Asymmetric Synthesis of 1,2-fluorohydrin: Iridium Catalyzed Hydrogenation of Fluorinated Allylic Alcohol

Sudipta Ponra,[!a] Jianping Yang,[!a] Haibo Wu,[a] Wangchuk Rabten[a] and Pher G. Andersson*[a,b]

[a] Department ofOrganic Chemistry, Stockholm University, Svante Arrhenius väg 16C, SE-10691 Stockholm, Sweden

[b] School of Chemistry and Physics, University of KwaZulu-Natal, Private Bag X54001, Durban, 4000, South Africa.

! Authors contributed equally to this work

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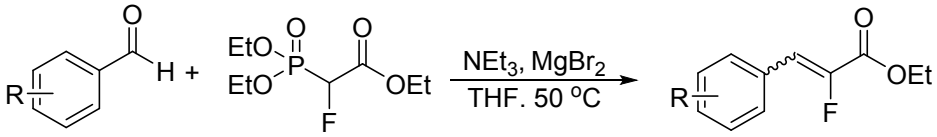
1. General methods

All reactions were conducted under inert atmosphere using magnetic stirring. CH_2Cl_2, used in the hydrogenation, was freshly distilled from CaH_2 under nitrogen. THF was freshly distilled from sodium-benzophenone under nitrogen. All reagents were used as supplied commercially without further purification. Chromatographic separations were performed on Kiesel gel 60 H silica gel (particle size: 0.063-0.100 mm). Thin layer chromatography (TLC) was performed on aluminium plates coated with Kiesel gel 60 (0.20 mm, UV254) and visualized under ultraviolet light ($\nu = 254$ nm). ^{1}H NMR spectra were recorded on a Bruker 400 or 500 at 400/500 MHz in $CDCl_3$ and referenced internally to the residual $CHCl_3$ peak (7.26 ppm). ^{13}C NMR spectra were recorded at 100/125 MHz in $CDCl_3$ and referenced to the central peak of $CDCl_3$ (77.16 ppm). Chemical shifts are reported in ppm (δ scale). Enantiomeric excesses were determined either using chiral HPLC or SFC with a diode array detector at 210 and 254 nm. Racemic compounds were used for comparison. HRMS data were obtained using a Bruker MicroTOF-Q II instrument operation at ambient temperature. Optical rotations were recorded on an Autopol IV polarimeter from Rudolp Research Analytical, equipped with a sodium lamp (589 nm) and a 10 cm cell.

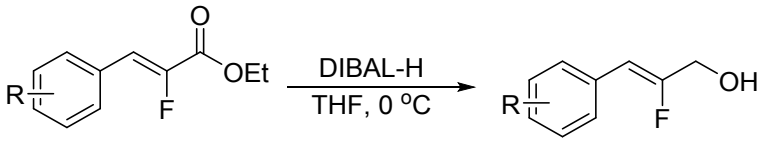
2. General procedure for substrates synthesis

2.1. General procedure for the Horner-Wadsworth-Emmons reaction[1]



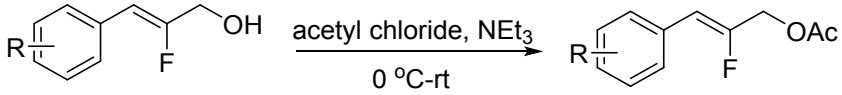
2-fluoro-triethylphosphonoacetate (4.84 g, 20 mmol, 1.0 equiv) was dissolved in dry THF (100 ml) at ambient temperature. Triethylamine (2.8 ml, 40 mmol, 2.0 equiv) was added, followed by magnesium bromide (3.68 g, 10 mmol, 1.0 equiv). An exotherm is observed, and while the reaction was hot (ca. 50 °C), the corresponding aldehydes (20 mmol, 1.0 equiv) was added. The reaction was stirred and monitored by TLC. Upon completion (ca. 1h), the reaction was diluted with 100 ml diethyl ether, then filtered on a medium porosity fritted funnel. The filtrate was washed with saturated ammonium chloride solution, which was then extracted with ether (2 x 100 ml). The organic layers were combined, washed with brine, dried over magnesium sulfate, filtered and concentrated to give mixture of olefins (major product is *Z* isomer).

2.2 General procedure for preparation of fluorinated allylic alcohol

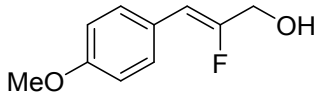


The corresponding ester (1.0 mmol) prepared according to procedure in section 2.1 was dissolved in dry THF (5 ml) in dry glassware. DIBAL-H (1.5 M in toluene, 3 equiv., 2.0 ml) was added slowly at 0 °C and stirred at room temperature for 1 hour. It was then quenched with saturated solution of Rochelles salt under vigorous stirring, extracted with CH_2Cl_2 (3 × 15 ml), washed with water (2 × 15 ml), dried over Na_2SO_4 and evaporated. Product was separated by column chromatography (*n*-pentane/Et_2O 9:1).

2.3 general procedure for preparation of fluorinated allylic acetates

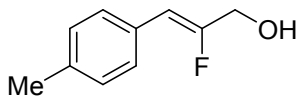


The corresponding fluorinated allylic alcohol (1mmol, 1equiv.) and triethylamine (1.2 mmol, 1.2 equiv.) were dissolved in CH_2Cl_2 (3ml). Acetyl chloride (1.2 mmol, 1.2 equiv.) was added slowly at 0 °C. The reaction was allowed to warm to rt and stirred until the fluorinated allylic alcohol was consumed completely. It was then quenched with H_2O, extracted with CH_2Cl_2 (3 × 3 ml), washed with water (2 × 5 ml), dried over Na_2SO_4 and evaporated. Product was separated by column chromatography (*n*-pentane/Et_2O 20:1).



(*Z*)-2-fluoro-3-(4-methoxyphenyl)prop-2-en-1-ol (1a)

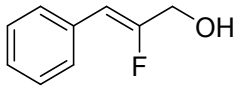
The characterization data is in agreement with the reported data.[2]



(*Z*)-2-fluoro-3-(p-tolyl)prop-2-en-1-ol (1b)

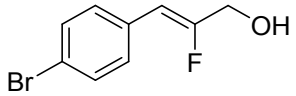
White solid, ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.41 (d, *J* = 8.1 Hz, 2H), 7.16 (d, *J* = 8.0 Hz, 2H), 5.75 (d, *J* = 38.9 Hz, 1H), 4.27 (d, *J* = 14.9 Hz, 2H), 2.35 (s, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ 157.7 (d, *J* = 265.6 Hz), 137.5 (d, J = 2.4 Hz), 129.9 (d, J = 2.8 Hz), 129.3, 128.8 (d, J = 7.2

Hz), 107.6 (d, J = 6.9 Hz), 62.1 (d, J = 32.4 Hz), 21.4. ^{19}F NMR ($CDCl_3$, 376 MHz) δ -114.3. HRMS-ESI calcd for $[M+Na]^+$: 189.0686, found: 189.0687.



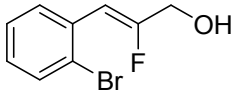
(*Z*)-2-fluoro-3-phenylprop-2-en-1-ol (1c)

The characterization data is in agreement with the reported data.[3]



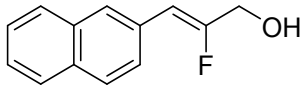
(*Z*)-3-(4-bromophenyl)-2-fluoroprop-2-en-1-ol (1d)

The characterization data is in agreement with the reported data.[2]



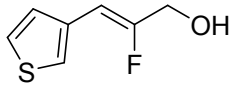
(*Z*)-3-(2-bromophenyl)-2-fluoroprop-2-en-1-ol (1e)

White solid, ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.66 (t, *J* = 1.6 Hz, 1H), 7.46 – 7.32 (m, 2H), 7.19 (t, *J* = 7.9 Hz, 1H), 5.72 (d, *J* = 38.1 Hz, 1H), 4.28 (dd, *J* = 13.5, 5.5 Hz, 2H), 2.22 (t, *J* = 5.9 Hz, 1H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ 159.2 (d, *J* = 268.7 Hz), 134.8 (d, *J* = 2.7 Hz), 131.6 (d, *J* = 7.9 Hz), 130.5 (d, *J* = 2.1 Hz), 130.1 (s), 127.3 (d, *J* = 7.2 Hz), 122.7 (s), 106.2 (d, *J* = 6.4 Hz), 61.7 (d, *J* = 32.9 Hz). ^{19}F NMR ($CDCl_3$, 376 MHz) δ -111.1 (s). HRMS-ESI calcd for $[M+Na]^+$: 252.9635 (254.9615), found: 252.9633 (254.9621).



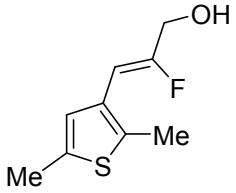
(*Z*)-2-fluoro-3-(naphthalen-2-yl)prop-2-en-1-ol (1f)

The characterization data is in agreement with the reported data.[2]



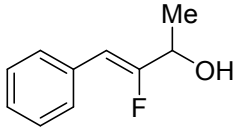
(*Z*)-2-fluoro-3-(thiophen-3-yl)prop-2-en-1-ol (1g)

The characterization data is in agreement with the reported data.[4]



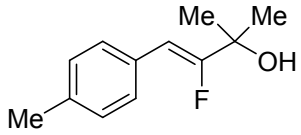
(*Z*)-3-(2,5-dimethylthiophen-3-yl)-2-fluoroprop-2-en-1-ol (1h)

Brown solid, ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.03 – 6.97 (m, 1H), 5.72 (d, *J* = 38.9 Hz, 1H), 4.26 (d, *J* = 15.1 Hz, 2H), 2.43 – 2.32 (m, 6H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ 156.3 (d, *J* = 263.6 Hz), 135.7, 134.6 (d, *J* = 2.3 Hz), 129.0 (d, *J* = 2.9 Hz), 126.2 (d, *J* = 9.6 Hz), 101.1 (d, *J* = 9.4 Hz), 62.1 (d, *J* = 32.3 Hz), 15.3, 13.3. ^{19}F NMR ($CDCl_3$, 376 MHz) δ -115.2. HRMS-ESI calcd for $[M+Na]^+$: 209.0407, found: 209.0428.



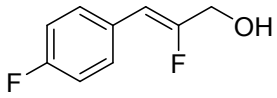
(*Z*)-3-fluoro-4-phenylbut-3-en-2-ol (1i)

The characterization data is in agreement with the reported data.[5]



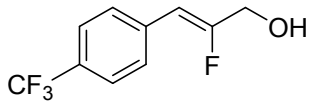
(*Z*)-3-fluoro-2-methyl-4-*p*-tolylbut-3-en-2-ol (1j)

Yellowish solid, ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.41 (d, J = 8.0 Hz, 2H), 7.15 (d, J = 8.0 Hz, 2H), 5.86 (d, J = 40.3 Hz, 1H), 2.35 (s, 3H), 1.97 (dd, J = 14.6, 5.9 Hz, 1H), 1.51 (s, 6H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ 163.5 (d, J = 269.1 Hz), 137.1 (d, J = 2.3 Hz), 130.3 (d, J = 2.0 Hz), 129.3, 128.7 (d, J = 7.3 Hz), 103.1 (d, J = 7.7 Hz), 71.0 (d, J = 29.0 Hz), 27.7, 21.3. ^{19}F NMR ($CDCl_3$, 376 MHz) δ -116.6 (s). HRMS-ESI calcd for $[M+Na]^+$: 217.0999, found: 217.0982.



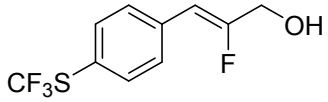
(*Z*)-2-fluoro-3-(4-fluorophenyl)prop-2-en-1-ol (1k)

The characterization data is in agreement with the reported data.[2]



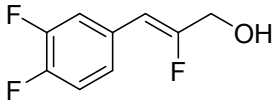
(*Z*)-2-fluoro-3-(4-(trifluoromethyl)phenyl)prop-2-en-1-ol (1l)

The characterization data is in agreement with the reported data.[6]



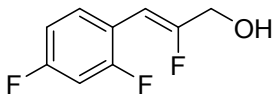
(*Z*)-2-fluoro-3-(4-(trifluoromethylthio)phenyl)prop-2-en-1-ol (1m)

White solid, ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.60 (d, J = 8.3 Hz, 2H), 7.55 – 7.50 (m, 2H), 5.80 (d, J = 38.1 Hz, 1H), 4.29 (dd, J = 13.2, 6.2 Hz, 2H), 2.65 (t, J = 6.3 Hz, 1H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ 159.9 (d, J = 269.9 Hz), 136.5 (s), 135.5 (d, J = 2.7 Hz), 129.7 (d, J = 308.2 Hz), 129.6 (d, J = 7.5 Hz), 123.31 – 122.97 (m), 106.3 (d, J = 6.1 Hz), 61.6 (d, J = 32.9 Hz). ^{19}F NMR ($CDCl_3$, 376 MHz) δ -110.0 (s), -42.7 (s). HRMS-ESI calcd for $[M+Na]^+$: 275.0124, found: 275.0098



(*Z*)-3-(3,4-difluorophenyl)-2-fluoroprop-2-en-1-ol (1n)

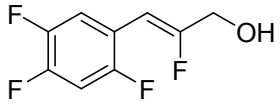
White solid, ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.39 (ddd, J = 11.7, 7.7, 1.8 Hz, 1H), 7.21 – 7.04 (m, 2H), 5.73 (d, J = 37.6 Hz, 1H), 4.29 (dd, J = 13.4, 6.1 Hz, 2H), 1.82 (t, J = 6.3 Hz, 1H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ 160.1 (d, J = 2.3 Hz), 152.1 – 150.3 (m), 149.3 – 148.1 (m), 130.2 – 129.2 (m), 125.0 (td, J = 6.4, 3.6 Hz), 117.9 – 117.4 (m), 117.4 – 117.1 (m), 105.8 (dt, J = 6.3, 1.8 Hz), 61.6 (d, J = 32.7 Hz). ^{19}F NMR ($CDCl_3$, 376 MHz) δ -112.8 (t, J = 1.5 Hz), -137.6 (dd, J = 21.7, 1.8 Hz), -138.4 (dd, J = 21.3, 2.1 Hz). HRMS-ESI calcd for $[M+Na]^+$: 211.0341, found: 211.0358.



(*Z*)-3-(2,4-difluorophenyl)-2-fluoroprop-2-en-1-ol (1o)

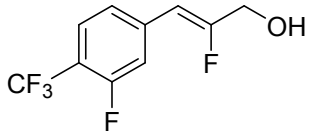
White solid, ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.86 – 7.68 (m, 1H), 6.92 – 6.69 (m, 2H), 5.97 (d, J = 38.2 Hz, 1H), 4.29 (dd, J = 14.0, 5.5 Hz, 2H), 2.81 – 2.28 (m, 1H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ 163.4 (dd, J = 12.2, 2.8 Hz), 161.2 – 160.7 (m), 160.7 – 157.8 (m), 131.0 (ddd, J =

13.2, 9.4, 4.2 Hz), 117.2 – 116.5 (m), 111.6 (dd, J = 21.2, 3.7 Hz), 103.8 (t, J = 25.7 Hz), 98.4 (t, J = 6.2 Hz), 61.8 (d, J = 32.3 Hz). ^{19}F NMR ($CDCl_3$, 376 MHz) δ -110.0 (dd, J = 7.5, 1.3 Hz), -112.5 (dd, J = 4.1, 1.4 Hz), -112.6 (dd, J = 7.5, 4.1 Hz) . HRMS-ESI calcd for $[M+Na]^+$: HRMS-ESI calcd for $[M+Na]^+$: 211.0341, found: 211.0350.



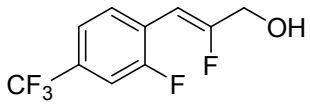
(*Z*)-2-fluoro-3-(2,4,5-trifluorophenyl)prop-2-en-1-ol (1p)

White solid, ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.65 – 7.54 (m, 1H), 6.87 (td, J = 9.9, 6.7 Hz, 1H), 5.94 (d, J = 37.5 Hz, 1H), 4.28 (d, J = 13.5 Hz, 2H), 3.17 (s, 1H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ 160.0 (d, J = 269.9 Hz), 154.8 (dd, J = 248.5, 9.1 Hz), 150.8 – 145.3 (m), 148.2 – 147.7 (m), 117.5 (ddd, J = 20.1, 14.0, 4.0 Hz), 117.2 – 116.8 (m), 105.3 (dd, J = 28.3, 21.0 Hz), 98.2 – 96.9 (m), 61.4 (d, J = 32.5 Hz). ^{19}F NMR ($CDCl_3$, 376 MHz) δ -142.4 (dd, J = 21.6, 14.5 Hz), -133.6 (ddd, J = 5.1, 3.5, 1.1 Hz), -118.4 (dt, J = 14.5, 3.6 Hz), -110.8 (dd, J = 3.4, 1.1 Hz). HRMS-ESI calcd for $[M+Na]^+$: 229.0247, found: 229.0255.



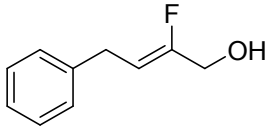
(*Z*)-2-fluoro-3-(3-fluoro-4-(trifluoromethyl)phenyl)prop-2-en-1-ol (1q)

White solid, ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.51 (t, J = 7.9 Hz, 1H), 7.35 (d, J = 11.9 Hz, 1H), 7.26 (d, J = 8.2 Hz, 1H), 5.81 (d, J = 37.4 Hz, 1H), 4.31 (dd, J = 12.2, 5.6 Hz, 2H), 2.58 (t, J = 5.9 Hz, 1H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ 162.3, 161.2 – 158.3 (m), 159.6, 138.9 (d, J = 8.9 Hz), 127.4 – 127.0 (m), 124.3 (dd, J = 6.6, 3.5 Hz), 122.7 (d, J = 271.8 Hz), 116.6 (dd, J = 22.0, 8.9 Hz), 105.3 (dd, J = 5.5, 2.0 Hz), 61.3 (d, J = 33.3 Hz). ^{19}F NMR ($CDCl_3$, 376 MHz) δ -114.0 (q, J = 12.8 Hz), -103.2 (s), -61.3 (d, J = 12.6 Hz). HRMS-ESI calcd for $[M+Na]^+$: 261.0309, found: 261.0328.



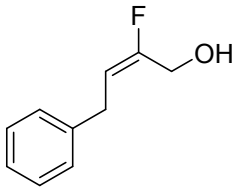
(*Z*)-2-fluoro-3-(2-fluoro-4-(trifluoromethyl)phenyl)prop-2-en-1-ol (1r)

White solid, ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.92 (t, J = 7.7 Hz, 1H), 7.39 (d, J = 8.3 Hz, 1H), 7.30 (d, J = 10.2 Hz, 1H), 6.09 (d, J = 37.9 Hz, 1H), 4.34 (dd, J = 12.3, 5.3 Hz, 2H), 2.19 (d, J = 65.3 Hz, 1H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ 161.5 (d, J = 225.1 Hz), 158.9 (d, J = 204.6 Hz), 130.7 (dd, J = 13.0, 3.0 Hz), 124.7 (d, J = 2.8 Hz), 124.4 (d, J = 11.3 Hz), 122.1 (d, J = 2.7 Hz), 121.2 (p, J = 3.8 Hz), 112.8 (dq, J = 25.4, 3.6 Hz), 97.9 (t, J = 6.1 Hz), 61.6 (d, J = 33.1 Hz). ^{19}F NMR ($CDCl_3$, 376 MHz) δ -114.7 (d, J = 4.4 Hz), -108.6 (d, J = 4.4 Hz), -62.9 (s). HRMS-ESI calcd for $[M+Na]^+$: 261.0309, found: 261.0324.



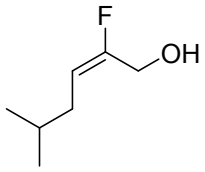
(*Z*)-2-fluoro-4-phenylbut-2-en-1-ol (1s)

Colorless oil, ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.35 – 7.27 (m, 2H), 7.24 – 7.17 (m, 3H), 5.07 (dt, J = 35.8, 7.7 Hz, 1H), 4.16 (d, J = 15.3 Hz, 2H), 3.47 (d, J = 7.7 Hz, 2H), 1.75 (br, J = 6.8 Hz, 1H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ 159.2, 156.7, 140.0, 128.6 (d, J = 24.2 Hz), 126.4, 107.0 (d, J = 13.5 Hz), 61.4 (d, J = 32.5 Hz), 29.8 (d, J = 4.9 Hz). ^{19}F NMR ($CDCl_3$, 376 MHz) δ -120.8. HRMS-ESI calcd for $[M+Na]^+$: 189.0686, found: 189.0678.



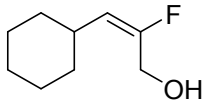
(*E*)-2-fluoro-4-phenylbut-2-en-1-ol (1t)

Colorless oil, ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.35 – 7.28 (m, 2H), 7.25 – 7.16 (m, 3H), 5.44 (dt, *J* = 20.3, 8.3 Hz, 1H), 4.34 (d, *J* = 21.0 Hz, 2H), 3.39 (d, *J* = 8.3 Hz, 2H), 1.87 (br, 1H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ 159.7, 157.3, 139.6 (d, *J* = 2.4 Hz), 128.5 (d, *J* = 52.8 Hz), 126.6, 108.1 (d, *J* = 21.6 Hz), 57.4 (d, *J* = 30.5 Hz), 31.4 (d, *J* = 9.0 Hz). ^{19}F NMR ($CDCl_3$, 376 MHz) δ -112.9 (s). HRMS-ESI calcd for $[M+Na]^+$: 189.0686, found: 189.0690.



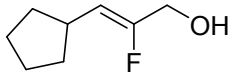
(*E*)-2-fluoro-5-methylhex-2-en-1-ol (1u)

Colorless oil, ^{1}H NMR ($CDCl_3$, 400 MHz) δ 4.93 – 4.73 (m, 1H), 4.11 (dd, *J* = 15.9, 0.8 Hz, 2H), 1.99 (dddt, *J* = 7.7, 6.9, 1.8, 0.8 Hz, 2H), 1.96 – 1.82 (br, 1H), 1.63 (dp, *J* = 13.4, 6.7 Hz, 1H), 0.90 (d, *J* = 6.7 Hz, 6H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ 158.0 (d, *J* = 253.5 Hz), 106.9 (d, *J* = 14.0 Hz), 61.6 (d, *J* = 32.7 Hz), 32.4 (d, *J* = 3.5 Hz), 28.4 (d, *J* = 1.8 Hz), 22.3. ^{19}F NMR ($CDCl_3$, 376 MHz) δ -120.9. HRMS-ESI calcd for $[M+Na]^+$: 155.0843, found: 155.0843.



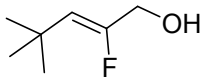
(*E*)-3-cyclohexyl-2-fluoroprop-2-en-1-ol (1v)

Colorless oil, ^{1}H NMR ($CDCl_3$, 400 MHz) δ 5.09 (dd, *J* = 21.3, 10.2 Hz, 1H), 4.23 (d, *J* = 21.4 Hz, 2H), 2.15 – 2.00 (m, 1H), 1.80 – 1.57 (m, 6H), 1.37 – 1.03 (m, 5H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ 158.0, 155.6, 115.4 (d, *J* = 16.9 Hz), 57.7 (d, *J* = 30.6 Hz), 35.2 (d, *J* = 7.7 Hz), 34.1 (d, *J* = 2.3 Hz), 25.9. ^{19}F NMR ($CDCl_3$, 376 MHz) δ -116.7 (s). HRMS-ESI calcd for $[M+Na]^+$: 181.0999, found: 181.0991.



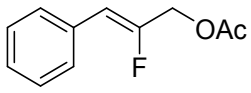
(*Z*)-3-cyclopentyl-2-fluoroprop-2-en-1-ol (1w)

Colorless oil, ^{1}H NMR ($CDCl_3$, 400 MHz) δ 5.12 (ddd, *J* = 21.1, 10.3, 2.1 Hz, 1H), 4.23 (d, *J* = 21.5 Hz, 2H), 2.59 – 2.38 (m, 1H), 2.35 – 1.92 (m, 1H), 1.80 (dt, *J* = 11.4, 8.8 Hz, 2H), 1.72 – 1.48 (m, 4H), 1.32 – 1.18 (m, 2H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ 156.8 (d, *J* = 246.7 Hz), 114.5 (d, *J* = 18.0 Hz), 57.5 (d, *J* = 30.3 Hz), 36.7 (d, *J* = 7.9 Hz), 34.2 (d, *J* = 2.2 Hz), 25.2. ^{19}F NMR ($CDCl_3$, 376 MHz) δ -116.0 (s). HRMS-ESI calcd for $[M+Na]^+$: 167.0837, found: 167.0841.



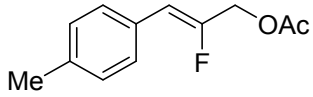
(*Z*)-2-fluoro-4,4-dimethylpent-2-en-1-ol (2x)

Colorless oil, ^{1}H NMR ($CDCl_3$, 400 MHz) δ 4.74 (d, *J* = 42.4 Hz, 1H), 4.04 (d, *J* = 15.8 Hz, 2H), 1.85 (br, 1H), 1.13 (s, 9H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ 156.2 (d, *J* = 257.6 Hz), 117.5 (d, *J* = 8.9 Hz), 62.4 (d, *J* = 32.5 Hz), 30.9 (d, *J* = 96.9 Hz), 30.5 (d, *J* = 3.3 Hz). ^{19}F NMR ($CDCl_3$, 376 MHz) δ -119.0. HRMS-ESI calcd for $[M+Na]^+$: 155.0843, found: 155.0869.



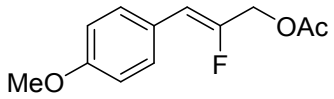
(*Z*)-2-fluoro-3-phenylallyl acetate (6a)

The characterization data is in agreement with the reported data.[3]



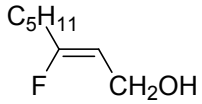
(*Z*)-2-fluoro-3-(p-tolyl)allyl acetate (6b)

White solid, ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.42 (d, *J* = 8.1 Hz, 2H), 7.16 (d, *J* = 8.0 Hz, 2H), 5.81 (d, *J* = 37.6 Hz, 1H), 4.73 (d, *J* = 18.1 Hz, 2H), 2.35 (s, 3H), 2.13 (s, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ 170.6, 153.6 (d, *J* = 265.0 Hz), 138.0 (d, *J* = 2.4 Hz), 129.5 (d, *J* = 3.3 Hz), 129.4, 128.9 (d, *J* = 7.4 Hz), 111.1 (d, *J* = 7.0 Hz), 63.2 (d, *J* = 30.7 Hz), 21.4, 20.9. ^{19}F NMR ($CDCl_3$, 376 MHz) δ -112.2. HRMS-ESI calcd for $[M+Na]^+$: 231.0792, found: 231.0793.



(*Z*)-2-fluoro-3-(4-methoxyphenyl)allyl acetate (6c) (unstable)

White solid, ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.51 – 7.37 (m, 2H), 6.88 (d, *J* = 8.9 Hz, 2H), 5.78 (d, *J* = 37.6 Hz, 1H), 4.71 (d, *J* = 18.5 Hz, 2H), 3.82 (s, 3H), 2.13 (s, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ 170.7, 159.4, 152.8 (d, *J* = 263.3 Hz), 130.4 (d, *J* = 7.6 Hz), 125.1, 114.1, 110.9 (d, *J* = 7.3 Hz), 63.3 (d, *J* = 30.5 Hz), 55.4, 21.0. ^{19}F NMR ($CDCl_3$, 376 MHz) δ -114.1. HRMS-ESI calcd for $[M+Na]^+$: 247.0741, found: 247.0766.

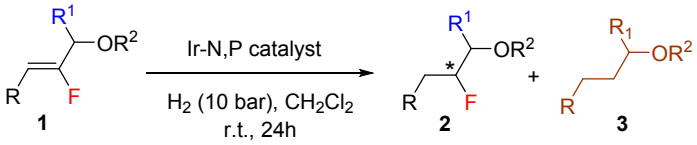


(*Z*)-3-fluorooct-2-en-1-ol (1y)

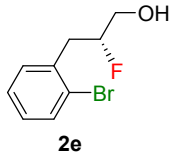
The compound was prepared according the reported procedure.[7]

3. Additional condition optimization

Table S1. Comparison study of catalyst **E** and catalyst **F** with various fluorinated allylic alcohols

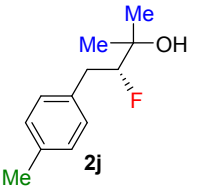


Cat-F > Cat-E



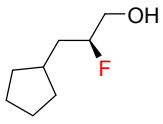
2e

Cat-**E**	Cat-ent-**F**
97% yield	97% yield
15% de-F	12% de-F
90% ee	93% ee



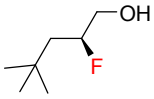
2j

Cat-**E**	Cat-ent-**F**
95% yield	97% yield
7% de-F	5% de-F
52% ee	95% ee



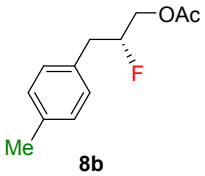
2w

Cat-**E**	Cat-**F**
99% yield	99% yield
0% de-F	0% de-F
43% ee	91% ee



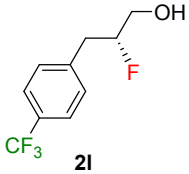
2x

Cat-**E**	Cat-**F**
31% conv.	71% yield
0% de-F	0% de-F
23% ee	71% ee



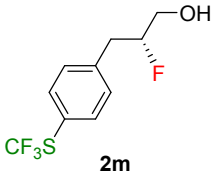
8b

Cat-**E**	Cat-ent-**F**
40% conv.	60% yield
24% de-F	8% de-F
93% ee	93% ee



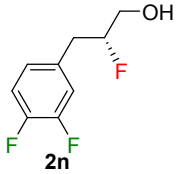
2l

Cat-**E**	Cat-ent-**F**
98% conv.	97% yield
9% de-F	7% de-F
85% ee	98% ee



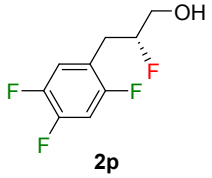
2m

Cat-**E**	Cat-ent-**F**
97% yield	97% yield
8% de-F	6% de-F
33% ee	95% ee



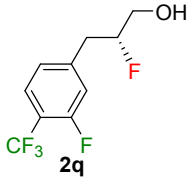
2n

Cat-**E**	Cat-ent-**F**
98% conv.	71% yield
8% de-F	5% de-F
83% ee	96% ee



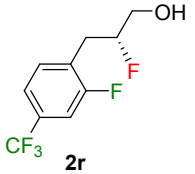
2p

Cat-**E**	Cat-ent-**F**
57% conv.	85% yield
19% de-F	4% de-F
48% ee	96% ee



2q

Cat-**E**	Cat-ent-**F**
73% conv.	98% yield
12% de-F	0% de-F
83% ee	98.5% ee



2r

Cat-**E**	Cat-ent-**F**
65% conv.	70% yield
20% de-F	9% de-F
38% ee	>99% ee

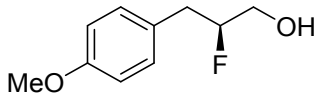
Reaction conditions: 0.25 mmol of substrate, 1 mol% catalyst, H_2 (10 bar), 2.0 mL CH_2Cl_2, r.t., 24 h. Yields are isolated hydrogenated product. Conversion was determined by ^{1}H-NMR spectroscopy. Enantiomeric excess was determined by SFC or GC/MS using chiral stationary phases.

4. General procedure for asymmetric hydrogenation

A vial was charged with substrate (0.015 mmol) and Ir-complex (1 mol%). Dry CH_2Cl_2 (1.5 ml) was added (so that the concentration of the substrate was 0.1 M) and the vial was placed in a high-pressure hydrogenation apparatus. The reactor was purged three times with Ar gas, then filled with H_2. The reaction was stirred at room temperature for 24 hours before the H_2 pressure was released and the solvent was removed *in vacuo*. The crude product was filtered through on a short plug of silica. Conversions were determined by ^{1}H NMR spectroscopy and *ee* values were determined by HPLC or SFC using a chiral stationary phase.

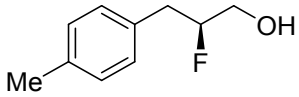
The full characterizations of the new hydrogenated products are available below (in some specific cases the hydrogenated product are characterized in the mixture with de-fluorinated product).

The characterization of the hydrogenated compounds:



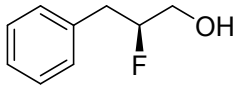
(*S*)-2-fluoro-3-(4-methoxyphenyl)propan-1-ol (2a)

The characterization data is in agreement with the reported data.[8]



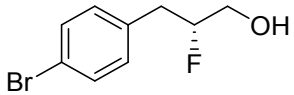
(*S*)-2-fluoro-3-(4-methylphenyl)propan-1-ol (2b)

Colorless oil, ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.13 – 7.11 (m, 4H), 4.71 (dtd, *J* = 31.0, 8.7, 7.0 Hz, 2H), 3.79 – 3.67(m, 2H), 2.34 (s, 3H), 2.02 (t, *J* = 6.3 Hz, 1H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ 136.5, 133.4 (d, *J* = 6.0 Hz), 129.4, 129.3, 95.4 (d, *J* = 170.1 Hz), 63.3 (d, *J* = 22.0 Hz), 37.1 (d, *J* = 21.4 Hz), 21.2. ^{19}F NMR ($CDCl_3$, 376 MHz) δ -187.5 (s). HRMS-ESI calcd for $C_{15}H_{21}NO_2$ $[M+Na]^+$: 191.0843, found: 191.0856.



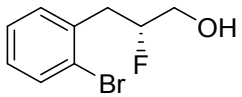
(*S*)-2-fluoro-3-phenylpropan-1-ol (2c)

The characterization data is in agreement with the reported data.[3]



(*R*)-3-(4-bromophenyl)-2-fluoropropan-1-ol (2d)

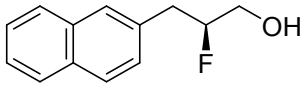
White solid, ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.49 – 7.38 (m, 2H), 7.12 (t, *J* = 5.3 Hz, 2H), 4.73 (ddtd, *J* = 48.5, 7.5, 5.7, 3.0 Hz, 1H), 3.89 – 3.57 (m, 2H), 2.94 (dqd, *J* = 19.9, 14.3, 6.5 Hz, 2H), 1.94 (t, *J* = 6.3 Hz, 1H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ 135.5 (d, *J* = 5.3 Hz), 131.8, 131.2, 120.9, 94.3 (d, *J* = 172.2 Hz), 64.1 (d, *J* = 21.9 Hz), 36.9 (d, *J* = 21.5 Hz). ^{19}F NMR ($CDCl_3$, 376 MHz) δ -188.2 (s). HRMS-ESI calcd for $[M+Na]^+$: 254.9791(256.9771), found: 254.9782 (256.9760).



(*R*)-3-(2-bromophenyl)-2-fluoropropan-1-ol (2e)

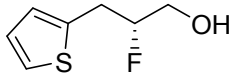
White solid, ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.44 – 7.33 (m, 2H), 7.21 – 7.12 (m, 2H), 4.75 (ddtd, *J* = 48.5, 7.6, 5.6, 3.0 Hz, 1H), 3.88 – 3.56 (m, 2H), 2.95 (dqd, *J* = 19.8, 14.3, 6.5 Hz, 2H), 1.98 (t, *J* = 6.3 Hz, 1H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ 138.9 (d, *J* = 5.2 Hz), 132.4, 130.2,

130.1, 128.1, 122.7, 94.3 (d, J = 172.4 Hz), 64.1 (d, J = 21.9 Hz), 37.1 (d, J = 21.6 Hz). ^{19}F NMR ($CDCl_3$, 376 MHz) δ -188.1 (s). HRMS-ESI calcd for $[M+Na]^+$: 254.9791(256.9771), found: 254.9802 (256.9787).



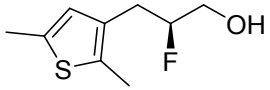
(*S*)-2-fluoro-3-(naphthalen-2-yl)propan-1-ol (2f)

White solid, ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.82 (ddd, J = 9.6, 6.9, 3.1 Hz, 3H), 7.70 (s, 1H), 7.51 – 7.44 (m, 2H), 7.38 (dd, J = 8.4, 1.6 Hz, 1H), 4.88 (ddtd, J = 48.6, 7.2, 5.9, 2.9 Hz, 1H), 3.96 – 3.64 (m, 2H), 3.29 – 3.03 (m, 2H), 2.00 – 1.91 (m, 1H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ 134.0 (d, J = 6.1 Hz), 133.6, 132.5, 128.4, 128.0, 127.8, 127.7, 127.6, 126.3, 125.8, 94.7 (d, J = 171.9 Hz), 64.3 (d, J = 21.8 Hz), 37.7 (d, J = 21.5 Hz). ^{19}F NMR ($CDCl_3$, 376 MHz) δ -187.3 (s). HRMS-ESI calcd for $[M+Na]^+$: 227.0843, found: 227.0856.



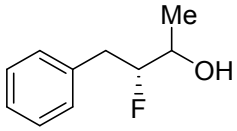
(*R*)-2-fluoro-3-(thiophen-2-yl)propan-1-ol (2g)

Brown oil, ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.19 (dd, J = 5.1, 1.2 Hz, 1H), 6.96 (dd, J = 5.1, 3.5 Hz, 1H), 6.92 – 6.88 (m, 1H), 4.78 (ddtd, J = 48.4, 6.9, 5.8, 3.0 Hz, 1H), 3.96 – 3.58 (m, 2H), 3.33 – 3.10 (m, 2H), 1.88 (t, J = 6.4 Hz, 1H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ 138.0 (d, J = 6.3 Hz), 127.2, 126.51, 124.6, 94.1 (d, J = 172.7 Hz), 64.0 (d, J = 21.8 Hz), 31.6 (d, J = 23.0 Hz). ^{19}F NMR ($CDCl_3$, 376 MHz) δ -187.3 (s). HRMS-ESI calcd for $[M+Na]^+$: 183.0250, found: 183.0245.



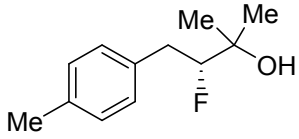
(*S*)-3-(2,5-dimethylthiophen-3-yl)-2-fluoropropan-1-ol (2h)

Brown solid, ^{1}H NMR ($CDCl_3$, 400 MHz) δ 6.49 (s, 1H), 4.70 (dqd, J = 48.7, 6.6, 2.8 Hz, 1H), 3.86 – 3.52 (m, 2H), 2.95 – 2.72 (m, 2H), 2.38 (s, 3H), 2.31 (s, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ 135.9, 132.7, 131.2 (d, J = 7.2 Hz), 127.2, 94.2 (d, J = 171.6 Hz), 64.3 (d, J = 21.7 Hz), 30.0 (d, J = 22.3 Hz), 15.2, 13.0. ^{19}F NMR ($CDCl_3$, 376 MHz) δ -186.7. HRMS-ESI calcd for $[M+Na]^+$: 211.0563, found: 211.0555.



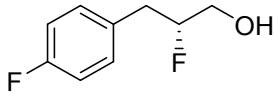
(*3R*)-3-fluoro-4-phenylbutan-2-ol (2i)

The characterization data is in agreement with the reported data.[5]



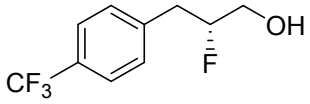
(*R*)-3-fluoro-2-methyl-4-p-tolylbutan-2-ol (2j)

White solid, ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.19 – 7.11 (m, 4H), 4.42 (ddd, J = 48.1, 8.7, 3.7 Hz, 1H), 3.03 – 2.79 (m, 2H), 2.34 (d, J = 2.6 Hz, 3H), 1.96 (d, J = 1.5 Hz, 1H), 1.30 (s, 6H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ 136.2, 134.9, 129.3, 129.1, 100.1 (d, J = 175.8 Hz), 72.1 (d, J = 20.4 Hz), 35.9 (d, J = 21.7 Hz), 25.5 (d, J = 4.1 Hz), 24.8 (d, J = 3.5 Hz), 21.2. ^{19}F NMR ($CDCl_3$, 376 MHz) δ -190.1 (s). HRMS-ESI calcd for $[M+Na]^+$: 219.1156, found: 219.1168.



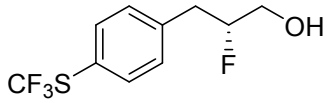
(*R*)-2-fluoro-3-(4-fluorophenyl)propan-1-ol (2k)

The characterization data is in agreement with the reported data.[8]



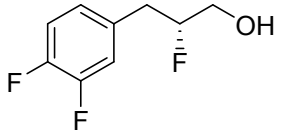
(*R*)-2-fluoro-3-(4-(trifluoromethyl)phenyl)propan-1-ol (2l)

White solid, ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.58 (d, *J* = 8.0 Hz, 2H), 7.36 (d, *J* = 8.1 Hz, 2H), 4.97 – 4.62 (m, 1H), 3.90 – 3.61 (m, 2H), 3.04 (dqd, *J* = 19.5, 14.4, 6.4 Hz, 2H), 2.05 (t, *J* = 6.2 Hz, 1H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ 140.7 (d, *J* = 4.8 Hz), 129.8, 129.6 – 128.7 (m), 125.6 (q, *J* = 3.8 Hz), 125.0 (d, *J* = 402.7 Hz), 94.2 (d, *J* = 172.6 Hz), 64.2 (d, *J* = 22.0 Hz), 37.3 (d, *J* = 21.5 Hz). ^{19}F NMR ($CDCl_3$, 376 MHz) δ -188.4 (s), -62.5 (s). HRMS-ESI calcd for $[M+Na]^+$: 245.0560, found: 245.0568.



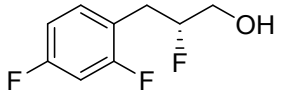
(*R*)-2-fluoro-3-(4-(trifluoromethylthio)phenyl)propan-1-ol (2m)

White solid, ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.61 (d, *J* = 8.1 Hz, 2H), 7.30 (d, *J* = 8.0 Hz, 2H), 4.93 – 4.62 (m, 1H), 3.76 (dddt, *J* = 23.7, 18.2, 12.4, 4.3 Hz, 2H), 3.13 – 2.88 (m, 2H), 1.95 (t, *J* = 6.3 Hz, 1H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ 139.9 (d, *J* = 4.9 Hz), 136.7, 130.6, 130.5 (d, *J* = 148.7 Hz), 128.3 – 122.6 (m), 94.2 (d, *J* = 172.5 Hz), 64.2 (d, *J* = 22.0 Hz), 37.2 (d, *J* = 21.6 Hz). ^{19}F NMR ($CDCl_3$, 376 MHz) δ -188.3 (s), -42.8 (s). HRMS-ESI calcd for $[M+Na]^+$: 275.0124, found: 275.0098.



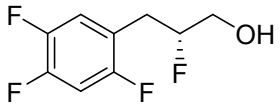
(*R*)-3-(3,4-difluorophenyl)-2-fluoropropan-1-ol (2n)

White solid, ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.16 – 7.00 (m, 2H), 6.99 – 6.91 (m, 1H), 4.87 – 4.58 (m, 1H), 3.88 – 3.57 (m, 2H), 3.06 – 2.80 (m, 2H), 2.00 (t, *J* = 6.3 Hz, 1H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ 150.3 (dd, *J* = 248.2, 12.7 Hz), 149.5 (dd, *J* = 247.1, 12.5 Hz), 133.5 (dd, *J* = 9.4, 5.3 Hz), 125.4 (dd, *J* = 6.1, 3.6 Hz), 118.3 (d, *J* = 17.1 Hz), 117.4 (d, *J* = 17.1 Hz), 94.2 (d, *J* = 172.3 Hz), 64.1 (d, *J* = 22.0 Hz), 36.7 (dd, *J* = 21.6, 1.1 Hz). ^{19}F NMR ($CDCl_3$, 376 MHz) δ -188.6 (s), -140.8 (d, *J* = 21.3 Hz), -137.8 (d, *J* = 21.2 Hz). HRMS-ESI calcd for $[M+Na]^+$: 213.0498, found: 213.0542.



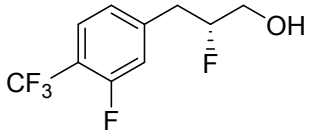
(*R*)-3-(2,4-difluorophenyl)-2-fluoropropan-1-ol (2o)

White solid, ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.31 – 7.14 (m, 1H), 6.89 – 6.73 (m, 2H), 4.91 – 4.62 (m, 1H), 3.94 – 3.57 (m, 2H), 2.96 (ddd, *J* = 20.7, 15.4, 5.7 Hz, 2H), 1.94 (t, *J* = 6.4 Hz, 1H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ 162.2 (dd, *J* = 247.8, 12.0 Hz), 161.2 (dd, *J* = 247.8, 11.9 Hz), 132.5 (dd, *J* = 9.5, 6.2 Hz), 119.3 (ddd, *J* = 15.9, 5.5, 3.9 Hz), 111.5 (dd, *J* = 21.1, 3.8 Hz), 104.2 – 103.7 (m), 93.4 (d, *J* = 172.1 Hz), 64.2 (d, *J* = 21.7 Hz), 30.3 (dd, *J* = 22.5, 1.8 Hz). ^{19}F NMR ($CDCl_3$, 376 MHz) δ -188.7 (d, *J* = 3.0 Hz), -113.7 (dd, *J* = 7.1, 3.1 Hz), -111.9 (d, *J* = 7.0 Hz). HRMS-ESI calcd for $[M+Na]^+$: 213.0498, found: 213.0519.



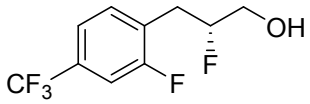
(*R*)-2-fluoro-3-(2,4,5-trifluorophenyl)propan-1-ol (2p)

White solid, ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.11 (ddd, *J* = 10.3, 8.7, 6.9 Hz, 1H), 7.00 – 6.85 (m, 1H), 4.91 – 4.59 (m, 1H), 3.91 – 3.56 (m, 2H), 2.96 (ddd, *J* = 12.2, 5.7, 3.4 Hz, 2H), 1.91 (t, *J* = 6.4 Hz, 1H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ 156.2 (ddd, *J* = 244.3, 9.2, 2.6 Hz), 150.6 – 145.4 (m), 148.2 – 147.7 (m), 119.9 (dd, *J* = 18.1, 5.7 Hz), 119.6 – 119.2 (m), 105.6 (dd, *J* = 28.5, 20.8 Hz), 93.0 (d, *J* = 172.6 Hz), 64.2 (d, *J* = 21.8 Hz), 30.2 (d, *J* = 22.5 Hz). ^{19}F NMR ($CDCl_3$, 376 MHz) δ -189.2 (d, *J* = 3.0 Hz), -142.8 (dd, *J* = 21.5, 15.3 Hz), -135.3 (dd, *J* = 21.4, 3.4 Hz), -119.4 (dt, *J* = 15.3, 3.2 Hz). HRMS-ESI calcd for $[M+Na]^+$: 231.0403, found: 231.0440.



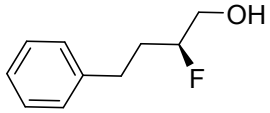
(*R*)-2-fluoro-3-(3-fluoro-4-(trifluoromethyl)phenyl)propan-1-ol (2q)

White solid, ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.54 (t, *J* = 7.9 Hz, 1H), 7.12 (dd, *J* = 9.1, 5.9 Hz, 2H), 4.94 – 4.61 (m, 1H), 3.96 – 3.57 (m, 2H), 3.18 – 2.88 (m, 2H), 1.97 (t, *J* = 5.9 Hz, 1H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ 159.9 (d, *J* = 256.2 Hz), 143.9, 127.4 (dd, *J* = 4.5, 1.9 Hz), 125.1 (d, *J* = 3.4 Hz), 124.3 – 121.4 (m), 117.9 (d, *J* = 20.6 Hz), 117.0 (dd, *J* = 33.1, 12.4 Hz), 93.7 (d, *J* = 173.1 Hz), 64.1 (d, *J* = 22.2 Hz), 37.1 (d, *J* = 21.6 Hz). ^{19}F NMR ($CDCl_3$, 376 MHz) δ -188.8 (s), -114.5 (q, *J* = 12.8 Hz), -61.3 (d, *J* = 12.5 Hz). HRMS-ESI calcd for $[M+Na]^+$: 263.0466, found: 263.0502.



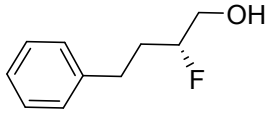
(*R*)-2-fluoro-3-(2-fluoro-4-(trifluoromethyl)phenyl)propan-1-ol (2r)

White solid, ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.45 – 7.35 (m, 2H), 7.33 (t, *J* = 6.4 Hz, 1H), 4.93 – 4.69 (m, 1H), 3.91 – 3.61 (m, 2H), 3.15 – 3.03 (m, 2H), 2.00 (t, *J* = 6.3 Hz, 1H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ 160.9 (d, *J* = 247.8 Hz), 132.6 (d, *J* = 4.7 Hz), 131.4 (dd, *J* = 33.5, 8.0 Hz), 127.9 (dd, *J* = 16.6, 4.5 Hz), 123.4 (dd, *J* = 272.2, 2.7 Hz), 121.5 – 121.0 (m), 113.0 (dd, *J* = 25.6, 3.9 Hz), 93.0 (d, *J* = 172.7 Hz), 64.3 (d, *J* = 21.7 Hz), 30.8 (dd, *J* = 22.4, 1.9 Hz). ^{19}F NMR ($CDCl_3$, 376 MHz) δ -189.0 (d, *J* = 3.6 Hz), -115.5 (d, *J* = 3.9 Hz), -62.7 (s). HRMS-ESI calcd for $[M+Na]^+$: 263.0466, found: 263.0477.



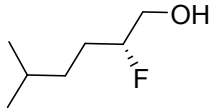
(*S*)-2-fluoro-4-phenylbutan-1-ol (2s)

The characterization data is in agreement with the reported data.[9]



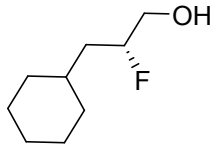
(*R*)-2-fluoro-4-phenylbutan-1-ol (2t)

The characterization data is in agreement with the reported data.[9]



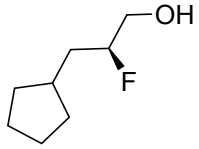
(*R*)-2-fluoro-5-methylhexan-1-ol (2u) (volatile)

Colorless oil, ^{1}H NMR ($CDCl_3$, 400 MHz) δ 4.66 – 4.44 (m, 1H), 3.80 – 3.58 (m, 2H), 1.88 (br, 1H), 1.77 – 1.45 (m, 3H), 1.43 – 1.14 (m, 2H), 0.90 (dd, J = 6.6, 1.8 Hz, 6H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ 95.2 (d, J = 167.6 Hz), 65.2 (d, J = 21.7 Hz), 34.1 (d, J = 4.6 Hz), 29.0 (d, J = 20.4 Hz), 28.1, 22.6 (d, J = 8.0 Hz). ^{19}F NMR ($CDCl_3$, 376 MHz) δ -189.3. HRMS-ESI calcd for $[M+Na]^+$: 157.0999, found: 157.0982.



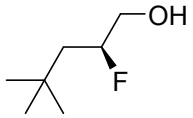
(*R*)-3-cyclohexyl-2-fluoropropan-1-ol (2v)

Colorless oil, ^{1}H NMR ($CDCl_3$, 400 MHz) δ 4.82 – 4.56 (m, 1H), 3.77 – 3.56 (m, 2H), 1.89 – 1.06 (m, 12H), 0.92 (ddt, J = 15.3, 12.4, 7.8 Hz, 2H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ 93.0 (d, J = 167.0 Hz), 65.7 (d, J = 21.7 Hz), 38.6 (d, J = 19.9 Hz), 34.0 (d, J = 3.5 Hz), 33.5 (d, J = 103.8 Hz), 26.6 (s), 26.3 (d, J = 14.0 Hz). ^{19}F NMR ($CDCl_3$, 376 MHz) δ -189.7 (s). HRMS-ESI calcd for $[M+Na]^+$: 183.1156, found: 183.1171.



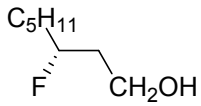
(*R*)-3-cyclopentyl-2-fluoropropan-1-ol (2w) (volatile)

Colorless oil, ^{1}H NMR ($CDCl_3$, 400 MHz) δ 4.76 – 4.49 (m, 1H), 3.79 – 3.58 (m, 2H), 2.04 – 1.67 (m, 5H), 1.68 – 1.38 (m, 5H), 1.16 – 1.04 (m, 2H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ 94.6 (d, J = 167.2 Hz), 65.5 (d, J = 21.7 Hz), 37.1 (d, J = 19.8 Hz), 36.3 (d, J = 4.0 Hz), 32.9 (d, J = 48.8 Hz), 25.1 (d, J = 16.6 Hz). ^{19}F NMR ($CDCl_3$, 376 MHz) δ -189.6 (s). HRMS-ESI calcd for $[M+Na]^+$: 169.0999, found: 169.0992.



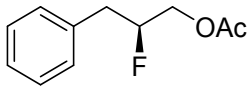
(*S*)-2-fluoro-4,4-dimethylpentan-1-ol (2x)

Colorless oil, ^{1}H NMR ($CDCl_3$, 400 MHz) δ 4.82 – 4.64 (m, 1H), 3.68 – 3.57 (m, 2H), 1.88 (br, 1H), 1.67 – 1.60 (m, 1H), 1.46 – 1.24 (m, 1H), 0.98 (d, J = 0.9 Hz, 9H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ 92.8 (d, J = 167.2 Hz), 66.4 (d, J = 22.2 Hz), 44.5 (d, J = 19.2 Hz), 29.9 (d, J = 1.4 Hz), 29.7 (d, J = 42.7 Hz). ^{19}F NMR ($CDCl_3$, 376 MHz) δ -185.9. HRMS-ESI calcd for $[M+Na]^+$: 157.0999, found:157.0985.



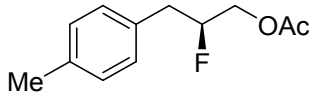
(*R*)-3-fluorooctan-1-ol (2y)

Colorless oil, ^{1}H NMR ($CDCl_3$, 400 MHz) δ 4.70 (dtt, J = 49.63, 7.87, 3.88 Hz, 1H), 3.89 – 3.74 (m, 2H), 1.95 – 1.6 1(m, 3H), 1.54 – 1.42 (m, 2H), 1.40 – 1.24 (m, 5H), 0.90 (t, J = 6.73 Hz, 3H). 19F NMR ($CDCl_3$, 376 MHz,) δ -182.3. ^{13}C NMR ($CDCl_3$, 100 MHz) δ 92.9 (d, J = 165.40 Hz), 59.7 (d, J = 4.23 Hz), 38.0 (d, J = 20.11 Hz), 35.5 (d, J = 20.52 Hz), 31.8, 24.8 (d, J = 4.65 Hz), 22.7, 14.1. HRMS-ESI calcd for $[M+Na]^+$: 171.1156, found: 171.1164.



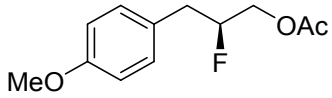
(*S*)-2-fluoro-3-phenylpropyl acetate (7a)

The characterization data is in agreement with the reported data.[3]



(*S*)-2-fluoro-3-(p-tolyl)propyl acetate (7b)

Colorless oil, ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.15 – 7.05 (m, 4H), 4.97 – 4.73 (m, 1H), 4.31 – 4.03 (m, 2H), 3.12 – 2.78 (m, 2H), 2.33 (s, 3H), 2.11 (s, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ 170.9, 136.7, 132.8 (d, J = 5.6 Hz), 129.5, 129.3, 91.7 (d, J = 175.8 Hz), 65.2 (d, J = 22.1 Hz), 37.6 (d, J = 21.3 Hz), 21.2, 20.9. ^{19}F NMR ($CDCl_3$, 376 MHz) δ -185.0. HRMS-ESI calcd for $[M+Na]^+$: 233.0948, found: 233.0926.

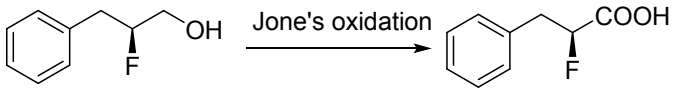


(*S*)-2-fluoro-3-(4-methoxyphenyl)propyl acetate (7c) (unstable)

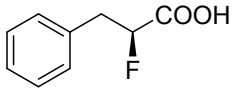
Colorless oil, ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.14 (d, J = 8.5 Hz, 2H), 6.92 – 6.76 (m, 2H), 4.84 (dqd, J = 48.5, 6.4, 2.8 Hz, 1H), 4.31 – 4.04 (m, 2H), 3.79 (s, 3H), 3.09 – 2.78 (m, 2H), 2.11 (s, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ 170.9, 158.8, 130.4, 127.9 (d, J = 5.6 Hz), 114.2, 91.7 (d, J = 175.6 Hz), 65.2 (d, J = 22.1 Hz), 55.4, 37.2 (d, J = 21.3 Hz), 20.9. ^{19}F NMR ($CDCl_3$, 376 MHz) δ -185.1. HRMS-ESI calcd for $[M+Na]^+$: 249.0897, found: 249.0869.

5. Synthesis of chiral fluorine molecule with different functional group.

1) Jone's oxidation



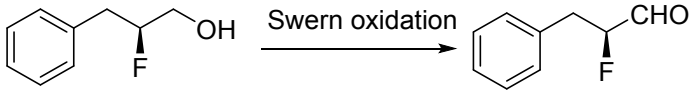
To a solution of (*S*)-2-fluoro-3-phenylpropan-1-ol (0.4 g, 2.6 mmol) in acetone, Jone's reagent (2 ml) was slowly added under ice bath. The solution then was slowly warmed to room temperature and reacted for 1h. Isopropanol was added dropwise to quench the excess Jone's regent. The reaction mixture was treated sodium bicarbonate until PH ~ 5, then was extracted twice with DCM. The aqueous phase was acidified using 1M HCl solution and was extracted 3 times with ether. The combined ether was washed with brine, dried over Na_2SO_4, crystallized to give white solid (0.36g, 82% yield).



