



Supporting Information

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A Highly Enantioselective Brønsted Acid Catalyzed Reaction Cascade

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General: Unless otherwise noted, all commercially available compounds were used as provided without further purification. Solvents for chromatography were technical grade and distilled prior to use. Benzene used in reaction was reagent grade and distilled from P₂O₅. Analytical thin-layer chromatography (TLC) was performed on Merck silica gel aluminium plates with F-254 indicator, visualised by irradiation with UV light. Column chromatography was performed using silica gel Merck 60 (particle size 0.040-0.063 mm). Solvent mixtures are understood as volume/volume.

¹H-NMR and ¹³C-NMR were recorded on a Bruker AM 250 or a Bruker AV 300 spectrometer in CDCl₃. Data are reported in the following order: chemical shift (δ) in ppm; multiplicities are indicated br s (broadened singlet), s (singlet), d (doublet), t (triplet), q (quartet), m (multiplet); coupling constants (J) are in Hertz (Hz). Mass spectra (MS-EI, 70 eV) were conducted on GC-MS Shimadzu QP2010 (column: Equity[®]-5, length × I.D. 30 m × 0.25 mm, d_f 0.25 μm, lot # 28089-U, Supelco). IR spectra were recorded on a Jasco FT/IR-420 spectrometer and are reported in terms of frequency of absorption (cm⁻¹). Optical rotations were measured on a Perkin Elmer 241 polarimeter. The enantiomeric excesses were determined by HPLC analysis using a chiral stationary phase column (column: CHIRALCEL OD-H or CHIRALCEL AS-H or CHIRALPAK AD-H; eluent: hexane/2-propanol). The chiral HPLC methods were calibrated with the corresponding racemic mixtures. Chemical yields refer to pure isolated substances. The yields and enantiomeric excesses are given in table.

General procedure: Enamine (0.250 mmol, 3-aminocyclohex-2-en-1-one or 3-aminobut-2-enenitrile or 4-aminopent-3-en-2-one or methyl 3-aminobut-2-enoate), phosphoric acid (5 mol%), Hantzsch dihydropyridine (1.1 equiv.), vinyl ketone (1.2 equiv.) and molecular sieves (3Å, Alfa Aesar®, Item #:L05335) were suspended in benzene (2 mL) or in chloroform (3 mL, for 3-aminocyclohex-2-enone) in a screw-capped vial and flushed with argon. The resulting mixture was allowed to stir at 50°C for 12-18 h. The solvent was removed under reduced pressure and purification of the crude product by column chromatography on silica gel (ethyl acetate/hexane) afforded the pure product.

Physical data:

(2S)-2-Phenyl-2,3,4,6,7,8-hexahydroquinolin-5(1H)-one

¹H-NMR (300 MHz, CDCl₃, 25 °C, TMS): δ=7.32-7.16 (m, 5H), 4.87 (br s, 1H), 4.31 (ddd, 1H, J=1.3, 3.7, 8.4 Hz), 2.41-2.16 (m, 6H), 2.03-1.52 (m, 3H), 1.80-1.65 ppm (m, 1H); ¹³C-NMR (75 MHz, CDCl₃, 25 °C, TMS): δ=194.49, 158.78, 142.72, 128.74, 127.81, 126.35, 105.17, 55.95, 36.42, 29.93, 29.31, 21.77, 18.05 ppm; IR (KBr): $\tilde{\nu}$ =3274, 2937, 2915, 1599, 1564, 1516, 1402, 1287, 1187, 1107, 1020 cm⁻¹; MS-EI: m/z(%): 228 (4) [M+H]⁺, 227 (26) [M]⁺, 212 (16), 170 (23), 156 (13), 148 (16), 136 (30), 130 (11), 128 (10), 120 (14), 115 (21), 104 (76), 103 (37), 94 (19), 93 (19), 91 (49), 78 (96), 77 (100), 65 (31), 51 (53); [α]_D^{RT}=+180.0 (c=1.0 in CHCl₃); HPLC conditions: OD-H column, n-hexane/2-propanol =

80/20, flow rate = 0.6 mL min⁻¹, major enantiomer: t_R=32.7 min;
minor enantiomer: t_R=50.3 min.

(2S)-2-(4-Methylphenyl)-2,3,4,6,7,8-hexahydroquinolin-5(1H)-one

¹H-NMR (300 MHz, CDCl₃, 25 °C, TMS): δ=7.12-7.04 (m, 4H), 4.76 (br s, 1H), 4.26 (ddd, 1H, J=1.3, 3.6, 8.6 Hz), 2.43-2.14 (m, 9H), 2.01-1.82 (m, 3H), 1.78-1.62 ppm (m, 1H); ¹³C-NMR (75 MHz, CDCl₃, 25 °C, TMS): δ=194.41, 158.62, 139.74, 137.55, 129.40, 126.29, 105.13, 55.77, 36.48, 30.00, 29.33, 21.78, 21.05, 18.25 ppm; IR (KBr): $\tilde{\nu}$ =3219, 3033, 2934, 1571, 1514, 1401, 1328, 1284, 1186, 1106, 1020 cm⁻¹; MS-EI: m/z(%): 242 (9) [M+H]⁺, 241 (26) [M]⁺, 240 (5), 226 (12), 170 (11), 148 (18), 136 (40), 118 (47), 117 (42), 115 (26), 105 (21), 91 (100), 89 (22), 77 (37), 65 (43), 63 (12), 55 (26); [α]_D^{RT}=+212,3 (c=1.0 in CHCl₃); HPLC conditions: OD-H column, n-hexane/2-propanol = 80/20, flow rate = 0.6 mL min⁻¹, major enantiomer: t_R=13.0 min; minor enantiomer: t_R=71.6 min.

(2S)-2-(4-Bromophenyl)-2,3,4,6,7,8-hexahydroquinolin-5(1H)-one

¹H-NMR (300 MHz, CDCl₃, 25 °C, TMS): δ=7.39 (d, 2H, J=8.4 Hz), 7.05 (d, 2H, J=8.4 Hz), 5.12 (br s, 1H), 4.31-4.23 (m, 1H), 2.41-2.11 (m, 6H), 2.00-1.81 (m, 3H), 1.76-1.60 ppm (m, 1H); ¹³C-NMR (75 MHz, CDCl₃, 25 °C, TMS): δ=194.45, 158.71, 141.88, 131.78, 128.11, 121.46, 105.11, 55.21, 36.46, 29.76, 29.19, 21.74, 17.72 ppm; IR (KBr): $\tilde{\nu}$ =3271, 2945, 2924, 1562, 1512, 1488, 1400, 1283, 1183, 1022 cm⁻¹; MS-EI: m/z(%): 308 (7) [M+H]⁺

(C₁₅H₁₇⁸¹BrNO), 307 (23) [M]⁺ (C₁₅H₁₆⁸¹BrNO), 306 (11) [M+H]⁺
 (C₁₅H₁₇⁷⁹BrNO), 305 (18) [M]⁺ (C₁₅H₁₆⁷⁹BrNO), 290 (16), 250 (10), 248
 (13), 198 (19), 184 (24), 182 (24), 169 (22), 155 (16), 148
 (32), 136 (68), 128 (29), 115 (32), 103 (48), 94 (37), 80 (26),
 77 (100), 65 (51), 55 (64), 53 (66); [α]_D^{RT}=+191.4 (c=1.0 in
 CHCl₃); HPLC conditions: OD-H column, n-hexane/2-propanol =
 80/20, flow rate = 0.6 mL min⁻¹, major enantiomer: t_R=13.5 min;
 minor enantiomer: t_R=48.9 min.

**(2S)-2-(1,3-Benzodioxol-5-yl)-2,3,4,6,7,8-hexahydroquinolin-
 5(1H)-one**

¹H-NMR (300 MHz, CDCl₃, 25 °C, TMS): δ=6.75-6.59 (m, 3H), 5.88
 (s, 2H), 4.73 (br s, 1H), 4.27-4.18 (m, 1H), 2.42-2.15 (m, 6H),
 2.00-1.82 (m, 3H), 1.76-1.60 ppm (m, 1H); ¹³C-NMR (75 MHz,
 CDCl₃, 25 °C, TMS): δ=194.46, 158.45, 147.99, 147.14, 136.68,
 119.71, 108.31, 106.74, 105.20, 101.13, 55.77, 36.46, 30.07,
 29.31, 21.76, 18.17 ppm; IR (KBr): $\tilde{\nu}$ =3249, 2942, 2854, 1568,
 1514, 1401, 1283, 1250, 1186, 1107, 1039 cm⁻¹; MS-EI: m/z(%): 271
 (36) [M]⁺, 256 (10), 214 (7), 184 (7), 156 (5), 148 (100), 136
 (68), 131 (12), 121 (37), 94 (32), 91 (30), 77 (30), 65 (55), 63
 (37), 55 (46); [α]_D^{RT}=+190.7 (c=1.0 in CHCl₃); HPLC conditions: OD-
 H column, n-hexane/2-propanol = 80/20, flow rate = 0.6 mL min⁻¹,
 major enantiomer: t_R=23.0 min; minor enantiomer: t_R=68.8 min.

(2S)-2-[4-(Trifluoromethyl)phenyl]-2,3,4,6,7,8-hexahydroquinolin-5(1H)-one

¹H-NMR (300 MHz, CDCl₃, 25 °C, TMS): δ=7.53 (d, 2H, *J*=8.1 Hz), 7.29 (d, 2H, *J*=8.1 Hz), 5.09 (br s, 1H), 4.45-4.34 (m, 1H), 2.44-2.10 (m, 6H), 2.02-1.82 (m, 3H), 1.81-1.64 ppm (m, 1H); ¹³C-NMR (75 MHz, CDCl₃, 25 °C, TMS): δ=194.53, 158.49, 146.89 (q, *J*=1.3 Hz), 126.71, 125.66 (q, *J*=3.8 Hz), 105.33, 55.32, 36.44, 29.68, 29.19, 21.72, 17.51 ppm; IR (KBr): $\tilde{\nu}$ =3223, 3047, 2944, 1576, 1508, 1402, 1331, 1287, 1190, 1162, 1119, 1067, 1018 cm⁻¹; MS-EI: *m/z*(%): 296 (5) [M+H]⁺, 295 (21) [M]^{+•}, 294 (11), 280 (17), 267 (7), 238 (15), 172 (20), 159 (13), 153 (10), 151 (11), 148 (13), 146 (11), 145 (21), 136 (33), 127 (32), 120 (16), 115 (10), 103 (21), 94 (25), 77 (31), 69 (100), 66 (27), 55 (44); [α]_D^{RT}=+134.9 (c=1.0 in CHCl₃); HPLC conditions: OD-H column, n-hexane/2-propanol = 80/20, flow rate = 0.6 mL min⁻¹, major enantiomer: *t*_R=10.6 min; minor enantiomer: *t*_R=21.2 min.

(2S)-2-(2,4-Difluorophenyl)-2,3,4,6,7,8-hexahydroquinolin-5(1H)-one

¹H-NMR (300 MHz, CDCl₃, 25 °C, TMS): δ=7.12 (dt, 1H, *J*=6.5, 8.5 Hz), 6.84-6.67 (m, 2H), 4.94 (br s, 1H), 4.73-4.62 (m, 1H), 2.44-2.21 (m, 5H), 2.21-2.06 (m, 1H), 2.00-1.84 (m, 3H), 1.84-1.68 ppm (m, 1H); ¹³C-NMR (75 MHz, CDCl₃, 25 °C, TMS): δ=194.53, 162.66 (dd, 1C, *J*=12.0, 187.7 Hz), 159.36 (dd, 1C, *J*=12.0, 187.7 Hz), 158.55, 128.58 (dd, 1C, *J*=5.7, 9.6 Hz), 125.66 (dd, 1C, *J*=3.8, 13.3 Hz), 111.40 (dd, 1C, *J*=3.7, 21.1 Hz), 105.21, 103.98

(t, 1C, $J=25.5$ Hz), 48.47 (d, 1C, $J=3.1$ Hz) 36.46, 29.24, 27.74, 21.75, 17.13 ppm; IR (KBr): $\tilde{\nu}=3229, 3059, 2937, 1580, 1501, 1400, 1351, 1287, 1194, 1136, 1087$ cm⁻¹; MS-EI: $m/z(\%)$: 264 (6) [M+H]⁺, 263 (24) [M]^{+•}, 262 (7), 248 (10), 235 (10), 206 (17), 192 (8), 164 (9), 151 (10), 148 (16), 140 (100), 136 (49), 127 (64), 120 (37), 114 (65), 107 (14), 101 (12), 94 (30), 80 (20), 77 (24), 66 (39), 55 (68); $[\alpha]_D^{RT}=+148.4$ (c=1.0 in CHCl₃); HPLC conditions: OD-H column, n-hexane/2-propanol = 80/20, flow rate = 0.6 mL min⁻¹, major enantiomer: $t_R=9.9$ min; minor enantiomer: $t_R=21.2$ min.

(2S)-2-(5-Methyl-2-thienyl)-2,3,4,6,7,8-hexahydroquinolin-5(1H)-one

¹H-NMR (300 MHz, CDCl₃, 25 °C, TMS): $\delta=6.67$ (d, 1H, $J=3.4$ Hz), 6.55-6.49 (m, 1H), 4.74 (br s, 1H), 4.54-4.46 (m, 1H), 2.50-2.34 (m, 4H), 2.33-2.16 (m, 5H), 2.10-1.95 (m, 1H), 1.93-1.76 ppm (m, 3H); ¹³C-NMR (62.5 MHz, CDCl₃, 25 °C, TMS): $\delta=194.69, 157.91, 143.63, 139.27, 124.76, 124.33, 105.27, 51.72, 36.49, 30.30, 29.25, 21.74, 18.31, 15.39$ ppm; IR (KBr): $\tilde{\nu}=3262, 3220, 2943, 1637, 1565, 1547, 1513, 1402, 1278, 1180, 1137, 1104$ cm⁻¹; MS-EI: $m/z(\%)$: 248 (5) [M+H]⁺, 247 (23) [M]^{+•}, 232 (4), 219 (7), 190 (7), 149 (14), 136 (80), 124 (100), 111 (26), 97 (79), 93 (31), 77 (23), 67 (39), 59 (34), 53 (69); $[\alpha]_D^{RT}=+159.2$ (c=1.0 in CHCl₃); HPLC conditions: OD-H column, n-hexane/2-propanol = 80/20, flow rate = 0.6 mL min⁻¹, major enantiomer: $t_R=15.6$ min; minor enantiomer: $t_R=50.7$ min.

(2R)-2-Pentyl-2,3,4,6,7,8-hexahydroquinolin-5(1H)-one

The physical data were identical in respect to those previously reported.^[1]

(2S)-2-(4-Methoxyphenyl)-2,3,4,6,7,8-hexahydroquinolin-5(1H)-one

¹H-NMR (250 MHz, CDCl₃, 25 °C, TMS): δ=7.12 (d, 2H, J=8.7 Hz), 6.81 (d, 2H, J=8.7 Hz), 4.68 (br s, 1H), 4.31-4.18 (m, 1H), 3.73 (s, 3H), 2.46-2.13 (m, 6H), 2.02-1.82 (m, 3H), 1.80-1.60 ppm (m, 1H); ¹³C-NMR (62.5 MHz, CDCl₃, 25 °C, TMS): δ=194.44, 159.24, 158.56, 134.77, 127.56, 114.13, 105.15, 55.51, 55.33, 36.50, 30.07, 29.35, 21.79, 18.37 ppm; IR (KBr): $\tilde{\nu}$ =3235, 2937, 1568, 1509, 1403, 1284, 1247, 1188, 1103, 1031 cm⁻¹; MS-EI: m/z(%): 258 (5) [M+H]⁺, 257 (27) [M]⁺, 242 (11), 148 (29), 136 (66), 134 (100), 121 (32), 108 (49), 103 (12), 91 (60), 77 (47), 65 (39), 55 (42); [α]_D^{RT}=+127.0 (c=1.0 in CHCl₃); HPLC conditions: OD-H column, n-hexane/2-propanol = 80/20, flow rate = 1.0 mL min⁻¹, major enantiomer: t_R=9.3 min; minor enantiomer: t_R=29.3 min.

