Silver-catalysed trifluoromethylation of arenes at room temperature

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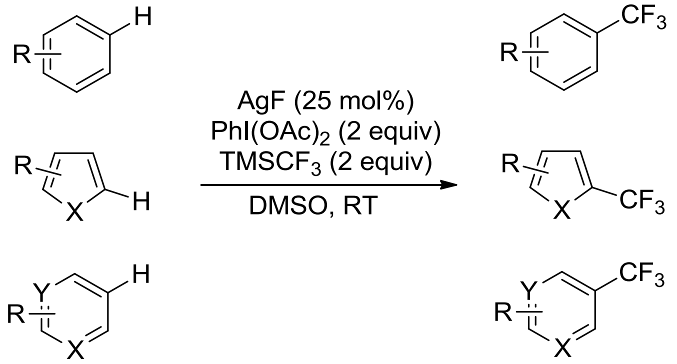
Supporting Information

I. Experimental Procedures

General Methods:

Melting points are uncorrected. ^{1}H, ^{13}C and ^{19}F NMR spectra were recorded on a Brüker Ava400 (400 MHz) instrument and calibrated to residual solvent peaks: proton ($CDCl_3$: 7.26 ppm) and carbon ($CDCl_3$: 77.0 ppm). ^{19}F NMR yields were determined using 4-fluoroanisole as internal standard (δ = -124.8 ppm). Data for ^{1}H and ^{19}F NMR are presented as follows: chemical shift (in ppm on the δ scale), multiplicity (bs = broad singlet, s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet), the coupling constant (J, in Hertz) and integration. ^{13}C data are reported as the ppm on the δ scale followed by the interpretation and multiplicity where appropriate. Gas chromatography-mass spectrometry (GC/MS) was performed using Agilent 5975C Triple Axis GCMS (EI/CI). High Resolution Mass spectra were obtained from the EPSRC mass spectrometry service at the University of Swansea or from the analytical service at Syngenta, Jealott's Hill International Research Centre, UK. The data is recorded as the method followed by the calculated and measured masses. TLC was performed on Merck 60F$_{254}$ silica plates and visualised by UV light and potassium permanganate stains. The compounds were purified by flash chromatography using Aldrich silica gel (particle size 40-63 μm) under a positive pressure. The eluent is quoted as a percentage. Anhydrous DMSO used for the trifluoromethylation reaction was bought from Sigma-Aldrich and used as received. All other chemicals were purchased from a chemical supplier and used as received.

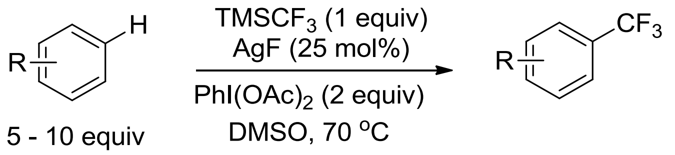
Trifluoromethylation of electron-rich (hetero)arenes:



Scheme S1. Trifluoromethylation of electron rich (hetero)arenes.

General procedure A: An oven-dried reaction vial (5 mL) was charged with (hetero)arene **1** (0.3 mmol), (diacetoxyiodo)benzene (193.3 mg, 0.6 mmol), trimethyl(trifluoromethyl)silane (88.7 µL, 0.6 mmol) and anhydrous DMSO (1 mL). The mixture was stirred at room temperature for 1 min and AgF (9.5 mg, 0.075 mmol) was slowly added to the stirring mixture. The vial was sealed with a septum cap and the reaction was kept stirring at the same temperature for 20 h. The resulting mixture was quenched with water (5 mL) and extracted with Et_2O (3 × 5 mL). The combined organic layers were dried over $MgSO_4$, filtered and concentrated under reduced pressure. The crude material was purified by column chromatography (SiO_2, using the noted solvent mixture) to yield the desired trifluoromethylated product **2**. For volatile compounds, 4-fluoroanisole (3 equiv) was added as an internal standard to the crude, and the reaction was analysed by ^{19}F NMR spectroscopy in $CDCl_3$. The identity of the products was further confirmed by ^{1}H NMR of the crude mixture (and GC/MS analysis for unknown compounds).

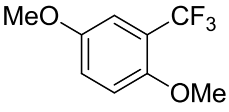
Trifluoromethylation of unactivated arenes (1p, 1q and 1r):



Scheme S2. Trifluoromethylation of unactivated arenes.

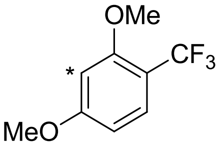
General procedure B: An oven-dried reaction vial (5 mL) was charged with trimethyl(trifluoromethyl)silane (73.9 µL, 0.5 mmol), arene (2.5 mmol (**1r**) or 5.0 mmol (**1p** and **1q**)), (diacetoxyiodo)benzene (322.1 mg, 1.0 mmol), AgF (15.9 mg, 0.125 mmol) and anhydrous DMSO (0.5 mL). The vial was sealed with a septum cap and the reaction was heated at 70 °C for 20 h. The resulting mixture was quenched with water (5 mL) and extracted with Et_2O (3 × 5 mL). The combined organic layers were dried over $MgSO_4$, filtered and concentrated under reduced pressure. 4-Fluoroanisole (3 equiv) was added as an internal standard to the crude, and the reaction was analysed by ^{19}F NMR spectroscopy in $CDCl_3$.

1,4-Dimethoxy-2-(trifluoromethyl)benzene (2a)[1]



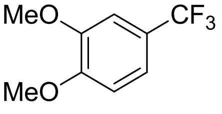
Prepared following general procedure A using 1,4-dimethoxybenzene (41.4 mg, 0.3 mmol). The reaction mixture was purified by flash chromatography using 20% DCM in pentane to afford **2a** as a colourless oil (Yield = 58%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.12 (d, J = 3.1 Hz, 1H), 7.02 (dd, J = 9.1, 3.0 Hz, 1H), 6.94 (d, J = 9.0 Hz, 1H), 3.86 (s, 3H), 3.79 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 152.9 (C), 151.5 (C), 123.4 (q, J_{C-F} = 272.4 Hz, CF_3), 119.4 (q, J_{C-F} = 31.1 Hz, C), 118.1 (CH), 113.5 (CH), 112.8 (q, J_{C-F} = 5.5 Hz, CH), 56.5 (CH_3), 55.9 (CH_3); ^{19}F NMR (376 MHz, $CDCl_3$): δ -62.4 (s, CF_3).

1,3-Dimethoxy-4-(trifluoromethyl)benzene 2b[1] and 1,3-dimethoxy-2-(trifluoromethyl)benzene (2b*)[1]



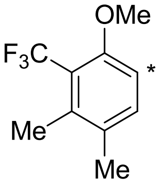
Prepared following general procedure A using 1,3-dimethoxybenzene (41.4 mg (39.3 µL), 0.3 mmol). The reaction mixture was purified by flash chromatography using 20% DCM in pentane to afford **2b** as a mixture of isomers as a colourless oil (Yield = 77%, **1b**:**1b*** = 2:1). **1,3-Dimethoxy-4-(trifluoromethyl)benzene:** ^{1}H NMR (400 MHz, CDCl$_3$): δ 7.47 (d, J = 8.6 Hz, 1H), 6.52 (s, 1H), 6.48 (d, J = 8.6 Hz, 1H), 3.87 (s, 3H), 3.84 (s, 3H); ^{13}C NMR (100 MHz, CDCl$_3$): δ 163.6 (C), 158.8 (C), 128.2 (q, J_{C-F} = 5.4 Hz, CH), 124.0 (q, J_{C-F} = 271.2 Hz, CF$_3$), 111.6 (q, J_{C-F} = 31.3 Hz, C), 103.7 (CH), 99.3 (CH), 55.8 (CH$_3$), 55.5 (CH$_3$); ^{19}F NMR (376 MHz, CDCl$_3$): δ -61.3 (s, CF$_3$); **1,3-Dimethoxy-2-(trifluoromethyl)benzene:** ^{1}H NMR (400 MHz, CDCl$_3$): δ 7.38 (t, J = 8.4 Hz, 1H), 6.61 (d, J = 8.5 Hz, 2H), 3.86 (s, 6H); ^{13}C NMR (100 MHz, CDCl$_3$): δ 159.3 (C), 133.0 (CH), 124.1 (q, J_{C-F} = 274.5 Hz, CF$_3$), 107.1 (q, J_{C-F} = 29.5 Hz, C), 104.8 (CH), 56.3 (CH$_3$); ^{19}F NMR (376 MHz, CDCl$_3$): δ -54.9 (s, CF$_3$).

1,2-dimethoxy-4-(trifluoromethyl)benzene (2c)[1]



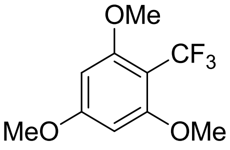
Prepared following general procedure A using 1,2-dimethoxybenzene (41.4 mg (38.2 µL), 0.3 mmol). The reaction mixture was purified by flash chromatography using 30% DCM in pentane to afford **2c** as a colourless oil (Yield = 55%). ^{1}H NMR (400 MHz, CDCl$_3$): δ 7.21 (ddd, J = 8.4, 2.0, 0.8 Hz, 1H), 7.07 (d, J = 2.0 Hz, 1H), 6.91 (d, J = 8.4 Hz, 1H), 3.92 (s, 3H), 3.91 (s, 3H); ^{13}C NMR (100 MHz, CDCl$_3$): δ 151.6 (C), 149.0 (C), 124.3 (q, J_{C-F} = 271.3 Hz, CF$_3$), 122.9 (q, J_{C-F} = 32.7 Hz, C), 118.3 (q, J_{C-F} = 4.2 Hz, CH), 110.6 (CH), 108.0 (q, J_{C-F} = 3.4 Hz, CH), 56.0 (CH$_3$); ^{19}F NMR (376 MHz, CDCl$_3$): δ -61.5 (s, CF$_3$).

3,4-Dimethyl-2-(trifluoromethyl)anisole (2d) and 3,4-dimethyl-6-(trifluoromethyl)anisole (2d*)



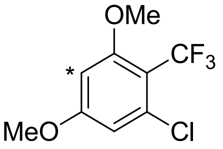
Prepared following general procedure A using 3,4-dimethylanisole (40.9 mg (41.9 µL), 0.3 mmol). The reaction mixture was purified by flash chromatography using 100% pentane to afford **2d** and **2d*** as colourless oils (Yield = 45%, **2d**:**2d*** = 1:1). **3,4-Dimethyl-2-(trifluoromethyl)anisole:** ^{1}H NMR (400 MHz, CDCl$_3$): δ 7.23 (d, J = 8.5 Hz, 1H), 6.77 (d, J = 8.5, Hz, 1H), 3.84 (s, 3H), 2.36 (q, J_{H-F} = 2.9 Hz, 3H), 2.26 (s, 3H); ^{13}C NMR (100 MHz, CDCl$_3$): δ 156.8 (C), 137.3 (q, J_{C-F} = 1.5 Hz, C), 133.5 (CH), 130.0 (C), 125.2 (q, J_{C-F} = 275.9 Hz, CF$_3$), 117.7 (q, J_{C-F} = 28.1 Hz, C), 110.0 (CH), 56.3 (CH$_3$), 20.3 (CH$_3$), 16.7 (q, J_{C-F} = 4.6 Hz, CH$_3$); ^{19}F NMR (376 MHz, CDCl$_3$): δ -53.5 (s, CF$_3$); HRMS (ES$^+$) cald. for (M+H)$^+$ $C_{10}H_{12}O_1F_3$: 205.0835, found: 205.0835; **3,4-Dimethyl-6-(trifluoromethyl)anisole:** ^{1}H NMR (400 MHz, CDCl$_3$): δ 7.30 (s, 1H), 6.79 (s, 1H), 3.87 (s, 3H), 2.30 (s, 3H), 2.22 (s, 3H); ^{13}C NMR (100 MHz, CDCl$_3$): δ 155.4 (C), 142.1 (C), 128.0 (C), 127.8 (q, J_{C-F} = 5.1 Hz, CH), 123.9 (q, J_{C-F} = 271.8 Hz, CF$_3$), 115.9 (q, J_{C-F} = 30.5 Hz, C), 113.6 (CH), 56.0 (CH$_3$), 20.3 (CH$_3$), 18.7 (CH$_3$); ^{19}F NMR (376 MHz, CDCl$_3$): δ -61.7 (s, CF$_3$); HRMS (ES$^+$) cald. for (M+H)$^+$ $C_{10}H_{12}O_1F_3$: 205.0835, found: 205.0835.

1,3,5-Trimethoxy-4-(trifluoromethyl)benzene (2e)



Prepared following general procedure A using 1,3,5-trimethoxybenzene (50.5 mg, 0.3 mmol). The reaction mixture was purified by flash chromatography using 20% Et$_2$O in pentane to afford **2e** as a white solid (Yield = 89%). Mp = 52 – 54 °C; ^{1}H NMR (400 MHz, CDCl$_3$): δ 6.13 (s, 2H), 3.84 (s, 9H); ^{13}C NMR (100 MHz, CDCl$_3$): δ 163.5 (C), 160.4 (C), 124.3 (q, J_{C-F} = 273.4 Hz, CF$_3$), 100.3 (q, J_{C-F} = 30.0 Hz, C), 91.2 (CH), 56.2 (CH$_3$), 55.3 (CH$_3$); ^{19}F NMR (376 MHz, CDCl$_3$): δ -54.1 (s, CF$_3$); HRMS (ES$^+$) cald. for (M+H)$^+$ $C_{10}H_{12}O_3F_3$: 237.0733, found: 237.0736.

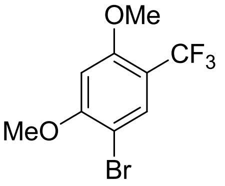
1-Chloro-3,5-dimethoxy-2-(trifluoromethyl)benzene (2f) and 1-chloro-3,5-dimethoxy-4-(trifluoromethyl)benzene (2f*)



Prepared following general procedure A using 1-chloro-3,5-dimethoxybenzene (51.8 mg, 0.3 mmol). The reaction mixture was purified by flash chromatography using 10% DCM in pentane to afford **2f (major)** as a colourless oil and **2f*** as a white solid (Yield = 83%, **2f**:**2f*** = 2:1). **1-Chloro-3,5-dimethoxy-2-(trifluoromethyl)benzene:** ^{1}H NMR (400 MHz, CDCl$_3$): δ 6.57 (d, J = 2.4 Hz, 1H), 6.41 (d, J = 2.0, Hz, 1H), 3.85 (s, 3H), 3.82 (s, 3H); ^{13}C NMR (100 MHz, CDCl$_3$): δ 162.3 (C), 160.5 (C), 134.8 (q, J_{C-F} = 1.8 Hz, C), 123.5 (q, J_{C-F} = 273.9 Hz, CF$_3$), 109.8 (q, J_{C-F} = 30.5 Hz, C), 108.2 (CH), 98.4 (CH), 56.4 (CH$_3$), 55.6 (CH$_3$); ^{19}F NMR

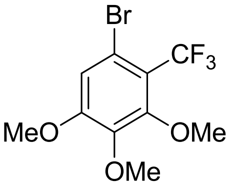
(376 MHz, $CDCl_3$): δ -54.5 (s, CF_3); HRMS (ES^+) cald. for $(M+H)^+$ $C_9H_9O_2Cl_1F_3$: 241.0238, found: 241.0242; **1-Chloro-3,5-dimethoxy-4-(trifluoromethyl)benzene:** Mp = 70 – 72 °C; ^1H NMR (400 MHz, $CDCl_3$): δ 6.61 (s, 2H), 3.85 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 159.6 (C), 139.1 (C), 123.7 (q, $J_{C\text{-}F}$ = 274.7 Hz, CF_3), 105.8 (q, $J_{C\text{-}F}$ = 30.0 Hz, C), 105.6 (CH), 56.5 (CH_3); ^{19}F NMR (376 MHz, $CDCl_3$): δ -55.1 (s, CF_3); HRMS (ES^+) cald. for $(M+H)^+$ $C_9H_9O_2Cl_1F_3$: 241.0238, found: 241.0242.

1-Bromo-2,4-dimethoxy-5-(trifluoromethyl)benzene (2g)



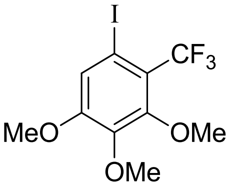
Prepared following general procedure A using 1-bromo-2,4-dimethoxybenzene (65.1 mg, 0.3 mmol). The reaction mixture was purified by flash chromatography using 50% Et_2O in iso-hexane to afford **2g** as a white solid (Yield = 40%). Mp = 130 – 133 °C; ^1H NMR (400 MHz, $CDCl_3$): δ 7.69 (s, 1H), 6.51 (s, 1H), 3.94 (s, 3H), 3.91 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 159.4 (C), 158.3 (q, $J_{C\text{-}F}$ = 2.3 Hz, C), 131.3 (q, $J_{C\text{-}F}$ = 5.4 Hz, CH), 123.0 (q, $J_{C\text{-}F}$ = 271.5 Hz, CF_3), 112.2 (q, $J_{C\text{-}F}$ = 32.0 Hz, C), 101.1 (C), 96.7 (CH), 56.4 (CH_3), 56.2 (CH_3); ^{19}F NMR (376 MHz, $CDCl_3$): δ -61.5 (s, CF_3). HRMS (ES^+) cald. for $(M+H)^+$ $C_9H_9O_2Br_1F_3$: 284.9733, found: 284.9741.

1-Bromo-3,4,5-trimethoxy-2-(trifluoromethyl)benzene (2h)



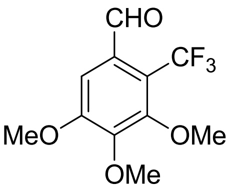
Prepared following general procedure A using 1-bromo-3,4,5-trimethoxybenzene (74.1 mg, 0.3 mmol). The reaction mixture was purified by flash chromatography using 40% DCM in pentane to afford **2h** as a yellow oil (Yield = 55%). ^1H NMR (400 MHz, $CDCl_3$): δ 6.98 (s, 1H), 3.91 (s, 3H), 3.89 (s, 3H), 3.86 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 155.8 (C), 154.3 (C), 142.6 (C), 122.9 (q, $J_{C\text{-}F}$ = 274.6 Hz, CF_3), 116.9 (q, $J_{C\text{-}F}$ = 29.8 Hz, C), 114.2 (CH), 114.1 (q, $J_{C\text{-}F}$ = 2.1 Hz, C), 62.1 (CH_3), 60.8 (CH_3), 56.2 (CH_3); ^{19}F NMR (376 MHz, $CDCl_3$): δ -55.5 (s, CF_3); HRMS (ES^+) cald. for $(M+H)^+$ $C_{10}H_{11}O_3Br_1F_3$: 314.9838, found: 314.9837.

1-Iodo-3,4,5-trimethoxy-2-(trifluoromethyl)benzene (2i)



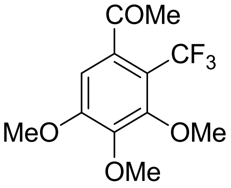
Prepared following general procedure A using 1-iodo-3,4,5-trimethoxybenzene (88.2 mg, 0.3 mmol). The reaction mixture was purified by flash chromatography using 40% DCM in pentane to afford **2i** (as a mixture with a small amount of an inseparable impurity) as a yellow oil (Yield = 51%). ^1H NMR (400 MHz, $CDCl_3$): δ 7.31 (s, 1H), 3.90 (s, 3H), 3.89 (s, 3H), 3.86 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 155.8 (C), 154.2 (C), 143.5 (C), 122.1 (q, $J_{C\text{-}F}$ = 275.0 Hz, CF_3), 121.5 (CH), 120.3 (q, $J_{C\text{-}F}$ = 29.8 Hz, C), 82.7 (q, $J_{C\text{-}F}$ = 2.5 Hz, C), 62.1 (CH_3), 60.8 (CH_3), 56.3 (CH_3); ^{19}F NMR (376 MHz, $CDCl_3$): δ -55.7 (s, CF_3); HRMS (ES^+) cald. for $(M+H)^+$ $C_{10}H_{11}O_3F_3I_1$: 362.9699, found: 362.9698.

2-(Trifluoromethyl)-3,4,5-trimethoxybenzaldehyde (2j)



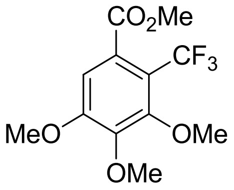
Prepared following general procedure A using 3,4,5-trimethoxybenzaldehyde (58.9 mg, 0.3 mmol). The reaction mixture was purified by flash chromatography using 40% DCM in pentane to afford **2j** as a yellow oil (Yield = 63%). ^1H NMR (400 MHz, $CDCl_3$): δ 10.32 (q, $J_{H\text{-}F}$ = 2.4 Hz, 1H), 7.34 (s, 1H), 3.95 (s, 6H), 3.93 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 189.2 (q, $J_{C\text{-}F}$ = 6.0 Hz, CO), 155.8 (C), 152.8 (q, $J_{C\text{-}F}$ = 2.5 Hz, C), 147.3 (C), 130.8 (C), 124.1 (q, $J_{C\text{-}F}$ = 275.1 Hz, CF_3), 117.9 (q, $J_{C\text{-}F}$ = 31.2 Hz, C), 107.2 (CH), 62.0 (CH_3), 61.0 (CH_3), 56.2 (CH_3); ^{19}F NMR (376 MHz, $CDCl_3$): δ -51.1 (s, CF_3); HRMS (ES^+) cald. for $(M+H)^+$ $C_{11}H_{12}O_4F_3$: 265.0682, found: 265.0682.

2’-(Trifluoromethyl)-3’,4’,5’-trimethoxyacetophenone (2k)



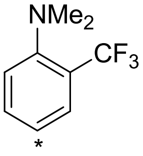
Prepared following general procedure A using 3’,4’,5’-trimethoxyacetophenone (63.1 mg, 0.3 mmol). The reaction mixture was purified by flash chromatography using 100% DCM to afford **2k** as a yellow oil (Yield = 61%). ^1H NMR (400 MHz, $CDCl_3$): δ 6.47 (s, 1H), 3.93 (s, 3H), 3.88 (s, 3H), 3.87 (s, 3H), 2.45 (q, $J_{H\text{-}F}$ = 1.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 202.4 (CO), 156.2 (C), 152.7 (q, $J_{C\text{-}F}$ = 1.9 Hz, C), 143.4 (C), 137.6 (q, $J_{C\text{-}F}$ = 2.6 Hz, C), 123.4 (q, $J_{C\text{-}F}$ = 273.1 Hz, CF_3), 112.8 (q, $J_{C\text{-}F}$ = 31.0 Hz, C), 104.4 (CH), 61.7 (CH_3), 60.8 (CH_3), 56.2 (CH_3), 31.3 (q, $J_{C\text{-}F}$ = 3.1 Hz, CH_3); ^{19}F NMR (376 MHz, $CDCl_3$): δ -55.0 (s, CF_3); HRMS (ES^+) cald. for $(M+H)^+$ $C_{12}H_{14}O_4F_3$: 279.0839, found: 279.0839.

Methyl 2-(trifluoromethyl)-3,4,5-trimethoxybenzoate (2l)



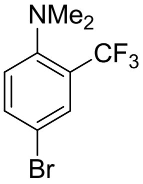
Prepared following general procedure A using methyl 3,4,5-trimethoxybenzoate (67.9 mg, 0.3 mmol). The reaction mixture was purified by flash chromatography using 100% DCM to afford **2l** as a yellow oil (Yield = 54%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 6.74 (s, 1H), 3.93 (s, 3H), 3.89 (s, 3H), 3.87 (s, 3H), 3.86 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 168.4 (CO), 155.9 (C), 152.9 (q, $J_{C\text{-}F}$ = 1.7 Hz, C), 144.1 (C), 128.4 (q, $J_{C\text{-}F}$ = 2.9 Hz, C), 123.0 (q, $J_{C\text{-}F}$ = 273.0 Hz, CF_3), 114.5 (q, $J_{C\text{-}F}$ = 30.9 Hz, C), 106.8 (CH), 61.8 (CH_3), 60.8 (CH_3), 56.2 (CH_3), 52.9 (CH_3); ^{19}F NMR (376 MHz, $CDCl_3$): δ -56.9 (s, CF_3); HRMS (ES^+) cald. for (M) $C_{12}H_{13}O_5F_3$: 294.0710, found: 294.0709.

N,N-Dimethyl-2-(trifluoromethyl)aniline (2m) and *N,N*-Dimethyl-4-(trifluoromethyl)aniline (2m*)[2]



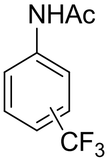
Prepared following general procedure A using *N,N*-dimethylaniline (53.2 mg (58.4 µL), 0.3 mmol). The reaction mixture was purified by flash chromatography using 100% pentane to afford a mixture of **2m** and **2m*** as a colourless oil (Yield = 75%, **2l**:**2l*** = 2:1). ***N,N*-Dimethyl-2-(trifluoromethyl)aniline (2m):** ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.62 (dd, J = 7.9, 1.5 Hz, 1H), 7.51 (t, J = 7.7 Hz, 1H), 7.36 (d, J = 8.1 Hz, 1H), 7.17 (t, J = 7.6 Hz, 1H), 2.76 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 153.8 (C), 132.6 (CH), 127.3 (q, $J_{C\text{-}F}$ = 5.5 Hz, CH), 125.6 (q, $J_{C\text{-}F}$ = 28.9 Hz, C), 123.6 (CH), 124.2 (q, $J_{C\text{-}F}$ = 273.0 Hz, CF_3), 122.7 (CH), 45.8 (CH_3); ^{19}F NMR (376 MHz, $CDCl_3$): δ -60.1 (s, CF_3); ***N,N*-Dimethyl-4-(trifluoromethyl)aniline (2m*):** ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.47 (d, J = 8.6 Hz, 2H), 6.71 (d, J = 8.8 Hz, 2H), 3.02 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 152.3 (C), 126.3 (q, $J_{C\text{-}F}$ = 3.8 Hz, CH), 125.2 (q, $J_{C\text{-}F}$ = 270.2 Hz, CF_3), 117.4 (q, $J_{C\text{-}F}$ = 32.8 Hz, C), 111.1 (CH), 40.0 (CH_3); ^{19}F NMR (376 MHz, $CDCl_3$): δ -60.8 (s, CF_3).

4-Bromo-*N,N*-dimethyl-2-(trifluoromethyl)aniline (2n)



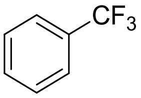
Prepared following general procedure A using 4-bromo-*N,N*-dimethylaniline (60.0 mg, 0.3 mmol). The reaction mixture was purified by flash chromatography using 100% pentane to afford **2n** (as a mixture with a small amount of an inseparable impurity) as a yellow oil (Yield = 64%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.72 (d, J = 2.4 Hz, 1H), 7.58 (dd, J = 8.8, 2.4 Hz, 1H), 7.19 (d, J = 8.8 Hz, 1H), 2.72 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 152.7 (C), 135.5 (CH), 130.5 (q, $J_{C\text{-}F}$ = 5.8 Hz, CH), 127.1 (q, $J_{C\text{-}F}$ = 29.7 Hz, C), 124.4 (CH), 123.2 (q, $J_{C\text{-}F}$ = 273.6 Hz, CF_3), 116.0 (C), 45.5 (CH_3); ^{19}F NMR (376 MHz, $CDCl_3$): δ -60.3 (s, CF_3); HRMS (ES^+) cald. for $(M+H)^+$ $C_9H_{10}N_1Br_1F_3$: 267.9943, found: 267.9942.

2-(Trifluoromethyl)acetanilide (2o^o), 3-(trifluoromethyl)acetanilide (2o^m)[3] and 4-(trifluoromethyl)acetanilide (2o^p)[4]



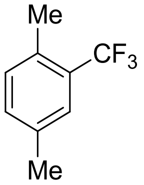
Prepared following general procedure A using acetanilide (40.6 mg, 0.3 mmol). The reaction mixture was purified by flash chromatography using 10% Et_2O in pentane to afford **2o^o** and an inseparable mixture of **2o^m** and **2o^p**, each as off-white solids (Yield = 48%, ***o*:*m*:*p*** = 3:1:4.3). **2-(Trifluoromethyl)acetanilide:** Mp = 72 – 74 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.15 (d, J = 7.9 Hz, 1H), 7.60 (d, J = 7.8 Hz, 1H), 7.55 (t, J = 7.8 Hz, 1H), 7.42 (bs, NH), 7.23 (t, J = 7.5 Hz, 1H), 2.22 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 168.4 (CO), 135.2 (C), 132.8 (CH), 126.0 (q, $J_{C\text{-}F}$ = 3.5 Hz, CH), 124.7 (CH), 124.5 (CH), 24.6 (CH_3); ^{19}F NMR (376 MHz, $CDCl_3$): δ -60.6 (s, CF_3); HRMS (ES^+) cald. for $(M+H)^+$ $C_9H_9O_1N_1F_3$: 204.0631, found: 204.0632. **3-(Trifluoromethyl)acetanilide:** ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.79 (s, 1H), 7.71 (d, J = 8.7 Hz, 1H), 7.63 (bs, NH), 7.42 (t, J = 7.9, 1H), 7.35 (t, J = 7.7 Hz, 1H), 2.20 (s, 3H); ^{19}F NMR (376 MHz, $CDCl_3$): δ -62.8 (s, CF_3). **4-(Trifluoromethyl)acetanilide:** ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.63 (d, J = 8.5 Hz, 2H), 7.63 (bs, NH), 7.55 (d, J = 8.6 Hz, 2H), 2.20 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 168.7 (CO), 140.9 (C), 126.2 (q, $J_{C\text{-}F}$ = 3.7 Hz, CH), 125.9 (C), 124.1 (q, $J_{C\text{-}F}$ = 271.4 Hz, CF_3), 119.3 (CH), 24.7 (CH_3); ^{19}F NMR (376 MHz, $CDCl_3$): δ -62.1 (s, CF_3).

1,1,1-Trifluorotoluene (2p)



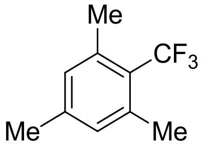
Prepared following general procedure B using benzene (390.6 mg (447 µL), 5.0 mmol). The reaction mixture was analysed directly by ^{19}F NMR (Yield = 60%). ^{19}F NMR (376 MHz, $CDCl_3$): δ -62.8 (s, CF_3).

1,4-Dimethyl-2-(trifluoromethyl)benzene (2q)



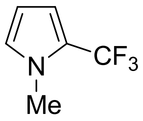
Prepared following general procedure B using p-xylene (530.9 mg (617 μL), 5.0 mmol). The reaction mixture was analysed directly by ^{19}F NMR (Yield = 67%). ^{19}F NMR (376 MHz, $CDCl_3$): δ -61.8 (s, CF_3).

1,3,5-Trimethyl-2-(trifluoromethyl)benzene (2r)



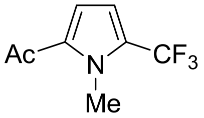
Prepared following general procedure B using mesitylene (300.5 mg (348 μL), 2.5 mmol). The reaction mixture was analysed directly by ^{19}F NMR (Yield = 71%). ^{19}F NMR (376 MHz, $CDCl_3$): δ -53.8 (s, CF_3).

N-Methyl-2-(trifluoromethyl)pyrrole (2s)[5]



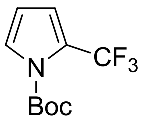
Prepared following general procedure A using *N*-methylpyrrole (24.3 mg (26.6 μL), 0.3 mmol). The reaction mixture was analysed directly by ^{1}H and ^{19}F NMR (Yield = 94%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 6.70 (t, J = 2.1 Hz, 1H), 6.56 – 6.54 (m, 1H), 6.10 (t, J = 3.2 Hz, 1H), 3.72 (s, 3H); ^{19}F NMR (376 MHz, $CDCl_3$): δ -58.8 (s, CF_3).

2-Acetyl-*N*-methyl-5-(trifluoromethyl)pyrrole (2t)[6]



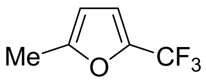
Prepared following general procedure A using *N*-methyl-2-acetylpyrrole (36.9 mg (35.5 μL), 0.3 mmol). The reaction mixture was analysed directly by ^{1}H and ^{19}F NMR (Yield = 93%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 6.88 (d, J = 4.3 Hz, 1H), 6.54 (d, J = 4.3 Hz, 1H), 4.00 (s, 3H), 2.47 (s, 3H); ^{19}F NMR (376 MHz, $CDCl_3$): δ -59.8 (s, CF_3).

N-Boc-2-(trifluoromethyl)pyrrole (2u)[5]



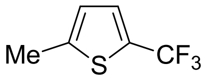
Prepared following general procedure A using *N*-Boc-pyrrole (50.2 mg (50.2 μL), 0.3 mmol). The reaction mixture was analysed directly by ^{1}H and ^{19}F NMR (Yield = 50%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.44 (dd, J = 3.3, 1.9 Hz, 1H), 6.74 – 6.72 (m, 1H), 6.19 (t, J = 3.4 Hz, 1H), 1.61 (s, 9H); ^{19}F NMR (376 MHz, $CDCl_3$): δ -58.3 (s, CF_3).

2-Methyl-5-(trifluoromethyl)furan (2v)[5]



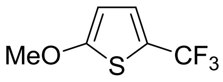
Prepared following general procedure A using 2-methylfuran (24.6 mg (27.1 μL), 0.3 mmol). The reaction mixture was analysed directly by ^{1}H and ^{19}F NMR (Yield = 51%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 6.64 (d, J = 1.8 Hz, 1H), 6.03 (d, J = 3.3 Hz, 1H), 2.32 (s, 3H); ^{19}F NMR (376 MHz, $CDCl_3$): δ -63.9 (s, CF_3).

2-Methyl-5-(trifluoromethyl)thiophene (2w)[5]



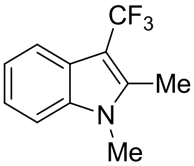
Prepared following general procedure A using 2-methylthiophene (29.5 mg (29.0 μL), 0.3 mmol). The reaction mixture was analysed directly by ^{1}H and ^{19}F NMR (Yield = 42%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.20 (dd, J = 3.6, 1.1 Hz, 1H), 6.68 (m, 1H), 2.48 (s, 3H); ^{19}F NMR (376 MHz, $CDCl_3$): δ -55.1 (s, CF_3).

2-Methoxy-5-(trifluoromethyl)thiophene (2x)



Prepared following general procedure A using 2-methoxythiophene (34.3 mg (30.2 μL), 0.3 mmol). The reaction mixture was analysed directly by ^{1}H and ^{19}F NMR and the identity of the product was further confirmed by GC/MS (Yield = 76%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.06 – 7.04 (m, 1H), 6.11 (dd, J = 4.1, 0.7 Hz, 1H), 3.87 (s, 3H); ^{19}F NMR (376 MHz, $CDCl_3$): δ -55.3 (s, CF_3); GC/MS: M($C_6H_5OSF_3$) = 182.0, found = 182.0.

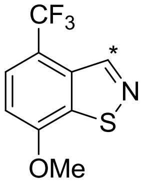
1,2-Dimethyl-3-(trifluoromethyl)indole (2v)[7]



Prepared following general procedure A using 1,2-dimethylindole (43.6 mg, 0.3 mmol). The reaction mixture was purified by flash chromatography using 10% DCM in pentane to afford **2v** as a yellow solid (Yield = 46%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.71 (d, J = 8.0 Hz, 1H), 7.27 – 7.16 (m, 3H), 3.62 (s, 3H), 2.50 (q, $J_{H\text{-}F}$ = 1.3 Hz, 3H); ^{13}C NMR (100

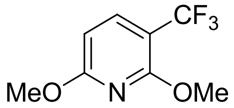
MHz, $CDCl_3$): δ 137.3 (C), 136.1 (C), 125.5 (q, $J_{C\text{-}F}$ = 266.7 Hz, CF_3), 124.4 (q, $J_{C\text{-}F}$ = 1.6 Hz, C), 121.9 (CH), 121.0 (CH), 119.0 (CH), 109.2 (CH), 102.5 (q, $J_{C\text{-}F}$ = 35.1 Hz, C), 29.4 (CH_3), 10.9 (CH_3); ^{19}F NMR (376 MHz, $CDCl_3$): δ -53.6 (s, CF_3).

7-Methoxy-4-(trifluoromethyl)-1,2-benzisothiazole (2z) and 7-methoxy-3-(trifluoromethyl)-1,2-benzisothiazole (2z*)



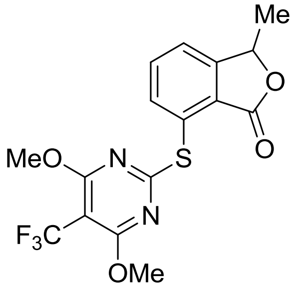
Prepared following general procedure A using 7-methoxy-1,2-benzisothiazole (49.5 mg, 0.3 mmol). The reaction mixture was purified by flash chromatography using 20% DCM in iso-hexane to afford a mixture of **2w** and **2w*** as a white solid (Yield = 41%, **2w**:**2w*** = 5:1). **7-Methoxy-4-(trifluoromethyl)-1,2-benzisothiazole (2w):** ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.04 (q, $J_{H\text{-}F}$ = 1.6 Hz, 1H), 7.68 (d, J = 8.0 Hz, 1H), 6.86 (d, J = 8.0 Hz, 1H), 4.06 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 155.4 (C), 152.9 (q, $J_{C\text{-}F}$ = 2.1 Hz, CH), 144.0 (C), 133.6 (q, $J_{C\text{-}F}$ = 1.3 Hz, C), 125.5 (q, $J_{C\text{-}F}$ = 5.1 Hz, CH), 124.1 (q, $J_{C\text{-}F}$ = 271.5 Hz, CF_3), 118.0 (q, $J_{C\text{-}F}$ = 34.1 Hz, C), 105.0 (CH), 56.2 (CH_3); ^{19}F NMR (376 MHz, $CDCl_3$): δ -59.9 (s, CF_3); **7-Methoxy-3-(trifluoromethyl)-1,2-benzisothiazole (2w*):** ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.73 (d, J = 8.2 Hz, 1H), 7.47 (t, J = 8.0 Hz, 1H), 6.93 (d, J = 7.7 Hz, 1H), 4.02 (s, 3H); ^{19}F NMR (376 MHz, $CDCl_3$): δ -63.6 (s, CF_3); HRMS (ES$^+$) cald. for $(M+H)^+$ $C_9H_7O_1N_1F_3S_1$: 234.0195, found: 234.0194.

2,6-dimethoxy-3-(trifluoromethyl)pyridine (2aa)



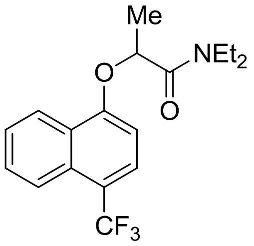
Prepared following general procedure A using 2,6-dimethoxypyridine (41.7 mg (39.6 μL), 0.3 mmol). The reaction mixture was purified by flash chromatography using 100% pentane to afford **2x** as a white solid (Yield = 72%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.71 (d, J = 8.3 Hz, 1H), 6.32 (d, J = 8.3 Hz, 1H), 4.02 (s, 3H), 3.96 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 165.1 (C), 160.4 (C), 138.8 (q, $J_{C\text{-}F}$ = 4.5 Hz, CH), 123.7 (q, $J_{C\text{-}F}$ = 270.1 Hz, CF_3), 104.3 (q, $J_{C\text{-}F}$ = 33.5 Hz, C), 100.8 (CH), 53.9 (CH_3), 53.8 (CH_3); ^{19}F NMR (376 MHz, $CDCl_3$): δ -61.9 (s, CF_3); HRMS (ES$^+$) cald. for $(M+H)^+$ $C_8H_9O_2N_1F_3$: 208.0580, found: 208.0582.

Pyriftalid-CF$_3$ (3)



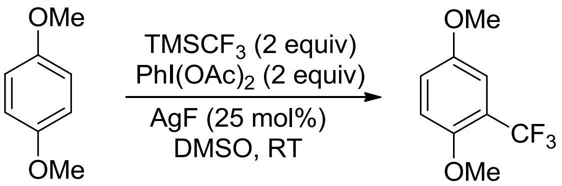
Prepared following general procedure A using (±)-pyriftalid (95.5 mg, 0.3 mmol). The reaction mixture was purified by flash chromatography using 70% DCM in iso-hexane to afford **3** as a white solid (Yield = 42%). Mp = 154 – 156 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.78 (d, J = 7.6 Hz, 1H), 7.70 (t, J = 7.6 Hz, 1H), 7.50 (d, J = 7.7 Hz, 1H), 5.53 (q, J = 6.7 Hz, 1H), 3.76 (s, 6H), 1.64 (d, J = 6.7 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 171.7 (C), 167.9 (C), 167.3 (C), 152.7 (C), 136.3 (CH), 133.9 (CH), 129.5 (C), 127.2 (C), 123.1 (q, $J_{C\text{-}F}$ = 272.4 Hz, CF_3), 122.6 (CH), 91.6 (q, $J_{C\text{-}F}$ = 34.3 Hz, C), 76.2 (CH), 54.8 (CH_3), 20.5 (CH_3); ^{19}F NMR (376 MHz, $CDCl_3$): δ -56.3 (s, CF_3). HRMS (ES$^+$) cald. for $(M+H)^+$ $C_{16}H_{14}O_4N_2F_3S_1$: 387.0621, found: 387.0620.

Napropamide-CF$_3$ (4)



Prepared following general procedure A using (±)-napropamide (81.4 mg, 0.3 mmol). The reaction mixture was purified by flash chromatography using 20% EtOAc in iso-hexane to afford **4** as a white solid (Yield = 51%). Mp = 77 – 81 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.41 (d, J = 9.0 Hz, 1H), 8.12 (d, J = 8.7 Hz, 1H), 7.74 (d, J = 8.2 Hz, 1H), 7.63 (ddd, J = 8.5, 6.8, 1.5 Hz, 1H), 7.56 (ddd, J = 8.2, 6.9, 1.2 Hz, 1H), 6.77 (d, J = 8.2 Hz, 1H), 5.17 (q, J = 6.7 Hz, 1H), 3.59 – 3.34 (m, 4H), 1.76 (d, J = 6.7 Hz, 3H), 1.12 (t, J = 7.1 Hz, 3H), 1.05 (t, J = 7.1 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 169.4 (CO), 156.2 (C), 130.2 (C), 128.1 (CH), 126.0 (CH), 125.9 (C), 125.5 (q, $J_{C\text{-}F}$ = 6.1 Hz, CH), 124.9 (q, $J_{C\text{-}F}$ = 272.3 Hz, CF_3), 124.0 (q, $J_{C\text{-}F}$ = 2.4 Hz, CH), 122.7 (CH), 118.9 (q, $J_{C\text{-}F}$ = 30.3 Hz, C), 103.3 (CH), 74.3 (CH), 41.1 (CH_2), 40.4 (CH_2), 17.9 (CH_3), 14.1 (CH_3), 12.6 (CH_3); ^{19}F NMR (376 MHz, $CDCl_3$): δ -59.1 (s, CF_3). HRMS (ES$^+$) cald. for $(M+H)^+$ $C_{18}H_{21}O_2N_1F_3$: 340.1519, found: 340.1518.