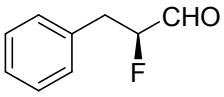
(*S*)-2-fluoro-3-phenylpropanoic acid (3)

The characterization data is in agreement with the reported data.[10]

2) Swern oxidation



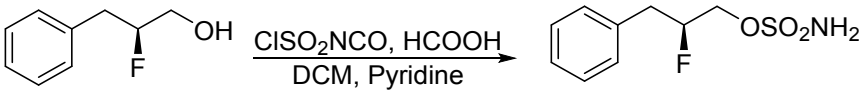
To a stirred solution of $(COCl)_2$ (0.4 g, 3.17 mmol) in anhydrous CH_2C1_2 (5 ml) at -78°C was added a solution of DMSO (0.47 g, 6.0 mmol) in anhydrous CH_2C1_2 (3 ml) slowly. The mixture was stirred at -78°C for 15 min. (*S*)-2-fluoro-3-phenylpropan-1-ol (0.4 g, 2.6 mmol) in CH_2C1_2 (10 ml) was added slowly and the mixture was stirred at -78°C for 45 min. TEA (0.79 g, 7.8 mmol) was added and the mixture was stirred at -78°C for another l h, followed by warming up to 0°C in 40 min. Water (4 ml) was added to quench the reaction and the mixture was extracted with CH_2C1_2 (40 ml x3). The combined organic layers were washed with brine, dried over Na_2SO_4, filtered and concentrated. The crude was purified by column chromatography.



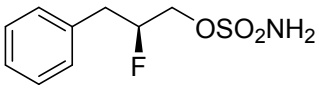
(*S*)-2-fluoro-3-phenylpropanal (4)

The characterization data is in agreement with the reported data.[11]

3) Synthesis of (*S*)-2-fluoro-3-phenylpropyl sulfamate



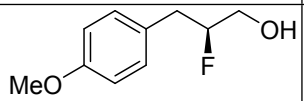
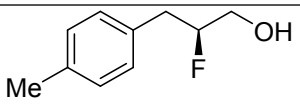
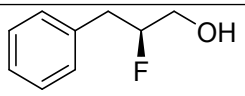
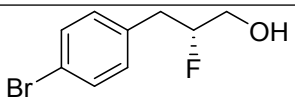
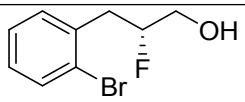
To chlorosulfonyl isocyanate (1.5 eq), formic acid (1.5 eq) was added dropwise at 0 °C. The resulting solid was allowed to stir at 0 °C for a further 20 minutes. The residue was diluted with dichloromethane and warmed to room temperature for one hour. The reaction mixture was cooled in an ice/salt bath and a solution of (*S*)-2-fluoro-3-phenylpropan-1-ol (1.0 eq) in pyridine (1.5 eq) and dichloromethane was added, keeping the temperature below 7 °C. After 2 hours, the reaction was concentrated in vacuo, diluted with ethyl acetate, washed with saturated sodium bicarbonate solution and brine. The organic layer was dried over sodium sulfate, filtered and concentrated in vacuo. The residue was purified by column chromatography on silica gel to give a white solid.

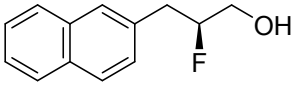
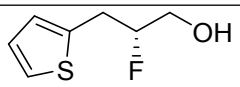
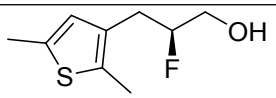
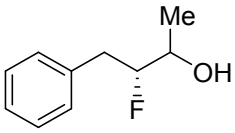
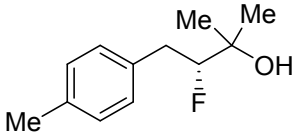
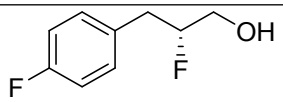
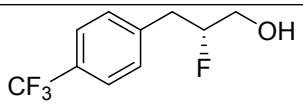
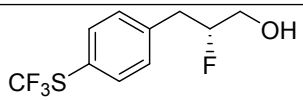
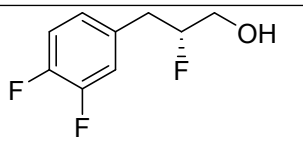
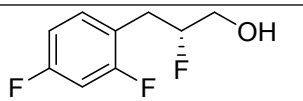


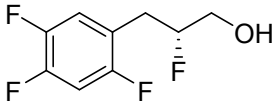
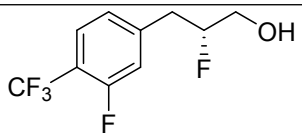
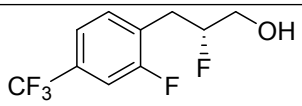
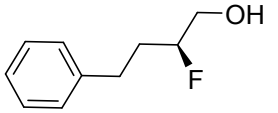
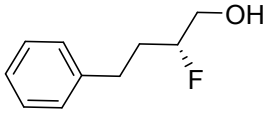
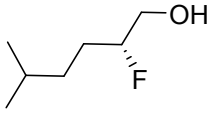
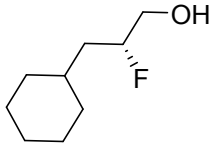
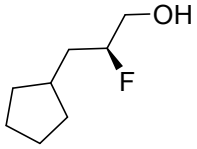
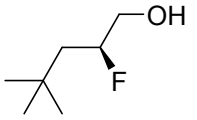
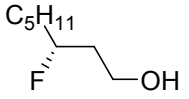
(*S*)-2-fluoro-3-phenylpropyl sulfamate (5)

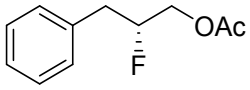
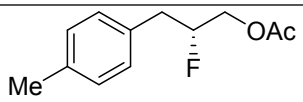
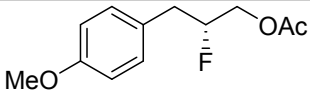
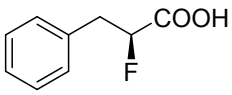
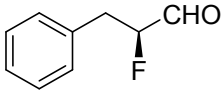
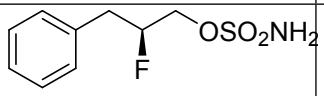
White solid, 87% yield. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.40 – 7.17 (m, 5H), 5.01 – 4.57 (m, 3H), 4.37 – 4.07 (m, 2H), 3.11 – 2.88 (m, 2H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ 136.0, 129.4, 128.8, 127.1, 91.9 (d, J = 175.8 Hz), 66.0 (d, J = 21.8 Hz), 37.9 (d, J = 21.2 Hz). ^{19}F NMR ($CDCl_3$, 376 MHz) δ -185.5. HRMS-ESI calcd for $[M+Na]^+$: 256.0414, found: 256.0405.

6. Separation method data and specific rotation of chiral compounds

Entry	Product	Separation method	Optical rotation	*ee* (%)
1		**HPLC**, ASH column, 5% MeOH, 0.5 ml/min, t_R = 40.6 min (major) / 47.4 (minor)	$[\alpha]_D^{25.0}$ = -19 (C= 0.10 in $CHCl_3$)	97
2		**SFC**, IA column, 10% MeOH, 2 ml/min, t_R = 4.1 min (minor)/5.1 (major)	$[\alpha]_D^{25.0}$ = -20 (C= 0.10 in $CHCl_3$)	93
3		**SFC**, IF column, 5% MeOH, 2 ml/min, t_R = 6.3 min (minor) / 9.9 (major)	$[\alpha]_D^{25.0}$ = +13 (C= 0.10 in $CHCl_3$)	97
4		**SFC**, AYH column, 5% MeOH, 2 ml/min, t_R = 10.7 min (major) / 13.1 (minor)	$[\alpha]_D^{25.0}$ = +13 (C= 0.10 in $CHCl_3$)	95
5		**SFC**, AYH column, 5% MeOH, 2 ml/min,	$[\alpha]_D^{25.0}$ = +20 (C= 0.10 in $CHCl_3$)	93

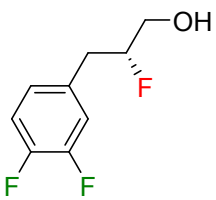
		t_R = 11.3 min (major) / 12.7 (minor)		
6		**SFC**, IB column, 5% MeOH, 2 ml/min, t_R = 12.6 min (minor) / 14.3 (major)	$[\alpha]_D^{25.0}$ = -15 (C= 0.10 in $CHCl_3$)	96
7		**SFC**, IA column, 5% MeOH, 2 ml/min, t_R = 6.2 min (minor) / 8.1 (major)	$[\alpha]_D^{25.0}$ = +9 (C= 0.10 in $CHCl_3$)	97
8		**GC-MS**, Hydrodex β-6TBDM, 120 °C iso, 1 degree/min, t_R = 58.8min (major) / 64.5 (minor)	$[\alpha]_D^{25.0}$ = -12 (C= 0.10 in $CHCl_3$)	98
9		**SFC**, ID column, 5% MeOH, 2 ml/min, t_{R1} = 4.4 min (major) / 6.2 (minor); t_{R2}=5.7 min (only)	$[\alpha]_D^{25.0}$ = +21 (C= 0.10 in $CHCl_3$)	91 and 99
10		**GC-MS**, Hydrodex β-6TBDM, 100 °C iso 150 min, 1 degree/min, t_R = 138.0 min (minor) / 139.7 (major)	$[\alpha]_D^{25.0}$ = +40 (C= 0.54 in $CHCl_3$)	95
11		**GC-MS**, Hydrodex β-DM, 100 °C iso 120 min, 1 degree/min, t_R = 83.3 min (major) / 88.2 (minor)	$[\alpha]_D^{25.0}$ = +16 (C= 0.10 in $CHCl_3$)	98
12		**GC-MS**, Hydrodex β-DM, 100 °C iso 200 min, 1 degree/min, t_R = 77.8 min (major) / 82.8 (minor)	$[\alpha]_D^{25.0}$ = +15 (C= 0.10 in $CHCl_3$)	98
13		**GC-MS**, Hydrodex β-DM, 100 °C iso 240 min, 1 degree/min, t_R = 187.0 min (major) /207.1 (minor)	$[\alpha]_D^{25.0}$ = +6 (C= 0.10in $CDCl_3$)	95
14		**SFC**, IA column, 5% MeOH, 2 ml/min, t_R = 9.2 min (minor)/9.8 (major)	$[\alpha]_D^{25.0}$ = +9 (C= 0.10 in $CHCl_3$)	96
15		**SFC**, IF column, 5% MeOH, 2 ml/min, t_R = 7.2 min (minor)/8.6	$[\alpha]_D^{25.0}$ = +15 (C= 0.77 in $CHCl_3$)	92

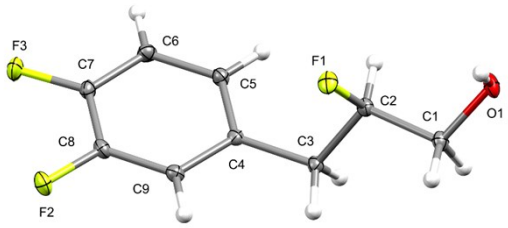
		(major)		
16		**GC-MS**, Hydrodex β-DM, 70 °C iso 150 min, 1 degree/min, t_R = 57.0 min (major) /61.6 (minor)	$[\alpha]_D^{25.0}$ = +20 (C= 0.73 in $CHCl_3$)	96
17		**GC-MS**, Hydrodex β-6TBDM, 100 °C iso 300 min, 1 degree/min, t_R = 188.3 min (major) /203.1 (minor)	$[\alpha]_D^{25.0}$ = +11 (C= 0.10 in $CHCl_3$)	99
18		**SFC**, IA column, 5% MeOH, 2 ml/min, t_R = 6.4 (only)	$[\alpha]_D^{25.0}$ = +19 (C= 0.45in $CHCl_3$)	99
19		**GC-MS**, Hydrodex β-DM, 90 °C iso 100 min, 1 degree/min, t_R = 70.2 min (major) /75.7 (minor)	$[\alpha]_D^{25.0}$ = -20.3 (C= 0.30 in $CHCl_3$)	85
20		**GC-MS**, Hydrodex β-DM, 90 °C iso 100 min, 1 degree/min, t_R = 71.7 min (minor) /75.2 (major)	$[\alpha]_D^{25.0}$ = +21 (C= 0.10 in $CHCl_3$)	89
21		**GC-MS**, Hydrodex β-DM, 90 °C iso 100 min, 1 degree/min, t_R = 67.9 min (major) /72.23 (minor)	$[\alpha]_D^{25.0}$ = +10 (C= 0.10 in $CHCl_3$)	89
22		**GC-MS**, Hydrodex β-DM, 90 °C iso 100 min, 1 degree/min, t_R = 45.9 min (minor) /54.0 (major)	$[\alpha]_D^{25.0}$ = +1 (C= 0.10 in $CHCl_3$)	92
23		**GC-MS**, Hydrodex β-DM, 70 °C iso 180 min, 1 degree/min, t_R = 92.6 min (minor) /95.7 (major)	$[\alpha]_D^{25.0}$ = -14 (C= 0.10 in $CHCl_3$)	91
24		**GC-MS**, Hydrodex β-DM, 70 °C iso 180 min, 1 degree/min, t_R = 29.6 min (minor) /31.3 (major)	$[\alpha]_D^{25.0}$ = -6 (C= 0.10 in $CHCl_3$)	71
25		**GC-MS**, Hydrodex β-DM, 50 °C iso 180	$[\alpha]_D^{25.0}$ = -6	83

		min, 1 degree/min, t_R = 128.7 min (minor) /129.6 (major)	(C= 0.10 in $CHCl_3$)	
26		**SFC**, OJH column, 5% MeOH, 2 ml/min, t_R = 4.1 min (minor)/4.5 (major)	$[\alpha]_D^{25.0}$ = -14 (C= 0.10 in $CHCl_3$)	94
27		**SFC**, OJH column, 5% MeOH, 2 ml/min, t_R = 5.6 min (minor)/ 6.0 (major)	$[\alpha]_D^{25.0}$ = -17 (C= 0.10 in $CHCl_3$)	93
28		**SFC**, OJH column, 5% MeOH, 2 ml/min, t_R = 4.3 min (minor)/4.5 (major)	$[\alpha]_D^{25.0}$ = -12 (C= 0.10 in $CHCl_3$)	94
29		**SFC**, OJH column, 5% MeOH, 2 ml/min, t_R = 15.2 min (minor)/17.2 (major)	$[\alpha]_D^{25.0}$ = -6 (C= 0.10 in $CHCl_3$)	97
30		**SFC**, AYH column, 5% MeOH, 2 ml/min, t_R = 12.9 min (major)/14.3 (minor)	$[\alpha]_D^{25.0}$ = -5 (C= 0.10 in $CHCl_3$)	97
31		**SFC**, AYH column, 5% MeOH, 2 ml/min, t_R = 7.6 min (major)/8.2 (minor)	$[\alpha]_D^{25.0}$ = -16 (C= 0.10 in $CHCl_3$)	97

7. Absolute configuration determination

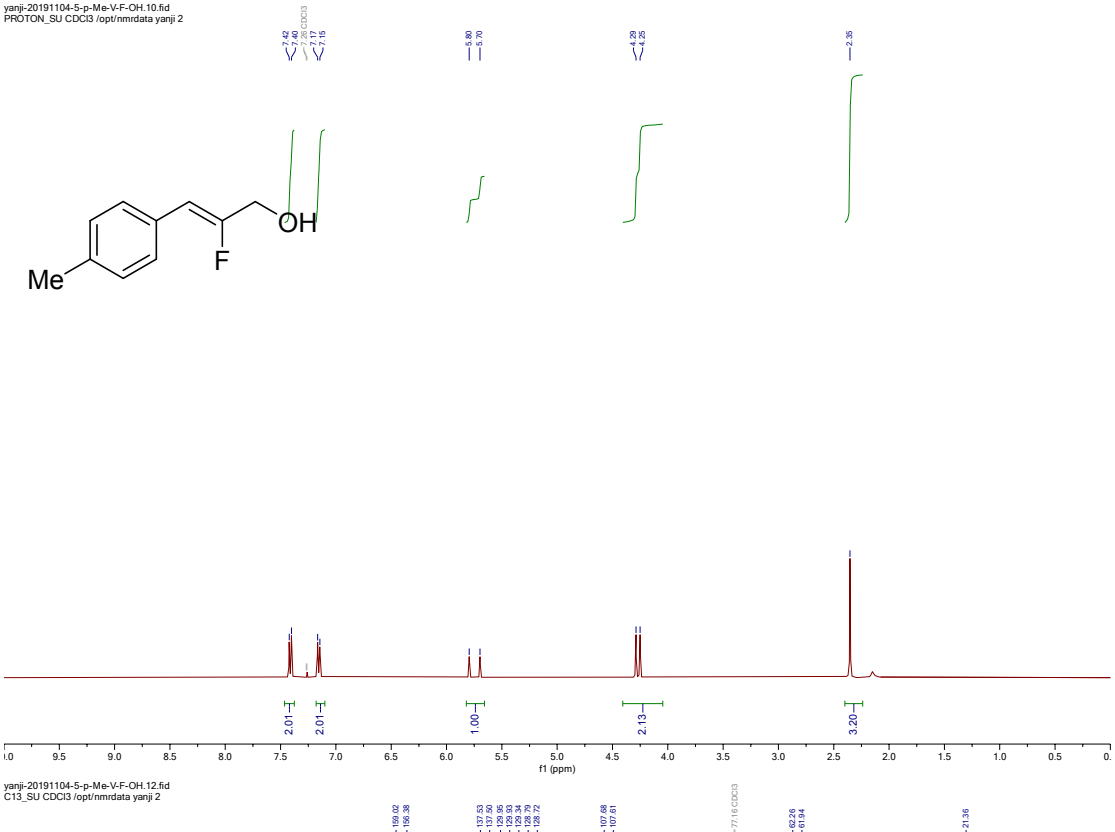
Single crystal of **2n** was grown by dissolving in pentane/diethyl ether mixture and slow evaporation at room temperature. Detailed information for this crystal is available in CCDC 1976216.

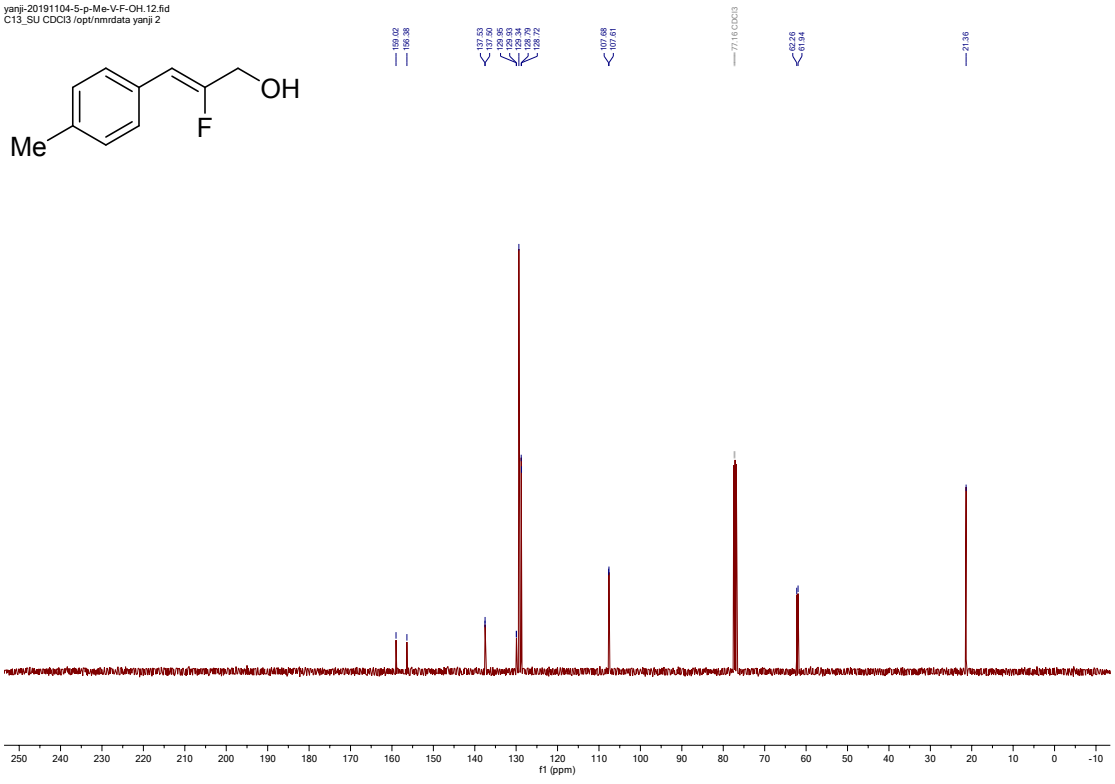


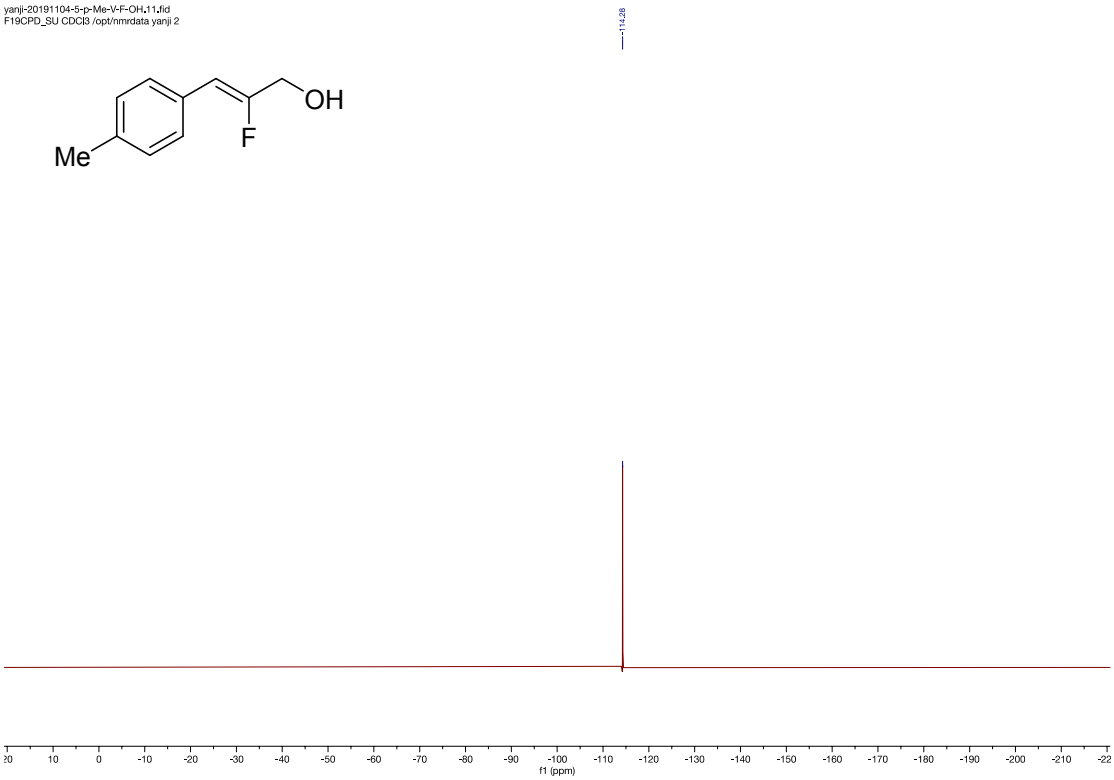


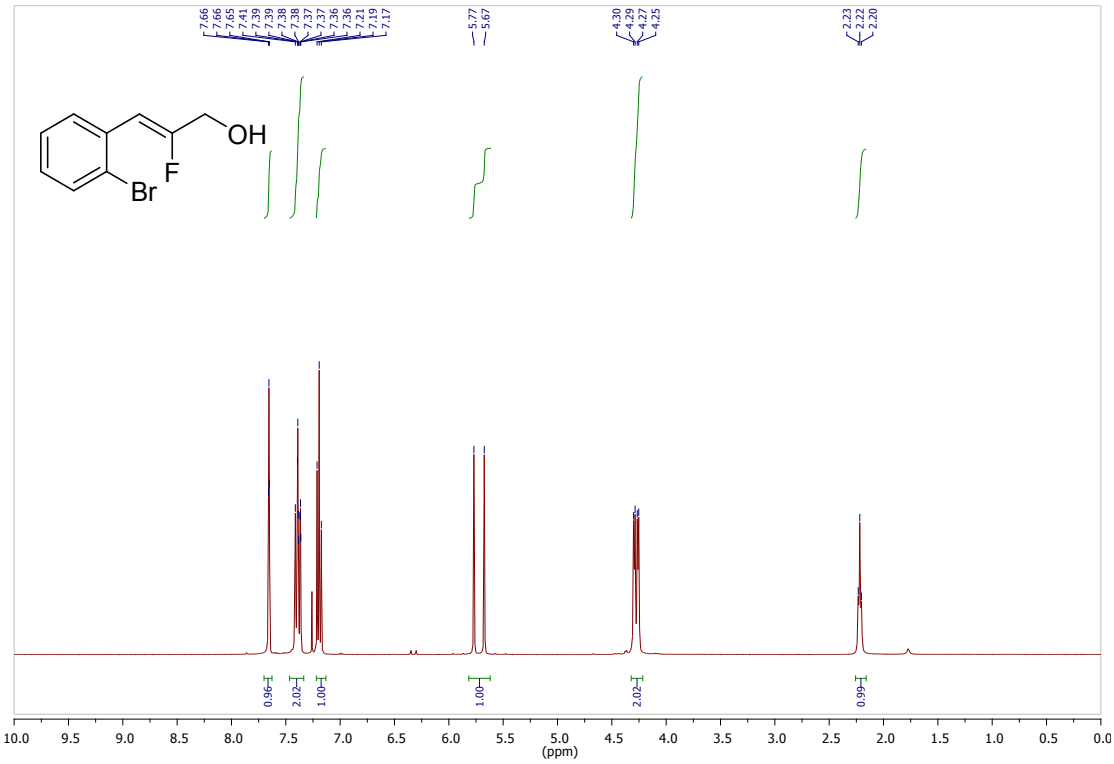
X-ray crystal structure of **2n**

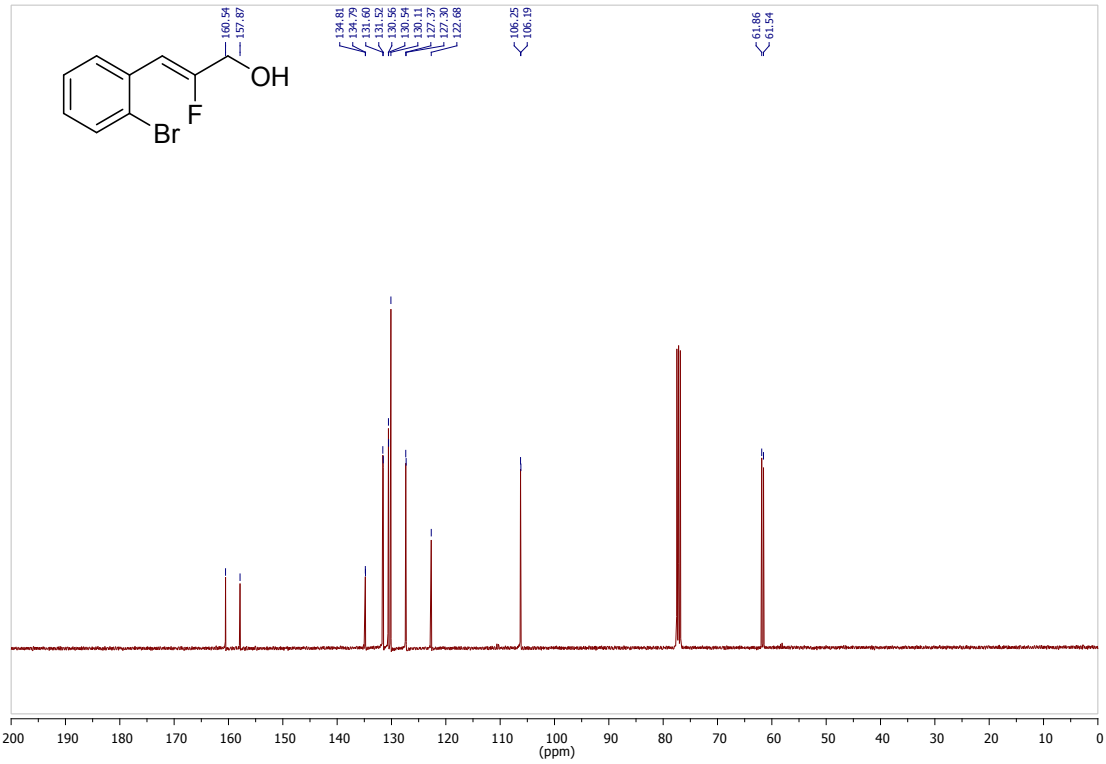
8. NMR **Spectra**

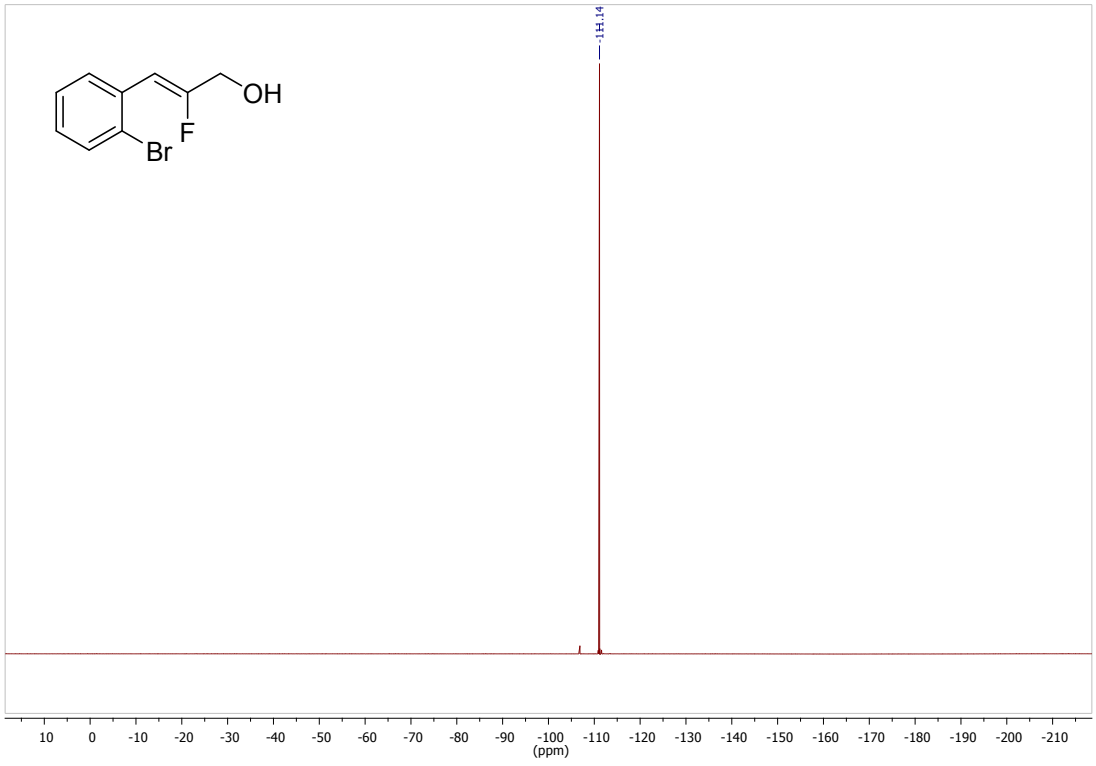




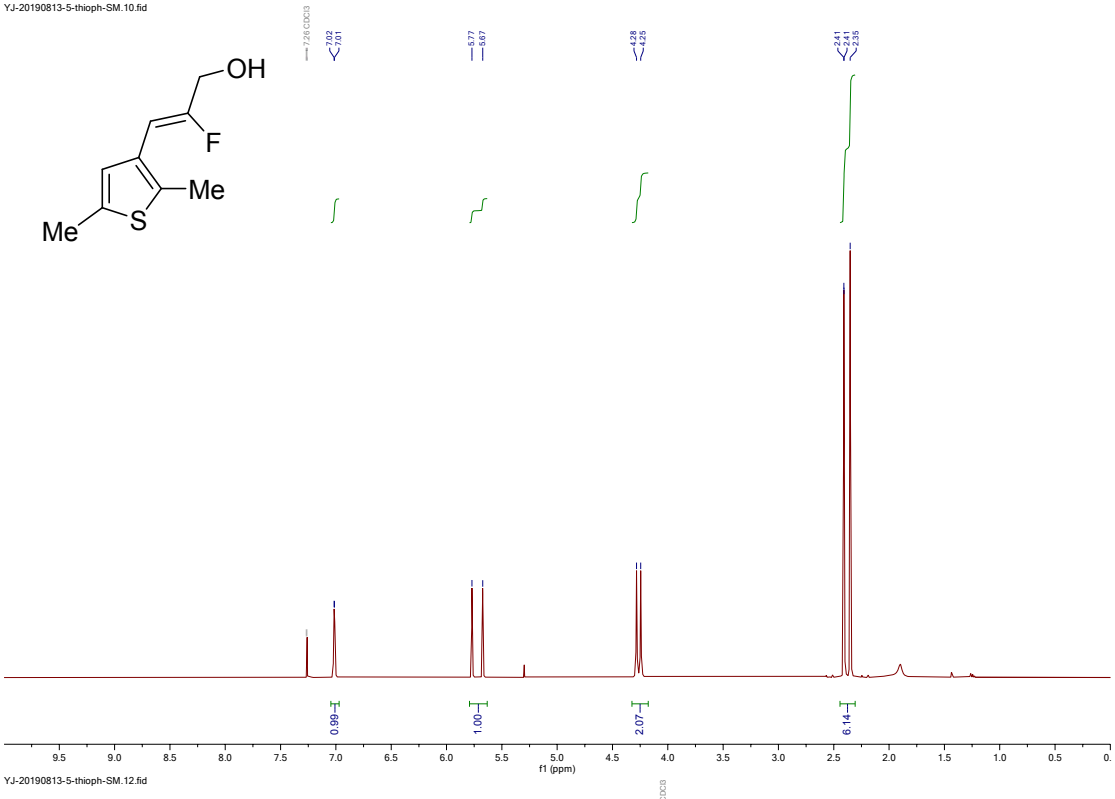

yanji-20191104-5-p-Me-V-F-OH,11.fid
F19CPD_SU CDCl3 /opt/nmrdata yanji 2
-114.28
OH
F
Me
f1 (ppm)


7.66
7.66
7.65
7.41
7.39
7.39
7.38
7.38
7.37
7.37
7.36
7.36
7.21
7.19
7.17
5.77
5.67
4.30
4.29
4.27
4.25
2.23
2.22
2.20
OH
F
Br
0.96
2.02
1.00
1.00
2.02
0.99
(ppm)

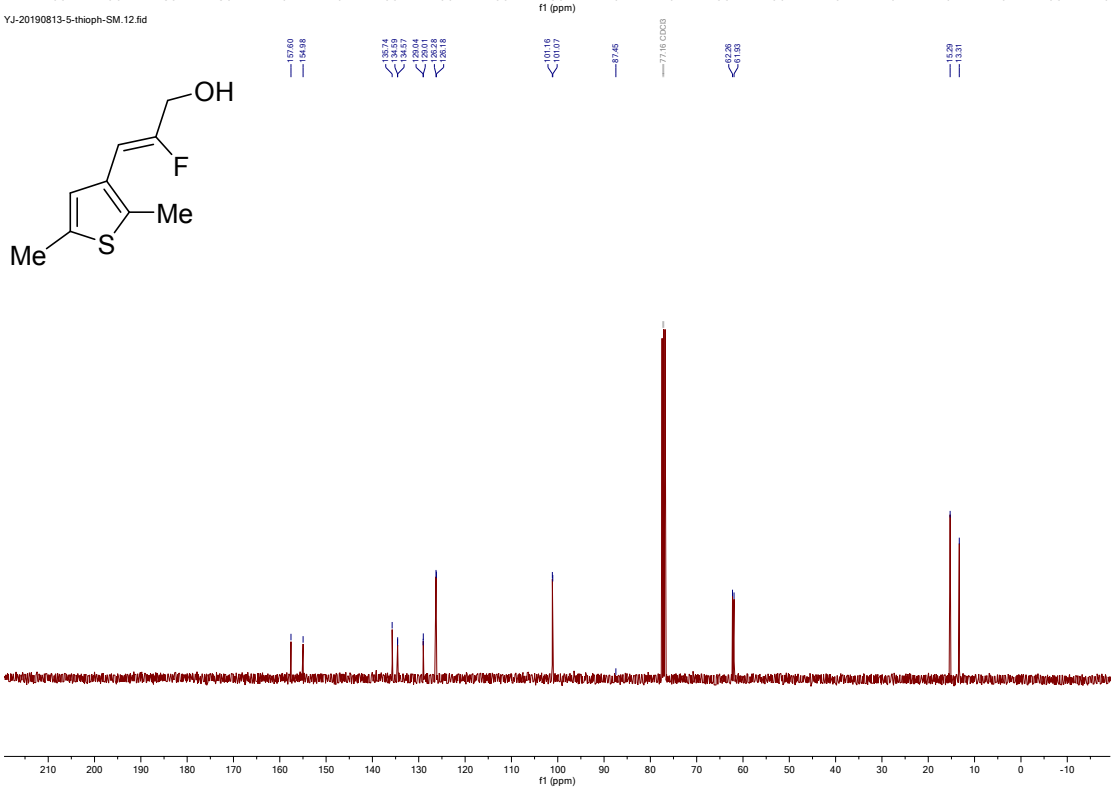

160.54
157.87
134.81
134.79
131.60
131.52
130.56
130.54
130.11
127.37
127.30
122.68
106.25
106.19
61.86
61.54
OH
F
Br
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
(ppm)

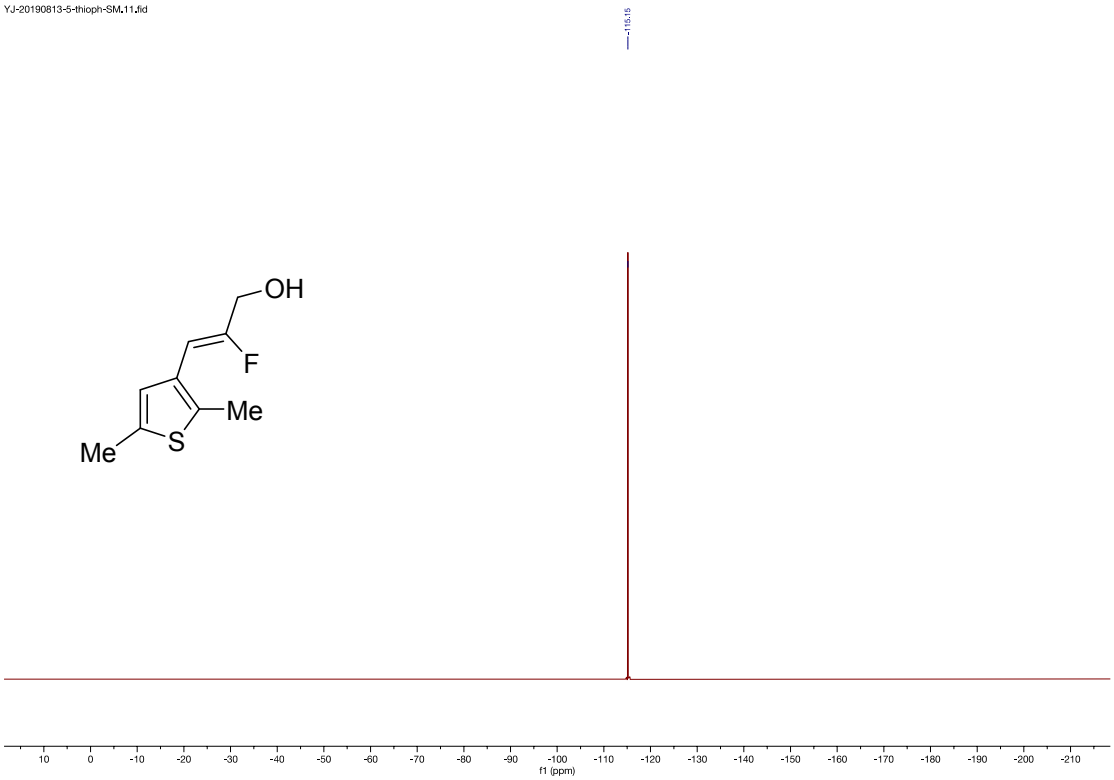

-111.14
OH
F
Br
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
(ppm)

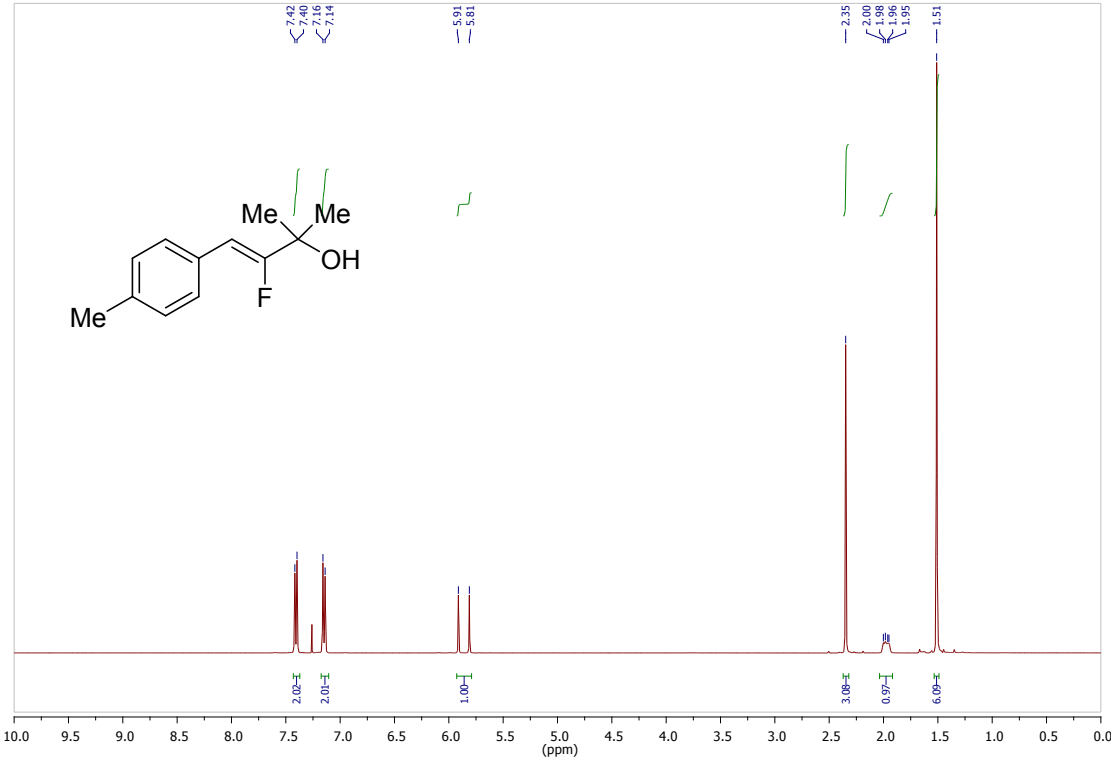
YJ-20190813-5-thioph-SM.10.fid

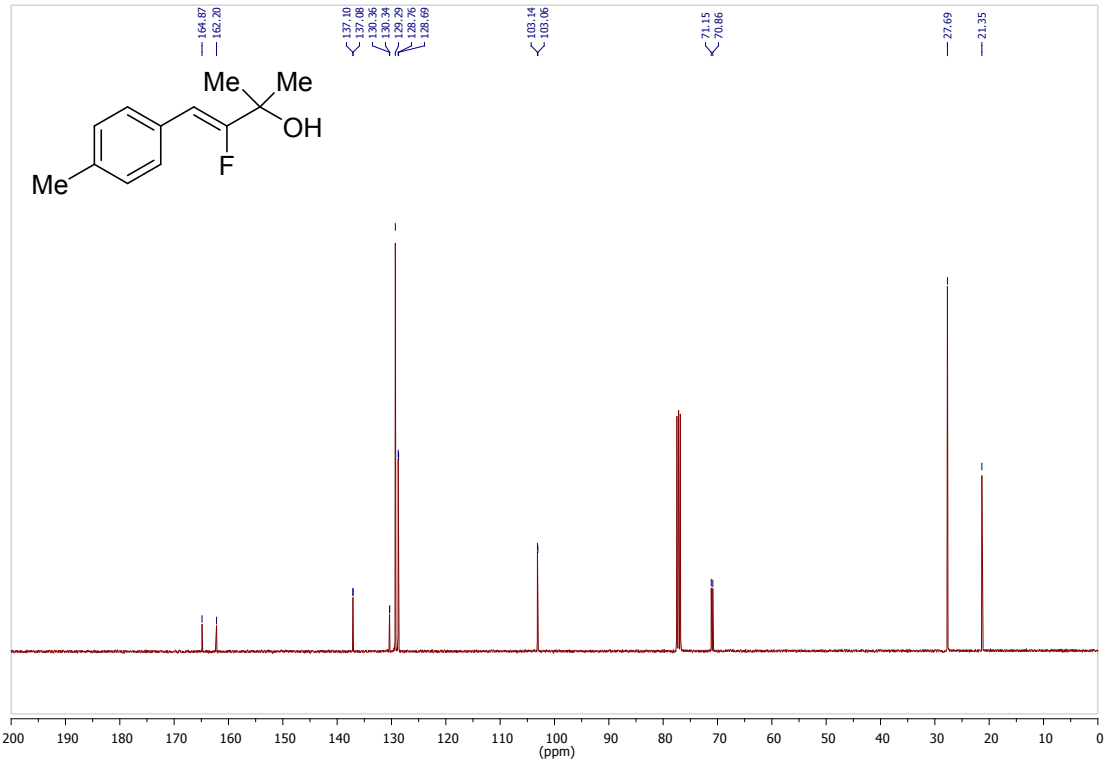


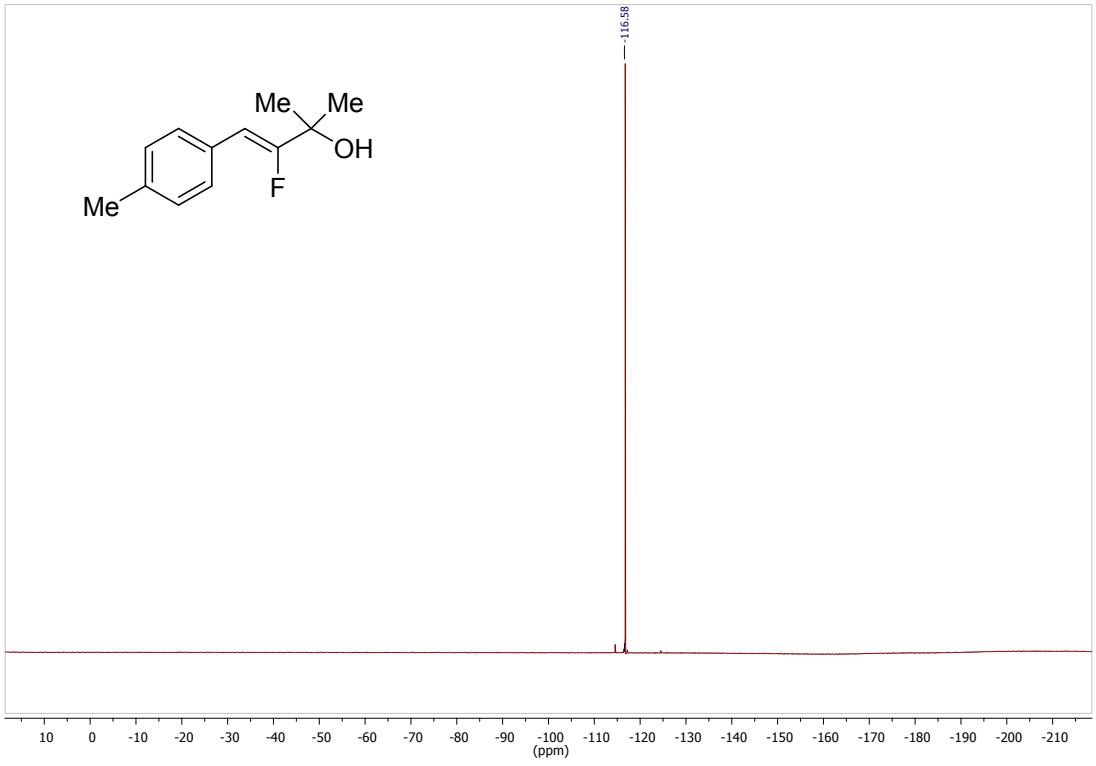
YJ-20190813-5-thioph-SM.12.fid

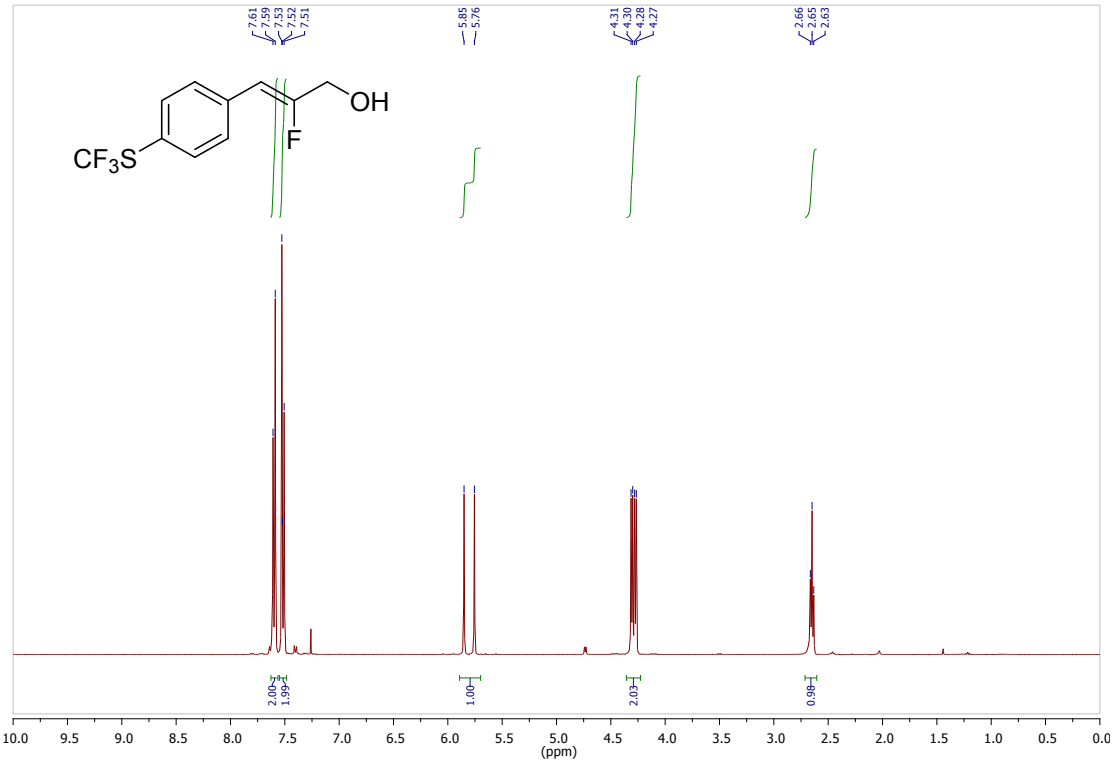


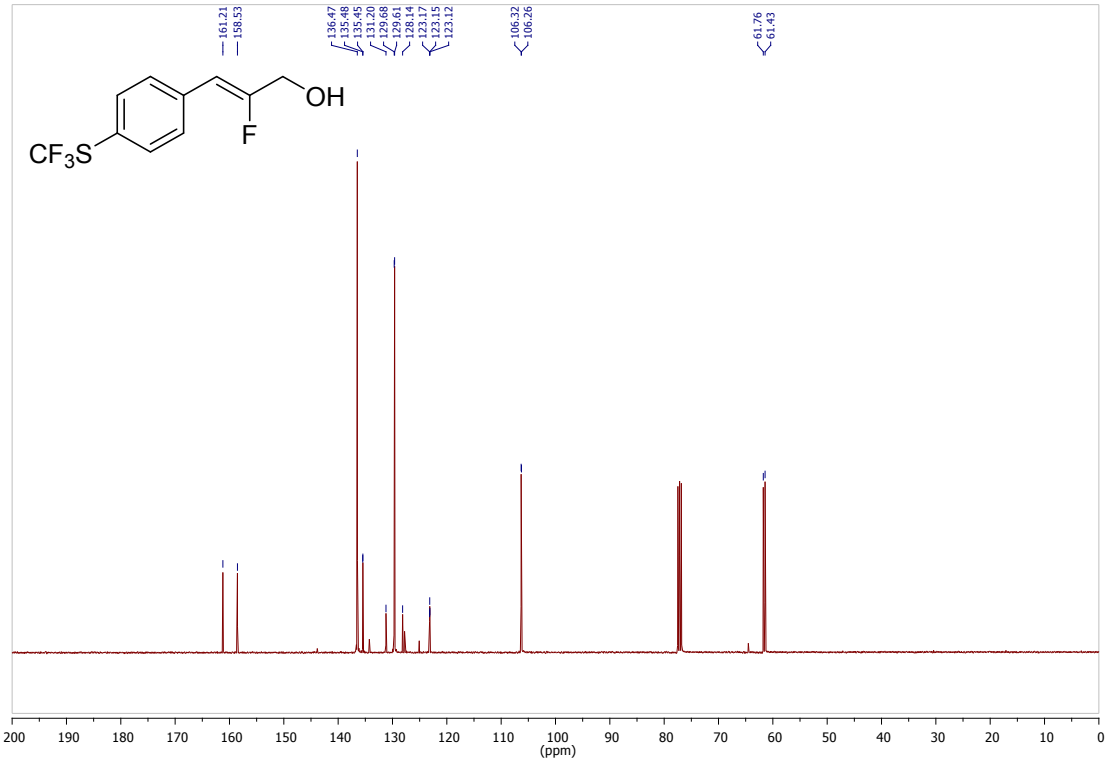

YJ-20190813-5-thioph-SM.11.fid
-115.15
OH
F
Me
Me
S
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)

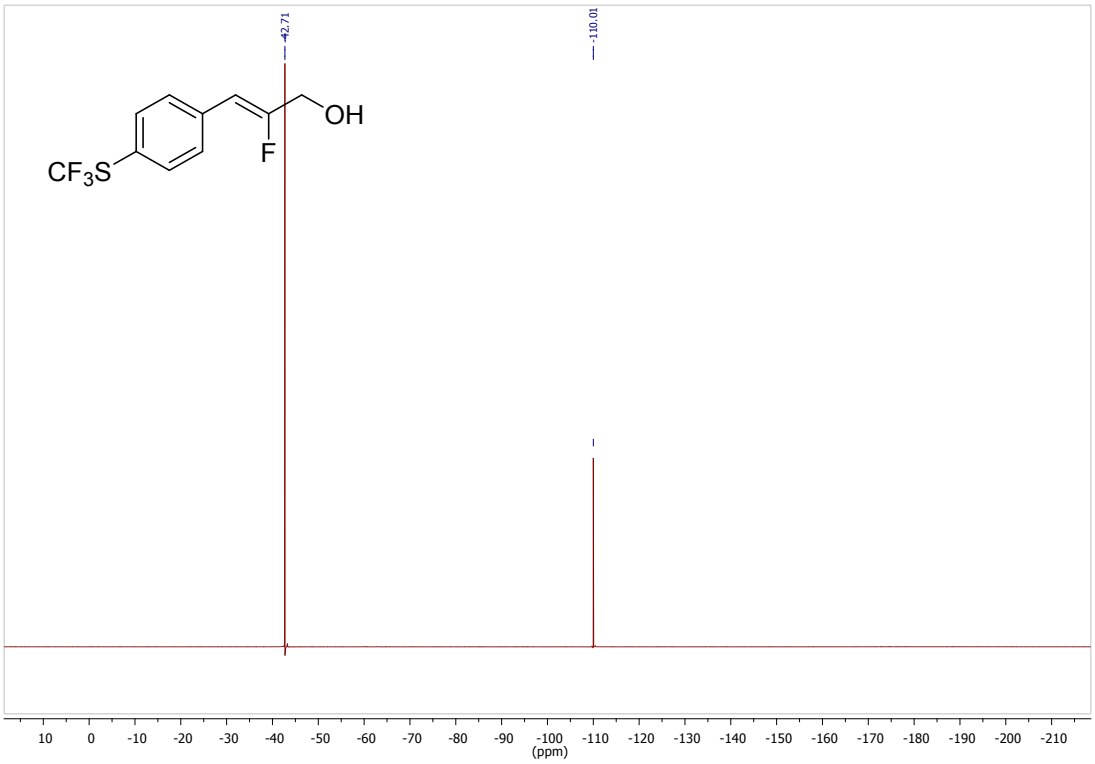

7.42
7.40
7.16
7.14
5.91
5.81
2.35
2.00
1.98
1.96
1.95
1.51
Me
Me
OH
F
Me
2.02
2.01
1.00
3.08
0.97
6.09
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
(ppm)

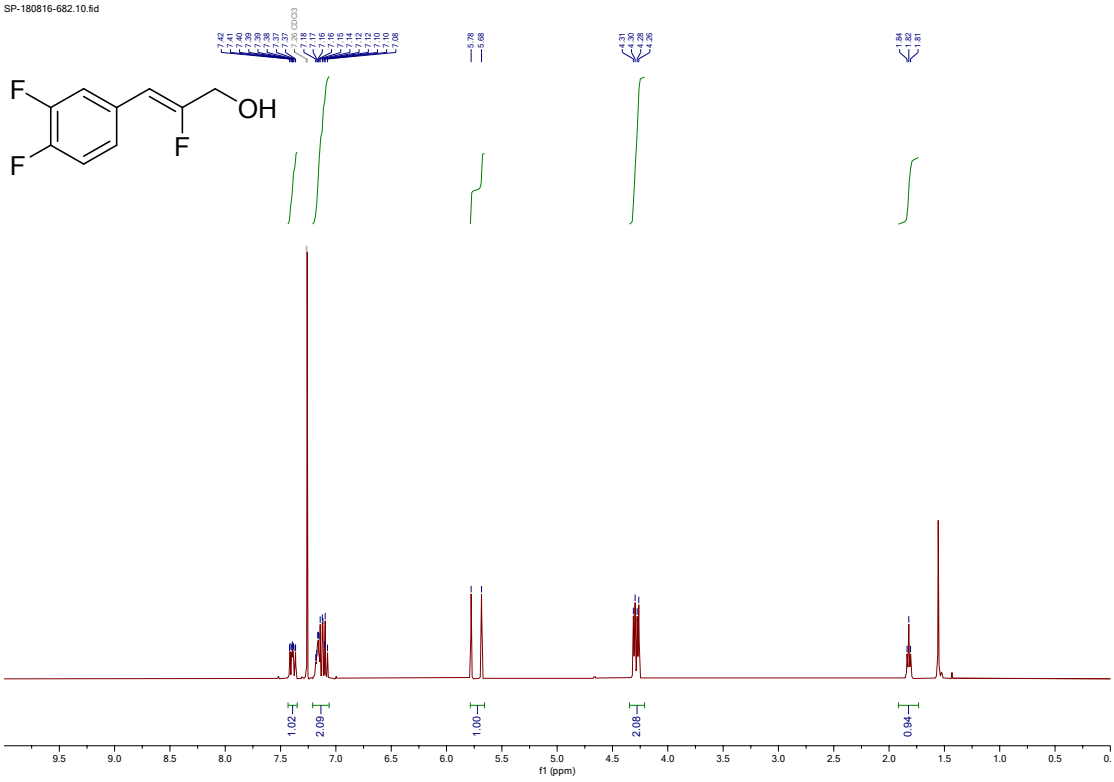

164.87
162.20
137.10
137.08
130.36
130.34
129.29
128.76
128.69
103.14
103.06
71.15
70.86
27.69
21.35
Me
Me
OH
F
Me
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
(ppm)


