Supporting Information

Unstrained C-C Bond Activation and Directed Fluorination through Photocatalytically-Generated Radical Cations

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Contents:

General. Unless otherwise stated, all reactions were carried out under strictly anhydrous conditions under N_2 atmosphere. All solvents were dried and distilled by standard methods. All ^1H and ^{13}C NMR spectra were acquired on a 400 MHz NMR spectrometer in $CDCl_3$ or CD_3OD, and ^{19}F spectra were acquired on a 300 MHz NMR spectrometer in $CDCl_3$, CD_3OD, or CD_3CN. The ^1H, ^{13}C, and ^{19}F NMR chemical shifts are given in parts per million (δ) with respect to an internal tetramethylsilane (TMS, δ = 0.00 ppm) standard and/or 3-chlorobenzotrifluoride (δ = −64.2 ppm relative to $CFCl_3$).[1] NMR data are reported in the following format: chemical shift (integration, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet), coupling constants (Hz)). IR data were obtained using an ATR-IR instrument. The 2-aryl ketone precursors for compounds **1-6**, **9-14**, and **18-20** were synthesized using the Pd-catalyzed 2-arylation procedure by Kawatsura and Hartwig;[2] the precursors for compounds **7**, **15**, and **17** were synthesized using standard Grignard reactions[3] followed by PCC oxidations;[4] the precursor for compound **8** was synthesized using the Pd-catalyzed 2-arylation procedure by Willis, Taylor, and Gillmore.[5] The ethylene glycol acetals were synthesized according to a general literature procedure.[6] Characterization data for **16** is consistent with literature.[7] Spectral data were analyzed with the ACD/NMR Processor Academic Edition[8] and processed on Bruker software. The Gaussian '09 package was used for all calculations.[9] Geometry optimizations were performed at the B3PW91/6-311++G** level of theory employing the default MeCN solvent continuum.

Representative Procedures.

Selectfluor (195 mg, 0.55 mmol, 2.2 equiv.), 9-fluorenone (9 mg, 0.25 mmol, 0.2 equiv.), and the substrate (0.25 mmol, 1.0 equiv.) were added to an oven-dried microwave vial equipped with a stir bar. The microwave vial was sealed via crimper with a cap w/ septum; it was evacuated and refilled with N_2 multiple times. Anhydrous CH_3CN (3 mL) was then added to the vial via syringe under N_2 atmosphere. The reaction mixture was stirred in a Rayonet reactor and irradiated at 300 nm for 12 h.

To obtain carboxylic acid: The reaction mixture was diluted with approximately equal parts H_2O. $LiOH{\cdot}H_2O$ (63 mg, 1.25 mmol, 5.0 equiv.) was added, and the reaction mixture was stirred for 25 min. open to air. The mixture was acidified with 1 M HCl (pH ~2) and extracted into CH_2Cl_2. The combined organic layers were dried with $MgSO_4$, filtered through Celite, and concentrated. Products typically columned on Florisil,

[1] D. Naumann and J. Kischkewitz, *J. Fluorine Chem*., 1990, **47**, 283-299.
[2] M. Kawatsura and J. F. Hartwig, *J. Am. Chem. Soc.*, 1999, **121**, 1473-1478.
[3] a) G. F. Woods and F. Scotti, *J. Org. Chem.*, 1961, **26**, 312-318. b) E. Pinard, S. M. Ceccarelli, H. Stalder, and D. Alberati, *Bioorg. Med. Chem. Lett.*, 2006, **16**, 349-352.
[4] M. Ceylan, S. Yalcin, H. Secen, Y. Suetbeyaz, and M. Balci, *J. Chem. Res-S.*, 2003, **1**, 21-23.
[5] M. C. Willis, D. Taylor, and A. T. Gillmore, *Tetrahedron*, 2006, **62**, 11513-11520.
[6] C. Djerassi, G. von Mutzenbecher, J. Fajkos, D. H. Williams, and H. Budzikiewicz, *J. Am. Chem. Soc.*, 1965, **87**, 817-826.
[7] J-B. Xia, C. Zhu, and C. Chen, *J. Am. Chem. Soc.*, 2013, **135**, 17494-17500.
[8] ACD/NMR Processor Academic Edition, version 12.0, Advanced Chemistry Development, Inc., Toronto, ON, Canada, www.acdlabs.com, **2012**.
[9] A. Huczynski, J. Rutkowski, and B. Brzezinski, *Struct. Chem.*, 2011, **22**, 627-634.

eluting with 5:94:1 EtOAc:Hexanes:AcOH. (Do not column on silica – it promotes dehydrofluorination.) Better results can be achieved by flushing the loaded column with a few column volumes of EtOAc:Hexanes before acidifying it. Analytical purity can be obtained via subsequent gradient C18 column chromatography, eluting with MeCN/H_2O.

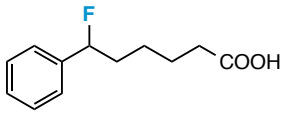
To obtain methyl ester: The reaction mixture was diluted with approximately equal parts H_2O. LiOMe (47 mg, 1.25 mmol, 5.0 equiv.) was added, and the reaction mixture was stirred for 25 min. open to air. The mixture was extracted into CH_2Cl_2. The combined organic layers were dried with $MgSO_4$, filtered through Celite, and concentrated. Products typically columned on Florisil, eluting with 5:95 EtOAc:Hexanes. (Do not column on silica – it promotes dehydrofluorination.) Analytical purity can be obtained via subsequent gradient C18 column chromatography, eluting with MeCN/H_2O, or via flash chromatography on silica gel, eluting with 10:90 EtOAc:Toluene.

To obtain alcohol: The reaction mixture was concentrated and dissolved in 10 mL anhydrous THF under N_2 atmosphere. After cooling to 0 °C, $LiAlH_4$ (57 mg, 1.50 mmol, 6.0 equiv.) was added to the reaction mixture; the mixture slowly warmed to rt and was stirred vigorously for 1 h. The reaction was quenched and worked up via the standard Fieser method. Products typically columned on Florisil, eluting with 5:95 EtOAc:Hexanes. (Do not column on silica – it promotes dehydrofluorination.) Analytical purity can be obtained via subsequent gradient C18 column chromatography, eluting with MeCN/H_2O.

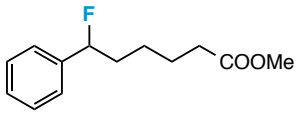
To obtain ketone/fragmentation product: The reaction mixture was diluted with approximately equal parts H_2O and was stirred for 25 min. open to air. The mixture was extracted into CH_2Cl_2. The combined organic layers were dried with $MgSO_4$, filtered through Celite, and concentrated. Products typically columned on Florisil, eluting with 5:95 EtOAc:Hexanes. (Do not column on silica – it promotes dehydrofluorination.) Analytical purity can be obtained via subsequent gradient C18 column chromatography, eluting with MeCN/H_2O.

Gram Scale Example: Selectfluor (3.90 g, 11.0 mmol, 2.2 equiv.), 9-fluorenone (0.180 g, 1.0 mmol, 0.2 equiv.), and 6-phenyl-1,4-dioxaspiro[4.5]decane (1.09 g, 5.0 mmol, 1.0 equiv.) were added to an oven-dried round bottom flask equipped with a stir bar. The flask was evacuated and refilled with N_2 multiple times. Anhydrous CH_3CN (60 mL) was then added to the flask via syringe under N_2 atmosphere. The reaction mixture was stirred in a Rayonet reactor and irradiated at 300 nm for 12 h. The reaction was worked up to obtain 6-fluoro-6-phenyl-hexanoic acid as outlined above in 54% yield (568 mg).

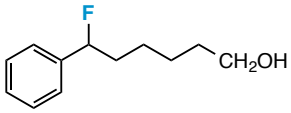
Compound Characterization



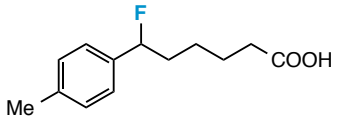
6-fluoro-6-phenyl-hexanoic acid (**1**). 60% yield. Clear oil. υ_{max}/cm^{-1} 3300-2500 (COOH) and 1708 (CO). ^{1}H NMR ($CDCl_3$): 11.26 (1H, br s), 7.38-7.30 (5H, m), 5.42 (1H, ddd, *J* = 47.9, 8.0, 4.9 Hz), 2.36 (2H, t, *J* = 7.4 Hz), 2.05-1.92 (1H, m), 1.91-1.75 (1H, m), 1.68 (2H, quint, *J* = 7.5 Hz), 1.59-1.48 (1H, m), 1.48-1.37 (1H, m); ^{13}C NMR ($CDCl_3$): 180.2, 140.2 (d, *J* = 19.9 Hz), 128.4, 128.2, 125.5 (d, *J* = 7.4 Hz), 94.3 (d, *J* = 170.3 Hz), 36.8 (d, *J* = 23.6 Hz), 33.9, 24.5 (d, *J* = 4.4 Hz), 24.3; ^{19}F NMR ($CDCl_3$): -174.31 (1F, ddd, *J* = 47.0, 28.7, 17.2 Hz).



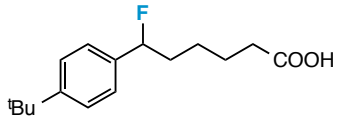
methyl 6-fluoro-6-phenylhexanoate (**2**). 59% yield. Clear oil. υ_{max}/cm^{-1} 1733 (CO). ^{1}H NMR ($CDCl_3$): 7.41-7.29 (5H, m), 5.42 (1H, ddd, *J* = 47.8, 8.0, 4.8 Hz), 3.66 (3H, s), 2.32 (2H, t, *J* = 7.5 Hz), 2.09-1.92 (1H, m), 1.76-1.74 (1H, m), 1.72-1.64 (2H, m), 1.56-1.36 (2H, m); ^{13}C NMR ($CDCl_3$): 173.9, 140.4, 140.2, 128.4, 128.23, 128.21, 125.51, 125.44, 94.3 (d, *J* = 171 Hz), 51.5, 37.0, 36.7, 33.9, 24.7, 24.6; ^{19}F NMR ($CDCl_3$): -174.24 (1F, ddd, *J* = 47.0, 27.5, 16.1 Hz).



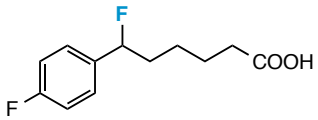
6-fluoro-6-phenylhexan-1-ol (**3**). 55% yield. Clear oil. υ_{max}/cm^{-1} 3381 (OH). ^{1}H NMR ($CDCl_3$): 7.40-7.35 (2H, m), 7.34-7.30 (3H, m), 5.43 (1H, ddd, *J* = 47.7, 8.0, 4.9 Hz), 3.64 (2H, m), 2.06-1.91 (1H, m), 1.90-1.75 (1H, m), 1.61-1.47 (3H, m), 1.47-1.37 (3H, m); ^{13}C NMR ($CDCl_3$): 140.6, 140.4, 128.4, 128.18, 128.17, 125.53, 125.46, 94.5 (d, *J* = 170.3 Hz), 62.8, 37.3, 37.0, 32.6, 25.5, 24.90, 24.86; ^{19}F NMR ($CDCl_3$): -173.96 (1F, ddd, *J* = 45.9, 27.5, 16.1 Hz).



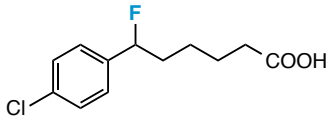
6-fluoro-6-(*p*-tolyl)hexanoic acid (**4**). 42% yield. White solid; m.p. 49-51 °C. υ_{max}/cm^{-1} 3300-2500 (COOH) and 1695 (CO). ^{1}H NMR ($CDCl_3$): 8.77 (1H, br s), 7.23-7.17 (4H, m), 5.39 (1H, ddd, *J* = 47.7, 8.2, 4.9 Hz), 2.43-2.33 (5H, m), 2.06-1.93 (1H, m), 1.90-1.76 (1H, m), 1.74-1.66 (2H, m), 1.59-1.50 (1H, m), 1.48-1.39 (1H, m); ^{13}C NMR ($CDCl_3$): 138.10, 138.07, 137.3, 137.1, 129.1, 125.6, 125.5, 94.3 (d, *J* = 169.5 Hz), 36.8, 36.6, 24.69, 24.65, 24.4, 21.2.^{19}F NMR ($CDCl_3$): -172.10 (1F, ddd, *J* = 45.9, 27.5, 16.1 Hz).



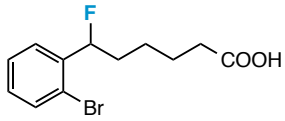
6-(4-(*tert*-butyl)phenyl)-6-fluorohexanoic acid (**5**). 64% yield. Clear oil. υ_{max}/cm^{-1} 3300-2500 (COOH) and 1706 (CO). ^{1}H NMR ($CDCl_3$): 11.47 (1H, br s), 7.40 (2H, dm, *J* = 8.6 Hz), 7.38 (2H, dm, *J* = 8.2 Hz), 5.40 (1H, ddd, *J* = 47.7, 8.2, 4.7 Hz), 2.36 (2H, t, *J* = 7.4 Hz), 2.09-1.93 (1H, m), 1.91-1.74 (1H, m), 1.70 (2H, quint, *J* = 7.8 Hz), 1.61-1.51 (1H, m), 1.50-1.38 (1H, m), 1.32 (9H, s); ^{13}C NMR ($CDCl_3$): 180.1, 151.30, 151.28, 137.3, 137.1, 125.38, 125.35, 125.31, 93.4 (d, *J* = 169.5 Hz), 36.7, 36.5, 34.6, 33.9, 31.31, 31.29, 24.73, 24.68, 24.4; ^{19}F NMR ($CDCl_3$): -172.34 (1F, ddd, *J* = 45.9, 28.7, 16.1 Hz).



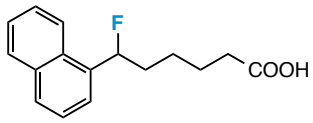
6-fluoro-6-(4-fluoro)phenyl-hexanoic acid (**6**). 70% yield. Clear oil. υ_{max}/cm^{-1} 3300-2500 (COOH) and 1705 (CO). ^{1}H NMR ($CDCl_3$): 11.27 (1H, br s), 7.31-7.26 (2H, m), 7.06 (2H, t, *J* = 8.4 Hz), 5.40 (1H, ddd, *J* = 47.9, 8.0, 4.9 Hz), 2.37 (2H, t, *J* = 7.4 Hz), 2.05-1.91 (1H, m), 1.89-1.75 (1H, m), 1.69 (2H, quint, *J* = 7.6 Hz), 1.58-1.48 (1H, m), 1.48-1.36 (1H, m); ^{13}C NMR ($CDCl_3$): 179.7, 162.6 (dd, *J* = 246.2, 2.2 Hz), 127.4 (d, *J* = 6.6 Hz), 127.3 (d, *J* = 6.6 Hz), 124.0 (d, *J* = 3.7 Hz), 115.4 (d, *J* = 21.4 Hz), 93.7 (d, *J* = 171.8 Hz), 36.8 (d, *J* = 24.3 Hz), 33.8, 24.6 (d, *J* = 4.4 Hz), 24.29; ^{19}F NMR ($CDCl_3$): -113.2 (1F, m), -172.0 (1F, ddd, *J* = 48.2, 28.7, 17.2 Hz).



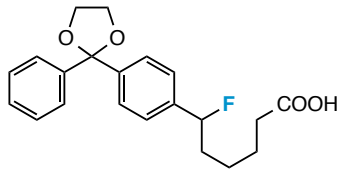
6-(4-chlorophenyl)-6-fluorohexanoic acid (**7**). 54% yield. Clear oil. υ_{max}/cm^{-1} 3300-2500 (COOH) and 1684 (CO). ^{1}H NMR ($CDCl_3$): 8.65 (1H, br s), 7.34 (2H, d, J = 7.8 Hz), 7.24 (2H, d, J = 8.6 Hz), 5.40 (1H, ddd, J = 47.3, 8.0, 4.7 Hz), 2.37 (1H, t, J = 7.0 Hz), 2.03-1.90 (1H, m), 1.89-1.75 (1H, m), 1.69 (2H, quint, J = 7.4 Hz), 1.58-1.48 (1H, m), 1.47-1.37 (1H, m); ^{13}C NMR ($CDCl_3$): 179.5, 138.8, 138.6, 134.02, 134.00, 128.6, 126.9, 126.8, 93.3 (J = 171.2 Hz), 36.86, 36.85, 36.63, 36.61, 24.5, 24.4, 24.3; ^{19}F NMR ($CDCl_3$): -174.74 (1F, ddd, J = 45.9, 27.5, 17.2 Hz).



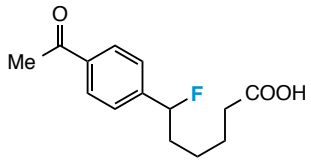
6-(2-bromophenyl)-6-fluorohexanoic acid (**8**). 63% yield. Clear oil. υ_{max}/cm^{-1} 3300-2500 (COOH) and 1685 (CO). ^{1}H NMR ($CDCl_3$): 7.52 (1H, dt, J = 8.0, 1.1 Hz), 7.48 (1H, dd, J = 7.8, 1.6 Hz), 7.36 (1H, td, J = 7.5, 1.2 Hz), 7.18 (1H, td, J = 7.8, 1.8 Hz), 5.76 (1H, ddd, J = 47.3, 8.4, 3.5 Hz), 2.40 (2H, t, J = 7.4 Hz), 2.02-1.82 (2H, m), 1.80-1.67 (2H, m), 1.66-1.54 (2H, m); ^{13}C NMR ($CDCl_3$): 178.7, 140.0, 139.8, 132.6, 129.4, 127.7, 126.8, 126.7, 120.64, 120.58, 93.1 (d, J = 172.5 Hz), 35.9, 35.6, 33.7, 24.61, 24.59, 24.3; ^{19}F NMR ($CDCl_3$): -181.16 (1F, ddd, J = 47.0, 32.1, 20.7 Hz).



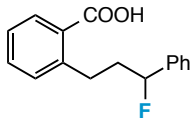
6-fluoro-6-(naphthalen-1-yl)hexanoic acid (**9**). 47% yield. Light brown oil. υ_{max}/cm^{-1} 3300-2500 (COOH) and 1704 (CO). ^{1}H NMR ($CDCl_3$): 11.22 (1H, br s), 7.96-7.93 (1H, m), 7.88-7.86 (1H, m), 7.81 (1H, d, J = 8.2 Hz), 7.57-7.45 (4H, m), 6.14 (1H, ddd, J = 47.1, 8.0, 4.3 Hz), 2.36 (2H, t, J = 7.2 Hz), 2.20-1.97 (2H, m), 1.78-1.51 (4H, m); ^{13}C NMR ($CDCl_3$): 179.8, 136.0, 135.8, 133.7, 129.85, 129.81, 128.9, 128.70, 128.68, 126.3, 125.7, 125.2, 123.1, 122.99, 122.94, 92.3 (d, J = 171.0 Hz), 36.4, 36.2, 25.09, 25.06, 24.4; ^{19}F NMR ($CDCl_3$): -178.13 (1F, ddd, J = 48.2, 29.8, 19.5 Hz).



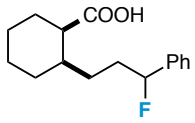
6-fluoro-6-(4-(2-phenyl-1,3-dioxolan-2-yl)phenyl)hexanoic acid (**10**). 51% yield. Clear oil. υ_{max}/cm^{-1} 3300-2500 (COOH) and 1706 (OH). ^{1}H NMR (CD_3OD): 7.48-7.45 (4H, m), 7.33-7.24 (5H, m), 5.42 (1H, ddd, J = 47.9, 8.2, 4.9 Hz), 4.02 (4H, s), 2.25 (2H, t, J = 7.3 Hz), 2.00-1.73 (2H, m), 1.63 (2H, quint, J = 7.2 Hz), 1.54-1.44 (1H, m), 1.43-1.33 (1H, m); ^{13}C NMR (CD_3OD): 178.5, 143.7, 143.6, 142.0, 141.8, 131.0, 129.1, 127.4, 127.3, 126.4, 126.3, 110.4, 95.2 (d, J = 169.5 Hz), 65.9, 38.2, 37.9, 35.6, 26.1, 25.89, 25.85; ^{19}F NMR (CD_3OD): -175.90 (1F, ddd, J = 45.9, 28.7, 17.2 Hz).



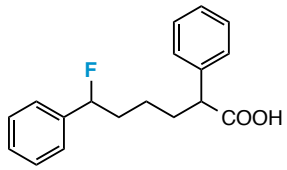
6-(4-acetylphenyl)-6-fluorohexanoic acid (**11**). 28% yield. Clear oil. υ_{max}/cm^{-1} 3300-2500 (COOH) and 1668 (CO). ^{1}H NMR (CD_3OD): 8.00 (2H, d, J = 7.8 Hz), 7.48 (2H, d, J = 8.4 Hz), 5.54 (1H, ddd, J = 48.1, 7.8, 5.1 Hz), 2.61 (3H, s), 2.16 (t, J = 7.5 Hz), 2.02-1.75 (2H, m), 1.64 (2H, quint, J = 7.2 Hz), 1.54-1.36 (2H, m); ^{13}C NMR (CD_3OD): 200.1, 182.6, 147.8, 147.6, 138.0, 129.6, 126.72, 126.65, 94.8 (d, J = 171.8 Hz), 39.0, 38.3, 38.1, 27.4, 26.7, 26.10, 26.06; ^{19}F NMR (CD_3OD): -178.70 (1F, ddd, J = 47.0, 28.7, 18.4 Hz).



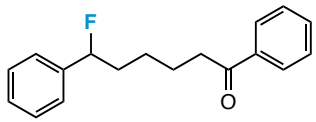
2-(3-fluoro-3-phenylpropyl)benzoic acid (**12**). 40% yield. Clear oil. υ_{max}/cm^{-1} 3300-2500 (COOH) and 1687 (CO). ^{1}H NMR ($CDCl_3$): 11.67 (1H, br s), 8.09 (1H, d, J = 7.6 Hz), 7.50 (1H, m), 7.36-7.28 (7H, m), 5.50 (1H, ddd, J = 47.9, 8.2, 3.9 Hz), 3.28-3.21 (1H, m), 3.18-3.11 (1H, m), 2.38-2.22 (1H, m), 2.20-2.11 (1H, m); ^{13}C NMR ($CDCl_3$): 173.0, 144.4, 140.2, 140.0, 133.2, 132.0, 131.6, 128.54, 128.50, 128.4, 128.24, 128.22, 126.4, 125.6, 125.5, 94.1 (d, J = 171.0 Hz), 38.9, 38.7, 30.6, 30.5; ^{19}F NMR ($CDCl_3$): -175.12 (1F, ddd, J = 47.0, 29.8, 16.1 Hz).



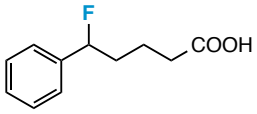
cis-2-(3-fluoro-3-phenylpropyl)cyclohexane-1-carboxylic acid (**13**). 58% yield. Clear oil. υ_{max}/cm^{-1} 3300-2500 (COOH), 1702 (CO), and 1699 (CO). ^{1}H NMR ($CDCl_3$): 11.32 (1H, br s), 7.38-7.28 (5H, m), 5.49-5.29 (1H, m), 2.15-2.02 (1H, m), 2.01-1.83 (3H, m), 1.82-1.71 (2H, m), 1.70-1.59 (2H, m), 1.58-1.46 (1H, m), 1.44-1.35 (1H, m), 1.34-1.13 (2H, m), 1.00-0.87 (1H, m); ^{13}C NMR ($CDCl_3$): 182.4, 140.5, 140.3, 140.2, 128.39, 128.37, 128.25, 128.23, 128.12, 128.11, 125.7, 125.6, 125.5, 125.4, 95.0 (d, J = 170.3 Hz), 94.4 (d, J = 171.8 Hz), 49.7, 49.5, 38.3, 38.2, 34.3, 34.1, 34.0, 33.8, 30.5, 30.4, 30.18, 30.15, 30.13, 30.00, 29.97, 25.5, 25.30, 25.28; ^{19}F NMR ($CDCl_3$): -171.99 (1F, m), -175.23 (1F, ddd, J = 48.2, 31.0, 17.2 Hz).



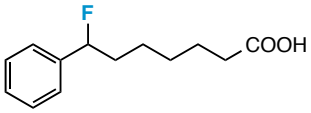
6-fluoro-2,6-diphenylhexanoic acid (**14**). 56% yield. Clear oil. υ_{max}/cm^{-1} 3300-2500 (COOH) and 1704 (CO). ^{1}H NMR ($CDCl_3$): 7.37-7.25 (10H, m), 5.38 (1H, ddd, J = 47.7, 8.2, 4.5 Hz), 3.59 (1H, br s), 2.19-2.07 (1H, m), 2.06-1.91 (1H, m), 1.91-1.72 (2H, m), 1.57-1.28 (3H, m); ^{13}C NMR ($CDCl_3$): 140.3, 140.1, 128.7, 128.4, 128.24, 128.23, 128.0, 127.5, 125.5, 125.4, 95.13, 95.08, 93.44, 93.38, 37.0, 36.8, 32.8, 23.3; ^{19}F NMR ($CDCl_3$): -174.16 (1F, ddd, J = 47.0, 29.8, 17.2 Hz), -174.39 (1F, ddd, J = 47.0, 29.8, 16.1 Hz).



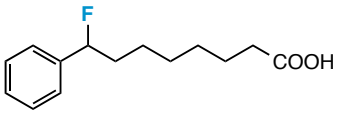
6-fluoro-1,6-diphenyl-hexanone (**15**). 30% yield. White solid; 30-32 °C. υ_{max}/cm^{-1} 2938 (CH), 2863 (CH), and 1684 (CO). ^{1}H NMR ($CDCl_3$): 7.96-7.93 (2H, m), 7.59-7.53 (1H, m), 7.49-7.43 (2H, m), 7.39-7.30 (5H, m), 5.45 (1H, ddd, J = 47.5, 7.8, 5.0 Hz), 2.99 (1H, t, 7.3 Hz), 2.17-1.87 (2H, m), 1.86-1.74 (2H, m), 1.65-1.55 (1H, m), 1.53-1.40 (1H, m); ^{13}C NMR ($CDCl_3$): 200.1, 133.0, 128.64, 128.60, 128.50, 128.45, 128.2, 128.1, 128.0, 125.6, 125.5, 94.4 (d, J = 169.5 Hz), 38.4, 37.1 (d, J = 23.6 Hz), 24.9, 23.9; ^{19}F NMR ($CDCl_3$): -174.1 (1F, ddd, J = 47.0, 28.7, 16.1 Hz).



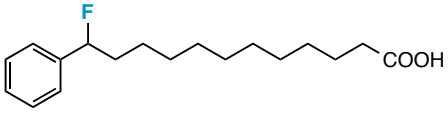
5-fluoro-5-phenylpentanoic acid (**17**). 58% yield. Clear oil. υ_{max}/cm^{-1} 3300-2500 (COOH) and 1705 (CO). ^{1}H NMR ($CDCl_3$): 11.19 (1H, br s), 7.39-7.35 (2H, m), 7.33-7.31 (3H, m), 5.45 (1H, ddd, *J* = 48.1, 7.8, 4.1 Hz), 2.44-2.41 (2H, m), 2.09-1.98 (1H, m), 1.96-1.81 (2H, m), 1.79-1.69 (1H, m); ^{13}C NMR ($CDCl_3$): 179.5, 140.1, 139.9, 128.5, 128.3, 125.5, 125.4, 94.1 (d, *J* = 171.8 Hz), 36.5, 36.2, 20.4, 20.3; ^{19}F NMR ($CDCl_3$): -174.90 (1F, ddd, *J* = 45.9, 28.7, 18.4 Hz).



