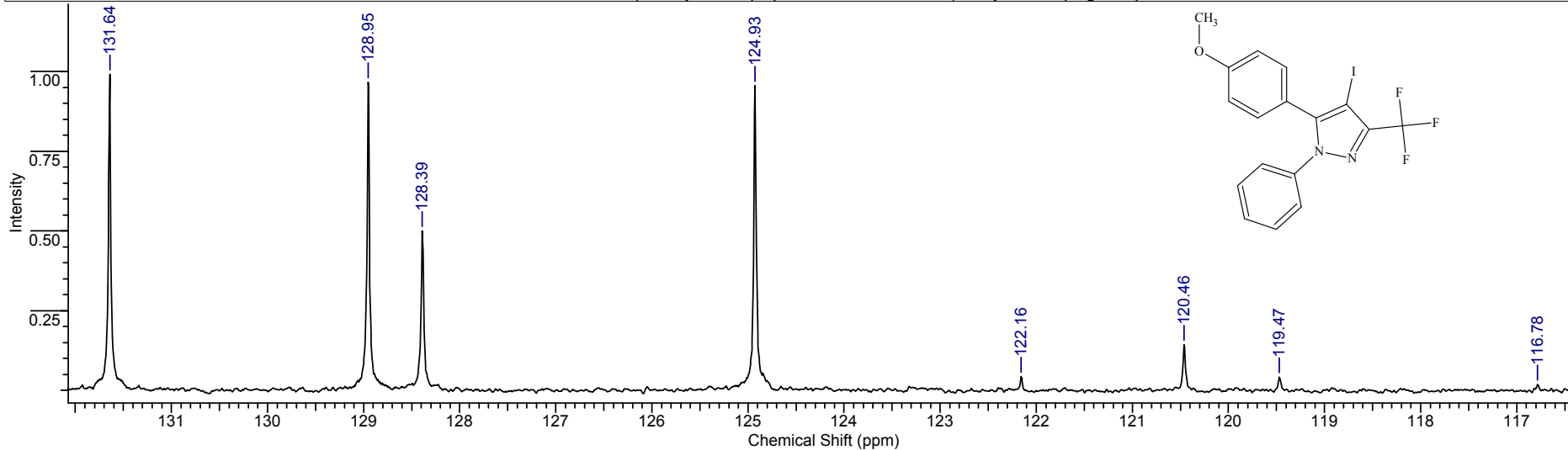
FW 444.1897 **Formula** C₁₇H₁₂F₃IN₂O

Acquisition Time (sec)	2.9295	Comment	Imported from UXNMR.	Date	24 May 2017 23:15:02
File Name	D:\BN\output\2017\05.i à\BM-1076\BM-1076_001001r	Frequency (MHz)	400.13	Nucleus	¹ H
Number of Transients	8	Original Points Count	16384	Points Count	65536
Solvent	CHLOROFORM-D	Sweep Width (Hz)	5592.84	Pulse Sequence	zg30
				Temperature (degree C)	27.000



FW 444.1897 **Formula** C₁₇H₁₂F₃IN₂O

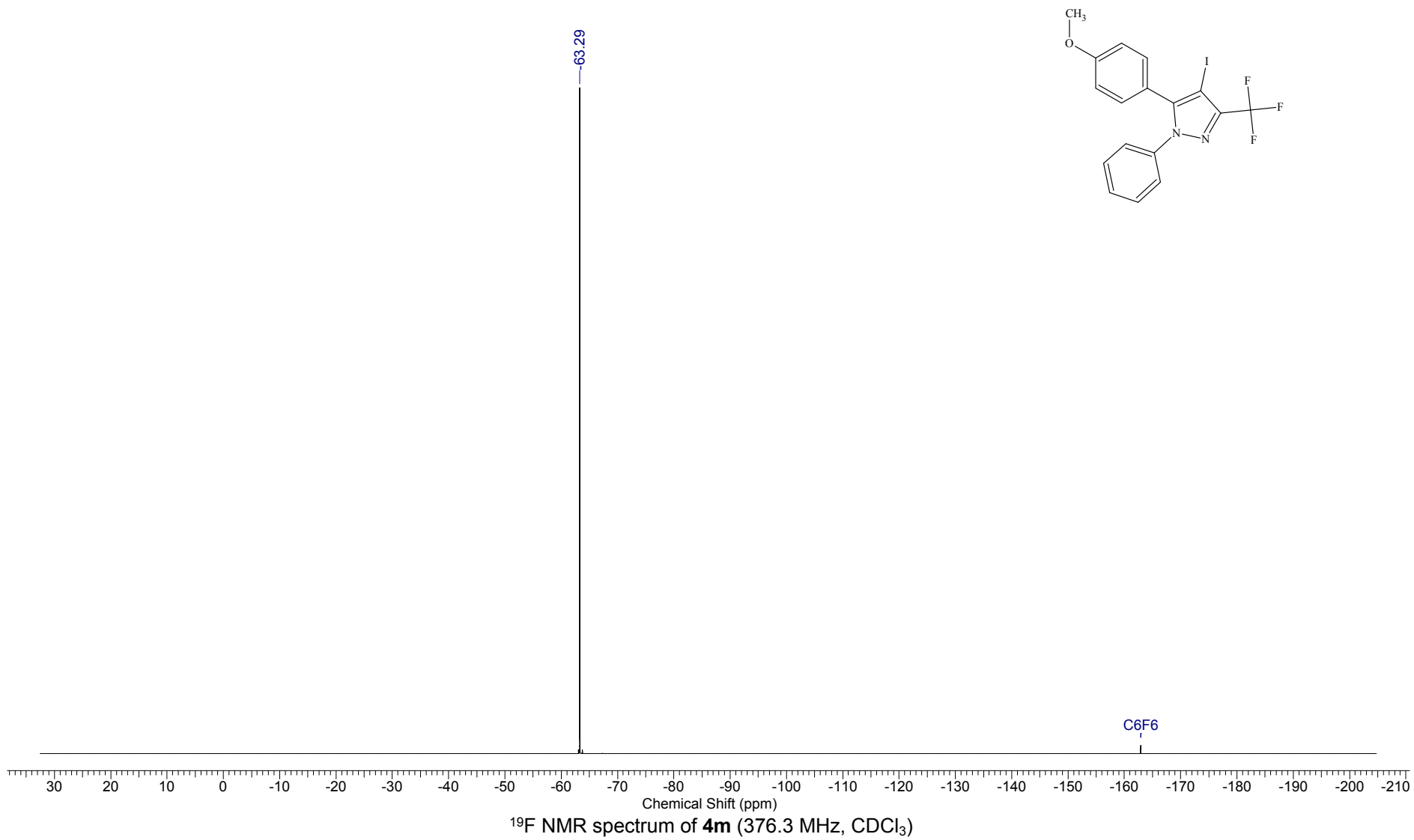
Acquisition Time (sec)	0.4999	Comment	Imported from UXNMR.	Date	25 May 2017 17:43:48
File Name	D:\BN\output\2017\05.i à à\BM-1076.C_002001r	Frequency (MHz)	100.61	Nucleus	13C
Number of Transients	64	Original Points Count	12076	Points Count	65536
Solvent	CHLOROFORM-D	Sweep Width (Hz)	24154.59	Pulse Sequence	zgpg30
				Temperature (degree C)	27.000



¹³C NMR spectrum of **4m** (100.6 MHz, CDCl₃)

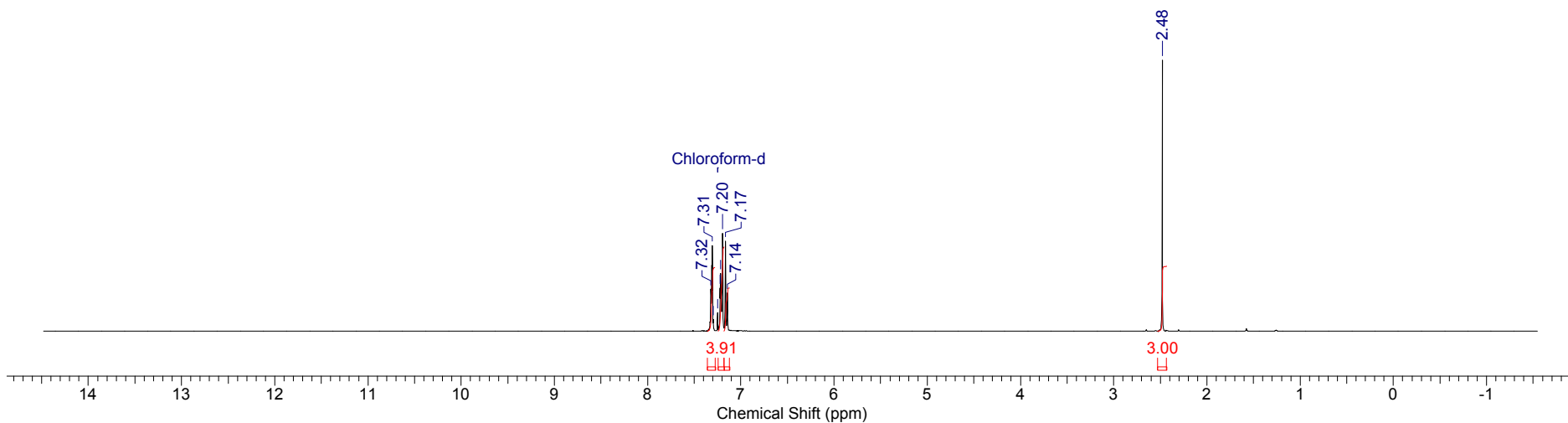
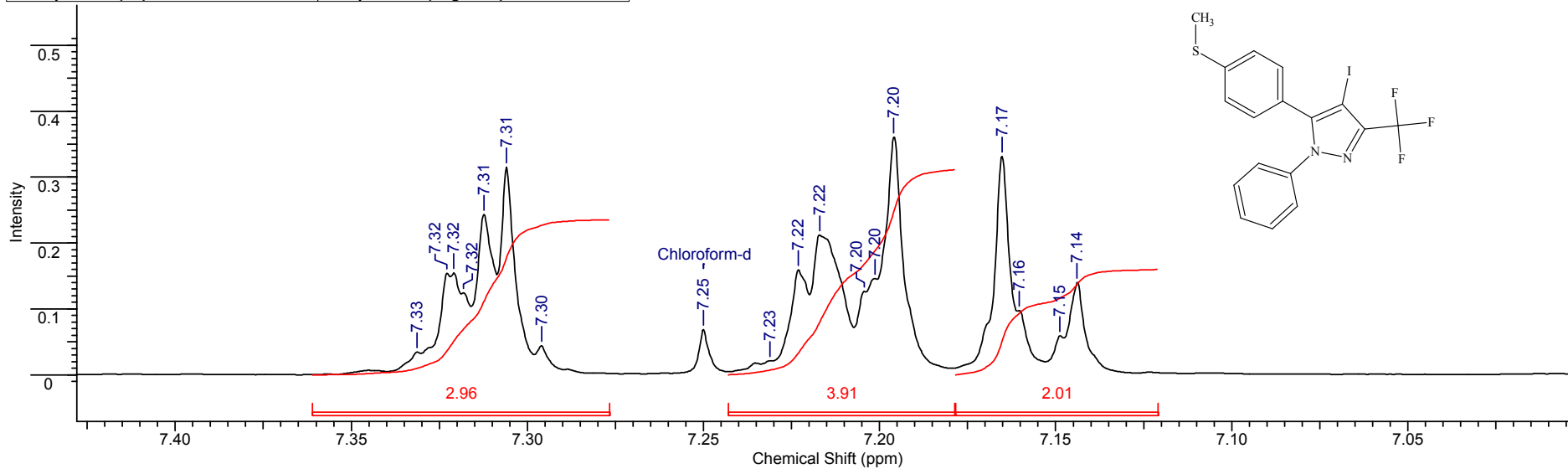
FW	444.1897	Formula	C ₁₇ H ₁₂ F ₃ IN ₂ O
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Acquisition Time (sec)	1.5000	Date	May 29 2017	File Name	D:\BN\output\F19\F_2017\2017.05.29\BM-1076_20170529_01\FLUORINE_01		
Frequency (MHz)	376.31	Nucleus	¹⁹ F	Number of Transients	16	Original Points Count	133929
Points Count	262144	Pulse Sequence	s2pul	Solvent	BENZENE-D6	Sweep Width (Hz)	89285.71
Temperature (degree C)	25.000						



FW 460.2563 **Formula** C₁₇H₁₂F₃IN₂S

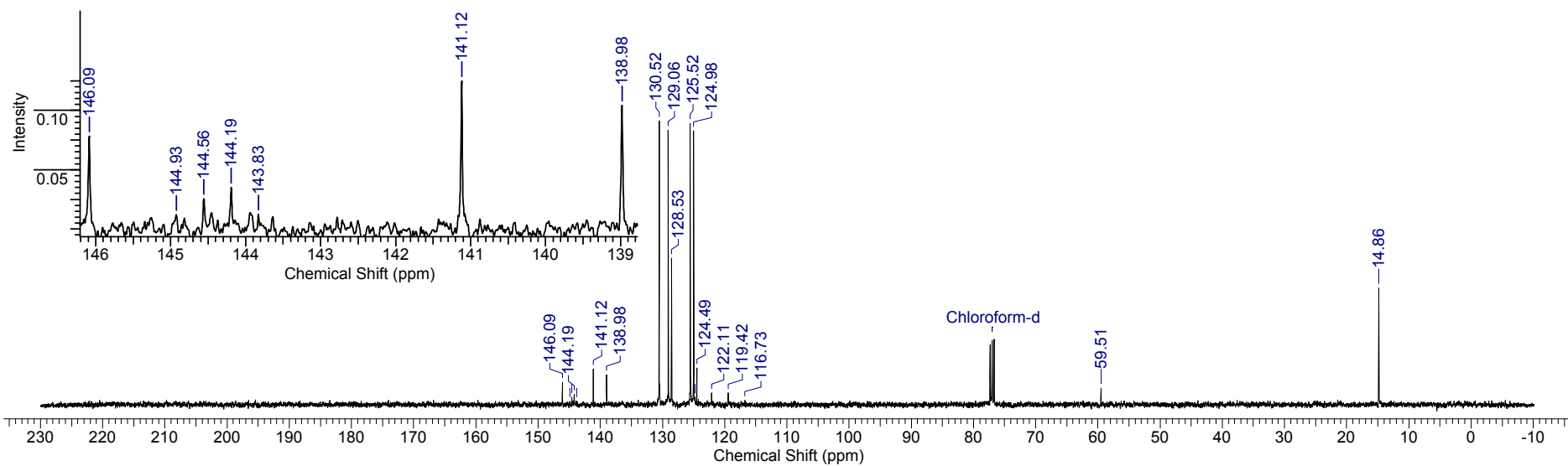
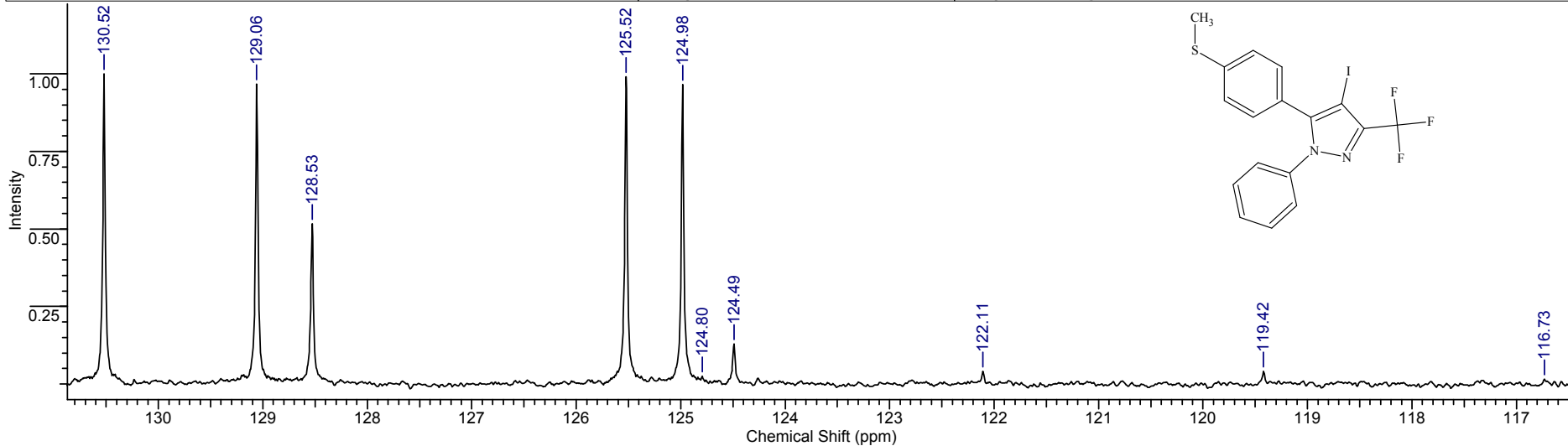
Acquisition Time (sec)	2.5559	Comment	Imported from UXNMR.		Date	02 Jun 2017 15:21:52	
File Name	D:\BN\output\2017\06.epi\BM-1098.H_001001r	Frequency (MHz)	400.13	Nucleus	1H	Number of Transients	4
Original Points Count	16384	Points Count	65536	Pulse Sequence	zg30	Solvent	CHLOROFORM-D
Sweep Width (Hz)	6410.26	Temperature (degree C)	27.000				



¹H NMR spectrum of **4n** (400.1 MHz, CDCl₃)

FW 460.2563 **Formula** C₁₇H₁₂F₃I₂S

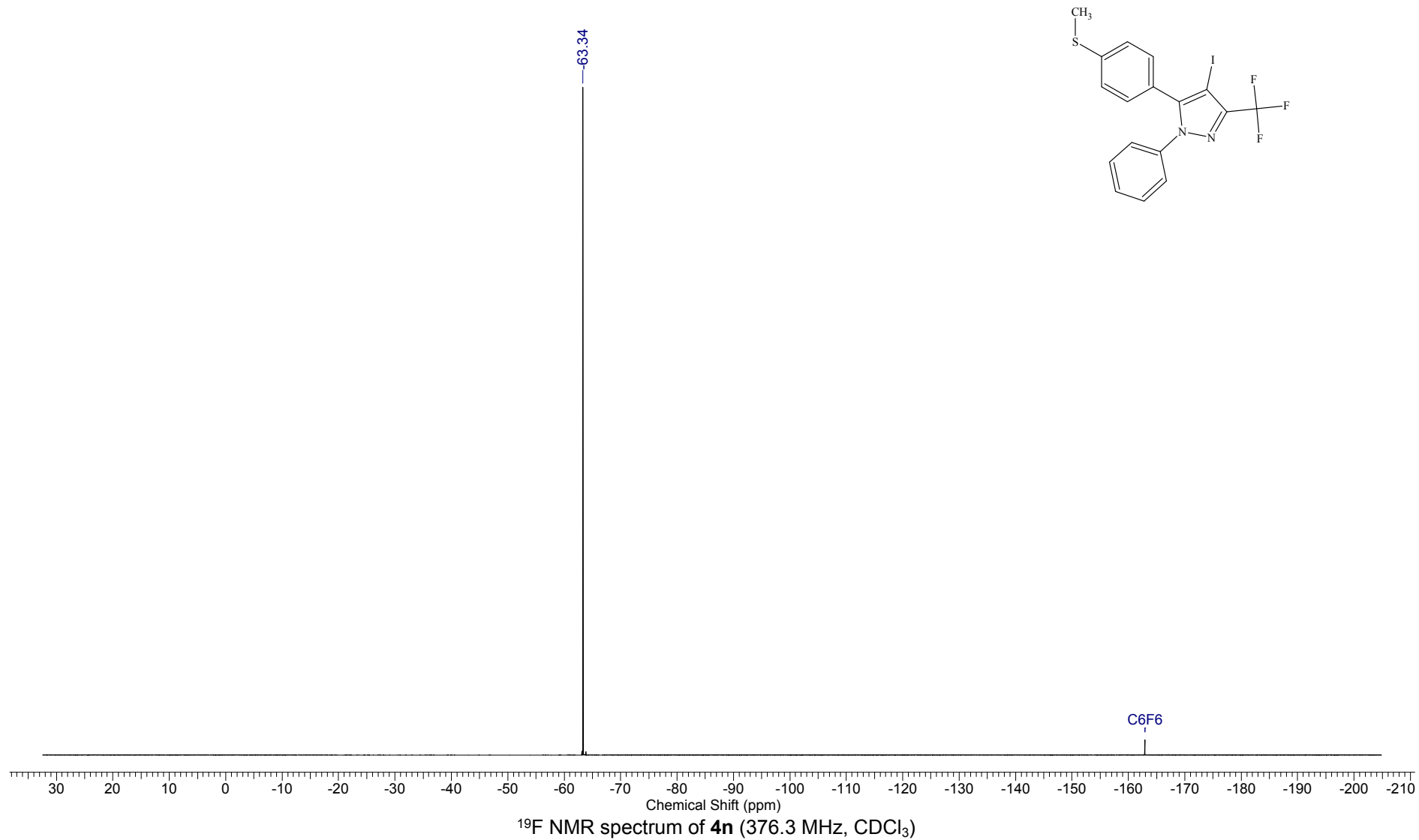
Acquisition Time (sec)	0.4999	Comment	Imported from UXNMR.		Date	02 Jun 2017 15:25:52
File Name	D:\BN\output\2017\06.ep f \BM-1098.C_002001r	Frequency (MHz)	100.61	Nucleus	13C	
Number of Transients	128	Original Points Count	12076	Points Count	Pulse Sequence zgpg30	
Solvent	CHLOROFORM-D	Sweep Width (Hz)	24154.59	Temperature (degree C)	27.000	



¹³C NMR spectrum of **4n** (100.6 MHz, CDCl₃)

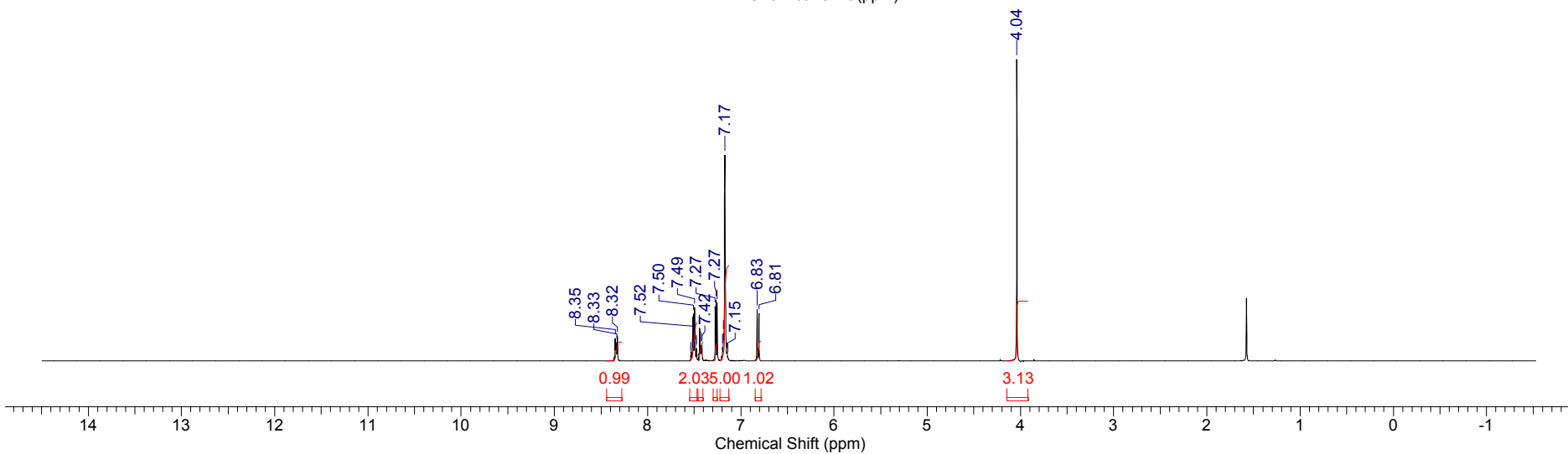
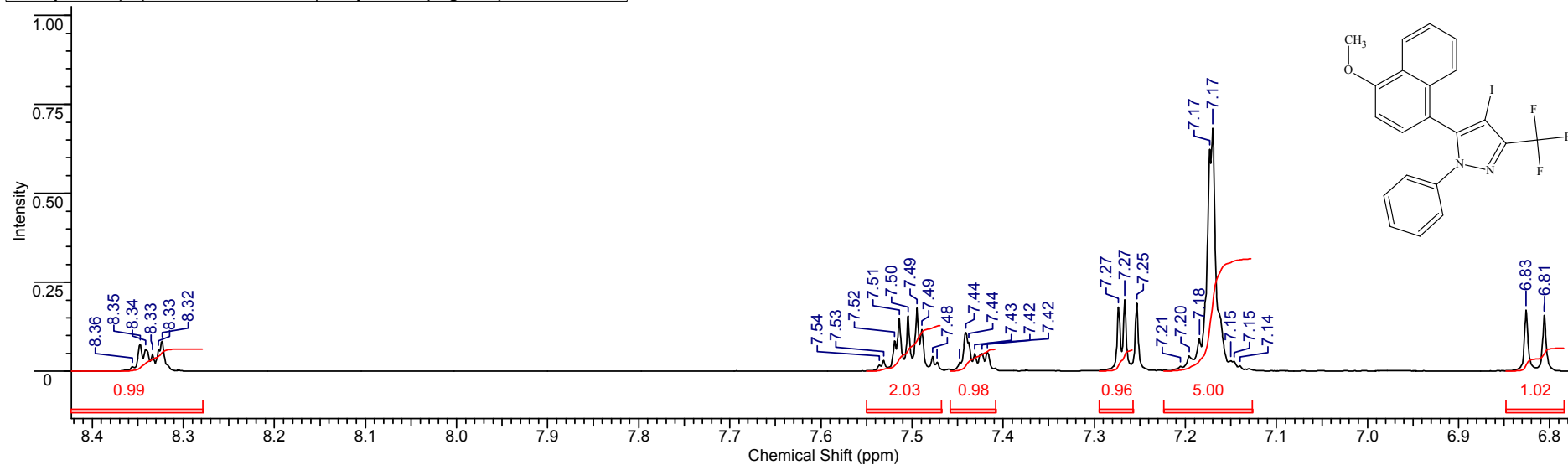
FW	460.2563	Formula	C ₁₇ H ₁₂ F ₃ IN ₂ S
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Acquisition Time (sec)	0.7340	Date	Jun 7 2017	File Name	D:\BN\output\F19\F_2017\2017.06.07\BM-1098_20170607_01\FLUORINE_01		
Frequency (MHz)	376.31	Nucleus	¹⁹ F	Number of Transients	16	Original Points Count	65536
Points Count	65536	Pulse Sequence	s2pul	Solvent	CHLOROFORM-D		
Sweep Width (Hz)	89285.71	Temperature (degree C)	25.000				