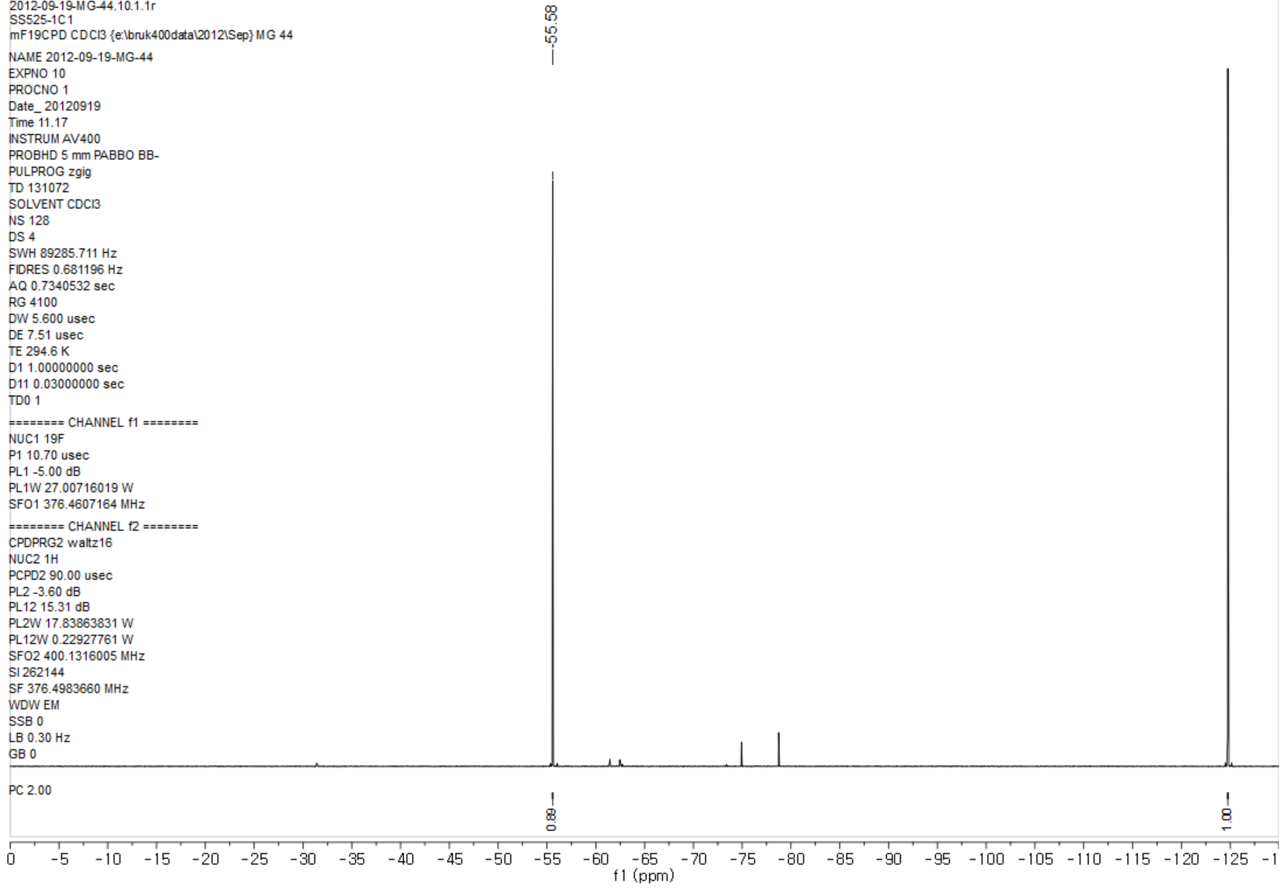
Trifluoromethylation in the presence of radical scavengers:



Additive	Yield (%)
TEMPO	<1
Galvinoxyl	<1

Scheme S3. Reaction with radical scavengers

To an oven-dried reaction vial (5 mL) charged with 1,4-dimethoxybenzene (41.4 mg, 0.3 mmol), (diacetoxyiodo)benzene (193.3 mg, 0.6 mmol), a radical scavenger (0.6 mmol) and trimethyl(trifluoromethyl)silane (88.7 µL, 0.6 mmol) in anhydrous DMSO (1 mL) was slowly added AgF (9.5 mg, 0.075 mmol). The vial was sealed with a septum cap and the reaction was stirred at room temperature for 20 h. The resulting mixture was quenched with water (5 mL) and extracted with Et_2O (3 × 5 mL). The combined organic layers were dried over $MgSO_4$, filtered and concentrated under reduced pressure. The crude material was analysed by ^{19}F NMR spectroscopy (4-fluoroanisole as the internal standard) in $CDCl_3$. With TEMPO, a characteristic TEMPO-CF_3 peak[8] was obtained at ^{19}F NMR: δ -55.6 (89% NMR yield). No trifluoromethylation product was formed with either TEMPO or galvinoxyl.



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PROCNO 1
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Time 11.17
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PULPROG zgig
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DS 4
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DE 7.51 usec
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D11 0.03000000 sec
TD0 1

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P1 10.70 usec
PL1 -5.00 dB
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SFO1 376.4607164 MHz

======== CHANNEL f2 ========
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PL12 15.31 dB
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PL12W 0.22927761 W
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SI 262144
SF 376.4983660 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0

PC 2.00
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II. References

1 Y. Ye, S. H. Lee and M. S. Sanford, *Org. Lett.*, 2011, **13**, 5464.

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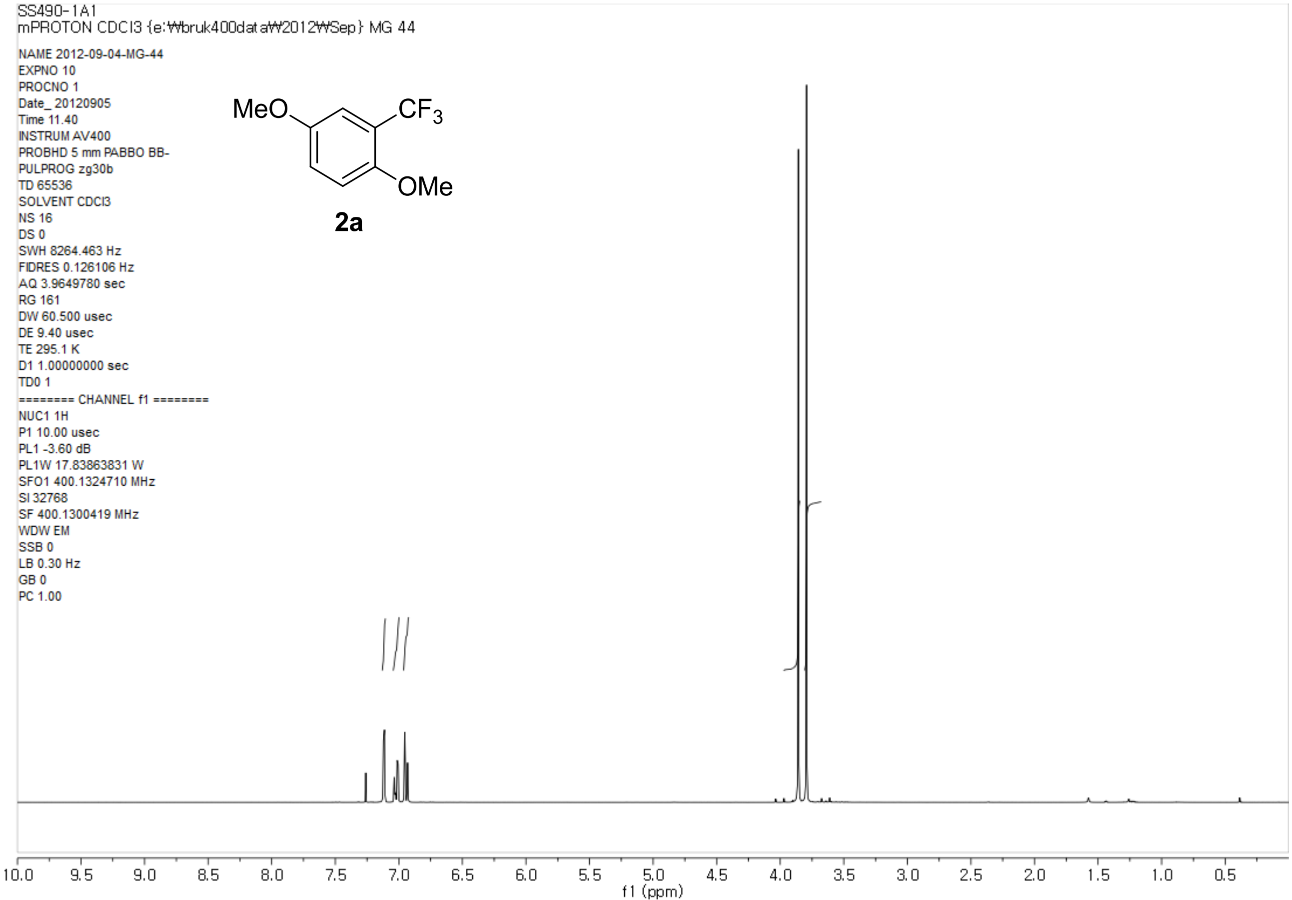
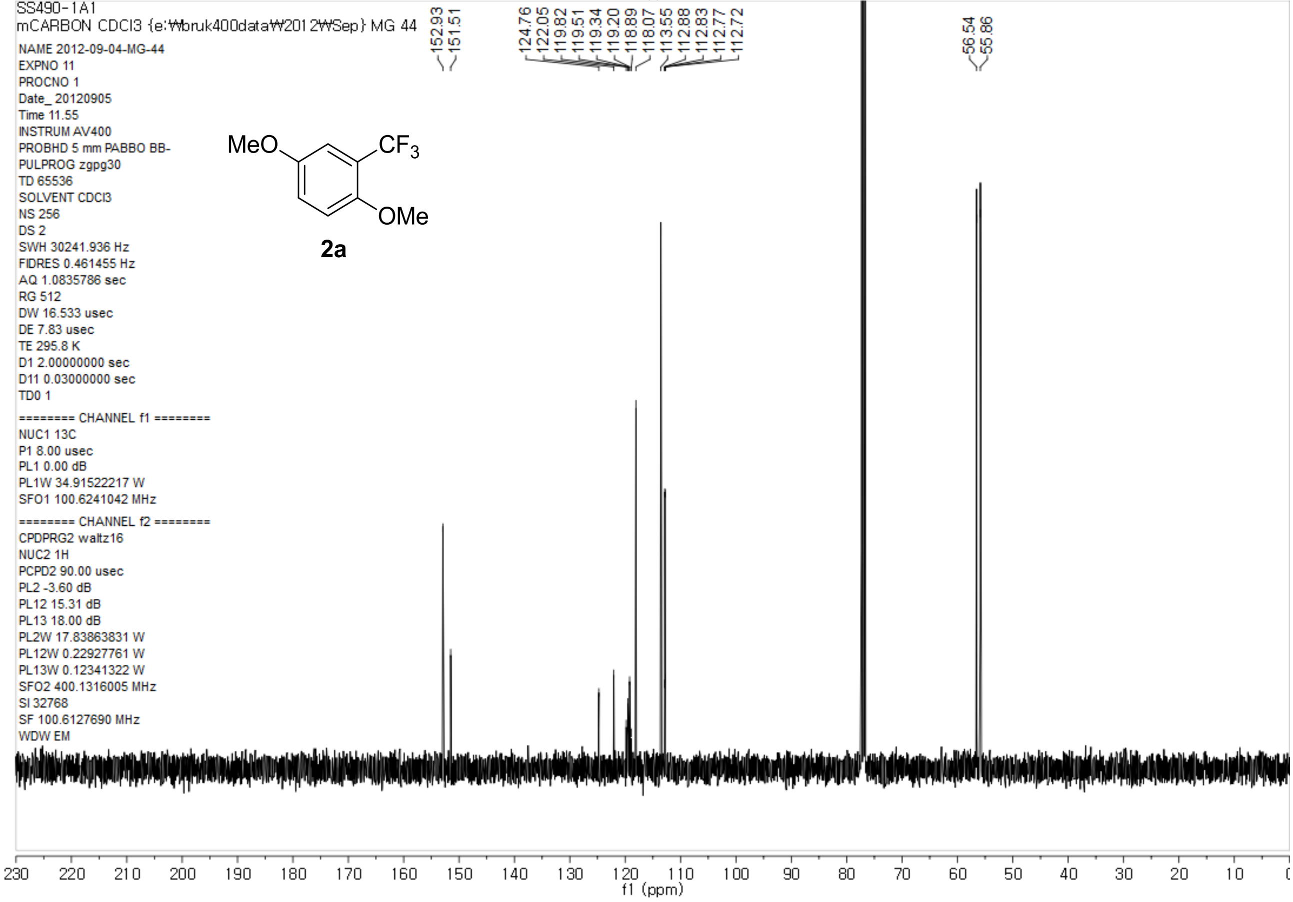
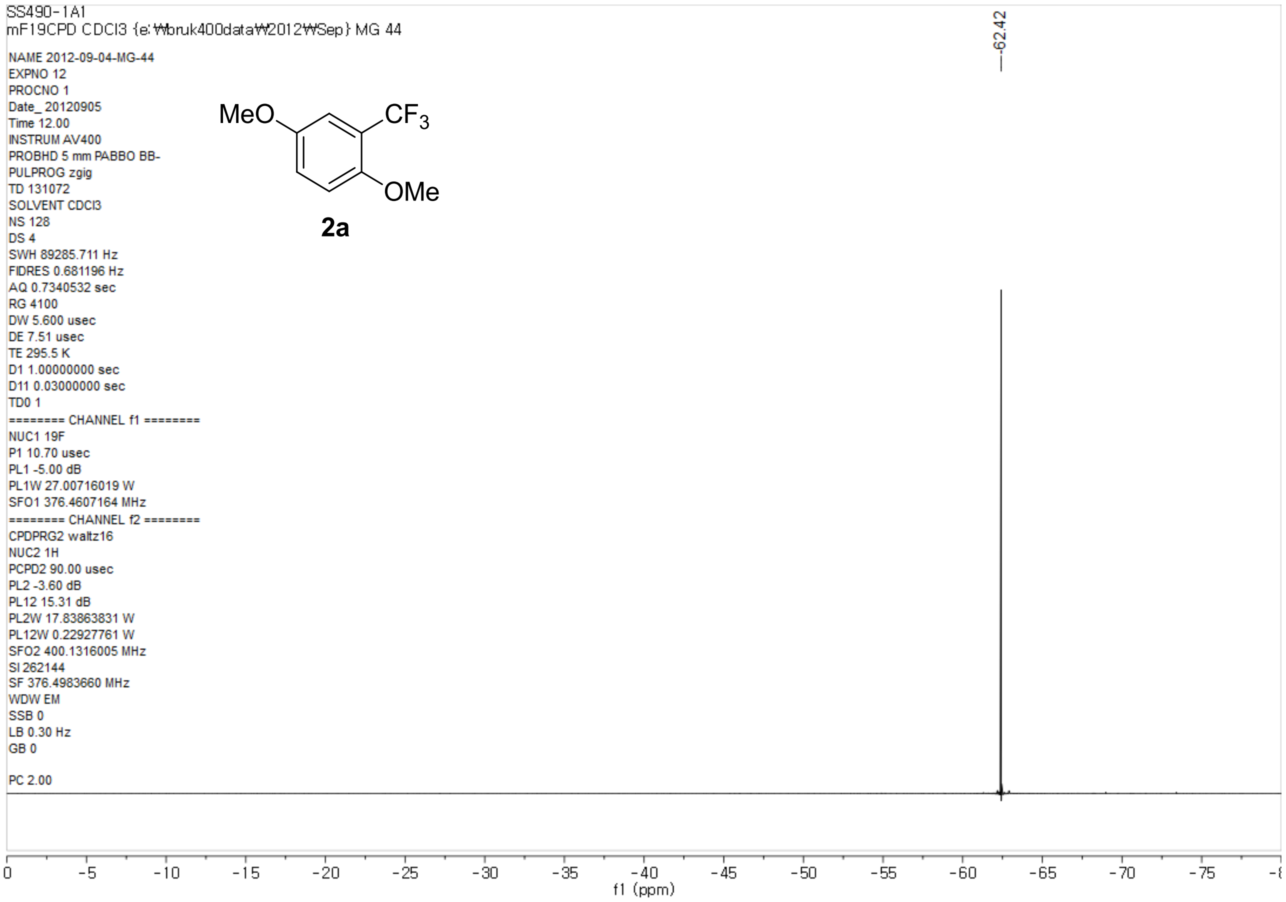
III. NMR Spectra of Isolated Compounds

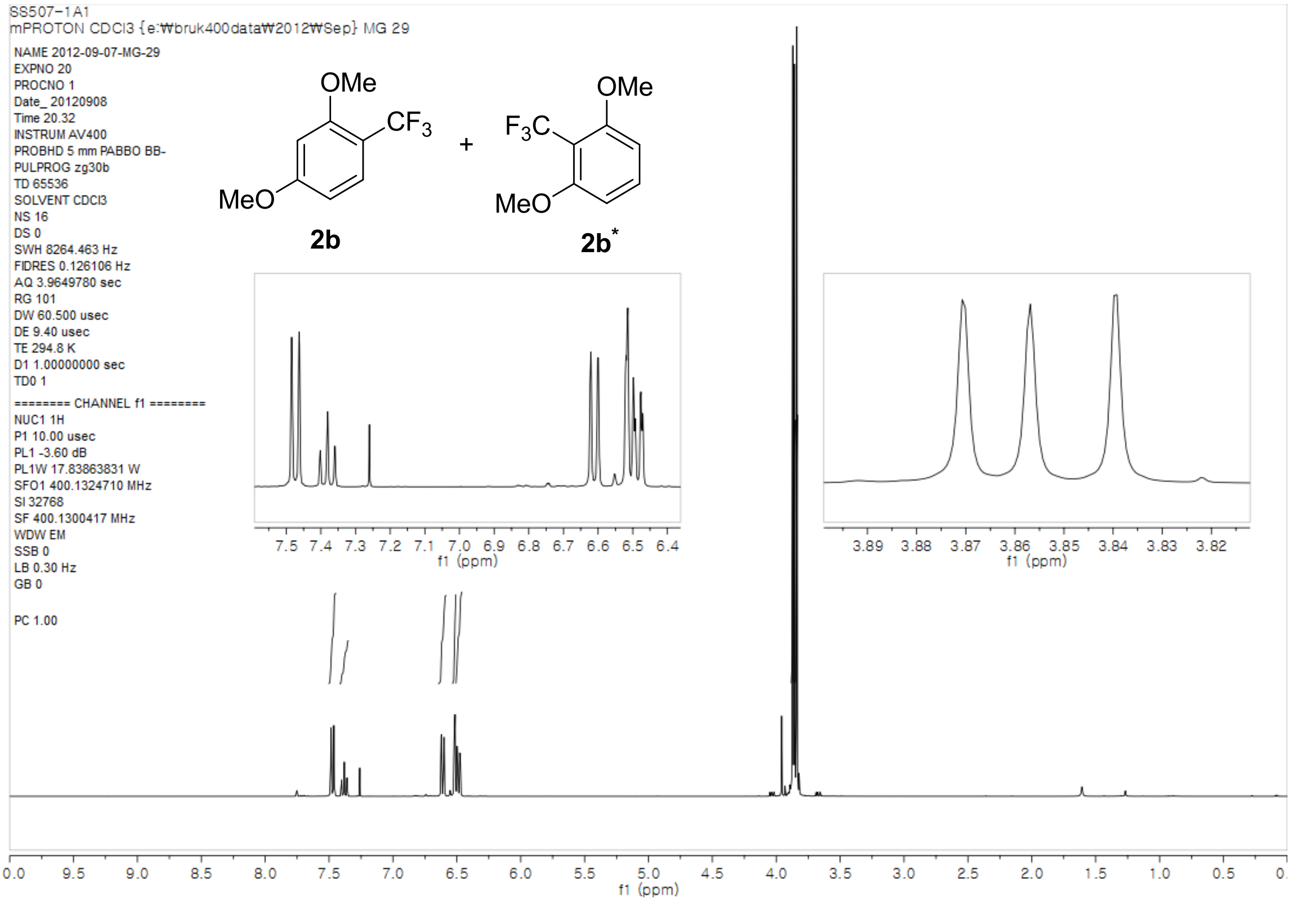






```
SS490-1A1
mF19CPD CDCl3 {e:₩bruk400data₩2012₩Sep} MG 44
NAME 2012-09-04-MG-44
EXPNO 12
PROCNO 1
Date_ 20120905
Time 12.00
INSTRUM AV400
PROBHD 5 mm PABBO BB-
PULPROG zgig
TD 131072
SOLVENT CDCl3
NS 128
DS 4
SWH 89285.711 Hz
FIDRES 0.681196 Hz
AQ 0.7340532 sec
RG 4100
DW 5.600 usec
DE 7.51 usec
TE 295.5 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 19F
P1 10.70 usec
PL1 -5.00 dB
PL1W 27.00716019 W
SFO1 376.4607164 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -3.60 dB
PL12 15.31 dB
PL2W 17.83863831 W
PL12W 0.22927761 W
SFO2 400.1316005 MHz
SI 262144
SF 376.4983660 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0

PC 2.00
```



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SS507-1A1
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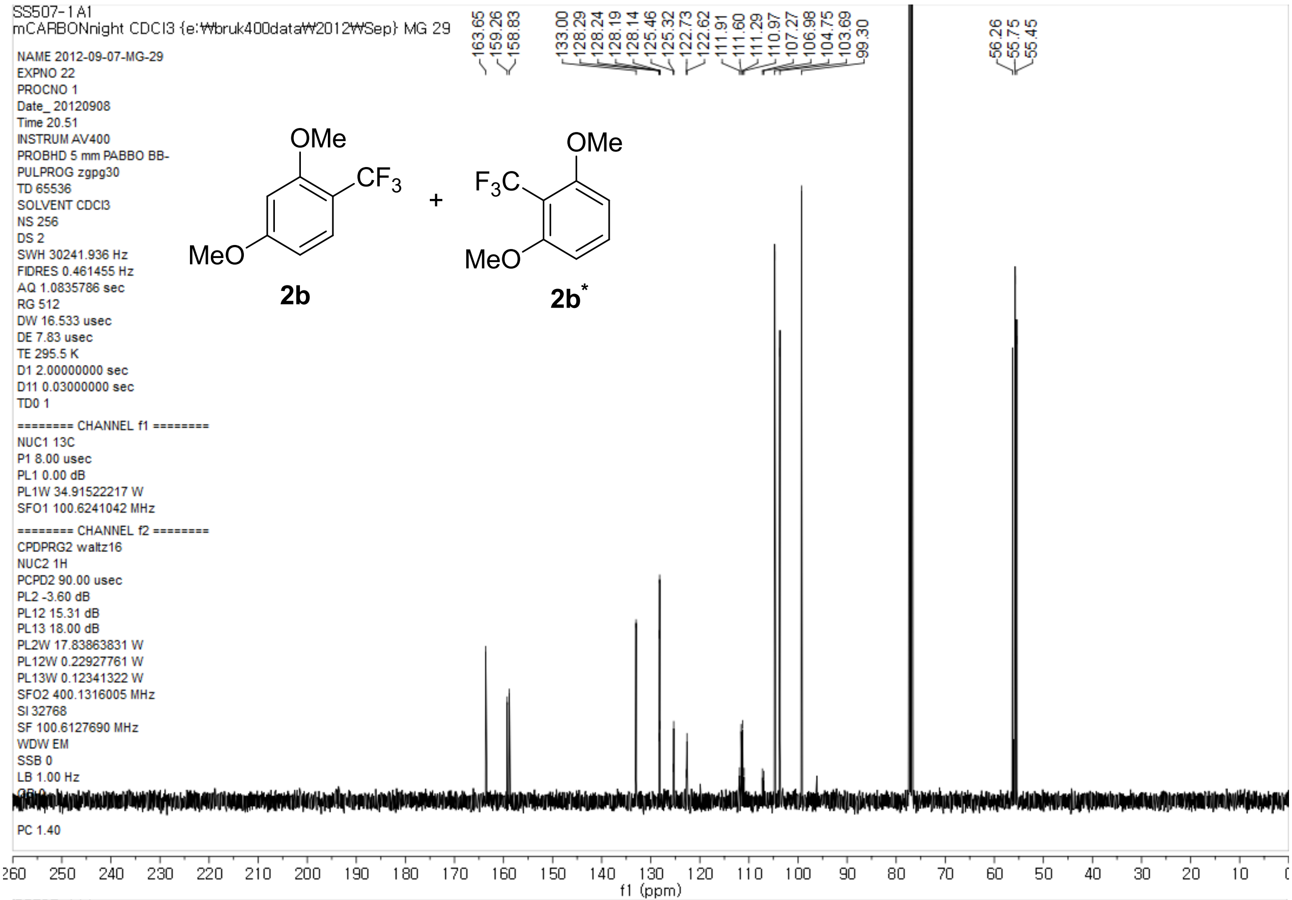
NAME 2012-09-07-MG-29
EXPNO 20
PROCNO 1
Date_ 20120908
Time 20.32
INSTRUM AV400
PROBHD 5 mm PABBO BB-
PULPROG zg30b
TD 65536
SOLVENT CDCl3
NS 16
DS 0
SWH 8264.463 Hz
FIDRES 0.126106 Hz
AQ 3.9649780 sec
RG 101
DW 60.500 usec
DE 9.40 usec
TE 294.8 K
D1 1.00000000 sec
TD0 1

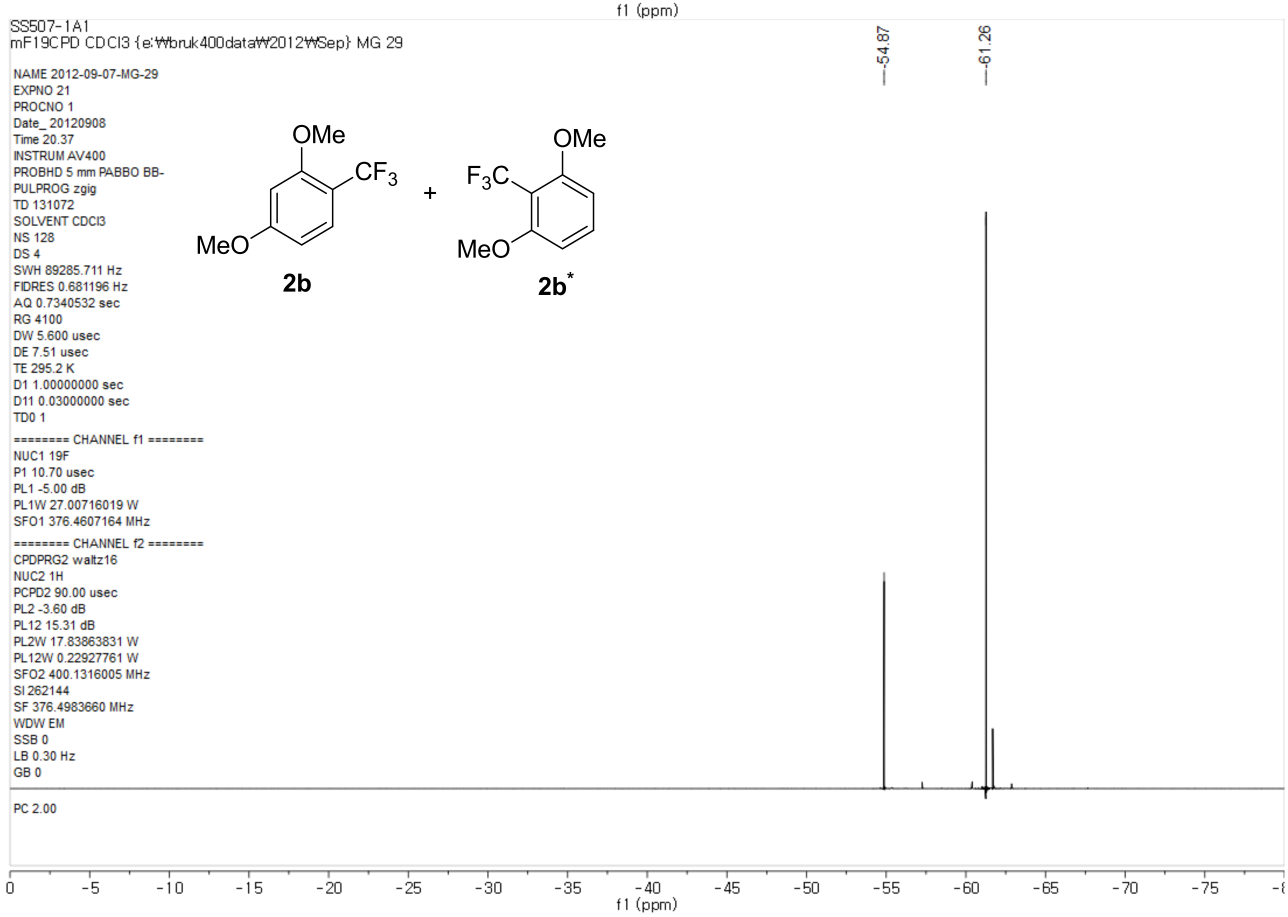
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 -3.60 dB
PL1W 17.83863831 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300417 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0

PC 1.00
```



```
SS507-1A1
mCARBONnight CDCl3 {e:\bruk400data\2012\Sep} MG 29

NAME 2012-09-07-MG-29
EXPNO 22
PROCNO 1
Date_ 20120908
Time 20.51
INSTRUM AV400
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 256
DS 2
SWH 30241.936 Hz
FIDRES 0.461455 Hz
AQ 1.0835786 sec
RG 512
DW 16.533 usec
DE 7.83 usec
TE 295.5 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 8.00 usec
PL1 0.00 dB
PL1W 34.91522217 W
SFO1 100.6241042 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -3.60 dB
PL12 15.31 dB
PL13 18.00 dB
PL2W 17.83863831 W
PL12W 0.22927761 W
PL13W 0.12341322 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
```



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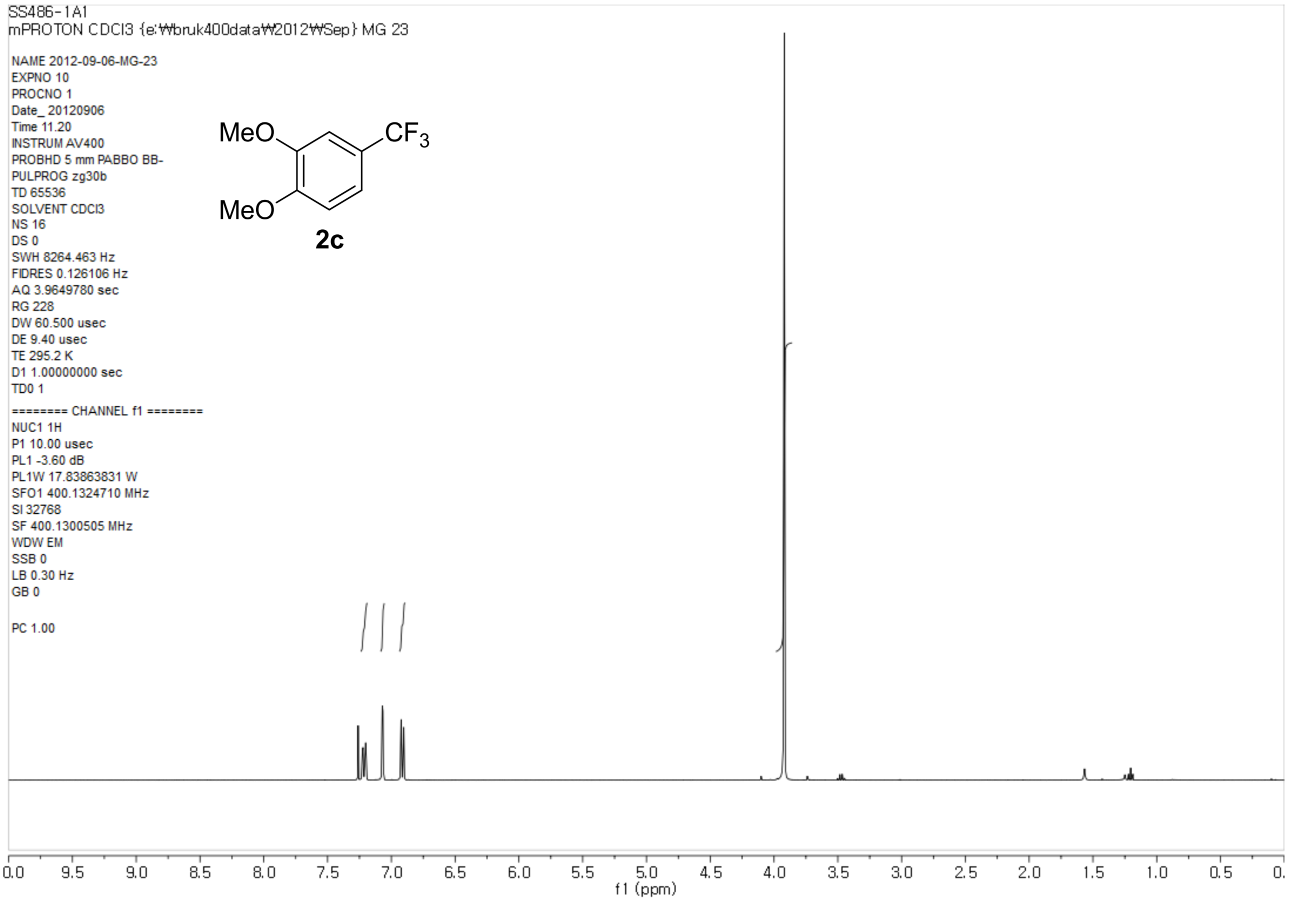
SS507-1A1
mF19CPD CDCl3 {e:\bruk400data\2012\Sep} MG 29

NAME 2012-09-07-MG-29
EXPNO 21
PROCNO 1
Date_ 20120908
Time 20.37
INSTRUM AV400
PROBHD 5 mm PABBO BB-
PULPROG zgig
TD 131072
SOLVENT CDCl3
NS 128
DS 4
SWH 89285.711 Hz
FIDRES 0.681196 Hz
AQ 0.7340532 sec
RG 4100
DW 5.600 usec
DE 7.51 usec
TE 295.2 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 19F
P1 10.70 usec
PL1 -5.00 dB
PL1W 27.00716019 W
SFO1 376.4607164 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -3.60 dB
PL12 15.31 dB
PL2W 17.83863831 W
PL12W 0.22927761 W
SFO2 400.1316005 MHz
SI 262144
SF 376.4983660 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 2.00
```



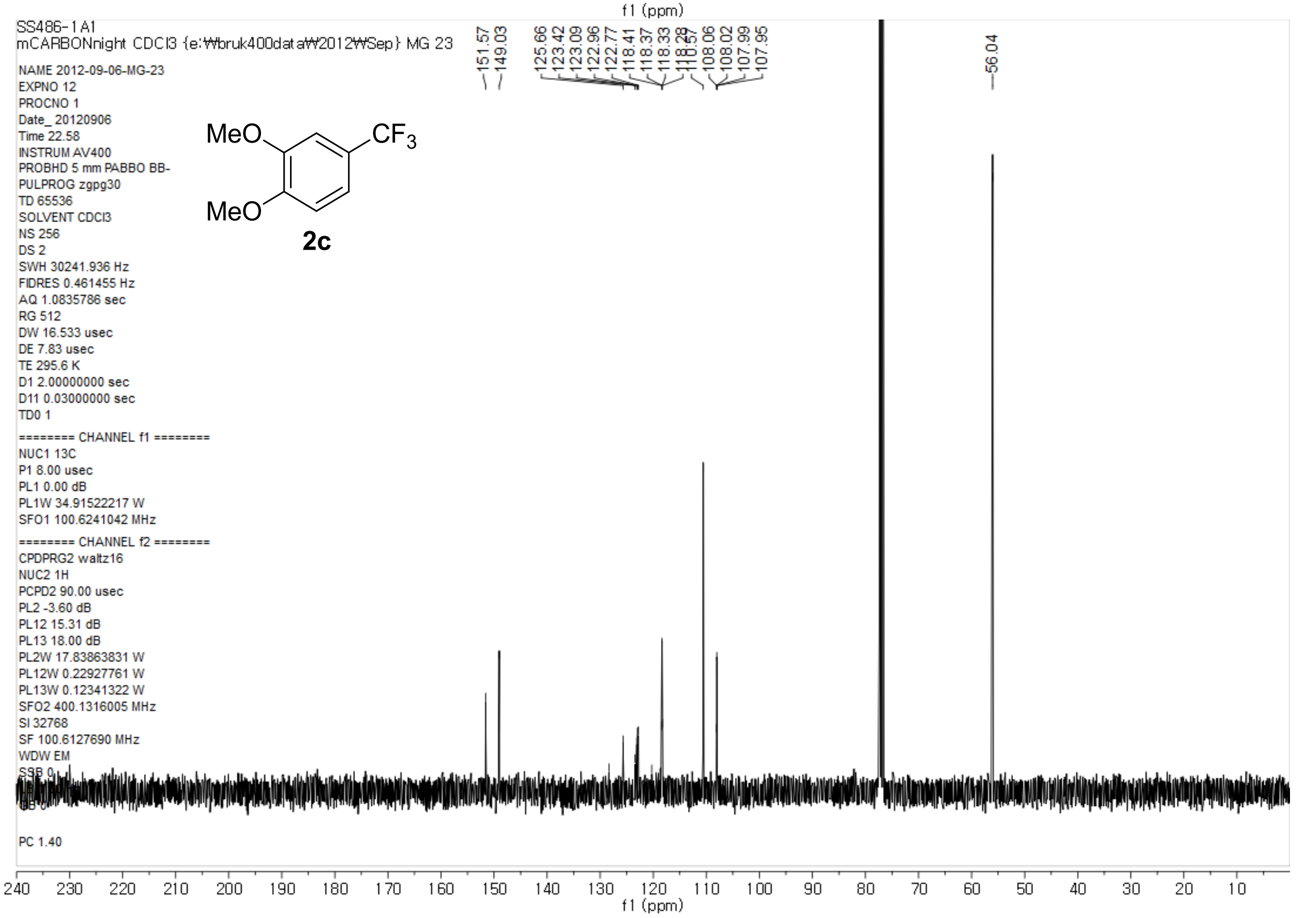
SS486-1A1
mPROTON CDCl3 {e:₩bruk400data₩2012₩Sep} MG 23

NAME 2012-09-06-MG-23
EXPNO 10
PROCNO 1
Date_ 20120906
Time 11.20
INSTRUM AV400
PROBHD 5 mm PABBO BB-
PULPROG zg30b
TD 65536
SOLVENT CDCl3
NS 16
DS 0
SWH 8264.463 Hz
FIDRES 0.126106 Hz
AQ 3.9649780 sec
RG 228
DW 60.500 usec
DE 9.40 usec
TE 295.2 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 -3.60 dB
PL1W 17.83863831 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300505 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0

PC 1.00

2c



SS486-1A1
mCARBONnight CDCl3 {e:₩bruk400data₩2012₩Sep} MG 23

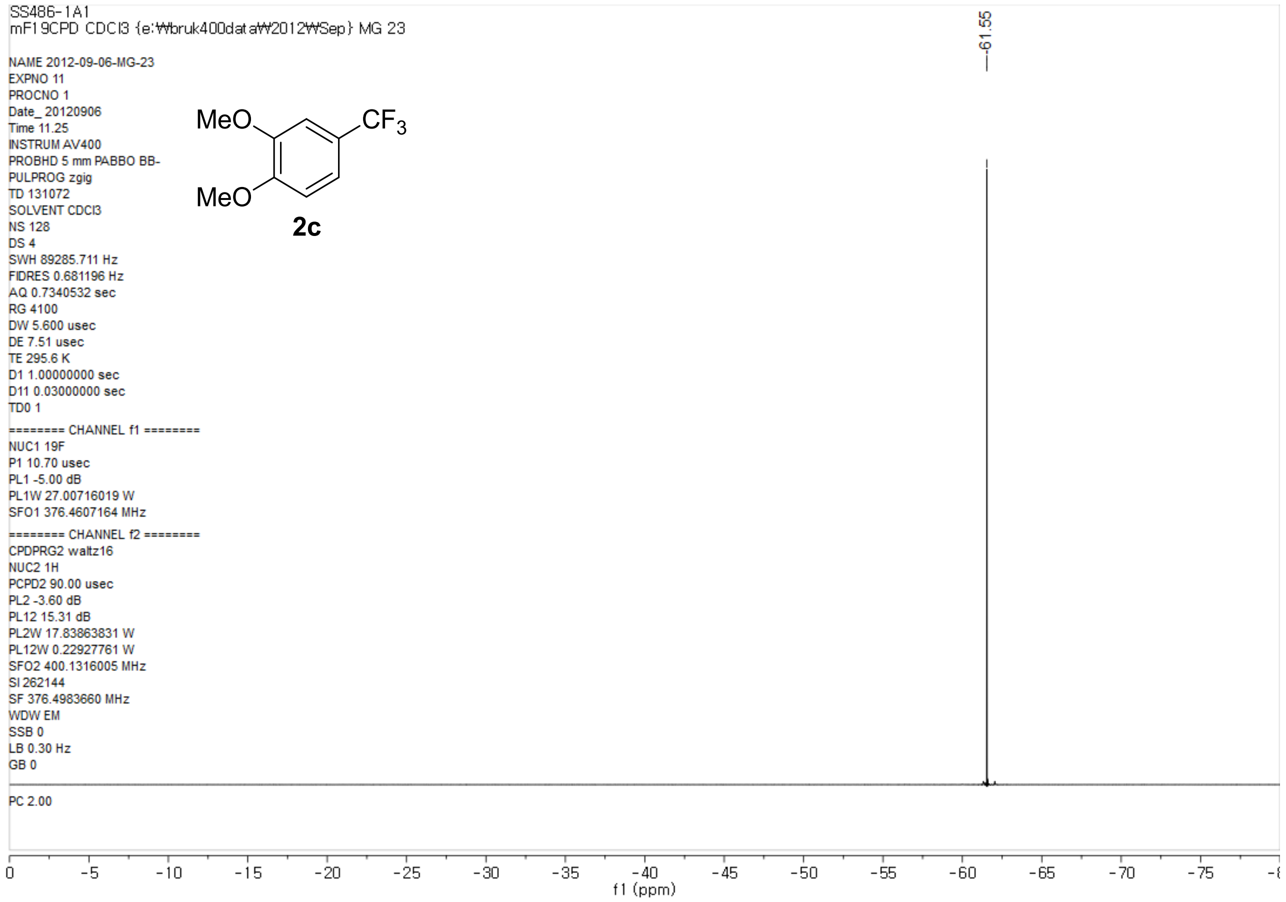
NAME 2012-09-06-MG-23
EXPNO 12
PROCNO 1
Date_ 20120906
Time 22.58
INSTRUM AV400
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 256
DS 2
SWH 30241.936 Hz
FIDRES 0.461455 Hz
AQ 1.0835786 sec
RG 512
DW 16.533 usec
DE 7.83 usec
TE 295.6 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 8.00 usec
PL1 0.00 dB
PL1W 34.91522217 W
SFO1 100.6241042 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -3.60 dB
PL12 15.31 dB
PL13 18.00 dB
PL2W 17.83863831 W
PL12W 0.22927761 W
PL13W 0.12341322 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
[illegible]
GB 0

