

Supporting Information

Mechanochemical Decarbonylative Transformation of Amide Group to OCF₃ and CF₃ Functionalities under Ruthenium Catalysis.

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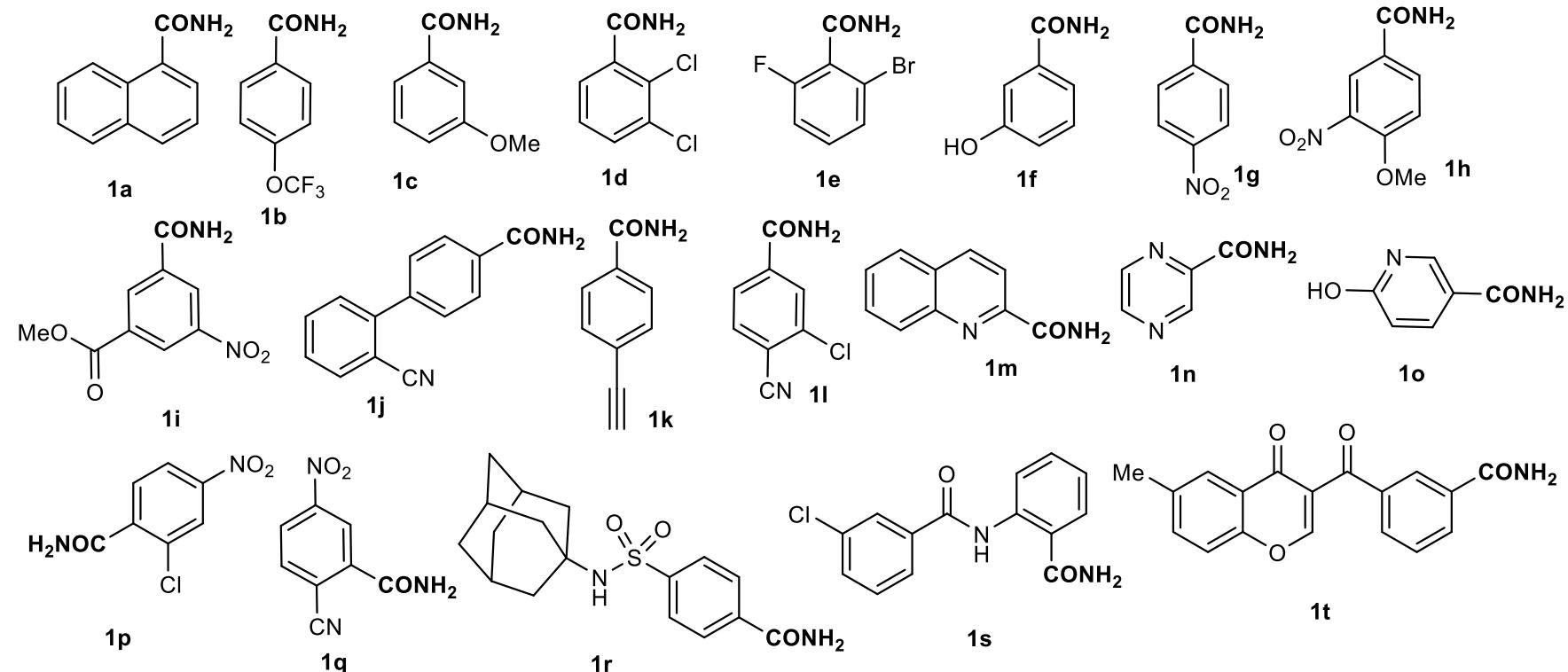
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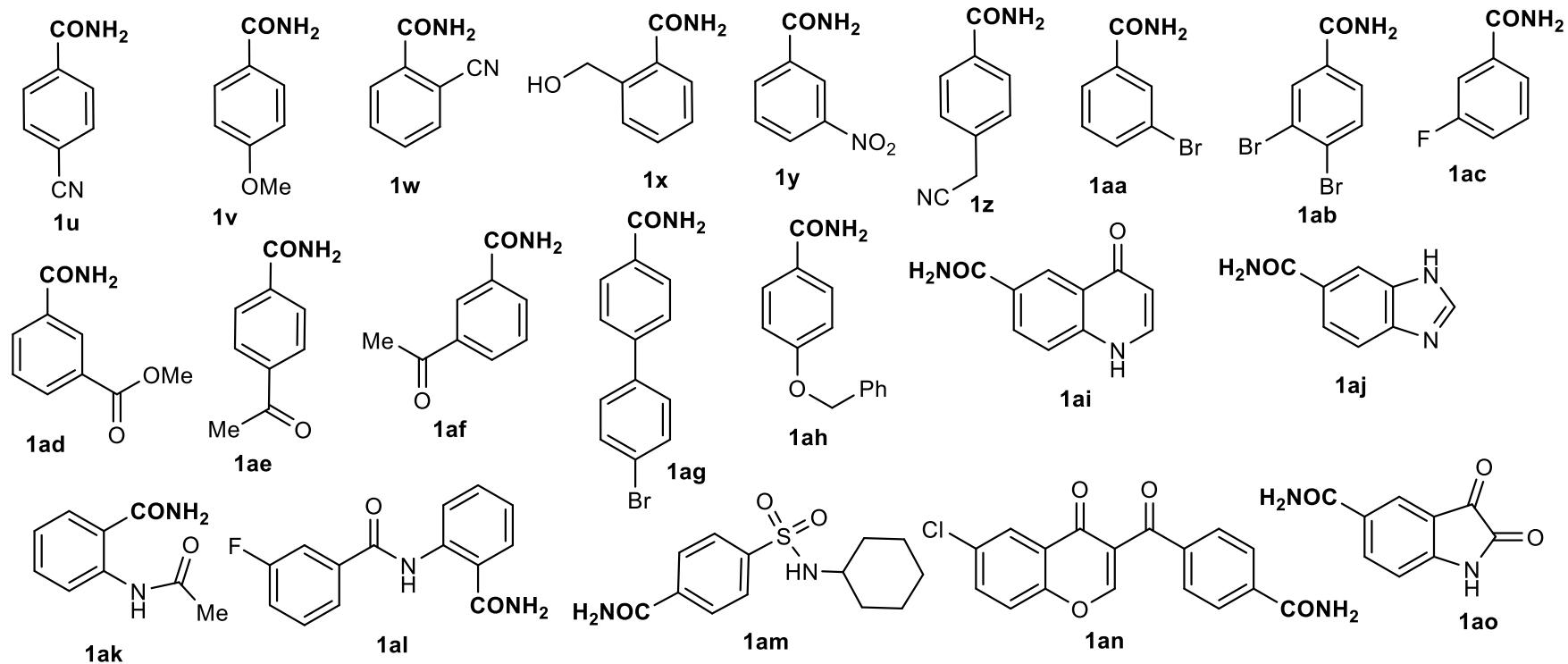
(A) Experimental Section.

Commercially available starting materials, reagents, catalysts, anhydrous and degassed solvents were used without further purification. Flash column chromatography was performed with Merck Silica gel 60 (230-400 mesh). The solvents for column chromatography were distilled before the use. Thin layer chromatography was carried out using Merck TLC Silica gel 60 F₂₅₄ and visualized by short-wavelength ultraviolet light or by treatment with potassium permanganate (KMnO₄) stain. ¹H, ¹³C and ¹⁹F NMR spectra were recorded on a Bruker 400 and 600 MHz at 20°C. All ¹H NMR spectra are reported in parts per million (ppm) downfield of TMS and were measured relative to the signals for CHCl₃ (7.26 ppm) and DMSO (2.50 ppm). All ¹³C{¹H} and ¹⁹F{¹H} NMR spectra were reported in ppm relative to residual CHCl₃ (77.00 ppm) or DMSO (39.70 ppm) and were obtained with ¹H decoupling. Coupling constants, *J*, are reported in Hertz (Hz). Gas chromatographic analyses was performed on Gas Chromatograph Mass Spectrometer GCMS-QP2010 Ultra instrument. Mechanochemical synthesis was performed using the Retsch MM400 mill. Liquid chemicals were dosed using gas tight micro syringes. Isolation of obtained compounds was achieved by column chromatography on Silica gel. All commercially available compounds were purchased from appropriate vendors.

(A-1) Scope of reagents used



Scheme S1. List of amide substrates used for trifluoromethylation.



Scheme S2. List of amide substrates used for trifluoromethylation.

(A-2) Reaction procedures with optimised reaction conditions.

Synthesis of trifluoromethyl arenes.

General procedure for the in-solution attempts:

Inside a glovebox, starting amide (1.0 mmol, 1.0 equiv.), pyrlyium tetrafluoroborate (185 mg, 1.1 mmol, 1.1 equiv.), CF_3SiMe_3 (185 mg, 1.3 mmol, 1.3 equiv.), ruthenium(III) acetylacetone (8 mg, 0.02 mmol, 0.02 equiv.), BaTiO_3 (700 mg, 3.0 mmol, 3.0 equiv.) were weighed and placed successively into an Ace Pressure Tube equipped with a magnetic stir bar. Finally, 10 mL of an appropriate solvent was added inside the glovebox, then the reaction vessel was capped with a stopper. Subsequently, the Pressure Tube was taken out of

the glovebox and heated at appropriate temperature for 24 hours. Upon completion, the reaction mixture was cooled to room temperature and analysed by TLC and GS MS. Finally, the reaction mixture was concentrated under vacuum, the formed crude was washed with water, filtrated and dried. The residue was subjected to preparative column chromatography on Silica gel using hexane/ethyl acetate mixtures.

General procedure for the solid-state reaction:

Inside a glovebox, a stainless steel 5 mL grinding vessel equipped with four balls (stainless steel, $\phi=5$ mm) was loaded consecutively with an appropriate amide (1.0 mmol, 1.0 equiv.), pyrlyium tetrafluoroborate (185 mg, 1.1 mmol, 1.1 equiv.), BaTiO_3 (700 mg, 3.0 mmol, 3.0 equiv.), ruthenium(III) acetylacetone (8 mg, 0.02 mmol, 0.02 equiv.) and 0.1 mL of 1,4-dioxane. Lastly, CF_3SiMe_3 (185 mg, 1.3 mmol, 1.3 equiv.) was added and the reaction vessel was properly sealed. The reaction vessel was installed on the ball mill and the content was pulverized at 30Hz for 90 minutes. After completion of the reaction, the content of the vessel was directly subjected to flash chromatography on silica gel to isolate the desired compound using gradient elution.

Synthesis of aryl trifluoromethyl ethers.

General procedure for the in-solution attempts:

Inside a glovebox, a starting amide (1.0 mmol, 1.0 equiv.), pyrlyium tetrafluoroborate (185 mg, 1.1 mmol, 1.1 equiv.), 1-methyl-1,4-diazabicyclo[2.2.2]octan-1-iun trifluoromethanolate (**3**) (318 mg, 1.5 mmol, 1.5 equiv.) BaTiO_3 (700 mg, 3.0 mmol, 3.0 equiv.), ruthenium(III) acetylacetone (8 mg, 0.02 mmol, 0.02 equiv.) were weighed and placed successively into an Ace Pressure Tube equipped with a magnetic stir bar. Finally, 10 mL of an appropriate solvent were added inside the glovebox, then the reaction vessel was capped with a stopper. Subsequently, the Pressure Tube was taken out of the glovebox and heated at appropriate temperature for 24 hours. Upon completion, the reaction mixture was cooled to room temperature and analysed by TLC and GS MS. Finally, the reaction mixture was concentrated under vacuum, the formed crude was washed with water, filtrated and dried. The residue was subjected to preparative column chromatography on Silica gel using hexane/ethyl acetate mixtures.

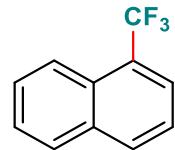
General procedure for the solid-state reaction:

Inside a glovebox, a stainless steel 5 mL grinding vessel equipped with four balls (stainless steel, $\phi=5$ mm) was loaded consecutively with an appropriate amide (1.0 mmol, 1.0 equiv.), pyrlyium tetrafluoroborate (185 mg, 1.1 mmol, 1.1 equiv.), BaTiO_3 (700 mg, 3.0 mmol, 3.0 equiv.), ruthenium(III) acetylacetone (8 mg, 0.02 mmol, 0.02 equiv.) and 0.1 mL of 1,4-dioxane. Lastly, freshly prepared salt **3** (1-methyl-1,4-diazabicyclo[2.2.2]octan-1-iun trifluoromethoxide) (318 mg, 1.5 mmol, 1.5 equiv.) was added and the reaction vessel was properly sealed. The reaction vessel was installed on the ball mill and the contents were pulverized at 30Hz for 90 minutes. After

completion of the reaction, the content of the vessel was directly subjected to flash chromatography on silica gel to isolate the desired compound using gradient elution.

(B) Characterization of products.

1-(trifluoromethyl)naphthalene 2a



The title compound was prepared starting from amide **1a** (171 mg, 1.0 mmol, 1.0 equiv.), pyrlyium tetrafluoroborate (185 mg, 1.1 mmol, 1.1 equiv.), BaTiO_3 (700 mg, 3.0 mmol, 3.0 equiv.), ruthenium(III) acetylacetone (8 mg, 0.02 mmol, 0.02 equiv.), 0.1 mL of 1,4-dioxane and CF_3SiMe_3 (185 mg, 1.3 mmol, 1.3 equiv.). The purification was accomplished by column chromatography on silica gel to provide the desired product **2a** (164 mg, 0.84 mmol, 84%).

Colourless liquid. **$^1\text{H NMR}$** (400 MHz, CDCl_3): δ 7.50 (t, 1H, $^3J = 7.8$ Hz, CH_{Ar}), 7.55 – 7.65 (m, 2H, CH_{Ar}), 7.86 (d, 1H, $^3J = 7.3$ Hz, CH_{Ar}), 7.92 (dd, 1H, $^3J = 7.5$ Hz, $^4J = 1.1$ Hz, CH_{Ar}), 8.02 (d, 1H, $^3J = 8.3$ Hz, CH_{Ar}), 8.2 (dd, 1H, $^3J = 8.4$ Hz, $^4J = 0.8$ Hz, CH_{Ar}).

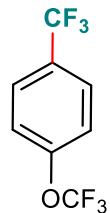
$^{13}\text{C}\{^1\text{H}\} \text{NMR}$ (100 MHz, CDCl_3): δ 124.2, 124.3 (q, $J_{\text{C-F}} = 2.3$ Hz), 124.7 (q, $J_{\text{C-F}} = 6.0$ Hz), 124.8 (q, $^1J_{\text{C-F}} = 274.0$ Hz,), 126.0, 126.6, 127.6, 128.8, 129.0, 133.7, 133.9.

$^{19}\text{F NMR}$ (376 MHz, CDCl_3): δ -59.74 (s, 3F, CF_3).

MS (GC, 70eV): m/z (%) = 196 (M+, 100), 177 (16), 146 (31).

Anal. calcd. for $\text{C}_{11}\text{H}_7\text{F}$: C, 67.35; H, 3.60. Found: C, 67.49; H, 3.53.

1-(trifluoromethoxy)-4-(trifluoromethyl)benzene 2b



The title compound was prepared starting from amide **1b** (205 mg, 1.0 mmol, 1.0 equiv.), pyrlyium tetrafluoroborate (185 mg, 1.1 mmol, 1.1 equiv.), BaTiO₃ (700 mg, 3.0 mmol, 3.0 equiv.), ruthenium(III) acetylacetone (8 mg, 0.02 mmol, 0.02 equiv.), 0.1 mL of 1,4-dioxane and CF₃SiMe₃ (185 mg, 1.3 mmol, 1.3 equiv.). The purification was accomplished by column chromatography on silica gel to provide the desired product **2b** (174 mg, 0.85 mmol, 85%).

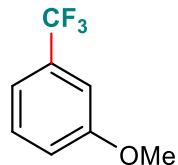
Colourless liquid. ¹H NMR (400 MHz, CDCl₃): δ 7.33 (d, 2H, ³J = 8.5 Hz, CH_{Ar}), 7.68 (d, 2H, ³J = 8.7 Hz, CH_{Ar}).

¹³C{¹H} NMR (100 MHz, CDCl₃): δ 120.3 (q, ¹J_{C-F} = 259.0 Hz, OCF₃), 120.9, 123.6 (q, ¹J_{C-F} = 272.0 Hz, CF₃), 127.3 (q, J_{C-F} = 3.7 Hz), 129.1 (q, J_{C-F} = 33.8 Hz), 151.6.

¹⁹F NMR (376 MHz, CDCl₃): δ -62.55 (S, 3F, CF₃), -57.92 (S, 3F, OCF₃).

Anal. calcd. for C₈H₄F₆O: C, 41.76; H, 1.75. Found: C, 41.92; H, 1.69.

1-methoxy-3-(trifluoromethyl)benzene **2c**



The title compound was prepared starting from amide **1c** (151 mg, 1.0 mmol, 1.0 equiv.), pyrlyium tetrafluoroborate (185 mg, 1.1 mmol, 1.1 equiv.), BaTiO₃ (700 mg, 3.0 mmol, 3.0 equiv.), ruthenium(III) acetylacetone (8 mg, 0.02 mmol, 0.02 equiv.), 0.1 mL of 1,4-dioxane and CF₃SiMe₃ (185 mg, 1.3 mmol, 1.3 equiv.). The purification was accomplished by column chromatography on silica gel to provide the desired product **2c** (146 mg, 0.83 mmol, 83%).

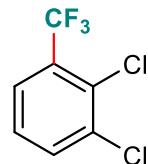
Colourless liquid. ¹H NMR (600 MHz, CDCl₃): δ 3.90 (s, 3H, OCH₃), 7.13 (dd, 1H, ³J = 8.4 Hz, ⁴J = 2.5 Hz, CH_{Ar}), 7.19 (d, 1H, ⁴J = 2.6 Hz, CH_{Ar}), 7.27 (s, 1H, CH_{Ar}), 7.44 (t, 1H, ³J = 8.0 Hz, CH_{Ar}).

$^{13}\text{C}\{\text{H}\}$ NMR (151 MHz, CDCl_3): δ 55.4, 110.8 (q, $J_{\text{C-F}} = 3.0$ Hz), 117.3 (q, $J_{\text{C-F}} = 4.5$ Hz), 117.5, 124.0 (q, $^1J_{\text{C-F}} = 273.3$ Hz), 129.9, 131.8 (q, $J_{\text{C-F}} = 31.7$ Hz), 159.7.

^{19}F NMR (564 MHz, CDCl_3) δ -62.8 (s, 3F, CF_3).

Anal. calcd. for $\text{C}_8\text{H}_7\text{F}_3\text{O}$: C, 54.55; H, 4.01. Found: C, 54.51; H, 3.92.

1,2-dichloro-3-(trifluoromethyl)benzene 2d



The title compound was prepared starting from amide **1d** (190 mg, 1.0 mmol, 1.0 equiv.), pyrlyium tetrafluoroborate (185 mg, 1.1 mmol, 1.1 equiv.), BaTiO_3 (700 mg, 3.0 mmol, 3.0 equiv.), ruthenium(III) acetylacetone (8 mg, 0.02 mmol, 0.02 equiv.), 0.1 mL of 1,4-dioxane and CF_3SiMe_3 (185 mg, 1.3 mmol, 1.3 equiv.). The purification was accomplished by column chromatography on silica gel to provide the desired product **2d** (195 mg, 0.91 mmol, 91%).

Colourless liquid. **^1H NMR** (600 MHz, CDCl_3): δ 7.33 (t, 1H, $^3J = 8.0$ Hz, CH_{Ar}), 7.65 (m, 2H, CH_{Ar}).

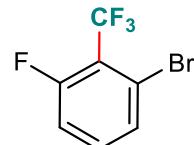
$^{13}\text{C}\{\text{H}\}$ NMR (151 MHz, CDCl_3): δ 122.4 (q, $^1J_{\text{C-F}} = 273.3$ Hz), 125.8 (q, $J_{\text{C-F}} = 6.0$ Hz), 127.2, 130.4 (q, $J_{\text{C-F}} = 31.7$ Hz), 131.0, 133.7, 135.3.

^{19}F NMR (564 MHz, CDCl_3) δ -63.0 (s, 3F, CF_3).

MS (GC, 70eV): m/z (%) = 214 (M+, 100), 216 (64), 197 (13), 195 (17), 181 (18), 179 (52).

Anal. calcd. for $\text{C}_7\text{H}_3\text{F}_3\text{Cl}_2\text{O}$: C, 39.11; H, 1.41. Found: C, 39.23; H, 1.52.

1-bromo-3-fluoro-2-(trifluoromethyl)benzene 2e



The title compound was prepared starting from amide **1e** (218 mg, 1.0 mmol, 1.0 equiv.), pyrlyium tetrafluoroborate (185 mg, 1.1 mmol, 1.1 equiv.), BaTiO_3 (700 mg, 3.0 mmol, 3.0 equiv.), ruthenium(III) acetylacetone (8 mg, 0.02 mmol, 0.02 equiv.), 0.1 mL of 1,4-

dioxane and CF_3SiMe_3 (185 mg, 1.3 mmol, 1.3 equiv.). The purification was accomplished by column chromatography on silica gel to provide the desired product **2e** (194 mg, 0.80 mmol, 80%).

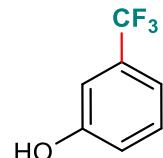
Colourless liquid. **$^1\text{H NMR}$** (400 MHz, CDCl_3): δ 7.15 (dd, 1H, $^3J = 11.1$ Hz, $^4J = 8.4$ Hz, CH_{Ar}), 7.35 (td, 1H, $^3J = 8.2$ Hz, $^4J = 5.3$ Hz, CH_{Ar}), 7.52 (d, 1H, $^3J = 8.1$ Hz, CH_{Ar}).

$^{13}\text{C}\{^1\text{H}\} \text{NMR}$ (100 MHz, CDCl_3): δ 116.5 (d, $J_{\text{C-F}} = 23.6$ Hz), 118.6 (qd, $J_{\text{C-F}} = 32.3$ Hz, $J_{\text{C-F}} = 12.0$ Hz), 121.1, 122.1 (qd, $^1J_{\text{C-F}} = 274.6$ Hz, $J_{\text{C-F}} = 2.5$ Hz), 130.9 (d, $J_{\text{C-F}} = 3.6$ Hz), 133.7 (d, $J_{\text{C-F}} = 10.2$ Hz), 160.8 (d, $^1J_{\text{C-F}} = 261.2$ Hz).

$^{19}\text{F NMR}$ (376 MHz, CDCl_3): δ -107.9 (qdd, 1F, $J = 31.7$ Hz, $J = 11.0$ Hz, $J = 5.1$ Hz, CF), -56.6 (d, 3F, $J = 31.7$ Hz, CF_3).

Anal. calcd. for $\text{C}_7\text{H}_3\text{F}_4\text{Br}$: C, 34.60; H, 1.24. Found: C, 34.49; H, 1.11.

3-(trifluoromethyl)phenol **2f**



The title compound was prepared starting from amide **1f** (218 mg, 1.0 mmol, 1.0 equiv.), pyrlyium tetrafluoroborate (185 mg, 1.1 mmol, 1.1 equiv.), BaTiO_3 (700 mg, 3.0 mmol, 3.0 equiv.), ruthenium(III) acetylacetone (8 mg, 0.02 mmol, 0.02 equiv.), 0.1 mL of 1,4-dioxane and CF_3SiMe_3 (185 mg, 1.3 mmol, 1.3 equiv.). The purification was accomplished by column chromatography on silica gel to provide the desired product **2f** (125 mg, 0.77 mmol, 77%).

Yellowish liquid. **$^1\text{H NMR}$** (600 MHz, CDCl_3): δ 5.05 (s, 1H, OH), 7.00 (dd, 1H, $^3J = 8.2$ Hz, $^4J = 2.6$ Hz, CH_{Ar}), 7.08 (s, 1H, CH_{Ar}), 7.20 (d, 1H, $J = 7.7$ Hz, CH_{Ar}), 7.35 (t, 1H, $^3J = 7.9$ Hz, CH_{Ar}).

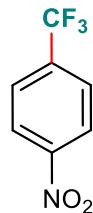
$^{13}\text{C}\{^1\text{H}\} \text{NMR}$ (151 MHz, CDCl_3): δ 112.3 (q, $J_{\text{C-F}} = 3.0$ Hz), 117.6 (q, $J_{\text{C-F}} = 3.0$ Hz), 118.8, 123.7 (q, $^1J_{\text{C-F}} = 271.8$ Hz), 130.2, 132.1 (q, $J_{\text{C-F}} = 31.7$ Hz), 155.6.

$^{19}\text{F NMR}$ (564 MHz, CDCl_3): δ -62.8 (s, 3F, CF_3).

MS (GC, 70eV): m/z (%) = 162 (M+, 100), 143 (32), 114 (20).

Anal. calcd. for $\text{C}_7\text{H}_5\text{F}_3\text{O}$: C, 51.86; H, 3.11. Found: C, 51.96; H, 3.23.

1-nitro-4-(trifluoromethyl)benzene **2g**



The title compound was prepared starting from amide **1g** (166 mg, 1.0 mmol, 1.0 equiv.), pyrlyium tetrafluoroborate (185 mg, 1.1 mmol, 1.1 equiv.), BaTiO_3 (700 mg, 3.0 mmol, 3.0 equiv.), ruthenium(III) acetylacetone (8 mg, 0.02 mmol, 0.02 equiv.), 0.1 mL of 1,4-dioxane and CF_3SiMe_3 (185 mg, 1.3 mmol, 1.3 equiv.). The purification was accomplished by column chromatography on silica gel to provide the desired product **2g** (153 mg, 0.80 mmol, 80%).

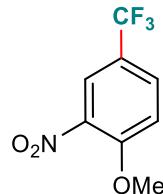
Yellowish solid, mp 39 °C. $^1\text{H NMR}$ (400 MHz, CDCl_3): δ 7.85 (d, 2H, $^3J = 8.7$ Hz, CH_{Ar}), 8.37 (d, 2H, $^3J = 8.6$ Hz, CH_{Ar}).

$^{13}\text{C}\{\text{H}\}$ NMR (100 MHz, CDCl_3): δ 123.0 (q, $^1J_{\text{C-F}} = 272.8$ Hz), 124.1, 124.8, 126.8 (q, $J_{\text{C-F}} = 3.7$ Hz), 136.2 (q, $J_{\text{C-F}} = 33.7$ Hz), 138.7, 150.1.

$^{19}\text{F NMR}$ (376 MHz, CDCl_3): δ -63.24 (s, 3F, $-\text{CF}_3$).

Anal. calcd. for $\text{C}_7\text{H}_4\text{F}_3\text{NO}_2$: C, 43.99; H, 2.11; N, 7.33. Found: C, 44.06; H, 2.17; N, 7.25.

1-methoxy-2-nitro-4-(trifluoromethyl)benzene 2h



The title compound was prepared starting from amide **1h** (196 mg, 1.0 mmol, 1.0 equiv.), pyrlyium tetrafluoroborate (185 mg, 1.1 mmol, 1.1 equiv.), BaTiO_3 (700 mg, 3.0 mmol, 3.0 equiv.), ruthenium(III) acetylacetone (8 mg, 0.02 mmol, 0.02 equiv.), 0.1 mL of 1,4-dioxane and CF_3SiMe_3 (185 mg, 1.3 mmol, 1.3 equiv.). The purification was accomplished by column chromatography on silica gel to provide the desired product **2h** (181 mg, 0.82 mmol, 82%).

Yellow solid, mp 48-49 °C. $^1\text{H NMR}$ (600 MHz, CDCl_3): δ 4.03 (s, 3H, OCH_3), 7.21 (d, 1H, $^3J = 8.8$ Hz, CH_{Ar}), 7.80 (dd, 1H, $^3J = 8.8$ Hz, $^4J = 2.4$ Hz, CH_{Ar}), 8.11 (d, 1H, $^4J = 2.5$ Hz, CH_{Ar}).

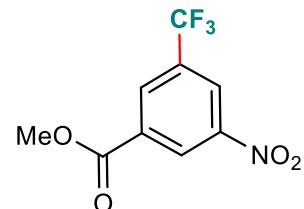
$^{13}\text{C}\{\text{H}\}$ NMR (151 MHz, CDCl_3): δ 57.0, 114.0, 122.9 (q, $J_{\text{C-F}} = 34.7$ Hz), 123.3 (q, $^1J_{\text{C-F}} = 271.8$ Hz), 123.4 (q, $J_{\text{C-F}} = 3.0$ Hz), 131.1 (q, $J_{\text{C-F}} = 3.0$ Hz), 139.4, 155.4.

^{19}F NMR (564 MHz, CDCl_3): δ -62.0 (s, 3F, CF_3).

MS (GC, 70eV): m/z (%) = 221 (M+, 44), 202 (26), 191 (62), 174 (100), 161 (40), 1610 (66), 145 (88), 141 (18), 132 (39), 126 (32).

Anal. calcd. for $\text{C}_8\text{H}_6\text{F}_3\text{NO}_3$: C, 43.45; H, 2.73; N, 6.33. Found: C, 43.61; H, 2.80; N, 6.36.

methyl 3-nitro-5-(trifluoromethyl)benzoate 2i



The title compound was prepared starting from amide **1i** (224 mg, 1.0 mmol, 1.0 equiv.), pyrlyium tetrafluoroborate (185 mg, 1.1 mmol, 1.1 equiv.), BaTiO_3 (700 mg, 3.0 mmol, 3.0 equiv.), ruthenium(III) acetylacetone (8 mg, 0.02 mmol, 0.02 equiv.), 0.1 mL of 1,4-dioxane and CF_3SiMe_3 (185 mg, 1.3 mmol, 1.3 equiv.). The purification was accomplished by column chromatography on silica gel to provide the desired product **2i** (206 mg, 0.83 mmol, 83%).

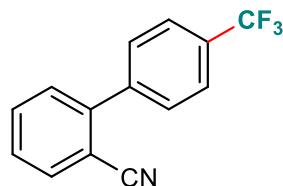
Pale white solid, mp 35-37 °C. **^1H NMR** (400 MHz, CDCl_3): δ 4.04 (s, 3H, OCH_3), 8.63 (s, 1H, CH_{Ar}), 8.68 (s, 1H, CH_{Ar}), 9.05 (s, 1H, CH_{Ar}).

$^{13}\text{C}\{\text{H}\}$ NMR (100 MHz, CDCl_3): δ 53.3, 122.4 (q, $^1J_{\text{C-F}} = 273.4$ Hz), 124.4 (q, $J_{\text{C-F}} = 3.7$ Hz), 127.5, 131.9 (q, $J_{\text{C-F}} = 3.5$ Hz), 132.8 (q, $J_{\text{C-F}} = 34.7$ Hz), 133.2, 148.5, 163.7.

^{19}F NMR (376 MHz, CDCl_3): δ -62.96 (s, 3F, CF_3).

Anal. calcd. for $\text{C}_9\text{H}_6\text{F}_3\text{NO}_4$: C, 43.39; H, 2.43; N, 5.62. Found: C, 43.29; H, 2.52; N, 5.70.

4'-(trifluoromethyl)-[1,1'-biphenyl]-2-carbonitrile 2j



The title compound was prepared starting from amide **1j** (222 mg, 1.0 mmol, 1.0 equiv.), pyrlyium tetrafluoroborate (185 mg, 1.1 mmol, 1.1 equiv.), BaTiO₃ (700 mg, 3.0 mmol, 3.0 equiv.), ruthenium(III) acetylacetone (8 mg, 0.02 mmol, 0.02 equiv.), 0.1 mL of 1,4-dioxane and CF₃SiMe₃ (185 mg, 1.3 mmol, 1.3 equiv.). The purification was accomplished by column chromatography on silica gel to provide the desired product **2j** (220 mg, 0.89 mmol, 89%).

White solid, mp 103-104 °C. ¹H NMR (400 MHz, CDCl₃): δ 7.47 – 7.52 (m, 2H, CH_{Ar}), 77.66 – 7.70 (m, 3H, CH_{Ar}), 7.73 – 7.75 (m, 2H, CH_{Ar}), 7.78 (dd, 1H, ³J = 7.8 Hz, ⁴J = 0.8 Hz, CH_{Ar}).

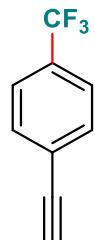
¹³C{¹H} NMR (100 MHz, CDCl₃): δ 111.3, 118.2, 124.0 (q, ¹J_{C-F} = 272.7 Hz), 125.7 (q, ¹J_{C-F} = 3.7 Hz), 128.4, 130.0, 130.8 (q, ¹J_{C-F} = 32.5 Hz), 133.1, 133.9, 141.7, 143.8.

¹⁹F NMR (376 MHz, CDCl₃): δ -62.65 (s, 3F, CF₃).

MS (GC, 70eV): m/z (%) = 247 (M+, 100).

Anal. calcd. for C₁₄H₈F₃N: C, 68.02; H, 3.26; N, 5.67. Found: C, 68.13; H, 3.33; N, 5.51.

1-ethynyl-4-(trifluoromethyl)benzene 2k



The title compound was prepared starting from amide **1k** (145 mg, 1.0 mmol, 1.0 equiv.), pyrlyium tetrafluoroborate (185 mg, 1.1 mmol, 1.1 equiv.), BaTiO₃ (700 mg, 3.0 mmol, 3.0 equiv.), ruthenium(III) acetylacetone (8 mg, 0.02 mmol, 0.02 equiv.), 0.1 mL of 1,4-dioxane and CF₃SiMe₃ (185 mg, 1.3 mmol, 1.3 equiv.). The purification was accomplished by column chromatography on silica gel to provide the desired product **2k** (220 mg, 0.63 mmol, 63%).

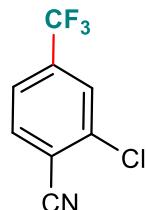
Colorless liquid. **¹H NMR** (400 MHz, CDCl₃): δ 3.19 (s, 1H, CH), 7.59 (br s, 4H, CH_{Ar}).

¹³C{¹H} NMR (100 MHz, CDCl₃): δ 77.7, 80.3, 121.9 (q, $^{1}J_{C-F}$ = 272.6 Hz), 123.3 (q, J_{C-F} = 3.8 Hz), 124.0 (d, J_{C-F} = 1.2 Hz), 128.6 (q, J_{C-F} = 32.8 Hz), 130.5.

¹⁹F NMR (376 MHz, CDCl₃): δ -63.0 (s, 3F, CF₃).

Anal. calcd. for C₉H₅F₃: C, 63.54; H, 2.96. Found: C, 63.42; H, 3.01.

2-chloro-4-(trifluoromethyl)benzonitrile 2l



The title compound was prepared starting from amide **1l** (180 mg, 1.0 mmol, 1.0 equiv.), pyrlyium tetrafluoroborate (185 mg, 1.1 mmol, 1.1 equiv.), BaTiO₃ (700 mg, 3.0 mmol, 3.0 equiv.), ruthenium(III) acetylacetone (8 mg, 0.02 mmol, 0.02 equiv.), 0.1 mL of 1,4-dioxane and CF₃SiMe₃ (185 mg, 1.3 mmol, 1.3 equiv.). The purification was accomplished by column chromatography on silica gel to provide the desired product **2l** (185 mg, 0.90 mmol, 90%).

White solid, mp 83-84 °C. **¹H NMR** (400 MHz, CDCl₃): δ 7.66 (d, 1H, ^{3}J = 8.2 Hz, CH_{Ar}), 7.80 (s, 1H, CH_{Ar}), 7.84 (d, 1H, ^{3}J = 8.1 Hz, CH_{Ar}).

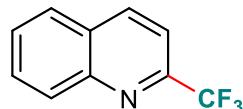
¹³C{¹H} NMR (100 MHz, CDCl₃): δ 114.7, 117.0, 121.0 (q, $^{1}J_{C-F}$ = 273.6 Hz), 124.1 (q, J_{C-F} = 3.6), 127.2 (q, J_{C-F} = 3.8), 134.6, 135.7 (q, J_{C-F} = 34.2), 137.8.

¹⁹F NMR (376 MHz, CDCl₃): δ -63.64 (s, 3F, CF₃).

MS (GC, 70eV): m/z (%) = 205 (M+, 100), 186 (23), 170 (34).

Anal. calcd. for C₈H₃F₃CIN: C, 46.74; H, 1.47; N, 6.81. Found: C, 46.61; H, 1.52; N, 6.95.

2-(trifluoromethyl)quinoline 2m



The title compound was prepared starting from amide **1m** (172 mg, 1.0 mmol, 1.0 equiv.), pyrlyium tetrafluoroborate (185 mg, 1.1 mmol, 1.1 equiv.), BaTiO₃ (700 mg, 3.0 mmol, 3.0 equiv.), ruthenium(III) acetylacetone (8 mg, 0.02 mmol, 0.02 equiv.), 0.1 mL of 1,4-dioxane and CF₃SiMe₃ (185 mg, 1.3 mmol, 1.3 equiv.). The purification was accomplished by column chromatography on silica gel to provide the desired product **2m** (155 mg, 0.79 mmol, 79%).

White solid, mp 60-61 °C. **¹H NMR** (400 MHz, CDCl₃): δ 7.67 (ddd, 1H, ³J = 8.1 Hz, ⁴J = 6.8 Hz, J = 1.2 Hz, CH_{Ar}), 7.73 (d, 1H, ³J = 8.5 Hz, CH_{Ar}), 7.81 (ddd, 1H, ³J = 8.5 Hz, ⁴J = 6.9 Hz, J = 1.5 Hz, CH_{Ar}), 7.89 (d, 1H, ³J = 8.1, 1.4 Hz, CH_{Ar}), 8.22 (d, 1H, ³J = 8.5, 1.1 Hz, CH_{Ar}), 8.34 (d, 1H, ³J = 8.5 Hz, CH_{Ar}).

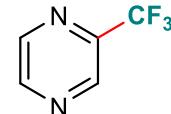
¹³C{¹H} NMR (100 MHz, CDCl₃): δ 116.8 (d, J_{C-F} = 2.10 Hz), 121.6 (q, ¹J_{C-F} = 275.1 Hz), 127.7, 128.6, 128.9, 130.1, 130.8, 138.1, 147.2, 147.9 (q, J_{C-F} = 34.6 Hz).

¹⁹F NMR (376 MHz, CDCl₃): δ -67.5 (s, 3F, CF₃).

MS (GC, 70eV): m/z (%) = 197 (M+, 100), 128 (77), 101 (16).

Anal. calcd. for C₁₀H₆F₃N: C, 60.92; H, 3.07; N, 7.10. Found: C, 61.04; H, 3.19; N, 6.98.

2-(trifluoromethyl)pyrazine **2n**



The title compound was prepared starting from amide **1n** (180 mg, 1.0 mmol, 1.0 equiv.), pyrlyium tetrafluoroborate (185 mg, 1.1 mmol, 1.1 equiv.), BaTiO₃ (700 mg, 3.0 mmol, 3.0 equiv.), ruthenium(III) acetylacetone (8 mg, 0.02 mmol, 0.02 equiv.), 0.1 mL of 1,4-dioxane and CF₃SiMe₃ (185 mg, 1.3 mmol, 1.3 equiv.). The purification was accomplished by column chromatography on silica gel to provide the desired product **2n** (185 mg, 0.71 mmol, 71%).

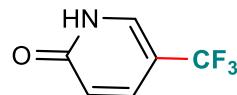
Colorless liquid. **¹H NMR** (400 MHz, CDCl₃): δ 8.73 (s, 1H, CH_{Ar}), 8.83 (d, 1H, J = 2.3 Hz, CH_{Ar}), 7.73 (s, 1H, CH_{Ar}),

¹³C{¹H} NMR (100 MHz, CDCl₃): δ 121.0 (q, ¹J_{C-F} = 272.8 Hz), 141.9 (q, J_{C-F} = 3.3 Hz), 144.1 (q, J_{C-F} = 35.5 Hz), 144.4, 147.8.

¹⁹F NMR (376 MHz, CDCl₃): δ -67.85 (s, 3F, CF₃).

Anal. calcd. for C₅H₃F₃N₂: C, 40.55; H, 2.04; N, 18.92. Found: C, 40.45; H, 1.96; N, 19.03.

5-(trifluoromethyl)pyridin-2-ol **2o**



The title compound was prepared starting from amide **1o** (138 mg, 1.0 mmol, 1.0 equiv.), pyrylium tetrafluoroborate (185 mg, 1.1 mmol, 1.1 equiv.), BaTiO₃ (700 mg, 3.0 mmol, 3.0 equiv.), ruthenium(III) acetylacetone (8 mg, 0.02 mmol, 0.02 equiv.), 0.1 mL of 1,4-dioxane and CF₃SiMe₃ (185 mg, 1.3 mmol, 1.3 equiv.). The purification was accomplished by column chromatography on silica gel to provide the desired product **4o** (106 mg, 0.65 mmol, 65%).

White solid, mp 145–146 °C. ¹H NMR (400 MHz, DMSO-d₆): δ 6.51 (d, 1H, ³J = 9.7 Hz, CH_{Ar}), 7.66 (dd, 1H, J = 9.7, 2.8 Hz, CH_{Ar}), 7.95 (q, 1H, J = 1.6 Hz, CH_{Ar}), 12.22 (s, 1H, -OH).

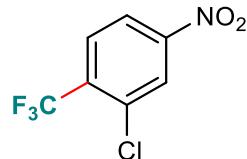
¹³C{¹H} NMR (100 MHz, CDCl₃): δ 107.8 (q, J_{C-F} = 34.4 Hz), 121.4, 124.5 (q, ¹J_{C-F} = 269.1 Hz), 136.7, 162.7.

¹⁹F{¹H} NMR (376 MHz, CDCl₃): δ –55.99 (s, 3F, CF₃).

MS (GC, 70eV): m/z (%) = 163 (M+, 100), 144 (23), 135 (65), 116 (56).

Anal. calcd. for C₆H₄F₃ON: C, 44.19; H, 2.47; N, 8.59. Found: C, 43.98; H, 2.23; N, 8.68.

2-chloro-4-nitro-1-(trifluoromethyl)benzene **2p**



The title compound was prepared starting from amide **1p** (200 mg, 1.0 mmol, 1.0 equiv.), pyrylium tetrafluoroborate (185 mg, 1.1 mmol, 1.1 equiv.), BaTiO₃ (700 mg, 3.0 mmol, 3.0 equiv.), ruthenium(III) acetylacetone (8 mg, 0.02 mmol, 0.02 equiv.), 0.1 mL of 1,4-dioxane and CF₃SiMe₃ (185 mg, 1.3 mmol, 1.3 equiv.). The purification was accomplished by column chromatography on silica gel to provide the desired product **2p** (182 mg, 0.81 mmol, 81%).

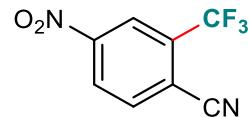
Colourless liquid. ¹H NMR (500 MHz, DMSO-d₆): δ 8.08 (d, 1H, ¹J = 8.6 Hz, CH_{Ar}), 8.28 (d, 1H, ¹J = 8.6 Hz, CH_{Ar}), 8.43 (s, 1H, CH_{Ar}).

¹³C{¹H} NMR (125 MHz, DMSO-d₆): δ 122.4 (q, ¹J_{C-F} = 274.1 Hz), 123.2, 126.7, 130.1 (q, J_{C-F} = 5.2 Hz), 132.2 (q, J_{C-F} = 31.6 Hz), 132.7, 150.7.

HRMS (TOF MS ES⁻) m/z: [M - H]⁺: Calcd for C₇H₃F₃O₂NCl (M-H) 224.9802. Found 224.9804.

Anal. calcd. for C₇H₃F₃O₂NCl: C, 37.28; H, 1.34; N, 6.21. Found: C, 37.39; H, 1.48; N, 6.09.

4-nitro-2-(trifluoromethyl)benzonitrile 2q



The title compound was prepared starting from amide **1q** (191 mg, 1.0 mmol, 1.0 equiv.), pyrlyium tetrafluoroborate (185 mg, 1.1 mmol, 1.1 equiv.), BaTiO₃ (700 mg, 3.0 mmol, 3.0 equiv.), ruthenium(III) acetylacetone (8 mg, 0.02 mmol, 0.02 equiv.), 0.1 mL of 1,4-dioxane and CF₃SiMe₃ (185 mg, 1.3 mmol, 1.3 equiv.). The purification was accomplished by column chromatography on silica gel to provide the desired product **2q** (166 mg, 0.77 mmol, 77%).

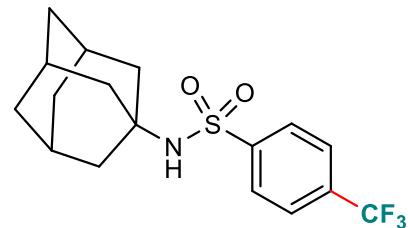
Yellowish solid, mp 52-53 °C. ¹H NMR (500 MHz, CDCl₃): δ 8.13 (d, 1H, ³J = 8.4 Hz, CH_{Ar}), 8.57 (dd, 1H, ³J = 8.5 Hz, ⁴J = 2.2 Hz, CH_{Ar}), 8.65 (d, 1H, ⁴J = 2.3 Hz, CH_{Ar}).

¹³C{¹H} NMR (125 MHz, CDCl₃): δ 113.7, 115.8, 121.3 (q, ¹J_{C-F} = 274.5 Hz), 122.2 (q, J_{C-F} = 4.7 Hz), 127.2, 134.8 (q, J_{C-F} = 33.8 Hz), 136.5, 149.7.

MS (GC, 70eV): m/z (%) = 216 (M+, 40), 186 (32), 170 (100), 150 (14), 143 (14), 120 (19), 100 (17).

Anal. calcd. for C₈H₃F₃O₂N₂: C, 44.46; H, 1.40; N, 12.96. Found: C, 44.60; H, 1.19; N, 13.09.

N-((1s,3s)-adamantan-1-yl)-4-(trifluoromethyl)benzenesulfonamide 2r



The title compound was prepared starting from amide **1r** (334 mg, 1.0 mmol, 1.0 equiv.), pyrlyium tetrafluoroborate (185 mg, 1.1 mmol, 1.1 equiv.), BaTiO₃ (700 mg, 3.0 mmol, 3.0 equiv.), ruthenium(III) acetylacetone (8 mg, 0.02 mmol, 0.02 equiv.), 0.1 mL of 1,4-dioxane and CF₃SiMe₃ (185 mg, 1.3 mmol, 1.3 equiv.). The purification was accomplished by column chromatography on silica gel to provide the desired product **2r** (320 mg, 0.89 mmol, 89%).

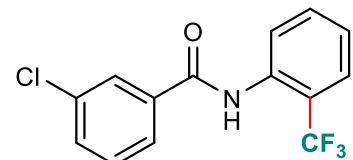
White solid, mp 135 °C. **¹H NMR (500 MHz, DMSO-d₆)**: δ 1.42 – 1.49 (m, 6H, CH), 1.65 (d, 6H, ¹J = 3.0 Hz, CH), 1.87 (s, 3H, CH), 7.81 (s, 1H, NH), 7.92 (d, 2H, ¹J = 8.3 Hz, CH_{Ar}), 8.01 (d, 2H, ¹J = 8.2 Hz, CH_{Ar}).

¹³C{¹H} NMR (125 MHz, DMSO-d₆): δ 29.3, 35.9, 42.9, 54.6, 124.1 (q, ¹J_{C-F} = 272.2 Hz), 126.8, 127.5, 132.1 (q, ¹J_{C-F} = 32.2 Hz), 149.3.

MS (GC, 70eV): m/z (%) = 359 (M+, 45), 302 (55), 145 (26), 132 (20), 93 (100).

Anal. calcd. for C₁₇H₂₀F₃O₂SN: C, 56.81; H, 5.61; N, 3.90. Found: C, 56.63; H, 5.49; N, 4.03.

3-chloro-N-(2-(trifluoromethyl)phenyl)benzamide 2s



The title compound was prepared starting from amide **1s** (274 mg, 1.0 mmol, 1.0 equiv.), pyrylium tetrafluoroborate (185 mg, 1.1 mmol, 1.1 equiv.), BaTiO₃ (700 mg, 3.0 mmol, 3.0 equiv.), ruthenium(III) acetylacetone (8 mg, 0.02 mmol, 0.02 equiv.), 0.1 mL of 1,4-dioxane and CF₃SiMe₃ (185 mg, 1.3 mmol, 1.3 equiv.). The purification was accomplished by column chromatography on silica gel to provide the desired product **2s** (212 mg, 0.71 mmol, 71%).

White solid, mp 166–167 °C. **¹H NMR (400 MHz, CDCl₃)**: δ 7.28 (t, 1H, ¹J = 7.7 Hz, CH_{Ar}), 7.44 (t, 1H, ¹J = 7.8 Hz, CH_{Ar}), 7.55 (d, 1H, ¹J = 8.0 Hz, CH_{Ar}), 7.61 (t, 1H, ¹J = 7.9 Hz, CH_{Ar}), 7.66 (d, 1H, ¹J = 8.0 Hz, CH_{Ar}), 7.70 (d, 1H, ¹J = 7.7 Hz, CH_{Ar}), 7.88 (s, 1H, CH_{Ar}), 8.17 (s, 1H, NH), 8.33 (d, 1H, ¹J = 8.3 Hz, CH_{Ar}).

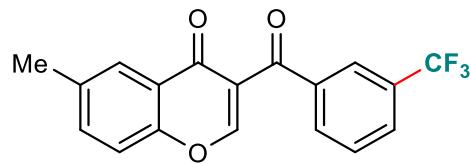
¹³C{¹H} NMR (100 MHz, CDCl₃): δ 120.6 (q, ¹J_{C-F} = 29.6 Hz), 124.2 (q, ¹J_{C-F} = 272.7 Hz), 124.5, 124.7, 124.9, 126.2 (q, ¹J_{C-F} = 5.3 Hz), 127.7, 130.3, 132.4, 133.1, 135.1, 135.3, 136.1, 164.2.

¹⁹F{¹H} NMR (376 MHz, CDCl₃): δ – 60.38 (s, 3F, CF₃).

MS (GC, 70eV): m/z (%) = 299 (M+, 36), 139 (100), 111 (34).

Anal. calcd. for C₁₄H₉ClF₃ON: C, 56.11; H, 3.03; N, 4.67. Found: C, 56.32; H, 2.97; N, 4.79.

6-methyl-3-(3-(trifluoromethyl)benzoyl)-4H-chromen-4-one 2t



The title compound was prepared starting from amide **1t** (327 mg, 1.0 mmol, 1.0 equiv.), pyrlyium tetrafluoroborate (185 mg, 1.1 mmol, 1.1 equiv.), BaTiO₃ (700 mg, 3.0 mmol, 3.0 equiv.), ruthenium(III) acetylacetone (8 mg, 0.02 mmol, 0.02 equiv.), 0.1 mL of 1,4-dioxane and CF₃SiMe₃ (185 mg, 1.3 mmol, 1.3 equiv.). The purification was accomplished by column chromatography on silica gel to provide the desired product **2t** (272 mg, 0.74 mmol, 74%).

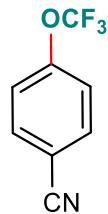
White solid, mp 157-158 °C. **¹H NMR (500 MHz, CDCl₃)**: δ 2.47 (s, 3H, CH₃), 7.45 (d, 1H, ¹J = 8.6 Hz, CH_{Ar}), 7.56 (dd, 1H, ¹J = 8.4 Hz, J = 2.1 Hz, CH_{Ar}), 7.59 (d, 1H, ¹J = 7.8 Hz, CH_{Ar}), 7.82 (d, 1H, ¹J = 7.8 Hz, CH_{Ar}), 7.97 (d, 1H, ¹J = 7.8 Hz, CH_{Ar}), 8.01 (d, 1H, J = 1.0 Hz, CH_{Ar}), 8.10 (s, 1H, CH_{Ar}), 8.36 (s, 1H, CH_{Ar}).

¹³C{¹H NMR (125 MHz, CDCl₃): δ 21.0, 118.2, 123.7 (q, ¹J_{C-F} = 272.3 Hz), 124.3, 124.6, 125.8, 126.2 (q, J_{C-F} = 3.9 Hz), 128.9, 129.7 (q, J_{C-F} = 3.1 Hz), 131.0 (q, J_{C-F} = 32.9 Hz), 132.9, 135.9, 136.6, 137.9, 154.4, 159.6, 174.7, 191.1.

MS (GC, 70eV): m/z (%) = 368 (M+, 58), 303 (100), 283 (23), 254 (21), 207 (28), 189 (70), 128 (26), 154 (49), 126 (13).

Anal. calcd. for C₁₇H₈ClF₃O₄: C, 55.38; H, 2.19. Found: C, 55.16; H, 2.32.

4-(trifluoromethoxy)benzonitrile **4a**



The title compound was prepared starting from amide **1u** (146 mg, 1.0 mmol, 1.0 equiv.), pyrlyium tetrafluoroborate (185 mg, 1.1 mmol, 1.1 equiv.), BaTiO₃ (700 mg, 3.0 mmol, 3.0 equiv.), ruthenium(III) acetylacetone (8 mg, 0.02 mmol, 0.02 equiv.), 0.1 mL of 1,4-dioxane and freshly prepared salt **3** (1-methyl-1,4-diazabicyclo[2.2.2]octan-1-ium trifluoromethoxide) (318 mg, 1.5 mmol, 1.5 equiv.). The purification was accomplished by column chromatography on silica gel to provide the desired product **4a** (153 mg, 0.82 mmol, 82%).

Colorless liquid. **¹H NMR** (400 MHz, CDCl₃): δ 7.33 (d, 2H, ³J = 8.4 Hz, CH_{Ar}), 7.73 (dt, 2H, ³J = 8.8 Hz, ⁴J = 2.3 Hz, CH_{Ar}).

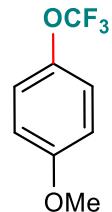
¹³C{¹H} NMR (100 MHz, CDCl₃): δ 110.9, 117.6, 120.2 (q, ¹J_{C-F} = 259.8 Hz), 121.2, 134.2, 152.2.

¹⁹F NMR (376 MHz, CDCl₃): δ -57.83 (S, 3F, OCF₃).

MS (GC, 70eV): m/z (%) = 187 (M+, 100), 90 (19).

Anal. calcd. for C₈H₄F₃NO: C, 51.35; H, 2.15; N, 7.49. Found: C, 51.39; H, 2.07; N, 7.56.

1-methoxy-4-(trifluoromethoxy)benzene 4b



The title compound was prepared starting from amide **1v** (151 mg, 1.0 mmol, 1.0 equiv.), pyrlyium tetrafluoroborate (185 mg, 1.1 mmol, 1.1 equiv.), BaTiO₃ (700 mg, 3.0 mmol, 3.0 equiv.), ruthenium(III) acetylacetone (8 mg, 0.02 mmol, 0.02 equiv.), 0.1 mL of 1,4-dioxane and freshly prepared salt **3** (1-methyl-1,4-diazabicyclo[2.2.2]octan-1-ium trifluoromethoxide) (318 mg, 1.5 mmol, 1.5 equiv.). The purification was accomplished by column chromatography on silica gel to provide the desired product **4b** (153 mg, 0.80 mmol, 80%).

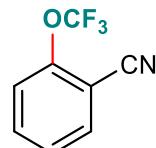
Colorless liquid. **¹H NMR** (600 MHz, CDCl₃): δ 3.92 (s, 3H, OCH₃). 7.00 (d, 2H, ³J = 8.6 Hz, CH_{Ar}), 7.27 (d, 2H, ³J = 8.6 Hz, CH_{Ar}).

¹³C{¹H} NMR (151 MHz, CDCl₃): δ 158.3, 142.9, 122.6, 120.8 (q, ¹J_{C-F} = 255.2 Hz), 114.8, 55.7.

¹⁹F{¹H} NMR (564 MHz, CDCl₃): δ -58.50 (s, 3F, OCF₃).

Anal. calcd. for C₈H₇F₃O₂: C, 50.01; H, 3.67. Found: C, 49.96; H, 3.77.

2-(trifluoromethoxy)benzonitrile 4c



The title compound was prepared starting from amide **1w** (146 mg, 1.0 mmol, 1.0 equiv.), pyrylium tetrafluoroborate (185 mg, 1.1 mmol, 1.1 equiv.), BaTiO₃ (700 mg, 3.0 mmol, 3.0 equiv.), ruthenium(III) acetylacetone (8 mg, 0.02 mmol, 0.02 equiv.), 0.1 mL of 1,4-dioxane and freshly prepared salt **3** (1-methyl-1,4-diazabicyclo[2.2.2]octan-1-ium trifluoromethoxide) (318 mg, 1.5 mmol, 1.5 equiv.). The purification was accomplished by column chromatography on silica gel to provide the desired product **4c** (142 mg, 0.76 mmol, 76%).

Colorless liquid. ¹H NMR (400 MHz, CDCl₃): δ 7.43 (t, 2H, ³J = 7.7 Hz, CH_{Ar}), 7.67 (td, 1H, ³J = 8.0 Hz, ⁴J = 1.7 Hz, CH_{Ar}), 7.73 (dd, 1H, ³J = 7.7 Hz, ⁴J = 7.7 Hz, CH_{Ar}).

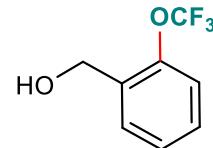
¹³C{¹H} NMR (100 MHz, CDCl₃): δ 107.3, 114.3, 120.2 (q, ¹J_{C-F} = 260.4 Hz), 121.2, 127.2, 134.1, 134.4, 150.0.

¹⁹F{¹H} NMR (376 MHz, CDCl₃): δ -57.89 (s, 3F, OCF₃).

MS (GC, 70eV): m/z (%) = 187 (M+, 100), 102 (14).

Anal. calcd. for C₈H₇F₃ON: C, 51.35; H, 2.15; N, 7.49. Found: C, 51.46; H, 2.03; N, 7.55.

(2-(trifluoromethoxy)phenyl)methanol **4d**



The title compound was prepared starting from amide **1x** (151 mg, 1.0 mmol, 1.0 equiv.), pyrylium tetrafluoroborate (185 mg, 1.1 mmol, 1.1 equiv.), BaTiO₃ (700 mg, 3.0 mmol, 3.0 equiv.), ruthenium(III) acetylacetone (8 mg, 0.02 mmol, 0.02 equiv.), 0.1 mL of 1,4-dioxane and freshly prepared salt **3** (1-methyl-1,4-diazabicyclo[2.2.2]octan-1-ium trifluoromethoxide) (318 mg, 1.5 mmol, 1.5 equiv.). The purification was accomplished by column chromatography on silica gel to provide the desired product **4d** (150 mg, 0.78 mmol, 78%).

Colorless oil. ¹H NMR (400 MHz, CDCl₃): δ 2.30 (br s, 1H, OH), 4.73 (d, 2H, ³J = 5.8 Hz, CH₂), 7.20 – 7.23 (m, 1H, CH_{Ar}), 7.27 – 7.33 (m, 2H, CH_{Ar}), 7.50 – 7.53 (m, 1H, CH_{Ar}).

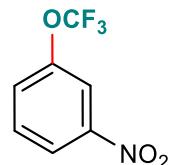
¹³C{¹H} NMR (100 MHz, CDCl₃): δ 59.7, 120.4, 120.6 (q, ¹J_{C-F} = 257.5 Hz), 127.0, 128.8, 129.1, 133.3, 146.7.

¹⁹F NMR (376 MHz, CDCl₃): δ -57.40 (s, 3F, OCF₃).

MS (GC, 70eV): m/z (%) = 187 (M+, 100), 102 (14).

Anal. calcd. for $C_8H_7F_3ON$: C, 51.35; H, 2.15; N, 7.49. Found: C, 51.46; H, 2.03; N, 7.55.

1-nitro-3-(trifluoromethoxy)benzene 4e



The title compound was prepared starting from amide **1y** (166 mg, 1.0 mmol, 1.0 equiv.), pyrlyium tetrafluoroborate (185 mg, 1.1 mmol, 1.1 equiv.), BaTiO₃ (700 mg, 3.0 mmol, 3.0 equiv.), ruthenium(III) acetylacetone (8 mg, 0.02 mmol, 0.02 equiv.), 0.1 mL of 1,4-dioxane and freshly prepared salt **3** (1-methyl-1,4-diazabicyclo[2.2.2]octan-1-ium trifluoromethoxide) (318 mg, 1.5 mmol, 1.5 equiv.). The purification was accomplished by column chromatography on silica gel to provide the desired product **4e** (190 mg, 0.92 mmol, 92%).