(6S)-6-(4-Methoxyphenyl)-2-methyl-1,4,5,6-tetrahydropyridine-3-carbonitrile

¹H-NMR (250 MHz, CDCl₃, 25 °C, TMS): δ=7.10 (d, 2H, J=8.7 Hz), 6.81 (d, 2H, J=8.7 Hz), 4.30 (br s, 1H), 4.26-4.17 (m, 1H), 3.73 (s, 3H), 2.37-2.21 (m, 1H), 2.18-2.04 (m, 1H), 2.01 (s, 3H), 1.97-1.82 (m, 1H), 1.80-1.63 ppm (m, 1H); ¹³C-NMR (62.5 MHz,

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CDCl₃, 25 °C, TMS): δ =159.31, 152.79, 134.64, 127.47, 123.14, 114.18, 72.43, 55.37, 55.11, 29.45, 22.56, 19.90 ppm; IR (KBr): $\tilde{\nu}$ =3331, 2921, 2846, 2177, 1618, 1510, 1435, 1293, 1243, 1167, 1097, 1034 cm⁻¹; MS-EI: m/z (%): 229 (5) [M+H]⁺, 228 (19) [M]⁺, 227 (4), 213 (6), 187 (4), 172 (4), 169 (3), 145 (4), 134 (88), 119 (100), 108 (35), 103 (10), 91 (78), 77 (33), 65 (51), 51 (24); [α]_D^{RT}=+113.2 (c=1.0 in CHCl₃); HPLC conditions: AD-H column, n-hexane/2-propanol = 95/5, flow rate = 1.0 mL min⁻¹, major enantiomer: t_R =24.8 min; minor enantiomer: t_R =26.1 min.

1-[(6*S*)-6-(4-Methoxyphenyl)-2-methyl-1,4,5,6-tetrahydropyridin-3-yl]ethanone

¹H-NMR (250 MHz, CDCl₃, 25 °C, TMS): δ =7.12 (d, 2H, J =8.7 Hz), 6.82 (d, 2H, J =8.7 Hz), 4.30 (br s, 1H), 4.29-4.19 (m, 1H), 3.74 (s, 3H), 2.50-2.31 (m, 2H), 2.62 (s, 3H), 2.08 (s, 3H), 2.04-1.90 (m, 1H), 1.85-1.70 ppm (m, 1H); ¹³C-NMR (62.5 MHz, CDCl₃, 25 °C, TMS): δ =196.24, 159.26, 153.00, 135.02, 127.52, 114.16, 102.56, 55.41, 55.36, 30.36, 29.28, 23.54, 22.94 ppm; IR (KBr): $\tilde{\nu}$ =3283, 3077, 2928, 2837, 1617, 1497, 1370, 1338, 1246, 1182, 1035 cm⁻¹; MS-EI: m/z (%): 246 (4) [M+H]⁺, 245 (33) [M]⁺, 230 (20), 228 (4), 202 (24), 186 (9), 147 (15), 136 (22), 134 (100), 121 (27), 119 (41), 115 (15), 108 (34), 103 (12), 96 (16), 94 (27), 91 (65), 77 (31), 67 (28), 65 (39), 55 (26); [α]_D^{RT}=+122.3 (c=1.0 in CHCl₃); HPLC conditions: OD-H column, n-hexane/2-propanol = 80/20, flow rate = 1.0 mL min⁻¹, major enantiomer: t_R =12.0 min; minor enantiomer: t_R =19.8 min.

Methyl (6S)-6-(4-methoxyphenyl)-2-methyl-1,4,5,6-tetrahydropyridine-3-carboxylate

$^1\text{H-NMR}$ (250 MHz, CDCl_3 , 25 °C, TMS): δ =7.13 (d, 2H, J =8.7 Hz), 6.81 (d, 2H, J =8.7 Hz), 4.26-4.17 (m, 1H), 4.12 (br s, 1H), 3.74 (s, 3H), 3.60 (s, 3H), 2.40-2.29 (m, 2H), 2.23 (s, 3H), 1.99-1.85 (m, 1H), 1.79-1.65 ppm (m, 1H); $^{13}\text{C-NMR}$ (62.5 MHz, CDCl_3 , 25 °C, TMS): δ =169.28, 159.17, 152.74, 135.43, 127.54, 114.09, 92.28, 55.50, 55.35, 50.36, 30.24, 21.88, 21.66 ppm; IR (KBr): $\tilde{\nu}$ =3335, 2943, 2855, 1732, 1663, 1576, 1532, 1509, 1276, 1246, 1175, 1089, 1038 cm^{-1} ; MS-EI: m/z (%): 262 (3) $[\text{M}+\text{H}]^+$, 261 (23) $[\text{M}]^{+\bullet}$, 202 (29), 200 (8), 152 (8), 147 (10), 134 (100), 121 (24), 119 (37), 115 (13), 108 (34), 103 (12), 96 (11), 94 (32), 91 (53), 80 (10), 78 (25), 67 (29), 65 (30), 59 (56); $[\alpha]_{\text{D}}^{\text{RT}}$ =+91.8 (c=1.0 in CHCl_3); HPLC conditions: AS-H column, n-hexane/2-propanol = 98/2, flow rate = 0.6 mL min^{-1} , major enantiomer: t_{R} =126.1 min; minor enantiomer: t_{R} =117.7 min.

(6S)-6-(4-Bromophenyl)-2-methyl-1,4,5,6-tetrahydropyridine-3-carbonitrile

$^1\text{H-NMR}$ (300 MHz, CDCl_3 , 25 °C, TMS): δ =7.41 (d, 2H, J =8.5 Hz), 7.05 (d, 2H, J =8.3 Hz), 4.33 (br s, 1H), 4.31-4.22 (m, 1H), 2.34-2.19 (m, 1H), 2.15-2.04 (m, 1H), 2.03 (s, 3H), 1.97-1.84 (m, 1H), 1.80-1.64 ppm (m, 1H); $^{13}\text{C-NMR}$ (62.5 MHz, CDCl_3 , 25 °C, TMS): δ =152.59, 141.66, 131.96, 128.01, 122.74, 121.72, 73.09, 54.96, 29.19, 22.07, 19.92 ppm; IR (KBr): $\tilde{\nu}$ =3310, 2920, 2850,

2178, 1656, 1615, 1529, 1487, 1295, 1211 cm^{-1} ; MS-EI: $m/z(\%)$: 279 (2) $[\text{M}+\text{H}]^+$ ($\text{C}_{13}\text{H}_{14}^{81}\text{BrN}_2$), 278 (19) $[\text{M}]^{+\bullet}$ ($\text{C}_{13}\text{H}_{13}^{81}\text{BrN}_2$), 277 (10) $[\text{M}+\text{H}]^+$ ($\text{C}_{13}\text{H}_{14}^{79}\text{BrN}_2$), 276 (20) $[\text{M}]^{+\bullet}$ ($\text{C}_{13}\text{H}_{13}^{79}\text{BrN}_2$), 261 (10), 184 (15), 182 (22), 169 (36), 158 (11), 156 (17), 140 (12), 128 (15), 127 (15), 119 (70), 115 (28), 103 (81), 90 (20), 77 (100), 65 (38), 51 (51); $[\alpha]_{\text{D}}^{\text{RT}}=+94.7$ ($c=1.0$ in CHCl_3); HPLC conditions: AD-H column, n-hexane/2-propanol = 98/2, flow rate = 0.6 mL min^{-1} , major enantiomer: $t_{\text{R}}=110.1 \text{ min}$; minor enantiomer: $t_{\text{R}}=114.1 \text{ min}$.

1-{(6S)-2-Methyl-6-[4-(trifluoromethyl)phenyl]-1,4,5,6-tetrahydropyridin-3-yl}ethanone

$^1\text{H-NMR}$ (250 MHz, CDCl_3 , 25 $^{\circ}\text{C}$, TMS): $\delta=7.54$ (d, 2H, $J=8.1 \text{ Hz}$), 7.30 (d, 2H, $J=8.1 \text{ Hz}$), 4.54 (br s, 1H), 4.46-4.35 (m, 1H), 2.49-2.33 (m, 1H), 2.29 (s, 3H), 2.31-2.18 (m, 1H), 2.06 (s, 3H), 2.08-1.97 (m, 1H), 1.89-1.73 ppm (m, 1H); $^{13}\text{C-NMR}$ (75 MHz, CDCl_3 , 25 $^{\circ}\text{C}$, TMS): $\delta=196.34$, 152.55, 147.11 (d, $J=1.2 \text{ Hz}$), 126.62, 125.68 (q, $J=3.8 \text{ Hz}$), 102.95, 55.18, 29.84, 29.20, 22.67, 22.52 ppm; IR (KBr): $\tilde{\nu}=3262$, 3053, 2921, 2857, 1622, 1491, 1420, 1324, 1288, 1161, 1132, 1065, 1014 cm^{-1} ; MS-EI: $m/z(\%)$: 283 (15) $[\text{M}]^{+\bullet}$, 269 (10), 268 (33), 253 (16), 240 (20), 224 (83), 208 (28), 196 (63), 180 (23), 172 (14), 159 (13), 151 (47), 145 (13), 136 (21), 134 (40), 127 (14), 122 (20), 106 (100), 96 (32), 94 (25), 79 (31), 77 (42), 69 (42), 67 (40), 65 (39); $[\alpha]_{\text{D}}^{\text{RT}}=+92.8$ ($c=1.0$ in CHCl_3); HPLC conditions: OD-H column,

n-hexane/2-propanol = 90/10, flow rate = 0.6 mL min⁻¹, major enantiomer: t_R=53.2 min; minor enantiomer: t_R=27.5 min.

Methyl (6S)-6-(4-bromophenyl)-2-methyl-1,4,5,6-tetrahydropyridine-3-carboxylate

¹H-NMR (300 MHz, CDCl₃, 25 °C, TMS): δ=7.39 (d, 2H, J=8.4 Hz), 7.06 (d, 2H, J=8.4 Hz), 4.29-4.22 (m, 1H), 4.20 (br s, 1H), 3.58 (s, 3H), 2.40-2.17 (m, 2H), 2.24 (s, 3H), 1.98-1.86 (m, 1H), 1.76-1.64 ppm (m, 1H); ¹³C-NMR (75 MHz, CDCl₃, 25 °C, TMS): δ=169.08, 152.34, 142.46, 131.76, 128.03, 121.34, 92.75, 55.23, 50.36, 29.87, 21.49, 21.17 ppm; IR (KBr): $\tilde{\nu}$ =3348, 2935, 2898, 2847, 1659, 1578, 1568, 1522, 1429, 1276, 1177, 1119, 1094 cm⁻¹; MS-EI: m/z(%): 311 (11) [M]^{+•} (C₁₄H₁₆⁸¹BrNO₂), 309 (11) [M]^{+•} (C₁₄H₁₆⁷⁹BrNO₂), 278 (10), 252 (21), 250 (21), 184 (16), 182 (21), 171 (13), 156 (12), 154 (10), 152 (14), 128 (21), 115 (19), 103 (44), 94 (32), 89 (15), 77 (60), 67 (30), 59 (100), 53 (35); [α]_D^{RT}=+119.0 (c=1.0 in CHCl₃); HPLC conditions: AD-H column, n-hexane/2-propanol = 99/1, flow rate = 0.6 mL min⁻¹, major enantiomer: t_R=88.3 min; minor enantiomer: t_R=81.8 min.

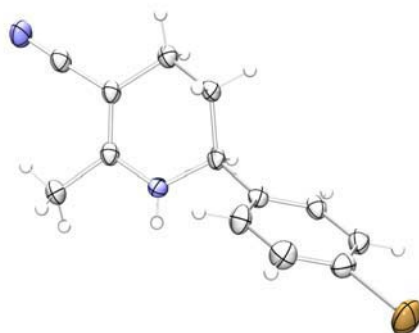
Methyl (6S)-6-(2,4-difluorophenyl)-2-methyl-1,4,5,6-tetrahydropyridine-3-carboxylate

¹H-NMR (300 MHz, CDCl₃, 25 °C, TMS): δ=7.15 (dt, 1H, J=6.6, 8.7 Hz), 6.83-6.67 (m, 2H), 4.69-4.60 (m, 1H), 4.20 (br s, 1H), 3.58 (s, 3H), 2.44-2.32 (m, 1H), 2.26 (s, 3H), 2.21-2.08 (m, 1H), 1.99-1.86 (m, 1H), 1.83-1.70 ppm (m, 1H); ¹³C-NMR (75 MHz,

CDCl₃, 25 °C, TMS): δ =169.05, 162.55 (dd, 1C, J =12.0, 189.3 Hz), 159.25 (dd, 1C, J =12.0, 189.8 Hz), 152.33, 128.63 (dd, 1C, J =5.8, 9.6 Hz), 126.25 (dd, 1C, J =3.8, 13.3 Hz), 111.31 (dd, 1C, J =3.7, 21.1 Hz), 103.85 (dd, 1C, J =25.6, 25.6 Hz), 92.78, 50.36, 48.46 (d, 1C, J =3.1 Hz), 27.77, 21.43, 20.48 ppm; IR (KBr): $\tilde{\nu}$ =3337, 2980, 2950, 2853, 1667, 1577, 1531, 1497, 1364, 1273, 1180, 1116, 1088 cm⁻¹; MS-EI: m/z (%): 267 (19) [M]⁺, 252 (8), 236 (17), 208 (40), 206 (11), 192 (10), 165 (8), 153 (12), 145 (9), 140 (98), 127 (30), 122 (10), 114 (42), 99 (10), 94 (21), 68 (25), 59 (100), 55 (29); $[\alpha]_D^{RT}$ =+92.9 (c=1.0 in CHCl₃); HPLC conditions: AD-H column, n-hexane/2-propanol = 99/1, flow rate = 0.6 mL min⁻¹, major enantiomer: t_R =59.3 min; minor enantiomer: t_R =86.8 min.

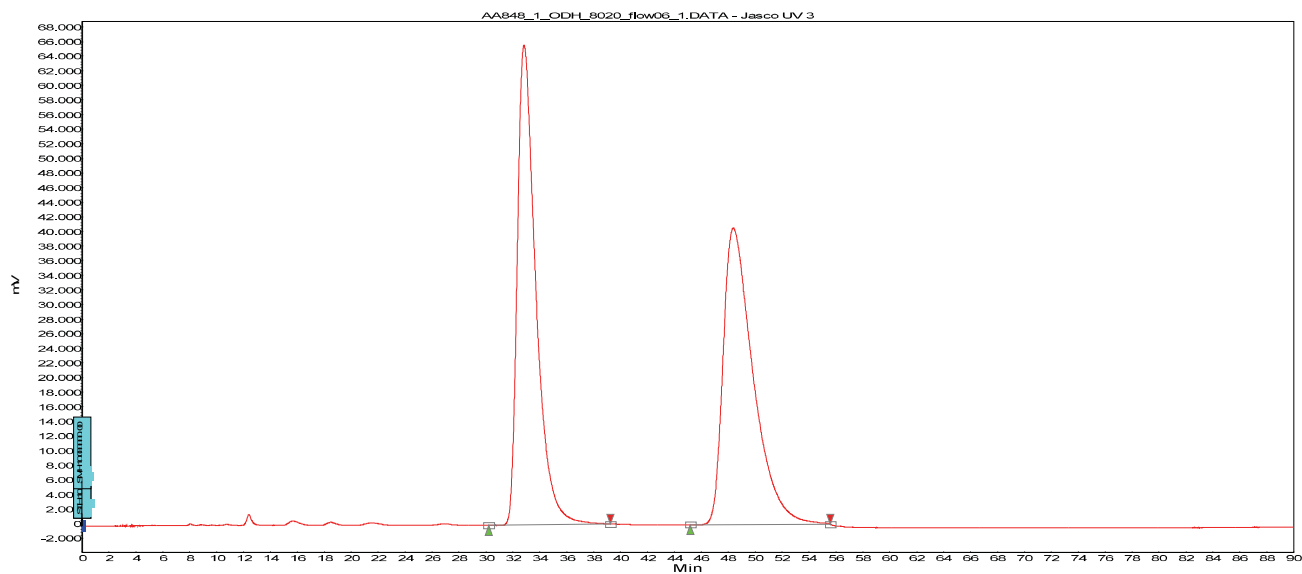
Determination of the absolute configuration

The determination of absolute configuration was achieved by an X-ray crystal structure (Figure 1S) of compound **9b** (Table 1). All other compounds were assigned based on this crystal structure or by comparison with known $[\alpha]_D^{RT}$ -values.^[1]



