A green, acid switchable approach to trifluoromethylated triazoles and isoxazoles via reaction of CF_3-ynones with sodium azide

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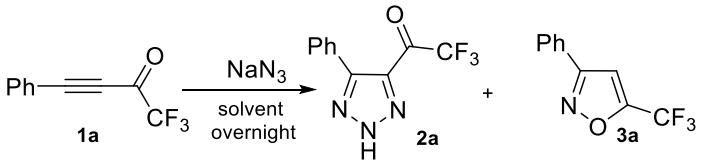
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Experimental section

General remarks. ^{1}H, ^{13}C and ^{19}F NMR spectra were recorded on Bruker AVANCE 400 MHz spectrometer in acetone-d_6, CD_3CN and $CDCl_3$ at 400, 100 and 376 MHz respectively. Chemical shifts (δ) in ppm are reported with the use of the residual acetone-d_5, CHD_2CN and chloroform signals (2.04, 1.94 and 7.25 for ^{1}H and 29.8, 1.3, 77.0 for ^{13}C) as internal reference. The ^{19}F chemical shifts were referenced to C_6F_6, (-162.9 ppm). The coupling constants (J) are given in Hertz (Hz). ESI-MS spectra were measured with an Orbitrap Elite instrument. One FT-IR spectrometer using consoles of internal reflection iS3 with ATR element from ZnSe, dip angle 45 °C. TLC analysis was performed on "Merck 60 F_{254}" plates. Column chromatography was performed on silica gel "Macherey-Nagel 0.063-0.2nm (Silica 60)". In all cases gravity column chromatography was used.. All reagents were of reagent grade and were used as such or were distilled prior to use. CF_3-ynones **1** were prepared as reported previously. Melting points were determined on an Electrothermal 9100 apparatus.

Investigation of reaction of CF_3-ynones with NaN_3 in various solvents. A 4 mL vial with a screw cap was charged with CF_3-ynone **1a** (0.099 g, 0.5 mmol), corresponding solvent (2 mL, see Table 1) and NaN_3 (0.039 g, 0.6 mmol, 1.2 equiv.). The reaction mixture was stirred overnight using magnetic stirrer. Composition of the reaction mixture was established by ^{19}F NMR using $PhCF_3$ as a standard for calculation of the products yields. Attention! All manipulations with any azides demand significant care due to safety reasons!

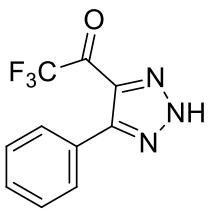
Table S1. Investigation of the solvent nature in the reaction of sodium azide with CF_3-ynone **1**.



Entry	Solvent	Yield of **2a**, %[a]	Yield of **3a**, %
1	PhMe	2	12
2	Acetone-H_2O	12	5
3	MeCN	26	7
4	THF	19	12
5	EtOAc-H_2O	23	14
6	DMF	49	2
7	DMSO	48	1
8	NMP	52	2
9	MeOH	77	4
10	EtOH	85(81[b])	3

[a]- by ^{19}F NMR; [b]-isolated yield.

Synthesis of triazoles 2 (general procedure). A 8 mL vial with a screw cap was charged with corresponding CF_3-ynone **1** (1 mmol), ethanol (4 mL) and NaN_3 (0.078 g, 1.2 mmol). The reaction mixture was stirred overnight using magnetic stirrer. Next, ethanol was evaporated in vacuo; the residue was suspended in the mixture of heptane-ethylacetate (1:1, 0.5-1 mL) and purified by column chromatography using gradient eluation by mixtures of heptane-ethylacetate (9:1, 3:1 and 1:1). Evaporation of the solvents afforded pure triazoles **2**.



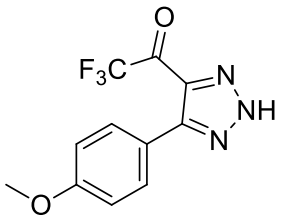
2,2,2-Trifluoro-1-(5-phenyl-2*H*-1,2,3-triazol-4-yl)ethanone (2a). Obtained from **1a** (0.202 g, 1.02 mmol). White crystals, m.p. 105-108 °C, yield 0.199 g (81%). ^1H NMR ($CDCl_3$, 400.1 MHz): δ 12.75 (br.s, 1H), 7.89-7.75 (m, 2H), 7.58-7.45 (m, 3H). $^{13}C\{^1H\}$ NMR ($CDCl_3$, 100.6 MHz): δ 174.4 (q, $^2J_{CF}$ = 37.2 Hz), 147.7, 136.1, 131.3, 129.0, 128.9, 125.1, 116.2 (q, $^1J_{CF}$ = 290.6 Hz). ^{19}F NMR ($CDCl_3$, 376.5 MHz): δ -75.0 (s, 3F). ^1H NMR (CD_3CN, 400.1 MHz): δ 12.75 (br.s, 1H), 7.85-7.74 (m, 2H), 7.61-7.49 (m, 3H). $^{13}C\{^1H\}$ NMR (CD_3CN, 100.6 MHz): δ 175.2 (q, $^2J_{CF}$ = 36.3 Hz), 148.1, 137.0, 131.7, 130.1, 129.6, 127.1, 117.4 (q, $^1J_{CF}$ = 290.2 Hz). ^{19}F NMR (CD_3CN, 376.5 MHz): δ -73.0 (s, 3F). ^1H NMR (Acetone-d6,

400.1 MHz): δ, 8.06-7.98 (m, 2H), 7.41-7.28 (m, 3H), 5.14 (br.s, 1H). $^{13}C\{^1H\}$ NMR (Acetone-d6, 100.6 MHz): δ 174.7 (q, $^2J_{CF}$ = 33.4 Hz), 152.0, 136.1, 133.5, 129.5, 128.51, 128.45, 118.6 (q, $^1J_{CF}$ = 291.6 Hz). ^{19}F NMR (Acetone-d6, 376.5 MHz): δ -70.7 (s, 3F).

HRMS (ESI-TOF): m/z $[M+H]^+$ Calcd for $C_{10}H_7F_3N_3O^+$: 242.0536; found: 242.0536.

IR (ν, cm^{-1}): 1719 (C=O).

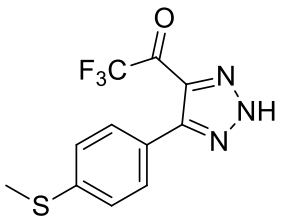
2,2,2-Trifluoro-1-(5-(4-methoxyphenyl)-2*H*-1,2,3-triazol-4-yl)ethanone (2b). Obtained from **1b** (0.228 g, 1 mmol). Pale brown solid, m.p. 100-102 °C, yield 0.216 g (80%). ^1H NMR ($CDCl_3$, 400.1 MHz): δ 13.87 (br.s, 1H), 7.84 (d, 2H, ^3J = 8.8 Hz), 7.97 (d, 2H, ^3J = 8.8 Hz), 3.84 (s, 3H). $^{13}C\{^1H\}$ NMR ($CDCl_3$, 100.6 MHz): δ 174.2 (q, $^2J_{CF}$ = 37.0 Hz), 162.0, 146.7, 135.5, 130.7, 116.5, 116.3 (q, $^1J_{CF}$ = 290.7 Hz), 114.3, 55.4. ^{19}F NMR ($CDCl_3$, 376.5 MHz): δ -74.7 (s, 3F). ^1H NMR (Acetone-d6, 400.1 MHz): δ 13.41 (br.s, 1H), 7.91 (d, 2H, ^3J = 7.9 Hz), 7.08 (d, 2H, ^3J = 8.0 Hz), 3.88 (s, 3H). $^{13}C\{^1H\}$ NMR (Acetone-d6, 100.6 MHz): δ 175.0 (q, $^2J_{CF}$ = 36.0 Hz), 162.4, 147.9, 136.2, 131.5, 127.8, 117.5 (q, $^1J_{CF}$ = 290.6 Hz), 114.7, 55.7. ^{19}F NMR (Acetone-d6, 376.5 MHz): δ -72.6 (s, 3F).



HRMS (ESI-TOF): m/z $[M+H]^+$ Calcd for $C_{11}H_9F_3N_3O_2^+$: 272.0641; found: 272.0641.

IR (ν, cm^{-1}): 1719 (C=O).

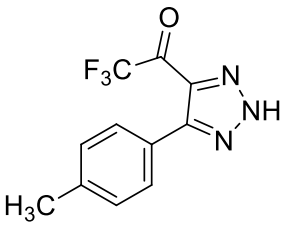
2,2,2-Trifluoro-1-(5-(4-methylthio)phenyl)-2*H*-1,2,3-triazol-4-yl)ethanone (2c). Obtained from **1c** (0.123 g, 0.504 mmol). Pale yellow-brown solid, m.p. 102-104 °C, yield 0.110 g (76%). ^1H NMR ($CDCl_3$, 400.1 MHz): δ 13.99 (br.s, 1H), 7.75 (d, 2H, ^3J = 8.4 Hz), 7.26 (d, 2H, ^3J = 7.9 Hz), 2.5 (s, 3H). $^{13}C\{^1H\}$ NMR ($CDCl_3$, 100.6 MHz): δ 174.2 (q, $^2J_{CF}$ = 37.2 Hz), 147.0, 143.7, 135.7, 129.1, 125.5, 120.7 (d, $^4J_{CF}$ = 1.6 Hz), 116.2 (q, $^1J_{CF}$ = 290.8 Hz), 14.7. ^{19}F NMR ($CDCl_3$, 376.5 MHz): δ -74.8 (s, 3F).



HRMS (ESI-TOF): m/z $[M+H]^+$ Calcd for $C_{11}H_9F_3N_3OS^+$: 288.0413; found: 288.0417.

IR (ν, cm^{-1}): 1722 (C=O).

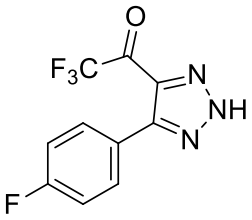
2,2,2-Trifluoro-1-(5-(*p*-tolyl)-2*H*-1,2,3-triazol-4-yl)ethanone (2d). Obtained from **1d** (0.424 g, 2 mmol). Pale beige powder, m.p. 128-130 °C, yield 0.395 g (77%). ^{1}H NMR ($CDCl_3$, 400.1 MHz): δ 13.41 (br.s, 1H), 7.72 (d, 2H, ^{3}J = 7.9 Hz), 7.28 (d, 2H, ^{3}J = 8.0 Hz), 2.41 (s, 3H). $^{13}C\{^{1}H\}$ NMR ($CDCl_3$, 100.6 MHz): δ 174.2 (q, $^{2}J_{CF}$ = 37.1 Hz), 146.9 (q, $^{4}J_{CF}$ = 2.3 Hz), 142.0, 135.6, 129.5, 128.9, 121.4, 116.2 (q, $^{1}J_{CF}$ = 290.7 Hz), 21.4. ^{19}F NMR ($CDCl_3$, 376.5 MHz): δ -75.0 (s, 3F).



HRMS (ESI-TOF): m/z $[M+H]^+$ Calcd for $C_{11}H_9F_3N_3O^+$: 256.0692; found: 256.0692.

IR (ν, cm^{-1}): 1719 (C=O).

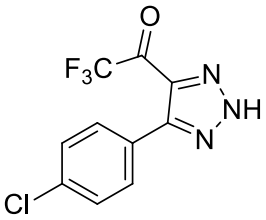
2,2,2-Trifluoro-1-(5-(4-fluorophenyl)-2*H*-1,2,3-triazol-4-yl)ethanone (2e). Obtained from **1e** (0.110 g, 0.509 mmol). Pale beige solid, m.p. 85-87 °C, yield 0.092 g (70%). ^{1}H NMR ($CDCl_3$, 400.1 MHz): δ 11.12 (br.s, 1H), 7.90-7.79 (m, 2H), 7.15 (t, 2H, ^{3}J = 8.3 Hz). $^{13}C\{^{1}H\}$ NMR ($CDCl_3$, 100.6 MHz): δ 174.3 (q, $^{2}J_{CF}$ = 37.4 Hz), 164.3 (d, $^{1}J_{CF}$ = 252.8 Hz), 147.5, 136.0, 131.3 (d, $^{3}J_{CF}$ = 8.8 Hz), 121.7, 116.2 (q, $^{1}J_{CF}$ = 290.5 Hz), 116.0 (d, $^{2}J_{CF}$ = 22.1 Hz). ^{19}F NMR ($CDCl_3$, 376.5 MHz): δ -75.0 (s, 3F), 109.1 (s, 1F).



HRMS (ESI-TOF): m/z $[M+H]^+$ Calcd for $C_{10}H_6F_4N_3O^+$: 260.0442; found: 260.0447.

IR (ν, cm^{-1}): 1726 (C=O).

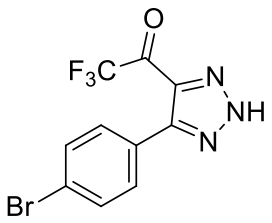
1-(5-(4-Chlorophenyl)-2*H*-1,2,3-triazol-4-yl)-2,2,2-trifluoroethanone (2f). Obtained from **1f** (0.233 g, 1 mmol). Pale beige solid, m.p. 83-85 °C, yield 0.203 g (74%). ^{1}H NMR ($CDCl_3$, 400.1 MHz): δ 14.05 (br.s, 1H), 7.75 (d, 2H, ^{3}J = 8.3 Hz), 7.42 (d, 2H, ^{3}J = 8.2 Hz). $^{13}C\{^{1}H\}$ NMR ($CDCl_3$, 100.6 MHz): δ 174.3 (q, $^{2}J_{CF}$ = 37.3 Hz), 147.1, 137.5, 136.0, 130.3, 129.1, 123.6, 116.1 (q, $^{1}J_{CF}$ = 290.6 Hz). ^{19}F NMR ($CDCl_3$, 376.5 MHz): δ -74.9 (s, 3F).



HRMS (ESI-TOF): m/z $[M+H]^+$ Calcd for $C_{10}H_6[^{35}Cl]F_3N_3O^+$: 276.0146; found: 276.0151; Calcd for $C_{10}H_6[^{37}Cl]F_3N_3O^+$: 278.0117; found: 278.0121.

IR (ν, cm^{-1}): 1726 (C=O).

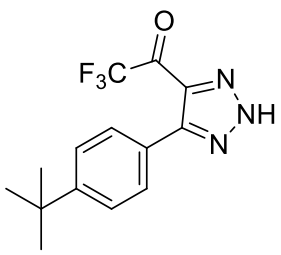
1-(5-(4-Bromophenyl)-2*H*-1,2,3-triazol-4-yl)-2,2,2-trifluoroethanone (2g). Obtained from **1g** (0.186 g, 0.671 mmol). Pale beige solid, m.p. 82-84 °C, yield 0.166 g (77%). ^{1}H NMR ($CDCl_3$, 400.1 MHz): δ 13.39 (br.s, 1H), 7.69 (d, 2H, ^{3}J = 8.5 Hz), 7.59 (d, 2H, ^{3}J = 8.5 Hz). $^{13}C\{^{1}H\}$ NMR ($CDCl_3$, 100.6 MHz): δ 174.3 (q, $^{2}J_{CF}$ = 37.7 Hz), 147.5, 136.1, 132.1, 130.5, 125.8, 124.4, 116.1 (q, $^{1}J_{CF}$ = 290.3 Hz). ^{19}F NMR ($CDCl_3$, 376.5 MHz): δ -75.0 (s, 3F).



HRMS (ESI-TOF): m/z $[M+H]^+$ Calcd for $C_{10}H_6[^{79}Br]F_3N_3O^+$: 319.9641; found: 319.9646; m/z $[M+H]^+$ Calcd for $C_{10}H_6[^{81}Br]F_3N_3O^+$: 321.9620; found: 321.9625.

IR (ν, cm^{-1}): 1723 (C=O).

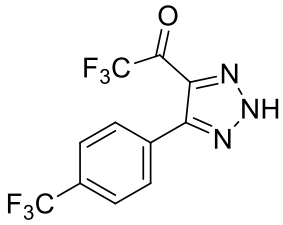
1-(5-(4-(*Tret*-butyl)phenyl)-2*H*-1,2,3-triazol-4-yl)-2,2,2-trifluoroethanone (2h). Obtained from **1h** (0.130 g, 0.512 mmol). Light brown powder, m.p. 140-143 °C, yield 0.123 g (81%). ^{1}H NMR ($CDCl_3$, 400.1 MHz): δ 14.12 (br.s, 1H), 7.82 (d, 2H, ^{3}J = 8.3 Hz), 7.53 (d, 2H, ^{3}J = 8.2 Hz), 1.35 (s, 9H). $^{13}C\{^{1}H\}$ NMR ($CDCl_3$, 100.6 MHz): δ 174.3 (q, $^{2}J_{CF}$ = 37.1 Hz), 155.1, 147.0, 135.9, 128.8, 126.0, 121.6, 116.3 (q, $^{1}J_{CF}$ = 290.7 Hz), 35.0, 31.0. ^{19}F NMR ($CDCl_3$, 376.5 MHz): δ -74.9 (s, 3F).



HRMS (ESI-TOF): m/z $[M+H]^+$ Calcd for $C_{14}H_{15}F_3N_3O^+$: 298.1162; found: 298.1166.

IR (ν, cm^{-1}): 1713 (C=O).

2,2,2-Trifluoro-1-(5-(4-trifluoromethyl)phenyl)-2*H*-1,2,3-triazol-4-yl)ethanone (2i). Obtained from **1i** (0.268 g, 1.01 mmol). Pale yellow solid, m.p. 67-69 °C, yield 0.230 g (74%). ^{1}H NMR ($CDCl_3$, 400.1 MHz): δ 10.94 (br.s, 1H), 7.94 (d, 2H, ^{3}J = 8.2 Hz), 7.71 (d, 2H, ^{3}J = 8.3 Hz). $^{13}C\{^{1}H\}$ NMR ($CDCl_3$, 100.6 MHz): δ 174.5 (q, $^{2}J_{CF}$ = 37.8 Hz), 148.2, 136.5, 132.6 (q, $^{2}J_{CF}$ = 32.9 Hz), 129.8, 129.5, 125.7 (q, $^{3}J_{CF}$ = 3.6 Hz), 123.6 (q, $^{1}J_{CF}$ = 272.4 Hz), 116.1 (q, $^{1}J_{CF}$ = 290.4 Hz). ^{19}F NMR ($CDCl_3$, 376.5 MHz): δ -64.2 (s, 3F), -75.1 (s, 3F).



HRMS (ESI-TOF): m/z $[M+H]^+$ Calcd for $C_{11}H_6F_6N_3O^+$: 310.0410; found: 310.0416.

IR (ν, cm^{-1}): 1718 (C=O).

1-(5-(3,4-Dimethylphenyl)-2*H*-1,2,3-triazol-4-yl)-2,2,2-trifluoroethanone (2j). Obtained from **1j** (0.118 g, 0.522 mmol). Pale brown solid, m.p. 76-78 °C, yield 0.114 g (81%). ^{1}H NMR ($CDCl_3$, 400.1 MHz): δ 14.05 (br.s, 1H), 7.63-7.50 (m, 2H), 7.21 (d, 1H, ^{3}J = 7.7 Hz), 2.30 (s, 3H), 2.28 (s, 3H). $^{13}C\{^{1}H\}$ NMR ($CDCl_3$, 100.6 MHz): δ 174.2 (q, $^{2}J_{CF}$ = 37.1 Hz), 146.9, 140.7, 137.4, 135.6, 130.1, 129.8, 126.4, 121.8, 116.3 (q, $^{1}J_{CF}$ = 290.7 Hz), 19.8, 19.6. ^{19}F NMR ($CDCl_3$, 376.5 MHz): δ -74.8 (s, 3F).

HRMS (ESI-TOF): m/z $[M+H]^+$ Calcd for $C_{12}H_{11}F_3N_3O^+$: 270.0849; found: 270.0856.

IR (ν, cm^{-1}): 1722 (C=O).

1-(5-(2,3-dihydrobenzo[*b*][1,4]dioxin-6-yl)-2*H*-1,2,3-triazol-4-yl)-2,2,2-trifluoroethanone (2k). Obtained from **1k** (0.240 g, 1.025 mmol). Slightly yellow oil, yield 0.218 g (71%). ^{1}H NMR ($CDCl_3$, 400.1 MHz): δ 13.85 (br.s, 1H), 7.35 (s, 1H), 7.31 (d, 1H, ^{3}J = 8.5 Hz), 6.90 (d, 1H, ^{3}J = 8.4 Hz), 4.31-4.23 (m, 4H). $^{13}C\{^{1}H\}$ NMR ($CDCl_3$, 100.6 MHz): δ 174.3 (q, $^{2}J_{CF}$ = 37.0 Hz), 146.9, 146.2, 143.5, 135.6, 122.5, 120.6, 118.1, 117.7, 117.8 (q, $^{4}J_{CF}$ = 3.1 Hz), 116.3 (q, $^{1}J_{CF}$ = 290.7 Hz), 64.5, 64.1. ^{19}F NMR ($CDCl_3$, 376.5 MHz): δ -74.8 (s, 3F).

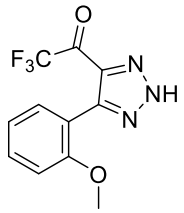
HRMS (ESI-TOF): m/z $[M+H]^+$ Calcd for $C_{12}H_9F_3N_3O_3^+$: 300.0591; found: 300.0595.

IR (ν, cm^{-1}): 1717 (C=O).

1-(5-(2-Chlorophenyl)-2*H*-1,2,3-triazol-4-yl)-2,2,2-trifluoroethanone (2l). Obtained from **1l** (0.237 g, 1.015 mmol). Pale brown viscous oil, yield 0.164 g (59%). ^{1}H NMR ($CDCl_3$, 400.1 MHz): δ 13.55 (br.s, 1H), 7.80-7.25 (m, 4H). $^{13}C\{^{1}H\}$ NMR ($CDCl_3$, 100.6 MHz): δ 173.9 (q, $^{2}J_{CF}$ = 38.1 Hz), 145.0, 137.7, 133.5, 131.8, 131.3, 129.9, 126.9, 125.3, 115.8 (q, $^{1}J_{CF}$ = 290.2 Hz). ^{19}F NMR ($CDCl_3$, 376.5 MHz): δ -75.6 (s, 3F).

HRMS (ESI-TOF): m/z $[M+H]^+$ Calcd for $C_{10}H_6[^{35}Cl]F_3N_3O^+$: 276.0146; found: 276.0149; Calcd for $C_{10}H_6[^{37}Cl]F_3N_3O^+$: 278.0117; found: 278.0118.

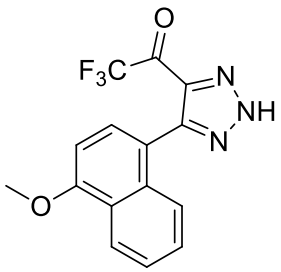
IR (ν, cm^{-1}): 1726 (C=O).



2,2,2-Trifluoro-1-(5-(2-methoxyphenyl)-2*H*-1,2,3-triazol-4-yl)ethanone (2m). Obtained from **1m** (0.195 g, 0.867 mmol). Pale brown solid, m.p. 130-132 °C, yield 0.097 g (41%). ^{1}H NMR ($CDCl_3$, 400.1 MHz): δ 10.67 (br.s, 1H), 7.61 (dd, 1H, ^{3}J = 8.5 Hz, ^{4}J = 8.5 Hz), 7.42-7.38 (m, 1H), 7.00-6.94 (m, 2H), 3.74 (s, 3H). $^{13}C\{^{1}H\}$ NMR ($CDCl_3$, 100.6 MHz): δ 174.6 (q, $^{2}J_{CF}$ = 36.5 Hz), 156.4, 142.0, 136.6, 132.1, 130.7, 120.3, 116.0 (q, $^{1}J_{CF}$ = 290.6 Hz), 113.7, 110.8, 55.2. ^{19}F NMR ($CDCl_3$, 376.5 MHz): δ -74.7 (s, 3F).

HRMS (ESI-TOF): m/z $[M+H]^+$ Calcd for $C_{11}H_9F_3N_3O_2^+$: 272.0641; found: 272.0625.

2,2,2-Trifluoro-1-(5-(4-methoxynaphthalen-1-yl)-2*H*-1,2,3-triazol-4-yl)ethanone (2n). Obtained from **1n** (0.215 g, 0.773 mmol). Slightly yellow oil,

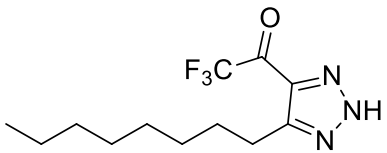


yield 0.127 g (51%). ^{1}H NMR ($CDCl_3$, 400.1 MHz): δ 13.00 (br.s, 1H), 8.36-8.30 (m, 1H), 7.53-7.36 (m, 4H), 6.81 (d, 1H, ^{3}J = 7.9 Hz), 4.04 (s, 3H). $^{13}C\{^{1}H\}$ NMR ($CDCl_3$, 100.6 MHz): δ 173.9 (q, $^{2}J_{CF}$ = 37.6 Hz), 157.7, 145.8, 137.8, 131.8, 129.6, 127.9, 125.9, 125.5, 123.7, 122.8, 116.0 (q, $^{1}J_{CF}$ = 290.4 Hz), 114.4 103.0, 55.7. ^{19}F NMR ($CDCl_3$, 376.5 MHz): δ -75.4 (s, 3F).

HRMS (ESI-TOF): m/z $[M+H]^+$ Calcd for $C_{15}H_{11}F_3N_3O_2^+$: 322.0798; found: 322.0805.

IR (ν, cm^{-1}): 1720 (C=O).

2,2,2-Trifluoro-1-(5-octyl-2*H*-1,2,3-triazol-4-yl)ethanone (2o). Obtained from **1o** (0.122 g, 0.521 mmol). Pale brown solid, m.p. 66-68 °C, yield 0.082 g



(56%). ^{1}H NMR ($CDCl_3$, 400.1 MHz): δ 13.73 (br.s, 1H), 3.21-3.07 (m, 2H), 1.75-1.65 (m, 2H), 1.37-1.19 (m, 10H), 0.87-0.81 (m, 3H). $^{13}C\{^{1}H\}$ NMR ($CDCl_3$, 100.6 MHz): δ 174.7 (q, $^{2}J_{CF}$ = 37.1 Hz), 149.3, 136.8, 116.1 (q, $^{1}J_{CF}$ = 290.4 Hz), 31.7, 29.1, 29.0, 28.3, 24.1, 22.6, 14.0. ^{19}F NMR ($CDCl_3$, 376.5 MHz): δ -75.4 (s, 3F).

HRMS (ESI-TOF): m/z $[M+H]^+$ Calcd for $C_{12}H_{19}F_3N_3O^+$: 278.1475; found: 278.1475.

IR (ν, cm^{-1}): 1721 (C=O).

Synthesis of triazoles 2a,b (sub-gram scale, general procedure). A 25 mL one-neck round-bottom flask was charged with corresponding CF_3-ynone **1** (5 mmol), ethanol (5 mL) and cooled down to 0 ºC at ice bath. Next, NaN_3 (0.390 g, 6 mmol) was added and the reaction mixture was stirred overnight using magnetic stirrer. Next, ethanol was evaporated *in vacuo*. The residue was dispersed in water (4 mL) and washed twice with a mixture heptane-ethylacetate

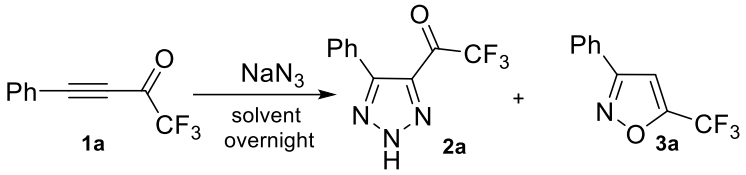
(1:1, 1 mL). Organic phase was thrown away; water phase was acidified by dropwise addition of concentrated HCl (0.8 mL, ~9-10 mmol) to form a precipitate. Water phase was decanted and the precipitate left was dried *in vacuo*.

2,2,2-Trifluoro-1-(5-phenyl-2*H*-1,2,3-triazol-4-yl)ethanone (2a), sub-gram scale synthesis. Obtained from **1a** (1.019 g, 5.146 mmol). White crystals, m.p. 105-108 °C, yield 0.994 g (80%). Calculation of E-factor: E-factor=(mass of all reagents and solvents used)/(mass of the isolated product)=(1.019+0.390+5mL(EtOH)*0.789+4mL(H_2O)*1+ 2mL(Heptane)*0.684+2mL(EtOAc)*0.902+0.8 mL (HCl)*1.2))/(0.994 g)=13.509/0.994=13.6.

2,2,2-Trifluoro-1-(5-(4-methoxyphenyl)-2*H*-1,2,3-triazol-4-yl)ethanone (2b), sub-gram scale synthesis. Obtained from **1b** (0.674 g, 1 mmol). Pale brown solid, m.p. 100-102 °C, yield 0.681 g (85%).

Investigation of reaction of CF_3-ynones with NaN_3 in various solvents in the presence of acids. A 4 mL vial with a screw cap was charged with CF_3-ynone **1a** (0.099 g, 0.5 mmol), corresponding solvent (2 mL, see Table SI2), corresponding acid (for quantity of acid see Table SI2) and NaN_3 (for quantity see Table SI2). The reaction mixture was stirred for 1 day using magnetic stirrer. Composition of the reaction mixture was established by ^{19}F NMR using $PhCF_3$ as a standard for calculation of the products yields.

Table S2. Investigation of the solvent and acid nature in the reaction of sodium azide with CF_3-ynone **1a**.



Entry	Solvents	Reagents	Yield of **2a**, %[a]	Yield of **3a**, %[a]
1	EtOH	NaN_3(2 eq)/ HCO_2H(4 eq.)	3	42
2	EtOH	NaN_3(2 eq)/ AcOH(4 eq.)	7	42 (34[b])
3	EtOH(dry)	NaN_3(2 eq)/ AcOH(4 eq.)	4	42
4	EtOH	NaN_3(2 eq)/ $ClCH_2CO_2H$(4 eq.)	4	41
5	EtOH	NaN_3(2 eq)/ TFA(4 eq.)	10	36
6	EtOH	NaN_3(2 eq)/ $MeSO_3H$(2.1 eq.)	9	9
7	EtOH	NaN_3(1.2 eq)/ HCl (~1 eq)	2	3
8	Heptane-H_2O (10/1)	NaN_3(2 eq)/ AcOH(4 eq.)	2	35
9	Heptane-H_2O (10/1)	NaN_3(5 eq)/ AcOH(6 eq.)	2	40(36[b])
10	Heptane-H_2O (10/1)	NaN_3(2 eq)/ HCO_2H(4 eq.)	2	35
11	Heptane-H_2O (10/1)	NaN_3(2 eq)/ $ClCH_2CO_2H$(4 eq.)	1	35
12	Heptane-H_2O (10/1)	NaN_3(4 eq)/ TEBAC (1 eq.)	-	traces
13	MeOH	NaN_3(2 eq)/ AcOH(4 eq.)	5	35

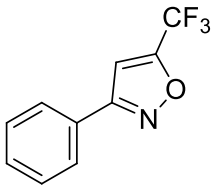
14	dioxane	NaN_3(5 eq), AcOH (5 eq.)	1	41
15	TCE	NaN_3(2 eq)/ AcOH(4 eq.)	-	34
16	toluene	NaN_3(5 eq), AcOH (5 eq.)	traces	41 (30[b])
17	EtOAc	NaN_3(5 eq), AcOH (6 eq.)	2	40
18	CF_3CH_2OH	NaN_3(1.2 eq)	-	37
19	AcOH	NaN_3(5 eq)	traces	36
20	AcOH	NaN_3(1.2 eq)	traces	35
21	Heptane-H_2O (10/1)	NaN_3(2 eq)/ $MeSO_3H$(2.1 eq.)	2	4 (conversion 7%)
22	dioxane	NaN_3(1.2 eq) $MeSO_3H$ (1 eq)	5	3 (conversion 11%)

[a]- by ^{19}F NMR; [b]-isolated yield.

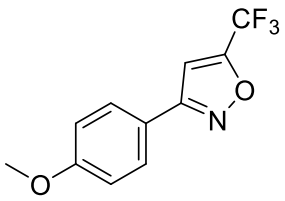
Synthesis of isoxazoles 3 in ethanol (general procedure A). A 8 mL vial with a screw cap was charged with corresponding CF_3-ynone **1** (0.5 mmol), ethanol (2 mL), acetic acid (0.120 g, 2 mmol, 4 equiv.) and NaN_3 (0.065 g, 1 mmol, 2 equiv.). The reaction mixture was stirred overnight using magnetic stirrer. Next, ethanol was evaporated in vacuo at room temperature (careful! isoxazoles 4a, 4x are quite volatile); the residue was suspended in the mixture of heptane-ethylacetate (3:1, 0.5) and passed through a short silica gel pad using gradient eluating by heptane and mixture of heptane-ethylacetate (9:1). Evaporation of the solvents afforded pure isoxazoles **3**.

Synthesis of isoxazoles 3 in heptane (general procedure B). A 8 mL vial with a screw cap was charged with corresponding CF_3-ynone **1** (0.5 mmol), heptane (4 mL), water (0.5 mL)acetic acid (0.120 g, 2 mmol, 4 equiv.) and NaN_3 (0.065 g, 1 mmol, 2 equiv.). The reaction mixture was stirred overnight using magnetic stirrer. Next, heptane phase was separated, water phase was extracted with a mixture of heptane-ethylacetate (9:1, 2x0.5 mL) combined extract was passed through a short silica gel pad using gradient eluating by heptane followed by mixtures of heptane-ethylacetate (9:1). Evaporation of the solvents afforded pure isoxazoles **3**.

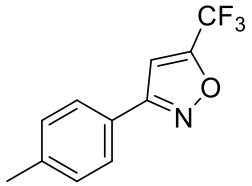
3-Phenyl-5-(trifluoromethyl)isoxazole (3a). Obtained from **1a** (0.099 g, 0.5 mmol (A); 0.100 g, 0.505 mmol (B)). White crystals, m.p. 74-77 °C (Lit.: 73.3-74 °C, 76-78 °C), yield 0.037 g (35%, (A)); 0.039 g (36%, (B)). ^{1}H NMR ($CDCl_3$, 400.1 MHz): δ 7.85-7.76 (m, 2H), 7.54-7.44 (m, 3H), 7.0 (s, 1H). $^{13}C\{^{1}H\}$ NMR ($CDCl_3$, 100.6 MHz): δ 162.5, 159.1 (q, $^{2}J_{CF}$ = 42.6 Hz), 130.9, 129.2, 127.3, 126.9, 117.9 (q, $^{1}J_{CF}$ = 270.3 Hz), 103.4 (q, $^{4}J_{CF}$ = 2.0 Hz). ^{19}F NMR ($CDCl_3$, 376.5 MHz): δ -65.3 (s, 3F). NMR data are in agreement with those in the literature[Error! Bookmark not defined.].



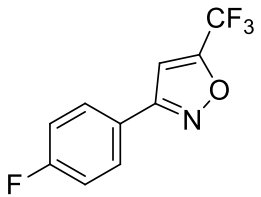
3-(4-Methoxyphenyl)-5-(trifluoromethyl)isoxazole (3b). Obtained from **1b** (0.114 g, 0.5 mmol (A); 0.110 g, 0.482 mmol (B)). Pale yellow solid, m.p. 72-74 °C (Lit.: 72-75 °C[Error! Bookmark not defined.]), yield 0.021 g (17%, (A)); 0.019 g (16%, (B)). ^{1}H NMR ($CDCl_3$, 400.1 MHz): δ 7.74 (d, 2H, ^{3}J = 8.9 Hz), 6.99 (d, 2H, ^{3}J = 8.9 Hz), 6.94 (*pseudo*-d, 1H, ^{4}J = 0.8 Hz), 3.86 (s, 3H). $^{13}C\{^{1}H\}$ NMR ($CDCl_3$, 100.6 MHz): δ 162.1, 161.7, 158.9 (q, $^{2}J_{CF}$ = 42.4 Hz), 128.4, 119.7, 117.9 (q, $^{1}J_{CF}$ = 270.0 Hz), 114.6, 103.2 (q, $^{4}J_{CF}$ = 1.8 Hz), 55.4. ^{19}F NMR ($CDCl_3$, 376.5 MHz): δ -65.4 (d, 3F, J = 0.9 Hz). NMR data are in agreement with those in the literature[Error! Bookmark not defined.].



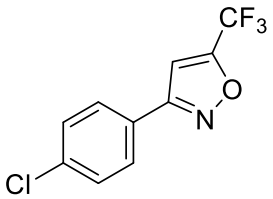
3-(4-Methylphenyl)-5-(trifluoromethyl)isoxazole (3d). Obtained from **1d** (0.106 g, 0.5 mmol (A); 0.115 g, 0.542 mmol (B)). Pale yellow solid, m.p. 78-80 °C (Lit.: 79-80 °C), yield 0.035 g (31%, (A)); 0.036 g (29%, (B)). ^{1}H NMR ($CDCl_3$, 400.1 MHz): δ 7.70 (d, 2H, ^{3}J = 8.0 Hz), 7.29 (d, 2H, ^{3}J = 8.0 Hz), 6.97 (*pseudo*-d, 1H, ^{4}J = 0.9 Hz), 2.41 (s, 3H). $^{13}C\{^{1}H\}$ NMR ($CDCl_3$, 100.6 MHz): δ 162.5, 159.0 (q, $^{2}J_{CF}$ = 42.4 Hz), 141.2, 129.9, 126.8, 124.4, 117.9 (q, $^{1}J_{CF}$ = 270.4 Hz), 103.3 (q, $^{4}J_{CF}$ = 2.0 Hz), 21.4. ^{19}F NMR ($CDCl_3$, 376.5 MHz): δ -65.4 (d, 3F, J = 0.9 Hz). NMR data are in agreement with those in the literature[Error! Bookmark not defined.].



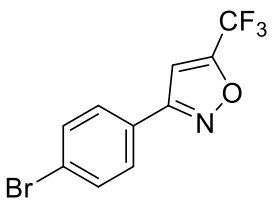
3-(4-Fluorophenyl)-5-(trifluoromethyl)isoxazole (3e). Obtained from **1e** (0.113 g, 0.5 mmol (A); 0.113 g, 0.5 mmol (B)). Pale beige crystals, m.p. 49-50 °C (Lit.: 48 °C), yield 0.036 g (31%, (A)); 0.035 g (30%, (B)). ^{1}H NMR ($CDCl_3$, 400.1 MHz): δ 7.83-7.78 (m, 2H), 7.21-7.15 (m, 2H), 6.97 (*pseudo*-d, 1H, ^{4}J = 0.9 Hz). $^{13}C\{^{1}H\}$ NMR ($CDCl_3$, 100.6 MHz): δ 164.3 (d, $^{1}J_{CF}$ = 251.7 Hz), 161.6, 159.4 (q, $^{2}J_{CF}$ = 42.7 Hz), 129.0 (d, $^{3}J_{CF}$ = 8.7 Hz), 123.5 (d, $^{4}J_{CF}$ = 3.5 Hz), 117.8 (q, $^{1}J_{CF}$ = 270.5 Hz), 116.4 (d, $^{2}J_{CF}$ = 22.1 Hz), 103.3 (q, $^{4}J_{CF}$ = 2.2 Hz). ^{19}F NMR ($CDCl_3$, 376.5 MHz): δ -65.4 (d, 3F, J = 0.8 Hz), -109.9--110.0 (m, 1F). NMR data are in agreement with those in the literature[Error! Bookmark not defined.].



3-(4-Chlorophenyl)-5-(trifluoromethyl)isoxazole (3f). Obtained from **1f** (0.117 g, 0.503 mmol (A); 0.114 g, 0.49 mmol (B)). Pale yellow solid, m.p. 51-53 °C (Lit.: 61-62 °C[Error! Bookmark not defined.]), yield 0.047 g (38%, (A)); 0.042 g (35%, (B)). ^{1}H NMR ($CDCl_3$, 400.1 MHz): δ 7.74 (d, 2H, ^{3}J = 8.7 Hz), 7.46 (d, 2H, ^{3}J = 8.7 Hz), 6.98 (*pseudo*-d, 1H, ^{4}J = 0.9 Hz). ^{13}C{^{1}H} NMR ($CDCl_3$, 100.6 MHz): δ 161.5, 159.5 (q, $^{2}J_{CF}$ = 42.6 Hz), 137.1, 129.5, 128.2, 125.7, 117.7 (q, $^{1}J_{CF}$ = 270.3 Hz), 103.3 (q, $^{4}J_{CF}$ = 2.0 Hz). ^{19}F NMR ($CDCl_3$, 376.5 MHz): δ -65.4 (d, 3F, J = 0.9 Hz). NMR data are in agreement with those in the literature[Error! Bookmark not defined.].

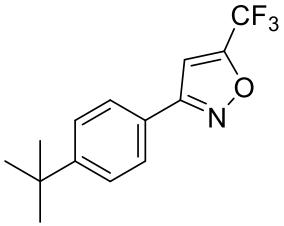


3-(4-Bromophenyl)-5-(trifluoromethyl)isoxazole (3g). Obtained from **1g** (0.140 g, 0.505 mmol (A); 0.143 g, 0.516 mmol (B)). Colorless solid, m.p. 71-73 °C (Lit.: 63-64 °C[Error! Bookmark not defined.]), yield 0.053 g (36%, (A)); 0.051 g (34%, (B)). ^{1}H NMR ($CDCl_3$, 400.1 MHz): δ 7.68 (d, 2H, ^{3}J = 8.6 Hz), 7.62 (d, 2H, ^{3}J = 8.6 Hz), 6.98 (*pseudo*-d, 1H, ^{4}J = 0.8 Hz). ^{13}C{^{1}H} NMR ($CDCl_3$, 100.6 MHz): δ 161.7, 159.5 (q, $^{2}J_{CF}$ = 42.8 Hz), 132.5, 128.4, 126.2, 125.4, 117.7 (q, $^{1}J_{CF}$ = 270.4 Hz), 103.3 (q, $^{4}J_{CF}$ = 2.0 Hz). ^{19}F NMR ($CDCl_3$, 376.5 MHz): δ -65.4 (d, 3F, J = 0.6 Hz). NMR data are in agreement with those in the literature[Error! Bookmark not defined.].

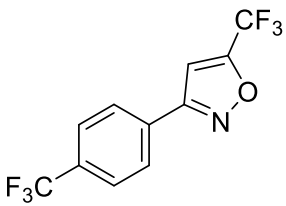


3-(4-(*tert*-Butyl)phenyl)-5-(trifluoromethyl)isoxazole (3h). Obtained from **1h** (0.121 g, 0.476 mmol (A); 0.122 g, 0.48 mmol (B)). Pale yellow viscous oil, yield 0.041 g (32%, (A)); 0.033 g (26%, (B)). ^{1}H NMR ($CDCl_3$, 400.1 MHz): δ 7.74 (d, 2H, ^{3}J = 8.7 Hz), 7.51 (d, 2H, ^{3}J = 8.7 Hz), 6.97 (*pseudo*-d, 1H, ^{4}J = 0.9 Hz), 2.41 (s, 3H). ^{13}C{^{1}H} NMR ($CDCl_3$, 100.6 MHz): δ 162.4, 159.0 (q, $^{2}J_{CF}$ = 42.4 Hz), 154.4, 126.7, 126.2, 124.4, 117.9 (q, $^{1}J_{CF}$ = 270.4 Hz), 103.4 (q, $^{4}J_{CF}$ = 2.0 Hz), 34.9, 31.1. ^{19}F NMR ($CDCl_3$, 376.5 MHz): δ -65.4 (d, 3F, J = 0.6 Hz).

HRMS (ESI-TOF): m/z $[M+H]^+$ Calcd for $C_{14}H_{15}F_3NO^+$: 270.1100; found: 270.1102.

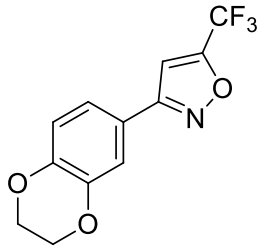


5-(Trifluoromethyl)-3-(4-(trifluoromethyl)phenyl)isoxazole (3i). Obtained from **1i** (0.134 g, 0.504 mmol (A); 0.137 g, 0.515 mmol (B)). Colorless solid, m.p. 55-57 °C (Lit.: 63-64 °C), yield 0.067 g (47%, (A)); 0.070 g (48%, (B)). ^{1}H NMR ($CDCl_3$, 400.1 MHz): δ 7.94 (d, 2H, ^{3}J = 8.2 Hz), 7.75 (d, 2H, ^{3}J = 8.2 Hz), 7.05 (*pseudo*-d, 1H, ^{4}J = 0.8 Hz). ^{13}C{^{1}H} NMR ($CDCl_3$, 100.6 MHz): δ 161.5, 159.8 (q, $^{2}J_{CF}$ = 42.9 Hz), 132.8 (q, $^{2}J_{CF}$ = 32.8 Hz), 130.7, 127.3, 126.2 (q, $^{3}J_{CF}$ = 3.9 Hz), 123.6 (q, $^{1}J_{CF}$ = 272.4 Hz), 117.7 (q, $^{1}J_{CF}$ = 270.5 Hz), 103.5 (q, $^{4}J_{CF}$ = 2.0 Hz). ^{19}F



NMR ($CDCl_3$, 376.5 MHz): δ -64.2 (d, 3F), -65.3 (d, 3F, *J* = 0.6 Hz). NMR data are in agreement with those in the literature[Error! Bookmark not defined.].

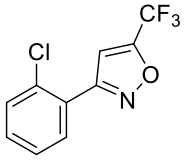
3-(2,3-diHydrobenzo[*b*][1,4]dioxin-6-yl)-5-(trifluoromethyl)isoxazole (3k). Obtained from **1k** (0.128 g, 0.5 mmol (A); 0.126 g, 0.492 mmol (B)).



Colorless solid, m.p. 102-104 °C, yield 0.026 g (19%, (A)); 0.021 g (16%, (B)). ^{1}H NMR ($CDCl_3$, 400.1 MHz): δ 7.34 (d, 1H, ^4J = 2.1 Hz), 7.30 (dd, 1H, ^3J = 8.4 Hz, ^4J = 2.1 Hz), 6.96 (d, 1H, ^3J = 8.4 Hz), 6.91 (*pseudo*-d, 1H, ^4J = 0.9 Hz), 4.34-4.29 m, 4H). ^{13}C{^{1}H} NMR ($CDCl_3$, 100.6 MHz): δ 162.0, 158.9 (q, $^2J_{CF}$ = 42.4 Hz), 145.9, 144.0, 120.5, 120.3, 118.0, 117.9 (q, $^1J_{CF}$ = 270.8 Hz), 116.0, 103.3 (q, $^4J_{CF}$ = 2.0 Hz), 64.5, 64.3. ^{19}F NMR ($CDCl_3$, 376.5 MHz): δ -65.4 (d, 3F, ^4J = 0.4 Hz).

HRMS (ESI-TOF): m/z $[M+H]^+$ Calcd for $C_{12}H_9F_3NO_3^+$: 272.0529; found: 272.0531.

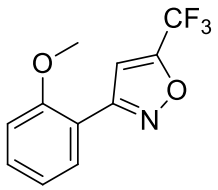
3-(2-Chlorophenyl)-5-(trifluoromethyl)isoxazole (3l). Obtained from **1l** (0.119 g, 0.512 mmol (A); 0.123 g, 0.529 mmol (B)). Pale yellow oil, yield 0.037



g (29%, (A)); 0.047 g (36%, (B)). ^{1}H NMR ($CDCl_3$, 400.1 MHz): δ 7.75 (dd, 1H, ^3J = 7.7 Hz, ^4J = 1.8 Hz), 7.52 (dd, 1H, ^3J = 7.7 Hz, ^4J = 1.4 Hz), 7.45 (td, 1H, ^3J = 7.7 Hz, ^4J = 1.8 Hz), 7.39 (td, 1H, ^3J = 7.7 Hz, ^4J = 1.4 Hz), 7.19 (*pseudo*-d, 1H, ^4J = 0.8 Hz). ^{13}C{^{1}H} NMR ($CDCl_3$, 100.6 MHz): δ 161.2, 158.5 (q, $^2J_{CF}$ = 42.6 Hz), 132.9, 131.7, 131.1, 130.6, 127.4, 126.5, 117.8 (q, $^1J_{CF}$ = 270.3 Hz), 106.6 (q, $^4J_{CF}$ = 2.0 Hz). ^{19}F NMR ($CDCl_3$, 376.5 MHz): δ -65.2 (d, 3F, ^4J = 0.9 Hz).

HRMS (ESI-TOF): m/z $[M+H_3O]^+$ Calcd for $C_{10}H_8[^{35}Cl]F_3NO_2^+$: 266.0190; found: 266.0190; Calcd for $C_{10}H_8[^{37}Cl]F_3NO_2^+$: 268.0161; found: 268.0156.

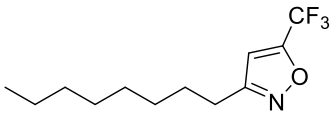
3-(2-Methoxyphenyl)-5-(trifluoromethyl)isoxazole (3m). Obtained from **1m** (0.113 g, 0.502 mmol (A); 0.108 g, 0.48 mmol (B)). Colorless oil, yield



0.026 g (21%, (A)); 0.030 g (26%, (B)). ^{1}H NMR ($CDCl_3$, 400.1 MHz): δ 7.91 (dd, 1H, ^3J = 7.7 Hz, ^4J = 1.7 Hz), 7.48-7.44 (m, 1H), 7.22 (s, 1H), 7.06 (*pseudo*-t, 1H, ^3J = 7.5 Hz), 7.02 (d, 1H, ^3J = 8.4 Hz), 3.92 (s, 1H). ^{13}C{^{1}H} NMR ($CDCl_3$, 100.6 MHz): δ 160.1, 157.9 (q, $^2J_{CF}$ = 42.2 Hz), 157.2, 132.1, 129.4, 121.1, 118.1 (q, $^1J_{CF}$ = 270.0 Hz), 116.1, 111.4, 106.9 (q, $^4J_{CF}$ = 2.0 Hz), 55.6. ^{19}F NMR ($CDCl_3$, 376.5 MHz): δ -65.3 (d, 3F, ^4J = 0.9 Hz).

HRMS (ESI-TOF): m/z $[M+H]^+$ Calcd for $C_{11}H_9F_3NO_2^+$: 244.0580; found: 244.0581.

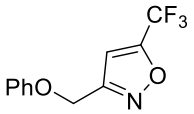
3-Octyl-5-(trifluoromethyl)isoxazole (3o). Obtained from **1o** (0.118 g, 0.504 mmol (A); 0.130 g, 0.556 mmol (B)). Colorless oil, yield 0.041 g (32%, (A));



0.046 g (33%, (B)). ^{1}H NMR ($CDCl_3$, 400.1 MHz): δ 6.53 (*pseudo*-d, 1H, ^{4}J = 0.7 Hz), 2.71 (t, 2H, ^{3}J = 7.7 Hz), 1.70-1.63 (m, 2H), 1.39-1.19 (m, 10H), 0.88-0.85 (m, 3H). $^{13}C\{^{1}H\}$ NMR ($CDCl_3$, 100.6 MHz): δ 164.2, 158.4 (q, $^{2}J_{CF}$ = 42.4 Hz), 118.0 (q, $^{1}J_{CF}$ = 270.2 Hz), 104.9 (q, $^{4}J_{CF}$ = 1.9 Hz), 31.8, 29.14, 29.08, 29.04, 28.0, 25.8, 22.6, 14.1. ^{19}F NMR ($CDCl_3$, 376.5 MHz): δ -65.4 (d, 3F, ^{4}J = 0.9 Hz).

HRMS (ESI-TOF): m/z $[M+H]^+$ Calcd for $C_{12}H_{19}F_3NO^+$: 250.14133; found: 250.141.

3-(Phenoxymethyl)-5-(trifluoromethyl)isoxazole (3p). Obtained from **1p** (0.117 g, 0.52 mmol (A); 0.125 g, 0.556 mmol (B)). Pale yellow oil, yield 0.065 g

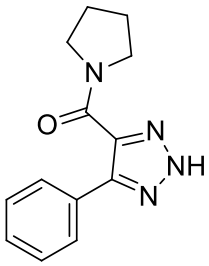


(51%, (A)); 0.064 g (47%, (B)). ^{1}H NMR ($CDCl_3$, 400.1 MHz): δ 7.36-7.30 (m, 2H), 7.05-7.01 (m, 1H), 6.99-6.96 (m, 2H), 6.86 (*pseudo*-d, 1H, ^{4}J = 0.4 Hz), 5.20 (s, 2H). $^{13}C\{^{1}H\}$ NMR ($CDCl_3$, 100.6 MHz): δ 161.2, 159.2 (q, $^{2}J_{CF}$ = 42.8 Hz), 157.6, 129.7, 122.0, 117.7 (q, $^{1}J_{CF}$ = 270.5 Hz), 114.6, 104.9 (q, $^{4}J_{CF}$ = 2.0 Hz), 61.0. ^{19}F NMR ($CDCl_3$, 376.5 MHz): δ -65.2 (d, 3F, ^{4}J = 0.6 Hz).

HRMS (ESI-TOF): m/z $[M+H]^+$ Calcd for $C_{11}H_9F_3NO_2^+$: 244.0580; found: 244.0585.

Synthesis of amides 4-6 (general procedure). A 4 mL vial with a screw cap was charged with 2,2,2-trifluoro-1-(5-phenyl-2*H*-1,2,3-triazol-4-yl)ethanone (**2a**). (0.054-0.059 g, 0.224-0.245 mmol) and corresponding amine (0.189-0.230 g, ~2.7 mmol, ~12 equiv.) The reaction mixture was heated at 90 °C for 2.5-8 h using magnetic stirrer with heating and then volatiles were evaporated in vacuo. The residue was passed through a short silica gel pad using CH_2Cl_2 followed by CH_2Cl_2 -MeOH (100:1) as eluents. Evaporation of volatiles afforded corresponding pure amide **4-6**.

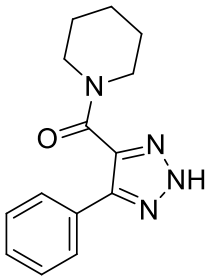
(5-Phenyl-2*H*-1,2,3-triazol-4-yl)(pyrrolidin-1-yl)methanone (4). Obtained from **2a** (0.054 g, 0.224 mmol) and pyrrolidine (0.189 g, 2.66 mmol) by heating for 2.5 h. Pale brown solid, m.p. 162-164 °C, yield 0.046 g (85%). ^{1}H NMR ($CDCl_3$, 400.1 MHz): δ 7.76-7.65 (m, 2H), 7.35-7.25 (m, 3H), 3.67 (t, 2H, ^3J = 6.9 Hz), 3.38 (t, 2H, ^3J = 6.9 Hz), 1.92-1.85 (m, 2H), 1.85-1.74 (m, 2H). ^{13}C{^{1}H} NMR ($CDCl_3$, 100.6 MHz): δ 162.5, 142.8, 138.0, 128.9, 128.6, 127.6, 48.6, 46.4, 25.9, 24.2.



HRMS (ESI-TOF): m/z $[M+Na]^+$ Calcd for $C_{13}H_{14}N_4ONa^+$: 265.1060; found: 265.1068.

IR (ν, cm^{-1}): 1595 (C=O).

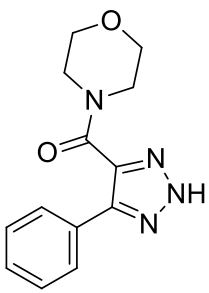
(5-Phenyl-2*H*-1,2,3-triazol-4-yl)(piperidin-1-yl)methanone (5). Obtained from **2a** (0.053 g, 0.220 mmol) and piperidine (0.228 g, 2.68 mmol) by heating for 8 h. Pale brown solid, m.p. 123-125 °C, yield 0.033 g (58%). ^{1}H NMR ($CDCl_3$, 400.1 MHz): δ 7.66 (dd, 2H, ^3J = 6.9 Hz, ^4J = 1.9 Hz), 7.41-7.38 (m, 3H), 3.82-3.62 (m, 2H), 3.28-3.10 (m, 2H), 1.68-1.48 (m, 4H), 1.34-1.21 (m, 2H). ^{13}C{^{1}H} NMR ($CDCl_3$, 100.6 MHz): δ 163.0, 142.9, 137.4, 128.9, 128.8, 128.5, 127.3, 48.3, 43.3, 26.0, 25.4, 24.3.



HRMS (ESI-TOF): m/z $[M+H]^+$ Calcd for $C_{14}H_{17}N_4O^+$: 257.1397; found: 257.1403.

IR (ν, cm^{-1}): 1592 (C=O).

Morpholino(5-phenyl-2*H*-1,2,3-triazol-4-yl)methanone (6). Obtained from **2a** (0.053 g, 0.220 mmol) and morpholine (0.230 g, 2.64 mmol) by heating for 8 h. Pale brown viscous sticky mass, yield 0.027 g (48%). ^{1}H NMR ($CDCl_3$, 400.1 MHz): δ 7.73-7.59 (m, 2H), 7.44-7.34 (m, 3H), 3.87-3.79 (m, 2H), 3.77-3.70 (m, 2H), 3.47-3.39 (m, 2H), 3.39-3.27 (m, 2H). ^{13}C{^{1}H} NMR ($CDCl_3$, 100.6 MHz): δ 163.0, 141.6, 136.9, 129.3, 128.9, 127.5, 127.3, 66.53, 66.48, 47.5, 42.7.

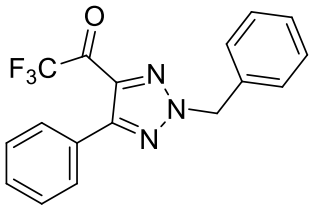


HRMS (ESI-TOF): m/z $[M+H]^+$ Calcd for $C_{13}H_{15}N_4O_2^+$: 259.1190; found: 259.1190.

IR (ν, cm^{-1}): 1604 (C=O).

Synthesis of triazoles 7-10 (general procedure). A 4 mL vial with a screw cap was charged with 2,2,2-trifluoro-1-(5-phenyl-2*H*-1,2,3-triazol-4-yl)ethanone (**2a**) (0.120 g, 0.498 mmol), DMF (1 mL), Na_2CO_3 (0.079 g, 0.745 mmol, 1.5 equiv.), and corresponding alkylating reagent (0.548 mmol, ~1.1 equiv.) The reaction mixture was stirred overnight, poured into water (20 mL) and extracted with CH_2Cl_2 (3x20 mL). Combined organic phase was washed with water (20 mL), dried over Na_2SO_4 and then volatiles were evaporated in vacuo. The residue was purified by column chromatography on silica gel using appropriate mixtures of hexane and CH_2Cl_2 as eluents.

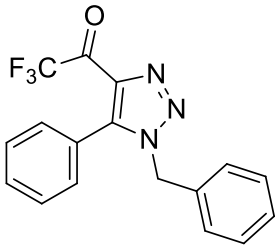
1-(2-Benzyl-5-phenyl-2*H*-1,2,3-triazol-4-yl)-2,2,2-trifluoroethanone (7). Obtained from **2a** (0.120 g, 0.498 mmol) and benzylbromide (0.094 g, 0.550 mmol). Purified using gradient eluating by hexane-CH_2Cl_2 (3:1) followed by hexane-CH_2Cl_2 (1:1) and CH_2Cl_2. Beige oil, yield 0.113 g (69%). ^{1}H NMR ($CDCl_3$, 400.1 MHz): δ 7.96-7.86 (m, 2H), 7.53-7.44 (m, 5H), 7.44-7.36(m, 3H), 5.71 (s, 2H). $^{13}C\{^1H\}$ NMR ($CDCl_3$, 100.6 MHz): δ 174.2 (q, $^2J_{CF}$ = 37.0 Hz), 152.7, 136.4, 133.5, 130.1, 129.1, 129.0, 128.9, 128.40, 128.35, 128.2, 116.3 (q, $^1J_{CF}$ = 290.7 Hz), 59.9. ^{19}F NMR ($CDCl_3$, 376.5 MHz): δ -74.9 (s, 3F).



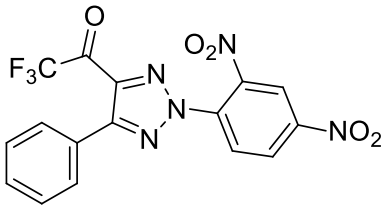
HRMS (ESI-TOF): m/z $[M+H]^+$ Calcd for $C_{17}H_{13}F_3N_3O^+$: 332.1005; found: 332.1005.

IR (ν, cm^{-1}): 1723 (C=O).

1-(1-Benzyl-5-phenyl-1*H*-1,2,3-triazol-4-yl)-2,2,2-trifluoroethanone (8). Obtained from **2a** as an admixture (81:19) in the synthesis of 7. Beige thick oil, yield 0.026 g (15%). ^{1}H NMR ($CDCl_3$, 400.1 MHz): δ 7.58-7.52 (m, 1H), 7.51-7.46 (m, 2H), 7.31-7.25 (m, 3H), 7.24-7.20 (m, 2H), 7.08-7.00 (m, 2H), 5.46 (s, 2H). $^{13}C\{^1H\}$ NMR ($CDCl_3$, 100.6 MHz): δ 174.2 (q, $^2J_{CF}$ = 37.3 Hz), 143.9, 138.1, 133.9, 130.9, 129.4, 129.0, 128.9, 128.7, 127.7, 124.4, 116.1 (q, $^1J_{CF}$ = 290.6 Hz), 52.2. ^{19}F NMR ($CDCl_3$, 376.5 MHz): δ -75.4 (s, 3F). NMR data are in agreement with those in the literature



1-(2-(2,4-Dinitrophenyl)-5-phenyl-2*H*-1,2,3-triazol-4-yl)-2,2,2-trifluoroethanone (9). Obtained from **2a** (0.057 g, 0.237 mmol) and 1-fluoro-2,4-dinitrobenzene (0.049 g, 0.263 mmol). Purified using gradient eluating by hexane-CH_2Cl_2 (3:1) followed by hexane-CH_2Cl_2 (1:1).

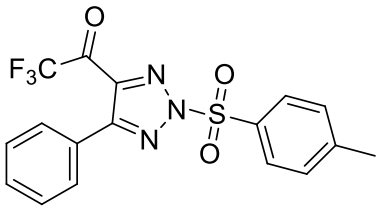


Pale yellow powder, m.p. 132-134 °C, yield 0.079 g (82%). ^{1}H NMR ($CDCl_3$, 400.1 MHz): δ 8.67 (d, 1H, ^{4}J = 2.4 Hz), 8.56 (dd, 1H, ^{3}J = 8.9 Hz, ^{4}J = 2.4 Hz), 8.31 (d, 1H, ^{3}J = 8.9 Hz), 7.83 (dd, 2H, ^{3}J = 7.7 Hz, ^{4}J = 1.7 Hz), 7.49-7.40 (m, 3H). $^{13}C\{^{1}H\}$ NMR ($CDCl_3$, 100.6 MHz): δ 173.7 (q, $^{2}J_{CF}$ = 38.2 Hz), 153.8, 147.1, 142.8, 138.7, 134.1, 130.8, 129.0, 128.4, 127.4, 126.4, 120.7, 115.6 (q, $^{1}J_{CF}$ = 290.5 Hz). ^{19}F NMR ($CDCl_3$, 376.5 MHz): δ -75.0 (s, 3F).

HRMS (ESI-TOF): m/z $[M+H]^+$ Calcd for $C_{16}H_9F_3N_5O_5^+$: 408.0550; found: 408.0549.

IR (ν, cm^{-1}): 1738 (C=O); 1545, 1540, 1349, 1335 (NO_2).

2,2,2-Trifluoro-1-(5-phenyl-2-tosyl-2*H*-1,2,3-triazol-4-yl)ethanone (10). Obtained from **2a** (0.060 g, 0.249 mmol) and 4-toluenesulfonyl chloride (0.052 g, 0.274 mmol). Purified using gradient eluating by hexane-CH_2Cl_2 (1:1) followed by CH_2Cl_2.White crystals, m.p. 156-160 °C, yield 0.073 g (74%). ^{1}H NMR ($CDCl_3$, 400.1 MHz): δ 8.08 (d, 2H, ^{3}J = 8.4 Hz), 7.83 (dd, 2H, ^{3}J = 7.9 Hz, ^{4}J = 1.4 Hz) 7.52-7.39 (m, 5H), 2.46 (s, 3H). $^{13}C\{^{1}H\}$ NMR ($CDCl_3$, 100.6 MHz): δ 174.5 (q, $^{2}J_{CF}$ = 37.9 Hz), 153.4, 148.1, 138.6, 131.6, 130.8, 130.6, 129.6, 129.3, 128.5, 126.9, 115.8 (q, $^{1}J_{CF}$ = 290.5 Hz), 21.9. ^{19}F NMR ($CDCl_3$, 376.5 MHz): δ -75.2 (s, 3F).



HRMS (ESI-TOF): m/z $[M+H]^+$ Calcd for $C_{17}H_{13}F_3N_3O_3S^+$: 396.0324; found: 396.0626.

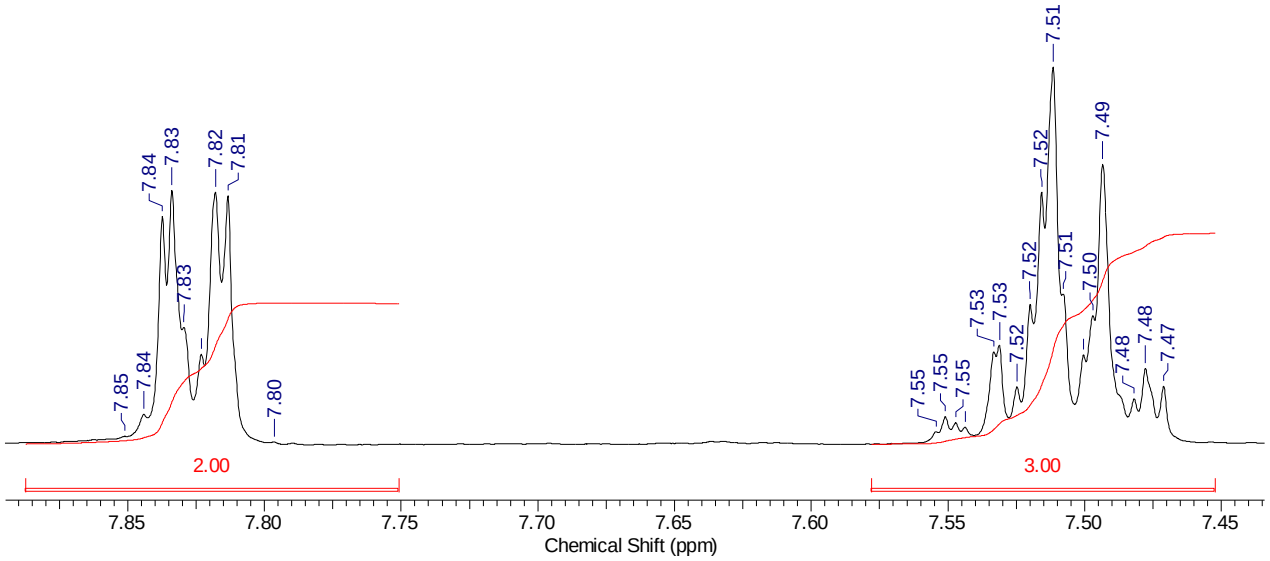
IR (ν, cm^{-1}): 1604 (C=O).

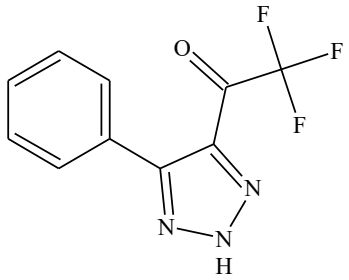
Synthesis of 1-(2,5-diphenyl-2*H*-1,2,3-triazol-4-yl)-2,2,2-trifluoroethanone (11). A 25 mL round-bottomed flask was charged with 2,2,2-trifluoro-1-(5-phenyl-2*H*-1,2,3-triazol-4-yl)ethanone (**2a**) (0.062 g, 0.257 mmol), DMSO (1.5 mL), $PhB(OH)_2$ (0.047 g, 0.385 mmol, 1.5 equiv.), and $Cu(OAc)_2xH_2O$ (0.0051, 0.257 mmol, 0.1 equiv.) The reaction mixture was heated at 100 °C for 5 h at air using magnetic stirrer with heating. The reaction mixture was poured into water (20 mL) and extracted with CH_2Cl_2 (3x20 mL). Combined organic phase was washed with water (20 mL), dried over Na_2SO_4 and then volatiles were evaporated in vacuo. The residue was purified by column chromatography on silica gel using using gradient eluating by hexane-CH_2Cl_2 (3:1) followed by hexane-CH_2Cl_2 (1:1) as eluents. Colorless crystals, m.p. 93-95 °C yield 0.032 g (50%). ^{1}H NMR ($CDCl_3$, 400.1 MHz): δ 8.28-8.18 (m, 2H), 8.03-7.95 (m, 2H), 7.59-7.46 (m, 6H). $^{13}C\{^1H\}$ NMR ($CDCl_3$, 100.6 MHz): δ 174.4 (q, $^2J_{CF}$ = 37.5 Hz), 152.9, 138.8, 137.1, 130.4, 129.6, 129.4, 129.2, 128.5, 128.1, 119.7, 116.3 (q, $^1J_{CF}$ = 290.9 Hz). ^{19}F NMR ($CDCl_3$, 376.5 MHz): δ -74.9 (s, 3F).

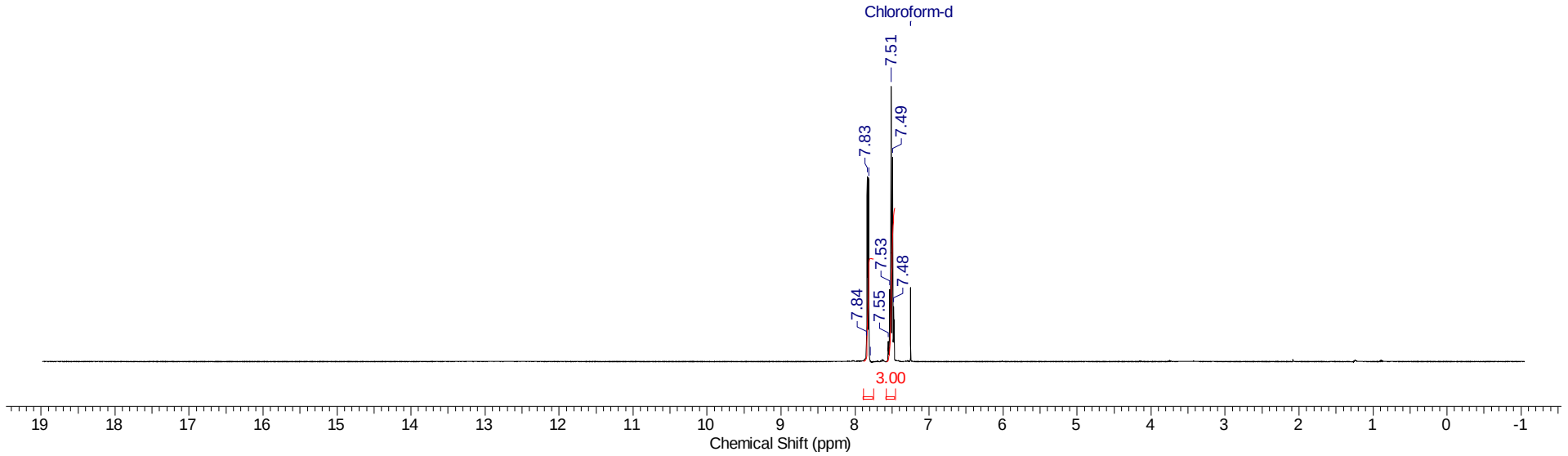
HRMS (ESI-TOF): m/z $[M+H]^+$ Calcd for $C_{16}H_{11}F_3N_3O^+$: 318.0849; found: 318.0851.

IR (ν, cm^{-1}): 1716 (C=O).

