Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Asymmetric Hydrogenation of Trifluoromethyl Ketones: Application in the Synthesis of Odanacatib and LX-1031

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Electronic Supplementary Information

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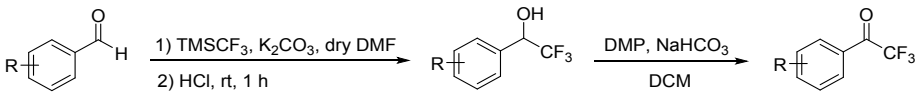
I. General Information

Unless otherwise mentioned, all experiments were carried out under an atmosphere of argon in a glovebox or using standard Schlenk techniques. Solvents were dried with standard procedures and degassed with N_2. Flash column chromatography was performed using Tsingdao silica gel (60, particle size 200-300 mesh). ^{1}H, ^{13}C and ^{19}F NMR spectra were recorded on Bruker Ascend TM 400MHz (^{1}H: 400 MHz, ^{13}C: 101 MHz, ^{19}F: 376 MHz). Chemical shifts (δ) for ^{1}H and ^{13}C NMR spectra were given in ppm and were referenced to residual solvent or TMS peaks. Enantioselective ratios were determined by chiral HPLC analysis using a chiral stationary phase on Agilent Technologies 1260 Infinity II instrument in comparison with the authentic racemates. Optical rotations were obtained on Rudolph Autopol I, serial number 35148. Exact ESI mass spectra were recorded on Orbitrap Fusion instrument.

II. Experimental procedure and characterization of secondary trifluoromethyl ketones

Scheme S1. General Preparation of fluorinated acetophenones

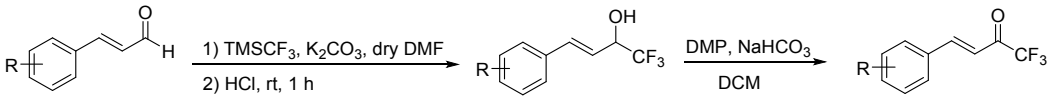
Method A:



General procedure for the fluorinated acetophenones[1]: To a 100 mL flask was added aldehyde (8.0 mmol), and DMF (15 mL), and K_2CO_3 (0.08 mmol), TMS-CF_3 (9.6 mmol) was added dropwise. Then the mixture was allowed to stir at rt for 1 h before HCl (1 M) was added, then the mixture was stirred at rt for another 1 h. After the reaction was finished, the reaction mixture was extracted with ethyl acetate (3 × 100 mL). The combined organic phase was dried with Na_2SO_4 and evaporated in vacuum. Purification of the residue by silica gel (hexanes/EtOAc 10/1~4/1) afforded the desired fluorinated phenylethanols as a white solid.

To a solution of the fluorinated phenylethanols (5.0 mmol) in DCM, DMP (12.0 mmol) and $NaHCO_3$ (20 mmol) were added successively. The solution was allowed to stir at rt for 3 h. Then water was added and the obtained suspension was stirred for another 1 h. After the reaction was finished, the reaction mixture was extracted with DCM (3 × 20 mL). The combined organic phase was dried with Na_2SO_4 and evaporated in vacuum. Purification of the residue by silica gel (hexanes/EtOAc 100/1~90/1) afforded the desired fluorinated acetophenones as a white solid.[2]

Method B:

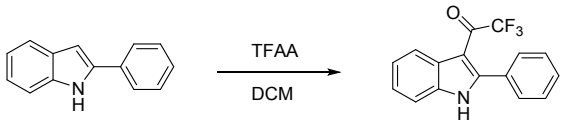


General procedure for the *α,β*-unsaturated trifluoromethyl ketones[2]: To a 100 mL flask was added *α,β*-unsaturated aldehyde (8.0 mmol), and DMF (20 mL), and K_2CO_3 (0.08 mmol), TMS-CF_3 (9.6 mmol) was added dropwise. Then the mixture was allowed to stir at rt for 1 h before HCl (1 M) was added, then the mixture was stirred at rt for another 1 h. After the reaction was finished, the reaction mixture was extracted with ethyl acetate (3 × 100 mL). The combined organic phase was dried with Na_2SO_4 and evaporated in vacuum. Purification of the residue by silica gel

(hexanes/EtOAc 10/1~4/1) afforded the desired *α,β*-unsaturated trifluoromethyl alcohols as light yellow oil.

To a solution of the *α,β*-unsaturated trifluoromethyl alcohols (5.0 mmol) in DCM, DMP (12.0 mmol) and $NaHCO_3$ (20 mmol) were added successively. The solution was allowed to stir at rt for 3 h. Then water was added and the obtained suspension was stirred for another 1 h. After the reaction was finished, the reaction mixture was extracted with DCM (3 × 20 mL). The combined organic phase was dried with Na_2SO_4 and evaporated in vacuum. Purification of the residue by silica gel (hexanes/EtOAc 100/1~90/1) afforded the desired *α,β*-unsaturated trifluoromethyl ketones as a white solid.[2]

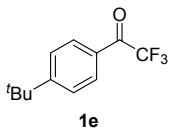
Method C:



General procedure for the fluorinated indolinone [3]: To a 100 mL oven-dried flask under argon was added the indole (5.2 mmol), and dry DCM (10 mL), and under stirring the mixture was cooled to 0 °C. The perfluoro anhydride (20.8 mmol) was then added dropwise using a syringe. After the reaction was finished, the reaction mixture is then dropwise added to a stirred, ice-cold saturated $NaHCO_3$ solution. Further DCM was added, the organic phases were separated, and the aqueous layer was extracted with DCM. The combined organic phase was dried with Na_2SO_4 and evaporated in vacuum. Purification of the residue by silica gel (hexanes/EtOAc 20/1~2/1) afforded the desired fluorinated indolinone as a yellow solid.

Characterization data of substrates

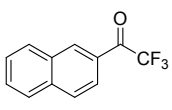
1-(4-(*tert*-butyl)phenyl)-2,2,2-trifluoroethan-1-one (1e)



1e

White solid, 86% yield. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.08 – 7.92 (m, 2H), 7.65 – 7.45 (m, 2H), 1.36 (s, 9H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 180.1 (q, *J* = 34.5 Hz), 159.8, 130.2, 127.3, 126.1, 116.8 (q, *J* = 291.3 Hz), 35.5, 30.9. **^{19}F NMR** (376 MHz, $CDCl_3$) δ -71.33.

2,2,2-trifluoro-1-(naphthalen-2-yl)ethan-1-one (1m)

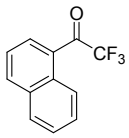


1m

White solid, 84% yield. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.62 (s, 1H), 8.07 (d, *J* =

8.7 Hz, 1H), 8.01 (d, *J* = 8.1 Hz, 1H), 7.95 (d, *J* = 8.7 Hz, 1H), 7.90 (d, *J* = 8.1 Hz, 1H), 7.69 (t, *J* = 7.5 Hz, 1H), 7.61 (t, *J* = 7.2 Hz, 1H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 180.5 (q, *J* = 35.0 Hz), 136.5, 133.2 (d, *J* = 3.2 Hz), 132.2, 130.2, 130.1, 129.1, 127.9, 127.4, 127.2, 124.2, 116.9 (q, *J* = 291.0 Hz). **^{19}F NMR** (376 MHz, $CDCl_3$) δ -70.73.

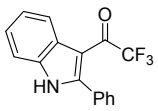
2,2,2-trifluoro-1-(naphthalen-1-yl)ethan-1-one (1n)



1n

Light yellow oil, 83% yield. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.78 (d, *J* = 8.7 Hz, 1H), 8.12 (d, *J* = 7.4 Hz, 1H), 8.00 (d, *J* = 8.2 Hz, 1H), 7.79 (d, *J* = 8.1 Hz, 1H), 7.59 (ddd, *J* = 8.6, 6.9, 1.5 Hz, 1H), 7.50 (ddd, *J* = 8.1, 6.8, 1.2 Hz, 1H), 7.43 (t, *J* = 7.8 Hz, 1H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 182.2 (q, *J* = 33.8 Hz), 136.1, 133.9, 131.6 (q, *J* = 4.0 Hz), 131.1, 129.4, 128.9, 127.0, 126.1, 125.1, 124.0, 116.7 (q, *J* = 293.2 Hz). **^{19}F NMR** (565 MHz, $CDCl_3$) δ -70.15.

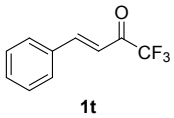
2,2,2-trifluoro-1-(2-phenyl-1H-indol-3-yl)ethan-1-one (1o)



1o

Yellow oil, 91% yield. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.77 (s, 1H), 8.21 (d, *J* = 5.9 Hz, 1H), 7.64 – 7.31 (m, 8H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 177.0 (q, *J* = 36.5 Hz), 148.1, 135.1, 131.3, 130.1, 129.5, 128.4, 126.9, 124.4, 123.6, 121.8 (q, *J* = 2.5 Hz), 116.5 (q, *J* = 290.3 Hz), 111.4, 108.4. **^{19}F NMR** (376 MHz, $CDCl_3$) δ -72.71. **HRMS (ESI)** calcd. for $C_{11}H_9F_3O_2$ [M-H]$^-$: 288.0642, Found: 288.0640.

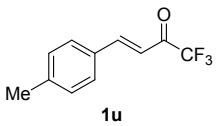
(*E*)-1,1,1-trifluoro-4-phenylbut-3-en-2-one (1t)



1t

Light yellow oil, 86% yield. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.97 (d, *J* = 16.0 Hz, 1H), 7.67 – 7.60 (m, 2H), 7.54 – 7.39 (m, 3H), 7.02 (d, *J* = 15.9 Hz, 1H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 180.0 (q, *J* = 35.3 Hz), 150.1, 133.3, 132.3, 129.2, 116.6, 116.4 (q, *J* = 290.6 Hz).**^{19}F NMR** (376 MHz $CDCl_3$) δ -77.60. **HRMS (ESI)** calcd. for $C_{10}H_7F_3O$ [M-H]$^-$: 199.0376, Found: 199.0368.

(*E*)-1,1,1-trifluoro-4-(p-tolyl)but-3-en-2-one (1u)

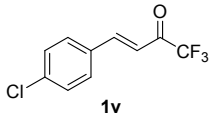


1u

Light yellow solid, 67% yield. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.95 (d, *J* = 15.9 Hz, 1H), 7.54 (d, *J* = 8.1 Hz, 2H), 7.34 – 7.17 (m, 2H), 6.97 (d, *J* = 15.9 Hz, 1H), 2.41 (s, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 180.0 (q, *J* = 34.9 Hz),

150.2, 143.4, 130.7, 123.0, 129.3, 116.4 (q, J = 291.2 Hz), 115.6, 21.7. **^{19}F NMR** (565 MHz, $CDCl_3$) δ -77.54.

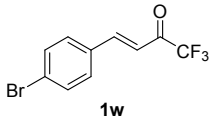
(*E*)-4-(4-chlorophenyl)-1,1,1-trifluorobut-3-en-2-one (1v)



1v

White solid, 90% yield. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.91 (d, J = 16.0 Hz, 1H), 7.58 (d, J = 8.4 Hz, 2H), 7.43 (d, J = 8.4 Hz, 2H), 6.99 (d, J = 16.0 Hz, 1H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 179.8 (q, J = 35.0 Hz), 148.5, 138.5, 131.8, 130.3, 129.6, 117.0, 116.3 (q, J = 290.2 Hz). **^{19}F NMR** (565 MHz, $CDCl_3$) δ -77.65 .

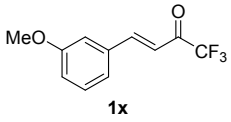
(*E*)-4-(4-bromophenyl)-1,1,1-trifluorobut-3-en-2-one (1w)



1w

Light yellow solid, 85% yield. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.90 (d, J = 16.0 Hz, 1H), 7.60 (d, J = 8.3 Hz, 2H), 7.50 (d, J = 8.3 Hz, 2H), 7.00 (d, J = 15.9 Hz, 1H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 179.8 (q, J = 35.6 Hz), 148.6, 132.5, 132.2, 130.4, 126.9, 117.1, 116.3 (q, J = 290.8 Hz). **^{19}F NMR** (376 MHz, $CDCl_3$) δ -77.65. **HRMS (ESI)** calcd. for $C_{10}H_6BrF_3O$ [M-H]$^-$: 276.9481, Found: 276.9478.

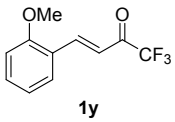
(*E*)-1,1,1-trifluoro-4-(3-methoxyphenyl)but-3-en-2-one (1x)



1x

Light yellow oil, 76% yield. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.93 (d, J = 16.0 Hz, 1H), 7.36 (t, J = 7.9 Hz, 1H), 7.28 – 7.21 (m, 1H), 7.13 (t, J = 2.1 Hz, 1H), 7.05 (ddd, J = 8.3, 2.6, 0.9 Hz, 1H), 6.99 (dd, J = 16.0, 1.0 Hz, 1H), 3.86 (s, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 178.0 (q, J = 35.0 Hz), 160.1, 150.1, 134.6, 130.2, 122.0, 118.3, 116.9, 116.4 (q, J = 290.7 Hz), 113.8, 55.4. **^{19}F NMR** (376 MHz, $CDCl_3$) δ -77.56. **HRMS (ESI)** calcd. for $C_{11}H_9F_3O_2$ [M-H]$^-$: 229.0482, Found: 229.0476.

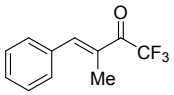
(*E*)-1,1,1-trifluoro-4-(2-methoxyphenyl)but-3-en-2-one (1y)



1y

Yellow oil, 67% yield. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 8.28 (d, J = 16.0 Hz, 1H), 7.59 (d, J = 7.5 Hz, 1H), 7.45 (t, J = 7.7 Hz, 1H), 7.14 (d, J = 16.0 Hz, 1H), 7.00 (t, J = 7.4 Hz, 1H), 6.96 (d, J = 8.3 Hz, 1H), 3.92 (s, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 180.5 (q, J = 34.8 Hz), 159.7, 145.8, 133.8, 130.2, 122.4, 120.9, 117.0, 116.6 (q, J = 290.7 Hz), 111.5, 55.6. **^{19}F NMR** (376 MHz, $CDCl_3$) δ -77.63. **HRMS (ESI)** calcd. for $C_{11}H_9F_3O_2$ [M-H]$^-$: 229.0482, Found: 229.0476.

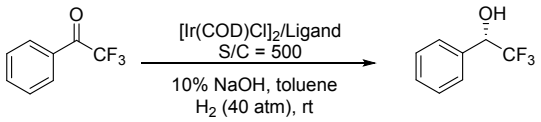
(*E*)-1,1,1-trifluoro-3-methyl-4-phenylbut-3-en-2-one (1z)



1z

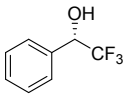
Yellow oil, 83% yield. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.74 (s, 1H), 7.60 – 7.34 (m, 5H), 2.17 (s, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 182.4 (dd, *J* = 33.3, 15.2 Hz), 145.9 (dt, *J* = 15.2, 3.5 Hz), 134.7 (d, *J* = 15.5 Hz), 131.0 (d, *J* = 15.2 Hz), 130.4 (d, *J* = 15.2 Hz), 130.0 (d, *J* = 15.1 Hz), 128.8 (d, *J* = 15.2 Hz), 116.9 (qd, *J* = 291.8, 15.1 Hz), 13.4 (d, *J* = 15.1 Hz). **^{19}F NMR** (376 MHz, $CDCl_3$) δ -68.91.

III. Representative procedure for asymmetric hydrogenation and characterization of secondary trifluoromethyl alcohols



General procedure for S/C = 500[4]: To a 4.0 mL vial was added the catalyst precursor $[Ir(COD)Cl]_2$ (6.7 mg, 9.97 μmol, 1.0 equiv), (S_C, R_C, S_C, R_{FC})-*f*-amphol **L2** (16.2 mg, 21.04 μmol, 2.1 equiv) and anhydrous ^{i}PrOH (2.0 mL) in the argon-filled glovebox. The mixture was stirred for 2.0 h at 25 °C. The resulting orange solution (20 μL) was transferred by syringe into a vial (5.0 mL) charged with substrate (0.2 mmol), NaOH (0.8 mg, 0.02 mmol) and anhydrous toluene (1.0 mL). The vial was transferred to an autoclave, which was then charged with of H_2 (40 atm) and stirred at rt for 16 h. The hydrogen gas was released slowly in a well-ventilated hood, the yield of the reaction was first determined by quantitative $^{19}F\{^1H\}$ NMR analysis. Then the solution was concentrated and purified by flash chromatography on silica gel (CH_2Cl_2/MeOH, 10:1) to afford the product. Pure product was afforded after column chromatography (hexanes/EtOAc 10/1~5/1).

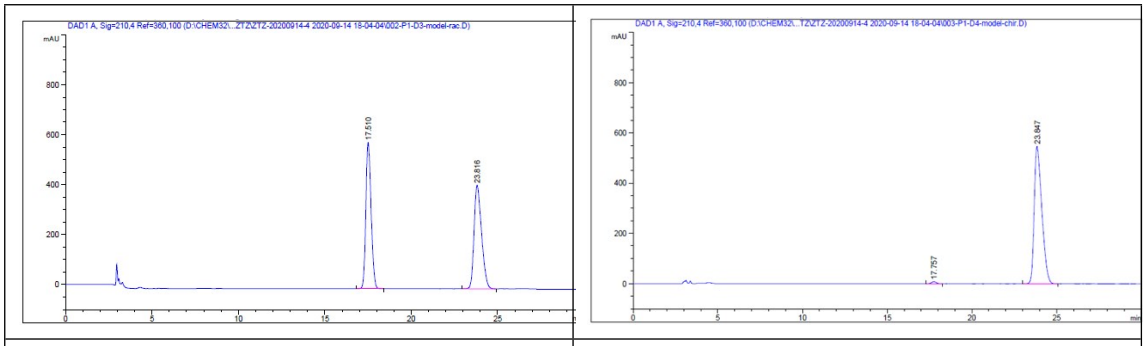
(*S*)-2, 2, 2-trifluoro-1-phenylethan-1-ol (2a)



2a

Colourless oil, >99% yield. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.41 – 7.29 (m, 5H), 4.84 (q, *J* = 6.8 Hz, 1H), 3.50 (s, 1H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 133.9, 129.5, 128.6, 127.4, 124.2 (q, *J* = 281.8 Hz), 72.7 (q, *J* = 32.2 Hz). **^{19}F NMR** (376 MHz, $CDCl_3$) δ -78.20.

Optical Rotation: $[\alpha]^{25}_D$ = +21.7 (c = 1.0, $CHCl_3$) (Lit:[5] $[\alpha]^{25}_D$ = +8.33 (c = 0.5, $CHCl_3$, *S*, 51% ee). The absolute configuration was determined to be (***S***). 98% ee. (HPLC condition: Daicel Chiralcel OJ-H Column, ^{n}hexane/^{i}PrOH = 95:5, flow rate = 1.0 mL/min, T = 25 °C, wavelength = 210 nm, t_{R1} = 17.8 min for minor isomer, t_{R2} = 23.8 min for major isomer).



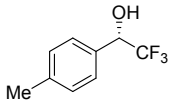
Signal 1: DAD1 A, Sig=210,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	17.510	BB	0.3271	1.24153e4	586.11285	49.8651
2	23.816	BB	0.4584	1.24824e4	415.54990	50.1349
Totals :				2.48977e4	1001.66275	

Signal 1: DAD1 A, Sig=210,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	17.757	BB	0.2926	152.29539	7.63775	0.8862
2	23.847	BB	0.4687	1.70328e4	547.90521	99.1138
Totals :				1.71851e4	555.54297	

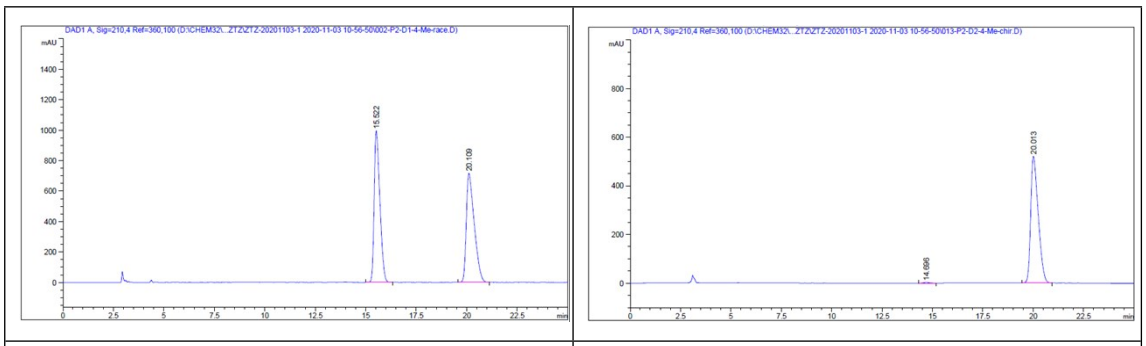
(*S*)-2,2,2-trifluoro-1-(p-tolyl)ethan-1-ol (2b)



2b

Colourless oil, 91% yield. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.36 (d, *J* = 7.9 Hz, 2H), 7.22 (d, *J* = 7.9 Hz, 2H), 4.98 (qd, *J* = 6.7, 4.0 Hz, 1H), 2.63 (d, *J* = 4.2 Hz, 1H), 2.37 (s, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 139.6, 131.1, 129.3, 127.3, 124.3 (q, *J* = 282.0 Hz), 72.7 (q, *J* = 32.0 Hz), 21.2 (d, *J* = 4.0 Hz). **^{19}F NMR** (376 MHz, $CDCl_3$) δ -78.41.

Optical Rotation: $[\alpha]^{20}_D$ = +28.7 (c = 1.0, $CHCl_3$) (Lit: [6]$[\alpha]^{25}_D$ = +28.0 (c = 1.6, $CHCl_3$, *S*, 86% ee). The absolute configuration was determined to be (***S***). 99% ee. (HPLC condition: Daicel Chiralcel OJ-H Column, ^{n}hexane/^{i}PrOH = 95:5, flow rate = 1.0 ml/min, T = 25 ^{o}C, wavelength = 210 nm, t_{R1} = 14.7 min for minor isomer, t_{R2} = 20.0 min for major isomer).



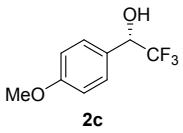
Signal 1: DAD1 A, Sig=210,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	15.522	BB	0.2999	1.94238e4	994.42737	49.8554
2	20.109	BB	0.4002	1.95364e4	716.29712	50.1446
Totals :				3.89602e4	1710.72449	

Signal 1: DAD1 A, Sig=210,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	14.696	BB	0.2416	52.45398	2.66591	0.3881
2	20.013	BB	0.3876	1.34625e4	520.68628	99.6119
Totals :				1.35150e4	523.35219	

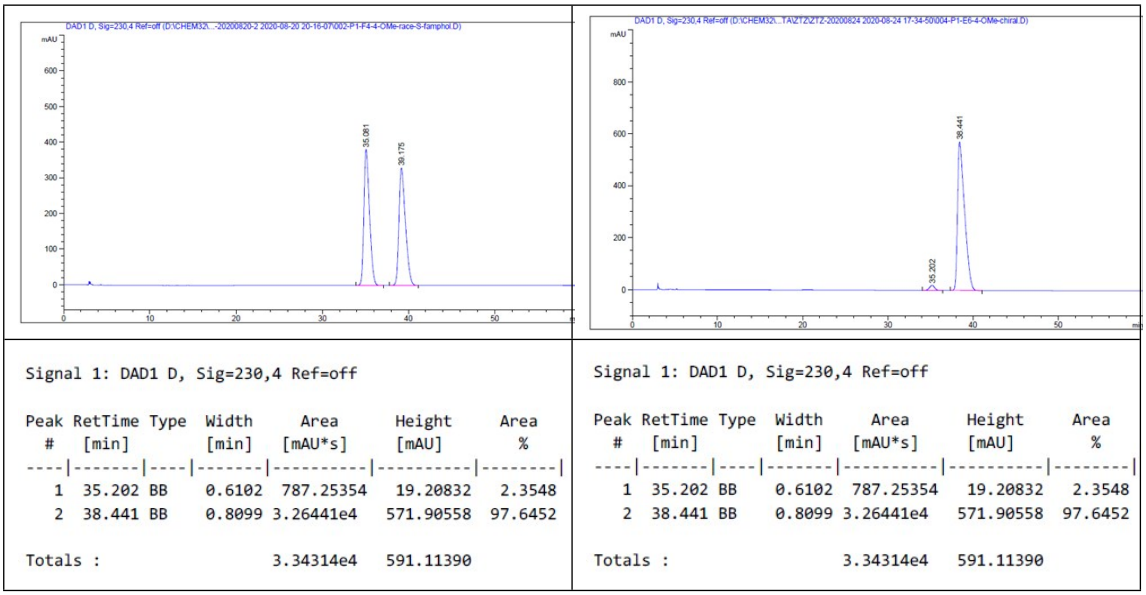
(*S*)-2,2,2-trifluoro-1-(4-methoxyphenyl)ethan-1-ol (2c)



2c

Colourless oil, >99% yield. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.48 – 7.30 (m, 2H), 7.07 – 6.79 (m, 2H), 4.95 (q, *J* = 6.7 Hz, 1H), 3.82 (s, 3H), 2.58 (s, 1H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 160.4, 128.8, 126.1, 124.3 (q, *J* = 282.3 Hz), 114.0, 72.4 (q, *J* = 32.0 Hz), 55.3. **^{19}F NMR** (565 MHz, $CDCl_3$) δ -78.55.

Optical Rotation: $[\alpha]^{25}_D$ = +30.2 (c = 1.0, $CHCl_3$). The absolute configuration was assigned to be **(*S*)** by analogy to **2a**. 95% ee. (HPLC condition: Daicel Chiralcel OJ-H Column, ^{n}hexane/^{i}PrOH = 95:5, flow rate = 1.0 ml/min, T = 25 °C, wavelength = 230 nm, t_{R1} = 35.2 min for minor isomer, t_{R2} = 38.4 min for major isomer).



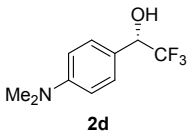
Signal 1: DAD1 D, Sig=230,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	35.202	BB	0.6102	787.25354	19.20832	2.3548
2	38.441	BB	0.8099	3.26441e4	571.90558	97.6452
Totals :				3.34314e4	591.11390	

Signal 1: DAD1 D, Sig=230,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	35.202	BB	0.6102	787.25354	19.20832	2.3548
2	38.441	BB	0.8099	3.26441e4	571.90558	97.6452
Totals :				3.34314e4	591.11390	

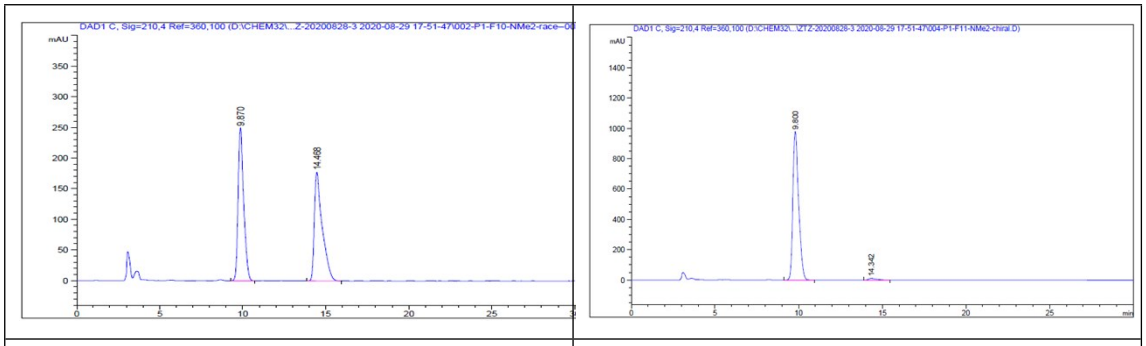
(*S*)-1-(4-(dimethylamino)phenyl)-2,2,2-trifluoroethan-1-ol (2d)



2d

White solid, 40.3 mg, 92% yield. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.29 (d, *J* = 8.5 Hz, 2H), 6.70 (d, *J* = 8.8 Hz, 2H), 4.85 (q, *J* = 6.8 Hz, 1H), 2.95 (s, 6H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 151.2, 128.4, 124.5(q, *J* = 282.2 Hz), 121.5, 112.2, 72.7 (q, *J* = 32.1 Hz), 40.4. **^{19}F NMR** (376 MHz, $CDCl_3$) δ -78.35. **HRMS (ESI)** calcd. for $C_{10}H_{12}F_3NO$ $[M+H]^+$: 220.0944, Found: 220.0945.

Optical Rotation: $[\alpha]^{25}_D$ = +30.5 (c = 1.0, $CHCl_3$). The absolute configuration was assigned to be **(*S*)** by analogy to **2a**. 97% ee. (HPLC condition: Daicel Chiralcel AS-H Column, ^{n}hexane/^{i}PrOH = 95:5, flow rate = 1.0 ml/min, T = 25 °C, wavelength = 210 nm, t_{R1} = 9.8 min for major isomer, t_{R2} = 14.3 min for minor isomer).



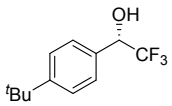
Signal 1: DAD1 C, Sig=210,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	9.870	BB	0.3513	5843.51318	249.45985	49.8462
2	14.468	BB	0.4624	5879.57422	177.53111	50.1538
Totals :				1.17231e4	426.99097	

Signal 1: DAD1 C, Sig=210,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	9.800	BB	0.3616	2.34495e4	978.58685	98.4590
2	14.342	BB	0.4410	367.02347	11.12269	1.5410
Totals :				2.38165e4	989.70954	

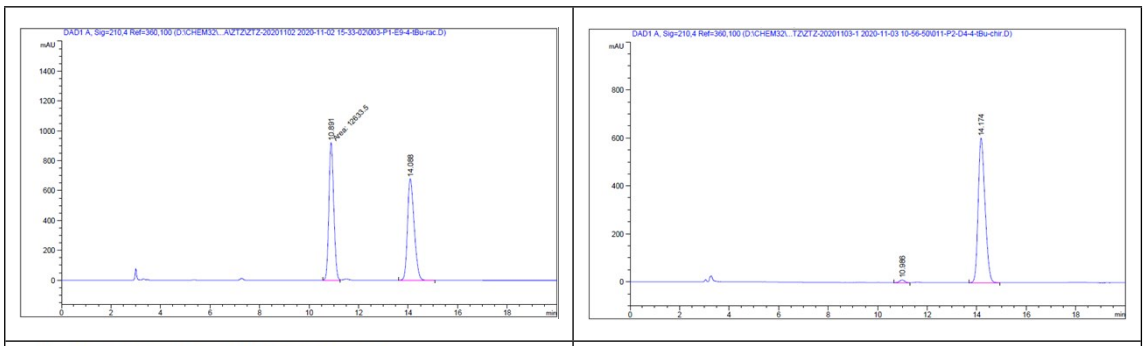
(*S*)-1-(4-(*tert*-butyl)phenyl)-2,2,2-trifluoroethan-1-ol (2e)



2e

White solid, >99% yield. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.38 – 7.29 (m, 4H), 4.90 (q, *J* = 6.8 Hz, 1H), 2.49 (s, 1H), 1.25 (s, 9H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 152.7, 131.0, 127.2, 125.6, 124.3(q, *J* = 282.0 Hz), 72.7(q, *J* = 32.0 Hz), 34.7, 31.2. **^{19}F NMR** (565 MHz, $CDCl_3$) δ -78.27.

Optical Rotation: $[\alpha]^{20}_D$ = +19.1 (c = 1.0, $CHCl_3$). The absolute configuration was assigned to be **(*S*)** by analogy to **2a**. 97% ee. (HPLC condition: Daicel Chiralcel OJ-H Column, ^{n}hexane/^{i}PrOH = 97/3, flow rate = 1.0 mL/min, T = 25 °C, wavelength = 210 nm, t_{R1} = 11.0 min for minor isomer, t_{R2} = 14.2 min for major isomer).



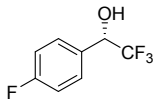
Signal 1: DAD1 A, Sig=210,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.891	MM	0.2283	1.26335e4	922.44647	49.9531
2	14.088	BB	0.2854	1.26573e4	679.16125	50.0469
Totals :				2.52908e4	1601.60773	

Signal 1: DAD1 A, Sig=210,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.986	BB	0.2185	157.15160	11.01138	1.3422
2	14.174	BB	0.2936	1.15518e4	602.79773	98.6578
Totals :				1.17089e4	613.80911	

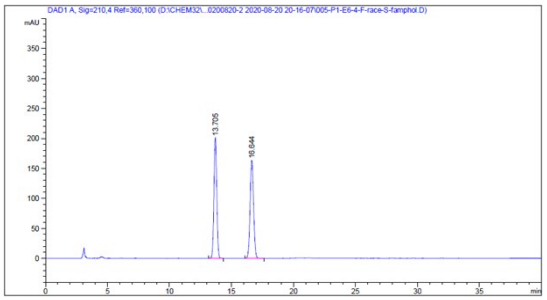
(*S*)-2,2,2-trifluoro-1-(4-fluorophenyl)ethan-1-ol (2f)



2f

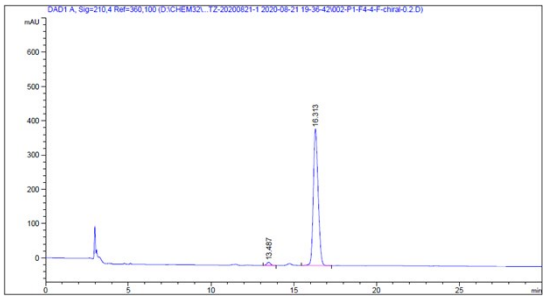
Colourless oil, >99% yield. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.46 (dd, J = 8.5, 5.2 Hz, 2H), 7.15 – 7.04 (m, 2H), 5.01 (q, J = 6.6 Hz, 1H), 2.81 (s, 1H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 163.4 (d, *J* = 248.5 Hz), 129.8, 129.3 (d, *J* = 8.5 Hz), 124.1 (q, *J* = 281.5 Hz), 115.7 (d, *J* = 21.8 Hz), 72.1 (q, *J* = 32.4 Hz). **^{19}F NMR** (376 MHz, $CDCl_3$) δ -78.64, -111.86. **HRMS (ESI)** calcd. for $C_8H_6F_4O$ [M-H]$^-$: 193.0282, Found: 193.0274.

Optical Rotation: $[\alpha]^{20}_D$ = +22.4 (c = 1.0, $CHCl_3$). The absolute configuration was assigned to be **(*S*)** by analogy to **2a**. 96% ee. (HPLC condition: Daicel Chiralcel OJ-H Column, ^{n}hexane/^{i}PrOH = 95/5, flow rate = 1.0 mL/min, T = 25 °C, wavelength = 210 nm, t_{R1} = 13.5 min for minor isomer, t_{R2} = 16.3 min for major isomer).



Signal 1: DAD1 A, Sig=210,4 Ref=360,100

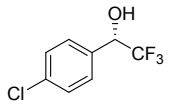
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	13.705	BB	0.2473	3193.30884	201.06387	49.9504
2	16.644	BB	0.3067	3199.65405	163.19508	50.0496
Totals :				6392.96289	364.25896	



Signal 1: DAD1 A, Sig=210,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	13.487	BB	0.2459	143.41727	9.20010	1.7523
2	16.313	BB	0.3090	8041.00391	399.18066	98.2477
Totals :				8184.42117	408.38076	

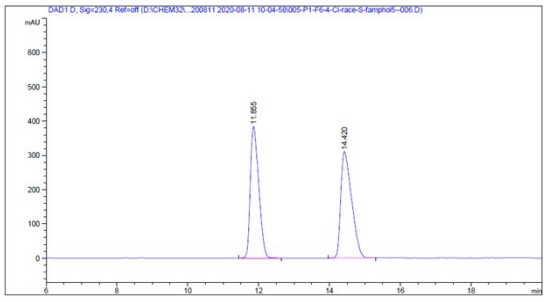
(*S*)-1-(4-chlorophenyl)-2,2,2-trifluoroethan-1-one (2g)



2g

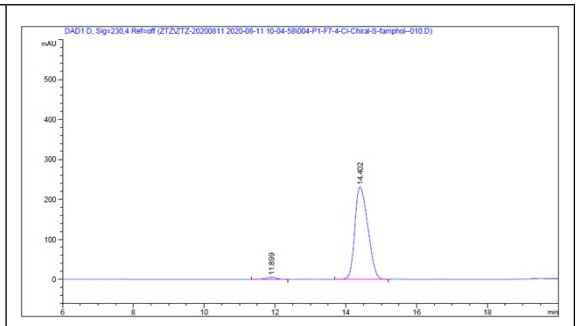
Colourless oil, >99% yield. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.49 – 7.30 (m, 4H), 5.02 (q, *J* = 6.2 Hz, 1H), 2.60 (s, 1H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 135.6, 132.2, 128.9, 128.8, 124.0 (q, *J* = 281.4 Hz), 72.2 (q, *J* = 32.6 Hz). **^{19}F NMR** (376 MHz, $CDCl_3$) δ -78.55. **HRMS (ESI)** calcd. for $C_8H_6ClF_3O$ [M+HCOO]$^-$: 255.0041, Found: 255.0038.

Optical Rotation: $[\alpha]^{20}_D$ = +25.4 (c = 1.0, $CHCl_3$) (Lit:[7] $[\alpha]^{20}_D$ = +26.1 (c = 1.0, $CHCl_3$, *S*, 98.7% ee). The absolute configuration was determined to be (***S***). 97% ee. (HPLC condition: Daicel Chiralcel OJ-H Column, ^{n}hexane/^{i}PrOH = 95/5, flow rate = 1.0 mL/min, T = 25 °C, wavelength = 230 nm, t_{R1} = 11.9 min for minor isomer, t_{R2} = 14.4 min for major isomer).



Signal 1: DAD1 D, Sig=230,4 Ref=off

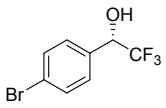
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	11.855	BB	0.2593	6310.78418	384.93372	48.9373
2	14.420	BB	0.3290	6584.86523	310.97110	51.0627
Totals :				1.28956e4	695.90482	



Signal 1: DAD1 D, Sig=230,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	11.899	BB	0.3254	101.26991	4.81388	1.7018
2	14.402	BB	0.4069	5849.52197	231.37939	98.2982

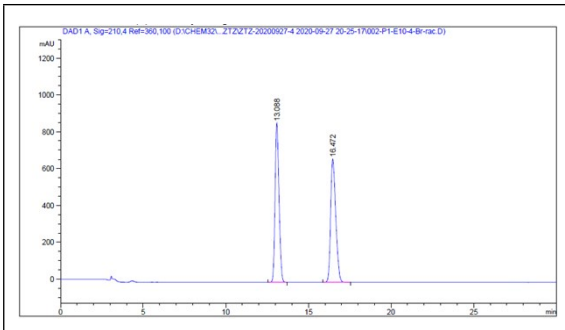
(*S*)-1-(4-bromophenyl)-2,2,2-trifluoroethan-1-ol (2h)



2h

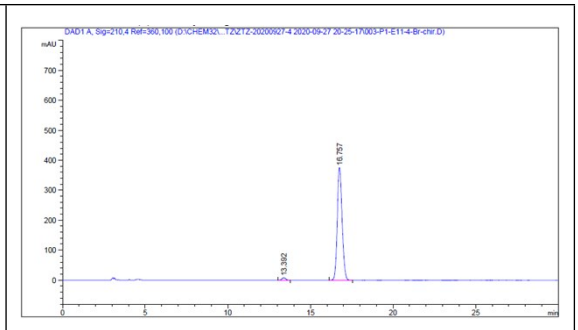
White solid, >99% yield. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.70 – 7.43 (m, 2H), 7.30 (d, *J* = 8.2 Hz, 2H), 4.93 (q, *J* = 6.6 Hz, 1H), 3.17 (s, 1H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 132.8, 131.9, 129.1, 124.0 (q, *J* = 281.9 Hz), 123.8, 72.2 (q, *J* = 32.3 Hz). **^{19}F NMR** (376 MHz, $CDCl_3$) δ -78.42. **HRMS (ESI)** calcd. for $C_8H_6BrF_3O$ [M+HCOO]$^-$: 298.9536, Found: 298.9535.

Optical Rotation: $[\alpha]^{20}_D$ = +18.1 (c = 1.0, $CHCl_3$). The absolute configuration was assigned to be **(*S*)** by analogy to **2a**. 97% ee. (HPLC condition: Daicel Chiralcel OJ-H Column, ^{n}hexane/^{i}PrOH = 95/5, flow rate = 1.0 mL/min, T = 25 °C, wavelength = 210 nm, t_{R1} = 13.4 min for minor isomer, t_{R2} = 16.8 min for major isomer).



Signal 1: DAD1 A, Sig=210,4 Ref=360,100

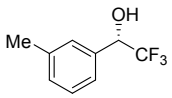
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	13.088	BB	0.2552	1.43035e4	863.65570	49.9246
2	16.472	BB	0.3281	1.43467e4	669.33801	50.0754
Totals :				2.86503e4	1532.99371	



Signal 1: DAD1 A, Sig=210,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	13.392	BB	0.2413	125.21133	8.05612	1.6169
2	16.757	BB	0.3123	7618.53125	376.06619	98.3831
Totals :				7743.74258	384.12232	

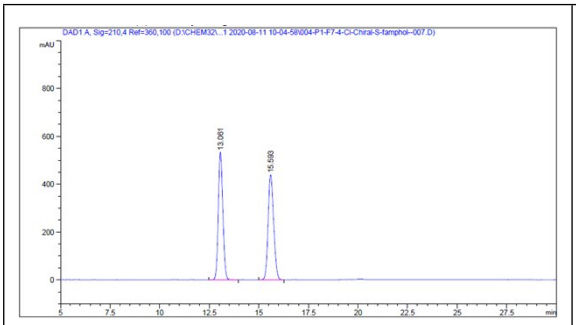
(*S*)-2,2,2-trifluoro-1-(m-tolyl)ethan-1-ol (2i)



2i

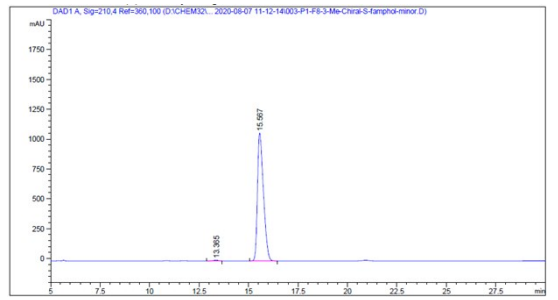
Colourless oil, >99% yield. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.39 – 7.04 (m, 4H), 4.94 (q, *J* = 6.5 Hz, 1H), 2.68 (s, 1H), 2.37 (s, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 138.5, 133.9, 130.3, 128.5, 128.0, 124.5, 124.3 (q, *J* = 282.0 Hz), 72.9 (q, *J* = 32.0 Hz), 21.3. **^{19}F NMR** (376 MHz, $CDCl_3$) δ -78.25. **HRMS (ESI)** calcd. for $C_9H_9F_3O$ [M-H]$^-$: 189.0533, Found: 189.0525.

Optical Rotation: $[\alpha]^{20}_D$ = +23.3 (c = 1.0, $CHCl_3$). The absolute configuration was assigned to be **(*S*)** by analogy to **2a**. 99% ee. (HPLC condition: Daicel Chiralcel OJ-H Column, ^{n}hexane/^{i}PrOH = 95/5, flow rate = 1.0 mL/min, T = 25 °C, wavelength = 210 nm, t_{R1} = 13.4 min for minor isomer, t_{R2} = 15.6 min for major isomer).



Signal 1: DAD1 A, Sig=210,4 Ref=360,100

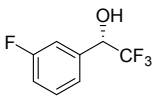
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	13.061	BB	0.2449	8464.75977	534.05096	49.9099
2	15.593	BB	0.2998	8495.32324	439.01605	50.0901
Totals :				1.69601e4	973.06702	



Signal 1: DAD1 A, Sig=210,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	13.365	BB	0.2350	102.10171	6.51080	0.4539
2	15.567	BB	0.3201	2.23910e4	1070.29395	99.5461
Totals :				2.24931e4	1076.80474	

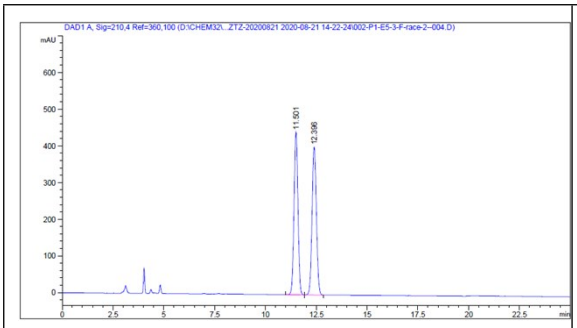
(*S*)-2,2,2-trifluoro-1-(3-fluorophenyl)ethan-1-ol (2j)



2j

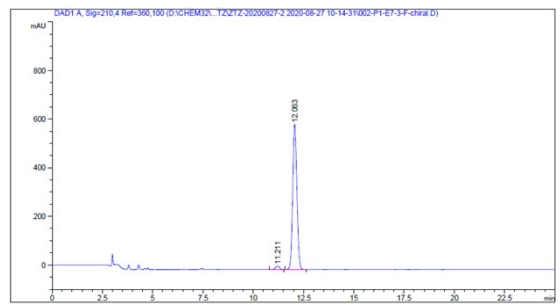
Colourless oil, >99% yield. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.38 (td, *J* = 8.2, 6.0 Hz, H), 7.30 – 7.16 (m, 2H), 7.17 – 7.03 (m, 1H), 5.02 (qd, *J* = 6.5, 3.9 Hz, 1H), 2.79 (d, *J* = 4.2 Hz, 1H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 162.8 (d, *J* = 246.4 Hz), 136.2 (d, *J* = 7.6 Hz), 130.2 (d, *J* = 7.8 Hz), 124.0 (q, *J* = 282.2 Hz), 123.1 (d, *J* = 3.0 Hz), 116.5 (d, *J* = 20.8 Hz), 114.5 (d, *J* = 23.4 Hz), 72.3 (t, *J* = 32.2 Hz). **^{19}F NMR** (376 MHz, $CDCl_3$) δ -78.41, -112.12. **HRMS (ESI)** calcd. for $C_8H_6F_4O$ [M-H]$^-$: 193.0282, Found: 193.0273.

Optical Rotation: $[\alpha]^{20}_D$ = +14.4 (c = 1.0, $CHCl_3$). The absolute configuration was assigned to be **(*S*)** by analogy to **2a**. 96% ee. (HPLC condition: Daicel Chiralcel OJ-H Column, ^{n}hexane/^{i}PrOH = 95/5, flow rate = 1.0 mL/min, T = 25 °C, wavelength = 210 nm, t_{R1} = 11.2 min for minor isomer, t_{R2} = 12.1 min for major isomer).



Signal 1: DAD1 A, Sig=210,4 Ref=360,100

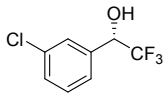
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	11.501	BB	0.2114	5988.49609	443.91724	49.9776
2	12.396	BB	0.2314	5993.87549	403.34689	50.0224
Totals :				1.19824e4	847.26413	



Signal 1: DAD1 A, Sig=210,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	11.211	BB	0.2047	182.89124	13.97279	2.0754
2	12.063	BB	0.2247	8629.45215	596.86493	97.9246
Totals :				8812.34338	610.83772	

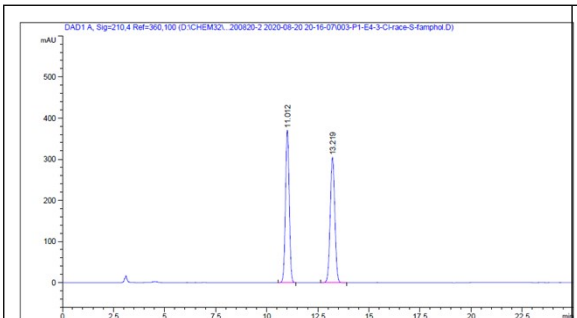
(*S*)-1-(3-chlorophenyl)-2,2,2-trifluoroethan-1-ol (2k)



2k

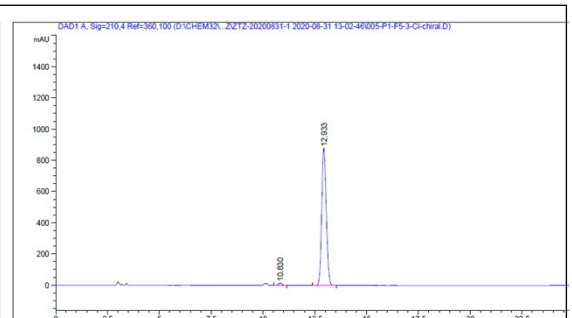
Colourless oil, >99% yield. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.49 (s, 1H), 7.42 – 7.31 (m, 3H), 5.00 (q, *J* = 6.6 Hz, 1H), 2.75 (s, 1H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 135.7, 134.6, 129.9, 129.7, 127.6, 125.6, 123.9 (q, *J* = 282.4 Hz), 72.2 (q, *J* = 32.1 Hz). **^{19}F NMR** (376 MHz, $CDCl_3$) δ -78.35. **HRMS (ESI)** calcd. for $C_8H_6ClF_3O$ [M-H]$^-$: 208.9987, Found: 208.9979.

Optical Rotation: $[\alpha]^{20}_D$ = +17.3 (c = 1.0, $CHCl_3$) (Lit:[7] $[\alpha]^{20}_D$ = +23.1 (c = 1.0, $CHCl_3$, *S*, 99.6% ee). The absolute configuration was determined to be (***S***). 98% ee. (HPLC condition: Daicel Chiralcel OJ-H Column, ^{n}hexane/^{i}PrOH = 95/5, flow rate = 1.0 mL/min, T = 25 °C, wavelength = 210 nm, t_{R1} = 10.8 min for minor isomer, t_{R2} = 12.9 min for major isomer).



Signal 1: DAD1 A, Sig=210,4 Ref=360,100

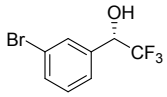
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	11.012	BB	0.2020	4766.61914	370.66928	49.9292
2	13.219	BB	0.2428	4780.12891	305.02029	50.0708
Totals :				9546.74805	675.68958	



Signal 1: DAD1 A, Sig=210,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.830	BB	0.1858	163.59911	13.45990	1.2112
2	12.933	BB	0.2351	1.33432e4	879.22192	98.7888
Totals :				1.35068e4	892.68182	

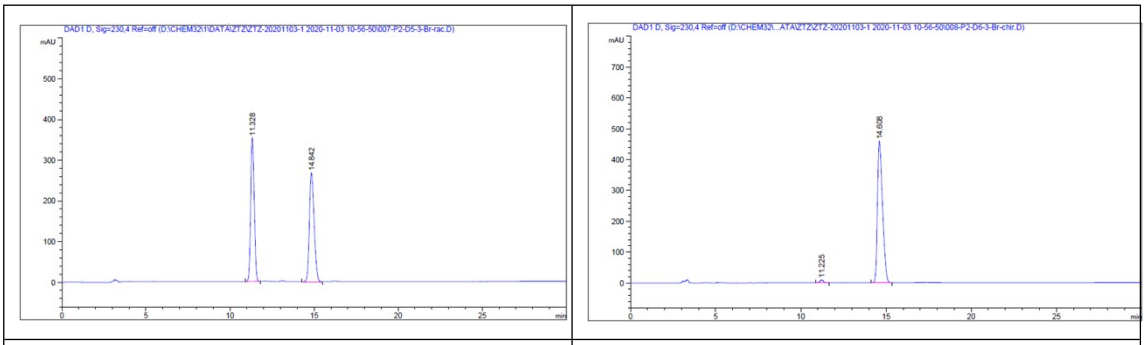
(*S*)-1-(3-bromophenyl)-2,2,2-trifluoroethan-1-ol (2l)



2l

Colourless oil, >99% yield. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.64 (s, 1H), 7.54 (ddd, *J* = 8.0, 2.0, 1.1 Hz, 1H), 7.40 (d, *J* = 7.8 Hz, 1H), 7.32 – 7.23 (m, 1H), 4.99 (qd, *J* = 6.5, 4.3 Hz, 1H), 2.73 (d, *J* = 4.4 Hz, 1H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 136.0, 132.7, 130.5, 130.1, 126.1, 124.0 (q, *J* = 282.4 Hz), 122.7, 72.1 (q, *J* = 32.5 Hz). **^{19}F NMR** (565 MHz, $CDCl_3$) δ -78.33. **HRMS (ESI)** calcd. for $C_8H_6BrF_3O$ [M-H]$^-$: 252.9481, Found: 252.9477.

Optical Rotation: $[\alpha]^{20}_D$ = +15.9 (c = 1.0, $CHCl_3$). The absolute configuration was assigned to be **(*S*)** by analogy to **2a**. 97% ee. (HPLC condition: Daicel Chiralcel OJ-H Column, ^{n}hexane/^{i}PrOH = 95/5, flow rate = 1.0 mL/min, T = 25 °C, wavelength = 230 nm, t_{R1} = 11.2 min for minor isomer, t_{R2} = 14.6 min for major isomer).



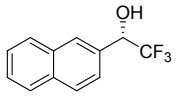
Signal 1: DAD1 D, Sig=230,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	11.328	BB	0.2290	5158.41064	352.03021	49.6313
2	14.842	BB	0.3040	5235.05859	267.85114	50.3687
Totals :				1.03935e4	619.88135	

Signal 1: DAD1 D, Sig=230,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	11.225	BB	0.2302	138.42287	9.48674	1.4350
2	14.608	BB	0.3176	9507.90723	459.05469	98.5650
Totals :				9646.33009	468.54143	

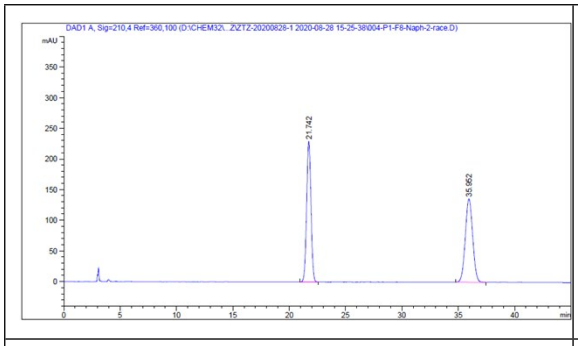
(*S*)-2,2,2-trifluoro-1-(naphthalen-2-yl)ethan-1-ol (2m)



2m

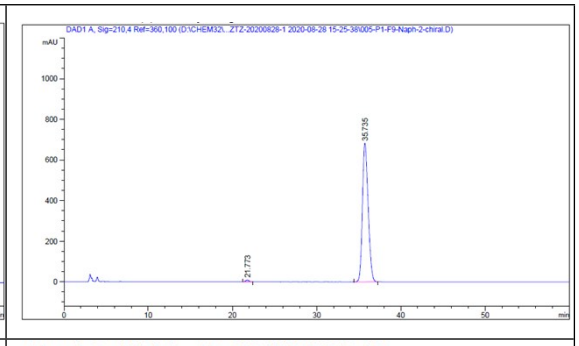
Colourless oil, 40.7 mg, 90% yield. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.98 (s, 1H), 7.97 – 7.84 (m, 3H), 7.68 – 7.50 (m, 3H), 5.21 (qd, *J* = 6.7, 4.3 Hz, 1H), 2.78 (d, *J* = 4.5 Hz, 1H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 133.7, 132.9, 131.2, 128.5, 128.2, 127.7, 127.3, 126.9, 126.6, 124.3 (q, *J* = 282.3 Hz), 124.3, 73.0 (q, *J* = 32.5 Hz). **^{19}F NMR** (376 MHz, $CDCl_3$) δ -78.00. **HRMS (ESI)** calcd. for $C_{12}H_9F_3O$ [M-H]$^-$: 225.0533, Found: 225.0526.