-116.58
Me
Me
OH
F
Me
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
(ppm)

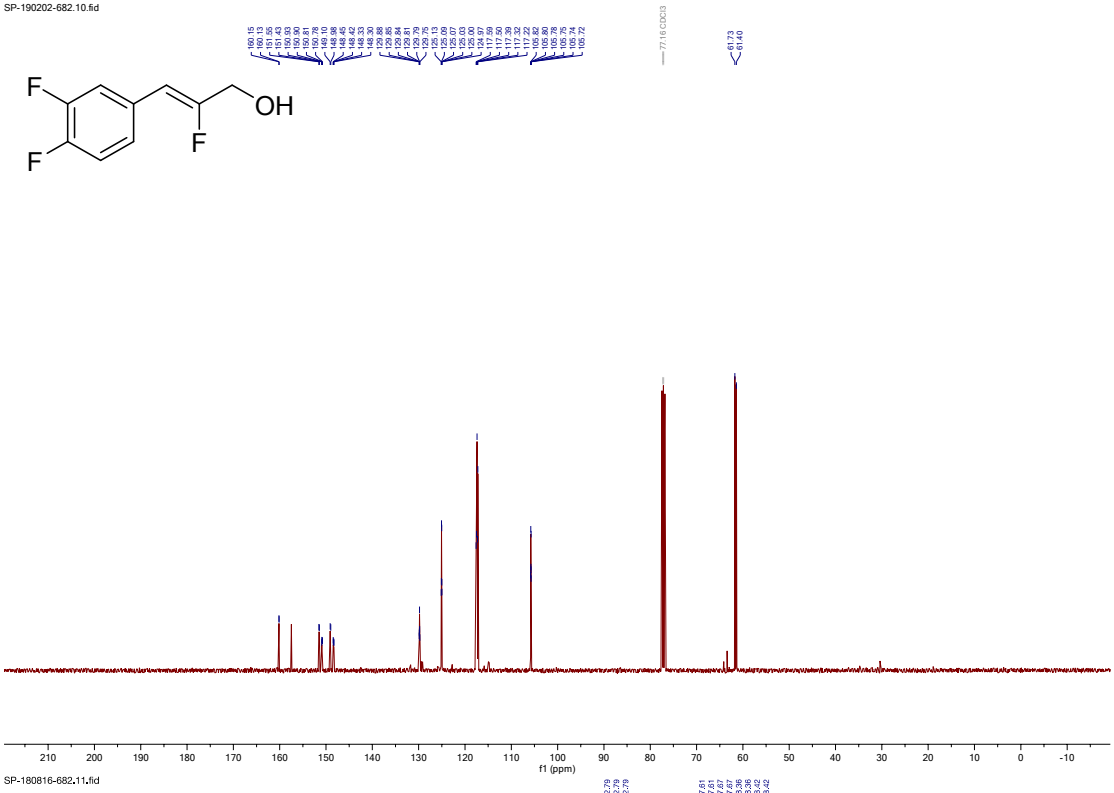

7.61
7.59
7.53
7.52
7.51
5.85
5.76
4.31
4.30
4.28
4.27
2.66
2.65
2.63
OH
F
CF3S
2.00
1.99
1.00
2.03
0.98
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
(ppm)


161.21
158.53
136.47
135.48
135.45
131.20
129.68
129.61
128.14
123.17
123.15
123.12
106.32
106.26
61.76
61.43
OH
F
CF3S
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
(ppm)

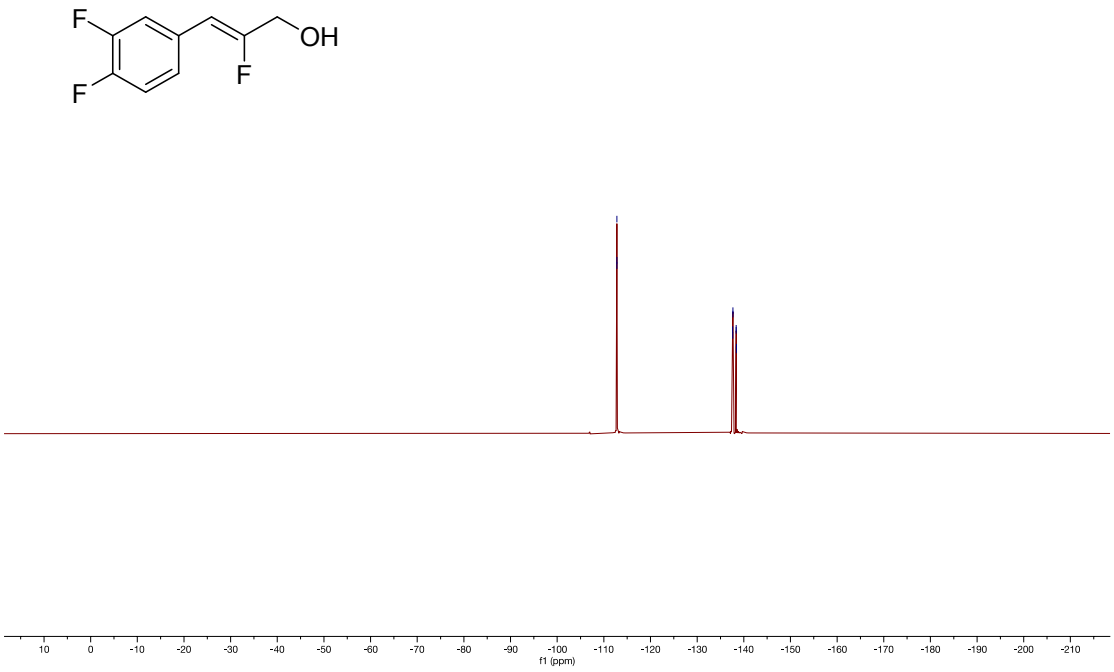

-42.71
-110.01
OH
F
CF3S
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
(ppm)

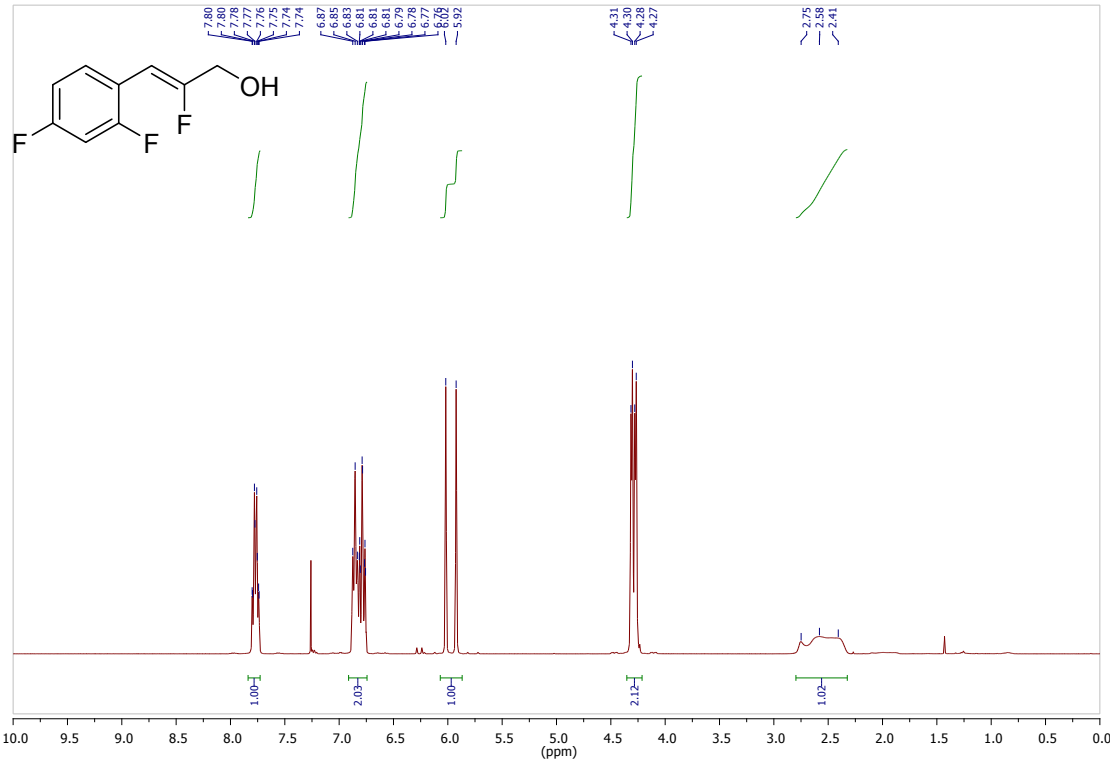

SP-180816-682.10.fid
F
F
OH
F
1.02
2.09
1.00
2.08
0.94
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)

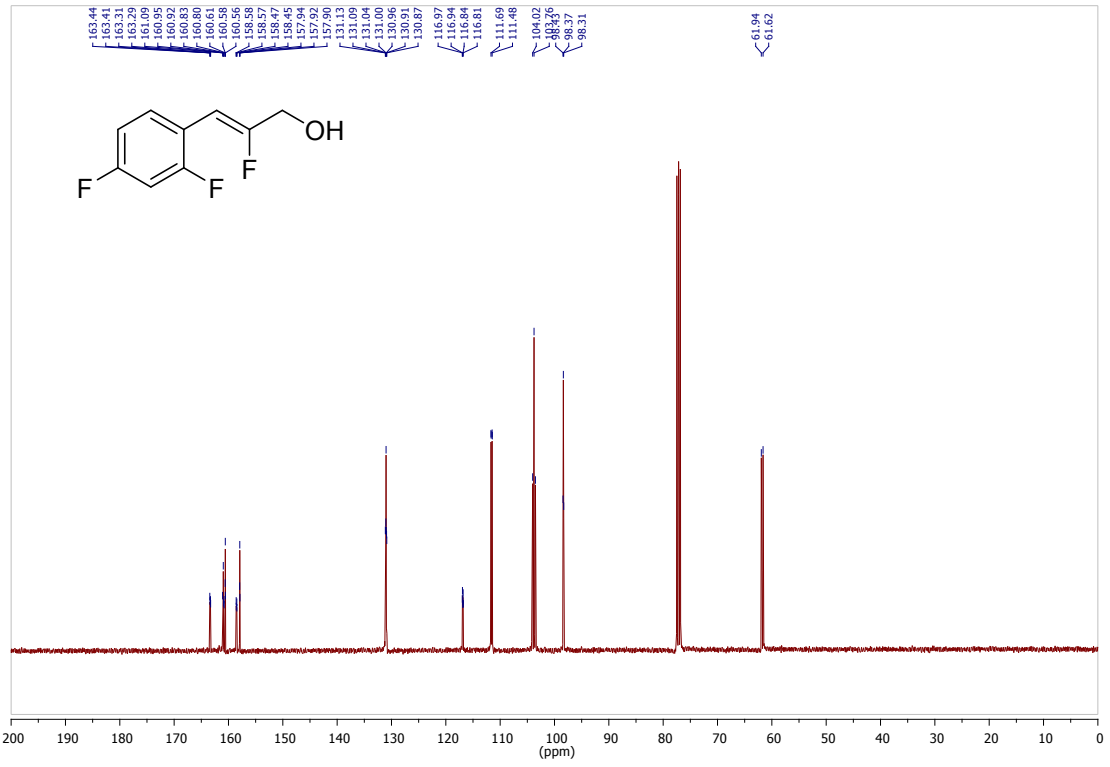
SP-190202-682.10.fid

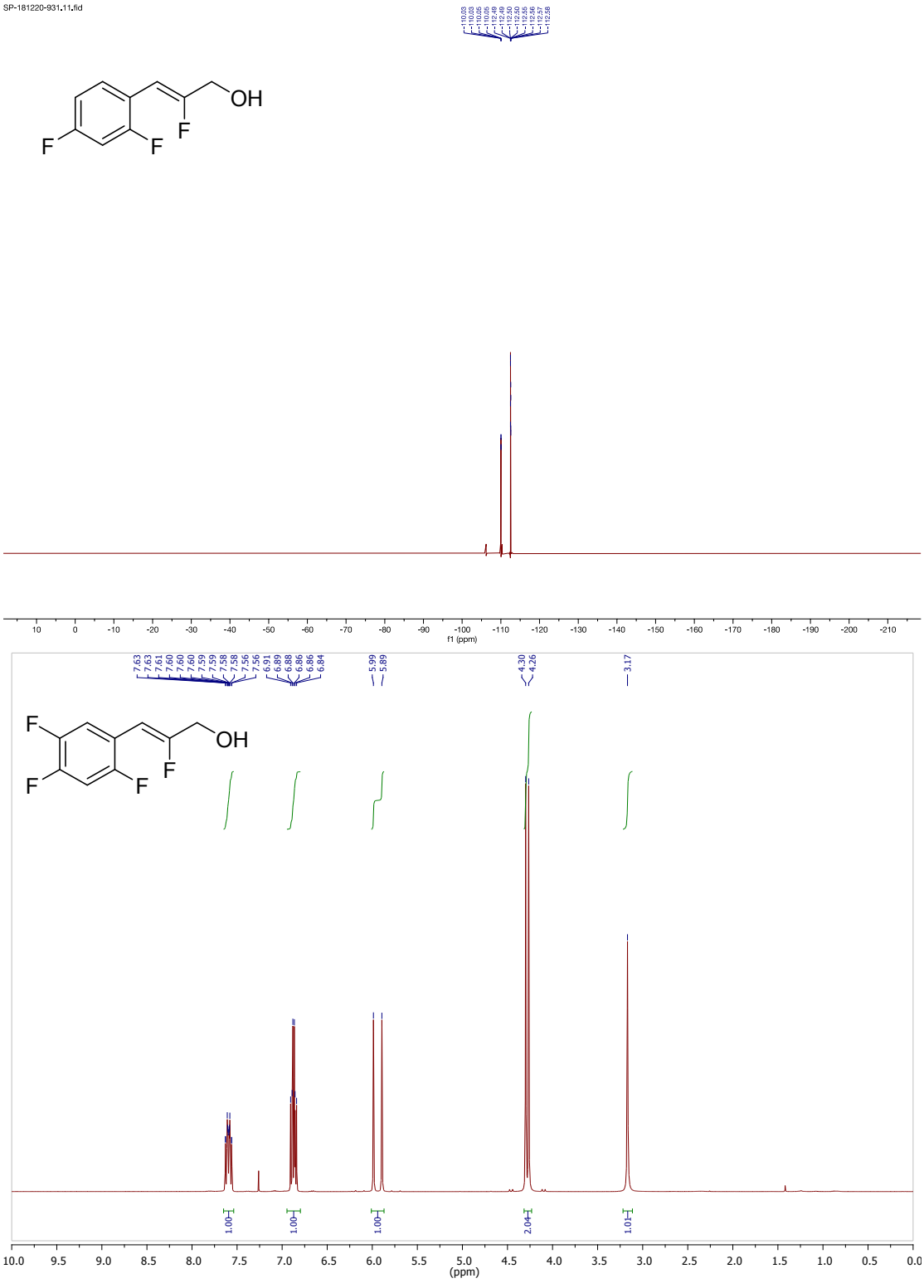


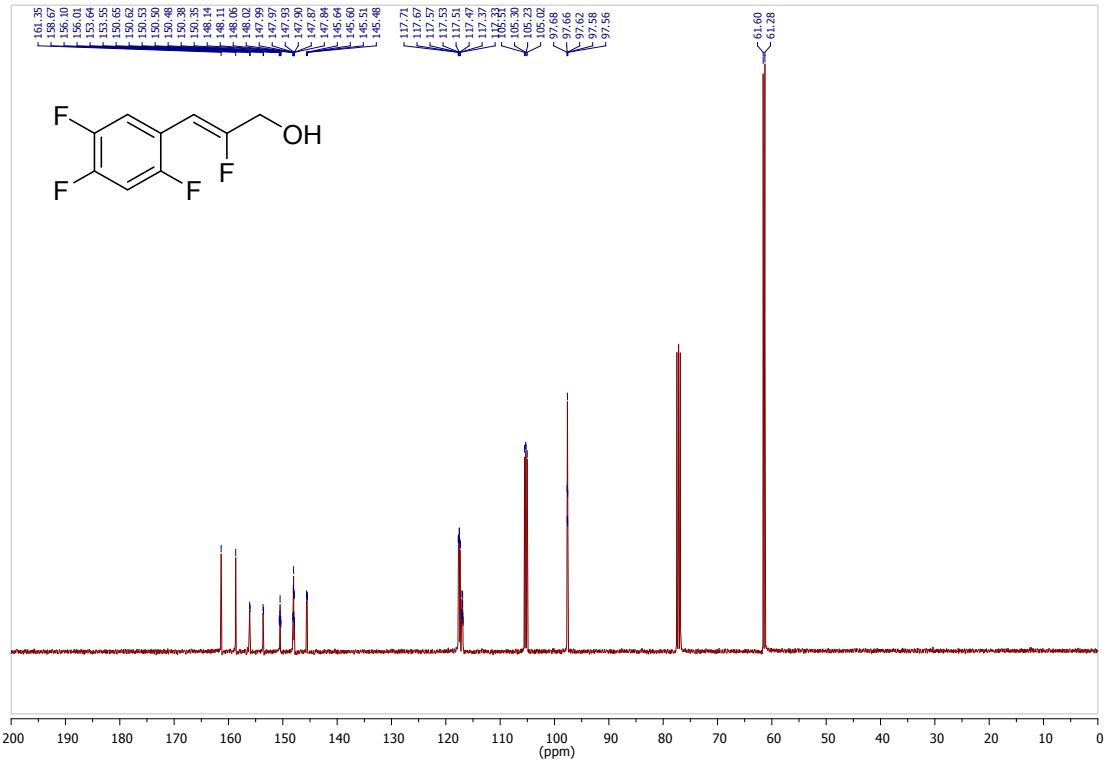
SP-180816-682.11.fid



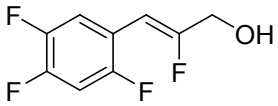

OH
F
F
F
7.80
7.80
7.78
7.77
7.77
7.76
7.75
7.74
7.74
6.87
6.85
6.83
6.81
6.81
6.81
6.79
6.78
6.77
6.09
6.07
5.92
4.31
4.30
4.28
4.27
2.75
2.58
2.41
1.00
2.03
1.00
2.12
1.02
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
(ppm)

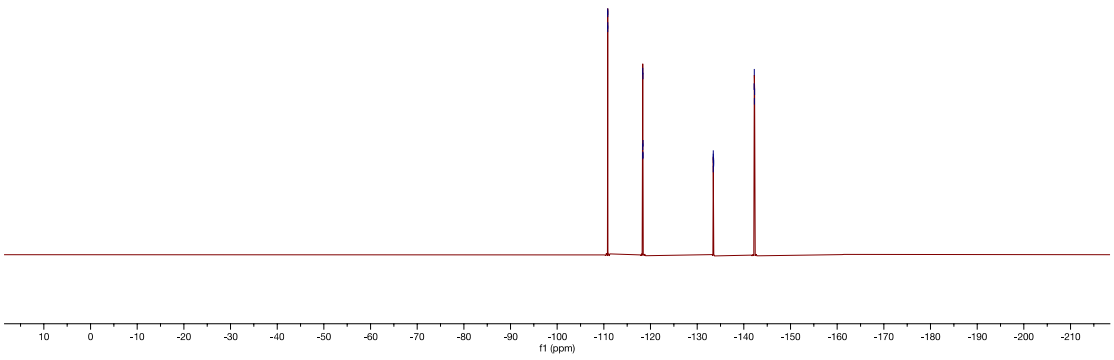

OH
F
F
F
163.44
163.41
163.31
163.29
161.09
160.95
160.92
160.83
160.80
160.61
160.58
160.55
158.58
158.57
158.47
158.45
157.94
157.92
157.90
131.13
131.09
131.04
131.00
130.96
130.91
130.87
116.97
116.94
116.84
116.81
111.69
111.48
104.02
98.37
98.31
61.94
61.62
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
(ppm)

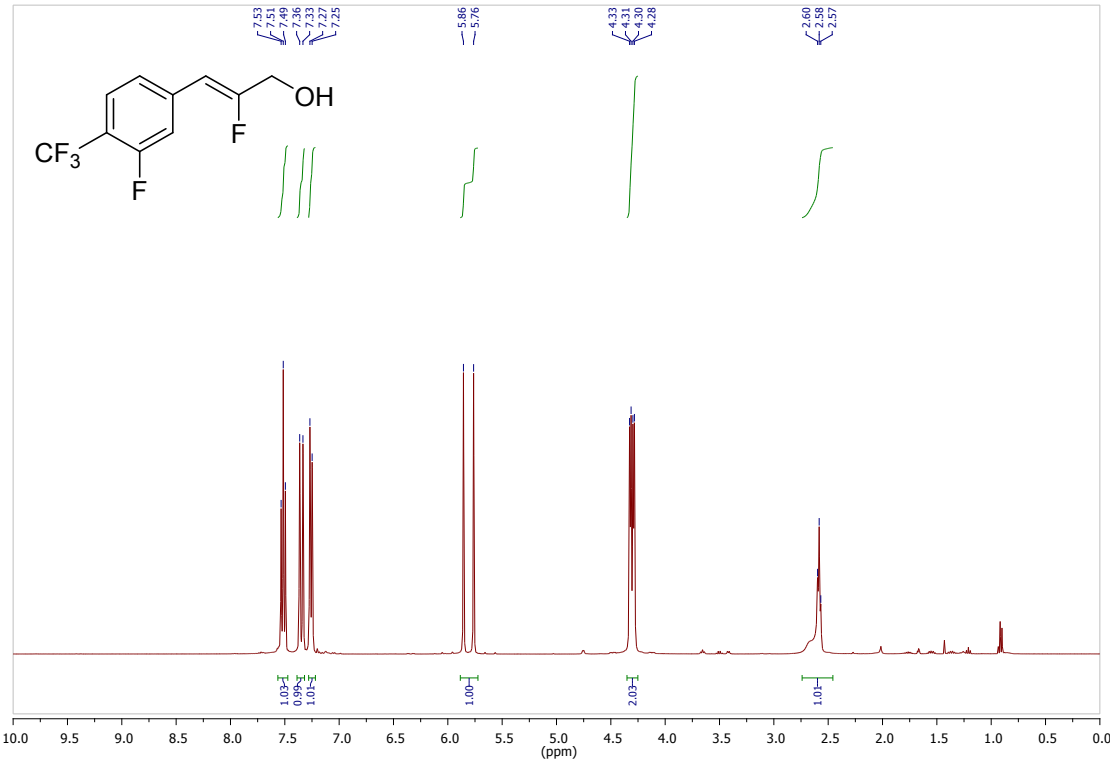

SP-181220-931.11.fid
OH
F
F
F
f1 (ppm)
OH
F
F
F
1.00
1.00
1.00
2.04
1.01
(ppm)

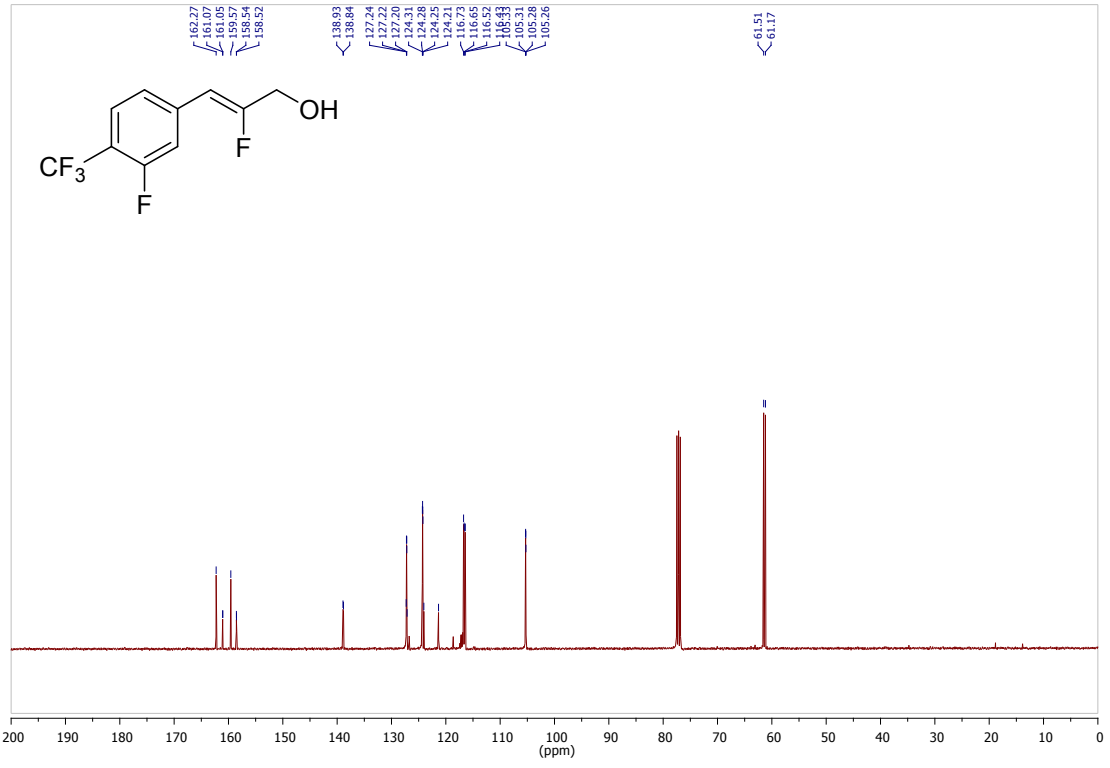


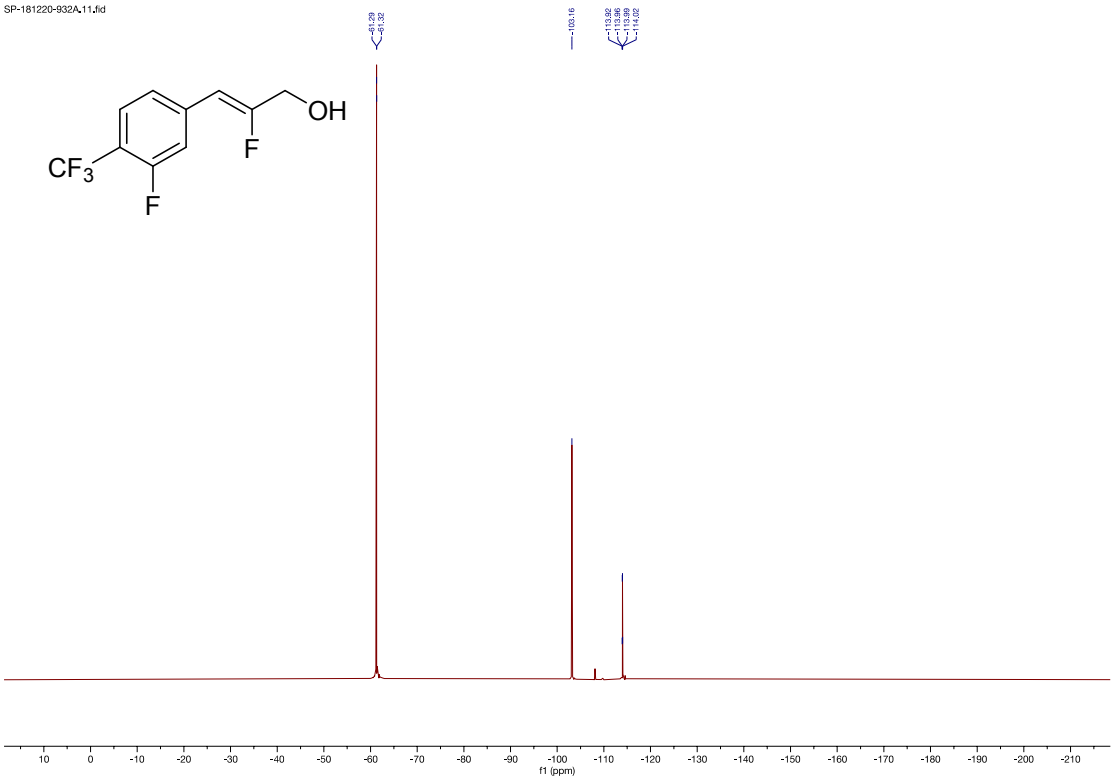
SP-181015-768.11.fid

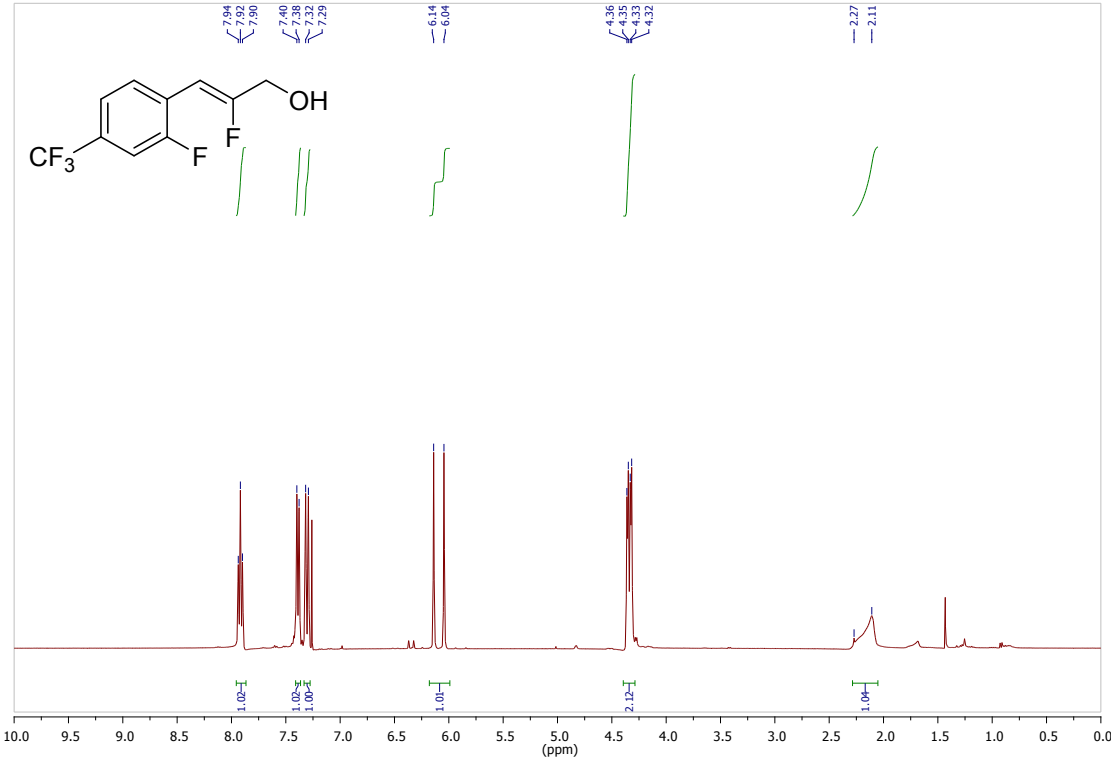


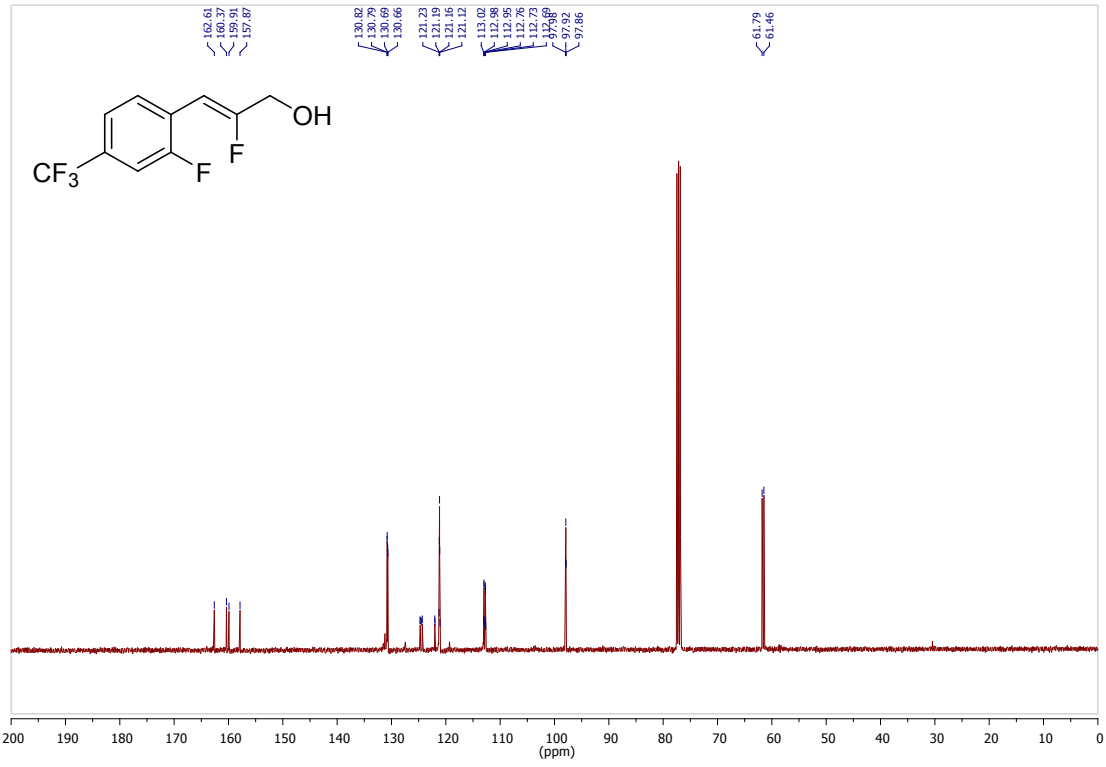



7.53
7.51
7.49
7.36
7.33
7.27
7.25
5.86
5.76
4.33
4.31
4.30
4.28
2.60
2.58
2.57
OH
F
CF3
F
1.03
0.99
1.01
1.00
2.03
1.01
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
(ppm)

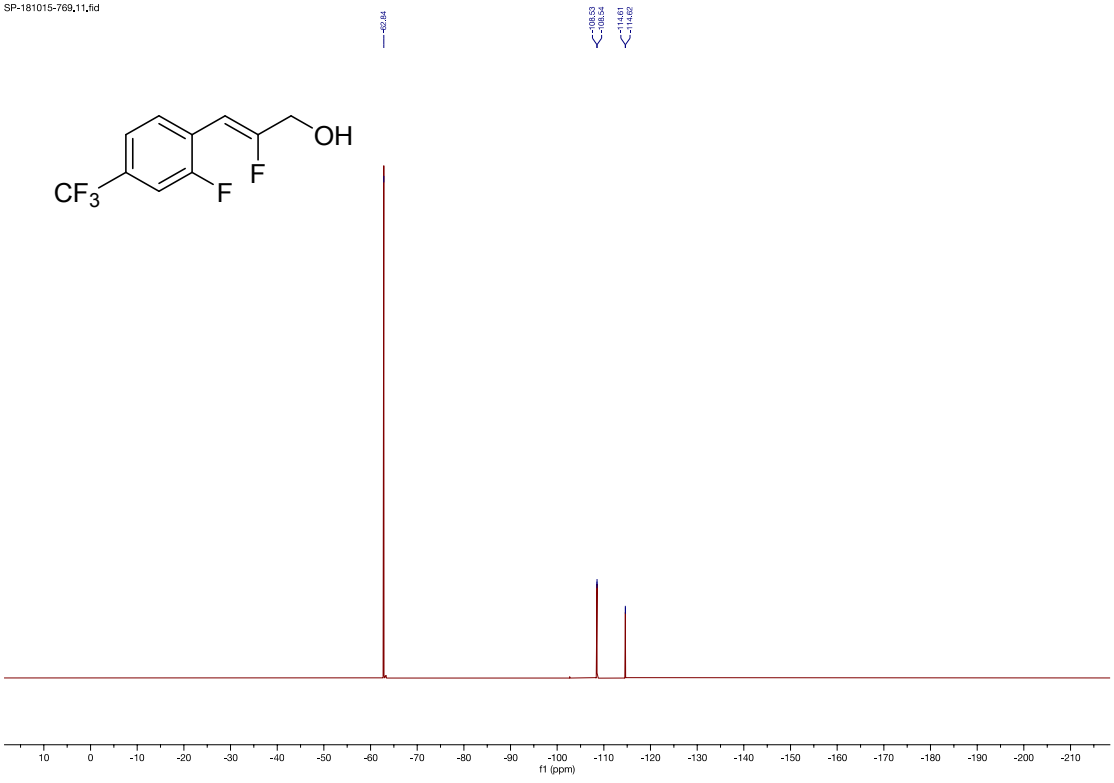

162.27
161.07
161.05
159.57
158.54
158.52
138.93
138.84
127.24
127.22
127.20
124.31
124.28
124.25
124.21
116.73
116.65
116.52
116.43
105.33
105.31
105.28
105.26
61.51
61.17
OH
F
CF3
F
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
(ppm)

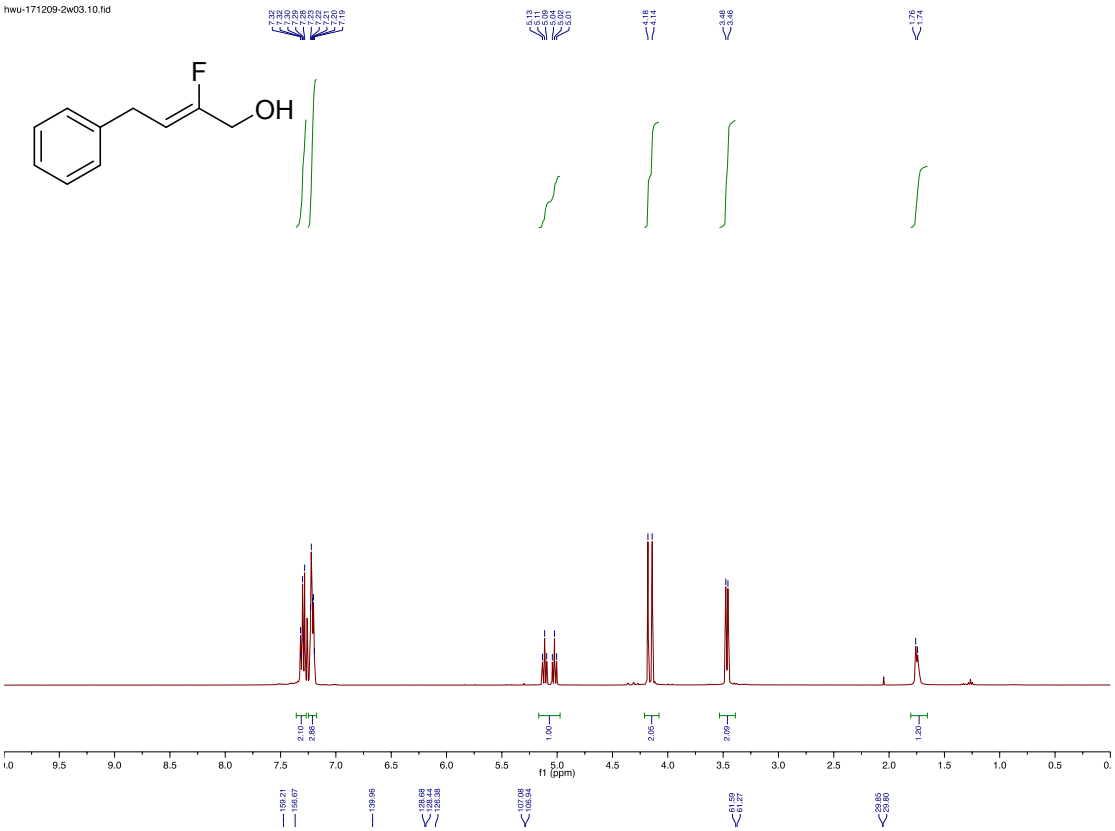

SP-181220-932A.11.fid
-61.29
-61.32
-103.16
-113.92
-113.96
-113.99
-114.02
OH
F
CF3
F
f1 (ppm)

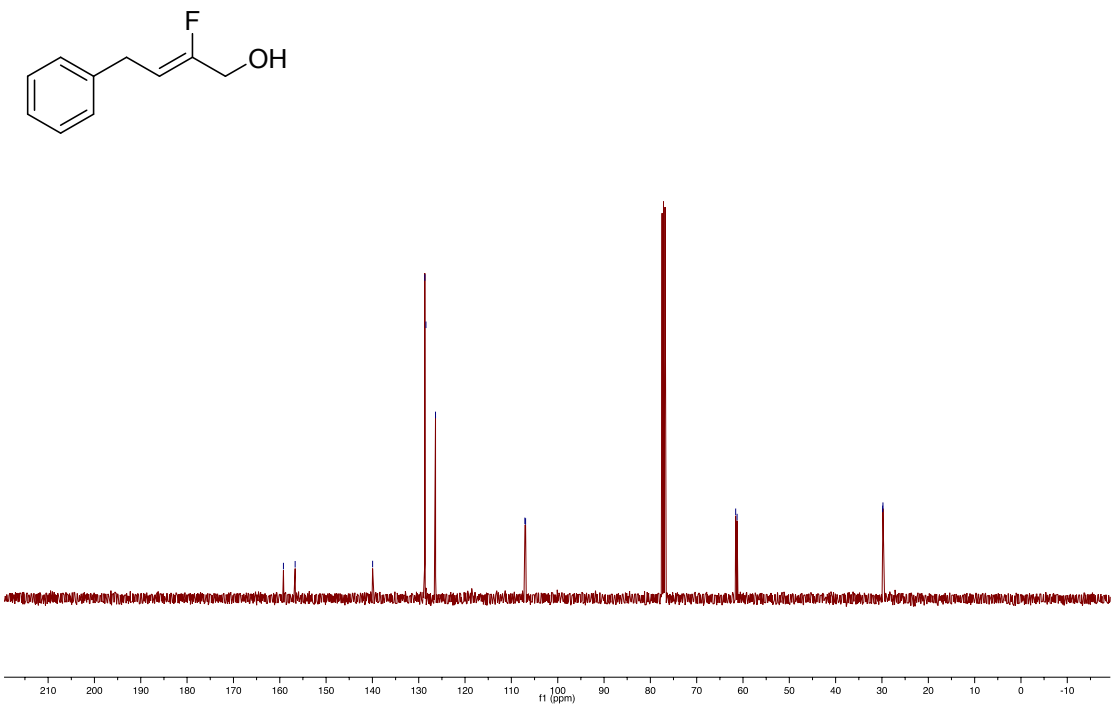

7.94
7.92
7.90
7.40
7.38
7.32
7.29
6.14
6.04
4.36
4.35
4.33
4.32
2.27
2.11
OH
F
CF3
F
1.02
1.03
1.00
1.01
2.12
1.04
(ppm)

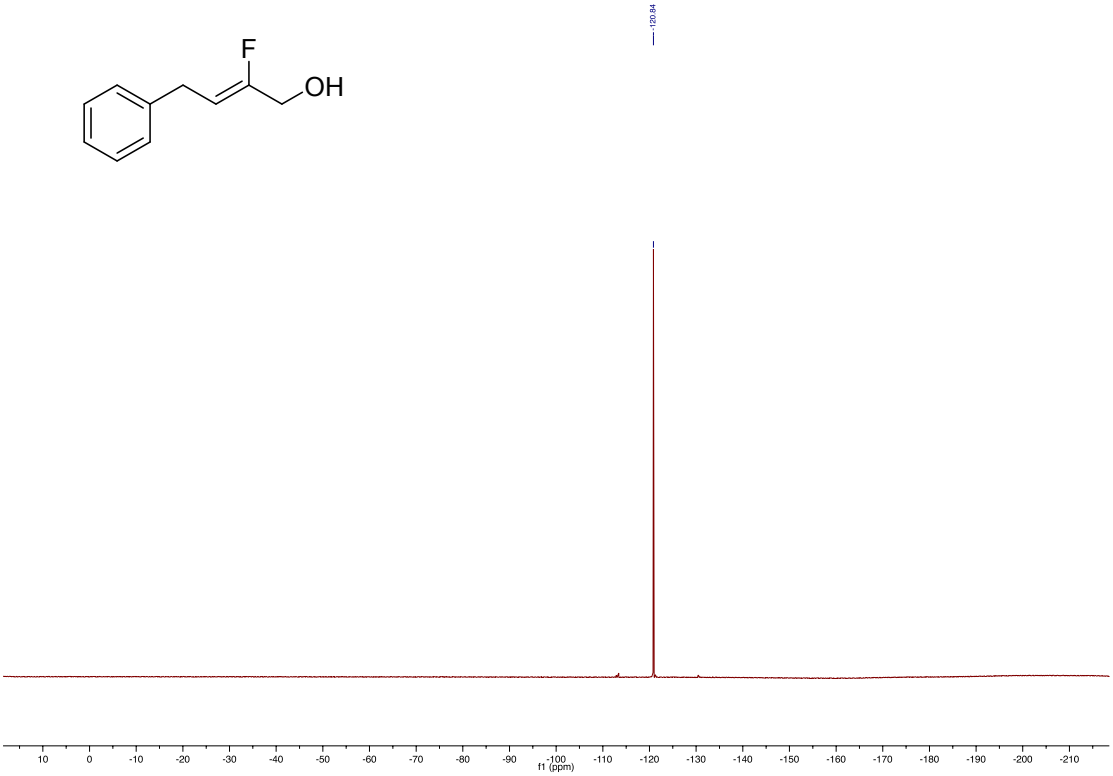


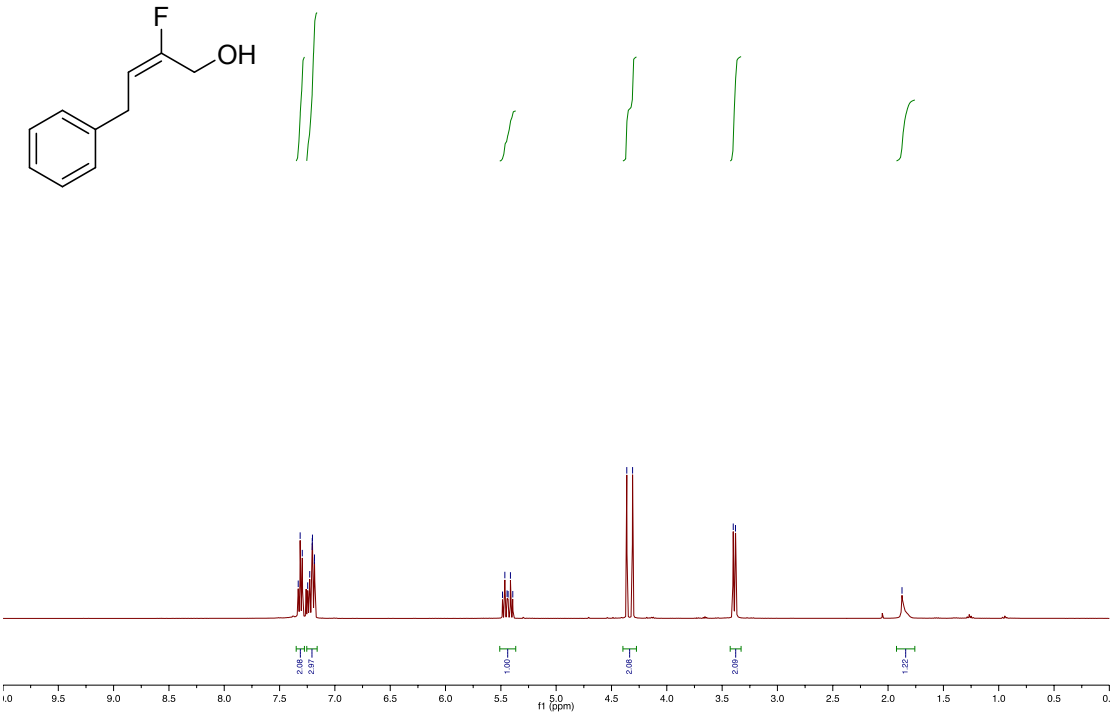
SP-181015-769.11.fid

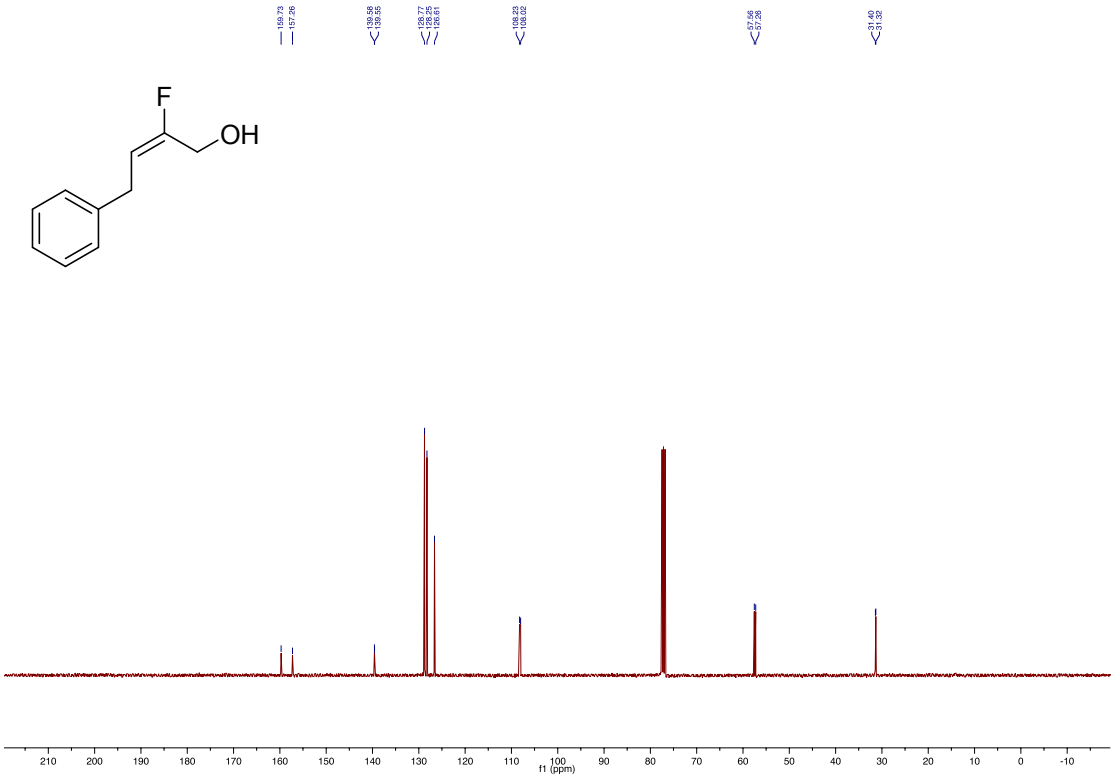


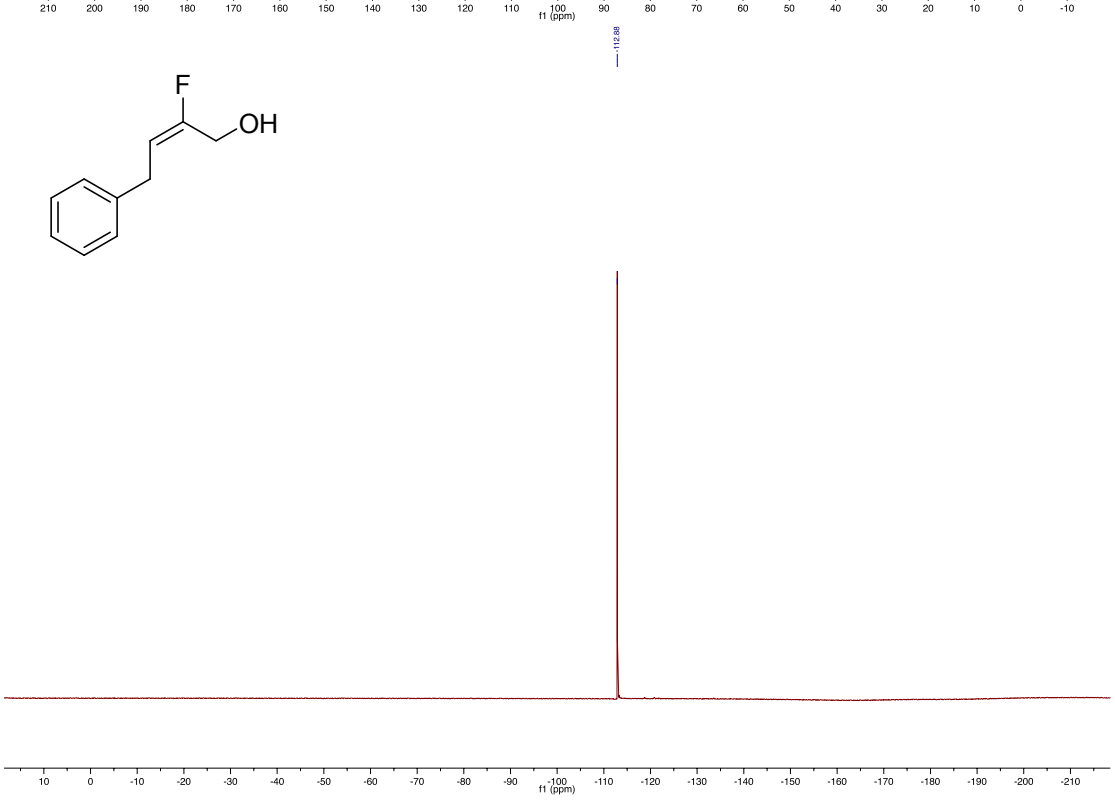

hwu-171209-2w03.10.fid
F
OH
f1 (ppm)


F
OH
f1 (ppm)

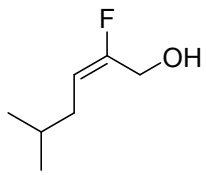

F
OH
-120.84
f1 (ppm)


F
OH
f1 (ppm)

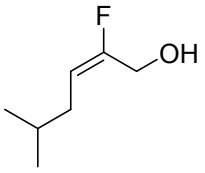

159.73
157.26
139.58
139.56
128.77
128.25
126.61
108.23
108.02
57.56
57.28
31.40
31.32
F
OH
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