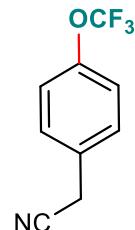
Yellowish liquid. ¹H NMR (400 MHz, CDCl₃): δ 7.58 (d, 1H, ³J = 8.25 Hz, CH_{Ar}), 7.64 (t, 1H, ³J = 8.2 Hz, CH_{Ar}), 8.11 (s, 1H, CH_{Ar}), 8.20 (dt, 1H, ³J = 8.1 Hz, ⁴J = 1.5 Hz, CH_{Ar}).

¹³C{¹H} NMR (100 MHz, CDCl₃): δ 116.4, 120.1 (q, ¹J_{C-F} = 259.6 Hz), 121.7, 126.9, 130.7, 149.0, 149.4.

¹⁹F NMR (376 MHz, CDCl₃): δ -58.18 (s, 3F, OCF₃).

Anal. calcd. for C₇H₄F₃O₃N: C, 40.60; H, 1.95; N, 6.76. Found: C, 40.69; H, 1.88; N, 6.83.

2-(4-(trifluoromethoxy)phenyl)acetonitrile 4f



The title compound was prepared starting from amide **1z** (160 mg, 1.0 mmol, 1.0 equiv.), pyrlyium tetrafluoroborate (185 mg, 1.1 mmol, 1.1 equiv.), BaTiO₃ (700 mg, 3.0 mmol, 3.0 equiv.), ruthenium(III) acetylacetone (8 mg, 0.02 mmol, 0.02 equiv.), 0.1 mL of 1,4-

dioxane and freshly prepared salt **3** (1-methyl-1,4-diazabicyclo[2.2.2]octan-1-ium trifluoromethoxide) (318 mg, 1.5 mmol, 1.5 equiv.). The purification was accomplished by column chromatography on silica gel to provide the desired product **4f** (168 mg, 0.84 mmol, 84%).

Yellowish liquid. **¹H NMR** (400 MHz, CDCl₃): δ 3.76 (s, 2H, CH₂), 7.24 (d, 2H, ³J = 8.4 Hz, CH_{Ar}), 7.38 (d, 2H, ³J = 8.5 Hz, CH_{Ar}).

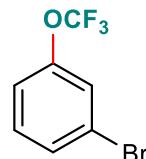
¹³C{¹H} NMR (100 MHz, CDCl₃): δ 23.1, 117.3, 120.2 (q, ¹J_{C-F} = 257.8 Hz), 121.7, 128.6, 129.5, 149.0.

¹⁹F NMR (376 MHz, CDCl₃): δ -57.99 (s, 3F, OCF₃).

MS (GC, 70eV): m/z (%) = 201 (M+, 100), 132 (19), 115 (38).

Anal. calcd. for C₉H₆F₃ON: C, 53.74; H, 3.01; N, 6.96. Found: C, 53.66; H, 3.12; N, 7.03.

1-bromo-3-(trifluoromethoxy)benzene **4g**



The title compound was prepared starting from amide **1aa** (200 mg, 1.0 mmol, 1.0 equiv.), pyrlyium tetrafluoroborate (185 mg, 1.1 mmol, 1.1 equiv.), BaTiO₃ (700 mg, 3.0 mmol, 3.0 equiv.), ruthenium(III) acetylacetone (8 mg, 0.02 mmol, 0.02 equiv.), 0.1 mL of 1,4-dioxane and freshly prepared salt **3** (1-methyl-1,4-diazabicyclo[2.2.2]octan-1-ium trifluoromethoxide) (318 mg, 1.5 mmol, 1.5 equiv.). The purification was accomplished by column chromatography on silica gel to provide the desired product **4g** (168 mg, 0.84 mmol, 84%).

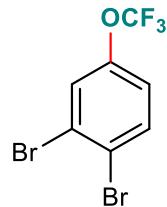
Colorless liquid. **¹H NMR** (600 MHz, CDCl₃): δ 7.16 – 7.17 (m, 1H, CH_{Ar}), 7.26 (t, 1H, ³J = 8.2 Hz, CH_{Ar}), 7.39 (s, 1H, CH_{Ar}), 7.43 – 7.44 (m, 1H, CH_{Ar}).

¹³C NMR{¹H} (151 MHz, CDCl₃): δ 149.8, 131.0, 130.2, 124.6, 122.9, 120.5 (q, ¹J_{C-F} = 258.2 Hz), 119.8.

¹⁹F NMR (564 MHz, CDCl₃): δ -58.0 (s, 3F, OCF₃).

Anal. calcd. for C₇H₄F₃OB_r: C, 34.89; H, 1.67. Found: C, 35.01; H, 1.81.

1,2-dibromo-4-(trifluoromethoxy)benzene **4h**



The title compound was prepared starting from amide **1ab** (279 mg, 1.0 mmol, 1.0 equiv.), pyrlyium tetrafluoroborate (185 mg, 1.1 mmol, 1.1 equiv.), BaTiO₃ (700 mg, 3.0 mmol, 3.0 equiv.), ruthenium(III) acetylacetone (8 mg, 0.02 mmol, 0.02 equiv.), 0.1 mL of 1,4-dioxane and freshly prepared salt **3** (1-methyl-1,4-diazabicyclo[2.2.2]octan-1-ium trifluoromethoxide) (318 mg, 1.5 mmol, 1.5 equiv.). The purification was accomplished by column chromatography on silica gel to provide the desired product **4h** (271 mg, 0.85 mmol, 85%).

Yellowish liquid. ¹H NMR (400 MHz, CDCl₃): δ 7.06 (dd, 1H, ³J = 8.8 Hz, ⁴J = 2.8 Hz, CH_{Ar}), 7.51 (d, 1H, ⁴J = 2.7 Hz, CH_{Ar}), 7.64 (d, 1H, ³J = 8.8 Hz, CH_{Ar}).

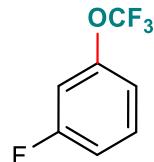
¹³C{¹H} NMR (100 MHz, CDCl₃): δ 120.2 (q, ¹J_{C-F} = 259.1 Hz), 121.2, 123.0, 125.5, 126.3, 134.3, 148.2.

¹⁹F NMR (376 MHz, CDCl₃): δ -58.17 (s, 3F, OCF₃).

MS (GC, 70eV): m/z (%) = 320 (M+, 100), 318 (53), 250 (21), 225 (16), 223 (34).

Anal. calcd. for C₇H₃F₃OBr₂: C, 26.28; H, 0.95. Found: C, 26.33; H, 1.04.

1-fluoro-3-(trifluoromethoxy)benzene **4i**



The title compound was prepared starting from amide **1ac** (139 mg, 1.0 mmol, 1.0 equiv.), pyrlyium tetrafluoroborate (185 mg, 1.1 mmol, 1.1 equiv.), BaTiO₃ (700 mg, 3.0 mmol, 3.0 equiv.), ruthenium(III) acetylacetone (8 mg, 0.02 mmol, 0.02 equiv.), 0.1 mL of 1,4-dioxane and freshly prepared salt **3** (1-methyl-1,4-diazabicyclo[2.2.2]octan-1-ium trifluoromethoxide) (318 mg, 1.5 mmol, 1.5 equiv.). The purification was accomplished by column chromatography on silica gel to provide the desired product **4i** (168 mg, 0.81 mmol, 81%).

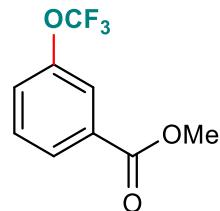
Colorless liquid. **¹H NMR** (400 MHz, CDCl₃): δ 6.96 (d, 1H, ³J = 9.3 Hz, CH_{Ar}), 7.00 – 7.04 (m, 2H, CH_{Ar}), 7.36 (dq, 1H, ³J = 8.3 Hz, ⁴J = 1.8 Hz, CH_{Ar}).

¹³C{¹H} NMR (100 MHz, CDCl₃): δ 109.0 (d, J_{C-F} = 28.0 Hz), 113.9 (d, J_{C-F} = 21.7 Hz), 116.5 (d, J_{C-F} = 2.8 Hz), 120.3 (q, ¹J_{C-F} = 257.3 Hz), 130.6 (d, J_{C-F} = 8.8 Hz), 149.9 (m), 162.9 (d, ¹J_{C-F} = 247.2 Hz).

¹⁹F NMR (376 MHz, CDCl₃): δ -109.86 (s, 1F, CF), -58.07 (s, 3F, OCF₃).

Anal. calcd. for C₇H₄F₄O: C, 46.68; H, 2.24. Found: C, 46.81; H, 2.29.

methyl 3-(trifluoromethoxy)benzoate 4j



The title compound was prepared starting from amide **1ad** (179 mg, 1.0 mmol, 1.0 equiv.), pyrlyium tetrafluoroborate (185 mg, 1.1 mmol, 1.1 equiv.), BaTiO₃ (700 mg, 3.0 mmol, 3.0 equiv.), ruthenium(III) acetylacetone (8 mg, 0.02 mmol, 0.02 equiv.), 0.1 mL of 1,4-dioxane and freshly prepared salt **3** (1-methyl-1,4-diazabicyclo[2.2.2]octan-1-ium trifluoromethoxide) (318 mg, 1.5 mmol, 1.5 equiv.). The purification was accomplished by column chromatography on silica gel to provide the desired product **4j** (199 mg, 0.87 mmol, 87%).

Colorless liquid. **¹H NMR** (600 MHz, CDCl₃): δ 3.73 (s, 3H, OCH₃), 7.20 (d, 1H, ³J = 8.4 Hz, CH_{Ar}), 7.27 (t, 1H, ³J = 8.4 Hz, CH_{Ar}), 7.67 (s, 1H, CH_{Ar}), 7.77 (d, 1H, ³J = 7.8 Hz, CH_{Ar}).

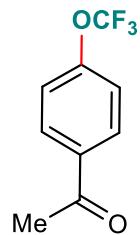
¹³C NMR{¹H} (151 MHz, CDCl₃): δ 52.6, 120.5 (q, ¹J_{C-F} = 258.2 Hz), 122.2, 125.5, 128.1, 130.0, 132.3, 149.4, 165.8.

¹⁹F NMR (376 MHz, CDCl₃): δ -58.0 (s, 3F, OCF₃).

MS (GC, 70eV): m/z (%) = 220 (M+, 33), 189 (100), 161 (27).

Anal. calcd. for C₉H₇F₃O₃: C, 49.10; H, 3.21. Found: C, 49.22; H, 3.06.

1-(4-(trifluoromethoxy)phenyl)ethan-1-one 4k



The title compound was prepared starting from amide **1ae** (163 mg, 1.0 mmol, 1.0 equiv.), pyrlyium tetrafluoroborate (185 mg, 1.1 mmol, 1.1 equiv.), BaTiO₃ (700 mg, 3.0 mmol, 3.0 equiv.), ruthenium(III) acetylacetone (8 mg, 0.02 mmol, 0.02 equiv.), 0.1 mL of 1,4-dioxane and freshly prepared salt **3** (1-methyl-1,4-diazabicyclo[2.2.2]octan-1-ium trifluoromethoxide) (318 mg, 1.5 mmol, 1.5 equiv.). The purification was accomplished by column chromatography on silica gel to provide the desired product **4k** (183 mg, 0.90 mmol, 90%).

Yellowish liquid. **¹H NMR** (400 MHz, CDCl₃): δ 2.61 (s, 3H, CH₃), 7.29 (d, 2H, ³J = 7.8 Hz, CH_{Ar}), 8.01 (dt, 2H, ³J = 8.8 Hz, ⁴J = 2.4 Hz, CH_{Ar}).

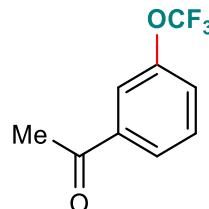
¹³C{¹H} NMR (100 MHz, CDCl₃): δ 26.5, 120.3 (q, ¹J_{C-F} = 258.7 Hz), 120.4, 130.3, 135.4, 152.6, 196.4.

¹⁹F NMR (376 MHz, CDCl₃): δ -63.0 (s, 3F, OCF₃).

MS (GC, 70eV): m/z (%) = 204 (M+, 21), 189 (100), 161 (20).

Anal. calcd. for C₉H₇F₃O₂: C, 52.95; H, 3.46. Found: C, 53.09; H, 3.56.

1-(3-(trifluoromethoxy)phenyl)ethan-1-one **4l**



The title compound was prepared starting from amide **1af** (163 mg, 1.0 mmol, 1.0 equiv.), pyrlyium tetrafluoroborate (185 mg, 1.1 mmol, 1.1 equiv.), BaTiO₃ (700 mg, 3.0 mmol, 3.0 equiv.), ruthenium(III) acetylacetone (8 mg, 0.02 mmol, 0.02 equiv.), 0.1 mL of 1,4-dioxane and freshly prepared salt **3** (1-methyl-1,4-diazabicyclo[2.2.2]octan-1-ium trifluoromethoxide) (318 mg, 1.5 mmol, 1.5 equiv.).

The purification was accomplished by column chromatography on silica gel to provide the desired product **4l** (180 mg, 0.89 mmol, 89%).

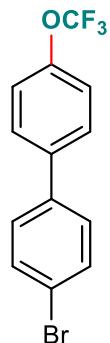
Yellowish liquid. **¹H NMR** (400 MHz, CDCl₃): δ 2.6 (s, 3H, CH₃), 7.42 (dt, 1H, ³J = 8.2 Hz, ⁴J = 1.1 Hz, CH_{Ar}), 7.52 (t, 1H, ³J = 7.9 Hz, CH_{Ar}), 7.80 (s, 1H, CH_{Ar}), 7.89 (d, 1H, ³J = 7.7 Hz, CH_{Ar}).

¹³C{¹H} NMR (100 MHz, CDCl₃): δ 26.5, 120.4 (q, ¹J_{C-F} = 257.85 Hz), 120.5, 125.4, 126.6, 130.1, 138.9, 149.5, 196.4.

¹⁹F NMR (376 MHz, CDCl₃): δ -57.98 (s, 3F, OCF₃).

Anal. calcd. for C₉H₇F₃O₂: C, 52.95; H, 3.46. Found: C, 52.81; H, 3.51.

4-bromo-4'-(trifluoromethoxy)-1,1'-biphenyl 4m



The title compound was prepared starting from amide **1ag** (276 mg, 1.0 mmol, 1.0 equiv.), pyrlyium tetrafluoroborate (185 mg, 1.1 mmol, 1.1 equiv.), BaTiO₃ (700 mg, 3.0 mmol, 3.0 equiv.), ruthenium(III) acetylacetone (8 mg, 0.02 mmol, 0.02 equiv.), 0.1 mL of 1,4-dioxane and freshly prepared salt **3** (1-methyl-1,4-diazabicyclo[2.2.2]octan-1-ium trifluoromethoxide) (318 mg, 1.5 mmol, 1.5 equiv.). The purification was accomplished by column chromatography on silica gel to provide the desired product **4m** (288 mg, 0.91 mmol, 91%).

White solid, mp 57-58 °C. **¹H NMR** (400 MHz, CDCl₃): δ 7.25 (d, 2H, ³J = 8.1 Hz, CH_{Ar}), 7.37 (dt, 2H, ³J = 8.6 Hz, ⁴J = 2.5 Hz, CH_{Ar}), 7.52 (m, 4H, CH_{Ar}).

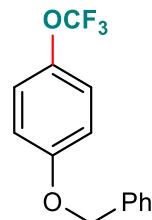
¹³C{¹H} NMR (100 MHz, CDCl₃): δ 120.6 (q, ¹J_{C-F} = 255.7 Hz), 121.4, 121.8, 128.3, 128.7, 132.1, 138.7, 148.9 (q, ¹J_{C-F} = 1.7 Hz).

¹⁹F NMR (376 MHz, CDCl₃): δ -57.80 (s, 3F, OCF₃).

MS (GC, 70eV): m/z (%) = 316 (M+, 100), 318 (98), 249 (17), 247 (18), 221 (18), 219 (18), 139 (33).

Anal. calcd. for $C_{13}H_8F_3OBr$: C, 49.24; H, 2.54. Found: C, 49.33; H, 2.43.

1-(benzyloxy)-4-(trifluoromethoxy)benzene 4n



The title compound was prepared starting from amide **1ah** (227 mg, 1.0 mmol, 1.0 equiv.), pyrlyium tetrafluoroborate (185 mg, 1.1 mmol, 1.1 equiv.), $BaTiO_3$ (700 mg, 3.0 mmol, 3.0 equiv.), ruthenium(III) acetylacetone (8 mg, 0.02 mmol, 0.02 equiv.), 0.1 mL of 1,4-dioxane and freshly prepared salt **3** (1-methyl-1,4-diazabicyclo[2.2.2]octan-1-ium trifluoromethoxide) (318 mg, 1.5 mmol, 1.5 equiv.). The purification was accomplished by column chromatography on silica gel to provide the desired product **4n** (249 mg, 0.93 mmol, 93%).

White solid mp 52-53 °C. **1H NMR** (400 MHz, $CDCl_3$): δ 5.03 (s, 2H, CH_2), 6.93 (dt, 2H, $^3J = 9.2$ Hz, $^4J = 2.3$ Hz, CH_{Ar}), 7.12 (d, 2H, $^3J = 8.5$ Hz, CH_{Ar}), 7.30 – 7.42 (m, 5H, CH_{Ar}).

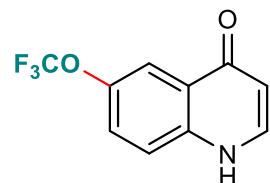
$^{13}C\{^1H\} NMR$ (100 MHz, $CDCl_3$): δ 70.5, 115.7, 120.6 (q, $^{1}J_{C-F} = 254.5$ Hz), 122.4, 127.5, 128.2, 128.7, 136.6, 142.9 (qt, $J_{C-F} = 1.8$ Hz), 157.3.

$^{19}F NMR$ (376 MHz, $CDCl_3$): δ -58.34 (s, 3F, OCF_3).

MS (GC, 70eV): m/z (%) = 268 (M+, 15), 91 (100), 249 (17).

Anal. calcd. for $C_{14}H_{11}F_3O_2$: C, 62.69; H, 4.13. Found: C, 62.78; H, 4.01.

6-(trifluoromethoxy)quinolin-4(1H)-one 4o



The title compound was prepared starting from amide **1ai** (188 mg, 1.0 mmol, 1.0 equiv.), pyrylium tetrafluoroborate (185 mg, 1.1 mmol, 1.1 equiv.), BaTiO₃ (700 mg, 3.0 mmol, 3.0 equiv.), ruthenium(III) acetylacetone (8 mg, 0.02 mmol, 0.02 equiv.), 0.1 mL of 1,4-dioxane and freshly prepared salt **3** (1-methyl-1,4-diazabicyclo[2.2.2]octan-1-ium trifluoromethoxide) (318 mg, 1.5 mmol, 1.5 equiv.). The purification was accomplished by column chromatography on silica gel to provide the desired product **4o** (181 mg, 0.79 mmol, 79%).

White solid, mp 233-234 °C. **¹H NMR** (400 MHz, DMSO-*d*₆): δ 6.11 (d, 1H, ³J = 7.4 Hz, CH_{Ar}), 7.65 – 7.73 (m, 2H, CH_{Ar}), 7.95 (s, 1H, CH_{Ar}), 8.01 (d, 1H, ³J = 7.4 Hz, CH_{Ar}), 12.0 (br s, 1H, NH).

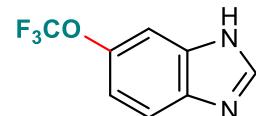
¹³C{¹H} NMR (100 MHz, DMSO-*d*₆): δ 109.0, 116.4, 120.6 (q, ¹J_{C-F} = 256.3 Hz), 121.6, 125.8, 126.8, 139.2, 140.6, 144.4, 176.4.

¹⁹F NMR (376 MHz, DMSO-*d*₆): δ -57.16 (s, 3F, OCF₃).

MS (GC, 70eV): m/z (%) = 229 (M+, 100), 91 (100), 201 (18), 160 (18), 132 (47), 104 (21).

Anal. calcd. for C₁₀H₆F₃NO₂: C, 52.41; H, 2.64; N, 6.11. Found: C, 52.52; H, 2.49; N, 6.19.

6-(trifluoromethoxy)-1*H*-benzo[d]imidazole **4p**



The title compound was prepared starting from amide **1aj** (161 mg, 1.0 mmol, 1.0 equiv.), pyrylium tetrafluoroborate (185 mg, 1.1 mmol, 1.1 equiv.), BaTiO₃ (700 mg, 3.0 mmol, 3.0 equiv.), ruthenium(III) acetylacetone (8 mg, 0.02 mmol, 0.02 equiv.), 0.1 mL of 1,4-dioxane and freshly prepared salt **3** (1-methyl-1,4-diazabicyclo[2.2.2]octan-1-ium trifluoromethoxide) (318 mg, 1.5 mmol, 1.5 equiv.). The purification was accomplished by column chromatography on silica gel to provide the desired product **4p** (151 mg, 0.75 mmol, 75%).

Brown solid, mp 99-100 °C. **¹H NMR** (400 MHz, DMSO-*d*₆): δ 7.20 (dd, 1H, ³J = 8.7 Hz, ⁴J = 1.0 Hz, CH_{Ar}), 7.61 (s, 1H, CH_{Ar}), 7.69 (d, 1H, ³J = 8.7 Hz, CH_{Ar}), 7.37 (s, 1H, CH_{Ar}), 12.72 (s, 1H, NH).

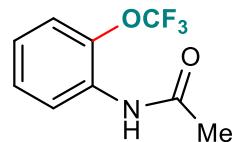
¹³C{¹H} NMR (100 MHz, DMSO-*d*₆): δ 109.2, 116.0, 120.8 (q, ¹J_{C-F} = 253.4 Hz), 144.0, 144.6, 163.5.

¹⁹F NMR (376 MHz, DMSO-*d*₆): δ 57.09 (s, 3F, OCF₃).

MS (GC, 70eV): m/z (%) = 229 (M+, 100), 91 (100), 201 (18), 160 (18), 132 (47), 104 (21).

Anal. calcd. for C₈H₅F₃N₂O: C, 47.54; H, 2.49; N, 13.86. Found: C, 47.62; H, 2.59; N, 13.69.

N-(2-(trifluoromethoxy)phenyl)acetamide 4q



The title compound was prepared starting from amide **1ak** (178 mg, 1.0 mmol, 1.0 equiv.), pyrlyium tetrafluoroborate (185 mg, 1.1 mmol, 1.1 equiv.), BaTiO₃ (700 mg, 3.0 mmol, 3.0 equiv.), ruthenium(III) acetylacetone (8 mg, 0.02 mmol, 0.02 equiv.), 0.1 mL of 1,4-dioxane and CF₃SiMe₃ (185 mg, 1.3 mmol, 1.3 equiv.). The purification was accomplished by column chromatography on silica gel to provide the desired product **4q** (164 mg, 0.75 mmol, 75%).

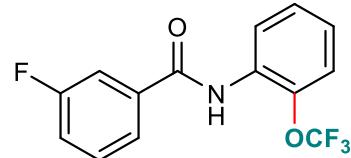
White solid, mp 68-69 °C. **¹H NMR (400 MHz, CDCl₃)**: δ 2.23 (s, 3H, CH₃), 7.09 (t, 1H, ³J = 8.0 Hz, CH_{Ar}), 7.23 – 7.29 (m, 2H, CH_{Ar}), 7.48 (s, 1H, -NH), 8.37 (d, 1H, ³J = 8.3 Hz, CH_{Ar}).

¹³C{¹H} NMR (100 MHz, CDCl₃): δ 24.7, 120.3, 120.6 (q, ¹J_{C-F} = 257.2 Hz), 122.1, 124.2, 127.5, 130.5, 138.1, 168.3.

MS (GC, 70eV): m/z (%) = 219 (M+, 30), 177 (100), 137 (17), 108 (39).

Anal. calcd. for C₉H₈F₃O₂N: C, 49.32; H, 3.68; N, 6.39. Found: C, 49.12; H, 3.45; N, 6.51.

3-fluoro-N-(2-(trifluoromethoxy)phenyl)benzamide 4r



The title compound was prepared starting from amide **1al** (258 mg, 1.0 mmol, 1.0 equiv.), pyrlyium tetrafluoroborate (185 mg, 1.1 mmol, 1.1 equiv.), BaTiO₃ (700 mg, 3.0 mmol, 3.0 equiv.), ruthenium(III) acetylacetone (8 mg, 0.02 mmol, 0.02 equiv.), 0.1 mL of 1,4-dioxane and CF₃SiMe₃ (185 mg, 1.3 mmol, 1.3 equiv.). The purification was accomplished by column chromatography on silica gel to provide the desired product **4r** (203 mg, 0.68 mmol, 68%).

White solid, mp 128 °C. **¹H NMR (400 MHz, CDCl₃)**: δ 7.17 (t, 1H, ³J = 7.9 Hz, CH_{Ar}), 7.26 – 7.37 (m, 3H, CH_{Ar}), 7.49 (td, 1H, ³J = 7.9 Hz, ⁴J = 5.4 Hz, CH_{Ar}), 7.61 (d, 2H, ³J = 7.7 Hz, CH_{Ar}), 8.16 (s, 1H, -NH), 8.53 (d, 1H, ³J = 8.3 Hz, CH_{Ar}).

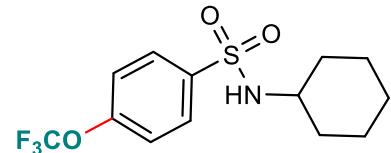
$^{13}\text{C}\{\text{H}\}$ NMR (100 MHz, CDCl_3): δ 114.7 (d, $J_{\text{C-F}} = 23.1$ Hz), 119.3 (d, $J_{\text{C-F}} = 21.3$ Hz), 120.5, 120.6 (q, $^{1}\text{J}_{\text{C-F}} = 259.8$ Hz), 122.0, 122.2 (d, $J_{\text{C-F}} = 3.0$ Hz), 124.7, 127.7, 130.4, 130.7 (d, $J_{\text{C-F}} = 8.0$ Hz), 136.8 (d, $J_{\text{C-F}} = 6.8$ Hz), 138.5 (d, $J_{\text{C-F}} = 1.0$ Hz), 162.9 (d, $^{1}\text{J}_{\text{C-F}} = 248.6$ Hz), 164.0 (d, $J_{\text{C-F}} = 2.8$ Hz).

$^{19}\text{F}\{\text{H}\}$ NMR (376 MHz, CDCl_3): δ -110.87 (m, 1F, CF), -57.10 (s, 3F, OCF_3).

MS (GC, 70eV): m/z (%) = 323 (M+, 44),

Anal. calcd. for $\text{C}_{14}\text{H}_9\text{F}_4\text{O}_2\text{N}$: C, 56.20; H, 3.03; N, 4.68. Found: C, 56.01; H, 3.21; N, 4.79.

N-cyclohexyl-4-(trifluoromethoxy)benzenesulfonamide 4s



The title compound was prepared starting from amide **1am** (282 mg, 1.0 mmol, 1.0 equiv.), pyrlyium tetrafluoroborate (185 mg, 1.1 mmol, 1.1 equiv.), BaTiO_3 (700 mg, 3.0 mmol, 3.0 equiv.), ruthenium(III) acetylacetone (8 mg, 0.02 mmol, 0.02 equiv.), 0.1 mL of 1,4-dioxane and CF_3SiMe_3 (185 mg, 1.3 mmol, 1.3 equiv.). The purification was accomplished by column chromatography on silica gel to provide the desired product **4s** (193 mg, 0.83 mmol, 83%).

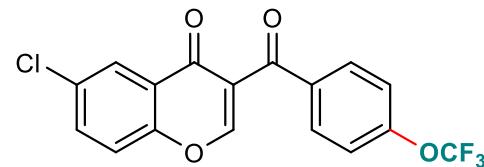
White solid, mp 66–67 °C. **^1H NMR (500 MHz, DMSO-d_6):** δ 0.96 – 1.00 (m, 1H, Cy), 1.04 – 1.10 (m, 4H, Cy), 1.37 – 1.40 (m, 1H, Cy), 1.51 – 1.53 (m, 4H, Cy), 2.92 (m, 1H, Cy), 7.53 (d, 2H, $^3\text{J} = 8.4$ Hz, CH_{Ar}), 7.77 (s, 1H, -NH), 7.90 (dt, 2H, $^3\text{J} = 8.9$ Hz, $^4\text{J} = 2.0$ Hz, CH_{Ar}).

$^{13}\text{C}\{\text{H}\}$ NMR (125 MHz, DMSO-d_6): δ 24.7, 25.2, 33.7, 52.6, 120.3 (q, $^{1}\text{J}_{\text{C-F}} = 257.1$ Hz), 121.8, 129.2, 141.8, 151.0.

MS (GC, 70eV): m/z (%) = 323 (M+, 44), 293 (11), 278 (99), 225 (100), 203 (10), 161 (94), 98 (71).

Anal. calcd. for $\text{C}_{13}\text{H}_{16}\text{F}_3\text{OSN}$: C, 48.29; H, 4.99; N, 4.33. Found: C, 48.06; H, 5.09; N, 4.12.

6-chloro-3-(4-(trifluoromethoxy)benzoyl)-4H-chromen-4-one 4t



The title compound was prepared starting from amide **1an** (327 mg, 1.0 mmol, 1.0 equiv.), pyrlyium tetrafluoroborate (185 mg, 1.1 mmol, 1.1 equiv.), BaTiO₃ (700 mg, 3.0 mmol, 3.0 equiv.), ruthenium(III) acetylacetone (8 mg, 0.02 mmol, 0.02 equiv.), 0.1 mL of 1,4-dioxane and CF₃SiMe₃ (185 mg, 1.3 mmol, 1.3 equiv.). The purification was accomplished by column chromatography on silica gel to provide the desired product **4t** (272 mg, 0.74 mmol, 74%).

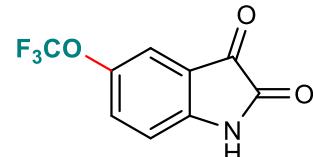
White solid, mp 157-158 °C. ¹H NMR (500 MHz, CDCl₃): δ 7.28 (d, 2H, ³J = 8.4 Hz, CH_{Ar}), 7.53 (d, 1H, ³J = 8.8 Hz, CH_{Ar}), 7.70 (d, 1H, ³J = 8.8 Hz, CH_{Ar}), 7.89 (d, 2H, ³J = 8.3 Hz, CH_{Ar}), 8.20 (s, 1H, CH_{Ar}), 8.34 (s, 1H, CH_{Ar}).

¹³C{¹H} NMR (125 MHz, CDCl₃): δ 120.1, 120.2, 120.3 (q, ¹J_{C-F} = 259.3 Hz), 124.8, 125.9, 131.7, 132.5, 134.9, 135.1, 153.0, 154.4, 159.3, 173.6, 190.0.

MS (GC, 70eV): m/z (%) = 368 (M+, 58), 303 (100), 283 (23), 254 (21), 207 (28), 189 (70), 128 (26), 154 (49), 126 (13).

Anal. calcd. for C₁₇H₈ClF₃O₄: C, 55.38; H, 2.19. Found: C, 55.16; H, 2.32.

5-(trifluoromethoxy)indoline-2,3-dione **4u**



The title compound was prepared starting from amide **1ao** (190 mg, 1.0 mmol, 1.0 equiv.), pyrlyium tetrafluoroborate (185 mg, 1.1 mmol, 1.1 equiv.), BaTiO₃ (700 mg, 3.0 mmol, 3.0 equiv.), ruthenium(III) acetylacetone (8 mg, 0.02 mmol, 0.02 equiv.), 0.1 mL of 1,4-dioxane and CF₃SiMe₃ (185 mg, 1.3 mmol, 1.3 equiv.). The purification was accomplished by column chromatography on silica gel to provide the desired product **4u** (196 mg, 0.85 mmol, 85%).

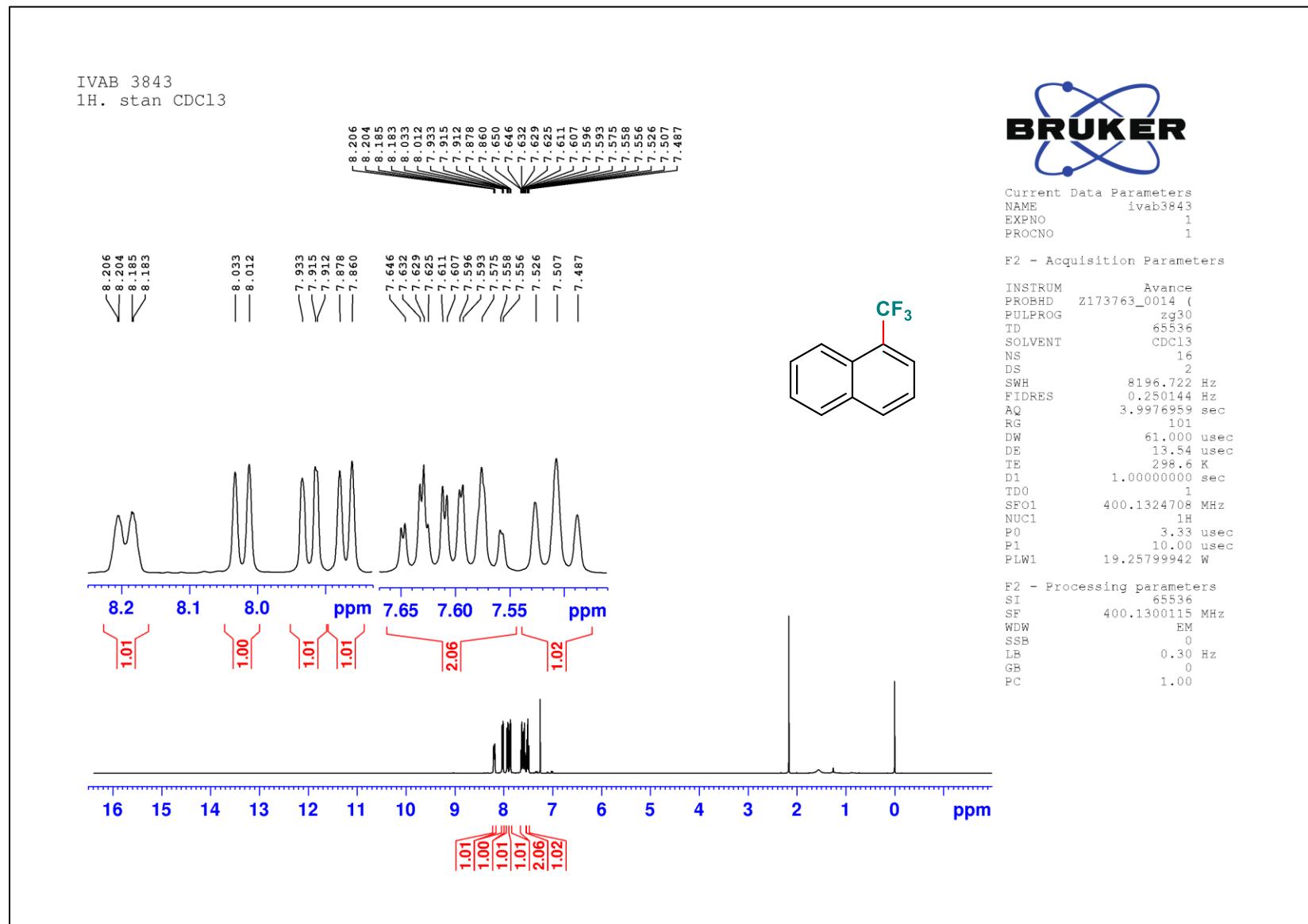
Yellow solid, mp 170-171 °C. ¹H NMR (500 MHz, DMSO-d₆): δ 6.95 (d, 1H, ³J = 8.5 Hz, CH_{Ar}), 7.47 (d, 1H, ⁴J = 2.6 Hz, CH_{Ar}), 7.54 (dd, 1H, ³J = 8.5 Hz, ⁴J = 2.5 Hz, CH_{Ar}), 11.16 (s, 1H, -NH).

¹³C{¹H} NMR (125 MHz, DMSO-d₆): δ 113.9, 118.2, 119.1, 120.6 (q, ¹J_{C-F} = 256.2 Hz), 131.3, 143.9, 149.9, 159.9, 183.8.

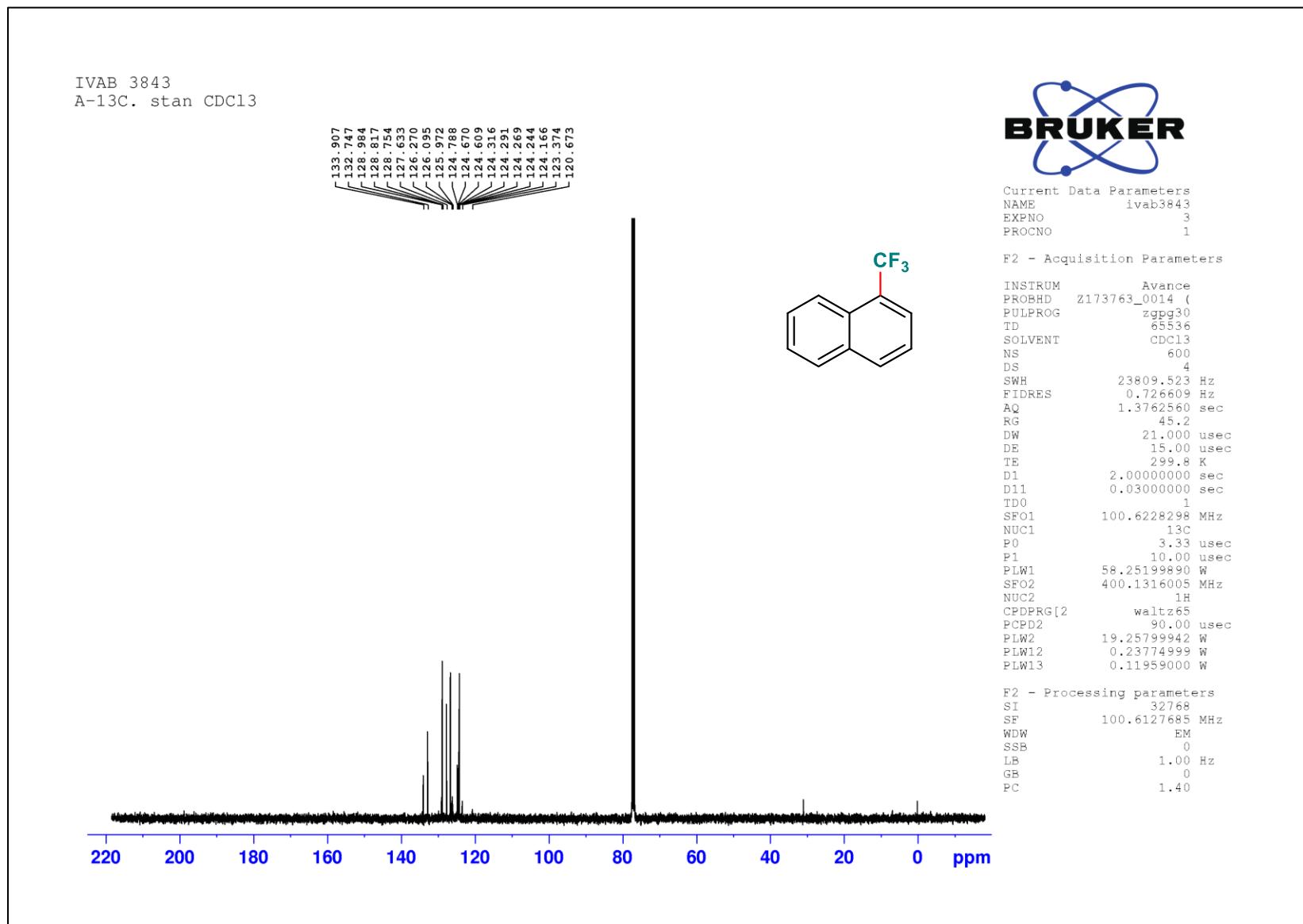
Anal. calcd. for C₉H₄F₃O₃N: C, 46.77; H, 1.74; N, 6.06. Found: C, 46.88; H, 1.58; N, 5.91.

(C) Copies ^1H and ^{13}C NMR spectra.

¹H NMR of Compound 2a

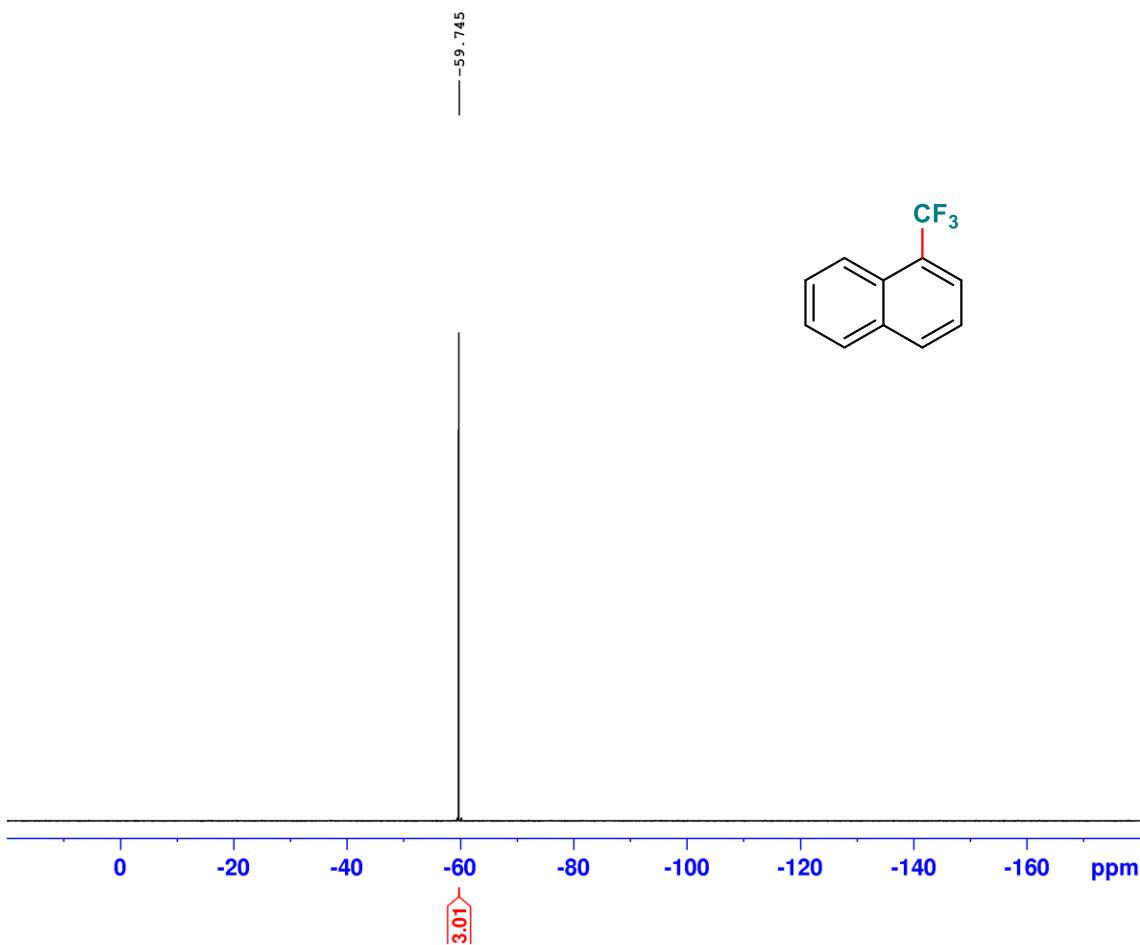


¹³C NMR of Compound 2a



¹⁹F NMR of Compound **2a**

IVAB 3843
19F. stan CDCl₃



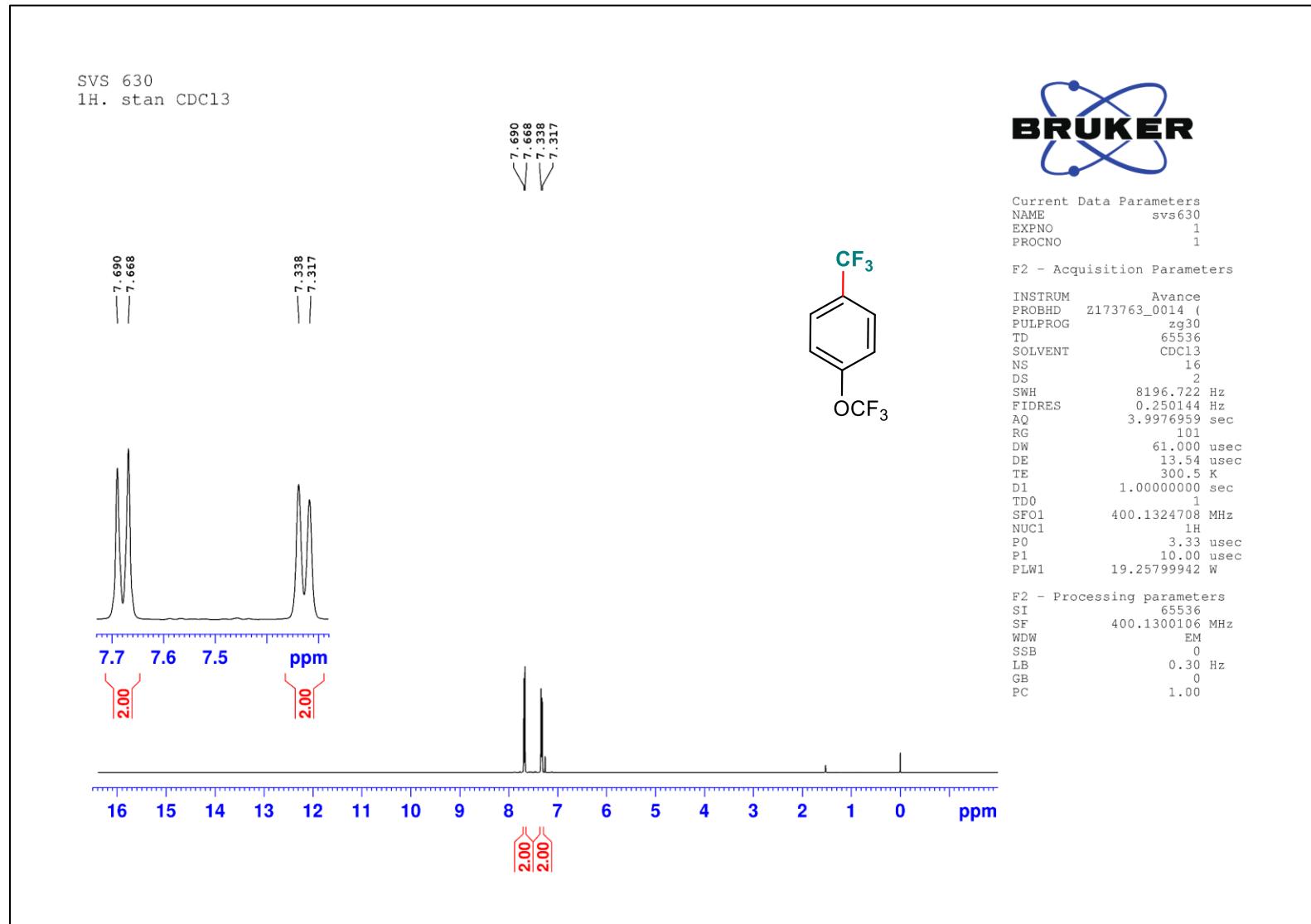
Current Data Parameters
NAME ivab3843
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters

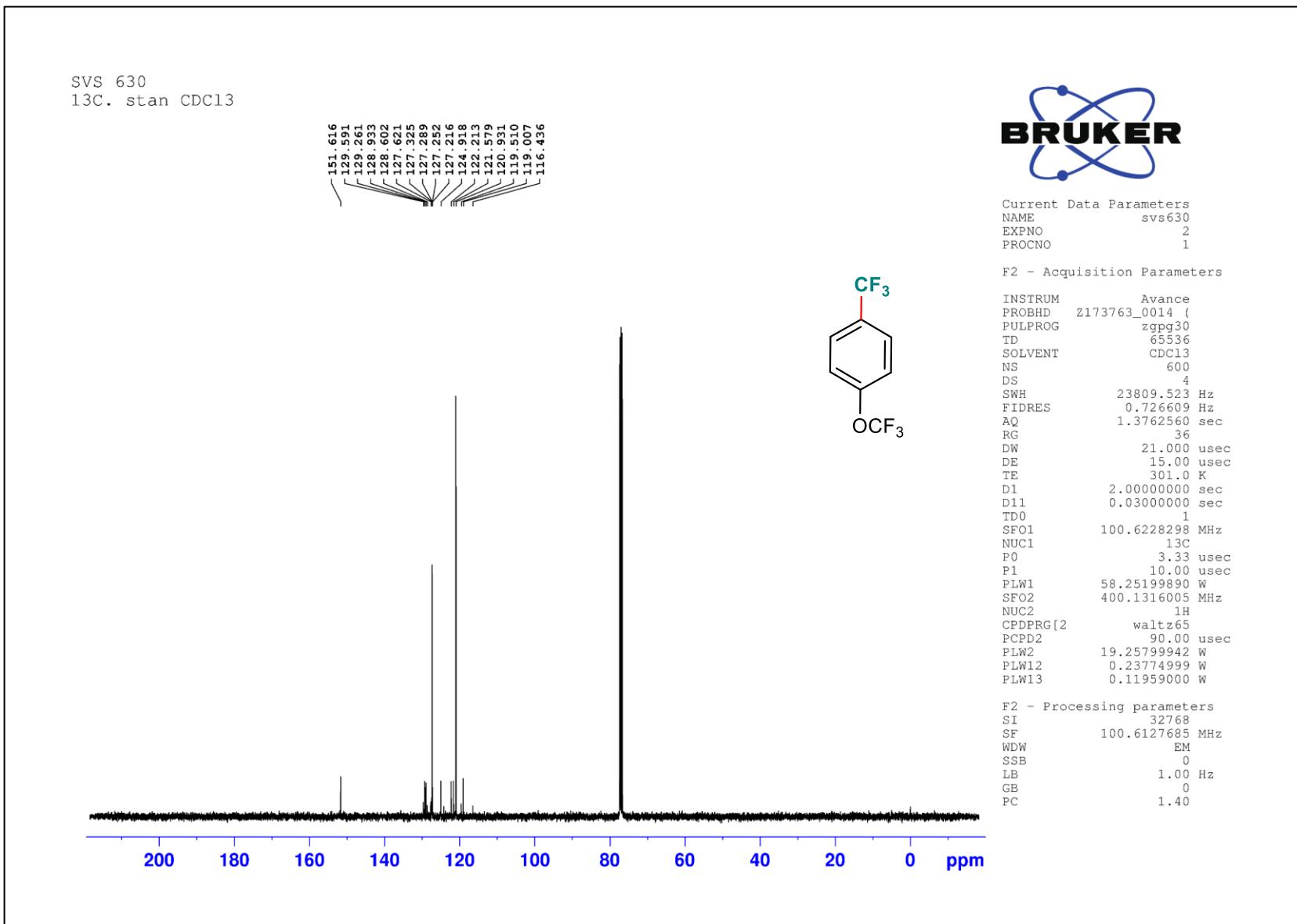
INSTRUM Avance
PROBHD Z173763_0014 (zg
PULPROG zg
TD 131072
SOLVENT CDCl₃
NS 16
DS 4
SWH 90909.094 Hz
FIDRES 1.387163 Hz
AQ 0.7208960 sec
RG 101
DW 5.500 usec
DE 6.50 usec
TE 298.8 K
D1 1.0000000 sec
TDO 1
SFO1 376.4607164 MHz
NUC1 ¹⁹F
P1 12.00 usec
PLW1 36.0000000 W

F2 - Processing parameters
SI 65536
SF 376.4983662 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

¹H NMR of Compound 2b



¹³C NMR of Compound **2b**



¹⁹F NMR of Compound **2b**

SVS 630
19F. stan CDC13

-57.919
-62.554

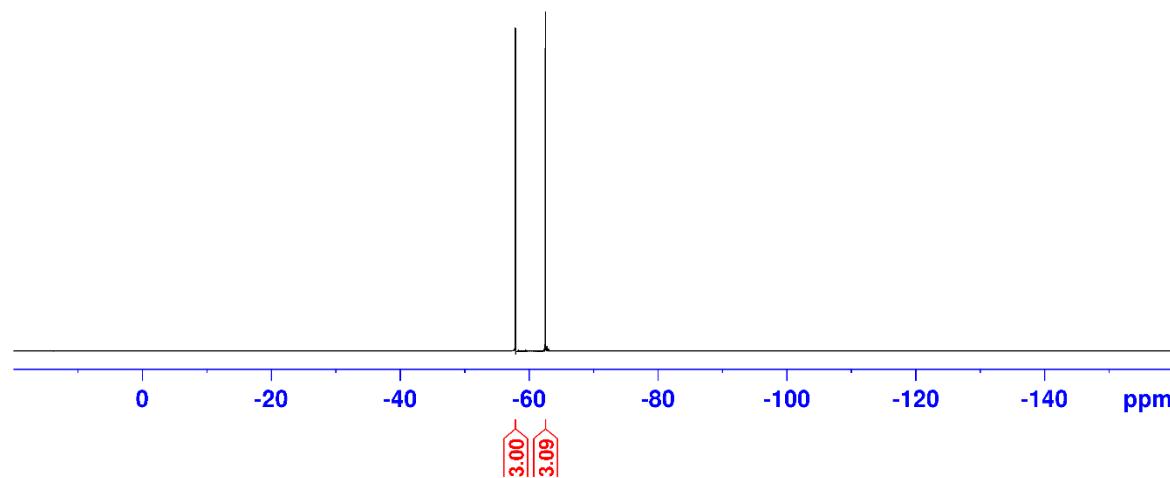
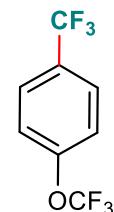


Current Data Parameters
NAME svs630
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters

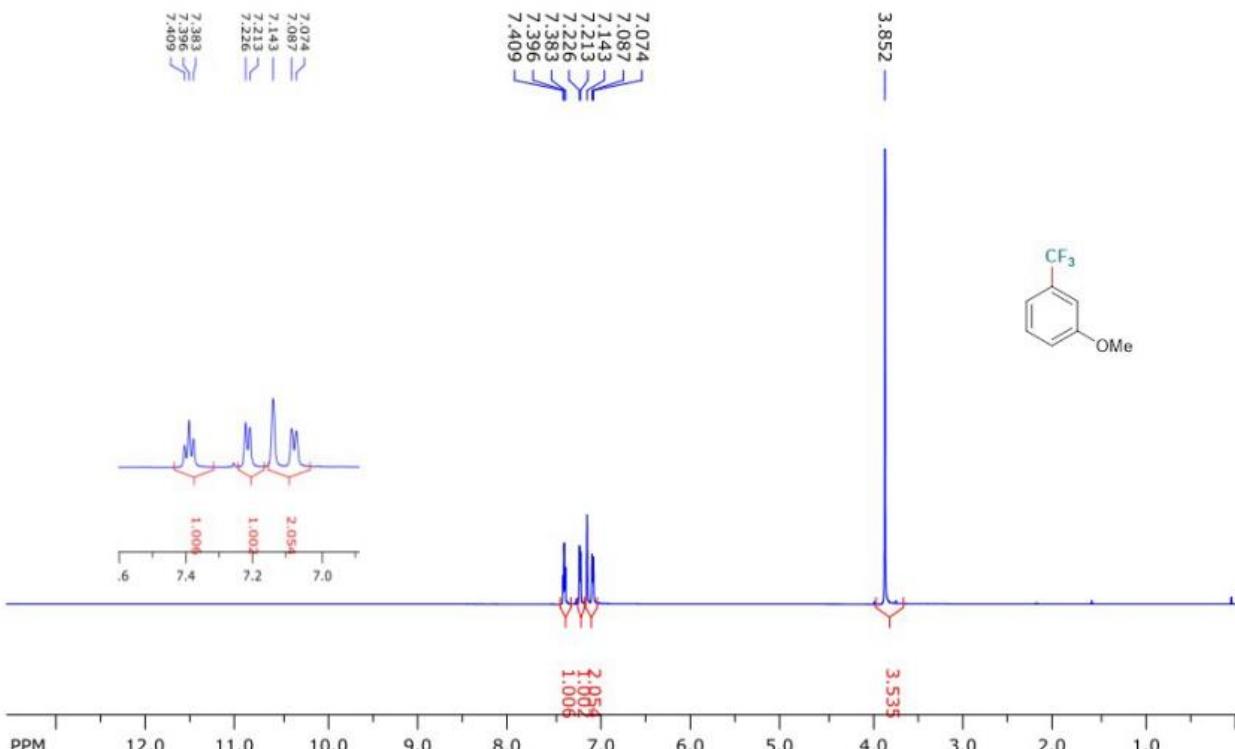
INSTRUM Avance
PROBHD Z173763_0014 (zg
PULPROG zg
TD 131072
SOLVENT CDCl3
NS 16
DS 4
SWH 90909.094 Hz
FIDRES 1.387163 Hz
AQ 0.7208960 sec
RG 101
DW 5.500 usec
DE 6.50 usec
TE 300.7 K
D1 1.0000000 sec
TD0 1
SF01 376.4607164 MHz
NUC1 ¹⁹F
P1 12.00 usec
PLW1 36.0000000 W

F2 - Processing parameters
SI 65536
SF 376.4983662 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



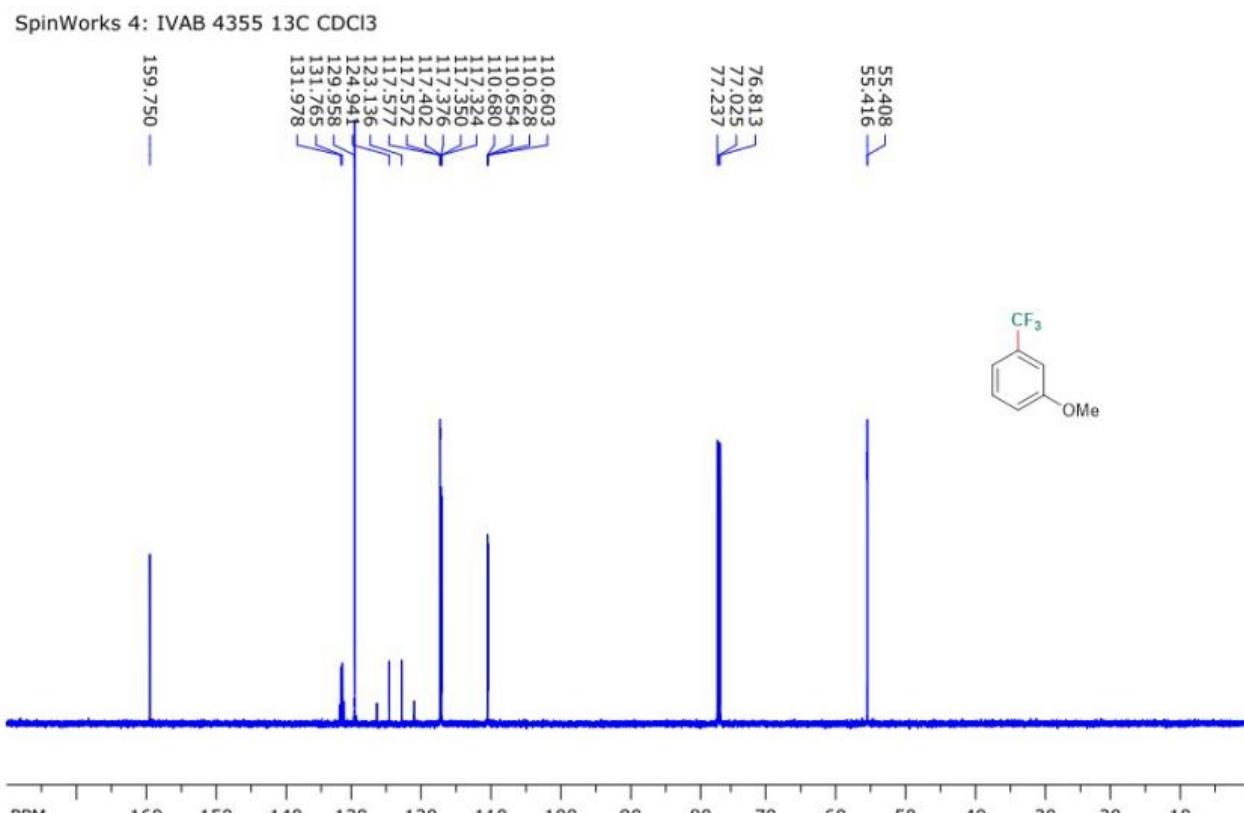
¹H NMR of Compound **2c**

SpinWorks 4: IVAB 4355 1H CDCl₃



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transmitter freq.: 599.770272 MHz processed size: 32768 complex points
time domain size: 57692 points LB: 1.500 GF: 0.0000
width: 9615.38 Hz = 16.0318 ppm = 0.166668 Hz/pt Hz/cm: 327.178 ppm/cm: 0.54551
number of scans: 16