Acquisition Time (sec)	4.0894	***Comment***	Imported from UXNMR.			***Date***	25 Apr 2022 15:23:00
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Pulse Sequence	zg30	***Solvent***	CHLOROFORM-D			***Sweep Width (Hz)***	8012.82
Temperature (degree C)	27.000						



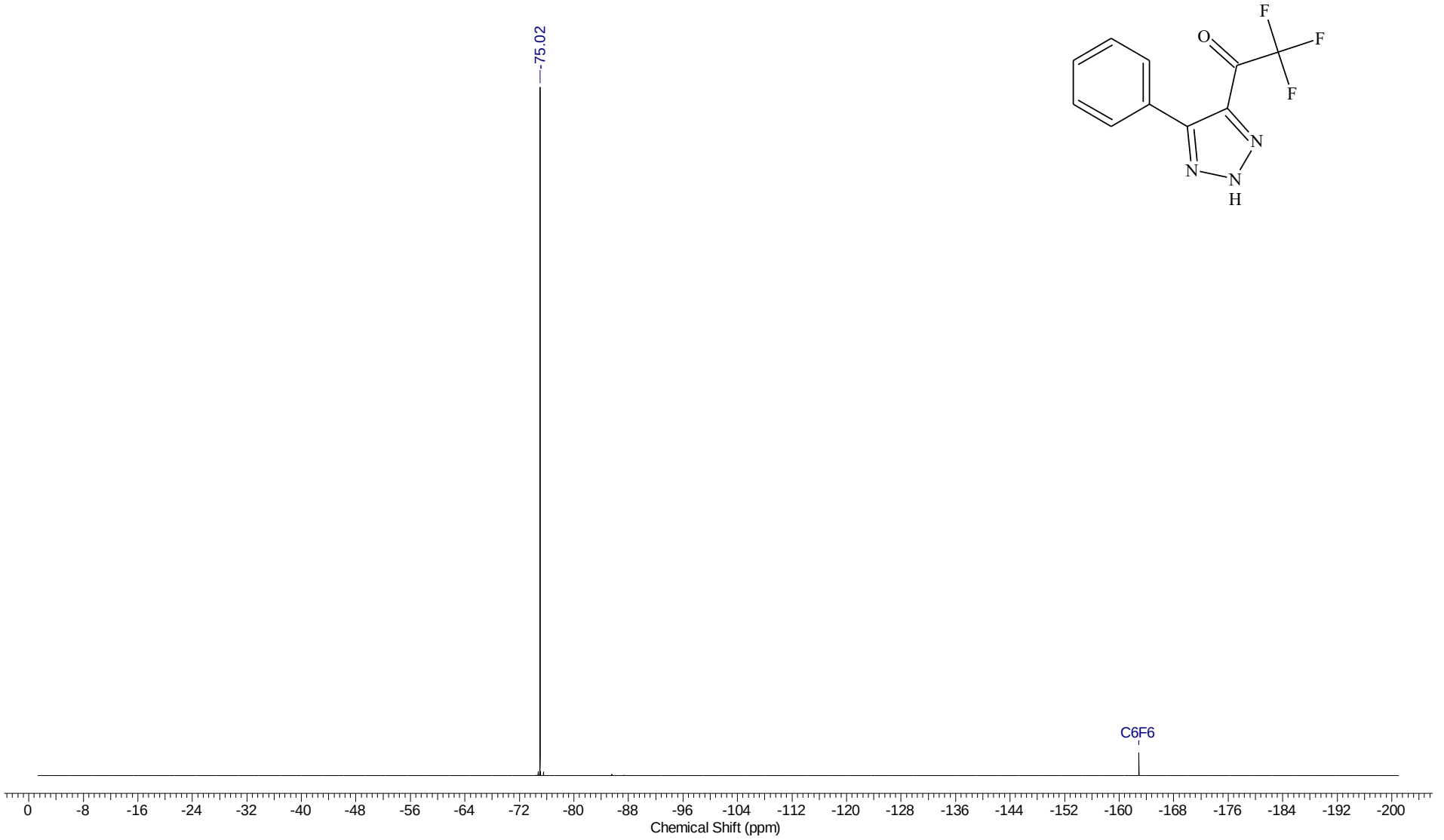




^{1}H NMR spectrum of **2a** (400.1 MHz, $CDCl_3$)

13 May 2022

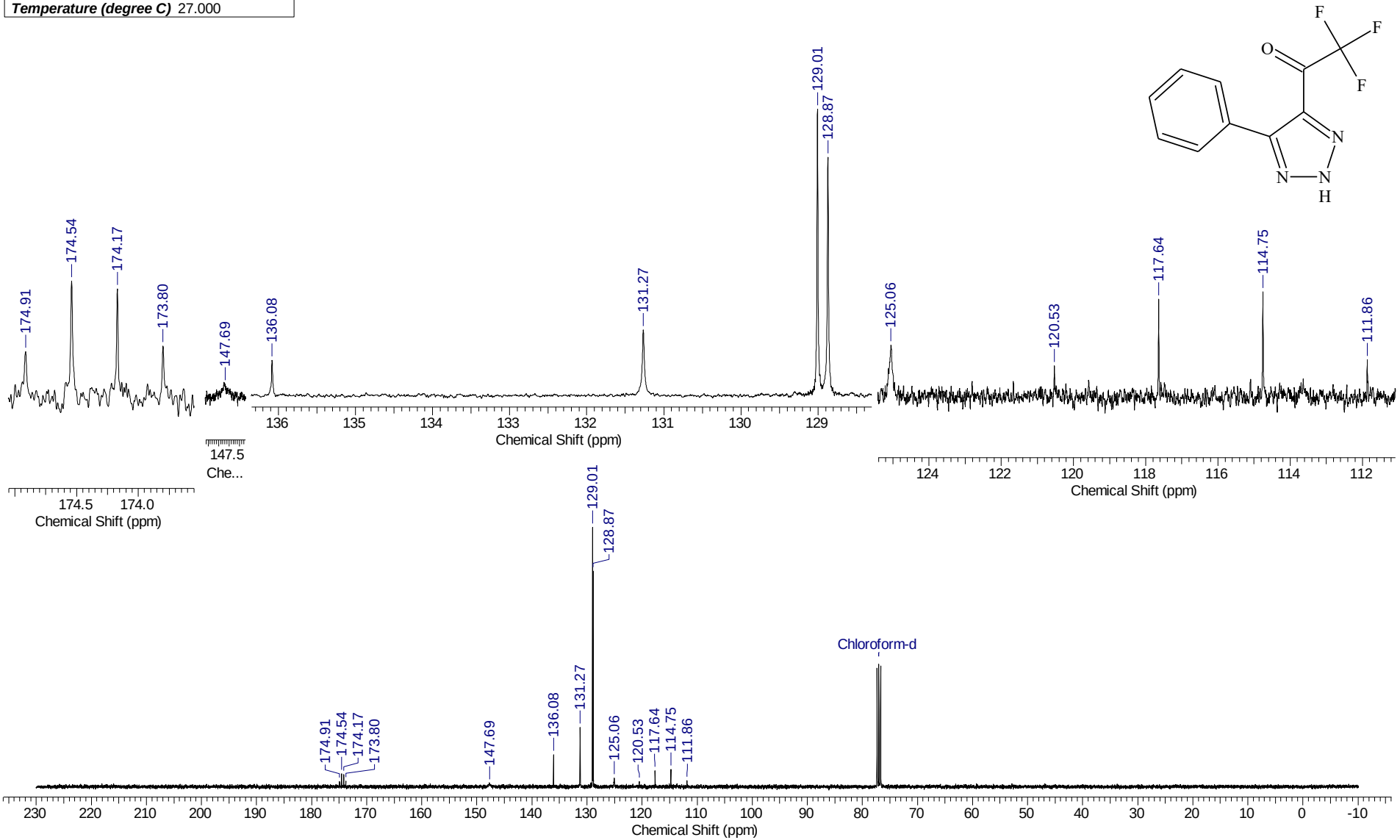
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Temperature (degree C)	27.000						



^{19}F NMR spectrum of **2a** (376.5 MHz, $CDCl_3$)

16 May 2022

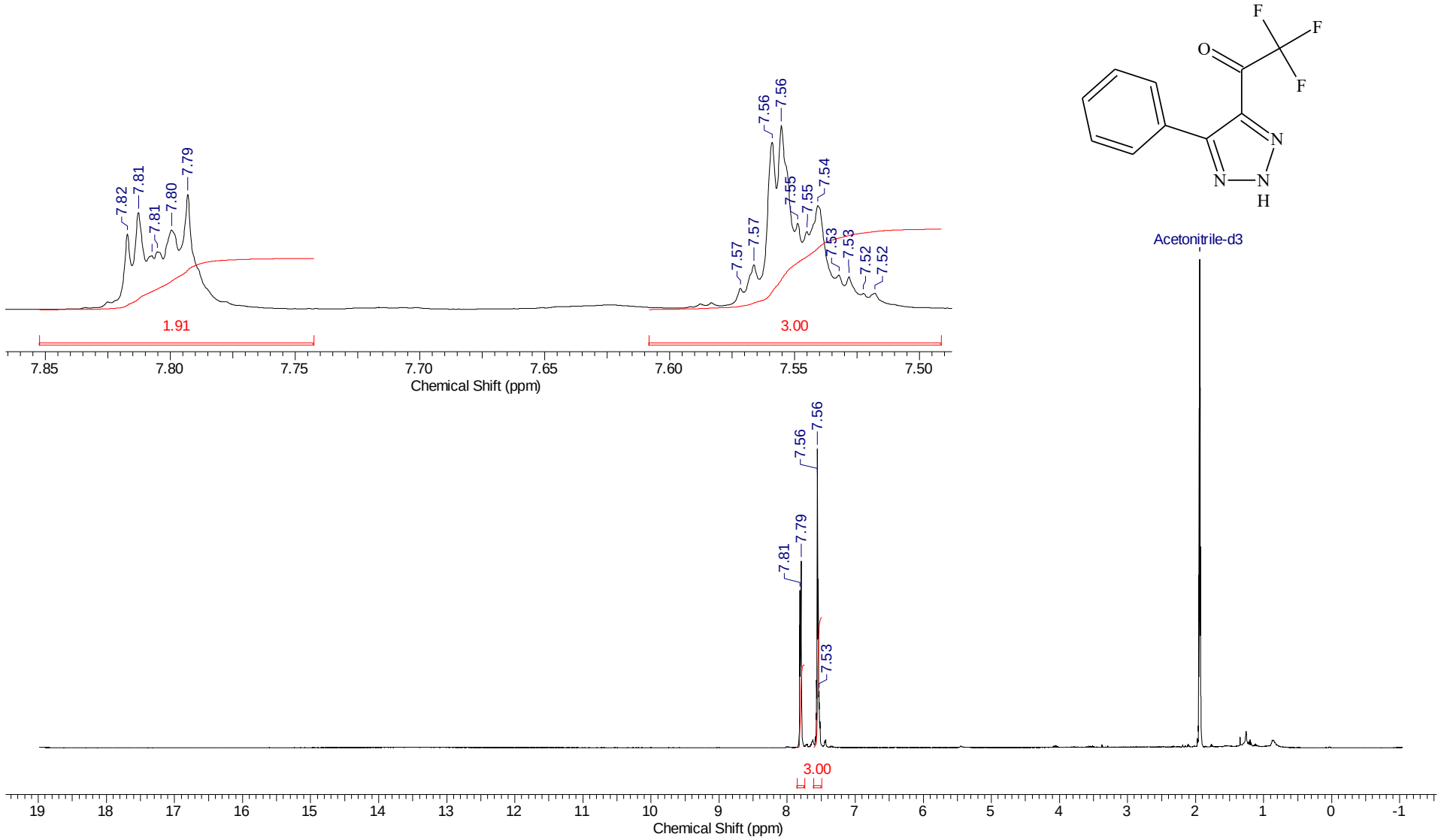
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Pulse Sequence	zgpg30	***Solvent***	CHLOROFORM-D			***Sweep Width (Hz)***	24154.59
Temperature (degree C)	27.000						



^{13}C NMR spectrum of **2a** (100.6 MHz, $CDCl_3$)

13 May 2022

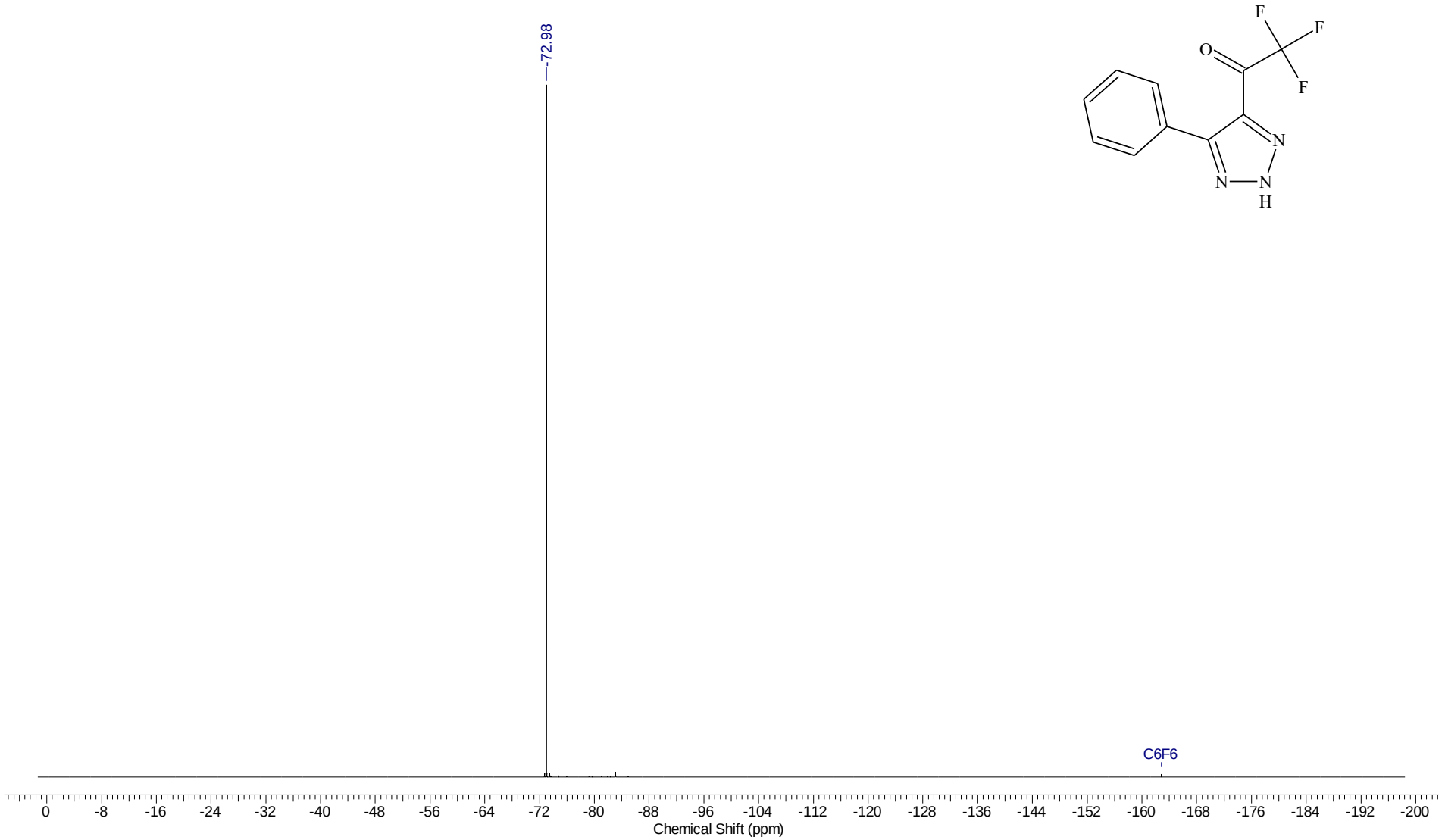
Acquisition Time (sec)	4.0894	***Comment***	Imported from UXNMR.			***Date***	04 Feb 2022 15:56:08
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Nucleus	1H	***Number of Transients***	4	***Original Points Count***	32768	***Points Count***	131072
Pulse Sequence	zg30	***Solvent***	ACETONITRILE-D3			***Sweep Width (Hz)***	8012.82
Temperature (degree C)	27.000						



^{1}H NMR spectrum of **2a** (400.1 MHz, CD_3CN)

13 May 2022

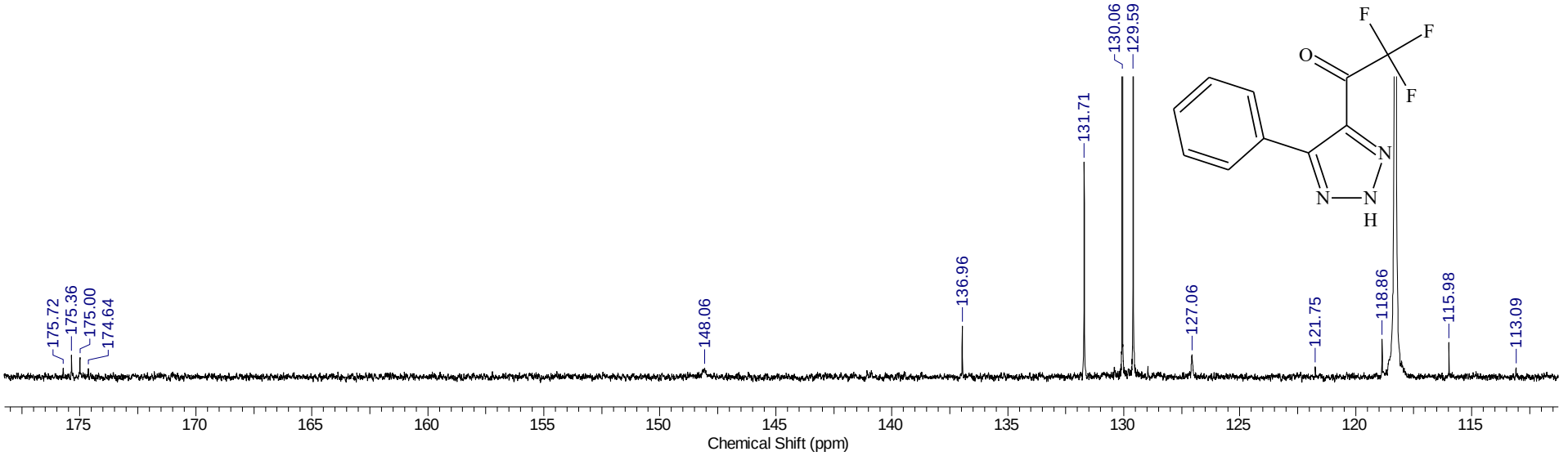
Acquisition Time (sec)	1.7433	***Comment***	Imported from UXNMR.			***Date***	07 Feb 2022 15:16:48
File Name	C:\DOCS\OUTPUT_301\2022\02.翦 怵嚾黑SZA-BM-2368-11.F_005001r					***Frequency (MHz)***	376.50
Nucleus	19F	***Number of Transients***	16	***Original Points Count***	131072	***Points Count***	262144
Pulse Sequence	zgflqn	***Solvent***	CHLOROFORM-D			***Sweep Width (Hz)***	75187.97
Temperature (degree C)	27.000						

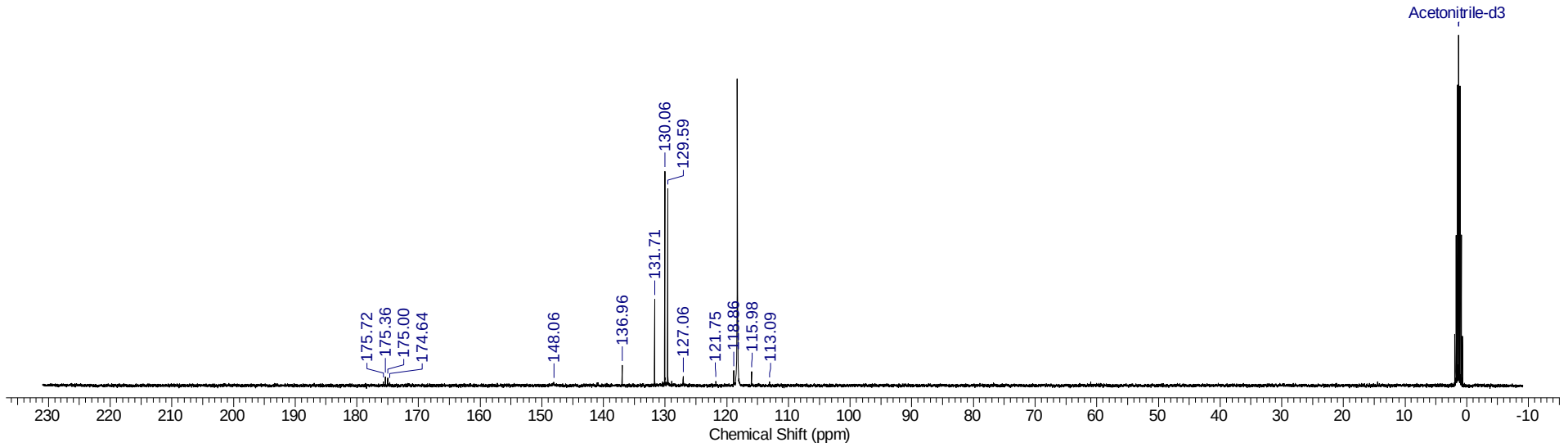


^{19}F NMR spectrum of **2a** (376.5 MHz, CD_3CN)

13 May 2022

Acquisition Time (sec)	0.6783	***Comment***	Imported from UXNMR.			***Date***	08 Feb 2022 16:02:02
File Name	C:\DOCS\OUTPUT_301\2022\02.翦 怵嚾黑SZA-BM-2368-11.C_002001r					***Frequency (MHz)***	100.61
Nucleus	13C	***Number of Transients***	248	***Original Points Count***	16384	***Points Count***	131072
Pulse Sequence	zgpg30	***Solvent***	ACETONITRILE-D3			***Sweep Width (Hz)***	24154.59
Temperature (degree C)	27.000						

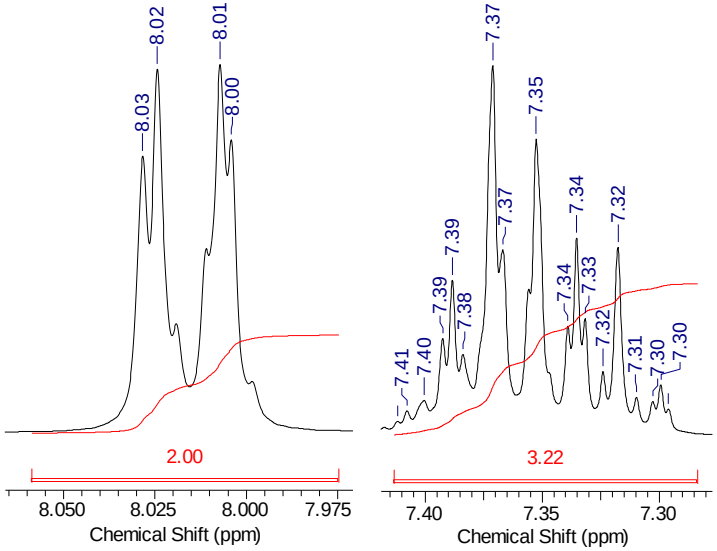


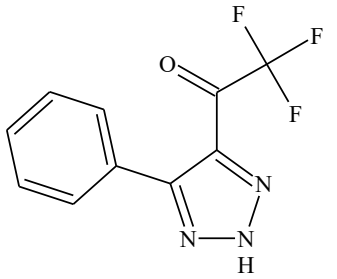


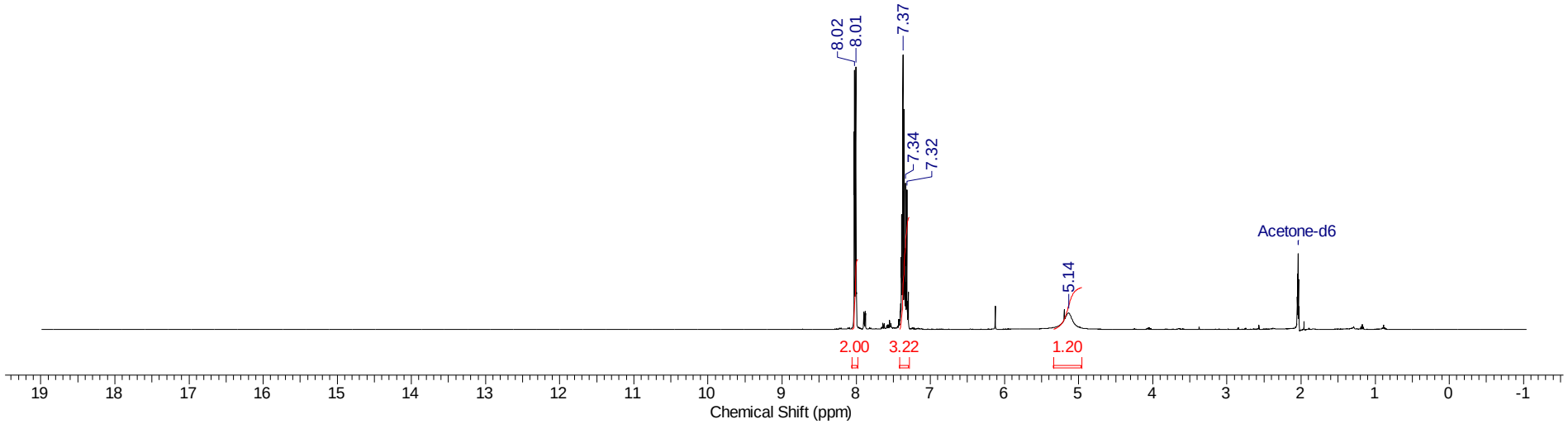
^{13}C NMR spectrum of **2a** (100.6 MHz, CD_3CN)

20 May 2022

Acquisition Time (sec)	4.0894	***Comment***	Imported from UXNMR.			***Date***	25 Jan 2022 15:01:30
File Name	C:\DOCS\OUTPUT_301\2022\01. 磺囧黑BM-2368-C-2.H_001001r					***Frequency (MHz)***	400.13
Nucleus	1H	***Number of Transients***	4	***Original Points Count***	32768	***Points Count***	131072
Pulse Sequence	zg30	***Solvent***	CHLOROFORM-D			***Sweep Width (Hz)***	8012.82
Temperature (degree C)	27.000						



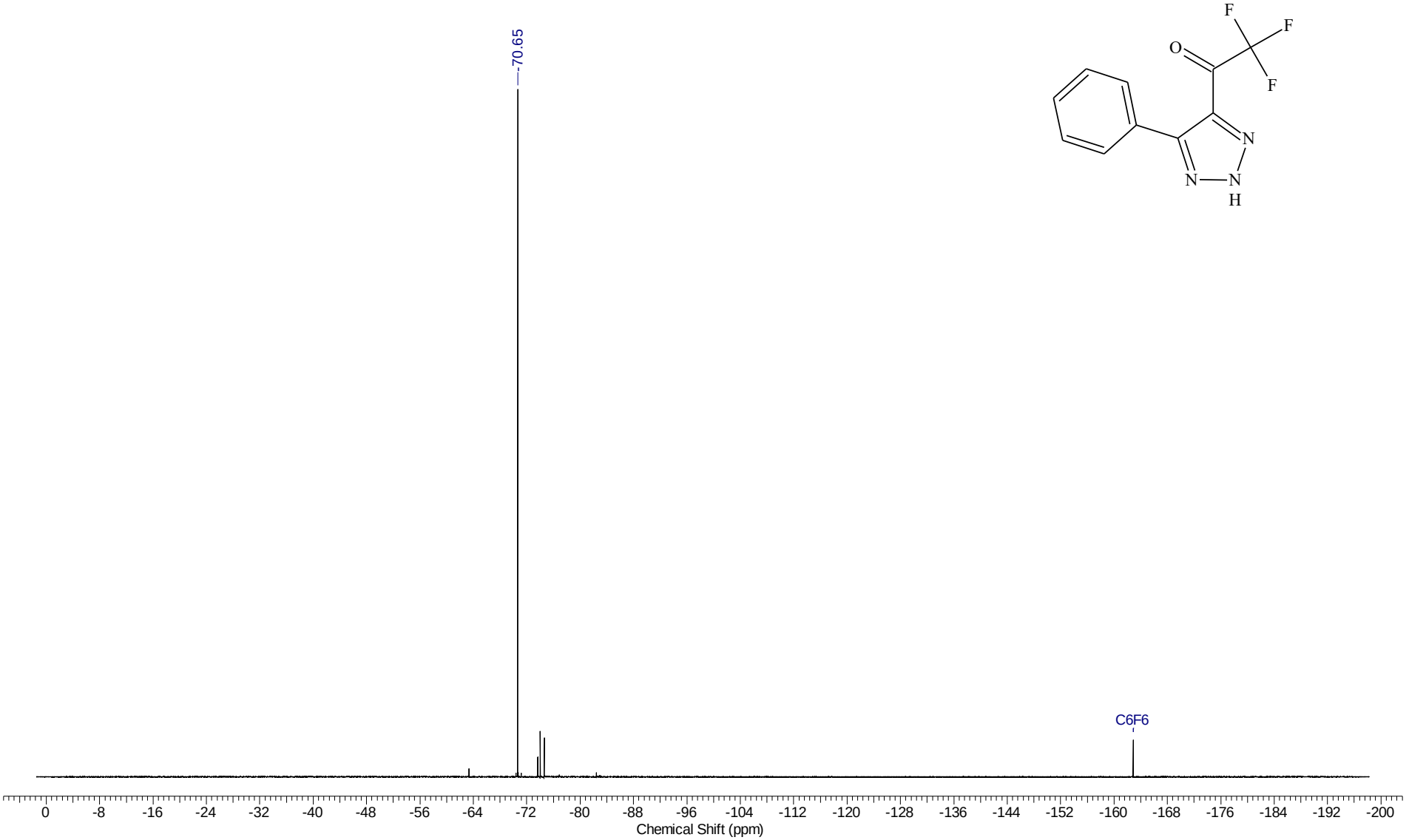




^{1}H NMR spectrum of **2a** (400.1 MHz, acetone-d_6)

20 May 2022

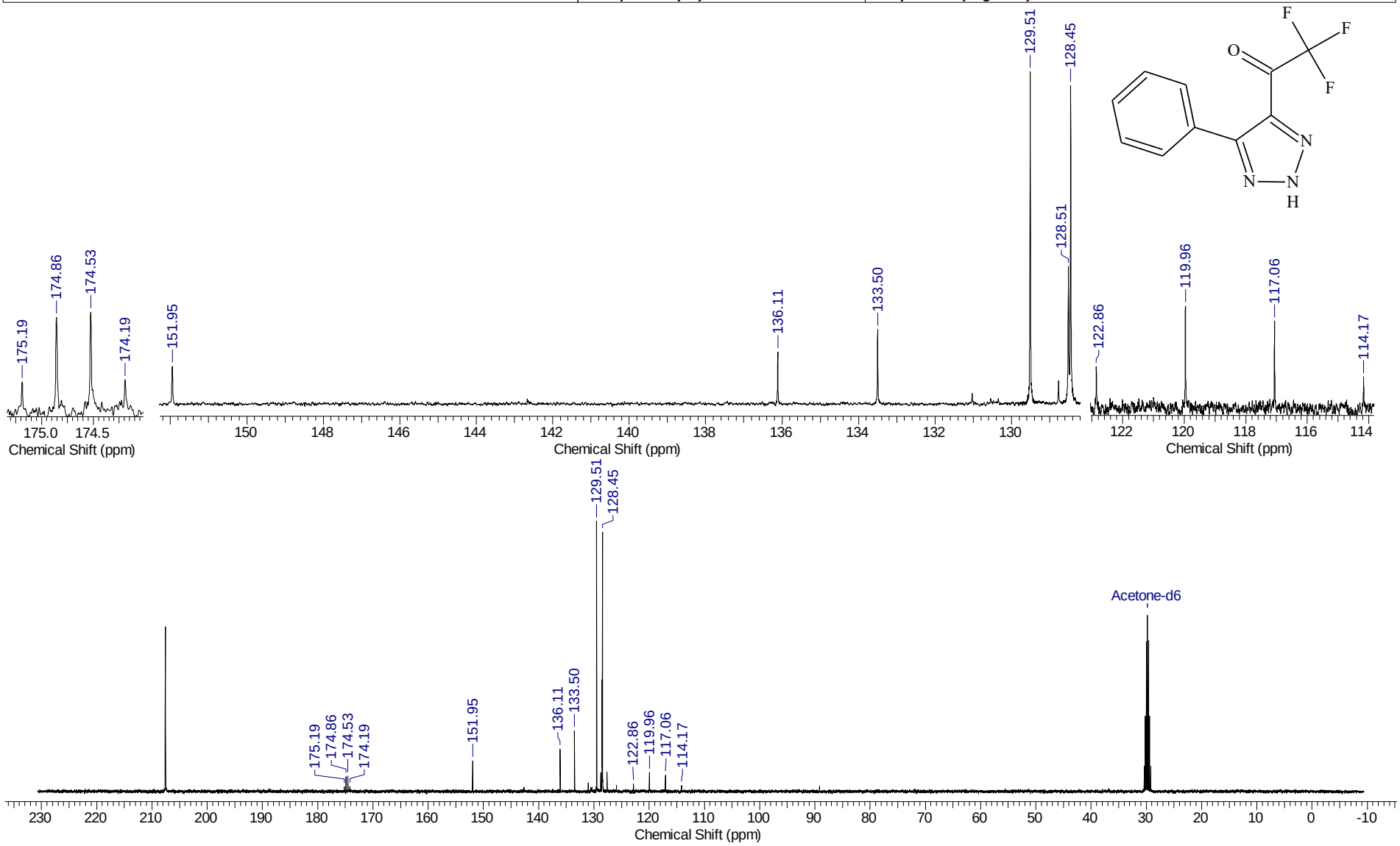
Acquisition Time (sec)	1.7433	***Comment***	Imported from UXNMR.			***Date***	18 Jan 2022 15:24:18
File Name	C:\DOCS\OUTPUT_301\2022\01. 磯囪黒BM-2368-2.F_005001r					***Frequency (MHz)***	376.50
Nucleus	19F	***Number of Transients***	16	***Original Points Count***	131072	***Points Count***	262144
Pulse Sequence	zgflqn	***Solvent***	Acetone	***Sweep Width (Hz)***	75187.97	***Temperature (degree C)***	27.000



^{19}F NMR spectrum of **2a** (376.5 MHz, acetone-d_6)

20 May 2022

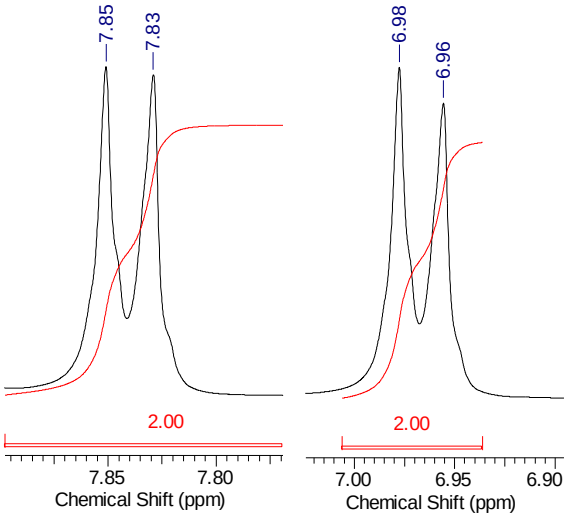
Acquisition Time (sec)	0.6783	***Comment***	Imported from UXNMR.			***Date***	25 Jan 2022 15:05:38
File Name	C:\DOCS\OUTPUT_301\2022\01. 磯囪黒BM-2368_002001r			***Frequency (MHz)***	100.61	***Nucleus***	13C
Number of Transients	57	***Original Points Count***	16384	***Points Count***	131072	***Pulse Sequence***	zgpg30
Solvent	CHLOROFORM-D			***Sweep Width (Hz)***	24154.59	***Temperature (degree C)***	27.000

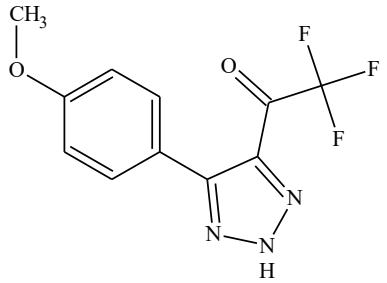


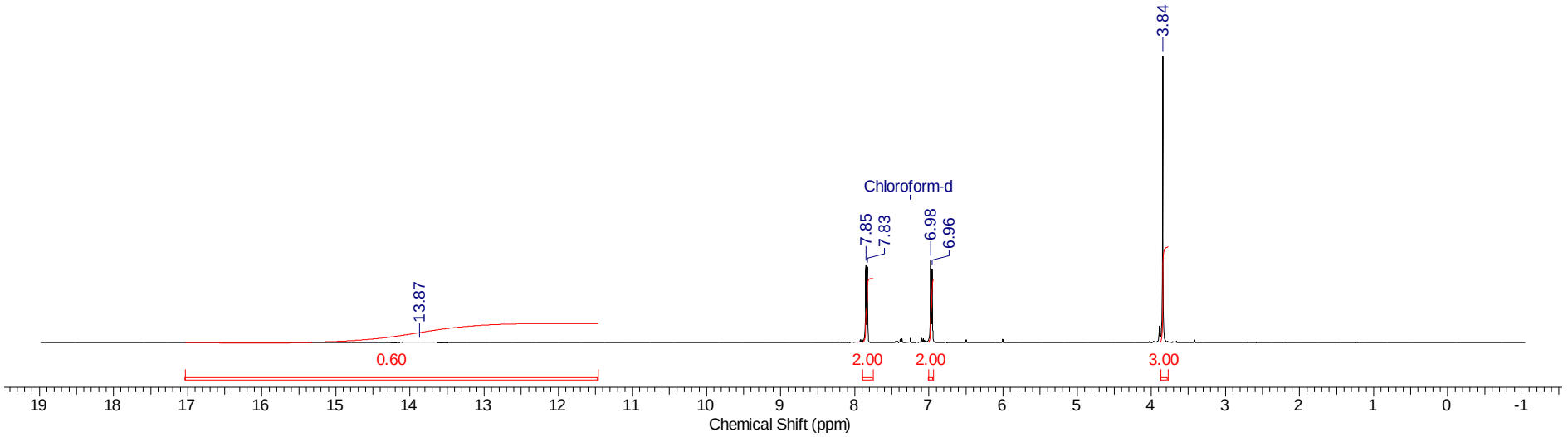
^{13}C NMR spectrum of **2a** (100.6 MHz, acetone-d_6)

1 Jun 2022

Acquisition Time (sec)	4.0894	***Comment***	Imported from UXNMR.			***Date***	27 May 2022 15:23:34
File Name	C:\DOCS\OUTPUT_301\2022\05.爨 閒BM-2511-2.H_001001r			***Frequency (MHz)***	400.13	***Nucleus***	1H
Number of Transients	4	***Original Points Count***	32768	***Points Count***	131072	***Pulse Sequence***	zg30
Solvent	CHLOROFORM-D			***Sweep Width (Hz)***	8012.82	***Temperature (degree C)***	27.000



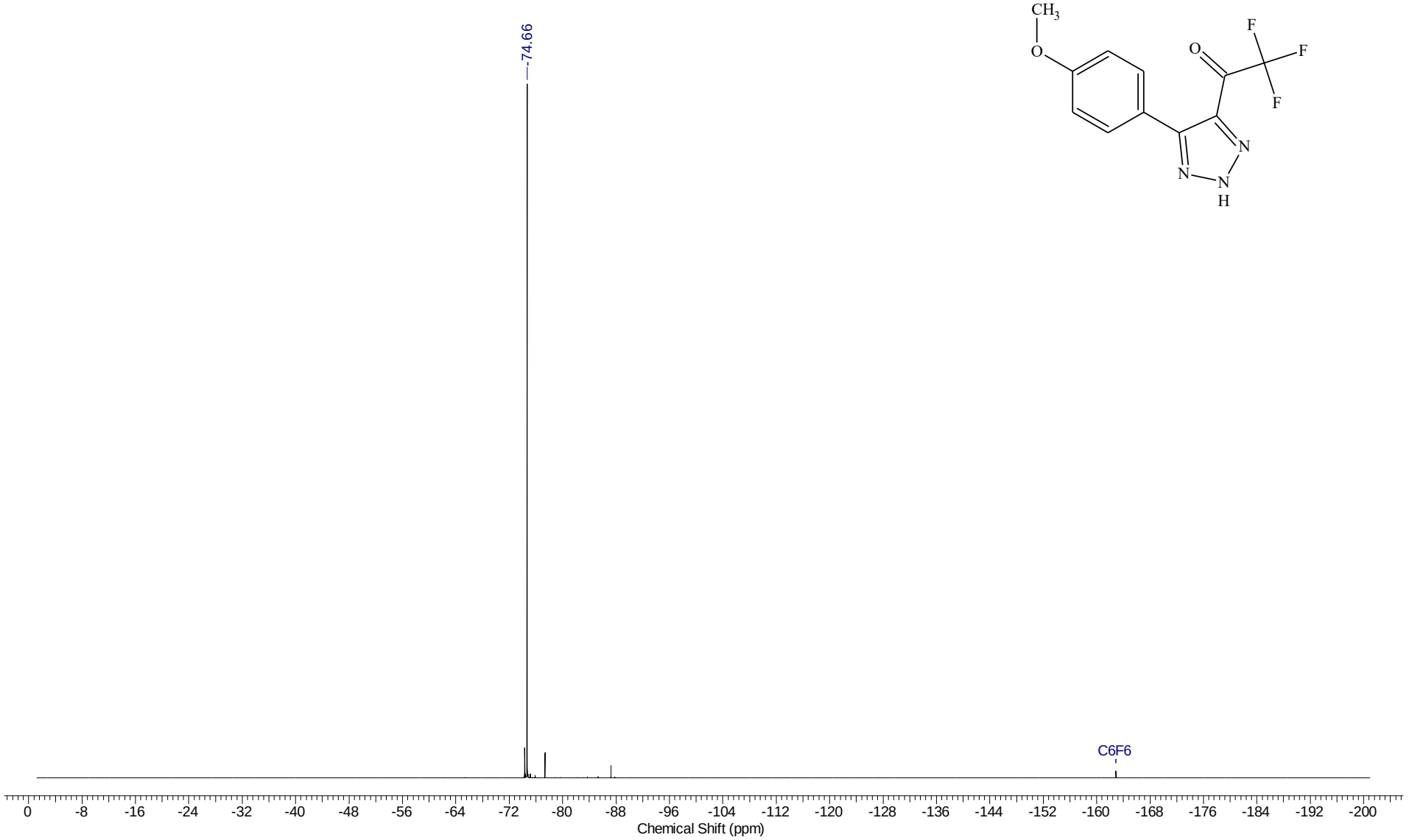




^{1}H NMR spectrum of **2b** (400.1 MHz, $CDCl_3$)

1 Jun 2022

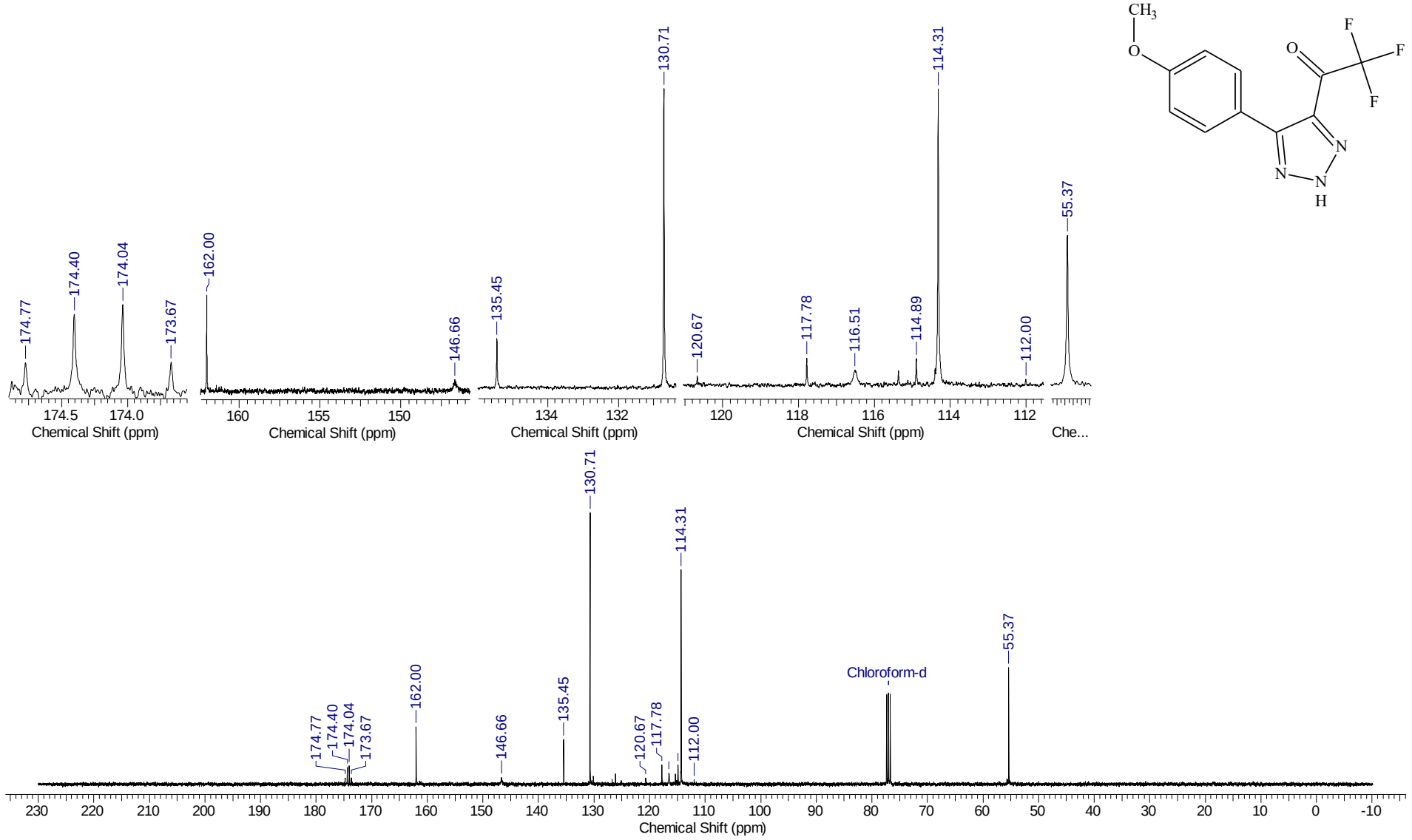
Acquisition Time (sec)	1.7433	***Comment***	Imported from UXNMR.			***Date***	27 May 2022 15:38:18
File Name	C:\DOCS\OUTPUT_301\2022\05.爨 閉BM-2511-2.F_005001r			***Frequency (MHz)***	376.50	***Nucleus***	19F
Number of Transients	16	***Original Points Count***	131072	***Points Count***	262144	***Pulse Sequence***	zgflqn
Solvent	CHLOROFORM-D			***Sweep Width (Hz)***	75187.97	***Temperature (degree C)***	27.000



^{19}F NMR spectrum of **2b** (376.5 MHz, $CDCl_3$)

1 Jun 2022

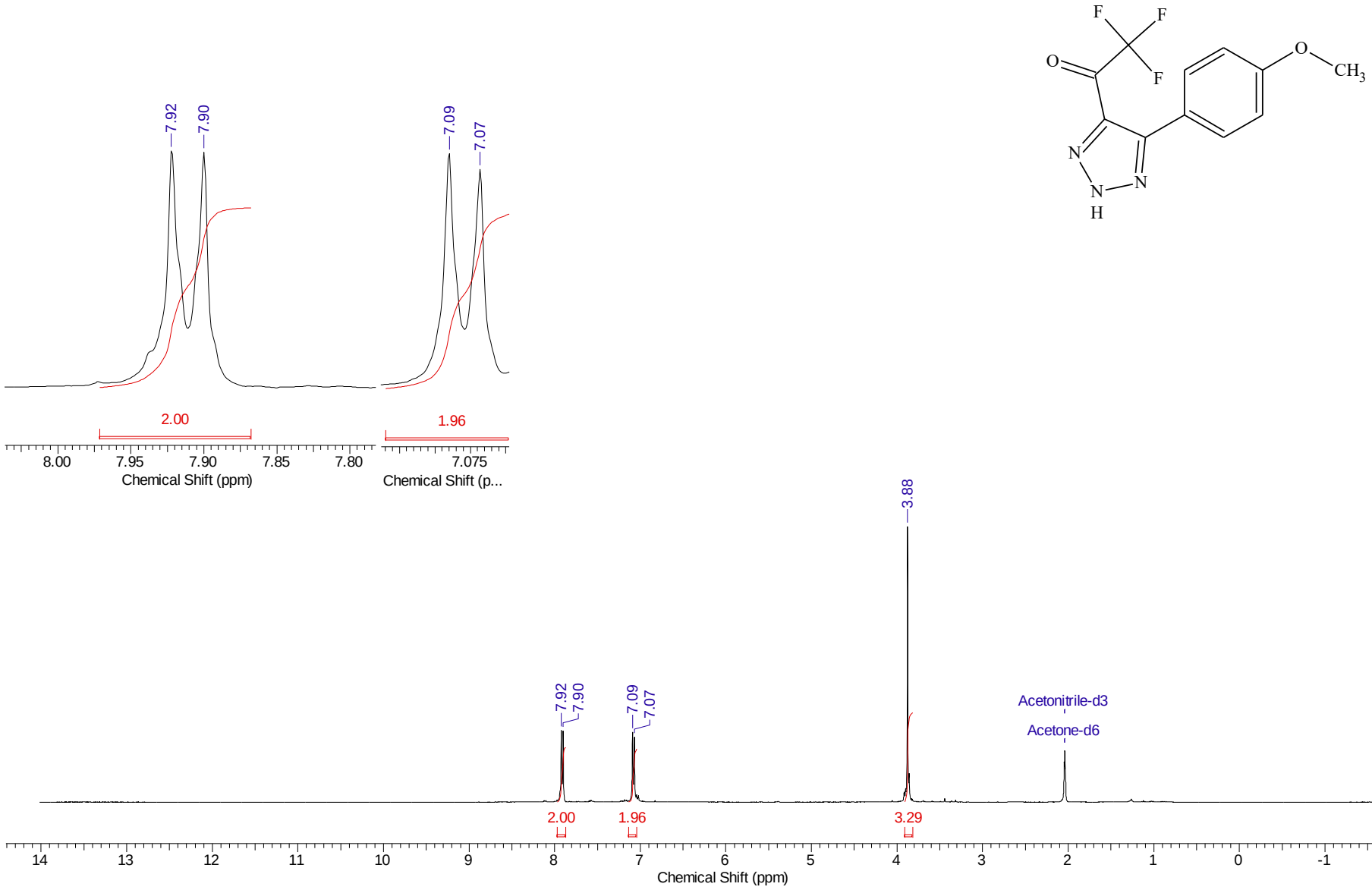
Acquisition Time (sec)	0.6783	***Comment***	Imported from UXNMR.			***Date***	27 May 2022 15:33:52
File Name	C:\DOCS\OUTPUT_301\2022\05.爨 閇BM-2511-2.C_002001r			***Frequency (MHz)***	100.61	***Nucleus***	13C
Number of Transients	209	***Original Points Count***	16384	***Points Count***	131072	***Pulse Sequence***	zgpg30
Solvent	CHLOROFORM-D			***Sweep Width (Hz)***	24154.59	***Temperature (degree C)***	27.000



^{13}C NMR spectrum of **2b** (100.6 MHz, $CDCl_3$)

12 May 2022

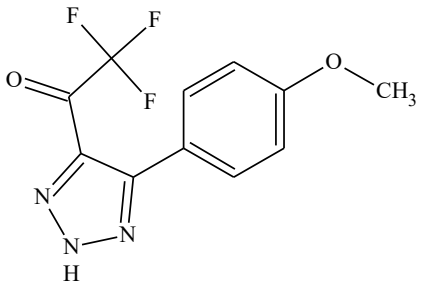
Acquisition Time (sec)	2.5559	***Date***	Apr 10 2018	***File Name***	I:\SPEC_BM_F_2018.12.25\bm1336-2-h_20180410_01\PROTON_01				
Frequency (MHz)	399.97	***Nucleus***	1H	***Number of Transients***	4	***Original Points Count***	16384	***Points Count***	16384
Pulse Sequence	s2pul	***Solvent***	acetone	***Sweep Width (Hz)***	6410.26	***Temperature (degree C)***	22.000		

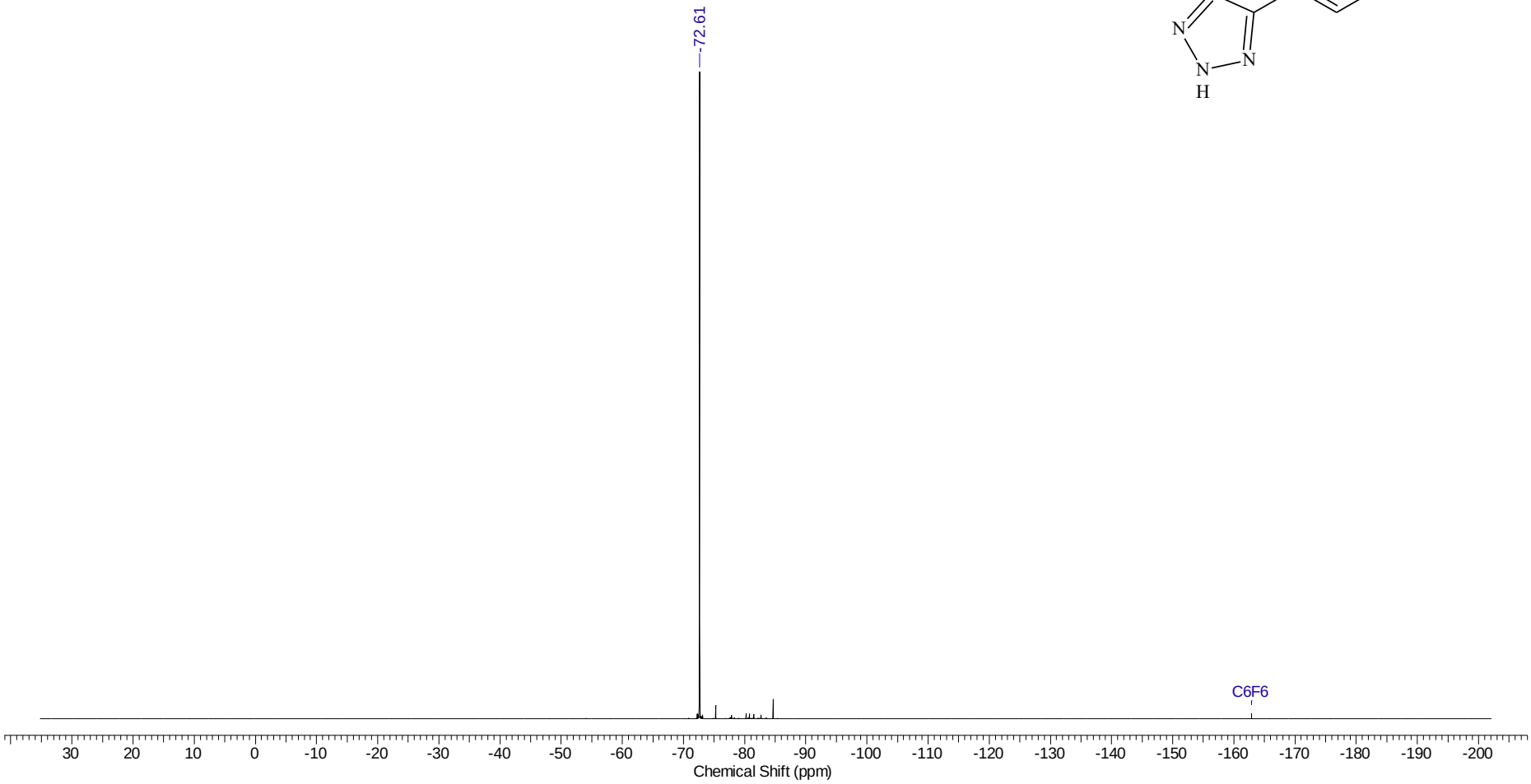


^{1}H NMR spectrum of **2b** (400.1 MHz, acetone-d_6)

12 May 2022

Acquisition Time (sec)	0.7340	***Date***	Apr 10 2018	***File Name***	C:\DOCS\OUTPUT_301\F19\2018.04.10\bm1336-2-f_20180410_01\FLUORINE_01		
Frequency (MHz)	376.31	***Nucleus***	19F	***Number of Transients***	100	***Original Points Count***	65536
Points Count	65536	***Pulse Sequence***	s2pul	***Solvent***	acetone	***Sweep Width (Hz)***	89285.71
Temperature (degree C)	22.000						

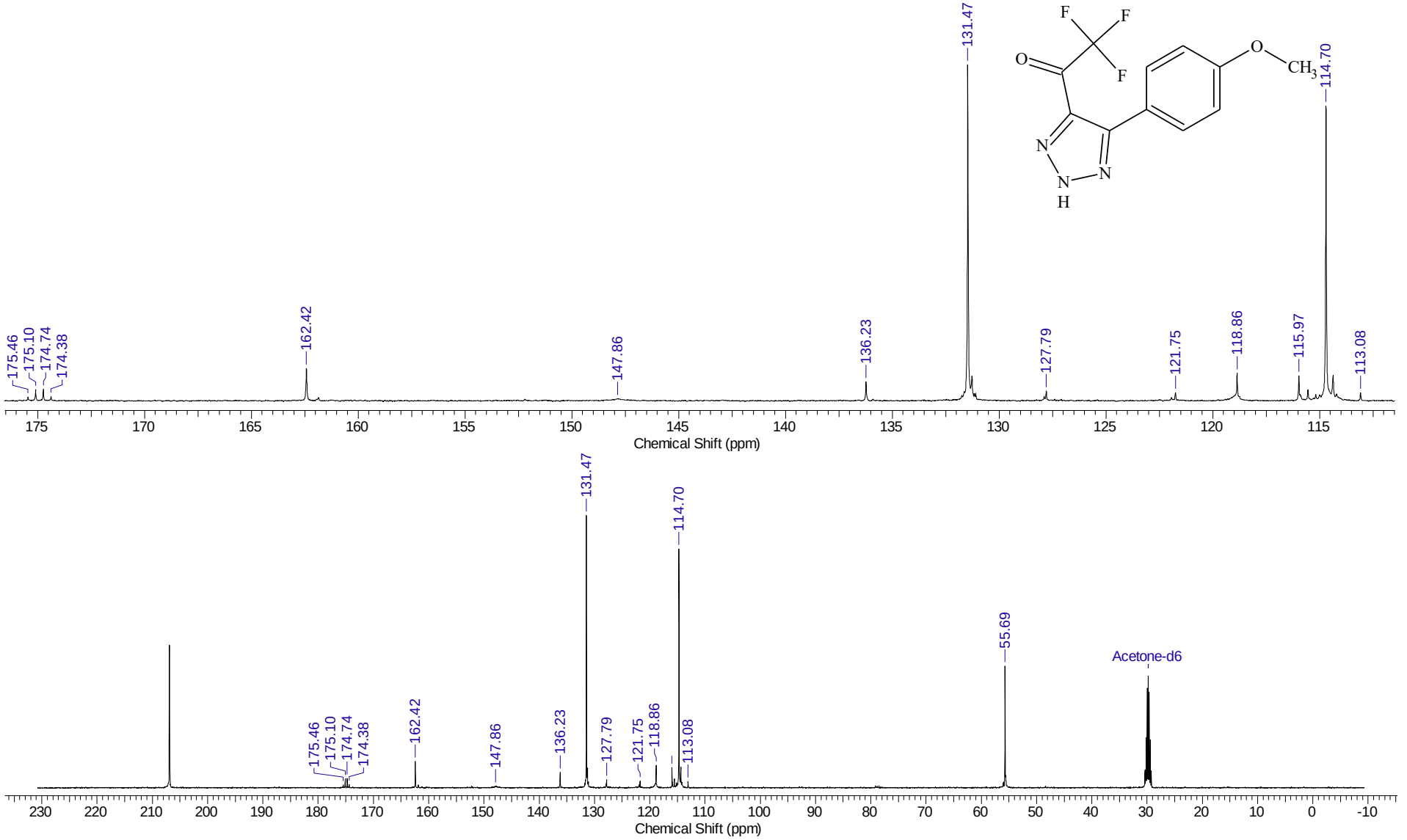




^{19}F NMR spectrum of **2b** (376.5 MHz, acetone-d_6)

12 May 2022

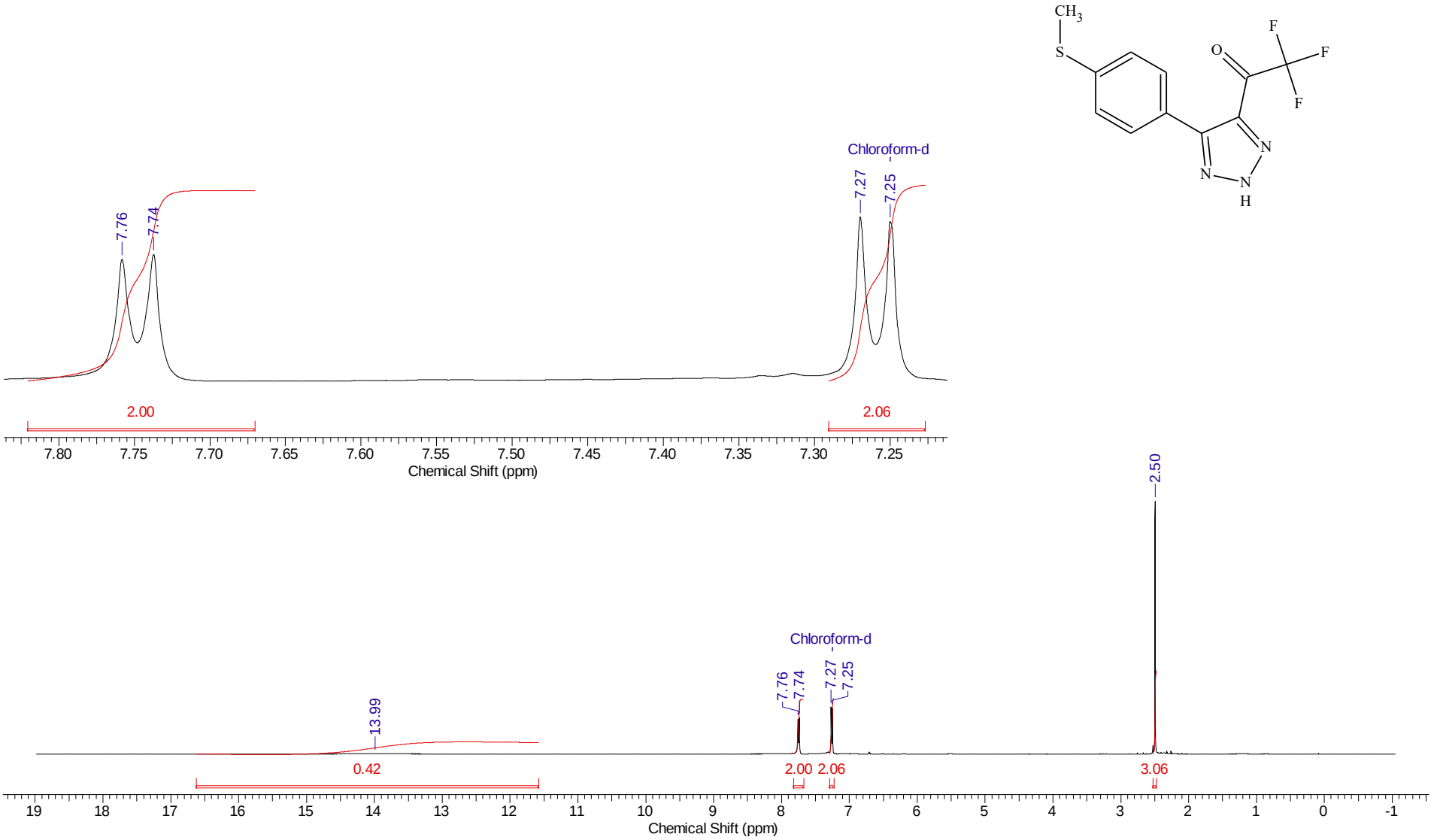
Acquisition Time (sec)	0.4999	***Comment***	Imported from UXNMR.			***Date***	10 Apr 2018 16:05:28
File Name	C:\BM_DATA\DOCS\SPEC_BM_H,C\BM-1336-2.C_002001r					***Frequency (MHz)***	100.61
Nucleus	13C	***Number of Transients***	1188	***Original Points Count***	12076	***Points Count***	65536
Pulse Sequence	zgpg30	***Solvent***	Acetone	***Sweep Width (Hz)***	24154.59	***Temperature (degree C)***	27.000



^{13}C NMR spectrum of **2b** (100.6 MHz, acetone-d_6)

3 May 2022

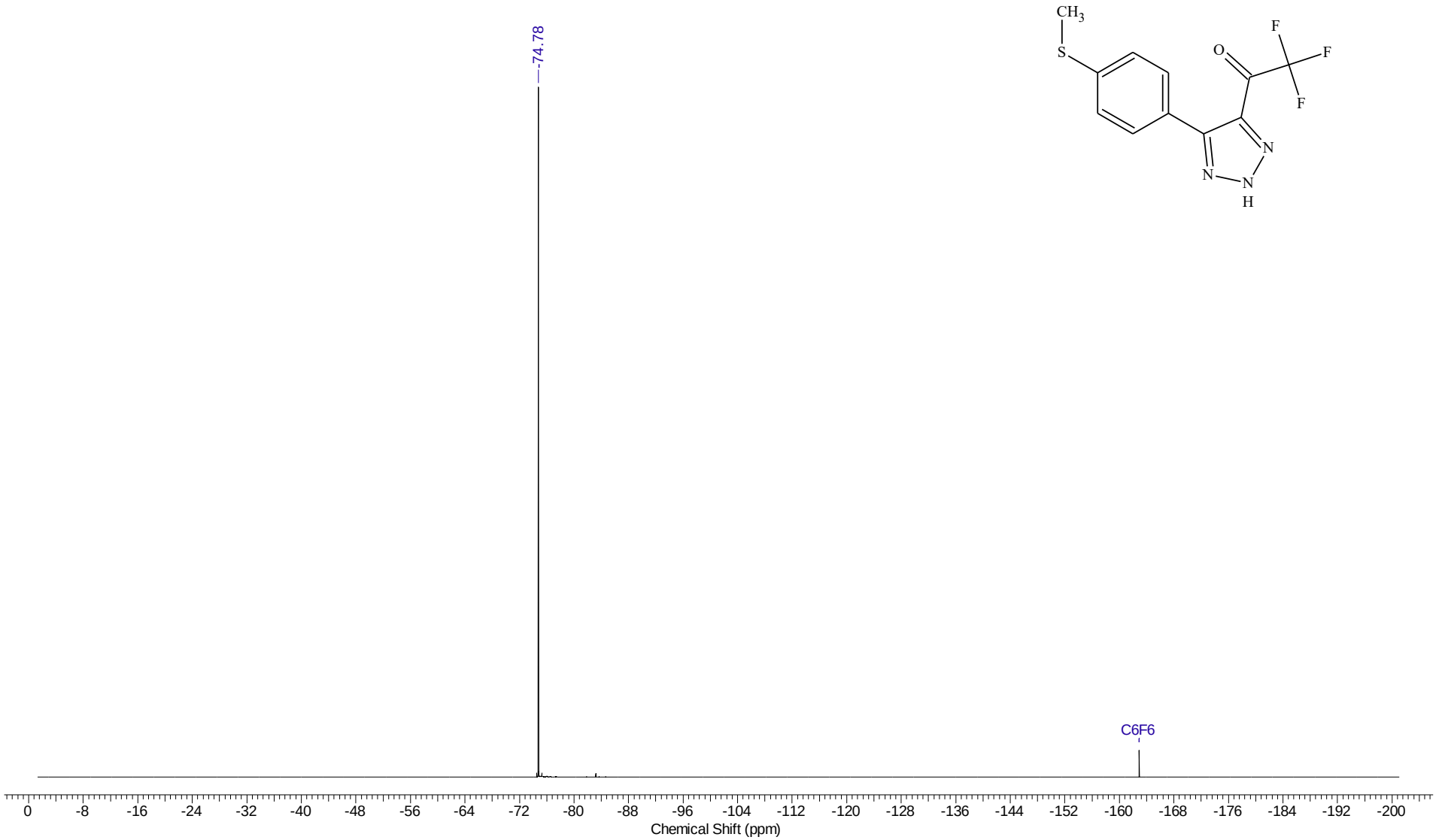
Acquisition Time (sec)	4.0894	***Comment***	Imported from UXNMR.			***Date***	16 Feb 2022 17:36:48
File Name	C:\DOCS\OUTPUT_301\2022\02.翦 怵嚾黑BM-2365-3.H_001001r					***Frequency (MHz)***	400.13
Nucleus	1H	***Number of Transients***	4	***Original Points Count***	32768	***Points Count***	131072
Pulse Sequence	zg30	***Solvent***	DEUTERIUM OXIDE			***Sweep Width (Hz)***	8012.82
Temperature (degree C)	27.000						



^{1}H NMR spectrum of **2c** (400.1 MHz, $CDCl_3$)

3 May 2022

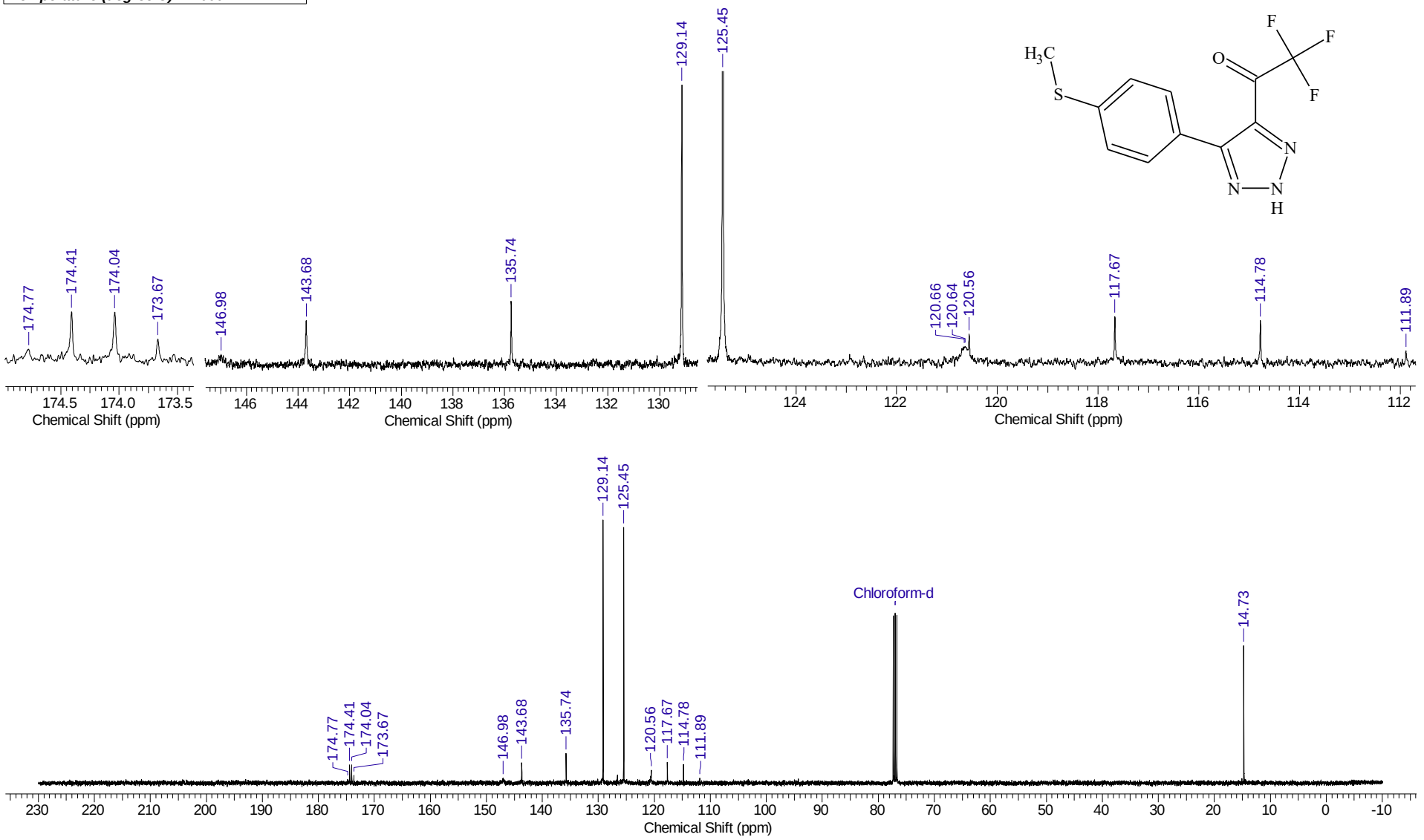
Acquisition Time (sec)	1.7433	***Comment***	Imported from UXNMR.			***Date***	16 Feb 2022 17:51:02
File Name	C:\DOCS\OUTPUT_301\2022\02.翦 怵嚏黑BM-2365-3.F_005001r					***Frequency (MHz)***	376.50
Nucleus	19F	***Number of Transients***	16	***Original Points Count***	131072	***Points Count***	262144
Pulse Sequence	zgflqn	***Solvent***	CHLOROFORM-D			***Sweep Width (Hz)***	75187.97
Temperature (degree C)	27.000						



^{19}F NMR spectrum of **2c** (376.5 MHz, $CDCl_3$)

3 May 2022

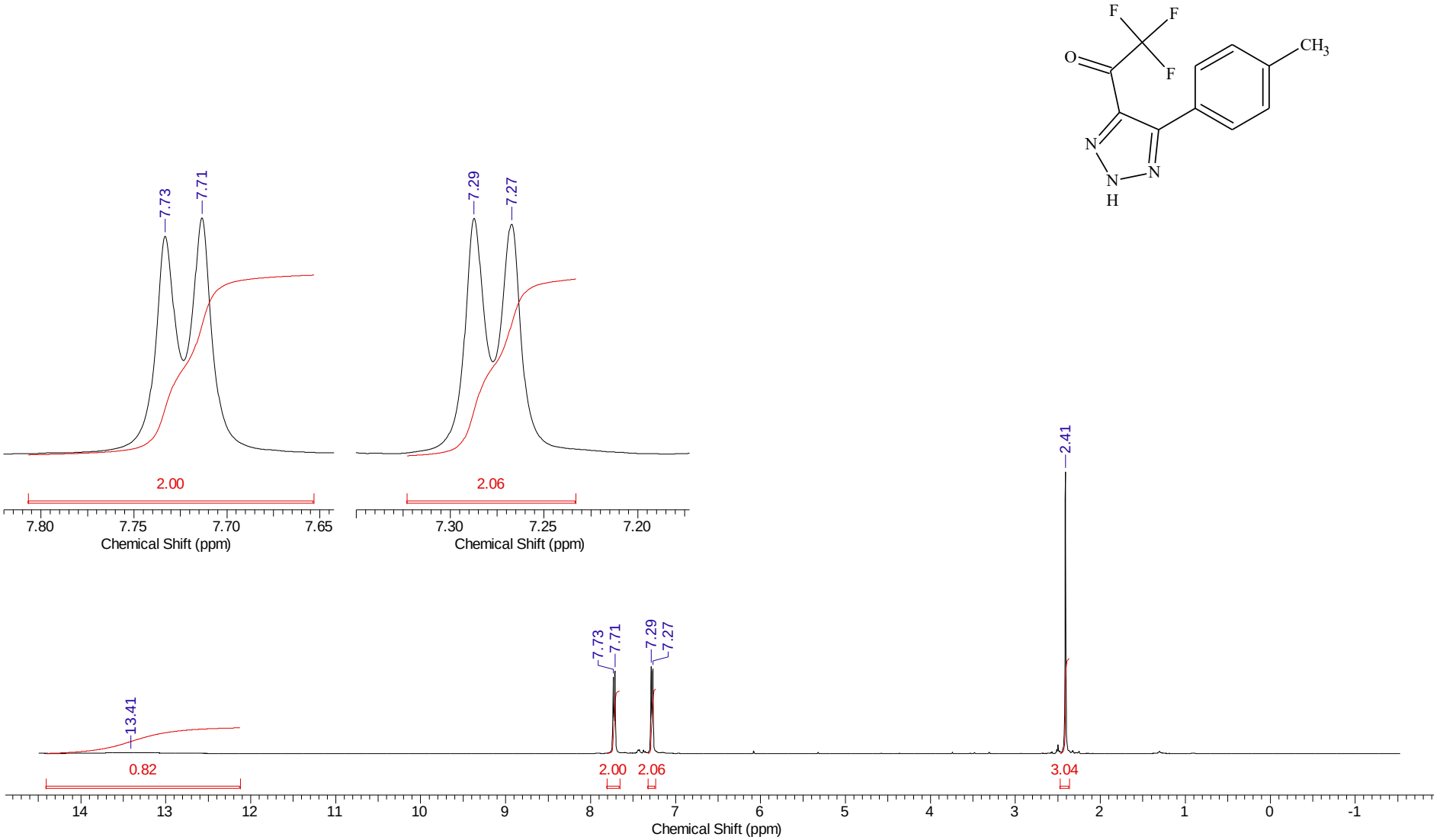
Acquisition Time (sec)	0.6783	***Comment***	Imported from UXNMR.			***Date***	17 Feb 2022 12:45:10
File Name	C:\BM_DATA\DOCS\吟 齂耦皴滂\2022\17_02_2022\BM-2365-3.C_002001r					***Frequency (MHz)***	100.61
Nucleus	13C	***Number of Transients***	161	***Original Points Count***	16384	***Points Count***	131072
Pulse Sequence	zgpg30	***Solvent***	ACETONITRILE-D3			***Sweep Width (Hz)***	24154.59
Temperature (degree C)	27.000						



^{13}C NMR spectrum of **2c** (100.6 MHz, $CDCl_3$)

12 May 2022

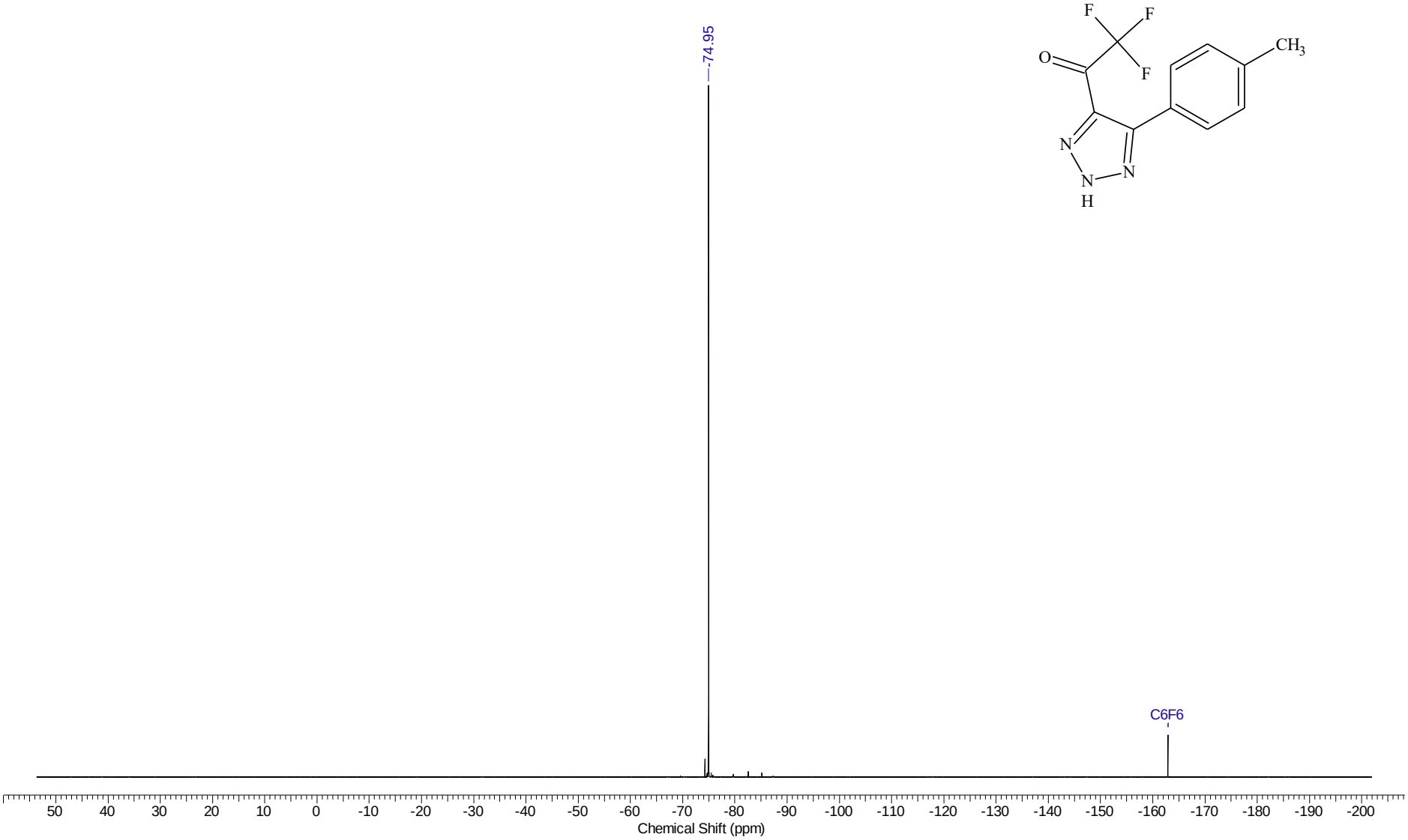
Acquisition Time (sec)	2.5559	***Comment***	Imported from UXNMR.			***Date***	06 Apr 2018 15:06:24
File Name	C:\BM_DATA\DOCS\SPEC_BM_H,C\BM-1327-3S.H_001001r					***Frequency (MHz)***	400.13
Nucleus	1H	***Number of Transients***	4	***Original Points Count***	16384	***Points Count***	65536
Pulse Sequence	zg30	***Solvent***	CHLOROFORM-D			***Sweep Width (Hz)***	6410.26
Temperature (degree C)	27.000						



^{1}H NMR spectrum of **2d** (400.1 MHz, $CDCl_3$)

12 May 2022

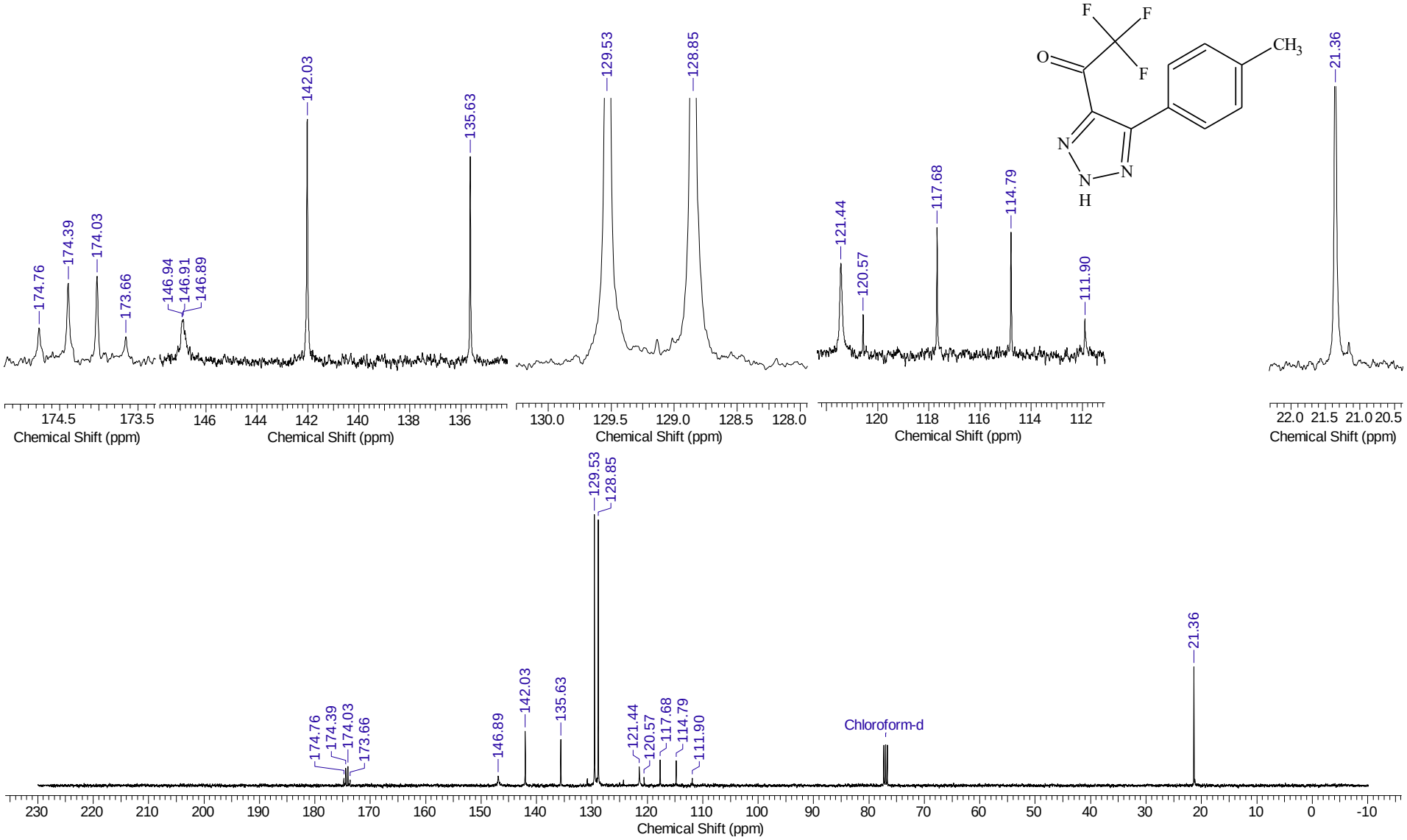
Acquisition Time (sec)	2.7263	***Date***	Apr 5 2018	***File Name***	I:\SPEC_BM_F_2018.12.25\BM-1327-3S-F_20180405_01\FLUORINE_01		
Frequency (MHz)	376.31	***Nucleus***	19F	***Number of Transients***	8	***Original Points Count***	262144
Points Count	262144	***Pulse Sequence***	s2pul	***Solvent***	CHLOROFORM-D		
Sweep Width (Hz)	96153.84	***Temperature (degree C)***	22.000				



^{19}F NMR spectrum of **2d** (376.5 MHz, $CDCl_3$)

12 May 2022

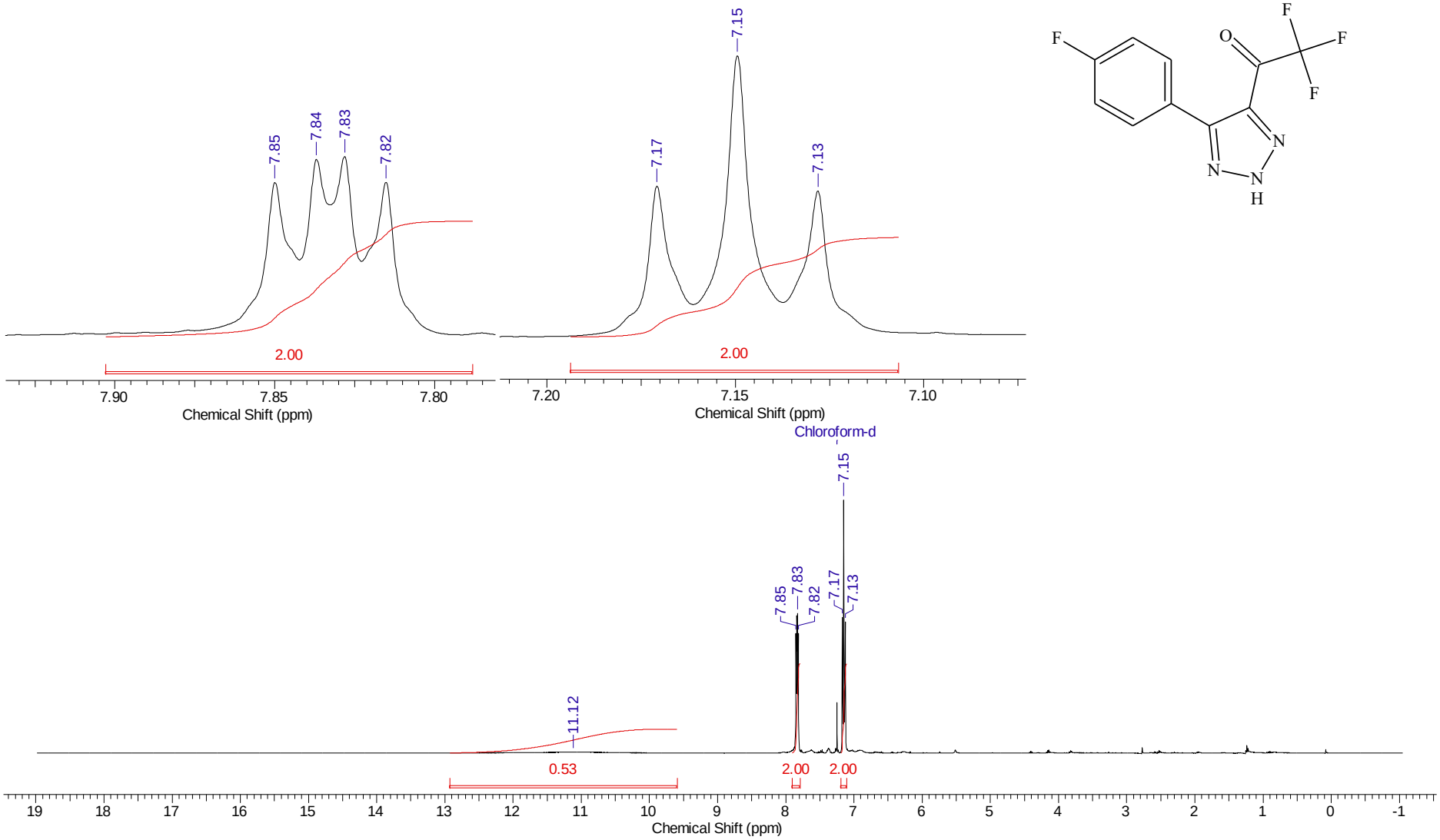
Acquisition Time (sec)	0.4999	***Comment***	Imported from UXNMR.			***Date***	06 Apr 2018 15:09:52
File Name	C:\BM_DATA\DOCS\SPEC_BM_H,C\BM-1327-3S.C_002001r			***Frequency (MHz)***	100.61	***Nucleus***	13C
Number of Transients	64	***Original Points Count***	12076	***Points Count***	65536	***Pulse Sequence***	zgpg30
Solvent	DEUTERIUM OXIDE			***Sweep Width (Hz)***	24154.59	***Temperature (degree C)***	27.000



^{13}C NMR spectrum of **2d** (100.6 MHz, $CDCl_3$)

