Ligand-Enabled Stereoselective *β*-C(sp^3)−H Fluorination: Synthesis of Unnatural Enantiopure *anti*-*β*-Fluoro-*α*-Amino Acids

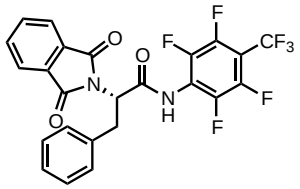
Ru-Yi Zhu, Keita Tanaka, Gen-Cheng Li, Jian He, Hai-Yan Fu, Su-Hua Li, and Jin-Quan Yu*
Department of Chemistry, The Scripps Research Institute, 10550 North Torrey Pines Road, La Jolla, California 92037

Table of Contents

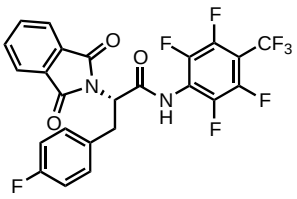
General Information

α-Amino acids and 2,3,5,6-tetrafluoro-4-(trifluoromethyl)aniline were obtained from the commercial sources or synthesized following literature procedures, and used to prepare the corresponding amides. Selectfluor was obtained from Oakwood. $Pd(TFA)_2$ was obtained from Strem. Ag_2CO_3 was purchased from Alfa-Aesar. Solvents were obtained from Sigma-Aldrich, Alfa-Aesar and Acros and used directly without further purification. Analytical thin layer chromatography was performed on 0.25 mm silica gel 60-F254. Visualization was carried out with UV light and Vogel's permanganate. ^{1}H NMR was recorded on Bruker AMX-400 instrument (400 MHz) or Bruker DRX-600 instrument (600 MHz). Chemical shifts were quoted in parts per million (ppm) referenced to 0.0 ppm for tetramethylsilane. The following abbreviations (or combinations thereof) were used to explain multiplicities: s = singlet, d = doublet, t = triplet, q =quartet, m = multiplet, br = broad. Coupling constants, *J*, were reported in Hertz unit (Hz). ^{13}C NMR spectra were recorded on Bruker AMX-400 instrument (100 MHz) or Bruker DRX-600 instrument (150 MHz), and were fully decoupled by broad band proton decoupling. ^{19}F NMR spectra were recorded on Bruker AMX-400 instrument (376 MHz), and were fully decoupled by broad band proton decoupling. Chemical shifts were reported in ppm referenced to either the center line of a triplet at 77.0 ppm of chloroform-*d* or the center line of a multiplet at 29.84 ppm of acetone-d^6. In the ^{13}C NMR analysis, peaks that correspond to those of the polyfluoroarylamide auxiliary appeared as nearly invisible, complex sets of multiplets; they were omitted in the following spectroscopic analysis. High-resolution mass spectra (HRMS) were recorded on an Agilent Mass spectrometer using ESI-TOF (electrospray ionization-time of flight).

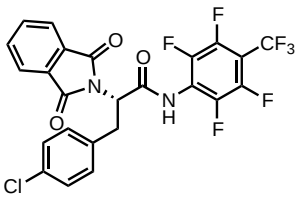
Substrate Structures



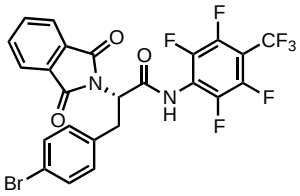
1a



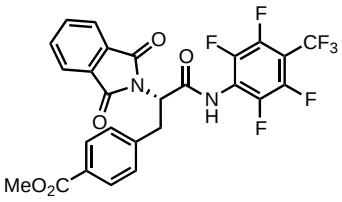
1b



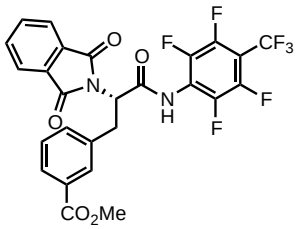
1c



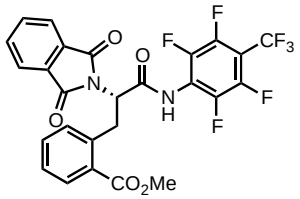
1d



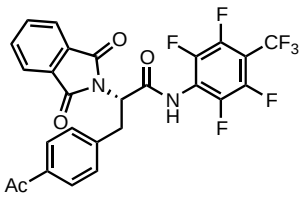
1e



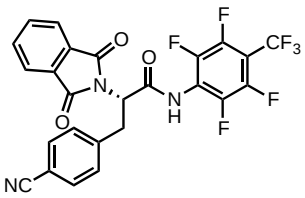
1f



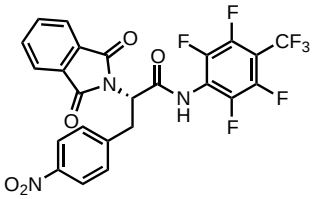
1g



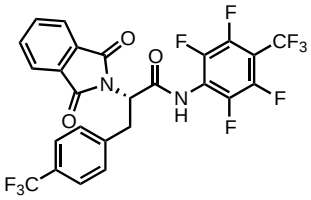
1h



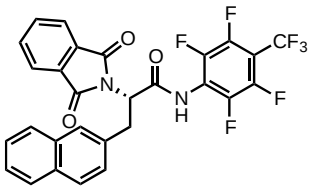
1i



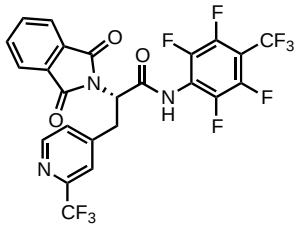
1j



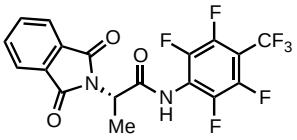
1k



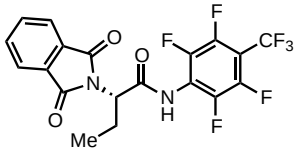
1l



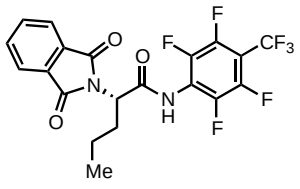
1m



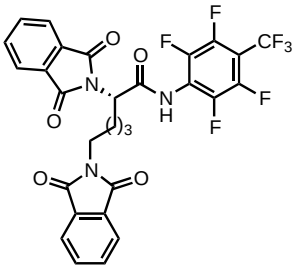
1n



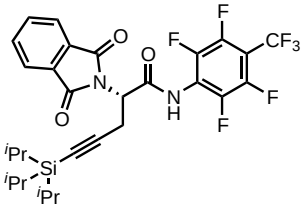
1o



1p



1q

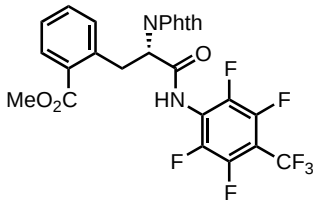


1r

Experimental Section

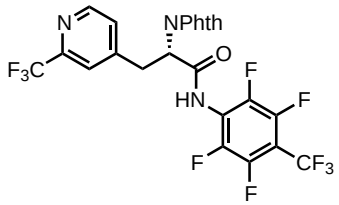
Substrate Preparation

Substrates **1a**, **1n-q** were prepared through traditional synthesis following literature procedure.[1] Substrates **1b-m** were prepared through C−H arylation method following literature procedure.[1] Substrate **1r** was prepared through C−H alkynylation method which is an unpublished result.



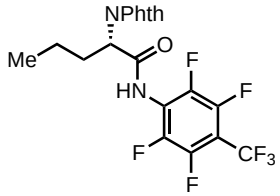
(*S*)-methyl 2-(2-(1,3-dioxoisoindolin-2-yl)-3-oxo-3-((2,3,5,6-tetrafluoro-4-(trifluoromethyl)phenyl)amino)propyl)benzoate (1g)

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.23 (br s, 1H), 8.14-8.11 (m, 1H), 7.85-7.83 (m, 2H), 7.74-7.72 (m, 2H), 7.36-7.30 (m, 2H), 7.11-7.09 (m, 1H), 5.38 (dd, J_1 = 2.4 Hz, J_2 = 10.4 Hz, 1H), 4.17-4.02 (m, 2H), 4.01 (s, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 168.28, 168.08, 166.46, 140.22, 134.28, 133.26, 132.20, 131.55, 127.78, 127.58, 123.65, 56.29, 52.72, 34.28. HRMS (ESI-TOF) Calcd for $C_{26}H_{14}F_7N_2O_5$ [M-H]$^-$: 567.0796, found: 567.0800.



(*S*)-2-(1,3-dioxoisoindolin-2-yl)-*N*-(2,3,5,6-tetrafluoro-4-(trifluoromethyl)phenyl)-3-(2-(trifluoromethyl)pyridin-4-yl)propanamide (1m)

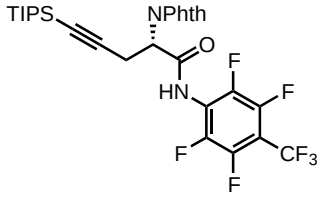
^{1}H NMR (600 MHz, $CDCl_3$) δ 8.59 (d, J = 5.4 Hz, 1H), 8.21 (br s, 1H), 7.86-7.85 (m, 2H), 7.80-7.79 (m, 2H), 7.51 (s, 1H), 7.38 (d, J = 4.8 Hz, 1H), 5.38 (dd, J_1 = 6.0 Hz, J_2 = 10.2 Hz, 1H), 3.78-3.68 (m, 2H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 167.72, 165.58, 150.42, 148.77 (q, J = 34.6 Hz), 146.95, 135.23, 130.69, 126.77, 124.20, 123.01 (q, J = 278.2 Hz), 120.98 (q, J = 2.7 Hz), 54.72, 34.37. HRMS (ESI-TOF) Calcd for $C_{24}H_{10}F_{10}N_3O_3$ [M-H]$^-$: 578.0568, found: 578.0570.



(*S*)-2-(1,3-dioxoisoindolin-2-yl)-*N*-(2,3,5,6-tetrafluoro-4-(trifluoromethyl)phenyl)pentanamide (1p)

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.63 (br s, 1H), 7.93-7.91 (m, 2H), 7.82-7.80 (m, 2H), 5.09 (dd,

J_1 = 6.4 Hz, J_2 = 10.0 Hz, 1H), 2.37-2.19 (m, 2H), 1.44-1.34 (m, 2H), 0.98 (t, J = 7.2 Hz, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 168.35, 167.19, 134.84, 131.25, 124.01, 55.59, 31.43, 19.41, 13.34. HRMS (ESI-TOF) Calcd for $C_{20}H_{12}F_7N_2O_3$ [M-H]$^-$: 461.0742, found: 461.0745.

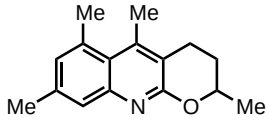


(*S*)-2-(1,3-dioxoisoindolin-2-yl)-*N*-(2,3,5,6-tetrafluoro-4-(trifluoromethyl)phenyl)-5-(triisopropylsilyl)pent-4-ynamide (1r)

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.41 (br s, 1H), 7.90-7.88 (m, 2H), 7.79-7.77 (m, 2H), 5.26 (dd, J_1 = 6.8 Hz, J_2 = 10.0 Hz, 1H), 3.41-3.24 (m, 2H), 0.87-0.85 (m, 21H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 167.72, 165.78, 134.72, 131.47, 123.95, 101.83, 85.56, 53.22, 21.08, 18.26, 10.95. HRMS (ESI-TOF) Calcd for $C_{29}H_{28}F_7N_2O_3Si$ [M-H]$^-$: 613.1763, found: 613.1764.

Ligand Synthesis

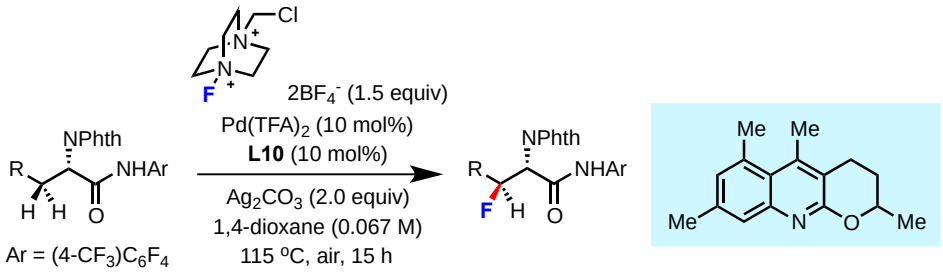
Ligands **4**-**10** were prepared following literature procedure.[2]



2,5,6,8-tetramethyl-3,4-dihydro-2*H*-pyrano[2,3-*b*]quinoline (L10)

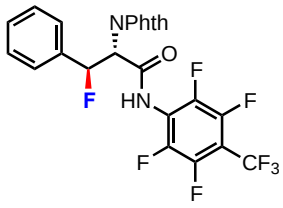
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.46 (s, 1H), 6.96 (s, 1H), 4.37-4.29 (m, 1H), 2.96-2.90 (m, 1H), 2.85-2.76 (m, 1H), 2.82 (s, 3H), 2.70 (s, 3H), 2.40 (s, 3H), 2.16-2.10 (m, 1H), 1.84-1.73 (m, 1H), 1.50 (d, J = 6.0 Hz, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 159.22, 147.59, 145.73, 137.88, 134.13, 130.10, 126.25, 123.67, 115.63, 72.74, 29.31, 26.00, 23.98, 21.35, 21.17, 18.83. HRMS (ESI-TOF) Calcd for $C_{16}H_{20}NO$ [M+H]$^+$: 242.1539, found: 242.1545.

C(sp^3)–H Fluorination



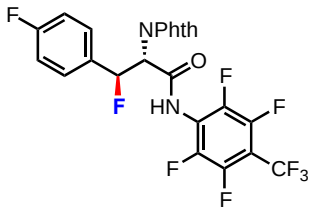
General Procedures for the C(sp^3)–H Fluorination: Substrate **1** (0.10 mmol), Selectfluor (0.15 mmol, 53.2 mg), $Pd(TFA)_2$ (0.01 mmol, 3.3 mg), **L10** (0.01 mmol, 2.4 mg) and Ag_2CO_3 (0.20 mmol, 55.2 mg) were weighed into a tube (10 mL) with a magnetic stir bar under air. 1,4-Dioxane (1.5 mL) was added, and the tube was sealed with a cap. The reaction mixture was stirred at 115 °C for 15 hours. Upon completion, the reaction mixture was cooled to room temperature and diluted with EtOAc. Then the reaction mixture was filtered through

a short celite tube and purified by preparative thin-layer chromatography using hexane/DCM mixtures as the eluent.



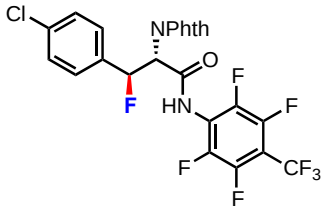
(2*R*,3*S*)-2-(1,3-dioxoisoindolin-2-yl)-3-fluoro-3-phenyl-*N*-(2,3,5,6-tetrafluoro-4-(trifluoromethyl)phenyl)propanamide (2a)

Substrate **1a** was fluorinated following the general fluorination procedure. Analysis of crude reaction mixture by ^{1}H NMR showed a > 20:1 diastereomer ratio. After purification by preparative thin-layer chromatography, **2a** was obtained as a colorless oil (41.9 mg, 79%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.33 (br d, J = 11.2 Hz, 1H), 7.77-7.74 (m, 2H), 7.71-7.67 (m, 2H), 7.43-7.40 (m, 2H), 7.32-7.31 (m, 3H), 6.57 (dd, J_1 = 10.0 Hz, J_2 = 47.6 Hz, 1H), 5.53 (dd, J_1 = 9.6 Hz, J_2 = 13.2 Hz, 1H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 167.01, 163.93 (d, J = 2.7 Hz), 134.52, 133.93 (d, J = 18.9 Hz), 131.13, 130.34 (d, J = 2.6 Hz), 128.90, 127.05 (d, J = 5.6 Hz), 123.84, 91.96 (d, J = 169.2 Hz), 56.42 (d, J = 36.2 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -56.35 (t, J = 21.8 Hz, 3F), -140.49-(-140.69) (m, 2F), -142.13-(-142.24) (m, 2F), -164.60 (s, 1F). HRMS (ESI-TOF) Calcd for $C_{24}H_{11}F_8N_2O_3$ [M-H]$^-$: 527.0647, found: 527.0644.



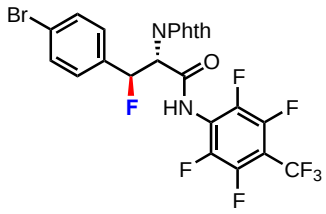
(2*R*,3*S*)-2-(1,3-dioxoisoindolin-2-yl)-3-fluoro-3-(4-fluorophenyl)-*N*-(2,3,5,6-tetrafluoro-4-(trifluoromethyl)phenyl)propanamide (2b)

Substrate **1b** was fluorinated following the general fluorination procedure. Analysis of crude reaction mixture by ^{1}H NMR showed a > 20:1 diastereomer ratio. After purification by preparative thin-layer chromatography, **2b** was obtained as a white solid (38.2 mg, 70%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.27 (br d, J = 10.8 Hz, 1H), 7.79-7.75 (m, 2H), 7.73-7.69 (m, 2H), 7.43-7.40 (m, 2H), 7.01 (t, J = 8.6 Hz, 2H), 6.57 (dd, J_1 = 9.6 Hz, J_2 = 47.2 Hz, 1H), 5.49 (dd, J_1 = 9.6 Hz, J_2 = 13.2 Hz, 1H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 167.01, 163.75 (d, J = 2.6 Hz), 163.62 (dd, J_1 = 3.0 Hz, J_2 = 249.0 Hz), 134.66, 131.05, 129.92 (dd, J_1 = 19.2 Hz, J_2 = 3.0 Hz), 129.20 (dd, J_1 = 8.7 Hz, J_2 = 5.4 Hz), 123.92, 116.11 (d, J = 21.8 Hz), 91.27 (d, J = 169.2 Hz), 56.37 (d, J = 36.3 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -56.36 (t, J = 22.2 Hz, 3F), -109.92 (d, J = 5.3 Hz, 1F), -140.42-(-140.62) (m, 2F), -142.17-(-142.29) (m, 2F), -163.03 (d, J = 4.5 Hz, 1F). HRMS (ESI-TOF) Calcd for $C_{24}H_{10}F_9N_2O_3$ [M-H]$^-$: 545.0553, found: 545.0554.



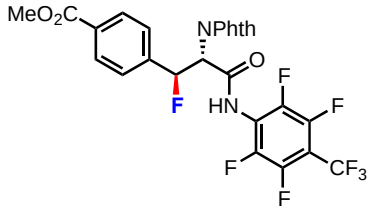
(2*R*,3*S*)-3-(4-chlorophenyl)-2-(1,3-dioxoisoindolin-2-yl)-3-fluoro-*N*-(2,3,5,6-tetrafluoro-4-(trifluoromethyl)phenyl)propanamide (2c)

Substrate **1c** was fluorinated following the general fluorination procedure. Analysis of crude reaction mixture by ^{1}H NMR showed a > 20:1 diastereomer ratio. After purification by preparative thin-layer chromatography, **2c** was obtained as a white solid (37.6 mg, 67%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.25 (br d, J = 10.8 Hz, 1H), 7.79-7.77 (m, 2H), 7.72-7.70 (m, 2H), 7.37 (d, J = 8.0 Hz, 2H), 7.30 (d, J = 8.8 Hz, 2H), 6.56 (dd, J_1 = 9.2 Hz, J_2 = 47.2 Hz, 1H), 5.48 (dd, J_1 = 10.0 Hz, J_2 = 13.6 Hz, 1H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 167.03, 163.67 (d, J = 2.7 Hz), 136.41 (d, J = 3.2 Hz), 134.69, 132.49 (d, J = 19.4 Hz), 131.05, 129.26, 128.47 (d, J = 5.4 Hz), 123.97, 91.21 (d, J = 169.5 Hz), 56.30 (d, J = 36.1 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -56.36 (t, J = 21.4 Hz, 3F), -140.36-(-140.55) (m, 2F), -140.60-(-142.25) (m, 2F), -164.51 (s, 1F). HRMS (ESI-TOF) Calcd for $C_{24}H_{10}ClF_8N_2O_3$ $[M-H]^-$: 561.0258, found: 561.0254.



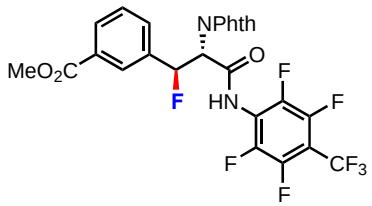
(2*R*,3*S*)-3-(4-bromophenyl)-2-(1,3-dioxoisoindolin-2-yl)-3-fluoro-*N*-(2,3,5,6-tetrafluoro-4-(trifluoromethyl)phenyl)propanamide (2d)

Substrate **1d** was fluorinated following the general fluorination procedure. Analysis of crude reaction mixture by ^{1}H NMR showed a > 20:1 diastereomer ratio. After purification by preparative thin-layer chromatography, **2d** was obtained as a white solid (41.3 mg, 68%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.28 (br d, J = 9.2 Hz, 1H), 7.81-7.79 (m, 2H), 7.74-7.72 (m, 2H), 7.48 (d, J = 8.0 Hz, 2H), 7.32 (d, J = 6.8 Hz, 2H), 6.57 (dd, J_1 = 10.4 Hz, J_2 = 46.8 Hz, 1H), 5.50 (dd, J_1 = 9.6 Hz, J_2 = 13.6 Hz, 1H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 167.04, 163.67 (d, J = 2.7 Hz), 134.70, 133.01 (d, J = 19.4 Hz), 132.21, 131.05, 128.70 (d, J = 5.4 Hz), 124.70 (d, J = 3.6 Hz), 123.98, 91.24 (d, J = 169.8 Hz), 56.25 (d, J = 35.8 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -56.36 (t, J = 22.2 Hz, 3F), -140.37-(-140.62) (m, 2F), -142.19-(-142.26) (m, 2F), -164.86 (s, 1F). HRMS (ESI-TOF) Calcd for $C_{24}H_{10}BrF_8N_2O_3$ $[M-H]^-$: 604.9753, found: 604.9750.



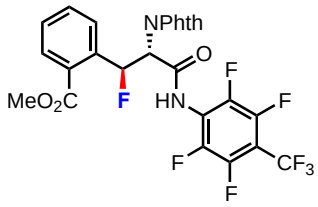
methyl 4-((1*S*,2*R*)-2-(1,3-dioxoisoindolin-2-yl)-1-fluoro-3-oxo-3-((2,3,5,6-tetrafluoro-4-(trifluoromethyl)phenyl)amino)propyl)benzoate (2e)

Substrate **1e** was fluorinated following the general fluorination procedure. Analysis of crude reaction mixture by ^{1}H NMR showed a > 20:1 diastereomer ratio. After purification by preparative thin-layer chromatography, **2e** was obtained as a colorless oil (45.3 mg, 77%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.31 (br d, *J* = 10.0 Hz, 1H), 7.98 (d, *J* = 8.0 Hz, 2H), 7.77-7.75 (m, 2H), 7.71-7.69 (m, 2H), 7.49 (d, *J* = 8.0 Hz, 2H), 6.62 (dd, J_1 = 9.6 Hz, J_2 = 47.2 Hz, 1H), 5.50 (dd, J_1 = 9.6 Hz, J_2 = 13.6 Hz, 1H), 3.87 (s, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 166.97, 166.17, 163.60 (d, *J* = 2.1 Hz), 138.65 (d, *J* = 18.8 Hz), 134.69, 131.84 (d, *J* = 2.2 Hz), 130.98, 130.08, 126.98 (d, *J* = 5.7 Hz), 123.95, 91.13 (d, *J* = 171.0 Hz), 56.38 (d, *J* = 35.4 Hz), 52.31. ^{19}F NMR (376 MHz, $CDCl_3$) δ -56.37 (t, *J* = 21.8 Hz, 3F), -140.40-(-140.64) (m, 2F), -142.16-(-142.26) (m, 2F), -167.88 (s, 1F). HRMS (ESI-TOF) Calcd for $C_{26}H_{13}F_8N_2O_5$ $[M-H]^-$: 585.0702, found: 585.0703.



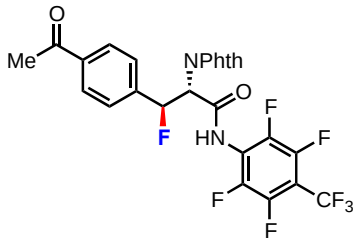
methyl 3-((1*S*,2*R*)-2-(1,3-dioxoisoindolin-2-yl)-1-fluoro-3-oxo-3-((2,3,5,6-tetrafluoro-4-(trifluoromethyl)phenyl)amino)propyl)benzoate (2f)

Substrate **1f** was fluorinated following the general fluorination procedure. Analysis of crude reaction mixture by ^{1}H NMR showed a > 20:1 diastereomer ratio. After purification by preparative thin-layer chromatography, **2f** was obtained as a colorless oil (45.8 mg, 78%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.34 (br d, *J* = 10.4 Hz, 1H), 8.10 (s, 1H), 8.00 (d, *J* = 7.6 Hz, 1H), 7.78-7.76 (m, 2H), 7.70-7.68 (m, 2H), 7.61 (d, *J* = 7.2 Hz, 1H), 7.41 (t, *J* = 7.6 Hz, 1H), 6.63 (dd, J_1 = 9.6 Hz, J_2 = 47.2 Hz, 1H), 5.54 (dd, J_1 = 9.6 Hz, J_2 = 12.8 Hz, 1H), 3.88 (s, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 167.01, 166.02, 163.70 (d, *J* = 2.7 Hz), 134.60 (d, *J* = 19.0 Hz), 134.63, 131.38 (d, *J* = 1.6 Hz), 131.28 (d, *J* = 5.2 Hz), 131.05, 130.94, 129.08, 128.19 (d, *J* = 6.0 Hz), 123.93, 91.21 (d, *J* = 170.6 Hz), 56.45 (d, *J* = 35.4 Hz), 52.34. ^{19}F NMR (376 MHz, $CDCl_3$) δ -56.37 (t, *J* = 21.4 Hz, 3F), -140.45-(-140.65) (m, 2F), -142.14-(-142.23) (m, 2F), -166.36 (s, 1F). HRMS (ESI-TOF) Calcd for $C_{26}H_{13}F_8N_2O_5$ $[M-H]^-$: 585.0702, found: 585.0706.



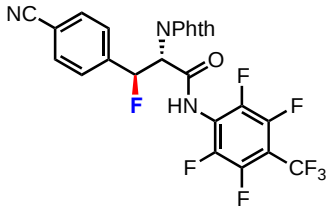
methyl 2-((1*S*,2*R*)-2-(1,3-dioxoisoindolin-2-yl)-1-fluoro-3-oxo-3-((2,3,5,6-tetrafluoro-4-(trifluoromethyl)phenyl)amino)propyl)benzoate (2g)

Substrate **1g** was fluorinated following the general fluorination procedure. Analysis of crude reaction mixture by ^{1}H NMR showed a > 20:1 diastereomer ratio. After purification by preparative thin-layer chromatography, **2g** was obtained as a colorless oil (44.9 mg, 77%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.91 (br d, *J* = 7.2 Hz, 1H), 7.87 (d, *J* = 8.0 Hz, 1H), 7.84-7.82 (m, 2H), 7.75-7.73 (m, 2H), 7.68 (d, *J* = 7.6 Hz, 1H), 7.57 (t, *J* = 7.6 Hz, 1H), 7.42 (t, *J* = 7.2 Hz, 1H), 7.16 (dd, J_1 = 7.2 Hz, J_2 = 46.8 Hz, 1H), 5.74 (dd, J_1 = 7.6 Hz, J_2 = 16.0 Hz, 1H), 3.90 (s, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 167.31, 167.10, 163.60, 135.68 (d, *J* = 19.8 Hz), 134.62, 132.56, 131.24, 130.91, 129.66 (d, *J* = 1.4 Hz), 129.03 (d, *J* = 3.6 Hz), 127.56 (d, *J* = 9.3 Hz), 123.89, 88.77 (d, *J* = 175.0 Hz), 58.09 (d, *J* = 30.9 Hz), 52.64. ^{19}F NMR (376 MHz, $CDCl_3$) δ -56.33 (t, *J* = 21.8 Hz, 3F), -140.76-(-141.00) (m, 2F), -141.97-(-142.08) (m, 2F), -173.97 (s, 1F). HRMS (ESI-TOF) Calcd for $C_{26}H_{13}F_8N_2O_5$ $[M-H]^-$: 585.0702, found: 585.0707.



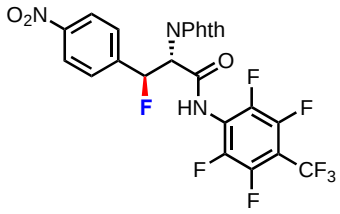
(2*R*,3*S*)-3-(4-acetylphenyl)-2-(1,3-dioxoisoindolin-2-yl)-3-fluoro-*N*-(2,3,5,6-tetrafluoro-4-(trifluoromethyl)phenyl)propanamide (2h)

Substrate **1h** was fluorinated following the general fluorination procedure. Analysis of crude reaction mixture by ^{1}H NMR showed a > 20:1 diastereomer ratio. After purification by preparative thin-layer chromatography, **2h** was obtained as a colorless oil (37.9 mg, 66%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.33 (br d, *J* = 10.0 Hz, 1H), 7.89 (d, *J* = 8.0 Hz, 2H), 7.78-7.76 (m, 2H), 7.71-7.69 (m, 2H), 7.62 (d, *J* = 8.0 Hz, 2H), 7.52 (d, *J* = 8.0 Hz, 2H), 6.63 (dd, J_1 = 9.6 Hz, J_2 = 47.2 Hz, 1H), 5.51 (dd, J_1 = 9.6 Hz, J_2 = 13.2 Hz, 1H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 197.34, 167.01, 163.58 (d, *J* = 2.5 Hz), 138.76 (d, *J* = 18.6 Hz), 138.38 (d, *J* = 2.5 Hz), 134.72, 131.00, 128.78, 127.23 (d, *J* = 5.7 Hz), 123.97, 91.08 (d, *J* = 171.0 Hz), 56.38 (d, *J* = 35.1 Hz), 26.63. ^{19}F NMR (376 MHz, $CDCl_3$) δ -56.36 (t, *J* = 21.8 Hz, 3F), -140.36-(-140.61) (m, 2F), -142.17-(-142.25) (m, 2F), -167.88 (s, 1F). HRMS (ESI-TOF) Calcd for $C_{26}H_{13}F_8N_2O_4$ $[M-H]^-$: 569.0753, found: 569.0757.



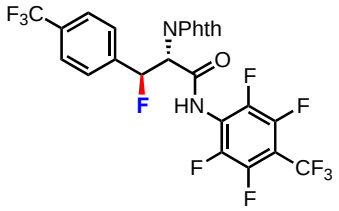
(2*R*,3*S*)-3-(4-cyanophenyl)-2-(1,3-dioxoisoindolin-2-yl)-3-fluoro-*N*-(2,3,5,6-tetrafluoro-4-(trifluoromethyl)phenyl)propanamide (2i)

Substrate **1i** was fluorinated following the general fluorination procedure. Analysis of crude reaction mixture by ^{1}H NMR showed a > 20:1 diastereomer ratio. After purification by preparative thin-layer chromatography, **2i** was obtained as a colorless oil (48.0 mg, 87%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.26 (br d, *J* = 8.4 Hz, 1H), 7.80-7.78 (m, 2H), 7.74-7.72 (m, 2H), 7.62 (d, *J* = 8.0 Hz, 2H), 7.54 (d, *J* = 8.0 Hz, 2H), 6.62 (dd, J_1 = 9.2 Hz, J_2 = 47.2 Hz, 1H), 5.47 (dd, J_1 = 9.6 Hz, J_2 = 14.0 Hz, 1H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 166.98, 163.33 (d, *J* = 1.6 Hz), 139.02 (d, *J* = 19.2 Hz), 134.90, 132.66, 130.87, 127.65 (d, *J* = 6.0 Hz), 124.05, 117.79, 114.16 (d, *J* = 2.4 Hz), 90.65 (d, *J* = 172.4 Hz), 56.32 (d, *J* = 34.6 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -56.38 (t, *J* = 21.4 Hz, 3F), -140.32-(-140.52) (m, 2F), -142.19-(-142.28) (m, 2F), -169.60 (s, 1F). HRMS (ESI-TOF) Calcd for $C_{25}H_{10}F_8N_3O_3$ $[M-H]^-$: 552.0600, found: 552.0604.