Optical Rotation: $[\alpha]^{20}_D$ = +17.7 (c = 0.5, $CHCl_3$). The absolute configuration was assigned to be **(*S*)** by analogy to **2a**. 99% ee. (HPLC condition: Daicel Chiralcel OJ-H Column, ^{n}hexane/^{i}PrOH = 92/8, flow rate = 1.0 mL/min, T = 25 °C, wavelength = 210 nm, t_{R1} = 21.8 min for minor isomer, t_{R2} = 35.7 min for major isomer).



Signal 1: DAD1 A, Sig=210,4 Ref=360,100

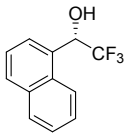
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	21.742	BB	0.4193	6164.46680	229.52333	49.8632
2	35.952	BB	0.6893	6198.29639	136.10626	50.1368
Totals :				1.23628e4	365.62959	



Signal 1: DAD1 A, Sig=210,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	21.773	BB	0.3797	237.57820	8.89130	0.7304
2	35.735	BB	0.7235	3.22906e4	683.07532	99.2696
Totals :				3.25281e4	691.96662	

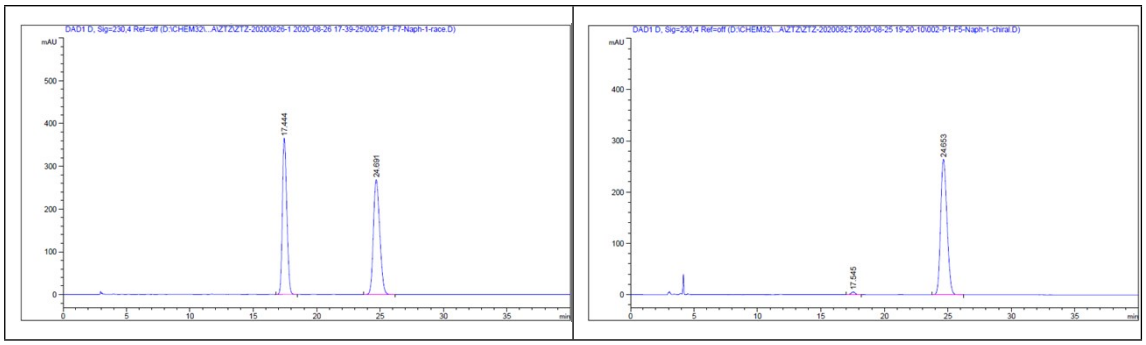
(*S*)-2,2,2-trifluoro-1-(naphthalen-1-yl)ethan-1-ol (2n)



2n

Colourless oil, 98% yield. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 8.06 (d, *J* = 8.5 Hz, 1H), 7.91 (t, *J* = 7.9 Hz, 2H), 7.84 (d, *J* = 7.2 Hz, 1H), 7.61 – 7.48 (m, 3H), 5.90 (q, *J* = 6.7 Hz, 1H), 2.64 (s, 1H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 133.7, 131.1, 130.2, 129.9, 129.0, 126.8, 125.9, 125.8, 125.2, 124.7 (q, *J* = 282.3 Hz), 122.8, 69.0 (q, *J* = 31.9 Hz). **^{19}F NMR** (376 MHz, $CDCl_3$) δ -76.87. **HRMS (ESI)** calcd. for $C_{12}H_9F_3O$ [M-H]$^-$: 225.0533, Found: 225.0527.

Optical Rotation: $[\alpha]^{20}_D$ = +18.2 (c = 1.0, $CHCl_3$). The absolute configuration was assigned to be **(*S*)** by analogy to **2a**. 98% ee. (HPLC condition: Daicel Chiralcel OJ-H Column, ^{n}hexane/^{i}PrOH = 92/8, flow rate = 1.0 mL/min, T = 25 °C, wavelength = 230 nm, t_{R1} = 17.5 min for minor isomer, t_{R2} = 24.7 min for major isomer).



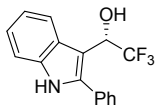
Signal 1: DAD1 D, Sig=230,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	17.444	BB	0.3790	8856.36426	365.13733	48.7160
2	24.691	BB	0.5405	9323.22949	268.92386	51.2840
Totals :				1.81796e4	634.06119	

Signal 1: DAD1 D, Sig=230,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	17.545	BB	0.3365	112.55531	5.12044	1.2081
2	24.653	BB	0.5420	9204.04297	264.45908	98.7919
Totals :				9316.59828	269.57951	

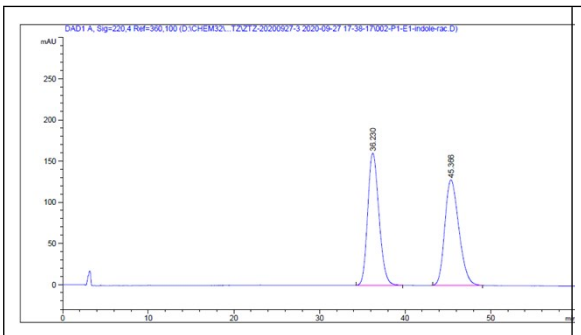
(*S*)-2,2,2-trifluoro-1-(2-phenyl-1H-indol-3-yl)ethan-1-ol (2o)

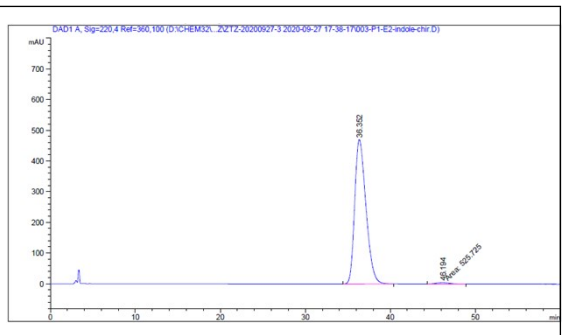


2o

White solid, 57.7 mg, >99% yield. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.27 (s, 1H), 7.93 (d, *J* = 7.9 Hz, 1H), 7.55 – 7.44 (m, 5H), 7.42 (d, *J* = 8.0 Hz, 1H), 7.28 (dd, *J* = 7.0, 1.2 Hz, 1H), 7.21 (ddd, *J* = 8.2, 7.1, 1.2 Hz, 1H), 5.32 (qd, *J* = 7.5, 2.6 Hz, 1H), 2.44 (s, 1H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 138.9, 135.9, 131.4, 129.1, 128.9, 126.0, 125.4 (q, *J* = 282.7 Hz), 123.1, 121.2 (q, *J* = 2.9 Hz), 120.9, 111.1, 106.1, 68.0 (q, *J* = 33.7 Hz). **^{19}F NMR** (376 MHz, $CDCl_3$) δ -75.73. **HRMS (ESI)** calcd. for $C_{16}H_{12}F_3NO$ $[M-H]^-$: 290.0798, Found: 290.0797.

Optical Rotation: $[\alpha]^{20}_D$ = +60.8 (c = 1.0, $CHCl_3$). The absolute configuration was assigned to be **(*S*)** by analogy to **2a**. 98% ee. (HPLC condition: Daicel Chiralcel OD-H Column, ^{n}hexane/^{i}PrOH = 90/10, flow rate = 1.0 mL/min, T = 25 °C, wavelength = 220 nm, t_{R1} = 36.4 min for major isomer, t_{R2} = 46.2 min for minor isomer).





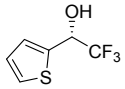
Signal 1: DAD1 A, Sig=220,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	36.230	BB	1.3404	1.46439e4	160.51514	50.1113
2	45.366	BB	1.5071	1.45789e4	128.16414	49.8887
Totals :				2.92228e4	288.67928	

Signal 1: DAD1 A, Sig=220,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	36.352	BB	1.3904	4.32037e4	470.00745	98.7978
2	46.194	MM	1.9561	525.72540	4.47946	1.2022
Totals :				4.37295e4	474.48690	

(*S*)-2,2,2-trifluoro-1-(thiophen-2-yl)ethan-1-ol (2p)

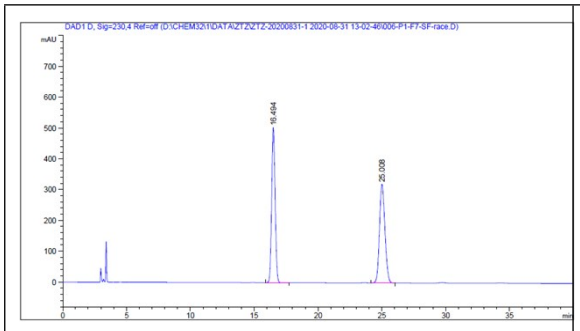


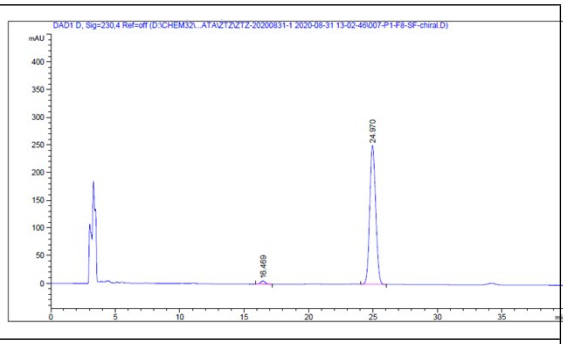
2p

Colourless oil, >99% yield. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.40 (dd, *J* = 5.0, 1.2 Hz, 1H), 7.20 (d, *J* = 3.5 Hz, 1H), 7.05 (dd, *J* = 5.1, 3.6 Hz, 1H), 5.28 (dt, *J* = 7.9, 5.1 Hz, 1H), 2.80 (s, 1H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 136.1, 127.5, 127.1, 127.0, 123.7 (q, *J* = 281.9 Hz), 69.3 (q, *J* = 34.0 Hz). **^{19}F NMR** (376 MHz, $CDCl_3$) δ -78.71. **HRMS (ESI)** calcd.

for $C_6H_5F_3OS$ [M+HCOO]$^-$: 226.9995, Found: 226.9990.

Optical Rotation: $[\alpha]^{20}_D$ = +15.9 (c = 1.0, $CHCl_3$) (Lit:[8] $[\alpha]^{25}_D$ = +24.2 (c = 1.0, $CHCl_3$, *S*, >98% ee). The absolute configuration was determined to be (***S***). 97% ee. (HPLC condition: Daicel Chiralcel OJ-H Column, ^{n}hexane/^{i}PrOH = 95/5, flow rate = 1.0 mL/min, T = 25 ^{o}C, wavelength = 230 nm, t_{R1} = 16.5 min for minor isomer, t_{R2} = 25.0 min for major isomer).





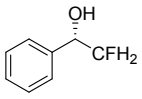
Signal 1: DAD1 D, Sig=230,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	16.494	BB	0.2917	9485.16016	503.69455	50.0505
2	25.008	BB	0.4564	9466.00391	320.62805	49.9495
Totals :				1.89512e4	824.32260	

Signal 1: DAD1 D, Sig=230,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	16.469	BB	0.3571	134.00116	5.76564	1.6266
2	24.970	BB	0.5020	8104.01709	251.47501	98.3734
Totals :				8238.01825	257.24065	

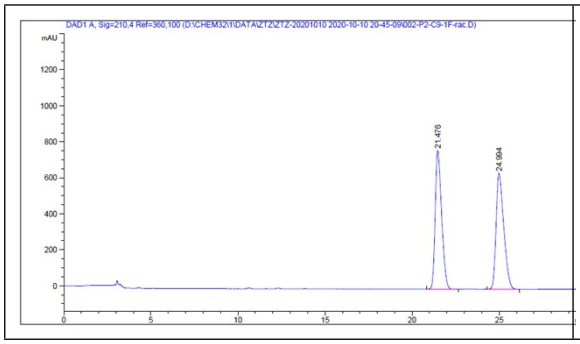
(*S*)-2-fluoro-1-phenylethan-1-ol (2q)

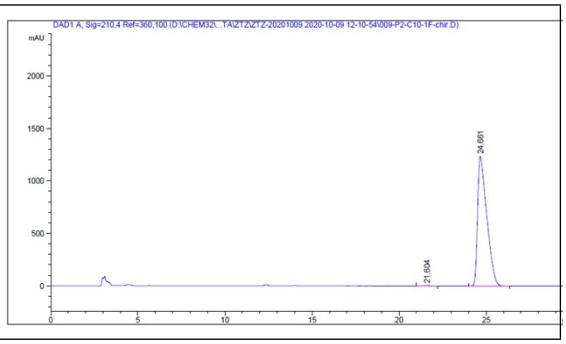


2q

Colourless oil, 92% yield. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.44 – 7.27 (m, 5H), 5.01 (ddd, J = 14.2, 7.7, 3.7 Hz, 1H), 4.68 – 4.20 (m, 2H), 2.64 (s, 1H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 138.1 (d, J = 8.4 Hz), 128.6, 128.4, 126.3, 87.1 (d, J = 174.4 Hz), 72.9 (d, J = 19.8 Hz). **^{19}F NMR** (376 MHz, $CDCl_3$) δ -220.56.

Optical Rotation: $[\alpha]^{20}_D$ = +69.5 (c = 1.0, $CHCl_3$) (Lit:[9] $[\alpha]^{20}_D$ = -56.8 (c = 1.2, $CHCl_3$, *R*, 98% ee). The absolute configuration was determined to be (***S***). 99% ee. (HPLC condition: Daicel Chiralcel OJ-H Column, ^{n}hexane/^{i}PrOH = 95/5, flow rate = 1.0 mL/min, T = 25 ^{o}C, wavelength = 210 nm, t_{R1} = 21.6 min for minor isomer, t_{R2} = 24.7 min for major isomer).





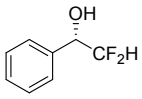
Signal 1: DAD1 A, Sig=210,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	21.476	BB	0.3902	1.97004e4	770.72473	49.9198
2	24.994	BB	0.4638	1.97637e4	644.35651	50.0802
Totals :				3.94641e4	1415.08124	

Signal 1: DAD1 A, Sig=210,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	21.604	BB	0.3418	112.93392	4.06852	0.2502
2	24.661	BB	0.5224	4.50219e4	1237.50769	99.7498
Totals :				4.51348e4	1241.57621	

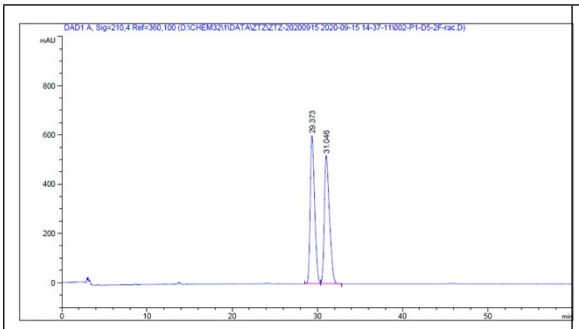
(*S*)-2,2-difluoro-1-phenylethan-1-ol (2r)

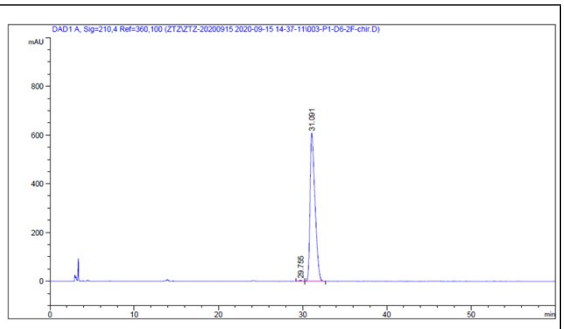


2r

Colourless oil, >99% yield. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.45 – 7.34 (m, 5H), 5.76 (td, *J* = 56.0, 4.7 Hz, 1H), 4.81 (td, *J* = 10.1, 4.6 Hz, 1H), 2.49 (s, 1H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 135.8 (t, *J* = 3.2 Hz), 129.0, 128.7, 127.1, 115.8 (t, *J* = 245.6 Hz), 73.7 (t, *J* = 24.4 Hz). **^{19}F NMR** (376 MHz, $CDCl_3$) δ -127.57 (q, *J* = 24.8 Hz).

Optical Rotation: $[\alpha]^{20}_D$ = +14.4 (c = 1.0, $CHCl_3$). The absolute configuration was assigned to be **(*S*)** by analogy to **2a**. 99% ee. (HPLC condition: Daicel Chiralcel OJ-H Column, ^{n}hexane/^{i}PrOH = 95/5, flow rate = 1.0 mL/min, T = 25 °C, wavelength = 210 nm, t_{R1} = 29.8 min for minor isomer, t_{R2} = 31.1 min for major isomer).





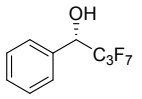
Signal 1: DAD1 A, Sig=210,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	29.373	BV	0.5507	2.17175e4	602.27856	49.8758
2	31.046	VB	0.6388	2.18257e4	520.91913	50.1242
Totals :				4.35432e4	1123.19769	

Signal 1: DAD1 A, Sig=210,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	29.755	BB	0.3545	81.76247	2.78515	0.3272
2	31.091	BB	0.6083	2.49098e4	607.65887	99.6728
Totals :				2.49916e4	610.44402	

(*S*)-2,2,3,3,4,4,4-heptafluoro-1-phenylbutan-1-ol (2s)

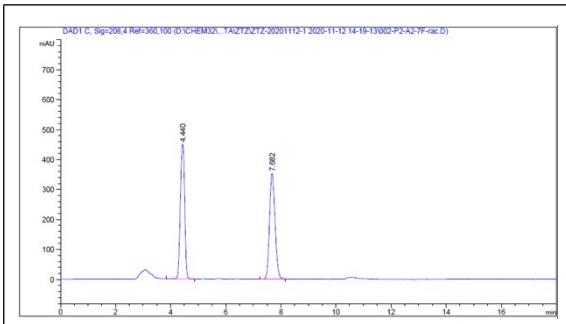


2s

Colourless oil, 97% yield. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.53 – 7.34 (m, 5H), 5.18 (dt, *J* = 17.7, 5.7 Hz, 1H), 2.58 (d, *J* = 5.2 Hz,1H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 133.9, 129.7, 128.6, 128.0, 72.1 (dd, *J* = 28.5, 22.0 Hz). **^{19}F NMR** (376 MHz, $CDCl_3$) δ -80.83 (d, *J* = 8.4 Hz), -114.59 – -121.33 (m), -122.47 – -129.21 (m). Note: Two of the carbon atoms from the CF_2-CF_2-CF_3 group are not reported in the data above, due to their low signal

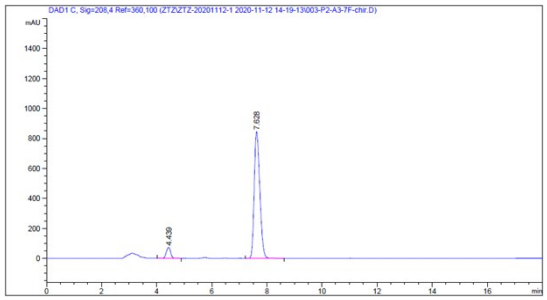
intensity and partial overlap with other signals.

Optical Rotation: $[\alpha]^{25}_D$ = +17.3 (c = 0.5, $CHCl_3$). The absolute configuration was assigned to be **(*S*)** by analogy to **2a**. 87% ee. (HPLC condition: Daicel Chiralcel OD-H Column, ^{n}hexane/^{i}PrOH = 85/15, flow rate = 1.0 mL/min, T = 25 °C, wavelength = 208 nm, t_{R1} = 4.4 min for minor isomer, t_{R2} = 7.6 min for major isomer).



Signal 1: DAD1 C, Sig=208,4 Ref=360,100

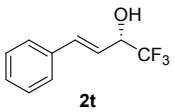
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.440	VV R	0.1767	4901.37793	449.81186	50.0768
2	7.682	VB R	0.2157	4886.34229	352.51266	49.9232
Totals :				9787.72021	802.32452	



Signal 1: DAD1 C, Sig=208,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.439	VB	0.1825	805.53235	71.99471	6.3244
2	7.628	BV R	0.2208	1.19313e4	844.41925	93.6756
Totals :				1.27368e4	916.41396	

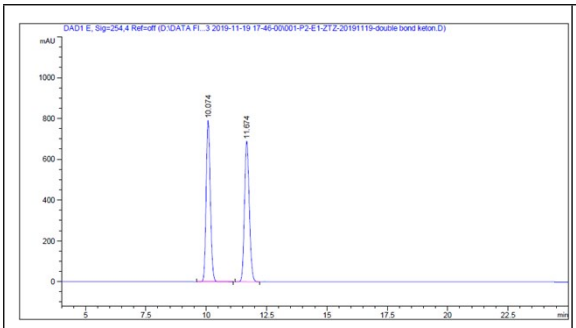
(*S*,*E*)-1,1,1-trifluoro-4-phenylbut-3-en-2-ol (2t)



2t

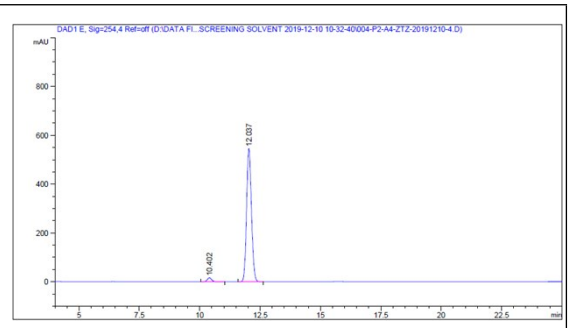
White solid, 93% yield. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.45 – 7.24 (m, 5H), 6.82 (d, *J* = 15.9 Hz, 1H), 6.18 (dd, *J* = 16.0, 6.6 Hz, 1H), 4.60 (q, *J* = 6.3 Hz, 1H), 2.70 (d, *J* = 5.6 Hz, 1H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 136.4, 135.3, 128.7 (d, *J* = 3.0 Hz), 126.9, 124.2 (q, *J* = 281.8 Hz), 120.5 (d, *J* = 2.2 Hz), 71.6 (q, *J* = 32.3 Hz). **^{19}F NMR** (376 MHz, $CDCl_3$) δ -78.97. **HRMS (ESI)** calcd. for $C_{10}H_9F_3O$ [M-H]$^{\cdot-}$: 201.0533, Found: 201.0525.

Optical Rotation: $[\alpha]^{20}_D$ = +14.3 (c = 1.0, MeOH). (Lit:[10] $[\alpha]^{20}_D$ = -20.3 (c = 0.17, MeOH, *R*, 67.6% ee). The absolute configuration was determined to be **(*S*)**. 95% ee. (HPLC condition: Daicel Chiralcel OJ-H Column, ^{n}hexane/^{i}PrOH = 92/8, flow rate = 1.0 mL/min, T = 25 °C, wavelength = 254 nm, t_{R1} = 10.4 min for minor isomer, t_{R2} = 12.0 min for major isomer).



Signal 1: DAD1 E, Sig=254,4 Ref=off

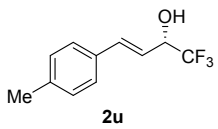
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.111	BB	0.1244	30.05438	3.35700	0.1577
2	10.074	BB	0.1864	9517.26465	790.62201	49.9370
3	11.674	BB	0.2149	9511.23438	689.55841	49.9053



Signal 1: DAD1 E, Sig=254,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.402	BB	0.1928	201.03569	16.19353	2.5496
2	12.037	BB	0.2181	7683.92236	546.30731	97.4504

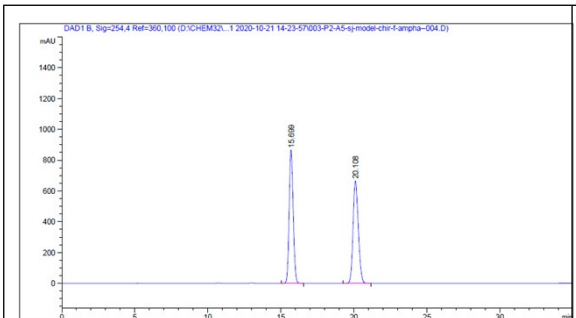
(*S*,*E*)-1,1,1-trifluoro-4-(p-tolyl)but-3-en-2-ol (2u)



2u

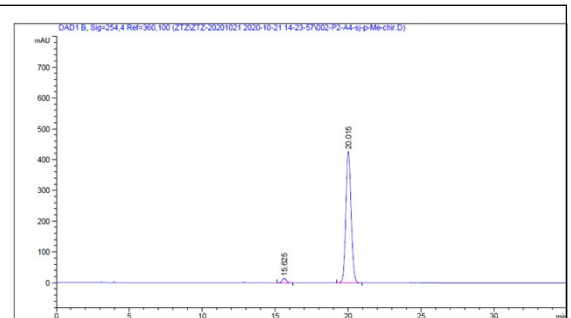
Light yellow solid, >99% yield. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.28 (d, *J* = 8.1 Hz, 2H), 7.13 (d, *J* = 7.9 Hz, 2H), 6.77 (d, *J* = 15.9 Hz, 1H), 6.12 (dd, *J* = 15.9, 6.8 Hz, 1H), 4.57 (p, *J* = 6.7 Hz, 1H), 2.71 (s, 1H), 2.33 (s, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 138.8, 136.4, 132.5, 129.4, 126.8, 124.3 (q, *J* = 281.9 Hz), 119.4, 71.7 (q, *J* = 32.3 Hz), 21.2. **^{19}F NMR** (376 MHz, $CDCl_3$) δ -78.99. **HRMS (ESI)** calcd. for $C_{11}H_{11}F_3O$ $[M-H]^-$: 215.0689, Found: 215.0682.

Optical Rotation: $[\alpha]^{20}_D$ = +17.1 (c = 1.0, MeOH). The absolute configuration was assigned to be **(*S*)** by analogy to **2t**. 95% ee. (HPLC condition: Daicel Chiralcel OJ-H Column, ^{n}hexane/^{i}PrOH = 95/5, flow rate = 1.0 mL/min, T = 25 °C, wavelength = 254 nm, t_{R1} = 15.6 min for minor isomer, t_{R2} = 20.0 min for major isomer).



Signal 1: DAD1 B, Sig=254,4 Ref=360,100

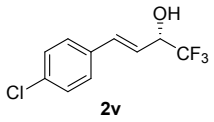
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	15.699	BB	0.2951	1.65717e4	866.70764	49.9564
2	20.108	BB	0.3854	1.66006e4	664.72754	50.0436
Totals :				3.31723e4	1531.43518	



Signal 1: DAD1 B, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	15.625	BB	0.3026	277.94705	14.30834	2.5419
2	20.015	BB	0.3872	1.06565e4	426.90356	97.4581
Totals :				1.09344e4	441.21191	

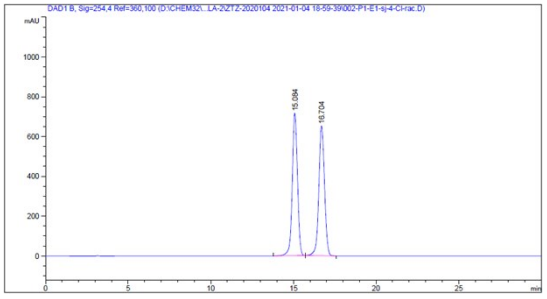
(*S*,*E*)-4-(4-chlorophenyl)-1,1,1-trifluorobut-3-en-2-ol (2v)



2v

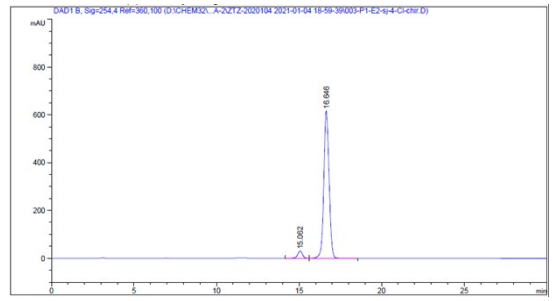
White solid, >99% yield. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.39 – 7.28 (m, 4H), 6.82 (d, *J* = 15.9 Hz, 1H), 6.18 (dd, *J* = 16.0, 6.3 Hz, 1H), 4.64 (q, *J* = 6.1 Hz, 1H), 2.30 (d, *J* = 5.8 Hz, 1H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 135.0, 134.5, 133.9, 129.0, 128.1, 124.2 (q, *J* = 281.9 Hz), 121.2, 71.5 (q, *J* = 31.8 Hz). **^{19}F NMR** (376 MHz, $CDCl_3$) δ -79.06 .

Optical Rotation: $[\alpha]^{20}_D$ = +12.6 (c = 1.0, MeOH). The absolute configuration was assigned to be **(*S*)** by analogy to **2t**. 92% ee. (HPLC condition: Daicel Chiralcel OJ-H Column, ^{n}hexane/^{i}PrOH = 95/5, flow rate = 1.0 mL/min, T = 25 °C, wavelength = 254 nm, t_{R1} = 15.1 min for minor isomer, t_{R2} = 16.6 min for major isomer).



Signal 1: DAD1 B, Sig=254,4 Ref=360,100

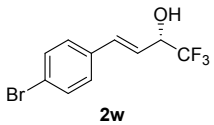
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	15.084	BB	0.3391	1.56476e4	715.65210	49.9959
2	16.704	BB	0.3719	1.56501e4	652.35553	50.0041
Totals :				3.12976e4	1368.00763	



Signal 1: DAD1 B, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	15.062	BB	0.3041	588.13251	29.82161	4.1424
2	16.646	BB	0.3414	1.36098e4	616.88849	95.8576
Totals :				1.41979e4	646.71010	

(*S*,*E*)-4-(4-bromophenyl)-1,1,1-trifluorobut-3-en-2-ol (2w)

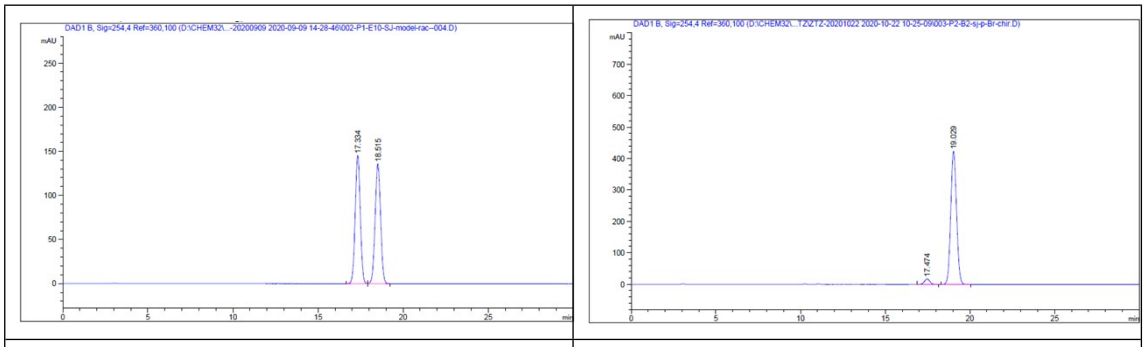


2w

Light yellow solid, 78% yield. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.64 – 7.38 (m, 2H), 7.35 – 7.15 (m, 2H), 6.79 (d, *J* = 15.9 Hz, 1H), 6.18 (dd, *J* = 16.0, 6.3 Hz, 1H), 4.63 (qd, *J* = 6.4, 1.4 Hz, 1H), 2.50 (d, *J* = 5.8 Hz, 1H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 135.0, 134.2, 131.9, 128.4, 124.1 (q, *J* = 281.9 Hz), 122.7, 121.3 (d, *J* = 2.2 Hz), 71.4 (q, *J* = 32.3 Hz). **^{19}F NMR** (376 MHz, $CDCl_3$) δ -78.99. **HRMS (ESI)** calcd. for $C_{10}H_8BrF_3O$ $[M-H]^-$: 278.9638, Found: 278.9636.

Optical Rotation: $[\alpha]^{23}_D$ = -2.5 (c = 1.0, $CHCl_3$) (Lit:[11] $[\alpha]_D$ = -9.1 (c = 1.6, $CHCl_3$, *S*, >99% ee). The absolute configuration was determined to be **(*S*)**. 93% ee. (HPLC condition: Daicel Chiralcel OJ-H Column, ^{n}hexane/^{i}PrOH = 95/5, flow rate = 1.0 mL/min, T = 25 °C, wavelength =

254 nm, t_{R1} = 17.5 min for minor isomer, t_{R2} = 19.0 min for major isomer).



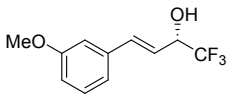
Signal 1: DAD1 B, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	17.334	BB	0.3236	3034.58276	145.32982	49.9879
2	18.515	BB	0.3486	3036.05298	135.92886	50.0121
Totals :				6070.63574	281.25868	

Signal 1: DAD1 B, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	17.474	BB	0.3346	370.48111	17.11268	3.5538
2	19.029	BB	0.3691	1.00546e4	423.32529	96.4462
Totals :				1.04250e4	440.43797	

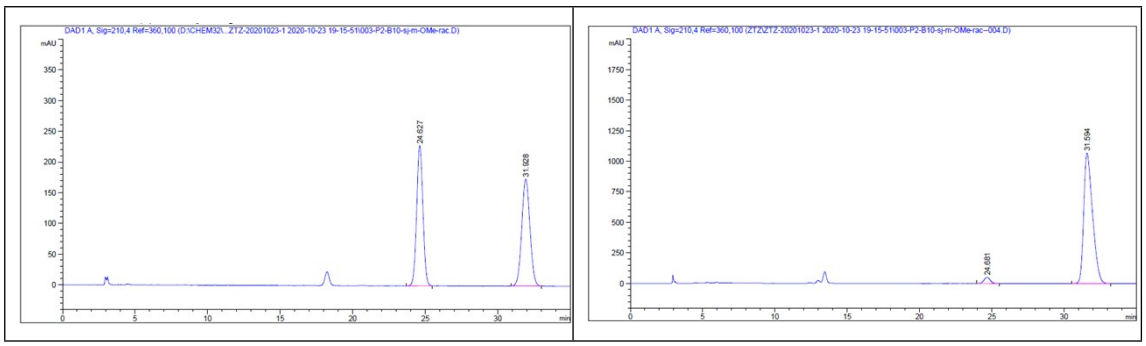
(*S*,*E*)-1,1,1-trifluoro-4-(3-methoxyphenyl)but-3-en-2-ol (2x)



2x

Light yellow oil, 87% yield. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.32 – 7.22 (m, 1H), 7.01 (d, *J* = 7.7 Hz, 1H), 6.94 (t, *J* = 2.1 Hz, 1H), 6.88 – 6.85 (m, 1H), 6.82 (d, *J* = 16.9 Hz, 1H), 6.19 (dd, *J* = 15.9, 6.5 Hz, 1H), 4.63 (pd, *J* = 6.5, 1.3 Hz, 1H), 3.82 (s, 3H), 2.53 (s, 1H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 159.8, 136.7, 136.1, 129.7, 124.2 (q, *J* = 281.9 Hz), 121.0 (d, *J* = 2.1 Hz), 119.5, 114.4, 112.1, 71.5 (q, *J* = 32.5 Hz), 55.3. **^{19}F NMR** (376 MHz, $CDCl_3$) δ -79.01. **HRMS (ESI)** calcd. for $C_{11}H_{11}F_3O_2$ $[M-H]^-$: 231.0638, Found: 231.0632.

Optical Rotation: $[\alpha]^{20}_D$ = +9.7 (c = 1.0, MeOH). The absolute configuration was assigned to be **(*S*)** by analogy to **2t**. 94% ee. (HPLC condition: Daicel Chiralcel OJ-H Column, ^{n}hexane/^{i}PrOH = 95/5, flow rate = 1.0 mL/min, T = 25 °C, wavelength = 210 nm, t_{R1} = 24.7 min for minor isomer, t_{R2} = 31.6 min for major isomer).



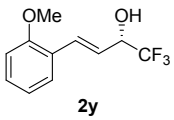
Signal 1: DAD1 A, Sig=210,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	24.627	BB	0.4602	6847.46826	228.10707	50.0786
2	31.928	BB	0.5939	6825.97070	173.91228	49.9214
Totals :				1.36734e4	402.01935	

Signal 1: DAD1 A, Sig=210,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	24.681	BB	0.4697	1505.14978	49.92312	3.2262
2	31.594	BB	0.6037	4.51494e4	1066.82153	96.7738
Totals :				4.66545e4	1116.74465	

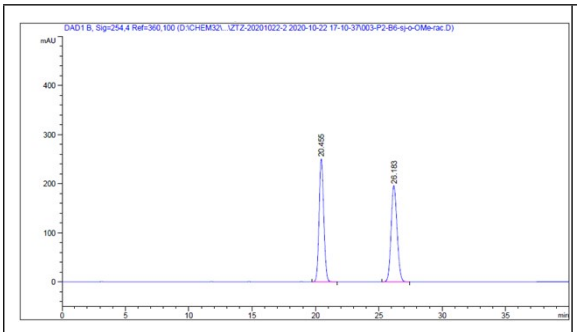
(*S*,*E*)-1,1,1-trifluoro-4-(2-methoxyphenyl)but-3-en-2-ol (2y)

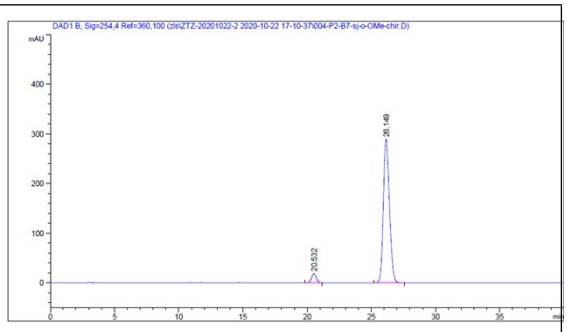


2y

Yellow oil, >99% yield. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.41 (dd, *J* = 7.6, 1.7 Hz, 1H), 7.30 – 7.23 (m, 1H), 7.14 (d, *J* = 16.1 Hz, 1H), 6.92 (t, *J* = 7.5 Hz, 1H), 6.87 (d, *J* = 8.3 Hz, 1H), 6.23 (dd, *J* = 16.1, 6.9 Hz, 1H), 4.59 (q, *J* = 6.7 Hz, 1H), 3.82 (s, 3H), 2.68 (d, *J* = 5.4 Hz, 1H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 157.0, 131.6, 129.8, 127.4, 124.3 (q, *J* = 281.7 Hz), 124.2, 121.2 (d, *J* = 2.2 Hz), 120.7, 111.0, 72.1 (q, *J* = 32.2 Hz), 55.4. **^{19}F NMR** (376 MHz, $CDCl_3$) δ -78.94. **HRMS (ESI)** calcd. for $C_{11}H_{11}F_3O_2$ $[M-H]^-$: 231.0638, Found: 231.0633.

Optical Rotation: $[\alpha]^{20}_D$ = +7.7 (c = 1.0, MeOH). The absolute configuration was assigned to be **(*S*)** by analogy to **2t**. 91% ee. (HPLC condition: Daicel Chiralcel OJ-H Column, ^{n}hexane/^{i}PrOH = 95/5, flow rate = 1.0 mL/min, T = 25 °C, wavelength = 254 nm, t_{R1} = 20.5 min for minor isomer, t_{R2} = 26.1 min for major isomer).





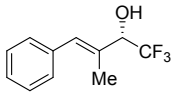
Signal 1: DAD1 B, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	20.455	BB	0.3989	6418.04199	250.47148	49.9988
2	26.183	BB	0.5083	6418.34277	195.89430	50.0012
Totals :				1.28364e4	446.36578	

Signal 1: DAD1 B, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	20.532	BB	0.3950	470.16525	18.59166	4.7177
2	26.149	BB	0.5028	9495.85254	289.39560	95.2823
Totals :				9966.01779	307.98726	

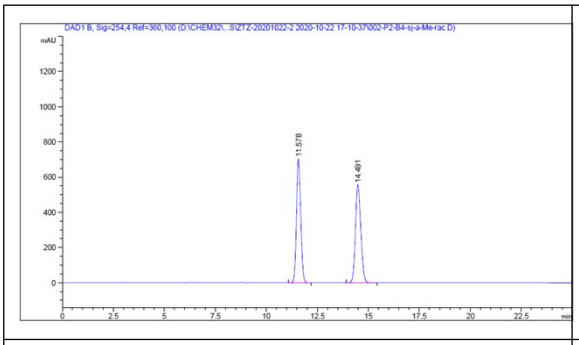
(*S*,*E*)-1,1,1-trifluoro-3-methyl-4-phenylbut-3-en-2-ol (2z)

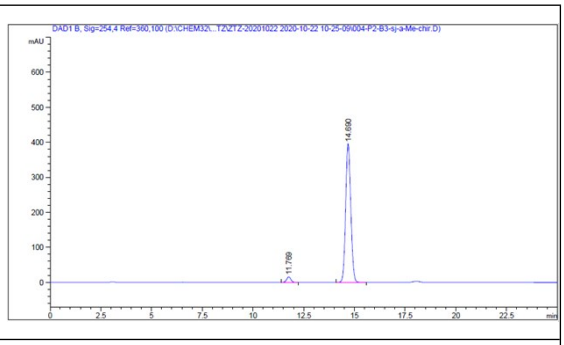


2z

Yellow oil, 98% yield. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.70 – 7.39 (m, 5H), 6.89 (s, 1H), 4.76 (p, *J* = 6.8 Hz, 1H), 4.14 (dd, *J* = 5.0, 1.9 Hz, 1H), 2.20 (s, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 136.2, 132.0, 131.0, 129.1, 128.2, 127.3, 124.6 (q, *J* = 283.2 Hz), 75.8 (q, *J* = 31.4 Hz), 13.3. **^{19}F NMR** (376 MHz, $CDCl_3$) δ -76.24. **HRMS (ESI)** calcd. for $C_{11}H_{11}F_3O$ [M-H]$^-$: 215.0689, Found: 215.0682.

Optical Rotation: $[\alpha]^{20}_D$ = -27.4 (c = 1.0, $CHCl_3$) (Lit:[11] $[\alpha]_D$ = -8 (c = 1.6, $CHCl_3$, *S*, 92% ee). The absolute configuration was assigned to be **(*S*)**. 94% ee. (HPLC condition: Daicel Chiralcel OJ-H Column, ^{n}hexane/^{i}PrOH = 95/5, flow rate = 1.0 mL/min, T = 25 °C, wavelength = 254 nm, t_{R1} = 11.8 min for minor isomer, t_{R2} = 14.7 min for major isomer).





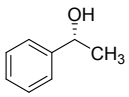
Signal 1: DAD1 B, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	11.578	BB	0.2232	1.02077e4	703.92010	49.9179
2	14.491	BB	0.2844	1.02413e4	557.31232	50.0821
Totals :				2.04490e4	1261.23242	

Signal 1: DAD1 B, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	11.769	BB	0.2198	220.20494	15.49078	3.0754
2	14.690	BB	0.2722	6940.05127	396.59366	96.9246
Totals :				7160.25621	412.08444	

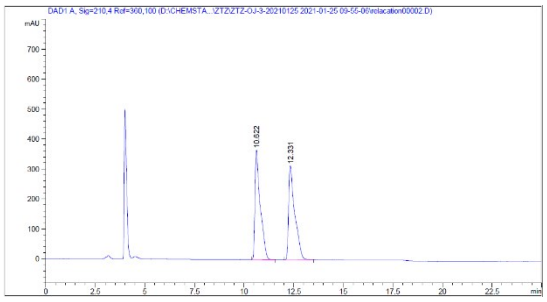
(*R*)-1-phenylethan-1-ol (4)



4

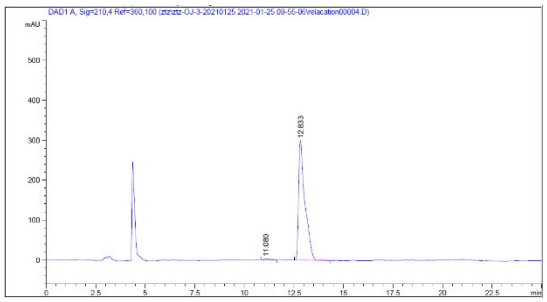
Colourless oil, 99% yield. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.38 – 7.31 (m, 4H), 7.29 – 7.23 (m, 1H), 4.88 (q, *J* = 6.5 Hz, 1H), 2.00 (s, 1H), 1.48 (d, *J* = 6.4 Hz, 3H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 145.8, 128.5, 127.4, 125.4, 70.4, 25.1.

Optical Rotation: $[\alpha]^{25}_D$ = +53.0 (c = 1.0, $CHCl_3$) (Lit:[12] $[\alpha]^{20}_D$ = +47.8 (c = 1.0, $CHCl_3$, *R*, 99% ee). The absolute configuration was determined to be (***R***). 98% ee. (HPLC condition: Daicel Chiralcel OJ-3 Column, ^{n}hexane/^{i}PrOH = 95/5, flow rate = 1.0 mL/min, T = 25 °C, wavelength = 210 nm, t_{R1} = 11.1 min for minor isomer, t_{R2} = 12.8min for major isomer).



Signal 1: DAD1 A, Sig=210,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.622	BB	0.2582	6776.92871	365.67569	49.9780
2	12.331	BB	0.3021	6782.89209	313.84119	50.0220

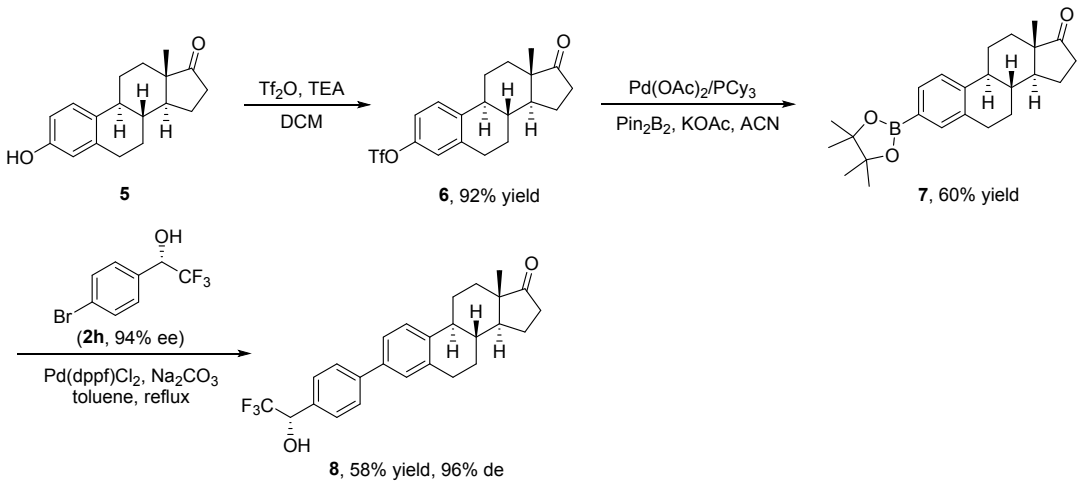


Signal 1: DAD1 A, Sig=210,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	11.080	BB	0.2301	68.23878	3.82601	1.0181
2	12.833	BV R	0.3104	6634.04736	299.55902	98.9819

IV. Applications of secondary trifluoromethyl alcohols

The late-stage modification of estrone with 2h

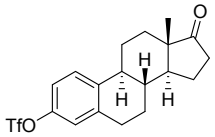


To a mixture of Estrone (8 mmol) and TEA (16 mmol) in DCM were dropwise added Tf_2O (9.6 mmol) under an argon at 0 °C, the reaction mixture was stirred at rt for 1.5 h. Then, saturated $NaHCO_3$ solution was added to the reaction mixture. Further ethyl acetate was added, the organic phases were separated, and the aqueous layer was extracted with ethyl acetate. The combined organic phase was dried with Na_2SO_4 and evaporated in vacuum. Purification of the residue by silica gel (hexanes/EtOAc 10/1) afforded the desired estrone trifluoromethanesulfonic ester **6** as a white solid.[13]

Tricyclohexylphosphine (1.9 mol%), palladium acetate (0.9 mol%), and triflate **6** (2.5 mmol) were added to a mixture of bis(pinacolato)diboron (2.75 mmol) and potassium acetate (5.0 mmol) in acetonitrile under nitrogen. The mixture was stirred at refluxing temperature until reaction completion, cooled to 30 – 40 °C, and filtered through a pad of cellulose powder. The filtercake was washed with acetonitrile. The combined filtrate was evaporated under reduced pressure and the residue was purified by column chromatography (hexanes/EtOAc 10/1~2/1) to afford pure **7** as a white solid.[14]

To a solution of **2h** (0.8 mmol) in toluene were added boronic acid **7** (0.76 mmol) and 2 M Na_2CO_3 aqueous (1.8 mL, 1.52 mmol) and $Pd(dppf)Cl_2$ (0.019 mmol). The solution was degassed with N_2 flowing for 30 min. Then the mixture solution was heated to reflux for 10 h. After the reaction was finished, the reaction mixture was cooled to rt and extracted with ethyl acetate (3 × 100 mL). The combined organic phase was dried with Na_2SO_4 and evaporated in vacuum. Purification of the residue by silica gel (hexanes/EtOAc 20/1~2/1) afforded **8** as a white solid.

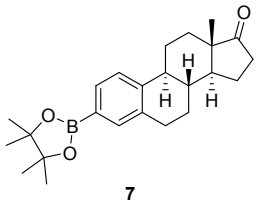
(8*R*,9*S*,13*S*,14*S*)-13-methyl-17-oxo-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopenta[a] phenanthren-3-yl trifluoromethanesulfonate (6)



6

White solid, 2.96 g, 92% yield. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.34 (d, *J* = 8.6 Hz, 1H), 7.04 (dd, *J* = 8.6, 2.8 Hz, 1H), 6.99 (d, *J* = 2.7 Hz, 1H), 2.94 (dd, *J* = 9.0, 4.4 Hz, 2H), 2.52 (dd, *J* = 18.8, 8.7 Hz, 1H), 2.45 – 2.37 (m, 1H), 2.30 (td, *J* = 10.7, 4.3 Hz, 1H), 2.22 – 1.91 (m, 4H), 1.72 – 1.59 (m, 2H), 1.59 – 1.41 (m, 4H), 0.92 (s, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 220.3, 147.5, 140.2, 139.3, 127.1, 121.2, 118.7 (d, *J* = 319.8 Hz), 118.2, 50.3, 47.8, 44.0, 37.7, 35.7, 31.4, 29.3, 26.0, 25.6, 21.5, 13.7. **^{19}F NMR** (376 MHz, $CDCl_3$) δ -72.97.

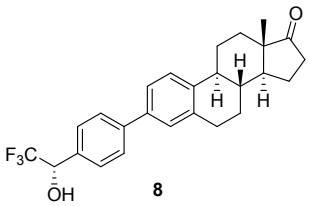
(8*R*,9*S*,13*S*,14*S*)-13-methyl-3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-6,7,8,9,11,12,13, 14,15,16-decahydro-17H-cyclopenta[a]phenanthren-17-one (7)



7

White solid, 570.5 mg, 60% yield. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.74 – 7.54 (m, 2H), 7.32 (d, *J* = 8.0 Hz, 1H), 3.11 – 2.79 (m, 2H), 2.57 – 2.41 (m, 2H), 2.33 (td, *J* = 10.8, 4.1 Hz, 1H), 2.21 – 1.89 (m, 4H), 1.74 – 1.39 (m, 7H), 1.34 (s, 12H), 0.91 (s, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 220.8, 143.1, 135.7, 135.5, 132.1, 124.7, 83.6, 50.5, 47.9, 44.6, 37.9, 35.8, 31.5, 29.1, 26.4, 25.5, 24.8, 24.7, 21.5, 13.8.

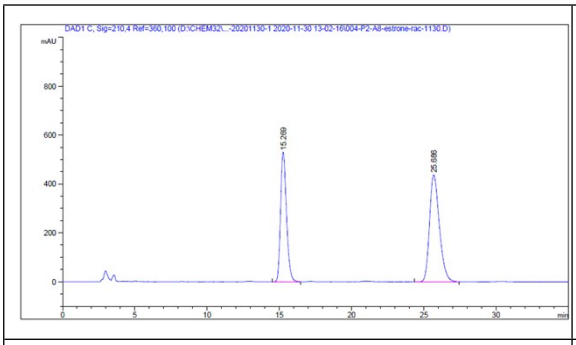
(8*R*,9*S*,13*S*,14*S*)-13-methyl-3-(4-((*S*)-2,2,2-trifluoro-1-hydroxyethyl)phenyl)-6,7,8,9,11,12,13, 14,15,16-decahydro-17H-cyclopenta[a]phenanthren-17-one (8)



8

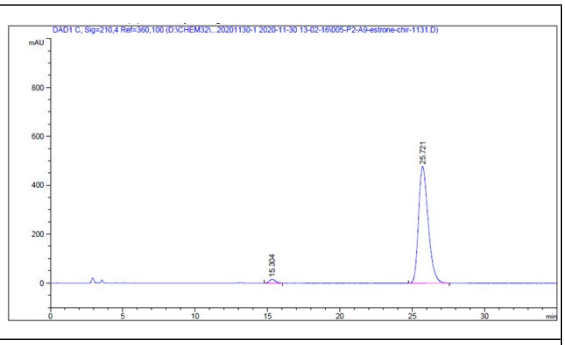
White solid, 188.9 mg, 58% yield. **^{1}H NMR** (600 MHz, DMSO-d_6) δ 7.66 (d, *J* = 7.9 Hz, 2H), 7.55 (d, *J* = 7.9 Hz, 2H), 7.43 (d, *J* = 8.1 Hz, 1H), 7.40 – 7.33 (m, 2H), 6.86 (s, 1H), 5.20 (q, *J* = 7.3 Hz, 1H), 3.04 – 2.83 (m, 2H), 2.48 – 2.37 (m, 2H), 2.28 (td, *J* = 11.0, 3.9 Hz, 1H), 2.07 (dt, *J* = 18.3, 8.8 Hz, 1H), 2.02 – 1.92 (m, 2H), 1.79 (d, *J* = 10.4 Hz, 1H), 1.64 – 1.31 (m, 6H), 0.84 (s, 3H). **^{13}C NMR** (151 MHz, DMSO-d_6) δ 219.6, 140.7, 139.3, 137.0, 136.9, 134.7, 128.2, 127.1, 126.3, 126.0, 125.2 (q, *J* = 282.5 Hz), 124.0, 70.3 (q, *J* = 30.4, 29.9 Hz), 49.7, 47.4, 43.9, 37.7, 35.4, 31.4, 29.1, 26.1, 25.4, 21.2, 13.6. **^{19}F NMR** (565 MHz, DMSO-d_6) δ -76.68. **HRMS (ESI)** calcd. for $C_{26}H_{27}F_3O_2$ [M+HCOO]$^-$: 473.1945, Found: 473.1941.

Optical Rotation: $[\alpha]^{23}_{D}$ = +43.4 (c = 1.0, MeOH). 96% de. (HPLC condition: Daicel Chiralcel AD-H Column, ^{n}hexane/^{i}PrOH = 90/10, flow rate = 1.0 ml/min, T = 25 ^{o}C, wavelength = 210 nm, t_{R1} = 15.3 min for minor isomer, t_{R2} = 25.7 min for major isomer).