FW	494.2484	Formula	C ₂₁ H ₁₄ F ₃ IN ₂ O
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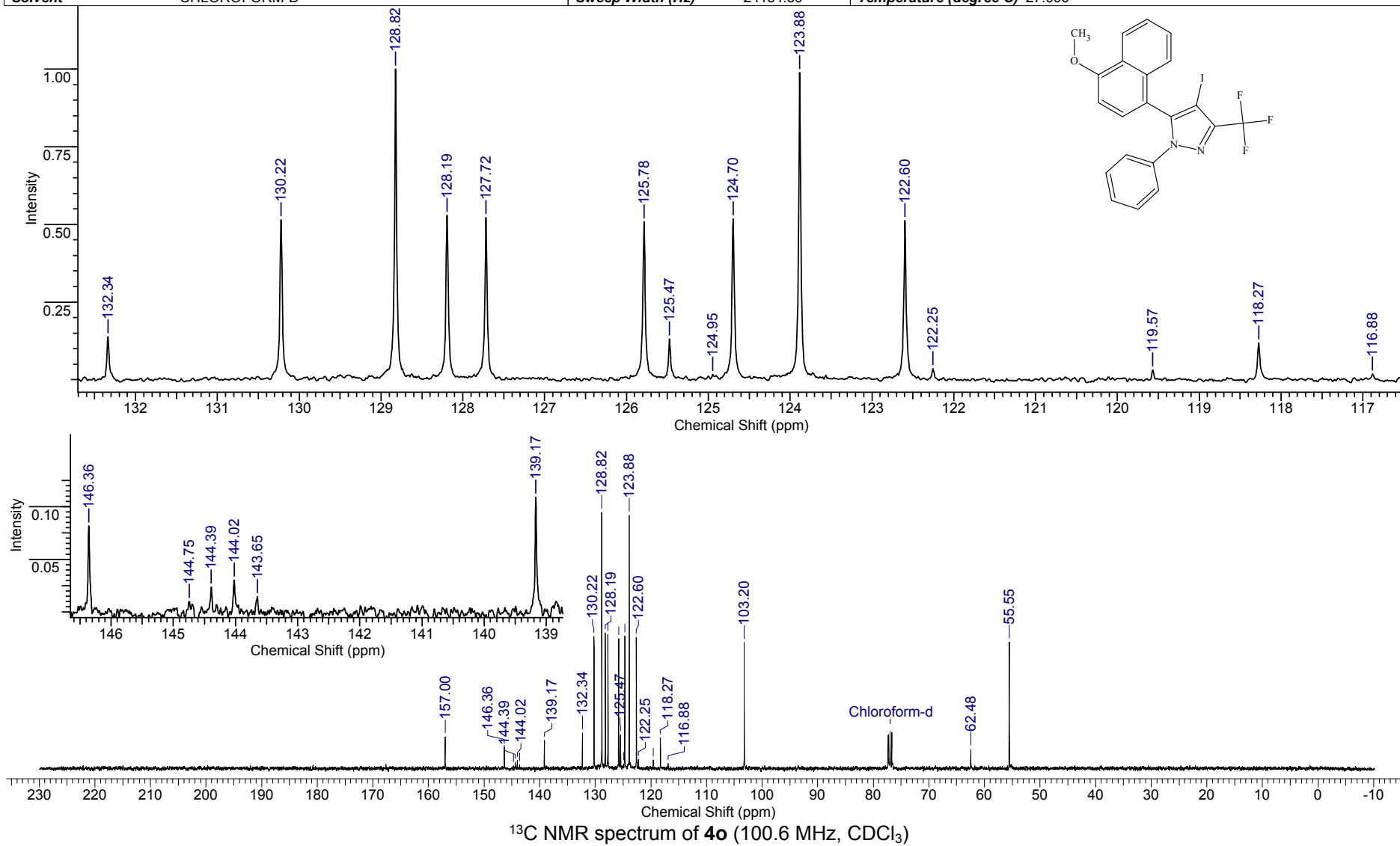
Acquisition Time (sec)	2.5559	Comment	Imported from UXNMR.		Date	23 May 2017 15:47:42	
File Name	D:\BN\output\2017\05.i àé\BM-1075.H_001001r	Frequency (MHz)	400.13	Nucleus	1H	Number of Transients	4
Original Points Count	16384	Points Count	65536	Pulse Sequence	zg30	Solvent	CHLOROFORM-D
Sweep Width (Hz)	6410.26	Temperature (degree C)	27.000				



¹H NMR spectrum of **4o** (400.1 MHz, CDCl₃)

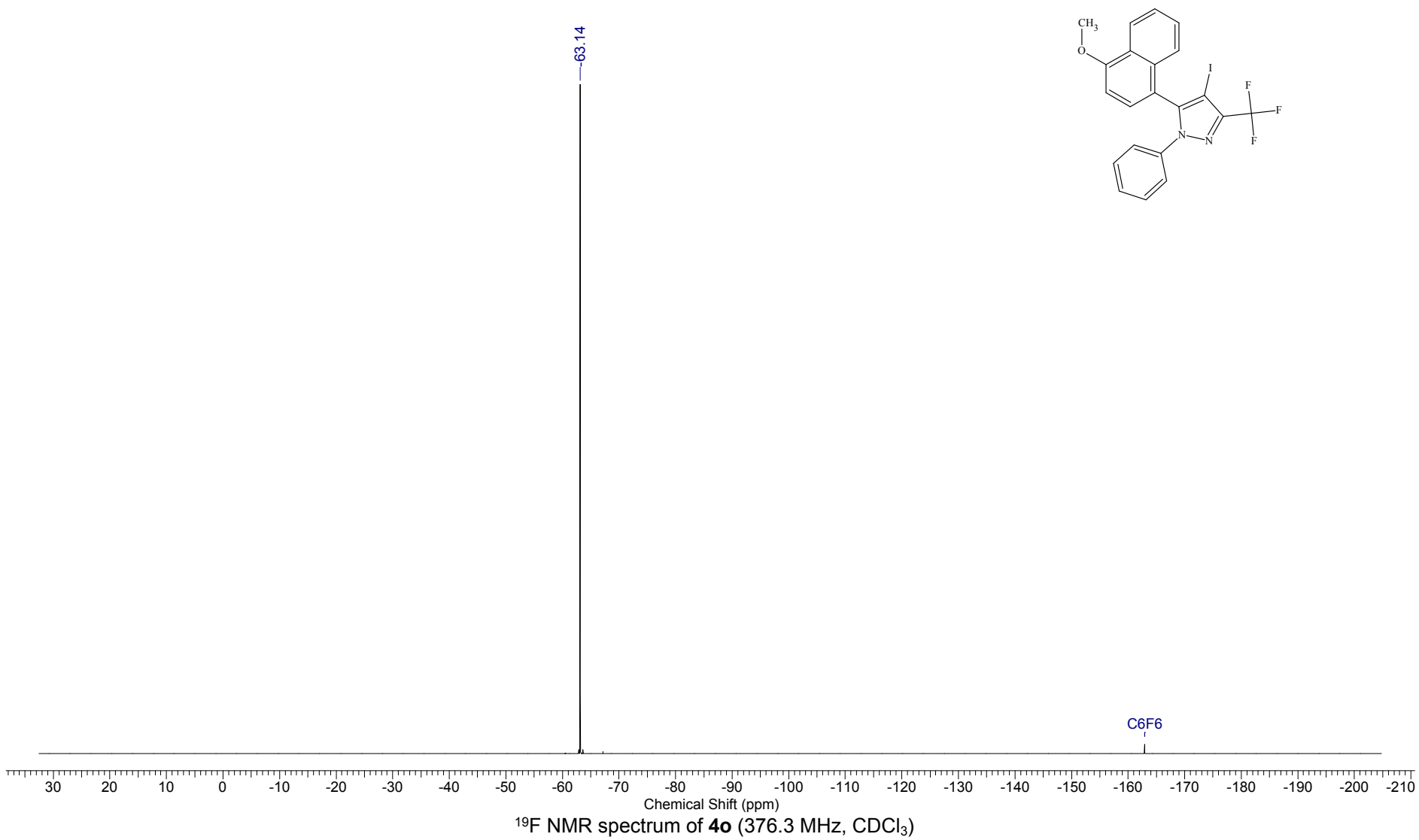
FW 494.2484 **Formula** C₂₁H₁₄F₃IN₂O

Acquisition Time (sec)	0.4999	Comment	Imported from UXMNR.	Date	24 May 2017 17:20:48
File Name	D:\BN\output\2017\05.i à\BM-1075.C_002001r	Frequency (MHz)	100.61	Nucleus	13C
Number of Transients	174	Original Points Count	12076	Points Count	65536
Solvent	CHLOROFORM-D	Sweep Width (Hz)	24154.59	Pulse Sequence	zgpg30
				Temperature (degree C)	27.000



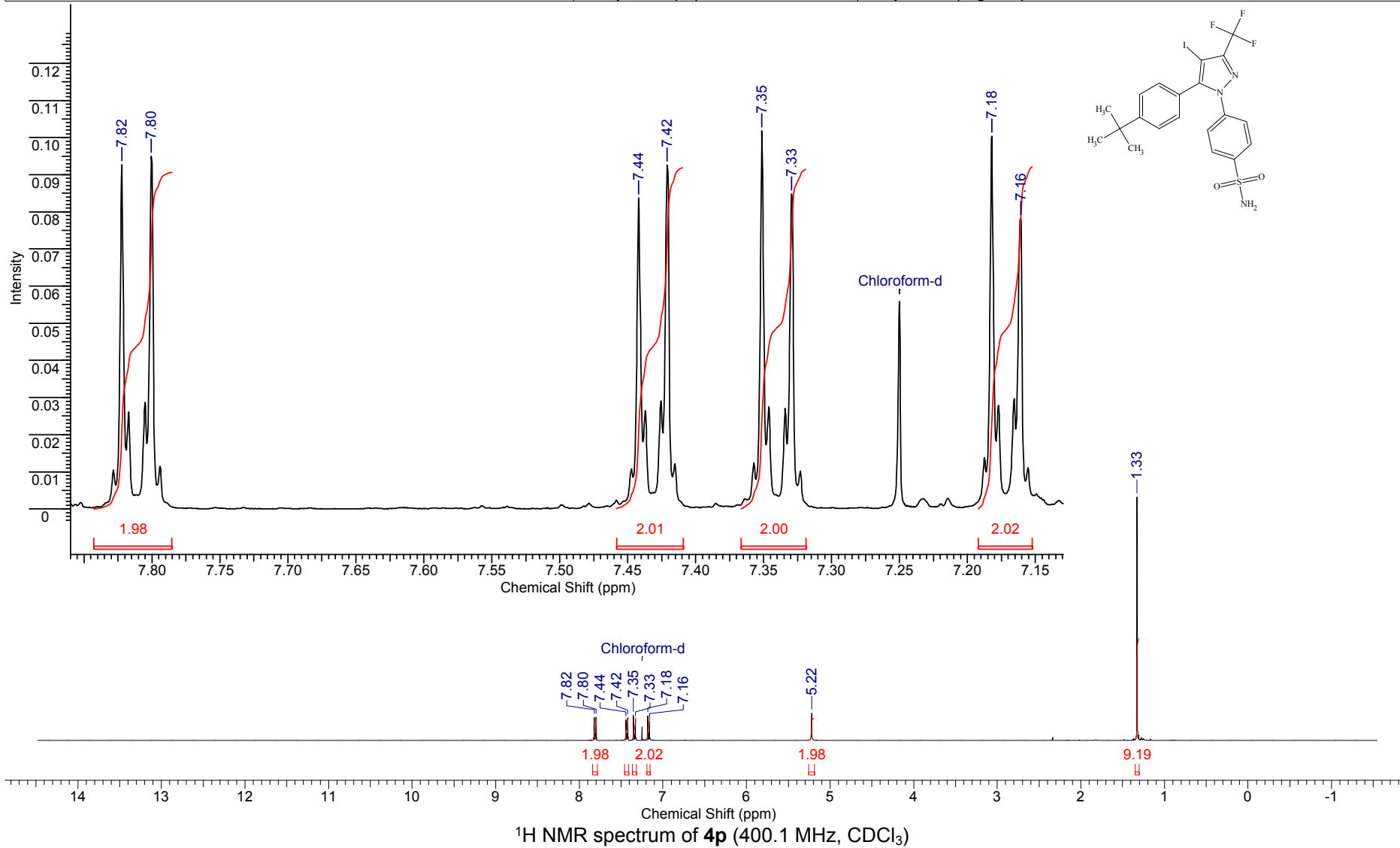
FW	494.2484	Formula	C ₂₁ H ₁₄ F ₃ IN ₂ O
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Acquisition Time (sec)	1.5000	Date	May 29 2017	File Name	D:\BN\output\F19\F_2017\2017.05.29\BM-1075_20170529_01\FLUORINE_01		
Frequency (MHz)	376.31	Nucleus	¹⁹ F	Number of Transients	16	Original Points Count	133929
Points Count	262144	Pulse Sequence	s2pul	Solvent	BENZENE-D6	Sweep Width (Hz)	89285.71
Temperature (degree C)	25.000						



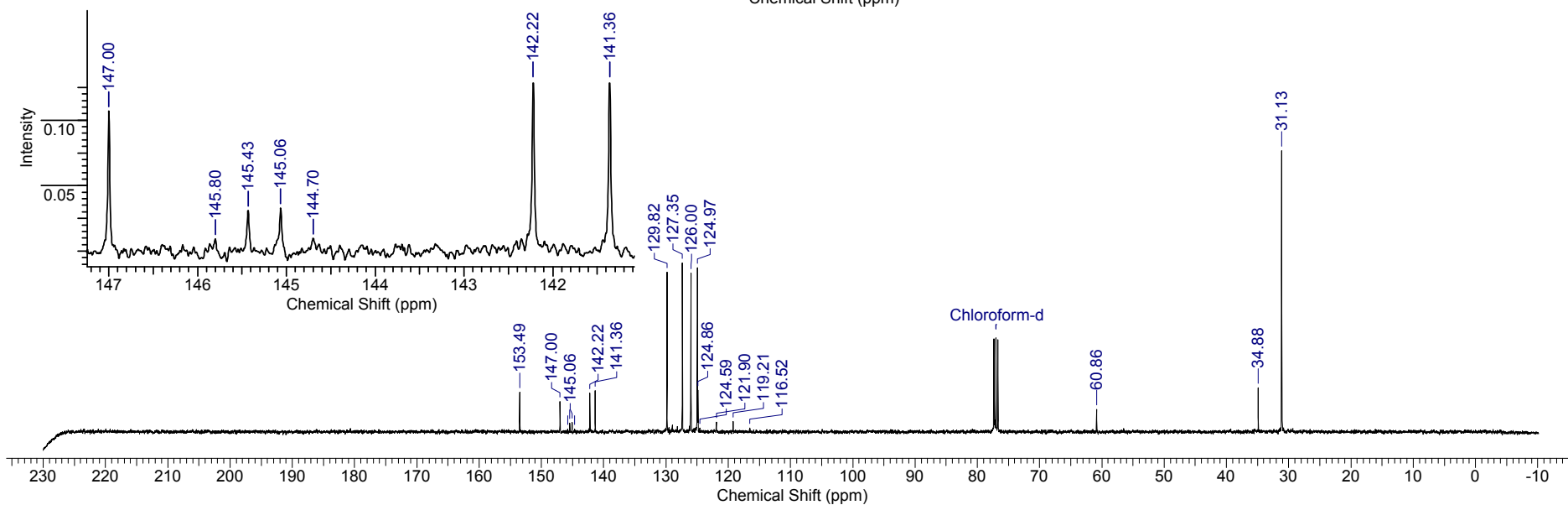
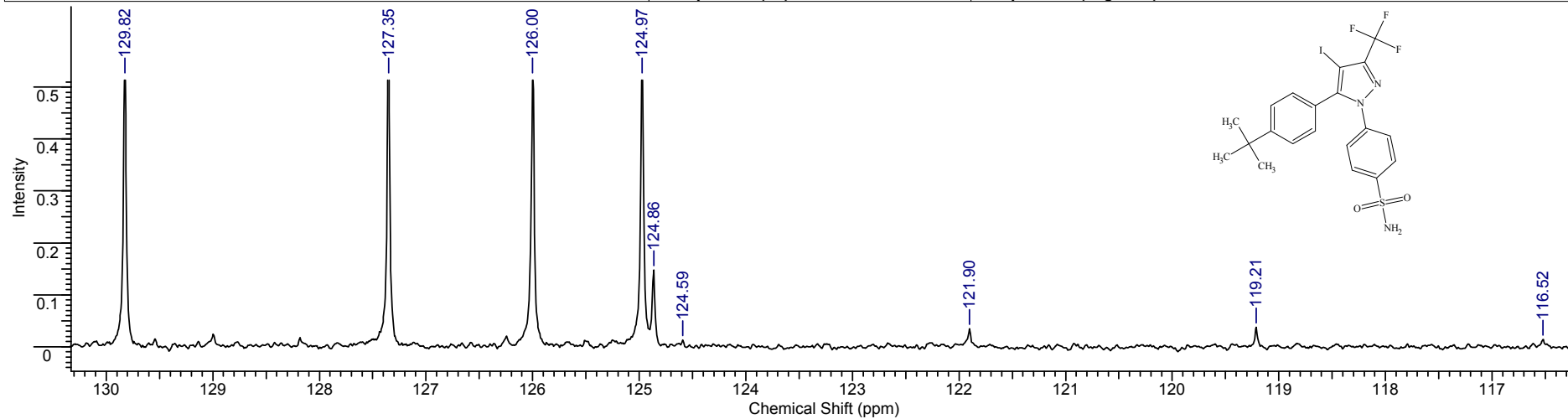
FW 549.3496 **Formula** C₂₀H₁₉F₃IN₃O₂S

Acquisition Time (sec)	2.5559	Comment	Imported from UXNMR.	Date	17 Apr 2014 18:38:56
File Name	C:\IBM_DATA\DOCS\SPEC_BM_H\CIBM-476.H_001001r	Frequency (MHz)	400.13	Nucleus	¹ H
Number of Transients	4	Original Points Count	16384	Points Count	65536
Solvent	CHLOROFORM-D	Sweep Width (Hz)	6410.26	Pulse Sequence	zg30
		Temperature (degree C)		Temperature (degree C)	27.000



FW	549.3496	Formula	C ₂₀ H ₁₉ F ₃ IN ₃ O ₂ S
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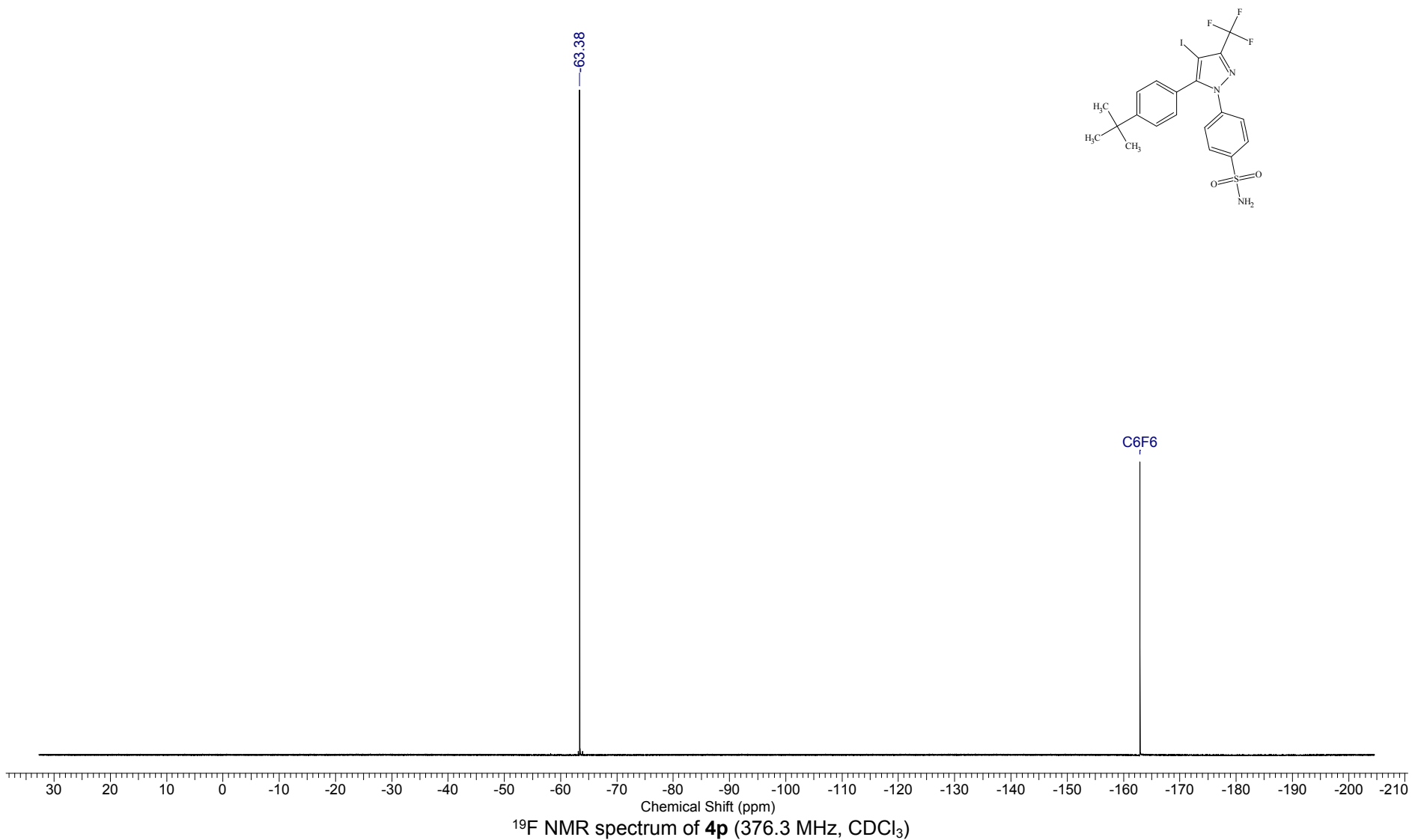
Acquisition Time (sec)	0.4999	Comment	Imported from UXNMR.		Date	17 Apr 2014 18:48:16
File Name	C:\BM_DATA\DOCS\SPEC_BM_H,C\BM-476.C_002001r	Frequency (MHz)	100.61	Nucleus	13C	
Number of Transients	256	Original Points Count	12076	Points Count	65536	
Solvent	CHLOROFORM-D	Sweep Width (Hz)	24154.59	Pulse Sequence	zpgp30	
				Temperature (degree C)	27.000	



¹³C NMR spectrum of **4p** (100.6 MHz, CDCl₃)

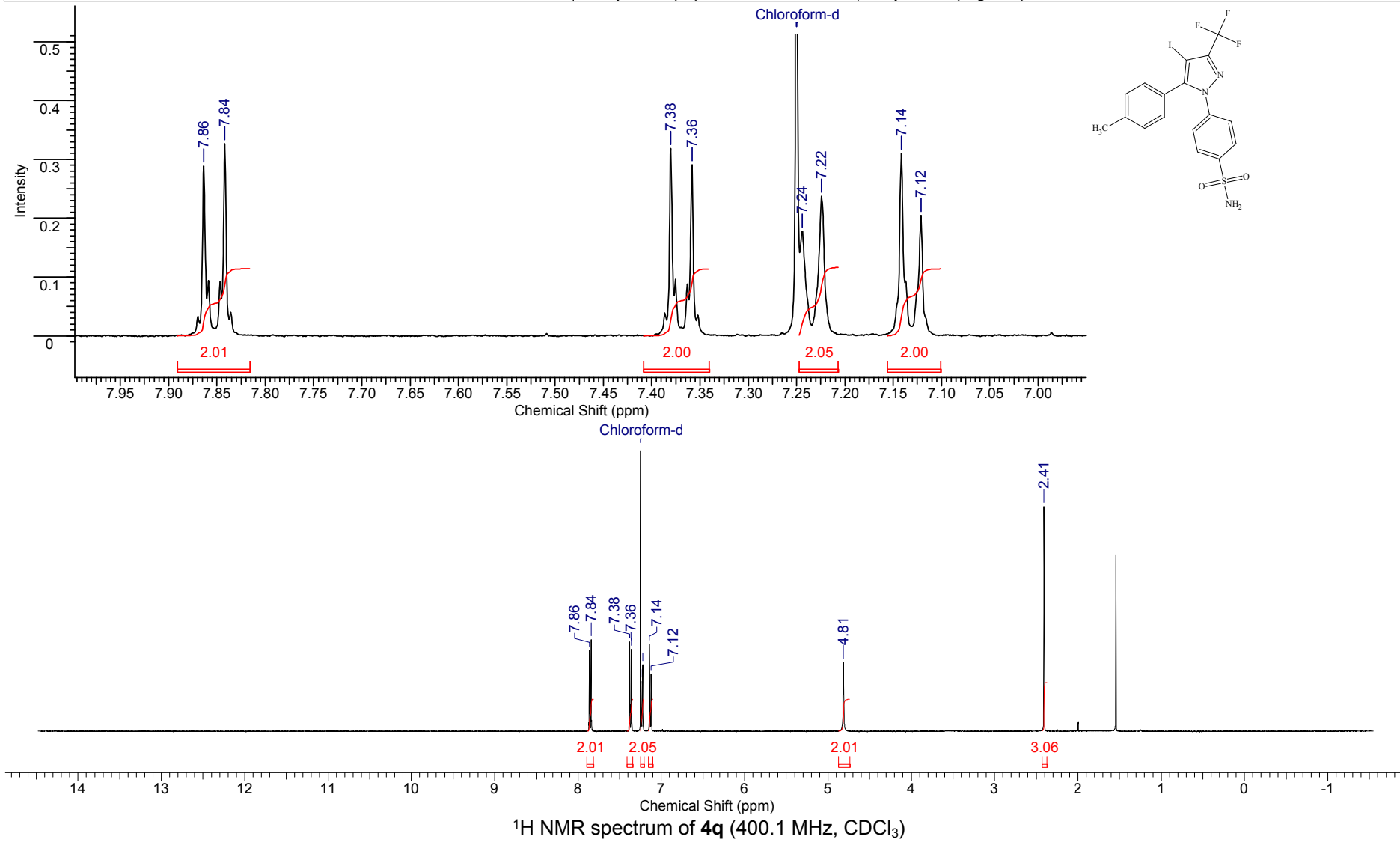
FW	549.3496	Formula	C ₂₀ H ₁₉ F ₃ IN ₃ O ₂ S
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Acquisition Time (sec)	1.0000	Date	Apr 11 2014	File Name	C:\BM_DATA\DOCS\SPEC_BM_FBM-476_20140411_01\FLUORINE_01		
Frequency (MHz)	376.31	Nucleus	19F	Number of Transients	8	Original Points Count	89286
Points Count	131072	Pulse Sequence	s2pul	Solvent	CHLOROFORM-D		
Sweep Width (Hz)	89285.71	Temperature (degree C)	30.000				