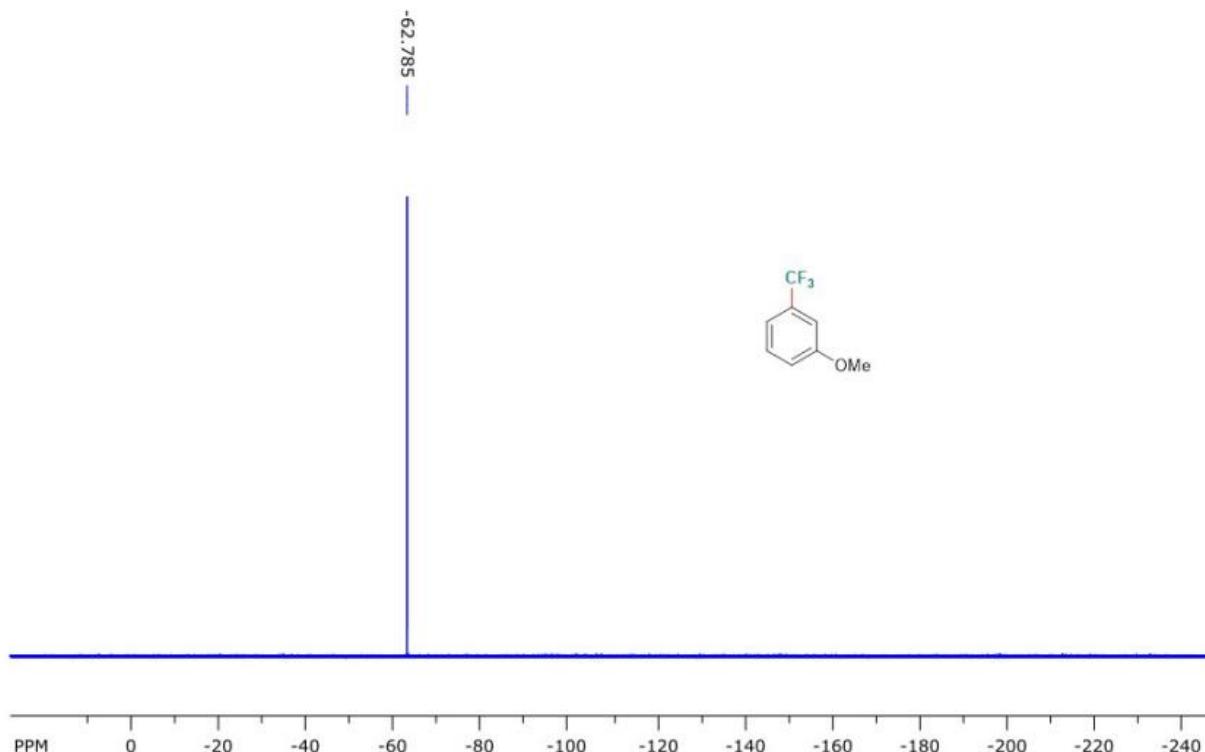
¹³C NMR of Compound **2c**



file: ...0418_01\ivab4355-CARBON_01.fid\fid block# 1 expt: "s2pul" freq. of 0 ppm: 150.811443 MHz
transmitter freq.: 150.828039 MHz processed size: 65536 complex points
time domain size: 65536 points LB: 0.500 GF: 0.0000
width: 37878.79 Hz = 251.1389 ppm = 0.577984 Hz/pt Hz/cm: 1091.110 ppm/cm: 7.23413
number of scans: 256

¹⁹F NMR of Compound **2c**

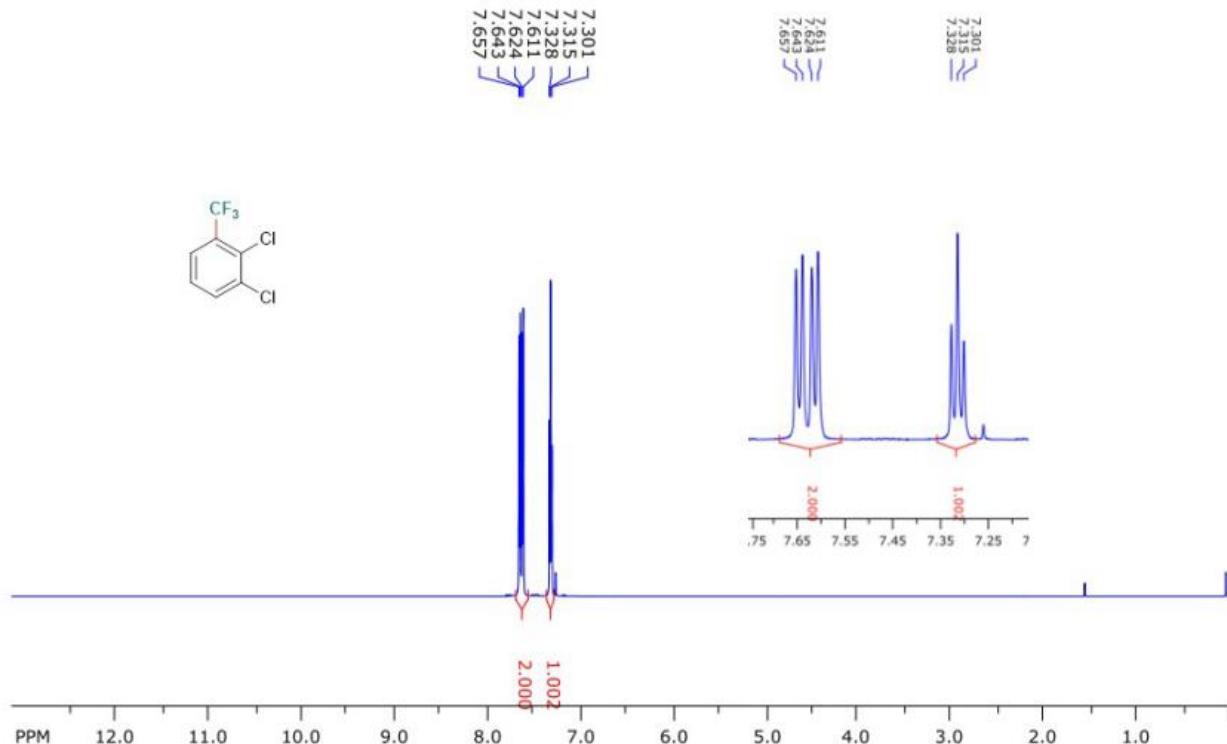
SpinWorks 4: IVAB 4355 19F



file: ...18_01\ivab4355-FLUORINE_01.fid\fid block# 1 expt: "s2pul" freq. of 0 ppm: 564.344520 MHz
transmitter freq.: 564.282442 MHz processed size: 262144 complex points
time domain size: 262144 points LB: 1.500 GF: 0.0000
width: 156250.00 Hz = 276.9003 ppm = 0.596046 Hz/pt Hz/cm: 6250.000 ppm/cm: 11.07601
number of scans: 32

¹H NMR of Compound 2d¹

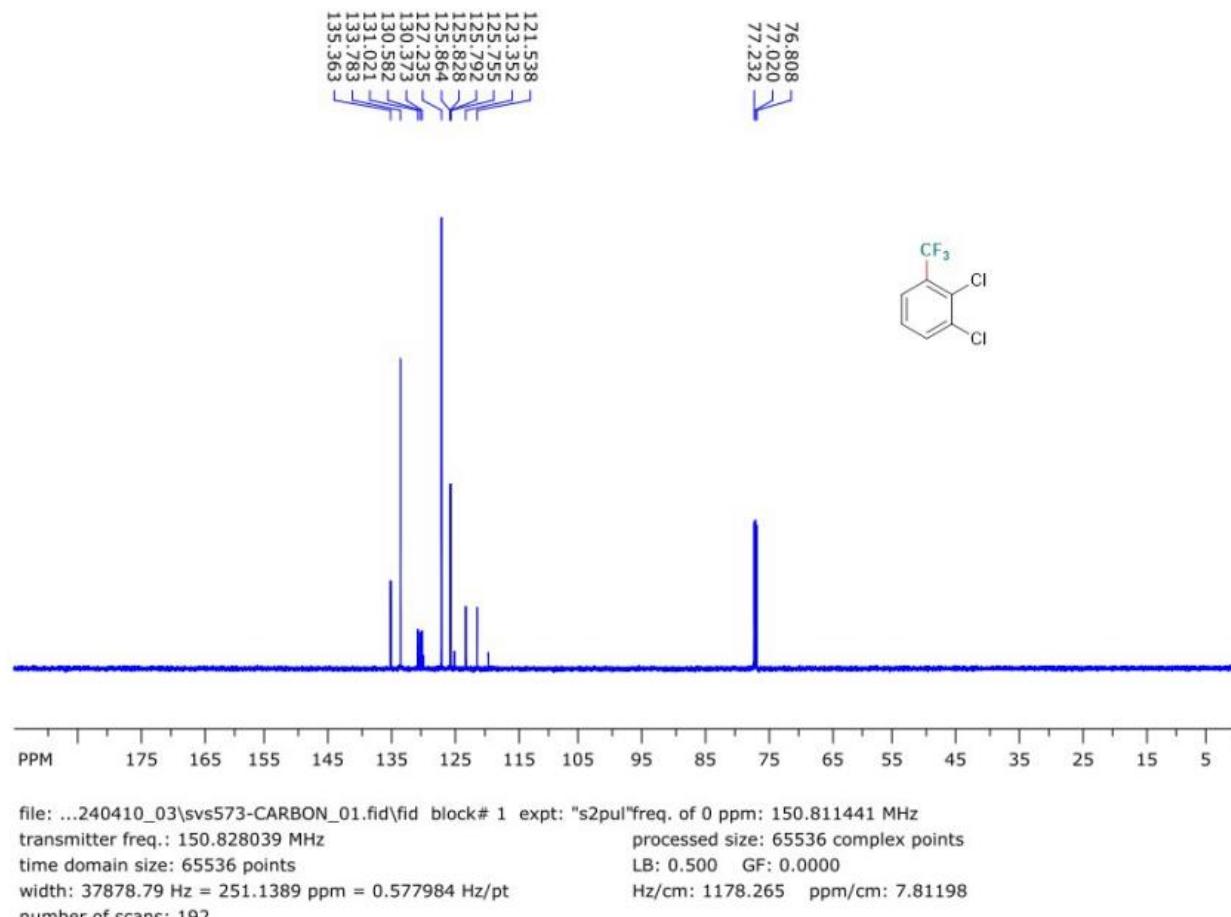
SpinWorks 4: SVS 573 1H CDCl₃



file: ...240410_01\svs573-PROTON_01.fid\fid block# 1 expt: "s2pul" freq. of 0 ppm: 599.7666671 MHz
transmitter freq.: 599.770272 MHz processed size: 65536 complex points
time domain size: 76924 points LB: 0.300 GF: 0.0000
width: 9615.38 Hz = 16.0318 ppm = 0.124999 Hz/pt Hz/cm: 317.393 ppm/cm: 0.52919
number of scans: 16

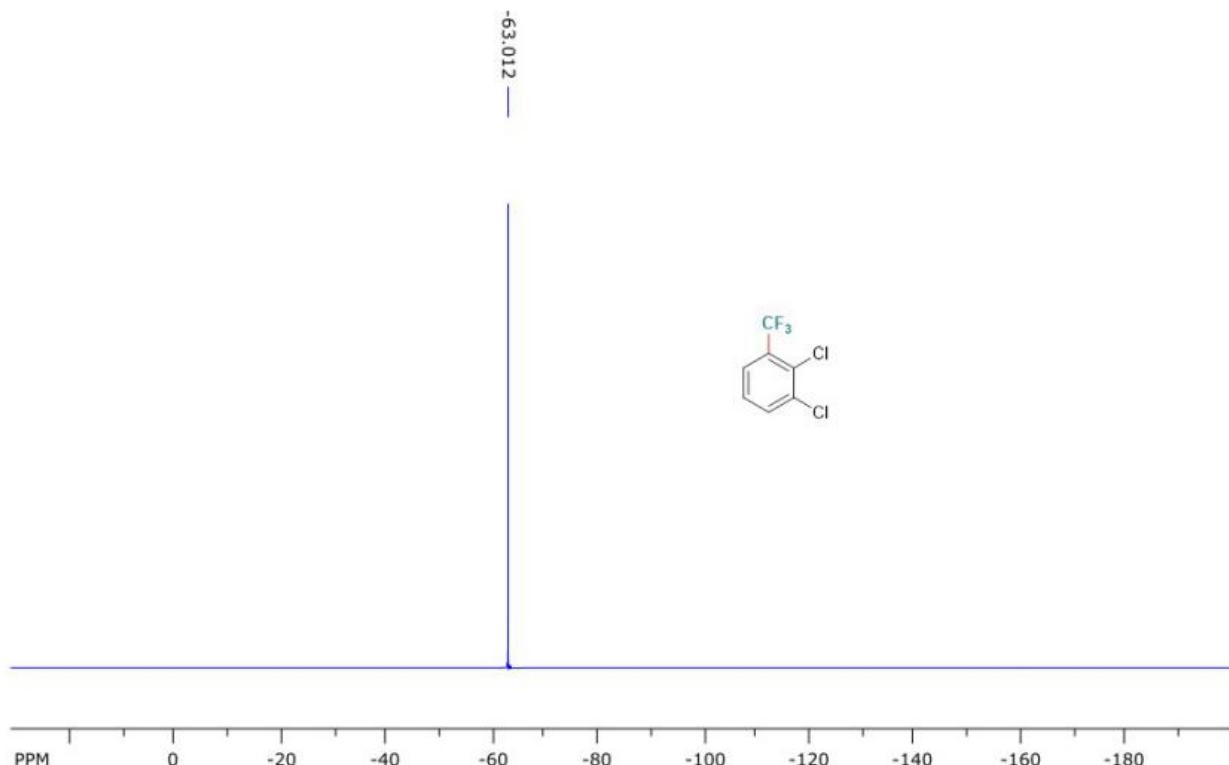
¹³C NMR of Compound **2d**

SpinWorks 4: SVS 573 13C CDCl₃



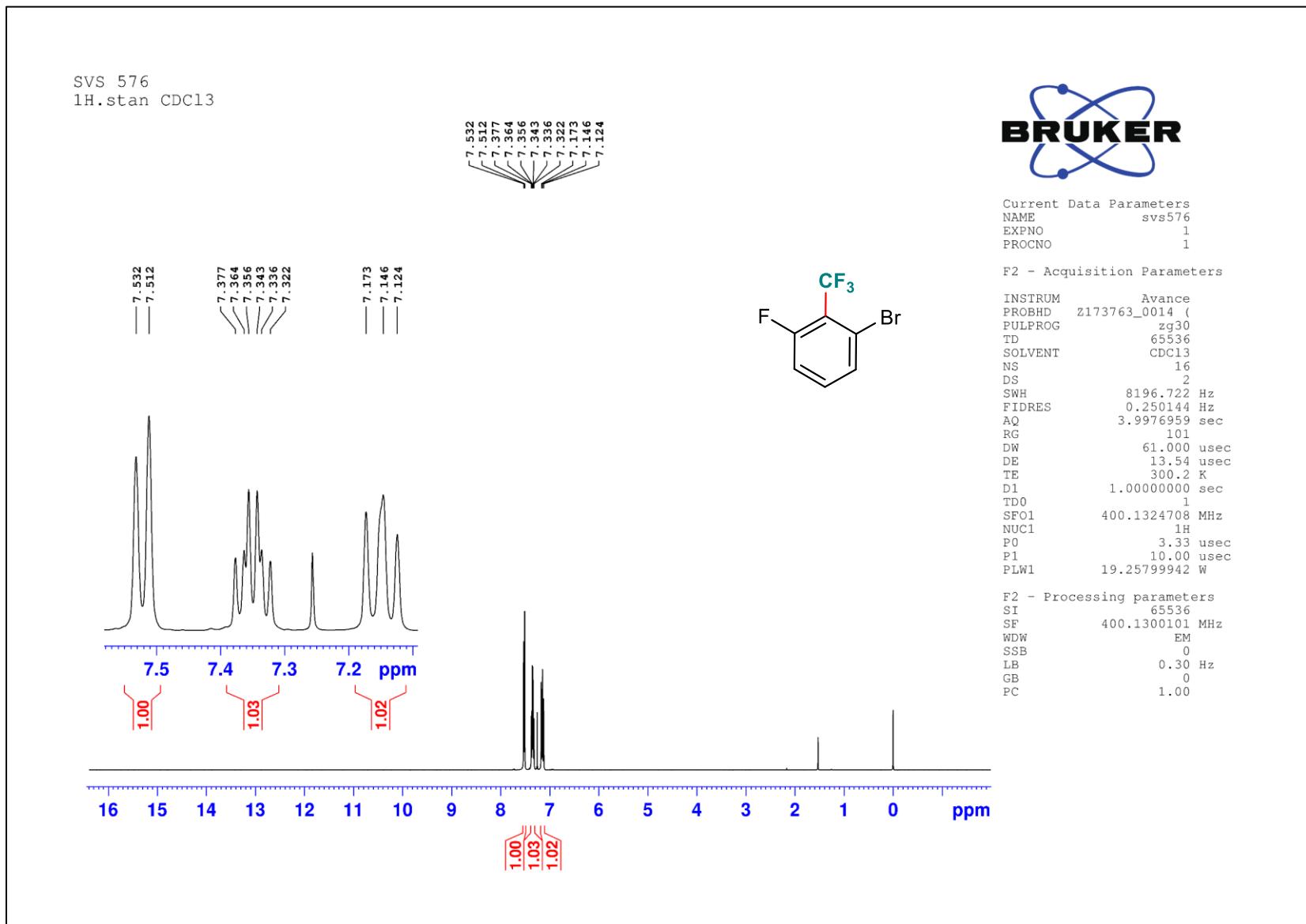
¹⁹F NMR of Compound **2d**

SpinWorks 4: SVS 573 19F

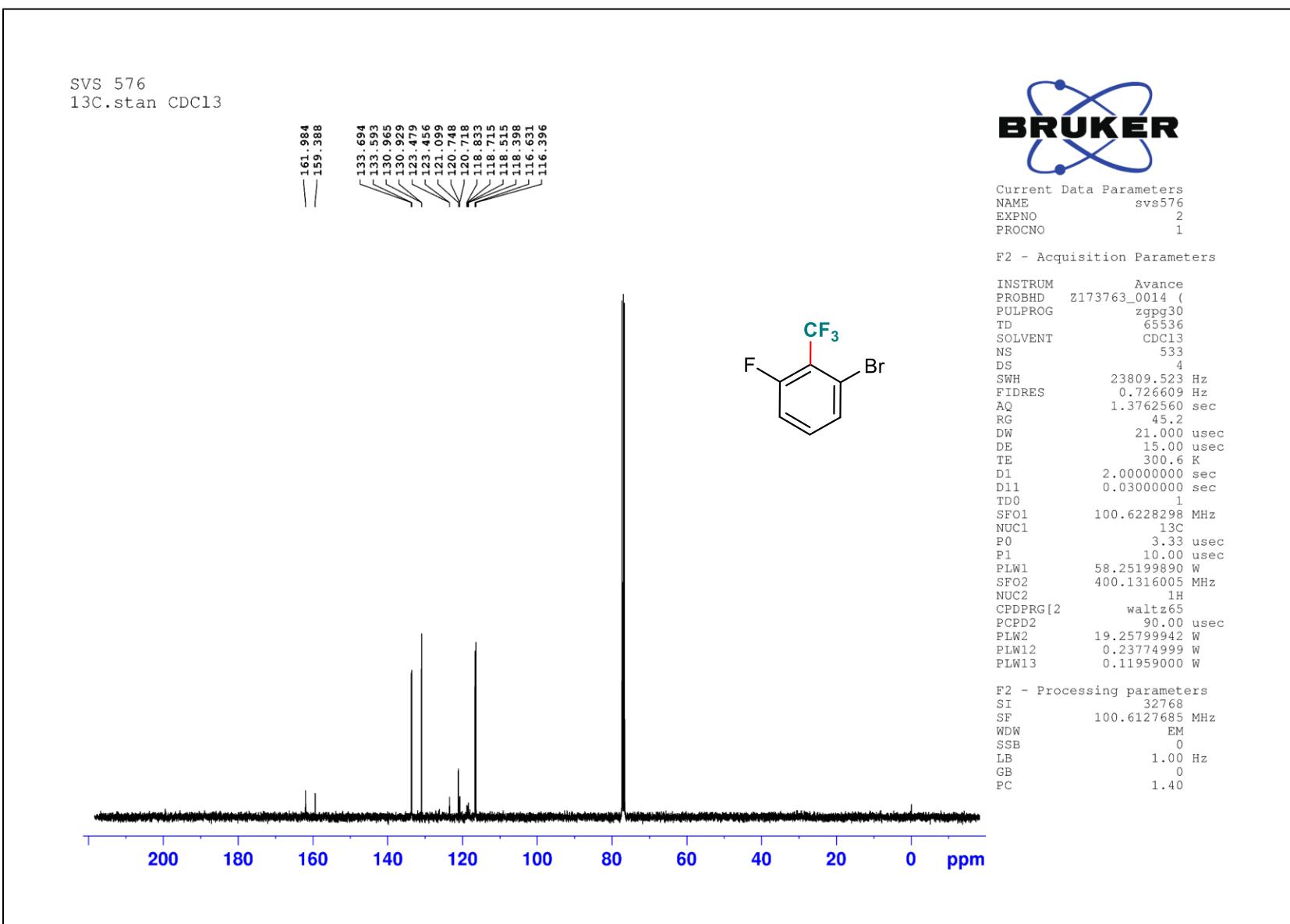


file: ...0410_02\svs573-FLUORINE_01.fid\fid block# 1 expt: "s2pul" freq. of 0 ppm: 564.344520 MHz
transmitter freq.: 564.296551 MHz processed size: 262144 complex points
time domain size: 262144 points LB: 1.500 GF: 0.0000
width: 131578.95 Hz = 233.1734 ppm = 0.501934 Hz/pt Hz/cm: 5263.158 ppm/cm: 9.32694
number of scans: 16

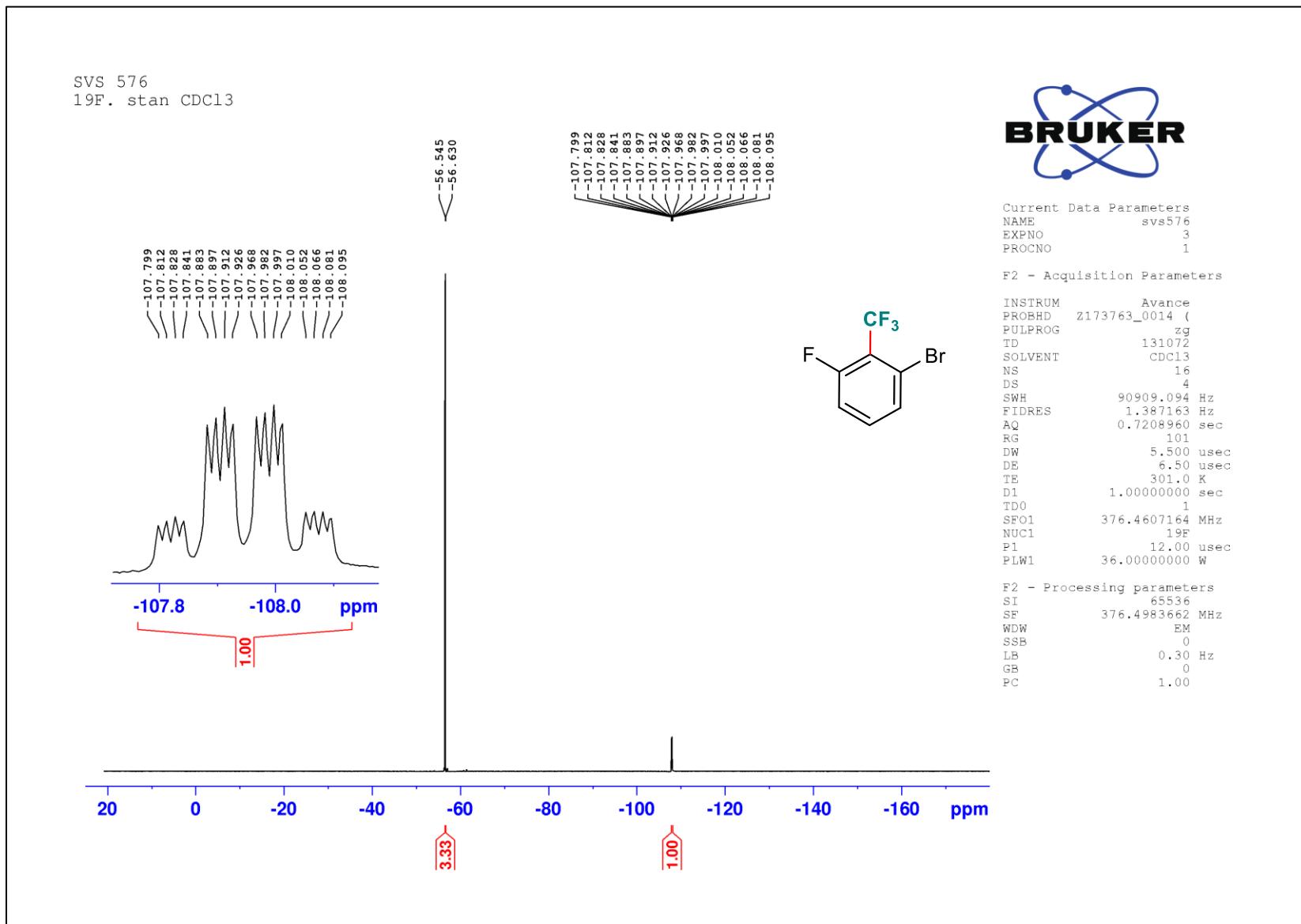
¹H NMR of Compound 2e



¹³C NMR of Compound 2e

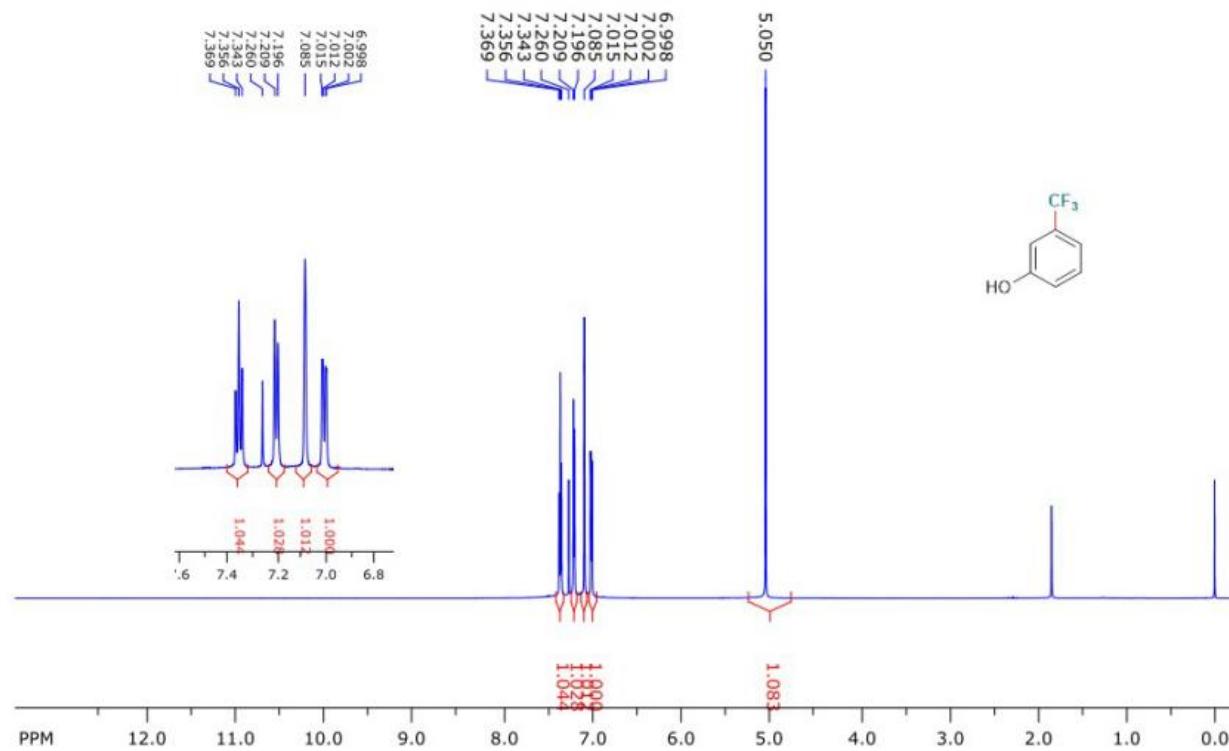


¹⁹F NMR of Compound 2e



¹H NMR of Compound 2f

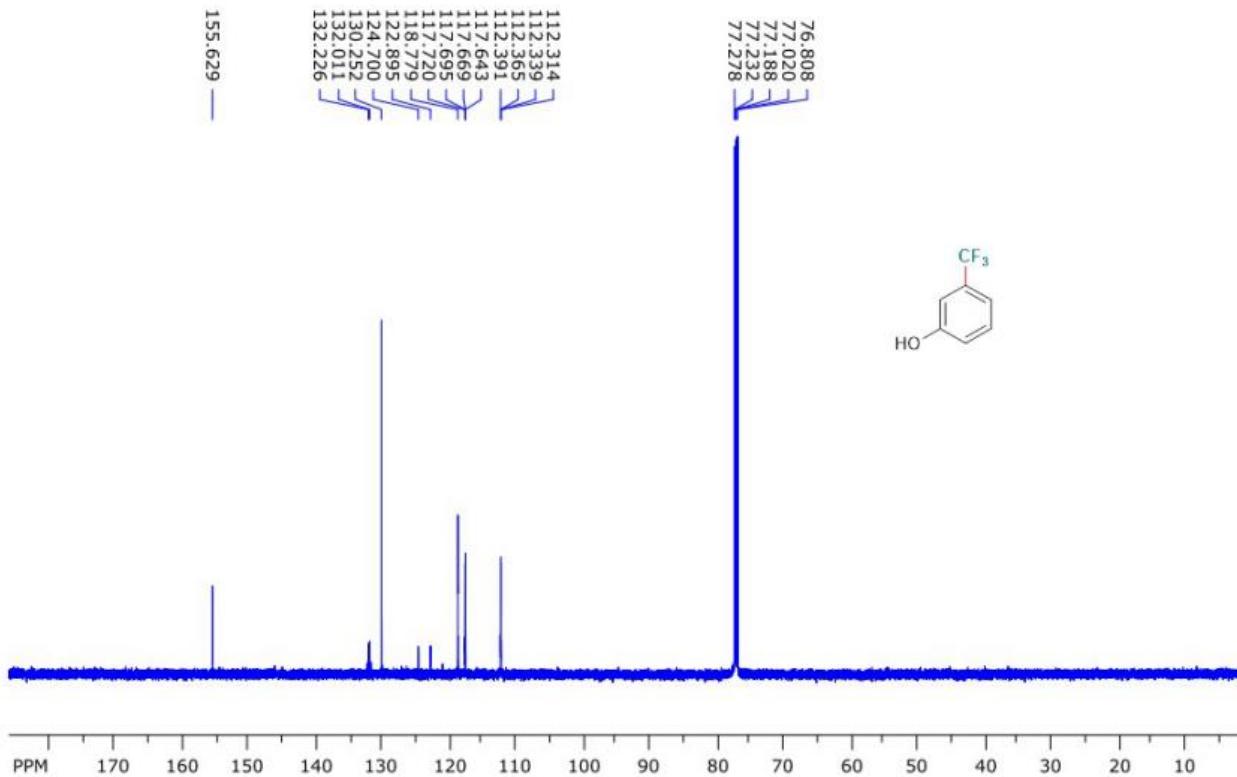
SpinWorks 4: SVS 583 1H CDCl₃



file: ...240410_01\svs583-PROTON_01.fid\fid block# 1 expt: "s2pul" freq. of 0 ppm: 599.766672 MHz
transmitter freq.: 599.770272 MHz processed size: 65536 complex points
time domain size: 76924 points LB: 0.300 GF: 0.0000
width: 9615.38 Hz = 16.0318 ppm = 0.124999 Hz/pt Hz/cm: 328.880 ppm/cm: 0.54834
number of scans: 16

¹³C NMR of Compound 2f

SpinWorks 4: SVS 583 13C CDCL₃



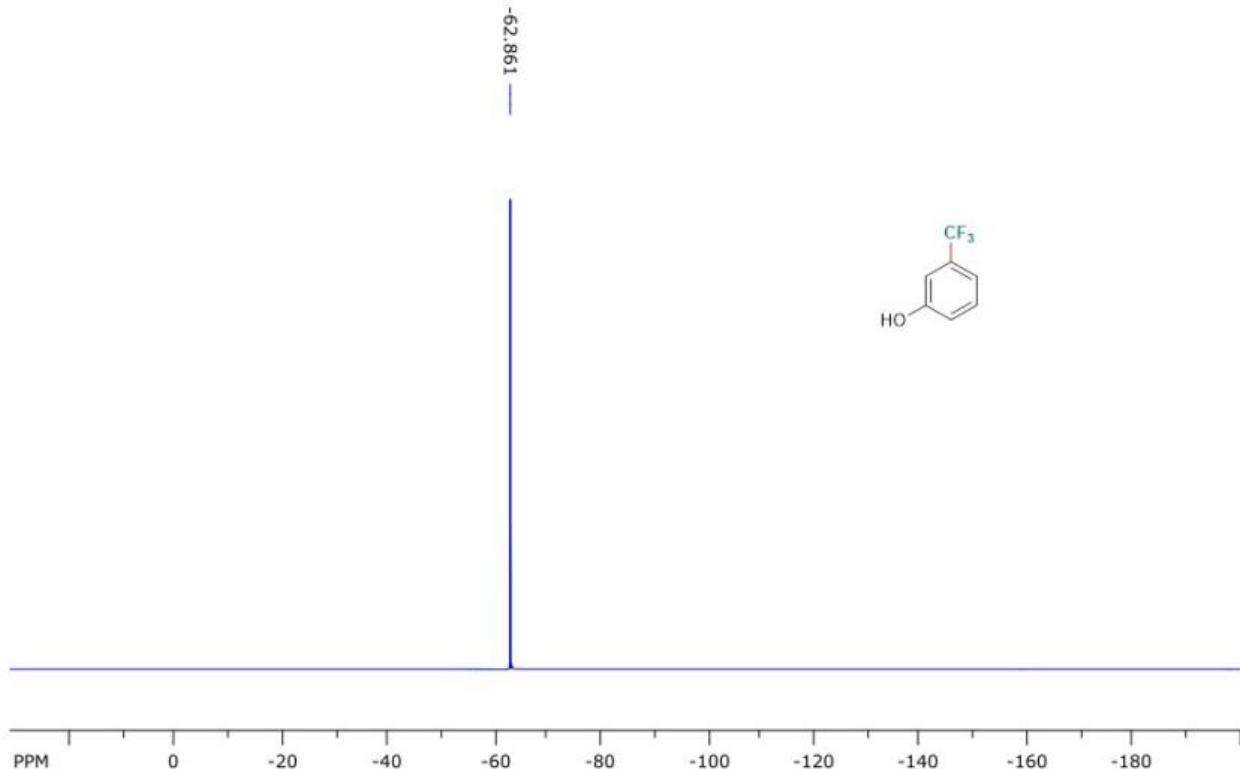
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transmitter freq.: 150.828039 MHz processed size: 65536 complex points
time domain size: 65536 points LB: 0.500 GF: 0.0000
width: 37878.79 Hz = 251.1389 ppm = 0.577984 Hz/pt Hz/cm: 1117.927 ppm/cm: 7.41193
number of scans: 576

¹⁹F

S50

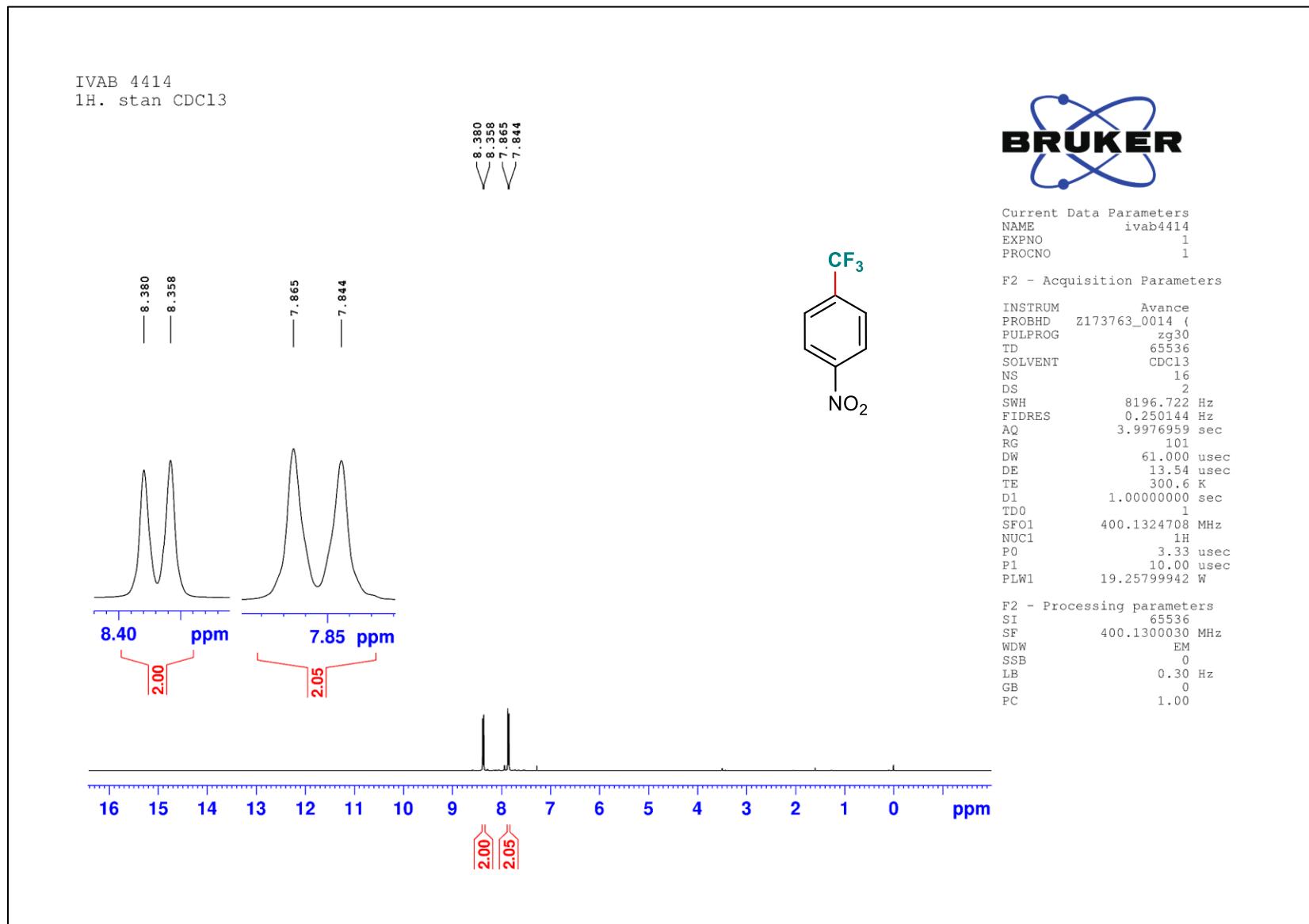
NMR of Compound 2f

SpinWorks 4: SVS 583 13C CDCl₃

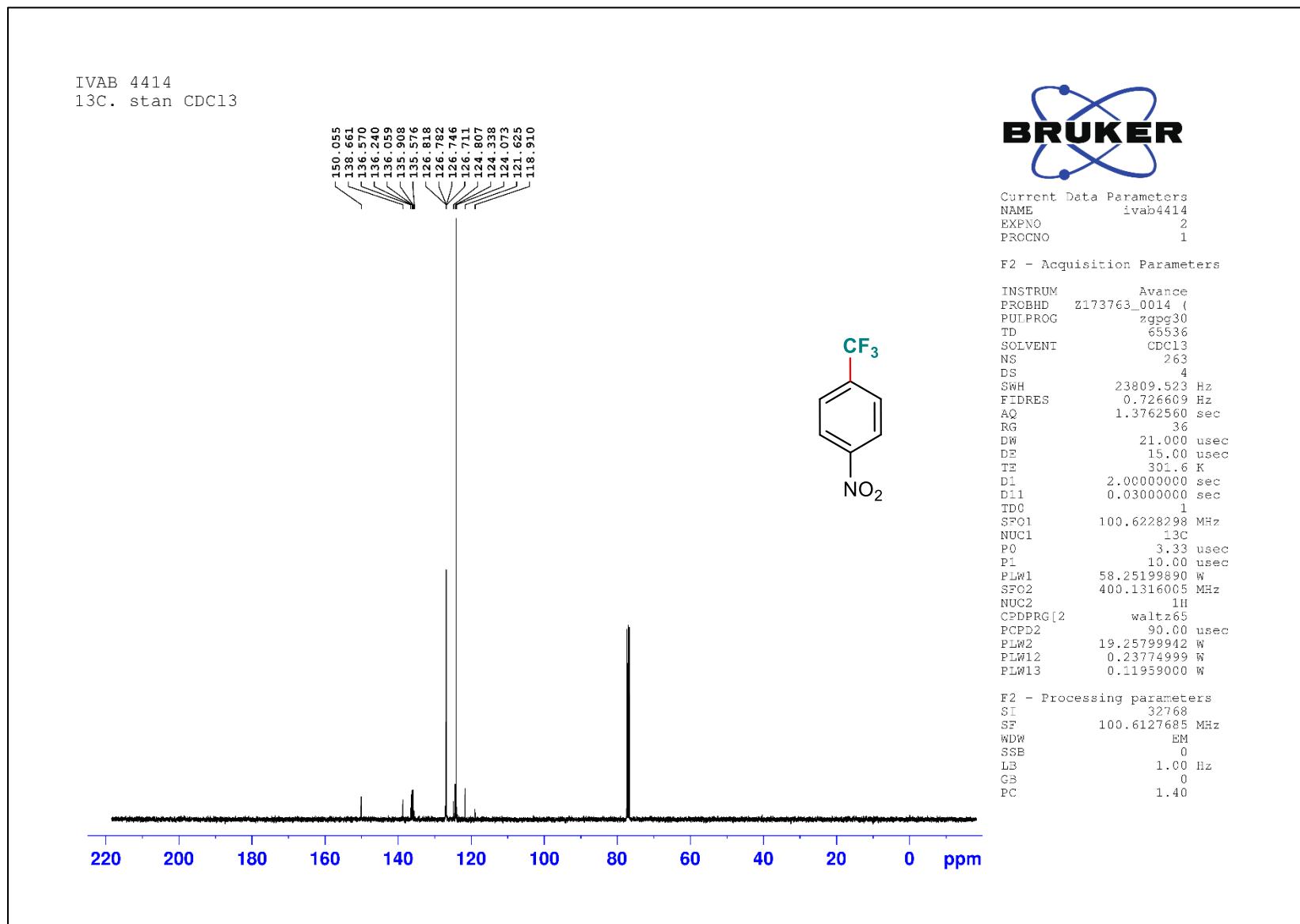


file: ...0410_02\svs583-FLUORINE_01.fid\fid block# 1 expt: "s2pul" freq. of 0 ppm: 564.344520 MHz
transmitter freq.: 564.296551 MHz processed size: 262144 complex points
time domain size: 262144 points LB: 1.500 GF: 0.0000
width: 131578.95 Hz = 233.1734 ppm = 0.501934 Hz/pt Hz/cm: 5263.158 ppm/cm: 9.32694
number of scans: 16

¹H NMR of Compound **2g**



¹³C NMR of Compound 2g

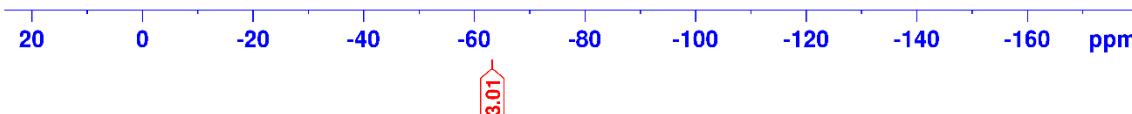
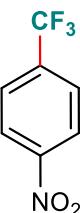


¹⁹F NMR of Compound 2g

IVAB 4414
19F. stan CDCl₃



-63.243



Current Data Parameters
NAME ivab4414
EXPNO 3
PROCNO 1

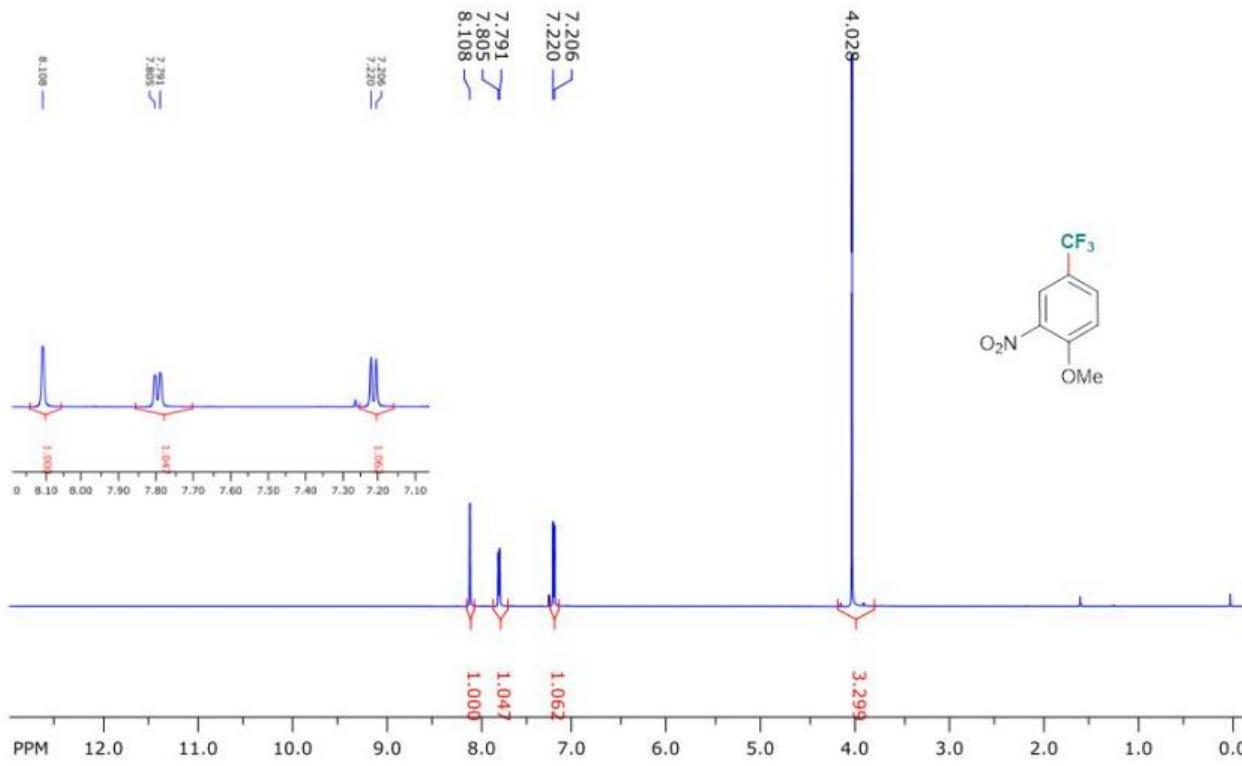
F2 - Acquisition Parameters

INSTRUM Avance
PROBHD Z173763_0014 (zg
PULPROG zg
TD 131072
SOLVENT CDCl₃
NS 16
DS 4
SWH 90909.094 Hz
FIDRES 1.387163 Hz
AQ 0.7208960 sec
RG 101
DW 5.500 usec
DE 6.50 usec
TE 301.3 K
D1 1.0000000 sec
TD0 1
SPO1 376.4607164 MHz
NUC1 ¹⁹F
P1 12.00 usec
PLW1 36.0000000 W

F2 - Processing parameters
SI 65536
SF 376.4983662 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

¹H NMR of Compound **2h**

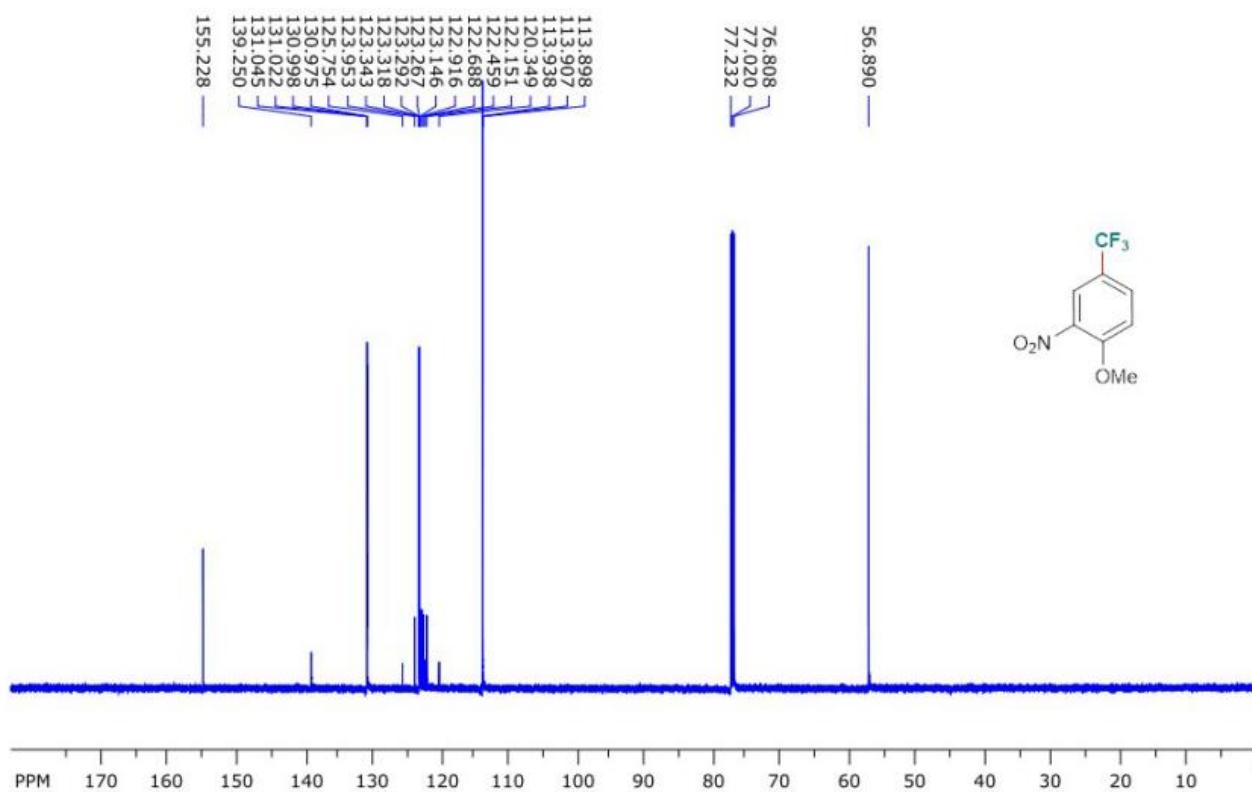
SpinWorks 4: IVAB 4372 1H CDCl₃



file: ...0409_01\ivab4372-PROTON_01.fid\fid block# 1 expt: "s2pul" freq. of 0 ppm: 599.766670 MHz
transmitter freq.: 599.770272 MHz processed size: 65536 complex points
time domain size: 76924 points LB: 0.300 GF: 0.0000
width: 9615.38 Hz = 16.0318 ppm = 0.124999 Hz/pt Hz/cm: 317.393 ppm/cm: 0.52919
number of scans: 16

¹³C NMR of Compound **2h**

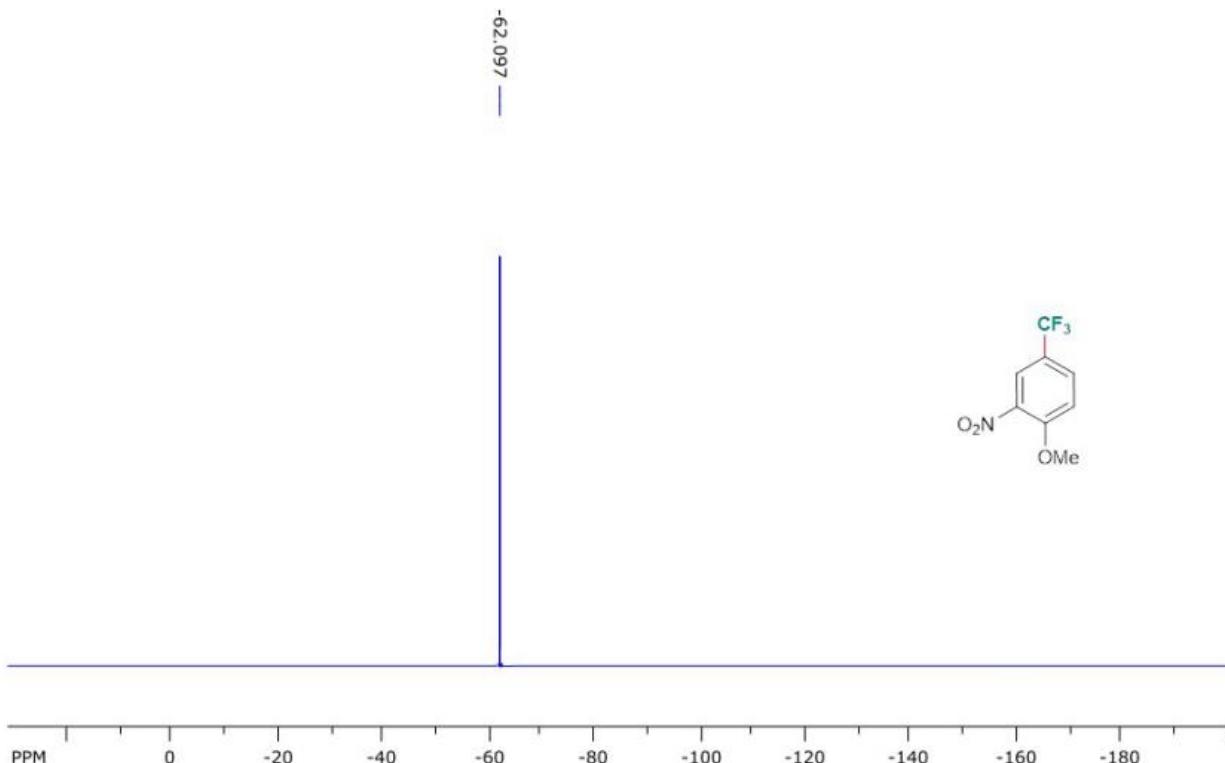
SpinWorks 4: IVAB 4372 13C CDCl₃



file: ...0409_02\ivab4372-CARBON_01.fid\fid block# 1 expt: "s2pul" freq. of 0 ppm: 150.811446 MHz
transmitter freq.: 150.828039 MHz processed size: 65536 complex points
time domain size: 65536 points LB: 0.500 GF: 0.0000
width: 37878.79 Hz = 251.1389 ppm = 0.577984 Hz/pt Hz/cm: 1114.575 ppm/cm: 7.38971
number of scans: 512

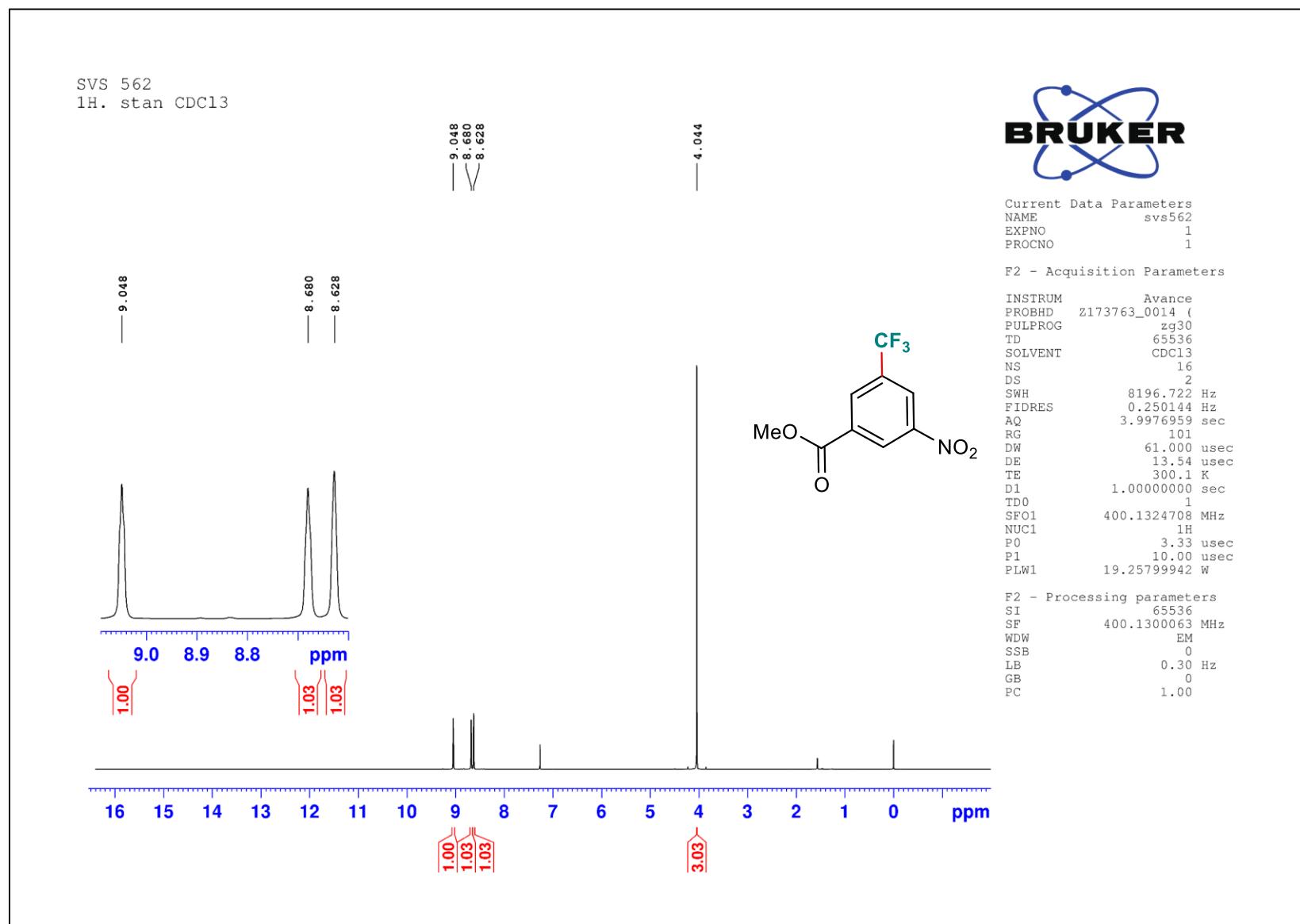
¹⁹F NMR of Compound **2h**

SpinWorks 4: IVAB 4372 19F

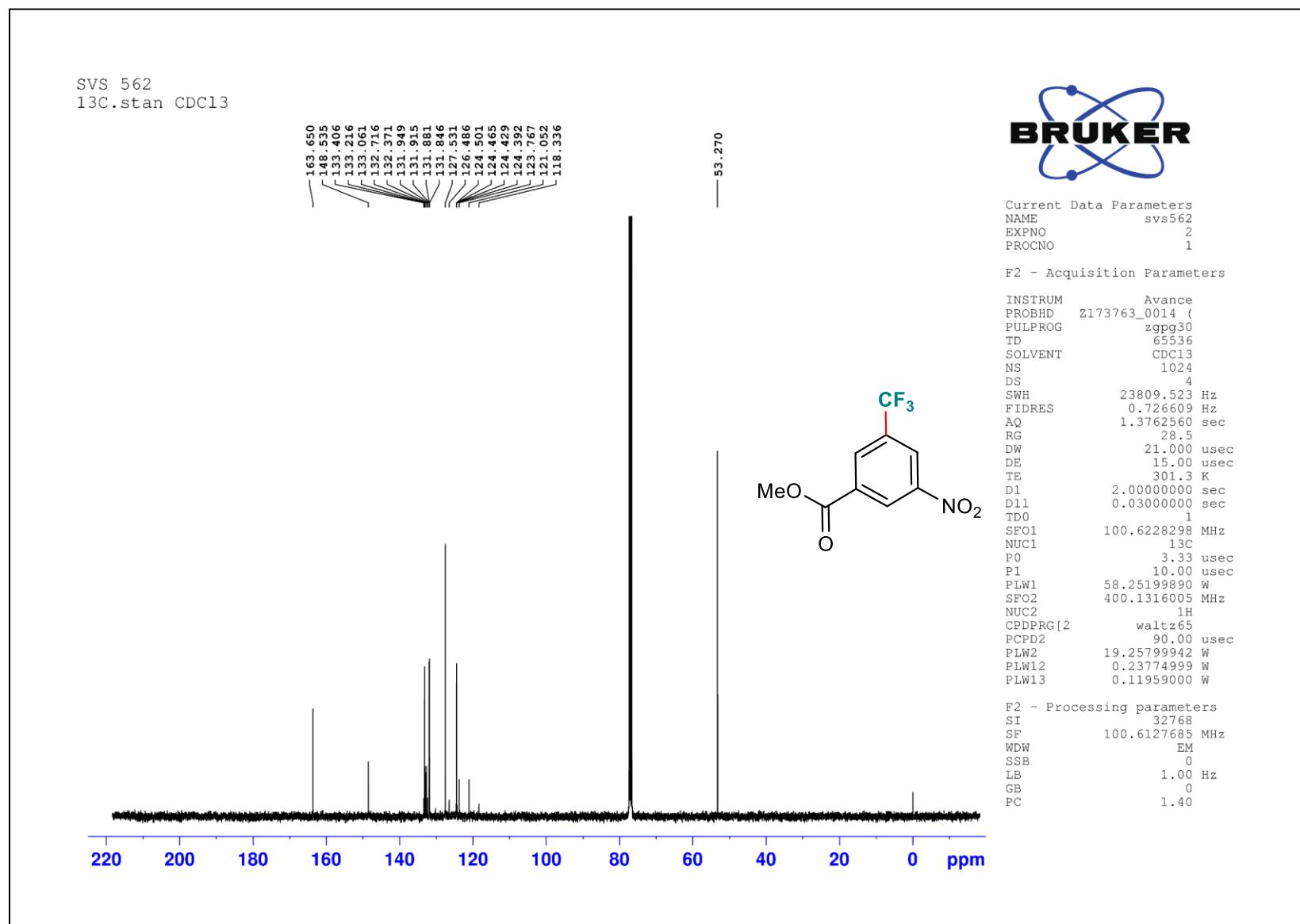


file: ...09_03\ivab4372-FLUORINE_01.fid\fid block# 1 expt: "s2pul" freq. of 0 ppm: 564.344520 MHz
transmitter freq.: 564.296551 MHz processed size: 262144 complex points
time domain size: 262144 points LB: 1.500 GF: 0.0000
width: 131578.95 Hz = 233.1734 ppm = 0.501934 Hz/pt Hz/cm: 5263.158 ppm/cm: 9.32694
number of scans: 16