7-fluoro-7-phenylheptanoic acid (**18**). 57% yield. Clear oil. υ_{max}/cm^{-1} 3300-2500 (COOH) and 1706 (CO). ^{1}H NMR ($CDCl_3$): 10.49 (1H, br s), 7.41-7.36 (2H, m), 7.35-7.31 (3H m), 5.43 (1H, ddd, *J* = 47.7, 8.0, 4.7 Hz), 2.35 (2H, t, *J* = 7.4 Hz), 2.06-1.92 (1H, m), 1.91-1.75 (1H, m), 1.65 (2H, quint, *J* = 7.4 Hz), 1.57-1.47 (1H, m), 1.45-1.38 (3H, m); ^{13}C NMR ($CDCl_3$): 180.2, 140.5, 140.3, 128.4, 128.17, 128.16, 125.5, 125.4, 94.5 (d, *J* = 171.0 Hz), 37.1, 36.8, 34.0, 28.7, 24.72, 24.68, 24.4; ^{19}F NMR ($CDCl_3$): -174.05 (1F, ddd, *J* = 47.0, 28.7, 17.2 Hz).

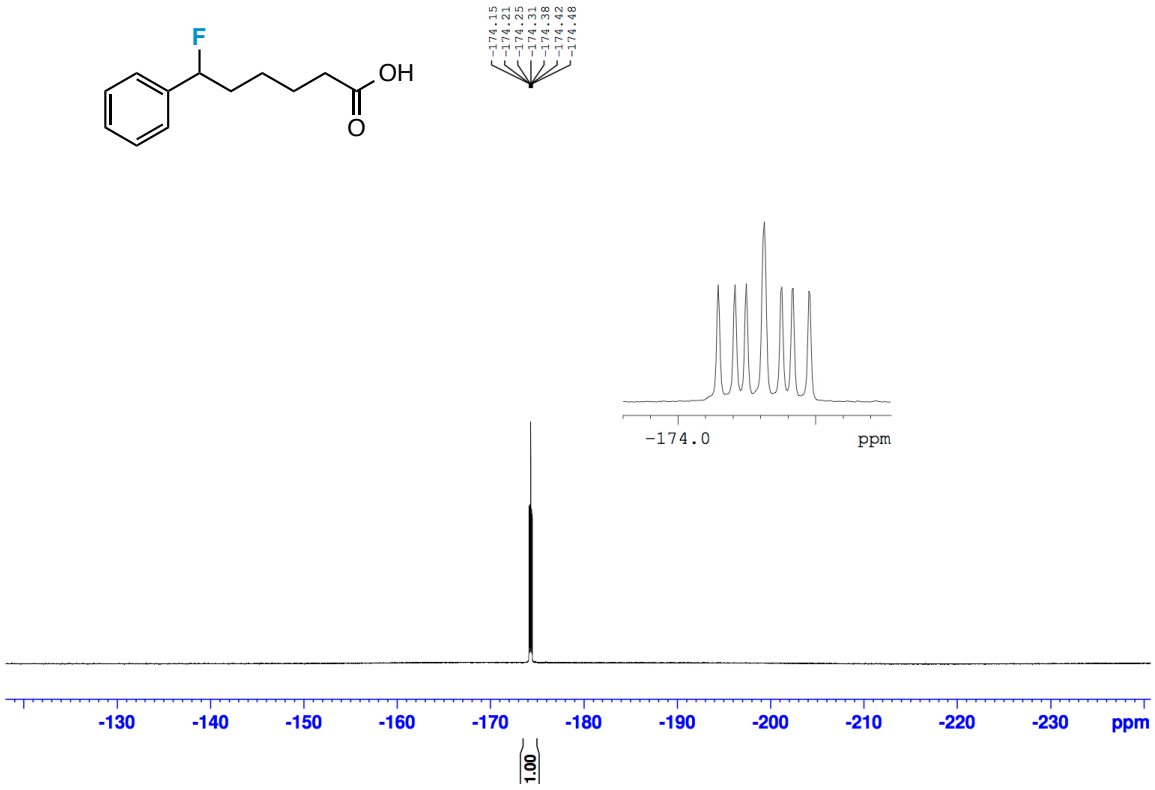


8-fluoro-8-phenyloctanoic acid (**19**). 46% yield. Clear oil. υ_{max}/cm^{-1} 3300-2500 (COOH) and 1705 (CO). ^{1}H NMR ($CDCl_3$): 9.97 (1H, br s), 7.40-7.35 (2H, m), 7.34-7.29 (3H, m), 5.41 (1H, ddd, *J* = 47.7, 8.0, 4.9 Hz), 2.34 (2H, t, *J* = 7.4 Hz), 2.03-1.90 (1H, m), 1.88-1.73 (1H, m), 1.62 (2H, quint, *J* = 7.2 Hz), 1.54-1.44 (1H, m), 1.43-1.31 (5H, m); ^{13}C NMR ($CDCl_3$): 180.1, 140.6, 140.4, 128.4, 128.3, 128.16, 128.14, 125.53, 125.46, 94.6 (d, *J* = 170.3 Hz), 37.2, 37.0, 34.0, 28.9, 28.8, 24.9, 24.8, 24.5; ^{19}F NMR ($CDCl_3$): -173.83 (1F, ddd, *J* = 47.0, 27.5, 17.2 Hz).

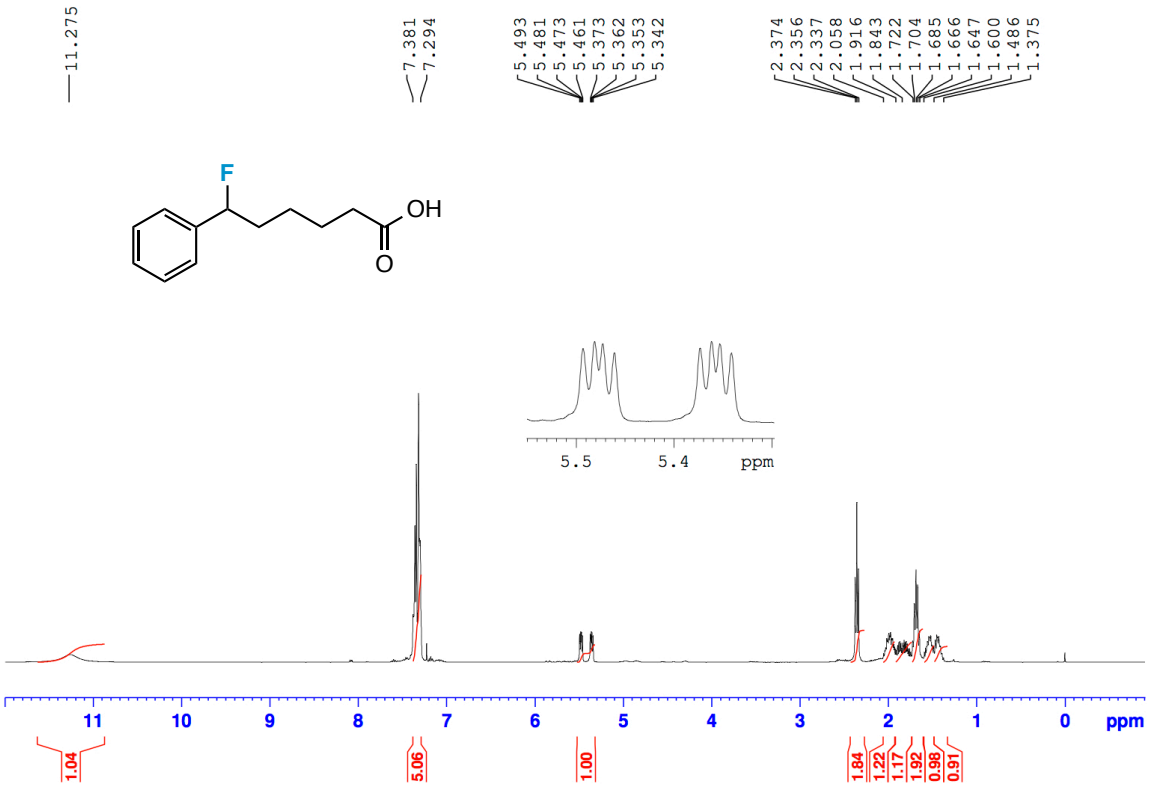


12-fluoro-12-phenyldodecanoic acid (**20**). 30% yield. White solid; m.p. 58-61 °C. υ_{max}/cm^{-1} 3300-2500 (COOH) and 1704 (CO). ^{1}H NMR ($CDCl_3$): 8.01 (1H, br s), 7.39-7.35 (2H, m), 7.33-7.29 (3H, m), 5.41 (1H, ddd, *J* = 47.9, 8.2, 5.1 Hz), 2.34 (2H, t, *J* = 7.4 Hz), 2.03-1.90 (1H, m), 1.88-1.72 (1H, m), 1.62 (2H, quint, *J* = 7.2 Hz), 1.52-1.41 (1H, m), 1.40-1.23 (13H, m); ^{13}C NMR ($CDCl_3$): 140.7, 140.5, 128.4, 128.13, 128.11, 125.6, 125.5, 94.7 (d, *J* = 171.0 Hz), 37.3, 37.1, 29.43, 29.41, 29.35, 29.33, 29.2, 29.0, 25.10, 25.05, 24.7; ^{19}F NMR ($CDCl_3$): -173.57 (1F, ddd, *J* = 47.0, 28.7, 17.2 Hz).