PC 1.40

2c



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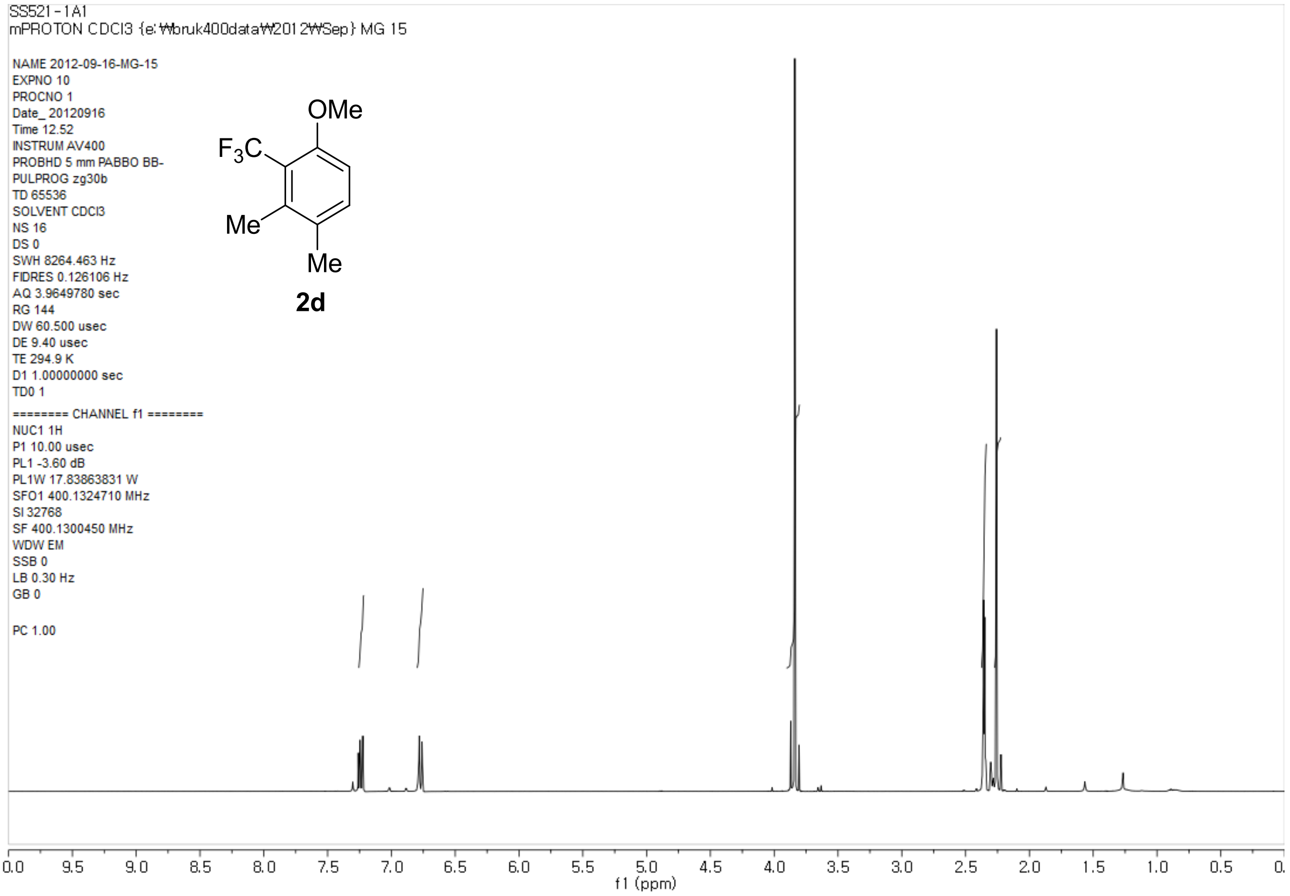
SS486-1A1
mF19CPD CDCl3 {e:₩bruk400data₩2012₩Sep} MG 23

NAME 2012-09-06-MG-23
EXPNO 11
PROCNO 1
Date_ 20120906
Time 11.25
INSTRUM AV400
PROBHD 5 mm PABBO BB-
PULPROG zgig
TD 131072
SOLVENT CDCl3
NS 128
DS 4
SWH 89285.711 Hz
FIDRES 0.681196 Hz
AQ 0.7340532 sec
RG 4100
DW 5.600 usec
DE 7.51 usec
TE 295.6 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 19F
P1 10.70 usec
PL1 -5.00 dB
PL1W 27.00716019 W
SFO1 376.4607164 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -3.60 dB
PL12 15.31 dB
PL2W 17.83863831 W
PL12W 0.22927761 W
SFO2 400.1316005 MHz
SI 262144
SF 376.4983660 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0

PC 2.00
```

2c

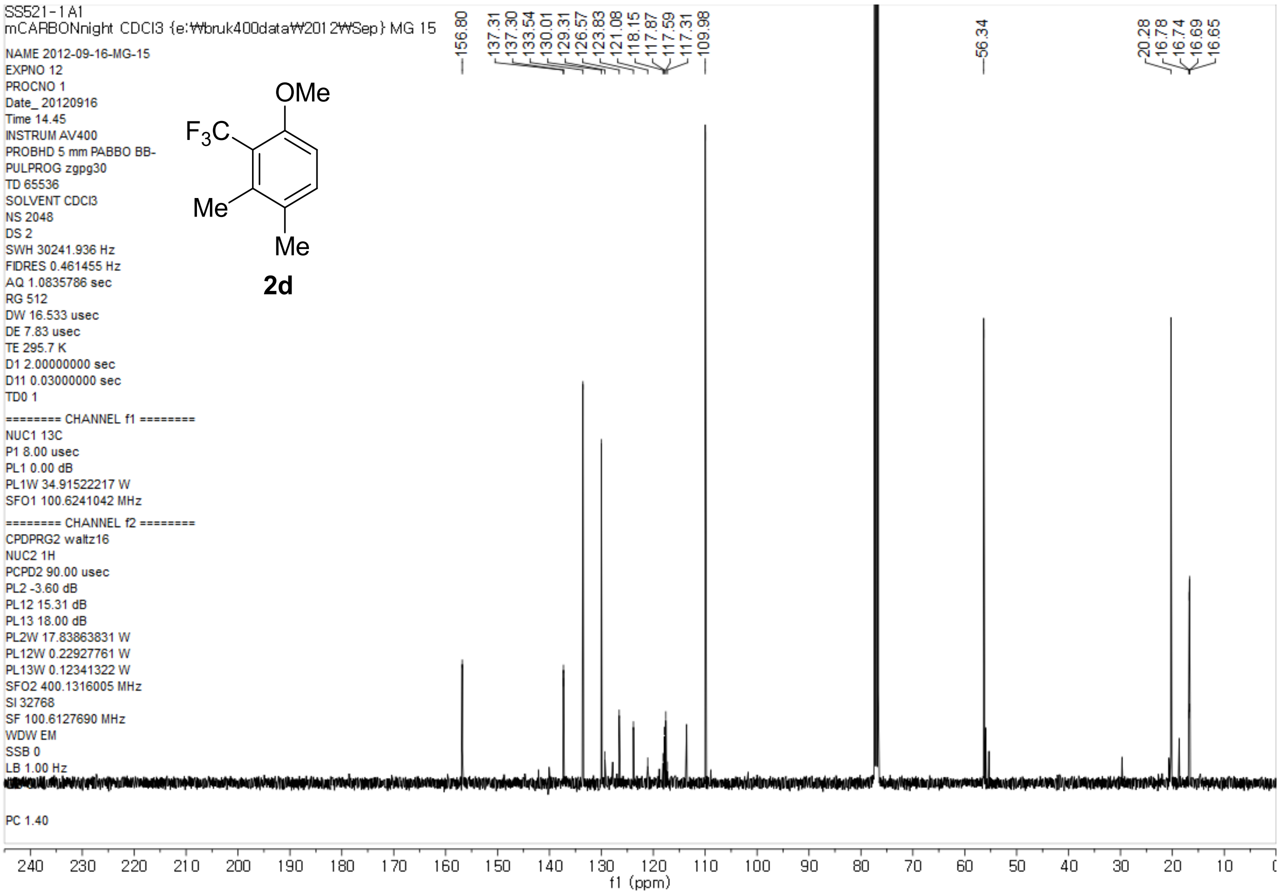


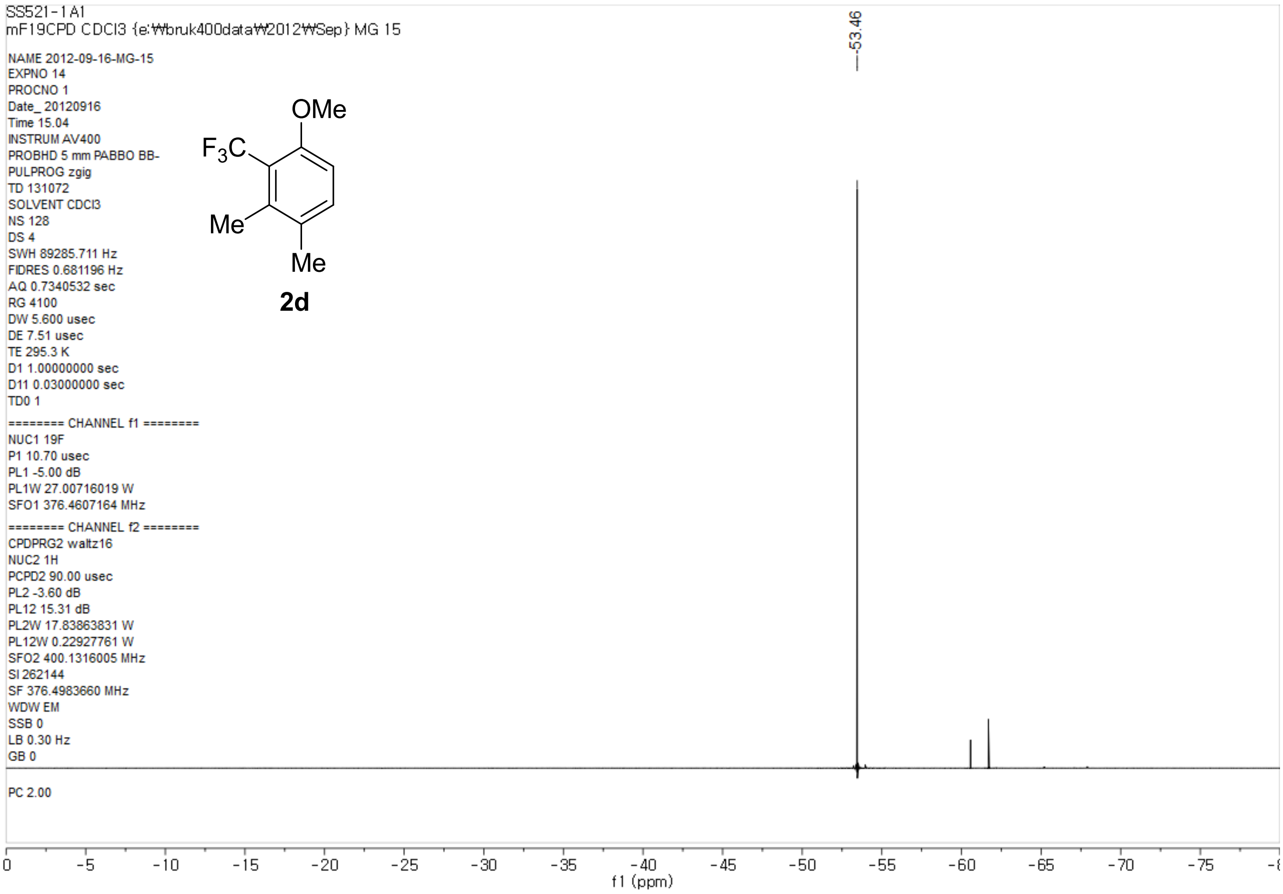
```
SS521-1A1
mPROTON CDCl3 {e:₩bruk400data₩2012₩Sep} MG 15

NAME 2012-09-16-MG-15
EXPNO 10
PROCNO 1
Date_ 20120916
Time 12.52
INSTRUM AV400
PROBHD 5 mm PABBO BB-
PULPROG zg30b
TD 65536
SOLVENT CDCl3
NS 16
DS 0
SWH 8264.463 Hz
FIDRES 0.126106 Hz
AQ 3.9649780 sec
RG 144
DW 60.500 usec
DE 9.40 usec
TE 294.9 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 -3.60 dB
PL1W 17.83863831 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300450 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0

PC 1.00
```

2d


SS521-1A1
mCARBONnight CDCl3 {e:₩bruk400data₩2012₩Sep} MG 15
NAME 2012-09-16-MG-15
EXPNO 12
PROCNO 1
Date_ 20120916
Time 14.45
INSTRUM AV400
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2048
DS 2
SWH 30241.936 Hz
FIDRES 0.461455 Hz
AQ 1.0835786 sec
RG 512
DW 16.533 usec
DE 7.83 usec
TE 295.7 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 8.00 usec
PL1 0.00 dB
PL1W 34.91522217 W
SFO1 100.6241042 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -3.60 dB
PL12 15.31 dB
PL13 18.00 dB
PL2W 17.83863831 W
PL12W 0.22927761 W
PL13W 0.12341322 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
PC 1.40
OMe
F3C
Me
Me
2d
156.80
137.31
137.30
133.54
130.01
129.31
126.57
123.83
121.08
118.15
117.87
117.59
117.31
109.98
56.34
20.28
16.78
16.74
16.69
16.65
240
230
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)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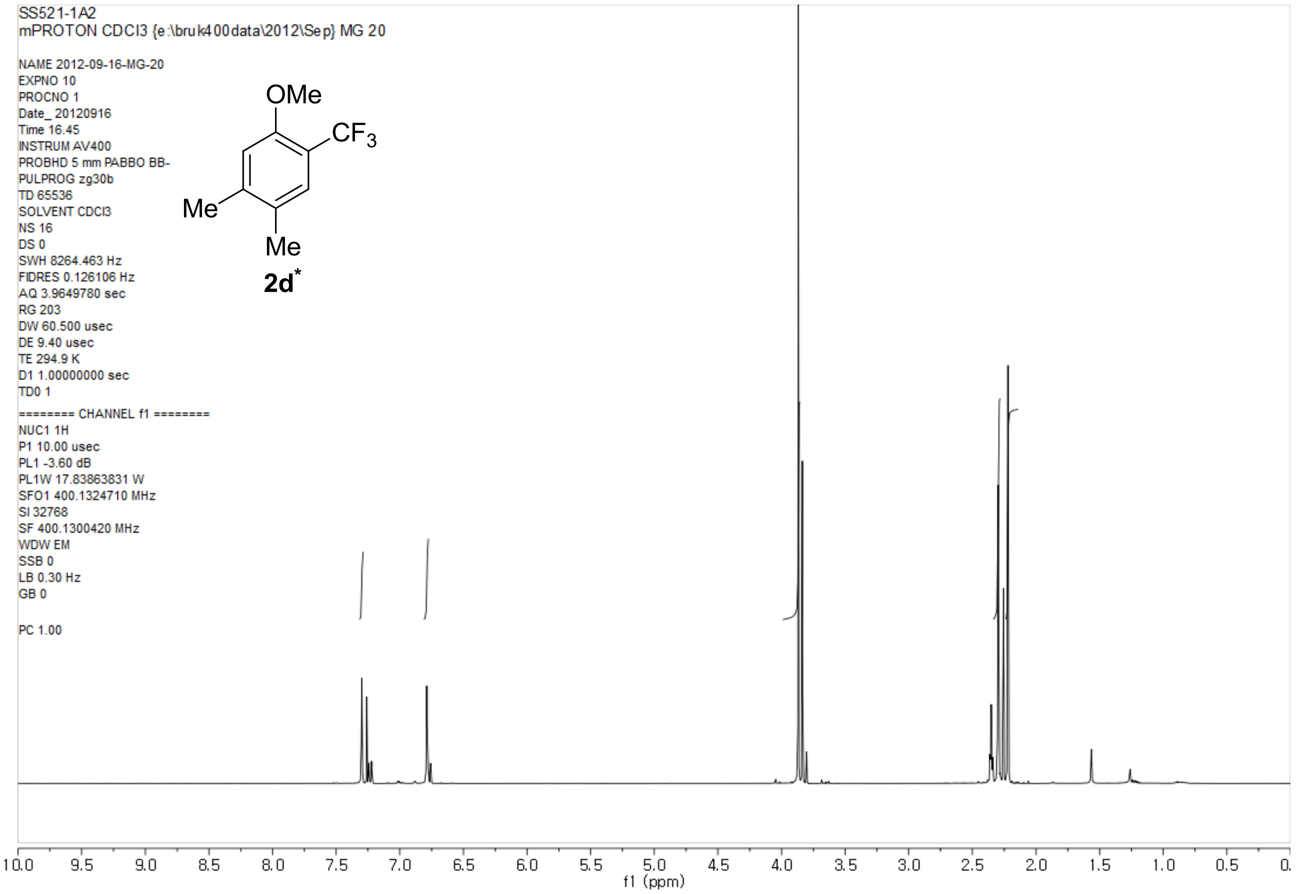
NAME 2012-09-16-MG-15
EXPNO 14
PROCNO 1
Date_ 20120916
Time 15.04
INSTRUM AV400
PROBHD 5 mm PABBO BB-
PULPROG zgig
TD 131072
SOLVENT CDCl3
NS 128
DS 4
SWH 89285.711 Hz
FIDRES 0.681196 Hz
AQ 0.7340532 sec
RG 4100
DW 5.600 usec
DE 7.51 usec
TE 295.3 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 19F
P1 10.70 usec
PL1 -5.00 dB
PL1W 27.00716019 W
SFO1 376.4607164 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -3.60 dB
PL12 15.31 dB
PL2W 17.83863831 W
PL12W 0.22927761 W
SFO2 400.1316005 MHz
SI 262144
SF 376.4983660 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 2.00
OMe
F3C
Me
Me
2d
-53.46
0
-5
-10
-15
-20
-25
-30
-35
-40
-45
-50
-55
-60
-65
-70
-75
f1 (ppm)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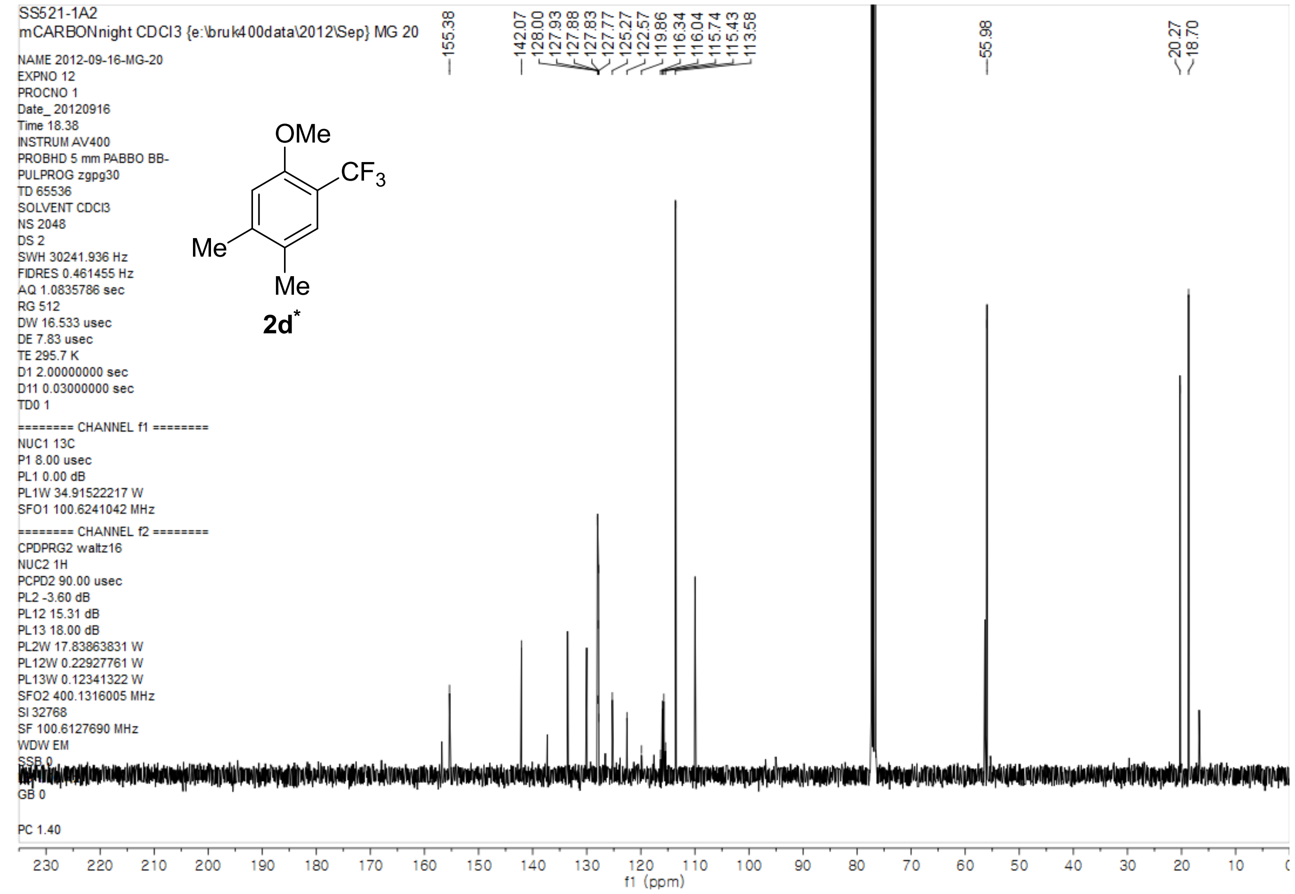
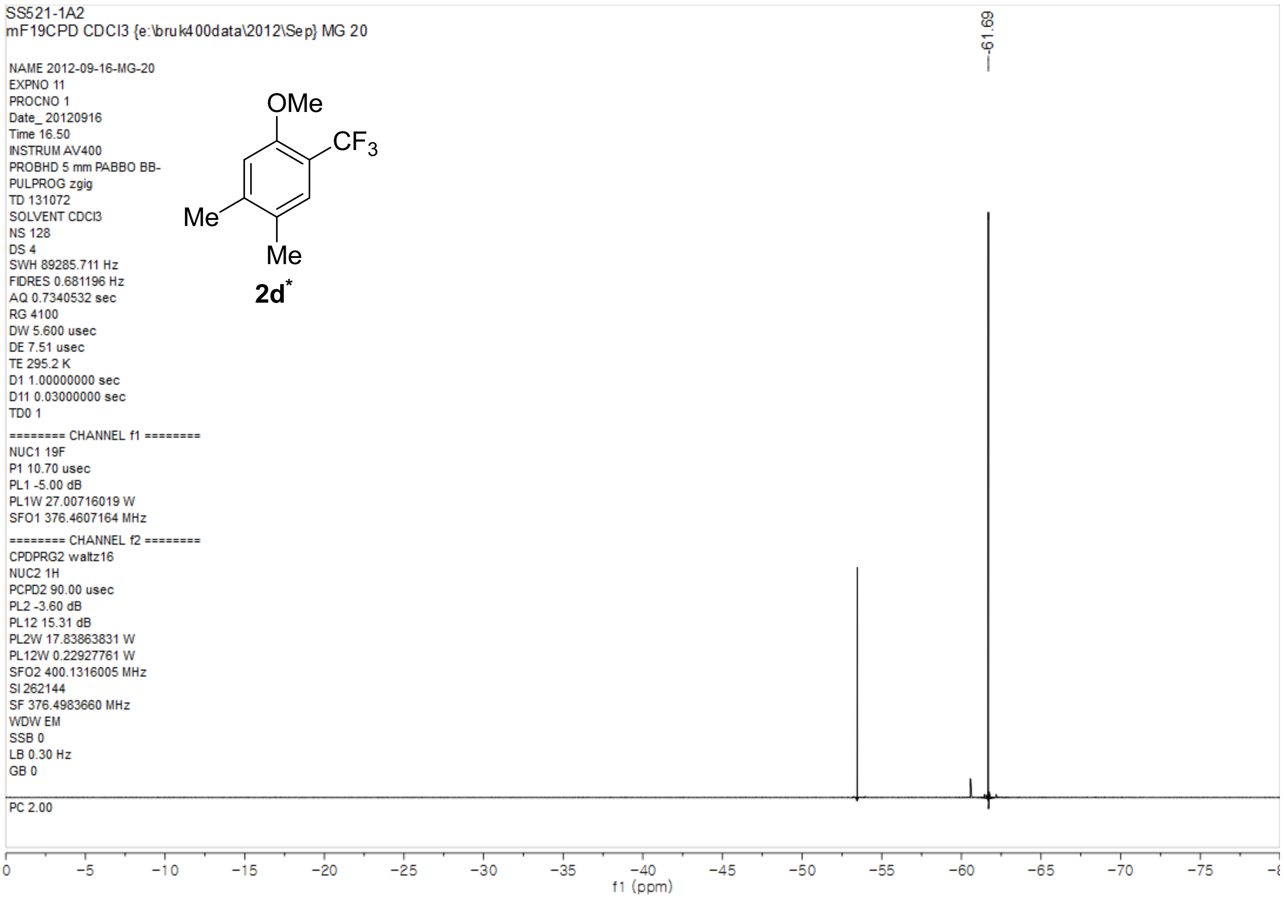
NAME 2012-09-16-MG-20
EXPNO 10
PROCNO 1
Date_ 20120916
Time 16.45
INSTRUM AV400
PROBHD 5 mm PABBO BB-
PULPROG zg30b
TD 65536
SOLVENT CDCl3
NS 16
DS 0
SWH 8264.463 Hz
FIDRES 0.126106 Hz
AQ 3.9649780 sec
RG 203
DW 60.500 usec
DE 9.40 usec
TE 294.9 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 -3.60 dB
PL1W 17.83863831 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300420 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0

PC 1.00


SS521-1A2
mCARBONnight CDCl3 {e:\bruk400data\2012\Sep} MG 20

NAME 2012-09-16-MG-20
EXPNO 12
PROCNO 1
Date_ 20120916
Time 18.38
INSTRUM AV400
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2048
DS 2
SWH 30241.936 Hz
FIDRES 0.461455 Hz
AQ 1.0835786 sec
RG 512
DW 16.533 usec
DE 7.83 usec
TE 295.7 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 8.00 usec
PL1 0.00 dB
PL1W 34.91522217 W
SFO1 100.6241042 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -3.60 dB
PL12 15.31 dB
PL13 18.00 dB
PL2W 17.83863831 W
PL12W 0.22927761 W
PL13W 0.12341322 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0

PC 1.40



2d*

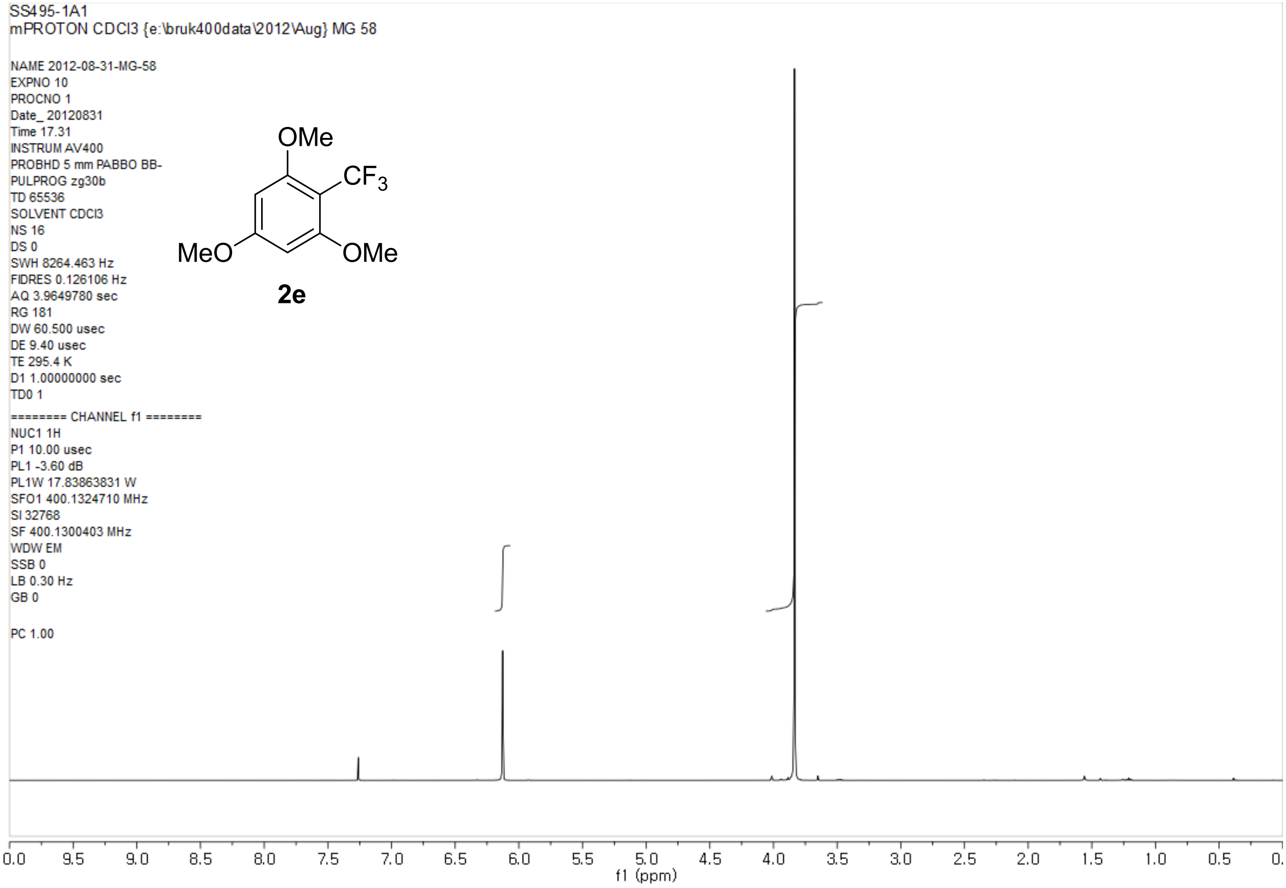
SS521-1A2
mF19CPD CDCl3 {e:\bruk400data\2012\Sep} MG 20

NAME 2012-09-16-MG-20
EXPNO 11
PROCNO 1
Date_ 20120916
Time 16.50
INSTRUM AV400
PROBHD 5 mm PABBO BB-
PULPROG zgig
TD 131072
SOLVENT CDCl3
NS 128
DS 4
SWH 89285.711 Hz
FIDRES 0.681196 Hz
AQ 0.7340532 sec
RG 4100
DW 5.600 usec
DE 7.51 usec
TE 295.2 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 19F
P1 10.70 usec
PL1 -5.00 dB
PL1W 27.00716019 W
SFO1 376.4607164 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -3.60 dB
PL12 15.31 dB
PL2W 17.83863831 W
PL12W 0.22927761 W
SFO2 400.1316005 MHz
SI 262144
SF 376.4983660 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0

PC 2.00



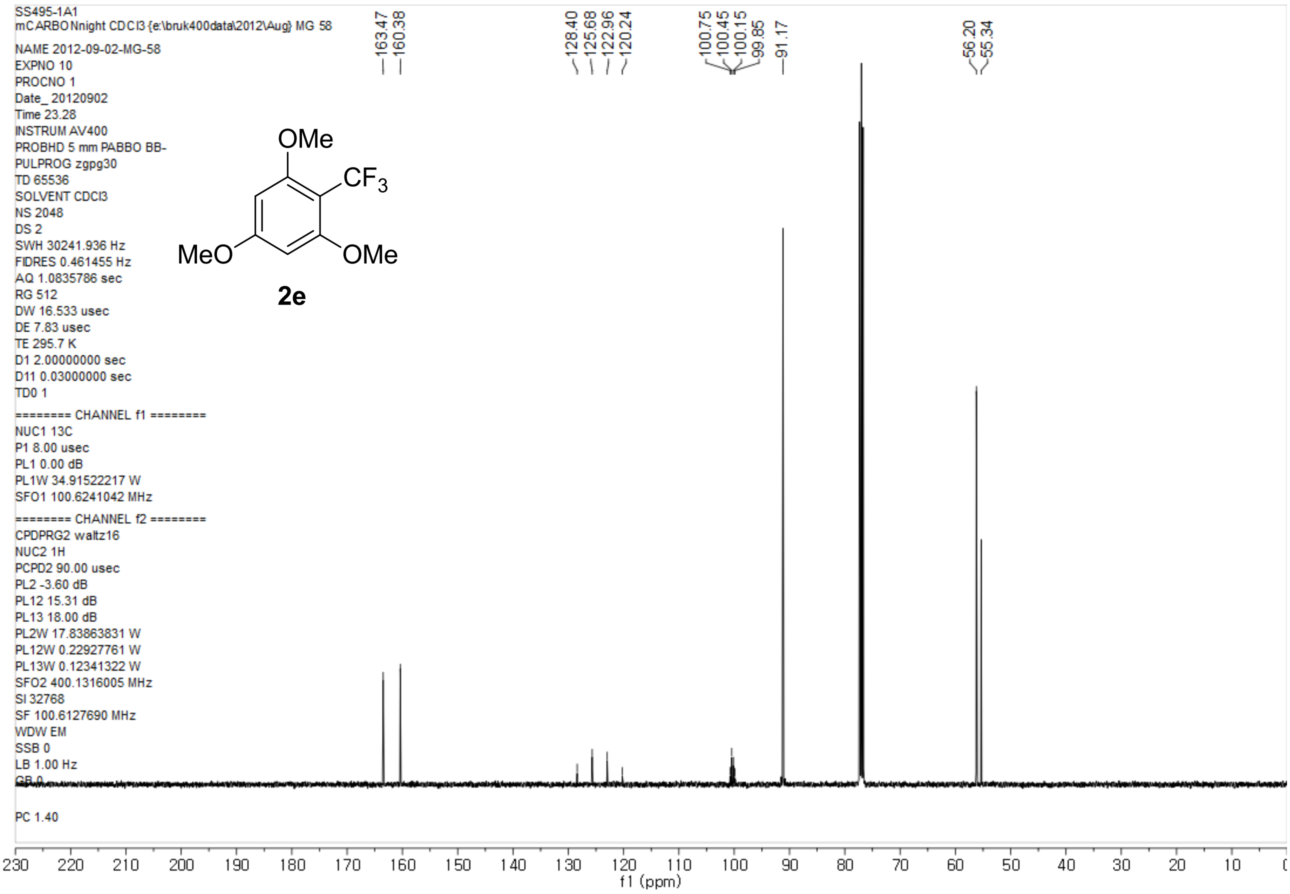
2e

SS495-1A1
mPROTON CDCl3 {e:\bruk400data\2012\Aug} MG 58

NAME 2012-08-31-MG-58
EXPNO 10
PROCNO 1
Date_ 20120831
Time 17.31
INSTRUM AV400
PROBHD 5 mm PABBO BB-
PULPROG zg30b
TD 65536
SOLVENT CDCl3
NS 16
DS 0
SWH 8264.463 Hz
FIDRES 0.126106 Hz
AQ 3.9649780 sec
RG 181
DW 60.500 usec
DE 9.40 usec
TE 295.4 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 -3.60 dB
PL1W 17.83863831 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300403 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0

PC 1.00

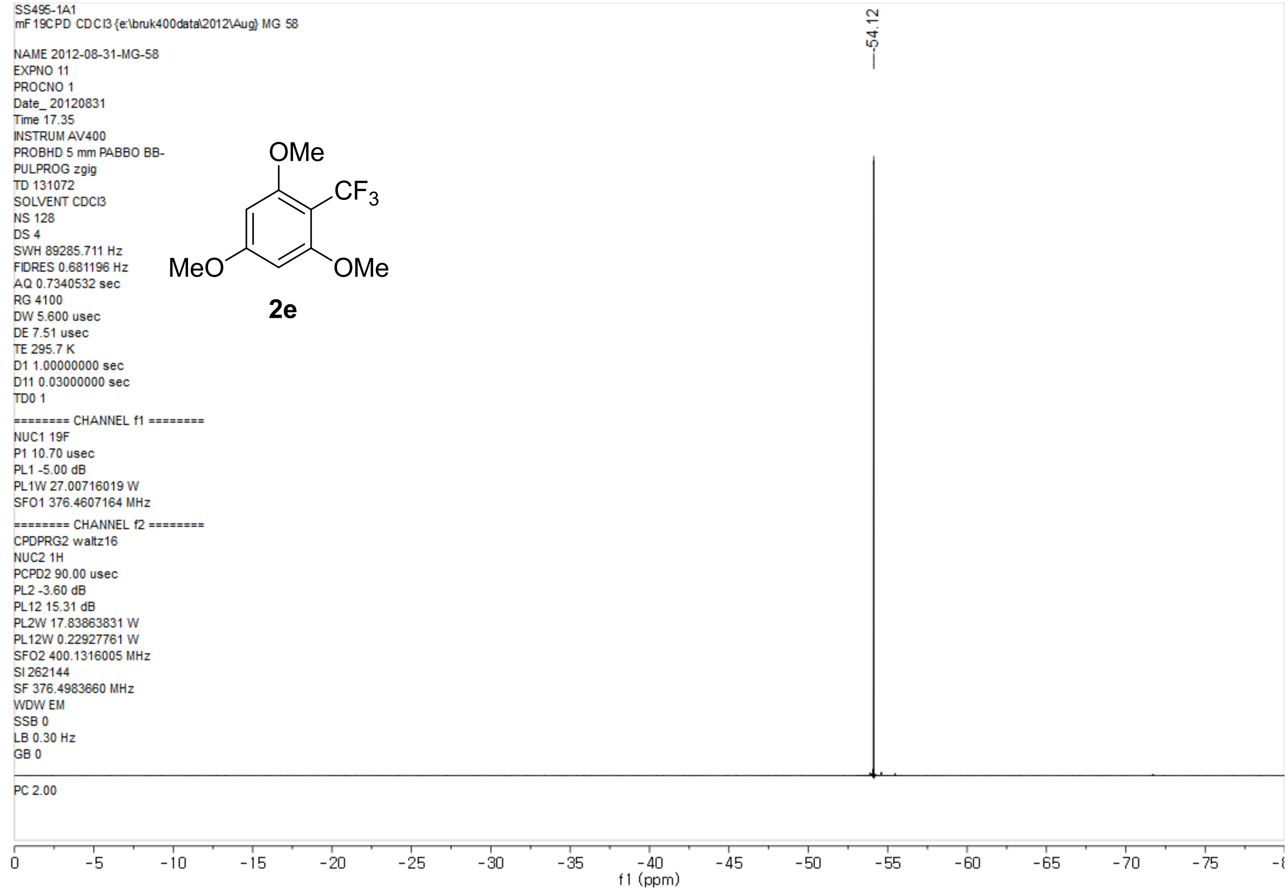

SS495-1A1
mCARBONnight CDCl3 {e:\bruk400data\2012\Aug} MG 58

NAME 2012-09-02-MG-58
EXPNO 10
PROCNO 1
Date_ 20120902
Time 23.28
INSTRUM AV400
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2048
DS 2
SWH 30241.936 Hz
FIDRES 0.461455 Hz
AQ 1.0835786 sec
RG 512
DW 16.533 usec
DE 7.83 usec
TE 295.7 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 8.00 usec
PL1 0.00 dB
PL1W 34.91522217 W
SFO1 100.6241042 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -3.60 dB
PL12 15.31 dB
PL13 18.00 dB
PL2W 17.83863831 W
PL12W 0.22927761 W
PL13W 0.12341322 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0

PC 1.40

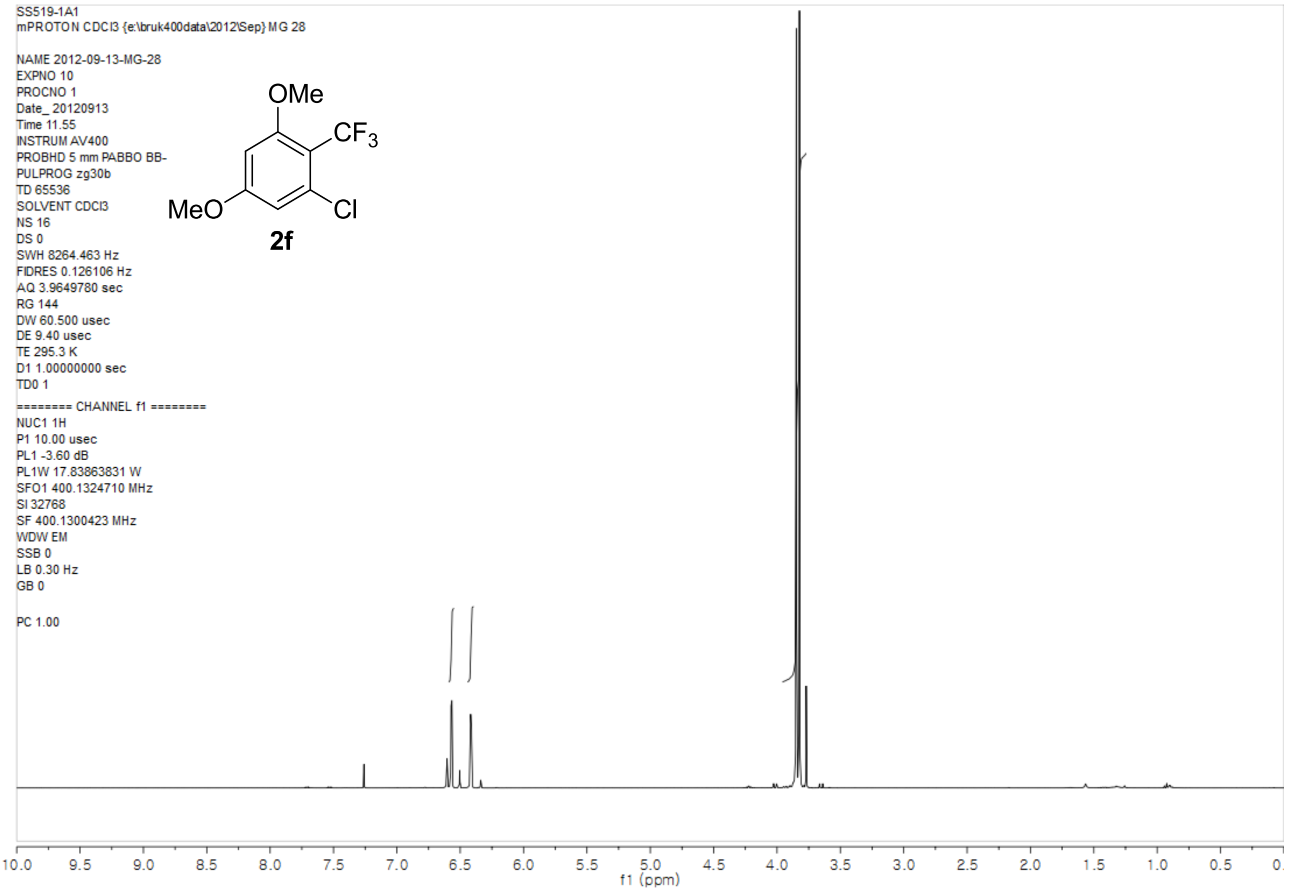

SS495-1A1
mF19CPD CDCl3 {e:\bruk400data\2012\Aug} MG 58

NAME 2012-08-31-MG-58
EXPNO 11
PROCNO 1
Date_ 20120831
Time 17.35
INSTRUM AV400
PROBHD 5 mm PABBO BB-
PULPROG zgig
TD 131072
SOLVENT CDCl3
NS 128
DS 4
SWH 89285.711 Hz
FIDRES 0.681196 Hz
AQ 0.7340532 sec
RG 4100
DW 5.600 usec
DE 7.51 usec
TE 295.7 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 19F
P1 10.70 usec
PL1 -5.00 dB
PL1W 27.00716019 W
SFO1 376.4607164 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -3.60 dB
PL12 15.31 dB
PL2W 17.83863831 W
PL12W 0.22927761 W
SFO2 400.1316005 MHz
SI 262144
SF 376.4983660 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0

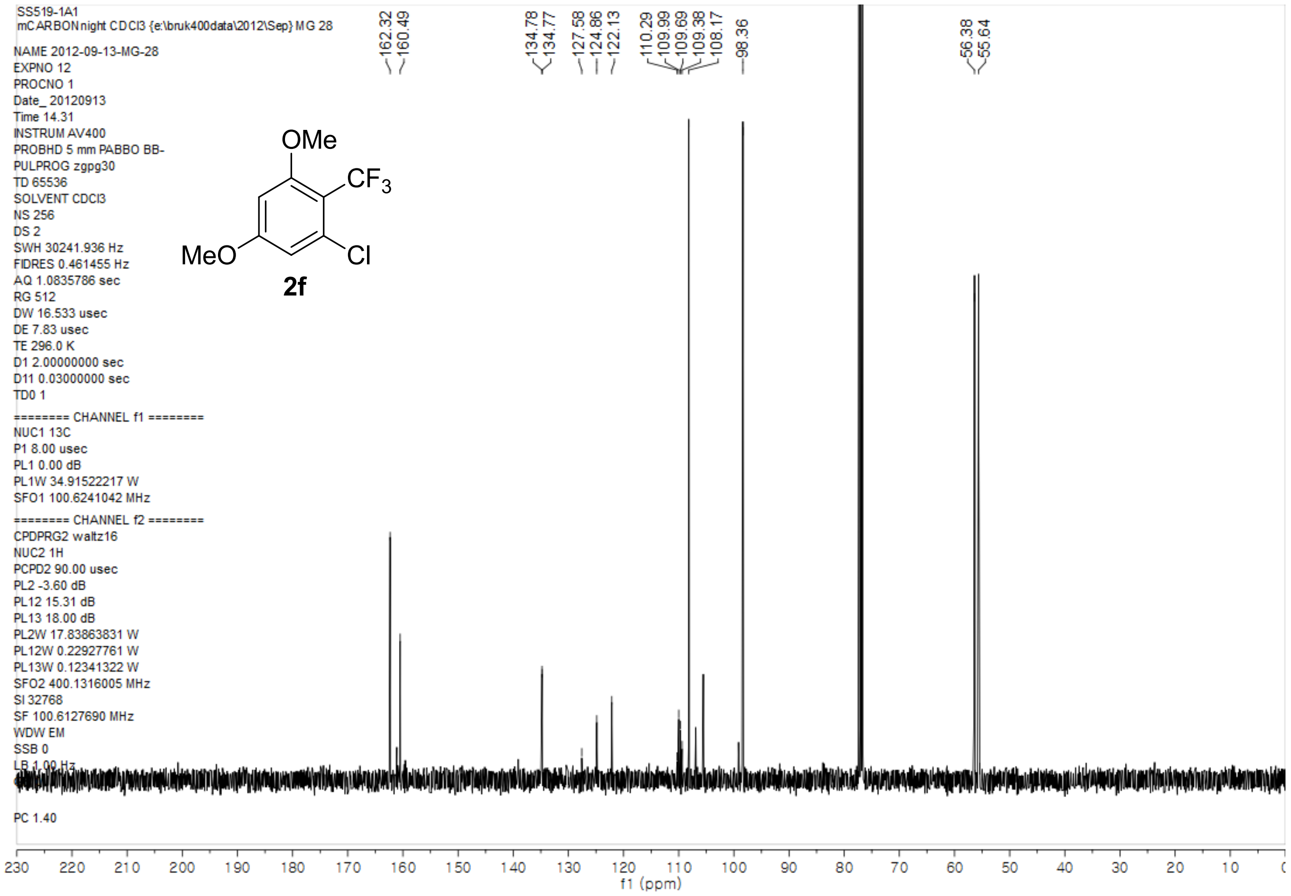
PC 2.00