3 May 2022

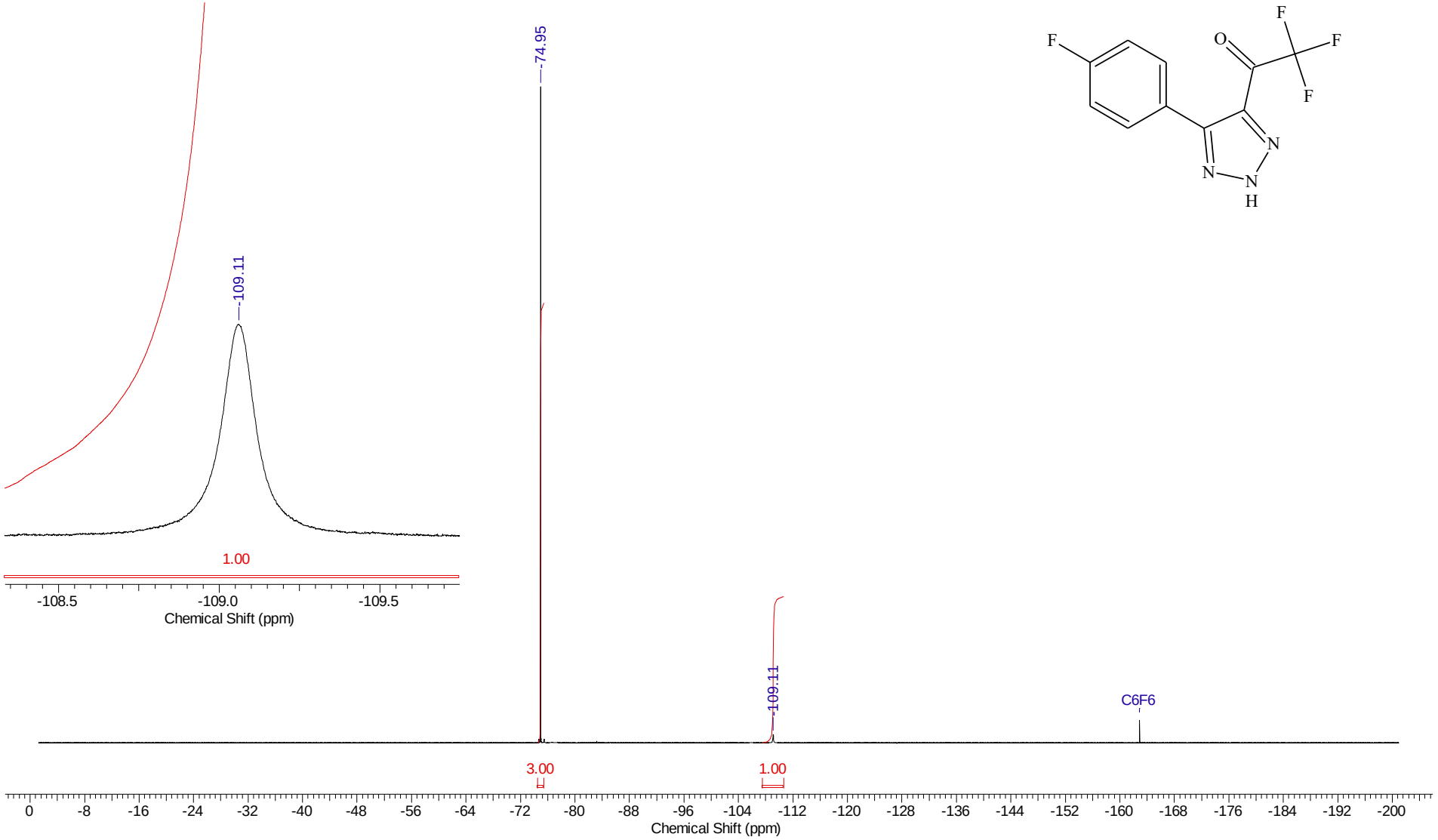
Acquisition Time (sec)	4.0894	***Comment***	Imported from UXNMR.			***Date***	15 Feb 2022 15:08:46
File Name	C:\DOCS\OUTPUT_301\2022\02.翦 怵曜黒BM-2214-2.H_001001r					***Frequency (MHz)***	400.13
Nucleus	1H	***Number of Transients***	4	***Original Points Count***	32768	***Points Count***	131072
Pulse Sequence	zg30	***Solvent***	DEUTERIUM OXIDE			***Sweep Width (Hz)***	8012.82
Temperature (degree C)	27.000						



^{1}H NMR spectrum of **2e** (400.1 MHz, $CDCl_3$)

3 May 2022

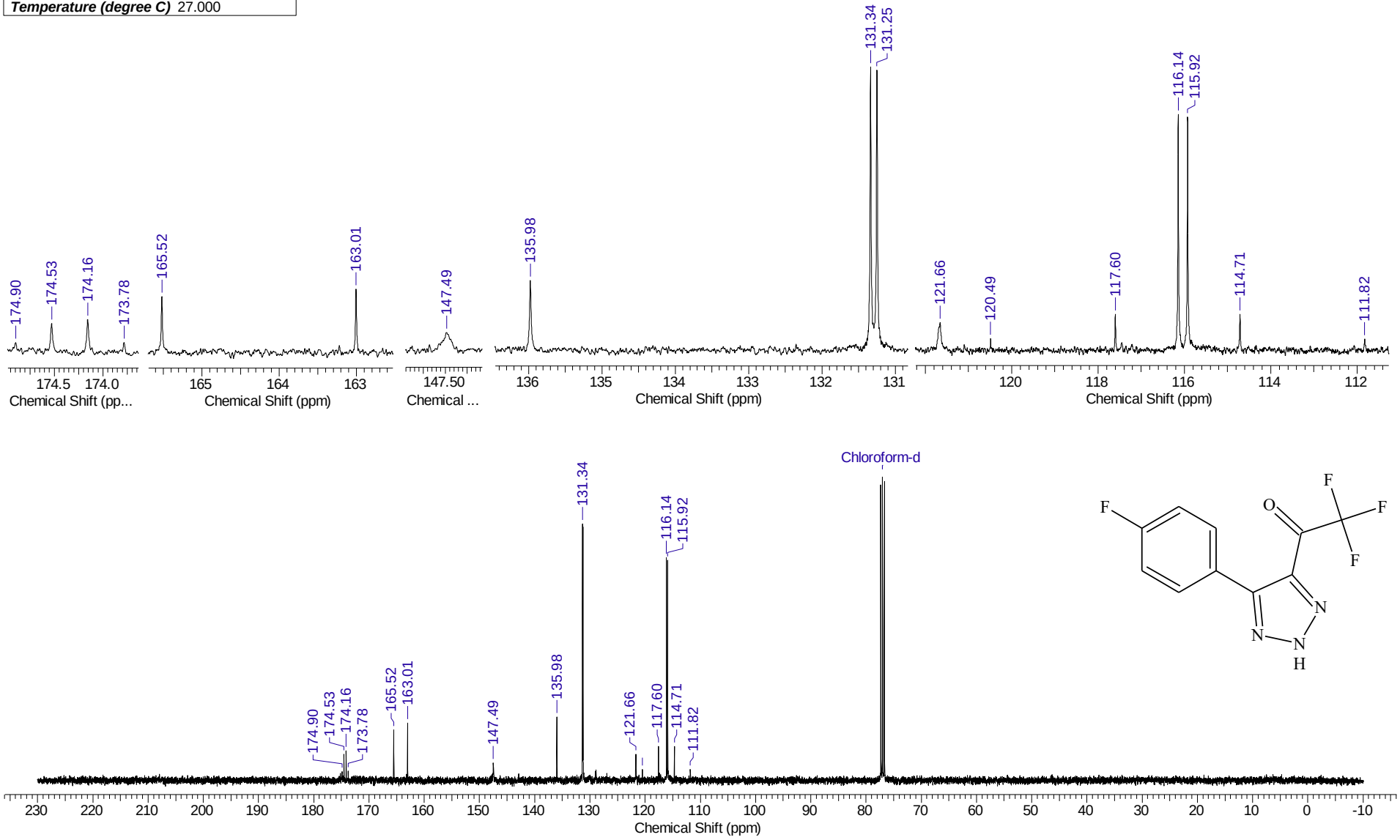
Acquisition Time (sec)	1.7433	***Comment***	Imported from UXNMR.			***Date***	15 Feb 2022 15:38:54
File Name	C:\DOCS\OUTPUT_301\2022\02.翦 怵嚾黑BM-2214-2.F_005001r					***Frequency (MHz)***	376.50
Nucleus	19F	***Number of Transients***	13	***Original Points Count***	131072	***Points Count***	262144
Pulse Sequence	zgflqn	***Solvent***	CHLOROFORM-D			***Sweep Width (Hz)***	75187.97
Temperature (degree C)	27.000						



^{19}F NMR spectrum of **2e** (376.5 MHz, $CDCl_3$)

3 May 2022

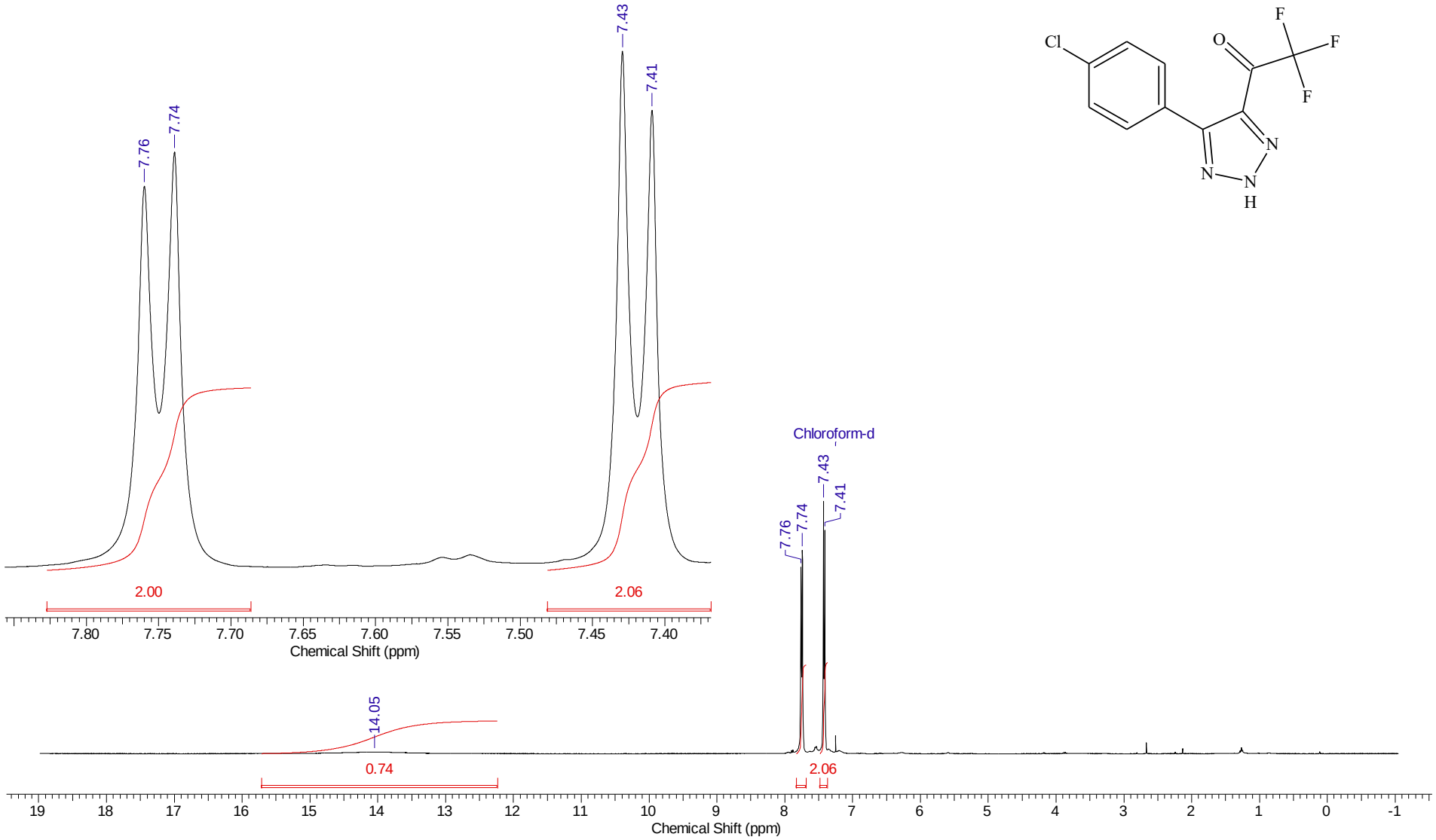
Acquisition Time (sec)	0.6783	***Comment***	Imported from UXNMR.			***Date***	15 Feb 2022 15:17:16
File Name	C:\DOCS\OUTPUT_301\2022\02.翦 怵嚏黑BM-2214-2.C_002001r					***Frequency (MHz)***	100.61
Nucleus	13C	***Number of Transients***	218	***Original Points Count***	16384	***Points Count***	131072
Pulse Sequence	zgpg30	***Solvent***	ACETONITRILE-D3			***Sweep Width (Hz)***	24154.59
Temperature (degree C)	27.000						



^{13}C NMR spectrum of **2e** (100.6 MHz, $CDCl_3$)

3 May 2022

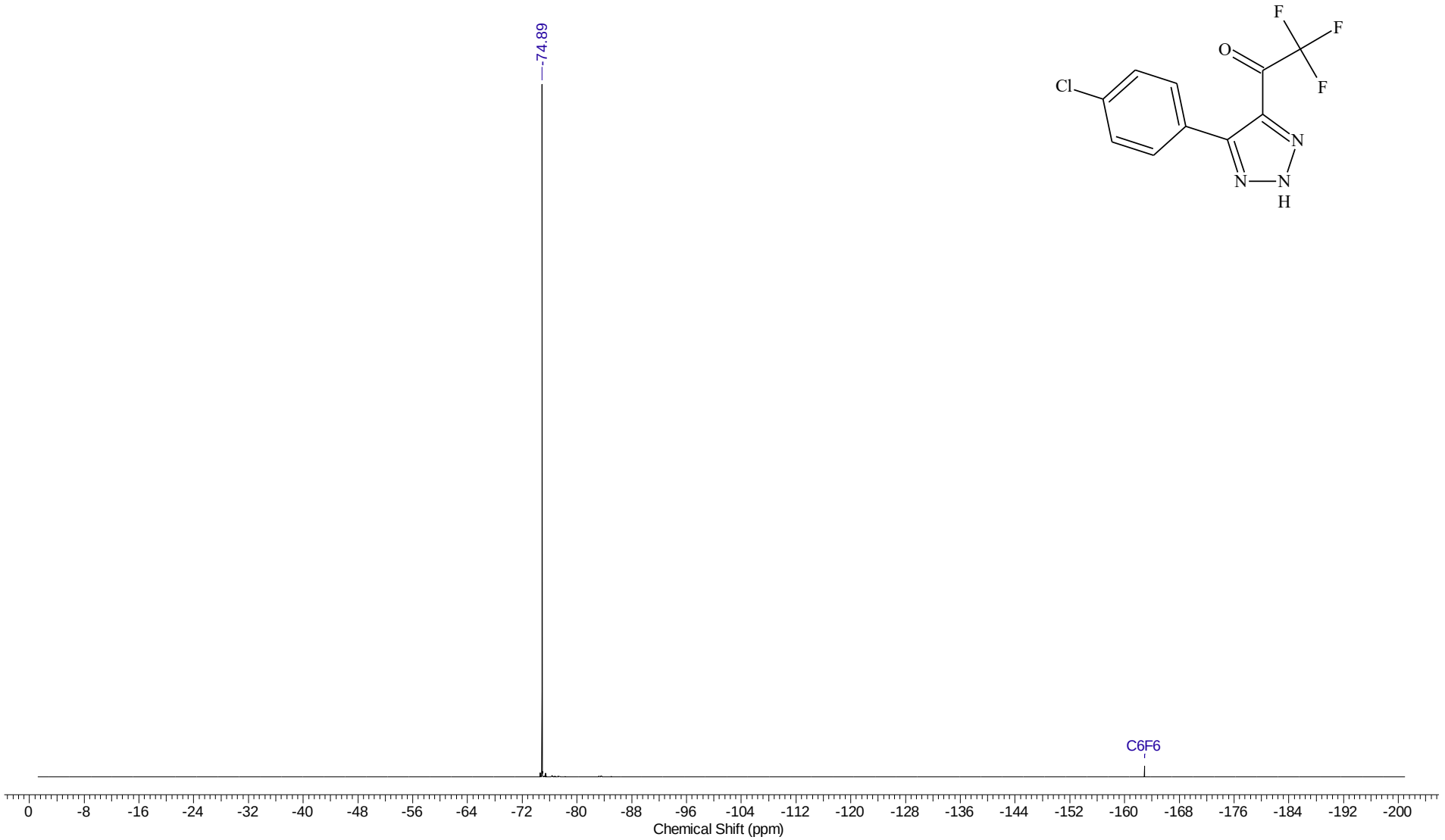
Acquisition Time (sec)	4.0894	***Comment***	Imported from UXNMR.			***Date***	14 Feb 2022 15:23:32
File Name	C:\DOCS\OUTPUT_301\2022\02.翦 怵嚾黑BM-2357-3.H_001001r					***Frequency (MHz)***	400.13
Nucleus	1H	***Number of Transients***	4	***Original Points Count***	32768	***Points Count***	131072
Pulse Sequence	zg30	***Solvent***	CHLOROFORM-D			***Sweep Width (Hz)***	8012.82
Temperature (degree C)	27.000						



^{1}H NMR spectrum of **2f** (400.1 MHz, $CDCl_3$)

3 May 2022

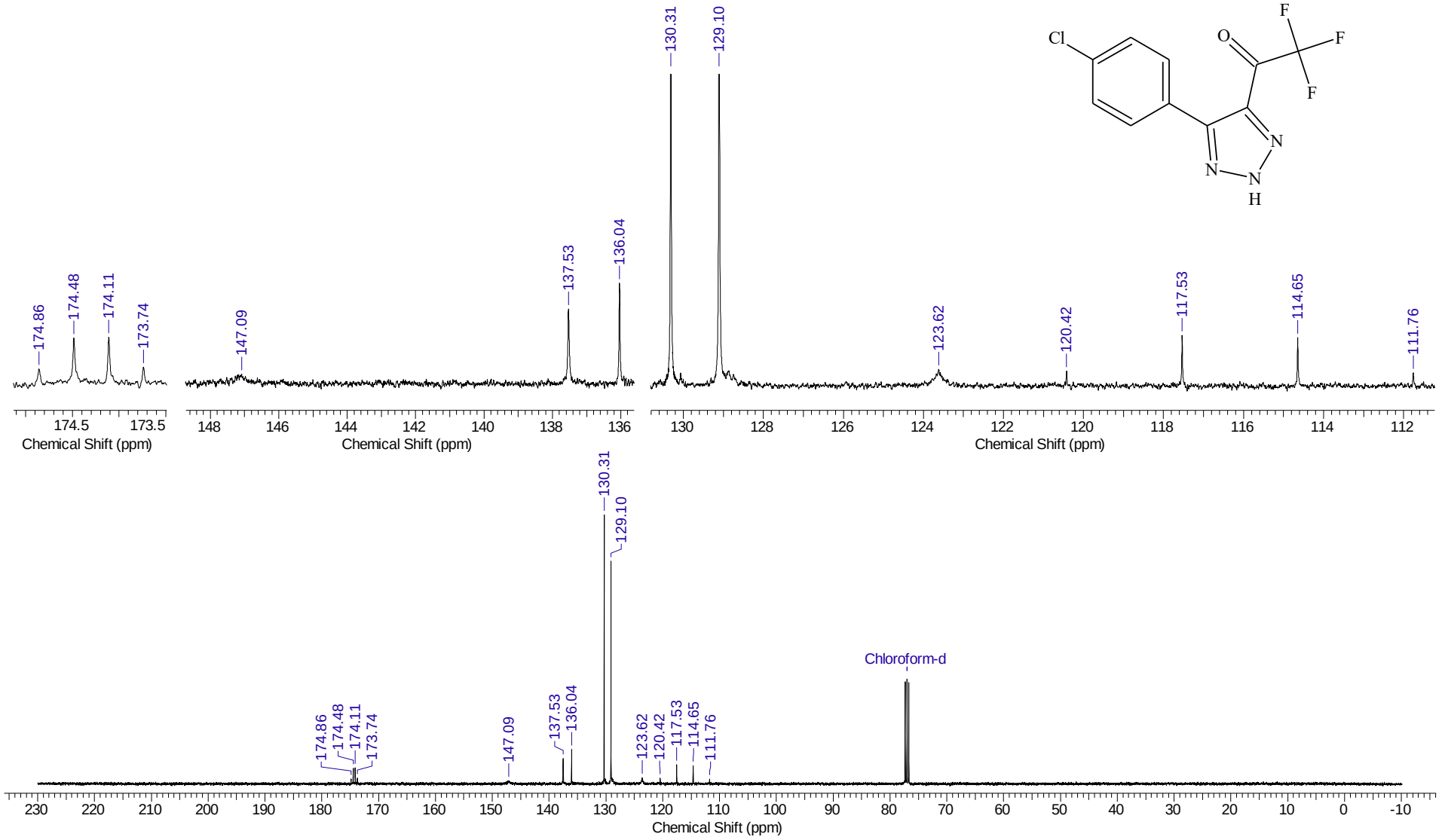
Acquisition Time (sec)	1.7433	***Comment***	Imported from UXNMR.			***Date***	12 Feb 2022 22:16:28
File Name	C:\BM_DATA\DOCS\吁 齁 耦皴滂\2022\bm220212\BM-2357-3_005001r					***Frequency (MHz)***	376.50
Nucleus	19F	***Number of Transients***	16	***Original Points Count***	131072	***Points Count***	262144
Pulse Sequence	zgflqn	***Solvent***	CHLOROFORM-D			***Sweep Width (Hz)***	75187.97
Temperature (degree C)	27.000						



^{19}F NMR spectrum of **2f** (376.5 MHz, $CDCl_3$)

3 May 2022

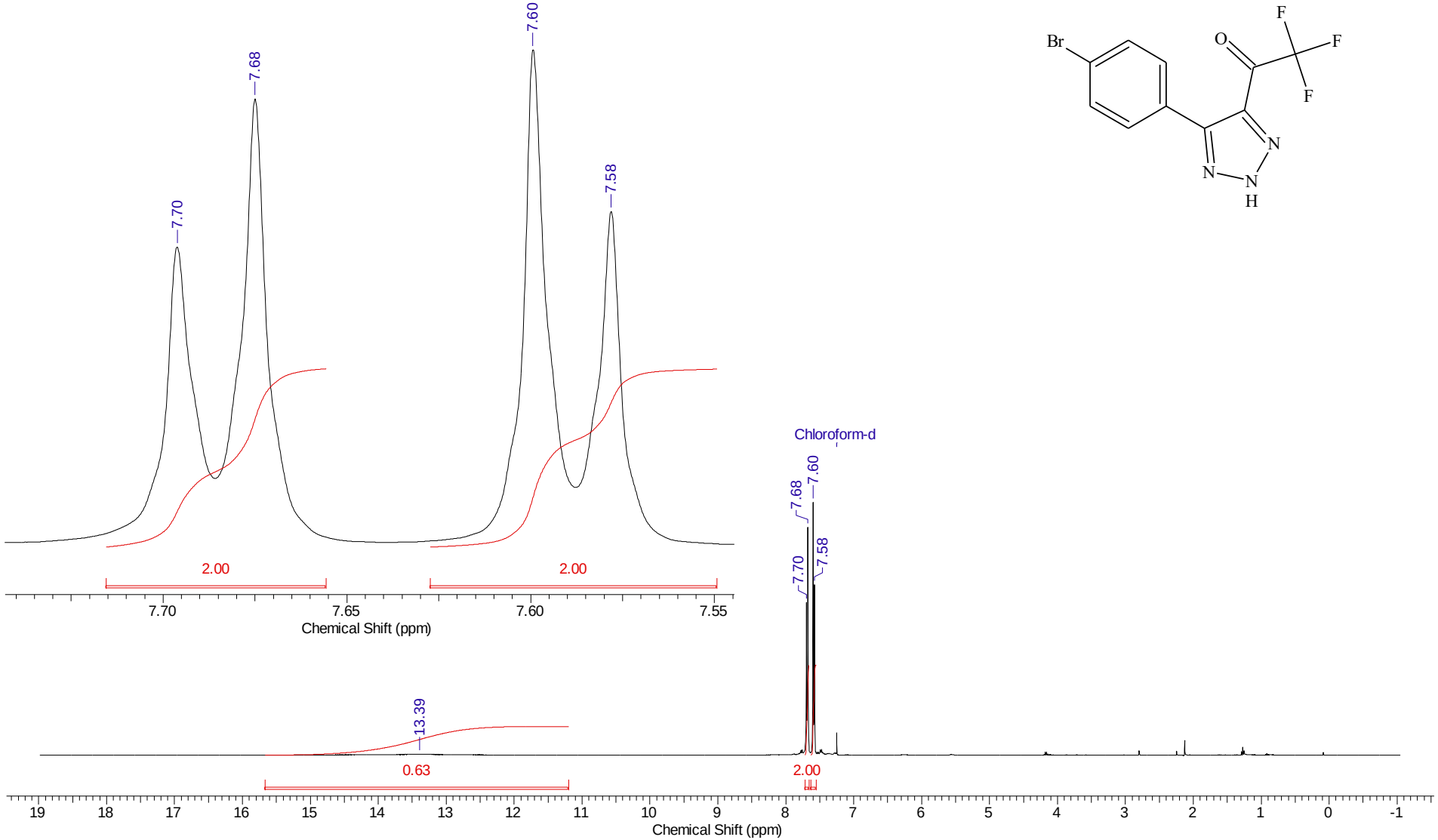
Acquisition Time (sec)	0.6783	***Comment***	Imported from UXNMR.			***Date***	14 Feb 2022 15:30:14
File Name	C:\DOCS\OUTPUT_301\2022\02.翦 怵嚏黑BM-2357-3.C_002001r					***Frequency (MHz)***	100.61
Nucleus	13C	***Number of Transients***	129	***Original Points Count***	16384	***Points Count***	131072
Pulse Sequence	zgpg30	***Solvent***	ACETONITRILE-D3			***Sweep Width (Hz)***	24154.59
Temperature (degree C)	27.000						



^{13}C NMR spectrum of **2f** (100.6 MHz, $CDCl_3$)

3 May 2022

Acquisition Time (sec)	4.0894	***Comment***	Imported from UXNMR.			***Date***	15 Feb 2022 16:05:56
File Name	C:\DOCS\OUTPUT_301\2022\02.翦 怵嚾黑BM-2363-3.H_001001r					***Frequency (MHz)***	400.13
Nucleus	1H	***Number of Transients***	4	***Original Points Count***	32768	***Points Count***	131072
Pulse Sequence	zg30	***Solvent***	DEUTERIUM OXIDE			***Sweep Width (Hz)***	8012.82
Temperature (degree C)	27.000						



^{1}H NMR spectrum of **2g** (400.1 MHz, $CDCl_3$)

3 May 2022

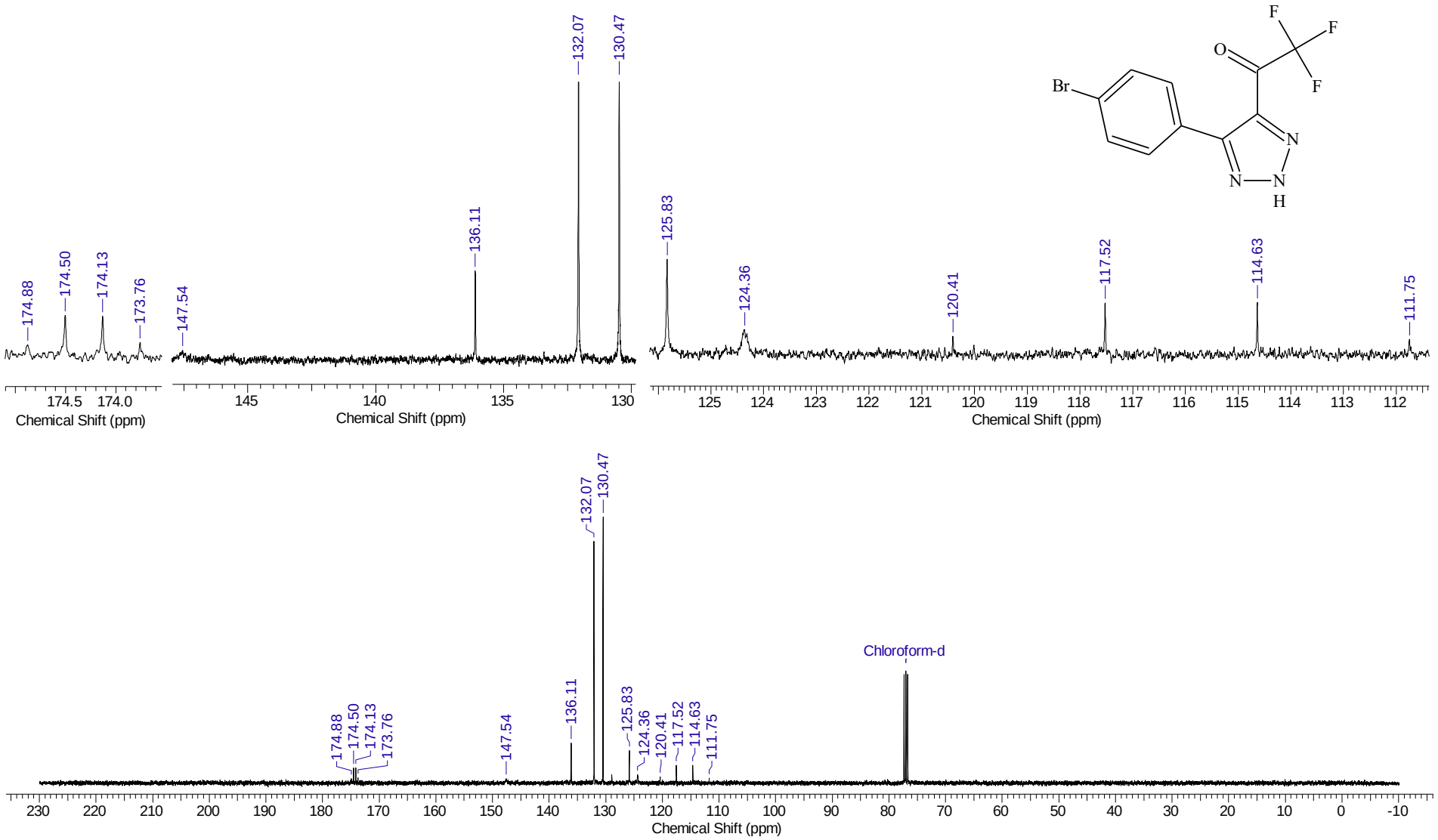
Acquisition Time (sec)	1.7433	***Comment***	Imported from UXNMR.			***Date***	15 Feb 2022 16:04:44
File Name	C:\DOCS\OUTPUT_301\2022\02.翦 怵曜黑BM-2363-3.F_005001r					***Frequency (MHz)***	376.50
Nucleus	19F	***Number of Transients***	6	***Original Points Count***	131072	***Points Count***	262144
Pulse Sequence	zgflqn	***Solvent***	CHLOROFORM-D			***Sweep Width (Hz)***	75187.97
Temperature (degree C)	27.000						



^{19}F NMR spectrum of **2g** (376.5 MHz, $CDCl_3$)

3 May 2022

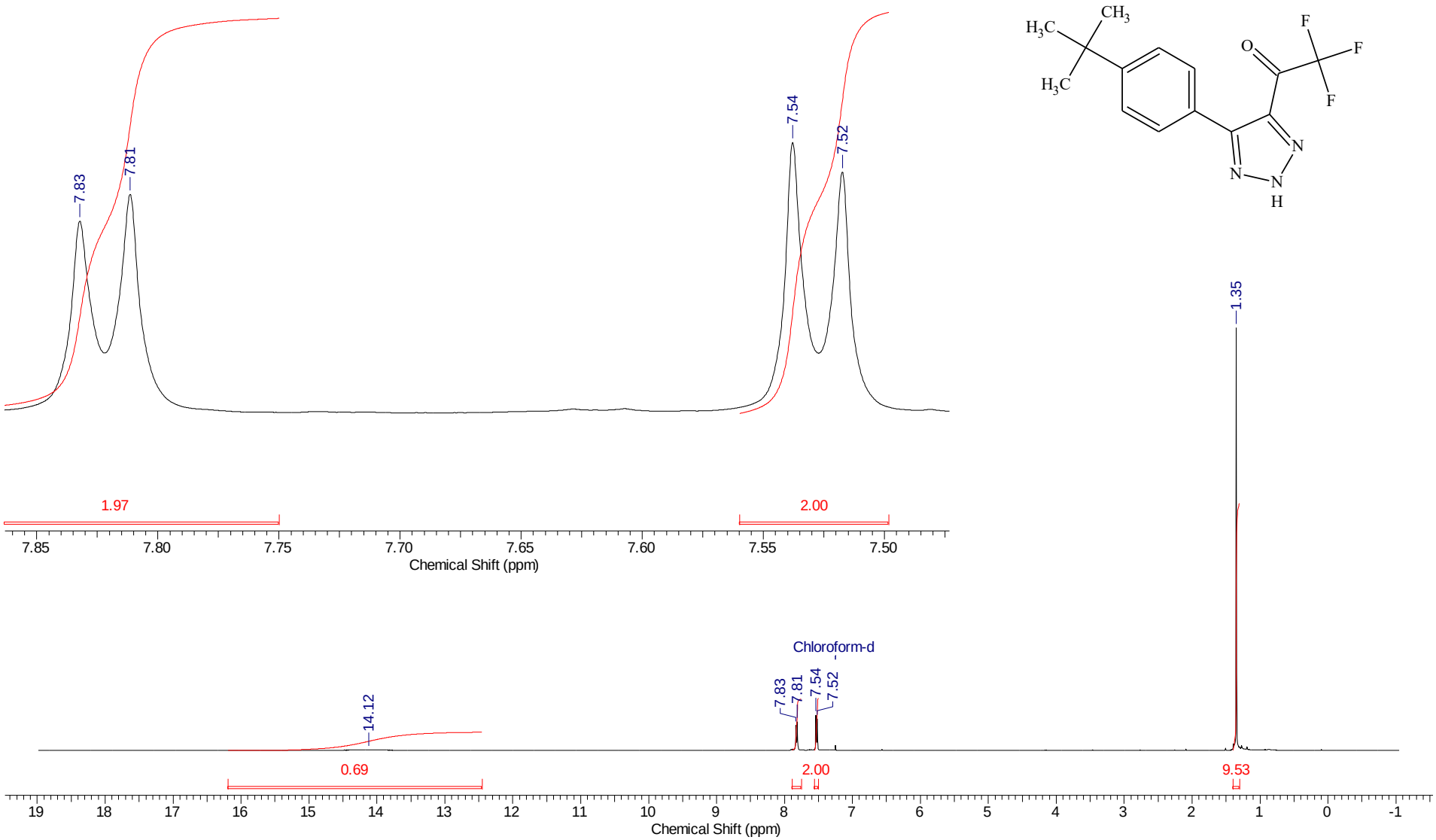
Acquisition Time (sec)	0.6783	***Comment***	Imported from UXNMR.			***Date***	17 Feb 2022 12:37:00
File Name	C:\BM_DATA\DOCS\吁 齂耦皴滂\2022\17_02_2022\BM-2363-3.C_002001r					***Frequency (MHz)***	100.61
Nucleus	13C	***Number of Transients***	81	***Original Points Count***	16384	***Points Count***	131072
Pulse Sequence	zgpg30	***Solvent***	ACETONITRILE-D3			***Sweep Width (Hz)***	24154.59
Temperature (degree C)	27.000						



^{13}C NMR spectrum of **2g** (100.6 MHz, $CDCl_3$)

13 May 2022

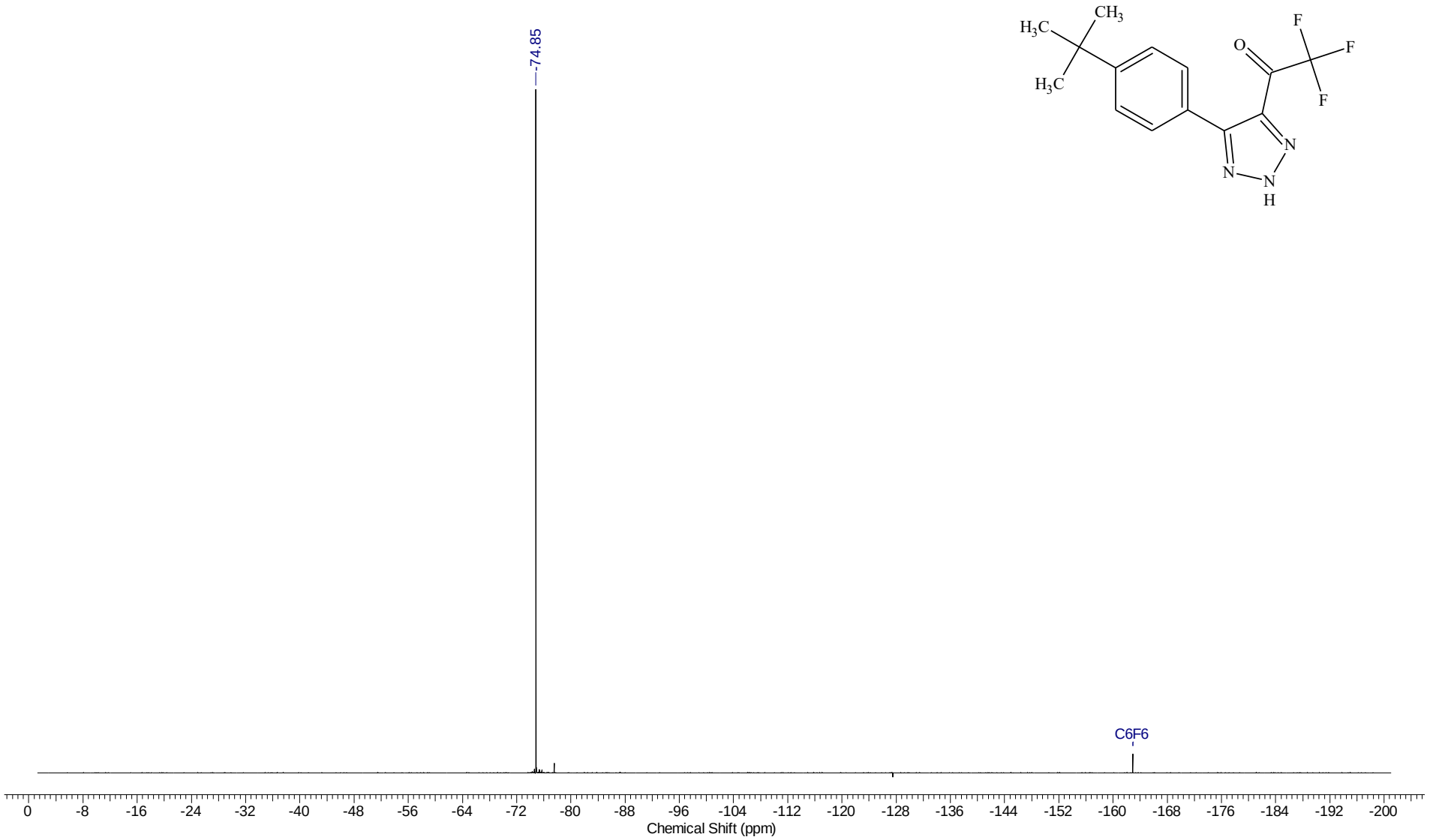
Acquisition Time (sec)	4.0894	***Comment***	Imported from UXNMR.			***Date***	02 Mar 2022 17:45:38
File Name	C:\DOCS\OUTPUT_301\2022\03.爨 痱\SZA-BM-2374.H_001001r					***Frequency (MHz)***	400.13
Nucleus	1H	***Number of Transients***	4	***Original Points Count***	32768	***Points Count***	131072
Pulse Sequence	zg30	***Solvent***	DEUTERIUM OXIDE			***Sweep Width (Hz)***	8012.82
Temperature (degree C)	27.000						



^{1}H NMR spectrum of **2h** (400.1 MHz, $CDCl_3$)

13 May 2022

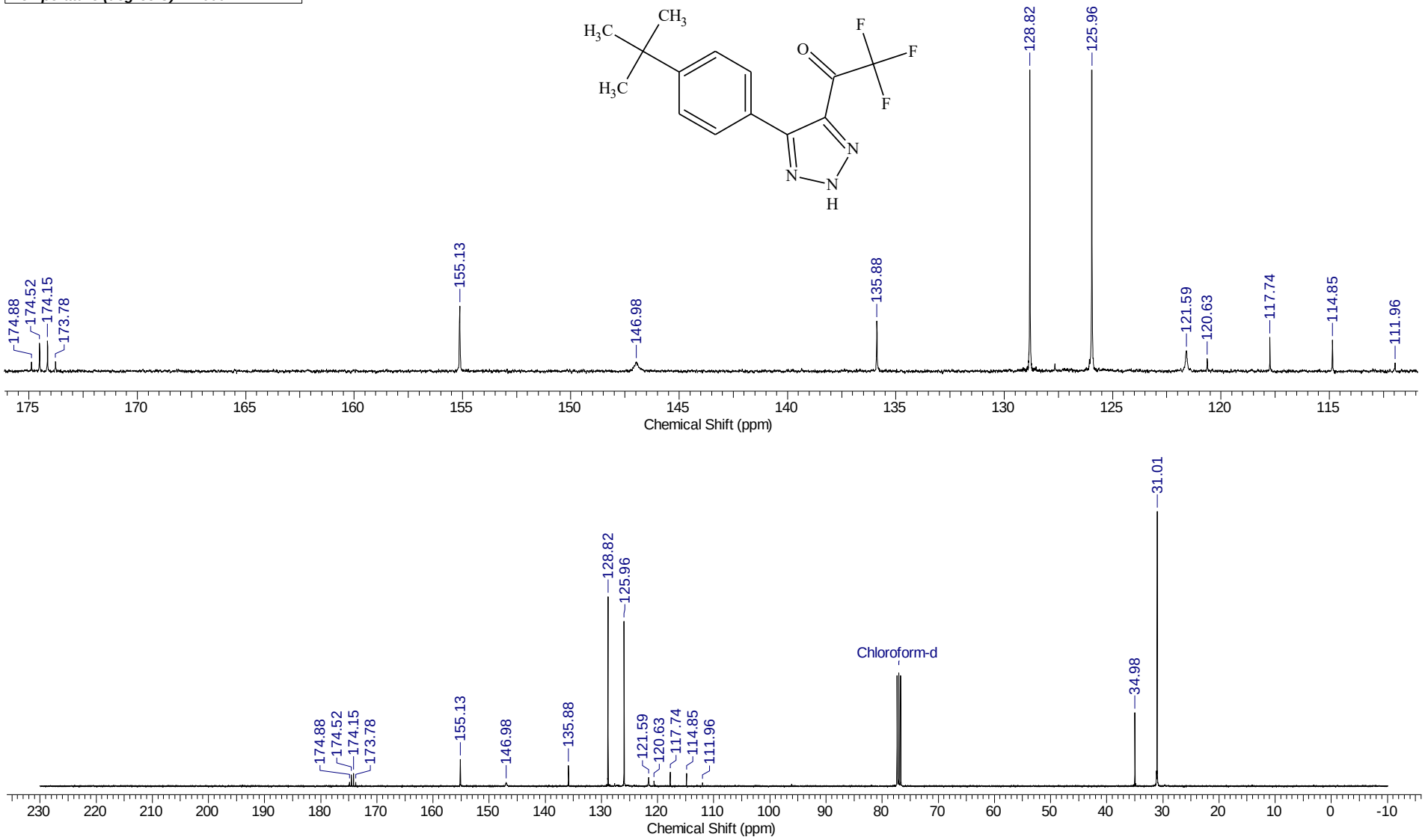
Acquisition Time (sec)	1.7433	***Comment***	Imported from UXNMR.			***Date***	02 Mar 2022 17:50:18
File Name	C:\DOCS\OUTPUT_301\2022\03.爨 痱\SZA-BM-2374.F_005001r					***Frequency (MHz)***	376.50
Nucleus	19F	***Number of Transients***	4	***Original Points Count***	131072	***Points Count***	262144
Pulse Sequence	zgflqn	***Solvent***	CHLOROFORM-D			***Sweep Width (Hz)***	75187.97
Temperature (degree C)	27.000						



^{19}F NMR spectrum of **2h** (376.5 MHz, $CDCl_3$)

13 May 2022

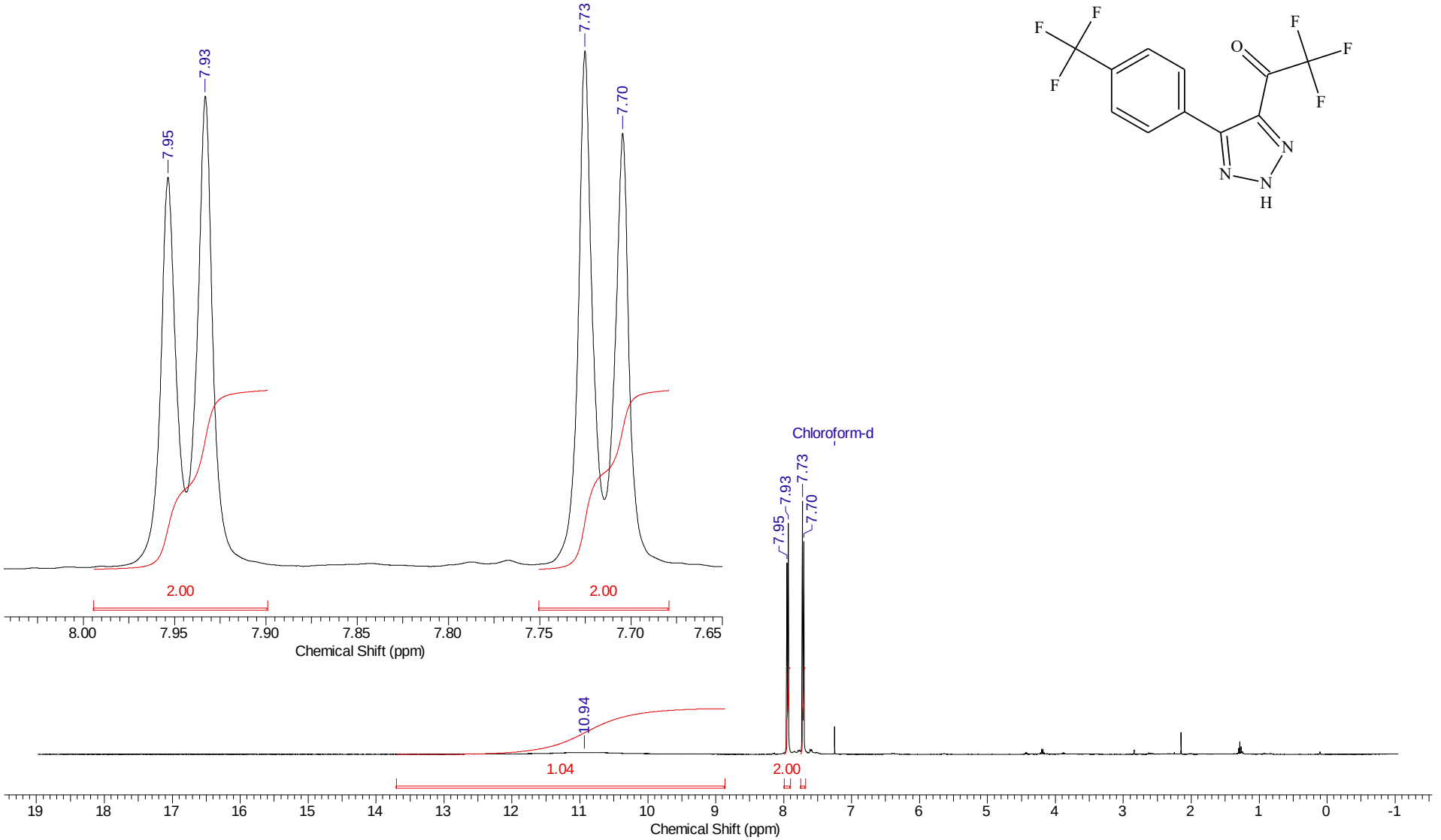
Acquisition Time (sec)	0.6783	***Comment***	Imported from UXNMR.			***Date***	03 Mar 2022 12:01:12
File Name	C:\DOCS\OUTPUT_301\2022\03.爨 痱\SZA-BM-2374.C_002001r					***Frequency (MHz)***	100.61
Nucleus	13C	***Number of Transients***	845	***Original Points Count***	16384	***Points Count***	131072
Pulse Sequence	zgpg30	***Solvent***	ACETONITRILE-D3			***Sweep Width (Hz)***	24154.59
Temperature (degree C)	27.000						



^{13}C NMR spectrum of **2h** (100.6 MHz, $CDCl_3$)

3 May 2022

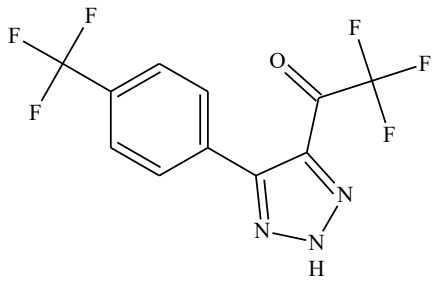
Acquisition Time (sec)	4.0894	***Comment***	Imported from UXNMR.			***Date***	15 Feb 2022 15:22:14
File Name	C:\DOCS\OUTPUT_301\2022\02.翦 怵曜黑BM-2362-3.H_001001r					***Frequency (MHz)***	400.13
Nucleus	1H	***Number of Transients***	4	***Original Points Count***	32768	***Points Count***	131072
Pulse Sequence	zg30	***Solvent***	DEUTERIUM OXIDE			***Sweep Width (Hz)***	8012.82
Temperature (degree C)	27.000						



^{1}H NMR spectrum of **2i** (400.1 MHz, $CDCl_3$)

3 May 2022

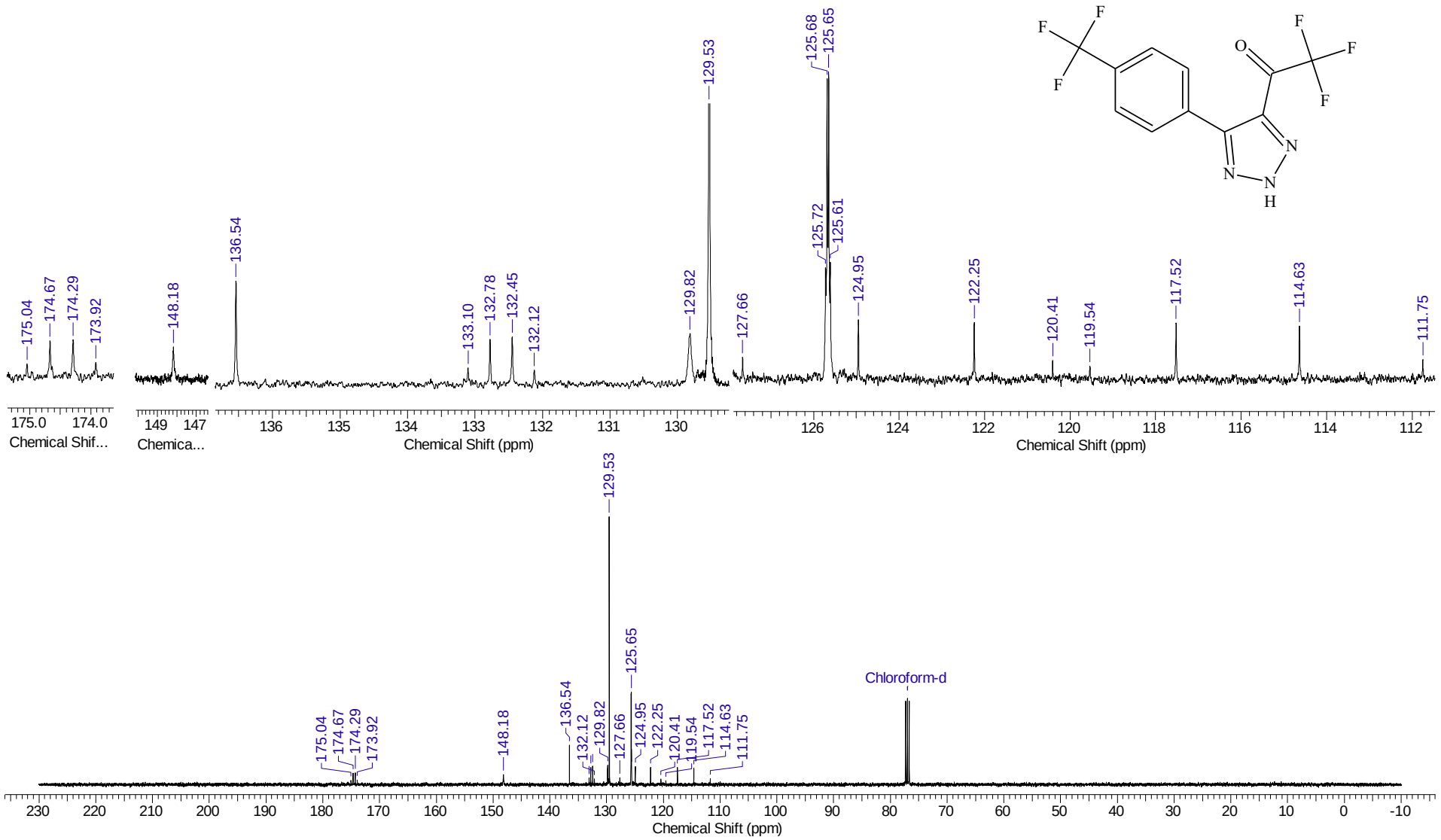
Acquisition Time (sec)	1.7433	***Comment***	Imported from UXNMR.			***Date***	15 Feb 2022 15:41:38
File Name	C:\DOCS\OUTPUT_301\2022\02.翦 怵嚾黑BM-2362-2.F_005001r					***Frequency (MHz)***	376.50
Nucleus	19F	***Number of Transients***	16	***Original Points Count***	131072	***Points Count***	262144
Pulse Sequence	zgflqn	***Solvent***	CHLOROFORM-D			***Sweep Width (Hz)***	75187.97
Temperature (degree C)	27.000						



^{19}F NMR spectrum of **2i** (376.5 MHz, $CDCl_3$)

3 May 2022

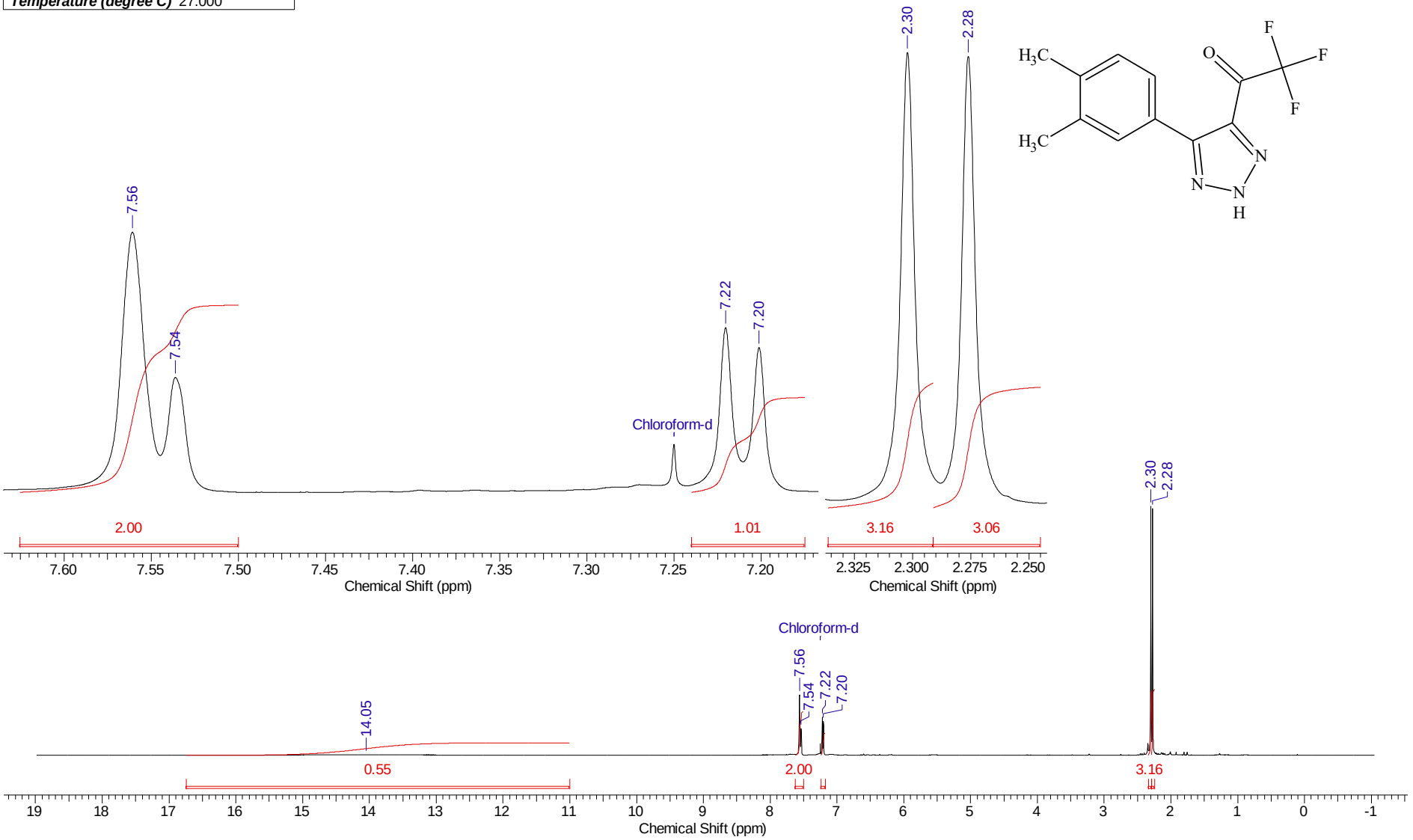
Acquisition Time (sec)	0.6783	***Comment***	Imported from UXNMR.			***Date***	15 Feb 2022 15:26:58
File Name	C:\DOCS\OUTPUT_301\2022\02.翦 怵曜黑BM-2362-3.C_002001r					***Frequency (MHz)***	100.61
Nucleus	13C	***Number of Transients***	105	***Original Points Count***	16384	***Points Count***	131072
Pulse Sequence	zgpg30	***Solvent***	ACETONITRILE-D3			***Sweep Width (Hz)***	24154.59
Temperature (degree C)	27.000						



^{13}C NMR spectrum of **2i** (100.6 MHz, $CDCl_3$)

3 May 2022

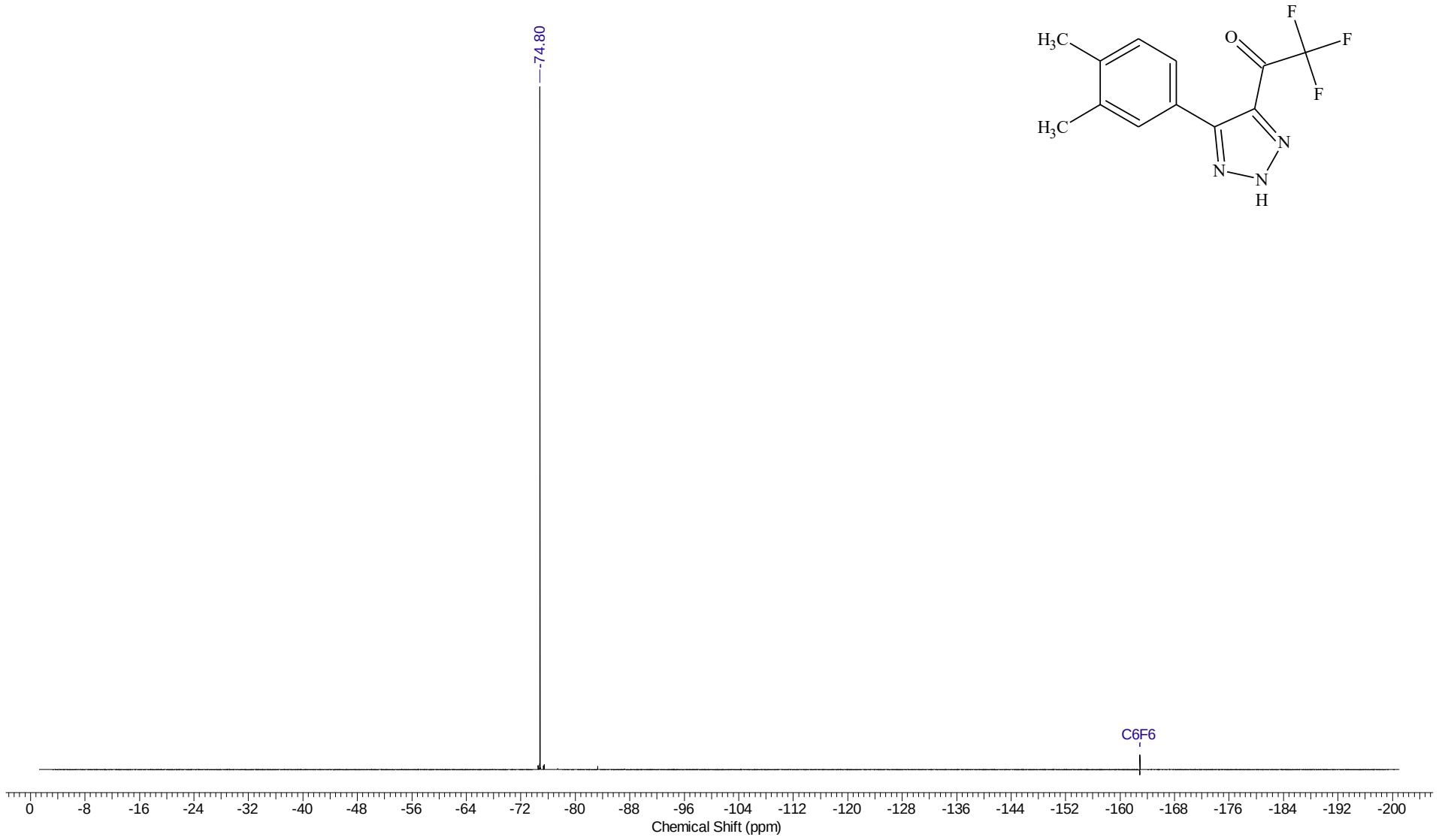
Acquisition Time (sec)	4.0894	***Comment***	Imported from UXNMR.			***Date***	16 Feb 2022 17:12:58
File Name	C:\DOCS\OUTPUT_301\2022\02.翦 怵嚯黑BM-2364-3.H_001001r					***Frequency (MHz)***	400.13
Nucleus	1H	***Number of Transients***	4	***Original Points Count***	32768	***Points Count***	131072
Pulse Sequence	zg30	***Solvent***	DEUTERIUM OXIDE			***Sweep Width (Hz)***	8012.82
Temperature (degree C)	27.000						



^{1}H NMR spectrum of **2j** (400.1 MHz, $CDCl_3$)

3 May 2022

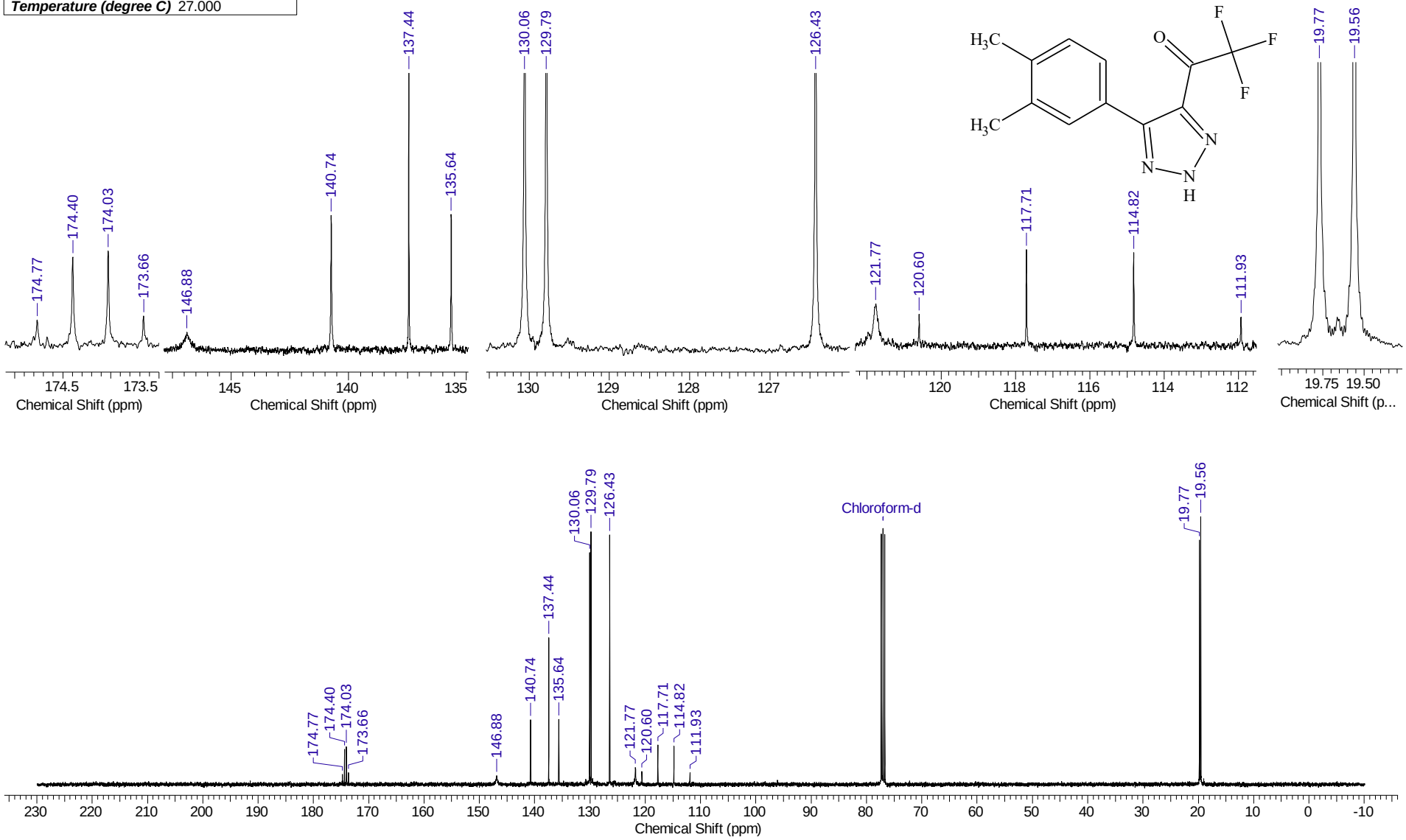
Acquisition Time (sec)	1.7433	***Comment***	Imported from UXNMR.			***Date***	16 Feb 2022 17:48:22
File Name	C:\DOCS\OUTPUT_301\2022\02.翦 怵嚏黑BM-2364-3.F_005001r					***Frequency (MHz)***	376.50
Nucleus	19F	***Number of Transients***	16	***Original Points Count***	131072	***Points Count***	262144
Pulse Sequence	zgflqn	***Solvent***	CHLOROFORM-D			***Sweep Width (Hz)***	75187.97
Temperature (degree C)	27.000						



^{19}F NMR spectrum of **2j** (376.5 MHz, $CDCl_3$)

3 May 2022

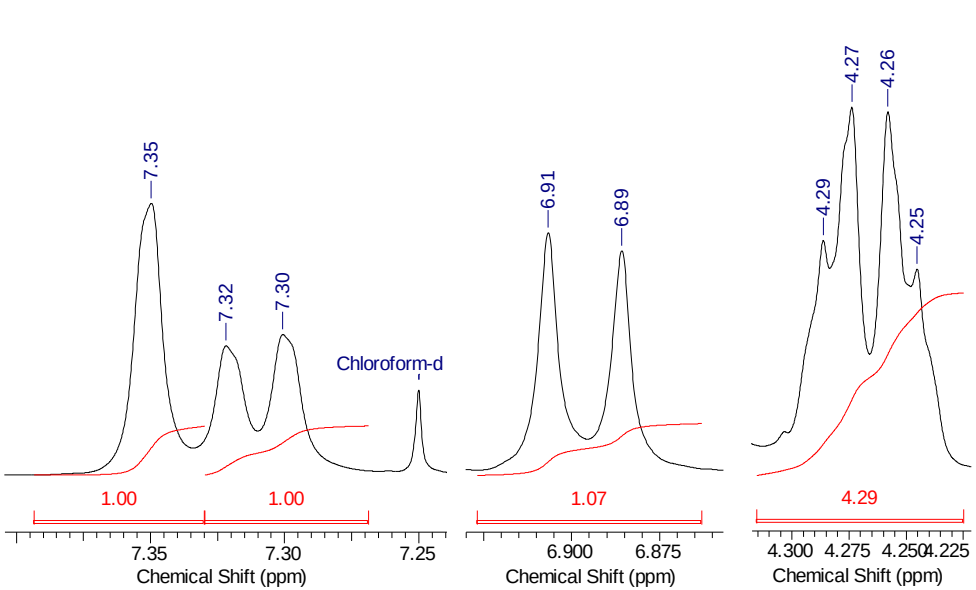
Acquisition Time (sec)	0.6783	***Comment***	Imported from UXNMR.			***Date***	16 Feb 2022 17:33:44
File Name	C:\DOCS\OUTPUT_301\2022\02.翦 怵嚾黑BM-2364-3.C_002001r					***Frequency (MHz)***	100.61
Nucleus	13C	***Number of Transients***	489	***Original Points Count***	16384	***Points Count***	131072
Pulse Sequence	zgpg30	***Solvent***	ACETONITRILE-D3			***Sweep Width (Hz)***	24154.59
Temperature (degree C)	27.000						

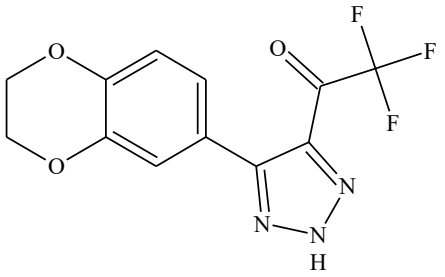


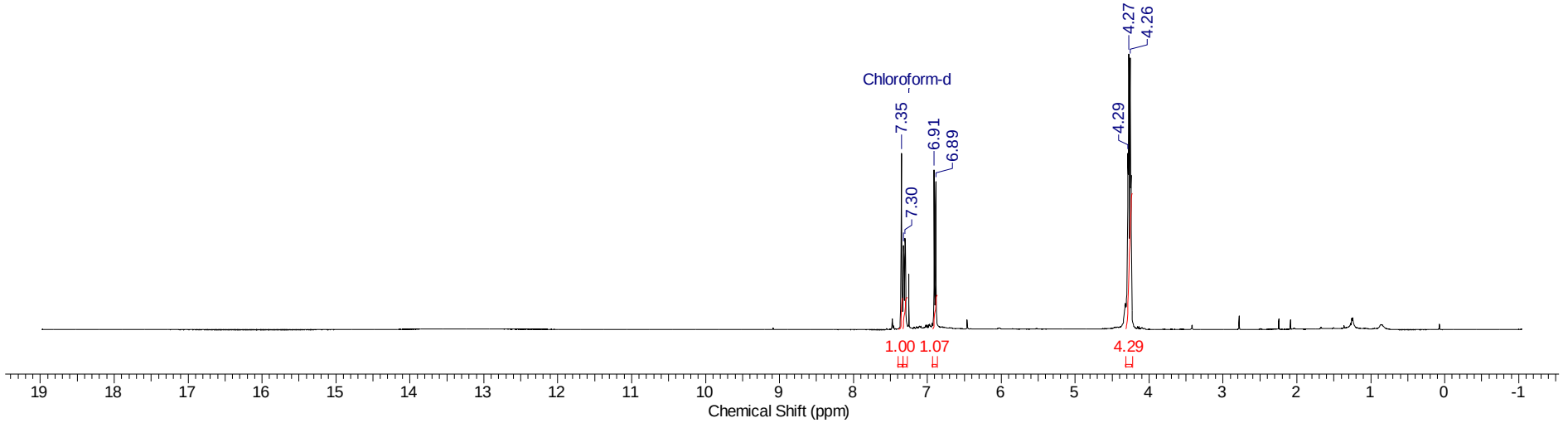
^{13}C NMR spectrum of **2j** (100.6 MHz, $CDCl_3$)

13 May 2022

Acquisition Time (sec)	4.0894	***Comment***	Imported from UXNMR.			***Date***	02 Mar 2022 17:24:00
File Name	C:\DOCS\OUTPUT_301\2022\03.爨 痱\SZA-BM-2359p.H_001001r					***Frequency (MHz)***	400.13
Nucleus	1H	***Number of Transients***	4	***Original Points Count***	32768	***Points Count***	131072
Pulse Sequence	zg30	***Solvent***	CHLOROFORM-D			***Sweep Width (Hz)***	8012.82
Temperature (degree C)	27.000						



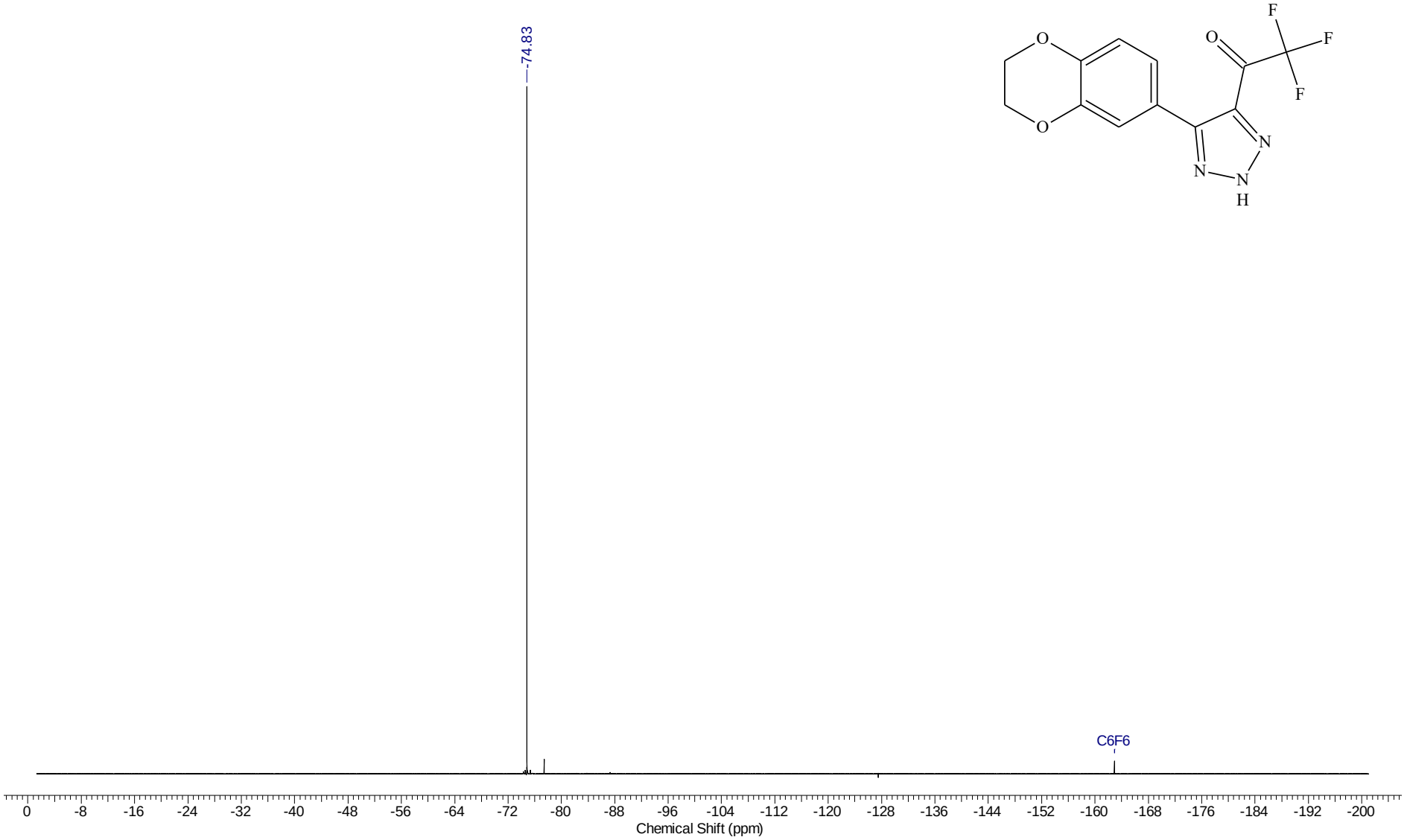




^{1}H NMR spectrum of **2k** (400.1 MHz, $CDCl_3$)

13 May 2022

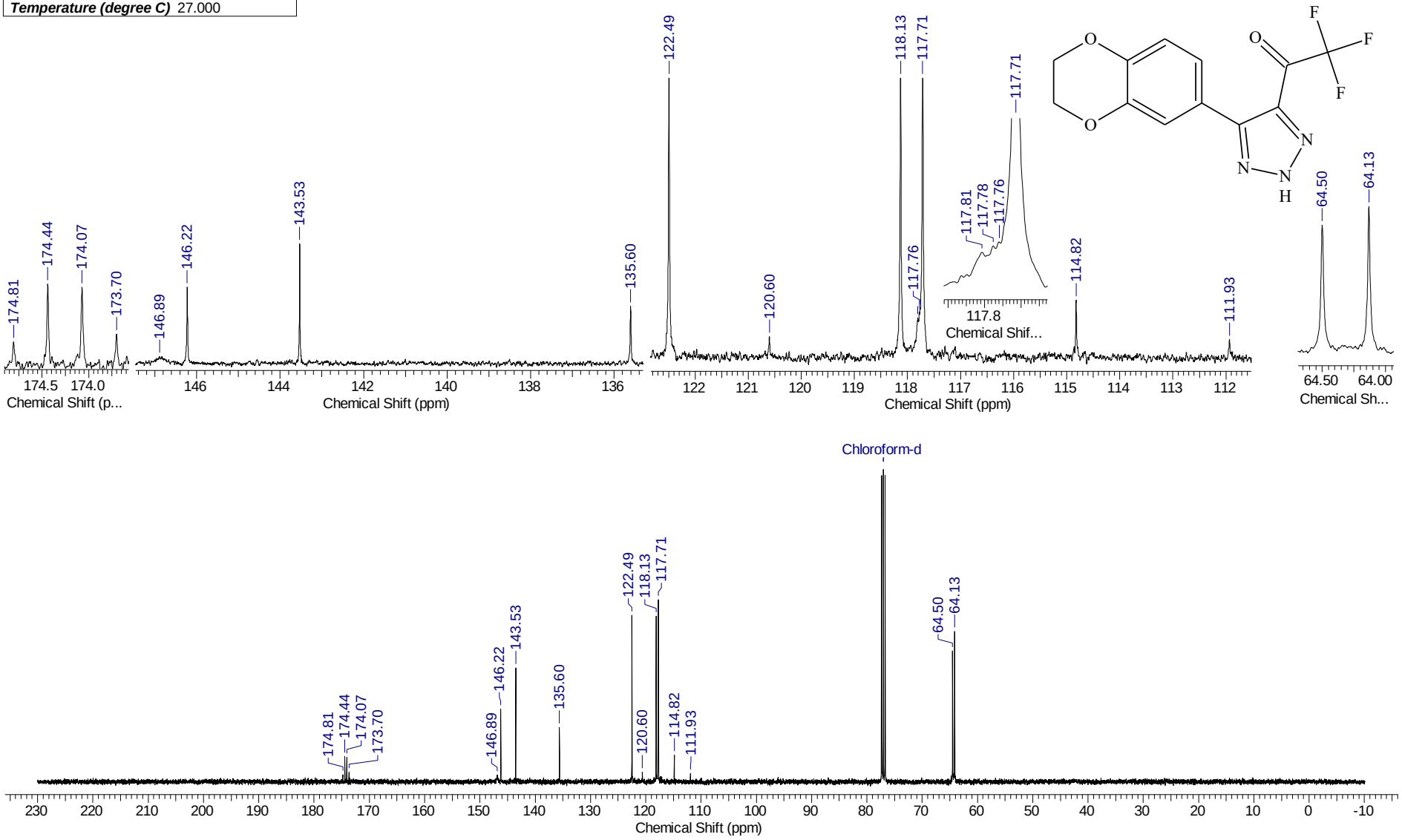
Acquisition Time (sec)	1.7433	***Comment***	Imported from UXNMR.			***Date***	01 Mar 2022 15:32:36
File Name	H:\吁 衆01.03.2022\SZA-BM-2359.F_005001r			***Frequency (MHz)***	376.50	***Nucleus***	19F
Original Points Count	131072	***Points Count***	262144	***Pulse Sequence***	zgflqn	***Solvent***	CHLOROFORM-D
Sweep Width (Hz)	75187.97	***Temperature (degree C)***	27.000				



^{19}F NMR spectrum of **2k** (376.5 MHz, $CDCl_3$)

13 May 2022

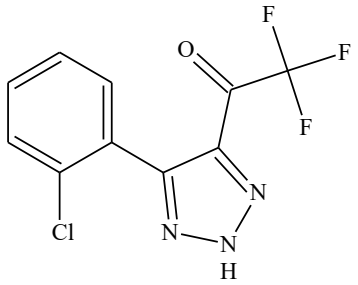
Acquisition Time (sec)	0.6783	***Comment***	Imported from UXNMR.			***Date***	02 Mar 2022 17:42:18
File Name	C:\DOCS\OUTPUT_301\2022\03.爨 痱\SZA-BM-2359p.C_002001r					***Frequency (MHz)***	100.61
Nucleus	13C	***Number of Transients***	417	***Original Points Count***	16384	***Points Count***	131072
Pulse Sequence	zgpg30	***Solvent***	ACETONITRILE-D3			***Sweep Width (Hz)***	24154.59
Temperature (degree C)	27.000						

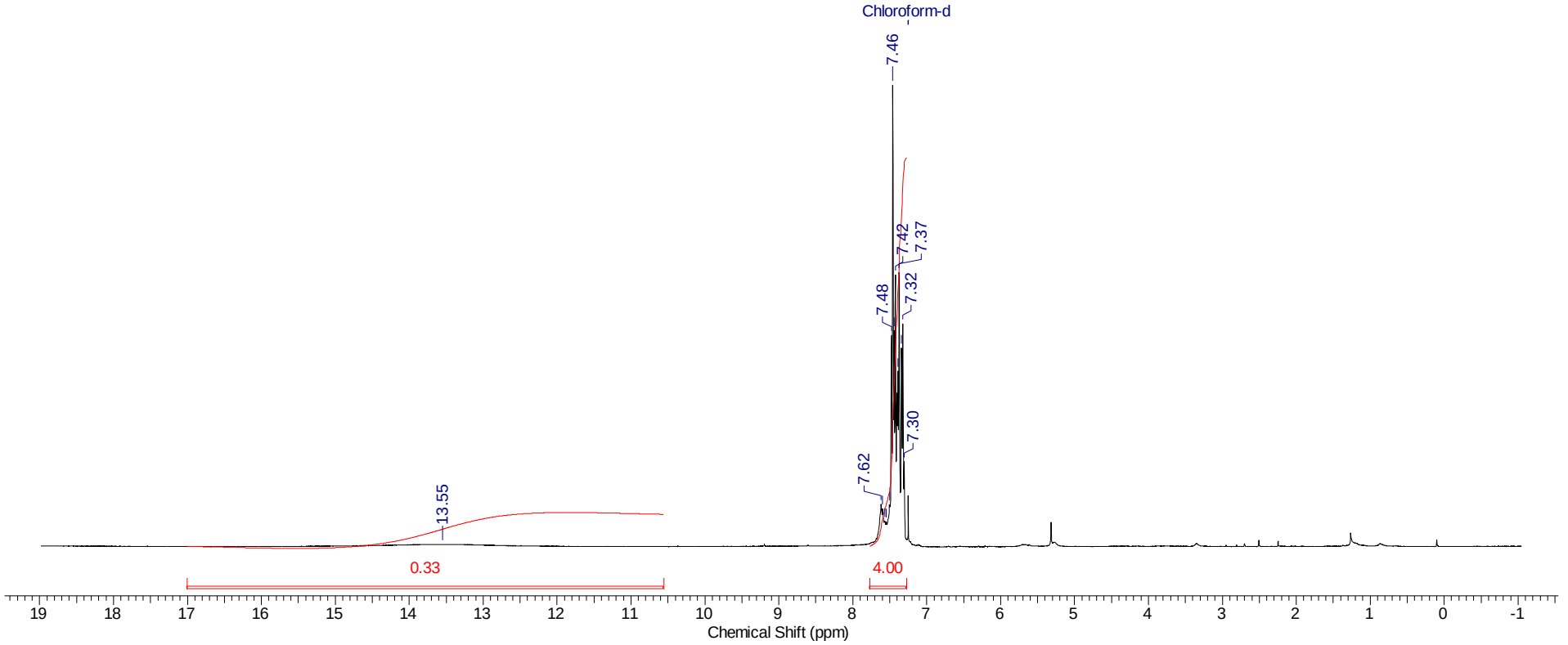


^{13}C NMR spectrum of **2k** (100.6 MHz, $CDCl_3$)

