

A General, Enantioselective Synthesis of β - and γ -Fluoroamines

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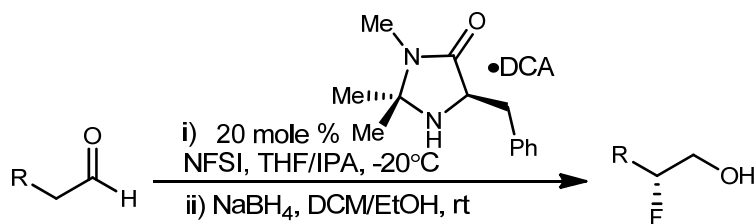
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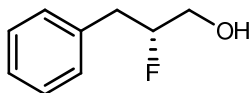
General Experimental

All reagents were purchased from commercial suppliers and were purified as needed according to the procedures of Armarego and Chai.¹ Analytical thin-layer chromatography (TLC) was performed on 250 μm silica plates from Sorbent Technologies. Visualization was accomplished via UV light, and/or the use of ninhydrin, iodine, and potassium permanganate solutions followed by application of heat. Chromatography was performed using Silica Gel 60 (230-400 mesh) from Sorbent Technologies or Silica RediSep Rf flash columns on a CombiFlash Rf automated flash chromatography system. All ^1H and ^{13}C NMR spectra were recorded on a Bruker AV-400 (400 MHz) instrument. Chemical shifts are reported in ppm relative to residual solvent peaks as an internal standard set to δ 7.26 and δ 77.16 (CDCl_3) or δ 3.31 and δ 49.00 (MeOD). Data are reported as follows: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, p = pentet, sx = sextet, sp = septet, br = broad, dd = doublet of doublets, dq = doublet of quartets, td = triplet of doublets, pd = pentet of doublets, m = multiplet), coupling constant (Hz), integration. Low resolution mass spectra (LCMS) were recorded on an Agilent 1200 LCMS with electrospray ionization. High resolution mass spectra (HRMS) were recorded on a Waters QToF-API-US plus Acuity system with ES as the ion source. Analytical high performance liquid chromatography (HPLC) was performed on an Agilent 1200 analytical LCMS with UV detection at 214 nm and 254 nm along with ELSD detection. Chiral separations were performed on a Thar Investigator II supercritical fluid chromatograph (SFC) utilizing Chiralcel[®] OD, OD-Cl, OJ, and Chiralpak[®] IA columns. Optical rotations were acquired on a Jasco P-2000 polarimeter at 23 $^{\circ}\text{C}$ and 589 nm. The specific rotations were calculated according to the equation $[\alpha]_{23}^D = 100\alpha/l \times c$ where l is the path length in decimeters and c is the concentration in g/100 mL.

General Procedure A—for fluorination and reduction of aldehydes.

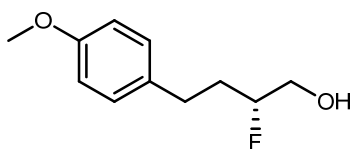


To a round-bottom flask equipped with a magnetic stir bar and charged with (*R*)-5-benzyl-2,2,3-trimethylimidazolidin-4-one dichloro acid salt (139 mg, 0.400 mmol) and *N*-fluorobenzenesulfonimide (3.15 g, 10.0 mmol) was added THF (8.0 mL) and *i*PrOH (1.0 mL). The mixture was stirred at room temperature until all solids were dissolved and was then cooled to -20^o C. The aldehyde substrate (2 mmol) was then slowly added to the reaction mixture dissolved in THF (1.0 mL) and the mixture was left to stirred for 16 hours. The reaction was then diluted with Et₂O (20 mL), cooled to -78^oC, and filtered through a pad of silica gel, eluting with cold Et₂O (~50 mL). The resultant organic layer was washed with saturated NaHCO₃ (3 x 75 mL), saturated brine (75 mL), dried over MgSO₄, filtered, and concentrated. The resultant oil was dissolved in DCM (12 mL) and EtOH (8 mL) and NaBH₄ (189 mg, 5.0 mmol) was added at room temperature, all at once. After 30 minutes, the reaction was cooled to 0^o C and was quenched with saturated NH₄Cl (~100 mL). The mixture was stirred vigorously and allowed to warm to room temperature and stirred for an additional 30 minutes. 75 mL DCM was added to the suspension when it was extracted with DCM (3 x 75 mL). The combined organic extracts were then washed with NaHCO₃ (3 x 75 mL) and brine (75 mL), dried with MgSO₄, filtered and concentrated. Purification of the resultant oil was performed by flash column chromatography.



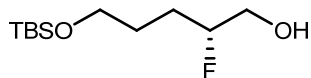
(*R*)-2-fluoro-3-phenylpropan-1-ol (4a)

The product was prepared according general procedure A, purified via flash column chromatography (15% ethyl acetate in hexanes) to afford the product was a clear oil (200 mg, 65% yield). ^1H NMR (400.1 MHz, CDCl_3) δ (ppm): 7.36-7.20 (m, 5H); 4.78 (dm, $J = 49.0$ Hz); 3.84-3.63 (m, 2H); 3.10-2.89 (m, 2H); 1.92 (s, br, 1H). ^{13}C NMR (100.6 MHz, CDCl_3) δ (ppm): 136.52 (d, $J = 5.5$ Hz), 129.33, 128.58, 126.75, 95.70 (d, $J = 171.9$ Hz), 64.01 (d, $J = 21.7$ Hz), 37.45 (d, $J = 21.2$ Hz). Specific rotation $[\alpha]_D^{23} = +14.9^\circ$ ($c = 100$, CHCl_3). HRMS (TOF, ES+) $\text{C}_9\text{H}_{11}\text{OFNa}$ $[\text{M}+\text{Na}]^+$ calc. mass 177.0692, found 177.0692.



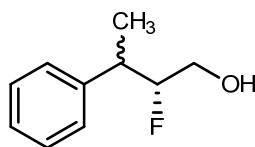
(*R*)-2-fluoro-4-(4-methoxyphenyl)butan-1-ol (4b)

The product was prepared according general procedure A, purified via flash column chromatography (25% ethyl acetate in hexanes) to afford the product was a waxy solid (291 mg, 73% yield). ^1H NMR (400.1 MHz, CDCl_3) δ (ppm): 7.13 (d, $J = 8.6$ Hz, 2H); 6.86 (d, $J = 8.6$ Hz, 2H); 4.56 (dm, $J = 49.9$ Hz, 1H); 3.79 (s, 3H); 3.74-3.59 (m, 2H); 2.92 (s, br, 1H); 2.82-2.56 (m, 2H); 2.07-1.92 (m, 1H); 1.89-1.71 (m, 1H). ^{13}C NMR (100.6 MHz, CDCl_3) δ (ppm): 157.89, 133.12, 129.33, 113.89, 93.72 (d, $J = 168.7$ Hz), 64.75 (d, $J = 21.9$), 55.20, 32.84 (d, $J = 20.7$), 30.11 (d, $J = 4.7$). Specific rotation $[\alpha]_D^{23} = +24.2^\circ$ ($c = 100$, CHCl_3). HRMS (TOF, ES+) $\text{C}_{11}\text{H}_{15}\text{O}_2\text{FNa}$ $[\text{M}+\text{Na}]^+$ calc. mass 221.0956, found 221.0954.



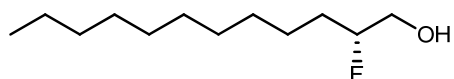
(*R*)-5-((*tert*-butyldimethylsilyloxy)-2-fluoropentan-1-ol (4c)

The product was prepared according general procedure A, purified via flash column chromatography (10% ethyl acetate in hexanes) to afford the product as a clear oil (365 mg, 77% yield). ^1H NMR (400.1 MHz, CDCl_3) δ (ppm): 4.52 (dm, $J = 49.4$ Hz, 1H); 3.70-3.53 (m, 4H); 3.31 (s, br, 1H); 1.69-1.48 (m, 4H); 0.84 (s, 9H); 0.00 (s, 6H). ^{13}C NMR (100.6 MHz, CDCl_3) δ (ppm): 94.12 (d, $J = 169.2$ Hz), 64.28 (d, $J = 22.2$ Hz), 62.47, 27.97 (d, $J = 4.2$ Hz), 27.37 (d, $J = 20.8$ Hz), 25.72, 18.04, -5.60. Specific rotation $[\alpha]_D^{23} = 5.9^0$ ($c = 100$, CHCl_3). HRMS (TOF, ES+) $\text{C}_{11}\text{H}_{26}\text{O}_2\text{FSi}$ $[\text{M}+\text{H}]^+$ calc. mass 237.1686, found 237.1688.



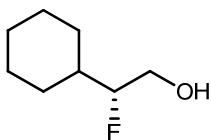
(*2R*)-2-fluoro-3-phenylbutan-1-ol (4d) (4e)

The product was prepared according general procedure A, purified via flash column chromatography (10% ethyl acetate in hexanes) to afford the product as a clear oil (249 mg, 74% yield, 1:1 dr). ^1H NMR—**Diastereomer A (less polar)** (400.1 MHz, CDCl_3) δ (ppm): 7.39-7.23 (m, 5H); 4.62 (dm, $J = 49.1$ Hz, 1H); 3.66-3.47 (m, 2H); 3.16-2.97 (m, 2H); 1.43 (d, $J = 7.1$ Hz, 3H). ^1H NMR—**Diastereomer B (more polar)** (400.1 MHz, CDCl_3) δ (ppm): 7.36-7.20 (m, 5H); 4.69 (dm, $J = 48.5$ Hz, 1H); 3.81-3.51 (m, 2H); 3.16-3.02 (m, 2H); 1.83 (s, br, 1H); 1.35 (d, $J = 7.2$ Hz, 3H). ^{13}C NMR—**Diastereomer A (less polar)** (100.6 MHz, CDCl_3) δ (ppm): 142.32 (d, $J = 7.7$ Hz), 128.66, 127.59, 126.89, 98.02 (d, $J = 175.5$ Hz), 63.02 (d, $J = 21.6$ Hz), 40.93 (d, $J = 20.5$ Hz), 17.19 (d, $J = 4.9$ Hz). ^{13}C NMR—**Diastereomer B (more polar)** (125 MHz, CDCl_3) δ (ppm): 141.94, 128.63, 128.08, 127.02, 97.57 (d, $J = 174.1$ Hz), 63.60 (d, $J = 22.6$ Hz), 41.13 (d, $J = 20.1$ Hz), 17.54 (d, $J = 6.1$ Hz). Specific rotation—**Diastereomer A (less polar)** $[\alpha]_D^{23} = +12.3^0$ ($c = 100$, CHCl_3). Specific rotation—**Diastereomer B (more polar)** $[\alpha]_D^{23} = +6.1^0$ ($c = 100$, CHCl_3). HRMS (TOF, ES+)—**Diastereomer A (less polar)**: $\text{C}_{10}\text{H}_{13}\text{OFNa}$ $[\text{M}+\text{Na}]^+$ calc. mass 191.0848, found 191.0848. HRMS (TOF, ES+)—**Diastereomer B (more polar)**: $\text{C}_{10}\text{H}_{13}\text{OFNa}$ $[\text{M}+\text{Na}]^+$ calc. mass 191.0848, found 191.0847.



(*R*)-2-fluorododecan-1-ol (4f)

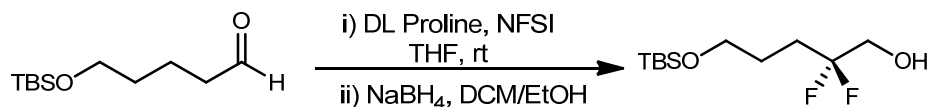
The product was prepared according general procedure A, purified via flash column chromatography (10% ethyl acetate in hexanes) to afford the product was a waxy solid (282 mg, 69% yield). ^1H NMR (400.1 MHz, CDCl_3) δ (ppm): 4.524 (dm, $J = 51.3$ Hz, 1H); 3.77-3.50 (m, 3H); 1.71-1.16 (m, 18H); 0.85 (t, $J = 6.6$ Hz, 3H). ^{13}C NMR (100.6 MHz, CDCl_3) δ (ppm): 94.83 (d, $J = 168.1$ Hz), 64.96 (d, $J = 22.1$ Hz), 31.99, 31.08 (d, $J = 20.6$ Hz), 29.69, 29.65, 29.57, 29.54, 29.42, 25.02 (d, $J = 4.8$ Hz), 22.76, 14.14. Specific rotation $[\alpha]_{\text{D}}^{23} = +9.6^\circ$ ($c = 100$, CHCl_3). HRMS (TOF, ES+) $\text{C}_{12}\text{H}_{25}\text{OFNa}$ $[\text{M}+\text{Na}]^+$ calc. mass 227.1787, found 227.1787.



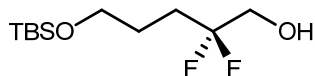
(*R*)-2-cyclohexyl-2-fluoroethanol (4g)

The product was prepared according general procedure A, purified via flash column chromatography (15% ethyl acetate in hexanes) to afford the product was a clear oil (236 mg, 81% yield). ^1H NMR (400.1 MHz, CDCl_3) δ (ppm): 4.20 (dm, $J = 49.2$ Hz, 1H); 3.70-3.57 (m, 2H); 3.21 (s, br, 1H); 1.79 (dm, br, $J = 12.7$, 1H); 1.73-1.49 (m, 5H); 1.26-0.93 (m, 5H). ^{13}C NMR (100.6 MHz, CDCl_3) δ (ppm): 98.38 (d, $J = 169.6$ Hz), 62.84 (d, $J = 22.2$ Hz), 38.79 (d, $J = 18.8$ Hz), 28.11 (dd, $J_1 = 51.2$ Hz, $J_2 = 5.6$ Hz), 26.14, 25.67 (d, $J = 17.4$ Hz). Specific rotation $[\alpha]_{\text{D}}^{23} = 2.4^\circ$ ($c = 100$, CHCl_3). HRMS (TOF, ES+) $\text{C}_8\text{H}_{15}\text{O}_2\text{FNa}$ $[\text{M}+\text{Na}]^+$ calc. mass 169.1005, found 169.005.

General procedure B—procedure for preparation of difluoro-alcohols



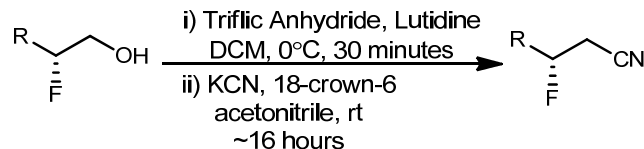
To a round-bottom flask equipped with a magnetic stir bar and charged with DL proline (103.5 mg, 0.9 mmol) and *N*-fluorobenzenesulfonimide (7.568 g, 24.0 mmol) was added THF (27 mL). The mixture was stirred at room temperature until all solids were dissolved and the aldehyde substrate (649.2 mg, 3 mmol) was then slowly added to the reaction mixture dissolved in THF (3.0 mL) and the mixture was stirred for 16 hours. The reaction was then diluted with Et₂O (20 mL), cooled to -78^oC, and filtered through a pad of silica gel, eluting with cold Et₂O (~75 mL). The resultant organic layer was washed with saturated NaHCO₃ (3x), saturated brine (1x), dried over MgSO₄, filtered, and concentrated. The resultant oil was dissolved in DCM (18 mL) and EtOH (12 mL) and NaBH₄ (283.7 mg, 7.5 mmol) was added at room temperature, all at once. After 30 minutes, the reaction was cooled to 0^oC and was quenched with saturated NH₄Cl (~100 mL). The mixture was stirred vigorously and allowed to warm to room temperature and stir for an additional 30 minutes. About 75 mL of DCM was added to the suspension and it was extracted with DCM (3x). The combined organic extracts were then washed with NaHCO₃ (3x) and brine (1x), dried with MgSO₄, filtered and concentrated. Purification of the resultant oil was performed by flash column chromatography.



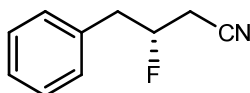
5-((*tert*-butyldimethylsilyl)oxy)-2,2-difluoropentan-1-ol

The product was prepared according general procedure B, purified via flash column chromatography (10% ethyl acetate in hexanes) to afford the product as a clear oil (586 mg, 77% yield). ¹H NMR (400.1 MHz, CDCl₃) δ (ppm): 3.73-3.60 (m, 4H); 3.49 (s, br, 1H); 2.03-1.85 (m, 2H); 1.75-1.63 (m, 2H); 0.87 (s, 9H); 0.03 (s, 6H). ¹³C NMR (100.6 MHz, CDCl₃) δ (ppm): 123.52 (t, *J* = 241.5 Hz), 63.85 (t, *J* = 31.8 Hz), 62.59, 29.89 (t, *J* = 24.2 Hz), 25.97, 25.14 (t, *J* = 4.3 Hz), 18.39, -5.34. HRMS (TOF, ES⁺) C₁₁H₂₅O₂F₂Si [M+H]⁺ calc. mass 255.1592, found 255.1592.

General Procedure C—procedure for preparation of fluoro-nitriles

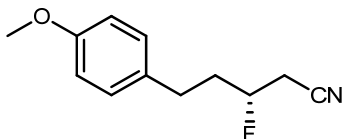


To a flame dried round-bottom flask equipped with a magnetic stir bar and charged with the chiral fluoro-alcohol (1 mmol) and lutidine (535 mg, 5.0 mmol) was added DCM (5 mL), and the mixture was cooled to 0°C with stirring. Trifluoromethanesulfonic anhydride (339 mg, 1.2 mmol) was added to the reaction dropwise, and the mixture was left to stir for 30 minutes. The reaction was then diluted with Et₂O and water was added to quench the reaction. The mixture was extracted with Et₂O (3x), dried with MgSO₄, filtered, and concentrated. The resultant oil was transferred to a round-bottom flask equipped with a magnetic stir bar where it was dissolved in acetonitrile (4 mL), and 18-crown-6 (53 mg, 0.2 mmol) was added and allowed to dissolve with stirring. Potassium cyanide (651 mg, 10 mmol) was added to the reaction at room temperature and the reaction was left with vigorous stirring for the following 16 hours. The reaction was then quenched via the addition of saturated NaHCO₃ and it was extracted with DCM (3x). The organic extract was dried with MgSO₄, filtered, and concentrated and the resultant crude oil was purified via flash column chromatography.



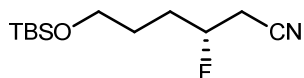
(*R*)-3-fluoro-4-phenylbutanenitrile (9a)

The product was prepared according general procedure C, purified via flash column chromatography (15% ethyl acetate in hexanes, visualized TLC with KMnO₄) to afford the product was a clear oil (126 mg, 77% yield). ¹H NMR (400.1 MHz, CDCl₃) δ (ppm): 7.41-7.23 (m, 5H); 4.93 (dp, *J*₁ = 46.7 Hz, *J*₂ = 5.6 Hz, 1H); 3.21-2.97 (m, 2H); 2.75-2.52 (m, 2H). ¹³C NMR (100.6 MHz, CDCl₃) δ (ppm): 134.77 (d, *J* = 5.6 Hz), 129.39, 128.86, 127.37, 116.07 (d, *J* = 5.4 Hz), 88.70 (d, *J* = 180.9 Hz), 40.17 (d, *J* = 20.8), 23.11 (d, *J* = 24.7 Hz). Specific rotation [α]_D²³ = -12.3° (*c* = 100, CHCl₃). HRMS (TOF, ES+) C₁₀H₁₀NFNa [M+Na]⁺ calc. mass 186.0695, found 186.0692.



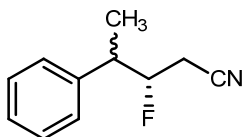
(*R*)-3-fluoro-5-(4-methoxyphenyl)pentanenitrile (9b)

The product was prepared according general procedure C, purified via flash column chromatography (20% ethyl acetate in hexanes, visualized TLC with KMnO_4) to afford the product was a clear oil (190 mg, 92% yield). ^1H NMR (400.1 MHz, CDCl_3) δ (ppm): 7.12 (d, $J = 8.6$ Hz, 2H); 6.86 (d, $J = 8.6$ Hz, 2H); 4.69 (dsx, $J_1 = 47.5$ Hz, $J_2 = 5.3$ Hz, 1H); 3.8 (s, 3H); 2.86-2.57 (m, 4H); 2.21-2.06 (m, 1H); 2.02-1.83 (m, 1H). ^{13}C NMR (100.6 MHz, CDCl_3) δ (ppm): 158.25, 132.05, 129.44, 114.97 (d, $J = 6.1$ Hz), 114.13, 87.49 (d, $J = 177.9$ Hz), 55.33, 36.16 (d, $J = 20.3$ Hz), 29.90 (d, $J = 4.2$ Hz), 24.10 (d, $J = 25.5$ Hz). Specific rotation $[\alpha]_D^{23} = +22.8^0$ ($c = 100$, CHCl_3). HRMS (TOF, ES+) $\text{C}_{12}\text{H}_{14}\text{NFNa}$ $[\text{M}+\text{Na}]^+$ calc. mass 230.0957, found 230.0955.



(*R*)-6-((*tert*-butyldimethylsilyl)oxy)-3-fluorohexanenitrile (9c)

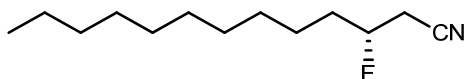
The product was prepared according general procedure C, purified via flash column chromatography (15% ethyl acetate in hexanes, visualized TLC with KMnO_4) to afford the product was a clear oil (175 mg, 71% yield). ^1H NMR (400.1 MHz, CDCl_3) δ (ppm): 4.76 (dm, $J = 47.5$ Hz, 1H); 3.69-3.59 (m, 2H); 2.78-2.59 (m, 2H); 1.90-1.53 (m, 4H); 0.87 (s, 9H); 0.03 (s, 6H). ^{13}C NMR (100.6 MHz, CDCl_3) δ (ppm): 116.03 (d, $J = 5.8$ Hz), 88.51 (d, $J = 177.4$ Hz), 62.24, 31.11 (d, $J = 20.4$ Hz), 27.85 (d, $J = 4.2$ Hz), 25.94, 24.09 (d, $J = 25.3$ Hz), 18.30, -5.35. Specific rotation $[\alpha]_D^{23} = +4.0^0$ ($c = 100$, CHCl_3). HRMS (TOF, ES+) $\text{C}_{12}\text{H}_{25}\text{NOFSi}$ $[\text{M}+\text{H}]^+$ calc. mass 246.1689, found 246.1690.



(3S)-3-fluoro-4-phenylpentanenitrile (9d) (9e)

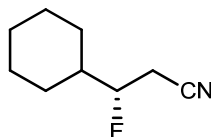
The product (**diastereomer A**) was prepared according to general procedure C, purified via flash column chromatography (10% ethyl acetate in hexanes, visualized TLC with KMnO_4) to afford the product was a clear oil (164 mg, 93% yield). The product (**diastereomer B**) was prepared according to general procedure C, purified via flash column chromatography (10% ethyl acetate in hexanes, visualized TLC with KMnO_4) to afford the product was a clear oil (137 mg, 77% yield). ^1H NMR—**Diastereomer A (less polar)** (400.1 MHz, CDCl_3) δ (ppm): 7.39-7.20 (m, 5H); 4.72 (dm, $J = 46.9$ Hz, 1H); 3.17-3.05 (m, 1H); 2.65-2.33 (m, 2H); 1.45 (dd, $J_1 = 6.9$ Hz, $J_2 = 1.3$ Hz, 3H). ^1H NMR—**Diastereomer B (more polar)** (400.1 MHz, CDCl_3) δ (ppm): 7.40-7.26 (m, 5H); 4.89 (dm, $J = 46.9$ Hz, 1H); 3.18-3.03 (m, 1H); 2.65-2.44 (m, 2H); 1.44 (d, $J = 7.3$ Hz, 3H). ^{13}C NMR—**Diastereomer A (less polar)** (100.6 MHz, CDCl_3) δ (ppm): 140.72 (d, $J = 8.3$ Hz), 129.23, 127.76, 127.59, 116.15 (d, $J = 3.3$ Hz), 92.21 (d, $J = 184.5$ Hz), 44.07 (d, $J = 20.0$ Hz), 22.56 (d, $J = 23.7$ Hz), 17.32 (d, $J = 4.1$ Hz). ^{13}C NMR—**Diastereomer B (more polar)** (100.6 MHz, CDCl_3) δ (ppm): 139.65 (d, $J = 1.2$ Hz), 128.78, 128.30, 127.53, 116.23 (d, $J = 7.7$ Hz), 91.58 (d, $J = 183.6$ Hz), 43.26 (d, $J = 19.1$ Hz), 22.04 (d, $J = 26.9$ Hz), 17.07 (d, $J = 5.5$ Hz). Specific rotation—**Diastereomer A (less polar)** $[\alpha]_D^{23} = -41.8^\circ$ ($c = 100$, CHCl_3).

Specific rotation—**Diastereomer B (more polar)** $[\alpha]_D^{23} = +41.0^\circ$ ($c = 100$, CHCl_3). HRMS—**Diastereomer A (less polar)** (TOF, ES+) $\text{C}_{11}\text{H}_{13}\text{NF}$ $[\text{M}+\text{H}]^+$ calc. mass 178.1032, found 178.1033. HRMS—**Diastereomer B (more polar)** (TOF, ES+) $\text{C}_{11}\text{H}_{13}\text{NF}$ $[\text{M}+\text{H}]^+$ calc. mass 178.1032, found 178.1033.



(R)-3-fluorotridecanenitrile (9f)

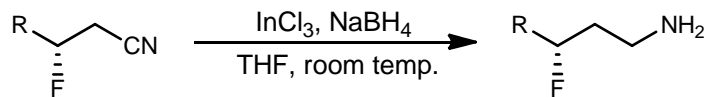
The product was prepared according to general procedure C, purified via flash column chromatography (10% ethyl acetate in hexanes, visualized TLC with KMnO_4) to afford the product was a waxy solid (175 mg, 82% yield). ^1H NMR (400.1 MHz, CDCl_3) δ (ppm): 4.69 (dm, $J = 47.7$ Hz, 1H); 2.76-2.56 (m, 2H); 1.87-1.55 (m, 2H); 1.51-1.17 (m, 16H), 0.86 (t, $J = 7.0$ Hz, 3H). ^{13}C NMR (100.6 MHz, CDCl_3) δ (ppm): 116.11 (d, $J = 6.1$ Hz), 88.54 (d, $J = 177.4$ Hz), 34.27 (d, $J = 20.1$ Hz), 31.92, 29.58, 29.51, 29.41, 29.33, 29.17, 24.66 (d, $J = 4.4$ Hz), 24.02 (d, $J = 25.6$ Hz), 22.70, 14.11. Specific rotation $[\alpha]_D^{23} = +8.5^\circ$ ($c = 100$, CHCl_3). HRMS (TOF, ES+) $\text{C}_{13}\text{H}_{24}\text{NFNa}$ $[\text{M}+\text{Na}]^+$ calc. mass 236.1790, found 236.1790.



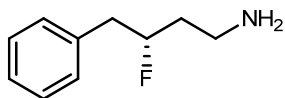
(S)-3-cyclohexyl-3-fluoropropanenitrile (9g)

The product was prepared according to general procedure C, purified via flash column chromatography (10% ethyl acetate in hexanes, visualized TLC with KMnO_4) to afford the product as a clear oil (131 mg, 84% yield). ^1H NMR (400.1 MHz, CDCl_3) δ (ppm): 4.44 (dq, $J_1 = 47.0$ Hz, $J_2 = 6.2$ Hz, 1H); 2.78-2.60 (m, 2H); 1.95-1.88 (m, 1H); 1.84-1.56 (m, 5H); 1.36-0.99 (m, 5H). ^{13}C NMR (100.6 MHz, CDCl_3) δ (ppm): 116.45 (d, $J = 5.4$ Hz), 92.18 (d, $J = 179.6$ Hz), 41.31 (d, $J = 18.7$ Hz), 27.84 (dd, $J_1 = 78.4$ Hz, $J_2 = 4.8$ Hz), 26.05, 25.55 (d, $J = 26.3$ Hz), 21.79 (d, $J = 25.9$ Hz). Specific rotation $[\alpha]_D^{23} = -4.2^0$ ($c = 100$, CHCl_3). HRMS (TOF, ES+) $\text{C}_9\text{H}_{14}\text{NFNa}$ $[\text{M}+\text{Na}]^+$ calc. mass 178.1008, found 178.1007.

General procedure D—preparation of γ -Fluoroamines

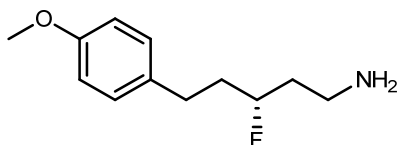


To a flame dried round-bottom flask equipped with a magnetic stir bar and charged with anhydrous InCl_3 (111 mg, 0.50 mmol) and NaBH_4 (56.7 mg, 1.50 mmol) was added anhydrous THF (1.2 mL) and the heterogeneous mixture was allowed to stir under argon for 1 hour. The nitrile substrate (0.5 mmol) was then slowly added to the reaction mixture in dissolved in THF (0.5 mL). The reaction was then allowed to stir and was monitored by TLC until completion (approx. 4 hrs). The solution was quenched by the dropwise addition of water (2 mL). This solution was then heated to 75 °C for 30 minutes, then MeOH (2 mL) was added to the mixture and it was again heated to 75 °C for an additional 30 minutes. The solution was then filtered, eluting with MeOH to remove any solid reaction components and the filtrate was concentrated under reduced pressure. The resultant crude material was purified via flash column chromatography (DCM/MeOH).



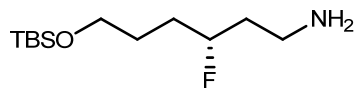
(*R*)-3-fluoro-4-phenylbutan-1-amine (3a)

The product was prepared according to general procedure D, purified via flash column chromatography (10% MeOH in DCM, visualize TLC with ninhydrin) to afford the product was a clear oil (73 mg, 87% yield), which was determined to have an ee of 94% by ^{19}F NMR of the (*R*) Mosher amide of the final amine (^{19}F NMR (300 MHz, CDCl_3) δ (ppm): δ (minor) -180.70, δ (major) -180.94, fluorine NMR of racemic and enantioenriched Mosher amides shown below. ^1H NMR (400.1 MHz, CDCl_3) δ (ppm): 7.33-7.18 (m, 5H); 4.81 (dm, $J = 49.0$ Hz, 1H); 3.05-2.78 (m, 4H); 1.88-1.60 (m, 2H); 1.49 (s, br, 2H). ^{13}C NMR (100.6 MHz, CDCl_3) δ (ppm): 137.10 (d, $J = 5.0$ Hz), 129.42, 128.49, 126.65, 92.97 (d, $J = 170.6$ Hz), 41.86 (d, $J = 21.1$ Hz), 38.40, 38.29 (d, $J = 14.5$ Hz). Specific rotation $[\alpha]_D^{23} = -2.1^0$ ($c = 100$, CHCl_3). HRMS (TOF, ES+) $\text{C}_{10}\text{H}_{15}\text{NF}$ $[\text{M}+\text{H}]^+$ calc. mass 168.1189, found 168.1190.



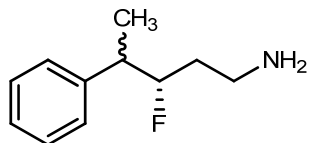
(*R*)-3-fluoro-5-(4-methoxyphenyl)pentan-1-amine (3b)

The product was prepared according to general procedure D, purified via flash column chromatography (10% MeOH in DCM, visualize TLC with ninhydrin) to afford the product was a clear oil (89 mg, 84% yield) which was determined to have an ee of 87% by ^{19}F NMR of the (*R*) Mosher amide of the final amine (^{19}F NMR (300 MHz, CDCl_3) δ (ppm): δ (minor) -184.15, δ (major) -184.32, fluorine NMR of racemic and enantioenriched Mosher amides shown below. ^1H NMR (400.1 MHz, MeOD) δ (ppm): 7.10 (d, $J = 8.5$ Hz, 2H); 6.82 (d, $J = 8.7$ Hz, 2H); 4.55 (dsp, $J_1 = 49.8$ Hz, $J_2 = 4.0$ Hz, 1H); 3.75 (s, 3H); 2.83-2.56 (m, 4H); 1.98-1.60 (m, 4H). ^{13}C NMR (100.6 MHz, MeOD) δ (ppm): 159.42, 134.76, 130.33, 114.87, 93.01 (d, $J = 166.7$ Hz), 55.63, 39.12 (d, $J = 20.4$ Hz), 38.81 (d, $J = 4.1$ Hz), 38.61 (d, $J = 20.6$ Hz), 31.40 (d, $J = 4.6$ Hz). Specific rotation $[\alpha]_D^{23} = +11.6^\circ$ ($c = 100$, CHCl_3). HRMS (TOF, ES+) $\text{C}_{12}\text{H}_{19}\text{NOF}$ $[\text{M}+\text{H}]^+$ calc. mass 212.1451, found 212.1447.



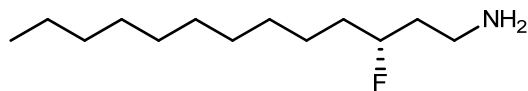
(*R*)-6-((*tert*-butyldimethylsilyloxy)-3-fluorohexan-1-amine (3c)

The product was prepared according general procedure D, purified via flash column chromatography (10% MeOH in DCM, visualize TLC with ninhydrin) to afford the product was a clear oil (107 mg, 86% yield) which was determined to have an ee of 92% by ^{19}F NMR of the (*R*) Mosher amide of the final amine (^{19}F NMR (300 MHz, CDCl_3) δ (ppm): δ (minor) -184.15, δ (major) -184.32, fluorine NMR of racemic and enantioenriched Mosher amides shown below. ^1H NMR (400.1 MHz, MeOD) δ (ppm): 4.60 (dm, $J = 50.2$ Hz, 1H); 3.71-3.55 (m, 2H); 2.84-2.70 (m, 2H); 1.87-1.53 (m, 6H); 0.91 (s, 9H); 0.07 (s, 6H). ^{13}C NMR (100.6 MHz, MeOD) δ (ppm): 93.73 (d, $J = 166.4$ Hz), 63.88, 39.27 (d, $J = 20.5$ Hz), 38.95 (d, $J = 4.4$ Hz), 32.97 (d, $J = 21.1$ Hz), 29.49 (d, $J = 4.1$ Hz), 26.41, 19.13, -5.18. Specific rotation $[\alpha]_D^{23} = -4.2^\circ$ ($c = 100$, CHCl_3). HRMS (TOF, ES+) $\text{C}_{12}\text{H}_{29}\text{NOFSi}$ $[\text{M}+\text{H}]^+$ calc. mass 250.2002, found 250.2001.



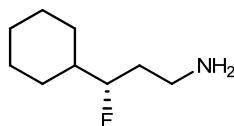
(3S)-3-fluoro-4-phenylpentan-1-amine (3d) (3e)

The product (**diastereomer A**) was prepared according to general procedure D, purified via flash column chromatography (10% MeOH in DCM, visualize TLC with ninhydrin) to afford the product was a clear oil (75 mg, 83% yield) which was determined to have an ee of 96% by ^{19}F NMR of the (*R*) mosher amide of the final amine (^{19}F NMR (300 MHz, CDCl_3) δ (ppm): δ (major) -186.34, δ (minor) -186.39, fluorine NMR of racemic and enantioenriched mosher amides shown below. The product (**diastereomer B**) was prepared according to general procedure D, purified via flash column chromatography (10% MeOH in DCM, stain visualize with ninhydrin) to afford the product was a clear oil (82 mg, 90% yield) which was determined to have an ee of 96% by ^{19}F NMR of the (*R*) mosher amide of the final amine (^{19}F NMR (300 MHz, CDCl_3) δ (ppm): δ (minor) -187.23, δ (major) -187.43, fluorine NMR of racemic and enantioenriched mosher amides shown below. ^1H NMR—**Diastereomer A (less polar)** (400.1 MHz, MeOD) δ (ppm): 7.33-7.26 (m, 2H); 7.25-7.18 (m, 3H); 4.65 (dm, $J = 49.0$ Hz); 2.97-2.83 (m, 1H); 2.79-2.61 (m, 2H); 1.81-1.44 (m, 2H); 1.35 (d, $J = 7.0$ Hz). ^1H NMR—**Diastereomer B (more polar)** (400.1 MHz, MeOD) δ (ppm): 7.32-7.17 (m, 5H); 4.71 (dm, $J = 48.9$ Hz, 1H); 2.99-2.85 (m, 1H); 2.83-2.69 (m, 2H); 1.78-1.58 (m, 2H); 1.33 (d, $J = 7.2$ Hz, 3H). ^{13}C NMR—**Diastereomer A (less polar)** (100.6 MHz, MeOD) δ (ppm): 144.49 (d, $J = 6.8$ Hz), 129.63, 128.89, 127.80, 97.34 (d, $J = 173.3$ Hz), 46.19 (d, $J = 20.5$ Hz), 39.10 (d, $J = 3.5$ Hz), 37.32 (d, $J = 20.7$ Hz), 17.67 (d, $J = 5.4$ Hz). ^{13}C NMR—**Diastereomer B (more polar)** (100.6 MHz, MeOD) δ (ppm): 143.62 (d, 2.3 Hz), 129.37, 129.28, 127.62, 96.81 (d, $J = 172.8$ Hz), 45.61 (d, $J = 19.8$ Hz), 38.98 (d, $J = 4.0$ Hz), 36.46 (d, $J = 20.8$ Hz), 17.96 (d, $J = 5.9$ Hz). Specific rotation—**Diastereomer A (less polar)** $[\alpha]_D^{23} = -9.1^0$ ($c = 100$, CHCl_3). Specific rotation—**Diastereomer B (more polar)** $[\alpha]_D^{23} = -14.0^0$ ($c = 100$, CHCl_3). HRMS—**Diastereomer A (less polar)** (TOF, ES+) $\text{C}_{11}\text{H}_{17}\text{NF}$ $[\text{M}+\text{H}]^+$ calc. mass 182.1345, found 182.1343. HRMS—**Diastereomer B (more polar)** (TOF, ES+) $\text{C}_{11}\text{H}_{17}\text{NF}$ $[\text{M}+\text{H}]^+$ calc. mass 182.1345, found 182.1346.



(*R*)-3-fluorotridecan-1-amine (3f)

The product was prepared according to general procedure D, purified via flash column chromatography (10% MeOH in DCM, visualize TLC with ninhydrin) to afford the product was a waxy solid (97 mg, 89% yield) which was determined to have an ee of 95% by ^{19}F NMR of the (*R*) mosher amide of the final amine (^{19}F NMR (300 MHz, CDCl_3) δ (ppm): δ (minor) -181.97, δ (major) -182.19, fluorine NMR of racemic and enantioenriched mosher amides shown below. ^1H NMR (400.1 MHz, MeOD) δ (ppm): 4.56 (dm, $J = 49.7$ Hz, 1H); 2.83-2.70 (m, 2H); 1.81-1.42 (m, 5H); 1.41-1.24 (m, 15H); 0.90 (t, $J = 7.1$ Hz, 3H). ^{13}C NMR (100.6 MHz, MeOD) δ (ppm): 93.81 (d, $J = 166.3$ Hz), 39.15 (d, $J = 20.7$ Hz), 38.95 (d, $J = 4.4$ Hz), 36.53 (d, $J = 20.7$ Hz), 33.08, 30.75, 30.73, 30.70, 30.62, 30.49, 26.22 (d, $J = 4.6$ Hz), 23.75, 14.47. Specific rotation $[\alpha]_D^{23} = -4.6^0$ ($c = 100$, CHCl_3). HRMS (TOF, ES+) $\text{C}_{13}\text{H}_{29}\text{NF}$ $[\text{M}+\text{H}]^+$ calc. mass 218.2284, found 218.2283.



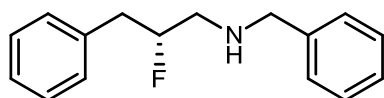
(*S*)-3-cyclohexyl-3-fluoropropan-1-amine (3g)

The product was prepared according to general procedure D, purified via flash column chromatography (10% MeOH in DCM, visualize TLC with ninhydrin) to afford the product was a clear oil (58 mg, 73% yield), which was determined to have an ee of 96% by ^{19}F NMR of the (*R*) mosher amide of the final amine (^{19}F NMR (300 MHz, CDCl_3) δ (ppm): δ (minor) -187.84, δ (major) -187.94, fluorine NMR of racemic and enantioenriched mosher amides shown below. ^1H NMR (400.1 MHz, MeOD) δ (ppm): 4.30 (dm, $J = 49.2$ Hz, 1H); 2.89-2.72 (m, 2H); 1.92-1.84 (m, 1H); 1.83-1.62 (m, 5H); 1.57-1.42 (m, 1H); 1.36-1.00 (m, 5H). ^{13}C NMR (100.6 MHz, MeOD) δ (ppm): 97.39 (d, $J = 168.6$ Hz), 43.61 (d, $J = 19.3$ Hz), 39.1 (d, $J = 3.8$ Hz), 35.74 (d, $J = 21.3$ Hz), 29.20 (dd, $J_1 = 97$ Hz, $J_2 = 5.7$ Hz), 27.30 (d, $J = 35.7$ Hz), 29.94. Specific rotation $[\alpha]_D^{23} = -19.0^0$ ($c = 100$, CHCl_3). HRMS (TOF, ES+) $\text{C}_9\text{H}_{19}\text{NF}$ $[\text{M}+\text{H}]^+$ calc. mass 160.1502, found 160.1502.

General Procedure E—preparation of β -fluoroamines or β,β -difluoroamines

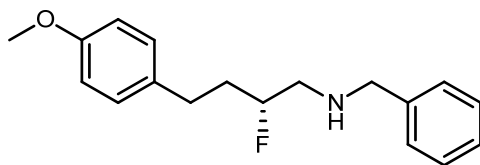


Triflic anhydride (339 mg, 1.2 mmol) was added dropwise to a flame dried round bottom flask equipped with a magnetic stir bar and charged with the chiral fluoro alcohol or difluoro alcohol (1 mmol) and lutidine (535 mg, 5 mmol) in DCM (5 mL) under argon at 0°C . The reaction mixture was allowed to stir for 30 minutes before it was removed from the stir plate while still being kept at 0°C . A separate round bottom flask equipped with a magnetic stir bar and charged with benzylamine (1.07 g, 10.0 mmol) in 2 mL of DCM was stirred at 0°C . The solution of the triflate was then added slowly to this new flask taking care to keep everything at 0°C , and after addition was complete, the flask was washed with an additional 2 mL of DCM and that was then added to the reaction to bring the total volume of DCM to 9 mL. The reaction was then allowed to warm to room temperature over the next hour and left to stir overnight (14-16 hours). The β,β -difluoroamines were allowed to react for 24 hours. A solution of saturated NaHCO_3 was added to quench the reaction and it was transferred to a separatory funnel. There it was extracted 3X with DCM and the combined organic extracts were dried with MgSO_4 , filtered, and concentrated under reduced pressure. The crude oil was then purified via flash column chromatography (hexanes/ethyl acetate).



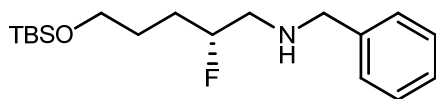
(*R*)-*N*-benzyl-2-fluoro-3-phenylpropan-1-amine (2a)

The product was prepared according to general procedure E, purified via flash column chromatography (20-50% ethyl acetate in hexanes, visualize TLC with ninhydrin) to afford the product was a clear oil (204 mg, 84% yield), which was determined to have an ee of 94% by chiral HPLC analysis (Chiralpak IA, t_R (major) = 4.87 minutes, t_R (minor) = 5.74 minutes, traces shown below). ^1H NMR (400.1 MHz, CDCl_3) δ (ppm): 7.42-7.23 (m, 10H); 4.91 (dm, J = 48.9 Hz, 1H); 3.91-3.81 (m, 2H); 3.13-2.78 (m, 4H); 1.86 (s, br, 1H). ^{13}C NMR (100.6 MHz, CDCl_3) δ (ppm): 140.09, 136.96 (d, J = 5.5 Hz), 129.40, 128.55, 128.50, 128.18, 127.10, 126.70, 94.07 (d, J = 171.2 Hz), 53.83, 52.38 (d, J = 21.0 Hz), 39.45 (d, J = 21.2 Hz). Specific rotation $[\alpha]_D^{23} = -2.3^\circ$ (c = 100, CHCl_3). HRMS (TOF, ES+) $\text{C}_{16}\text{H}_{19}\text{NF}$ $[\text{M}+\text{H}]^+$ calc. mass 244.1502, found 244.1503.



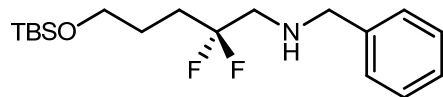
(*R*)-*N*-benzyl-2-fluoro-4-(4-methoxyphenyl)butan-1-amine (2b)

The product was prepared according to general procedure E, purified via flash column chromatography (20-50% ethyl acetate in hexanes, visualize TLC with ninhydrin) to afford the product was a clear oil (277 mg, 96% yield), which was determined to have an ee of 90% by chiral HPLC analysis (Chiralpak IB, t_R (major) = 6.56 minutes, t_R (minor) = 5.93 minutes, traces shown below). ^1H NMR (400.1 MHz, CDCl_3) δ (ppm): 7.41-7.25 (m, 5H); 7.14 (d, J = 8.6 Hz, 2H); 6.87 (d, J = 8.6 Hz, 2H); 4.68 (dm, J = 50.0 Hz, 1H); 3.85 (s, 2H); 3.81 (s, 3H); 2.94-2.63 (m, 4H); 2.10-1.95 (m, 1H); 1.93-1.80 (m, 1H); 1.78 (s, br, 1H). ^{13}C NMR (100.6 MHz, CDCl_3) δ (ppm): 157.97, 140.10, 133.30, 129.40, 128.47, 128.13, 127.07, 113.92, 93.05 (d, J = 167.8 Hz), 55.26, 53.83, 53.07 (d, J = 20.9 Hz), 35.00 (d, J = 20.6 Hz), 30.36 (d, J = 4.6 Hz). Specific rotation $[\alpha]_D^{23} = +11.8^\circ$ (c = 100, CHCl_3). HRMS (TOF, ES+) $\text{C}_{18}\text{H}_{23}\text{NOF}$ $[\text{M}+\text{H}]^+$ calc. mass 288.1764, found 288.1762.



(*R*)-*N*-benzyl-5-((*tert*-butyldimethylsilyloxy)-2-fluoropentan-1-amine (2c)

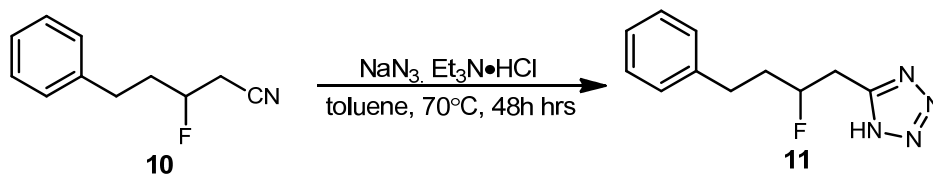
The product was prepared according to general procedure E, purified via flash column chromatography (20-50% ethyl acetate in hexanes, visualize TLC with ninhydrin) to afford the product was a clear oil (314 mg, 96% yield), which was determined to have an ee of 94% by chiral HPLC analysis (Chiralpak ID, t_R (major) = 9.74 minutes, t_R (minor) = 10.65 minutes, traces shown below). ^1H NMR (400.1 MHz, CDCl_3) δ (ppm): 7.39-7.22 (m, 5H); 4.68 (dm, J = 50.0 Hz, 1H); 3.87-3.79 (m, 2H); 3.69-3.58 (m, 2H); 2.90-2.68 (m, 2H); 1.81-1.54 (m, 5H); 0.90 (s, 9H); 0.06 (s, 6H). ^{13}C NMR (100.6 MHz, CDCl_3) δ (ppm): 140.18, 128.54, 128.19, 127.12, 93.89 (d, J = 167.8 Hz), 62.76, 53.90, 53.24 (d, J = 20.9 Hz), 29.62 (d, J = 20.7 Hz), 28.43 (d, J = 4.3 Hz), 26.06, 18.43, -5.20. Specific rotation $[\alpha]_D^{23} = +0.6^\circ$ (c = 100, CHCl_3). HRMS (TOF, ES+) $\text{C}_{18}\text{H}_{33}\text{NOFSi}$ $[\text{M}+\text{H}]^+$ calc. mass 326.2315, found 326.2318.



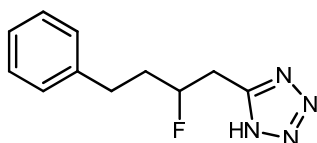
N-benzyl-5-((*tert*-butyldimethylsilyl)oxy)-2,2-difluoropentan-1-amine (5)

The product was prepared according to general procedure E, purified via flash column chromatography (20-50% ethyl acetate in hexanes, visualize TLC with ninhydrin) to afford the product as a clear oil (277 mg, 81% yield). ^1H NMR (400.1 MHz, CDCl_3) δ (ppm): 7.39-7.24 (m, 5H); 3.88 (s, 2H); 3.67 (t, $J = 6.3$ Hz, 2H); 2.95 (t, $J = 14.1$ Hz, 2H); 2.10-1.95 (m, 2H); 1.75-1.66 (m, 2H); 1.62 (s, 1H); 0.93 (s, 9H); 0.09 (s, 6H). ^{13}C NMR (100.6 MHz, CDCl_3) δ (ppm): 139.96, 128.55, 128.17, 127.23, 127.87 (t, $J = 240.9$ Hz), 62.52, 53.78, 52.70 (t, $J = 28.4$), 31.27 (t, $J = 24.6$ Hz), 26.04, 25.57 (t, $J = 4.3$ Hz), 18.41, -5.23. HRMS (TOF, ES+) $\text{C}_{18}\text{H}_{32}\text{NOF}_2\text{Si}$ $[\text{M}+\text{H}]^+$ calc. mass 344.2221, found 344.2219.

Procedure F—preparation of β -fluoro tetrazoles



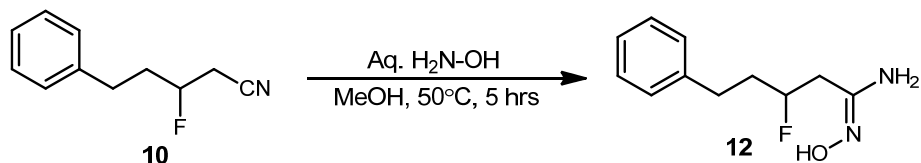
The mixture of fluoro-nitrile **10** (354 mg, 2 mmol), sodium azide (244 mg, 6 mmol), and triethylamine hydrochloride (517 mg, 6 mmol) in toluene (6 mL), in a round-bottomed flask equipped with a magnetic stir bar, was stirred and heated to 70°C for 48 hours. After cooling to room temperature, the product was extracted with water (2 X 6 mL), and the aqueous layer was acidified with 1 mL of concentrated hydrochloric acid (38%). If a white solid did not immediately crash out of solution upon acidification, air was blown on the water for to partially concentrate the water, and the β -fluoro-tetrazole then crashed out of solution as a white solid, which was collected using a Buchner funnel and was dried under reduced pressure. The solid was purified via reverse phase chromatography.



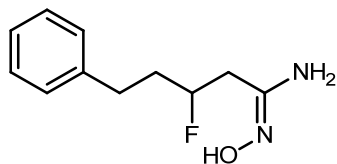
5-(2-fluoro-4-phenylbutyl)-1H-tetrazole (**11**)

The product was prepared according to general procedure F, and was purified via reverse phase chromatography (10-90% MeCN in water (0.1% TFA), to afford the product as a white solid (339 mg, 77% yield). ^1H NMR (400.1 MHz, MeOD) δ (ppm): 7.28-7.22 (m, 2H); 7.21-7.12 (m, 3H); 4.84 (dm, $J = 48.8$ Hz, 1H); 3.40-3.21 (m, 2H); 2.86-2.66 (m, 2H); 2.04-1.86 (m, 2H). ^{13}C NMR (100.6 MHz, MeOD) δ (ppm): 154.38, 142.11, 129.50, 129.41, 127.11, 91.62 (d, $J = 172.0$ Hz), 37.43 (d, $J = 20.5$ Hz), 31.92 (d, $J = 4.3$ Hz), 30.2 (d, $J = 22.3$ Hz). HRMS (TOF, ES+) $\text{C}_{11}\text{H}_{14}\text{N}_4\text{F}$ $[\text{M}+\text{H}]^+$ calc. mass 221.1202, found 221.1201.

Procedure G—preparation of β -fluoro amide oxime



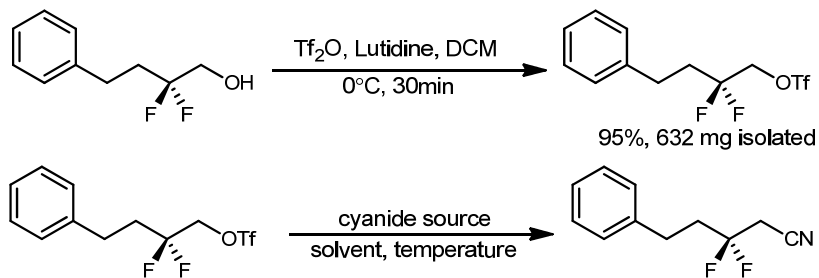
A mixture of fluoro-nitrile **10** (177 mg, 1 mmol) and aqueous hydroxylamine (66 mg, 2 mmol, from 50% aqueous solution) in methanol (1 mL) was added to a round-bottomed flask equipped with a magnetic stir bar and was heated to 50°C for 5 hours with stirring. The reaction was then concentrated under reduced pressure to evaporate all solvents and reagents. Crude product was pure enough for use in future reactions, but was purified via reverse phase chromatography to obtain spectroscopically pure material.