```
SS519-1A1
mPROTON CDCl3 {e:\bruk400data\2012\Sep} MG 28

NAME 2012-09-13-MG-28
EXPNO 10
PROCNO 1
Date_ 20120913
Time 11.55
INSTRUM AV400
PROBHD 5 mm PABBO BB-
PULPROG zg30b
TD 65536
SOLVENT CDCl3
NS 16
DS 0
SWH 8264.463 Hz
FIDRES 0.126106 Hz
AQ 3.9649780 sec
RG 144
DW 60.500 usec
DE 9.40 usec
TE 295.3 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 -3.60 dB
PL1W 17.83863831 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300423 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0

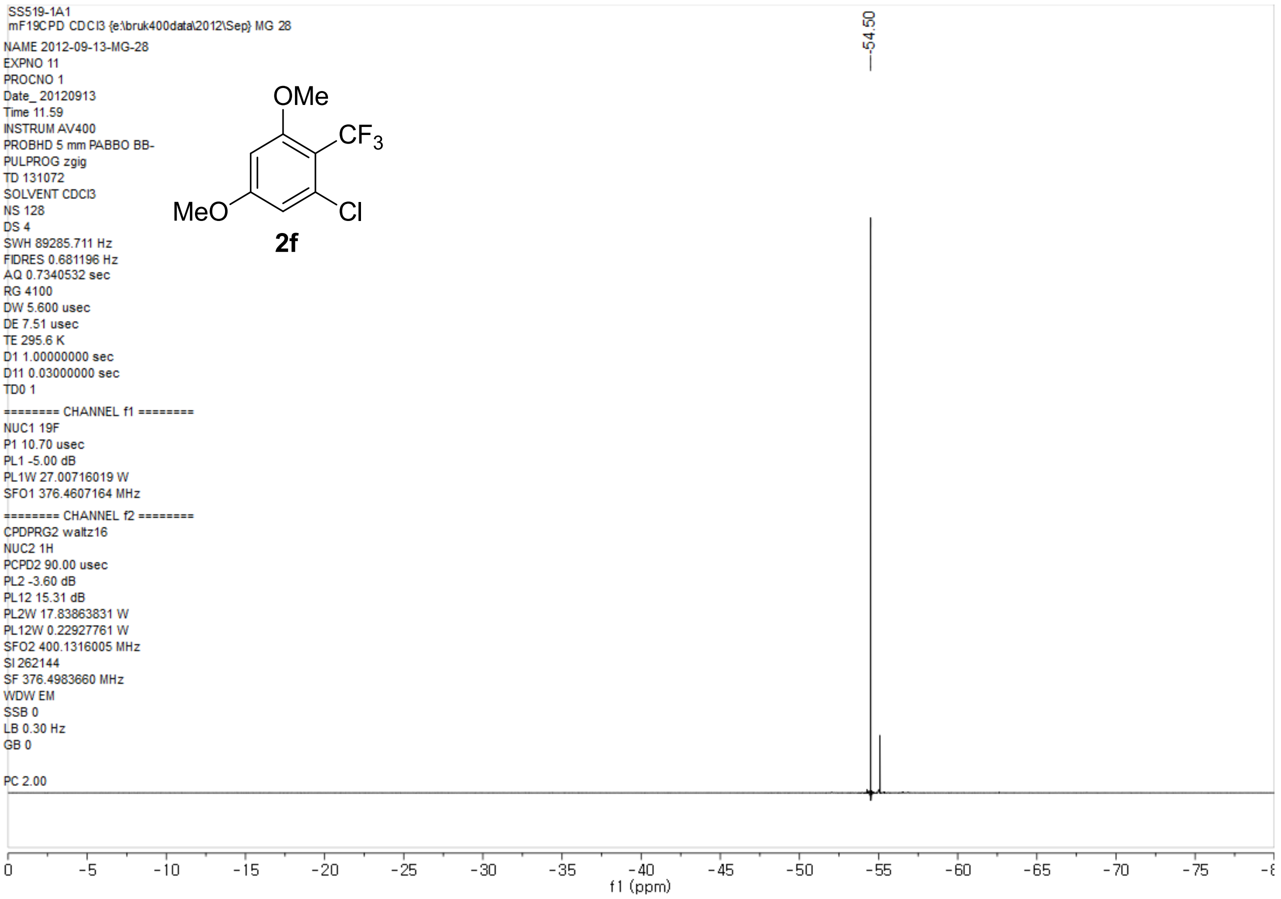
PC 1.00
```

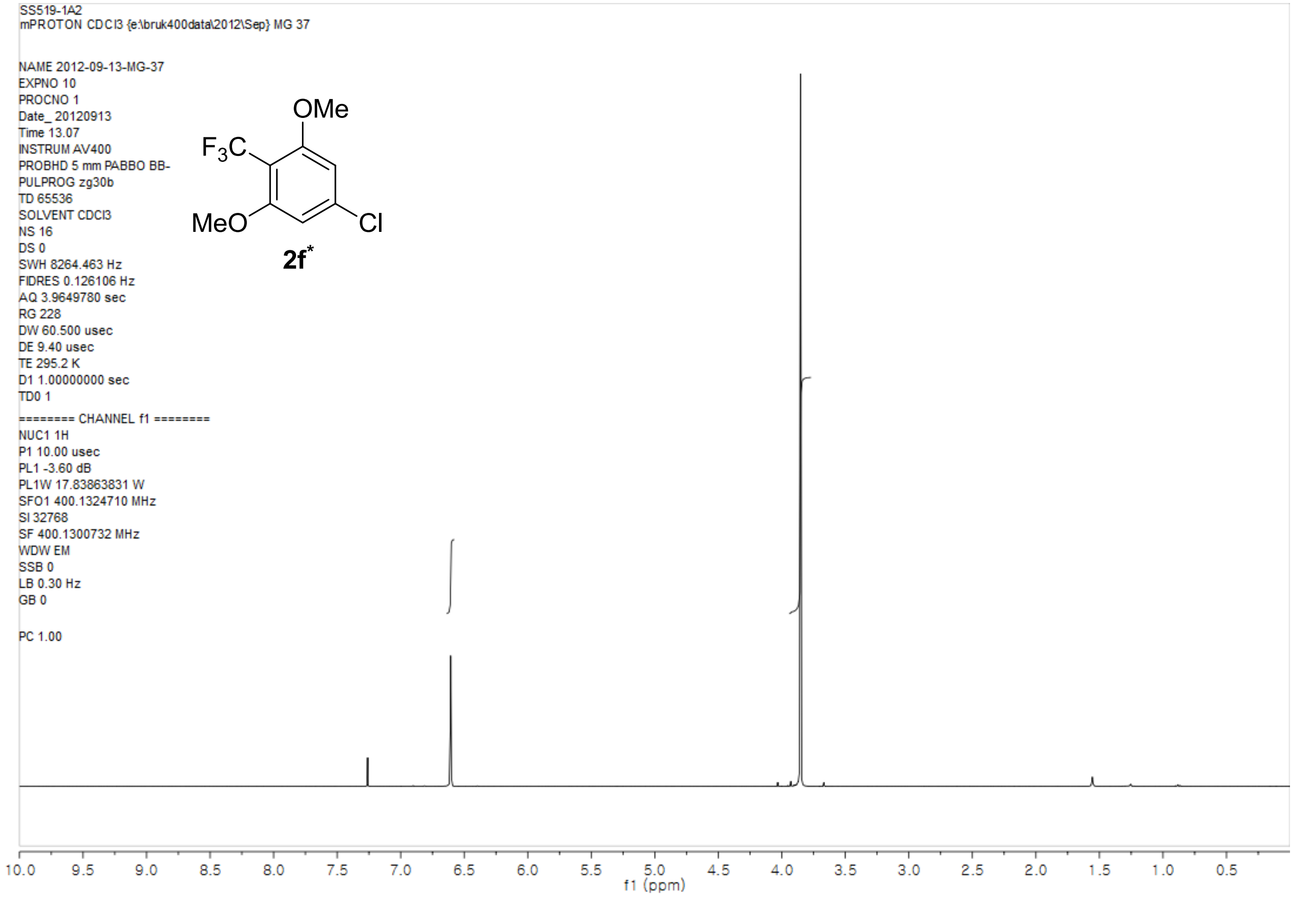


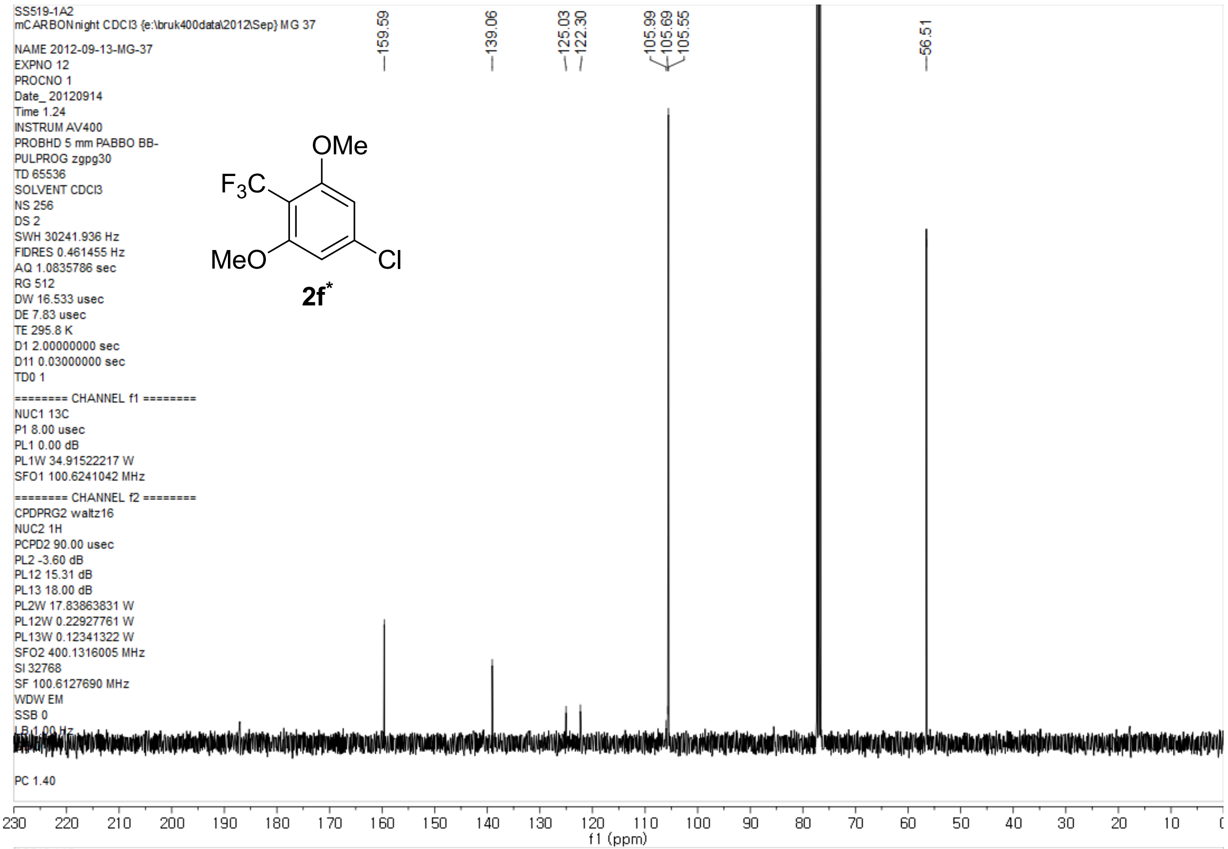
```
SS519-1A1
mCARBONnight CDCl3 {e:\bruk400data\2012\Sep} MG 28

NAME 2012-09-13-MG-28
EXPNO 12
PROCNO 1
Date_ 20120913
Time 14.31
INSTRUM AV400
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 256
DS 2
SWH 30241.936 Hz
FIDRES 0.461455 Hz
AQ 1.0835786 sec
RG 512
DW 16.533 usec
DE 7.83 usec
TE 296.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 8.00 usec
PL1 0.00 dB
PL1W 34.91522217 W
SFO1 100.6241042 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -3.60 dB
PL12 15.31 dB
PL13 18.00 dB
PL2W 17.83863831 W
PL12W 0.22927761 W
PL13W 0.12341322 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz

PC 1.40
```


```
SS519-1A1
mF19CPD CDCl3 {e:\bruk400data\2012\Sep} MG 28
NAME 2012-09-13-MG-28
EXPNO 11
PROCNO 1
Date_ 20120913
Time 11.59
INSTRUM AV400
PROBHD 5 mm PABBO BB-
PULPROG zgig
TD 131072
SOLVENT CDCl3
NS 128
DS 4
SWH 89285.711 Hz
FIDRES 0.681196 Hz
AQ 0.7340532 sec
RG 4100
DW 5.600 usec
DE 7.51 usec
TE 295.6 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 19F
P1 10.70 usec
PL1 -5.00 dB
PL1W 27.00716019 W
SFO1 376.4607164 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -3.60 dB
PL12 15.31 dB
PL2W 17.83863831 W
PL12W 0.22927761 W
SFO2 400.1316005 MHz
SI 262144
SF 376.4983660 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 2.00
```


```
SS519-1A2
mPROTON CDCl3 {e:\bruk400data\2012\Sep} MG 37
NAME 2012-09-13-MG-37
EXPNO 10
PROCNO 1
Date_ 20120913
Time 13.07
INSTRUM AV400
PROBHD 5 mm PABBO BB-
PULPROG zg30b
TD 65536
SOLVENT CDCl3
NS 16
DS 0
SWH 8264.463 Hz
FIDRES 0.126106 Hz
AQ 3.9649780 sec
RG 228
DW 60.500 usec
DE 9.40 usec
TE 295.2 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 -3.60 dB
PL1W 17.83863831 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300732 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
```



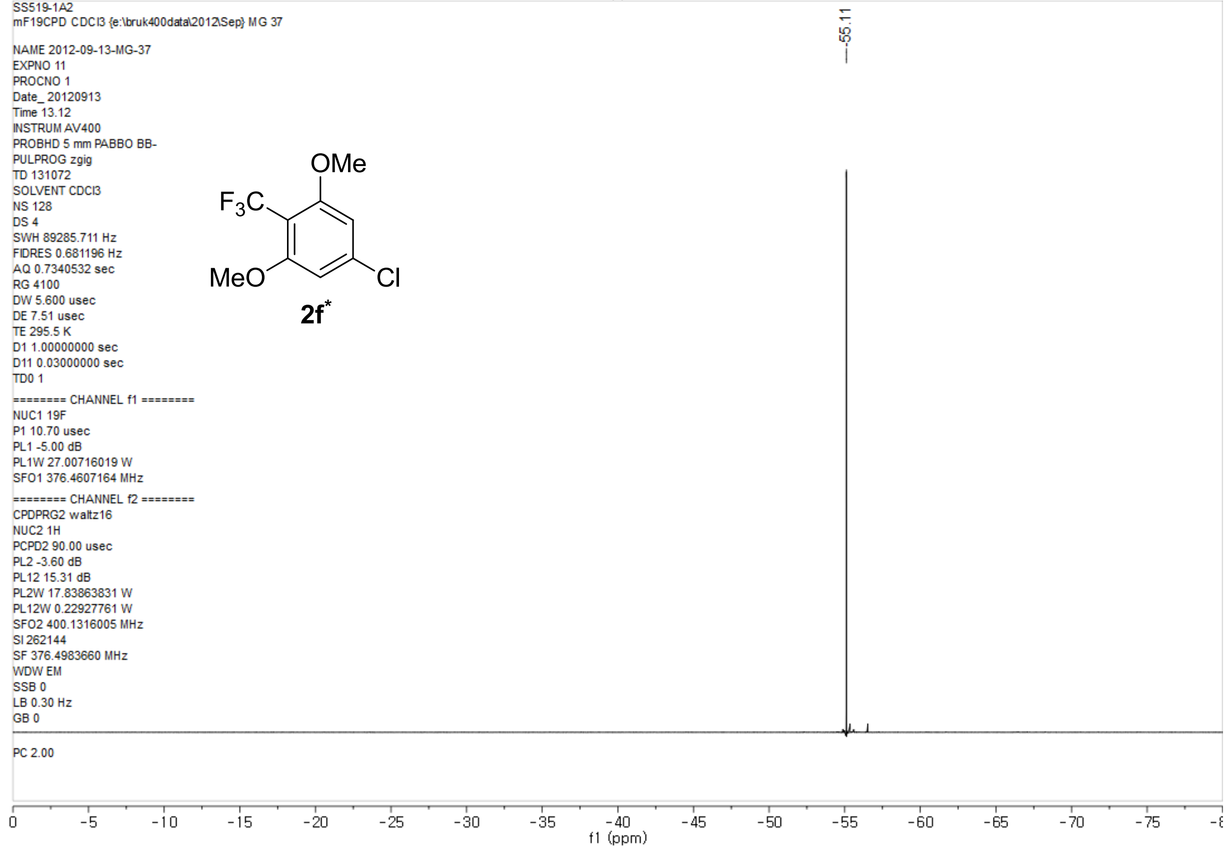
```
SS519-1A2
mCARBONnight CDCl3 {e:\bruk400data\2012\Sep} MG 37

NAME 2012-09-13-MG-37
EXPNO 12
PROCNO 1
Date_ 20120914
Time 1.24
INSTRUM AV400
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 256
DS 2
SWH 30241.936 Hz
FIDRES 0.461455 Hz
AQ 1.0835786 sec
RG 512
DW 16.533 usec
DE 7.83 usec
TE 295.8 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 8.00 usec
PL1 0.00 dB
PL1W 34.91522217 W
SFO1 100.6241042 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -3.60 dB
PL12 15.31 dB
PL13 18.00 dB
PL2W 17.83863831 W
PL12W 0.22927761 W
PL13W 0.12341322 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz

PC 1.40
```



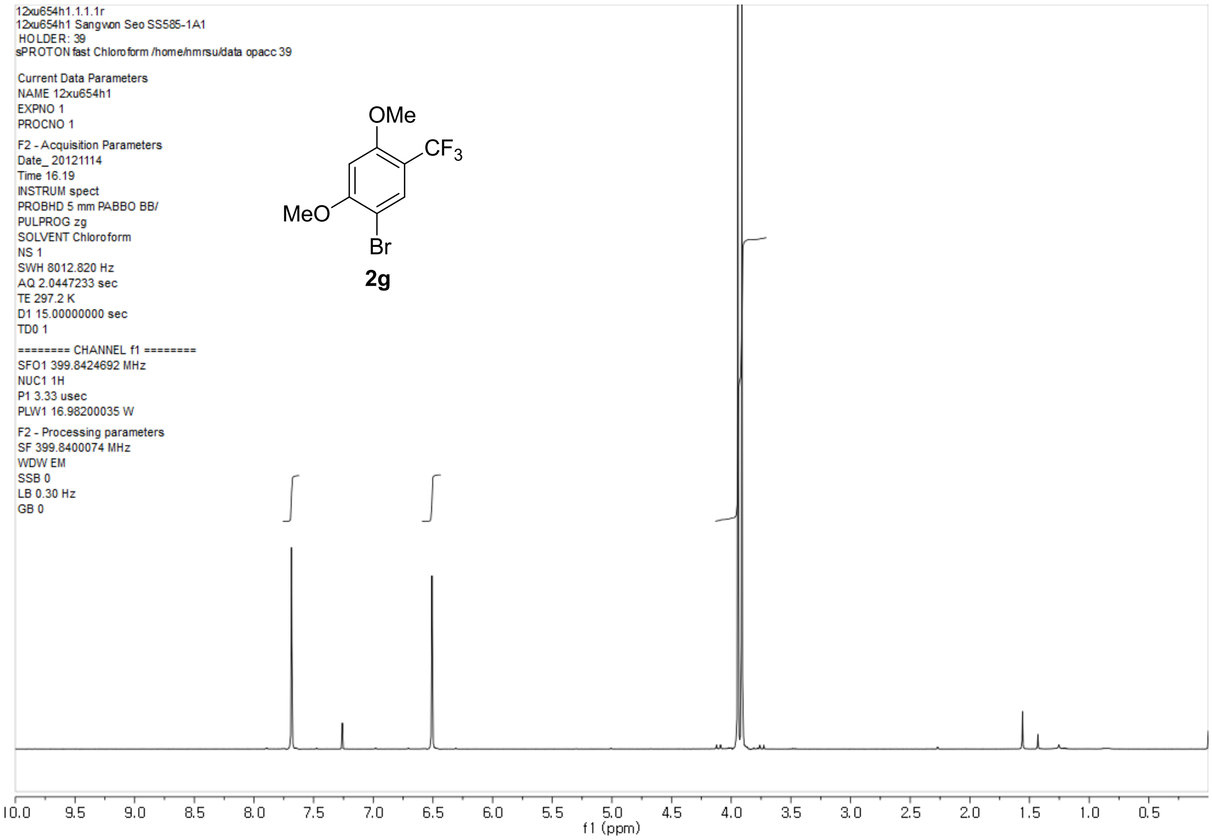
```
SS519-1A2
mF19CPD CDCl3 {e:\bruk400data\2012\Sep} MG 37

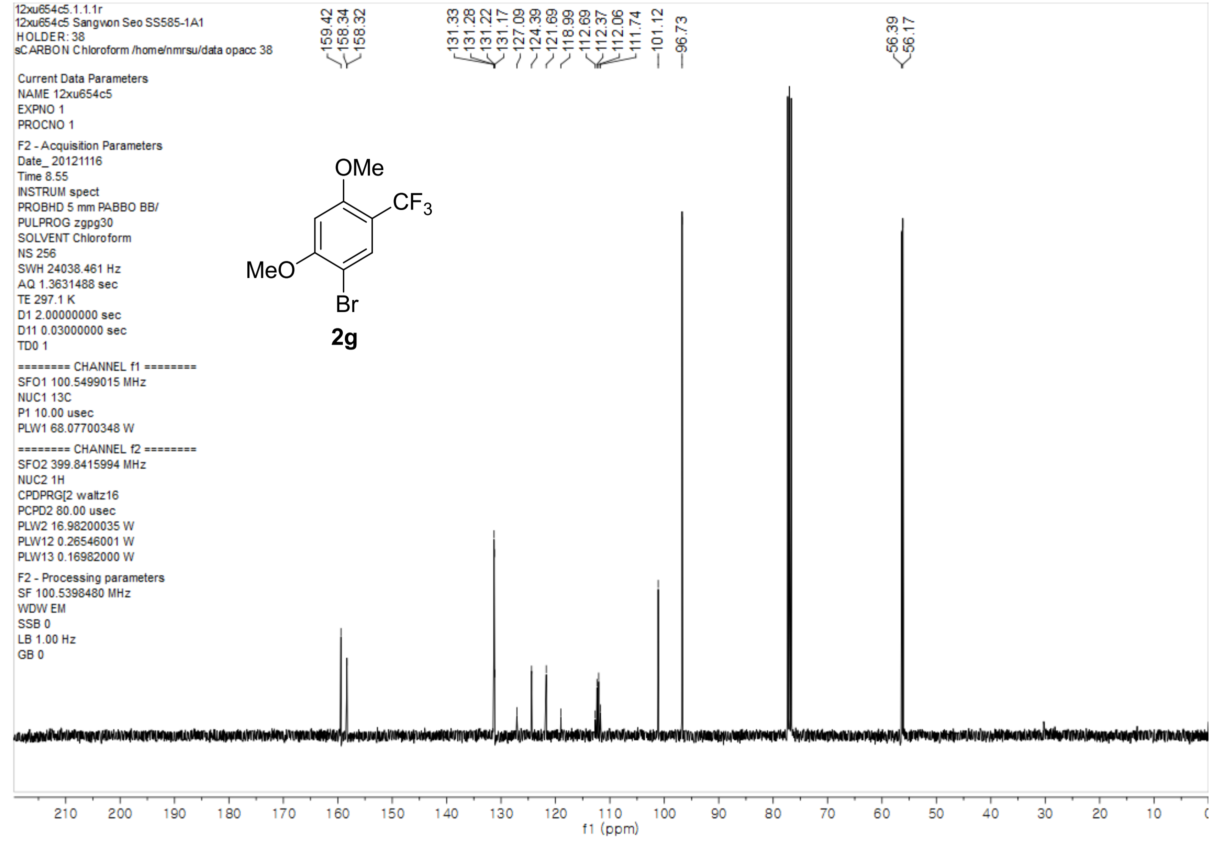
NAME 2012-09-13-MG-37
EXPNO 11
PROCNO 1
Date_ 20120913
Time 13.12
INSTRUM AV400
PROBHD 5 mm PABBO BB-
PULPROG zgig
TD 131072
SOLVENT CDCl3
NS 128
DS 4
SWH 89285.711 Hz
FIDRES 0.681196 Hz
AQ 0.7340532 sec
RG 4100
DW 5.600 usec
DE 7.51 usec
TE 295.5 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

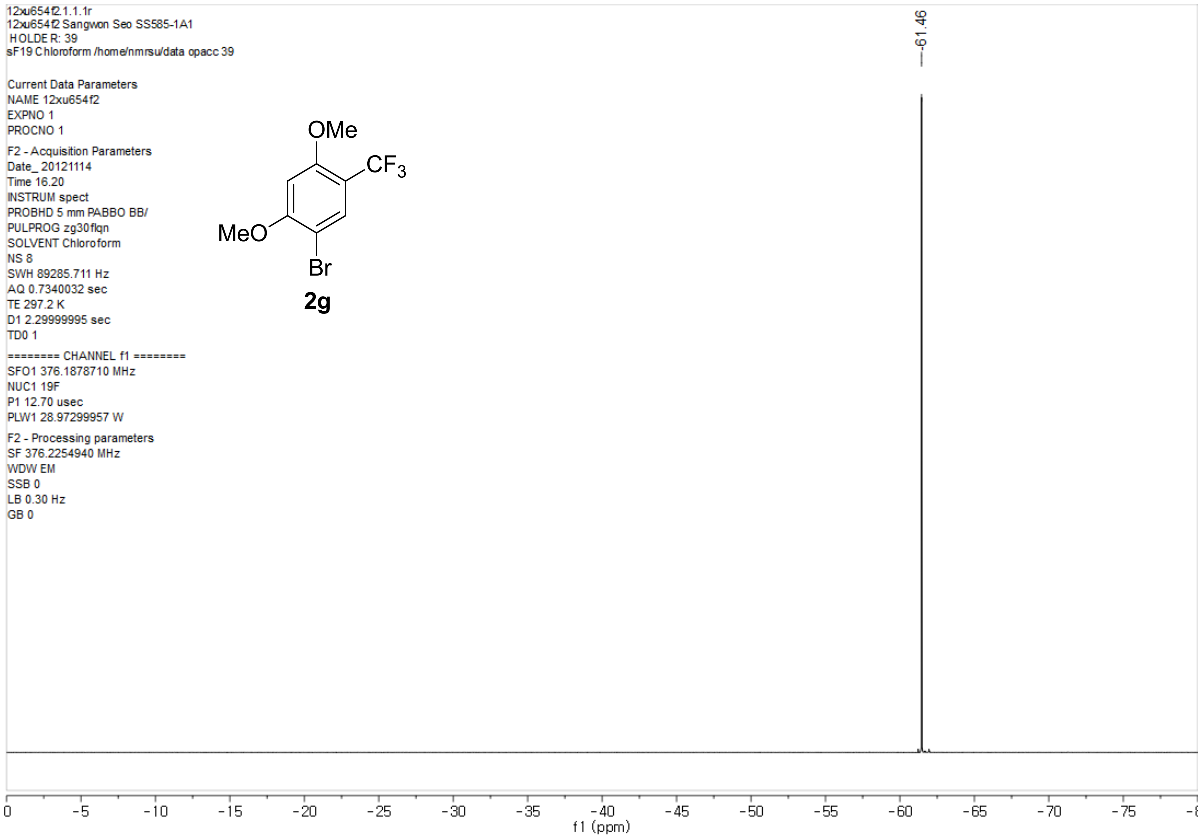
======== CHANNEL f1 ========
NUC1 19F
P1 10.70 usec
PL1 -5.00 dB
PL1W 27.00716019 W
SFO1 376.4607164 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -3.60 dB
PL12 15.31 dB
PL2W 17.83863831 W
PL12W 0.22927761 W
SFO2 400.1316005 MHz
SI 262144
SF 376.4983660 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0