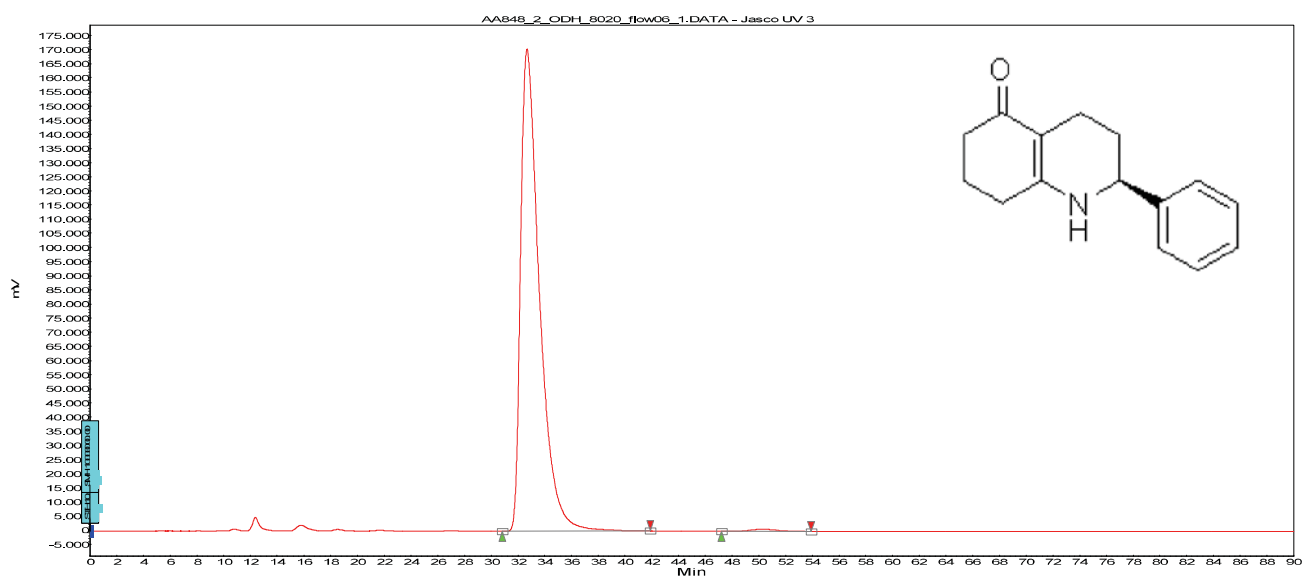
Chromatogram : AA848_1_ODH_8020_flow06_1

Data file: AA848_1_ODH_8020_flow06_1.DATA
Method: HPLC2_ODH_8020_flow06_acq90

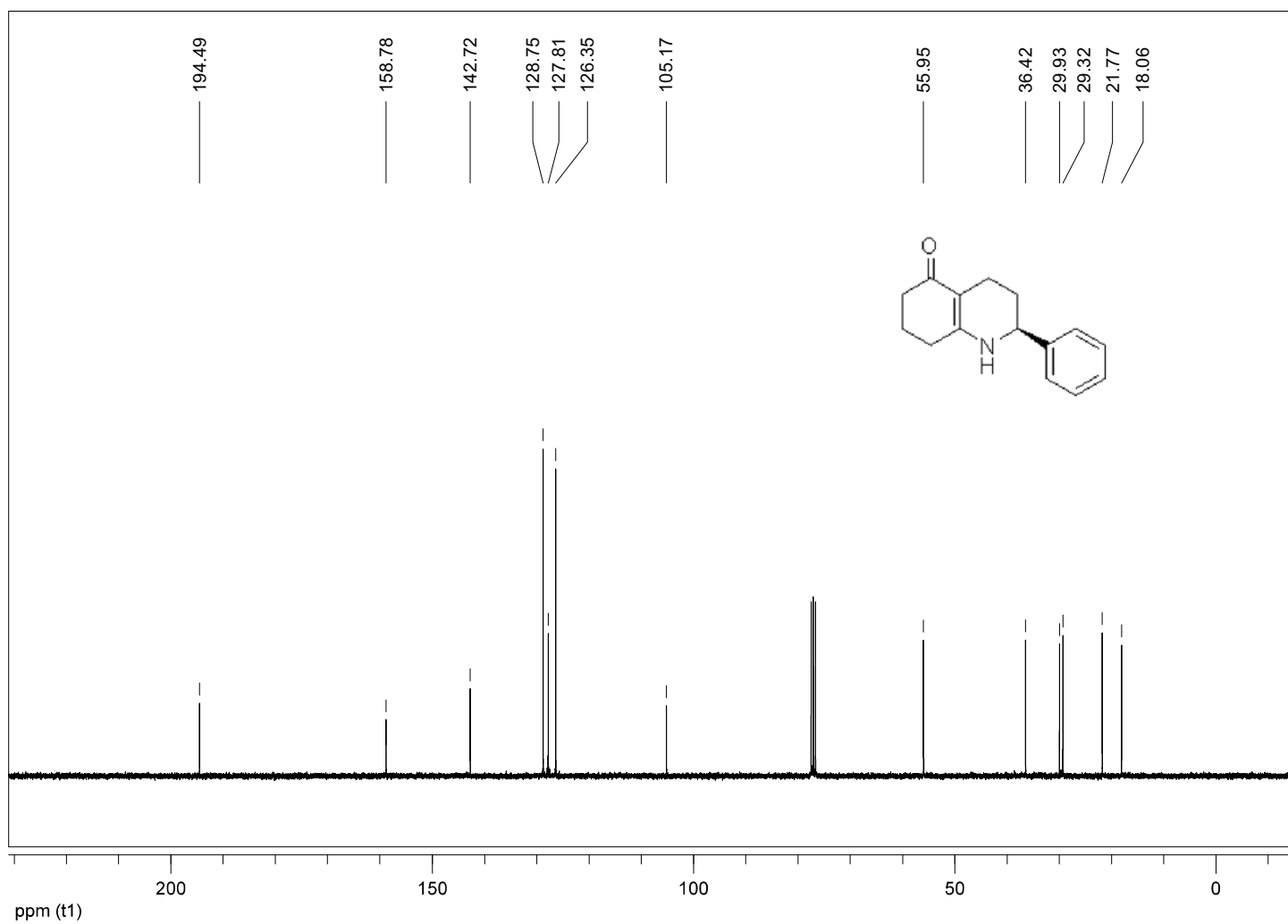
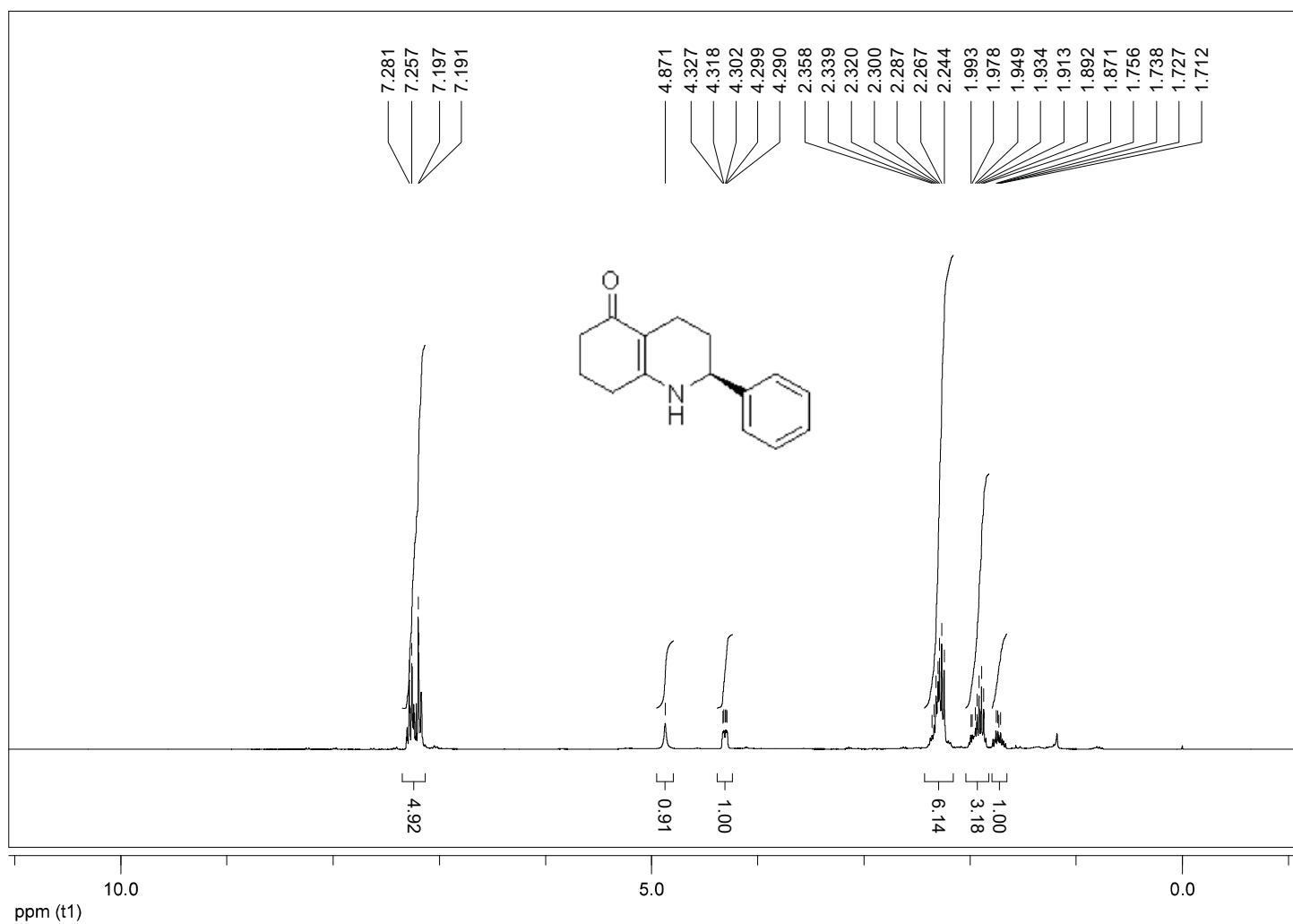


Chromatogram : AA848_2_ODH_8020_flow06_1

Data file: AA848_2_ODH_8020_flow06_1.DATA
Method: HPLC2_ODH_8020_flow06_acq90



Index	Start [Min]	Time [Min]	End [Min]	Area %
2	30,819	32,675	41,889	99,365
1	47,231	50,317	53,926	0,635
Total				100,000



Sample Information

Analyzed : 08.11.2007 10:06:35
 Sample Name : AA848_2

Method

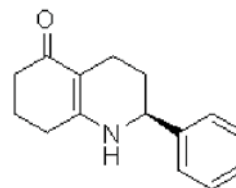
===== Analytical Line 1 =====

[GC-2010]

Column Oven Temp. : 60.0 °C
 Injection Temp. : 280.00 °C
 Injection Mode : Split
 Flow Control Mode : Linear Velocity
 Pressure : 29.2 kPa
 Total Flow : 17.2 mL/min
 Column Flow : 0.68 mL/min
 Linear Velocity : 30.0 cm/sec
 Purge Flow : 3.0 mL/min
 Split Ratio : 20.0

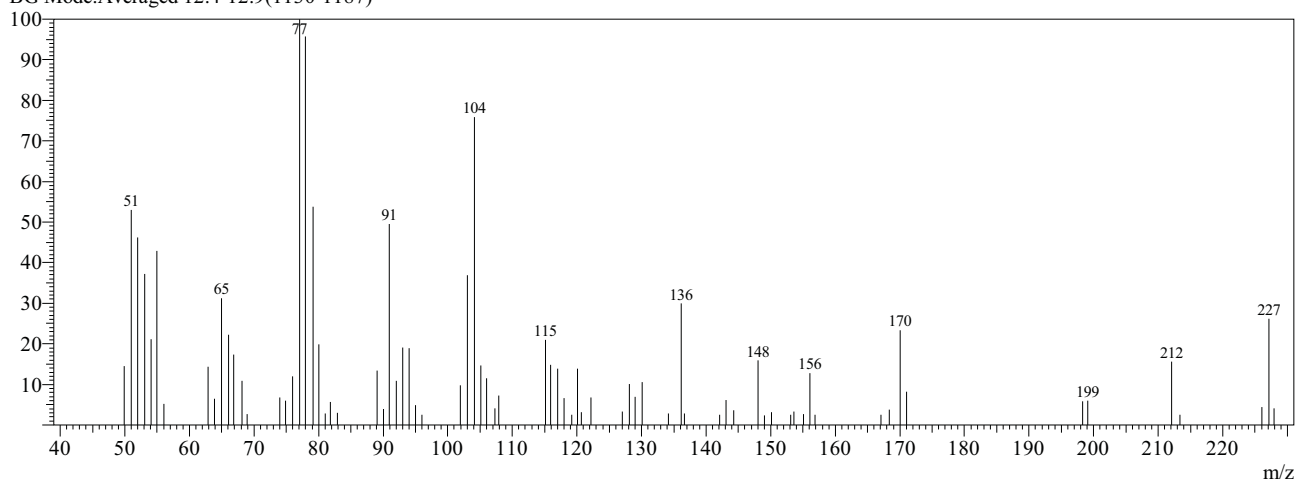
Oven Temp. Program

Rate	Temperature(°C)	Hold Time(min)
-	60.0	0.00
20.0	300.0	8.00



Spectrum

Line#:1 R.Time:12.1(Scan#:1096)
 MassPeaks:76 BasePeak:77(149238)
 RawMode:Averaged 12.1-12.1(1094-1097)
 BG Mode:Averaged 12.4-12.9(1130-1187)



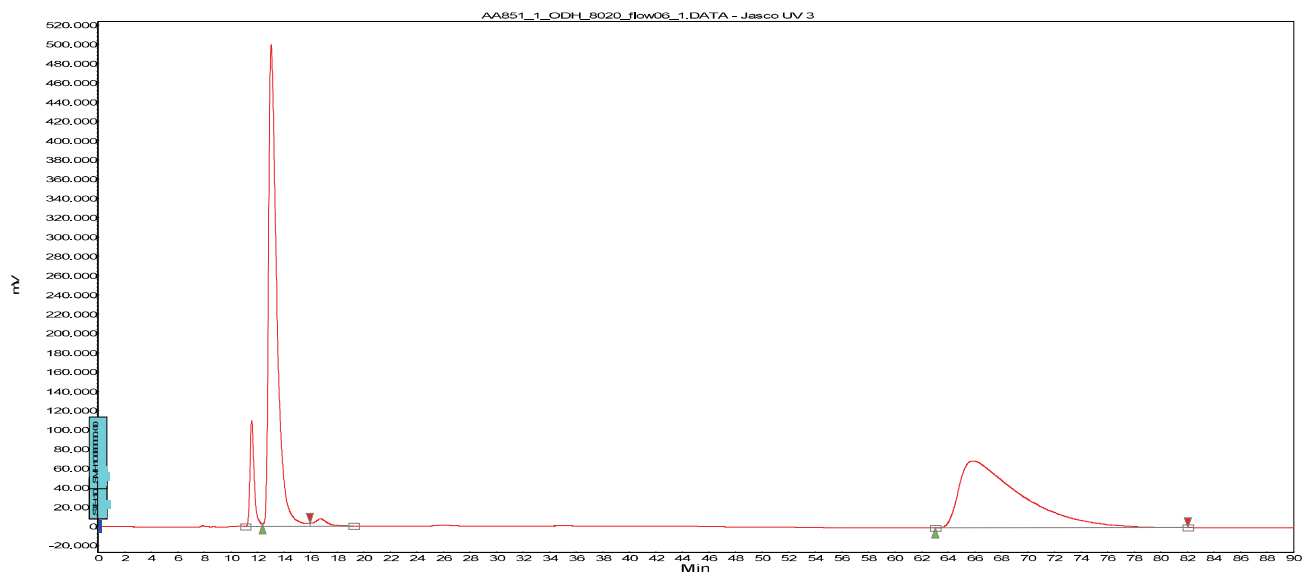
Mass Table

Line#:1 R.Time:12.1(Scan#:1096)
 MassPeaks:76 BasePeak:77(149238)
 RawMode:Averaged 12.1-12.1(1094-1097)
 BG Mode:Averaged 12.4-12.9(1130-1187)