13 May 2022

Acquisition Time (sec)	4.0894	***Comment***	Imported from UXNMR.			***Date***	14 Feb 2022 15:40:12
File Name	C:\DOCS\OUTPUT_301\2022\02.翦 怵嚾黑BM-2358-3.H_001001r					***Frequency (MHz)***	400.13
Nucleus	1H	***Number of Transients***	4	***Original Points Count***	32768	***Points Count***	131072
Pulse Sequence	zg30	***Solvent***	DMSO-D6	***Sweep Width (Hz)***	8012.82	***Temperature (degree C)***	27.000

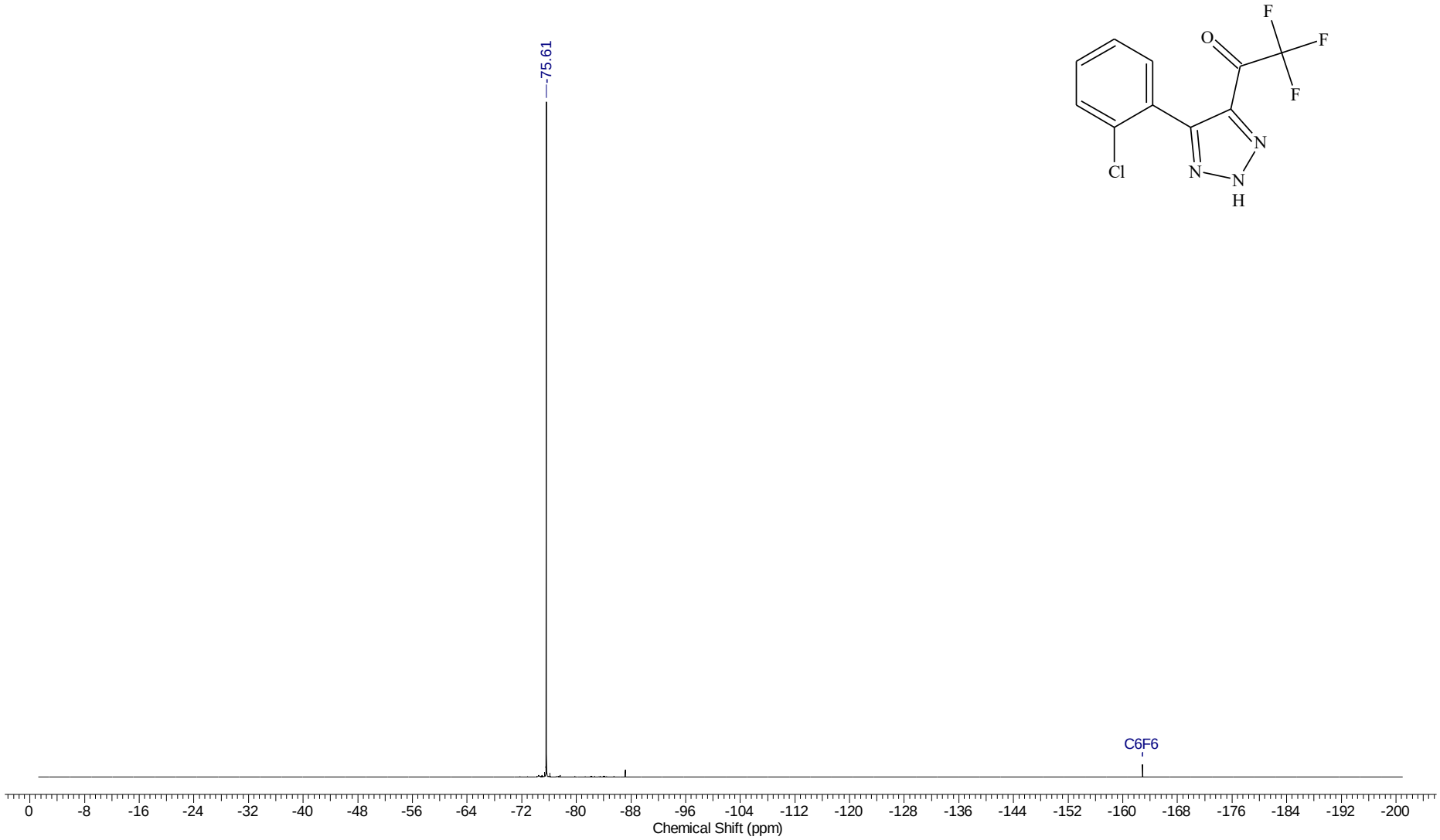




^{1}H NMR spectrum of **2l** (400.1 MHz, $CDCl_3$)

13 May 2022

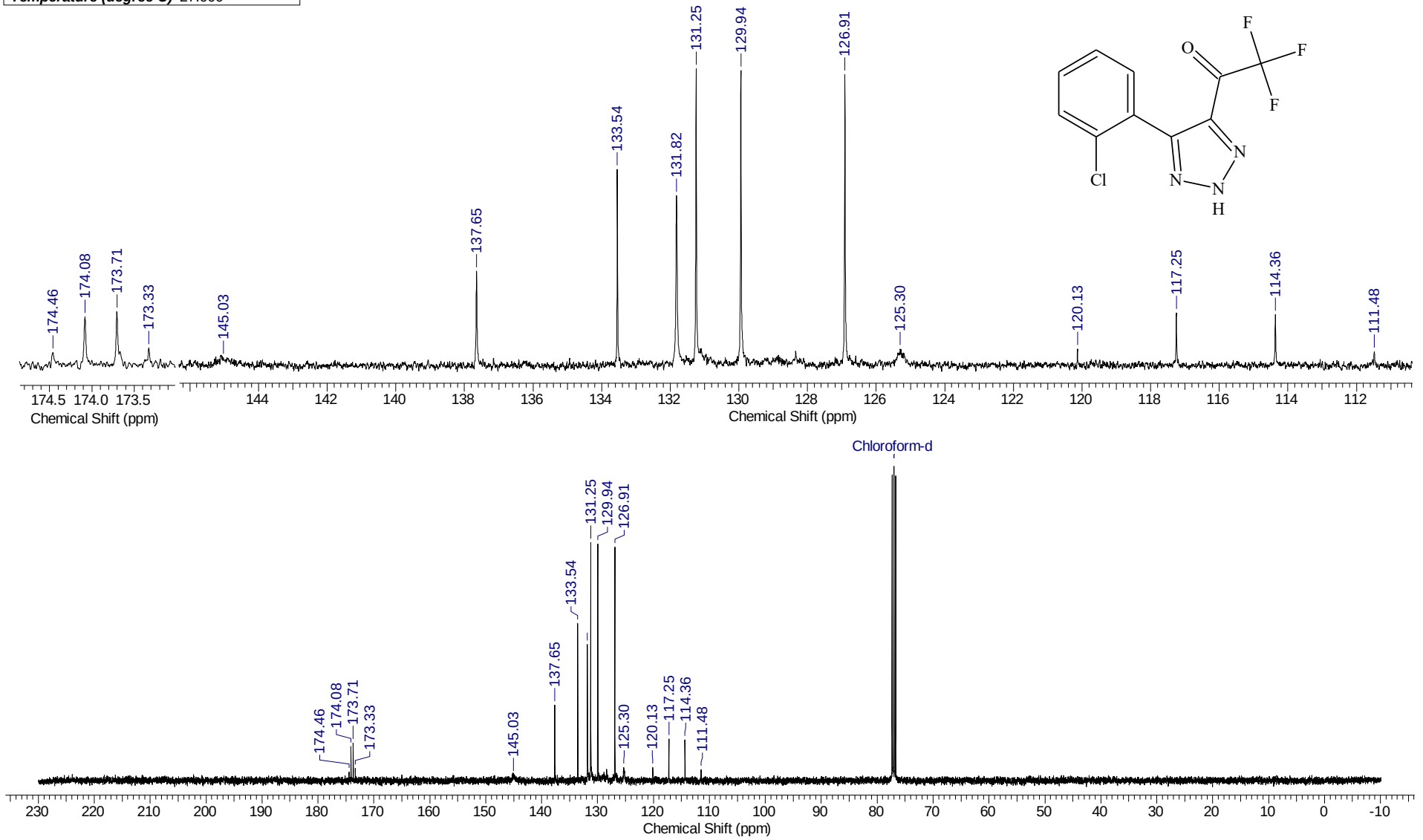
Acquisition Time (sec)	1.7433	***Comment***	Imported from UXNMR.			***Date***	12 Feb 2022 13:39:46
File Name	C:\DOCS\BM\吖 峪盐 雅 娜 \2022\bm220212\BM-2358-3_005001r					***Frequency (MHz)***	376.50
Nucleus	19F	***Number of Transients***	16	***Original Points Count***	131072	***Points Count***	262144
Pulse Sequence	zgflqn	***Solvent***	CHLOROFORM-D			***Sweep Width (Hz)***	75187.97
Temperature (degree C)	27.000						



^{19}F NMR spectrum of **2l** (376.5 MHz, $CDCl_3$)

13 May 2022

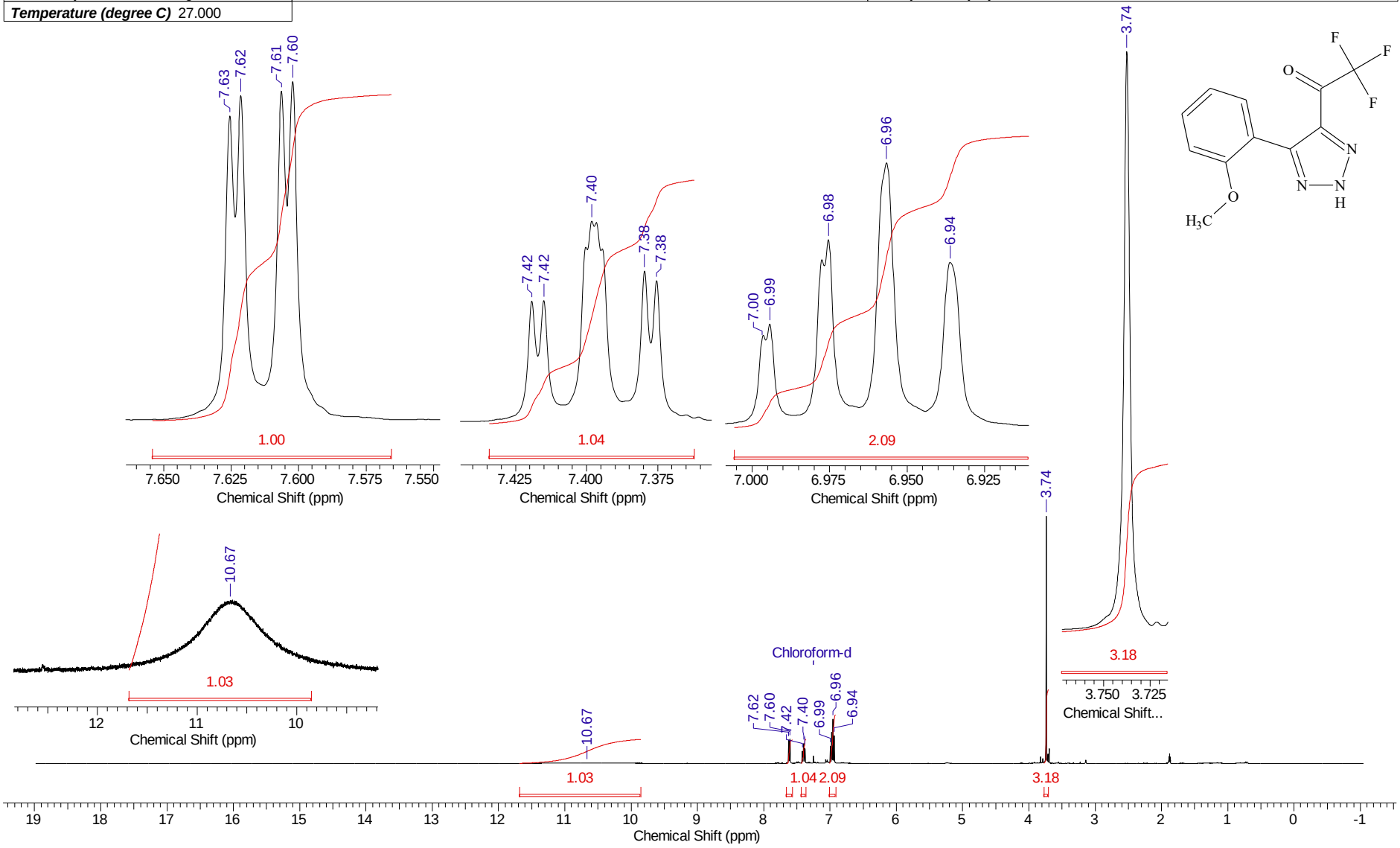
Acquisition Time (sec)	0.6783	***Comment***	Imported from UXNMR.			***Date***	14 Feb 2022 15:37:38
File Name	C:\DOCS\OUTPUT_301\2022\02.翦 怵嚾黑BM-2358-3.C_002001r					***Frequency (MHz)***	100.61
Nucleus	13C	***Number of Transients***	129	***Original Points Count***	16384	***Points Count***	131072
Pulse Sequence	zgpg30	***Solvent***	ACETONITRILE-D3			***Sweep Width (Hz)***	24154.59
Temperature (degree C)	27.000						



^{13}C NMR spectrum of **2l** (100.6 MHz, $CDCl_3$)

2 Aug 2022

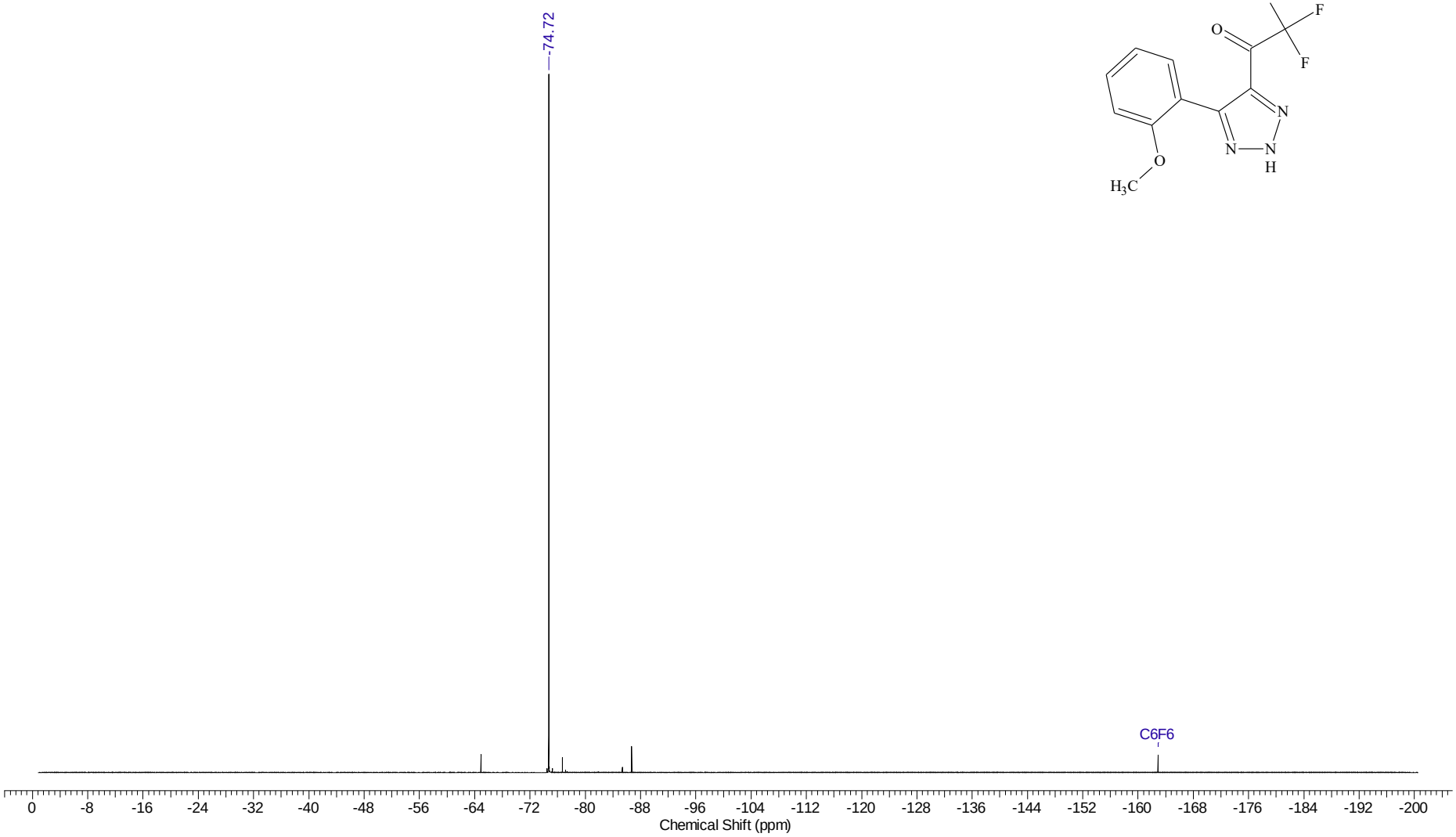
Acquisition Time (sec)	4.0894	***Comment***	Imported from UXNMR.			***Date***	07 Jun 2022 15:29:24
File Name	C:\DOCS\OUTPUT_301\2022\06.棹 睃\BM-2509-NEW.H_001001r					***Frequency (MHz)***	400.13
Nucleus	1H	***Number of Transients***	8	***Original Points Count***	32768	***Points Count***	131072
Pulse Sequence	zg30	***Solvent***	CHLOROFORM-D			***Sweep Width (Hz)***	8012.82
Temperature (degree C)	27.000						



^{1}H NMR spectrum of **2m** (400.1 MHz, $CDCl_3$)

2 Aug 2022

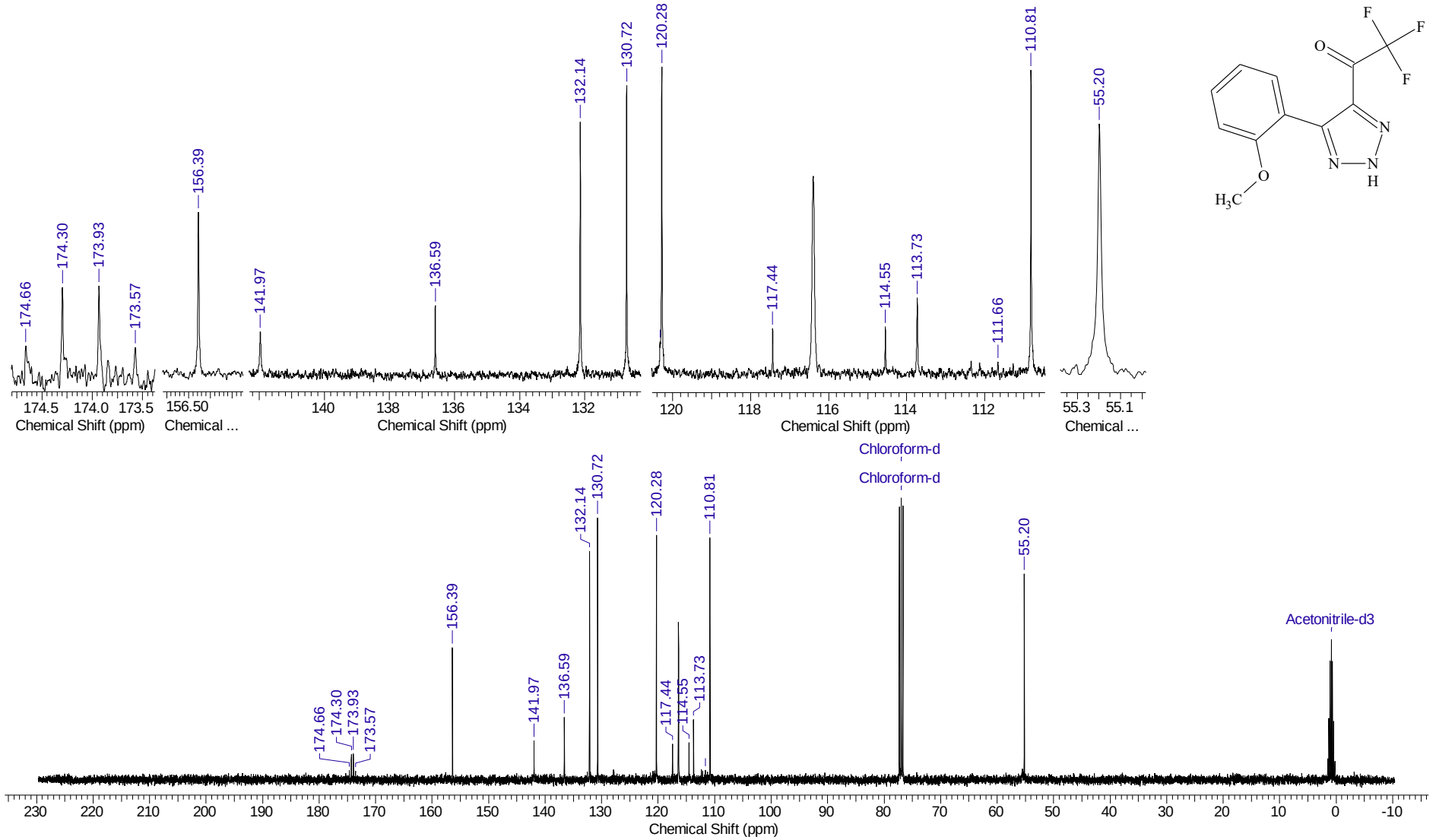
Acquisition Time (sec)	1.7433	***Comment***	Imported from UXNMR.			***Date***	07 Jun 2022 15:26:58
File Name	C:\DOCS\OUTPUT_301\2022\06.棹 睃\BM-2509-NEW.F_005001r					***Frequency (MHz)***	376.50
Nucleus	19F	***Number of Transients***	16	***Original Points Count***	131072	***Points Count***	262144
Pulse Sequence	zgflqn	***Solvent***	CHLOROFORM-D			***Sweep Width (Hz)***	75187.97
Temperature (degree C)	27.000						



^{19}F NMR spectrum of **2m** (376.5 MHz, $CDCl_3$)

2 Aug 2022

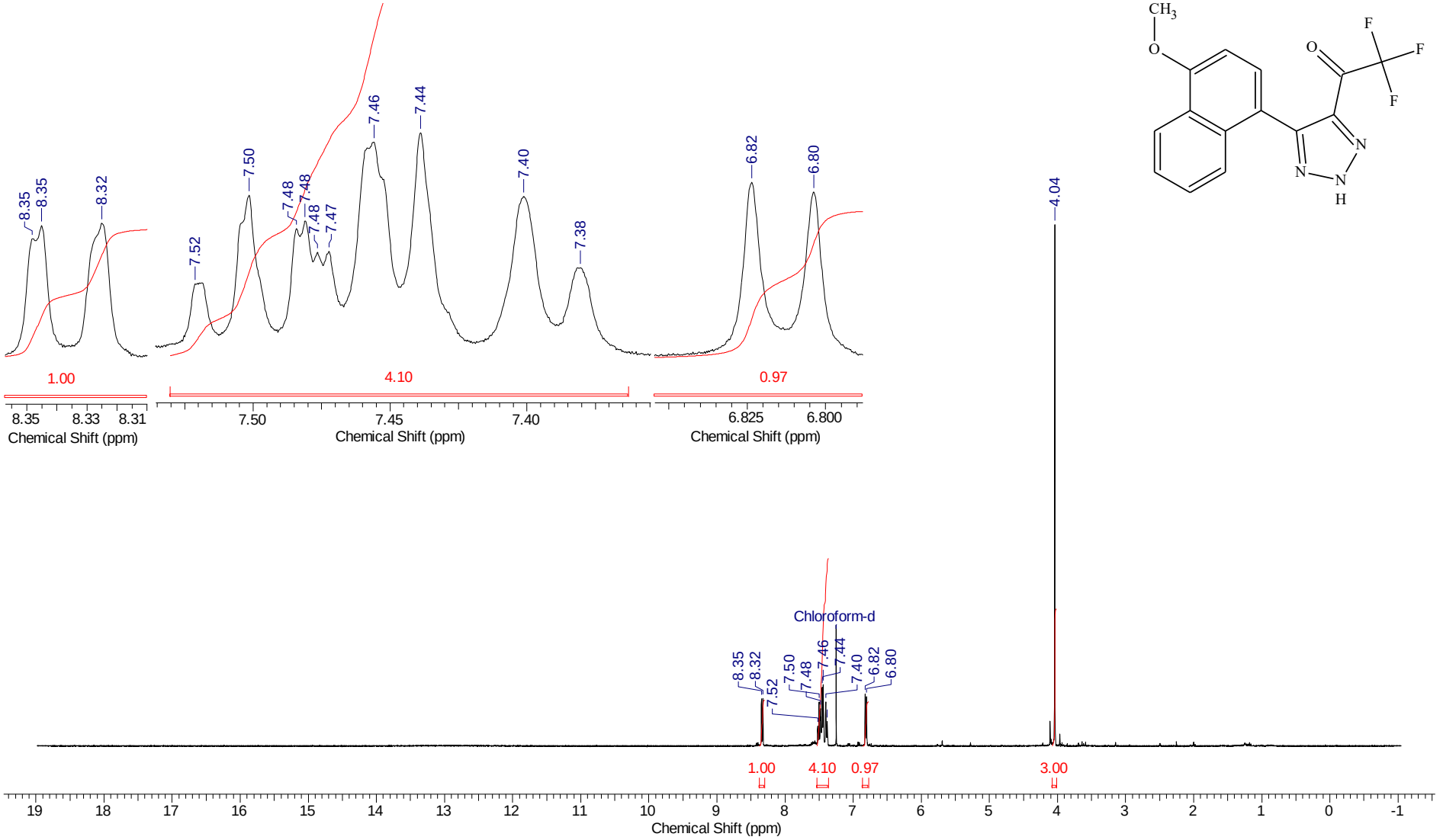
Acquisition Time (sec)	0.6783	***Comment***	Imported from UXNMR.			***Date***	07 Jun 2022 21:30:54
File Name	C:\DOCS\OUTPUT_301\2022\06.棹 睽\BM-2509-NEW\BM-2509-NEW_002001r					***Frequency (MHz)***	100.61
Nucleus	13C	***Number of Transients***	256	***Original Points Count***	16384	***Points Count***	131072
Pulse Sequence	zgpg30	***Solvent***	CHLOROFORM-D			***Sweep Width (Hz)***	24154.59
Temperature (degree C)	27.000						



^{13}C NMR spectrum of **2m** (100.6 MHz, $CDCl_3$)

13 May 2022

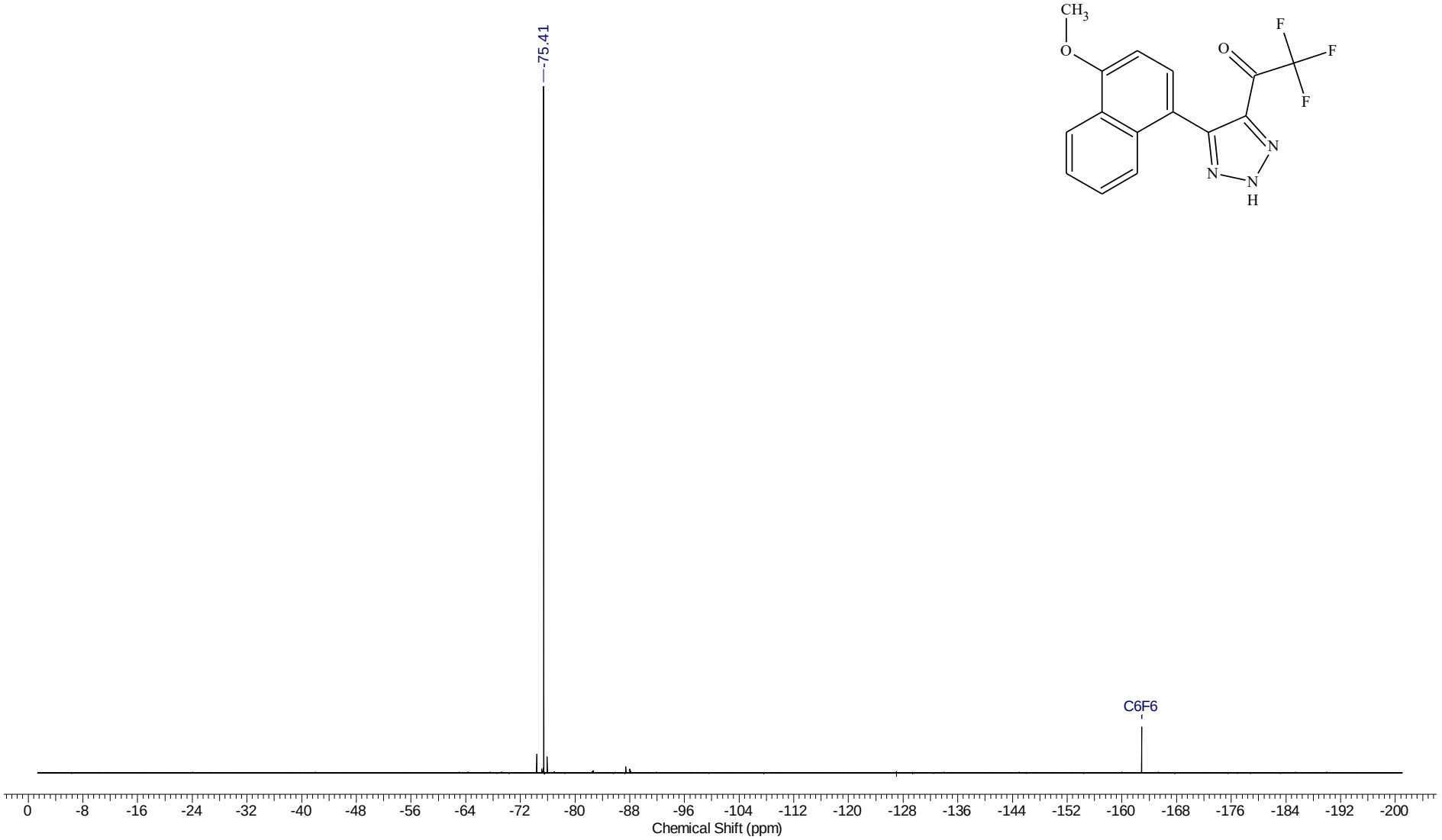
Acquisition Time (sec)	4.0894	***Comment***	Imported from UXNMR.			***Date***	03 Mar 2022 13:40:30
File Name	C:\DOCS\OUTPUT_301\2022\03.爨 痱\SZA-BM-2361-h_001001r					***Frequency (MHz)***	400.13
Nucleus	1H	***Number of Transients***	4	***Original Points Count***	32768	***Points Count***	131072
Pulse Sequence	zg30	***Solvent***	CHLOROFORM-D			***Sweep Width (Hz)***	8012.82
Temperature (degree C)	27.000						



^{1}H NMR spectrum of **2n** (400.1 MHz, $CDCl_3$)

13 May 2022

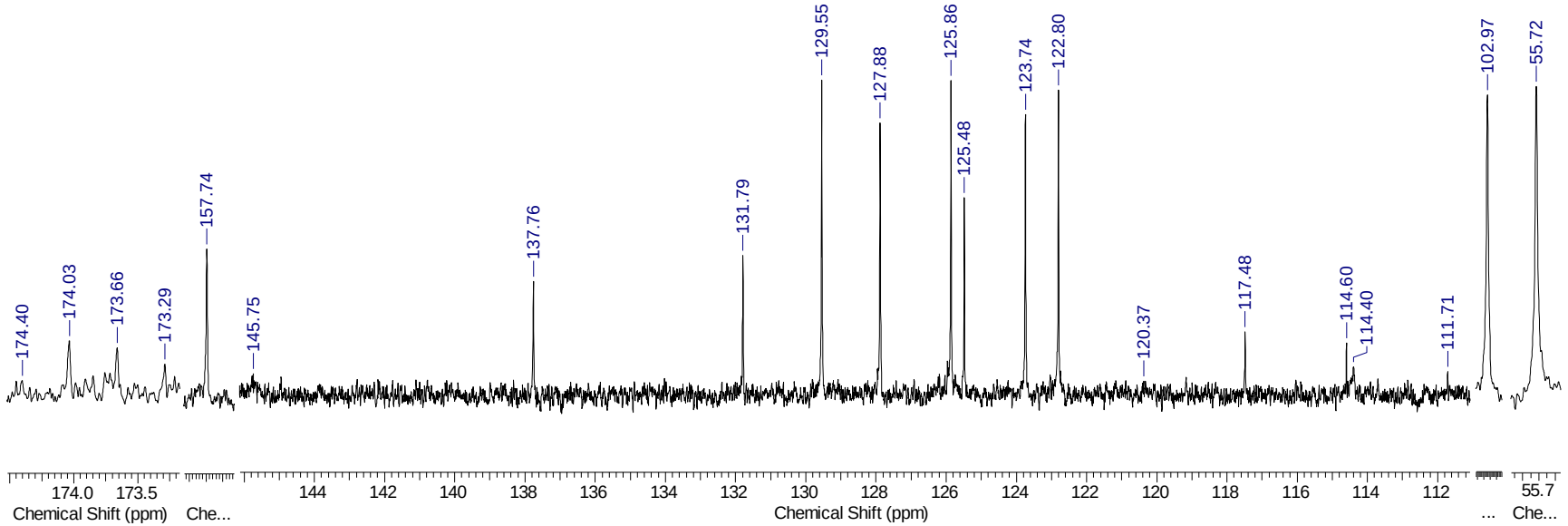
Acquisition Time (sec)	1.7433	***Comment***	Imported from UXNMR.			***Date***	04 Mar 2022 15:30:46
File Name	C:\DOCS\OUTPUT_301\2022\03.爨 痱\SZA-BM-2361.F_005001r					***Frequency (MHz)***	376.50
Nucleus	19F	***Number of Transients***	4	***Original Points Count***	131072	***Points Count***	262144
Pulse Sequence	zgflqn	***Solvent***	CHLOROFORM-D			***Sweep Width (Hz)***	75187.97
Temperature (degree C)	27.000						

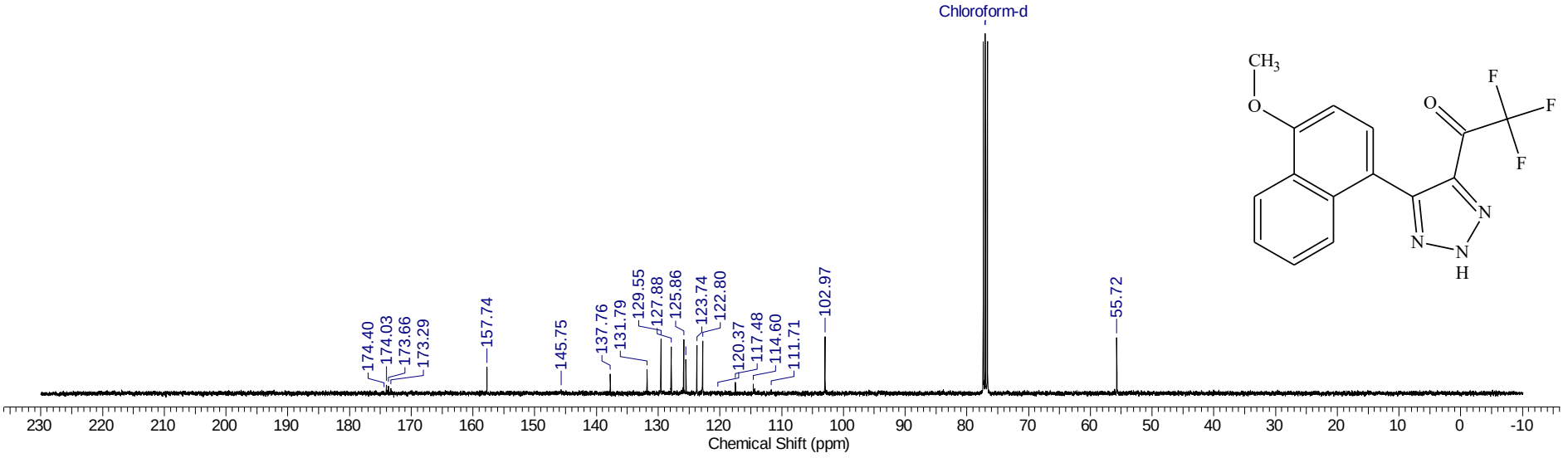


^{19}F NMR spectrum of **2n** (376.5 MHz, $CDCl_3$)

13 May 2022

Acquisition Time (sec)	0.6783	***Comment***	Imported from UXNMR.			***Date***	10 Mar 2022 14:52:34
File Name	C:\DOCS\OUTPUT_301\2022\03.爨 痱\SZA-BM-2361.C_002001r					***Frequency (MHz)***	100.61
Nucleus	13C	***Number of Transients***	894	***Original Points Count***	16384	***Points Count***	131072
Pulse Sequence	zgpg30	***Solvent***	DMSO-D6	***Sweep Width (Hz)***	24154.59	***Temperature (degree C)***	27.000

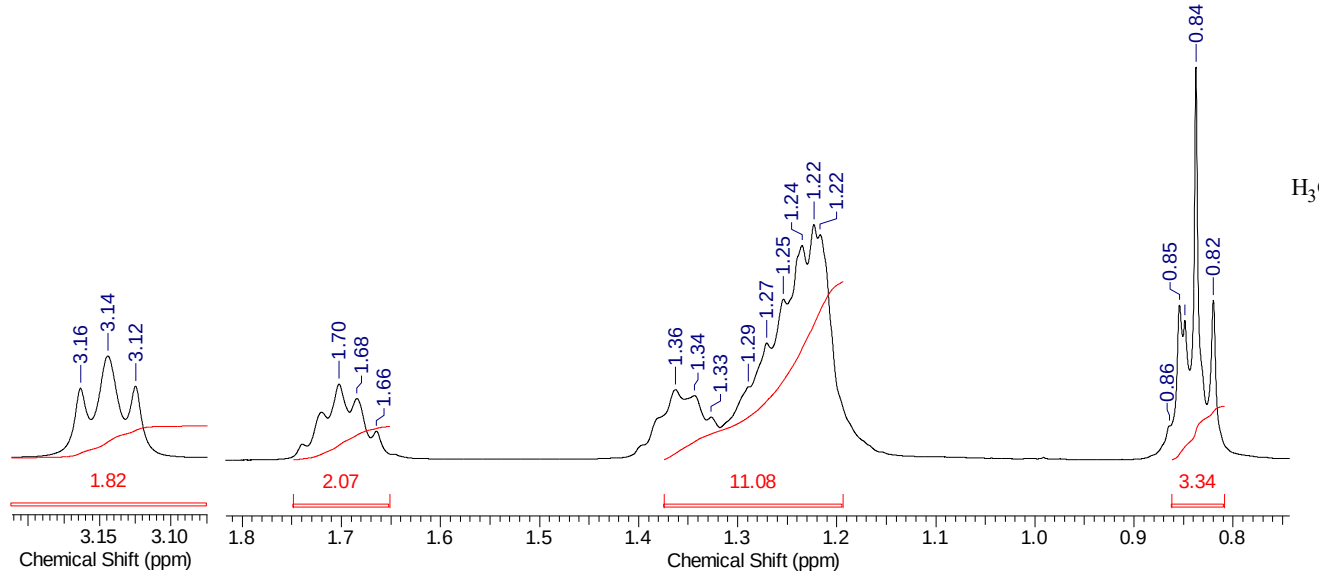


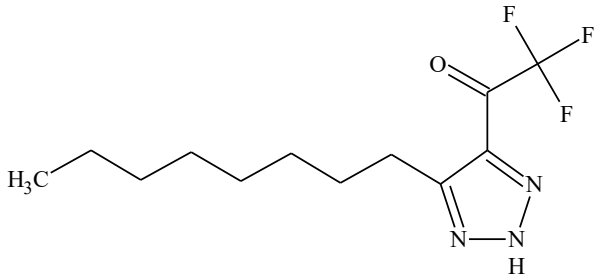


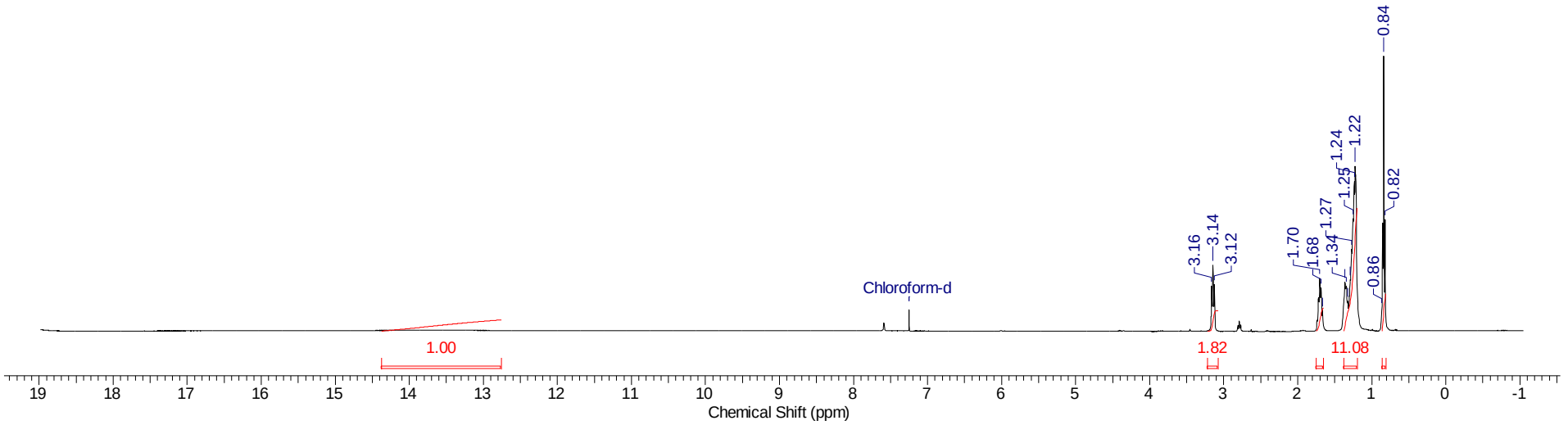
^{13}C NMR spectrum of **2n** (100.6 MHz, $CDCl_3$)

13 May 2022

Acquisition Time (sec)	4.0894	***Comment***	Imported from UXNMR.			***Date***	03 Dec 2021 15:15:22
File Name	C:\DOCS\OUTPUT_301\2021\12.溴赅狃黑BM-2356-3.H_001001r					***Frequency (MHz)***	400.13
Nucleus	1H	***Number of Transients***	4	***Original Points Count***	32768	***Points Count***	131072
Pulse Sequence	zg30	***Solvent***	CHLOROFORM-D			***Sweep Width (Hz)***	8012.82
Temperature (degree C)	27.000						



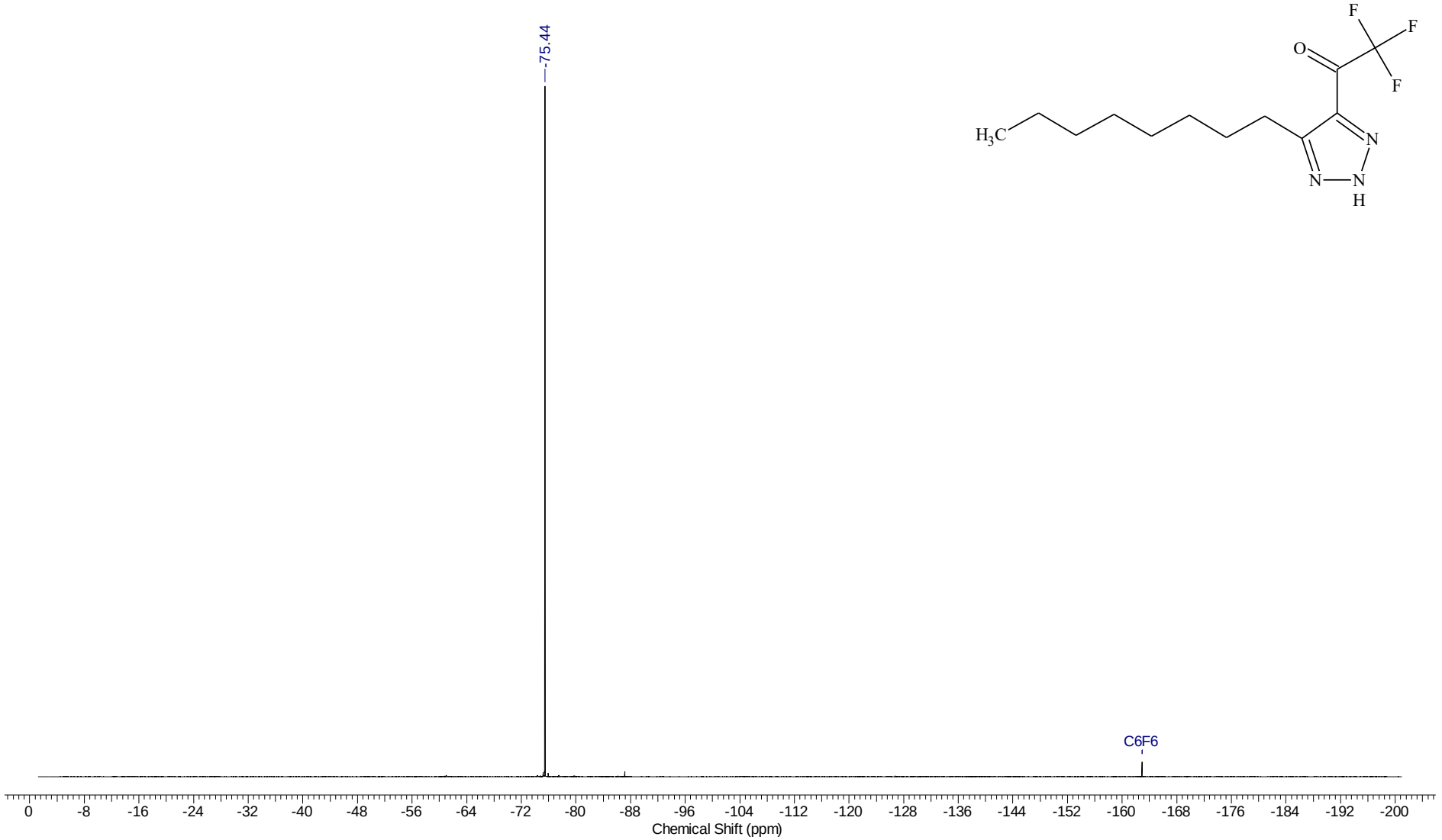




^{1}H NMR spectrum of **2o** (400.1 MHz, $CDCl_3$)

13 May 2022

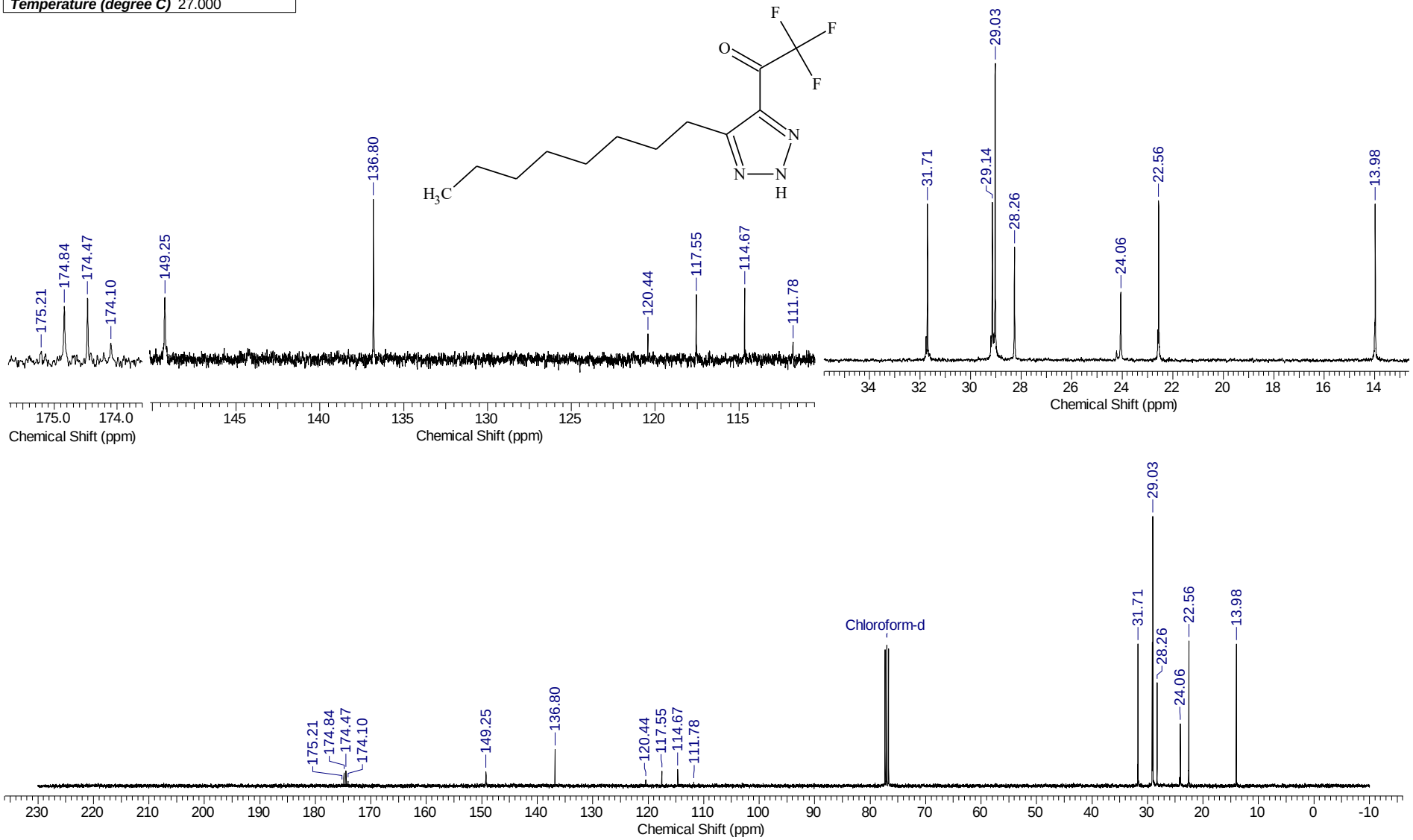
Acquisition Time (sec)	1.7433	***Comment***	Imported from UXNMR.			***Date***	03 Dec 2021 15:41:32
File Name	C:\DOCS\OUTPUT_301\2021\12.溴赅狃黑BM-2356-3.F_005001r					***Frequency (MHz)***	376.50
Nucleus	19F	***Number of Transients***	11	***Original Points Count***	131072	***Points Count***	262144
Pulse Sequence	zgflqn	***Solvent***	CHLOROFORM-D			***Sweep Width (Hz)***	75187.97
Temperature (degree C)	27.000						



^{19}F NMR spectrum of **2o** (376.5 MHz, $CDCl_3$)

13 May 2022

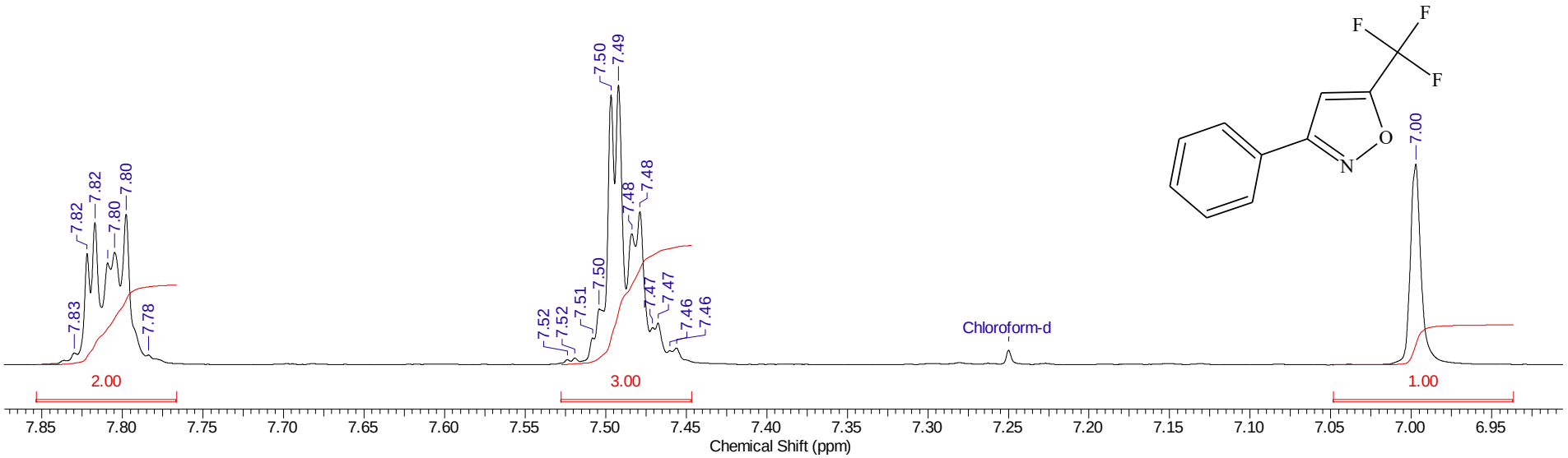
Acquisition Time (sec)	0.6783	***Comment***	Imported from UXNMR.			***Date***	04 Dec 2021 13:47:24
File Name	C:\DOCS\OUTPUT_301\2021\12.溴赅狃黑BM-2356-3.C_002001r					***Frequency (MHz)***	100.61
Nucleus	13C	***Number of Transients***	201	***Original Points Count***	16384	***Points Count***	131072
Pulse Sequence	zgpg30	***Solvent***	CHLOROFORM-D			***Sweep Width (Hz)***	24154.59
Temperature (degree C)	27.000						

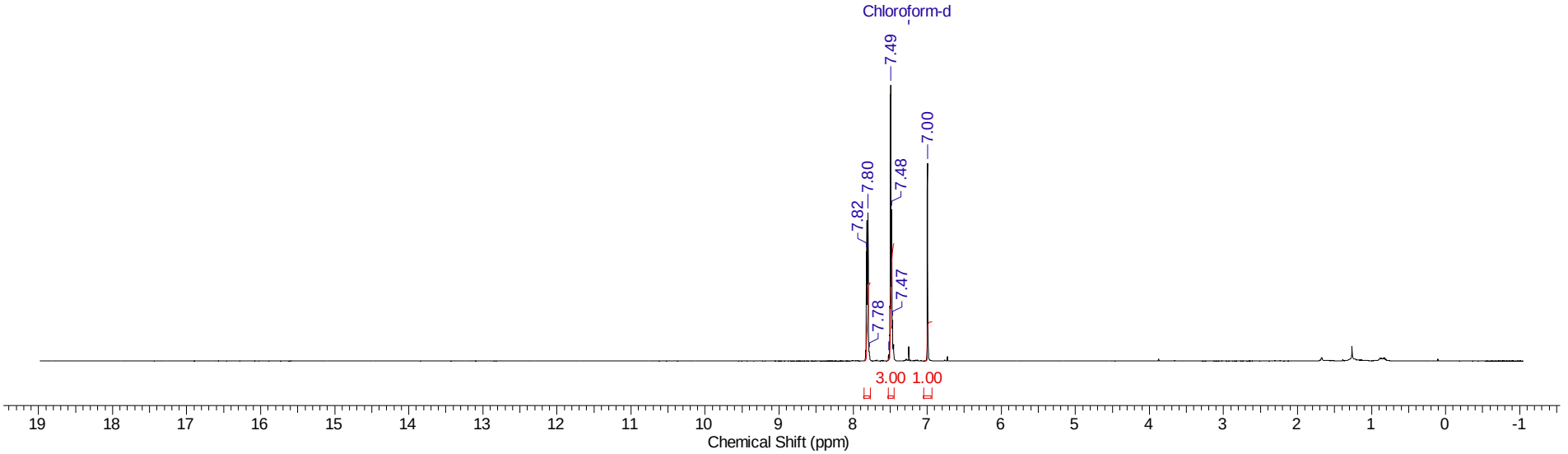


^{13}C NMR spectrum of **2o** (100.6 MHz, $CDCl_3$)

3 Aug 2022

Acquisition Time (sec)	4.0894	***Comment***	Imported from UXNMR.			***Date***	30 Nov 2021 14:27:30
File Name	C:\DOCS\OUTPUT_301\2021\11.躯 狃黑SZA-BM-2208.H_001001r					***Frequency (MHz)***	400.13
Nucleus	1H	***Number of Transients***	4	***Original Points Count***	32768	***Points Count***	131072
Pulse Sequence	zg30	***Solvent***	CHLOROFORM-D			***Sweep Width (Hz)***	8012.82
Temperature (degree C)	27.000						

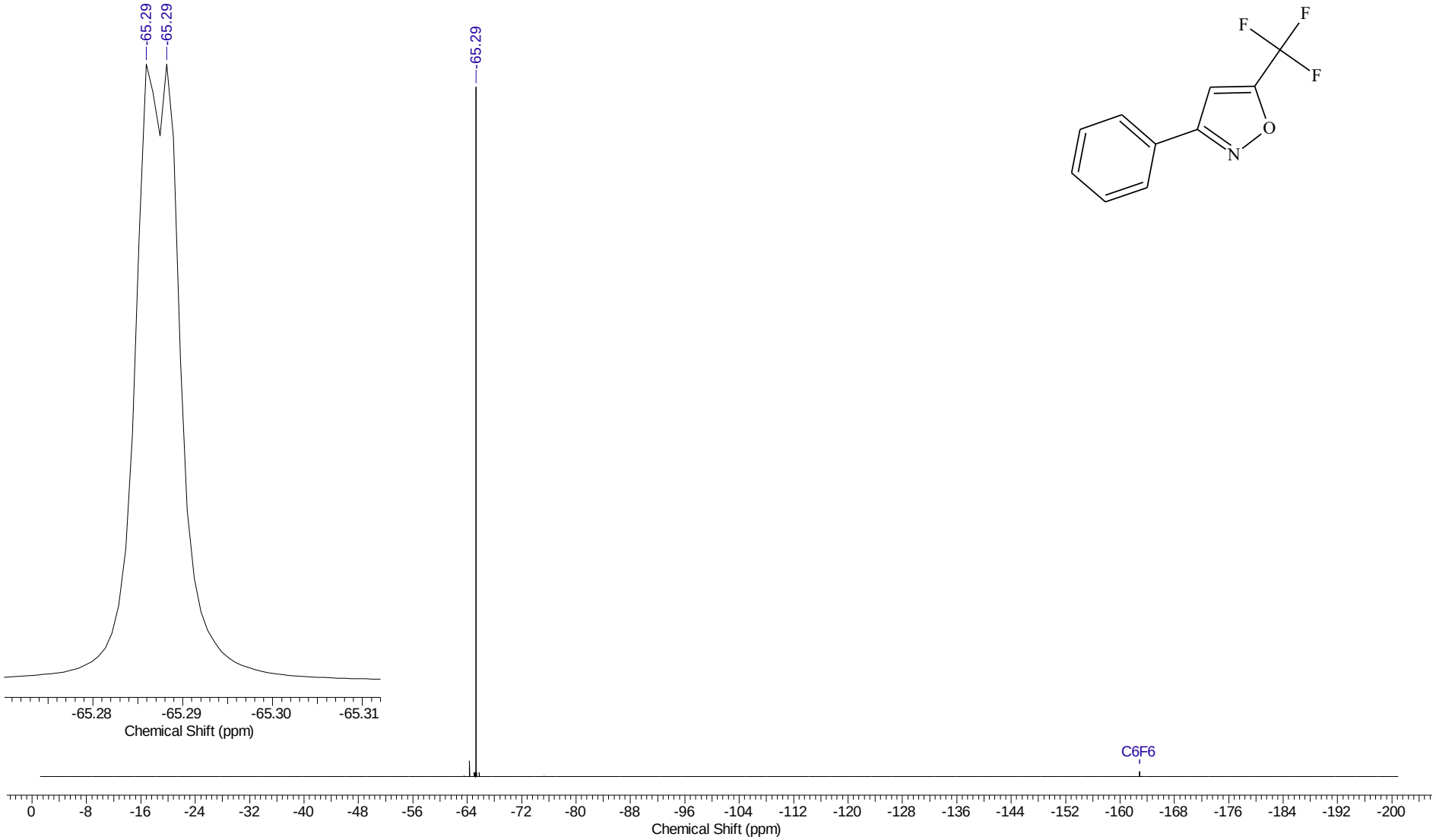




^{1}H NMR spectrum of **3a** (400.1 MHz, $CDCl_3$)

3 Aug 2022

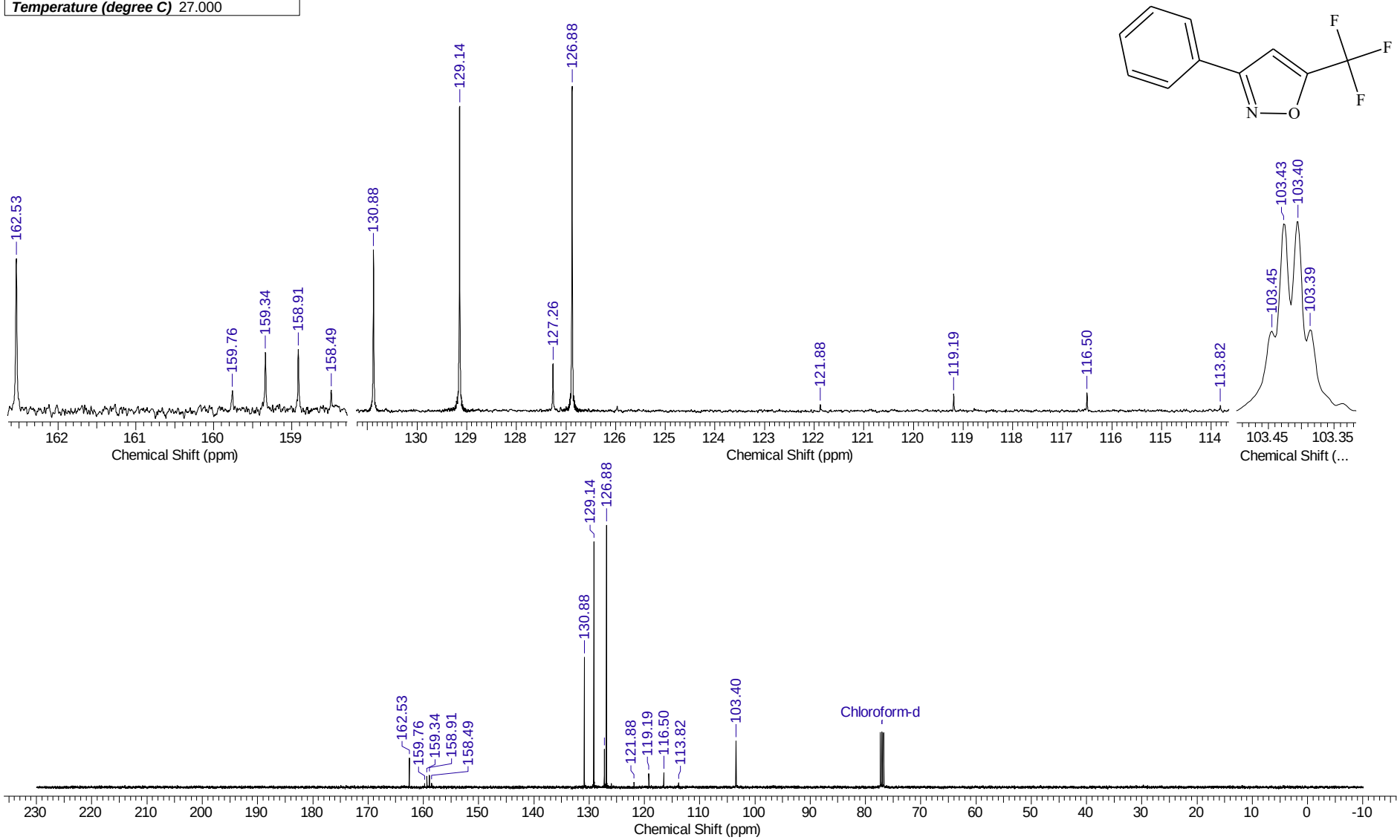
Acquisition Time (sec)	1.7433	***Comment***	Imported from UXNMR.			***Date***	30 Nov 2021 14:57:04
File Name	C:\DOCS\OUTPUT_301\2021\11.眶 狃黑SZA-BM-2208.F_005001r					***Frequency (MHz)***	376.50
Nucleus	19F	***Number of Transients***	16	***Original Points Count***	131072	***Points Count***	262144
Pulse Sequence	zgflqn	***Solvent***	CHLOROFORM-D			***Sweep Width (Hz)***	75187.97
Temperature (degree C)	27.000						



^{19}F NMR spectrum of **3a** (376.5 MHz, $CDCl_3$)

3 Aug 2022

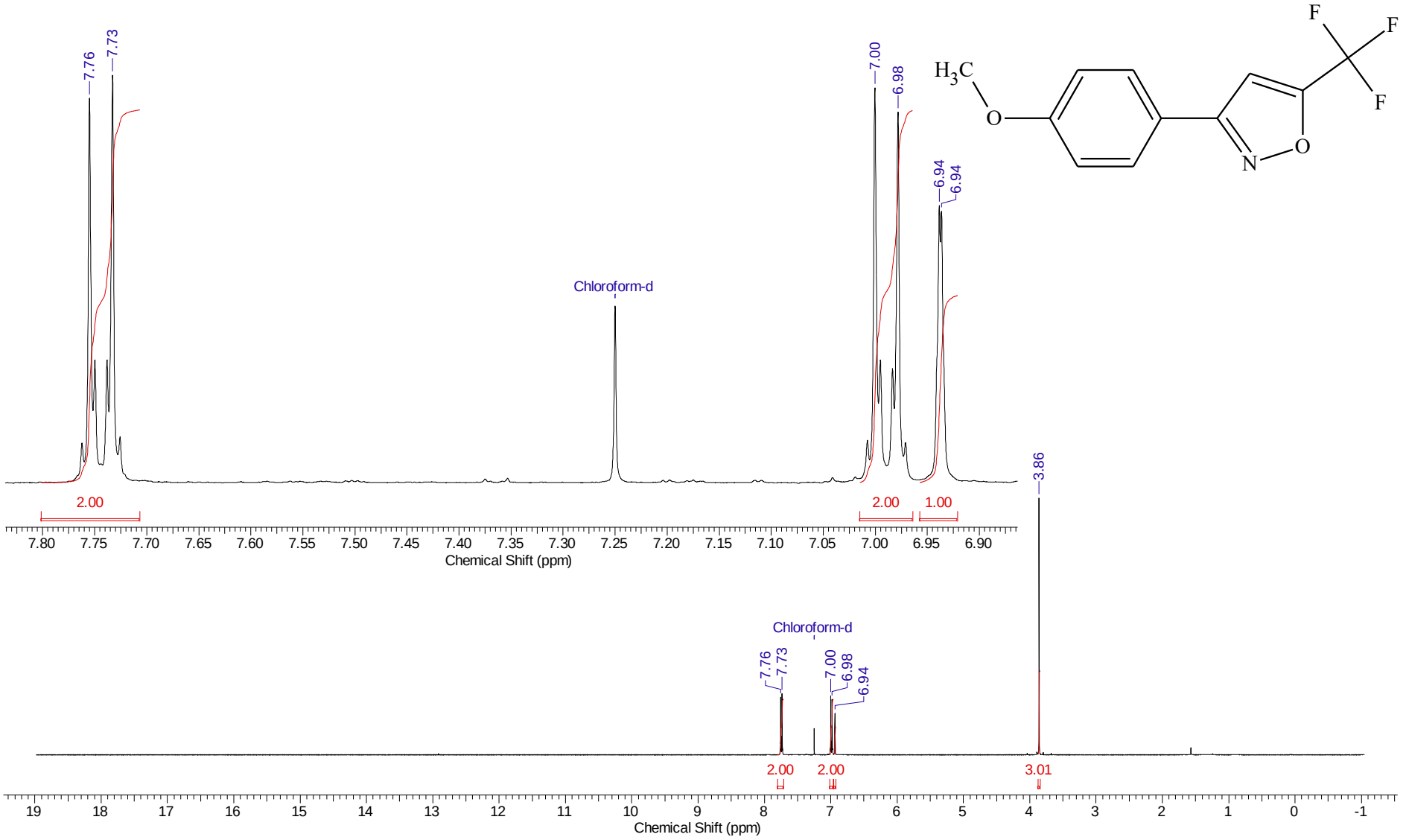
Acquisition Time (sec)	0.6783	***Comment***	Imported from UXNMR.			***Date***	02 Dec 2021 12:00:48
File Name	C:\DOCS\OUTPUT_301\2021\12.溴赅狃黑SZA-BM-2208.C.C_002001r					***Frequency (MHz)***	100.61
Nucleus	13C	***Number of Transients***	116	***Original Points Count***	16384	***Points Count***	131072
Pulse Sequence	zgpg30	***Solvent***	CHLOROFORM-D			***Sweep Width (Hz)***	24154.59
Temperature (degree C)	27.000						



^{13}C NMR spectrum of **3a** (100.6 MHz, $CDCl_3$)

3 Aug 2022

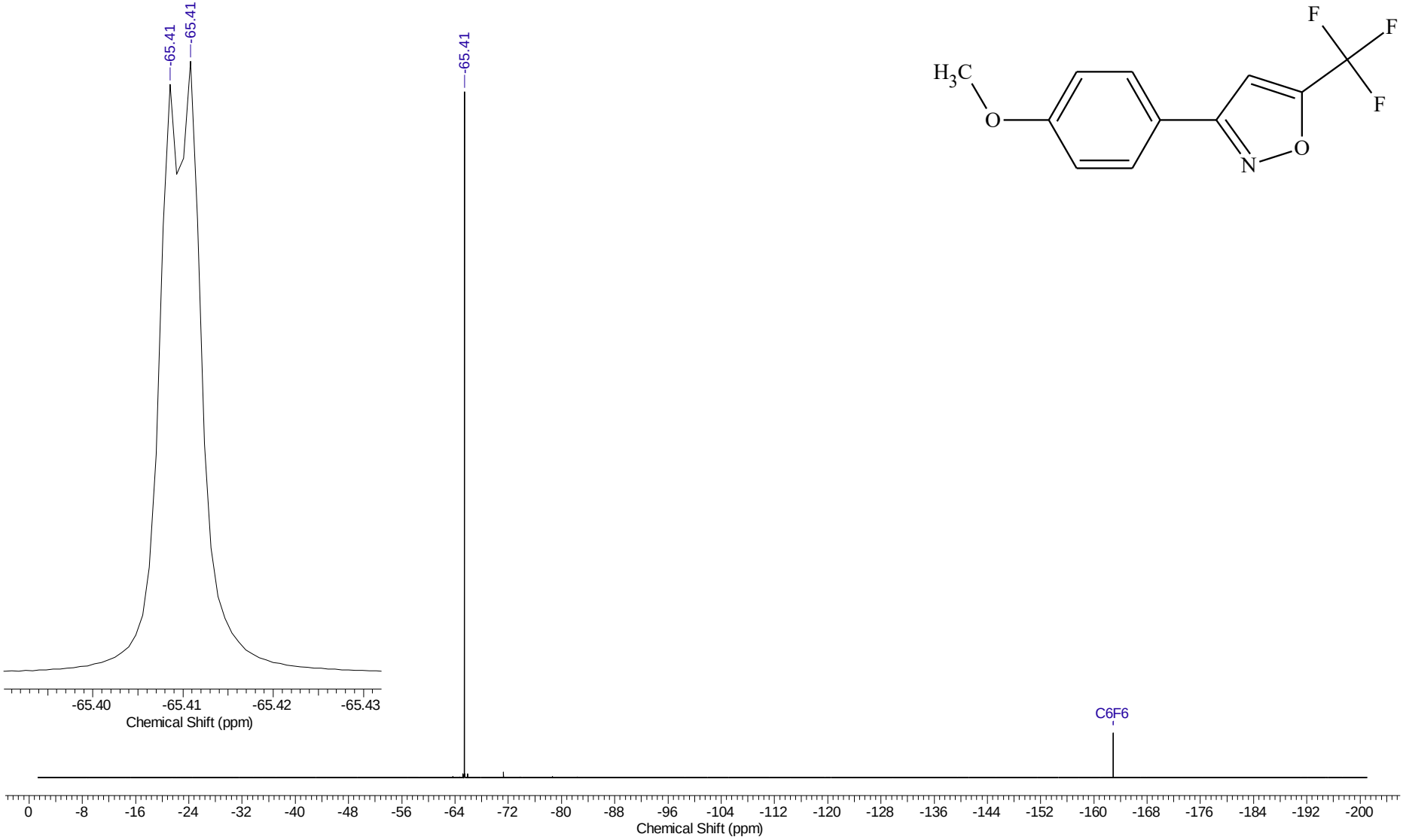
Acquisition Time (sec)	4.0894	***Comment***	Imported from UXNMR.			***Date***	17 Jan 2022 15:09:44
File Name	C:\DOCS\OUTPUT_301\2022\01. 磯囧黒BM-2399.H_001001r					***Frequency (MHz)***	400.13
Nucleus	1H	***Number of Transients***	4	***Original Points Count***	32768	***Points Count***	131072
Pulse Sequence	zg30	***Solvent***	BENZENE-D6	***Sweep Width (Hz)***	8012.82	***Temperature (degree C)***	27.000



^{1}H NMR spectrum of **3b** (400.1 MHz, $CDCl_3$)

3 Aug 2022

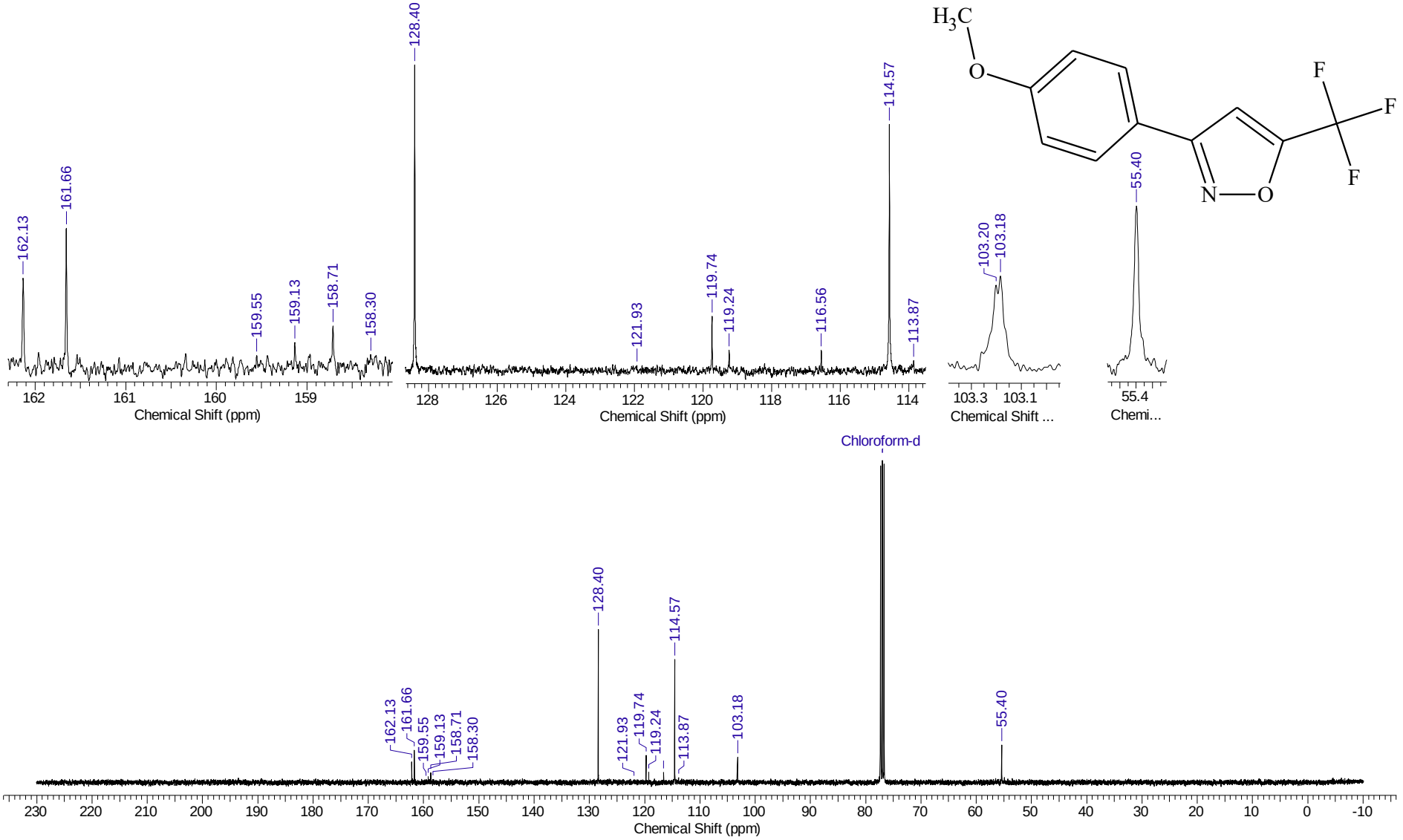
Acquisition Time (sec)	1.7433	***Comment***	Imported from UXNMR.			***Date***	17 Jan 2022 15:26:40
File Name	C:\DOCS\OUTPUT_301\2022\01. 磺囧黑BM-2399.F_005001r			***Frequency (MHz)***	376.50	***Nucleus***	19F
Number of Transients	15	***Original Points Count***	131072	***Points Count***	262144	***Pulse Sequence***	zgflqn
Solvent	CHLOROFORM-D			***Sweep Width (Hz)***	75187.97	***Temperature (degree C)***	27.000



^{19}F NMR spectrum of **3b** (376.5 MHz, $CDCl_3$)

3 Aug 2022

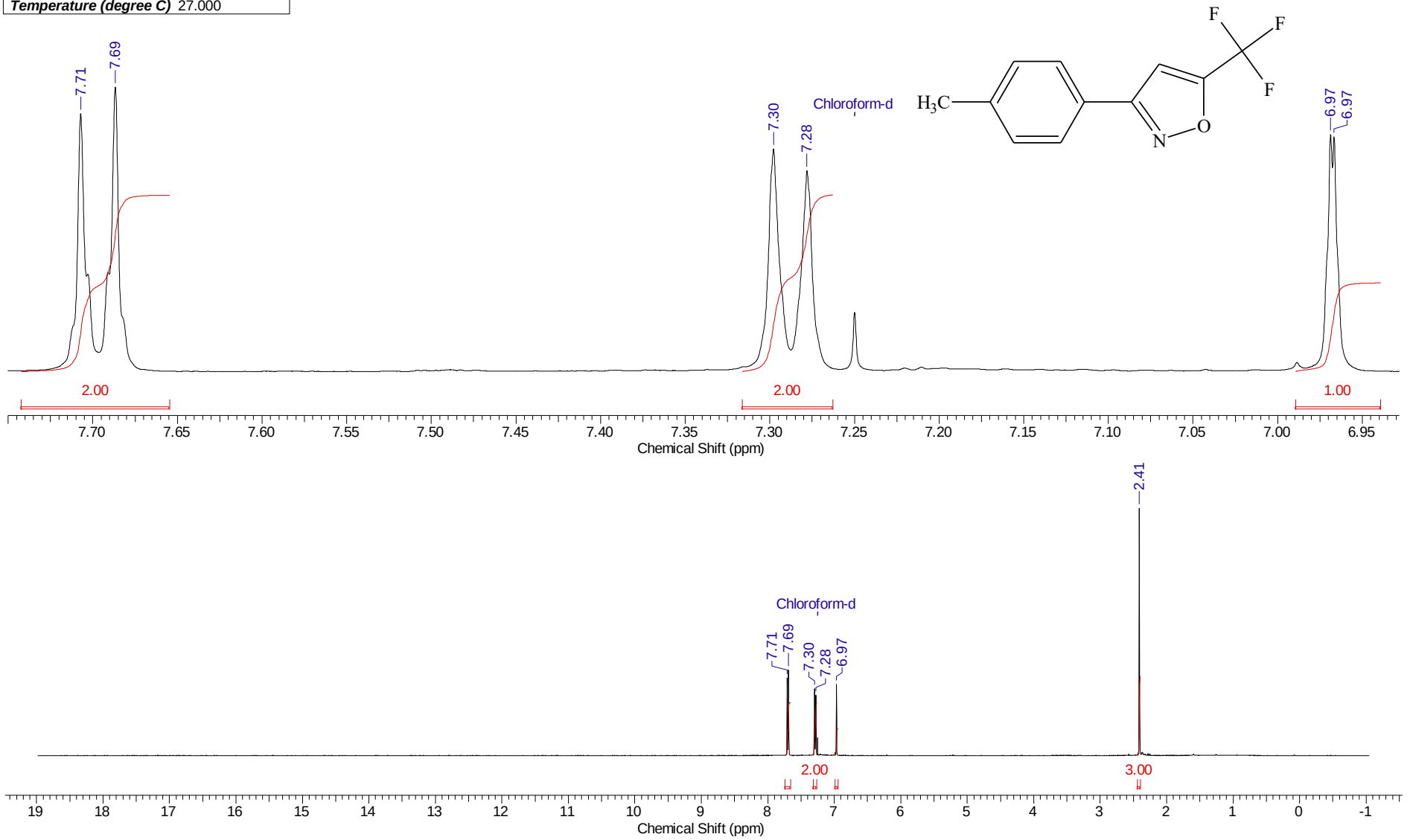
Acquisition Time (sec)	0.6783	***Comment***	Imported from UXNMR.			***Date***	08 Jul 2022 16:02:16
File Name	C:\DOCS\OUTPUT_301\2022\07.棹 朦\BM-2399-1.C_002001r			***Frequency (MHz)***	100.61	***Nucleus***	13C
Number of Transients	685	***Original Points Count***	16384	***Points Count***	131072	***Pulse Sequence***	zgpg30
Solvent	CHLOROFORM-D			***Sweep Width (Hz)***	24154.59	***Temperature (degree C)***	27.000