PC 2.00
```


12xu654h1.1.1.1r
12xu654h1 Sangwon Seo SS585-1A1
HOLDER: 39
sPROTON fast Chloroform /home/nmrsu/data opacc 39
Current Data Parameters
NAME 12xu654h1
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20121114
Time 16.19
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg
SOLVENT Chloroform
NS 1
SWH 8012.820 Hz
AQ 2.0447233 sec
TE 297.2 K
D1 15.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 399.8424692 MHz
NUC1 1H
P1 3.33 usec
PLW1 16.98200035 W
F2 - Processing parameters
SF 399.8400074 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
OMe
CF3
MeO
Br
2g
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)


12xu654c5.1.1.1r
12xu654c5 Sangwon Seo SS585-1A1
HOLDER: 38
sCARBON Chloroform /home/nmrsu/data opacc 38
Current Data Parameters
NAME 12xu654c5
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20121116
Time 8.55
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
SOLVENT Chloroform
NS 256
SWH 24038.461 Hz
AQ 1.3631488 sec
TE 297.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 100.5499015 MHz
NUC1 13C
P1 10.00 usec
PLW1 68.07700348 W
======== CHANNEL f2 ========
SFO2 399.8415994 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 16.98200035 W
PLW12 0.26546001 W
PLW13 0.16982000 W
F2 - Processing parameters
SF 100.5398480 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
159.42
158.34
158.32
131.33
131.28
131.22
131.17
127.09
124.39
121.69
118.99
112.69
112.37
112.06
111.74
101.12
96.73
56.39
56.17
OMe
CF3
MeO
Br
2g
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


12xu654f2.1.1.1r
12xu654f2 Sangwon Seo SS585-1A1
HOLDER: 39
sF19 Chloroform /home/nmrsu/data opacc 39

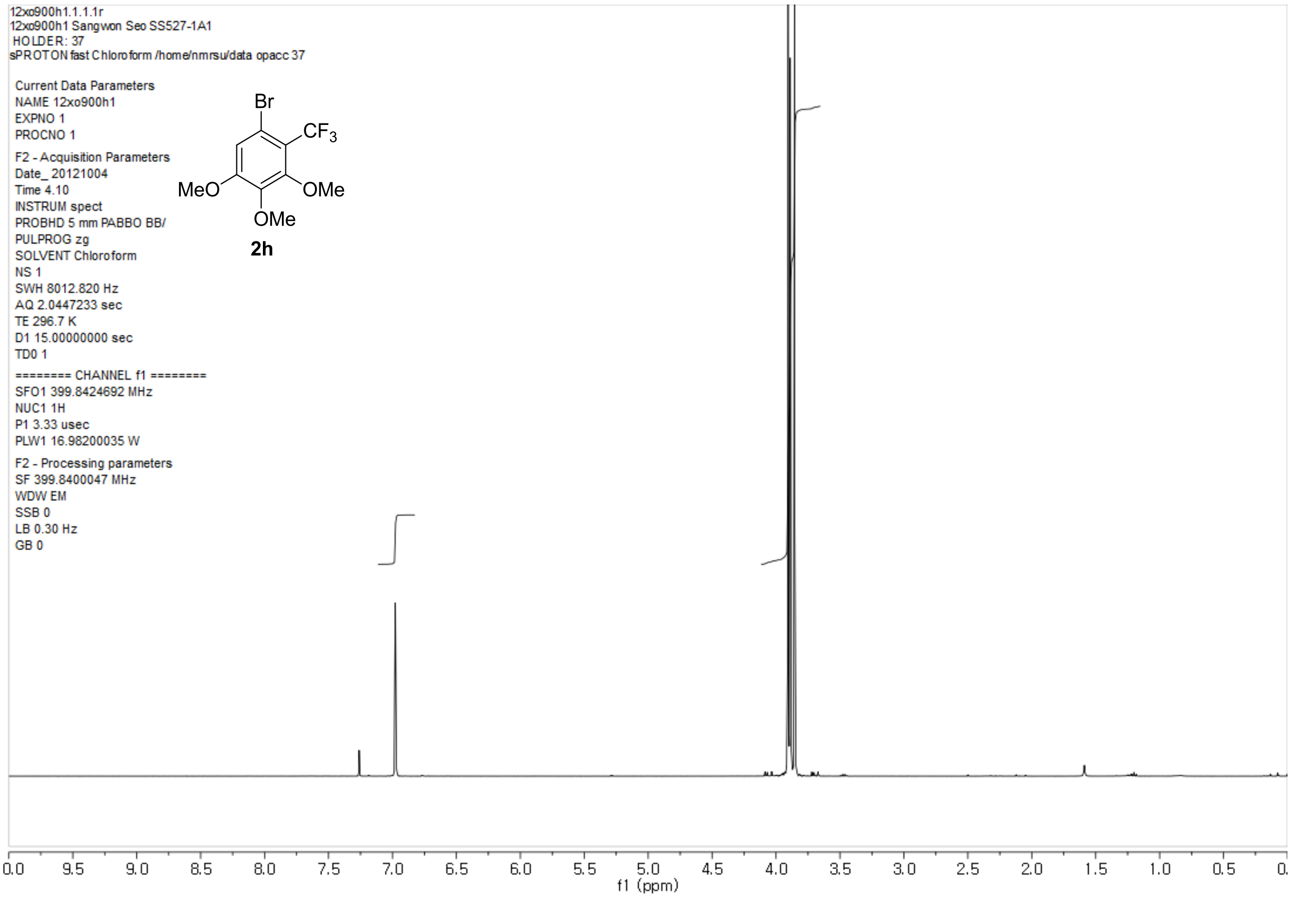
Current Data Parameters
NAME 12xu654f2
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20121114
Time 16.20
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30flqn
SOLVENT Chloroform
NS 8
SWH 89285.711 Hz
AQ 0.7340032 sec
TE 297.2 K
D1 2.29999995 sec
TD0 1

======== CHANNEL f1 ========
SFO1 376.1878710 MHz
NUC1 19F
P1 12.70 usec
PLW1 28.97299957 W

F2 - Processing parameters
SF 376.2254940 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0

2g


12xo900h1.1.1.1r
12xo900h1 Sangwon Seo SS527-1A1
HOLDER: 37
sPROTON fast Chloroform /home/nmrsu/data opacc 37

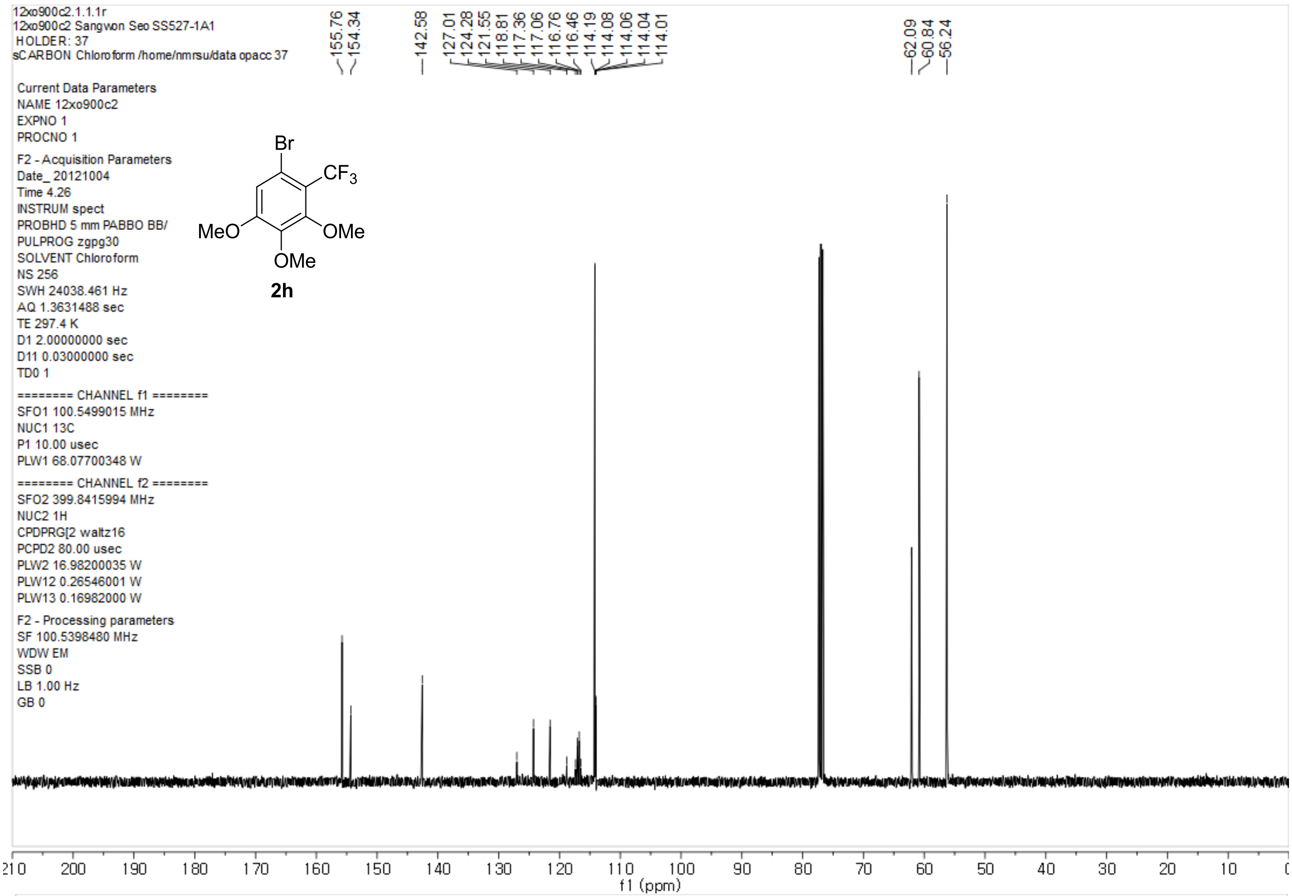
Current Data Parameters
NAME 12xo900h1
EXPNO 1
PROCNO 1

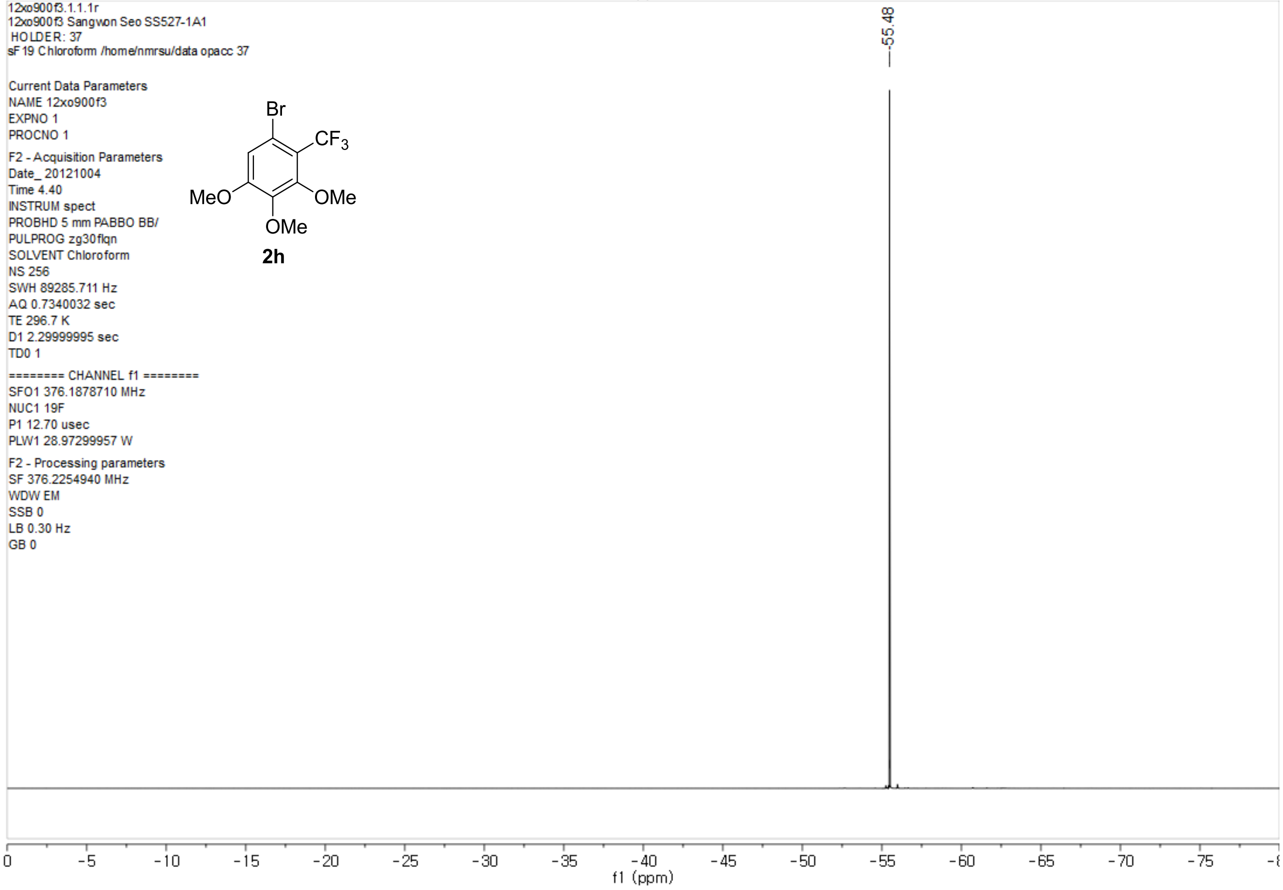
F2 - Acquisition Parameters
Date_ 20121004
Time 4.10
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg
SOLVENT Chloroform
NS 1
SWH 8012.820 Hz
AQ 2.0447233 sec
TE 296.7 K
D1 15.00000000 sec
TD0 1

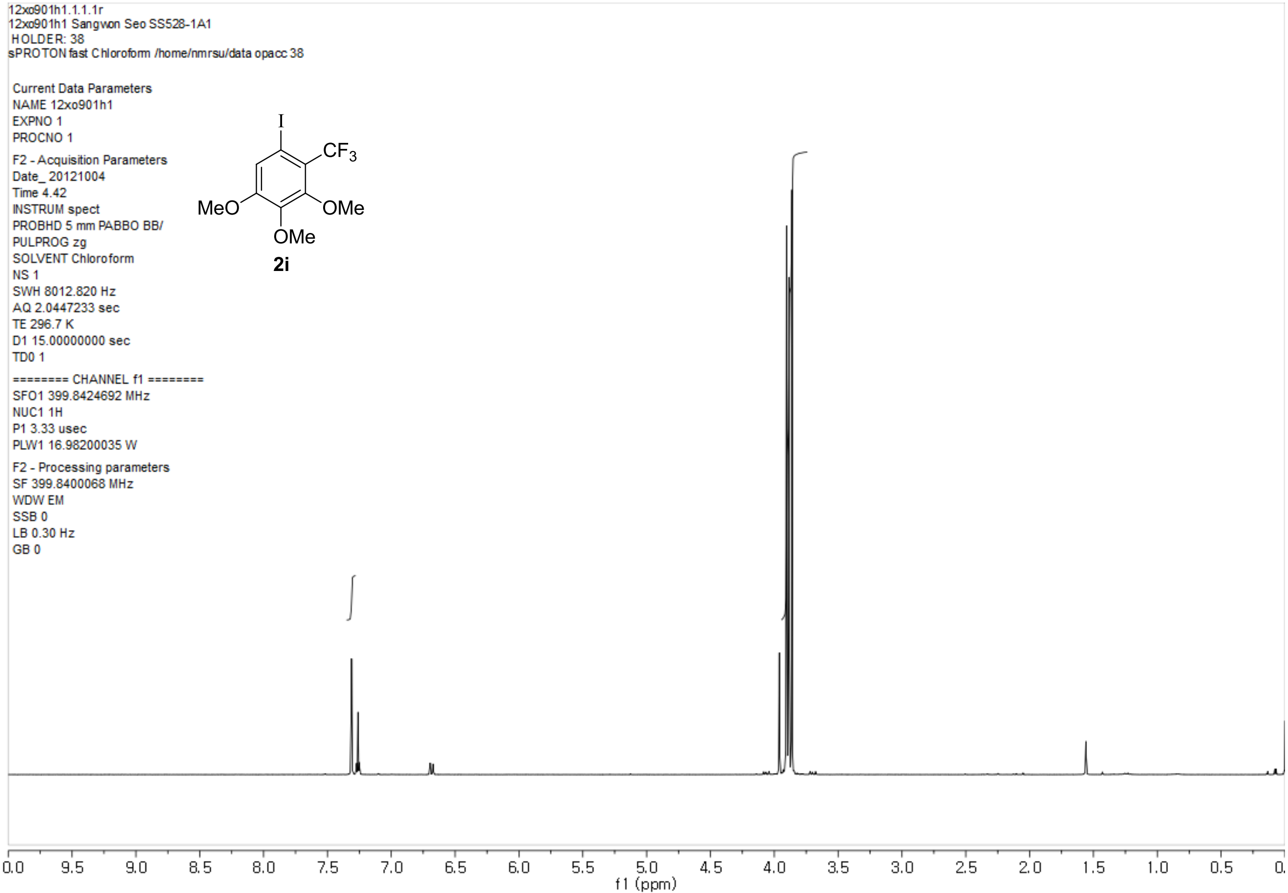
======== CHANNEL f1 ========
SFO1 399.8424692 MHz
NUC1 1H
P1 3.33 usec
PLW1 16.98200035 W

F2 - Processing parameters
SF 399.8400047 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0

2h


12xo900c2.1.1.1r
12xo900c2 Sangwon Seo SS527-1A1
HOLDER: 37
sCARBON Chloroform /home/nmrsu/data opacc 37
Current Data Parameters
NAME 12xo900c2
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20121004
Time 4.26
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
SOLVENT Chloroform
NS 256
SWH 24038.461 Hz
AQ 1.3631488 sec
TE 297.4 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 100.5499015 MHz
NUC1 13C
P1 10.00 usec
PLW1 68.07700348 W
======== CHANNEL f2 ========
SFO2 399.8415994 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 16.98200035 W
PLW12 0.26546001 W
PLW13 0.16982000 W
F2 - Processing parameters
SF 100.5398480 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
Br
CF3
MeO
OMe
OMe
2h
155.76
154.34
142.58
127.01
124.28
121.55
118.81
117.36
117.06
116.76
116.46
114.19
114.08
114.06
114.04
114.01
62.09
60.84
56.24
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


12xo900f3.1.1.1r
12xo900f3 Sangwon Seo SS527-1A1
HOLDER: 37
sF19 Chloroform /home/nmrsu/data opacc 37
Current Data Parameters
NAME 12xo900f3
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20121004
Time 4.40
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30flqn
SOLVENT Chloroform
NS 256
SWH 89285.711 Hz
AQ 0.7340032 sec
TE 296.7 K
D1 2.29999995 sec
TD0 1
======== CHANNEL f1 ========
SFO1 376.1878710 MHz
NUC1 19F
P1 12.70 usec
PLW1 28.97299957 W
F2 - Processing parameters
SF 376.2254940 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
Br
CF3
MeO
OMe
OMe
2h
-55.48
0
-5
-10
-15
-20
-25
-30
-35
-40
-45
-50
-55
-60
-65
-70
-75
f1 (ppm)



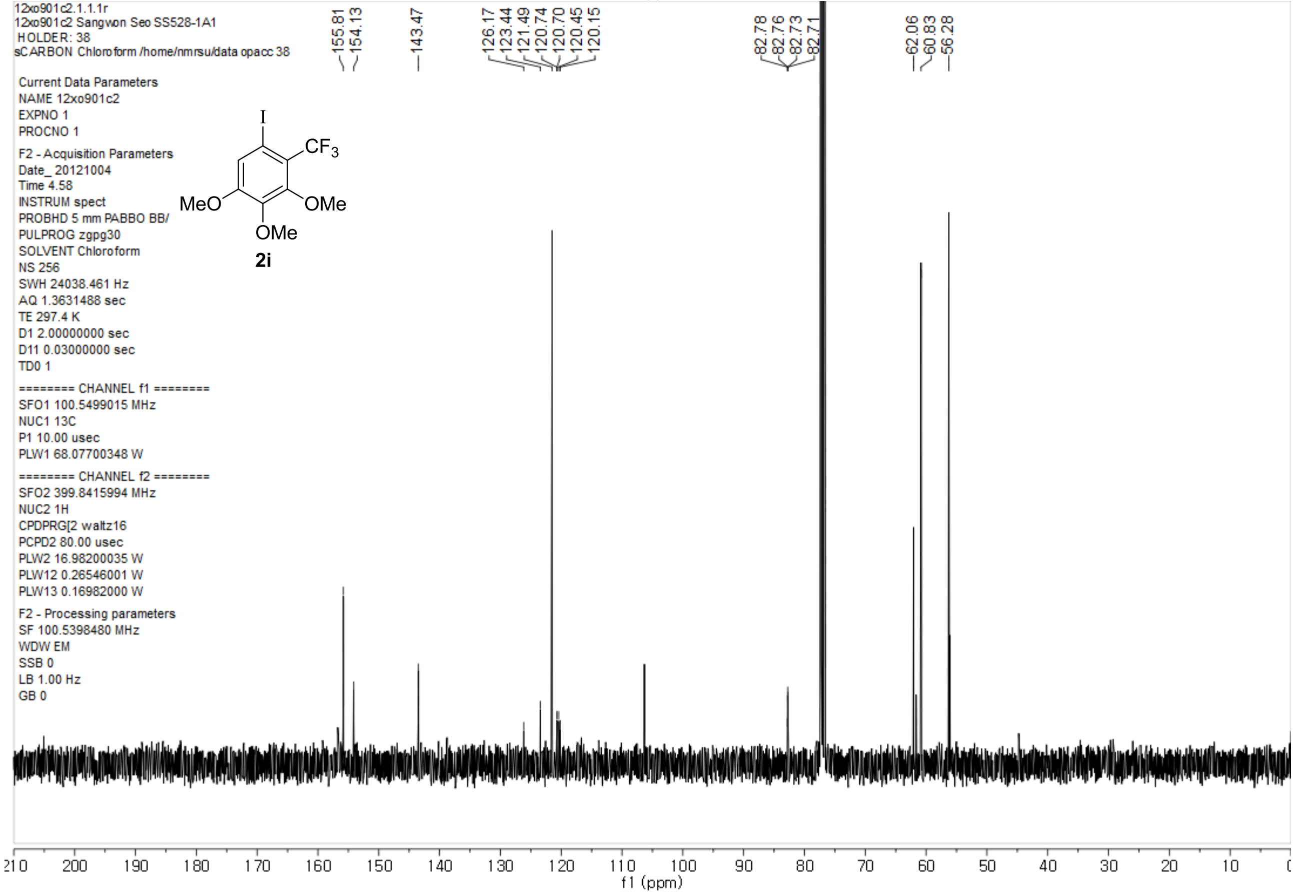
12xo901h1.1.1.1r
12xo901h1 Sangwon Seo SS528-1A1
HOLDER: 38
sPROTON fast Chloroform /home/nmrsu/data opacc 38

Current Data Parameters
NAME 12xo901h1
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20121004
Time 4.42
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg
SOLVENT Chloroform
NS 1
SWH 8012.820 Hz
AQ 2.0447233 sec
TE 296.7 K
D1 15.00000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 399.8424692 MHz
NUC1 1H
P1 3.33 usec
PLW1 16.98200035 W

F2 - Processing parameters
SF 399.8400068 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0



12xo901c2.1.1.1r
12xo901c2 Sangwon Seo SS528-1A1
HOLDER: 38
sCARBON Chloroform /home/nmrsu/data opacc 38

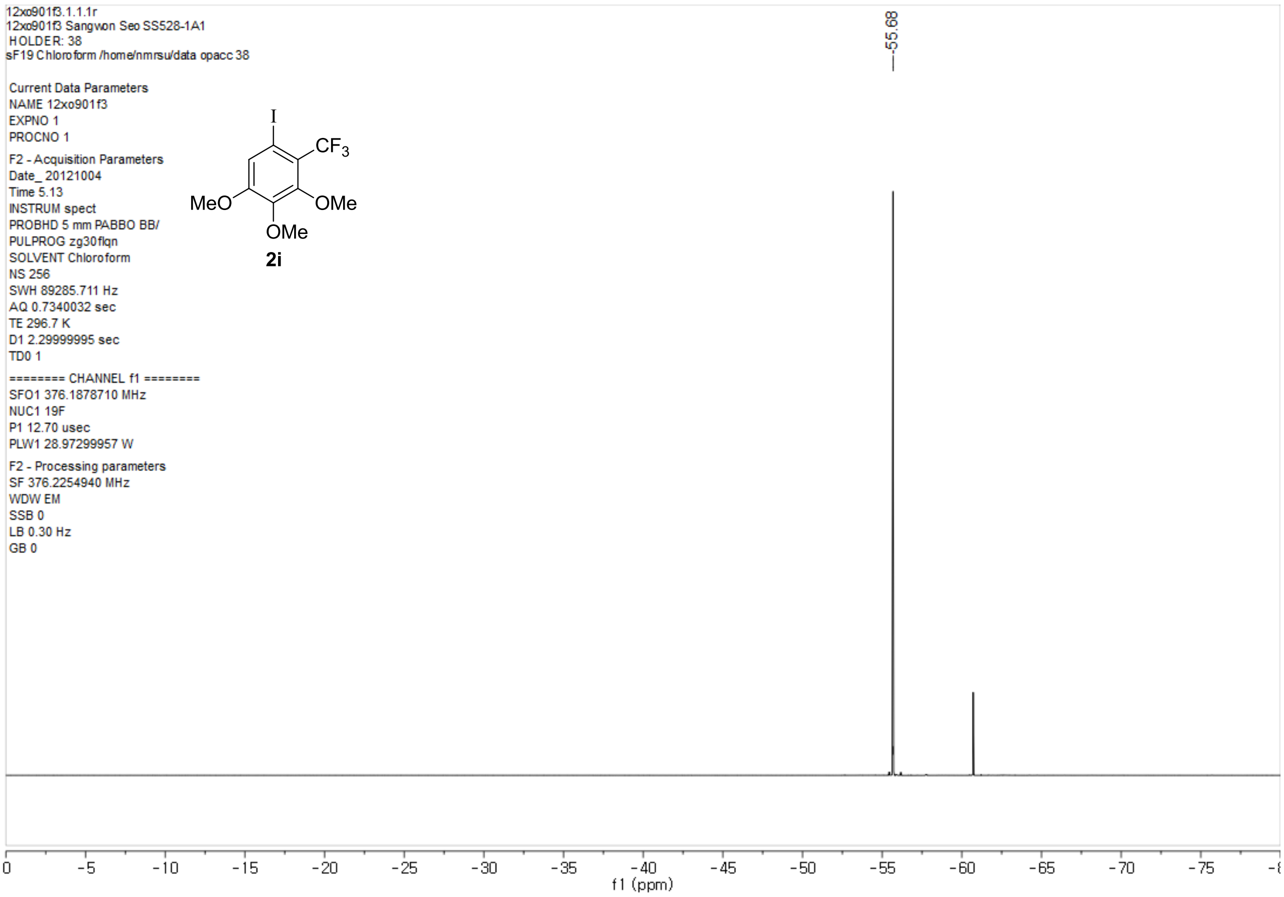
Current Data Parameters
NAME 12xo901c2
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20121004
Time 4.58
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
SOLVENT Chloroform
NS 256
SWH 24038.461 Hz
AQ 1.3631488 sec
TE 297.4 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 100.5499015 MHz
NUC1 13C
P1 10.00 usec
PLW1 68.07700348 W

======== CHANNEL f2 ========
SFO2 399.8415994 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 16.98200035 W
PLW12 0.26546001 W
PLW13 0.16982000 W

F2 - Processing parameters
SF 100.5398480 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0



2i

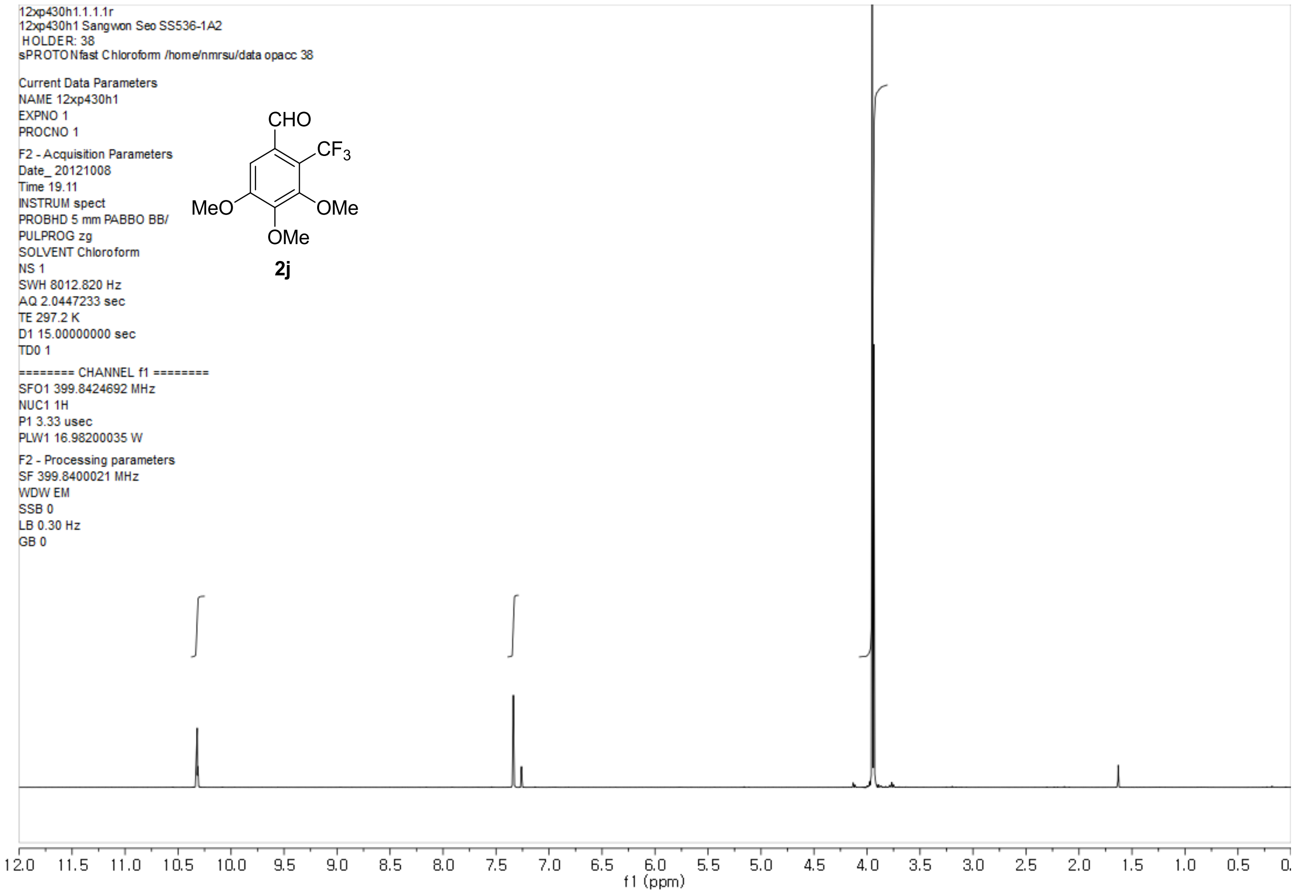
12xo901f3.1.1.1r
12xo901f3 Sangwon Seo SS528-1A1
HOLDER: 38
sF19 Chloroform /home/nmrsu/data opacc 38

Current Data Parameters
NAME 12xo901f3
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20121004
Time 5.13
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30flqn
SOLVENT Chloroform
NS 256
SWH 89285.711 Hz
AQ 0.7340032 sec
TE 296.7 K
D1 2.29999995 sec
TD0 1

======== CHANNEL f1 ========
SFO1 376.1878710 MHz
NUC1 19F
P1 12.70 usec
PLW1 28.97299957 W

F2 - Processing parameters
SF 376.2254940 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0



2j

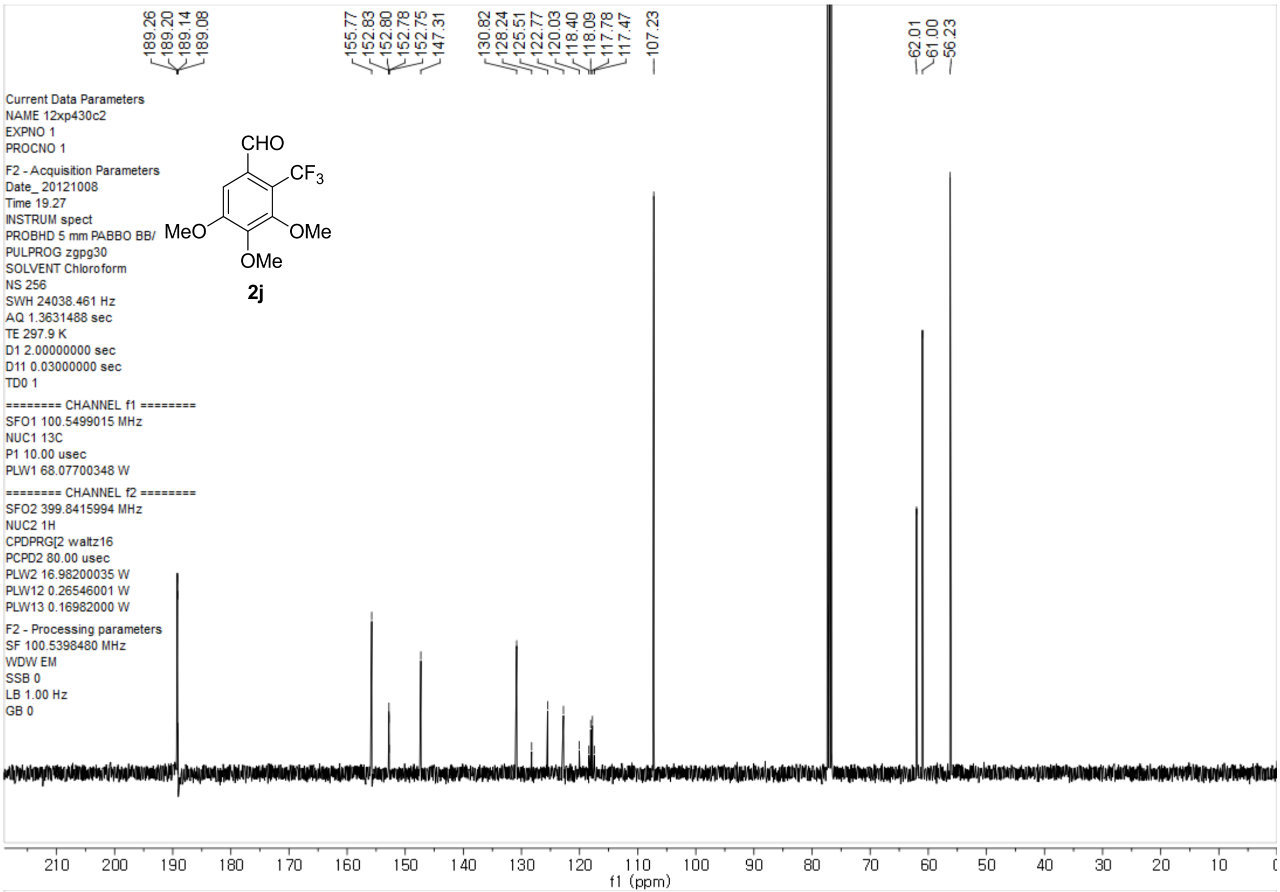
12xp430h1.1.1.1r
12xp430h1 Sangwon Seo SS536-1A2
HOLDER: 38
sPROTONfast Chloroform /home/nmrsu/data opacc 38

Current Data Parameters
NAME 12xp430h1
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20121008
Time 19.11
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg
SOLVENT Chloroform
NS 1
SWH 8012.820 Hz
AQ 2.0447233 sec
TE 297.2 K
D1 15.00000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 399.8424692 MHz
NUC1 1H
P1 3.33 usec
PLW1 16.98200035 W

F2 - Processing parameters
SF 399.8400021 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0



2j

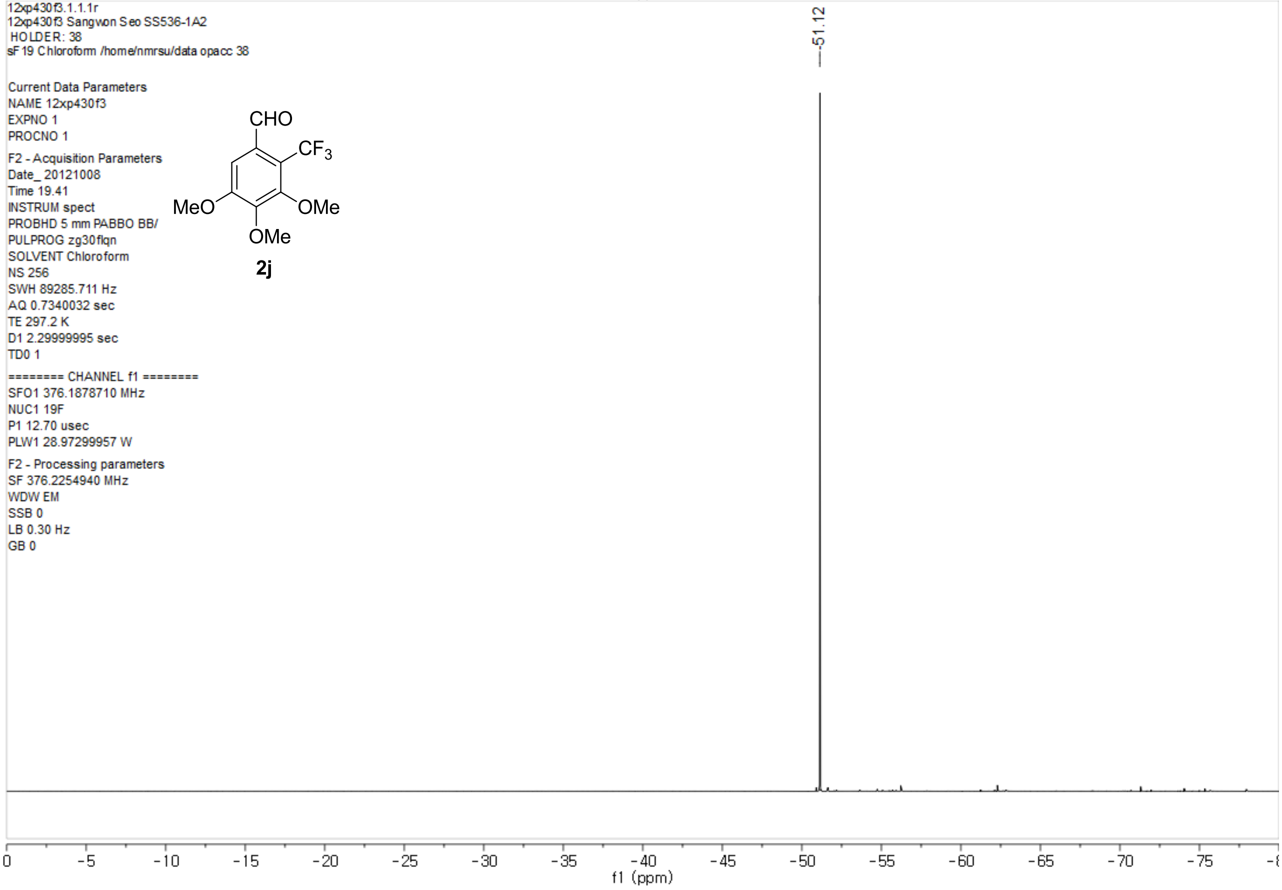
Current Data Parameters
NAME 12xp430c2
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20121008
Time 19.27
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
SOLVENT Chloroform
NS 256
SWH 24038.461 Hz
AQ 1.3631488 sec
TE 297.9 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 100.5499015 MHz
NUC1 13C
P1 10.00 usec
PLW1 68.07700348 W

======== CHANNEL f2 ========
SFO2 399.8415994 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 16.98200035 W
PLW12 0.26546001 W
PLW13 0.16982000 W

F2 - Processing parameters
SF 100.5398480 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0



2j

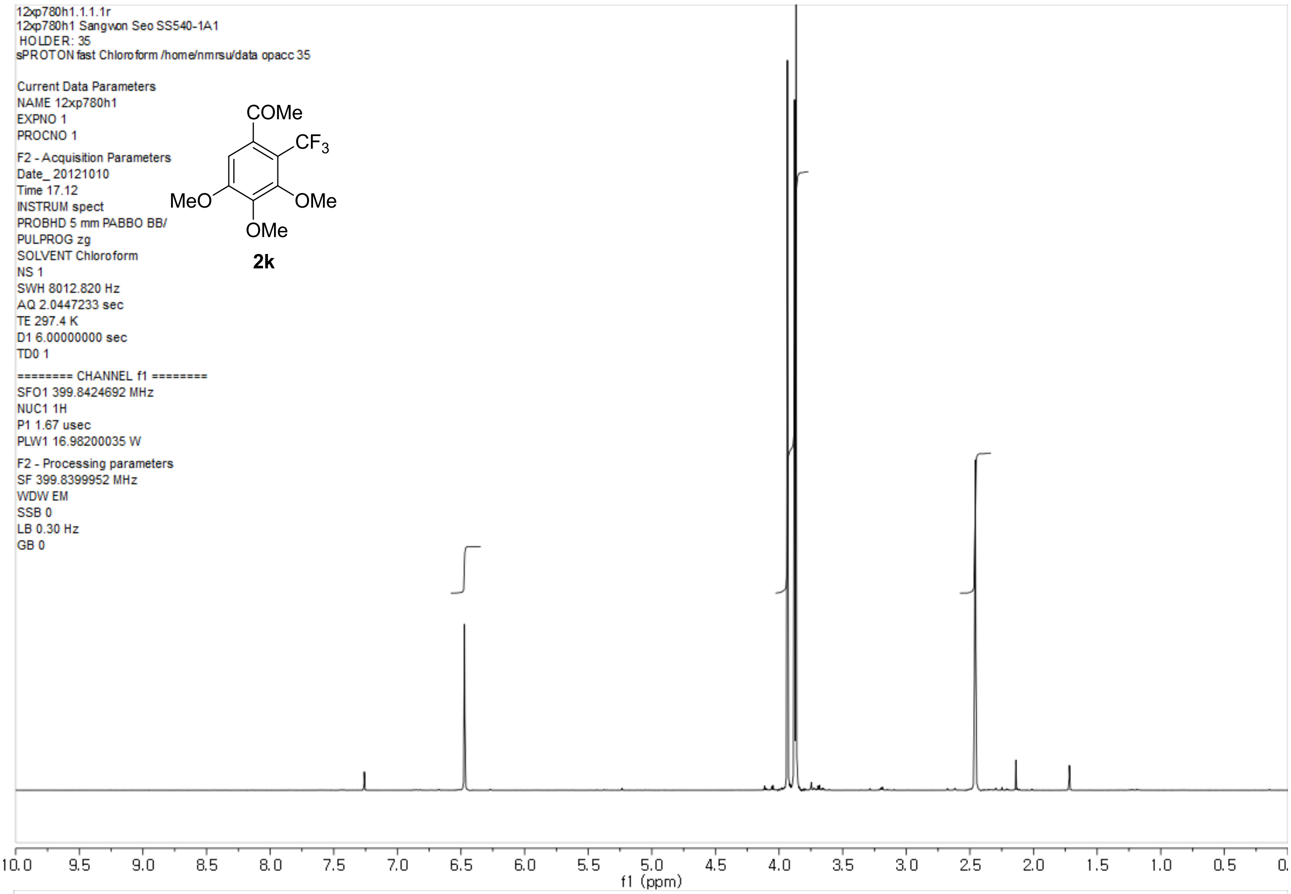
12xp430f3.1.1.1r
12xp430f3 Sangwon Seo SS536-1A2
HOLDER: 38
sF 19 Chloroform /home/nmrsu/data opacc 38

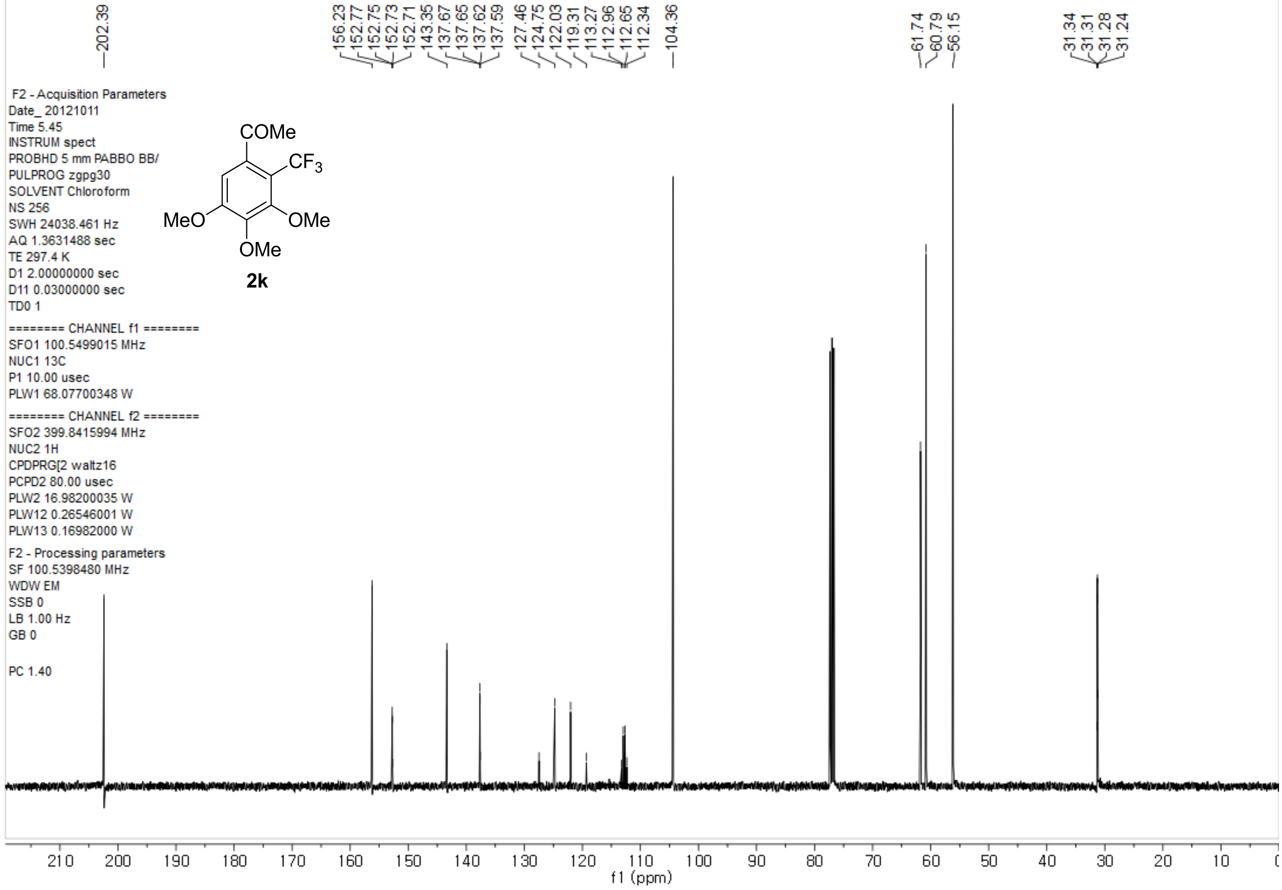
Current Data Parameters
NAME 12xp430f3
EXPNO 1
PROCNO 1

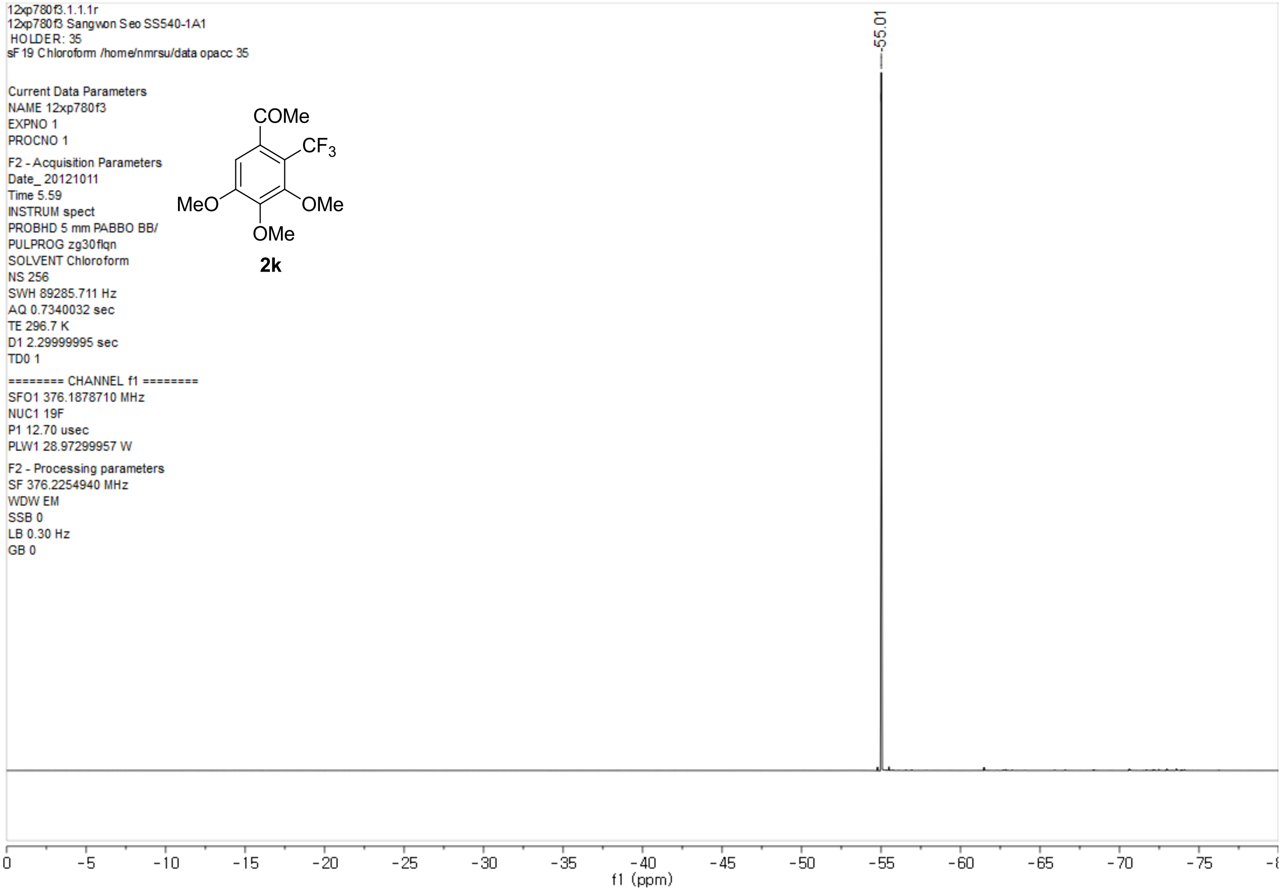
F2 - Acquisition Parameters
Date_ 20121008
Time 19.41
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30flqn
SOLVENT Chloroform
NS 256
SWH 89285.711 Hz
AQ 0.7340032 sec
TE 297.2 K
D1 2.29999995 sec
TD0 1

======== CHANNEL f1 ========
SFO1 376.1878710 MHz
NUC1 19F
P1 12.70 usec
PLW1 28.97299957 W

F2 - Processing parameters
SF 376.2254940 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0

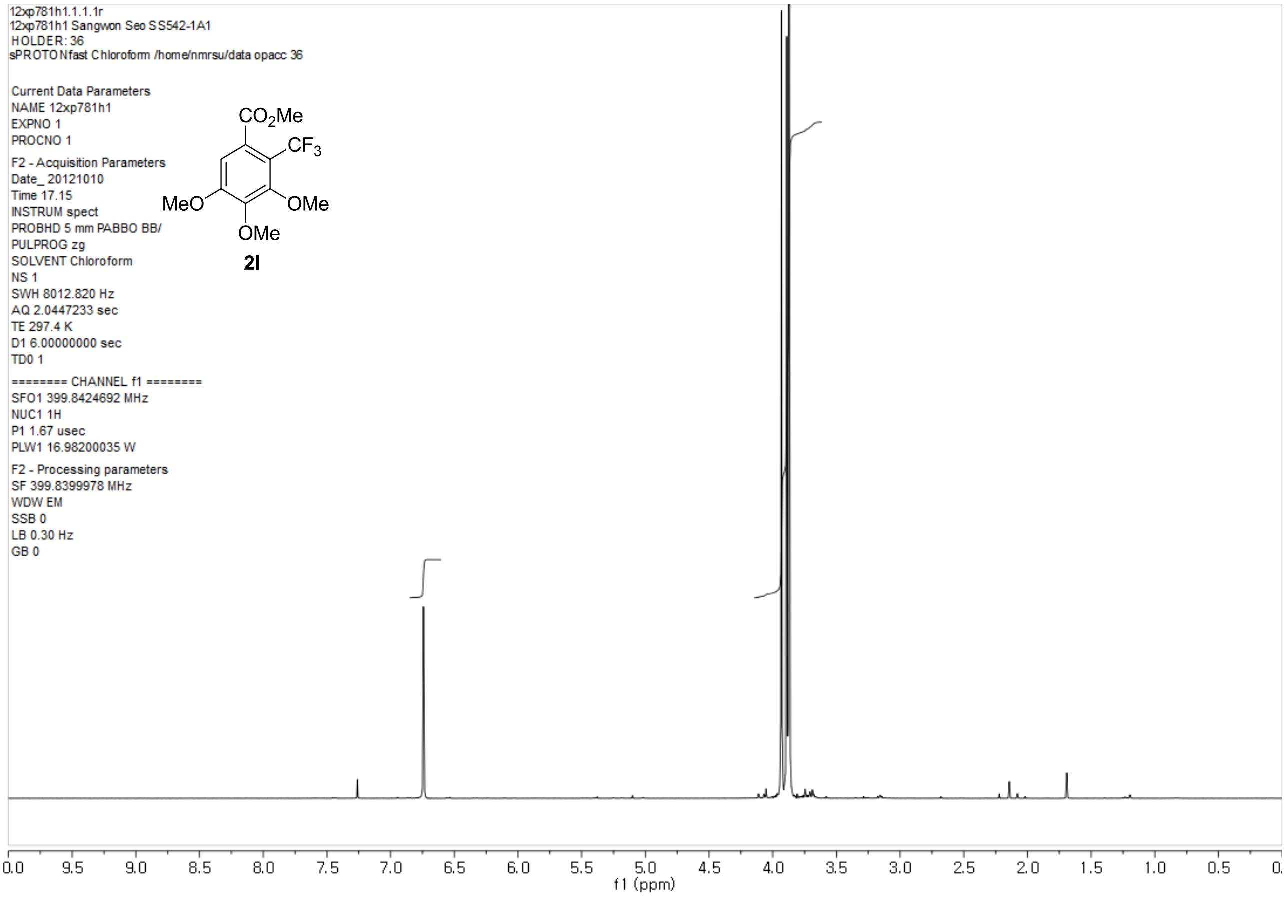

12xp780h1.1.1.1r
12xp780h1 Sangwon Seo SS540-1A1
HOLDER: 35
sPROTON fast Chloroform /home/nmrsu/data opacc 35
Current Data Parameters
NAME 12xp780h1
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20121010
Time 17.12
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg
SOLVENT Chloroform
NS 1
SWH 8012.820 Hz
AQ 2.0447233 sec
TE 297.4 K
D1 6.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 399.8424692 MHz
NUC1 1H
P1 1.67 usec
PLW1 16.98200035 W
F2 - Processing parameters
SF 399.8399952 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
COMe
CF3
MeO
OMe
OMe
2k
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.
f1 (ppm)


202.39
156.23
152.77
152.75
152.73
152.71
143.35
137.67
137.65
137.62
137.59
127.46
124.75
122.03
119.31
113.27
112.96
112.65
112.34
104.36
61.74
60.79
56.15
31.34
31.31
31.28
31.24
F2 - Acquisition Parameters
Date_ 20121011
Time 5.45
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
SOLVENT Chloroform
NS 256
SWH 24038.461 Hz
AQ 1.3631488 sec
TE 297.4 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 100.5499015 MHz
NUC1 13C
P1 10.00 usec
PLW1 68.07700348 W
======== CHANNEL f2 ========
SFO2 399.8415994 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 16.98200035 W
PLW12 0.26546001 W
PLW13 0.16982000 W
F2 - Processing parameters
SF 100.5398480 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
COMe
CF3
MeO
OMe
OMe
2k
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)



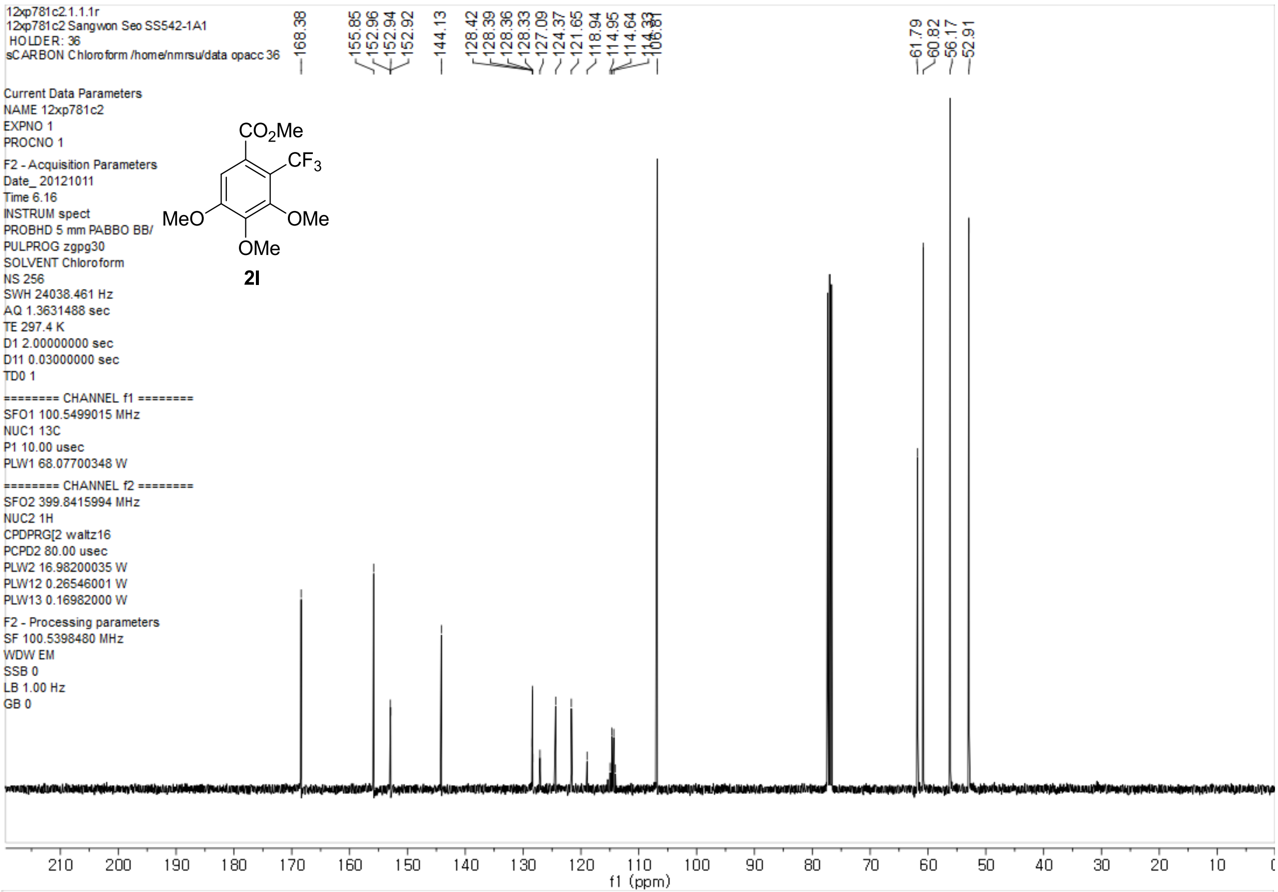
```
12xp780f3.1.1.1r
12xp780f3 Sangwon Seo SS540-1A1
 HOLDER: 35
sF19 Chloroform /home/nmrsu/data opacc 35