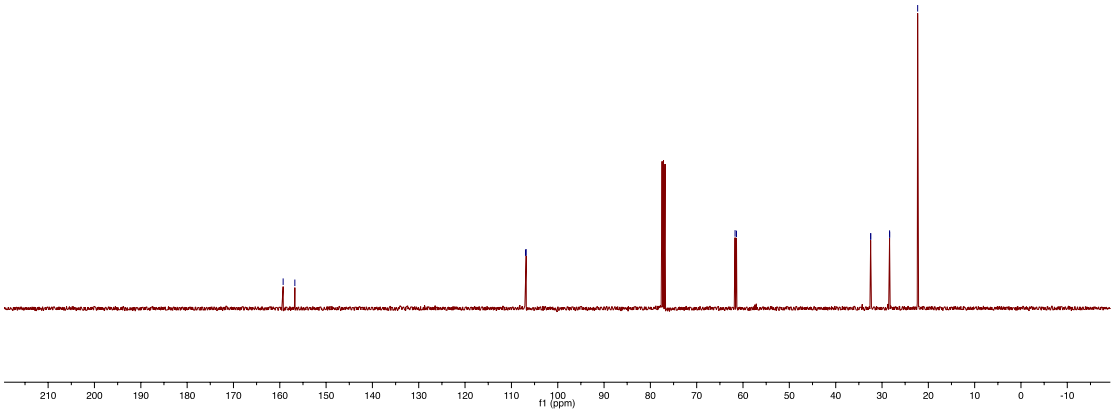

112.88
F
OH
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)

YJ-20190526-5-25-4/10

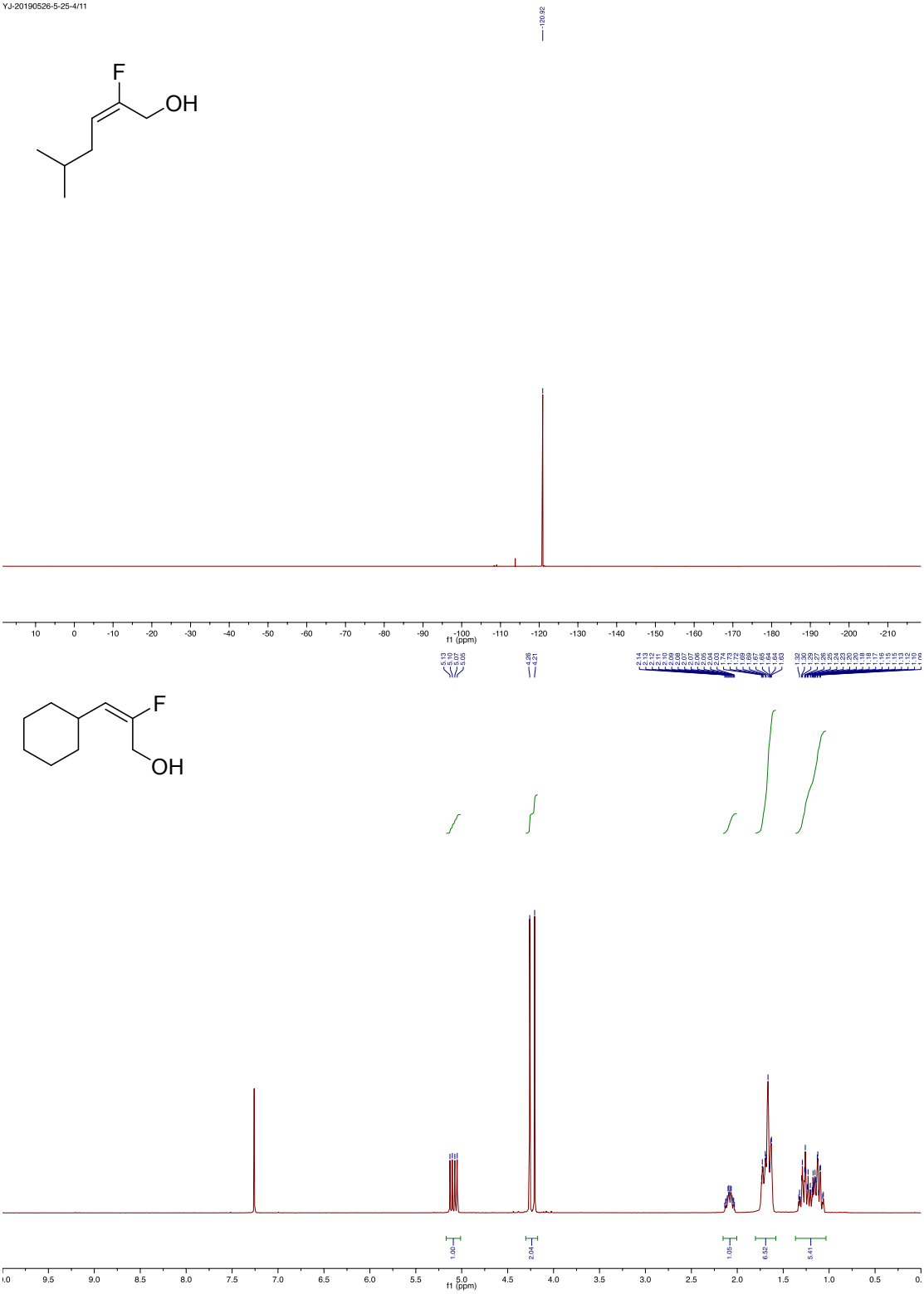


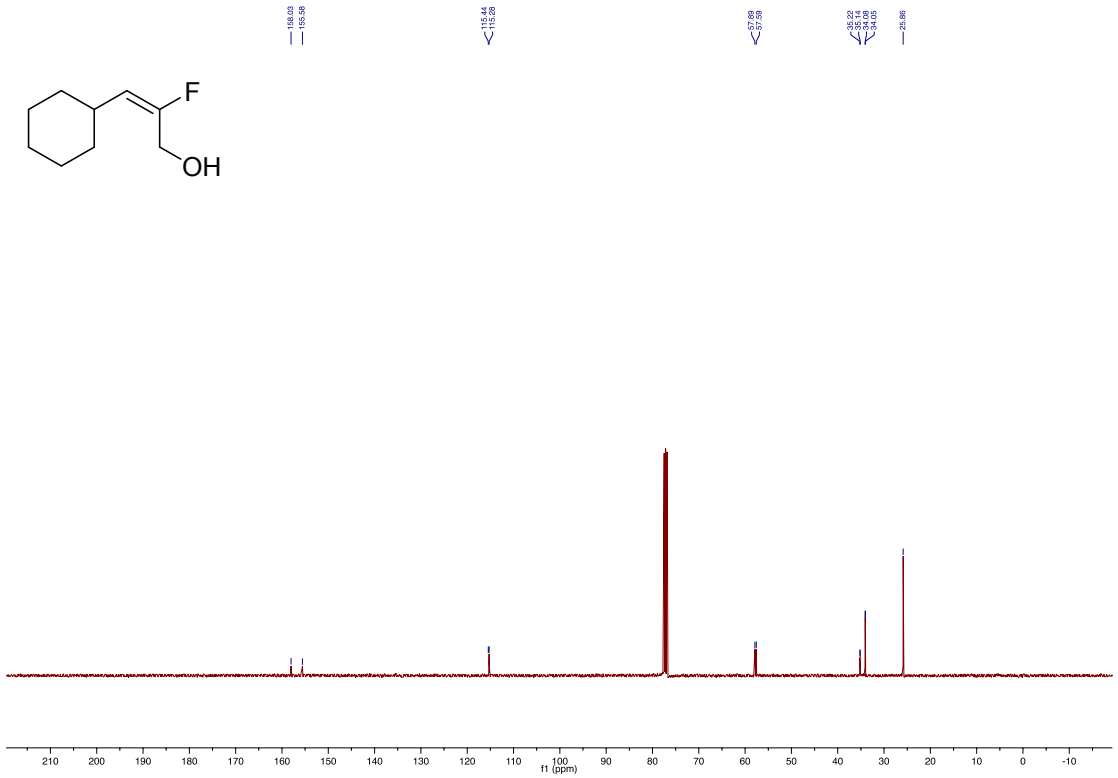
YJ-20190526-5-25-4/12

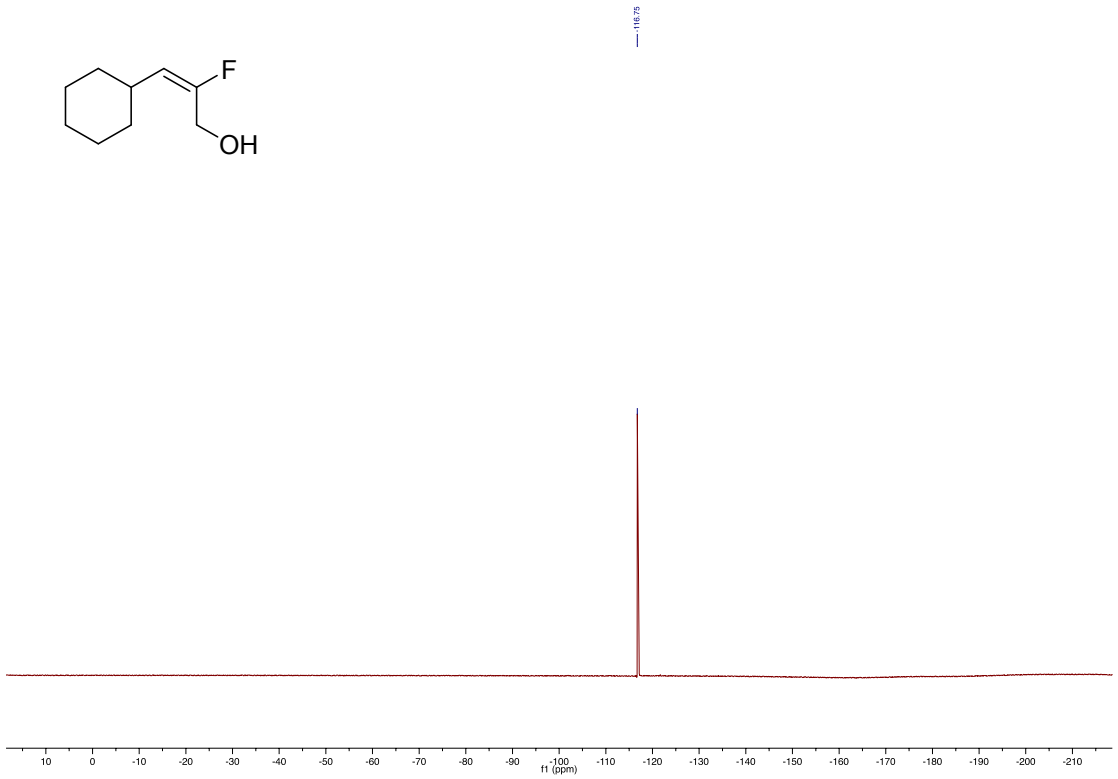


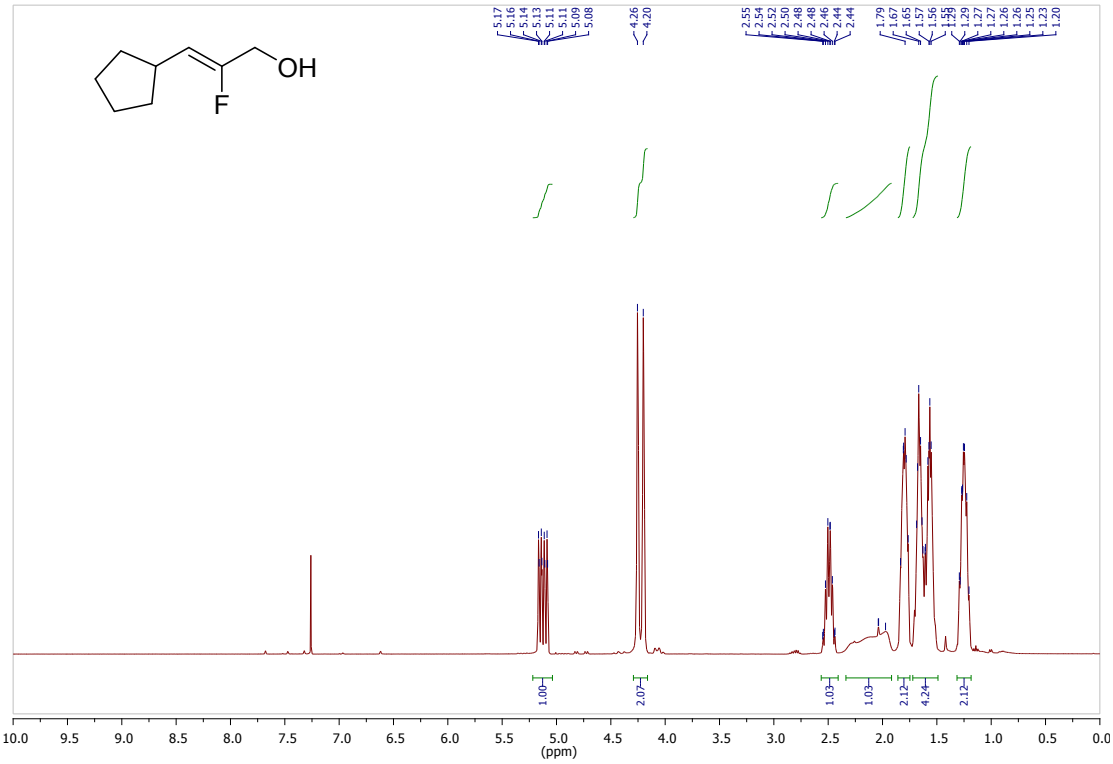


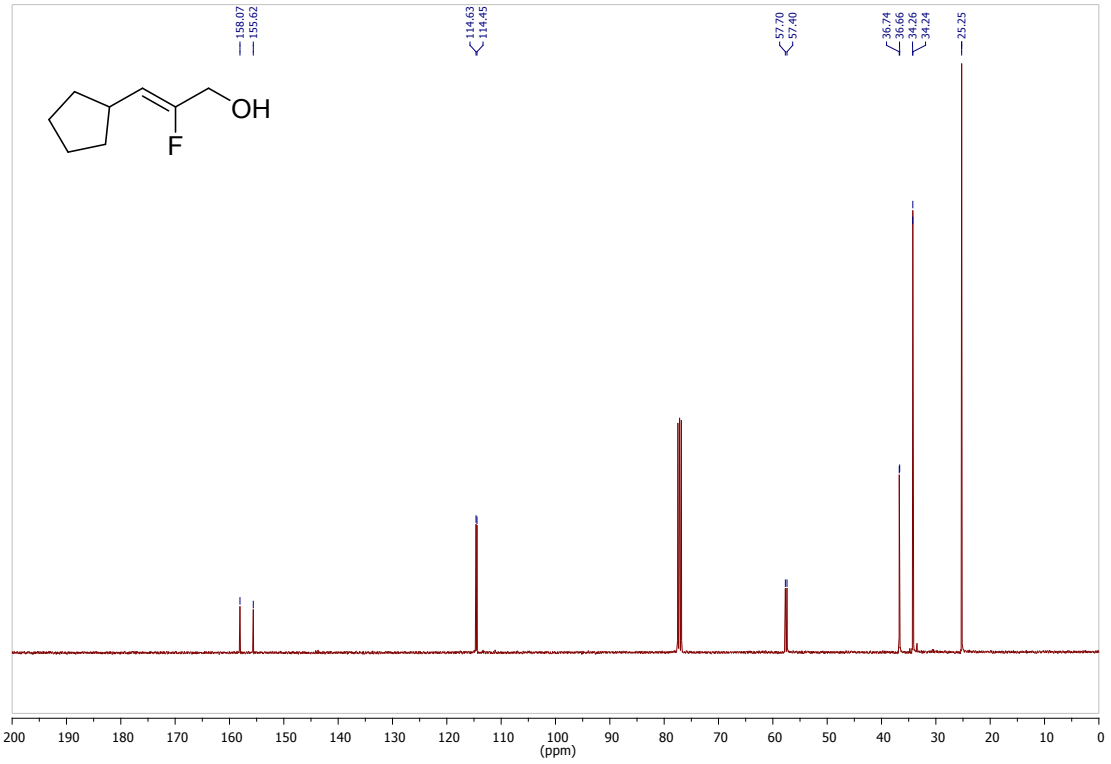
YJ-20190526-5-25-4/11

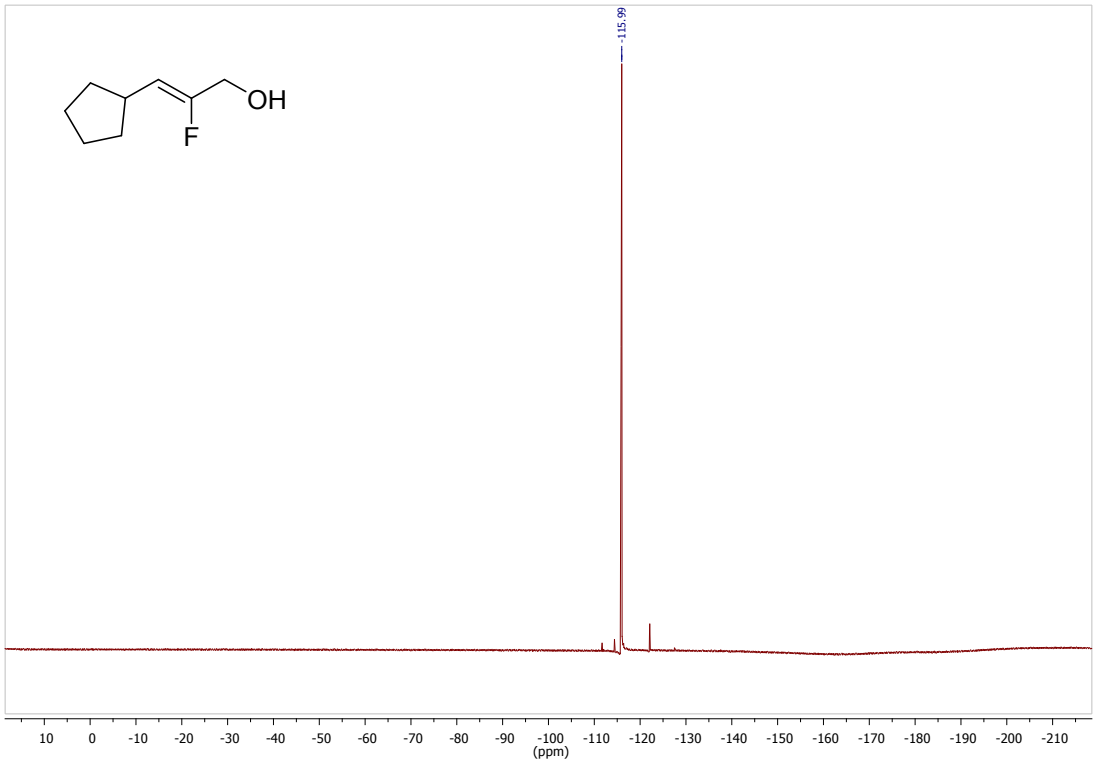


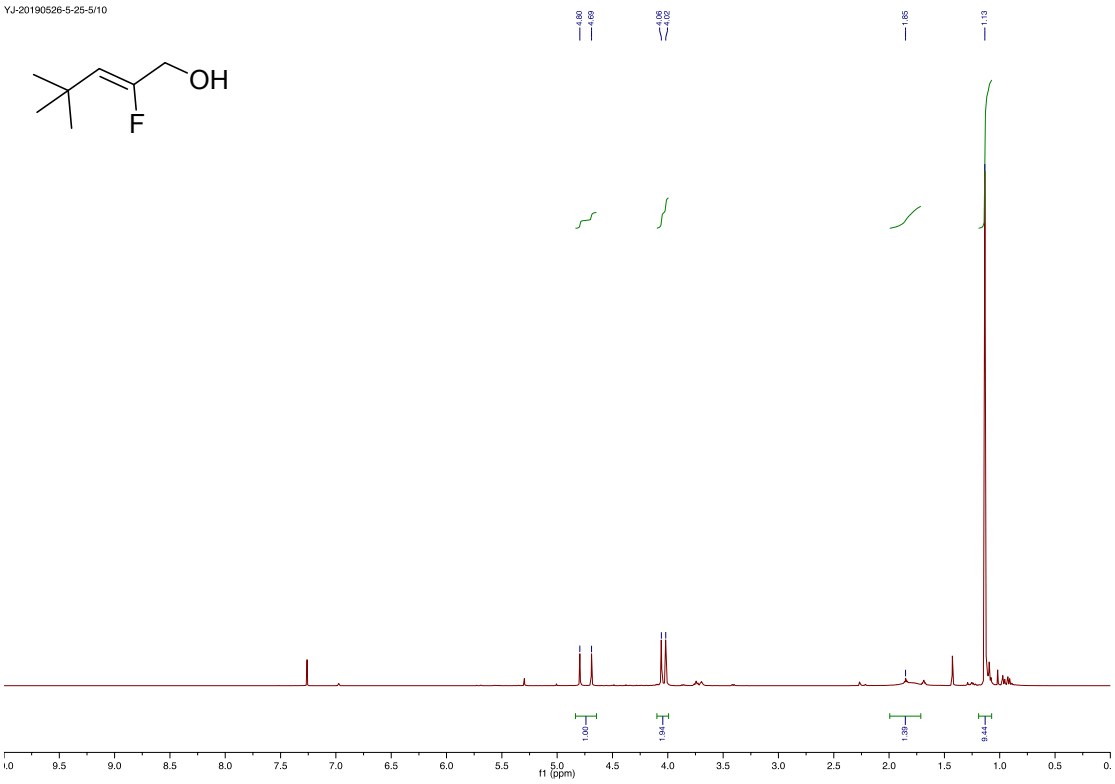

158.03
155.58
115.44
110.88
57.89
57.59
35.22
35.14
34.08
34.05
25.86
F
OH
f1 (ppm)


116.75
F
OH
f1 (ppm)

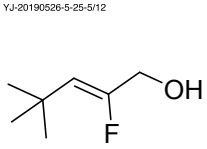

OH
F
5.17
5.16
5.14
5.13
5.11
5.11
5.09
5.08
4.26
4.20
2.55
2.54
2.52
2.50
2.48
2.48
2.46
2.44
2.44
1.79
1.67
1.65
1.57
1.56
1.29
1.27
1.27
1.26
1.26
1.25
1.23
1.20
1.00
2.07
1.03
1.03
2.12
4.24
2.12
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
(ppm)


OH
F
158.07
155.62
114.63
114.45
57.70
57.40
36.74
36.66
34.26
34.24
25.25
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
(ppm)

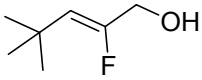

OH
F
-115.99
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
(ppm)

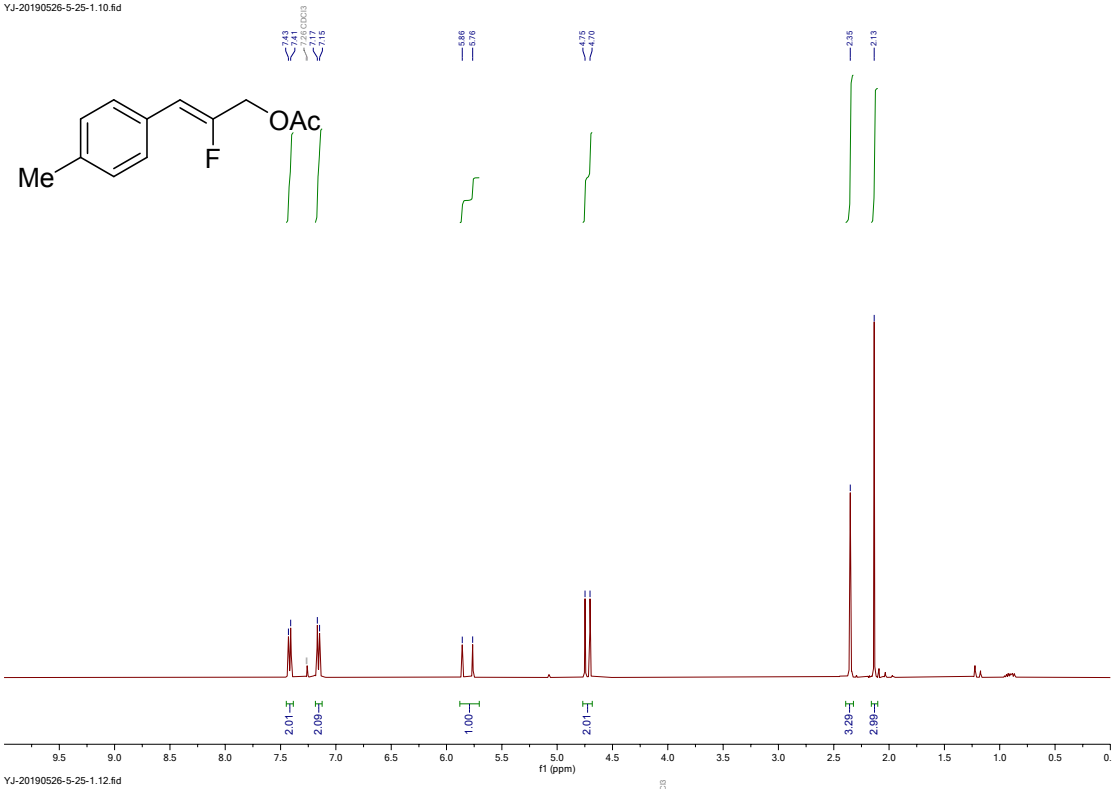

YJ-20190526-5-25-5/10
OH
F
4.80
4.69
4.06
4.02
1.85
1.13
1.00
1.94
1.39
9.44
f1 (ppm)

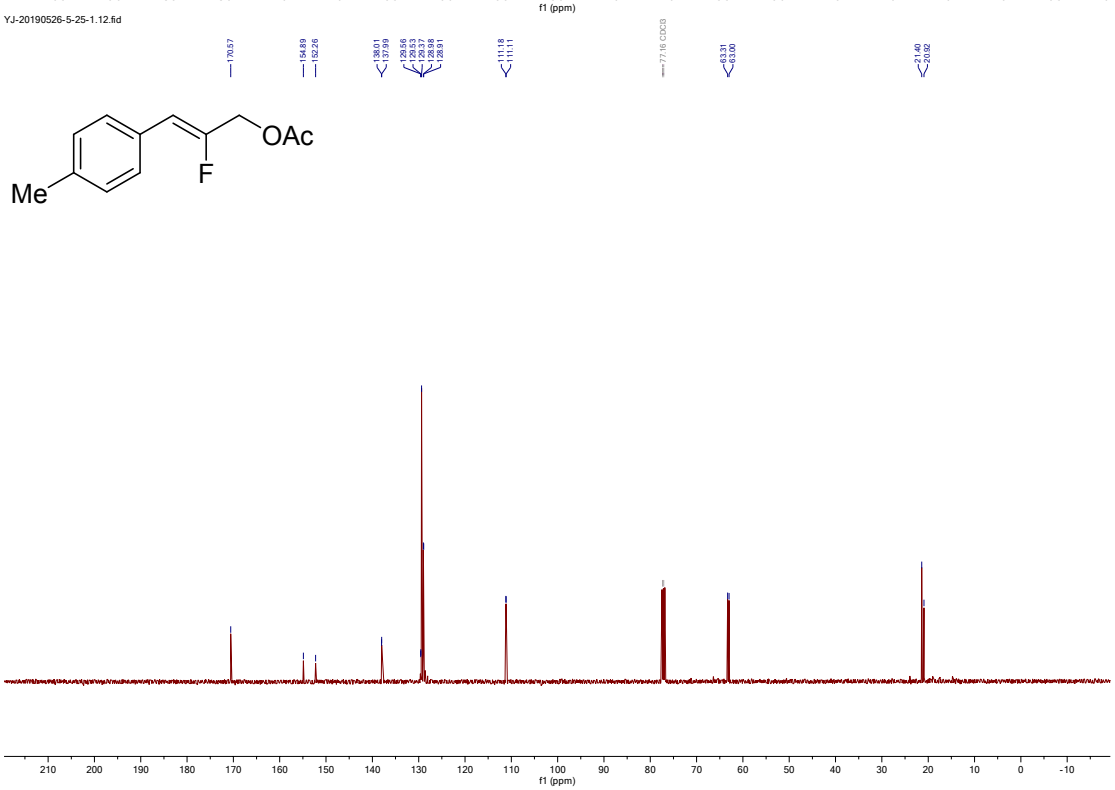
YJ-20190526-5-25-5/12



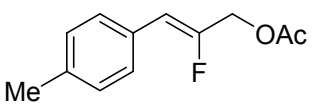
YJ-20190526-5-25-5/11



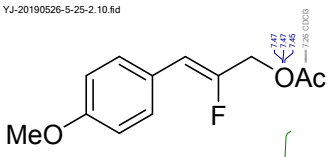

YJ-20190526-5-25-1.10.fid
OAc
F
Me
f1 (ppm)

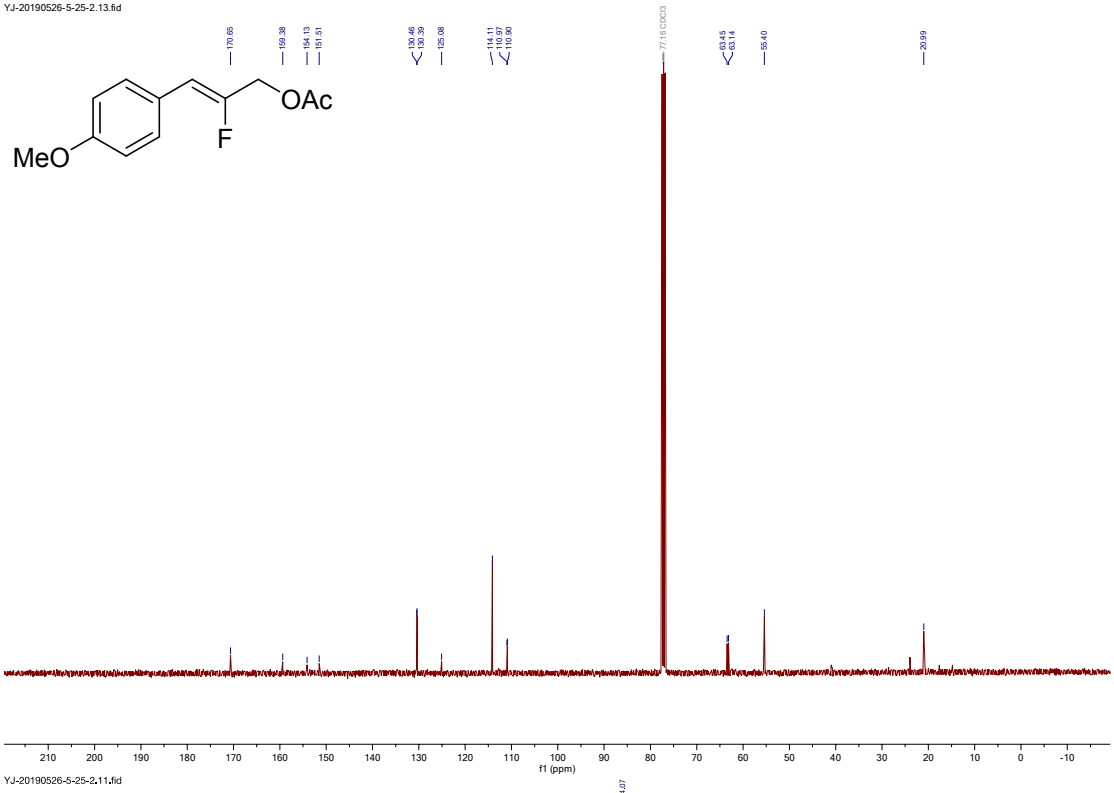

YJ-20190526-5-25-1.12.fid
OAc
F
Me
f1 (ppm)

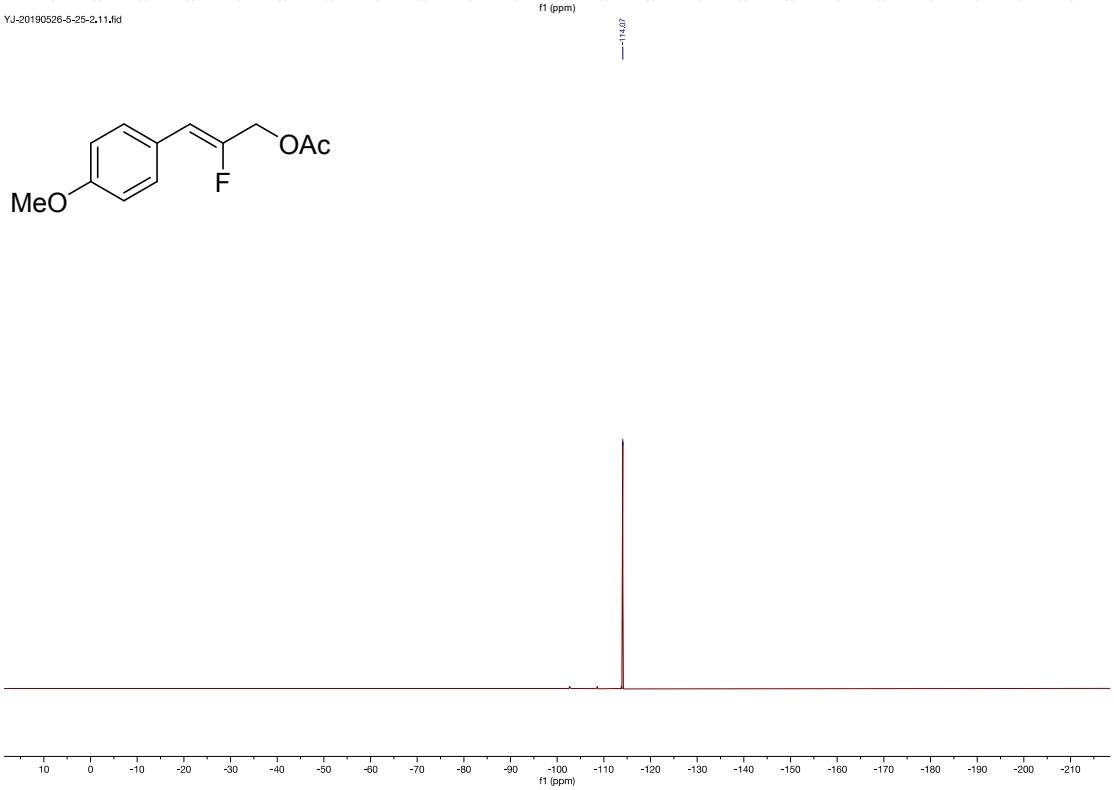
YJ-20190526-5-25-1.11.fid

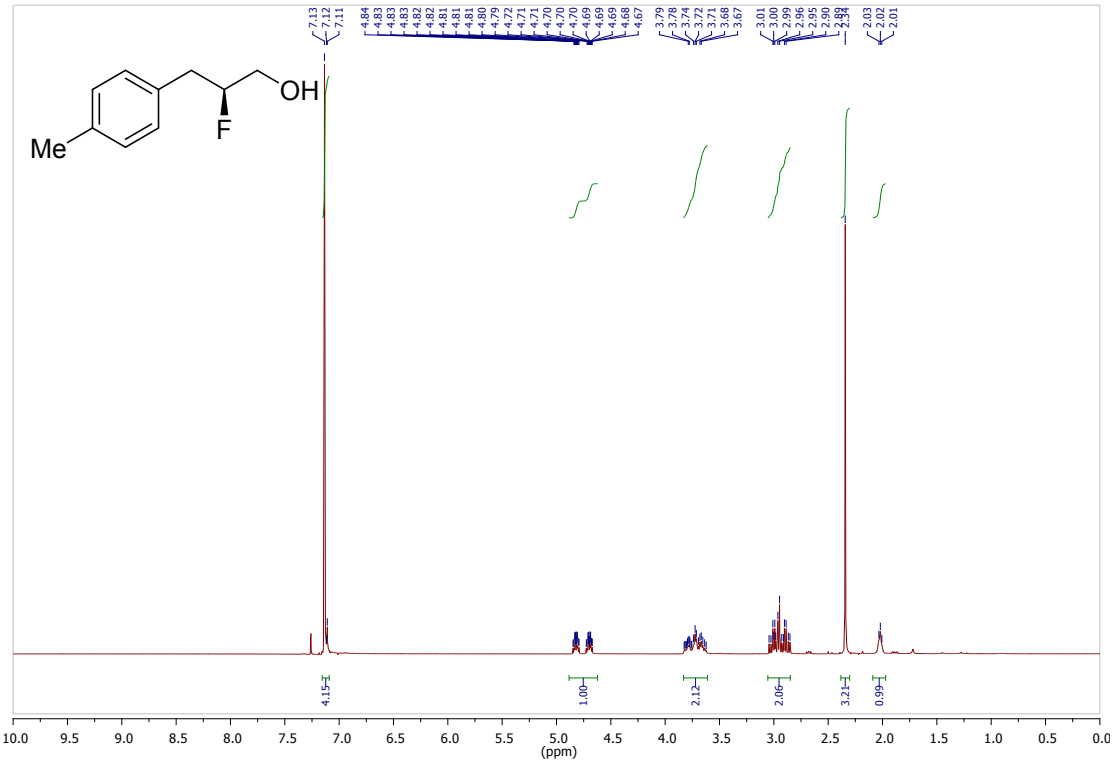


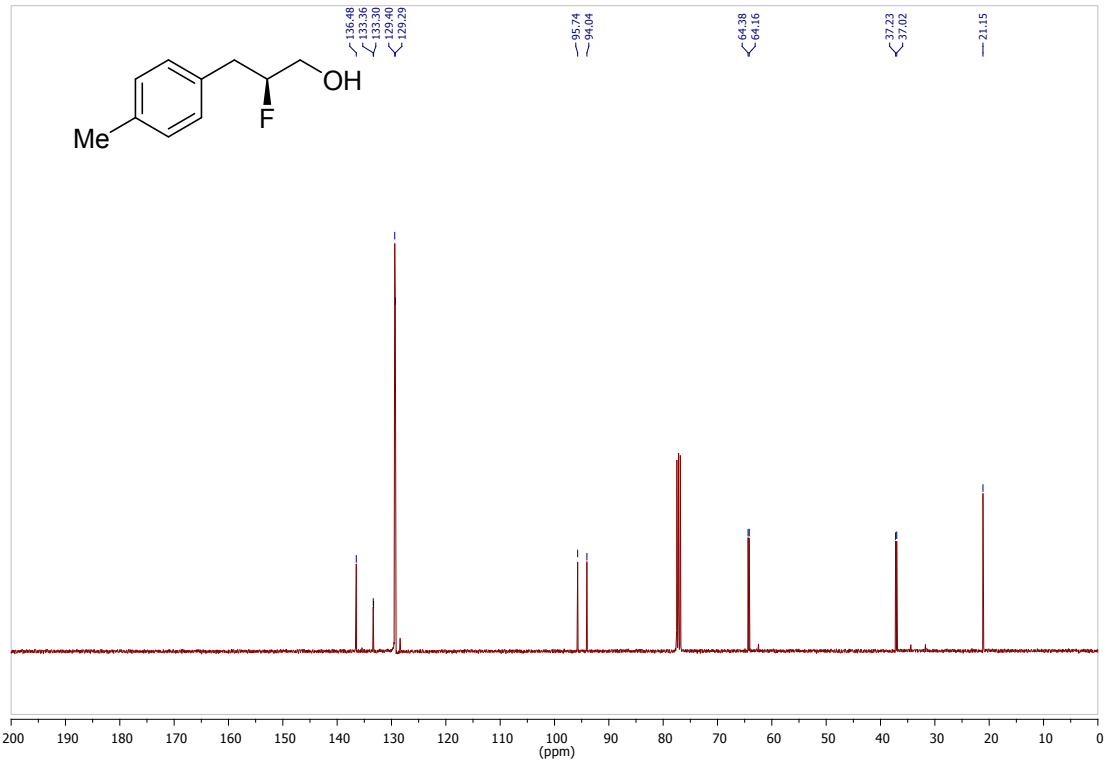
YJ-20190526-5-25-2.10.fid

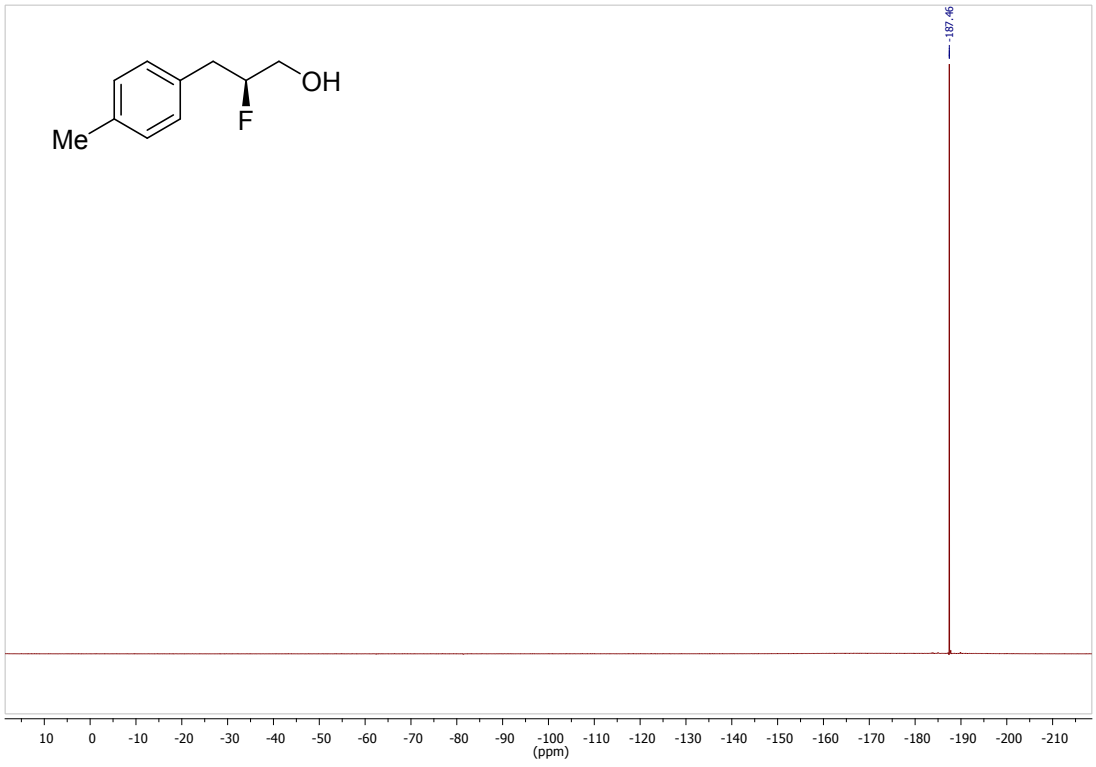


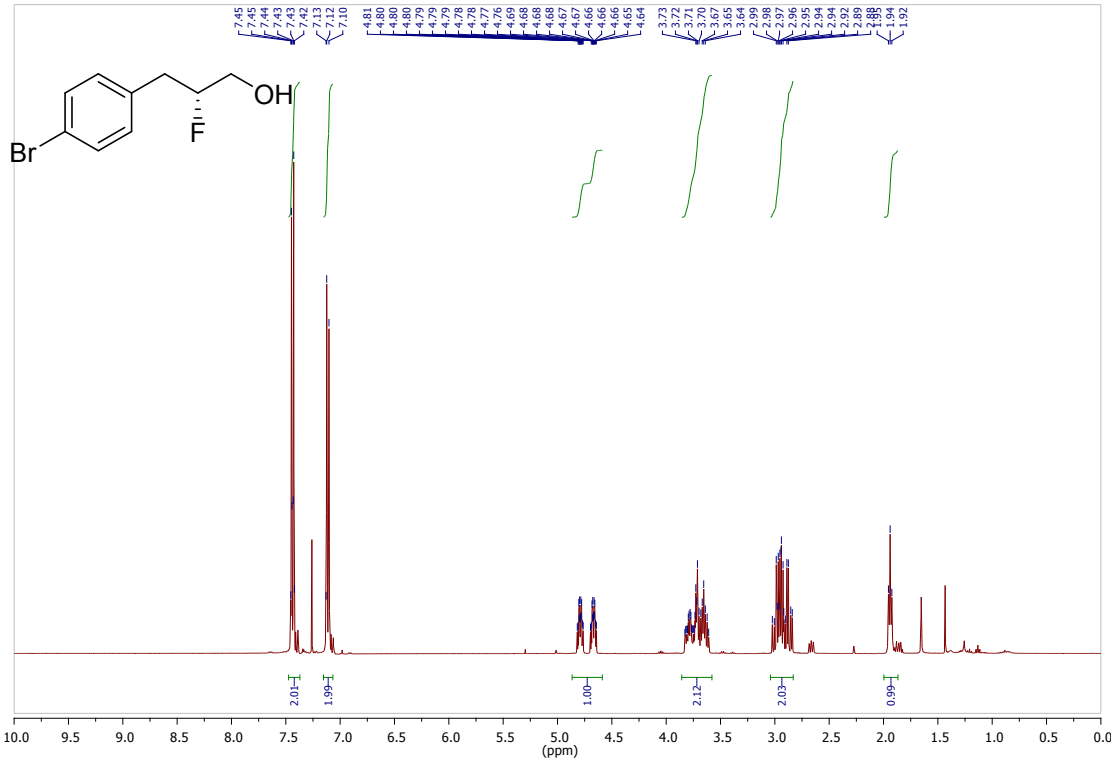

YJ-20190526-5-25-2.13.fid
170.65
159.38
154.13
151.51
130.46
130.39
125.08
114.11
110.97
110.90
77.16 CDCl3
63.45
63.14
55.40
20.99
OAc
F
MeO
f1 (ppm)

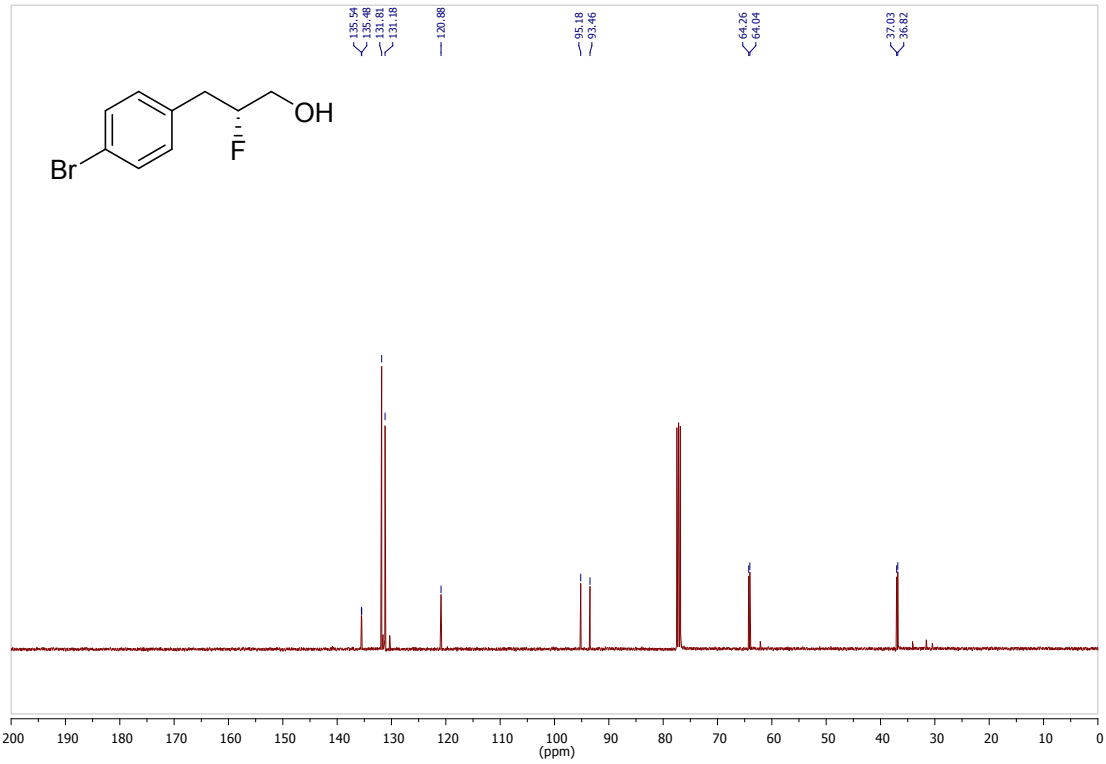

YJ-20190526-5-25-2.11.fid
-114.07
OAc
F
MeO
f1 (ppm)

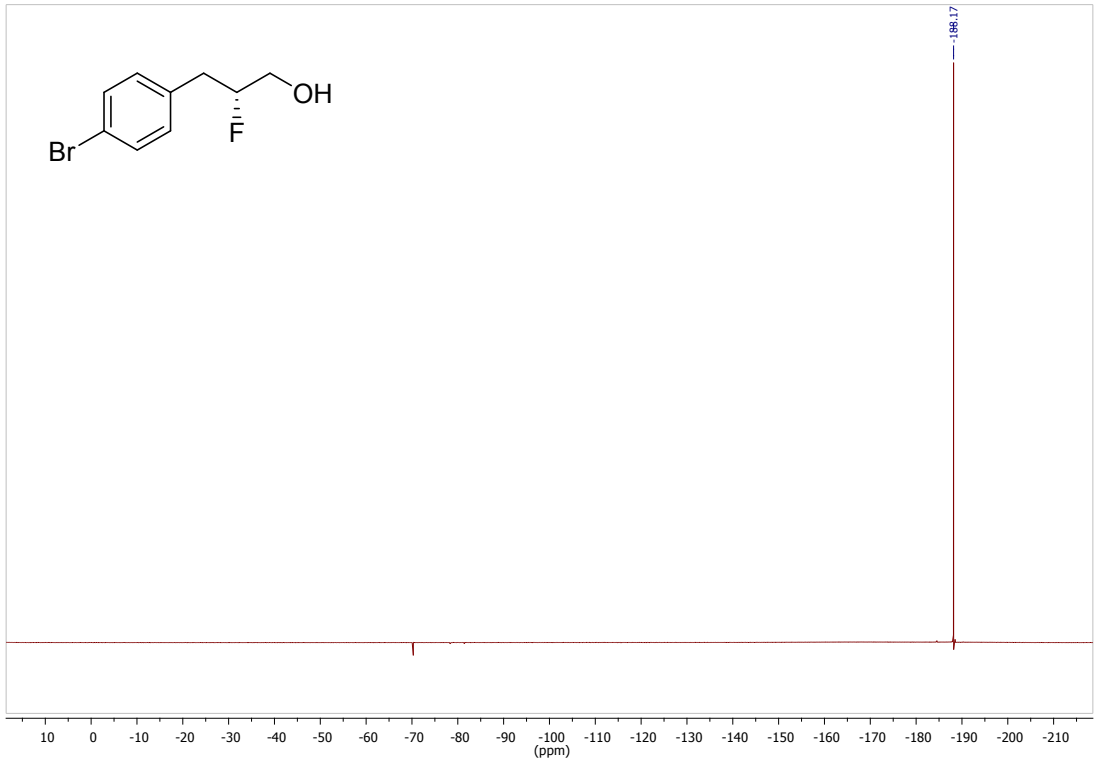

OH
F
Me
(ppm)

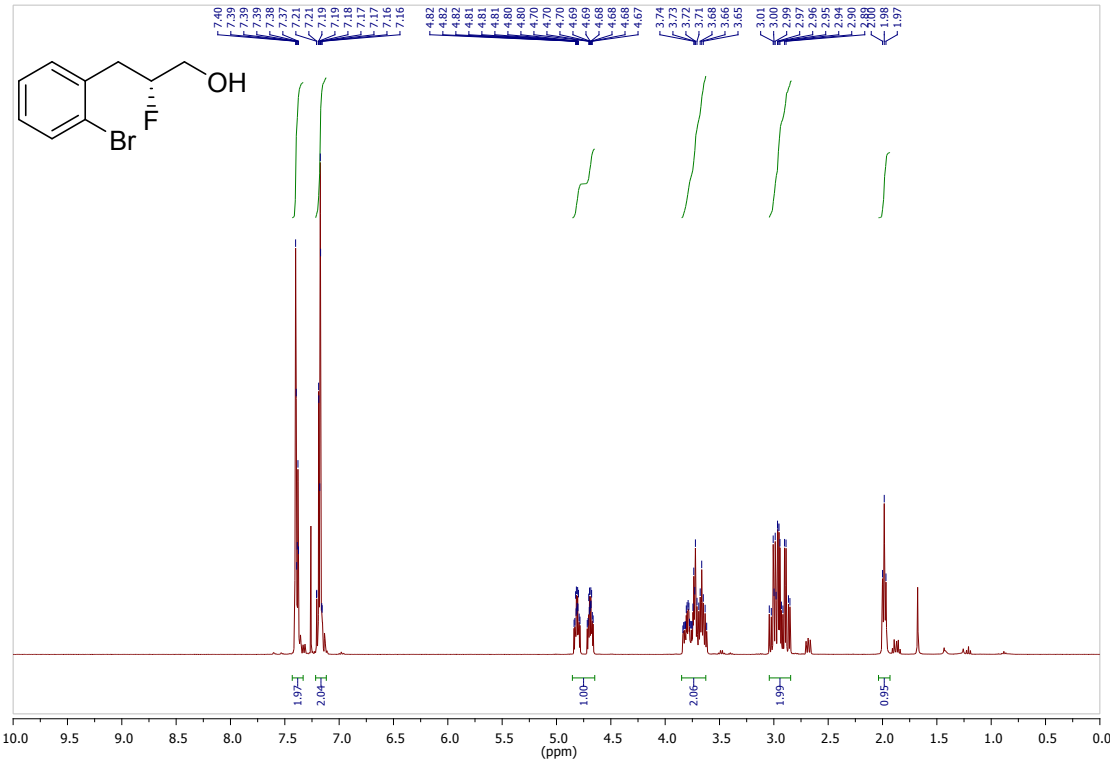

OH
F
Me
(ppm)

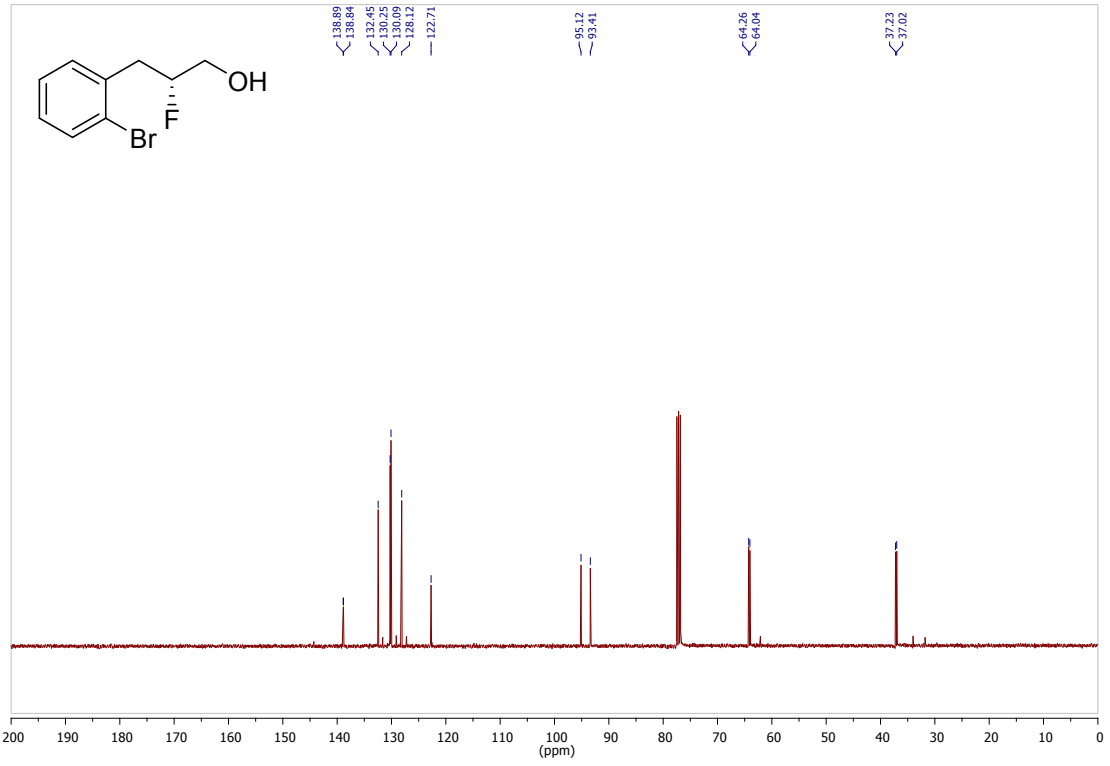

OH
F
Me
-187.46
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
(ppm)

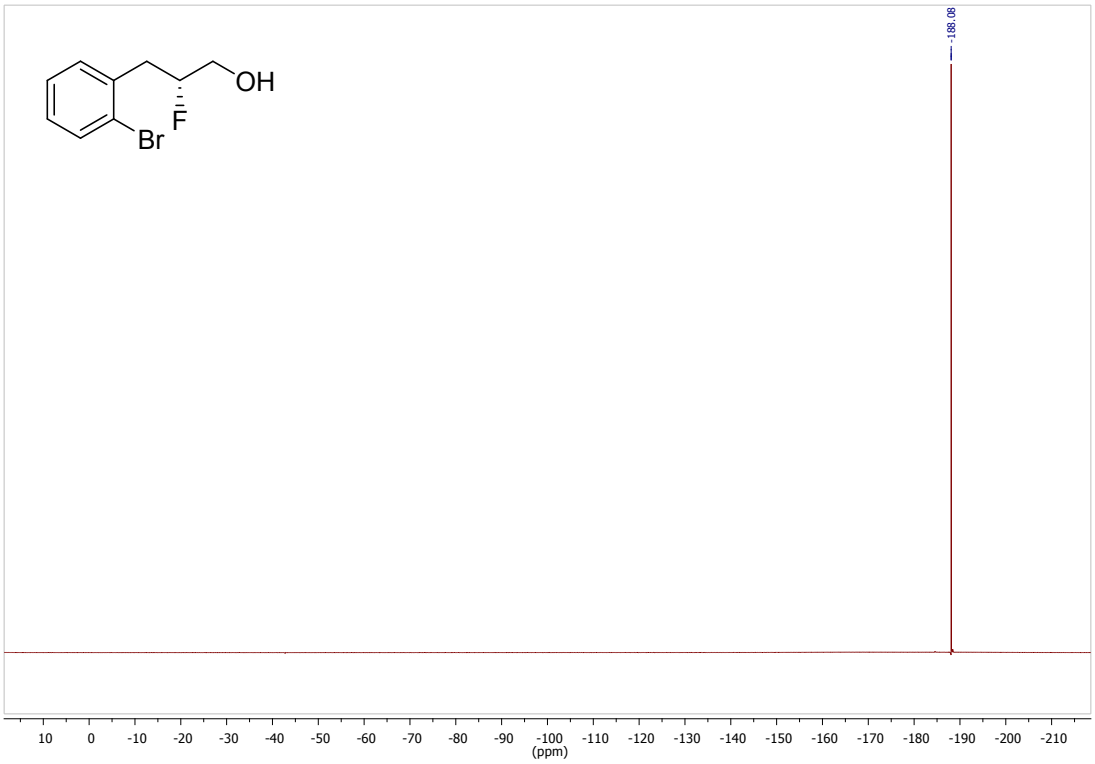

OH
F
Br
7.45 7.45 7.44 7.43 7.43 7.42 7.13 7.12 7.10
4.81 4.80 4.80 4.80 4.79 4.79 4.79 4.78 4.78 4.77 4.76 4.69 4.68 4.68 4.67 4.67 4.66 4.66 4.66 4.65 4.64
3.73 3.72 3.71 3.70 3.67 3.65 3.64
2.99 2.98 2.97 2.96 2.95 2.94 2.94 2.92 2.89 1.94 1.92
2.01 1.99 1.00 2.12 2.03 0.99
10.0 9.5 9.0 8.5 8.0 7.5 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
(ppm)

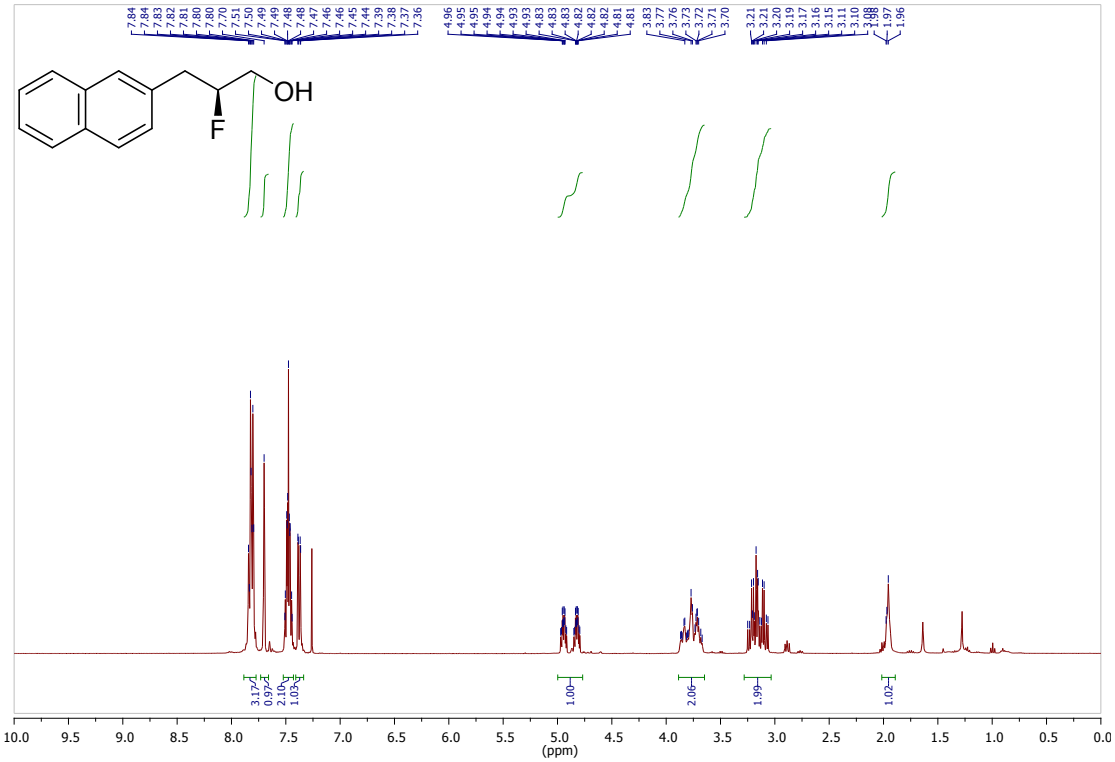

135.54
135.48
131.81
131.18
120.88
95.18
93.46
64.26
64.04
37.03
36.82
OH
F
Br
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
(ppm)