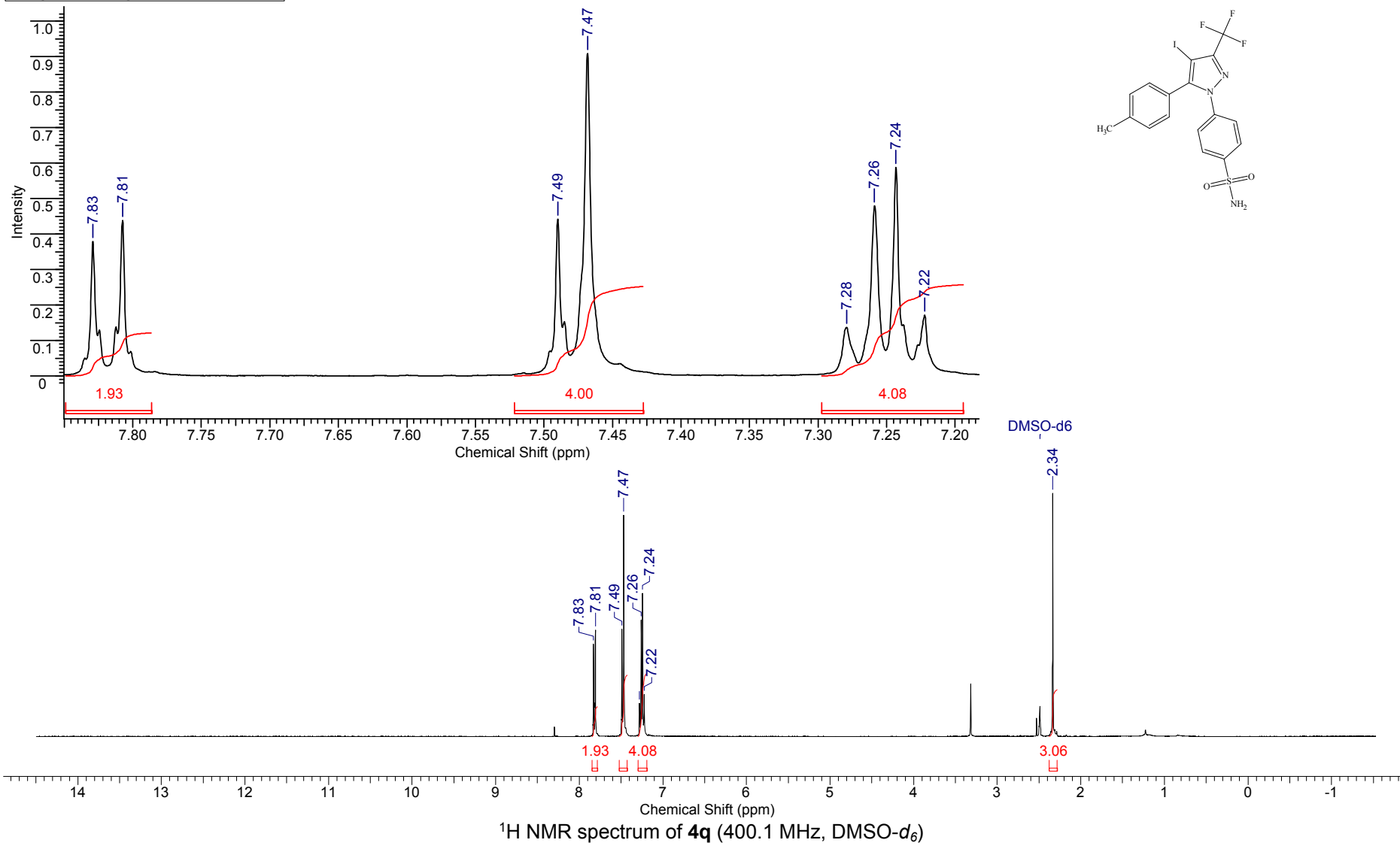
FW 507.2698 Formula C₁₇H₁₃F₃IN₃O₂S

Acquisition Time (sec)	2.5559	Comment	Imported from UXMNR.	Date	19 Jun 2014 18:58:36
File Name	C:\BM_DATA\DOCS\SPEC_BM_H\CIBM-508.H_001001r	Frequency (MHz)	400.13	Nucleus	¹ H
Number of Transients	4	Original Points Count	16384	Points Count	65536
Solvent	DEUTERIUM OXIDE	Sweep Width (Hz)	6410.26	Pulse Sequence	zg30
				Temperature (degree C)	27.000



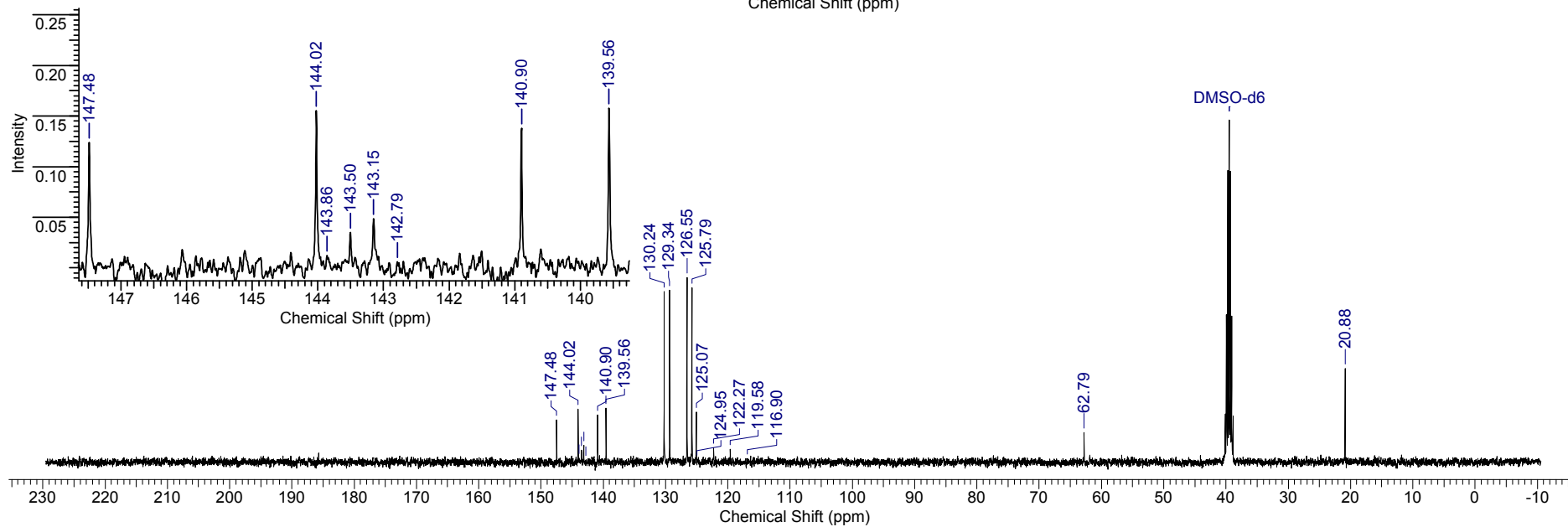
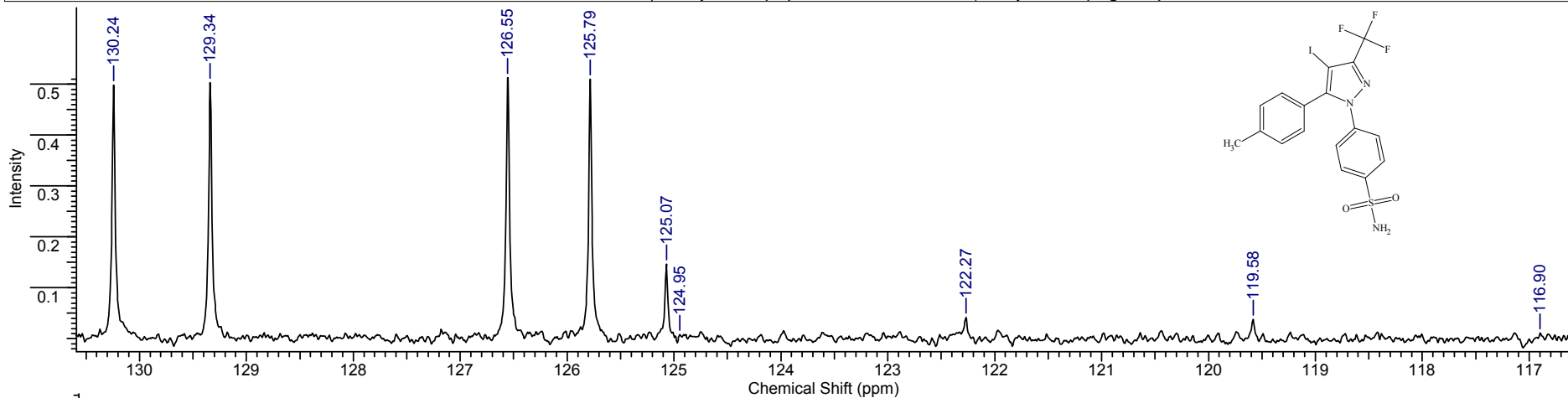
FW 507.2698 Formula C₁₇H₁₃F₃IN₃O₂S

Acquisition Time (sec)	2.5559	Comment	Imported from UXMNR.		Date	07 Jun 2014 20:29:48	
File Name	C:\IBM_DATA\DOCS\SPEC_BM_H\CIBM-499.H_001001r	Frequency (MHz)	400.13	Nucleus	1H	Number of Transients	4
Original Points Count	16384	Points Count	65536	Pulse Sequence	zg30	Solvent	DMSO-D6
Temperature (degree C)	27.000	Sweep Width (Hz)	6410.26				



FW	507.2698	Formula	C ₁₇ H ₁₃ F ₃ IN ₃ O ₂ S
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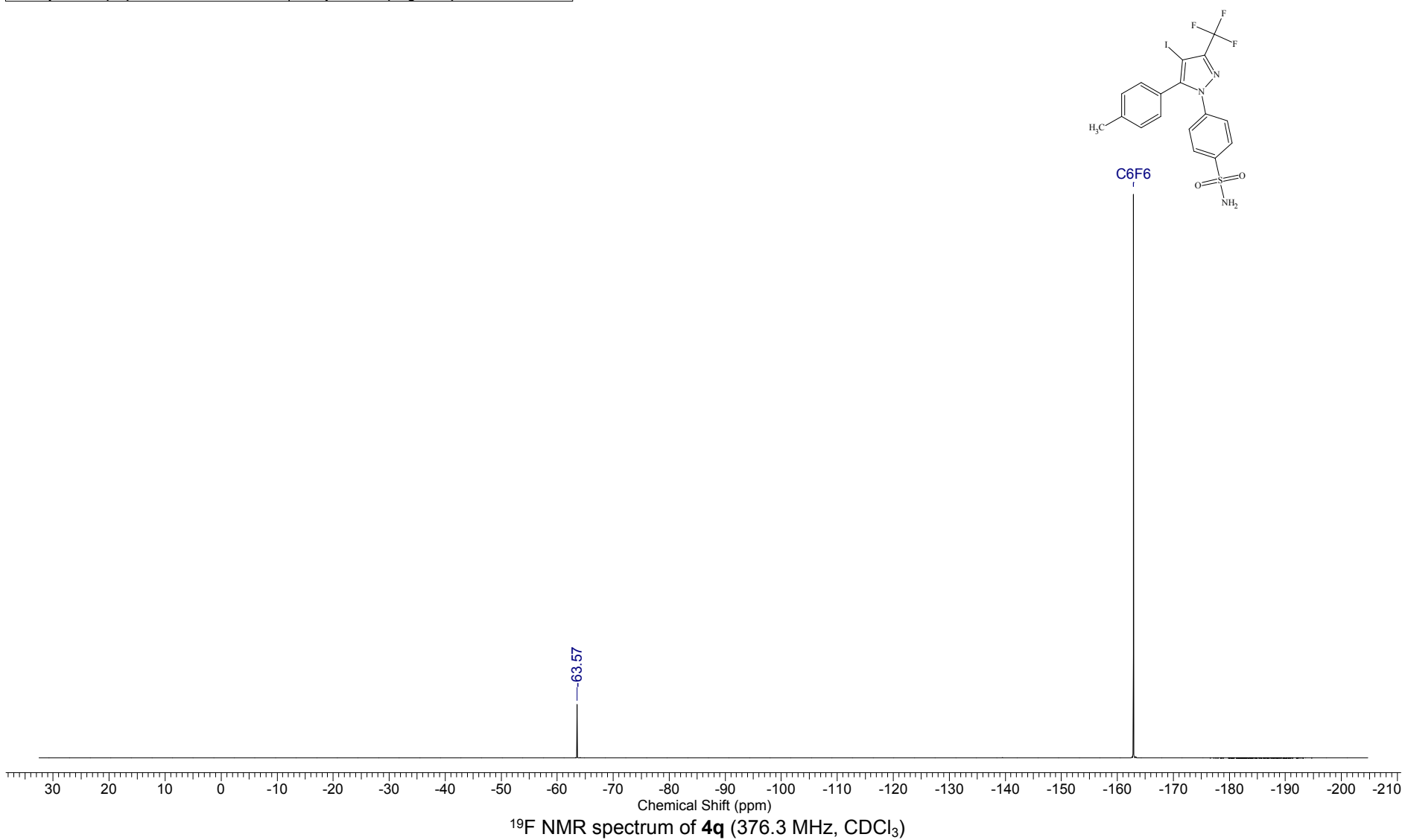
Acquisition Time (sec)	0.4999	Comment	Imported from UXMNR.		Date	07 Jun 2014 20:33:42
File Name	C:\BM_DATA\DOCS\SPEC_BM_H_C\BM-499.C_002001r	Frequency (MHz)	100.61	Nucleus	13C	
Number of Transients	120	Original Points Count	12076	Points Count	65536	
Solvent	DEUTERIUM OXIDE	Sweep Width (Hz)	24154.59	Pulse Sequence	zgpg30	
				Temperature (degree C)	27.000	



¹³C NMR spectrum of **4q** (100.6 MHz, DMSO-*d*₆)

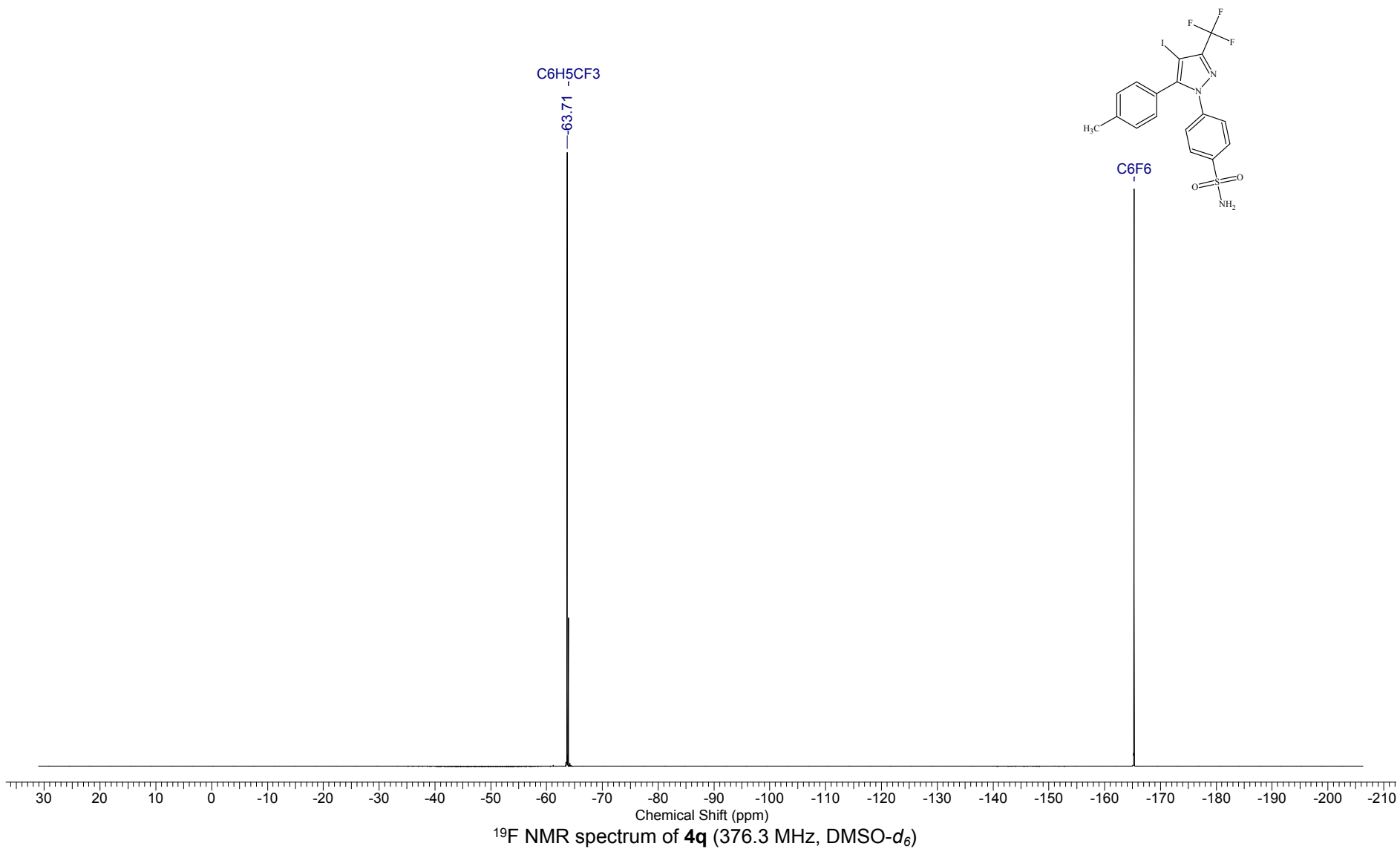
FW	507.2698	Formula	C ₁₇ H ₁₃ F ₃ IN ₃ O ₂ S
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Acquisition Time (sec)	1.0000	Date	Jun 20 2014	File Name	C:\BM_DATA\DOCS\SPEC_BM_FBM-508_20140620_01\FLUORINE_01		
Frequency (MHz)	376.31	Nucleus	¹⁹ F	Number of Transients	16	Original Points Count	89286
Points Count	131072	Pulse Sequence	s2pul	Solvent	CHLOROFORM-D		
Sweep Width (Hz)	89285.71	Temperature (degree C)	50.000				



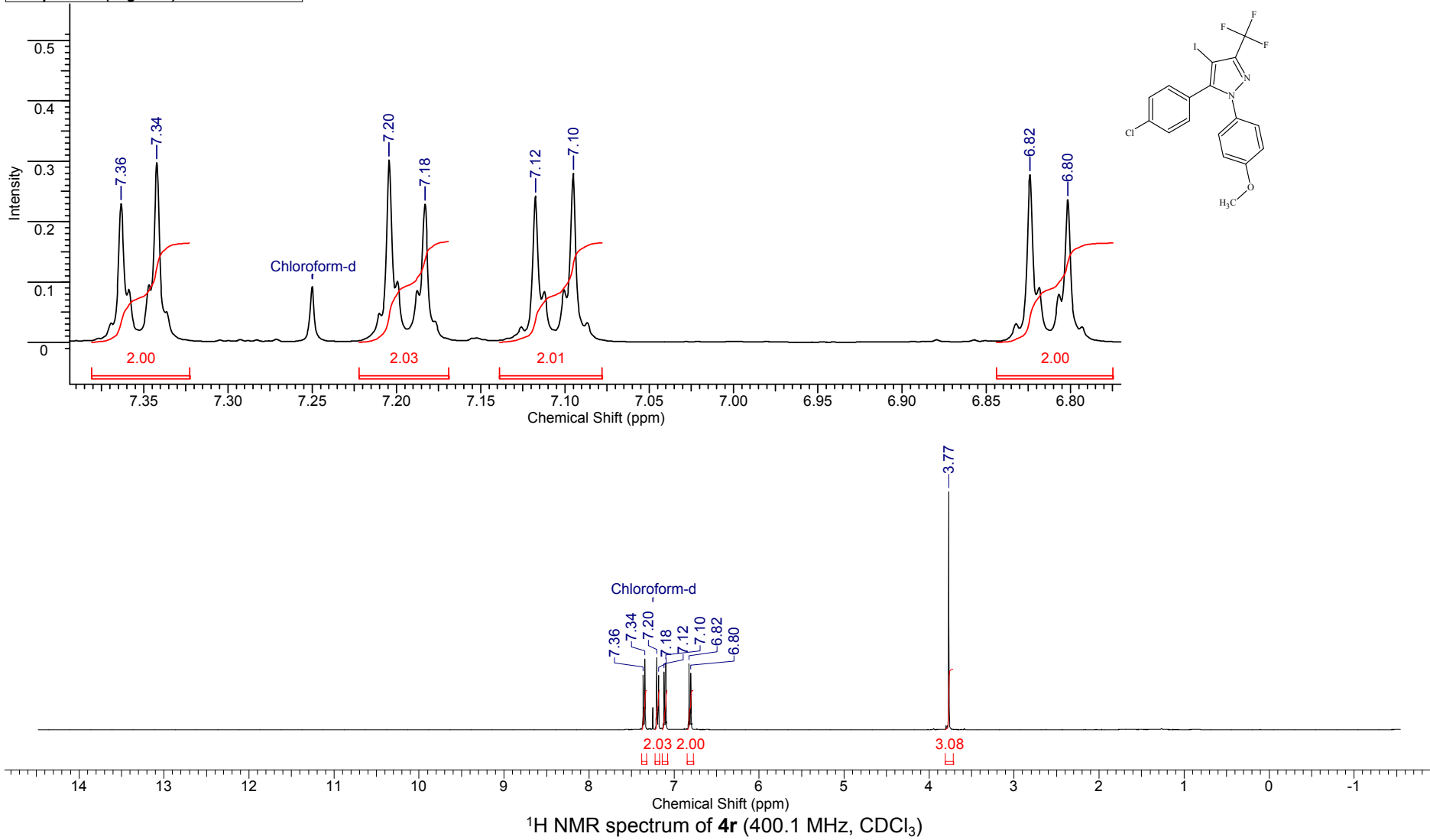
FW	507.2698	Formula	C ₁₇ H ₁₃ F ₃ IN ₃ O ₂ S
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Acquisition Time (sec)	2.0000	Date	Jun 17 2014	File Name	C:\BM_DATA\DOCS\SPEC_BM_FBM-499_20140617_01\FLUORINE_01				
Frequency (MHz)	376.31	Nucleus	¹⁹ F	Number of Transients	16	Original Points Count	178571	Points Count	262144
Pulse Sequence	s2pul	Solvent	DMSO-D6	Sweep Width (Hz)	89285.71	Temperature (degree C)	50.000		



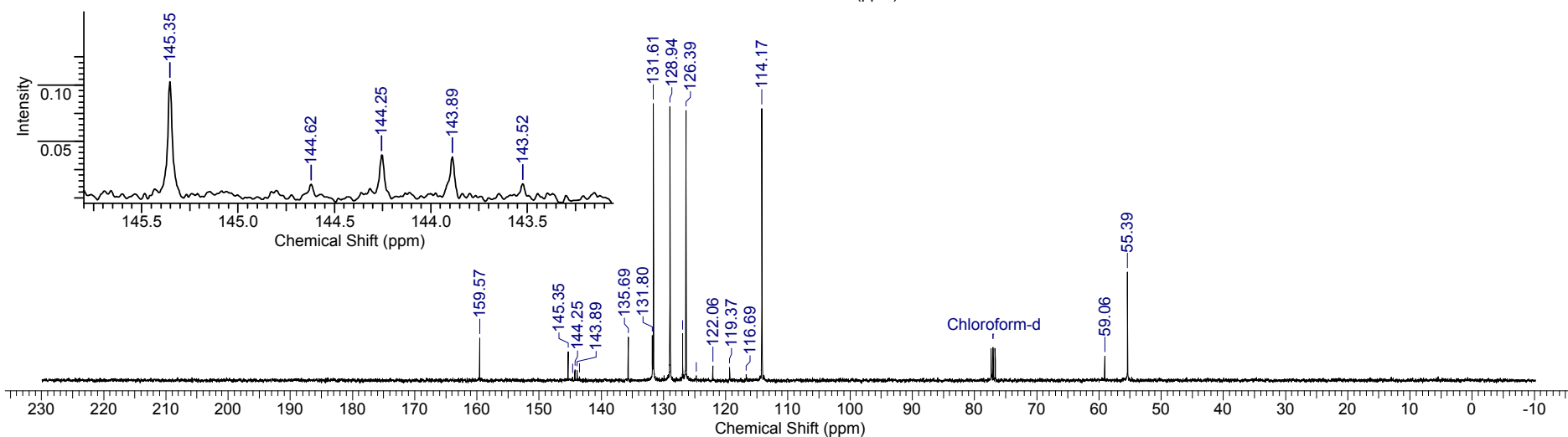
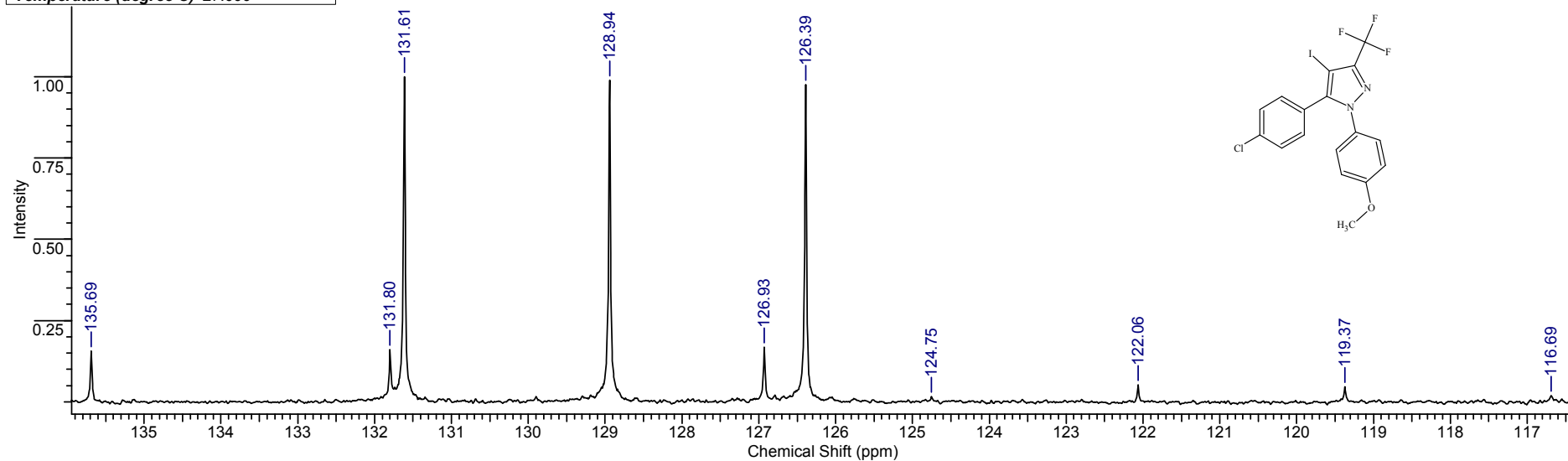
FW 478.6345 **Formula** C₁₇H₁₁ClF₃IN₂O