Signal 1: DAD1 C, Sig=210,4 Ref=360,100

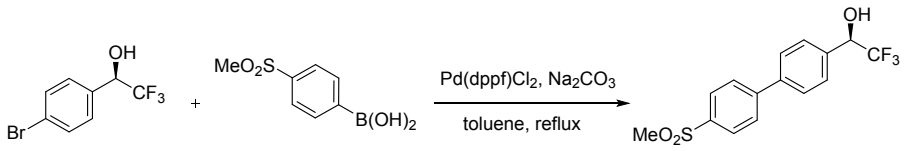
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	15.269	VB R	0.4298	1.50932e4	530.74524	42.1609
2	25.686	VV R	0.6296	2.07059e4	437.96472	57.8391
Totals :				3.57991e4	968.70996	



Signal 1: DAD1 C, Sig=210,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	15.304	BV R	0.3407	435.87131	15.56325	1.9347
2	25.721	BV R	0.6748	2.20931e4	478.40118	98.0653
Totals :				2.25290e4	493.96443	

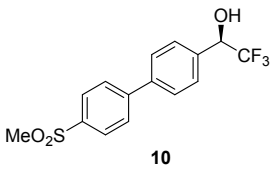
The synthesis of Odanacatib precursor



***ent*-2h**, 95% ee **9** **10**, 90% yield, 90% ee

To a solution of ***ent*-2h** (1.8 mmol) in toluene were added (4-(methylsulfonyl)phenyl)boronic acid **9** (1.9 mmol) and 2 M Na_2CO_3 aqueous (1.8 mL, 3.6 mmol) and $Pd(dppf)Cl_2$ (0.045 mmol). The solution was degassed with N_2 flowing for 30 min. Then the mixture solution was heated to reflux for 10 h. After the reaction was finished, the reaction mixture was cooled to rt and extracted with ethyl acetate (3 × 100 mL). The combined organic phase was dried with Na_2SO_4 and evaporated in vacuum. Purification of the residue by silica gel (hexanes/EtOAc 20/1~2/1) afforded **10** as a white solid.

(*R*)-2,2,2-trifluoro-1-(4'-(methylsulfonyl)-[1,1'-biphenyl]-4-yl)ethan-1-ol (10)

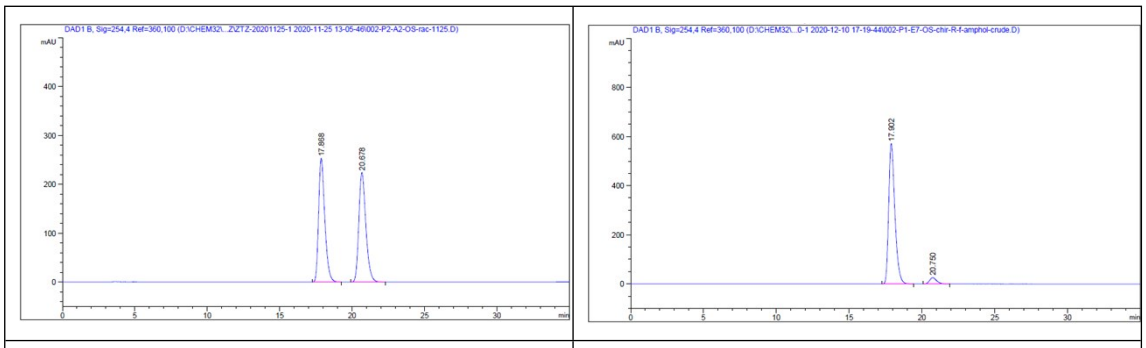


10

White solid, 535.1 mg, 90% yield. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.01 (d, *J* = 8.5 Hz, 2H), 7.76 (d, *J* = 8.5 Hz, 2H), 7.64 (t, *J* = 7.3 Hz, 4H), 5.12 (qd, *J* = 6.6, 4.5 Hz, 1H), 3.10 (s, 3H), 2.84 (d, *J* = 4.6 Hz, 1H). **^{13}C NMR** (101 MHz, DMSO-d_6) δ 144.7, 139.9, 138.9, 136.4, 128.5, 127.8

(d, J = 1.8 Hz), 127.2, 125.1 (q, J = 282.8 Hz), 70.2 (q, J = 30.5 Hz), 43.7. **^{19}F NMR** (376 MHz, $CDCl_3$) δ -78.27. **HRMS (ESI)** calcd. for $C_{15}H_{13}F_3O_2$ [M+HCOO]$^-$: 375.0525, Found: 375.0517.

Optical Rotation: $[\alpha]^{23}_D$ = -12.1 (c = 1.0, THF) (Lit:[15] $[\alpha]_D$ = -27.2 (c = 1.5, THF, *R*, > 99% ee). The absolute configuration of **10** was determined to be (***R***). 90% ee (HPLC condition: Daicel Chiralcel AD-H Column, ^{n}hexane/^{i}PrOH = 80/20, flow rate = 0.8 ml/min, T = 25 ^{o}C, wavelength = 254 nm, t_{R1} = 17.9 min for major isomer, t_{R2} = 20.8 min for minor isomer).



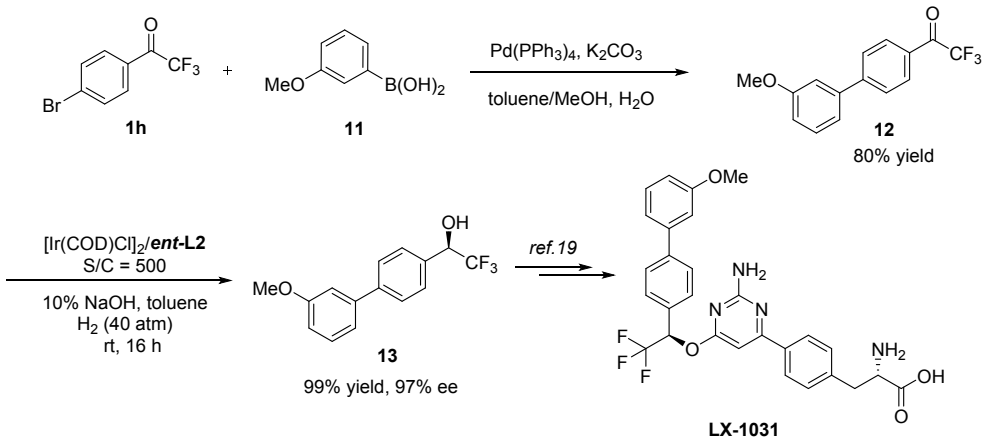
Signal 1: DAD1 B, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	17.868	BB	0.4509	7532.91016	253.31763	49.9756
2	20.678	BB	0.5085	7540.26123	224.12526	50.0244
Totals :				1.50732e4	477.44289	

Signal 1: DAD1 B, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	17.902	BB	0.4524	1.68907e4	572.14252	95.1837
2	20.750	BB	0.4914	854.67059	25.47475	4.8163
Totals :				1.77453e4	597.61727	

The synthesis of biaryl chiral alcohol (13) to LX1031

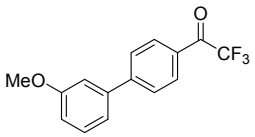


To a solution of 1-(4-bromophenyl)-2,2,2-trifluoroethan-1-one **1h** (8.0 mmol) in toluene and MeOH were added boronic (9.5 mmol), 4 M K_2CO_3 aqueous (6 mL, 24 mmol), and $Pd(PPh_3)_4$ (0.4 mmol). The solution was degassed with N_2 flowing for 30 min. The solution was heated to reflux for 6 h. After the reaction was finished, the reaction mixture was cooled to rt and extracted with ethyl acetate (3 × 100 mL). The combined organic phase was dried with Na_2SO_4 and evaporated in

vacuum. Purification of the residue by silica gel (hexanes/EtOAc 50/1~25/1) afforded the desired coupling product **12** as a white solid.[16]

To a 4.0 mL vial was added the catalyst precursor $[Ir(COD)Cl]_2$ (6.7 mg, 9.97 μmol, 1.0 equiv), (R_C, S_C, R_C, S_{FC})-*f*-amphol ***ent*-L2** (16.2 mg, 21.04 μmol, 2.1 equiv) and anhydrous ^{i}PrOH (2.0 mL) in the argon-filled glovebox. The mixture was stirred for 2.0 h at 25 °C. The resulting orange solution (20 μL) was transferred by syringe into a vial (5.0 mL) charged with compound (0.2 mmol), NaOH (0.8 mg, 0.02 mmol) and anhydrous toluene (1.0 mL). The vial was transferred to an autoclave, which was then charged with of H_2 (40 atm) and stirred at rt for 16 h. The hydrogen gas was released slowly in a well-ventilated hood, and the solution was concentrated and purified by silica gel (hexanes/EtOAc 50/1~25/1) afforded **13** as a white solid.

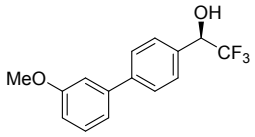
2,2,2-trifluoro-1-(3'-methoxy-[1,1'-biphenyl]-4-yl)ethan-1-one (12)



12

White solid, 1.79 g, 80% yield. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.15 (d, *J* = 7.9 Hz, 2H), 7.76 (d, *J* = 8.5 Hz, 2H), 7.41 (t, *J* = 8.0 Hz, 1H), 7.23 (d, *J* = 7.8 Hz, 1H), 7.18 – 7.14 (m, 1H), 6.99 (dd, *J* = 8.0, 2.2 Hz, 1H), 3.89 (s, 3H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 180.0 (q, *J* = 34.9 Hz), 160.1, 148.1, 140.5, 130.7, 130.1, 128.6, 127.7, 119.8, 116.7 (q, *J* = 291.3 Hz), 114.1, 113.2, 55.3. **^{19}F NMR** (376 MHz, $CDCl_3$) δ -71.32.

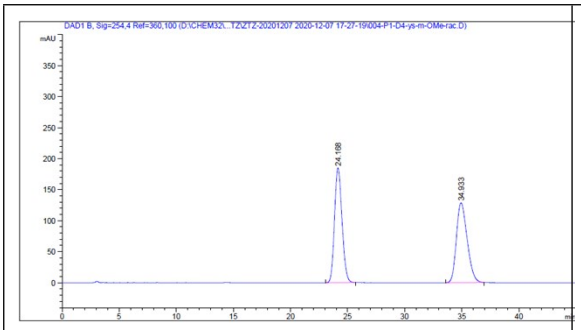
(*R*)-2,2,2-trifluoro-1-(3'-methoxy-[1,1'-biphenyl]-4-yl)ethan-1-ol (13)



13

White solid, 55.9 mg, 99% yield. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.63 (d, *J* = 8.3 Hz, 2H), 7.55 (d, *J* = 8.1 Hz, 2H), 7.37 (t, *J* = 7.9 Hz, 1H), 7.22 – 7.14 (m, 1H), 7.12 (dd, *J* = 2.6, 1.7 Hz, 1H), 6.92 (ddd, *J* = 8.3, 2.6, 1.0 Hz, 1H), 5.08 (qd, *J* = 6.7, 4.6 Hz, 1H), 3.87 (s, 3H), 2.60 (d, *J* = 4.6 Hz, 1H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 160.0, 142.4, 141.8, 133.0, 129.9, 127.8, 127.4, 124.3 (q, *J* = 282.1 Hz), 119.7, 113.0, 129.9, 72.6 (q, *J* = 31.9 Hz), 55.3. **^{19}F NMR** (376 MHz, $CDCl_3$) δ -78.27. **HRMS (ESI)** calcd. for $C_{15}H_{13}F_3O_2$ $[M-H]^-$: 281.0795, Found: 281.0791.

Optical Rotation: $[\alpha]^{22}_D$ = -22.2 (c = 1.0, EtOH) (Lit:[14] $[\alpha]_D$ = -31.85 (c = 1.067, EtOH, *R*, >99% ee). The absolute configuration was determined to be (***R***). 97% ee (HPLC condition: Daicel Chiralcel OD-H Column, ^{n}hexane/^{i}PrOH = 95/5, flow rate = 1.0 ml/min, T = 25 °C**,** wavelength = 254 nm, t_{R1} = 24.3 min for major isomer, t_{R2} = 35.1 min for minor isomer).



Signal 1: DAD1 C, Sig=210,4 Ref=off

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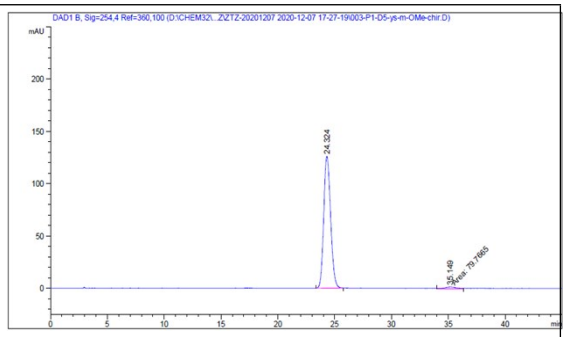
2	33.262	BB	0.8145	1863.71729	32.43040	49.4862
Totals :				3766.13708	92.95589	



Signal 1: DAD1 B, Sig=254,4 Ref=360,100

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2	35.149	MM	1.0080	79.76646	1.31895	1.4839
Totals :				5375.62730	127.36012	

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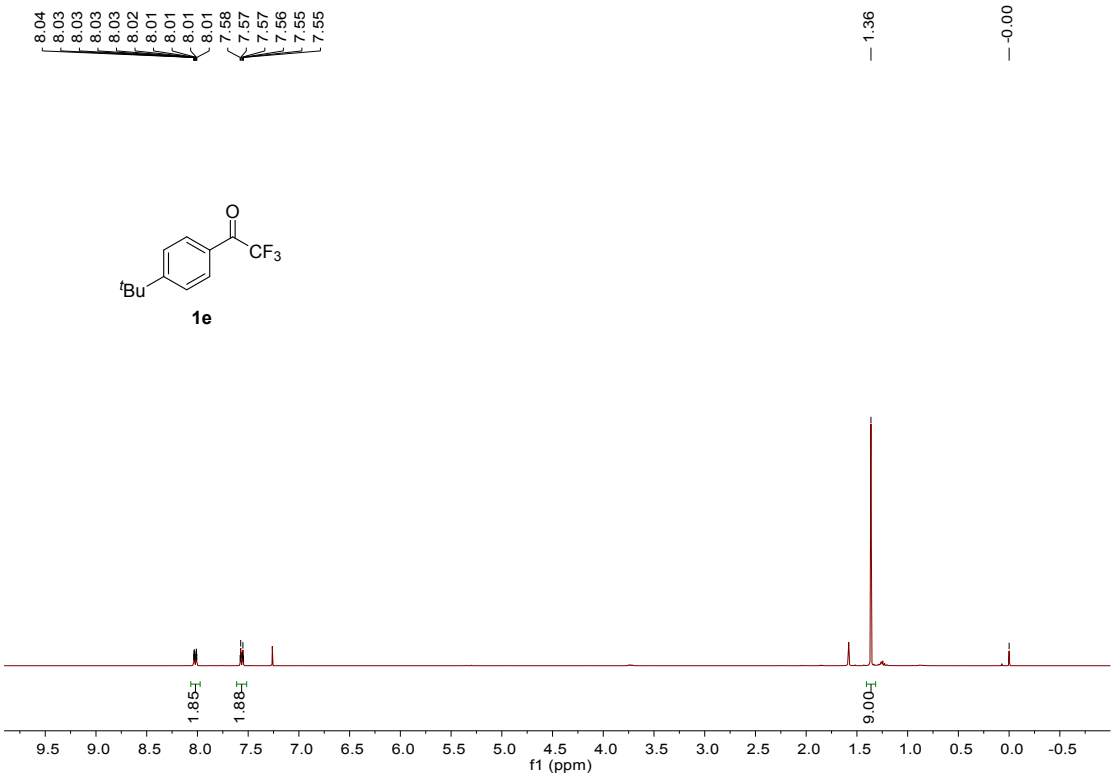
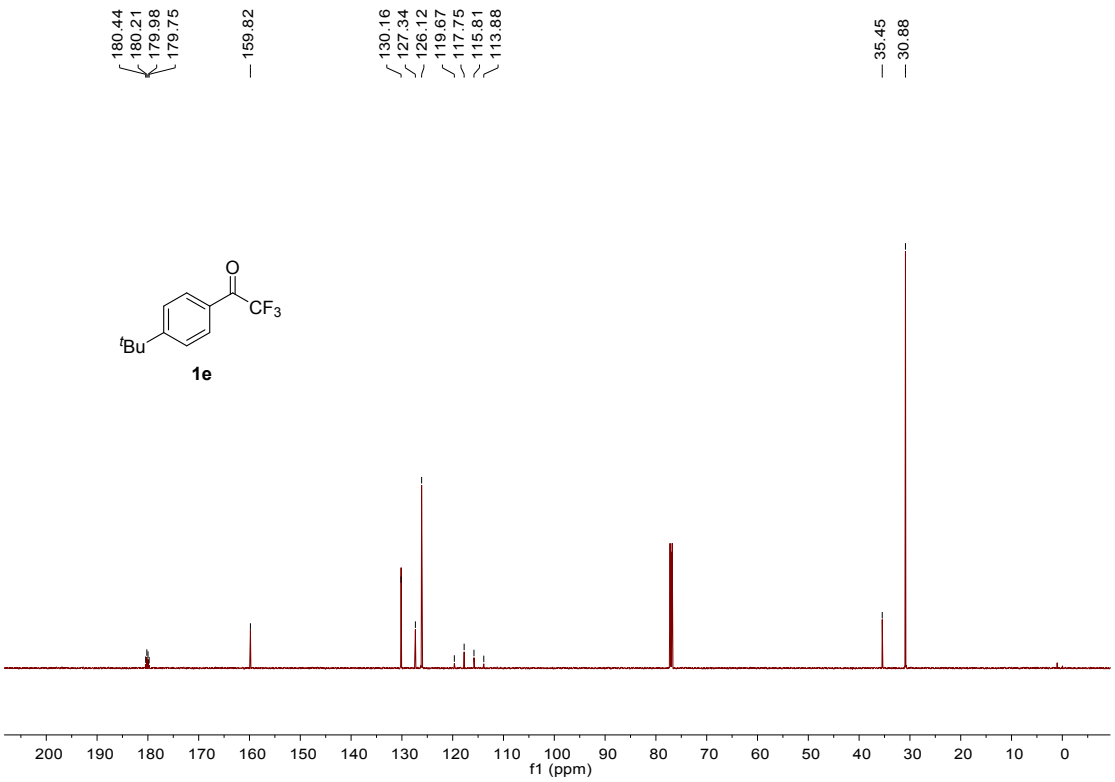
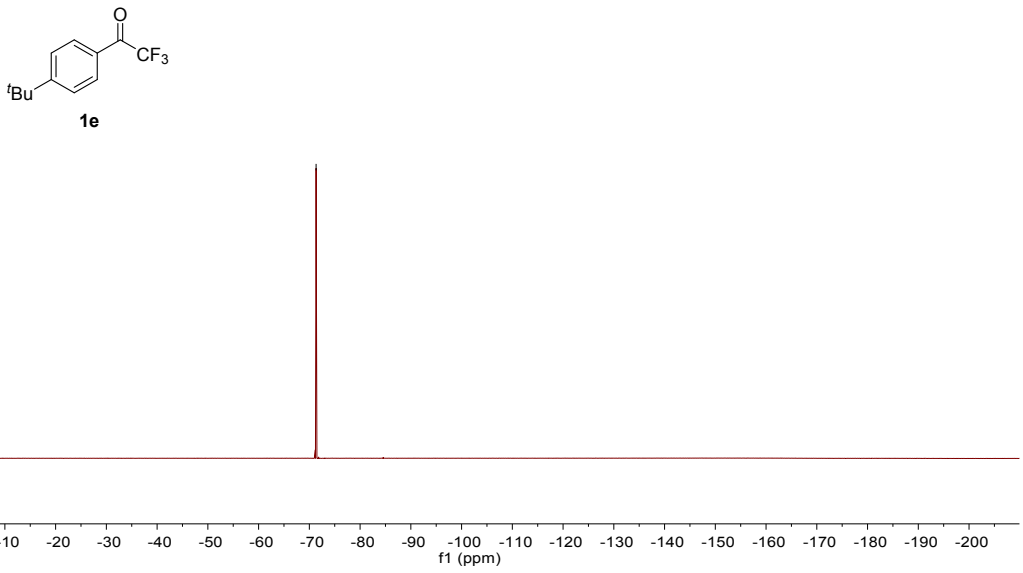
VIII. NMR spectrum



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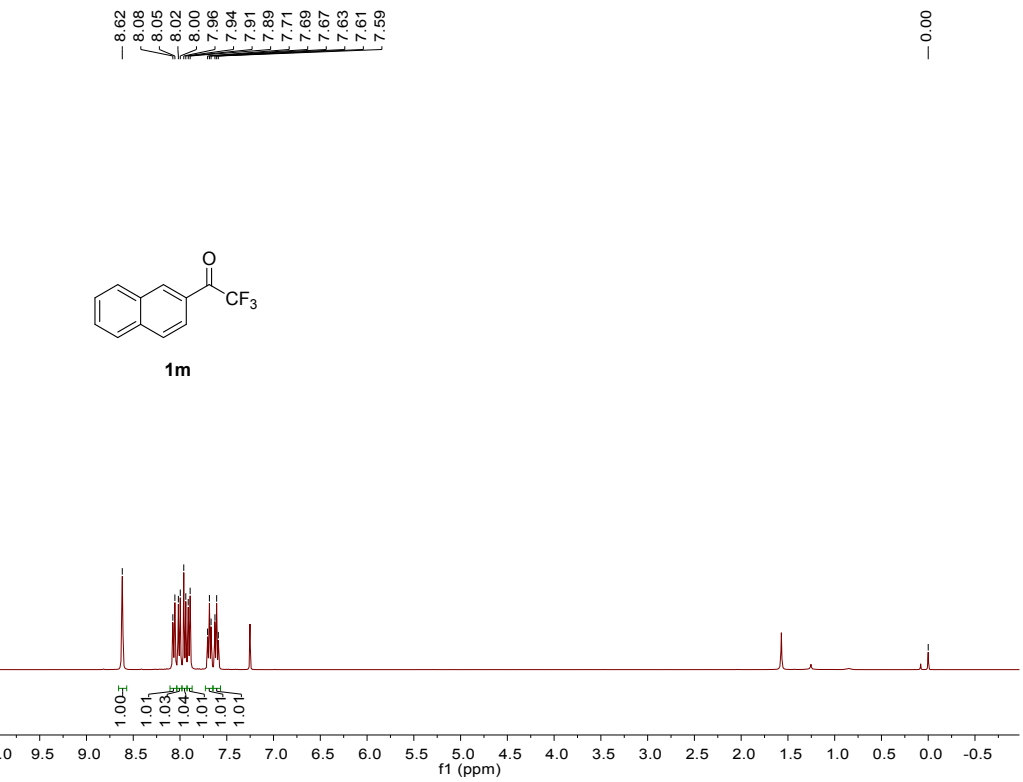
f1 (ppm)

1e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7.63
7.61
7.59
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CF3
1.00
1.01
1.03
1.04
1.01
1.01
1.01
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

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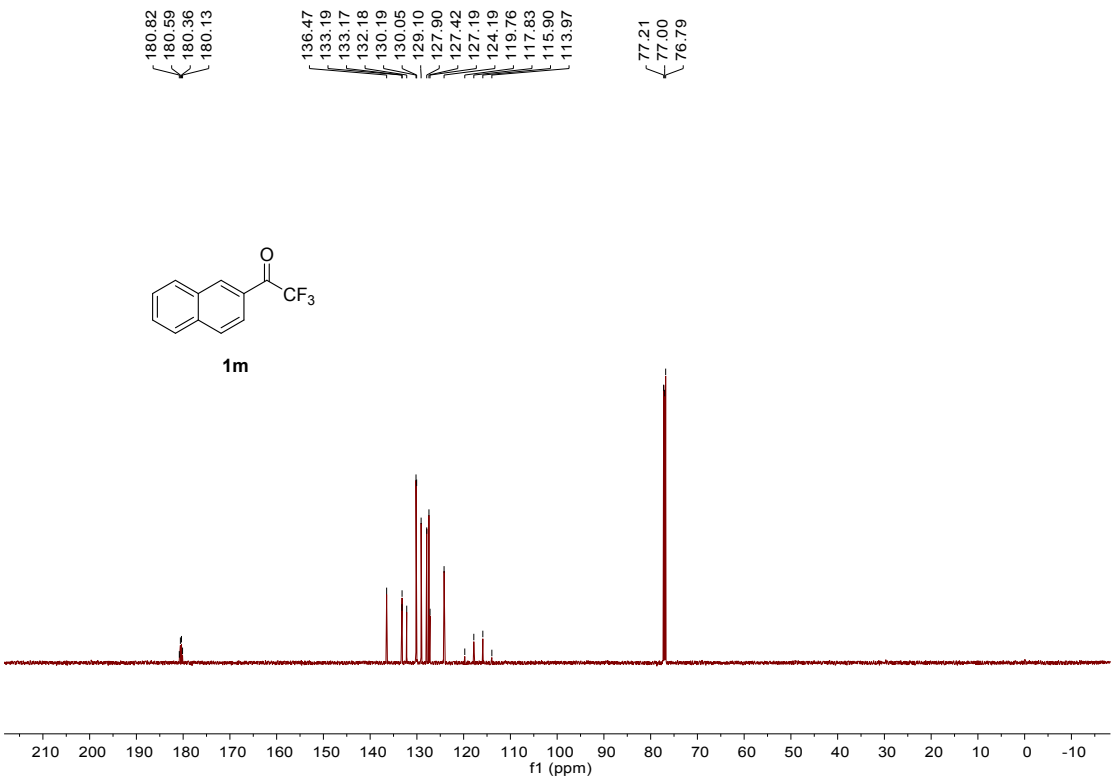
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127.19
124.19
119.76
117.83
115.90
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CF3
1m
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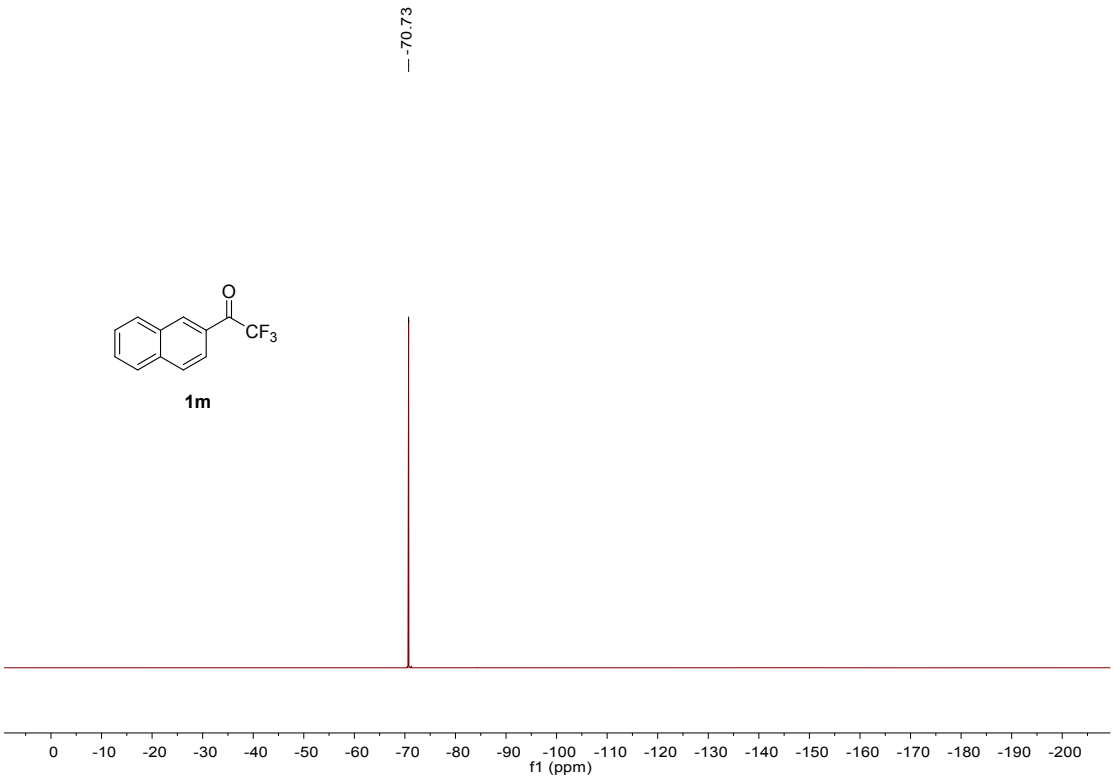
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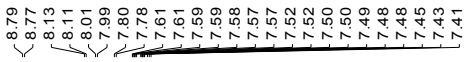
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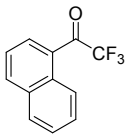
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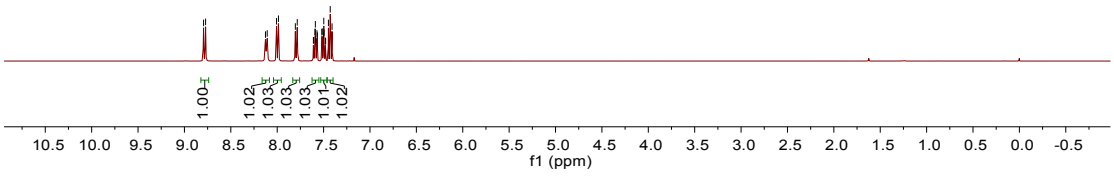
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f1 (ppm)


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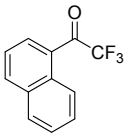
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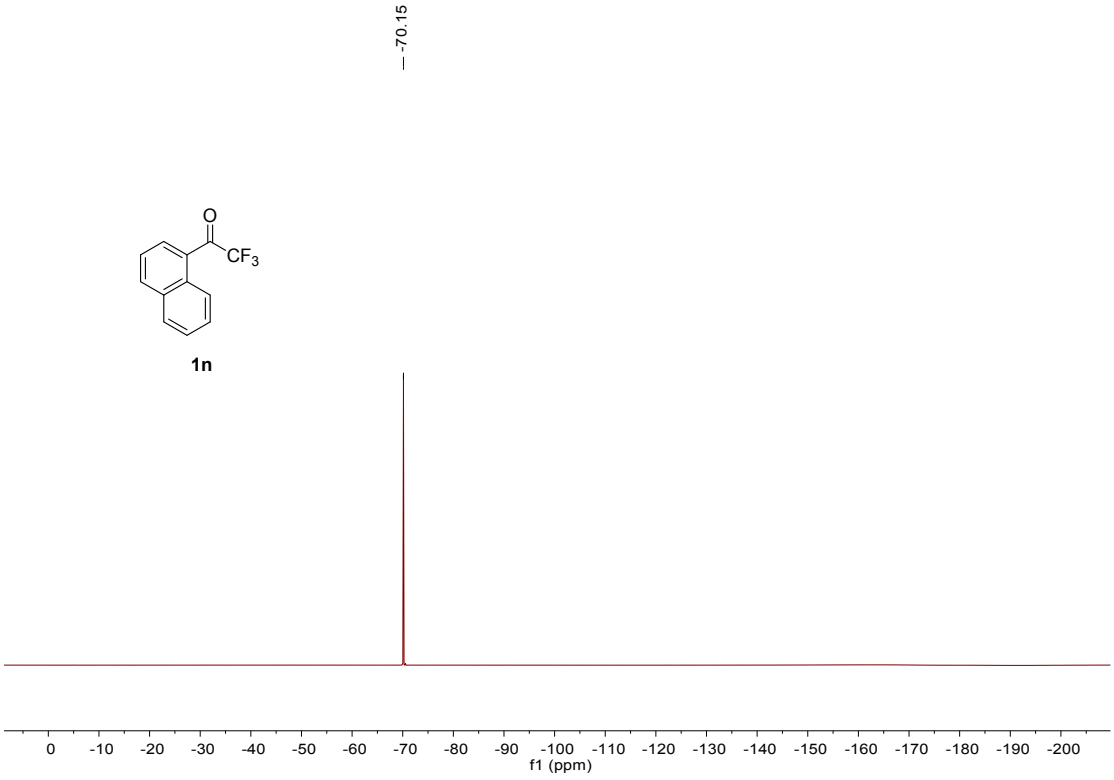
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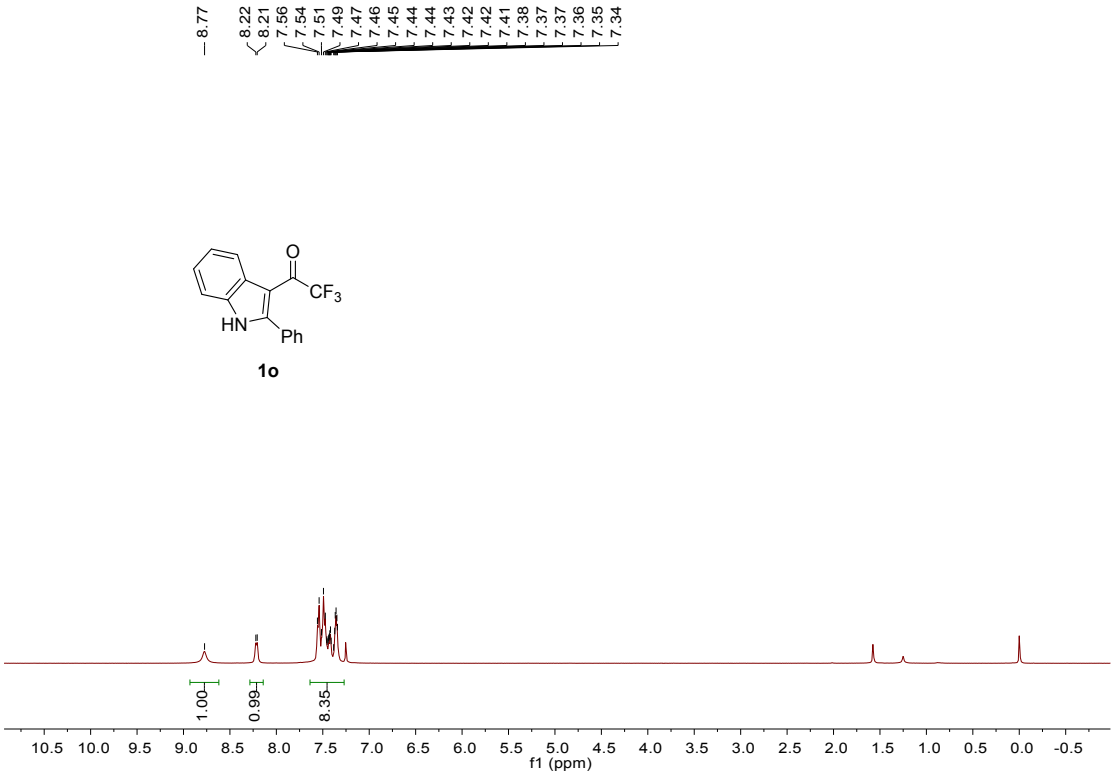
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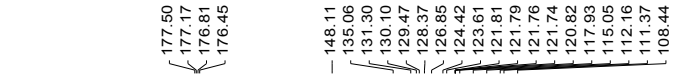
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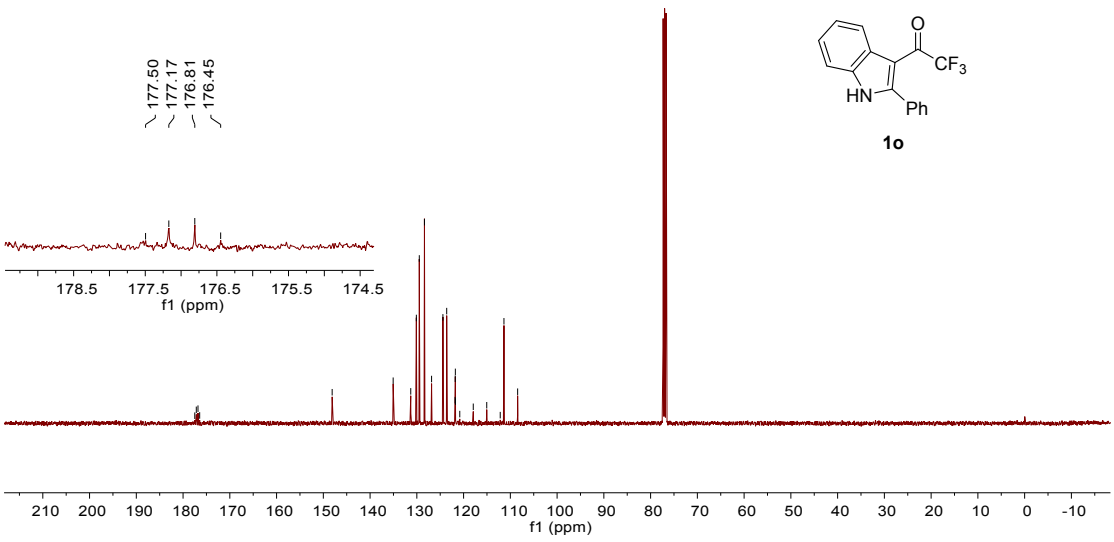
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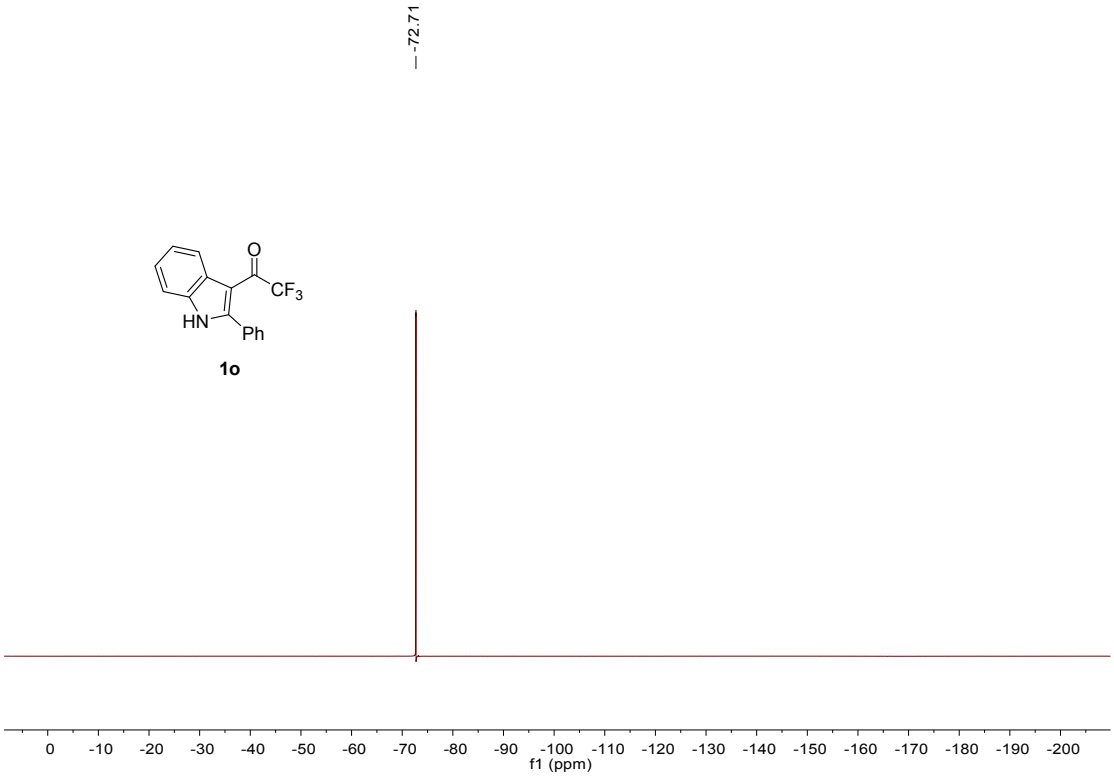
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Ph

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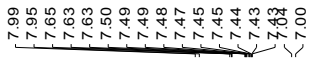
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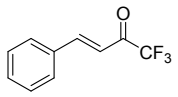
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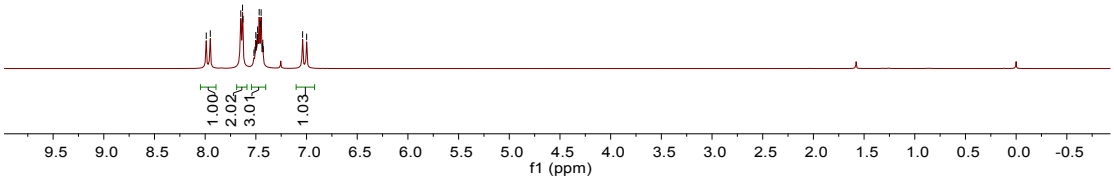
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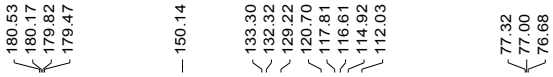
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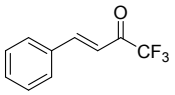
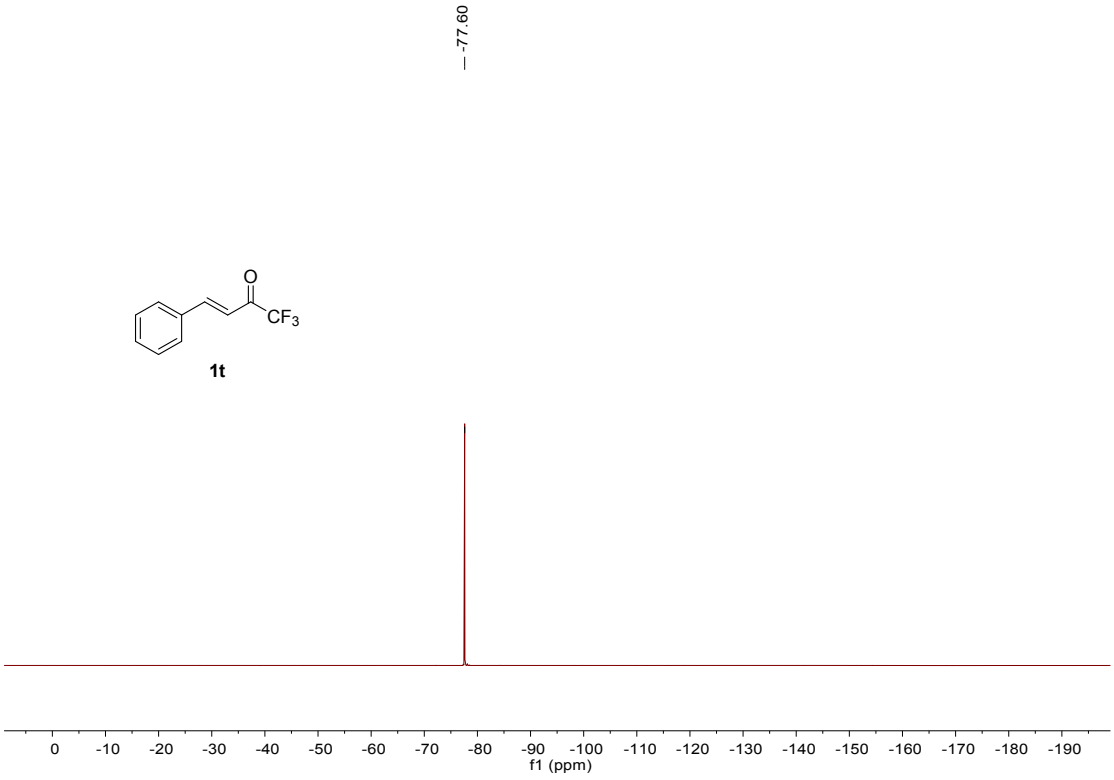
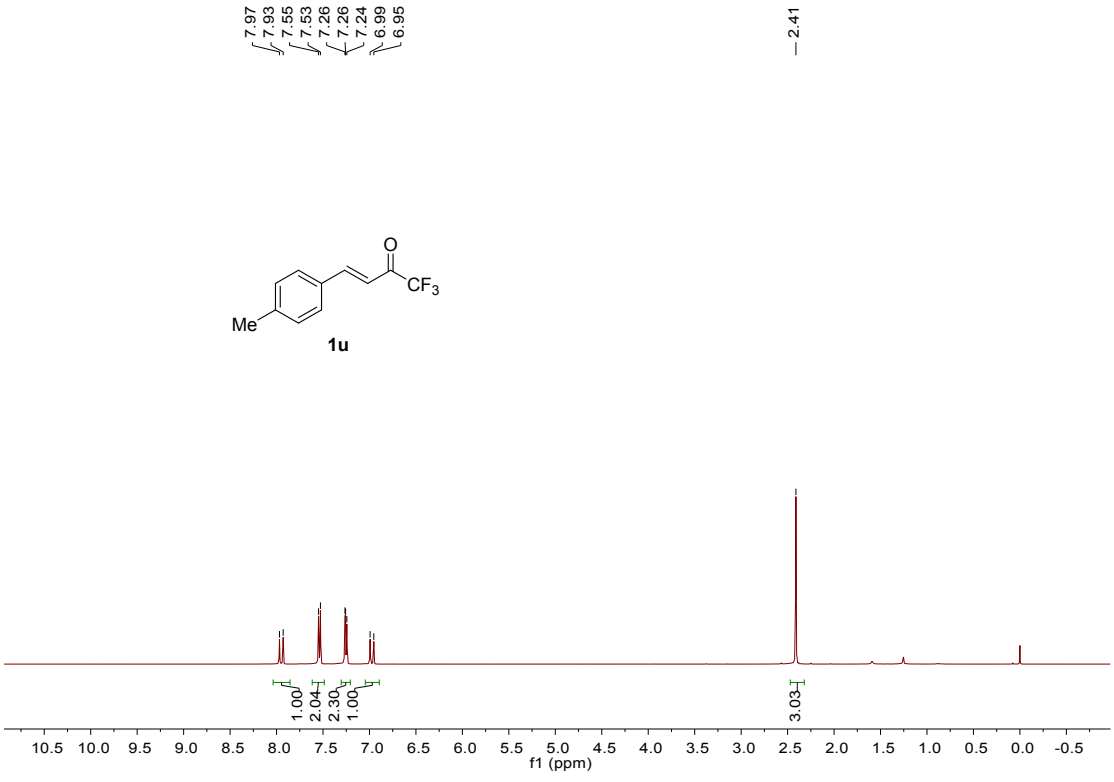
77.00
76.68

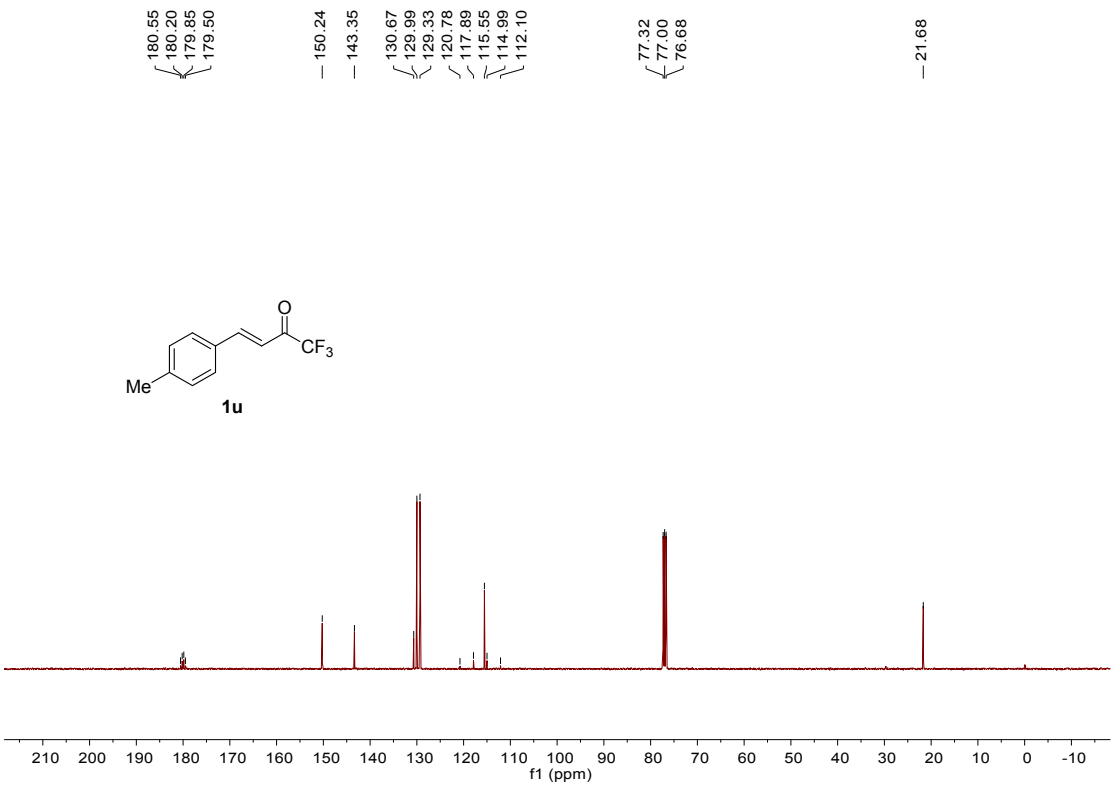

O
CF3

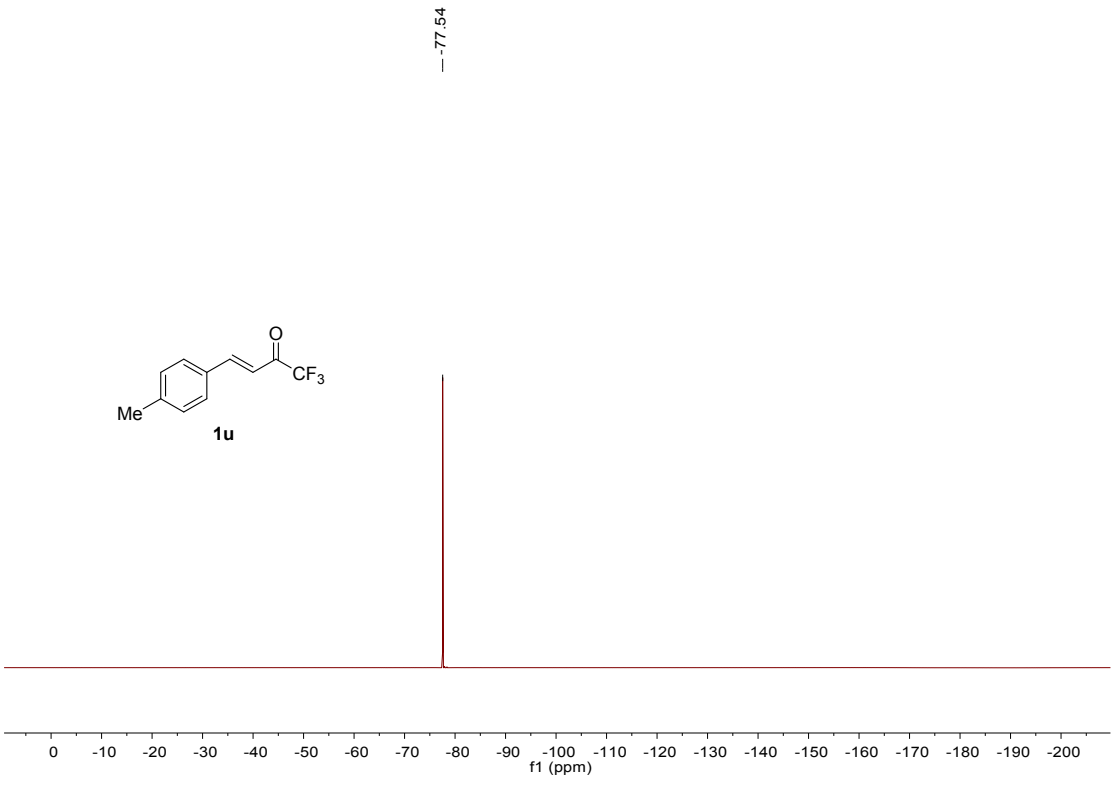
1t

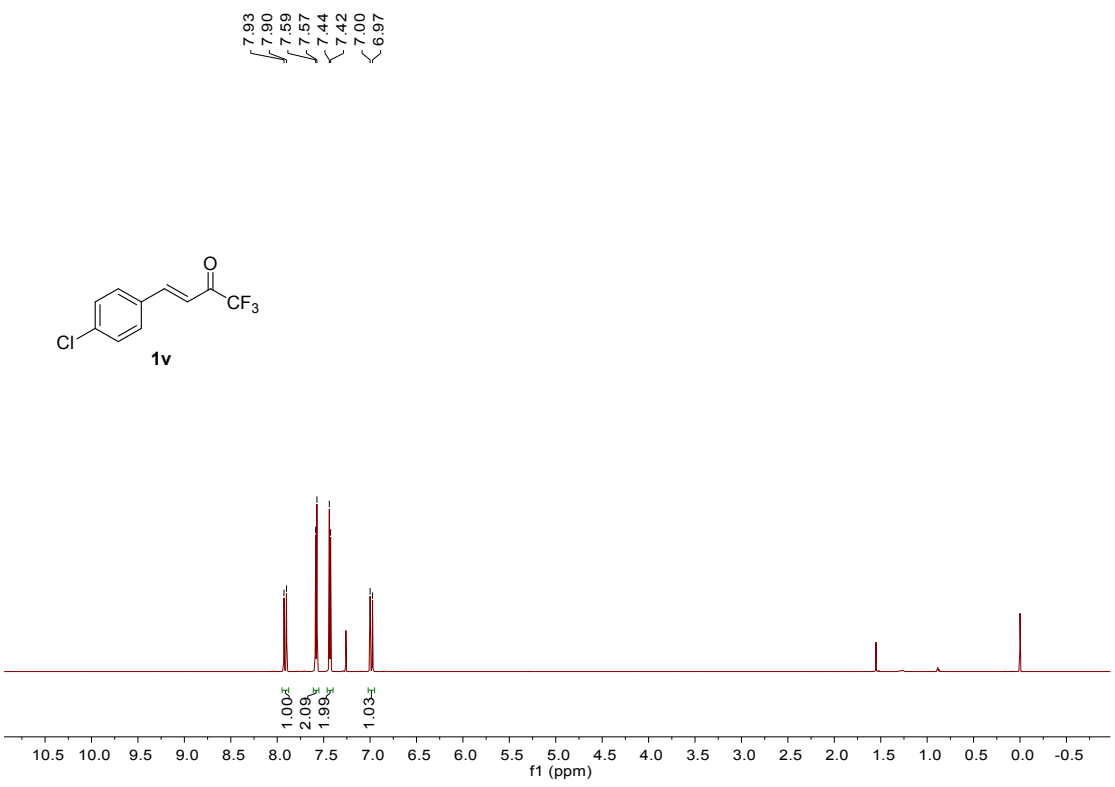
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