^{13}C NMR spectrum of **3b** (100.6 MHz, $CDCl_3$)

3 Aug 2022

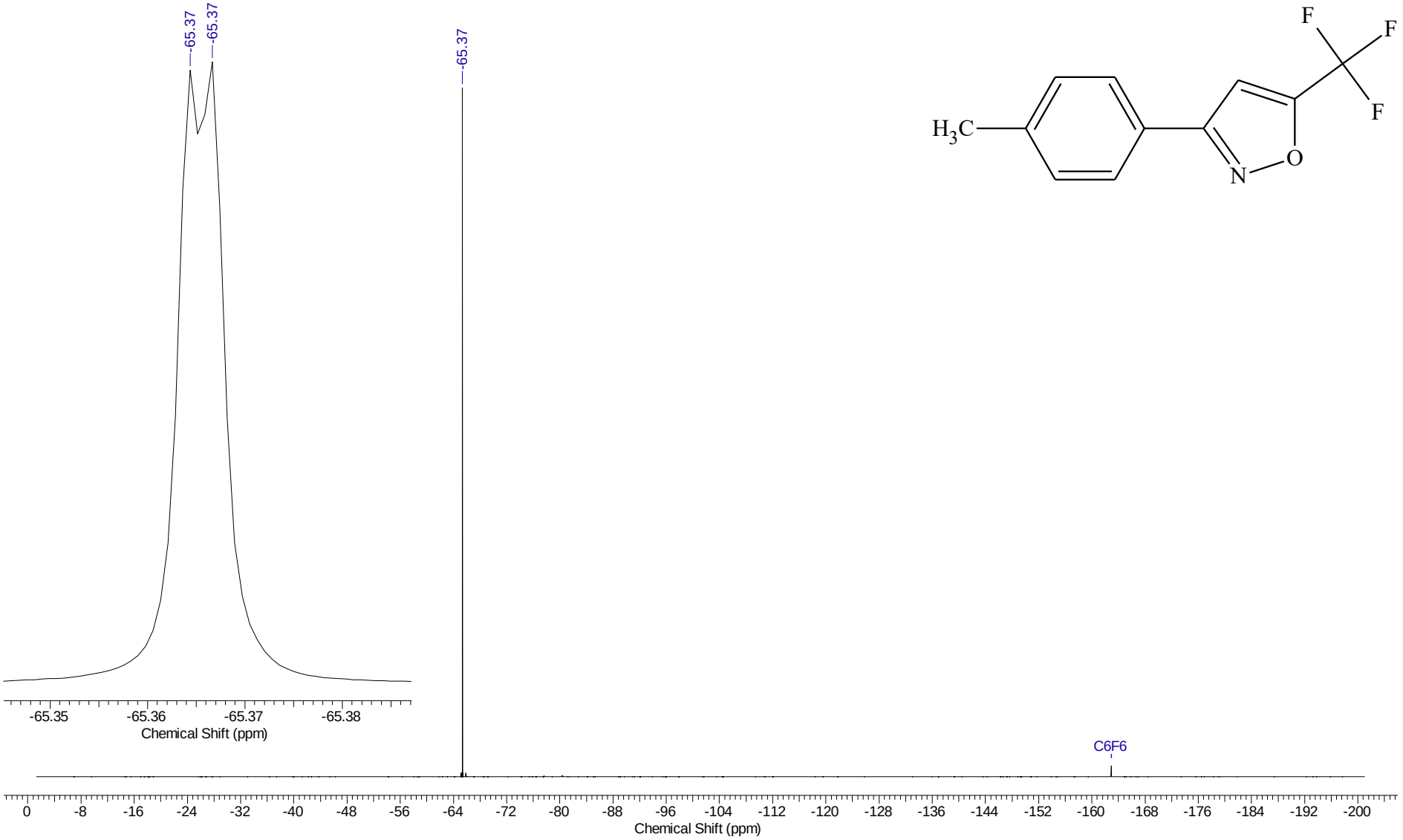
Acquisition Time (sec)	4.0894	***Comment***	Imported from UXNMR.			***Date***	21 Jan 2022 14:58:44
File Name	C:\DOCS\OUTPUT_301\2022\01. 磯囪黒BM-2408.H_001001r					***Frequency (MHz)***	400.13
Nucleus	1H	***Number of Transients***	4	***Original Points Count***	32768	***Points Count***	131072
Pulse Sequence	zg30	***Solvent***	CHLOROFORM-D			***Sweep Width (Hz)***	8012.82
Temperature (degree C)	27.000						



^{1}H NMR spectrum of **3d** (400.1 MHz, $CDCl_3$)

3 Aug 2022

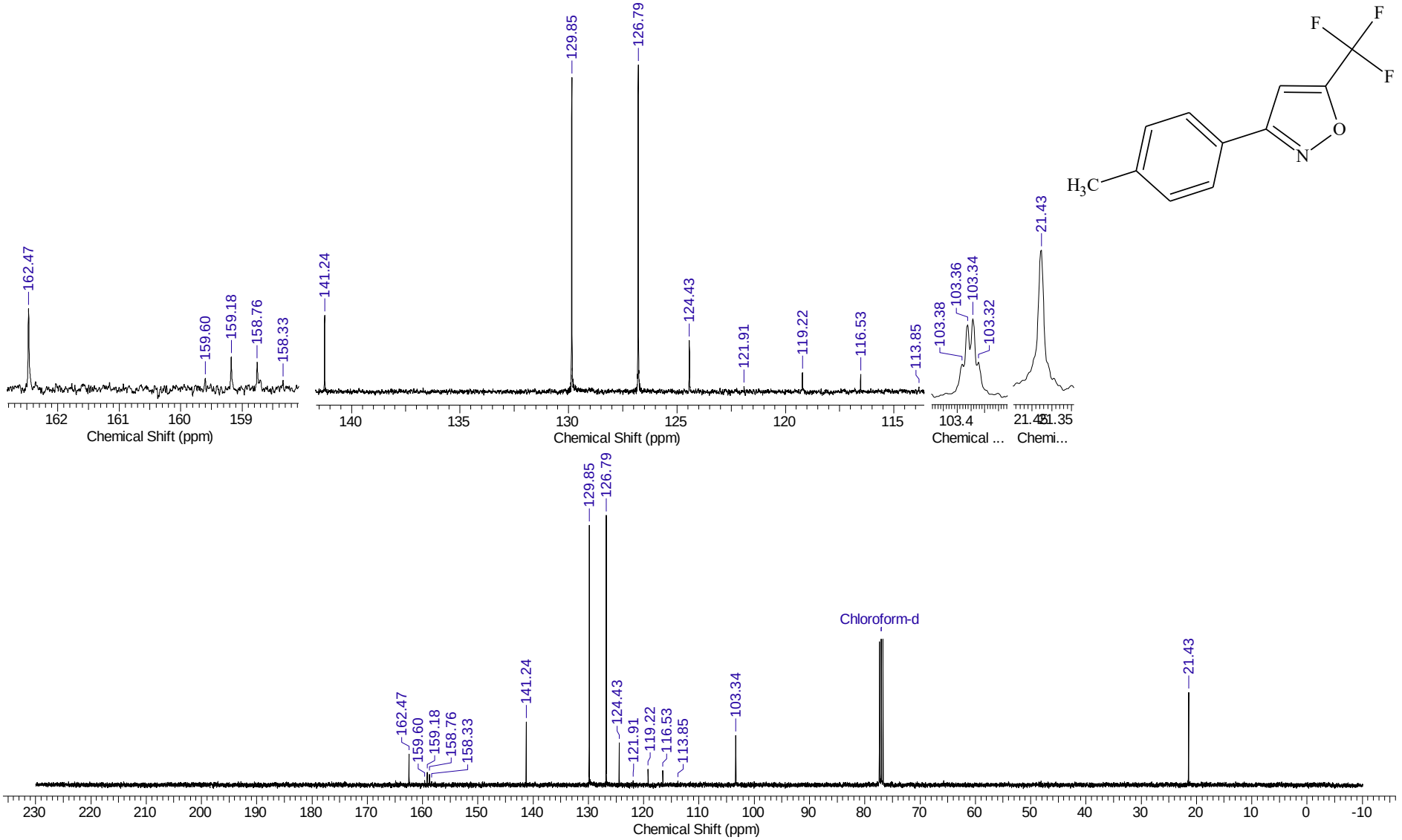
Acquisition Time (sec)	1.7433	***Comment***	Imported from UXNMR.			***Date***	21 Jan 2022 15:22:12
File Name	C:\DOCS\OUTPUT_301\2022\01. 磺囧黑BM-2408.F_005001r					***Frequency (MHz)***	376.50
Nucleus	19F	***Number of Transients***	10	***Original Points Count***	131072	***Points Count***	262144
Pulse Sequence	zgflqn	***Solvent***	Acetone	***Sweep Width (Hz)***	75187.97	***Temperature (degree C)***	27.000



^{19}F NMR spectrum of **3d** (376.5 MHz, $CDCl_3$)

3 Aug 2022

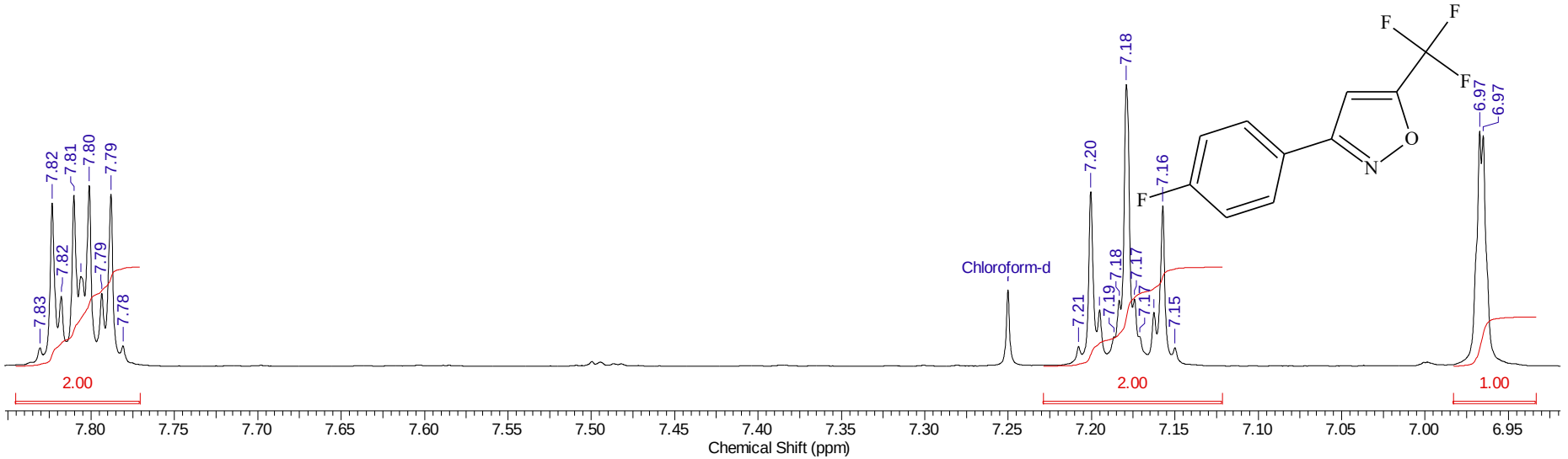
Acquisition Time (sec)	0.6783	***Comment***	Imported from UXNMR.			***Date***	24 Jan 2022 14:37:04
File Name	C:\DOCS\OUTPUT_301\2022\01. 磺囧黑BM-2408.C_002001r			***Frequency (MHz)***	100.61	***Nucleus***	13C
Number of Transients	201	***Original Points Count***	16384	***Points Count***	131072	***Pulse Sequence***	zgpg30
Solvent	CHLOROFORM-D			***Sweep Width (Hz)***	24154.59	***Temperature (degree C)***	27.000

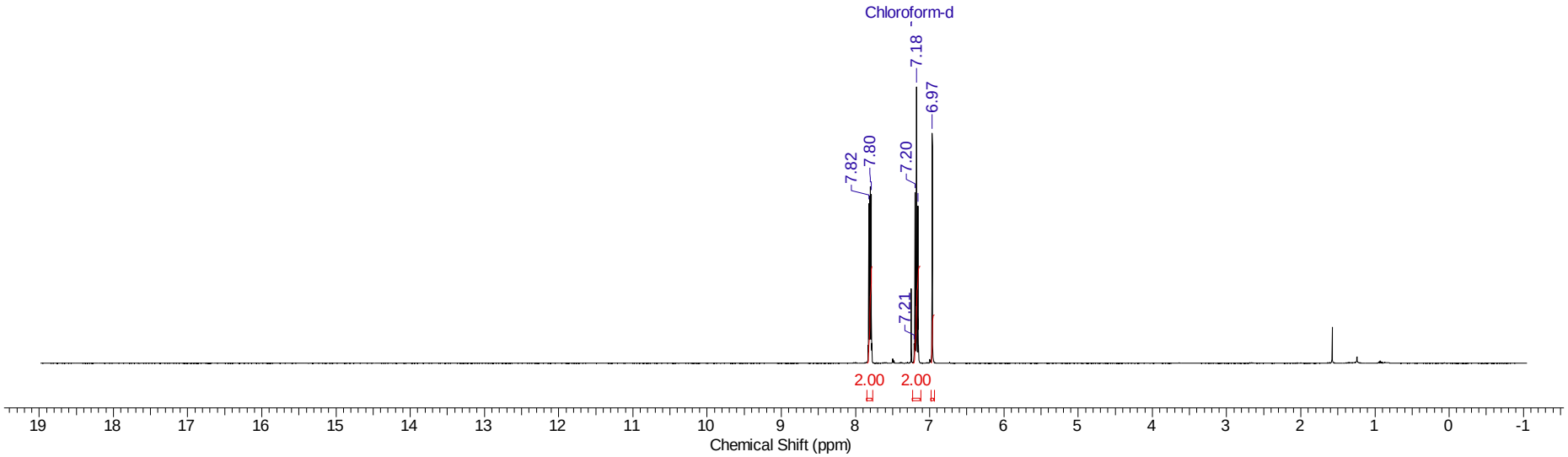


^{13}C NMR spectrum of **3d** (100.6 MHz, $CDCl_3$)

3 Aug 2022

Acquisition Time (sec)	4.0894	***Comment***	Imported from UXNMR.			***Date***	24 Jan 2022 15:19:32
File Name	C:\DOCS\OUTPUT_301\2022\01. 磯囪黒BM-2215.H_001001r					***Frequency (MHz)***	400.13
Nucleus	1H	***Number of Transients***	4	***Original Points Count***	32768	***Points Count***	131072
Pulse Sequence	zg30	***Solvent***	CHLOROFORM-D			***Sweep Width (Hz)***	8012.82
Temperature (degree C)	27.000						

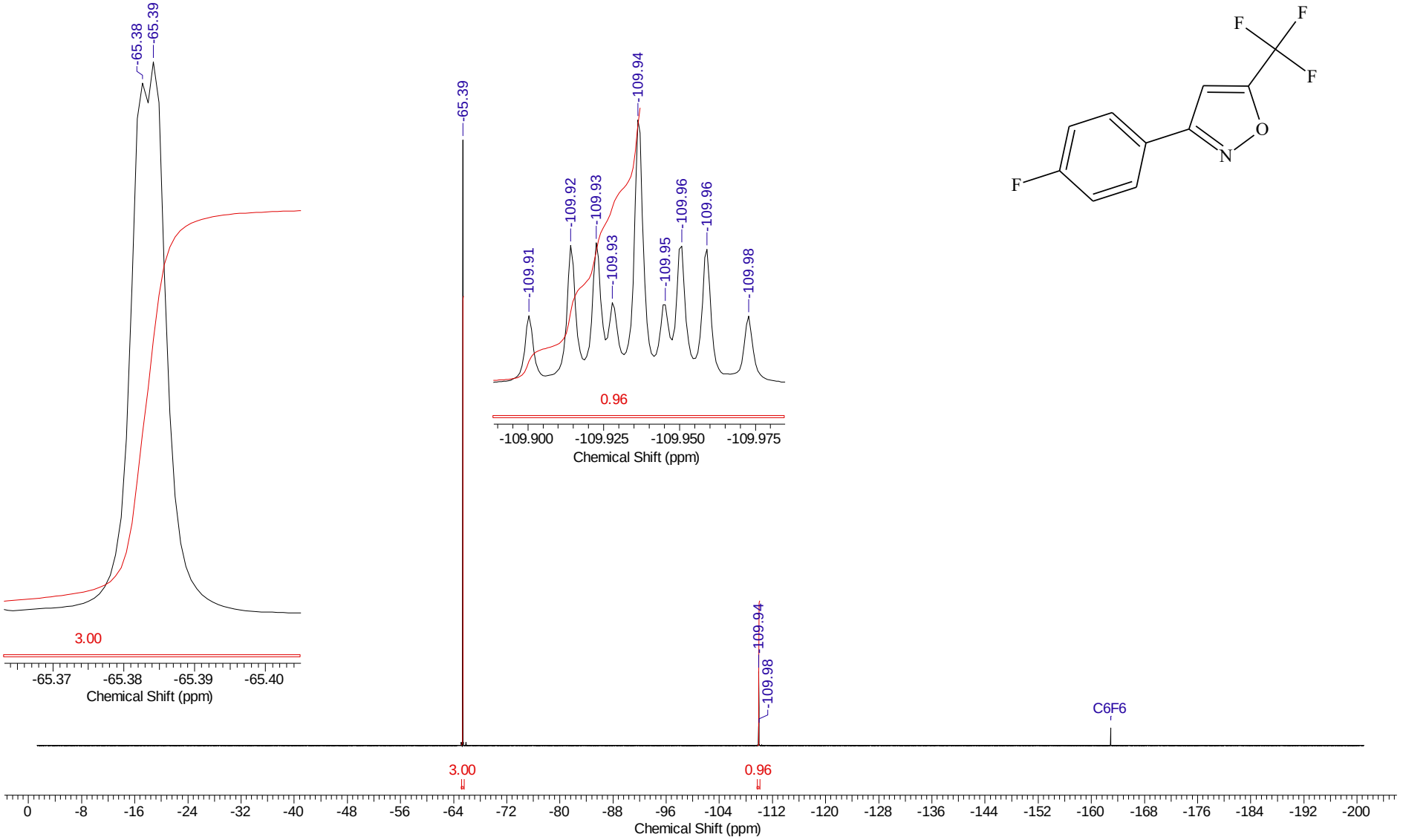




^{1}H NMR spectrum of **3e** (400.1 MHz, $CDCl_3$)

3 Aug 2022

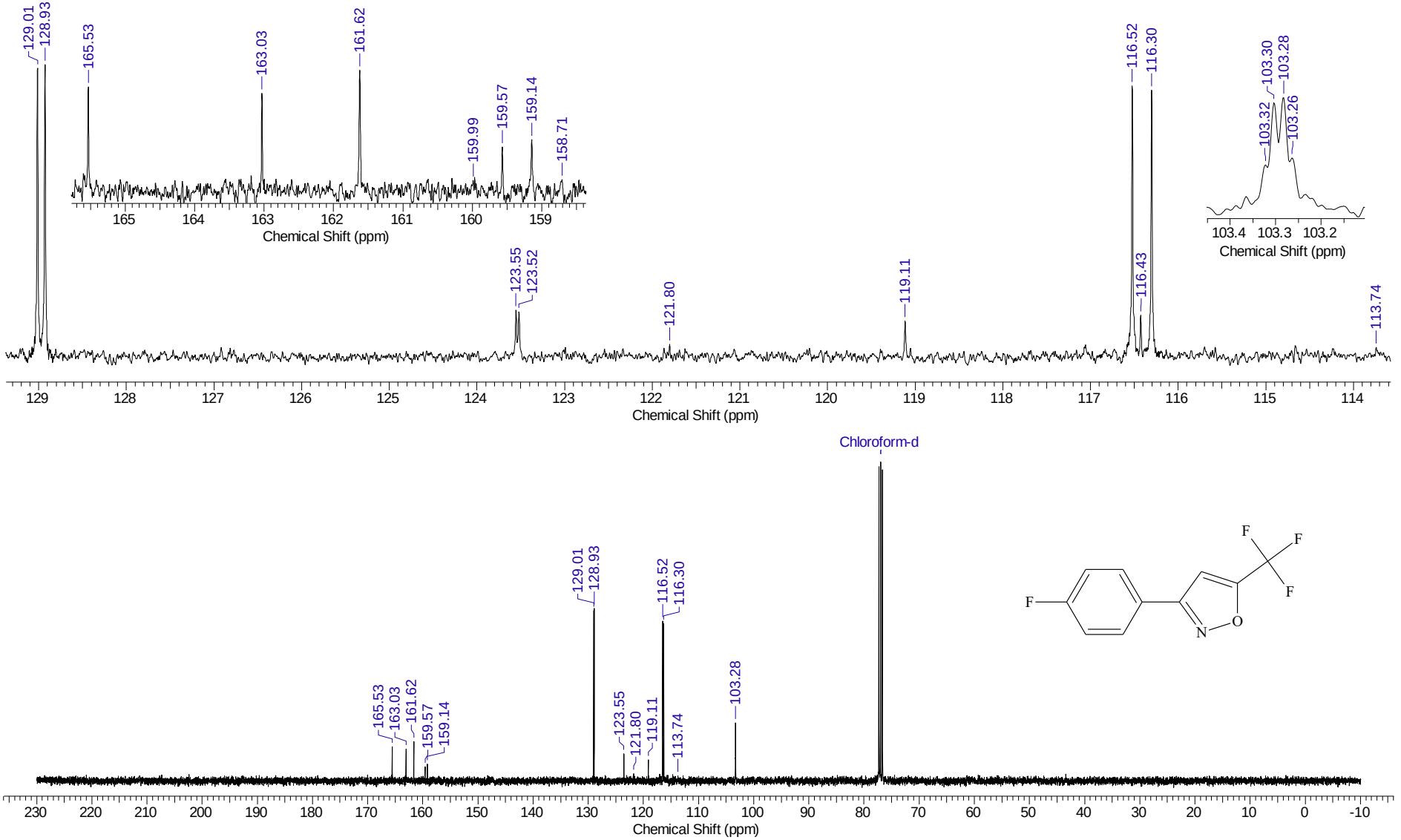
Acquisition Time (sec)	1.7433	***Comment***	Imported from UXNMR.			***Date***	24 Jan 2022 15:27:48
File Name	C:\DOCS\OUTPUT_301\2022\01. 磺囧黑BM-2215.F_005001r					***Frequency (MHz)***	376.50
Nucleus	19F	***Number of Transients***	16	***Original Points Count***	131072	***Points Count***	262144
Pulse Sequence	zgflqn	***Solvent***	Acetone	***Sweep Width (Hz)***	75187.97	***Temperature (degree C)***	27.000



^{19}F NMR spectrum of **3e** (376.5 MHz, $CDCl_3$)

3 Aug 2022

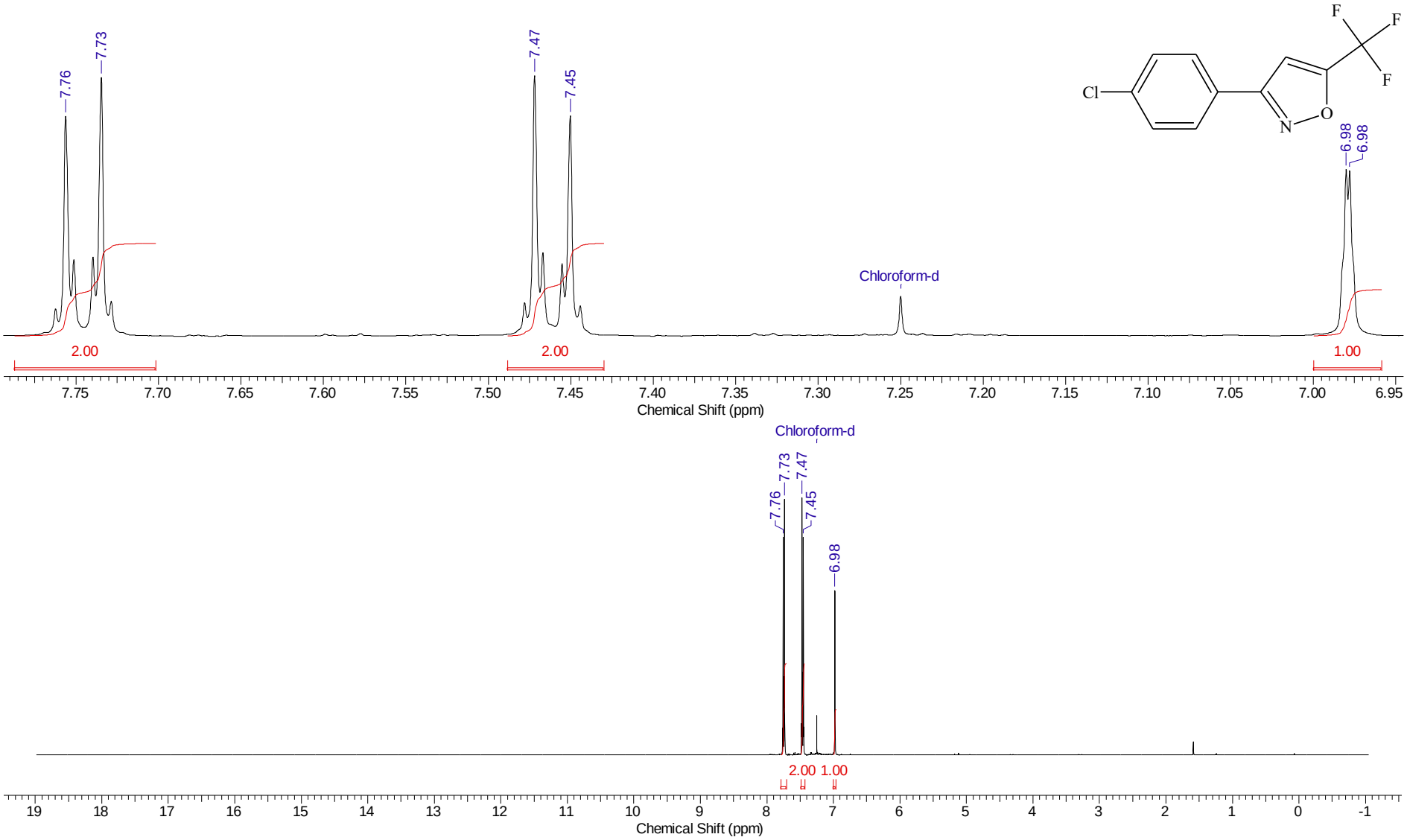
Acquisition Time (sec)	0.6783	***Comment***	Imported from UXNMR.			***Date***	25 Jan 2022 16:04:58
File Name	C:\DOCS\OUTPUT_301\2022\01. 磺囧黑BM-2215.C_002001r			***Frequency (MHz)***	100.61	***Nucleus***	13C
Number of Transients	273	***Original Points Count***	16384	***Points Count***	131072	***Pulse Sequence***	zgpg30
Solvent	CHLOROFORM-D			***Sweep Width (Hz)***	24154.59	***Temperature (degree C)***	27.000



^{13}C NMR spectrum of **3e** (100.6 MHz, $CDCl_3$)

3 Aug 2022

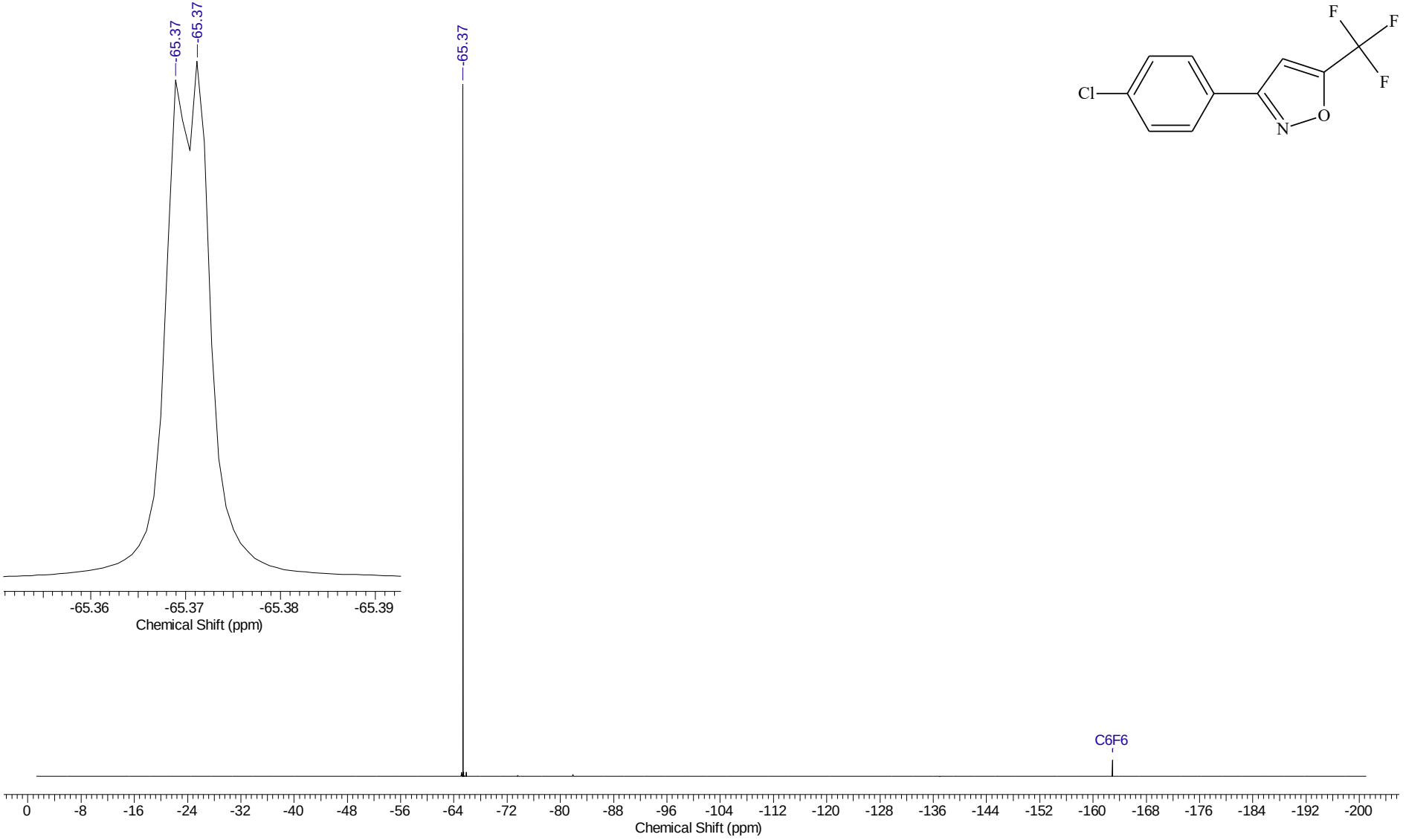
Acquisition Time (sec)	4.0894	***Comment***	Imported from UXNMR.			***Date***	17 Jan 2022 15:14:56
File Name	C:\DOCS\OUTPUT_301\2022\01. 磯囪黒BM-2402.H_001001r					***Frequency (MHz)***	400.13
Nucleus	1H	***Number of Transients***	4	***Original Points Count***	32768	***Points Count***	131072
Pulse Sequence	zg30	***Solvent***	BENZENE-D6	***Sweep Width (Hz)***	8012.82	***Temperature (degree C)***	27.000



^{1}H NMR spectrum of **3f** (400.1 MHz, $CDCl_3$)

3 Aug 2022

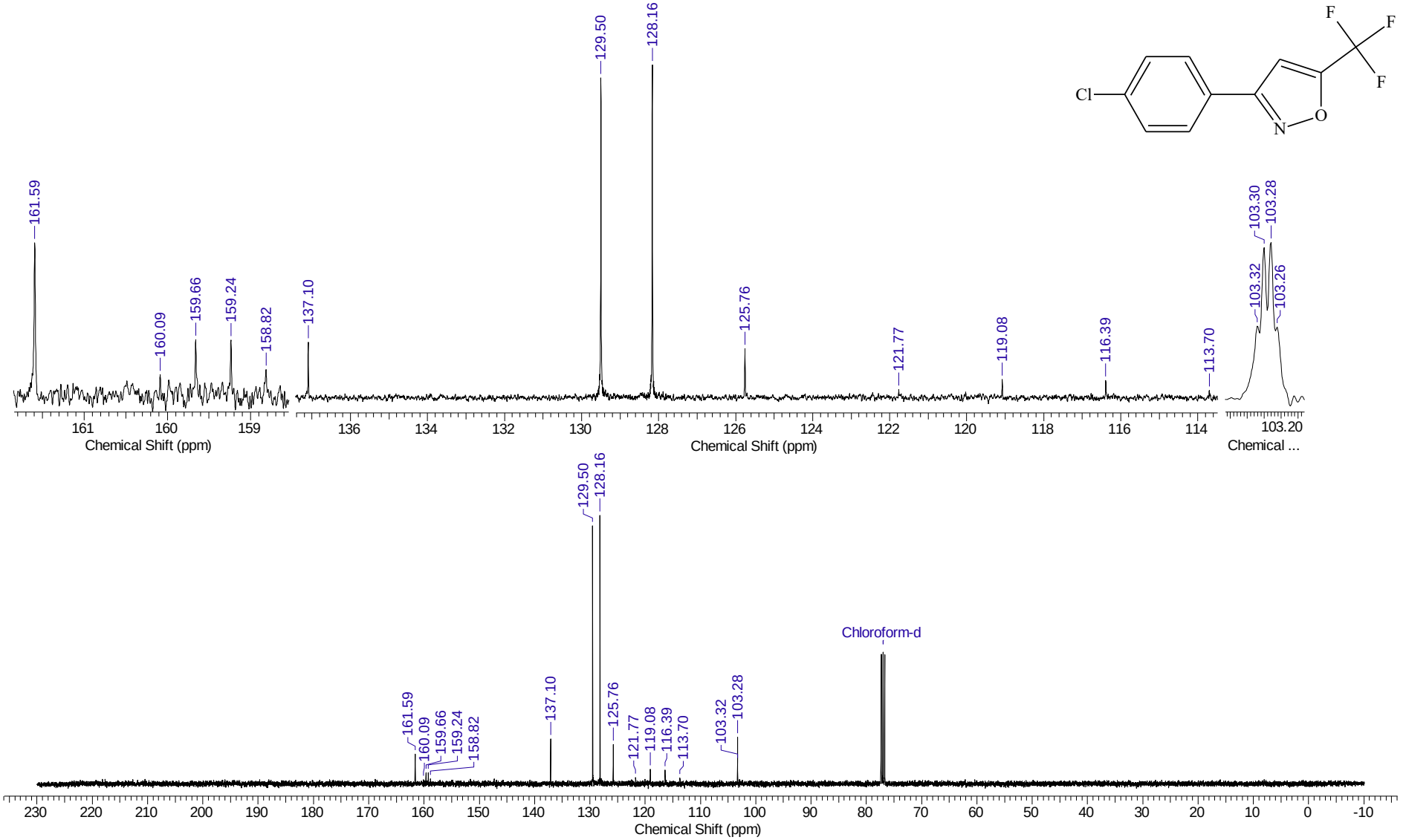
Acquisition Time (sec)	1.7433	***Comment***	Imported from UXNMR.			***Date***	17 Jan 2022 15:30:42
File Name	C:\DOCS\OUTPUT_301\2022\01. 磯囪黒BM-2402.F_005001r			***Frequency (MHz)***	376.50	***Nucleus***	19F
Number of Transients	9	***Original Points Count***	131072	***Points Count***	262144	***Pulse Sequence***	zgflqn
Solvent	CHLOROFORM-D			***Sweep Width (Hz)***	75187.97	***Temperature (degree C)***	27.000



^{19}F NMR spectrum of **3f** (376.5 MHz, $CDCl_3$)

3 Aug 2022

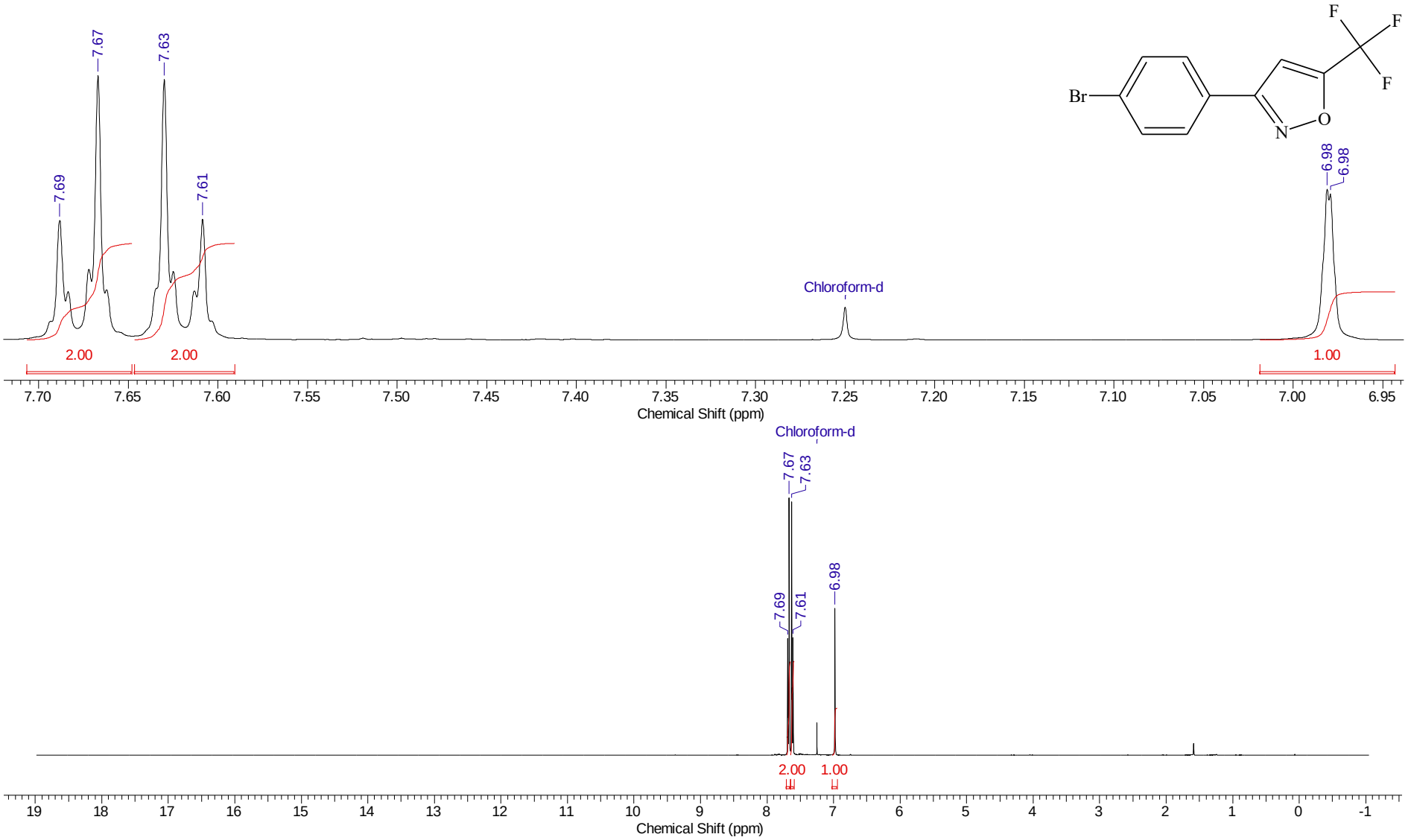
Acquisition Time (sec)	0.6783	***Comment***	Imported from UXNMR.			***Date***	18 Jan 2022 15:06:44
File Name	C:\DOCS\OUTPUT_301\2022\01. 磯囪黒BM-2402.C_002001r			***Frequency (MHz)***	100.61	***Nucleus***	13C
Number of Transients	121	***Original Points Count***	16384	***Points Count***	131072	***Pulse Sequence***	zgpg30
Solvent	CHLOROFORM-D			***Sweep Width (Hz)***	24154.59	***Temperature (degree C)***	27.000



^{13}C NMR spectrum of **3f** (100.6 MHz, $CDCl_3$)

3 Aug 2022

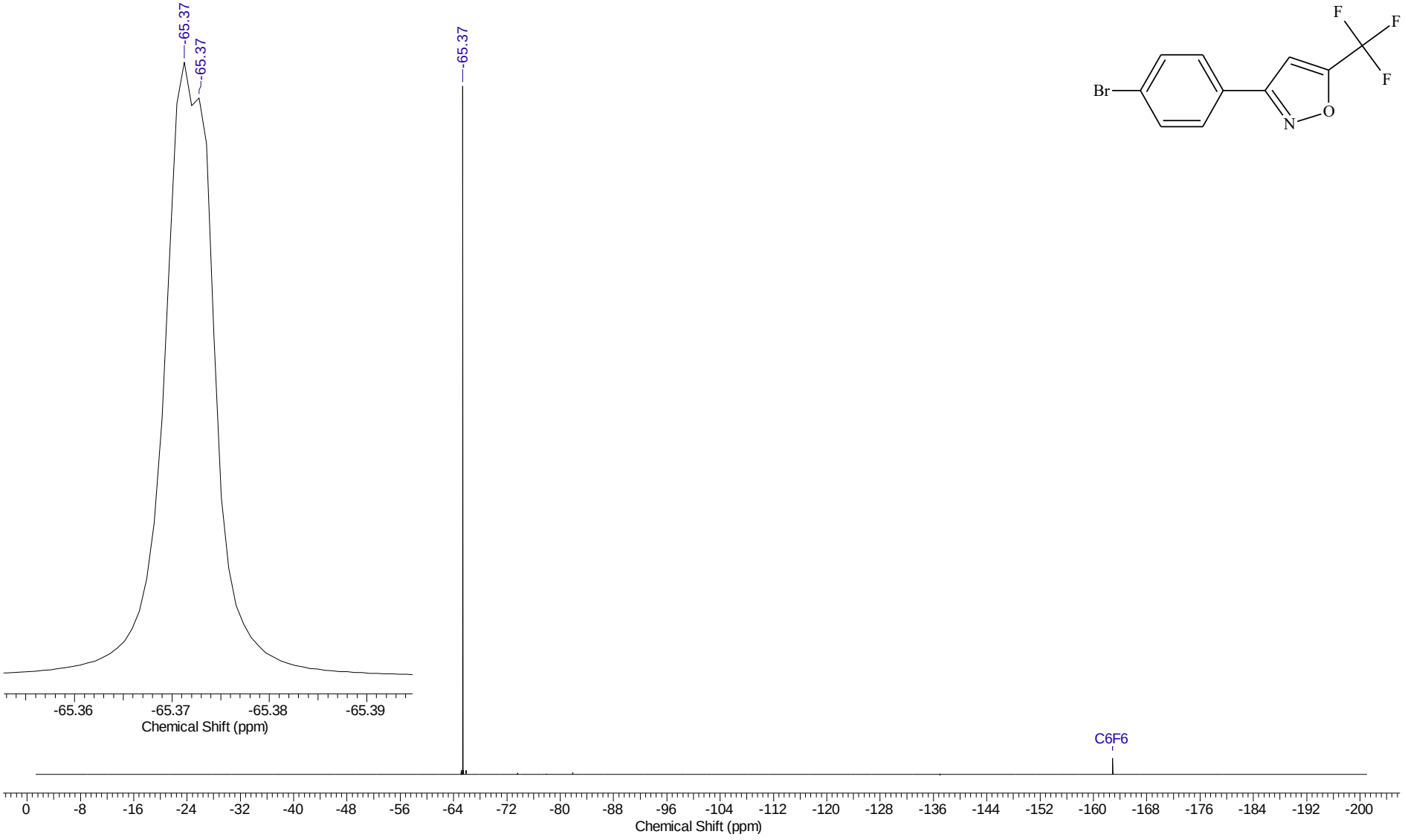
Acquisition Time (sec)	4.0894	***Comment***	Imported from UXNMR.			***Date***	17 Jan 2022 15:18:40
File Name	C:\DOCS\OUTPUT_301\2022\01. 磯囪黒BM-2405.H_001001r					***Frequency (MHz)***	400.13
Nucleus	1H	***Number of Transients***	4	***Original Points Count***	32768	***Points Count***	131072
Pulse Sequence	zg30	***Solvent***	BENZENE-D6	***Sweep Width (Hz)***	8012.82	***Temperature (degree C)***	27.000



^{1}H NMR spectrum of **3g** (400.1 MHz, $CDCl_3$)

3 Aug 2022

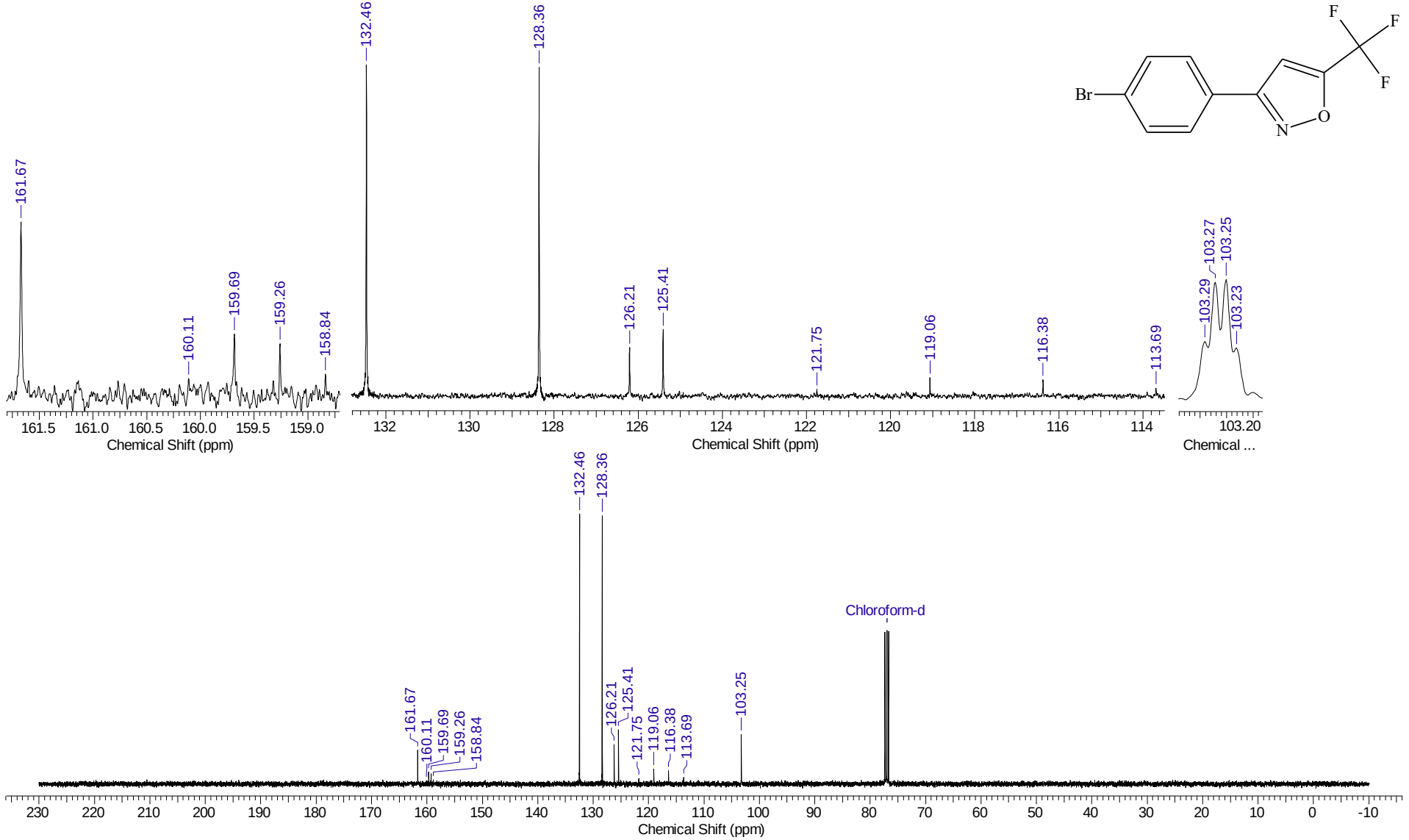
Acquisition Time (sec)	1.7433	***Comment***	Imported from UXNMR.			***Date***	17 Jan 2022 15:34:48
File Name	C:\DOCS\OUTPUT_301\2022\01. 徹囧黒BM-2405.F_005001r			***Frequency (MHz)***	376.50	***Nucleus***	19F
Number of Transients	11	***Original Points Count***	131072	***Points Count***	262144	***Pulse Sequence***	zgflqn
Solvent	CHLOROFORM-D			***Sweep Width (Hz)***	75187.97	***Temperature (degree C)***	27.000



^{19}F NMR spectrum of **3g** (376.5 MHz, $CDCl_3$)

3 Aug 2022

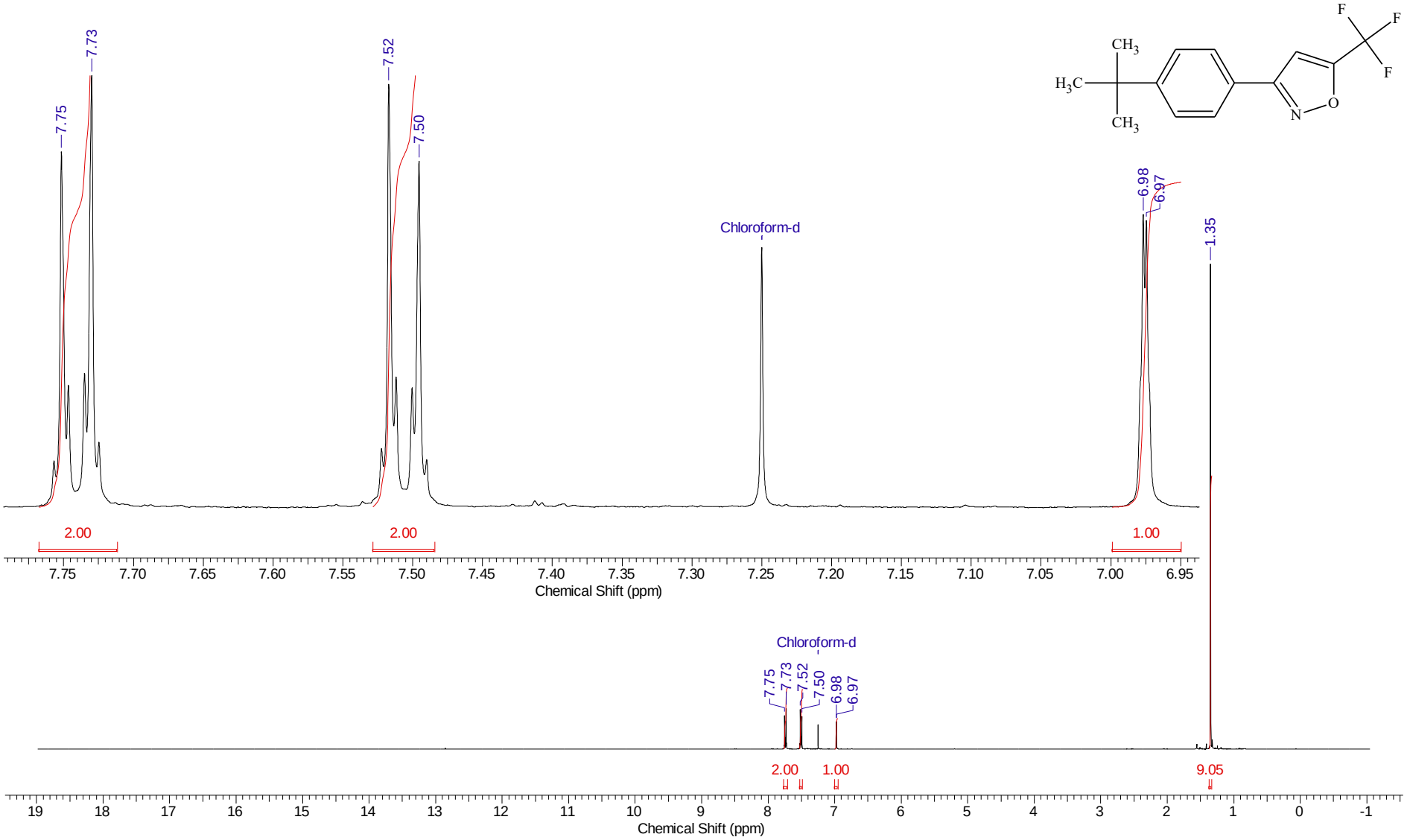
Acquisition Time (sec)	0.6783	***Comment***	Imported from UXNMR.			***Date***	18 Jan 2022 15:36:44
File Name	C:\DOCS\OUTPUT_301\2022\01. 磯囧黒BM-2405.C_002001r			***Frequency (MHz)***	100.61	***Nucleus***	13C
Number of Transients	177	***Original Points Count***	16384	***Points Count***	131072	***Pulse Sequence***	zgpg30
Solvent	CHLOROFORM-D			***Sweep Width (Hz)***	24154.59	***Temperature (degree C)***	27.000



^{13}C NMR spectrum of **3g** (100.6 MHz, $CDCl_3$)

3 Aug 2022

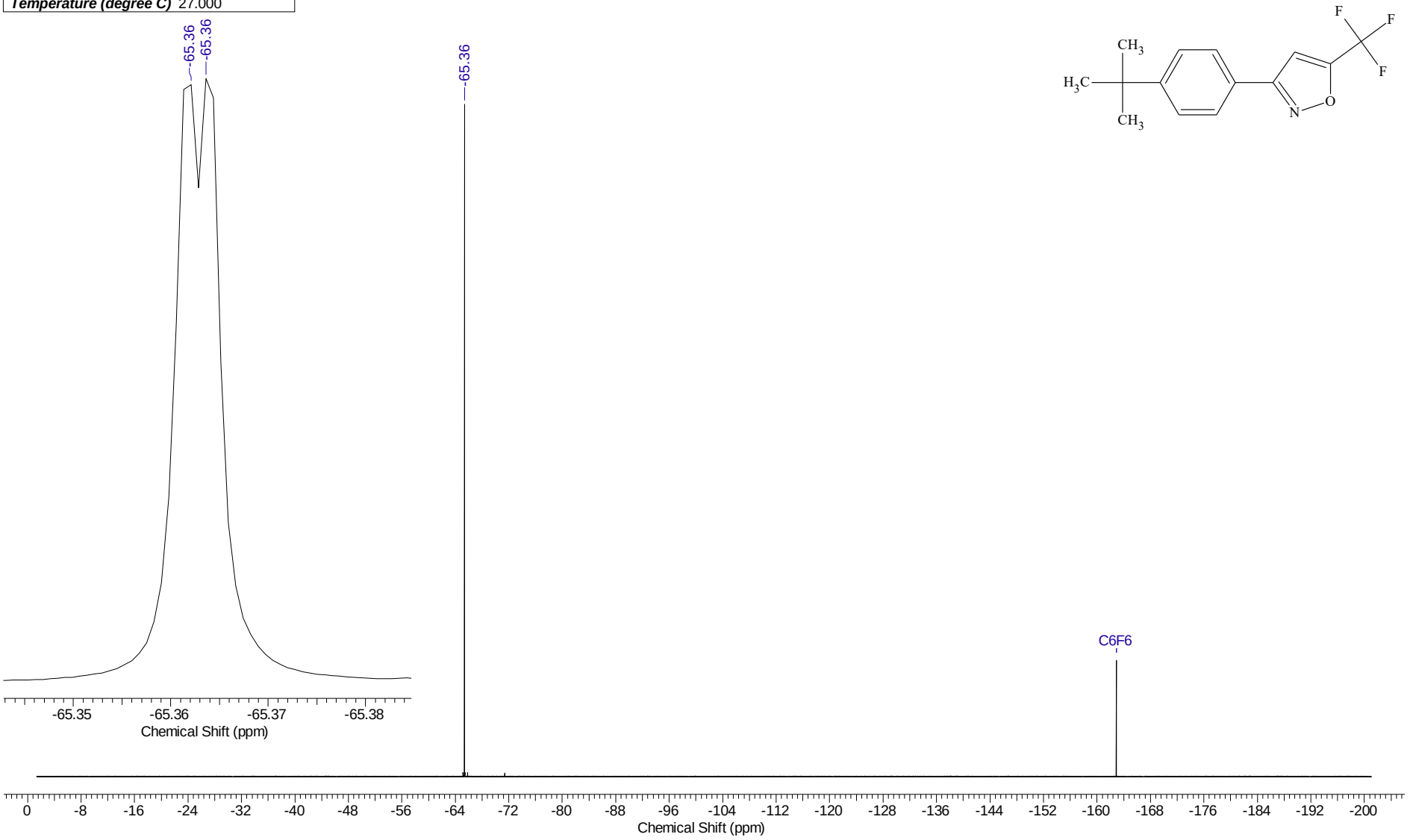
Acquisition Time (sec)	4.0894	***Comment***	Imported from UXNMR.			***Date***	18 Jan 2022 15:00:28
File Name	C:\DOCS\OUTPUT_301\2022\01. 磯囧黒BM-2404-3.H_001001r					***Frequency (MHz)***	400.13
Nucleus	1H	***Number of Transients***	4	***Original Points Count***	32768	***Points Count***	131072
Pulse Sequence	zg30	***Solvent***	BENZENE-D6	***Sweep Width (Hz)***	8012.82	***Temperature (degree C)***	27.000



^{1}H NMR spectrum of **3h** (400.1 MHz, $CDCl_3$)

3 Aug 2022

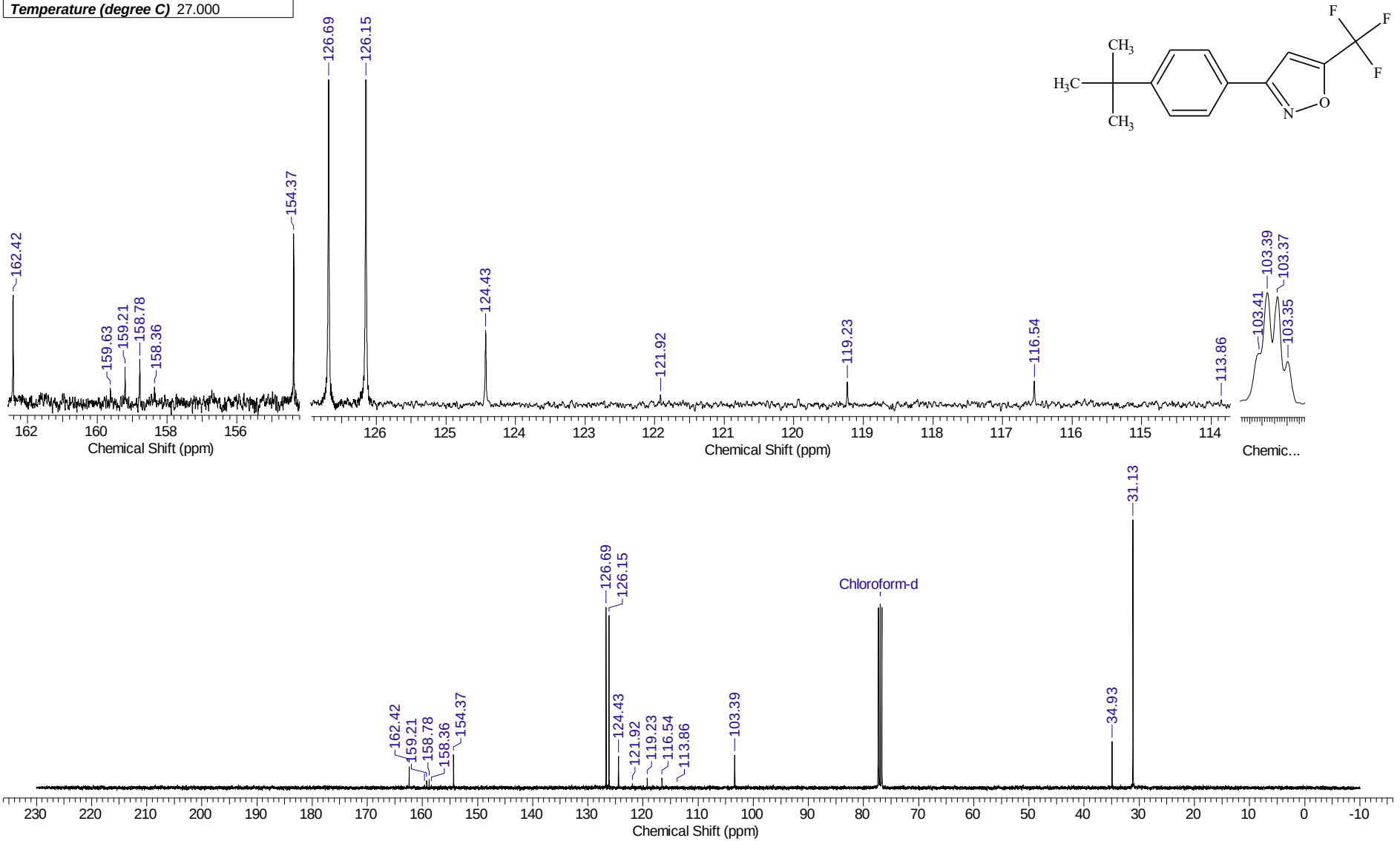
Acquisition Time (sec)	1.7433	***Comment***	Imported from UXNMR.			***Date***	18 Jan 2022 15:10:48
File Name	C:\DOCS\OUTPUT_301\2022\01. 磯囪黒BM-2404-4.F_005001r					***Frequency (MHz)***	376.50
Nucleus	19F	***Number of Transients***	16	***Original Points Count***	131072	***Points Count***	262144
Pulse Sequence	zgflqn	***Solvent***	CHLOROFORM-D			***Sweep Width (Hz)***	75187.97
Temperature (degree C)	27.000						



^{19}F NMR spectrum of **3h** (376.5 MHz, $CDCl_3$)

3 Aug 2022

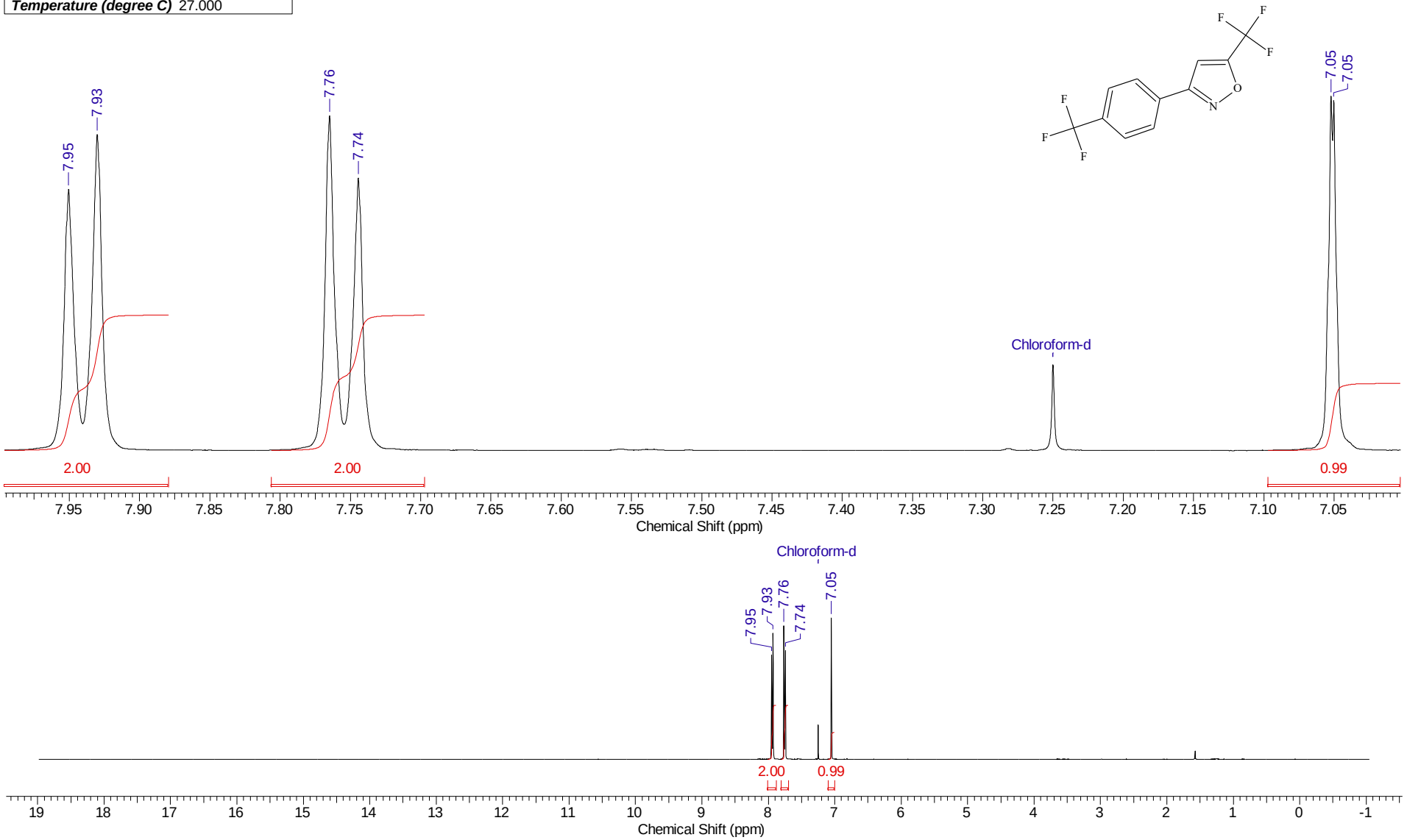
Acquisition Time (sec)	0.6783	***Comment***	Imported from UXNMR.			***Date***	20 Jan 2022 12:08:18
File Name	C:\DOCS\OUTPUT_301\2022\01. 磯囪黒BM-2404-3.C_002001r					***Frequency (MHz)***	100.61
Nucleus	13C	***Number of Transients***	637	***Original Points Count***	16384	***Points Count***	131072
Pulse Sequence	zgpg30	***Solvent***	CHLOROFORM-D			***Sweep Width (Hz)***	24154.59
Temperature (degree C)	27.000						



^{13}C NMR spectrum of **3h** (100.6 MHz, $CDCl_3$)

3 Aug 2022

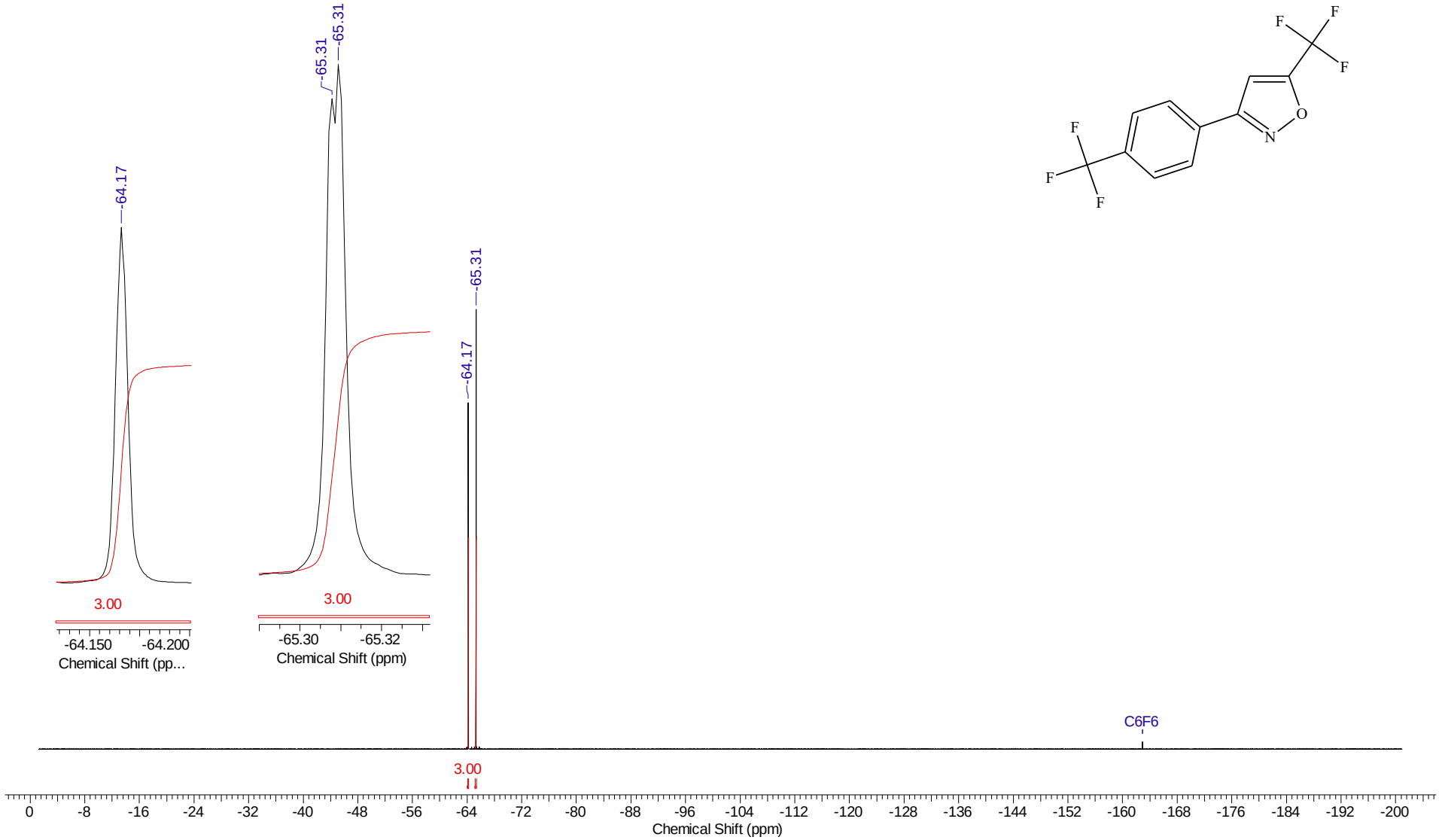
Acquisition Time (sec)	4.0894	***Comment***	Imported from UXNMR.			***Date***	24 Dec 2021 15:40:48
File Name	C:\DOCS\OUTPUT_301\2021\12.溴赅狃黑BM-2400-1.H_001001r					***Frequency (MHz)***	400.13
Nucleus	1H	***Number of Transients***	4	***Original Points Count***	32768	***Points Count***	131072
Pulse Sequence	zg30	***Solvent***	CHLOROFORM-D			***Sweep Width (Hz)***	8012.82
Temperature (degree C)	27.000						



^{1}H NMR spectrum of **3i** (400.1 MHz, $CDCl_3$)

3 Aug 2022

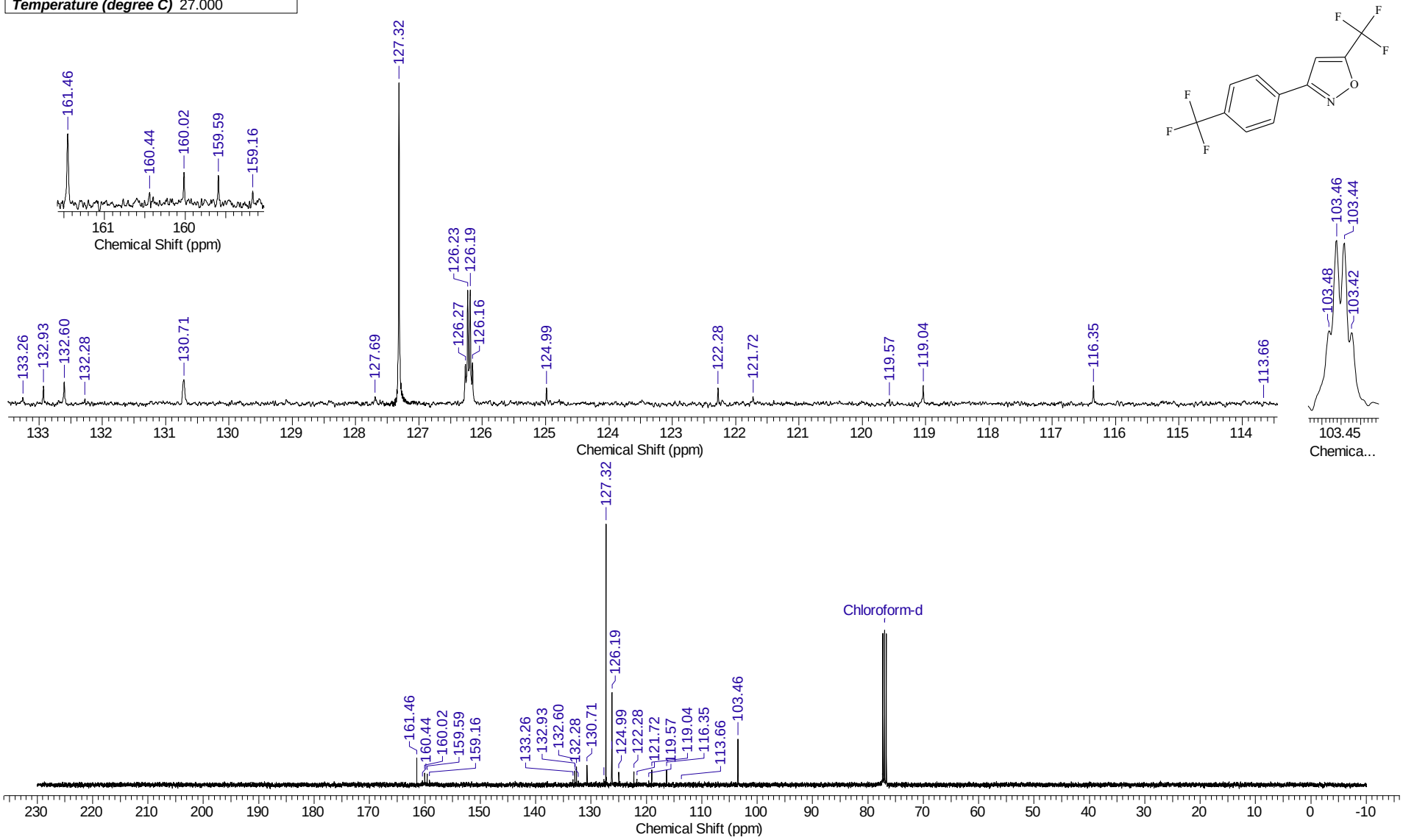
Acquisition Time (sec)	1.7433	***Comment***	Imported from UXNMR.			***Date***	24 Dec 2021 15:39:16
File Name	C:\DOCS\OUTPUT_301\2021\12.溴赅狃黑BM-2400-1.F_005001r					***Frequency (MHz)***	376.50
Nucleus	19F	***Number of Transients***	9	***Original Points Count***	131072	***Points Count***	262144
Pulse Sequence	zgflqn	***Solvent***	CHLOROFORM-D			***Sweep Width (Hz)***	75187.97
Temperature (degree C)	27.000						



^{19}F NMR spectrum of **3i** (376.5 MHz, $CDCl_3$)

3 Aug 2022

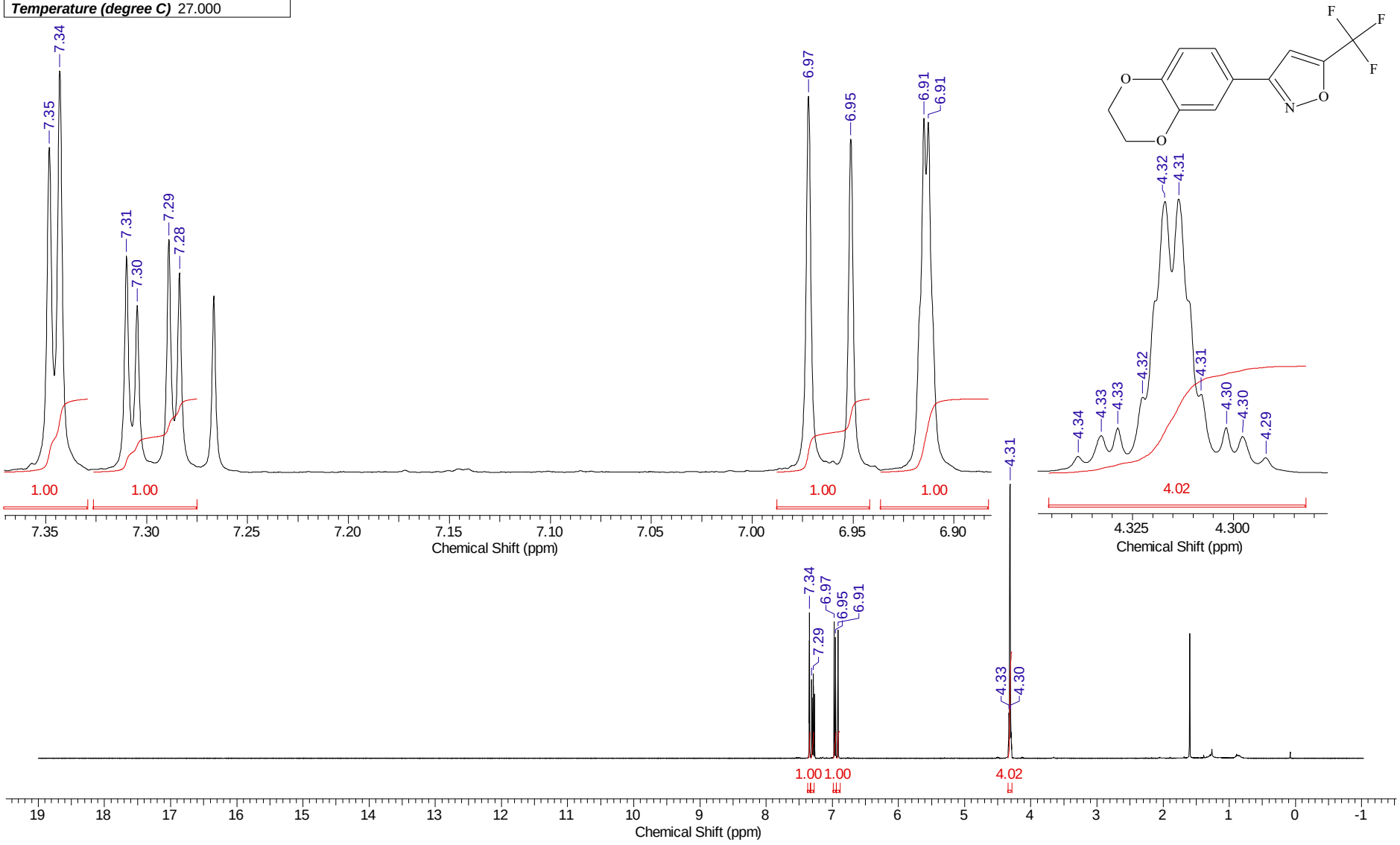
Acquisition Time (sec)	0.6783	***Comment***	Imported from UXNMR.			***Date***	24 Dec 2021 16:51:54
File Name	C:\DOCS\OUTPUT_301\2021\12.溴赅狃黑BM-2400-1.C_002001r					***Frequency (MHz)***	100.61
Nucleus	13C	***Number of Transients***	186	***Original Points Count***	16384	***Points Count***	131072
Pulse Sequence	zgpg30	***Solvent***	CHLOROFORM-D			***Sweep Width (Hz)***	24154.59
Temperature (degree C)	27.000						



^{13}C NMR spectrum of **3i** (100.6 MHz, $CDCl_3$)