Acquisition Time (sec)	2.5559	Comment	Imported from UXMNR.	Date	27 Jul 2017 18:16:12
File Name	C:\IBM_DATA\DOCS\SPEC_BM_H_C_V-VIII.2017\BM-1142.H_001001r			Frequency (MHz)	400.13
Nucleus	1H	Number of Transients	4	Original Points Count	16384
Pulse Sequence	zg30	Solvent	CHLOROFORM-D	Points Count	65536
Temperature (degree C)	27.000			Sweep Width (Hz)	6410.26



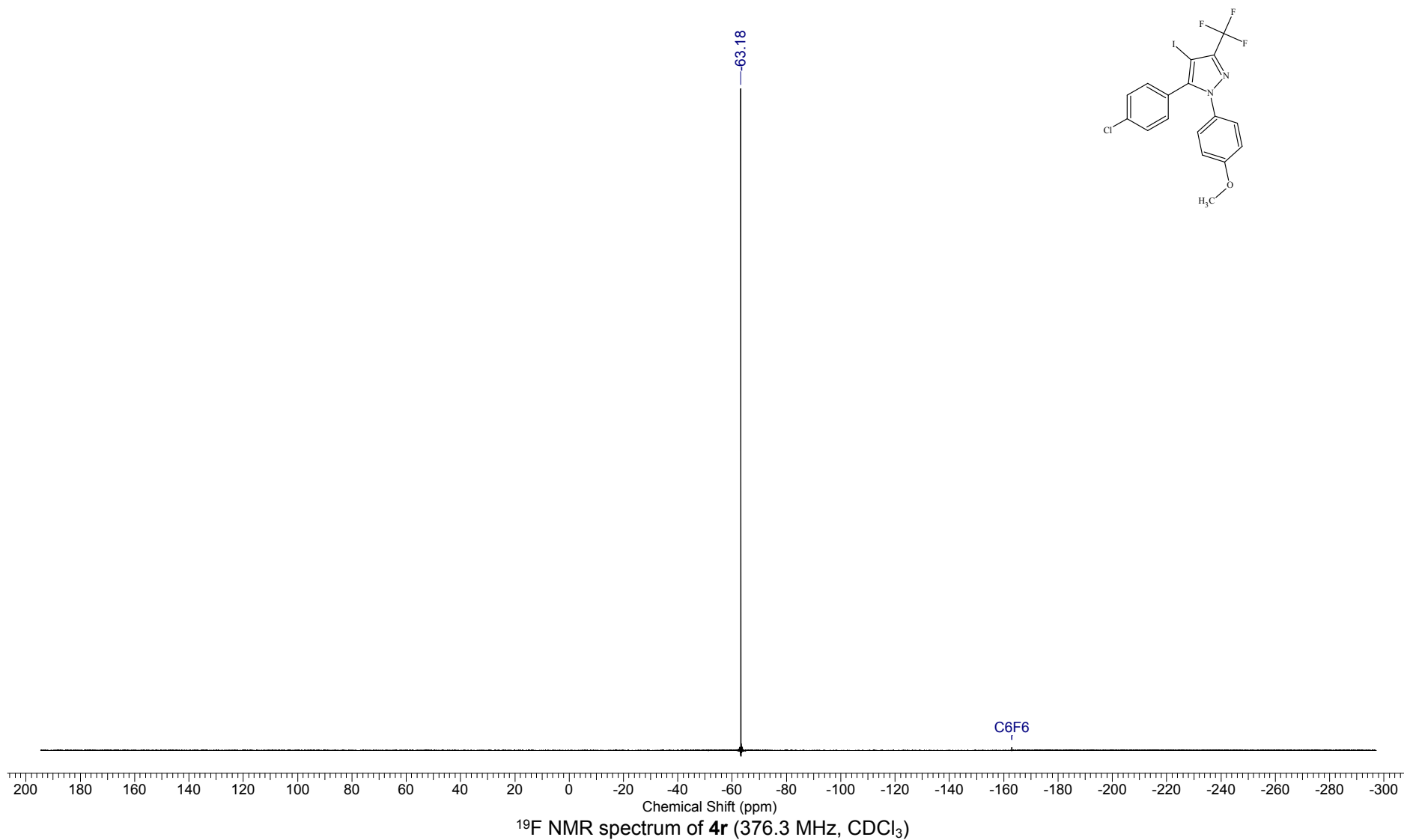
FW 478.6345 **Formula** C₁₇H₁₁ClF₃IN₂O

Acquisition Time (sec)	0.4999	Comment	Imported from UXMNR.		Date	27 Jul 2017 18:18:52	
File Name	C:\BM_DATA\DOCS\SPEC_BM_H,C_V-VIII.2017\BM-1142.C_002001r			Frequency (MHz)	100.61		
Nucleus	13C	Number of Transients	64	Original Points Count	12076	Points Count	65536
Pulse Sequence	zgpg30	Solvent	CHLOROFORM-D		Sweep Width (Hz)	24154.59	
Temperature (degree C)	27.000						



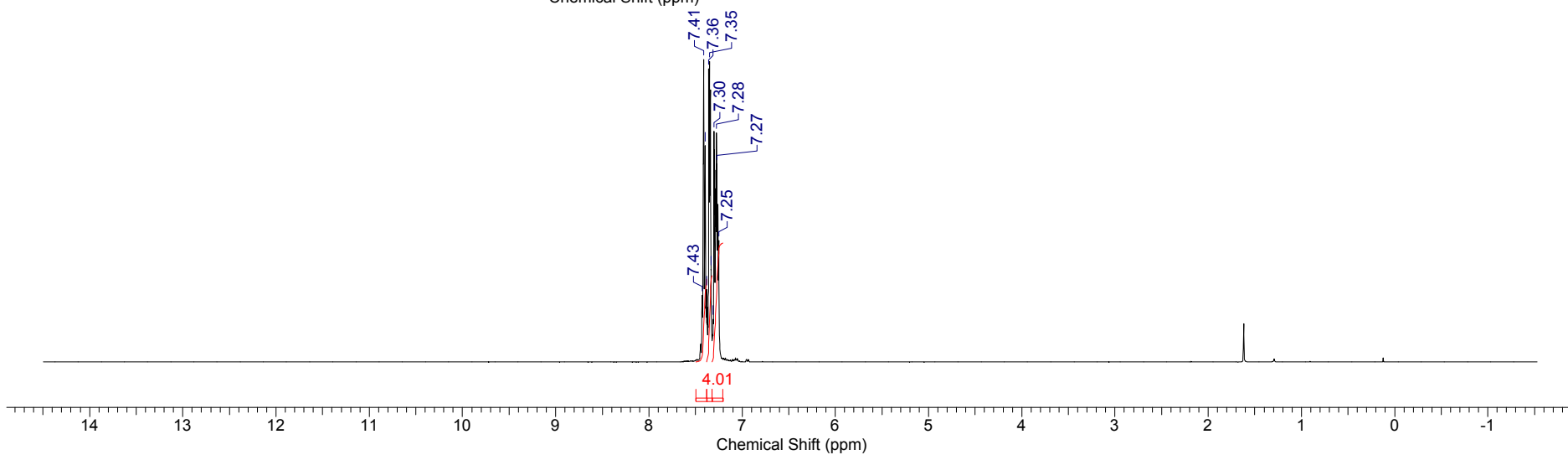
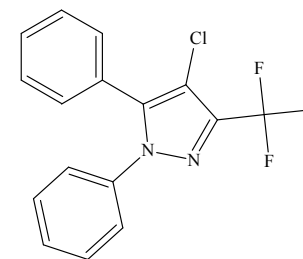
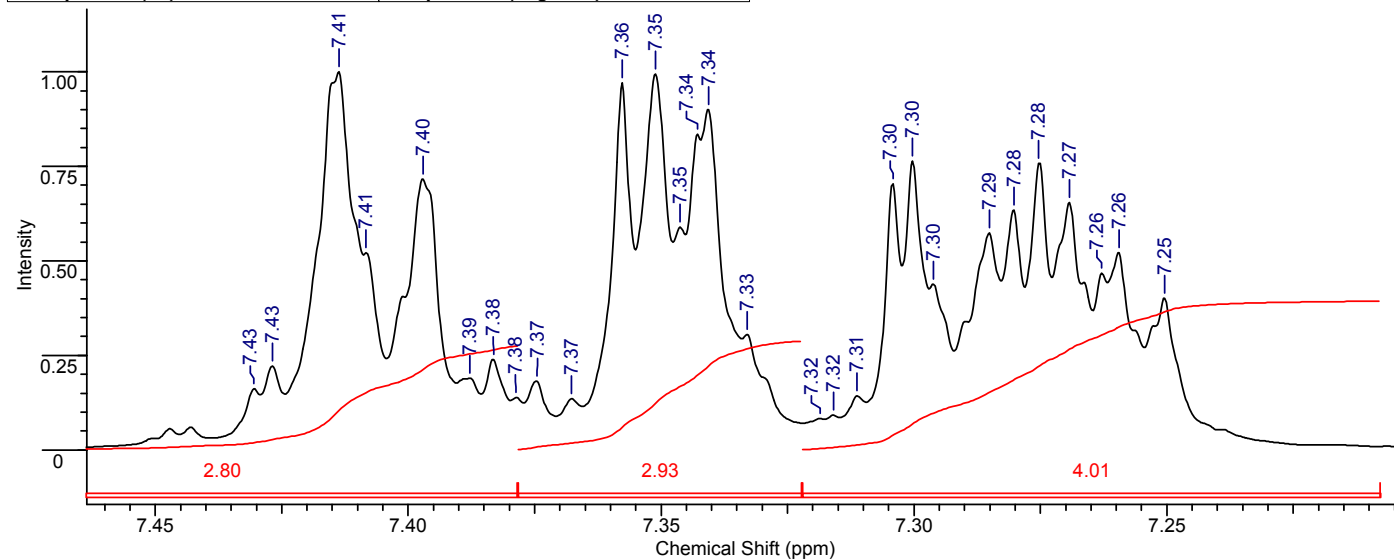
¹³C NMR spectrum of **4r** (100.6 MHz, CDCl₃)

FW	478.6345	Formula	C ₁₇ H ₁₁ ClF ₃ IN ₂ O				
Acquisition Time (sec)	0.2449	Date	31 Jul 2017 15:34:24				
File Name	C:\BM_DATA\DOCS\SPEC_F_IX-XII.2016\BM-1142.{19F}\BM-1142.{19F}\BM-1142.{19F}_019000fid			Frequency (MHz)	282.39		
Nucleus	19F	Number of Transients	1	Original Points Count	34018	Points Count	65536
Pulse Sequence	zg	Solvent	CHLOROFORM-D	Sweep Width (Hz)	138888.89	Temperature (degree C)	27.000



FW	322.7120	Formula	C ₁₆ H ₁₀ ClF ₃ N ₂
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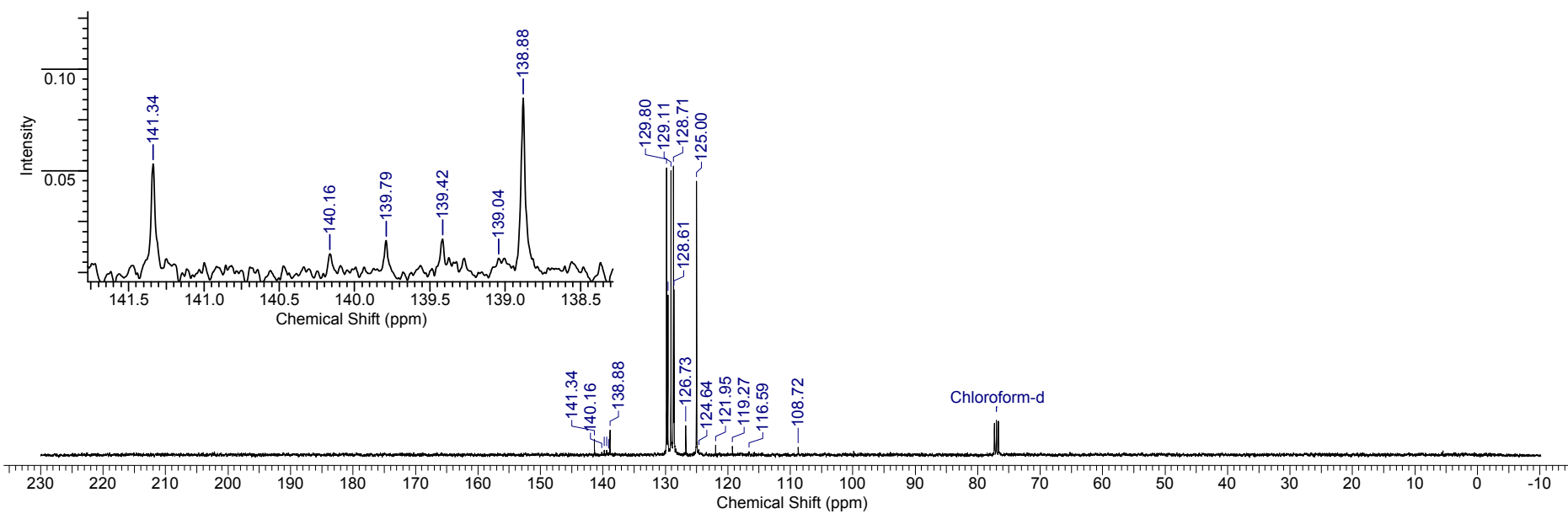
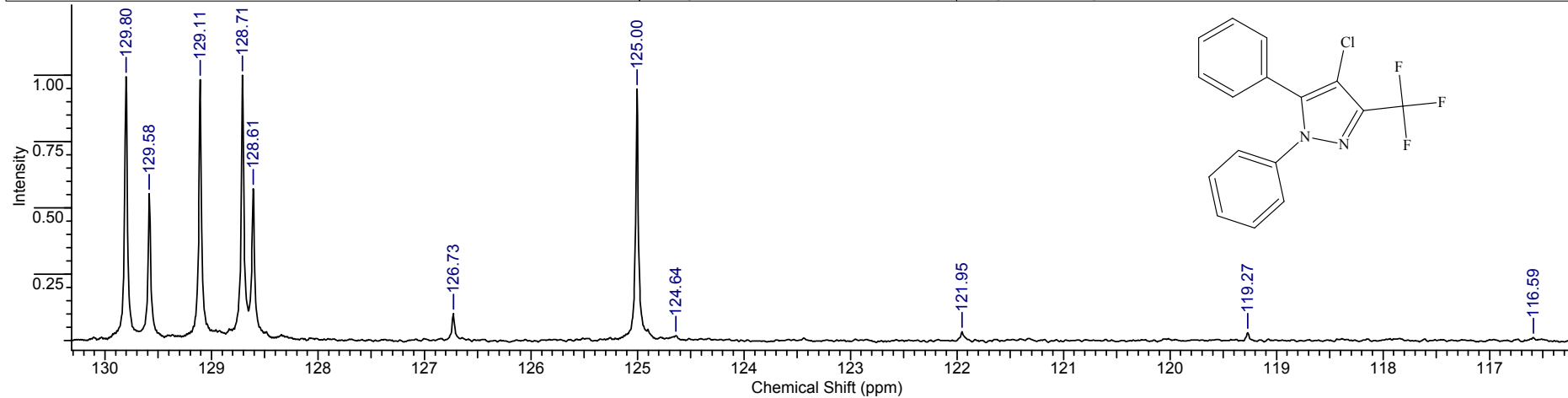
Acquisition Time (sec)	2.5559	Comment	Imported from UXMNR.		Date	24 May 2017 17:32:56		
File Name	D:\BN\output\2017\05.i à\BM-1071.H_001001r		Frequency (MHz)	400.13	Nucleus	1H	Number of Transients	6
Original Points Count	16384	Points Count	65536	Pulse Sequence	zg30	Solvent	CHLOROFORM-D	
Sweep Width (Hz)	6410.26	Temperature (degree C)	27.000					



¹H NMR spectrum of **5a** (400.1 MHz, CDCl₃)

FW 322.7120 **Formula** C₁₆H₁₀ClF₃N₂

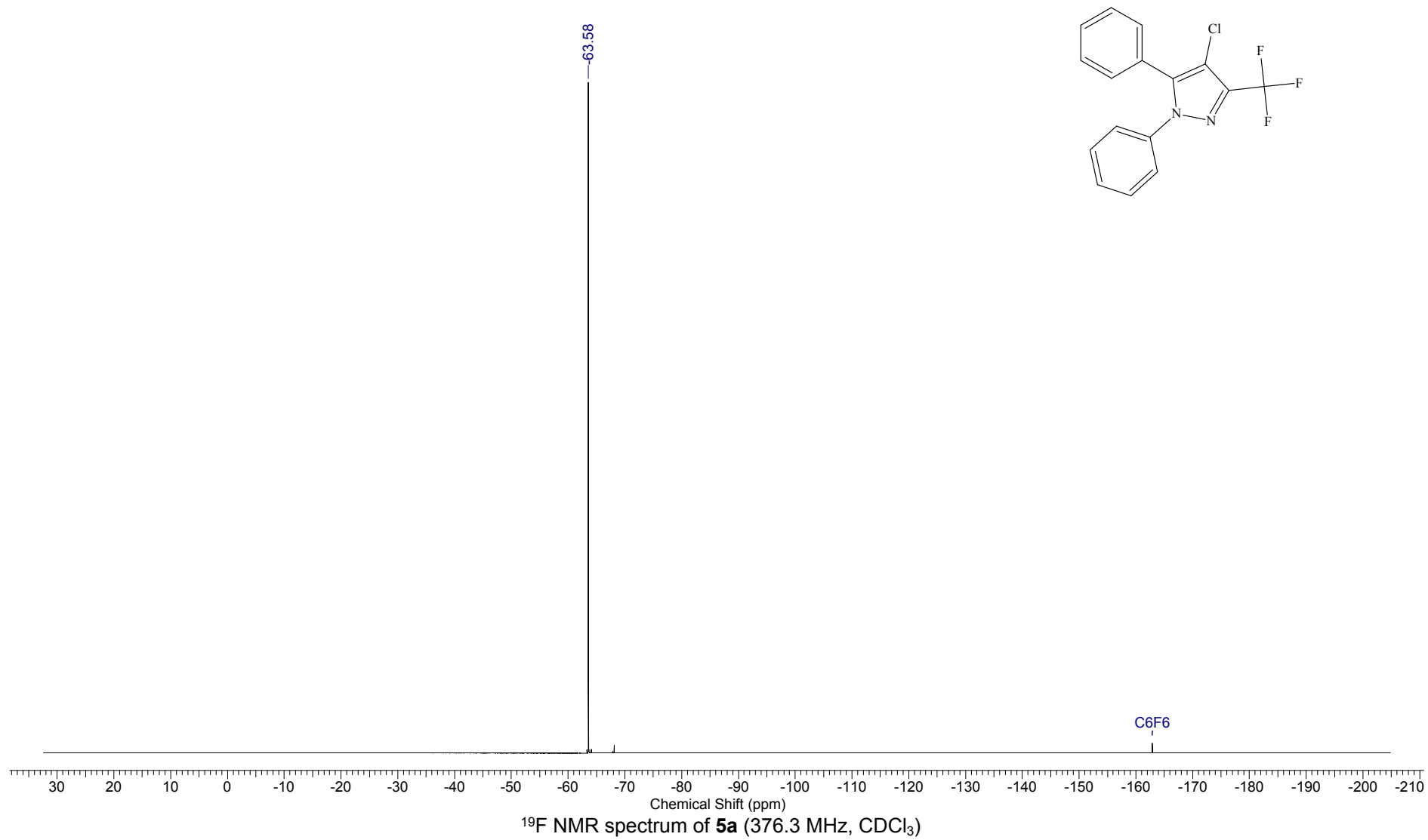
Acquisition Time (sec)	0.4999	Comment	Imported from UXMNR.		Date	24 May 2017 17:38:00
File Name	D:\BN\output\2017\05.i àé\BM-1071.C_002001r	Frequency (MHz)	100.61	Nucleus	13C	
Number of Transients	155	Original Points Count	12076	Points Count	Pulse Sequence zgpg30	
Solvent	CHLOROFORM-D	Sweep Width (Hz)	24154.59	Temperature (degree C)	27.000	



¹³C NMR spectrum of **5a** (100.6 MHz, CDCl₃)

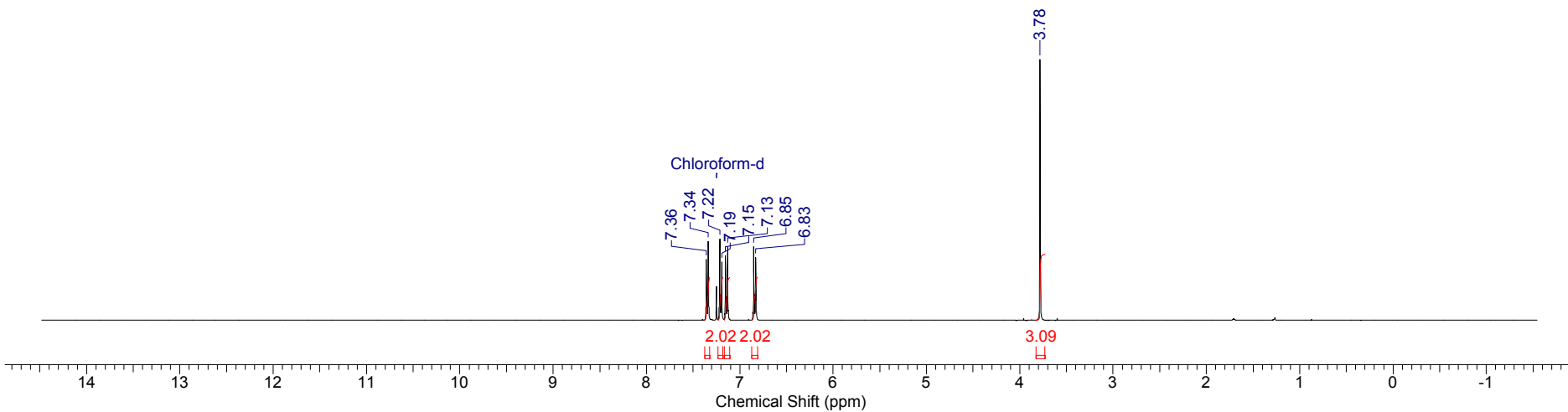
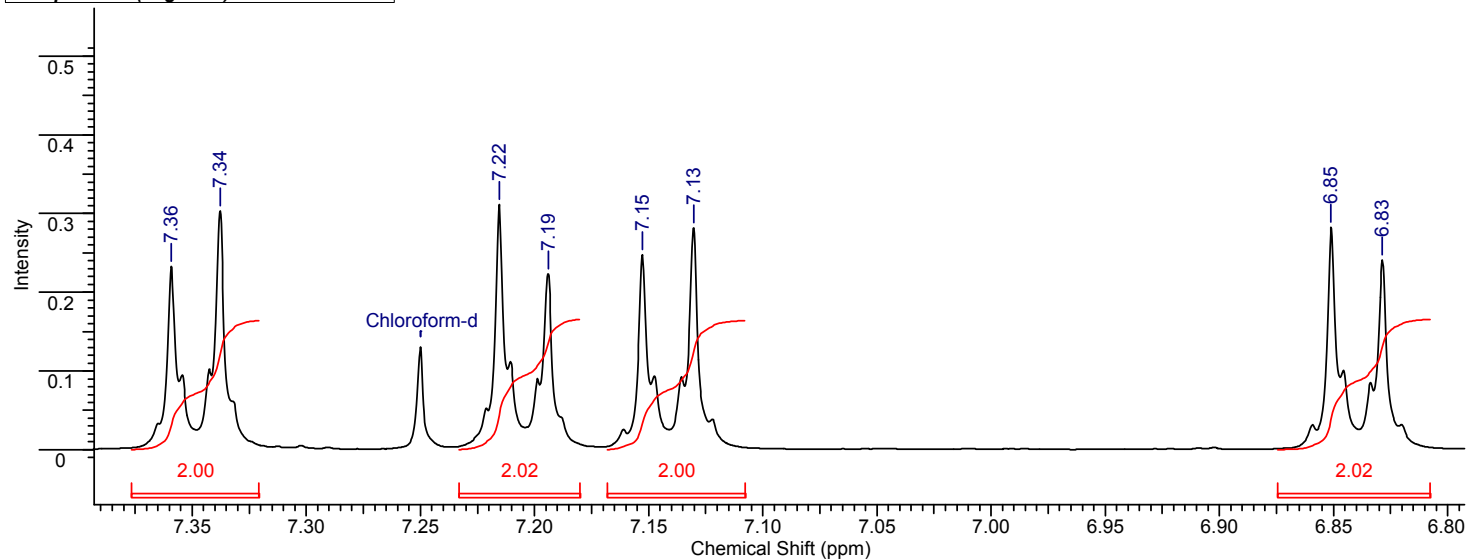
FW	322.7120	Formula	C ₁₆ H ₁₀ ClF ₃ N ₂
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Acquisition Time (sec)	0.7340	Date	May 30 2017	File Name	D:\BN\output\F19\F_2017\2017.05.30\bm1071-f_20170530_01\FLUORINE_01		
Frequency (MHz)	376.31	Nucleus	19F	Number of Transients	1000	Original Points Count	65536
Points Count	65536	Pulse Sequence	s2pul	Solvent	CHLOROFORM-D		
Sweep Width (Hz)	89285.71	Temperature (degree C)	25.000				