Current Data Parameters
NAME 12xp780f3
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20121011
Time 5.59
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30flqn
SOLVENT Chloroform
NS 256
SWH 89285.711 Hz
AQ 0.7340032 sec
TE 296.7 K
D1 2.29999995 sec
TD0 1
======== CHANNEL f1 ========
SFO1 376.1878710 MHz
NUC1 19F
P1 12.70 usec
PLW1 28.97299957 W
F2 - Processing parameters
SF 376.2254940 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
```



```
12xp781h1.1.1.1r
12xp781h1 Sangwon Seo SS542-1A1
 HOLDER: 36
sPROTONfast Chloroform /home/nmrsu/data opacc 36

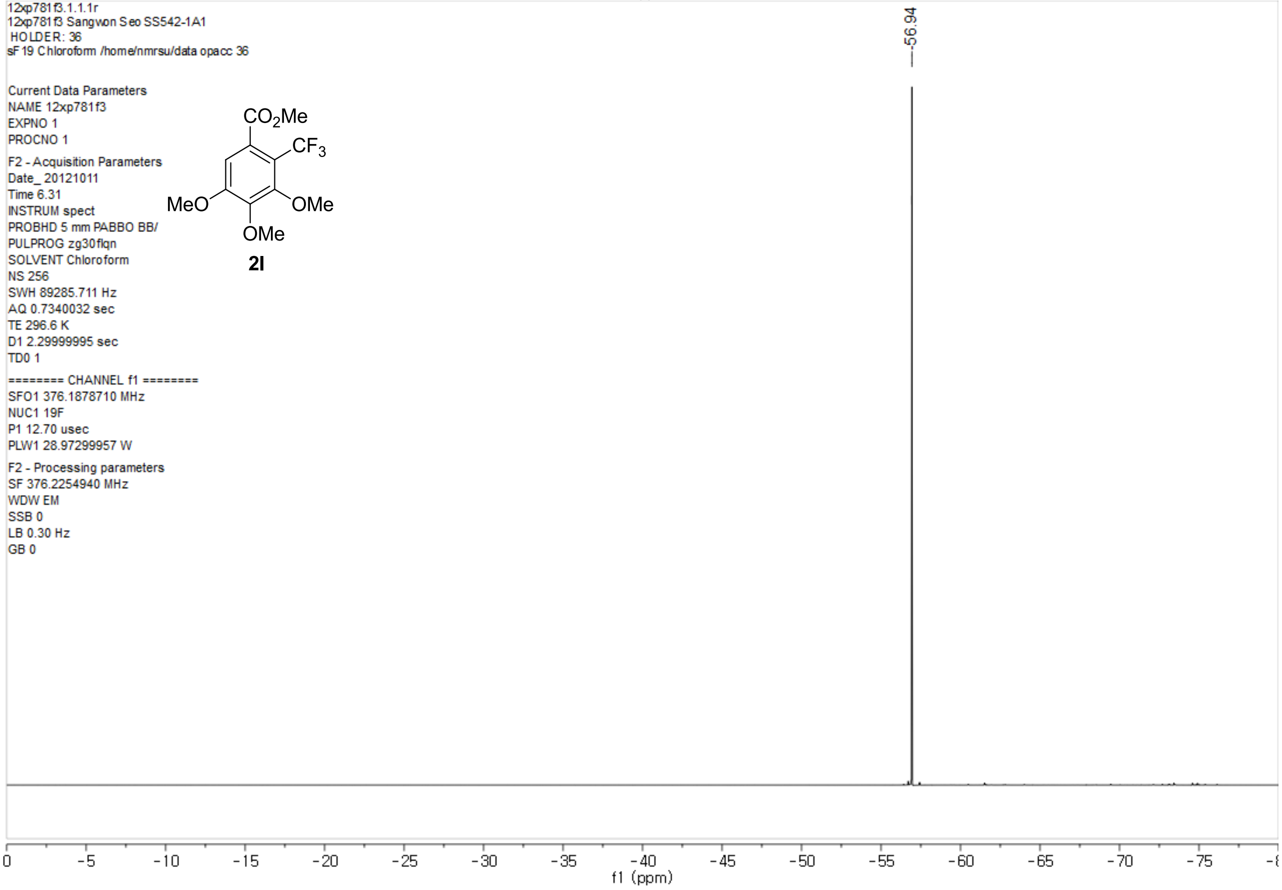
Current Data Parameters
NAME 12xp781h1
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20121010
Time 17.15
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg
SOLVENT Chloroform
NS 1
SWH 8012.820 Hz
AQ 2.0447233 sec
TE 297.4 K
D1 6.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 399.8424692 MHz
NUC1 1H
P1 1.67 usec
PLW1 16.98200035 W
F2 - Processing parameters
SF 399.8399978 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
```



2l

```
12xp781c2.1.1.1r
12xp781c2 Sangwon Seo SS542-1A1
 HOLDER: 36
sCARBON Chloroform /home/nmrsu/data opacc 36

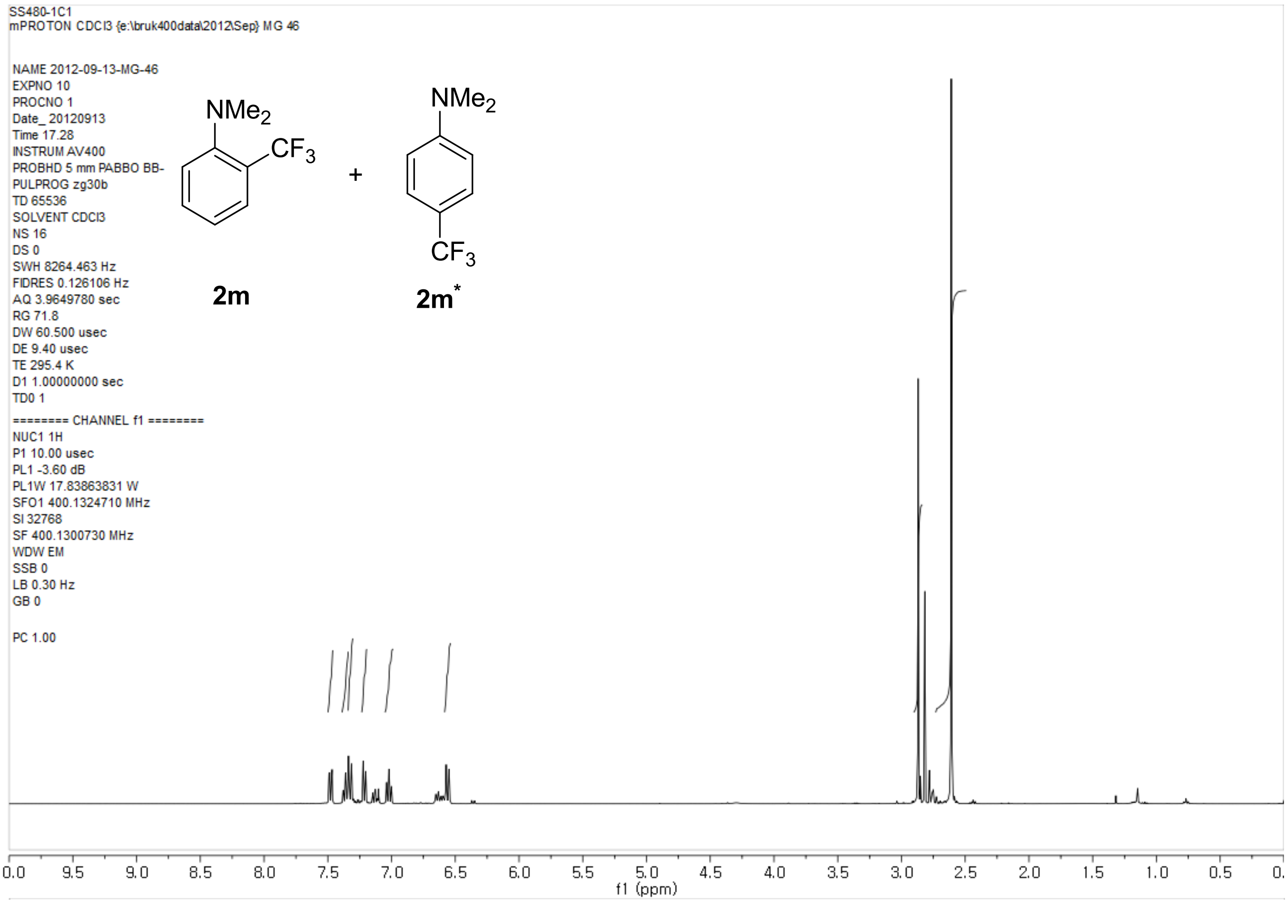
Current Data Parameters
NAME 12xp781c2
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20121011
Time 6.16
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
SOLVENT Chloroform
NS 256
SWH 24038.461 Hz
AQ 1.3631488 sec
TE 297.4 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 100.5499015 MHz
NUC1 13C
P1 10.00 usec
PLW1 68.07700348 W
======== CHANNEL f2 ========
SFO2 399.8415994 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 16.98200035 W
PLW12 0.26546001 W
PLW13 0.16982000 W
F2 - Processing parameters
SF 100.5398480 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
```



2l

```
12xp781f3.1.1.1r
12xp781f3 Sangwon Seo SS542-1A1
 HOLDER: 36
sF19 Chloroform /home/nmrsu/data opacc 36