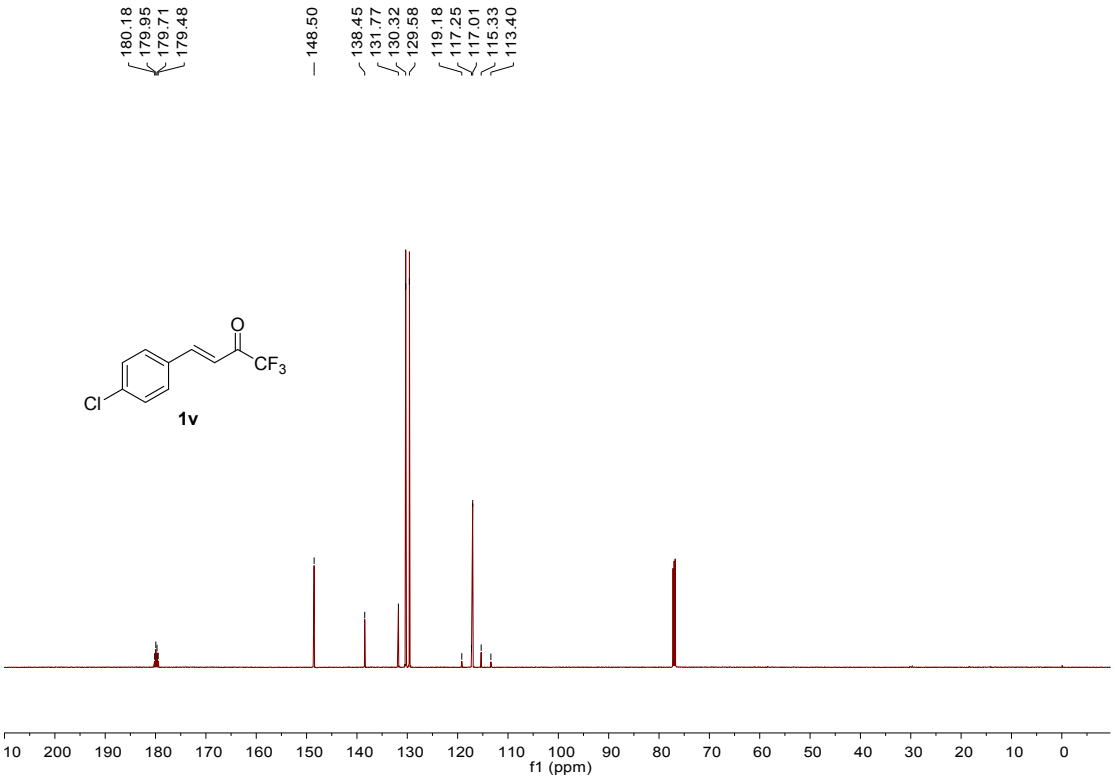

-77.60
O
CF3
1t
0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190
f1 (ppm)

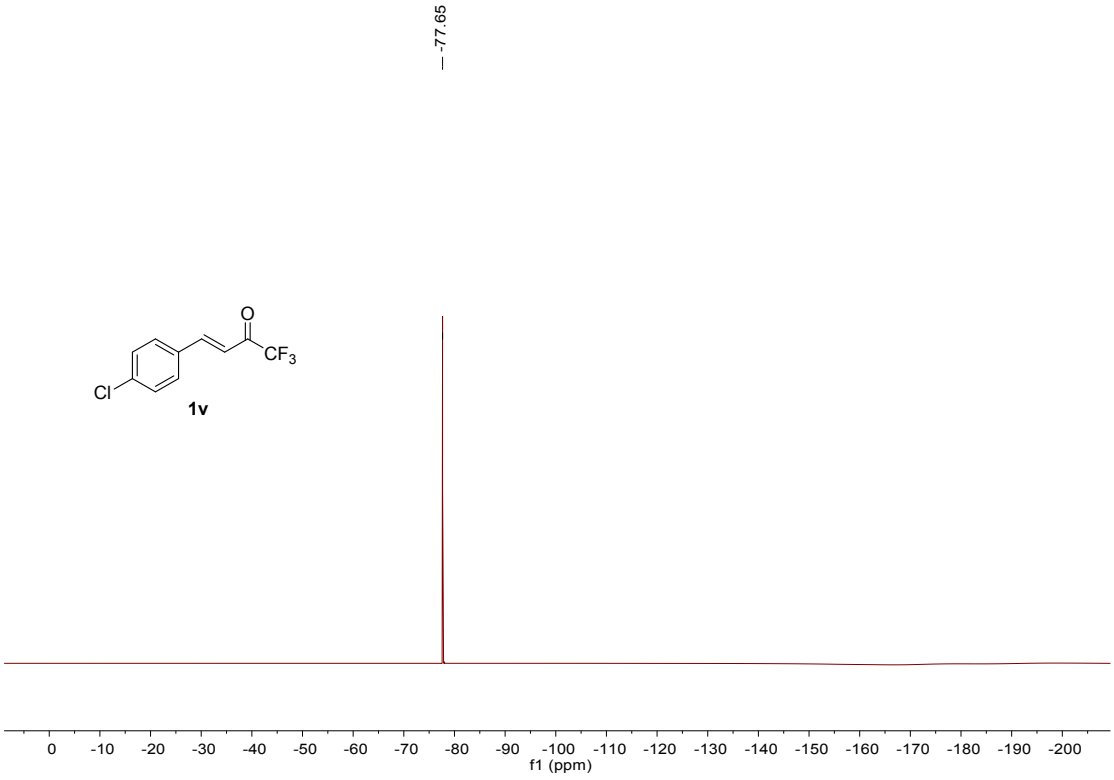

7.97
7.93
7.55
7.53
7.26
7.26
7.24
6.99
6.95
2.41
O
CF3
Me
1u
1.00
2.04
2.30
1.00
3.03
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

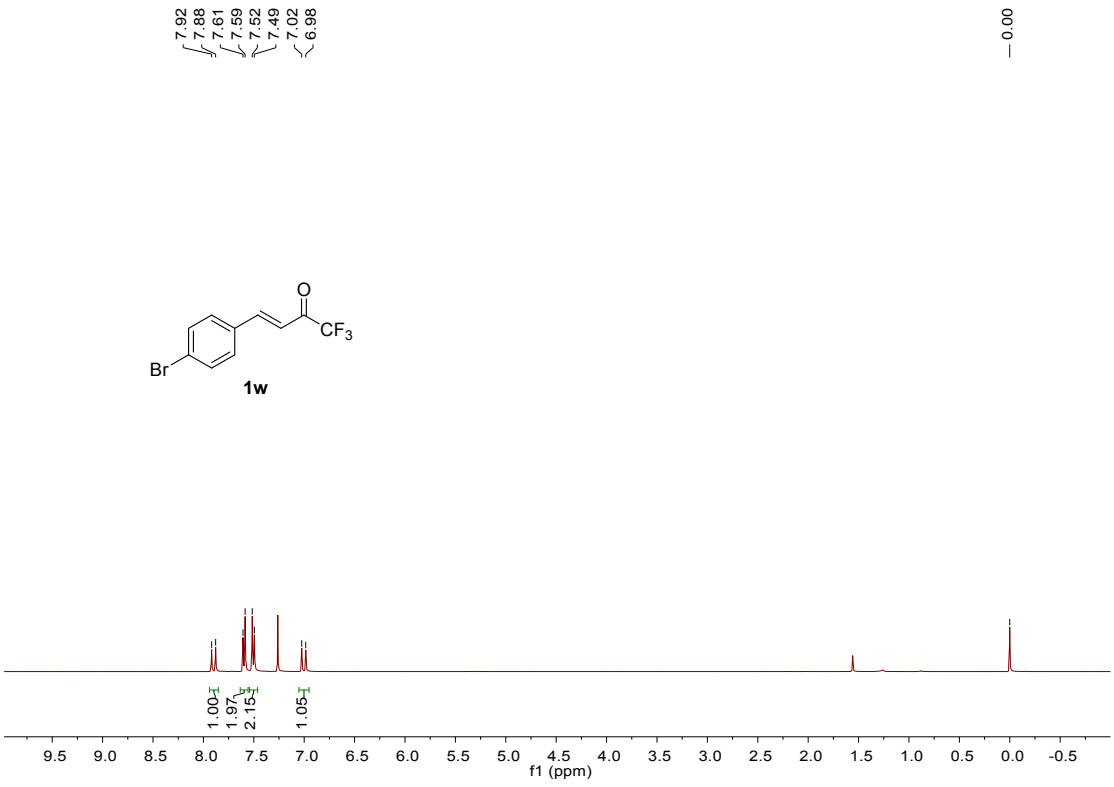

180.55
180.20
179.85
179.50
150.24
143.35
130.67
129.99
129.33
120.78
117.89
115.55
114.99
112.10
77.32
77.00
76.68
21.68
O
CF3
Me
1u
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

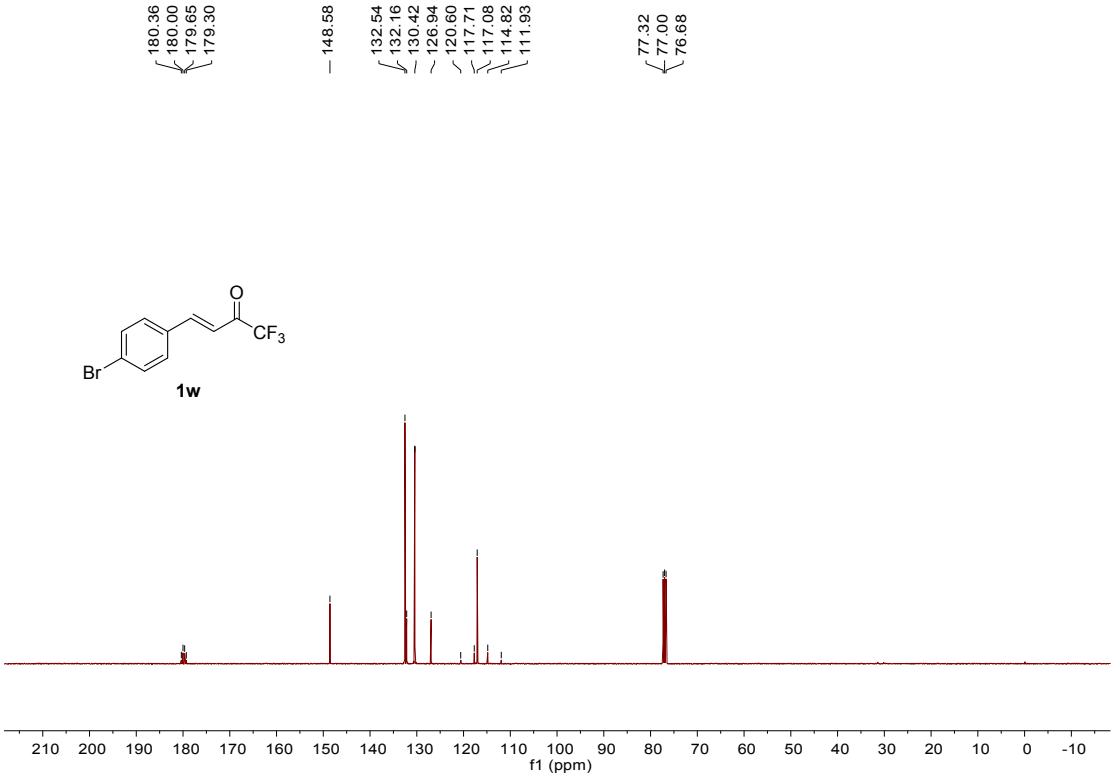

-77.54
O
CF3
Me
1u
0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200
f1 (ppm)

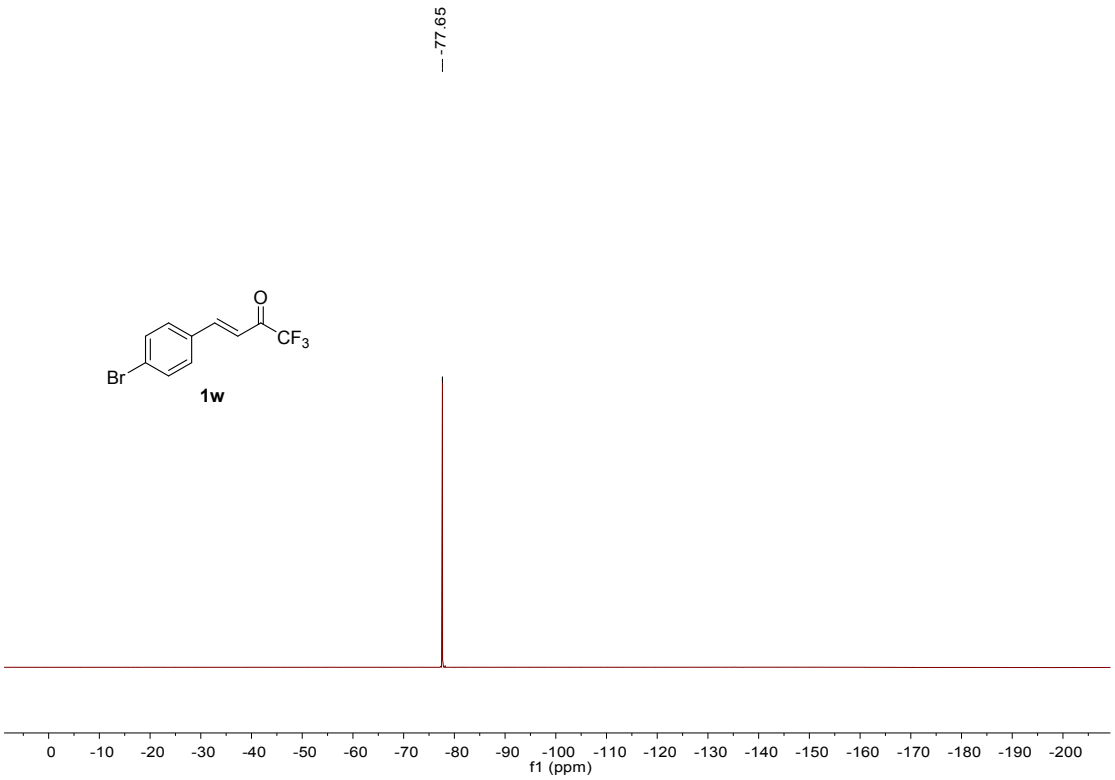

7.93
7.90
7.59
7.57
7.44
7.42
7.00
6.97
O
CF3
Cl
1v
1.00
2.09
1.99
1.03
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

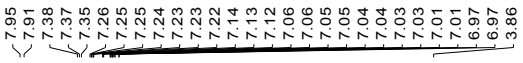

180.18
179.95
179.71
179.48
148.50
138.45
131.77
130.32
129.58
119.18
117.25
117.01
115.33
113.40
O
CF3
Cl
1v
10 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

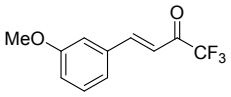

-77.65
O
CF3
Cl
1v
0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200
f1 (ppm)


7.92
7.88
7.61
7.59
7.52
7.49
7.02
6.98
0.00
O
CF3
Br
1w
1.00
1.97
2.15
1.05
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

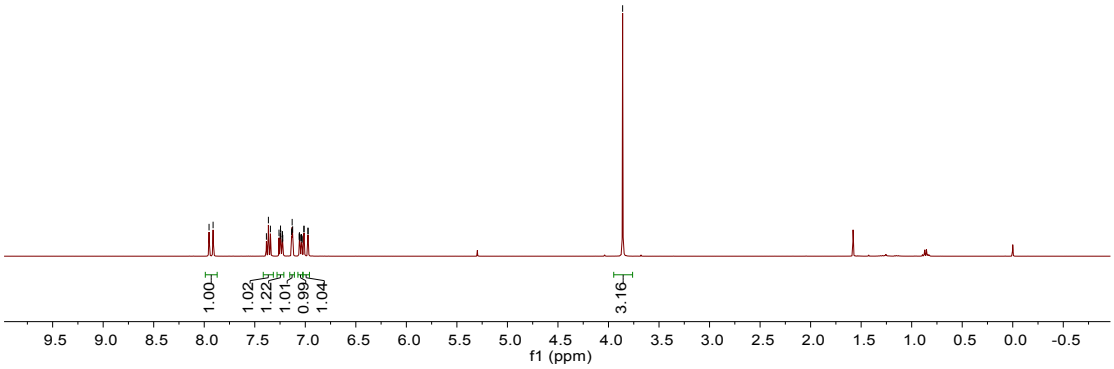

180.36
180.00
179.65
179.30
148.58
132.54
132.16
130.42
126.94
120.60
117.71
117.08
114.82
111.93
77.32
77.00
76.68
O
CF3
Br
1w
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

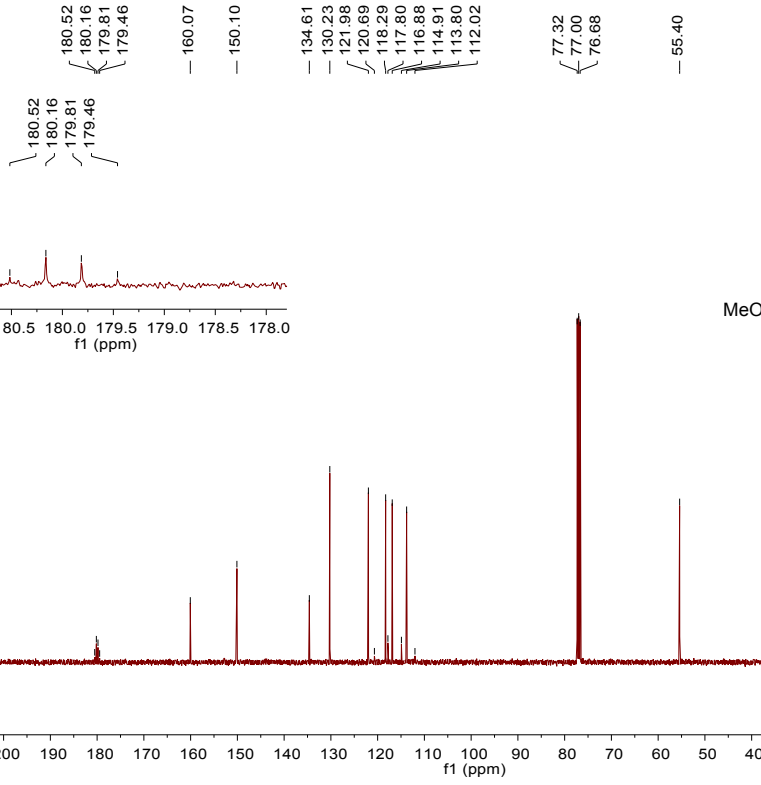

-77.65
O
CF3
Br
1w
0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200
f1 (ppm)


7.95
7.91
7.38
7.37
7.35
7.26
7.25
7.25
7.24
7.23
7.23
7.22
7.14
7.13
7.12
7.06
7.06
7.05
7.05
7.04
7.04
7.03
7.03
7.01
7.01
6.97
6.97
3.86

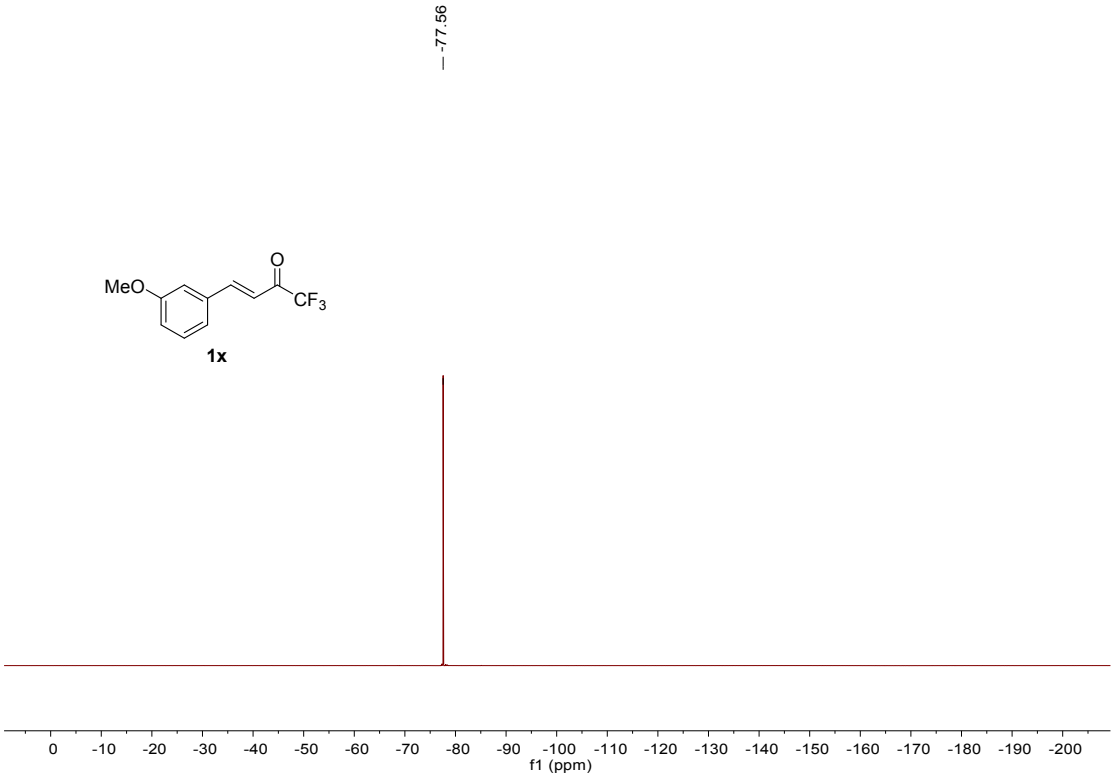

MeO
O
CF3

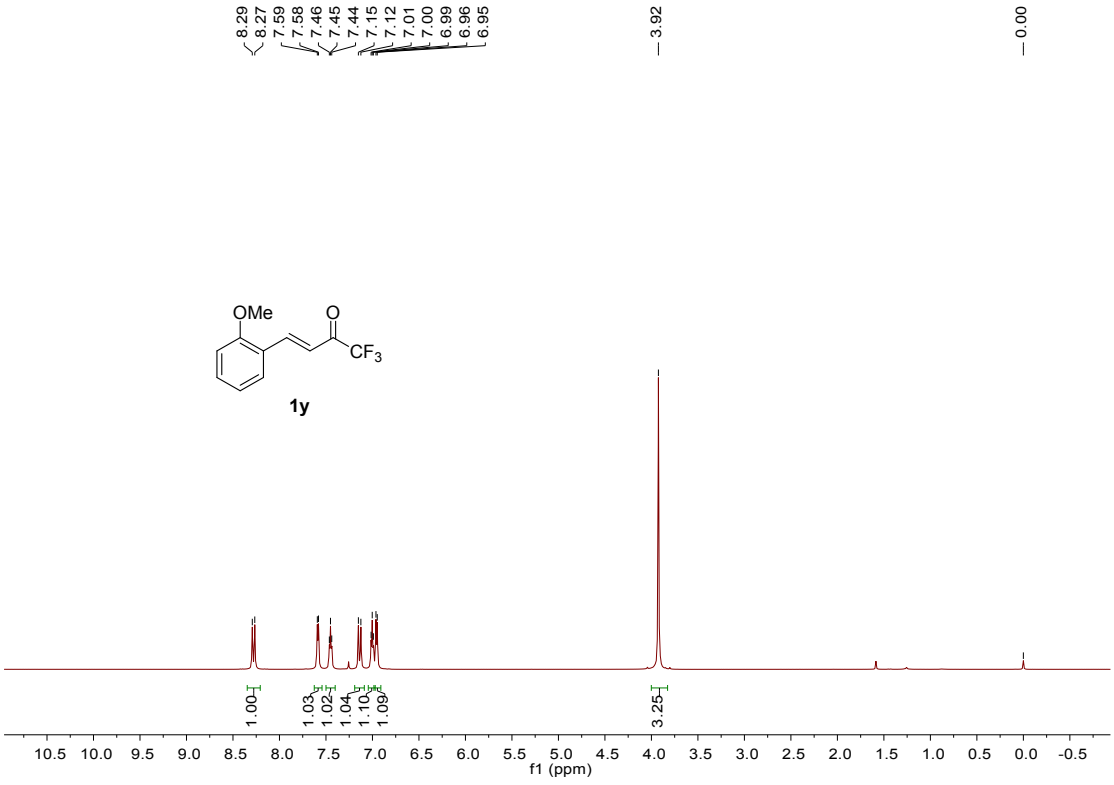
1x

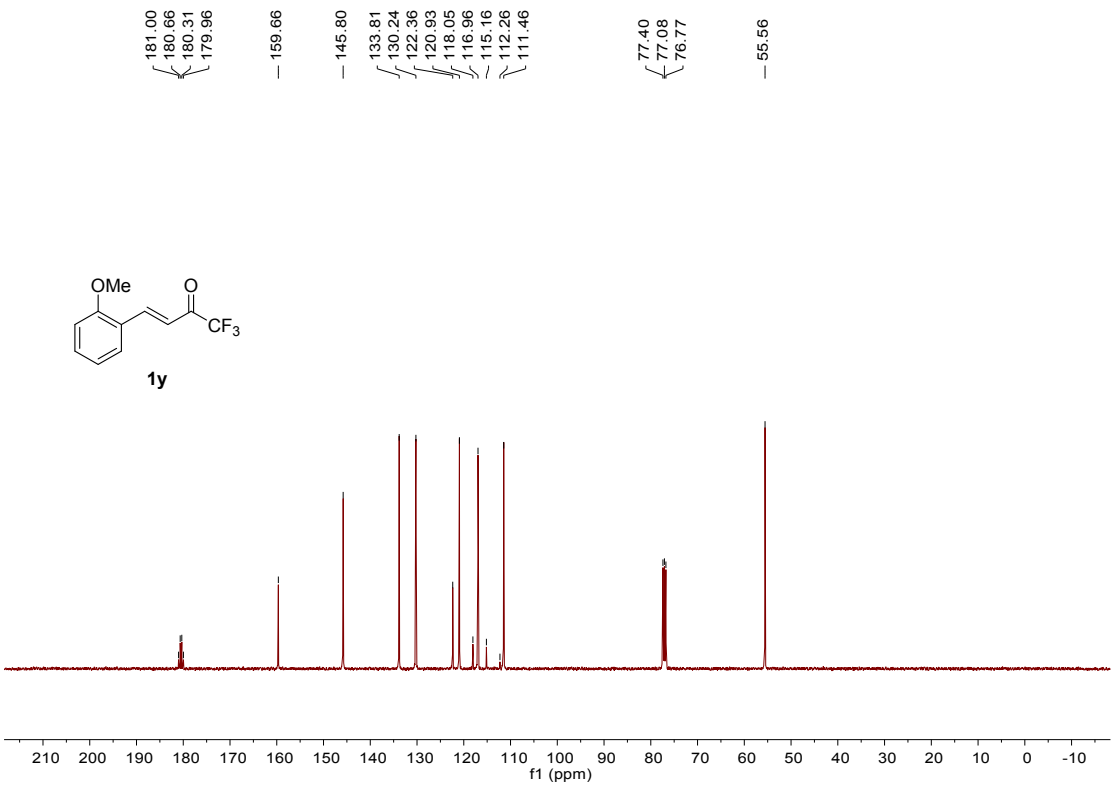

1.00
1.02
1.22
1.01
0.99
1.04
3.16
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

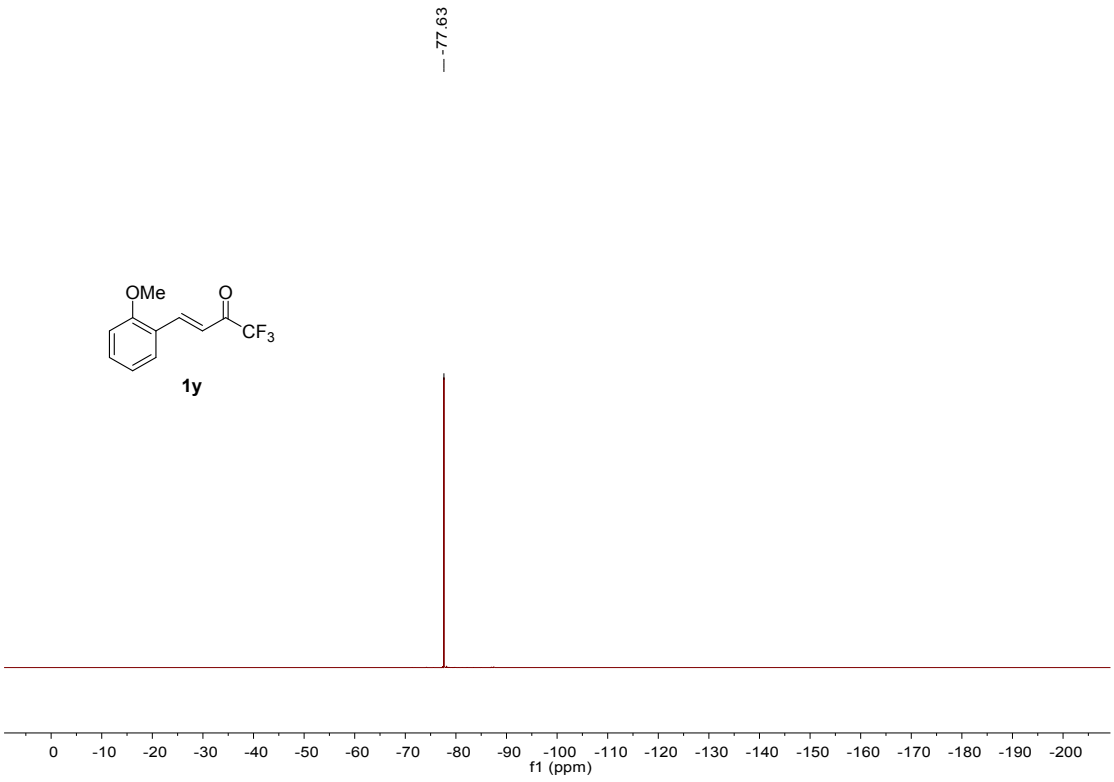

180.52
180.16
179.81
179.46
160.07
150.10
134.61
130.23
121.98
120.69
118.29
117.80
116.88
114.91
113.80
112.02
77.32
77.00
76.68
55.40
180.52
180.16
179.81
179.46
181.0 180.5 180.0 179.5 179.0 178.5 178.0
f1 (ppm)
MeO
O
CF3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

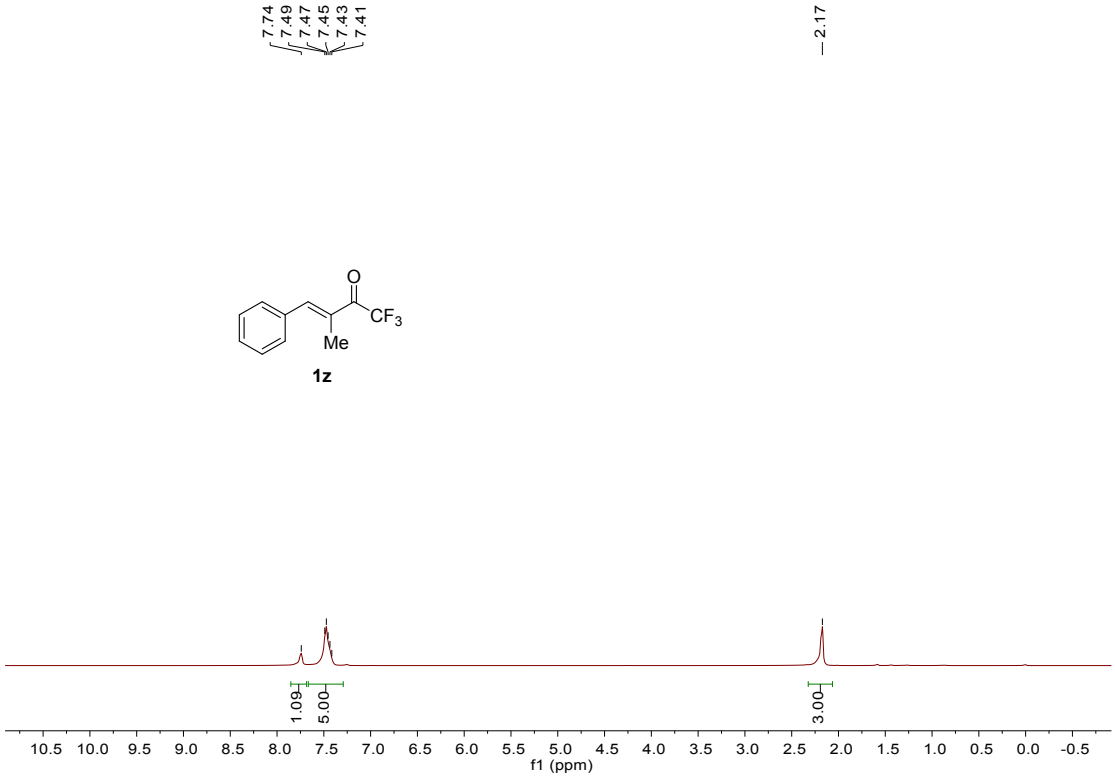
1x

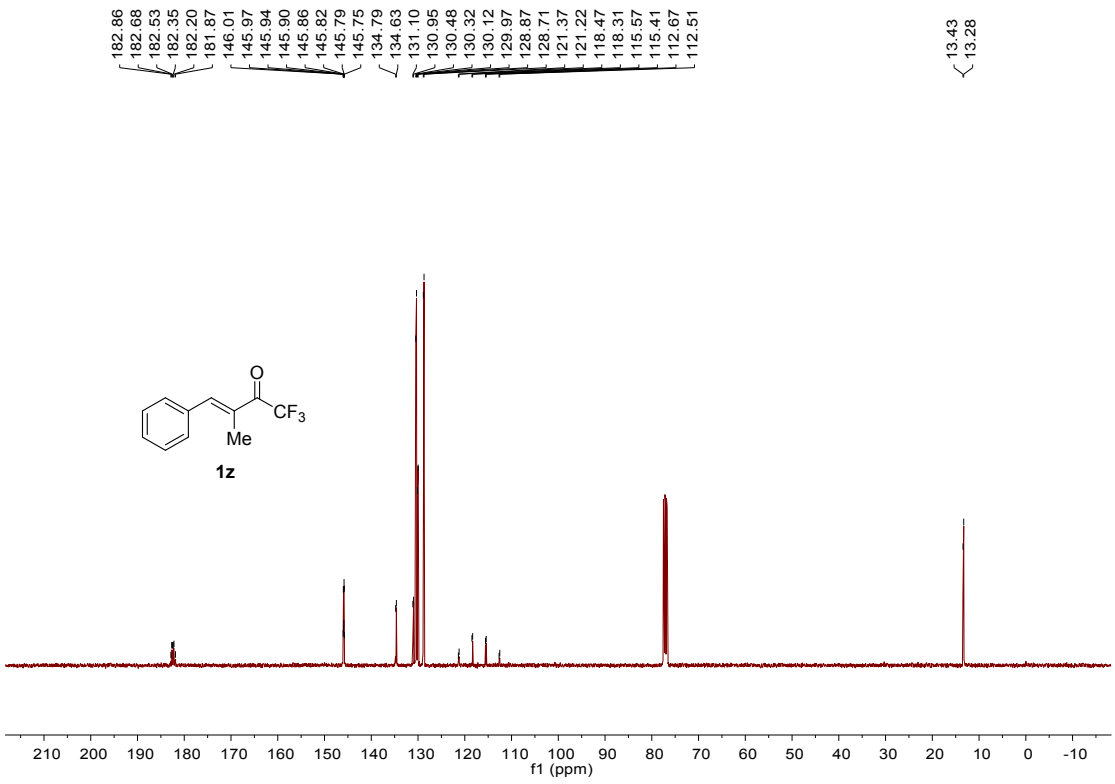

-77.56
MeO
O
CF3
1x
0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200
f1 (ppm)

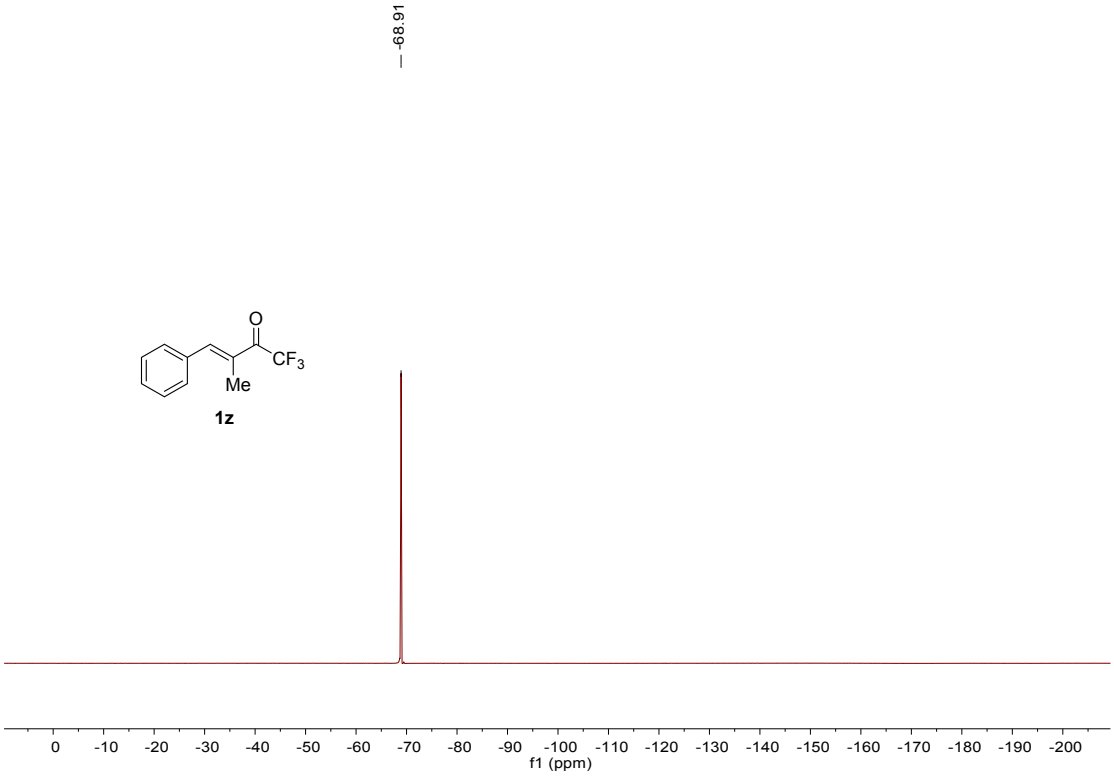

8.29
8.27
7.59
7.58
7.46
7.45
7.44
7.15
7.12
7.01
7.00
6.99
6.96
6.95
3.92
0.00
OMe
O
CF3
1y
1.00
1.03
1.02
1.04
1.10
1.09
3.25
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

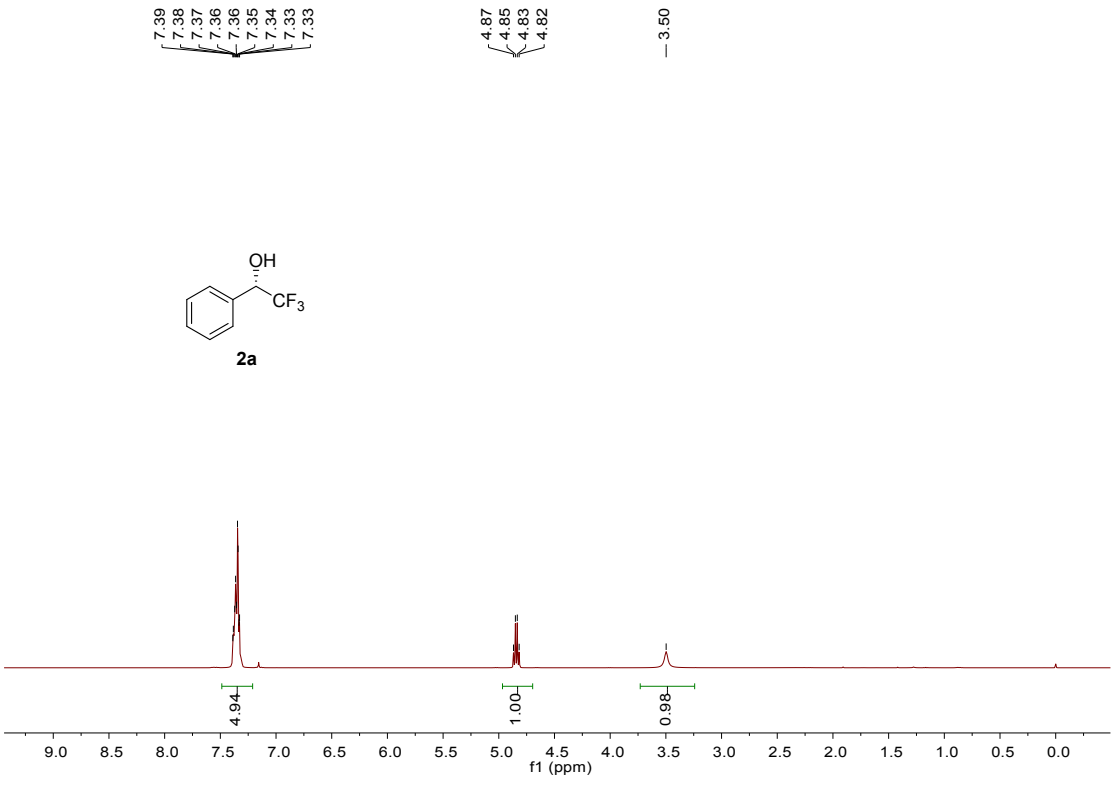

181.00
180.66
180.31
179.96
159.66
145.80
133.81
130.24
122.36
120.93
118.05
116.96
115.16
112.26
111.46
77.40
77.08
76.77
55.56
OMe
O
CF3
1y
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

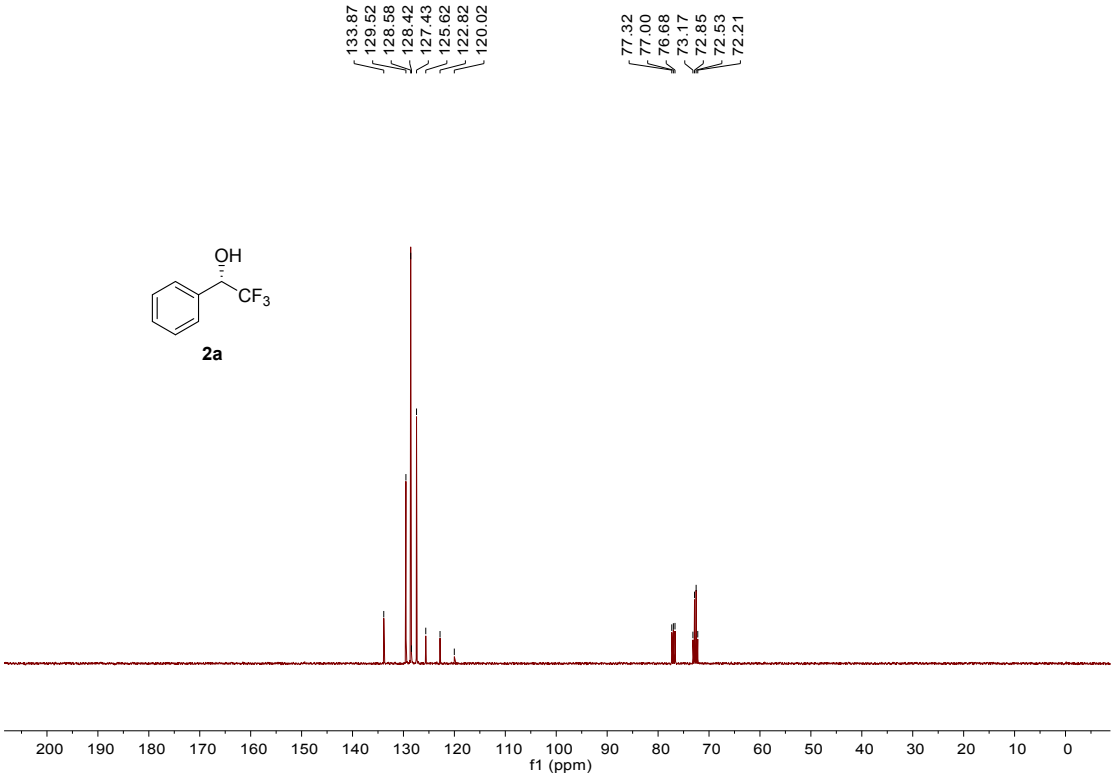

-77.63
OMe
O
CF3
1y
0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200
f1 (ppm)

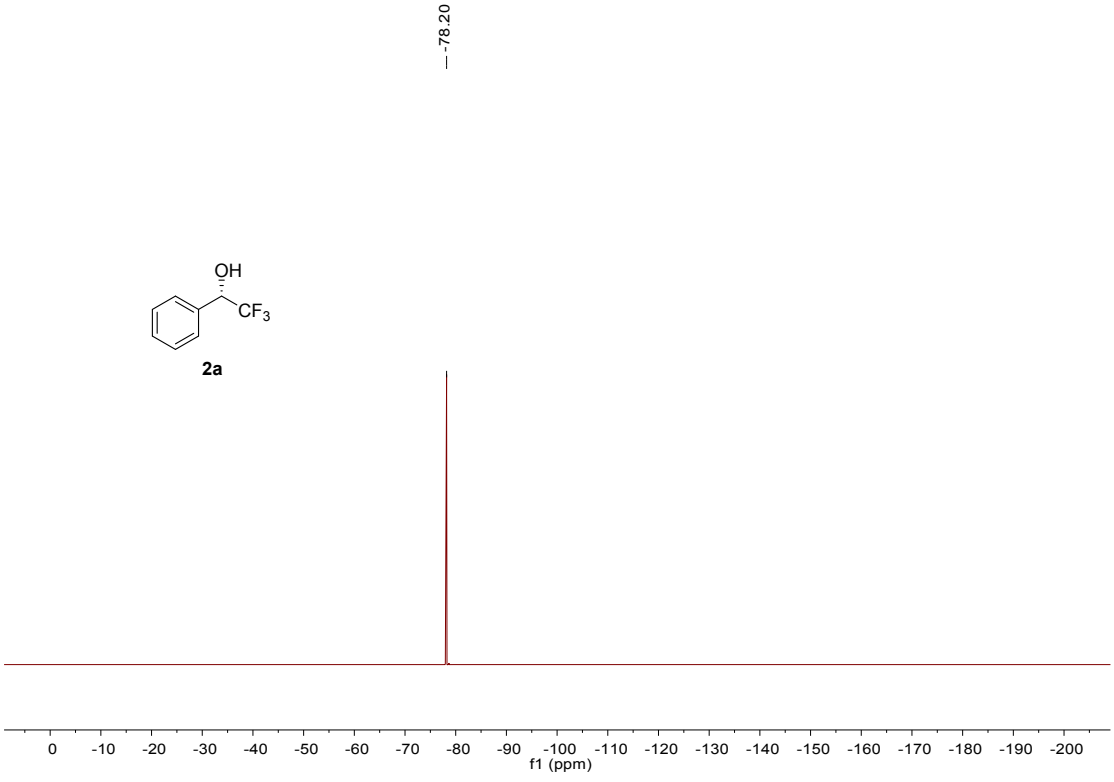

7.74
7.49
7.47
7.45
7.43
7.41
2.17
O
CF3
Me
1z
1.09
5.00
3.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

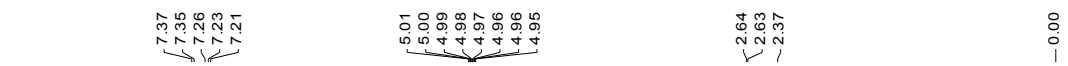

182.86
182.68
182.53
182.35
182.20
181.87
146.01
145.97
145.94
145.90
145.86
145.82
145.79
145.75
134.79
134.63
131.10
130.95
130.48
130.32
130.12
129.97
128.87
128.71
121.37
121.22
118.47
118.31
115.57
115.41
112.67
112.51
13.43
13.28
O
CF3
Me
1z
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

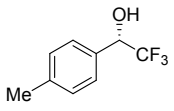

-68.91
O
CF3
Me
1z
0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200
f1 (ppm)


7.39
7.38
7.37
7.36
7.36
7.35
7.34
7.33
7.33
4.87
4.85
4.83
4.82
3.50
OH
CF3
2a
4.94
1.00
0.98
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

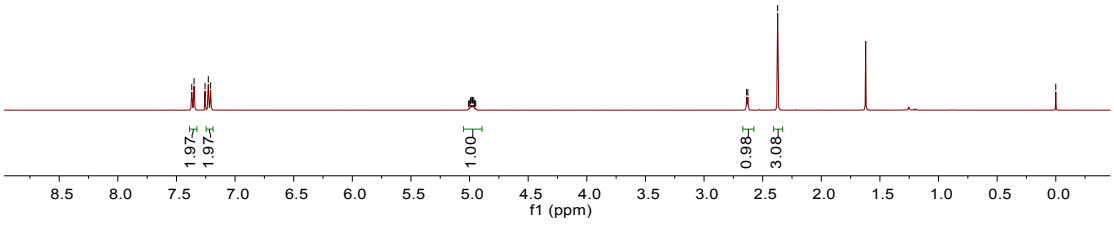

133.87
129.52
128.58
128.42
127.43
125.62
122.82
120.02
77.32
77.00
76.68
73.17
72.85
72.53
72.21
OH
CF3
2a
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

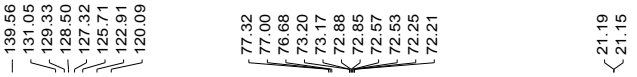

-78.20
OH
CF3
2a
0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200
f1 (ppm)

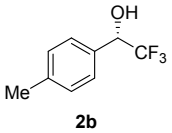

7.37
7.35
7.26
7.23
7.21
5.01
5.00
4.99
4.98
4.97
4.96
4.96
4.95
2.64
2.63
2.37
0.00


OH
CF3
Me

2b

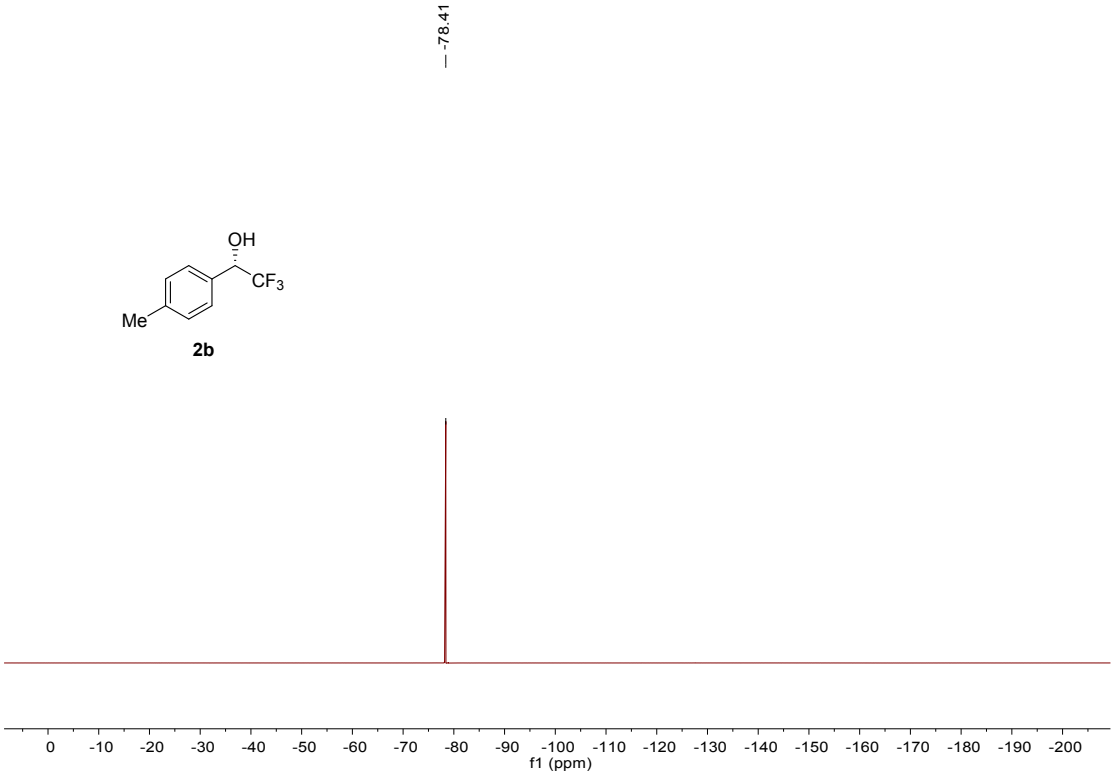

1.97
1.97
1.00
0.98
3.08
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

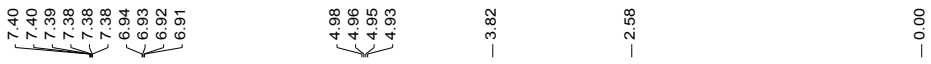

139.56
131.05
129.33
128.50
127.32
125.71
122.91
120.09
77.32
77.00
76.68
73.20
73.17
72.88
72.85
72.57
72.53
72.25
72.21
21.19
21.15