FW 387.1827 Formula C₁₇H₁₁Cl₂F₃N₂O

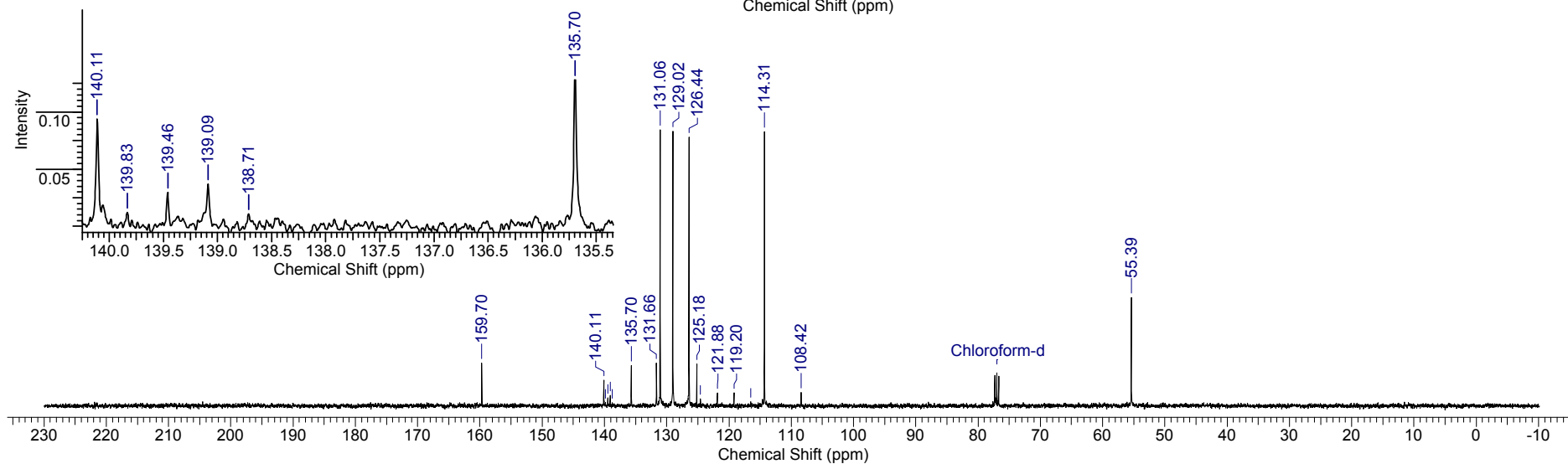
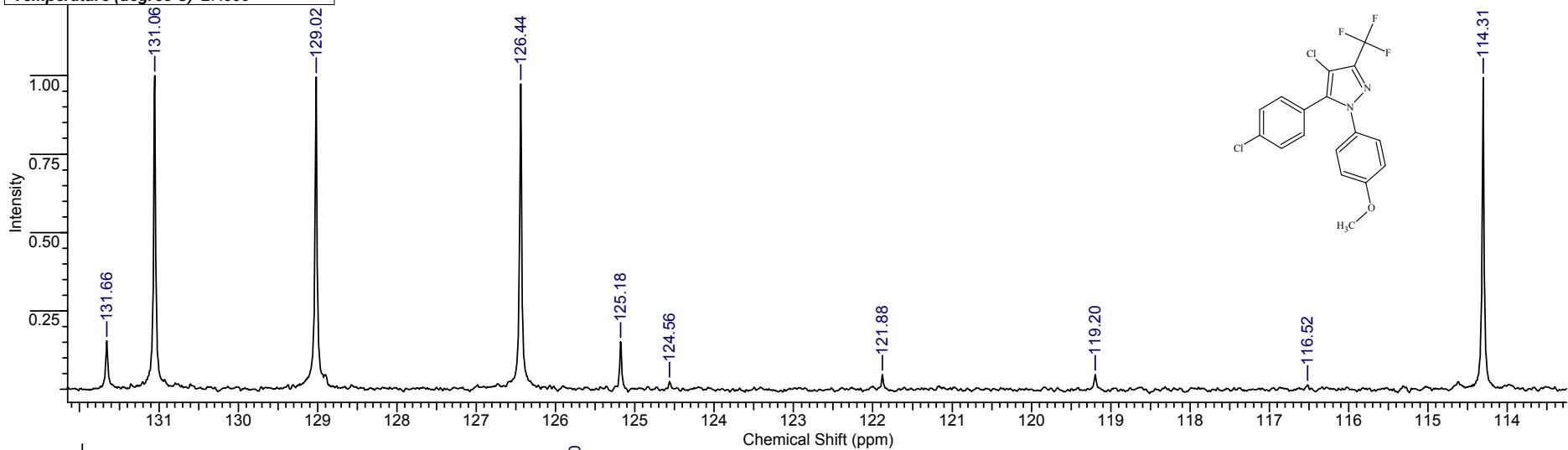
Acquisition Time (sec)	2.5559	Comment	Imported from UXMNR.	Date	28 Jul 2017 15:37:48
File Name	C:\BM_DATA\DOCS\SPEC_BM_H,C_V-VIII.2017\BM-1145.H_001001r			Frequency (MHz)	400.13
Nucleus	1H	Number of Transients	5	Original Points Count	16384
Pulse Sequence	zg30	Solvent	CHLOROFORM-D	Points Count	65536
Temperature (degree C)	27.000			Sweep Width (Hz)	6410.26



¹H NMR spectrum of **5b** (400.1 MHz, CDCl₃)

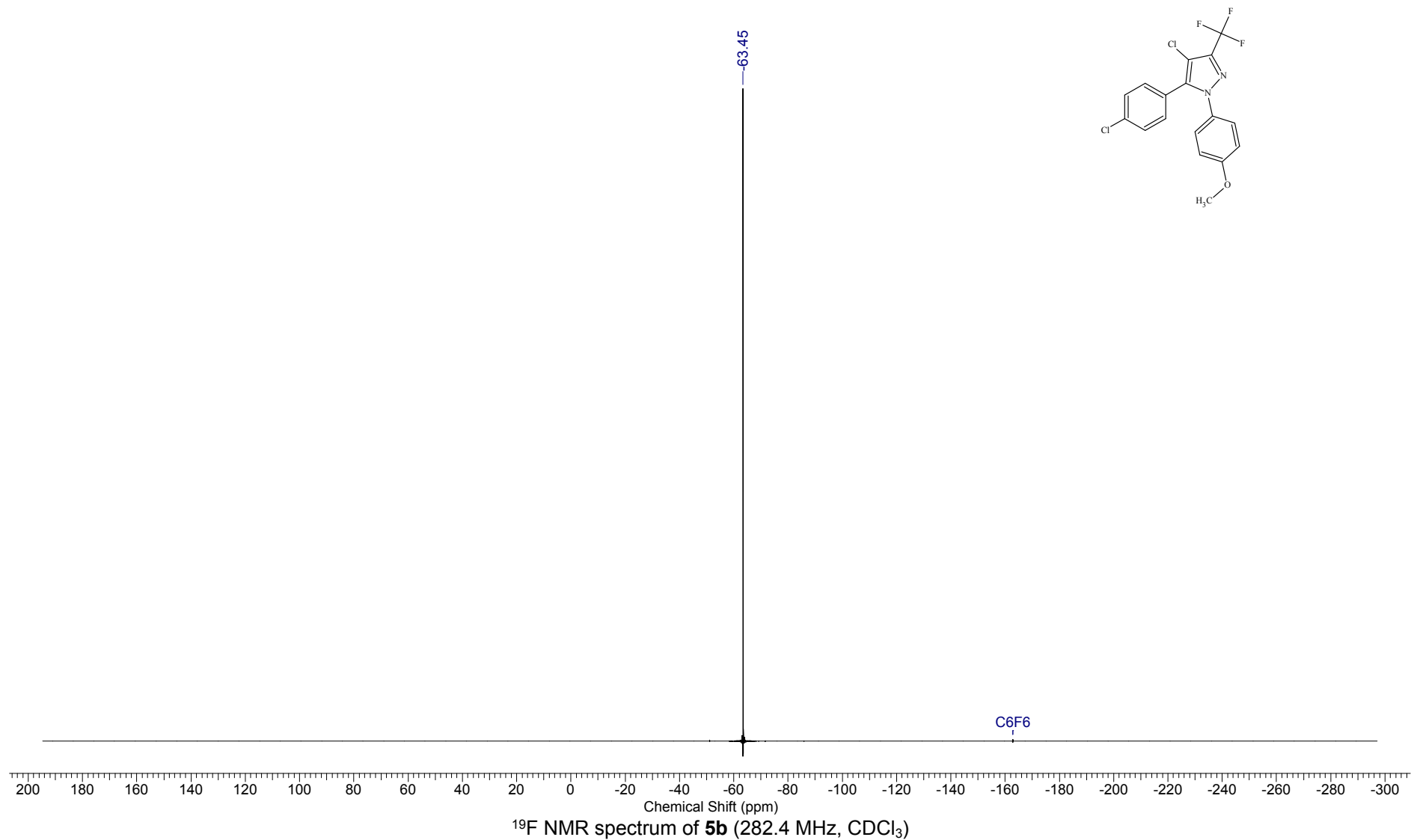
FW	387.1827	Formula	C ₁₇ H ₁₁ Cl ₂ F ₃ N ₂ O
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Acquisition Time (sec)	0.4999	Comment	Imported from UXNMR.	Date	28 Jul 2017 15:39:18
File Name	C:\BM_DATA\DOCS\SPEC_BM_H,C_V-VIII.2017\BM-1145.C_002001r			Frequency (MHz)	100.61
Nucleus	13C	Number of Transients	32	Original Points Count	12076
Pulse Sequence	zgpg30	Solvent	CHLOROFORM-D	Points Count	65536
Temperature (degree C)	27.000			Sweep Width (Hz)	24154.59



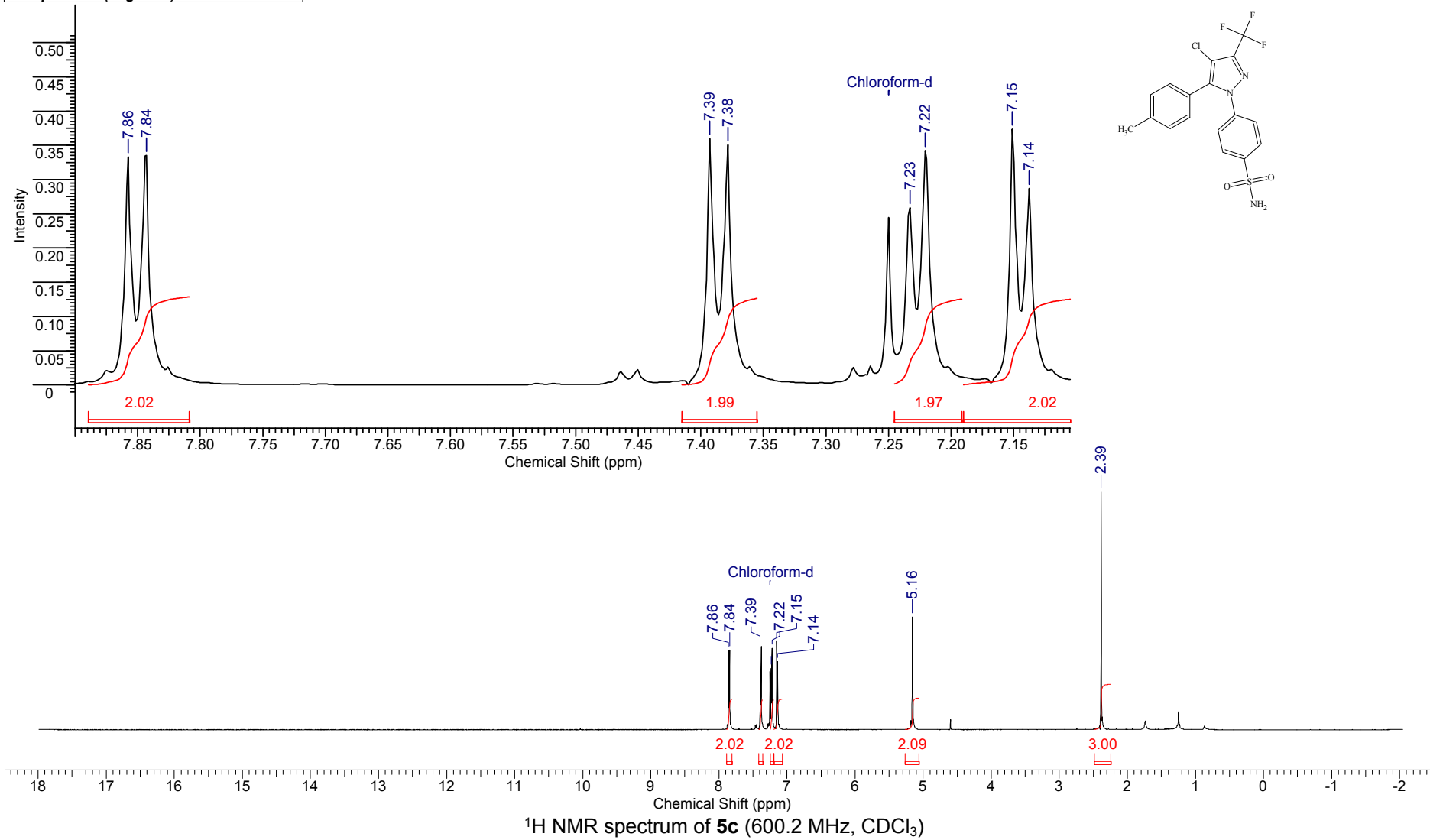
¹³C NMR spectrum of **5b** (100.6 MHz, CDCl₃)

FW	387.1827	Formula	C ₁₇ H ₁₁ Cl ₂ F ₃ N ₂ O				
Acquisition Time (sec)	0.2449	Date	31 Jul 2017 15:36:32				
File Name	C:\BM_DATA\DOCS\SPEC_F_IX-XII.2016\BM-1145.{19F}\BM-1145.{19F}\BM-1145.{19F}_019000fid			Frequency (MHz)	282.39		
Nucleus	19F	Number of Transients	1	Original Points Count	34018	Points Count	65536
Pulse Sequence	zg	Solvent	CHLOROFORM-D	Sweep Width (Hz)	138888.89	Temperature (degree C)	27.000



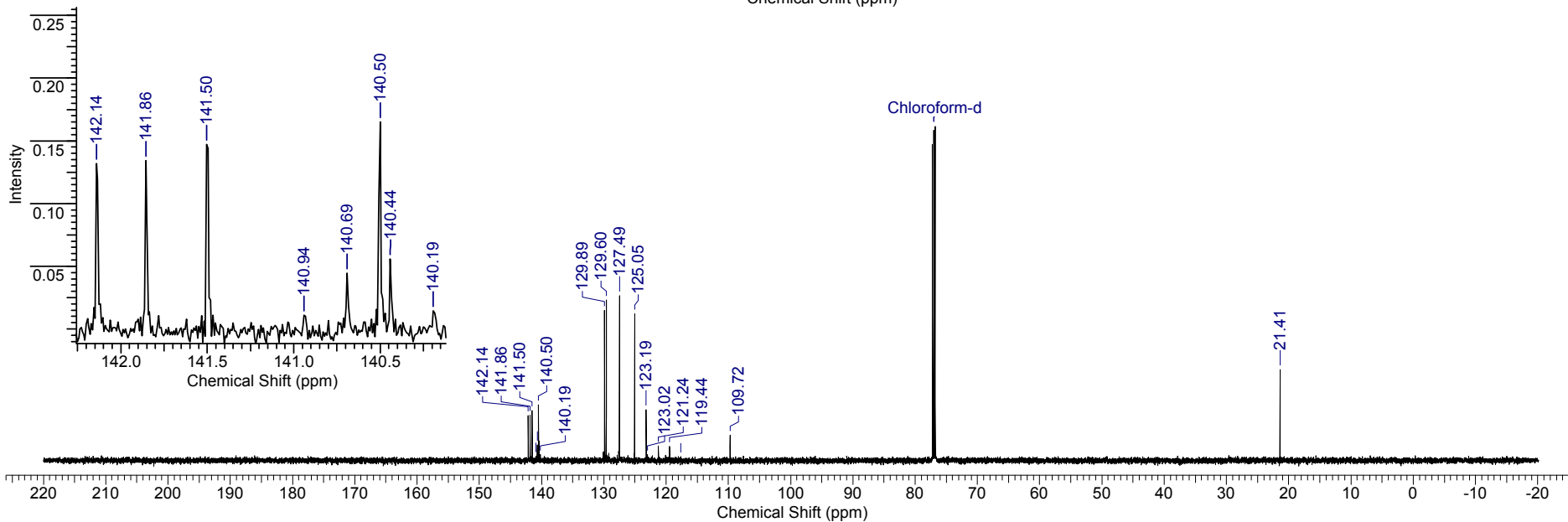
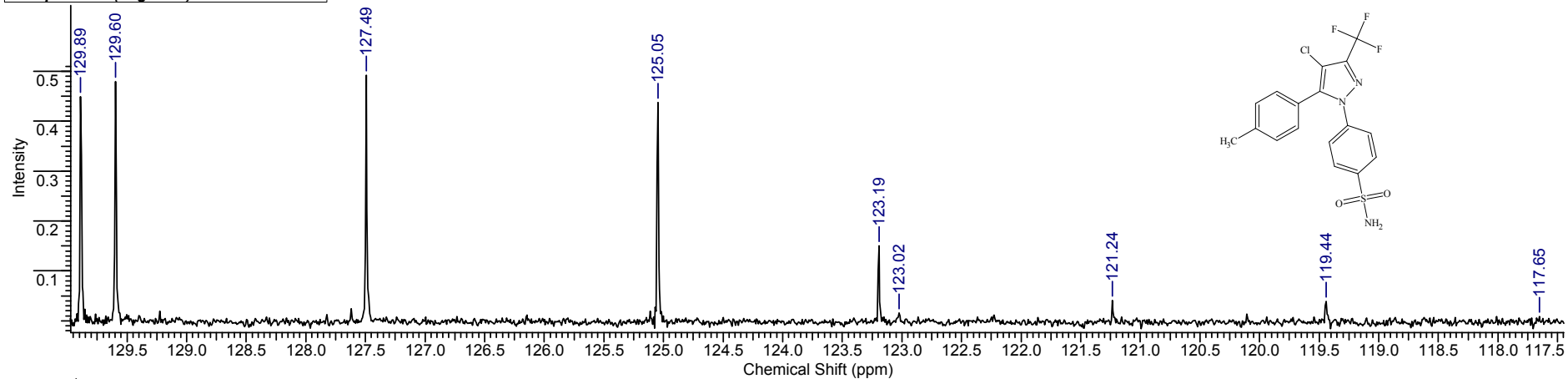
FW 415.8180 Formula $C_{17}H_{13}ClF_3N_3O_2S$

Acquisition Time (sec)	1.3631	Date	04 Aug 2017 07:51:28				
File Name	C:\BM_DATA\DOCS\SPEC_BM_H,C_V-VIII.2017\BM-1141\BM-1141_001000fid		Frequency (MHz)	600.13			
Nucleus	1H	Number of Transients	4	Original Points Count	16384	Points Count	16384
Pulse Sequence	zg30	Solvent	CHLOROFORM-D	Sweep Width (Hz)	12019.23		
Temperature (degree C)	25.000						



FW	415.8180	Formula	C ₁₇ H ₁₃ ClF ₃ N ₃ O ₂ S
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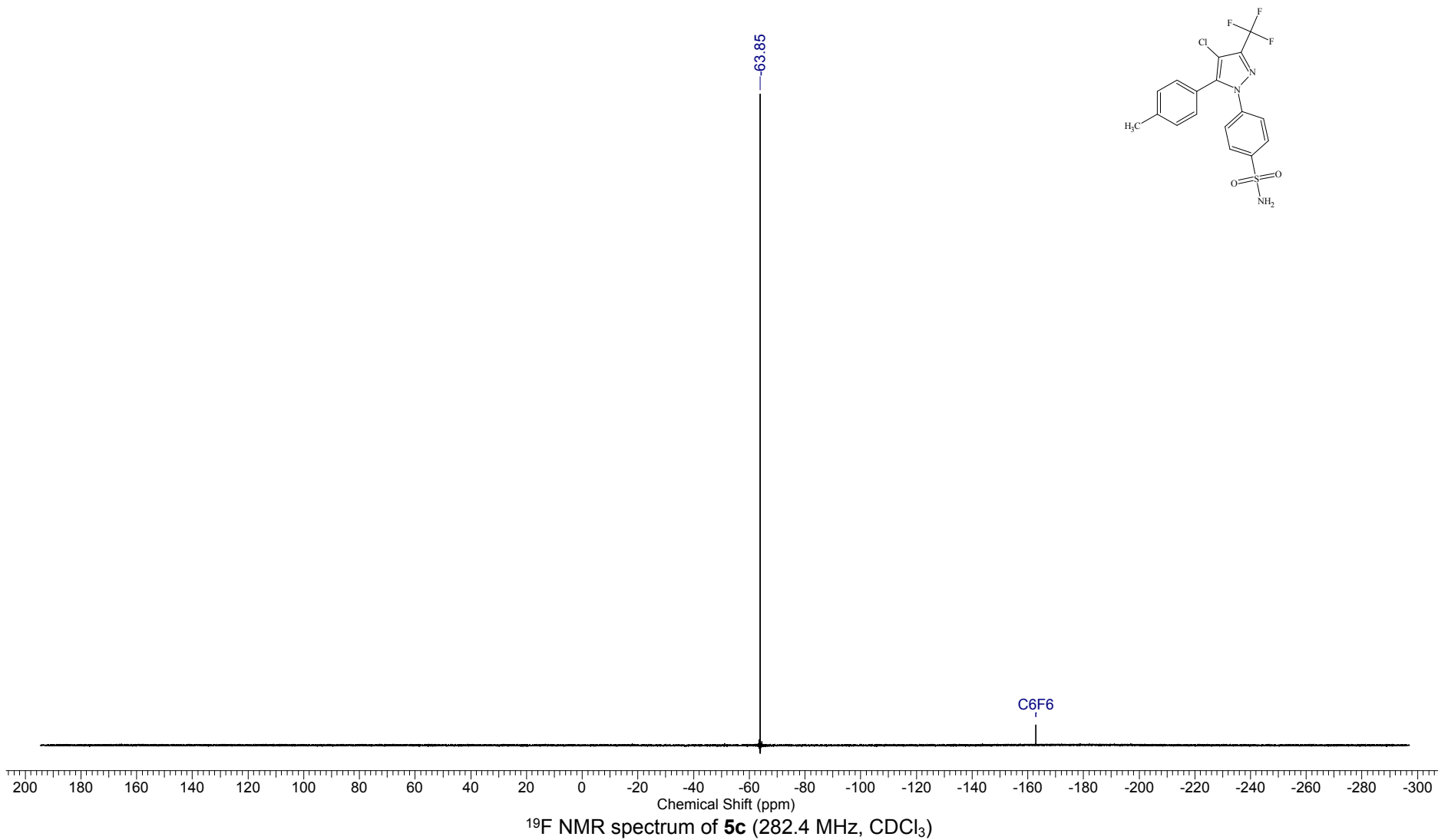
Acquisition Time (sec)	0.4522	Date	04 Aug 2017 10:50:36			
File Name	C:\BM_DATA\DOCS\SPEC_BM_H,C_V-VIII.2017\BM-1141_013001r			Frequency (MHz)	150.90	
Nucleus	13C	Number of Transients	151	Original Points Count	16384	
Pulse Sequence	zpgg30	Solvent	CHLOROFORM-D		Points Count	32768
Temperature (degree C)	25.000				Sweep Width (Hz)	36231.88



¹³C NMR spectrum of 5c (150.9 MHz, CDCl₃)