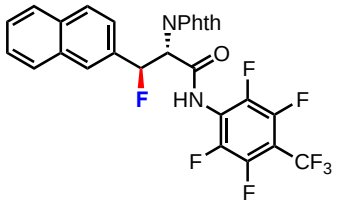
(2*R*,3*S*)-2-(1,3-dioxoisoindolin-2-yl)-3-fluoro-3-(4-nitrophenyl)-*N*-(2,3,5,6-tetrafluoro-4-(trifluoromethyl)phenyl)propanamide (2j)

Substrate **1j** was fluorinated following the general fluorination procedure. Analysis of crude reaction mixture by ^{1}H NMR showed a > 20:1 diastereomer ratio. After purification by preparative thin-layer chromatography, **2j** was obtained as a white solid (29.8 mg, 52%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.22 (br d, *J* = 8.8 Hz, 1H), 8.19 (d, *J* = 8.8 Hz, 2H), 7.81-7.78 (m, 2H), 7.75-7.72 (m, 2H), 7.63 (d, *J* = 8.0 Hz, 2H), 6.69 (dd, J_1 = 9.6 Hz, J_2 = 47.2 Hz, 1H), 5.50 (dd, J_1 = 9.6 Hz, J_2 = 14.0 Hz, 1H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 167.02, 163.19 (d, *J* = 1.6 Hz), 148.90 (d, *J* = 2.1 Hz), 140.76 (d, *J* = 19.2 Hz), 134.94, 130.88, 128.01 (d, *J* = 6.0 Hz), 124.13, 124.10, 90.48 (d, *J* = 172.4 Hz), 56.42 (d, *J* = 34.6 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -56.37 (t, *J* = 21.4 Hz, 3F), -140.18-(-140.43) (m, 2F), -142.16-(-142.25) (m, 2F), -169.29 (s, 1F). HRMS (ESI-TOF) Calcd for $C_{24}H_{10}F_8N_3O_5$ $[M-H]^-$: 572.0498, found: 572.0502.



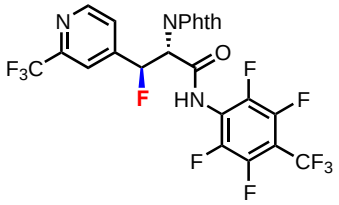
(2*R*,3*S*)-2-(1,3-dioxoisoindolin-2-yl)-3-fluoro-*N*-(2,3,5,6-tetrafluoro-4-(trifluoromethyl)phenyl)-3-(4-(trifluoromethyl)phenyl)propanamide (2k)

Substrate **1k** was fluorinated following the general fluorination procedure. Analysis of crude reaction mixture by ^{1}H NMR showed a > 20:1 diastereomer ratio. After purification by preparative thin-layer chromatography, **2k** was obtained as a white solid (45.0 mg, 76%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.25 (br d, J = 10.4 Hz, 1H), 7.80-7.78 (m, 2H), 7.73-7.71 (m, 2H), 7.61-7.55 (m, 4H), 6.71 (dd, J_1 = 9.2 Hz, J_2 = 47.2 Hz, 1H), 5.51 (dd, J_1 = 10.0 Hz, J_2 = 13.6 Hz, 1H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 167.09, 163.49 (d, J = 2.2 Hz), 137.86 (d, J = 19.4 Hz), 134.79, 132.34 (qd, J_1 = 2.8 Hz, J_2 = 32.7 Hz), 131.01, 127.47 (d, J = 5.6 Hz), 125.97 (q, J = 3.4 Hz), 124.03, 123.48 (q, J = 270.8 Hz), 91.00 (d, J = 170.7 Hz), 56.40 (d, J = 35.1 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -56.37 (t, J = 21.8 Hz, 3F), -63.26 (s, 3F), -140.31-(-140.52) (m, 2F), -142.18-(-142.25) (m, 2F), -167.26 (s, 1F). HRMS (ESI-TOF) Calcd for $C_{25}H_{10}F_{11}N_2O_3$ $[M-H]^-$: 595.0521, found: 595.0519.



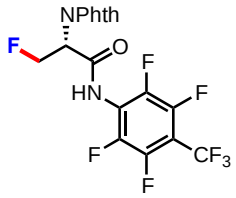
(2*R*,3*S*)-2-(1,3-dioxoisoindolin-2-yl)-3-fluoro-3-(naphthalen-2-yl)-*N*-(2,3,5,6-tetrafluoro-4-(trifluoromethyl)phenyl)propanamide (2l)

Substrate **1l** was fluorinated following the general fluorination procedure. Analysis of crude reaction mixture by ^{1}H NMR showed a > 7:1 diastereomer ratio. After purification by preparative thin-layer chromatography, **2l** was obtained as a major diastereoisomer and as a white solid (30.7 mg, 53%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.37 (br d, J = 11.2 Hz, 1H), 7.89 (s, 1H), 7.84-7.77 (m, 3H), 7.72-7.70 (m, 2H), 7.63-7.61 (m, 2H), 7.55 (d, J = 8.4 Hz, 1H), 7.51-7.45 (m, 2H), 6.76 (dd, J_1 = 10.0 Hz, J_2 = 48.0 Hz, 1H), 5.68 (dd, J_1 = 10.0 Hz, J_2 = 13.2 Hz, 1H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 167.10, 164.01 (d, J = 2.6 Hz), 134.48, 133.99 (d, J = 1.8 Hz), 132.69, 131.14 (d, J = 18.4 Hz), 131.12, 129.19, 128.39, 128.14 (d, J = 7.0 Hz), 127.74, 127.27, 126.71, 123.85, 123.02 (d, J = 4.4 Hz), 92.31 (d, J = 168.3 Hz), 56.24 (d, J = 36.2 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -56.33 (t, J = 21.8 Hz, 3F), -140.44-(-140.72) (m, 2F), -142.11-(-142.20) (m, 2F), -162.59 (s, 1F). HRMS (ESI-TOF) Calcd for $C_{28}H_{13}F_8N_2O_3$ $[M-H]^-$: 557.0804, found: 557.0806.



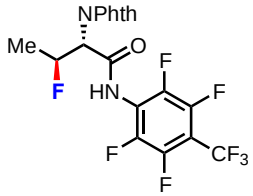
(2*R*,3*S*)-2-(1,3-dioxoisoindolin-2-yl)-3-fluoro-*N*-(2,3,5,6-tetrafluoro-4-(trifluoromethyl)phenyl)-3-(2-(trifluoromethyl)pyridin-4-yl)propanamide (2m)

Substrate **1m** was fluorinated following the general fluorination procedure. Analysis of crude reaction mixture by ^{1}H NMR showed a > 20:1 diastereomer ratio. A 2:1 mixture of **2m** to elimination byproduct was obtained after purification by preparative thin-layer chromatography,[3] **2m** and elimination byproduct were obtained as a colorless oil (25.9 mg, 43%). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.73 (d, J = 4.8 Hz, 1H), 8.15 (br d, J = 7.2 Hz, 1H), 7.83-7.82 (m, 2H), 7.77-7.76 (m, 2H), 7.72 (s, 1H), 7.55 (d, J = 4.8 Hz, 1H), 6.67 (dd, J_1 = 9.0 Hz, J_2 = 47.4 Hz, 1H), 5.47 (dd, J_1 = 9.0 Hz, J_2 = 14.4 Hz, 1H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 167.08, 165.92, 150.78, 149.20 (qd, J_1 = 7.6 Hz, J_2 = 35.0 Hz), 144.96 (d, J = 20.1 Hz), 135.13, 130.81, 124.24, 123.92 (d, J = 6.0 Hz), 120.93 (q, J = 273.0 Hz), 118.05 (qd, J_1 = 3.0 Hz, J_2 = 5.6 Hz), 89.61 (d, J = 174.8 Hz), 56.37 (d, J = 33.4 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -56.38 (t, J = 21.4 Hz, 3F), -68.49 (s, 3F), -140.06-(-140.33) (m, 2F), -142.14-(-142.26) (m, 2F), -175.06 (s, 1F). HRMS (ESI-TOF) Calcd for $C_{24}H_9F_{11}N_3O_3$ $[M-H]^-$: 596.0474, found: 596.0471.



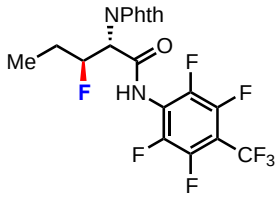
(*R*)-2-(1,3-dioxoisoindolin-2-yl)-3-fluoro-*N*-(2,3,5,6-tetrafluoro-4-(trifluoromethyl)phenyl)propanamide (2n)

Substrate **1n** was fluorinated following this procedure: Substrate **1n** (0.10 mmol, 43.4 mg), Selectfluor (0.125 mmol, 44.3 mg), $Pd(OAc)_2$ (0.01 mmol, 2.3 mg) and **L5** (0.02 mmol, 5.4 mg) were weighed into a tube (10 mL) with a magnetic stir bar under air. 1,4-Dioxane (1.25 mL) was added, and the tube was sealed with a cap. The reaction mixture was stirred at 115 ^{o}C for 15 hours. Upon completion, the reaction mixture was cooled to room temperature and diluted with EtOAc. Then the reaction mixture was filtered through a short celite tube and purified by preparative thin-layer chromatography using toluene/EtOAc mixtures as the eluent. After purification by preparative thin-layer chromatography, **2n** was obtained as a colorless oil (29.4 mg, 65%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03 (br d, J = 3.6 Hz, 1H), 7.94-7.92 (m, 2H), 7.82-7.80 (m, 2H), 5.44-5.23 (m, 2H), 5.05 (ddd, J_1 = 6.8 Hz, J_2 = 9.6 Hz, J_3 = 46.0 Hz, 1H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 167.47, 164.04 (d, J = 4.8 Hz), 134.92, 131.38, 124.12, 80.06 (d, J = 171.8 Hz), 53.08 (d, J = 24.0 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -56.38 (t, J = 21.8 Hz, 3F), -140.29-(-140.55) (m, 2F), -142.36-(-142.45) (m, 2F), -222.21 (s, 1F). HRMS (ESI-TOF) Calcd for $C_{18}H_7F_8N_2O_3$ $[M-H]^-$: 451.0334, found: 451.0336.



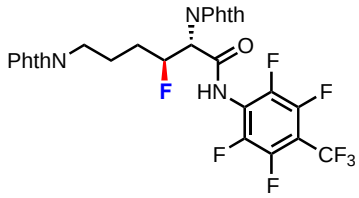
(2*R*,3*S*)-2-(1,3-dioxoisoindolin-2-yl)-3-fluoro-*N*-(2,3,5,6-tetrafluoro-4-(trifluoromethyl)phenyl)butanamide (2o)

Substrate **1o** was fluorinated following the general fluorination procedure. Analysis of crude reaction mixture by ^{1}H NMR showed a > 20:1 diastereomer ratio. After purification by preparative thin-layer chromatography, **2o** was obtained as a white solid (24.7 mg, 53%). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.20 (br d, J = 12.0 Hz, 1H), 7.92-7.91 (m, 2H), 7.80-7.79 (m, 2H), 5.87-5.75 (m, 1H), 5.10 (dd, J_1 = 9.0 Hz, J_2 = 13.8 Hz, 1H), 1.50 (dd, J_1 = 6.0 Hz, J_2 = 25.8 Hz, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 167.46, 164.08 (d, J = 2.0 Hz), 134.76, 131.47, 124.06, 88.87 (d, J = 165.0 Hz), 57.13 (d, J = 30.2 Hz), 18.77 (d, J = 21.9 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -56.36 (t, J = 22.2 Hz, 3F), -140.52-(-140.81) (m, 2F), -142.23-(-142.34) (m, 2F), -172.07 (s, 1F). HRMS (ESI-TOF) Calcd for $C_{19}H_9F_8N_2O_3$ [M-H]$^-$: 465.0491, found: 465.0490.



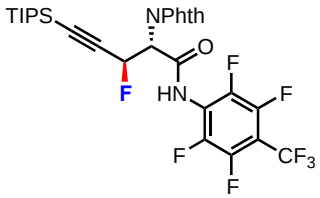
(2*R*,3*S*)-2-(1,3-dioxoisoindolin-2-yl)-3-fluoro-*N*-(2,3,5,6-tetrafluoro-4-(trifluoromethyl)phenyl)pentanamide (2p)

Substrate **1p** was fluorinated following the general fluorination procedure but using 20 mol% **L10** and adding 1.0 equiv of $KHCO_3$. Analysis of crude reaction mixture by ^{1}H NMR showed a > 20:1 diastereomer ratio. After purification by preparative thin-layer chromatography, **2p** was obtained as a white solid (14.4 mg, 30%). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.24 (br d, J = 12.6 Hz, 1H), 7.92-7.91 (m, 2H), 7.80-7.79 (m, 2H), 5.64 (dt, J_1 = 8.4 Hz, J_2 = 49.2 Hz, 1H), 5.16 (dd, J_1 = 10.2 Hz, J_2 = 13.2 Hz, 1H), 1.89-1.66 (m, 2H), 1.08 (t, J = 7.8 Hz, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 167.49, 164.34 (d, J = 2.0 Hz), 134.74, 131.50, 124.04, 92.56 (d, J = 167.4 Hz), 55.57 (d, J = 30.4 Hz), 25.48 (d, J = 20.8 Hz), 8.06 (d, J = 4.4 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -56.36 (t, J = 21.8 Hz, 3F), -140.57-(-140.82) (m, 2F), -142.24-(-142.34) (m, 2F), -183.02 (s, 1F). HRMS (ESI-TOF) Calcd for $C_{20}H_{11}F_8N_2O_3$ [M-H]$^-$: 479.0647, found: 479.0644.



(2*R*,3*S*)-2,6-bis(1,3-dioxoisoindolin-2-yl)-3-fluoro-*N*-(2,3,5,6-tetrafluoro-4-(trifluoromethyl)phenyl)hexanamide (2q)

Substrate **1q** was fluorinated following the general fluorination procedure but using 20 mol% **L10** and adding 1.0 equiv of $KHCO_3$. Analysis of crude reaction mixture by ^{1}H NMR showed a > 20:1 diastereomer ratio. After purification by preparative thin-layer chromatography, **2q** was obtained as a white solid (16.0 mg, 25%). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.27 (br d, *J* = 11.4 Hz, 1H), 7.89-7.88 (m, 2H), 7.80-7.77 (m, 4H), 7.71-7.69 (m, 2H), 5.76-5.64 (m, 1H), 5.15 (dd, J_1 = 9.0 Hz, J_2 = 13.2 Hz, 1H), 3.70 (t, *J* = 7.2 Hz, 2H), 2.01-1.76 (m, 4H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 168.22, 167.46, 164.01, 134.73, 134.00, 131.90, 131.45, 124.07, 123.25, 91.07 (d, *J* = 168.6 Hz), 55.89 (d, *J* = 29.7 Hz), 37.12, 29.59 (d, *J* = 20.6 Hz), 23.28 (d, *J* = 3.2 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -56.36 (t, *J* = 21.8 Hz, 3F), -140.57-(-140.81) (m, 2F), -142.15-(-142.22) (m, 2F), -181.85 (s, 1F). HRMS (ESI-TOF) Calcd for $C_{29}H_{16}F_8N_3O_5$ [M-H]$^-$: 638.0968, found: 638.0967.



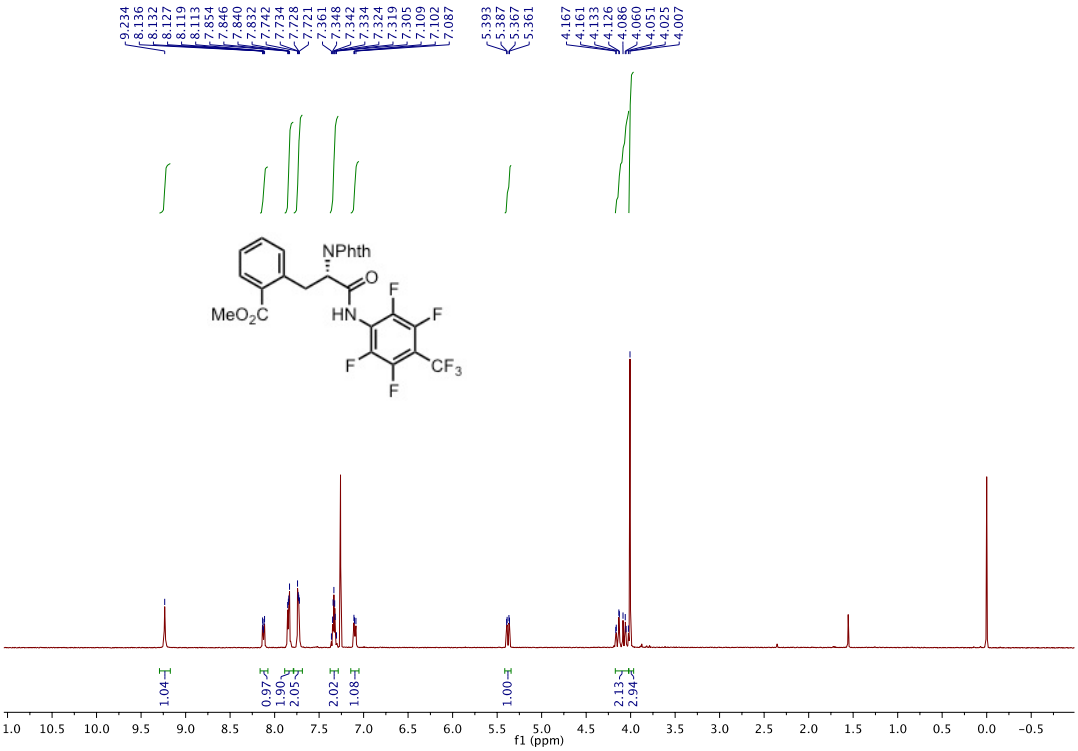
(2*R*,3*S*)-2-(1,3-dioxoisoindolin-2-yl)-3-fluoro-*N*-(2,3,5,6-tetrafluoro-4-(trifluoromethyl)phenyl)-5-(triisopropylsilyl)pent-4-ynamide (2r)

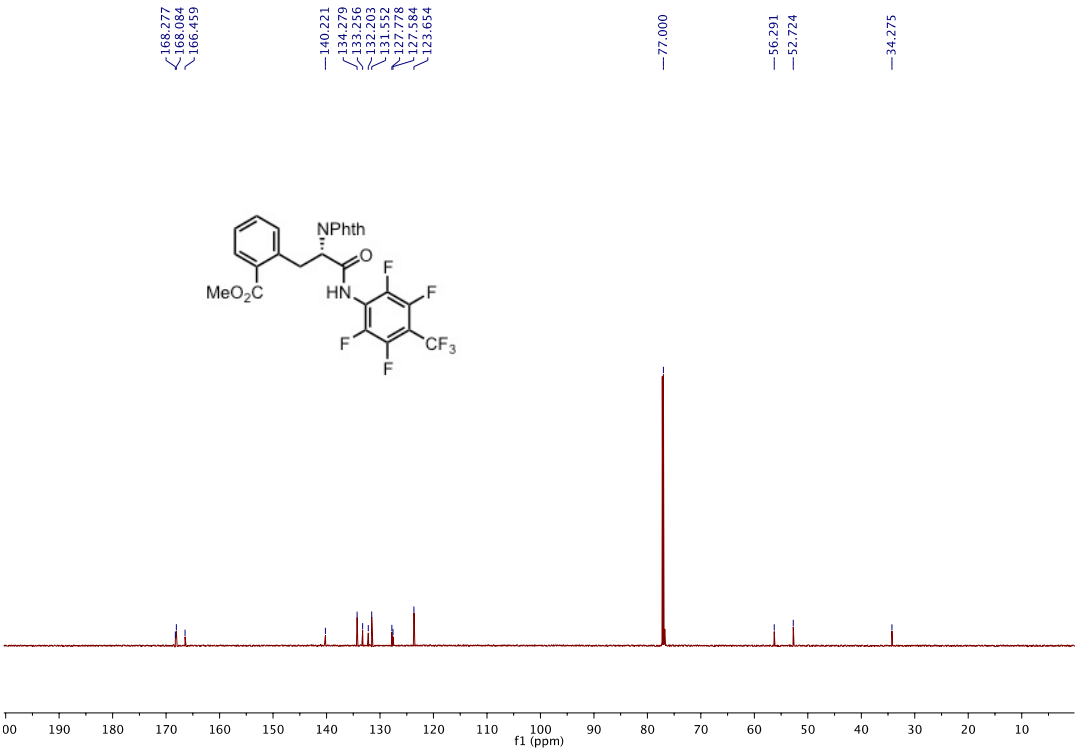
Substrate **1r** was fluorinated following this procedure: Substrate **1r** (0.10 mmol, 61.6 mg), Selectfluor (0.125 mmol, 44.3 mg), $Pd(OAc)_2$ (0.01 mmol, 2.3 mg) and **L5** (0.02 mmol, 5.4 mg) were weighed into a tube (10 mL) with a magnetic stir bar under air. 1,4-Dioxane (1.25 mL) was added, and the tube was sealed with a cap. The reaction mixture was stirred at 115 ^{o}C for 15 hours. Upon completion, the reaction mixture was cooled to room temperature and diluted with EtOAc. Then the reaction mixture was filtered through a short celite tube and purified by preparative thin-layer chromatography using toluene/EtOAc mixtures as the eluent. Analysis of crude reaction mixture by ^{1}H NMR showed a > 20:1 diastereomer ratio. After purification by preparative thin-layer chromatography, **2r** was obtained as a colorless oil (31.7 mg, 50%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00 (br d, *J* = 8.4 Hz, 1H), 7.91-7.89 (m, 2H), 7.80-7.76 (m, 2H), 6.30 (dd, J_1 = 9.2 Hz, J_2 = 49.6 Hz, 1H), 5.31 (dd, J_1 = 9.6 Hz, J_2 = 13.2 Hz, 1H), 0.86 (s, 21H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 166.88, 162.90 (d, *J* = 2.6 Hz), 134.69, 131.57, 123.98, 97.53 (d, *J* = 22.5 Hz), 95.37 (d, *J* = 8.8 Hz), 80.43 (d, *J* = 170.0 Hz), 55.70 (d, *J* = 32.2 Hz), 18.15, 10.71. ^{19}F NMR (376 MHz, $CDCl_3$) δ -56.38 (t, *J* = 21.4 Hz, 3F), -140.39-(-140.59) (m, 2F), -142.18-(-142.28) (m, 2F), -170.11 (s, 1F). HRMS (ESI-TOF) Calcd for $C_{29}H_{27}F_8N_2O_3Si$ [M-H]$^-$: 631.0742, found: 631.0745.

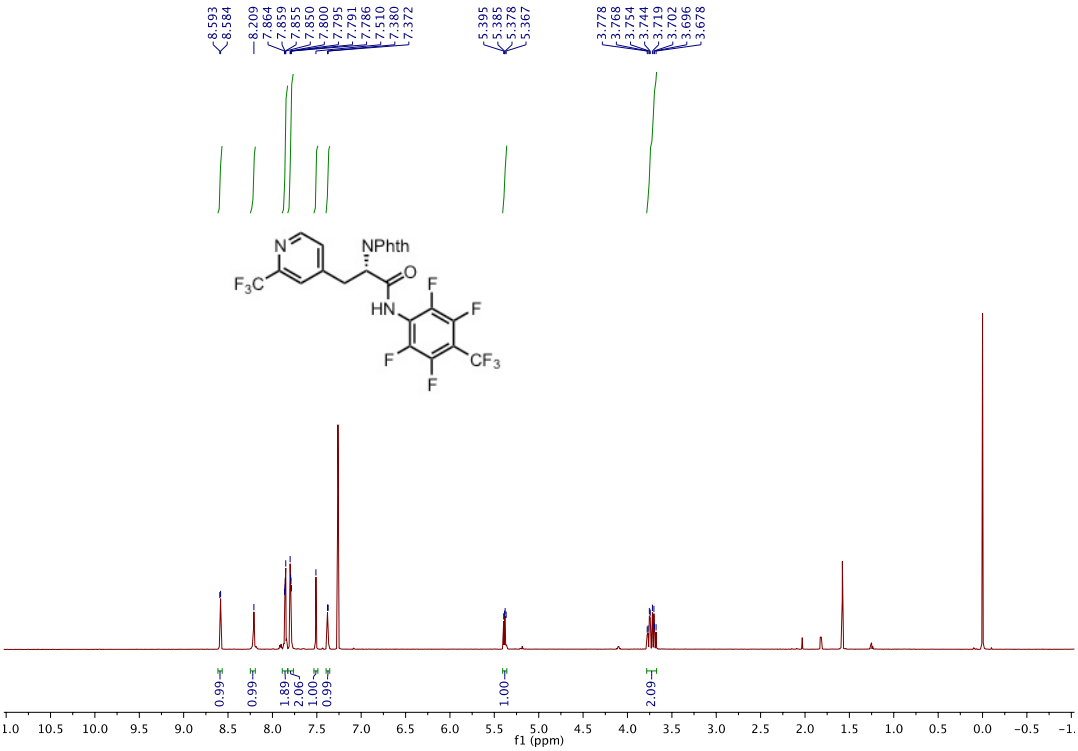
References

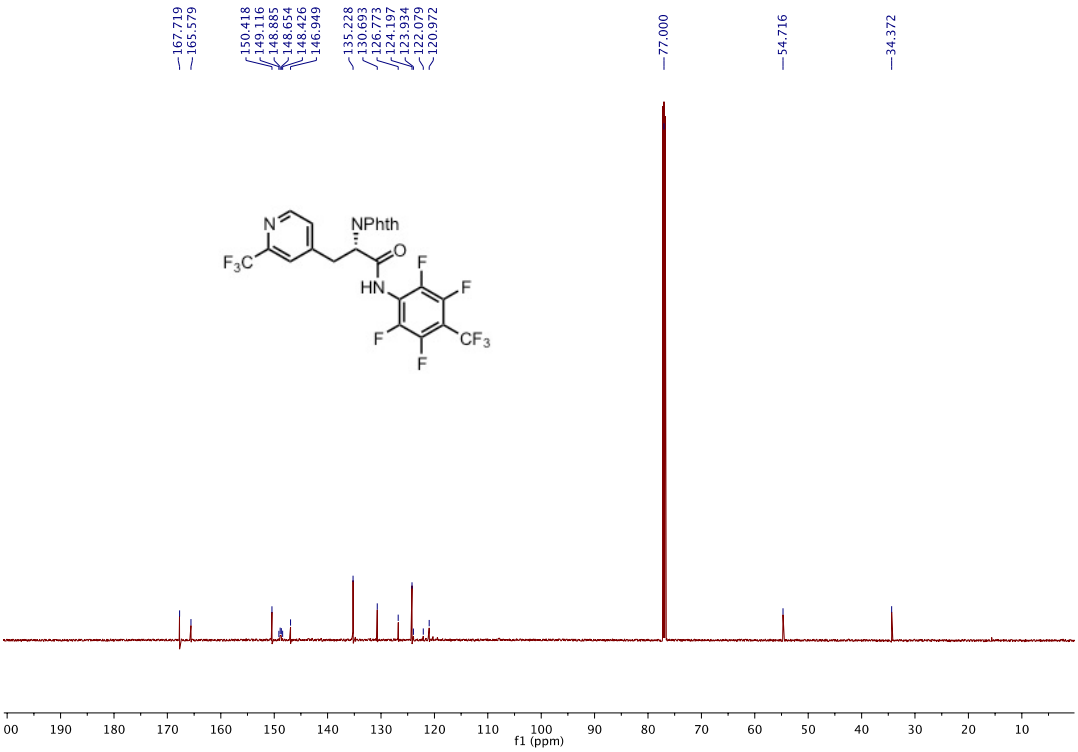
(1) He, J.; Li, S.-H.; Deng, Y.-Q.; Fu, H.-Y.; Laforteza, B. N.; Spangler, J. E.; Homs, A.; Yu, J.-Q. *Science* **2014**, *343*, 1216.
(2) Li, S.-H.; Chen, G.; Feng, C.-G.; Gong, W.; Yu, J.-Q. *J. Am. Chem. Soc.* **2014**, *136*, 5267.
(3) Xia, J.-B.; Zhu, C.; Chen, C. *J. Am. Chem. Soc.* **2013**, *135*, 9342.

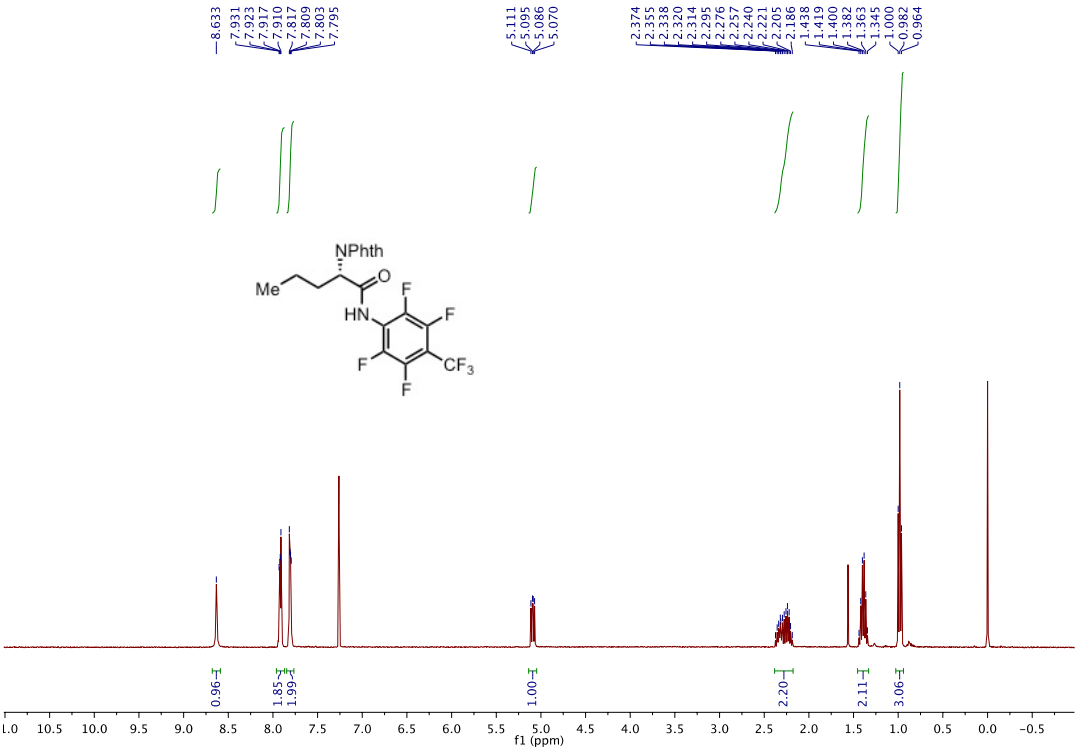
^{1}H and ^{13}C NMR Spectra

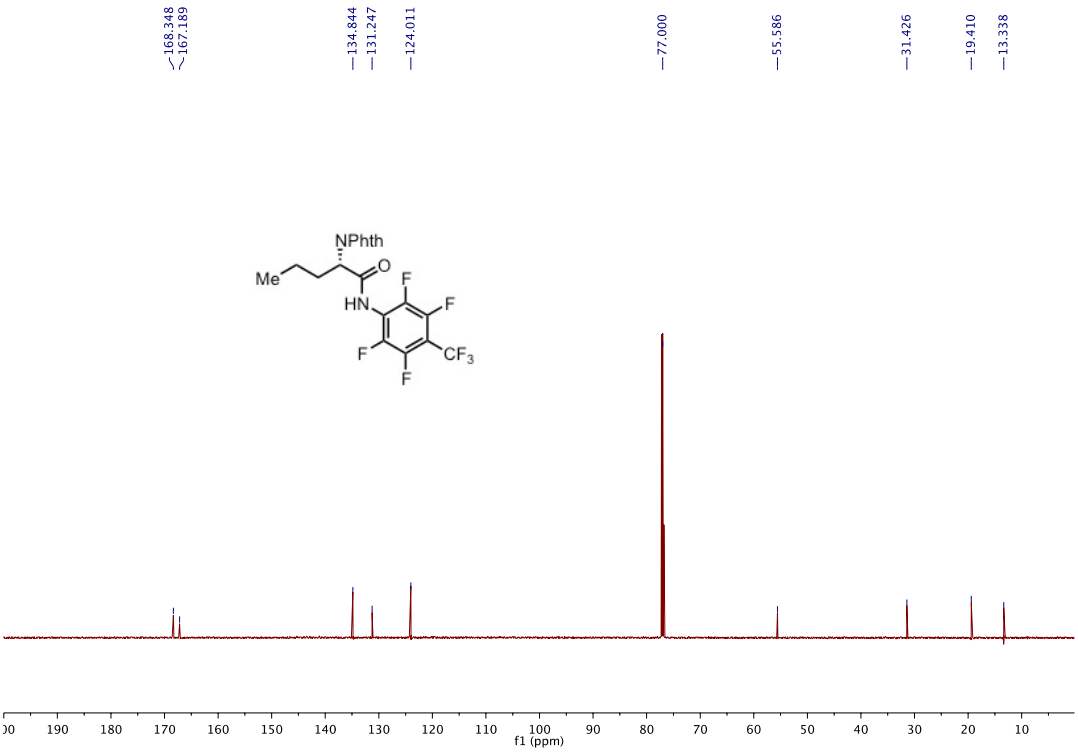

9.234
8.136
8.132
8.127
8.119
8.113
7.854
7.846
7.840
7.832
7.742
7.734
7.728
7.721
7.361
7.348
7.342
7.334
7.324
7.319
7.305
7.109
7.102
7.087
5.393
5.387
5.367
5.361
4.167
4.161
4.133
4.126
4.086
4.060
4.051
4.025
4.007
NPhth
O
HN
MeO2C
F
F
F
F
CF3
1.04
0.97
1.90
2.05
2.02
1.08
1.00
2.13
2.94
f1 (ppm)