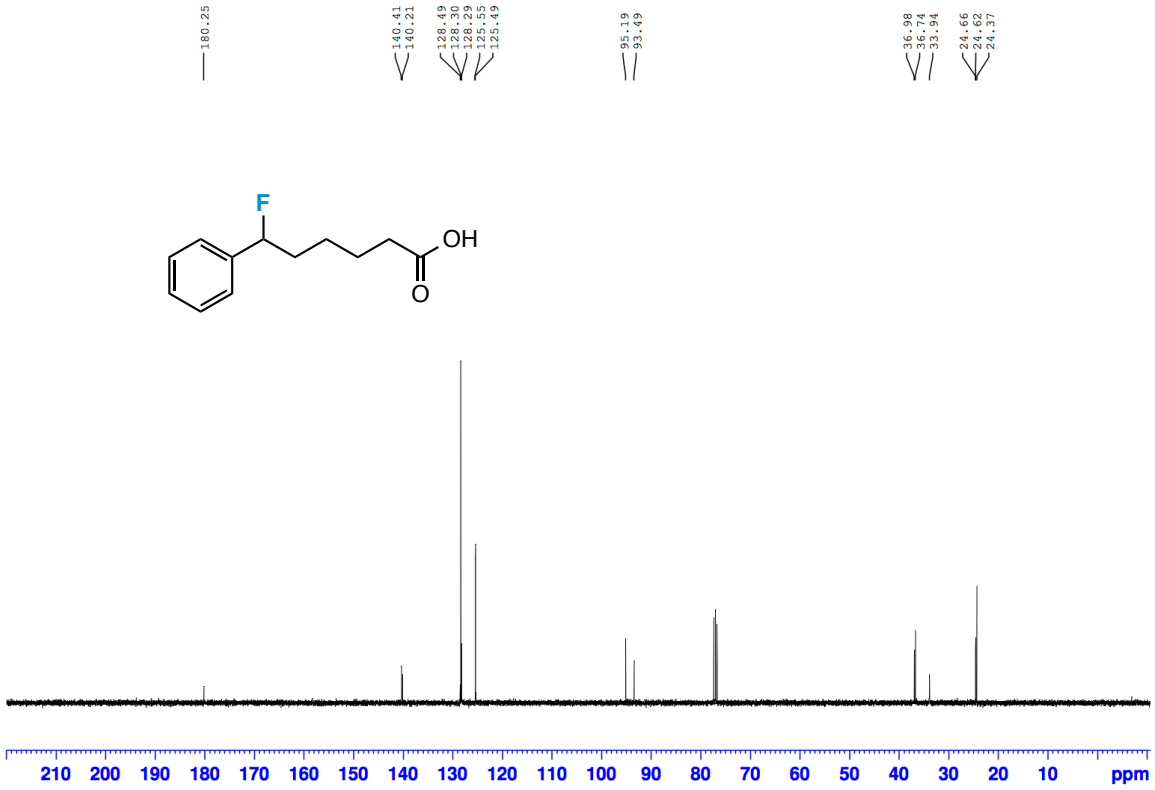
6-fluoro-6-phenyl-hexanoic acid



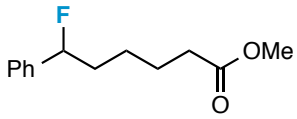
6-fluoro-6-phenyl-hexanoic acid

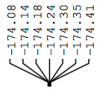


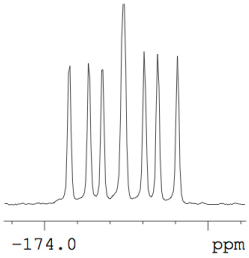
6-fluoro-6-phenyl-hexanoic acid

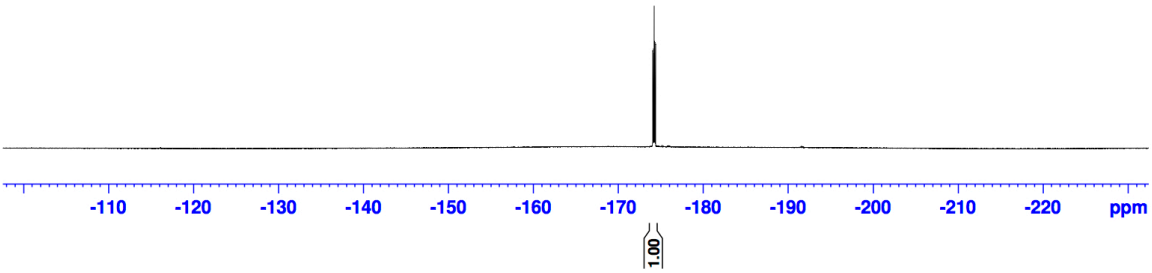


methyl 6-fluoro-6-phenylhexanoate

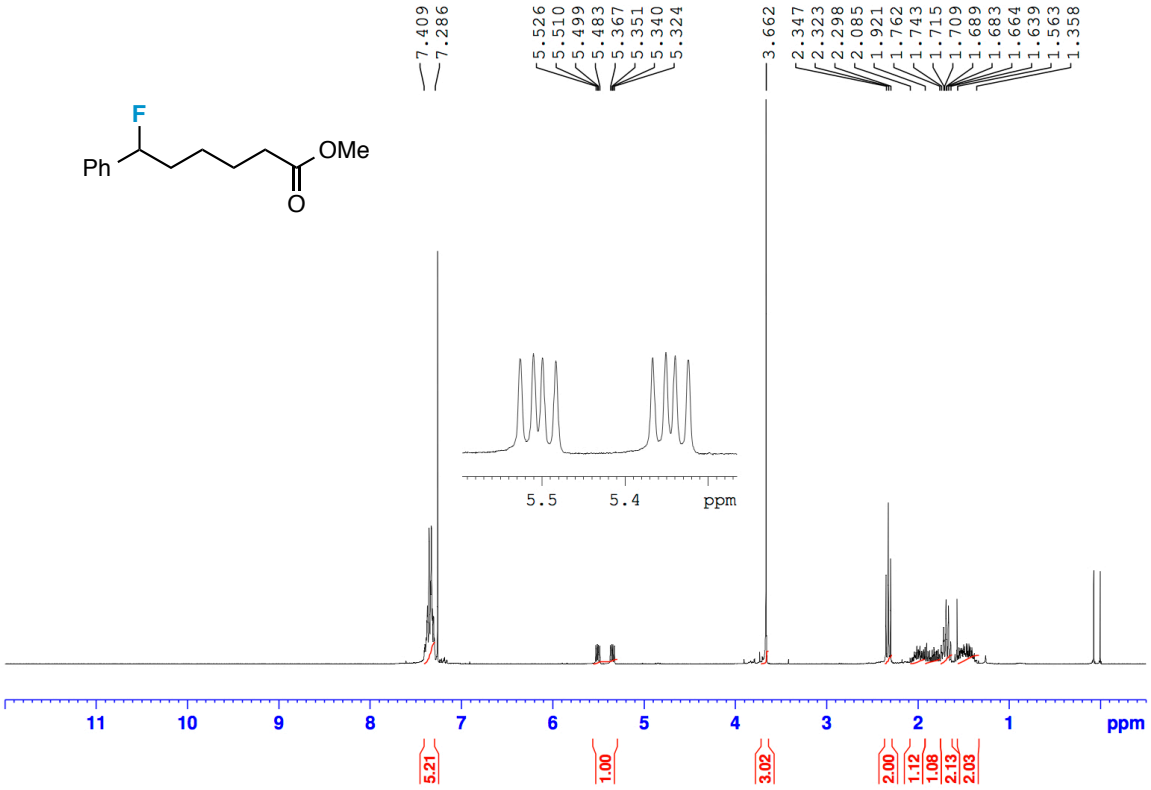




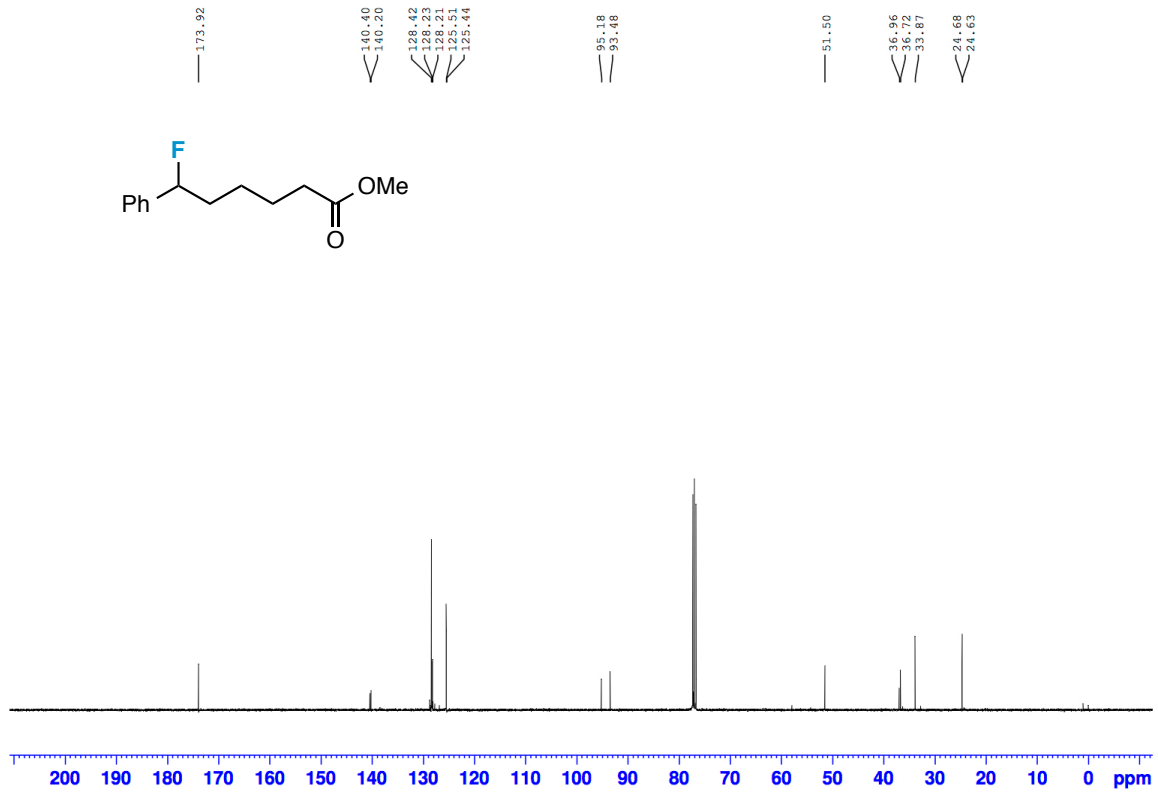




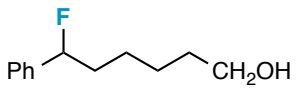
methyl 6-fluoro-6-phenylhexanoate

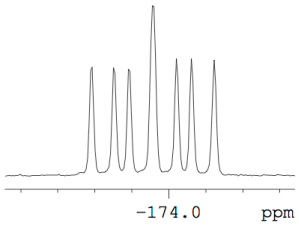


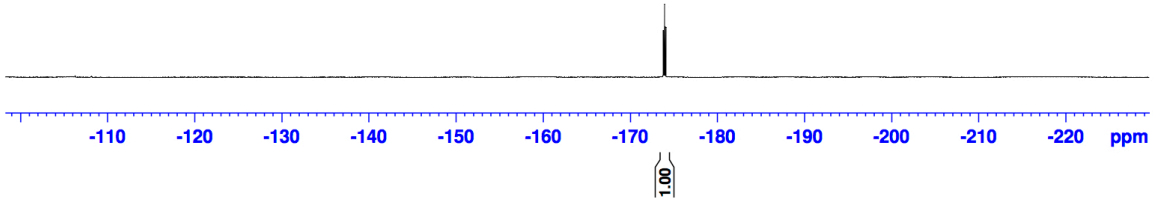
methyl 6-fluoro-6-phenylhexanoate



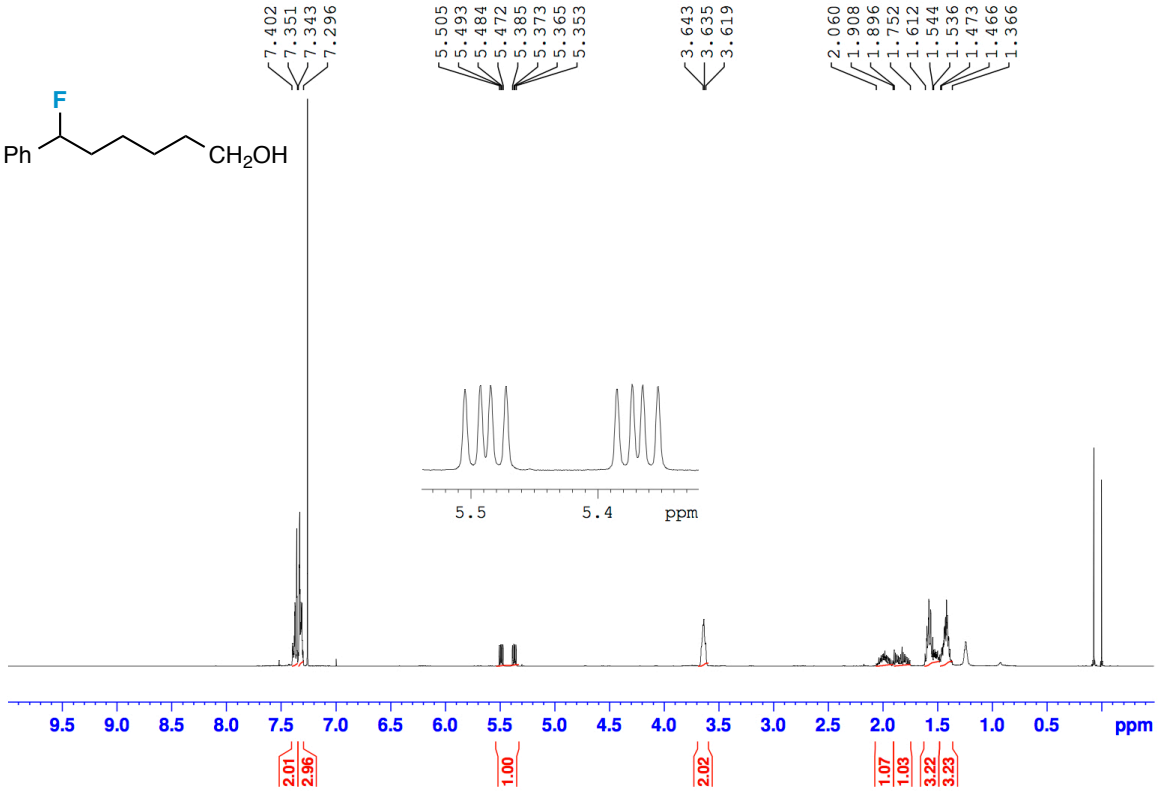
6-fluoro-6-phenylhexan-1-ol



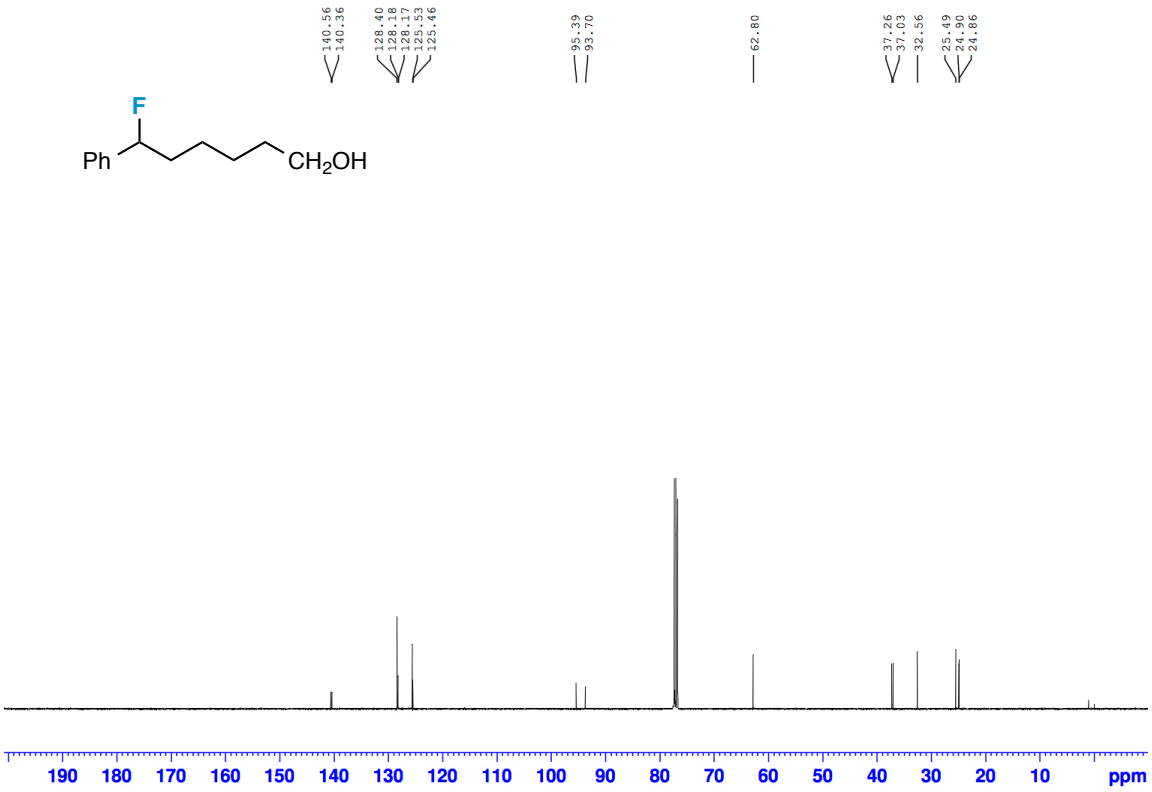




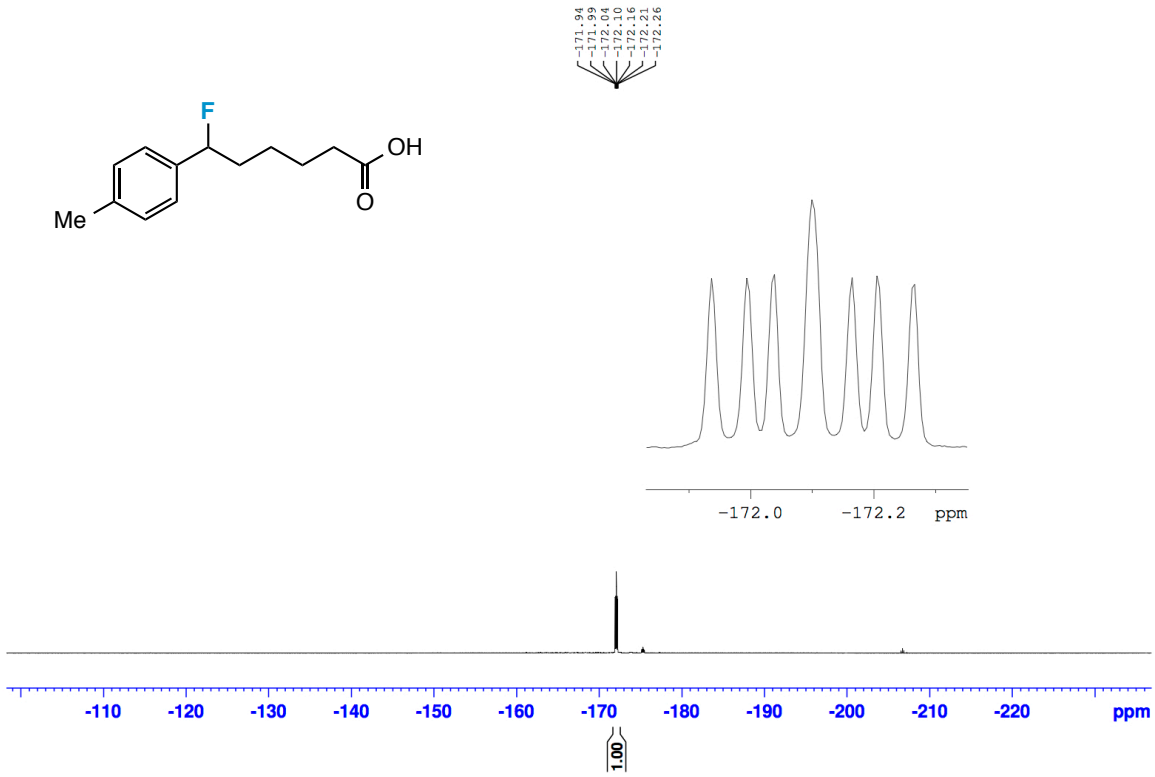
6-fluoro-6-phenylhexan-1-ol



6-fluoro-6-phenylhexan-1-ol

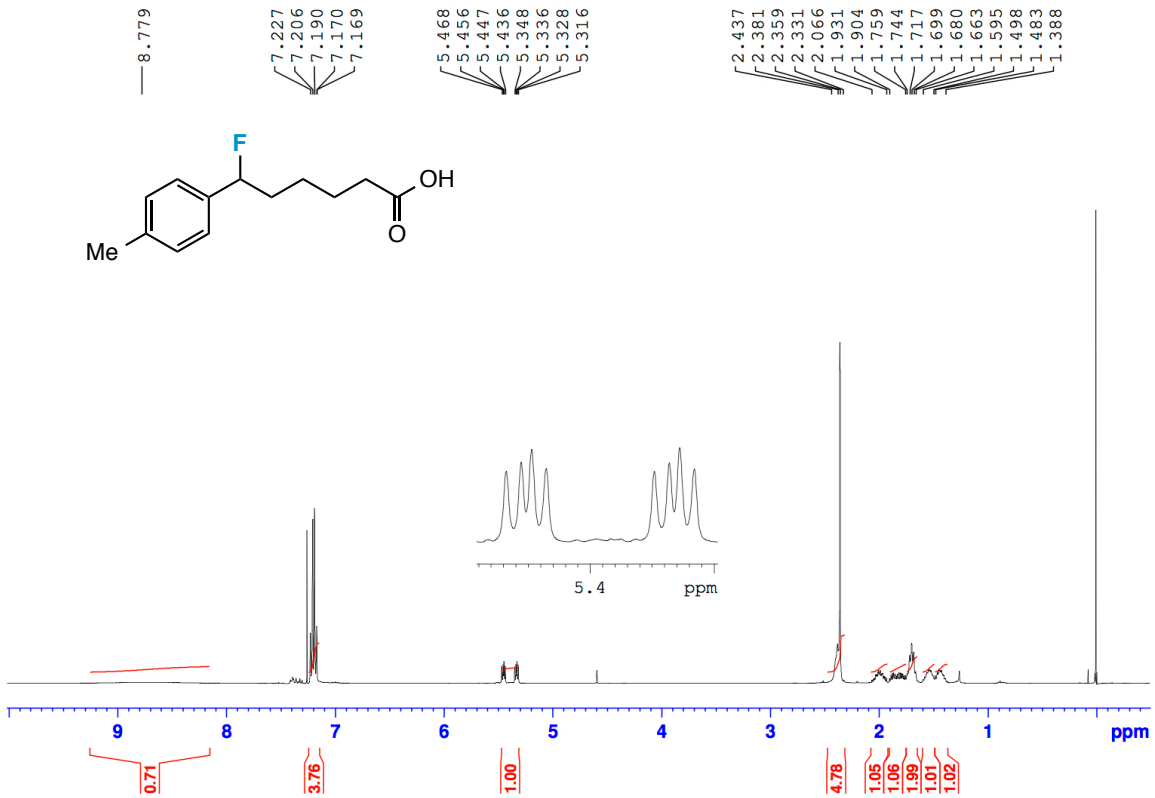


6-fluoro-6-(*p*-tolyl)hexanoic acid



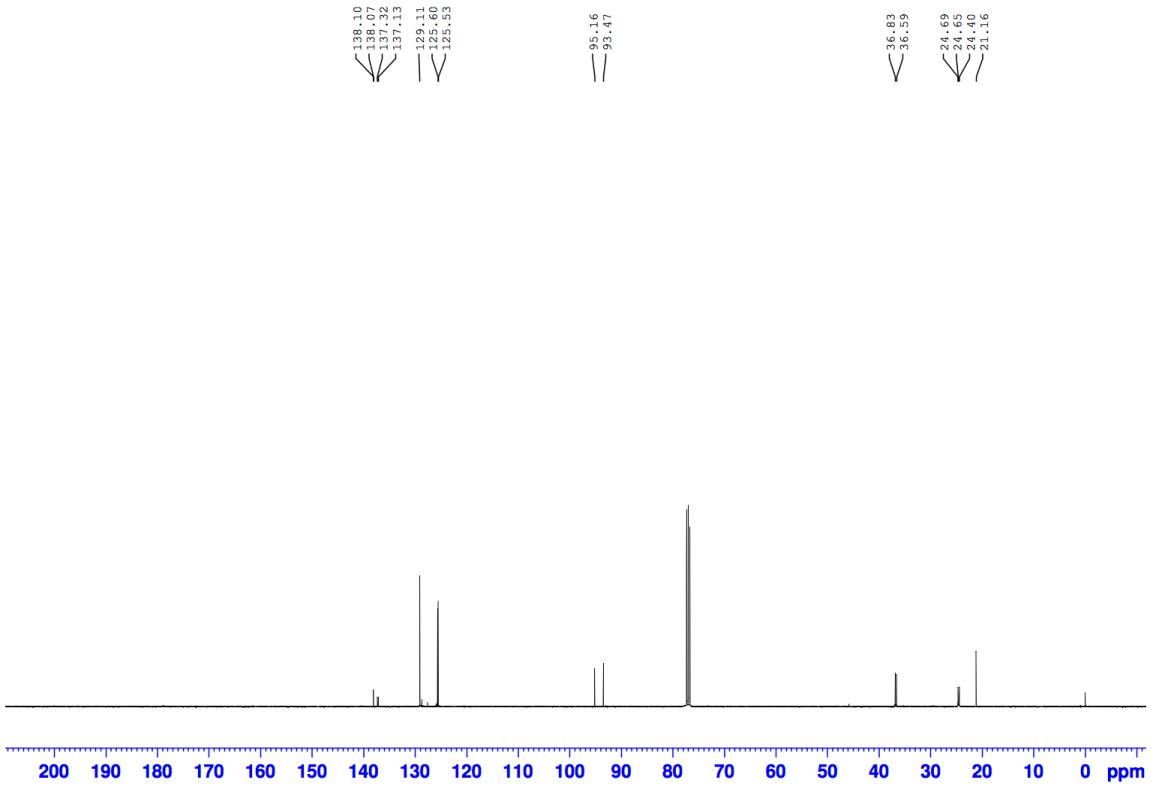
^{19}F NMR ($CDCl_3$):

6-fluoro-6-(*p*-tolyl)hexanoic acid

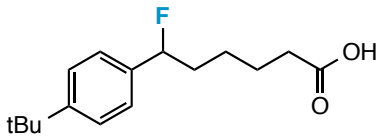


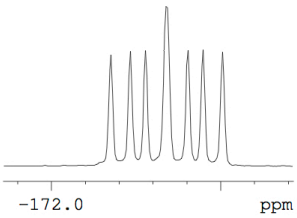
^{1}H NMR ($CDCl_3$):

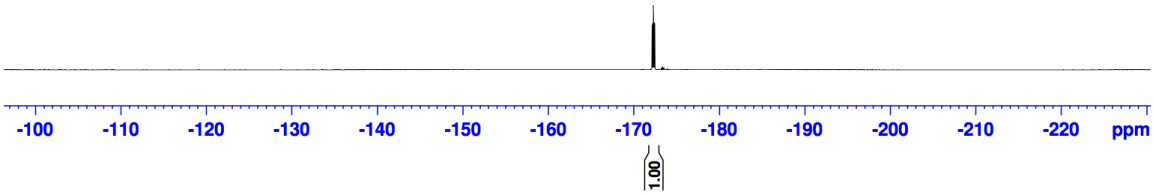
6-fluoro-6-(*p*-tolyl)hexanoic acid



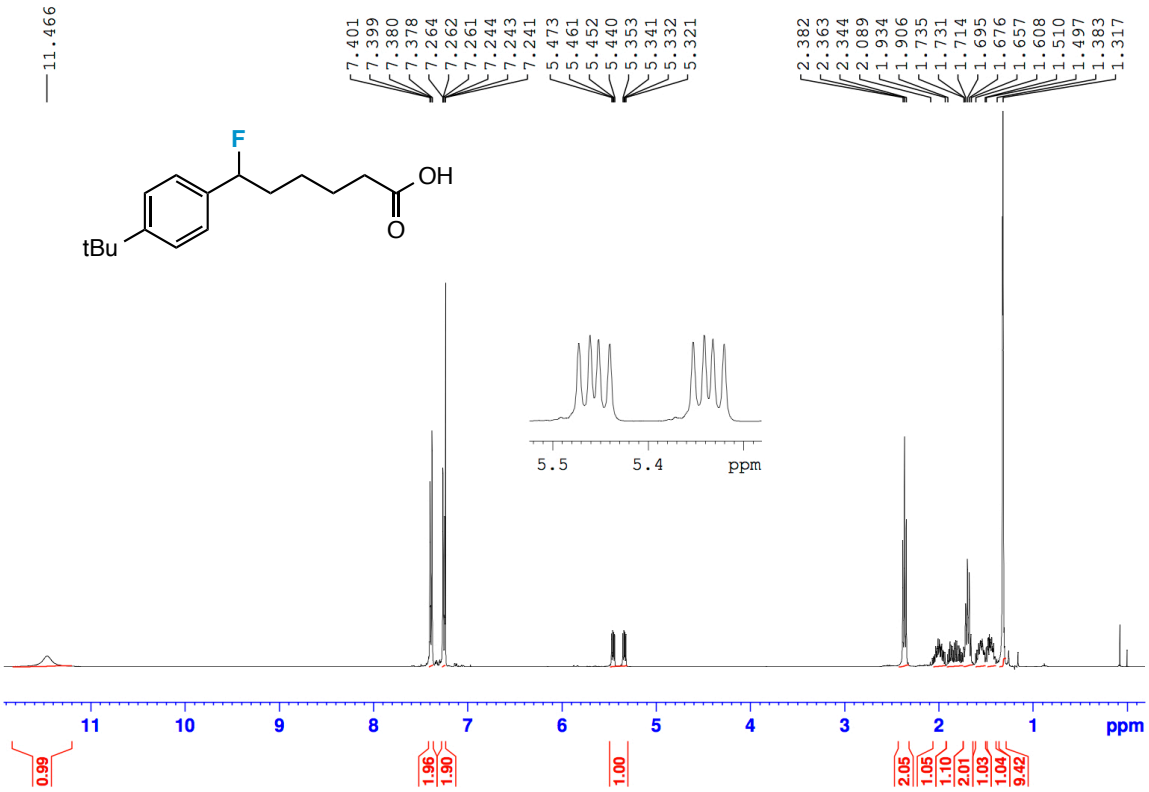
6-(4-(*tert*-butyl)phenyl)-6-fluorohexanoic acid



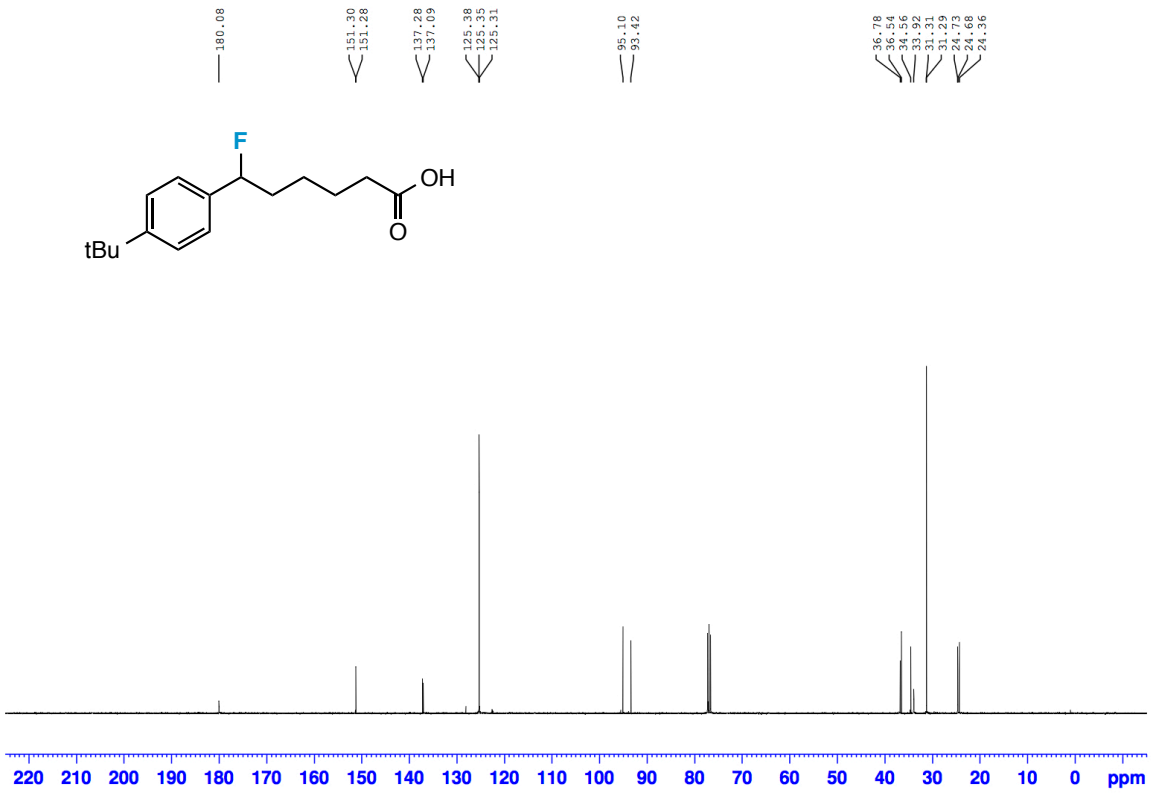




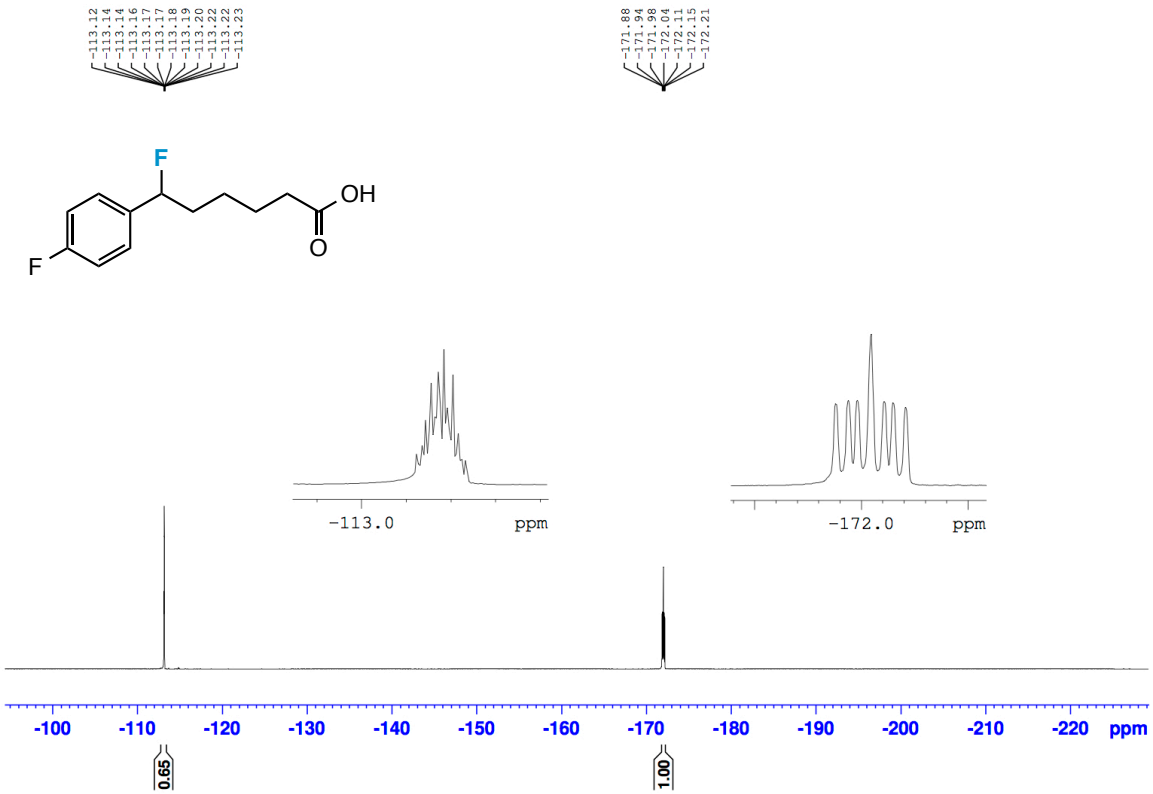
6-(4-(*tert*-butyl)phenyl)-6-fluorohexanoic acid



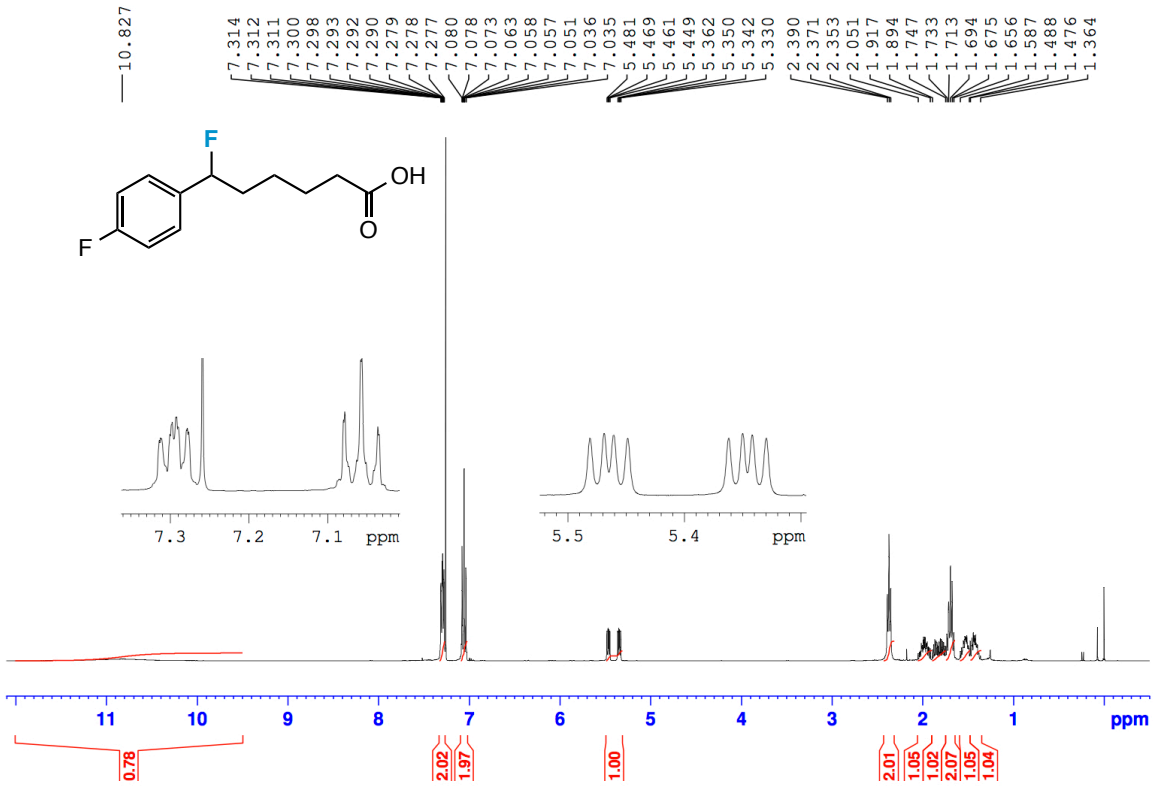
6-(4-(*tert*-butyl)phenyl)-6-fluorohexanoic acid



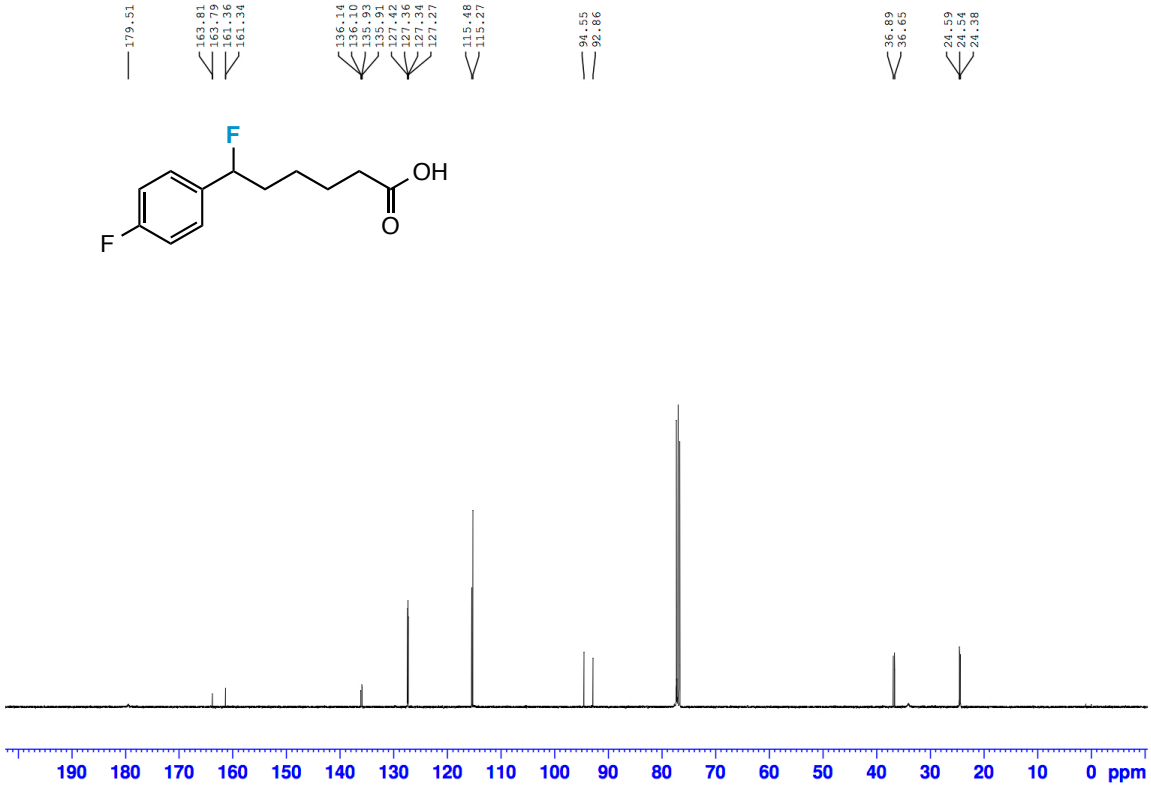
6-fluoro-6-(4-fluoro)phenyl-hexanoic acid



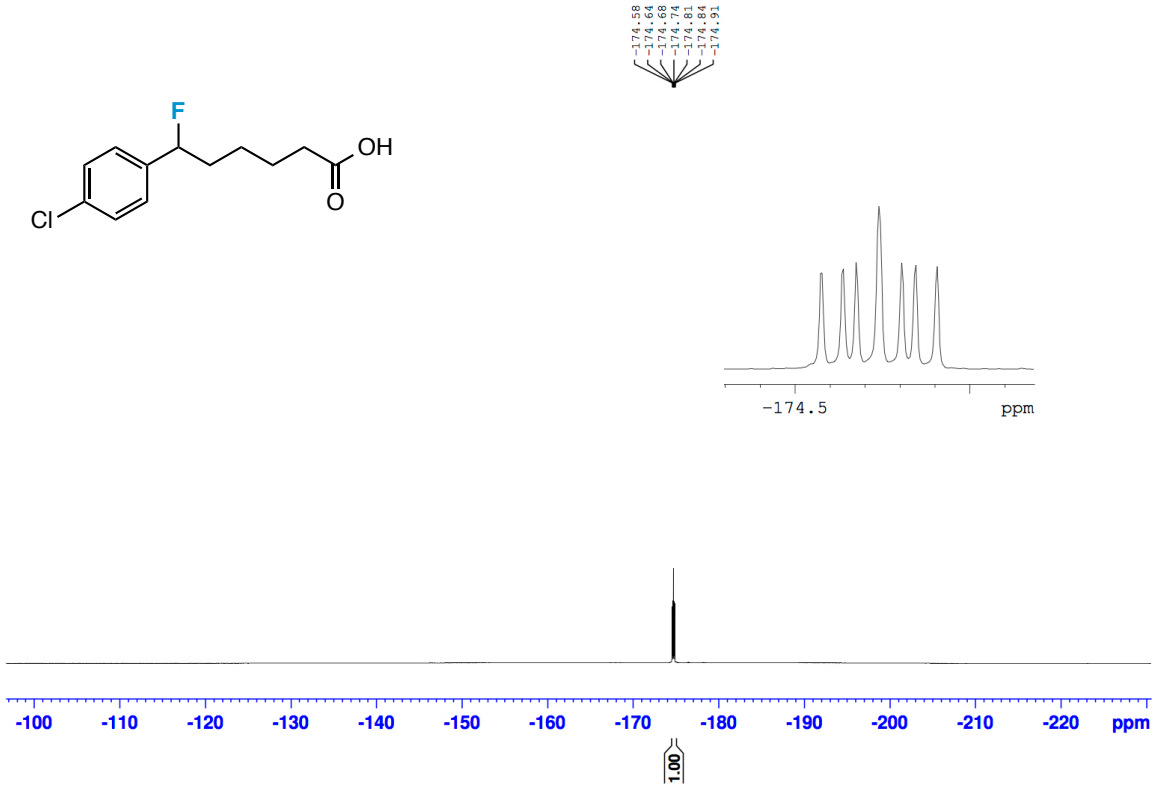
6-fluoro-6-(4-fluoro)phenyl-hexanoic acid