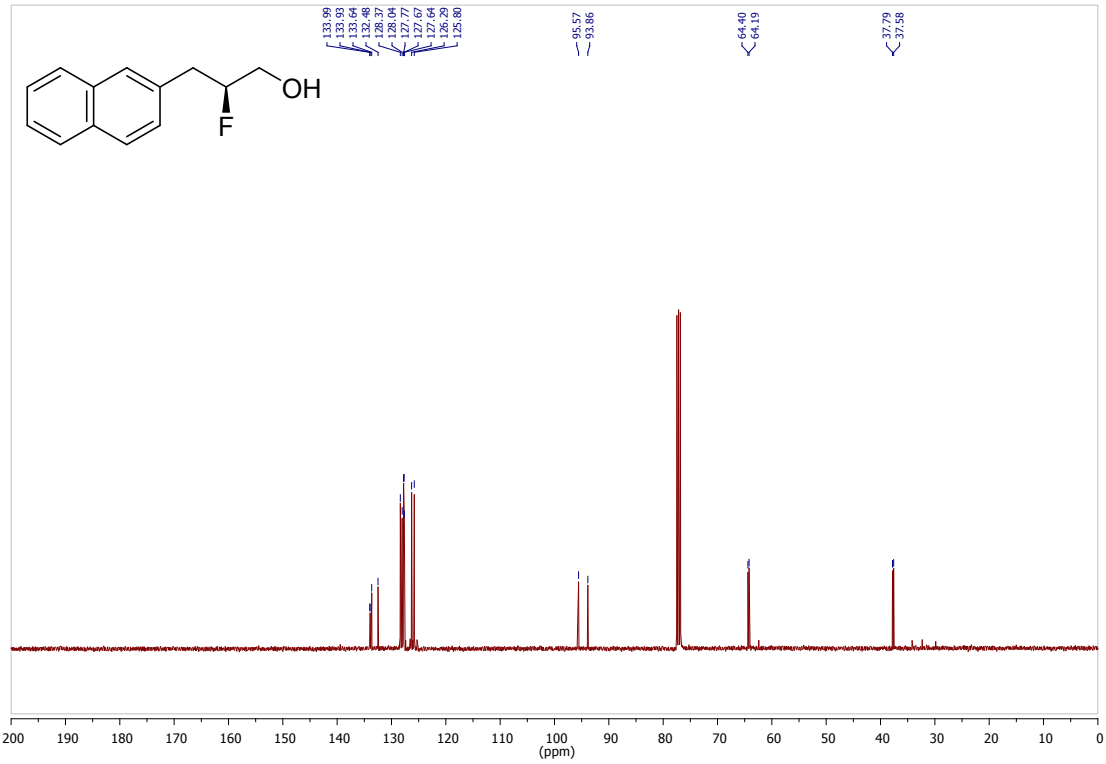

-188.17
OH
F
Br
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
(ppm)

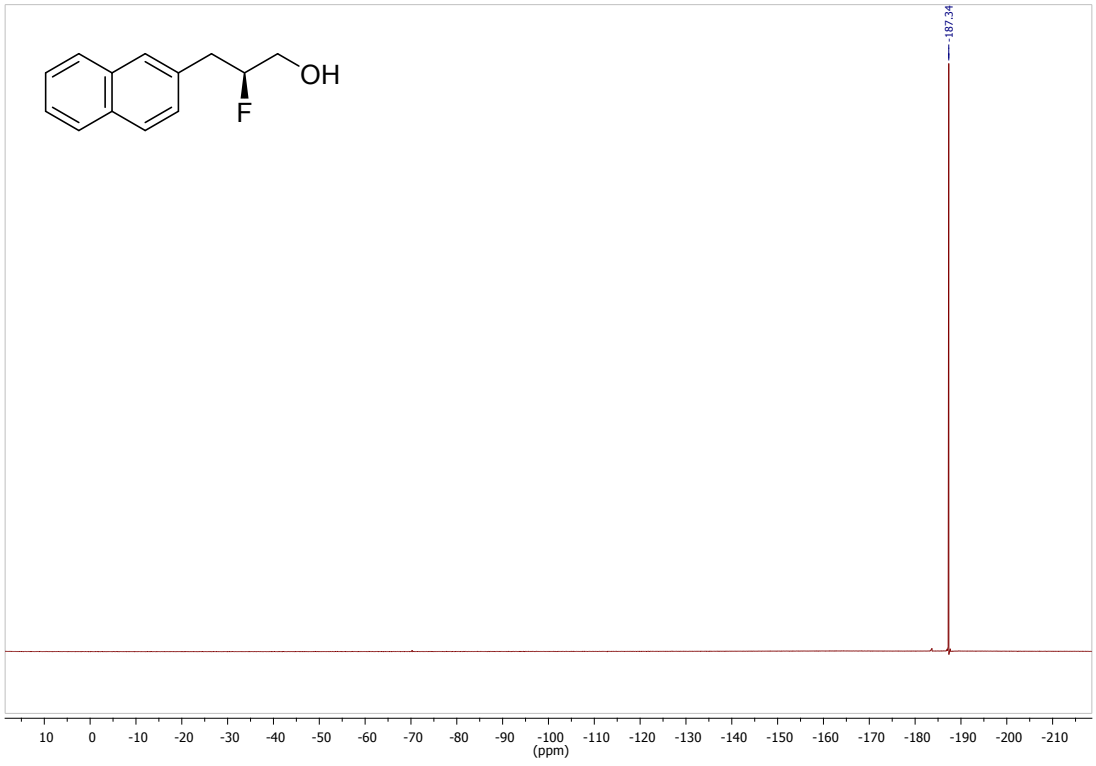

OH
F
Br
(ppm)

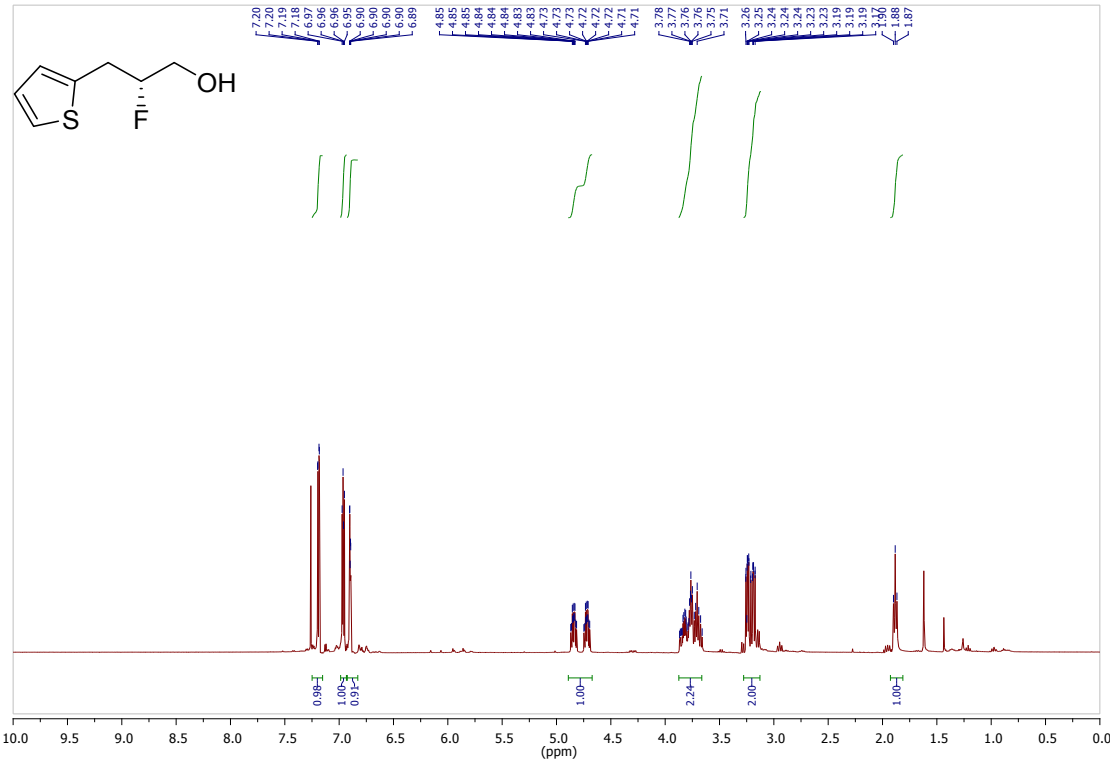

OH
F
Br
(ppm)

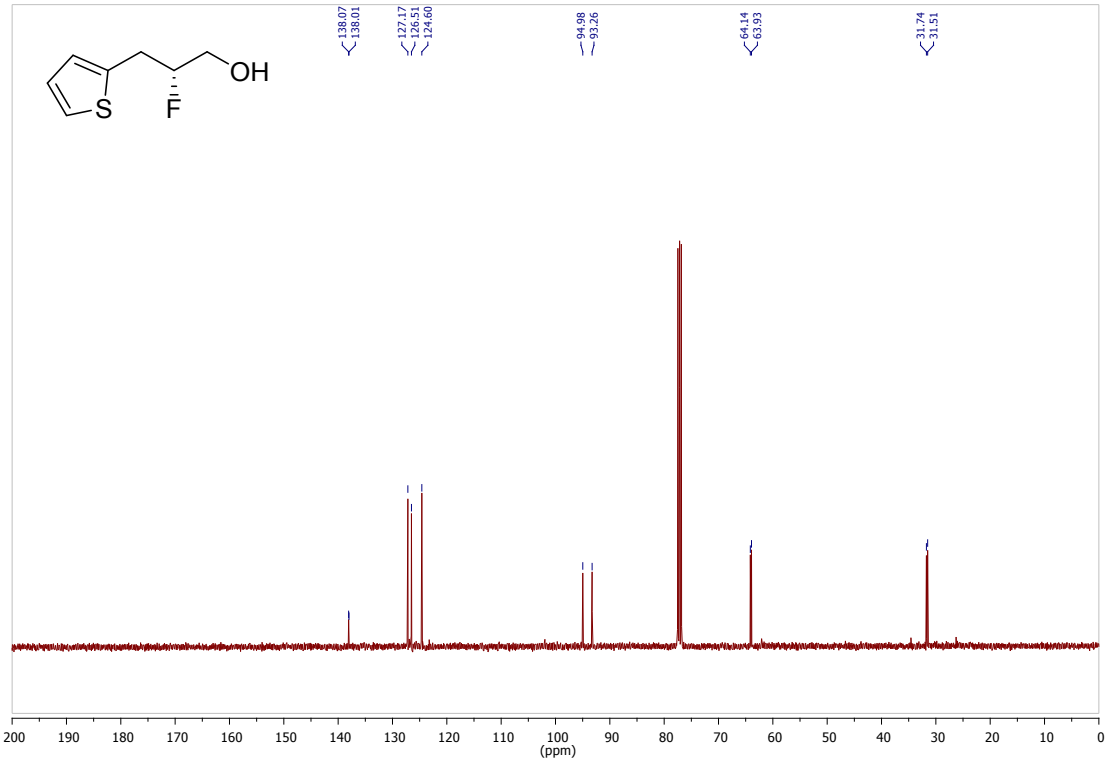

OH
F
Br
-188.08
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
(ppm)

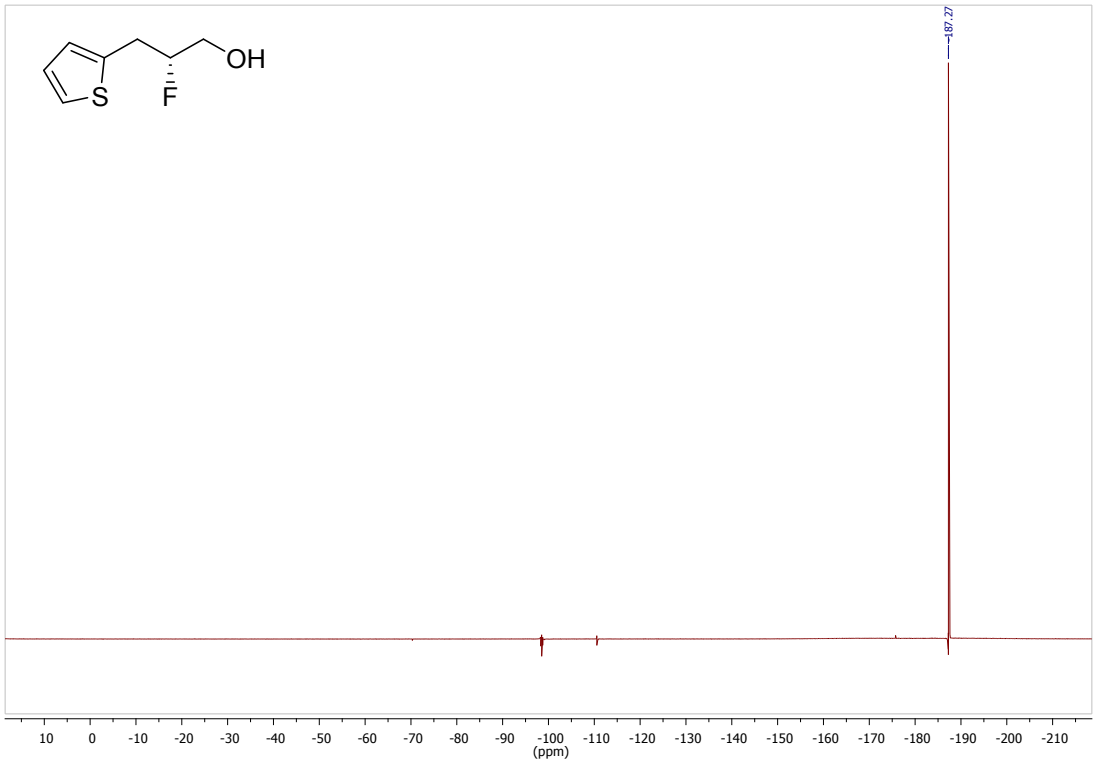

OH
F
7.84 7.84 7.83 7.82 7.81 7.80 7.80 7.70 7.51 7.50 7.49 7.49 7.48 7.48 7.47 7.46 7.46 7.45 7.44 7.39 7.38 7.37 7.36
4.96 4.95 4.95 4.94 4.94 4.93 4.93 4.83 4.83 4.82 4.82 4.82 4.81 4.81
3.83 3.77 3.76 3.73 3.72 3.71 3.70
3.21 3.21 3.20 3.19 3.17 3.16 3.15 3.11 3.10 1.98 1.97 1.96
3.17 0.97 2.16 1.03 1.00 2.06 1.99 1.02
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
(ppm)

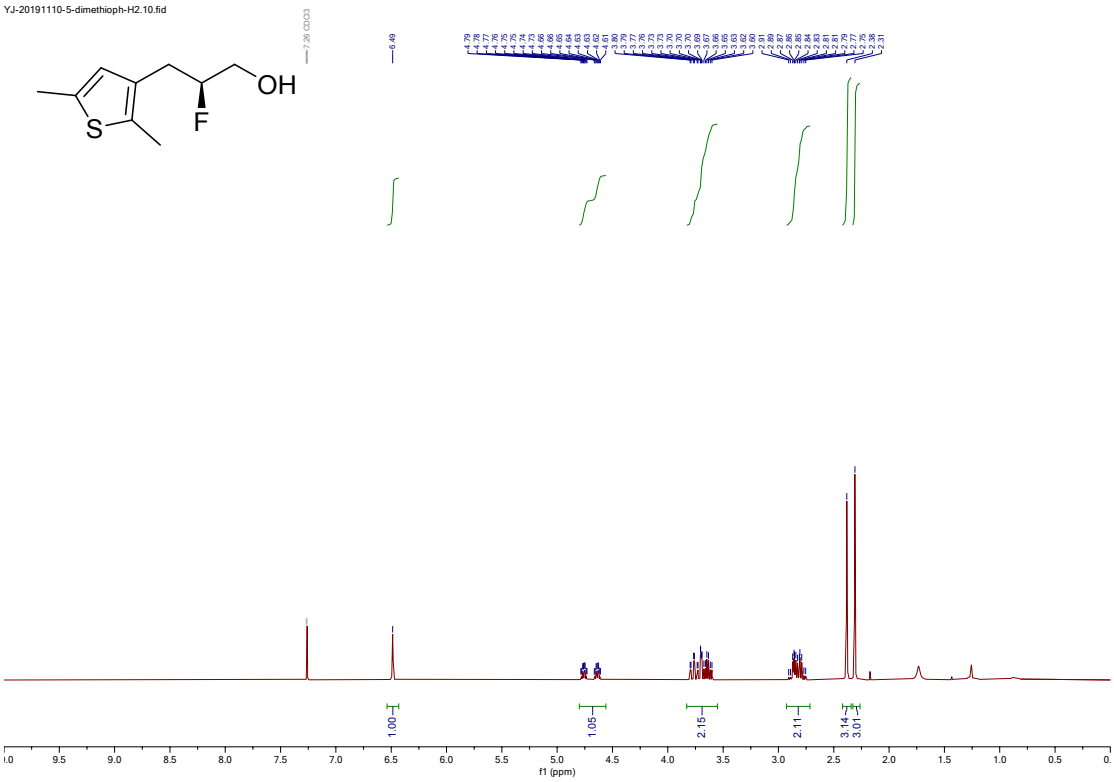

133.99
133.93
133.64
132.48
128.37
128.04
127.77
127.67
127.64
126.29
125.80
95.57
93.86
64.40
64.19
37.79
37.58
OH
F
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
(ppm)


-187.34
OH
F
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
(ppm)

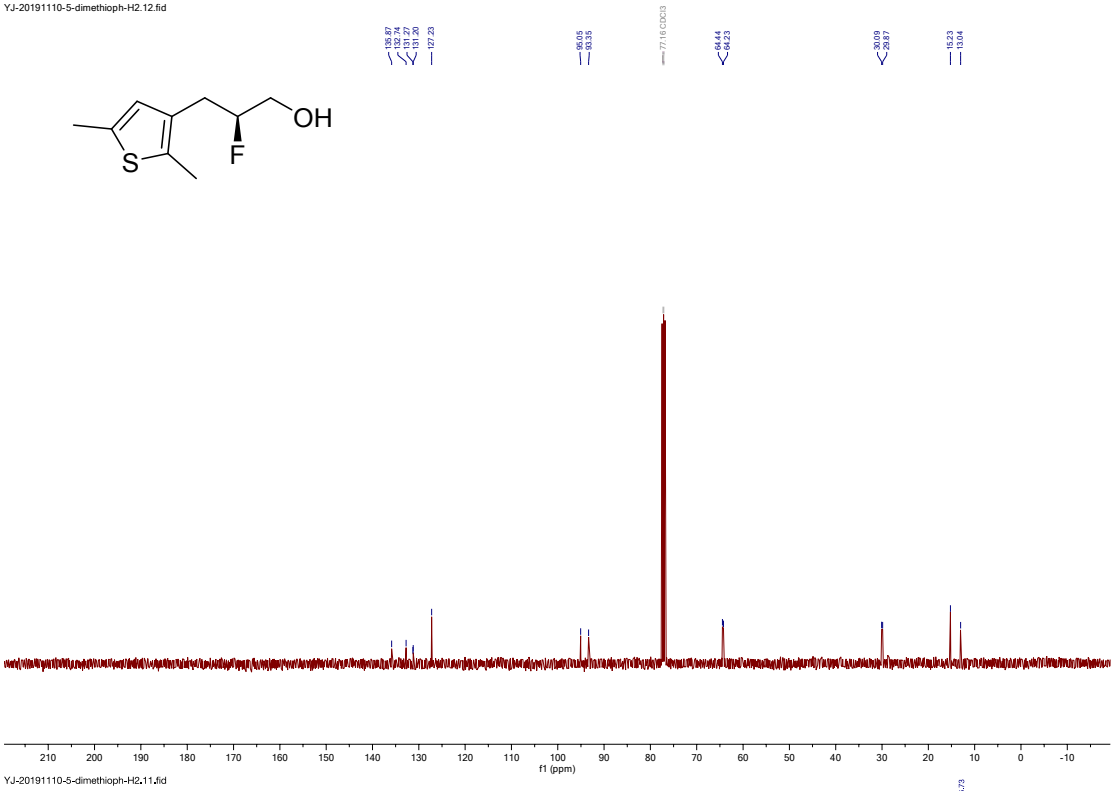

OH
S
F
(ppm)


OH
S
F
(ppm)

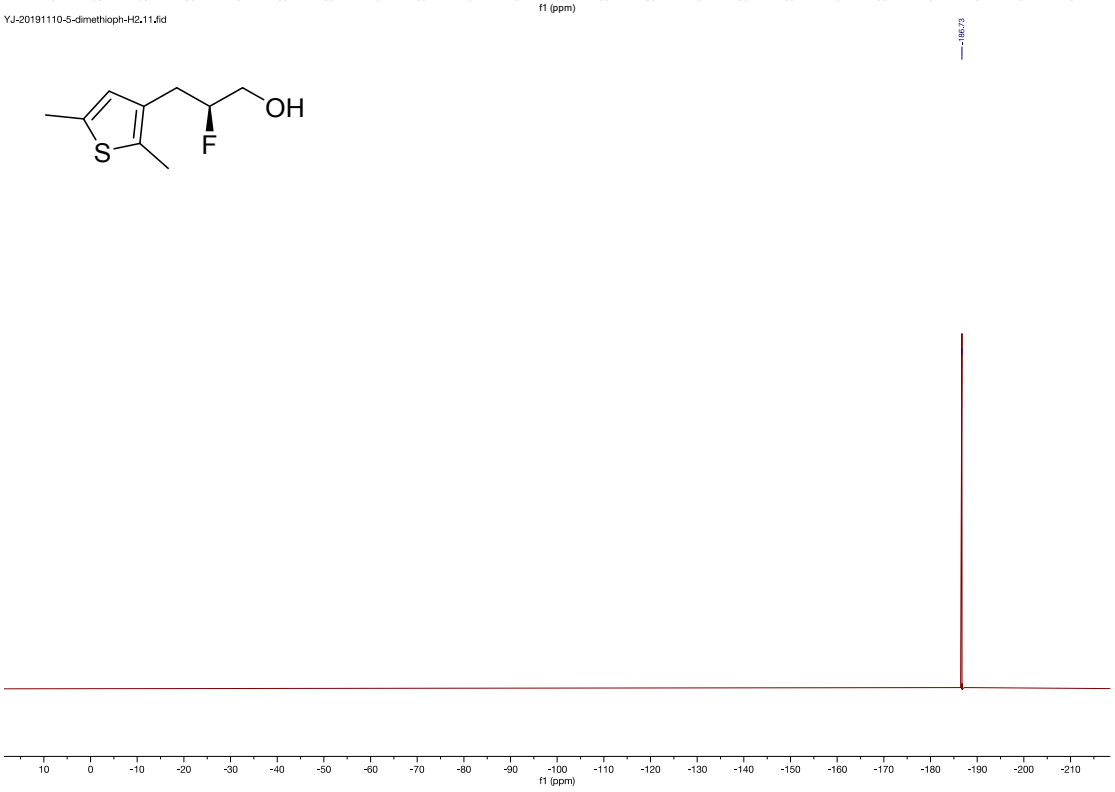

OH
S
F
-187.27
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
(ppm)

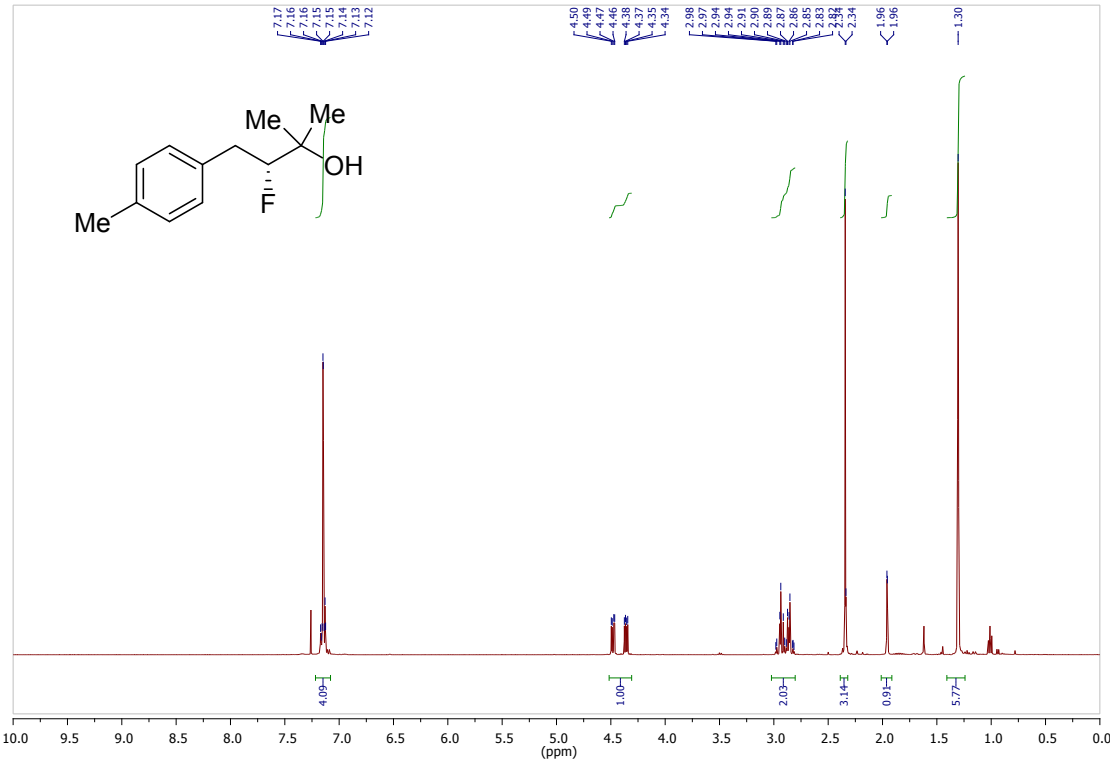

YJ-20191110-5-dimethioph-H2.10.fid
OH
S
F
7.26
6.49
1.00
1.05
2.15
2.11
3.14
3.01
f1 (ppm)

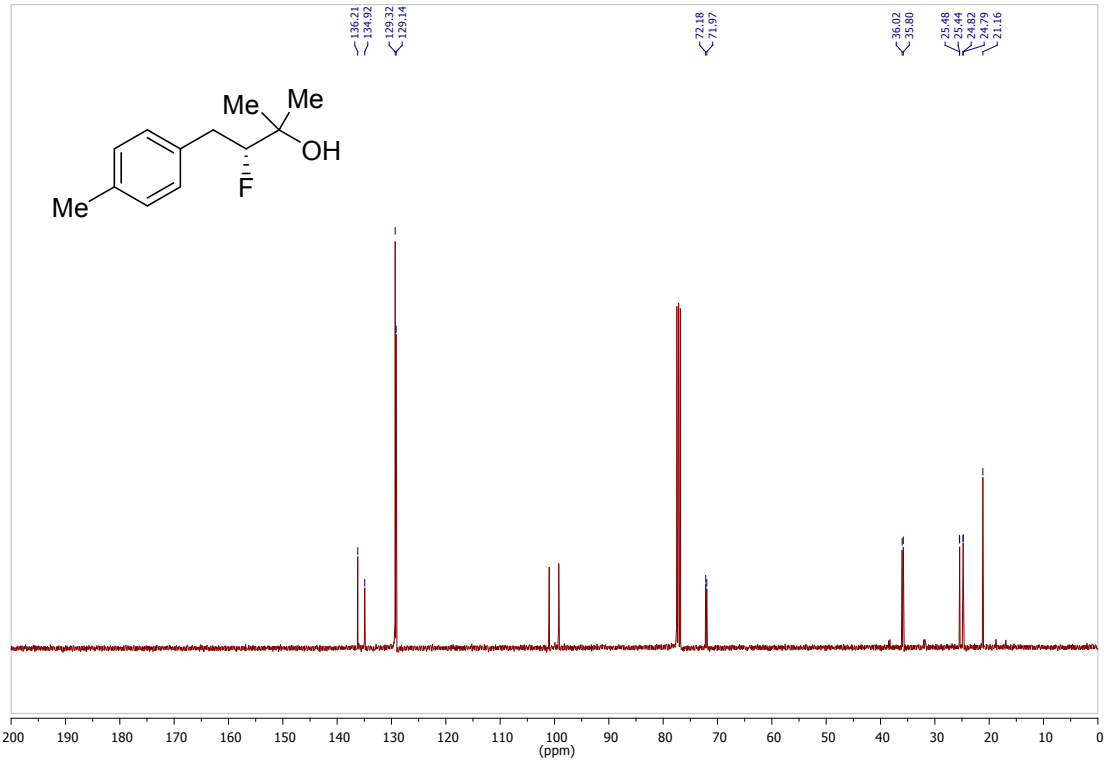
YJ-20191110-5-dimethioph-H2.12.fid

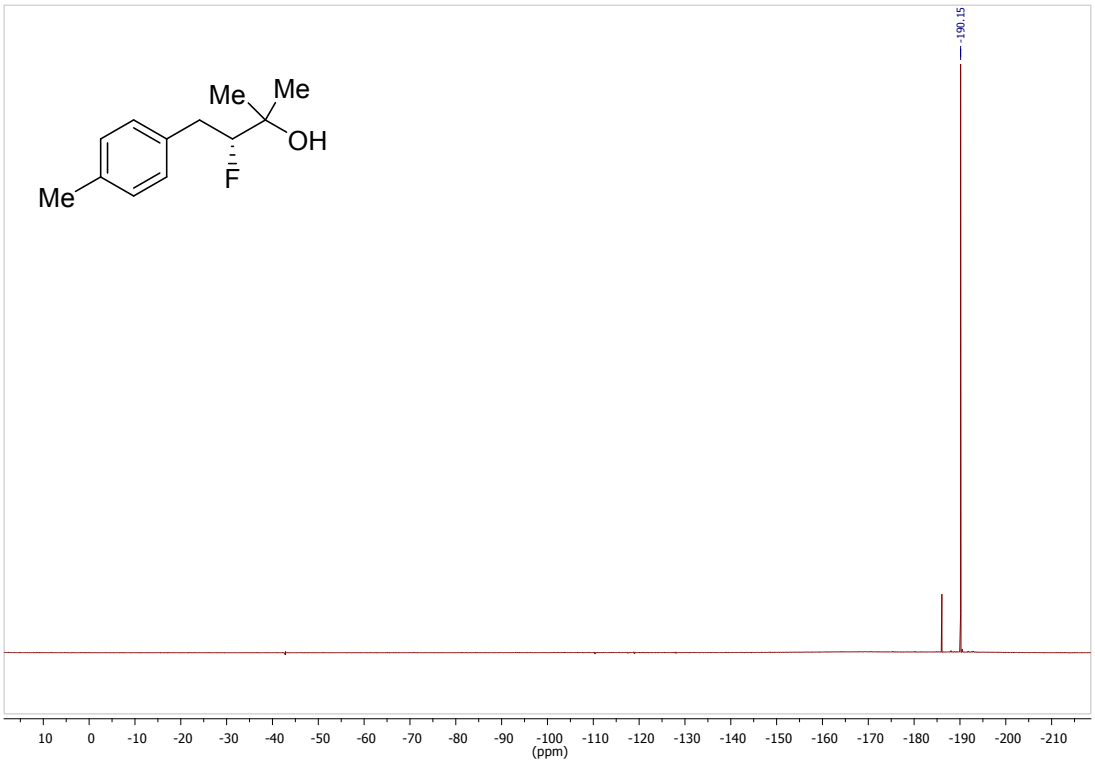


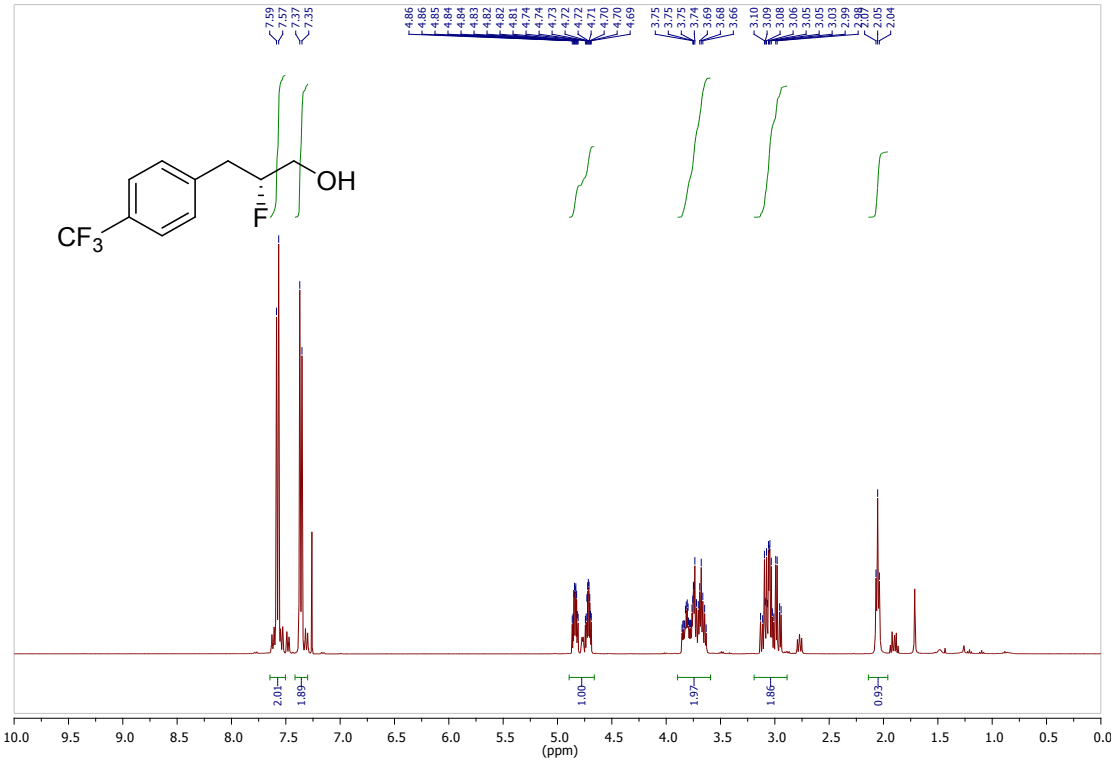
YJ-20191110-5-dimethioph-H2.11.fid

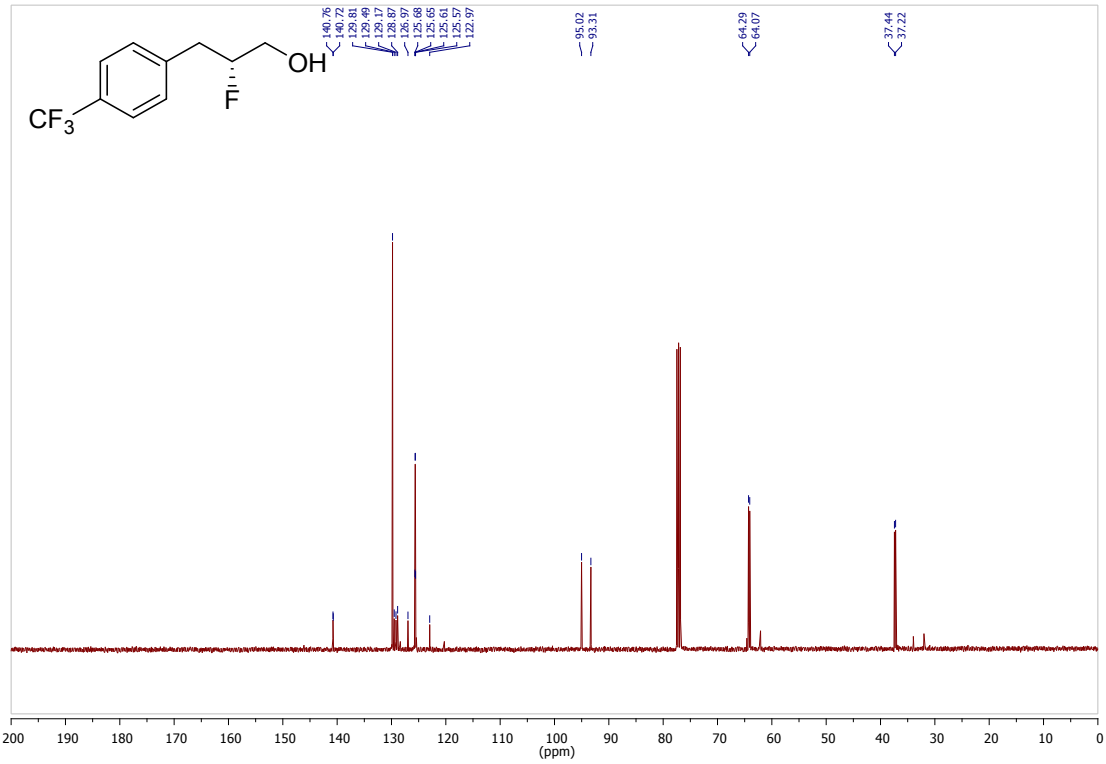


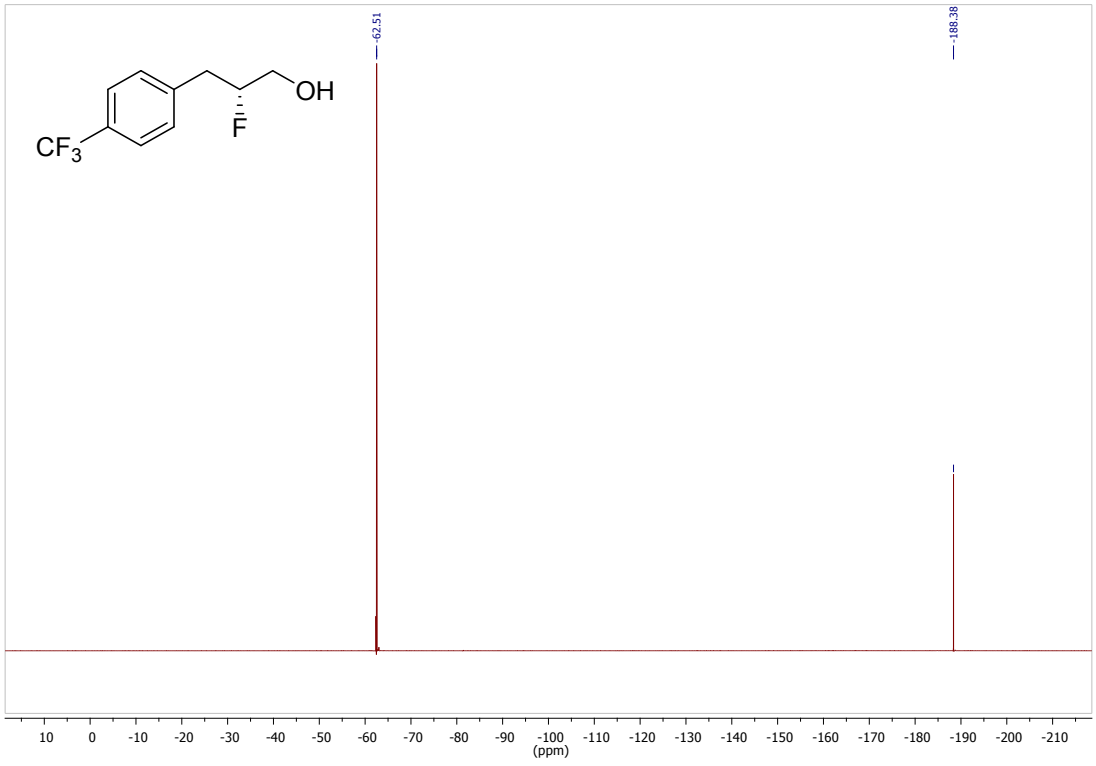

Me
Me
OH
F
Me
7.17
7.16
7.16
7.15
7.15
7.14
7.13
7.12
4.50
4.49
4.47
4.46
4.38
4.37
4.35
4.34
2.98
2.97
2.94
2.94
2.91
2.90
2.89
2.87
2.86
2.85
2.83
2.82
2.34
1.96
1.96
1.30
4.09
1.00
2.03
3.14
0.91
5.77
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
(ppm)

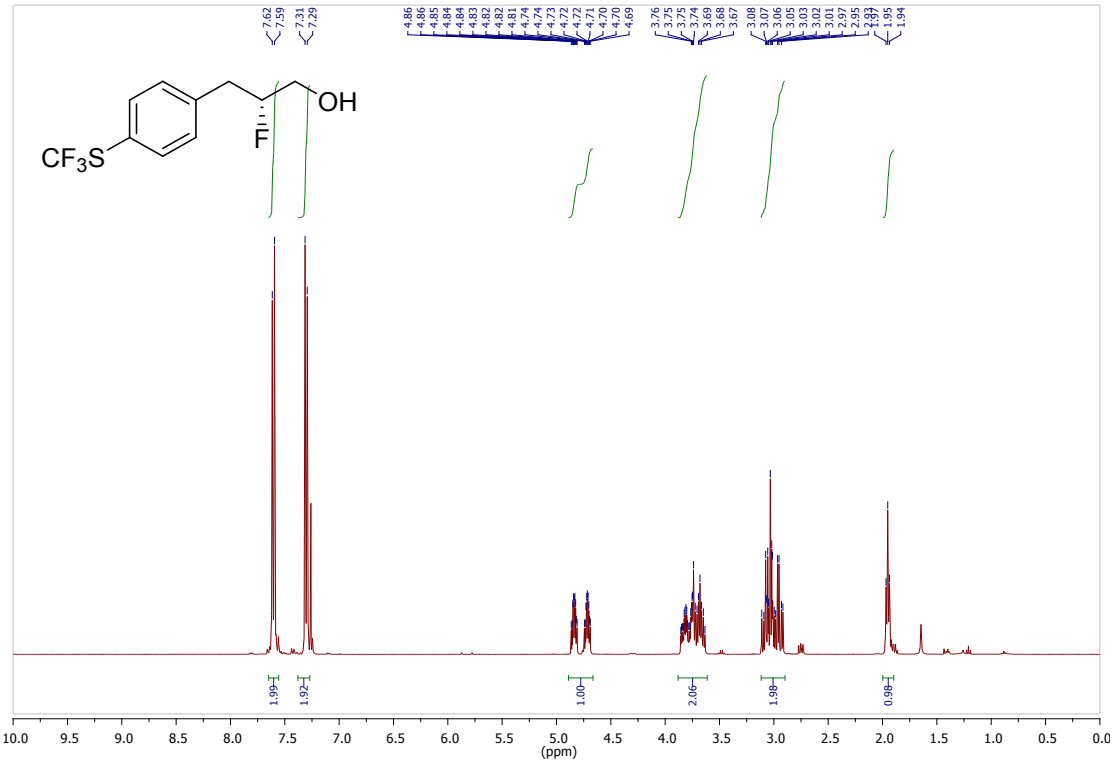

Me
Me
OH
F
Me
136.21
134.92
129.32
129.14
72.18
71.97
36.02
35.80
25.48
25.44
24.82
24.79
21.16
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
(ppm)

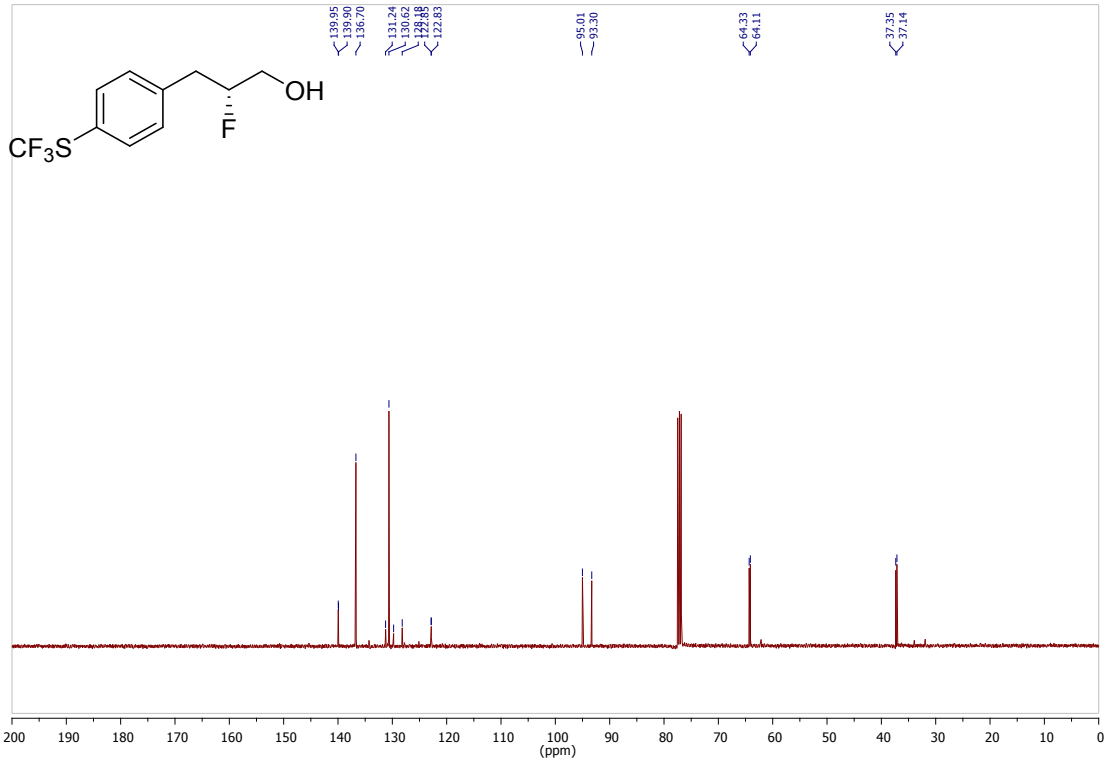

Me
Me
OH
F
Me
-190.15
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
(ppm)

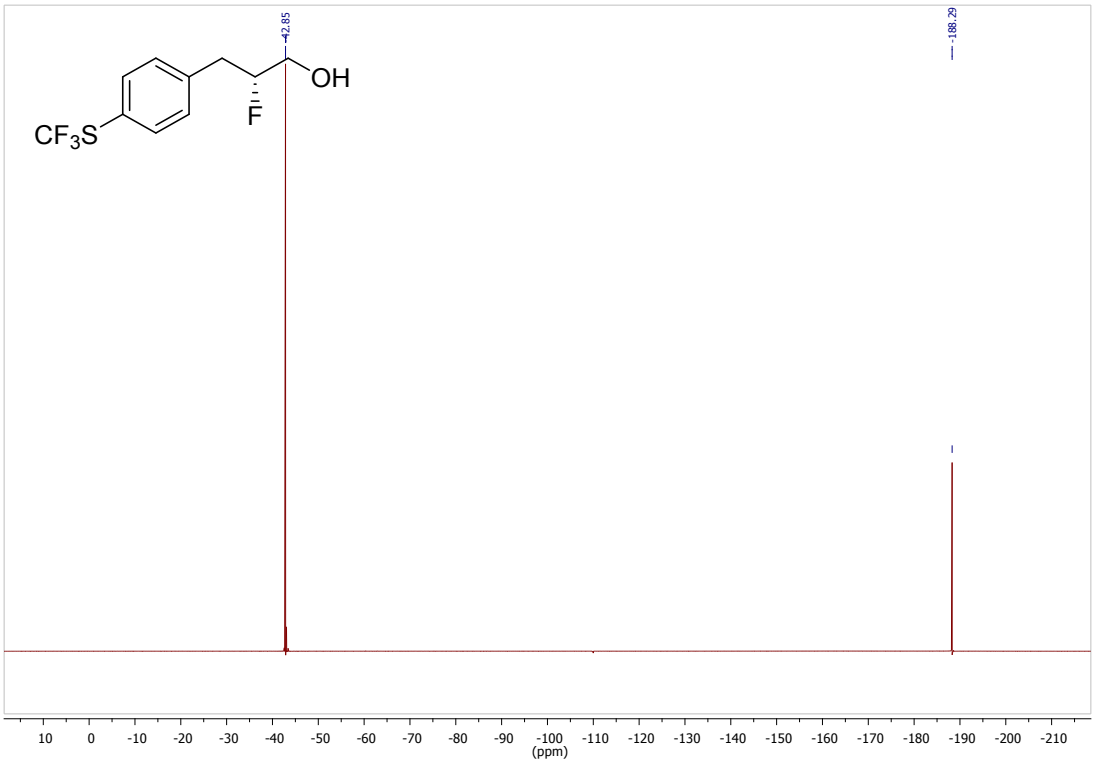

OH
F
CF3
2.01
1.89
1.00
1.97
1.86
0.93
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
(ppm)

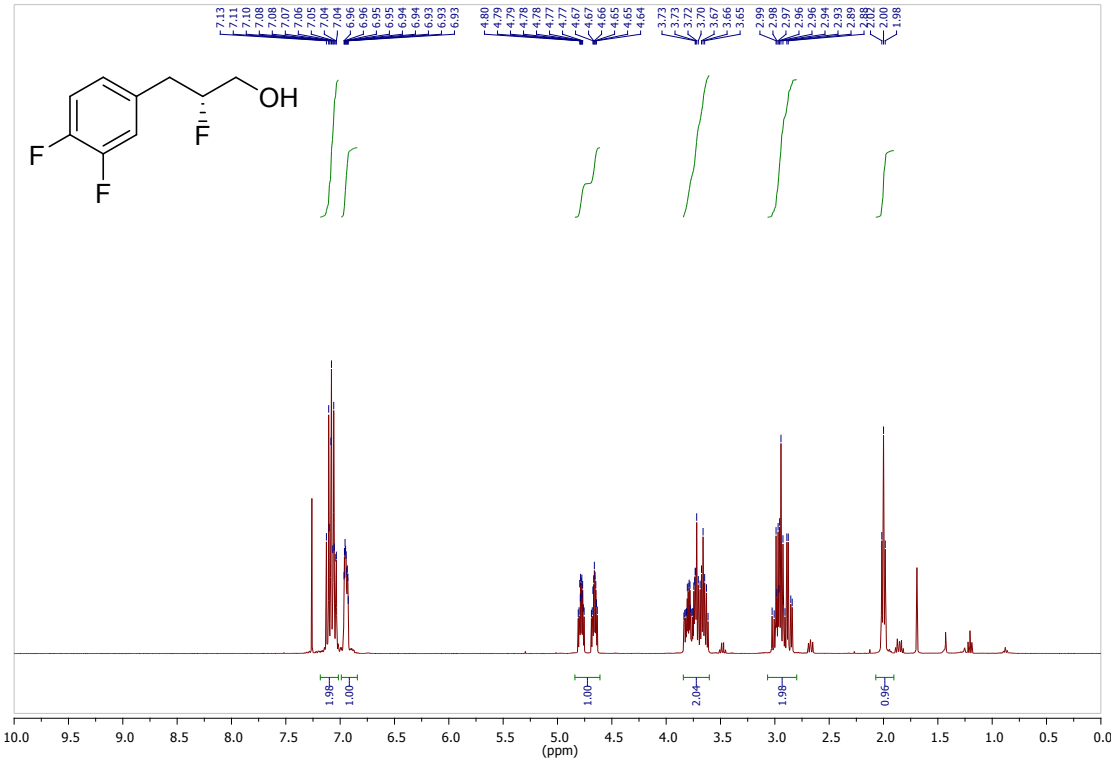

OH
F
CF3
140.76
140.72
129.81
129.49
129.17
128.87
125.67
125.65
125.61
125.57
122.97
95.02
93.31
64.29
64.07
37.44
37.22
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
(ppm)

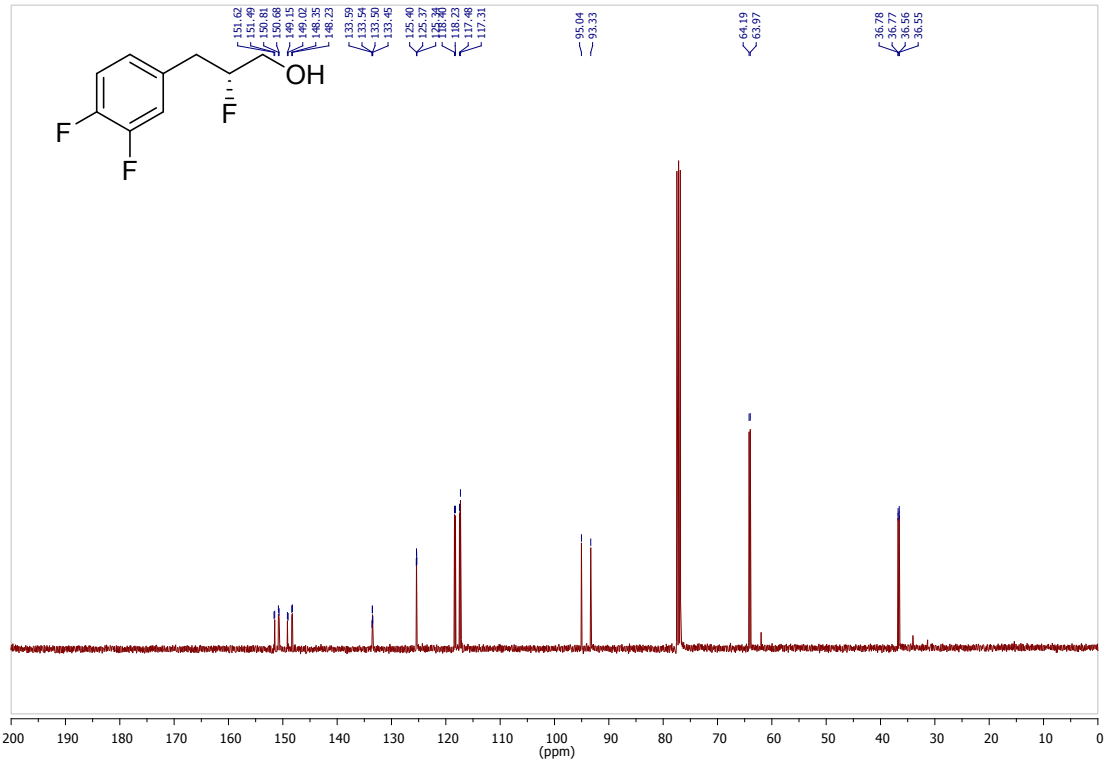

OH
F
CF3
-62.51
-188.38
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
(ppm)

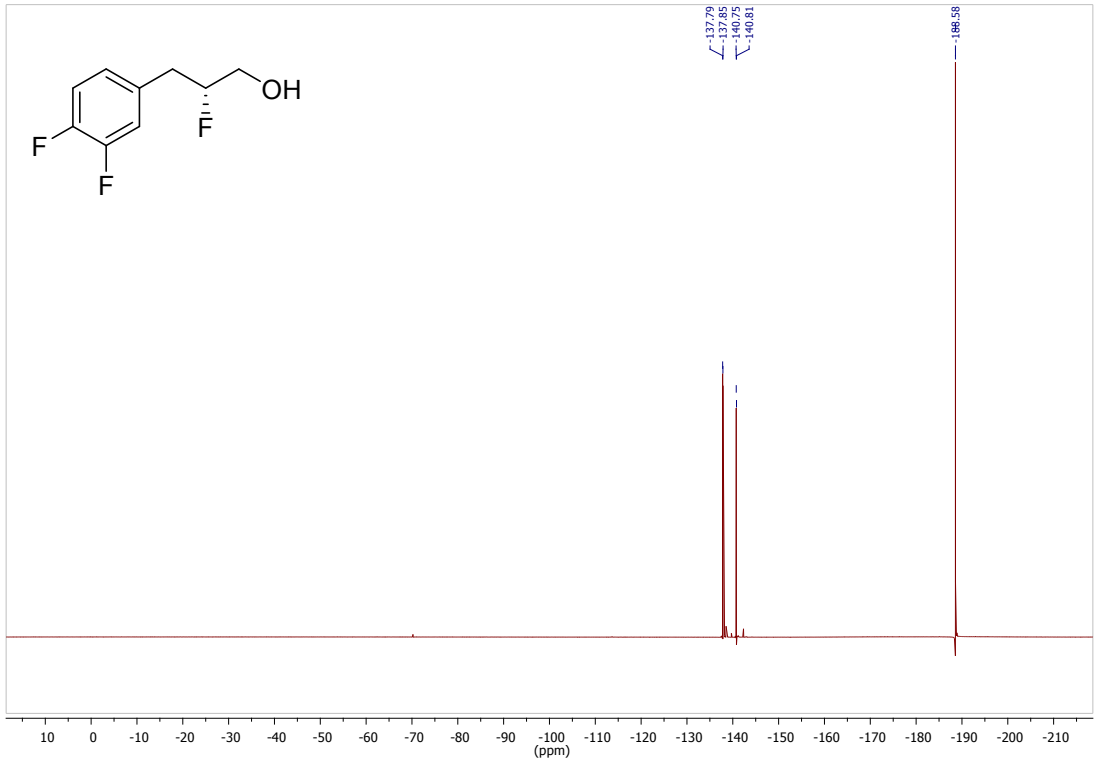

OH
F
CF3S
(ppm)