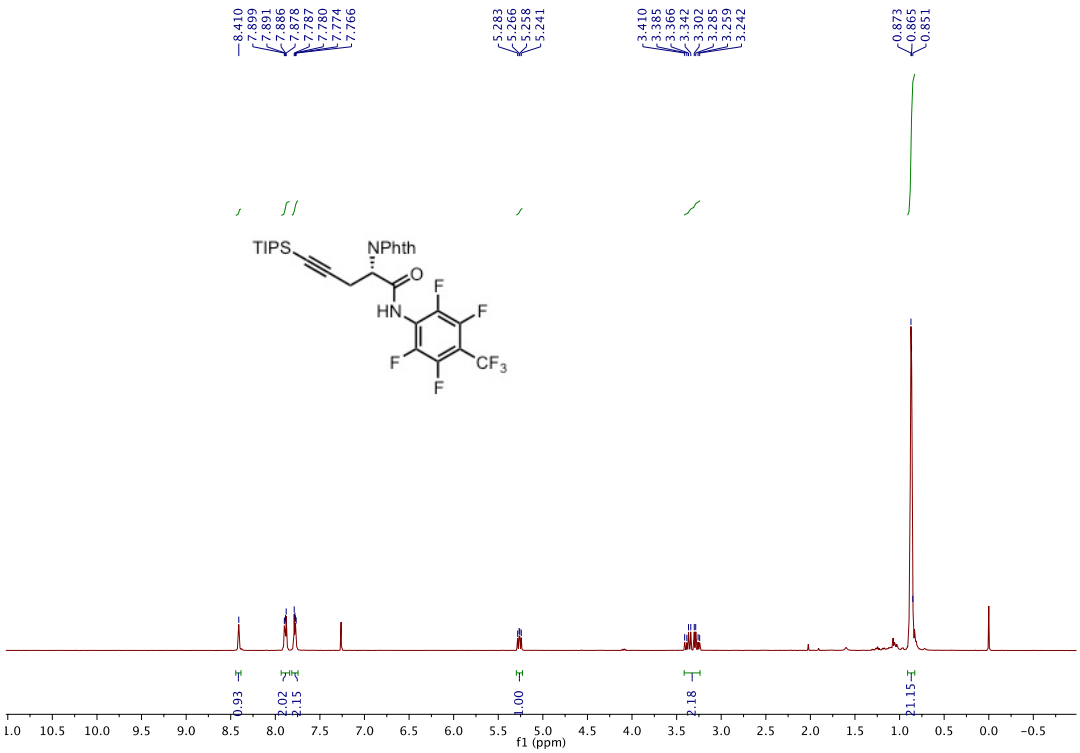

168.277
168.084
166.459
140.221
134.279
133.256
132.203
131.552
127.778
127.584
123.654
77.000
56.291
52.724
34.275
NPhth
O
HN
MeO2C
F
F
F
F
CF3
f1 (ppm)

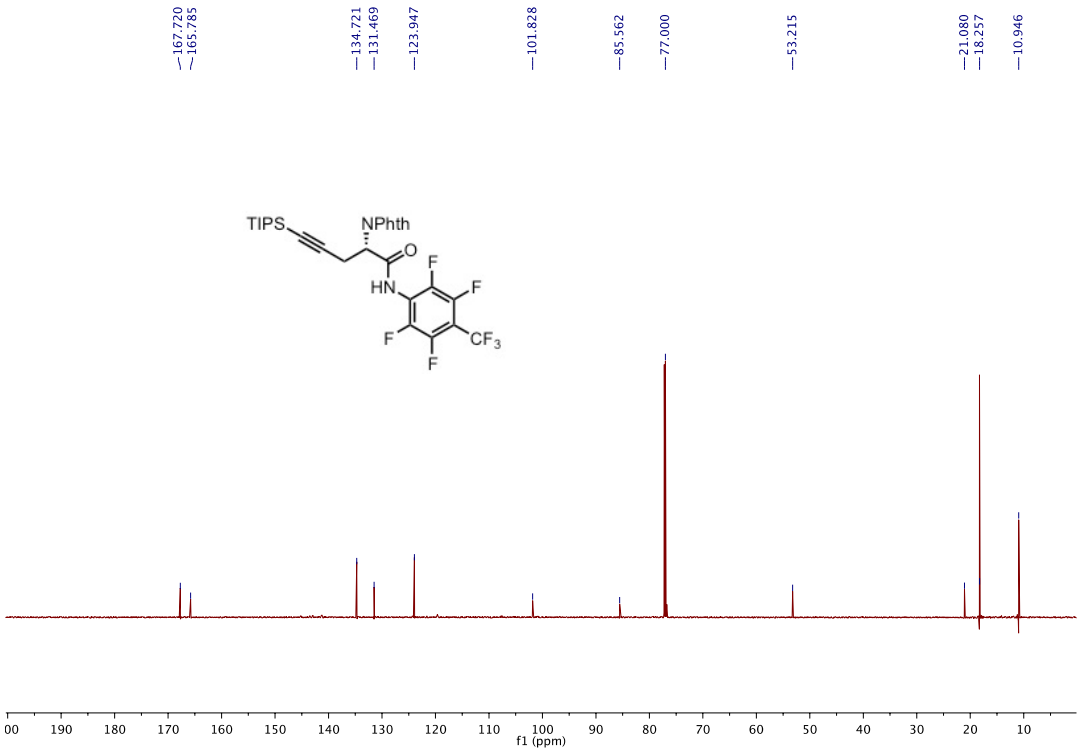

8.593
8.584
8.209
7.864
7.859
7.855
7.850
7.800
7.795
7.791
7.786
7.510
7.380
7.372
5.395
5.385
5.378
5.367
3.778
3.768
3.754
3.744
3.719
3.702
3.696
3.678
NPhth
O
HN
F
F
F
F
F
F3C
CF3
0.99
0.99
1.89
2.06
1.00
0.99
1.00
2.09
f1 (ppm)

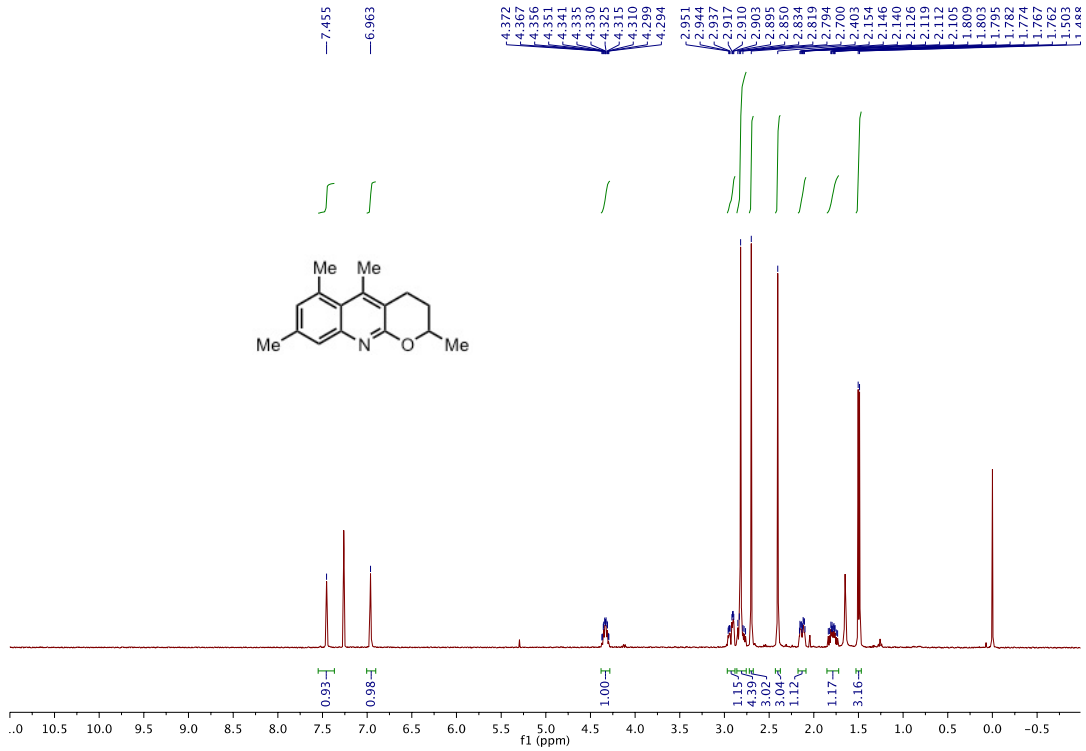

167.719
165.579
150.418
149.116
148.885
148.654
148.426
146.949
135.228
130.693
126.773
124.197
123.934
122.079
120.972
77.000
54.716
34.372
NPhth
O
HN
F
F
F
F
F
F3C
CF3
f1 (ppm)

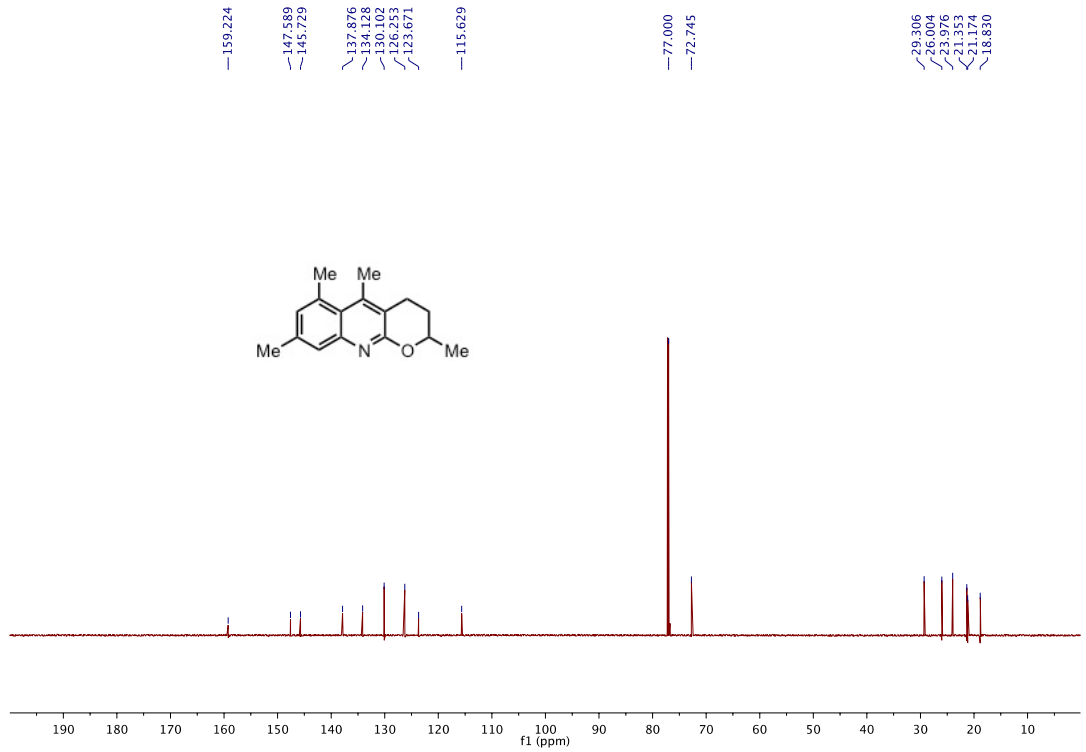

8.633
7.931
7.923
7.917
7.910
7.817
7.809
7.803
7.795
5.111
5.095
5.086
5.070
2.374
2.355
2.338
2.320
2.314
2.295
2.276
2.257
2.240
2.221
2.205
2.186
1.438
1.419
1.400
1.382
1.363
1.345
1.000
0.982
0.964
NPhth
Me
O
HN
F
F
F
F
CF3
0.96
1.85
1.99
1.00
2.20
2.11
3.06
f1 (ppm)

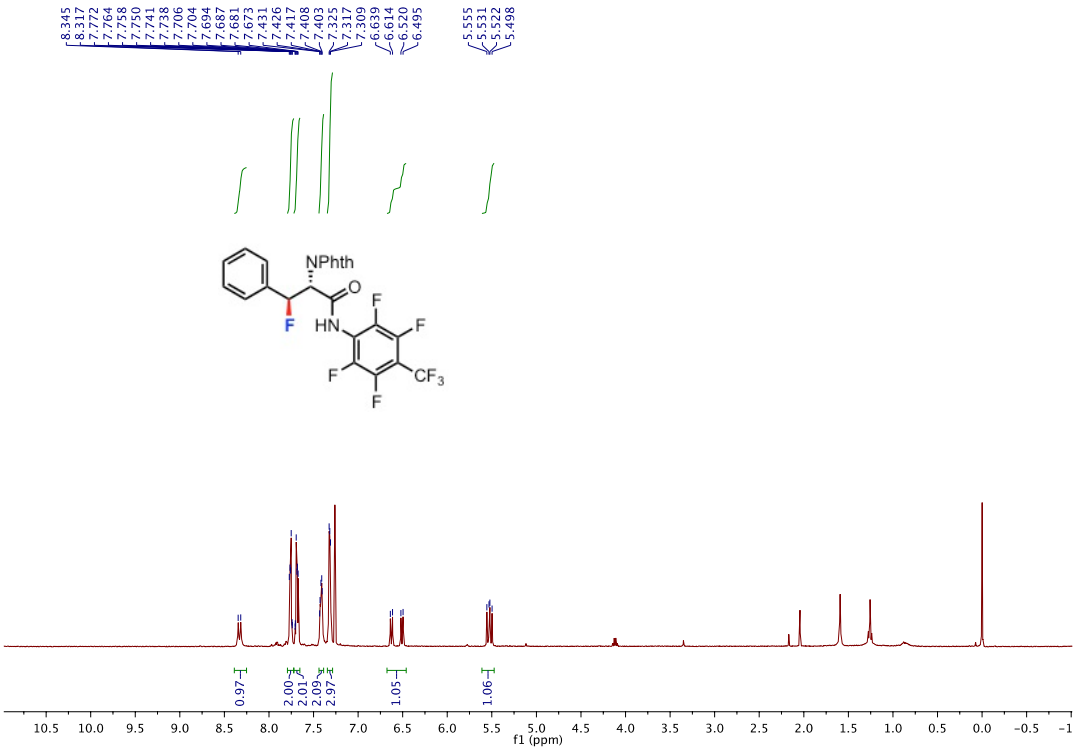

168.348
167.189
134.844
131.247
124.011
77.000
55.586
31.426
19.410
13.338
NPhth
Me
O
HN
F
F
F
F
CF3
f1 (ppm)

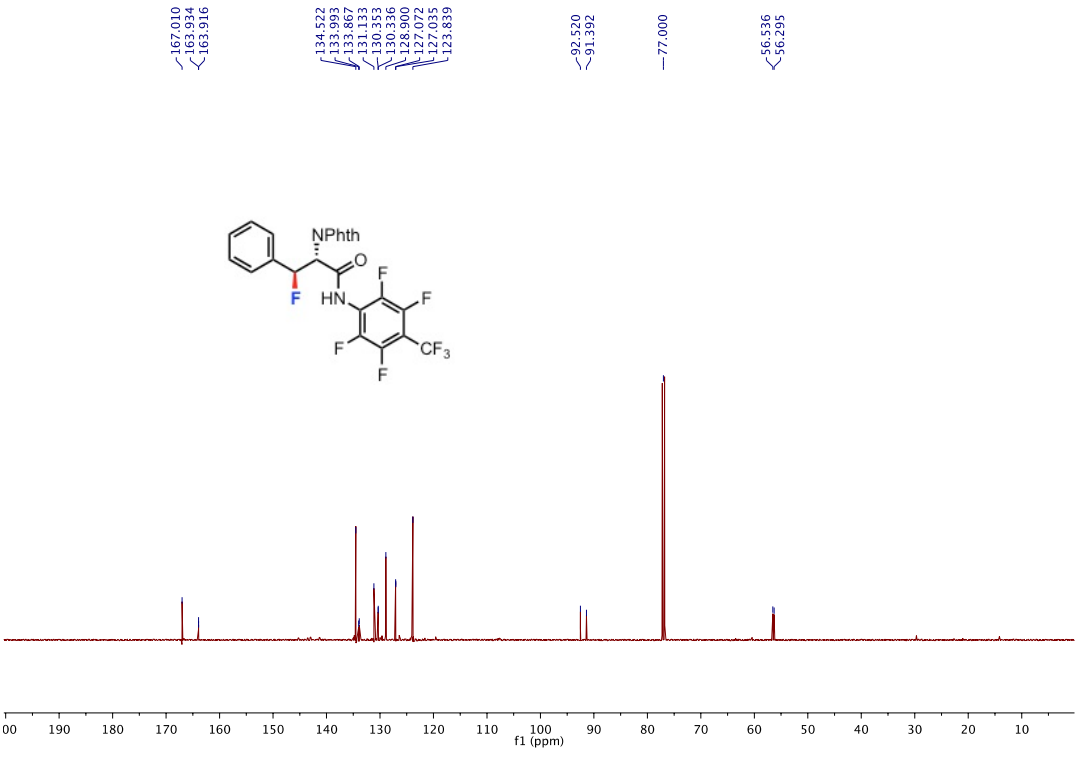

8.410
7.899
7.891
7.886
7.878
7.787
7.780
7.774
7.766
5.283
5.266
5.258
5.241
3.410
3.385
3.366
3.342
3.302
3.285
3.259
3.242
0.873
0.865
0.851
TIPS
NPhth
O
HN
F
F
F
F
F
CF3
0.93
2.02
2.15
1.00
2.18
21.15
f1 (ppm)

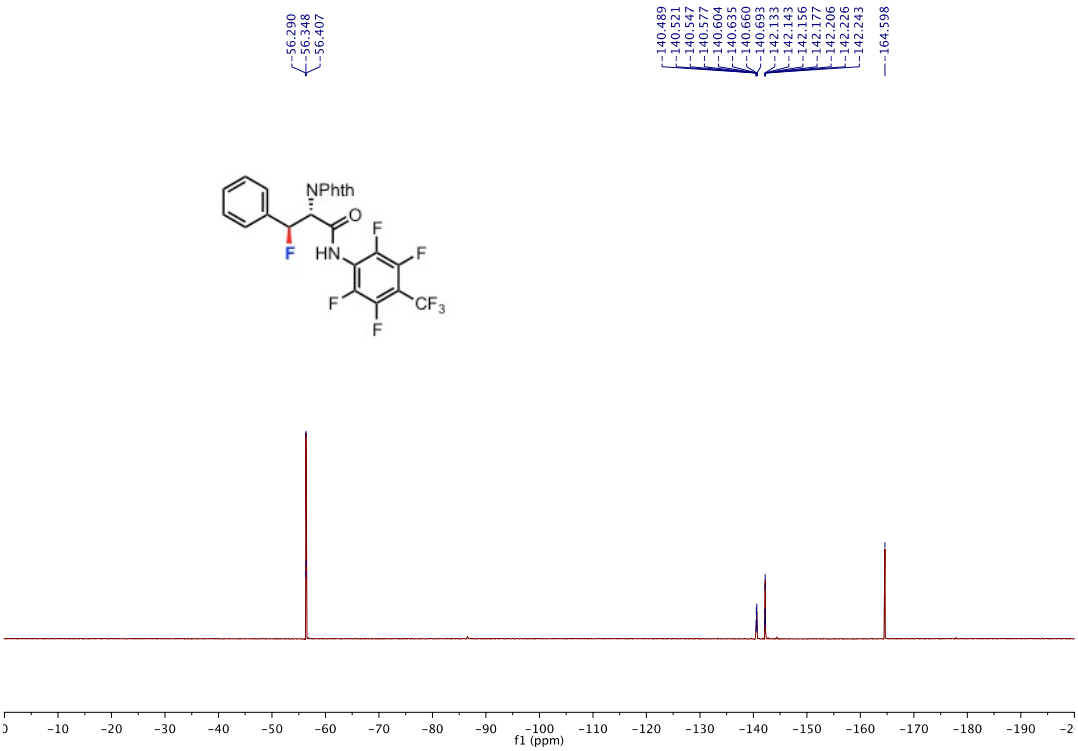

167.720
165.785
134.721
131.469
123.947
101.828
85.562
77.000
53.215
21.080
18.257
10.946
TIPS
NPhth
O
HN
F
F
F
F
F
CF3
f1 (ppm)

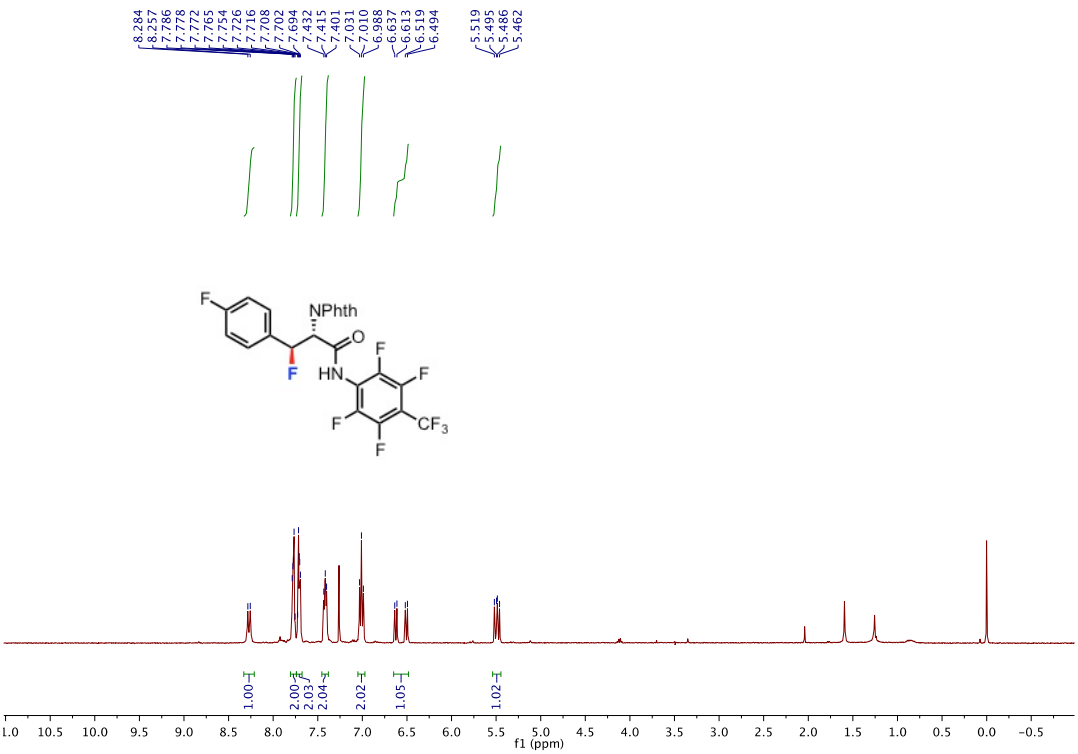

7.455
6.963
4.372
4.367
4.356
4.351
4.341
4.335
4.330
4.325
4.315
4.310
4.299
4.294
2.951
2.944
2.937
2.917
2.910
2.903
2.895
2.850
2.834
2.819
2.794
2.700
2.403
2.154
2.146
2.140
2.126
2.119
2.112
2.105
1.809
1.803
1.795
1.782
1.774
1.767
1.762
1.503
1.488
Me
Me
Me
Me
N
O
0.93
0.98
1.00
1.15
4.39
3.02
3.04
1.12
1.17
3.16
f1 (ppm)

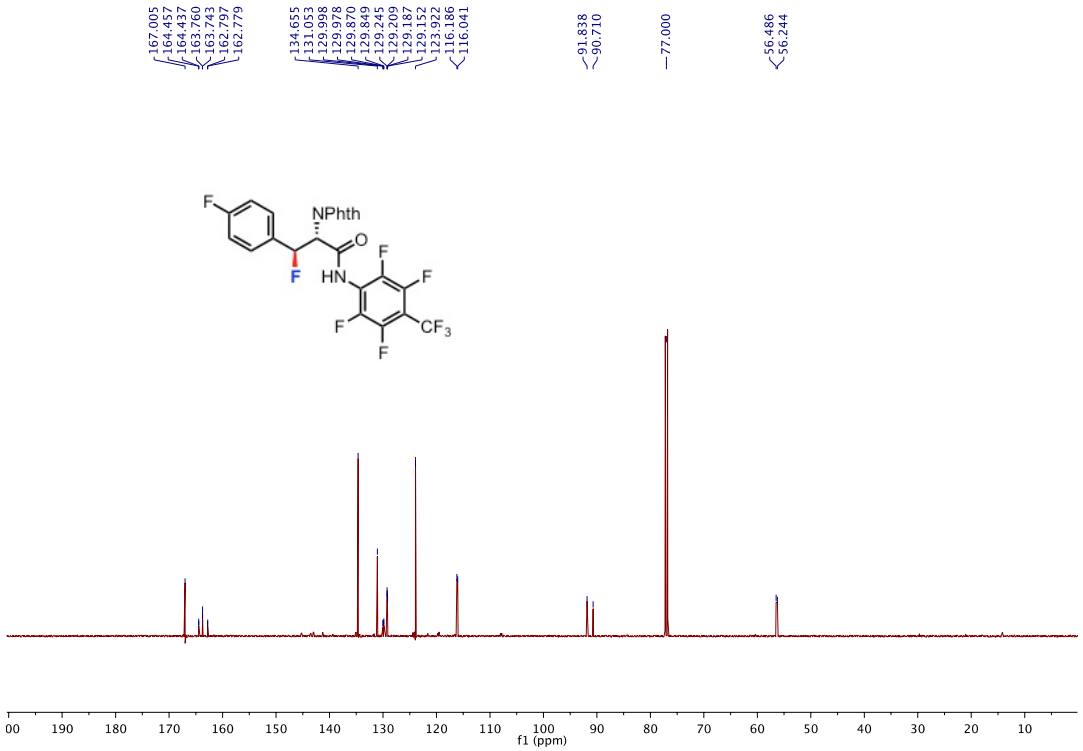

159.224
147.589
145.729
137.876
134.128
130.102
126.253
123.671
115.629
77.000
72.745
29.306
26.004
23.976
21.353
21.174
18.830
Me
Me
Me
Me
N
O
f1 (ppm)

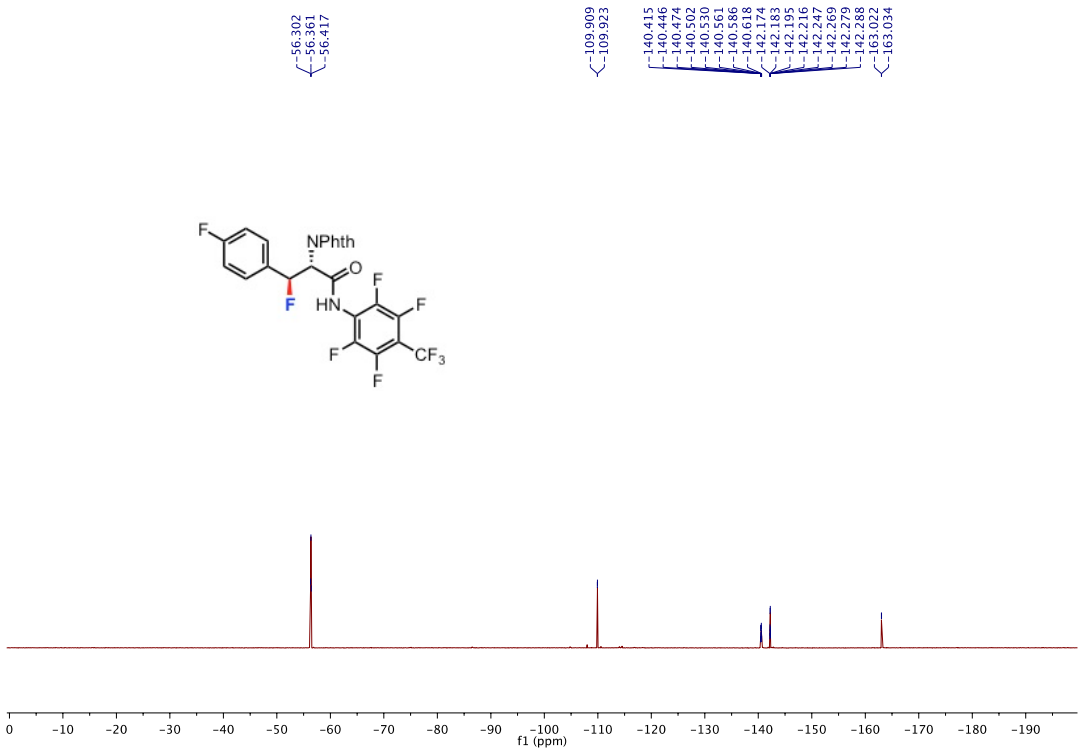

8.345
8.317
7.772
7.764
7.758
7.750
7.741
7.738
7.706
7.704
7.694
7.687
7.681
7.673
7.431
7.426
7.417
7.408
7.403
7.325
7.317
7.309
6.639
6.614
6.520
6.495
5.555
5.531
5.522
5.498
NPhth
O
F
HN
F
F
F
CF3
F
0.97
2.00
2.01
2.09
2.97
1.05
1.06
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 −0.5 −1
f1 (ppm)

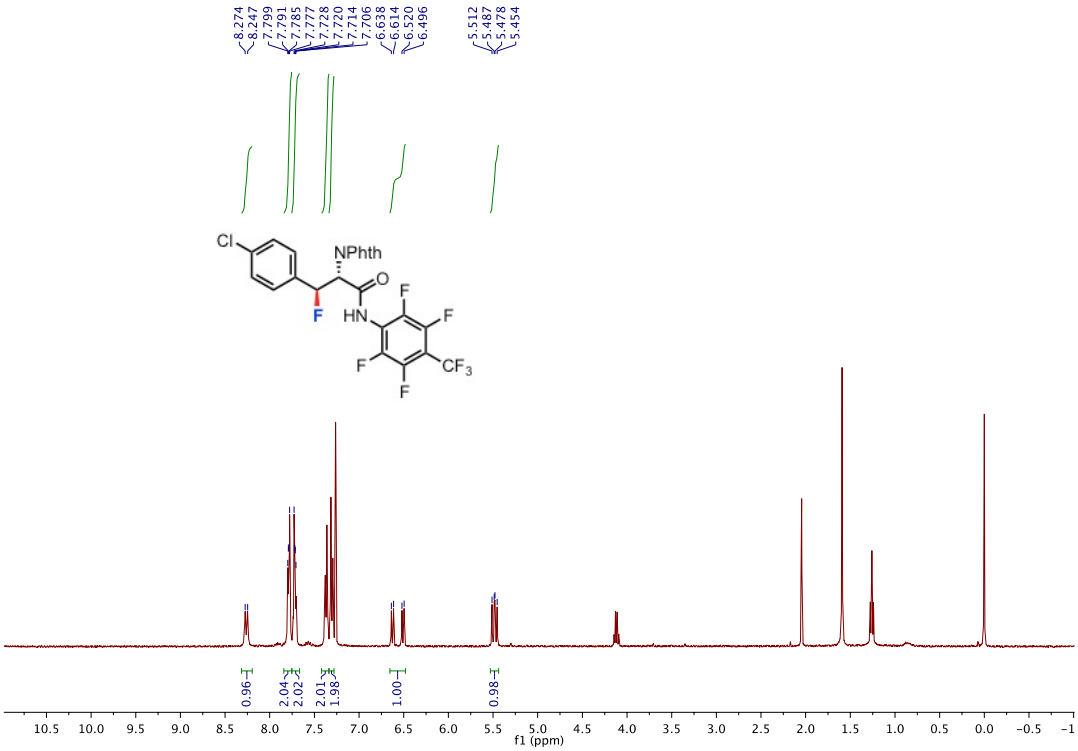

167.010
163.934
163.916
134.522
133.993
133.867
131.133
130.333
130.336
128.900
127.072
127.035
123.839
92.520
91.392
77.000
56.536
56.295
NPhth
O
F
HN
F
F
F
CF3
F
00 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)