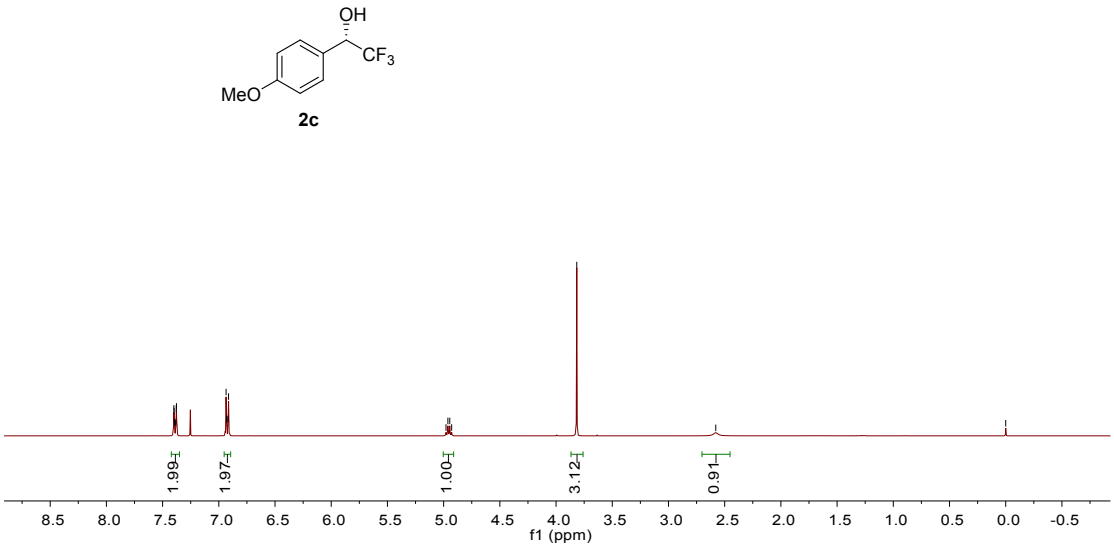

OH
CF3
Me

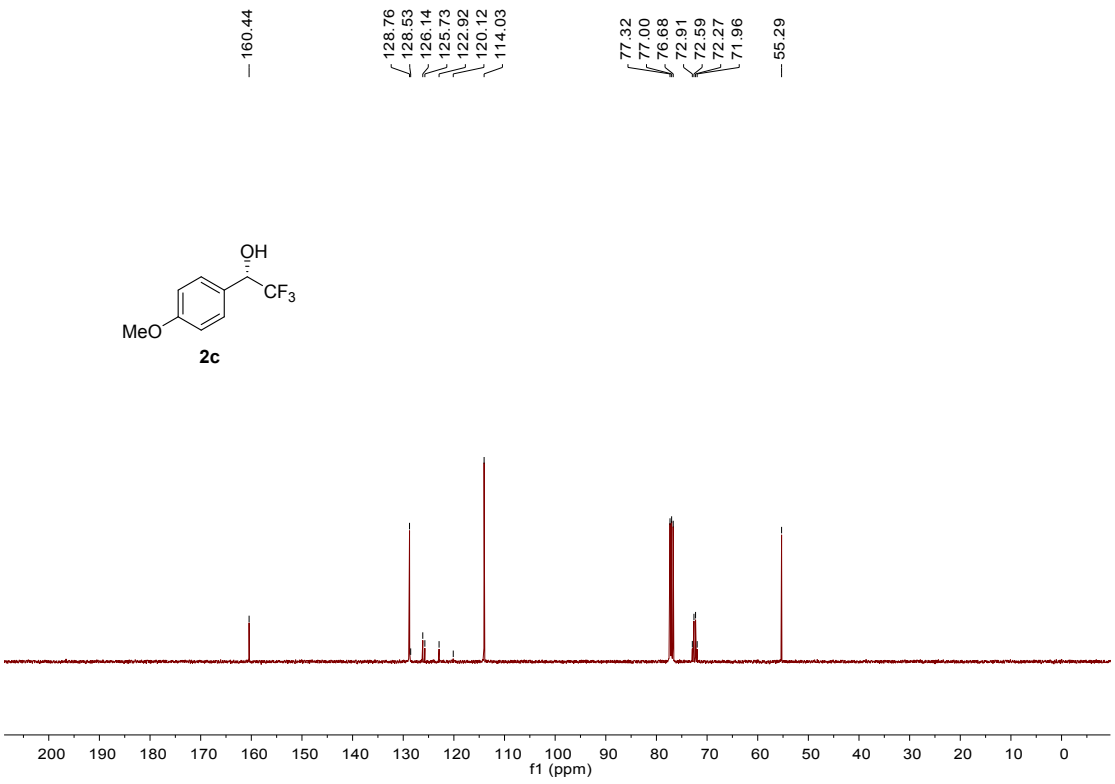
2b

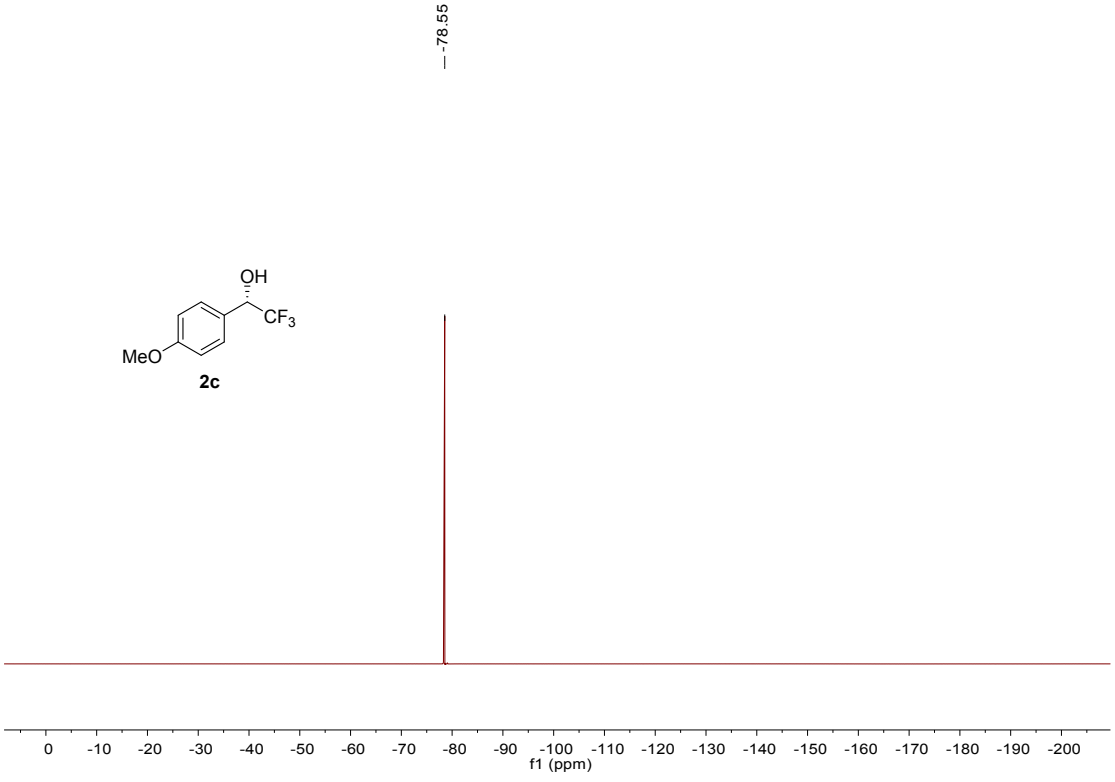
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

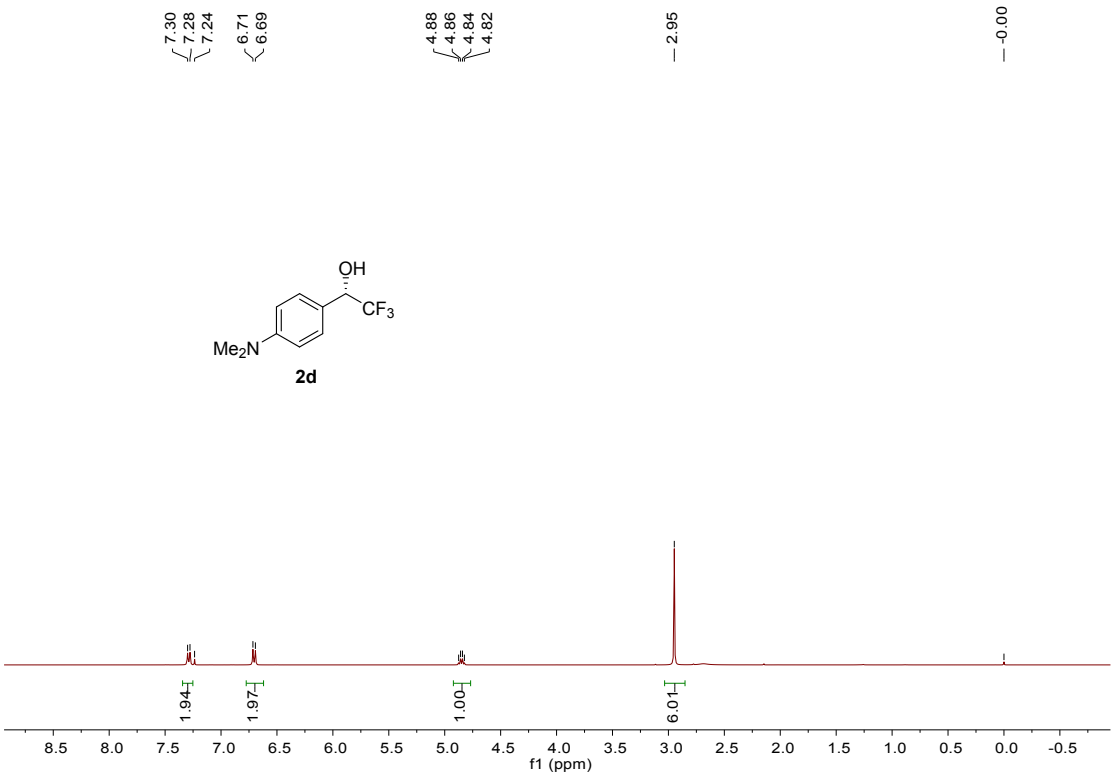

-78.41
OH
CF3
Me
2b
0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200
f1 (ppm)

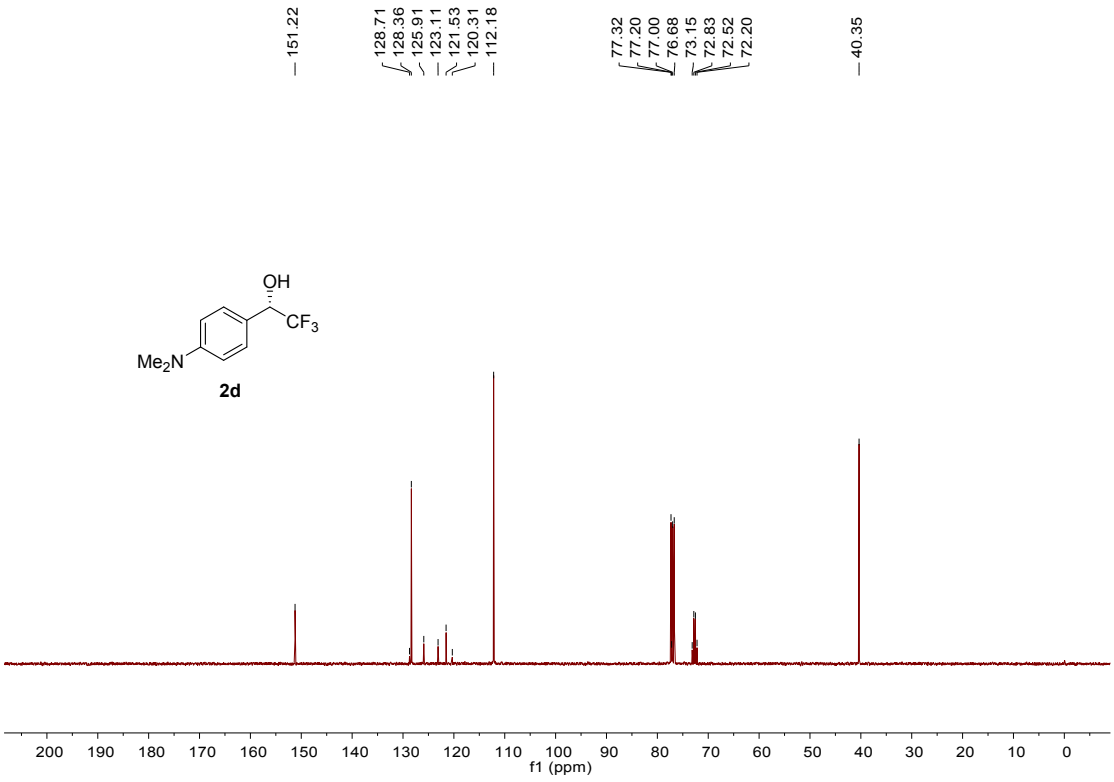

7.40
7.40
7.39
7.38
7.38
7.38
6.94
6.93
6.92
6.91
4.98
4.96
4.95
4.93
3.82
2.58
0.00

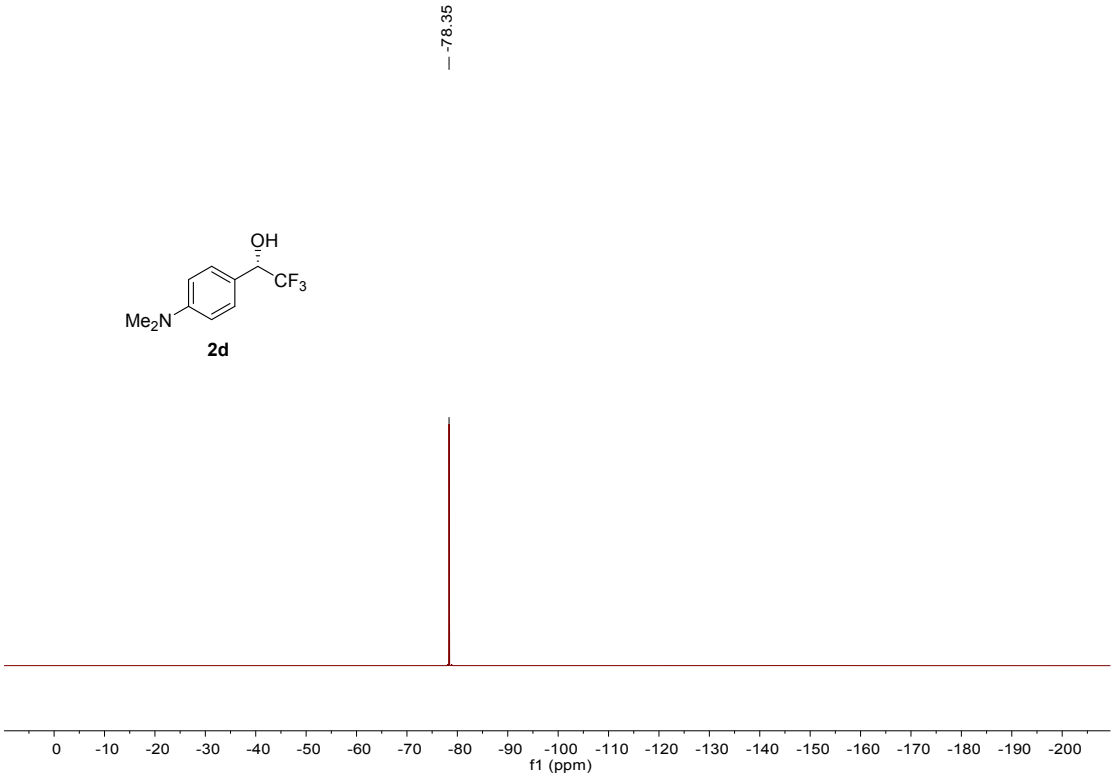

OH
CF3
MeO
2c
1.99
1.97
1.00
3.12
0.91
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


160.44
128.76
128.53
126.14
125.73
122.92
120.12
114.03
77.32
77.00
76.68
72.91
72.59
72.27
71.96
55.29
OH
CF3
MeO
2c
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

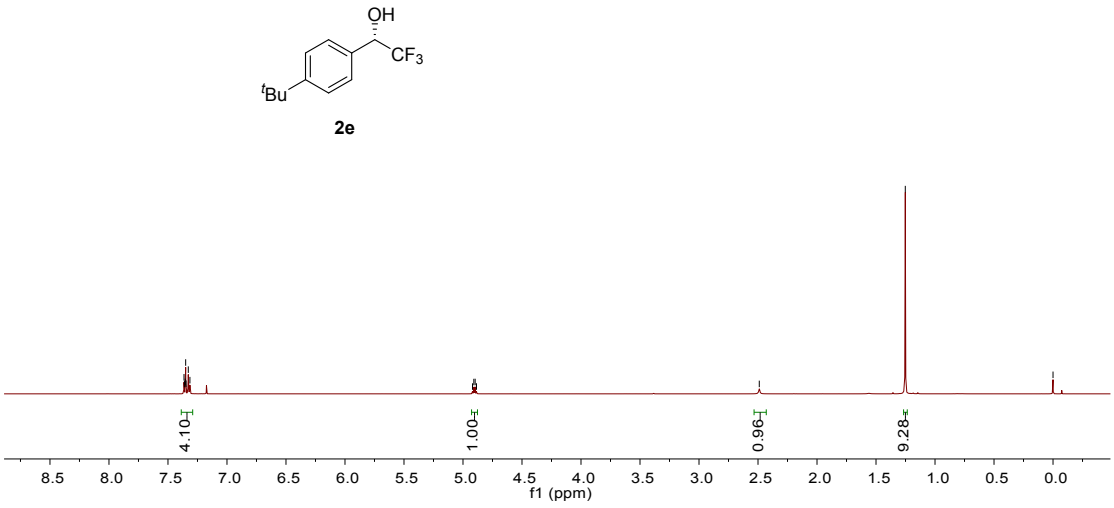

-78.55
OH
CF3
MeO
2c
0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200
f1 (ppm)

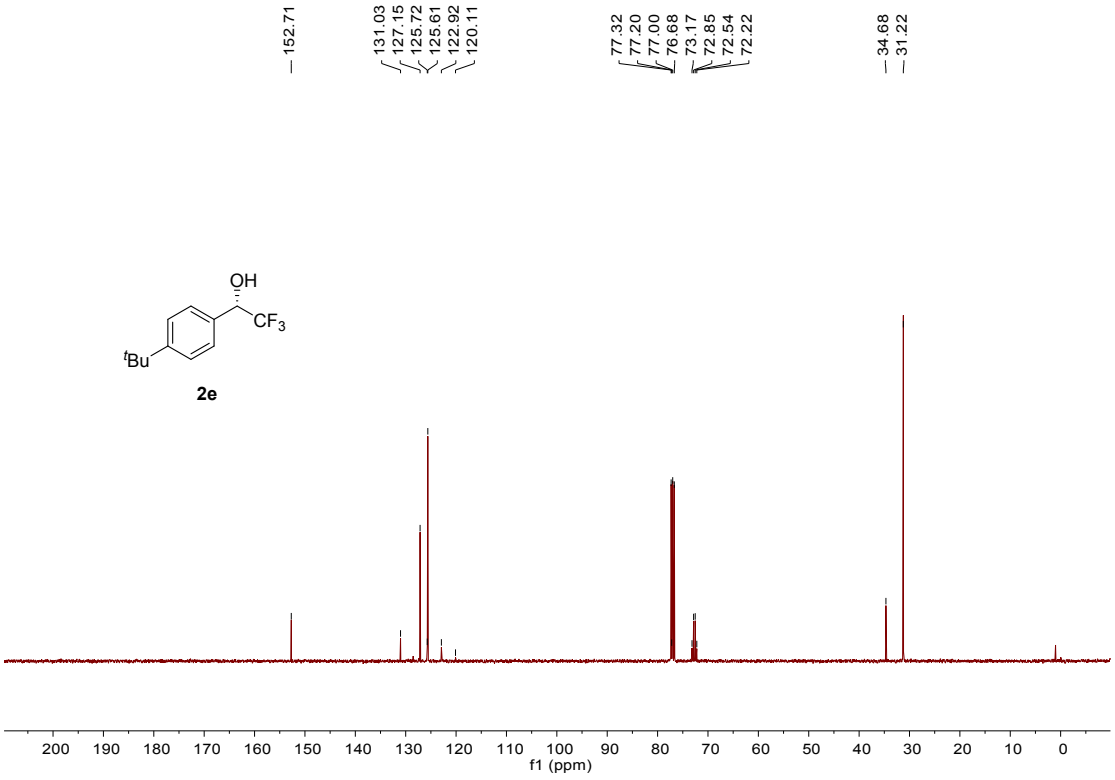

7.30
7.28
7.24
6.71
6.69
4.88
4.86
4.84
4.82
2.95
-0.00
OH
CF3
Me2N
2d
1.94
1.97
1.00
6.01
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

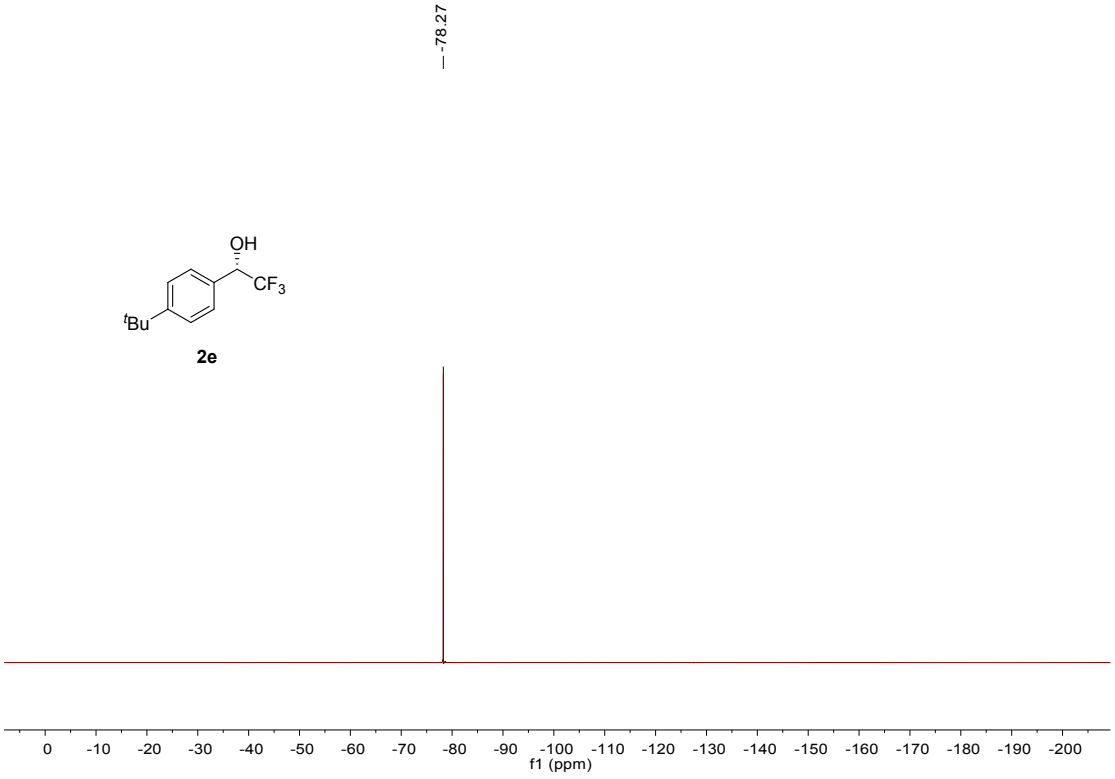

151.22
128.71
128.36
125.91
123.11
121.53
120.31
112.18
77.32
77.20
77.00
76.68
73.15
72.83
72.52
72.20
40.35
OH
CF3
Me2N
2d
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


-78.35
OH
CF3
Me2N
2d
0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200
f1 (ppm)

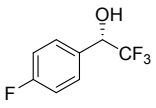

7.36
7.36
7.35
7.35
7.35
7.33
7.31
4.92
4.91
4.90
4.89
2.49
1.25
0.00


OH
CF3
tBu
2e
4.10
1.00
0.96
9.28
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

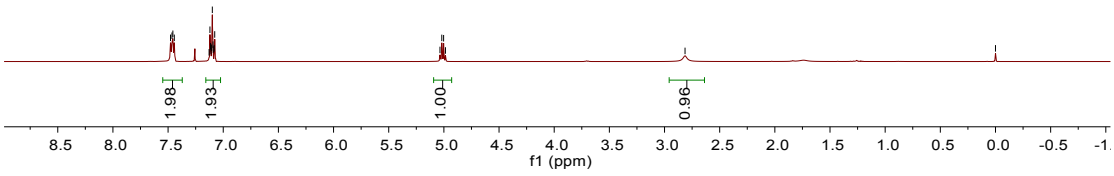

152.71
131.03
127.15
125.72
125.61
122.92
120.11
77.32
77.20
77.00
76.68
73.17
72.85
72.54
72.22
34.68
31.22
OH
CF3
tBu
2e
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

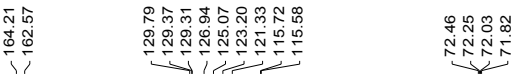

-78.27
OH
CF3
tBu
2e
0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200
f1 (ppm)

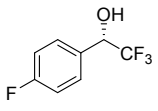

7.48
7.46
7.46
7.44
7.13
7.12
7.11
7.11
7.11
7.10
7.09
7.09
7.08
7.08
5.04
5.02
5.00
4.99
2.81
0.00


OH
CF3
F

2f

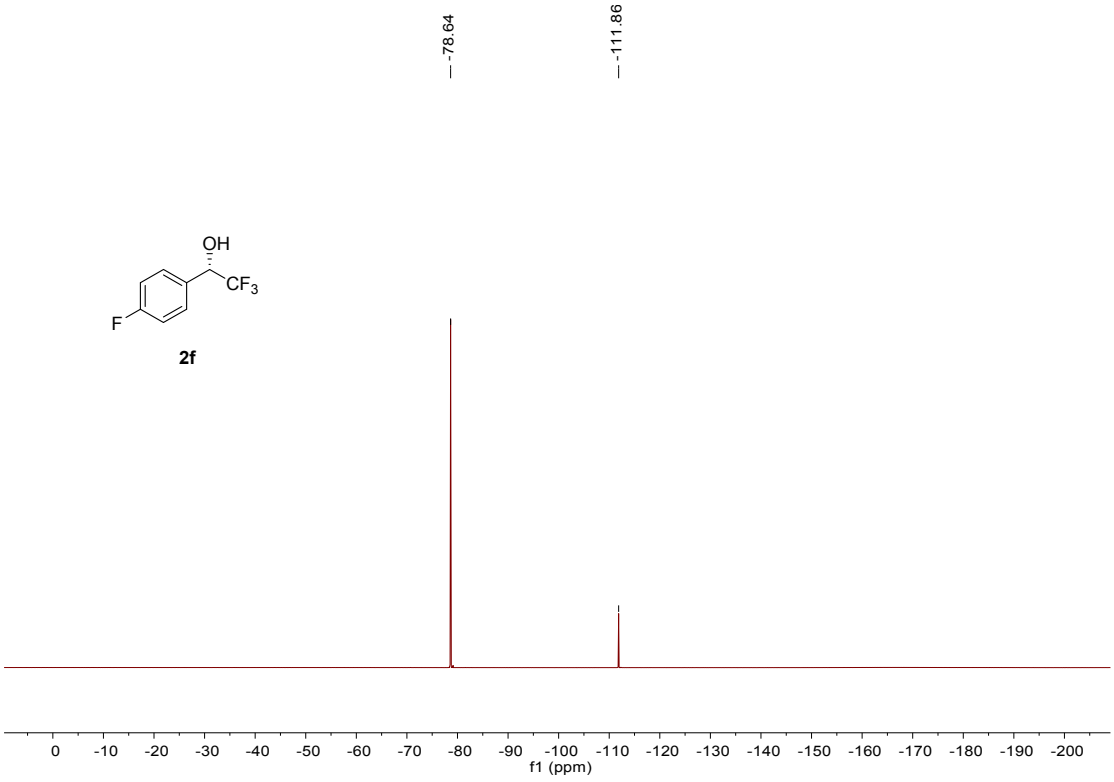

1.98
1.93
1.00
0.96
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

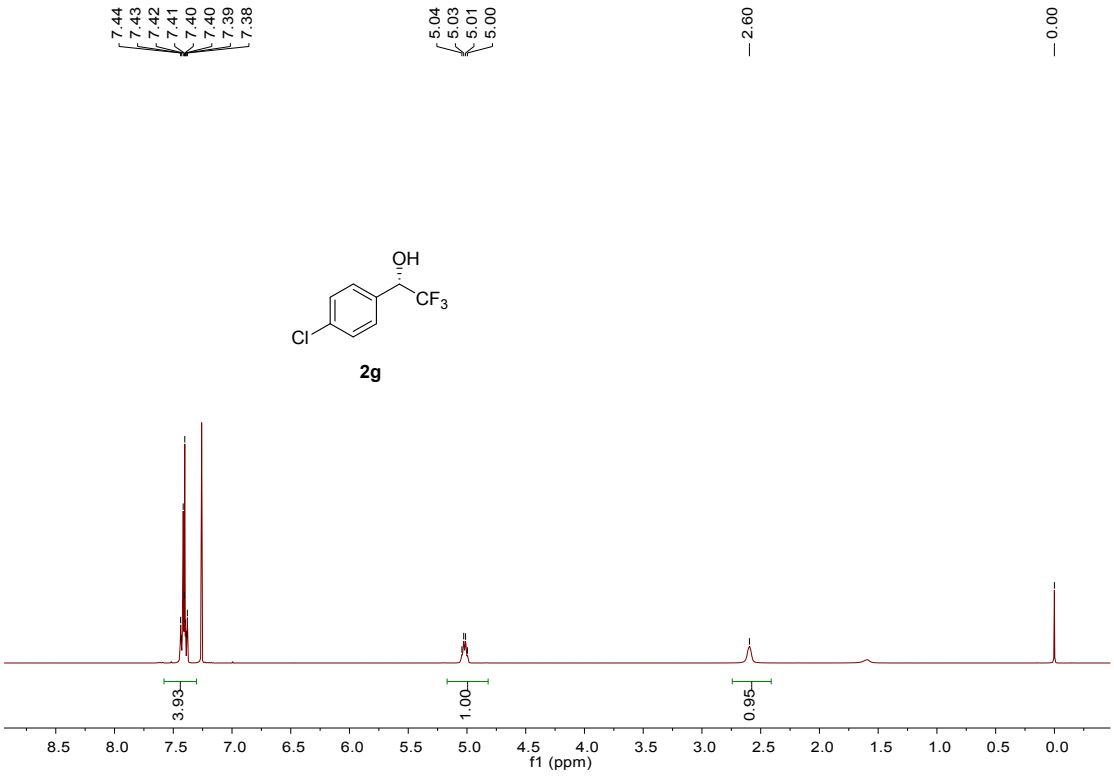

164.21
162.57
129.79
129.37
129.31
126.94
125.07
123.20
121.33
115.72
115.58
72.46
72.25
72.03
71.82

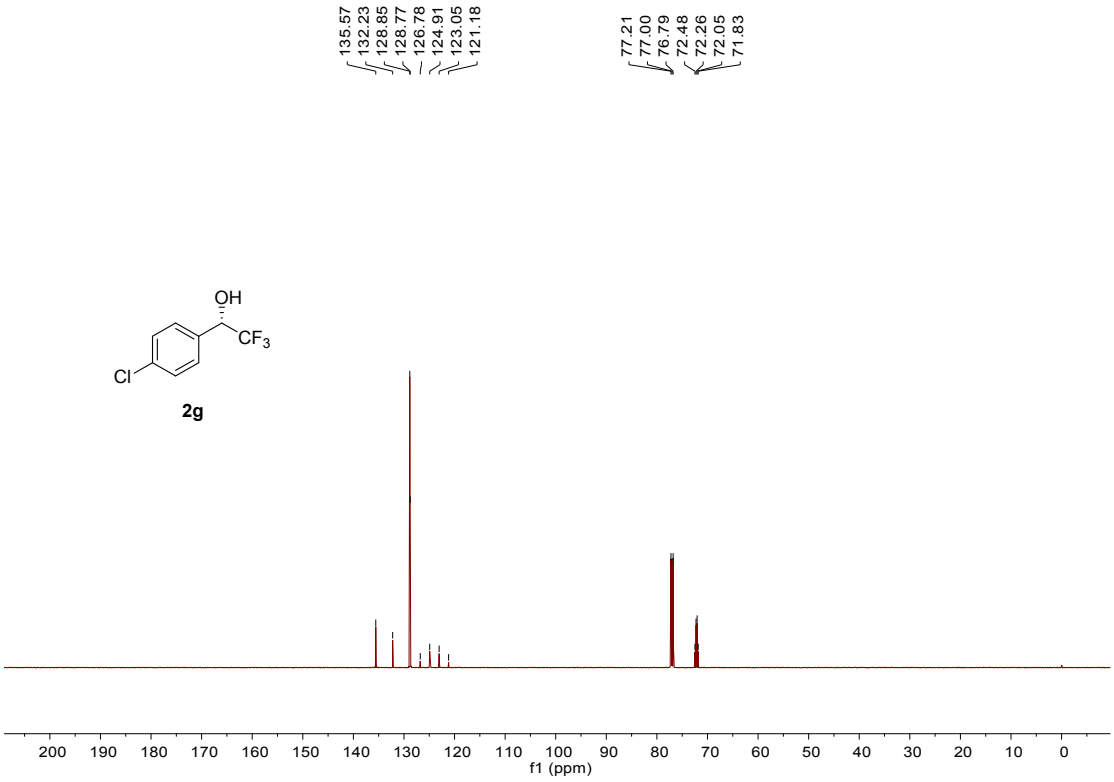

OH
CF3
F

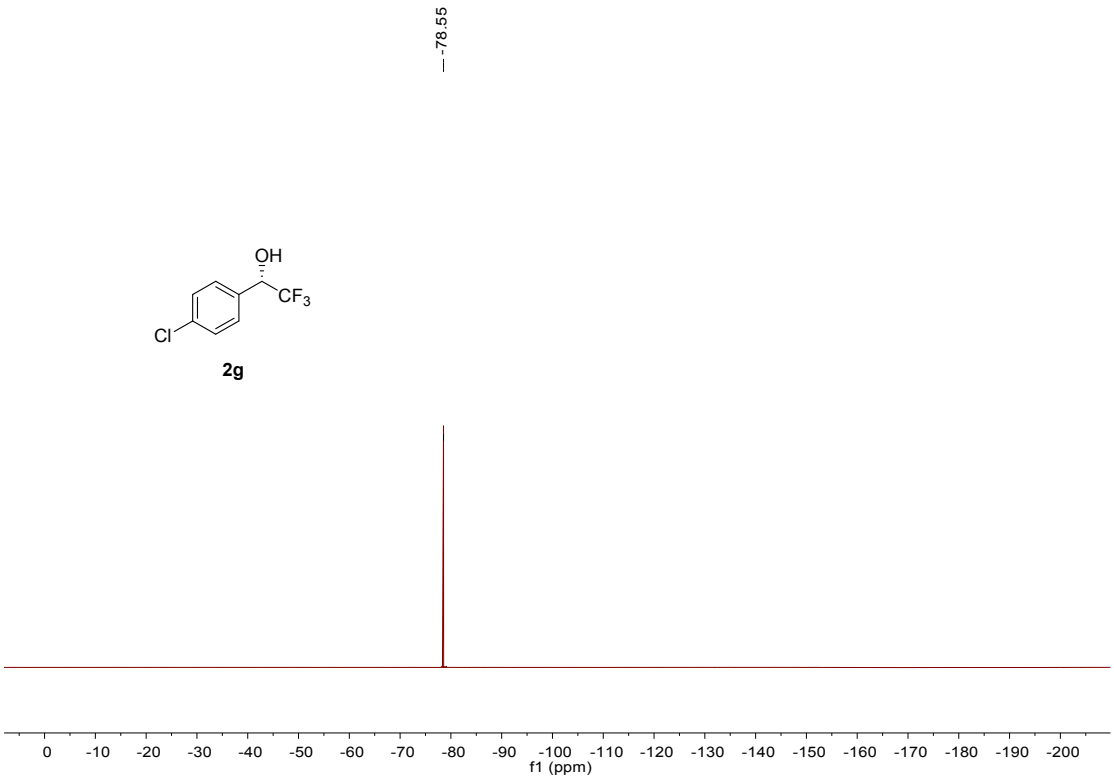
2f

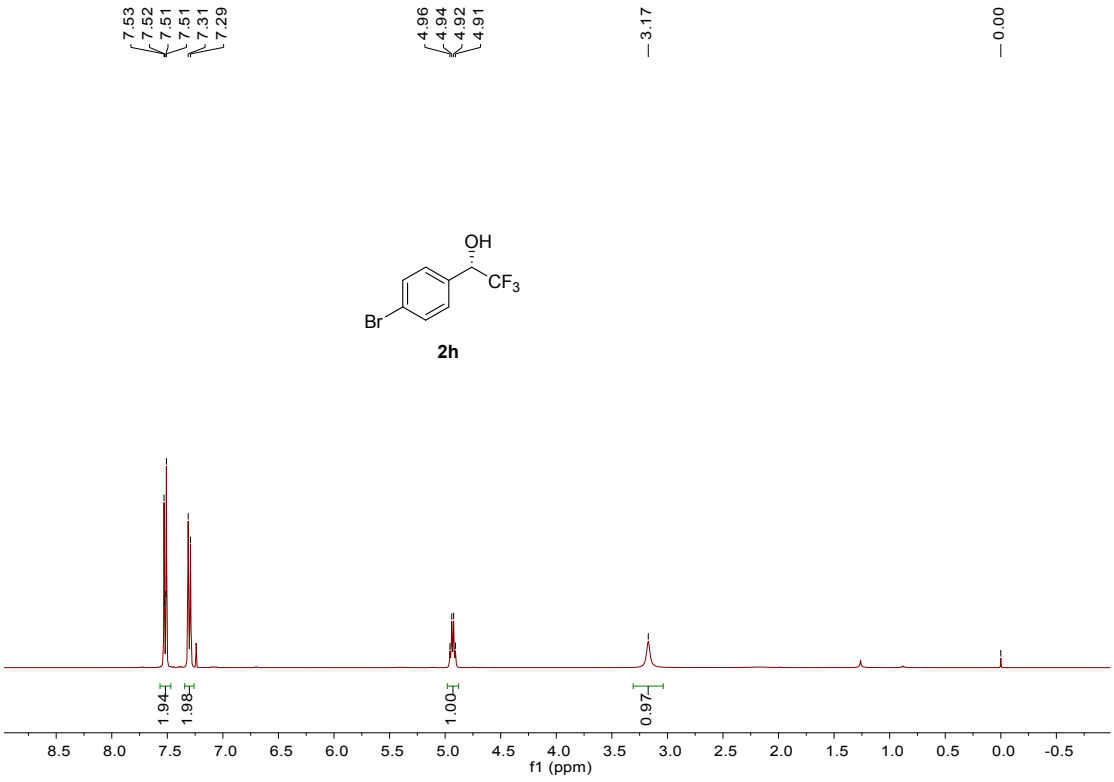
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

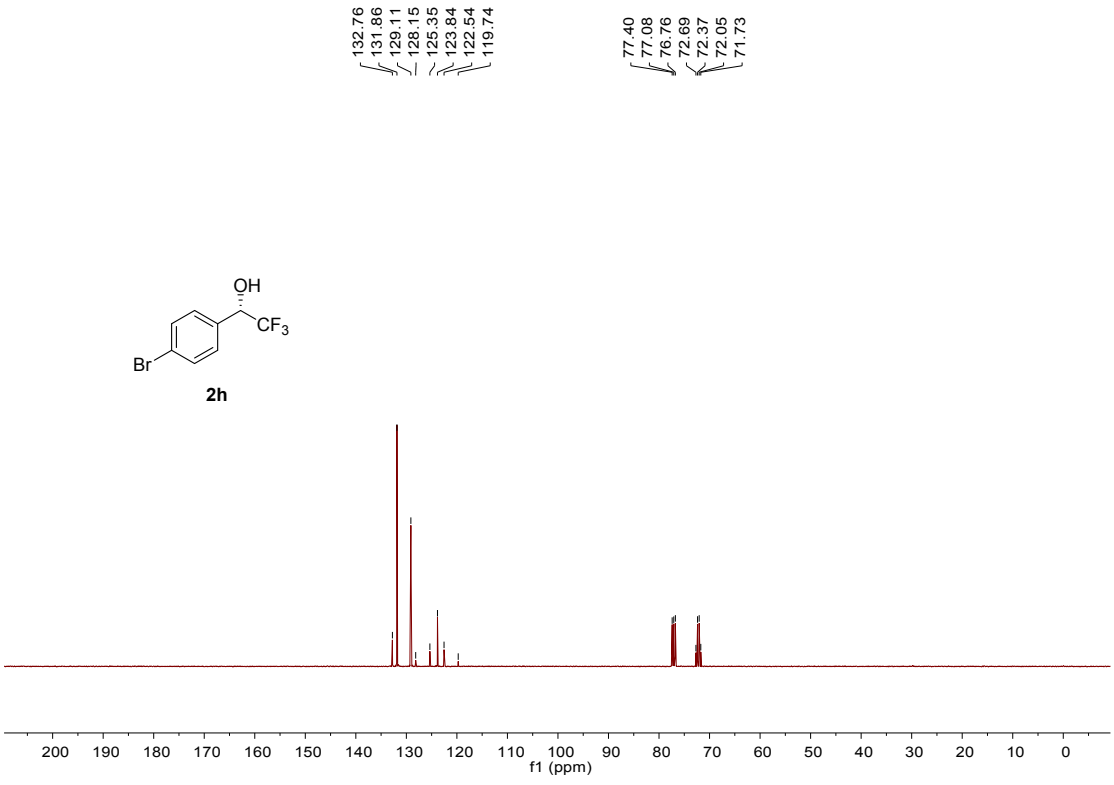

-78.64
-111.86
OH
CF3
F
2f
0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200
f1 (ppm)

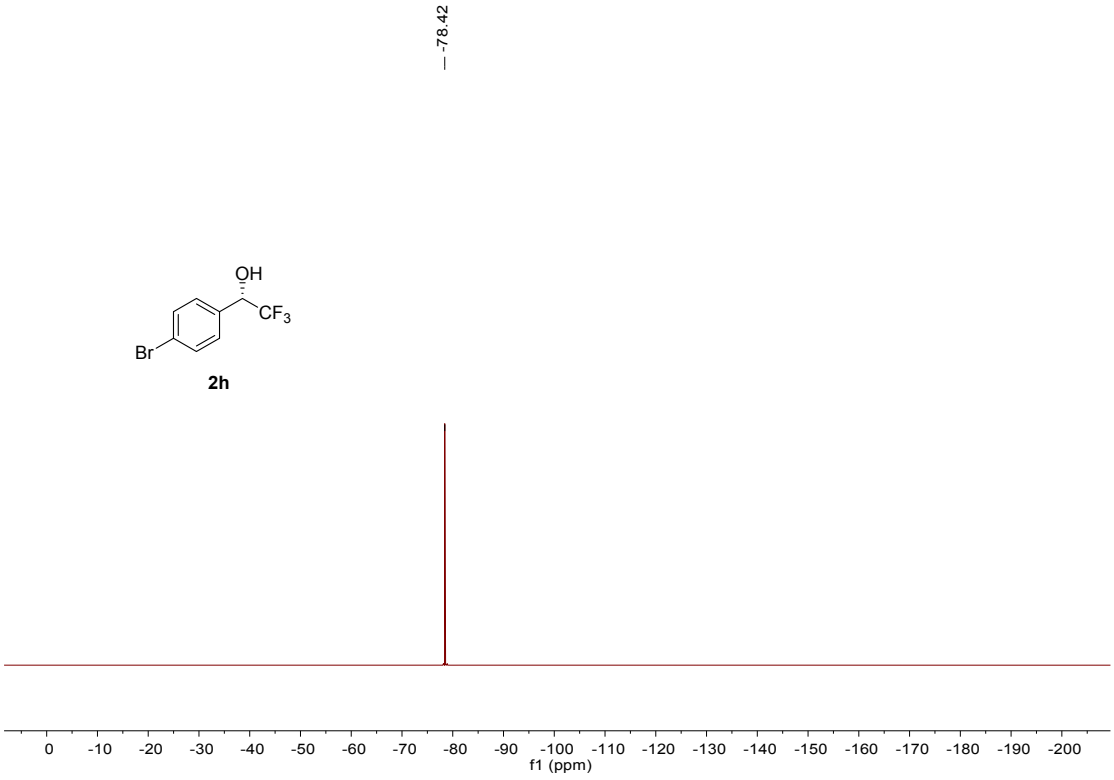

7.44
7.43
7.42
7.41
7.40
7.40
7.39
7.38
5.04
5.03
5.01
5.00
2.60
0.00
OH
CF3
Cl
2g
3.93
1.00
0.95
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


135.57
132.23
128.85
128.77
126.78
124.91
123.05
121.18
77.21
77.00
76.79
72.48
72.26
72.05
71.83
OH
CF3
Cl
2g
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

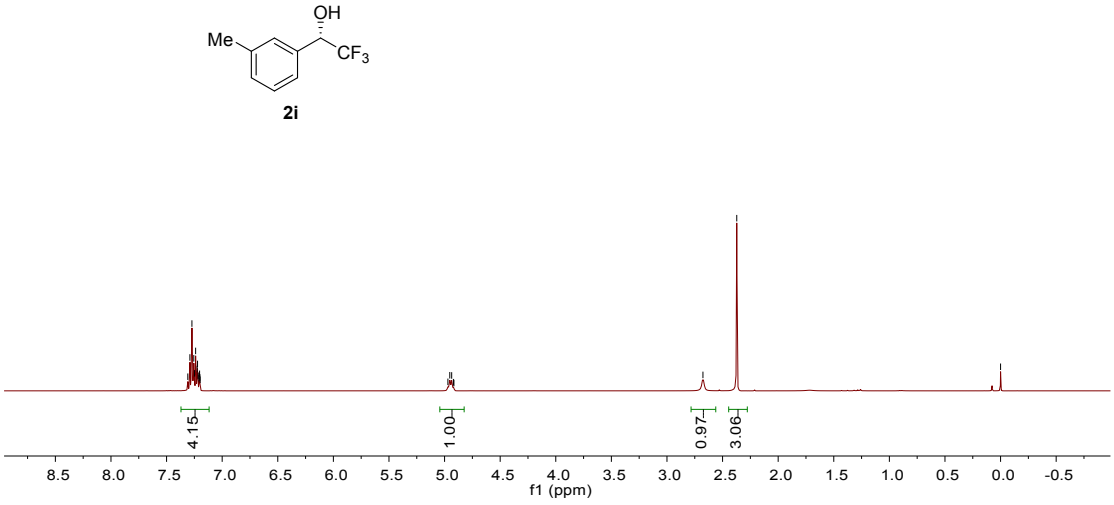

-78.55
OH
CF3
Cl
2g
0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200
f1 (ppm)

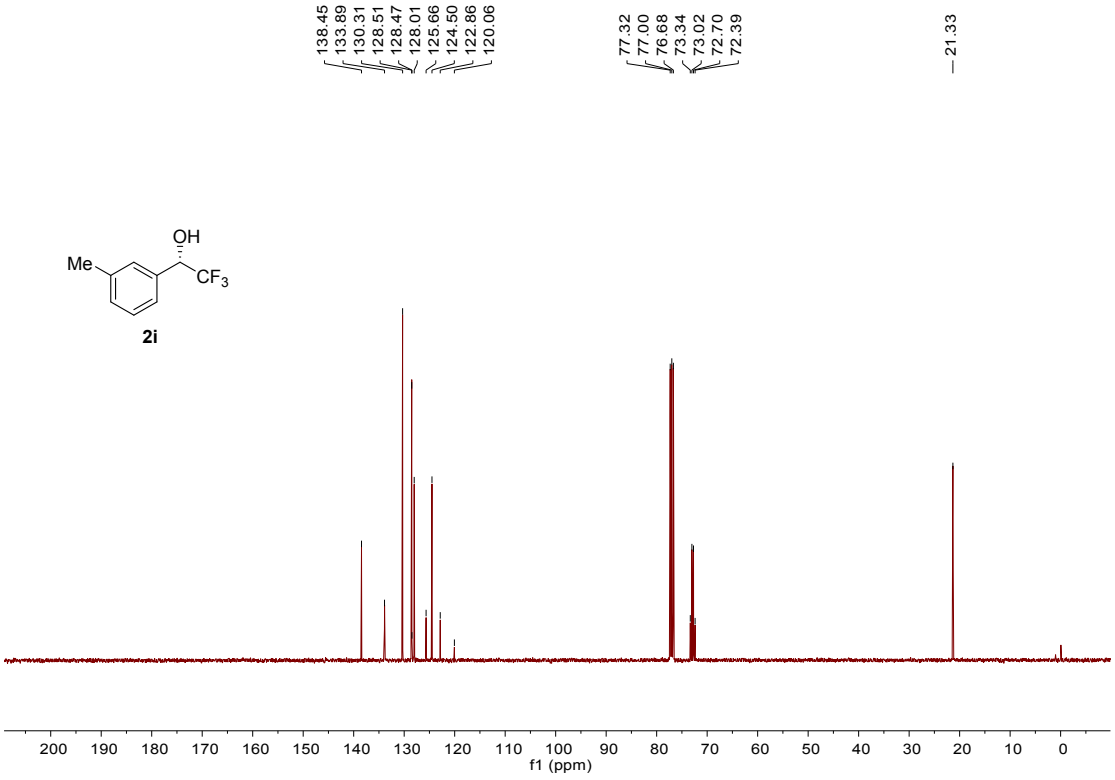

7.53
7.52
7.51
7.51
7.31
7.29
4.96
4.94
4.92
4.91
3.17
0.00
OH
CF3
Br
2h
1.94
1.98
1.00
0.97
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

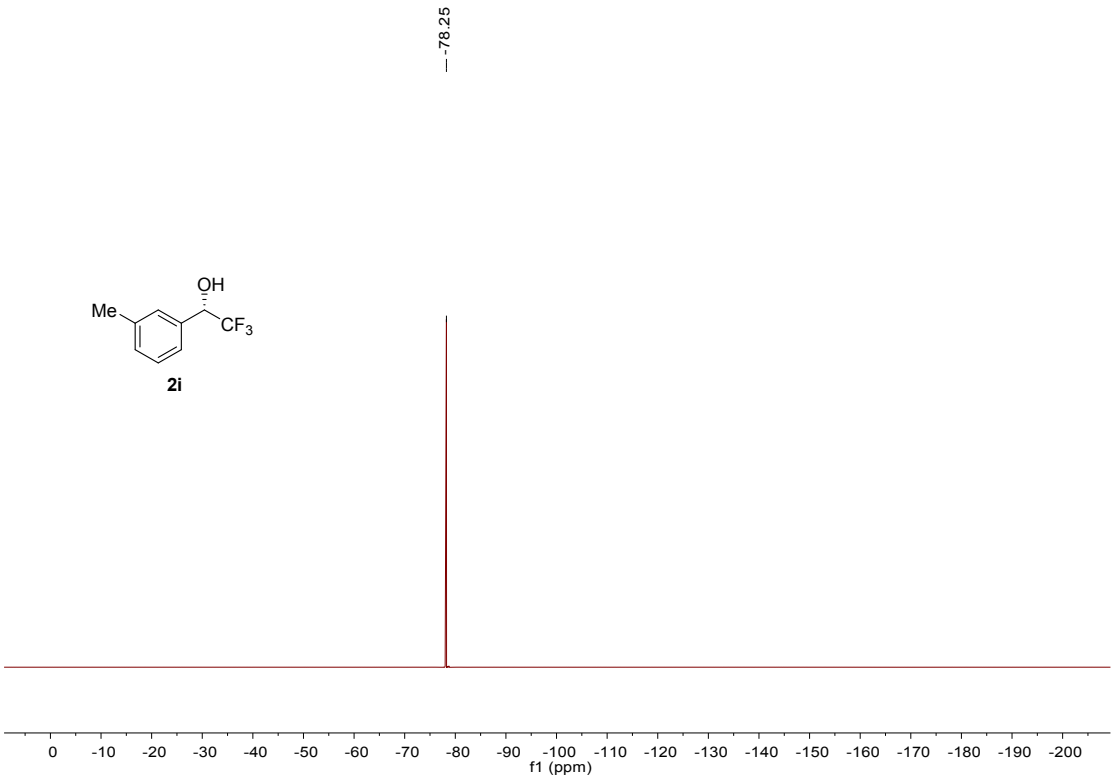

132.76
131.86
129.11
128.15
125.35
123.84
122.54
119.74
77.40
77.08
76.76
72.69
72.37
72.05
71.73
OH
CF3
Br
2h
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

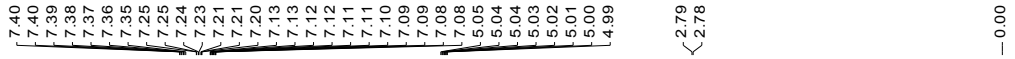

-78.42
OH
CF3
Br
2h
0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200
f1 (ppm)

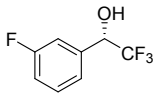

7.31
7.29
7.27
7.26
7.25
7.24
7.23
7.22
7.22
7.21
7.21
7.20
7.20
7.20
4.97
4.95
4.94
4.92
4.92
2.68
2.37
0.00


OH
Me
CF3
2i
4.15
1.00
0.97
3.06
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

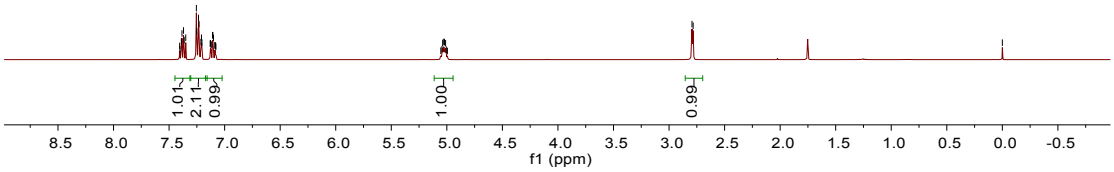

138.45
133.89
130.31
128.51
128.47
128.01
125.66
124.50
122.86
120.06
77.32
77.00
76.68
73.34
73.02
72.70
72.39
21.33
OH
Me
CF3
2i
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

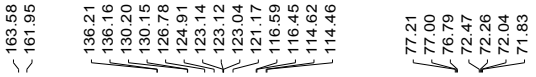

-78.25
OH
Me
CF3
2i
0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200
f1 (ppm)


7.40
7.40
7.39
7.38
7.37
7.36
7.35
7.25
7.24
7.23
7.21
7.21
7.20
7.13
7.13
7.12
7.12
7.11
7.11
7.10
7.09
7.09
7.08
7.08
5.05
5.04
5.04
5.03
5.02
5.01
5.00
4.99
2.79
2.78
0.00


OH
F
CF3

2j


1.01
2.11
0.99
1.00
0.99
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)