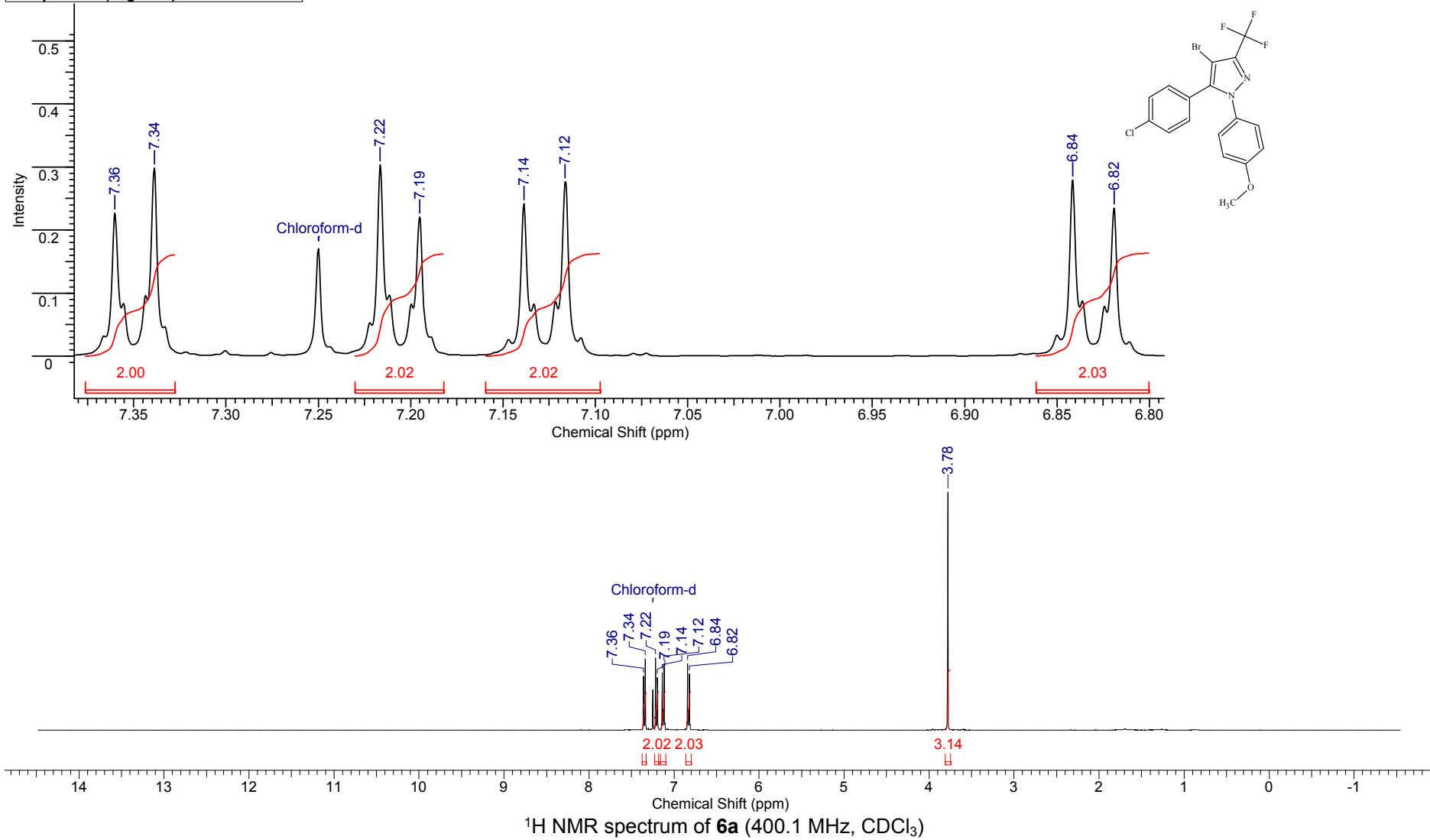
FW 415.8180	Formula C ₁₇ H ₁₃ ClF ₃ N ₃ O ₂ S
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Acquisition Time (sec) 0.2449	Date 07 Aug 2017 15:04:32	Frequency (MHz) 282.39
File Name C:\BM_DATA\DOCS\SPEC_F_IX-XII.2016\BM-1141.{19F}\BM-1141.{19F}_019000fid		Points Count 65536
Nucleus 19F	Number of Transients 1	Original Points Count 34018
Pulse Sequence zg	Solvent CHLOROFORM-D	Sweep Width (Hz) 138888.89
Temperature (degree C) 27.000		



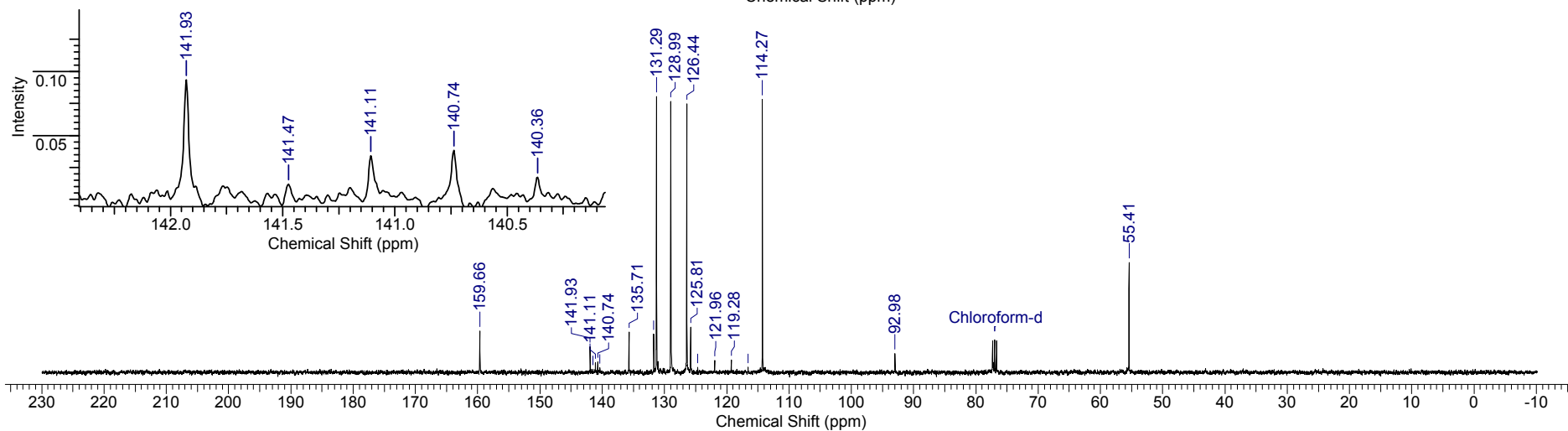
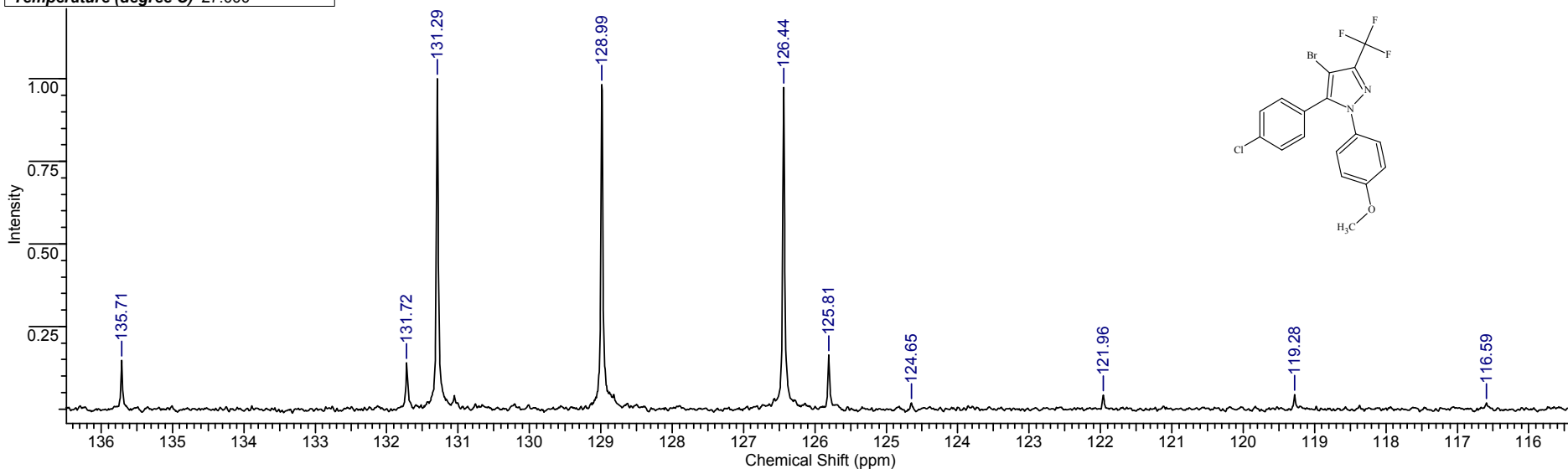
FW 431.6340 **Formula** C₁₇H₁₁BrClF₃N₂O

Acquisition Time (sec)	2.5559	Comment	Imported from UXMNR.	Date	27 Jul 2017 18:11:28
File Name	C:\BM_DATA\DOCS\SPEC_BM_H_C_V-VIII.2017\BM-1143.H_001001r			Frequency (MHz)	400.13
Nucleus	1H	Number of Transients	4	Original Points Count	16384
Pulse Sequence	zg30	Solvent	CHLOROFORM-D	Points Count	65536
Temperature (degree C)	27.000			Sweep Width (Hz)	6410.26



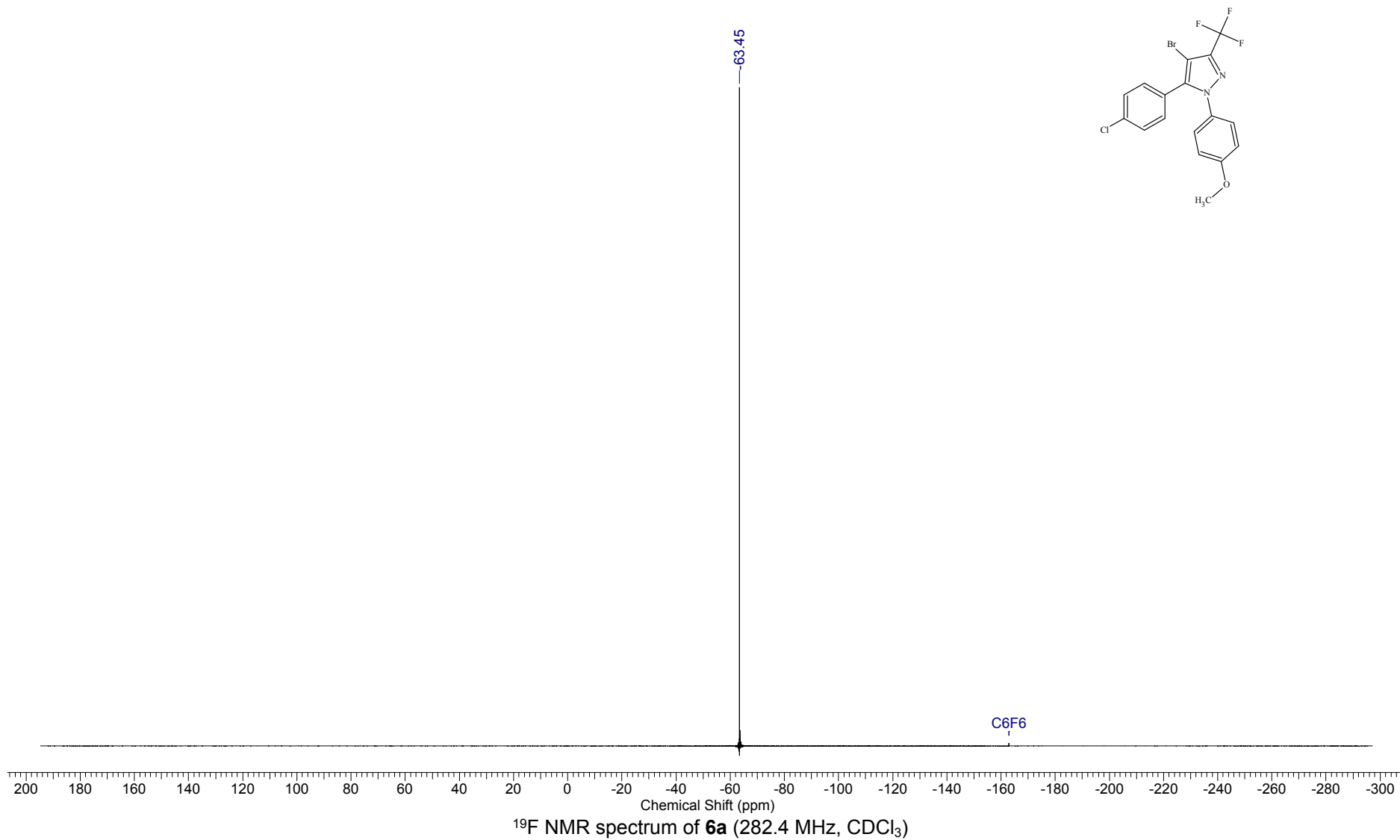
FW	431.6340	Formula	C ₁₇ H ₁₁ BrClF ₃ N ₂ O
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Acquisition Time (sec)	0.4999	Comment	Imported from UXMNR.	Date	27 Jul 2017 18:13:34
File Name	C:\BM_DATA\DOCS\SPEC_BM_H,C_V-VIII.2017\BM-1143.C_002001r			Frequency (MHz)	100.61
Nucleus	13C	Number of Transients	46	Original Points Count	12076
Pulse Sequence	zgpg30	Solvent	CHLOROFORM-D	Points Count	65536
Temperature (degree C)	27.000			Sweep Width (Hz)	24154.59



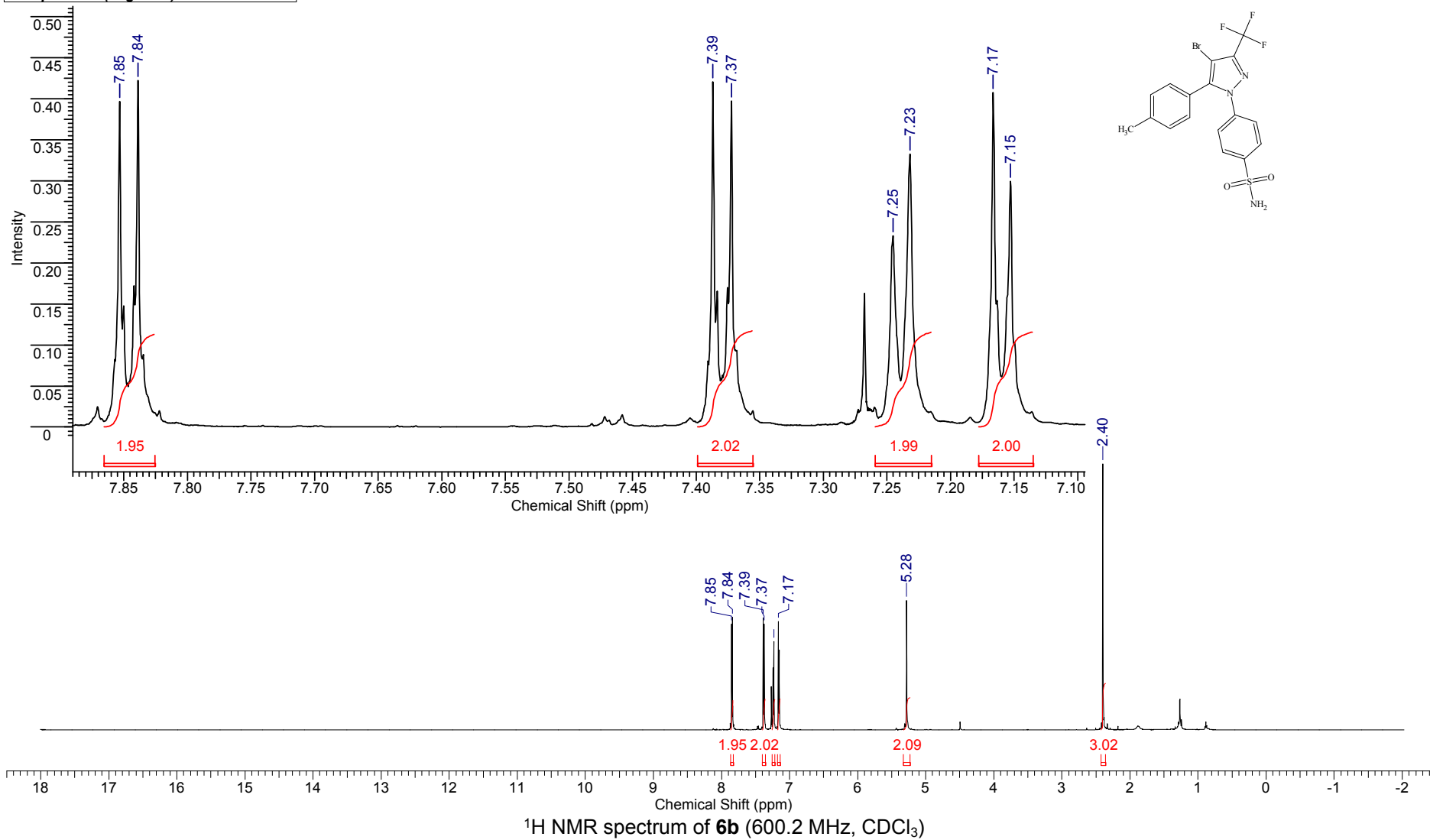
¹³C NMR spectrum of **6a** (100.6 MHz, CDCl₃)

FW	431.6340	Formula C ₁₇ H ₁₁ BrClF ₃ N ₂ O					
Acquisition Time (sec)	0.2449	Date	31 Jul 2017 15:34:24				
File Name	C:\BM_DATA\DOCS\SPEC_F_IX-XII.2016\BM-1143.{19F}\BM-1143.{19F}\BM-1143.{19F}_019000fid				Frequency (MHz)	282.39	
Nucleus	19F	Number of Transients	1	Original Points Count	34018	Points Count	65536
Pulse Sequence	zg	Solvent	CHLOROFORM-D	Sweep Width (Hz)	138888.89	Temperature (degree C)	27.000



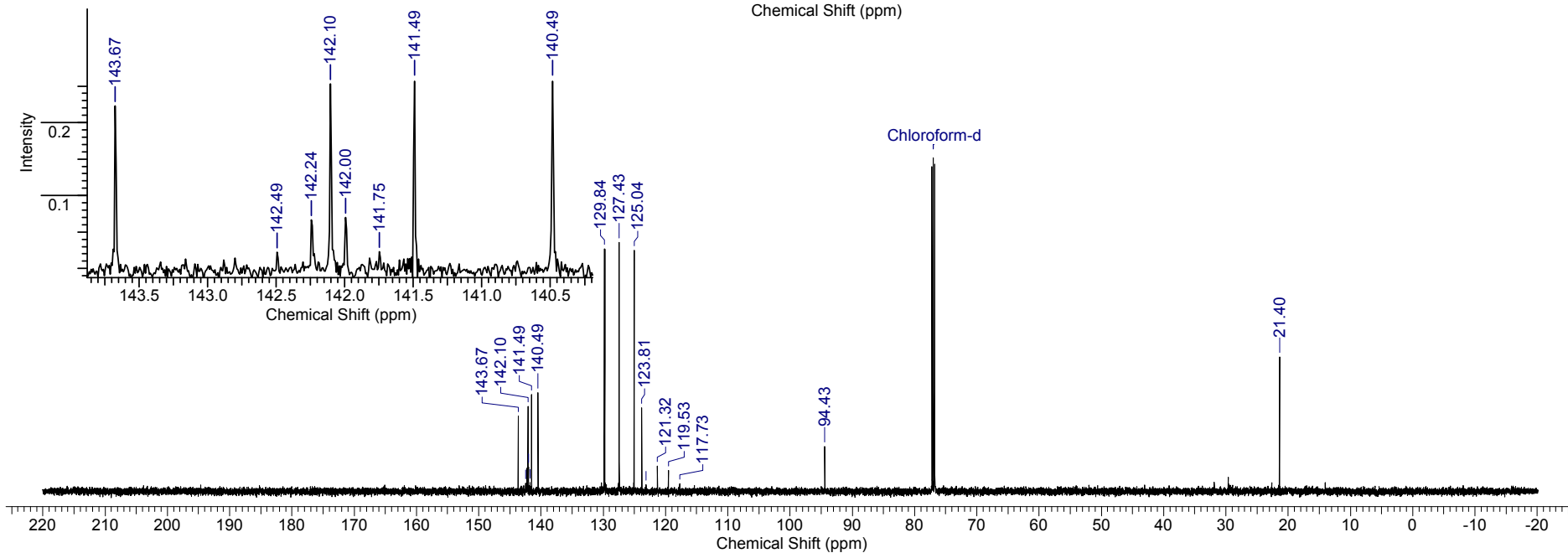
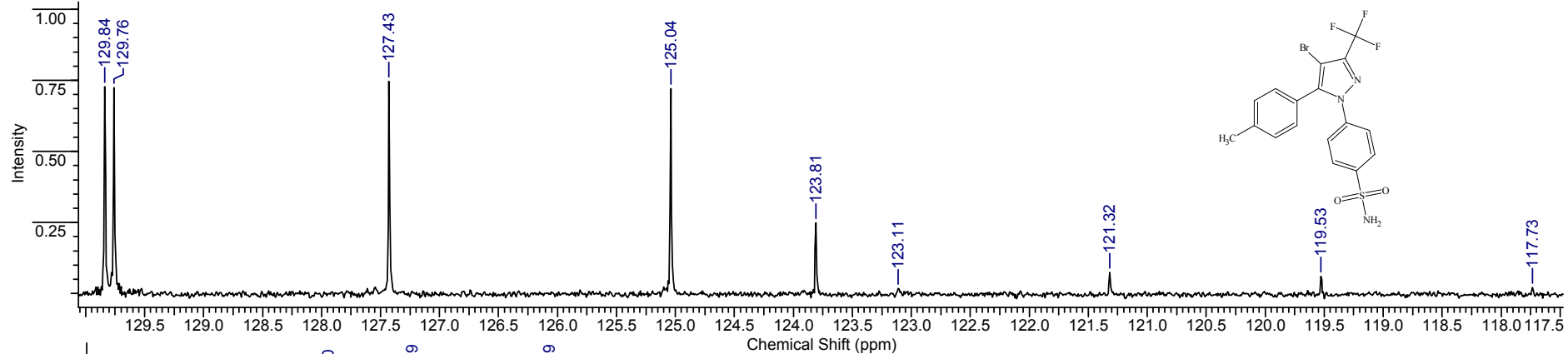
FW 460.2693 Formula C₁₇H₁₃BrF₃N₃O₂S

Acquisition Time (sec)	1.3631	Date	11 Aug 2017 10:43:30			
File Name	C:\BM_DATA\DOCS\SPEC_BM_H,C_V-VIII.2017\BM-1152_001001r			Frequency (MHz)	600.13	
Nucleus	1H	Number of Transients	4	Original Points Count	16384	
Pulse Sequence	zg30	Solvent	CHLOROFORM-D		Points Count	131072
Temperature (degree C)	25.000				Sweep Width (Hz)	12019.23



FW	460.2693	Formula	C ₁₇ H ₁₃ BrF ₃ N ₃ O ₂ S
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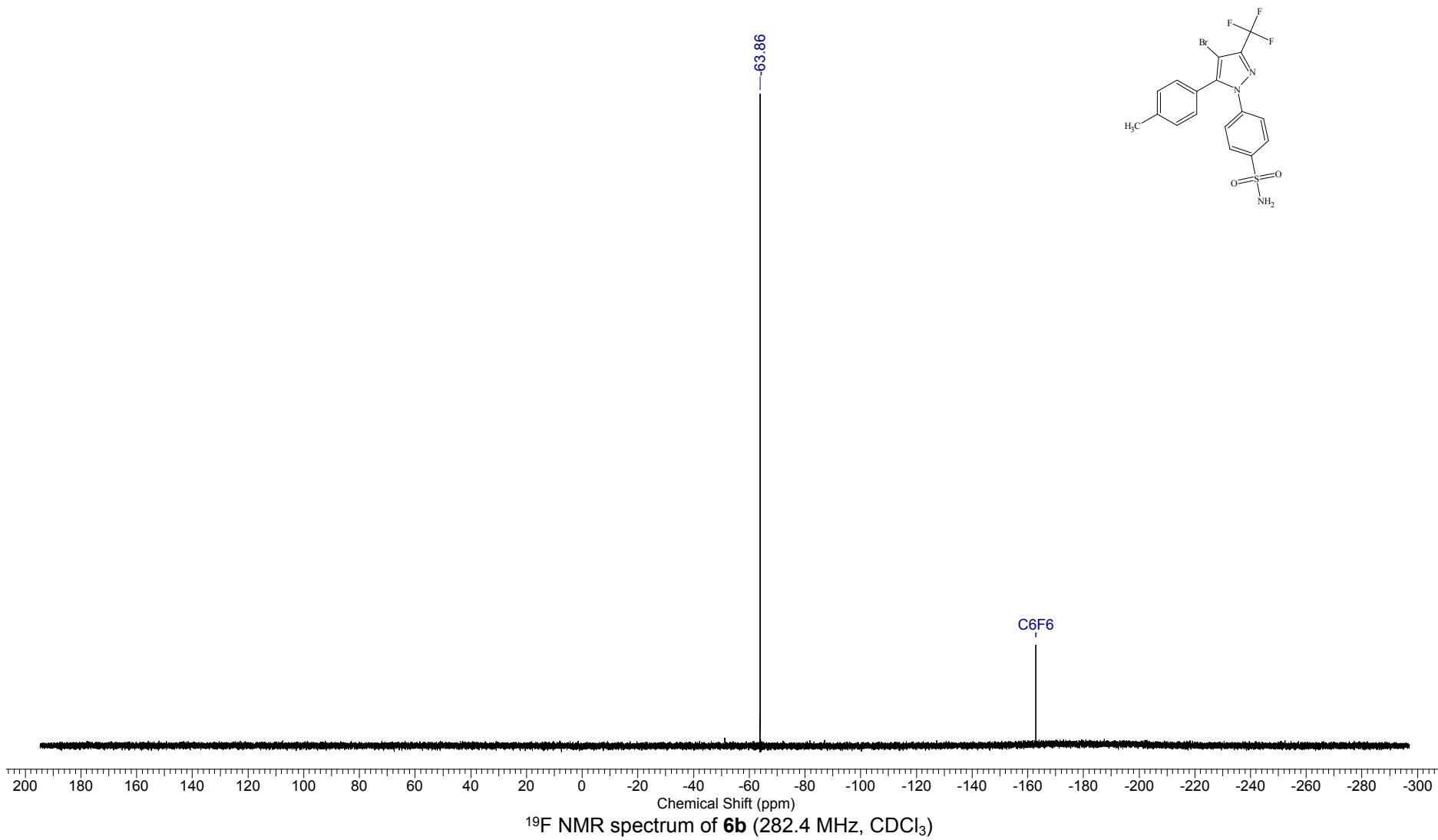
Acquisition Time (sec)	0.4522	Date	11 Aug 2017 10:41:00			
File Name	C:\BM_DATA\DOCS\SPEC_BM_H,C_V-VIII.2017\BM-1152_013001r			Frequency (MHz)	150.90	
Nucleus	13C	Number of Transients	105	Original Points Count	16384	
Pulse Sequence	zgpg30	Solvent	CHLOROFORM-D		Points Count	32768
Temperature (degree C)	25.000				Sweep Width (Hz)	36231.88



¹³C NMR spectrum of **6b** (150.9 MHz, CDCl₃)