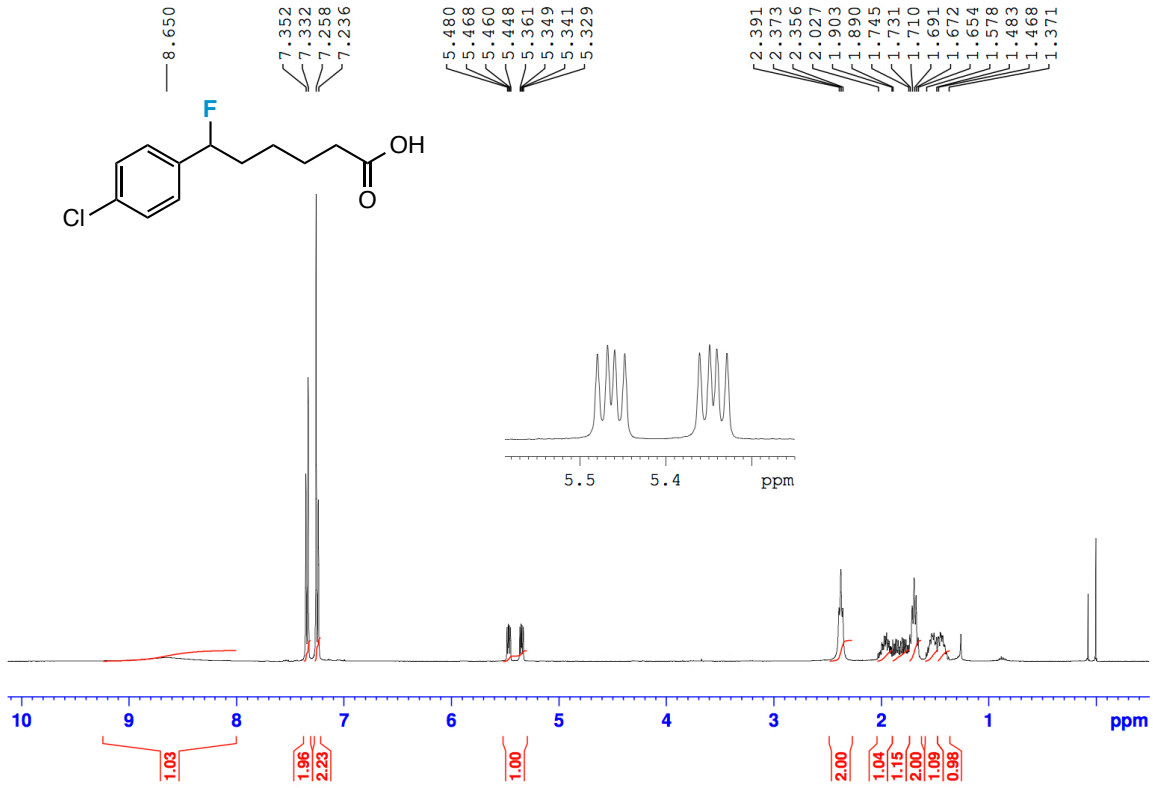
6-fluoro-6-(4-fluoro)phenyl-hexanoic acid



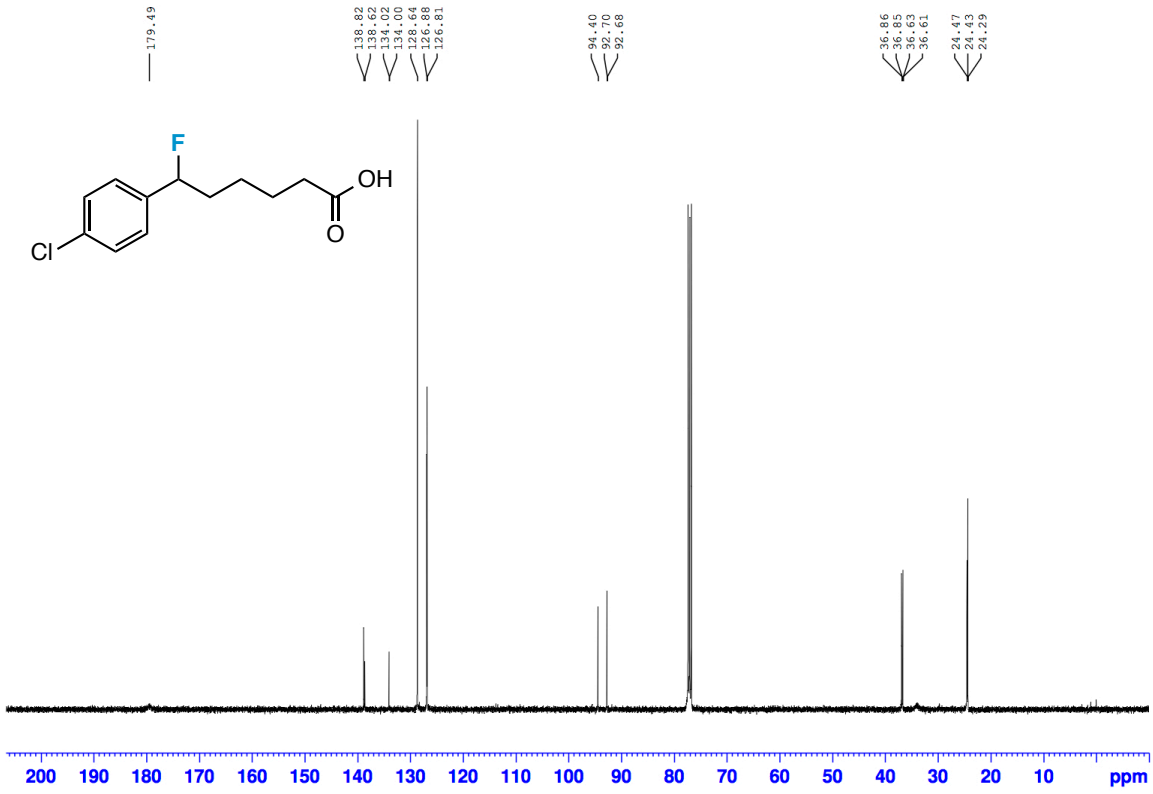
6-(4-chlorophenyl)-6-fluorohexanoic acid



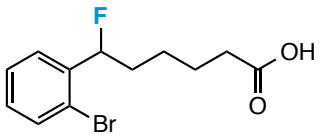
6-(4-chlorophenyl)-6-fluorohexanoic acid

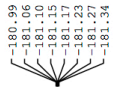


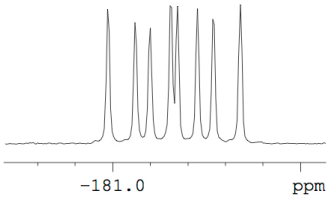
6-(4-chlorophenyl)-6-fluorohexanoic acid

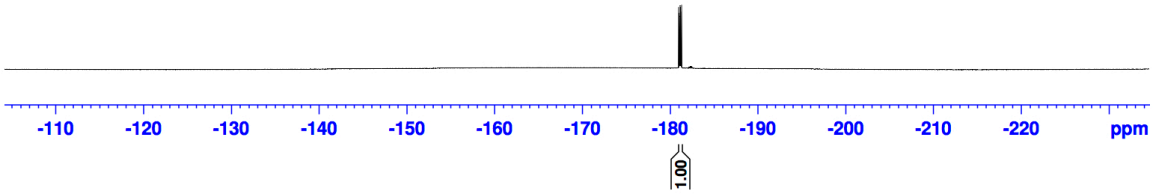


6-(2-bromophenyl)-6-fluorohexanoic acid

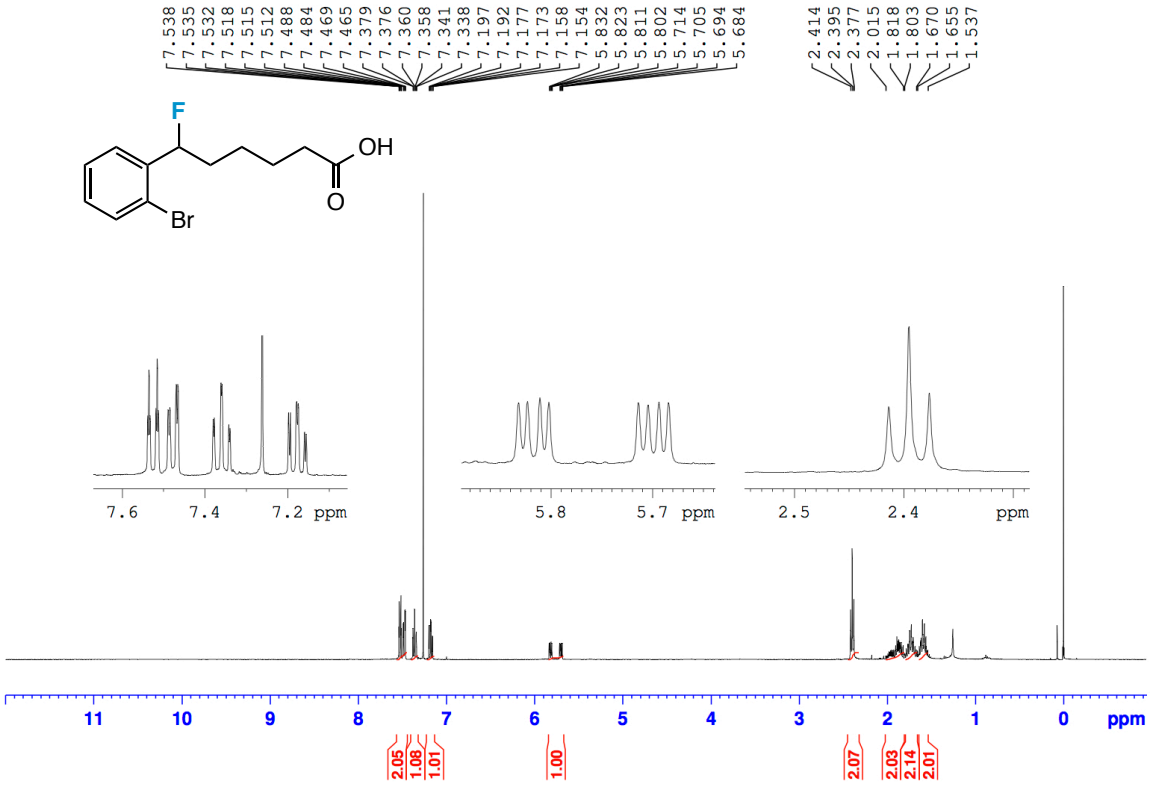




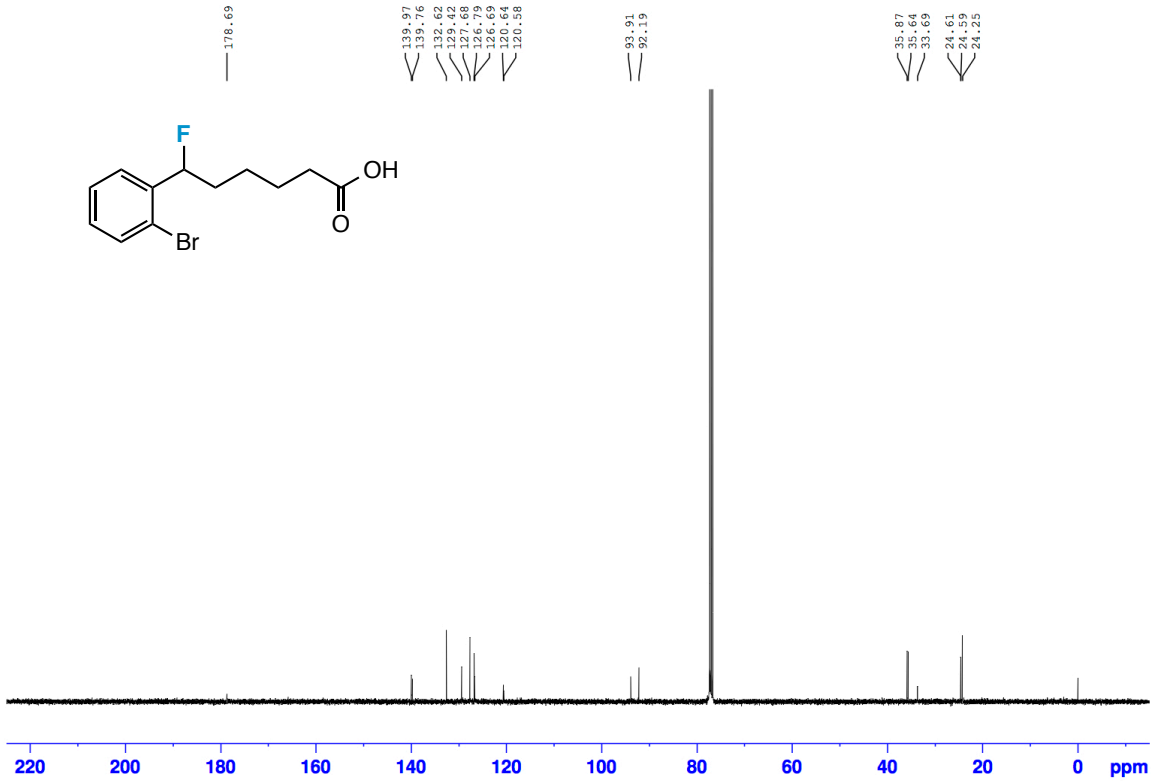




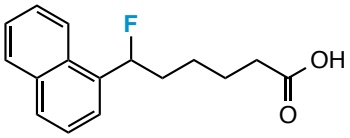
6-(2-bromophenyl)-6-fluorohexanoic acid

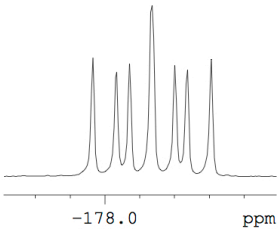


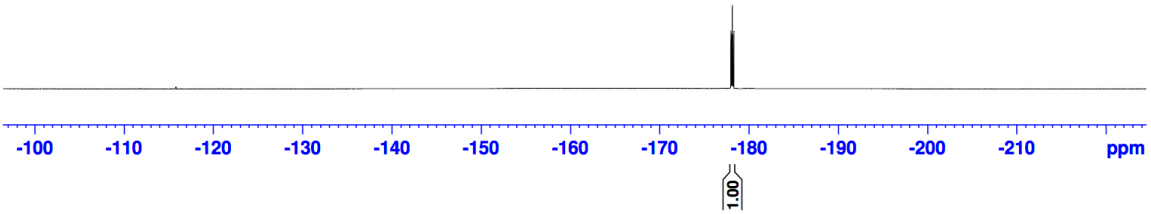
6-(2-bromophenyl)-6-fluorohexanoic acid



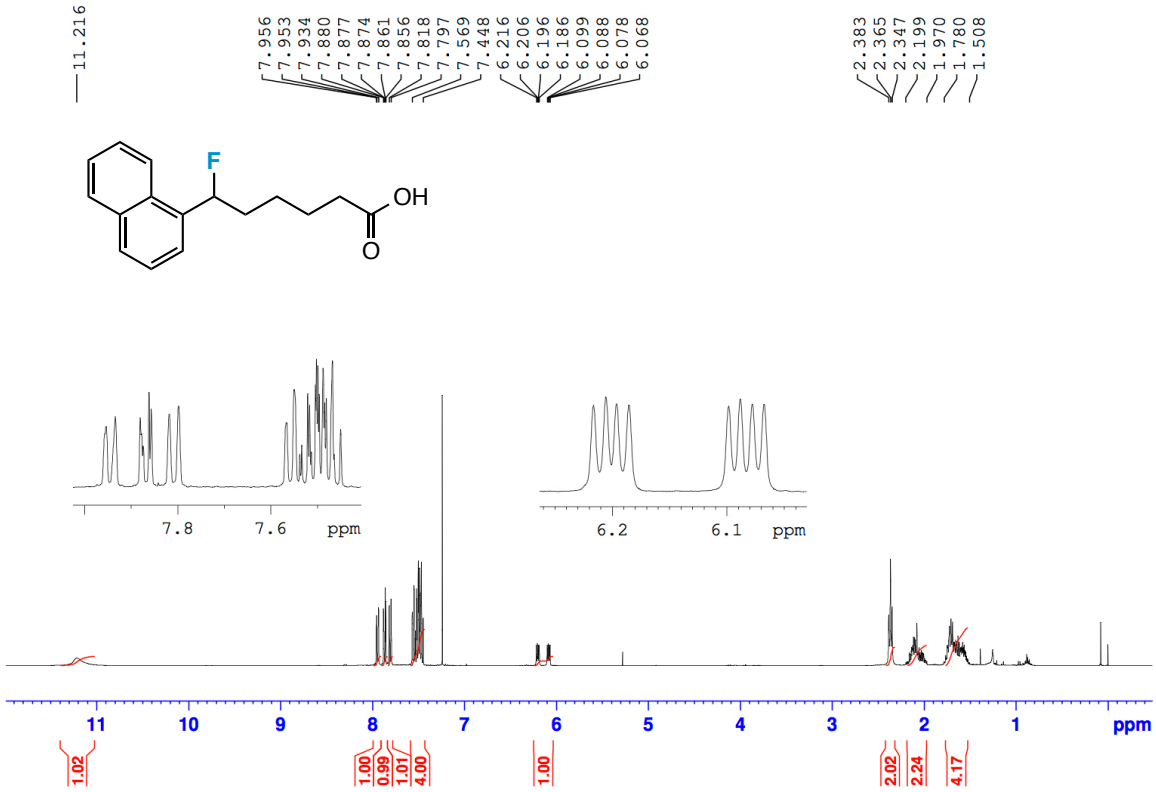
6-fluoro-6-(naphthalen-1-yl)hexanoic acid



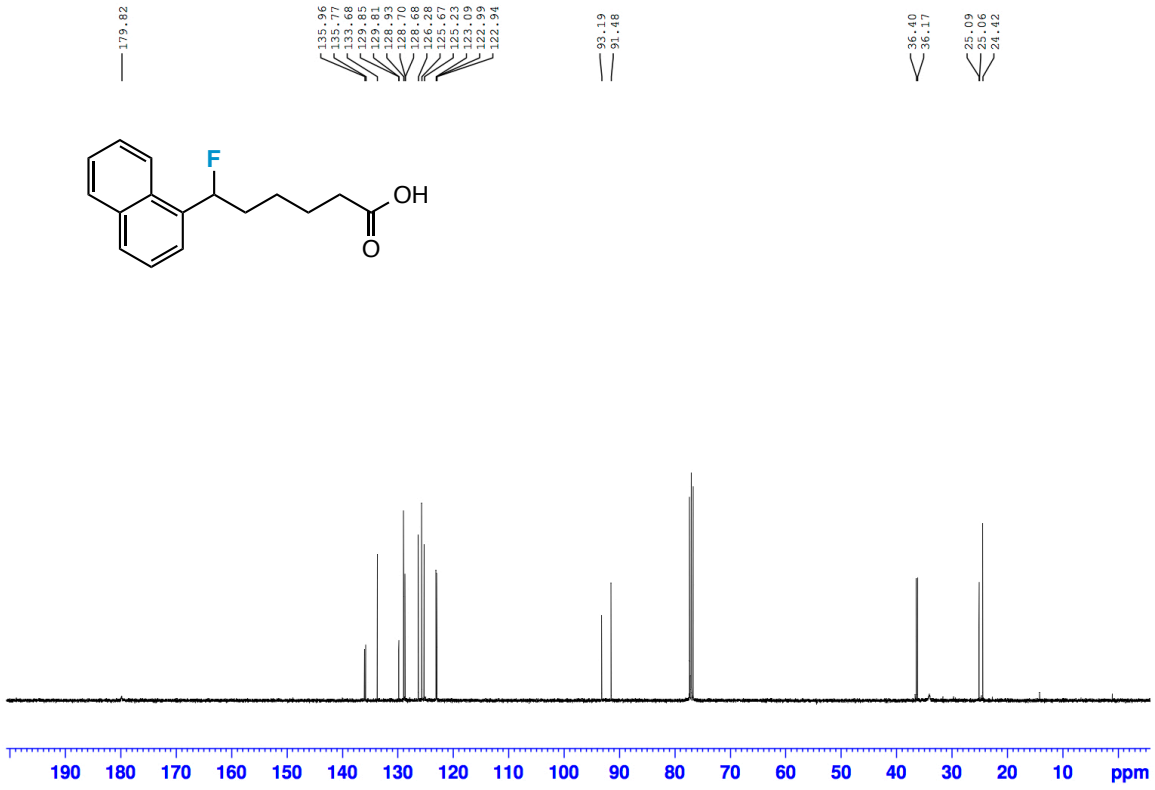




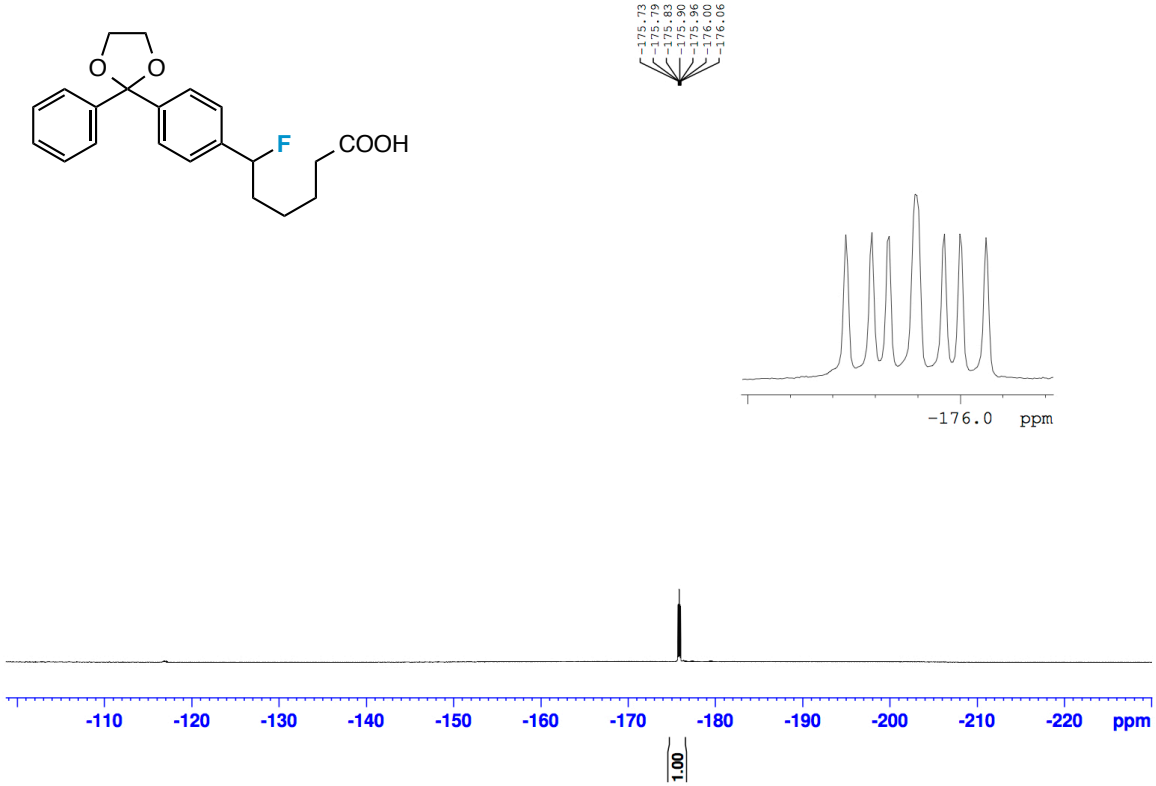
6-fluoro-6-(naphthalen-1-yl)hexanoic acid



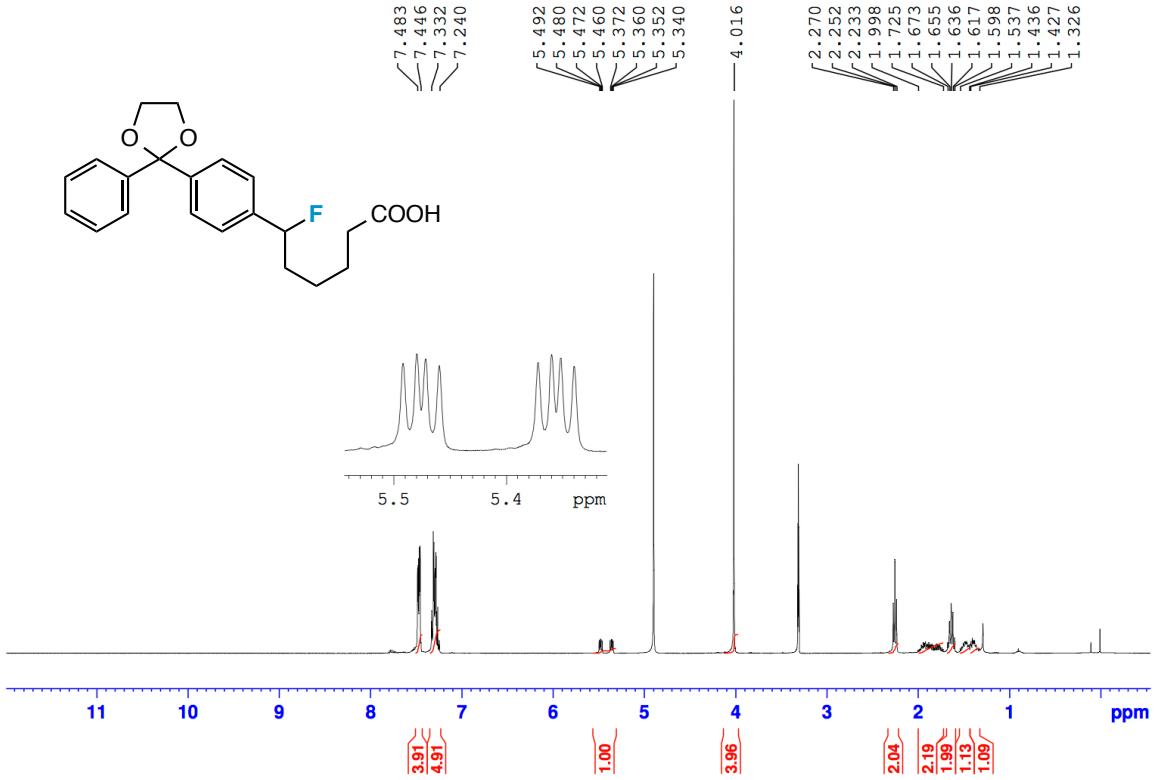
6-fluoro-6-(naphthalen-1-yl)hexanoic acid