#	m/z	Rel. Int.	#	m/z	Rel. Int.	#	m/z	Rel. Int.	#	m/z	Rel. Int.
1	49.90	14.54	20	79.10	53.74	39	107.90	7.32	58	148.00	15.92
2	51.00	52.98	21	80.00	19.90	40	115.10	20.95	59	149.00	2.37
3	51.95	46.21	22	81.05	2.78	41	115.95	14.89	60	150.15	3.10
4	53.05	37.24	23	81.85	5.66	42	117.05	13.89	61	153.05	2.53
5	54.05	21.10	24	82.90	3.02	43	118.05	6.62	62	153.60	3.30
6	54.95	42.94	25	89.10	13.40	44	119.20	2.54	63	155.05	2.63
7	56.00	5.19	26	90.05	4.02	45	120.05	13.88	64	156.05	12.78
8	62.90	14.38	27	90.95	49.47	46	120.70	3.12	65	156.90	2.52
9	63.90	6.54	28	92.05	10.87	47	122.20	6.71	66	167.10	2.53
10	65.00	31.25	29	93.00	19.02	48	127.00	3.36	67	168.40	3.73
11	66.05	22.23	30	94.05	18.86	49	128.10	10.11	68	170.05	23.34
12	66.90	17.34	31	95.00	4.97	50	129.05	7.01	69	171.05	8.27
13	68.10	10.95	32	95.95	2.52	51	130.10	10.58	70	198.25	5.83
14	68.95	2.69	33	101.90	9.84	52	134.15	2.80	71	199.05	6.06
15	73.95	6.78	34	103.00	36.87	53	136.15	29.90	72	212.05	15.64
16	74.90	6.07	35	104.10	75.81	54	136.60	2.78	73	213.35	2.54
17	76.00	11.96	36	105.10	14.62	55	142.10	2.60	74	226.05	4.41
18	77.05	100.00	37	106.05	11.57	56	143.10	6.15	75	227.10	26.19
19	78.00	95.74	38	107.25	4.06	57	144.25	3.66	76	227.95	4.16

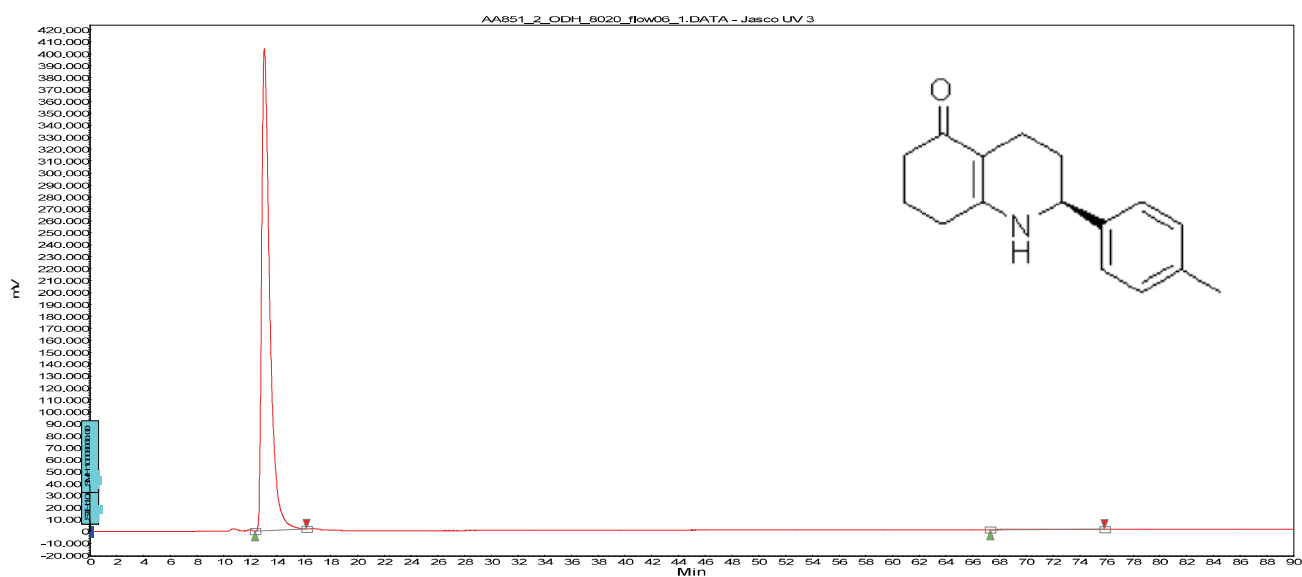
Chromatogram : AA851_1_ODH_8020_flow06_1

Data file: AA851_1_ODH_8020_flow06_1.DATA
Method: HPLC2_ODH_8020_flow06_acq90

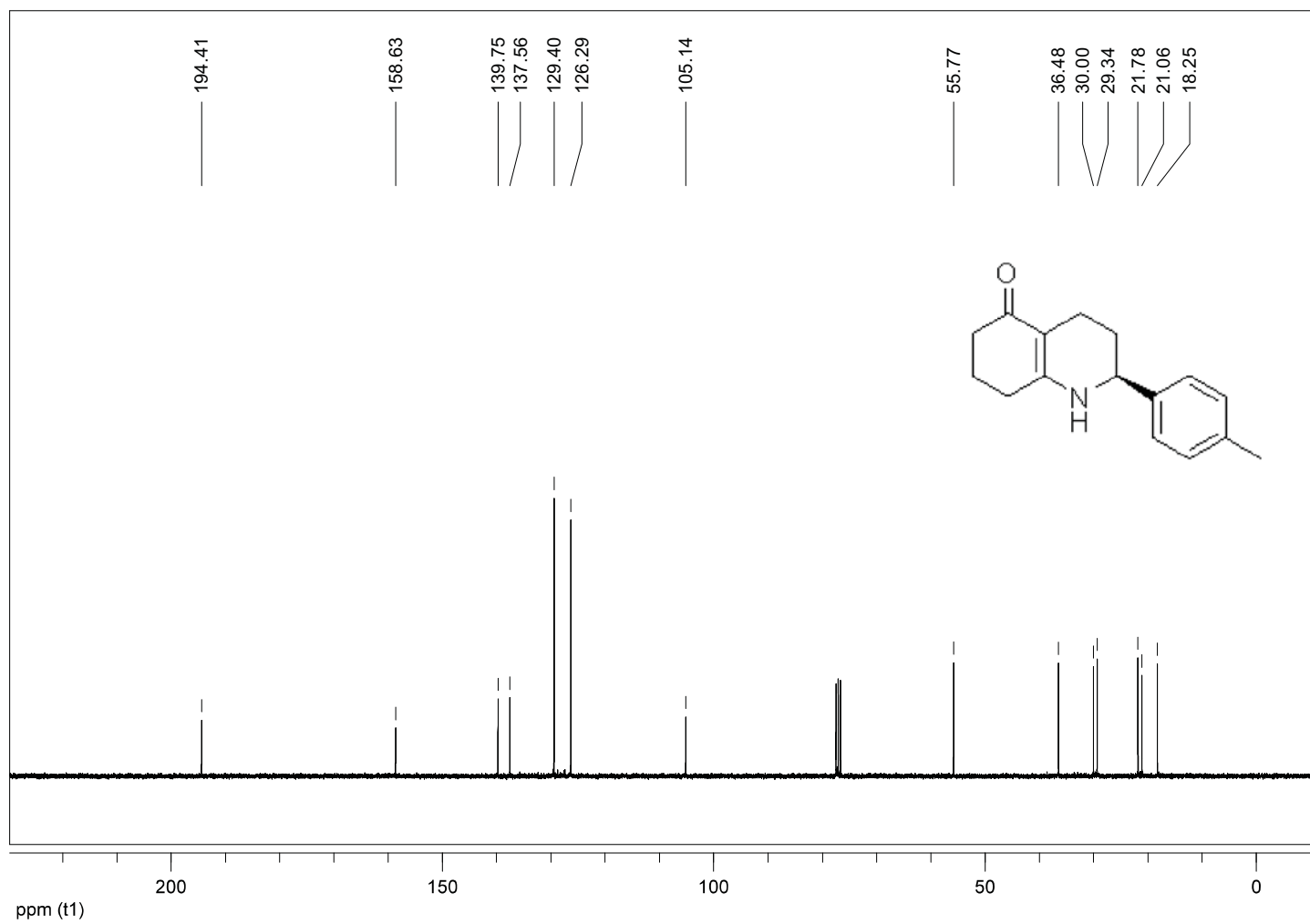
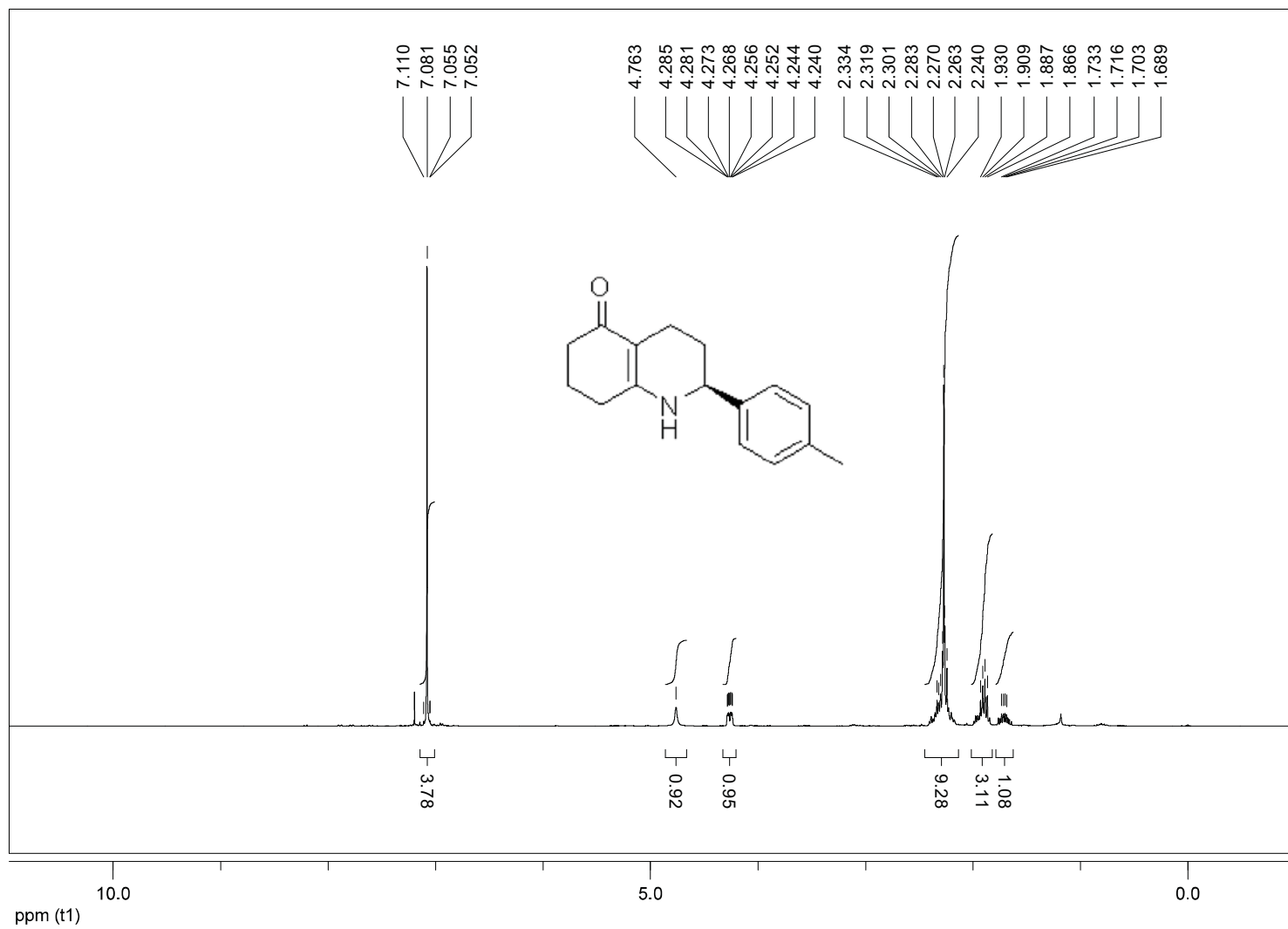


Chromatogram : AA851_2_ODH_8020_flow06_1

Data file: AA851_2_ODH_8020_flow06_1.DATA
Method: HPLC2_ODH_8020_flow06_acq90



Index	Start [Min]	Time [Min]	End [Min]	Area %
2	12,349	13,042	16,195	99,790
1	67,306	71,600	75,849	0,210
Total				100,000



Sample Information

Analyzed : 13.11.2007 13:37:58
 Sample Name : AA851_2

Method

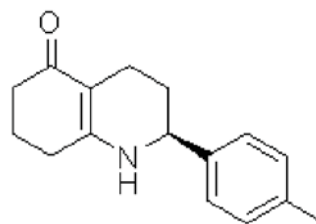
===== Analytical Line 1 =====

[GC-2010]

Column Oven Temp. : 60.0 °C
 Injection Temp. : 280.00 °C
 Injection Mode : Split
 Flow Control Mode : Linear Velocity
 Pressure : 29.2 kPa
 Total Flow : 17.2 mL/min
 Column Flow : 0.68 mL/min
 Linear Velocity : 30.0 cm/sec
 Purge Flow : 3.0 mL/min
 Split Ratio : 20.0

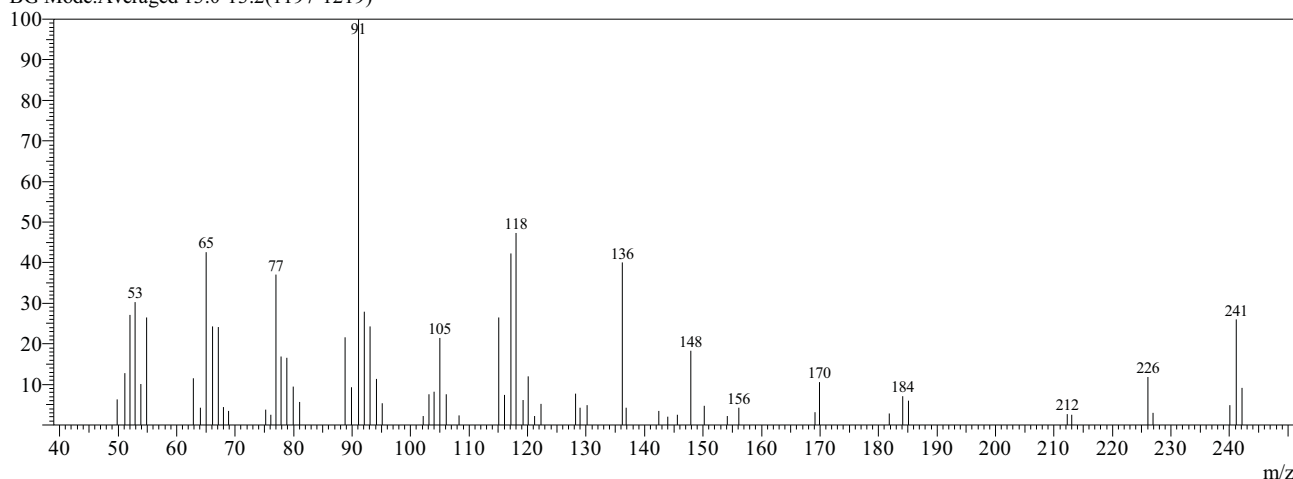
Oven Temp. Program

Rate	Temperature(°C)	Hold Time(min)
-	60.0	0.00
20.0	300.0	8.00



Spectrum

Line#:1 R.Time:12.6(Scan#:1158)
 MassPeaks:65 BasePeak:91(124703)
 RawMode:Averaged 12.6-12.7(1157-1160)
 BG Mode:Averaged 13.0-13.2(1197-1219)