(*E*)-3-fluoro-*N'*-hydroxy-5-phenylpentanimidamide (**12**)

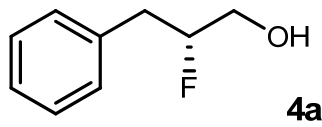
The product was prepared according to general procedure G, and was purified via reverse phase chromatography (10-90% MeCN in water (0.1% TFA), to afford the product as a white solid (191 mg, 91% yield). ¹H NMR (400.1 MHz, MeOD) δ (ppm): 7.31-7.24 (m, 2H); 7.23-7.15 (m, 3H); 4.79 (dm, $J = 49.0$ Hz, 1H); 2.89-2.63 (m, 4H); 2.09-1.85 (m, 2H). ¹³C NMR (100.6 MHz, MeOD) δ (ppm): 161.66, 141.94, 129.57, 129.46, 127.23, 90.89 (d, $J = 174.6$), 37.66 (d, $J = 20.1$ Hz), 35.9 (d, $J = 22.3$ Hz), = 22.3 Hz), 31.82 (d, $J = 3.9$ Hz). HRMS (TOF, ES⁺) C₁₁H₁₆N₂OF [M+H]⁺ calc. mass 211.1247, found 211.1245.

Attempted Reaction Conditions for the synthesis of β,β -difluoronitriles

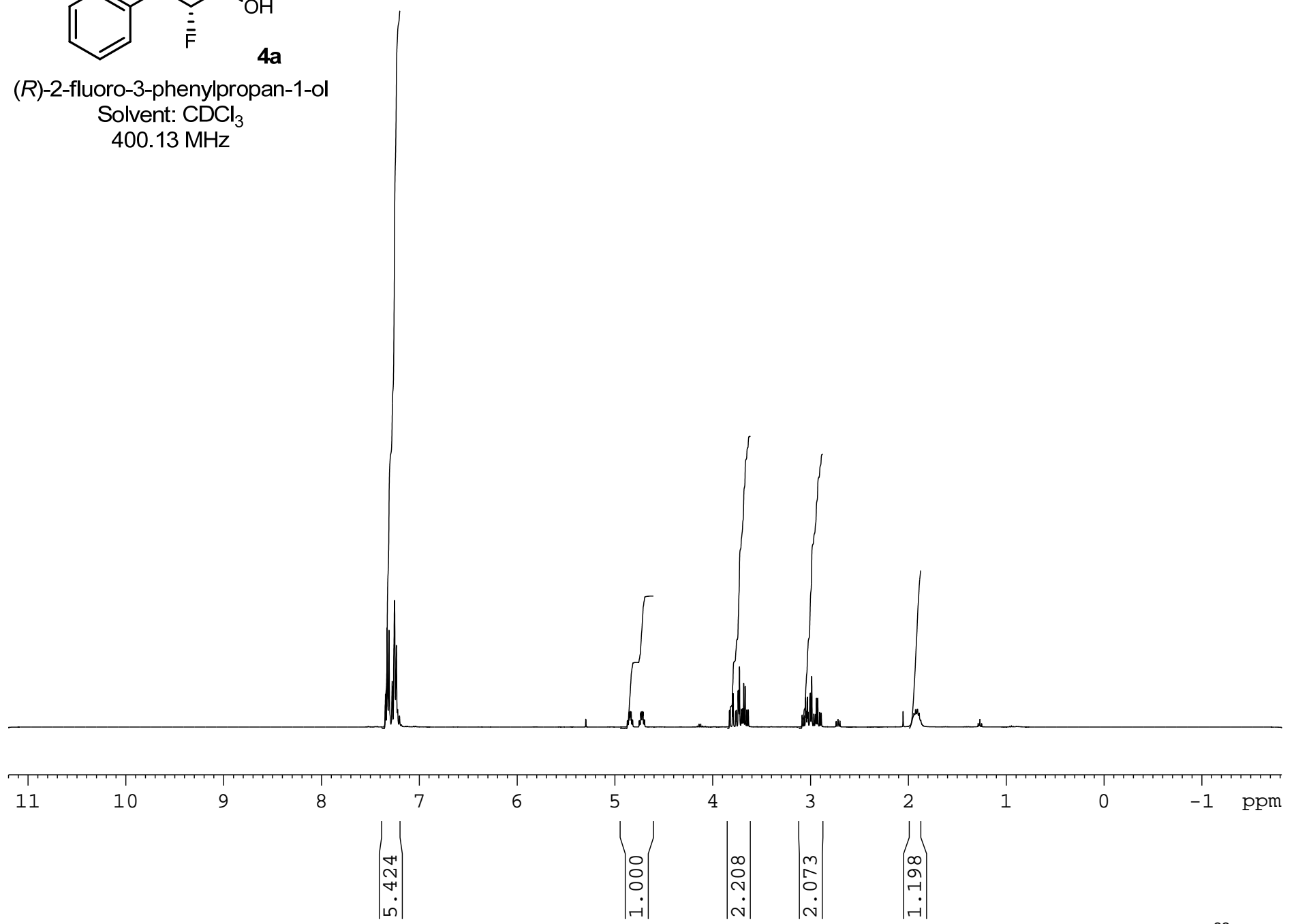


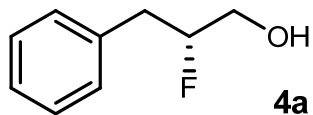
Solvent	Cyanide	Additive	Temperature	Result
MeCN	KCN	18-C-6	room temp (24 hrs)	decomposition
MeCN	KCN	water cosolvent	MW 90 (30min)	decomposition
MeCN	KCN	18-C-6	MW 120 (10min)	decomposition
THF	KCN	water cosolvent	room temp (16 hrs)	no conversion
THF	KCN	water cosolvent	50°C (16 hrs)	slow decomposition
THF	KCN	water cosolvent	MW 150 (45 min)	10% isolated yield (8mg) → Not Reproducible on Larger Scale
THF	KCN	water cosolvent	room temp (16 hrs)	no conversion
THF	KCN	MeOH cosolvent	MW 130 (30min)	slow decomposition
THF	KCN	18-C-6	MW 160 (45min)	decomposition
^t BuOH	KCN	none	MW 120 (10min)	little/no conversion
^t BuOH	KCN	none	MW 150 (45min)	some s.m. left, decomp.
DMSO	KCN	none	70°C (10min)	decomposition
DMSO	KCN	none	room temp (14 hrs)	decomposition
DCM	TBA • CN	none	room temp (2 hrs)	decomposition
MeCN	TBA • CN	none	room temp (15min)	decomposition

} no fluorine in products



(*R*)-2-fluoro-3-phenylpropan-1-ol
Solvent: CDCl₃
400.13 MHz





4a

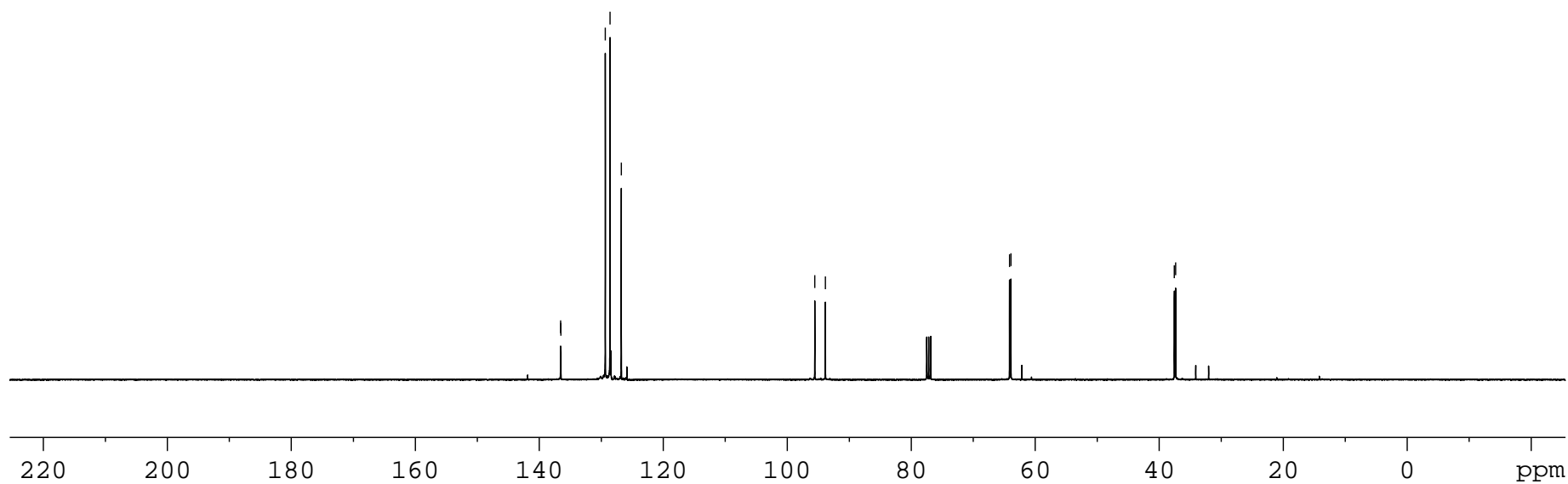
(*R*)-2-fluoro-3-phenylpropan-1-ol
Solvent: CDCl₃
100.6 MHz

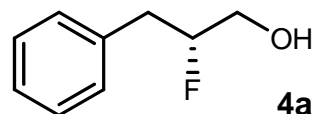
136.548
136.493
129.333
128.576
126.751

95.548
93.839

64.120
63.905

37.551
37.340





Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -0.5, max = 25.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron Ions

8 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

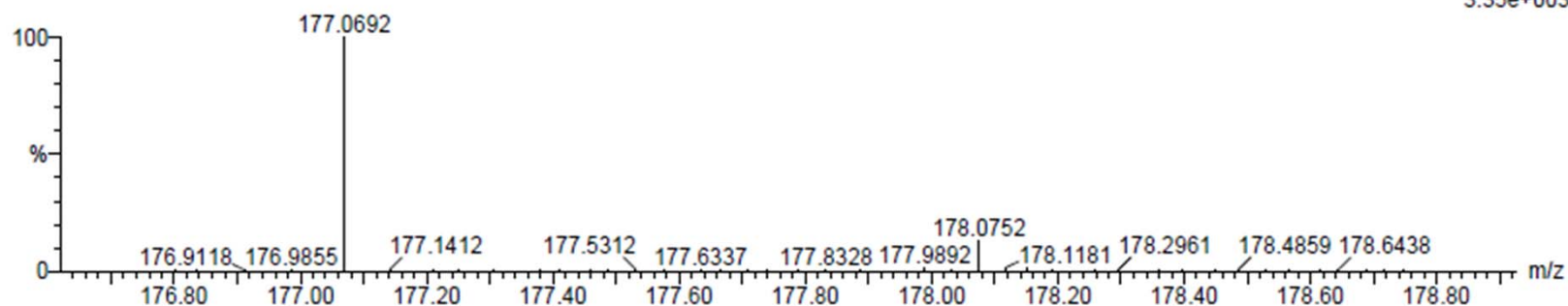
C: 8-500 H: 10-1000 O: 1-200 F: 1-1 Na: 1-1

MCO-IV-151

S/N: UH193

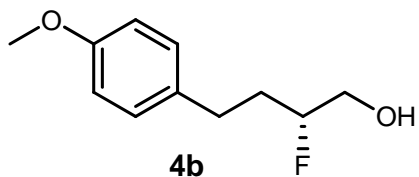
MCO-IV-151_120712_001 45 (0.842) AM (Cen,4, 80.00, Ar,8000.0,556.28,0.70); Sm (SG, 2x1.00); Cm (40:50)

07-Dec-2012
13:11:55
TOF MS ES+
3.35e+003



Minimum: -0.5
Maximum: 5.0 5.0 25.0

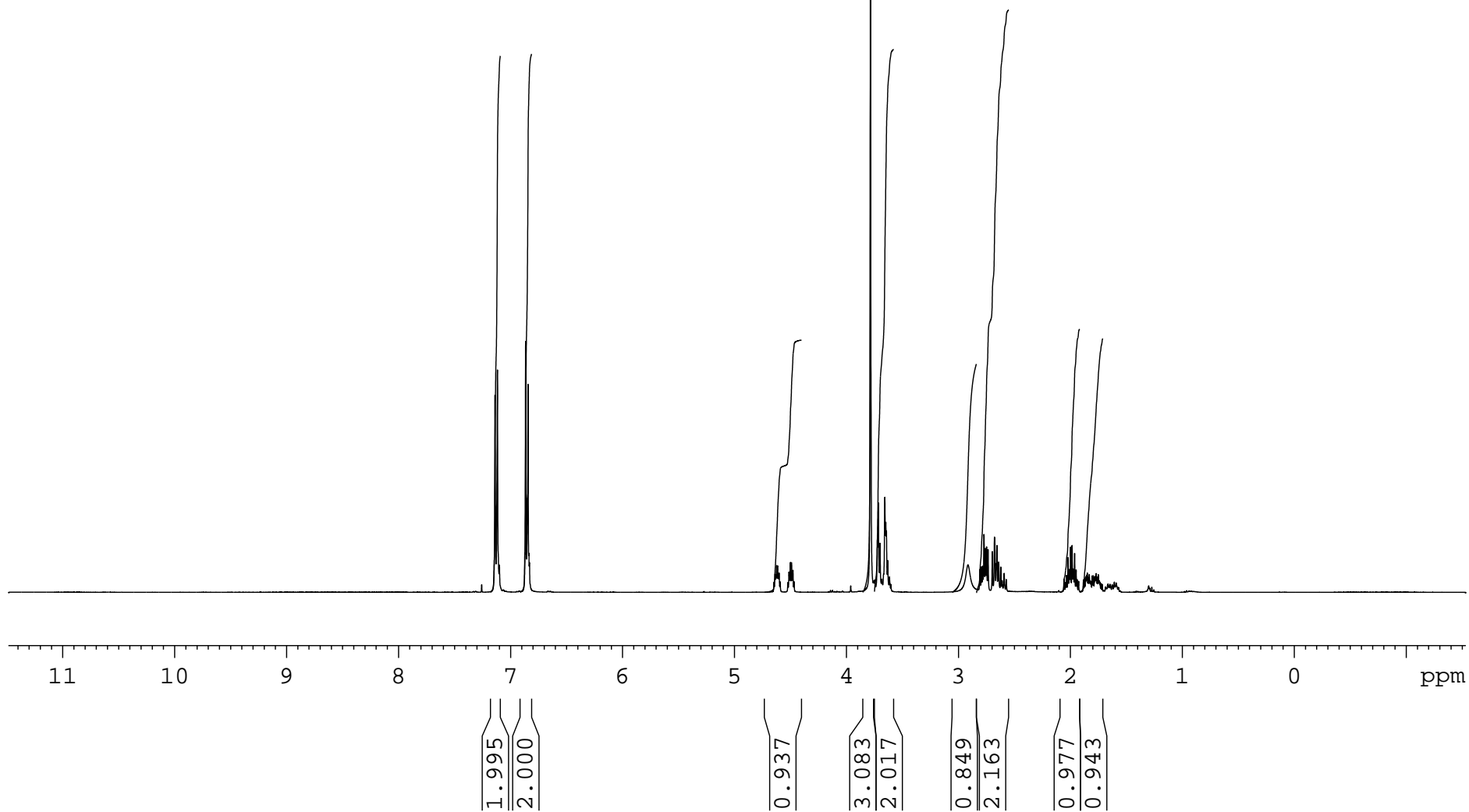
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
177.0692	177.0692	0.0	0.0	3.5	7.5	C9 H11 O F Na

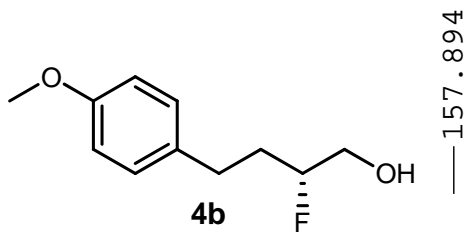


(*R*)-2-fluoro-4-(4-methoxyphenyl)butan-1-ol

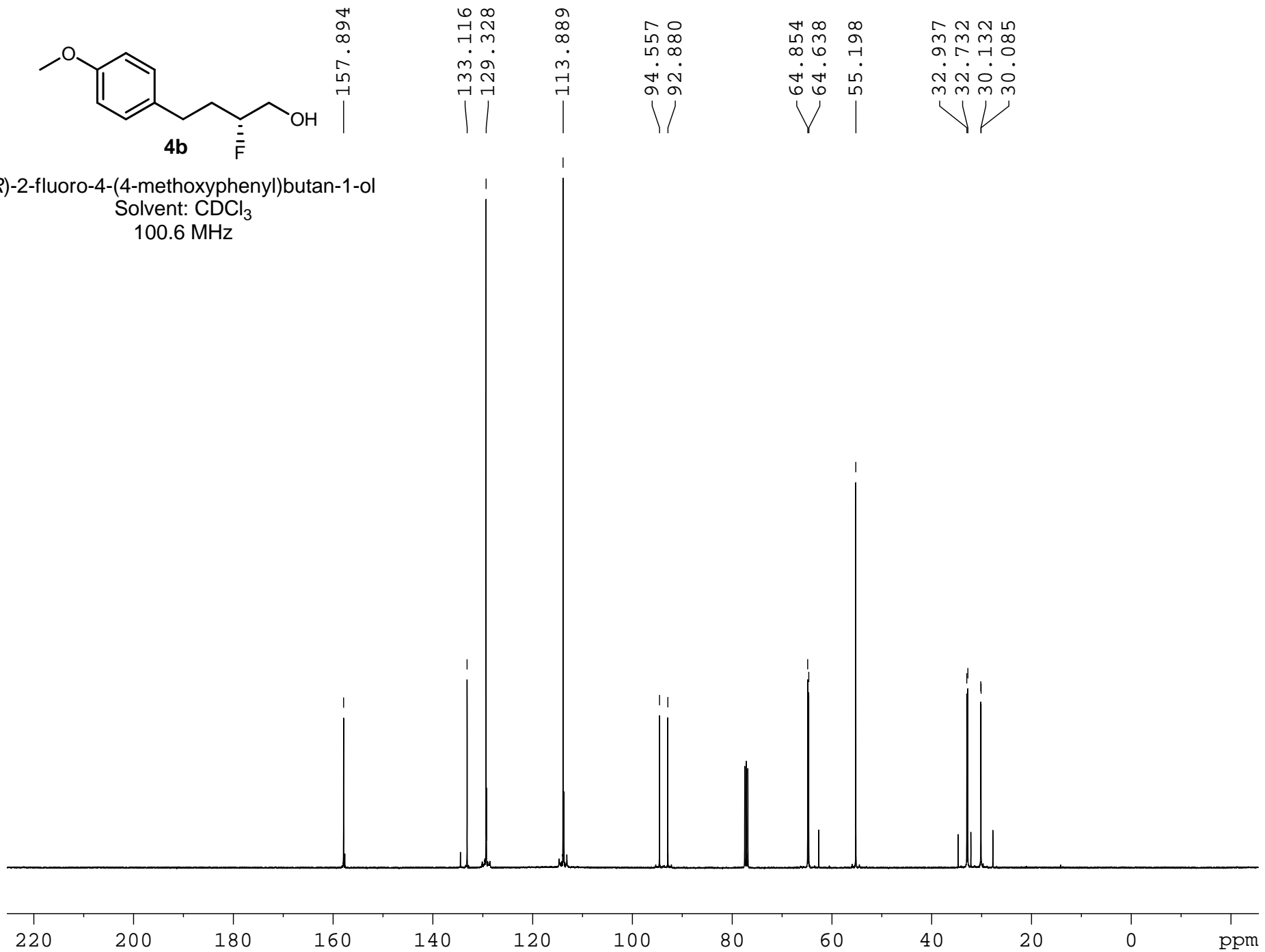
Solvent: CDCl₃

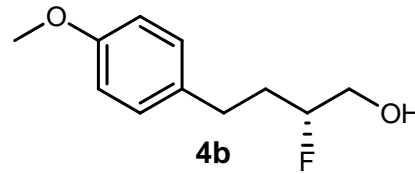
400.13 MHz





(*R*)-2-fluoro-4-(4-methoxyphenyl)butan-1-ol
Solvent: CDCl₃
100.6 MHz





Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -0.5, max = 25.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron Ions

12 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

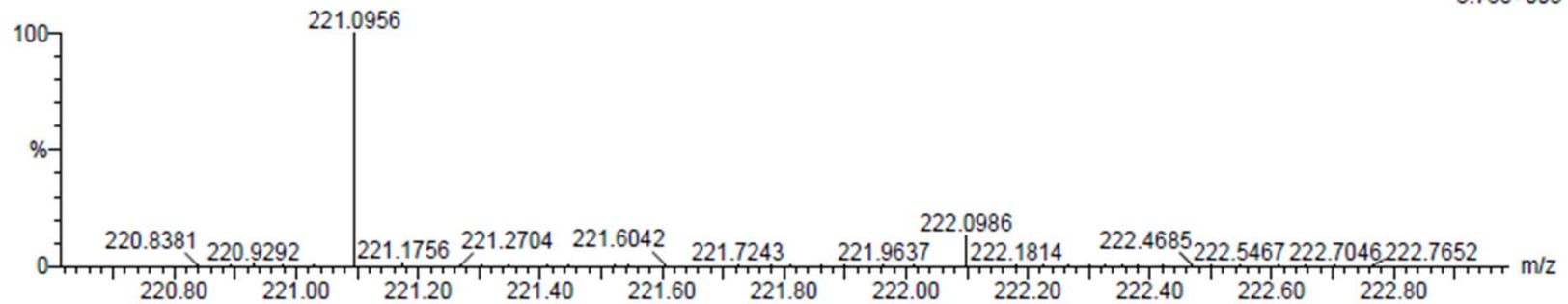
C: 10-500 H: 10-1000 O: 1-200 F: 1-1 Na: 1-1

MCO-IV-148

S/N: UH193

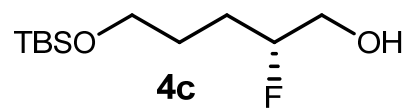
MCO-IV-148_120612_001 79 (1.473) AM (Cen,4, 80.00, Ar,8000.0,556.28,0.70); Sm (SG, 2x1.00); Cm (70:80)

06-Dec-2012
13:37:14
TOF MS ES+
3.78e+003



Minimum: -0.5
Maximum: 5.0 5.0 25.0

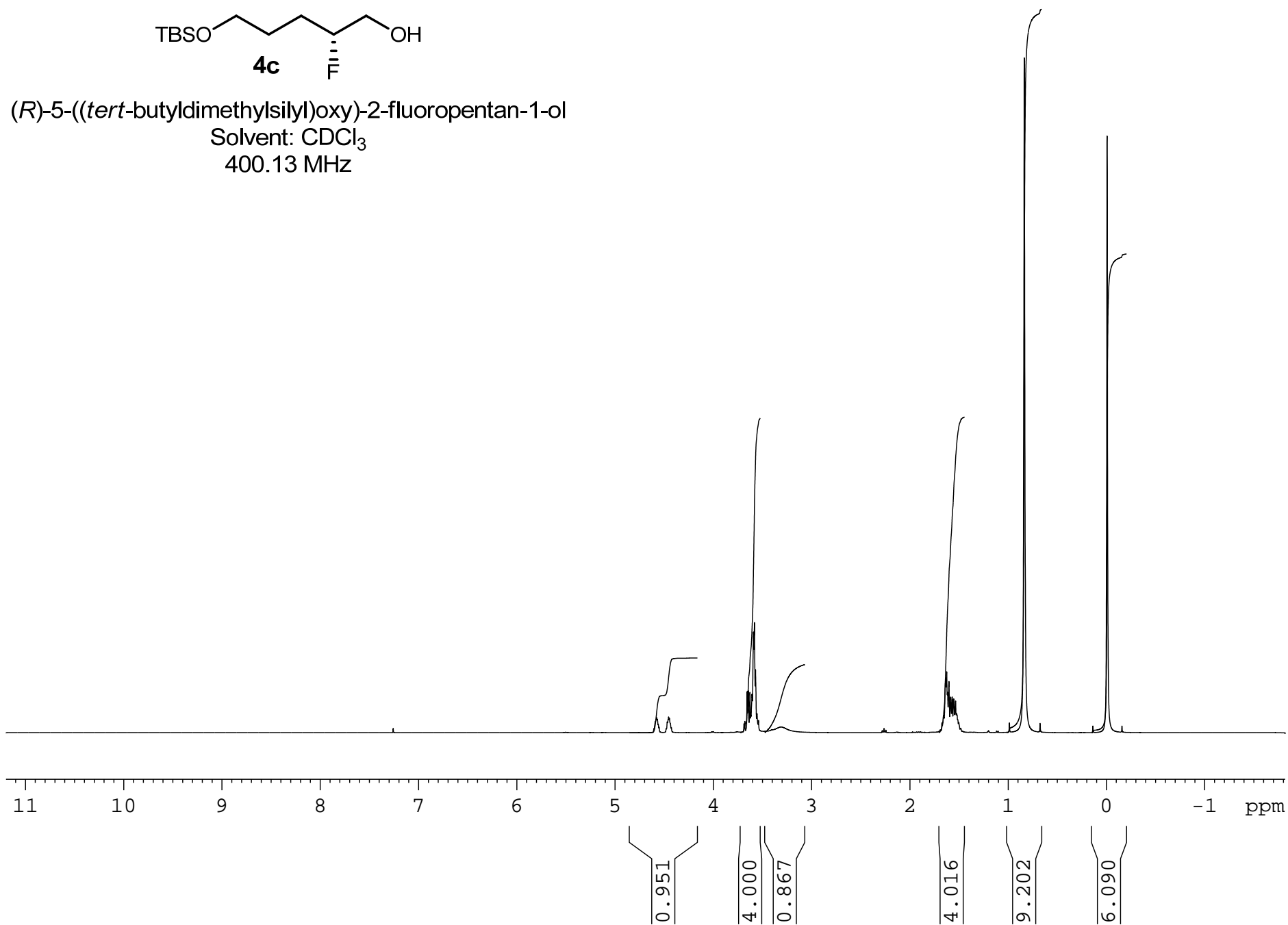
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
221.0956	221.0954	0.2	0.9	3.5	0.3	C11 H15 O2 F Na

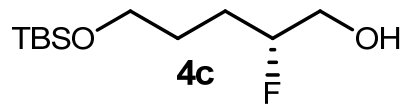


(*R*)-5-((*tert*-butyldimethylsilyl)oxy)-2-fluoropentan-1-ol

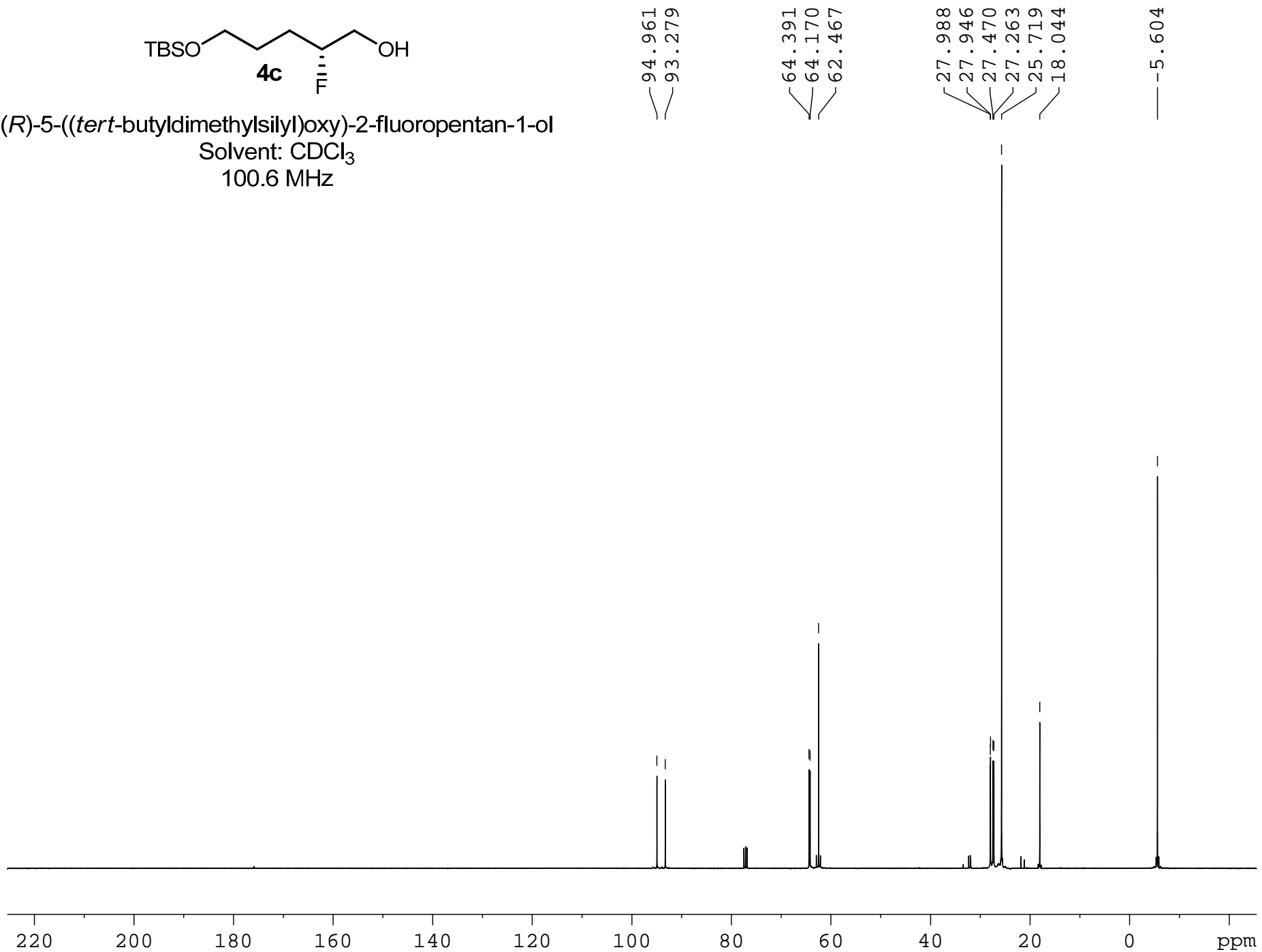
Solvent: CDCl₃

400.13 MHz

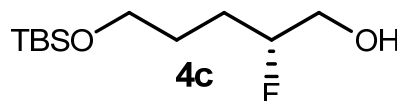




(*R*)-5-((*tert*-butyldimethylsilyl)oxy)-2-fluoropentan-1-ol
Solvent: CDCl₃
100.6 MHz



Elemental Composition Report



Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -0.5, max = 25.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron Ions

13 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

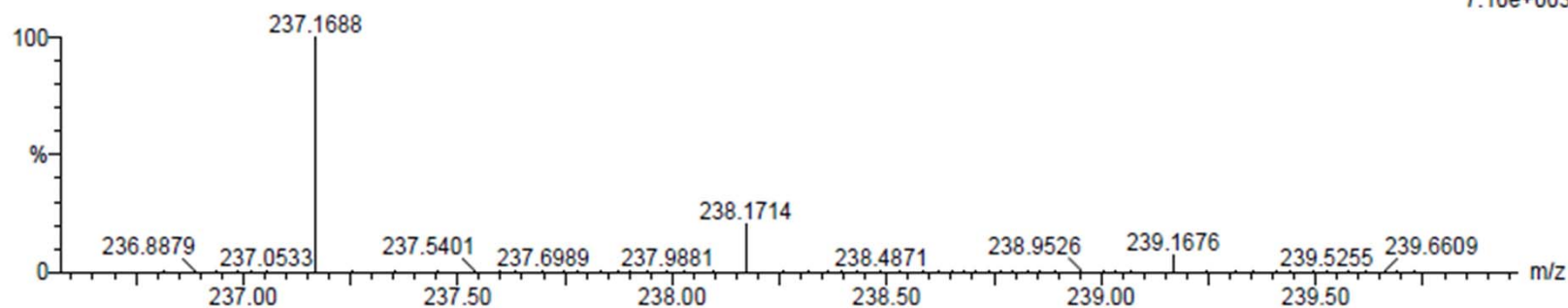
C: 10-500 H: 10-1000 O: 1-200 F: 1-1 Si: 1-1

MCO-IV-166

S/N: UH193

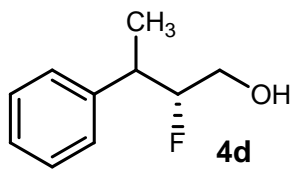
MCO-IV-166_120712_001 51 (0.954) AM (Cen,4, 80.00, Ar,8000.0,556.28,0.70); Sm (SG, 2x1.00); Cm (50:60)

07-Dec-2012
10:27:41
TOF MS ES+
7.10e+003

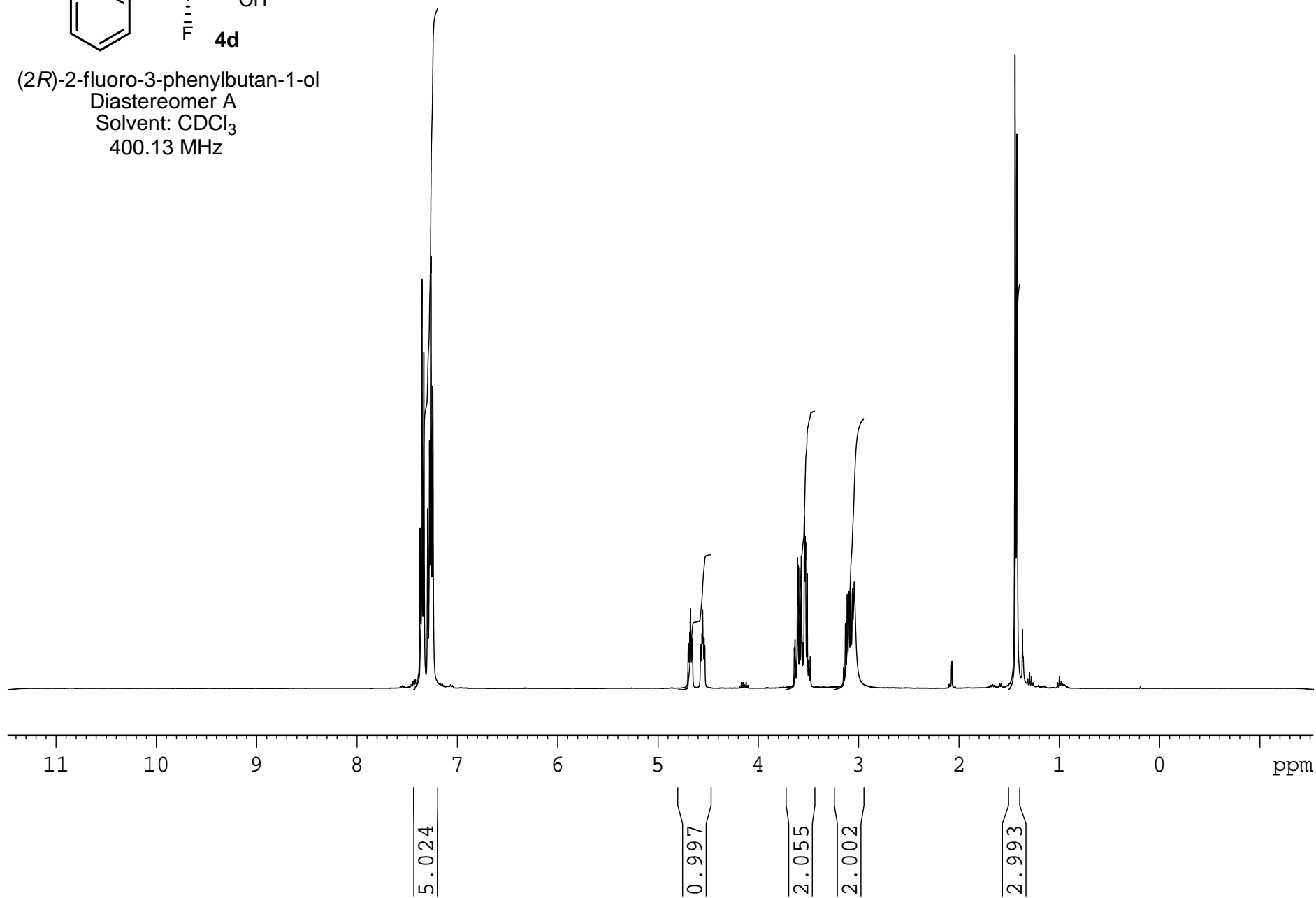


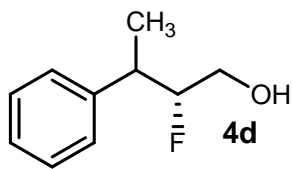
Minimum: -0.5
Maximum: 5.0 5.0 25.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
237.1688	237.1686	0.2	0.8	-0.5	7.8	C11 H26 O2 F Si

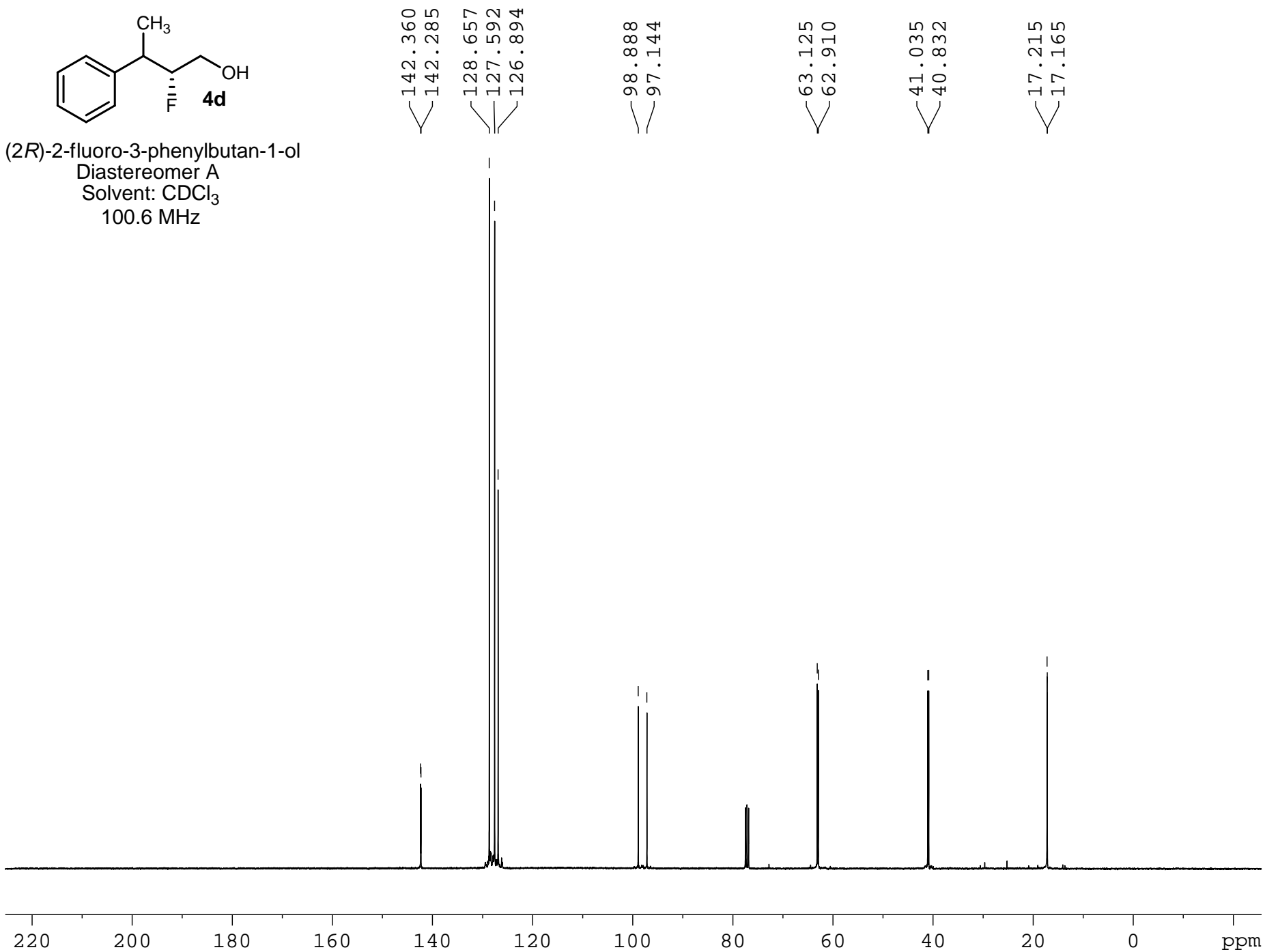


(2*R*)-2-fluoro-3-phenylbutan-1-ol
Diastereomer A
Solvent: CDCl₃
400.13 MHz





(2*R*)-2-fluoro-3-phenylbutan-1-ol
Diastereomer A
Solvent: CDCl₃
100.6 MHz



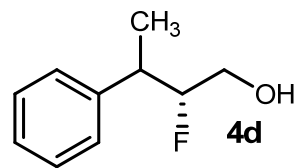
Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -0.5, max = 25.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 2



Diastereomer A

Page 1

Monoisotopic Mass, Even Electron Ions

8 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

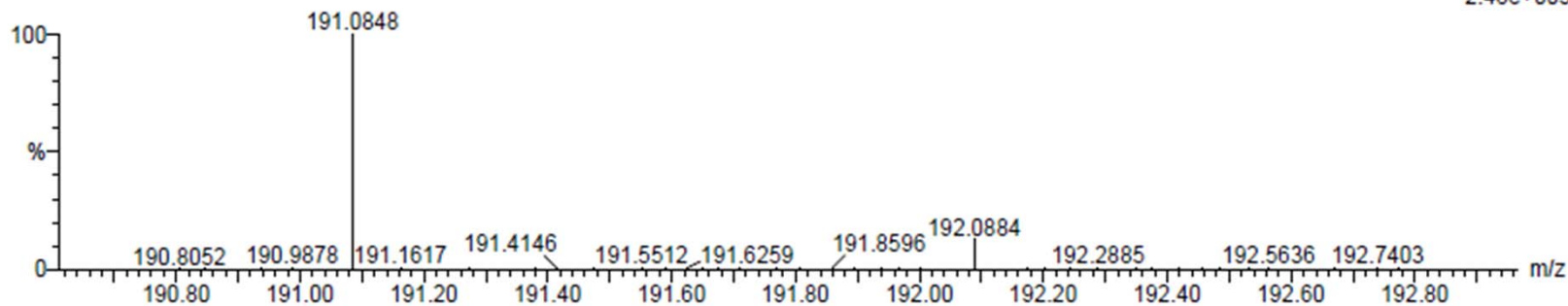
C: 10-500 H: 10-1000 O: 1-200 F: 1-1 Na: 1-1

MCO-IV-153 Non-Polar

S/N: UH193

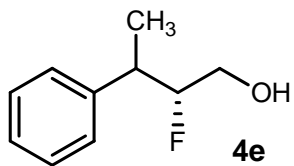
MCO-IV-153-NP_120612_001 60 (1.121) AM (Cen,4, 80.00, Ar,8000.0,556.28,0.70); Sm (SG, 2x1.00); Cm (50:60)

06-Dec-2012
15:53:48
TOF MS ES+
2.48e+003

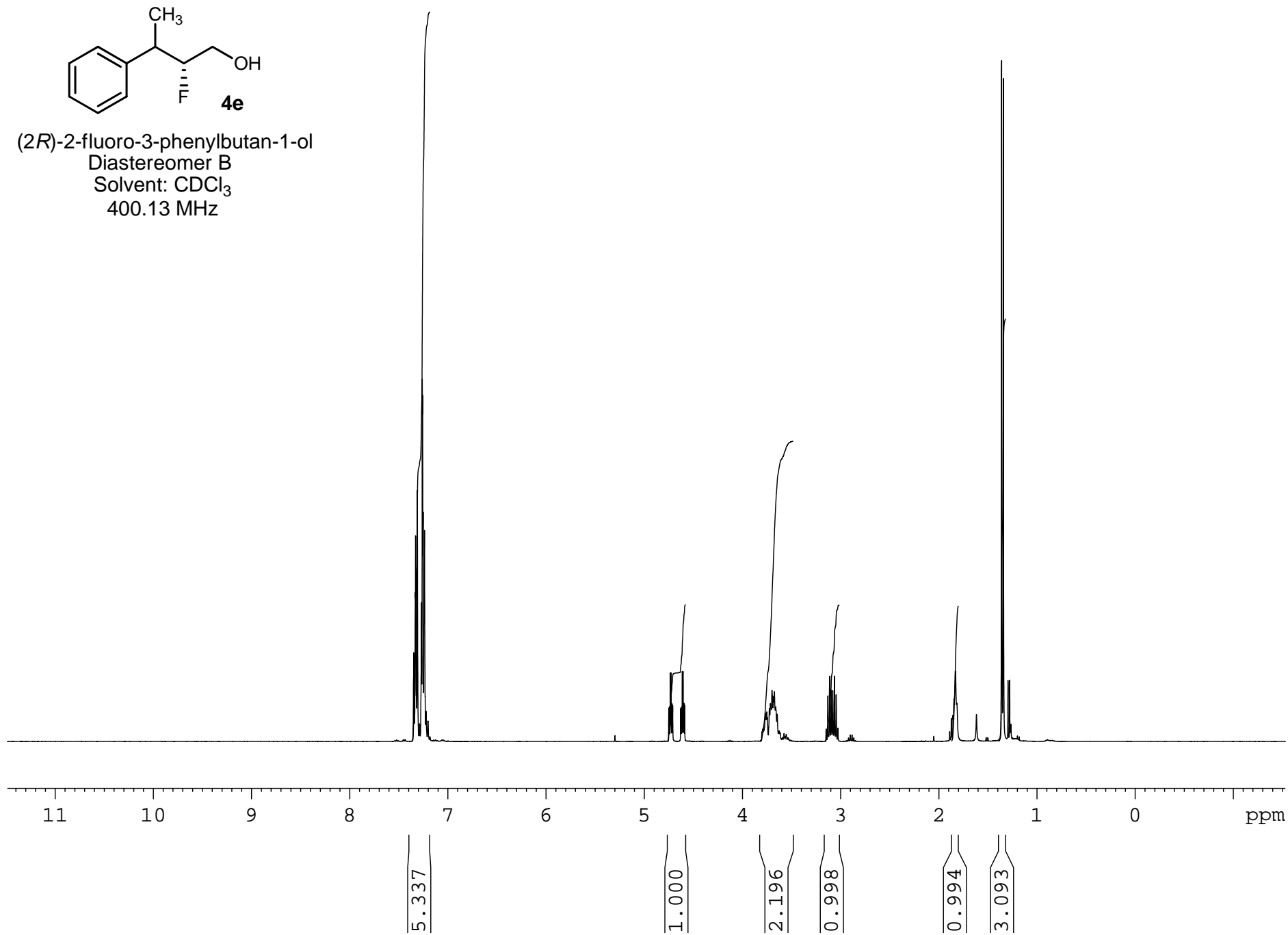


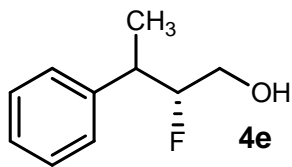
Minimum: -0.5
Maximum: 5.0 5.0 25.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
191.0848	191.0848	0.0	0.0	3.5	1.1	C10 H13 O F Na

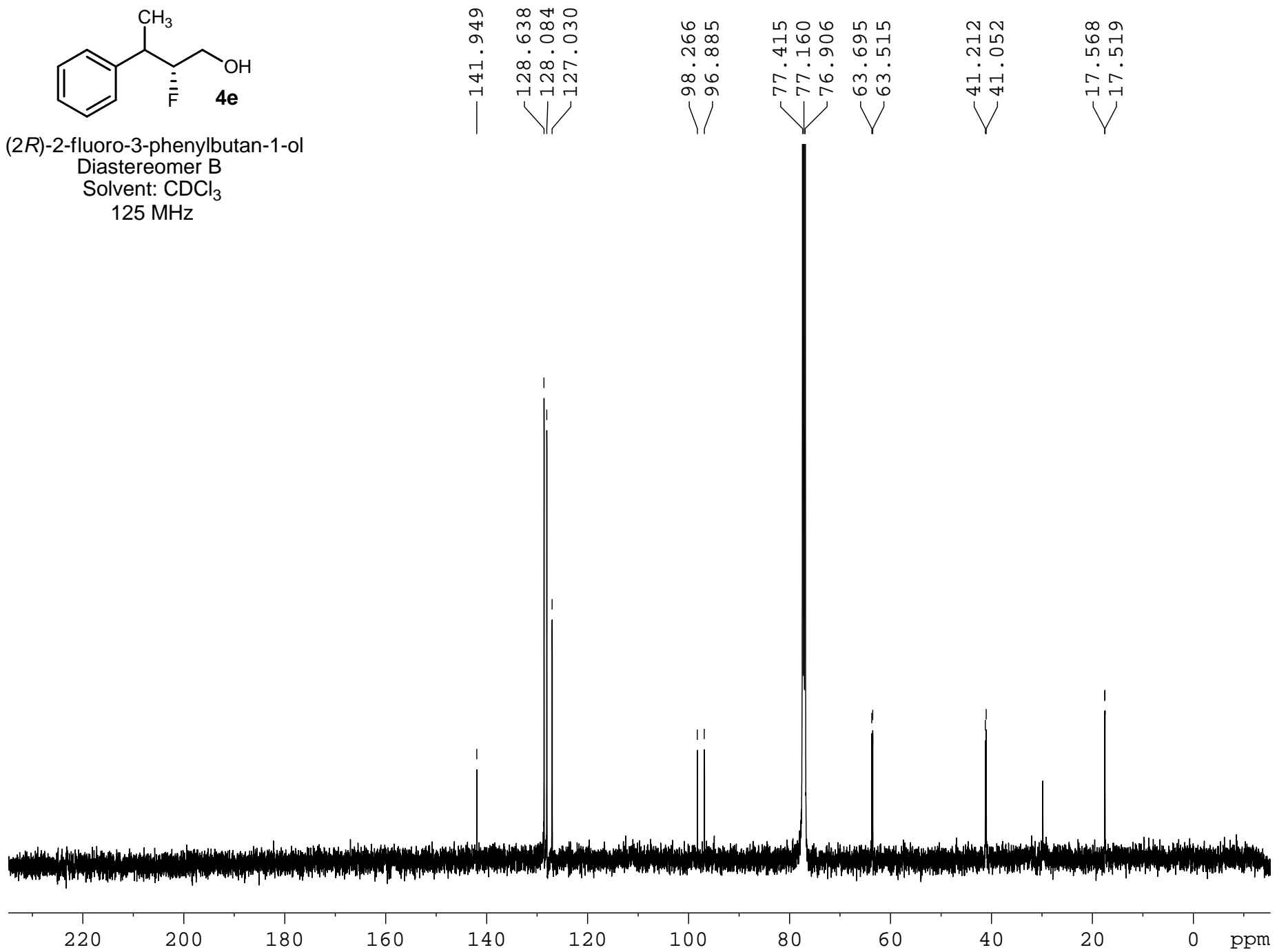


(2*R*)-2-fluoro-3-phenylbutan-1-ol
Diastereomer B
Solvent: CDCl₃
400.13 MHz





(2*R*)-2-fluoro-3-phenylbutan-1-ol
Diastereomer B
Solvent: CDCl₃
125 MHz



Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -0.5, max = 25.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron Ions

8 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

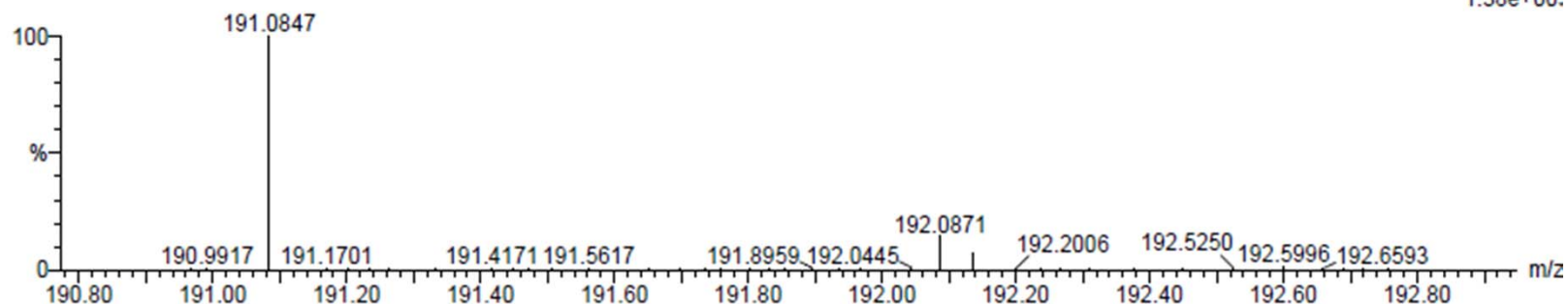
C: 10-500 H: 10-1000 O: 1-200 F: 1-1 Na: 1-1