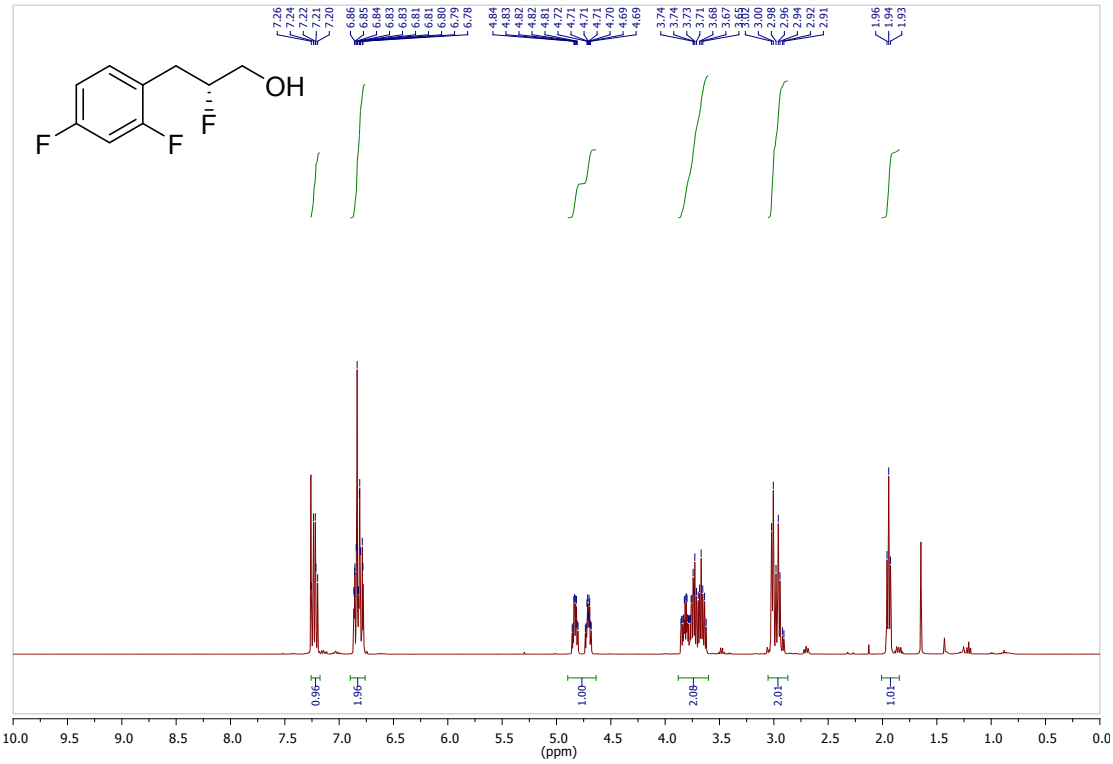

OH
F
CF3S
(ppm)

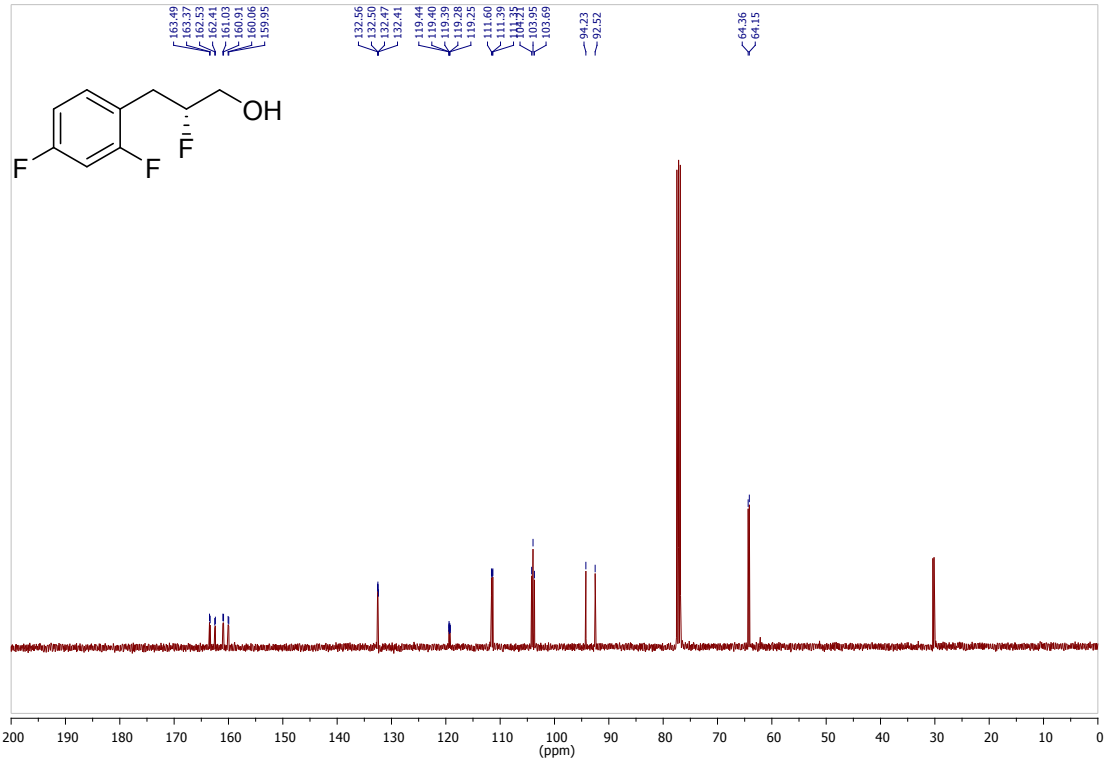

-42.85
-188.29
OH
F
CF_3S
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
(ppm)

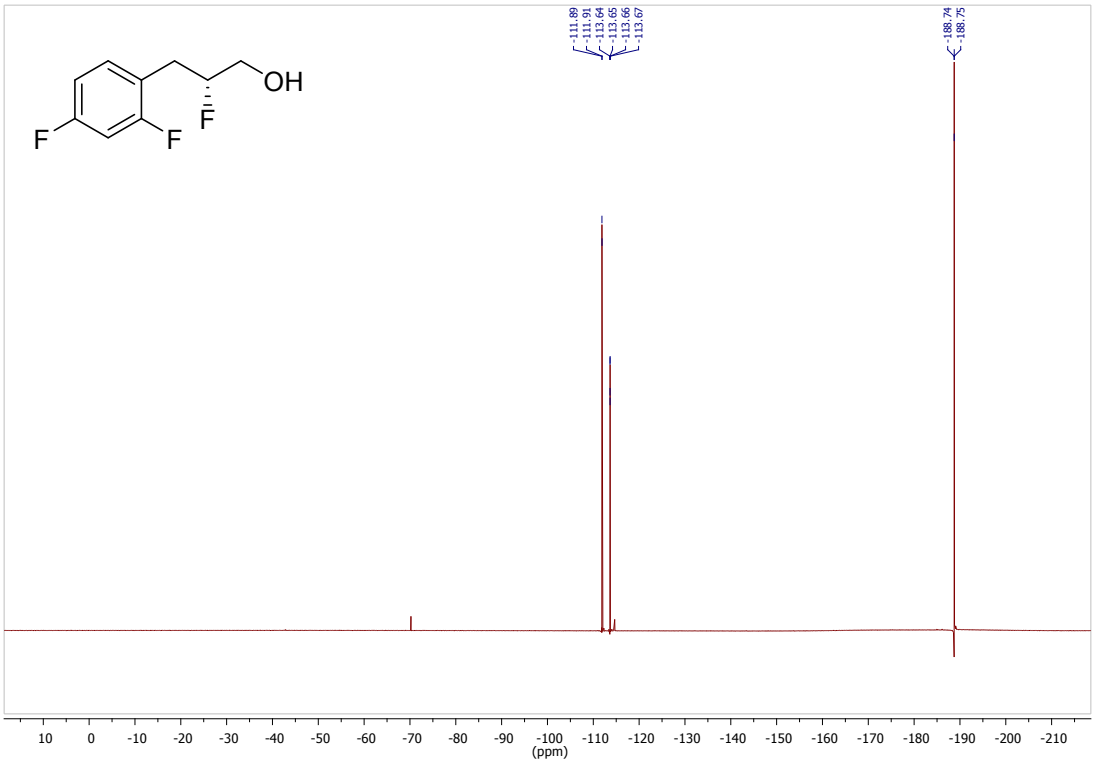

OH
F
F
F
1.98
1.00
1.00
2.04
1.98
0.96
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
(ppm)

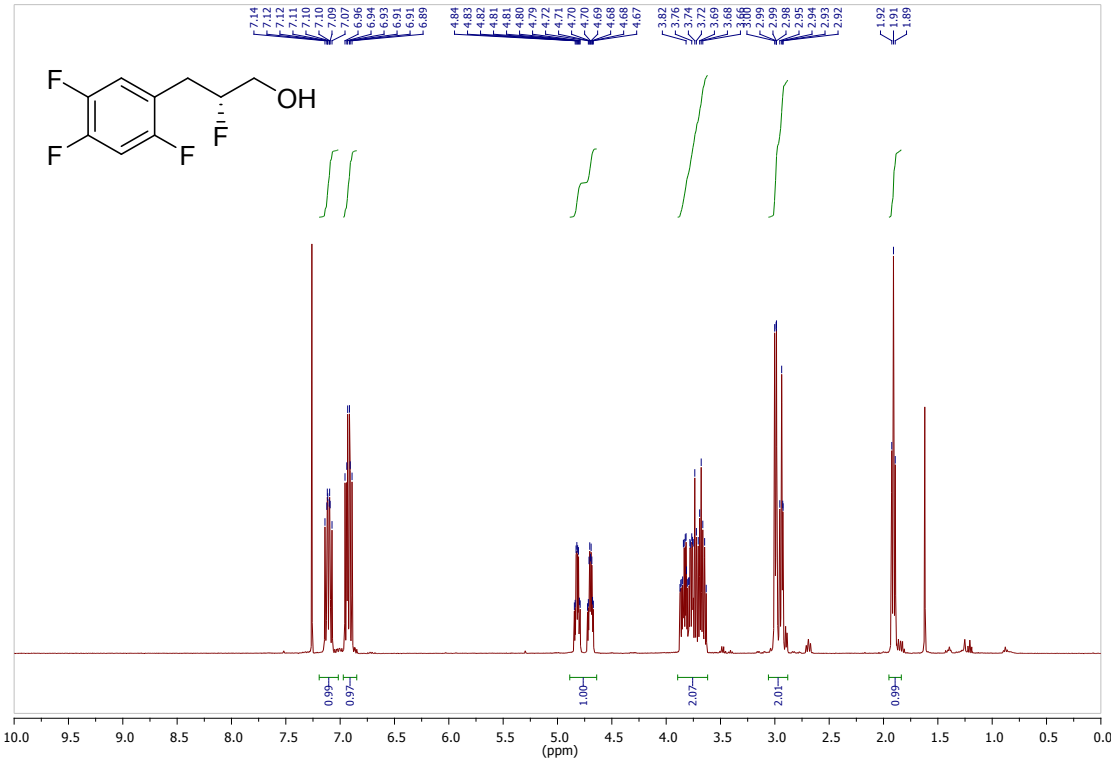

151.62
151.49
150.81
150.68
149.15
149.02
148.35
148.23
133.59
133.54
133.50
133.45
125.40
125.37
118.23
117.48
117.31
95.04
93.33
64.19
63.97
36.78
36.77
36.56
36.55
OH
F
F
F
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
(ppm)

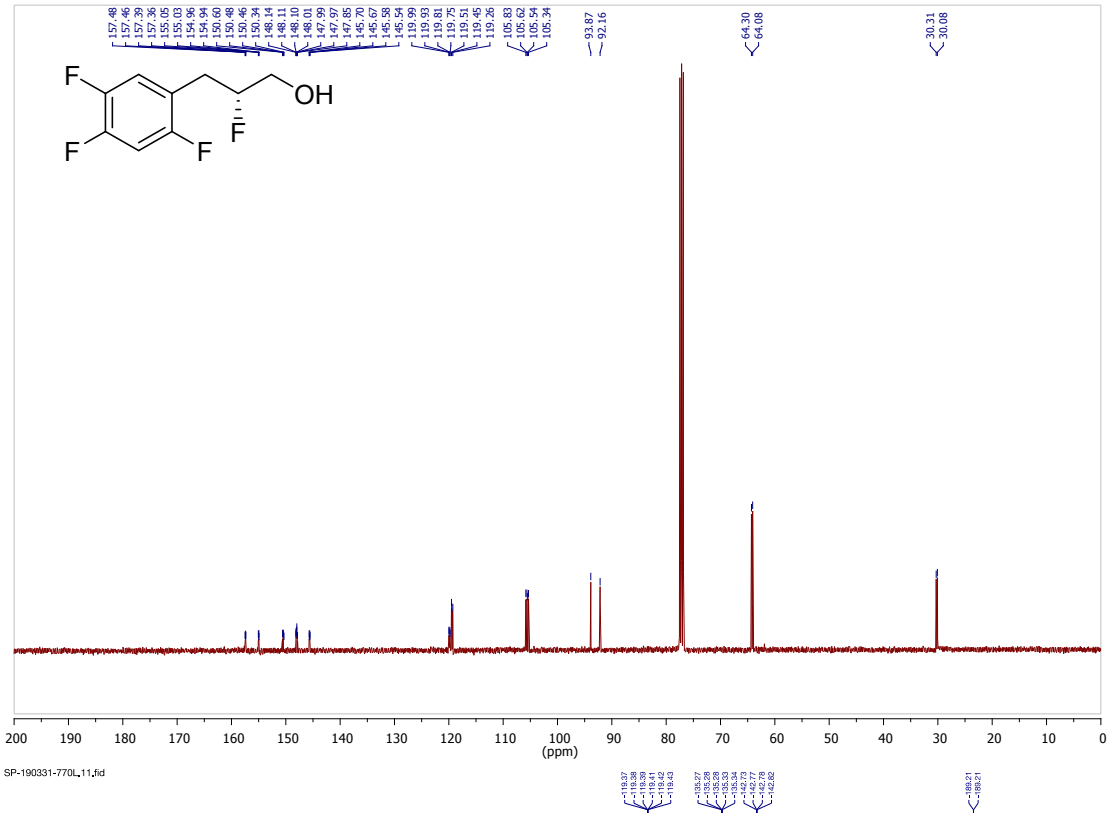

-137.79
-137.85
-140.75
-140.81
-186.58
OH
F
F
F
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
(ppm)


OH
F
F
F
7.26
7.24
7.22
7.21
7.20
6.86
6.85
6.84
6.83
6.81
6.80
6.79
6.78
4.84
4.83
4.82
4.82
4.81
4.72
4.71
4.71
4.71
4.70
4.69
4.69
3.74
3.74
3.73
3.71
3.68
3.67
3.65
3.02
3.00
2.98
2.96
2.94
2.92
2.91
1.96
1.94
1.93
0.96
1.96
1.00
2.08
2.01
1.01
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
(ppm)


OH
F
F
F
163.49
163.37
162.53
162.41
161.03
160.91
160.06
159.95
132.56
132.50
132.47
132.41
119.44
119.40
119.39
119.28
119.25
111.60
111.39
111.35
104.21
103.95
103.69
94.23
92.52
64.36
64.15
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
(ppm)


OH
F
F
F
-111.89
-111.91
-113.64
-113.65
-113.66
-113.67
-188.74
-188.75
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
(ppm)


OH
F
F
F
7.14 7.12 7.12 7.11 7.10 7.10 7.09 7.07 6.96 6.94 6.93 6.91 6.91 6.89
4.84 4.83 4.82 4.81 4.81 4.80 4.72 4.72 4.71 4.70 4.70 4.69 4.68 4.68 4.67
3.82 3.76 3.74 3.72 3.69 3.68 3.66 3.66 3.00 2.99 2.99 2.98 2.95 2.94 2.93 2.92
1.92 1.91 1.89
0.99 0.97 1.00 2.07 2.01 0.99
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
(ppm)


F
F
F
OH
F
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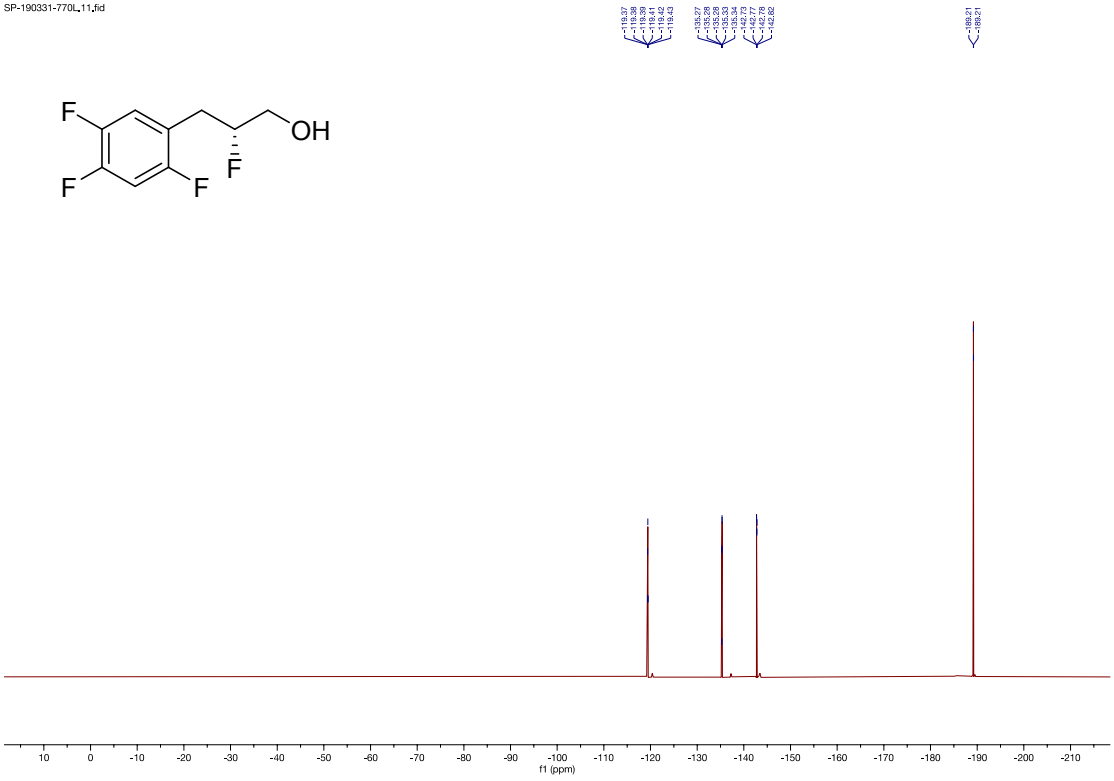
157.46
157.39
157.36
155.05
155.03
154.96
154.94
150.60
150.48
150.46
150.34
148.14
148.11
148.10
148.01
147.99
147.97
147.85
145.70
145.67
145.58
145.54
119.99
119.93
119.81
119.75
119.51
119.45
119.26
105.83
105.62
105.54
105.34
93.87
92.16
64.30
64.08
30.31
30.08
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
(ppm)
SP-190331-770L_11.fid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-118.38
-118.39
-118.41
-118.42
-118.43
-135.27
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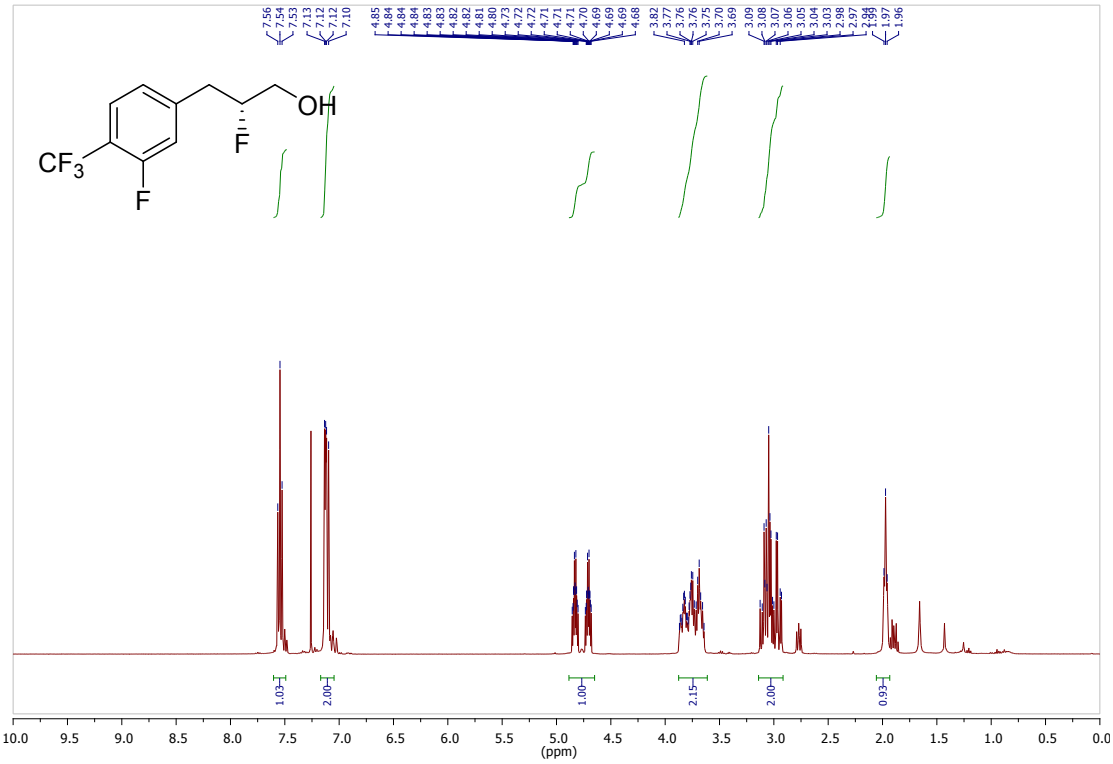
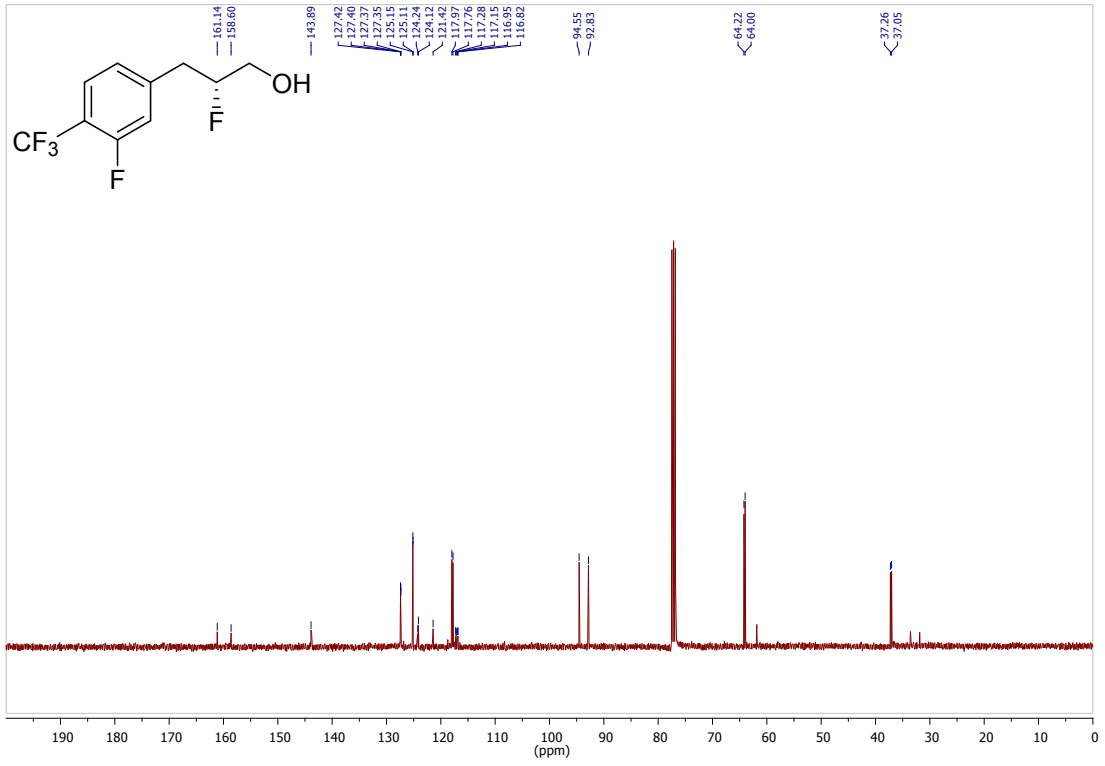
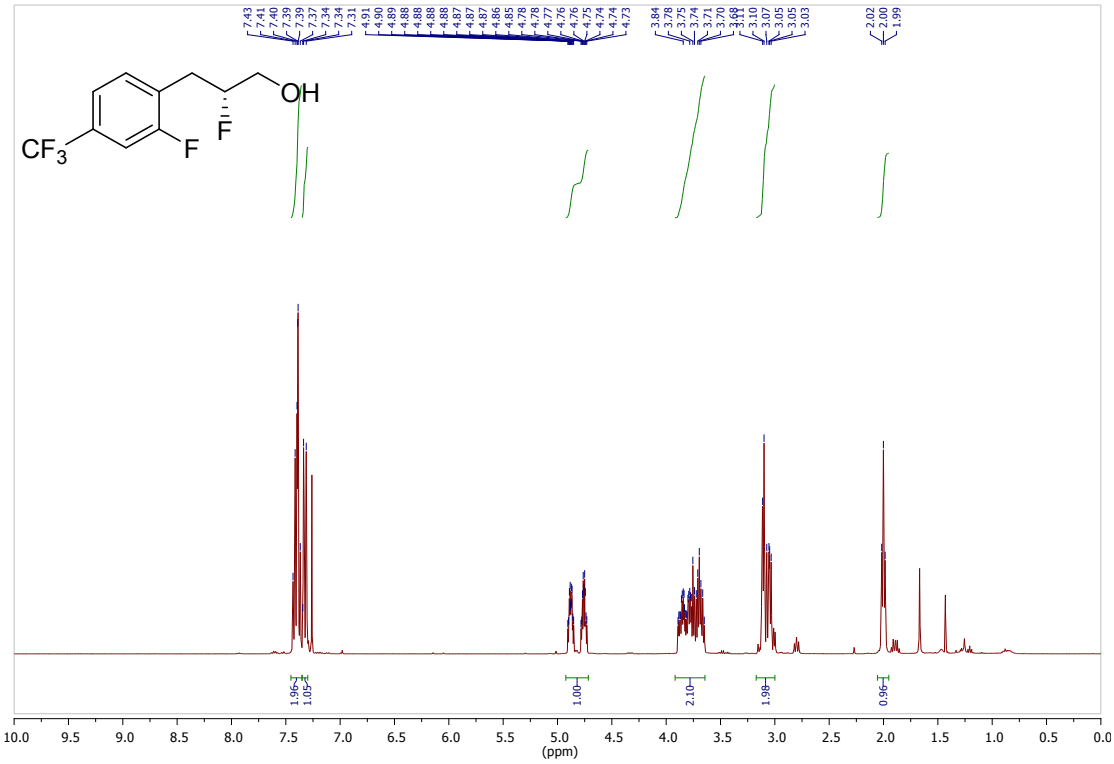
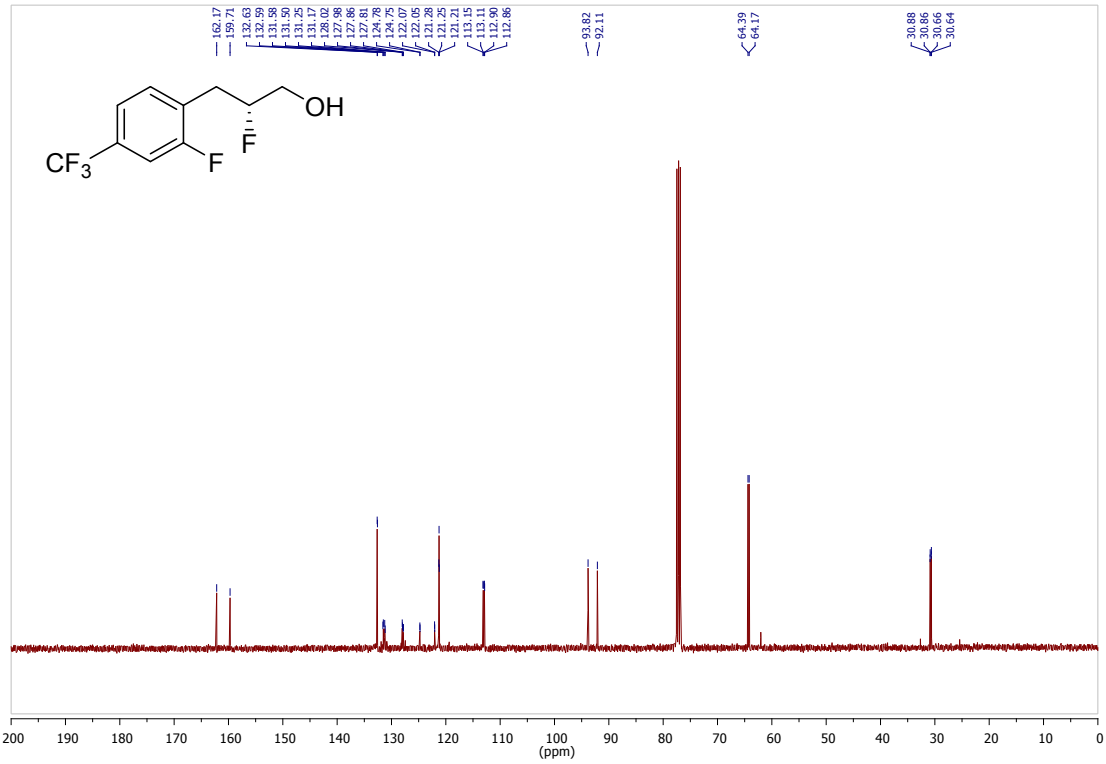
-135.29
-135.33
-135.34
-142.73
-142.77
-142.78
-142.82
-189.21
-189.21
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)


OH
F
CF3
F
(ppm)


OH
F
CF3
F
(ppm)


SP-190331-942L.11.fid
OH
F
CF3
F
f1 (ppm)


OH
F
CF3
F
(ppm)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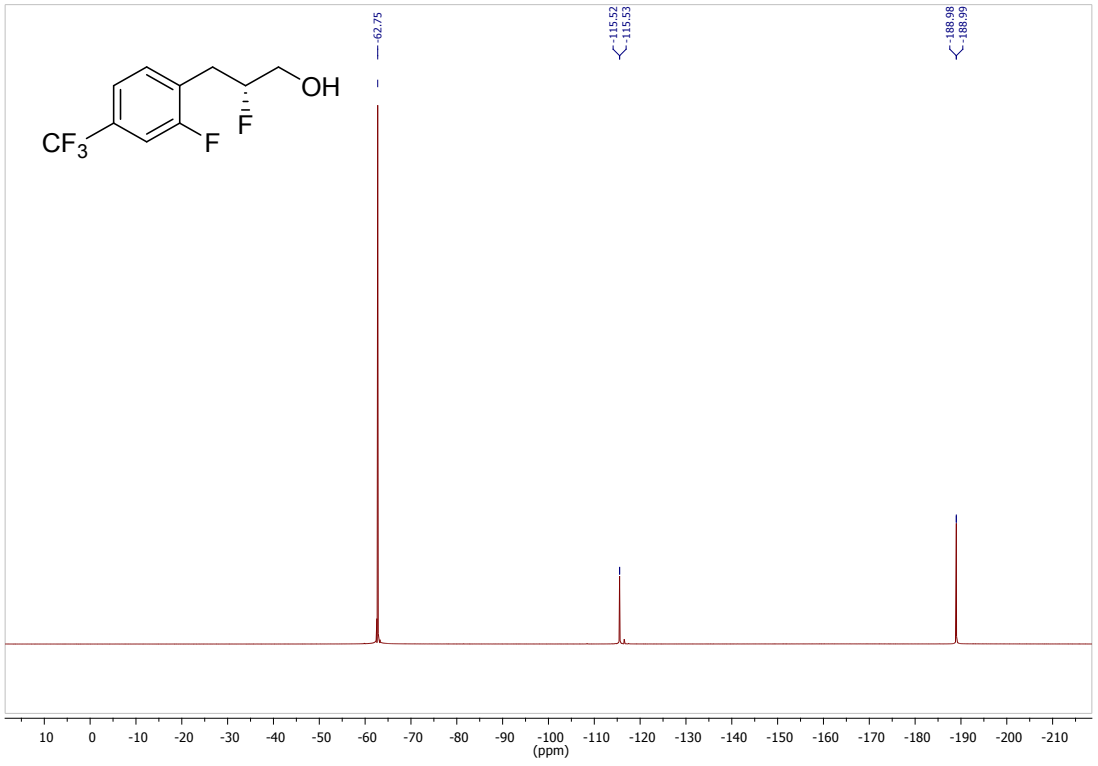
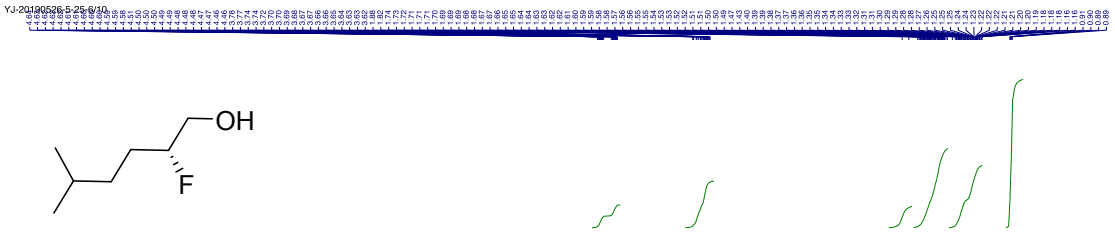
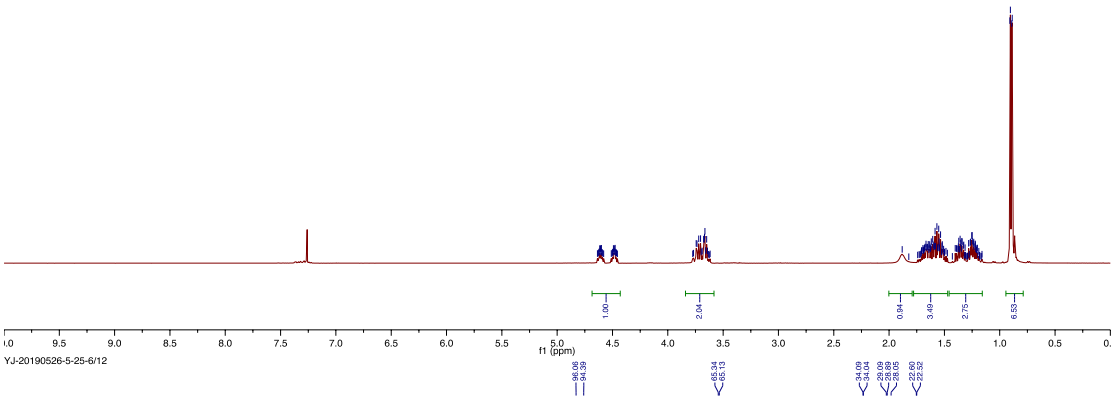
132.63
132.59
131.58
131.50
131.25
131.17
128.02
127.98
127.86
127.81
124.78
124.75
122.07
122.05
121.28
121.25
121.21
113.15
113.11
112.90
112.86
93.82
92.11
64.39
64.17
30.88
30.86
30.66
30.64
OH
F
CF3
F
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
(ppm)

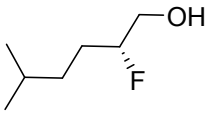

-62.75
-115.52
-115.53
-188.98
-188.99
OH
F
CF3
F
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
(ppm)

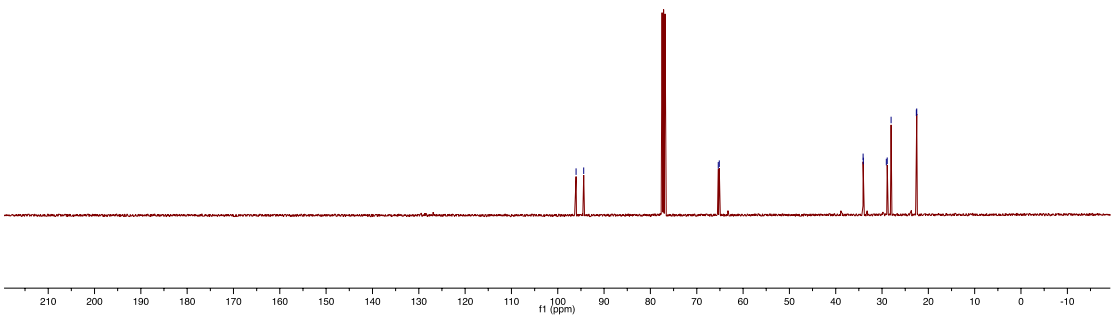




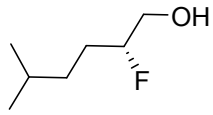
YJ-20190526-5-25-6/12

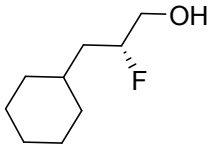
96.06
94.39
65.34
65.13
34.09
34.04
29.09
28.88
28.65
22.60
22.52

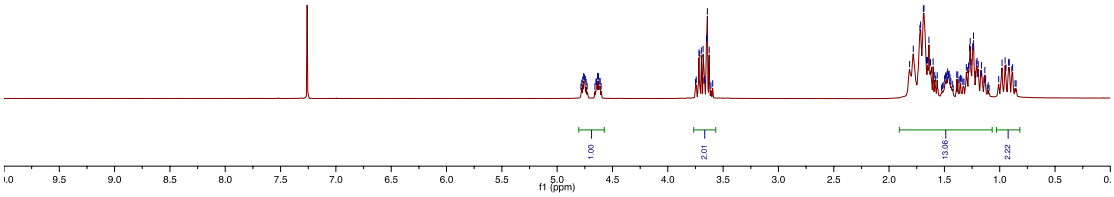


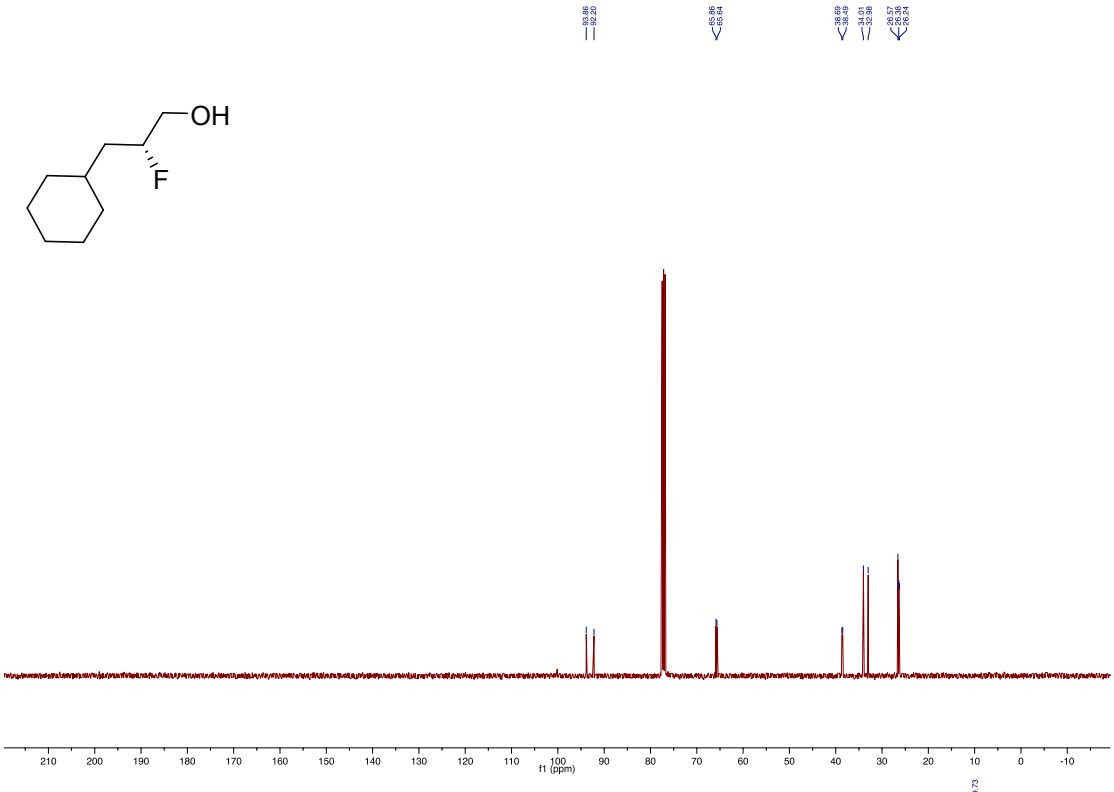


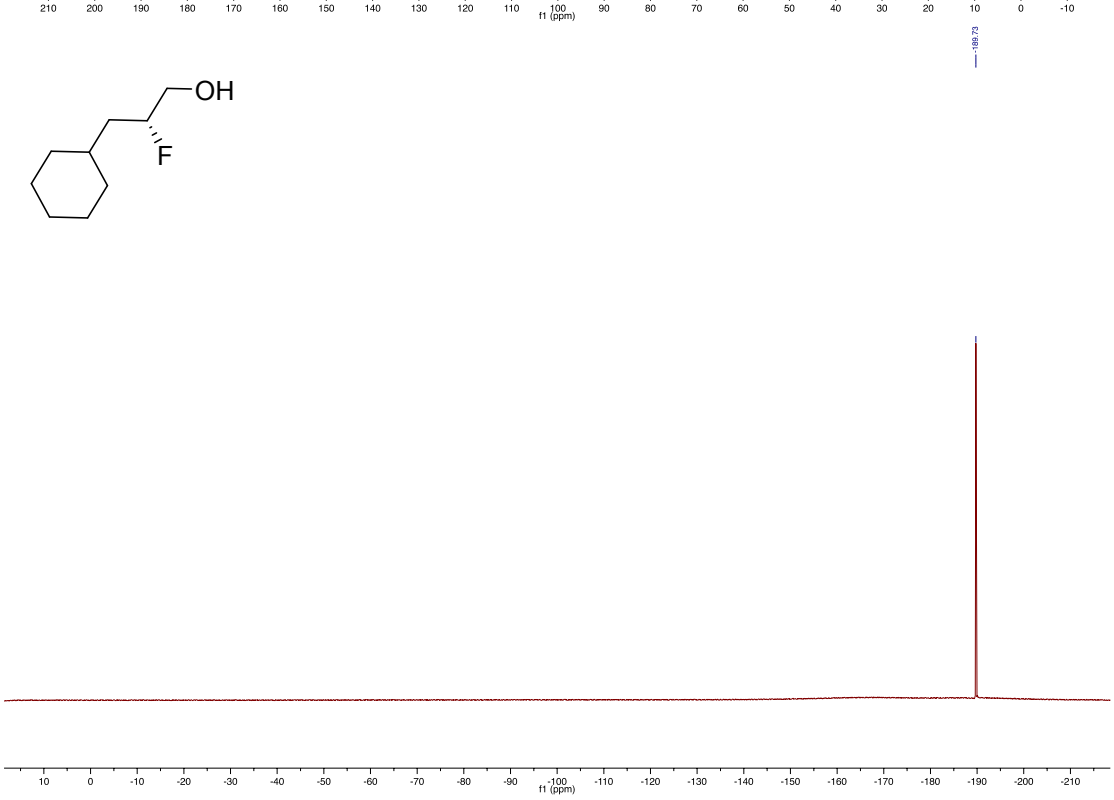
YJ-20190526-5-25-6/11

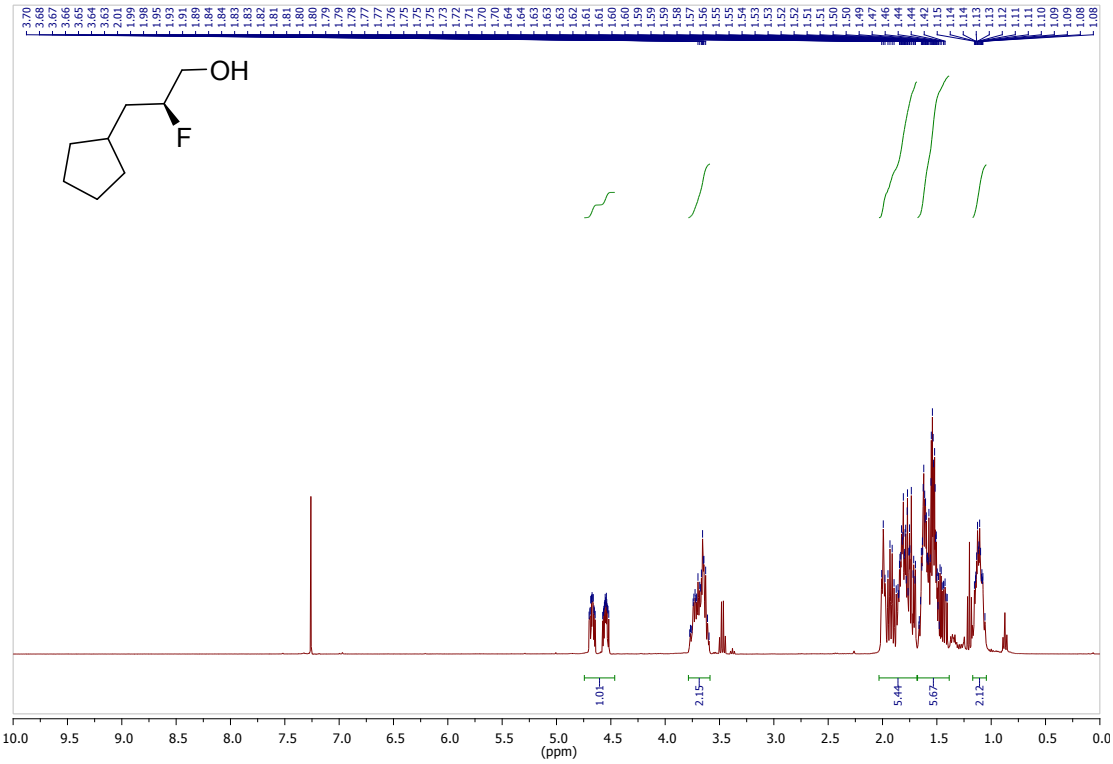


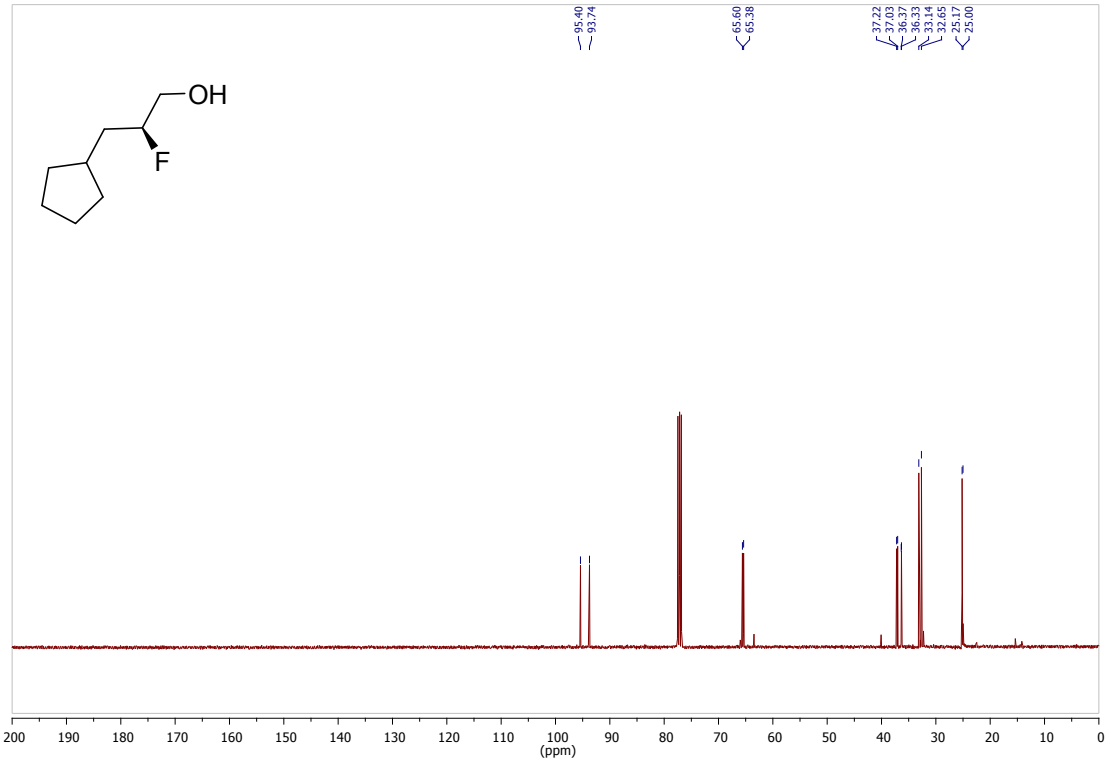


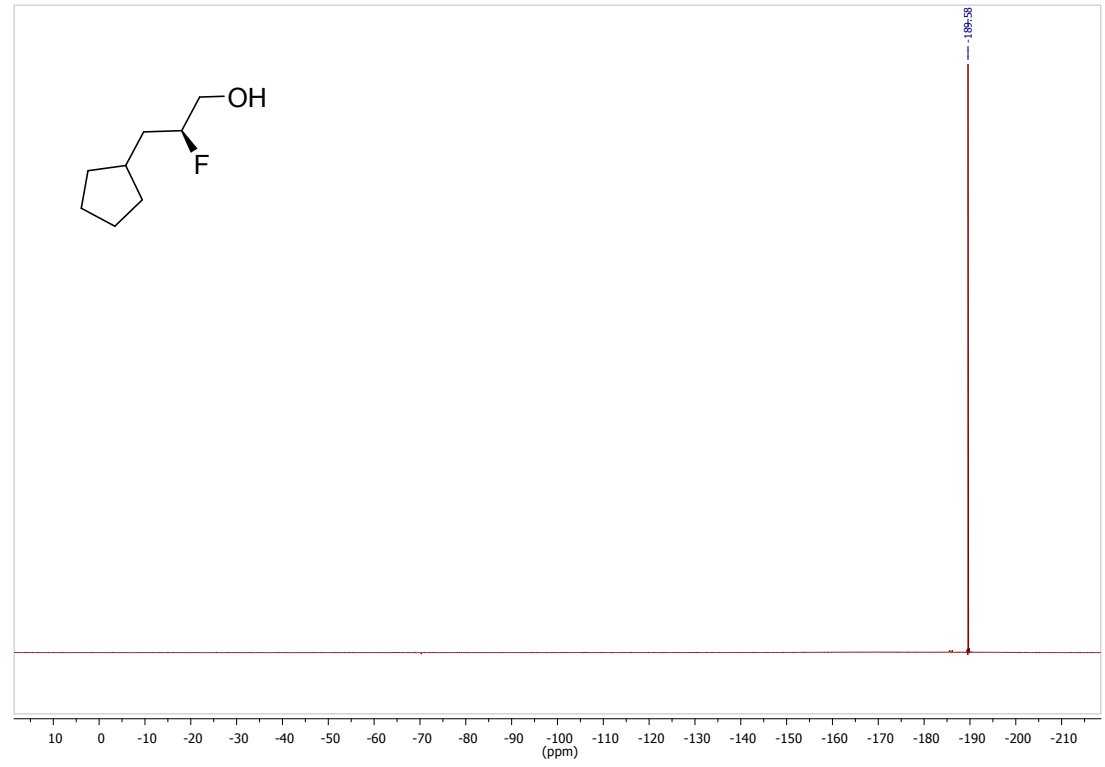



93.86
92.20
65.86
65.64
38.69
38.49
34.01
32.98
26.57
26.38
26.24
OH
F
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


-189.73
OH
F
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)


OH
F
1.01
2.15
5.44
5.67
2.12
(ppm)


OH
F
95.40
93.74
65.60
65.38
37.22
37.03
36.37
36.33
33.14
32.65
25.17
25.00
(ppm)



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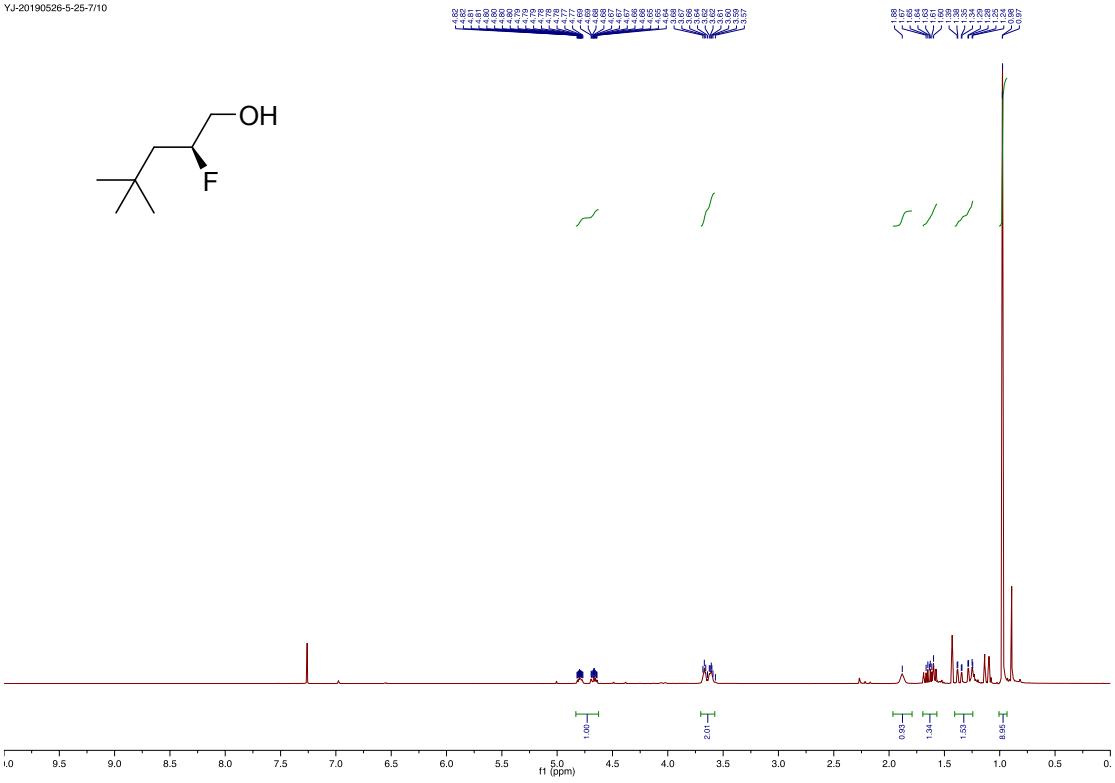
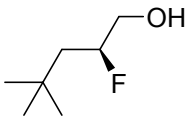
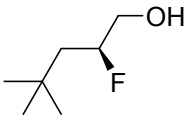


YJ-20190526-5-25-7/12



YJ-20190526-5-25-7/11



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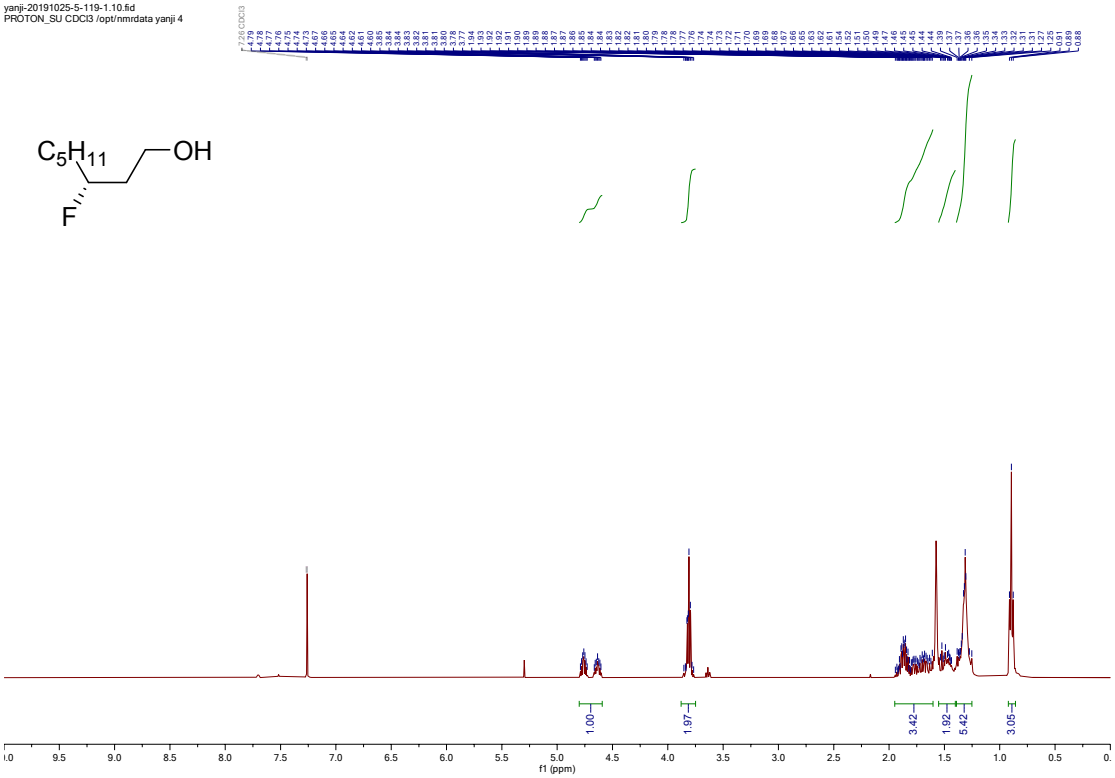