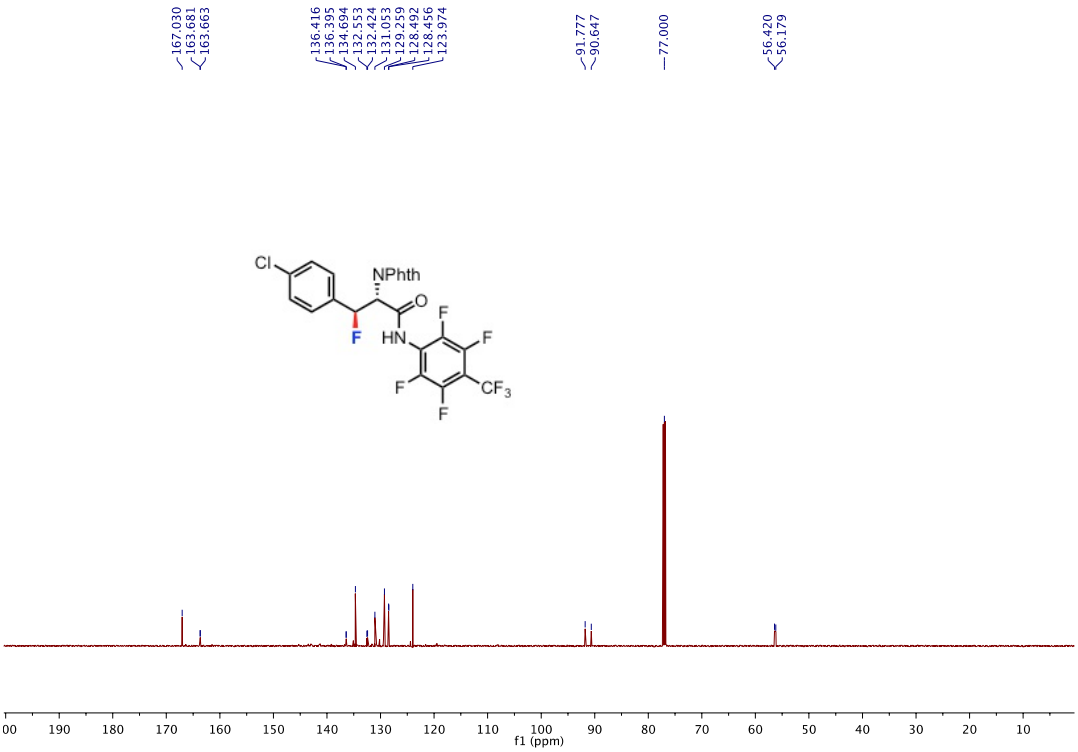

-56.290
-56.348
-56.407
-140.489
-140.521
-140.547
-140.577
-140.604
-140.635
-140.660
-140.693
-142.133
-142.143
-142.156
-142.177
-142.206
-142.226
-142.243
-164.598
NPhth
O
HN
F
F
F
F
F
F
CF3
f1 (ppm)

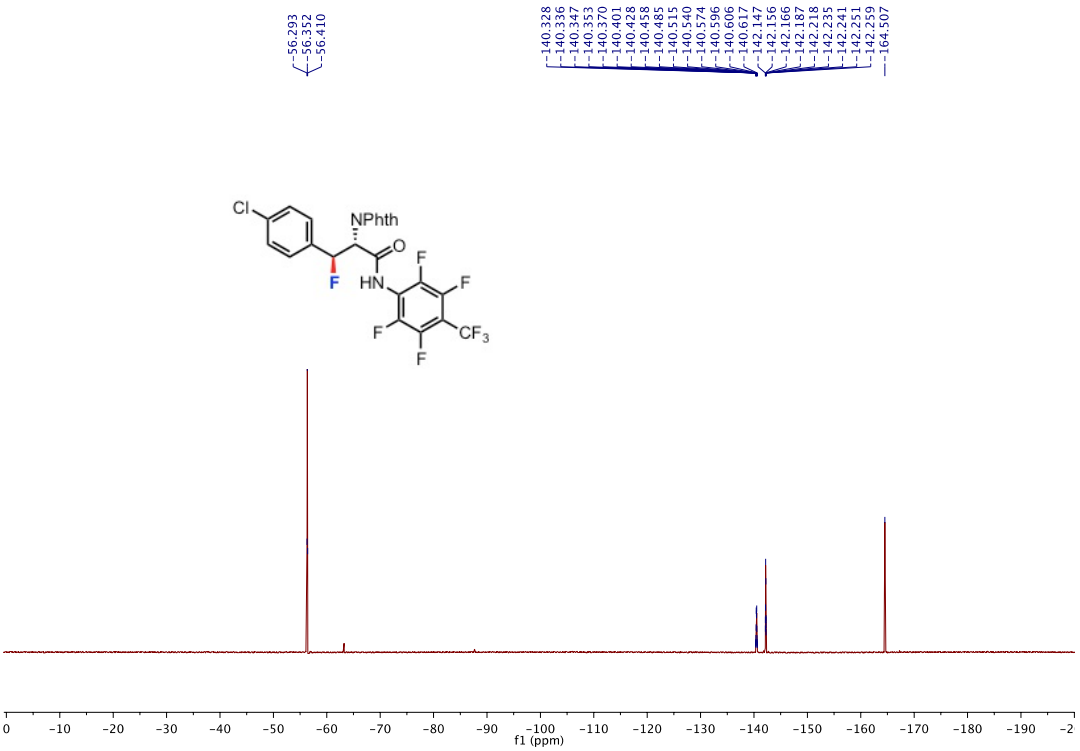

8.284
8.257
7.786
7.778
7.772
7.765
7.734
7.726
7.716
7.708
7.702
7.694
7.432
7.415
7.401
7.031
7.010
6.988
6.637
6.613
6.519
6.494
5.519
5.495
5.486
5.462
F
NPhth
O
HN
F
F
F
F
F
F
CF3
1.00
2.00
2.03
2.04
2.02
1.05
1.02
f1 (ppm)

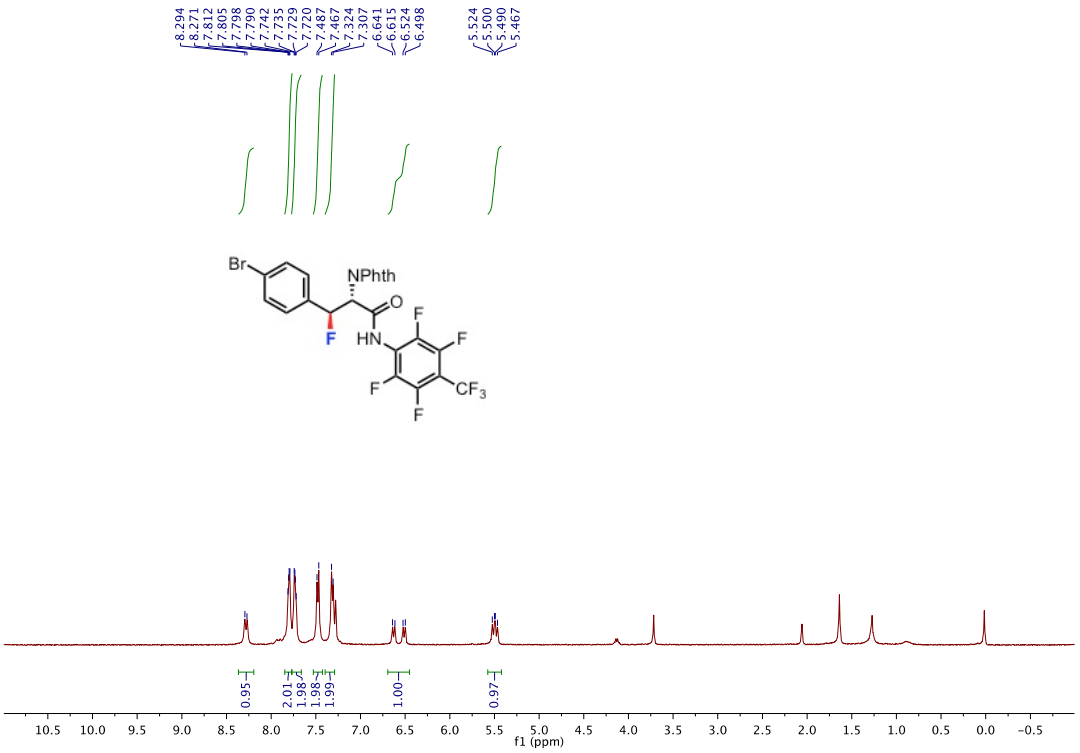

167.005
164.457
164.437
163.760
163.743
162.797
162.779
134.655
131.053
129.998
129.978
129.870
129.849
129.245
129.209
129.187
129.152
123.922
116.186
116.041
91.838
90.710
77.000
56.486
56.244
NPhth
HN
CF3
f1 (ppm)

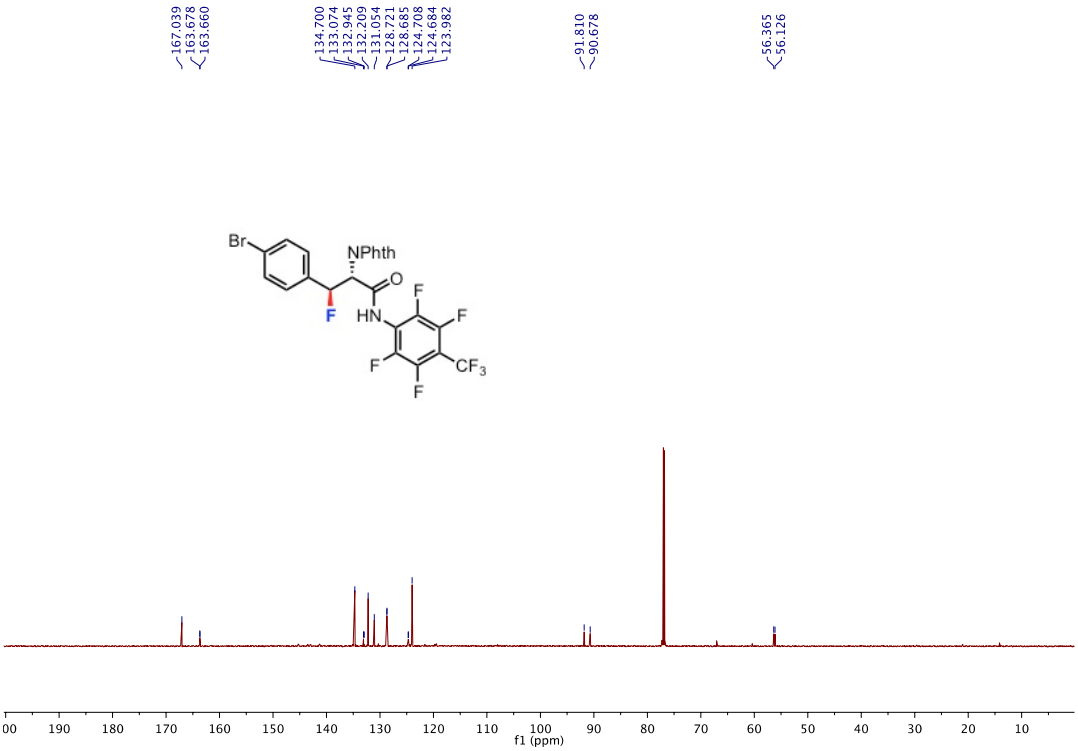

56.302
56.361
56.417
109.909
109.923
140.415
140.446
140.474
140.502
140.530
140.561
140.586
140.618
142.174
142.183
142.195
142.216
142.247
142.269
142.279
142.288
163.022
163.034
NPhth
HN
CF3
f1 (ppm)

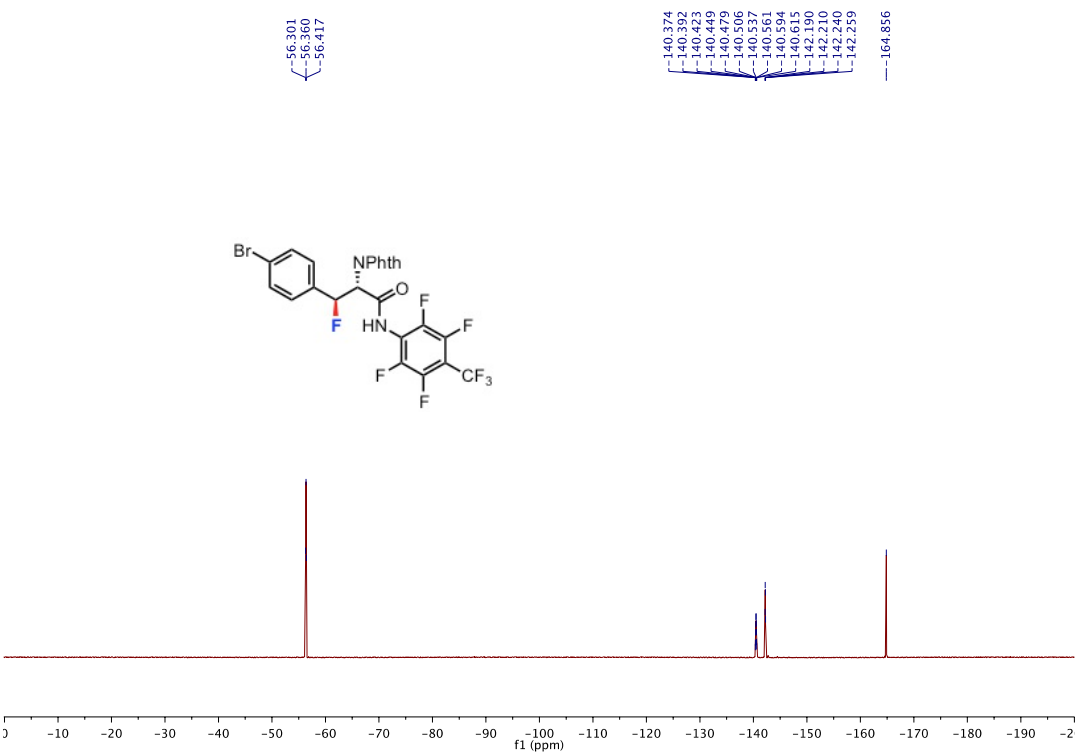

8.274
8.247
7.799
7.791
7.785
7.777
7.728
7.720
7.714
7.706
6.638
6.614
6.520
6.496
5.512
5.487
5.478
5.454
Cl
NPhth
O
F
HN
F
F
F
CF3
F
0.96
2.04
2.02
2.01
1.98
1.00
0.98
f1 (ppm)

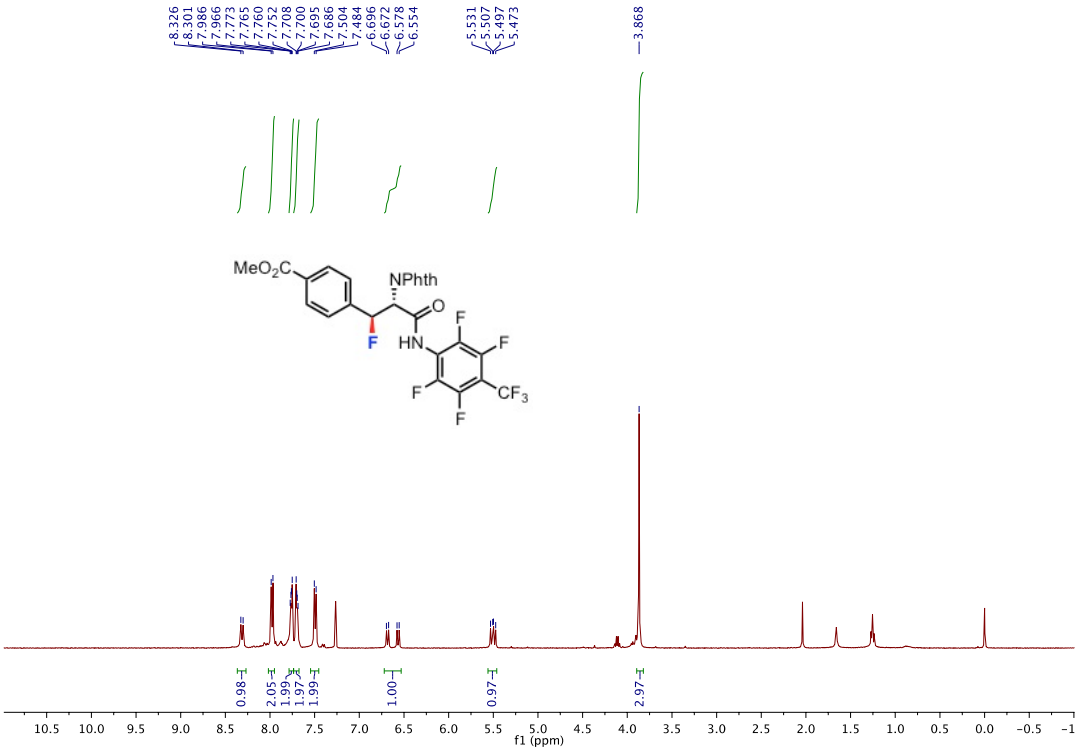

167.030
163.681
163.663
136.416
136.395
134.694
132.553
132.424
131.053
129.259
128.492
128.456
123.974
91.777
90.647
77.000
56.420
56.179
Cl
NPhth
O
F
HN
F
F
F
CF3
F
f1 (ppm)

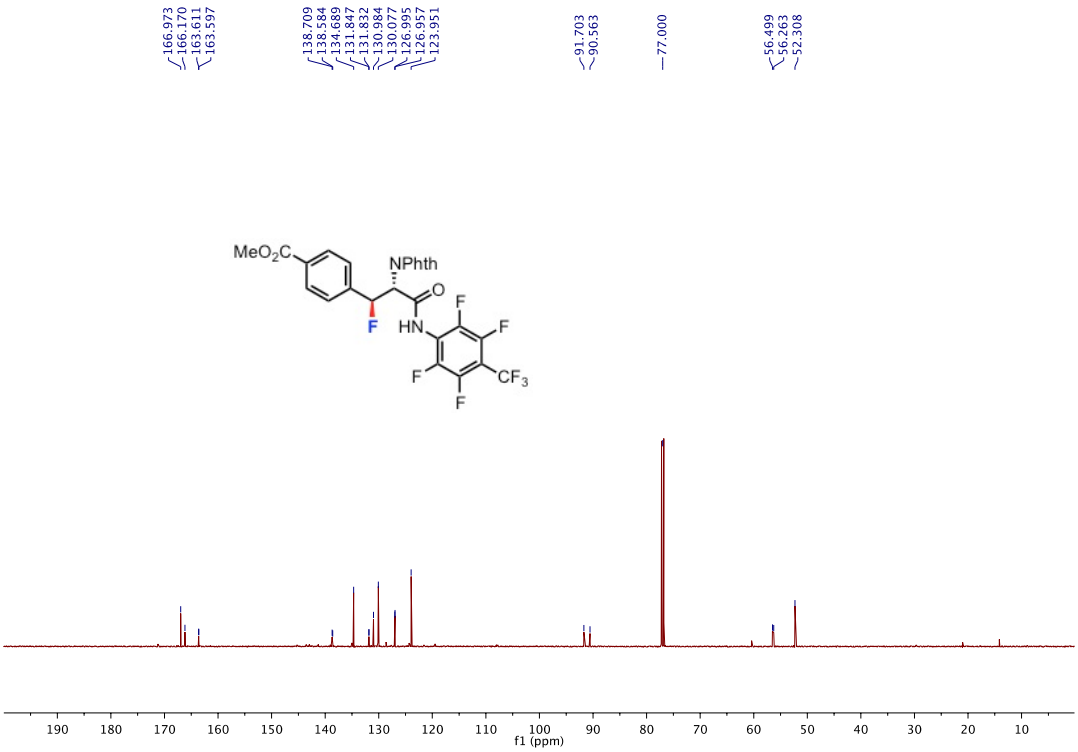

-56.293
-56.352
-56.410
140.328
140.336
140.347
140.353
140.370
140.401
140.428
140.458
140.485
140.515
140.540
140.574
140.596
140.606
140.617
142.147
142.156
142.166
142.187
142.218
142.235
142.241
142.251
142.259
164.507
Cl
NPhth
O
F
HN
F
F
F
CF3
F
f1 (ppm)

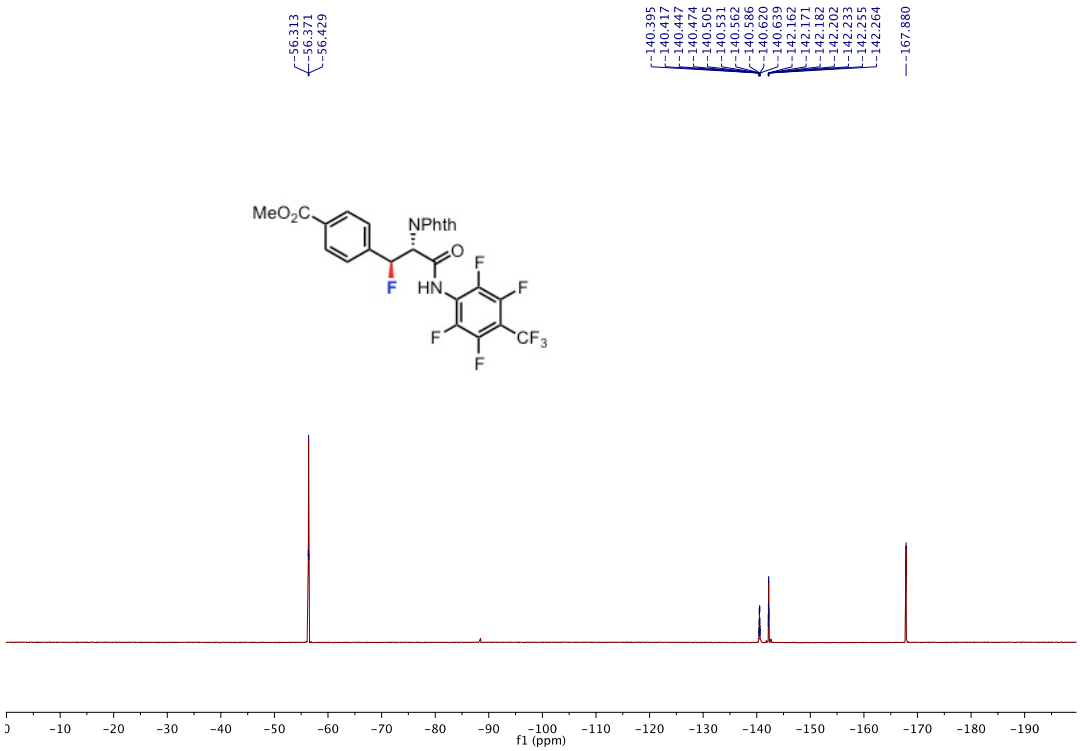

8.294
8.271
7.812
7.805
7.798
7.790
7.742
7.735
7.729
7.720
7.487
7.467
7.324
7.307
6.641
6.615
6.524
6.498
5.524
5.500
5.490
5.467
Br
NPhth
O
F
HN
F
F
F
CF3
F
0.95
2.01
1.98
1.98
1.99
1.00
0.97
f1 (ppm)

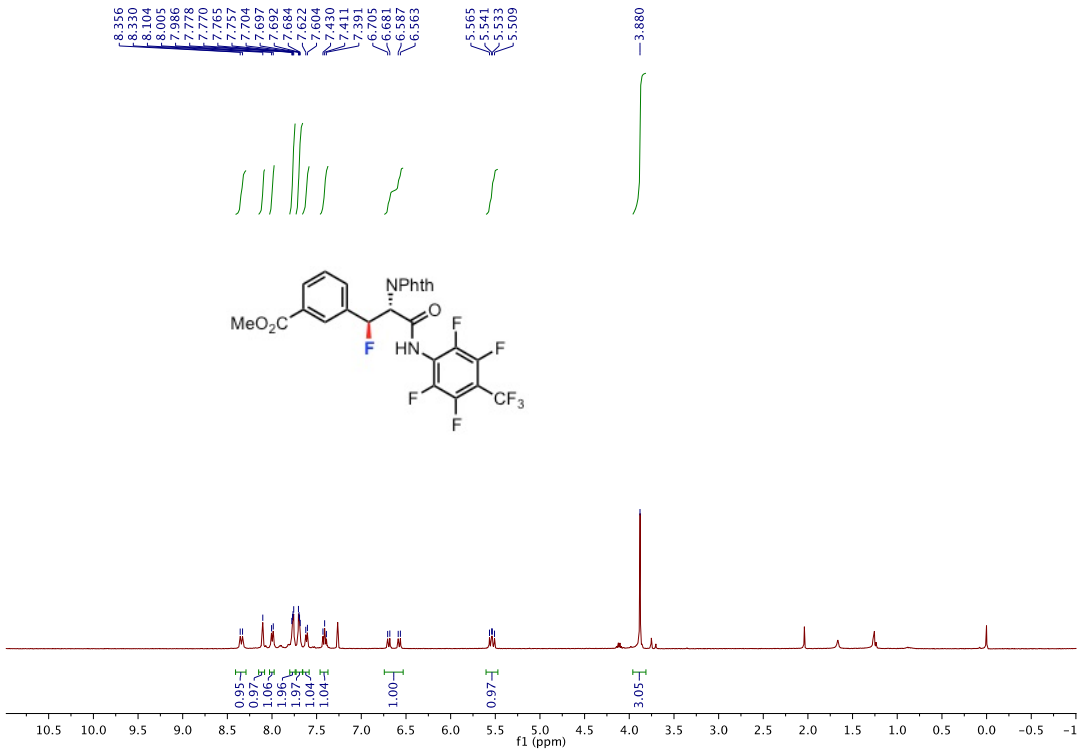

167.039
163.678
163.660
134.700
133.074
132.945
132.209
131.054
128.721
128.685
124.708
124.684
123.982
91.810
90.678
56.365
56.126
Br
NPhth
O
F
HN
F
F
F
CF3
F
f1 (ppm)

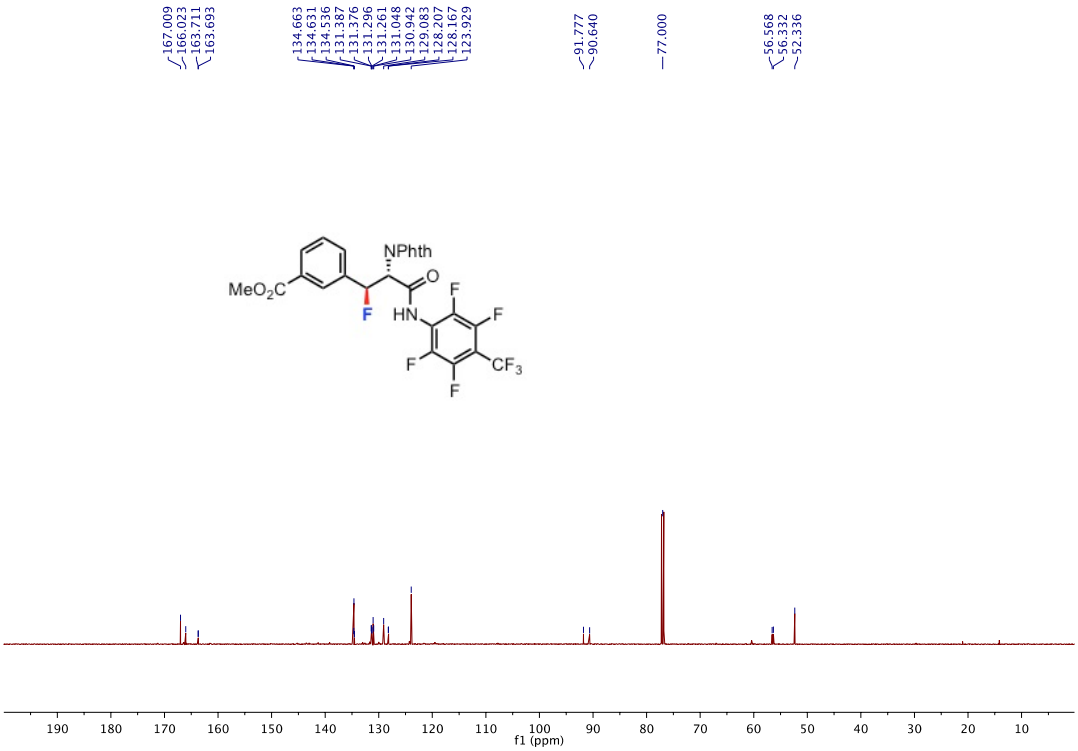

56.301
56.360
56.417
140.374
140.392
140.423
140.449
140.479
140.506
140.537
140.561
140.594
140.615
142.190
142.210
142.240
142.259
164.856
Br
NPhth
O
F
HN
F
F
F
CF3
F
f1 (ppm)

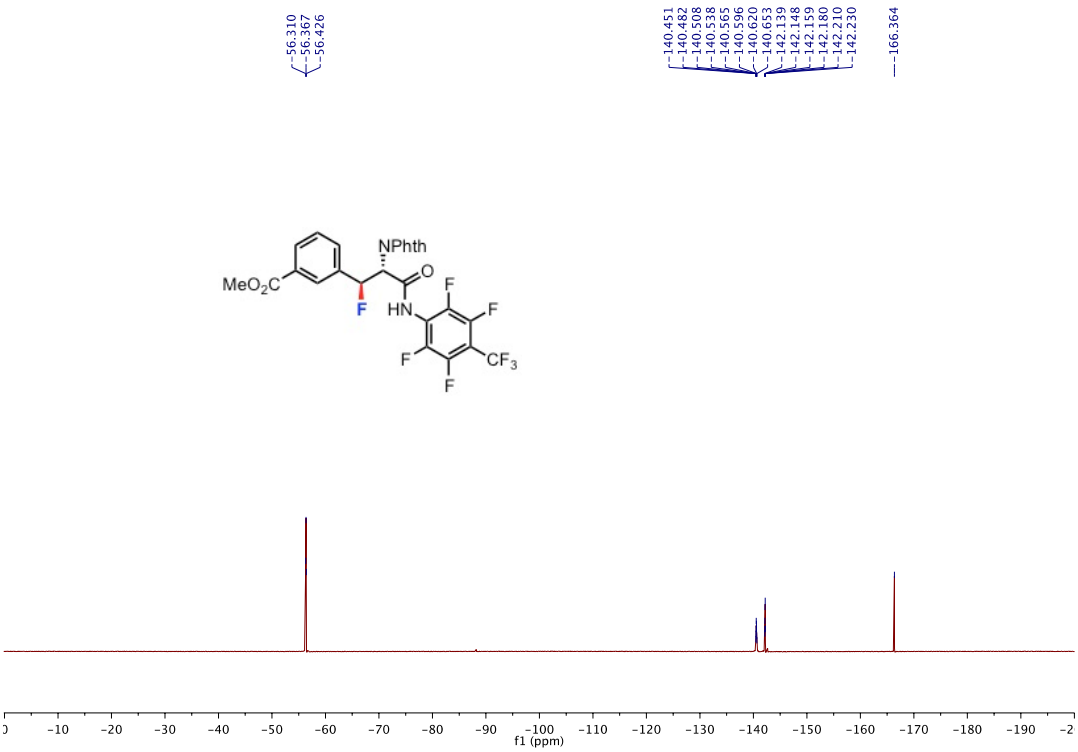

8.326
8.301
7.986
7.966
7.773
7.765
7.760
7.752
7.708
7.700
7.695
7.686
7.504
7.484
6.696
6.672
6.578
6.554
5.531
5.507
5.497
5.473
3.868
MeO2C
NPhth
O
F
HN
F
F
F
CF3
F
0.98
2.05
1.99
1.97
1.99
1.00
0.97
2.97
f1 (ppm)

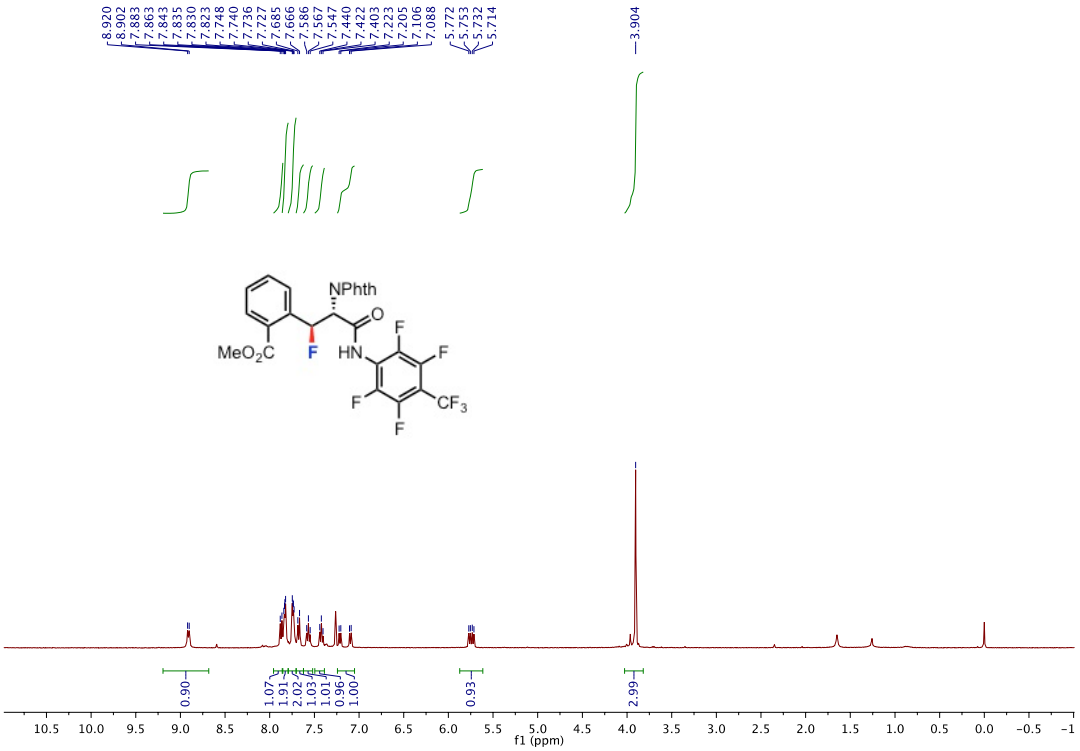

166.973
166.170
163.611
163.597
138.709
138.584
134.689
131.847
131.832
130.984
130.077
126.995
126.957
123.951
91.703
90.563
77.000
56.499
56.263
52.308
MeO2C
NPhth
O
F
HN
F
F
F
CF3
F
f1 (ppm)