Current Data Parameters
NAME 12xp781f3
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20121011
Time 6.31
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30flqn
SOLVENT Chloroform
NS 256
SWH 89285.711 Hz
AQ 0.7340032 sec
TE 296.6 K
D1 2.29999995 sec
TD0 1
======== CHANNEL f1 ========
SFO1 376.1878710 MHz
NUC1 19F
P1 12.70 usec
PLW1 28.97299957 W
F2 - Processing parameters
SF 376.2254940 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
```

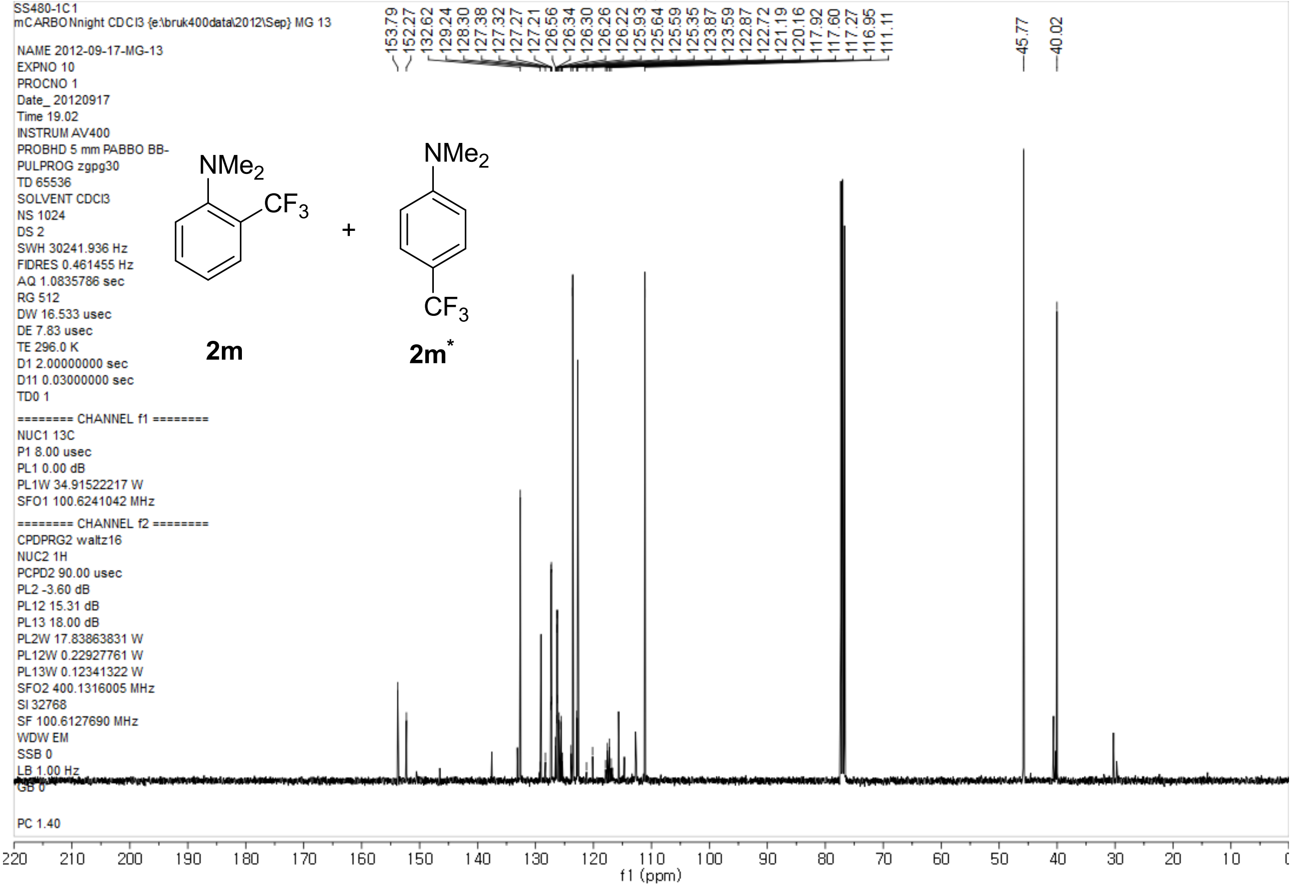


SS480-1C1
mPROTON CDCl3 {e:\bruk400data\2012\Sep} MG 46

NAME 2012-09-13-MG-46
EXPNO 10
PROCNO 1
Date_ 20120913
Time 17.28
INSTRUM AV400
PROBHD 5 mm PABBO BB-
PULPROG zg30b
TD 65536
SOLVENT CDCl3
NS 16
DS 0
SWH 8264.463 Hz
FIDRES 0.126106 Hz
AQ 3.9649780 sec
RG 71.8
DW 60.500 usec
DE 9.40 usec
TE 295.4 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 -3.60 dB
PL1W 17.83863831 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300730 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0

PC 1.00



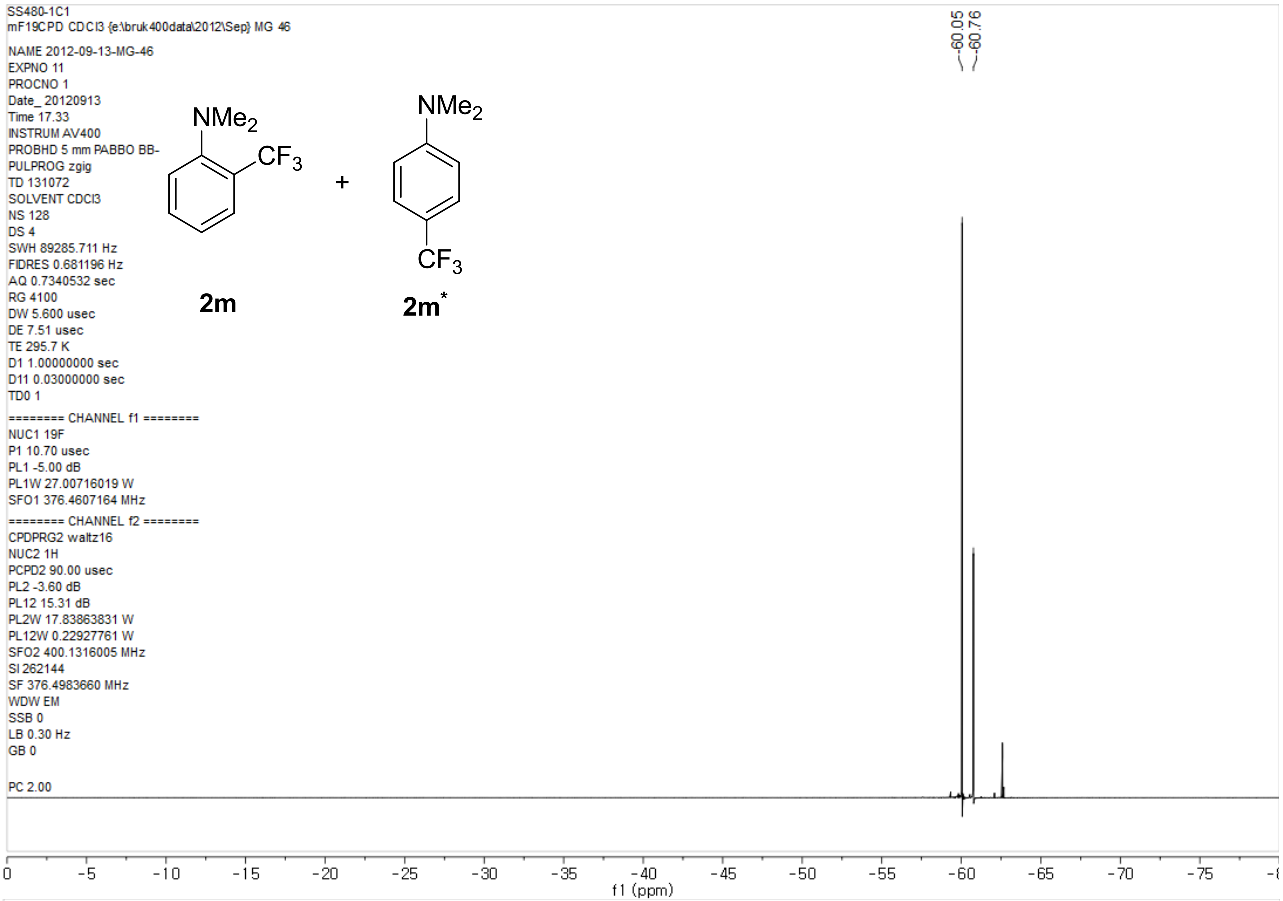
SS480-1C1
mCARBONnight CDCl3 {e:\bruk400data\2012\Sep} MG 13

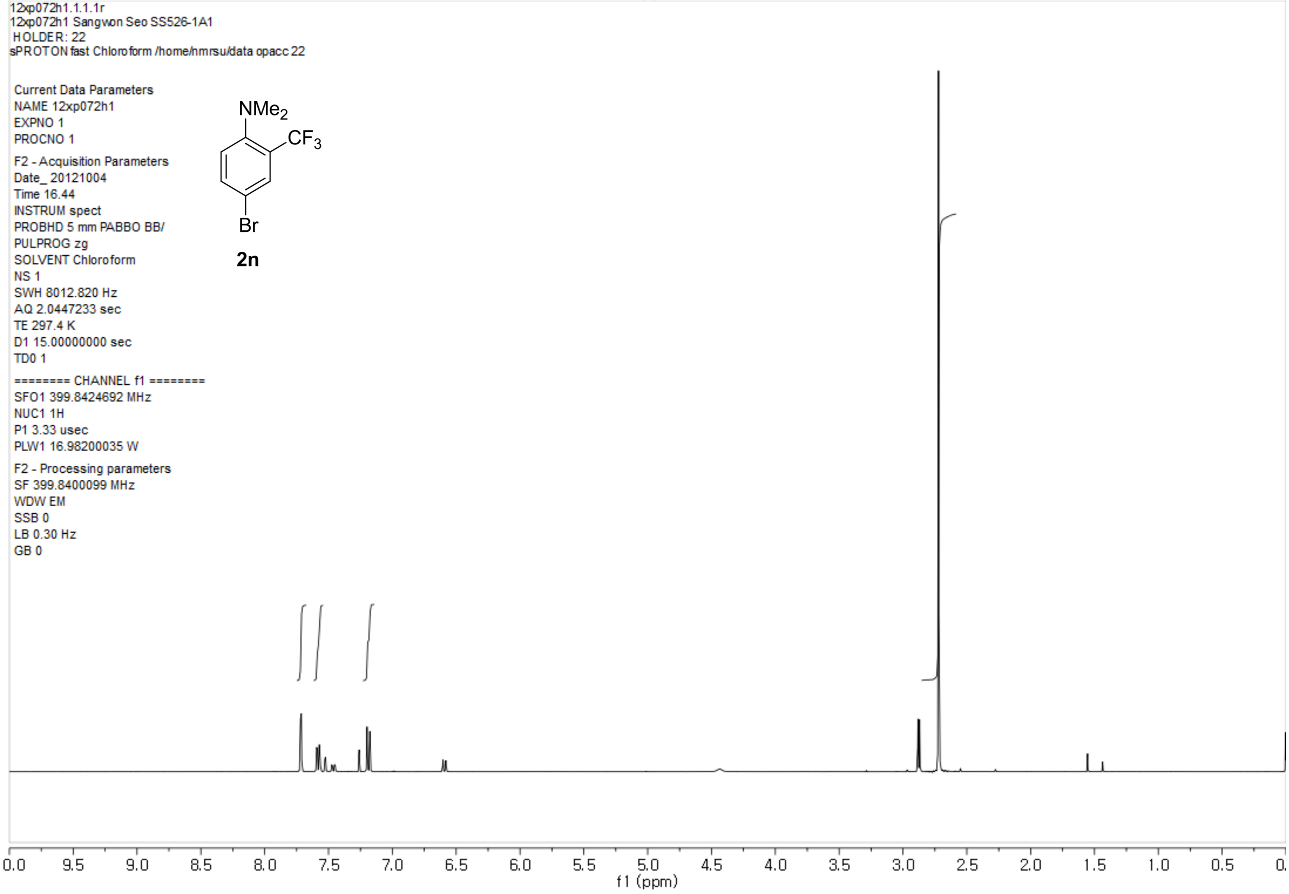
NAME 2012-09-17-MG-13
EXPNO 10
PROCNO 1
Date_ 20120917
Time 19.02
INSTRUM AV400
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 2
SWH 30241.936 Hz
FIDRES 0.461455 Hz
AQ 1.0835786 sec
RG 512
DW 16.533 usec
DE 7.83 usec
TE 296.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

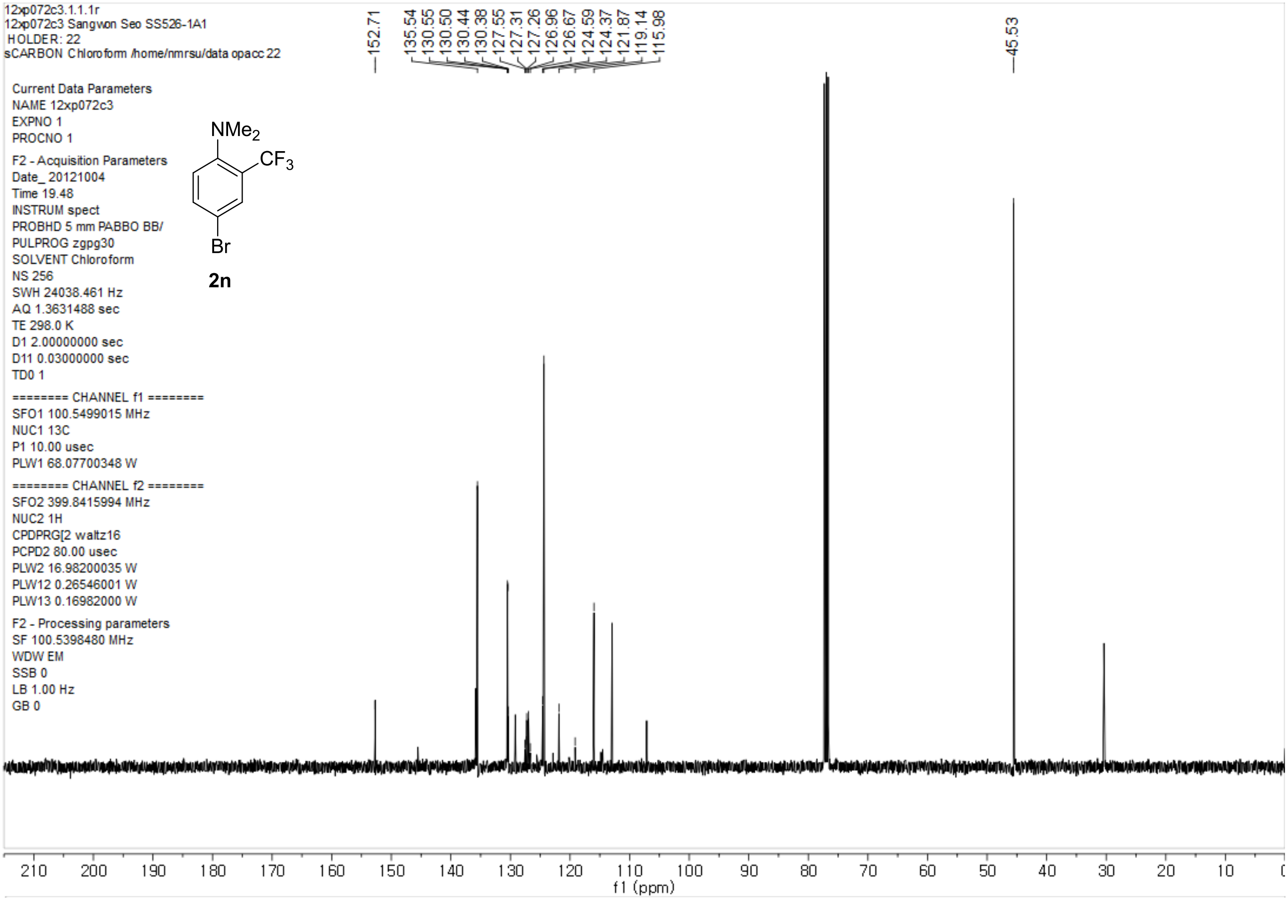
======== CHANNEL f1 ========
NUC1 13C
P1 8.00 usec
PL1 0.00 dB
PL1W 34.91522217 W
SFO1 100.6241042 MHz

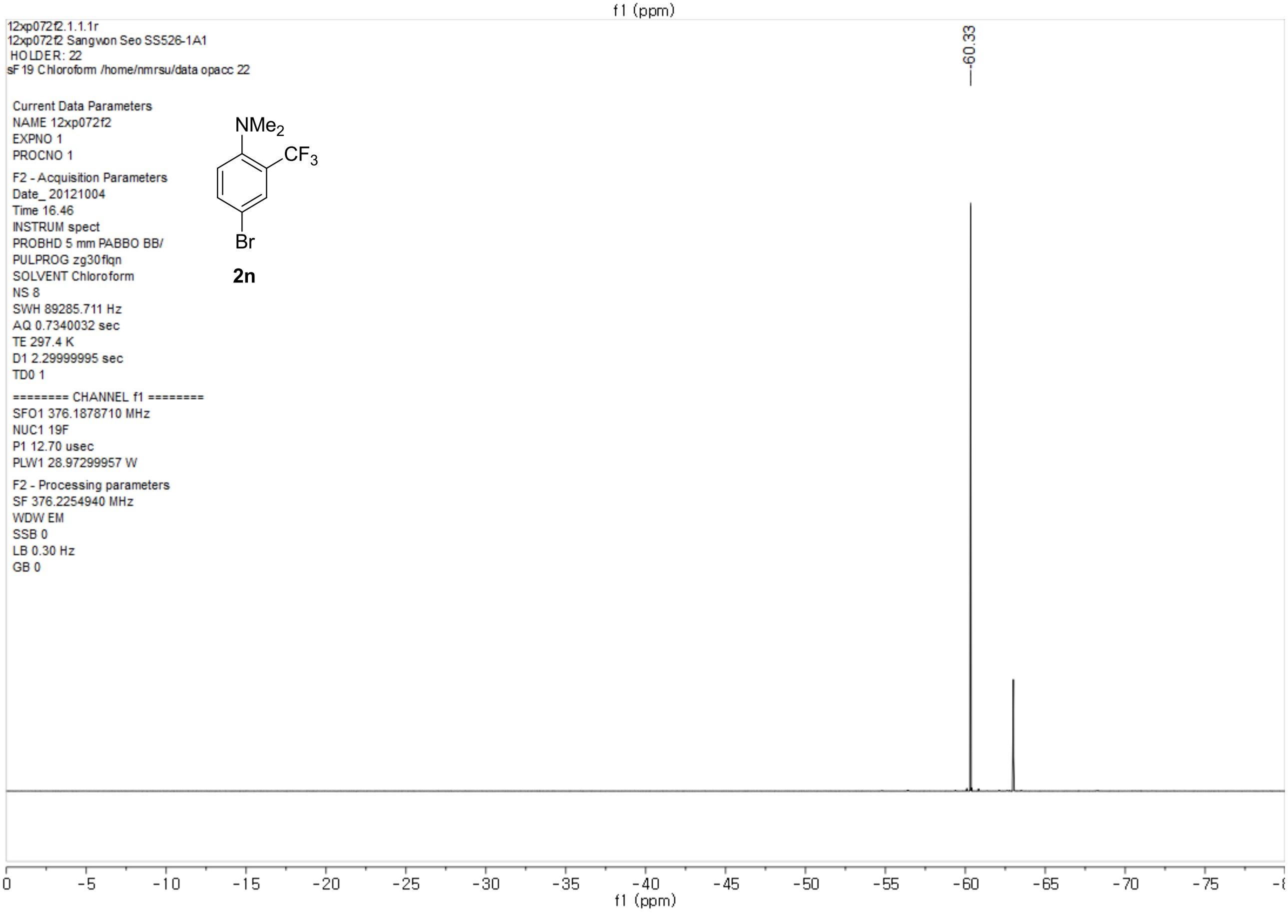
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -3.60 dB
PL12 15.31 dB
PL13 18.00 dB
PL2W 17.83863831 W
PL12W 0.22927761 W
PL13W 0.12341322 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0

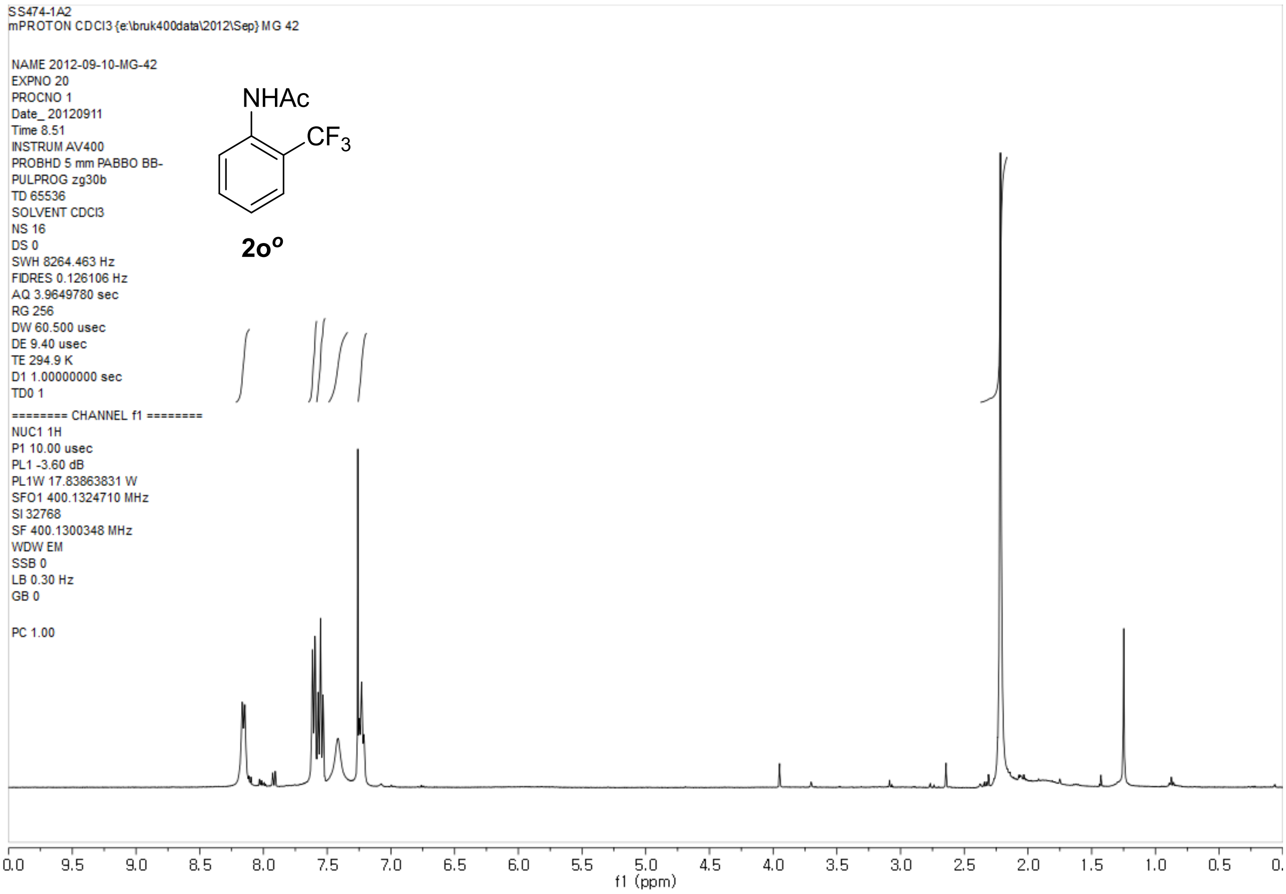
PC 1.40

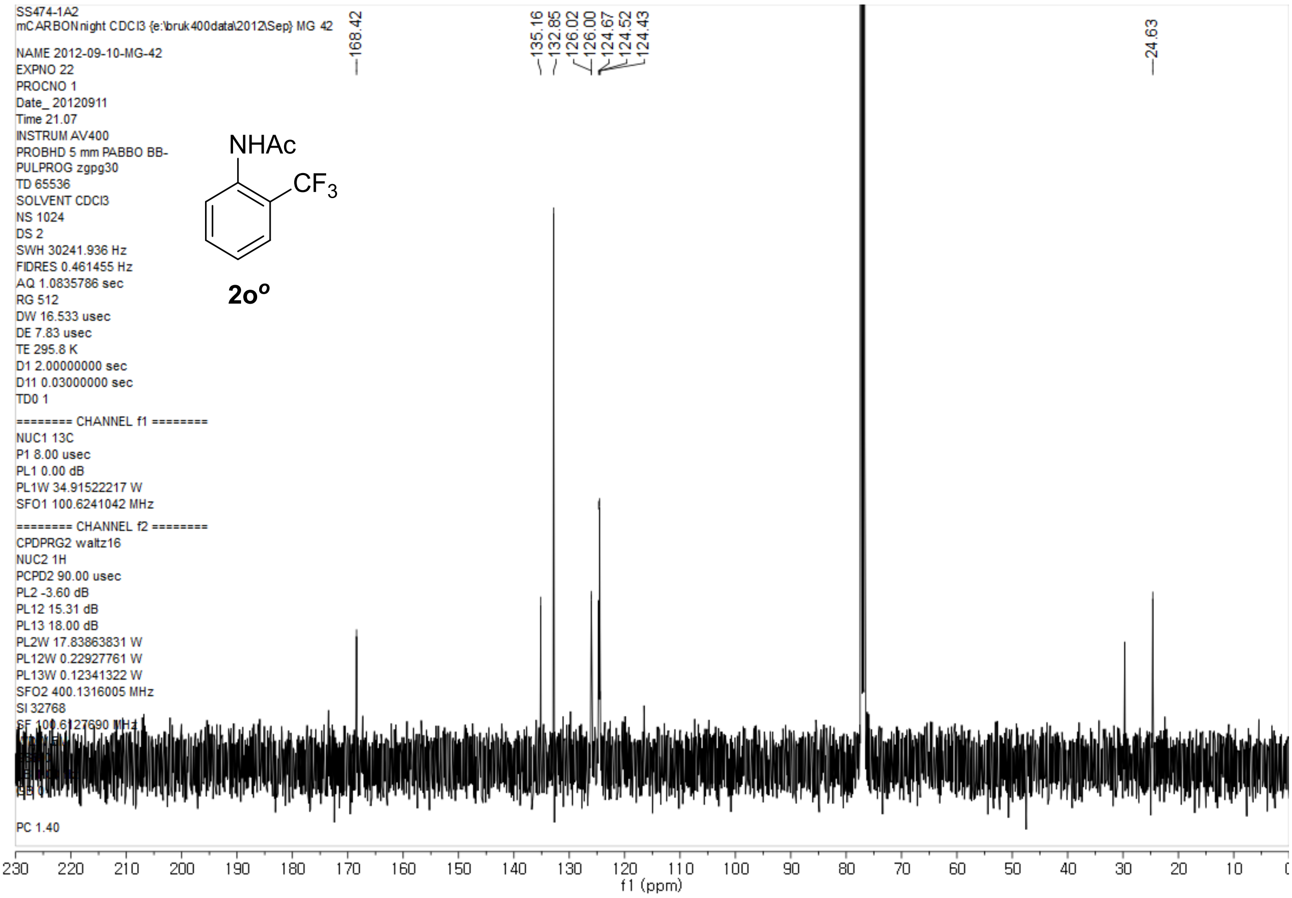

SS480-1C1
mF19CPD CDCl3 {e:\bruk400data\2012\Sep} MG 46
NAME 2012-09-13-MG-46
EXPNO 11
PROCNO 1
Date_ 20120913
Time 17.33
INSTRUM AV400
PROBHD 5 mm PABBO BB-
PULPROG zgig
TD 131072
SOLVENT CDCl3
NS 128
DS 4
SWH 89285.711 Hz
FIDRES 0.681196 Hz
AQ 0.7340532 sec
RG 4100
DW 5.600 usec
DE 7.51 usec
TE 295.7 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 19F
P1 10.70 usec
PL1 -5.00 dB
PL1W 27.00716019 W
SFO1 376.4607164 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -3.60 dB
PL12 15.31 dB
PL2W 17.83863831 W
PL12W 0.22927761 W
SFO2 400.1316005 MHz
SI 262144
SF 376.4983660 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 2.00
NMe2
CF3
+
NMe2
CF3
2m
2m*
-60.05
-60.76
0
-5
-10
-15
-20
-25
-30
-35
-40
-45
-50
-55
-60
-65
-70
-75
f1 (ppm)

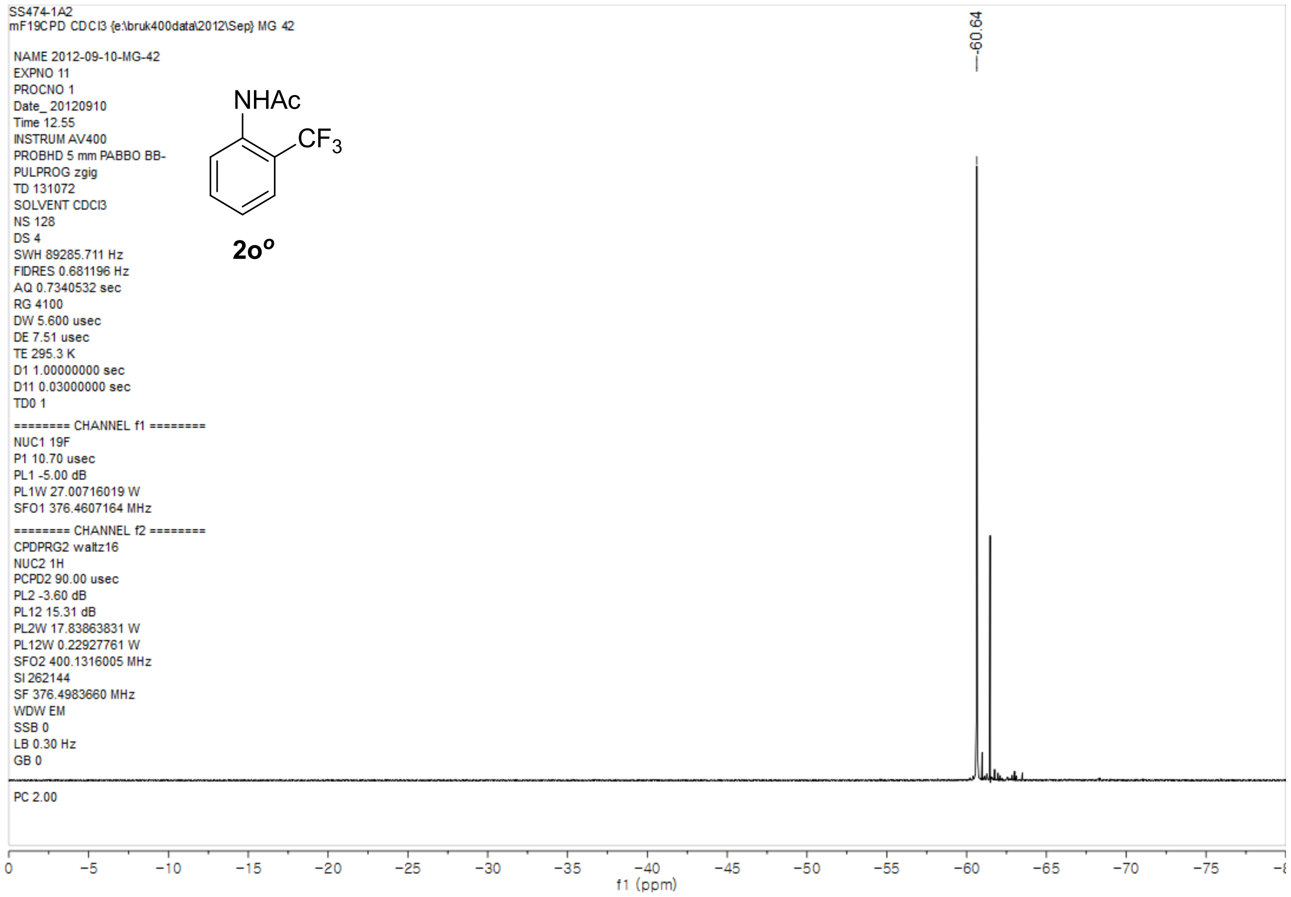

12xp072h1.1.1.1r
12xp072h1 Sangwon Seo SS526-1A1
HOLDER: 22
sPROTON fast Chloroform /home/nmrsu/data opacc 22
Current Data Parameters
NAME 12xp072h1
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20121004
Time 16.44
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg
SOLVENT Chloroform
NS 1
SWH 8012.820 Hz
AQ 2.0447233 sec
TE 297.4 K
D1 15.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 399.8424692 MHz
NUC1 1H
P1 3.33 usec
PLW1 16.98200035 W
F2 - Processing parameters
SF 399.8400099 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
NMe2
CF3
Br
2n
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)

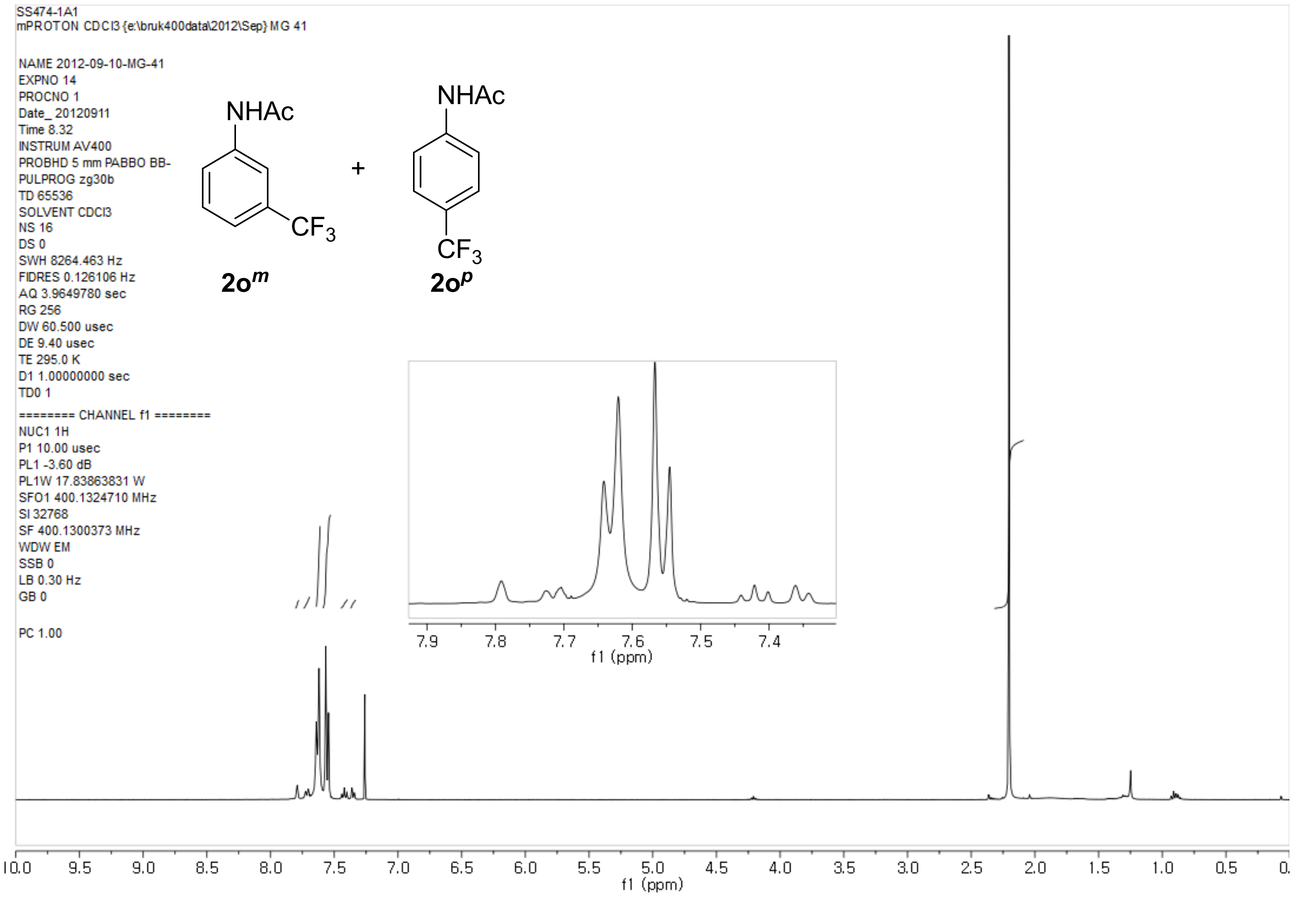

12xp072c3.1.1.1r
12xp072c3 Sangwon Seo SS526-1A1
HOLDER: 22
sCARBON Chloroform /home/nmrsu/data opacc 22
Current Data Parameters
NAME 12xp072c3
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20121004
Time 19.48
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
SOLVENT Chloroform
NS 256
SWH 24038.461 Hz
AQ 1.3631488 sec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 100.5499015 MHz
NUC1 13C
P1 10.00 usec
PLW1 68.07700348 W
======== CHANNEL f2 ========
SFO2 399.8415994 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 16.98200035 W
PLW12 0.26546001 W
PLW13 0.16982000 W
F2 - Processing parameters
SF 100.5398480 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
NMe2
CF3
Br
2n
152.71
135.54
130.55
130.50
130.44
130.38
127.55
127.31
127.26
126.96
126.67
124.59
124.37
121.87
119.14
115.98
45.53
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

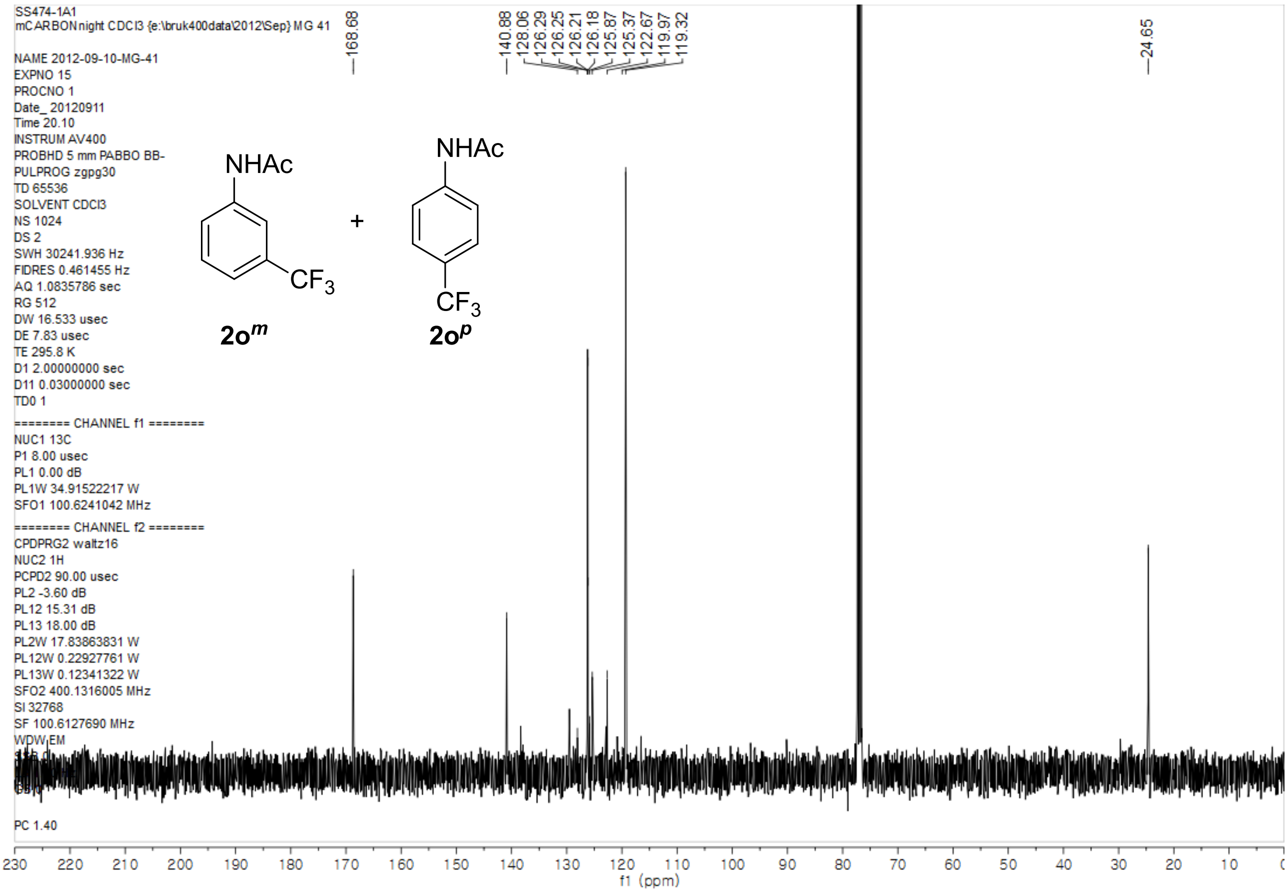

12xp072f2.1.1.1r
12xp072f2 Sangwon Seo SS526-1A1
HOLDER: 22
sF19 Chloroform /home/nmrsu/data opacc 22
Current Data Parameters
NAME 12xp072f2
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20121004
Time 16.46
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30flqn
SOLVENT Chloroform
NS 8
SWH 89285.711 Hz
AQ 0.7340032 sec
TE 297.4 K
D1 2.29999995 sec
TD0 1
======== CHANNEL f1 ========
SFO1 376.1878710 MHz
NUC1 19F
P1 12.70 usec
PLW1 28.97299957 W
F2 - Processing parameters
SF 376.2254940 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
NMe2
CF3
Br
2n
-60.33
0
-5
-10
-15
-20
-25
-30
-35
-40
-45
-50
-55
-60
-65
-70
-75
f1 (ppm)


SS474-1A2
mPROTON CDCl3 {e:\bruk400data\2012\Sep} MG 42
NAME 2012-09-10-MG-42
EXPNO 20
PROCNO 1
Date_ 20120911
Time 8.51
INSTRUM AV400
PROBHD 5 mm PABBO BB-
PULPROG zg30b
TD 65536
SOLVENT CDCl3
NS 16
DS 0
SWH 8264.463 Hz
FIDRES 0.126106 Hz
AQ 3.9649780 sec
RG 256
DW 60.500 usec
DE 9.40 usec
TE 294.9 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 -3.60 dB
PL1W 17.83863831 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300348 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
NHAc
CF3
2o^o
0.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.
f1 (ppm)

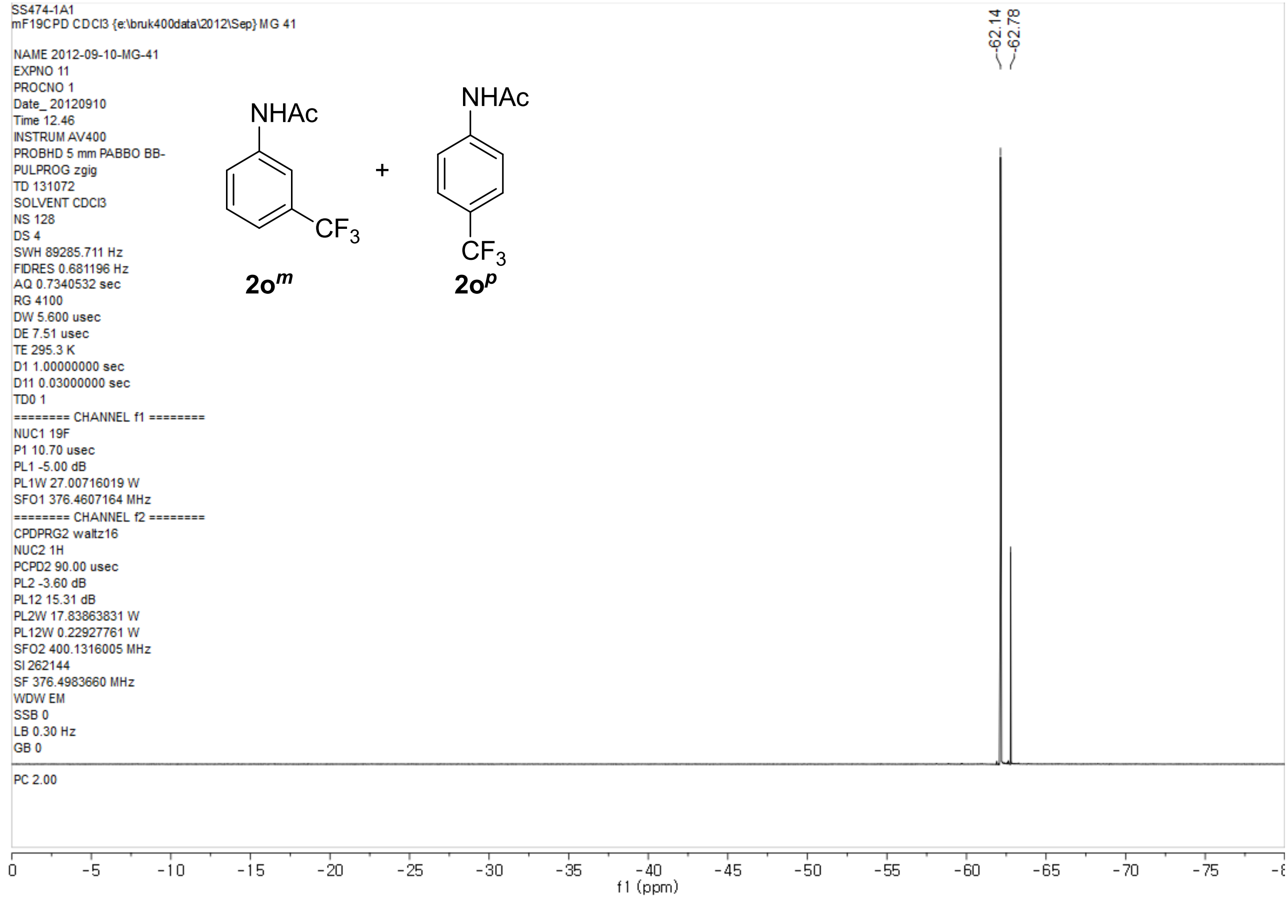

SS474-1A2
mCARBONnight CDCl3 {e:\bruk400data\2012\Sep} MG 42
NAME 2012-09-10-MG-42
EXPNO 22
PROCNO 1
Date_ 20120911
Time 21.07
INSTRUM AV400
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 2
SWH 30241.936 Hz
FIDRES 0.461455 Hz
AQ 1.0835786 sec
RG 512
DW 16.533 usec
DE 7.83 usec
TE 295.8 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 8.00 usec
PL1 0.00 dB
PL1W 34.91522217 W
SFO1 100.6241042 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -3.60 dB
PL12 15.31 dB
PL13 18.00 dB
PL2W 17.83863831 W
PL12W 0.22927761 W
PL13W 0.12341322 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127690 MHz
GB 0
PC 1.40
168.42
135.16
132.85
126.02
126.00
124.67
124.52
124.43
24.63
NHAc
CF3
2o^o
230
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
(
f1 (ppm)


SS474-1A2
mF19CPD CDCl3 {e:\bruk400data\2012\Sep} MG 42
NAME 2012-09-10-MG-42
EXPNO 11
PROCNO 1
Date_ 20120910
Time 12.55
INSTRUM AV400
PROBHD 5 mm PABBO BB-
PULPROG zgig
TD 131072
SOLVENT CDCl3
NS 128
DS 4
SWH 89285.711 Hz
FIDRES 0.681196 Hz
AQ 0.7340532 sec
RG 4100
DW 5.600 usec
DE 7.51 usec
TE 295.3 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 19F
P1 10.70 usec
PL1 -5.00 dB
PL1W 27.00716019 W
SFO1 376.4607164 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -3.60 dB
PL12 15.31 dB
PL2W 17.83863831 W
PL12W 0.22927761 W
SFO2 400.1316005 MHz
SI 262144
SF 376.4983660 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 2.00
NHAc
CF3
2o^o
-60.64
0
-5
-10
-15
-20
-25
-30
-35
-40
-45
-50
-55
-60
-65
-70
-75
f1 (ppm)

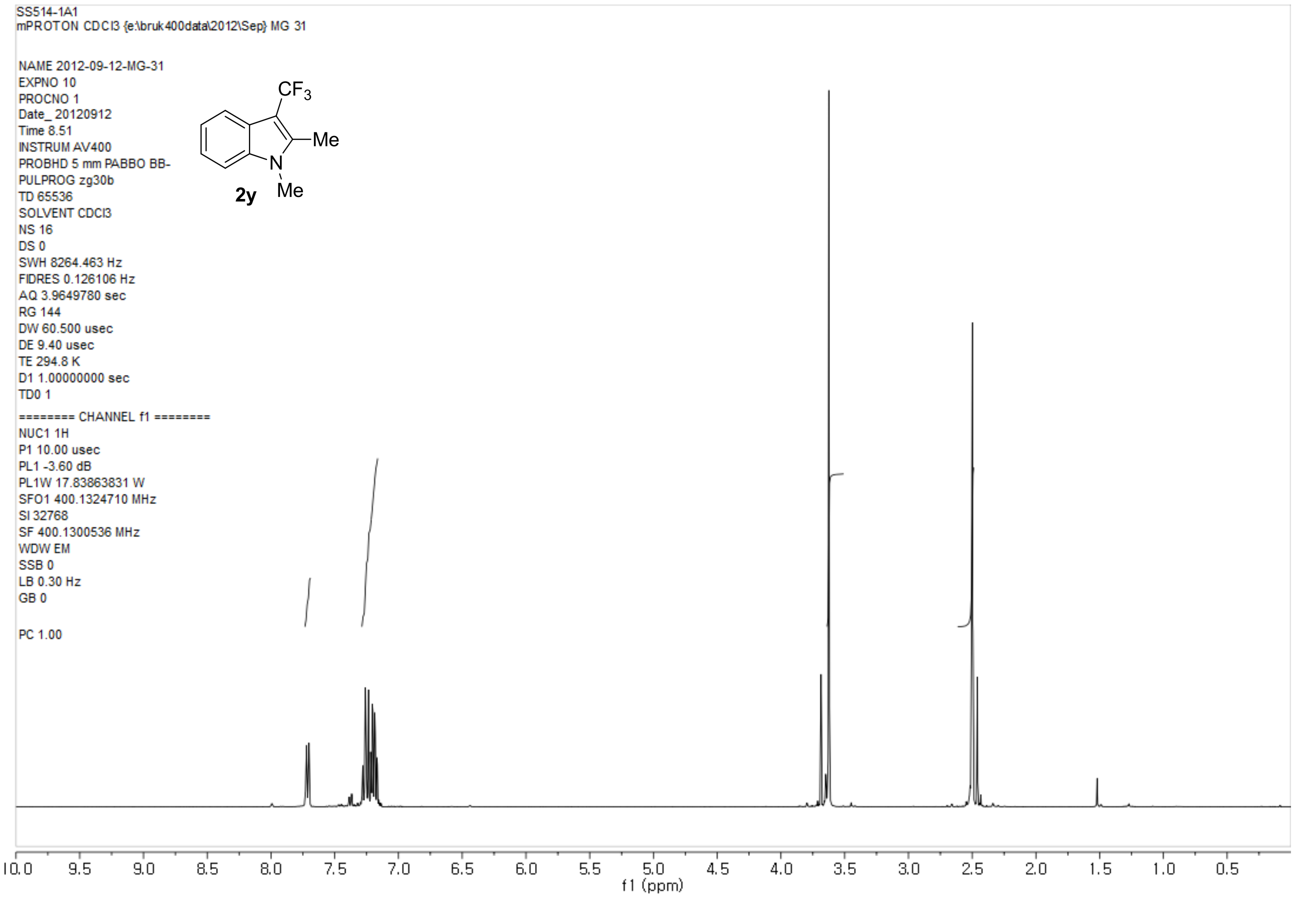

SS474-1A1
mPROTON CDCl3 {e:\bruk400data\2012\Sep} MG 41
NAME 2012-09-10-MG-41
EXPNO 14
PROCNO 1
Date_ 20120911
Time 8.32
INSTRUM AV400
PROBHD 5 mm PABBO BB-
PULPROG zg30b
TD 65536
SOLVENT CDCl3
NS 16
DS 0
SWH 8264.463 Hz
FIDRES 0.126106 Hz
AQ 3.9649780 sec
RG 256
DW 60.500 usec
DE 9.40 usec
TE 295.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 -3.60 dB
PL1W 17.83863831 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300373 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
NHAc
CF3
2o^m
+
NHAc
CF3
2o^p
7.9
7.8
7.7
7.6
7.5
7.4
f1 (ppm)
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)


SS474-1A1
mCARBONnight CDCl3 {e:\bruk400data\2012\Sep} MG 41

NAME 2012-09-10-MG-41
EXPNO 15
PROCNO 1
Date_ 20120911
Time 20.10
INSTRUM AV400
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 2
SWH 30241.936 Hz
FIDRES 0.461455 Hz
AQ 1.0835786 sec
RG 512
DW 16.533 usec
DE 7.83 usec
TE 295.8 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 8.00 usec
PL1 0.00 dB
PL1W 34.91522217 W
SFO1 100.6241042 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -3.60 dB
PL12 15.31 dB
PL13 18.00 dB
PL2W 17.83863831 W
PL12W 0.22927761 W
PL13W 0.12341322 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127690 MHz
WDW EM
PC 1.40


SS474-1A1
mF19CPD CDCl3 {e:\bruk400data\2012\Sep} MG 41

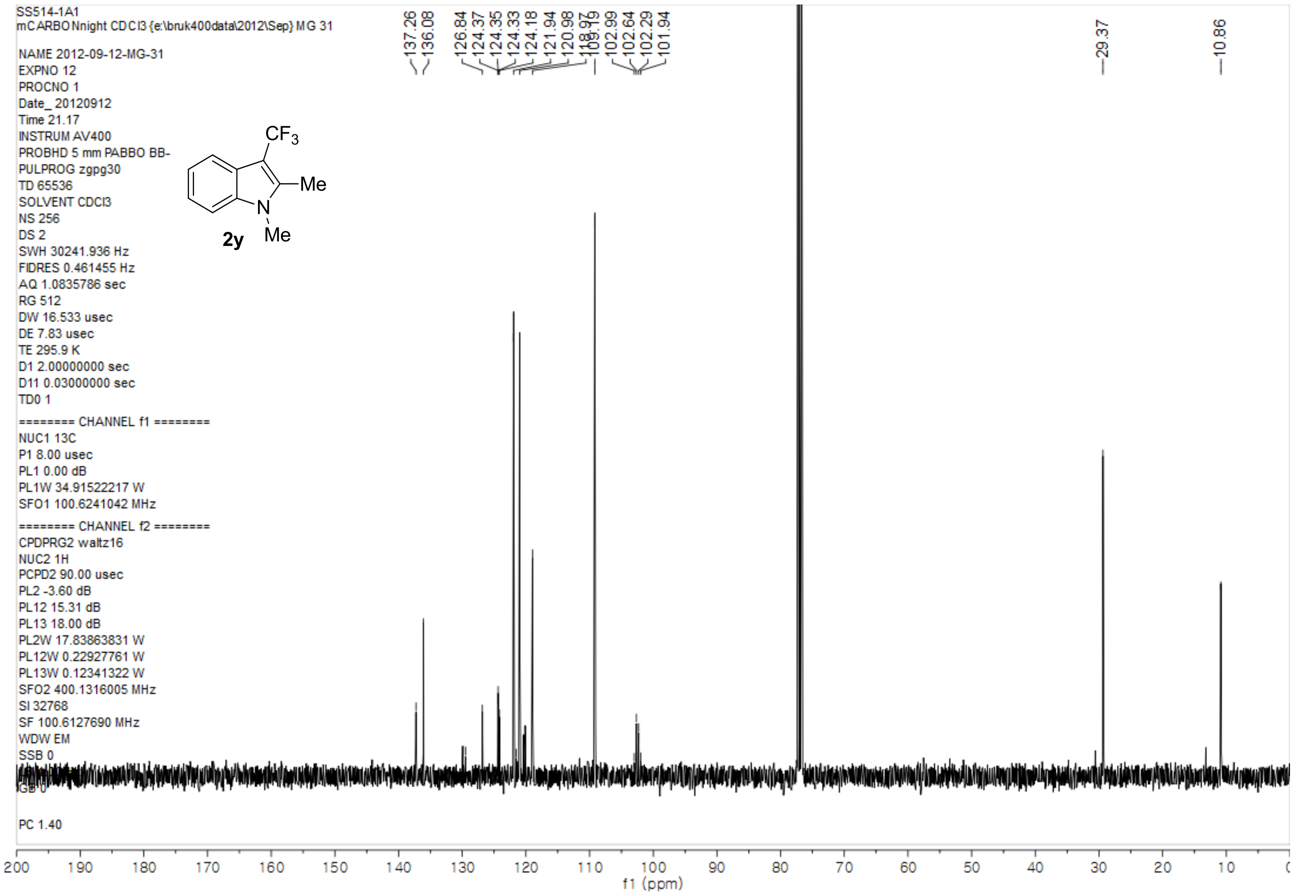
NAME 2012-09-10-MG-41
EXPNO 11
PROCNO 1
Date_ 20120910
Time 12.46
INSTRUM AV400
PROBHD 5 mm PABBO BB-
PULPROG zgig
TD 131072
SOLVENT CDCl3
NS 128
DS 4
SWH 89285.711 Hz
FIDRES 0.681196 Hz
AQ 0.7340532 sec
RG 4100
DW 5.600 usec
DE 7.51 usec
TE 295.3 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 19F
P1 10.70 usec
PL1 -5.00 dB
PL1W 27.00716019 W
SFO1 376.4607164 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -3.60 dB
PL12 15.31 dB
PL2W 17.83863831 W
PL12W 0.22927761 W
SFO2 400.1316005 MHz
SI 262144
SF 376.4983660 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 2.00



```
SS514-1A1
mPROTON CDCl3 {e:\bruk400data\2012\Sep} MG 31

NAME 2012-09-12-MG-31
EXPNO 10
PROCNO 1
Date_ 20120912
Time 8.51
INSTRUM AV400
PROBHD 5 mm PABBO BB-
PULPROG zg30b
TD 65536
SOLVENT CDCl3
NS 16
DS 0
SWH 8264.463 Hz
FIDRES 0.126106 Hz
AQ 3.9649780 sec
RG 144
DW 60.500 usec
DE 9.40 usec
TE 294.8 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 -3.60 dB
PL1W 17.83863831 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300536 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0

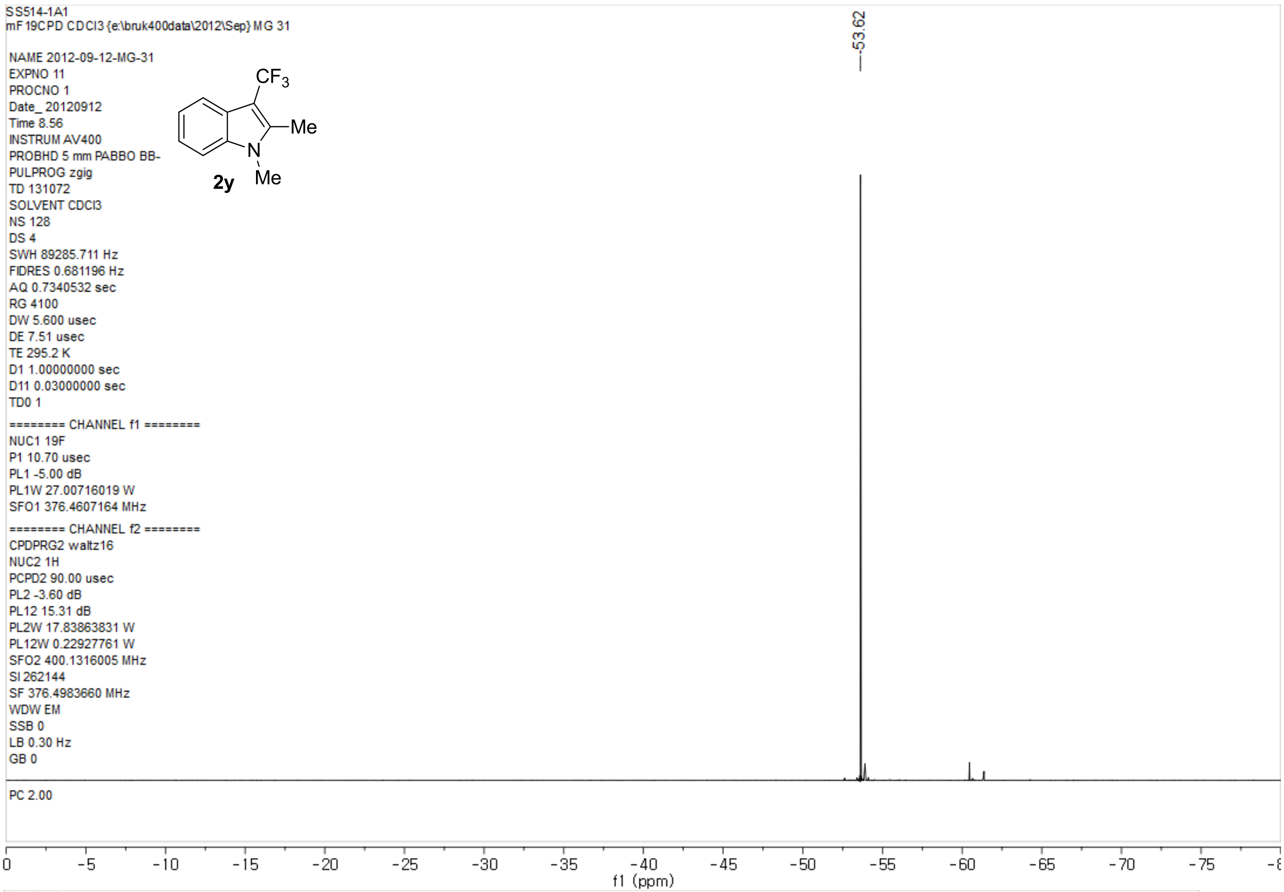
PC 1.00
```



```
SS514-1A1
mCARBONnight CDCl3 {e:\bruk400data\2012\Sep} MG 31

NAME 2012-09-12-MG-31
EXPNO 12
PROCNO 1
Date_ 20120912
Time 21.17
INSTRUM AV400
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 256
DS 2
SWH 30241.936 Hz
FIDRES 0.461455 Hz
AQ 1.0835786 sec
RG 512
DW 16.533 usec
DE 7.83 usec
TE 295.9 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 8.00 usec
PL1 0.00 dB
PL1W 34.91522217 W
SFO1 100.6241042 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -3.60 dB
PL12 15.31 dB
PL13 18.00 dB
PL2W 17.83863831 W
PL12W 0.22927761 W
PL13W 0.12341322 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0

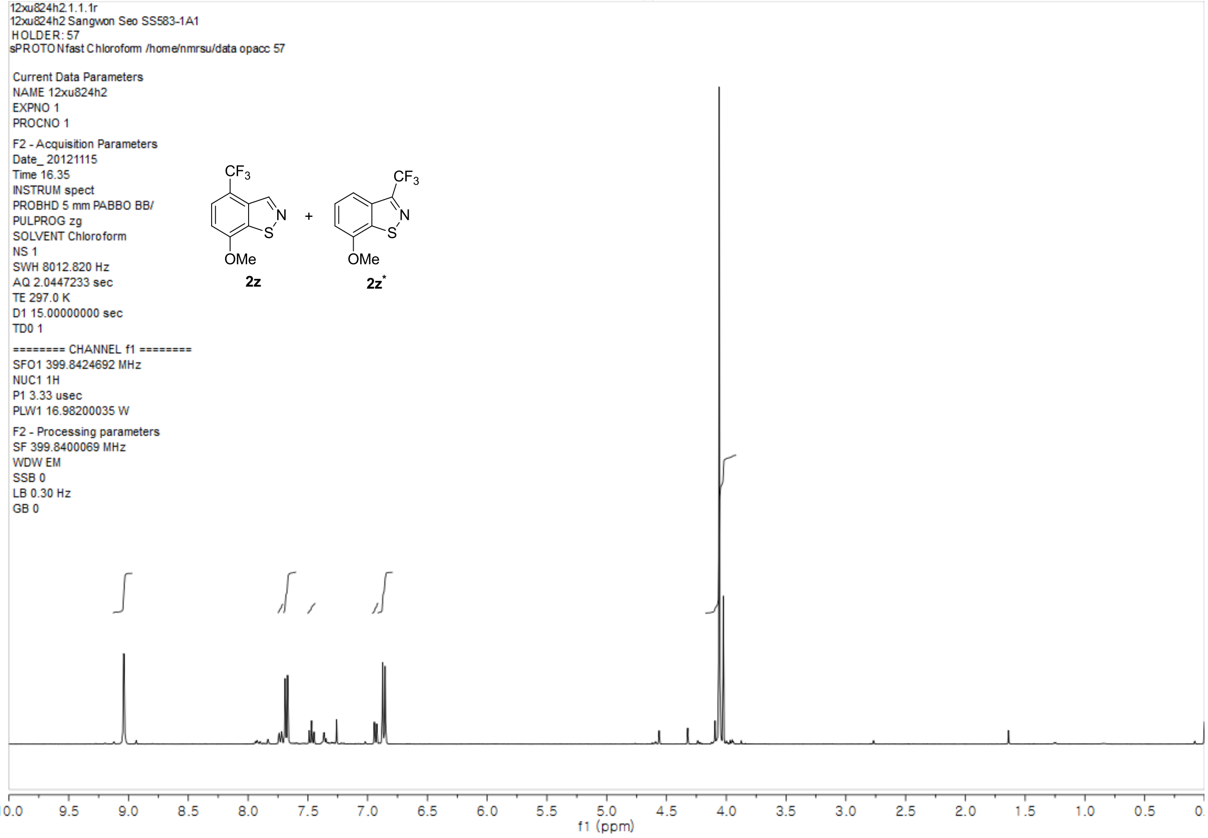
PC 1.40
```



```
SS514-1A1
mF 19CPD CDCl3 {e:\bruk400data\2012\Sep} MG 31

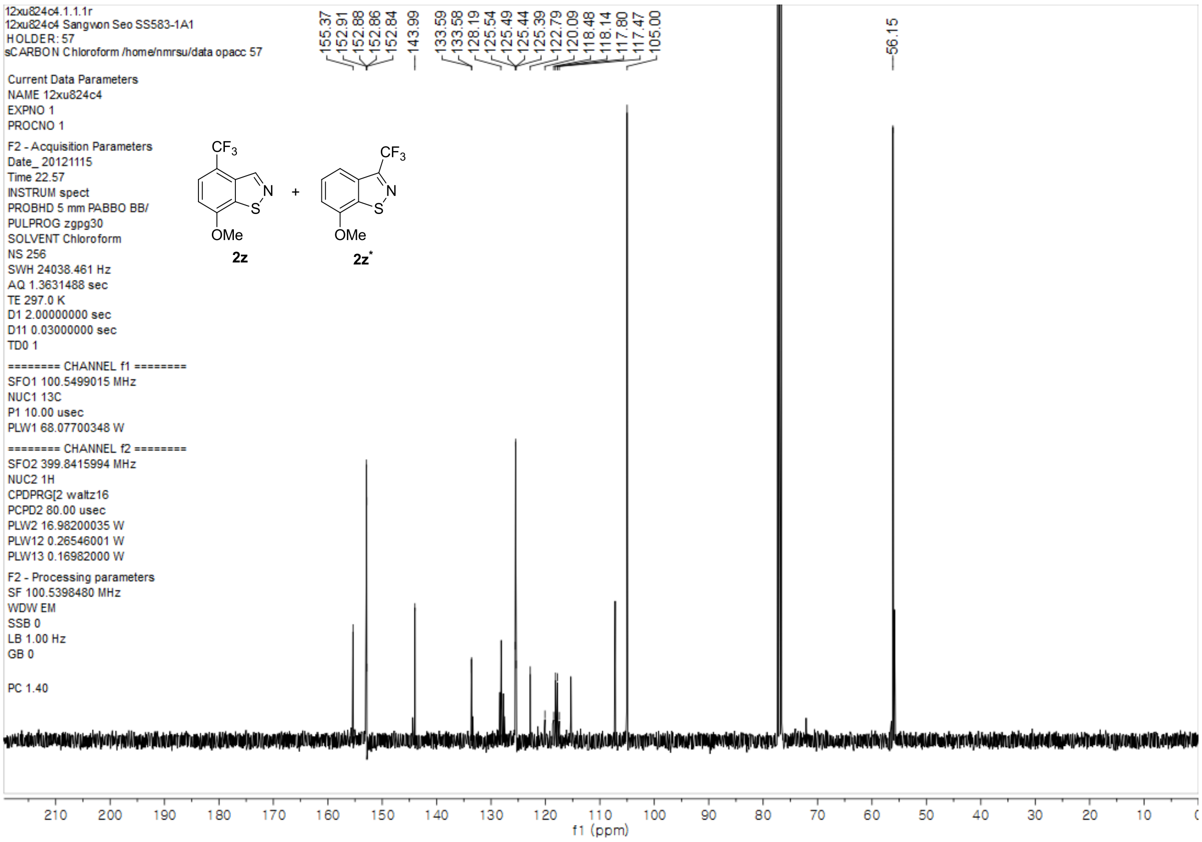
NAME 2012-09-12-MG-31
EXPNO 11
PROCNO 1
Date_ 20120912
Time 8.56
INSTRUM AV400
PROBHD 5 mm PABBO BB-
PULPROG zgig
TD 131072
SOLVENT CDCl3
NS 128
DS 4
SWH 89285.711 Hz
FIDRES 0.681196 Hz
AQ 0.7340532 sec
RG 4100
DW 5.600 usec
DE 7.51 usec
TE 295.2 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 19F
P1 10.70 usec
PL1 -5.00 dB
PL1W 27.00716019 W
SFO1 376.4607164 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -3.60 dB
PL12 15.31 dB
PL2W 17.83863831 W
PL12W 0.22927761 W
SFO2 400.1316005 MHz
SI 262144
SF 376.4983660 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0