MCO-IV-153 Polar

S/N: UH193

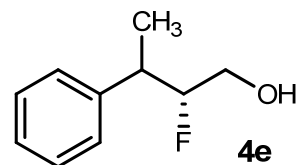
MCO-IV-153-P_120612_001 98 (1.825) AM (Cen,4, 80.00, Ar,8000.0,556.28,0.70); Sm (SG, 2x1.00); Cm (90:100)

06-Dec-201:
16:00:21
TOF MS ES+
1.38e+00:

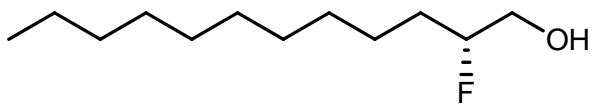


Minimum: -0.5
Maximum: 5.0 5.0 25.0

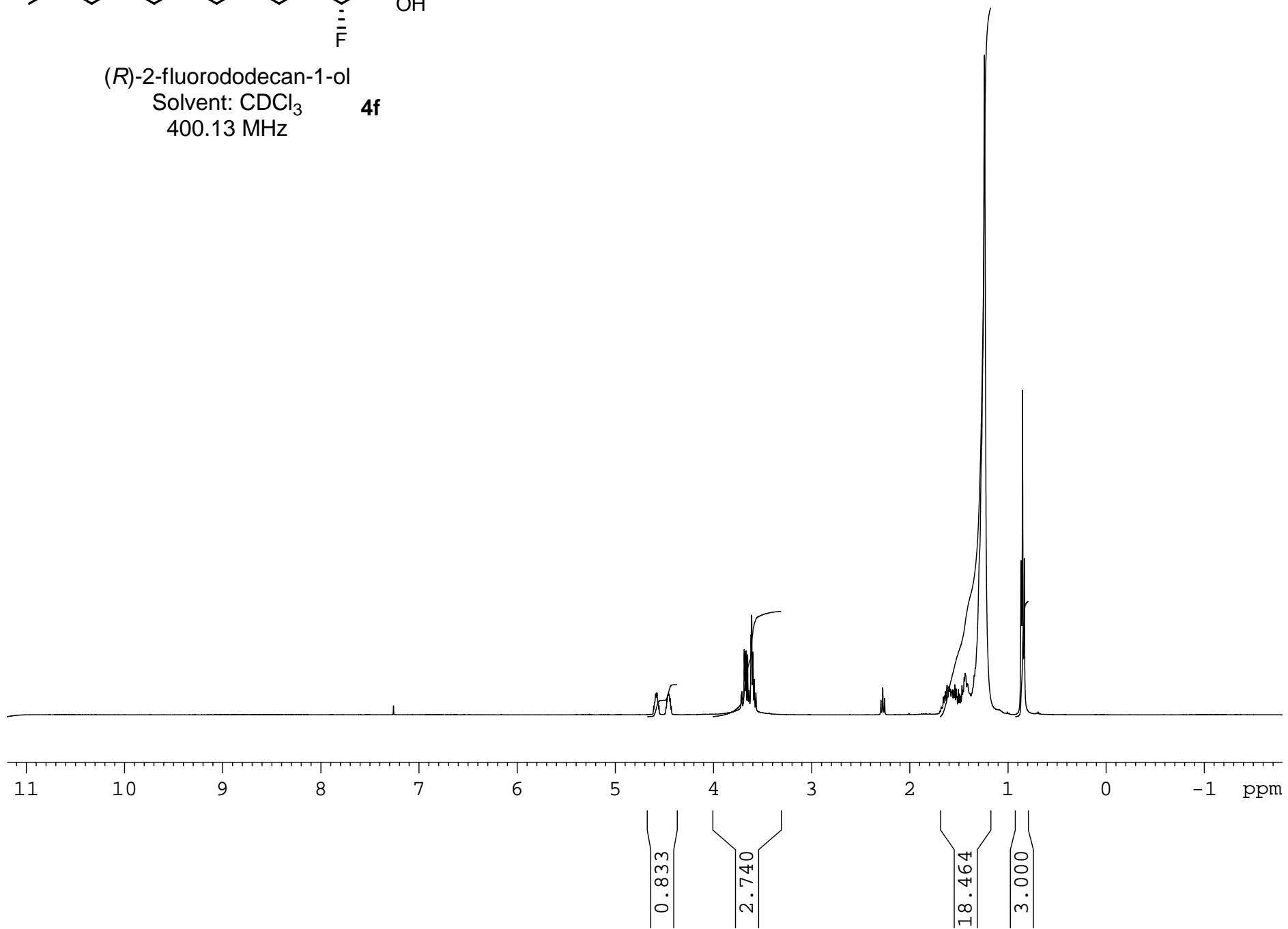
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
191.0847	191.0848	-0.1	-0.5	3.5	3.6	C10 H13 O F Na

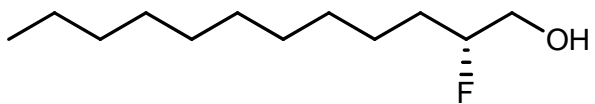


Diastereomer B



(*R*)-2-fluorododecan-1-ol
Solvent: CDCl₃ **4f**
400.13 MHz



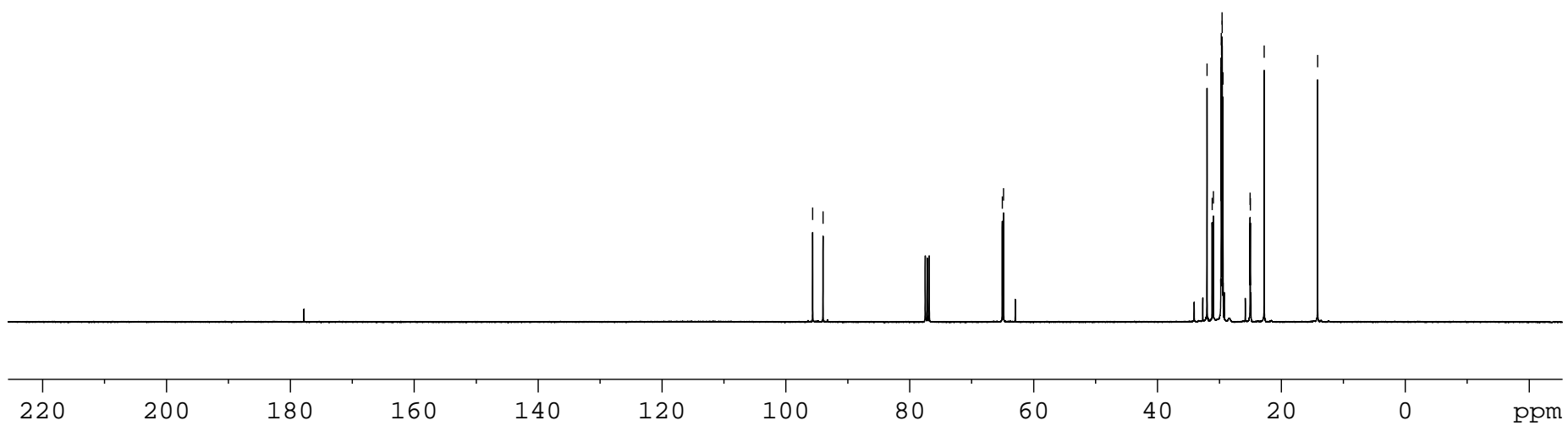


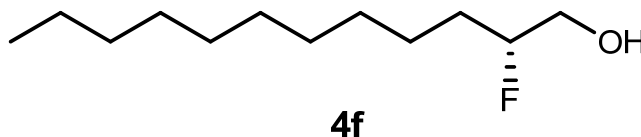
(*R*)-2-fluorododecan-1-ol
Solvent: CDCl₃
100.6 MHz **4f**

95.662
93.992

65.063
64.846

31.993
31.171
30.968
29.688
29.650
29.566
29.541
29.418
25.044
24.997
22.757
14.139





Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -0.5, max = 25.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron Ions

13 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

C: 10-500 H: 10-1000 O: 1-200 F: 1-1 Na: 1-1

MCO-IV-147

S/N: UH193

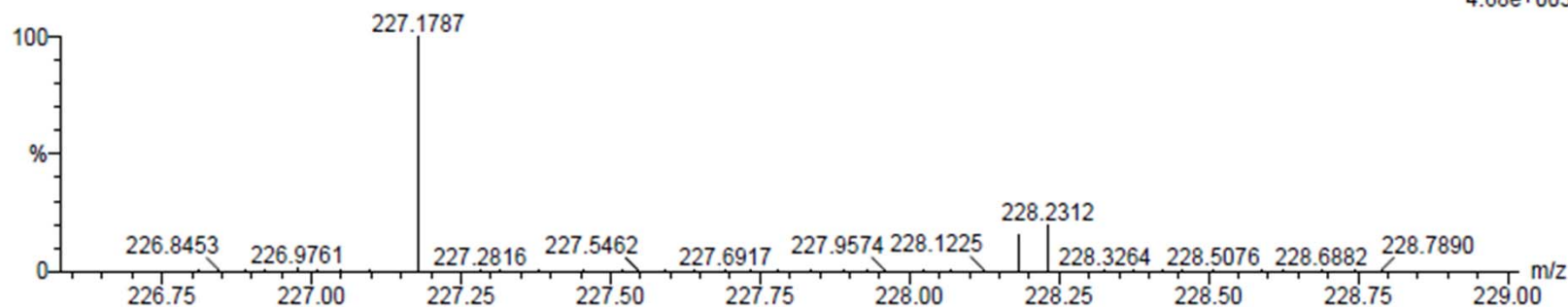
MCO-IV-147_120612_001 70 (1.306) AM (Cen,4, 80.00, Ar,8000.0,556.28,0.70); Sm (SG, 2x1.00); Cm (60:70)

06-Dec-2012

13:14:46

TOF MS ES+

4.68e+003



Minimum:

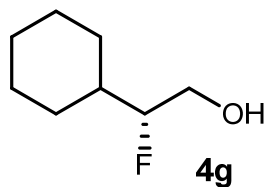
Maximum:

5.0 5.0 -0.5

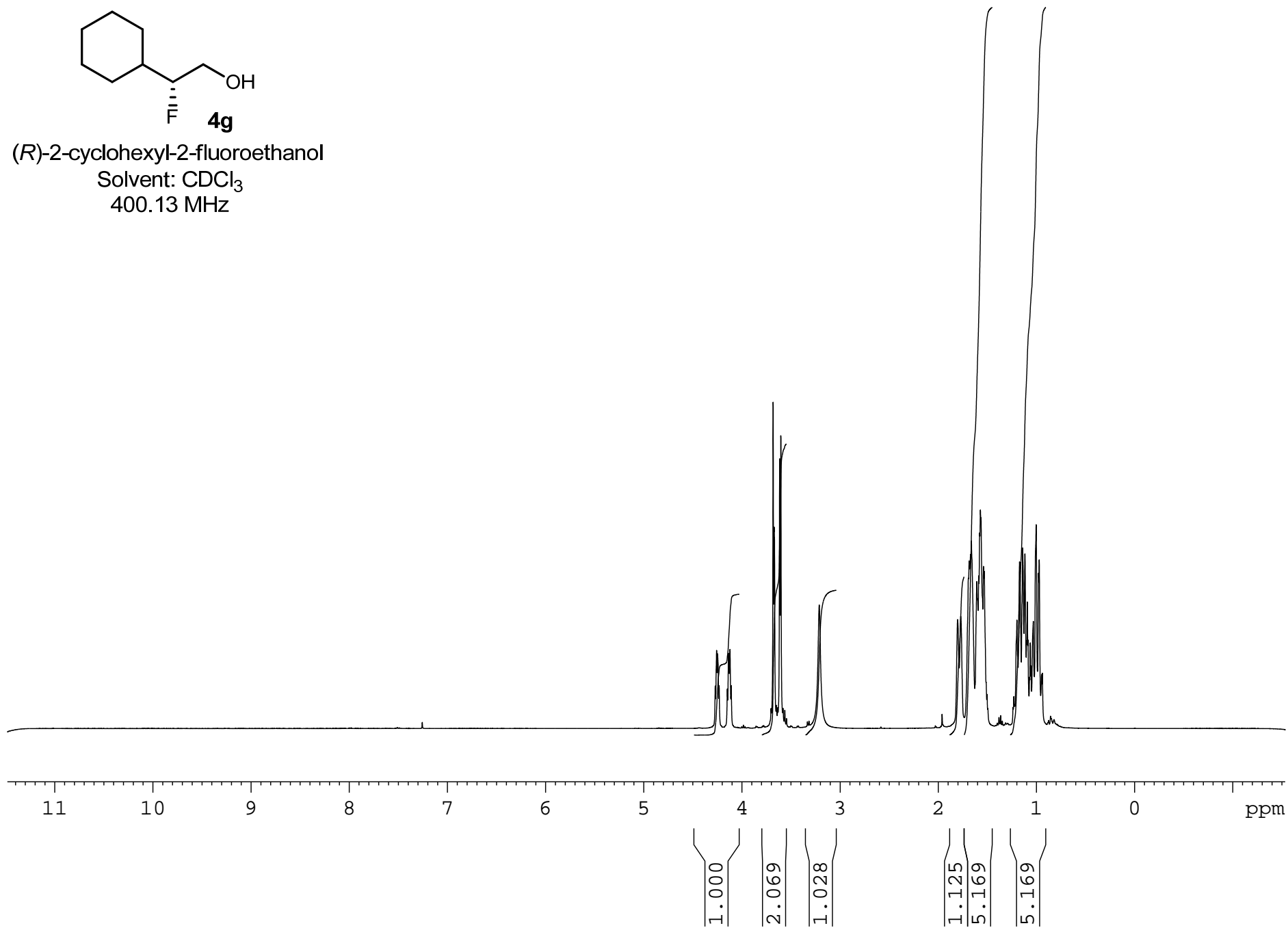
5.0 25.0

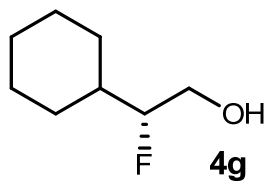
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
------	------------	-----	-----	-----	-------	---------

227.1787	227.1787	0.0	0.0	-0.5	4.0	C12 H25 O F Na
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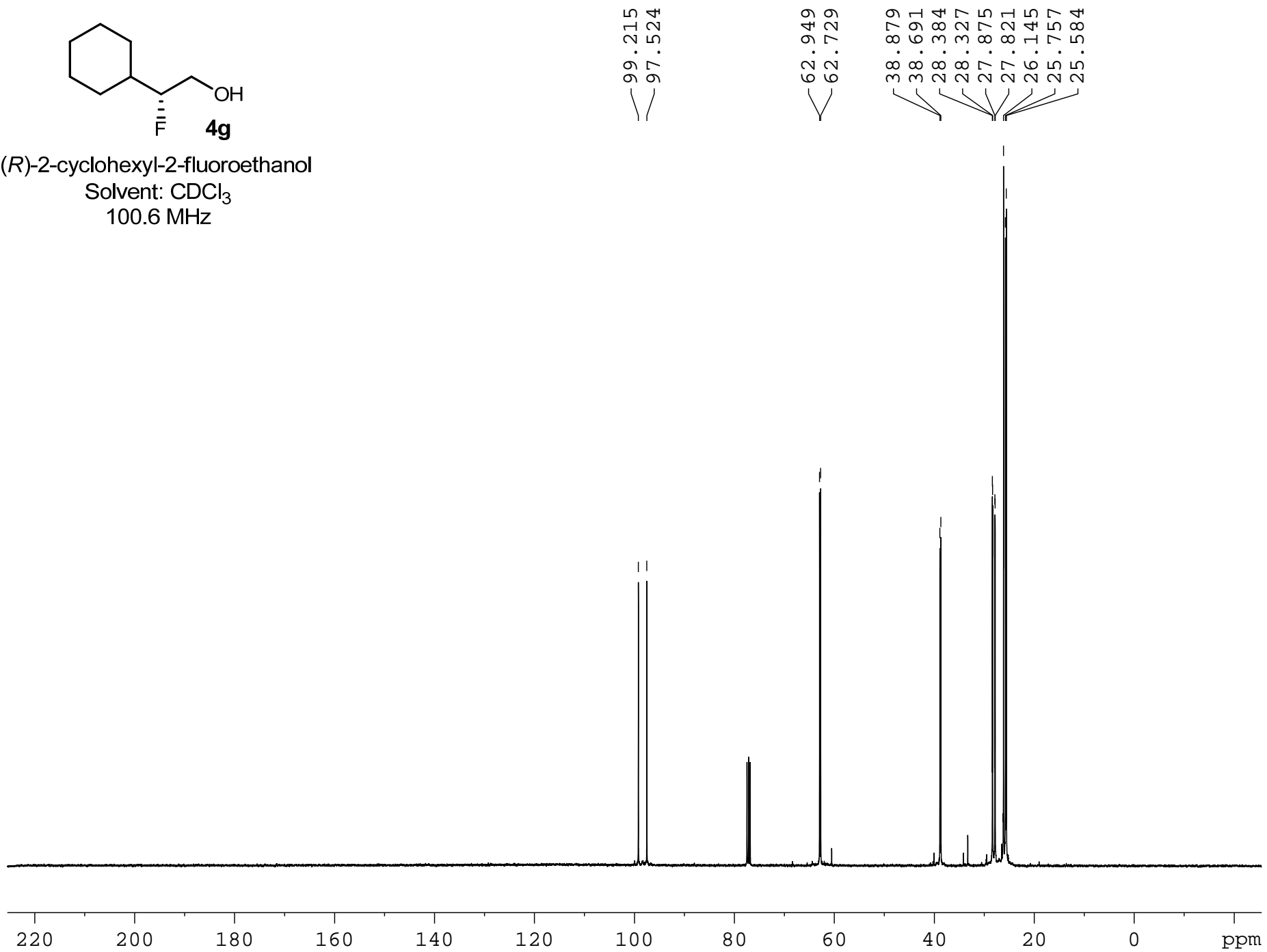


(*R*)-2-cyclohexyl-2-fluoroethanol
Solvent: CDCl₃
400.13 MHz

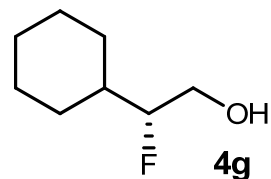




(*R*)-2-cyclohexyl-2-fluoroethanol
Solvent: CDCl₃
100.6 MHz



Elemental Composition Report



Page 1

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -0.5, max = 25.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron Ions

8 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

C: 5-500 H: 10-1000 O: 1-200 F: 1-1 Na: 1-1

MCO-IV-154

S/N: UH193

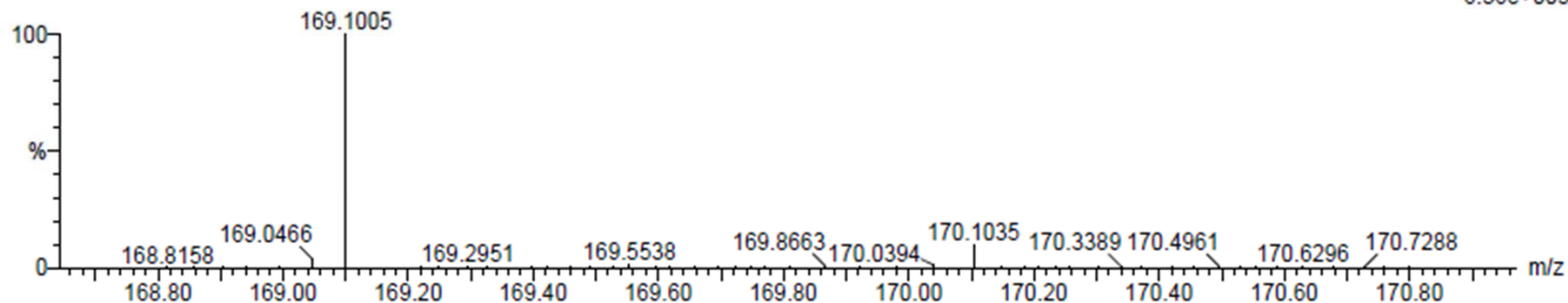
MCO-IV-154_120612_001 69 (1.287) AM (Cen,4, 80.00, Ar,8000.0,556.28,0.70); Sm (SG, 2x1.00); Cm (60:70)

06-Dec-2012

16:57:28

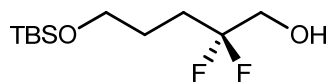
TOF MS ES+

6.36e+003



Minimum: -0.5
Maximum: 5.0 5.0 25.0

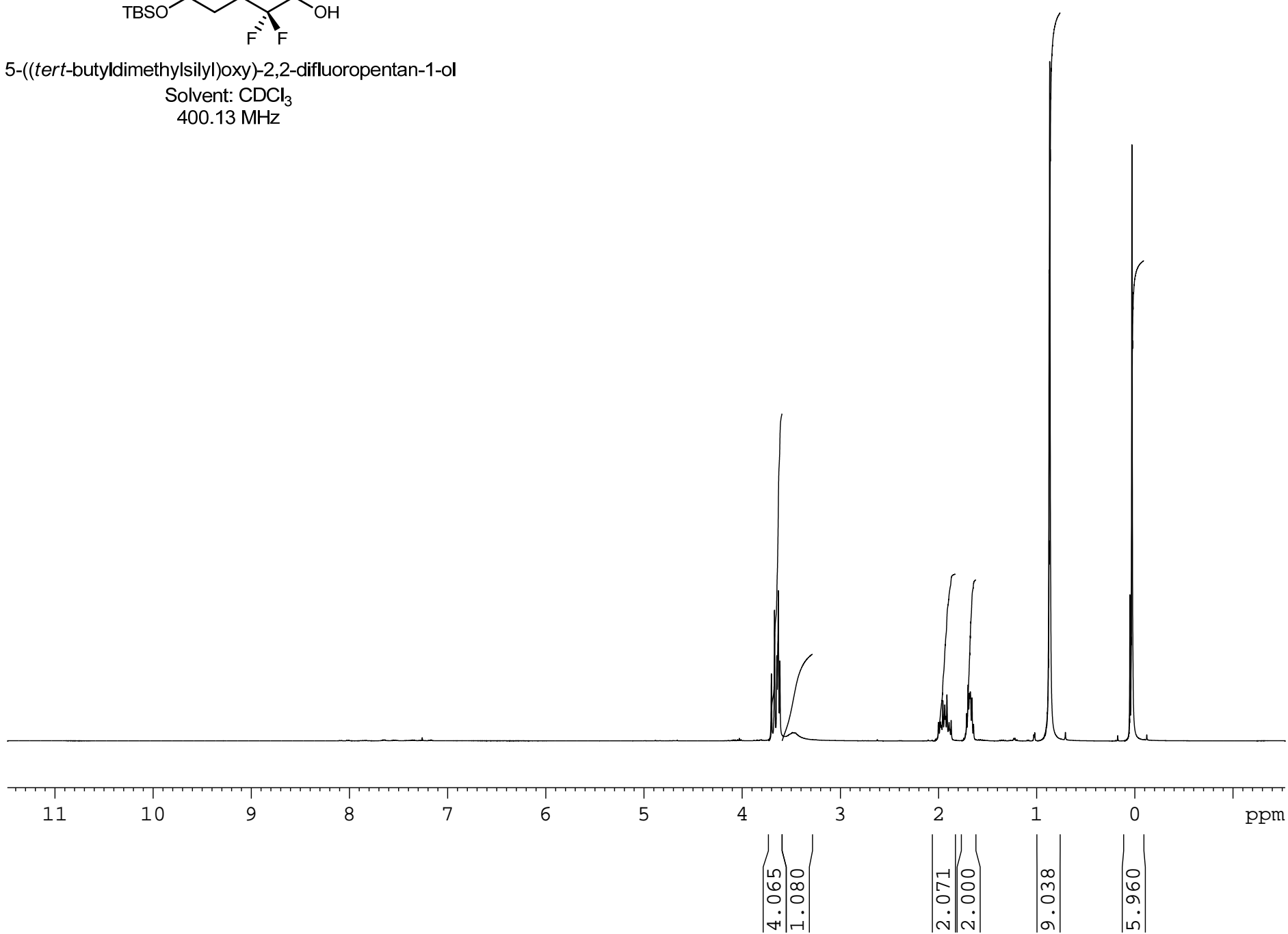
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
169.1005	169.1005	0.0	0.0	0.5	1.1	C8 H15 O F Na

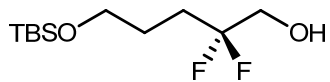


5-((*tert*-butyldimethylsilyl)oxy)-2,2-difluoropentan-1-ol

Solvent: CDCl₃

400.13 MHz





5-((*tert*-butyldimethylsilyl)oxy)-2,2-difluoropentan-1-ol

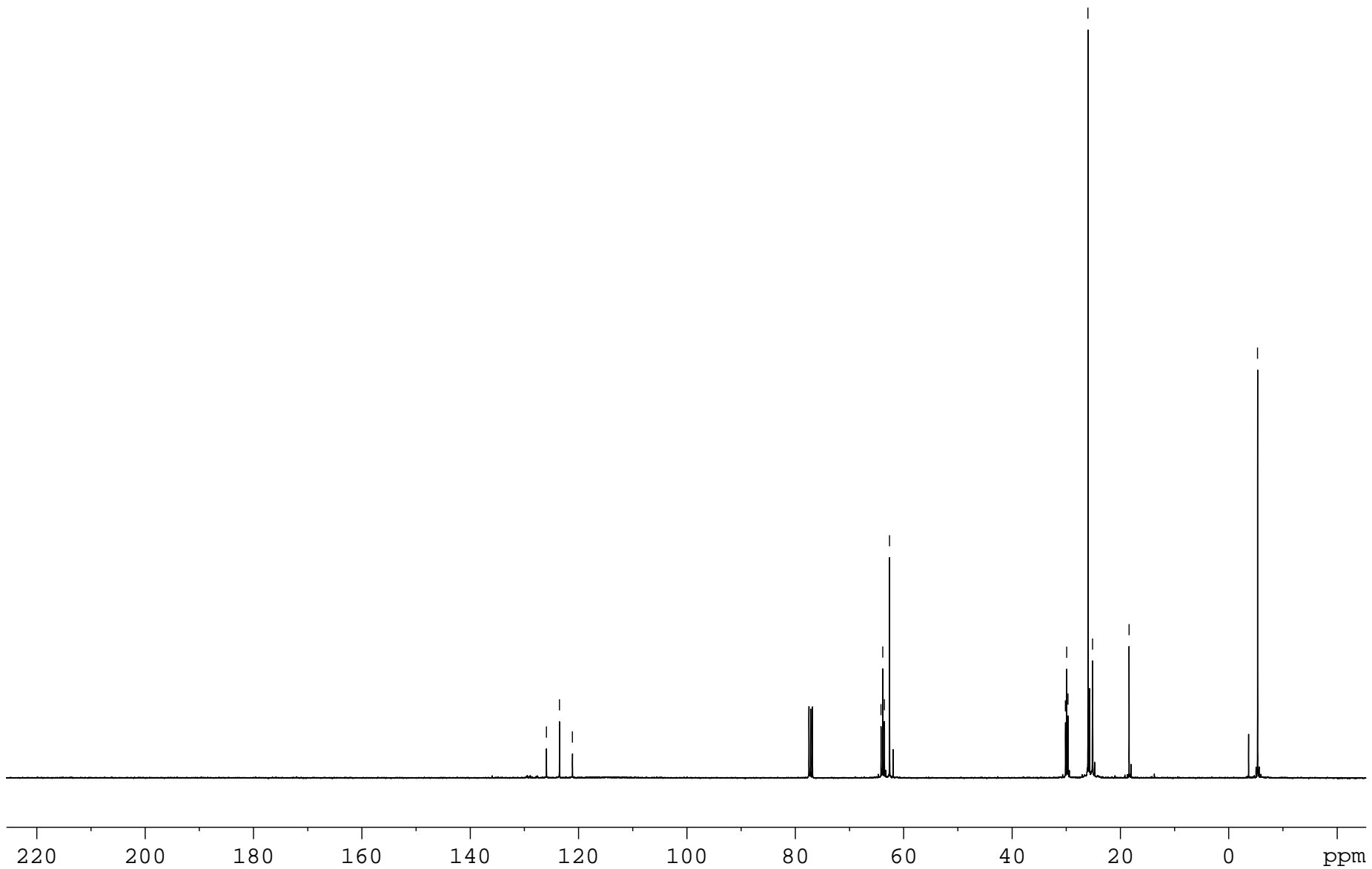
Solvent: CDCl₃
100.6 MHz

125.922
123.520
121.119

64.171
63.853
63.537
62.592

30.134
29.892
29.652
25.973
25.178
25.137
25.095
18.386

-5.336



Elemental Composition Report

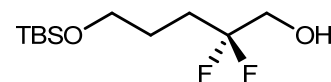
Page 1

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -0.5, max = 25.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 2



Monoisotopic Mass, Even Electron Ions

13 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

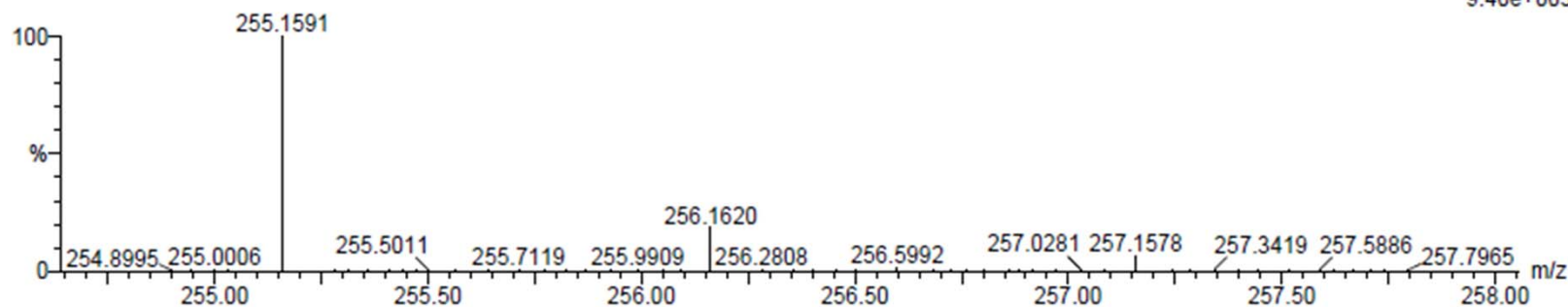
C: 10-500 H: 10-1000 O: 1-200 F: 2-2 Si: 1-1

MCO-V-15

S/N: UH193

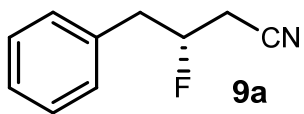
MCO-V-15_120712_001 97 (1.807) AM (Cen,4, 80.00, Ar,8000.0,556.28,0.70); Sm (SG, 2x1.00); Cm (90:100)

07-Dec-2012
11:50:46
TOF MS ES+
9.40e+003



Minimum: -0.5
Maximum: 5.0 5.0 25.0

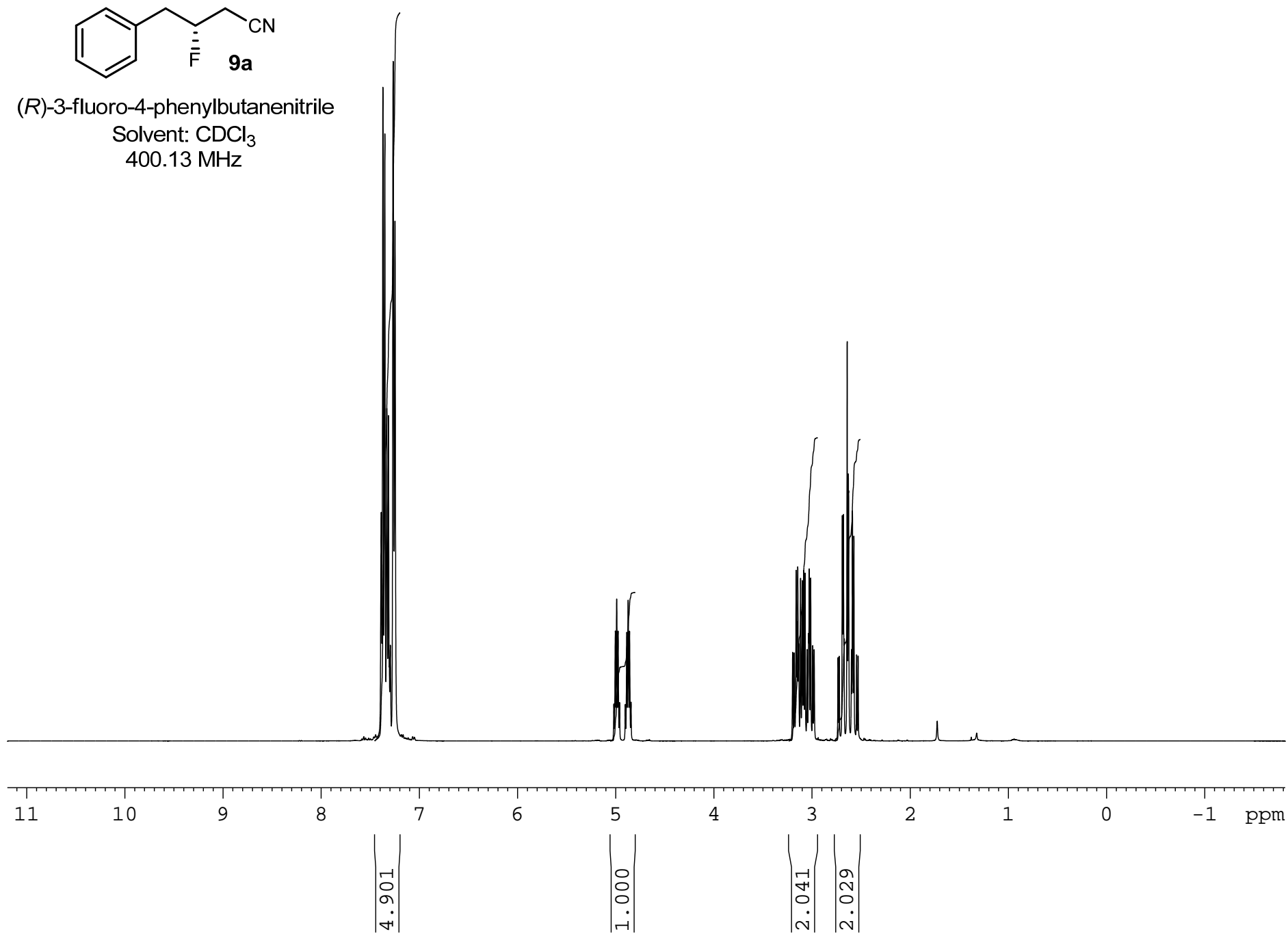
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
255.1591	255.1592	-0.1	-0.4	-0.5	0.8	C11 H25 O2 F2 Si1

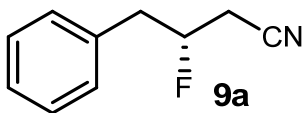


(*R*)-3-fluoro-4-phenylbutanenitrile

Solvent: CDCl₃

400.13 MHz

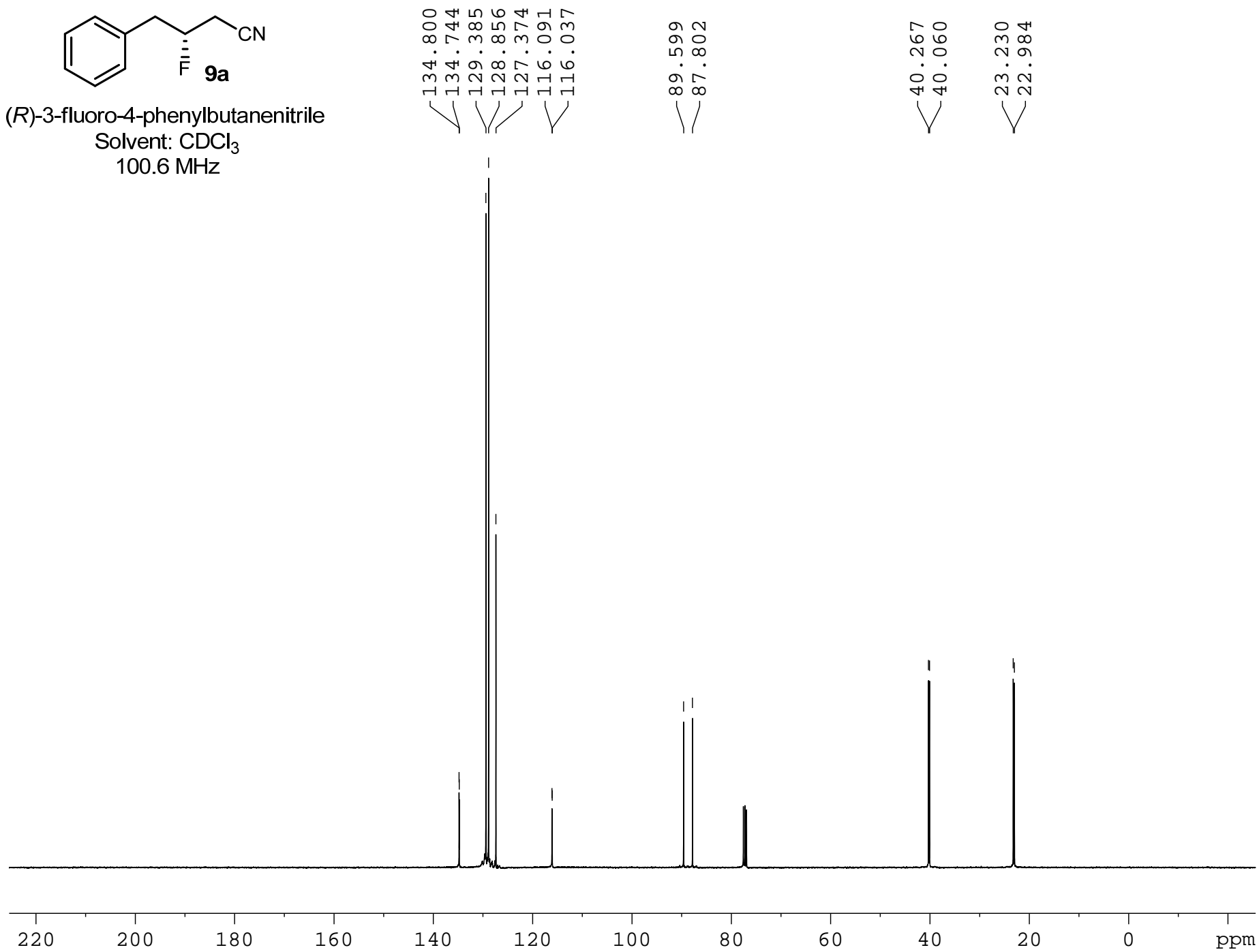




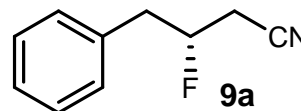
(*R*)-3-fluoro-4-phenylbutanenitrile

Solvent: CDCl₃

100.6 MHz



Elemental Composition Report



Page 1

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -0.5, max = 25.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron Ions

9 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

C: 10-500 H: 10-1000 N: 1-200 F: 1-1 Na: 1-1

MCO-IV-155

S/N: UH193

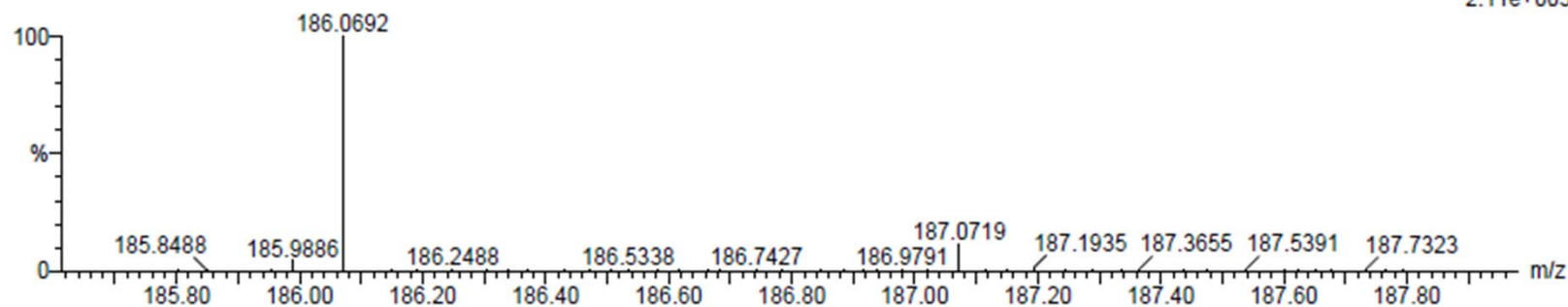
MCO-IV-155_120612_001 87 (1.621) AM (Cen,4, 80.00, Ar,8000.0,556.28,0.70); Sm (SG, 2x1.00); Cm (80:90)

06-Dec-2012

17:11:33

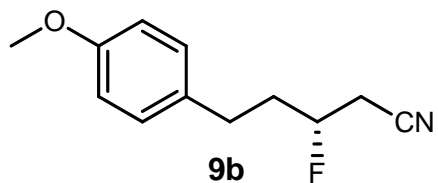
TOF MS ES+

2.11e+03

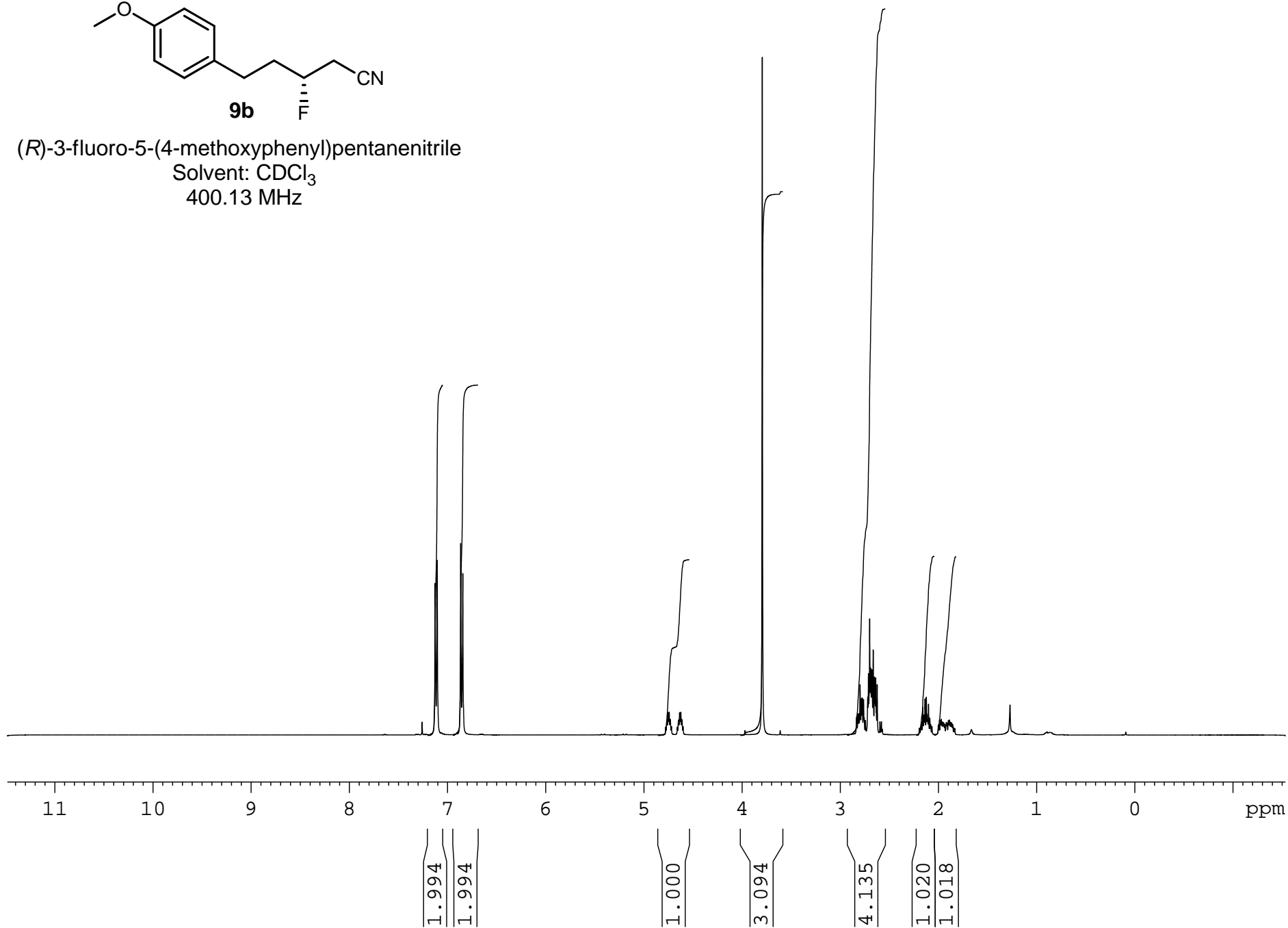


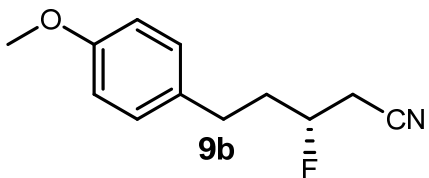
Minimum: -0.5
Maximum: 5.0 5.0 25.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
186.0692	186.0695	-0.3	-1.6	5.5	0.0	C10 H10 N F Na



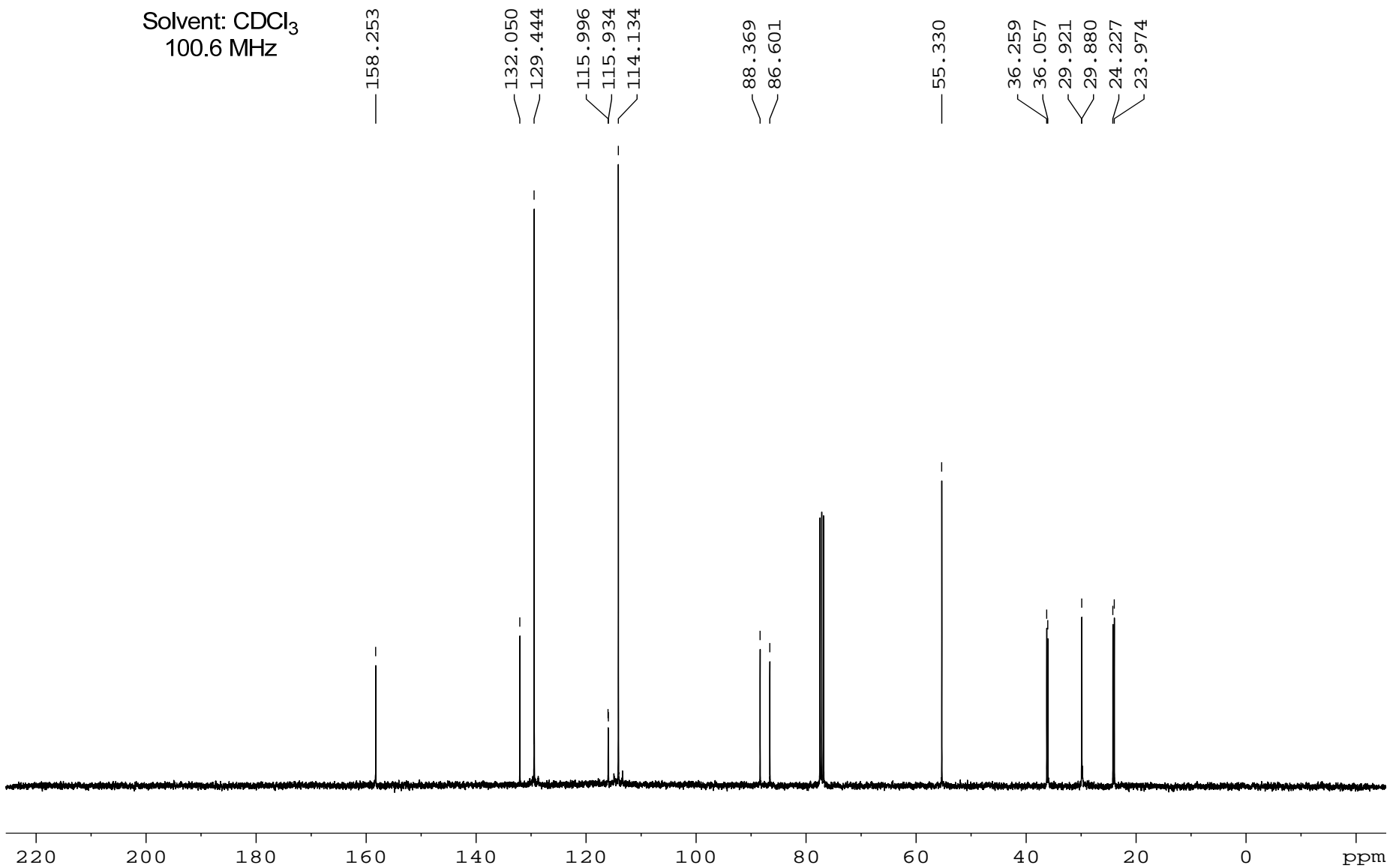
(*R*)-3-fluoro-5-(4-methoxyphenyl)pentanenitrile
Solvent: CDCl₃
400.13 MHz

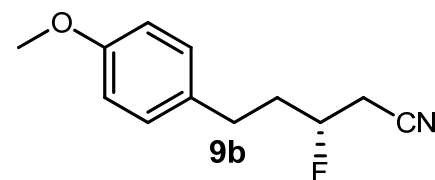




(*R*)-3-fluoro-5-(4-methoxyphenyl)pentanenitrile

Solvent: CDCl₃
100.6 MHz





Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -0.5, max = 25.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron Ions

155 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

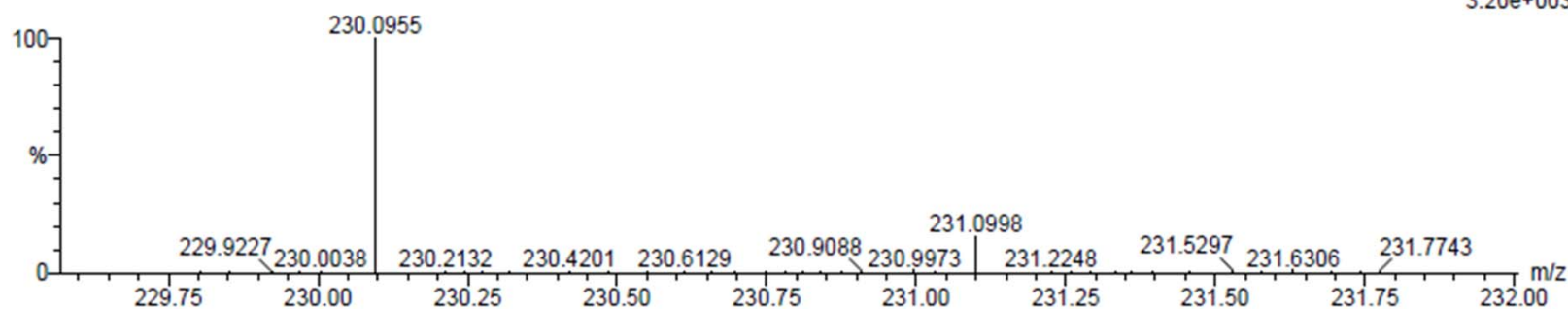
C: 10-500 H: 10-1000 N: 1-200 O: 1-200 F: 1-1 Na: 0-1

MCO-IV-150

S/N: UH193

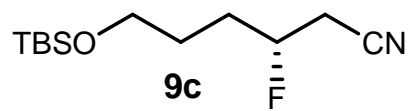
MCO-IV-150_120612_001 60 (1.121) AM (Cen,4, 80.00, Ar,8000.0,556.28,0.70); Sm (SG, 2x1.00); Cm (50:60)