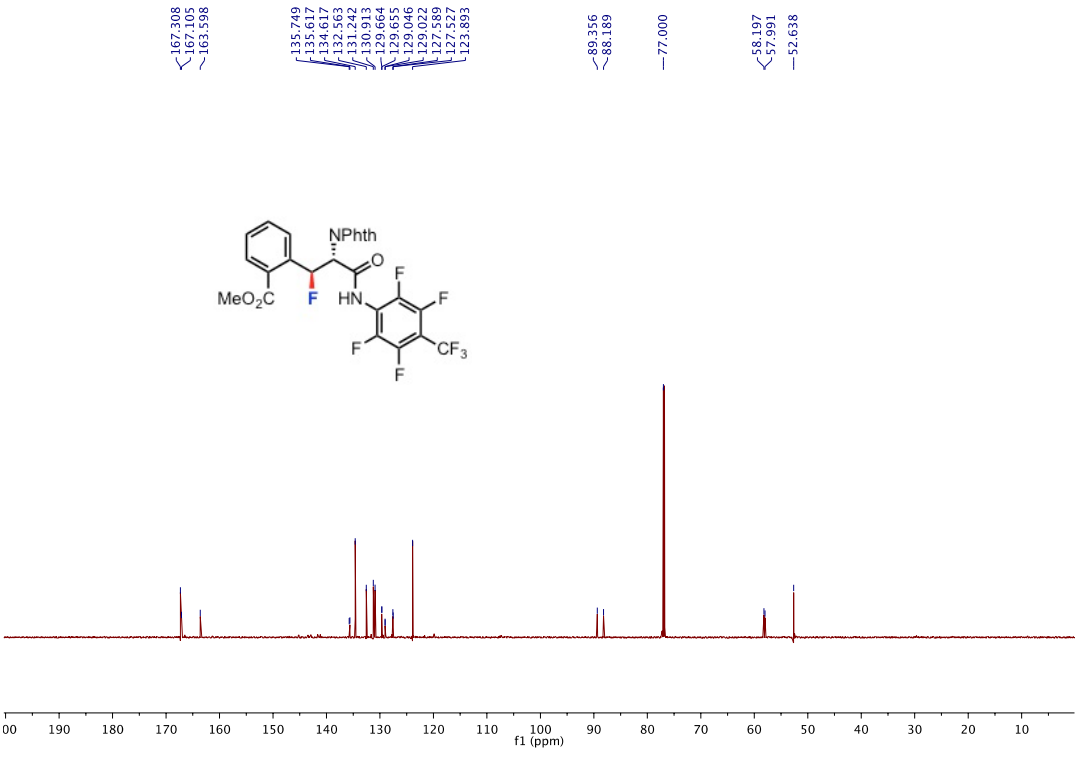

-56.313
-56.371
-56.429
140.395
140.417
140.447
140.474
140.505
140.531
140.562
140.586
140.620
140.639
142.162
142.171
142.182
142.202
142.233
142.255
142.264
167.880
MeO2C
NPhth
O
F
HN
F
F
F
CF3
F
f1 (ppm)

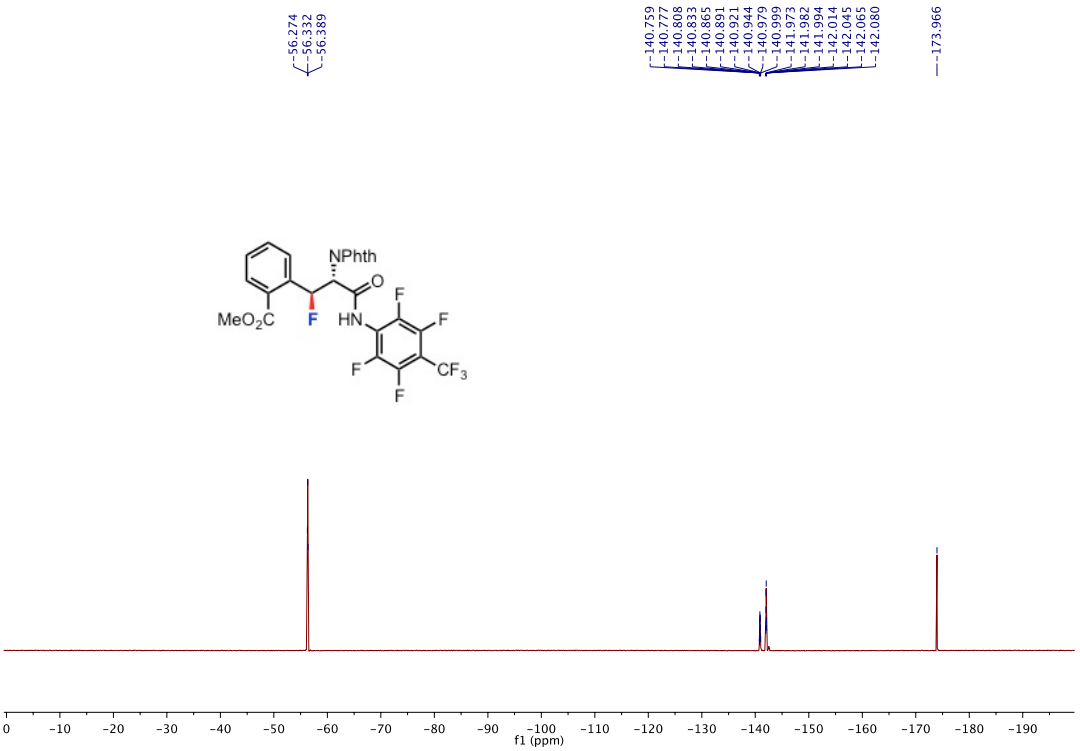

8.356
8.330
8.104
8.005
7.986
7.778
7.770
7.765
7.757
7.704
7.697
7.692
7.684
7.622
7.604
7.430
7.411
7.391
6.705
6.681
6.587
6.563
5.565
5.541
5.533
5.509
3.880
MeO2C
NPhth
O
F
HN
F
F
F
CF3
F
0.95
0.97
1.06
1.96
1.97
1.04
1.04
1.00
0.97
3.05
f1 (ppm)

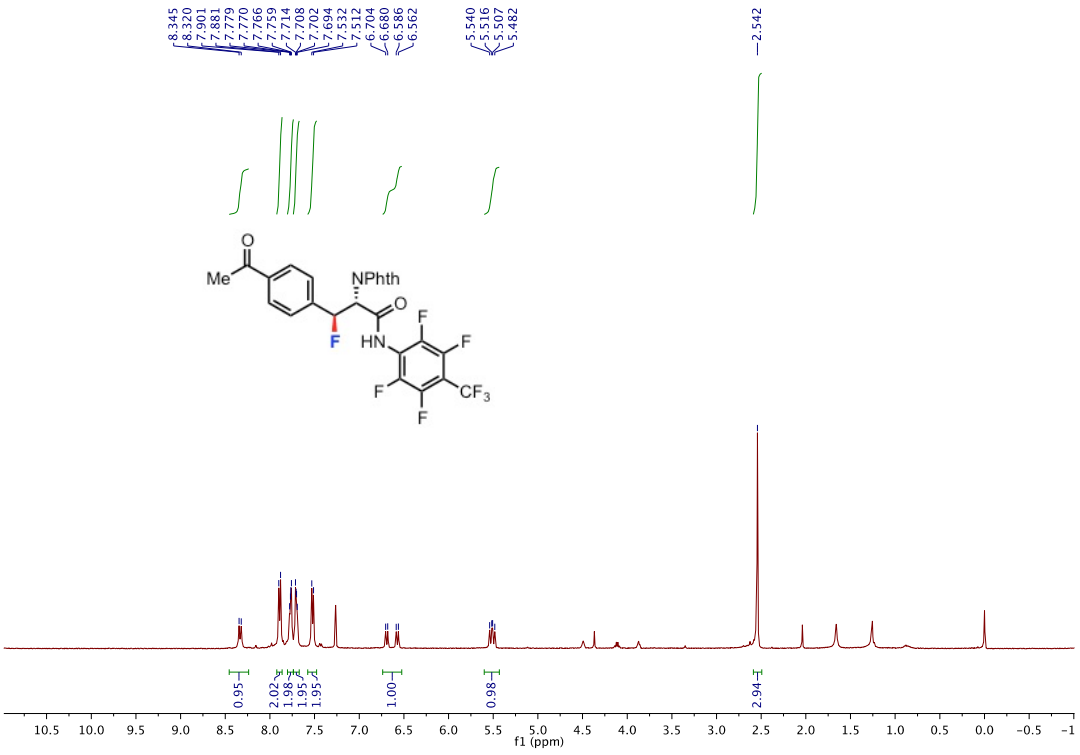

167.009
166.023
163.711
163.693
134.663
134.631
134.536
131.387
131.376
131.296
131.261
131.048
130.942
129.083
128.207
128.167
123.929
91.777
90.640
77.000
56.568
56.332
52.336
NPhth
MeO2C
O
F
HN
F
F
F
CF3
F
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)

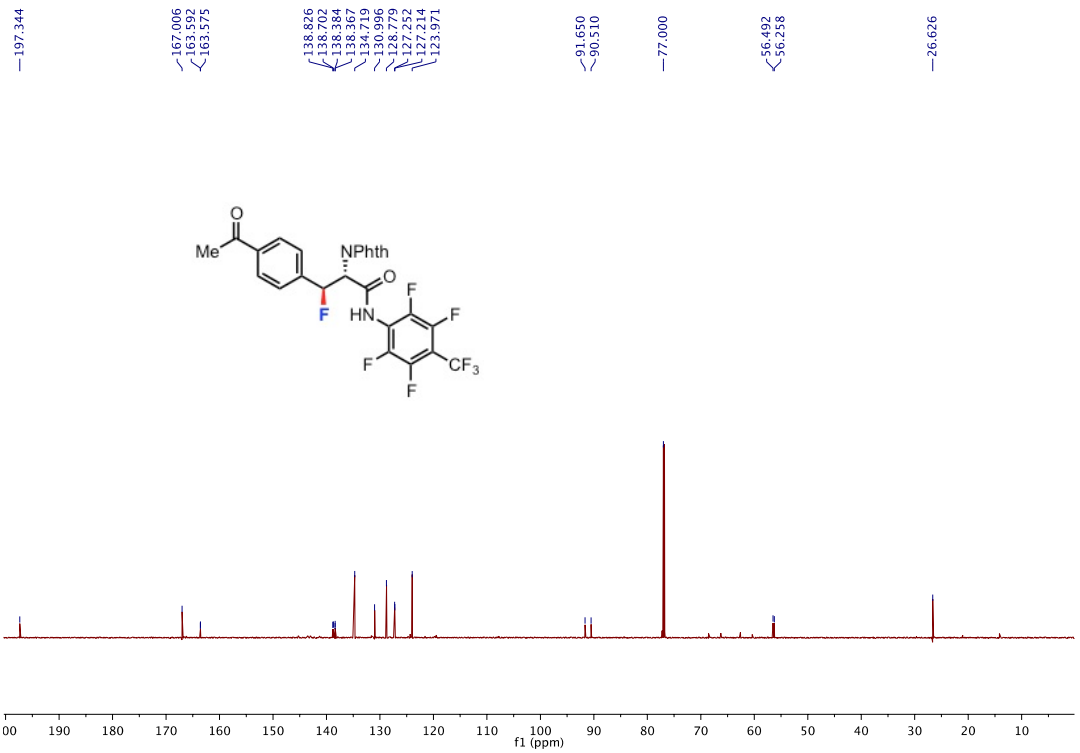

56.310
56.367
56.426
140.451
140.482
140.508
140.538
140.565
140.596
140.620
140.653
142.139
142.148
142.159
142.180
142.210
142.230
166.364
NPhth
MeO2C
O
F
HN
F
F
F
CF3
F
0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -2
f1 (ppm)

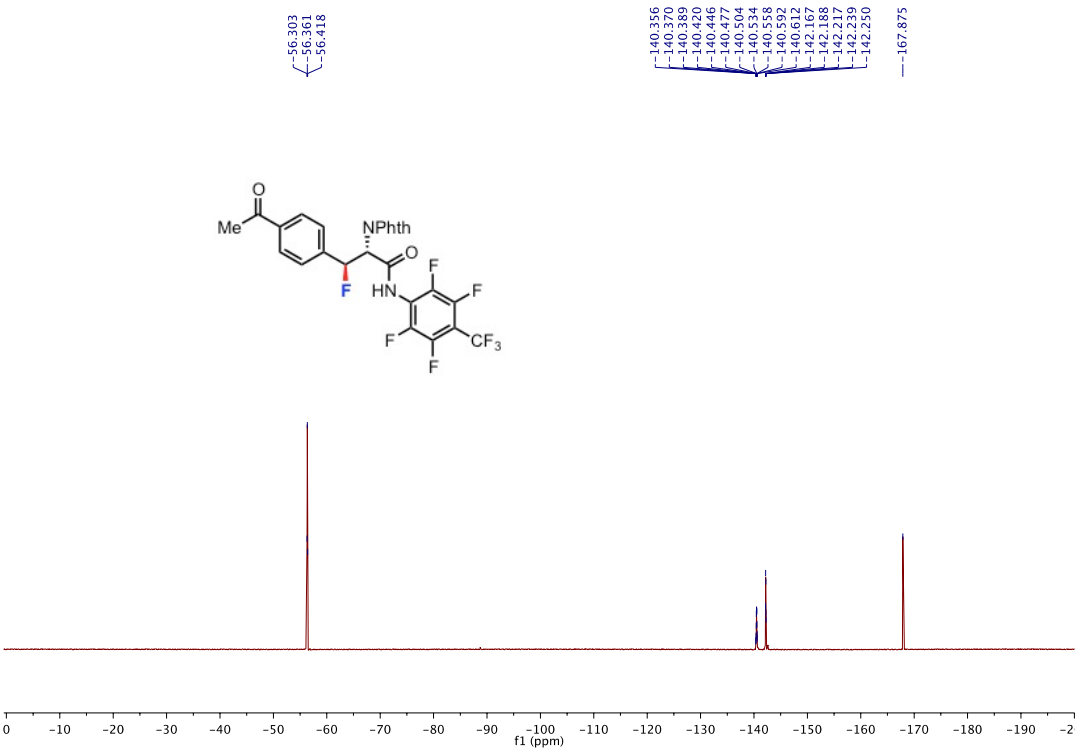

8.920
8.902
7.883
7.863
7.843
7.835
7.830
7.823
7.748
7.740
7.736
7.727
7.685
7.666
7.586
7.567
7.547
7.440
7.422
7.403
7.223
7.205
7.106
7.088
5.772
5.753
5.732
5.714
3.904
NPhth
MeO2C
F
HN
F
F
F
F
CF3
0.90
1.07
1.91
2.02
1.03
1.01
0.96
1.00
0.93
2.99
f1 (ppm)

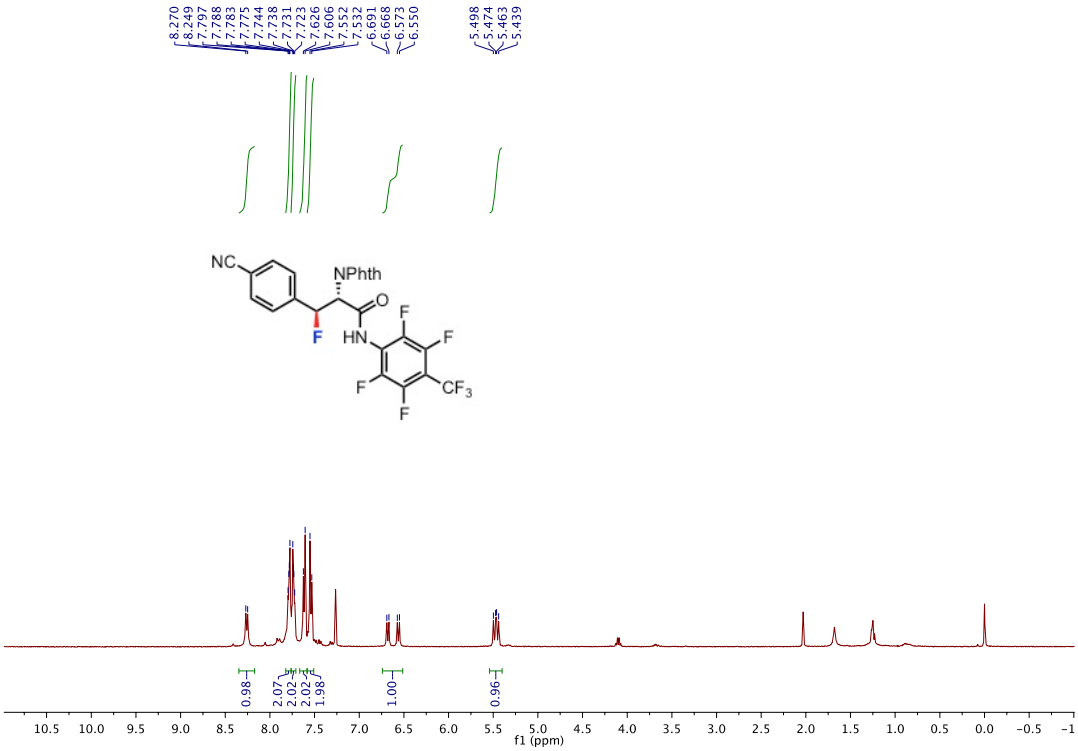

167.308
167.105
163.598
135.749
135.617
134.617
132.563
131.242
130.913
129.664
129.655
129.046
129.022
127.589
127.527
123.893
89.356
88.189
77.000
58.197
57.991
52.638
NPhth
MeO2C
F
HN
F
F
F
F
CF3
f1 (ppm)

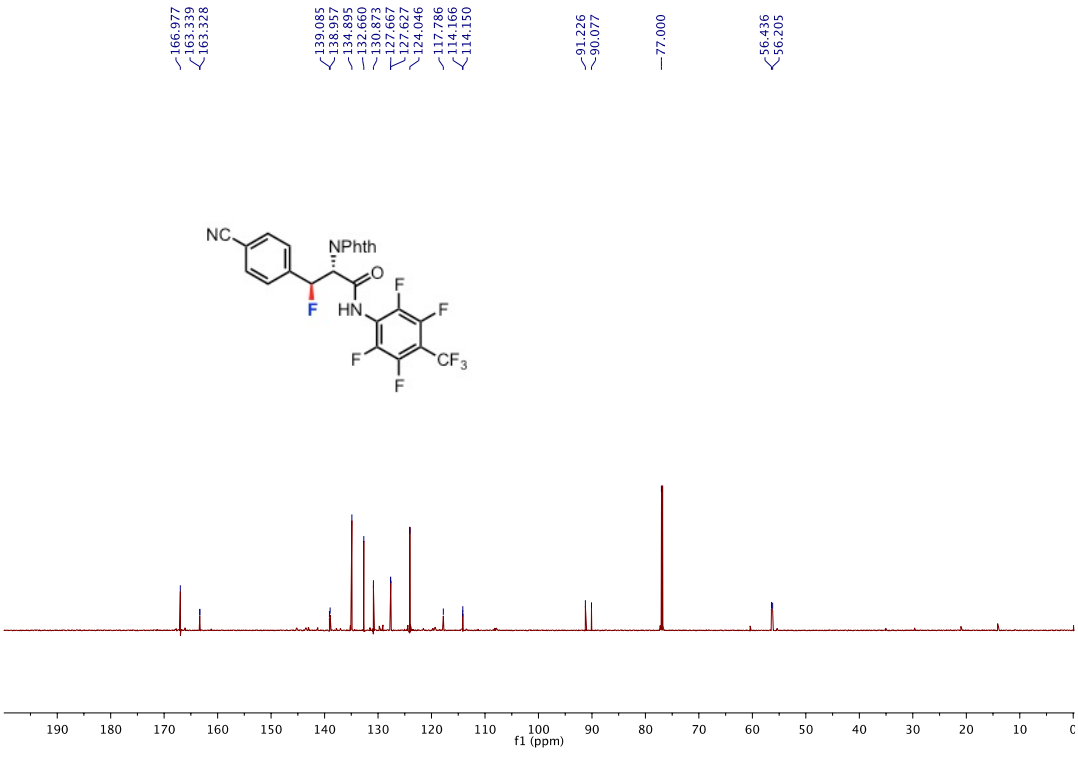

-56.274
-56.332
-56.389
-140.759
-140.777
-140.808
-140.833
-140.865
-140.891
-140.921
-140.944
-140.979
-140.999
-141.973
-141.982
-141.994
-142.014
-142.045
-142.065
-142.080
-173.966
NPhth
O
F
HN
F
F
F
F
CF3
MeO2C
F
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
f1 (ppm)

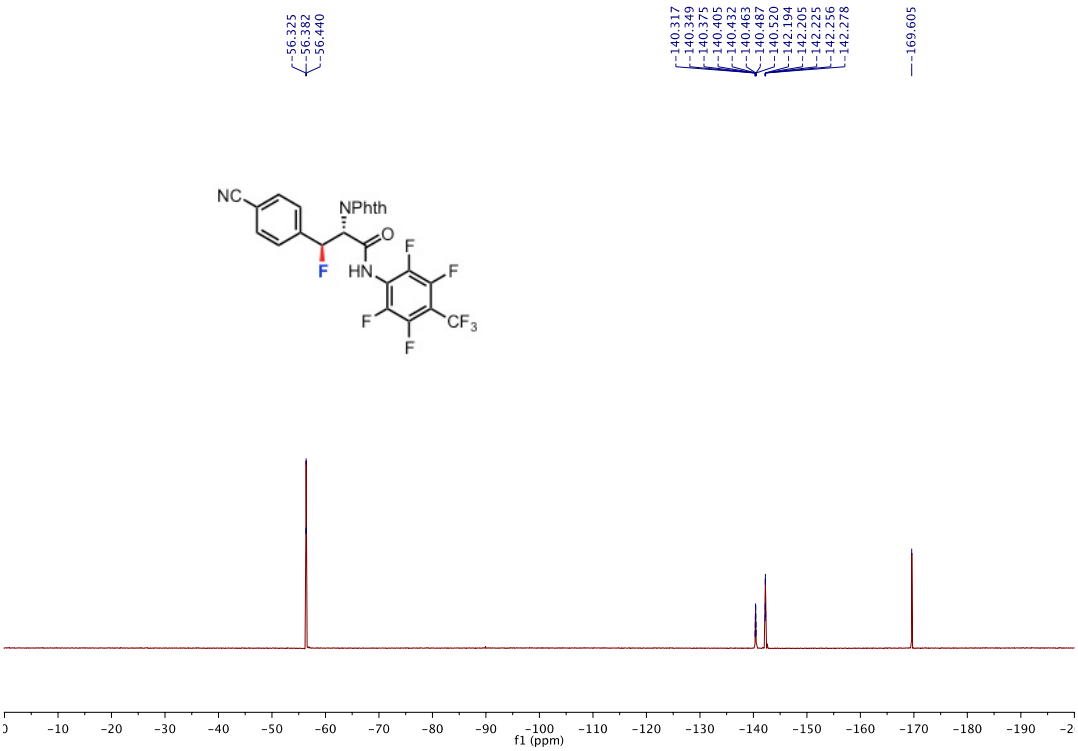

8.345
8.320
7.901
7.881
7.779
7.770
7.766
7.759
7.714
7.708
7.702
7.694
7.532
7.512
6.704
6.680
6.586
6.562
5.540
5.516
5.507
5.482
2.542
O
Me
NPhth
O
F
F
HN
F
F
F
CF3
0.95
2.02
1.98
1.95
1.95
1.00
0.98
2.94
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1
f1 (ppm)

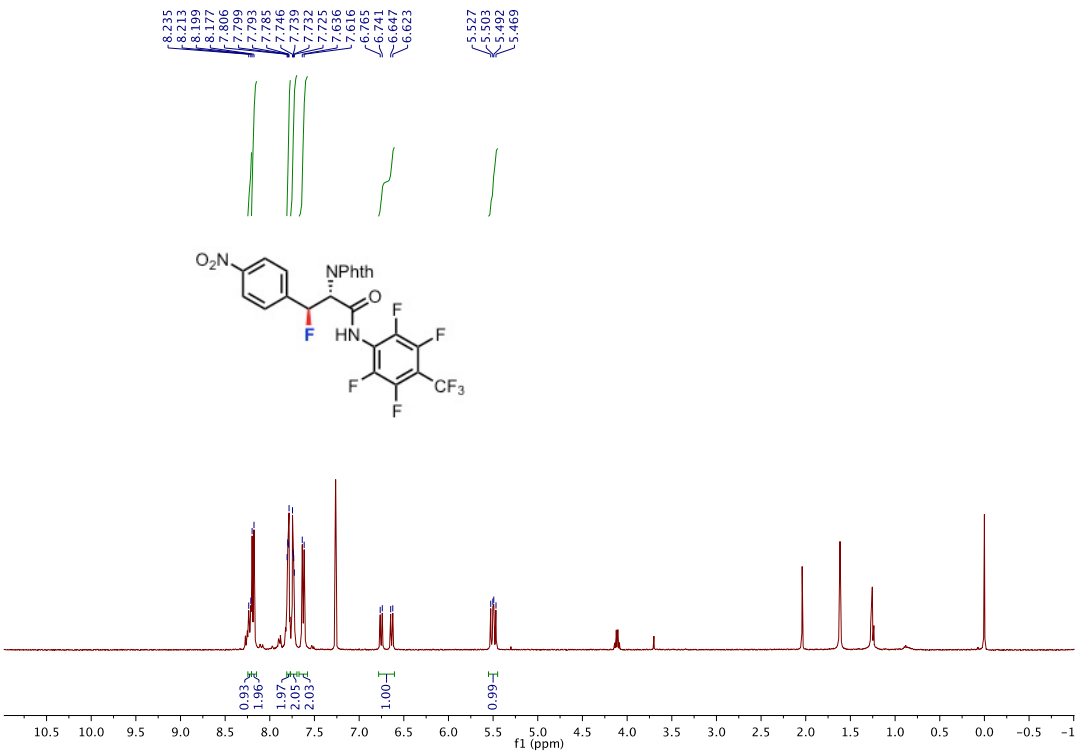

197.344
167.006
163.592
163.575
138.826
138.702
138.384
138.367
134.719
130.996
128.779
127.252
127.214
123.971
91.650
90.510
77.000
56.492
56.258
26.626
Me
O
NPhth
O
F
HN
F
F
F
F
F
CF3
f1 (ppm)

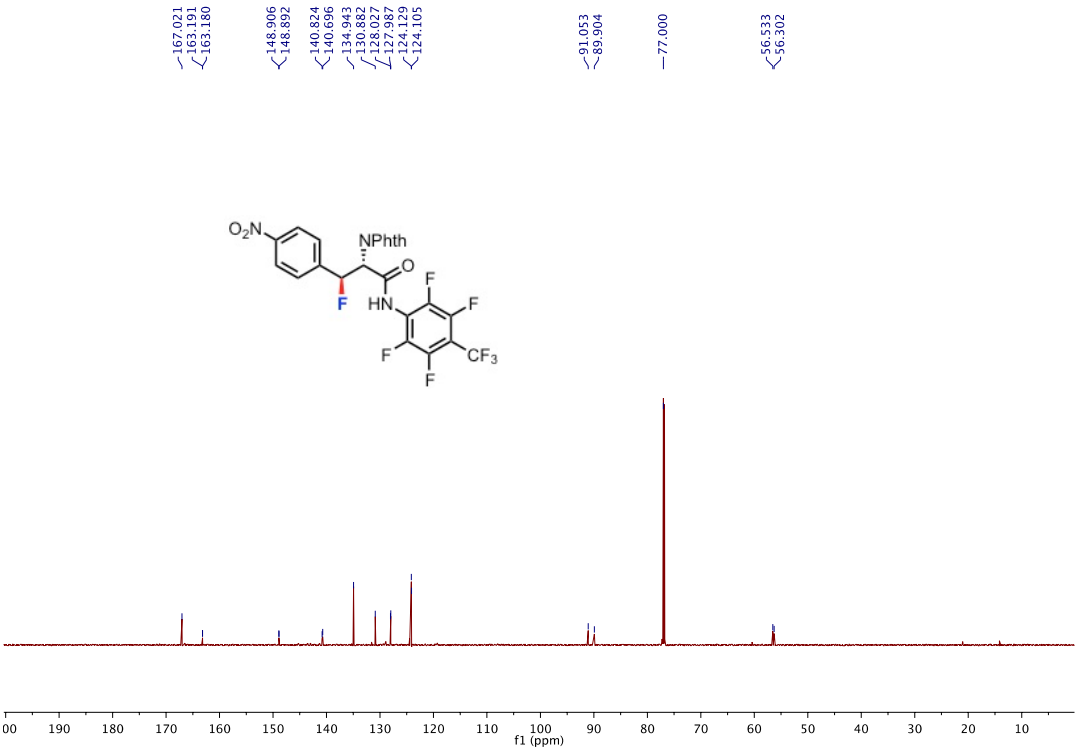

56.303
56.361
56.418
140.356
140.370
140.389
140.420
140.446
140.477
140.504
140.534
140.558
140.592
140.612
142.167
142.188
142.217
142.239
142.250
167.875
Me
O
NPhth
O
F
HN
F
F
F
F
F
CF3
f1 (ppm)

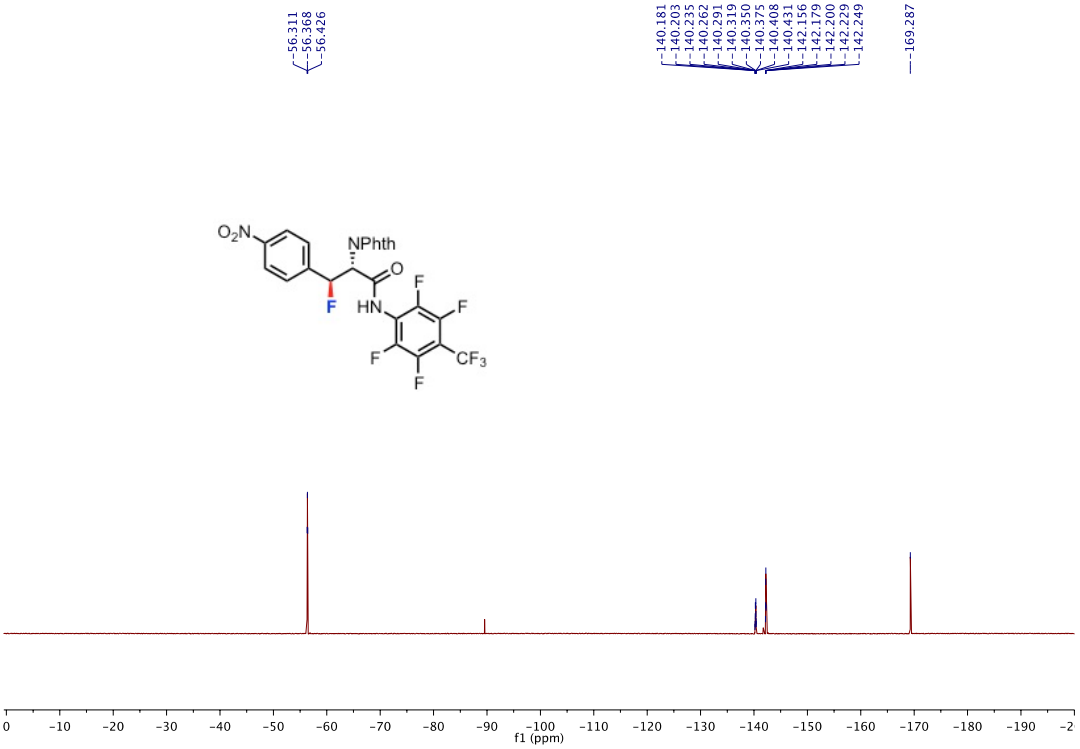

8.270
8.249
7.797
7.788
7.783
7.775
7.744
7.738
7.731
7.723
7.626
7.606
7.552
7.532
6.691
6.668
6.573
6.550
5.498
5.474
5.463
5.439
NC
NPhth
O
F
HN
F
F
F
F
CF3
F
0.98
2.07
2.02
2.02
1.98
1.00
0.96
f1 (ppm)