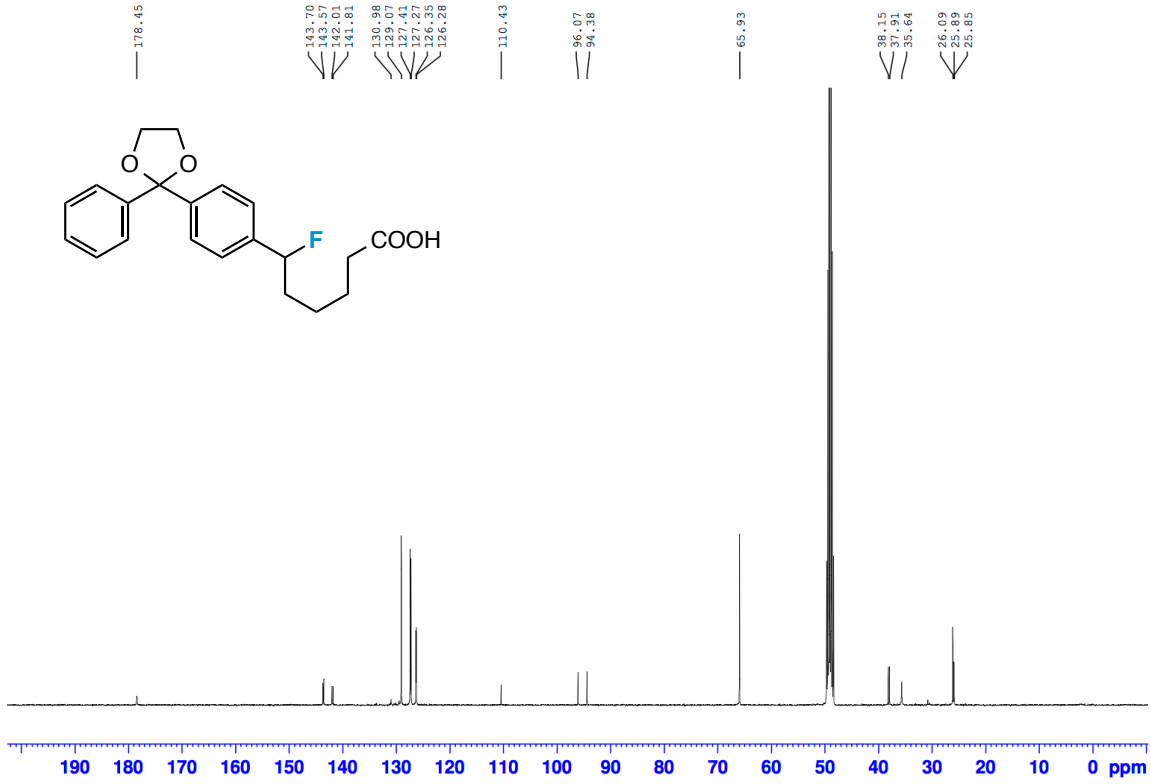
6-fluoro-6-(4-(2-phenyl-1,3-dioxolan-2-yl)phenyl)hexanoic acid



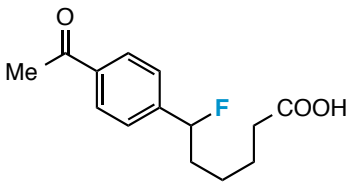
6-fluoro-6-(4-(2-phenyl-1,3-dioxolan-2-yl)phenyl)hexanoic acid

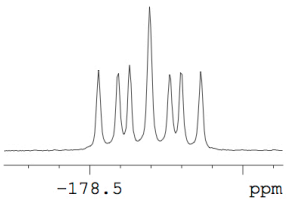


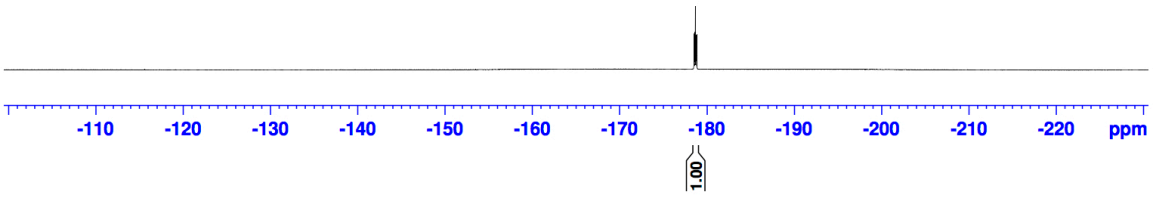
6-fluoro-6-(4-(2-phenyl-1,3-dioxolan-2-yl)phenyl)hexanoic acid



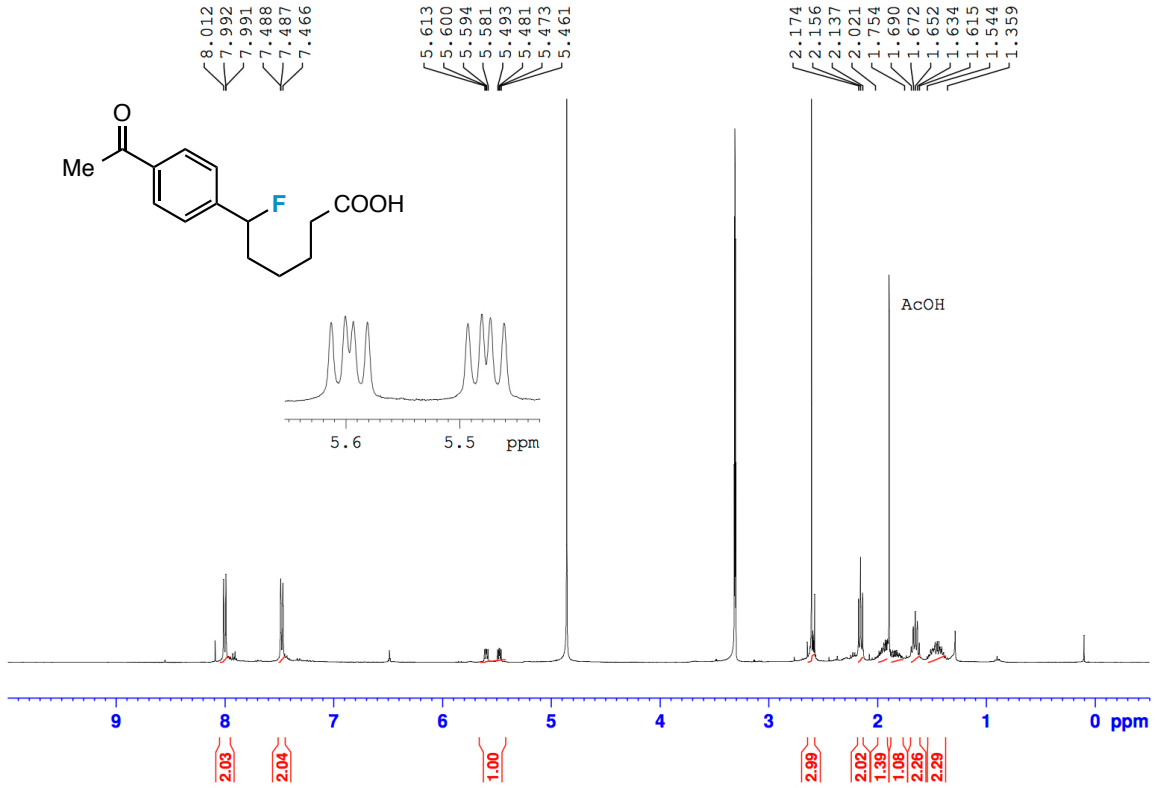
6-(4-acetylphenyl)-6-fluorohexanoic acid



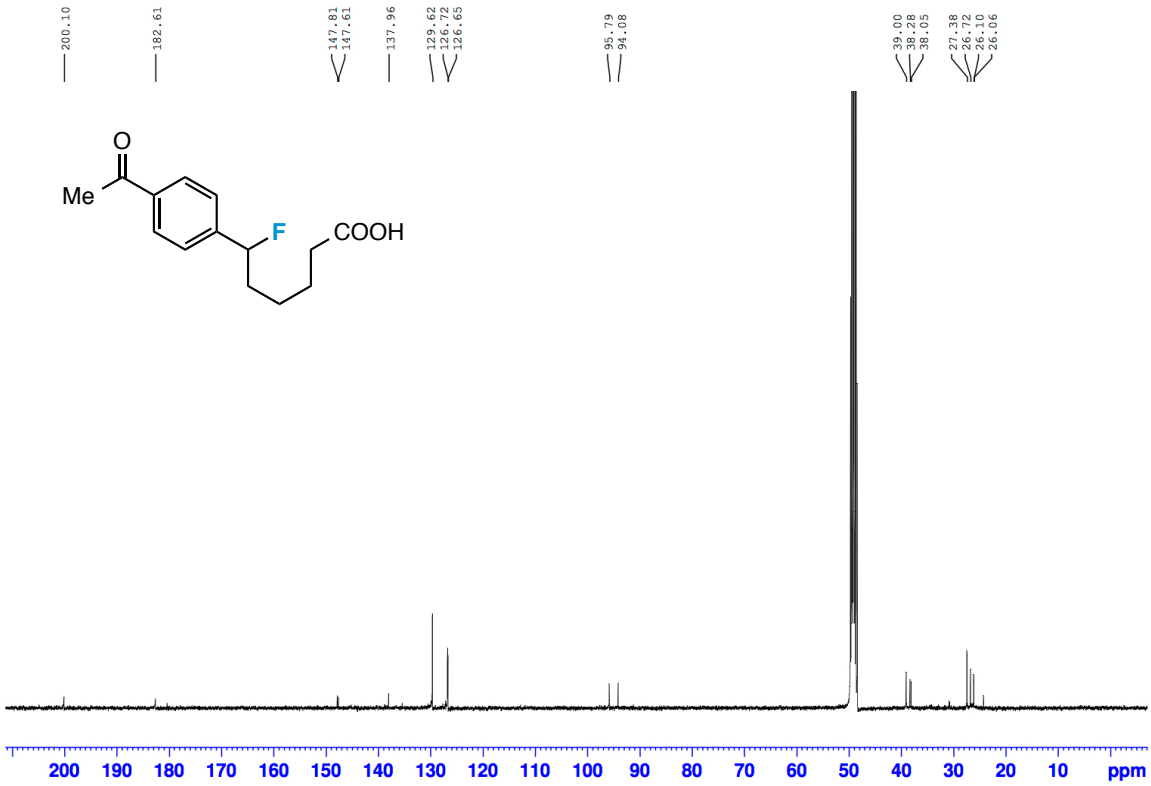




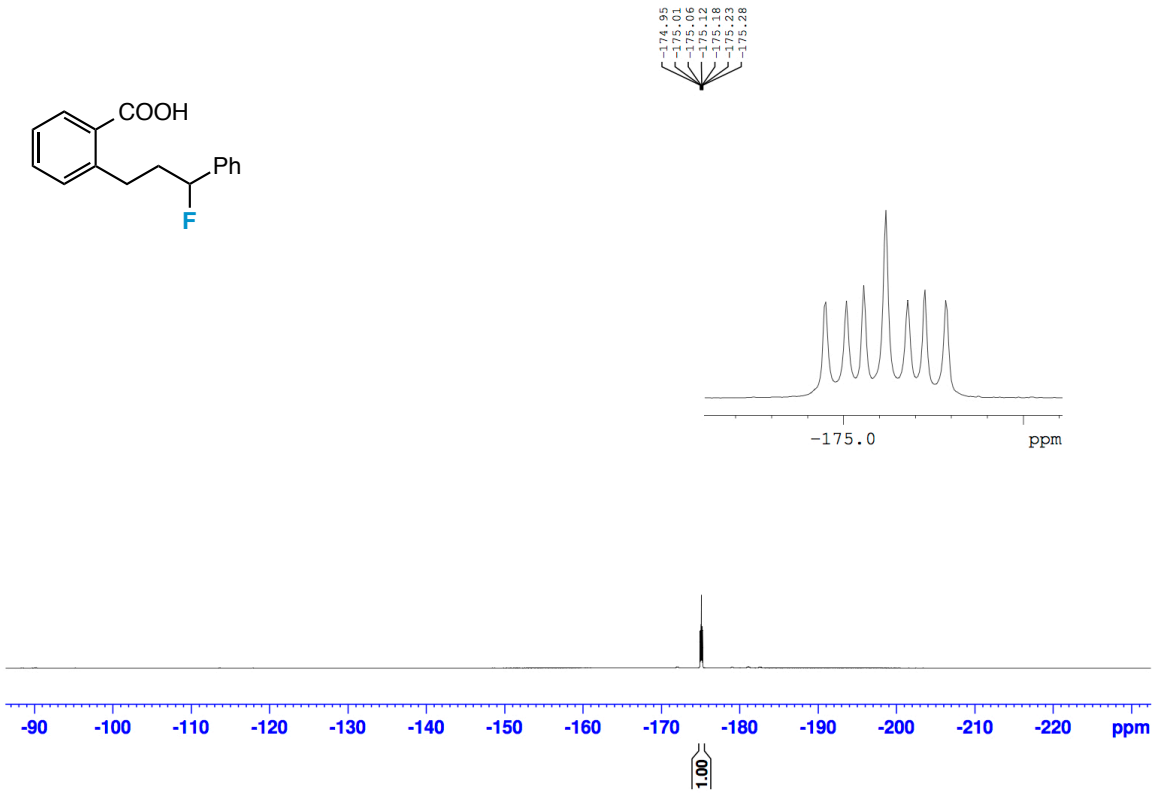
6-(4-acetylphenyl)-6-fluorohexanoic acid



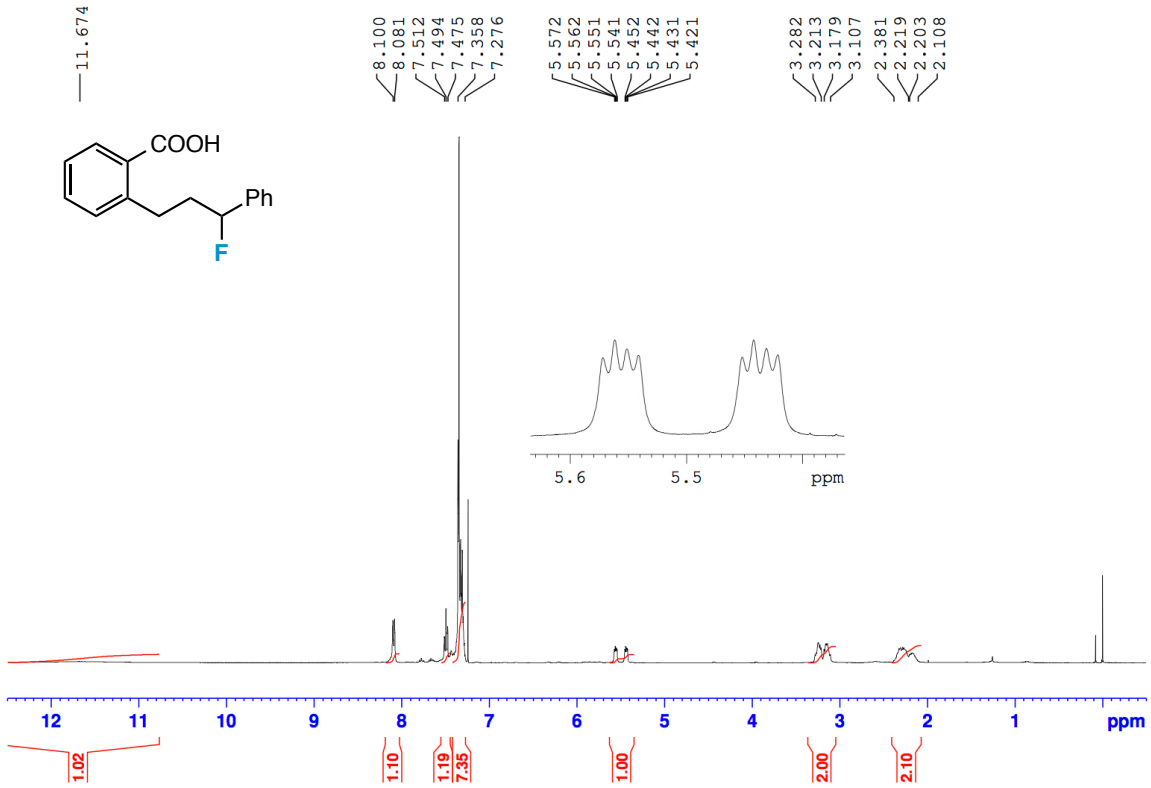
6-(4-acetylphenyl)-6-fluorohexanoic acid