06-Dec-2012
14:26:21
TOF MS ES+
3.20e+003



Minimum: -0.5
Maximum: 5.0 5.0 25.0

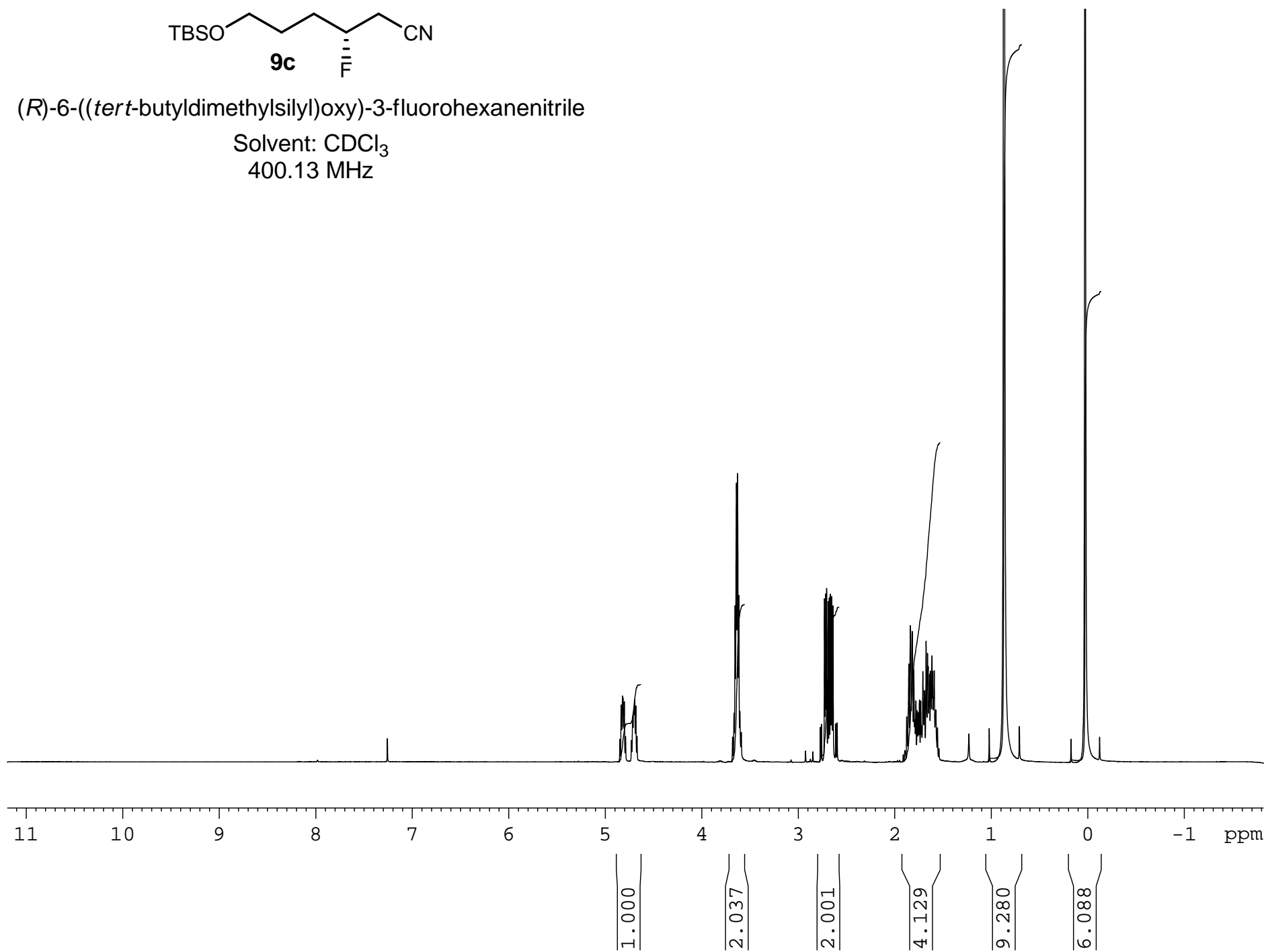
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
230.0955	230.0957	-0.2	-0.9	5.5	2.9	C12 H14 N O F Na

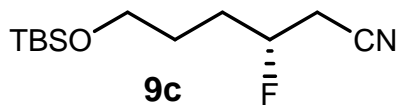


(*R*)-6-((*tert*-butyldimethylsilyl)oxy)-3-fluorohexanenitrile

Solvent: CDCl₃

400.13 MHz





(*R*)-6-((*tert*-butyldimethylsilyl)oxy)-3-fluorohexanenitrile

Solvent: CDCl₃

100.6 MHz

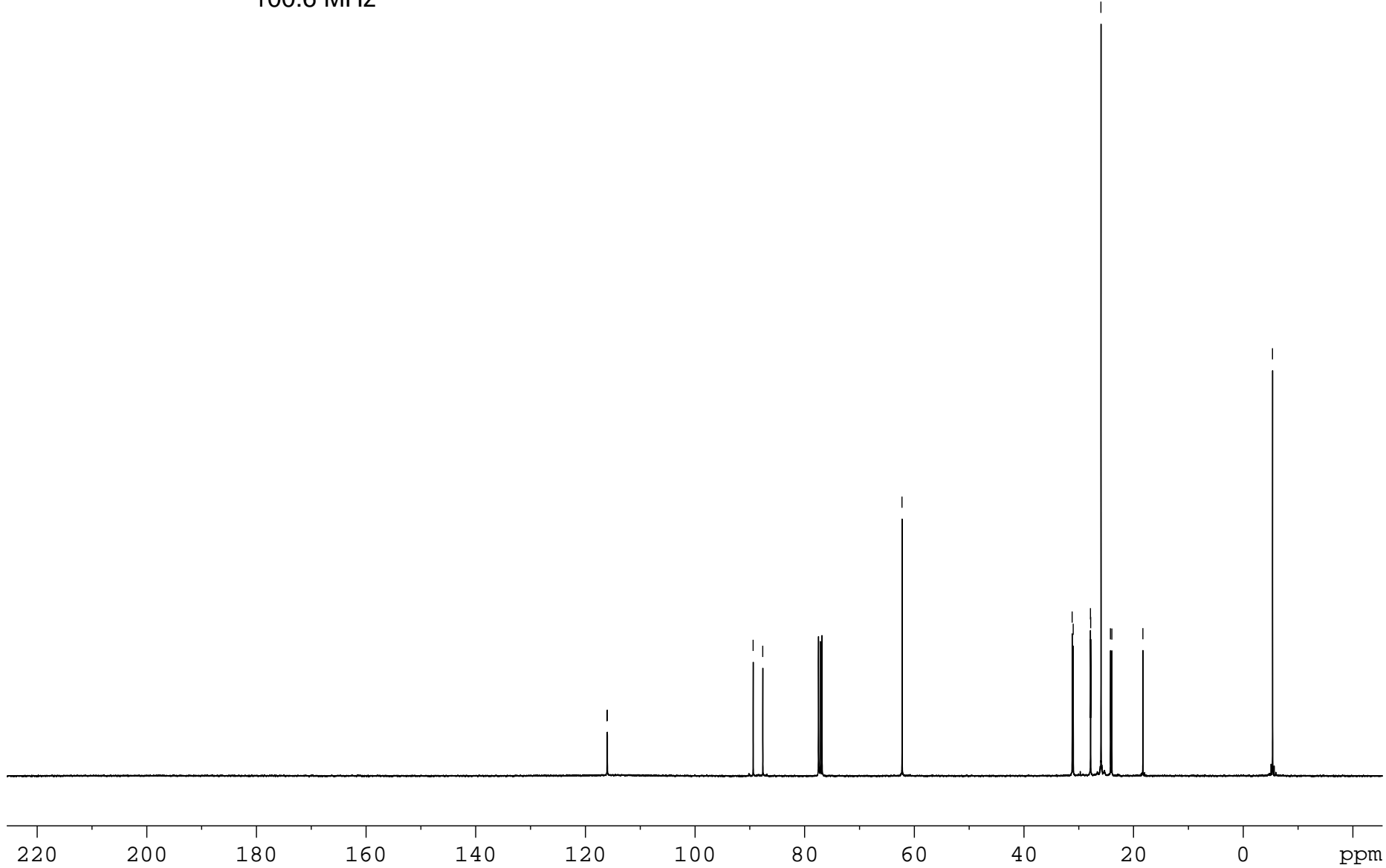
116.061
116.003

89.396
87.633

62.240

31.206
31.003
27.867
27.824
25.941
24.210
23.958
18.300

5.350



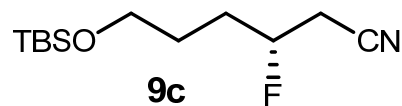
Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -0.5, max = 25.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 2



Page 1

Monoisotopic Mass, Even Electron Ions

76 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

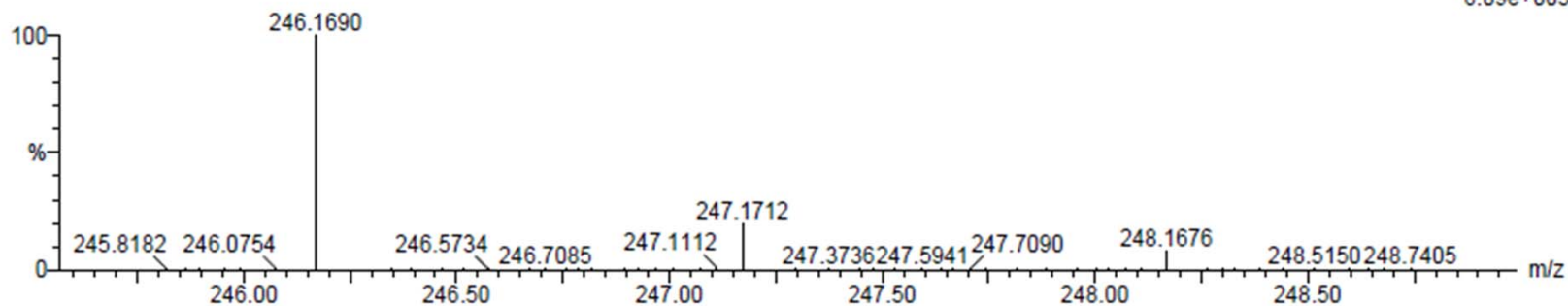
C: 10-500 H: 10-1000 N: 1-200 O: 1-200 F: 1-1 Si: 1-1

MCO-IV-171

S/N: UH193

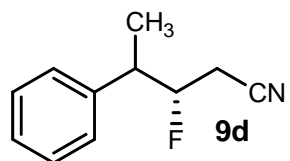
MCO-IV-171_120712_001 60 (1.120) AM (Cen,4, 80.00, Ar,8000.0,556.28,0.70); Sm (SG, 2x1.00); Cm (60:70)

07-Dec-2012
10:58:05
TOF MS ES+
6.09e+003

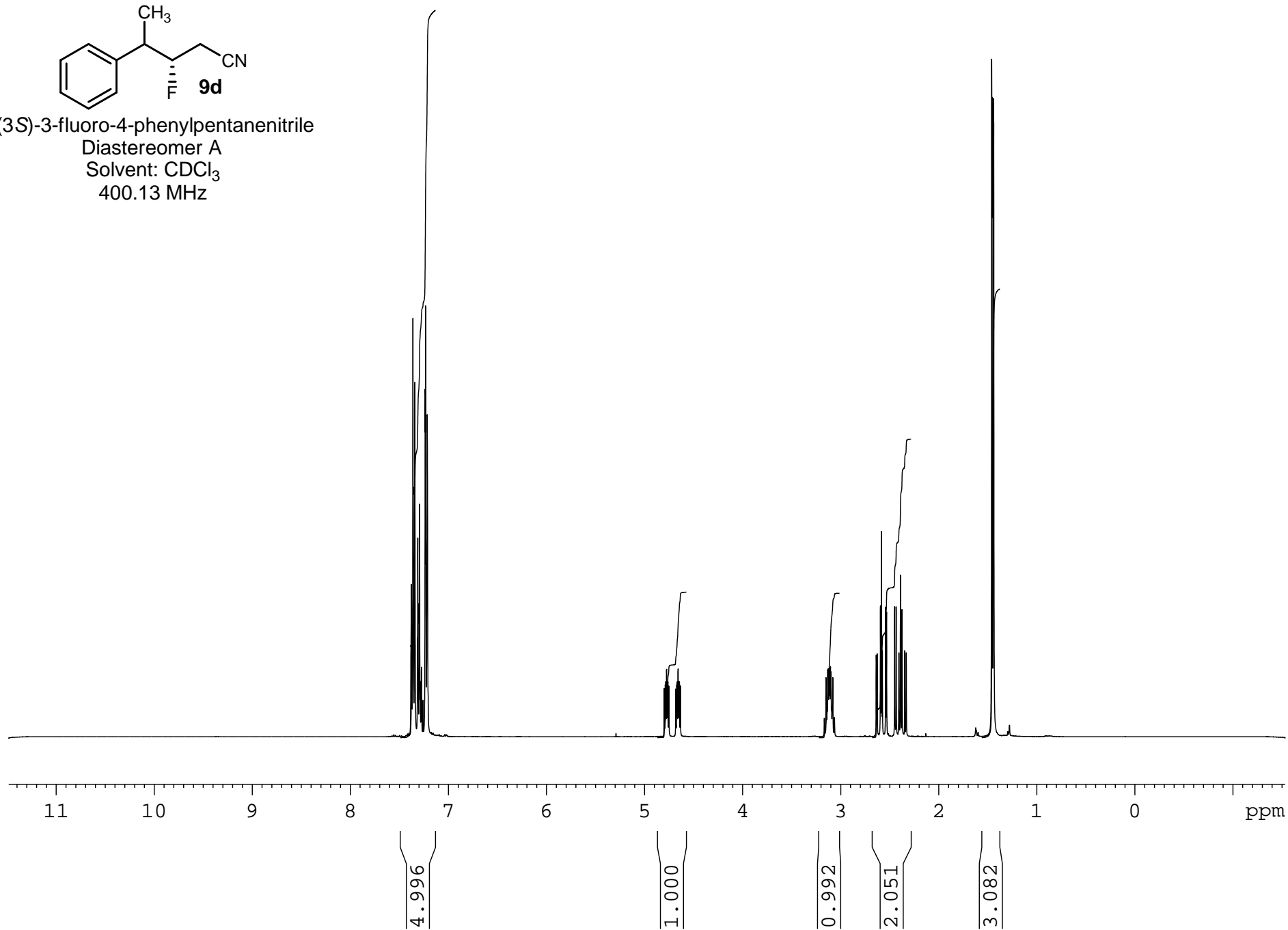


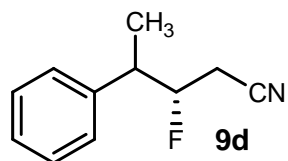
Minimum: -0.5
Maximum: 5.0 5.0 25.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
246.1690	246.1689	0.1	0.4	1.5	0.5	C12 H25 N O F Si

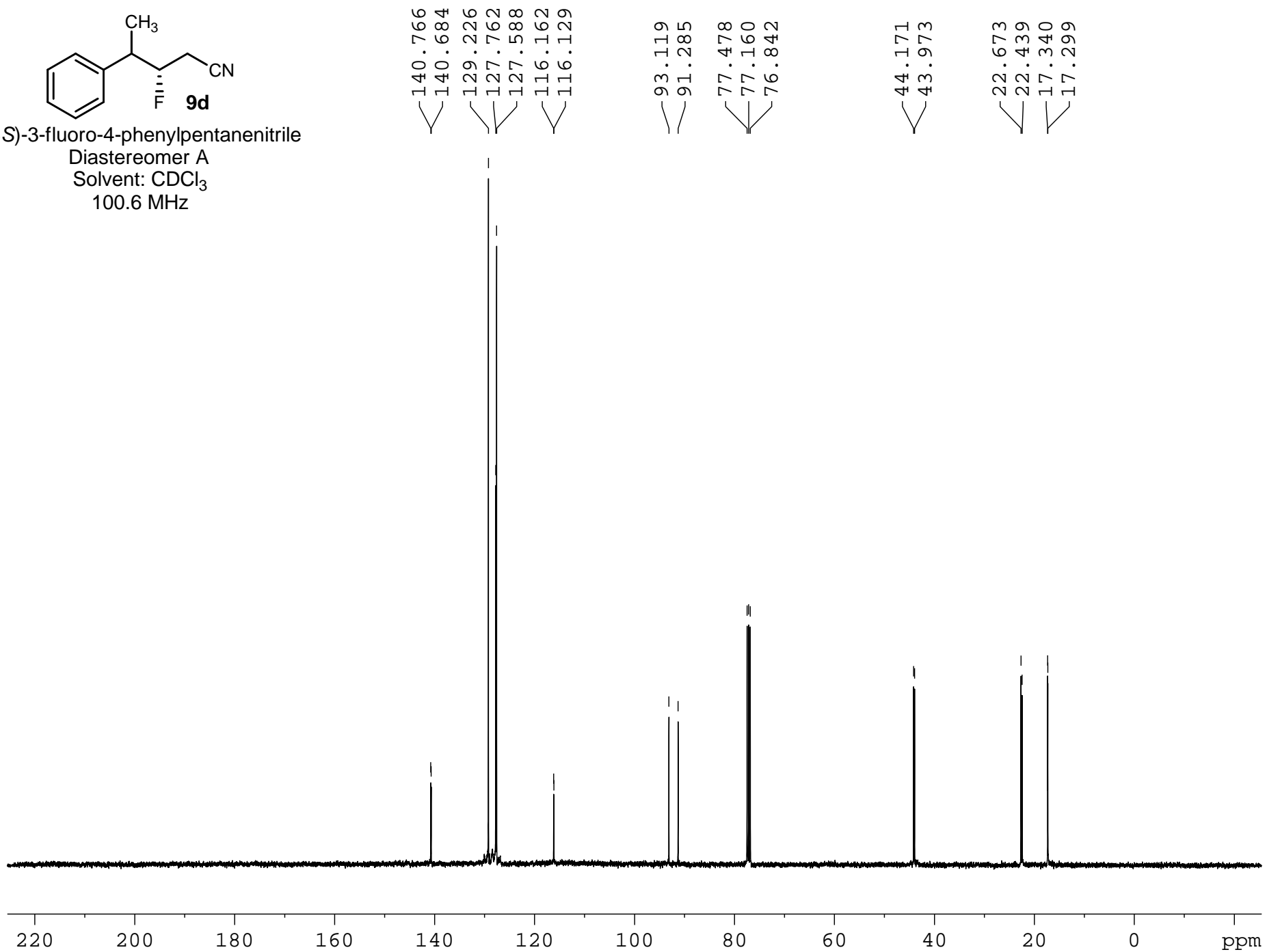


(3S)-3-fluoro-4-phenylpentanenitrile
Diastereomer A
Solvent: CDCl₃
400.13 MHz





(3S)-3-fluoro-4-phenylpentanenitrile
Diastereomer A
Solvent: CDCl₃
100.6 MHz



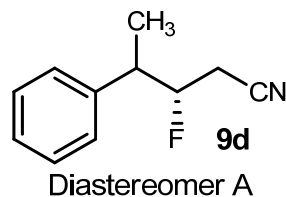
Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -0.5, max = 25.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 2



Page 1

Monoisotopic Mass, Even Electron Ions

11 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

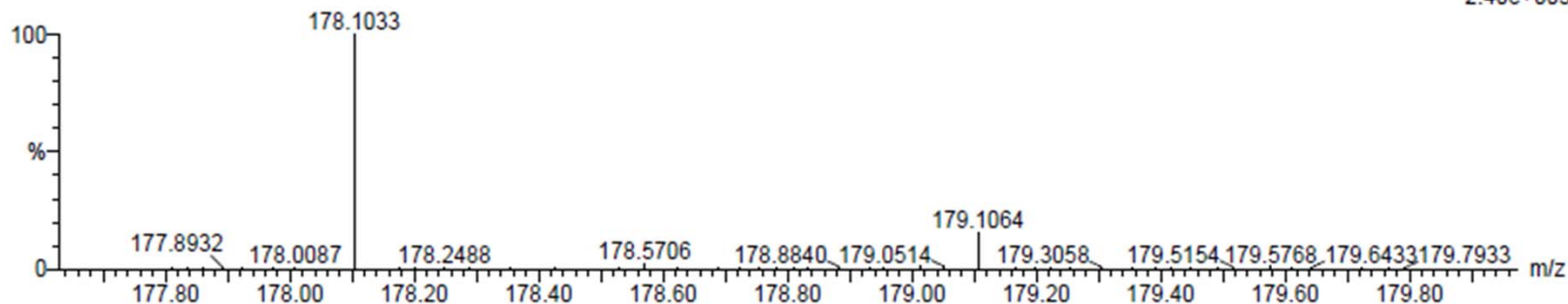
C: 10-500 H: 10-1000 N: 1-200 F: 1-1

MCO-IV-160

S/N: UH193

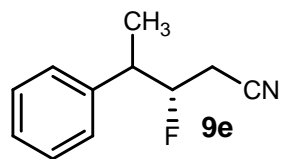
MCO-IV-160_120712_001 52 (0.972) AM (Cen,4, 80.00, Ar,8000.0,556.28,0.70); Sm (SG, 2x1.00); Cm (50:60)

07-Dec-2012
09:28:39
TOF MS ES+
2.40e+003

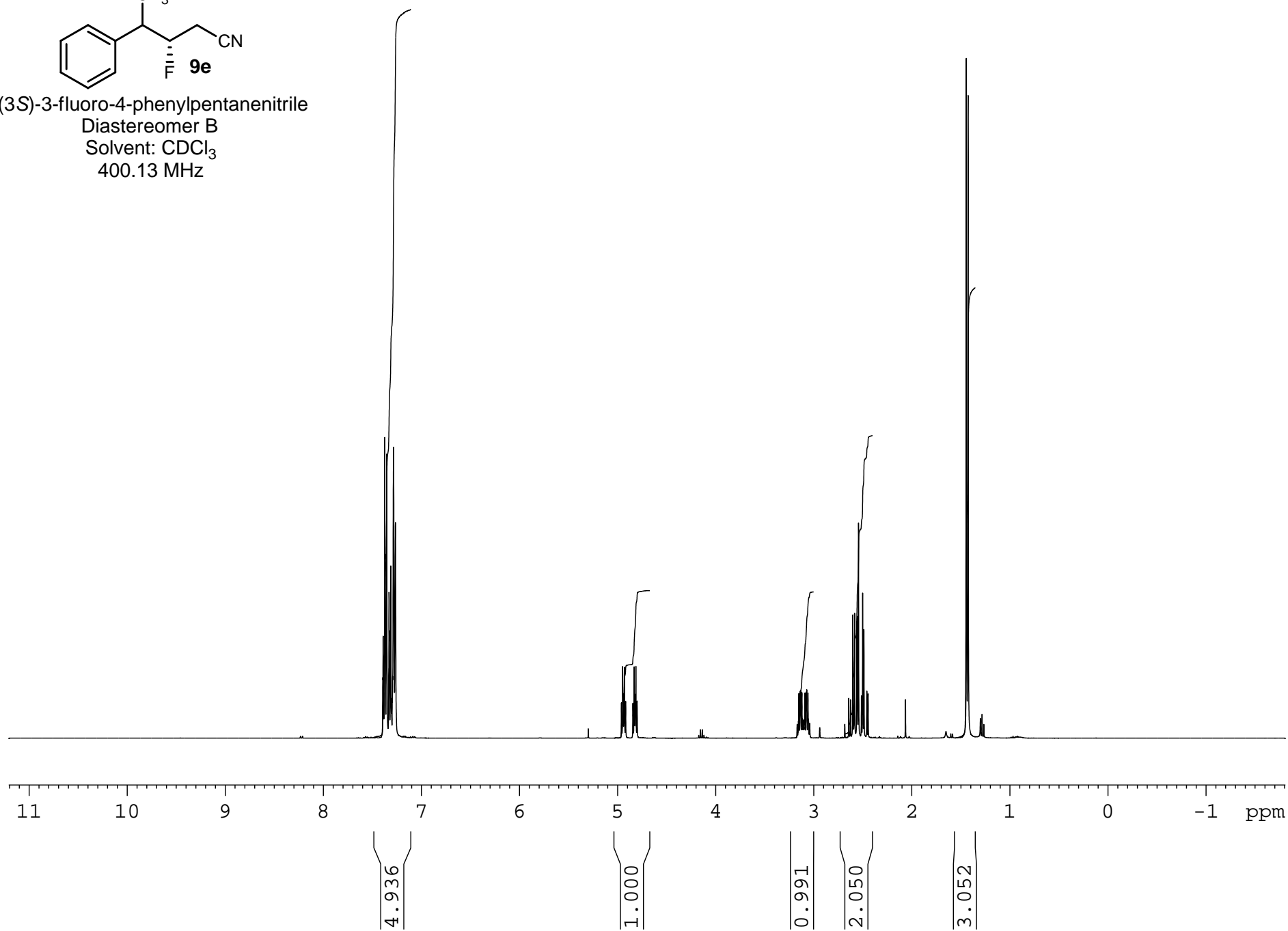


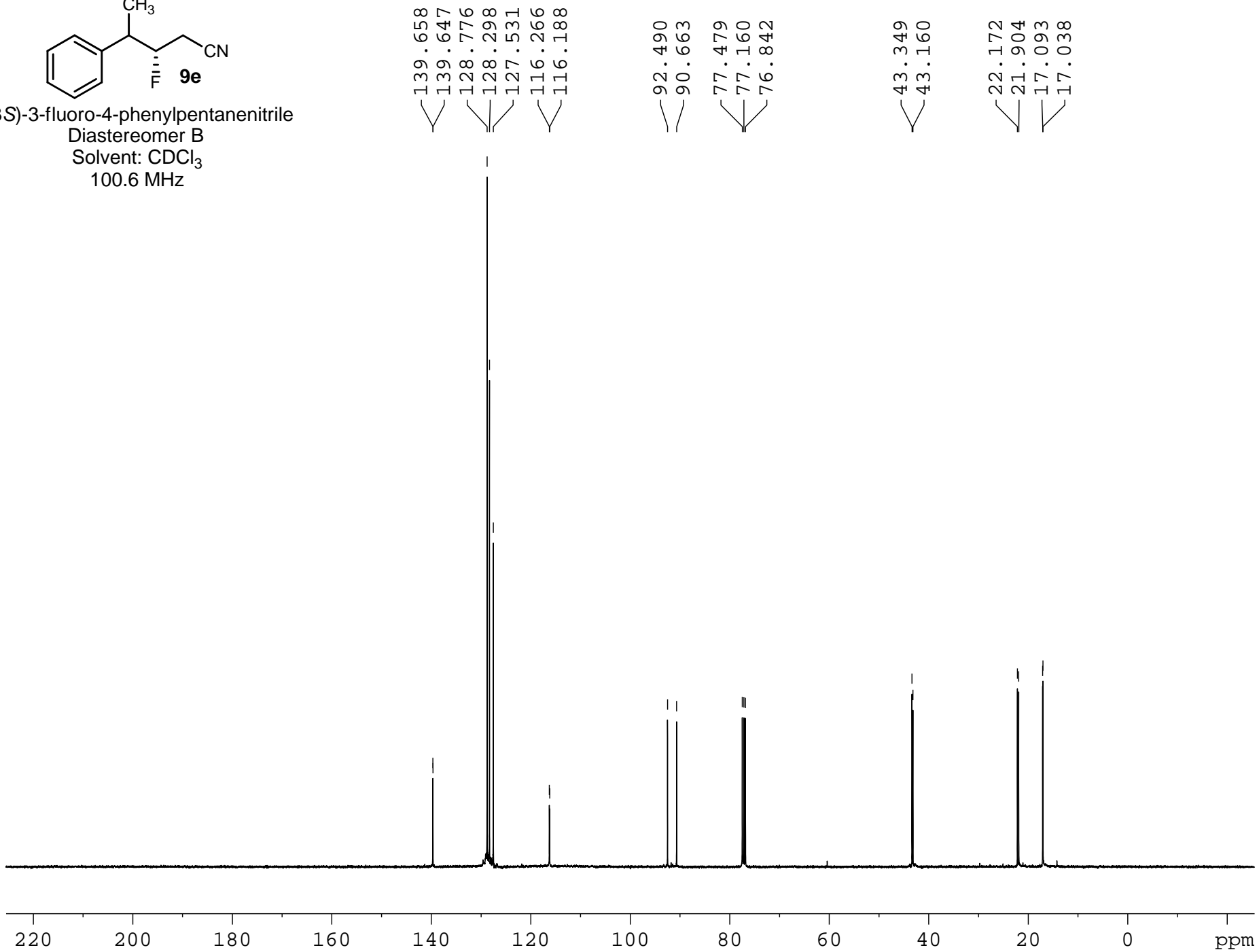
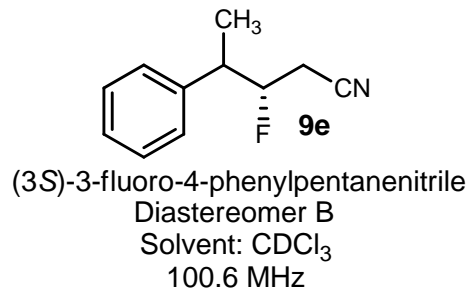
Minimum: -0.5
Maximum: 5.0 5.0 25.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
178.1033	178.1032	0.1	0.6	5.5	3.9	C11 H13 N F



(3S)-3-fluoro-4-phenylpentanenitrile
Diastereomer B
Solvent: CDCl₃
400.13 MHz





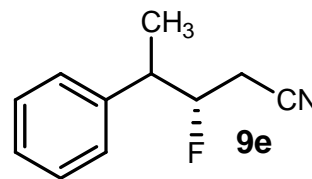
Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -0.5, max = 25.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 2



Diastereomer B

Page 1

Monoisotopic Mass, Even Electron Ions

11 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

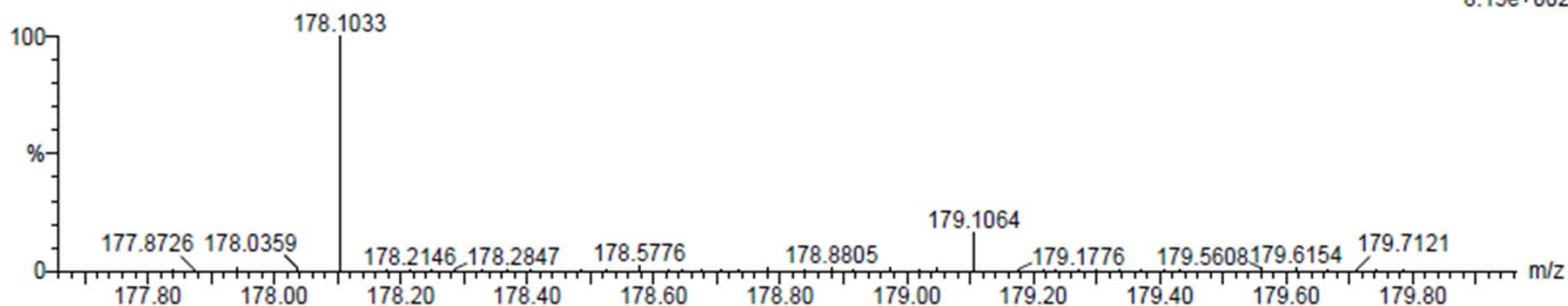
C: 10-500 H: 10-1000 N: 1-200 F: 1-1

MCO-IV-161

S/N: UH193

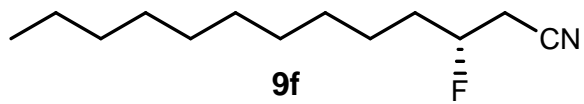
MCO-IV-161_120712_001 80 (1.492) AM (Cen,4, 80.00, Ar,8000.0,556.28,0.70); Sm (SG, 2x1.00); Cm (80:90)

07-Dec-2012
09:40:43
TOF MS ES+
8.15e+002

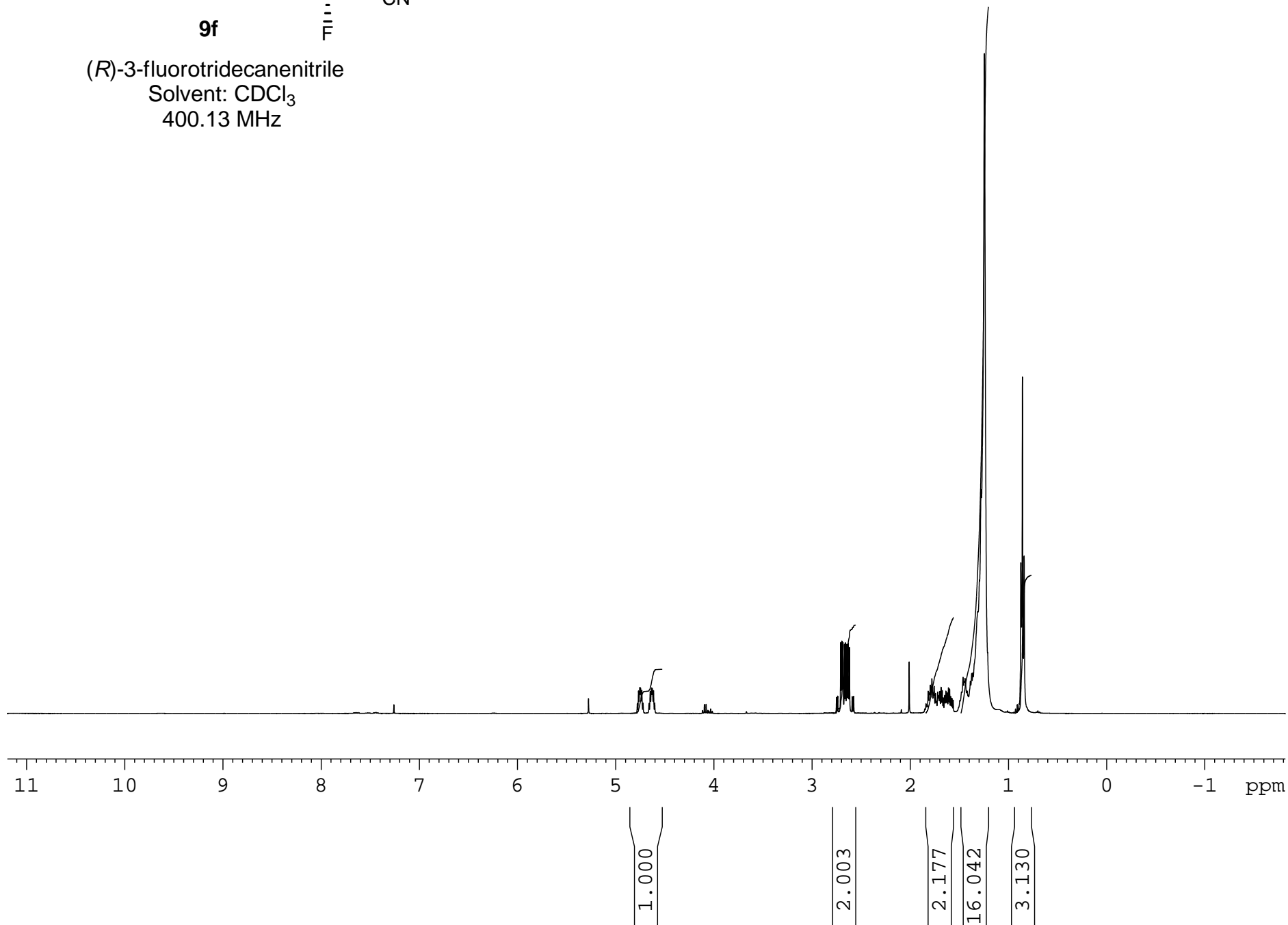


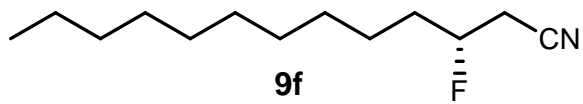
Minimum: -0.5
Maximum: 5.0 5.0 25.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
178.1033	178.1032	0.1	0.6	5.5	2.5	C11 H13 N F



(*R*)-3-fluorotridecanenitrile
Solvent: CDCl₃
400.13 MHz



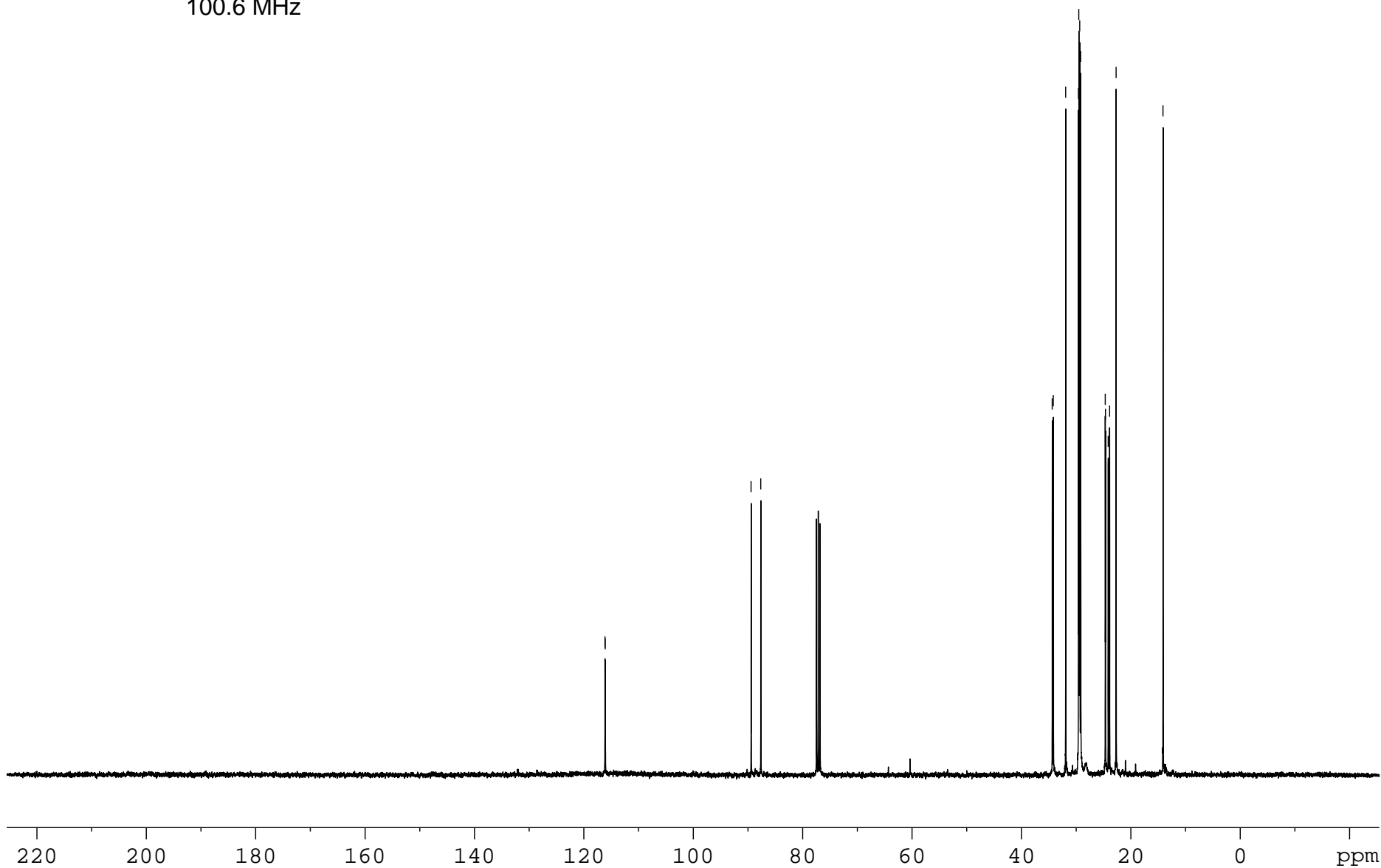


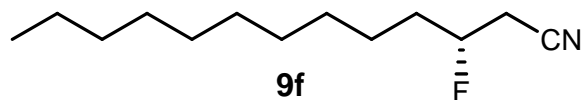
9f
(R)-3-fluorotridecanenitrile
Solvent: CDCl₃
100.6 MHz

116.139
116.078

89.424
87.661

34.374
34.174
31.916
29.583
29.516
29.406
29.335
29.171
24.684
24.641
24.144
23.889
22.700
14.114





Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -0.5, max = 25.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron Ions

37 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

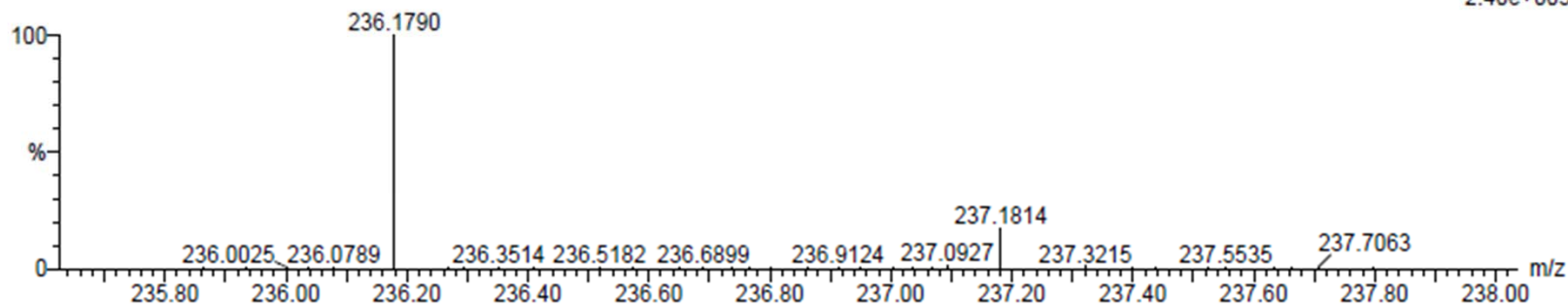
C: 10-500 H: 10-1000 N: 1-200 F: 1-1 Na: 0-1

MCO-IV-149

S/N: UH193

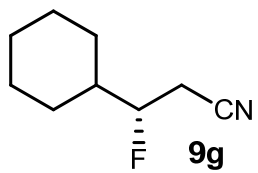
MCO-IV-149_120612_001 72 (1.343) AM (Cen,4, 80.00, Ar,8000.0,556.28,0.70); Sm (SG, 2x1.00); Cm (70:80)

06-Dec-2012
14:14:20
TOF MS ES+
2.40e+003



Minimum: -0.5
Maximum: 5.0 5.0 25.0

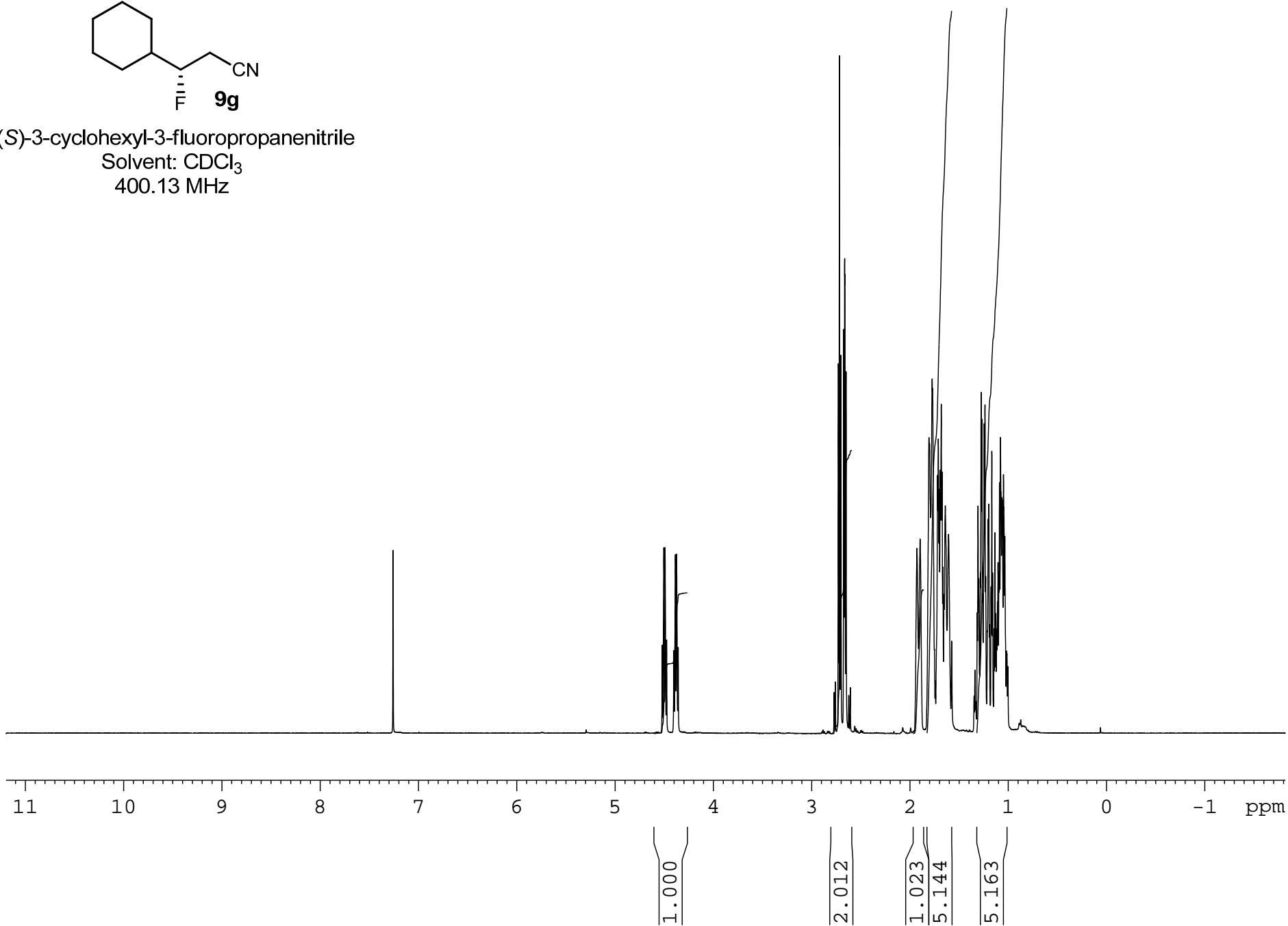
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
236.1790	236.1790	0.0	0.0	1.5	2.1	C13 H24 N F Na

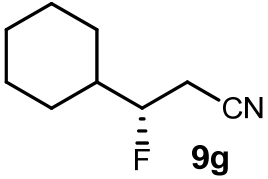


(S)-3-cyclohexyl-3-fluoropropanenitrile

Solvent: CDCl₃

400.13 MHz



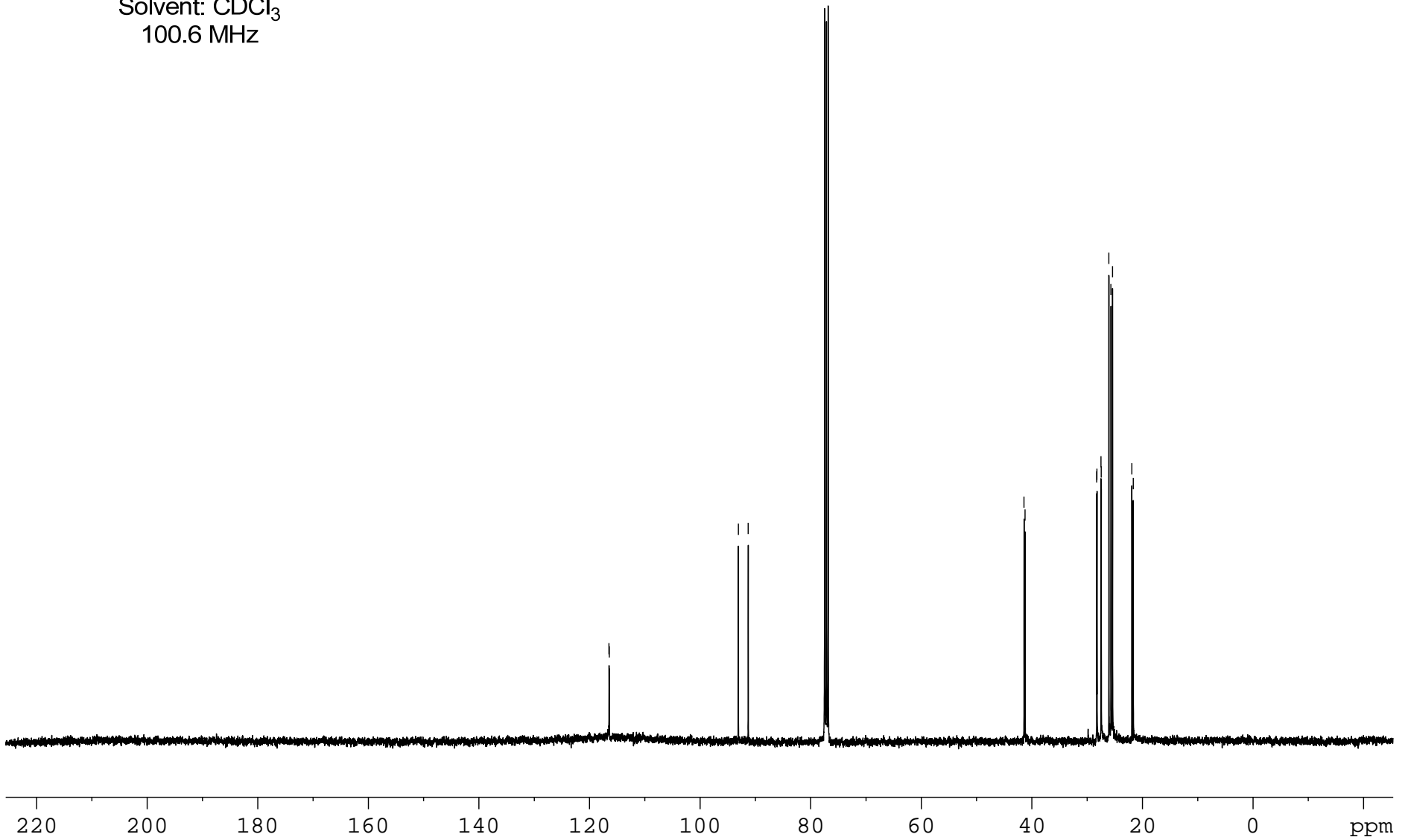


(S)-3-cyclohexyl-3-fluoropropanenitrile
Solvent: CDCl₃
100.6 MHz

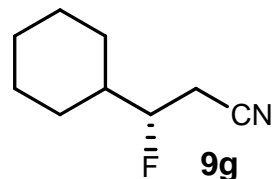
116.473
116.419

93.068
91.282

41.402
41.215
28.257
28.201
27.478
27.429
26.050
25.676
25.414
21.916
21.659



Elemental Composition Report



Page 1

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -0.5, max = 25.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron Ions

11 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

C: 5-500 H: 10-1000 N: 1-200 F: 1-1 Na: 1-1

MCO-IV-157

S/N: UH193

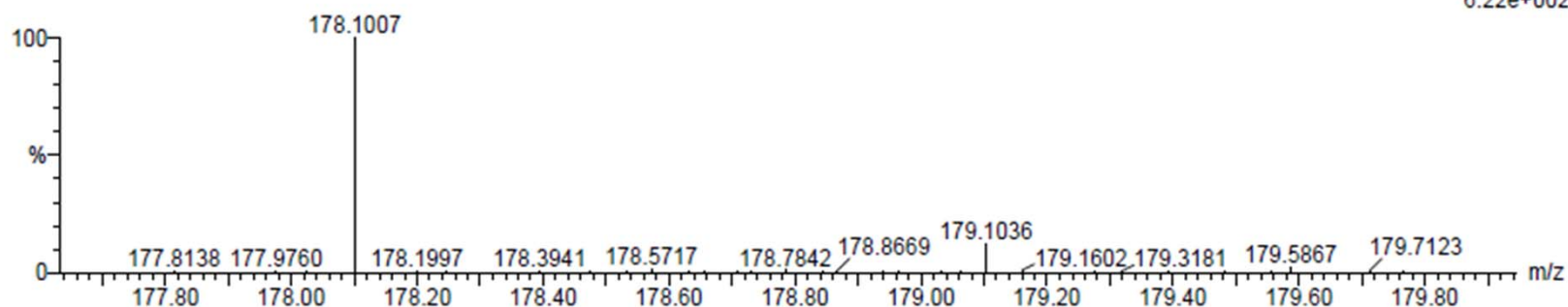
MCO-IV-157_120612_001 50 (0.935) AM (Cen,4, 80.00, Ar,8000.0,556.28,0.70); Sm (SG, 2x1.00); Cm (40:50)

06-Dec-2012

17:26:07

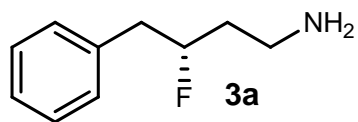
TOF MS ES+

6.22e+002



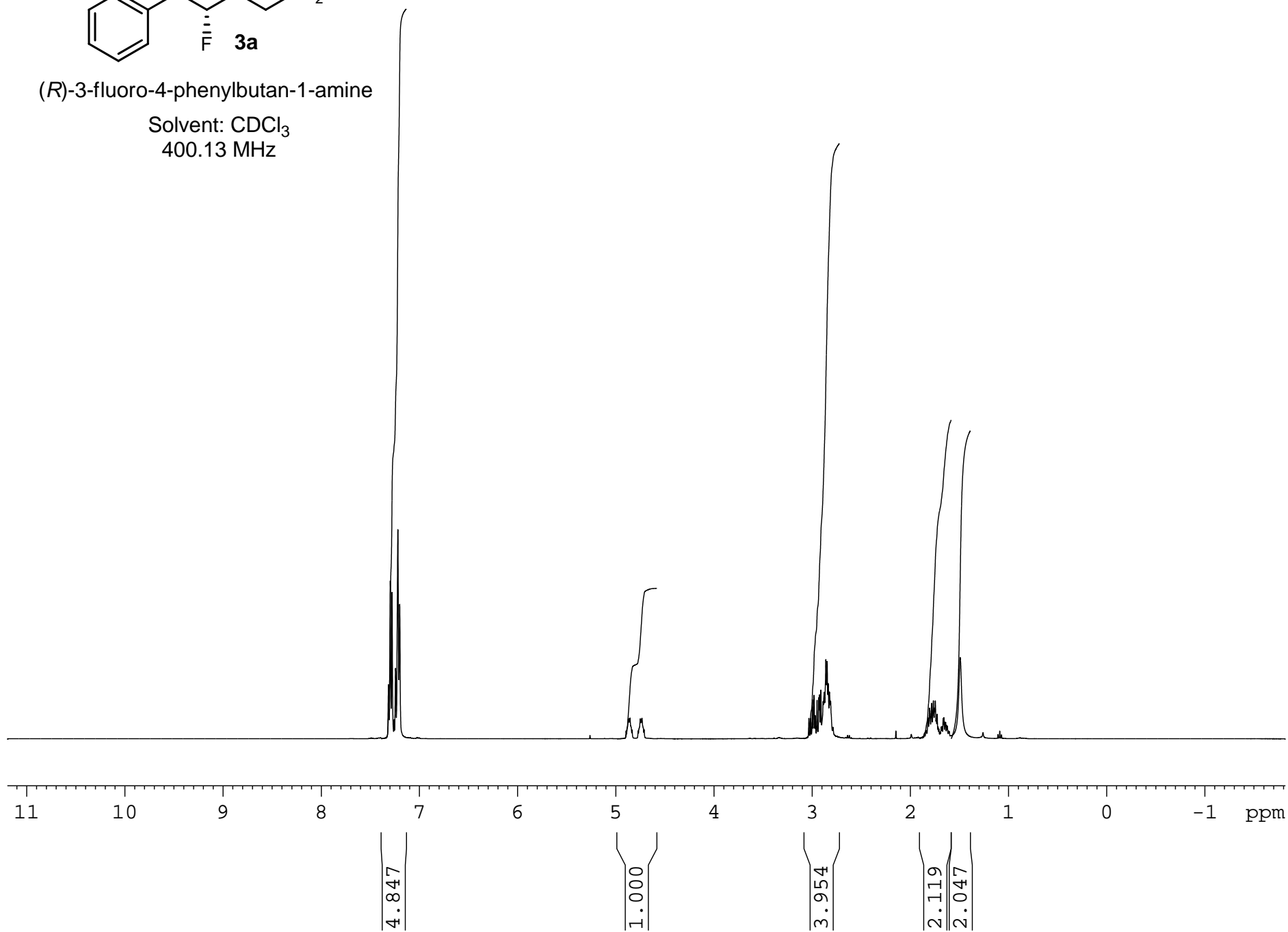
Minimum: -0.5
Maximum: 5.0 5.0 25.0

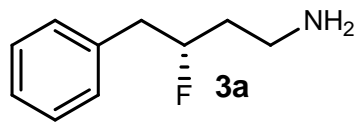
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
178.1007	178.1008	-0.1	-0.6	2.5	0.4	C9 H14 N F Na