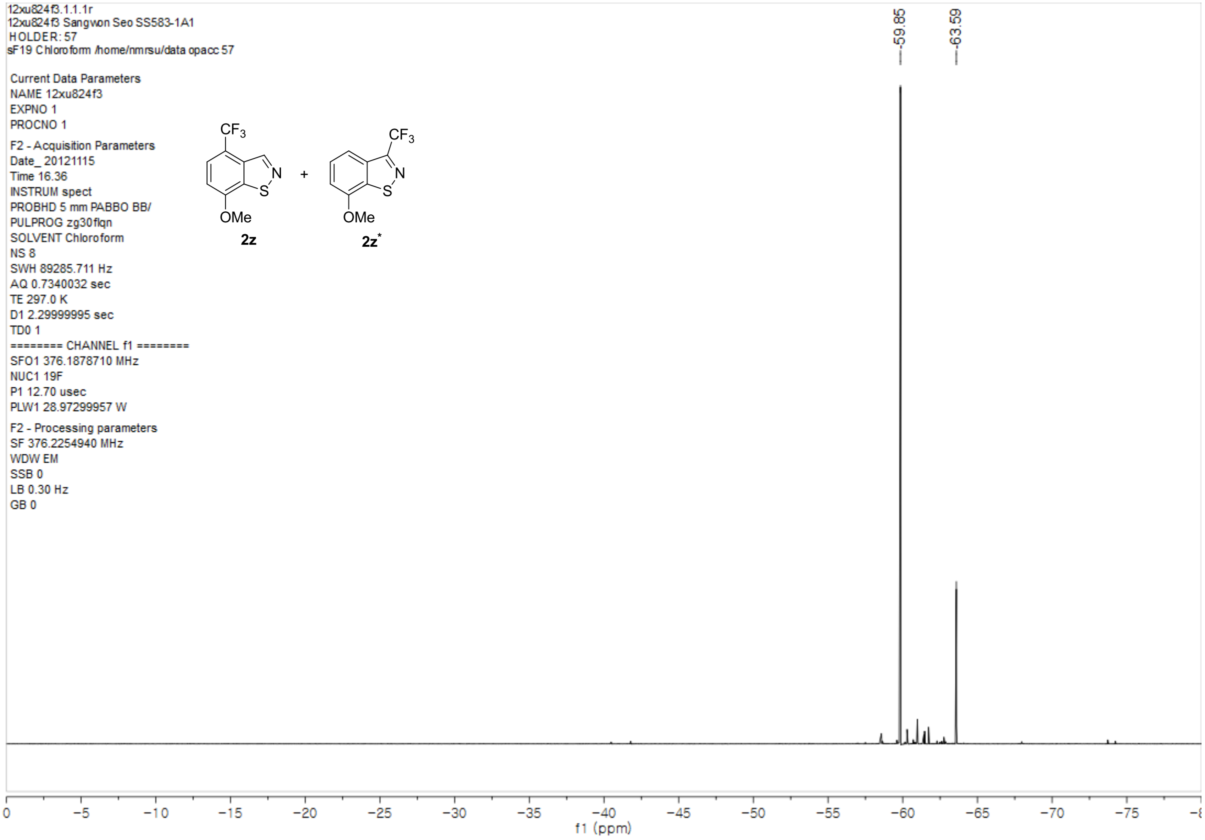
PC 2.00
```

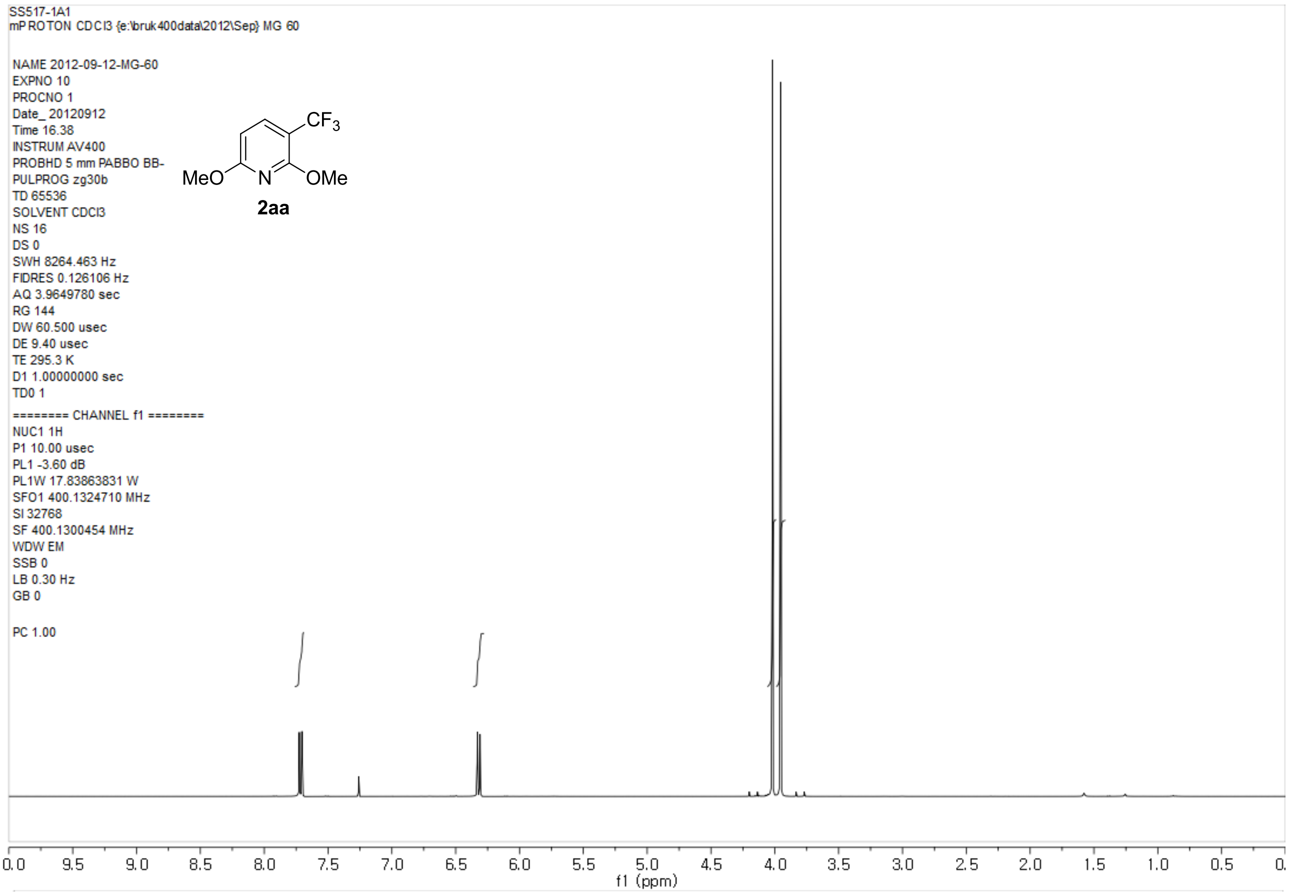


```
12xu824h2.1.1.1r
12xu824h2 Sangwon Seo SS583-1A1
HOLDER: 57
sPROTONfast Chloroform /home/nmrsu/data opacc 57

Current Data Parameters
NAME 12xu824h2
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20121115
Time 16.35
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg
SOLVENT Chloroform
NS 1
SWH 8012.820 Hz
AQ 2.0447233 sec
TE 297.0 K
D1 15.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 399.8424692 MHz
NUC1 1H
P1 3.33 usec
PLW1 16.98200035 W
F2 - Processing parameters
SF 399.8400069 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
```


12xu824c4.1.1.1r
12xu824c4 Sangwon Seo SS583-1A1
HOLDER: 57
sCARBON Chloroform /home/nmrsu/data opacc 57
Current Data Parameters
NAME 12xu824c4
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20121115
Time 22.57
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
SOLVENT Chloroform
NS 256
SWH 24038.461 Hz
AQ 1.3631488 sec
TE 297.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 100.5499015 MHz
NUC1 13C
P1 10.00 usec
PLW1 68.07700348 W
======== CHANNEL f2 ========
SFO2 399.8415994 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 16.98200035 W
PLW12 0.26546001 W
PLW13 0.16982000 W
F2 - Processing parameters
SF 100.5398480 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
CF3
N
S
OMe
2z
+
CF3
N
S
OMe
2z*
155.37
152.91
152.88
152.86
152.84
143.99
133.59
133.58
128.19
125.54
125.49
125.44
125.39
122.79
120.09
118.48
118.14
117.80
117.47
105.00
56.15
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


12xu824f3.1.1.1r
12xu824f3 Sangwon Seo SS583-1A1
HOLDER: 57
sF19 Chloroform /home/nmrsu/data opacc 57
Current Data Parameters
NAME 12xu824f3
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20121115
Time 16.36
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30flqn
SOLVENT Chloroform
NS 8
SWH 89285.711 Hz
AQ 0.7340032 sec
TE 297.0 K
D1 2.29999995 sec
TD0 1
======== CHANNEL f1 ========
SFO1 376.1878710 MHz
NUC1 19F
P1 12.70 usec
PLW1 28.97299957 W
F2 - Processing parameters
SF 376.2254940 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
CF3
N
S
OMe
2z
+
CF3
N
S
OMe
2z*
-59.85
-63.59
0
−5
−10
−15
−20
−25
−30
−35
−40
−45
−50
−55
−60
−65
−70
−75
f1 (ppm)

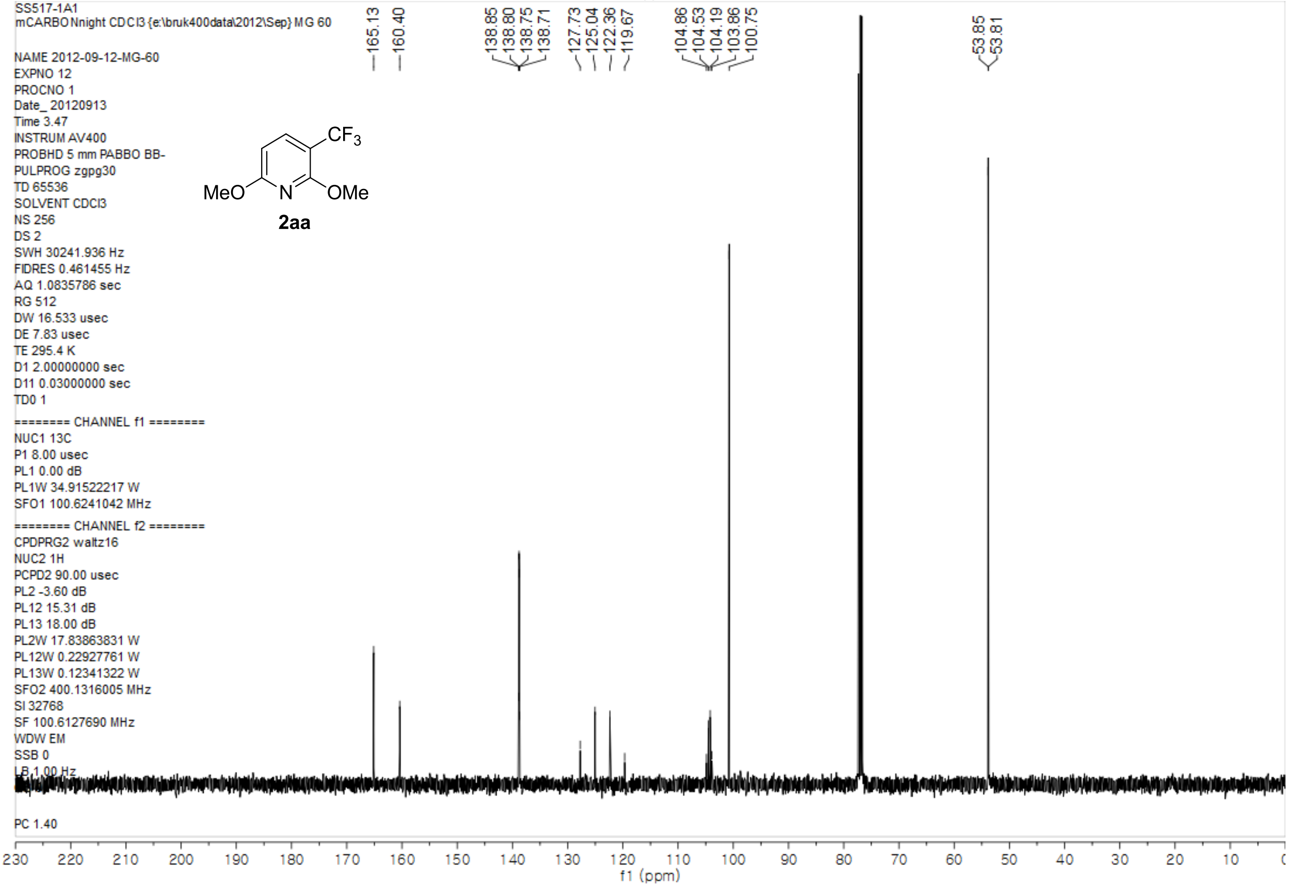


```
SS517-1A1
mPROTON CDCl3 {e:\bruk400data\2012\Sep} MG 60

NAME 2012-09-12-MG-60
EXPNO 10
PROCNO 1
Date_ 20120912
Time 16.38
INSTRUM AV400
PROBHD 5 mm PABBO BB-
PULPROG zg30b
TD 65536
SOLVENT CDCl3
NS 16
DS 0
SWH 8264.463 Hz
FIDRES 0.126106 Hz
AQ 3.9649780 sec
RG 144
DW 60.500 usec
DE 9.40 usec
TE 295.3 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 -3.60 dB
PL1W 17.83863831 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300454 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0

PC 1.00
```



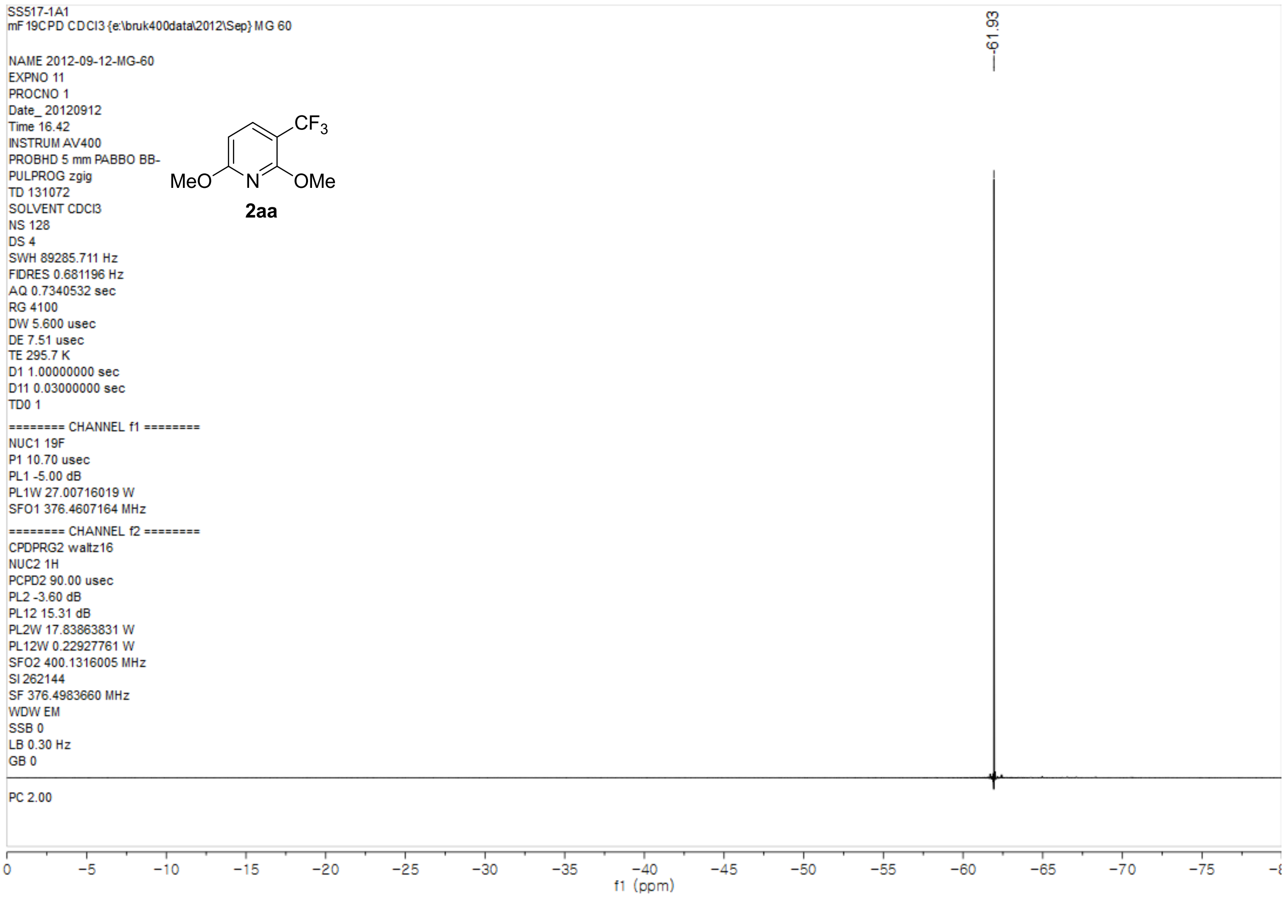
```
SS517-1A1
mCARBONnight CDCl3 {e:\bruk400data\2012\Sep} MG 60

NAME 2012-09-12-MG-60
EXPNO 12
PROCNO 1
Date_ 20120913
Time 3.47
INSTRUM AV400
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 256
DS 2
SWH 30241.936 Hz
FIDRES 0.461455 Hz
AQ 1.0835786 sec
RG 512
DW 16.533 usec
DE 7.83 usec
TE 295.4 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 8.00 usec
PL1 0.00 dB
PL1W 34.91522217 W
SFO1 100.6241042 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -3.60 dB
PL12 15.31 dB
PL13 18.00 dB
PL2W 17.83863831 W
PL12W 0.22927761 W
PL13W 0.12341322 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz

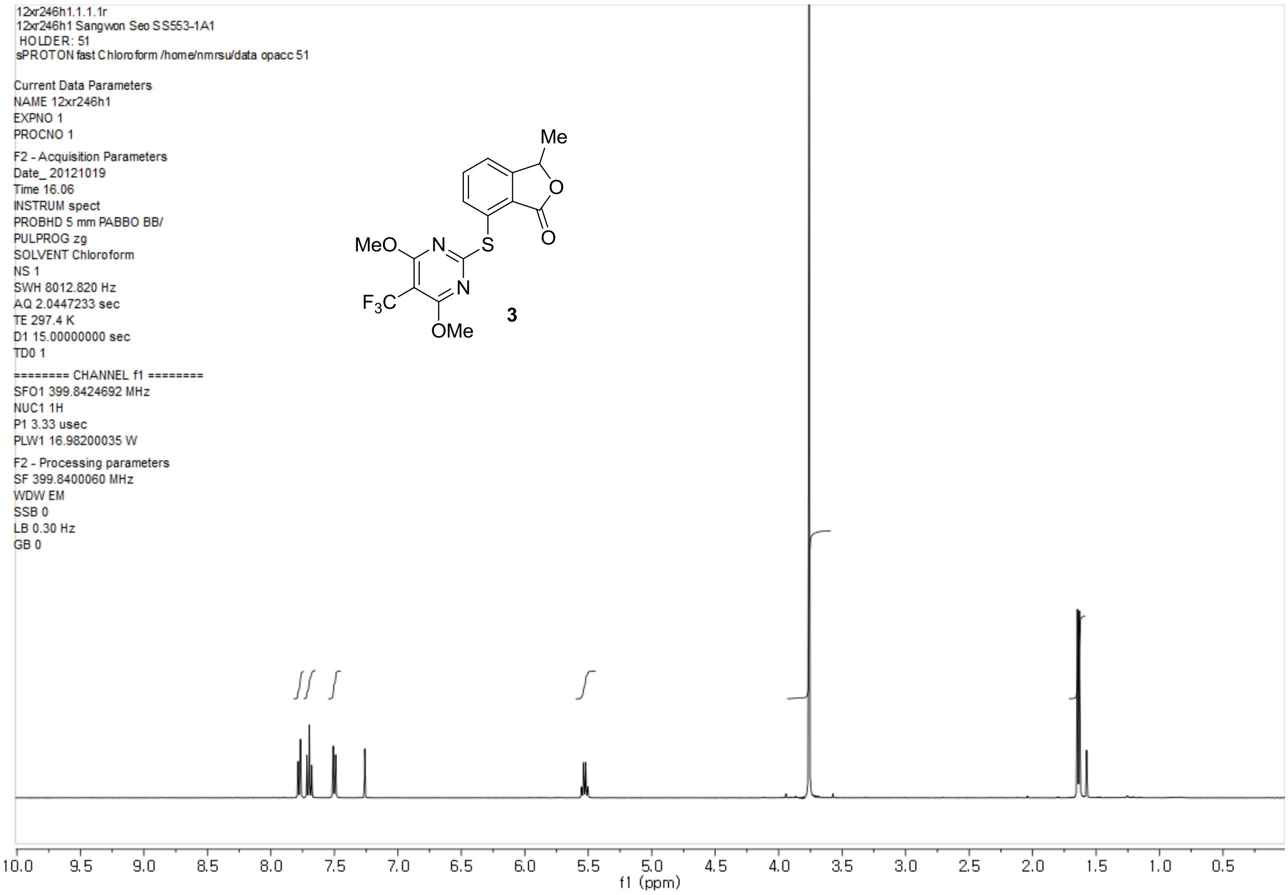
PC 1.40
```



SS517-1A1
mF 19CPD CDCl3 {e:\bruk400data\2012\Sep} MG 60

NAME 2012-09-12-MG-60
EXPNO 11
PROCNO 1
Date_ 20120912
Time 16.42
INSTRUM AV400
PROBHD 5 mm PABBO BB-
PULPROG zgig
TD 131072
SOLVENT CDCl3
NS 128
DS 4
SWH 89285.711 Hz
FIDRES 0.681196 Hz
AQ 0.7340532 sec
RG 4100
DW 5.600 usec
DE 7.51 usec
TE 295.7 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 19F
P1 10.70 usec
PL1 -5.00 dB
PL1W 27.00716019 W
SFO1 376.4607164 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -3.60 dB
PL12 15.31 dB
PL2W 17.83863831 W
PL12W 0.22927761 W
SFO2 400.1316005 MHz
SI 262144
SF 376.4983660 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 2.00

2aa



12xr246h1.1.1.1r
12xr246h1 Sangwon Seo SS553-1A1
HOLDER: 51
sPROTON fast Chloroform /home/nmrsu/data opacc 51

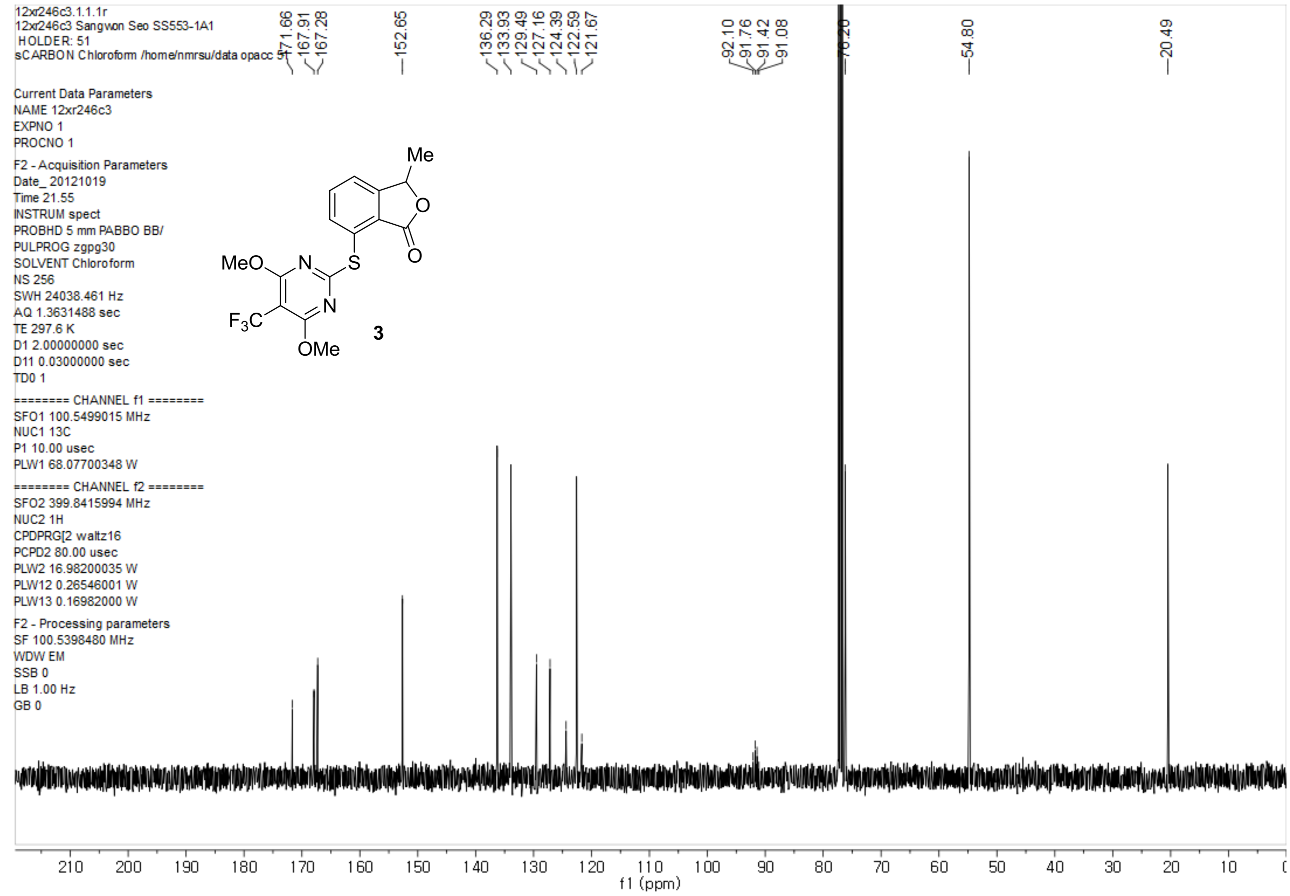
Current Data Parameters
NAME 12xr246h1
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20121019
Time 16.06
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg
SOLVENT Chloroform
NS 1
SWH 8012.820 Hz
AQ 2.0447233 sec
TE 297.4 K
D1 15.00000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 399.8424692 MHz
NUC1 1H
P1 3.33 usec
PLW1 16.98200035 W

F2 - Processing parameters
SF 399.8400060 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0

3



12xr246c3.1.1.1r
12xr246c3 Sangwon Seo SS553-1A1
HOLDER: 51
sCARBON Chloroform /home/nmrsu/data opacc 51

Current Data Parameters
NAME 12xr246c3
EXPNO 1
PROCNO 1

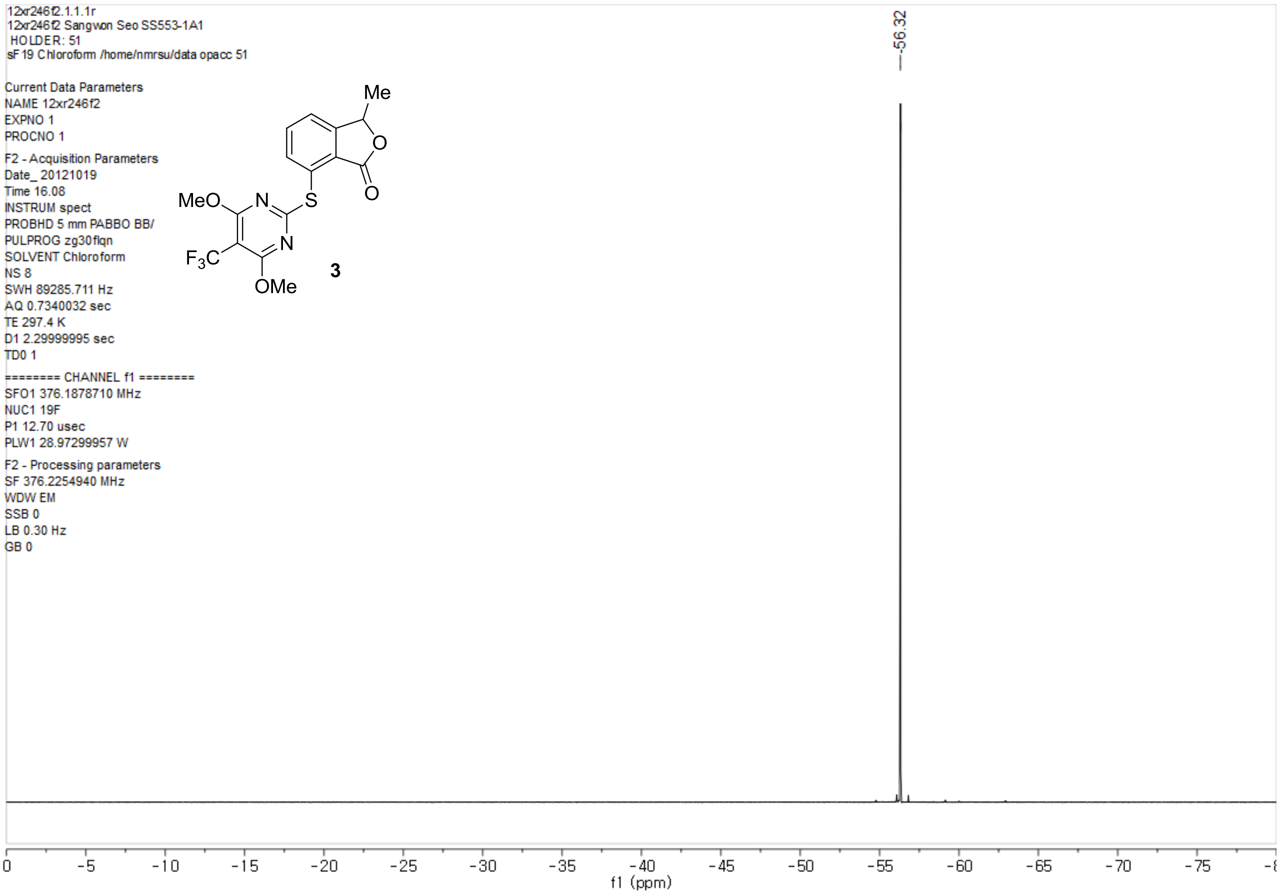
F2 - Acquisition Parameters
Date_ 20121019
Time 21.55
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
SOLVENT Chloroform
NS 256
SWH 24038.461 Hz
AQ 1.3631488 sec
TE 297.6 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

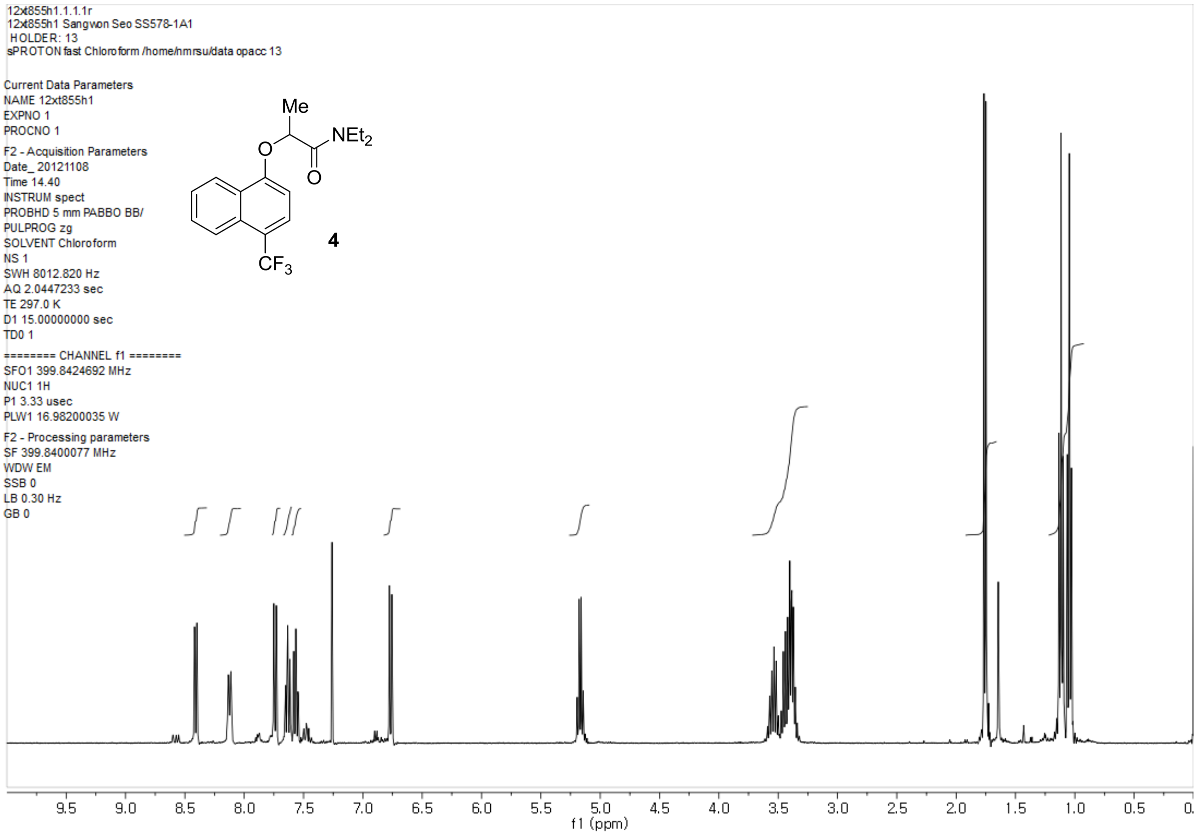
======== CHANNEL f1 ========
SFO1 100.5499015 MHz
NUC1 13C
P1 10.00 usec
PLW1 68.07700348 W

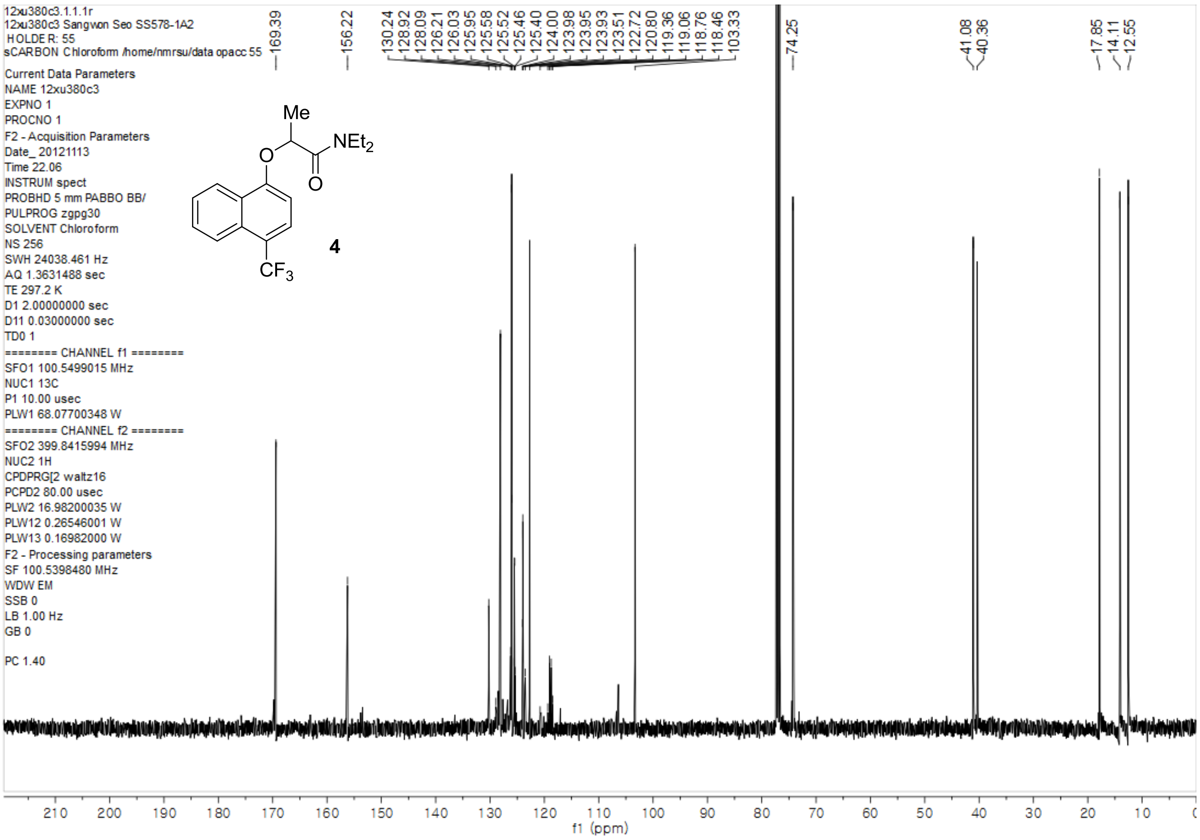
======== CHANNEL f2 ========
SFO2 399.8415994 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 16.98200035 W
PLW12 0.26546001 W
PLW13 0.16982000 W

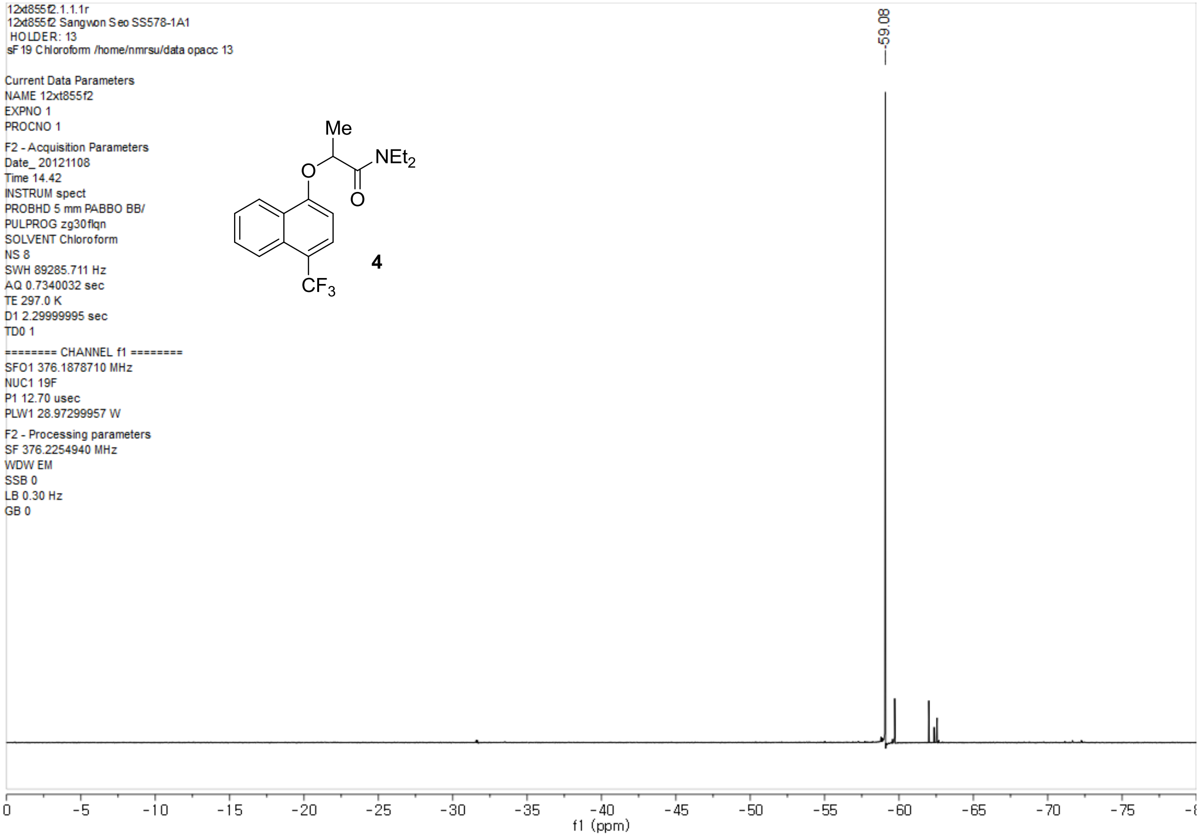
F2 - Processing parameters
SF 100.5398480 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0

3


12xr246f2.1.1.1r
12xr246f2 Sangwon Seo SS553-1A1
HOLDER: 51
sF 19 Chloroform /home/nmrsu/data opacc 51
Current Data Parameters
NAME 12xr246f2
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20121019
Time 16.08
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30flqn
SOLVENT Chloroform
NS 8
SWH 89285.711 Hz
AQ 0.7340032 sec
TE 297.4 K
D1 2.29999995 sec
TD0 1
======== CHANNEL f1 ========
SFO1 376.1878710 MHz
NUC1 19F
P1 12.70 usec
PLW1 28.97299957 W
F2 - Processing parameters
SF 376.2254940 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
Me
O
O
S
MeO
N
N
F3C
OMe
3
-56.32
0
-5
-10
-15
-20
-25
-30
-35
-40
-45
-50
-55
-60
-65
-70
-75
f1 (ppm)


12xt855h1.1.1.1r
12xt855h1 Sangwon Seo SS578-1A1
HOLDER: 13
sPROTON fast Chloroform /home/nmrsu/data opacc 13
Current Data Parameters
NAME 12xt855h1
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20121108
Time 14.40
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg
SOLVENT Chloroform
NS 1
SWH 8012.820 Hz
AQ 2.0447233 sec
TE 297.0 K
D1 15.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 399.8424692 MHz
NUC1 1H
P1 3.33 usec
PLW1 16.98200035 W
F2 - Processing parameters
SF 399.8400077 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
Me
O
NEt2
O
CF3
4
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.
f1 (ppm)


12xu380c3.1.1.1r
12xu380c3 Sangwon Seo SS578-1A2
HOLDER: 55
sCARBON Chloroform /home/nmrsu/data opacc 55
Current Data Parameters
NAME 12xu380c3
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20121113
Time 22.06
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
SOLVENT Chloroform
NS 256
SWH 24038.461 Hz
AQ 1.3631488 sec
TE 297.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 100.5499015 MHz
NUC1 13C
P1 10.00 usec
PLW1 68.07700348 W
======== CHANNEL f2 ========
SFO2 399.8415994 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 16.98200035 W
PLW12 0.26546001 W
PLW13 0.16982000 W
F2 - Processing parameters
SF 100.5398480 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
Me
NEt2
O
O
CF3
4
169.39
156.22
130.24
128.92
128.09
126.21
126.03
125.95
125.58
125.52
125.46
125.40
124.00
123.98
123.95
123.93
123.51
122.72
120.80
119.36
119.06
118.76
118.46
103.33
74.25
41.08
40.36
17.85
14.11
12.55
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


12xt855f2.1.1.1r
12xt855f2 Sangwon Seo SS578-1A1
HOLDER: 13
sF19 Chloroform /home/nmrsu/data opacc 13
Current Data Parameters
NAME 12xt855f2
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20121108
Time 14.42
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30flqn
SOLVENT Chloroform
NS 8
SWH 89285.711 Hz
AQ 0.7340032 sec
TE 297.0 K
D1 2.29999995 sec
TD0 1
======== CHANNEL f1 ========
SFO1 376.1878710 MHz
NUC1 19F
P1 12.70 usec
PLW1 28.97299957 W
F2 - Processing parameters
SF 376.2254940 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
Me
NEt2
O
O
CF3
4
-59.08
0
-5
-10
-15
-20
-25
-30
-35
-40
-45
-50
-55
-60
-65
-70
-75
f1 (ppm)