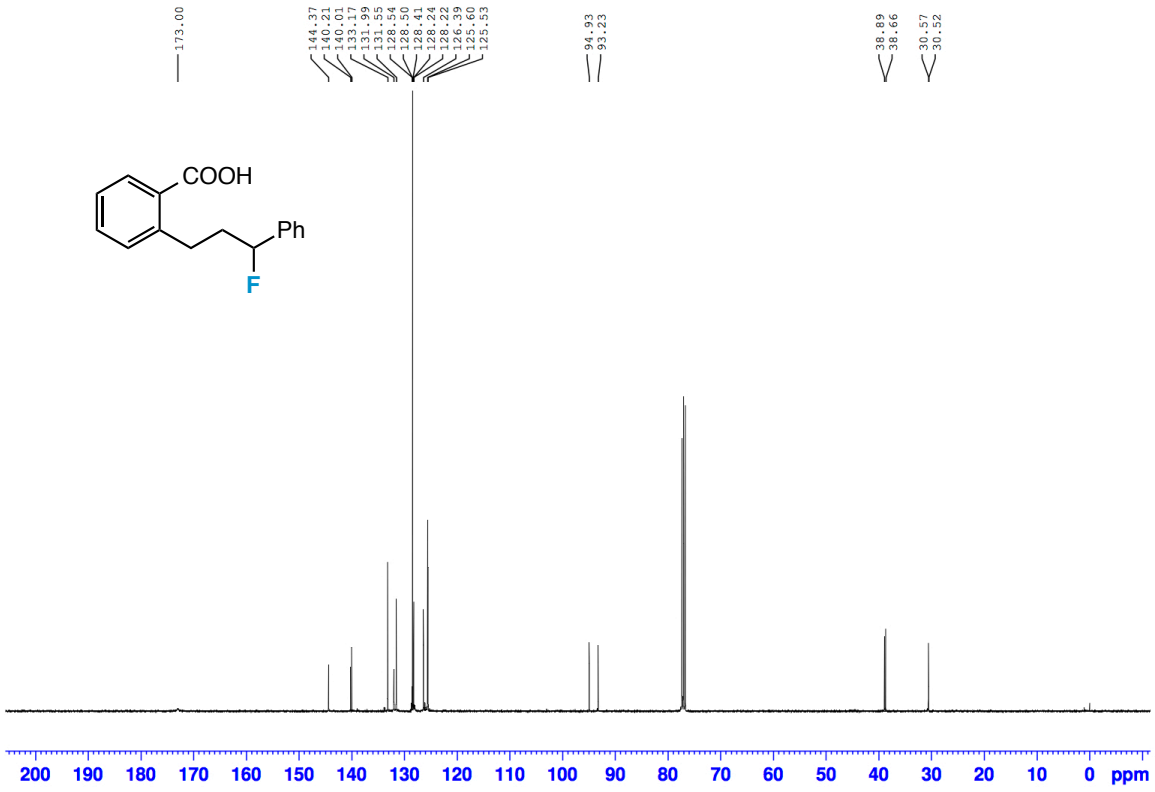
2-(3-fluoro-3-phenylpropyl)benzoic acid



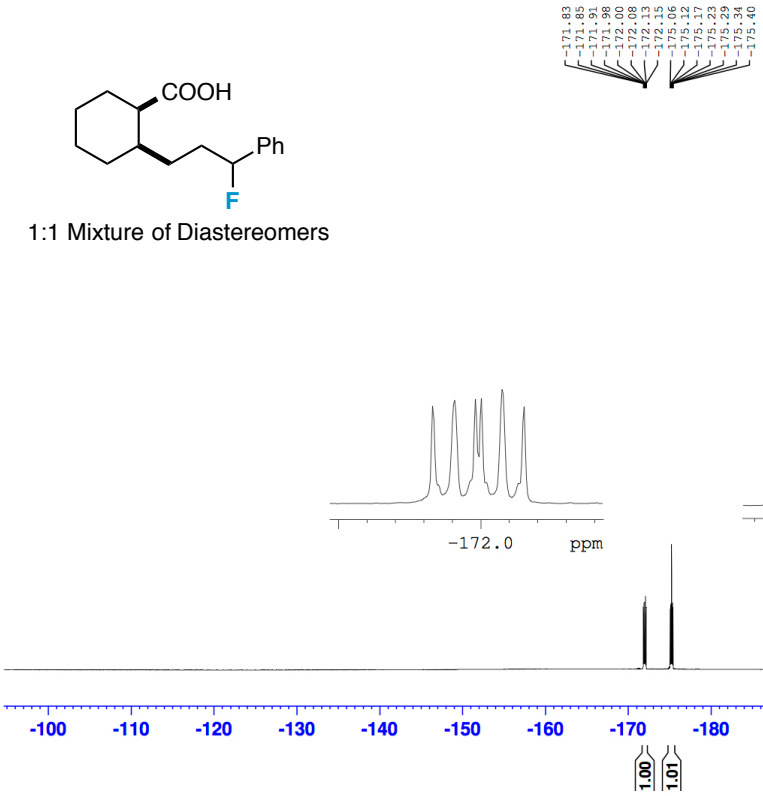
2-(3-fluoro-3-phenylpropyl)benzoic acid



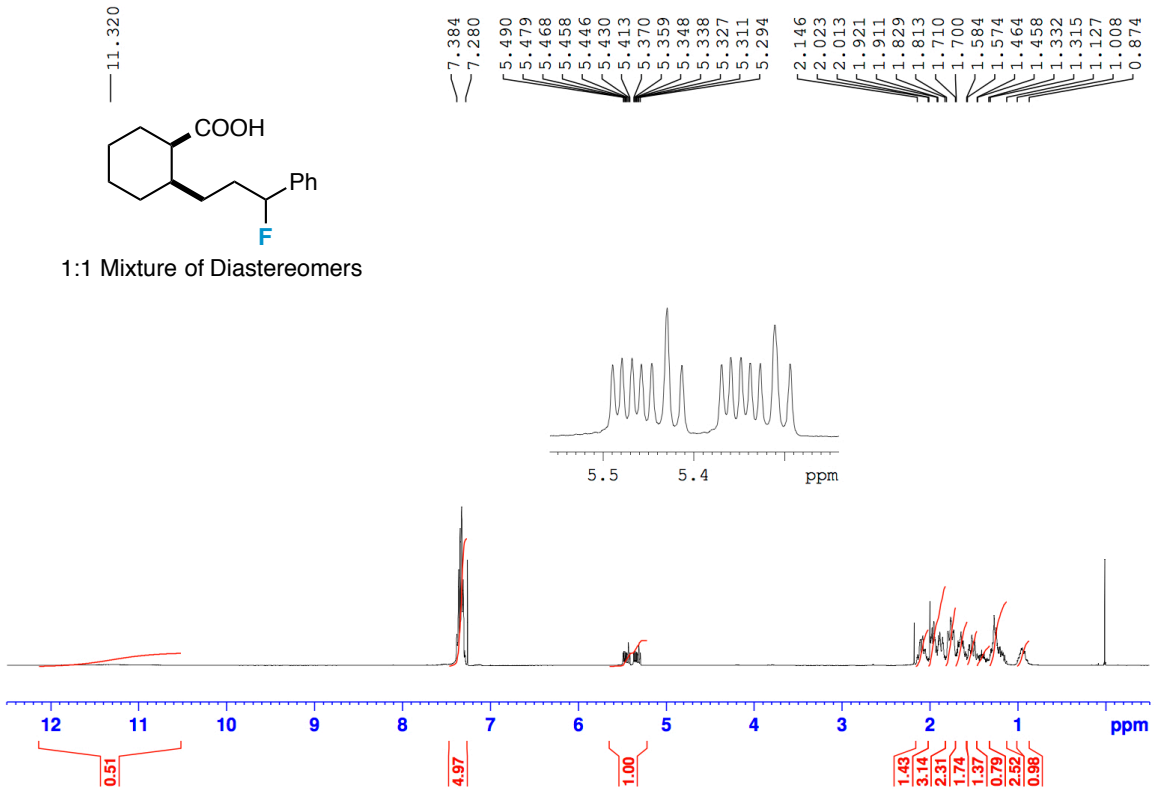
2-(3-fluoro-3-phenylpropyl)benzoic acid



cis-2-(3-fluoro-3-phenylpropyl)cyclohexane-1-carboxylic acid

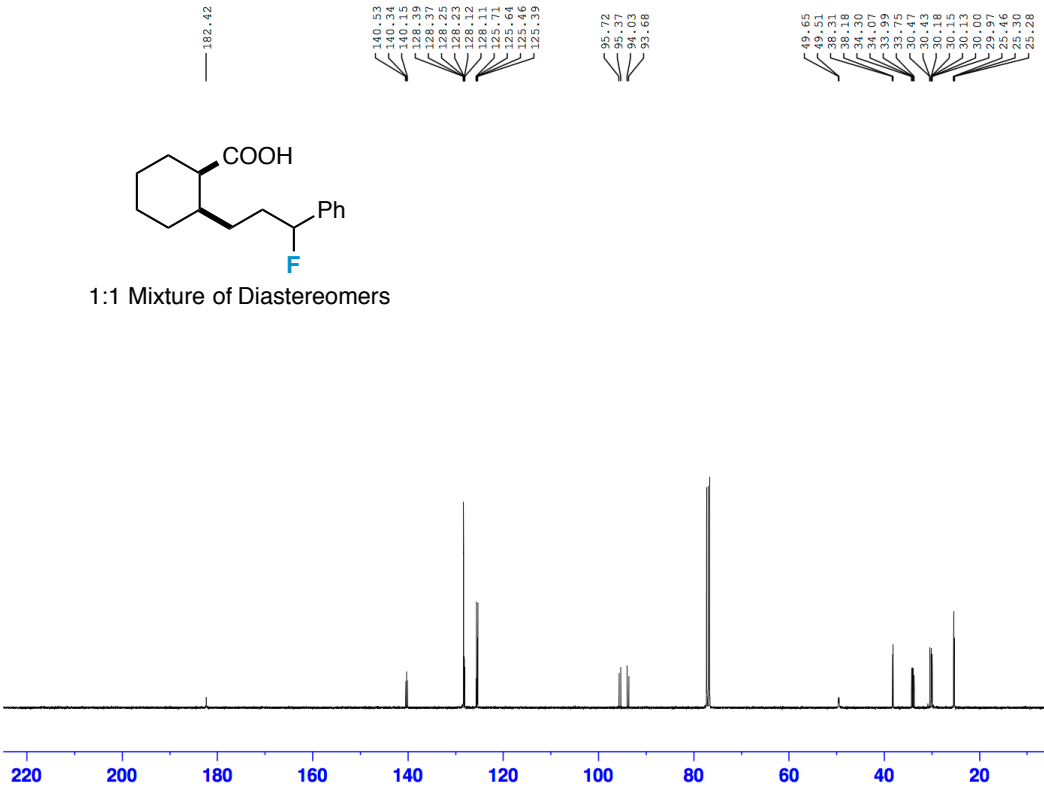


cis-2-(3-fluoro-3-phenylpropyl)cyclohexane-1-carboxylic acid

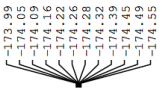


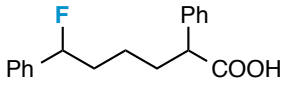
1:1 Mixture of Diastereomers

cis-2-(3-fluoro-3-phenylpropyl)cyclohexane-1-carboxylic acid

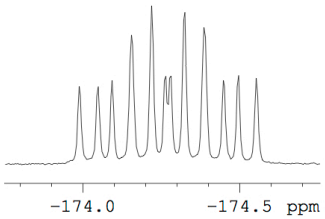


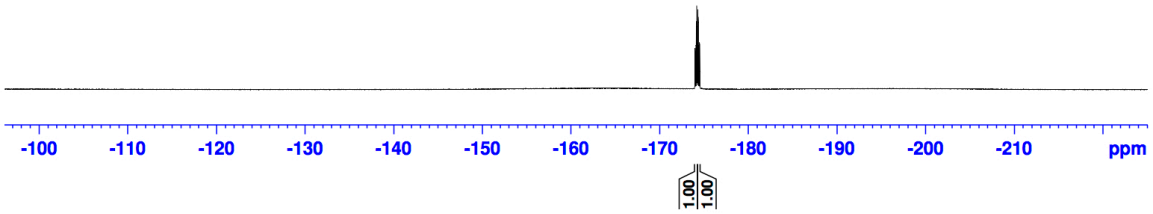
6-fluoro-2,6-diphenylhexanoic acid



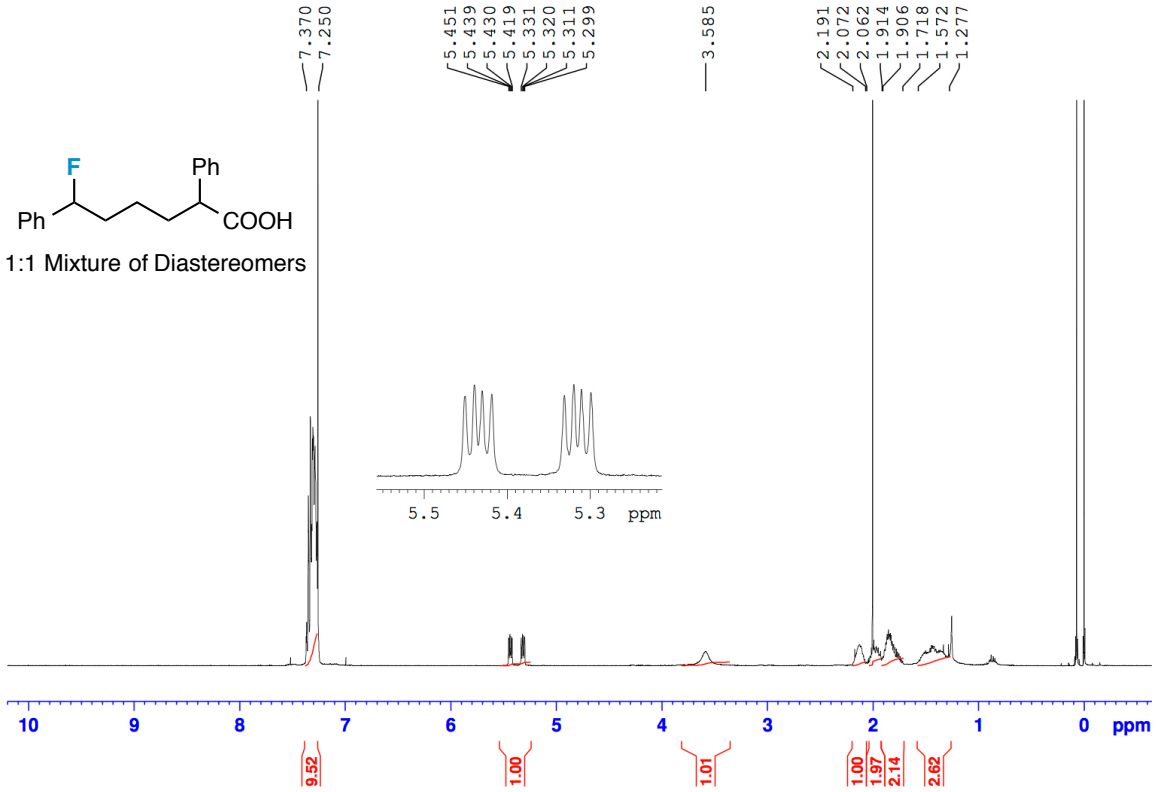


1:1 Mixture of Diastereomers

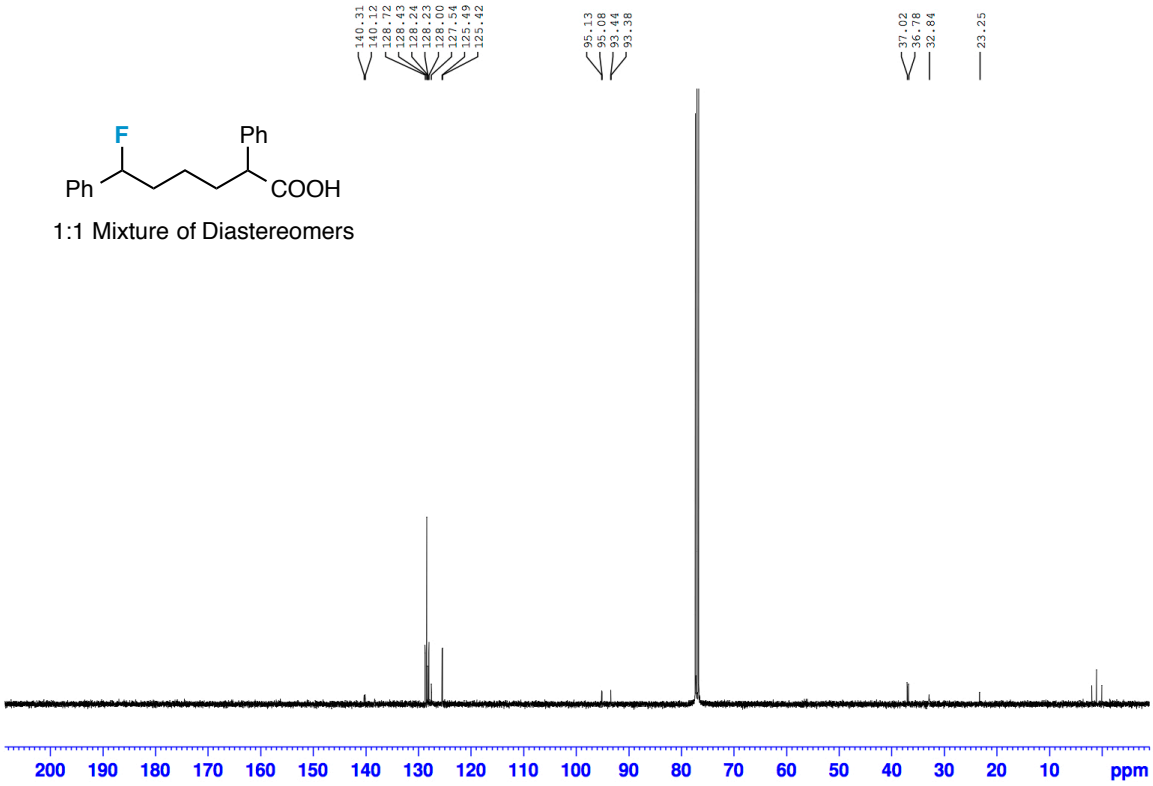




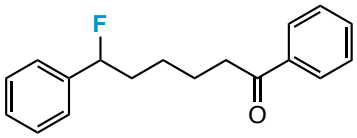
6-fluoro-2,6-diphenylhexanoic acid

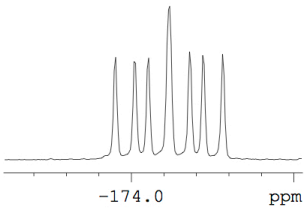


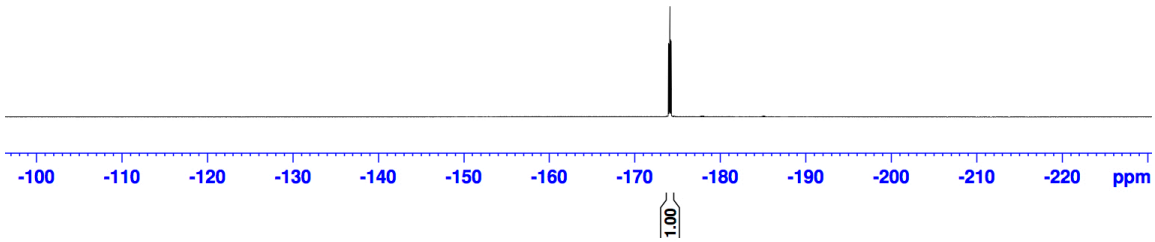
6-fluoro-2,6-diphenylhexanoic acid



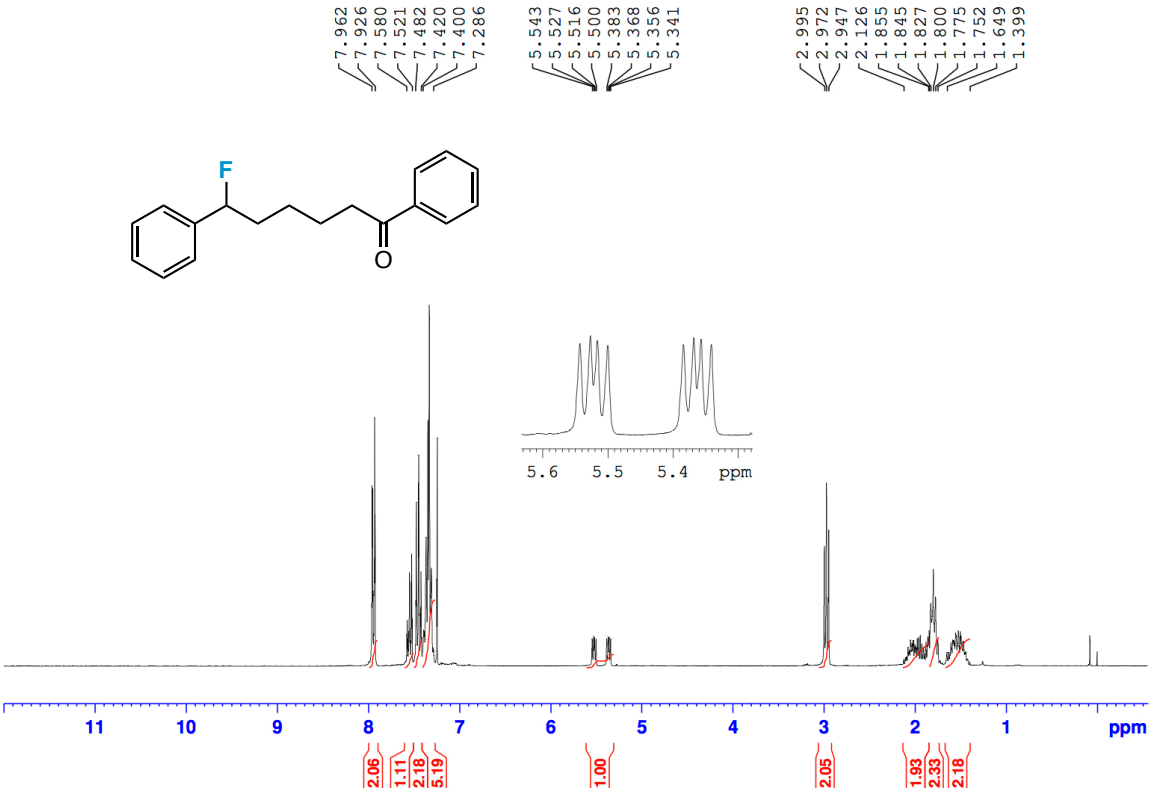
6-fluoro-1,6-diphenyl-hexanone



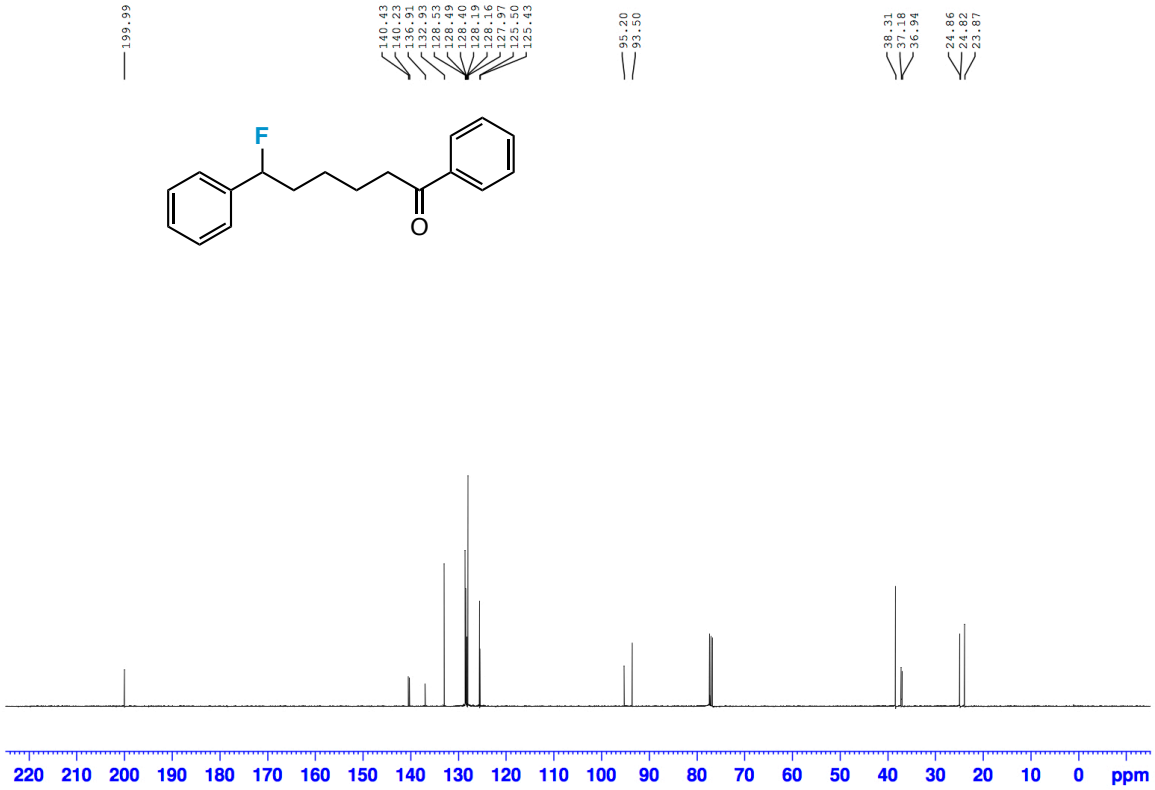




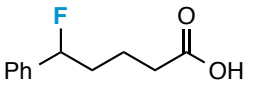
6-fluoro-1,6-diphenyl-hexanone

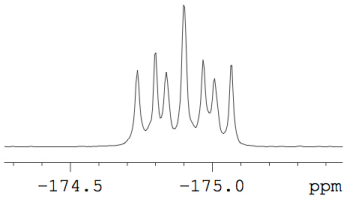