(*R*)-3-fluoro-4-phenylbutan-1-amine

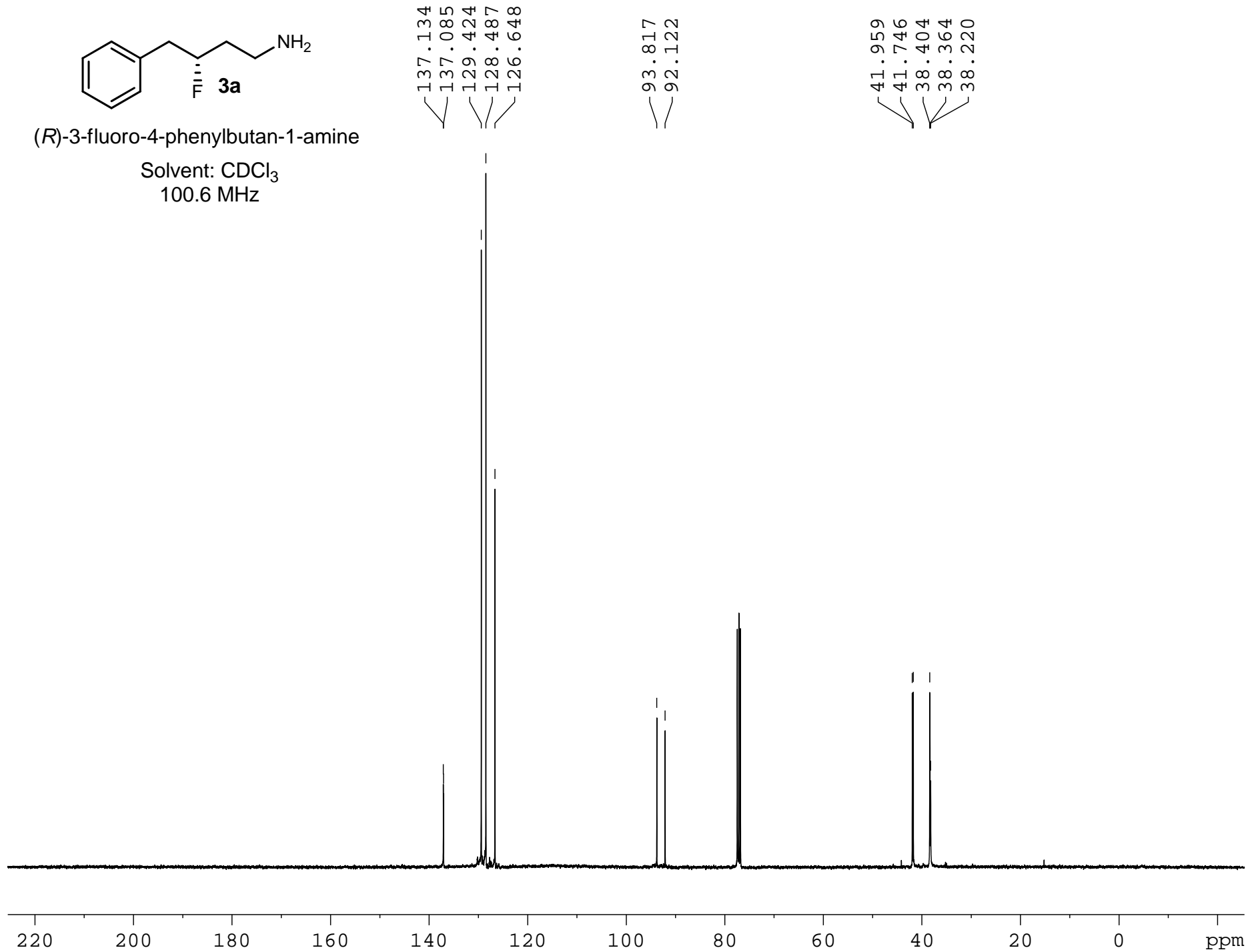
Solvent: CDCl₃
400.13 MHz





(*R*)-3-fluoro-4-phenylbutan-1-amine

Solvent: CDCl₃
100.6 MHz



Elemental Composition Report

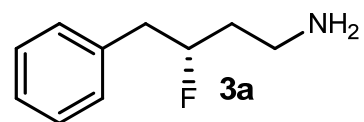
Page 1

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -0.5, max = 25.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 2



Monoisotopic Mass, Even Electron Ions

9 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

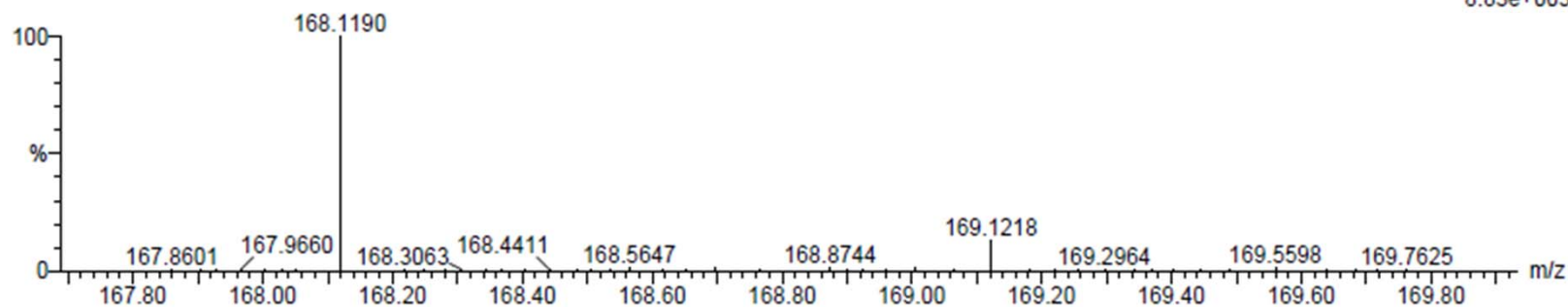
C: 10-500 H: 10-1000 N: 1-200 F: 1-1

MCO-IV-169

S/N: UH193

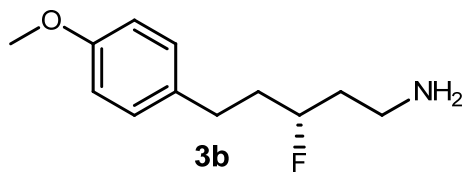
MCO-IV-169_120712_001 93 (1.733) AM (Cen,4, 80.00, Ar,8000.0,556.28,0.70); Sm (SG, 2x1.00); Cm (90:100)

07-Dec-2012
10:37:01
TOF MS ES+
8.83e+003



Minimum: -0.5
Maximum: 5.0 5.0 25.0

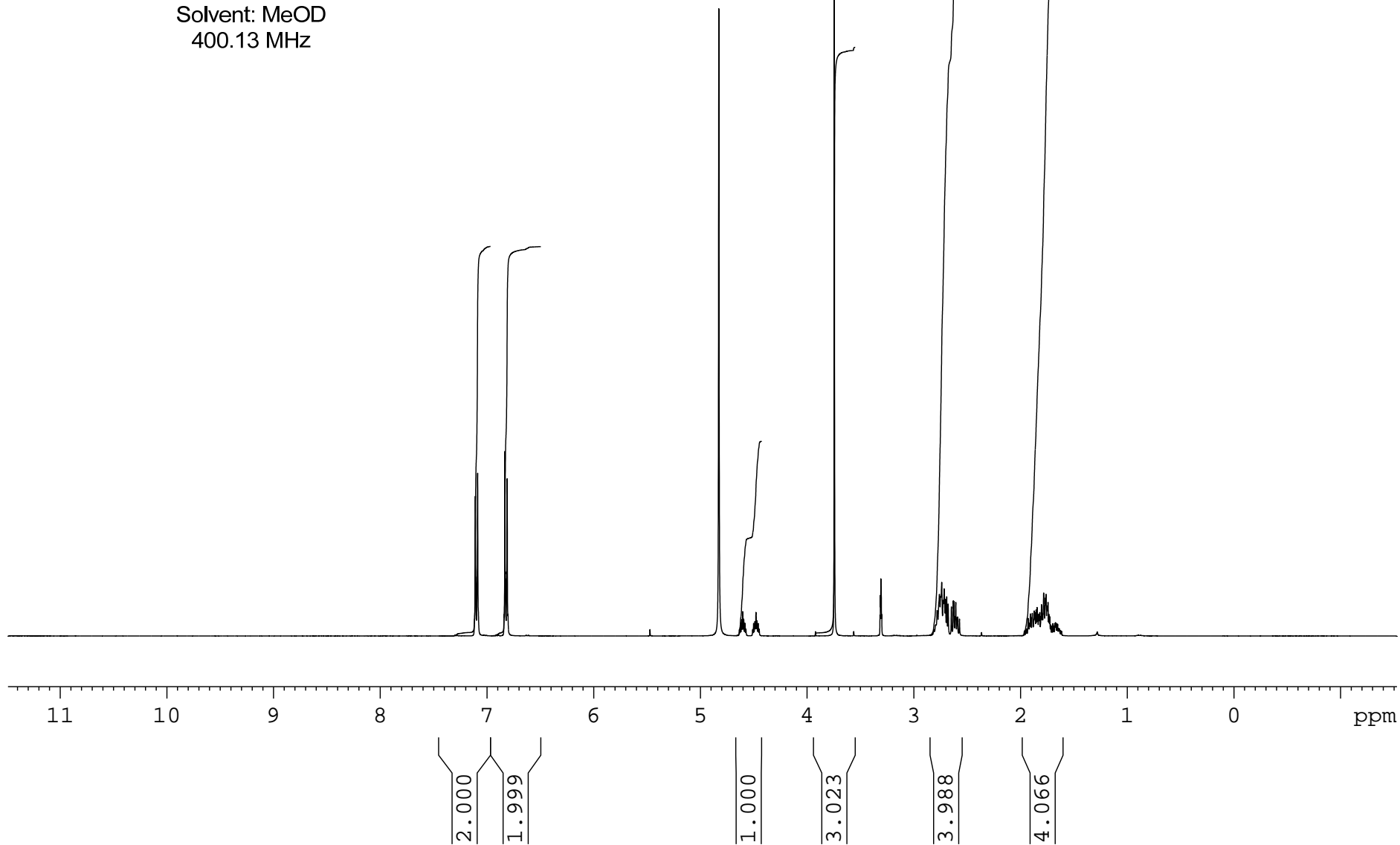
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
168.1190	168.1189	0.1	0.6	3.5	6.2	C10 H15 N F

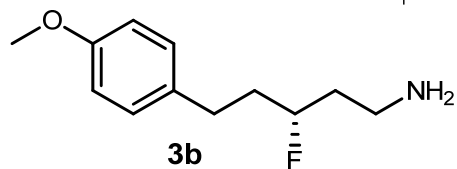


(*R*)-3-fluoro-5-(4-methoxyphenyl)pentan-1-amine

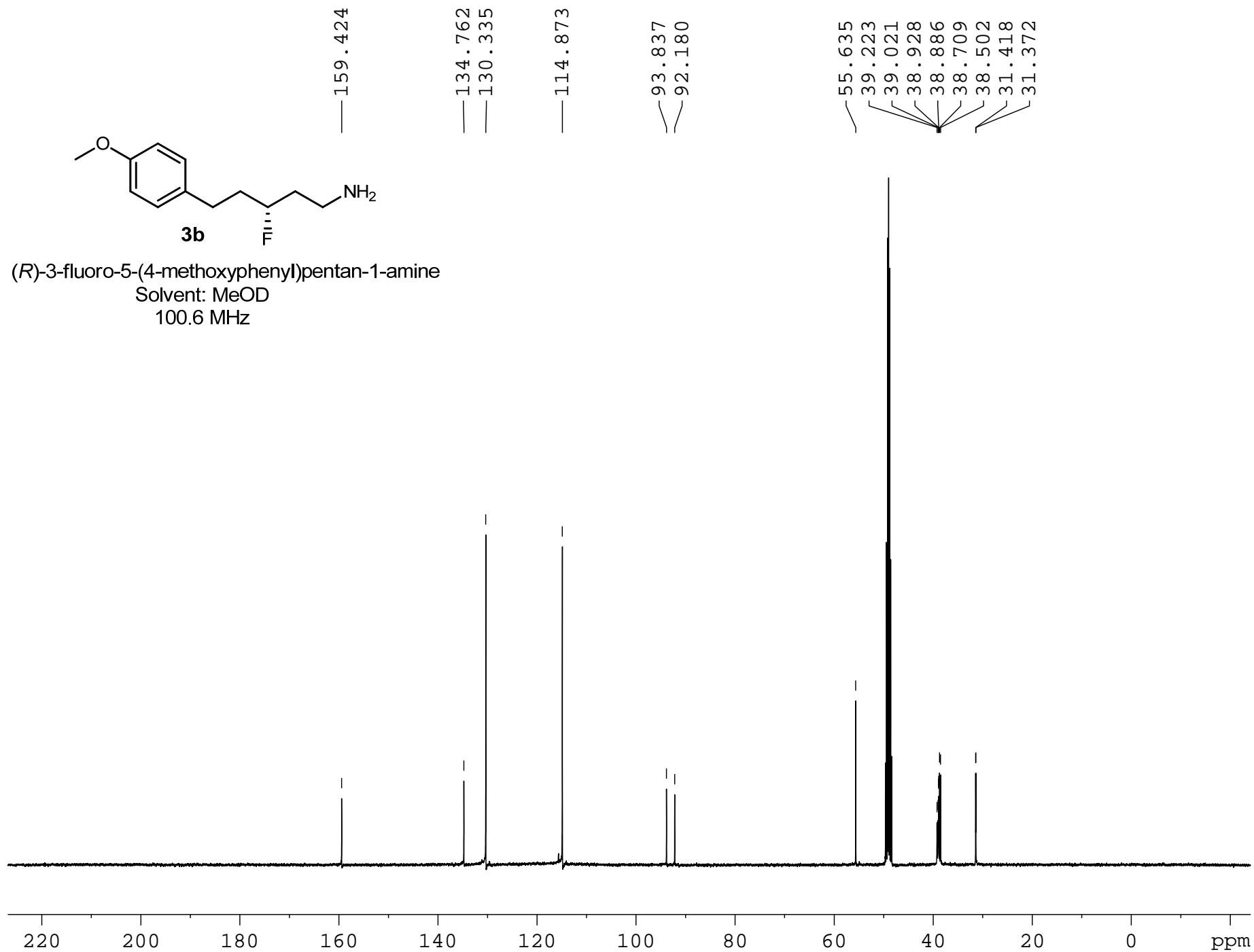
Solvent: MeOD

400.13 MHz





(*R*)-3-fluoro-5-(4-methoxyphenyl)pentan-1-amine
Solvent: MeOD
100.6 MHz



Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -0.5, max = 25.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron Ions

70 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

C: 10-500 H: 10-1000 N: 1-200 O: 1-200 F: 1-1

MCO-IV-159

S/N: UH193

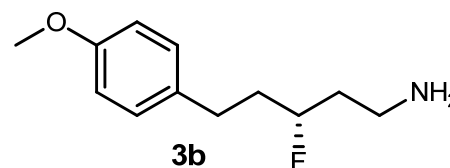
MCO-IV-159_120712_001 58 (1.083) AM (Cen,4, 80.00, Ar,8000.0,556.28,0.70); Sm (SG, 2x1.00); Cm (50:60)

07-Dec-2012

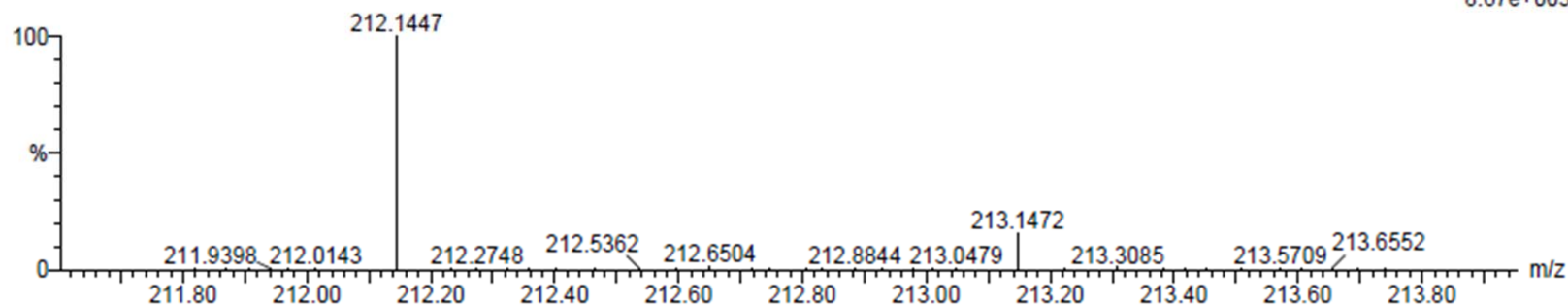
09:08:00

TOF MS ES+

8.67e+003



Page 1



Minimum:

Maximum:

5.0 5.0 -0.5
25.0

Mass

Calc. Mass

mDa

PPM

DBE

i-FIT

Formula

212.1447

212.1451

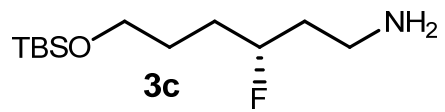
-0.4

-1.9

3.5

5.5

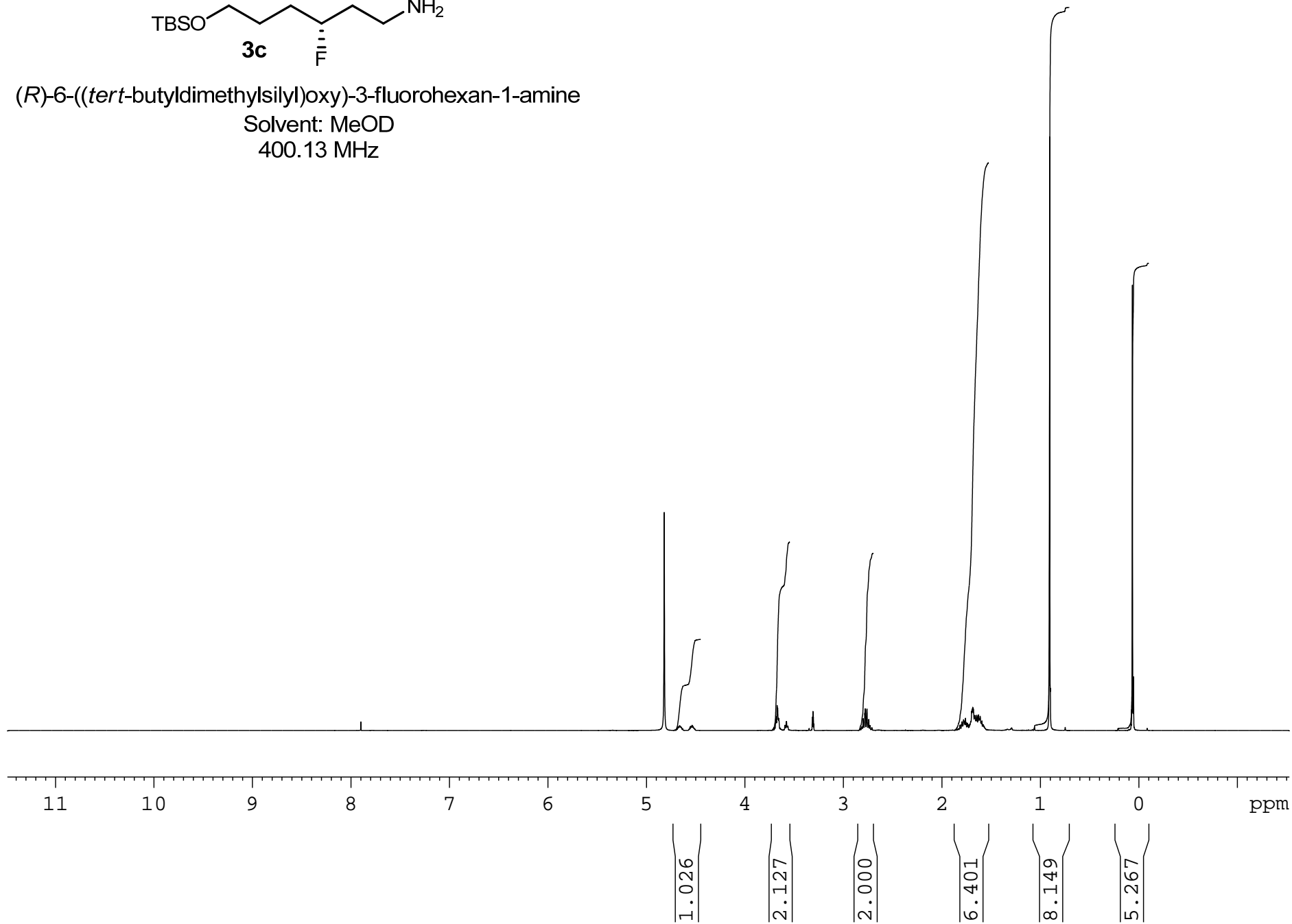
C12 H19 N O F

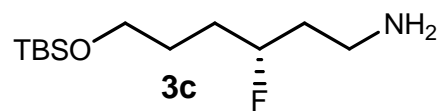


(*R*)-6-((*tert*-butyldimethylsilyl)oxy)-3-fluorohexan-1-amine

Solvent: MeOD

400.13 MHz





(*R*)-6-((*tert*-butyldimethylsilyl)oxy)-3-fluorohexan-1-amine

Solvent: MeOD

100.6 MHz

94.555
92.901

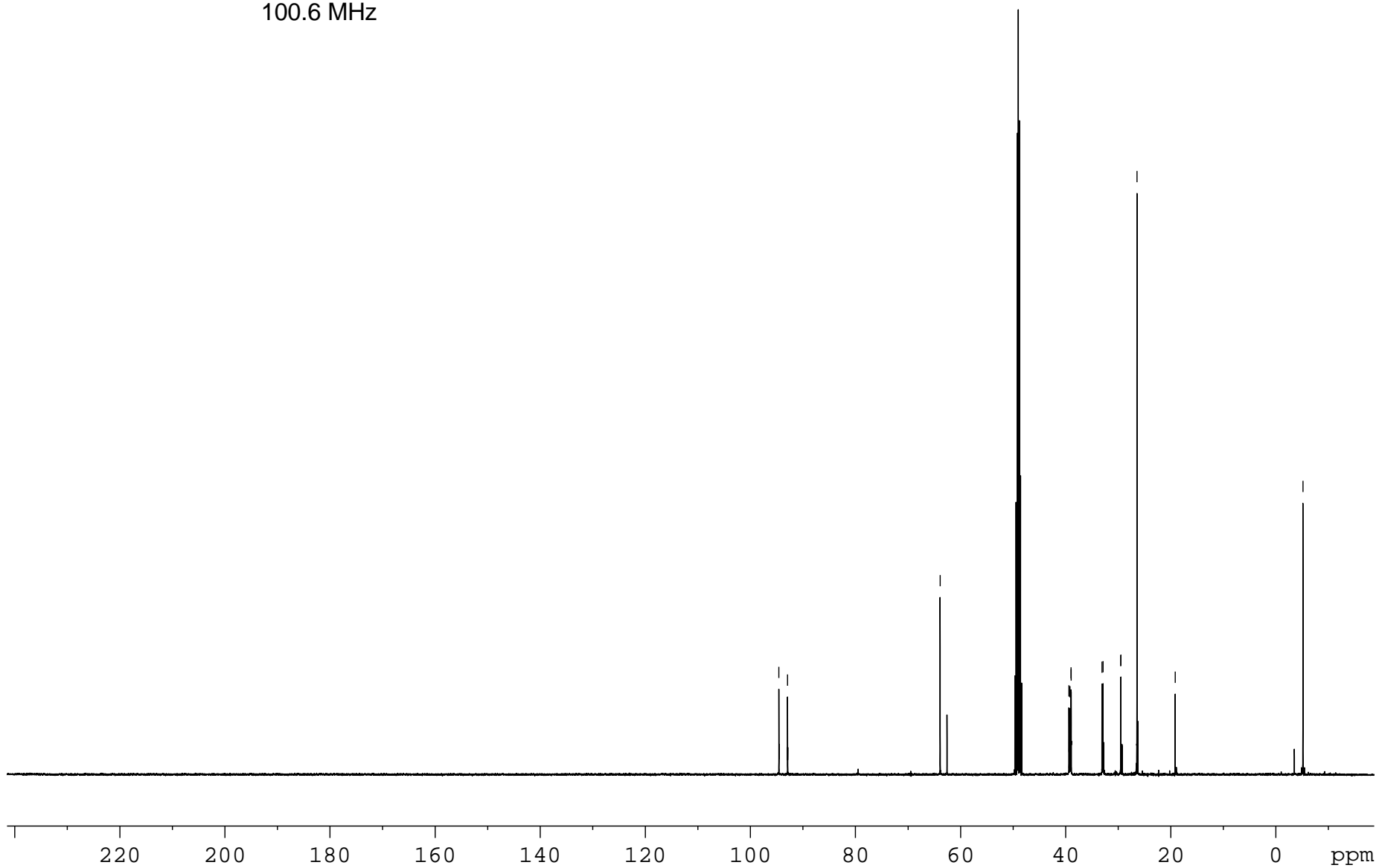
63.880

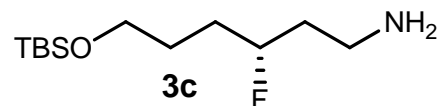
39.369
39.164
38.972
38.928

33.071
32.861

29.509
29.468
26.413
19.132

-5.184





Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -0.5, max = 25.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron Ions

80 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

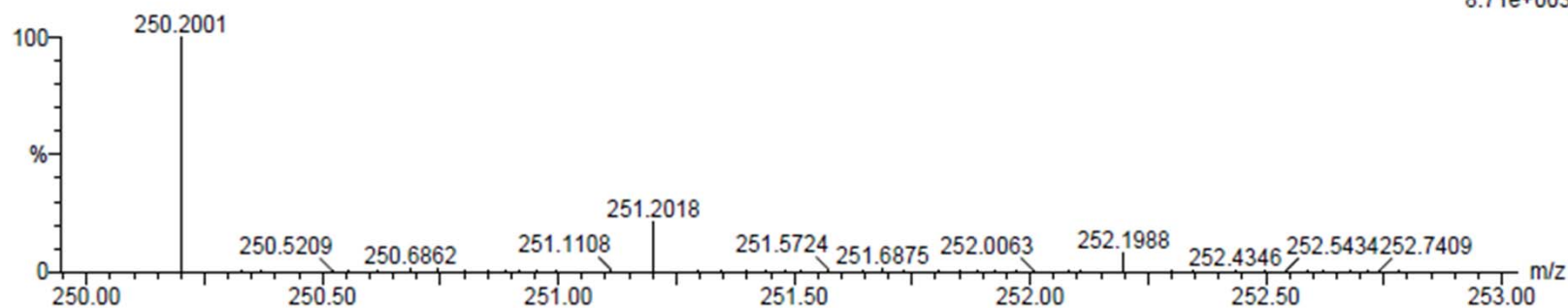
C: 10-500 H: 10-1000 N: 1-200 O: 1-200 F: 1-1 Si: 1-1

MCO-IV-172

S/N: UH193

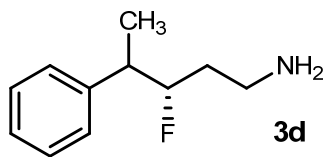
MCO-IV-172_120712_001 98 (1.825) AM (Cen,4, 80.00, Ar,8000.0,556.28,0.70); Sm (SG, 2x1.00); Cm (90:100)

07-Dec-2012
11:26:36
TOF MS ES+
8.71e+003



Minimum: -0.5
Maximum: 5.0 5.0 25.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
250.2001	250.2002	-0.1	-0.4	-0.5	7.0	C12 H29 N O F Si

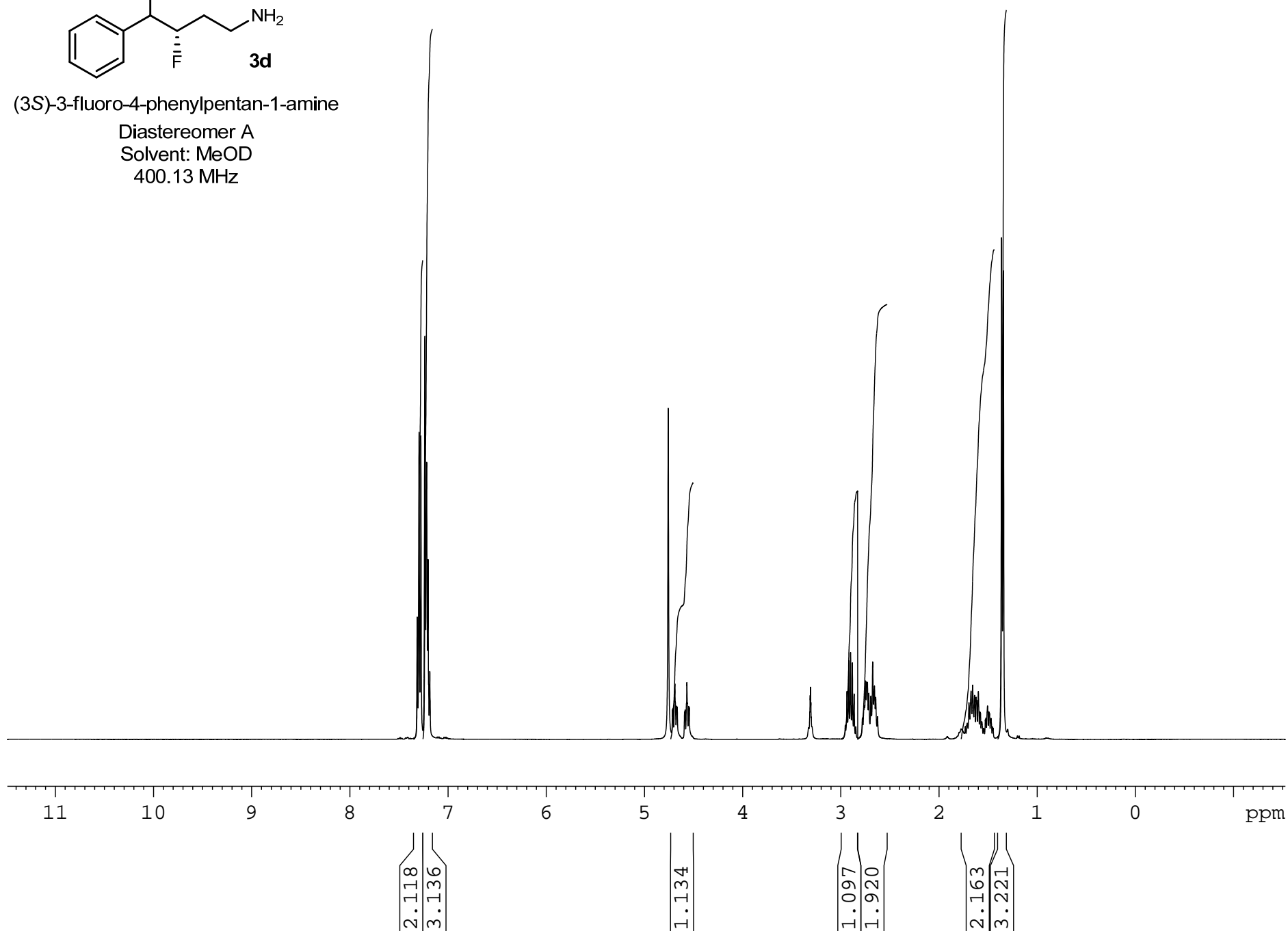


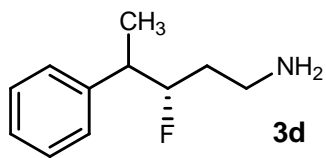
(3S)-3-fluoro-4-phenylpentan-1-amine

Diastereomer A

Solvent: MeOD

400.13 MHz



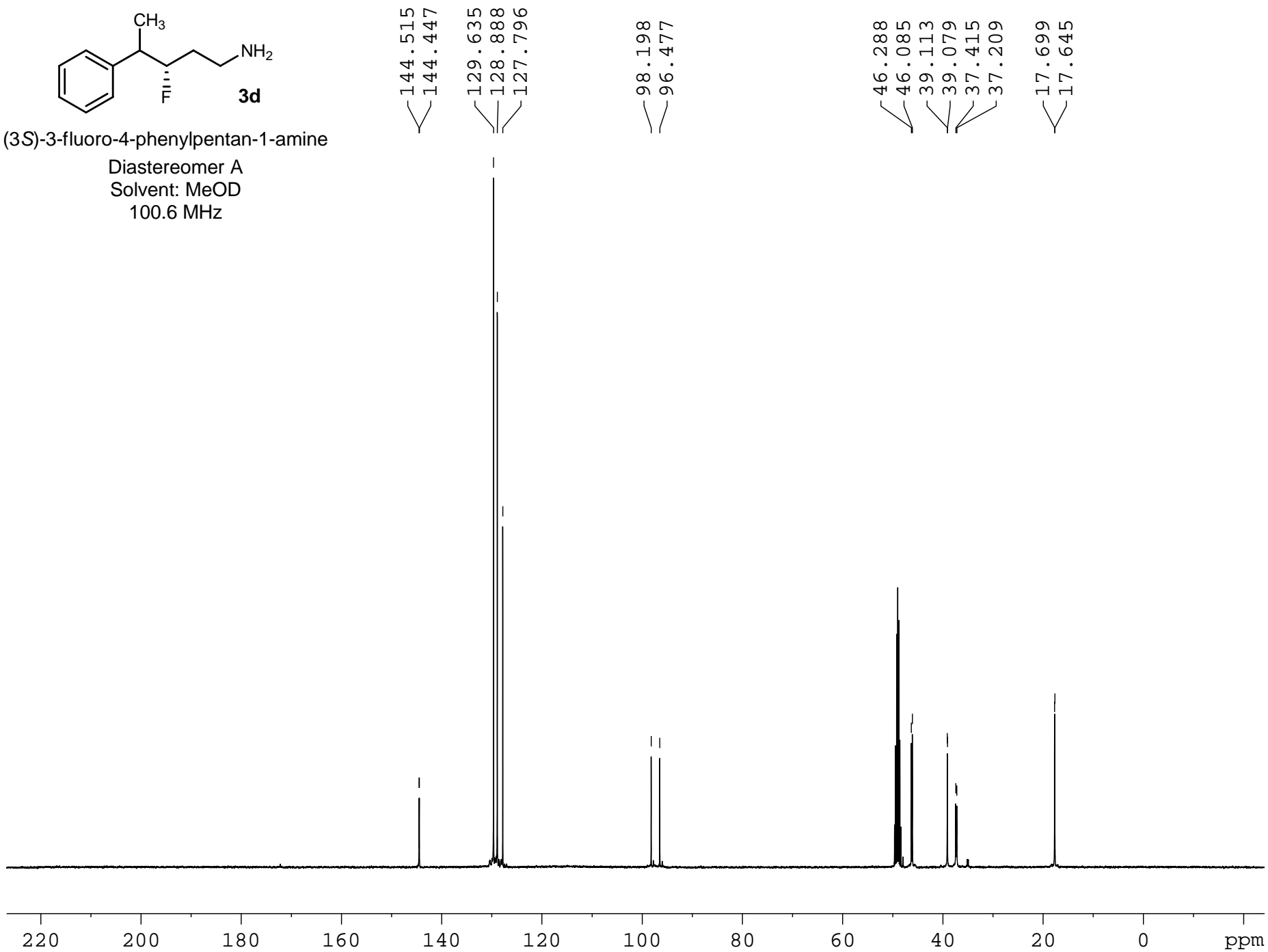


(3S)-3-fluoro-4-phenylpentan-1-amine

Diastereomer A

Solvent: MeOD

100.6 MHz



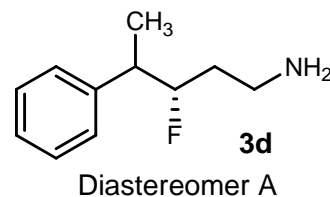
Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -0.5, max = 25.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 2



Page 1

Monoisotopic Mass, Even Electron Ions

11 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

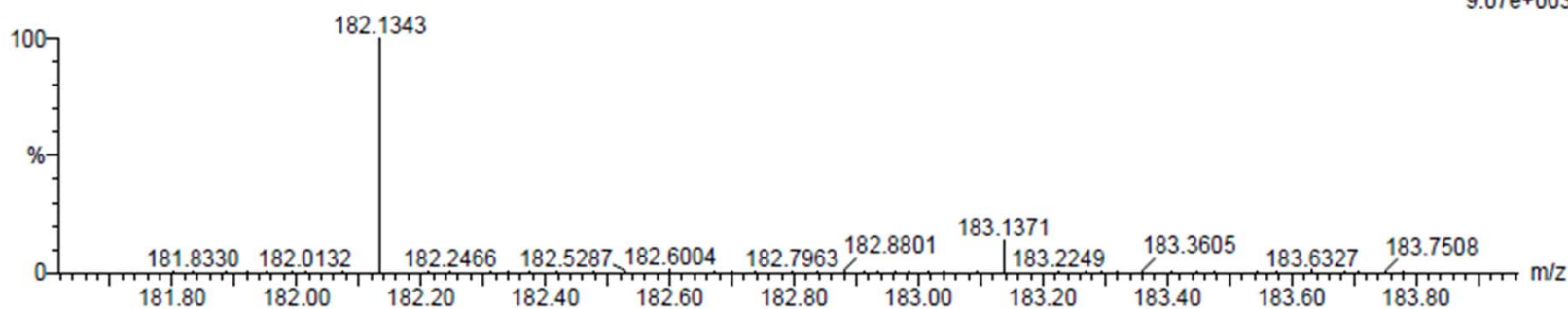
C: 10-500 H: 10-1000 N: 1-200 F: 1-1

MCO-IV-163

S/N: UH193

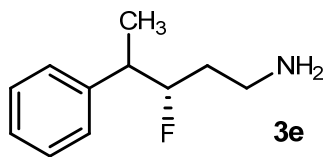
MCO-IV-163_120712_001 59 (1.102) AM (Cen,4, 80.00, Ar,8000.0,556.28,0.70); Sm (SG, 2x1.00); Cm (50:60)

07-Dec-2012
10:01:45
TOF MS ES+
9.07e+003



Minimum: -0.5
Maximum: 5.0 5.0 25.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
182.1343	182.1345	-0.2	-1.1	3.5	1.5	C11 H17 N F

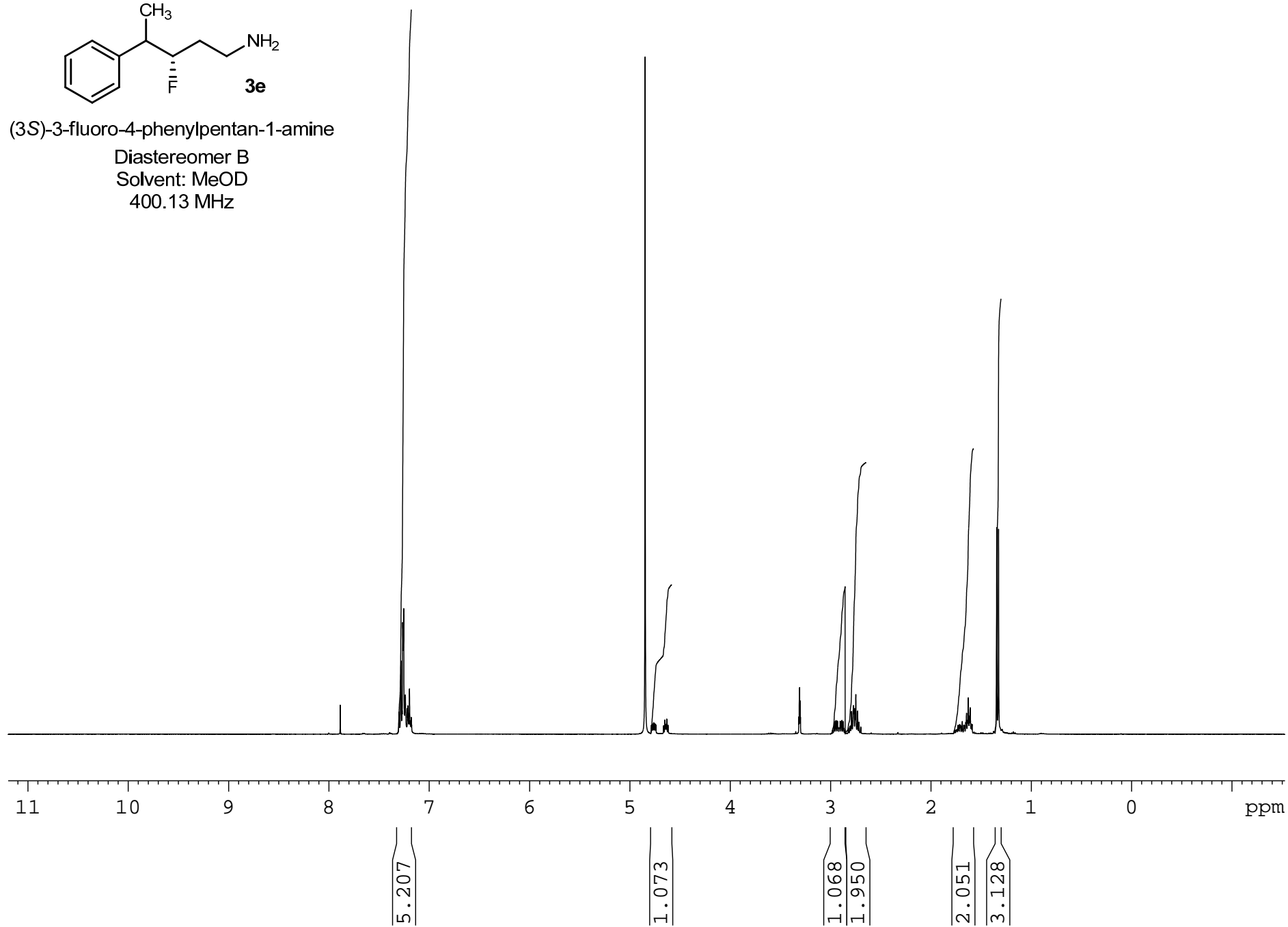


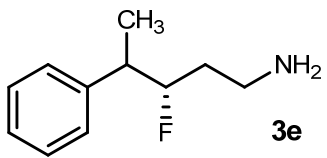
(3S)-3-fluoro-4-phenylpentan-1-amine

Diastereomer B

Solvent: MeOD

400.13 MHz





(3S)-3-fluoro-4-phenylpentan-1-amine

Diastereomer B

Solvent: MeOD

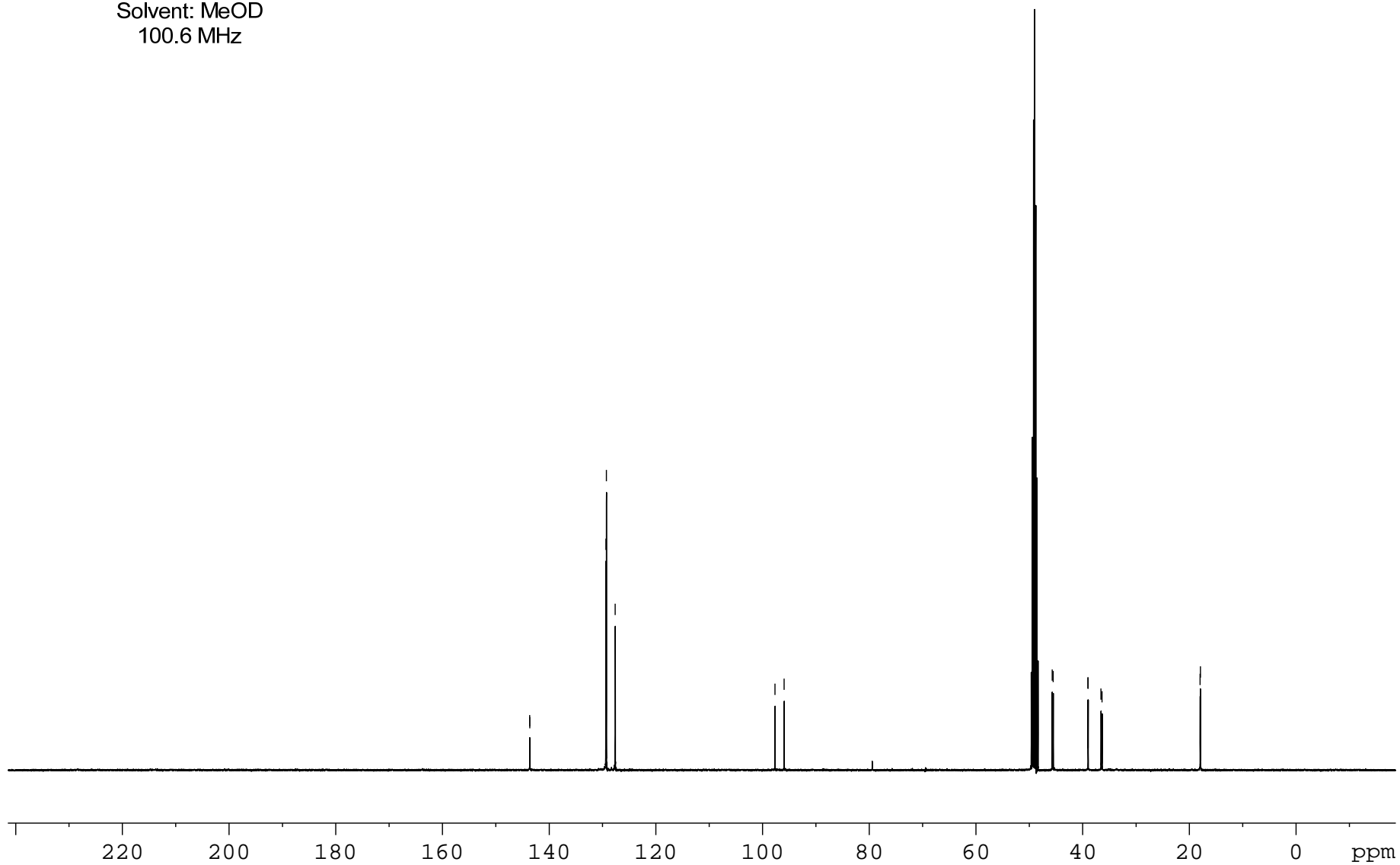
100.6 MHz

143.633
143.611
129.375
129.278
127.618

97.667
95.949

45.703
45.506
39.001
38.961
36.555
36.348

17.987
17.930



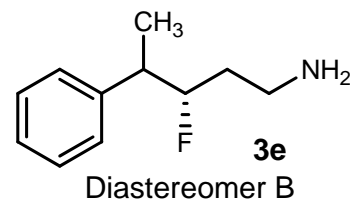
Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -0.5, max = 25.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 2



Page 1

Monoisotopic Mass, Even Electron Ions

11 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

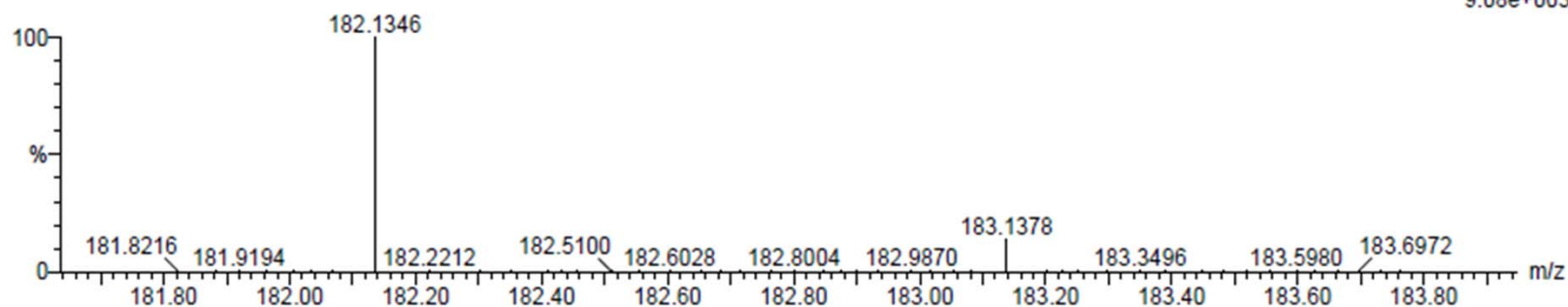
C: 10-500 H: 10-1000 N: 1-200 F: 1-1

MCO-IV-170

S/N: UH193

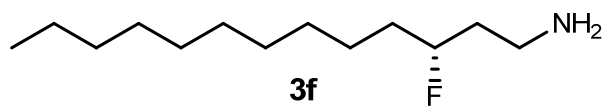
MCO-IV-170_120712_001 60 (1.120) AM (Cen,4, 80.00, Ar,8000.0,556.28,0.70); Sm (SG, 2x1.00); Cm (60:70)

07-Dec-2012
10:45:32
TOF MS ES+
9.08e+003

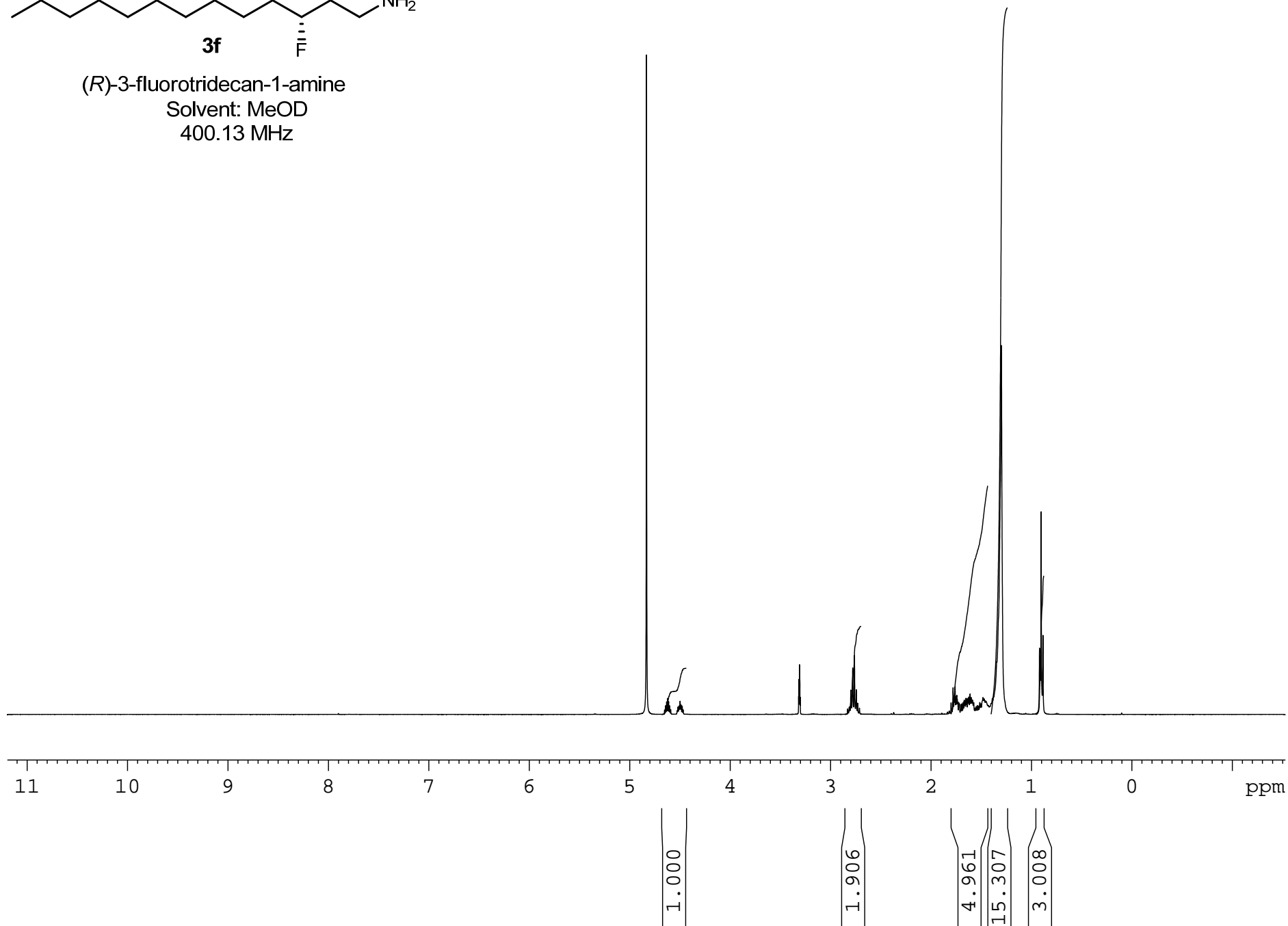


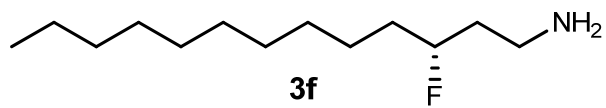
Minimum: -0.5
Maximum: 5.0 5.0 25.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
182.1346	182.1345	0.1	0.5	3.5	3.1	C11 H17 N F