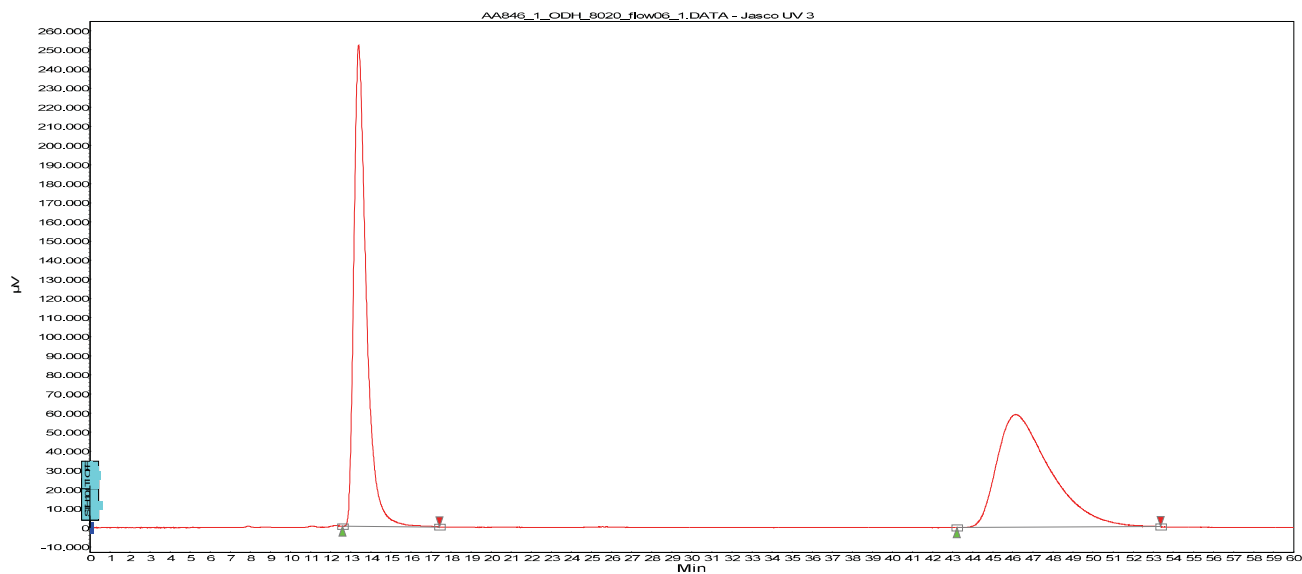
Mass Table

Line#:1 R.Time:12.6(Scan#:1158)
 MassPeaks:65 BasePeak:91(124703)
 RawMode:Averaged 12.6-12.7(1157-1160)
 BG Mode:Averaged 13.0-13.2(1197-1219)

#	m/z	Rel. Int.	#	m/z	Rel. Int.	#	m/z	Rel. Int.	#	m/z	Rel. Int.
1	49.85	6.36	18	78.85	16.50	35	116.00	7.36	52	154.10	2.22
2	51.10	12.85	19	79.90	9.40	36	117.15	42.26	53	156.15	4.22
3	52.05	27.12	20	81.05	5.67	37	118.05	47.37	54	169.15	3.23
4	52.90	30.30	21	88.80	21.68	38	119.25	6.23	55	169.90	10.54
5	53.85	10.10	22	89.85	9.33	39	120.10	12.05	56	181.80	2.85
6	54.90	26.49	23	91.05	100.00	40	121.20	2.22	57	184.10	7.03
7	62.85	11.58	24	92.05	27.91	41	122.30	5.16	58	185.10	6.02
8	64.05	4.20	25	93.10	24.34	42	128.15	7.80	59	212.25	2.72
9	65.00	42.62	26	94.20	11.37	43	129.00	4.19	60	213.05	2.52
10	66.10	24.28	27	95.10	5.31	44	130.15	4.96	61	226.10	11.83
11	67.10	24.13	28	102.20	2.24	45	136.15	40.10	62	226.95	3.02
12	67.95	4.46	29	103.15	7.60	46	136.80	4.27	63	240.05	4.88
13	68.90	3.41	30	104.00	8.16	47	142.45	3.46	64	241.15	26.10
14	75.25	3.75	31	105.00	21.43	48	143.95	2.00	65	242.15	9.21
15	76.05	2.54	32	106.05	7.61	49	145.55	2.57			
16	77.00	37.14	33	108.25	2.32	50	147.95	18.27			
17	77.90	16.92	34	115.10	26.42	51	150.15	4.70			

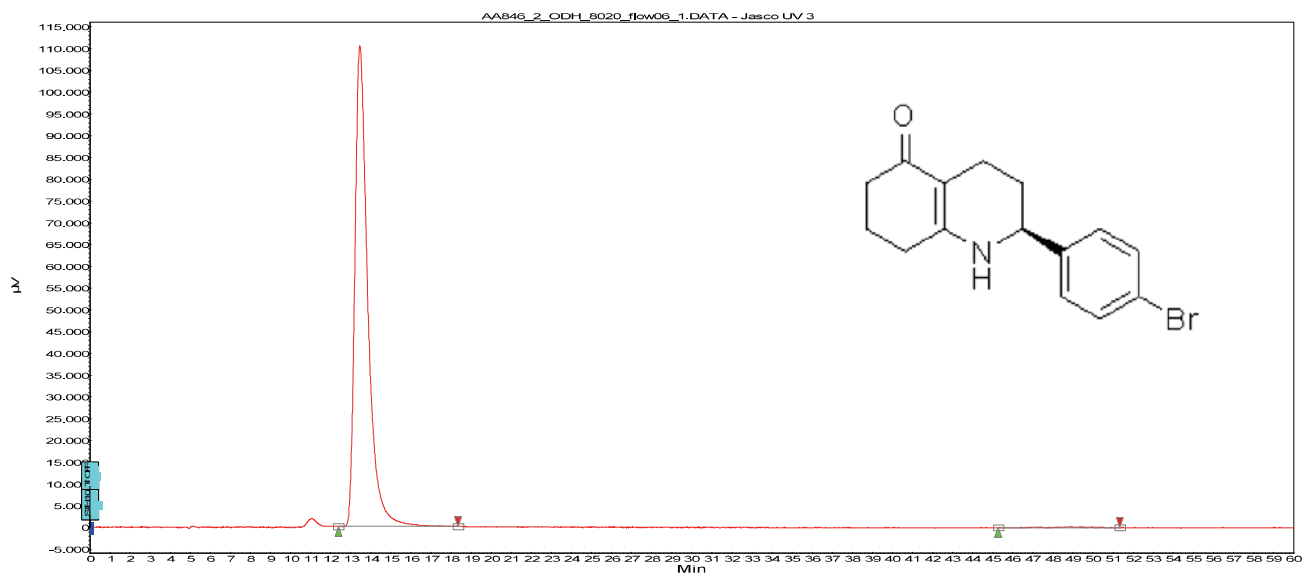
Chromatogram : AA846_1_ODH_8020_flow06_1

Data file: AA846_1_ODH_8020_flow06_1.DATA
Method: HPLC1_ODH_8020_flow06_acq_60

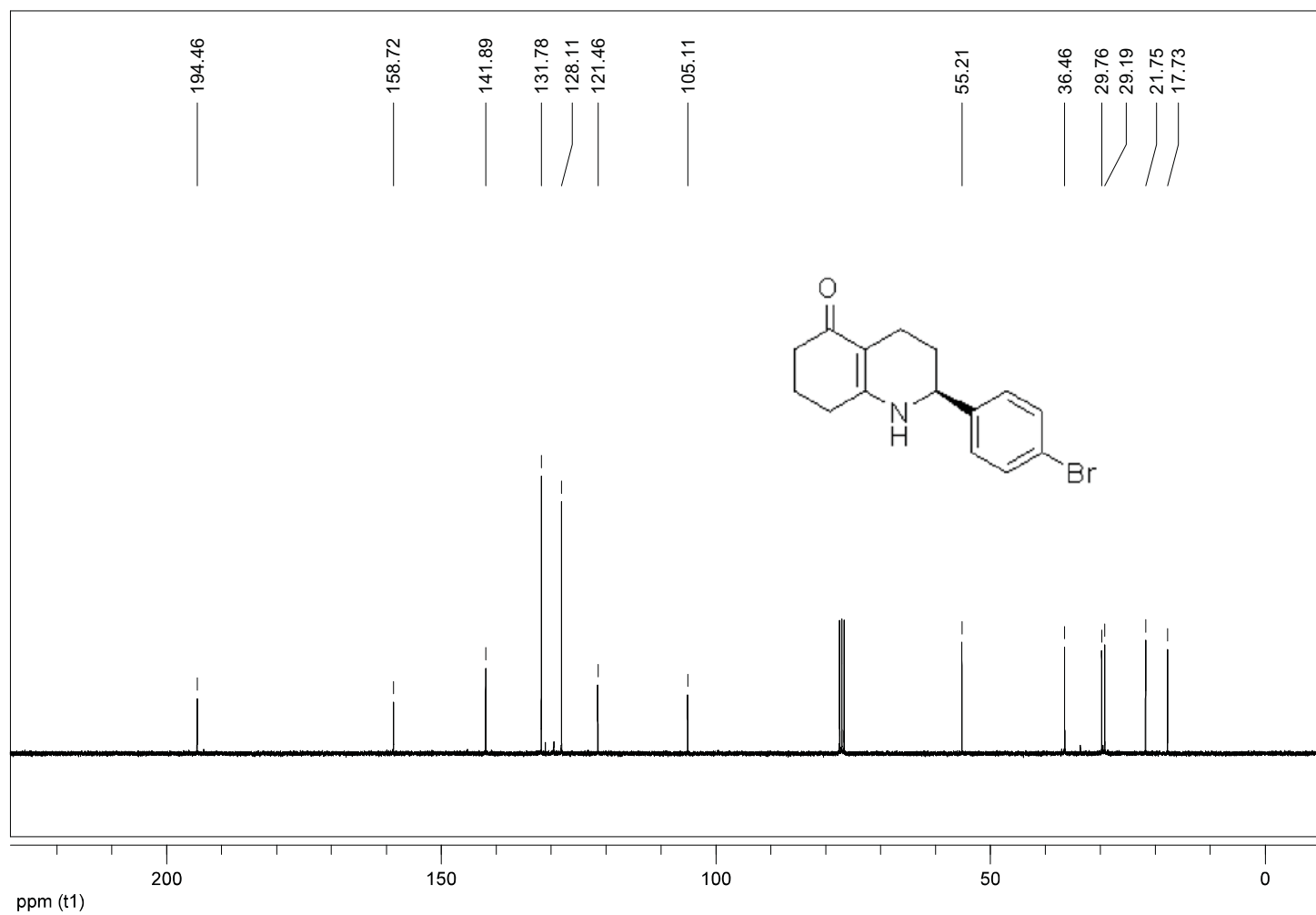
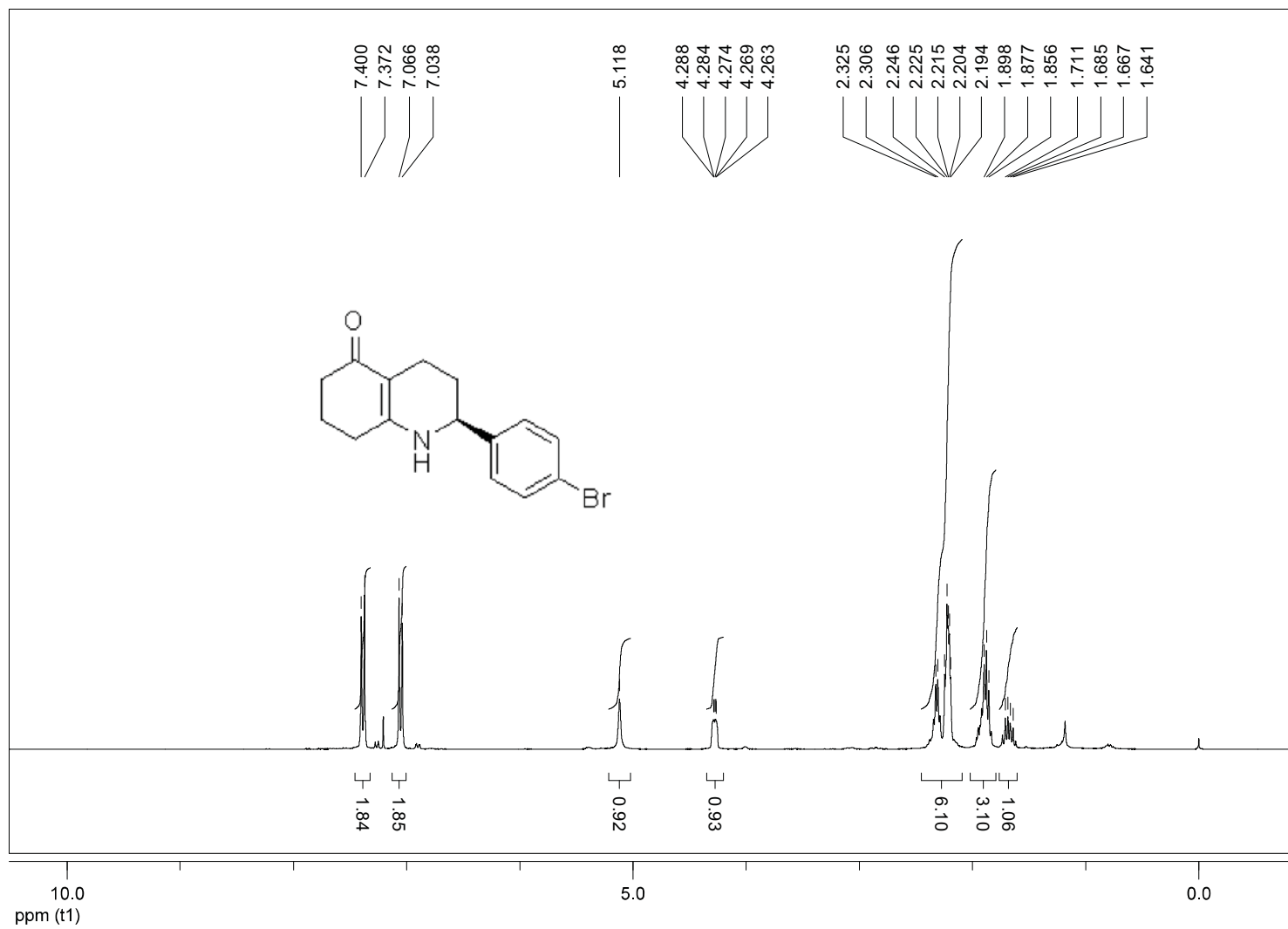


Chromatogram : AA846_2_ODH_8020_flow06_1

Data file: AA846_2_ODH_8020_flow06_1.DATA
Method: HPLC1_ODH_8020_flow06_acq_60



Index	Start [Min]	Time [Min]	End [Min]	Area %
1	12,386	13,458	18,343	99,832
2	45,257	48,875	51,337	0,168
Total				100,000



Sample Information

Analyzed : 06.11.2007 12:09:27
 Sample Name : AA846_2

Method

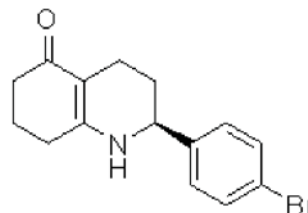
===== Analytical Line 1 =====

[GC-2010]

Column Oven Temp. : 60.0 °C
 Injection Temp. : 280.00 °C
 Injection Mode : Split
 Flow Control Mode : Linear Velocity
 Pressure : 29.2 kPa
 Total Flow : 17.2 mL/min
 Column Flow : 0.68 mL/min
 Linear Velocity : 30.0 cm/sec
 Purge Flow : 3.0 mL/min
 Split Ratio : 20.0

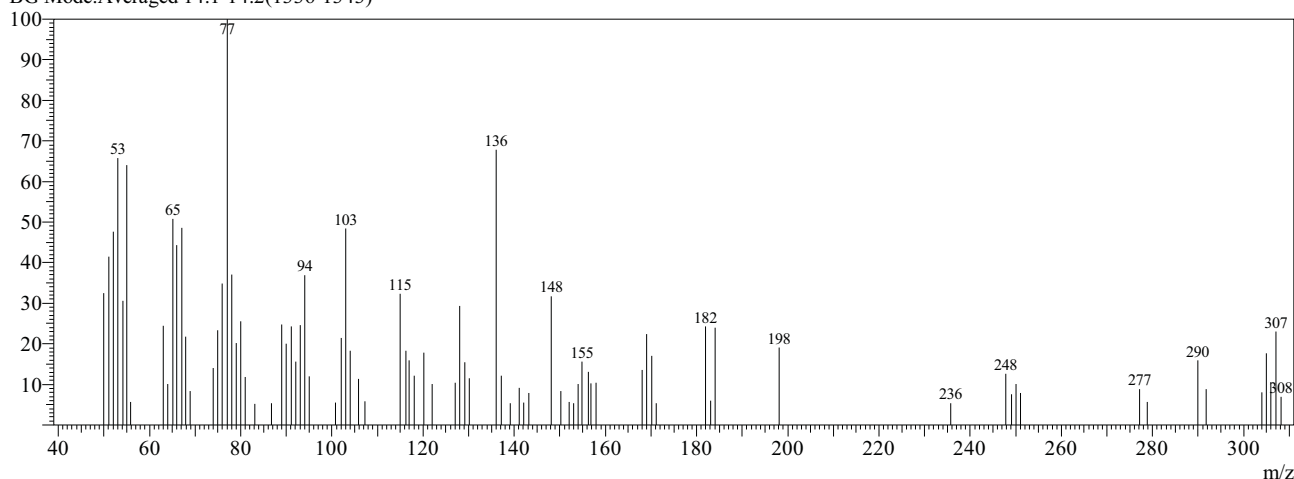
Oven Temp. Program

Rate	Temperature(°C)	Hold Time(min)
-	60.0	0.00
20.0	300.0	8.00



Spectrum

Line#:1 R.Time:14.0(Scan#:1324)
 MassPeaks:84 BasePeak:77(140621)
 RawMode:Averaged 14.0-14.0(1320-1325)
 BG Mode:Averaged 14.1-14.2(1336-1343)