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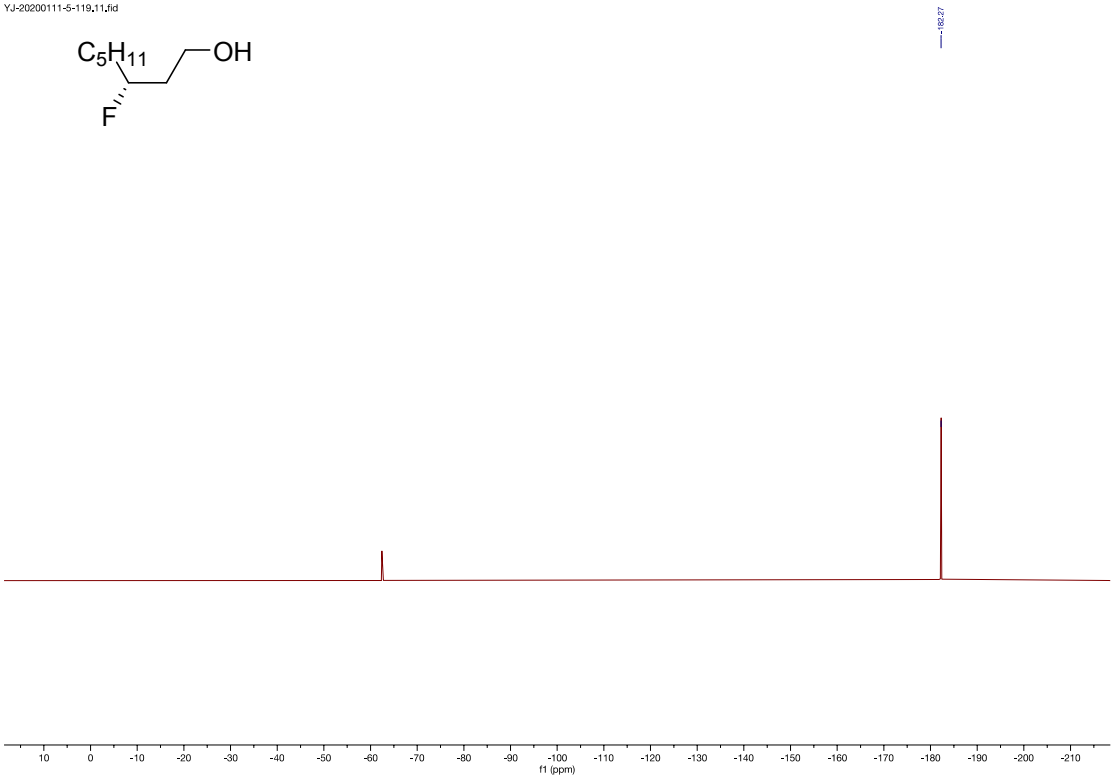

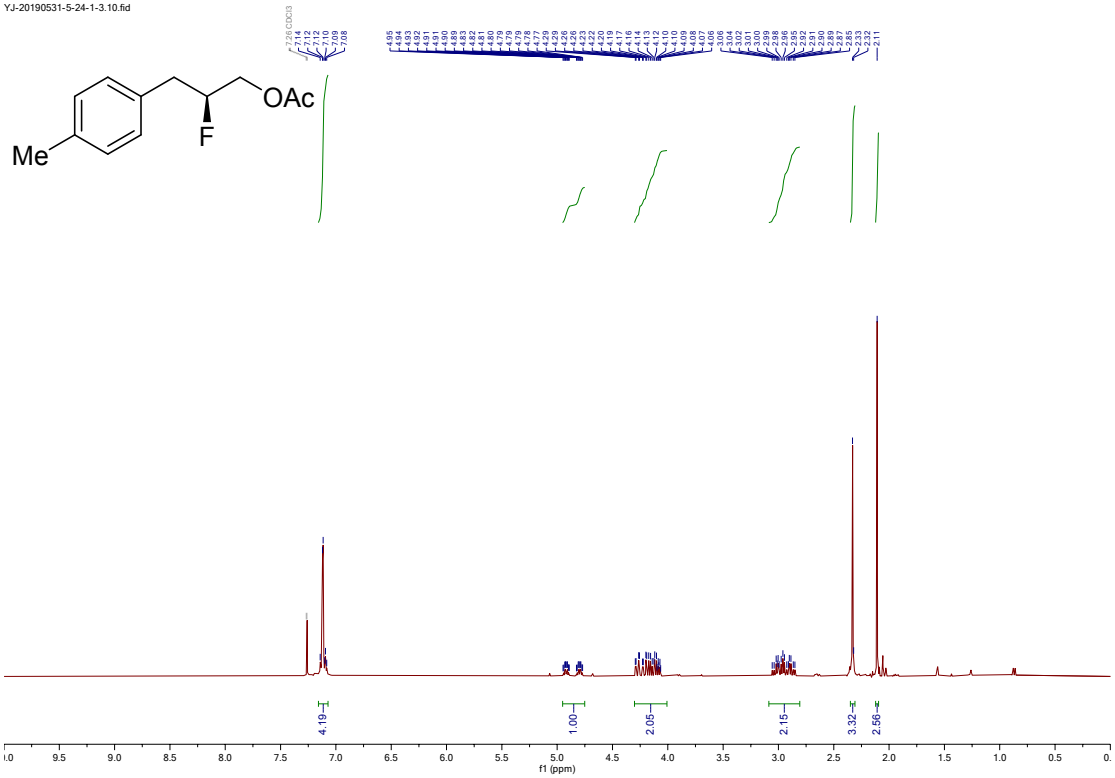
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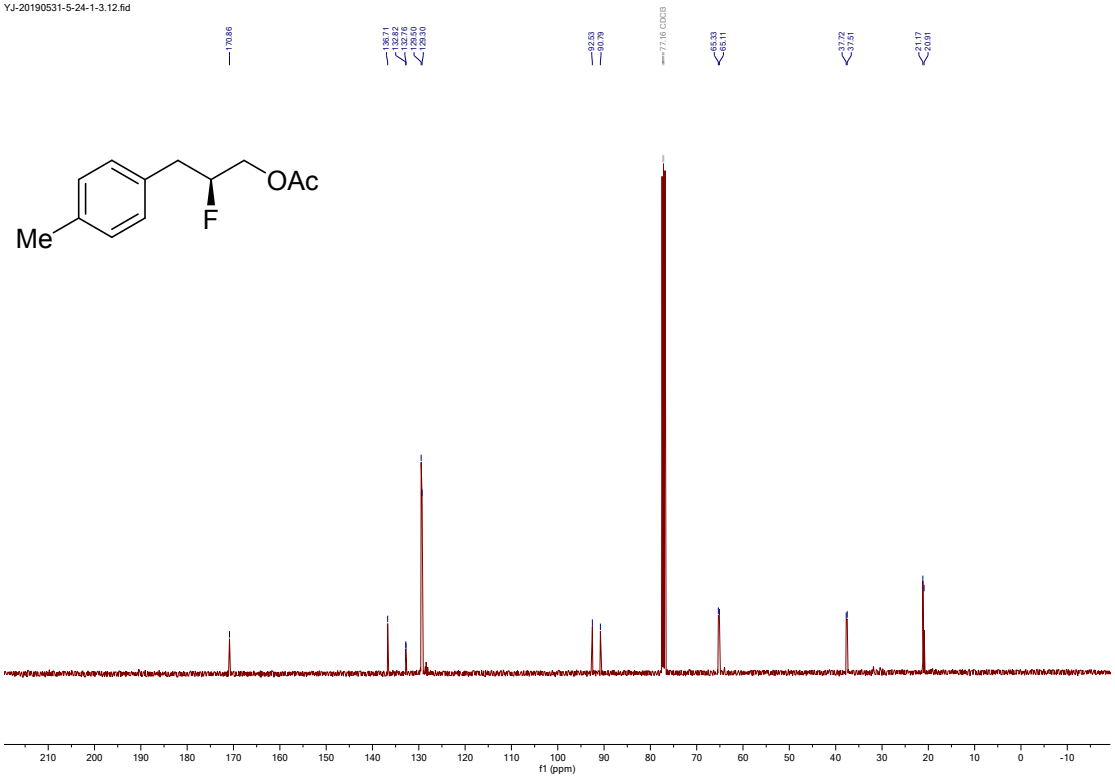
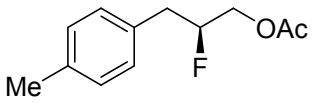
OAc
F
Me
4.19
1.00
2.05
2.15
3.32
2.56
f1 (ppm)


YJ-20190531-5-24-1-3.12.fid
OAc
F
Me
f1 (ppm)

YJ-20190531-5-24-1-3.11.fid



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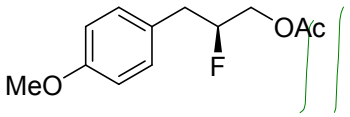

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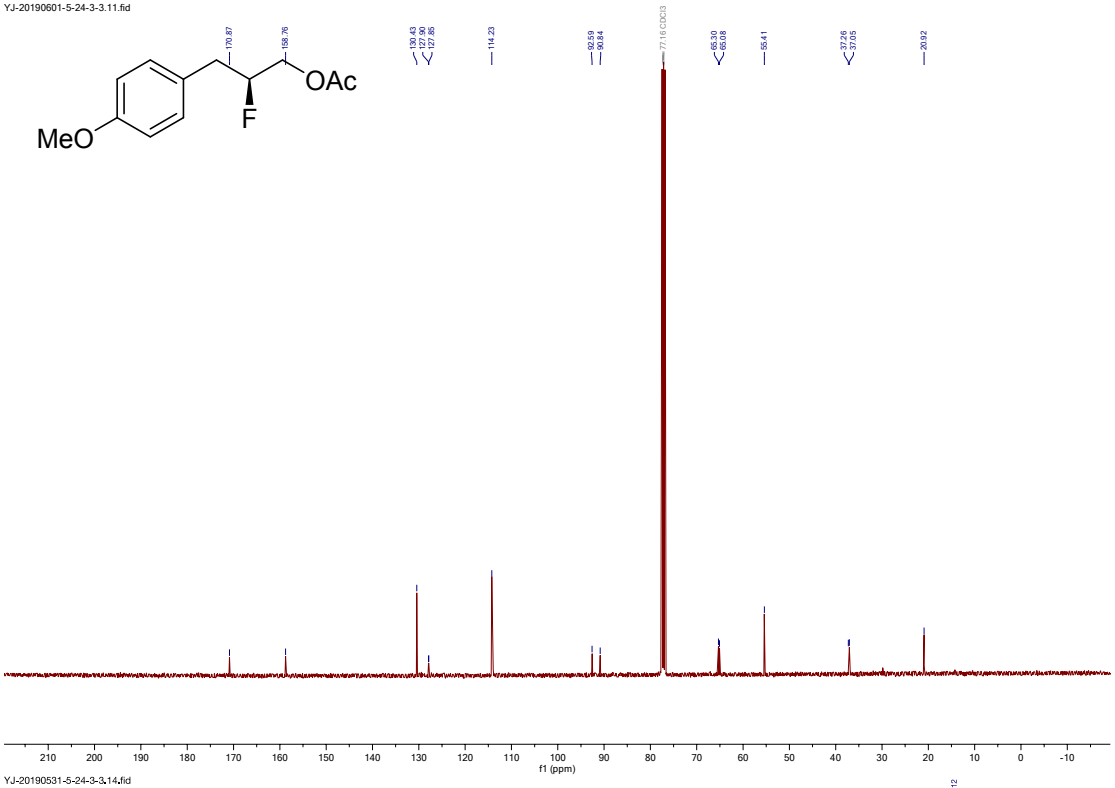

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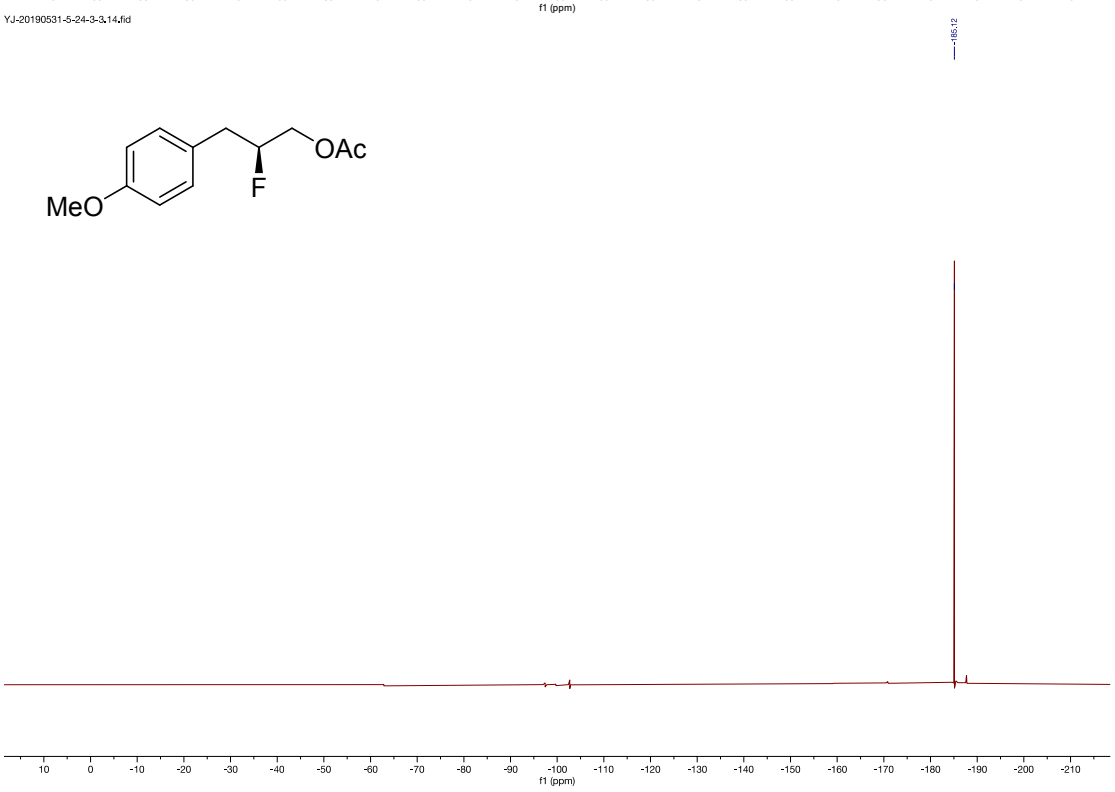

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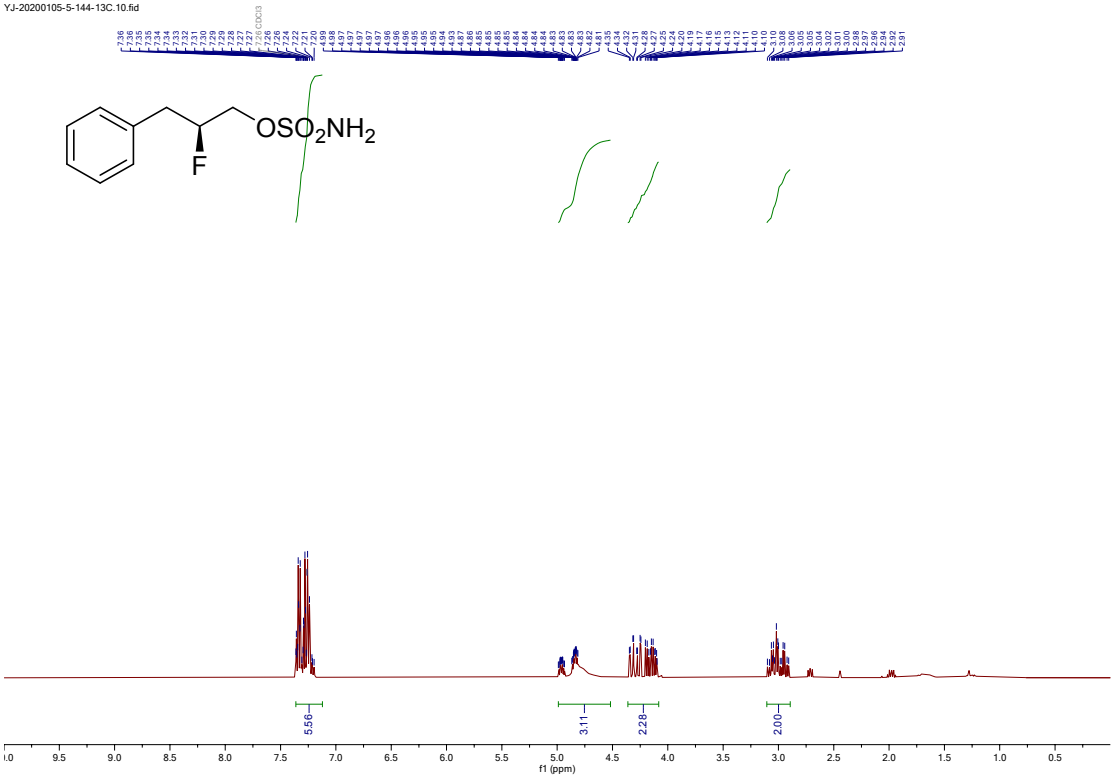
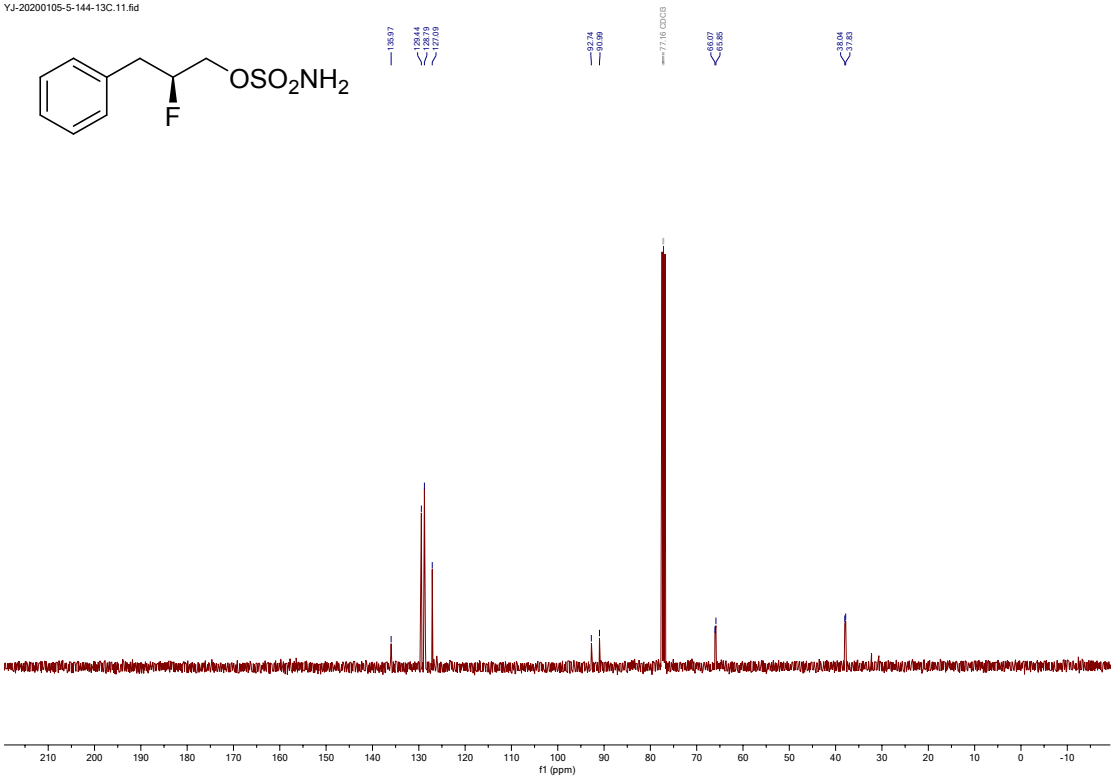


YJ-20200105-5-144-13C.11.fid



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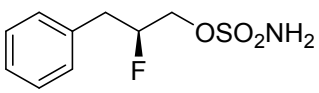
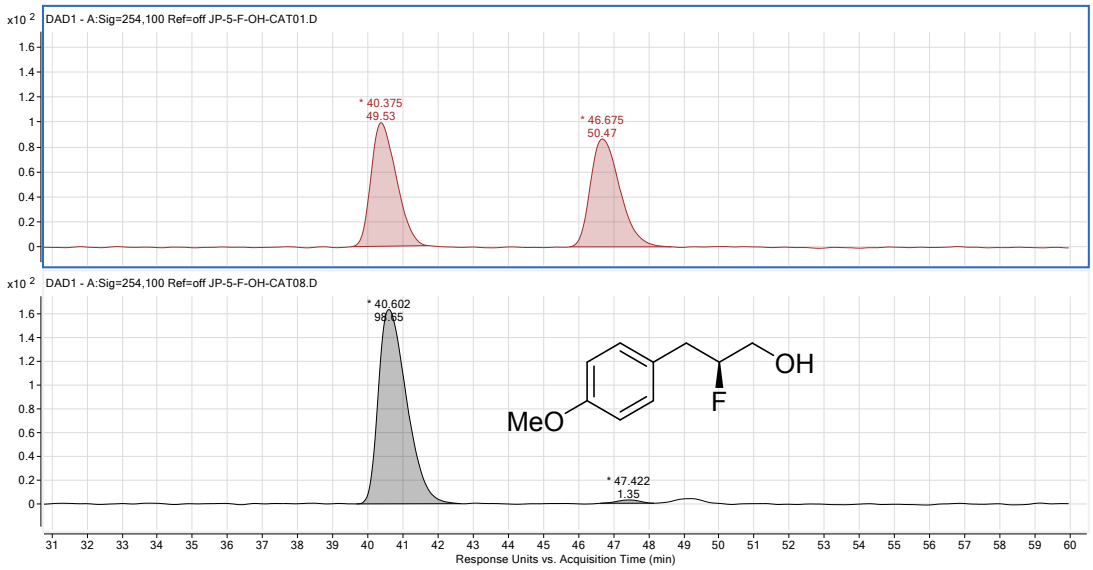
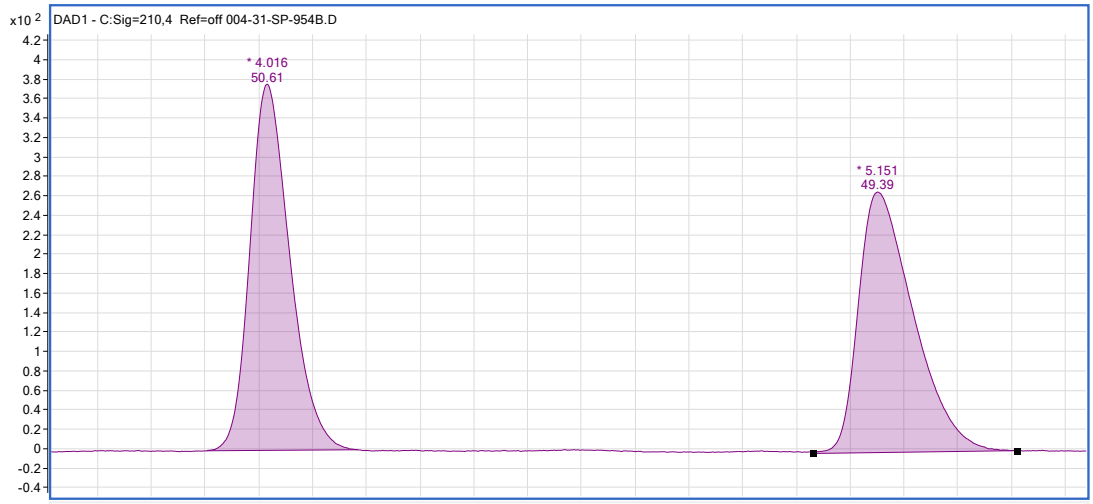
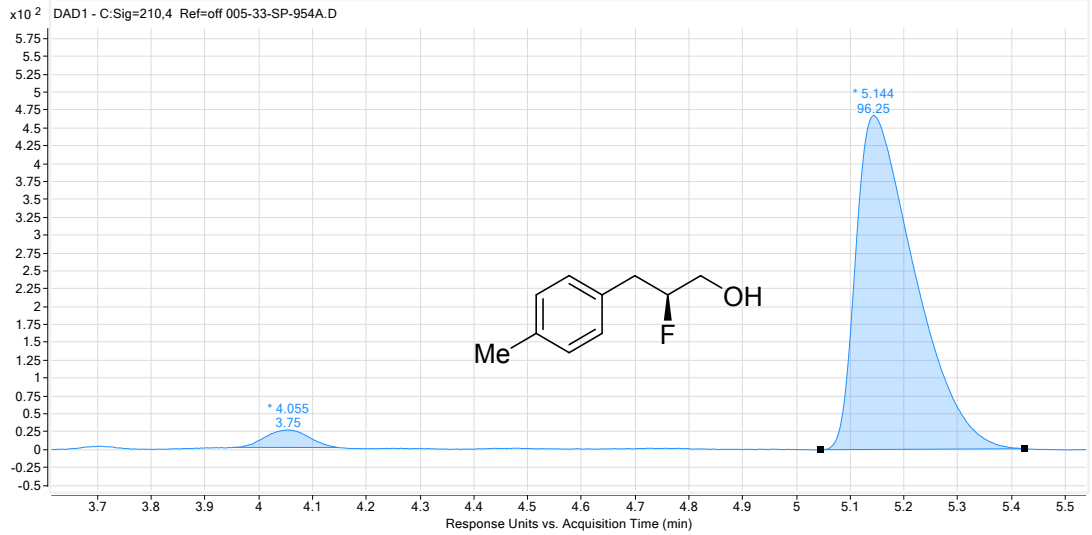
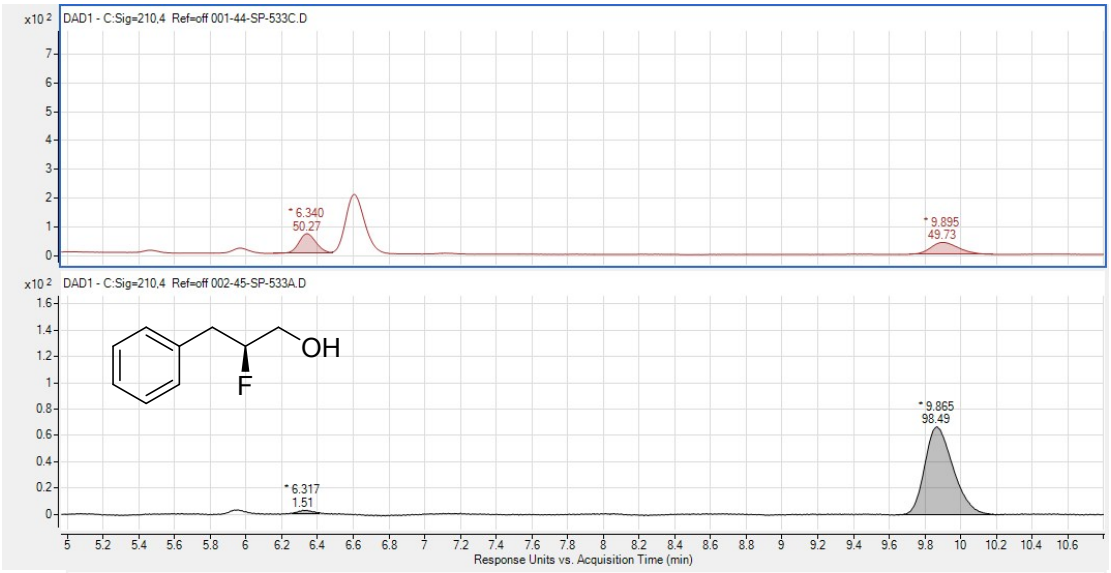


9. Chromatography

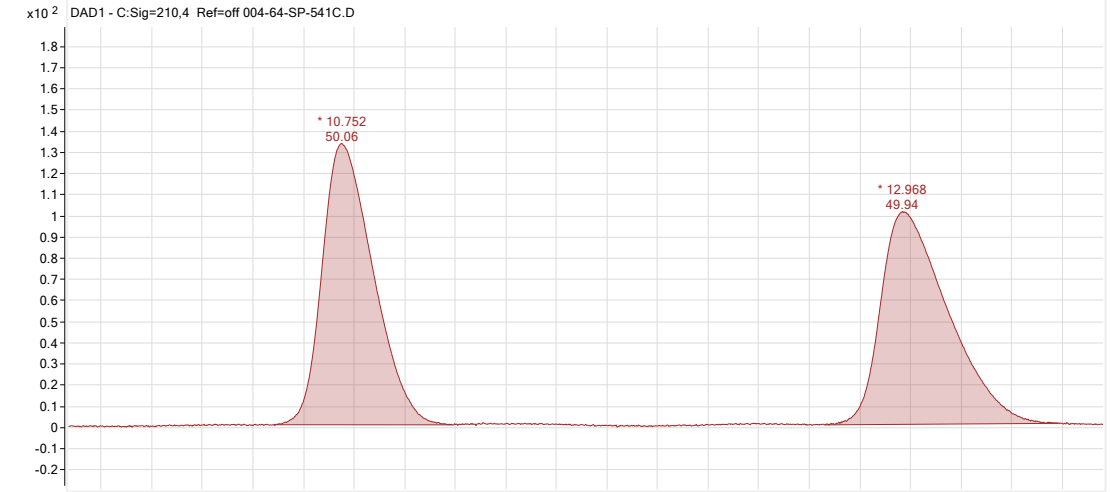


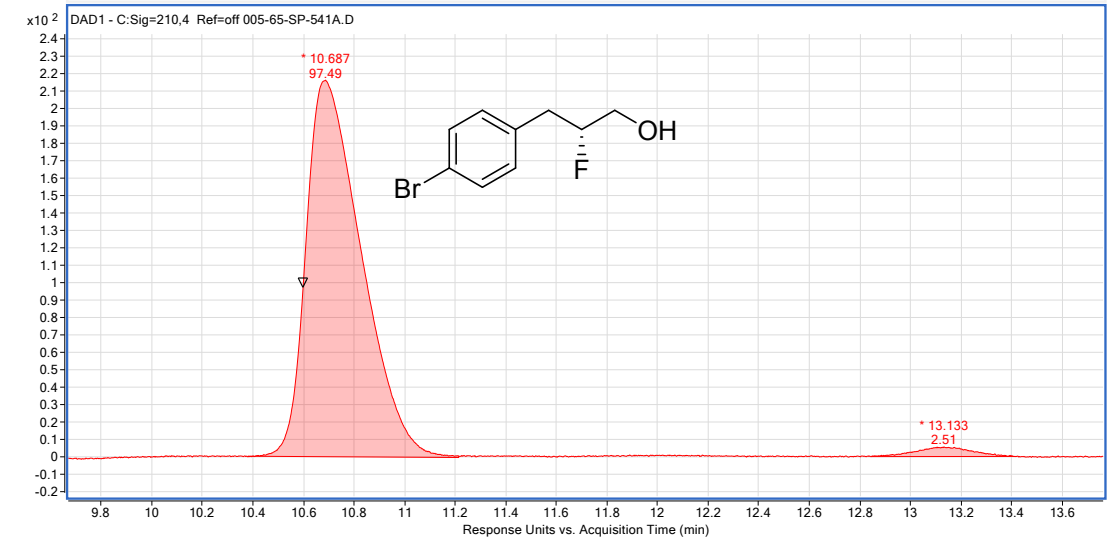


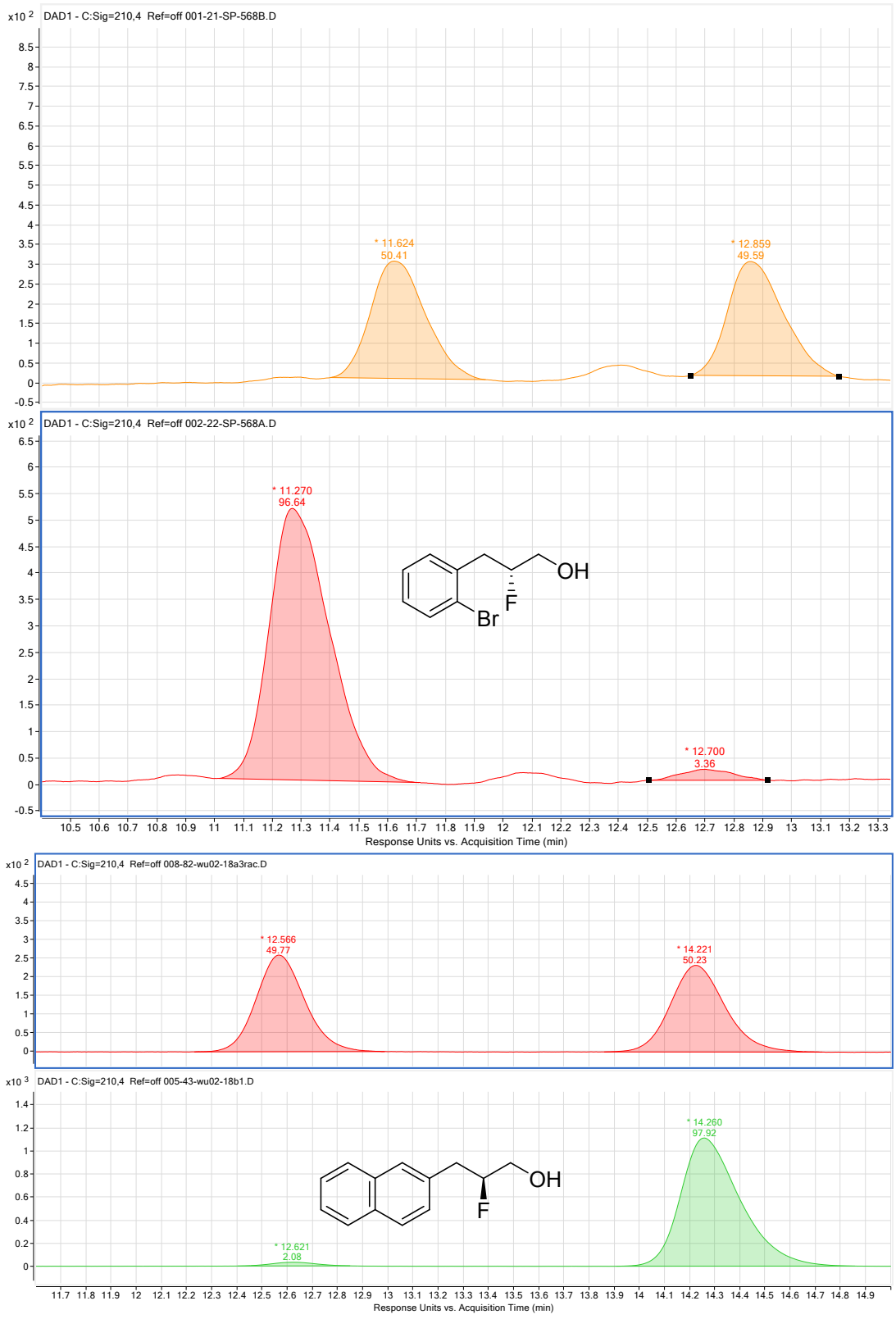


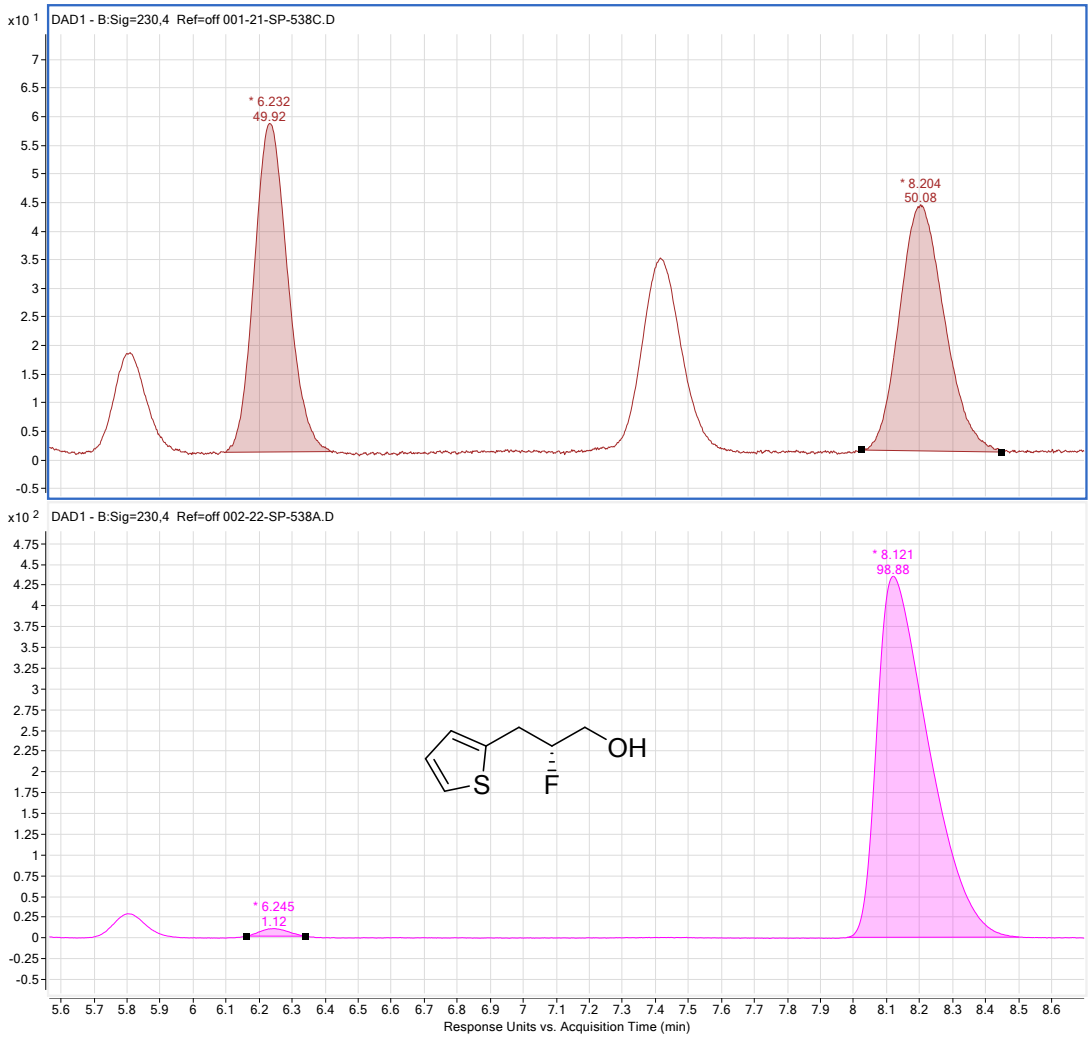

x10 2
DAD1 - C:Sig=210,4 Ref=off 001-44-SP-533C.D
* 6.340
50.27
* 9.895
49.73

x10 2
DAD1 - C:Sig=210,4 Ref=off 002-45-SP-533A.D
OH
F
* 9.865
98.49
* 6.317
1.51
Response Units vs. Acquisition Time (min)

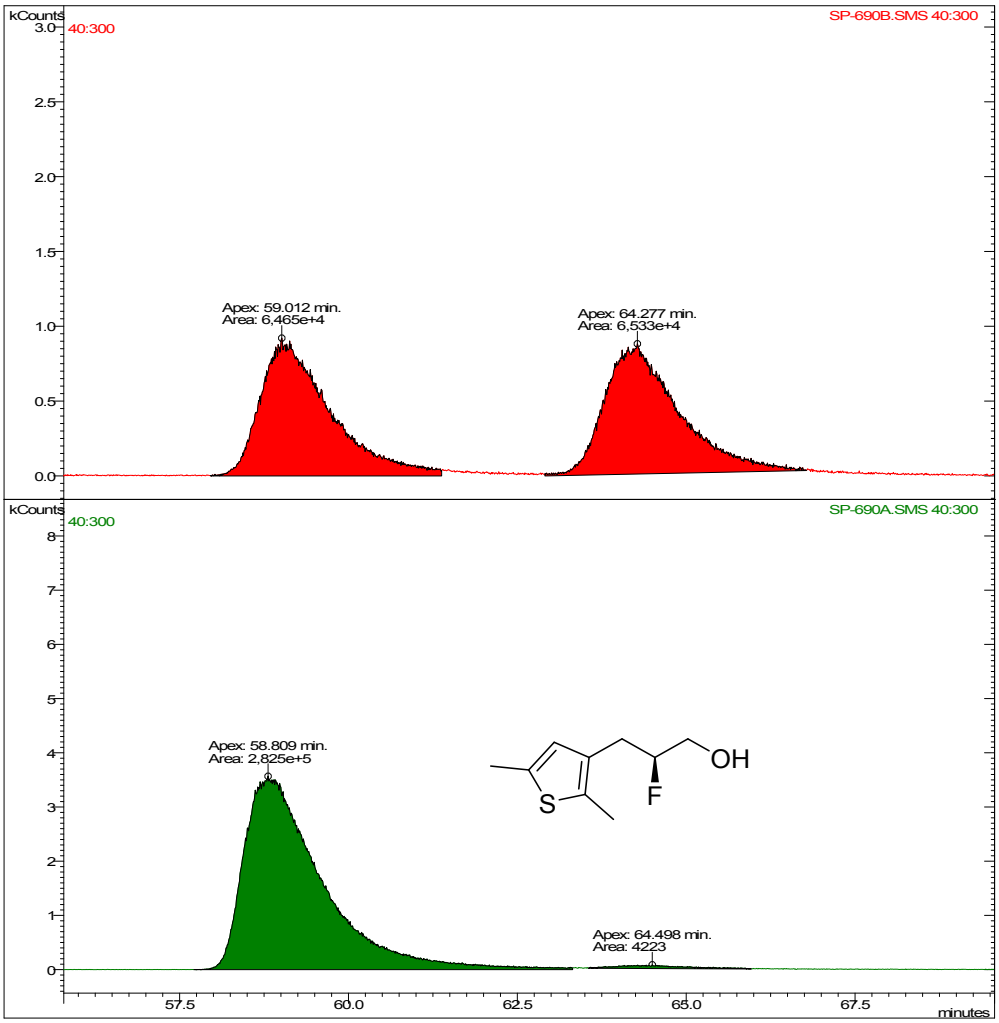

x10 2
DAD1 - C:Sig=210,4 Ref=off 004-64-SP-541C.D
* 10.752
50.06
* 12.968
49.94

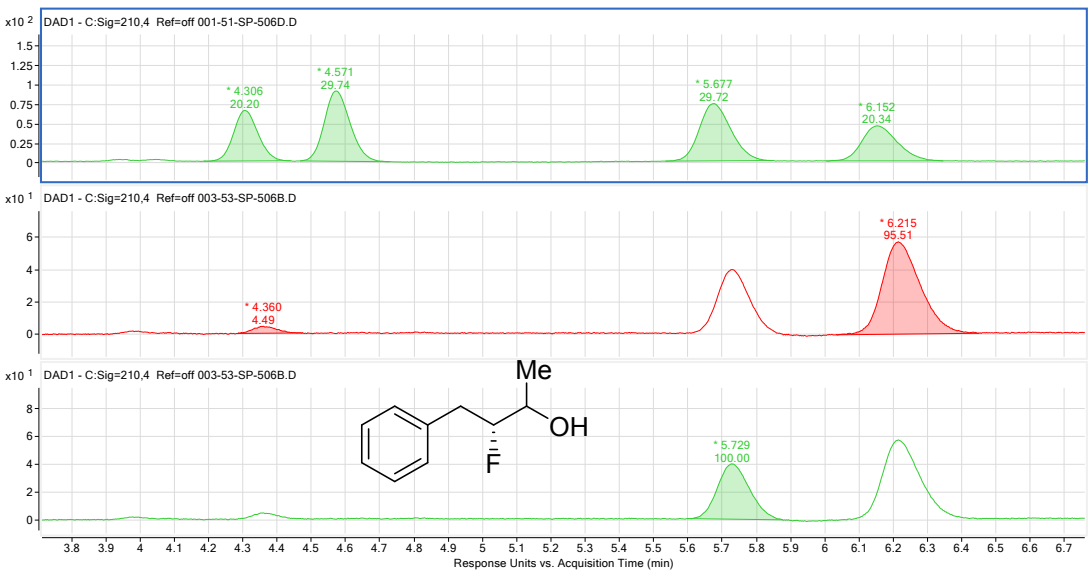

x10 2
DAD1 - C:Sig=210,4 Ref=off 005-65-SP-541A.D
* 10.687
97.49
OH
F
Br
* 13.133
2.51
Response Units vs. Acquisition Time (min)


x10 2
DAD1 - C:Sig=210,4 Ref=off 001-21-SP-568B.D
* 11.624
50.41
* 12.859
49.59
x10 2
DAD1 - C:Sig=210,4 Ref=off 002-22-SP-568A.D
* 11.270
96.64
OH
F
Br
* 12.700
3.36
Response Units vs. Acquisition Time (min)
x10 2
DAD1 - C:Sig=210,4 Ref=off 008-82-wu02-18a3rac.D
* 12.566
49.77
* 14.221
50.23
x10 3
DAD1 - C:Sig=210,4 Ref=off 005-43-wu02-18b1.D
* 14.260
97.92
OH
F
* 12.621
2.08
Response Units vs. Acquisition Time (min)


x10 1
DAD1 - B:Sig=230,4 Ref=off 001-21-SP-538C.D
* 6.232
49.92
* 8.204
50.08
x10 2
DAD1 - B:Sig=230,4 Ref=off 002-22-SP-538A.D
* 8.121
98.88
* 6.245
1.12
OH
S
F
Response Units vs. Acquisition Time (min)

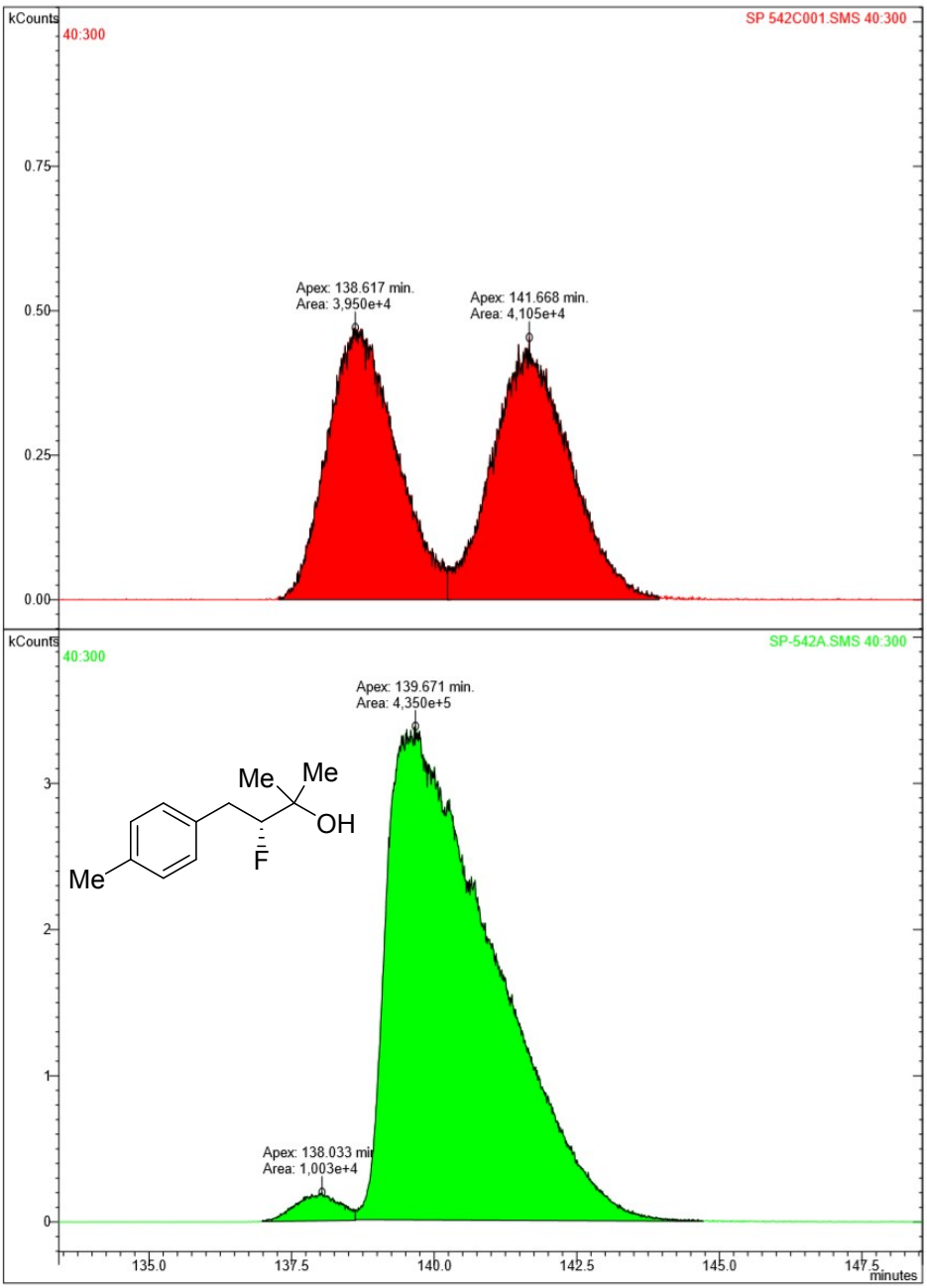
Chromatogram Plots





Print Date: 18 Apr 2019 15:18:24

Chromatogram Plots



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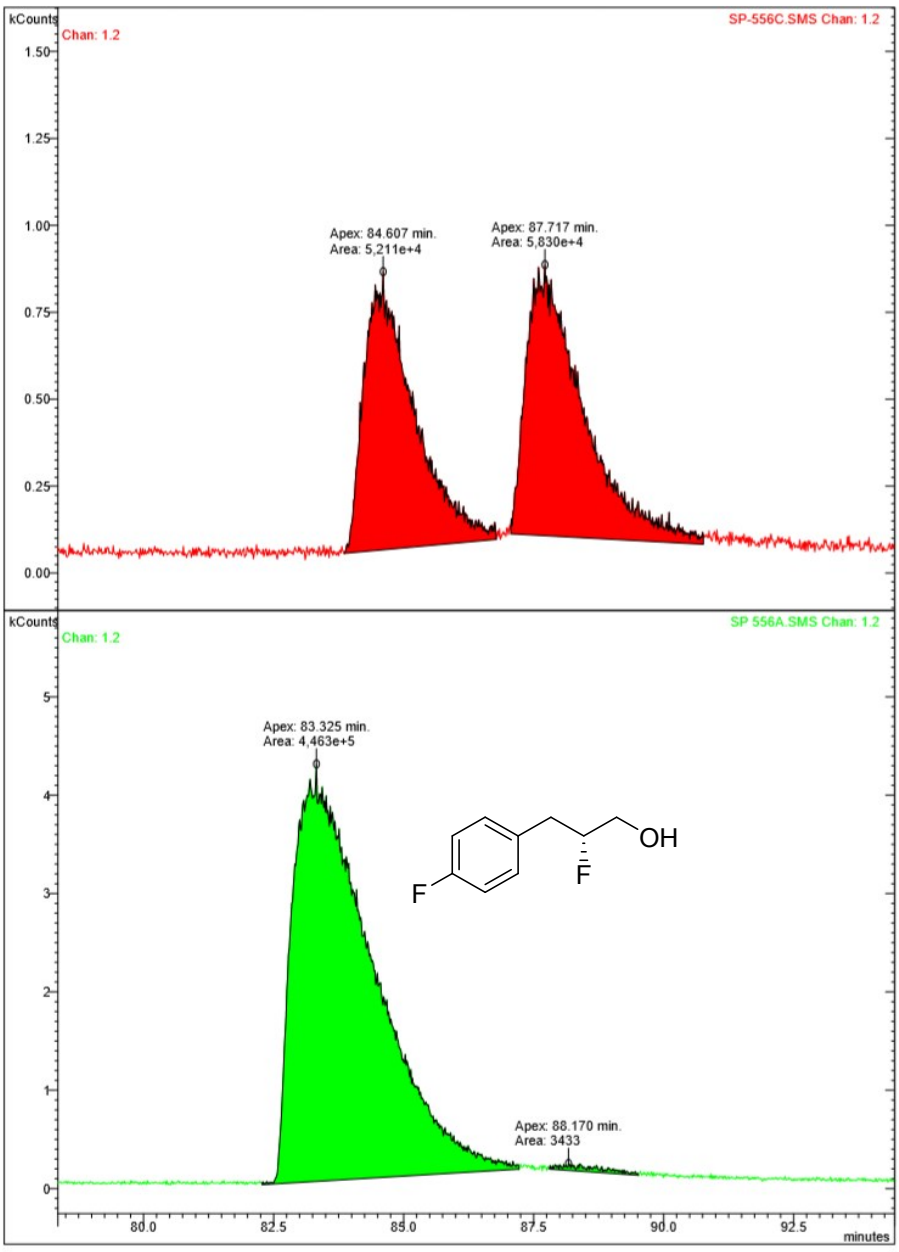
Chromatogram Plots



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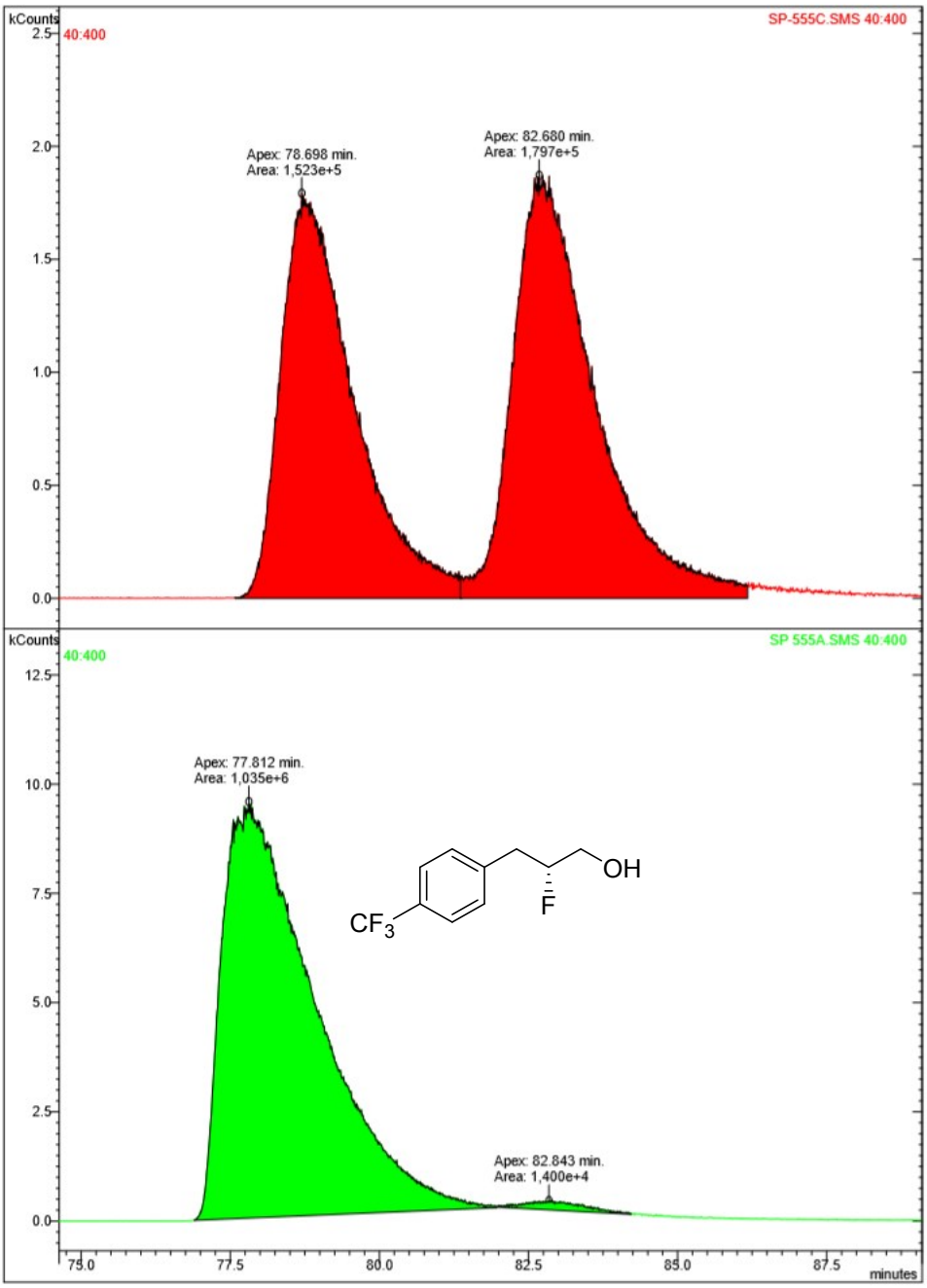
Chromatogram Plots