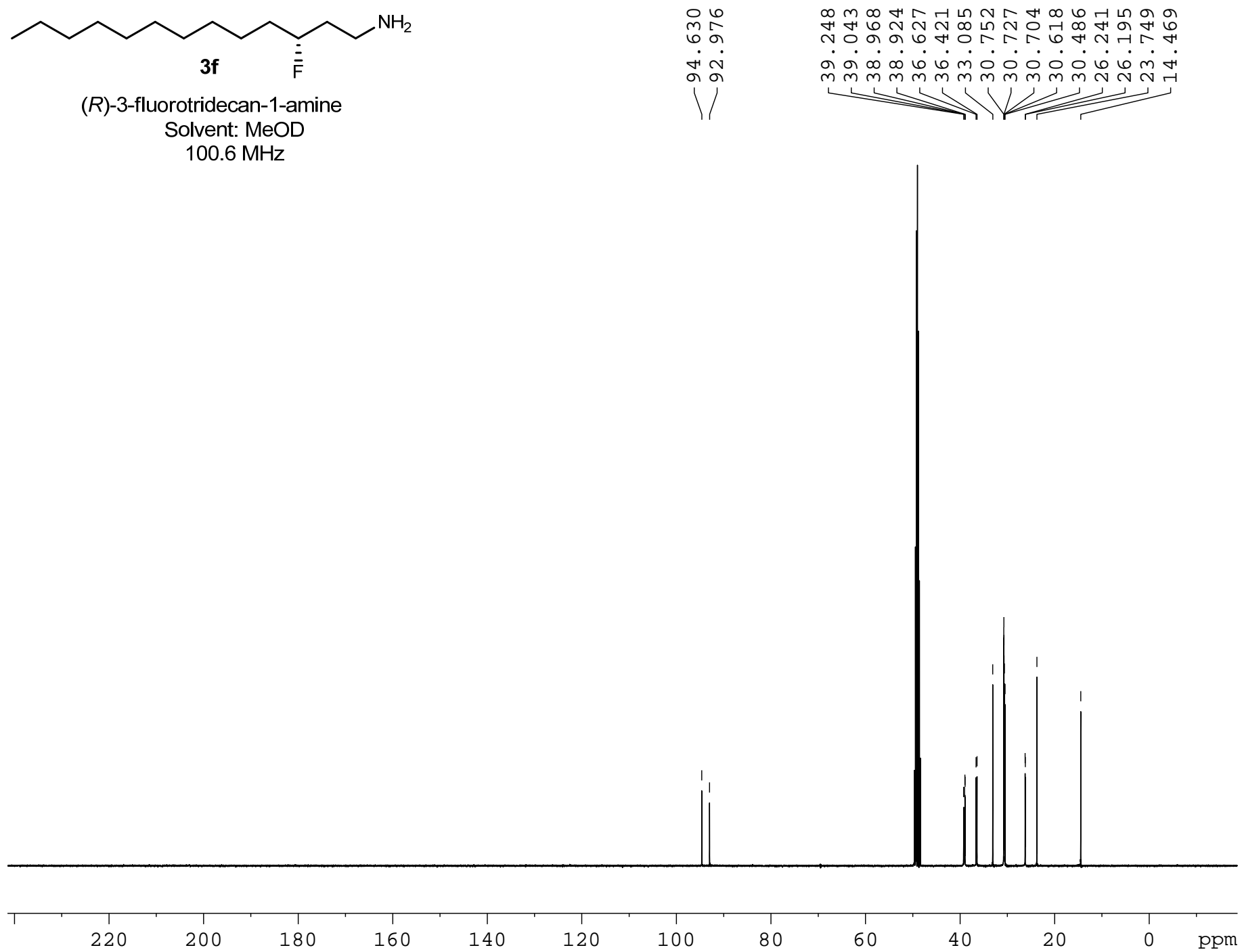


(*R*)-3-fluorotridecan-1-amine
Solvent: MeOD
400.13 MHz





3f
(*R*)-3-fluorotridecan-1-amine
Solvent: MeOD
100.6 MHz



Elemental Composition Report

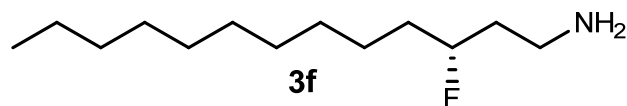
Page 1

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -0.5, max = 25.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 2



Monoisotopic Mass, Even Electron Ions

19 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

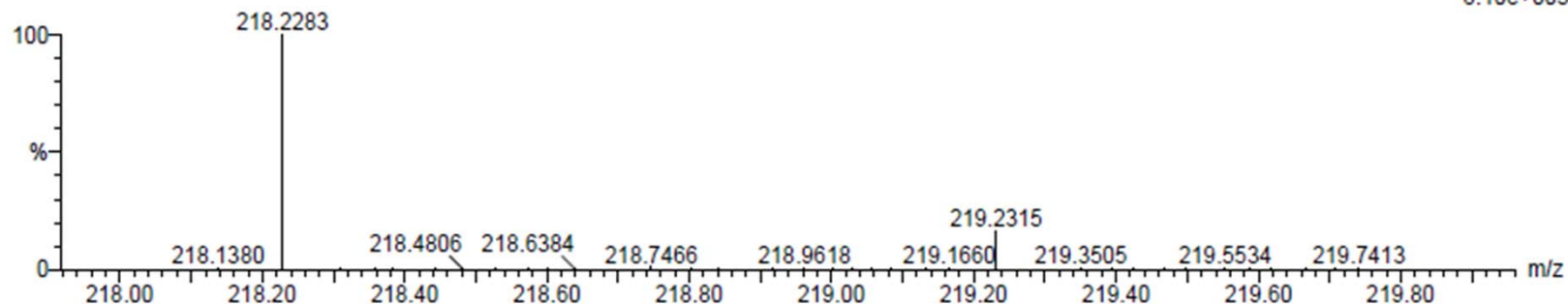
C: 10-500 H: 10-1000 N: 1-200 F: 1-1

MCO-IV-158

S/N: UH193

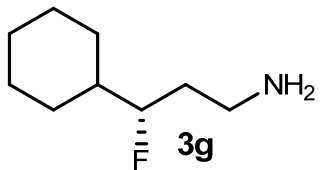
MCO-IV-158_120612_001 74 (1.380) AM (Cen,4, 80.00, Ar,8000.0,556.28,0.70); Sm (SG, 2x1.00); Cm (70:80)

06-Dec-2012
17:50:51
TOF MS ES+
8.10e+003



Minimum: -0.5
Maximum: 5.0 5.0 25.0

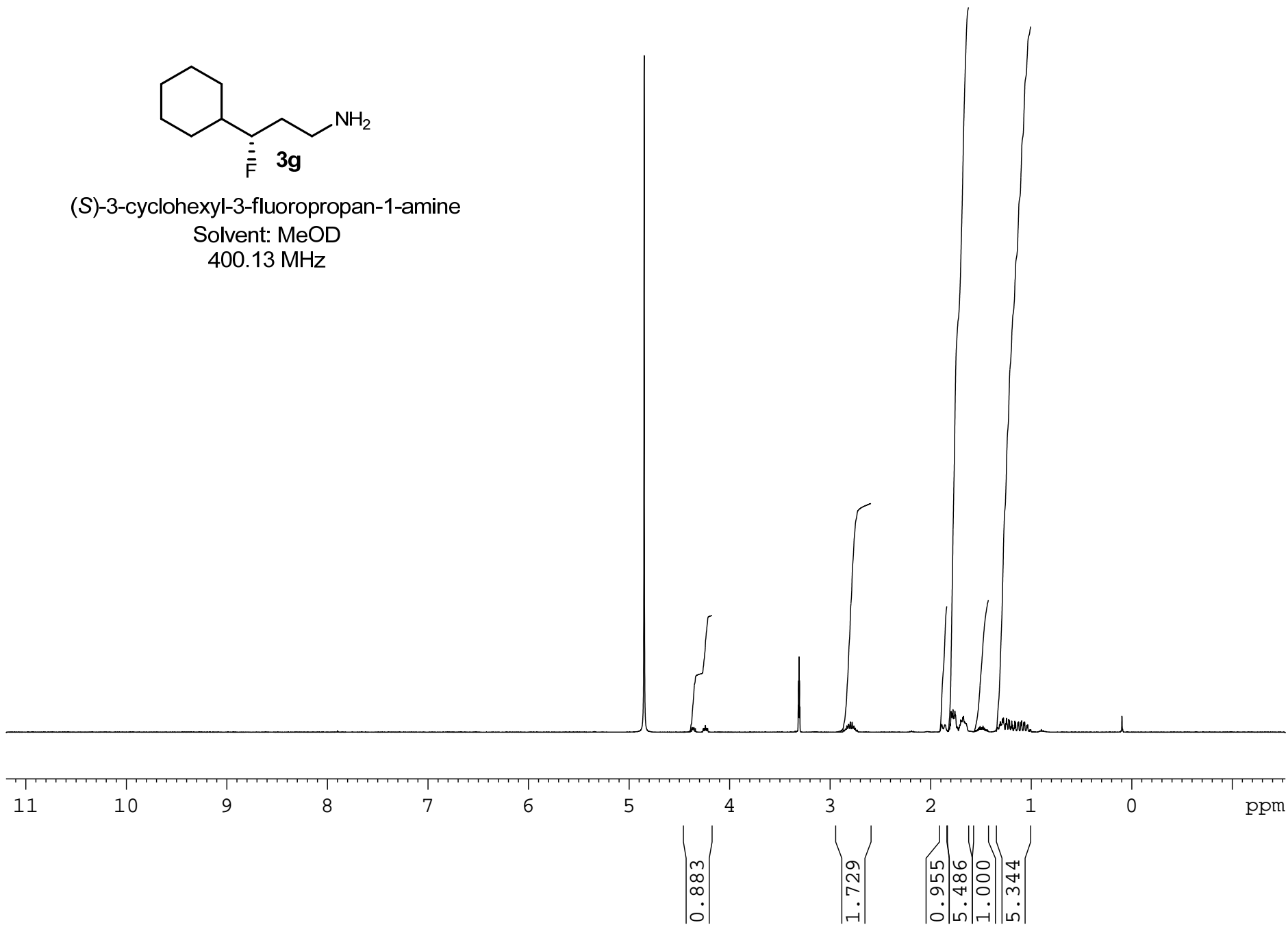
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
218.2283	218.2284	-0.1	-0.5	-0.5	2.1	C13 H29 N F

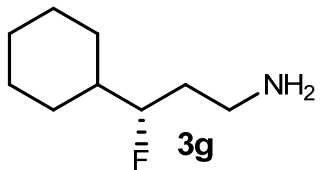


(S)-3-cyclohexyl-3-fluoropropan-1-amine

Solvent: MeOD

400.13 MHz





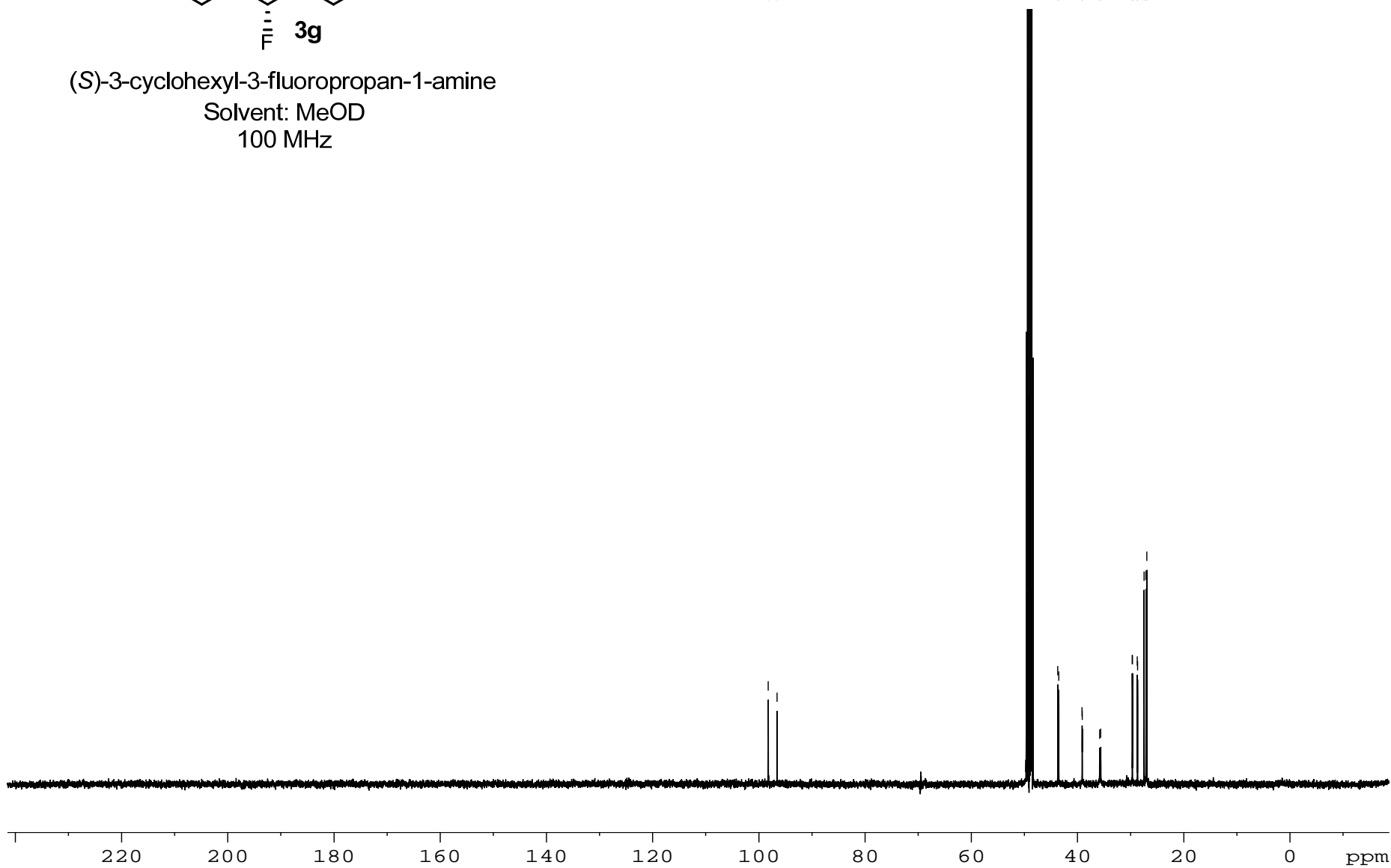
(S)-3-cyclohexyl-3-fluoropropan-1-amine

Solvent: MeOD

100 MHz

98.230
96.553

43.704
43.513
39.118
39.079
35.838
35.627
29.704
29.652
28.745
28.688
27.470
27.116
26.935



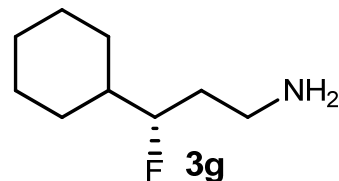
Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -0.5, max = 25.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 2



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Monoisotopic Mass, Even Electron Ions

10 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

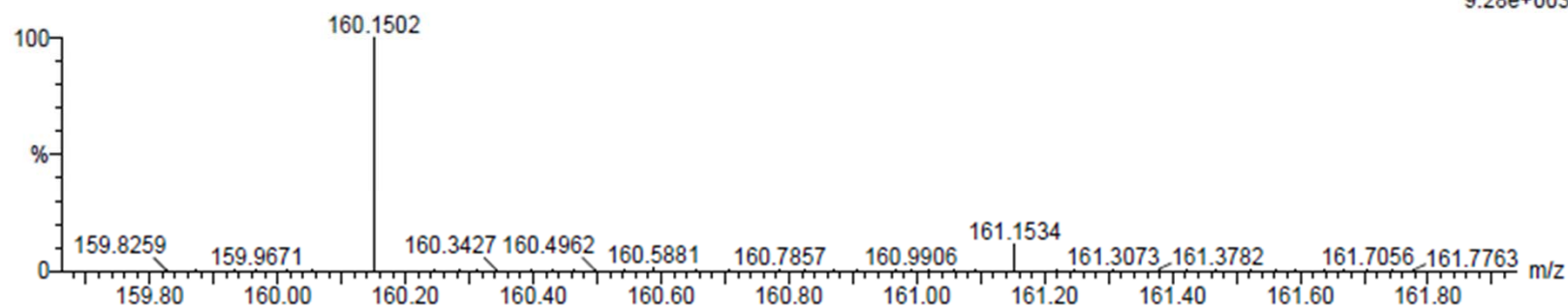
C: 8-500 H: 10-1000 N: 1-200 F: 1-1

MCO-IV-162

S/N: UH193

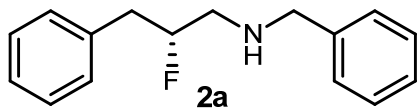
MCO-IV-162_120712_001 70 (1.306) AM (Cen,4, 80.00, Ar,8000.0,556.28,0.70); Sm (SG, 2x1.00); Cm (60:70)

07-Dec-2012
09:51:53
TOF MS ES+
9.28e+003



Minimum: -0.5
Maximum: 5.0 5.0 25.0

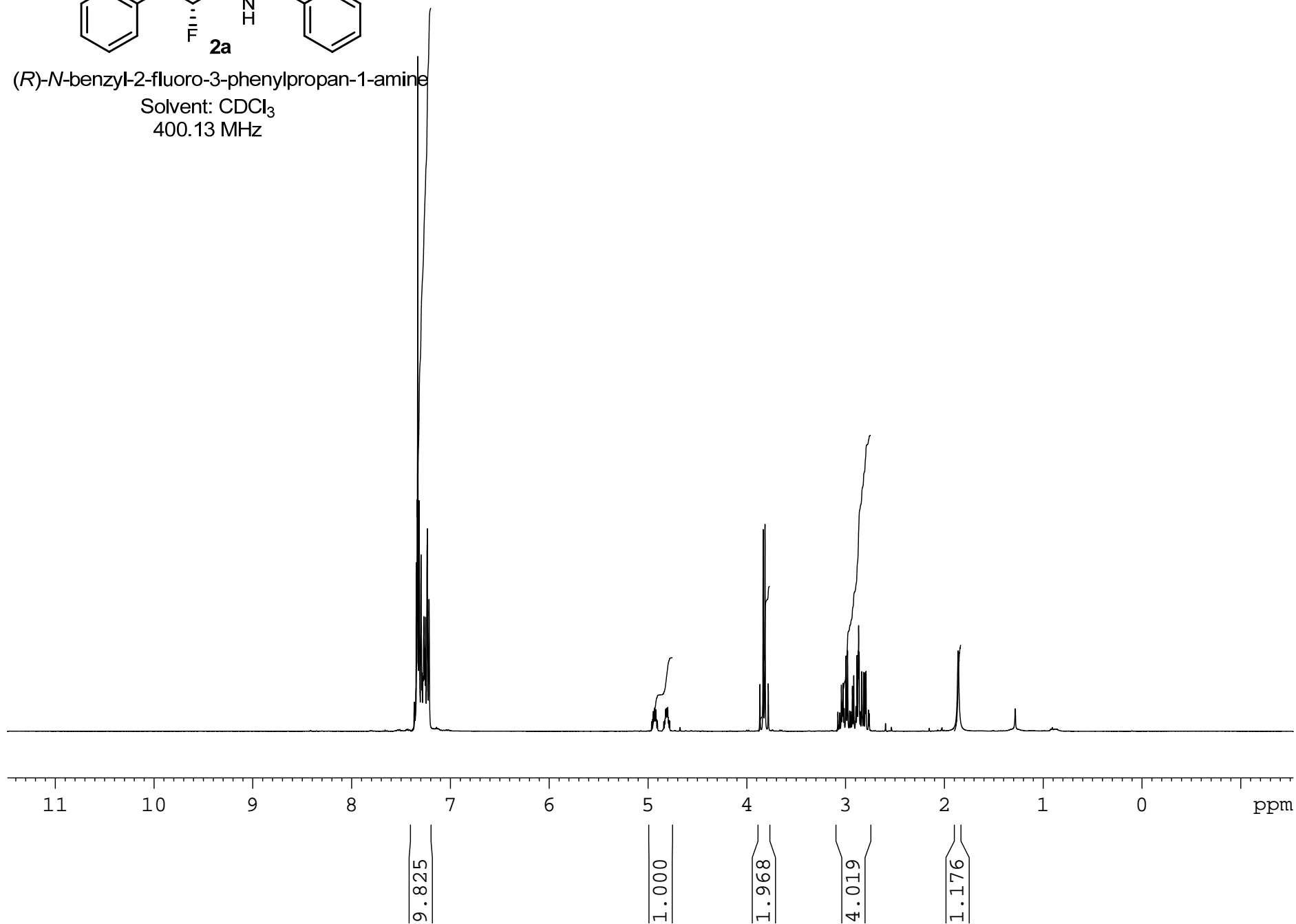
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
160.1502	160.1502	0.0	0.0	0.5	3.2	C9 H19 N F

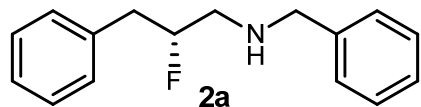


(*R*)-*N*-benzyl-2-fluoro-3-phenylpropan-1-amine

Solvent: CDCl₃

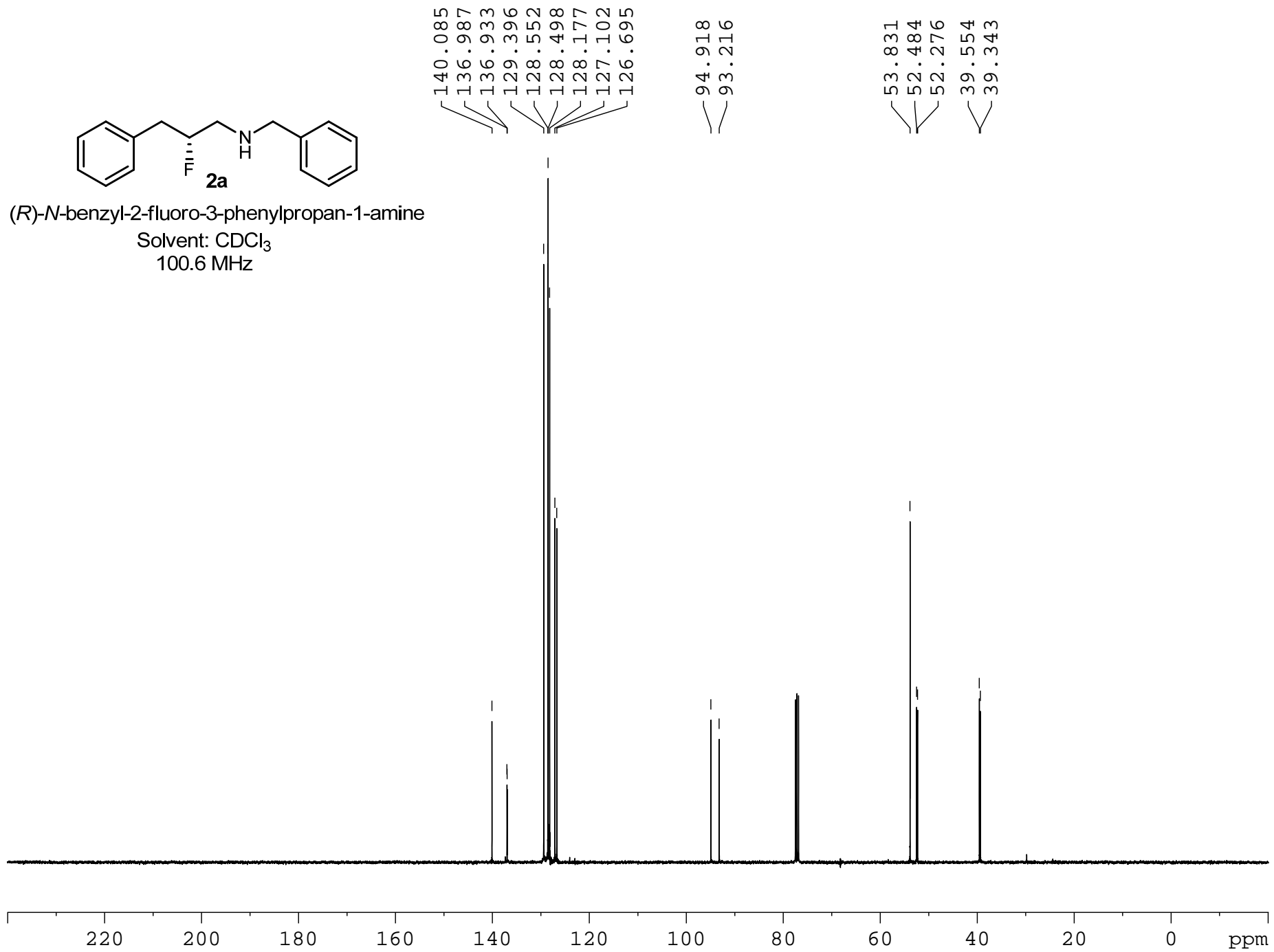
400.13 MHz





(*R*)-*N*-benzyl-2-fluoro-3-phenylpropan-1-amine

Solvent: CDCl₃
100.6 MHz



Elemental Composition Report

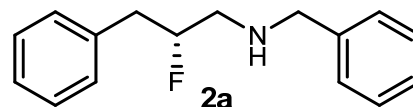
Page 1

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -0.5, max = 25.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 2



Monoisotopic Mass, Even Electron Ions

25 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

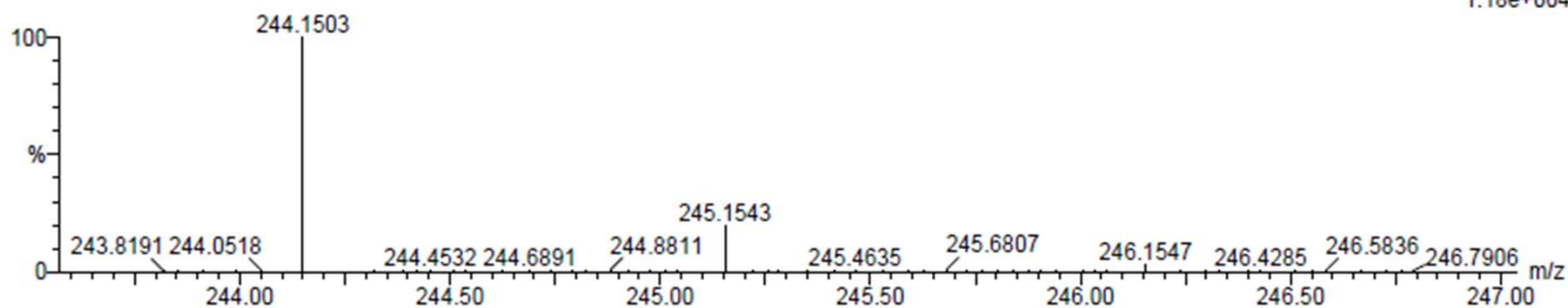
C: 10-500 H: 10-1000 N: 1-200 F: 1-1

MCO-V-20

S/N: UH193

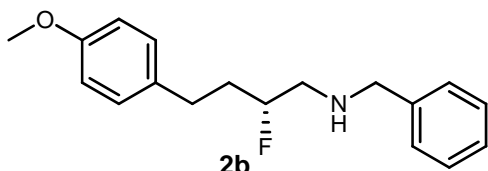
MCO-V-20_120712_001 50 (0.935) AM (Cen,4, 80.00, Ar,8000.0,556.28,0.70); Sm (SG, 2x1.00); Cm (50:60)

07-Dec-2012
12:03:38
TOF MS ES+
1.18e+004



Minimum: -0.5
Maximum: 5.0 5.0 25.0

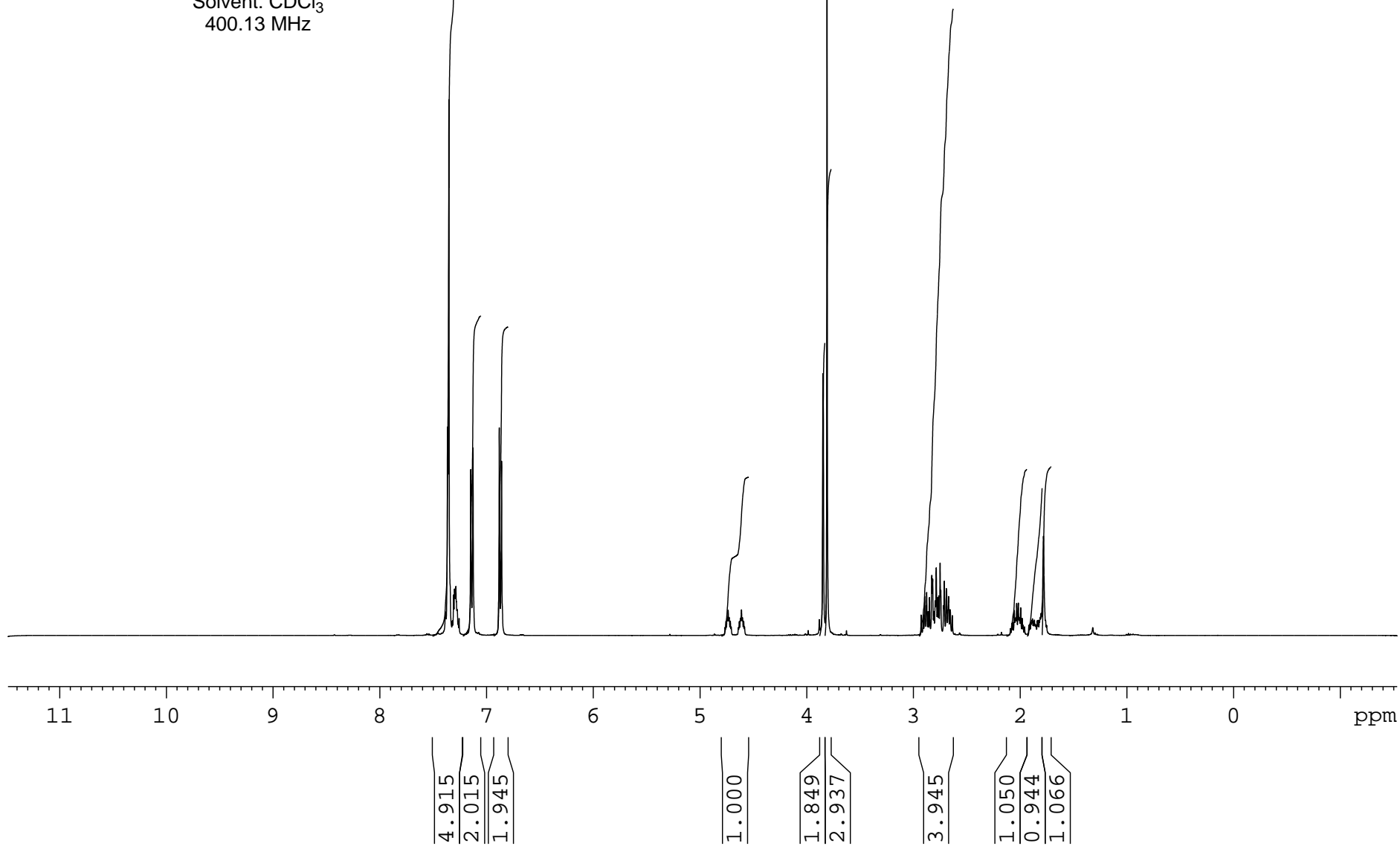
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
244.1503	244.1502	0.1	0.4	7.5	1.9	C16 H19 N F

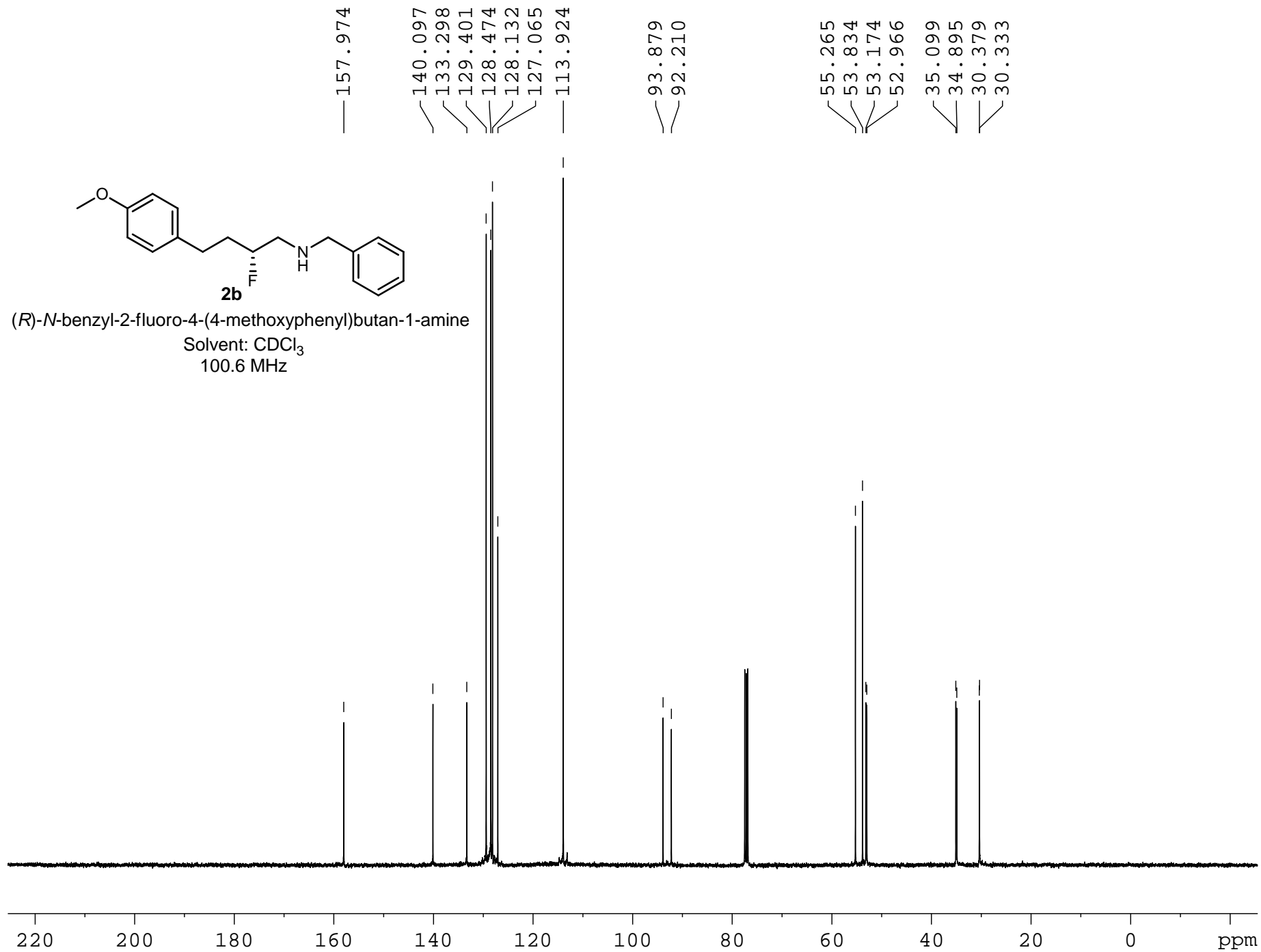


(*R*)-*N*-benzyl-2-fluoro-4-(4-methoxyphenyl)butan-1-amine

Solvent: CDCl₃

400.13 MHz

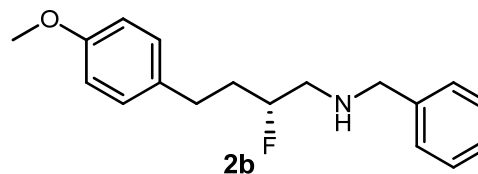




Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -0.5, max = 25.0
 Element prediction: Off
 Number of isotope peaks used for i-FIT = 2



Page 1

Monoisotopic Mass, Even Electron Ions

149 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

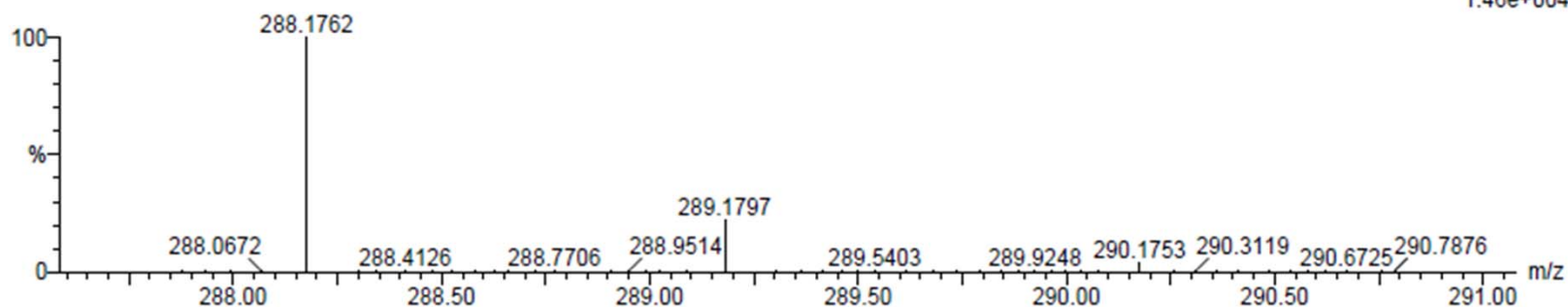
C: 15-500 H: 10-1000 N: 1-200 O: 1-200 F: 1-1

MCO-V-25

S/N: UH193

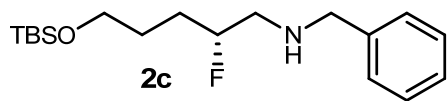
MCO-V-25_120712_001 98 (1.825) AM (Cen,4, 80.00, Ar,8000.0,556.28,0.70); Sm (SG, 2x1.00); Cm (90:100)

07-Dec-2012
 12:48:33
 TOF MS ES+
 1.46e+004



Minimum: -0.5
 Maximum: 5.0 5.0 25.0

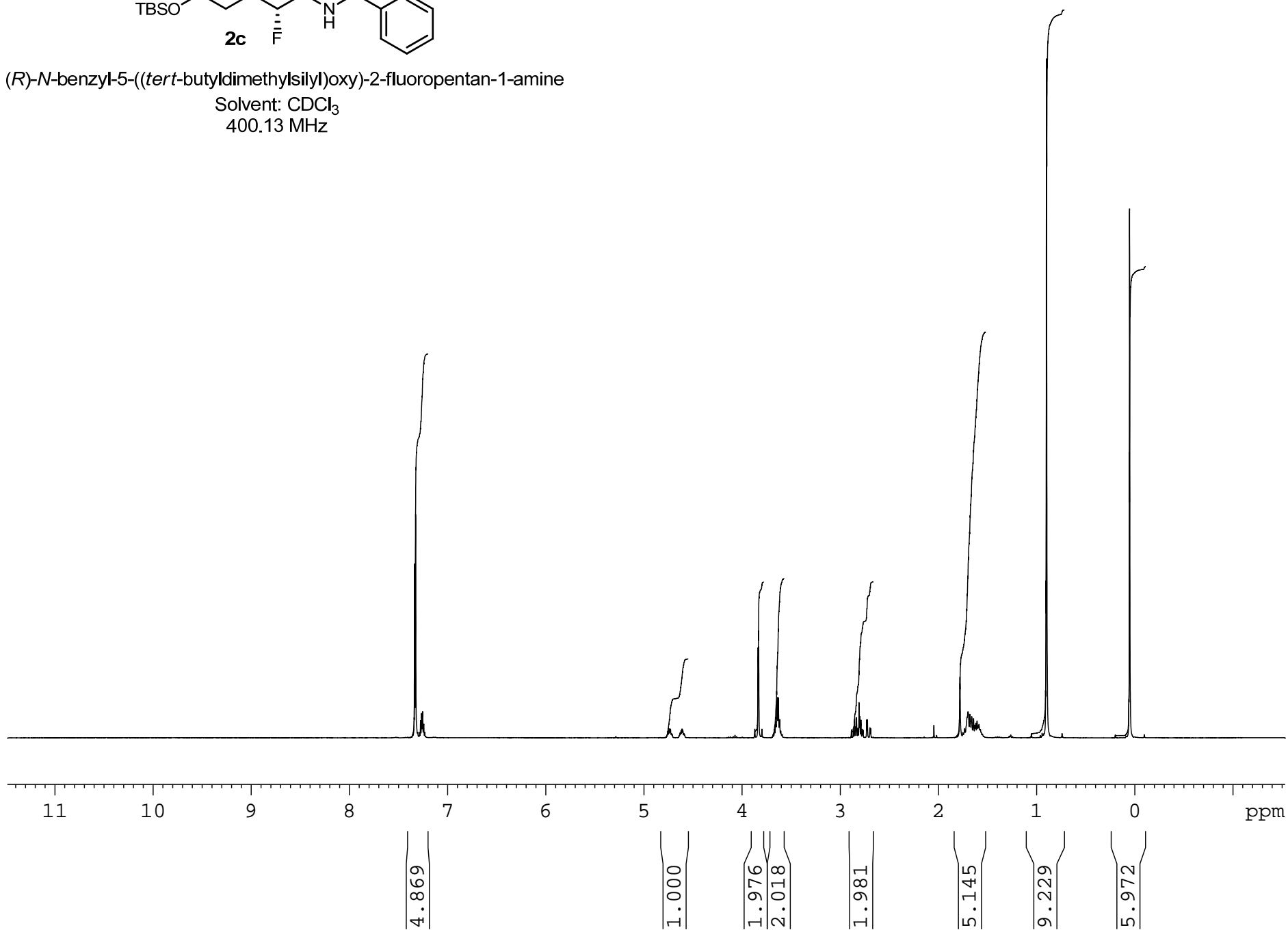
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
288.1762	288.1764	-0.2	-0.7	7.5	4.2	C18 H23 N O F

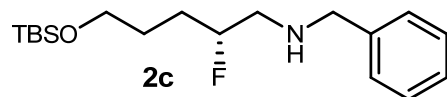


(*R*)-*N*-benzyl-5-((*tert*-butyldimethylsilyl)oxy)-2-fluoropentan-1-amine

Solvent: CDCl₃

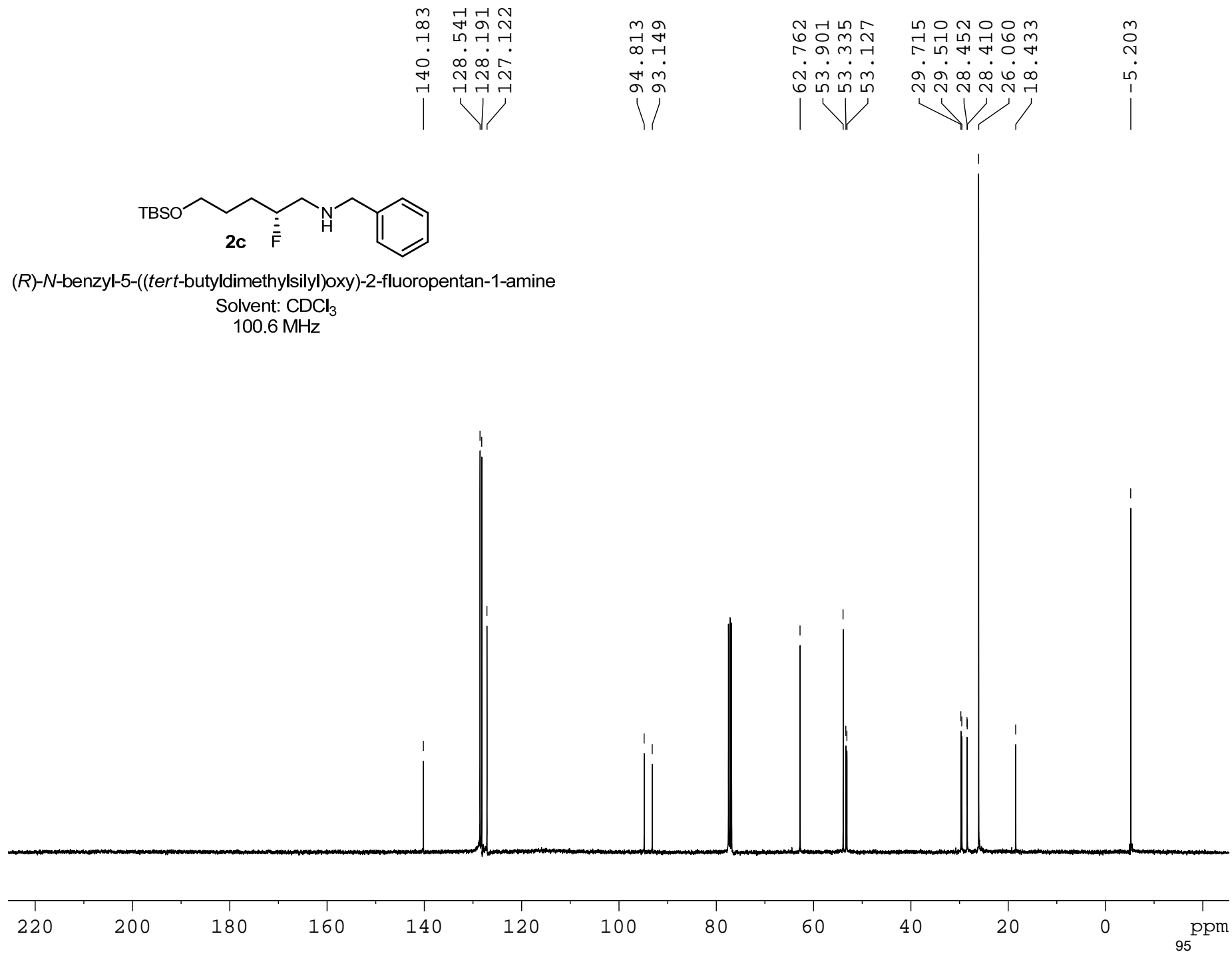
400.13 MHz





(*R*)-*N*-benzyl-5-((*tert*-butyldimethylsilyl)oxy)-2-fluoropentan-1-amine

Solvent: CDCl₃
100.6 MHz



Elemental Composition Report

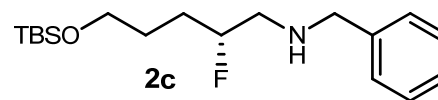
Page 1

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -0.5, max = 25.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 2



Monoisotopic Mass, Even Electron Ions

164 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

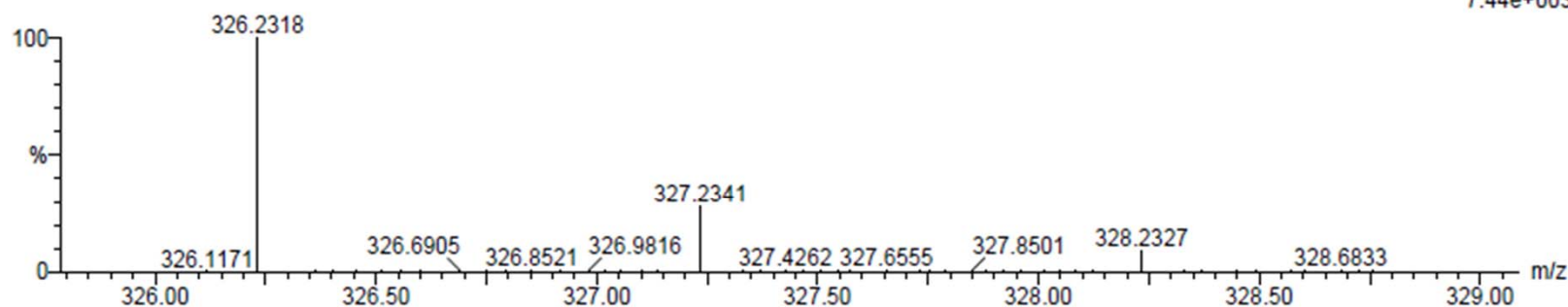
C: 15-500 H: 10-1000 N: 1-200 O: 1-200 F: 1-1 Si: 1-1

MCO-V-24

S/N: UH193

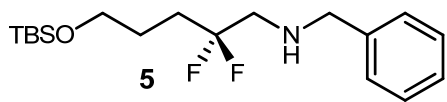
MCO-V-24_120712_001 97 (1.807) AM (Cen,4, 80.00, Ar,8000.0,556.28,0.70); Sm (SG, 2x1.00); Cm (90:100)

07-Dec-2012
12:34:55
TOF MS ES+
7.44e+003



Minimum: -0.5
Maximum: 5.0 5.0 25.0

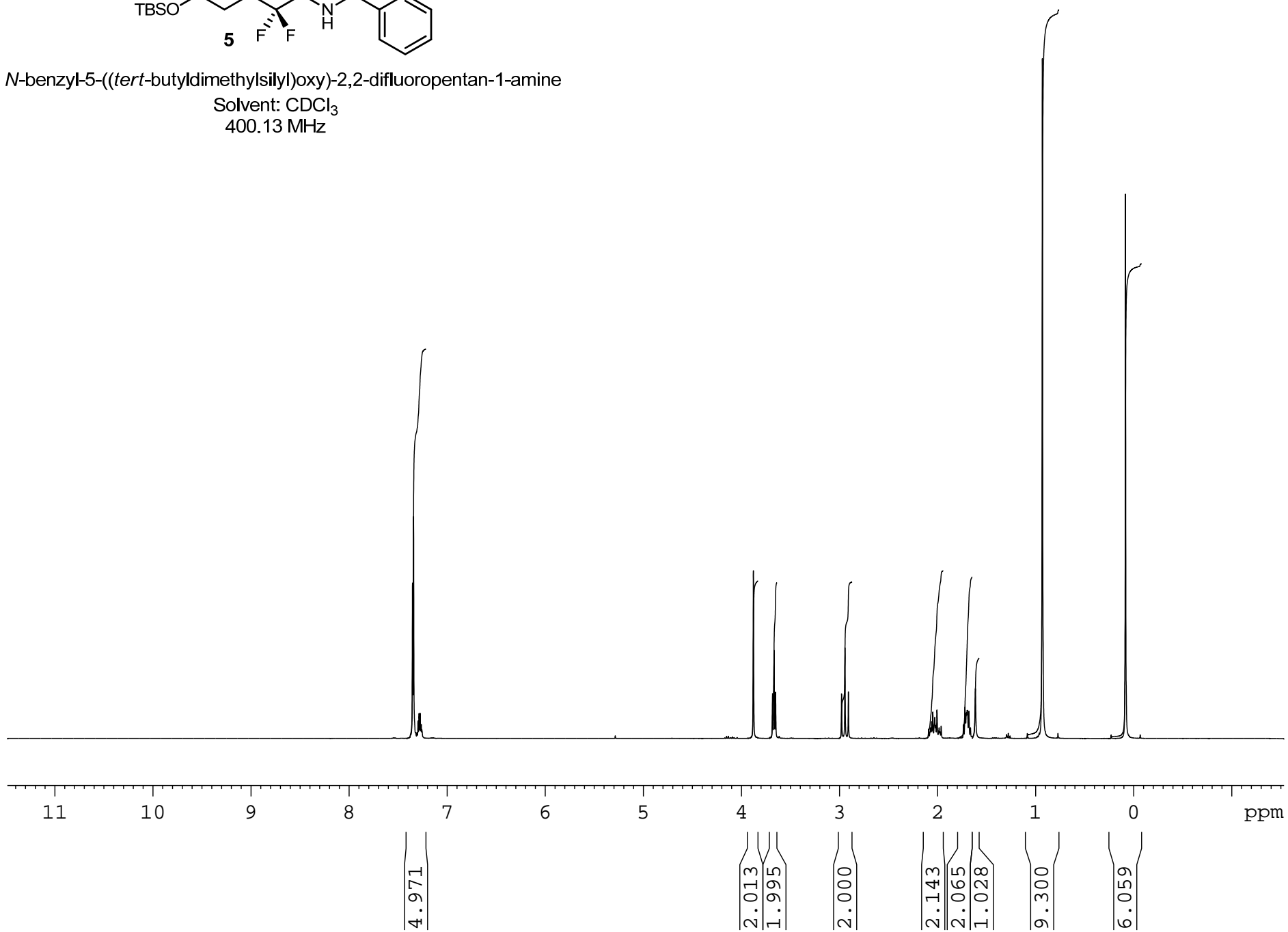
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
326.2318	326.2315	0.3	0.9	3.5	3.4	C18 H33 N O F Si