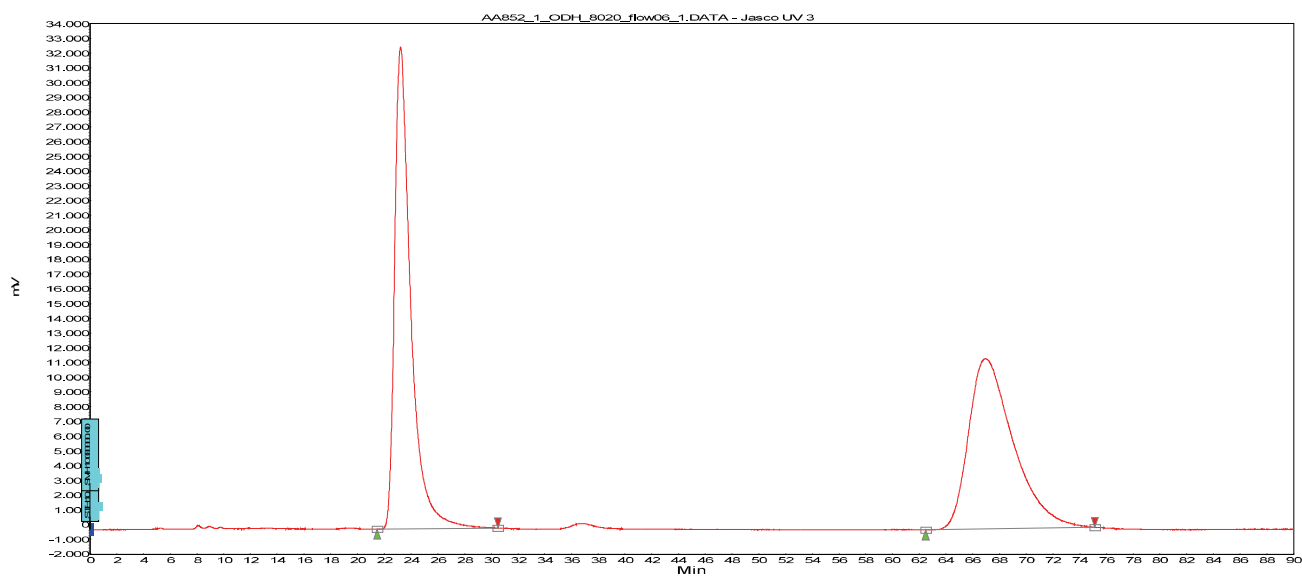
Mass Table

Line#:1 R.Time:14.0(Scan#:1324)
 MassPeaks:84 BasePeak:77(140621)
 RawMode:Averaged 14.0-14.0(1320-1325)
 BG Mode:Averaged 14.1-14.2(1336-1343)

#	m/z	Rel. Int.	#	m/z	Rel. Int.	#	m/z	Rel. Int.	#	m/z	Rel. Int.
1	49.95	32.50	22	80.95	11.76	43	121.95	10.14	64	169.10	22.35
2	51.05	41.45	23	83.10	5.22	44	127.00	10.33	65	170.10	17.10
3	52.00	47.56	24	86.80	5.36	45	128.00	29.40	66	171.15	5.40
4	53.05	65.73	25	89.00	24.77	46	129.15	15.47	67	181.90	24.33
5	54.10	30.52	26	90.00	20.05	47	130.10	11.45	68	183.05	6.01
6	55.00	64.01	27	91.10	24.32	48	136.10	67.78	69	184.00	23.92
7	55.90	5.69	28	92.10	15.55	49	137.15	12.20	70	198.10	19.14
8	63.05	24.39	29	93.10	24.65	50	139.10	5.43	71	235.75	5.29
9	64.05	10.09	30	94.00	36.98	51	141.10	9.11	72	247.85	12.54
10	65.05	50.85	31	95.00	12.00	52	142.10	5.50	73	249.05	7.58
11	66.00	44.36	32	100.80	5.49	53	143.20	7.93	74	250.00	10.06
12	67.10	48.61	33	102.00	21.49	54	148.10	31.68	75	251.05	7.94
13	67.90	21.80	34	103.05	48.39	55	150.15	8.36	76	277.10	8.77
14	68.90	8.34	35	104.00	18.29	56	152.10	5.67	77	278.90	5.75
15	74.00	13.96	36	105.85	11.40	57	153.00	5.44	78	289.90	15.86
16	75.00	23.31	37	107.25	5.77	58	154.05	10.15	79	291.80	8.78
17	76.00	34.92	38	114.95	32.41	59	154.90	15.67	80	303.95	8.11
18	77.00	100.00	39	116.20	18.32	60	156.20	13.02	81	304.90	17.73
19	78.00	37.12	40	117.00	15.92	61	156.80	10.22	82	305.90	10.62
20	79.05	20.24	41	118.05	12.10	62	157.90	10.43	83	307.00	23.07
21	80.00	25.56	42	120.10	17.76	63	168.10	13.53	84	308.20	6.93

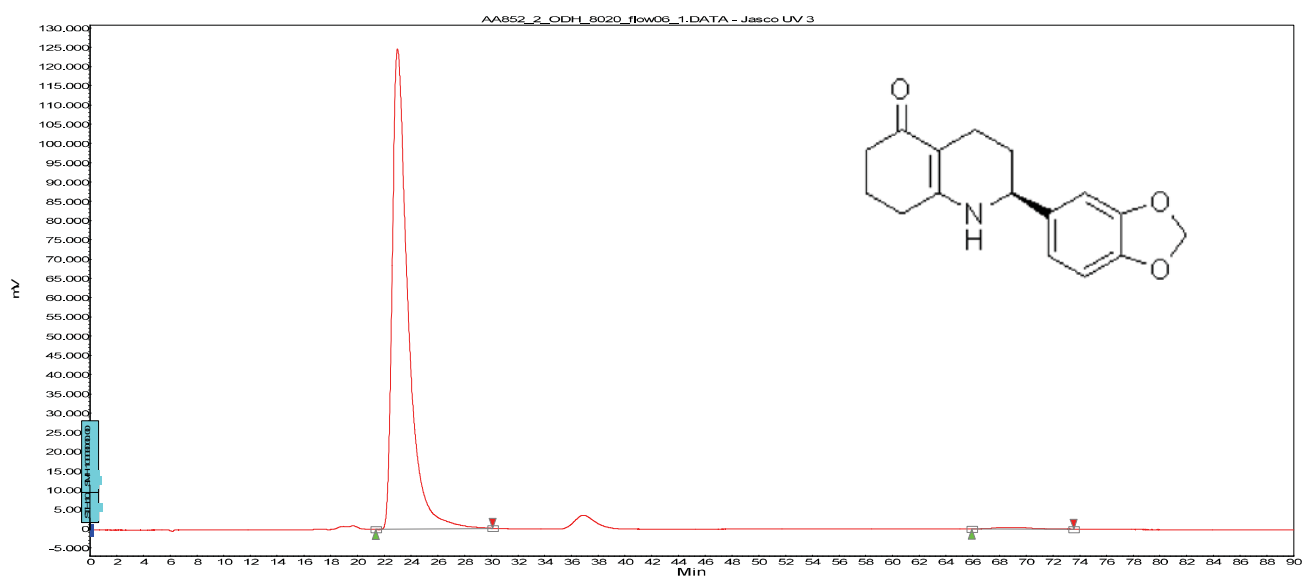
Chromatogram : AA852_1_ODH_8020_flow06_1

Data file: AA852_1_ODH_8020_flow06_1.DATA
Method: HPLC2_ODH_8020_flow06_acq90

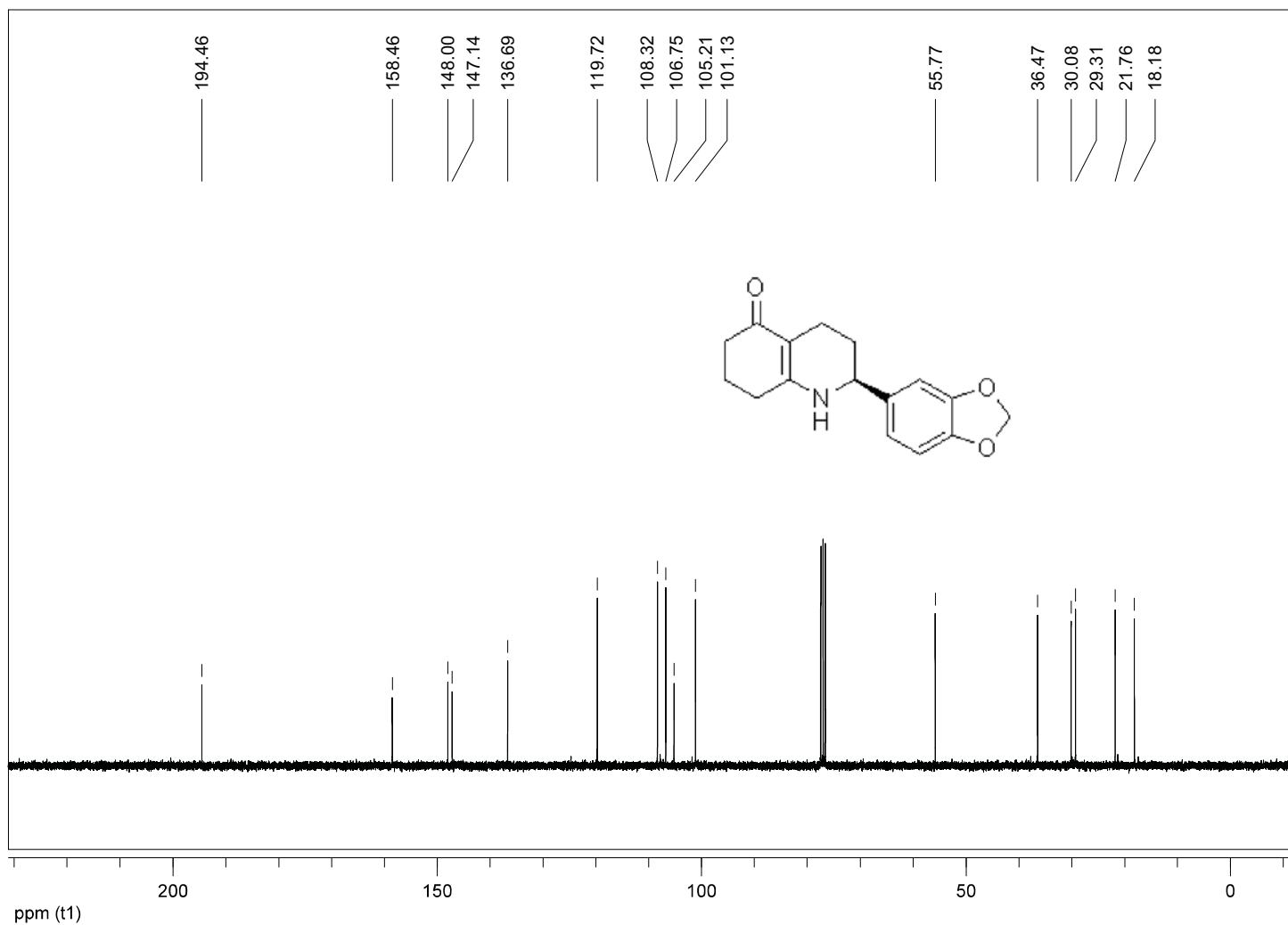
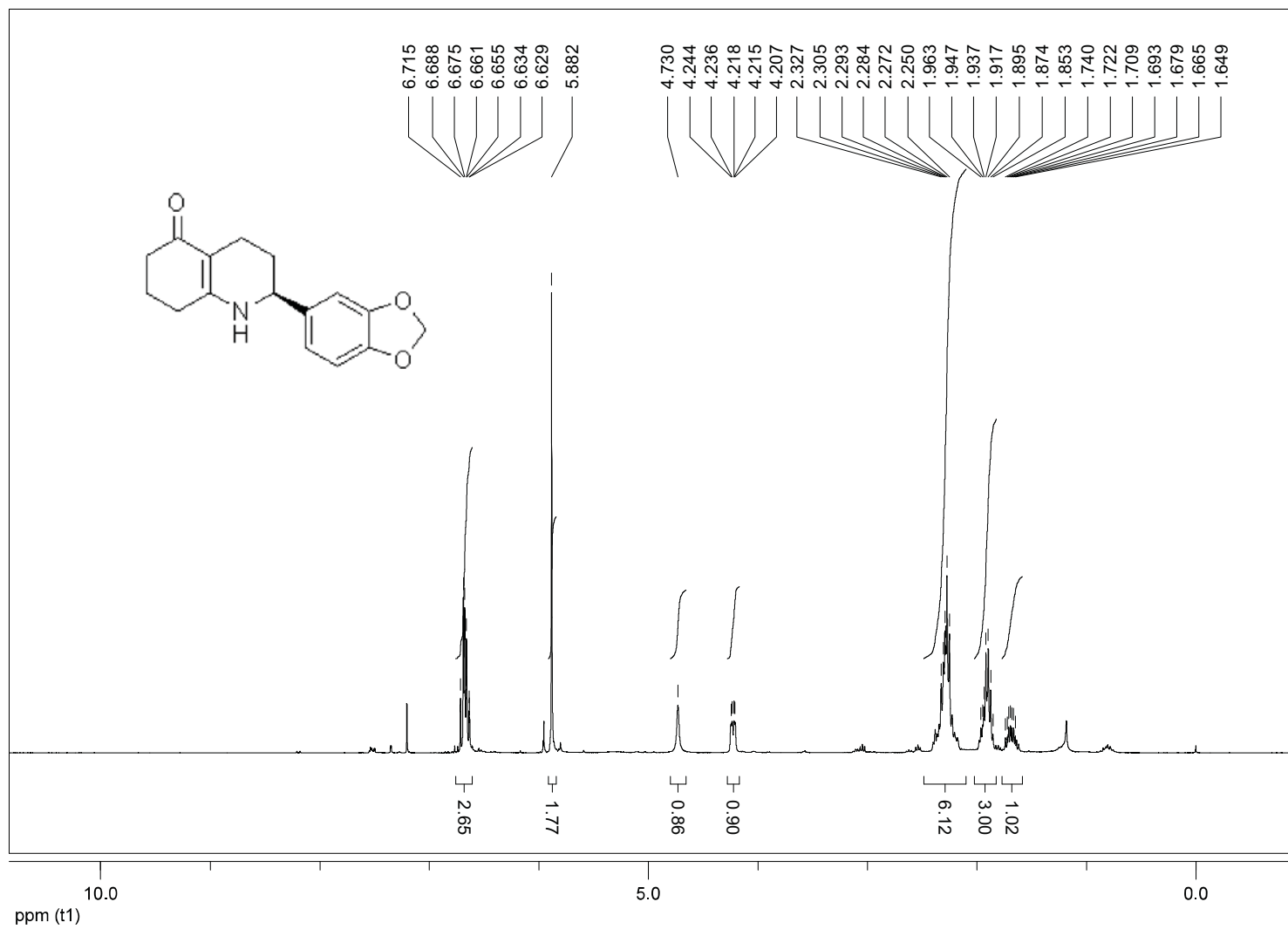


Chromatogram : AA852_2_ODH_8020_flow06_1

Data file: AA852_2_ODH_8020_flow06_1.DATA
Method: HPLC2_ODH_8020_flow06_acq90



Index	Start [Min]	Time [Min]	End [Min]	Area %
1	21,384	23,000	30,101	99,187
2	65,919	68,800	73,543	0,813
Total				100,000