163.58
161.95
136.21
136.16
130.20
130.15
126.78
124.91
123.14
123.12
123.04
121.17
116.59
116.45
114.62
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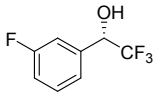
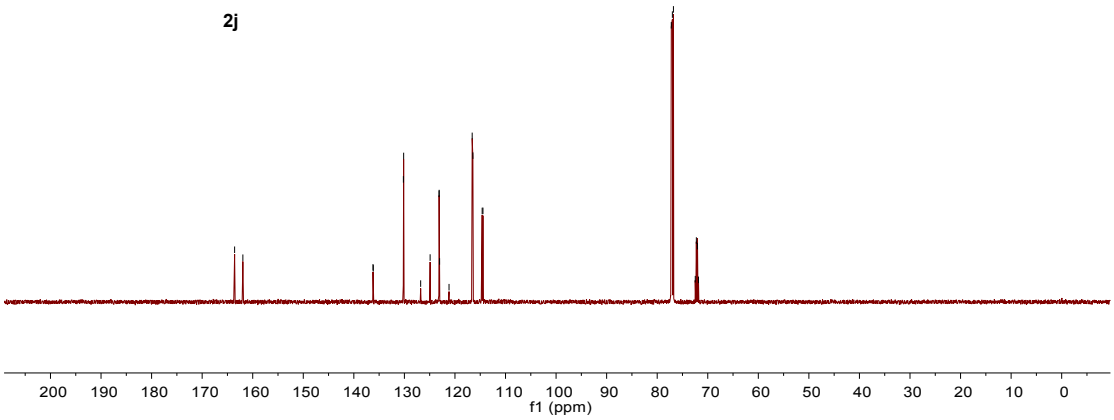
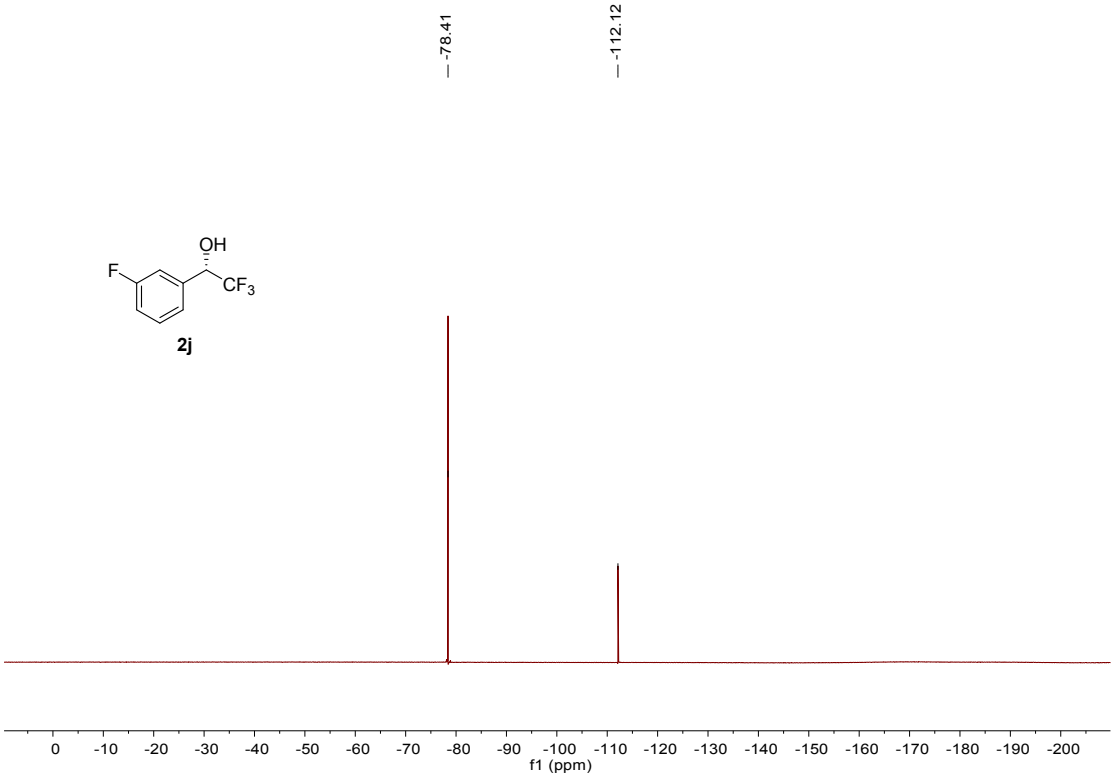
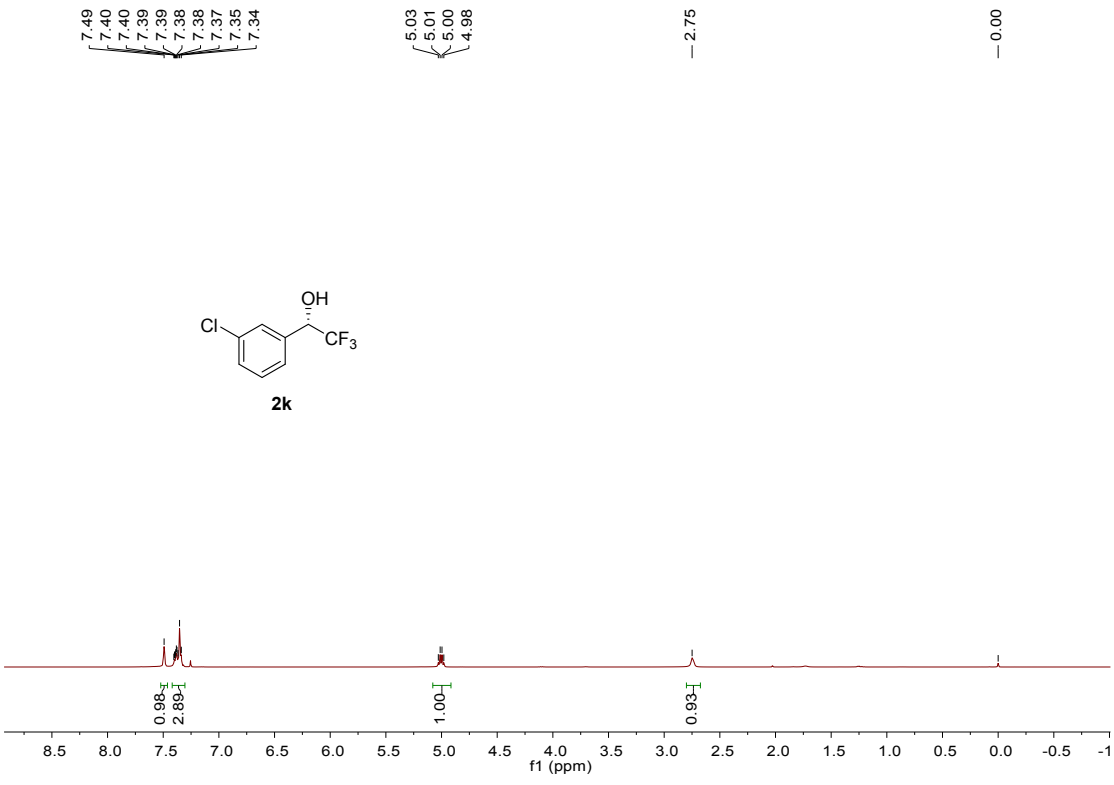
77.21
77.00
76.79
72.47
72.26
72.04
71.83

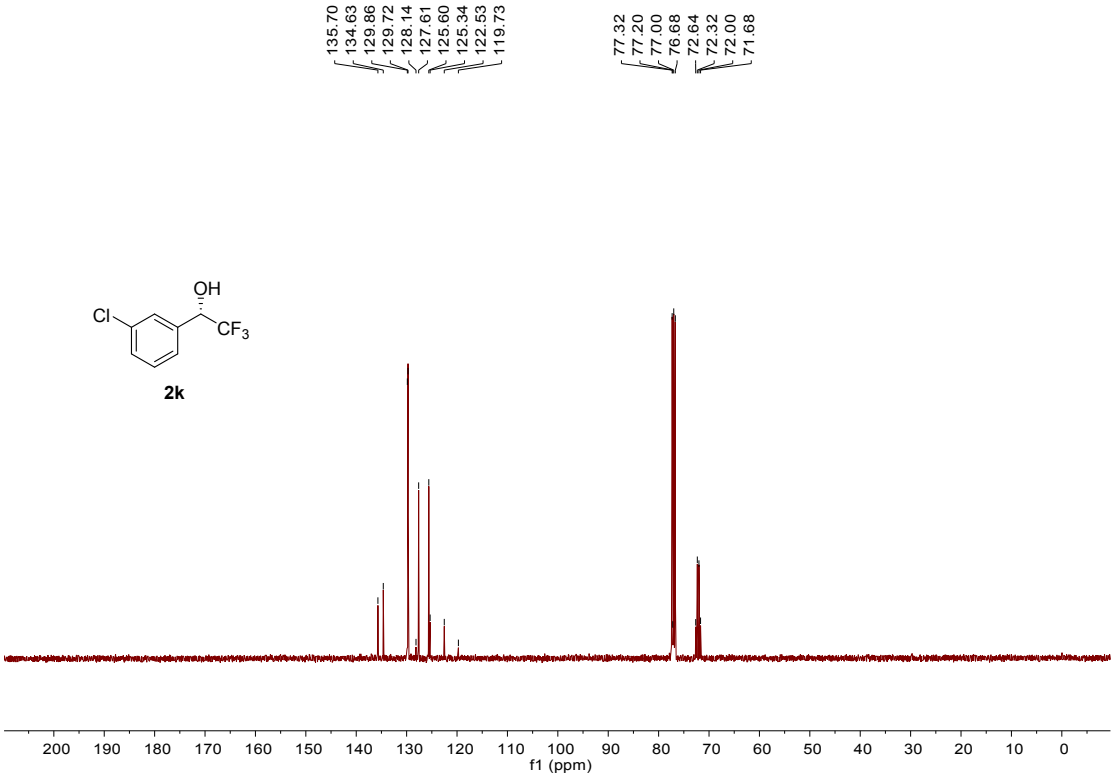

OH
F
CF3

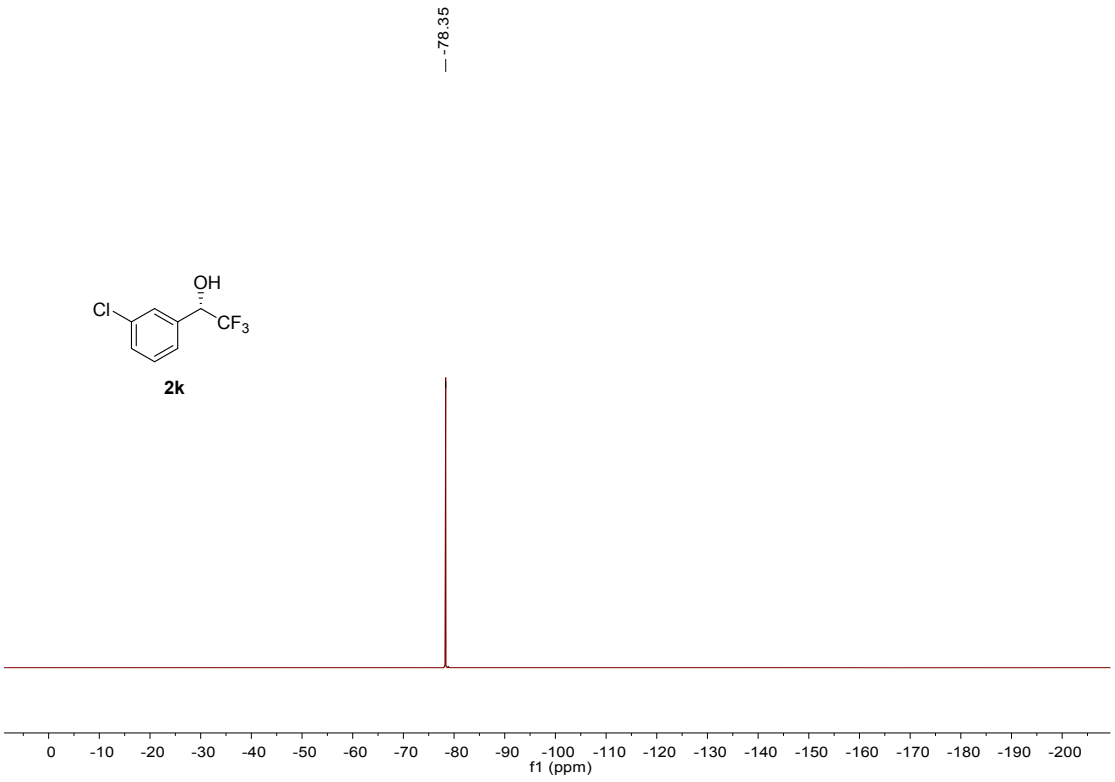
2j


200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

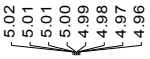

-78.41
-112.12
OH
F
CF3
2j
0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200
f1 (ppm)


7.49
7.40
7.40
7.39
7.39
7.38
7.38
7.37
7.35
7.34
5.03
5.01
5.00
4.98
2.75
0.00
OH
Cl
CF3
2k
0.98
2.89
1.00
0.93
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1
f1 (ppm)

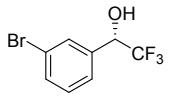

135.70
134.63
129.86
129.72
128.14
127.61
125.60
125.34
122.53
119.73
77.32
77.20
77.00
76.68
72.64
72.32
72.00
71.68
OH
Cl
CF3
2k
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


-78.35
OH
Cl
CF3
2k
0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200
f1 (ppm)

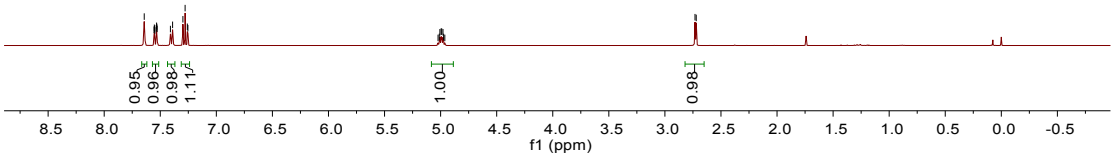

7.64
7.56
7.55
7.55
7.55
7.54
7.53
7.53
7.53
7.41
7.39
7.30
7.28
7.26
7.25

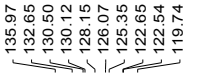

5.02
5.01
5.01
5.00
4.99
4.98
4.97
4.96


2.73
2.72

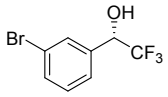

OH
Br
CF3

2l

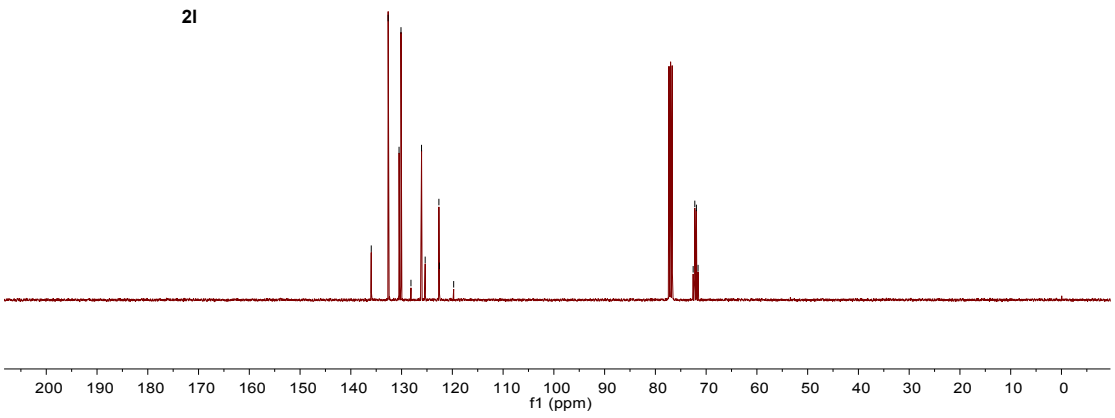

0.95
0.96
0.98
1.11
1.00
0.98
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

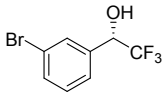

135.97
132.65
130.50
130.12
128.15
126.07
125.35
122.65
122.54
119.74


72.56
72.23
71.92
71.59


OH
Br
CF3

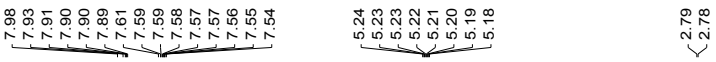
2l

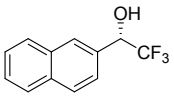

200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


OH
Br
CF3

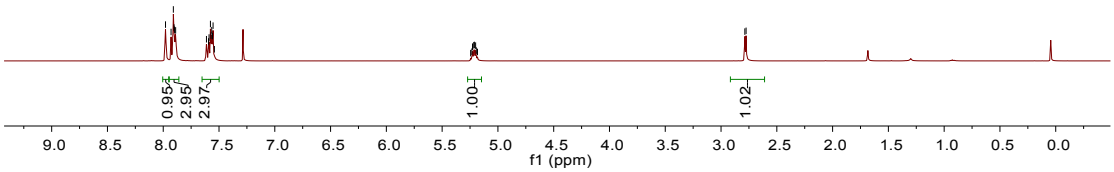
2l

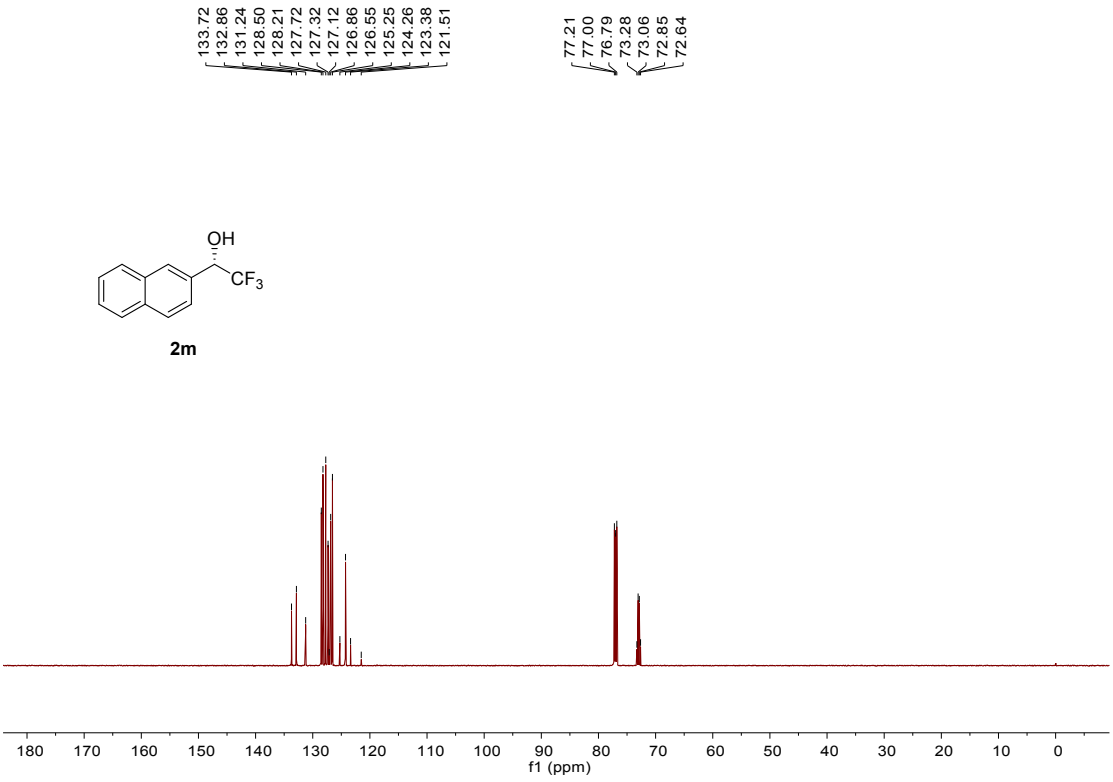
-78.33
0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200
f1 (ppm)


7.98
7.93
7.91
7.90
7.90
7.89
7.61
7.59
7.59
7.58
7.57
7.57
7.56
7.55
7.54
5.24
5.23
5.23
5.22
5.21
5.20
5.19
5.18
2.79
2.78

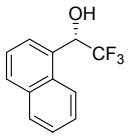

OH
CF3

2m

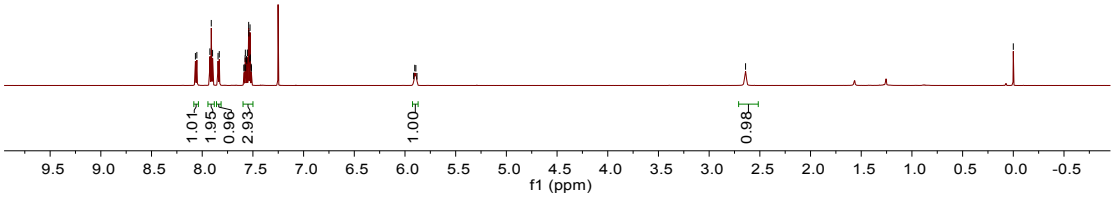

0.95
2.95
2.97
1.00
1.02
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

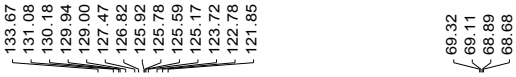

133.72
132.86
131.24
128.50
128.21
127.72
127.32
127.12
126.86
126.55
125.25
124.26
123.38
121.51
77.21
77.00
76.79
73.28
73.06
72.85
72.64
OH
CF3
2m
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)
-78.00
OH
CF3
2m
0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200
f1 (ppm)


8.07
8.05
7.92
7.91
7.90
7.84
7.83
7.59
7.58
7.57
7.57
7.56
7.56
7.55
7.54
7.54
7.53
7.53
7.53
5.92
5.90
5.89
5.88
2.64
0.00

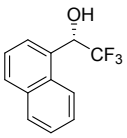

OH
CF3

2n

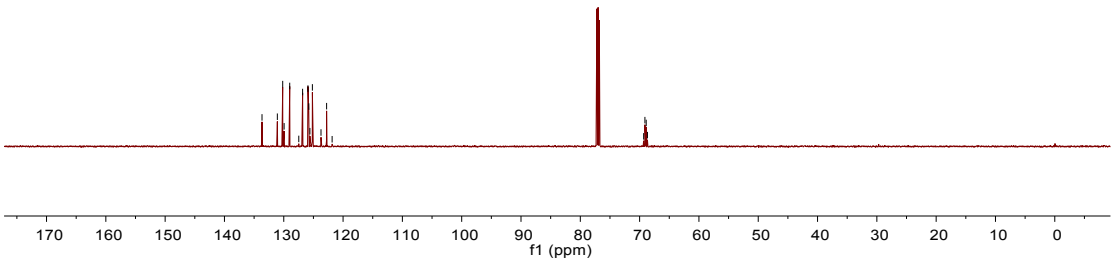

1.01
1.95
0.96
2.93
1.00
0.98
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

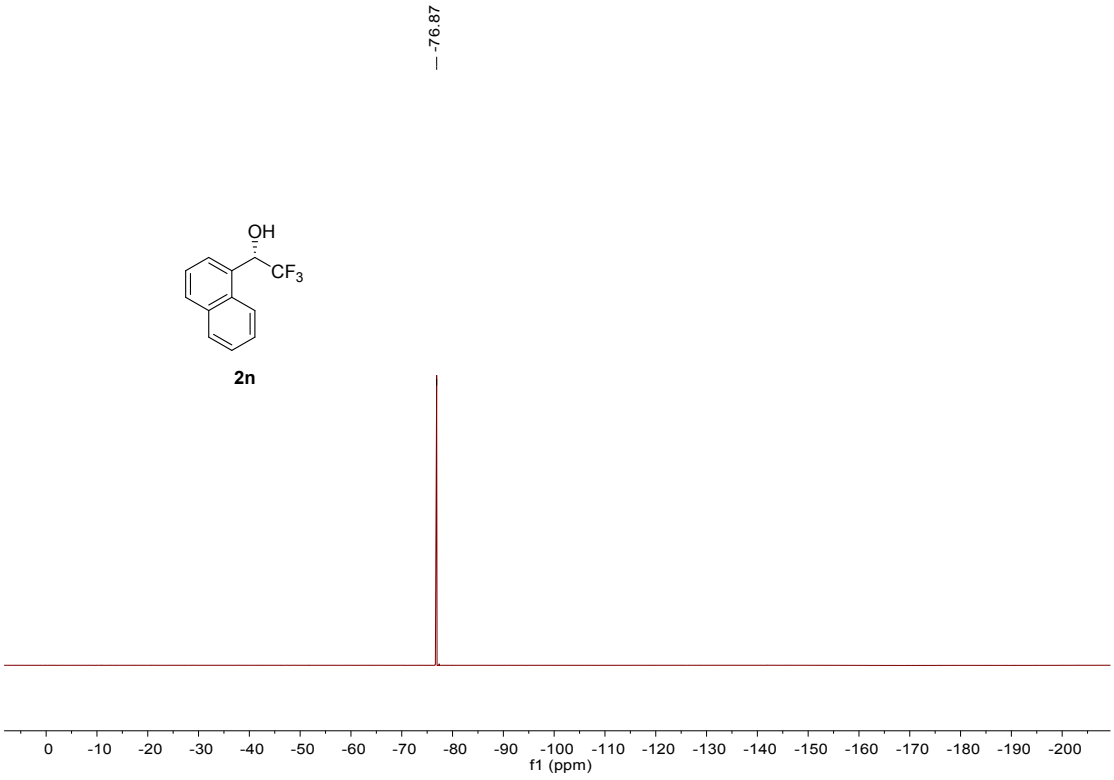

133.67
131.08
130.18
129.94
129.00
127.47
126.82
125.92
125.78
125.59
125.17
123.72
122.78
121.85

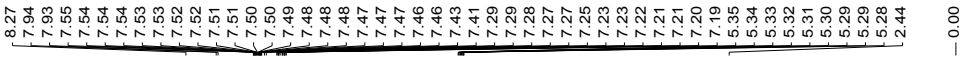
69.32
69.11
68.89
68.68

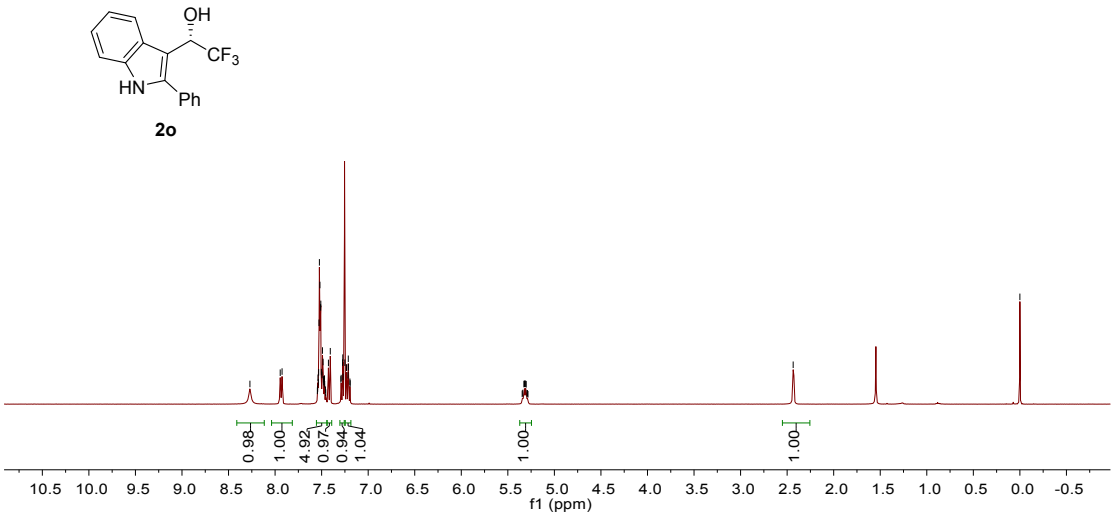

OH
CF3

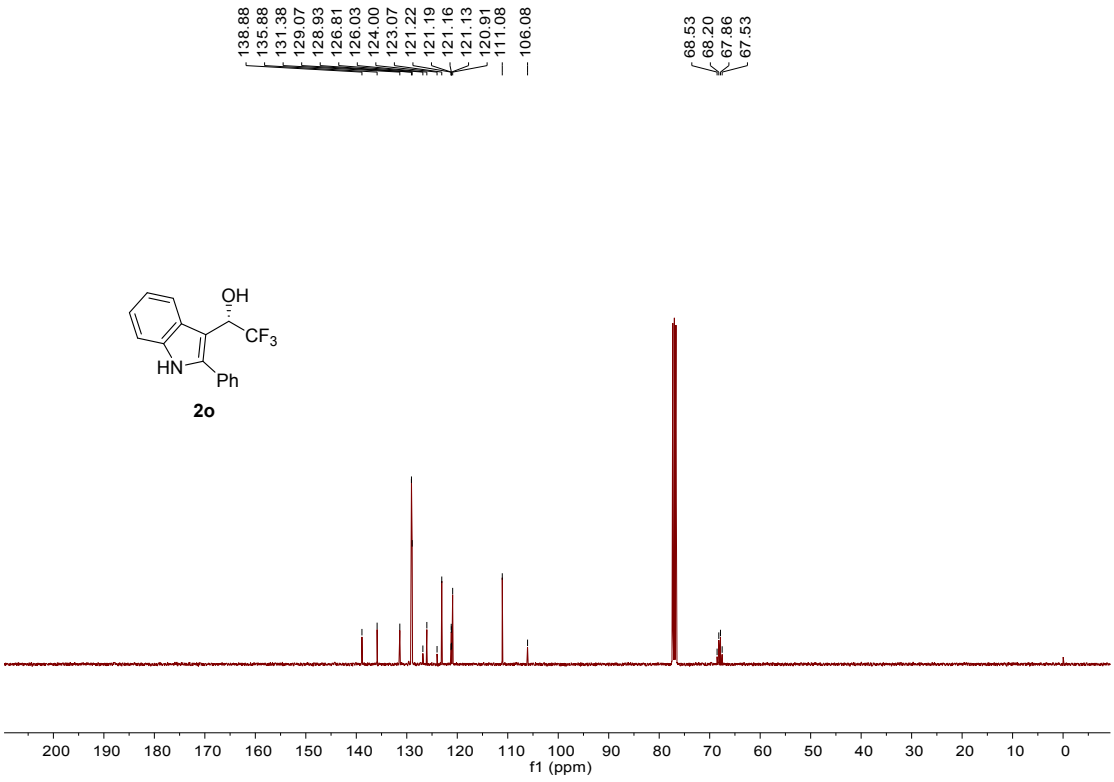
2n

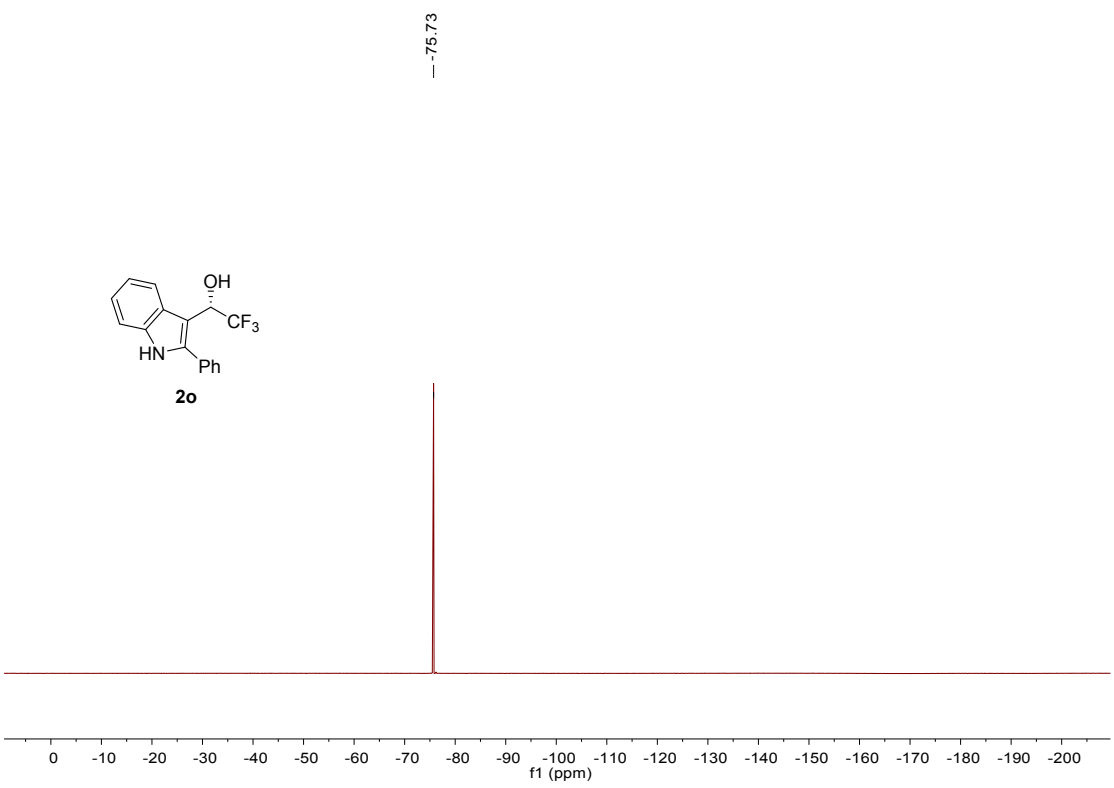

170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

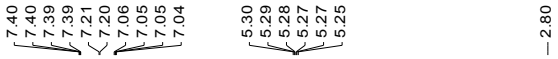

-76.87
OH
CF3
2n
0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200
f1 (ppm)

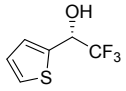

8.27 7.94 7.93 7.55 7.54 7.54 7.54 7.53 7.53 7.52 7.52 7.51 7.51 7.50 7.50 7.49 7.48 7.48 7.48 7.47 7.47 7.47 7.46 7.46 7.43 7.41 7.29 7.29 7.28 7.27 7.27 7.25 7.23 7.23 7.22 7.21 7.21 7.20 7.19 5.35 5.34 5.33 5.32 5.31 5.30 5.29 5.29 5.28 2.44
0.00


OH
CF3
HN
Ph
2o
0.98 1.00 4.92 0.97 0.94 1.04 1.00 1.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

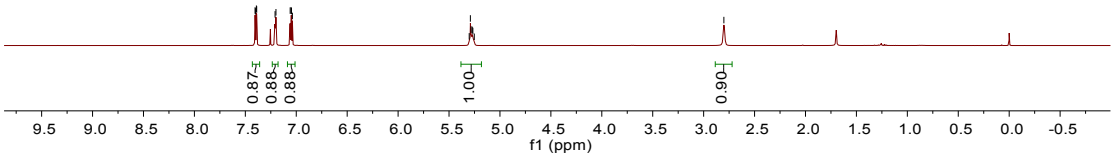

138.88
135.88
131.38
129.07
128.93
126.81
126.03
124.00
123.07
121.22
121.19
121.16
121.13
120.91
111.08
106.08
68.53
68.20
67.86
67.53
OH
CF3
HN
Ph
2o
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


-75.73
OH
CF3
HN
Ph
2o
0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200
f1 (ppm)

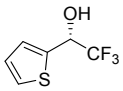

7.40
7.40
7.39
7.39
7.21
7.20
7.06
7.05
7.05
7.04
5.30
5.29
5.28
5.27
5.27
5.25
2.80


OH
CF3
S

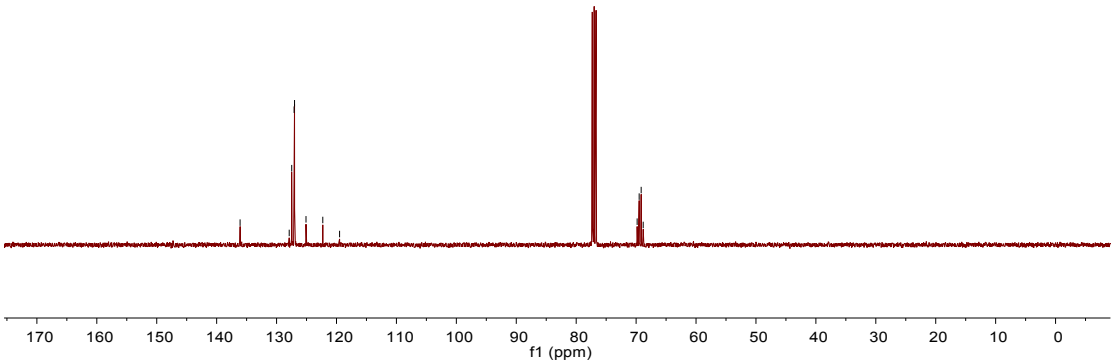
2p

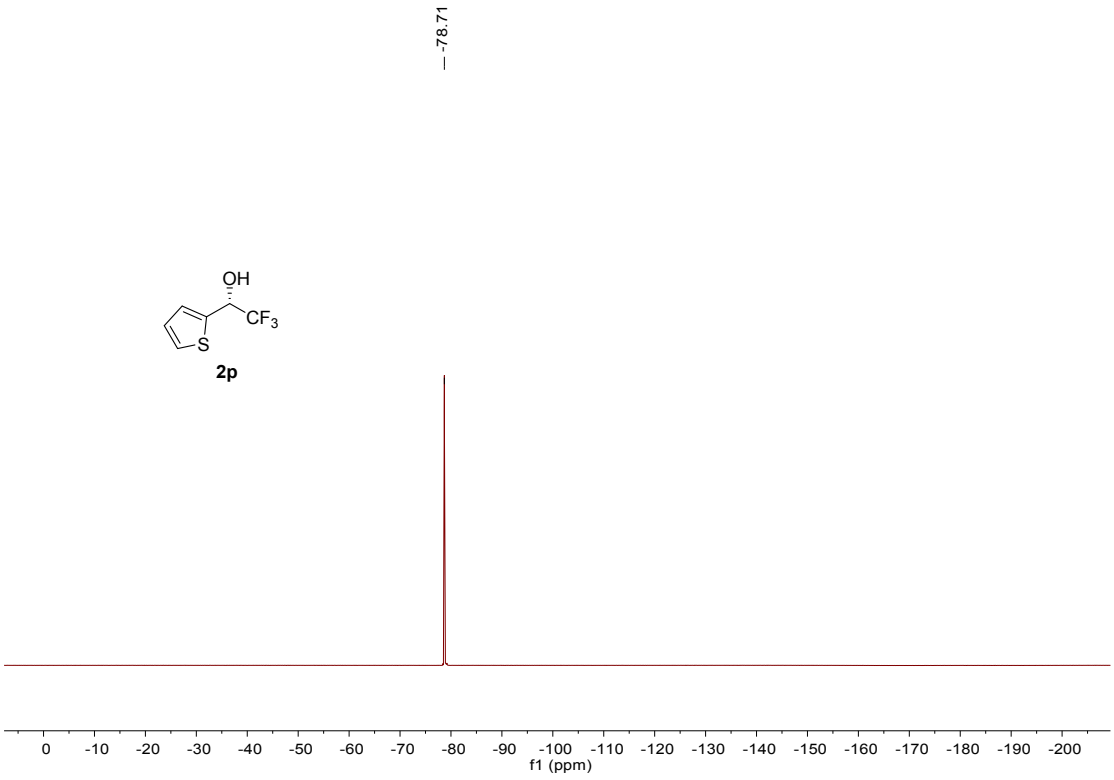

0.87
0.88
0.88
1.00
0.90
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

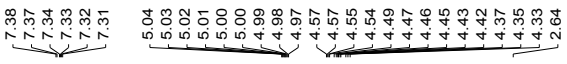

136.09
127.89
127.47
127.08
127.00
125.09
122.29
119.49
69.83
69.49
69.16
68.82

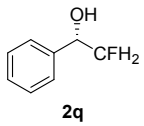

OH
CF3
S

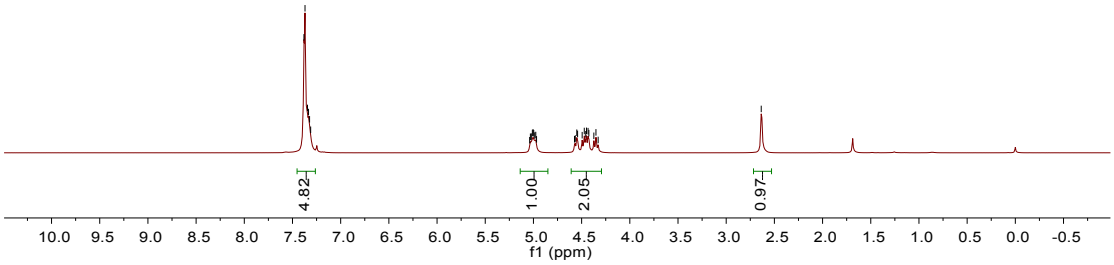
2p

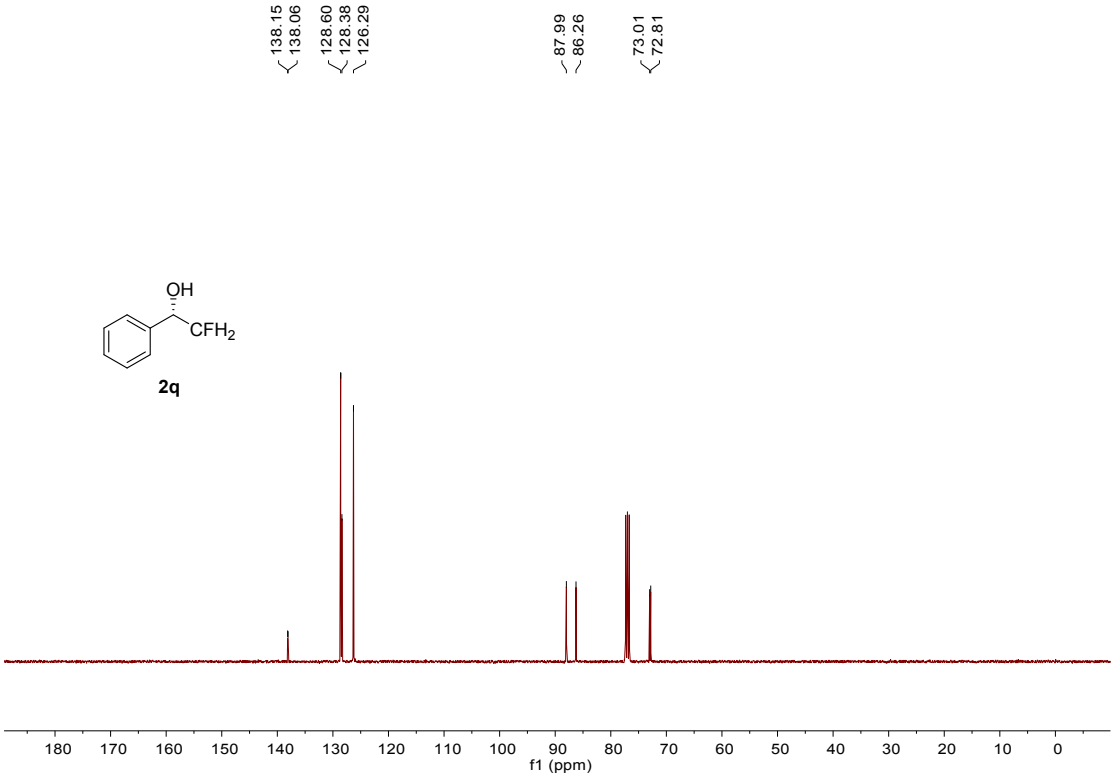

170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

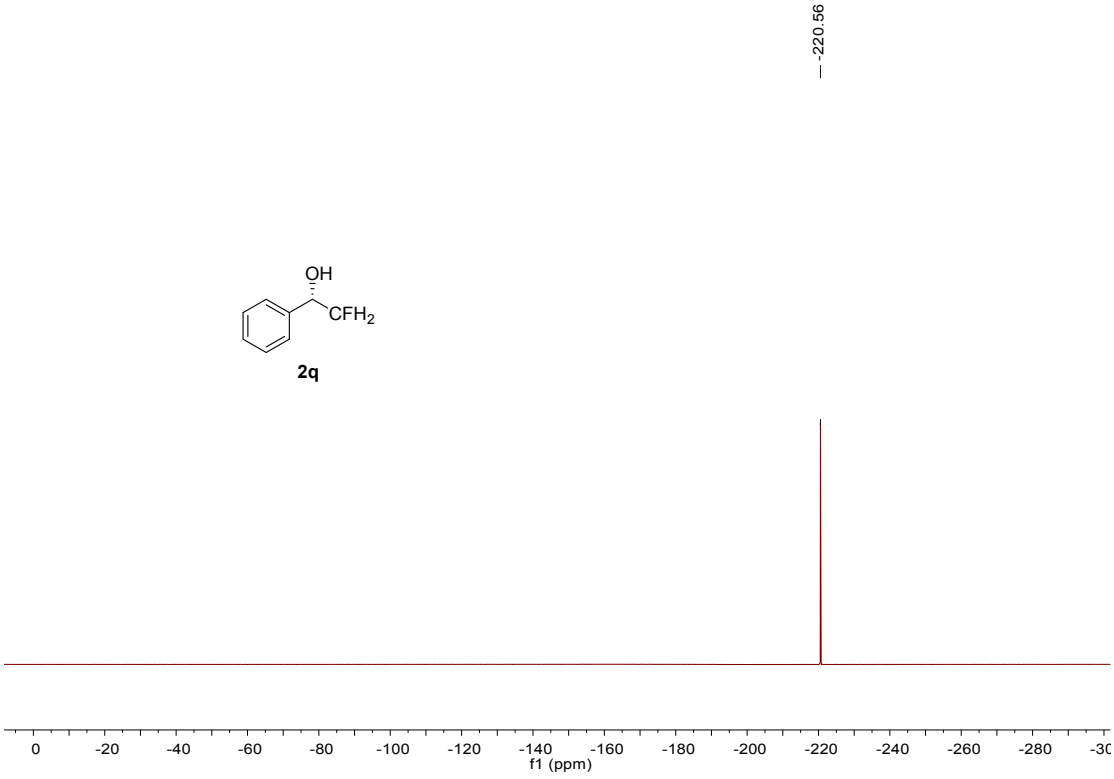

-78.71
OH
CF3
S
2p
0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200
f1 (ppm)

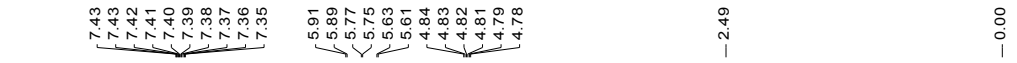

7.38 7.37 7.34 7.33 7.32 7.31
5.04 5.03 5.02 5.01 5.00 5.00 4.99 4.98 4.97 4.57 4.57 4.55 4.54 4.49 4.47 4.46 4.45 4.43 4.42 4.37 4.35 4.33 2.64

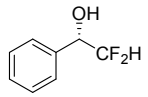

OH
CFH2
2q


4.82
1.00
2.05
0.97
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

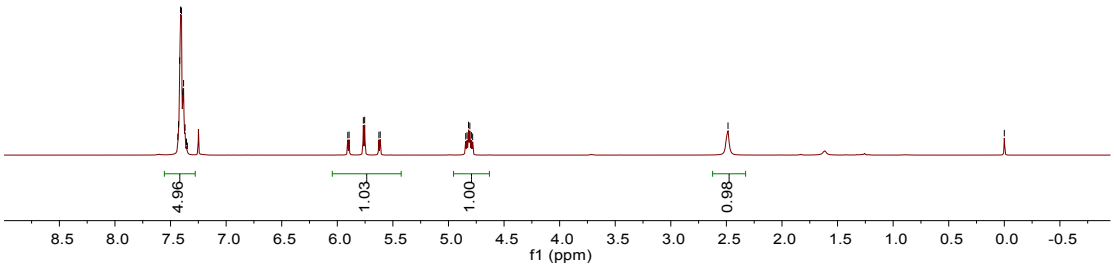

138.15
138.06
128.60
128.38
126.29
87.99
86.26
73.01
72.81
OH
CFH2
2q
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

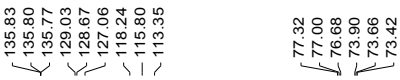

-220.56
OH
CFH2
2q
0 -20 -40 -60 -80 -100 -120 -140 -160 -180 -200 -220 -240 -260 -280 -30
f1 (ppm)


7.43
7.43
7.42
7.41
7.40
7.39
7.38
7.37
7.36
7.35
5.91
5.89
5.77
5.75
5.63
5.61
4.84
4.83
4.82
4.81
4.79
4.78
2.49
0.00

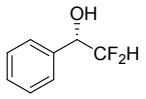

OH
CF2H

2r

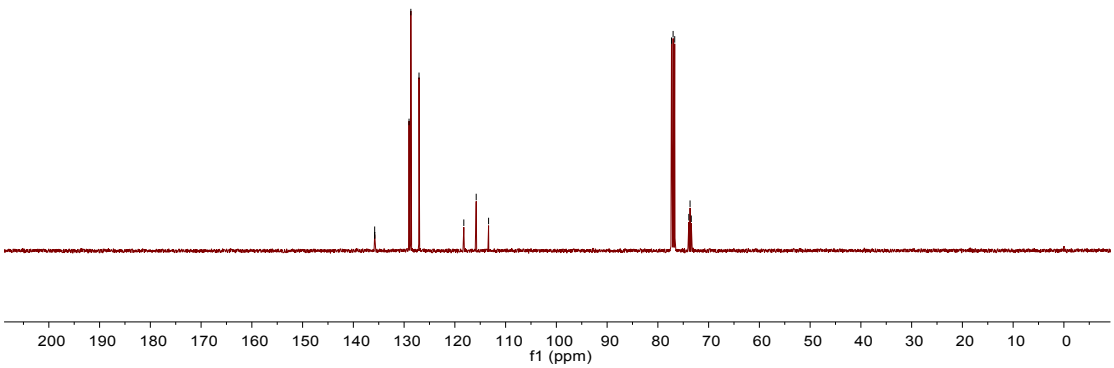

4.96
1.03
1.00
0.98
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

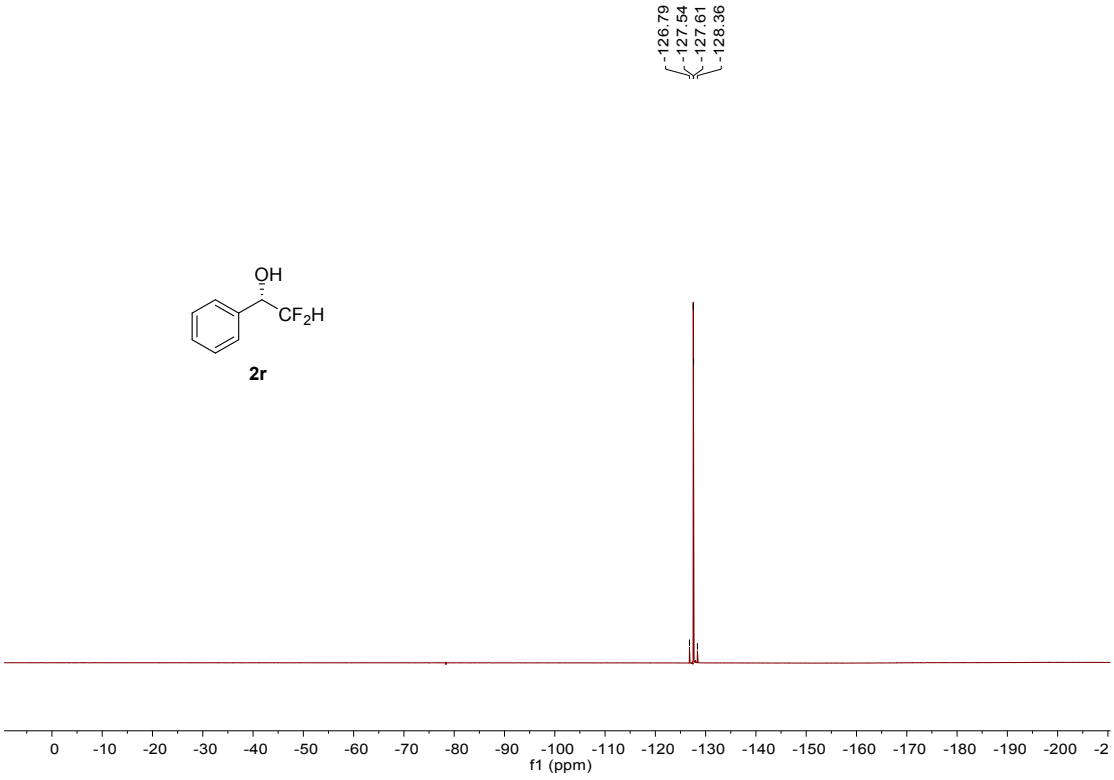

135.83
135.80
135.77
129.03
128.67
127.06
118.24
115.80
113.35

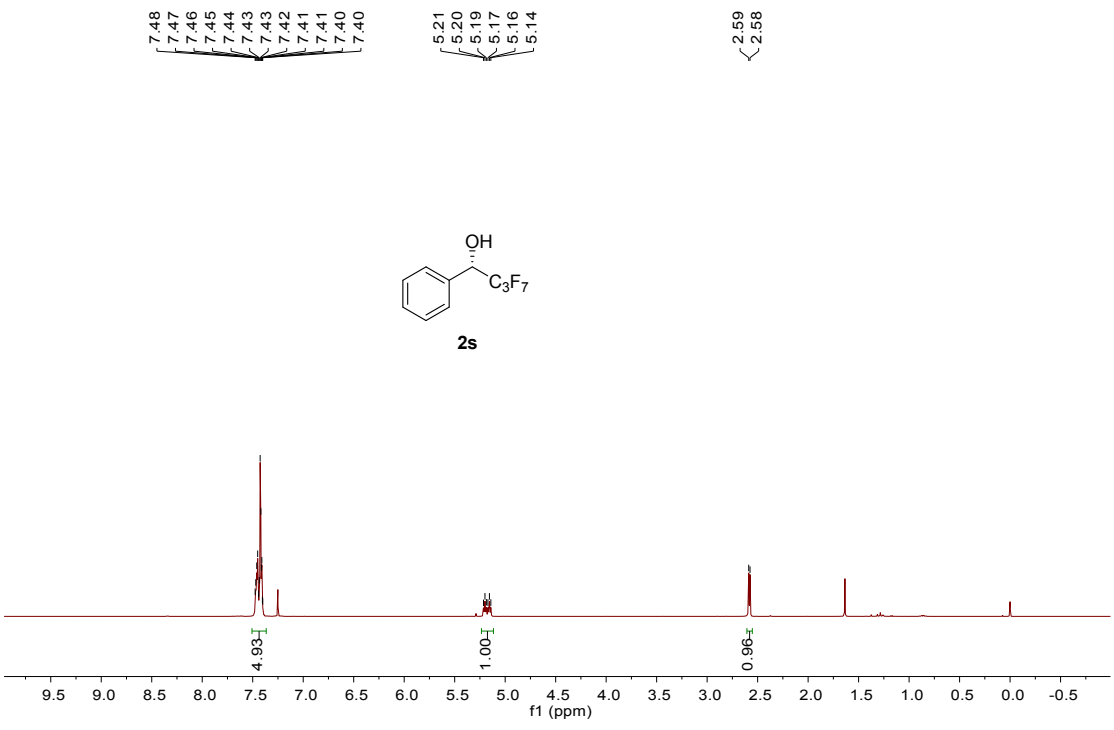
77.32
77.00
76.68
73.90
73.66
73.42

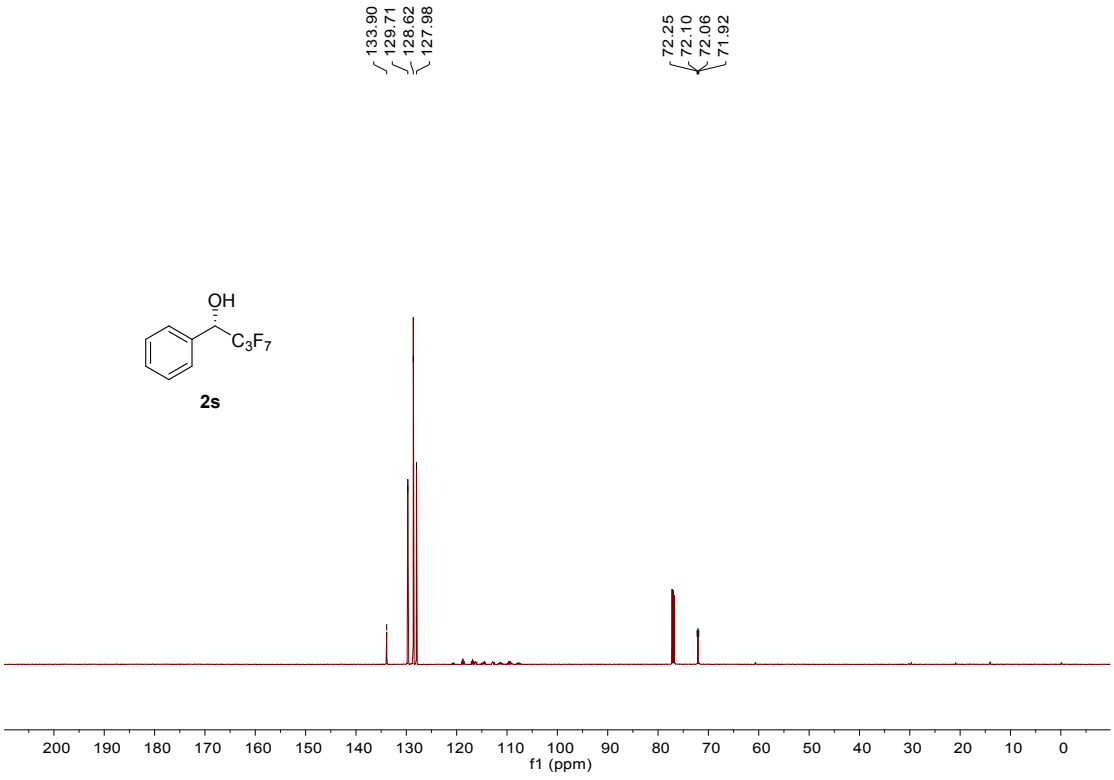

OH
CF2H

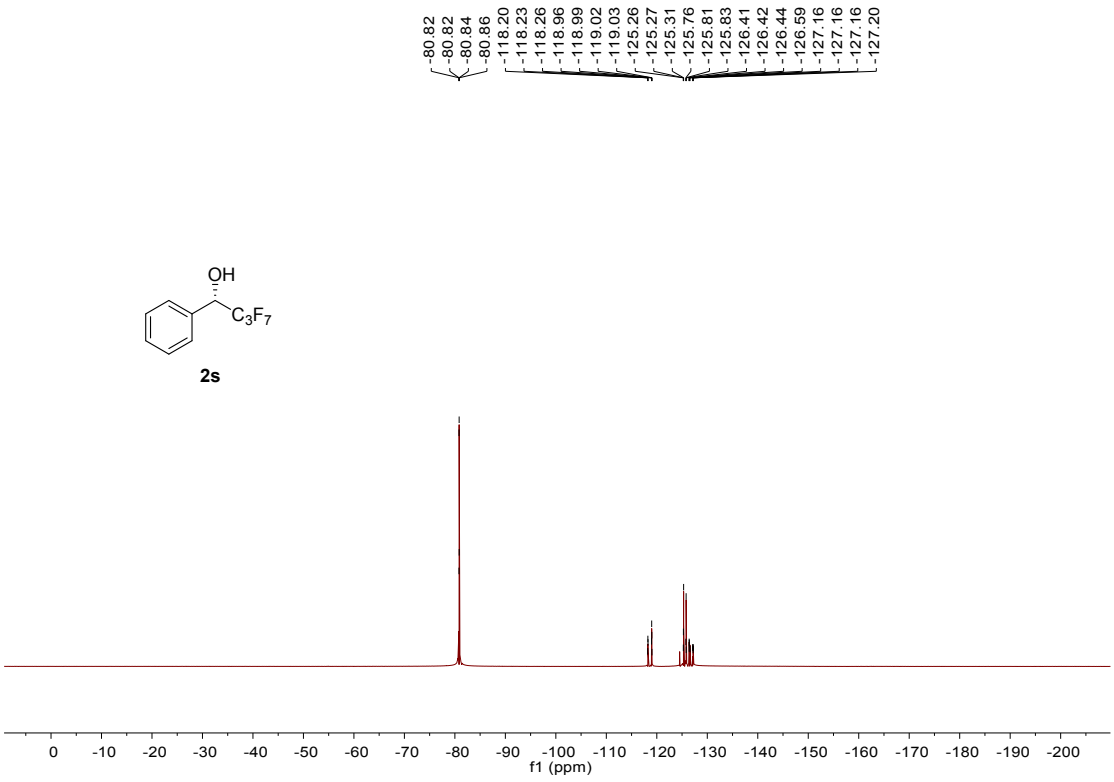
2r

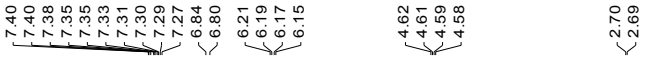

200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

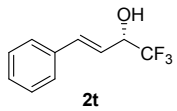

-126.79
-127.54
-127.61
-128.36
OH
CF2H
2r
0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -2
f1 (ppm)