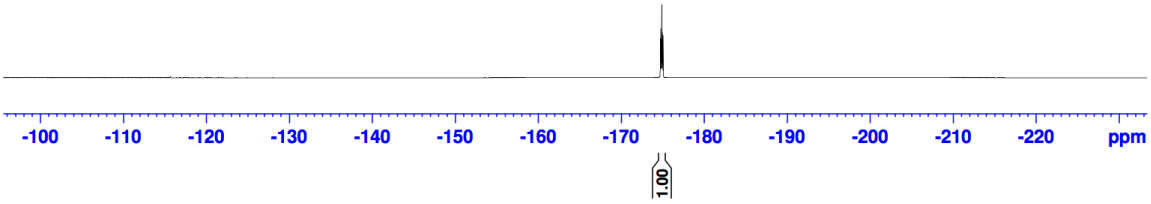
6-fluoro-1,6-diphenyl-hexanone



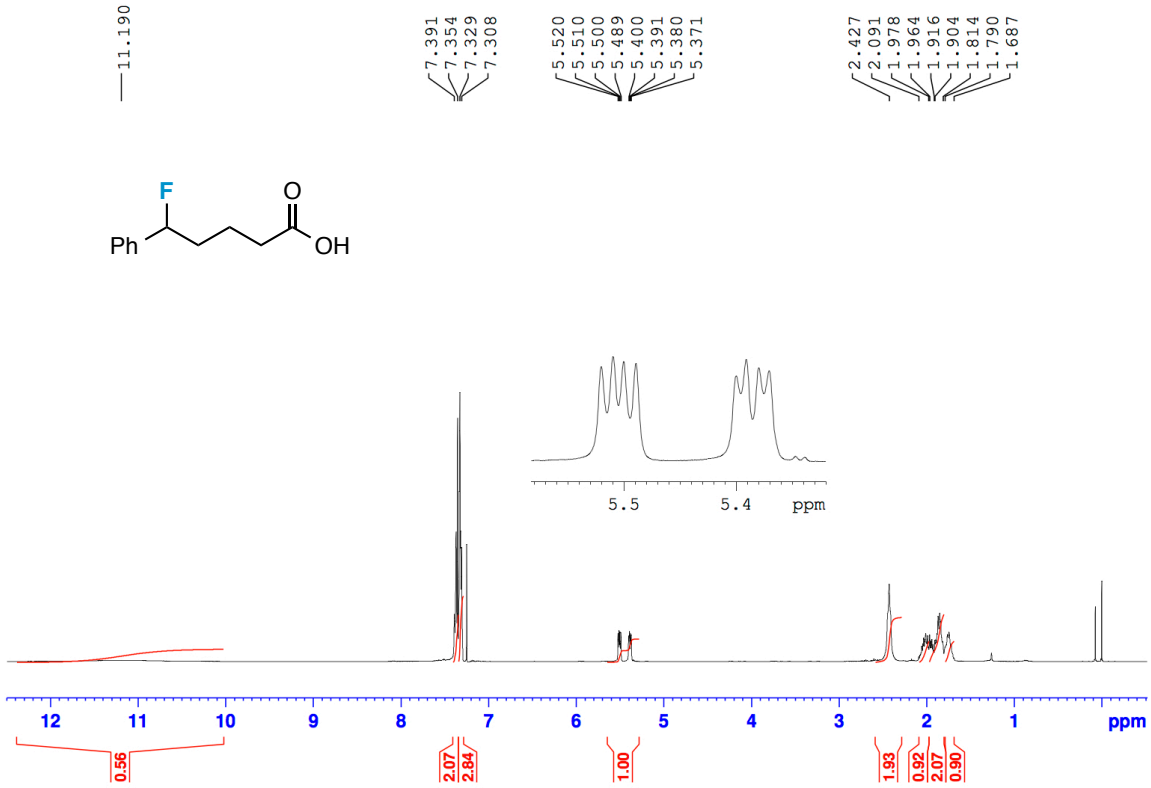
5-fluoro-5-phenylpentanoic acid



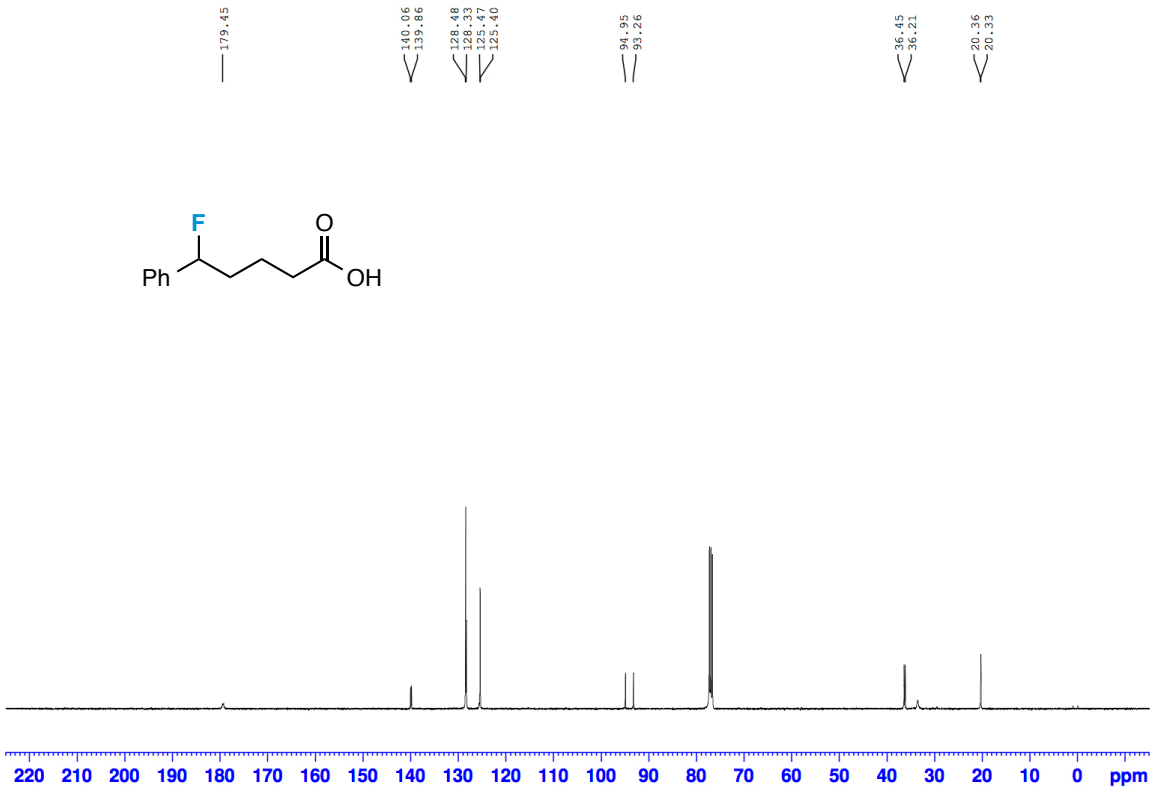




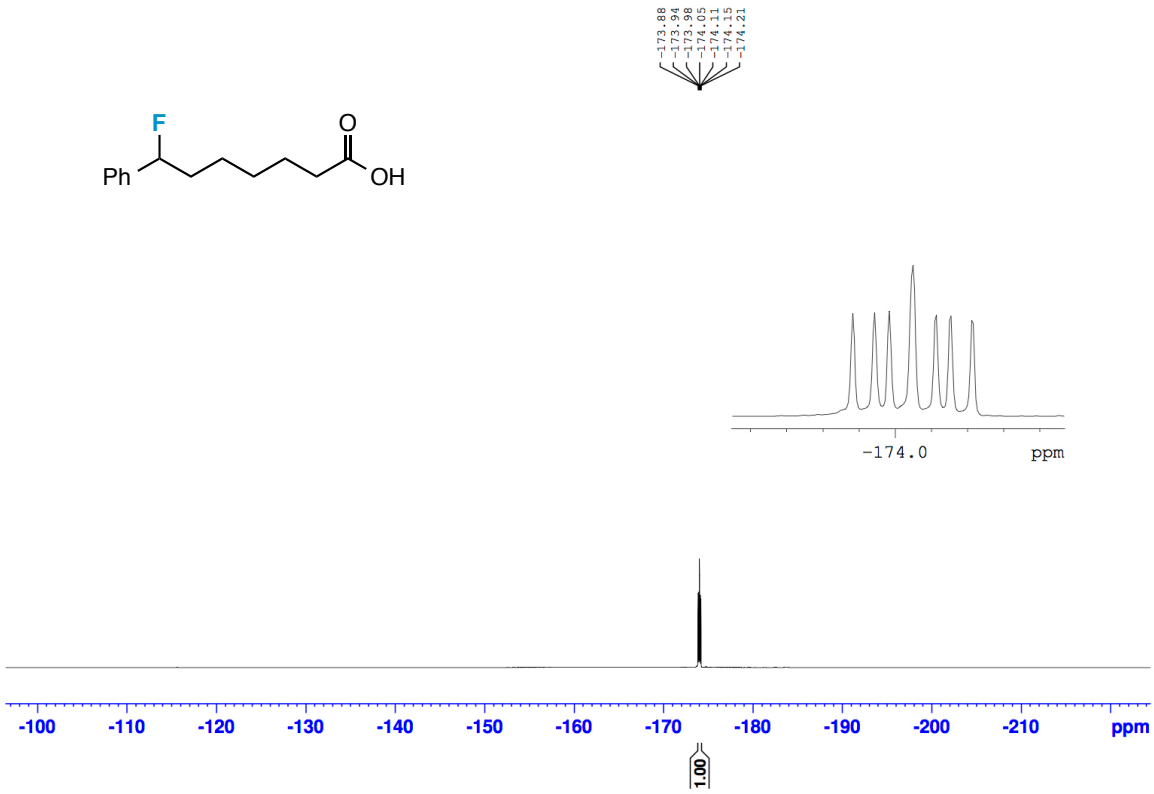
5-fluoro-5-phenylpentanoic acid



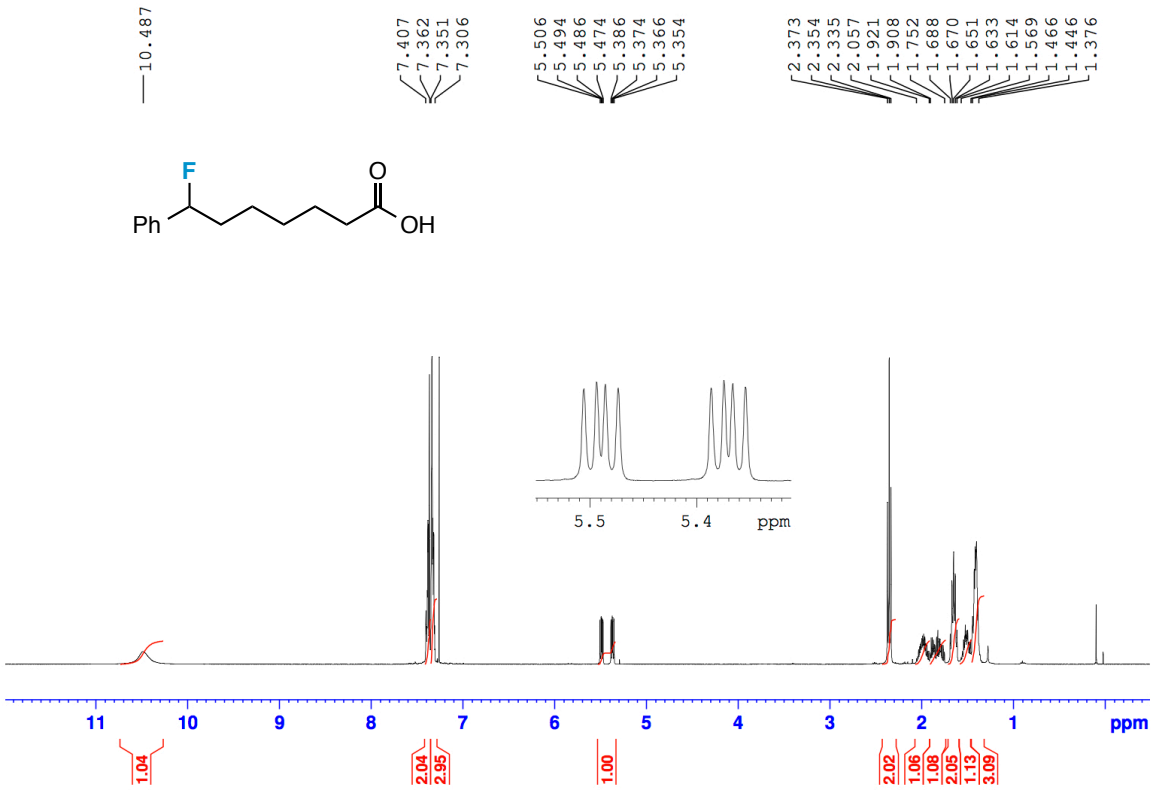
5-fluoro-5-phenylpentanoic acid



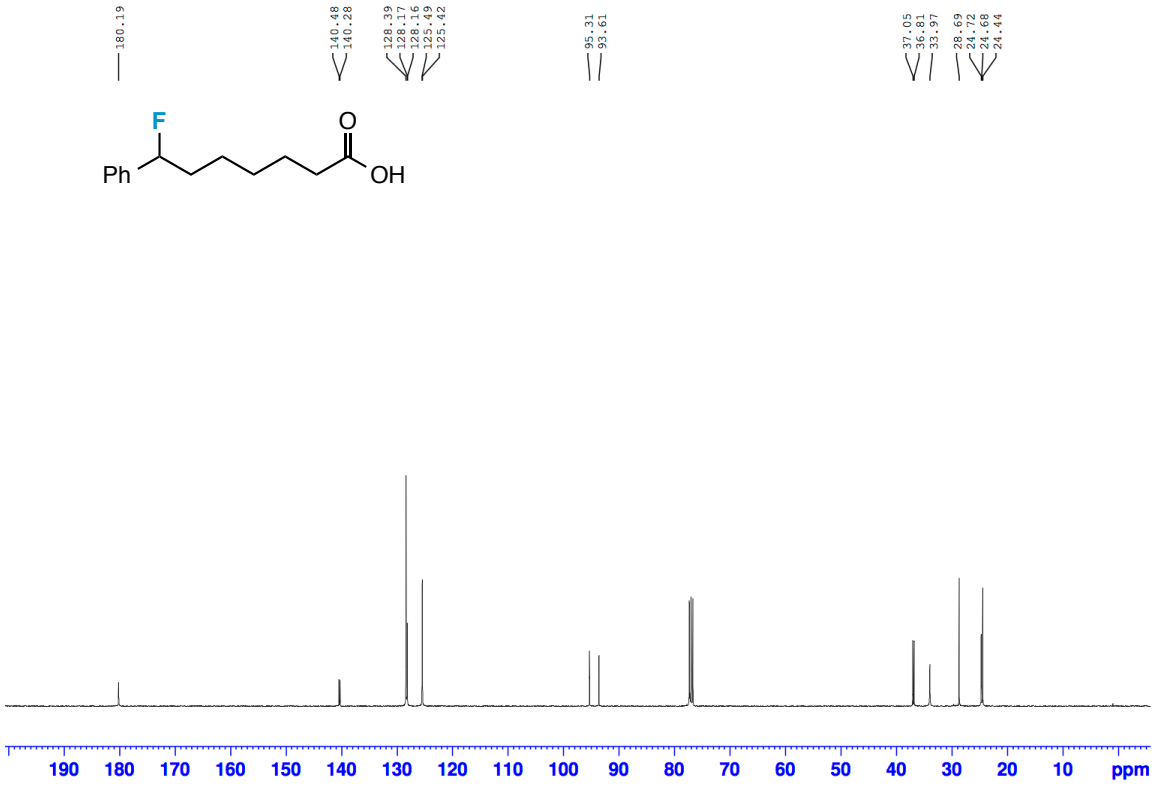
7-fluoro-7-phenylheptanoic acid



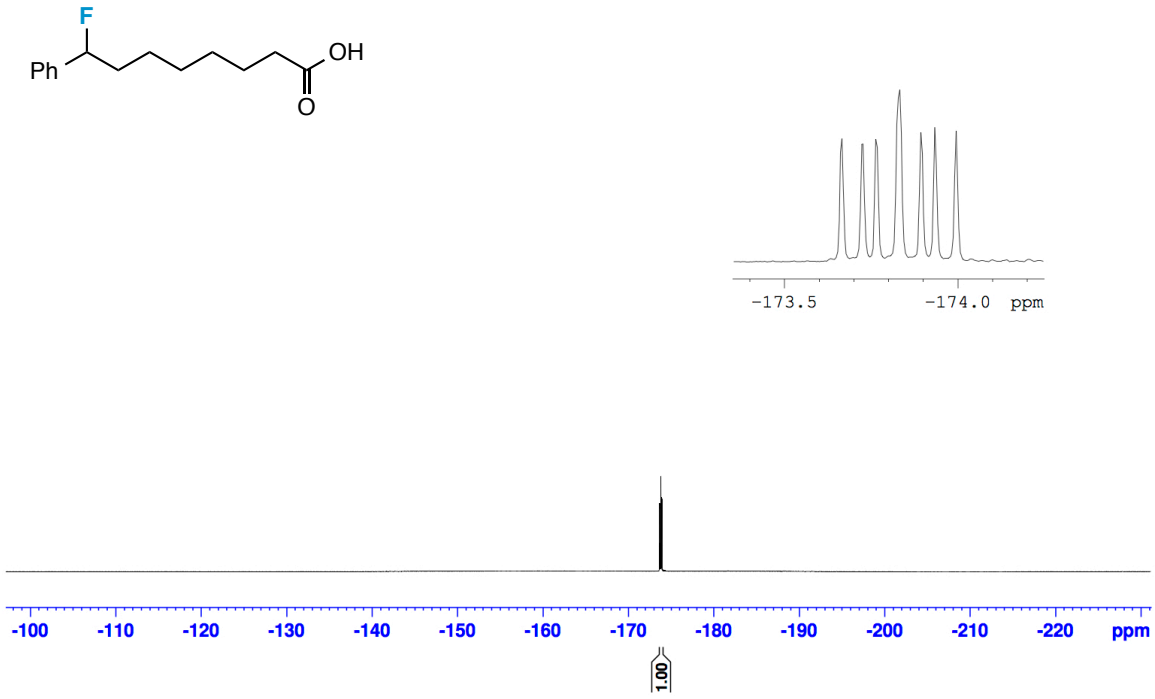
7-fluoro-7-phenylheptanoic acid



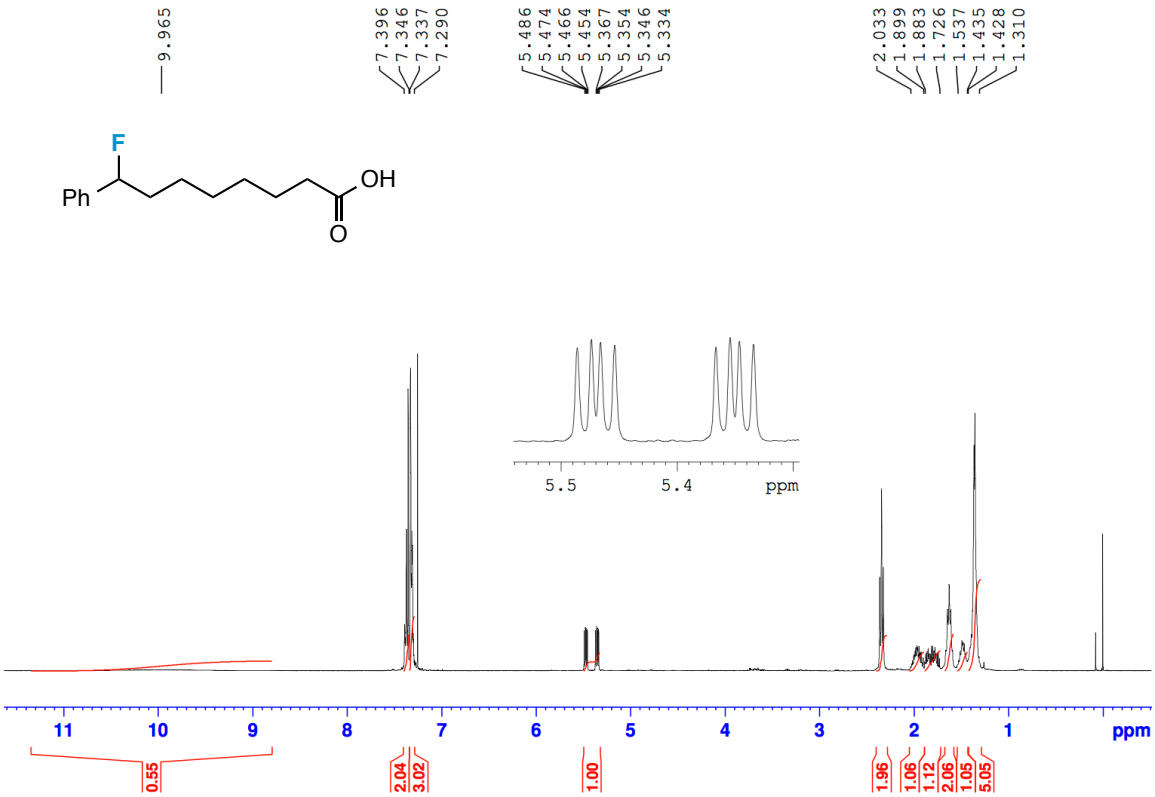
7-fluoro-7-phenylheptanoic acid



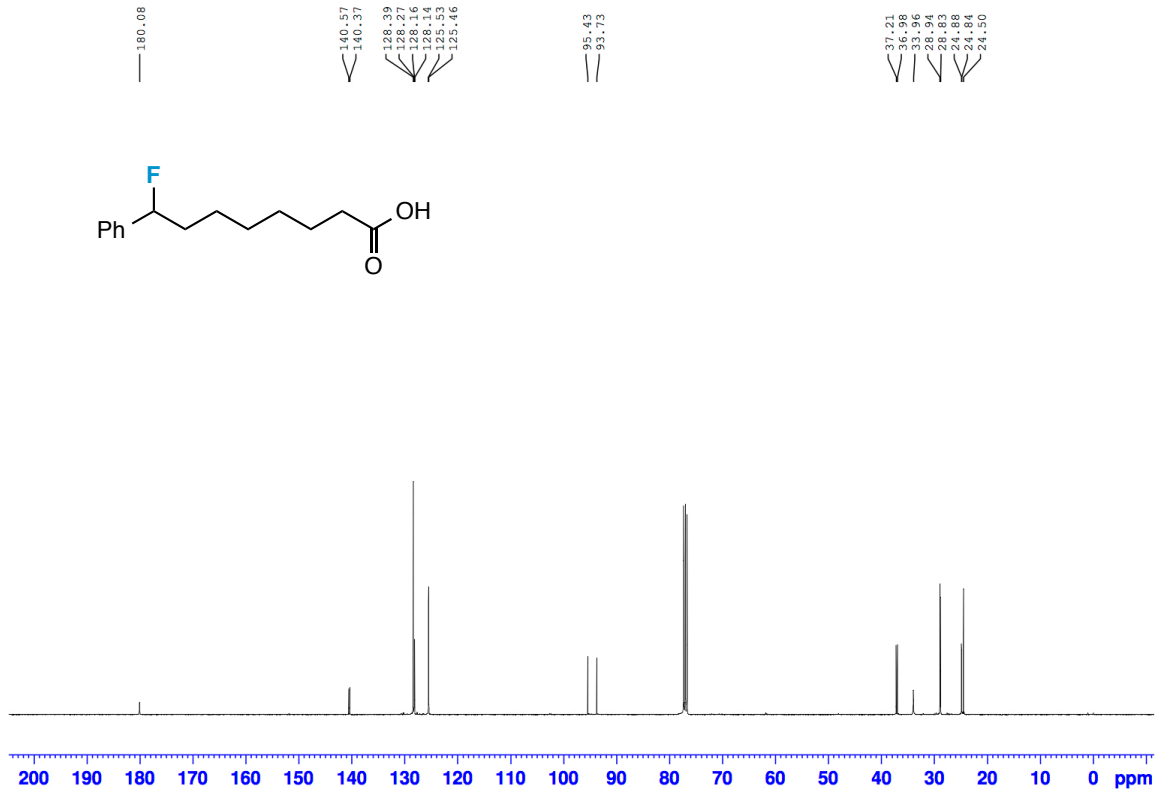
8-fluoro-8-phenyloctanoic acid



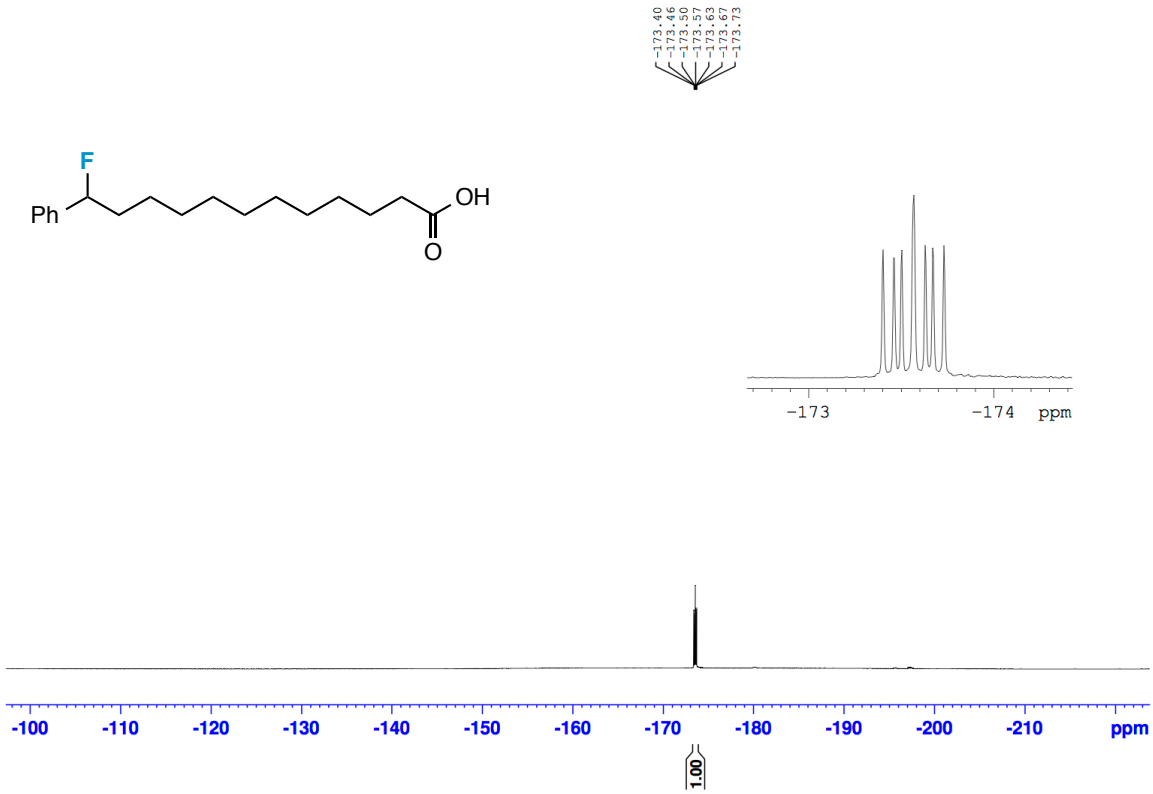
8-fluoro-8-phenyloctanoic acid



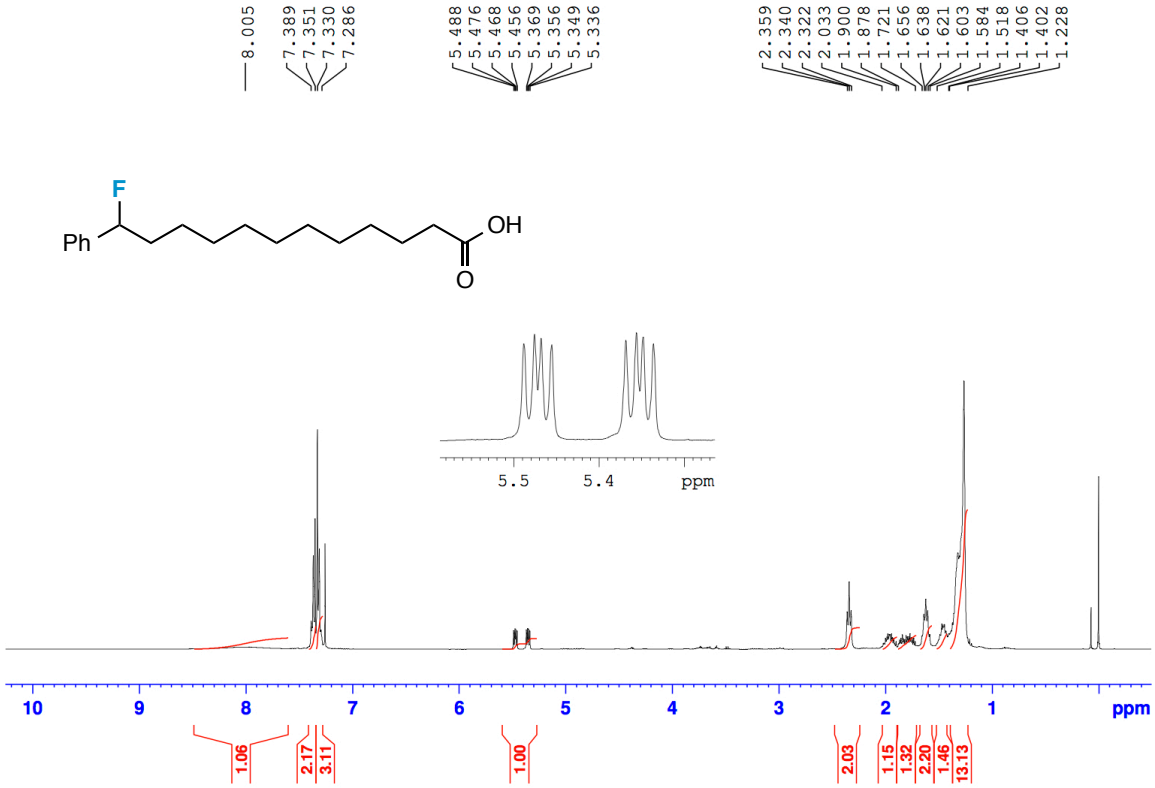
8-fluoro-8-phenyloctanoic acid



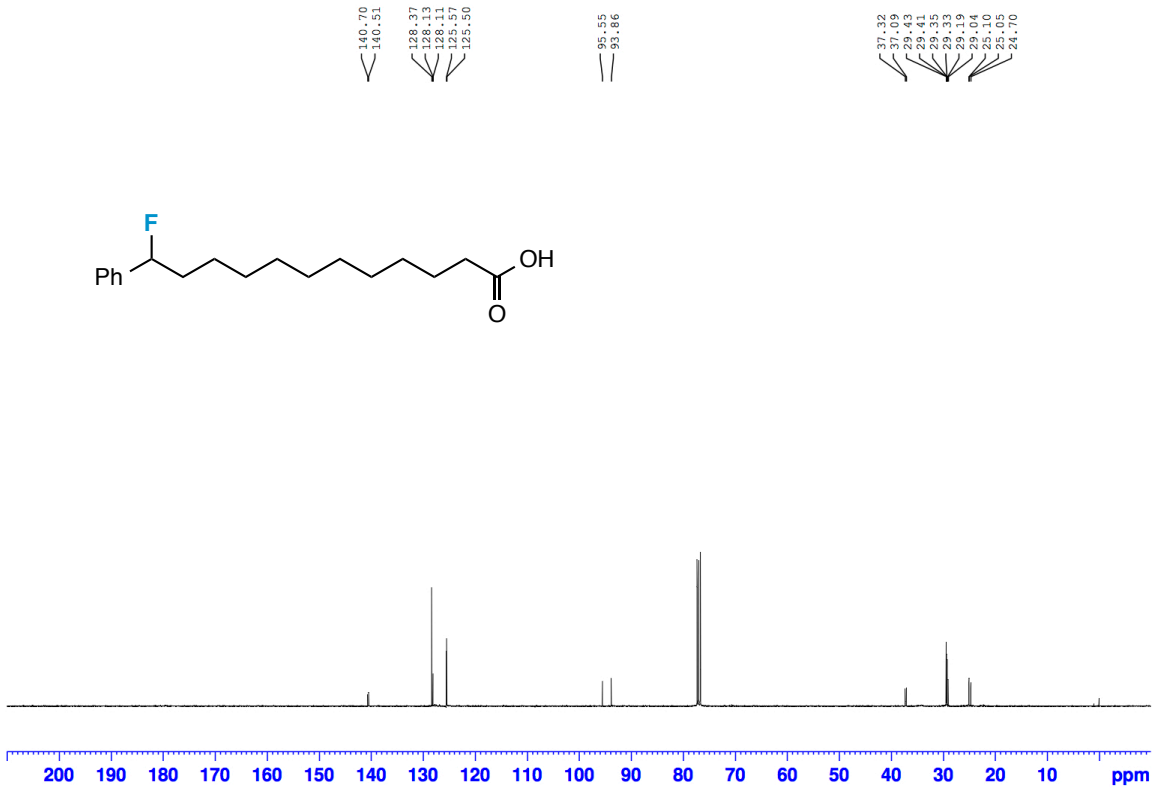
12-fluoro-12-phenyldodecanoic acid



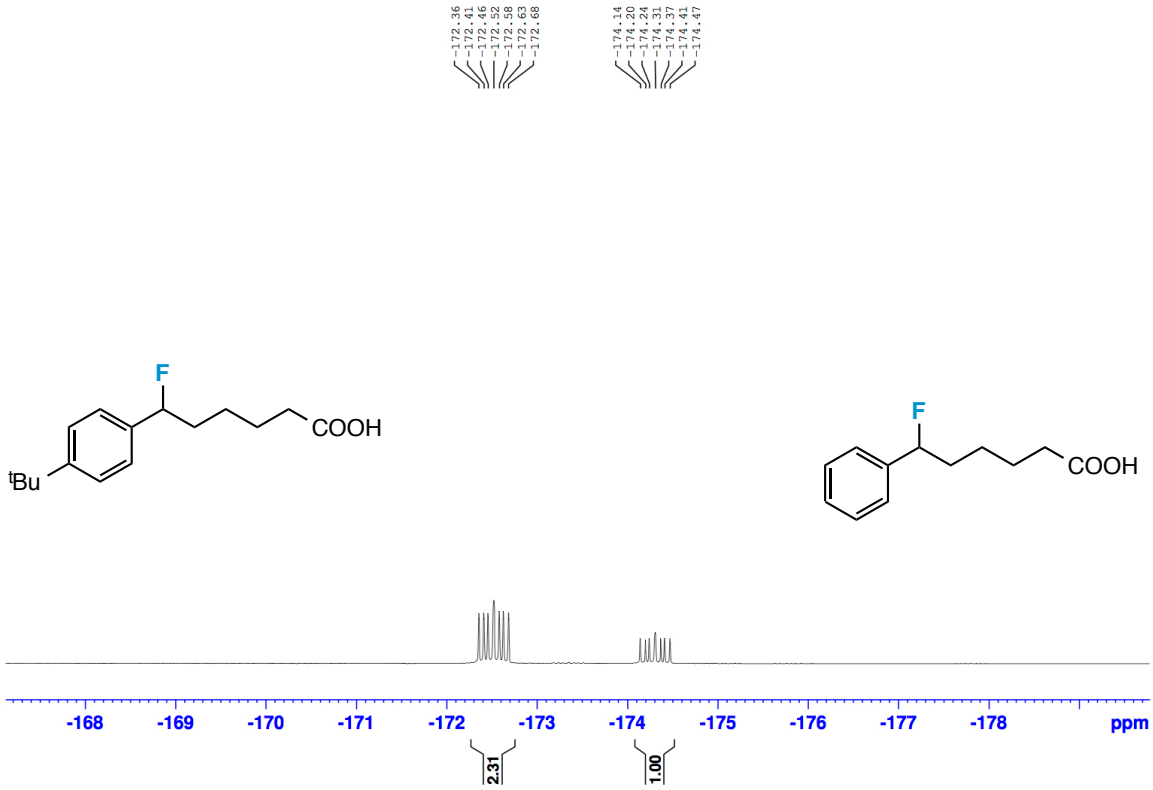
12-fluoro-12-phenyldodecanoic acid



12-fluoro-12-phenyldodecanoic acid

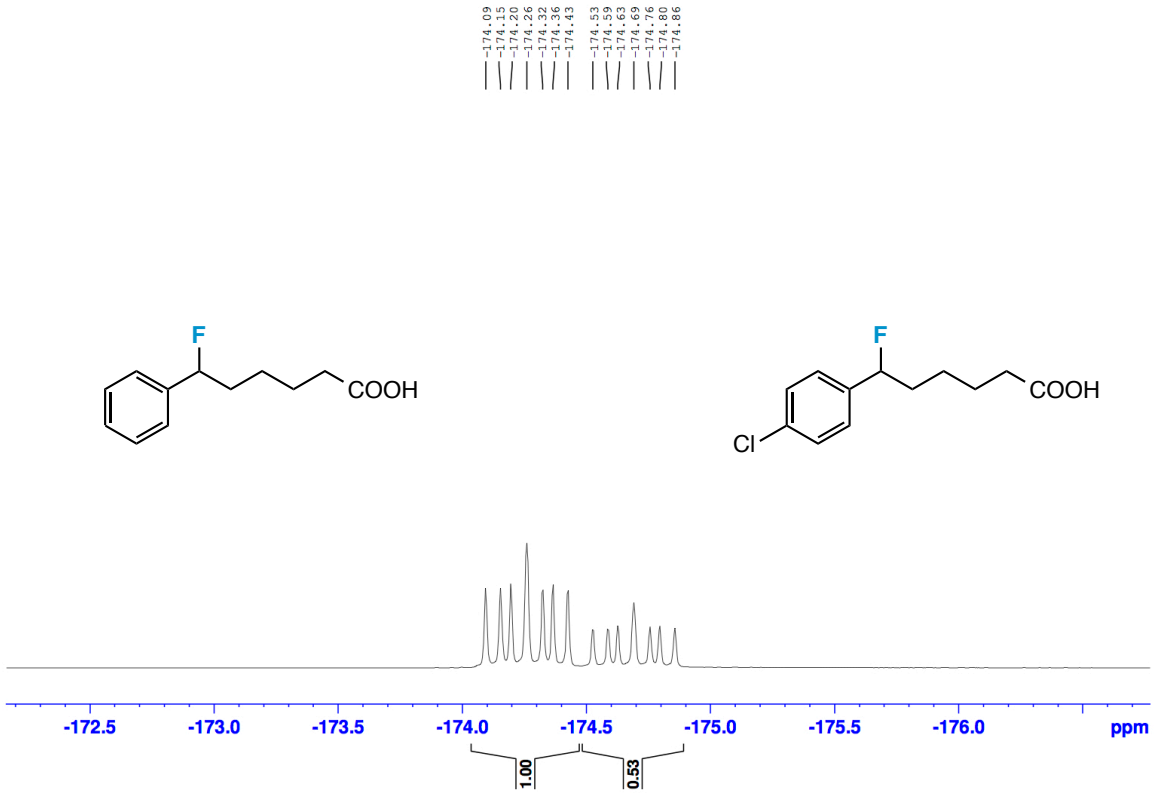


Intermolecular Competition (tBu vs. H)



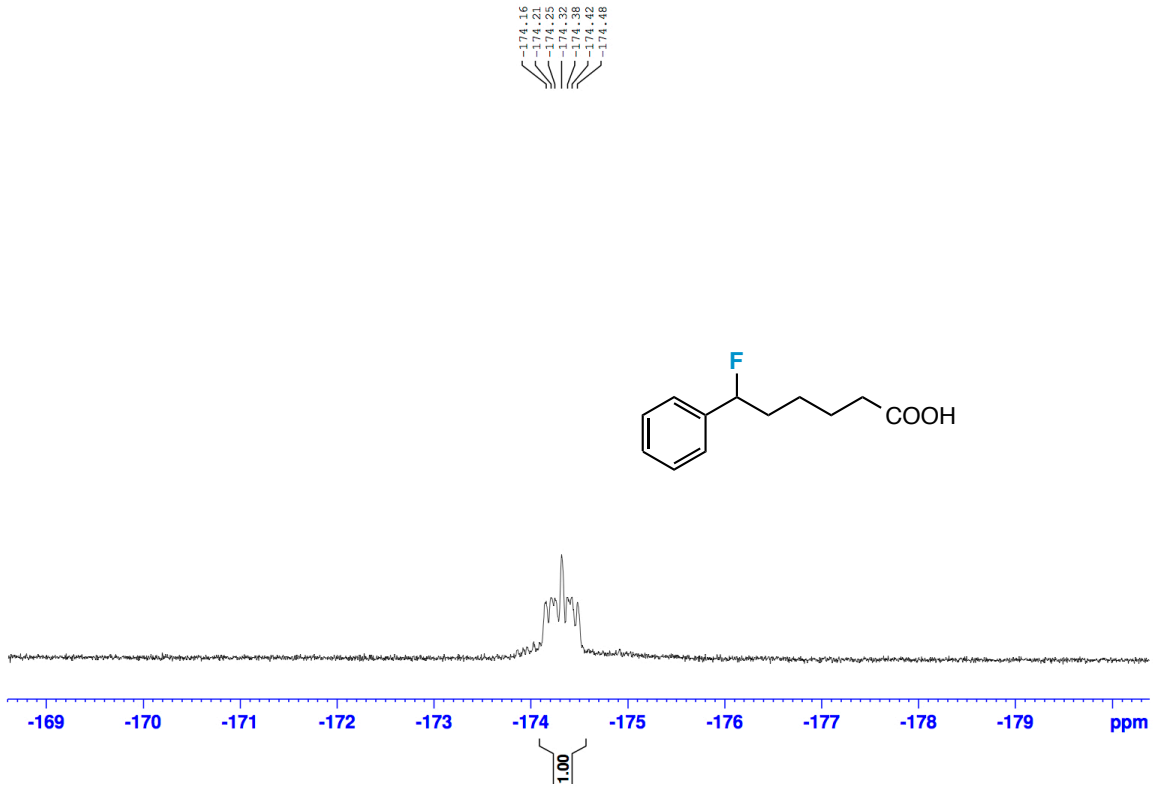
^{19}F NMR ($CDCl_3$): -172.52 (1F, ddd, J = 47.0, 28.7, 16.1 Hz), -174.31 (1F, ddd, J = 47.0, 28.7, 16.1 Hz).