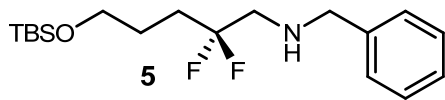


N-benzyl-5-((*tert*-butyldimethylsilyl)oxy)-2,2-difluoropentan-1-amine

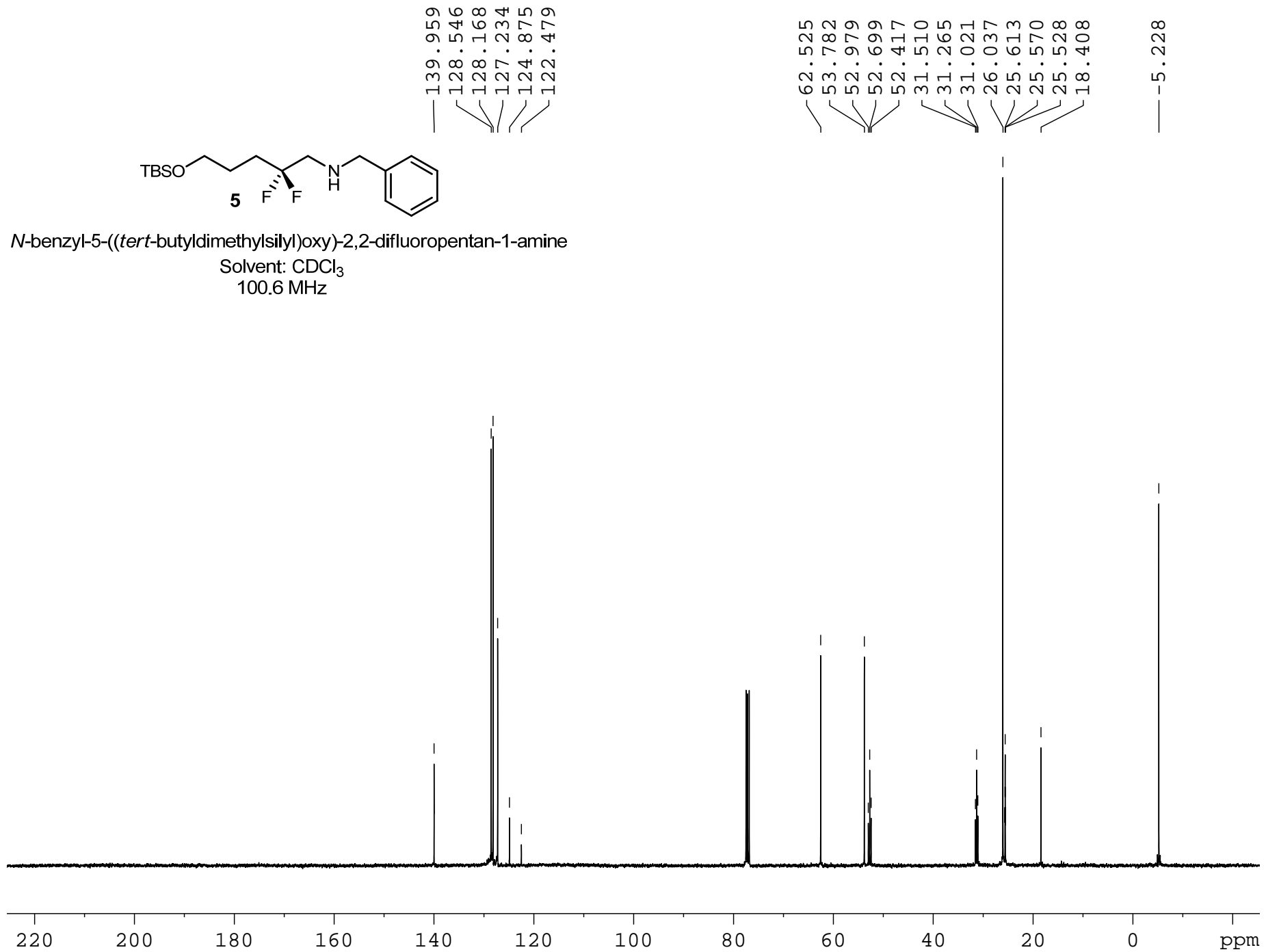
Solvent: CDCl₃

400.13 MHz





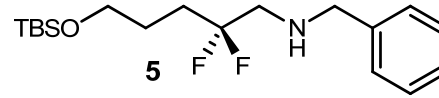
N-benzyl-5-((*tert*-butyldimethylsilyl)oxy)-2,2-difluoropentan-1-amine
 Solvent: CDCl₃
 100.6 MHz



Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -0.5, max = 25.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2



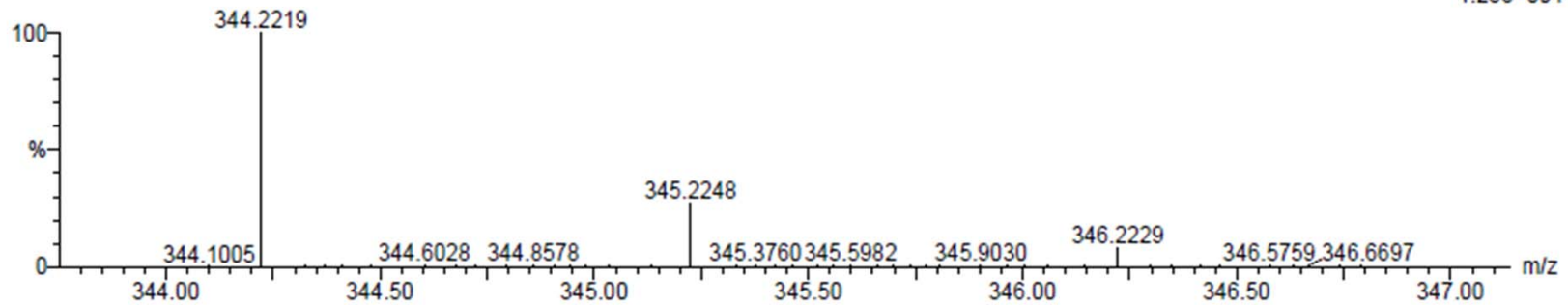
Monoisotopic Mass, Even Electron Ions
164 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 15-500 H: 10-1000 N: 1-200 O: 1-200 F: 2-2 Si: 1-1

MCO-V-45

S/N: UH193

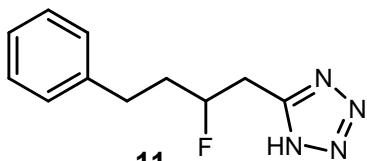
MCO-V-45_120712_001 49 (0.916) AM (Cen,4, 80.00, Ar,8000.0,556.28,0.70); Sm (SG, 2x1.00); Cm (40:50)

07-Dec-2012
13:00:23
TOF MS ES+
1.25e+004



Minimum: -0.5
Maximum: 5.0 5.0 25.0

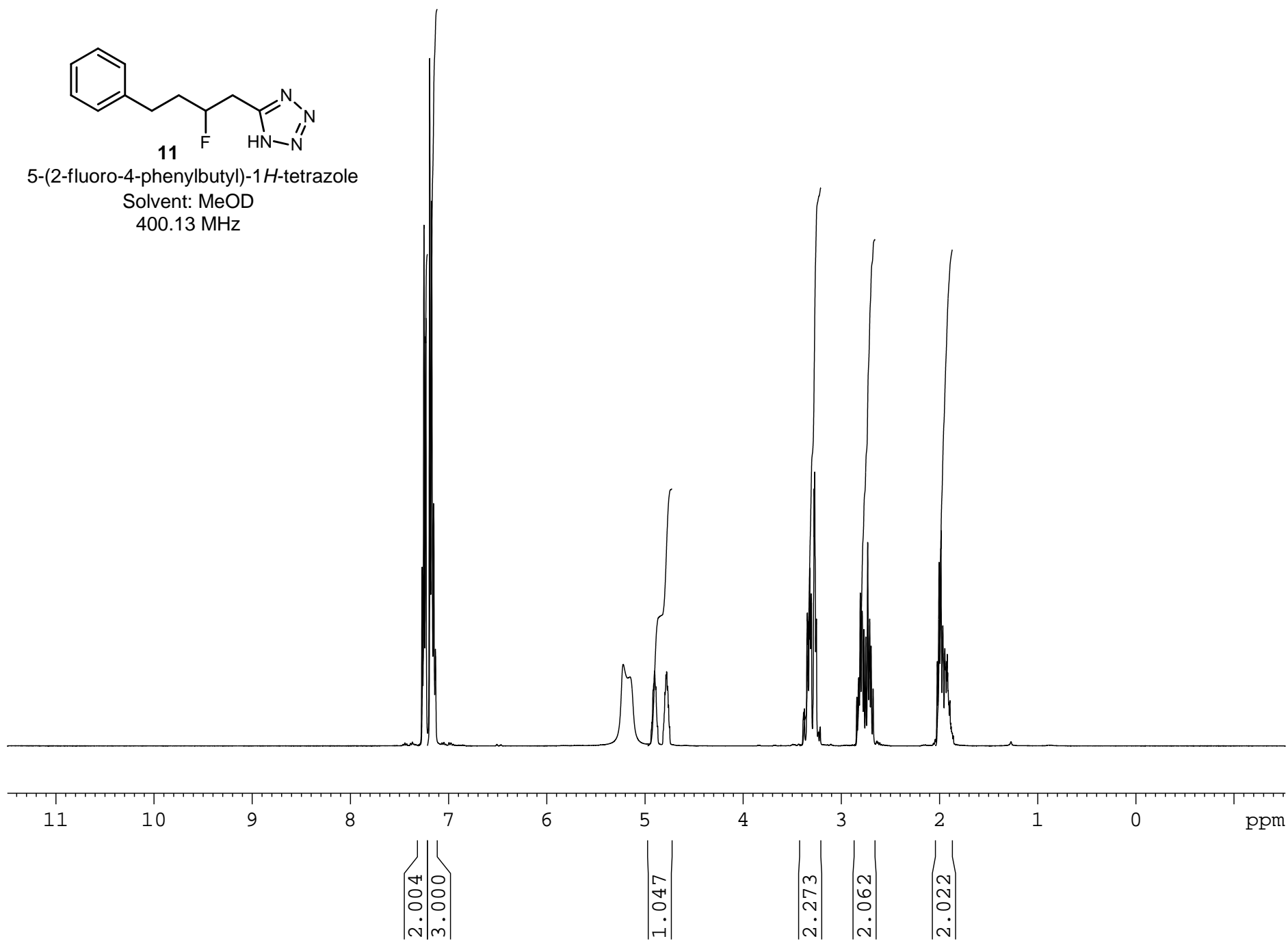
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
344.2219	344.2221	-0.2	-0.6	3.5	2.6	C18 H32 N O F2 Si

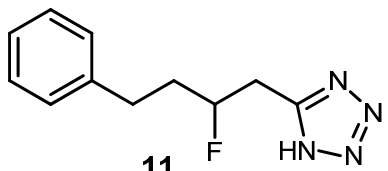


5-(2-fluoro-4-phenylbutyl)-1H-tetrazole

Solvent: MeOD

400.13 MHz



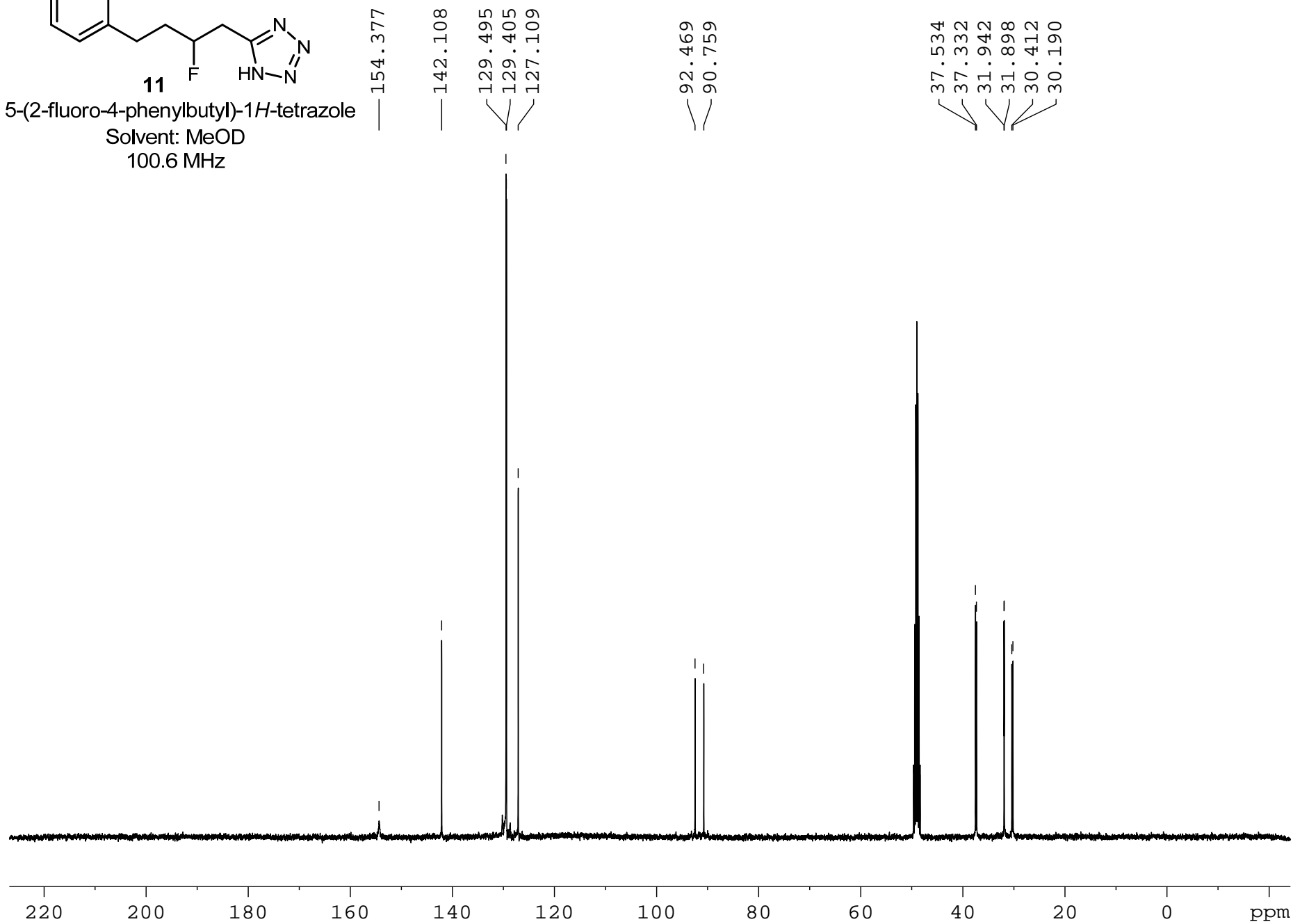


11

5-(2-fluoro-4-phenylbutyl)-1H-tetrazole

Solvent: MeOD

100.6 MHz



Elemental Composition Report

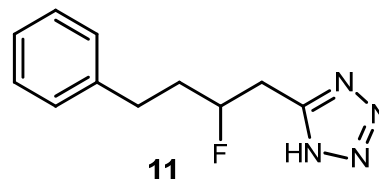
Page 1

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -0.5, max = 25.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 2



11
5-(2-fluoro-4-phenylbutyl)-1H-tetrazole

Monoisotopic Mass, Even Electron Ions

17 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

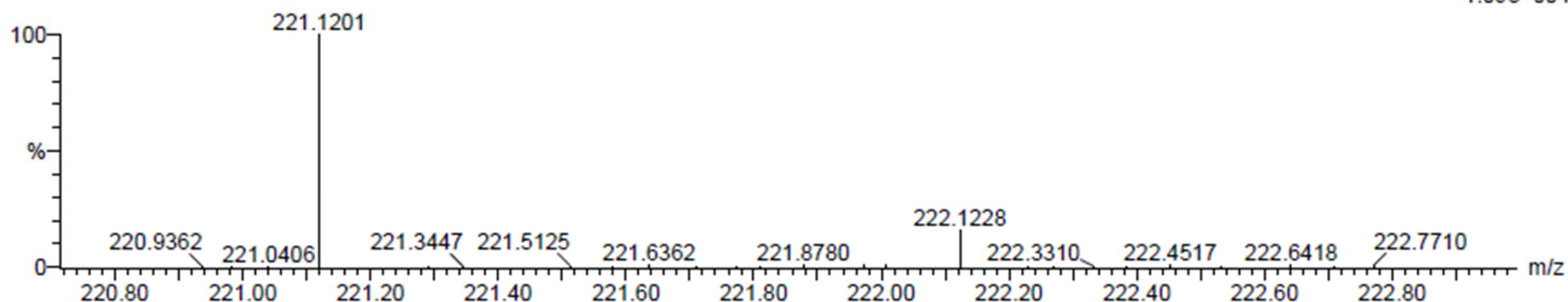
C: 10-500 H: 10-1000 N: 1-200 F: 1-1

MCO-V-184

S/N: UH193

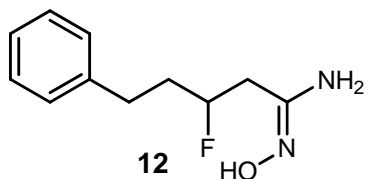
MCO-V-184_041013_001 95 (1.770) AM (Cen,5, 80.00, Ar,8000.0,556.28,0.70); Sm (SG, 2x1.00); Cm (90:100)

10-Apr-2013
10:56:47
1: TOF MS ES+
1.09e+004



Minimum: -0.5
Maximum: 5.0 5.0 25.0

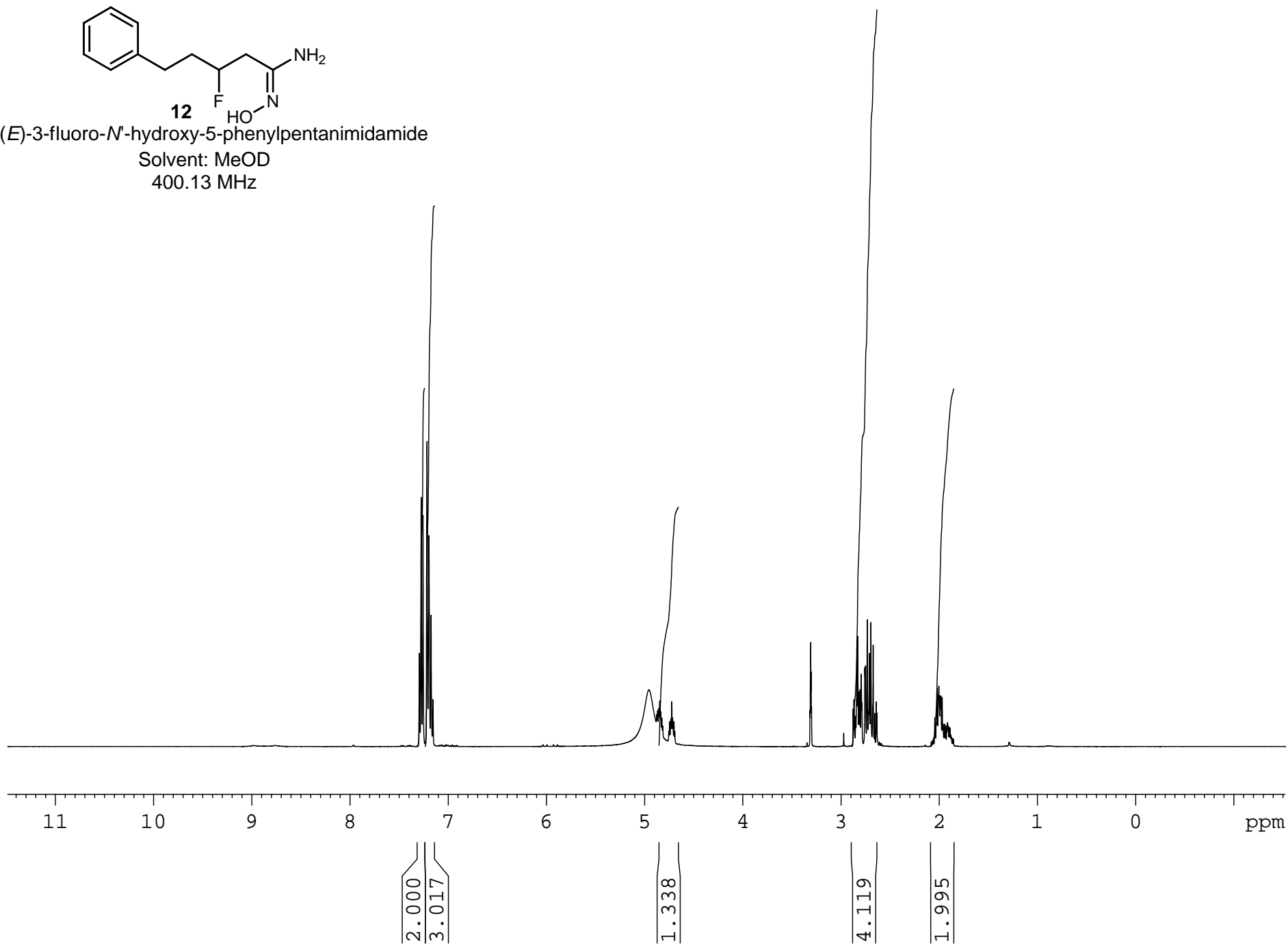
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
221.1201	221.1202	-0.1	-0.5	6.5	5.7	C11 H14 N4 F

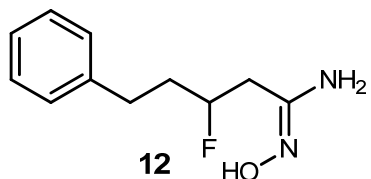


(*E*)-3-fluoro-*N*-hydroxy-5-phenylpentanimidamide

Solvent: MeOD

400.13 MHz



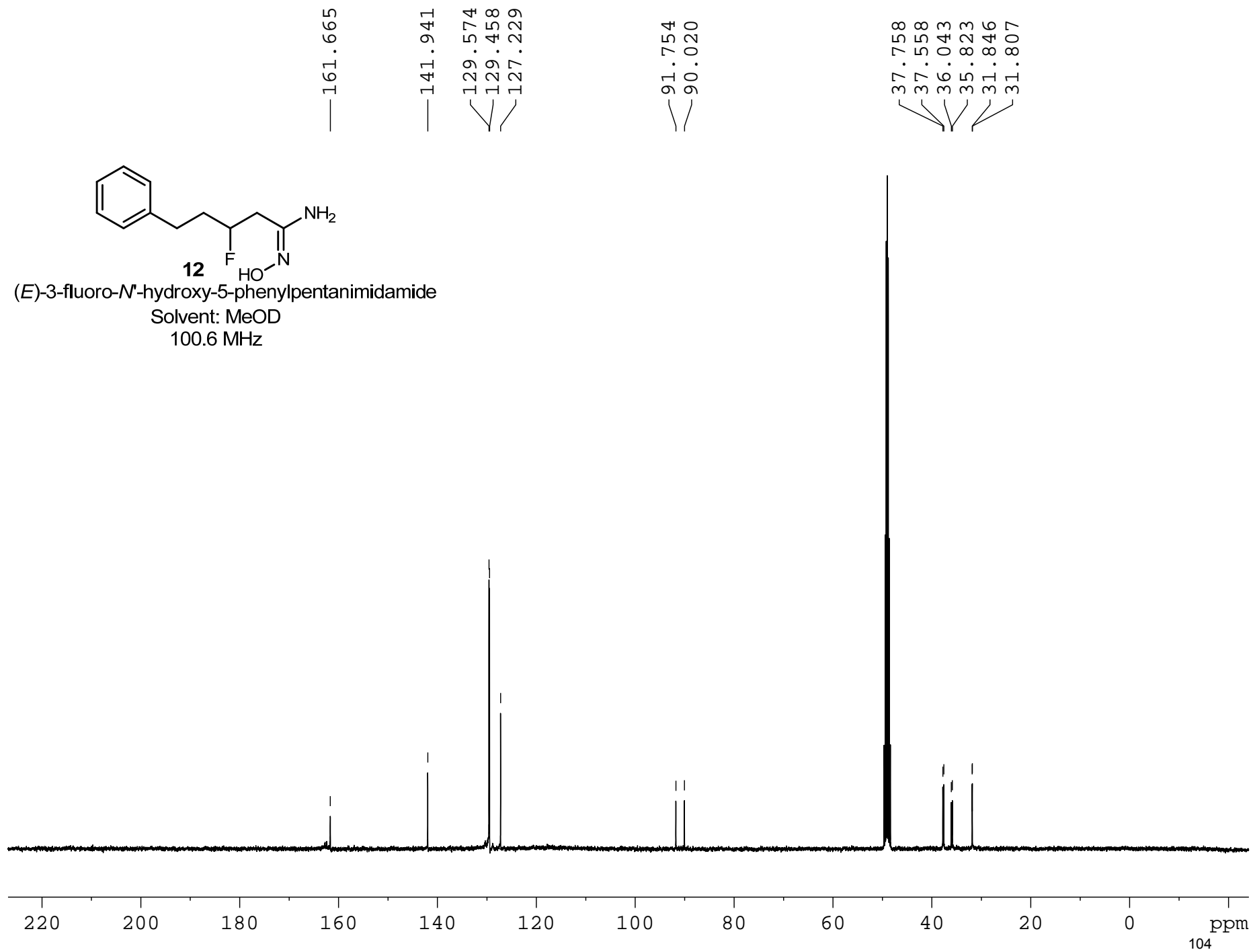


12

(*E*)-3-fluoro-*N*-hydroxy-5-phenylpentanimidamide

Solvent: MeOD

100.6 MHz



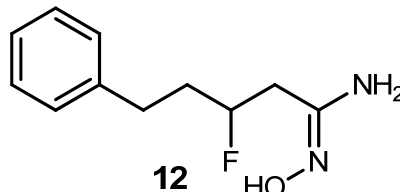
Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -0.5, max = 25.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 2



12
(E)-3-fluoro-N'-hydroxy-5-phenylpentanimidamide

Monoisotopic Mass, Even Electron Ions

70 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

C: 10-500 H: 10-1000 N: 1-200 O: 1-200 F: 1-1

MCO-V-183

S/N: UH193

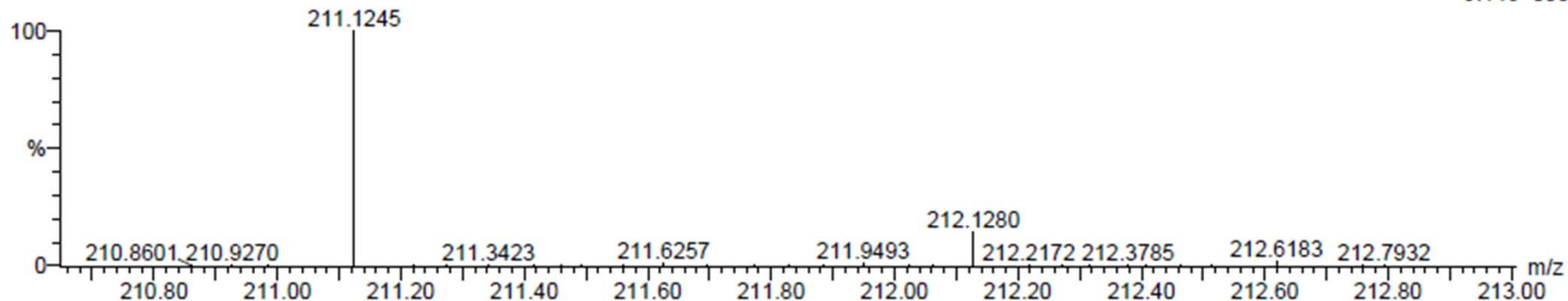
MCO-V-183_041013_001 80 (1.491) AM (Cen,5, 80.00, Ar,8000.0,556.28,0.70); Sm (SG, 2x1.00); Cm (80:90)

10-Apr-2013

10:29:04

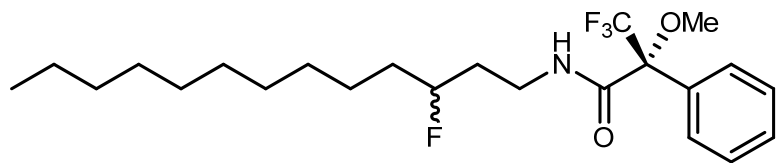
1: TOF MS ES+

9.14e+003

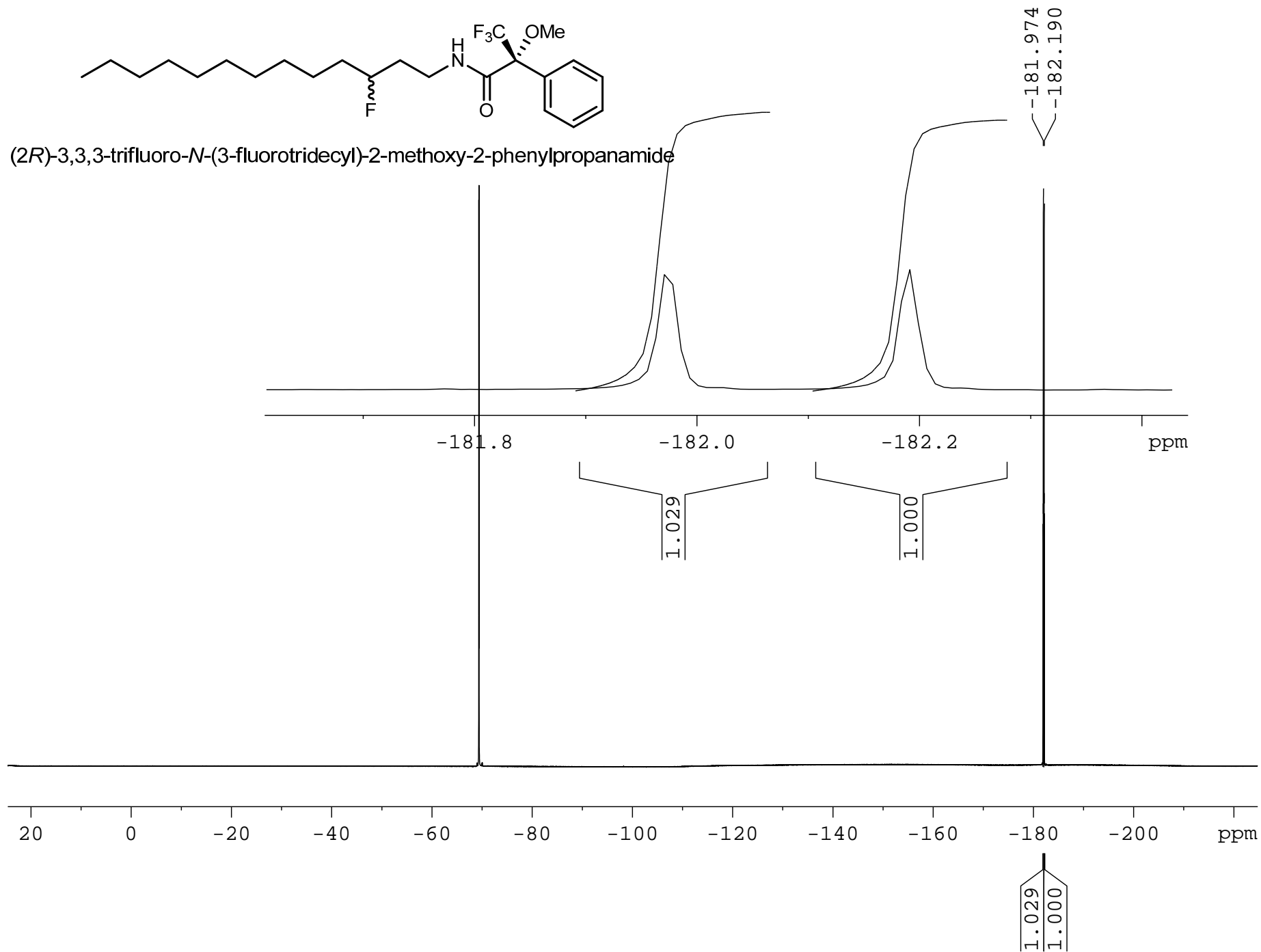


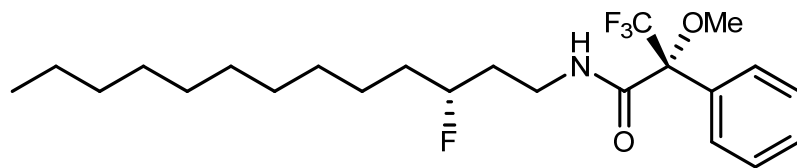
Minimum: -0.5
Maximum: 5.0 5.0 25.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
211.1245	211.1247	-0.2	-0.9	4.5	2.4	C11 H16 N2 O F

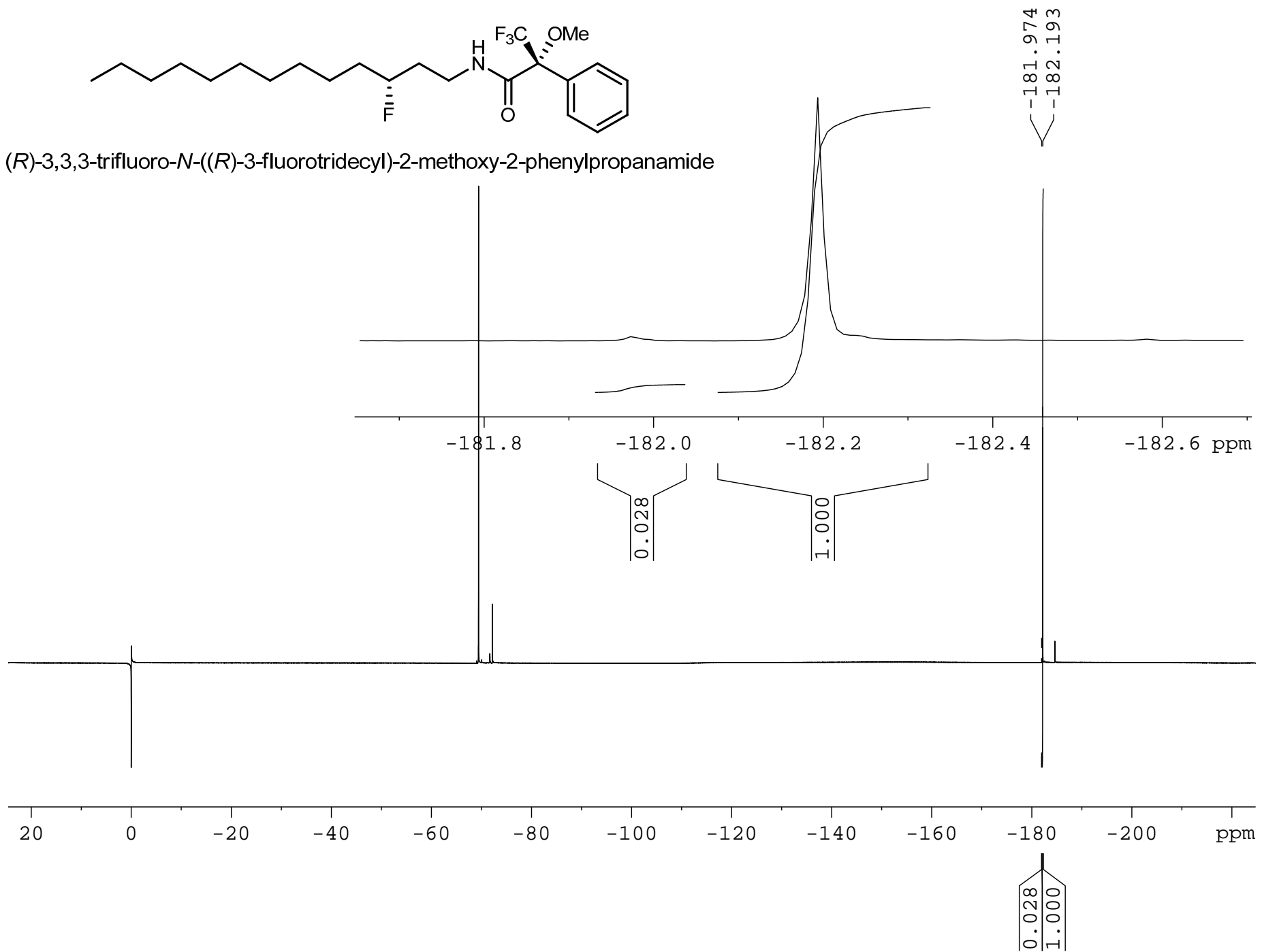


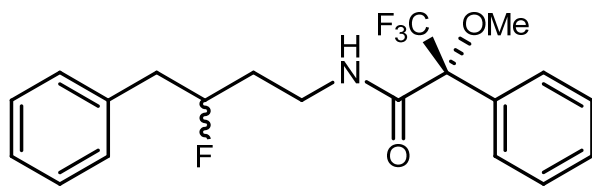
(2R)-3,3,3-trifluoro-N-(3-fluorotridecyl)-2-methoxy-2-phenylpropanamide



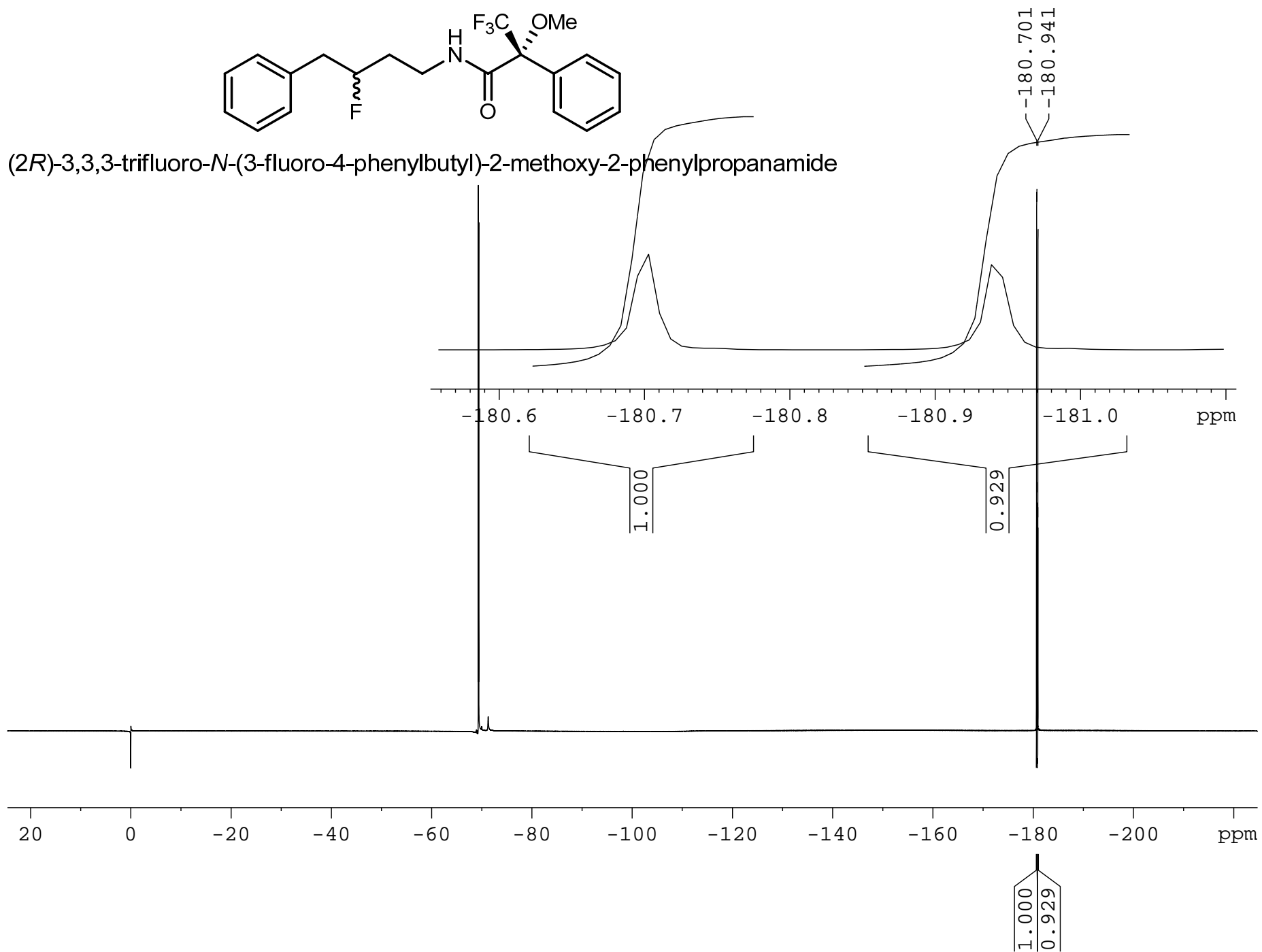


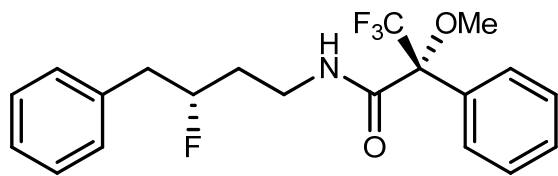
(R)-3,3,3-trifluoro-N-((R)-3-fluorotridecyl)-2-methoxy-2-phenylpropanamide



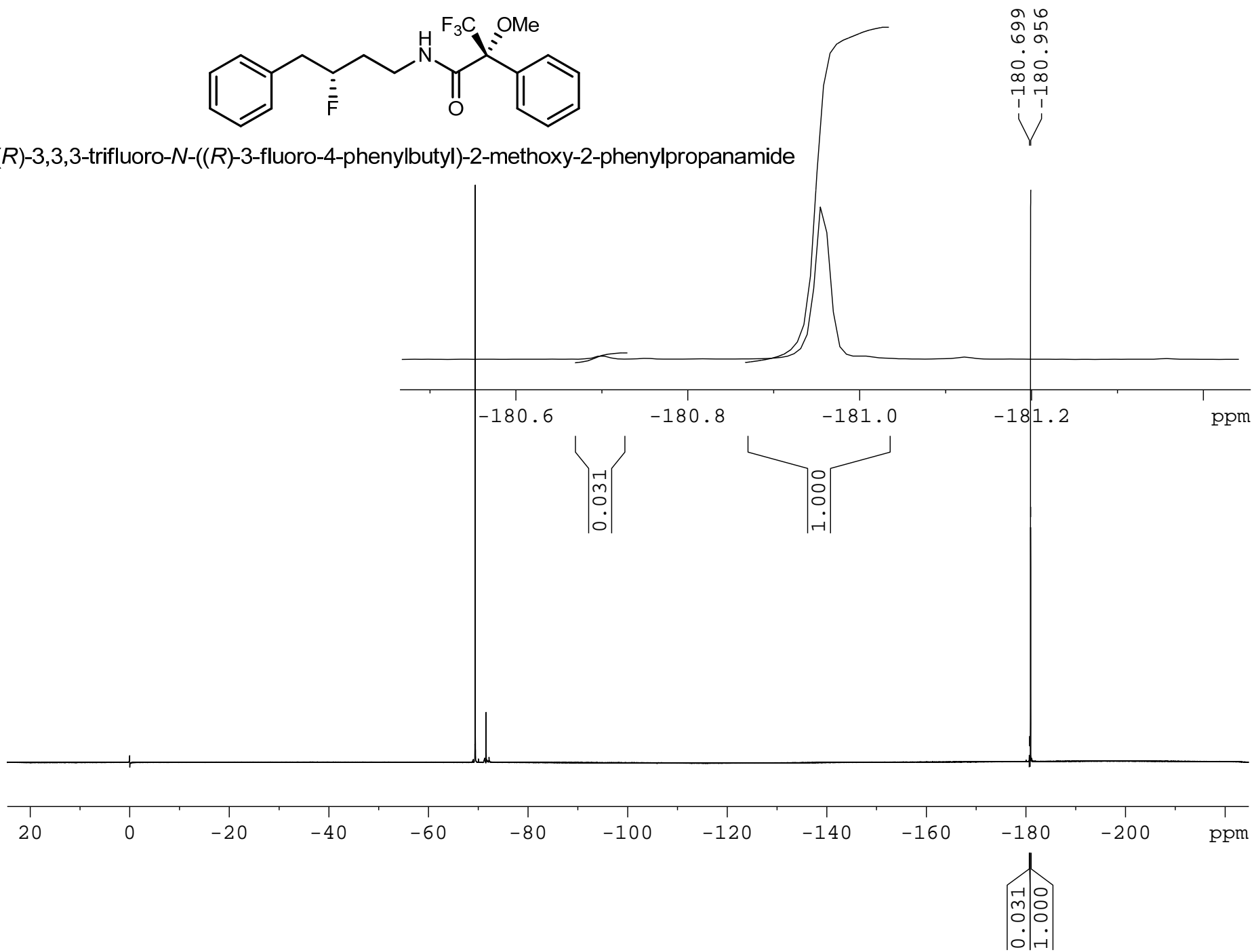


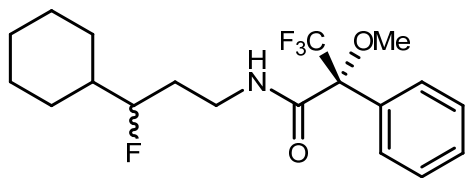
(2R)-3,3,3-trifluoro-N-(3-fluoro-4-phenylbutyl)-2-methoxy-2-phenylpropanamide



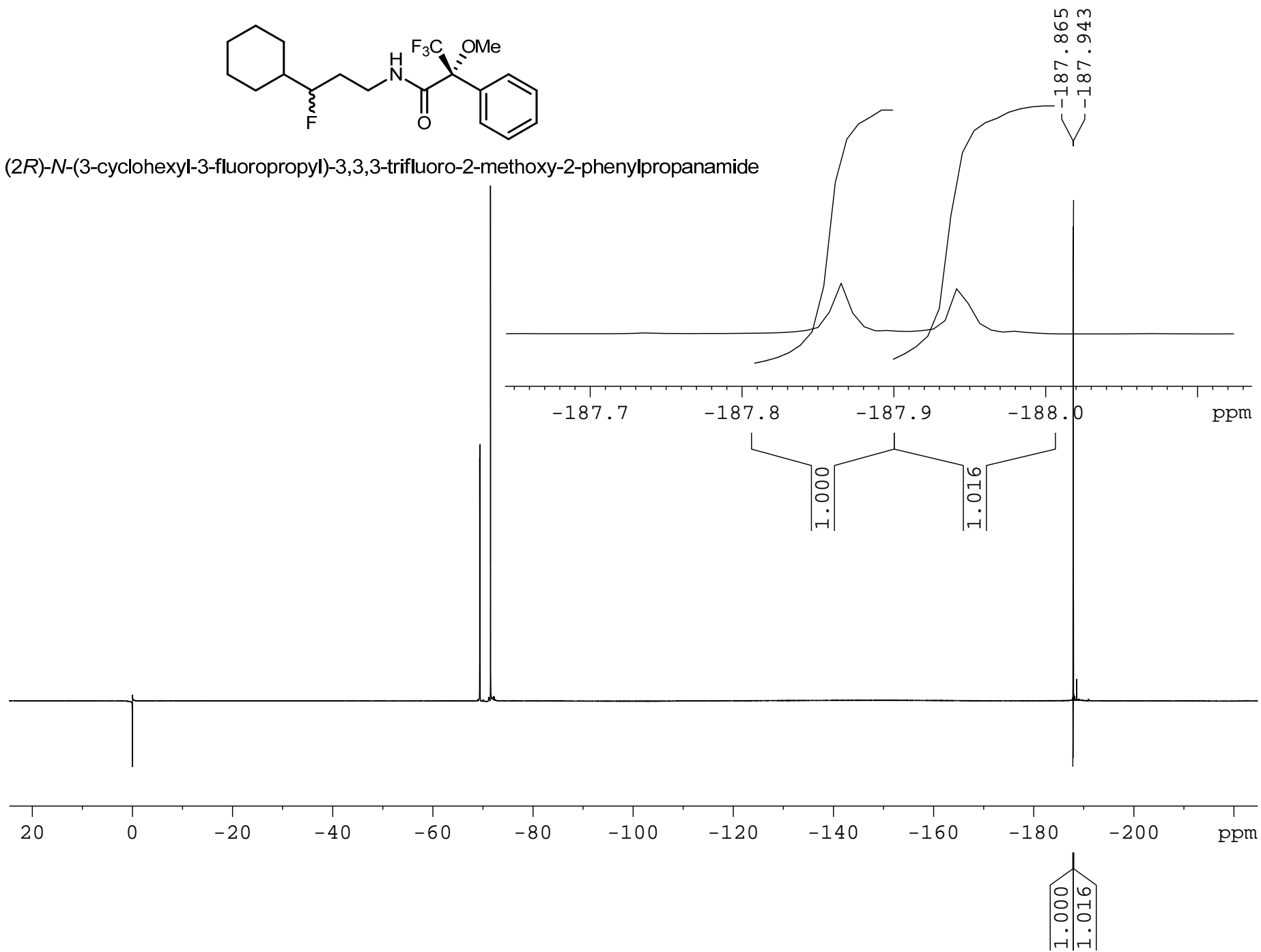


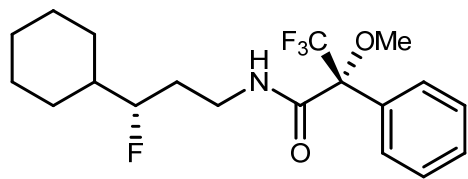
(*R*)-3,3,3-trifluoro-*N*-((*R*)-3-fluoro-4-phenylbutyl)-2-methoxy-2-phenylpropanamide



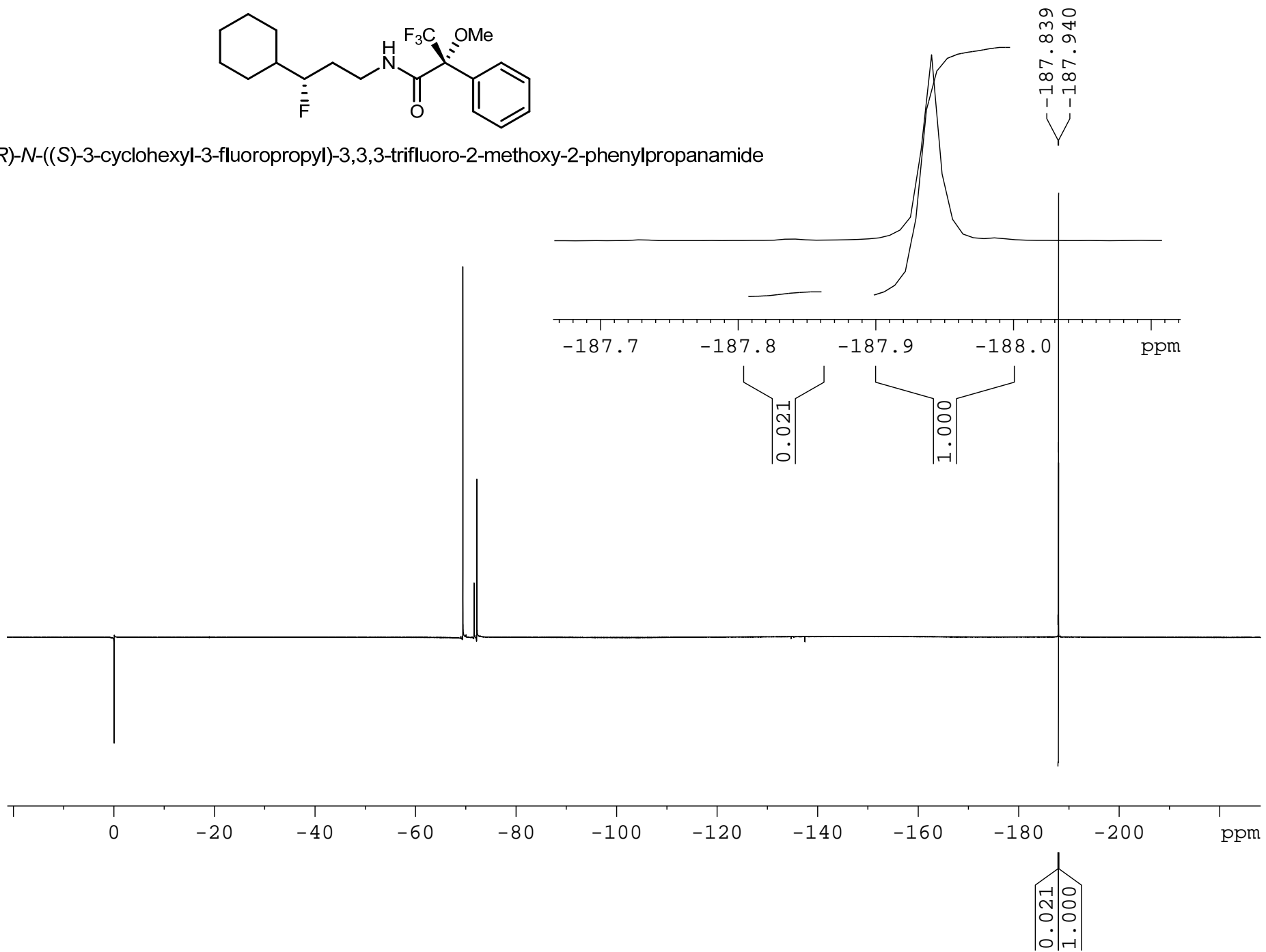


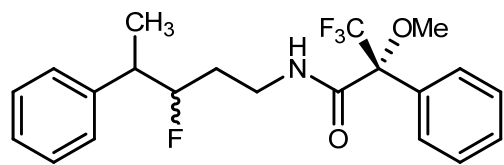
(2R)-N-(3-cyclohexyl-3-fluoropropyl)-3,3,3-trifluoro-2-methoxy-2-phenylpropanamide