¹H NMR of Compound 2i



¹³C NMR of Compound 2i



¹⁹F NMR of Compound 2i

SVS 562
19F. stan CDCl₃

-62.966

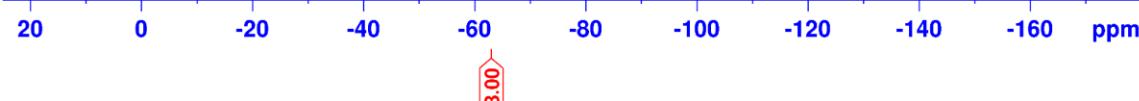
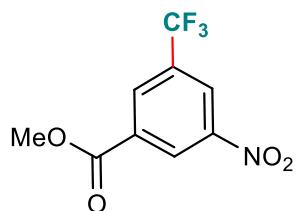


Current Data Parameters
NAME svs562
EXPNO 3
PROCNO 1

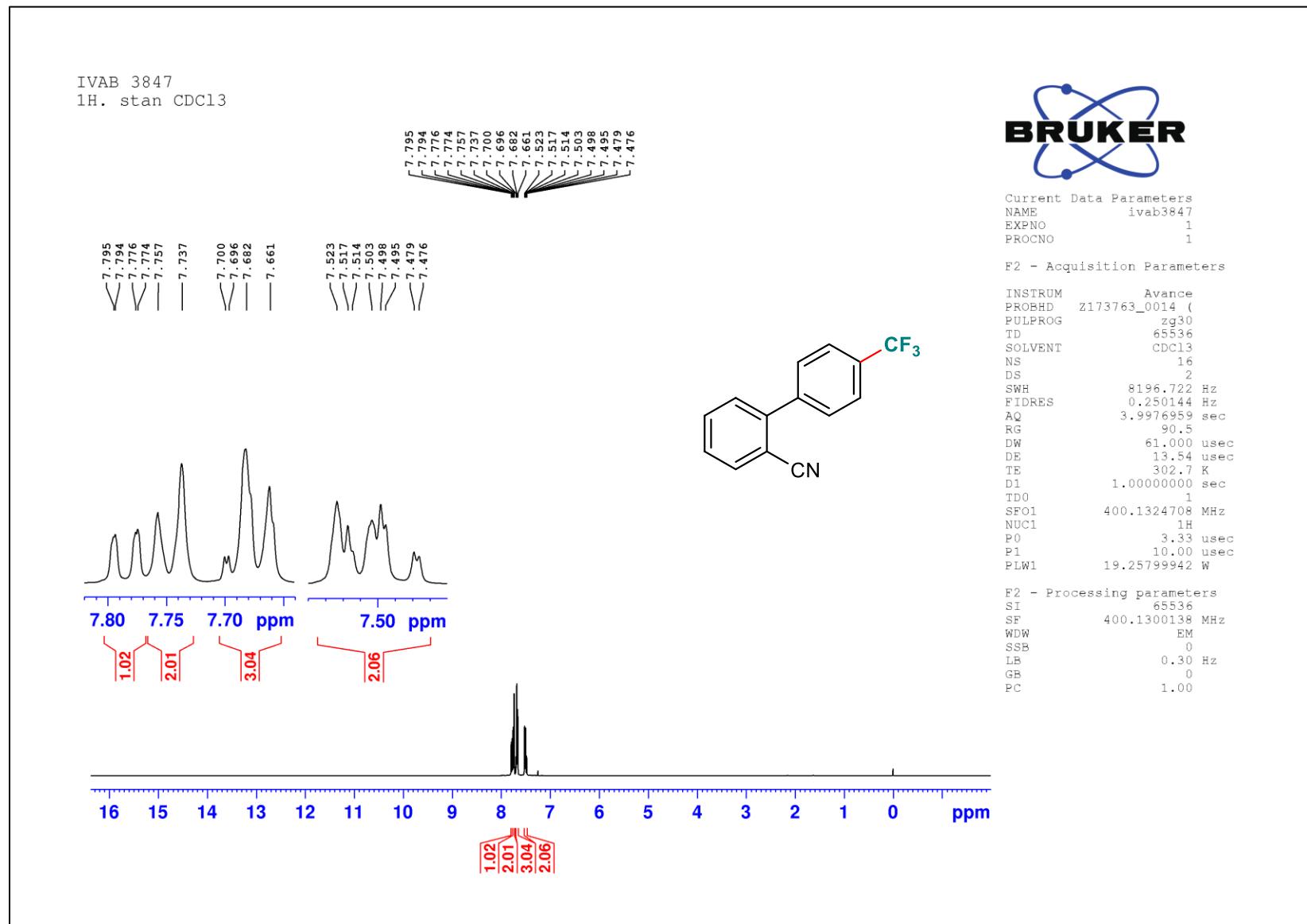
F2 - Acquisition Parameters

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PULPROG zg
TD 131072
SOLVENT CDCl₃
NS 16
DS 4
SWH 90909.094 Hz
FIDRES 1.387163 Hz
AQ 0.7208960 sec
RG 101
DW 5.500 usec
DE 6.50 usec
TE 301.0 K
D1 1.0000000 sec
TDO 1
SF01 376.4607164 MHz
NUC1 ¹⁹F
P1 12.00 usec
PLW1 36.0000000 W

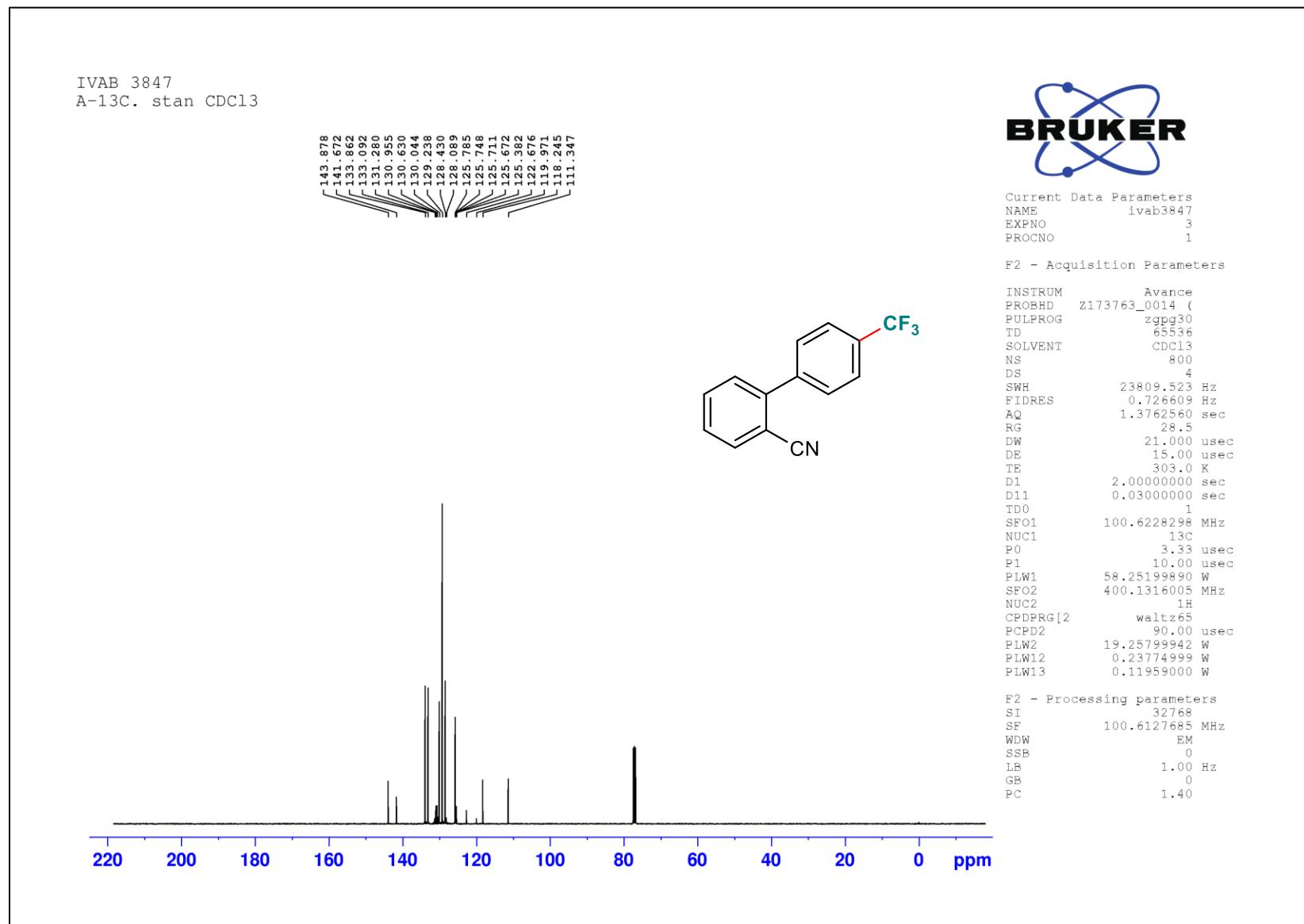
F2 - Processing parameters
SI 65536
SF 376.4983662 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



¹H NMR of Compound 2j



¹³C NMR of Compound 2j



¹⁹F NMR of Compound 2j

IVAB 3847
19F. stan CDCl₃

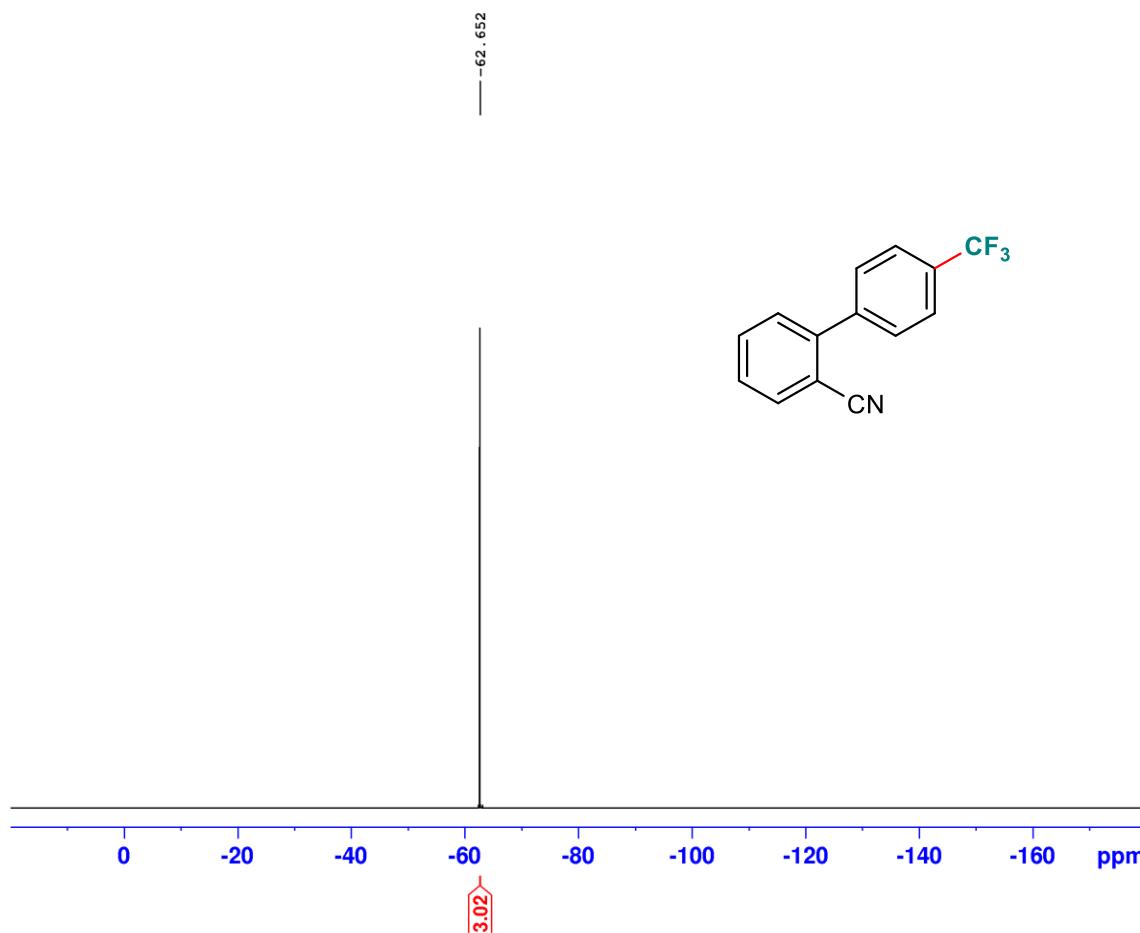


Current Data Parameters
NAME ivab3847
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters

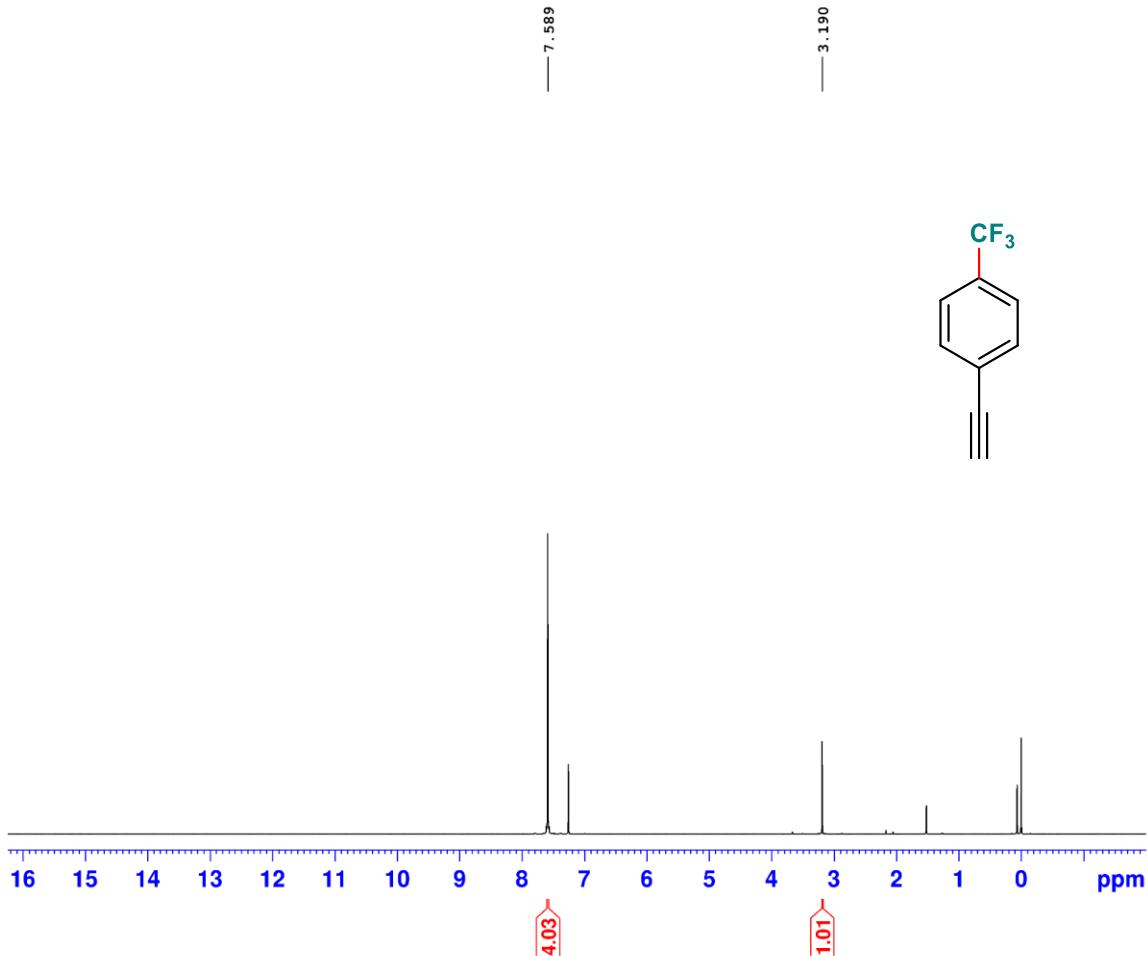
INSTRUM Avance
PROBHD Z173763_0014 (zg
PULPROG zg
TD 131072
SOLVENT CDCl₃
NS 16
DS 4
SWH 90909.094 Hz
FIDRES 1.387163 Hz
AQ 0.7208960 sec
RG 101
DW 5.500 usec
DE 6.50 usec
TE 302.7 K
D1 1.0000000 sec
TDO 1
SFO1 376.4607164 MHz
NUC1 ¹⁹F
P1 12.00 usec
PLW1 36.0000000 W

F2 - Processing parameters
SI 65536
SF 376.4983662 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



¹H NMR of Compound **2k**

SVS 614
1H. stan CDCl₃

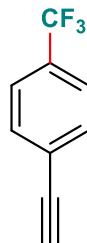


Current Data Parameters
NAME svs614
EXPNO 1
PROCNO 1

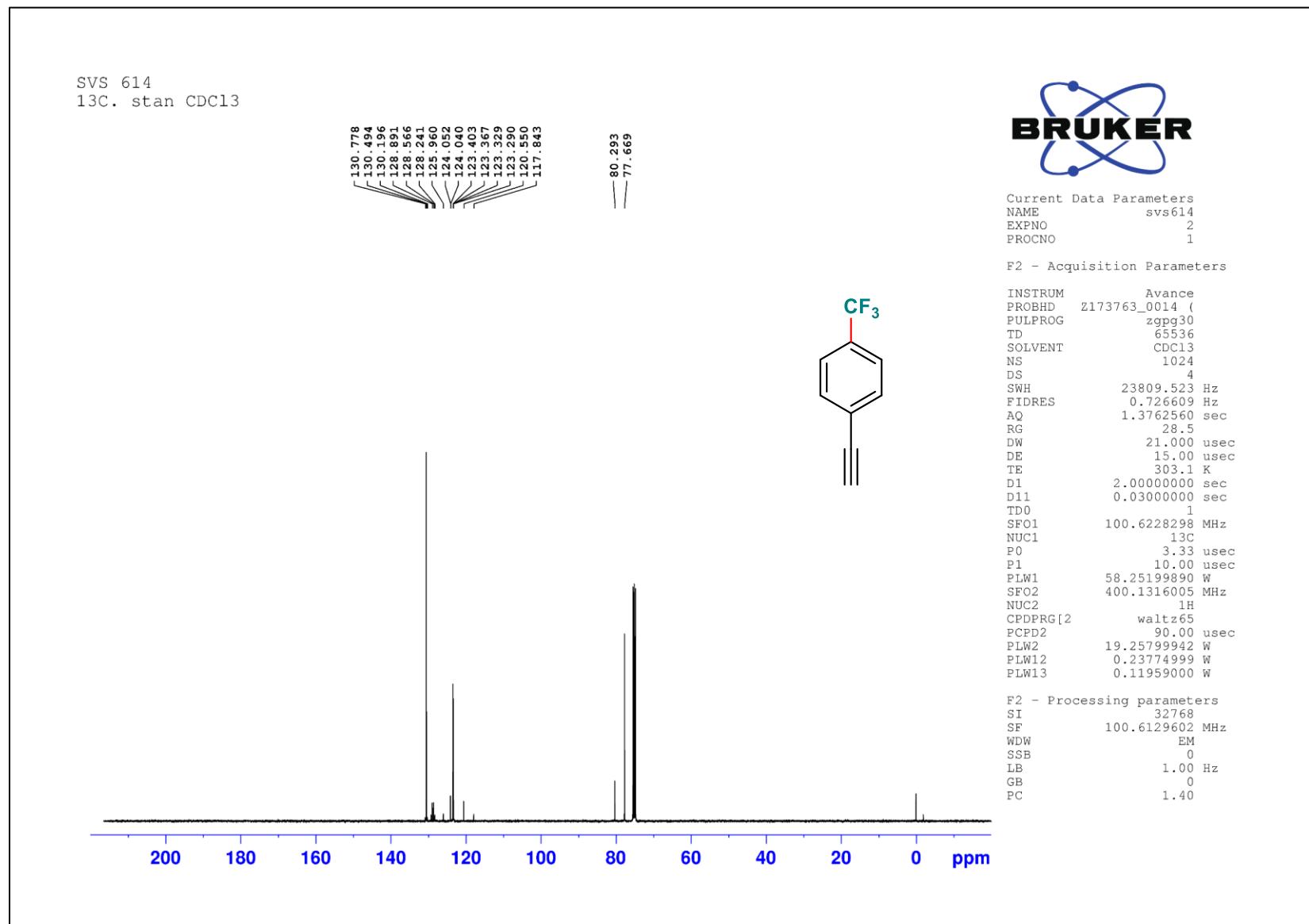
F2 - Acquisition Parameters

INSTRUM Avance
PROBHD z173763_0014_ (zg30
PULPROG zg30
TD 65536
SOLVENT CDCl₃
NS 16
DS 2
SWH 8196.722 Hz
FIDRES 0.250144 Hz
AQ 3.9976959 sec
RG 101
DW 61.000 usec
DE 13.54 usec
TE 302.2 K
D1 1.0000000 sec
TD0 1
SFO1 400.1324708 MHz
NUC1 1H
P0 3.33 usec
P1 10.00 usec
PLW1 19.25799942 W

F2 - Processing parameters
SI 65536
SF 400.1300099 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

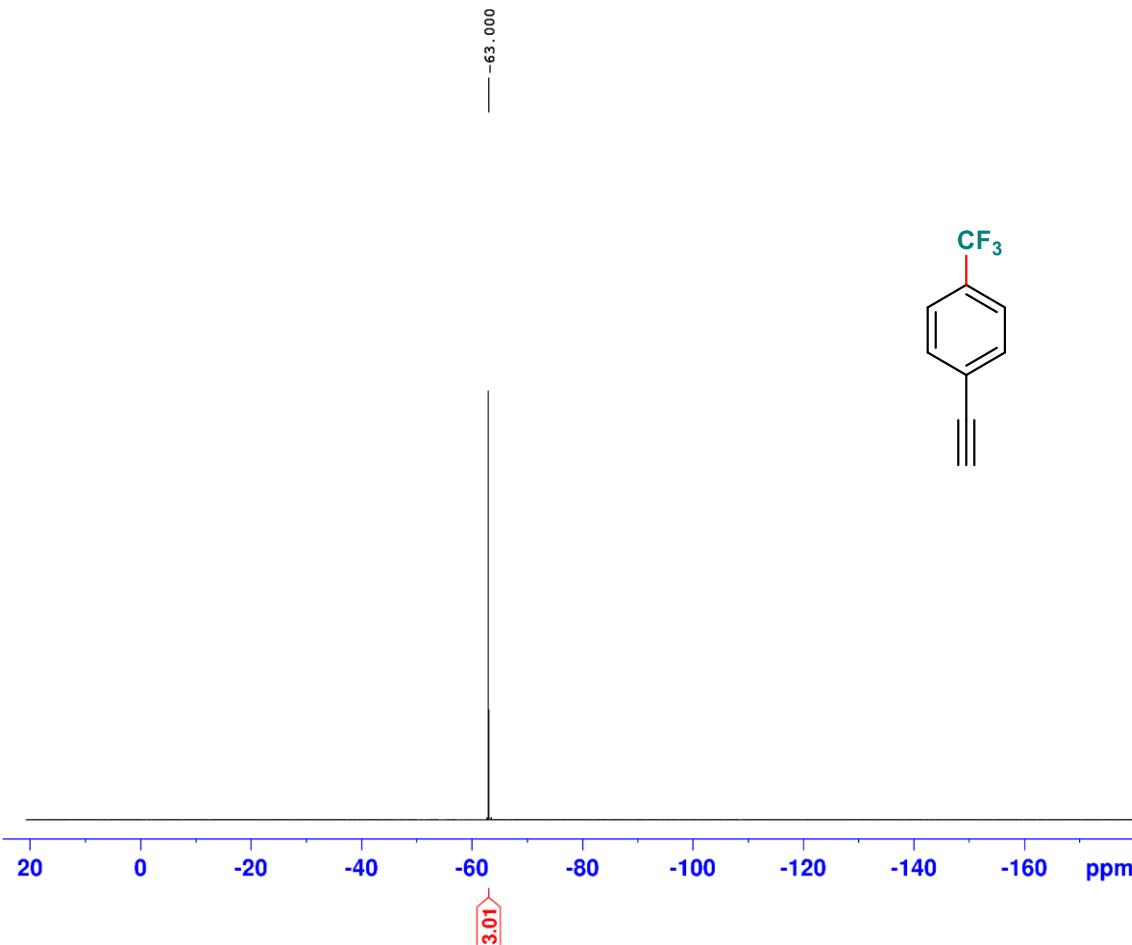


¹³C NMR of Compound 2k



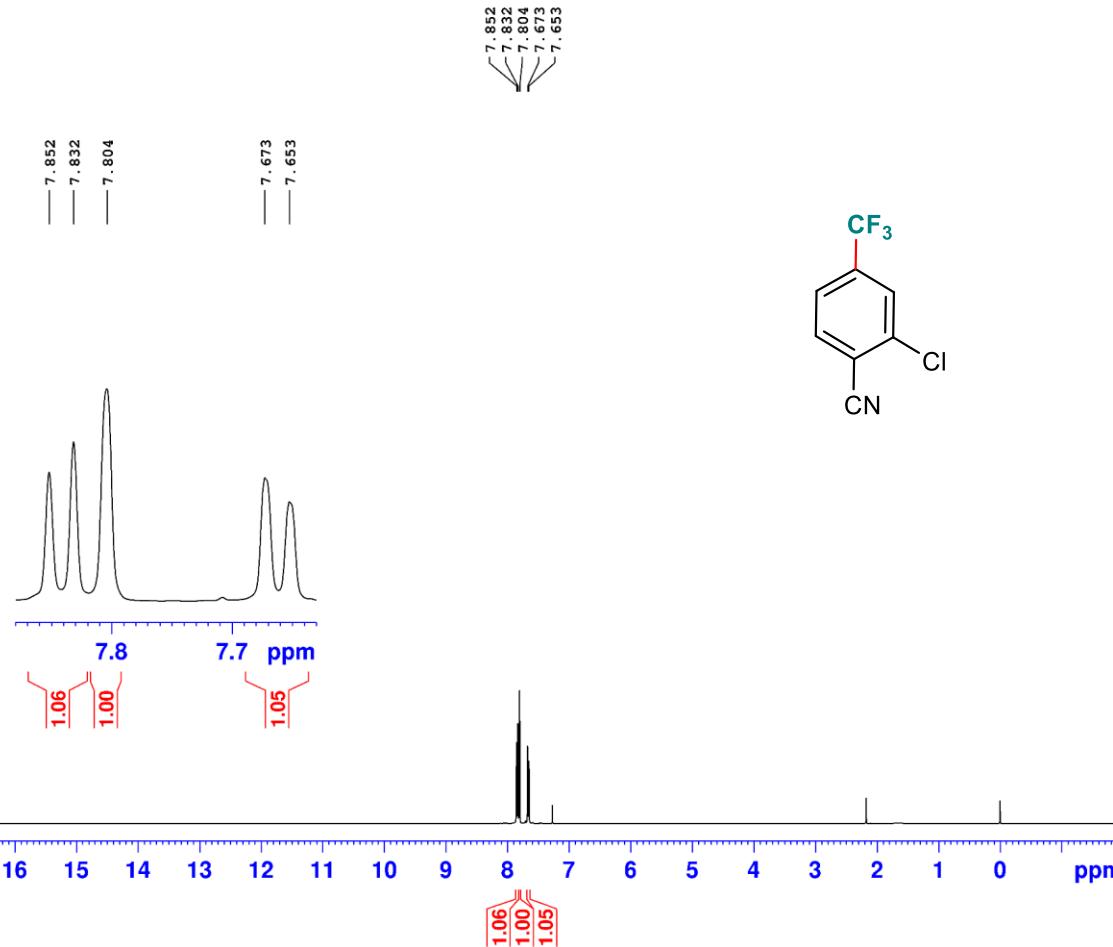
¹⁹F NMR of Compound **2k**

SVS 614
19F. stan CDCl₃



¹H NMR of Compound 2I

SVS 633
1H. stan CDC13





BRUKER

Current Data Parameters
NAME svs633
EXPNO 1
PROCNO 1

```

F2 - Acquisition Parameters
INSTRUM      Avance
PROBHD      Z173763_0014 (
PULPROG      zg30
TD          65536
SOLVENT      CDC13
NS           16
DS            2
SWH         8196.722 Hz
FIDRES      0.250144 Hz
AQ          3.9976959 sec
RG           101
DW           61.0000 usec
DE           13.54 usec
TE           300.8 K
D1          1.00000000 sec
TDO           1
SFO1        400.1324708 MHz
NUC1         1H
PO           3.33 usec
P1           10.00 usec
PLW1        19.25799942 W

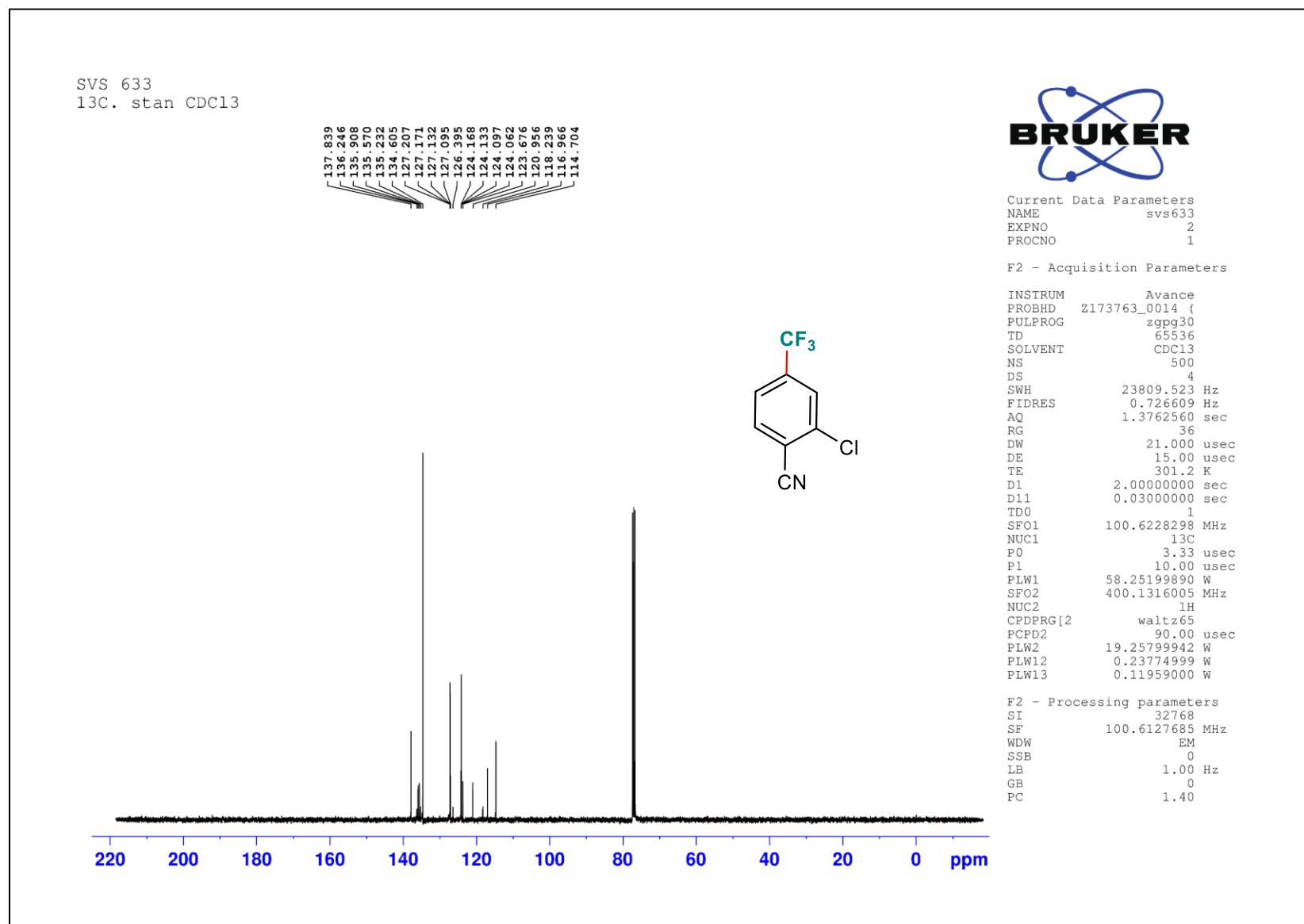
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F2 - Processing parameters
SI          65536
SF         400.1300046 MHz
WDW          EM
SSB          0
LB          0.30 Hz
GB          0
PC          1.00

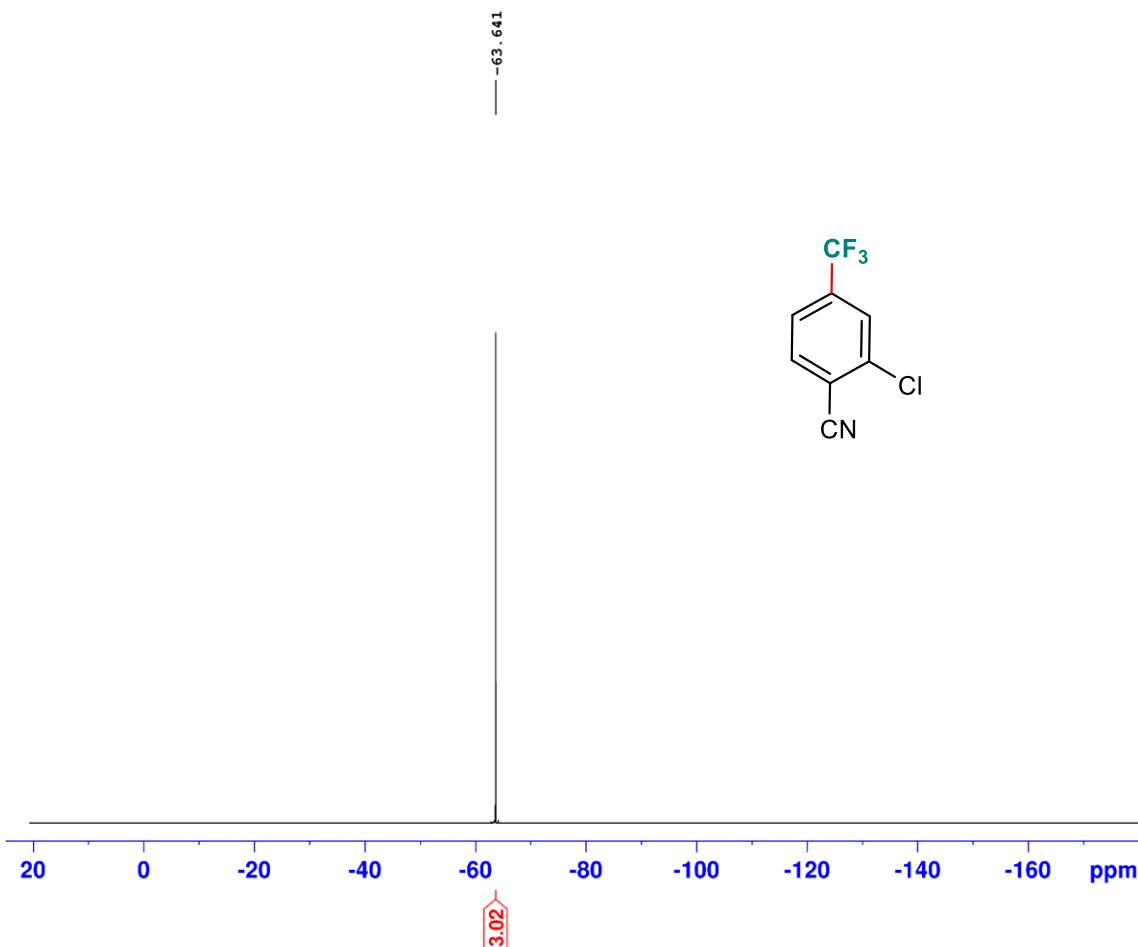
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¹³C NMR of Compound 2I



¹⁹F NMR of Compound 2I

SVS 633
19F. stan CDCl₃



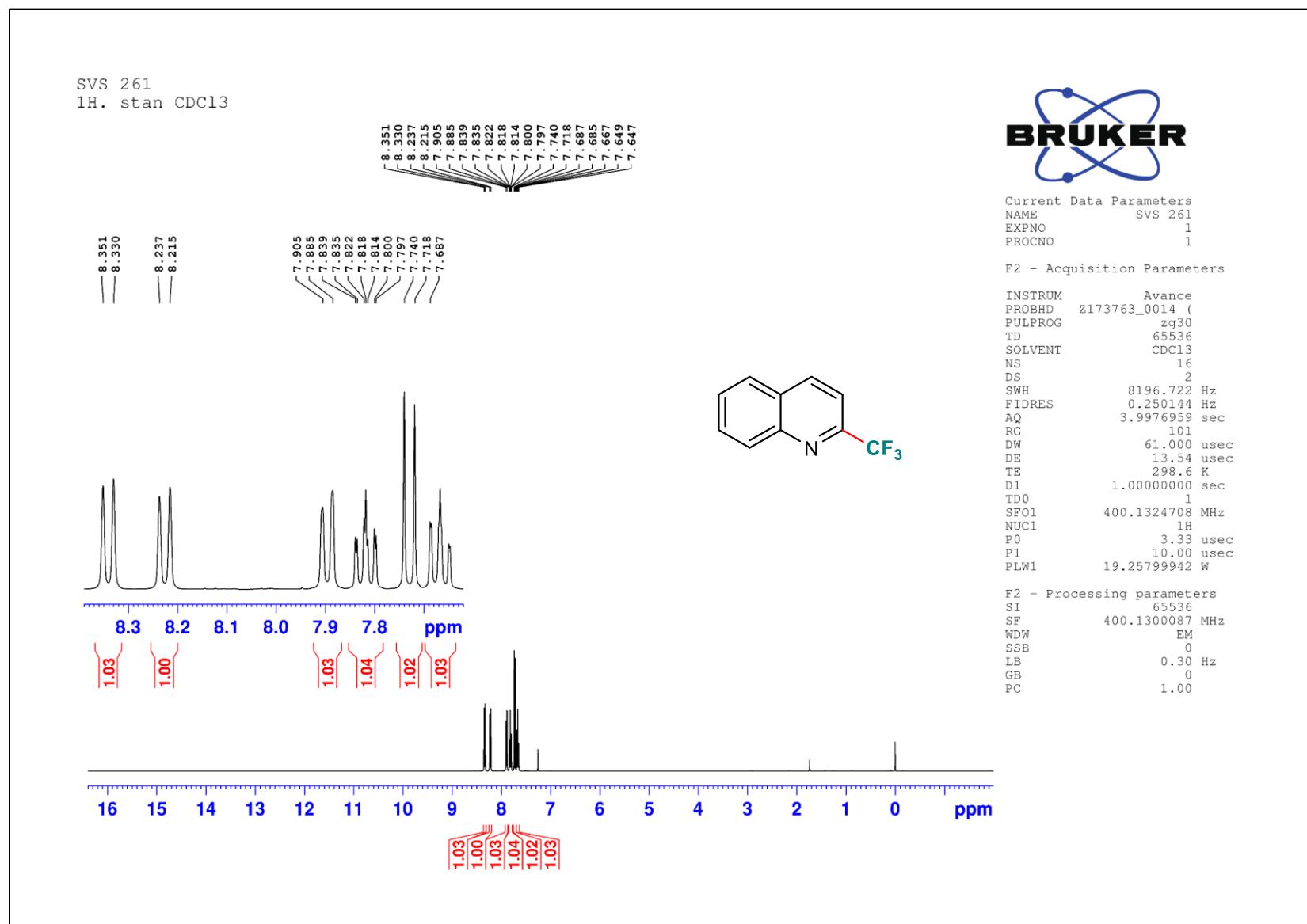
Current Data Parameters
NAME svs633
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters

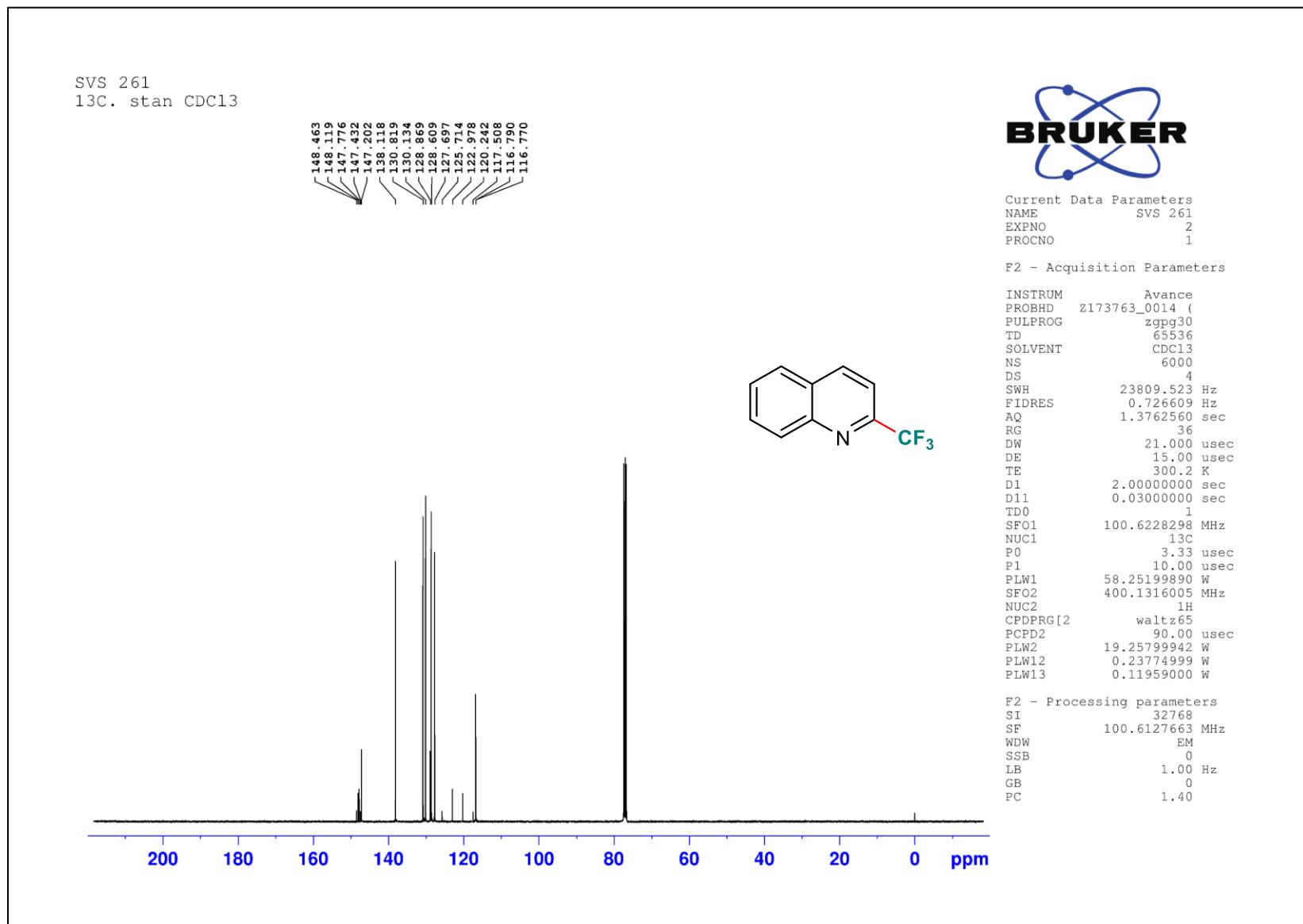
INSTRUM Avance
PROBHD Z173763_0014 ('
PULPROG zg
TD 131072
SOLVENT CDCl₃
NS 16
DS 4
SWH 90909.094 Hz
FIDRES 1.387163 Hz
AQ 0.7208960 sec
RG 101
DW 5.500 usec
DE 6.50 usec
TE 300.9 K
D1 1.0000000 sec
TD0 1
SFO1 376.4607164 MHz
NUC1 ¹⁹F
P1 12.00 usec
PLW1 36.0000000 W

F2 - Processing parameters
SI 65536
SF 376.4983662 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

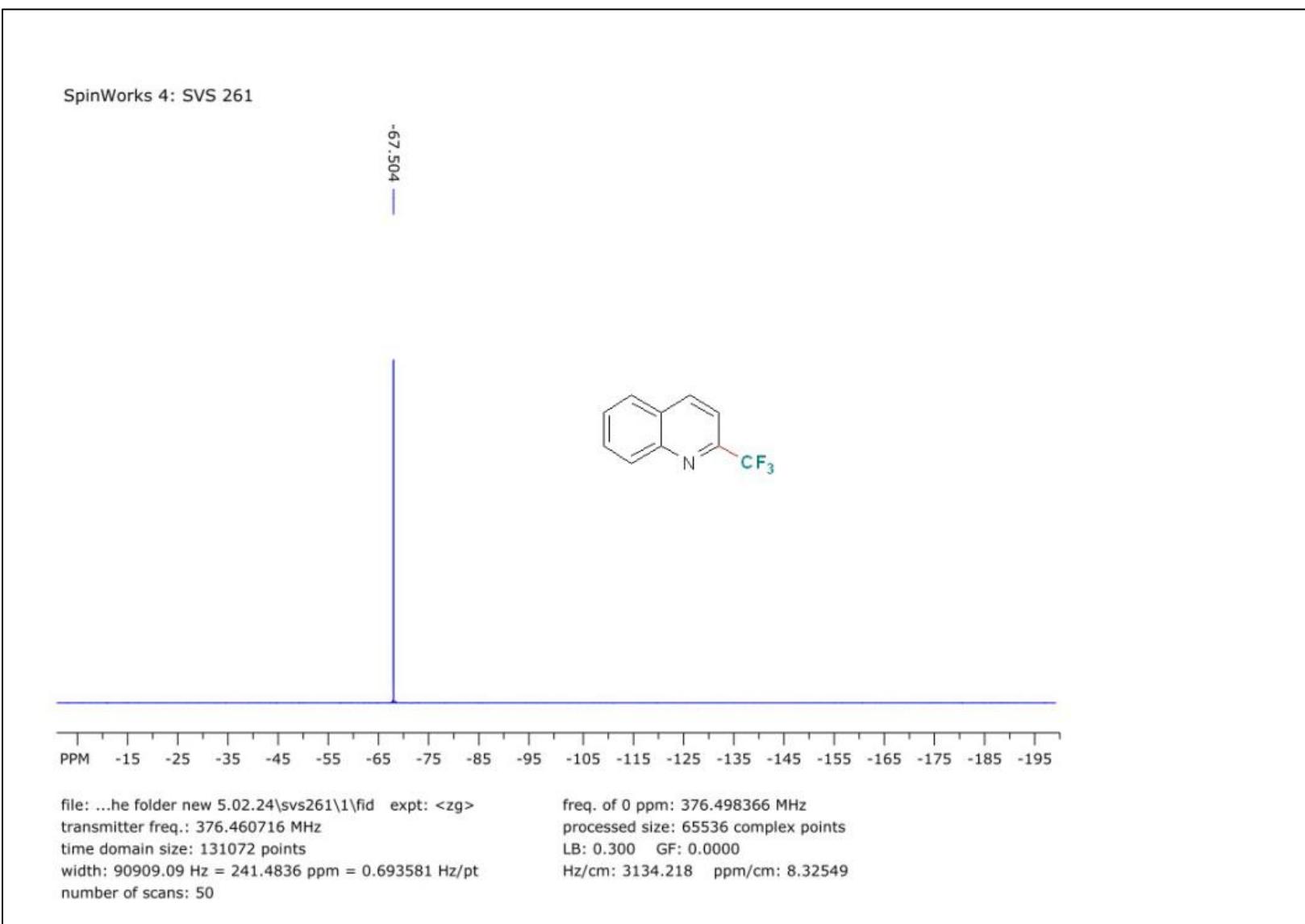
¹H NMR of Compound 2m



¹³C NMR of Compound 2m

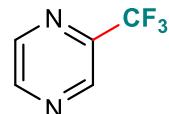
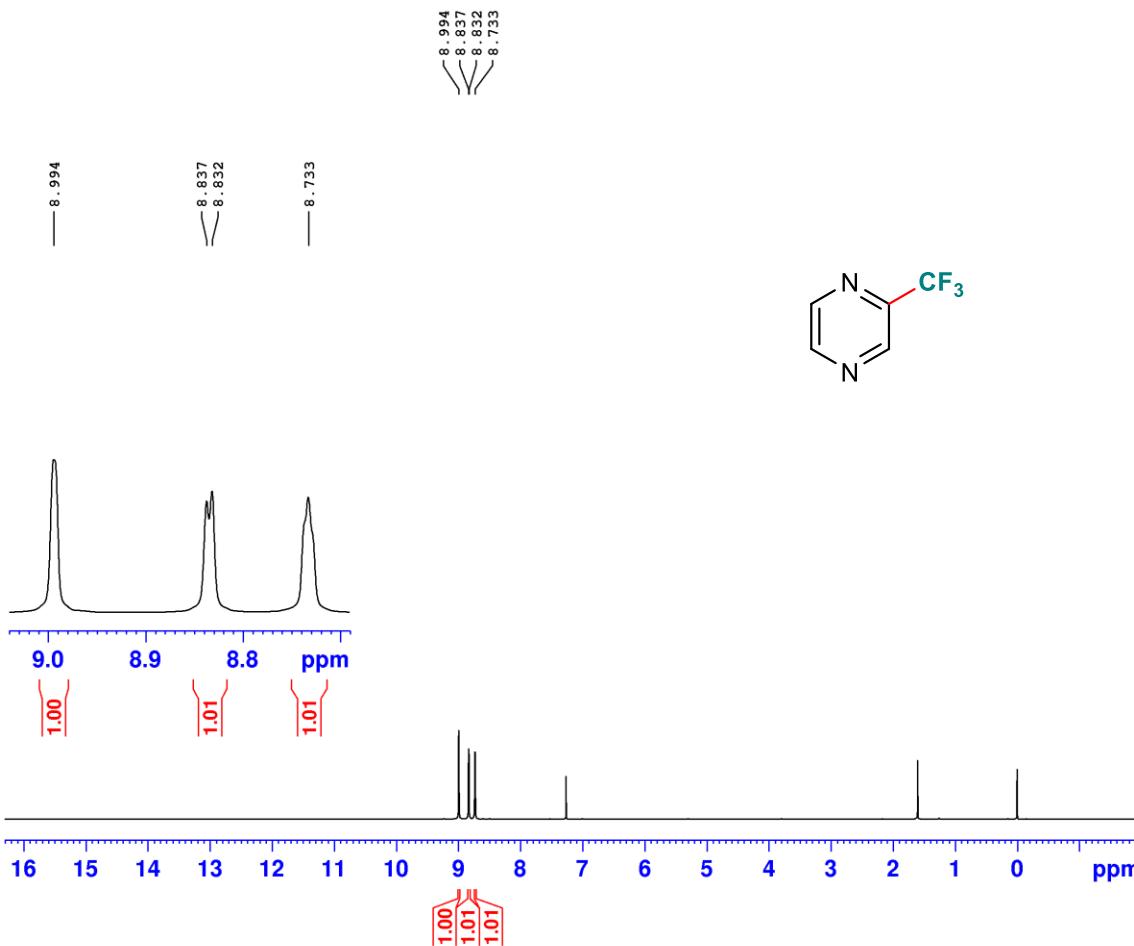


¹⁹F NMR of Compound **2m**



¹H NMR of Compound 2n

SVS 299
1H. stan CDC13



The Bruker logo consists of the word "BRUKER" in a bold, black, sans-serif font. Above the letter "B", there is a blue stylized atom symbol with three orbiting electrons.

Current Data Parameters	
NAME	svs299
EXPNO	1
PROCNO	1

F2 - Acquisition Parameters

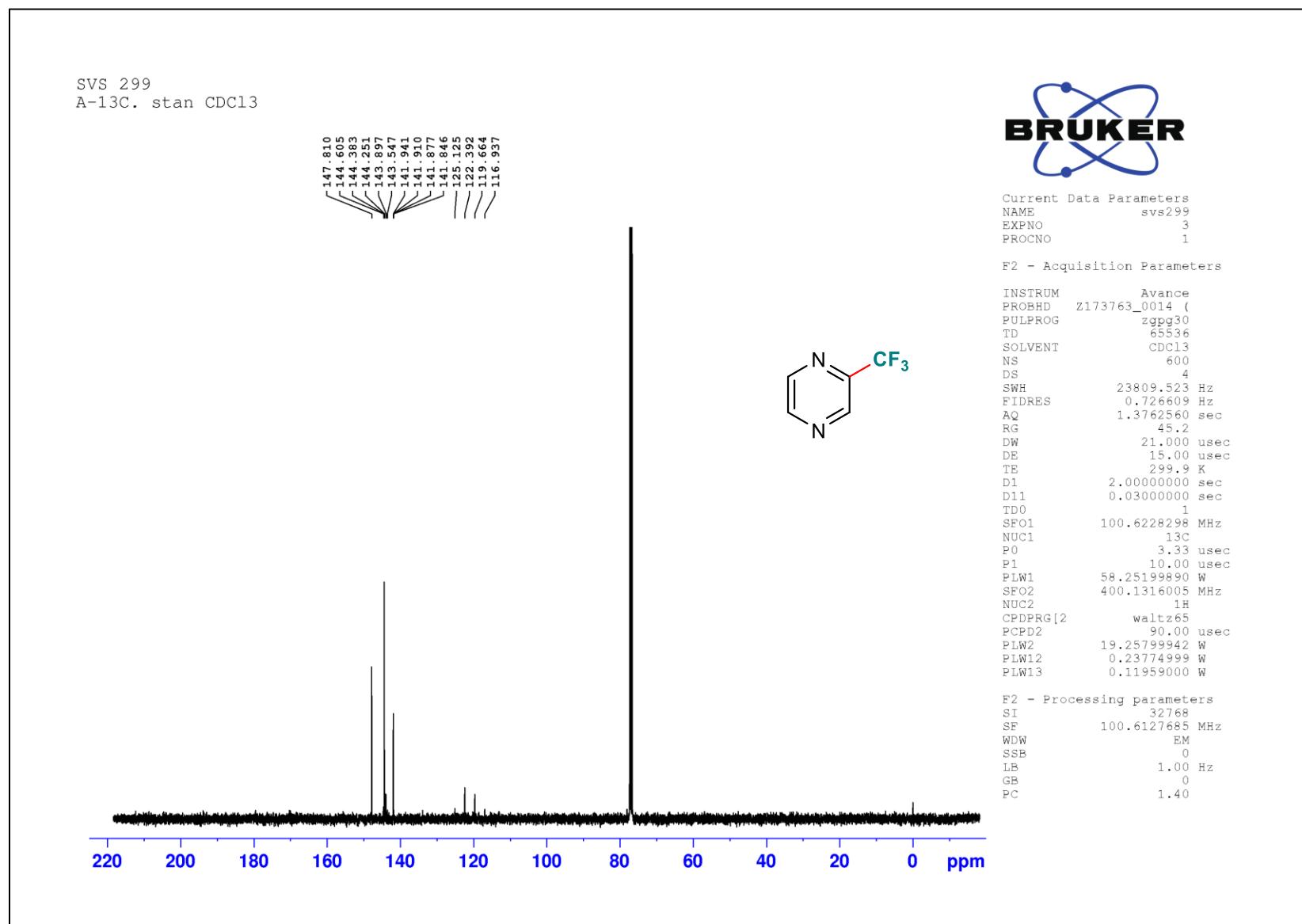
INSTRUM	Avance
PROBHD	Z173763_0014 (
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8196.722 Hz
FIDRES	0.250144 Hz
AQ	3.9976959 sec
RG	101
DW	61.000 usec
DE	13.54 usec
TE	299.4 K
D1	1.0000000 sec
TDO	1
SFO1	400.1324708 MHz
NUC1	1H
P0	3.33 usec
P1	10.00 usec
PLW1	19.25799942 W