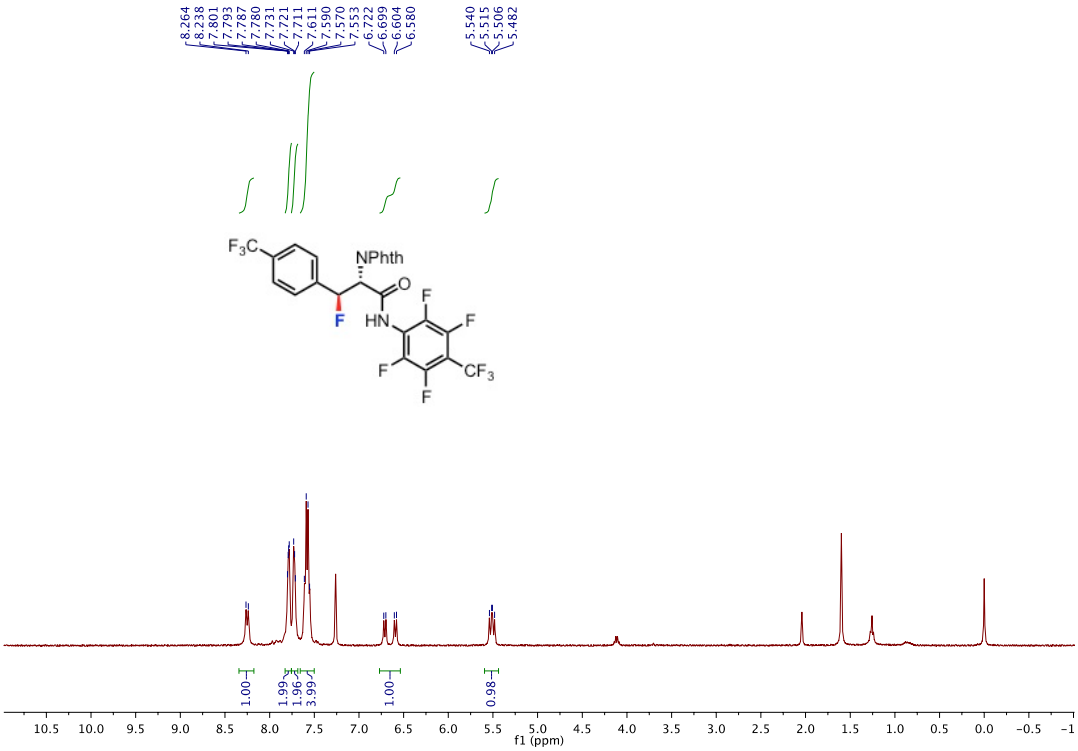

166.977
163.339
163.328
139.085
138.957
134.895
132.660
130.873
127.667
127.627
124.046
117.786
114.166
114.150
91.226
90.077
77.000
56.436
56.205
NC
NPhth
O
F
HN
F
F
F
F
CF3
f1 (ppm)

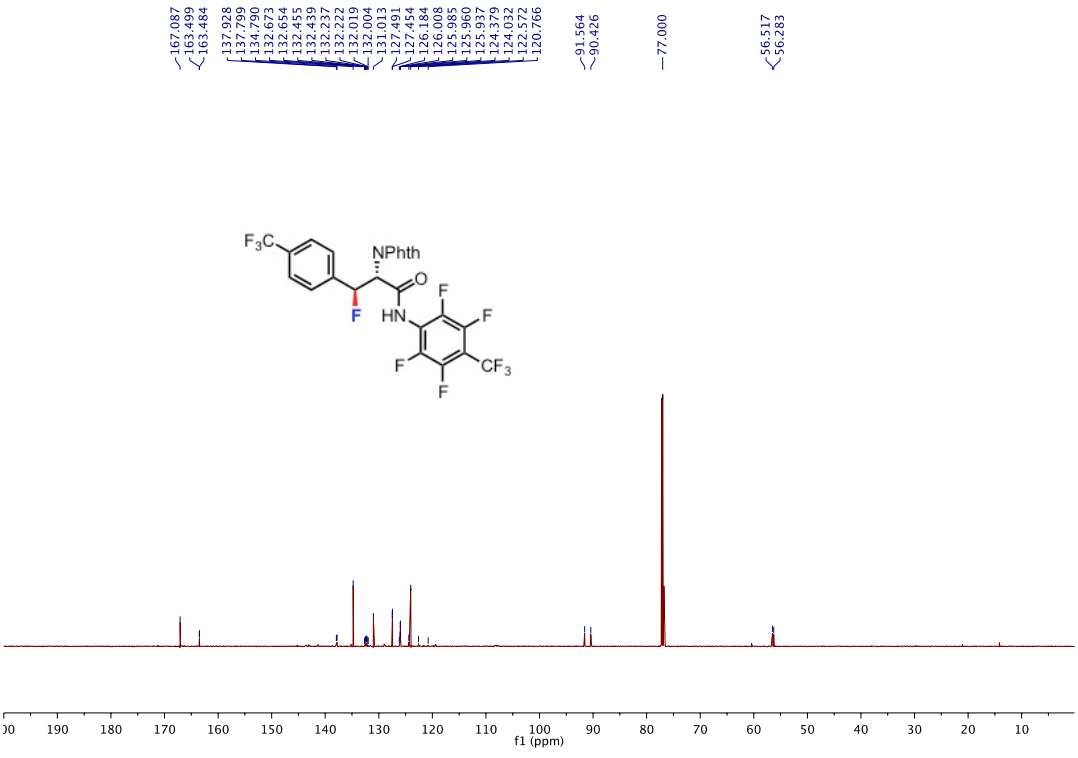

-56.325
-56.382
-56.440
140.317
140.349
140.375
140.405
140.432
140.463
140.487
140.520
142.194
142.205
142.225
142.256
142.278
169.605
NC
NPhth
O
F
HN
F
F
F
CF3
F
f1 (ppm)

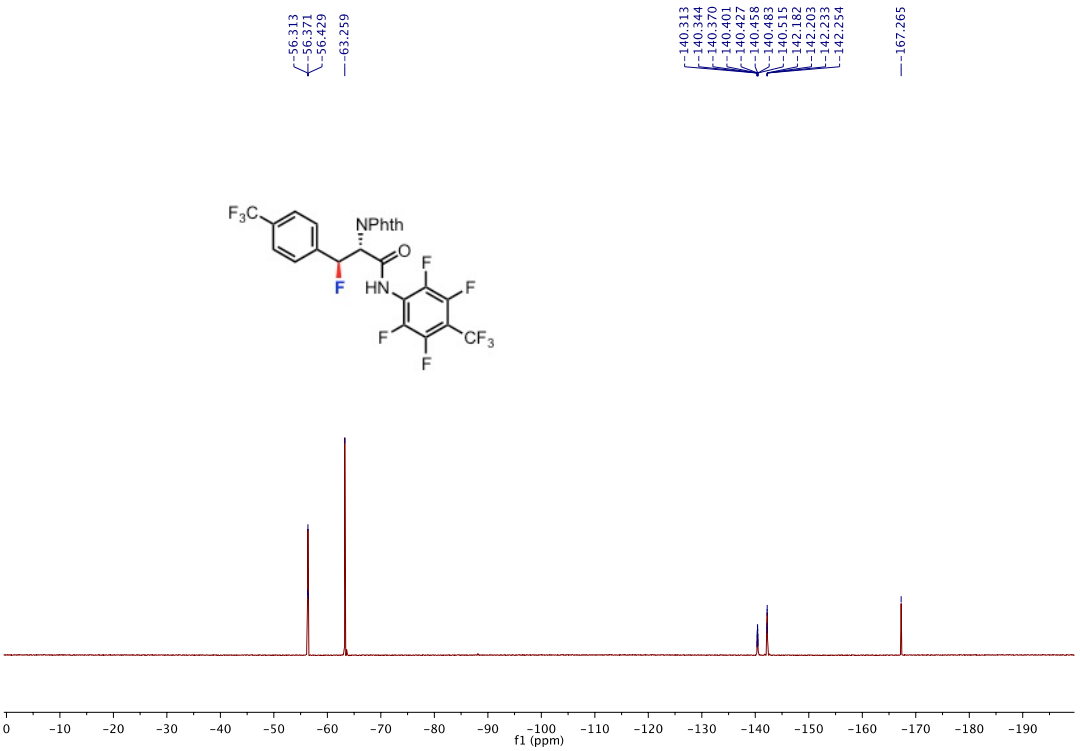

8.235
8.213
8.199
8.177
7.806
7.799
7.793
7.785
7.746
7.739
7.732
7.725
7.636
7.616
6.765
6.741
6.647
6.623
5.527
5.503
5.492
5.469
O2N
NPhth
O
F
HN
F
F
F
CF3
F
0.93
1.96
1.97
2.05
2.03
1.00
0.99
f1 (ppm)

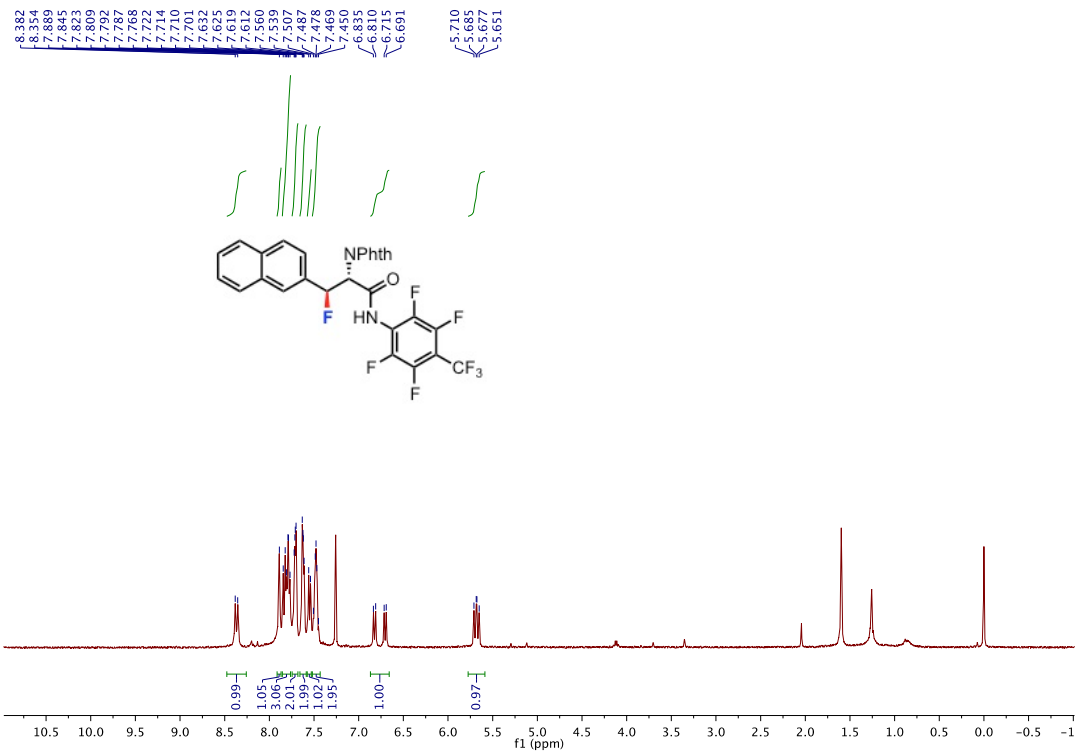

167.021
163.191
163.180
148.906
148.892
140.824
140.696
134.943
130.882
129.827
127.987
124.129
124.105
91.053
89.904
77.000
56.533
56.302
O2N
NPhth
O
F
HN
F
F
F
F
CF3
F
00 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)

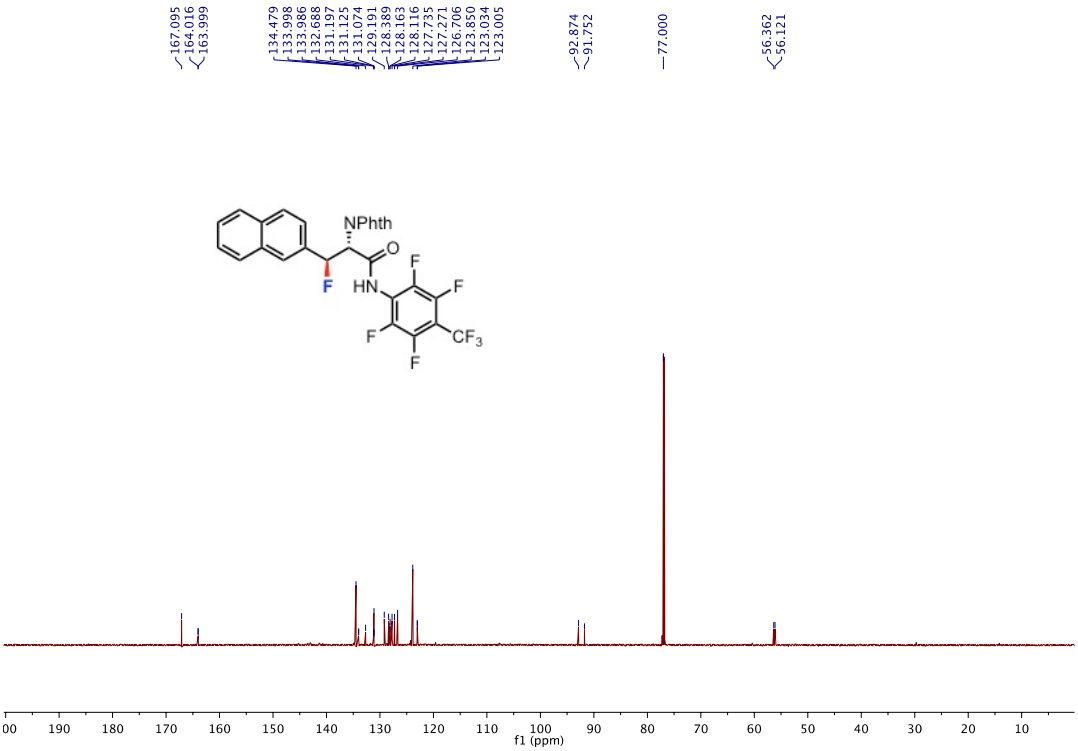

56.311
56.368
56.426
140.181
140.203
140.235
140.262
140.291
140.319
140.350
140.375
140.408
140.431
142.156
142.179
142.200
142.229
142.249
169.287
O2N
NPhth
O
F
HN
F
F
F
F
CF3
F
0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -2
f1 (ppm)

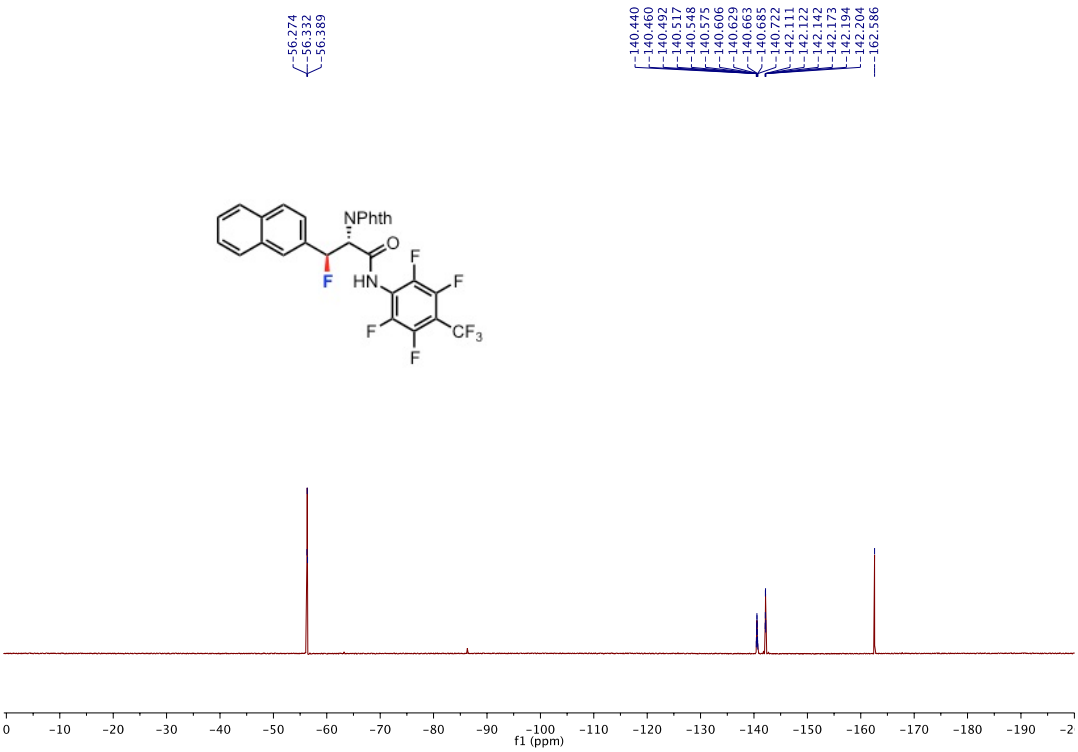

8.264
8.238
7.801
7.793
7.787
7.780
7.731
7.721
7.711
7.611
7.590
7.570
7.553
6.722
6.699
6.604
6.580
5.540
5.515
5.506
5.482
F3C
NPhth
O
F
HN
F
F
F
CF3
F
1.00
1.99
1.96
3.99
1.00
0.98
f1 (ppm)

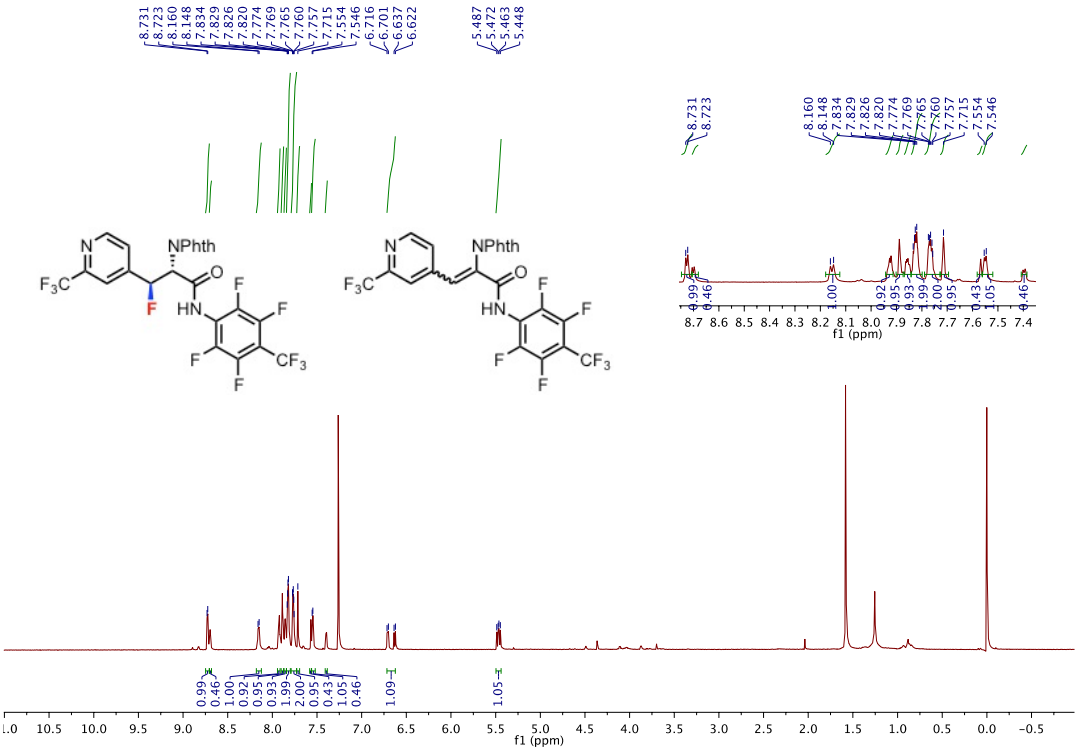

167.087
163.499
163.484
137.928
137.799
134.790
132.673
132.654
132.455
132.439
132.237
132.222
132.019
132.004
131.013
127.491
127.454
126.184
126.008
125.985
125.960
125.937
124.379
124.032
122.572
120.766
91.564
90.426
77.000
56.517
56.283
F3C
NPhth
O
F
HN
F
F
F
CF3
F
f1 (ppm)

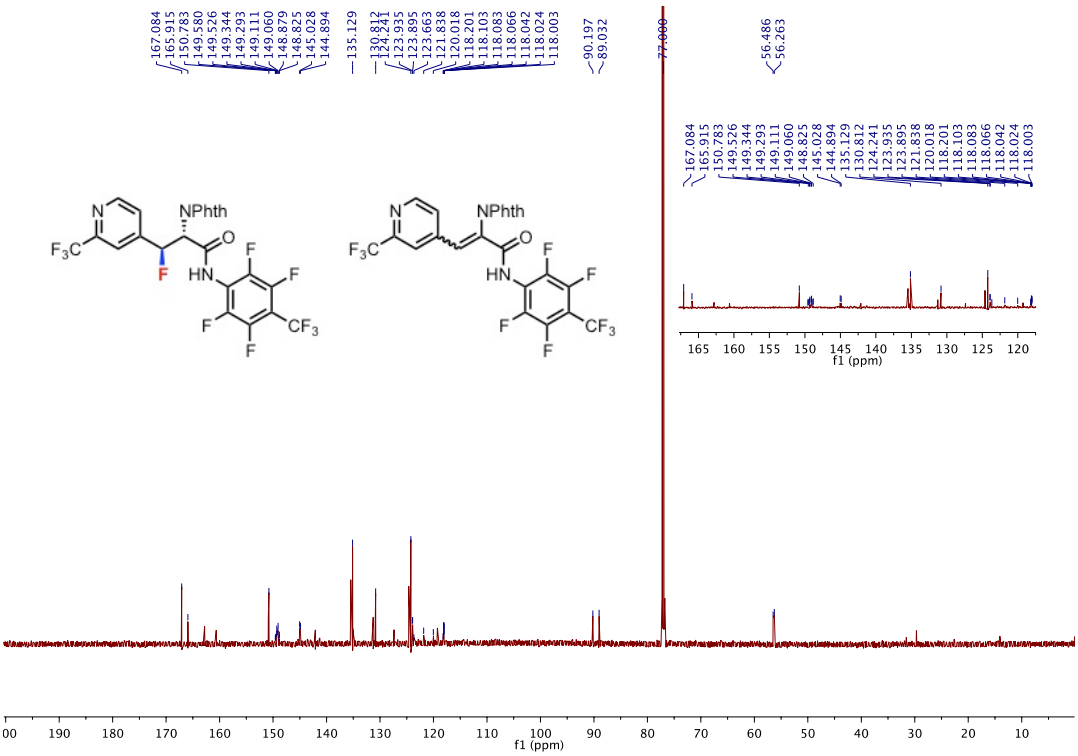

-56.313
-56.371
-56.429
-63.259
-140.313
-140.344
-140.370
-140.401
-140.427
-140.458
-140.483
-140.515
-142.182
-142.203
-142.233
-142.254
-167.265
NPhth
O
HN
F
F
F
F
F
F
F
F3C
CF3
f1 (ppm)

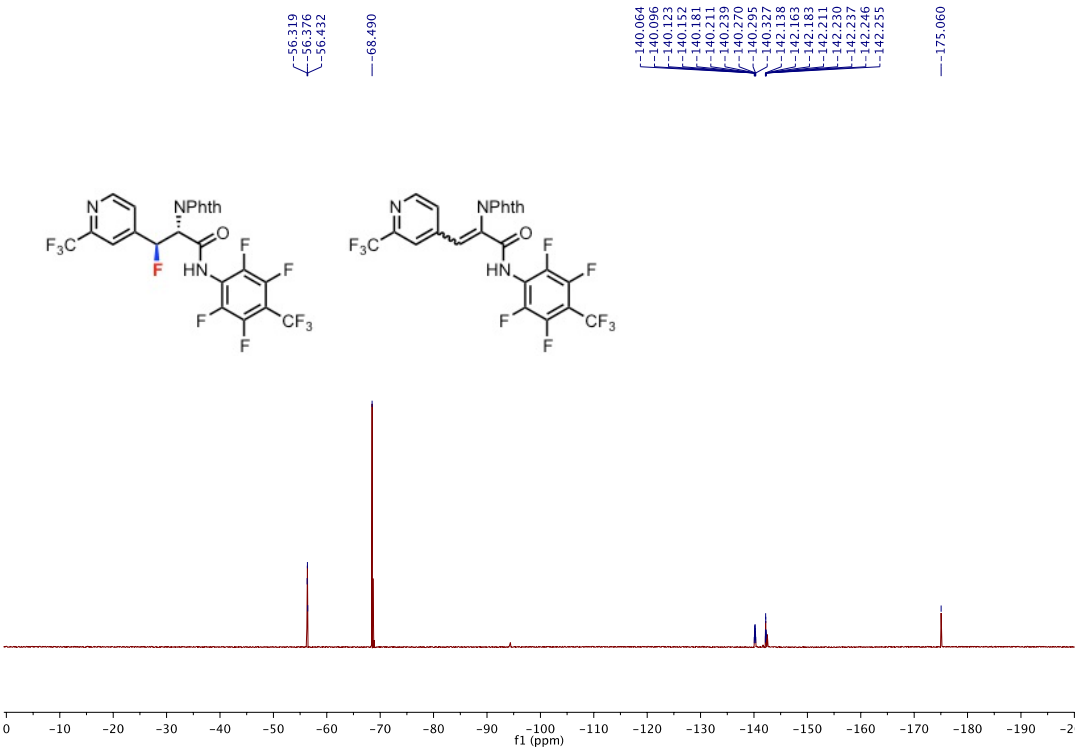

8.382
8.354
7.889
7.845
7.823
7.809
7.792
7.787
7.768
7.722
7.714
7.710
7.701
7.632
7.625
7.619
7.612
7.560
7.539
7.507
7.487
7.478
7.469
7.450
6.835
6.810
6.715
6.691
5.710
5.685
5.677
5.651
NPhth
O
HN
F
F
F
F
F
F
F
CF3
0.99
1.05
3.06
2.01
1.99
1.02
1.95
1.00
0.97
f1 (ppm)

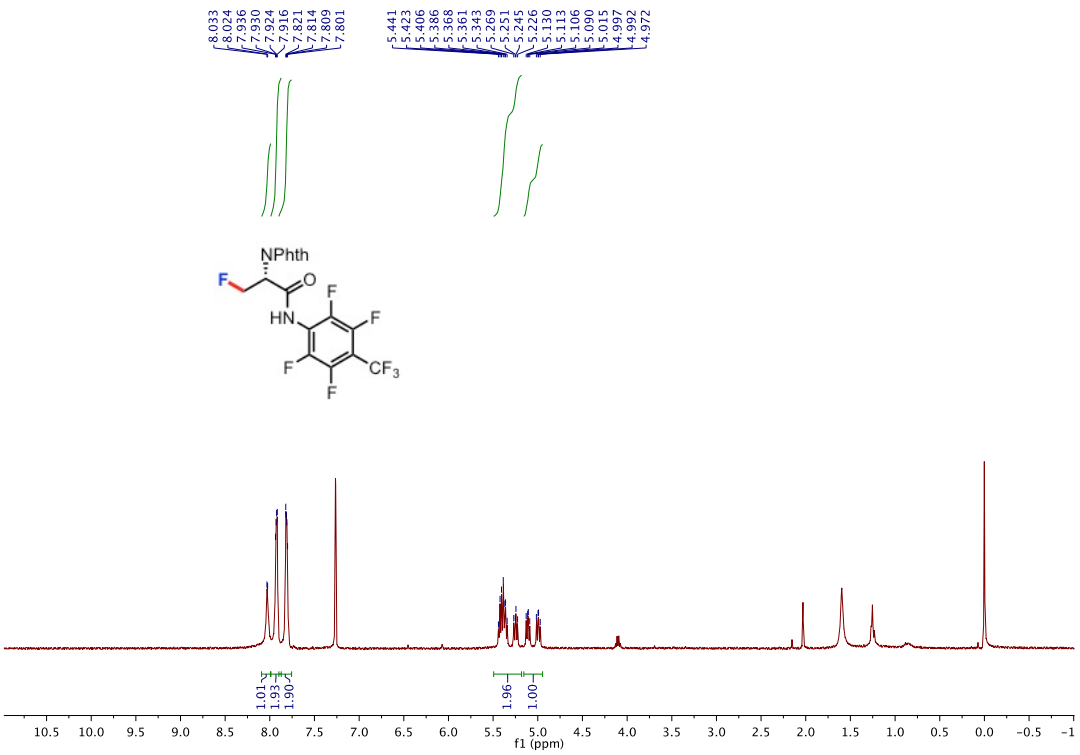

167.095
164.016
163.999
134.479
133.998
133.986
132.688
131.197
131.125
131.074
129.191
128.389
128.163
128.116
127.735
127.271
126.706
123.850
123.034
123.005
92.874
91.752
77.000
56.362
56.121
NPhth
O
F
HN
F
F
F
CF3
F
00 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)

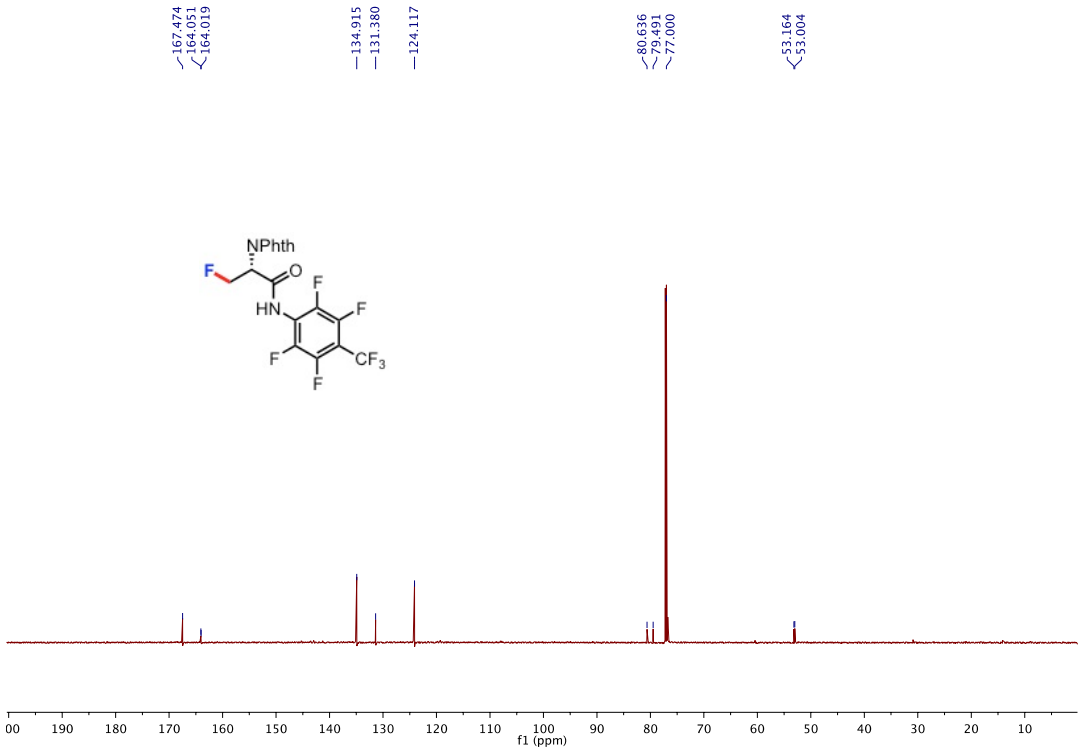

56.274
56.332
56.389
140.440
140.460
140.492
140.517
140.548
140.575
140.606
140.629
140.663
140.685
140.722
142.111
142.122
142.142
142.173
142.194
142.204
162.586
NPhth
O
F
HN
F
F
F
CF3
F
0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -2
f1 (ppm)

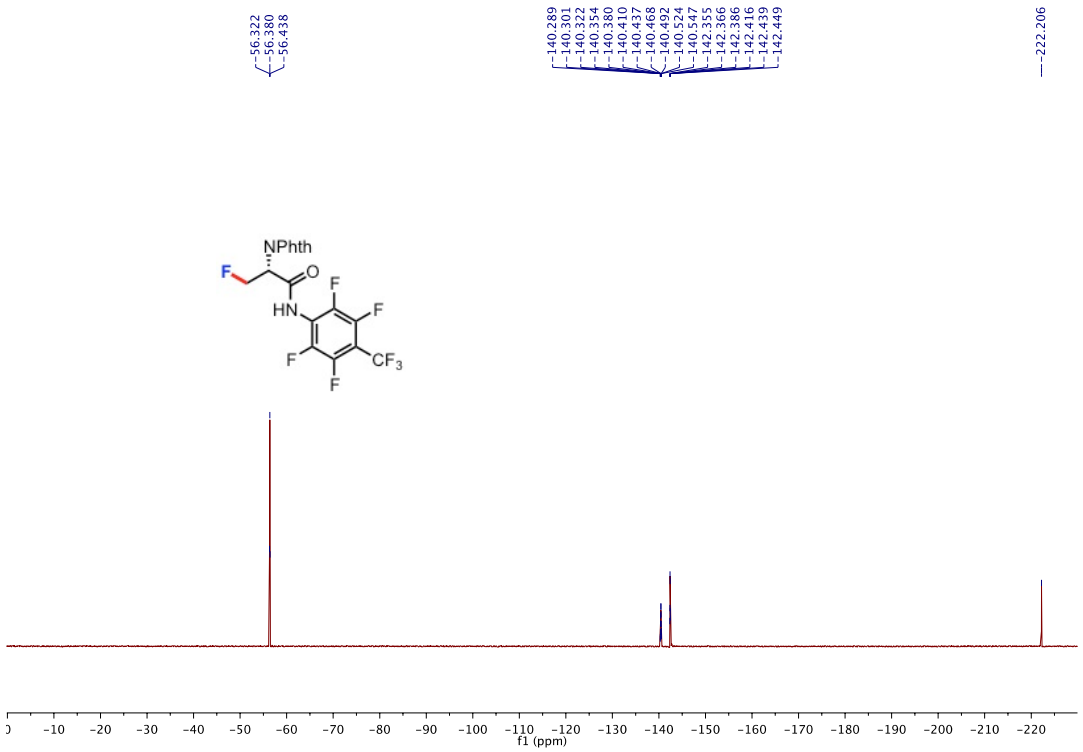

8.731
8.723
8.160
8.148
7.834
7.829
7.826
7.820
7.774
7.769
7.765
7.760
7.757
7.715
7.554
7.546
6.716
6.701
6.637
6.622
5.487
5.472
5.463
5.448
NPhth
F3C
F
HN
O
CF3
0.99
0.46
1.00
0.92
0.95
0.93
1.99
2.00
0.95
0.43
1.05
0.46
1.09
1.05
f1 (ppm)