Intermolecular Competition (Cl vs. H)



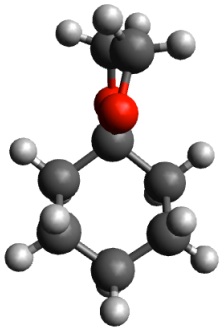
^{19}F NMR ($CDCl_3$): -174.31 (1F, ddd, J = 47.0, 28.7, 17.2 Hz), -174.74 (1F, ddd, J = 47.0, 28.7, 17.2 Hz).

Intermolecular Competition (CF_3 vs. H) – Crude Spectrum



^{19}F NMR (CD_3CN): -174.31 (1F, ddd, J = 47.0, 29.8, 17.2 Hz).

1,4-dioxaspiro[4.5]decane radical cation



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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
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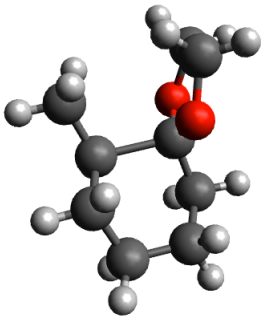
2	6	0	-1.798623	-1.290812	0.120762
3	6	0	-0.556771	-1.183402	-0.717397
4	6	0	0.373327	0.084645	-0.243229
5	6	0	-0.596470	1.347584	-0.358578
6	6	0	-1.841500	1.181860	0.476871
7	1	0	0.121133	-2.032470	-0.612592
8	1	0	-1.540827	-1.543246	1.153315
9	1	0	-2.365924	-2.142526	-0.282435
10	1	0	-3.047566	0.104361	-0.955052
11	1	0	-3.530221	-0.146002	0.720725
12	1	0	0.033418	2.176940	-0.026869
13	1	0	-0.813181	1.457548	-1.422321
14	1	0	-1.582609	1.134322	1.538876
15	1	0	-2.440209	2.091485	0.336279
16	1	0	-0.758335	-0.989142	-1.771884
17	8	0	1.419318	0.190894	-1.094481
18	8	0	0.802921	-0.098619	1.026287
19	6	0	2.651997	0.201547	-0.336963
20	1	0	2.992306	1.238622	-0.285460
21	1	0	3.380599	-0.406526	-0.869091
22	6	0	2.224364	-0.367151	1.007346
23	1	0	2.361602	-1.447947	1.090077
24	1	0	2.670427	0.132378	1.864656

6-methyl-1,4-dioxaspiro[4.5]decane radical cation



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opt b3pw91/6-311++g(d,p) scrf=(solvent=acetonitrile) maxdisk=24GB geom=connectivity

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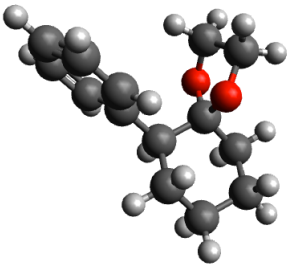
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.703666	-0.010994	0.094993
2	6	0	-2.013276	-1.364263	0.236053
3	6	0	-0.769642	-1.458675	-0.632234
4	6	0	0.344633	-0.501453	-0.243330
5	6	0	-0.545586	1.208064	-0.477392
6	6	0	-1.748210	1.134313	0.407989
7	1	0	-0.302103	-2.447315	-0.544885
8	1	0	-1.748681	-1.552251	1.281525
9	1	0	-2.695529	-2.164071	-0.065175
10	1	0	-3.088269	0.102877	-0.925168
11	1	0	-3.564866	0.039348	0.765991
12	1	0	-0.746839	1.060397	-1.540107
13	1	0	-1.440732	1.126841	1.459442
14	1	0	-2.268560	2.094531	0.256125
15	1	0	-0.996600	-1.296916	-1.688147
16	8	0	1.375981	-0.439361	-1.087071
17	8	0	0.731218	-0.527175	1.032085
18	6	0	2.616745	-0.358502	-0.339373
19	1	0	3.170298	0.512887	-0.684585
20	1	0	3.177700	-1.267374	-0.556319
21	6	0	2.153742	-0.257760	1.114276
22	1	0	2.586539	-1.014939	1.765187
23	1	0	2.290776	0.730654	1.550933
24	6	0	0.453250	2.280453	-0.196574
25	1	0	1.353052	2.194603	-0.806295
26	1	0	-0.020706	3.231452	-0.477251
27	1	0	0.708986	2.354464	0.862176

6-phenyl-1,4-dioxaspiro[4.5]decane



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opt b3pw91/6-311++g(d,p) scrf=(solvent=acetonitrile) maxdisk=24GB geom=connectivity

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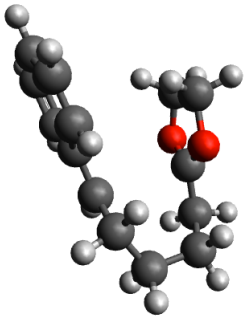
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.977598	-1.940150	0.423070
2	6	0	0.351431	-0.822385	-0.427506
3	6	0	1.168596	0.481485	-0.284160
4	6	0	2.636483	0.245303	-0.635799
5	6	0	3.254634	-0.885417	0.185125
6	6	0	2.442259	-2.172259	0.055517
7	1	0	0.471325	-1.105937	-1.480773
8	1	0	0.904549	-1.679018	1.484617
9	1	0	0.397933	-2.858545	0.283288
10	1	0	2.690387	0.009653	-1.705072
11	1	0	3.177840	1.185096	-0.486336
12	1	0	4.288858	-1.049255	-0.134720
13	1	0	3.295108	-0.584693	1.238702
14	1	0	2.502751	-2.540776	-0.977312
15	1	0	2.867082	-2.955203	0.692602
16	8	0	1.036545	0.984236	1.041727
17	8	0	0.660644	1.498359	-1.151342
18	6	0	0.066724	2.518942	-0.352359
19	1	0	-1.003717	2.327289	-0.217770
20	1	0	0.210388	3.479097	-0.850915
21	6	0	0.823008	2.389538	0.954888
22	1	0	1.778577	2.927981	0.924151
23	1	0	0.254944	2.707361	1.830290
24	6	0	-1.129275	-0.633425	-0.185224
25	6	0	-2.009198	-0.576705	-1.270961
26	6	0	-1.665808	-0.519190	1.102579
27	6	0	-3.378460	-0.403730	-1.083825
28	1	0	-1.614512	-0.669296	-2.278887
29	6	0	-3.034247	-0.347582	1.295224
30	1	0	-1.008113	-0.556995	1.963138
31	6	0	-3.896960	-0.287287	0.203094
32	1	0	-4.039856	-0.363708	-1.943848
33	1	0	-3.428128	-0.261337	2.303375
34	1	0	-4.963640	-0.155305	0.354404

6-phenyl-1,4-dioxaspiro[4.5]decane radical cation



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opt b3pw91/6-311++g(d,p) scrf=(solvent=acetonitrile) maxdisk=24GB geom=connectivity

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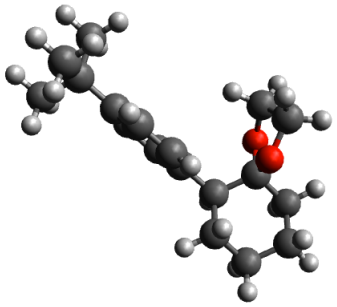
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.085559	-2.146509	0.315723
2	6	0	0.179984	-1.415871	-0.617412
3	6	0	1.547303	1.149616	-0.152635
4	6	0	2.765200	0.462220	-0.619161
5	6	0	3.251255	-0.721059	0.224974
6	6	0	2.569900	-2.061988	-0.052590
7	1	0	0.504028	-1.326455	-1.652911
8	1	0	0.942688	-1.812393	1.350316
9	1	0	0.795383	-3.209878	0.315904
10	1	0	2.630177	0.209840	-1.673025
11	1	0	3.521560	1.262528	-0.598761
12	1	0	4.318177	-0.829389	0.014663
13	1	0	3.175032	-0.468708	1.287068
14	1	0	2.698784	-2.326366	-1.109292
15	1	0	3.111039	-2.822711	0.518219
16	8	0	1.232600	1.212690	1.088861
17	8	0	0.828889	1.848652	-0.953910
18	6	0	-0.190467	2.571940	-0.181810
19	1	0	-1.157447	2.282928	-0.584517
20	1	0	-0.001520	3.631913	-0.332669
21	6	0	0.062762	2.088631	1.246848
22	1	0	0.351644	2.875645	1.938652
23	1	0	-0.736065	1.476798	1.657756
24	6	0	-1.146269	-1.005234	-0.332293
25	6	0	-1.940159	-0.425953	-1.361088
26	6	0	-1.744206	-1.148856	0.949311
27	6	0	-3.236662	-0.009415	-1.119118
28	1	0	-1.511489	-0.316612	-2.352958
29	6	0	-3.044018	-0.728430	1.179028
30	1	0	-1.181371	-1.599324	1.759336
31	6	0	-3.799604	-0.153781	0.153310
32	1	0	-3.820046	0.428233	-1.922850
33	1	0	-3.479116	-0.851064	2.165776
34	1	0	-4.816838	0.172418	0.341153

6-(4-(*tert*-butyl)phenyl)-1,4-dioxaspiro[4.5]decane



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opt b3pw91/6-311++g(d,p) scrf=(solvent=acetonitrile) maxdisk=24GB geom=connectivity

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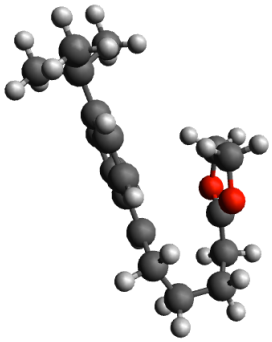
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.222395	-1.952142	0.418056
2	6	0	1.639768	-0.824521	-0.449803
3	6	0	2.456621	0.473357	-0.257351
4	6	0	3.937789	0.233403	-0.545021
5	6	0	4.512956	-0.907234	0.293202
6	6	0	3.701164	-2.188815	0.115870
7	1	0	1.806517	-1.099192	-1.499276
8	1	0	2.102428	-1.698672	1.477202
9	1	0	1.645290	-2.866528	0.244997
10	1	0	4.038942	0.006504	-1.612832
11	1	0	4.476413	1.169093	-0.363227
12	1	0	5.559942	-1.073671	0.019362
13	1	0	4.506871	-0.615256	1.350072
14	1	0	3.807192	-2.548722	-0.916355
15	1	0	4.093172	-2.979212	0.764778
16	8	0	2.268533	0.963139	1.067057
17	8	0	1.994014	1.503014	-1.135083
18	6	0	1.365438	2.514990	-0.351901
19	1	0	0.290309	2.321922	-0.266359
20	1	0	1.531149	3.480385	-0.833217
21	6	0	2.063417	2.369885	0.985629
22	1	0	3.020978	2.905522	1.001773
23	1	0	1.458778	2.681188	1.838645
24	6	0	0.150943	-0.629776	-0.273727
25	6	0	-0.680870	-0.528690	-1.393460
26	6	0	-0.456673	-0.548930	0.980142
27	6	0	-2.052634	-0.347059	-1.265123
28	1	0	-0.245066	-0.592621	-2.386933
29	6	0	-1.833875	-0.370412	1.107943
30	1	0	0.147627	-0.618382	1.877782
31	6	0	-2.667298	-0.263147	-0.008698
32	1	0	-2.651196	-0.273434	-2.168013
33	1	0	-2.252065	-0.315356	2.106551
34	6	0	-4.182596	-0.058974	0.094453
35	6	0	-4.669044	-0.040214	1.548354
36	1	0	-4.447917	-0.979943	2.063676
37	1	0	-4.219758	0.778134	2.119143
38	1	0	-5.753824	0.100834	1.568275
39	6	0	-4.907605	-1.201966	-0.640644
40	1	0	-4.661772	-2.170886	-0.195064
41	1	0	-5.991906	-1.063713	-0.576203
42	1	0	-4.638958	-1.239562	-1.699687
43	6	0	-4.558169	1.284419	-0.558965
44	1	0	-4.063350	2.117281	-0.049719
45	1	0	-4.270582	1.314984	-1.613416
46	1	0	-5.639962	1.445037	-0.501487

6-(4-(*tert*-butyl)phenyl)-1,4-dioxaspiro[4.5]decane radical cation



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opt b3pw91/6-311++g(d,p) scrf=(solvent=acetonitrile) maxdisk=24GB geom=connectivity

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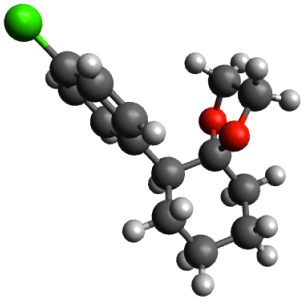
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.405375	-2.101720	0.347393
2	6	0	1.517962	-1.411079	-0.633266
3	6	0	2.739672	1.175805	-0.117374
4	6	0	4.015846	0.558761	-0.524245
5	6	0	4.521332	-0.604694	0.335016
6	6	0	3.899608	-1.970922	0.040491
7	1	0	1.889333	-1.307147	-1.651310
8	1	0	2.207087	-1.757303	1.369728
9	1	0	2.149942	-3.173937	0.352297
10	1	0	3.948711	0.310264	-1.585612
11	1	0	4.726053	1.398149	-0.459248
12	1	0	5.597768	-0.671143	0.157896
13	1	0	4.402335	-0.354466	1.393782
14	1	0	4.079887	-2.237339	-1.008199
15	1	0	4.443143	-2.708495	0.638781
16	8	0	2.358661	1.216896	1.107309
17	8	0	2.035415	1.853327	-0.950736
18	6	0	0.952682	2.531791	-0.226973
19	1	0	0.018592	2.222970	-0.688049
20	1	0	1.118094	3.599541	-0.348928
21	6	0	1.138352	2.029823	1.205543
22	1	0	1.341375	2.814356	1.929973
23	1	0	0.346968	1.369411	1.550520
24	6	0	0.158386	-1.078285	-0.417467
25	6	0	-0.621057	-0.535147	-1.475806
26	6	0	-0.503752	-1.265155	0.822245
27	6	0	-1.947233	-0.200698	-1.295973
28	1	0	-0.156297	-0.387198	-2.446501
29	6	0	-1.838058	-0.924369	0.984991
30	1	0	0.034279	-1.689638	1.663019
31	6	0	-2.599554	-0.381839	-0.060006
32	1	0	-2.494610	0.208536	-2.139078
33	1	0	-2.292609	-1.092562	1.954163
34	6	0	-4.073040	-0.001589	0.091213
35	6	0	-4.602094	-0.274184	1.504283
36	1	0	-4.534469	-1.333797	1.768233
37	1	0	-4.062758	0.304436	2.260341
38	1	0	-5.656117	0.013105	1.559180
39	6	0	-4.913989	-0.821097	-0.907097
40	1	0	-4.809686	-1.893662	-0.717136
41	1	0	-5.972507	-0.559700	-0.808686
42	1	0	-4.618191	-0.630473	-1.942065
43	6	0	-4.245631	1.499918	-0.208664
44	1	0	-3.665596	2.107102	0.493049
45	1	0	-3.923392	1.752153	-1.222335
46	1	0	-5.298782	1.783139	-0.112228

6-(4-chlorophenyl)-1,4-dioxaspiro[4.5]decane



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opt b3pw91/6-311++g(d,p) scrf=(solvent=acetonitrile) maxdisk=24GB geom=connectivity

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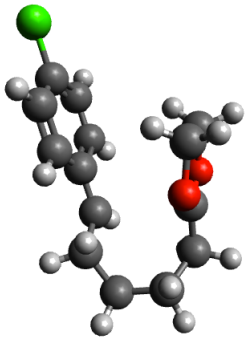
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.102369	-2.181054	-0.118911
2	6	0	-3.911395	-0.896500	-0.286940
3	6	0	-3.331392	0.238312	0.555985
4	6	0	-1.850968	0.477244	0.264726
5	6	0	-1.037837	-0.824612	0.446278
6	6	0	-1.624204	-1.947103	-0.425842
7	1	0	-3.868776	1.175978	0.381345
8	1	0	-3.907909	-0.598786	-1.342172
9	1	0	-4.957756	-1.062120	-0.010675
10	1	0	-3.205387	-2.546355	0.911601
11	1	0	-3.497982	-2.967008	-0.770776
12	1	0	-1.197913	-1.105132	1.494701
13	1	0	-1.508128	-1.688863	-1.484254
14	1	0	-1.048607	-2.863427	-0.258839
15	1	0	-3.429316	0.006025	1.622855
16	8	0	-1.663279	0.973390	-1.056255
17	8	0	-1.378936	1.497783	1.147812
18	6	0	-1.476032	2.382571	-0.966442
19	6	0	-0.772667	2.526967	0.368481
20	1	0	-0.879805	2.706668	-1.820408
21	1	0	-2.440511	2.905410	-0.974362
22	1	0	0.305153	2.353067	0.275208
23	1	0	-0.950547	3.485673	0.858581
24	6	0	0.449011	-0.627744	0.261403
25	6	0	1.286417	-0.555700	1.377967
26	6	0	1.034994	-0.516155	-1.003920
27	6	0	2.660144	-0.371218	1.251585
28	1	0	0.859817	-0.644382	2.372470
29	6	0	2.406079	-0.332973	-1.153597
30	1	0	0.416563	-0.564010	-1.892108
31	6	0	3.205765	-0.259763	-0.020044
32	1	0	3.294235	-0.317700	2.128876
33	1	0	2.846232	-0.247576	-2.140391
34	17	0	4.935005	-0.027675	-0.199323

6-(4-chlorophenyl)-1,4-dioxaspiro[4.5]decane radical cation



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opt b3pw91/6-311++g(d,p) scrf=(solvent=acetonitrile) maxdisk=24GB geom=connectivity

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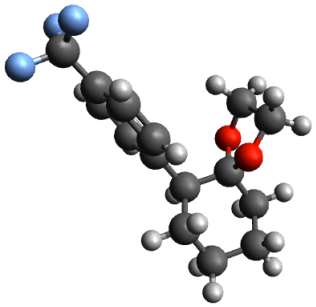
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.217747	1.171814	0.161298
2	6	0	-1.755079	-2.111806	-0.405629
3	6	0	-3.920388	-0.681387	-0.284085
4	6	0	-3.245548	-2.035790	-0.059860
5	6	0	-3.433315	0.467500	0.607045
6	6	0	-0.862933	-1.451888	0.591050
7	1	0	-1.586245	-1.714080	-1.414143
8	1	0	-3.841044	-0.386723	-1.334911
9	1	0	-3.392787	-2.350184	0.980528
10	1	0	-3.296239	0.175933	1.650318
11	1	0	-1.225854	-1.384913	1.614860
12	1	0	-1.474598	-3.175789	-0.468763
13	1	0	-4.988104	-0.795049	-0.081049
14	1	0	-3.780431	-2.765600	-0.675060
15	1	0	-4.190188	1.267430	0.617901
16	8	0	-1.481867	1.825969	0.983338
17	8	0	-1.914658	1.282444	-1.079155
18	6	0	0.484047	-1.077146	0.373983
19	6	0	3.164694	-0.306928	0.024665
20	6	0	1.132786	-1.206122	-0.884113
21	6	0	1.253652	-0.551858	1.448808
22	6	0	2.570386	-0.170618	1.281016
23	6	0	2.451873	-0.826419	-1.055978
24	1	0	0.595249	-1.615671	-1.731675
25	1	0	0.792697	-0.451531	2.426420
26	1	0	3.139822	0.226816	2.113020
27	1	0	2.932107	-0.933978	-2.021633
28	6	0	-0.746163	2.163198	-1.215619
29	1	0	-1.050227	2.989677	-1.852718
30	1	0	0.039348	1.576153	-1.684111
31	6	0	-0.455219	2.562326	0.232029
32	1	0	0.510169	2.227020	0.602052
33	1	0	-0.611224	3.617463	0.442070
34	17	0	4.827851	0.173910	-0.194366

6-(4-(trifluoromethyl)phenyl)-1,4-dioxaspiro[4.5]decane



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opt b3pw91/6-311++g(d,p) scrf=(solvent=acetonitrile) maxdisk=24GB geom=connectivity

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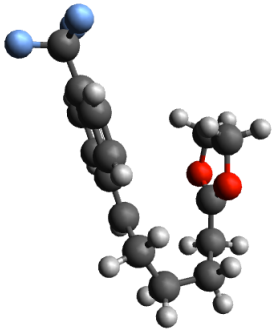
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.164963	-1.956952	-0.424576
2	6	0	-1.601343	-0.828291	0.454937
3	6	0	-2.421690	0.467490	0.259429
4	6	0	-3.903561	0.215956	0.531825
5	6	0	-4.462359	-0.925067	-0.317054
6	6	0	-3.644953	-2.202552	-0.136252
7	1	0	-1.772811	-1.108191	1.501515
8	1	0	-2.037466	-1.698231	-1.481407
9	1	0	-1.583929	-2.868134	-0.248936
10	1	0	-4.013577	-0.015077	1.597736
11	1	0	-4.446422	1.148712	0.348312
12	1	0	-5.510799	-1.099298	-0.054517
13	1	0	-4.447306	-0.628820	-1.372577
14	1	0	-3.758390	-2.567459	0.893226
15	1	0	-4.024959	-2.992614	-0.792312
16	8	0	-2.219964	0.961647	-1.059420
17	8	0	-1.968439	1.492799	1.146651
18	6	0	-1.372975	2.532792	0.372731
19	1	0	-0.290944	2.379699	0.292814
20	1	0	-1.574580	3.488506	0.859388
21	6	0	-2.057315	2.374169	-0.970523
22	1	0	-3.030115	2.880760	-0.991754
23	1	0	-1.455850	2.705918	-1.817735
24	6	0	-0.114903	-0.617763	0.288622
25	6	0	0.707010	-0.540581	1.417146
26	6	0	0.482168	-0.497512	-0.971279
27	6	0	2.077540	-0.342909	1.302624
28	1	0	0.266397	-0.634160	2.404676
29	6	0	1.851153	-0.300520	-1.099386
30	1	0	-0.128161	-0.547454	-1.864449
31	6	0	2.650711	-0.217417	0.039294
32	1	0	2.693525	-0.283258	2.192710
33	1	0	2.293696	-0.204767	-2.084456
34	6	0	4.131959	-0.054884	-0.098808
35	9	0	4.476254	0.631523	-1.208421
36	9	0	4.773123	-1.249525	-0.181697
37	9	0	4.682850	0.592730	0.948734

6-(4-(trifluoromethyl)phenyl)-1,4-dioxaspiro[4.5]decane



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opt b3pw91/6-311++g(d,p) scrf=(solvent=acetonitrile) maxdisk=24GB geom=connectivity

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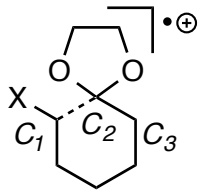
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.302695	-2.136108	-0.407976
2	6	0	-1.412729	-1.493454	0.600359
3	6	0	-2.796119	1.182884	0.154984
4	6	0	-4.004498	0.456534	0.583362
5	6	0	-4.466825	-0.694954	-0.318757
6	6	0	-3.796606	-2.049356	-0.078502
7	1	0	-1.784608	-1.427666	1.621045
8	1	0	-2.117467	-1.738932	-1.413441
9	1	0	-2.031443	-3.202613	-0.469623
10	1	0	-3.873823	0.162496	1.626858
11	1	0	-4.773558	1.244634	0.590857
12	1	0	-5.538398	-0.811751	-0.139717
13	1	0	-4.365448	-0.401085	-1.367816
14	1	0	-3.957351	-2.358394	0.961380
15	1	0	-4.326690	-2.780431	-0.696197
16	8	0	-2.478736	1.304147	-1.079883
17	8	0	-2.069314	1.827020	0.991478
18	6	0	-1.034875	2.573057	0.259409
19	1	0	-0.073780	2.230454	0.634050
20	1	0	-1.191078	3.625266	0.483113
21	6	0	-1.314292	2.194369	-1.196113
22	1	0	-1.620016	3.028281	-1.822571
23	1	0	-0.522940	1.618871	-1.669071
24	6	0	-0.066202	-1.112251	0.394039
25	6	0	0.692577	-0.590442	1.478541
26	6	0	0.588482	-1.231935	-0.861609
27	6	0	2.007647	-0.206620	1.317700
28	1	0	0.221618	-0.495557	2.451636
29	6	0	1.906972	-0.848458	-1.017724
30	1	0	0.054971	-1.635523	-1.714131
31	6	0	2.622717	-0.327343	0.064923
32	1	0	2.561731	0.190515	2.160648
33	1	0	2.385100	-0.950007	-1.985185
34	6	0	4.064426	0.036223	-0.092424
35	9	0	4.377717	0.375162	-1.358981
36	9	0	4.890322	-0.989093	0.240725
37	9	0	4.421928	1.073847	0.693160

Table of calculated C-C bond lengths in radical cation geometries.



X	$d(C_1\text{-}C_2)$	$d(C_2\text{-}C_3)$
H	1.64	1.60
Me	1.94	1.52
Ph	2.94	1.47
p-tBuPh	2.91	1.47
p-ClPh	2.98	1.47
p-CF_3Ph	3.06	1.47

Calculated at B3PW91/6-311++G** (MeCN). Distances reported in Angstroms.