Sample Information

Analyzed : 13.11.2007 11:39:10
 Sample Name : AA852_2

Method

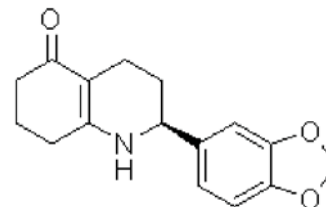
===== Analytical Line 1 =====

[GC-2010]

Column Oven Temp. : 60.0 °C
 Injection Temp. : 280.00 °C
 Injection Mode : Split
 Flow Control Mode : Linear Velocity
 Pressure : 29.2 kPa
 Total Flow : 17.2 mL/min
 Column Flow : 0.68 mL/min
 Linear Velocity : 30.0 cm/sec
 Purge Flow : 3.0 mL/min
 Split Ratio : 20.0

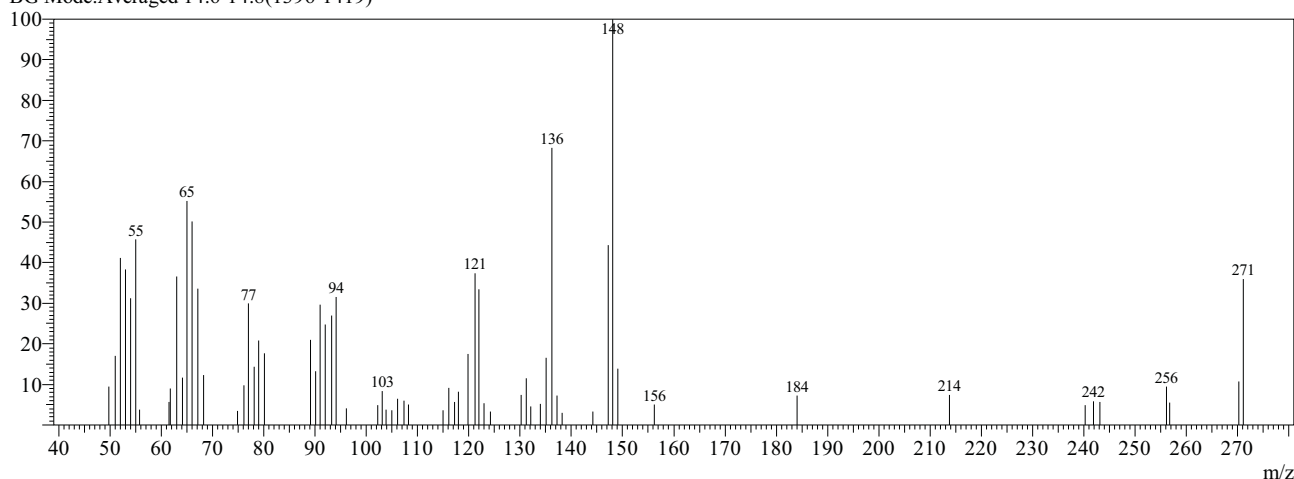
Oven Temp. Program

Rate	Temperature(°C)	Hold Time(min)
-	60.0	0.00
20.0	300.0	8.00



Spectrum

Line#:1 R.Time:14.4(Scan#:1364)
 MassPeaks:66 BasePeak:148(41885)
 RawMode:Averaged 14.3-14.4(1362-1366)
 BG Mode:Averaged 14.6-14.8(1396-1419)



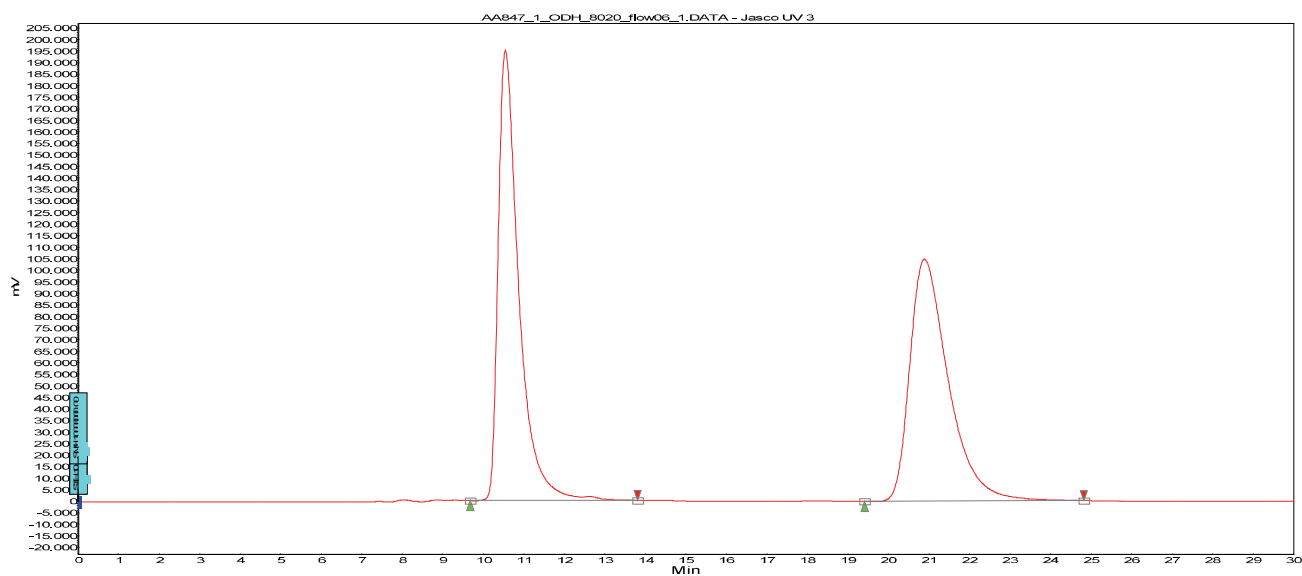
Mass Table

Line#:1 R.Time:14.4(Scan#:1364)
 MassPeaks:66 BasePeak:148(41885)
 RawMode:Averaged 14.3-14.4(1362-1366)
 BG Mode:Averaged 14.6-14.8(1396-1419)

#	m/z	Rel. Int.	#	m/z	Rel. Int.	#	m/z	Rel. Int.	#	m/z	Rel. Int.
1	49.80	9.41	18	77.00	30.03	35	108.20	5.02	52	138.25	3.07
2	51.00	17.03	19	78.10	14.30	36	114.95	3.56	53	144.25	3.35
3	52.00	41.20	20	79.00	20.85	37	116.05	9.18	54	147.15	44.29
4	53.05	38.35	21	80.15	17.65	38	117.15	5.73	55	148.05	100.00
5	54.05	31.29	22	89.05	21.04	39	118.00	8.15	56	149.05	13.82
6	54.95	45.77	23	90.05	13.20	40	119.80	17.45	57	156.15	5.04
7	55.80	3.86	24	91.00	29.62	41	121.15	37.31	58	184.05	7.24
8	61.50	5.70	25	92.00	24.72	42	122.00	33.46	59	213.80	7.42
9	61.80	8.99	26	93.20	27.03	43	122.95	5.33	60	240.30	4.96
10	63.00	36.55	27	94.10	31.58	44	124.20	3.28	61	241.95	5.86
11	64.10	11.66	28	96.05	4.03	45	130.20	7.36	62	243.15	5.68
12	65.00	55.15	29	102.25	4.91	46	131.15	11.59	63	256.10	9.53
13	66.00	50.20	30	103.10	8.36	47	132.10	4.64	64	256.75	5.52
14	67.10	33.58	31	103.85	3.76	48	133.90	5.20	65	270.25	10.66
15	68.20	12.36	32	104.95	3.70	49	135.05	16.53	66	271.15	35.95
16	74.90	3.52	33	106.05	6.48	50	136.15	68.22			
17	76.05	9.83	34	107.30	5.92	51	137.20	7.28			

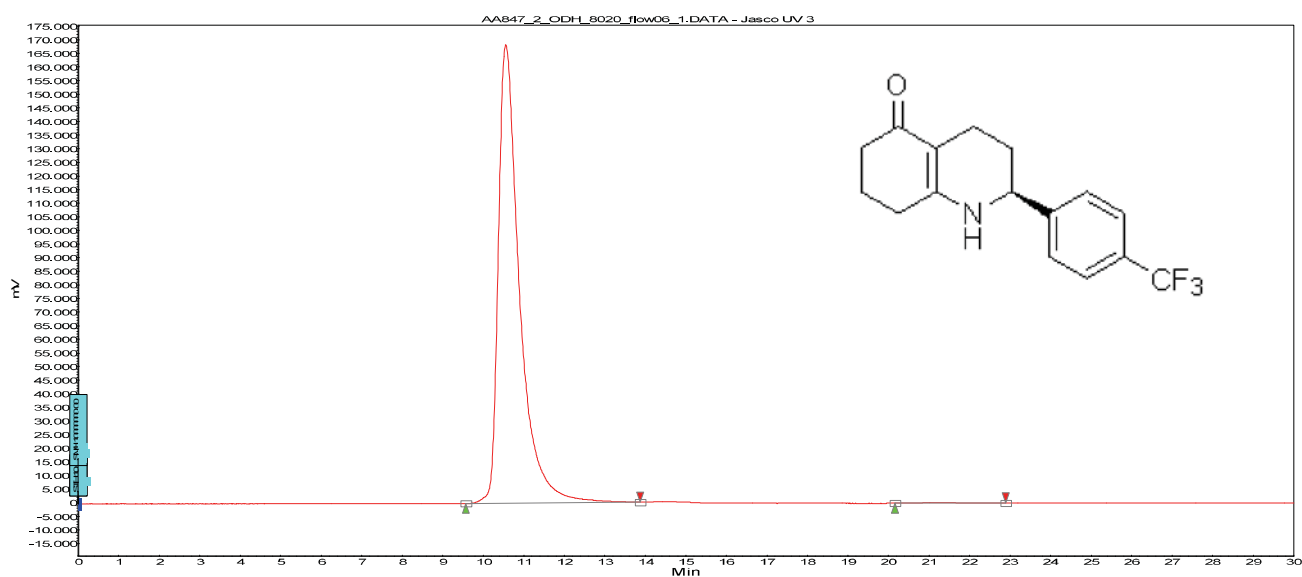
Chromatogram : AA847_1_ODH_8020_flow06_1

Data file: AA847_1_ODH_8020_flow06_1.DATA
Method: HPLC2_ODH_8020_flow06_acq90

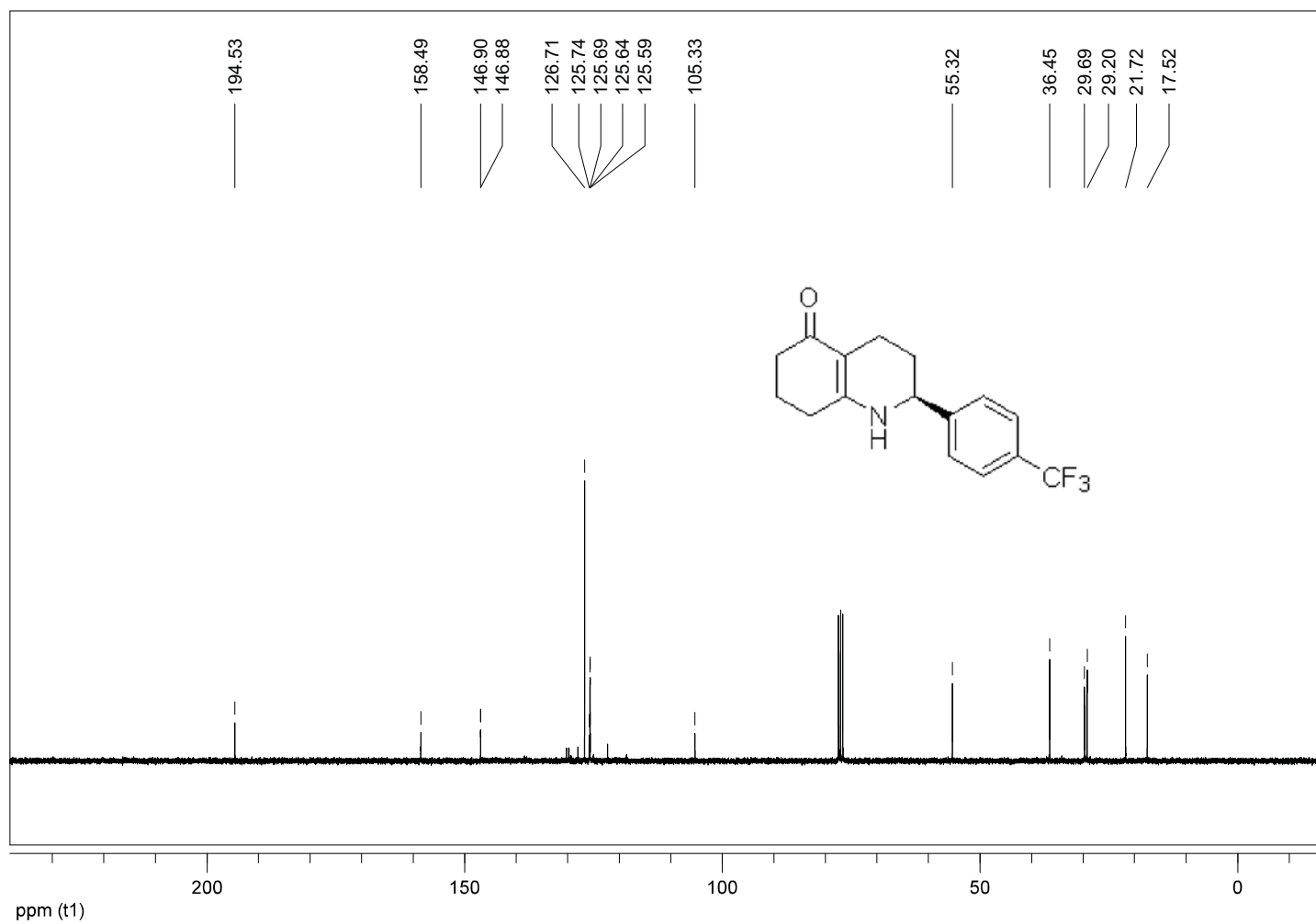
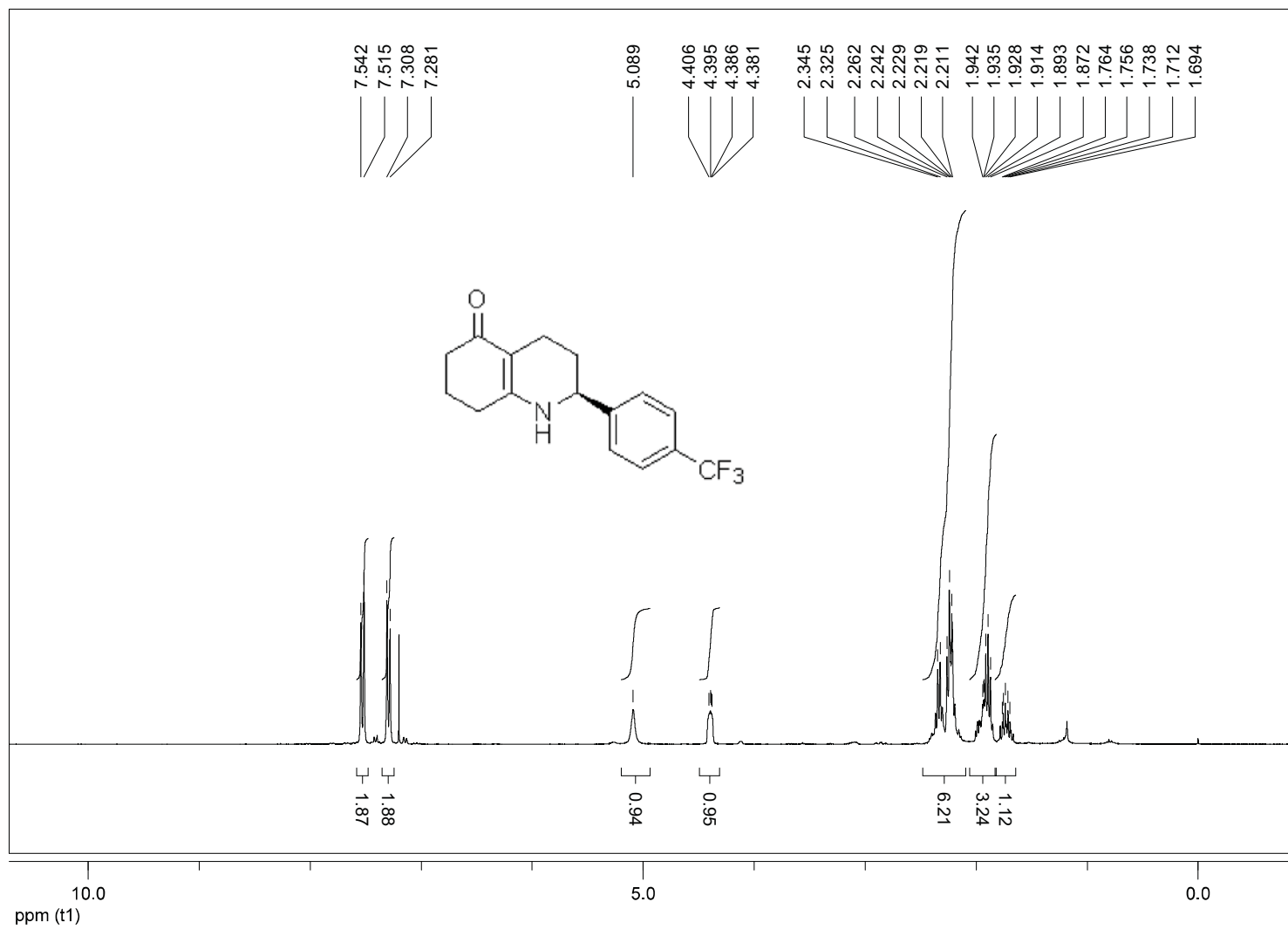