```

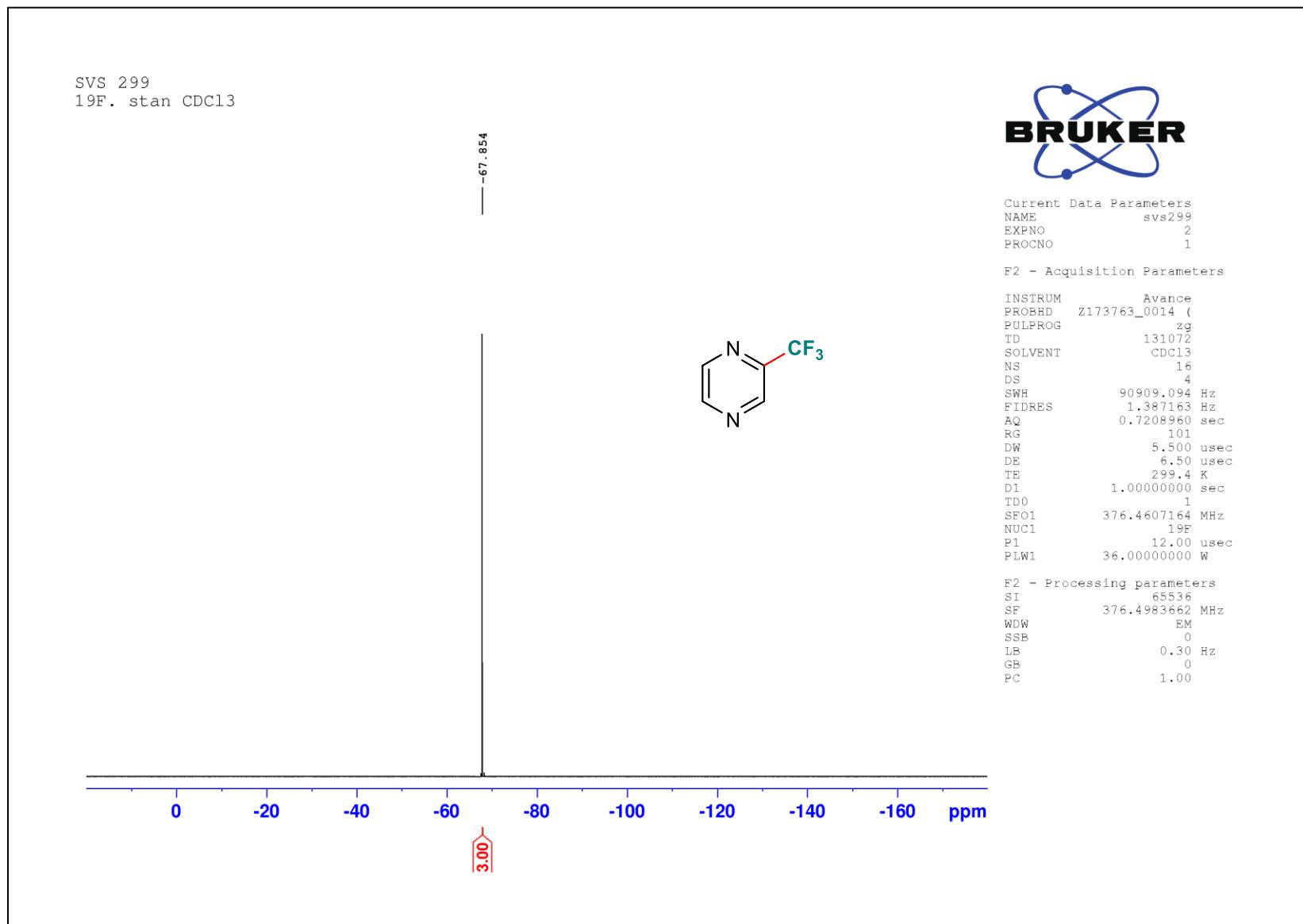
F2 - Processing parameters
SI          65536
SF        400.1300062 MHz
WDW         EM
SSB          0
LB        0.30 Hz
GB          0
PC        1.00

```

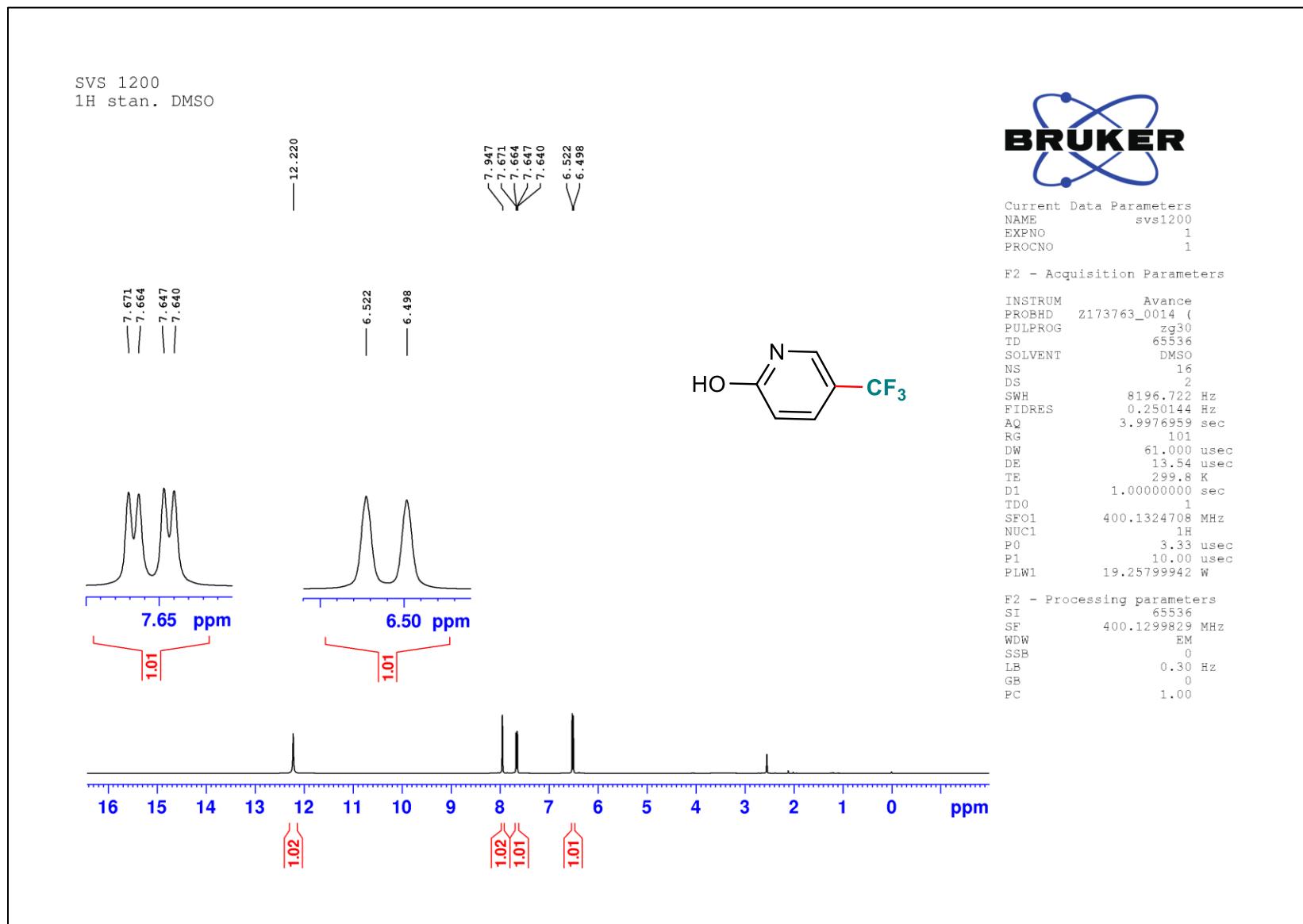
¹³C NMR of Compound 2n



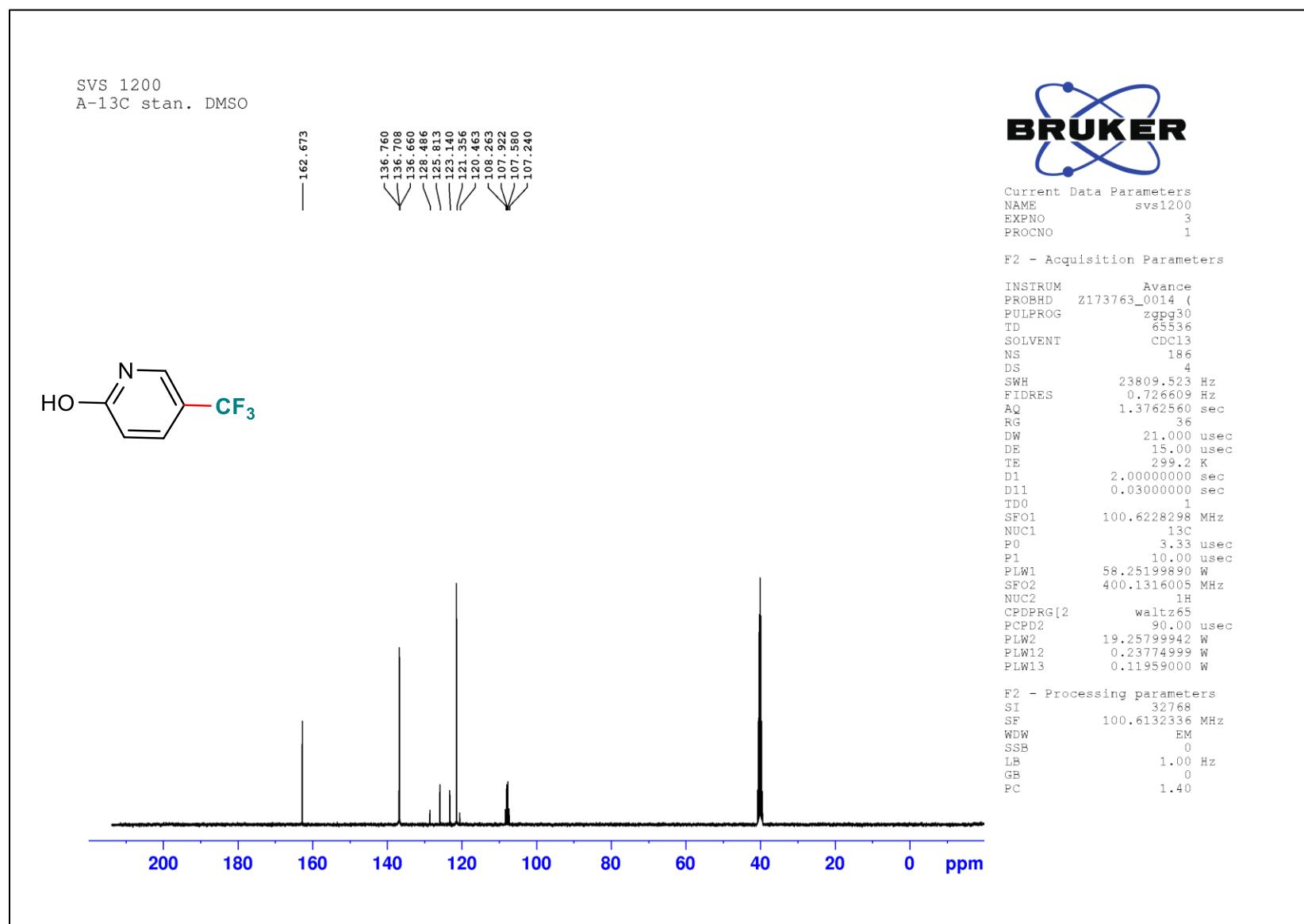
¹⁹F NMR of Compound 2n



¹H NMR of Compound 2o



¹³C NMR of Compound 2o



¹⁹F NMR of Compound 2o

SVS 1200
19F stan. DMSO

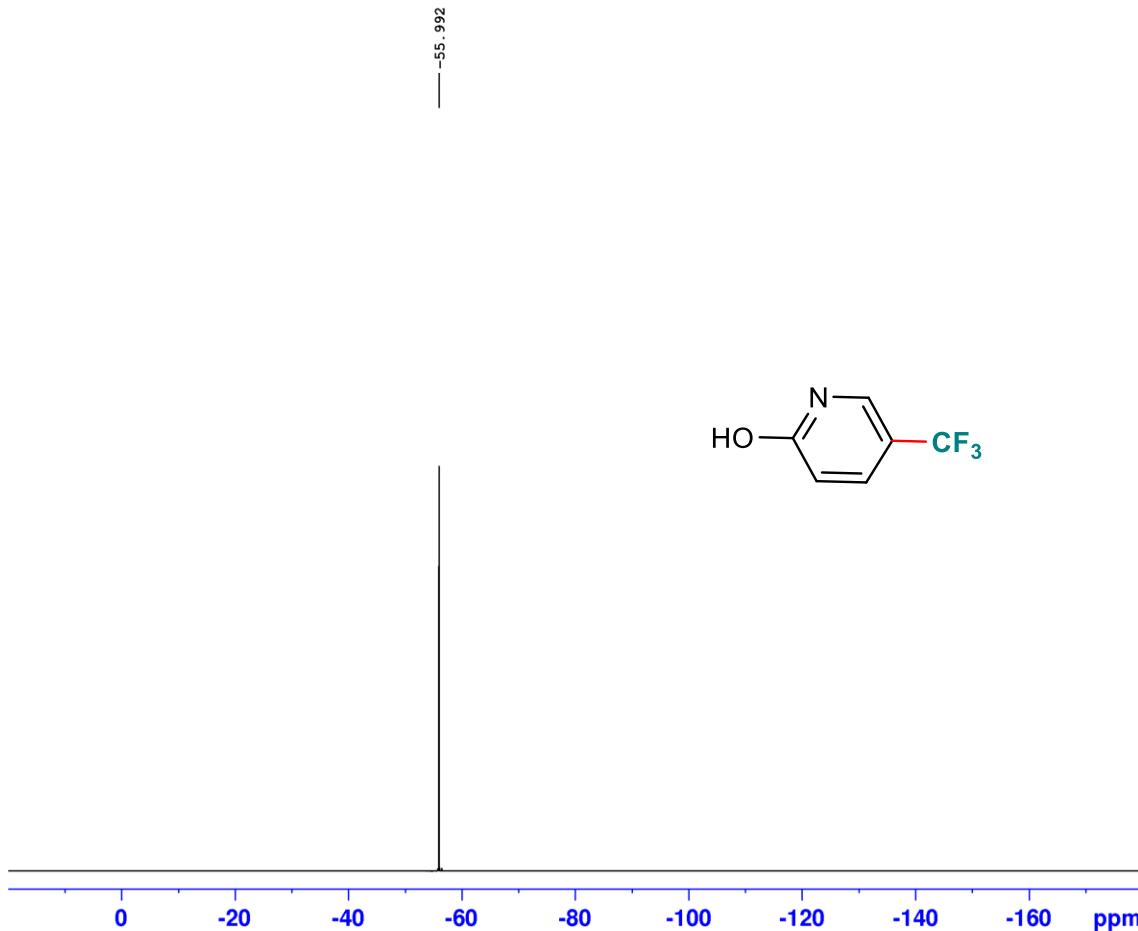
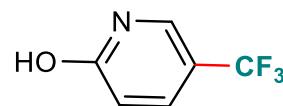


Current Data Parameters
NAME svs1200
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters

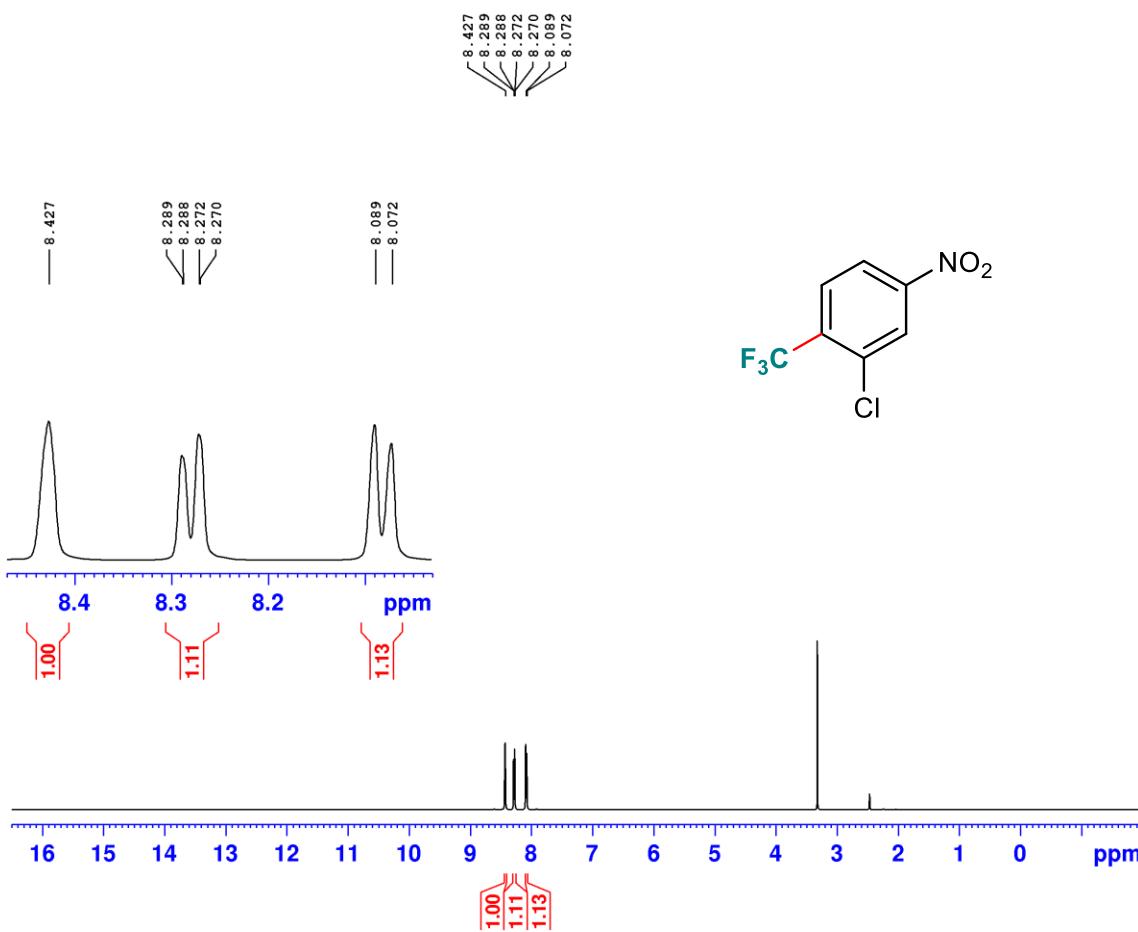
INSTRUM Avance
PROBHD Z173763_0014 (zg
PULPROG zg
TD 131072
SOLVENT CDCl3
NS 16
DS 4
SWH 90909.094 Hz
FIDRES 1.387163 Hz
AQ 0.7208960 sec
RG 101
DW 5.500 usec
DE 6.50 usec
TE 299.1 K
D1 1.0000000 sec
TDO 1
SFO1 376.4607164 MHz
NUC1 19F
P1 12.00 usec
PLW1 36.00000000 W

F2 - Processing parameters
SI 65536
SF 376.4983662 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



¹H NMR of Compound 2p

IVA 2477
1H stan DMSO



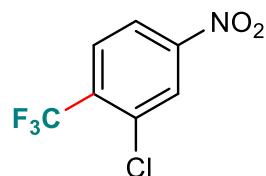
 BRUKER

Current Data Parameters
NAME IVA 2477
EXPNO 3
PROCNO 1

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F2 - Acquisition Parameters
INSTRUM      AV_III_500
PROBHD      5 mm Multincl
PULPROG      zg30
TD          65536
SOLVENT      DMSO
NS           24
DS            0
SWH         12335.526 Hz
FIDRES      0.188225 Hz
AQ        2.6563926 sec
RG           71.8
DW          40.533 used
DE           6.50 used
TE          295.0 K
D1       1.00000000 sec
TDO          1

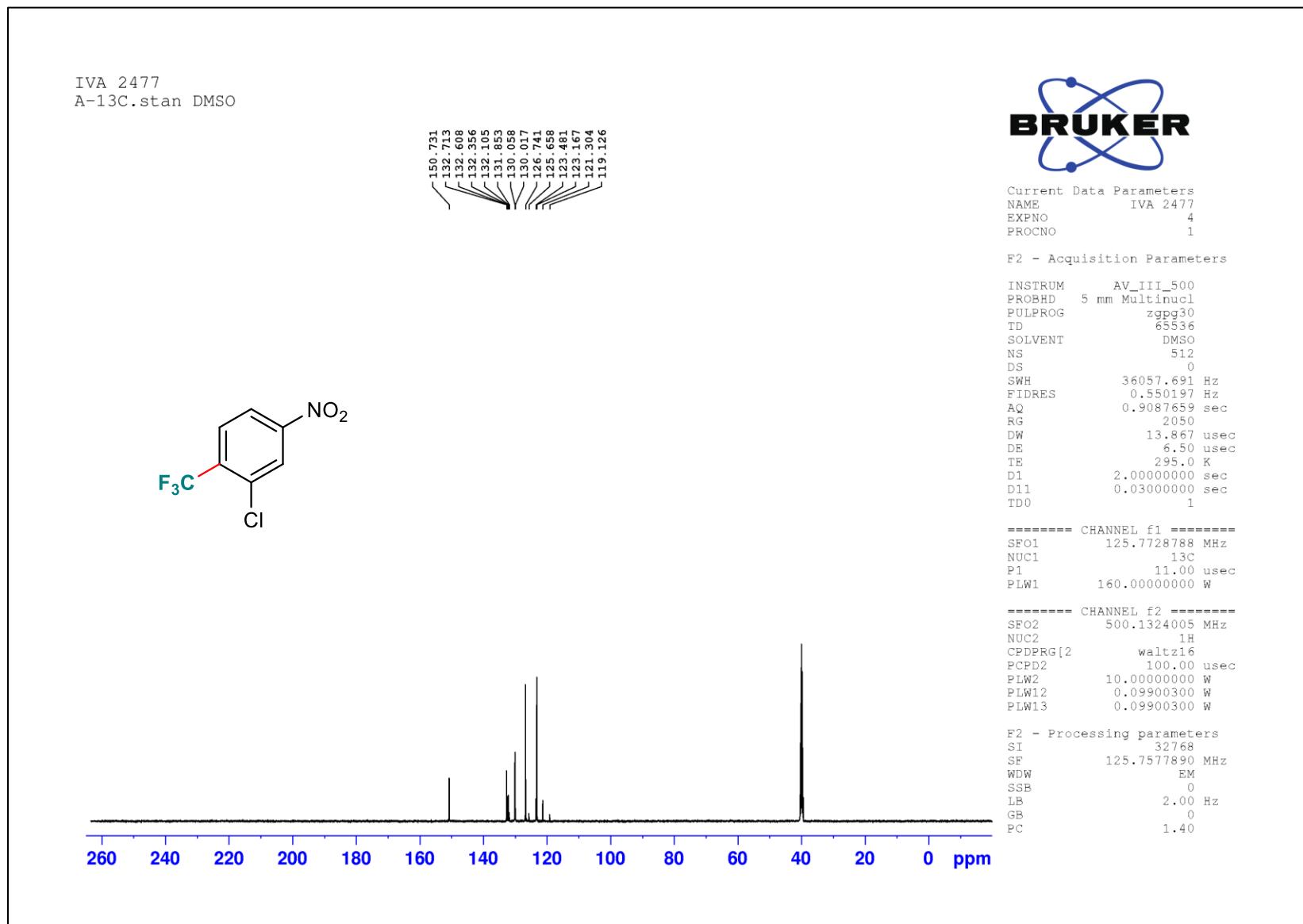
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===== CHANNEL f1 =====
SFO1 500.1330008 MHz
NUC1 1H
P1 9.95 usec
PLW1 9.69999981 W

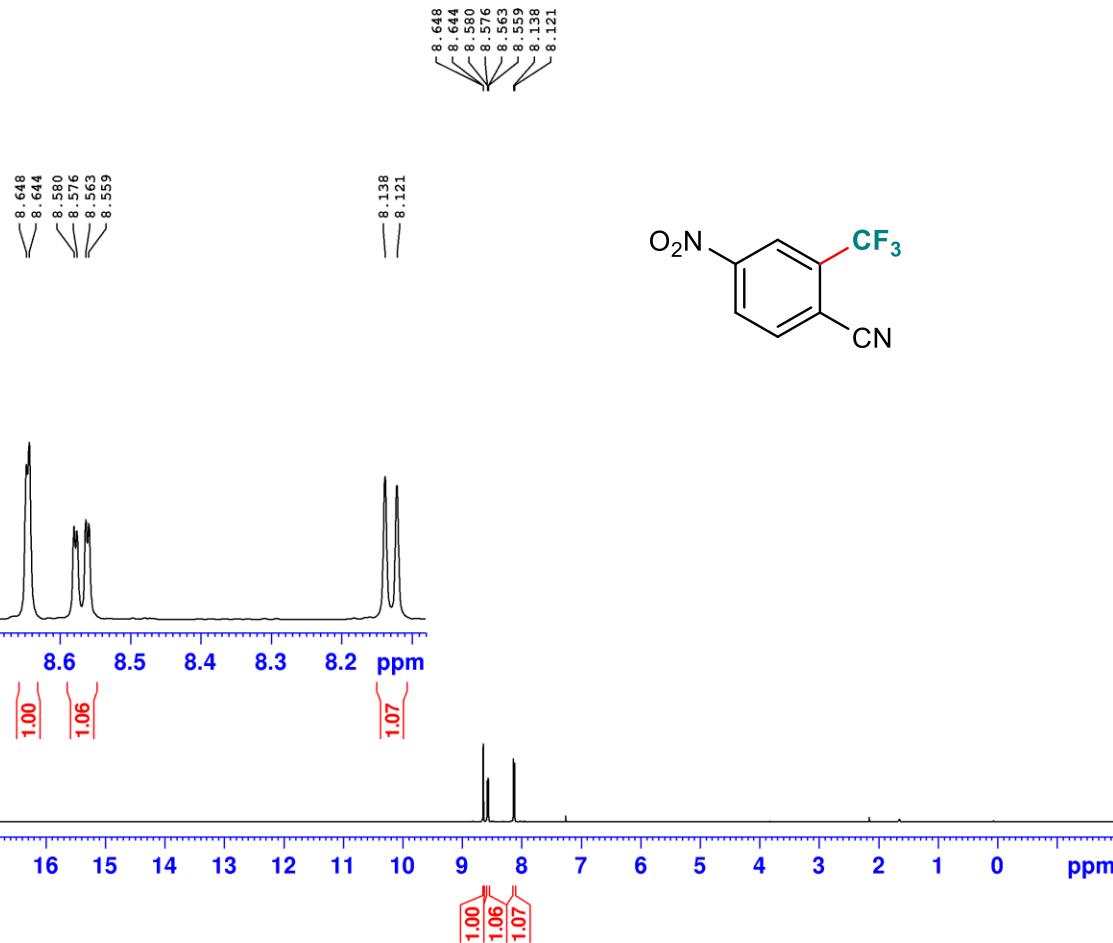
F2 - Processing parameters
SI 65536
SF 500.1300236 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

¹³C NMR of Compound 2p



¹H NMR of Compound 2q

IVA 2428
1H. stan CDC13





Current Data Parameter
NAME IVA 242
EXPNO
PROCNO

```

F2 - Acquisition Parameters
INSTRUM      AV_III_500
PROBHD      5 mm Multinucl
PULPROG      zg30
TD          65536
SOLVENT      CDC13
NS           24
DS            0
SWH         12335.526 Hz
FIDRES      0.188225 Hz
AQ        2.6563926 sec
RG           114
DW          40.533 usec
DE           6.50 usec
TE          295.0 K
D1       1.0000000 sec
TDO          1

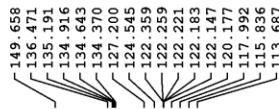
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===== CHANNEL f1 =====
SFO1 500.1330008 MHz
NUC1 1H
P1 9.95 usec
PLW1 9.69999981 W

F2 - Processing parameters
SI 65536
SF 500.1300236 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

¹³C NMR of Compound 2q

IVA 2428
A-13C. stan CDCl₃



Current Data Parameters
NAME IVA 2428
EXPNO 10
PROCNO 1

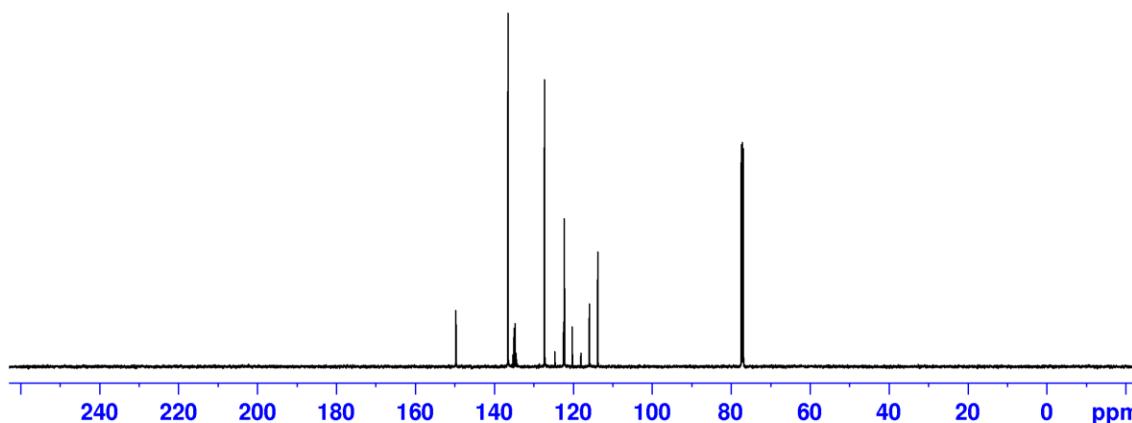
F2 - Acquisition Parameters

INSTRUM AV_III_500
PROBHD 5 mm Multinucl
PULPROG zgppg30
TD 65536
SOLVENT CDCl₃
NS 1024
DS 0
SWH 36057.691 Hz
FIDRES 0.550197 Hz
AQ 0.9087659 sec
RG 2050
DW 13.867 usec
DE 6.50 usec
TE 295.0 K
D1 2.0000000 sec
D11 0.03000000 sec
TDO 2

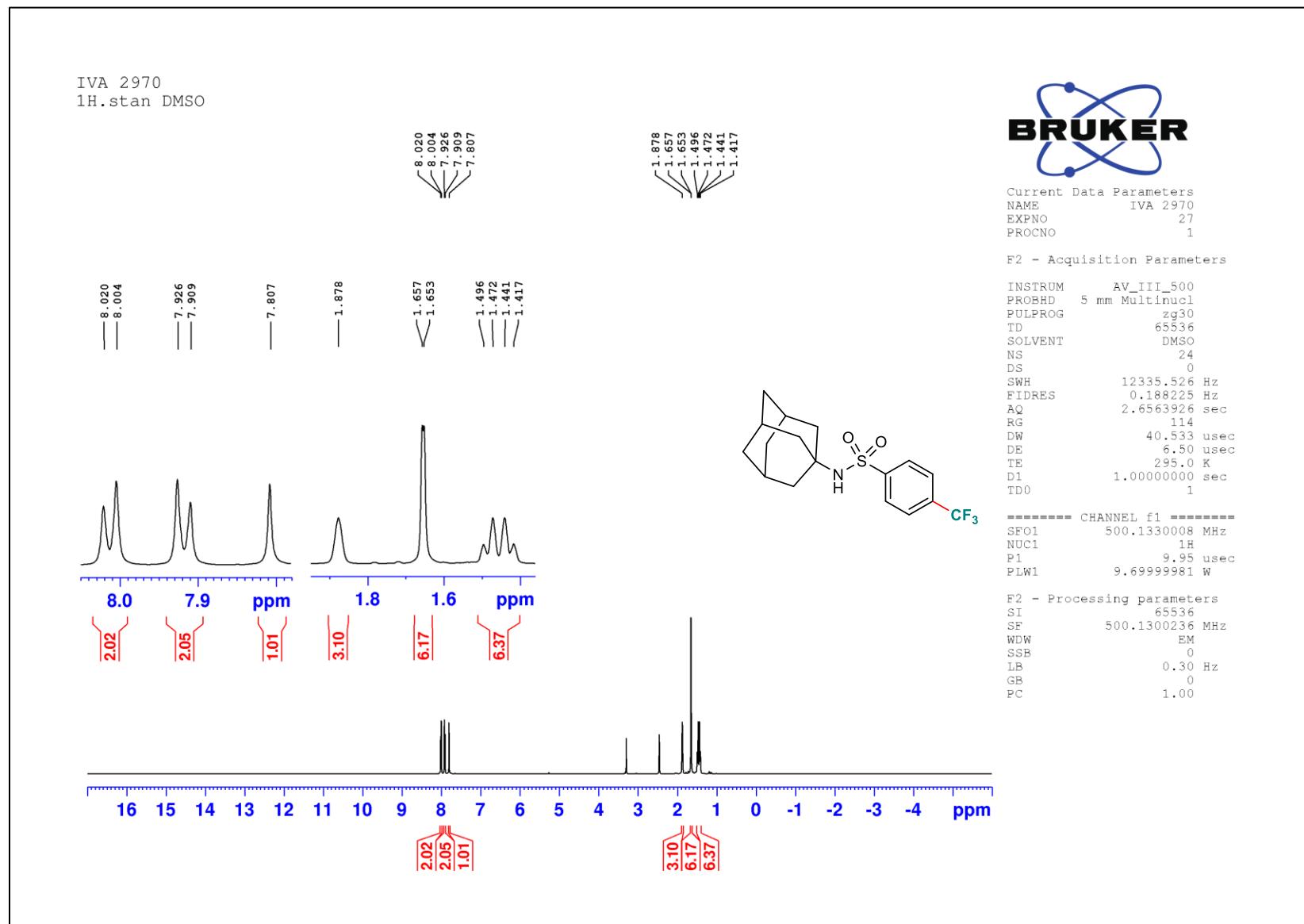
===== CHANNEL f1 =====
SFO1 125.7728788 MHz
NUC1 ¹³C
P1 11.00 usec
PLW1 160.00000000 W

===== CHANNEL f2 =====
SFO2 500.1324005 MHz
NUC2 ¹H
CPDPRG[2] waltz16
PCPD2 100.00 usec
PLW2 10.0000000 W
PLW12 0.09900300 W
PLW13 0.09900300 W

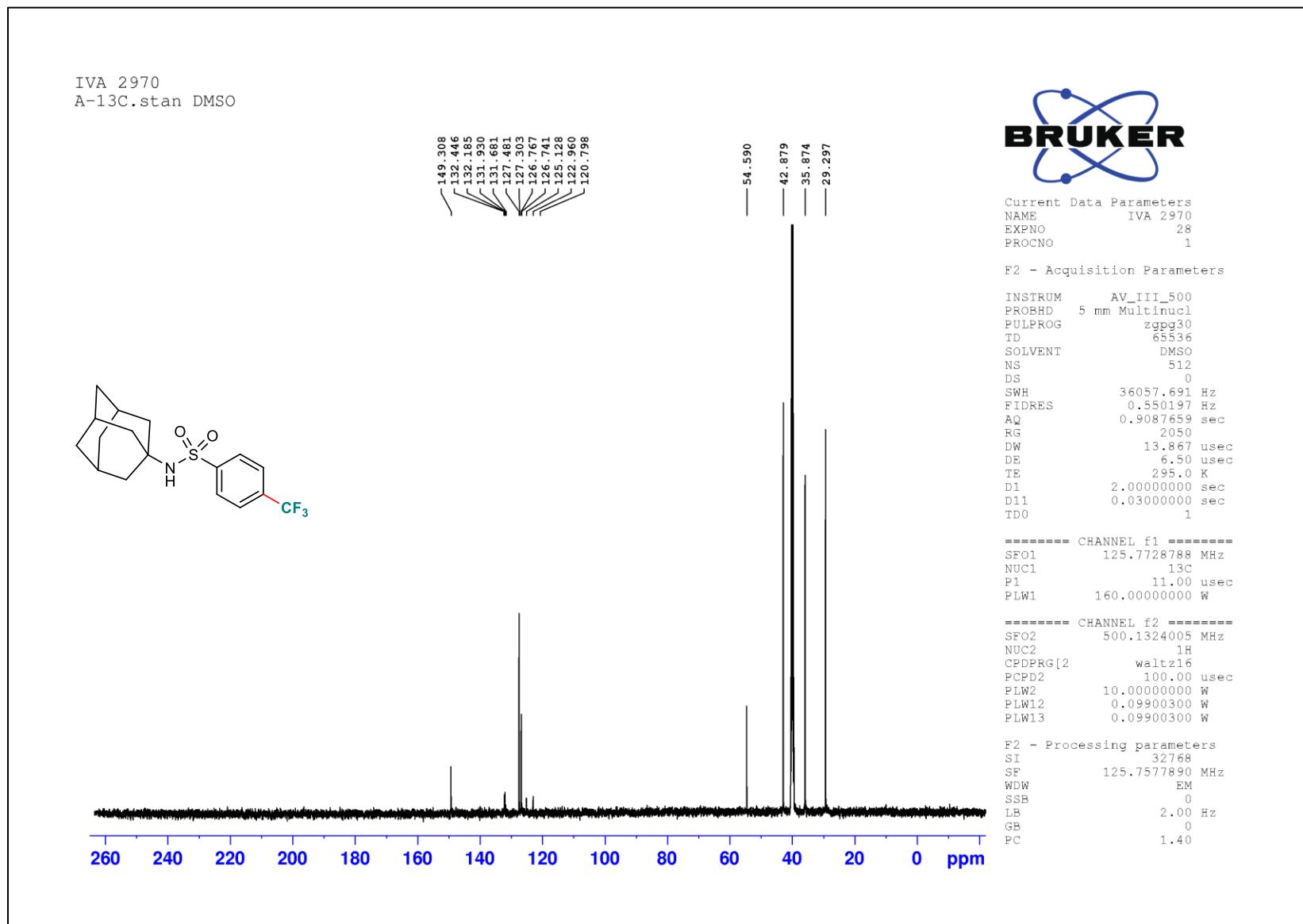
F2 - Processing parameters
SI 32768
SF 125.7577890 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40



¹H NMR of Compound 2r

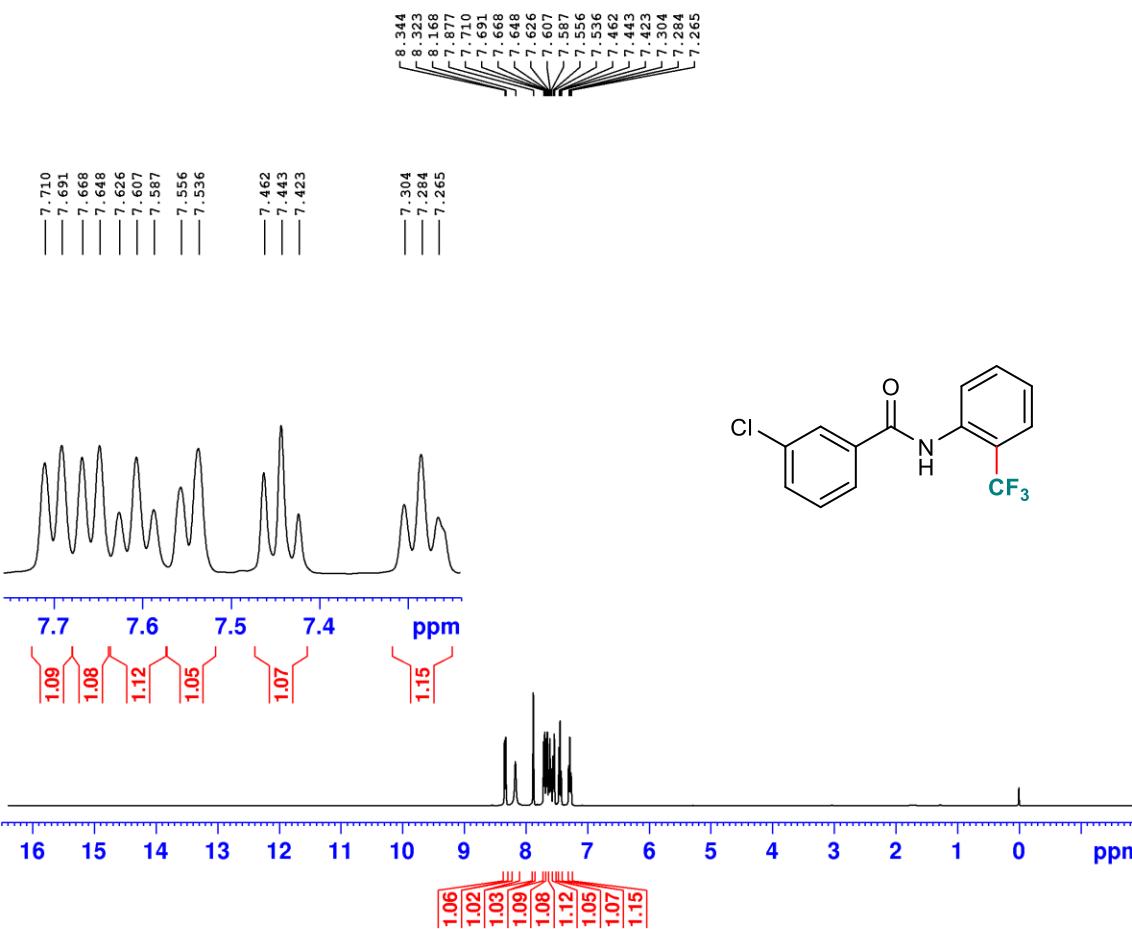


¹³C NMR of Compound 2r



¹H NMR of Compound 2s

ETH 238
1H. stan CDCl₃



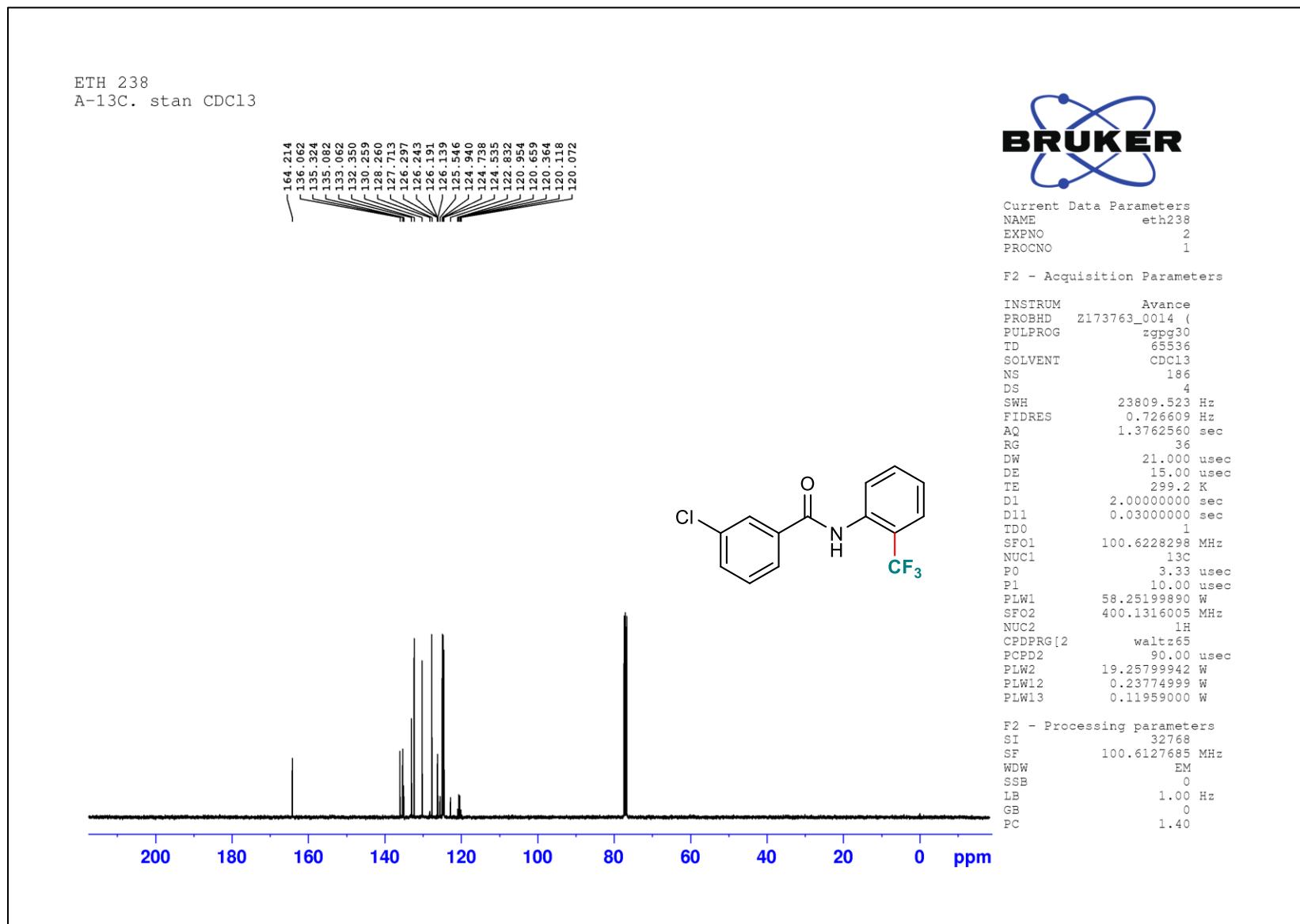
Current Data Parameters
NAME eth238
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters

INSTRUM Avance
PROBHD Z173763_0014 (zg30
PULPROG zg30
TD 65536
SOLVENT CDCl₃
NS 16
DS 2
SWH 8196.721 Hz
FIDRES 0.250144 Hz
AQ 3.9976959 sec
RG 101
DW 61.000 usec
DE 13.54 usec
TE 298.1 K
D1 1.0000000 sec
TDO 1
SFO1 400.1324708 MHz
NUC1 1H
P0 3.33 usec
P1 10.00 usec
PLW1 19.25799942 W

F2 - Processing parameters
SI 65536
SF 400.1300095 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

¹³C NMR of Compound **2s**



¹⁹F NMR of Compound **2s**

ETH 238
19F. stan CDCl₃

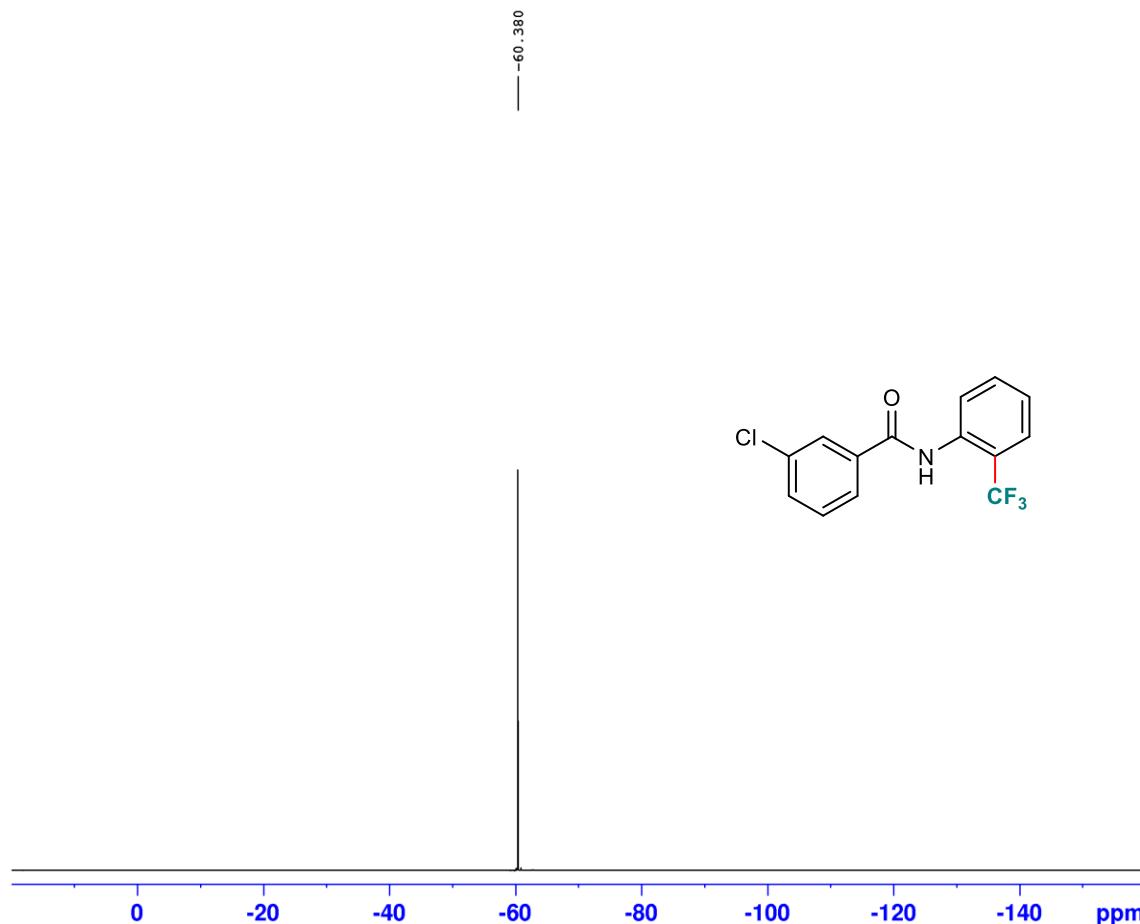
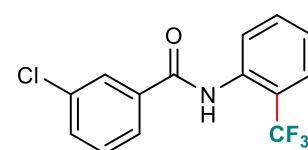


Current Data Parameters
NAME eth238
EXPNO 3
PROCNO 1

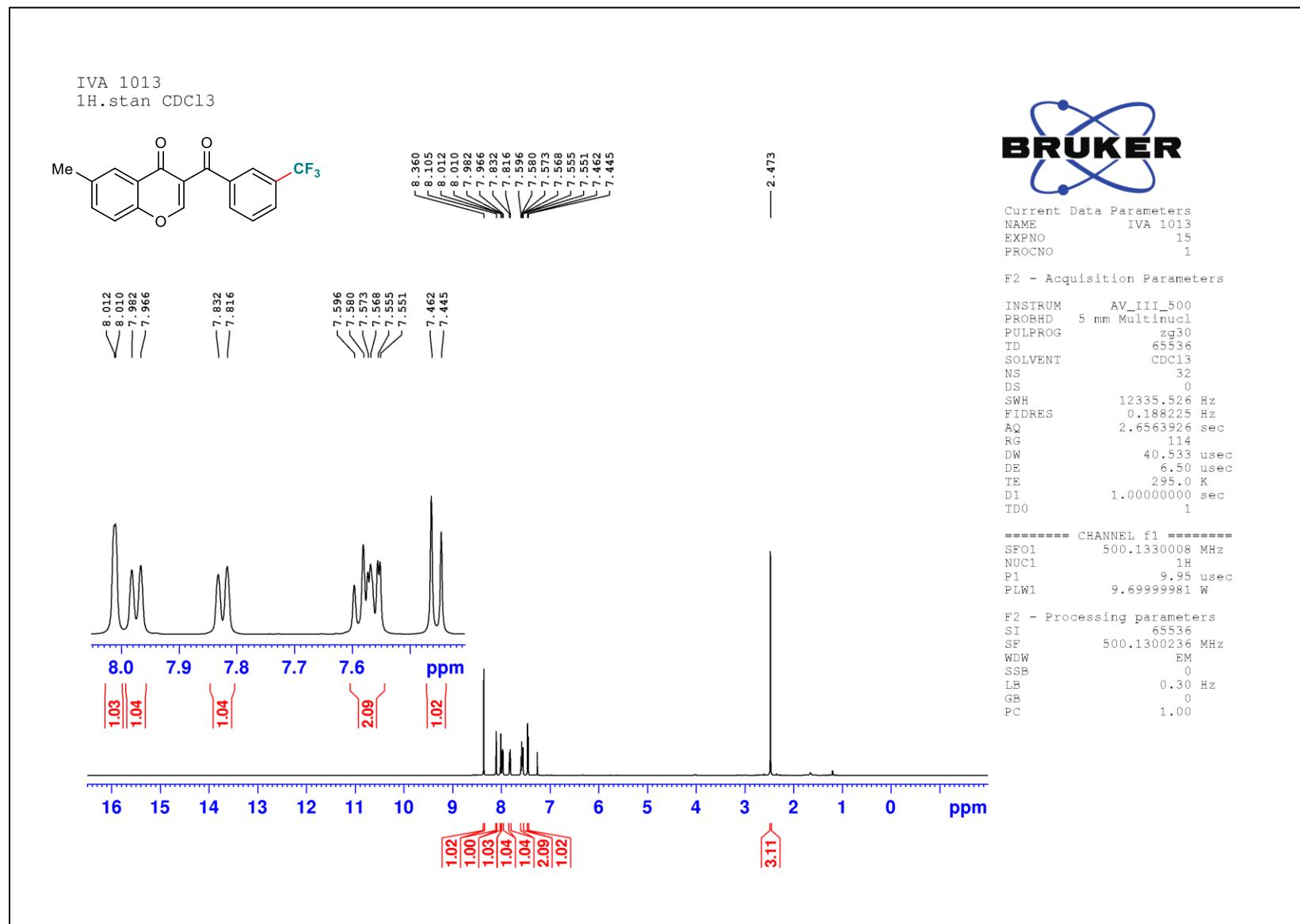
F2 - Acquisition Parameters

INSTRUM Avance
PROBHD Z173763_0014 (zg
PULPROG zg
TD 131072
SOLVENT CDCl₃
NS 16
DS 4
SWH 90909.091 Hz
FIDRES 1.387163 Hz
AQ 0.7208960 sec
RG 101
DW 5.500 usec
DE 6.50 usec
TE 298.1 K
D1 1.0000000 sec
TD0 1
SFO1 376.4607164 MHz
NUC1 ¹⁹F
P1 12.00 usec
PLW1 36.0000000 W

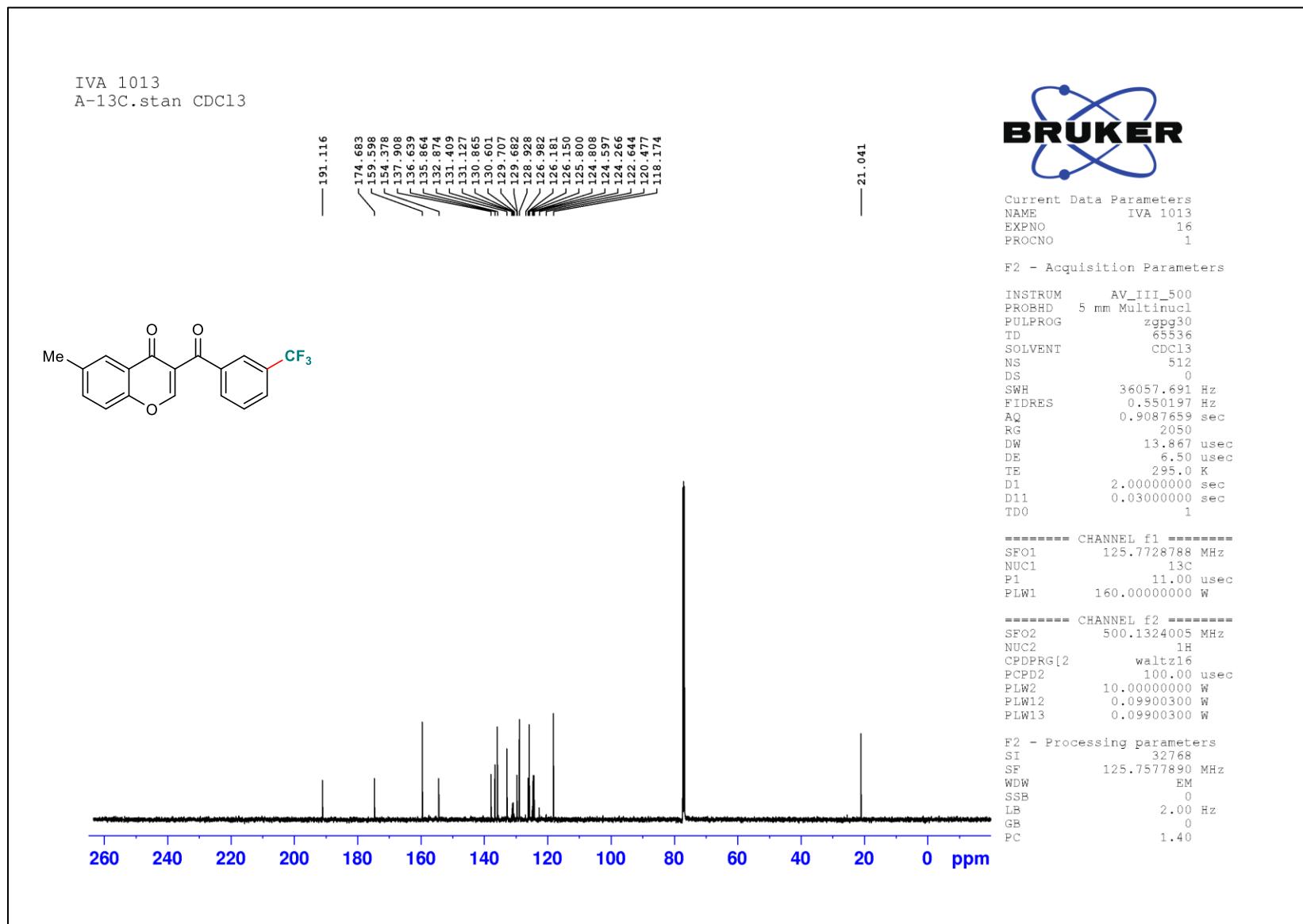
F2 - Processing parameters
SI 65536
SF 376.4983662 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