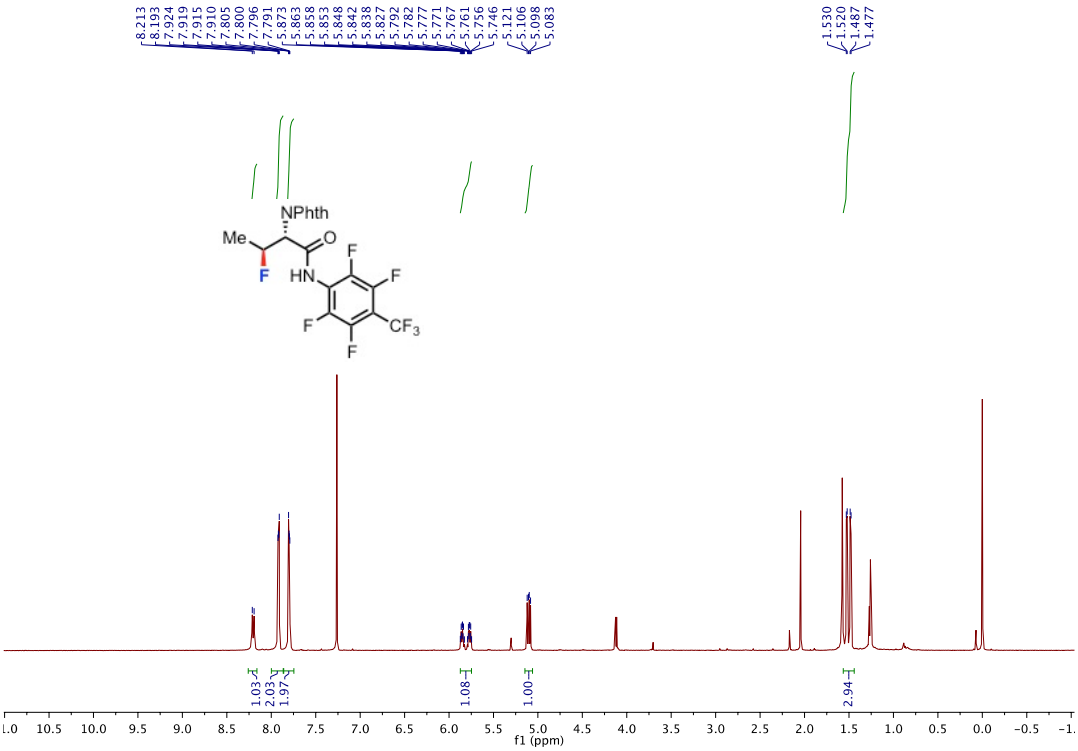

167.084
165.915
150.783
149.580
149.526
149.344
149.293
149.111
149.060
148.879
148.825
145.028
144.894
135.129
130.812
124.241
123.935
123.895
123.663
121.838
120.018
118.201
118.103
118.083
118.066
118.042
118.024
118.003
90.197
89.032
77.000
56.486
56.263
NPhth
F3C
F
HN
O
CF3
f1 (ppm)

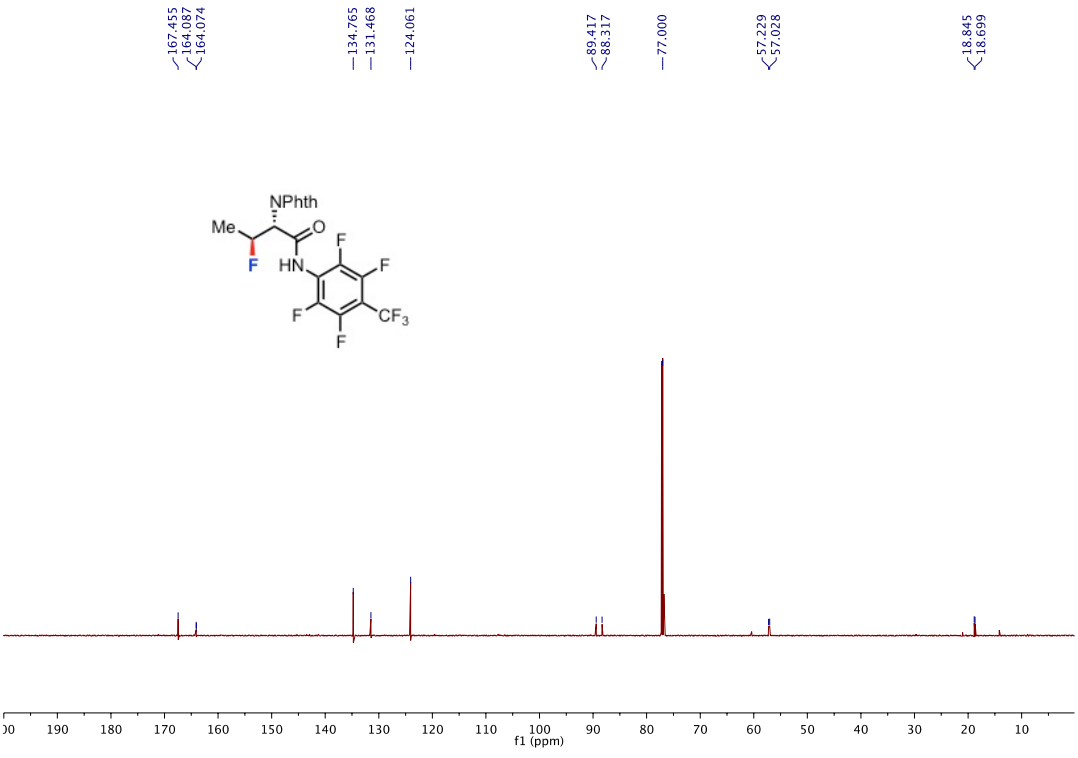

-56.319
-56.376
-56.432
-68.490
140.064
140.096
140.123
140.152
140.181
140.211
140.239
140.270
140.295
140.327
142.138
142.163
142.183
142.211
142.230
142.237
142.246
142.255
-175.060
NPhth
F3C
F
HN
O
F
CF3
f1 (ppm)

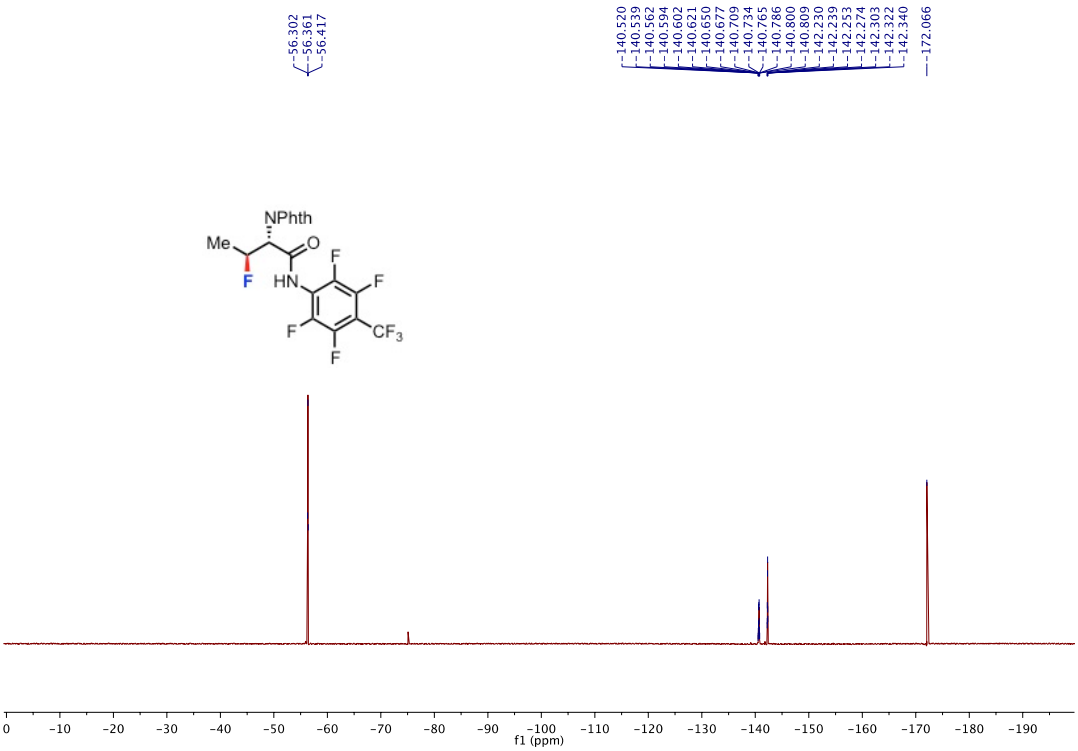

8.033
8.024
7.936
7.930
7.924
7.916
7.821
7.814
7.809
7.801
5.441
5.423
5.406
5.386
5.368
5.361
5.343
5.269
5.251
5.245
5.226
5.130
5.113
5.106
5.090
5.015
4.997
4.992
4.972
NPhth
F
HN
O
CF3
1.01
1.93
1.90
1.96
1.00
f1 (ppm)

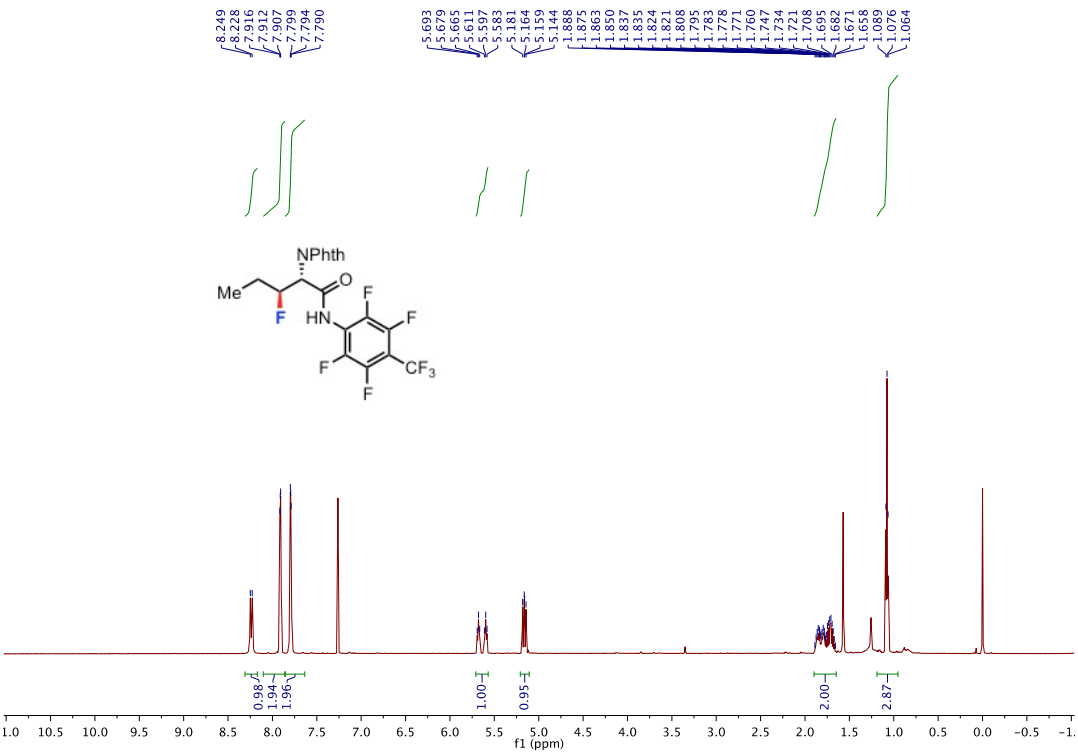

167.474
164.051
164.019
134.915
131.380
124.117
80.636
79.491
77.000
53.164
53.004
NPhth
F
O
HN
F
F
F
F
CF3
f1 (ppm)

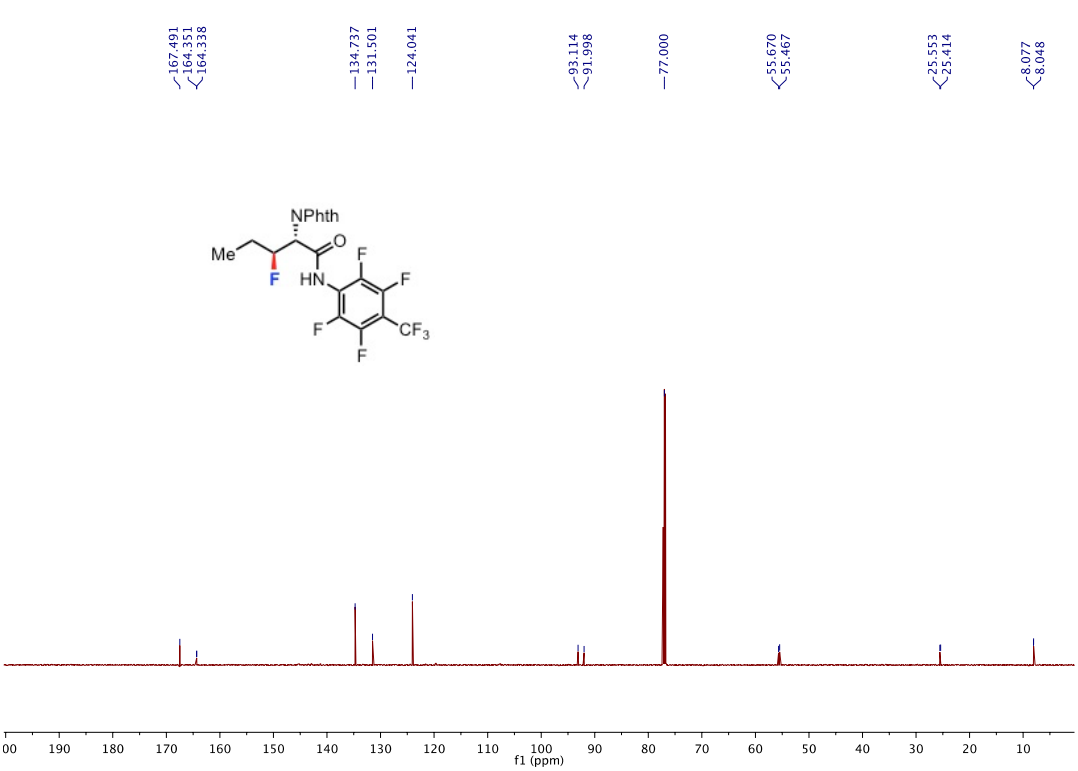

56.322
56.380
56.438
140.289
140.301
140.322
140.354
140.380
140.410
140.437
140.468
140.492
140.524
140.547
142.355
142.366
142.386
142.416
142.439
142.449
222.206
NPhth
F
O
HN
F
F
F
F
CF3
f1 (ppm)

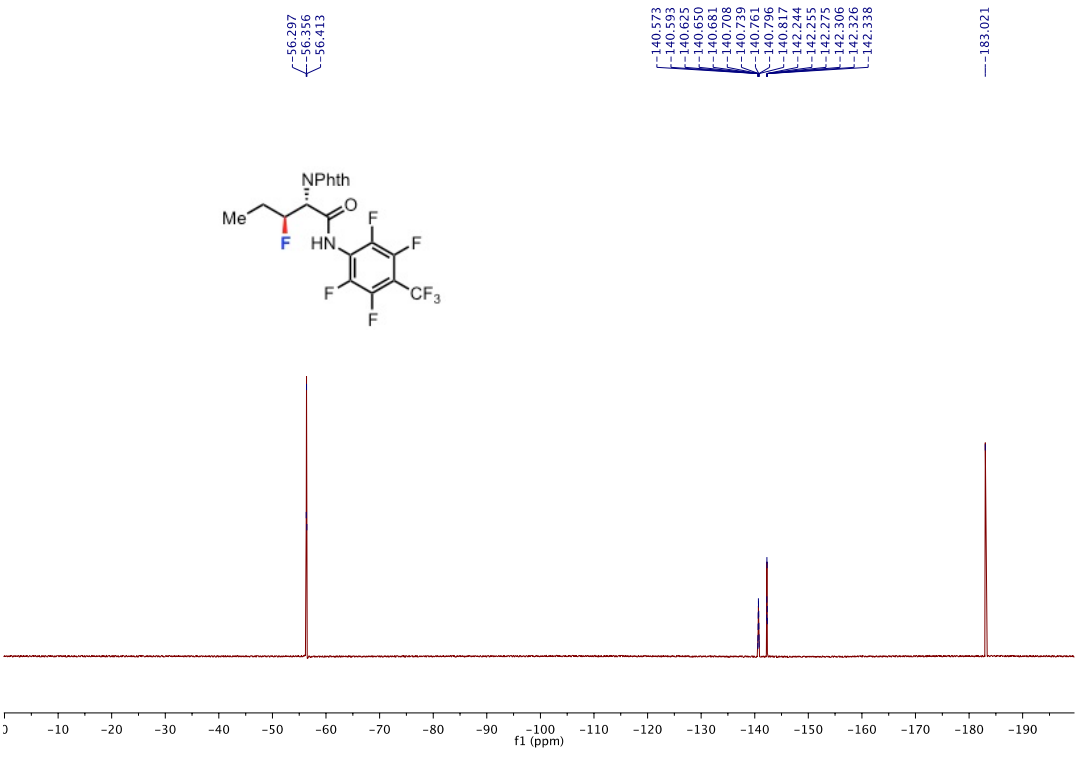

8.213
8.193
7.924
7.919
7.915
7.910
7.805
7.800
7.796
7.791
5.873
5.863
5.858
5.853
5.848
5.842
5.838
5.827
5.792
5.782
5.777
5.771
5.767
5.761
5.756
5.746
5.121
5.106
5.098
5.083
1.530
1.520
1.487
1.477
NPhth
Me
F
O
HN
F
F
F
CF3
F
1.03
2.03
1.97
1.08
1.00
2.94
f1 (ppm)

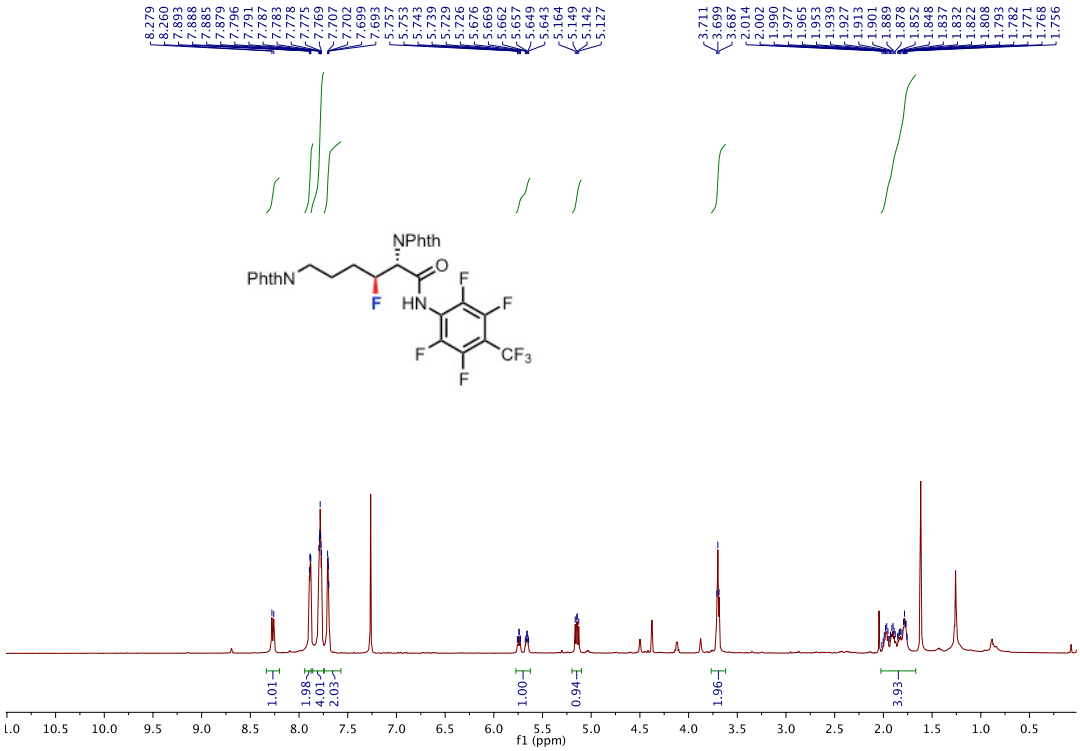

167.455
164.087
164.074
134.765
131.468
124.061
89.417
88.317
77.000
57.229
57.028
18.845
18.699
NPhth
Me
F
O
HN
F
F
F
CF3
F
f1 (ppm)

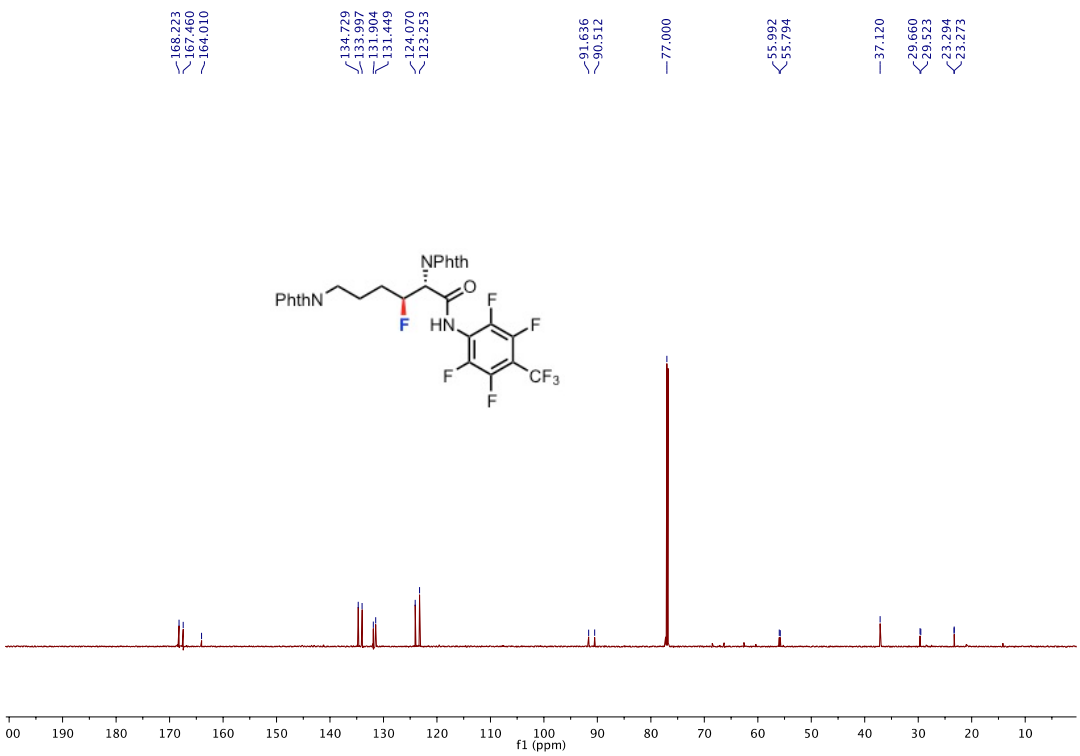

-56.302
-56.361
-56.417
-140.520
-140.539
-140.562
-140.594
-140.602
-140.621
-140.650
-140.677
-140.709
-140.734
-140.765
-140.786
-140.800
-140.809
-142.230
-142.239
-142.253
-142.274
-142.303
-142.322
-142.340
-172.066
NPhth
Me
F
HN
O
F
F
F
F
CF3
f1 (ppm)

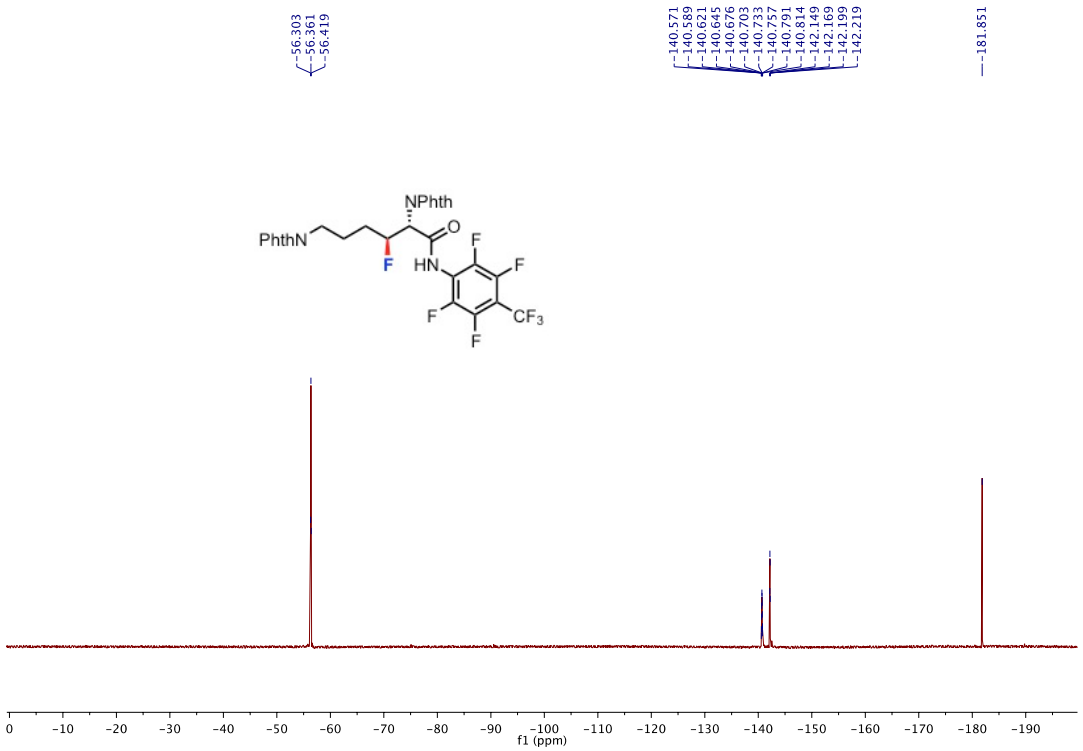

8.249
8.228
7.916
7.912
7.907
7.799
7.794
7.790
5.693
5.679
5.665
5.611
5.597
5.583
5.181
5.164
5.159
5.144
1.888
1.875
1.863
1.850
1.837
1.835
1.824
1.821
1.808
1.795
1.783
1.778
1.771
1.760
1.747
1.734
1.721
1.708
1.695
1.682
1.671
1.658
1.089
1.076
1.064
NPhth
Me
F
HN
O
F
F
F
F
CF3
0.98
1.94
1.96
1.00
0.95
2.00
2.87
f1 (ppm)

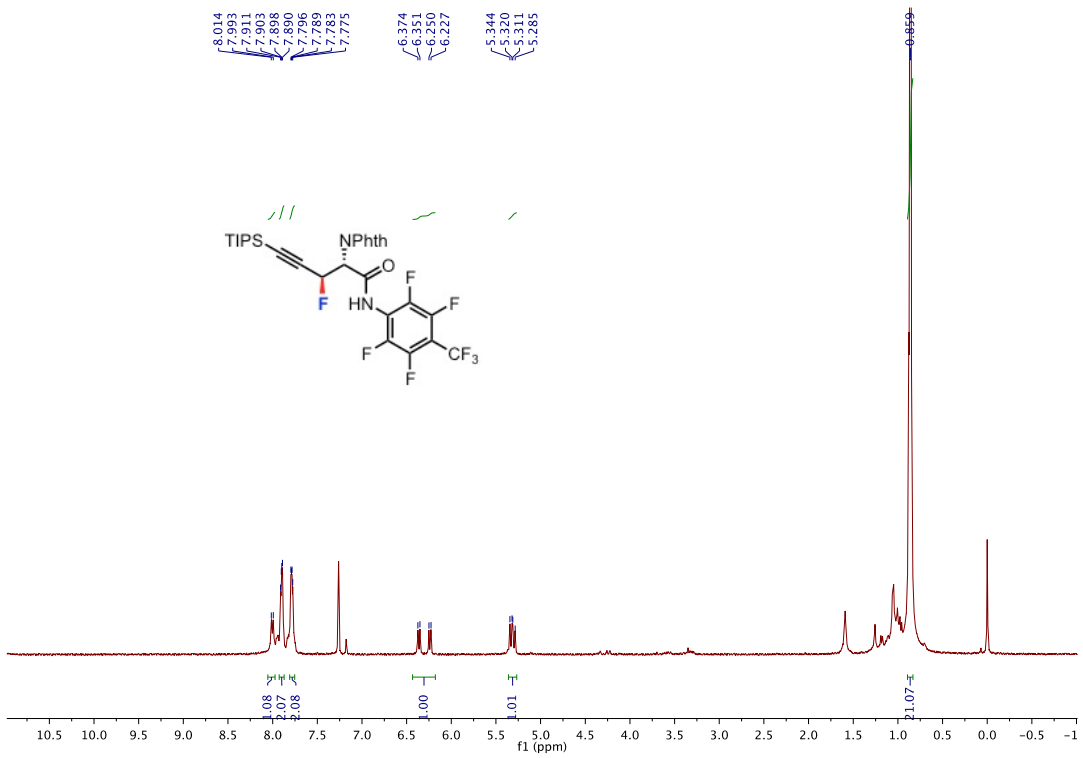

167.491
164.351
164.338
134.737
131.501
124.041
93.114
91.998
77.000
55.670
55.467
25.553
25.414
8.077
8.048
NPhth
Me
F
HN
O
F
F
F
F
CF3
f1 (ppm)

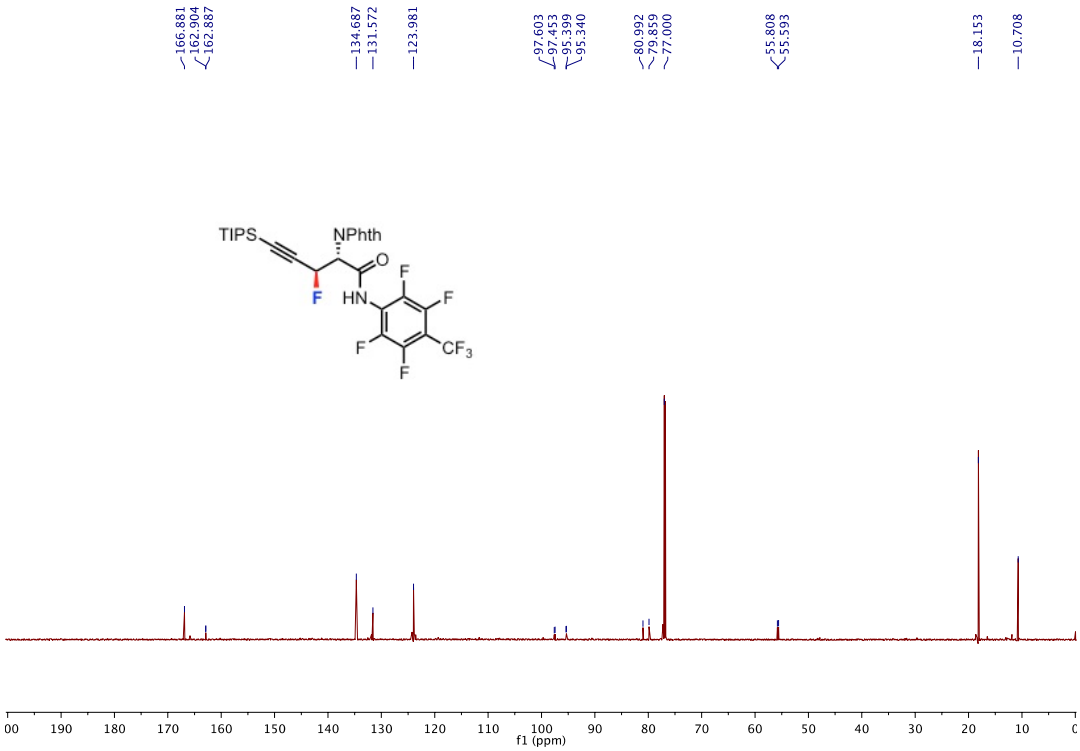

56.297
56.356
56.413
140.573
140.593
140.625
140.650
140.681
140.708
140.739
140.761
140.796
140.817
142.244
142.255
142.275
142.306
142.326
142.338
183.021
NPhth
Me
F
HN
O
F
F
F
F
CF3
f1 (ppm)