7.48
7.47
7.46
7.45
7.44
7.43
7.43
7.42
7.41
7.41
7.40
7.40
5.21
5.20
5.19
5.17
5.16
5.14
2.59
2.58
OH
C3F7
2s
4.93
1.00
0.96
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

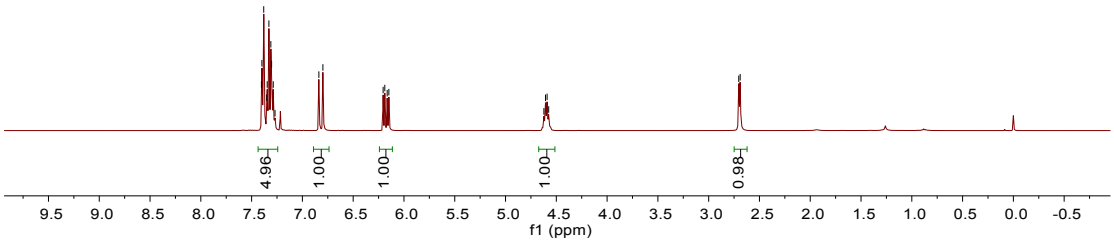

133.90
129.71
128.62
127.98
72.25
72.10
72.06
71.92
OH
C_3F_7
2s
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


-80.82
-80.82
-80.84
-80.86
-118.20
-118.23
-118.26
-118.96
-118.99
-119.02
-119.03
-125.26
-125.27
-125.31
-125.76
-125.81
-125.83
-126.41
-126.42
-126.44
-126.59
-127.16
-127.16
-127.16
-127.20
OH
C_3F_7
2s
0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200
f1 (ppm)

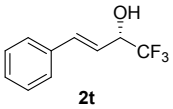

7.40
7.40
7.38
7.35
7.35
7.33
7.31
7.30
7.29
7.27
6.84
6.80
6.21
6.19
6.17
6.15
4.62
4.61
4.59
4.58
2.70
2.69


OH
CF3

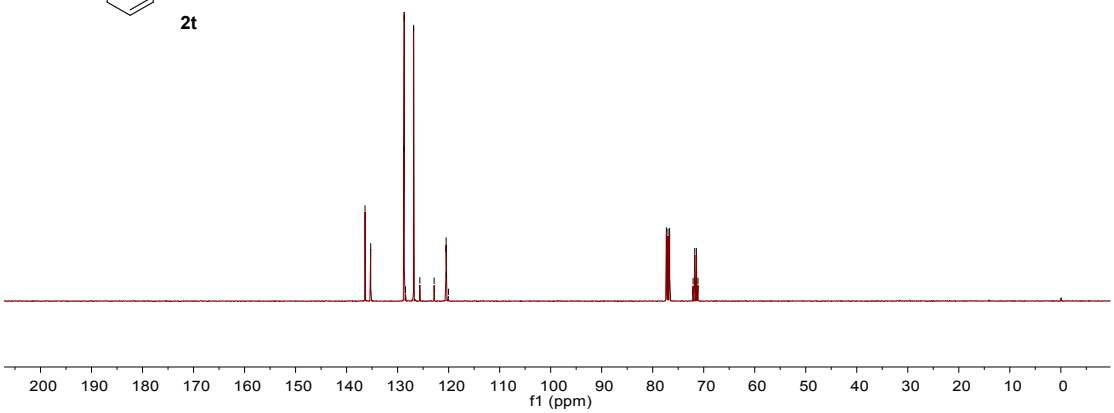
2t

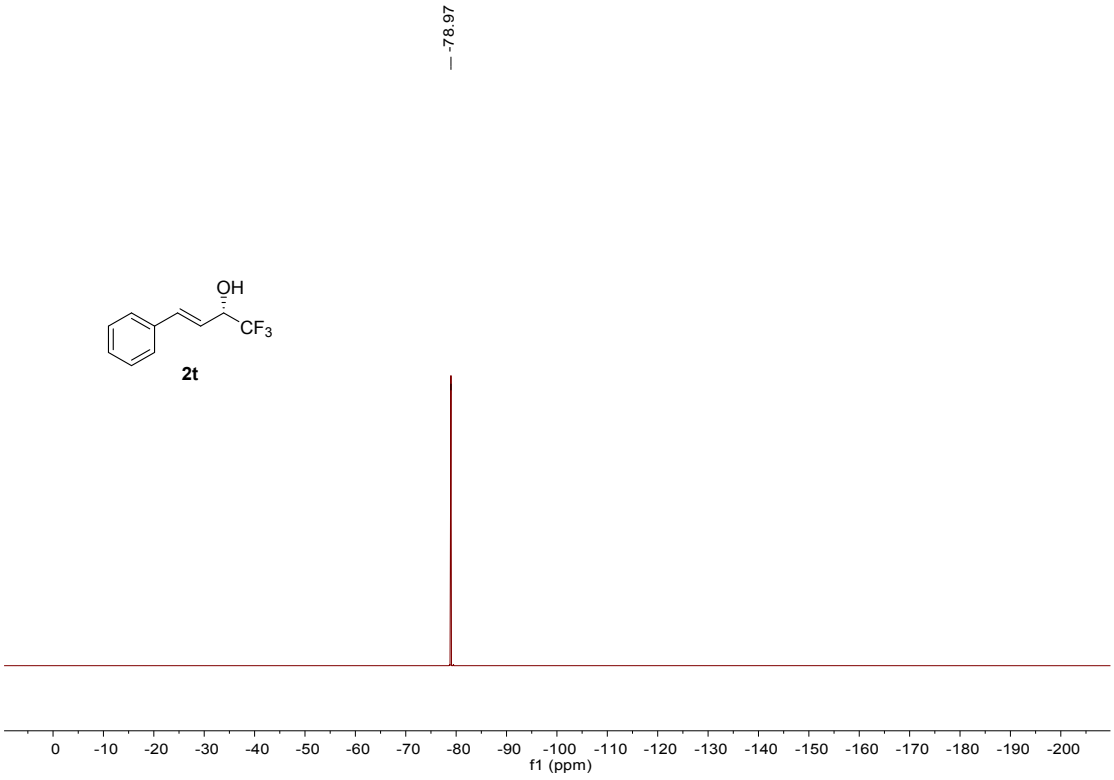

4.96
1.00
1.00
1.00
0.98
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

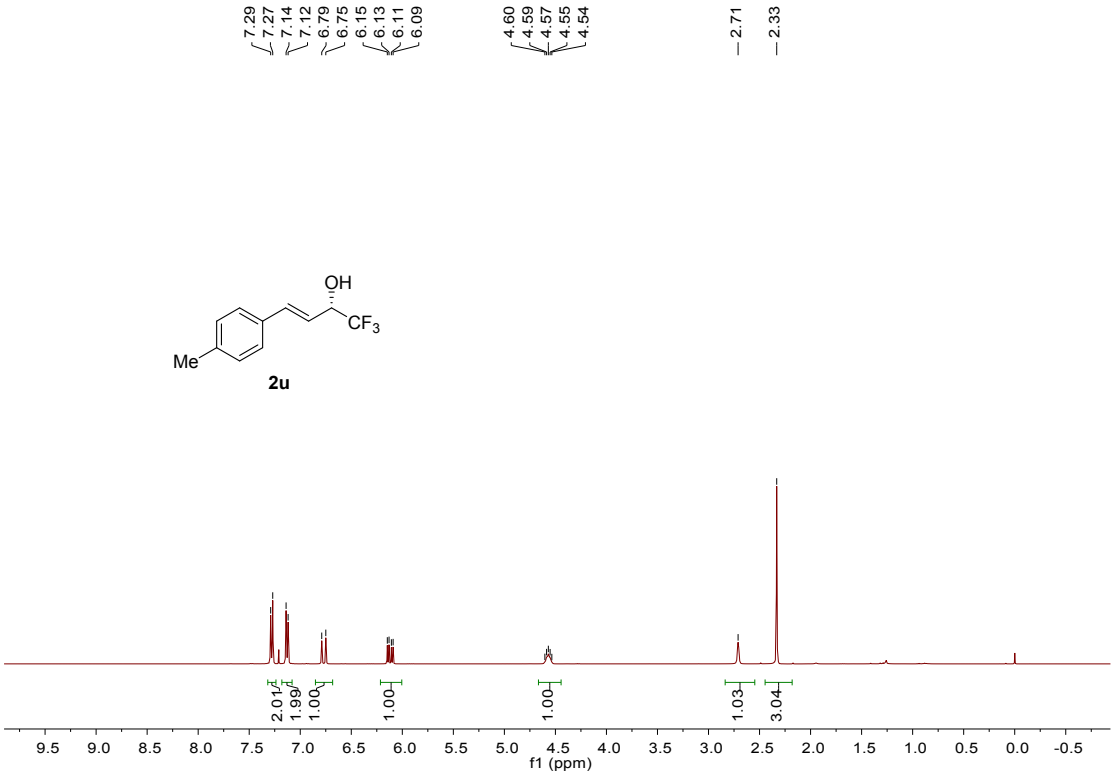

136.38
135.28
128.74
128.71
128.45
126.86
125.64
122.84
120.51
120.49
120.47
120.04
77.32
77.00
76.68
72.08
71.76
71.44
71.12

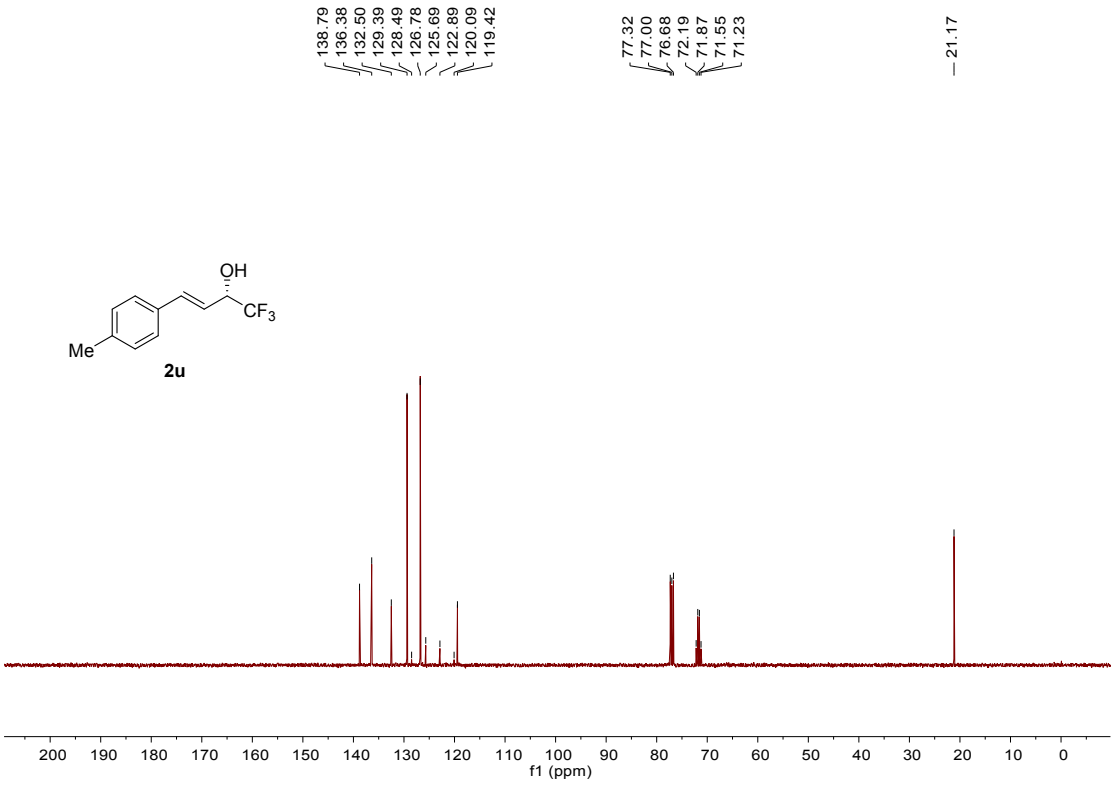

OH
CF3

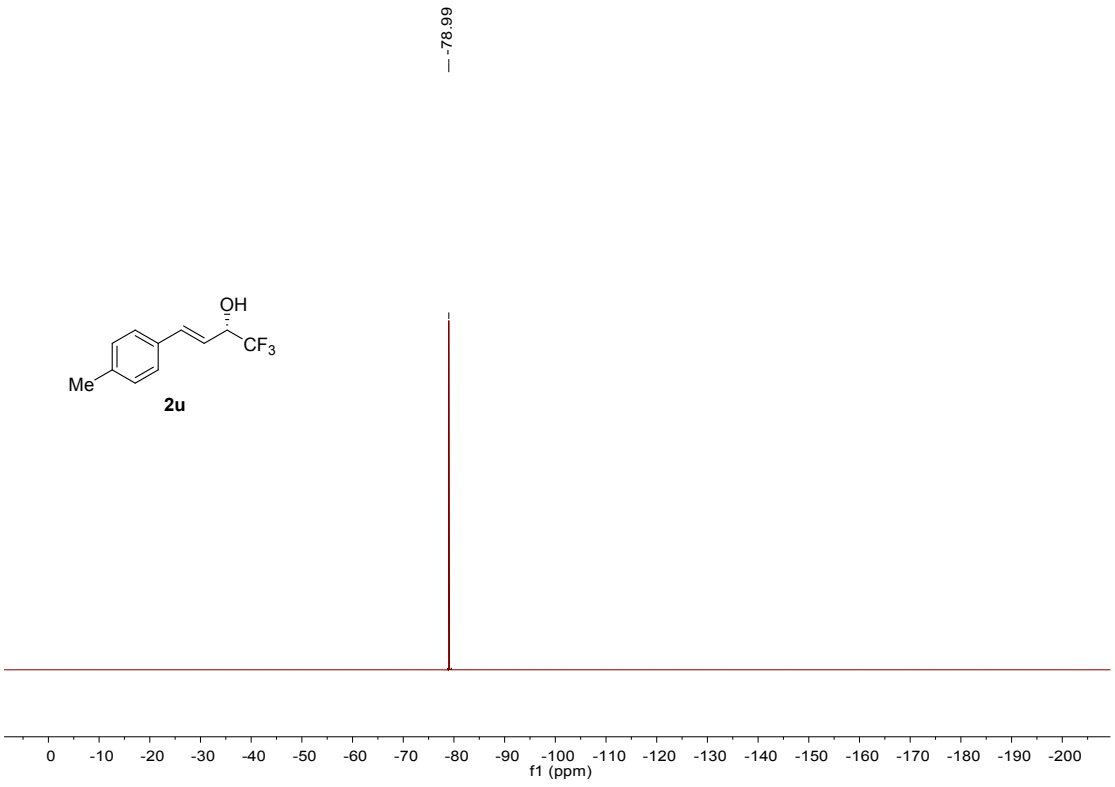
2t

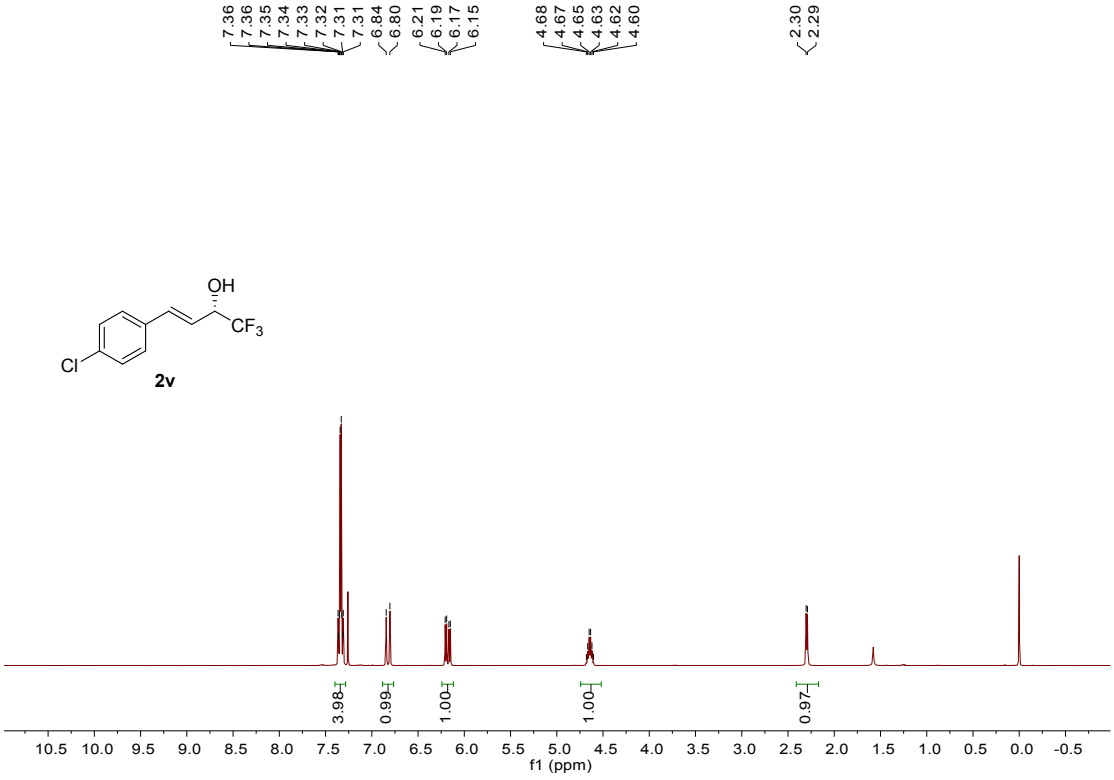

200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

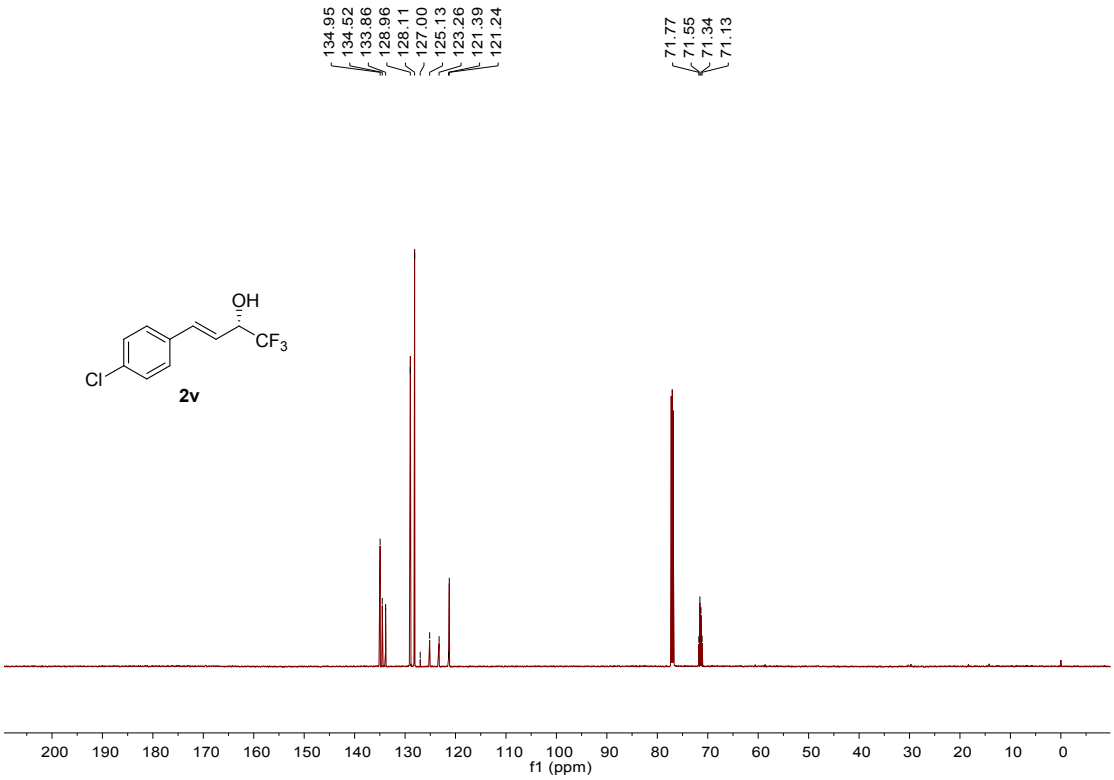

-78.97
OH
CF3
2t
0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200
f1 (ppm)

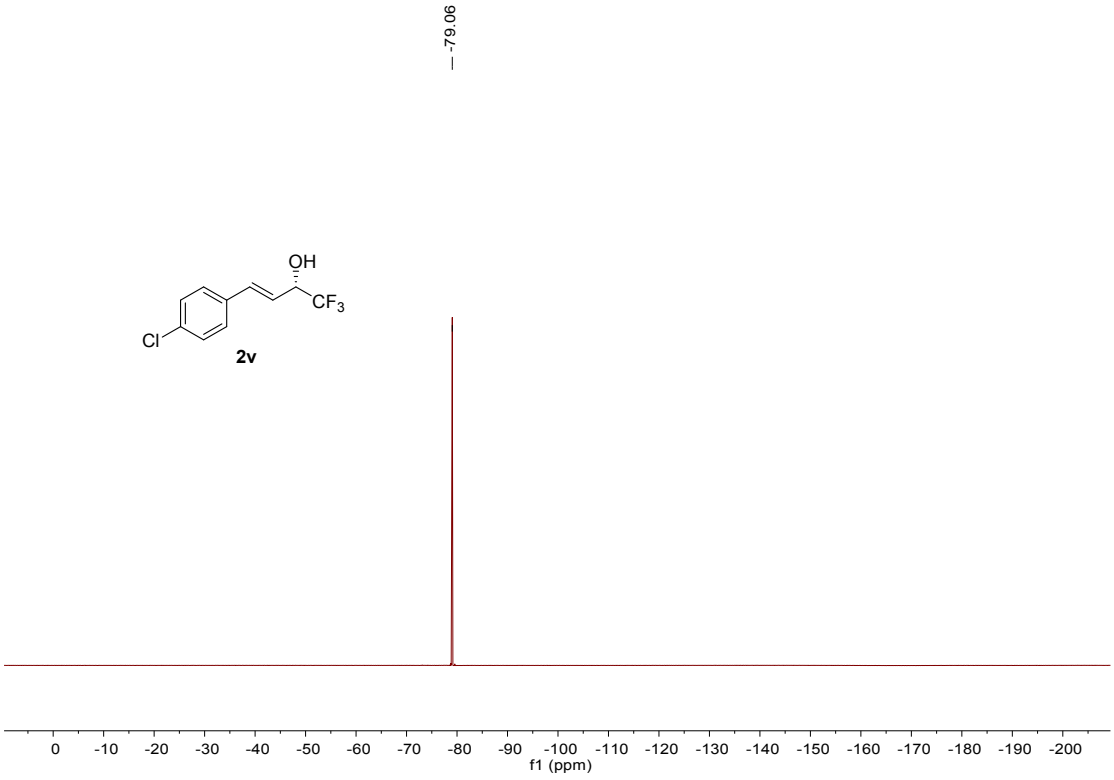

7.29
7.27
7.14
7.12
6.79
6.75
6.15
6.13
6.11
6.09
4.60
4.59
4.57
4.55
4.54
2.71
2.33
OH
CF3
Me
2u
2.01
1.99
1.00
1.00
1.00
1.03
3.04
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

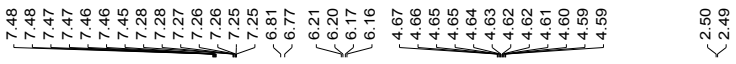

138.79
136.38
132.50
129.39
128.49
126.78
125.69
122.89
120.09
119.42
77.32
77.00
76.68
72.19
71.87
71.55
71.23
21.17
OH
CF3
Me
2u
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

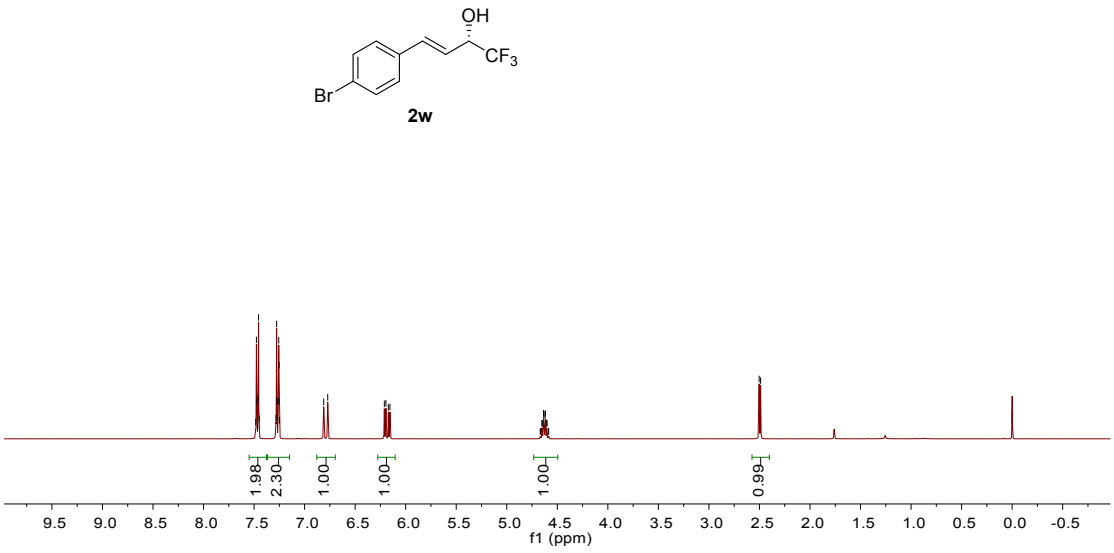

-78.99
OH
CF3
Me
2u
0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200
f1 (ppm)

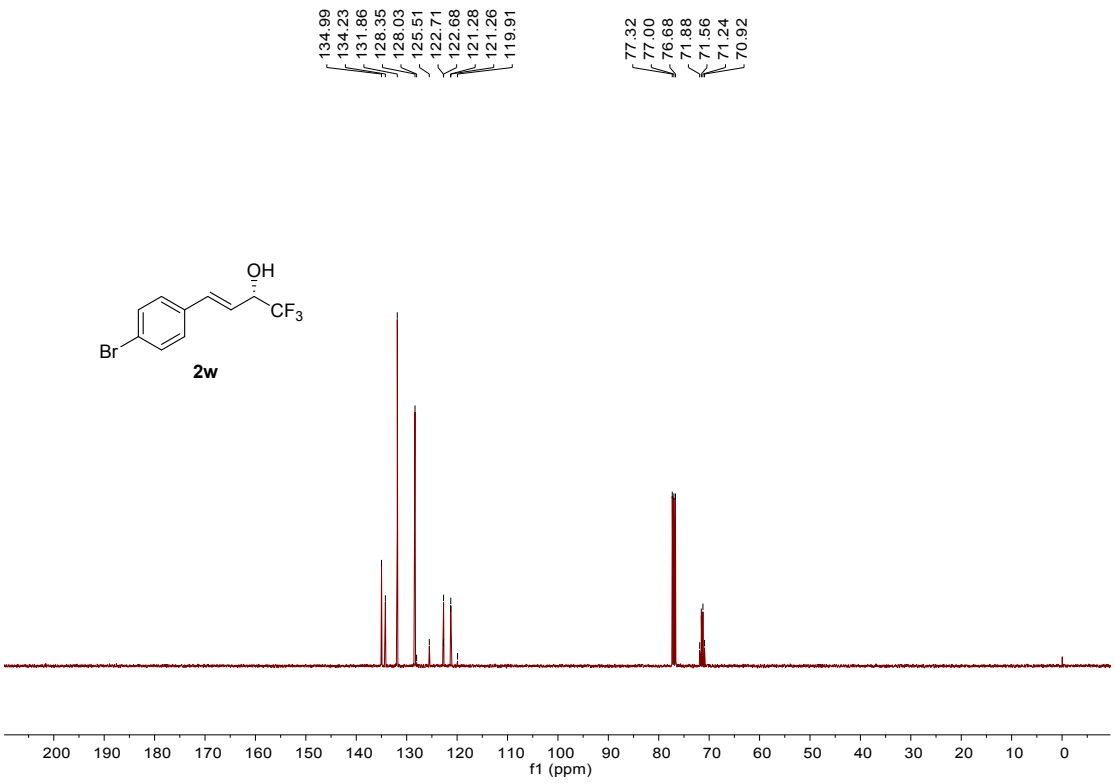

7.36
7.36
7.35
7.34
7.33
7.32
7.31
7.31
6.84
6.80
6.21
6.19
6.17
6.15
4.68
4.67
4.65
4.63
4.62
4.60
2.30
2.29
OH
CF3
Cl
2v
3.98
0.99
1.00
1.00
0.97
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

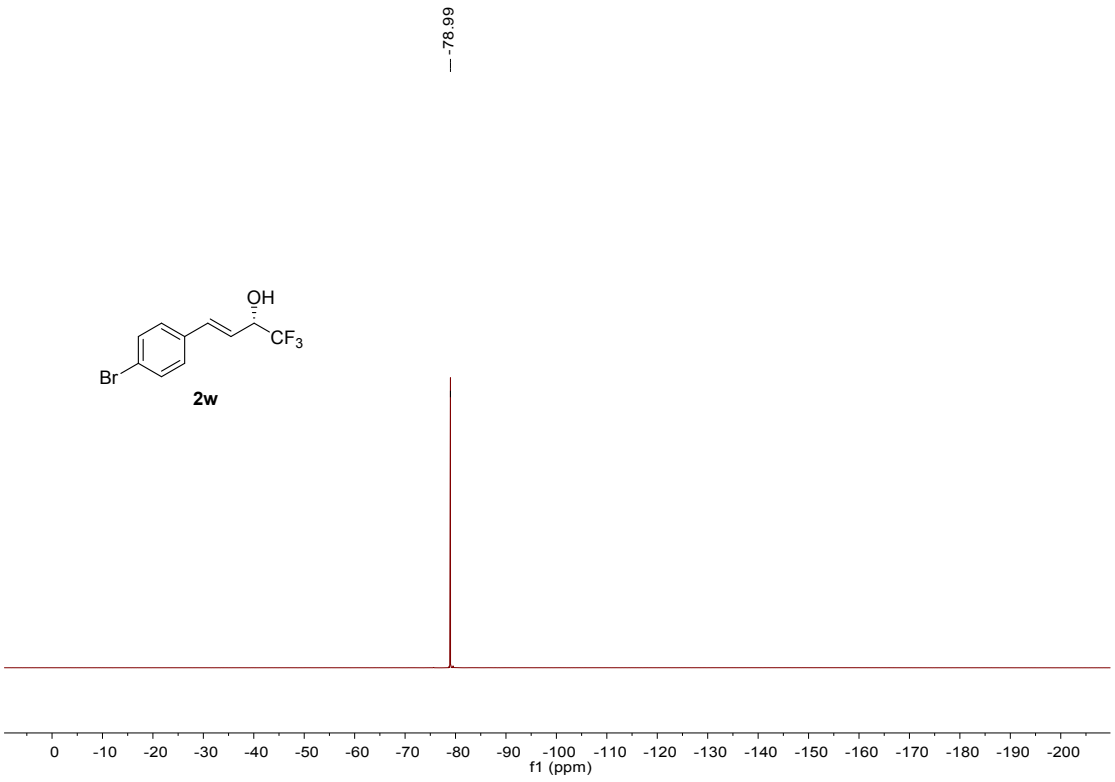

134.95
134.52
133.86
128.96
128.11
127.00
125.13
123.26
121.39
121.24
71.77
71.55
71.34
71.13
OH
CF3
Cl
2v
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

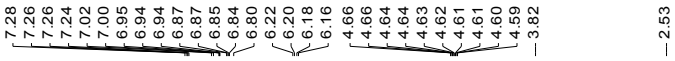

-79.06
OH
CF3
Cl
2v
0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200
f1 (ppm)

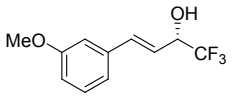

7.48 7.48 7.47 7.47 7.46 7.46 7.45 7.28 7.28 7.27 7.26 7.26 7.25 7.25
6.81 6.77
6.21 6.20 6.17 6.16
4.67 4.66 4.65 4.65 4.64 4.63 4.62 4.62 4.61 4.60 4.59 4.59
2.50 2.49


OH
CF3
Br
2w
1.98 2.30 1.00 1.00 1.00 0.99
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

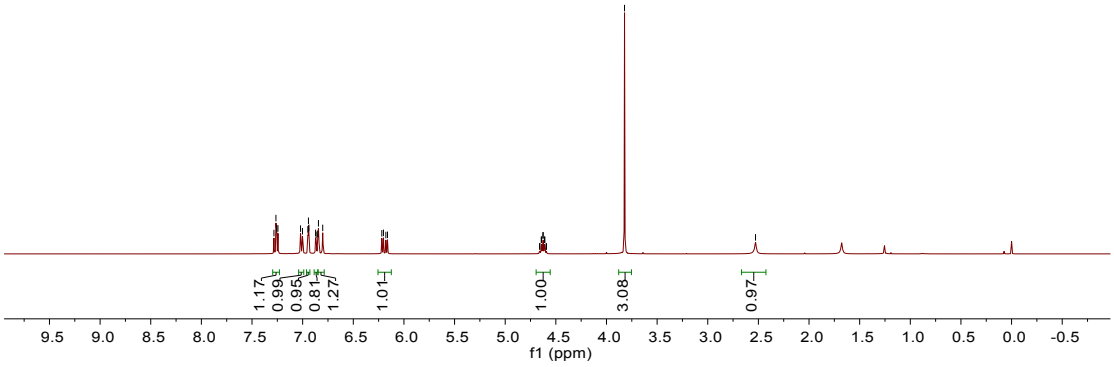

134.99
134.23
131.86
128.35
128.03
125.51
122.71
122.68
121.28
121.26
119.91
77.32
77.00
76.68
71.88
71.56
71.24
70.92
OH
CF3
Br
2w
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

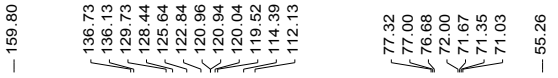

-78.99
OH
CF3
Br
2w
0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200
f1 (ppm)

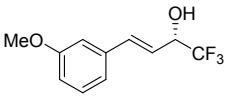

7.28
7.26
7.26
7.24
7.02
7.00
6.95
6.94
6.94
6.87
6.87
6.85
6.84
6.80
6.22
6.20
6.18
6.16
4.66
4.66
4.64
4.64
4.63
4.62
4.61
4.61
4.60
4.59
3.82
2.53


OH
MeO
CF3

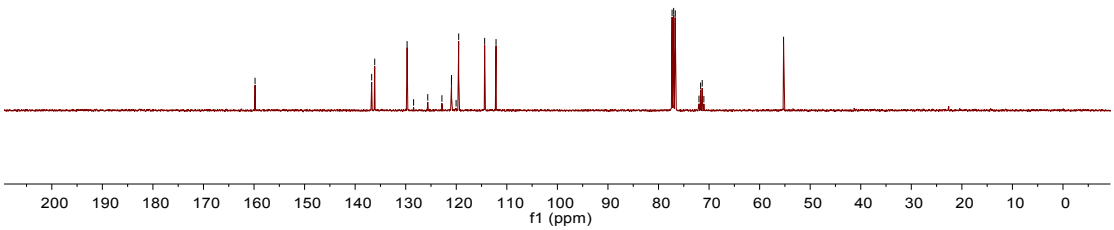
2x

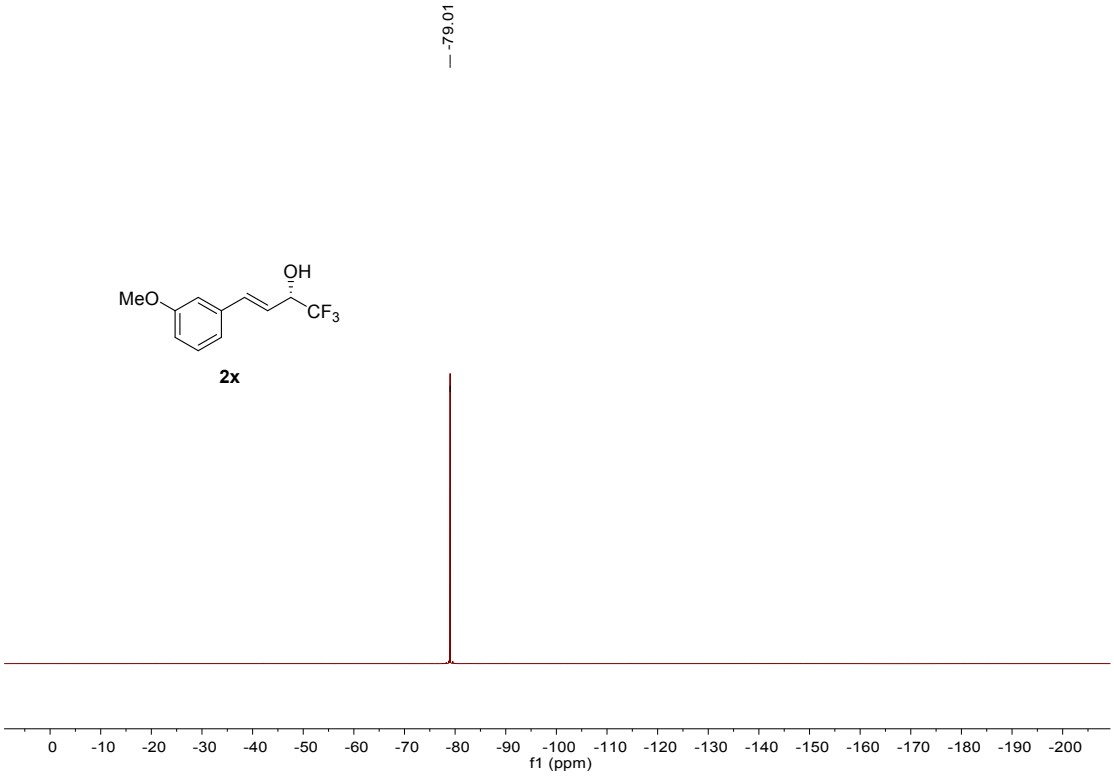

1.17
0.99
0.95
0.81
1.27
1.01
1.00
3.08
0.97
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

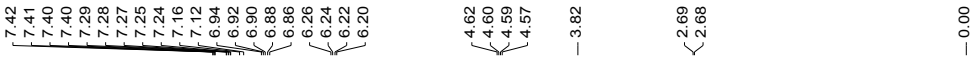

159.80
136.73
136.13
129.73
128.44
125.64
122.84
120.96
120.94
120.04
119.52
114.39
112.13
77.32
77.00
76.68
72.00
71.67
71.35
71.03
55.26

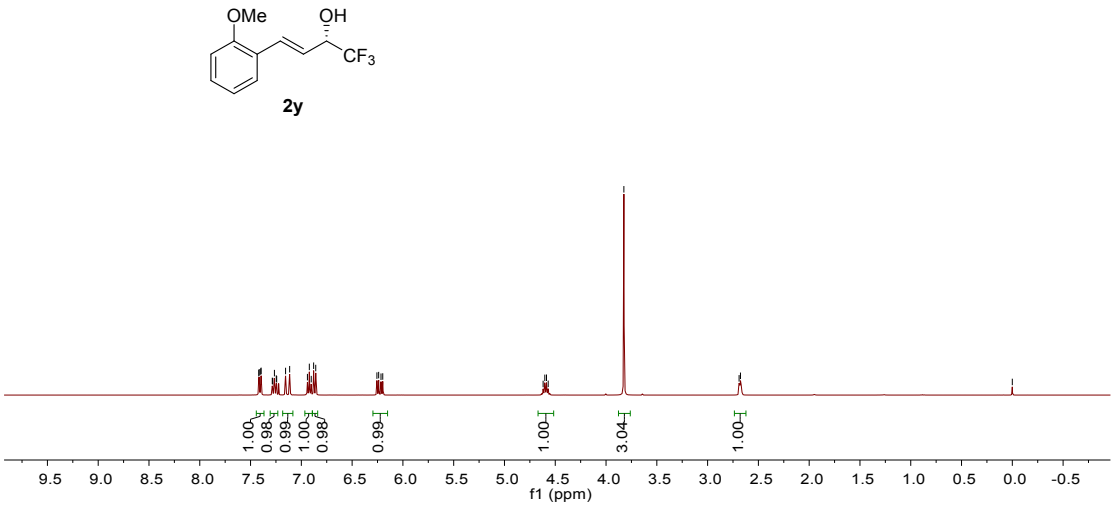

OH
MeO
CF3

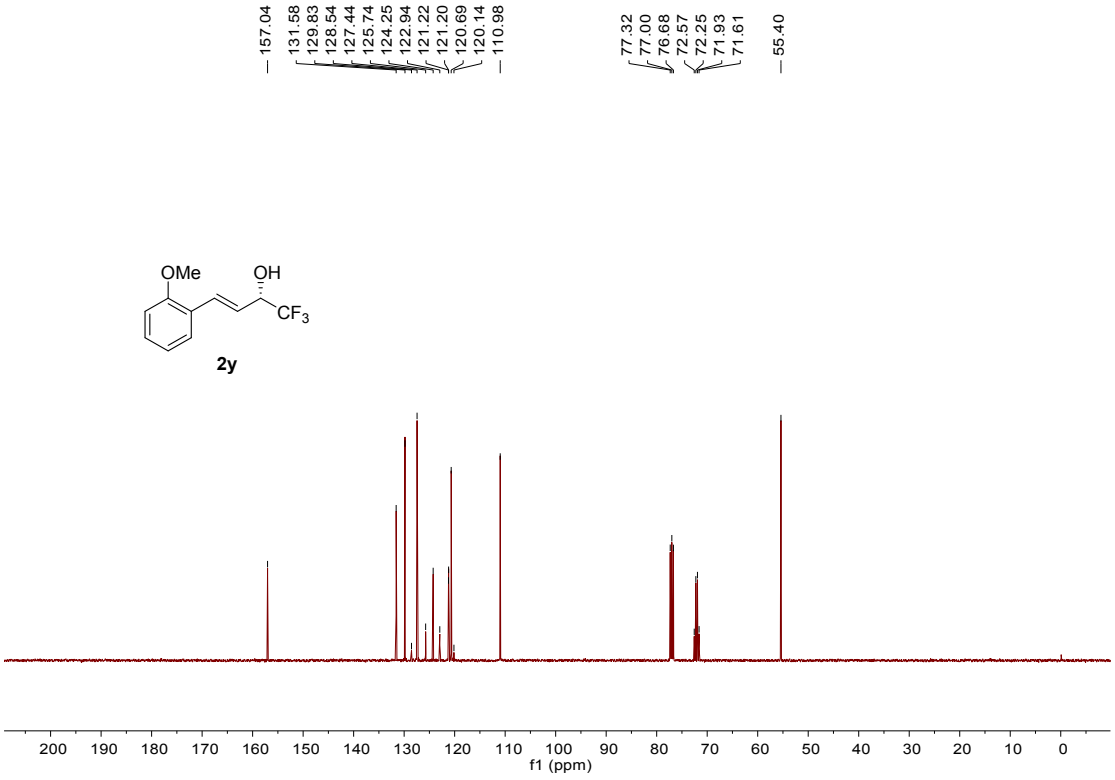
2x

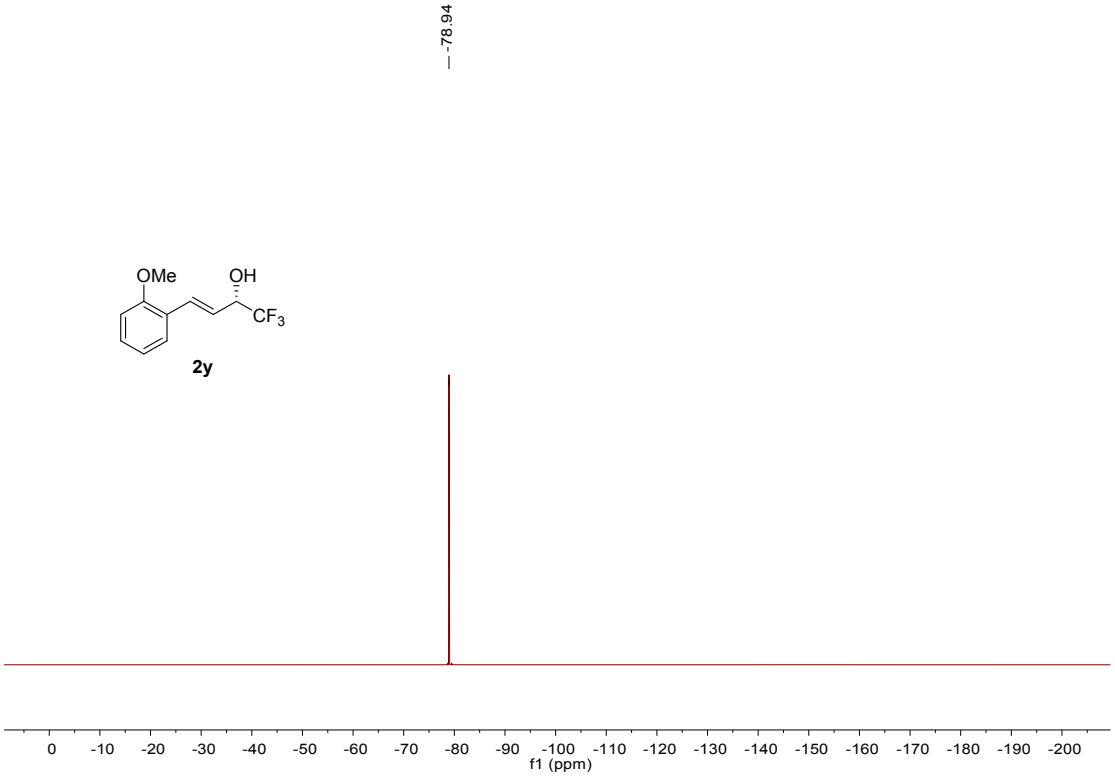

200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


-79.01
MeO
OH
CF3
2x
0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200
f1 (ppm)

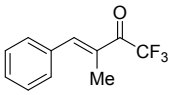

7.42
7.41
7.40
7.40
7.29
7.28
7.27
7.25
7.24
7.16
7.12
6.94
6.92
6.90
6.88
6.86
6.26
6.24
6.22
6.20
4.62
4.60
4.59
4.57
3.82
2.69
2.68
0.00


OMe
OH
CF3
2y
1.00
0.98
0.99
1.00
0.98
0.99
1.00
3.04
1.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

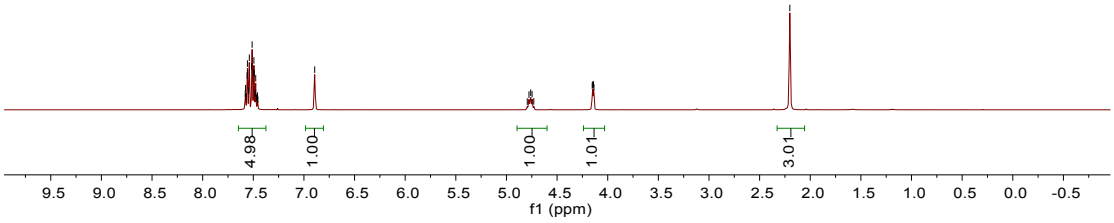

157.04
131.58
129.83
128.54
127.44
125.74
124.25
122.94
121.22
121.20
120.69
120.14
110.98
77.32
77.00
76.68
72.57
72.25
71.93
71.61
55.40
OMe
OH
CF3
2y
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

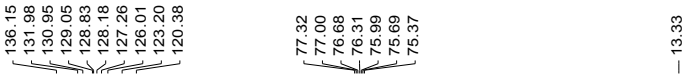

-78.94
OMe
OH
CF3
2y
0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200
f1 (ppm)

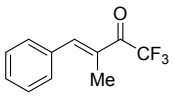

7.58
7.58
7.57
7.56
7.56
7.55
7.55
7.54
7.52
7.51
7.50
7.49
7.49
7.48
7.48
7.46
7.46
6.89
4.79
4.78
4.76
4.75
4.73
4.15
4.15
4.14
4.14
2.20


O
CF3
Me

1z

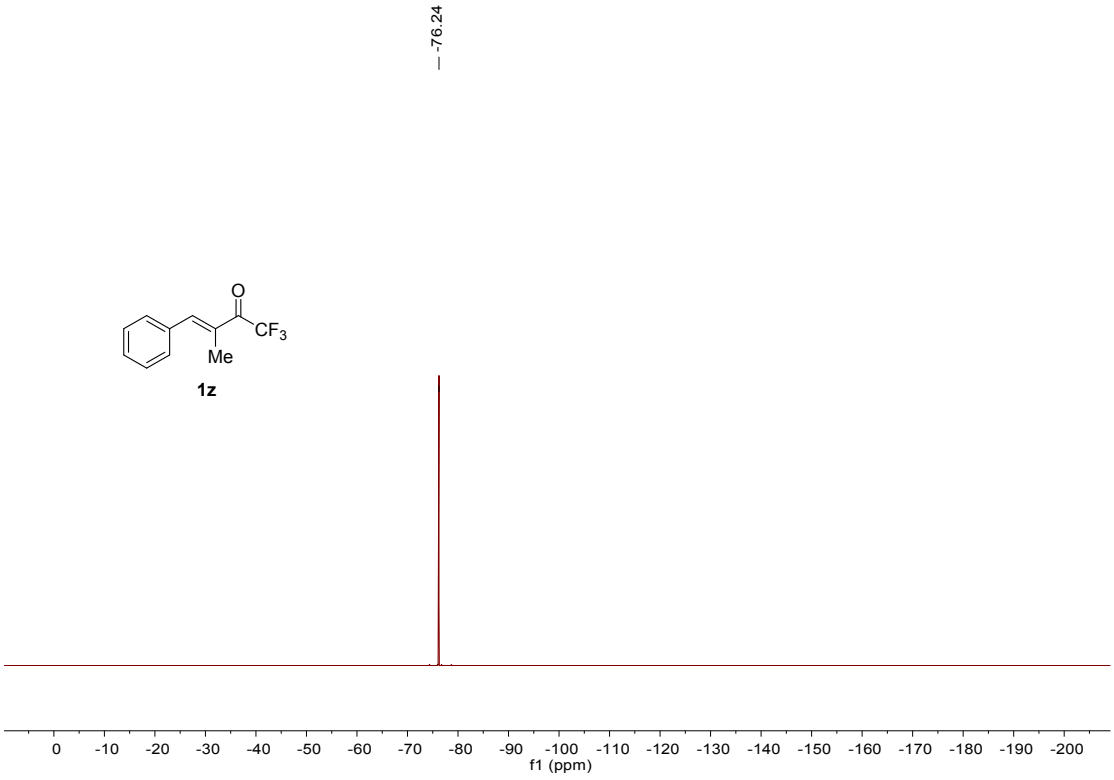

4.98
1.00
1.00
1.01
3.01
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

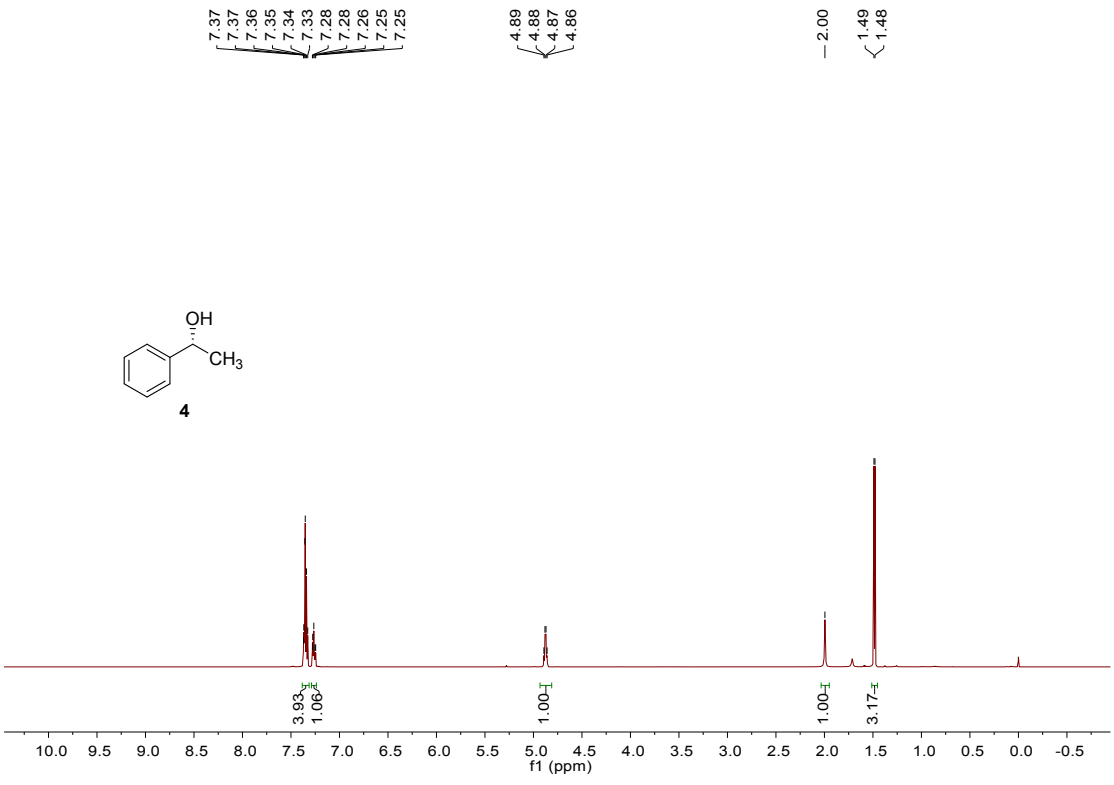

136.15
131.98
130.95
129.05
128.83
128.18
127.26
126.01
123.20
120.38
77.32
77.00
76.68
76.31
75.99
75.69
75.37
13.33