3 Aug 2022

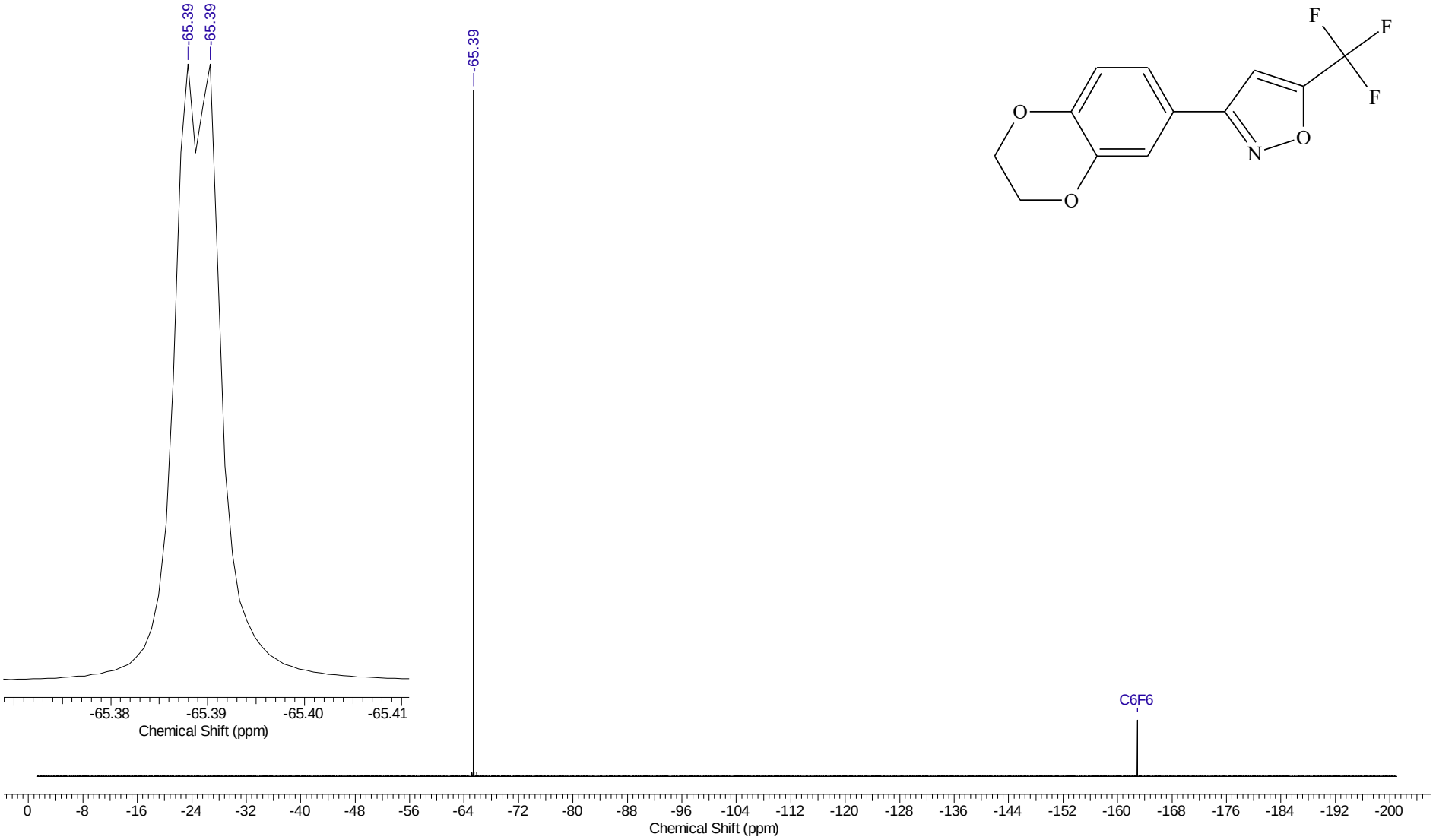
Acquisition Time (sec)	4.0894	***Comment***	Imported from UXNMR.			***Date***	12 Jul 2022 15:13:36
File Name	C:\BM_DATA\DOCS\12.07.22\12.07.22\SZA-BM-2554.H_001001r					***Frequency (MHz)***	400.13
Nucleus	1H	***Number of Transients***	4	***Original Points Count***	32768	***Points Count***	131072
Pulse Sequence	zg30	***Solvent***	CHLOROFORM-D			***Sweep Width (Hz)***	8012.82
Temperature (degree C)	27.000						



^{1}H NMR spectrum of **3k** (400.1 MHz, $CDCl_3$)

3 Aug 2022

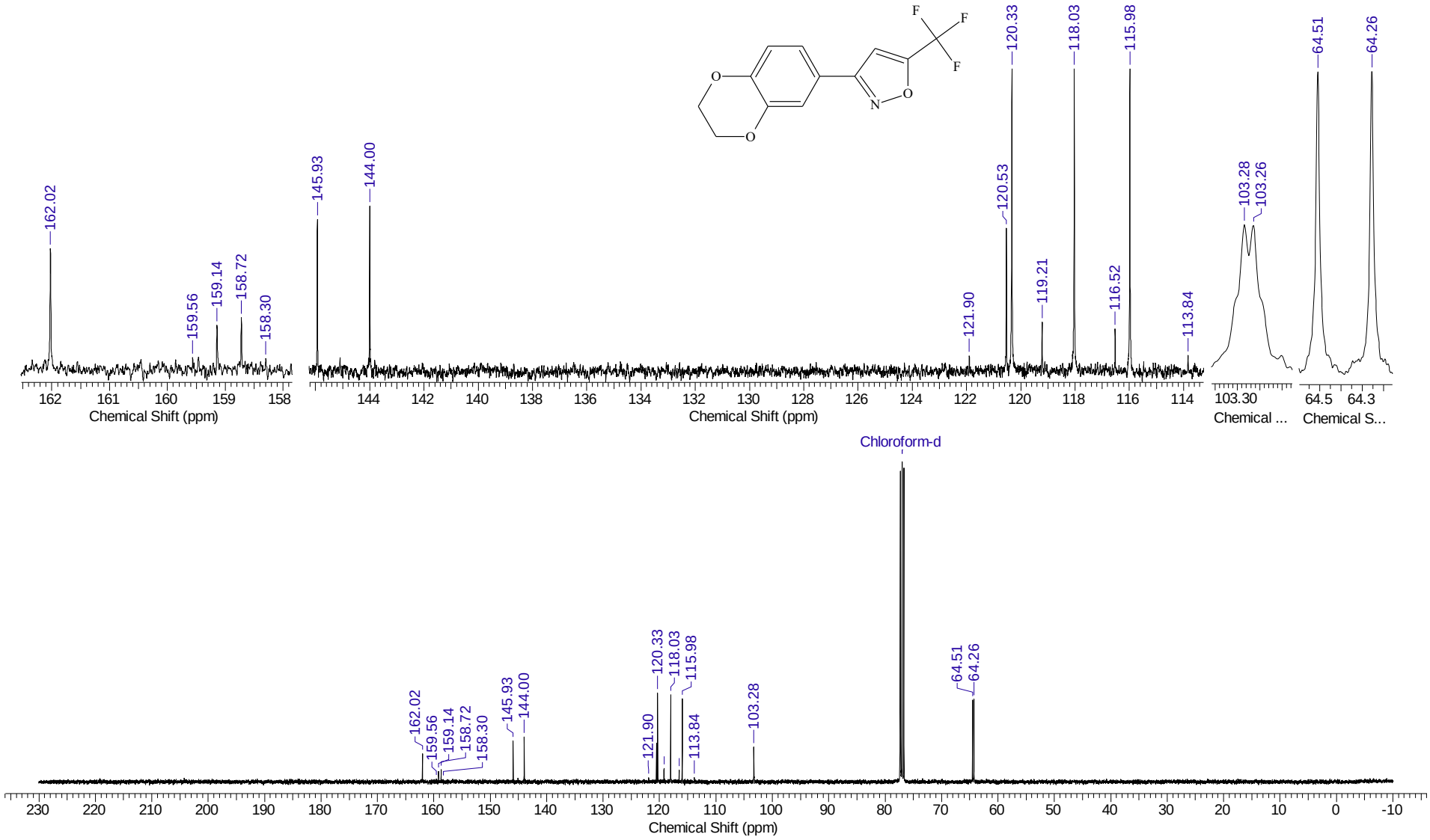
Acquisition Time (sec)	1.7433	***Comment***	Imported from UXNMR.			***Date***	12 Jul 2022 15:17:18
File Name	C:\BM_DATA\DOCS\12.07.22\12.07.22\SZA-BM-2554.F_005001r					***Frequency (MHz)***	376.50
Nucleus	19F	***Number of Transients***	16	***Original Points Count***	131072	***Points Count***	262144
Pulse Sequence	zgflqn	***Solvent***	CHLOROFORM-D			***Sweep Width (Hz)***	75187.97
Temperature (degree C)	27.000						



^{19}F NMR spectrum of **3k** (376.5 MHz, $CDCl_3$)

3 Aug 2022

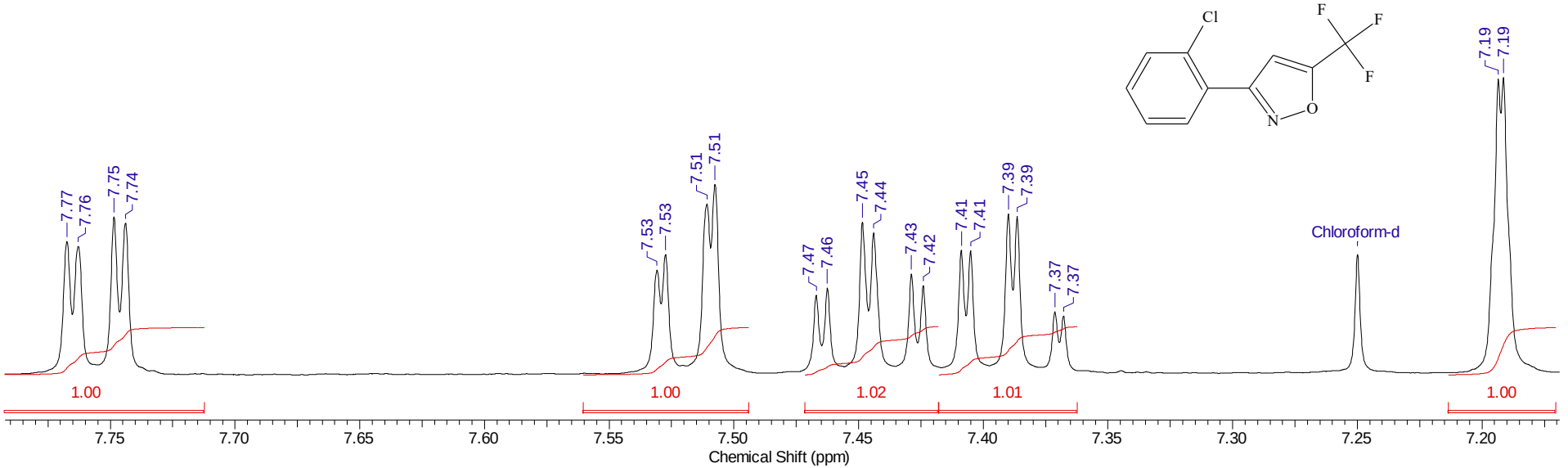
Acquisition Time (sec)	0.6783	***Comment***	Imported from UXNMR.			***Date***	14 Jul 2022 15:58:04
File Name	C:\BM_DATA\DOCS\14.07.22\14.07.22\SZA-BM-2554.C_002001r					***Frequency (MHz)***	100.61
Nucleus	13C	***Number of Transients***	1154	***Original Points Count***	16384	***Points Count***	131072
Pulse Sequence	zgpg30	***Solvent***	CHLOROFORM-D			***Sweep Width (Hz)***	24154.59
Temperature (degree C)	27.000						

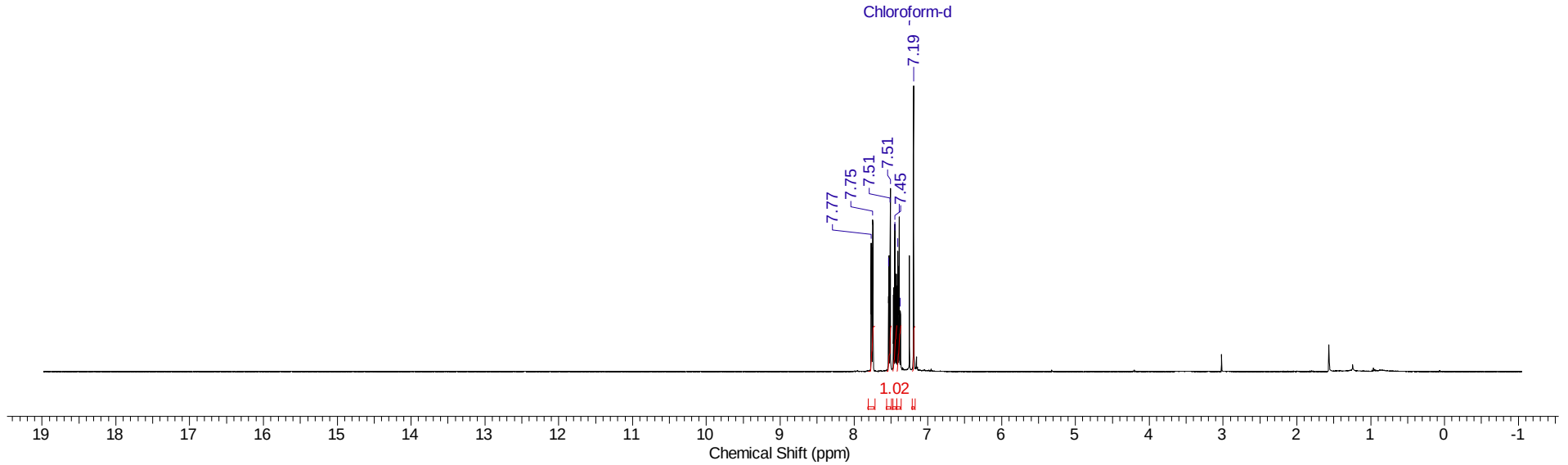


^{13}C NMR spectrum of **3k** (100.6 MHz, $CDCl_3$)

3 Aug 2022

Acquisition Time (sec)	4.0894	***Comment***	Imported from UXNMR.			***Date***	17 Jan 2022 15:12:28
File Name	C:\DOCS\OUTPUT_301\2022\01. 磯囧黑BM-2401.H_001001r					***Frequency (MHz)***	400.13
Nucleus	1H	***Number of Transients***	4	***Original Points Count***	32768	***Points Count***	131072
Pulse Sequence	zg30	***Solvent***	BENZENE-D6	***Sweep Width (Hz)***	8012.82	***Temperature (degree C)***	27.000

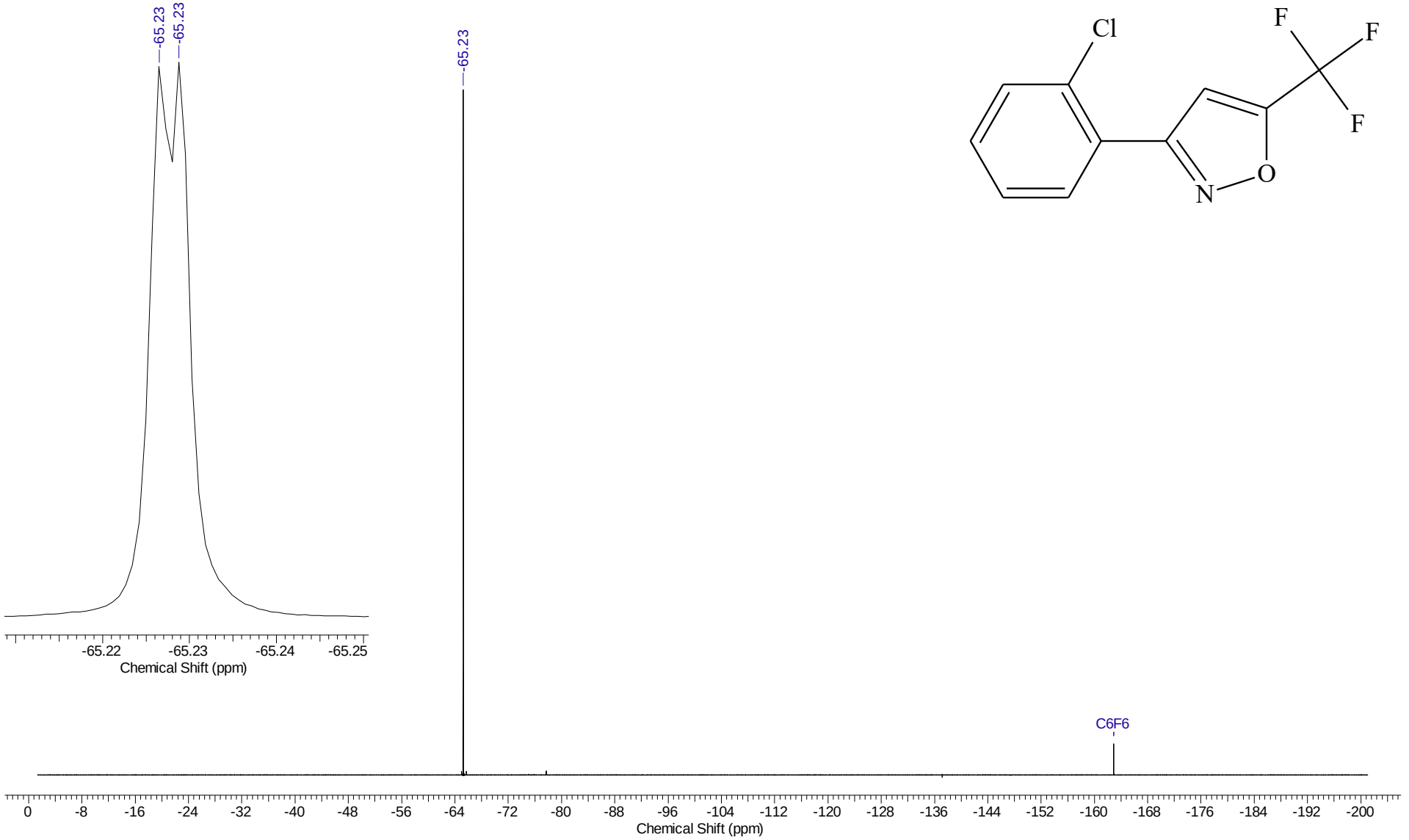




^{1}H NMR spectrum of **3l** (400.1 MHz, $CDCl_3$)

3 Aug 2022

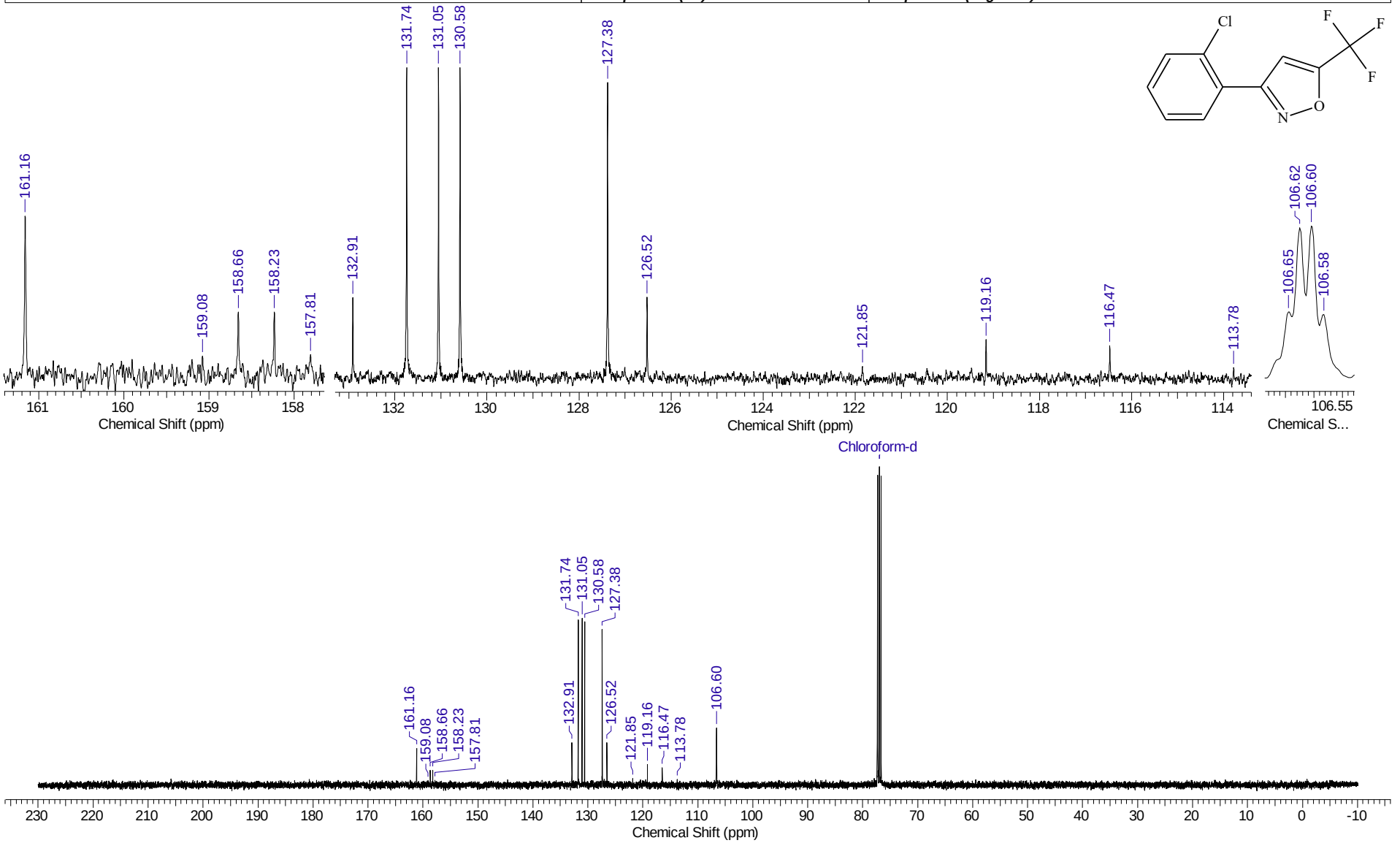
Acquisition Time (sec)	1.7433	***Comment***	Imported from UXNMR.			***Date***	17 Jan 2022 15:28:34
File Name	C:\DOCS\OUTPUT_301\2022\01. 磯囧黒BM-2401.F_005001r			***Frequency (MHz)***	376.50	***Nucleus***	19F
Number of Transients	13	***Original Points Count***	131072	***Points Count***	262144	***Pulse Sequence***	zgflqn
Solvent	CHLOROFORM-D			***Sweep Width (Hz)***	75187.97	***Temperature (degree C)***	27.000



^{19}F NMR spectrum of **3l** (376.5 MHz, $CDCl_3$)

3 Aug 2022

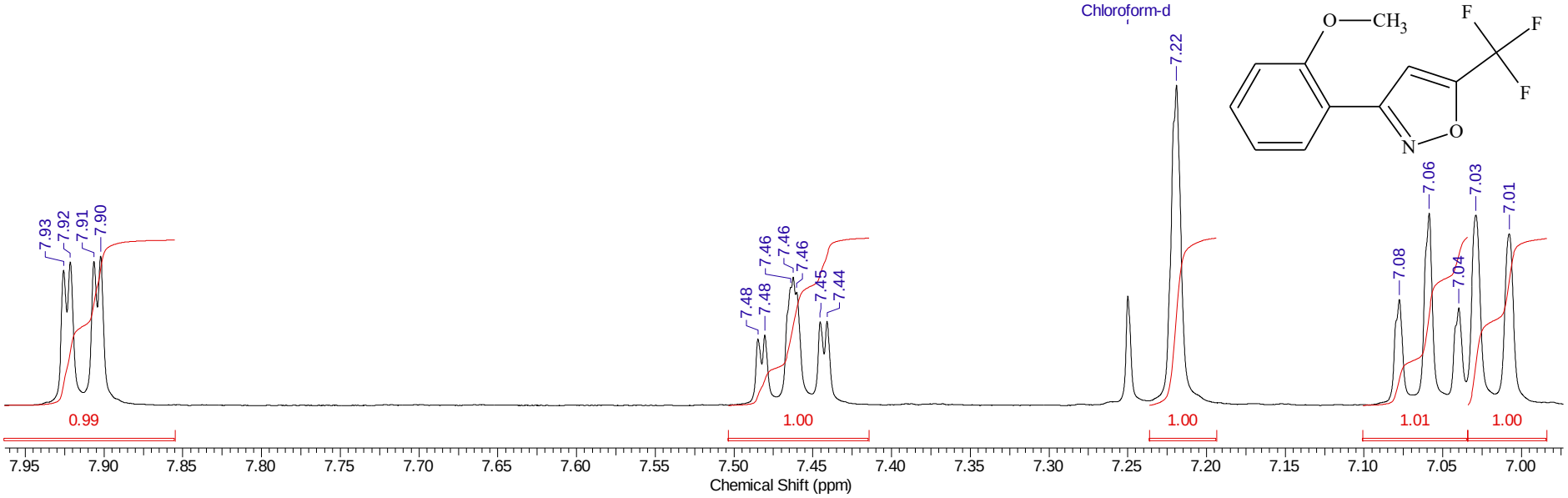
Acquisition Time (sec)	0.6783	***Comment***	Imported from UXNMR.			***Date***	18 Jan 2022 16:05:08
File Name	C:\DOCS\OUTPUT_301\2022\01. 磯囪黒BM-2401.C_002001r			***Frequency (MHz)***	100.61	***Nucleus***	13C
Number of Transients	364	***Original Points Count***	16384	***Points Count***	131072	***Pulse Sequence***	zgpg30
Solvent	CHLOROFORM-D			***Sweep Width (Hz)***	24154.59	***Temperature (degree C)***	27.000

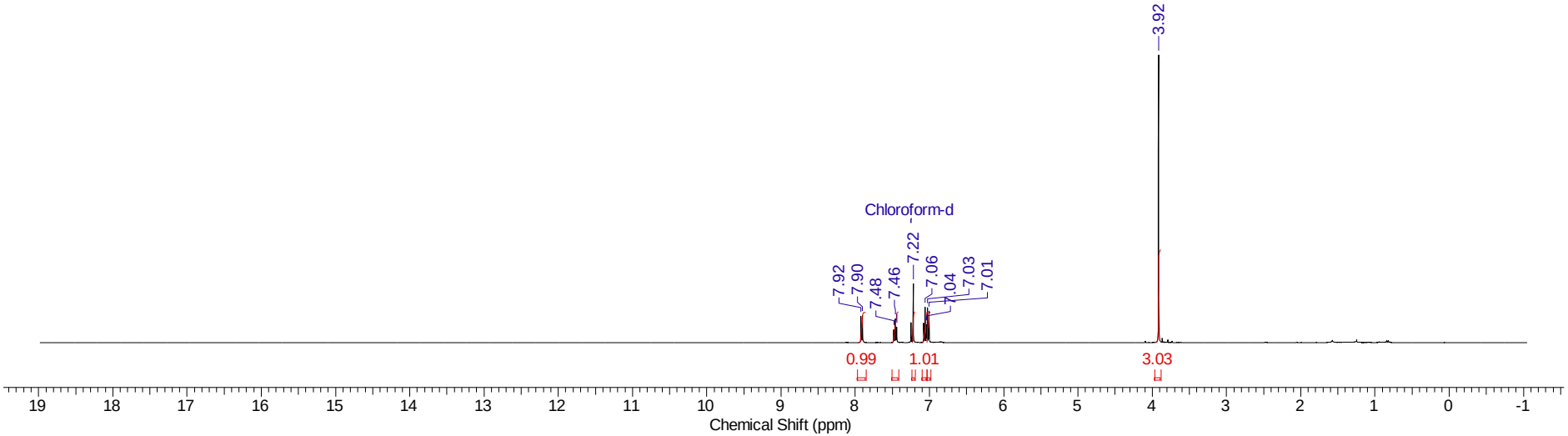


^{13}C NMR spectrum of **3l** (100.6 MHz, $CDCl_3$)

3 Aug 2022

Acquisition Time (sec)	4.0894	***Comment***	Imported from UXNMR.			***Date***	19 Jan 2022 17:43:48
File Name	C:\DOCS\OUTPUT_301\2022\01. 磯囧黒BM-2403-p.H_001001r					***Frequency (MHz)***	400.13
Nucleus	1H	***Number of Transients***	4	***Original Points Count***	32768	***Points Count***	131072
Pulse Sequence	zg30	***Solvent***	BENZENE-D6	***Sweep Width (Hz)***	8012.82	***Temperature (degree C)***	27.000

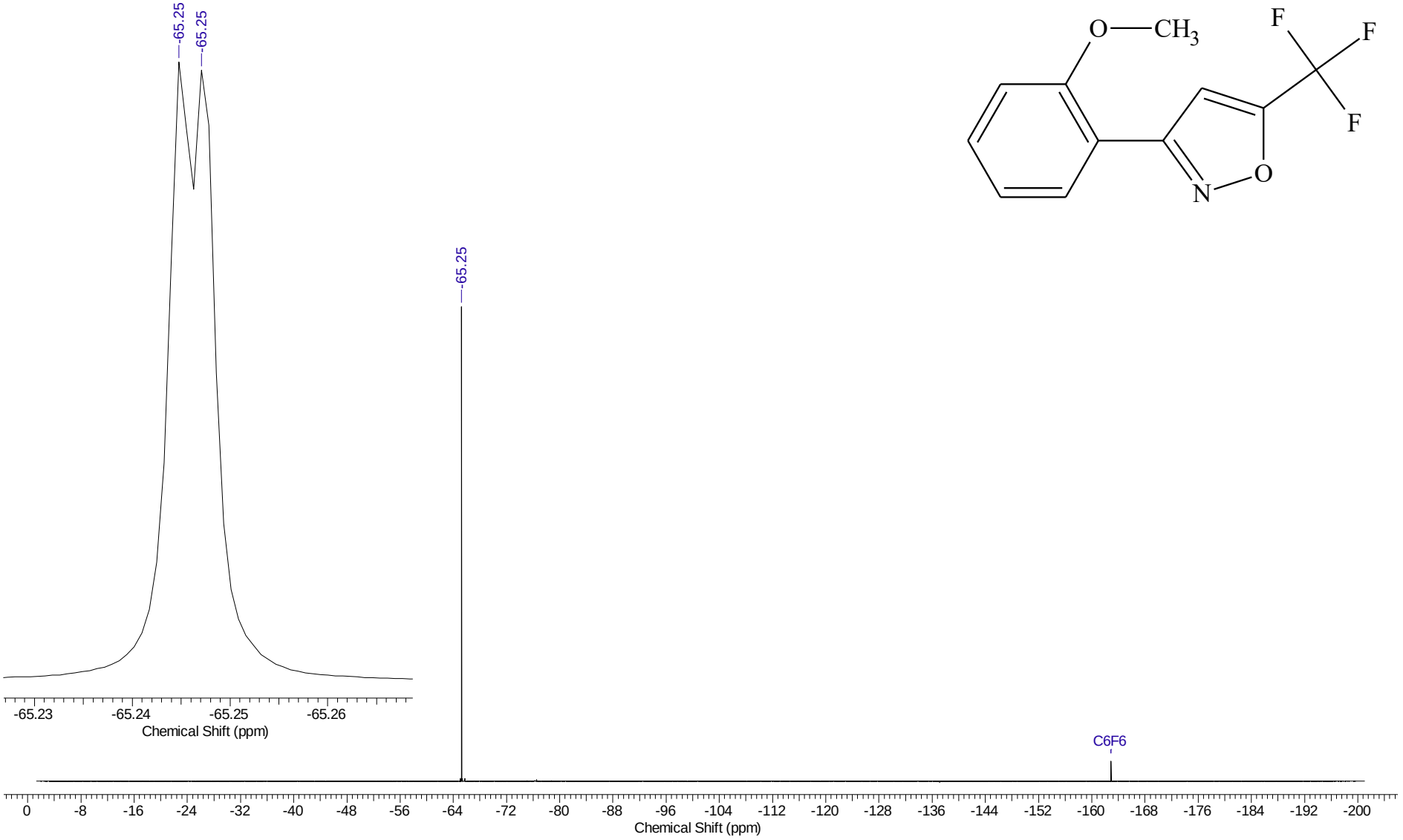




^{1}H NMR spectrum of **3m** (400.1 MHz, $CDCl_3$)

3 Aug 2022

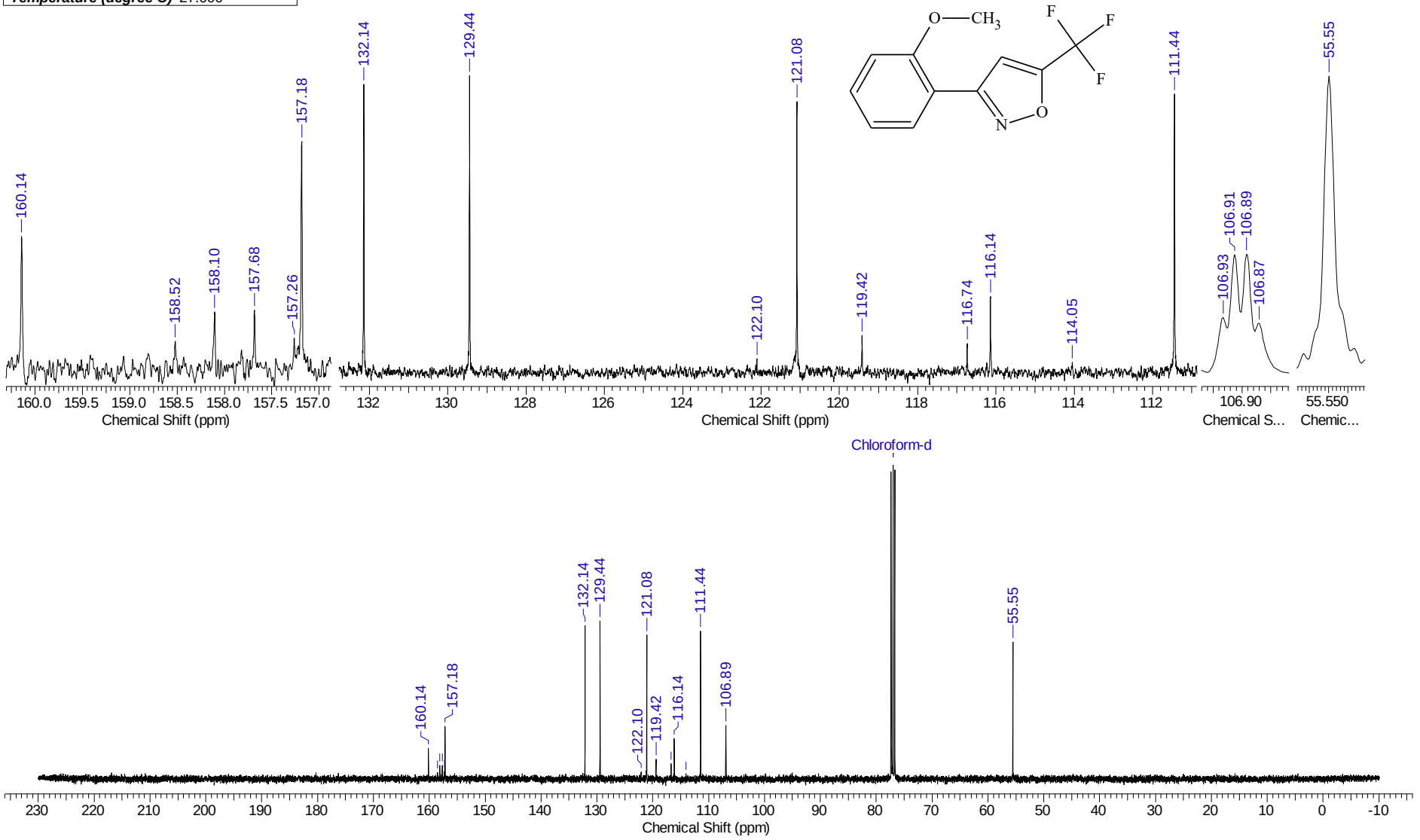
Acquisition Time (sec)	1.7433	***Comment***	Imported from UXNMR.			***Date***	17 Jan 2022 15:32:46
File Name	C:\DOCS\OUTPUT_301\2022\01. 磯囪黒BM-2403.F_005001r			***Frequency (MHz)***	376.50	***Nucleus***	19F
Number of Transients	12	***Original Points Count***	131072	***Points Count***	262144	***Pulse Sequence***	zgflqn
Solvent	CHLOROFORM-D			***Sweep Width (Hz)***	75187.97	***Temperature (degree C)***	27.000



^{19}F NMR spectrum of **3m** (376.5 MHz, $CDCl_3$)

3 Aug 2022

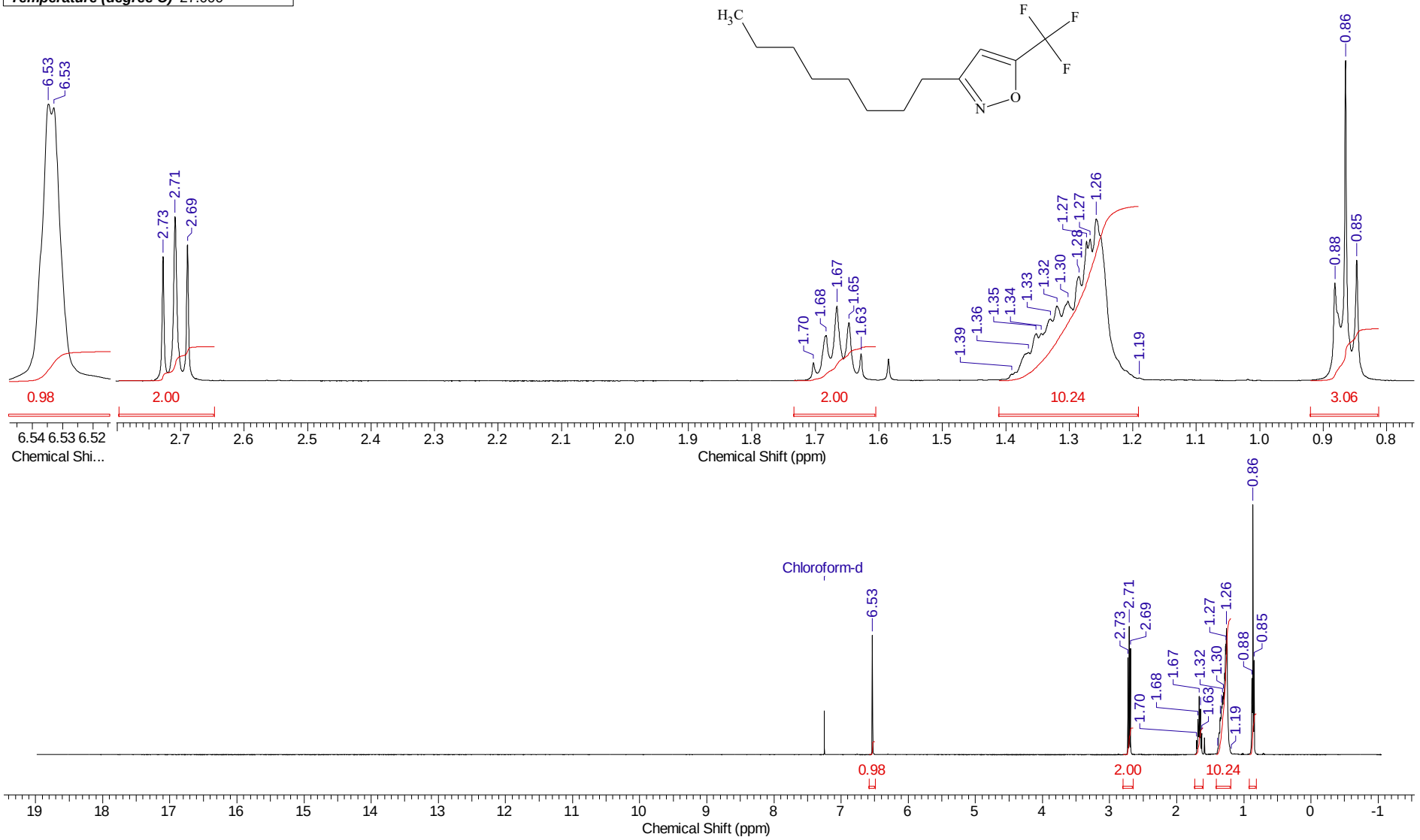
Acquisition Time (sec)	0.6783	***Comment***	Imported from UXNMR.			***Date***	20 Jan 2022 12:24:22
File Name	C:\DOCS\OUTPUT_301\2022\01. 磯囧黒BM-2403-p.C_002001r					***Frequency (MHz)***	100.61
Nucleus	13C	***Number of Transients***	351	***Original Points Count***	16384	***Points Count***	131072
Pulse Sequence	zgpg30	***Solvent***	CHLOROFORM-D			***Sweep Width (Hz)***	24154.59
Temperature (degree C)	27.000						



^{13}C NMR spectrum of **3m** (100.6 MHz, $CDCl_3$)

3 Aug 2022

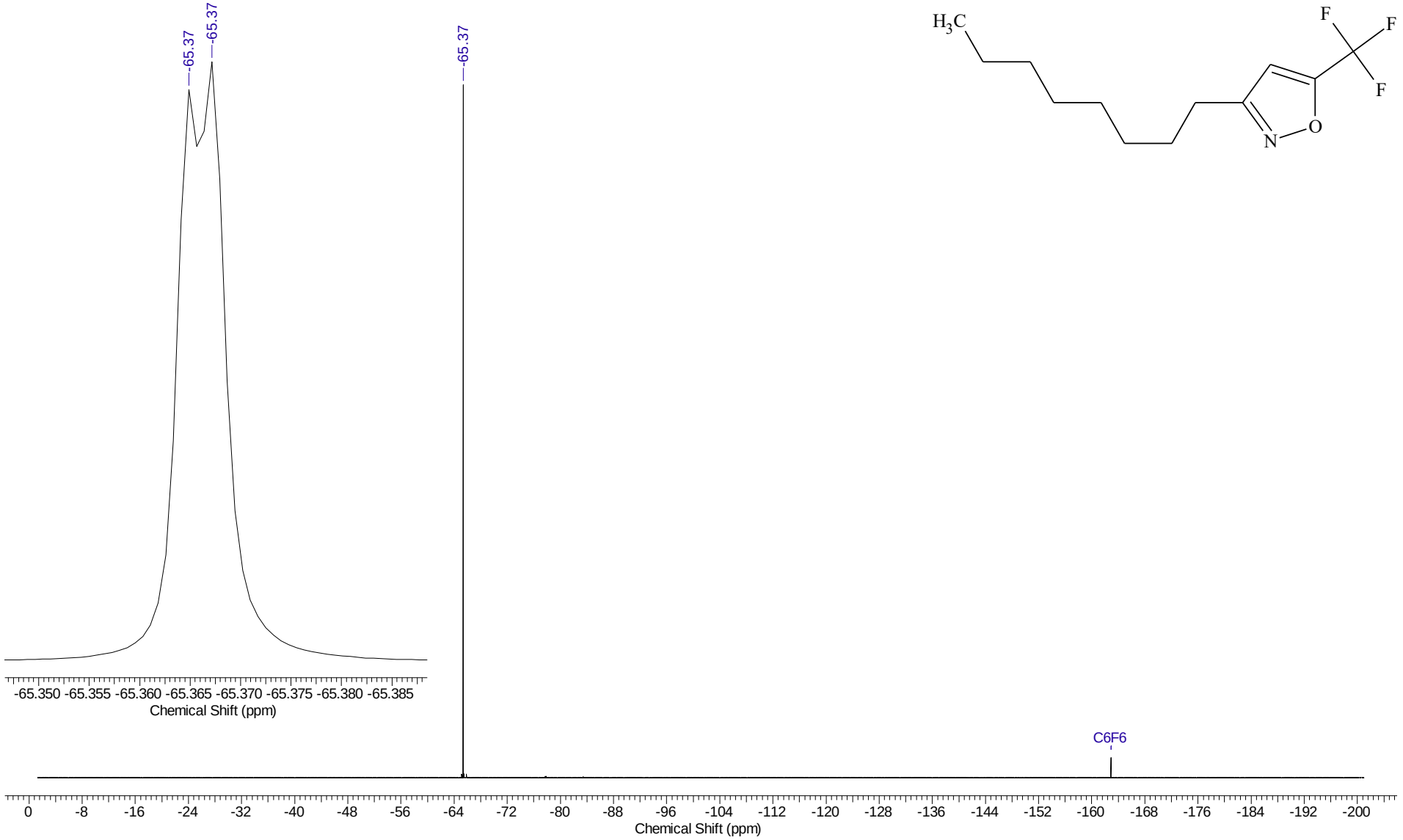
Acquisition Time (sec)	4.0894	***Comment***	Imported from UXNMR.			***Date***	21 Jan 2022 15:00:58
File Name	C:\DOCS\OUTPUT_301\2022\01. 磯囪黒BM-2412-1.H_001001r					***Frequency (MHz)***	400.13
Nucleus	1H	***Number of Transients***	4	***Original Points Count***	32768	***Points Count***	131072
Pulse Sequence	zg30	***Solvent***	CHLOROFORM-D			***Sweep Width (Hz)***	8012.82
Temperature (degree C)	27.000						



^{1}H NMR spectrum of **3o** (400.1 MHz, $CDCl_3$)

3 Aug 2022

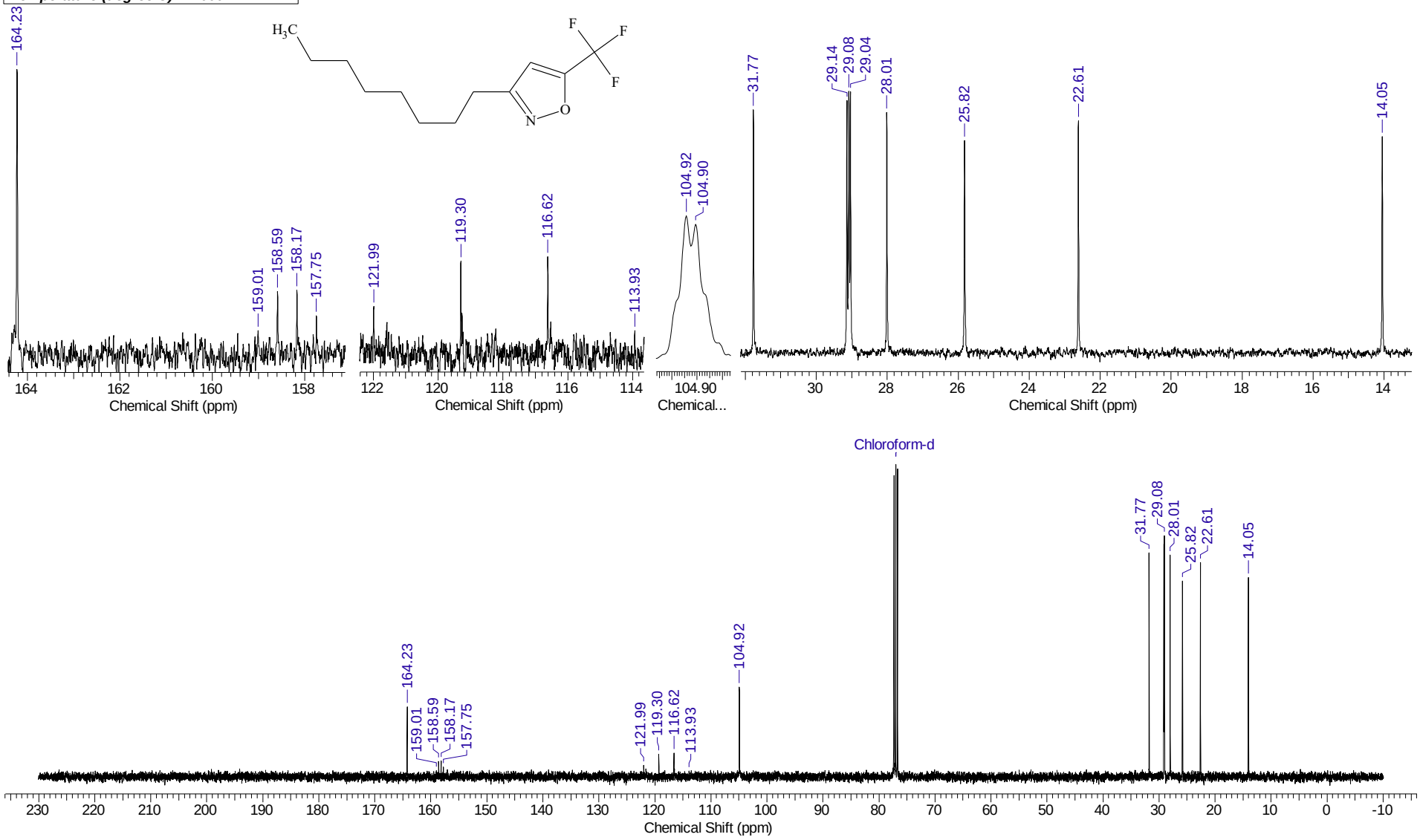
Acquisition Time (sec)	1.7433	***Comment***	Imported from UXNMR.			***Date***	21 Jan 2022 15:20:12
File Name	C:\DOCS\OUTPUT_301\2022\01. 磯囧黒BM-2412-1.F_005001r					***Frequency (MHz)***	376.50
Nucleus	19F	***Number of Transients***	8	***Original Points Count***	131072	***Points Count***	262144
Pulse Sequence	zgflqn	***Solvent***	Acetone	***Sweep Width (Hz)***	75187.97	***Temperature (degree C)***	27.000



^{19}F NMR spectrum of **3o** (376.5 MHz, $CDCl_3$)

3 Aug 2022

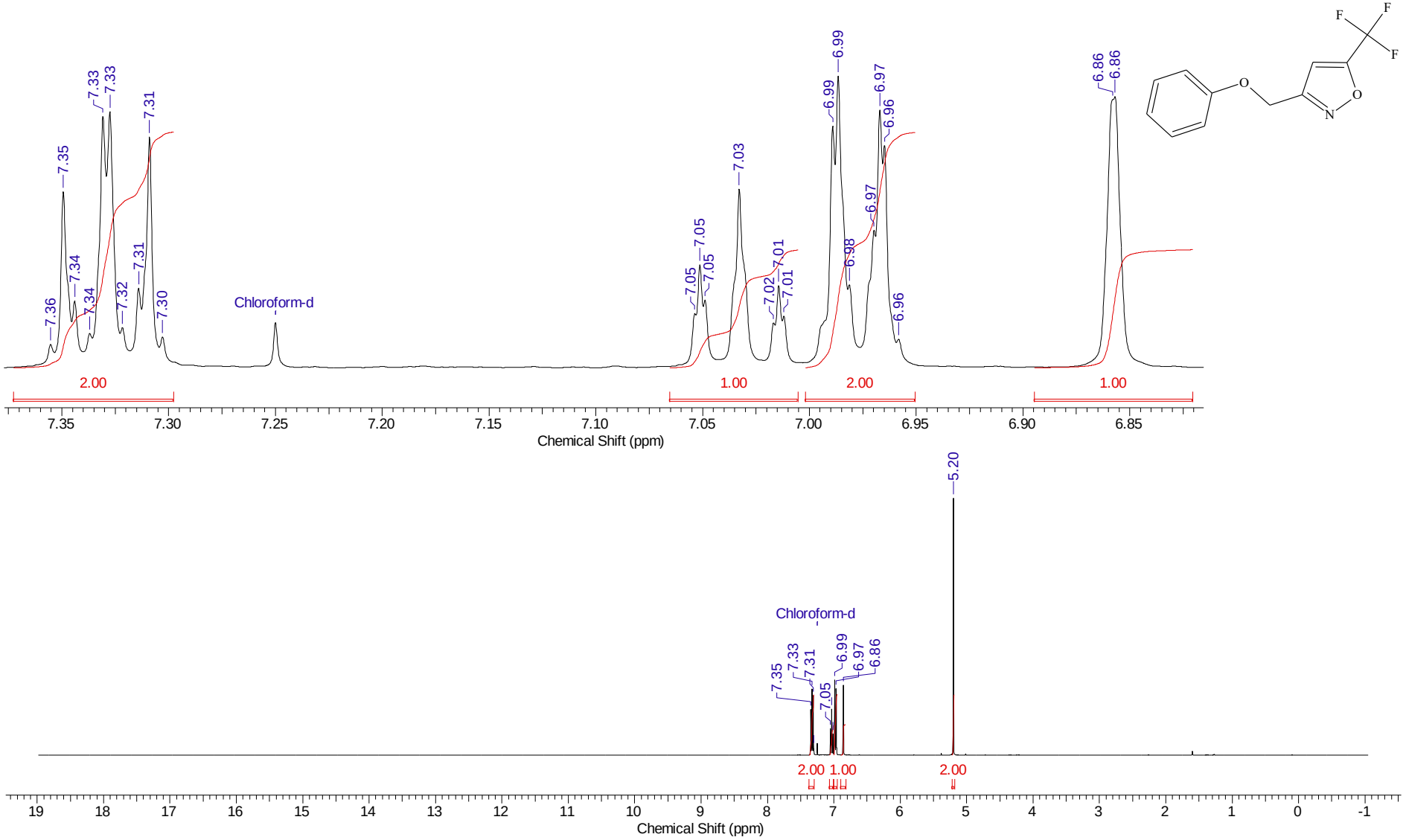
Acquisition Time (sec)	0.6783	***Comment***	Imported from UXNMR.			***Date***	24 Jan 2022 14:48:52
File Name	C:\DOCS\OUTPUT_301\2022\01. 磯囪黒BM-2412-1.C_002001r					***Frequency (MHz)***	100.61
Nucleus	13C	***Number of Transients***	257	***Original Points Count***	16384	***Points Count***	131072
Pulse Sequence	zgpg30	***Solvent***	CHLOROFORM-D			***Sweep Width (Hz)***	24154.59
Temperature (degree C)	27.000						



^{13}C NMR spectrum of **3o** (100.6 MHz, $CDCl_3$)

3 Aug 2022

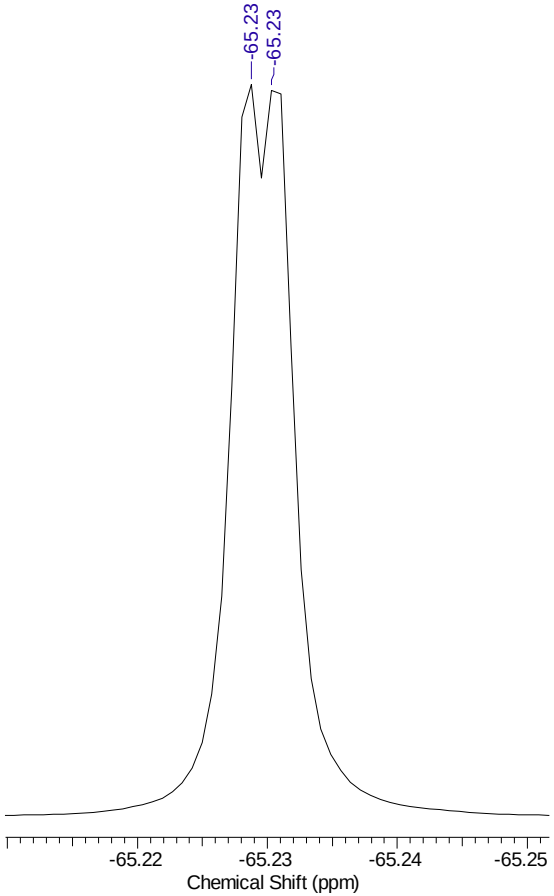
Acquisition Time (sec)	4.0894	***Comment***	Imported from UXNMR.			***Date***	20 Jan 2022 12:26:24
File Name	C:\DOCS\OUTPUT_301\2022\01. 磯囪黒BM-2411-1.H_001001r					***Frequency (MHz)***	400.13
Nucleus	1H	***Number of Transients***	4	***Original Points Count***	32768	***Points Count***	131072
Pulse Sequence	zg30	***Solvent***	BENZENE-D6	***Sweep Width (Hz)***	8012.82	***Temperature (degree C)***	27.000

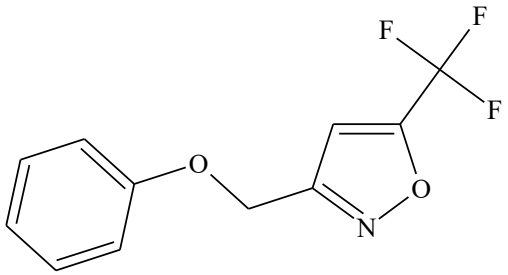


^{1}H NMR spectrum of **3p** (400.1 MHz, $CDCl_3$)

3 Aug 2022

Acquisition Time (sec)	1.7433	***Comment***	Imported from UXNMR.			***Date***	20 Jan 2022 13:02:40
File Name	C:\DOCS\OUTPUT_301\2022\01. 磯囧黒BM-2411-1.F_005001r					***Frequency (MHz)***	376.50
Nucleus	19F	***Number of Transients***	16	***Original Points Count***	131072	***Points Count***	262144
Pulse Sequence	zgflqn	***Solvent***	Acetone	***Sweep Width (Hz)***	75187.97	***Temperature (degree C)***	27.000

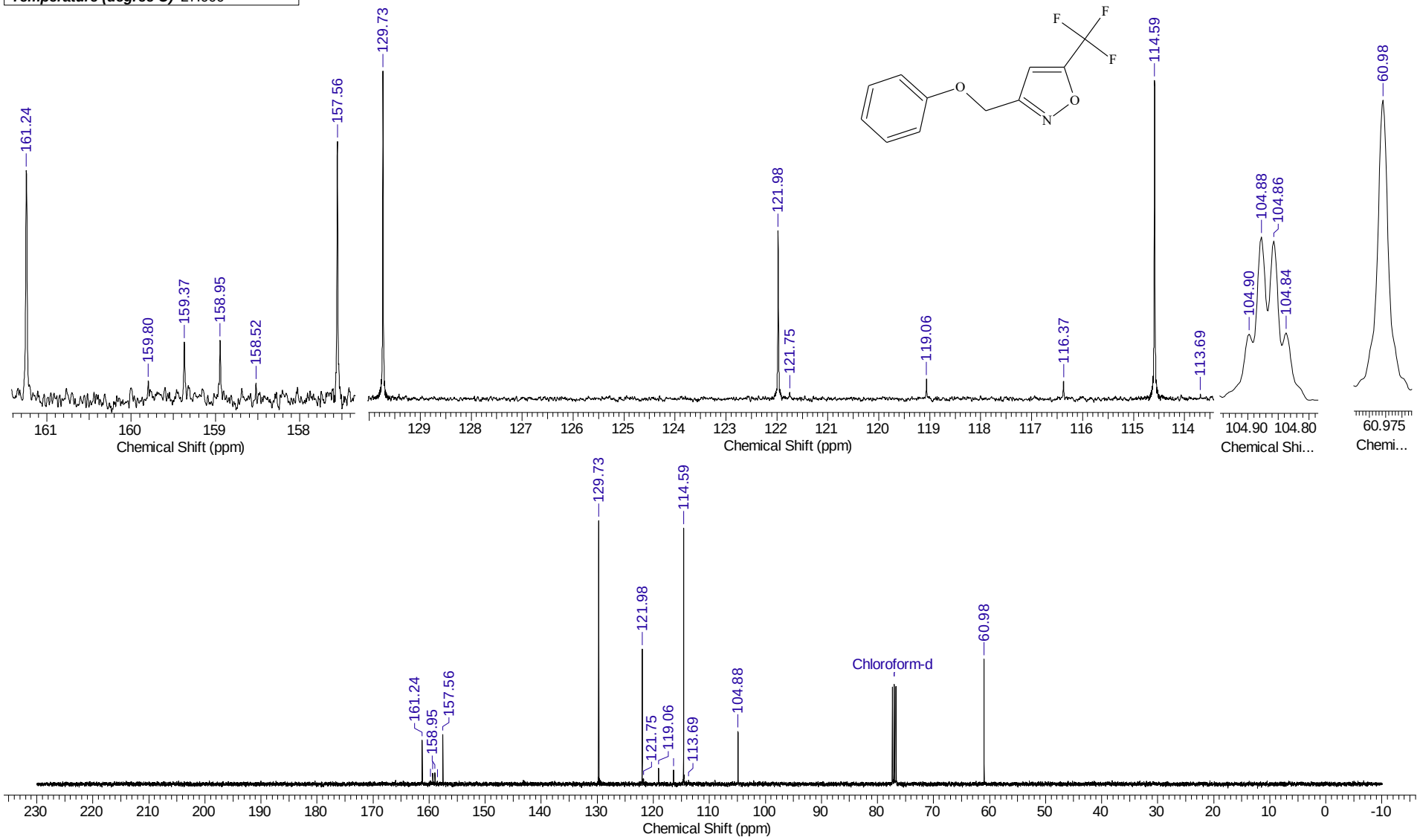




^{19}F NMR spectrum of **3p** (376.5 MHz, $CDCl_3$)

3 Aug 2022

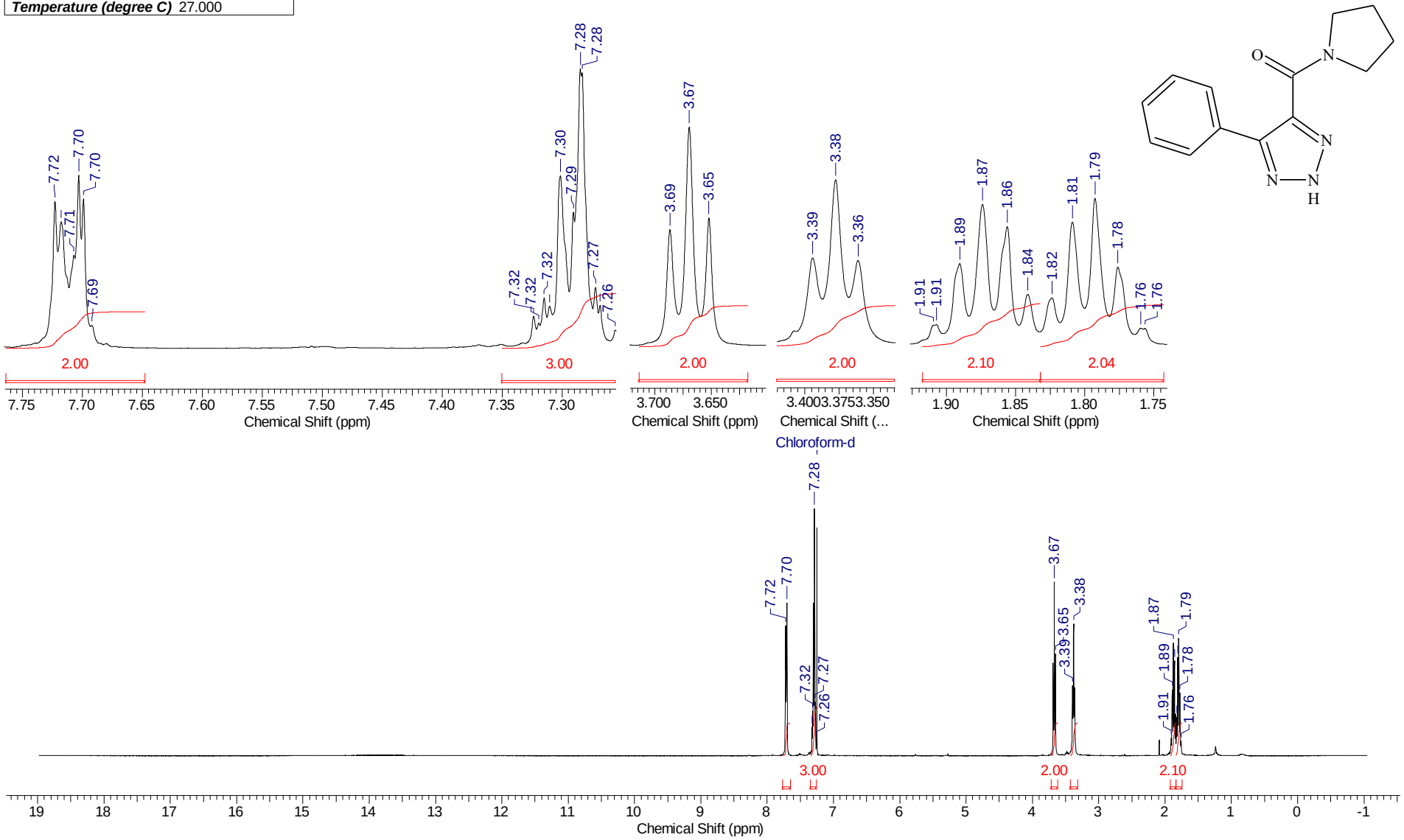
Acquisition Time (sec)	0.6783	***Comment***	Imported from UXNMR.			***Date***	20 Jan 2022 12:31:36
File Name	C:\DOCS\OUTPUT_301\2022\01. 磯囧黒BM-2411-1.C_002001r					***Frequency (MHz)***	100.61
Nucleus	13C	***Number of Transients***	106	***Original Points Count***	16384	***Points Count***	131072
Pulse Sequence	zgpg30	***Solvent***	CHLOROFORM-D			***Sweep Width (Hz)***	24154.59
Temperature (degree C)	27.000						



^{13}C NMR spectrum of **3p** (100.6 MHz, $CDCl_3$)

20 May 2022

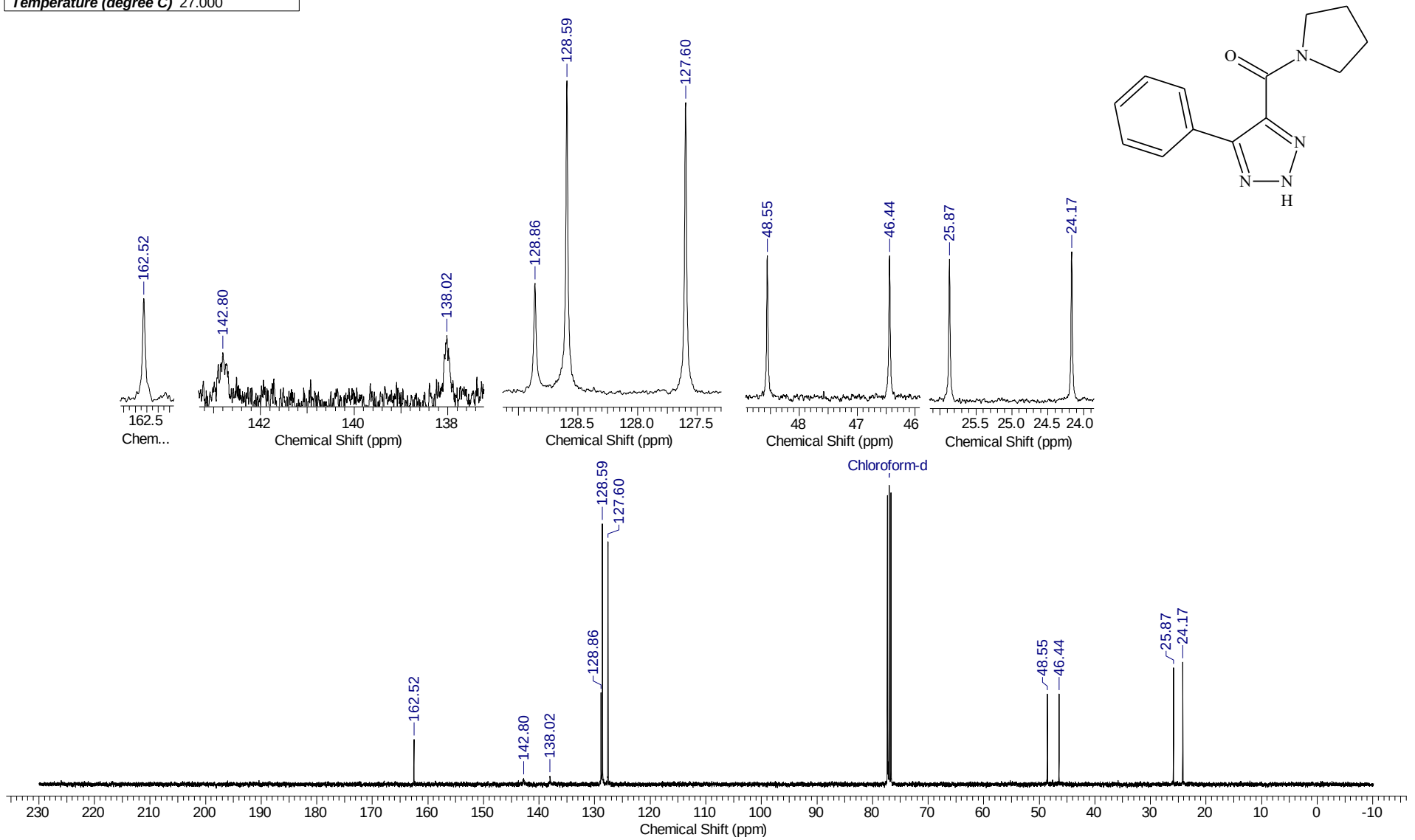
Acquisition Time (sec)	4.0894	***Comment***	Imported from UXNMR.			***Date***	08 Feb 2022 22:22:36
File Name	C:\DOCS\BM\吖 齁盐 雅 娜 \2022\BM-2447-3\BM-2447-3_001001r					***Frequency (MHz)***	400.13
Nucleus	1H	***Number of Transients***	8	***Original Points Count***	32768	***Points Count***	131072
Pulse Sequence	zg30	***Solvent***	CHLOROFORM-D			***Sweep Width (Hz)***	8012.82
Temperature (degree C)	27.000						



^{1}H NMR spectrum of **4** (400.1 MHz, $CDCl_3$)

20 May 2022

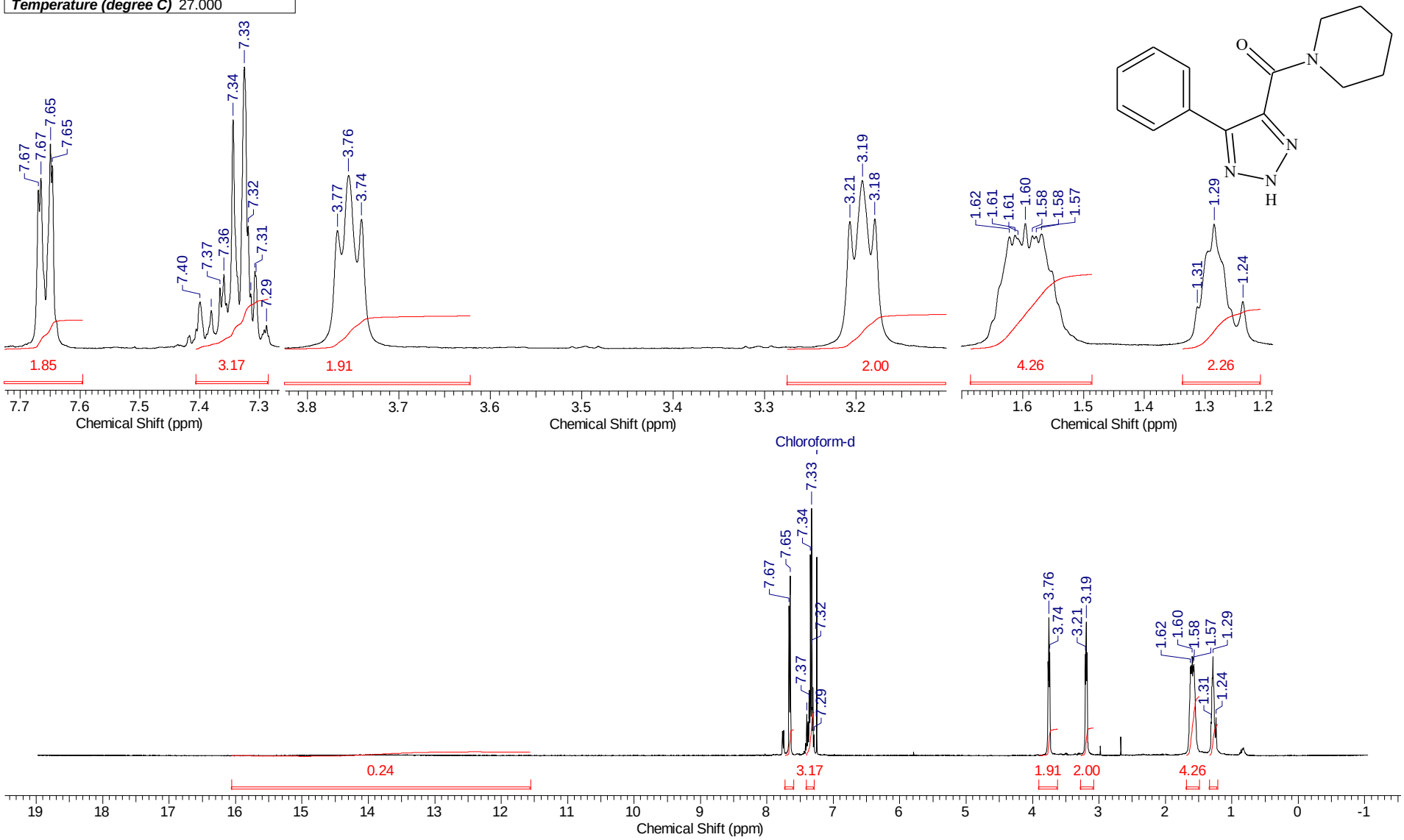
Acquisition Time (sec)	0.6783	***Comment***	Imported from UXNMR.			***Date***	08 Feb 2022 22:50:58
File Name	C:\DOCS\BM\吲 峪盐 雅 娜 \2022\BM-2447-3\BM-2447-3_002001r					***Frequency (MHz)***	100.61
Nucleus	13C	***Number of Transients***	648	***Original Points Count***	16384	***Points Count***	131072
Pulse Sequence	zgpg30	***Solvent***	CHLOROFORM-D			***Sweep Width (Hz)***	24154.59
Temperature (degree C)	27.000						



^{13}C NMR spectrum of **4** (100.6 MHz, $CDCl_3$)

20 May 2022

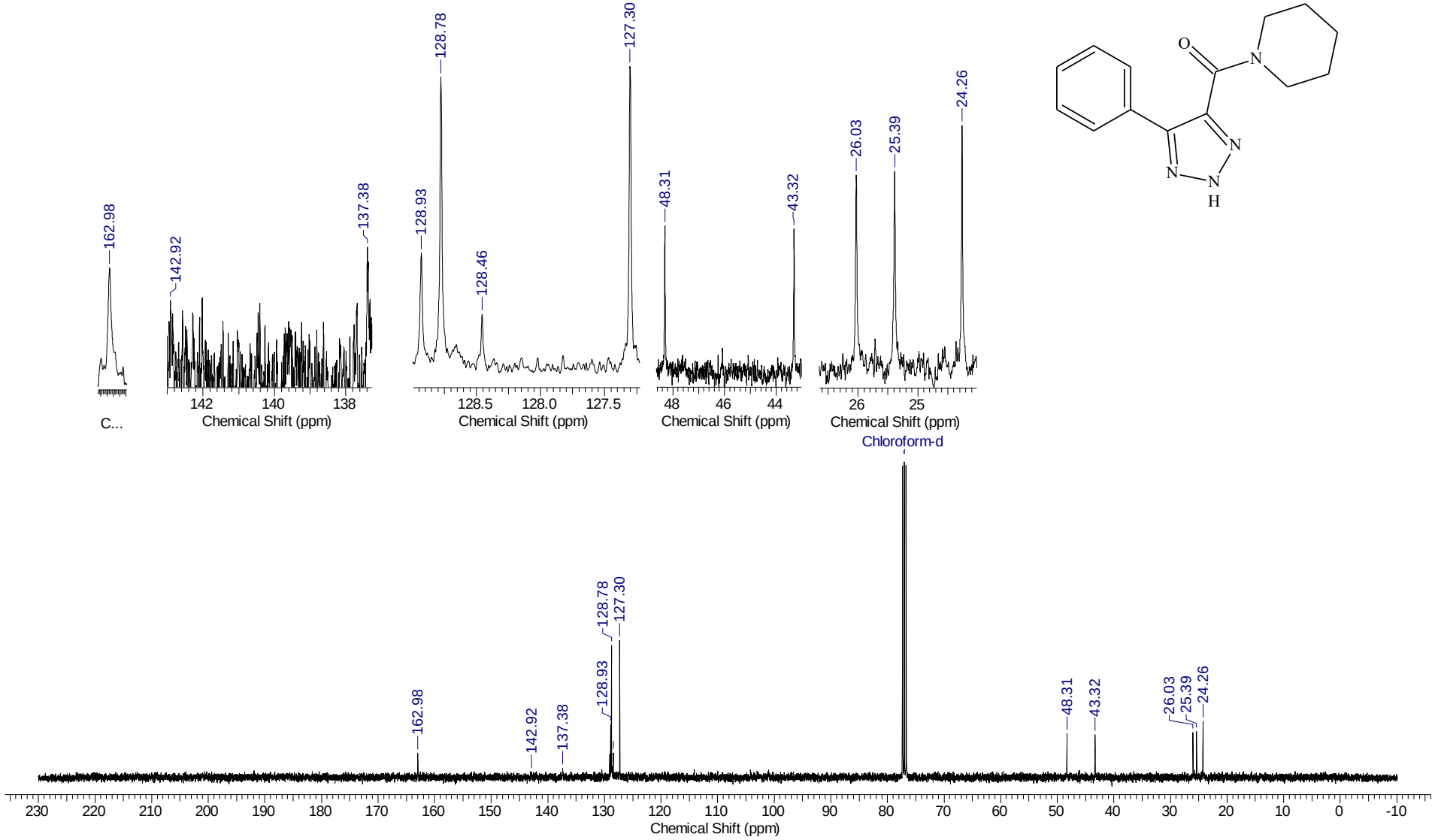
Acquisition Time (sec)	4.0894	***Comment***	Imported from UXNMR.			***Date***	09 Mar 2022 22:11:46
File Name	C:\DOCS\BM\吟 峪盐 雅 娜 \2022\BM-2449-2p\BM-2449-2p_001001r					***Frequency (MHz)***	400.13
Nucleus	1H	***Number of Transients***	8	***Original Points Count***	32768	***Points Count***	131072
Pulse Sequence	zg30	***Solvent***	CHLOROFORM-D			***Sweep Width (Hz)***	8012.82
Temperature (degree C)	27.000						



^{1}H NMR spectrum of **5** (400.1 MHz, $CDCl_3$)

20 May 2022

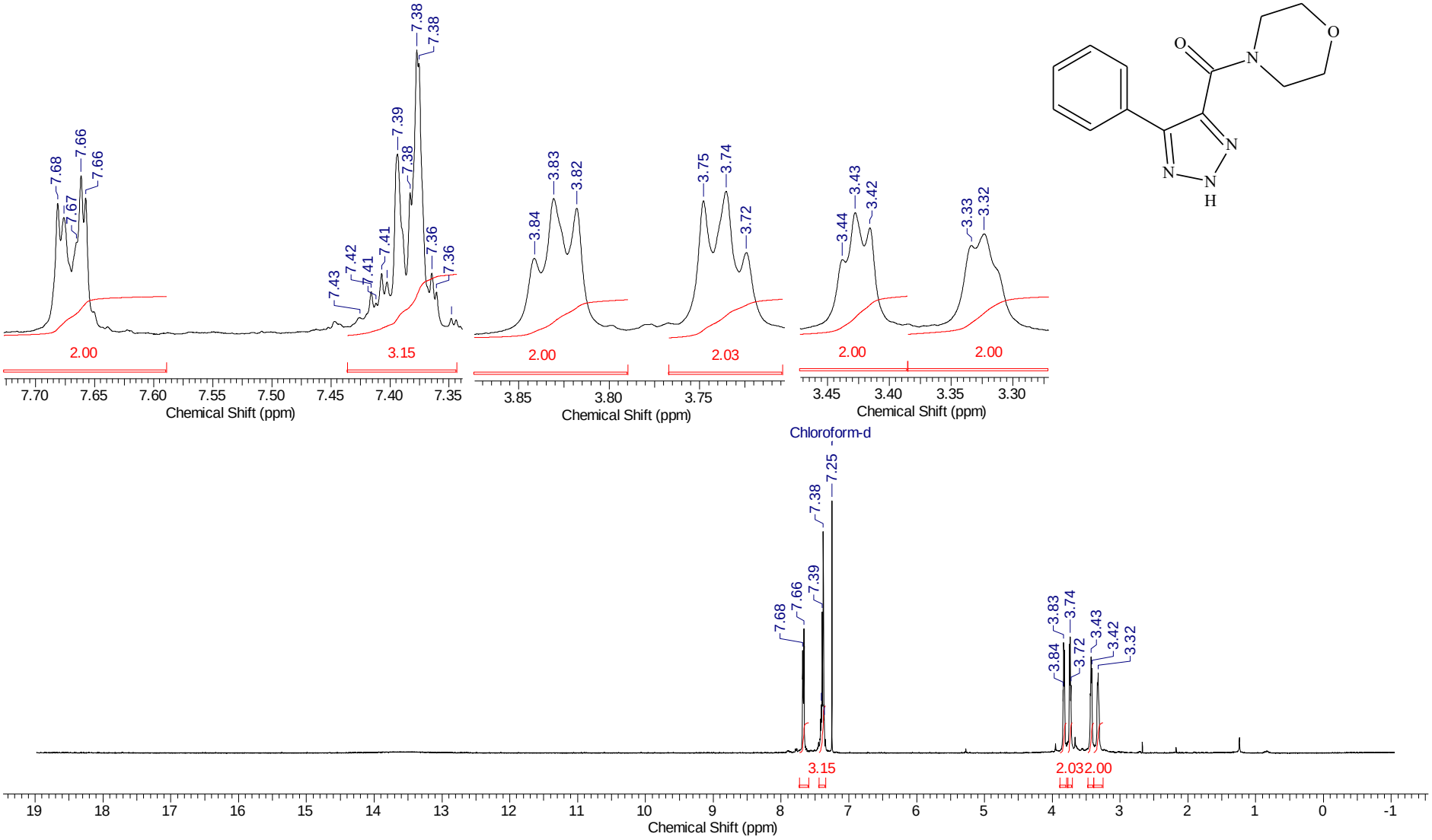
Acquisition Time (sec)	0.6783	***Comment***	Imported from UXNMR.			***Date***	10 Mar 2022 12:24:32
File Name	C:\DOCS\OUTPUT_301\2022\03.爨 痱\BM-2449-2p.C_002001r					***Frequency (MHz)***	100.61
Nucleus	13C	***Number of Transients***	244	***Original Points Count***	16384	***Points Count***	131072
Pulse Sequence	zgpg30	***Solvent***	ACETONITRILE-D3			***Sweep Width (Hz)***	24154.59
Temperature (degree C)	27.000						



^{13}C NMR spectrum of **5** (100.6 MHz, $CDCl_3$)