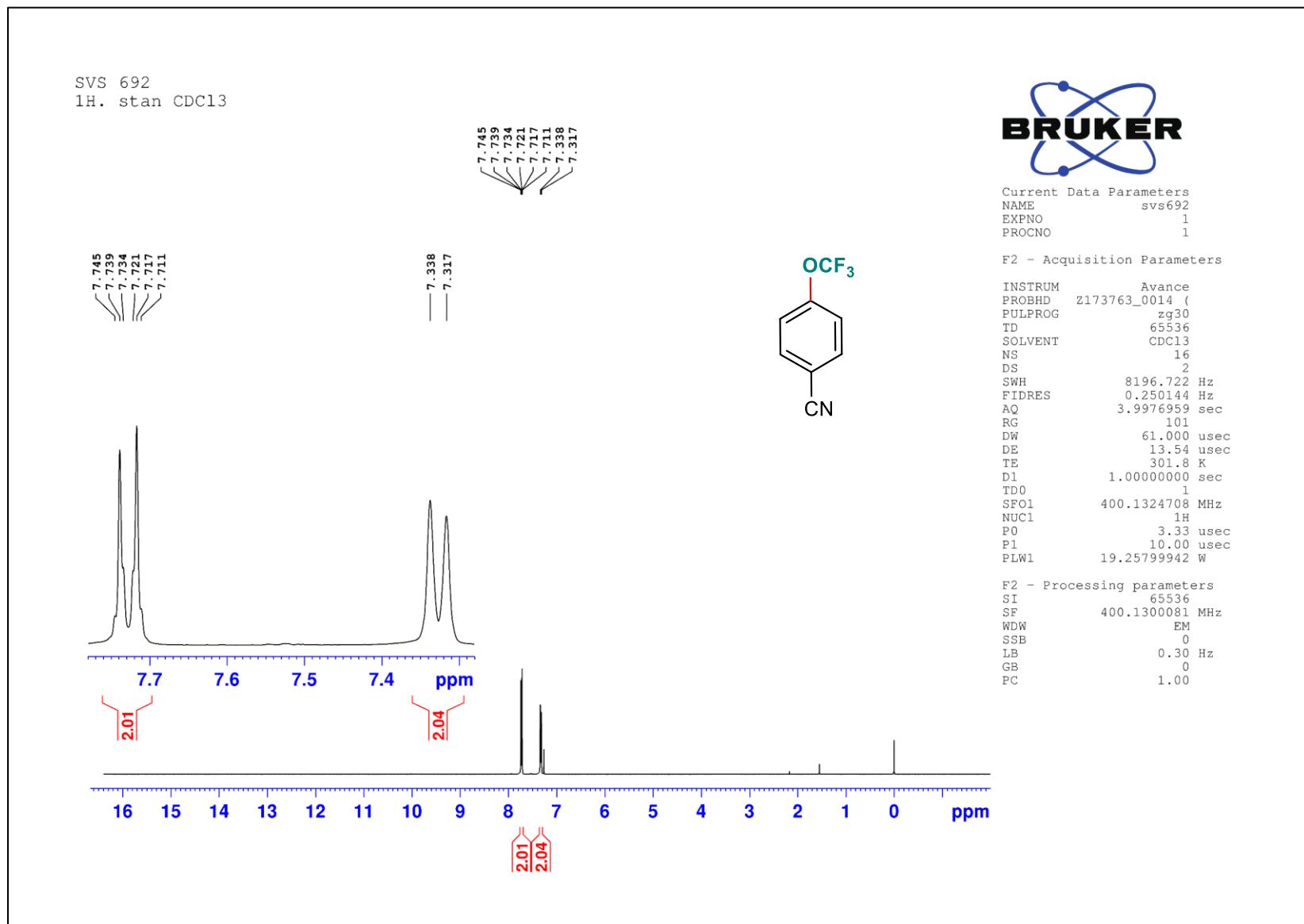
¹H NMR of Compound 2t



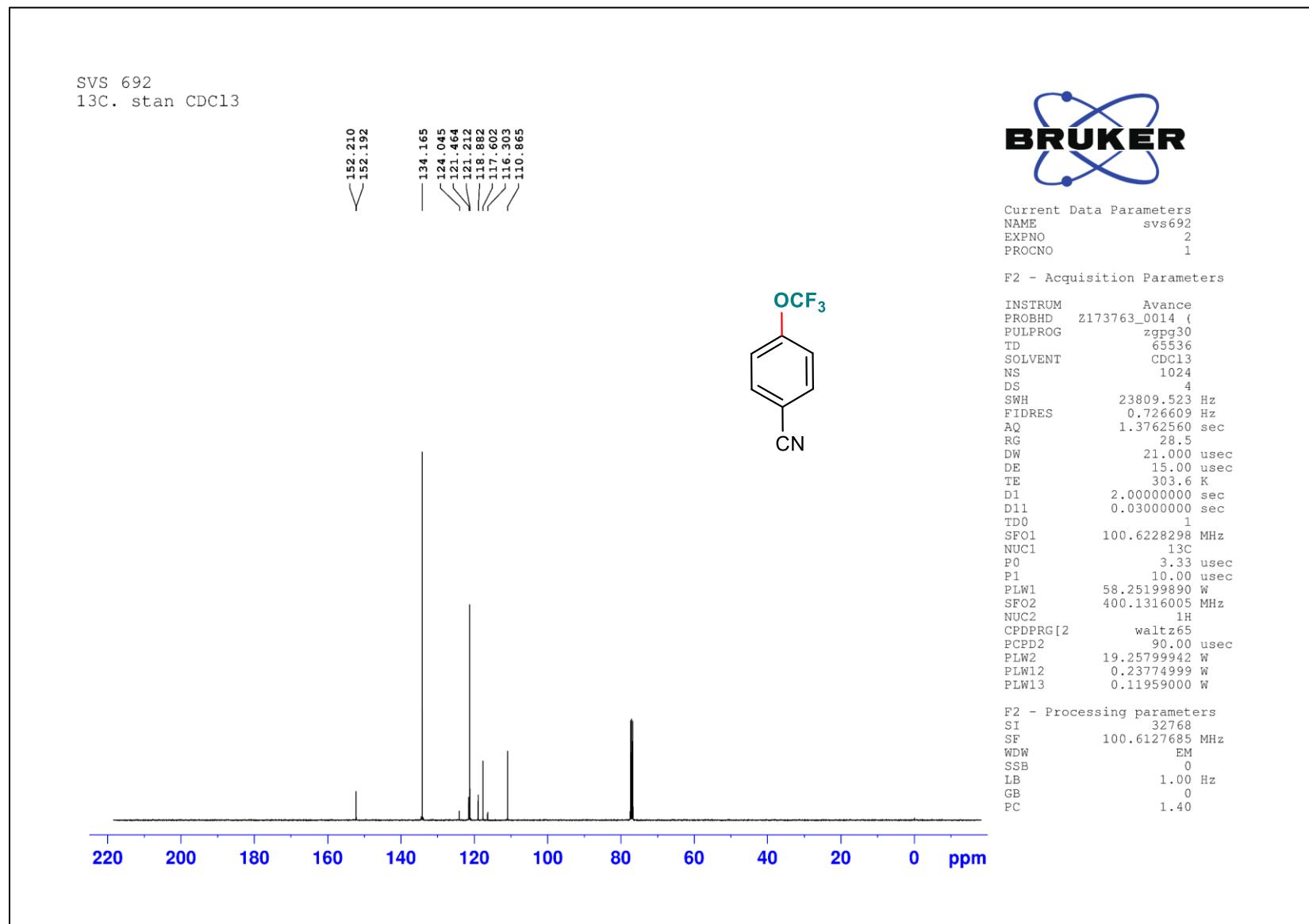
¹³C NMR of Compound 2t



¹H NMR of Compound 4a



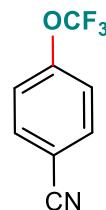
¹³C NMR of Compound 4a



¹⁹F NMR of Compound 4a

SVS 692
19F. stan CDCl₃

-57.83



Current Data Parameters
NAME svs692
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters

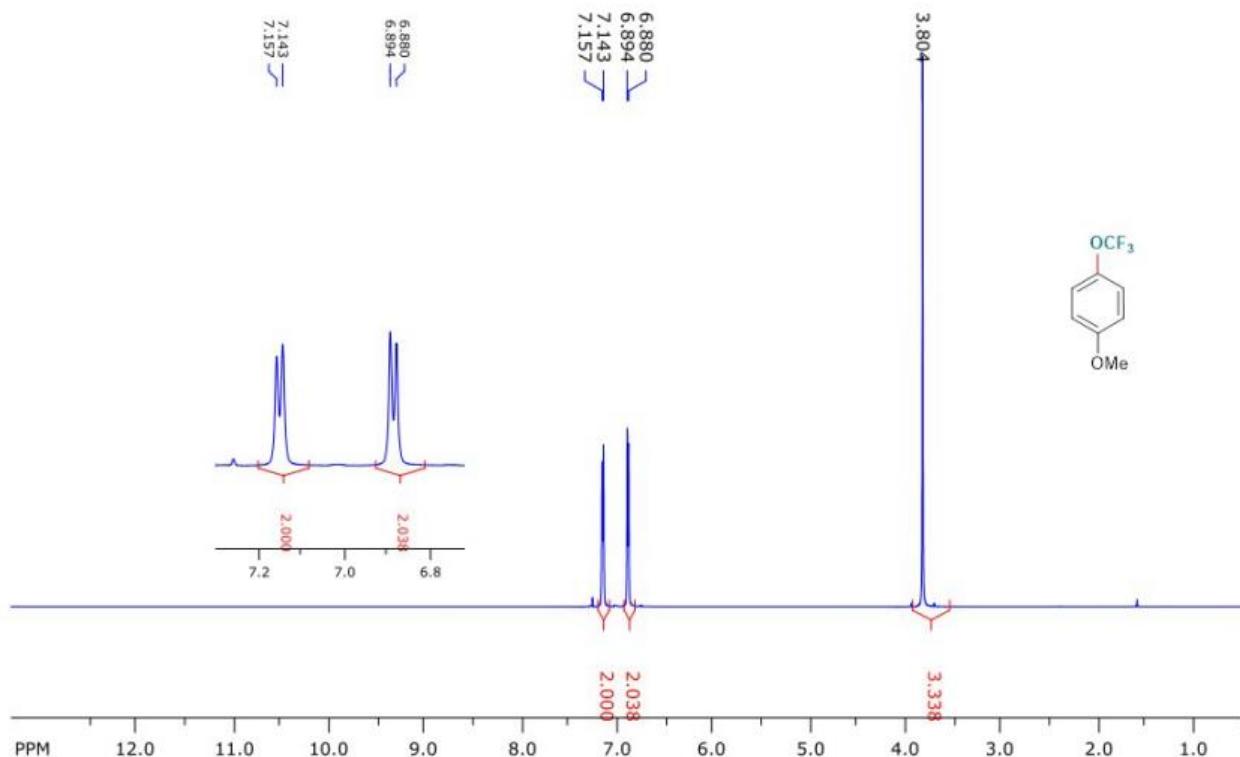
INSTRUM Avance
PROBHD Z173763_0014 (zg
PULPROG zg
TD 131072
SOLVENT CDCl₃
NS 16
DS 4
SWH 90909.094 Hz
FIDRES 1.387163 Hz
AQ 0.7208960 sec
RG 101
DW 5.500 usec
DE 6.50 usec
TE 302.4 K
D1 1.0000000 sec
TD0 1
SF01 376.4607164 MHz
NUC1 ¹⁹F
P1 12.00 usec
PLW1 36.00000000 W

F2 - Processing parameters
SI 65536
SF 376.4983662 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

20 0 -20 -40 -60 -80 -100 -120 -140 -160 ppm

¹H NMR of Compound 4b

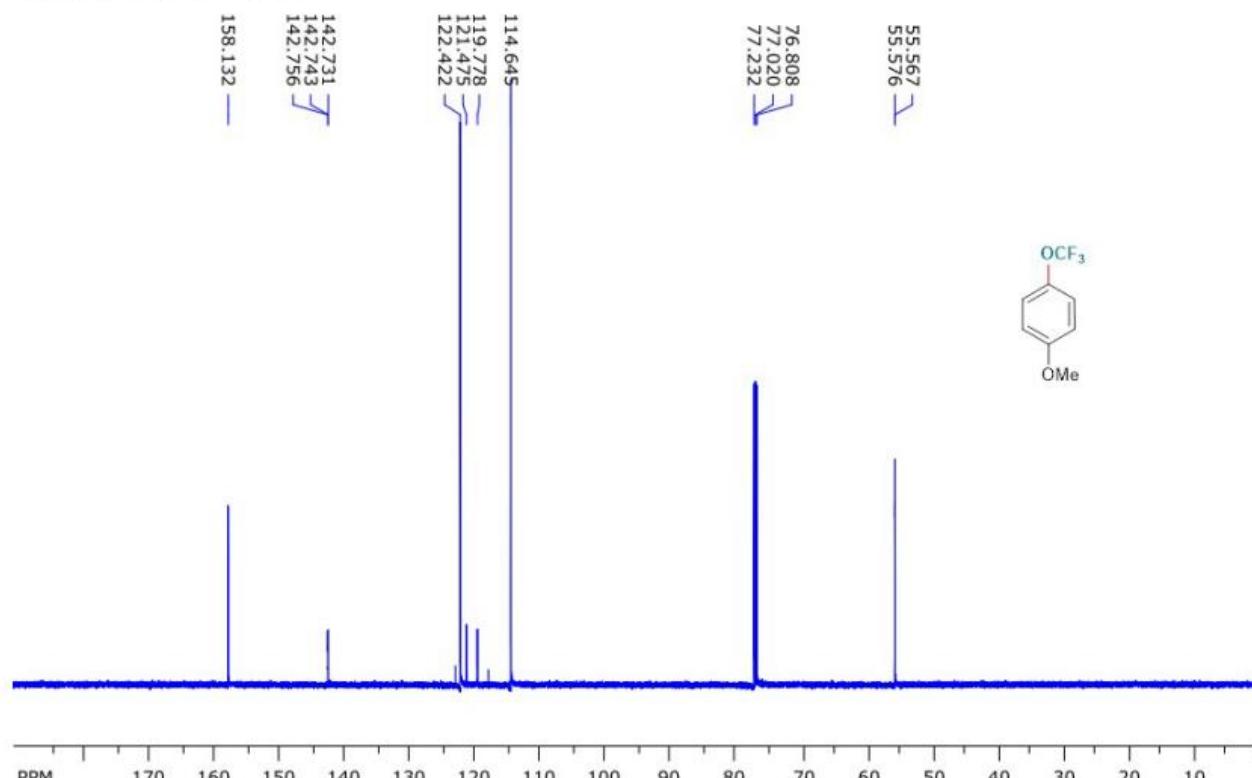
SpinWorks 4: IVAB 4374 1H CDCl₃



file: ...0418_01\ivab4374-PROTON_01.fid\fid block# 1 expt: "s2pul" freq. of 0 ppm: 599.766672 MHz
transmitter freq.: 599.770272 MHz processed size: 32768 complex points
time domain size: 57692 points LB: 1.500 GF: 0.0000
width: 9615.38 Hz = 16.0318 ppm = 0.166668 Hz/pt Hz/cm: 310.585 ppm/cm: 0.51784
number of scans: 16

¹³C NMR of Compound 4b

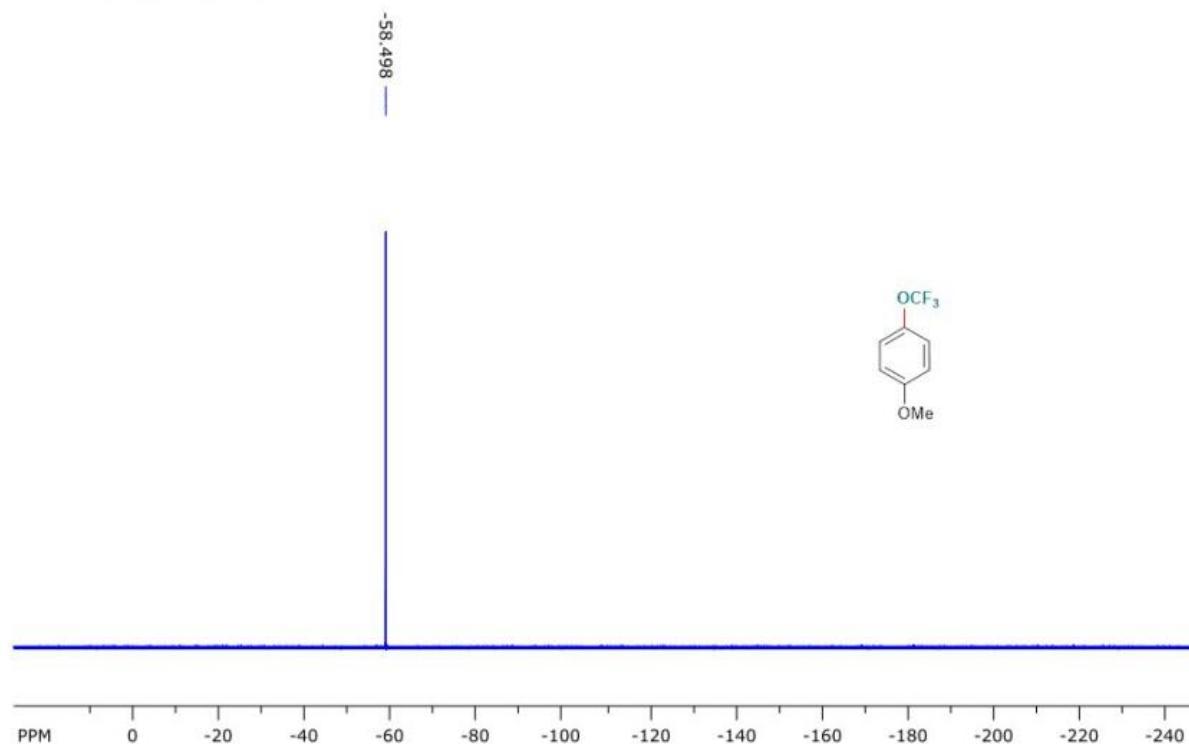
SpinWorks 4: IVAB 4374 13C



file: ...0418_01\ivab4374-CARBON_01.fid\fid block# 1 expt: "s2pul" freq. of 0 ppm: 150.811442 MHz
transmitter freq.: 150.828039 MHz processed size: 65536 complex points
time domain size: 65536 points LB: 0.500 GF: 0.0000
width: 37878.79 Hz = 251.1389 ppm = 0.577984 Hz/pt Hz/cm: 1156.476 ppm/cm: 7.66752
number of scans: 256

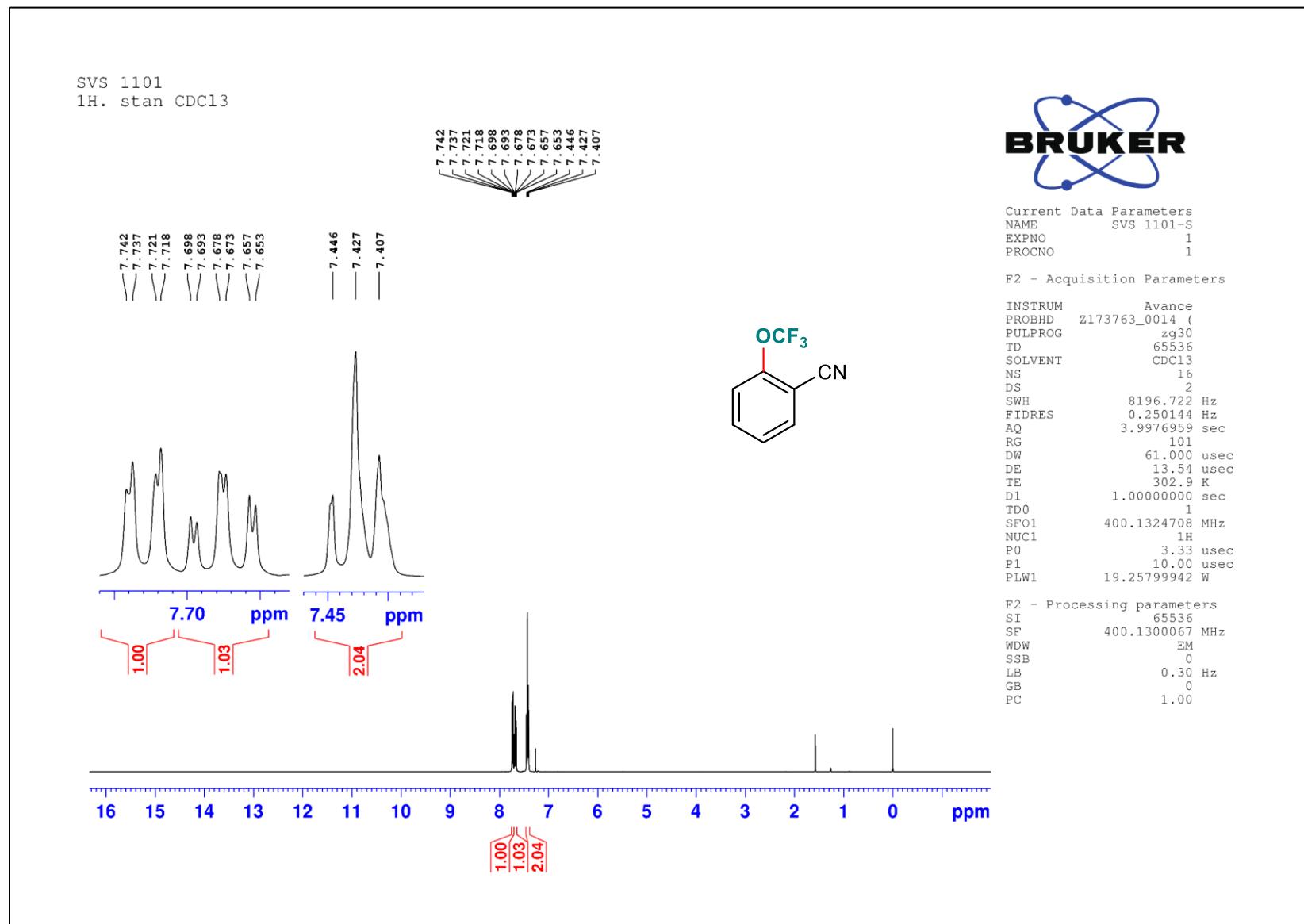
¹⁹F NMR of Compound **4b**

SpinWorks 4: IVAB 4374 19F

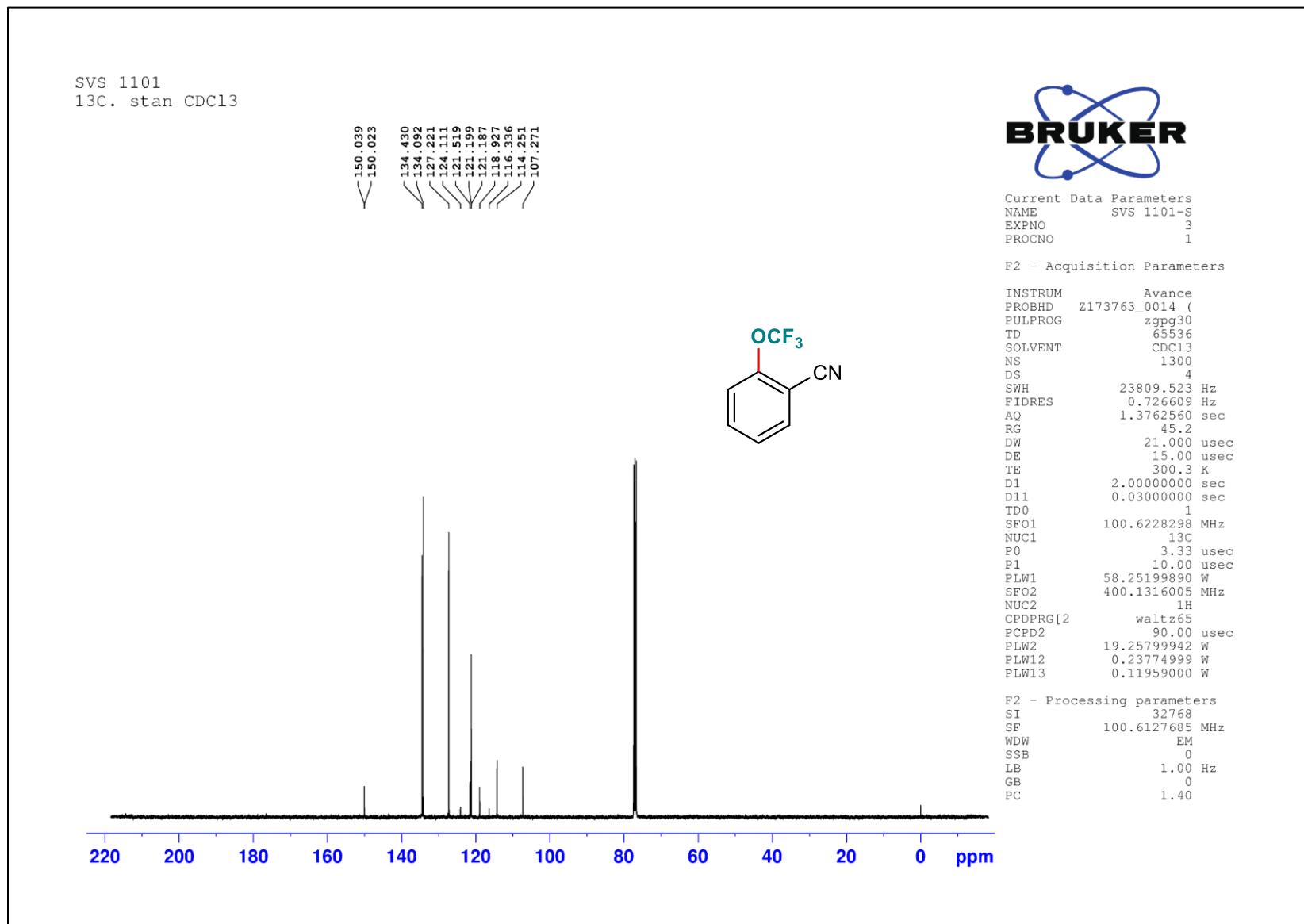


file: ...18_01\ivab4374-FLUORINE_01.fid\fid block# 1 expt: "s2pul" freq. of 0 ppm: 564.344520 MHz
transmitter freq.: 564.282442 MHz processed size: 262144 complex points
time domain size: 262144 points LB: 1.500 GF: 0.0000
width: 156250.00 Hz = 276.9003 ppm = 0.596046 Hz/pt Hz/cm: 6250.000 ppm/cm: 11.07601
number of scans: 32

¹H NMR of Compound 4c



¹³C NMR of Compound 4c

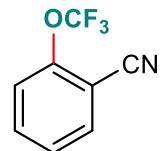


¹⁹F NMR of Compound 4c

SVS 1101
19F. stan CDC13



-57.891



Current Data Parameters
NAME SVS 1101-S
EXPNO 2
PROCNO 1

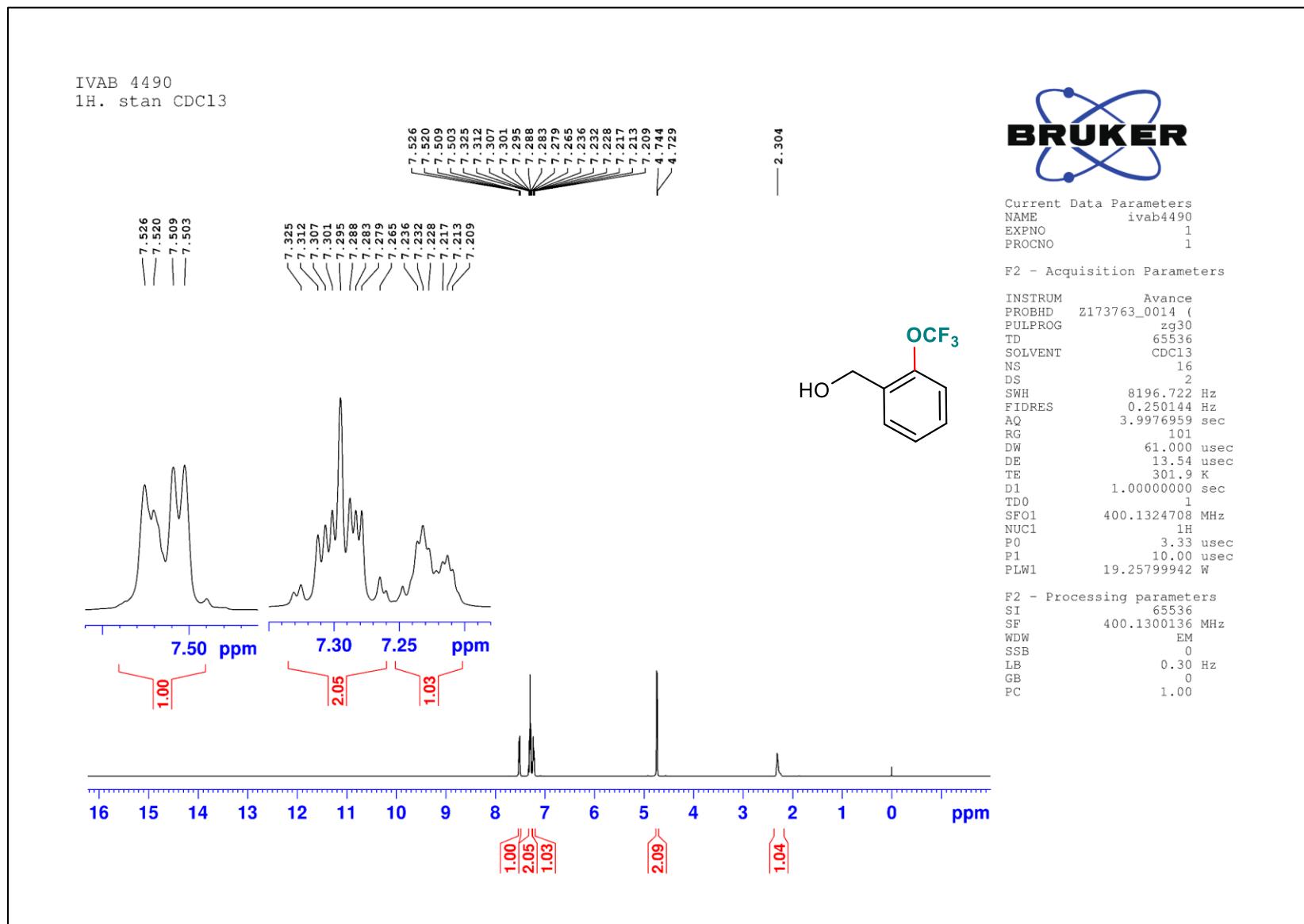
F2 - Acquisition Parameters

INSTRUM Avance
PROBHD Z173763_0014 (zg
PULPROG zg
TD 131072
SOLVENT CDC13
NS 16
DS 4
SWH 90909.094 Hz
FIDRES 1.387163 Hz
AQ 0.7208960 sec
RG 101
DW 5.500 usec
DE 6.50 usec
TE 302.5 K
D1 1.0000000 sec
TDO 1
SF01 376.4607164 MHz
NUC1 ¹⁹F
P1 12.00 usec
PLW1 36.00000000 W

F2 - Processing parameters
SI 65536
SF 376.4983662 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

20 0 -20 -40 -60 -80 -100 -120 -140 -160 ppm

¹H NMR of Compound 4d

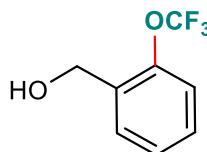


¹³C NMR of Compound 4d

IVAB 4490
13C. stan CDC13

146.706
146.695
133.327
129.053
128.829
127.024
124.413
121.852
120.405
119.293
116.734

59.666



220 200 180 160 140 120 100 80 60 40 20 0 ppm



Current Data Parameters
NAME ivab4490
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters

INSTRUM Avance
PROBHD Z173763_0014 (zgpg30
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 23809.523 Hz
FIDRES 0.726609 Hz
AQ 1.3762560 sec
RG 28.5
DW 21.000 usec
DE 15.00 usec
TE 302.7 K
D1 2.0000000 sec
D11 0.03000000 sec
TDO 1
SFO1 100.6228298 MHz
NUC1 13C
P0 3.33 usec
P1 10.00 usec
PLW1 58.25199890 W
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2] waltz65
PCPD2 90.00 usec
PLW2 19.25799942 W
PLW12 0.23774999 W
PLW13 0.11959000 W

F2 - Processing parameters

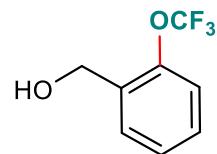
SI 32768
SF 100.6127685 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

¹⁹F NMR of Compound 4d

IVAB 4490
19F. stan CDCl₃

-57.404

20 0 -20 -40 -60 -80 -100 -120 -140 -160 ppm



Current Data Parameters
NAME ivab4490
EXPNO 3
PROCNO 1

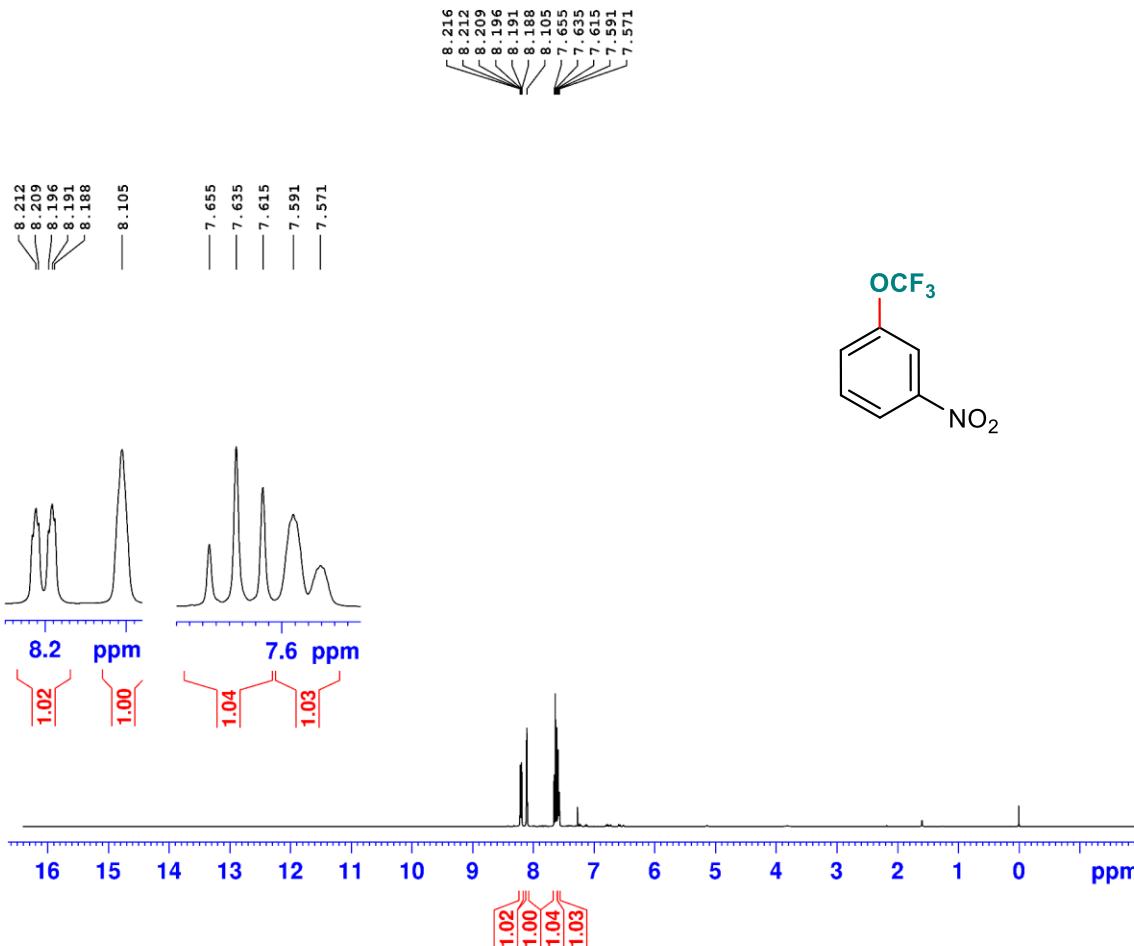
F2 - Acquisition Parameters

INSTRUM Avance
PROBHD Z173763_0014 (zg
PULPROG zg
TD 131072
SOLVENT CDCl₃
NS 16
DS 4
SWH 90909.094 Hz
FIDRES 1.387163 Hz
AQ 0.7208960 sec
RG 101
DW 5.500 usec
DE 6.50 usec
TE 302.7 K
D1 1.0000000 sec
TD0 1
SF01 376.4607164 MHz
NUC1 ¹⁹F
P1 12.00 usec
PLW1 36.0000000 W

F2 - Processing parameters
SI 65536
SF 376.4983662 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

¹H NMR of Compound 4e

IVAB 4318
1H. stan CDC13



Current	Data	Parameters
NAME	ivab4318	
EXPNO	1	
PROCNO	1	

F2 - Acquisition Parameters

INSTRUM	Avance
PROBHD	Z173763_0014 (
PULPROG	zg30
TD	65536
SOLVENT	CDC13
NS	16
DS	2
SWH	8196.722 Hz
FIDRES	0.250144 Hz
AQ	3.9976959 sec
RG	101
DW	61.000 usec
DE	13.54 usec
TE	300.4 K
D1	1.0000000 sec
TD0	1
SFO1	400.1324708 MHz
NUC1	1H
P0	3.33 usec
P1	10.00 usec
PLW1	19.2579942 W

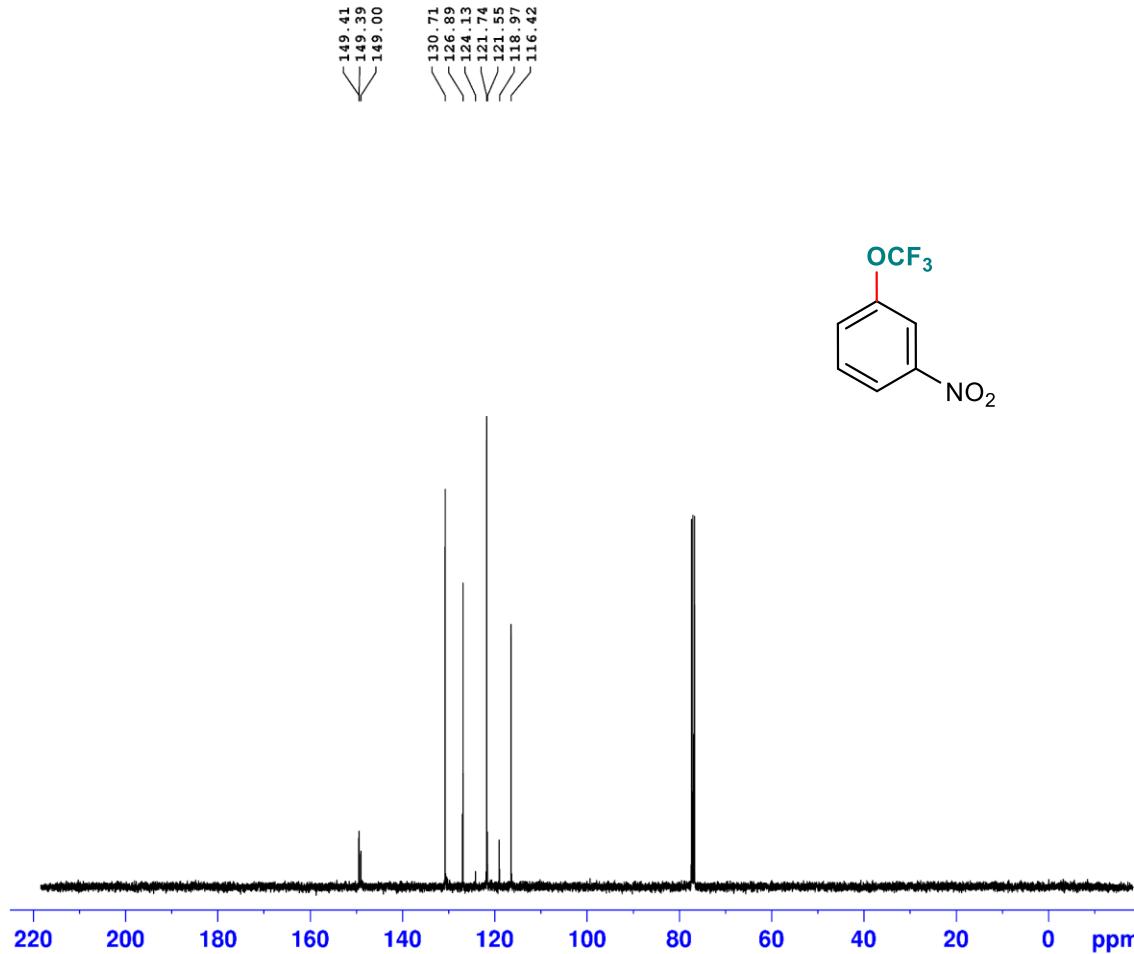
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F2 - Processing parameters
SI          65536
SF          400.1300053 MHz
WDW         EM
SSB         0
LB          0.30 Hz
GB          0
PC          1.00

```

¹³C NMR of Compound 4e

IVAB 4318
13C. stan CDC13





Current	Data	Parameters
NAME	ivab4318	
EXPNO	2	
PROCNO	1	

F2 - Acquisition Parameters

```

INSTRUM      Avance
PROBHD      Z173763_0014
PULPROG     zpgpg30
TD          65536
SOLVENT    CDC13
NS          207
DS           4
SWH        23809.523 Hz
FIDRES     0.726609 Hz
AQ        1.3762560 sec
RG          45.2
DW        21.0000 usec
DE          15.00 usec
TE         300.8 K
D1        2.00000000 sec
D11       0.03000000 sec
TD0          1
SFO1       100.6228298 MHz
NUC1          13C
P0            3.33 usec
P1            10.00 usec
PLW1       58.25199890 W
SFO2       400.1316005 MHz
NUC2          1H
CPDRG[2]    waltz65
PCPD2        90.00 usec
PLW2       19.25799492 W
PLW12      0.23774999 W
PLW13      0.11959000 W

```

```

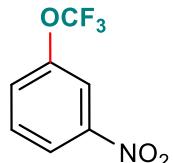
F2 - Processing parameters
SI           32768
SF          100.6127685 MHz
WDW          EM
SSB          0
LB           1.00 Hz
GB          0
PC          1.40

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¹⁹F NMR of Compound 4e

IVAB 4318
19F. stan CDCl₃

-58.175



Current Data Parameters
NAME ivab4318
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters

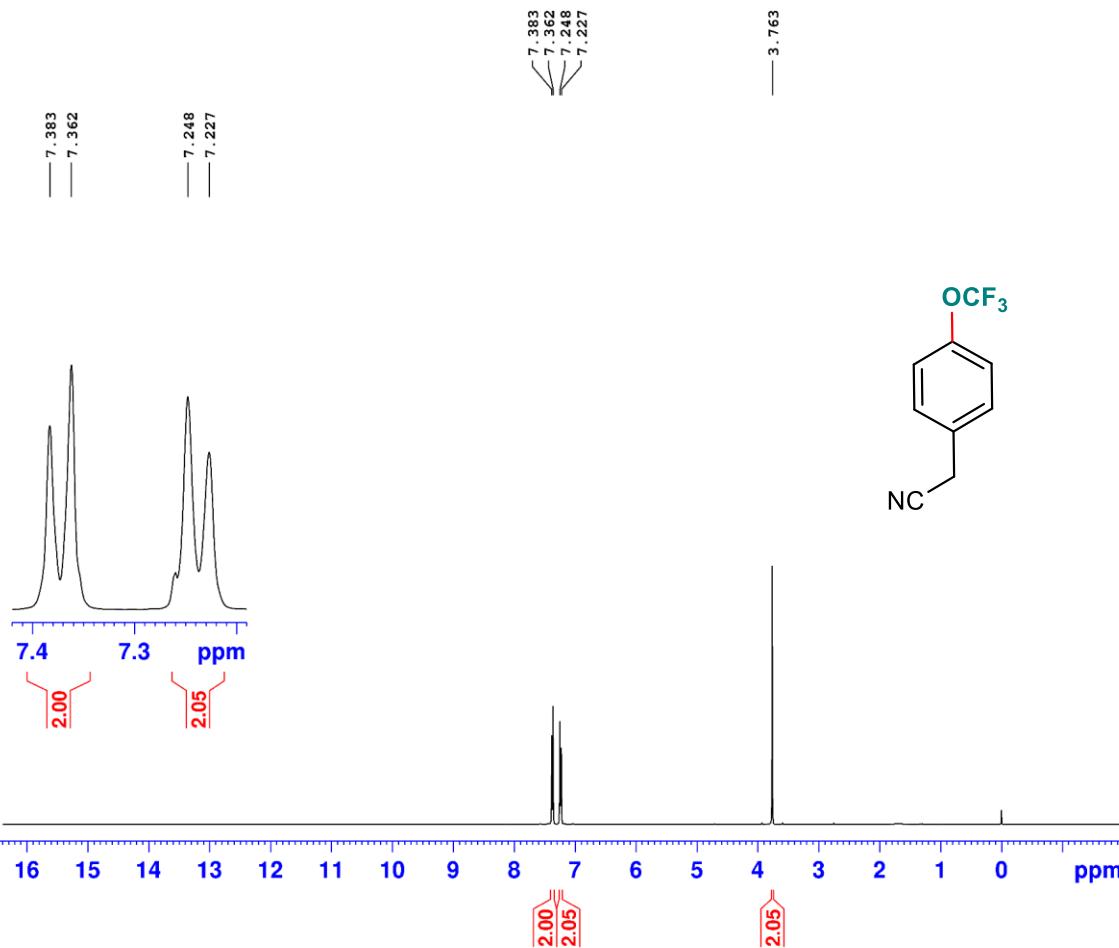
INSTRUM Avance
PROBHD Z173763_0014 (
PULPROG zg
TD 131072
SOLVENT CDCl₃
NS 16
DS 4
SWH 90909.094 Hz
FIDRES 1.387163 Hz
AQ 0.7208960 sec
RG 101
DW 5.500 usec
DE 6.50 usec
TE 300.6 K
D1 1.0000000 sec
TD0 1
SFO1 376.4607164 MHz
NUC1 ¹⁹F
P1 12.00 usec
PLW1 36.0000000 W

F2 - Processing parameters
SI 65536
SF 376.4983662 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

20 0 -20 -40 -60 -80 -100 -120 -140 -160 ppm

¹H NMR of Compound 4f

SVS 111
1H. stan CDC13



The Bruker logo consists of the word "BRUKER" in a bold, black, sans-serif font. Behind the text are three blue, stylized atomic orbits that intersect and overlap.

Current Data Parameters	
NAME	SVS 111
EXPNO	1
PROCNO	1

```

F2 - Acquisition Parameters
INSTRUM Avance
PROBHD Z173763_0014 (
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 8196.722 Hz
FIDRES 0.250144 Hz
AQ 3.9976959 sec
RG 101
DW 61.0000 usec
DE 13.54 usec
TE 298.9 K
D1 1.00000000 sec
TDO 1
SFO1 400.1324708 MHz
NUC1 1H
P0 3.33 usec
P1 10.00 usec
PLW1 19.25799942 W

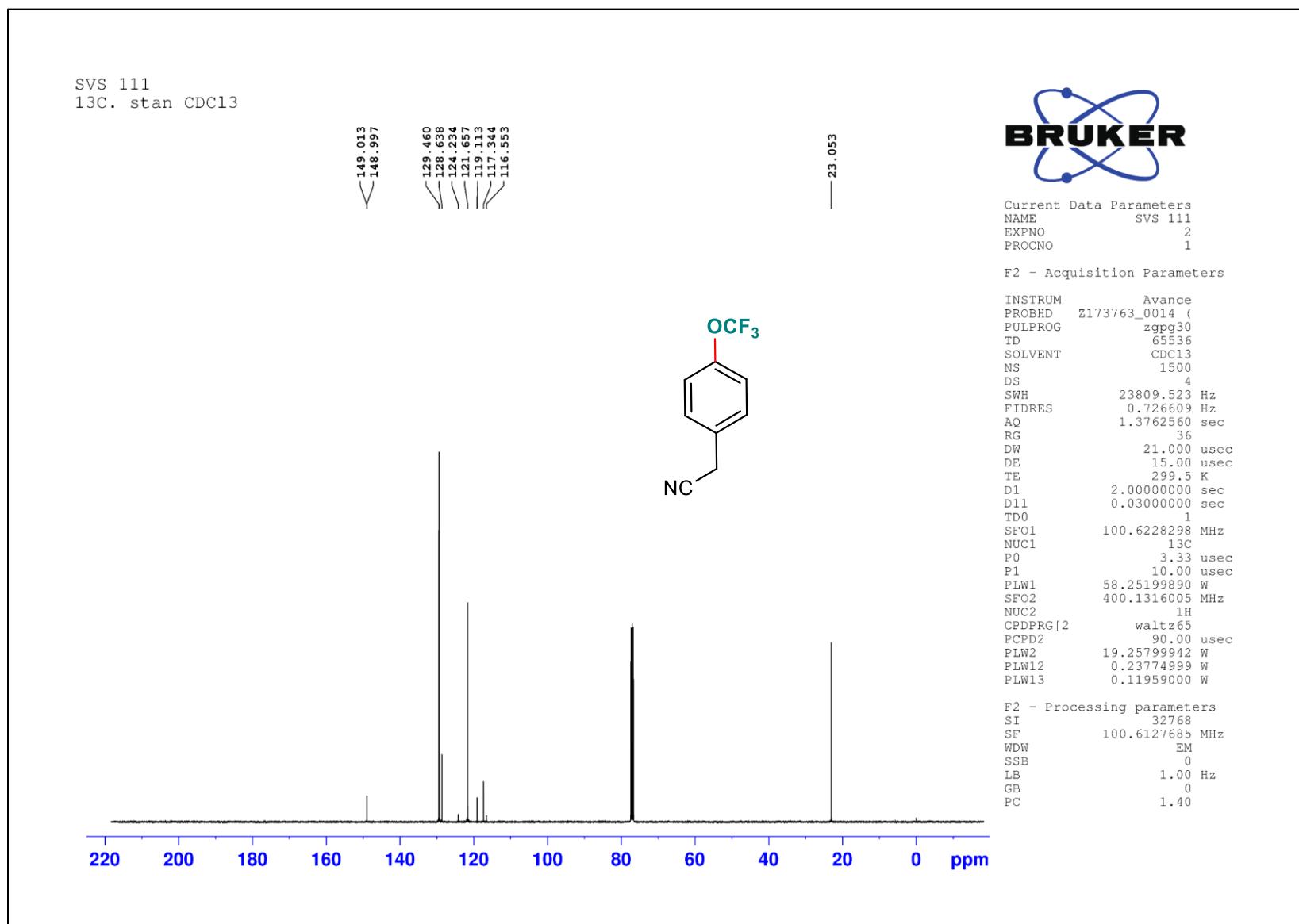
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```

F2 - Processing parameters
SI          65536
SF          400.1300083 MHz
WDW         EM
SSB         0
LB          0.30 Hz
GB          0
PC          1.00

```

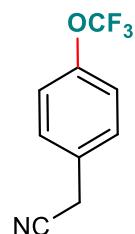
¹³C NMR of Compound 4f



¹⁹F NMR of Compound 4f

SVS 111
19F. stan CDC13

-57.990



Current Data Parameters
NAME SVS 111
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters

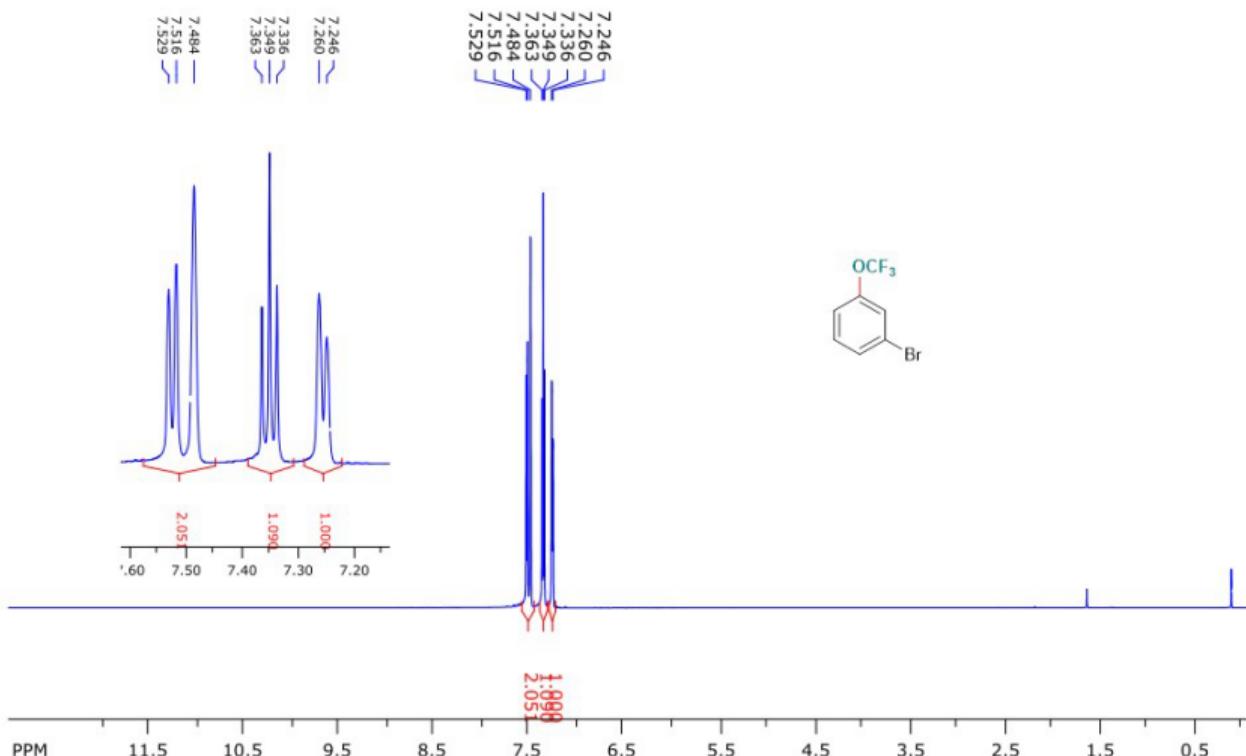
INSTRUM Avance
PROBHD Z173763_0014 (zg
PULPROG zg
TD 131072
SOLVENT CDC13
NS 50
DS 4
SWH 90909.094 Hz
FIDRES 1.387163 Hz
AQ 0.7208960 sec
RG 101
DW 5.500 usec
DE 6.50 usec
TE 299.1 K
D1 1.0000000 sec
TDO 1
SF01 376.4607164 MHz
NUC1 ¹⁹F
P1 12.00 usec
PLW1 36.0000000 W

F2 - Processing parameters
SI 65536
SF 376.4983662 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

20 0 -20 -40 -60 -80 -100 -120 -140 -160 ppm

¹H NMR of Compound 4g

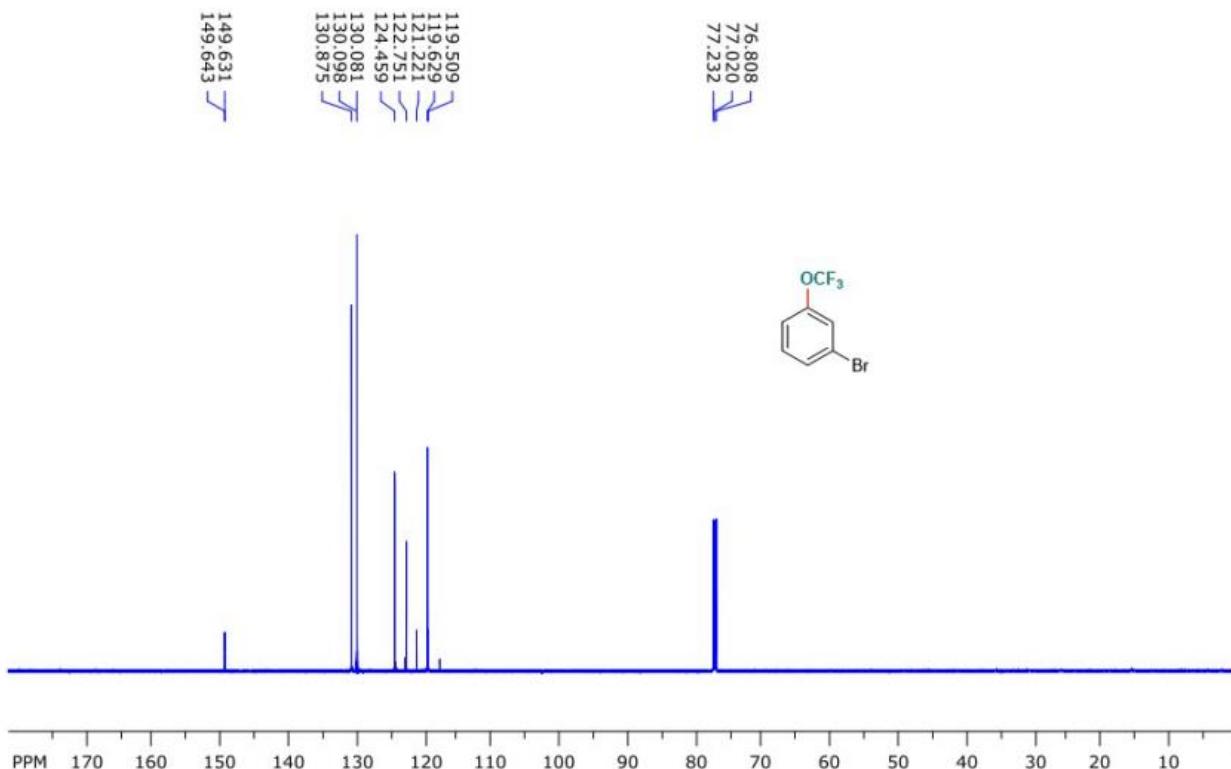
SpinWorks 4: SVS 601 1H CDCl₃



file: ...240410_01\svs601-PROTON_01.fid\fid block# 1 expt: "s2pul" freq. of 0 ppm: 599.766625 MHz
transmitter freq.: 599.770272 MHz processed size: 65536 complex points
time domain size: 76924 points LB: 0.300 GF: 0.0000
width: 9615.38 Hz = 16.0318 ppm = 0.124999 Hz/pt Hz/cm: 314.415 ppm/cm: 0.52422
number of scans: 16

¹³C NMR of Compound 4g

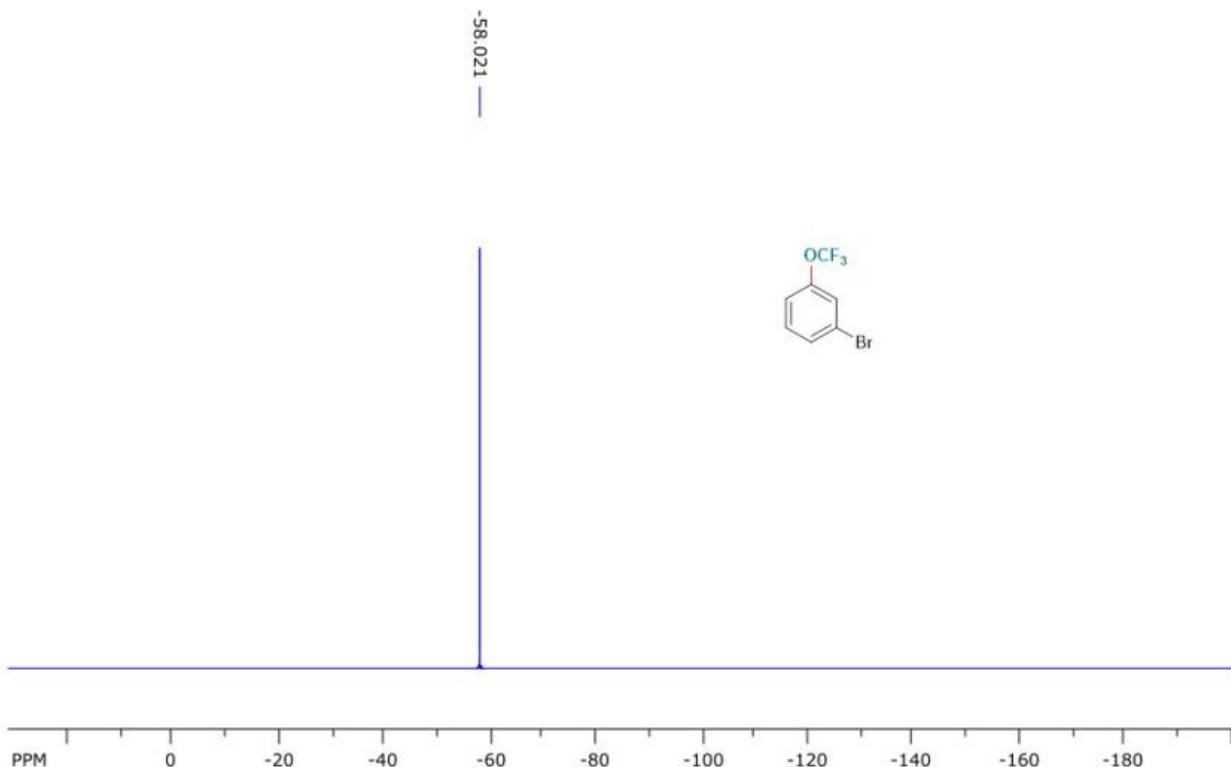
SpinWorks 4: SVS 601 13C CDCl₃



file: ...240410_02\svs601-CARBON_01.fid\fid block# 1 expt: "s2pul" freq. of 0 ppm: 150.811441 MHz
transmitter freq.: 150.828039 MHz processed size: 65536 complex points
time domain size: 65536 points LB: 0.500 GF: 0.0000
width: 37878.79 Hz = 251.1389 ppm = 0.577984 Hz/pt Hz/cm: 1094.462 ppm/cm: 7.25636
number of scans: 512