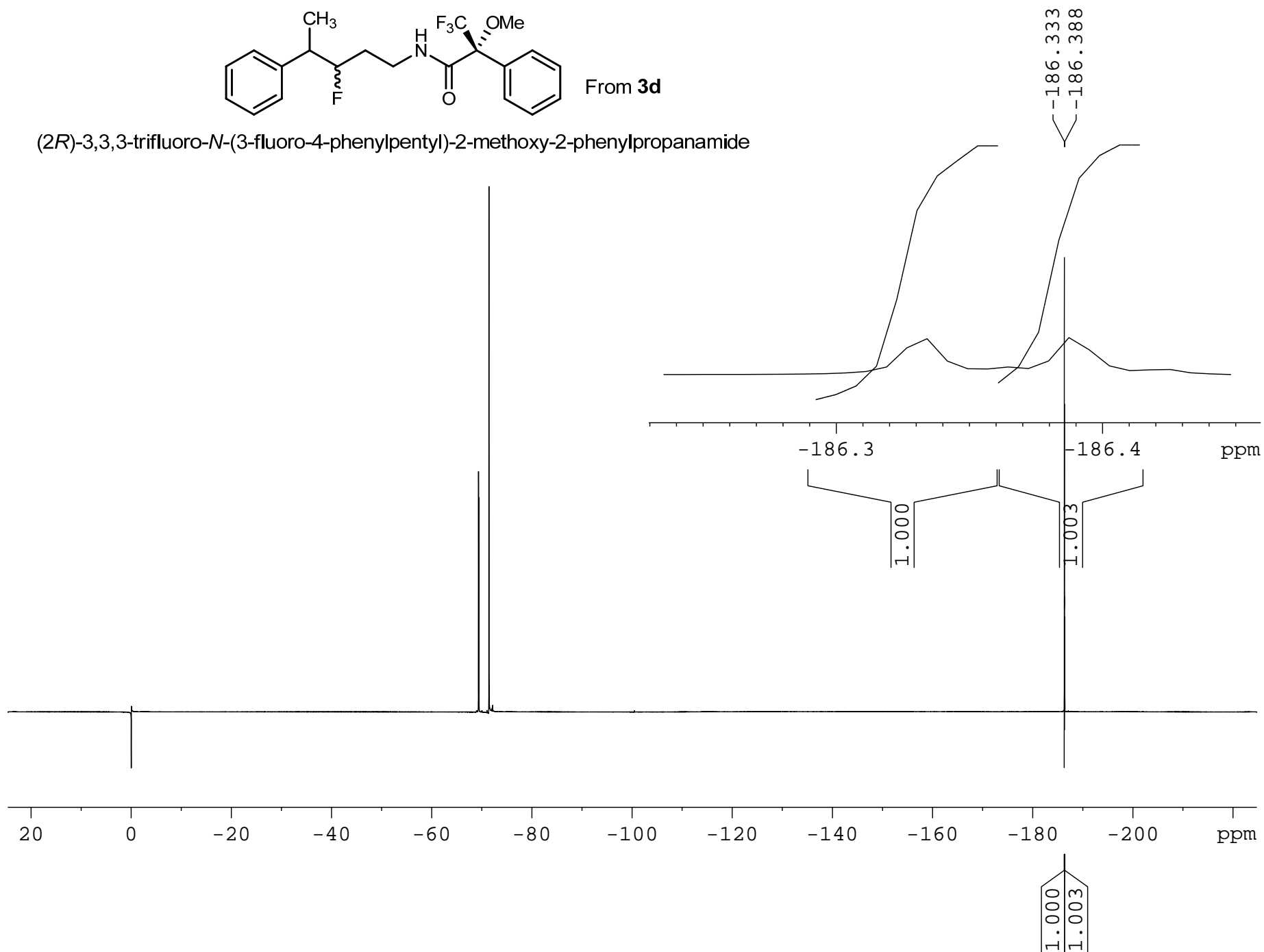
(R)-N-((S)-3-cyclohexyl-3-fluoropropyl)-3,3,3-trifluoro-2-methoxy-2-phenylpropanamide

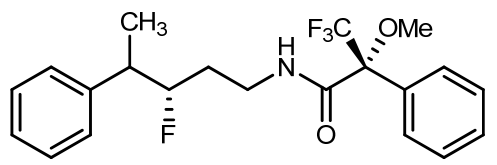




From **3d**

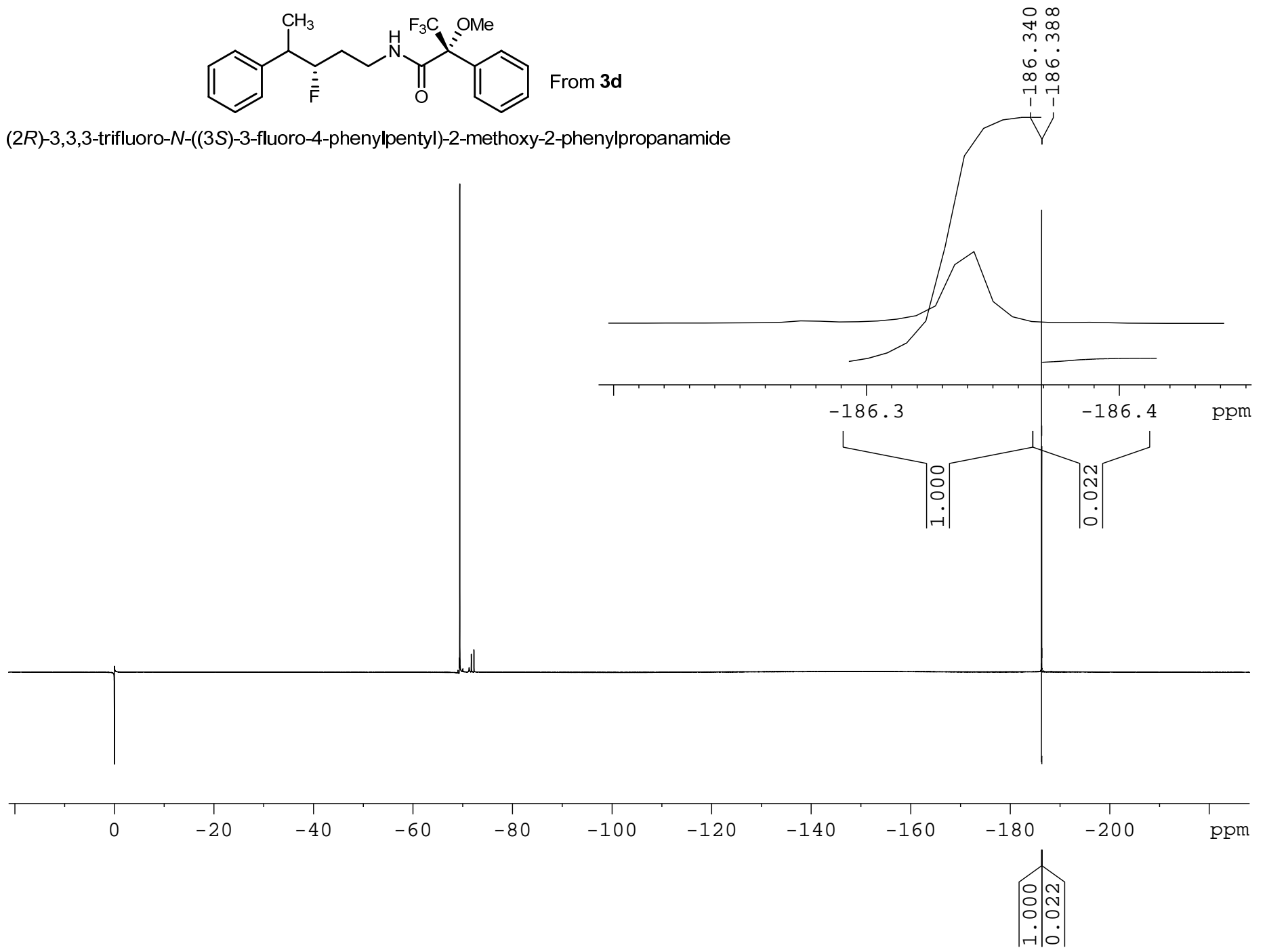
(2*R*)-3,3,3-trifluoro-*N*-(3-fluoro-4-phenylpentyl)-2-methoxy-2-phenylpropanamide

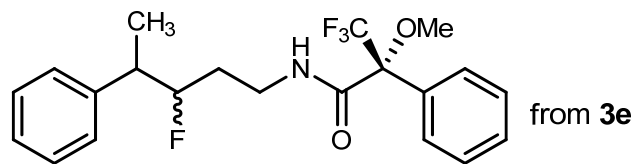




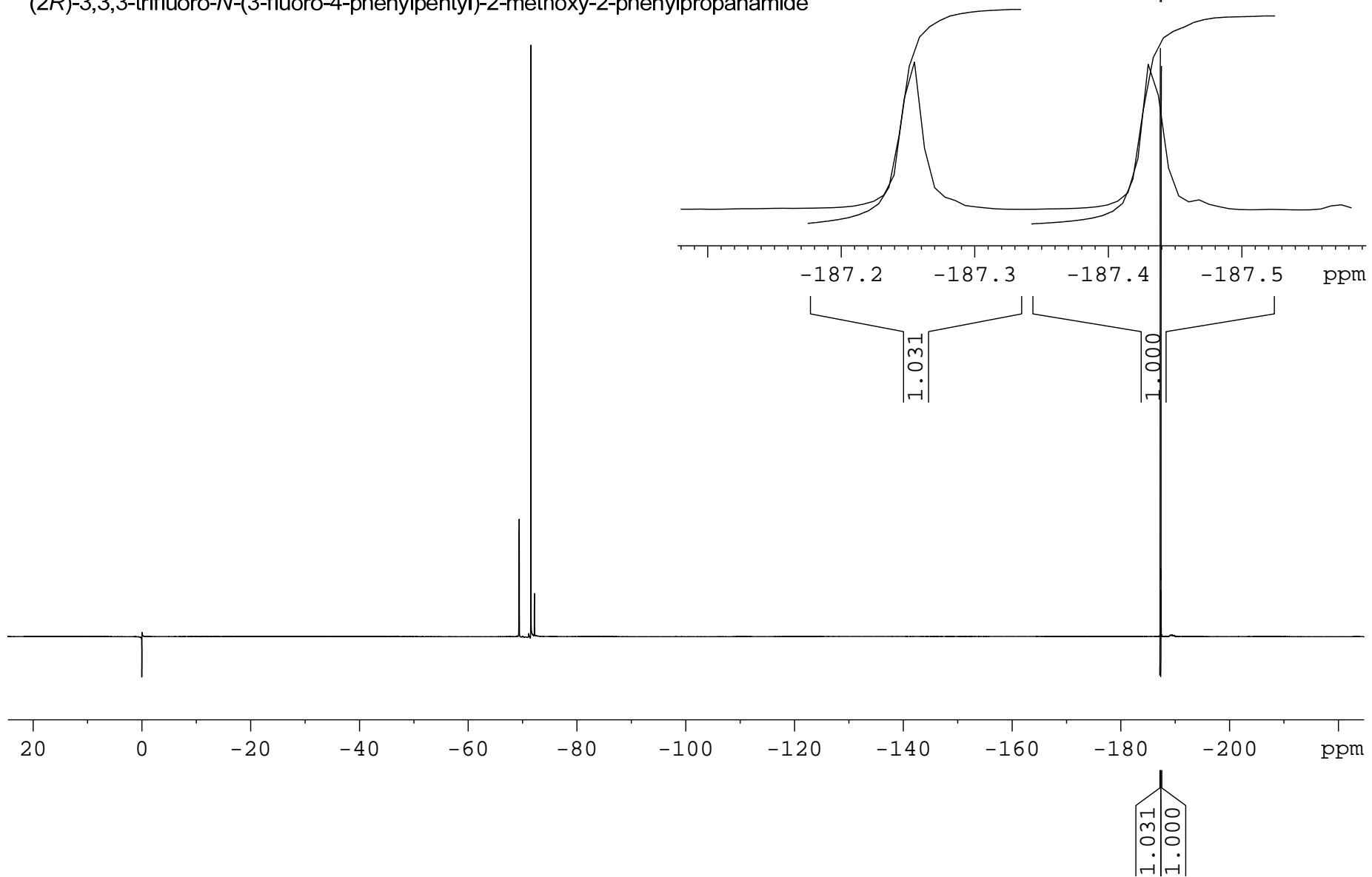
From **3d**

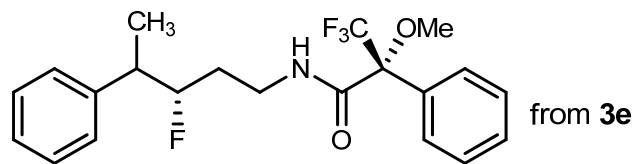
(2*R*)-3,3,3-trifluoro-*N*-((3*S*)-3-fluoro-4-phenylpentyl)-2-methoxy-2-phenylpropanamide



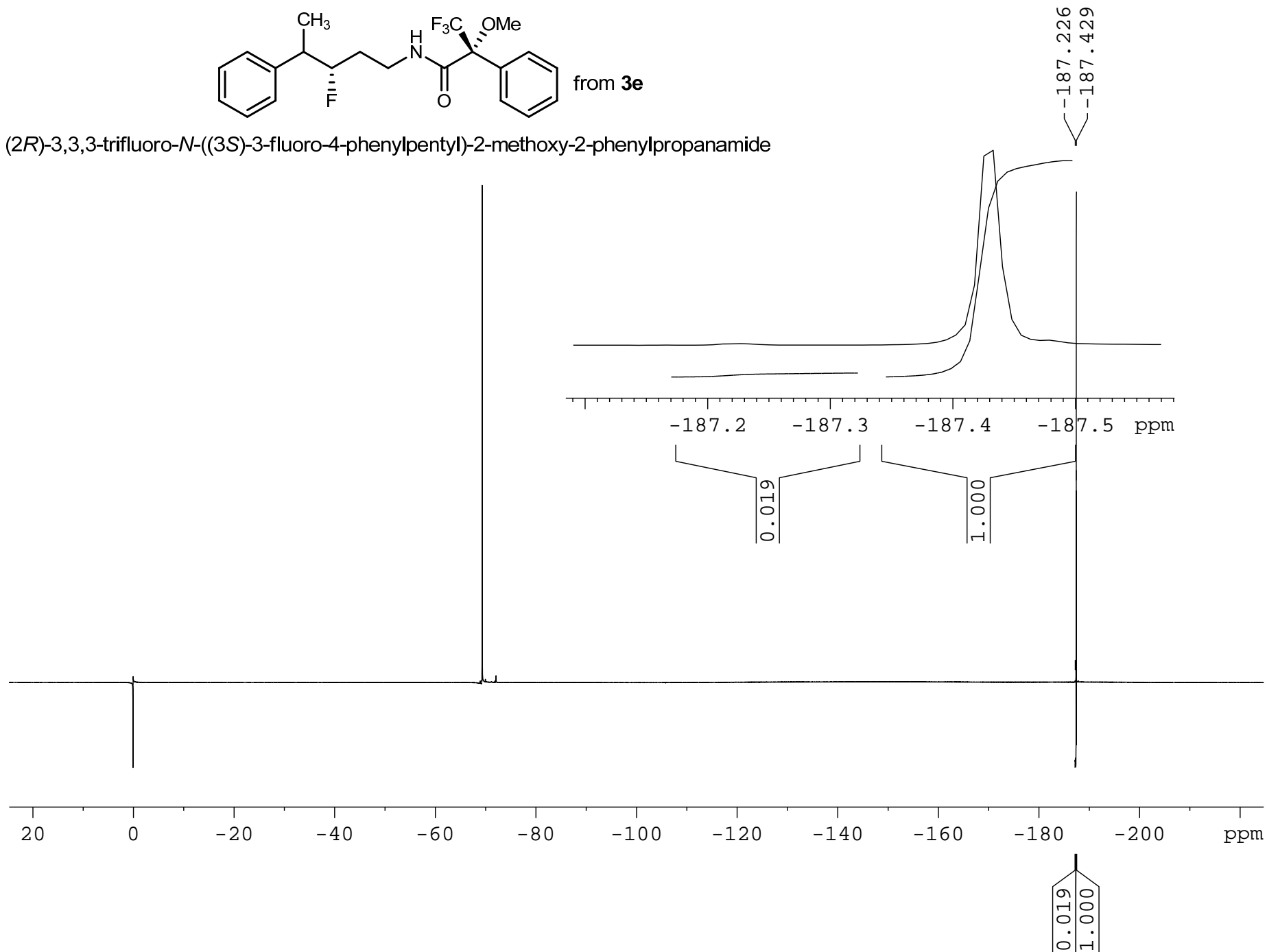


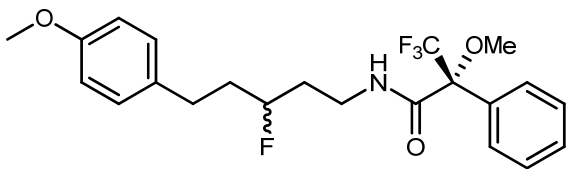
(2*R*)-3,3,3-trifluoro-*N*-(3-fluoro-4-phenylpentyl)-2-methoxy-2-phenylpropanamide





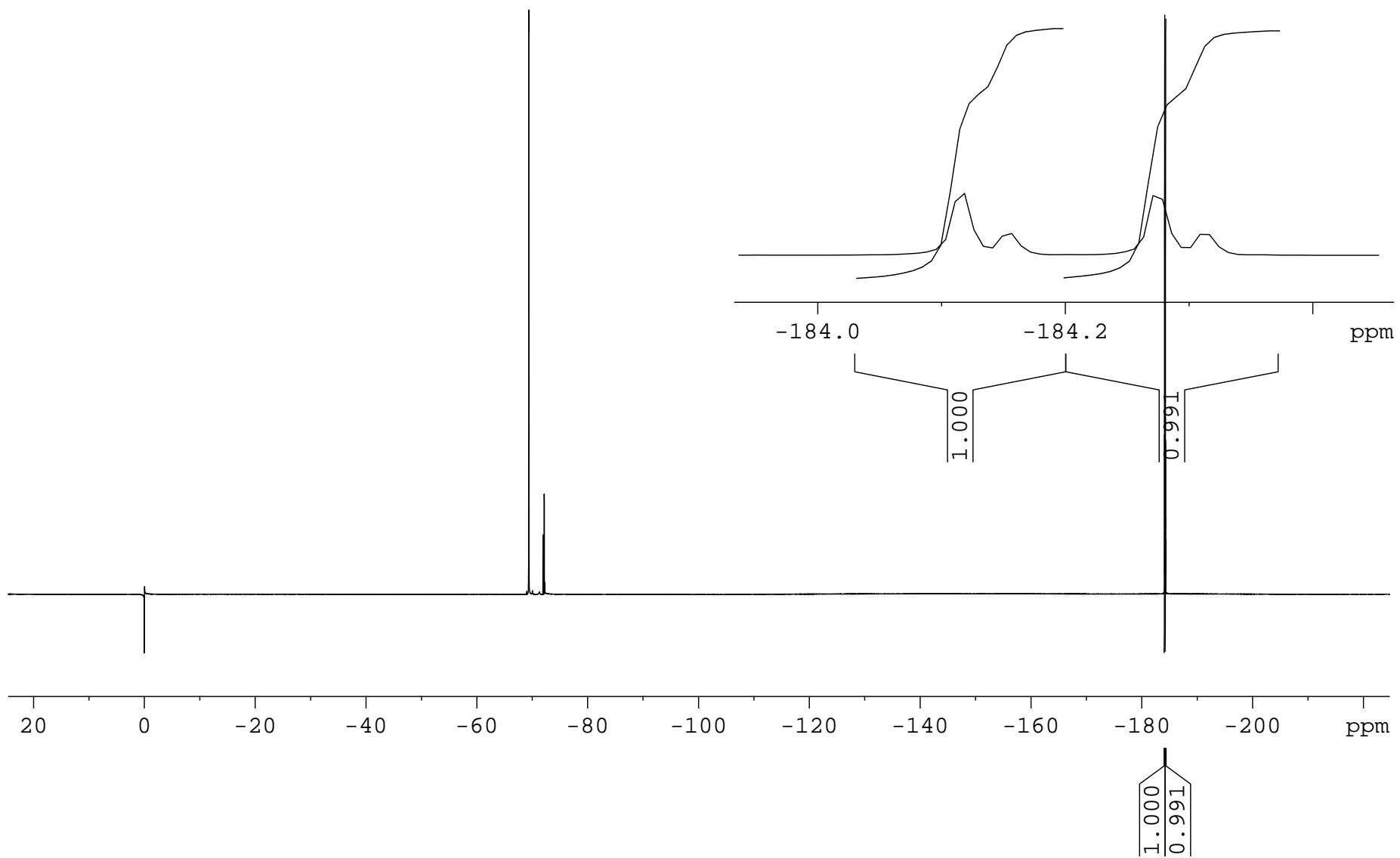
(2*R*)-3,3,3-trifluoro-*N*-((3*S*)-3-fluoro-4-phenylpentyl)-2-methoxy-2-phenylpropanamide

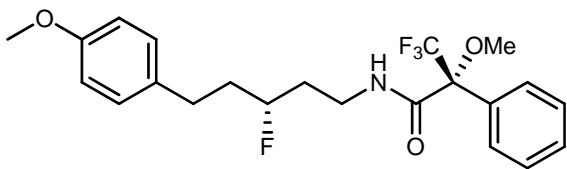




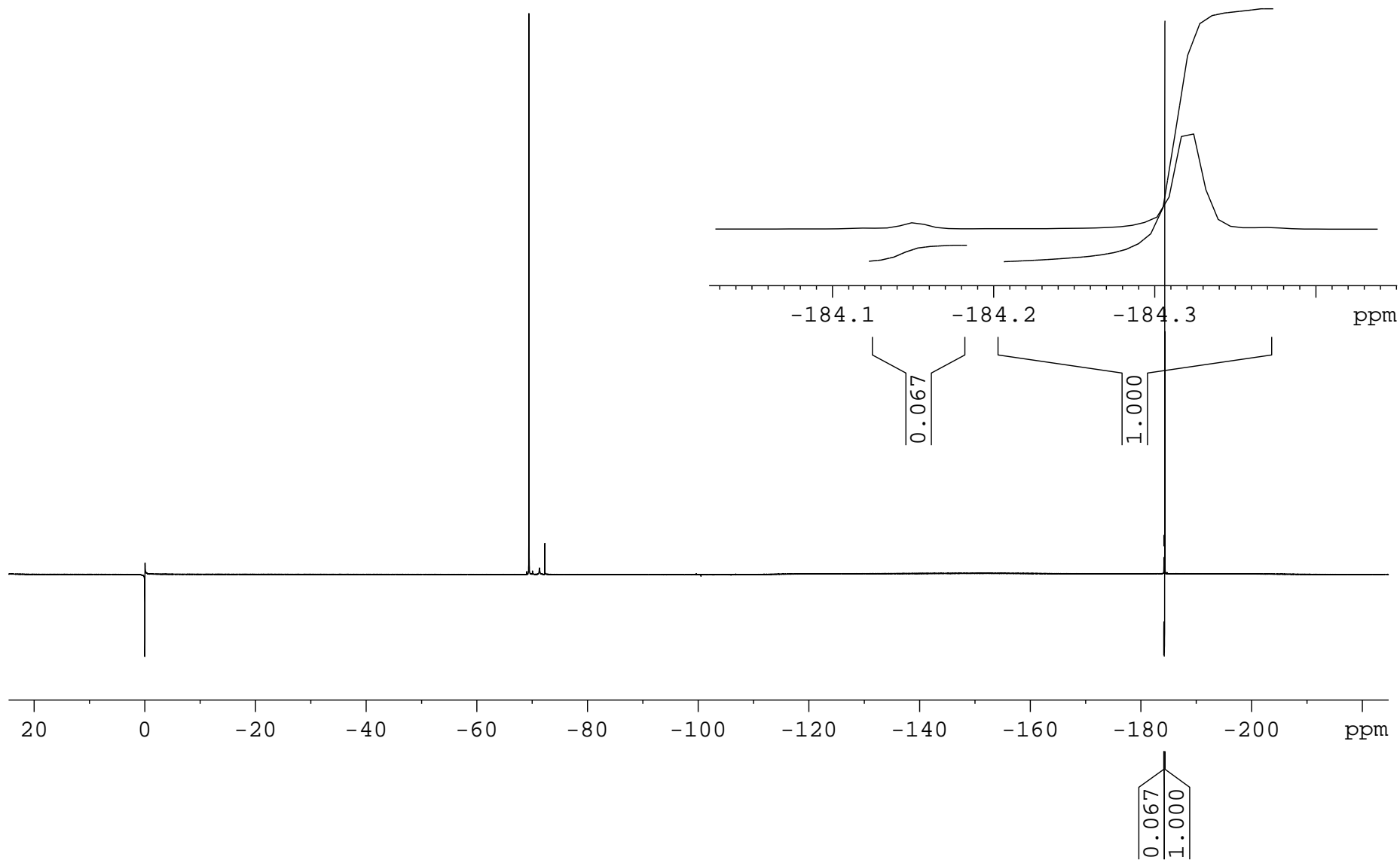
(2R)-3,3,3-trifluoro-N-(3-fluoro-5-(4-methoxyphenyl)pentyl)-2-methoxy-2-phenylpropanamide

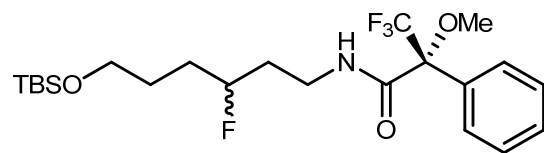
-184.1116
 -184.154
 -184.274
 -184.313



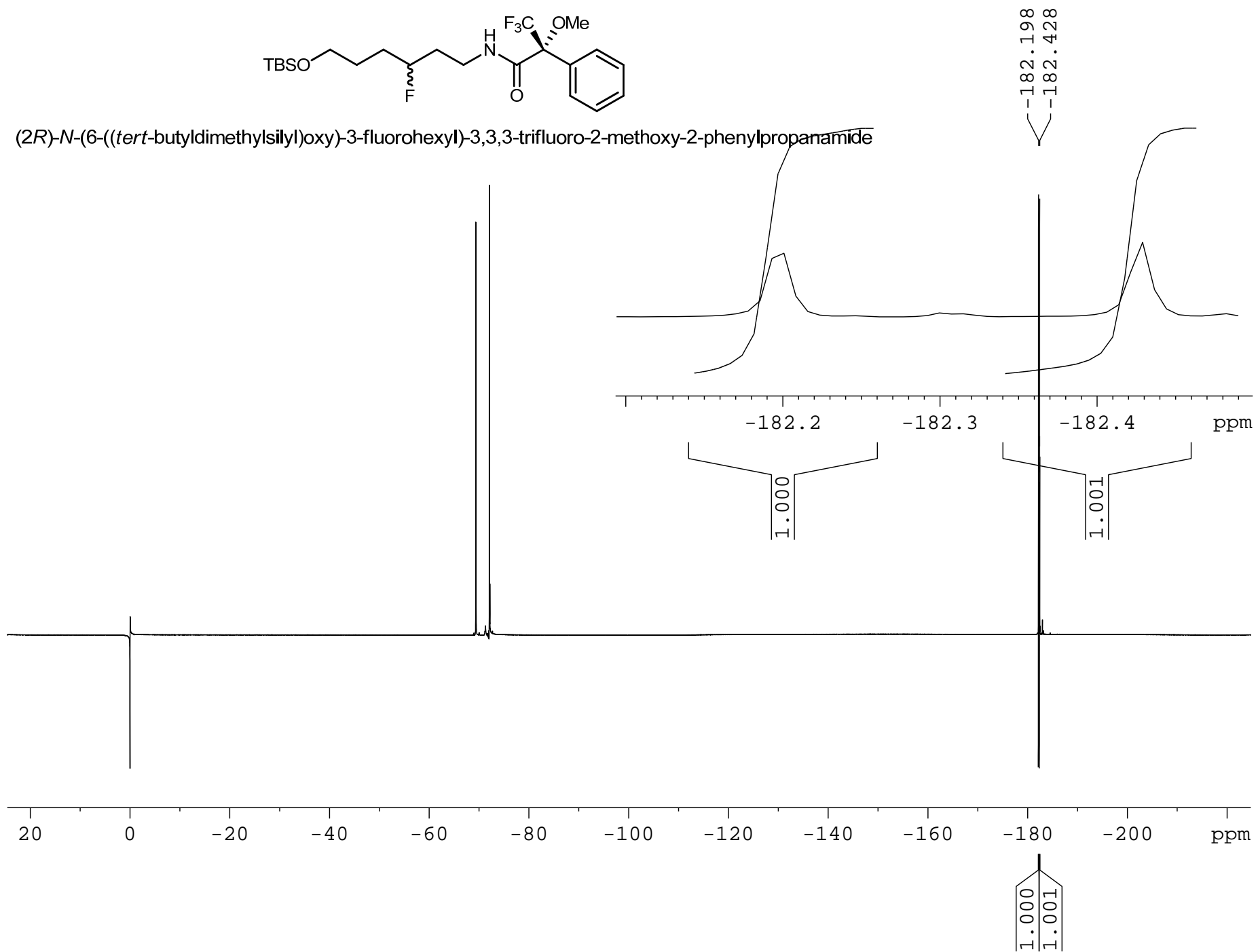


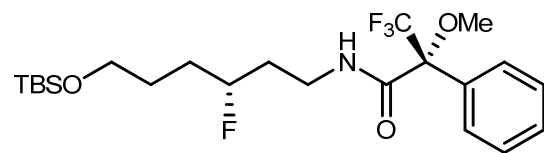
(R)-3,3,3-trifluoro-N-((R)-3-fluoro-5-(4-methoxyphenyl)pentyl)-2-methoxy-2-phenylpropanamide



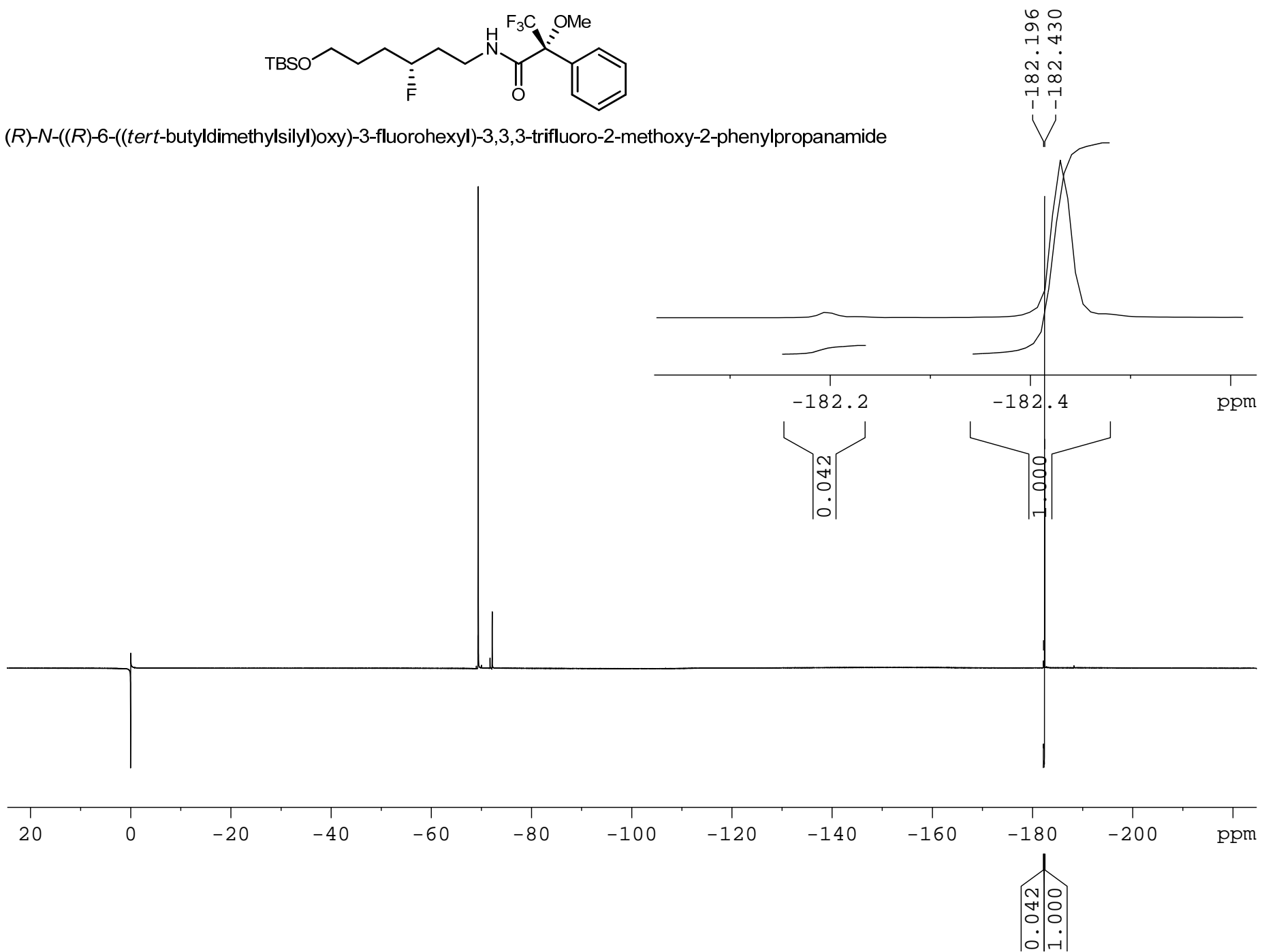


(2R)-N-(6-((*tert*-butyldimethylsilyl)oxy)-3-fluorohexyl)-3,3,3-trifluoro-2-methoxy-2-phenylpropanamide





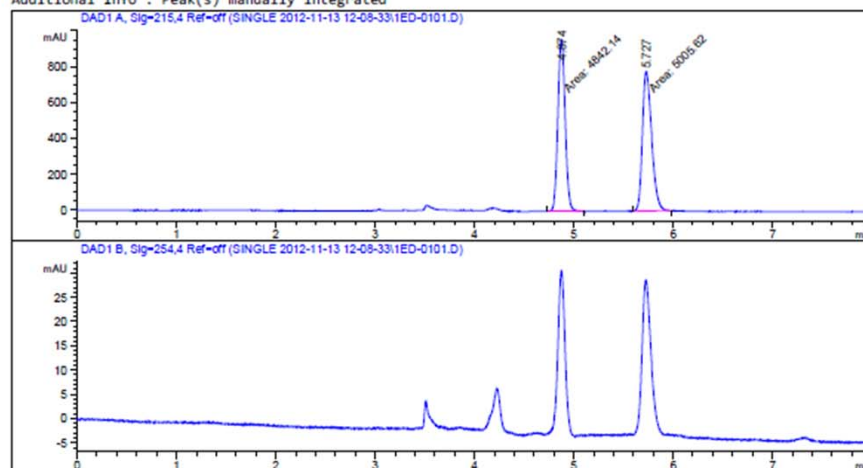
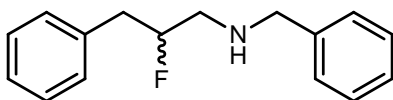
(R)-N-((R)-6-((*tert*-butyldimethylsilyl)oxy)-3-fluorohexyl)-3,3,3-trifluoro-2-methoxy-2-phenylpropanamide



Data File C:\CHEM32\2\DATA\SINGLE 2012-11-13 12-08-33\1ED-0101.D
 Sample Name: MCO-IV-184

```

=====
Acq. Operator   :                               Seq. Line :    1
Acq. Instrument : 12475 LC on SFC                Location  : P1-E-04
Injection Date  : 11/13/2012 12:09:10 PM        Inj       :    1
                                                Inj Volume: 5.000 µl
Different Inj Volume from Sequence ! Actual Inj Volume : 1.000 µl
Acq. Method    : C:\CHEM32\2\DATA\SINGLE 2012-11-13 12-08-33\CHIRALPAK_IA_5_MEOH.M
Last changed   : 11/13/2012 12:08:57 PM
                (modified after loading)
Analysis Method : C:\CHEM32\2\METHODS\CHIRALPAK_IC_5_MEOH.M
Last changed   : 11/13/2012 11:19:48 AM
                (modified after loading)
Additional Info : Peak(s) manually integrated
  
```



Area Percent Report

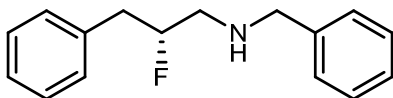
```

Sorted By      :      Signal
Multiplier:    :      1.0000
Dilution:      :      1.0000
Use Multiplier & Dilution Factor with ISTDs
  
```

Signal 1: DAD1 A, Sig=215,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.874	MM	0.0841	4842.13574	959.32269	49.1699
2	5.727	MM	0.1071	5005.61963	778.75336	50.8301

Totals : 9847.75537 1738.07605

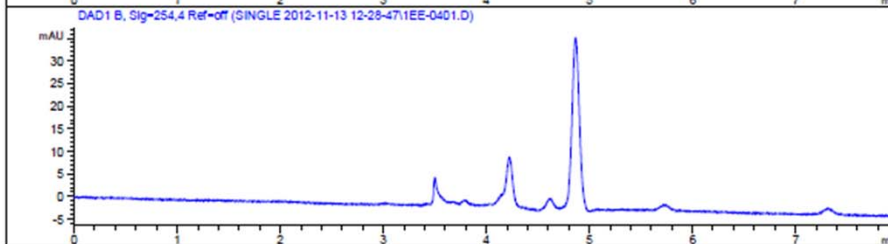
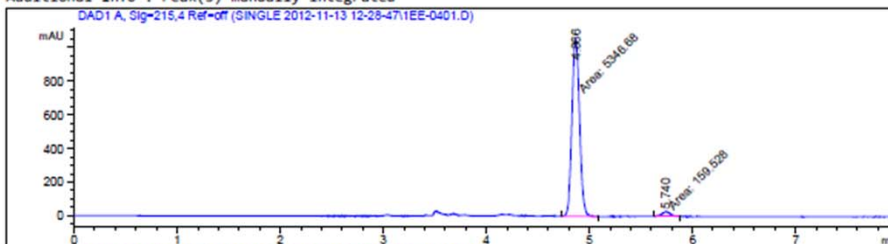


94% ee

Data File C:\CHEM32\2\DATA\SINGLE 2012-11-13 12-28-47\1EE-0401.D
 Sample Name: MCO-V-20

```

=====
Acq. Operator   :                               Seq. Line :    4
Acq. Instrument : 12475 LC on SFC                 Location  : P1-E-05
Injection Date  : 11/13/2012 12:53:32 PM         Inj       :    1
                                                Inj Volume: 5.000 µl
Different Inj Volume from Sequence !   Actual Inj Volume : 1.000 µl
Acq. Method    : C:\CHEM32\2\DATA\SINGLE 2012-11-13 12-28-47\CHIRALPAK_IA_5_MEOH.M
Last changed   : 11/13/2012 12:35:48 PM
                (modified after loading)
Analysis Method: C:\CHEM32\2\METHODS\CHIRALPAK_IC_5_MEOH.M
Last changed   : 11/13/2012 11:19:48 AM
                (modified after loading)
Additional Info : Peak(s) manually integrated
  
```



=====
 Area Percent Report
 =====

```

Sorted By      :      Signal
Multiplier:    :      1.0000
Dilution:      :      1.0000
Use Multiplier & Dilution Factor with ISTDs
  
```

Signal 1: DAD1 A, Sig=215,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.866	MM	0.0839	5346.67529	1062.06238	97.1028
2	5.740	MM	0.0988	159.52835	26.91542	2.8972

Totals : 5506.20364 1088.97780

Data File C:\CHEM32\2\DATA\SINGLE 2012-11-13 10-55-36\1EC-0101.D
Sample Name: MCO-IV-185

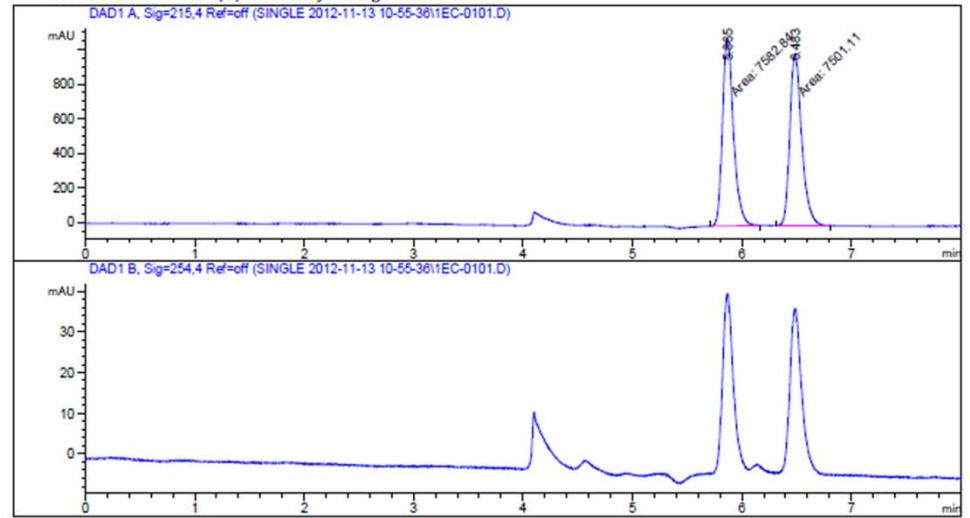
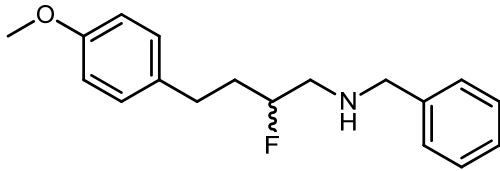
=====

Acq. Operator	:		Seq. Line	:	1
Acq. Instrument	:	12475 LC on SFC	Location	:	P1-E-03
Injection Date	:	11/13/2012 11:01:13 AM	Inj	:	1
			Inj Volume	:	5.000 µl

Different Inj Volume from Sequence ! Actual Inj Volume : 2.000 µl

Acq. Method	:	C:\CHEM32\2\DATA\SINGLE 2012-11-13 10-55-36\CHIRALPAK_IB_3_MEOH.M
Last changed	:	11/13/2012 11:08:26 AM (modified after loading)
Analysis Method	:	C:\CHEM32\2\METHODS\CHIRALPAK_IC_5_MEOH.M
Last changed	:	11/13/2012 11:19:48 AM (modified after loading)

Additional Info : Peak(s) manually integrated



=====
Area Percent Report
=====

Sorted By : Signal
Multiplier: : 1.0000
Dilution: : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=215,4 Ref=off

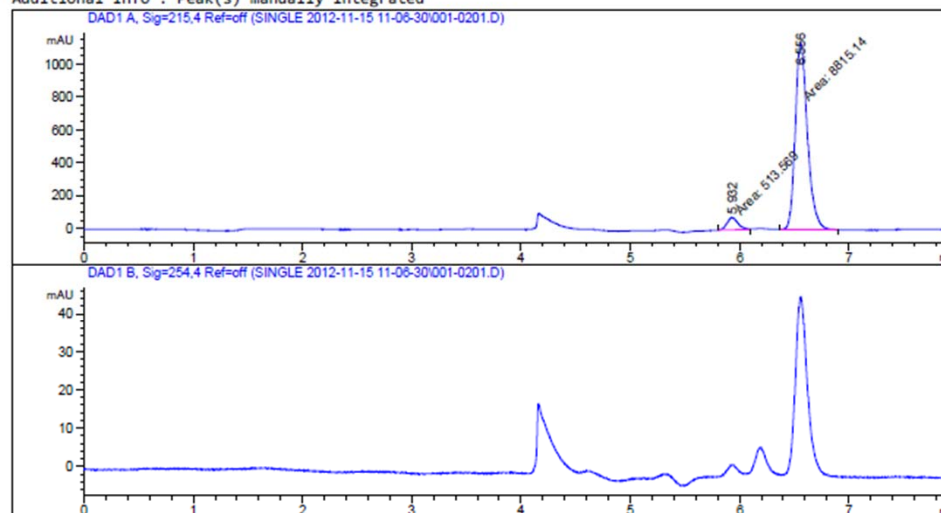
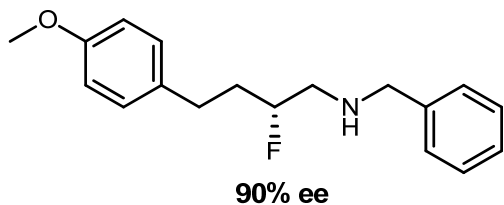
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.865	MM	0.1166	7582.83887	1083.60217	50.2709
2	6.483	MM	0.1255	7501.11475	996.49432	49.7291

Totals : 1.50840e4 2080.09650

Data File C:\CHEM32\2\DATA\SINGLE 2012-11-15 11-06-30\001-0201.D
 Sample Name: MCO-V-25

```

=====
Acq. Operator   :                               Seq. Line :    2
Acq. Instrument : 12475 LC on SFC                Location  : Vial 1
Injection Date  : 11/15/2012 11:16:55 AM        Inj       :    1
                                                Inj Volume: 5.000 µl
Different Inj Volume from Sequence !      Actual Inj Volume : 2.500 µl
Acq. Method    : C:\CHEM32\2\DATA\SINGLE 2012-11-15 11-06-30\CHIRALPAK_IB_3_MEOH.M
Last changed   : 11/15/2012 10:55:44 AM
Analysis Method : C:\CHEM32\2\DATA\SINGLE 2012-11-15 11-06-30\001-0201.D\DA.M (CHIRALPAK_IB_
                3_MEOH.M, From Data File)
Last changed   : 11/15/2012 11:26:56 AM
                (modified after loading)
Additional Info : Peak(s) manually integrated
  
```



Area Percent Report

```

Sorted By      :      Signal
Multiplier:    :      1.0000
Dilution:      :      1.0000
Use Multiplier & Dilution Factor with ISTDs
  
```

Signal 1: DAD1 A, Sig=215,4 Ref=off

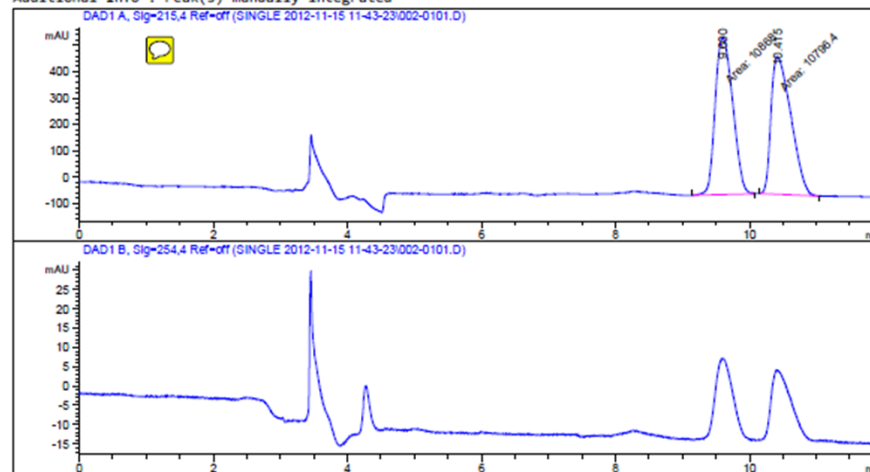
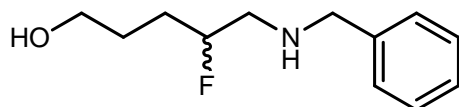
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.932	MM	0.1156	513.56860	74.04364	5.5052
2	6.556	MM	0.1293	8815.13965	1136.69775	94.4948

Totals : 9328.70825 1210.74139

Data File C:\CHEM32\2\DATA\SINGLE 2012-11-15 11-43-23\002-0101.D
 Sample Name: MCO-V-14

```

=====
Acq. Operator   :                               Seq. Line :    1
Acq. Instrument : 12475 LC on SFC                Location  : Vial 2
Injection Date  : 11/15/2012 11:44:39 AM        Inj       :    1
                                                Inj Volume: 5.000 µl
Different Inj Volume from Sequence !   Actual Inj Volume : 15.000 µl
Acq. Method    : C:\CHEM32\2\DATA\SINGLE 2012-11-15 11-43-23\CHIRALPAK_ID_7_MEOH.M
Last changed   : 11/15/2012 11:36:24 AM
Analysis Method: C:\CHEM32\2\DATA\SINGLE 2012-11-15 11-43-23\002-0101.D\DA.M (CHIRALPAK_ID_
7_MEOH.M, From Data File)
Last changed   : 11/15/2012 2:24:41 PM
                (modified after loading)
Additional Info : Peak(s) manually integrated
  
```



Area Percent Report

```

Sorted By      :      Signal
Multiplier:    :      1.0000
Dilution:      :      1.0000
Use Multiplier & Dilution Factor with ISTDs
  
```

Signal 1: DAD1 A, Sig=215,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	9.600	MM	0.3032	1.08680e4	597.32648	50.1652
2	10.415	MM	0.3431	1.07964e4	524.43738	49.8348

Totals : 2.16643e4 1121.76385

Data File C:\CHEM32\2\DATA\SINGLE 2012-11-15 12-27-32\003-0101.D
Sample Name: MCO-V-26

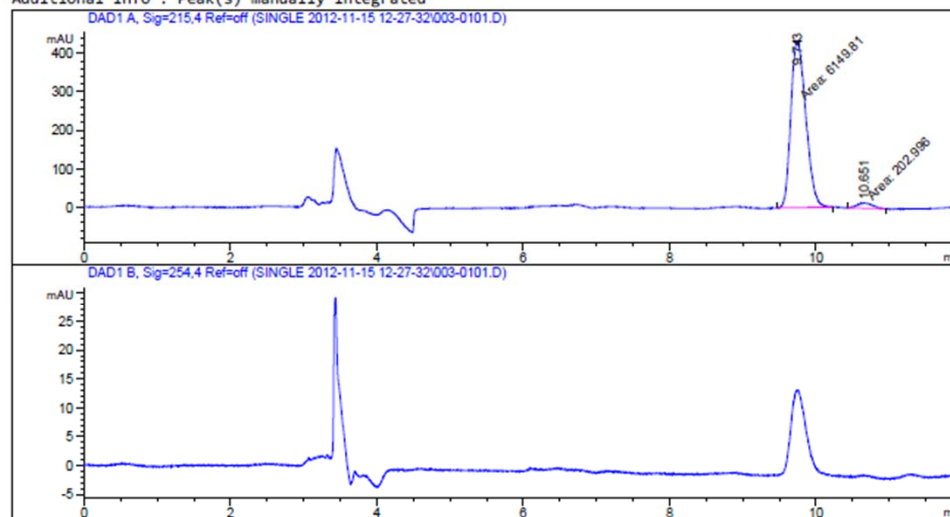
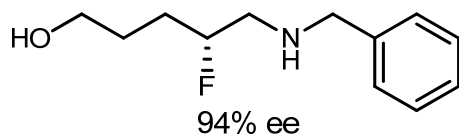
=====

Acq. Operator	:		Seq. Line	:	1
Acq. Instrument	:	12475 LC on SFC	Location	:	Vial 3
Injection Date	:	11/15/2012 12:28:55 PM	Inj	:	1
			Inj Volume	:	5.000 µl

Different Inj Volume from Sequence ! Actual Inj Volume : 10.000 µl

Acq. Method	:	C:\CHEM32\2\DATA\SINGLE 2012-11-15 12-27-32\CHIRALPAK_ID_7_MEOH.M
Last changed	:	11/15/2012 12:40:48 PM (modified after loading)
Analysis Method	:	C:\CHEM32\2\DATA\SINGLE 2012-11-15 12-27-32\003-0101.D\DA.M (CHIRALPAK_ID_7_MEOH.M, From Data File)
Last changed	:	11/15/2012 12:41:31 PM (modified after loading)

Additional Info : Peak(s) manually integrated



=====
Area Percent Report
=====

Sorted By : Signal
Multiplier: : 1.0000
Dilution: : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=215,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	9.743	MM	0.2379	6149.81494	430.90405	96.8046
2	10.651	MM	0.2380	202.99626	14.21245	3.1954

Totals : 6352.81120 445.11650