20 May 2022

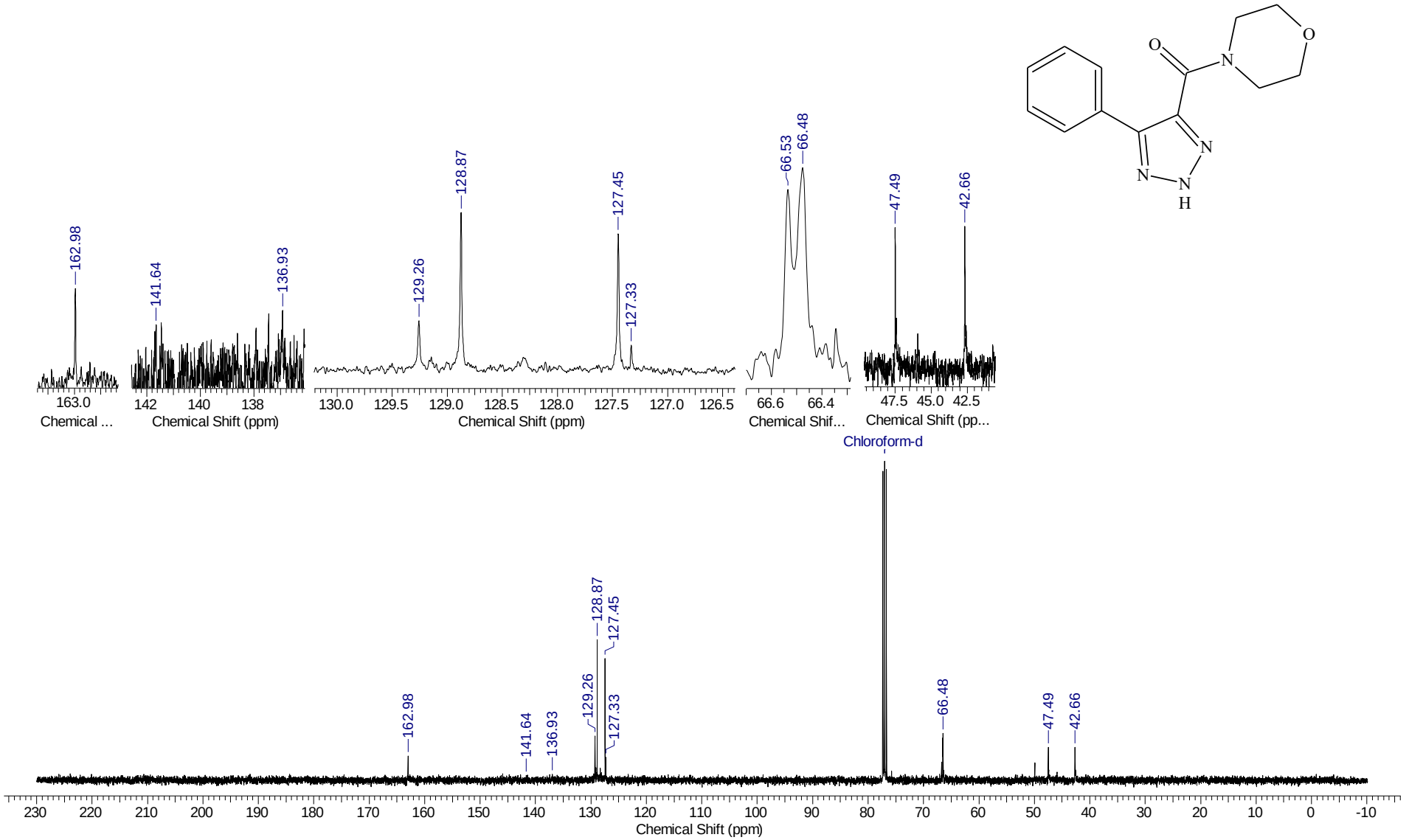
Acquisition Time (sec)	4.0894	***Comment***	Imported from UXNMR.			***Date***	12 Mar 2022 23:41:18
File Name	C:\DOCS\BM\吁 鄂盐 雅 娜 \2022\BM-2450\BM-2450_001001r					***Frequency (MHz)***	400.13
Nucleus	1H	***Number of Transients***	8	***Original Points Count***	32768	***Points Count***	131072
Pulse Sequence	zg30	***Solvent***	CHLOROFORM-D			***Sweep Width (Hz)***	8012.82
Temperature (degree C)	27.000						



^{1}H NMR spectrum of **6** (400.1 MHz, $CDCl_3$)

20 May 2022

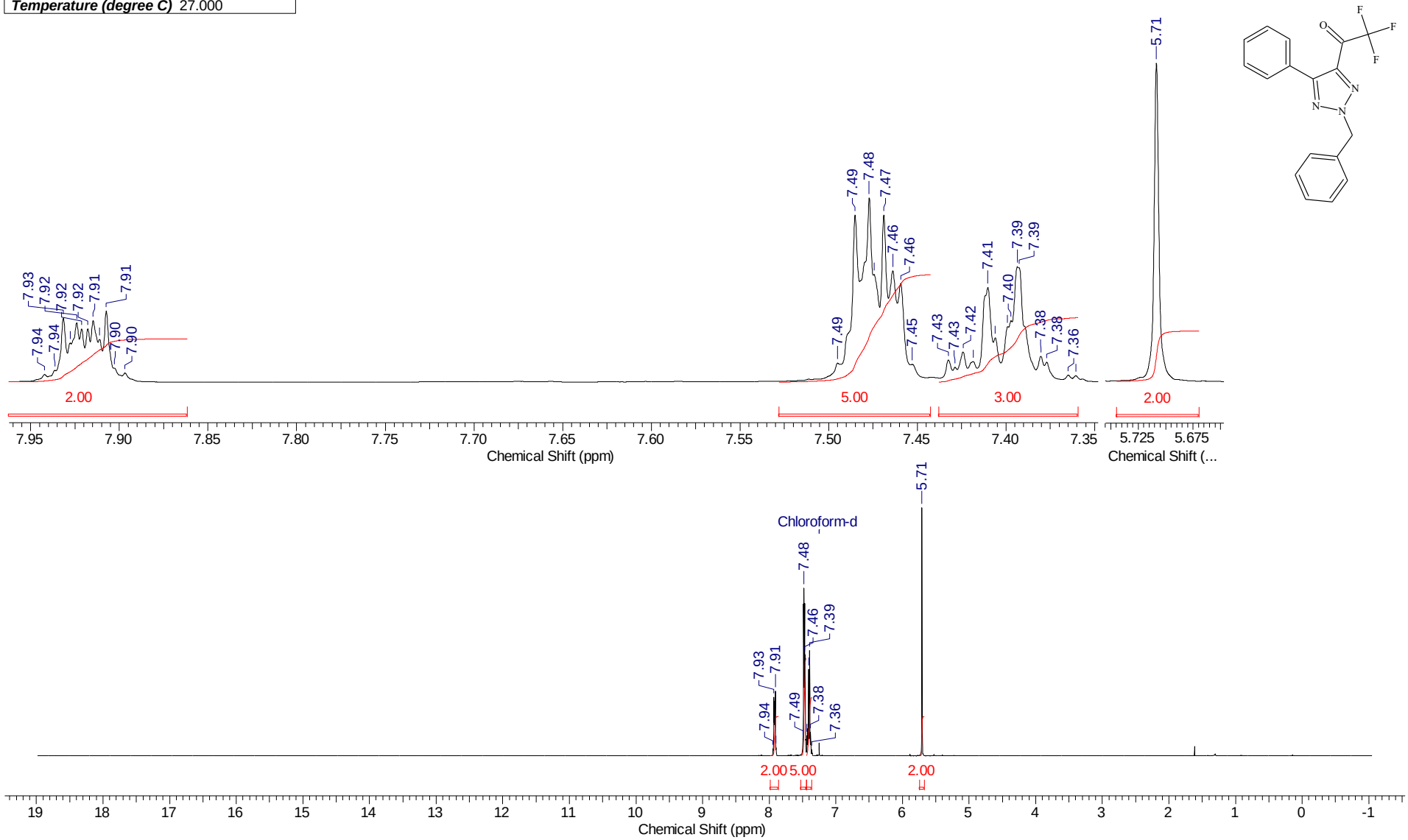
Acquisition Time (sec)	0.6783	***Comment***	Imported from UXNMR.			***Date***	14 Mar 2022 15:38:42
File Name	C:\DOCS\OUTPUT_301\2022\03.爨 痱\BM-2450-2.C_002001r					***Frequency (MHz)***	100.61
Nucleus	13C	***Number of Transients***	201	***Original Points Count***	16384	***Points Count***	131072
Pulse Sequence	zgpg30	***Solvent***	DMSO-D6	***Sweep Width (Hz)***	24154.59	***Temperature (degree C)***	27.000



^{13}C NMR spectrum of **6** (100.6 MHz, $CDCl_3$)

18 May 2022

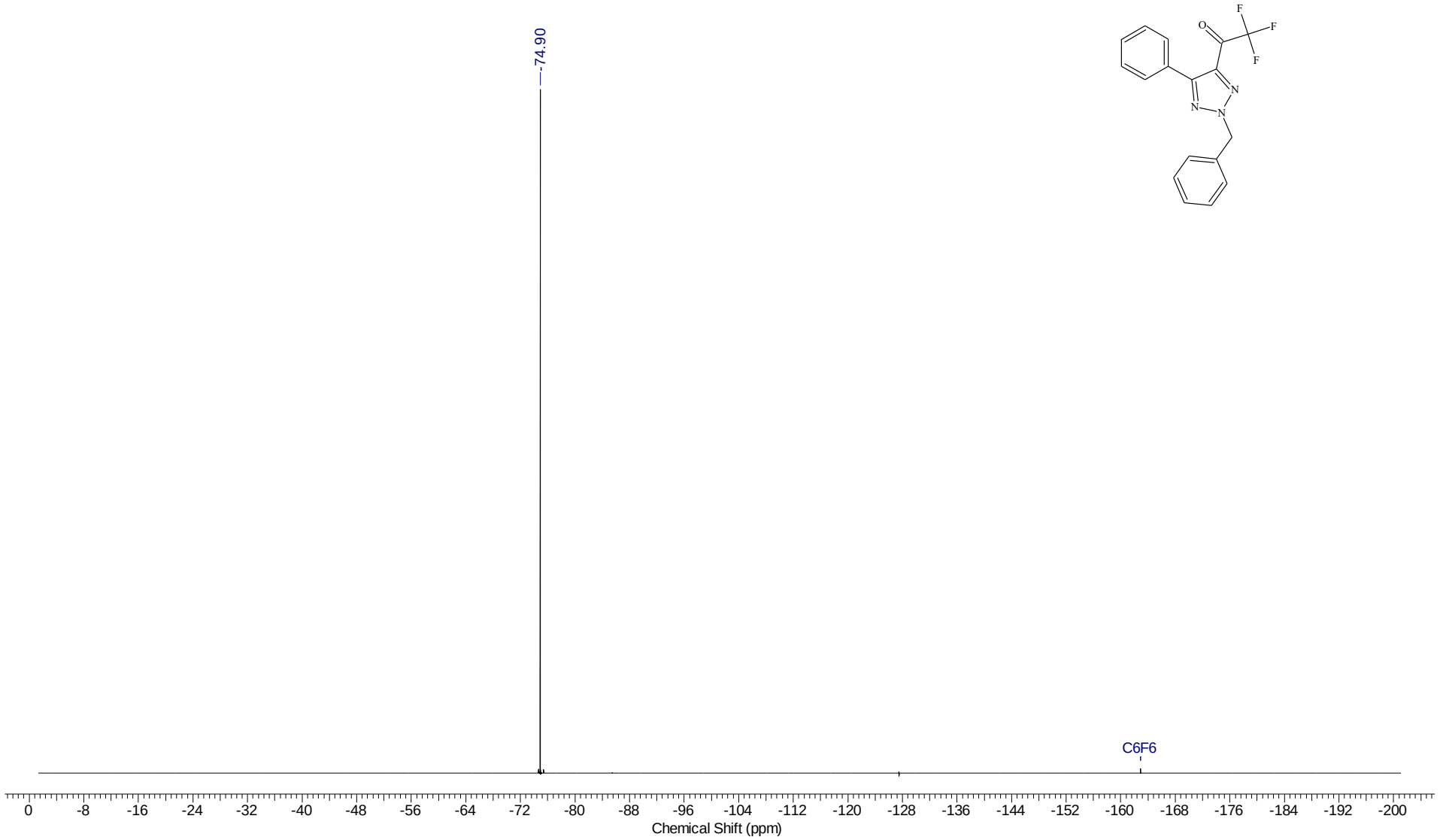
Acquisition Time (sec)	4.0894	***Comment***	Imported from UXNMR.			***Date***	29 Mar 2022 14:45:06
File Name	C:\DOCS\OUTPUT_301\2022\03.爨 菲\SZA-BM-2448-7.H.H_001001r					***Frequency (MHz)***	400.13
Nucleus	1H	***Number of Transients***	4	***Original Points Count***	32768	***Points Count***	131072
Pulse Sequence	zg30	***Solvent***	CHLOROFORM-D			***Sweep Width (Hz)***	8012.82
Temperature (degree C)	27.000						



^{1}H NMR spectrum of **7** (400.1 MHz, $CDCl_3$)

18 May 2022

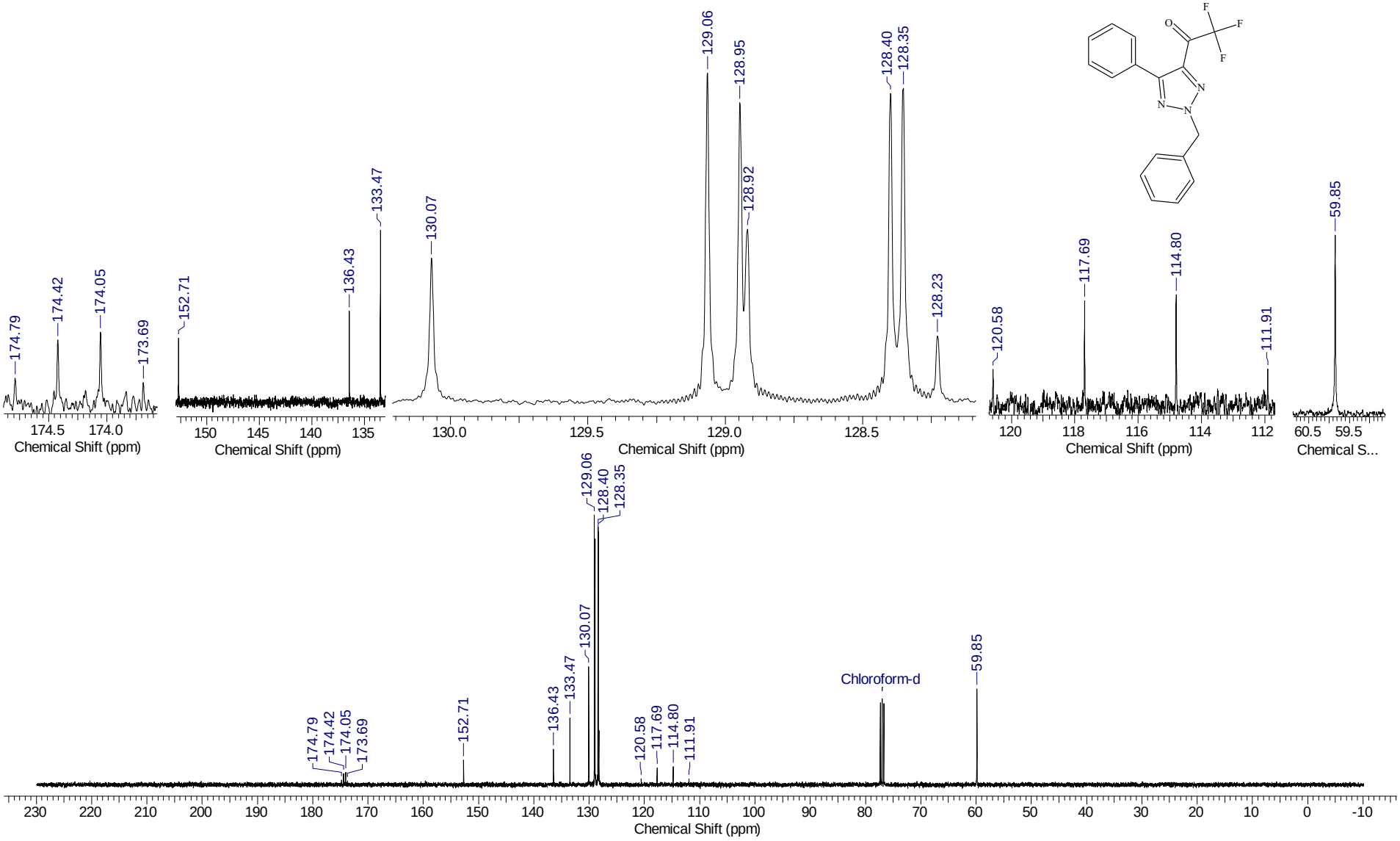
Acquisition Time (sec)	1.7433	***Comment***	Imported from UXNMR.			***Date***	29 Mar 2022 14:56:42
File Name	C:\DOCS\OUTPUT_301\2022\03.爨 痱\SZA-BM-2448-7.F_005001r					***Frequency (MHz)***	376.50
Nucleus	19F	***Number of Transients***	4	***Original Points Count***	131072	***Points Count***	262144
Pulse Sequence	zgflqn	***Solvent***	CHLOROFORM-D			***Sweep Width (Hz)***	75187.97
Temperature (degree C)	27.000						



^{19}F NMR spectrum of **7** (376.5 MHz, $CDCl_3$)

18 May 2022

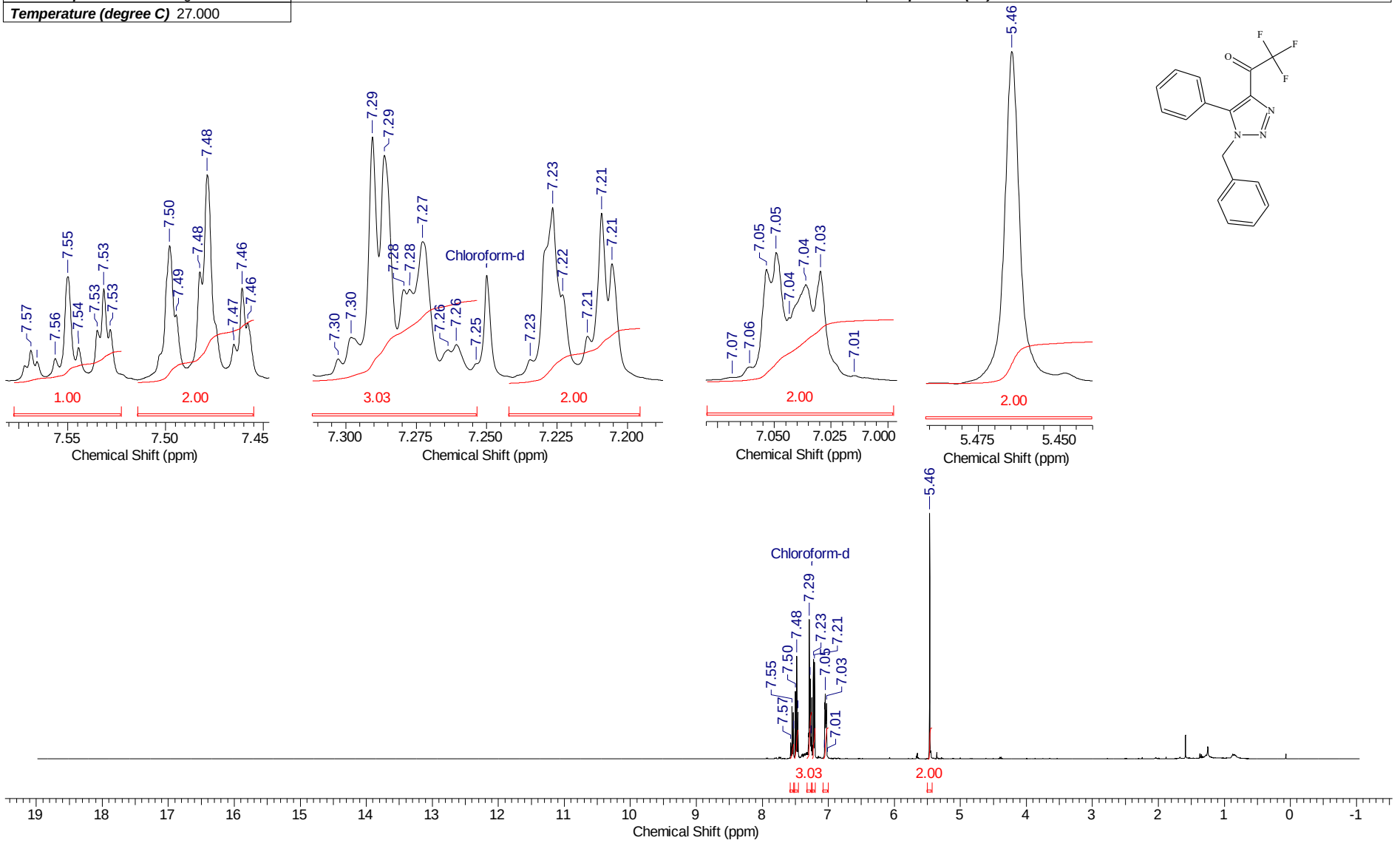
Acquisition Time (sec)	0.6783	***Comment***	Imported from UXNMR.			***Date***	31 Mar 2022 12:08:00
File Name	C:\DOCS\OUTPUT_301\2022\03.爨 痱\SZA-BM-2448-7.C_002001r					***Frequency (MHz)***	100.61
Nucleus	13C	***Number of Transients***	73	***Original Points Count***	16384	***Points Count***	131072
Pulse Sequence	zgpg30	***Solvent***	DMSO-D6	***Sweep Width (Hz)***	24154.59	***Temperature (degree C)***	27.000



^{13}C NMR spectrum of **7** (100.6 MHz, $CDCl_3$)

18 May 2022

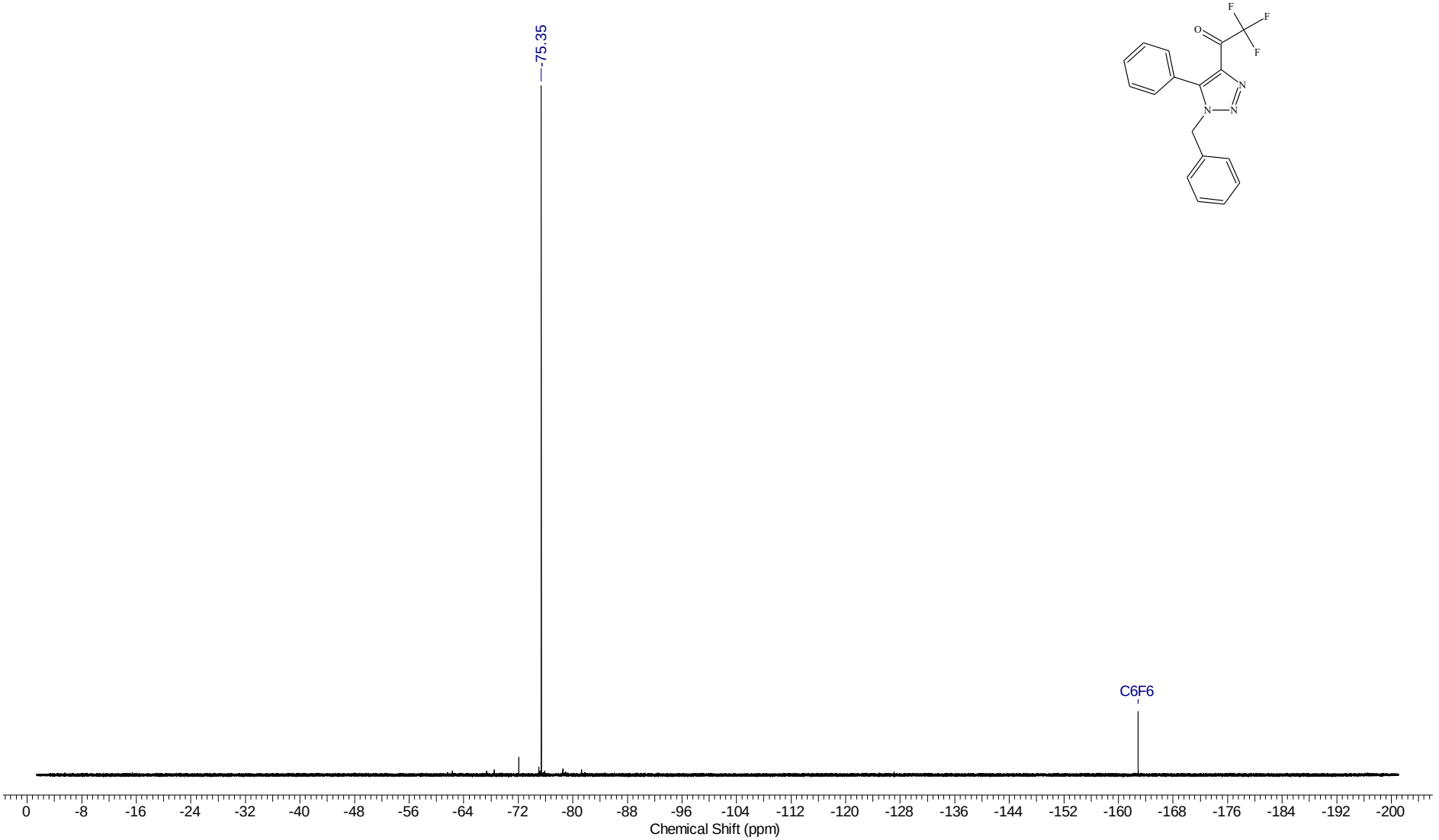
Acquisition Time (sec)	4.0894	***Comment***	Imported from UXNMR.			***Date***	30 Mar 2022 17:43:12
File Name	C:\DOCS\OUTPUT_301\2022\03.爨 痱\SZA-BM-2448-25.H_001001r					***Frequency (MHz)***	400.13
Nucleus	1H	***Number of Transients***	4	***Original Points Count***	32768	***Points Count***	131072
Pulse Sequence	zg30	***Solvent***	CHLOROFORM-D			***Sweep Width (Hz)***	8012.82
Temperature (degree C)	27.000						



^{1}H NMR spectrum of **8** (400.1 MHz, $CDCl_3$)

18 May 2022

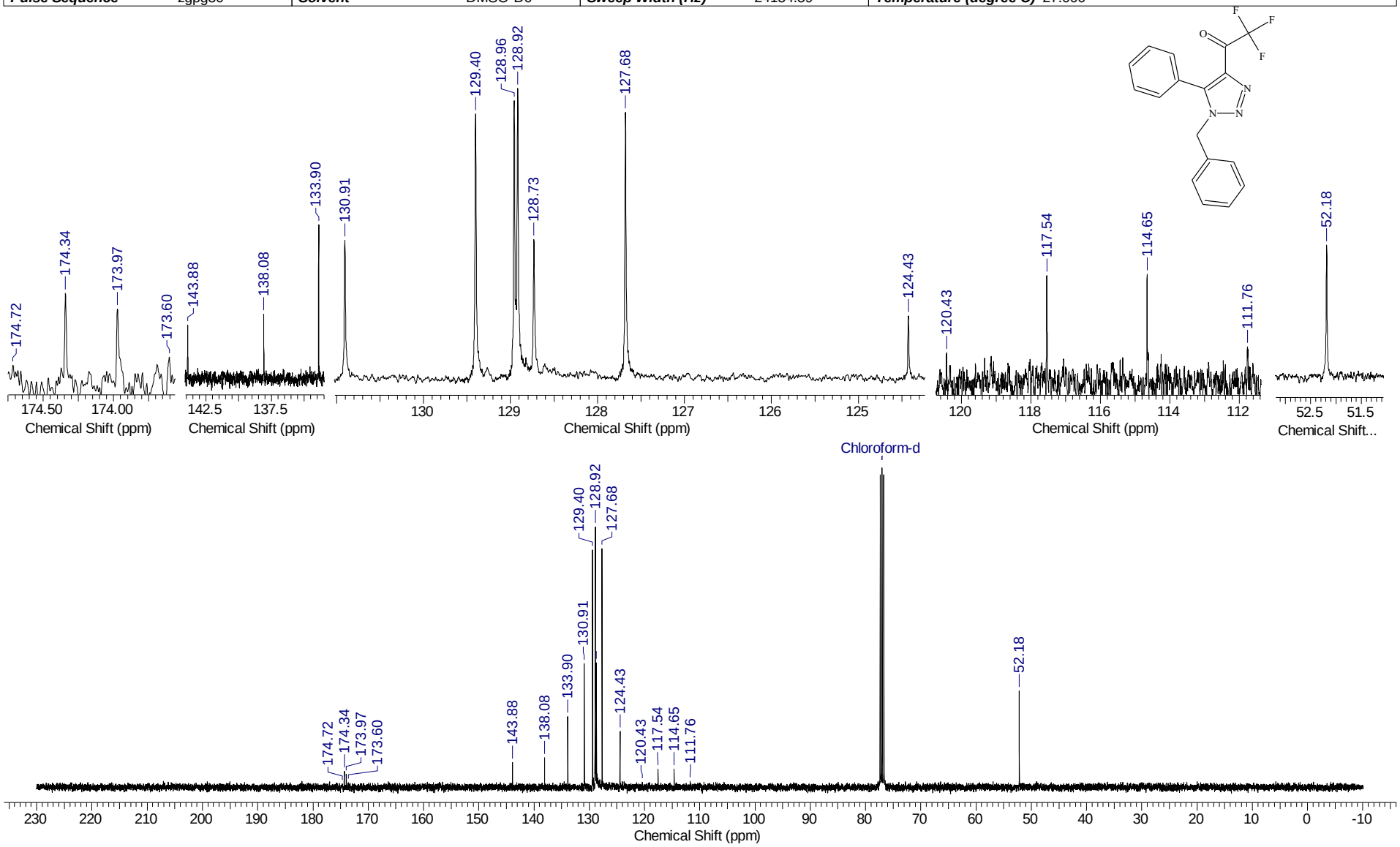
Acquisition Time (sec)	1.7433	***Comment***	Imported from UXNMR.			***Date***	29 Mar 2022 15:15:50
File Name	C:\DOCS\OUTPUT_301\2022\03.爨 痱\SZA-BM-2448-21.F_005001r					***Frequency (MHz)***	376.50
Nucleus	19F	***Number of Transients***	4	***Original Points Count***	131072	***Points Count***	262144
Pulse Sequence	zgflqn	***Solvent***	CHLOROFORM-D			***Sweep Width (Hz)***	75187.97
Temperature (degree C)	27.000						



^{19}F NMR spectrum of **8** (376.5 MHz, $CDCl_3$)

18 May 2022

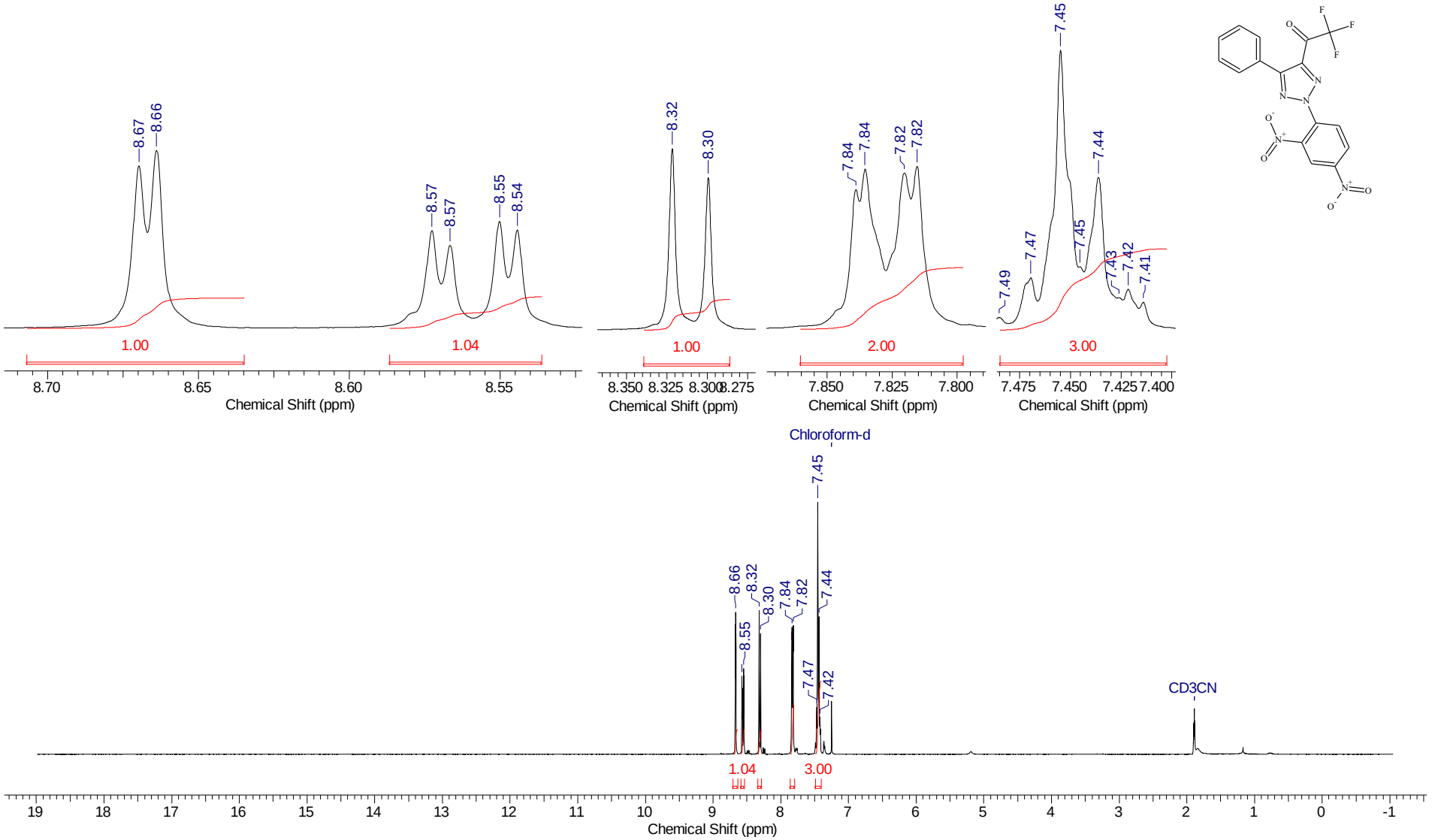
Acquisition Time (sec)	0.6783	***Comment***	Imported from UXNMR.			***Date***	31 Mar 2022 15:24:40
File Name	C:\DOCS\OUTPUT_301\2022\03.爨 痱\SZA-BM-2448-25.C_002001r					***Frequency (MHz)***	100.61
Nucleus	13C	***Number of Transients***	347	***Original Points Count***	16384	***Points Count***	131072
Pulse Sequence	zgpg30	***Solvent***	DMSO-D6	***Sweep Width (Hz)***	24154.59	***Temperature (degree C)***	27.000



^{13}C NMR spectrum of **8** (100.6 MHz, $CDCl_3$)

19 May 2022

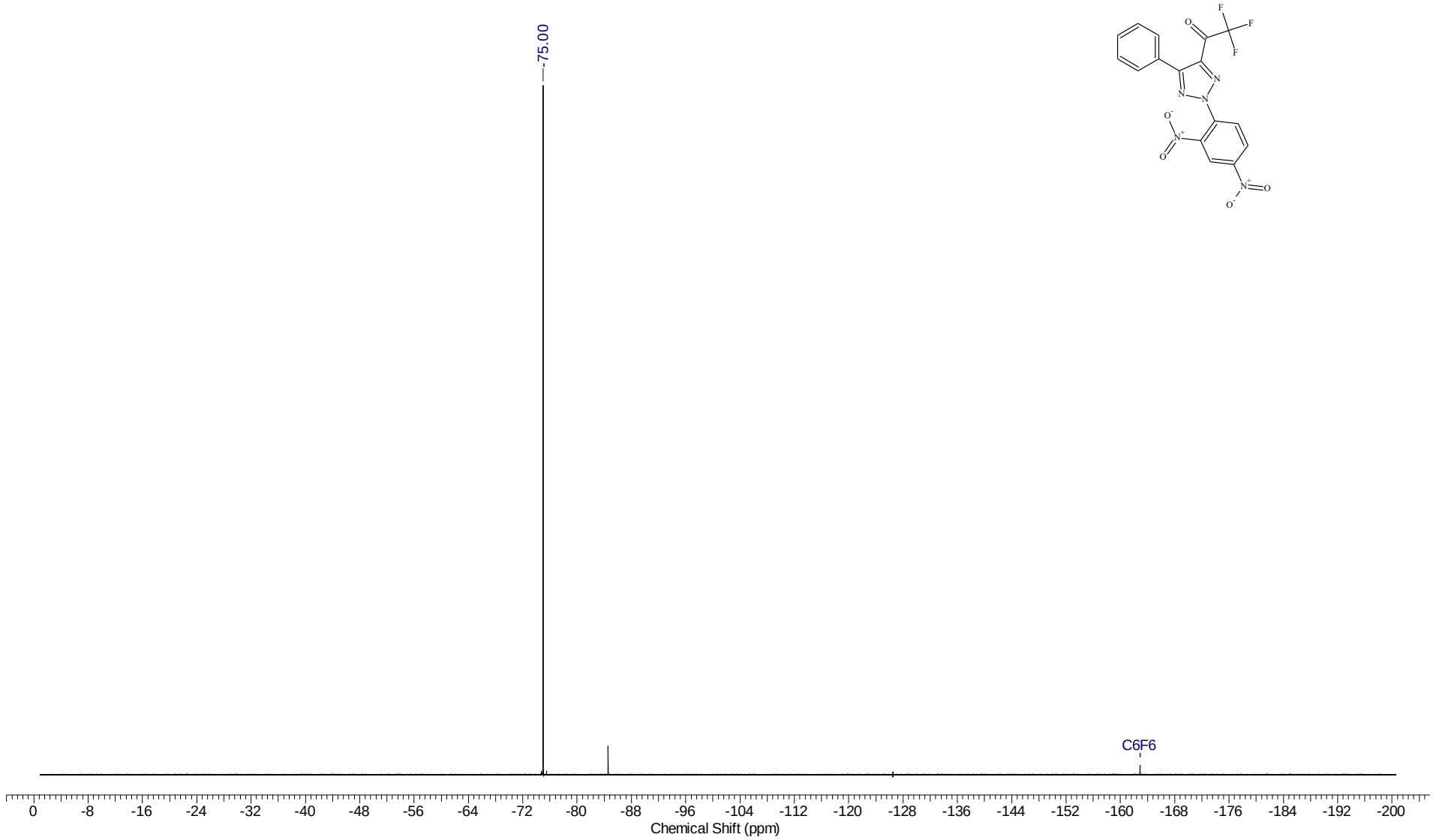
Acquisition Time (sec)	4.0894	***Comment***	Imported from UXNMR.			***Date***	22 Mar 2022 15:43:50
File Name	C:\DOCS\OUTPUT_301\2022\03.爨 痱\BM-2461-1p.H_001001r					***Frequency (MHz)***	400.13
Nucleus	1H	***Number of Transients***	4	***Original Points Count***	32768	***Points Count***	131072
Pulse Sequence	zg30	***Solvent***	CHLOROFORM-D			***Sweep Width (Hz)***	8012.82
Temperature (degree C)	27.000						



^{1}H NMR spectrum of **9** (400.1 MHz, $CDCl_3$)

19 May 2022

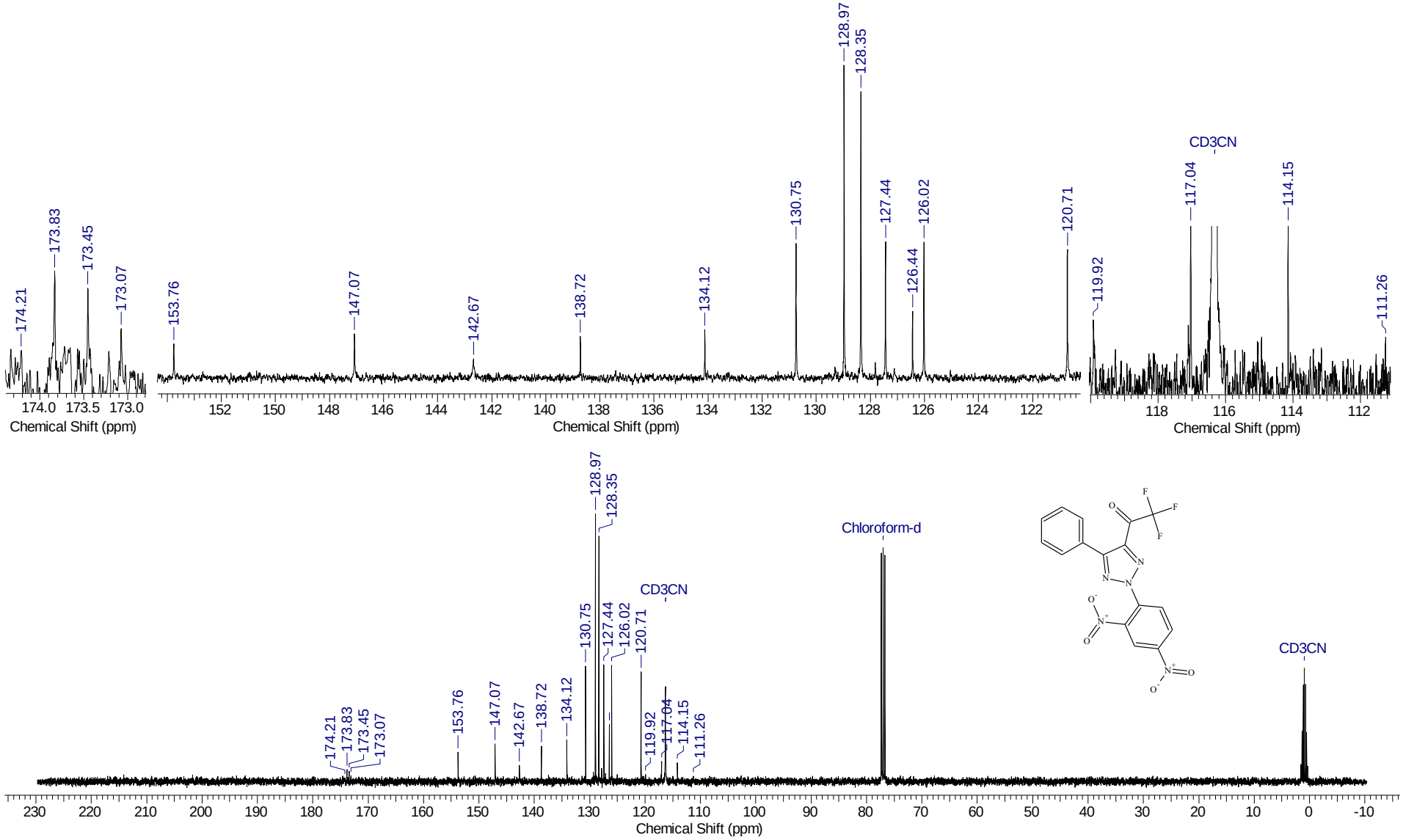
Acquisition Time (sec)	1.7433	***Comment***	Imported from UXNMR.			***Date***	22 Mar 2022 15:28:42
File Name	C:\DOCS\OUTPUT_301\2022\03.爨 痱\BM-2461-1p.F_005001r					***Frequency (MHz)***	376.50
Nucleus	19F	***Number of Transients***	4	***Original Points Count***	131072	***Points Count***	262144
Pulse Sequence	zgflqn	***Solvent***	CHLOROFORM-D			***Sweep Width (Hz)***	75187.97
Temperature (degree C)	27.000						



^{19}F NMR spectrum of **9** (376.5 MHz, $CDCl_3$)

19 May 2022

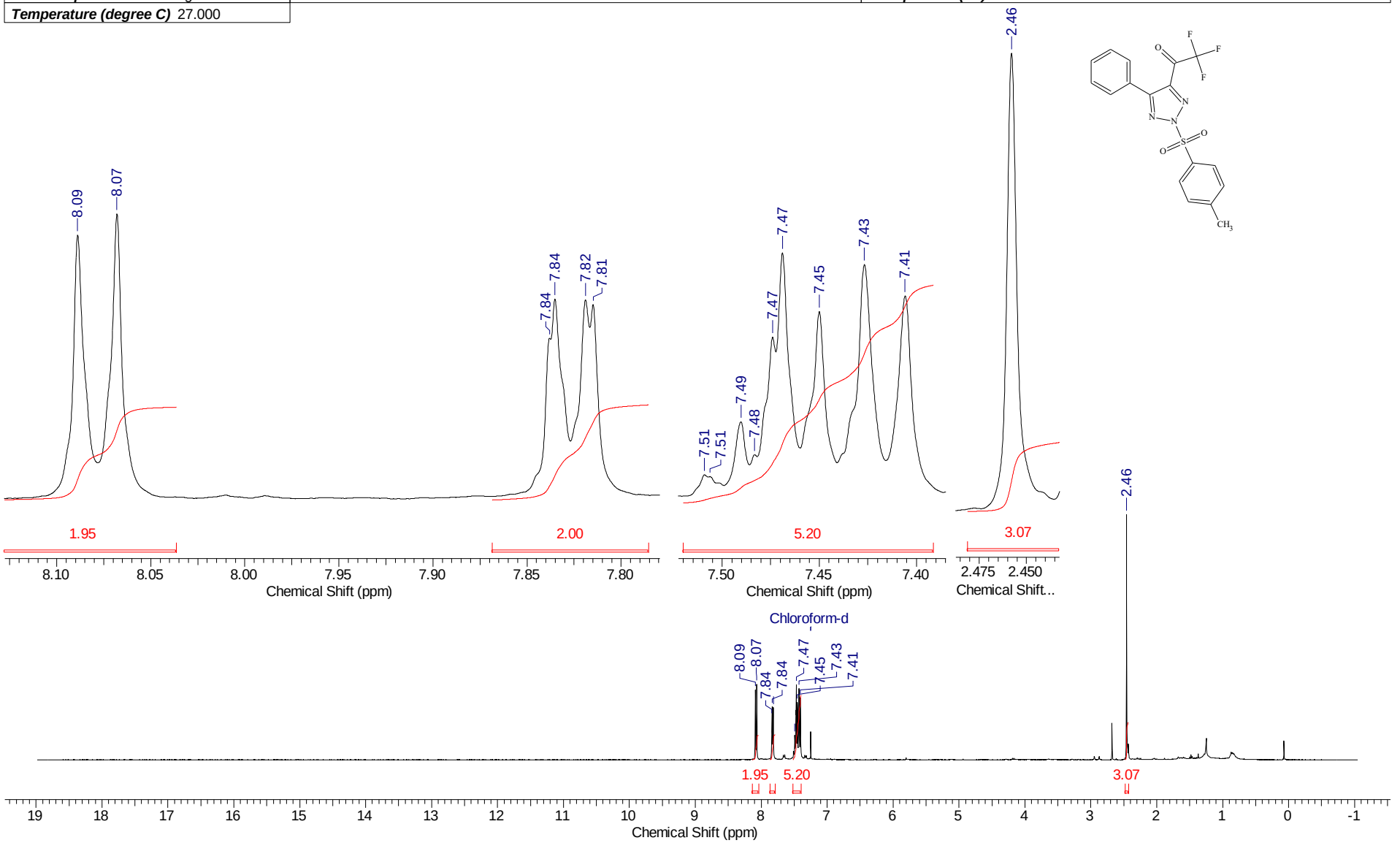
Acquisition Time (sec)	0.6783	***Comment***	Imported from UXNMR.			***Date***	22 Mar 2022 15:54:02
File Name	C:\DOCS\OUTPUT_301\2022\03.爨 菲\BM-2461-1p.C_002001r					***Frequency (MHz)***	100.61
Nucleus	13C	***Number of Transients***	266	***Original Points Count***	16384	***Points Count***	131072
Pulse Sequence	zgpg30	***Solvent***	DMSO-D6	***Sweep Width (Hz)***	24154.59	***Temperature (degree C)***	27.000



^{13}C NMR spectrum of **9** (100.6 MHz, $CDCl_3$)

19 May 2022

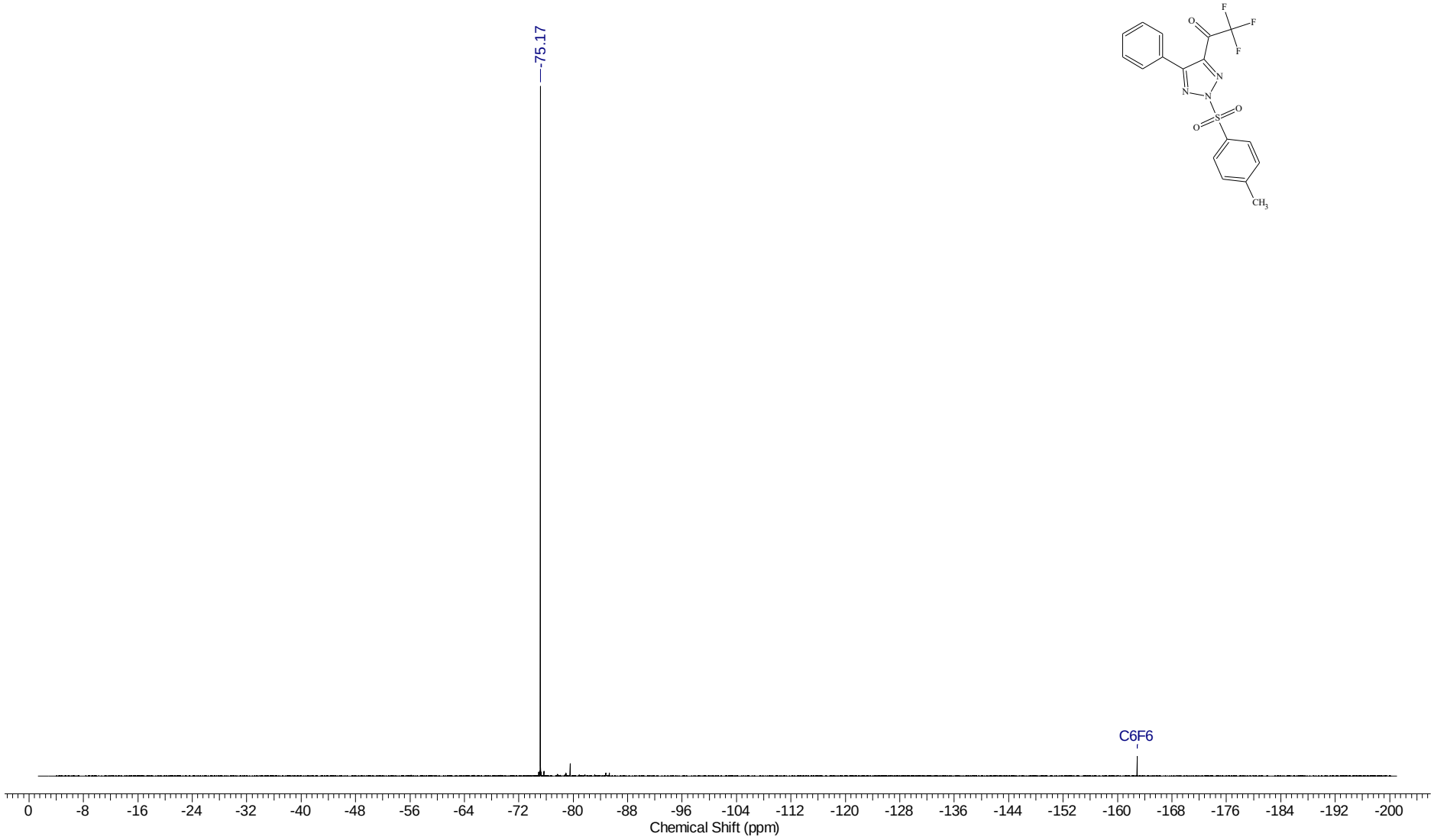
Acquisition Time (sec)	4.0894	***Comment***	Imported from UXNMR.			***Date***	30 Mar 2022 17:23:40
File Name	C:\DOCS\OUTPUT_301\2022\03.爨 痱\SZA-BM-2470.H_001001r					***Frequency (MHz)***	400.13
Nucleus	1H	***Number of Transients***	4	***Original Points Count***	32768	***Points Count***	131072
Pulse Sequence	zg30	***Solvent***	CHLOROFORM-D			***Sweep Width (Hz)***	8012.82
Temperature (degree C)	27.000						



^{1}H NMR spectrum of **10** (400.1 MHz, $CDCl_3$)

19 May 2022

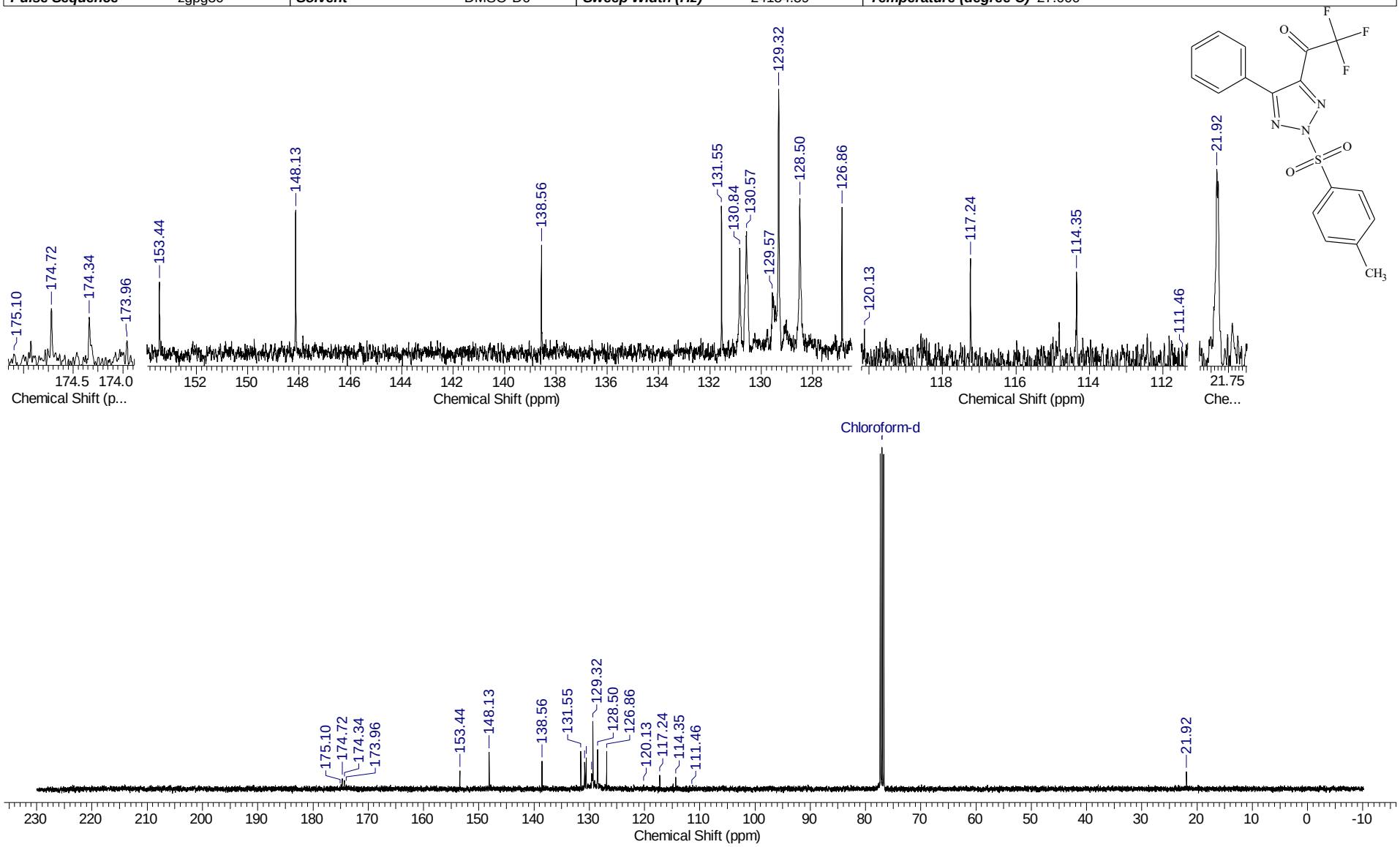
Acquisition Time (sec)	1.7433	***Comment***	Imported from UXNMR.			***Date***	30 Mar 2022 17:49:38
File Name	C:\DOCS\OUTPUT_301\2022\03.爨 痱\SZA-BM-2470.F_005001r					***Frequency (MHz)***	376.50
Nucleus	19F	***Number of Transients***	16	***Original Points Count***	131072	***Points Count***	262144
Pulse Sequence	zgflqn	***Solvent***	CHLOROFORM-D			***Sweep Width (Hz)***	75187.97
Temperature (degree C)	27.000						



^{19}F NMR spectrum of **10** (376.5 MHz, $CDCl_3$)

19 May 2022

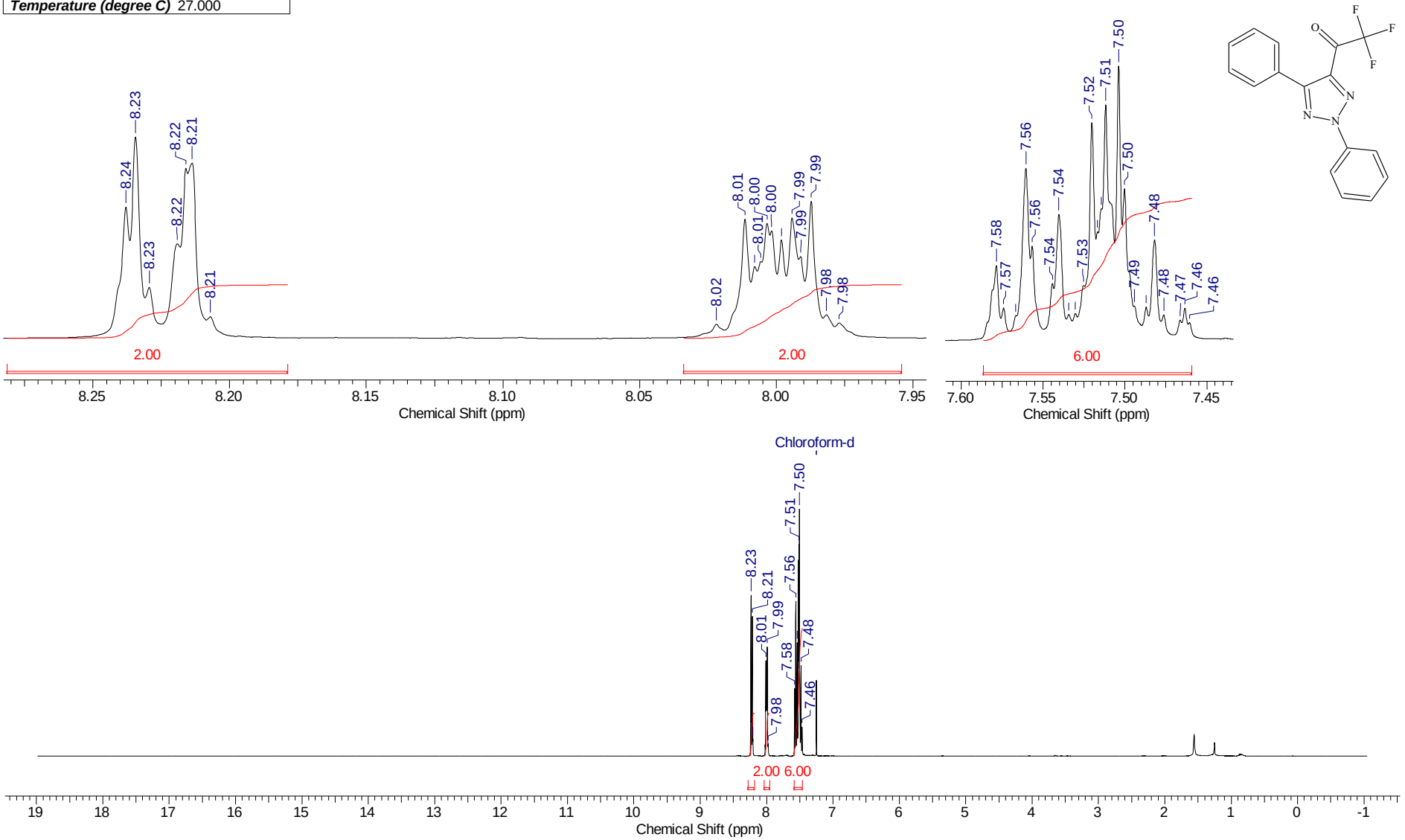
Acquisition Time (sec)	0.6783	***Comment***	Imported from UXNMR.			***Date***	31 Mar 2022 12:54:26
File Name	C:\DOCS\OUTPUT_301\2022\03.爨 痱\SZA-BM-2470.C_002001r					***Frequency (MHz)***	100.61
Nucleus	13C	***Number of Transients***	305	***Original Points Count***	16384	***Points Count***	131072
Pulse Sequence	zgpg30	***Solvent***	DMSO-D6	***Sweep Width (Hz)***	24154.59	***Temperature (degree C)***	27.000



^{13}C NMR spectrum of **10** (100.6 MHz, $CDCl_3$)

19 May 2022

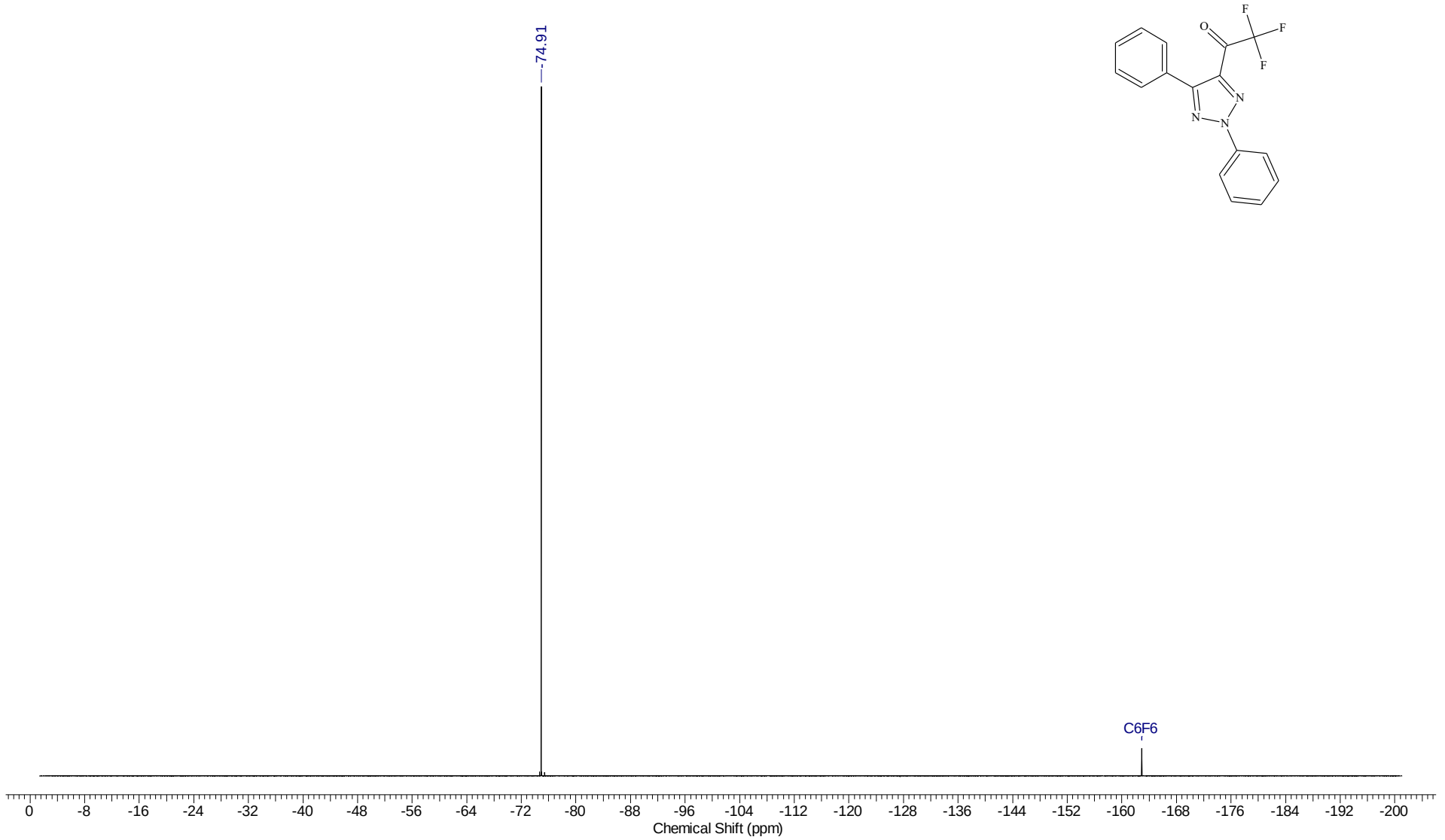
Acquisition Time (sec)	4.0894	***Comment***	Imported from UXNMR.			***Date***	21 Apr 2022 12:39:06
File Name	C:\DOCS\OUTPUT_301\2022\04.図疱膿\BM-2505-2.H_001001r					***Frequency (MHz)***	400.13
Nucleus	1H	***Number of Transients***	8	***Original Points Count***	32768	***Points Count***	131072
Pulse Sequence	zg30	***Solvent***	CHLOROFORM-D			***Sweep Width (Hz)***	8012.82
Temperature (degree C)	27.000						



^{1}H NMR spectrum of **11** (400.1 MHz, $CDCl_3$)

19 May 2022

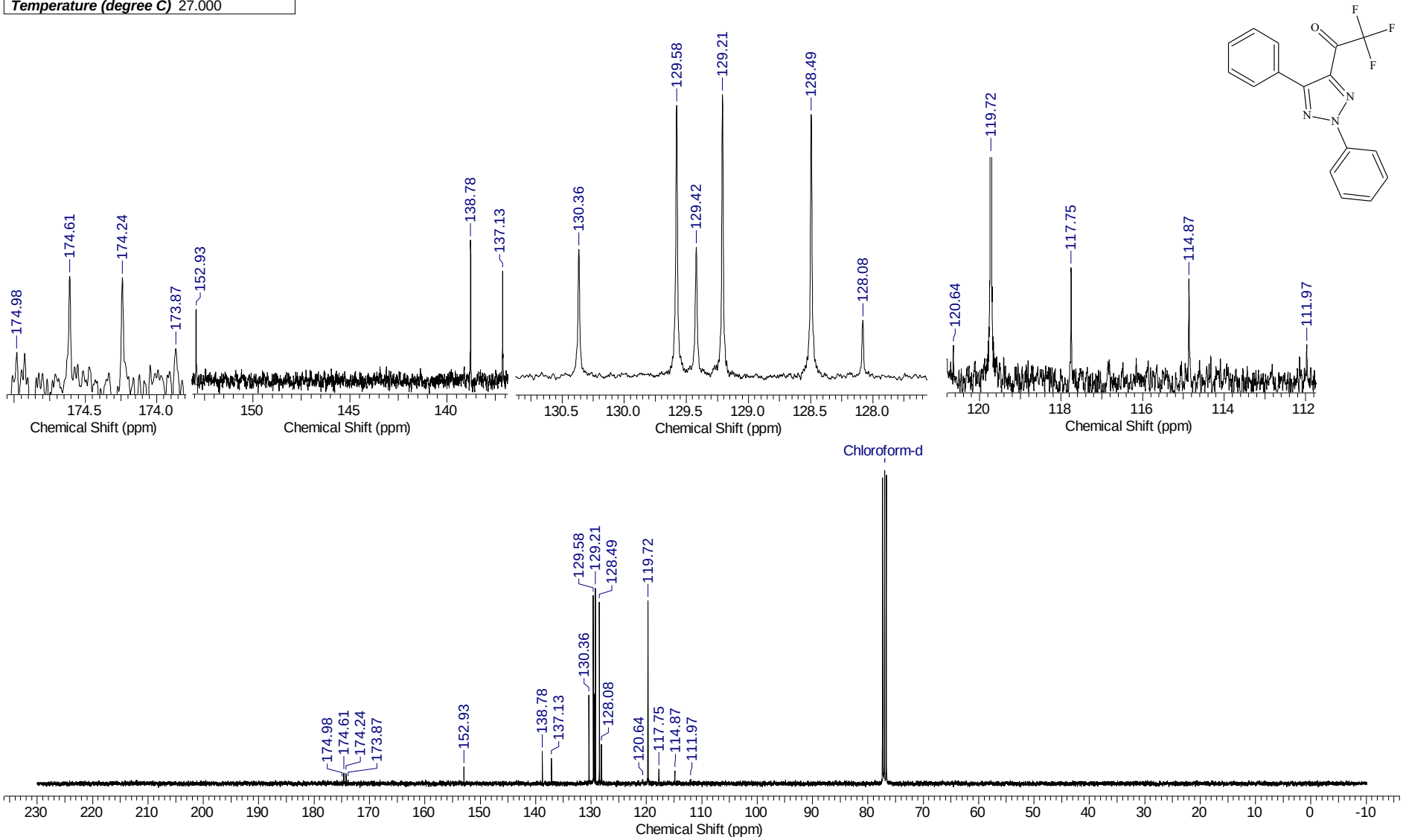
Acquisition Time (sec)	1.7433	***Comment***	Imported from UXNMR.			***Date***	21 Apr 2022 12:05:42
File Name	C:\DOCS\OUTPUT_301\2022\04.囡疱朦\BM-2505-2.F_005001r					***Frequency (MHz)***	376.50
Nucleus	19F	***Number of Transients***	11	***Original Points Count***	131072	***Points Count***	262144
Pulse Sequence	zgflqn	***Solvent***	CHLOROFORM-D			***Sweep Width (Hz)***	75187.97
Temperature (degree C)	27.000						



^{19}F NMR spectrum of **11** (376.5 MHz, $CDCl_3$)

19 May 2022

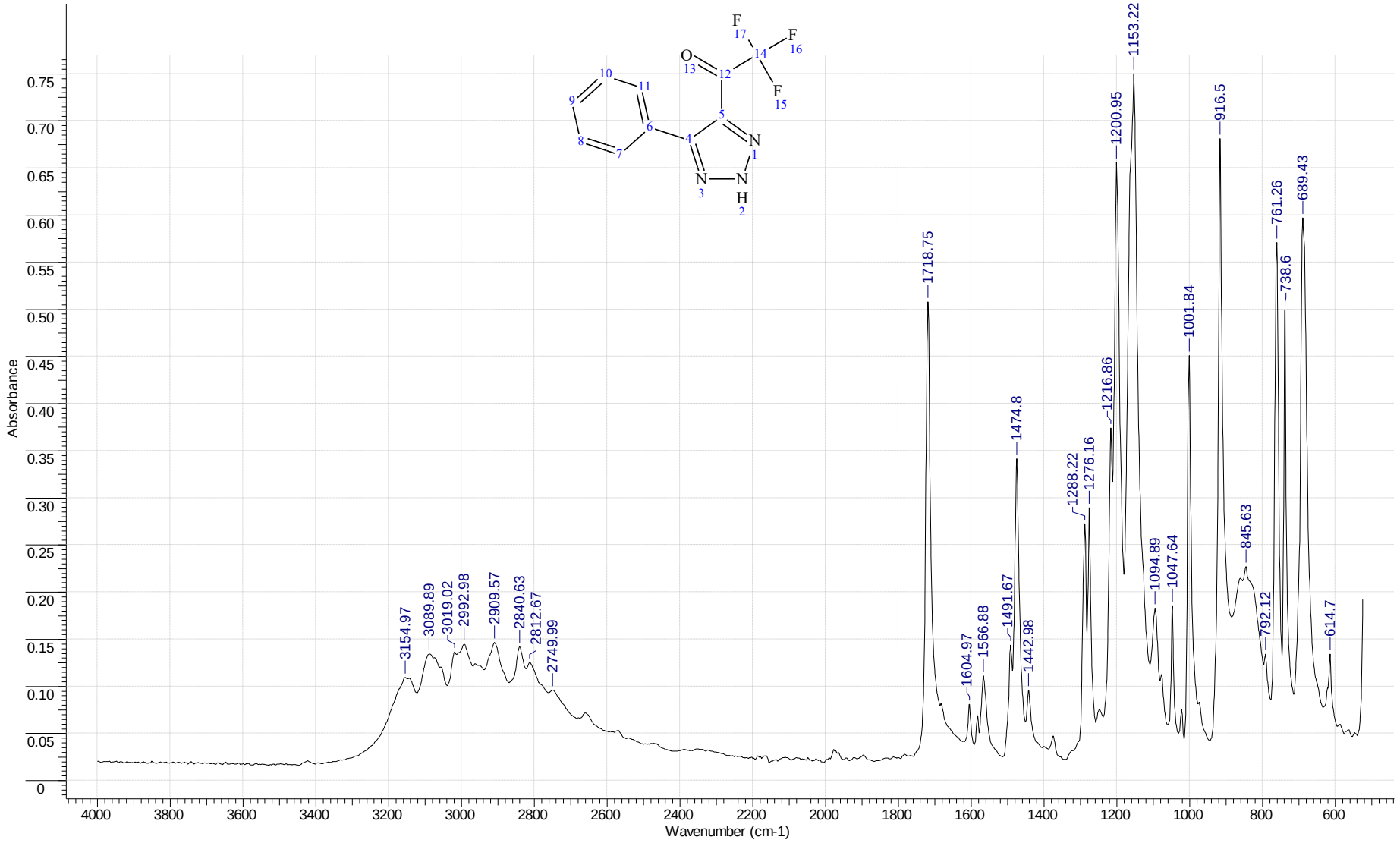
Acquisition Time (sec)	0.6783	***Comment***	Imported from UXNMR.			***Date***	21 Apr 2022 13:09:40
File Name	C:\DOCS\OUTPUT_301\2022\04.図疱膳\BM-2505-2.C_002001r					***Frequency (MHz)***	100.61
Nucleus	13C	***Number of Transients***	763	***Original Points Count***	16384	***Points Count***	131072
Pulse Sequence	zgpg30	***Solvent***	CHLOROFORM-D			***Sweep Width (Hz)***	24154.59
Temperature (degree C)	27.000						



^{13}C NMR spectrum of **11** (100.6 MHz, $CDCl_3$)
Copies of FT-IR spectra

8 Nov 2022

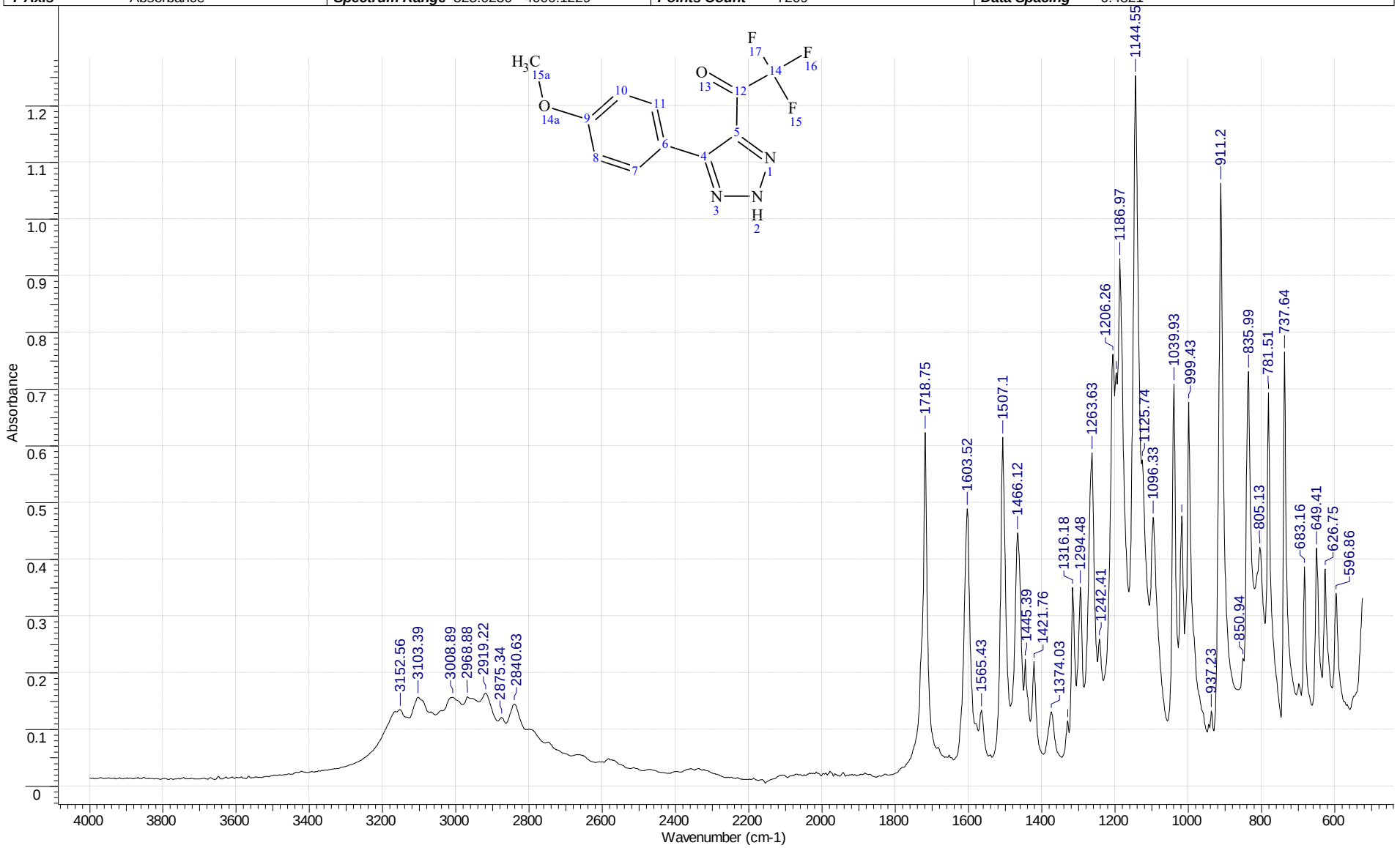
Title	腆玨脲怦觇? 绿 -2508-3 (窝 湾磬殇屑戳) iD7						
File Name	C:\DOCS\BM\IR SPECTRA\07-11-2022_15-26-24\腆玨脲怦觇? 绿 -2508-3 (窝 湾磬殇屑戳) ID7.SPA					***Date Stamp***	07 Nov 2022 11:16:05
Date	07 Nov 2022 18:49:50	***Technique***	Infrared	***Spectral Region***	IR	***X Axis***	Wavenumber (cm-1)
Y Axis	Absorbance	***Spectrum Range***	525.0250 - 4000.1229	***Points Count***	7209	***Data Spacing***	0.4821



FT-IR spectra of **2a**

8 Nov 2022

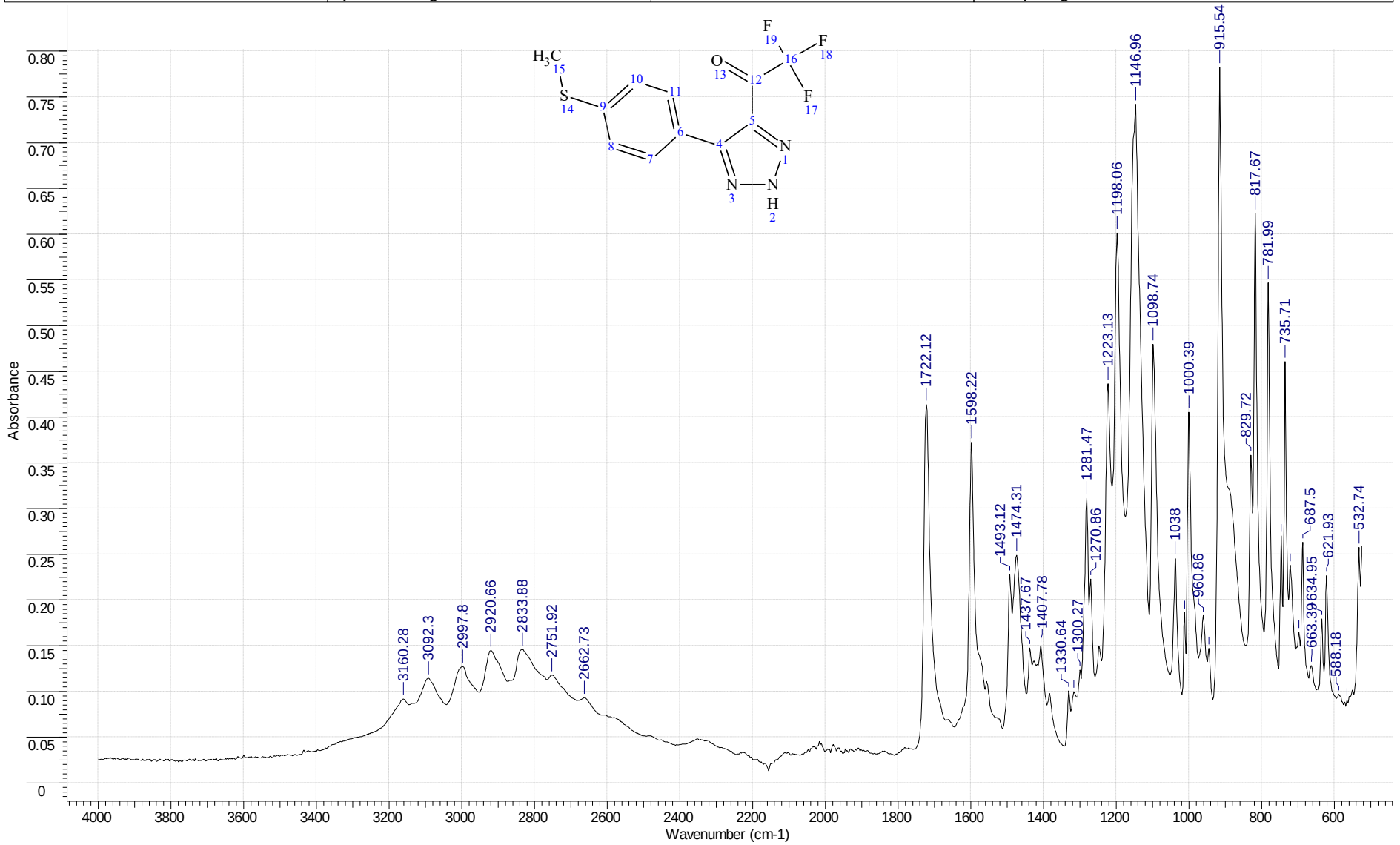
Title	腆 玎腺怦觇? 绿 -2511-2 （窝 湾 磬殇屑靓） iD7						
File Name	C:\DOCS\BM\IR SPECTRA\07-11-2022_15-26-24\腆 玎腺怦觇? 绿 -2511-2 （窝 湾 磬殇屑靓） ID7.SPA					***Date Stamp***	07 Nov 2022 11:52:12
Date	07 Nov 2022 18:49:52	***Technique***	Infrared	***Spectral Region***	IR	***X Axis***	Wavenumber (cm-1)
Y Axis	Absorbance	***Spectrum Range***	525.0250 - 4000.1229	***Points Count***	7209	***Data Spacing***	0.4821