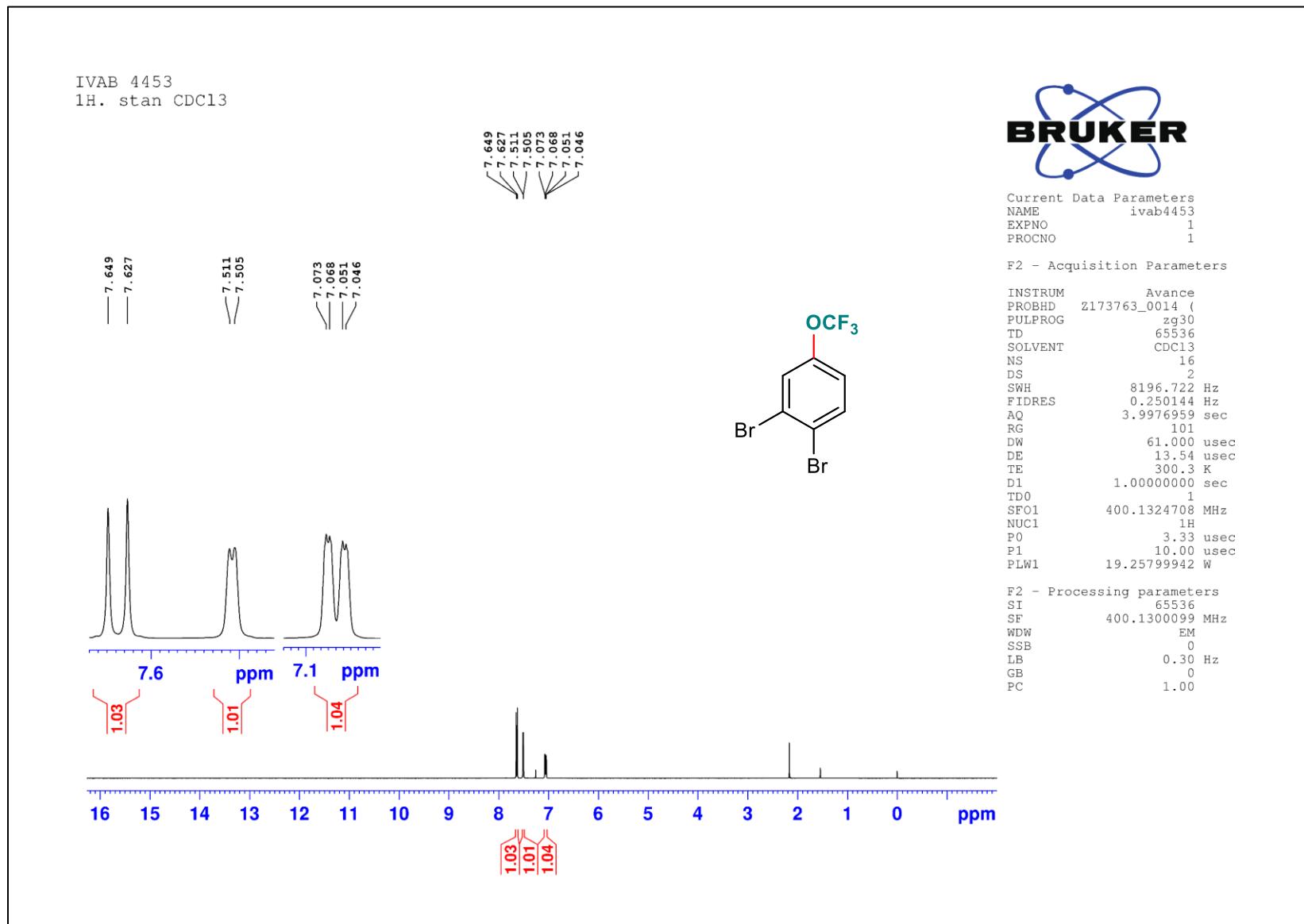
¹⁹F NMR of Compound 4g

SpinWorks 4: SVS 601 19F

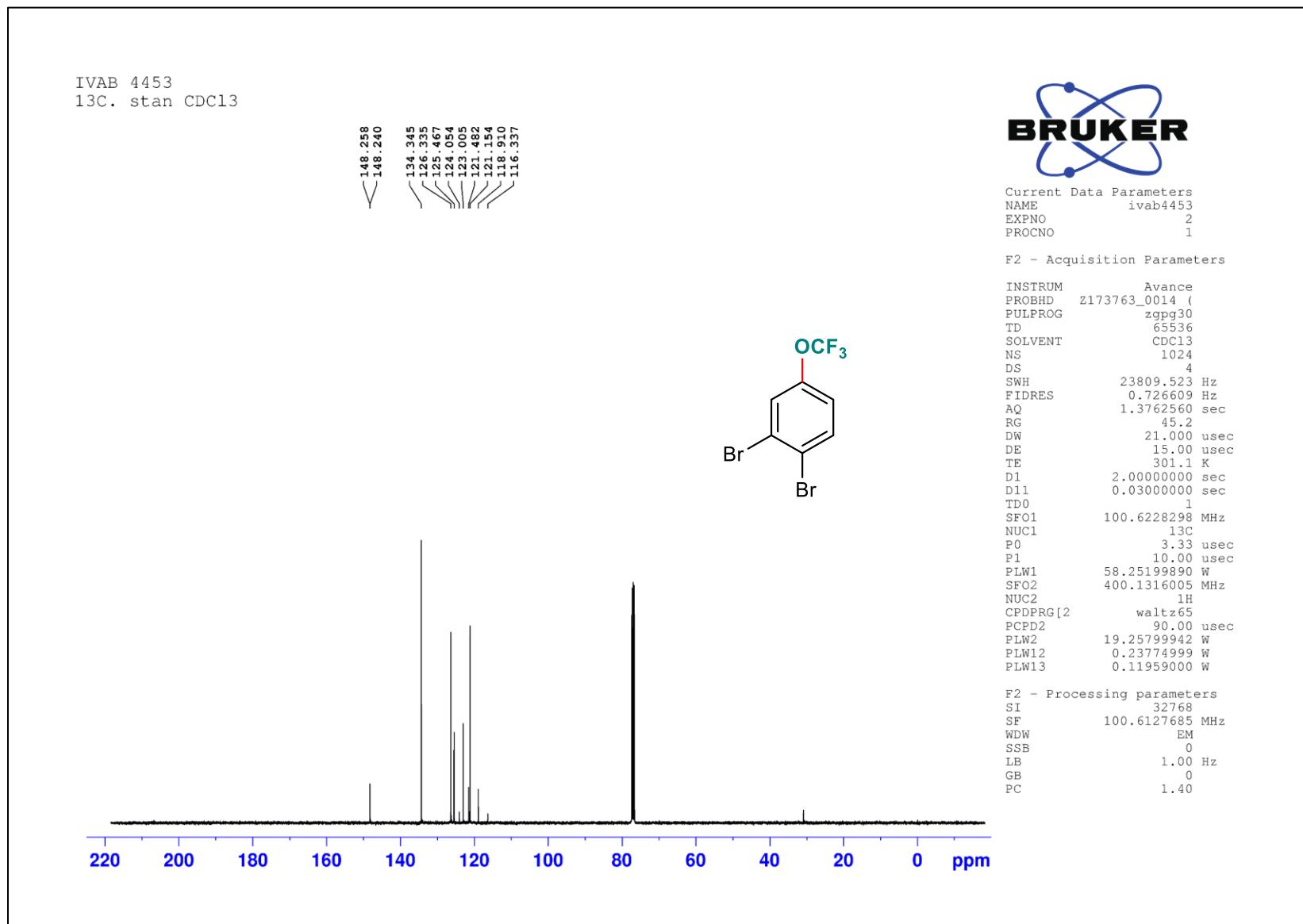


file: ...0410_03\svs601-FLUORINE_01.fid\fid block# 1 expt: "s2pul" freq. of 0 ppm: 564.344520 MHz
transmitter freq.: 564.296551 MHz processed size: 262144 complex points
time domain size: 262144 points LB: 1.500 GF: 0.0000
width: 131578.95 Hz = 233.1734 ppm = 0.501934 Hz/pt Hz/cm: 5263.158 ppm/cm: 9.32694
number of scans: 32

¹H NMR of Compound 4h



¹³C NMR of Compound 4h



¹⁹F NMR of Compound 4h

IVAB 4453
19F. stan CDCl₃

-58.169

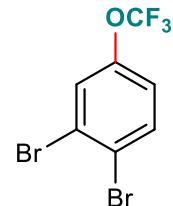


Current Data Parameters
NAME ivab4453
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters

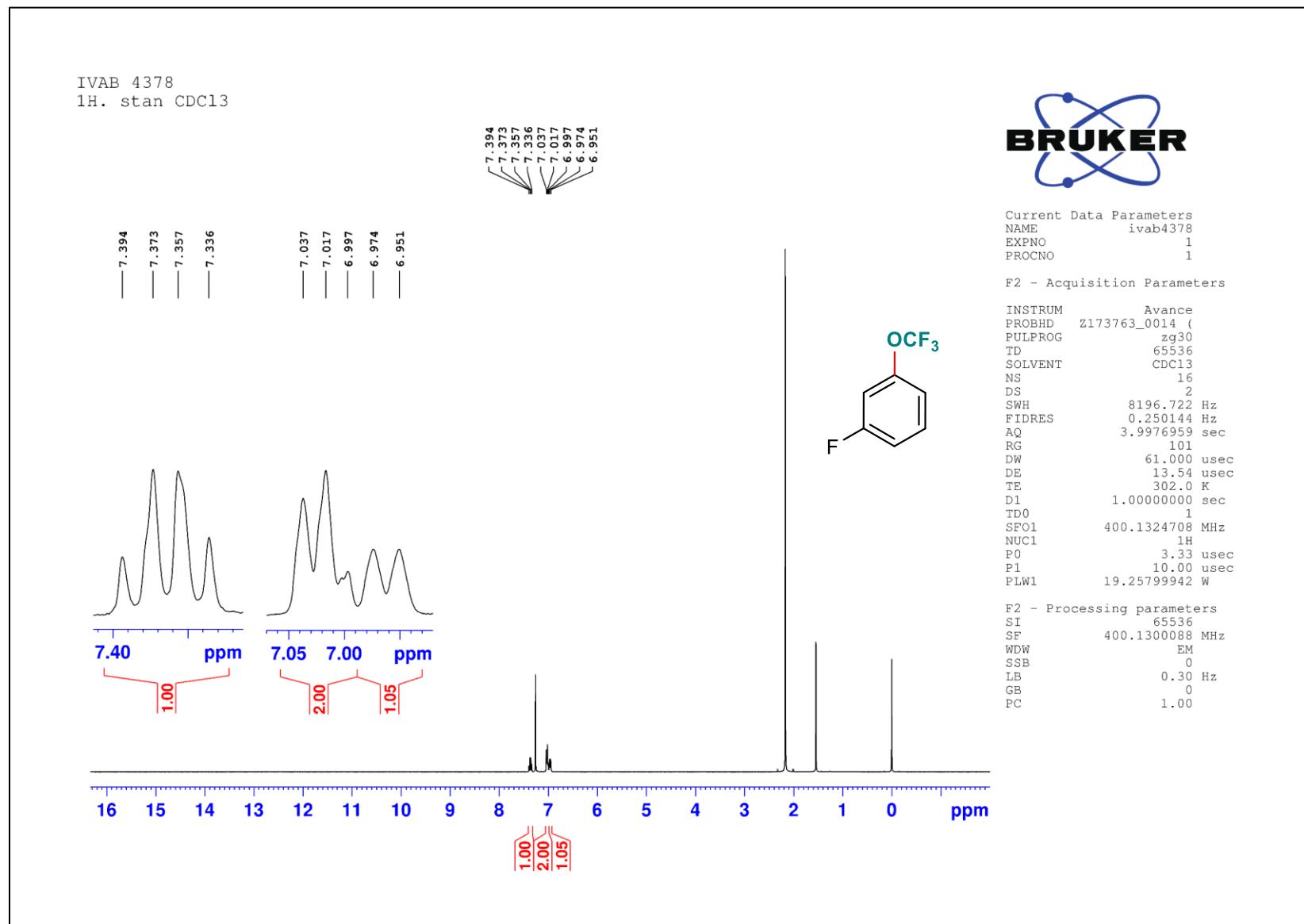
INSTRUM Avance
PROBHD Z173763_0014 (zg
PULPROG zg
TD 131072
SOLVENT CDCl₃
NS 16
DS 4
SWH 90909.094 Hz
FIDRES 1.387163 Hz
AQ 0.7208960 sec
RG 101
DW 5.500 usec
DE 6.50 usec
TE 300.8 K
D1 1.0000000 sec
TD0 1
SF01 376.4607164 MHz
NUC1 ¹⁹F
P1 12.00 usec
PLW1 36.0000000 W

F2 - Processing parameters
SI 65536
SF 376.4983662 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



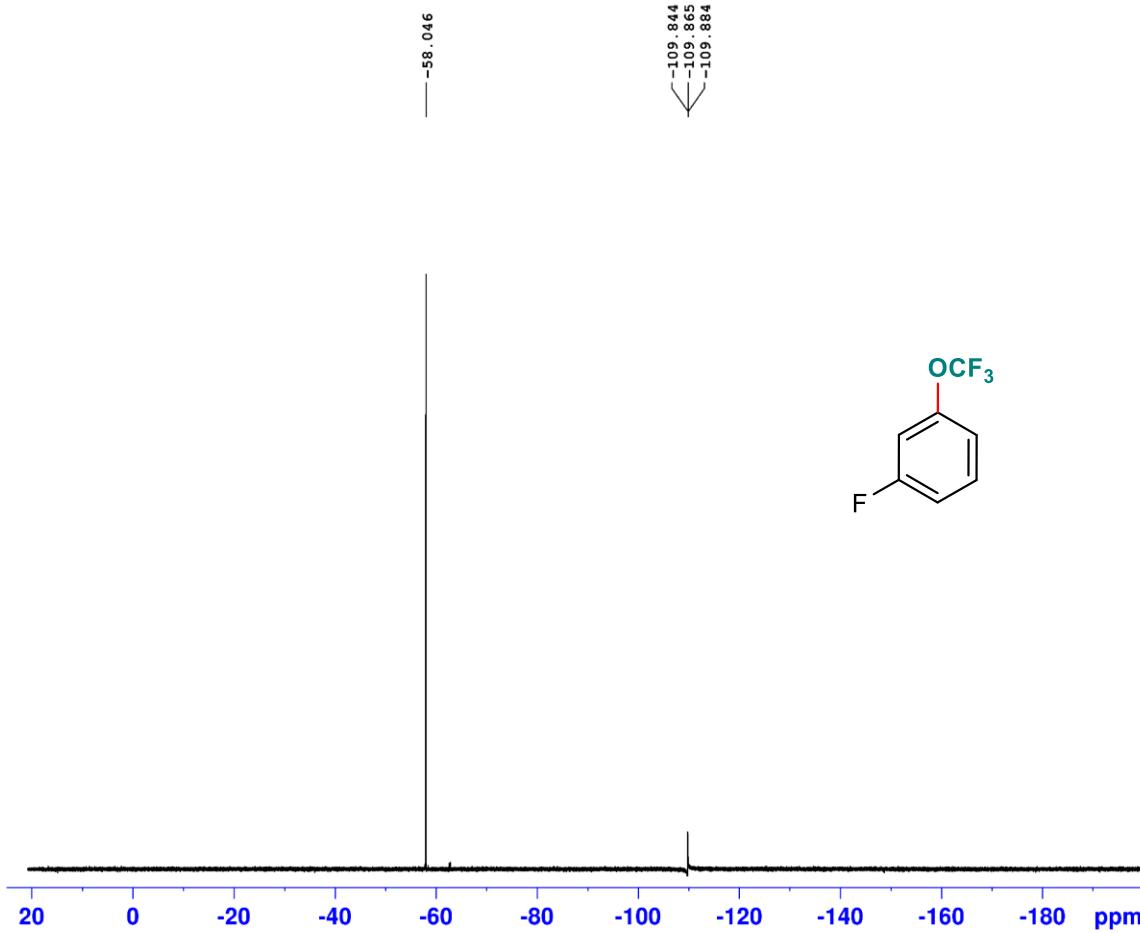
20 0 -20 -40 -60 -80 -100 -120 -140 -160 ppm

¹H NMR of Compound 4i



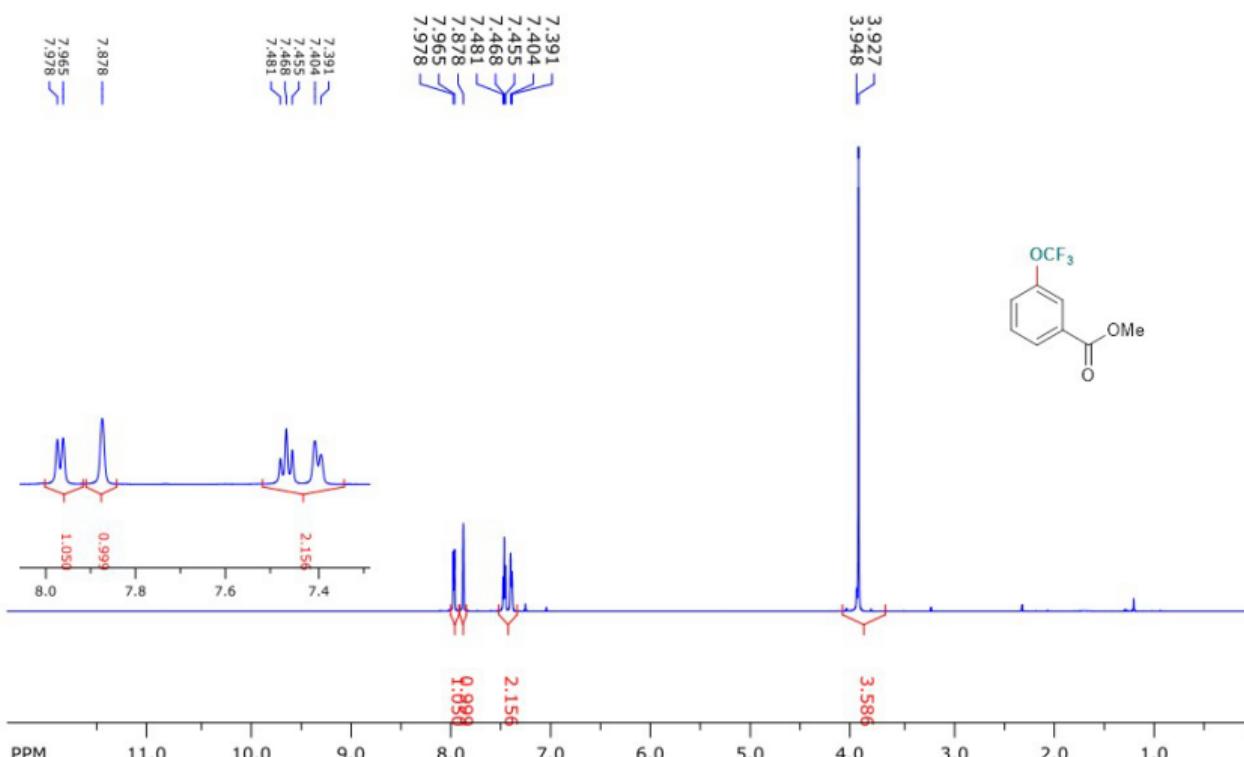
¹⁹F NMR of Compound 4i

IVAB 4378
19F. stan CDC13



¹H NMR of Compound 4j

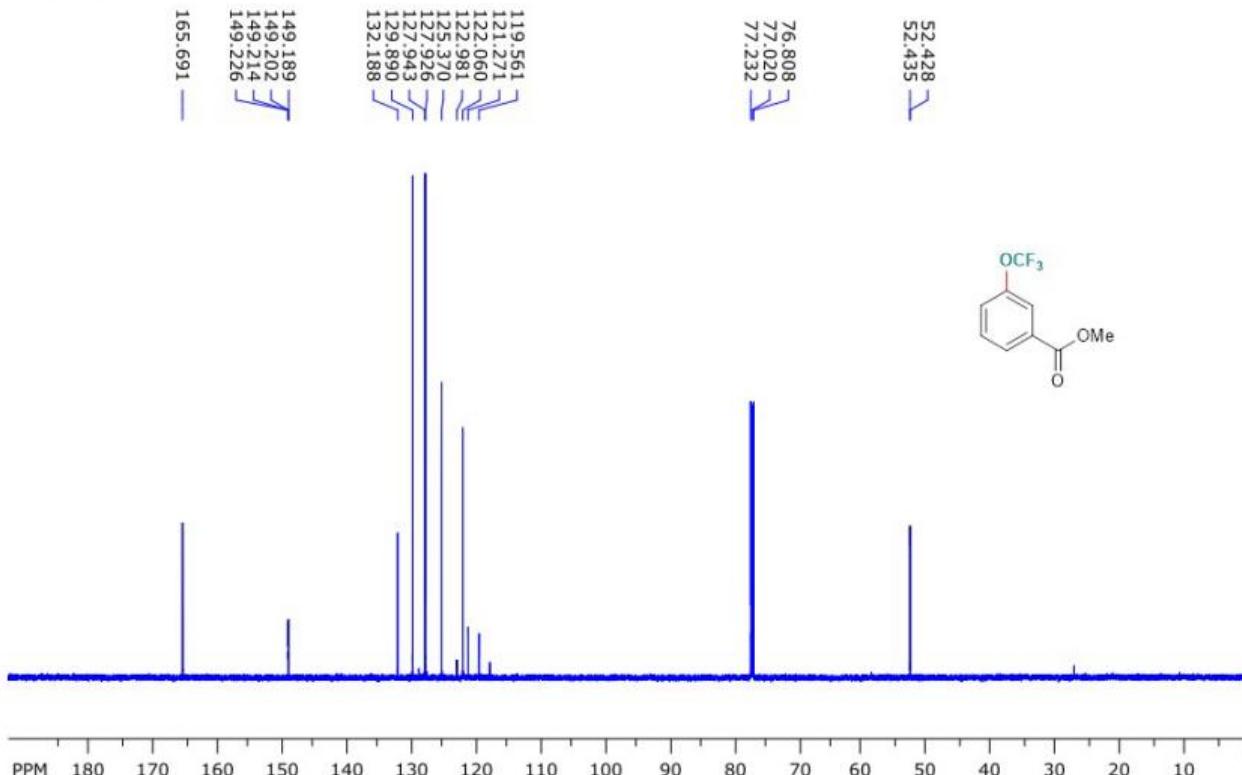
SpinWorks 4: SVS 644 1H CDCl₃



file: ...240418_01\svs644-PROTON_01.fid\fid block# 1 expt: "s2pul" freq. of 0 ppm: 599.766672 MHz
transmitter freq.: 599.770272 MHz processed size: 32768 complex points
time domain size: 57692 points LB: 1.500 GF: 0.0000
width: 9615.38 Hz = 16.0318 ppm = 0.166668 Hz/pt Hz/cm: 297.822 ppm/cm: 0.49656
number of scans: 16

¹³C NMR of Compound 4j

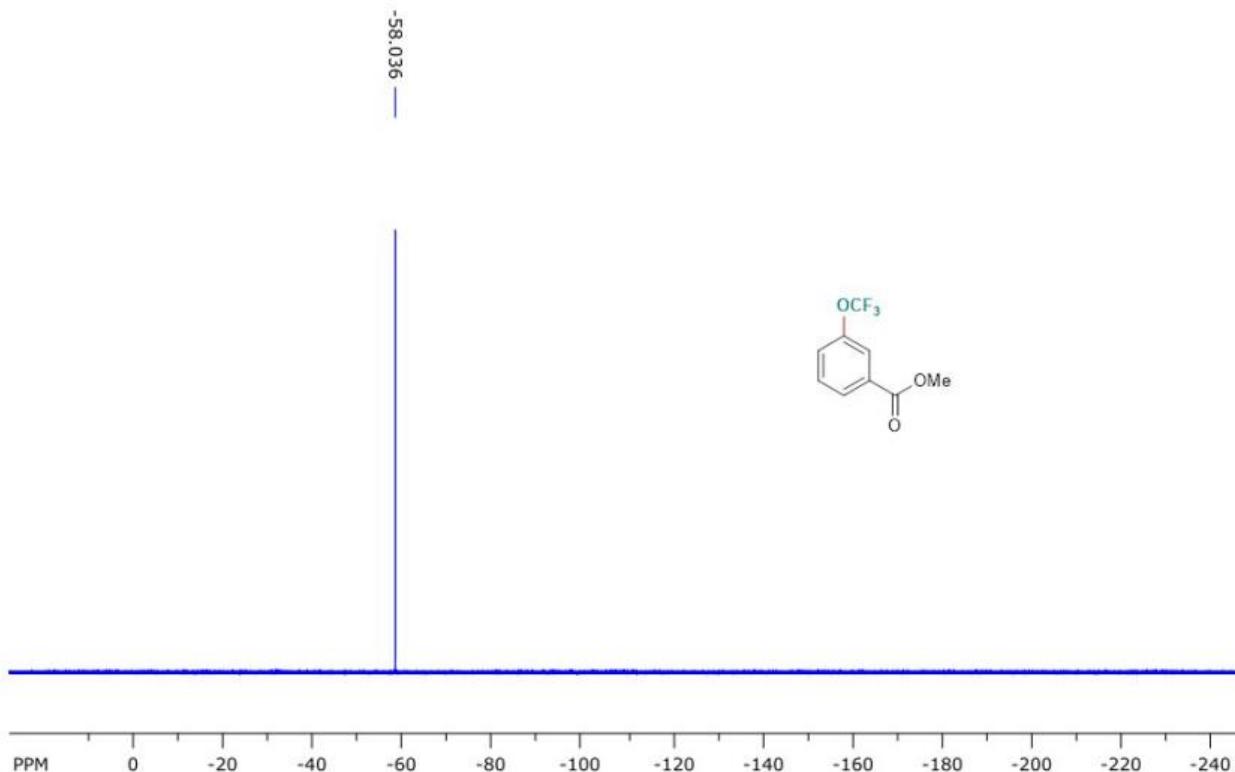
SpinWorks 4: SVS 644 13C CDCl₃



file: ...240418_01\svs644-CARBON_01.fid\fid block# 1 expt: "s2pul" freq. of 0 ppm: 150.811443 MHz
transmitter freq.: 150.828039 MHz processed size: 65536 complex points
time domain size: 65536 points LB: 0.500 GF: 0.0000
width: 37878.79 Hz = 251.1389 ppm = 0.577984 Hz/pt Hz/cm: 1164.857 ppm/cm: 7.72308
number of scans: 256

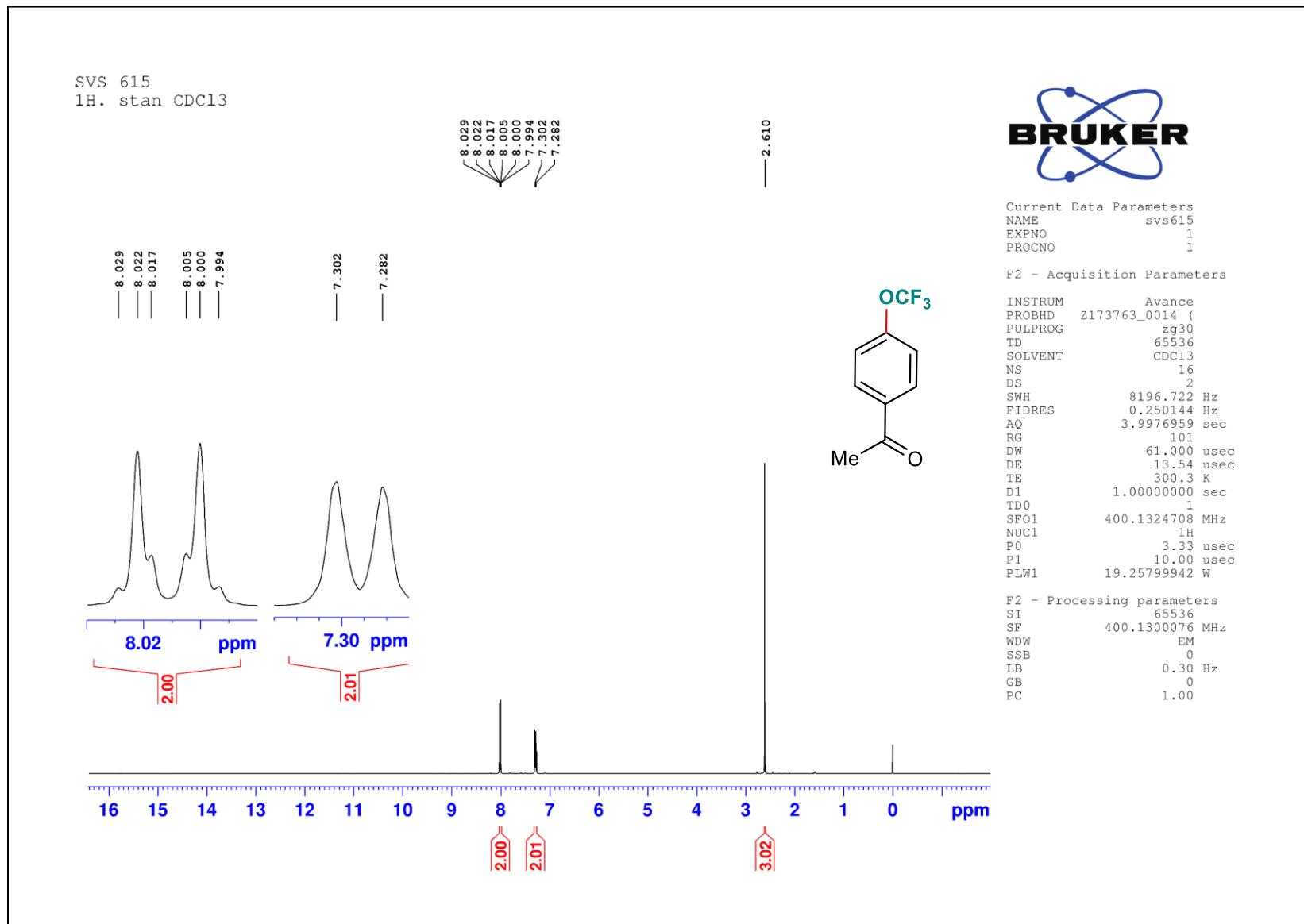
¹⁹F NMR of Compound 4j

SpinWorks 4: SVS 644 19F

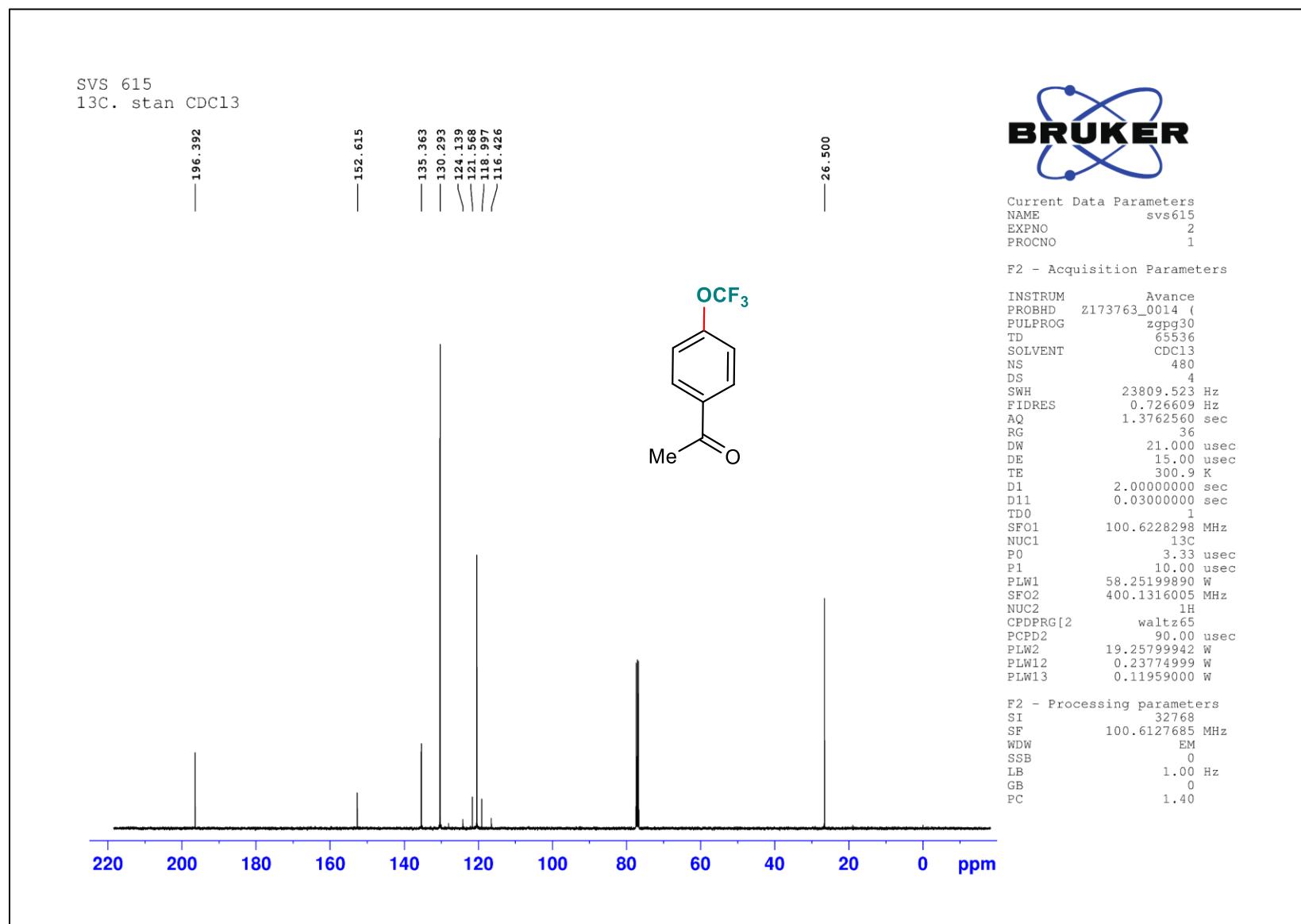


file: ...0418_01\svs644-FLUORINE_01.fid\fid block# 1 expt: "s2pul" freq. of 0 ppm: 564.344520 MHz
transmitter freq.: 564.282442 MHz processed size: 262144 complex points
time domain size: 262144 points LB: 1.500 GF: 0.0000
width: 156250.00 Hz = 276.9003 ppm = 0.596046 Hz/pt Hz/cm: 6250.000 ppm/cm: 11.07601
number of scans: 32

¹H NMR of Compound 4k

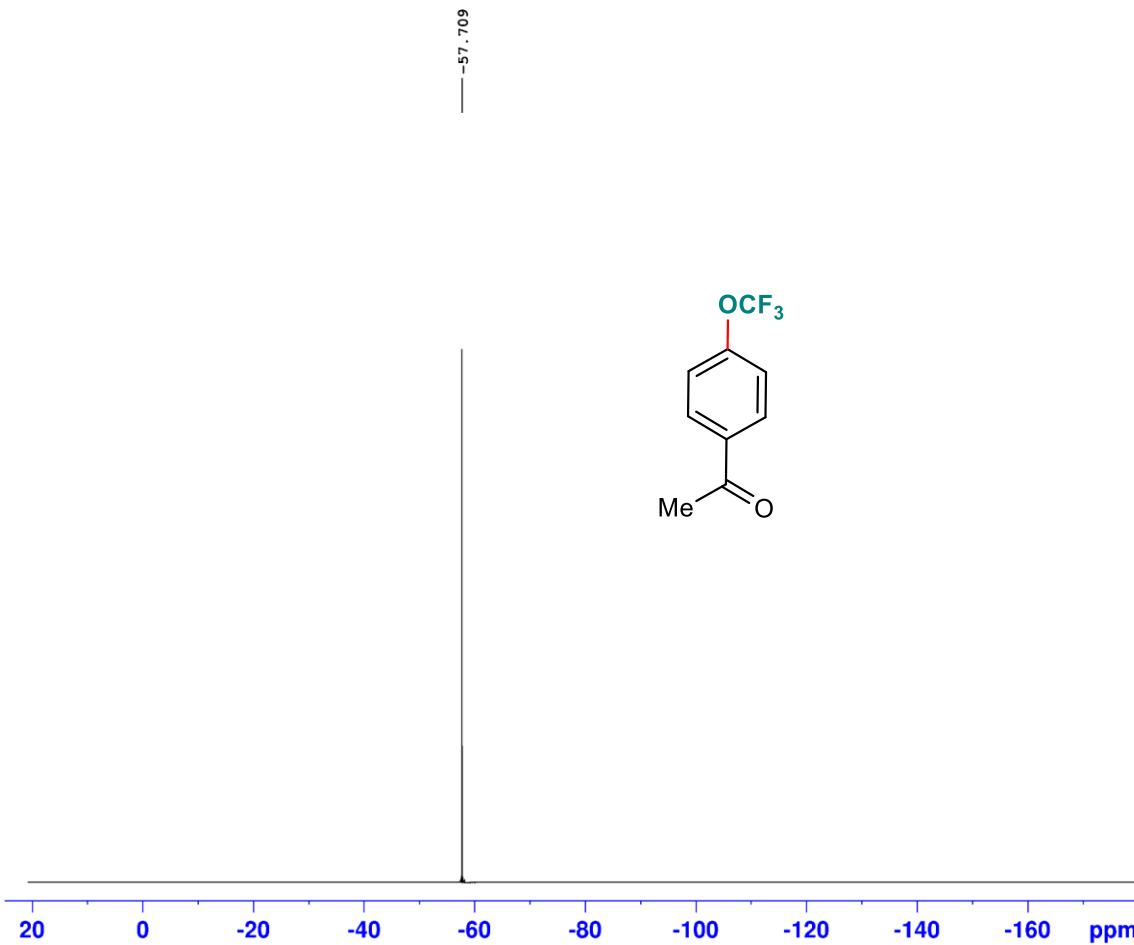


¹³C NMR of Compound 4k



¹⁹F NMR of Compound 4k

SVS 615
19F. stan CDC13



Current Data Parameters
NAME svs615
EXPNO 3
PROCNO 1

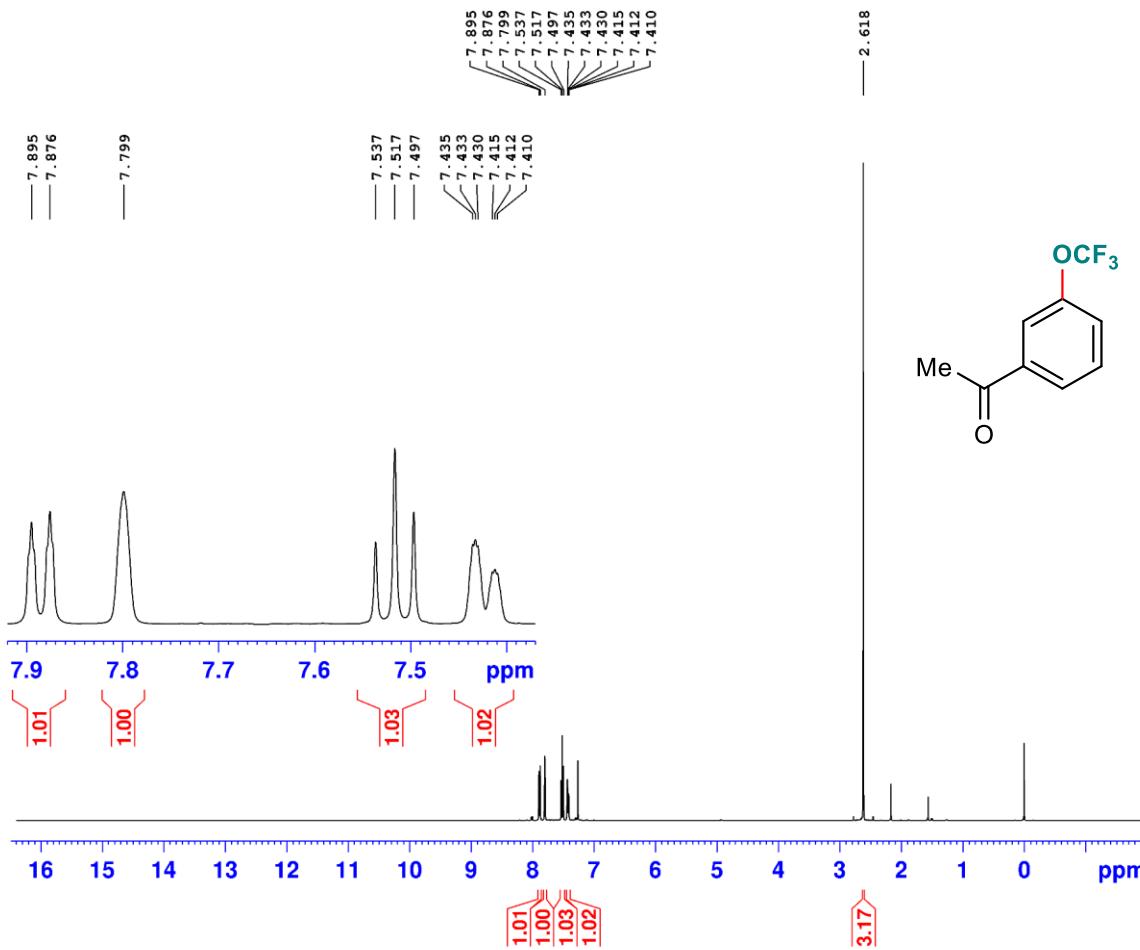
F2 - Acquisition Parameters

INSTRUM Avance
PROBHD Z173763_0014 (zg
PULPROG zg
TD 131072
SOLVENT CDC13
NS 16
DS 4
SWH 90909.094 Hz
FIDRES 1.387163 Hz
AQ 0.7208960 sec
RG 101
DW 5.500 usec
DE 6.50 usec
TE 300.6 K
D1 1.0000000 sec
TDO 1
SFO1 376.4607164 MHz
NUC1 ¹⁹F
P1 12.00 usec
PLW1 36.0000000 W

F2 - Processing parameters
SI 65536
SF 376.4983662 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

¹H NMR of Compound 4I

IVAB 4381
1H. stan CDC13



BRUKER

Current Data Parameters
NAME ivab4381
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters

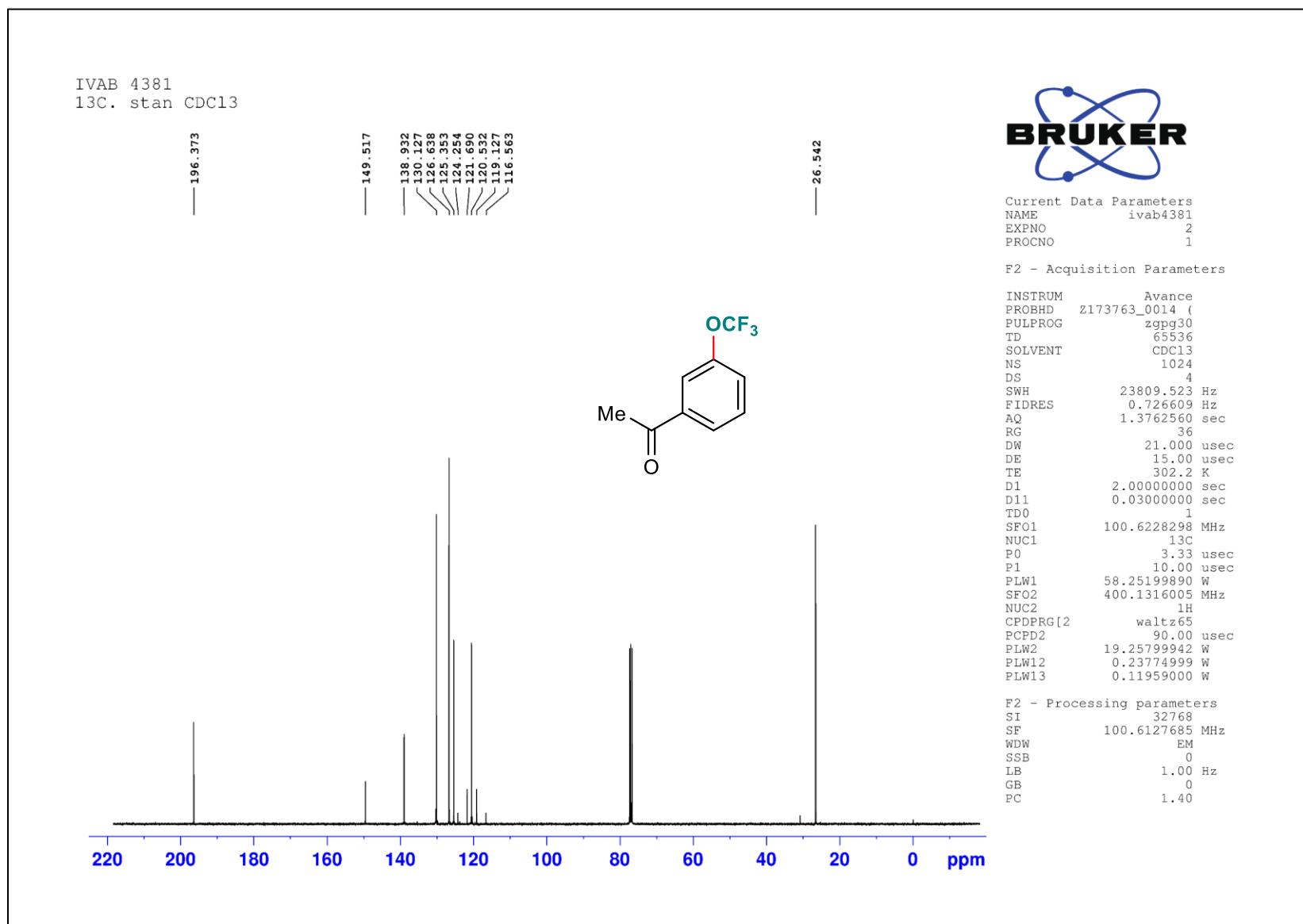
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INSTRUM      Avance
PROBHD      Z173763_0014 (
PULPROG      zg30
TD          65536
SOLVENT      CDC13
NS          16
DS           2
SWH         8196.722 Hz
FIDRES      0.250144 Hz
AQ         3.9976959 sec
RG          101
DW         61.0000 usec
DE         13.54 usec
TE          301.6 K
D1        1.0000000 sec
TD0          1
SFO1        400.1324708 MHz
NUC1          1H
PO          3.33 usec
P1          0.00 usec
PLW1        19.25799942 W

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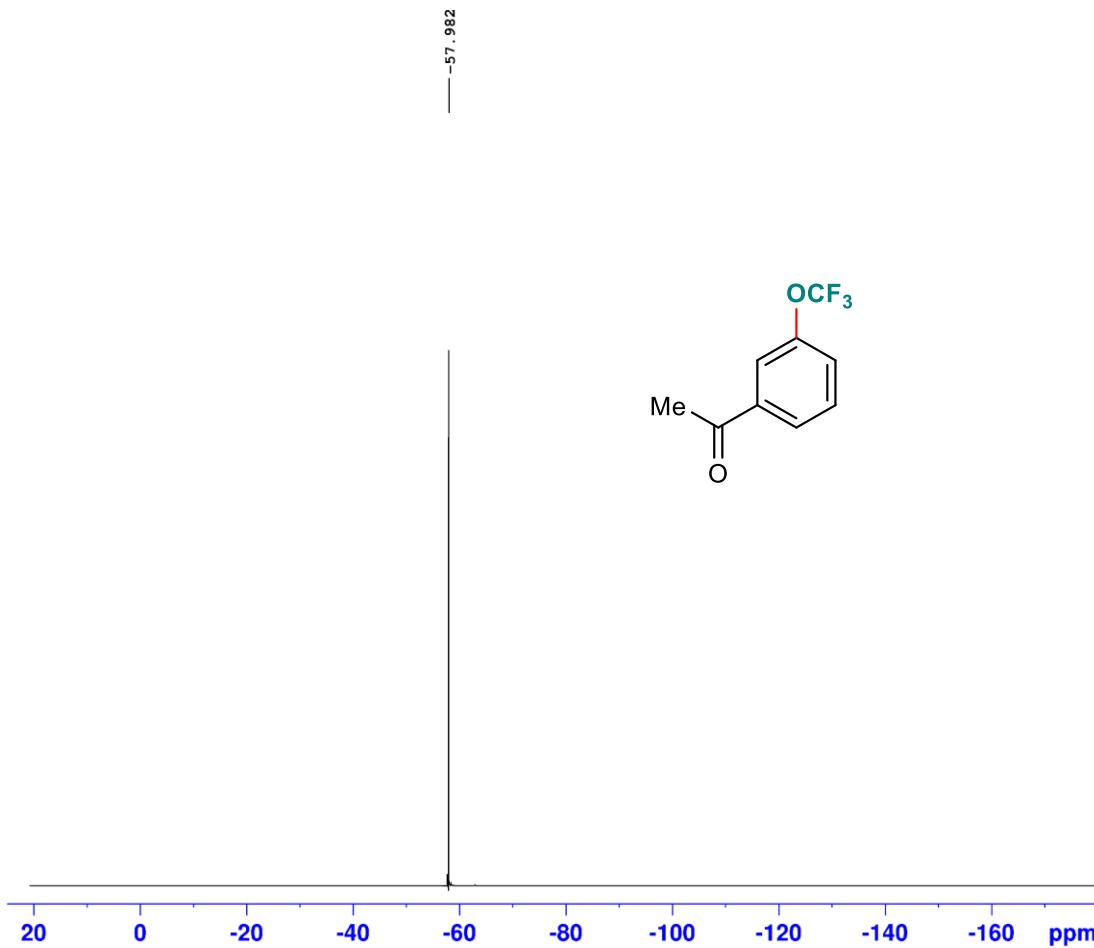
F2 - Processing parameters
SI 65536
SF 400.1300082 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

¹³C NMR of Compound 4I



¹⁹F NMR of Compound 4I

IVAB 4381
19F. stan CDCl₃



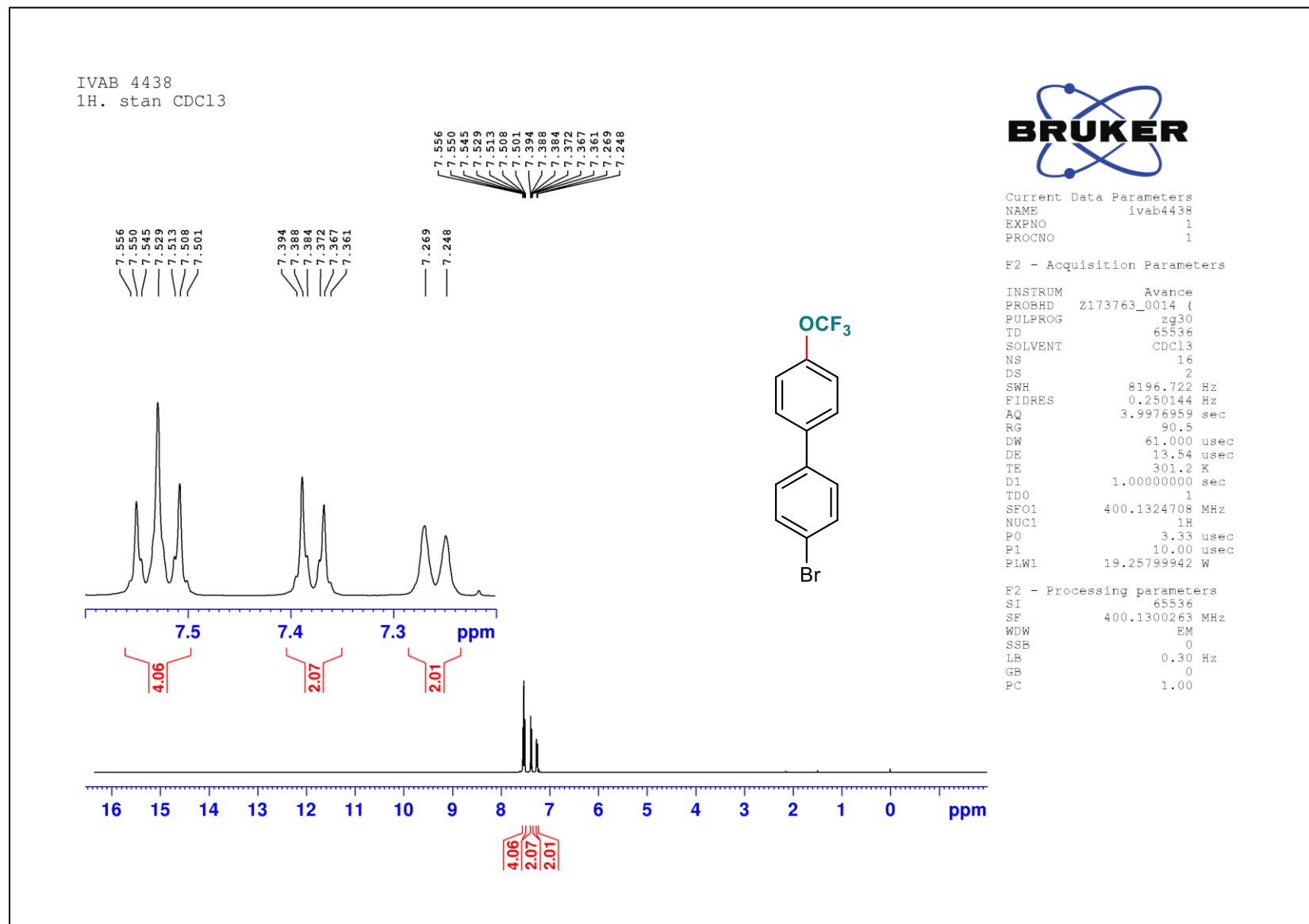
Current Data Parameters
NAME ivab4381
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters

INSTRUM Avance
PROBHD Z173763_0014 (zg
PULPROG zg
TD 131072
SOLVENT CDCl₃
NS 16
DS 4
SWH 90909.094 Hz
FIDRES 1.387163 Hz
AQ 0.7208960 sec
RG 101
DW 5.500 usec
DE 6.50 usec
TE 301.2 K
D1 1.0000000 sec
TDO 1
SF01 376.4607164 MHz
NUC1 ¹⁹F
P1 12.00 usec
PLW1 36.0000000 W

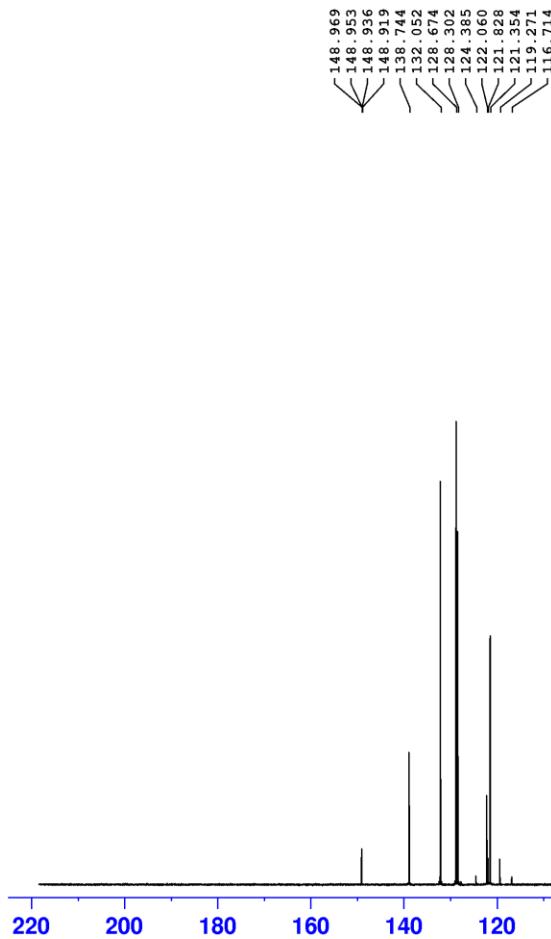
F2 - Processing parameters
SI 65536
SF 376.4983662 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

¹H NMR of Compound 4m



¹³C NMR of Compound 4m

IVAB 4438
A-13C. stan CDCl₃



Current Data Parameters
NAME ivab4438
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters

INSTRUM Avance
PROBHD Z173763_0014 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl₃
NS 600
DS 4
SWH 23809.523 Hz
FIDRES 0.726609 Hz
AQ 1.3762560 sec
RG 36
DW 21.000 usec
DE 15.00 usec
TE 300.9 K
D1 2.0000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6228298 MHz
NUC1 ¹³C
P0 3.33 usec
P1 10.00 usec
PLW1 58.25199890 W
SFO2 400.1316005 MHz
NUC2 ¹H
CPDPRG[2] waltz65
PCPD2 90.00 usec
PLW2 19.25799942 W
PLW12 0.23774999 W
PLW13 0.11959000 W

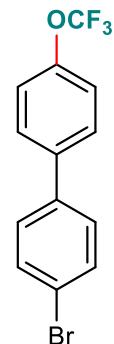
F2 - Processing parameters
SI 32768
SF 100.6127685 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

¹⁹F NMR of Compound 4m

IVAB 4438
19F. stan CDCl₃

-57.800

0 -20 -40 -60 -80 -100 -120 -140 -160 ppm



Current Data Parameters
NAME ivab4438
EXPNO 2
PROCNO 1

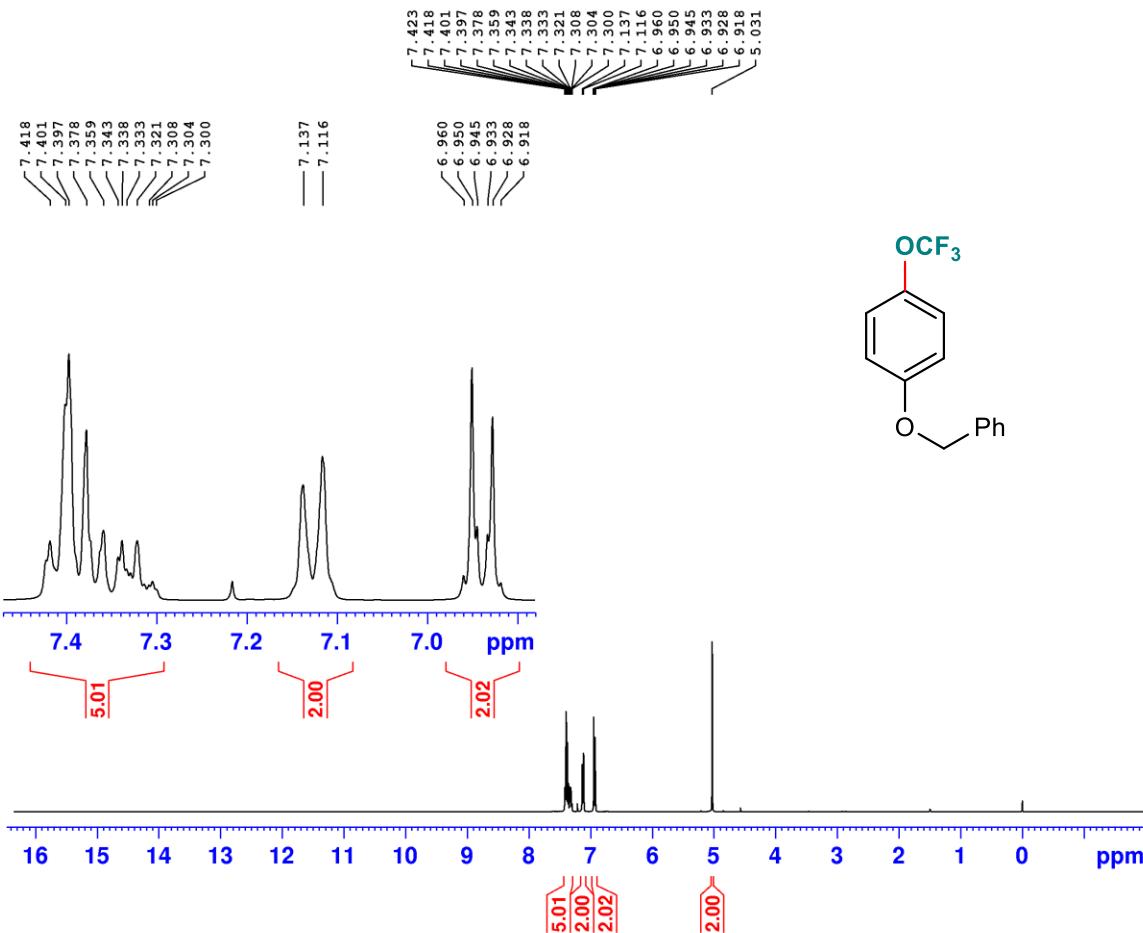
F2 - Acquisition Parameters

INSTRUM Avance
PROBHD Z173763_0014 ('
PULPROG zg
TD 131072
SOLVENT CDCl₃
NS 16
DS 4
SWH 90909.094 Hz
FIDRES 1.387163 Hz
AQ 0.7208960 sec
RG 101
DW 5.500 usec
DE 6.50 usec
TE 301.1 K
D1 1.0000000 sec
TDO 1
SFO1 376.4607164 MHz
NUC1 ¹⁹F
P1 12.00 usec
PLW1 36.00000000 W

F2 - Processing parameters
SI 65536
SF 376.4983662 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