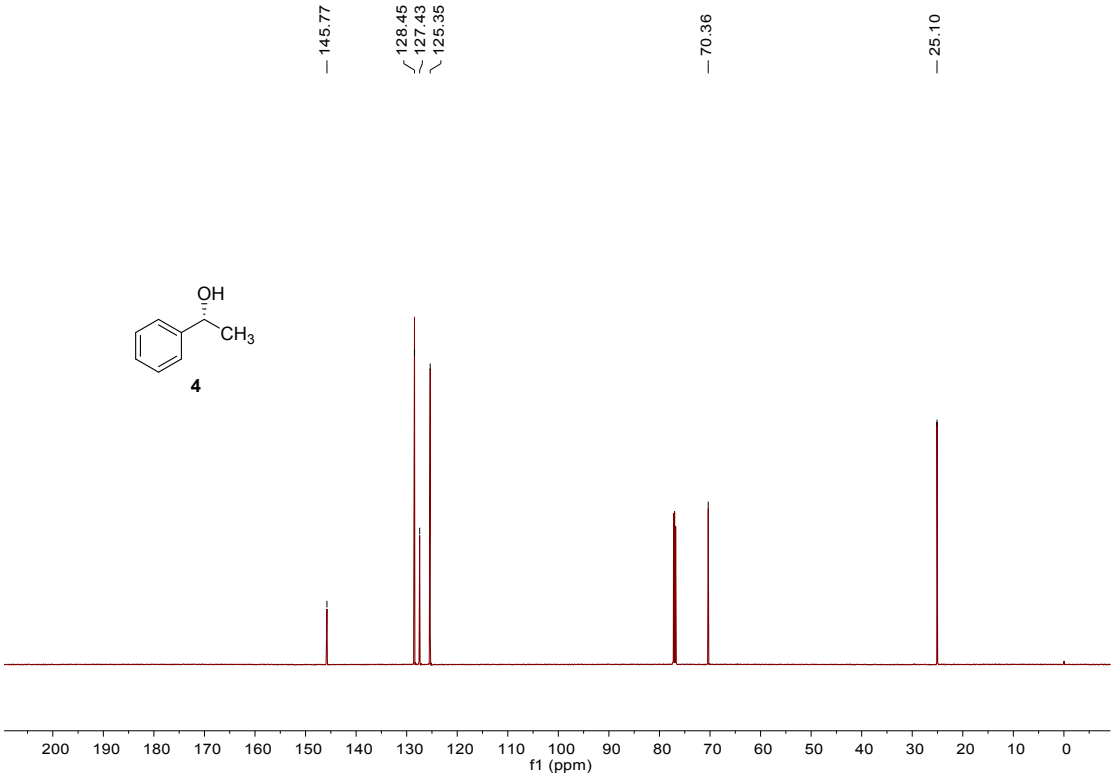

O
CF3
Me

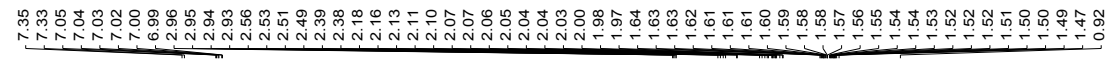
1z

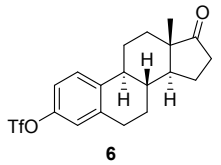
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

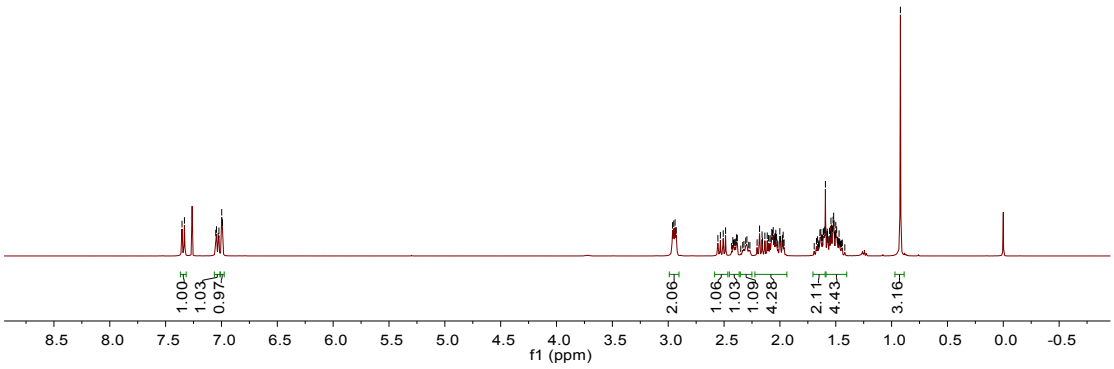

-76.24
O
CF3
Me
1z
0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200
f1 (ppm)

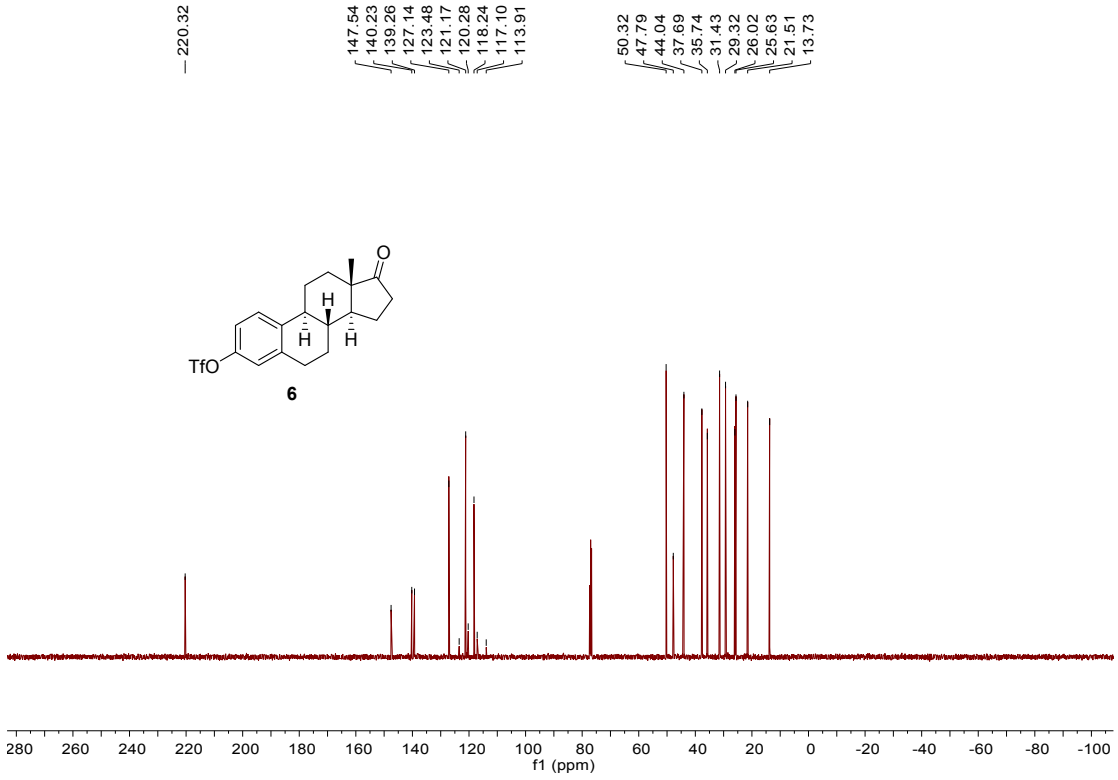

7.37
7.37
7.36
7.35
7.34
7.33
7.28
7.28
7.26
7.25
7.25
4.89
4.88
4.87
4.86
2.00
1.49
1.48
OH
CH3
4
3.93
1.06
1.00
1.00
3.17
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

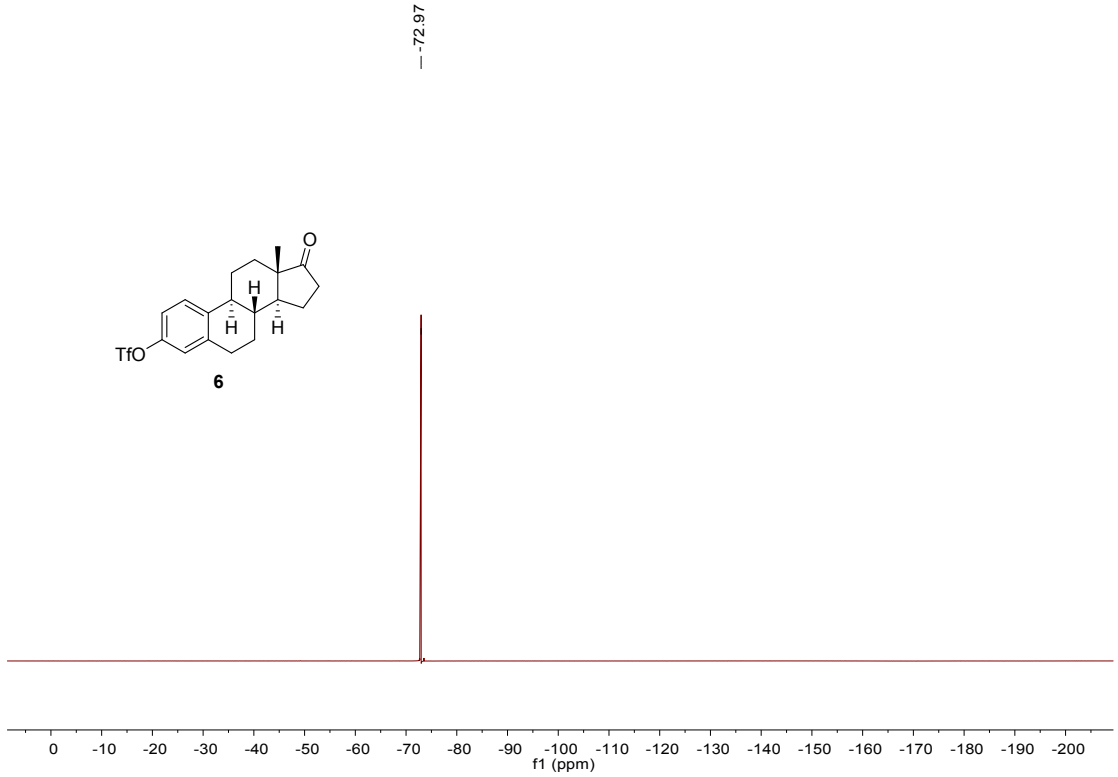

145.77
128.45
127.43
125.35
70.36
25.10
OH
CH3
4
f1 (ppm)

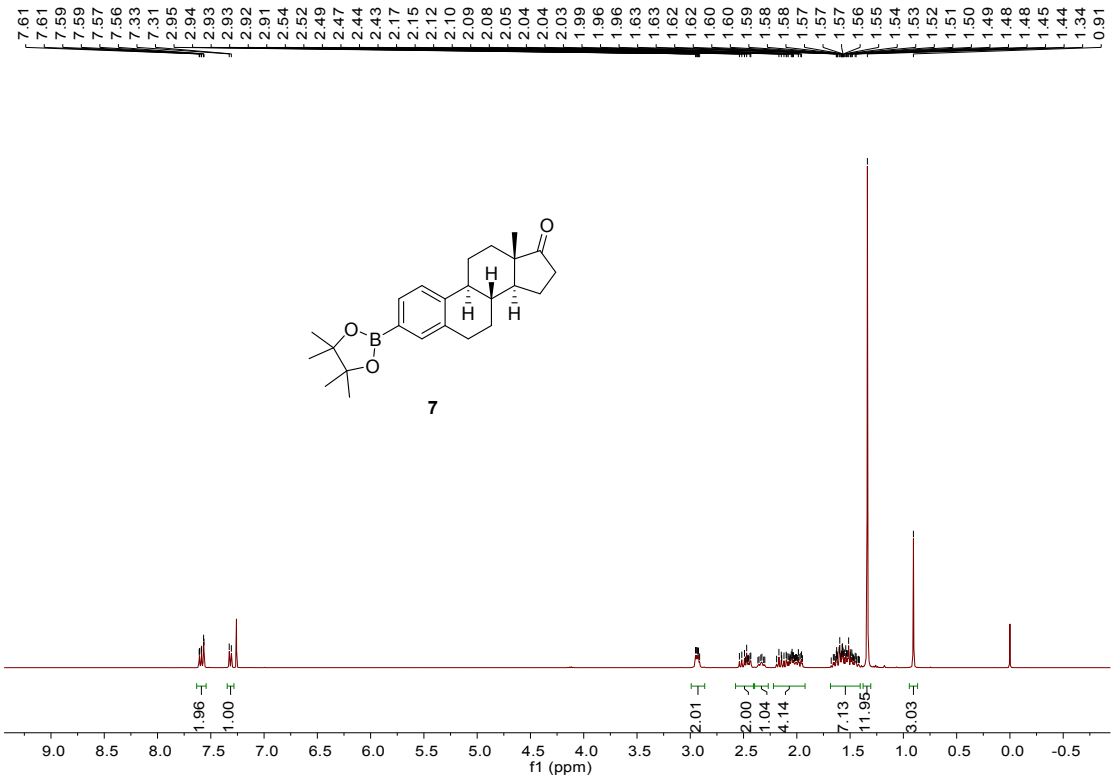

7.35
7.33
7.05
7.04
7.03
7.02
7.00
6.99
2.96
2.95
2.94
2.93
2.56
2.53
2.51
2.49
2.39
2.38
2.18
2.16
2.13
2.11
2.10
2.07
2.07
2.06
2.05
2.04
2.04
2.03
2.00
1.98
1.97
1.64
1.63
1.63
1.62
1.61
1.61
1.61
1.60
1.59
1.58
1.58
1.57
1.56
1.55
1.54
1.54
1.53
1.52
1.52
1.52
1.51
1.50
1.50
1.49
1.47
0.92

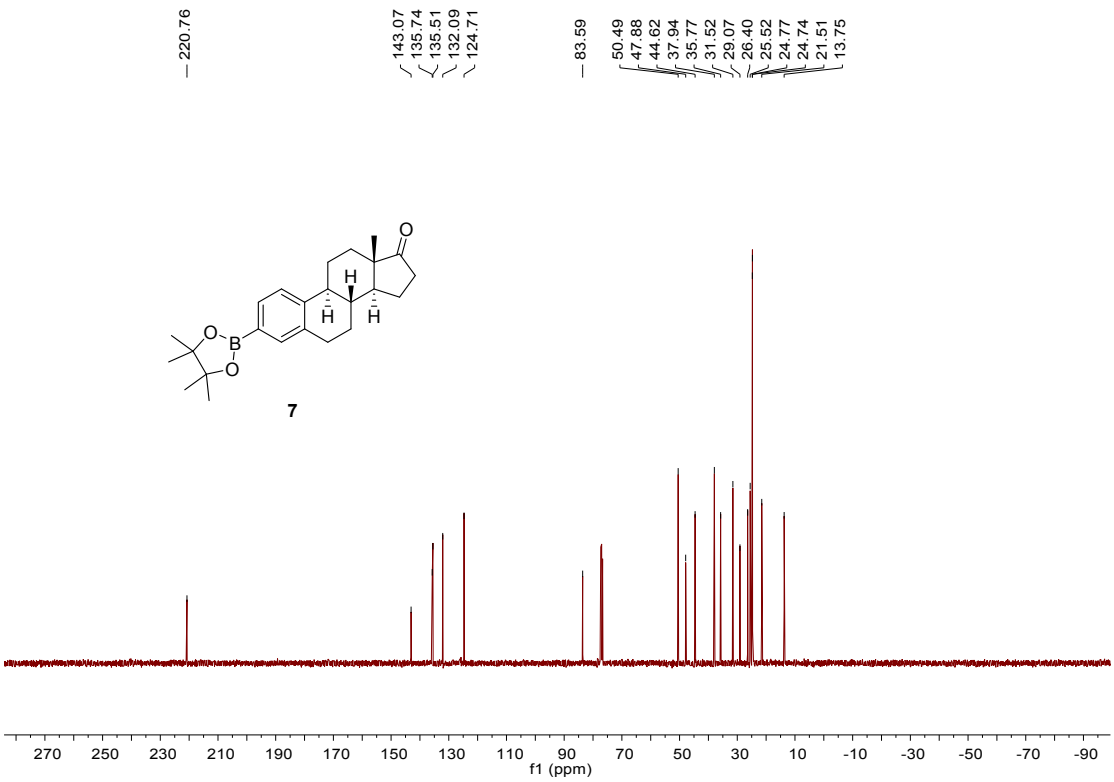

O
H
H
H
TfO
6

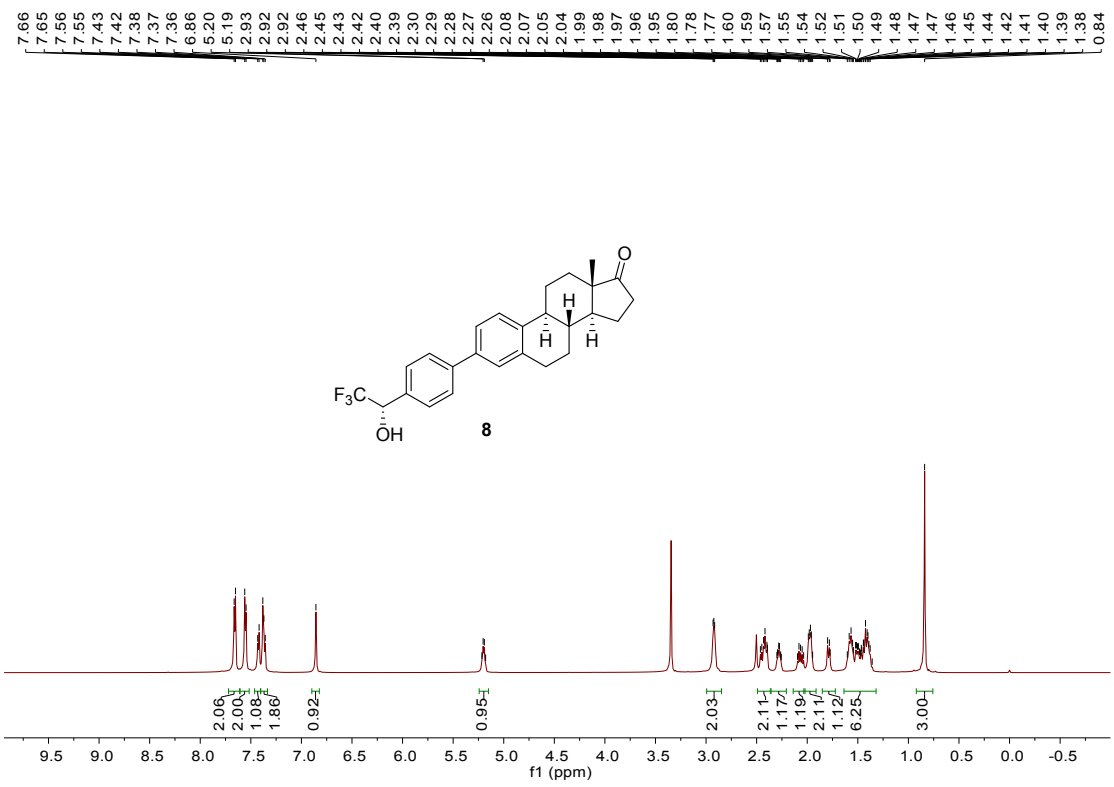

1.00
1.03
0.97
2.06
1.06
1.03
1.09
4.28
2.11
4.43
3.16
f1 (ppm)

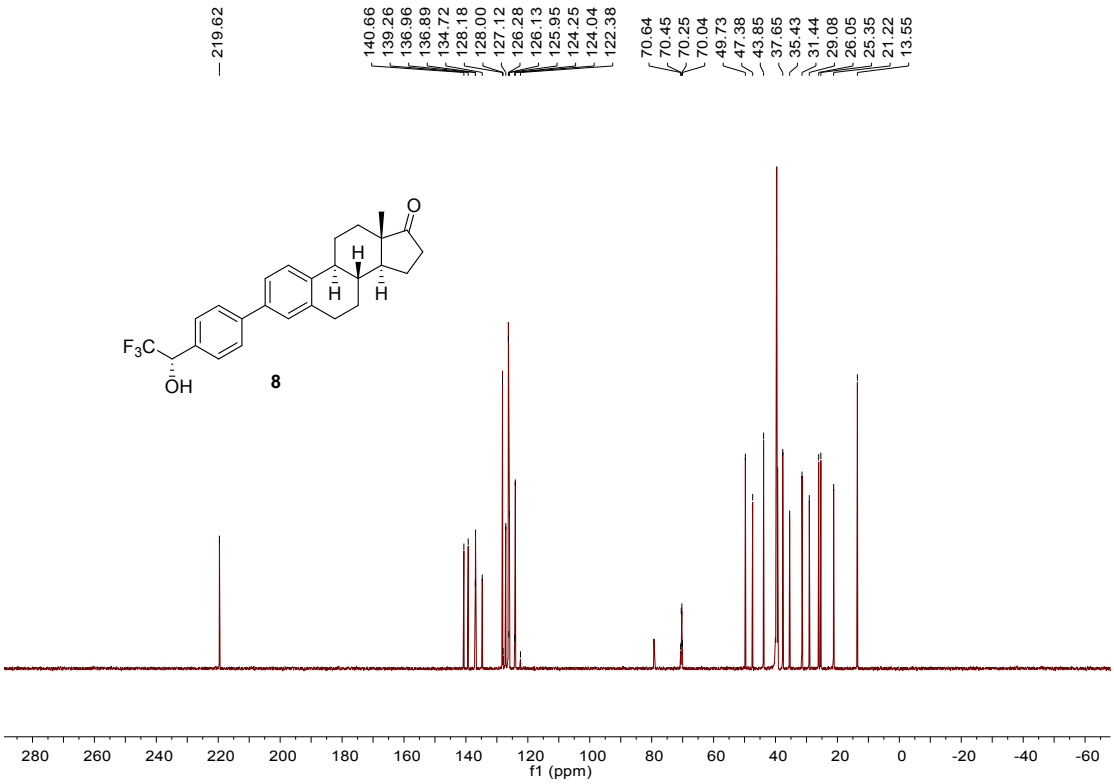

220.32
147.54
140.23
139.26
127.14
123.48
121.17
120.28
118.24
117.10
113.91
50.32
47.79
44.04
37.69
35.74
31.43
29.32
26.02
25.63
21.51
13.73
O
H
H
H
TfO
6
280 260 240 220 200 180 160 140 120 100 80 60 40 20 0 -20 -40 -60 -80 -100
f1 (ppm)

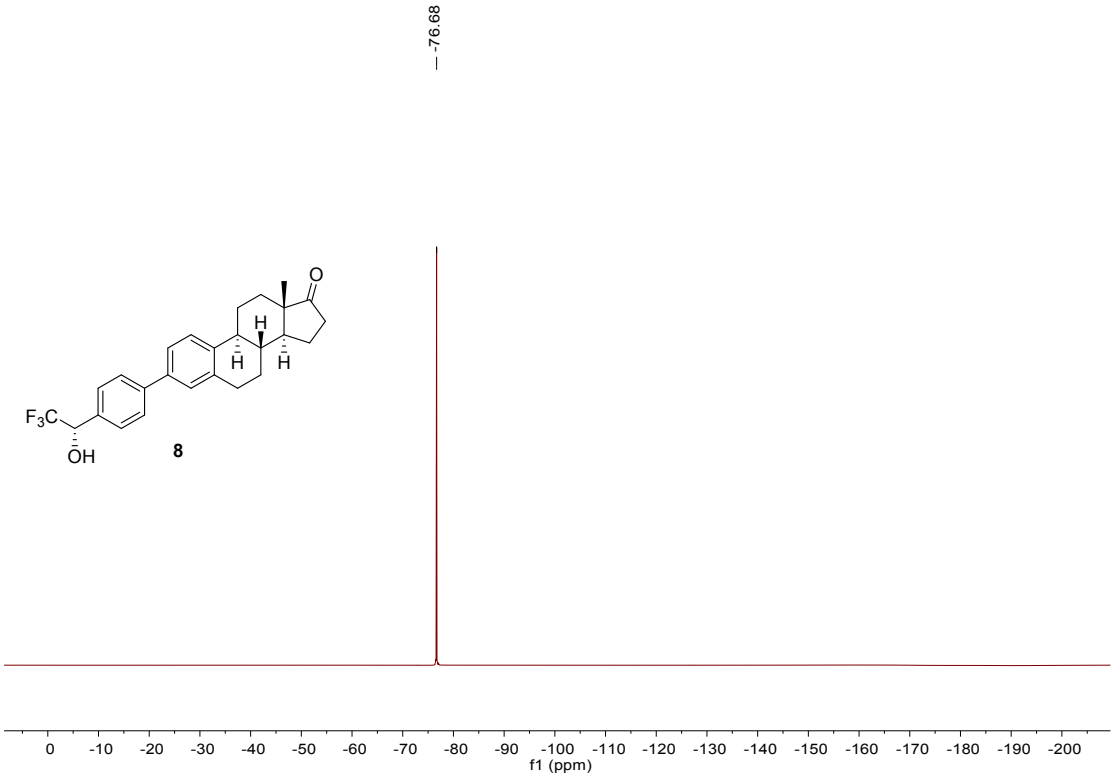

-72.97
O
H
H
H
TfO
6
0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200
f1 (ppm)

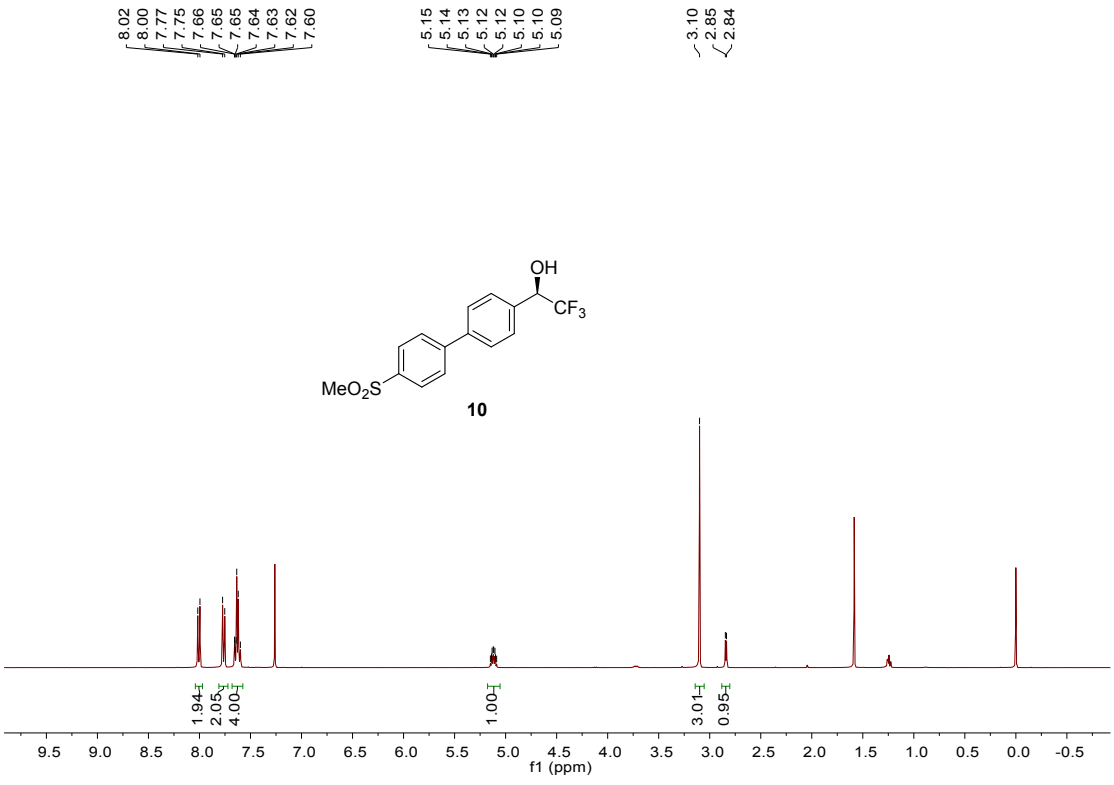

7.61 7.61 7.59 7.59 7.57 7.56 7.33 7.31 2.95 2.94 2.93 2.93 2.92 2.91 2.54 2.52 2.49 2.47 2.44 2.43 2.17 2.15 2.12 2.10 2.09 2.08 2.05 2.04 2.04 2.03 1.99 1.96 1.96 1.63 1.63 1.62 1.62 1.60 1.60 1.59 1.58 1.57 1.57 1.57 1.56 1.55 1.54 1.53 1.52 1.51 1.50 1.49 1.48 1.48 1.45 1.44 1.34 0.91
O
H
H
H
O
B
O
7
1.96
1.00
2.01
2.00
1.04
4.14
7.13
11.95
3.03
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

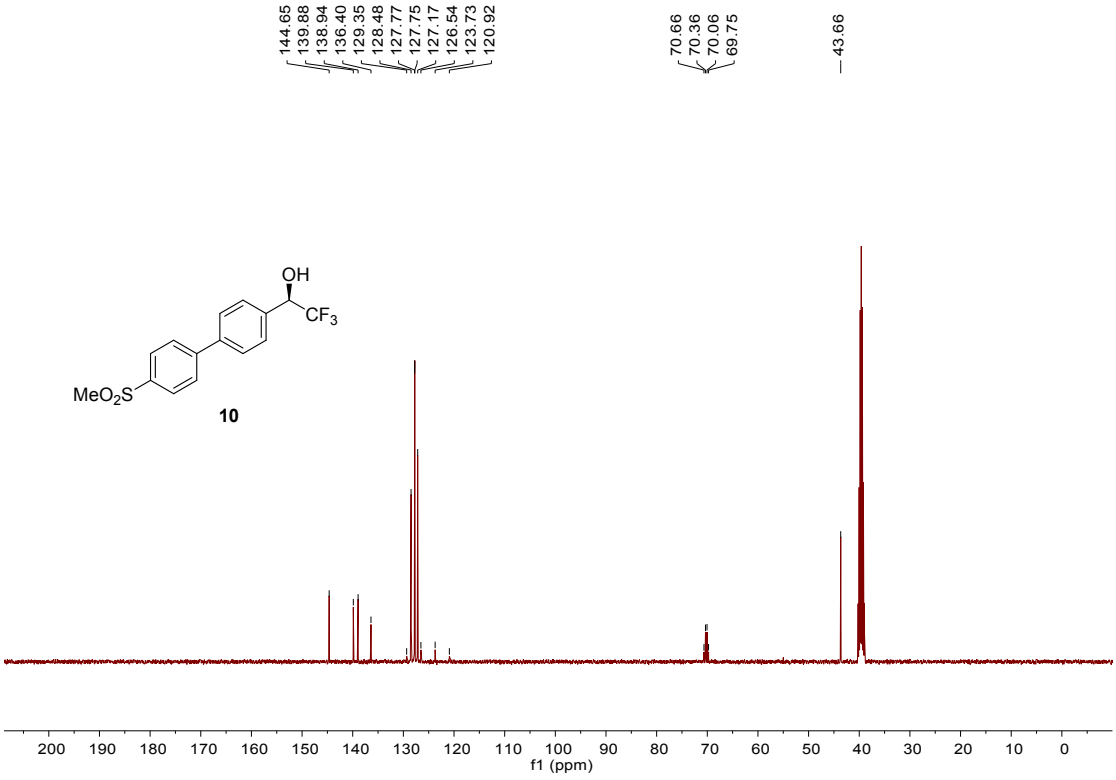

220.76
143.07
135.74
135.51
132.09
124.71
83.59
50.49
47.88
44.62
37.94
35.77
31.52
29.07
26.40
25.52
24.77
24.74
21.51
13.75
O
H
H
H
O
B
O
7
270 250 230 210 190 170 150 130 110 90 70 50 30 10 -10 -30 -50 -70 -90
f1 (ppm)

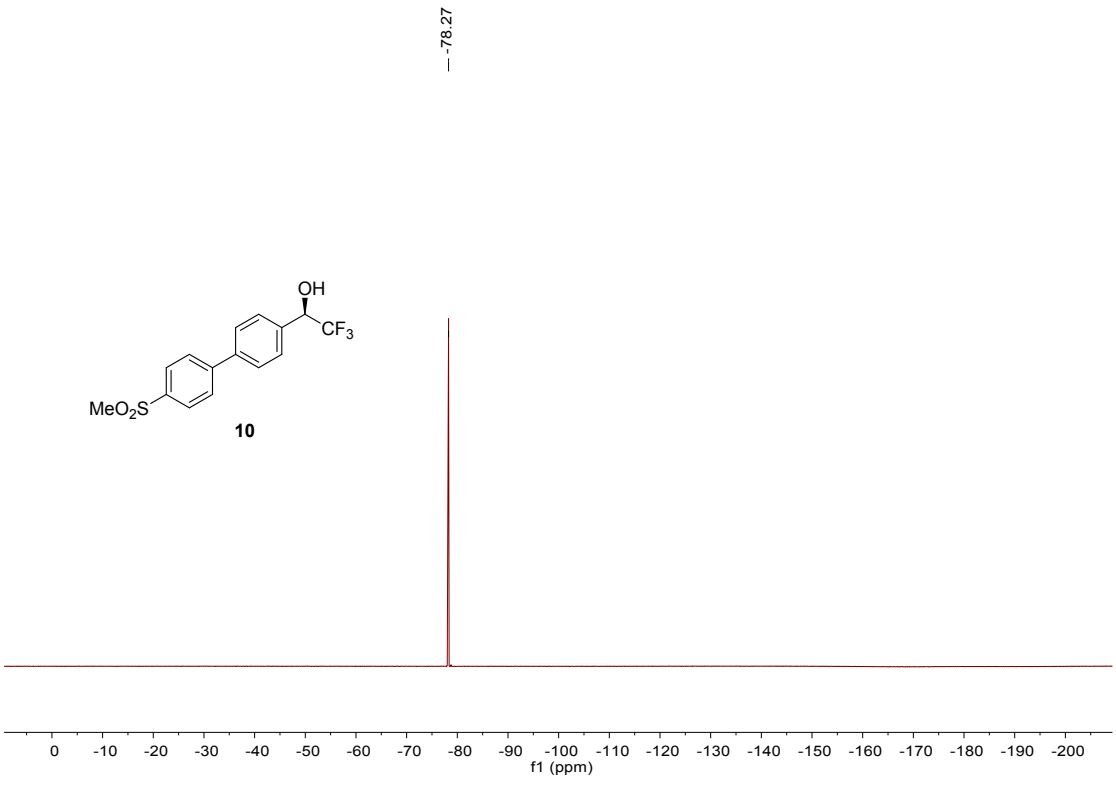

7.66 7.65 7.56 7.55 7.43 7.42 7.38 7.37 7.36 6.86 5.20 5.19 2.93 2.92 2.92 2.46 2.45 2.43 2.42 2.40 2.39 2.30 2.29 2.28 2.27 2.26 2.08 2.07 2.05 2.04 1.99 1.98 1.97 1.96 1.95 1.80 1.78 1.77 1.60 1.59 1.57 1.55 1.54 1.52 1.51 1.50 1.49 1.48 1.47 1.47 1.46 1.45 1.44 1.42 1.41 1.40 1.39 1.38 0.84
O
H
H
H
F3C
OH
8
2.06 2.00 1.08 1.86 0.92 0.95 2.03 2.11 1.17 1.19 2.11 1.12 6.25 3.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

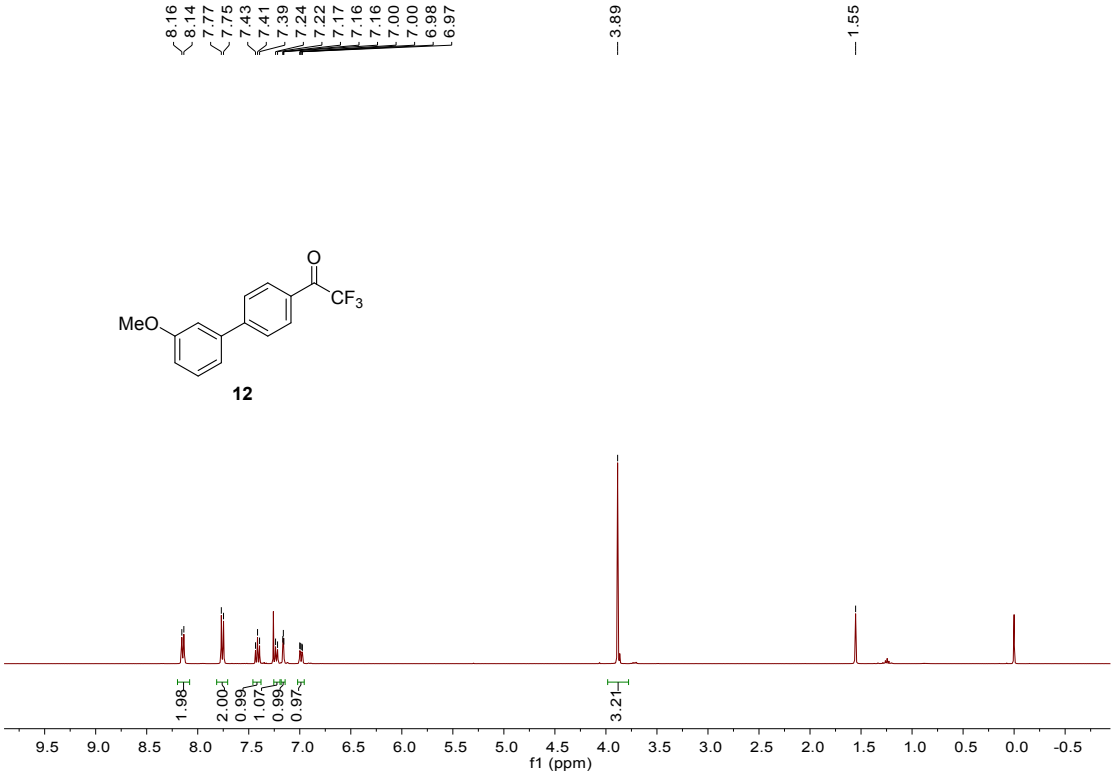

219.62
140.66 139.26 136.96 136.89 134.72 128.18 128.00 127.12 126.28 126.13 125.95 124.25 124.04 122.38
70.64 70.45 70.25 70.04 49.73 47.38 43.85 37.65 35.43 31.44 29.08 26.05 25.35 21.22 13.55
O
H
H
H
F3C
OH
8
280 260 240 220 200 180 160 140 120 100 80 60 40 20 0 -20 -40 -60
f1 (ppm)

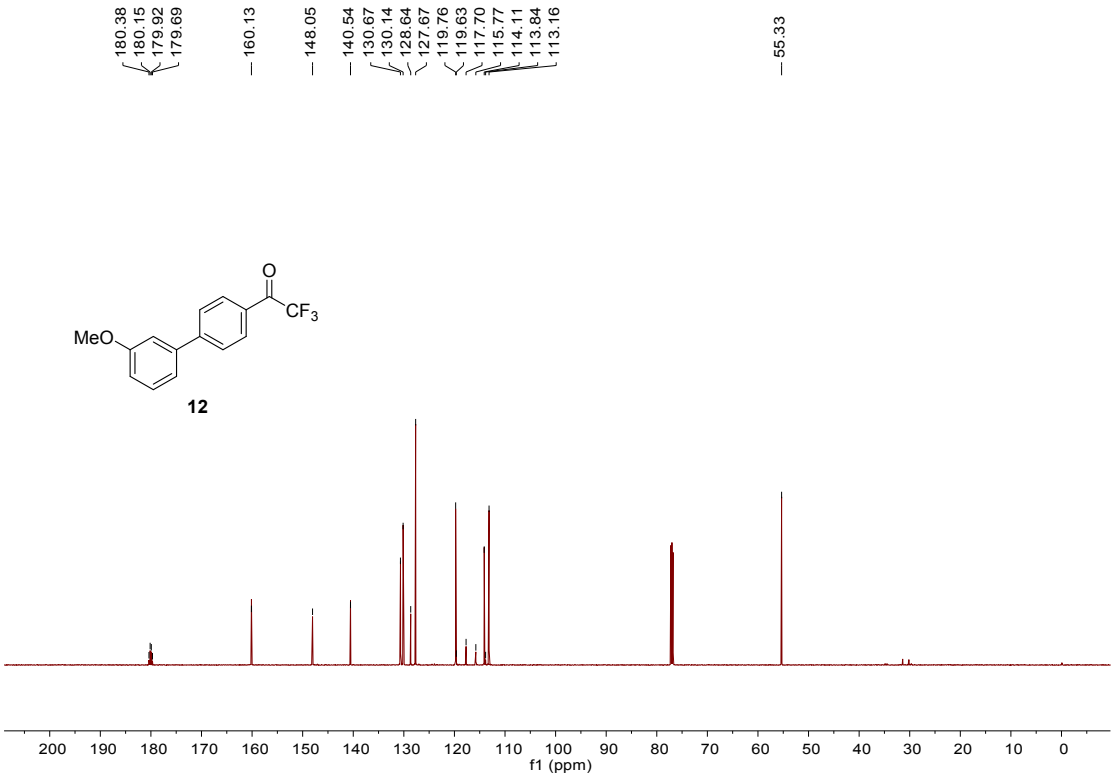

-76.68
O
H
H
H
F3C
OH
8
0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200
f1 (ppm)

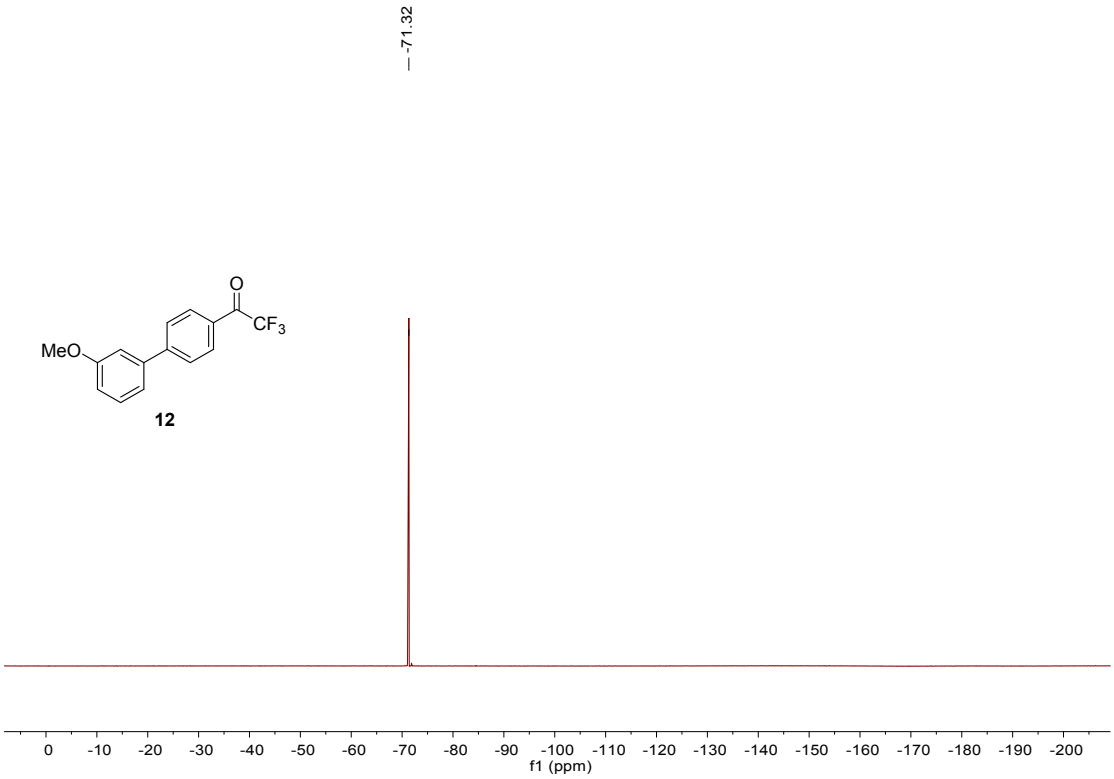

8.02
8.00
7.77
7.75
7.66
7.65
7.65
7.64
7.63
7.62
7.60
5.15
5.14
5.13
5.12
5.12
5.10
5.10
5.09
3.10
2.85
2.84
OH
CF3
MeO2S
10
1.94
2.05
4.00
1.00
3.01
0.95
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

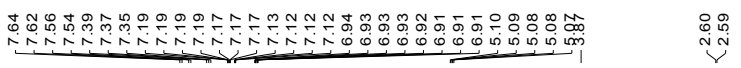

144.65
139.88
138.94
136.40
129.35
128.48
127.77
127.75
127.17
126.54
123.73
120.92
70.66
70.36
70.06
69.75
43.66
OH
CF3
MeO2S
10
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

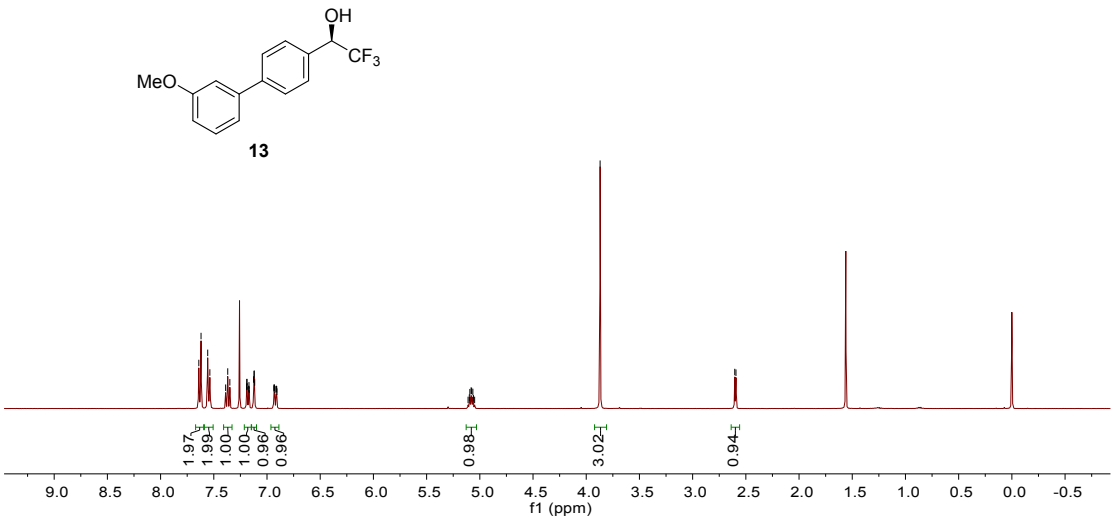

-78.27
OH
CF3
MeO2S
10
0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200
f1 (ppm)

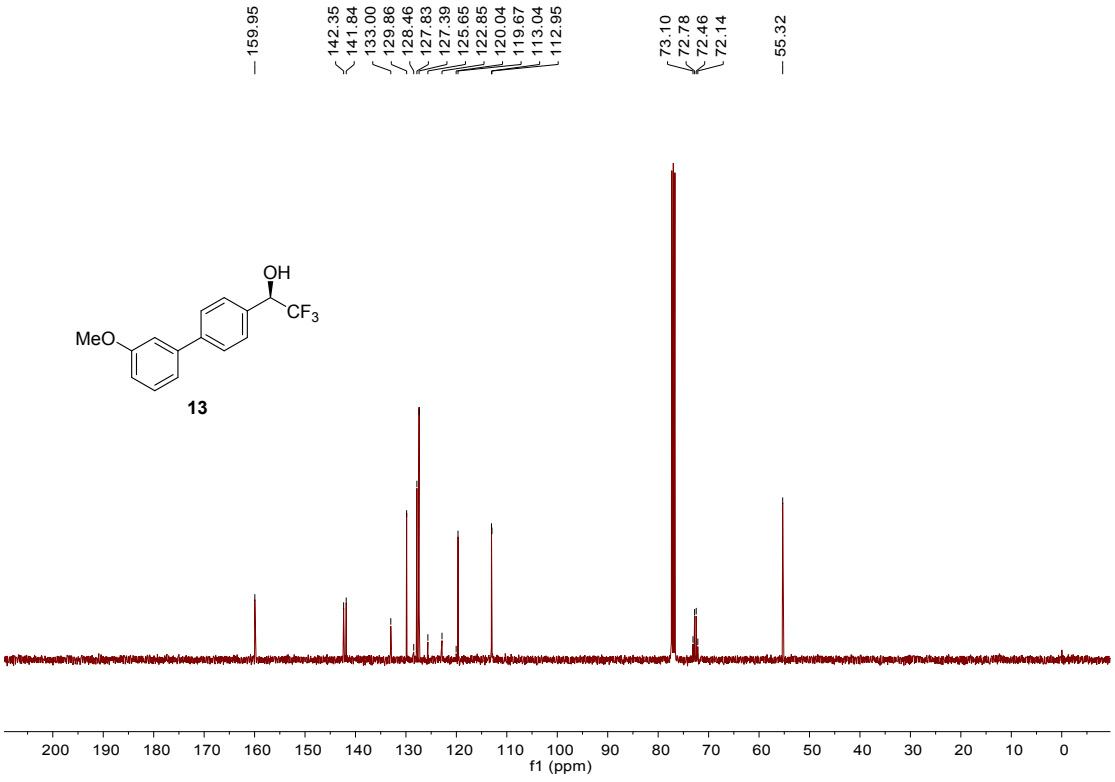

8.16
8.14
7.77
7.75
7.43
7.41
7.39
7.24
7.22
7.17
7.16
7.16
7.00
7.00
6.98
6.97
3.89
1.55
O
CF3
MeO
12
1.98
2.00
0.99
1.07
0.99
0.97
3.21
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

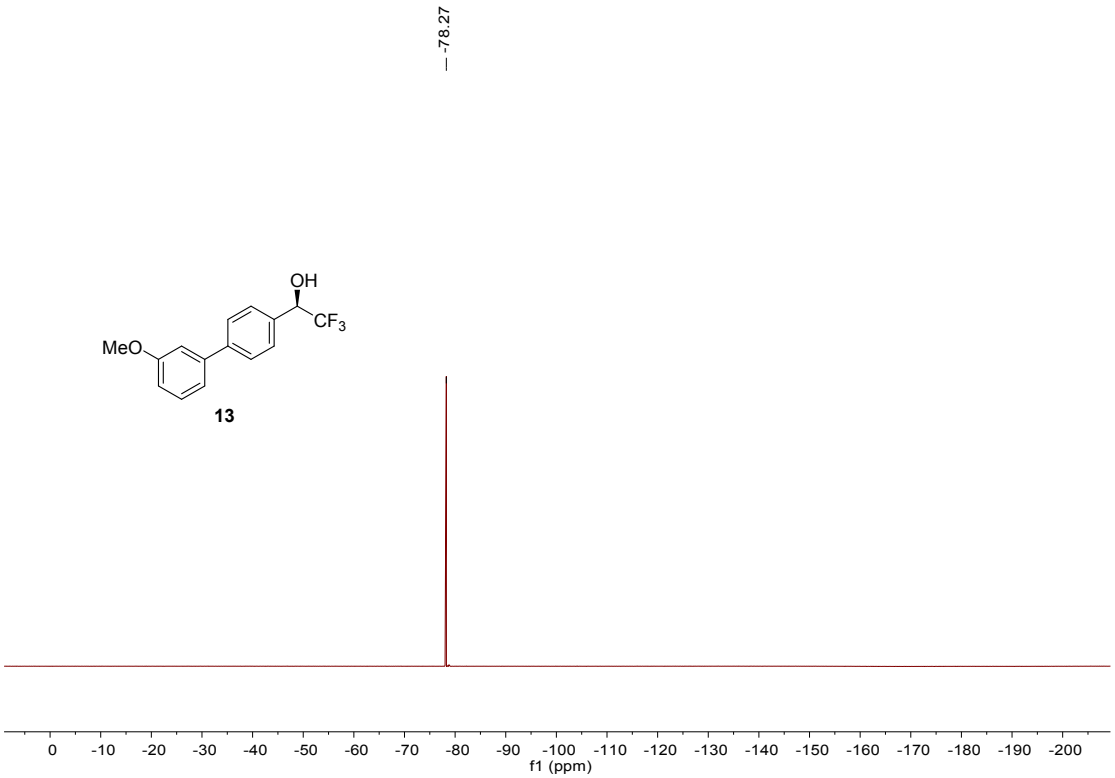

180.38
180.15
179.92
179.69
160.13
148.05
140.54
130.67
130.14
128.64
127.67
119.76
119.63
117.70
115.77
114.11
113.84
113.16
55.33
O
CF3
MeO
12
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


-71.32
MeO
O
CF3
12
0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200
f1 (ppm)


7.64 7.62 7.56 7.54 7.39 7.37 7.35 7.19 7.19 7.19 7.19 7.17 7.17 7.17 7.13 7.12 7.12 7.12 6.94 6.93 6.93 6.93 6.92 6.91 6.91 6.91 5.10 5.09 5.08 5.08 5.07
2.60 2.59


OH
CF3
MeO
13
1.97 1.99 1.00 1.00 0.96 0.96 0.98 3.02 0.94
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


159.95
142.35
141.84
133.00
129.86
128.46
127.83
127.39
125.65
122.85
120.04
119.67
113.04
112.95
73.10
72.78
72.46
72.14
55.32
OH
CF3
MeO
13
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


-78.27
OH
CF3
MeO
13
0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200
f1 (ppm)