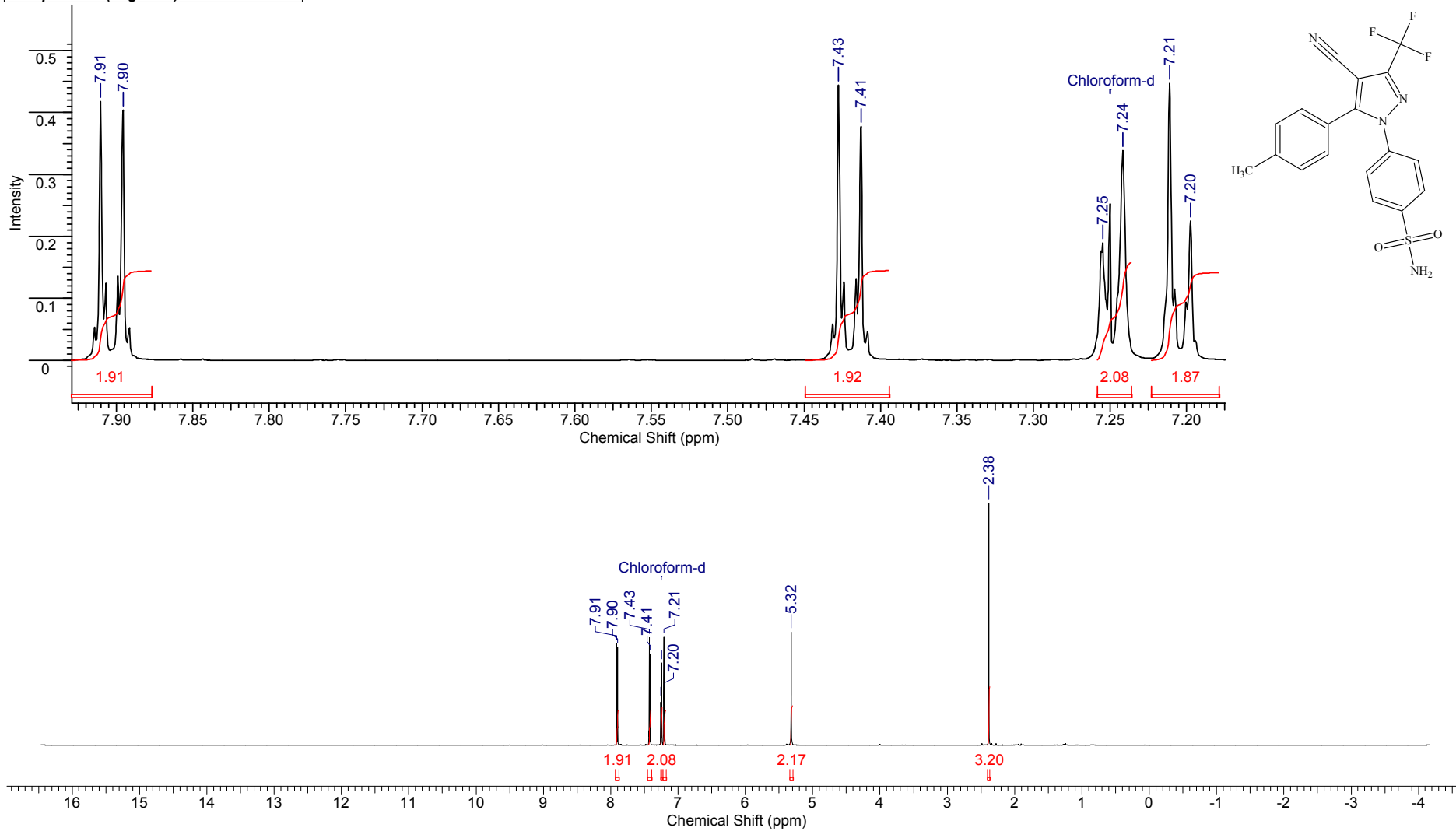
FW 460.2693	Formula C ₁₇ H ₁₃ BrF ₃ N ₃ O ₂ S
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Acquisition Time (sec) 0.2449	Date 07 Aug 2017 15:02:24	Frequency (MHz) 282.39
File Name C:\BM_DATA\DOCS\SPEC_F_IX-XII.2016\BM-1152.{19F}\BM-1152.{19F}_019000fid		Points Count 65536
Nucleus 19F	Number of Transients 1	Original Points Count 34018
Pulse Sequence zg	Solvent CHLOROFORM-D	Sweep Width (Hz) 138888.89
Temperature (degree C) 27.000		



FW 406.3828 Formula $C_{18}H_{13}F_3N_4O_2S$

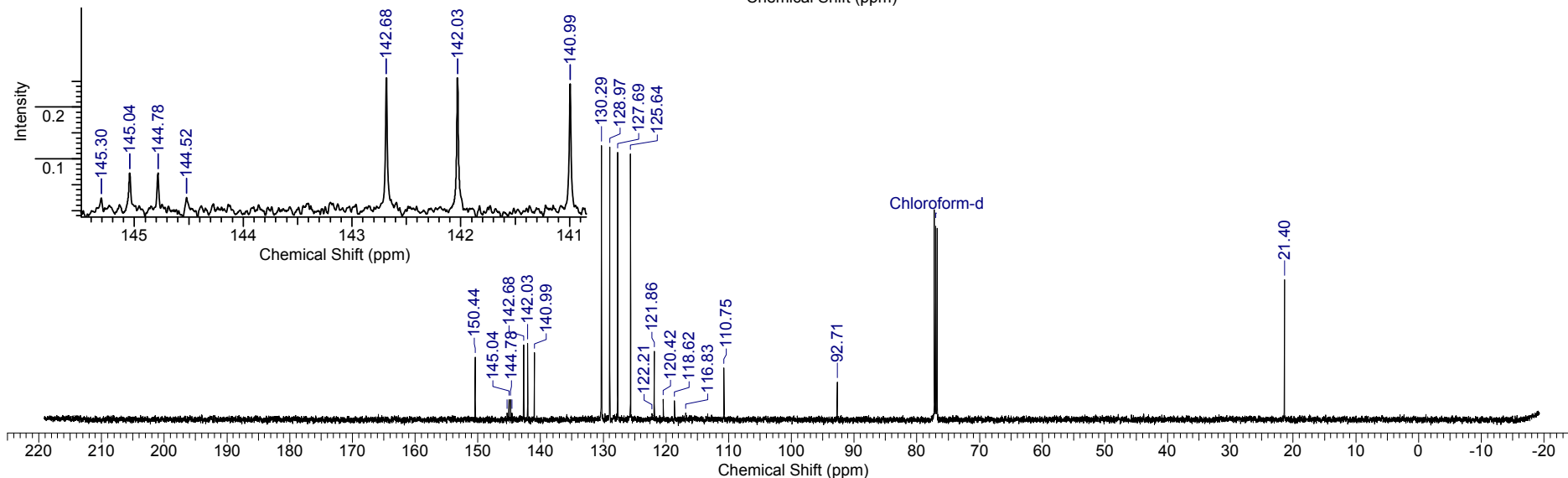
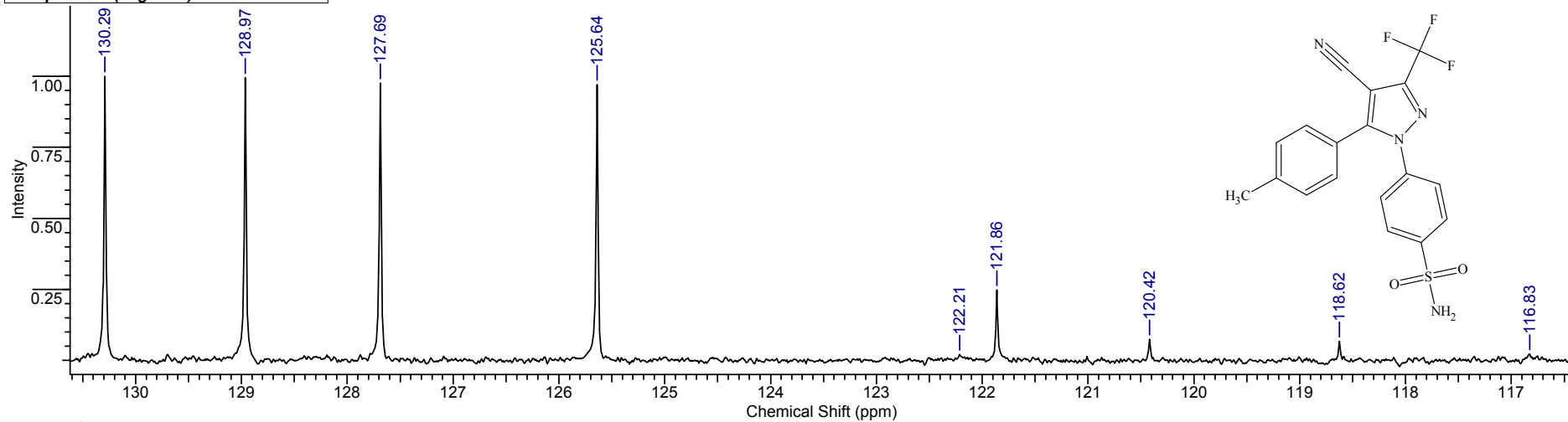
Acquisition Time (sec)	2.6477	Date	14 Aug 2017 23:57:00		Frequency (MHz)	600.13	
File Name	C:\BM_DATA\DOCS\SPEC_BM_H,C_V-VIII.2017\BM-1154-p_001001r				Points Count	131072	
Nucleus	1H	Number of Transients	16	Original Points Count	32768	Sweep Width (Hz)	12376.24
Pulse Sequence	zg	Solvent	CHLOROFORM-D				
Temperature (degree C)	30.000						



1H NMR spectrum of 7 (600.2 MHz, $CDCl_3$)

FW	406.3828	Formula	C ₁₈ H ₁₃ F ₃ N ₄ O ₂ S
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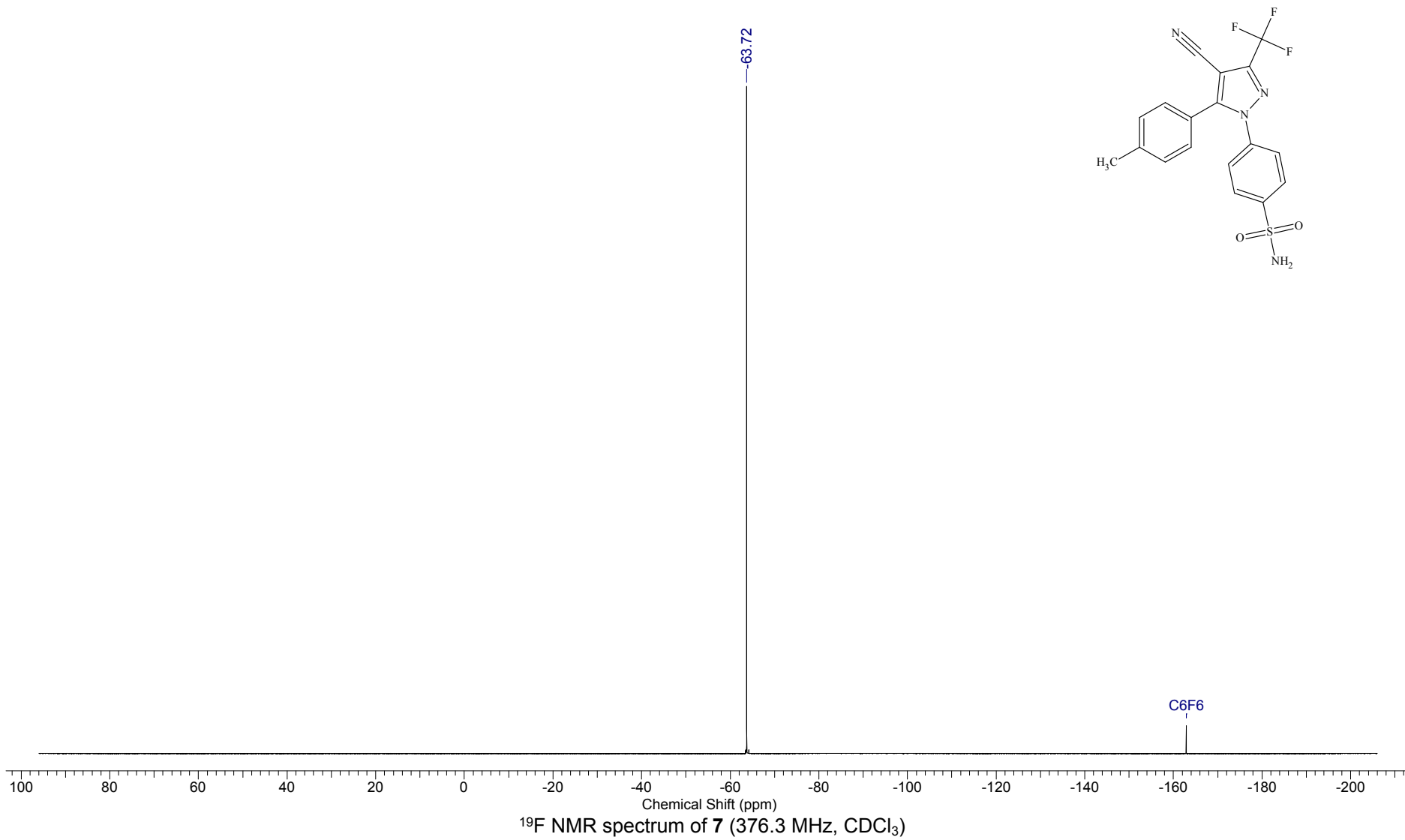
Acquisition Time (sec)	1.8219	Date	15 Aug 2017 00:02:16	Frequency (MHz)	150.90
File Name	C:\BM_DATA\DOCS\SPEC_BM_H,C_V-VIII.2017\BM-1154-p_002001r			Points Count	262144
Nucleus	13C	Number of Transients	50	Original Points Count	65536
Pulse Sequence	zpgpg	Solvent	CHLOROFORM-D	Sweep Width (Hz)	35971.22
Temperature (degree C)	30.100				



¹³C NMR spectrum of 7 (150.9 MHz, CDCl₃)

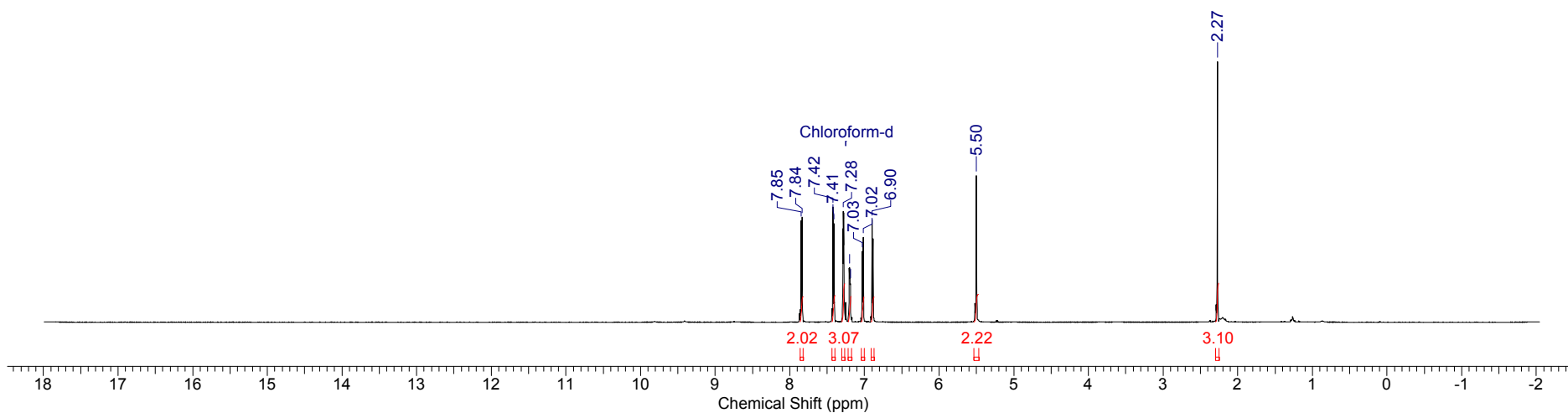
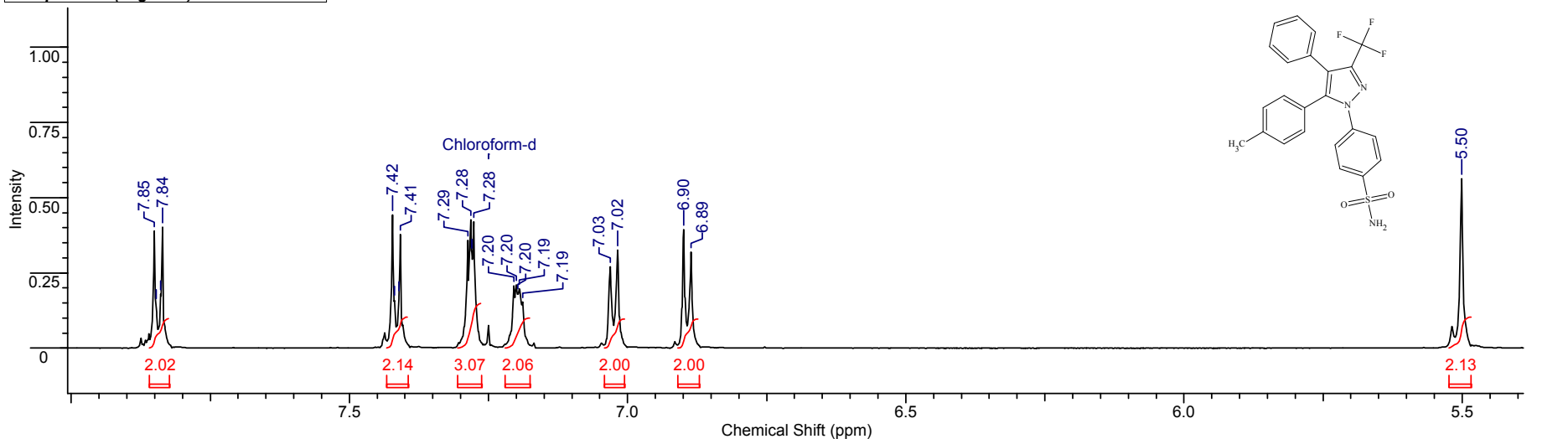
FW	406.3828	Formula	C ₁₈ H ₁₃ F ₃ N ₄ O ₂ S
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Acquisition Time (sec)	1.4680	Date	Sep 4 2017	File Name	D:\BN\output\F19\F_2017\2017.09.04\BM-1154-p-F_20170904_01\FLUORINE_01		
Frequency (MHz)	376.32	Nucleus	19F	Number of Transients	8	Original Points Count	166818
Points Count	262144	Pulse Sequence	s2pul	Solvent	CHLOROFORM-D		
Sweep Width (Hz)	113636.37	Temperature (degree C)	22.000				



FW 457.4692 Formula C₂₃H₁₈F₃N₃O₂S

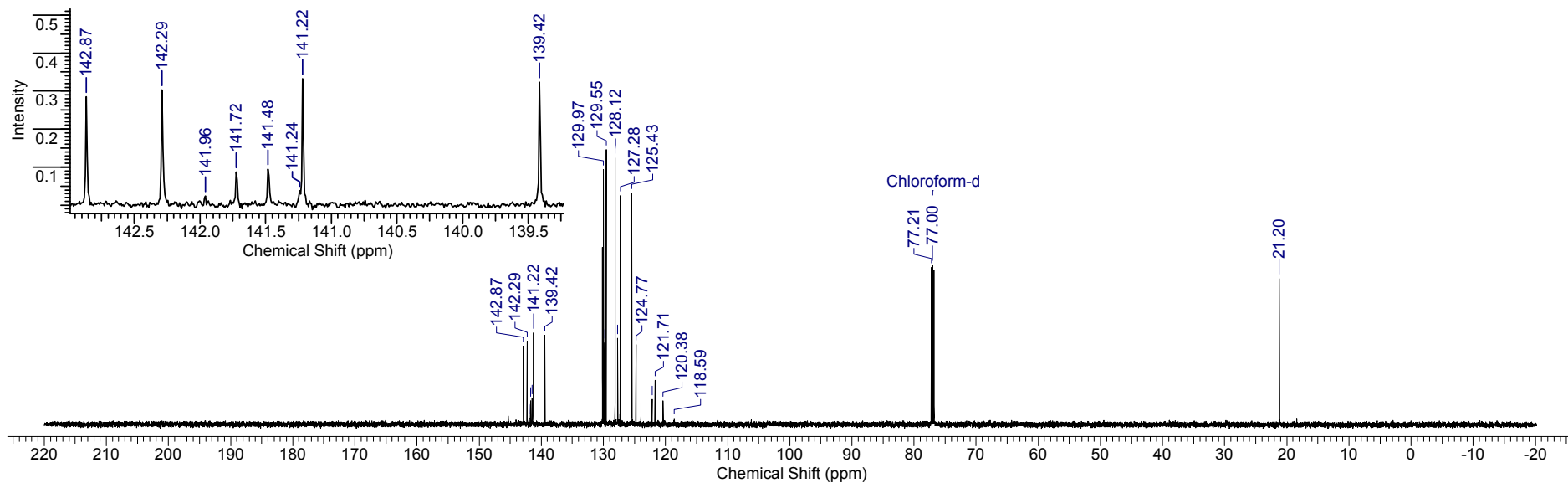
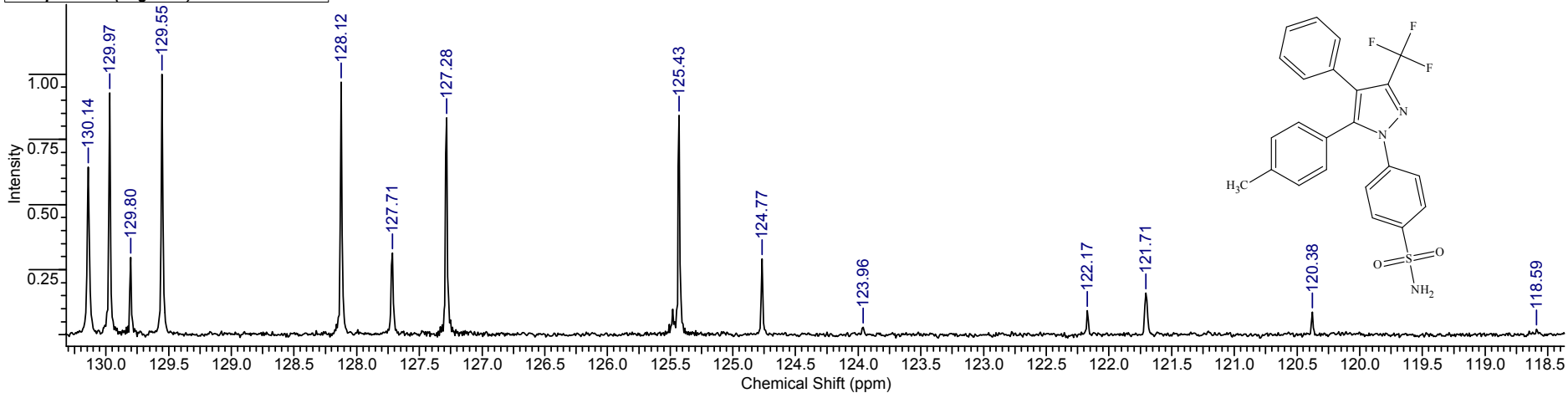
Acquisition Time (sec)	1.3631	Date	15 Aug 2017 10:51:42	Frequency (MHz)	600.13
File Name	C:\BM_DATA\DOCS\SPEC_BM_H,C_V-VIII.2017\BM-1155-p_001001r			Points Count	131072
Nucleus	1H	Number of Transients	4	Original Points Count	16384
Pulse Sequence	zg30	Solvent	CHLOROFORM-D	Sweep Width (Hz)	12019.23
Temperature (degree C)	25.000				



¹H NMR spectrum of 8 (600.2 MHz, CDCl₃)

FW	457.4692	Formula	C ₂₃ H ₁₈ F ₃ N ₃ O ₂ S
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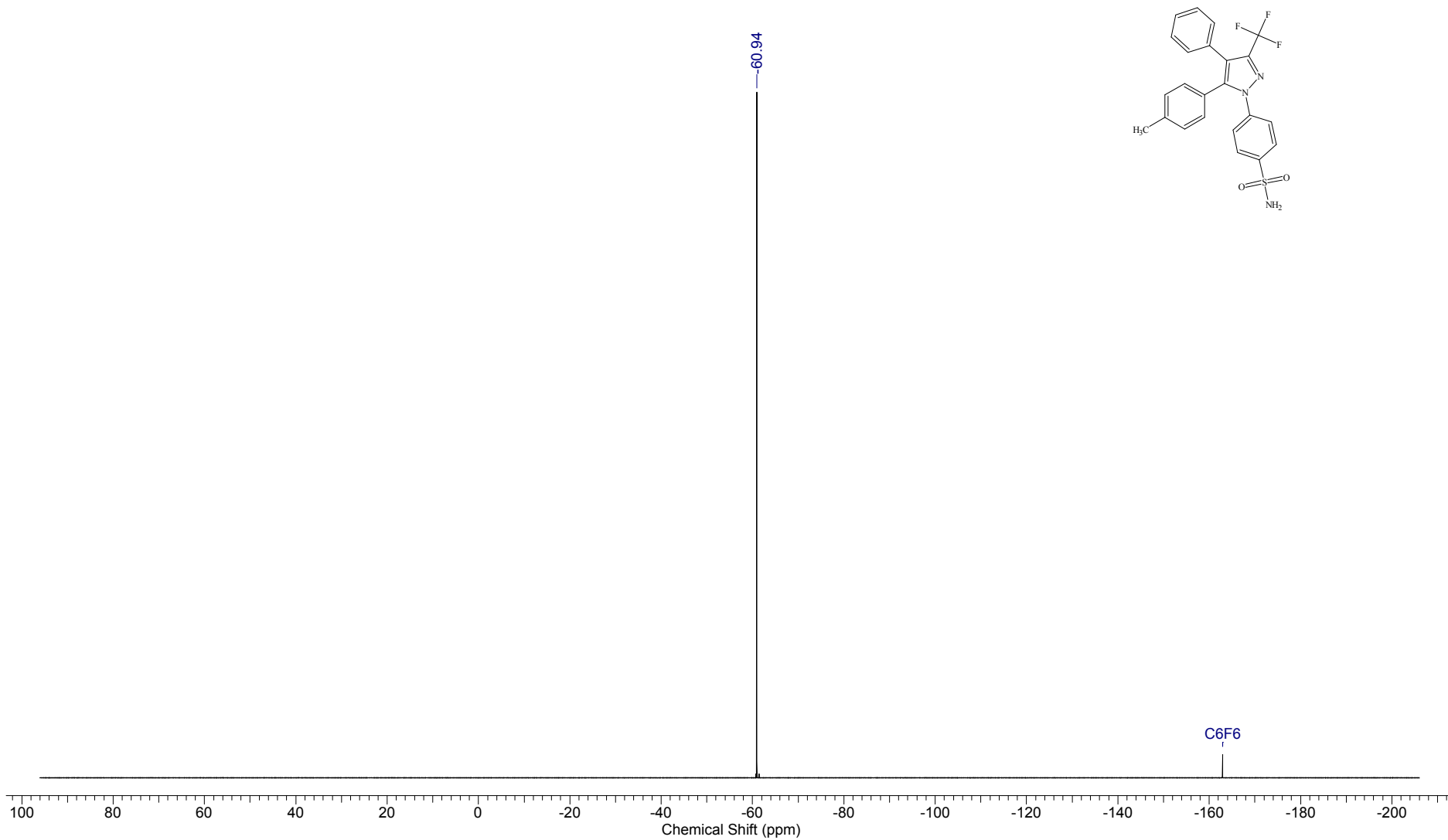
Acquisition Time (sec)	0.4522	Date	15 Aug 2017 10:49:50	Frequency (MHz)	150.90
File Name	C:\BM_DATA\DOCS\SPEC_BM_H,C_V-VIII.2017\BM-1155-p_013001r			Points Count	32768
Nucleus	¹³ C	Number of Transients	98	Original Points Count	16384
Pulse Sequence	zpgpg30	Solvent	CHLOROFORM-D	Sweep Width (Hz)	36231.88
Temperature (degree C)	25.000				