¹H NMR of Compound 4n

SVS 745
1H. stan CDC13



BRUKER

Current Data Parameters
NAME svs745
EXPNO 1
PROCNO 1

```

F2 - Acquisition Parameters
INSTRUM      Avance
PROBHD      Z173763_0014 (
PULPROG     zg30
TD          65536
SOLVENT      CDCl3
NS           16
DS            2
SWH         8196.722 Hz
FIDRES      0.250144 Hz
AQ          3.9976959 sec
RG           101
DW           61.0000 usec
DE           13.54 usec
TE           300.5 K
D1          1.00000000 sec
TD0           1
SF01        400.1324708 MHz
NUC1        1H
P0           3.33 usec
P1           10.00 usec
PLW1        19.25799942 W

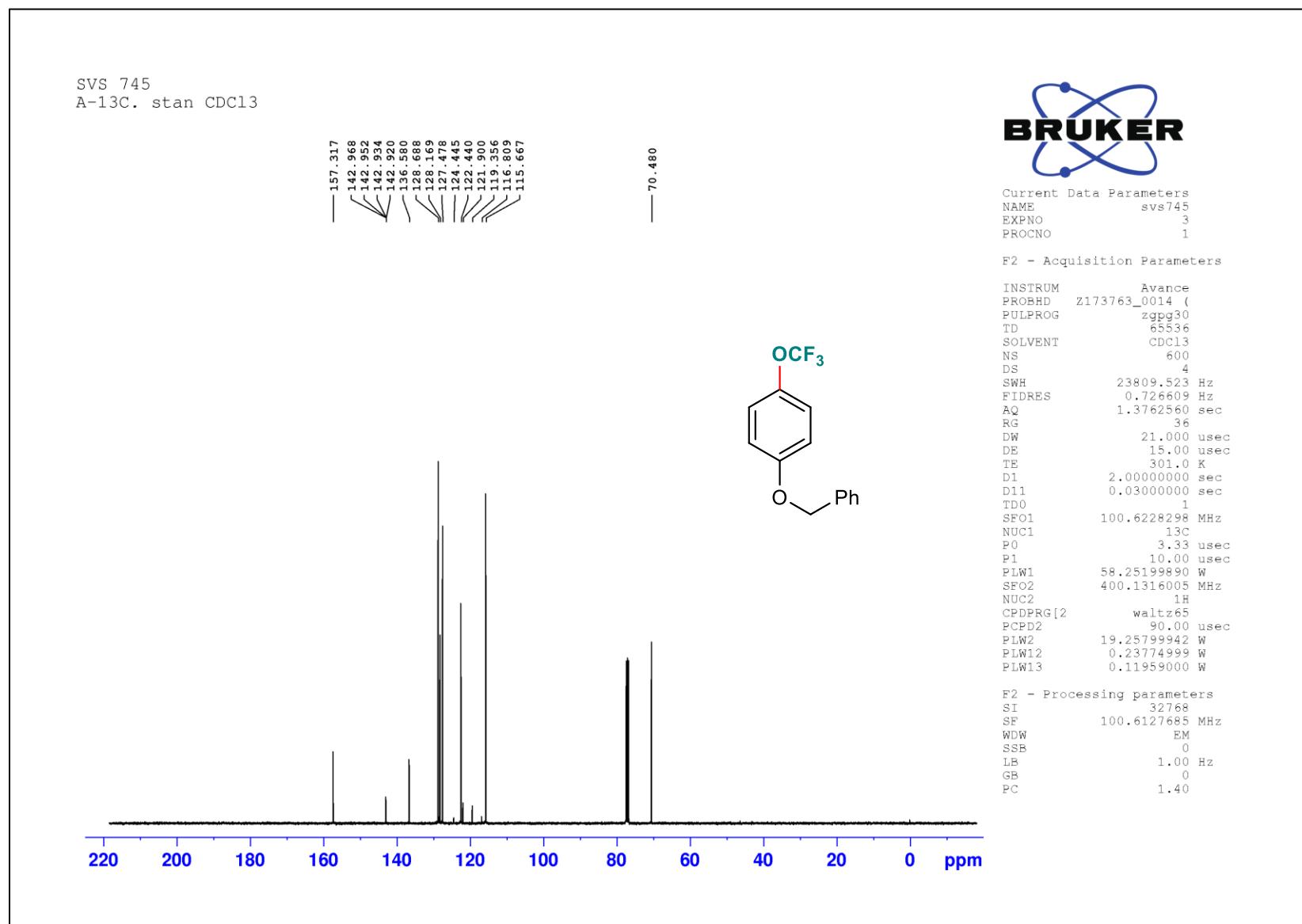
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F2 - Processing parameters
SI          65536
SF        400.1300263 MHz
WDW         EM
SSB          0
LB        0.30 Hz
GB          0
PC        1.00

```

¹³C NMR of Compound 4n



¹⁹F NMR of Compound 4n

SVS 745
19F. stan CDCl₃

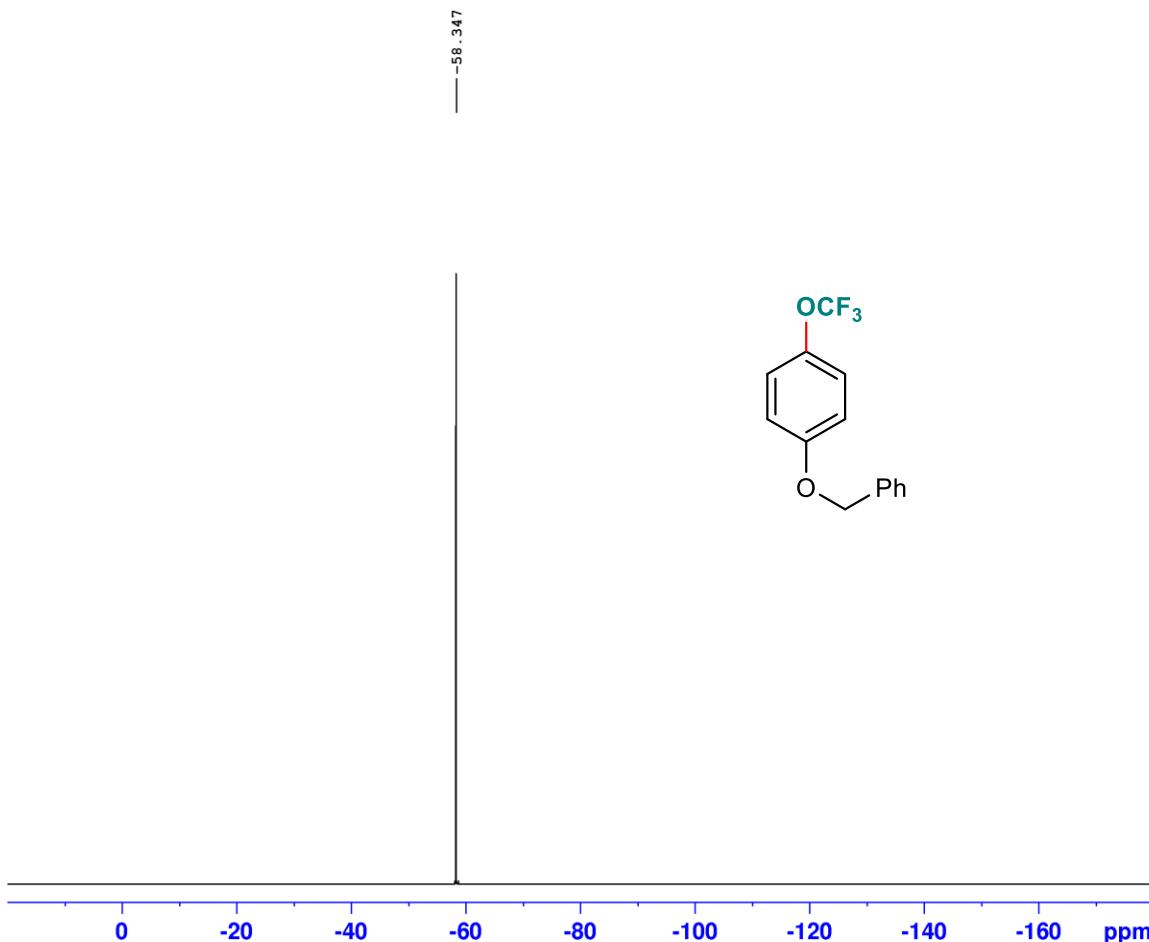
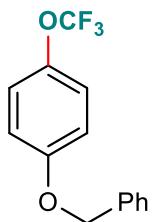


Current Data Parameters
NAME svs745
EXPNO 2
PROCNO 1

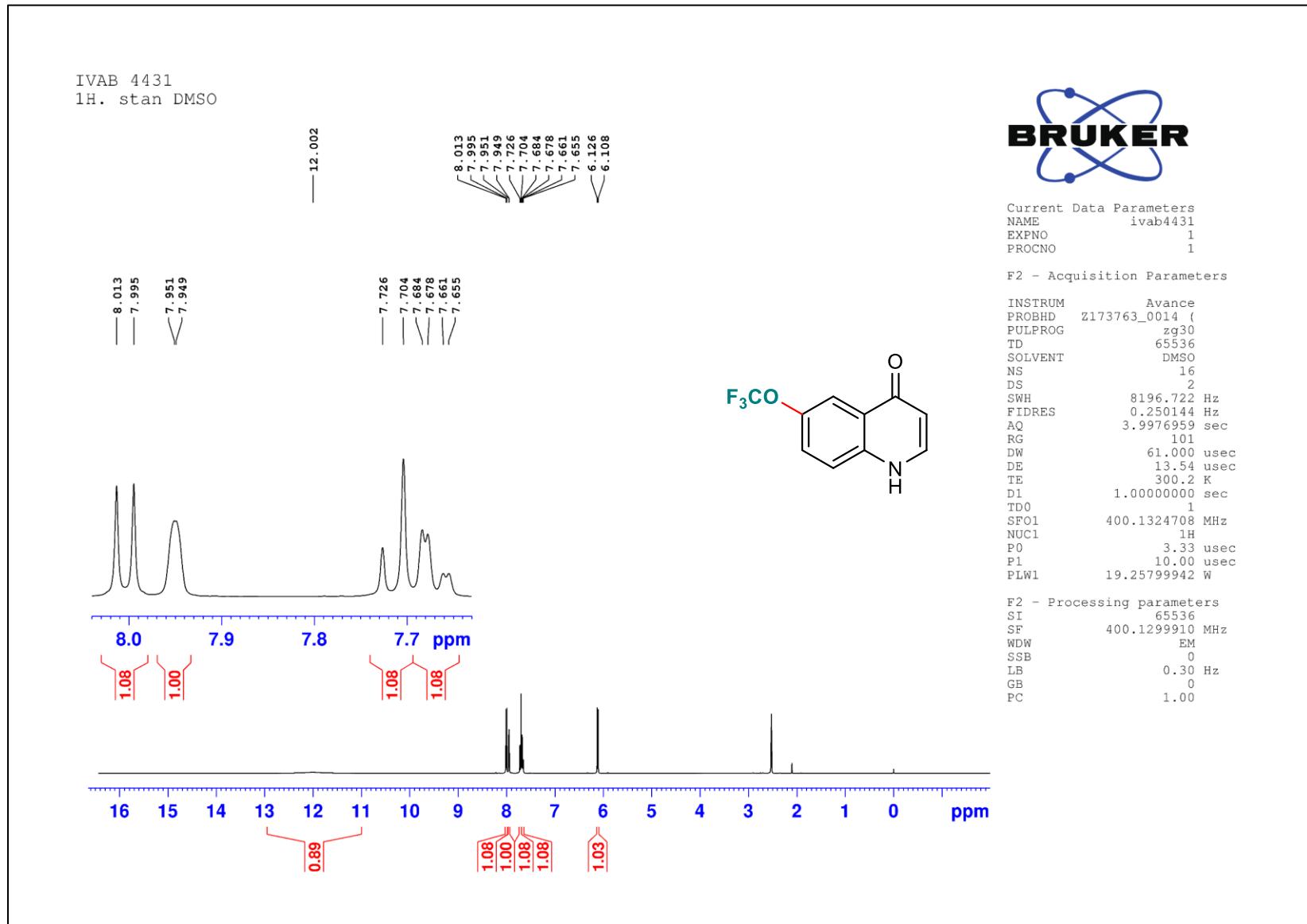
F2 - Acquisition Parameters

INSTRUM Avance
PROBHD Z173763_0014 (zg
PULPROG zg
TD 131072
SOLVENT CDCl₃
NS 16
DS 4
SWH 90909.094 Hz
FIDRES 1.387163 Hz
AQ 0.7208960 sec
RG 101
DW 5.500 usec
DE 6.50 usec
TE 300.6 K
D1 1.0000000 sec
TDO 1
SFO1 376.4607164 MHz
NUC1 ¹⁹F
P1 12.00 usec
PLW1 36.0000000 W

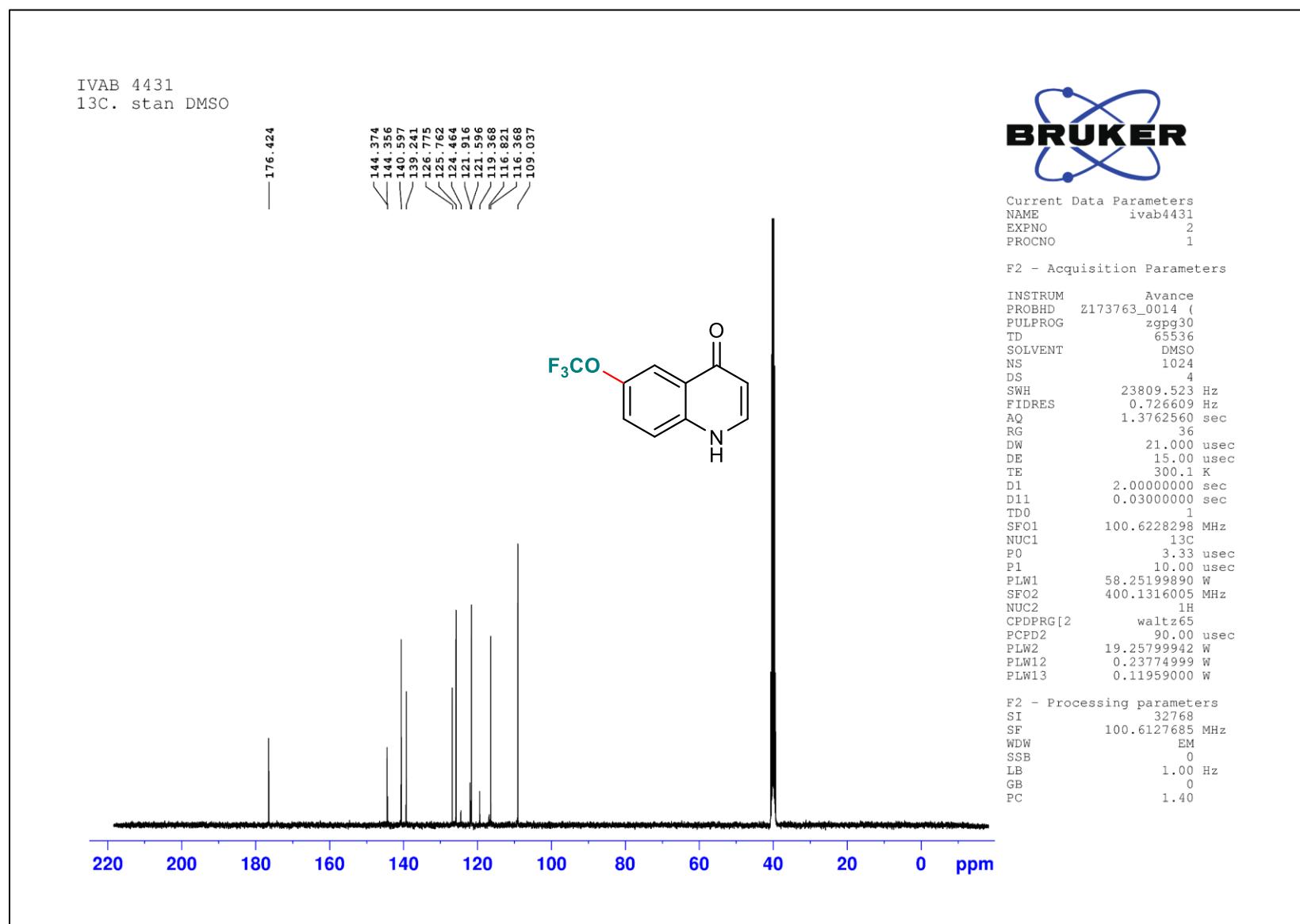
F2 - Processing parameters
SI 65536
SF 376.4983662 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
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¹H NMR of Compound 4o



¹³C NMR of Compound 4o



¹⁹F NMR of Compound 4o

IVAB 4431
19F. stan DMSO

-57.157

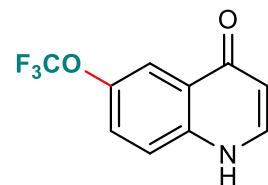


Current Data Parameters
NAME ivab4431
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters

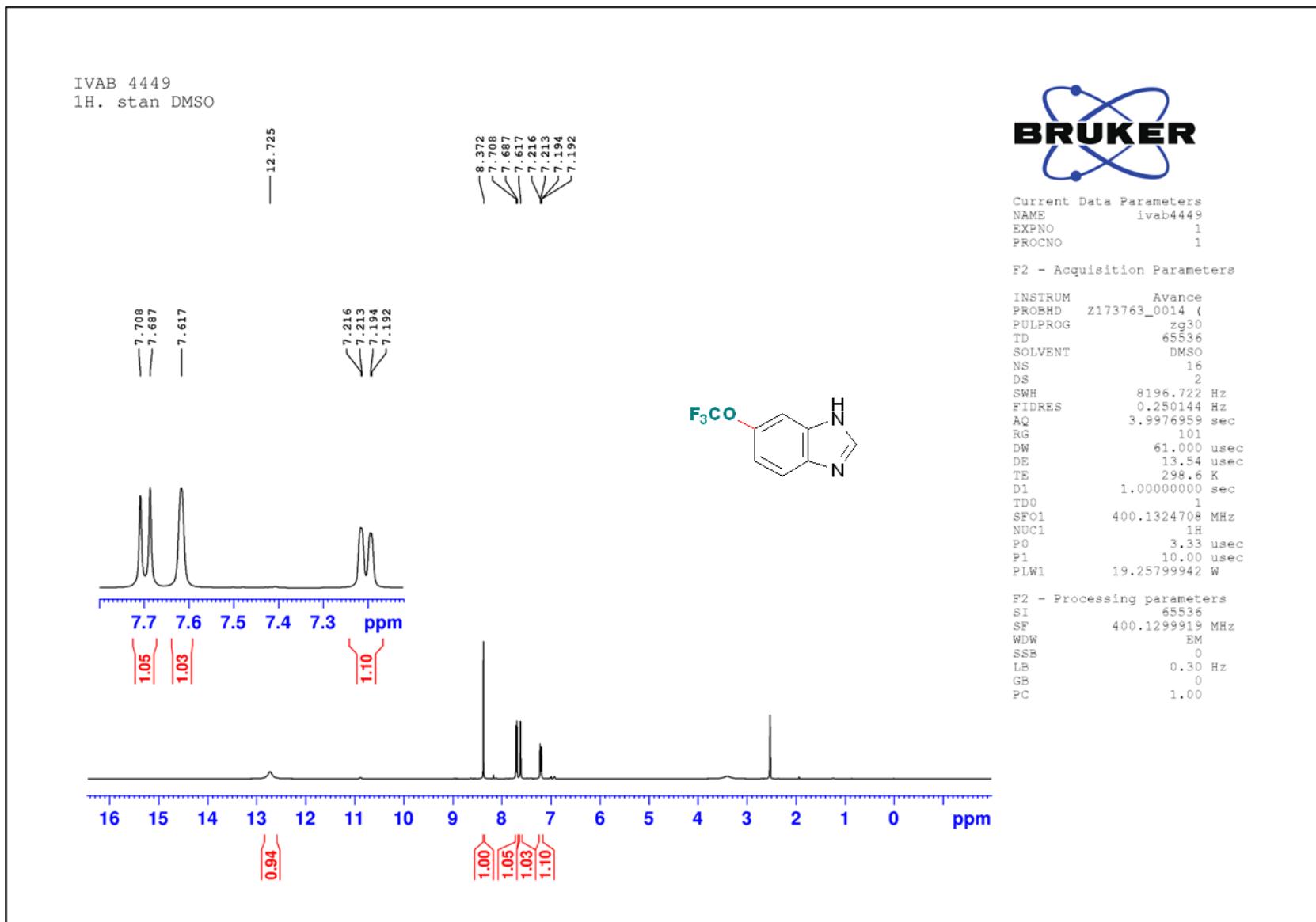
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PULPROG zg
TD 131072
SOLVENT DMSO
NS 16
DS 4
SWH 90909.094 Hz
FIDRES 1.387163 Hz
AQ 0.7208960 sec
RG 101
DW 5.500 usec
DE 6.50 usec
TE 299.8 K
D1 1.0000000 sec
TDO 1
SF01 376.4607164 MHz
NUC1 ¹⁹F
P1 12.00 usec
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F2 - Processing parameters
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SF 376.4983662 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

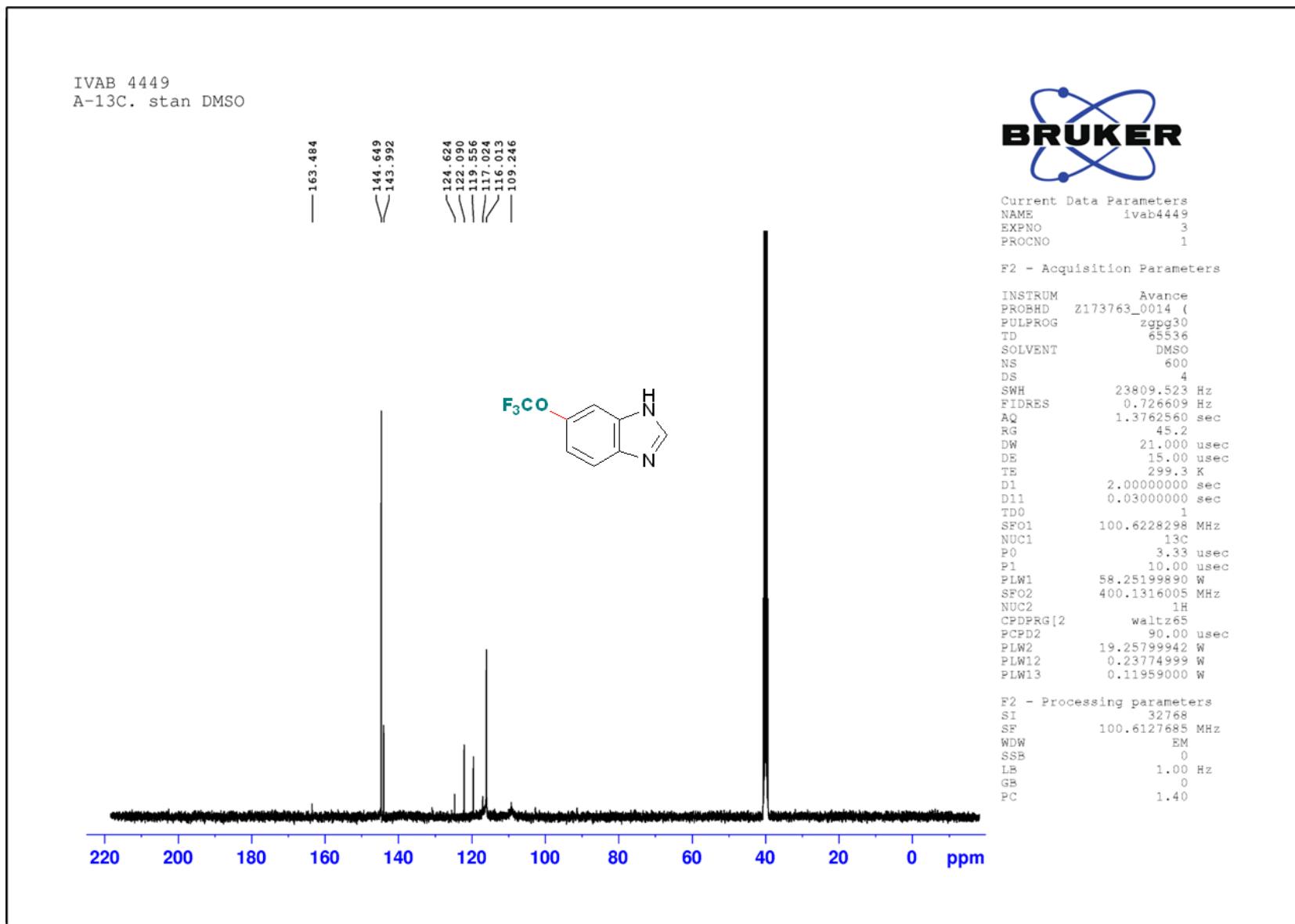


20 0 -20 -40 -60 -80 -100 -120 -140 -160 ppm

¹H NMR of Compound 4p



¹³C NMR of Compound 4p

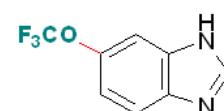


¹⁹F NMR of Compound 4p

IVAB 4449
19F. stan DMSO



-57.093



0 -20 -40 -60 -80 -100 -120 -140 -160 ppm

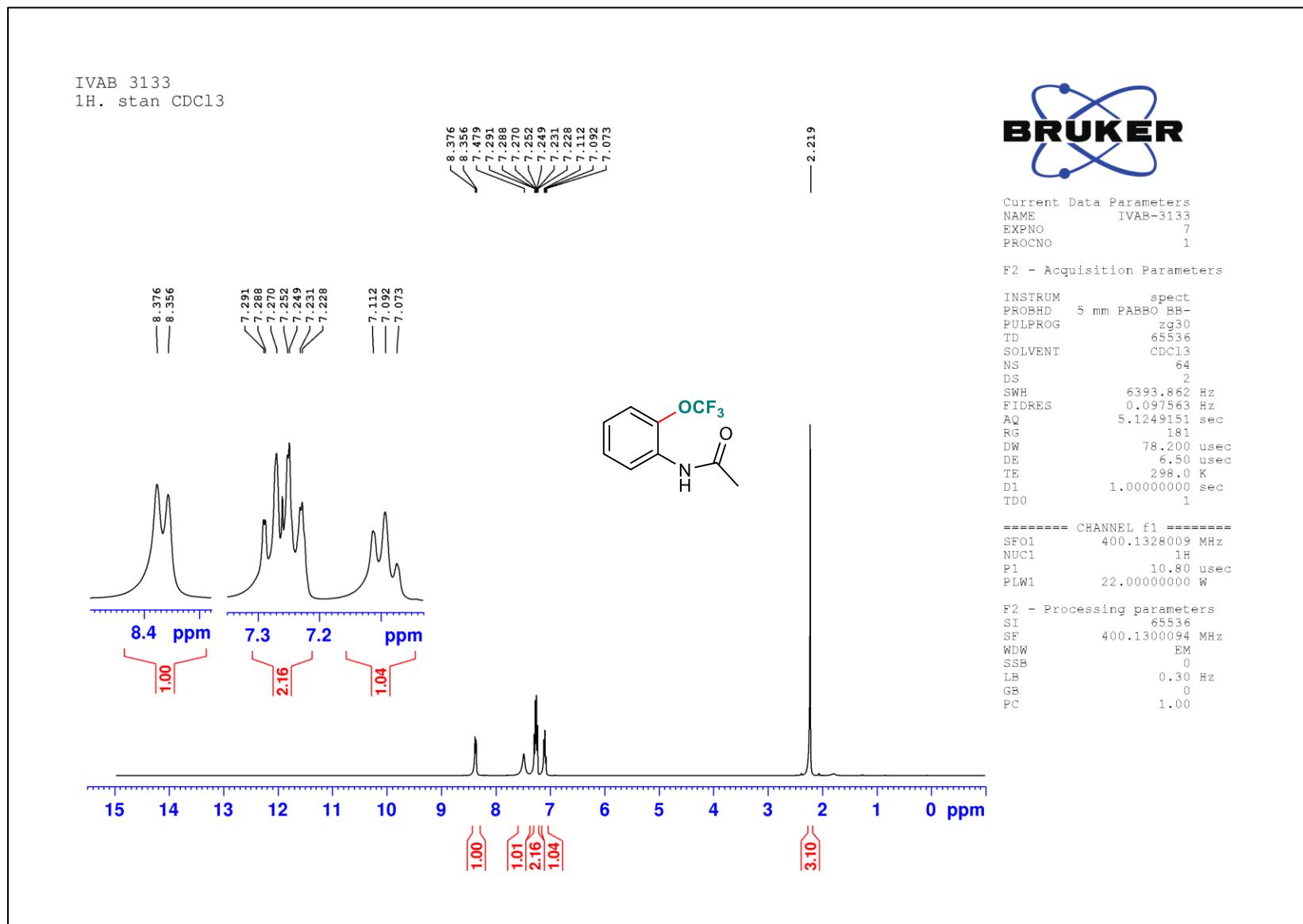
Current Data Parameters
NAME ivab4449
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters

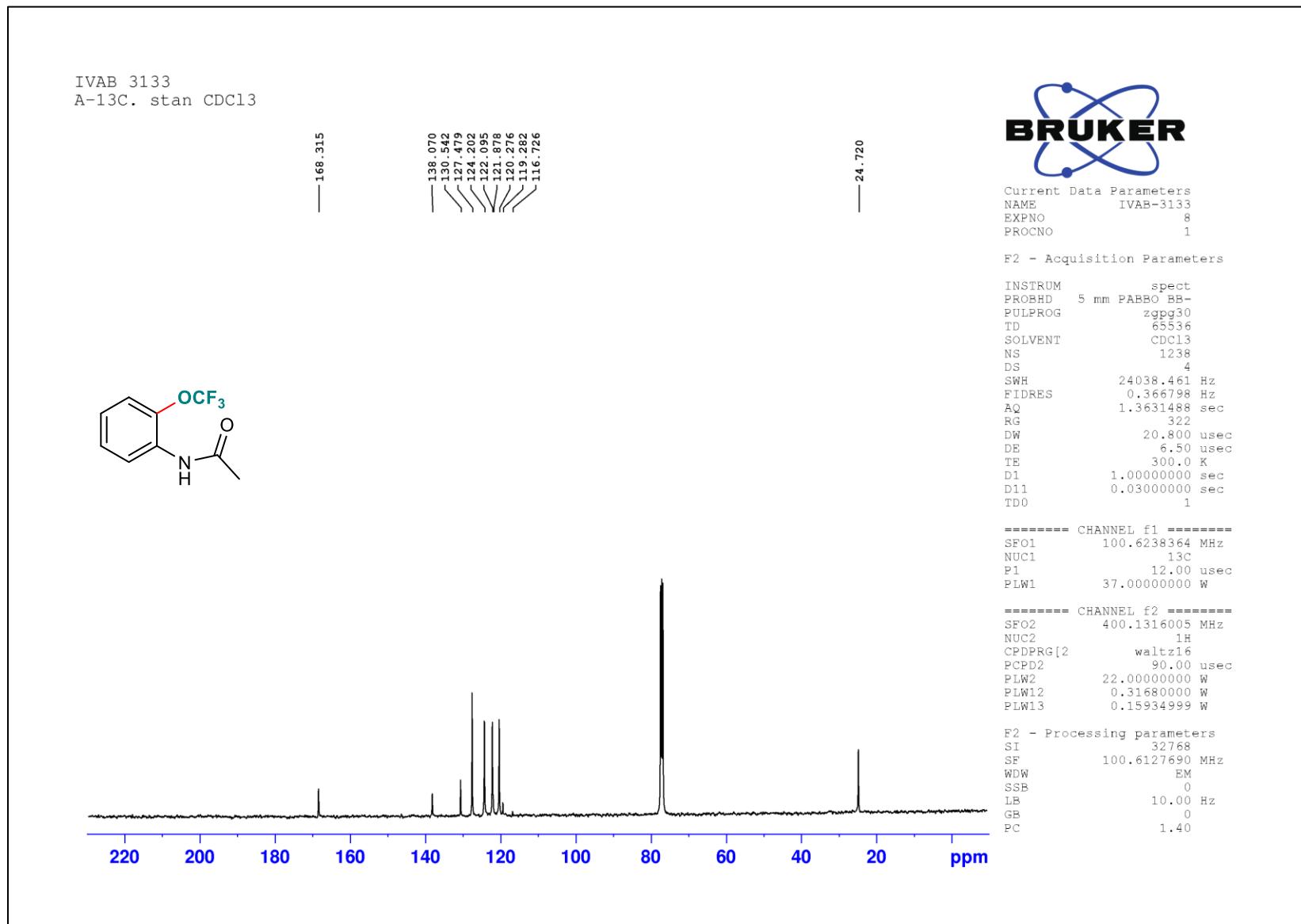
INSTRUM Avance
PROBHD Z173763_0014 (zg
PULPROG zg
TD 131072
SOLVENT DMSO
NS 16
DS 4
SWH 90909.094 Hz
FIDRES 1.387163 Hz
AQ 0.7208960 sec
RG 101
DW 5.500 usec
DE 6.50 usec
TE 298.7 K
D1 1.0000000 sec
TDO 1
SFO1 376.4607164 MHz
NUC1 ¹⁹F
P1 12.00 usec
PLW1 36.0000000 W

F2 - Processing parameters
SI 65536
SF 376.4983662 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

¹H NMR of Compound 4q

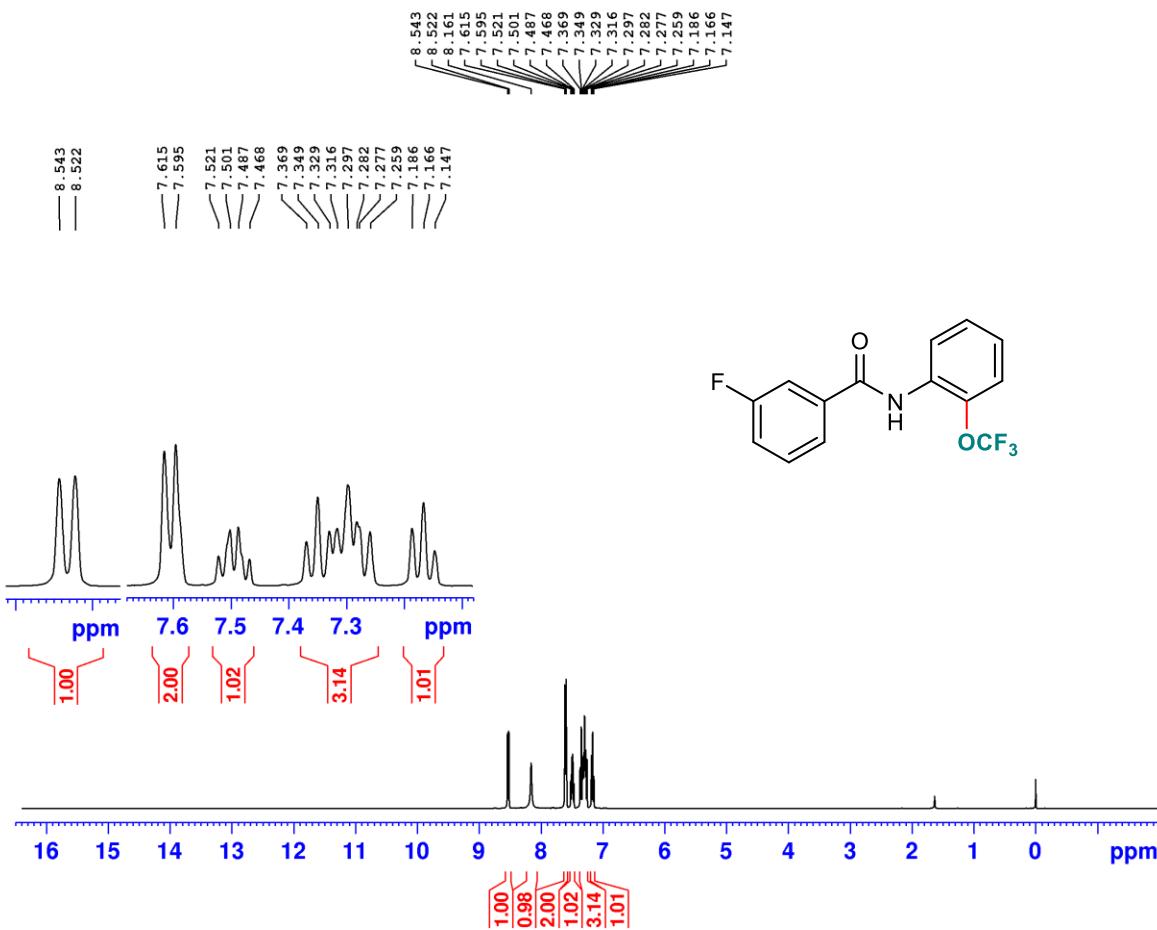


¹³C NMR of Compound 4q



¹H NMR of Compound 4r

ETH 219
1H. stan CDC13





Current Data Parameters
NAME eth219
EXPNO 1
PROCNO 1

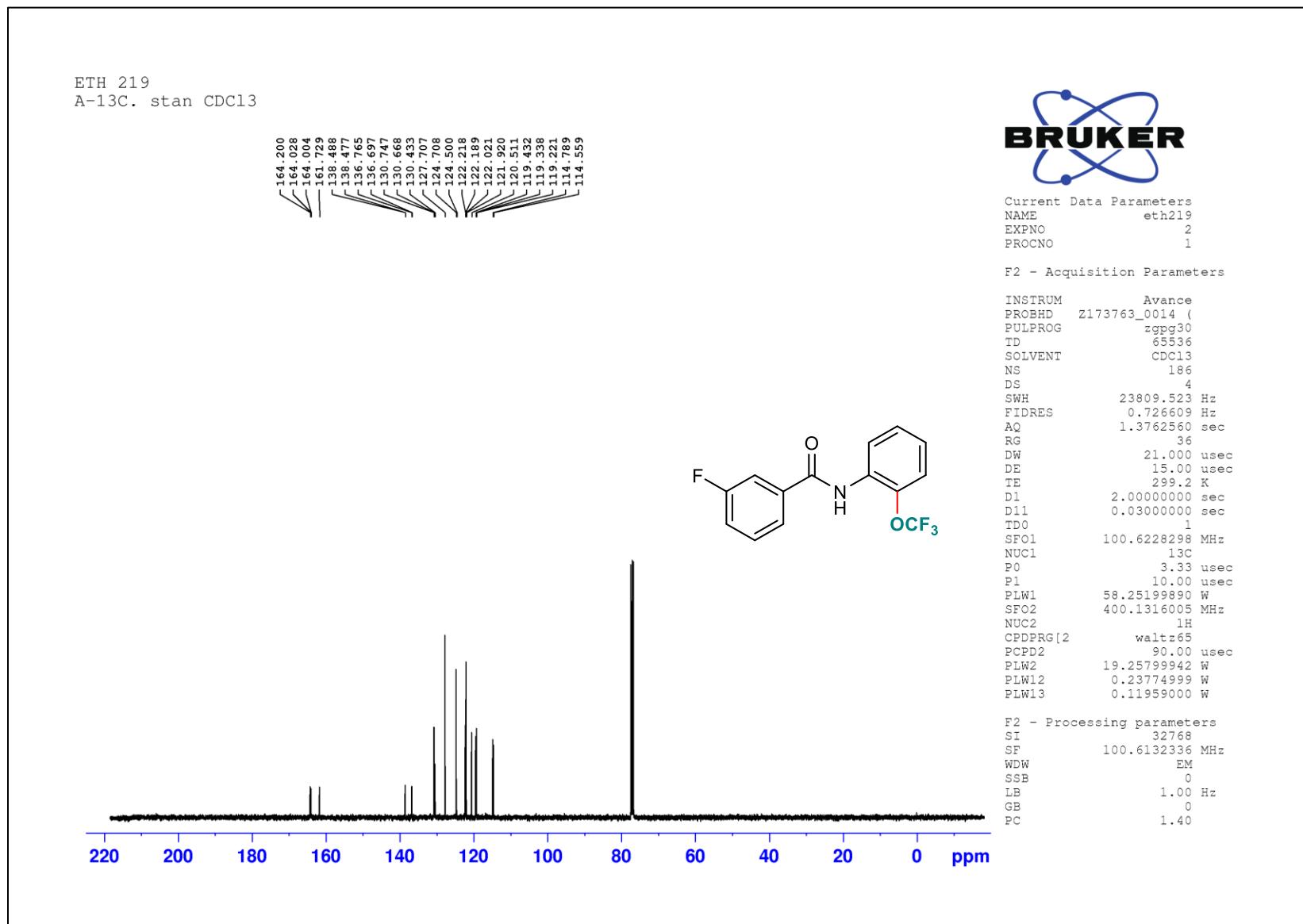
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F2 - Acquisition Parameters
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SOLVENT CDCl3
NS 16
DS 2
SWH 8196.721 Hz
FIDRES 0.250144 Hz
AQ 3.9976959 sec
RG 101
DW 61.000 usec
DE 13.54 usec
TE 298.1 K
D1 1.0000000 sec
TDO 1
SFO1 400.1324708 MHz
NUC1 1H
PO 3.33 usec
P1 10.00 usec
PLW1 19.25799942 W

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F2 - Processing parameters  
SI          65536  
SF        400.1300089 MHz  
WDW           EM  
SSB            0  
LB         0.30 Hz  
GB            0  
PC        1.00
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¹³C NMR of Compound 4r



¹⁹F NMR of Compound 4r

ETH 219
¹⁹F. stan CDCl₃



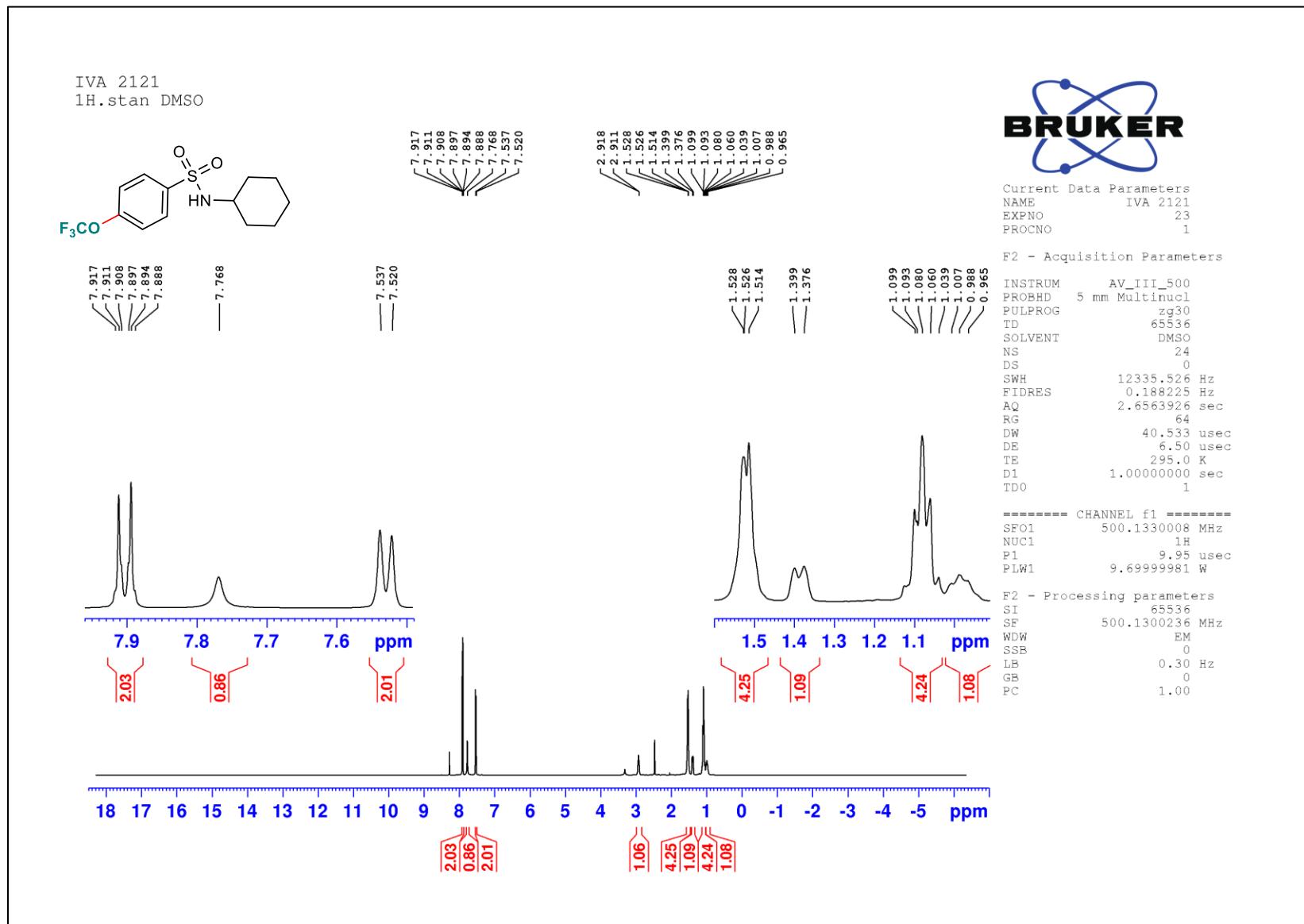
Current Data Parameters
NAME eth219
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters

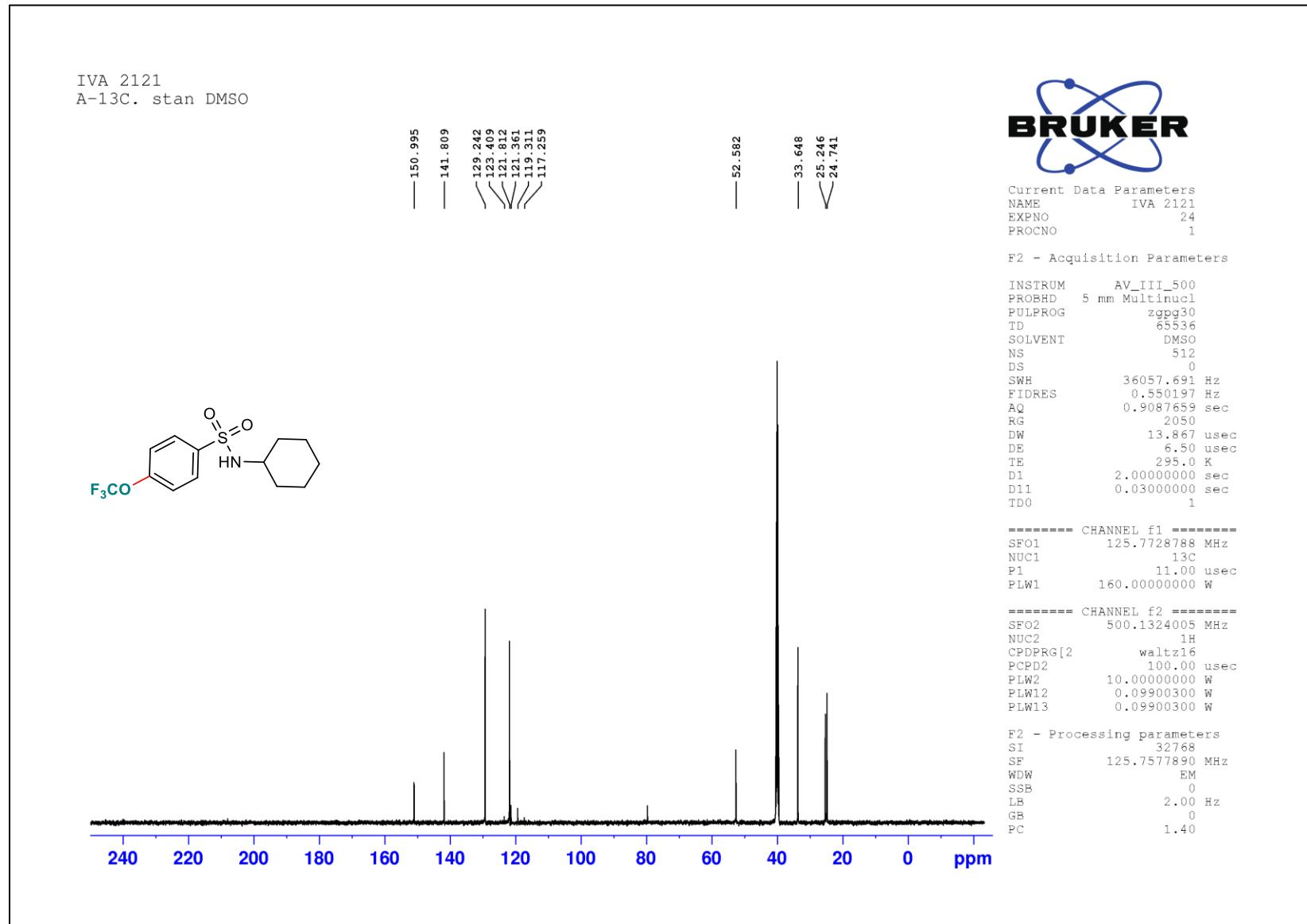
INSTRUM Avance
PROBHD Z173763_0014 (zg
PULPROG zg
TD 131072
SOLVENT CDCl₃
NS 16
DS 4
SWH 90909.091 Hz
FIDRES 1.387163 Hz
AQ 0.7208960 sec
RG 101
DW 5.500 usec
DE 6.50 usec
TE 298.0 K
D1 1.0000000 sec
TDO 1
SFO1 376.4607164 MHz
NUC1 ¹⁹F
P1 12.00 usec
PLW1 36.0000000 W

F2 - Processing parameters
SI 65536
SF 376.4983662 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

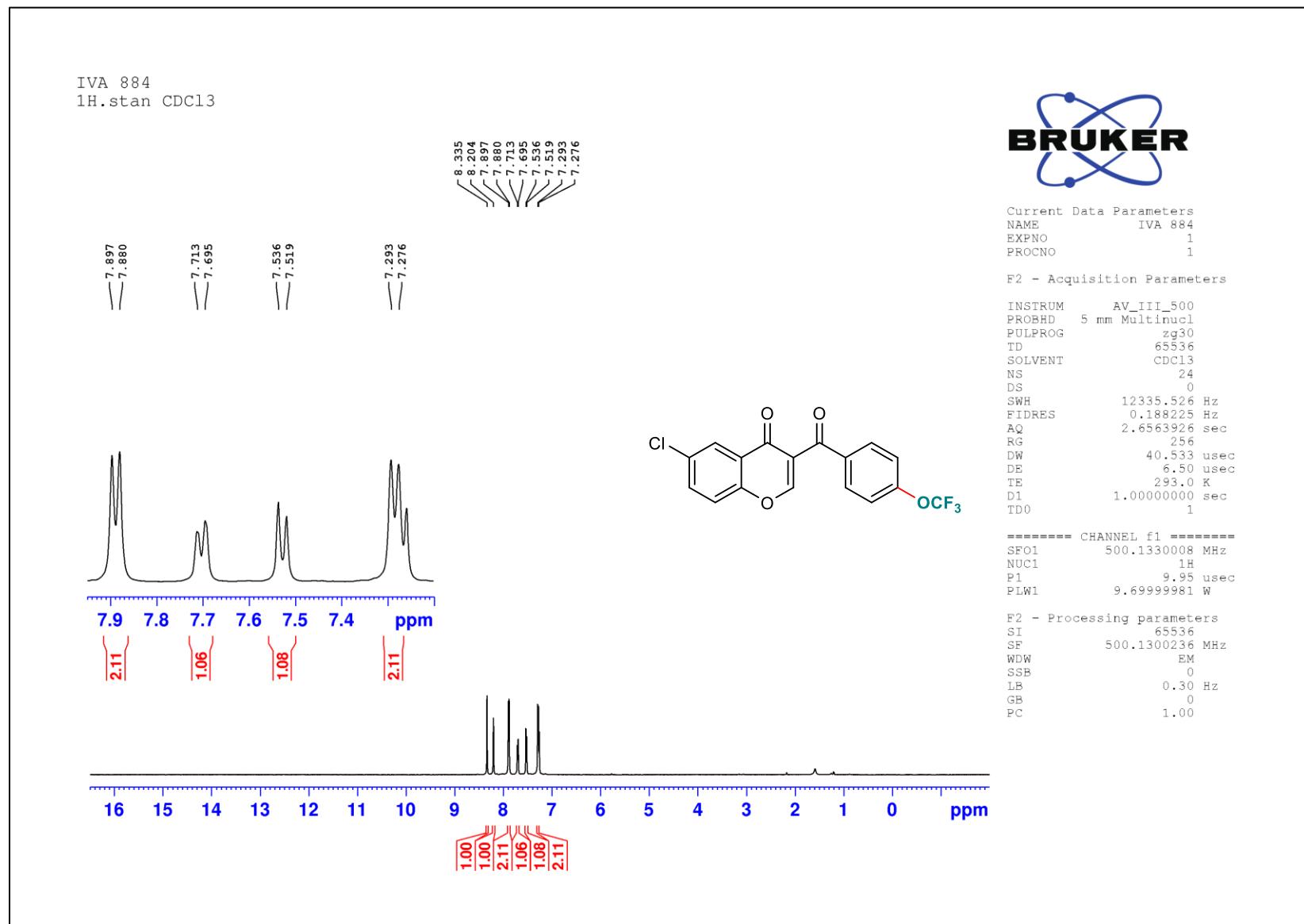
¹H NMR of Compound 4s



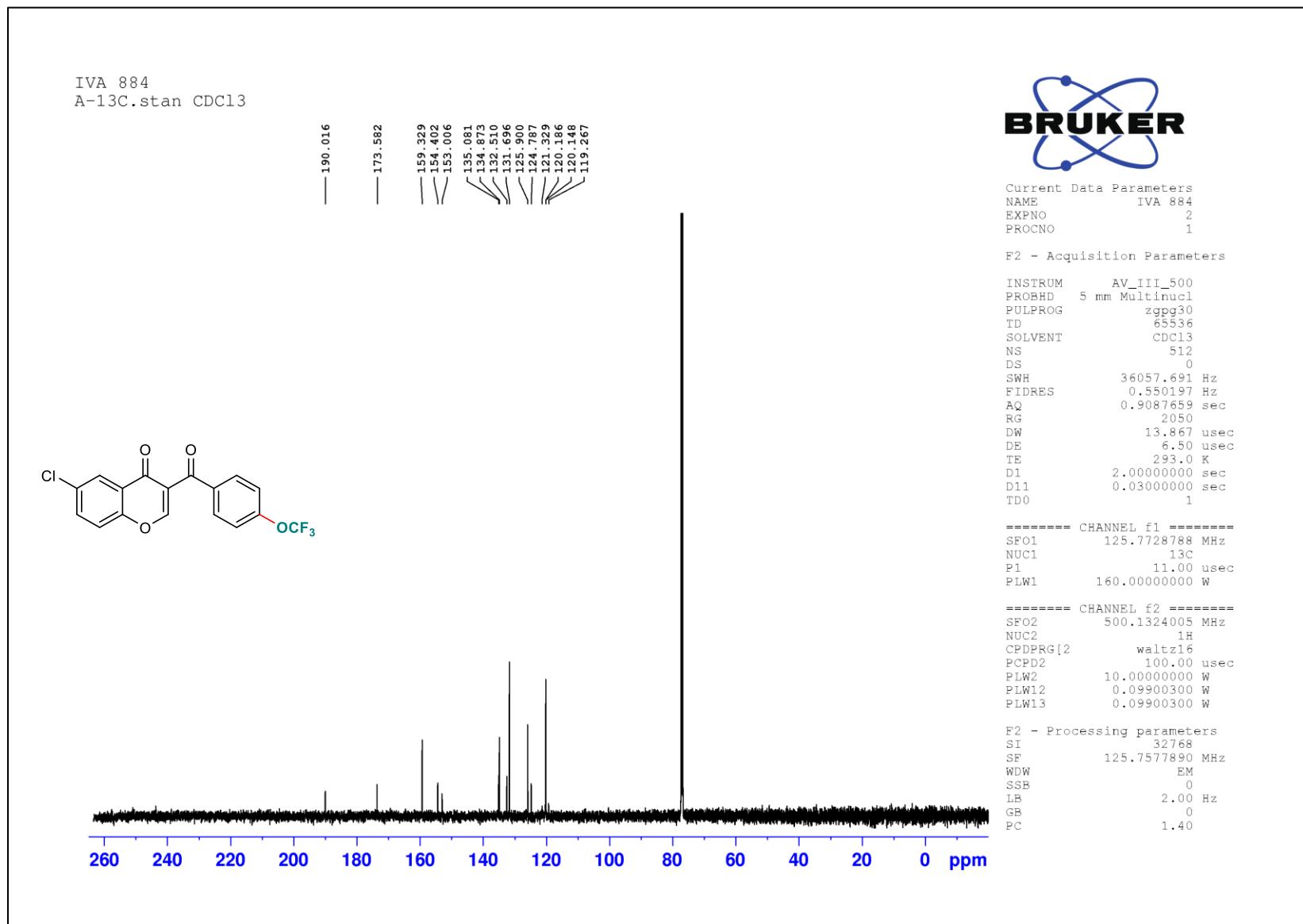
¹³C NMR of Compound 4s



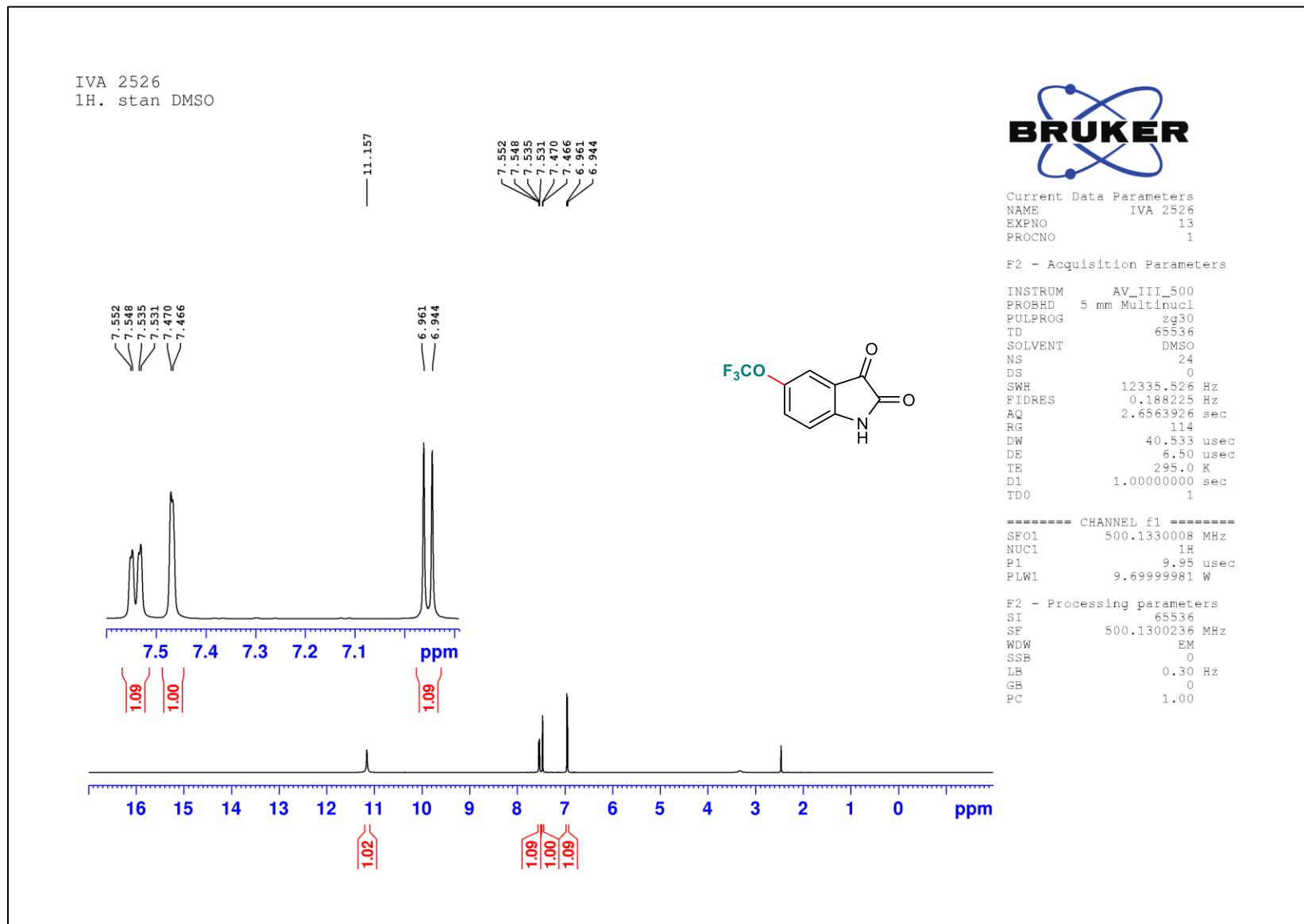
¹H NMR of Compound 4t



¹³C NMR of Compound 4t



¹H NMR of Compound 4u



¹³C NMR of Compound 4u