FT-IR spectra of **2b**

8 Nov 2022

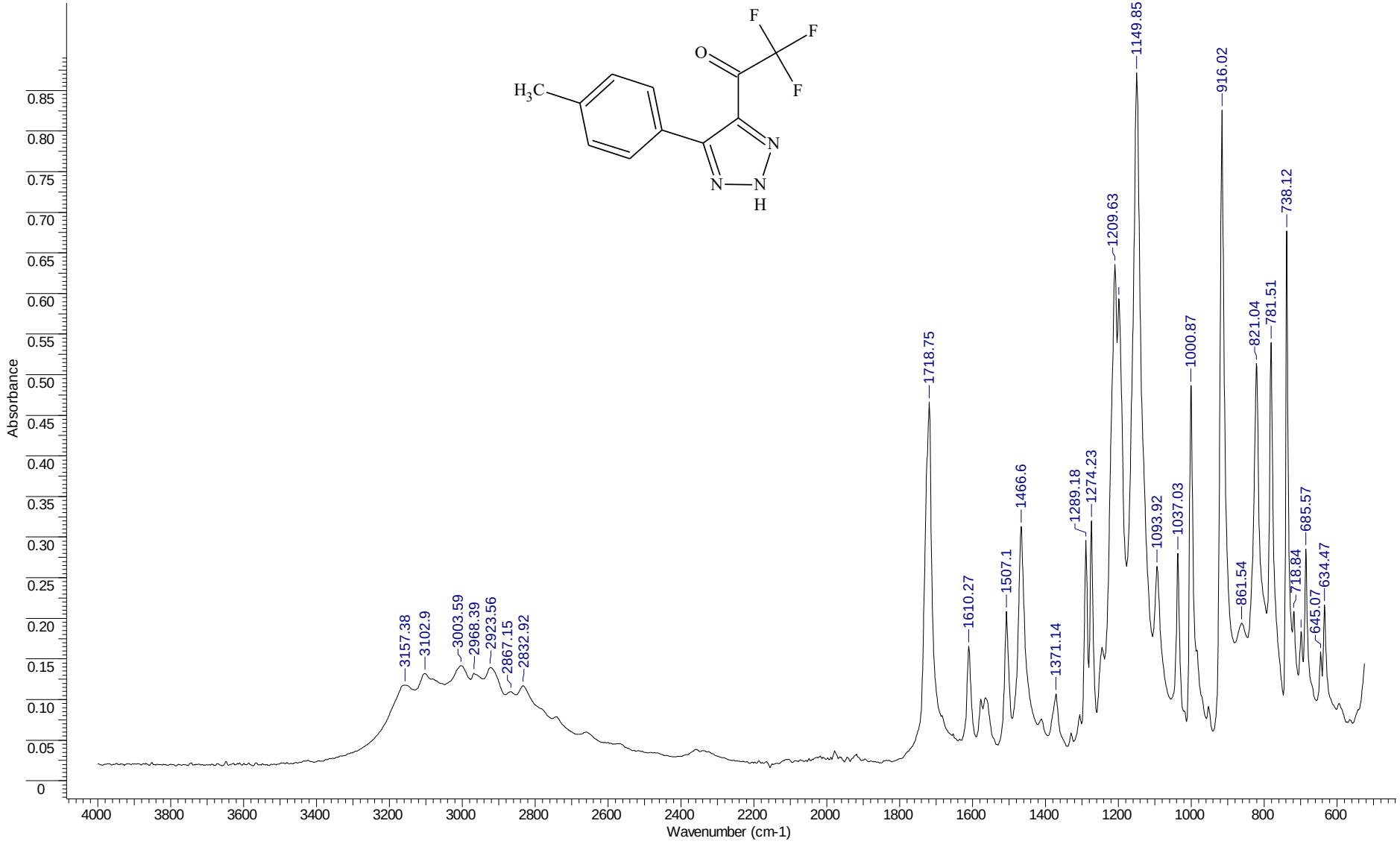
Title	腆玎脲怦觇? 绿 -2365-3 (窝 湾磬殇屑靓) iD7						
File Name	C:\DOCS\BM\IR SPECTRA\08-11-2022_13-23-31\腆玎脲怦觇? 绿 -2365-3 (窝 湾磬殇屑靓) ID7.SPA					***Date Stamp***	08 Nov 2022 09:42:25
Date	08 Nov 2022 13:56:40	***Technique***	Infrared	***Spectral Region***	IR	***X Axis***	Wavenumber (cm-1)
Y Axis	Absorbance	***Spectrum Range***	525.0250 - 4000.1229	***Points Count***	7209	***Data Spacing***	0.4821



FT-IR spectra of **2c**

8 Nov 2022

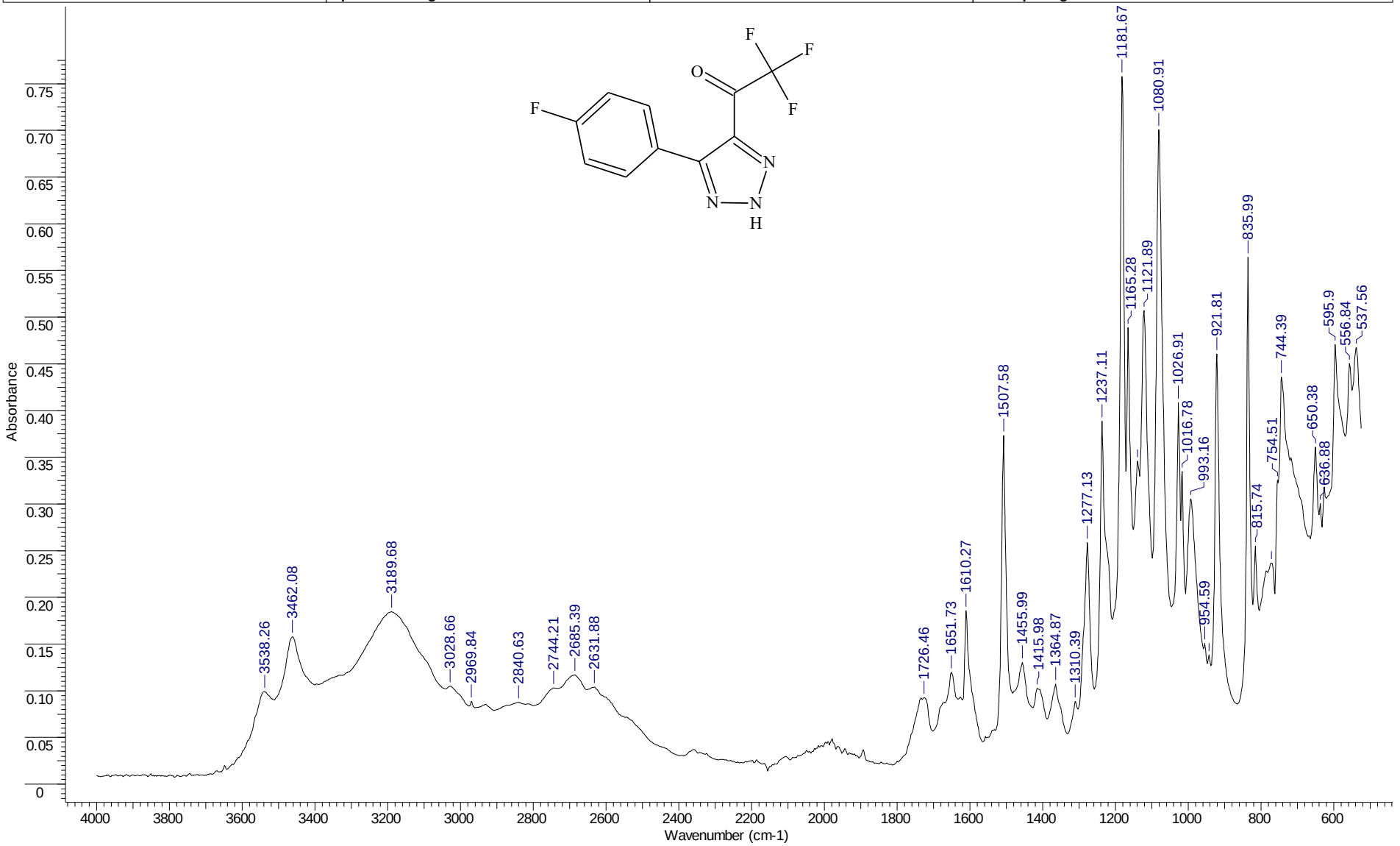
Title	腆 玎脲怦觇? 绿 -1327-3 (窝 湾 磬殇屑觐) iD7						
File Name	C:\DOCS\BM\IR SPECTRA\07-11-2022_15-26-24\腆 玎脲怦觇? 绿 -1327-3 (窝 湾 磬殇屑觐) ID7.SPA					***Date Stamp***	07 Nov 2022 11:42:47
Date	07 Nov 2022 18:49:52	***Technique***	Infrared	***Spectral Region***	IR	***X Axis***	Wavenumber (cm-1)
Y Axis	Absorbance	***Spectrum Range***	525.0250 - 4000.1229	***Points Count***	7209	***Data Spacing***	0.4821



FT-IR spectra of **2d**

8 Nov 2022

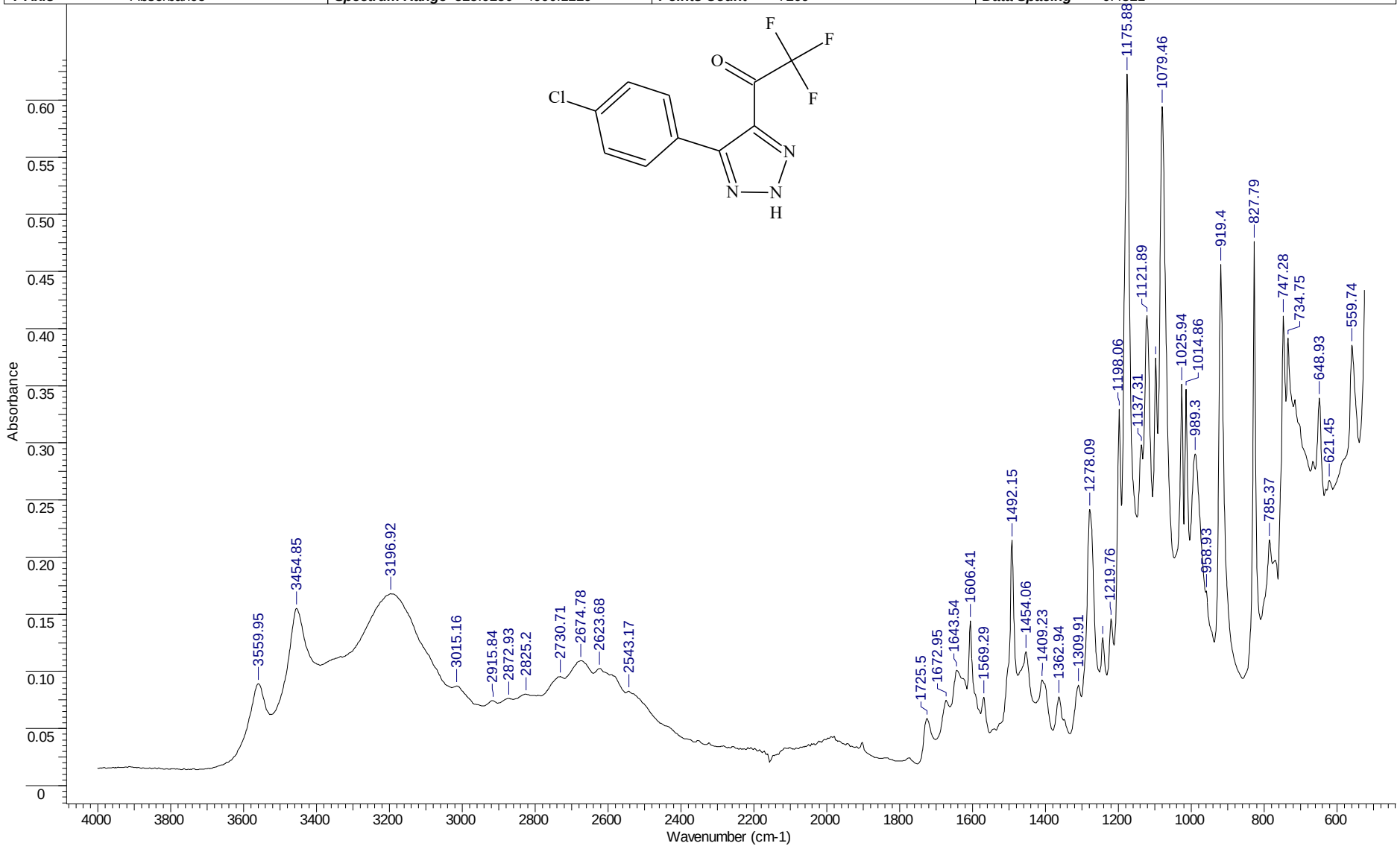
Title	腆 玨脲怦觇? 绿 -2214-2 (窝 湾 磬殇屑鹳) iD7						
File Name	C:\DOCS\BM\IR SPECTRA\07-11-2022_15-26-24\腆 玨脲怦觇? 绿 -2214-2 (窝 湾 磬殇屑鹳) ID7.SPA					***Date Stamp***	07 Nov 2022 11:47:33
Date	07 Nov 2022 18:49:52	***Technique***	Infrared	***Spectral Region***	IR	***X Axis***	Wavenumber (cm-1)
Y Axis	Absorbance	***Spectrum Range***	525.0250 - 4000.1229	***Points Count***	7209	***Data Spacing***	0.4821



FT-IR spectra of **2e**

8 Nov 2022

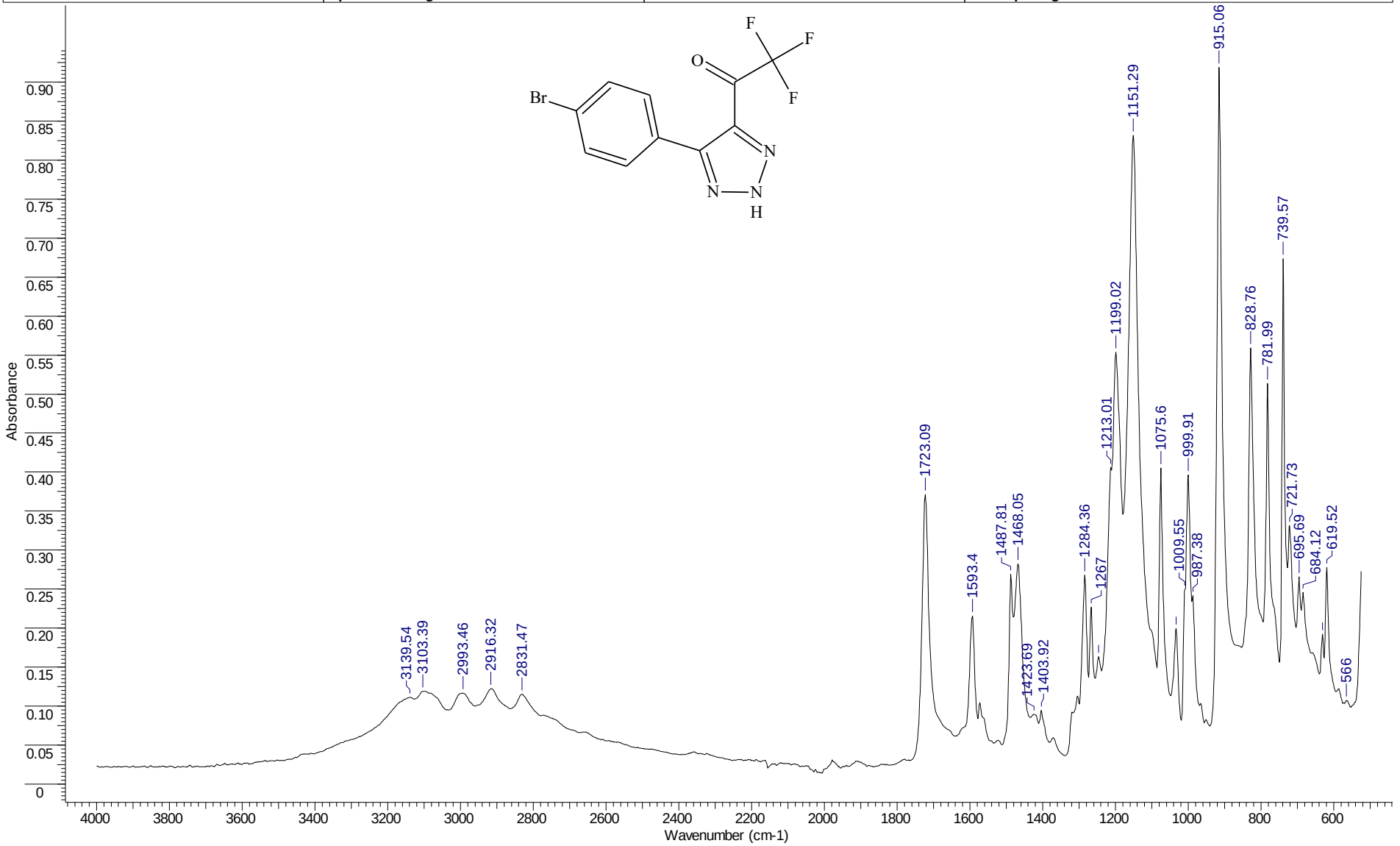
Title	腆 玎脲怦觇? 绿 -2357-3 (窝 湾 磬殇屑靓) iD7						
File Name	C:\DOCS\BM\IR SPECTRA\07-11-2022_15-26-24\腆 玎脲怦觇? 绿 -2357-3 (窝 湾 磬殇屑靓) ID7.SPA					***Date Stamp***	07 Nov 2022 12:02:20
Date	07 Nov 2022 18:49:50	***Technique***	Infrared	***Spectral Region***	IR	***X Axis***	Wavenumber (cm-1)
Y Axis	Absorbance	***Spectrum Range***	525.0250 - 4000.1229	***Points Count***	7209	***Data Spacing***	0.4821



FT-IR spectra of **2f**

8 Nov 2022

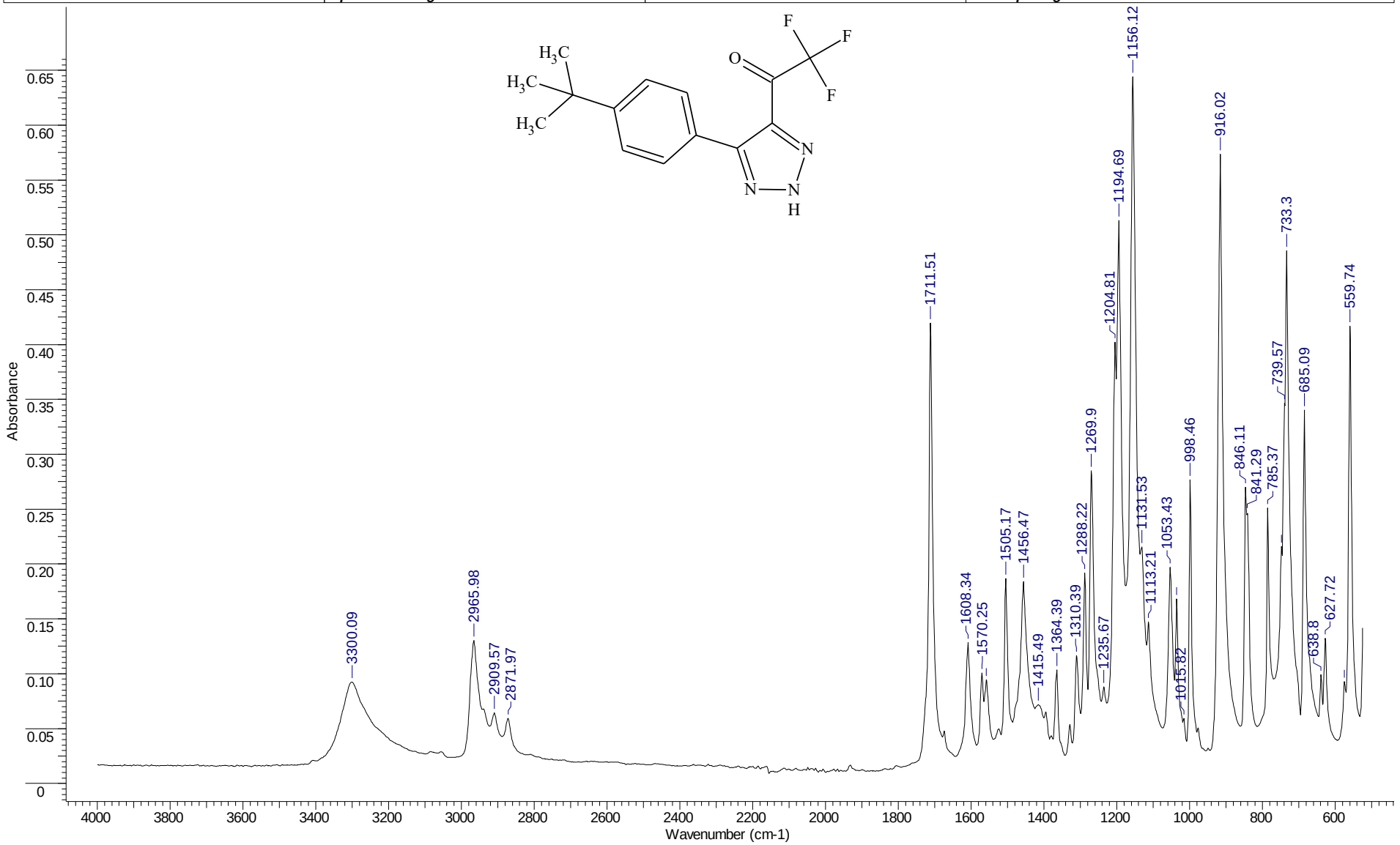
Title	腆 玨脲怦觇? 绿 -2363 (窝 湾 磬殇屑戳) iD7						
File Name	C:\DOCS\BM\IR SPECTRA\07-11-2022_15-26-24\腆 玨脲怦觇? 绿 -2363 (窝 湾 磬殇屑戳) ID7.SPA					***Date Stamp***	07 Nov 2022 11:29:32
Date	07 Nov 2022 18:49:52	***Technique***	Infrared	***Spectral Region***	IR	***X Axis***	Wavenumber (cm-1)
Y Axis	Absorbance	***Spectrum Range***	525.0250 - 4000.1229	***Points Count***	7209	***Data Spacing***	0.4821



FT-IR spectra of **2g**

8 Nov 2022

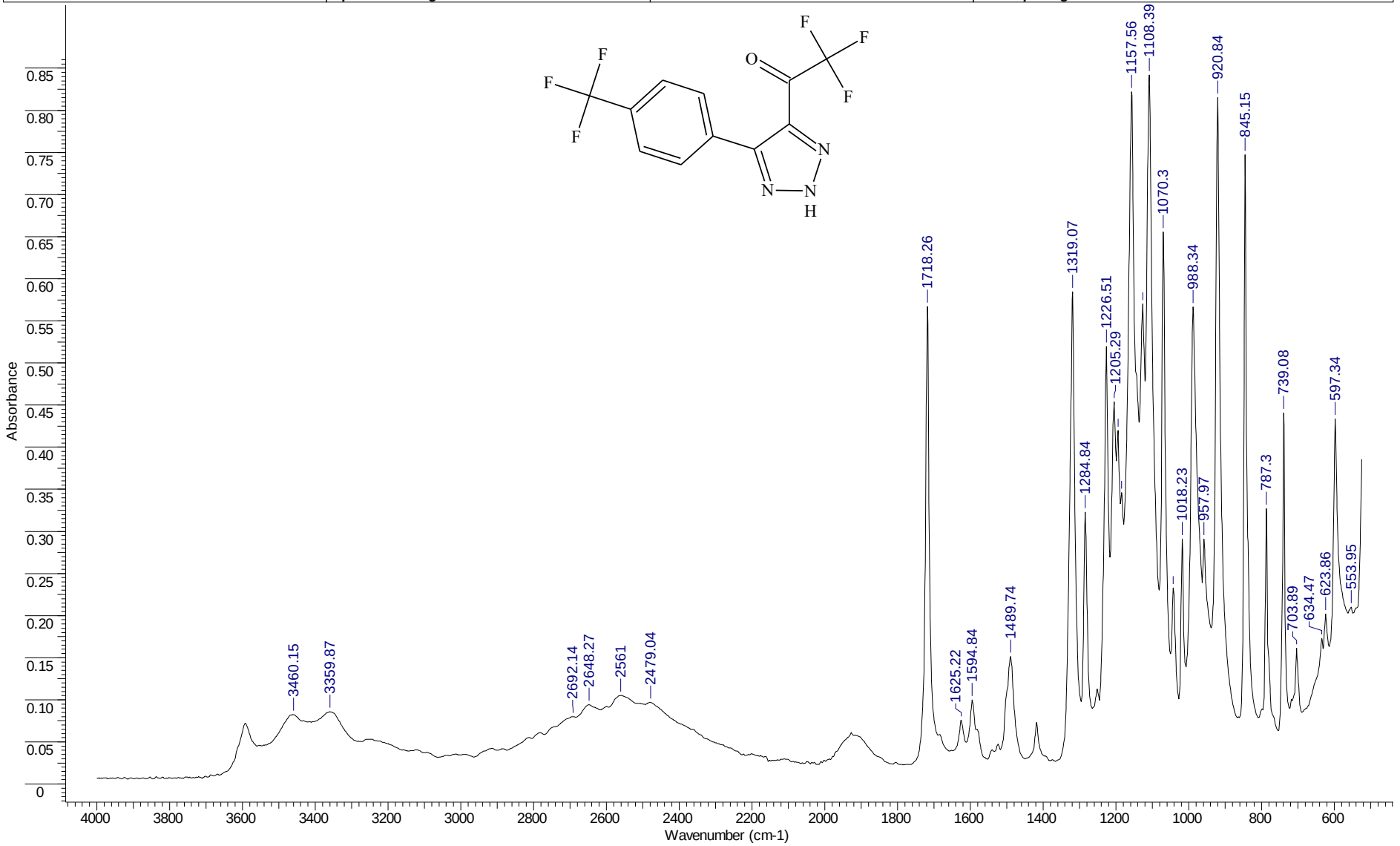
Title	腆 玎腺怦觇? 绿 -2374 (窝 湾 磬殇屑戳) iD7						
File Name	C:\DOCS\BM\IR SPECTRA\08-11-2022_13-23-31\腆 玎腺怦觇? 绿 -2374 (窝 湾 磬殇屑戳) ID7.SPA					***Date Stamp***	08 Nov 2022 09:19:57
Date	08 Nov 2022 13:56:38	***Technique***	Infrared	***Spectral Region***	IR	***X Axis***	Wavenumber (cm-1)
Y Axis	Absorbance	***Spectrum Range***	525.0250 - 4000.1229	***Points Count***	7209	***Data Spacing***	0.4821



FT-IR spectra of **2h**

8 Nov 2022

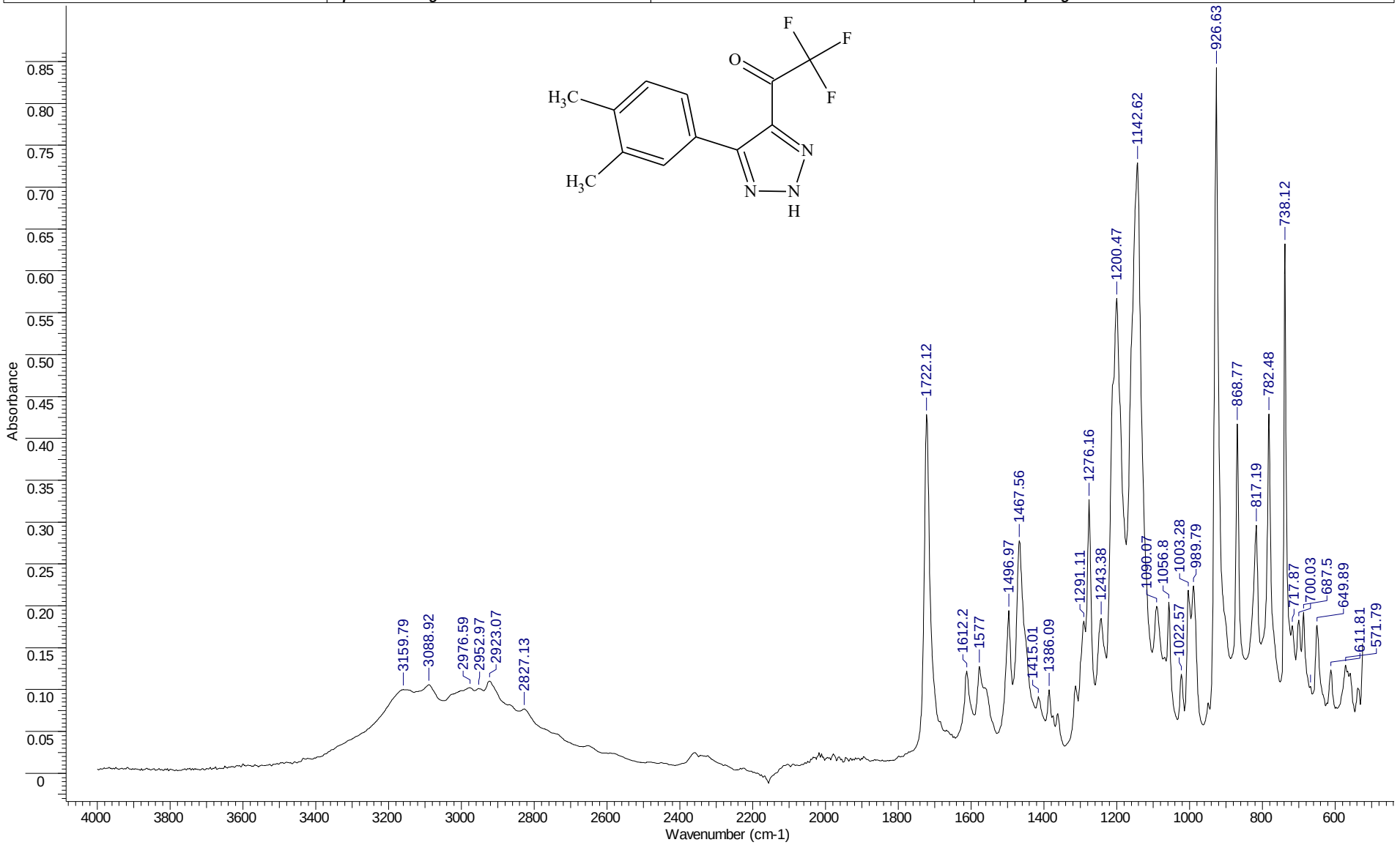
Title	腆玎脲怦觇? 绿 -2362-3 (窝 湾磬殇屑靶) iD7						
File Name	C:\DOCS\BM\IR SPECTRA\08-11-2022_13-23-31\腆玎脲怦觇? 绿 -2362-3 (窝 湾磬殇屑靶) ID7.SPA					***Date Stamp***	08 Nov 2022 10:18:30
Date	08 Nov 2022 13:56:38	***Technique***	Infrared	***Spectral Region***	IR	***X Axis***	Wavenumber (cm-1)
Y Axis	Absorbance	***Spectrum Range***	525.0250 - 4000.1229	***Points Count***	7209	***Data Spacing***	0.4821



FT-IR spectra of **2i**

8 Nov 2022

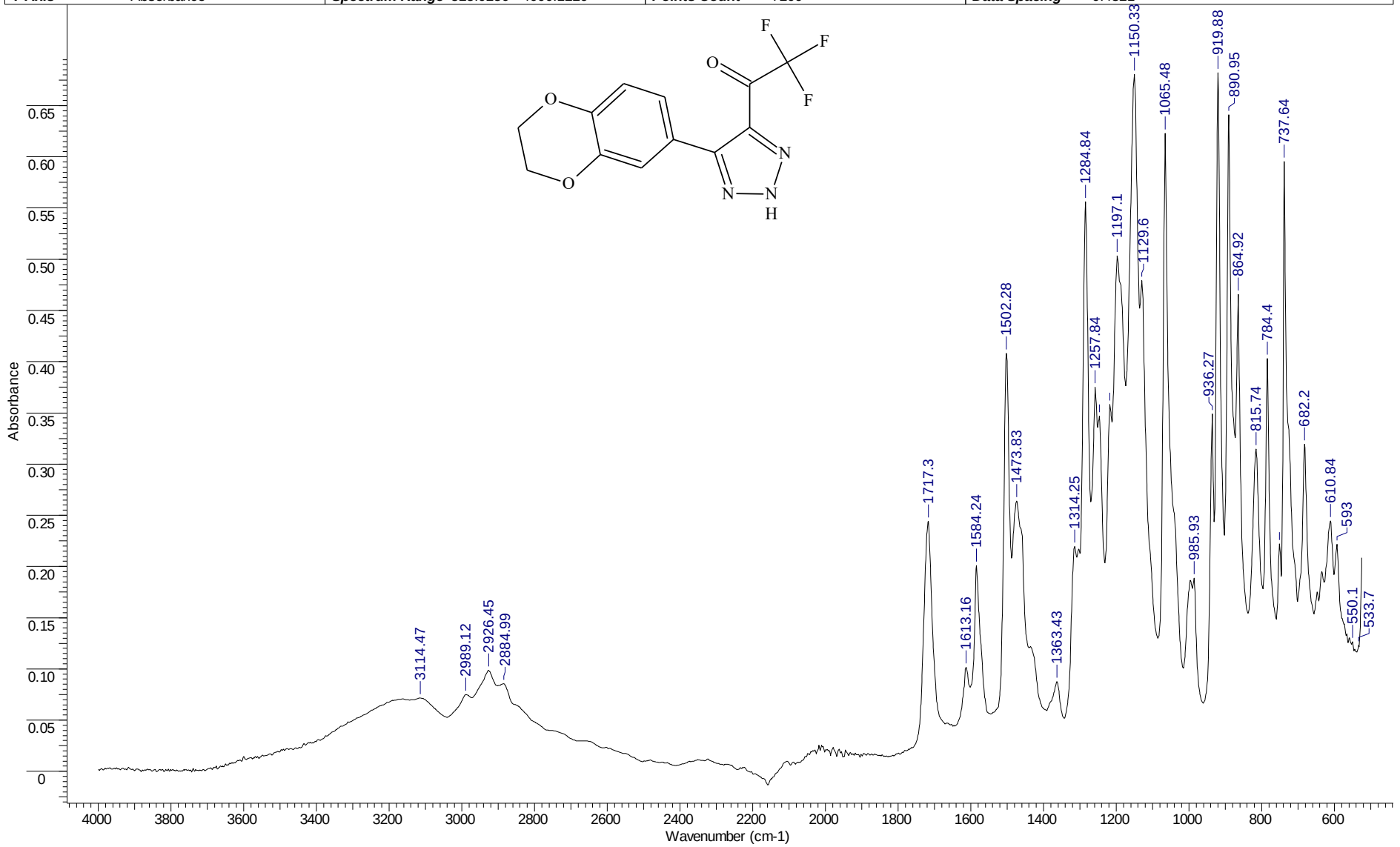
Title	腆 玎腺怦觇? 绿 -2364-3 (窝 湾 磬殇屑靓) iD7						
File Name	C:\DOCS\BM\IR SPECTRA\08-11-2022_13-23-31\腆 玎腺怦觇? 绿 -2364-3 (窝 湾 磬殇屑靓) ID7.SPA					***Date Stamp***	08 Nov 2022 09:56:29
Date	08 Nov 2022 13:56:38	***Technique***	Infrared	***Spectral Region***	IR	***X Axis***	Wavenumber (cm-1)
Y Axis	Absorbance	***Spectrum Range***	525.0250 - 4000.1229	***Points Count***	7209	***Data Spacing***	0.4821



FT-IR spectra of **2j**

8 Nov 2022

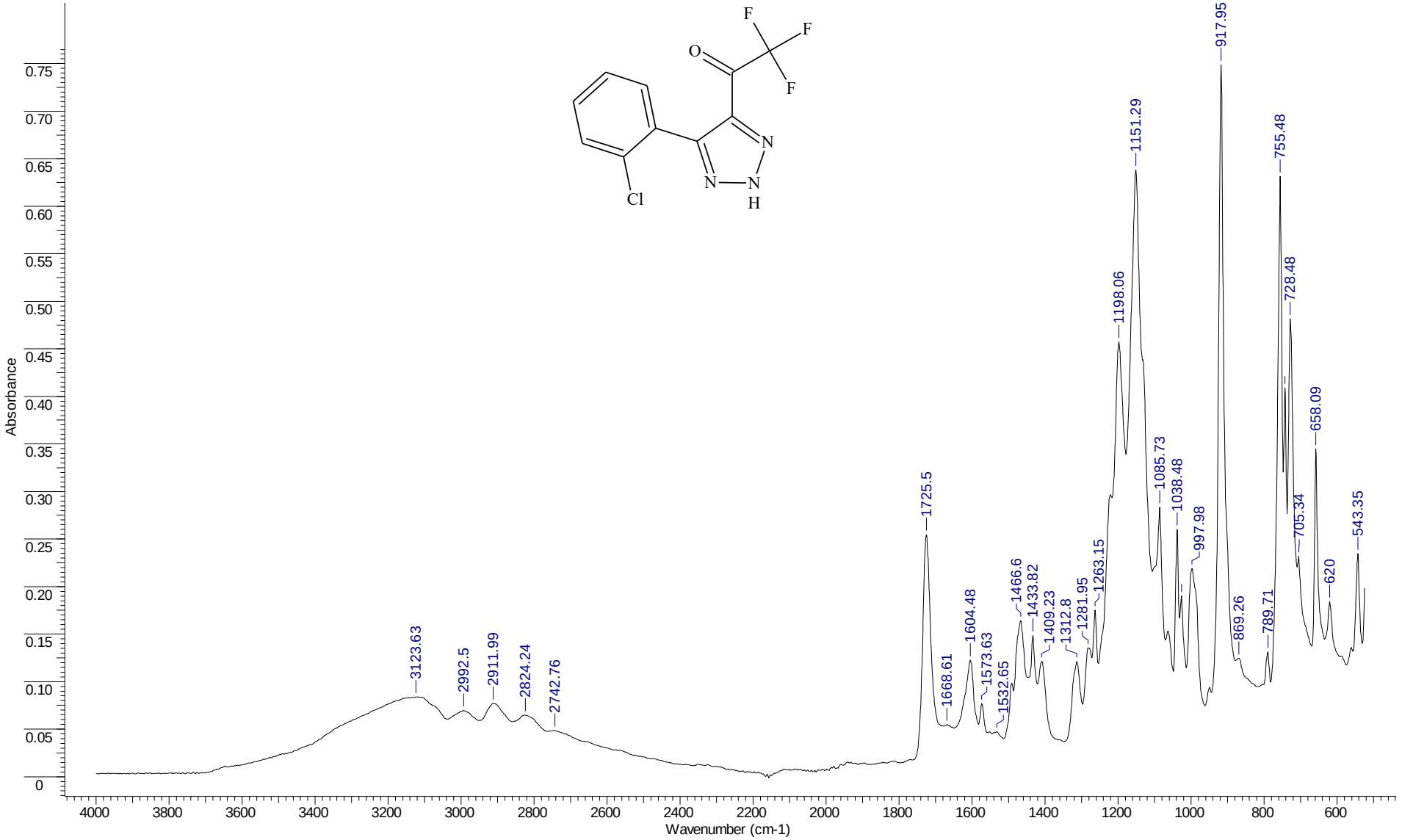
Title	腆玎脲怦觇? 绿 -2359 (窝 湾 磬殇屑靶) iD7						
File Name	C:\DOCS\BM\IR SPECTRA\08-11-2022_13-23-31\腆玎脲怦觇? 绿 -2359 (窝 湾 磬殇屑靶) ID7.SPA					***Date Stamp***	08 Nov 2022 09:38:16
Date	08 Nov 2022 13:56:40	***Technique***	Infrared	***Spectral Region***	IR	***X Axis***	Wavenumber (cm-1)
Y Axis	Absorbance	***Spectrum Range***	525.0250 - 4000.1229	***Points Count***	7209	***Data Spacing***	0.4821



FT-IR spectra of **2k**

8 Nov 2022

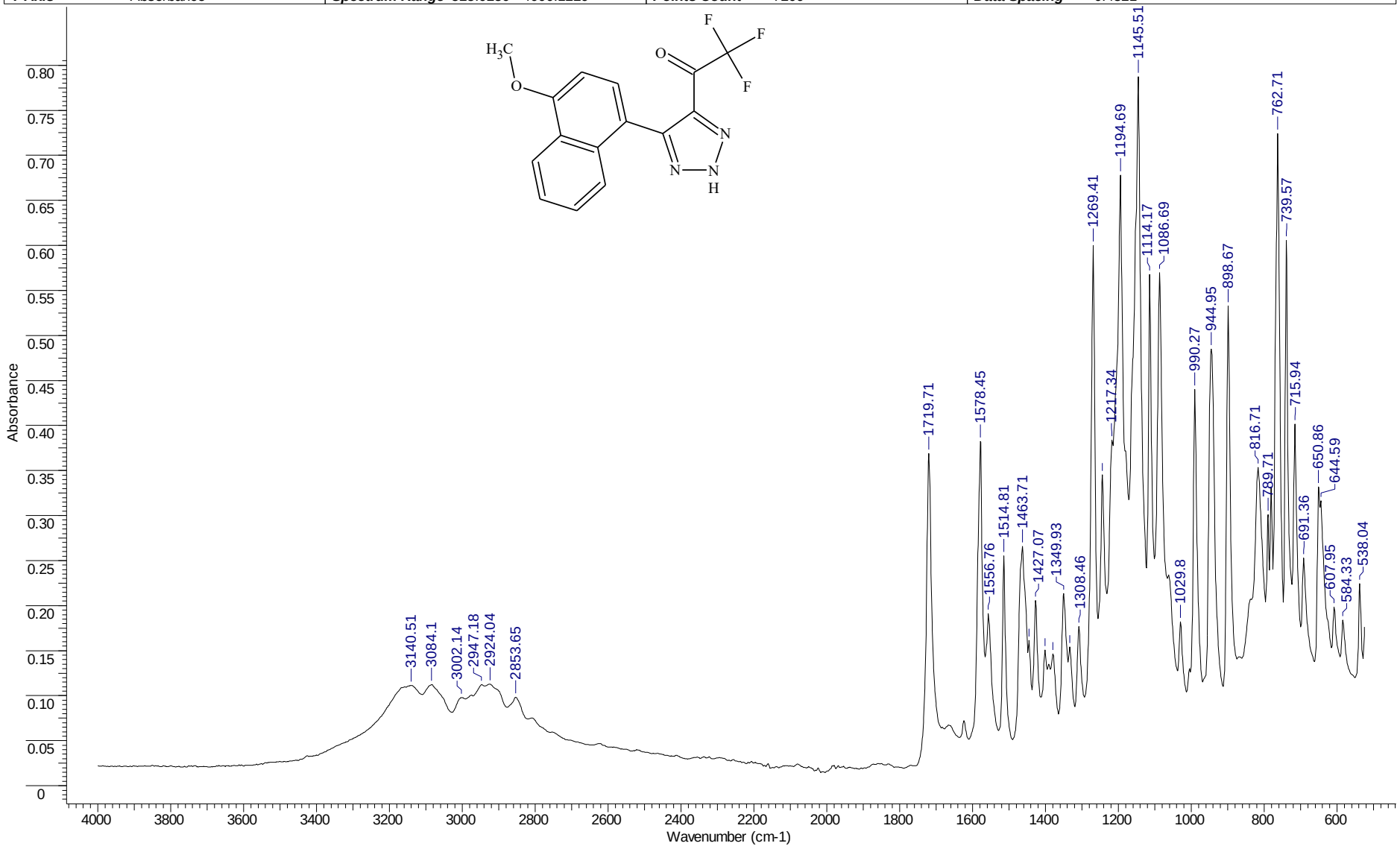
Title	腆 玨腺怦觇? 绿 -2358-3 (窝 湾 磬殇屑靓) iD7						
File Name	C:\DOCS\BM\IR SPECTRA\07-11-2022_15-26-24\腆 玨腺怦觇? 绿 -2358-3 (窝 湾 磬殇屑靓) ID7.SPA					***Date Stamp***	07 Nov 2022 12:19:57
Date	07 Nov 2022 18:49:50	***Technique***	Infrared	***Spectral Region***	IR	***X Axis***	Wavenumber (cm-1)
Y Axis	Absorbance	***Spectrum Range***	525.0250 - 4000.1229	***Points Count***	7209	***Data Spacing***	0.4821



FT-IR spectra of **2l**

8 Nov 2022

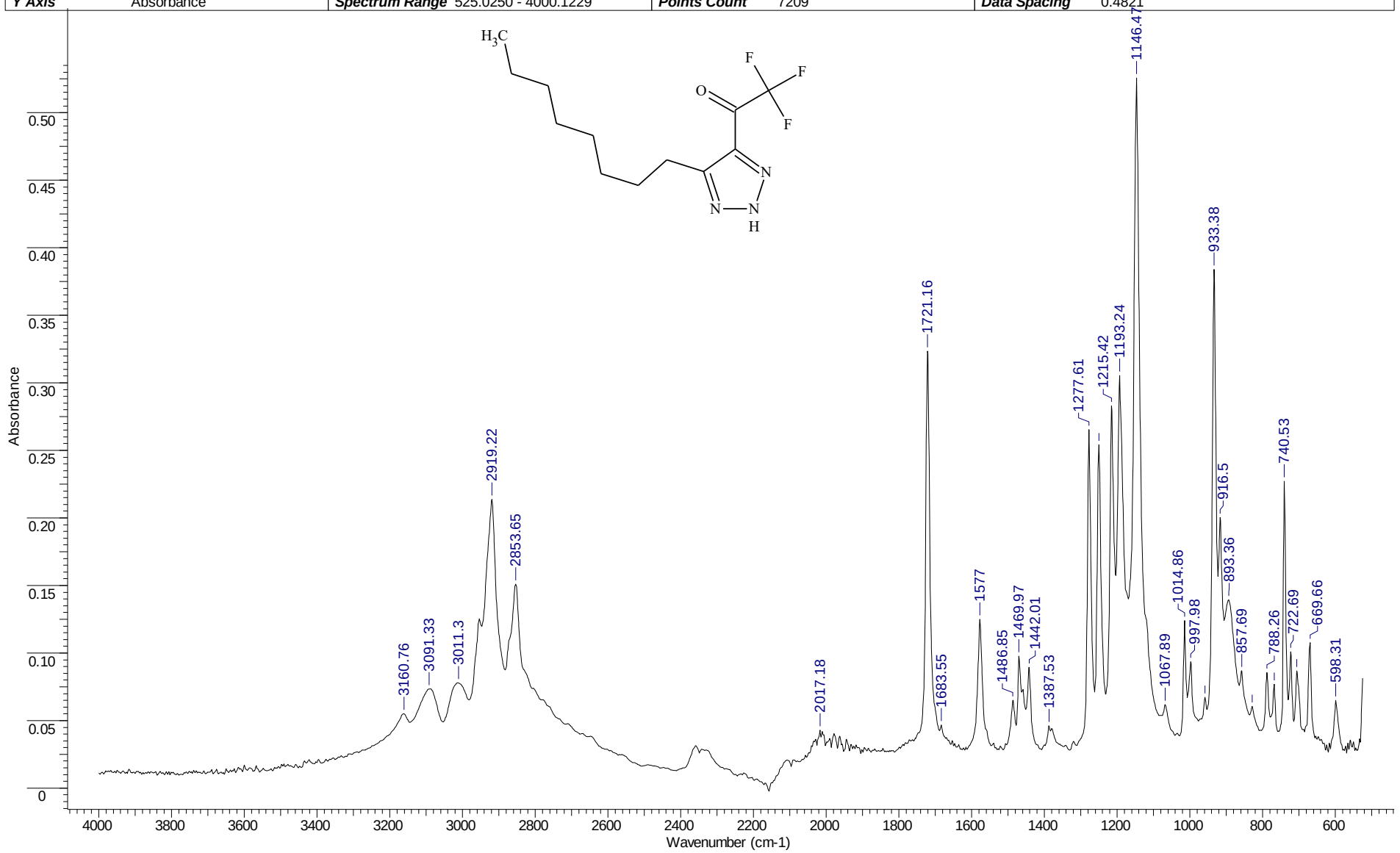
Title	腆 玎脲怦觇? 绿 -2361 (窝 湾 磬殇屑戳) iD7						
File Name	C:\DOCS\BM\IR SPECTRA\07-11-2022_15-26-24\腆 玎脲怦觇? 绿 -2361 (窝 湾 磬殇屑戳) ID7.SPA					***Date Stamp***	07 Nov 2022 12:08:13
Date	07 Nov 2022 18:49:50	***Technique***	Infrared	***Spectral Region***	IR	***X Axis***	Wavenumber (cm-1)
Y Axis	Absorbance	***Spectrum Range***	525.0250 - 4000.1229	***Points Count***	7209	***Data Spacing***	0.4821



FT-IR spectra of **2n**

8 Nov 2022

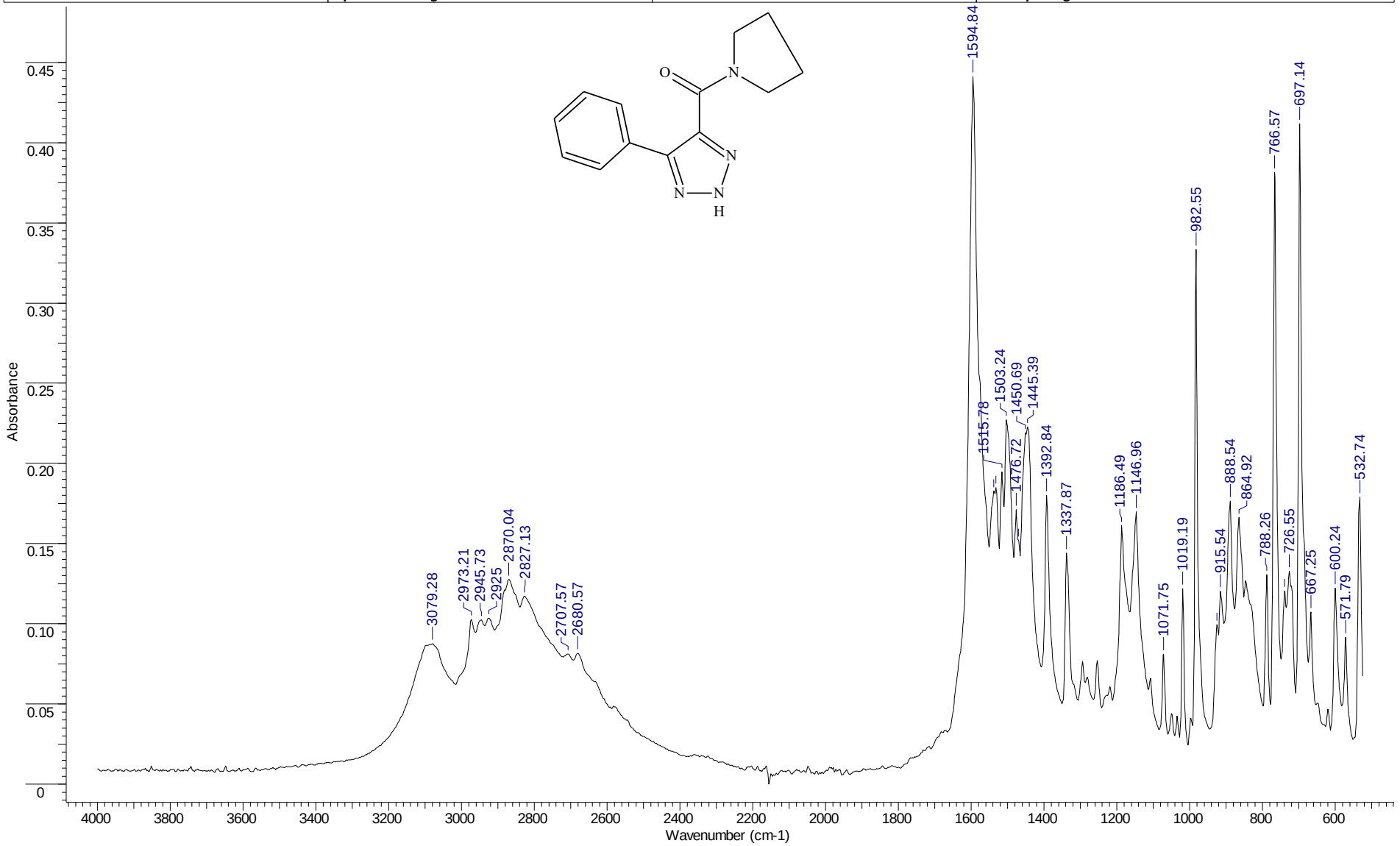
Title	腆 玨脲怦觇? 绿 -2356-3 (窝 湾 磬殇屑靓) iD7						
File Name	C:\DOCS\BM\IR SPECTRA\08-11-2022_13-23-31\腆 玨脲怦觇? 绿 -2356-3 (窝 湾 磬殇屑靓) ID7.SPA					***Date Stamp***	08 Nov 2022 10:06:09
Date	08 Nov 2022 13:56:38	***Technique***	Infrared	***Spectral Region***	IR	***X Axis***	Wavenumber (cm-1)
Y Axis	Absorbance	***Spectrum Range***	525.0250 - 4000.1229	***Points Count***	7209	***Data Spacing***	0.4821



FT-IR spectra of **2o**

8 Nov 2022

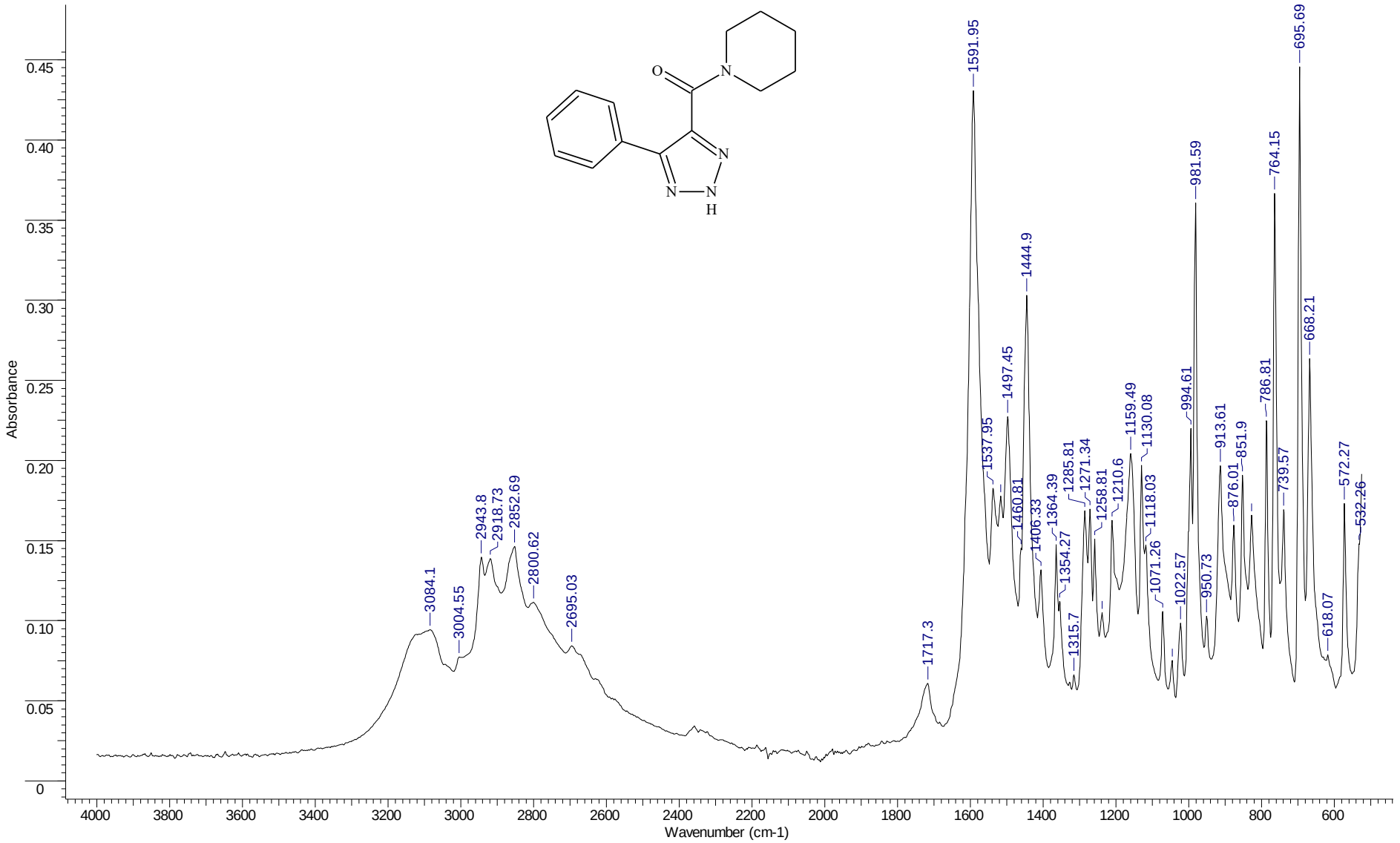
Title	*腆 玎脲怦觇? 绿 -2447-3 (窝 湾 磬殇屑戳) iD7						
File Name	C:\DOCS\BM\IR SPECTRA\07-11-2022_15-26-24\腆 玎脲怦觇? 绿 -2447-3 (窝 湾 磬殇屑戳) ID7.SPA					***Date Stamp***	07 Nov 2022 11:20:07
Date	07 Nov 2022 18:49:52	***Technique***	Infrared	***Spectral Region***	IR	***X Axis***	Wavenumber (cm-1)
Y Axis	Absorbance	***Spectrum Range***	525.0250 - 4000.1229	***Points Count***	7209	***Data Spacing***	0.4821



FT-IR spectra of **4**

8 Nov 2022

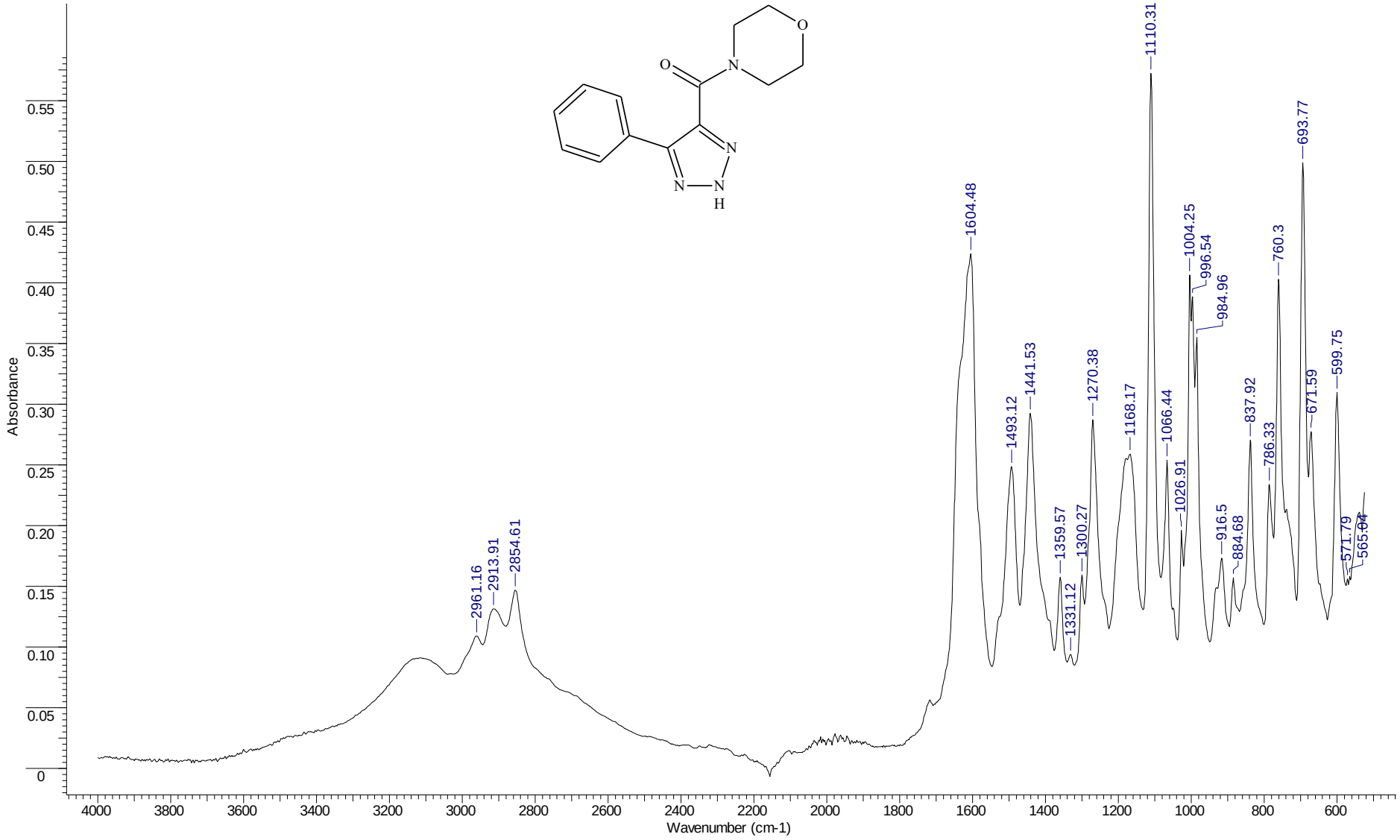
Title	腆玨脲怦觇? 绿 -2449-2? （窝　湾磬殇屑颤）iD7						
File Name	C:\DOCS\BM\IR SPECTRA\07-11-2022_15-26-24\腆玨脲怦觇? 绿 -2449-2? （窝　湾磬殇屑颤）ID7.SPA					***Date Stamp***	07 Nov 2022 11:38:08
Date	07 Nov 2022 18:49:52	***Technique***	Infrared	***Spectral Region***	IR	***X Axis***	Wavenumber (cm-1)
Y Axis	Absorbance	***Spectrum Range***	525.0250 - 4000.1229	***Points Count***	7209	***Data Spacing***	0.4821



FT-IR spectra of **5**

8 Nov 2022

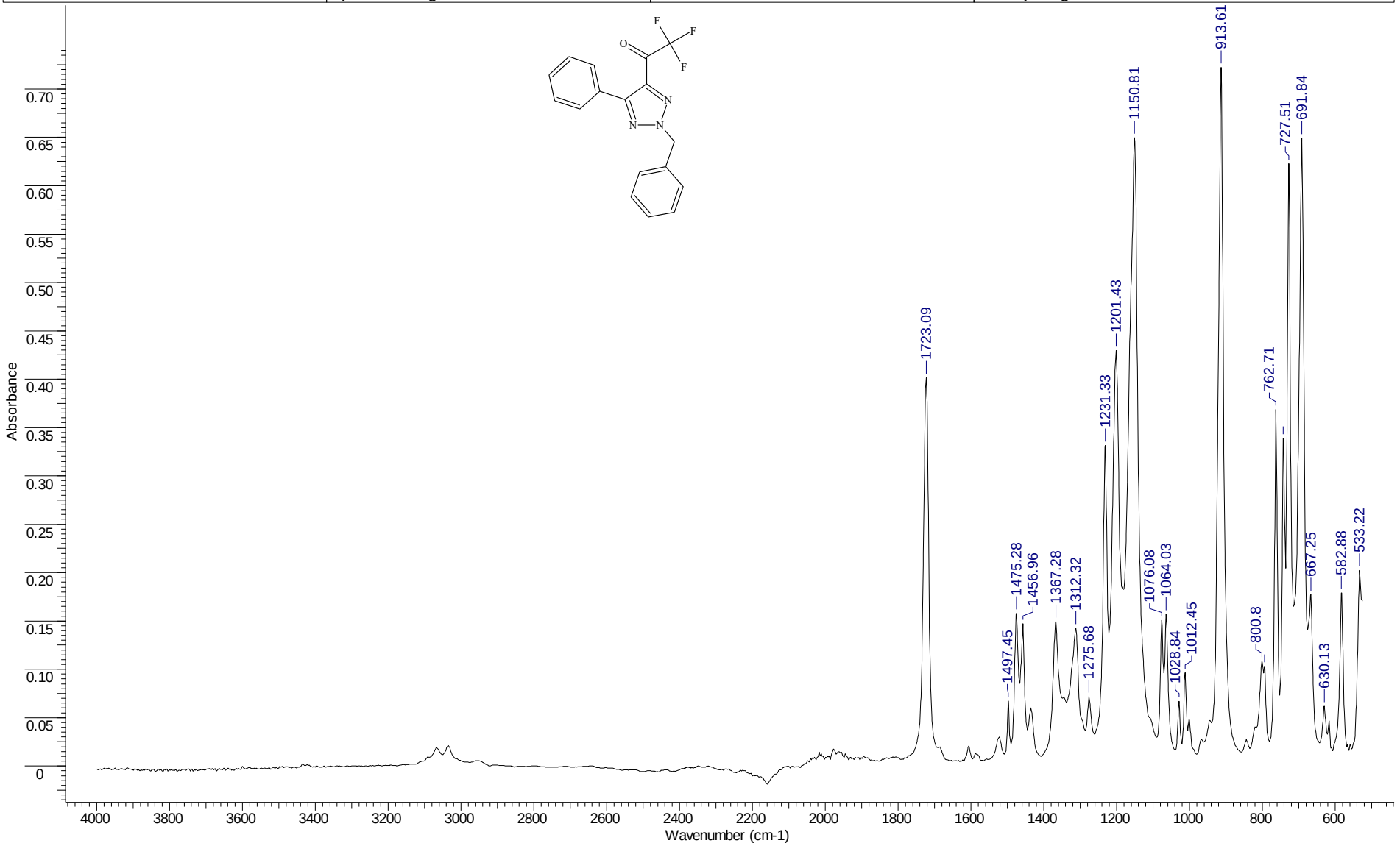
Title	腆 玎脲怦觇? 绿 -2450 (窝 湾 磬殇屑戮) iD7						
File Name	C:\DOCS\BM\IR SPECTRA\08-11-2022_13-23-31\腆 玎脲怦觇? 绿 -2450 (窝 湾 磬殇屑戮) ID7.SPA					***Date Stamp***	08 Nov 2022 09:29:32
Date	08 Nov 2022 13:56:38	***Technique***	Infrared	***Spectral Region***	IR	***X Axis***	Wavenumber (cm-1)
Y Axis	Absorbance	***Spectrum Range***	525.0250 - 4000.1229	***Points Count***	7209	***Data Spacing***	0.4821



FT-IR spectra of **6**

8 Nov 2022

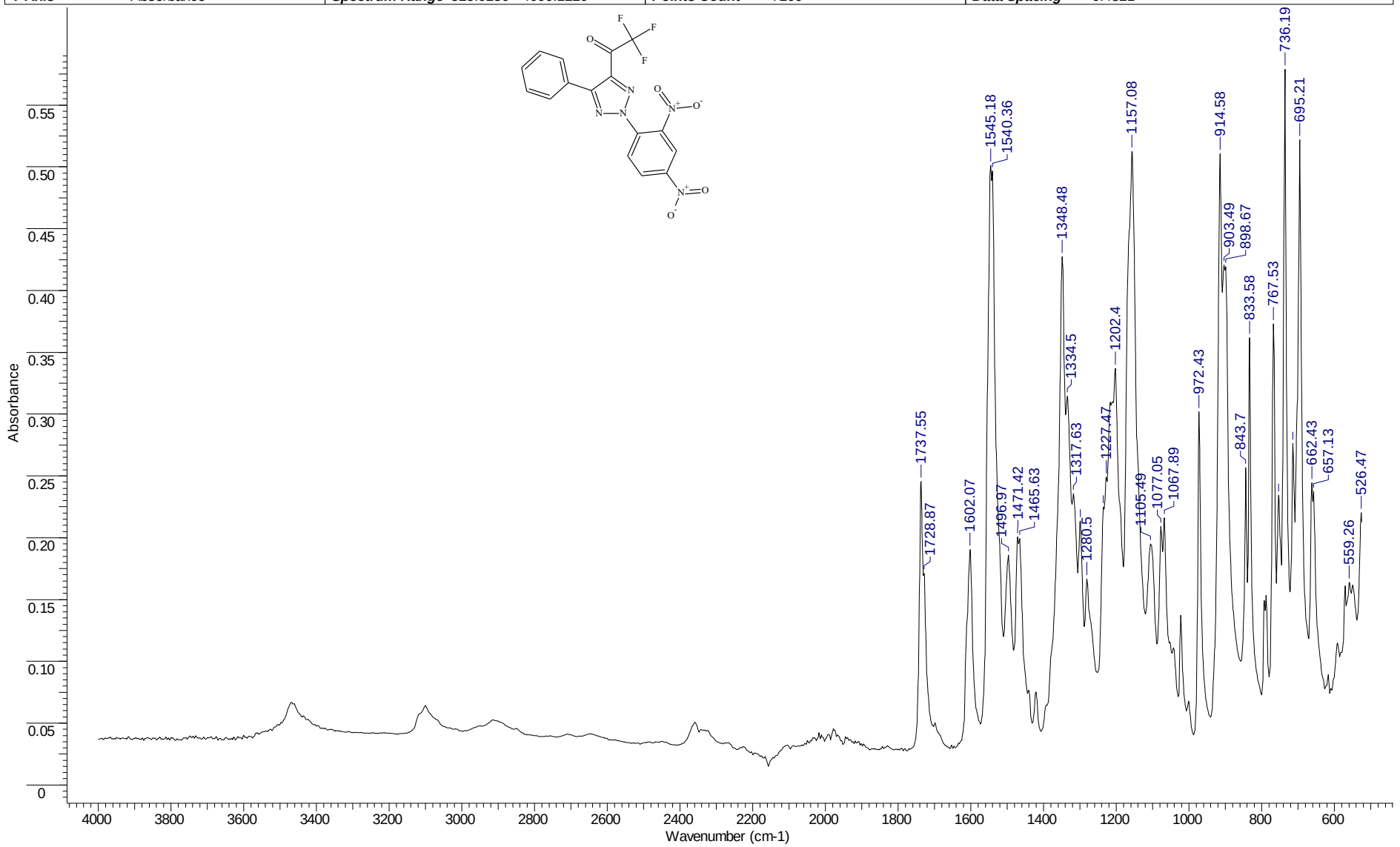
Title	腆 玨脲怦觇? 绿 -2448-7 (窝 湾 磬殇屑靶) iD7						
File Name	C:\DOCS\BM\IR SPECTRA\08-11-2022_13-23-31\腆 玨脲怦觇? 绿 -2448-7 (窝 湾 磬殇屑靶) ID7.SPA					***Date Stamp***	08 Nov 2022 09:33:50
Date	08 Nov 2022 13:56:40	***Technique***	Infrared	***Spectral Region***	IR	***X Axis***	Wavenumber (cm-1)
Y Axis	Absorbance	***Spectrum Range***	525.0250 - 4000.1229	***Points Count***	7209	***Data Spacing***	0.4821



FT-IR spectra of **7**

8 Nov 2022

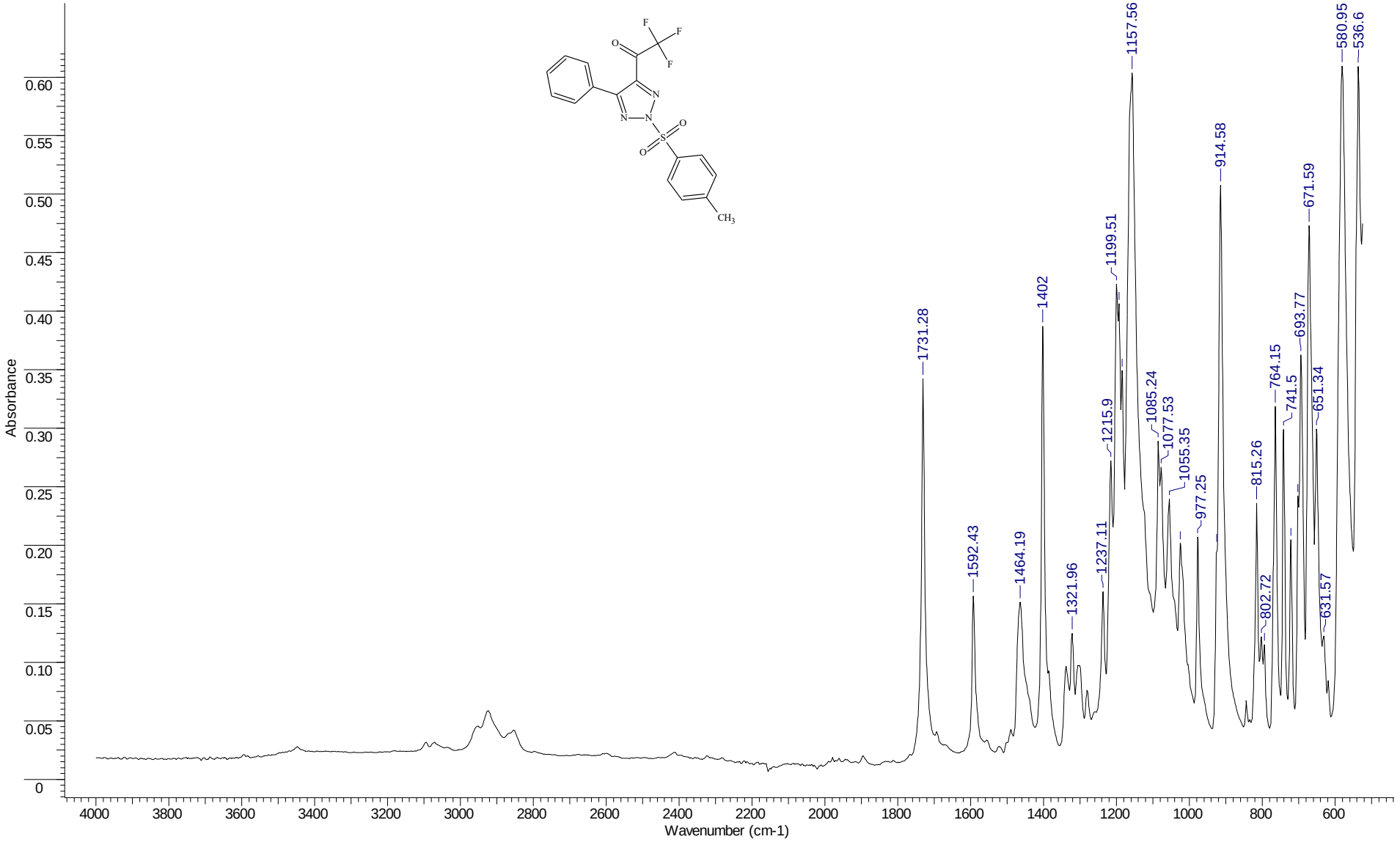
Title	腆玎脲怦觇? 绿 -2461 (窝 湾 磬殇屑靶) iD7						
File Name	C:\DOCS\BM\IR SPECTRA\08-11-2022_13-23-31\腆玎脲怦觇? 绿 -2461 (窝 湾 磬殇屑靶) ID7.SPA					***Date Stamp***	08 Nov 2022 10:00:55
Date	08 Nov 2022 13:56:38	***Technique***	Infrared	***Spectral Region***	IR	***X Axis***	Wavenumber (cm-1)
Y Axis	Absorbance	***Spectrum Range***	525.0250 - 4000.1229	***Points Count***	7209	***Data Spacing***	0.4821



FT-IR spectra of **9**

8 Nov 2022

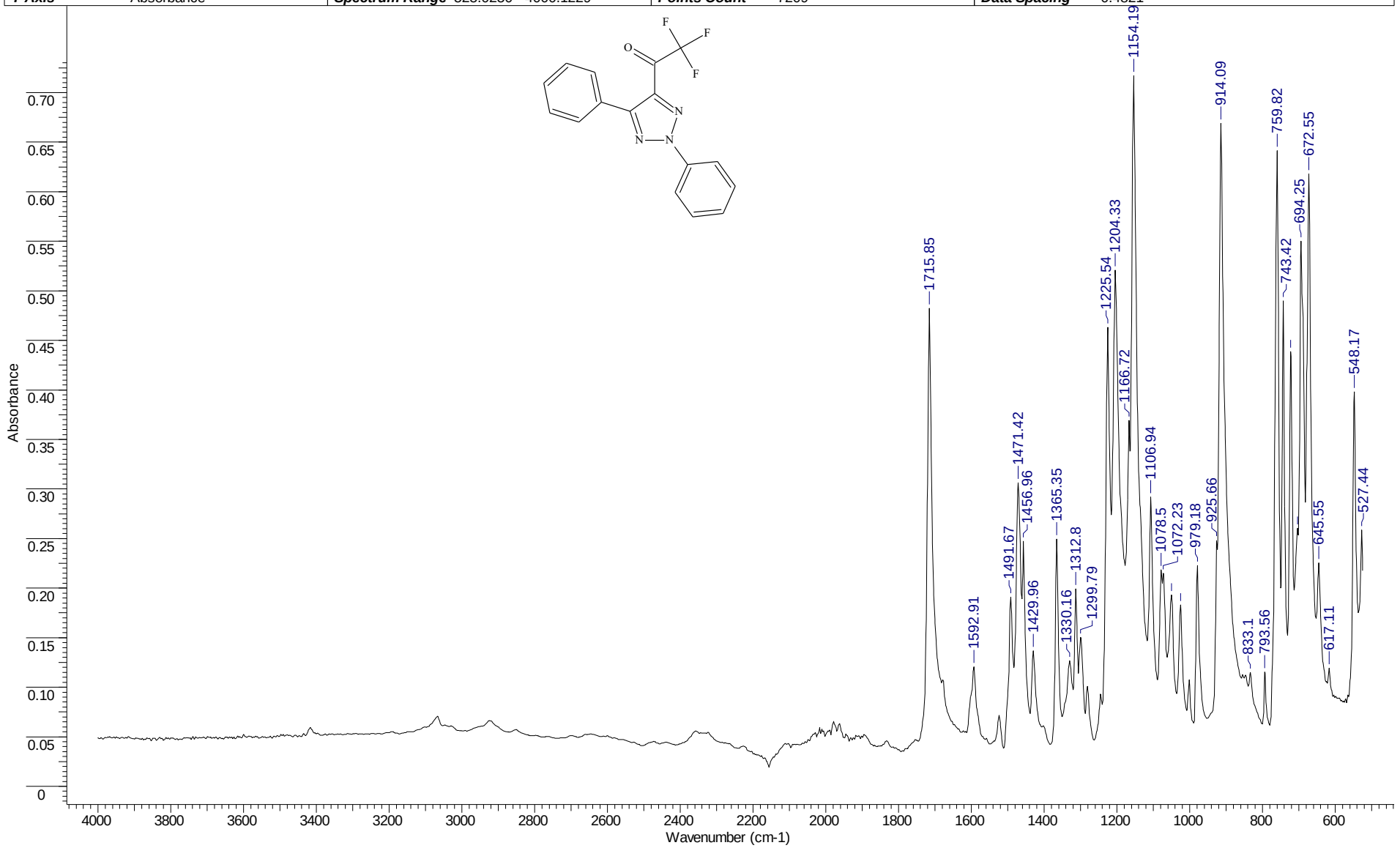
Title	腆 玎腺怦觇? 绿 -2470 (窝 湾 磬殇屑靓) iD7						
File Name	C:\DOCS\BM\IR SPECTRA\08-11-2022_13-23-31\腆 玎腺怦觇? 绿 -2470 (窝 湾 磬殇屑靓) ID7.SPA					***Date Stamp***	08 Nov 2022 10:14:22
Date	08 Nov 2022 13:56:38	***Technique***	Infrared	***Spectral Region***	IR	***X Axis***	Wavenumber (cm-1)
Y Axis	Absorbance	***Spectrum Range***	525.0250 - 4000.1229	***Points Count***	7209	***Data Spacing***	0.4821



FT-IR spectra of **10**

8 Nov 2022

Title	腆 玎腺怦觇? 绿 -2505-2 (窝 湾 磬殇屑靓) iD7						
File Name	C:\DOCS\BM\IR SPECTRA\08-11-2022_13-23-31\腆 玎腺怦觇? 绿 -2505-2 (窝 湾 磬殇屑靓) ID7.SPA					***Date Stamp***	08 Nov 2022 09:51:38
Date	08 Nov 2022 13:56:38	***Technique***	Infrared	***Spectral Region***	IR	***X Axis***	Wavenumber (cm-1)
Y Axis	Absorbance	***Spectrum Range***	525.0250 - 4000.1229	***Points Count***	7209	***Data Spacing***	0.4821



FT-IR spectra of **11**

Computational Details

Geometry optimizations were conducted at the DFT level using the Perdew-Burke-Ernzerhof (PBE) functional. Valence electrons were treated using a TZ2P basis set. The innermost electrons of non-hydrogen atoms were emulated using effective core potentials ECP-SBKJC. Stationary points were characterized as minima (i=0) or first order transition states (i=1) by calculations of normal modes of vibrations at the same level. Single point energy calculations were done using the long-range-corrected LPBE density functional, a scalar-relativistic approximation, L1 wavefunction, and density-fitting basis sets implemented in PRIRODA program.[10,11] Solvent effects using CPCM[12] approach and D4 dispersion corrections were calculated using PBE functional and def2-TZVP basis set using Orca 5.0.3 release. Optimized geometries are collected in separate .xyz file. Utilization of long-range-corrected functionals, combination of explicit and implicit solvent models, dispersion corrections for correct modeling of chemical reactions in condensed phase is comprehensively reviewed by Grimme et al. recently.

In modeling of the azide formation under non-acidic conditions we used combination of explicit solvation model to emulate first solvation shell of sodium cation with four ethanol molecules and CPCM approach for the outer shell. Modeling of transformation of neutral alleneole **D** was performed using three explicit ethanol molecules for correct description of hydrogen transfer reactions mediated by solvent molecules.

Table S3. Calculated energy parameters (E_t = E_{Total}(LPBE/L1) a.u.; G = G(PBE/TZ2p) kcal/mol; E_s = Solvation energy (PBE(CPCM)/def2-TZVP) a.u.; E_d = Van der Waals Correction E_d(PBE(CPCM)/def2-TZVP) a.u.; G = E_t + G + E_s + E_d kcal/mol).

Molecule	E_t	G	E_s	E_d	G
A	-1706.52455	229.4	-0.03466	-0.05853	0.0
TS-AB	-1706.51818	232.8	-0.02839	-0.06145	9.5
B	-1706.55538	232.9	-0.03108	-0.06295	-16.4
TS-BC	-1706.53316	234.2	-0.03356	-0.06484	-3.8
C	-1706.65590	236.2	-0.03263	-0.06465	-78.2
D	-1389.41392	196.1	-0.01544	-0.04982	0.0
TS-DE	-1389.38577	194.1	-0.02066	-0.05508	9.1
TS-DG	-1389.38029	195.5	-0.01699	-0.05163	18.5
E	-1389.41885	193.9	-0.02226	-0.04988	-9.5

TS-E3	-1389.38029	194.6	-0.02364	-0.05231	12.9
3 + N_2	-1389.49533	185.6	-0.01960	-0.04757	-62.8
TS-E2	-1389.37969	194.2	-0.01879	-0.05258	15.8
2	-1389.49415	199.3	-0.02084	-0.05250	-52.2