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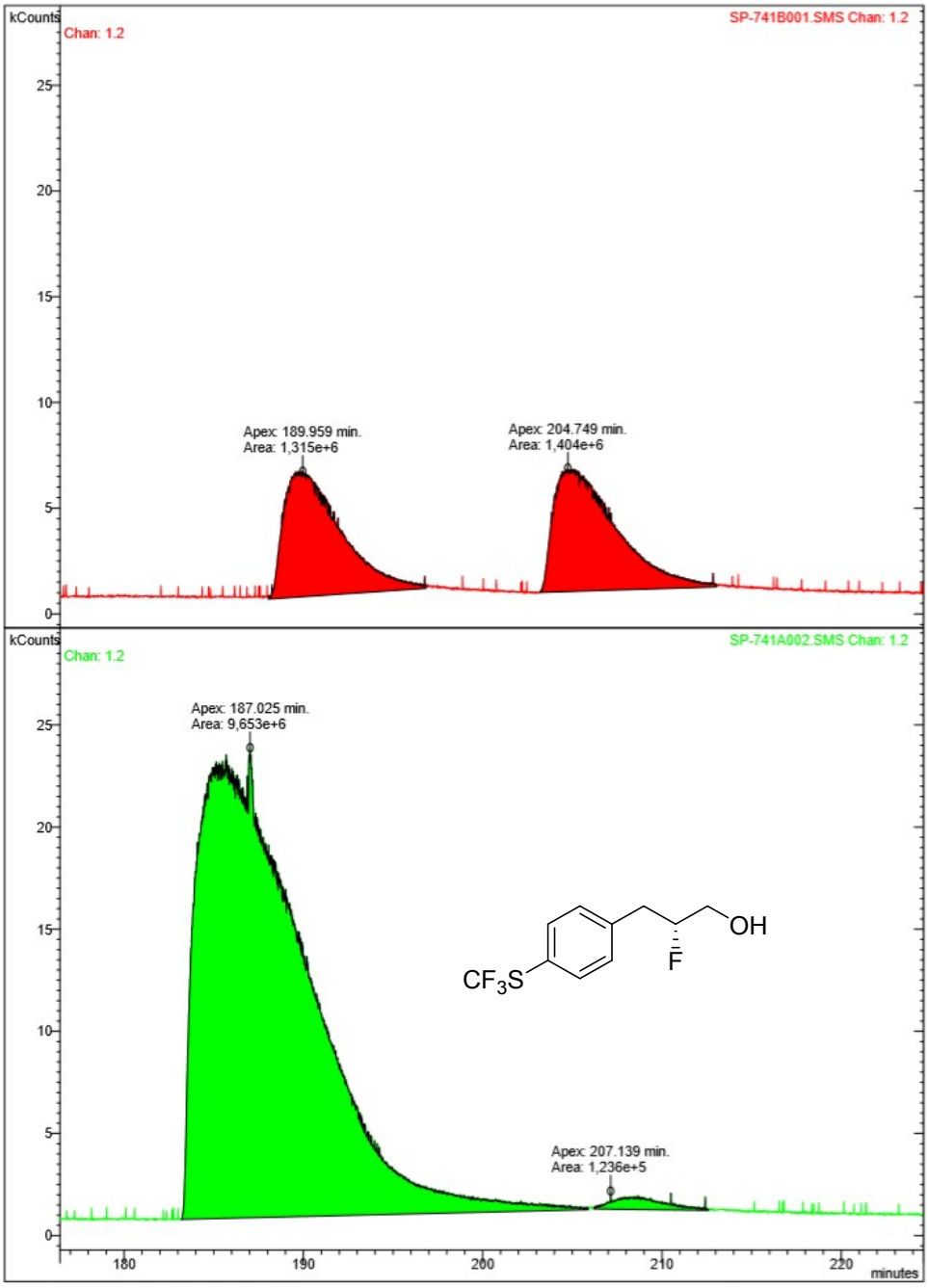
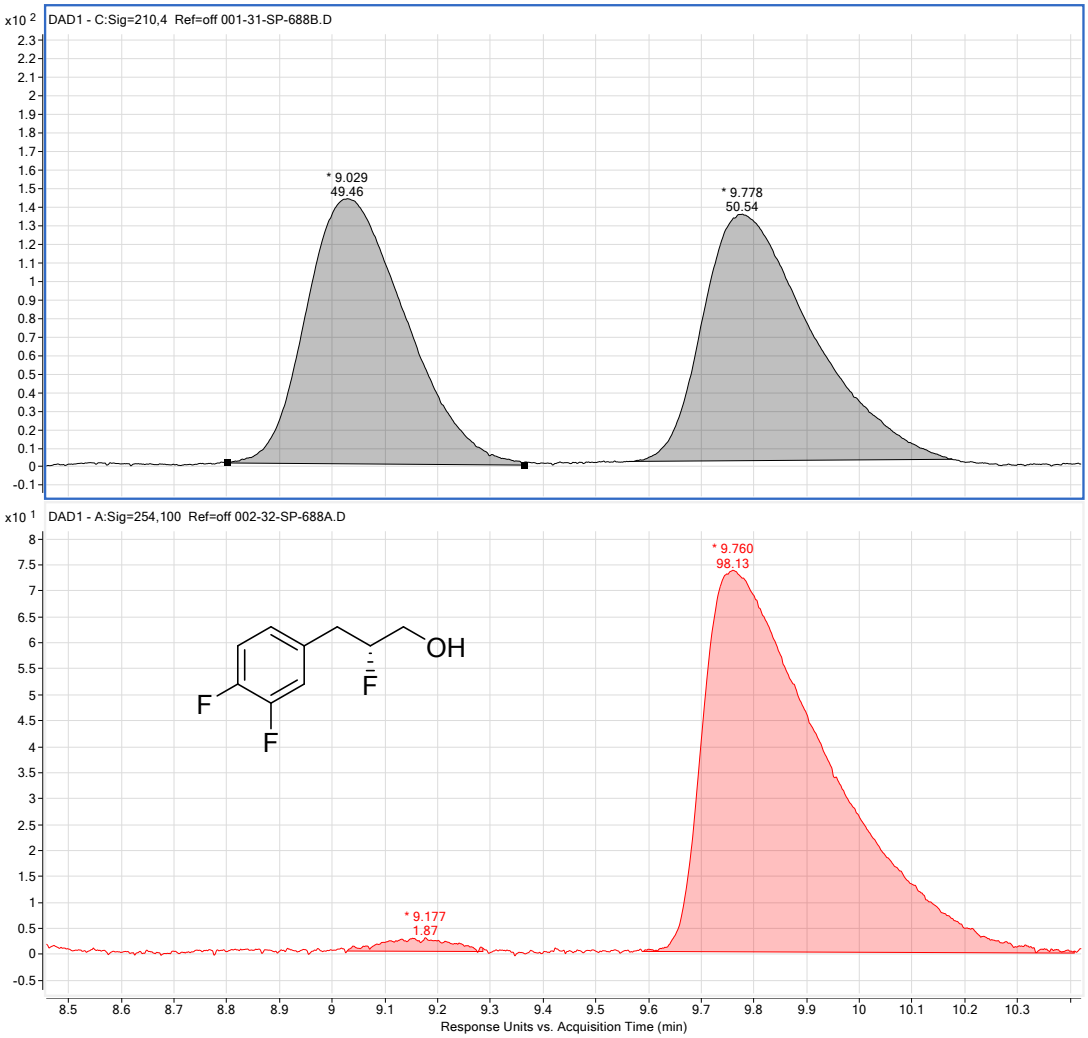
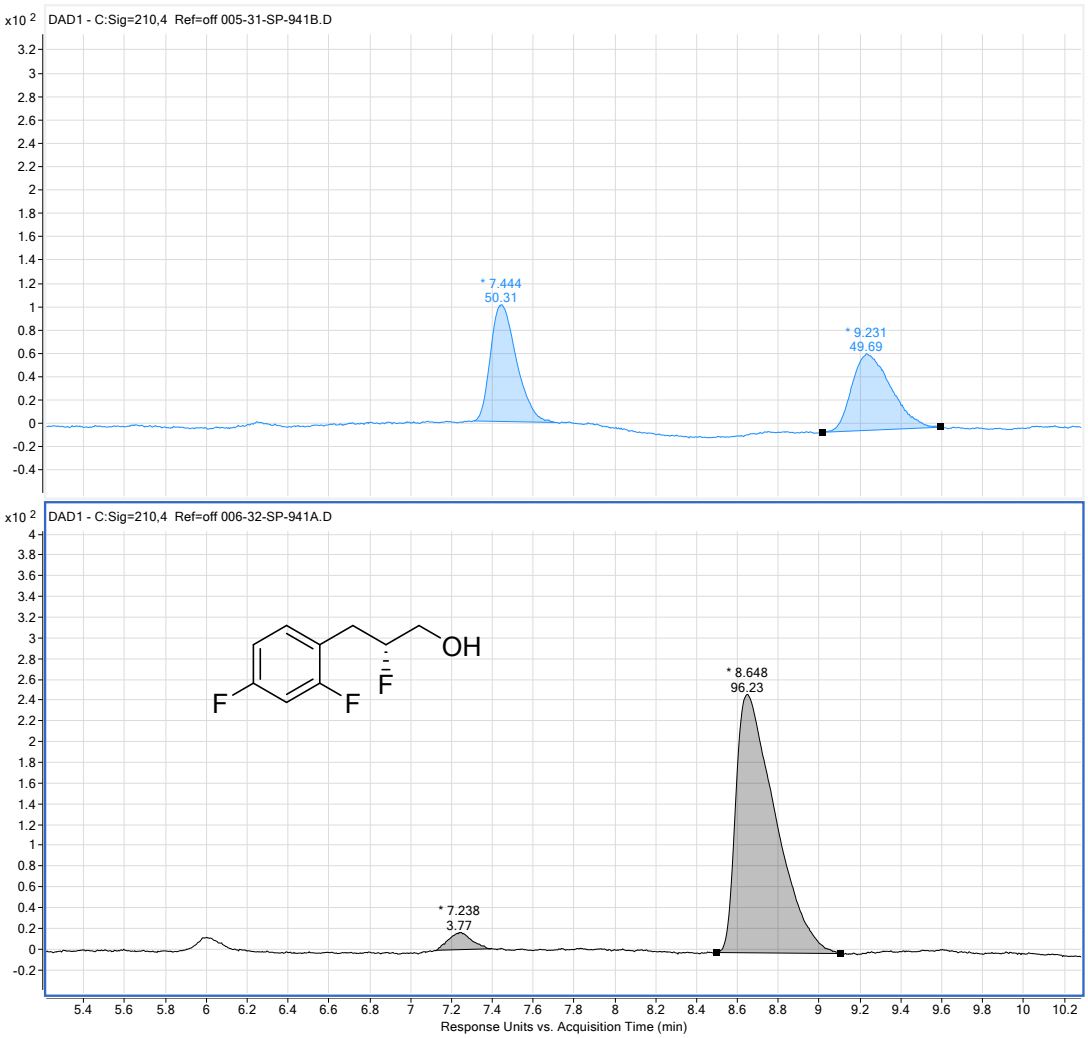
Chromatogram Plots

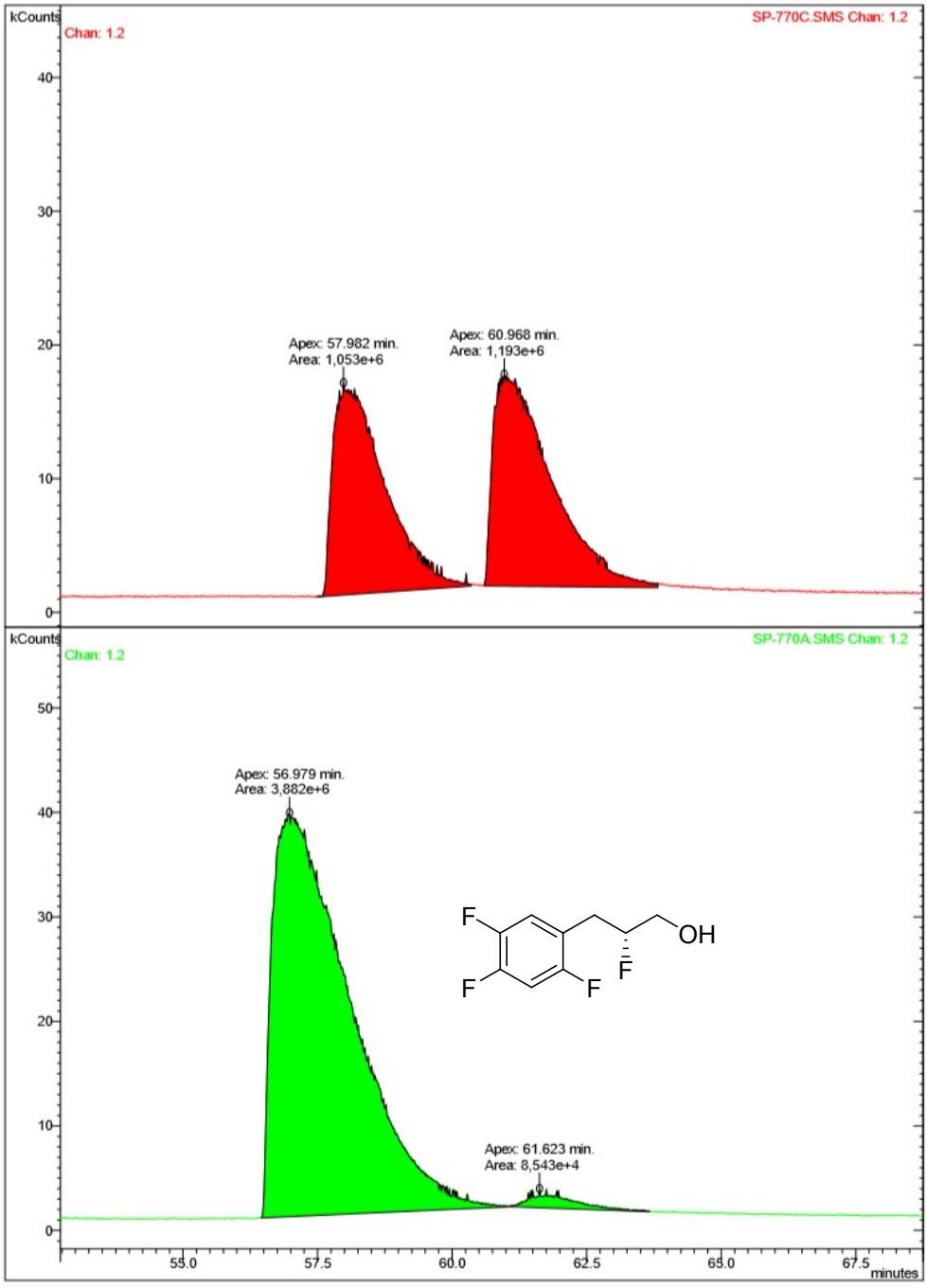



x10 2
DAD1 - C:Sig=210,4 Ref=off 001-31-SP-688B.D
* 9.029
49.46
* 9.778
50.54
x10 1
DAD1 - A:Sig=254,100 Ref=off 002-32-SP-688A.D
* 9.760
98.13
* 9.177
1.87
OH
F
F
F
Response Units vs. Acquisition Time (min)


x10 2
DAD1 - C:Sig=210,4 Ref=off 005-31-SP-941B.D
* 7.444
50.31
* 9.231
49.69
x10 2
DAD1 - C:Sig=210,4 Ref=off 006-32-SP-941A.D
OH
F
F
F
* 8.648
96.23
* 7.238
3.77
Response Units vs. Acquisition Time (min)

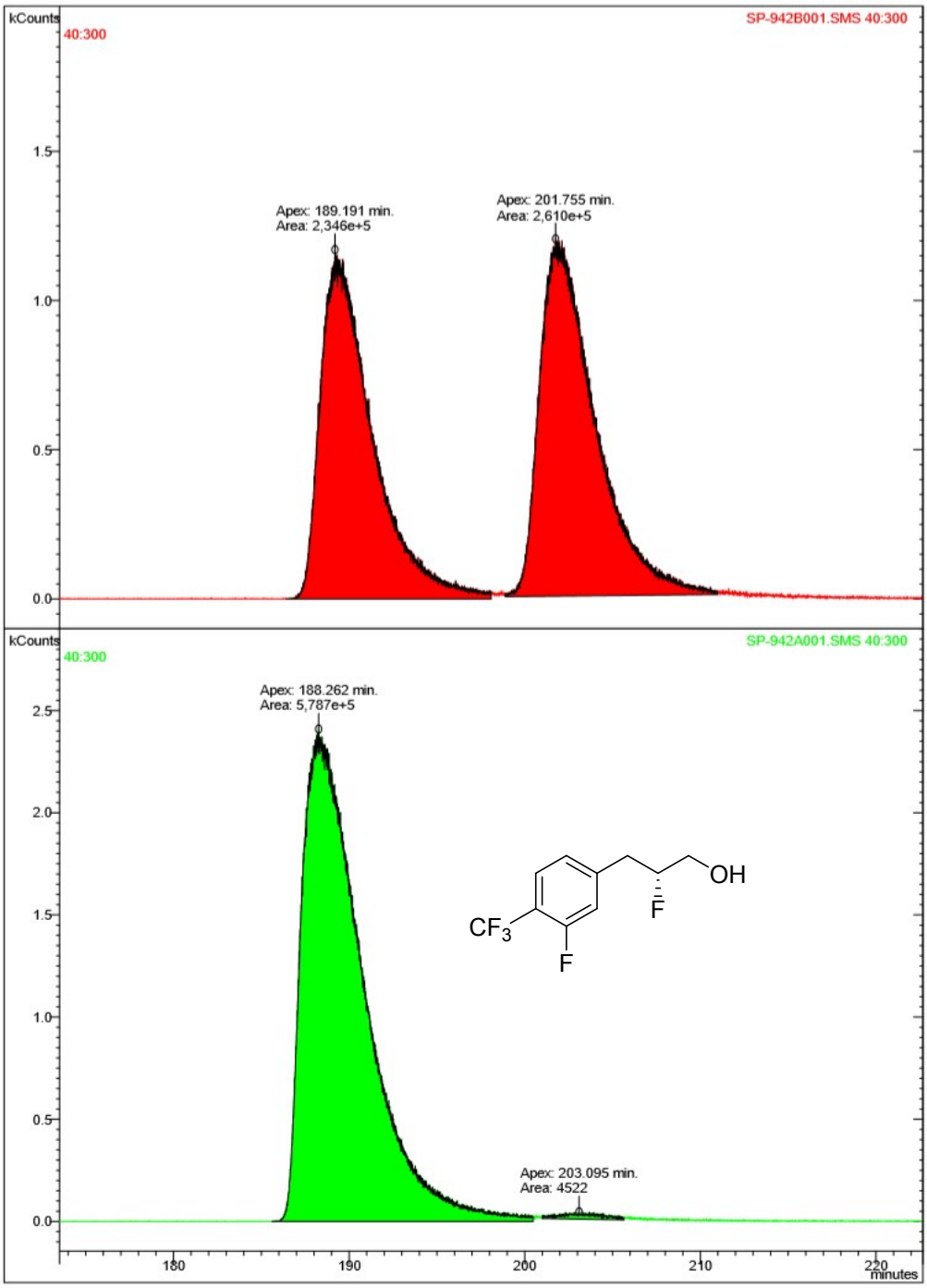
Print Date: 18 Apr 2019 11:04:02

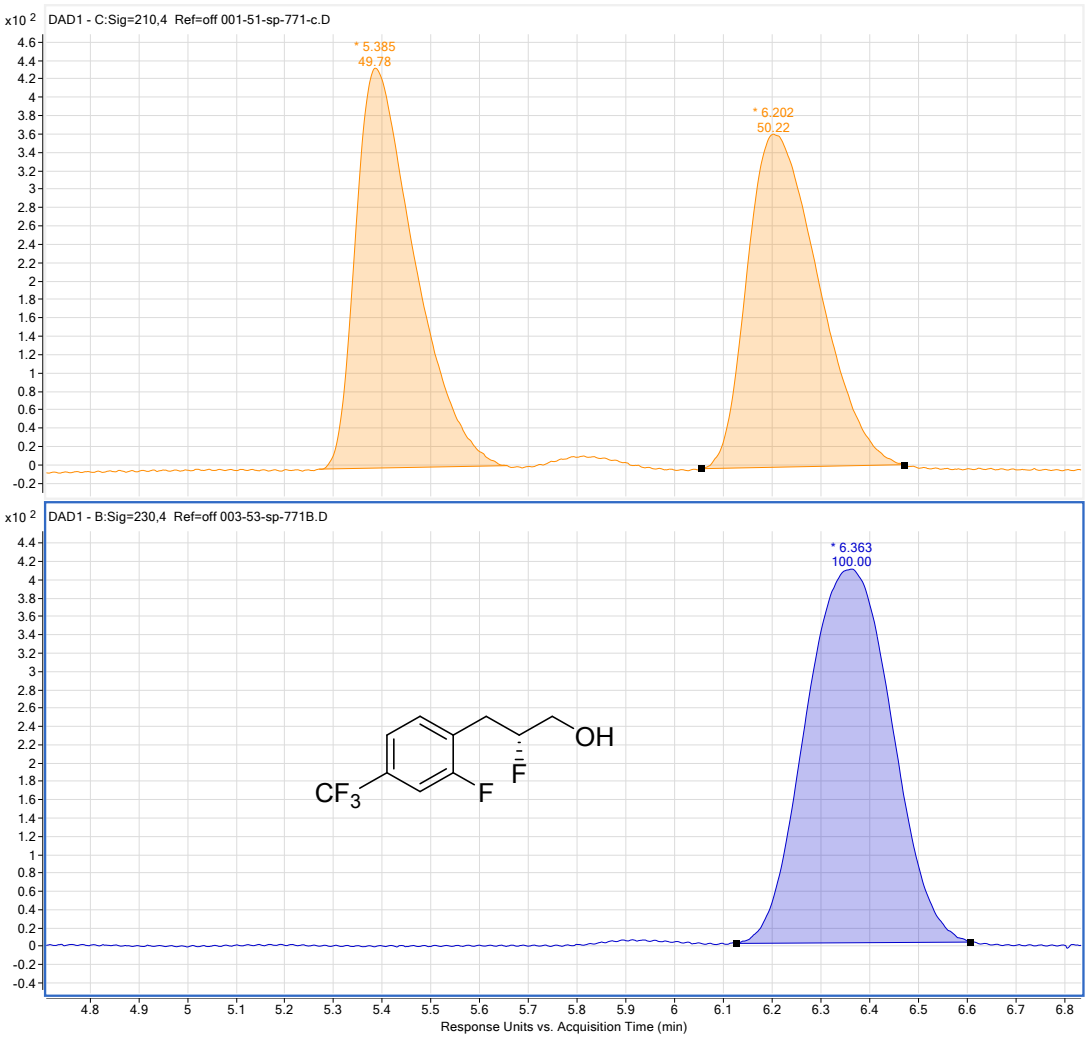
Chromatogram Plots



Print Date: 18 Apr 2019 09:57:30

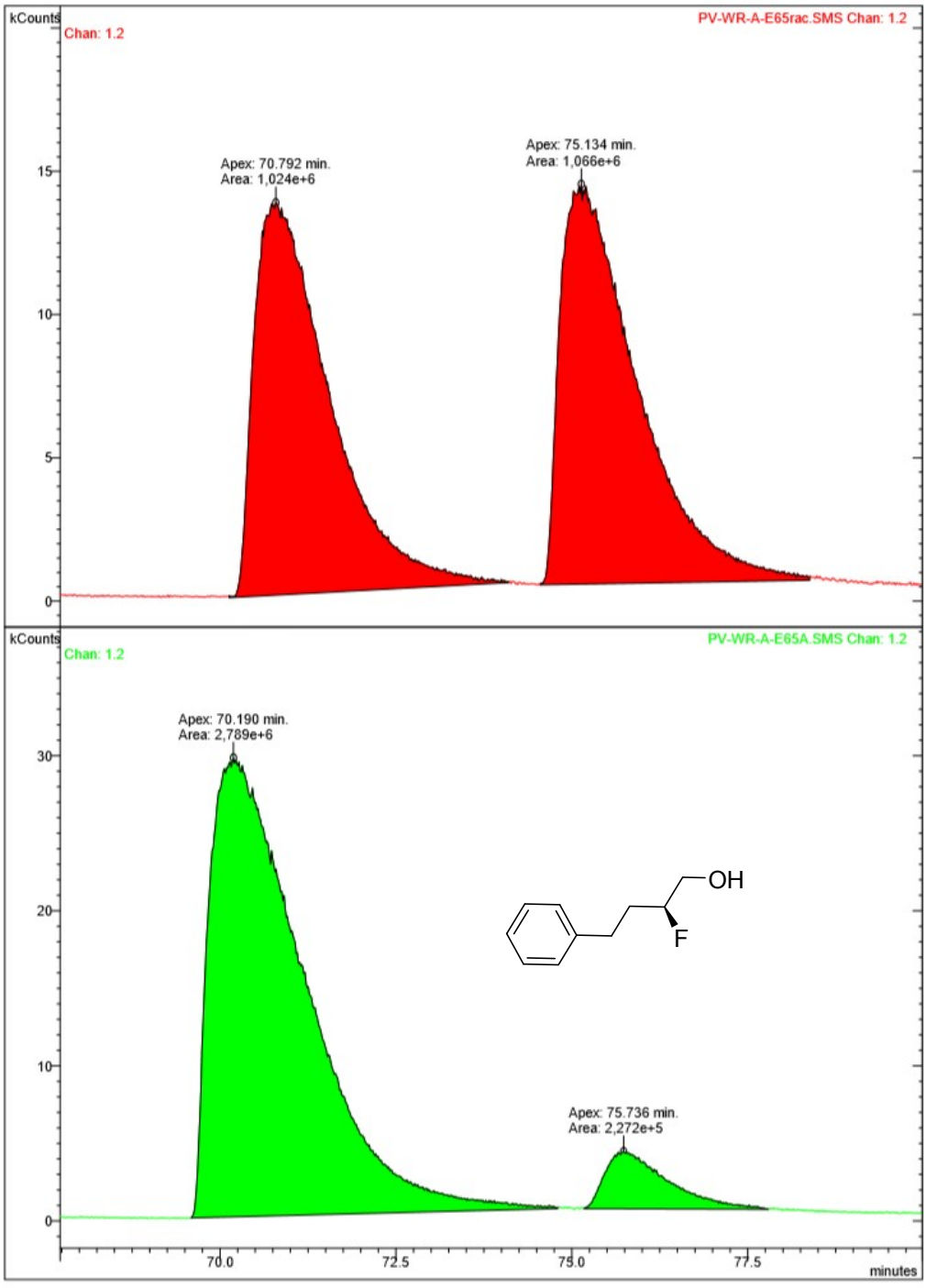
Chromatogram Plots




x10 2
DAD1 - C:Sig=210,4 Ref=off 001-51-sp-771-c.D
* 5.385
49.78
* 6.202
50.22
x10 2
DAD1 - B:Sig=230,4 Ref=off 003-53-sp-771B.D
* 6.363
100.00
OH
F
CF3
F
Response Units vs. Acquisition Time (min)

Print Date: 18 Apr 2019 12:16:26

Chromatogram Plots



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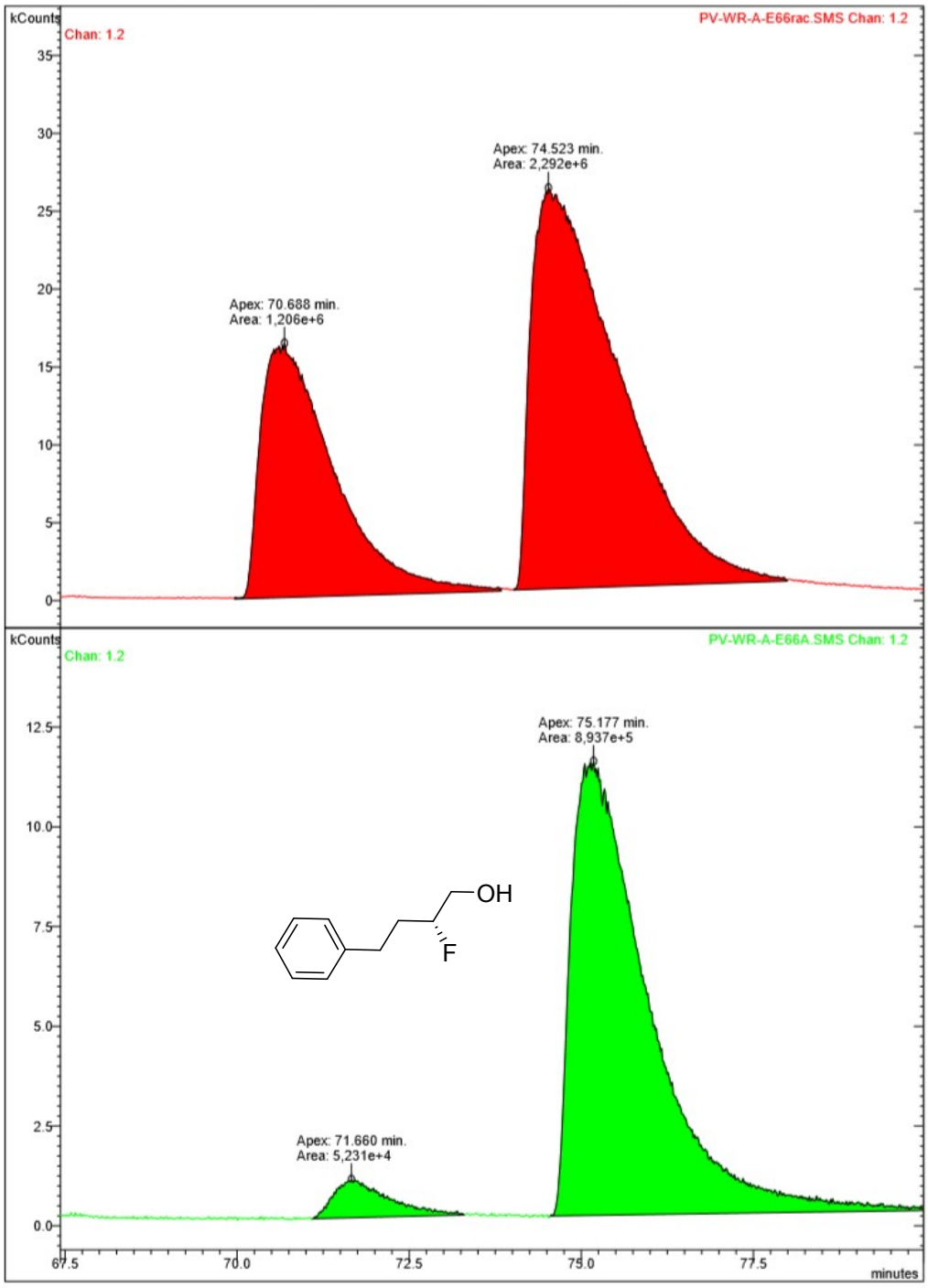
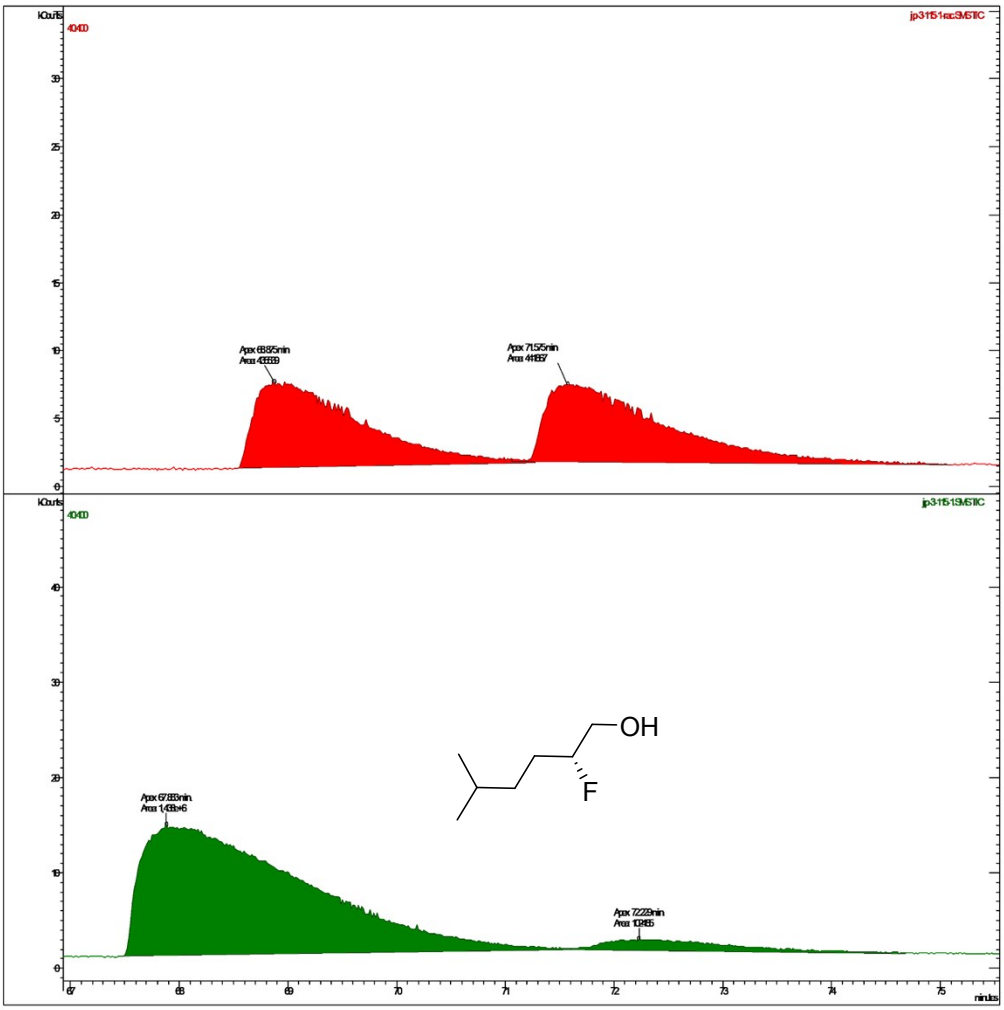
Chromatogram Plots



Chromatogram Plots



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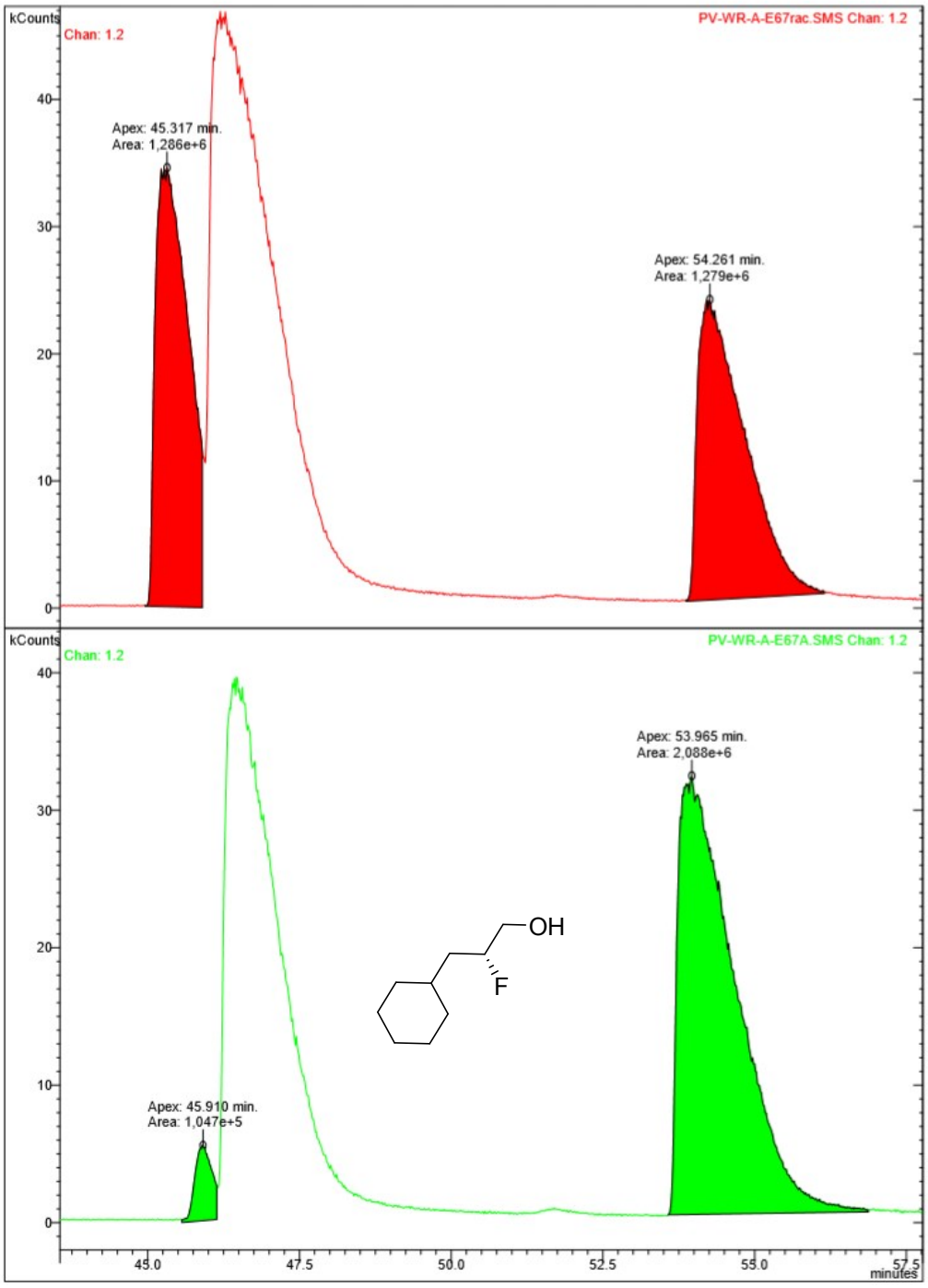

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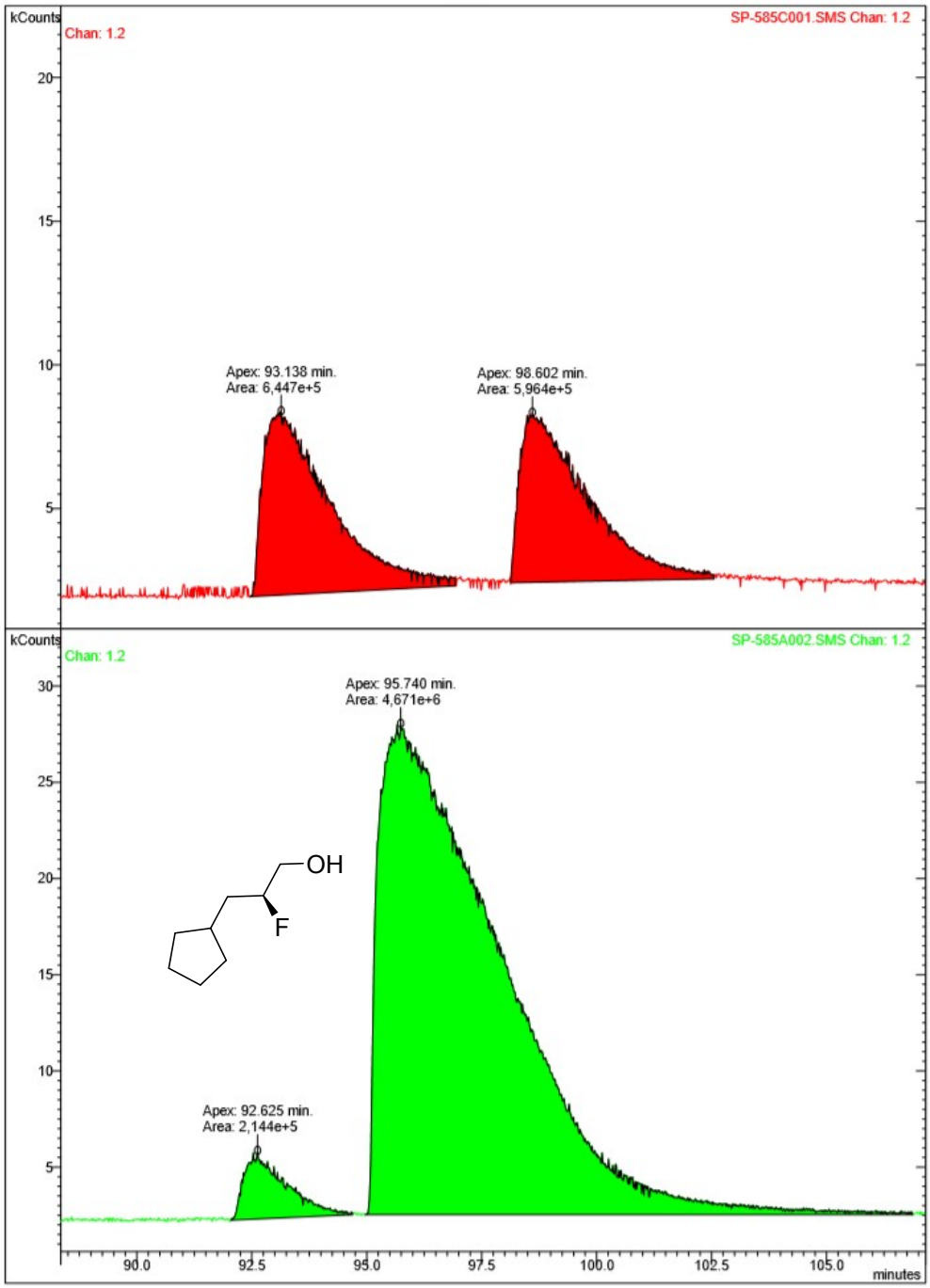
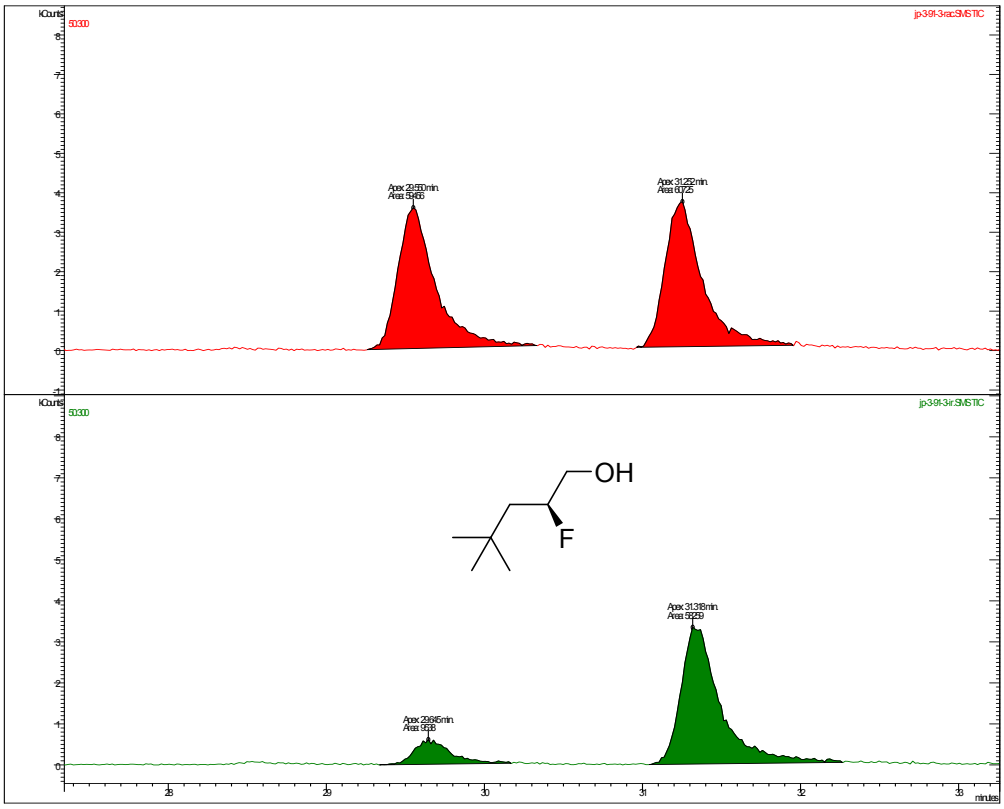
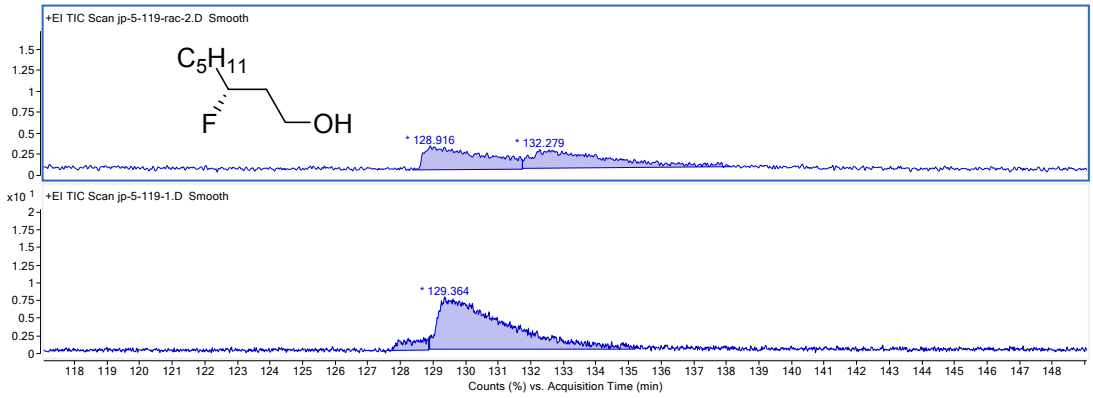
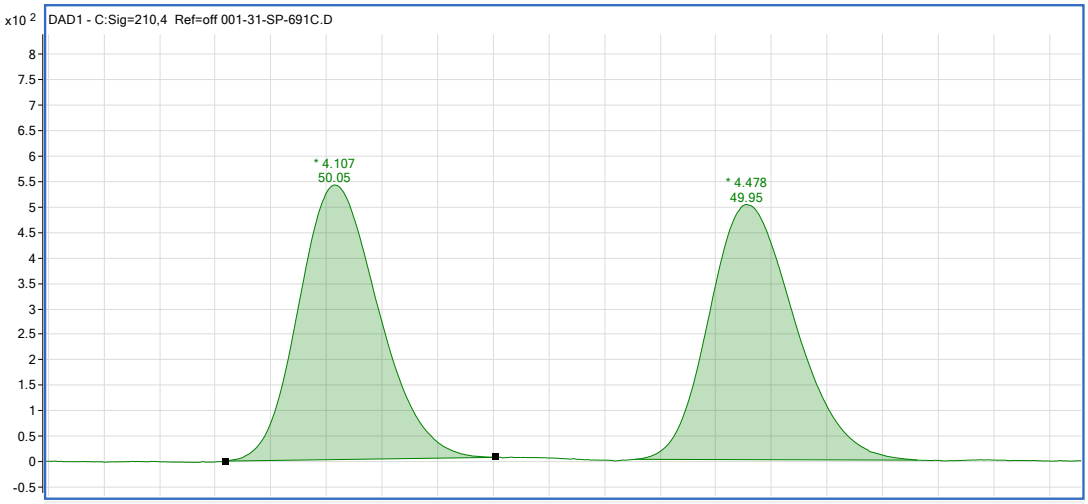
Chromatogram Plots

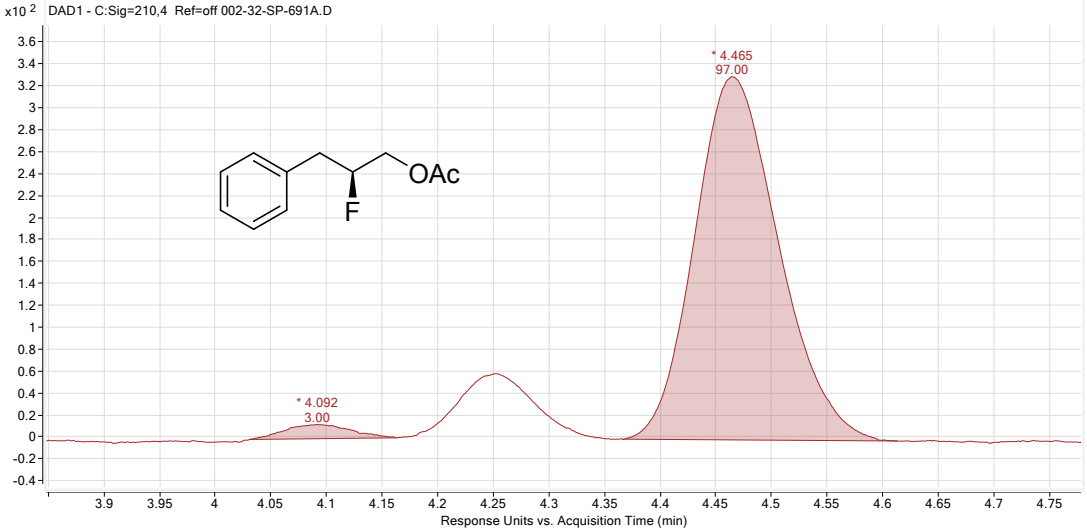


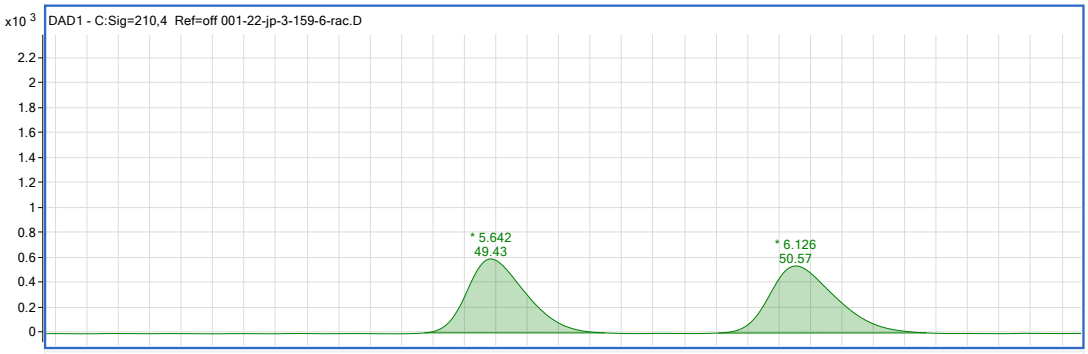
Chromatogram Plots

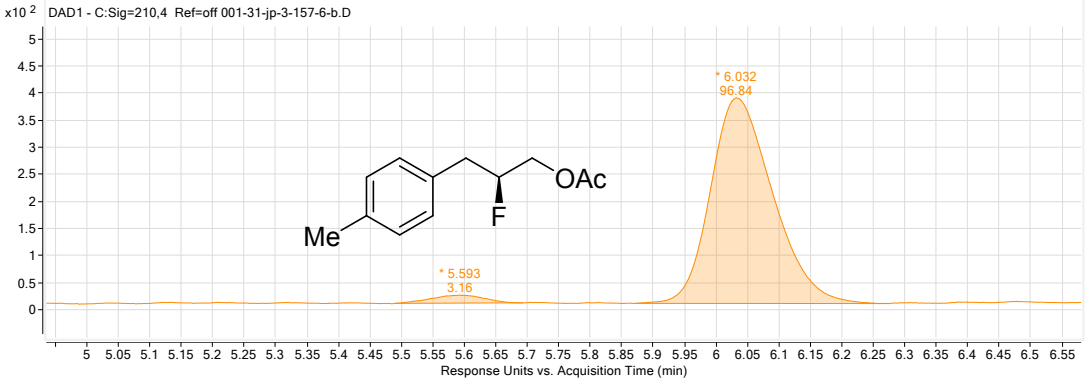


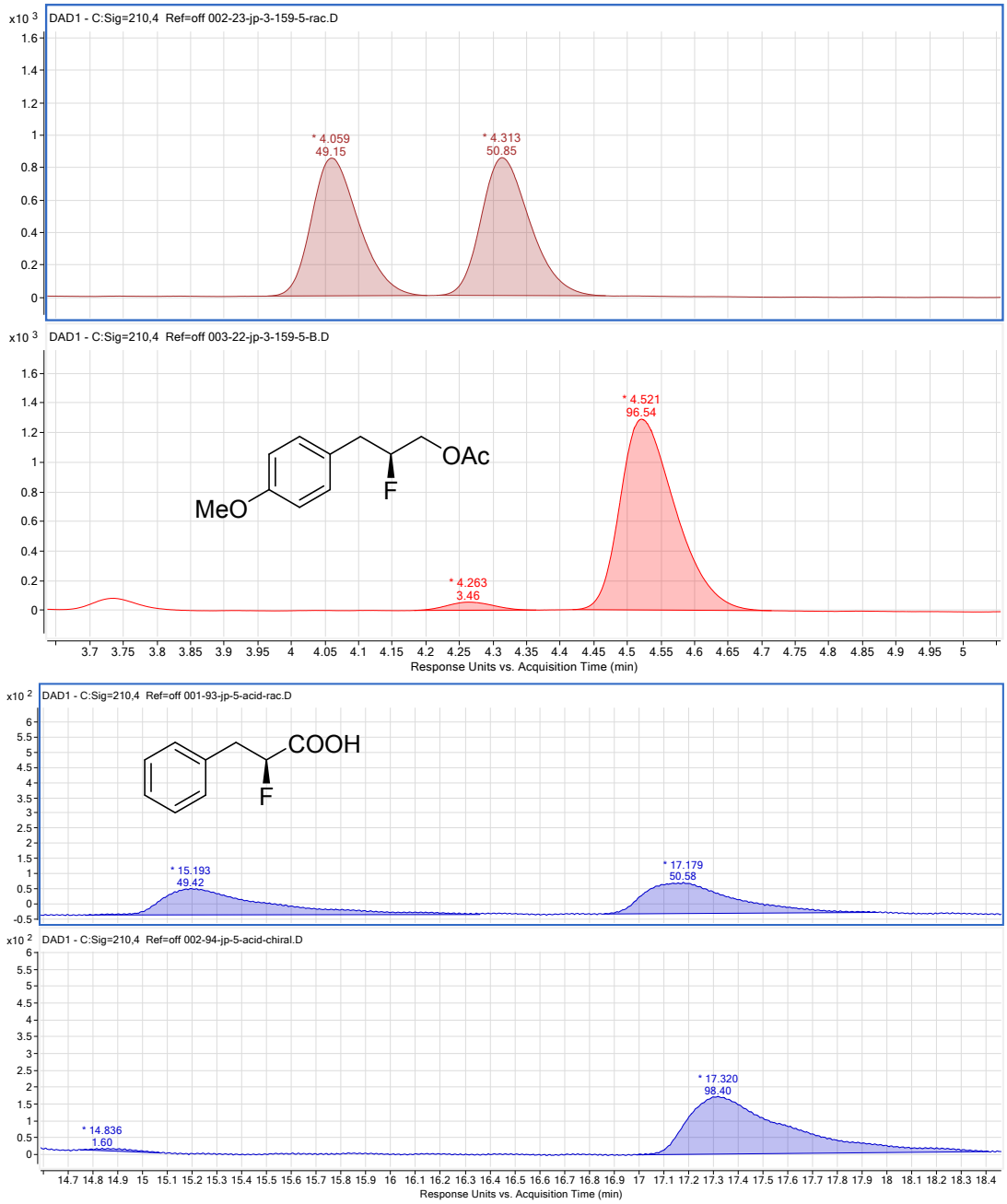


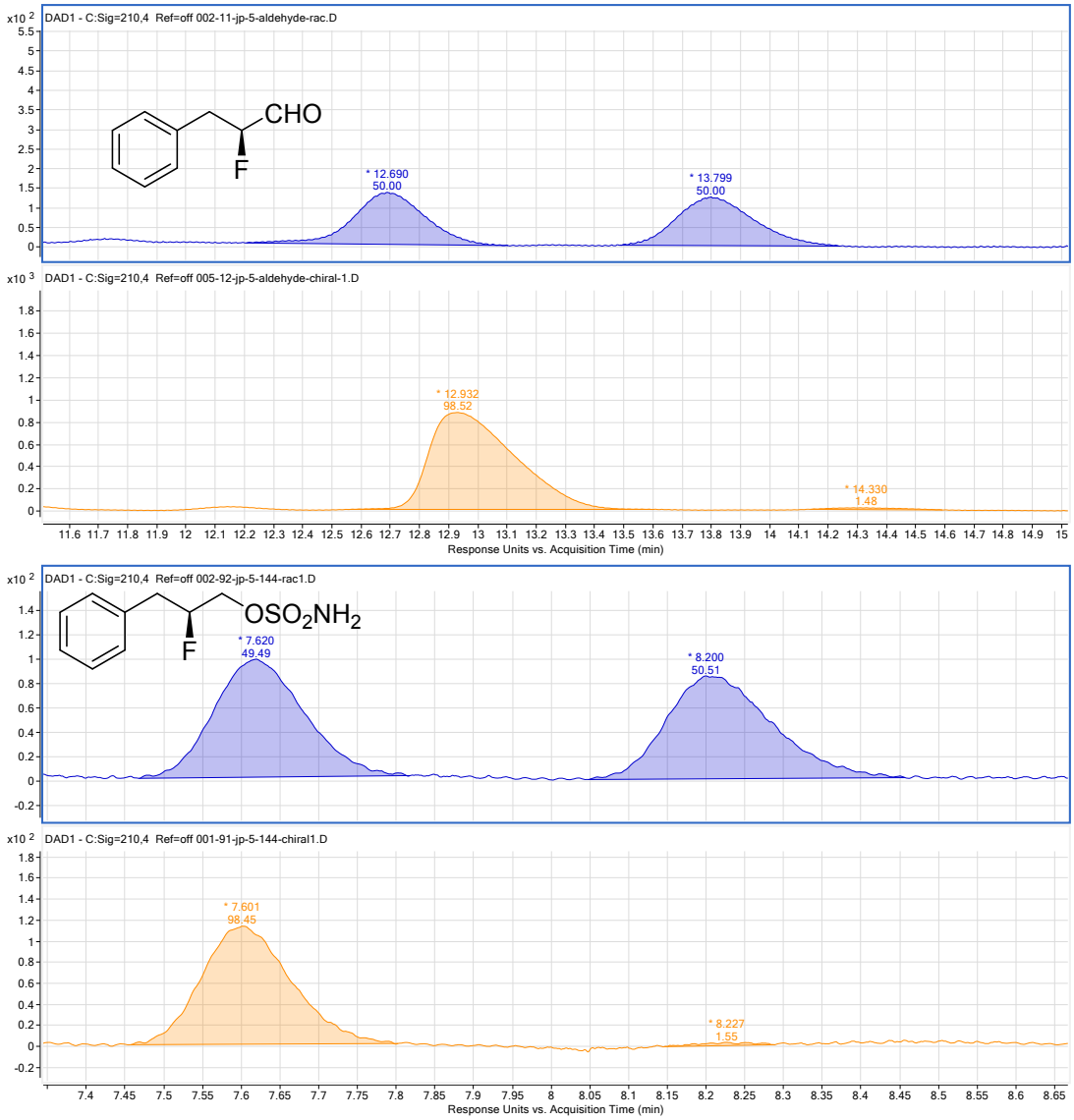

x10 2
DAD1 - C:Sig=210,4 Ref=off 001-31-SP-691C.D
* 4.107
50.05
* 4.478
49.95


x10 2
DAD1 - C:Sig=210,4 Ref=off 002-32-SP-691A.D
* 4.465
97.00
OAc
F
* 4.092
3.00
Response Units vs. Acquisition Time (min)


x10 3
DAD1 - C:Sig=210,4 Ref=off 001-22-jp-3-159-6-rac.D
* 5.642
49.43
* 6.126
50.57


x10 2
DAD1 - C:Sig=210,4 Ref=off 001-31-jp-3-157-6-b.D
* 6.032
96.84
OAc
F
Me
* 5.593
3.16
Response Units vs. Acquisition Time (min)


x10 3 DAD1 - C:Sig=210,4 Ref=off 002-23-jp-3-159-5-rac.D
* 4.059
49.15
* 4.313
50.85
x10 3 DAD1 - C:Sig=210,4 Ref=off 003-22-jp-3-159-5-B.D
* 4.521
96.54
OAc
F
MeO
* 4.263
3.46
Response Units vs. Acquisition Time (min)
x10 2 DAD1 - C:Sig=210,4 Ref=off 001-93-jp-5-acid-rac.D
COOH
F
* 15.193
49.42
* 17.179
50.58
x10 2 DAD1 - C:Sig=210,4 Ref=off 002-94-jp-5-acid-chiral.D
* 17.320
98.40
* 14.836
1.60
Response Units vs. Acquisition Time (min)


DAD1 - C:Sig=210,4 Ref=off 002-11-jp-5-aldehyde-rac.D
CHO
F
* 12.690
50.00
* 13.799
50.00
DAD1 - C:Sig=210,4 Ref=off 005-12-jp-5-aldehyde-chiral-1.D
* 12.932
98.52
* 14.330
1.48
Response Units vs. Acquisition Time (min)
DAD1 - C:Sig=210,4 Ref=off 002-92-jp-5-144-rac1.D
OSO2NH2
F
* 7.620
49.49
* 8.200
50.51
DAD1 - C:Sig=210,4 Ref=off 001-91-jp-5-144-chiral1.D
* 7.601
98.45
* 8.227
1.55
Response Units vs. Acquisition Time (min)

10**. References**

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