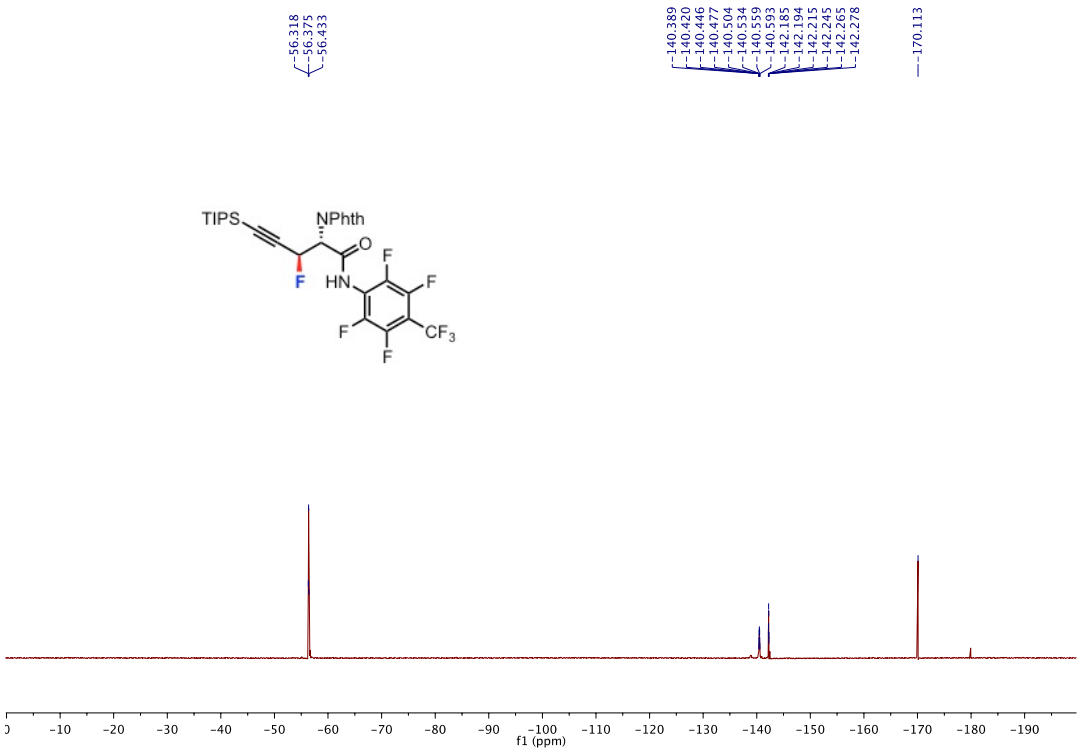

8.279
8.260
7.893
7.888
7.885
7.879
7.796
7.791
7.787
7.783
7.778
7.775
7.769
7.707
7.702
7.699
7.693
5.757
5.753
5.743
5.739
5.729
5.726
5.676
5.669
5.662
5.657
5.649
5.643
5.164
5.149
5.142
5.127
3.711
3.699
3.687
2.014
2.002
1.990
1.977
1.965
1.953
1.939
1.927
1.913
1.901
1.889
1.878
1.852
1.848
1.837
1.832
1.822
1.808
1.793
1.782
1.771
1.768
1.756
NPhth
PhthN
F
HN
O
F
F
F
F
CF3
F
1.01
1.98
4.01
2.03
1.00
0.94
1.96
3.93
f1 (ppm)


168.223
167.460
164.010
134.729
133.997
131.904
131.449
124.070
123.253
91.636
90.512
77.000
55.992
55.794
37.120
29.660
29.523
23.294
23.273
NPhth
PhthN
F
HN
O
F
F
F
F
CF3
F
f1 (ppm)


-56.303
-56.361
-56.419
-140.571
-140.589
-140.621
-140.645
-140.676
-140.703
-140.733
-140.757
-140.791
-140.814
-142.149
-142.169
-142.199
-142.219
-181.851
NPhth
PhthN
O
F
HN
F
F
F
CF3
F
f1 (ppm)


8.014
7.993
7.911
7.903
7.898
7.890
7.796
7.789
7.783
7.775
6.374
6.351
6.250
6.227
5.344
5.320
5.311
5.285
0.859
TIPS
NPhth
O
F
HN
F
F
F
CF3
F
1.08
2.07
2.08
1.00
1.01
21.07
f1 (ppm)


166.881
162.904
162.887
134.687
131.572
123.981
97.603
97.453
95.399
95.340
80.992
79.859
77.000
55.808
55.593
18.153
10.708
TIPS
NPhth
O
F
HN
F
F
F
CF3
F
f1 (ppm)


56.318
56.375
56.433
140.389
140.420
140.446
140.477
140.504
140.534
140.559
140.593
142.185
142.194
142.215
142.245
142.265
142.278
170.113
TIPS
NPhth
O
F
HN
F
F
F
CF3
F
f1 (ppm)

X-ray Crystallographic Data of 2c

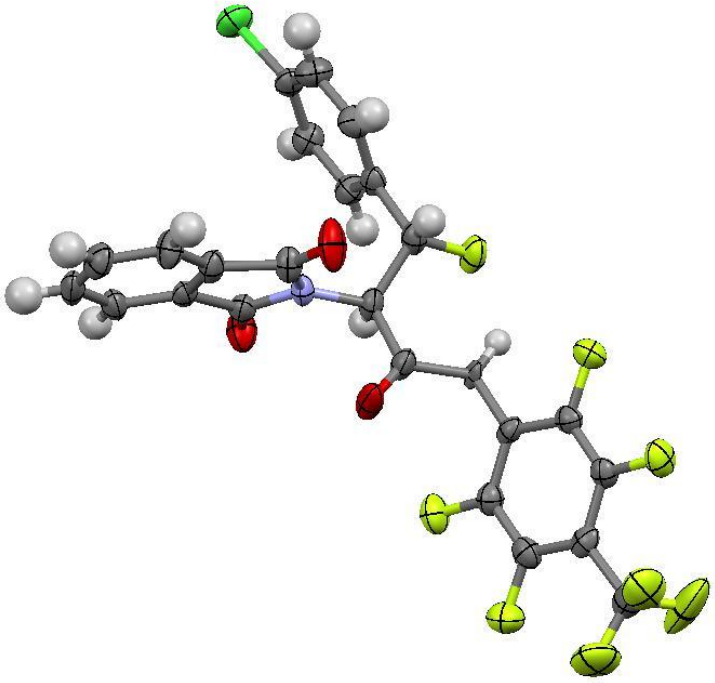


Table 1. Crystal data and structure refinement for **2c**.

Identification code	**2c**	
Empirical formula	$C_{24}H_{11}ClF_8N_2O_3$	
Formula weight	562.80	
Temperature	100.0 K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P1	
Unit cell dimensions	a = 8.4169(5) Å	α= 100.935(2)°.
	b = 9.1537(5) Å	β= 101.544(2)°.
	c = 15.6960(8) Å	γ = 104.301(2)°.
Volume	1111.12(11) $Å^3$	
Z	2	
Density (calculated)	1.682 Mg/m^3	
Absorption coefficient	0.272 mm^{-1}	
F(000)	564	
Crystal size	0.3 x 0.25 x 0.2 mm^3	
Theta range for data collection	1.368 to 26.373°.	
Index ranges	-6<=h<=10, -11<=k<=11, -19<=l<=19	
Reflections collected	11968	

Independent reflections	6275 [R(int) = 0.0352]
Completeness to theta = 26.000°	99.6 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.0932 and 0.0596
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6275 / 3 / 685
Goodness-of-fit on F^2	1.040
Final R indices [I>2sigma(I)]	R1 = 0.0419, wR2 = 0.1199
R indices (all data)	R1 = 0.0526, wR2 = 0.1347
Absolute structure parameter	0.15(5)
Extinction coefficient	n/a
Largest diff. peak and hole	0.390 and -0.379 e.$Å^{-3}$

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **2c**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Cl(2)	11029(2)	-1359(2)	9375(1)	50(1)
Cl(1)	-751(2)	11527(2)	636(1)	55(1)
F(9)	6400(4)	378(3)	5951(2)	40(1)
F(12)	2588(4)	4621(4)	3527(2)	47(1)
F(10)	616(5)	1261(4)	5824(2)	51(1)
F(13)	4836(4)	3678(4)	4559(2)	42(1)
F(5)	5349(4)	6778(3)	5493(2)	43(1)
F(4)	7391(4)	5658(3)	6548(2)	47(1)
F(11)	-1676(4)	2092(4)	4758(3)	60(1)
F(1)	4103(4)	10014(4)	4079(2)	49(1)
F(3)	11842(4)	7694(4)	5272(2)	58(1)
F(2)	9777(5)	8708(4)	4211(2)	51(1)
O(6)	4056(5)	500(4)	8204(2)	43(1)
O(5)	8432(6)	4764(4)	8442(3)	53(1)
N(3)	6248(5)	2497(4)	8113(2)	29(1)
O(1)	5977(6)	9957(4)	1445(3)	53(1)
O(4)	3720(6)	3226(5)	7110(2)	53(1)
F(6)	10115(6)	4597(5)	6605(3)	75(1)
O(3)	6624(6)	6981(5)	2942(2)	54(1)
N(1)	4376(5)	7972(4)	1900(3)	30(1)
N(4)	4048(6)	2050(5)	5778(3)	38(1)
O(2)	2580(7)	5648(4)	1931(3)	60(1)
F(15)	-2219(6)	3980(7)	3786(4)	101(2)
F(14)	-322(6)	5223(6)	3343(3)	89(2)
F(8)	12237(6)	5970(6)	6345(3)	80(1)
C(2)	4360(6)	7444(5)	413(3)	31(1)
N(2)	6365(6)	8293(5)	4255(3)	36(1)
C(32)	7415(7)	3874(5)	8680(3)	35(1)
F(7)	11249(8)	6913(6)	7402(3)	116(2)
C(15)	678(7)	8811(6)	2154(4)	40(1)
C(10)	2337(7)	9677(5)	2620(3)	33(1)
C(31)	7067(7)	3933(6)	9573(3)	33(1)
C(25)	5173(7)	1695(6)	8556(3)	32(1)

C(22)	8020(7)	6424(5)	5977(3)	34(1)
C(6)	2484(8)	4810(6)	-132(3)	46(1)
C(3)	4648(7)	7453(7)	-421(4)	40(1)
C(23)	6952(6)	6981(5)	5431(3)	32(1)
C(1)	5044(7)	8643(6)	1270(3)	34(1)
C(35)	7281(6)	-90(5)	7393(3)	31(1)
C(45)	367(7)	3405(6)	4104(3)	34(1)
C(44)	-61(7)	2548(6)	4707(4)	38(1)
C(33)	6029(7)	2100(5)	7155(3)	32(1)
C(13)	420(7)	10824(6)	1422(3)	38(1)
C(46)	2051(7)	3785(5)	4080(3)	33(1)
C(43)	1124(7)	2119(5)	5267(3)	35(1)
C(7)	3302(7)	6132(6)	553(3)	37(1)
C(26)	5744(6)	2636(6)	9511(3)	32(1)
C(18)	7476(7)	7726(5)	4810(3)	31(1)
C(39)	7891(7)	-1722(6)	8367(4)	39(1)
F(16)	-1473(9)	2852(7)	2709(4)	161(4)
C(48)	-935(8)	3849(7)	3471(4)	50(2)
C(40)	6747(6)	-1316(6)	7766(4)	37(1)
C(38)	9589(7)	-897(6)	8592(3)	38(1)
C(19)	9145(7)	7937(6)	4772(3)	36(1)
C(42)	2799(7)	2489(5)	5234(3)	32(1)
C(21)	9688(7)	6611(6)	5942(3)	34(1)
C(16)	6030(7)	7878(6)	3333(3)	37(1)
C(29)	7213(9)	4829(7)	11113(4)	50(2)
C(47)	3228(6)	3306(6)	4619(3)	31(1)
C(11)	2994(7)	11134(6)	2483(3)	38(1)
C(41)	4470(7)	2519(6)	6696(3)	38(1)
C(28)	5915(8)	3523(7)	11050(3)	48(1)
C(34)	6007(6)	401(5)	6792(3)	31(1)
C(12)	2038(7)	11727(5)	1895(3)	36(1)
C(8)	4906(7)	8743(6)	2859(3)	34(1)
C(9)	3408(7)	8980(6)	3209(3)	38(1)
C(14)	-272(7)	9392(6)	1558(4)	47(1)
C(01W)	3308(8)	6467(5)	1522(3)	36(1)
C(37)	10162(7)	300(6)	8207(4)	44(1)
C(20)	10236(7)	7410(6)	5335(3)	38(1)
C(4)	3846(8)	6111(7)	-1102(4)	47(1)

C(27)	5141(7)	2386(7)	10239(4)	43(1)
C(5)	2788(8)	4833(7)	-973(4)	46(1)
C(36)	9004(7)	704(6)	7608(4)	40(1)
C(24)	10847(9)	6072(8)	6589(4)	54(2)
C(30)	7828(8)	5046(6)	10380(3)	43(1)

Table 3. Bond lengths [Å] and angles [°] for **2c**.

Cl(2)-C(38)	1.736(5)
Cl(1)-C(13)	1.742(5)
F(9)-C(34)	1.422(5)
F(12)-C(46)	1.335(6)
F(10)-C(43)	1.345(6)
F(13)-C(47)	1.339(6)
F(5)-C(23)	1.342(6)
F(4)-C(22)	1.348(6)
F(11)-C(44)	1.343(6)
F(1)-C(9)	1.421(5)
F(3)-C(20)	1.339(7)
F(2)-C(19)	1.340(6)
O(6)-C(25)	1.200(6)
O(5)-C(32)	1.198(7)
N(3)-C(32)	1.400(6)
N(3)-C(25)	1.399(7)
N(3)-C(33)	1.440(6)
O(1)-C(1)	1.209(6)
O(4)-C(41)	1.203(7)
F(6)-C(24)	1.345(8)
O(3)-C(16)	1.198(7)
N(1)-C(1)	1.397(6)
N(1)-C(8)	1.462(6)
N(1)-C(01W)	1.387(6)
N(4)-H(4)	0.8800
N(4)-C(42)	1.405(6)
N(4)-C(41)	1.368(6)
O(2)-C(01W)	1.210(6)
F(15)-C(48)	1.297(8)
F(14)-C(48)	1.306(8)
F(8)-C(24)	1.320(8)
C(2)-C(3)	1.379(7)
C(2)-C(1)	1.471(7)
C(2)-C(7)	1.391(7)
N(2)-H(2)	0.8800
N(2)-C(18)	1.411(6)

N(2)-C(16)	1.376(6)
C(32)-C(31)	1.482(7)
F(7)-C(24)	1.289(7)
C(15)-H(15)	0.9500
C(15)-C(10)	1.392(7)
C(15)-C(14)	1.377(8)
C(10)-C(11)	1.387(7)
C(10)-C(9)	1.499(7)
C(31)-C(26)	1.385(7)
C(31)-C(30)	1.384(7)
C(25)-C(26)	1.496(7)
C(22)-C(23)	1.374(7)
C(22)-C(21)	1.386(8)
C(6)-H(6)	0.9500
C(6)-C(7)	1.375(7)
C(6)-C(5)	1.398(8)
C(3)-H(3)	0.9500
C(3)-C(4)	1.383(8)
C(23)-C(18)	1.372(7)
C(35)-C(40)	1.381(7)
C(35)-C(34)	1.495(7)
C(35)-C(36)	1.391(7)
C(45)-C(44)	1.387(8)
C(45)-C(46)	1.383(8)
C(45)-C(48)	1.514(8)
C(44)-C(43)	1.377(8)
C(33)-H(33)	1.0000
C(33)-C(41)	1.537(7)
C(33)-C(34)	1.545(6)
C(13)-C(12)	1.377(7)
C(13)-C(14)	1.372(8)
C(46)-C(47)	1.381(7)
C(43)-C(42)	1.380(8)
C(7)-C(01W)	1.492(7)
C(26)-C(27)	1.375(8)
C(18)-C(19)	1.385(8)
C(39)-H(39)	0.9500
C(39)-C(40)	1.380(7)

C(39)-C(38)	1.378(7)
F(16)-C(48)	1.277(7)
C(40)-H(40)	0.9500
C(38)-C(37)	1.380(8)
C(19)-C(20)	1.383(8)
C(42)-C(47)	1.380(7)
C(21)-C(20)	1.389(7)
C(21)-C(24)	1.503(8)
C(16)-C(8)	1.545(7)
C(29)-H(29)	0.9500
C(29)-C(28)	1.378(9)
C(29)-C(30)	1.379(8)
C(11)-H(11)	0.9500
C(11)-C(12)	1.380(7)
C(28)-H(28)	0.9500
C(28)-C(27)	1.400(8)
C(34)-H(34)	1.0000
C(12)-H(12)	0.9500
C(8)-H(8)	1.0000
C(8)-C(9)	1.518(8)
C(9)-H(9)	1.0000
C(14)-H(14)	0.9500
C(37)-H(37)	0.9500
C(37)-C(36)	1.384(8)
C(4)-H(4A)	0.9500
C(4)-C(5)	1.360(9)
C(27)-H(27)	0.9500
C(5)-H(5)	0.9500
C(36)-H(36)	0.9500
C(30)-H(30)	0.9500

C(32)-N(3)-C(33)	122.5(4)
C(25)-N(3)-C(32)	112.6(4)
C(25)-N(3)-C(33)	124.3(4)
C(1)-N(1)-C(8)	122.4(4)
C(01W)-N(1)-C(1)	112.4(4)
C(01W)-N(1)-C(8)	124.9(4)
C(42)-N(4)-H(4)	118.8

C(41)-N(4)-H(4)	118.8
C(41)-N(4)-C(42)	122.4(4)
C(3)-C(2)-C(1)	130.7(5)
C(3)-C(2)-C(7)	120.8(5)
C(7)-C(2)-C(1)	108.4(4)
C(18)-N(2)-H(2)	118.9
C(16)-N(2)-H(2)	118.9
C(16)-N(2)-C(18)	122.2(4)
O(5)-C(32)-N(3)	124.2(5)
O(5)-C(32)-C(31)	130.7(5)
N(3)-C(32)-C(31)	105.1(4)
C(10)-C(15)-H(15)	120.0
C(14)-C(15)-H(15)	120.0
C(14)-C(15)-C(10)	120.1(5)
C(15)-C(10)-C(9)	119.7(4)
C(11)-C(10)-C(15)	118.8(5)
C(11)-C(10)-C(9)	121.4(5)
C(26)-C(31)-C(32)	109.2(4)
C(30)-C(31)-C(32)	130.0(5)
C(30)-C(31)-C(26)	120.7(5)
O(6)-C(25)-N(3)	124.6(4)
O(6)-C(25)-C(26)	130.0(5)
N(3)-C(25)-C(26)	105.4(4)
F(4)-C(22)-C(23)	118.0(5)
F(4)-C(22)-C(21)	120.3(5)
C(23)-C(22)-C(21)	121.7(5)
C(7)-C(6)-H(6)	121.5
C(7)-C(6)-C(5)	117.0(5)
C(5)-C(6)-H(6)	121.5
C(2)-C(3)-H(3)	121.4
C(2)-C(3)-C(4)	117.2(5)
C(4)-C(3)-H(3)	121.4
F(5)-C(23)-C(22)	119.5(5)
F(5)-C(23)-C(18)	118.8(5)
C(18)-C(23)-C(22)	121.6(5)
O(1)-C(1)-N(1)	123.8(5)
O(1)-C(1)-C(2)	130.3(5)
N(1)-C(1)-C(2)	105.8(4)

C(40)-C(35)-C(34)	119.9(4)
C(40)-C(35)-C(36)	119.2(5)
C(36)-C(35)-C(34)	120.8(4)
C(44)-C(45)-C(48)	122.4(5)
C(46)-C(45)-C(44)	116.4(5)
C(46)-C(45)-C(48)	121.1(5)
F(11)-C(44)-C(45)	120.4(5)
F(11)-C(44)-C(43)	117.5(5)
C(43)-C(44)-C(45)	122.1(5)
N(3)-C(33)-H(33)	106.8
N(3)-C(33)-C(41)	109.1(4)
N(3)-C(33)-C(34)	112.2(4)
C(41)-C(33)-H(33)	106.8
C(41)-C(33)-C(34)	114.6(4)
C(34)-C(33)-H(33)	106.8
C(12)-C(13)-Cl(1)	118.8(4)
C(14)-C(13)-Cl(1)	120.0(4)
C(14)-C(13)-C(12)	121.2(5)
F(12)-C(46)-C(45)	120.8(5)
F(12)-C(46)-C(47)	117.8(5)
C(47)-C(46)-C(45)	121.5(5)
F(10)-C(43)-C(44)	119.0(5)
F(10)-C(43)-C(42)	119.7(5)
C(44)-C(43)-C(42)	121.2(5)
C(2)-C(7)-C(01W)	107.8(4)
C(6)-C(7)-C(2)	121.6(5)
C(6)-C(7)-C(01W)	130.5(5)
C(31)-C(26)-C(25)	107.7(4)
C(27)-C(26)-C(31)	122.1(5)
C(27)-C(26)-C(25)	130.2(5)
C(23)-C(18)-N(2)	120.9(5)
C(23)-C(18)-C(19)	117.4(5)
C(19)-C(18)-N(2)	121.6(5)
C(40)-C(39)-H(39)	120.3
C(38)-C(39)-H(39)	120.3
C(38)-C(39)-C(40)	119.3(5)
F(15)-C(48)-F(14)	103.4(6)
F(15)-C(48)-C(45)	112.8(5)

F(14)-C(48)-C(45)	112.1(5)
F(16)-C(48)-F(15)	109.1(7)
F(16)-C(48)-F(14)	108.5(6)
F(16)-C(48)-C(45)	110.6(5)
C(35)-C(40)-H(40)	119.6
C(39)-C(40)-C(35)	120.8(5)
C(39)-C(40)-H(40)	119.6
C(39)-C(38)-Cl(2)	119.7(4)
C(39)-C(38)-C(37)	121.0(5)
C(37)-C(38)-Cl(2)	119.3(4)
F(2)-C(19)-C(18)	121.2(5)
F(2)-C(19)-C(20)	117.6(5)
C(20)-C(19)-C(18)	121.1(5)
C(43)-C(42)-N(4)	123.3(5)
C(43)-C(42)-C(47)	117.1(5)
C(47)-C(42)-N(4)	119.6(5)
C(22)-C(21)-C(20)	116.7(5)
C(22)-C(21)-C(24)	120.1(5)
C(20)-C(21)-C(24)	123.0(6)
O(3)-C(16)-N(2)	122.7(5)
O(3)-C(16)-C(8)	123.5(5)
N(2)-C(16)-C(8)	113.7(4)
C(28)-C(29)-H(29)	119.4
C(28)-C(29)-C(30)	121.1(5)
C(30)-C(29)-H(29)	119.4
F(13)-C(47)-C(46)	119.2(4)
F(13)-C(47)-C(42)	119.0(5)
C(42)-C(47)-C(46)	121.7(5)
C(10)-C(11)-H(11)	119.4
C(12)-C(11)-C(10)	121.2(5)
C(12)-C(11)-H(11)	119.4
O(4)-C(41)-N(4)	123.4(5)
O(4)-C(41)-C(33)	122.7(4)
N(4)-C(41)-C(33)	113.9(4)
C(29)-C(28)-H(28)	119.2
C(29)-C(28)-C(27)	121.5(5)
C(27)-C(28)-H(28)	119.2
F(9)-C(34)-C(35)	110.0(4)

F(9)-C(34)-C(33)	104.4(3)
F(9)-C(34)-H(34)	109.7
C(35)-C(34)-C(33)	113.1(4)
C(35)-C(34)-H(34)	109.7
C(33)-C(34)-H(34)	109.7
C(13)-C(12)-C(11)	118.7(5)
C(13)-C(12)-H(12)	120.7
C(11)-C(12)-H(12)	120.7
N(1)-C(8)-C(16)	107.6(4)
N(1)-C(8)-H(8)	106.2
N(1)-C(8)-C(9)	111.3(4)
C(16)-C(8)-H(8)	106.2
C(9)-C(8)-C(16)	118.5(4)
C(9)-C(8)-H(8)	106.2
F(1)-C(9)-C(10)	109.6(4)
F(1)-C(9)-C(8)	106.3(4)
F(1)-C(9)-H(9)	109.6
C(10)-C(9)-C(8)	112.0(4)
C(10)-C(9)-H(9)	109.6
C(8)-C(9)-H(9)	109.6
C(15)-C(14)-H(14)	120.0
C(13)-C(14)-C(15)	119.9(5)
C(13)-C(14)-H(14)	120.0
N(1)-C(01W)-C(7)	105.5(4)
O(2)-C(01W)-N(1)	124.7(5)
O(2)-C(01W)-C(7)	129.8(5)
C(38)-C(37)-H(37)	120.4
C(38)-C(37)-C(36)	119.2(5)
C(36)-C(37)-H(37)	120.4
F(3)-C(20)-C(19)	117.5(5)
F(3)-C(20)-C(21)	121.1(5)
C(19)-C(20)-C(21)	121.4(5)
C(3)-C(4)-H(4A)	118.9
C(5)-C(4)-C(3)	122.2(5)
C(5)-C(4)-H(4A)	118.9
C(26)-C(27)-C(28)	116.7(5)
C(26)-C(27)-H(27)	121.7
C(28)-C(27)-H(27)	121.7

C(6)-C(5)-H(5)	119.5
C(4)-C(5)-C(6)	121.1(5)
C(4)-C(5)-H(5)	119.5
C(35)-C(36)-H(36)	119.8
C(37)-C(36)-C(35)	120.4(5)
C(37)-C(36)-H(36)	119.8
F(6)-C(24)-C(21)	111.0(5)
F(8)-C(24)-F(6)	102.4(5)
F(8)-C(24)-C(21)	113.2(6)
F(7)-C(24)-F(6)	107.0(6)
F(7)-C(24)-F(8)	109.7(6)
F(7)-C(24)-C(21)	112.9(5)
C(31)-C(30)-H(30)	121.0
C(29)-C(30)-C(31)	117.9(6)
C(29)-C(30)-H(30)	121.0

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **2c**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Cl(2)	43(1)	58(1)	50(1)	14(1)	-1(1)	25(1)
Cl(1)	52(1)	69(1)	56(1)	30(1)	9(1)	32(1)
F(9)	57(2)	49(2)	23(1)	5(1)	12(1)	31(2)
F(12)	56(2)	52(2)	41(2)	26(1)	15(2)	15(2)
F(10)	65(2)	50(2)	43(2)	22(1)	21(2)	11(2)
F(13)	33(2)	51(2)	44(2)	12(1)	13(1)	14(1)
F(5)	36(2)	52(2)	44(2)	12(1)	14(1)	18(1)
F(4)	59(2)	50(2)	46(2)	27(2)	21(2)	25(2)
F(11)	34(2)	75(2)	67(2)	18(2)	17(2)	5(2)
F(1)	64(2)	55(2)	28(2)	1(1)	6(2)	33(2)
F(3)	36(2)	80(2)	60(2)	20(2)	13(2)	15(2)
F(2)	62(2)	55(2)	42(2)	21(2)	23(2)	15(2)
O(6)	33(2)	50(2)	37(2)	2(2)	9(2)	1(2)
O(5)	71(3)	37(2)	37(2)	5(2)	14(2)	-6(2)
N(3)	31(2)	31(2)	23(2)	3(2)	7(2)	9(2)
O(1)	61(3)	42(2)	44(2)	6(2)	18(2)	-2(2)
O(4)	70(3)	69(3)	28(2)	0(2)	8(2)	51(2)
F(6)	91(3)	80(3)	82(3)	48(2)	28(2)	50(2)
O(3)	76(3)	69(3)	28(2)	3(2)	7(2)	50(2)
N(1)	39(2)	31(2)	21(2)	7(2)	7(2)	12(2)
N(4)	53(3)	43(2)	24(2)	7(2)	8(2)	30(2)
O(2)	99(4)	40(2)	39(2)	15(2)	28(2)	5(2)
F(15)	60(3)	145(4)	137(4)	79(4)	33(3)	62(3)
F(14)	81(3)	100(3)	107(4)	68(3)	11(3)	42(3)
F(8)	61(3)	105(3)	99(3)	47(3)	18(2)	53(3)
C(2)	31(2)	36(2)	32(2)	12(2)	7(2)	20(2)
N(2)	51(3)	39(2)	24(2)	2(2)	5(2)	29(2)
C(32)	45(3)	30(2)	30(2)	9(2)	8(2)	13(2)
F(7)	165(5)	134(4)	42(2)	-22(2)	-37(3)	115(4)
C(15)	37(3)	36(2)	49(3)	16(2)	10(2)	9(2)
C(10)	42(3)	36(2)	29(2)	6(2)	12(2)	22(2)
C(31)	39(3)	38(2)	23(2)	4(2)	2(2)	19(2)
C(25)	33(3)	40(3)	25(2)	6(2)	6(2)	15(2)

C(22)	42(3)	30(2)	28(2)	7(2)	8(2)	11(2)
C(6)	58(4)	40(3)	35(3)	3(2)	8(3)	11(3)
C(3)	43(3)	51(3)	36(3)	15(2)	15(2)	21(3)
C(23)	29(2)	34(2)	32(2)	0(2)	9(2)	13(2)
C(1)	35(3)	42(3)	32(2)	14(2)	9(2)	20(2)
C(35)	31(2)	32(2)	28(2)	4(2)	7(2)	11(2)
C(45)	33(3)	39(3)	23(2)	1(2)	1(2)	9(2)
C(44)	30(3)	37(3)	39(3)	1(2)	4(2)	10(2)
C(33)	40(3)	36(2)	21(2)	4(2)	7(2)	16(2)
C(13)	40(3)	43(3)	36(3)	13(2)	8(2)	23(2)
C(46)	45(3)	32(2)	24(2)	7(2)	9(2)	13(2)
C(43)	46(3)	30(2)	30(2)	9(2)	16(2)	6(2)
C(7)	45(3)	39(3)	30(2)	10(2)	8(2)	18(2)
C(26)	32(2)	43(3)	24(2)	9(2)	6(2)	21(2)
C(18)	39(3)	31(2)	22(2)	3(2)	2(2)	15(2)
C(39)	35(3)	35(2)	45(3)	16(2)	5(2)	9(2)
F(16)	211(7)	138(5)	78(3)	-60(3)	-97(4)	129(5)
C(48)	47(4)	59(4)	41(3)	5(3)	-1(3)	28(3)
C(40)	27(2)	38(3)	47(3)	11(2)	7(2)	11(2)
C(38)	35(3)	42(3)	40(3)	9(2)	8(2)	21(2)
C(19)	45(3)	31(2)	31(3)	8(2)	10(2)	7(2)
C(42)	42(3)	28(2)	26(2)	2(2)	7(2)	16(2)
C(21)	38(3)	35(2)	29(2)	3(2)	2(2)	17(2)
C(16)	47(3)	44(3)	22(2)	5(2)	6(2)	21(3)
C(29)	63(4)	55(3)	28(3)	-1(2)	1(3)	25(3)
C(47)	29(3)	35(2)	25(2)	5(2)	6(2)	8(2)
C(11)	41(3)	35(2)	34(2)	7(2)	7(2)	11(2)
C(41)	47(3)	37(3)	29(2)	8(2)	3(2)	18(2)
C(28)	52(3)	74(4)	26(3)	13(3)	16(3)	29(3)
C(34)	33(2)	37(2)	25(2)	7(2)	11(2)	14(2)
C(12)	39(3)	31(2)	39(3)	10(2)	10(2)	11(2)
C(8)	46(3)	34(2)	22(2)	5(2)	8(2)	15(2)
C(9)	52(3)	38(3)	25(2)	5(2)	10(2)	20(2)
C(14)	36(3)	46(3)	53(3)	15(3)	3(3)	10(3)
C(01W)	52(3)	30(2)	29(2)	8(2)	12(2)	15(2)
C(37)	28(3)	47(3)	57(3)	17(3)	9(3)	11(2)
C(20)	35(3)	40(3)	37(3)	4(2)	9(2)	14(2)
C(4)	60(4)	66(4)	27(3)	14(3)	13(3)	39(3)

C(27)	35(3)	57(3)	38(3)	12(2)	6(2)	16(3)
C(5)	52(3)	47(3)	32(3)	-2(2)	-1(3)	19(3)
C(36)	34(3)	44(3)	52(3)	22(2)	16(2)	15(2)
C(24)	59(4)	57(4)	40(3)	2(3)	-4(3)	30(3)
C(30)	52(3)	42(3)	31(3)	1(2)	5(2)	16(3)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^{3}) for **2c**.

	x	y	z	U(eq)
H(4)	4578	1450	5518	45
H(2)	5869	8935	4507	44
H(15)	201	7817	2247	48
H(6)	1745	3922	-37	55
H(3)	5367	8345	-522	49
H(33)	7042	2787	7036	38
H(39)	7514	-2563	8623	47
H(40)	5577	-1885	7606	45
H(29)	7694	5591	11670	60
H(11)	4124	11735	2800	45
H(28)	5536	3393	11570	57
H(34)	4845	-319	6698	37
H(12)	2486	12739	1818	43
H(8)	5668	9807	2922	40
H(9)	2697	7961	3254	45
H(14)	-1406	8802	1242	56
H(37)	11339	841	8352	52
H(4A)	4041	6081	-1680	56
H(27)	4244	1486	10194	52
H(5)	2248	3941	-1463	56
H(36)	9387	1528	7341	49
H(30)	8743	5932	10428	52