¹³C NMR spectrum of **8** (150.9 MHz, CDCl₃)

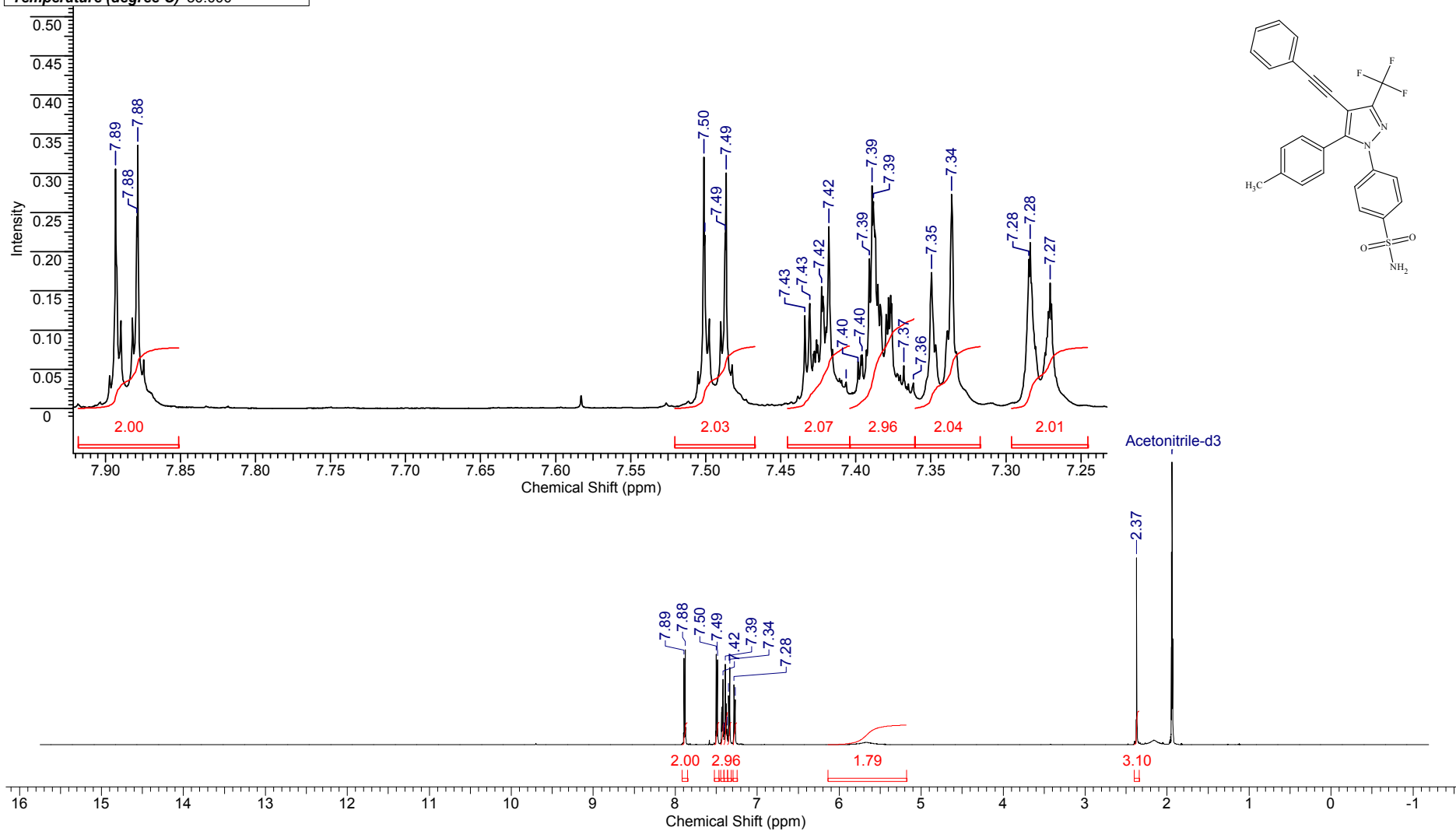
FW	457.4692	Formula	C ₂₃ H ₁₈ F ₃ N ₃ O ₂ S
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Acquisition Time (sec)	1.4680	Date	Sep 4 2017	File Name	D:\BN\output\F19\F_2017\2017.09.04\BM-1155-p-F_20170904_01\FLUORINE_01		
Frequency (MHz)	376.32	Nucleus	19F	Number of Transients	8	Original Points Count	166818
Points Count	262144	Pulse Sequence	s2pul	Solvent	CHLOROFORM-D		
Sweep Width (Hz)	113636.37	Temperature (degree C)	22.000				



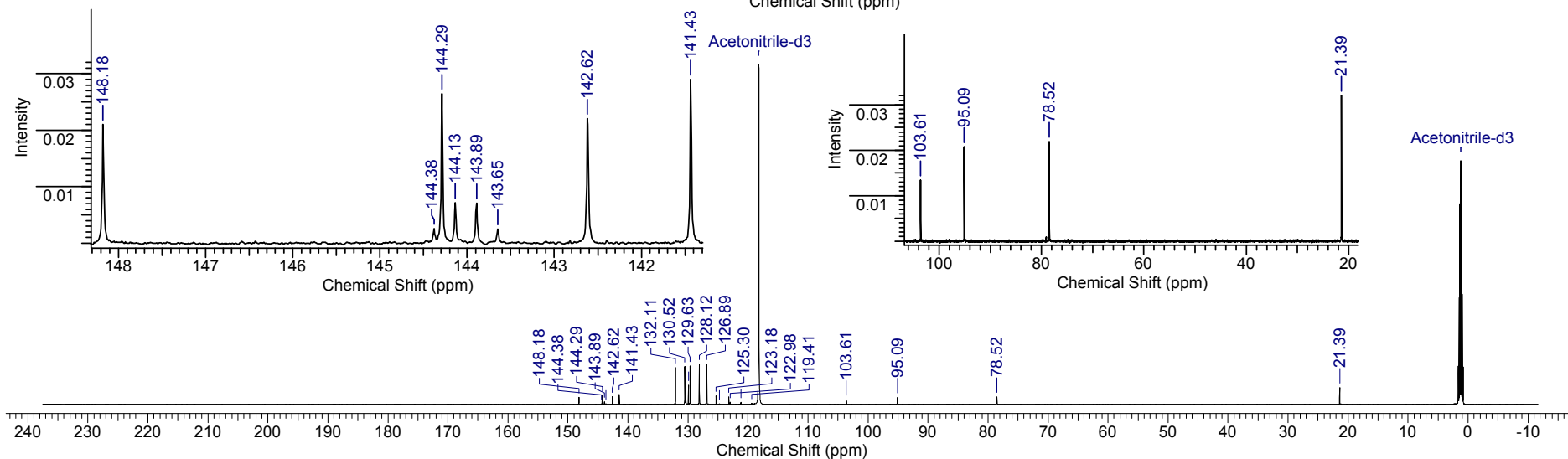
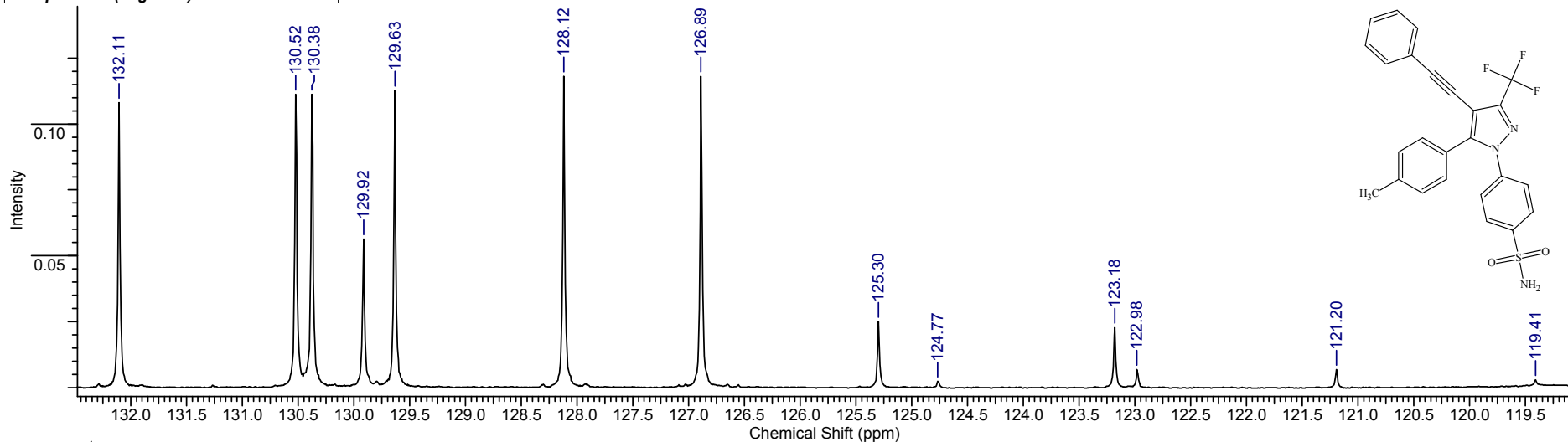
FW 481.4906 **Formula** C₂₅H₁₈F₃N₃O₂S

Acquisition Time (sec)	3.5479	Date	10 Aug 2017 19:29:02	Frequency (MHz)	600.13
File Name	C:\BM_DATA\DOCS\SPEC_BM_H,C_V-VIII.2017\BM-1156\BM-1156_001001r			Points Count	131072
Nucleus	1H	Number of Transients	9	Original Points Count	36056
Pulse Sequence	zg30	Solvent	ACETONITRILE-D3	Sweep Width (Hz)	10162.60
Temperature (degree C)	30.000				



FW 481.4906 Formula C₂₅H₁₈F₃N₃O₂S

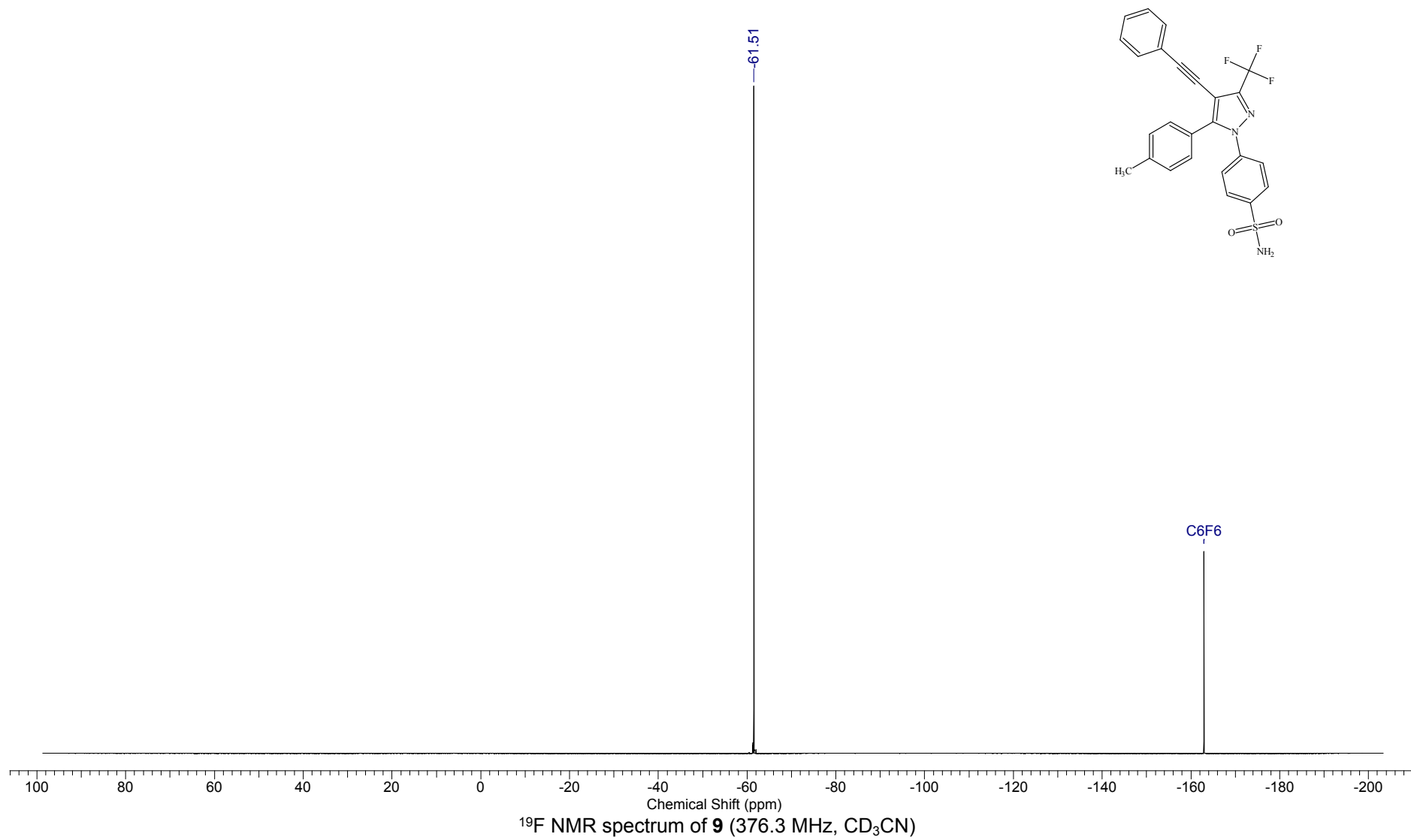
Acquisition Time (sec)	0.4783	Date	11 Aug 2017 16:37:22		
File Name	C:\BM_DATA\DOCS\SPEC_BM_H,C_V-VIII.2017\BM-1156\BM-1156_002001r			Frequency (MHz)	150.90
Nucleus	13C	Number of Transients	30586	Original Points Count	17983
Pulse Sequence	zgpg30	Solvent	ACETONITRILE-D3		
Temperature (degree C)	30.000			Sweep Width (Hz)	37593.98



¹³C NMR spectrum of **9** (150.9 MHz, CD₃CN)

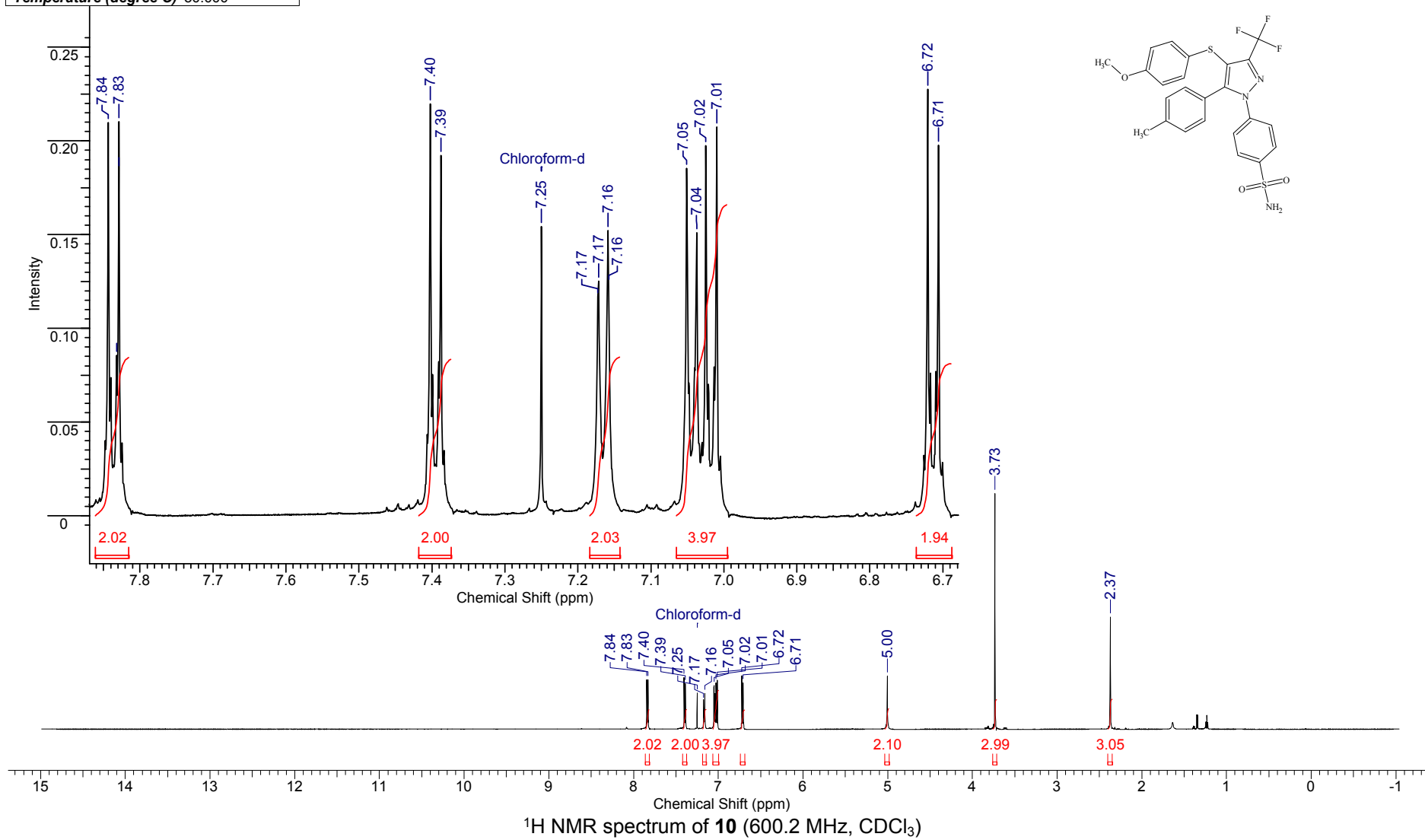
FW	481.4906	Formula	C ₂₅ H ₁₈ F ₃ N ₃ O ₂ S
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Acquisition Time (sec)	1.4680	Date	Sep 4 2017	File Name	D:\BN\output\F19\F_2017\2017.09.04\BM-1156-F_20170904_01\FLUORINE_01		
Frequency (MHz)	376.32	Nucleus	19F	Number of Transients	8	Original Points Count	166818
Points Count	262144	Pulse Sequence	s2pul	Solvent	ACETONITRILE-D3		
Sweep Width (Hz)	113636.37	Temperature (degree C)	22.000				



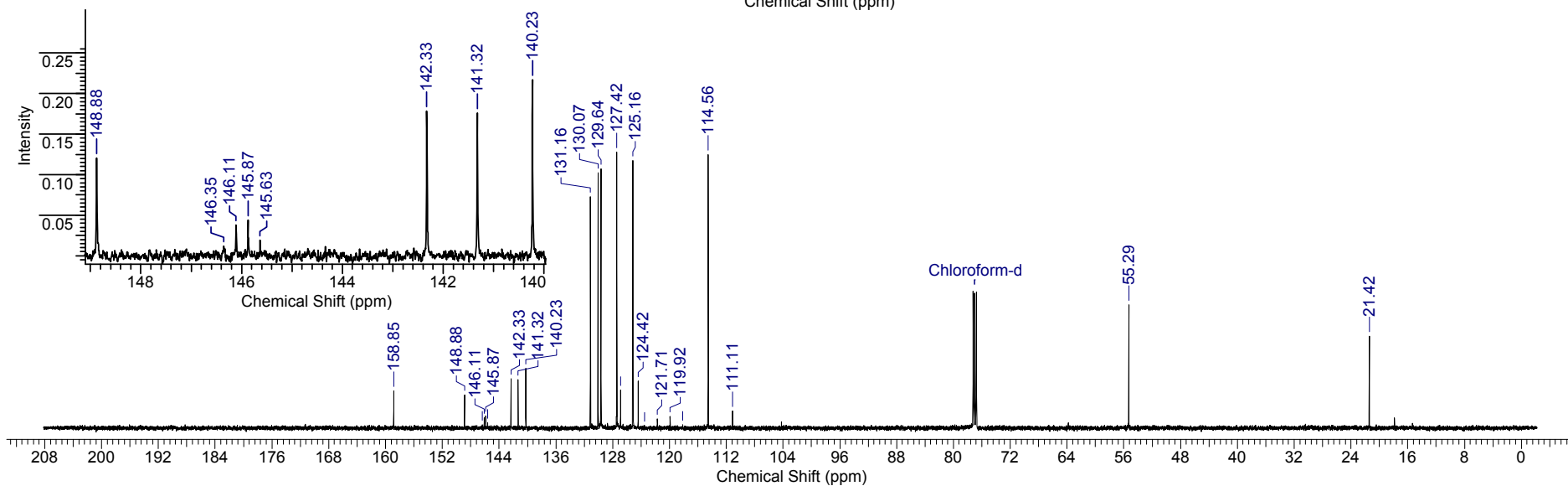
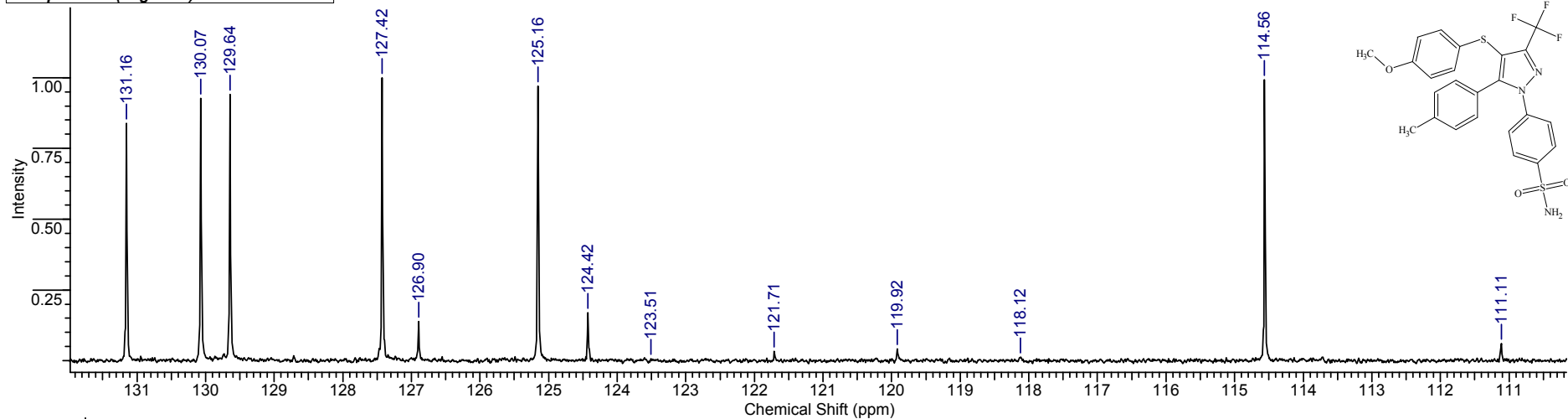
FW 519.5612 **Formula** C₂₄H₂₀F₃N₃O₃S₂

Acquisition Time (sec)	5.9999	Date	16 Aug 2017 19:47:56	Frequency (MHz)	600.13
File Name	C:\BM_DATA\DOCS\SPEC_BM_H,C_V-VIII.2017\BM-1157_cdcl3_001001r			Points Count	524288
Nucleus	1H	Number of Transients	16	Original Points Count	57691
Pulse Sequence	zg	Solvent	CHLOROFORM-D	Sweep Width (Hz)	9615.38
Temperature (degree C)	30.000				



FW	519.5612	Formula	C ₂₄ H ₂₀ F ₃ N ₃ O ₃ S ₂
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Acquisition Time (sec)	2.9999	Date	16 Aug 2017 20:16:08			
File Name	C:\BM_DATA\DOCS\SPEC_BM_H,C_V-VIII.2017\BM-1157_cdcl3_013001r			Frequency (MHz)	150.90	
Nucleus	13C	Number of Transients	256	Original Points Count	95236	
Pulse Sequence	zgpg	Solvent	CHLOROFORM-D		Points Count	262144
Temperature (degree C)	30.000			Sweep Width (Hz)	31746.03	



¹³C NMR spectrum of **10** (150.9 MHz, CDCl₃)

FW	519.5612	Formula	C ₂₄ H ₂₀ F ₃ N ₃ O ₃ S ₂
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Acquisition Time (sec)	2.0000	Date	Sep 4 2017	File Name	D:\BN\output\F19\F_2017\2017.09.04\BM-1157-F_20170904_01\FLUORINE_01		
Frequency (MHz)	376.32	Nucleus	19F	Number of Transients	8	Original Points Count	227273
Points Count	262144	Pulse Sequence	s2pul	Solvent	CHLOROFORM-D		
Sweep Width (Hz)	113636.37	Temperature (degree C)	22.000				