Chromatogram : AA847_2_ODH_8020_flow06_1

Data file: AA847_2_ODH_8020_flow06_1.DATA
Method: HPLC2_ODH_8020_flow06_acq90



Index	Start [Min]	Time [Min]	End [Min]	Area % [%]
1	9,567	10,558	13,872	99,706
2	20,155	21,200	22,891	0,294
Total				100,000



Sample Information

Analyzed : 08.11.2007 09:45:29
 Sample Name : AA847_2

Method

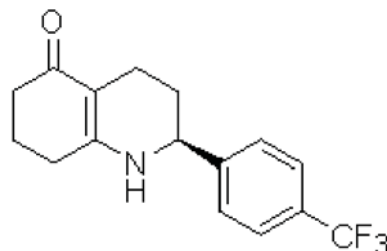
===== Analytical Line 1 =====

[GC-2010]

Column Oven Temp. : 60.0 °C
 Injection Temp. : 280.00 °C
 Injection Mode : Split
 Flow Control Mode : Linear Velocity
 Pressure : 29.2 kPa
 Total Flow : 17.2 mL/min
 Column Flow : 0.68 mL/min
 Linear Velocity : 30.0 cm/sec
 Purge Flow : 3.0 mL/min
 Split Ratio : 20.0

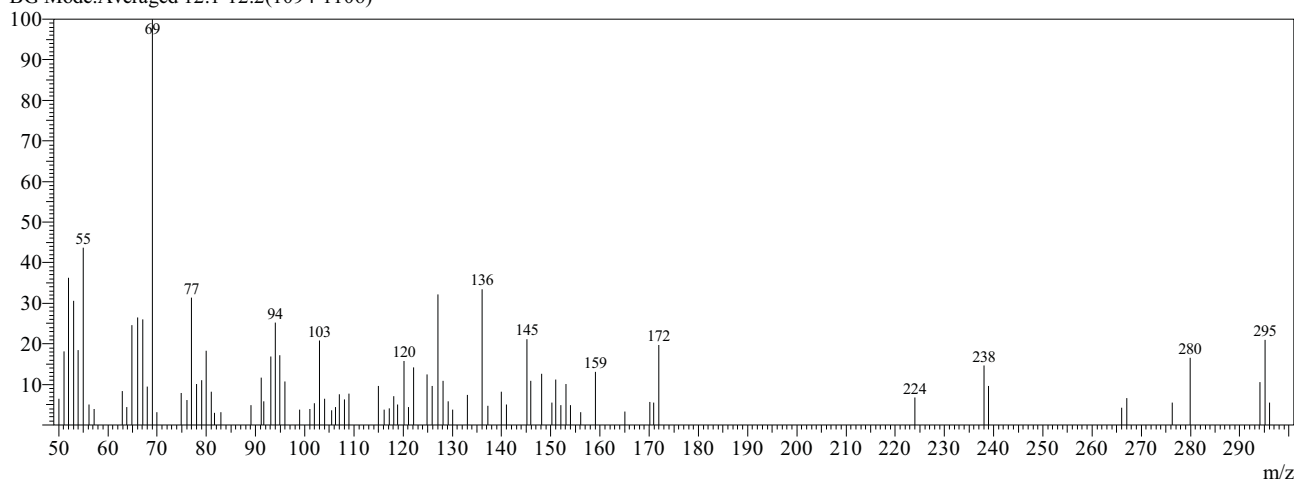
Oven Temp. Program

Rate	Temperature(°C)	Hold Time(min)
-	60.0	0.00
20.0	300.0	8.00



Spectrum

Line#:1 R.Time:12.0(Scan#:1082)
 MassPeaks:85 BasePeak:69(294494)
 RawMode:Averaged 12.0-12.0(1080-1083)
 BG Mode:Averaged 12.1-12.2(1094-1106)



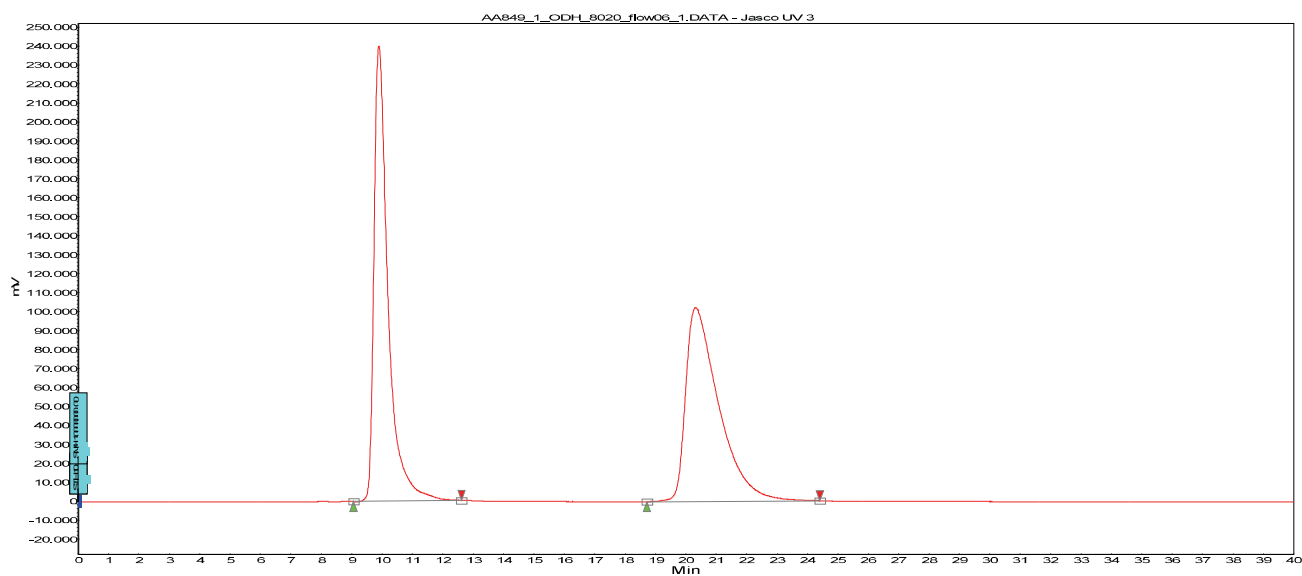
Mass Table

Line#:1 R.Time:12.0(Scan#:1082)
 MassPeaks:85 BasePeak:69(294494)
 RawMode:Averaged 12.0-12.0(1080-1083)
 BG Mode:Averaged 12.1-12.2(1094-1106)

#	m/z	Rel. Int.	#	m/z	Rel. Int.	#	m/z	Rel. Int.	#	m/z	Rel. Int.
1	50.00	6.44	23	81.00	8.21	45	117.20	4.05	67	152.10	4.96
2	51.05	18.16	24	81.60	3.05	46	118.10	7.05	68	153.10	10.02
3	52.00	36.30	25	82.90	3.13	47	118.80	4.99	69	154.05	4.92
4	53.00	30.66	26	89.05	4.89	48	120.10	15.74	70	156.05	3.12
5	53.95	18.40	27	91.10	11.75	49	121.05	4.37	71	159.10	13.07
6	55.00	43.70	28	91.70	5.86	50	122.15	14.26	72	165.05	3.33
7	56.10	4.98	29	93.05	16.90	51	124.90	12.43	73	170.10	5.63
8	57.15	4.01	30	94.00	25.28	52	125.95	9.57	74	170.85	5.57
9	62.95	8.34	31	94.90	17.13	53	127.05	32.15	75	172.00	19.68
10	63.85	4.42	32	96.00	10.66	54	128.10	10.84	76	224.00	6.74
11	64.90	24.61	33	99.00	3.75	55	129.10	5.91	77	238.05	14.61
12	66.05	26.50	34	101.10	3.93	56	130.05	3.78	78	238.90	9.67
13	67.05	25.98	35	101.95	5.32	57	133.05	7.37	79	266.05	4.27
14	68.05	9.43	36	103.00	20.89	58	136.00	33.49	80	267.10	6.60
15	69.00	100.00	37	104.05	6.48	59	137.20	4.73	81	276.25	5.51
16	70.00	3.15	38	105.50	3.57	60	139.90	8.19	82	279.95	16.61
17	74.95	7.82	39	106.20	4.41	61	140.95	5.02	83	294.05	10.50
18	76.05	6.14	40	107.00	7.57	62	145.10	21.09	84	295.10	21.01
19	77.00	31.46	41	108.00	6.27	63	145.95	10.91	85	296.05	5.47
20	77.95	10.14	42	108.95	7.69	64	148.10	12.65			
21	79.10	11.12	43	114.90	9.58	65	150.25	5.47			
22	80.00	18.37	44	116.15	3.78	66	151.00	11.25			

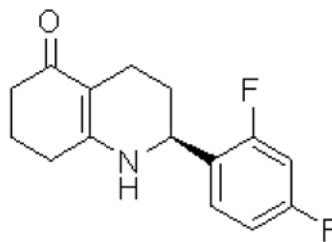
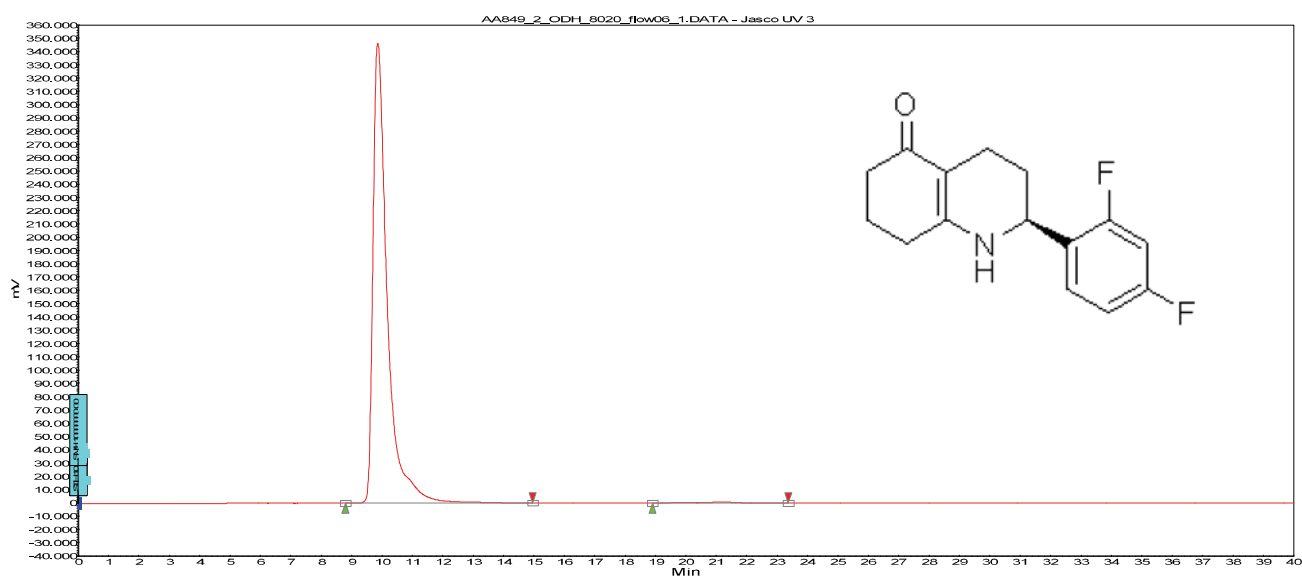
Chromatogram : AA849_1_ODH_8020_flow06_1

Data file: AA849_1_ODH_8020_flow06_1.DATA
Method: HPLC2_ODH_8020_flow06_acq90

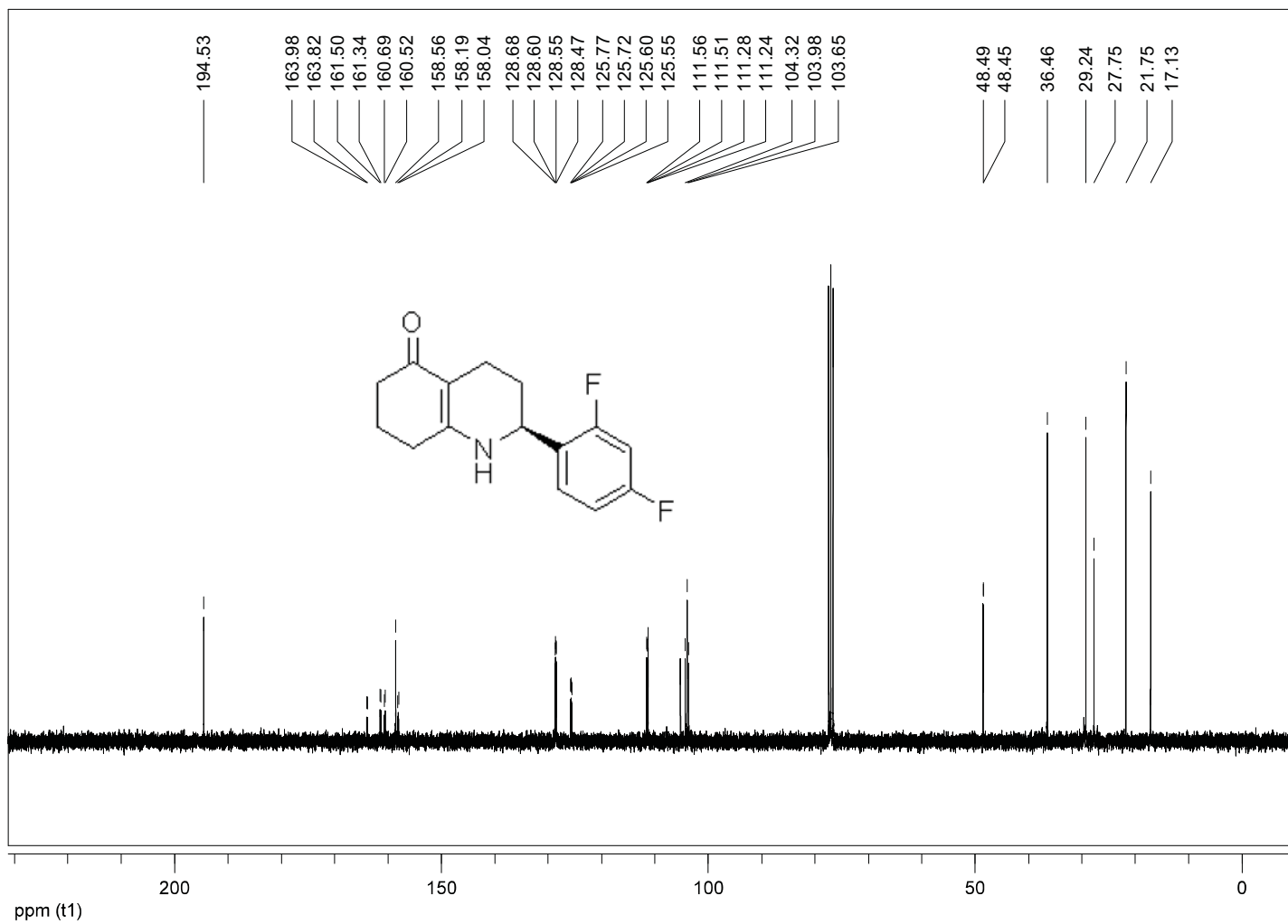
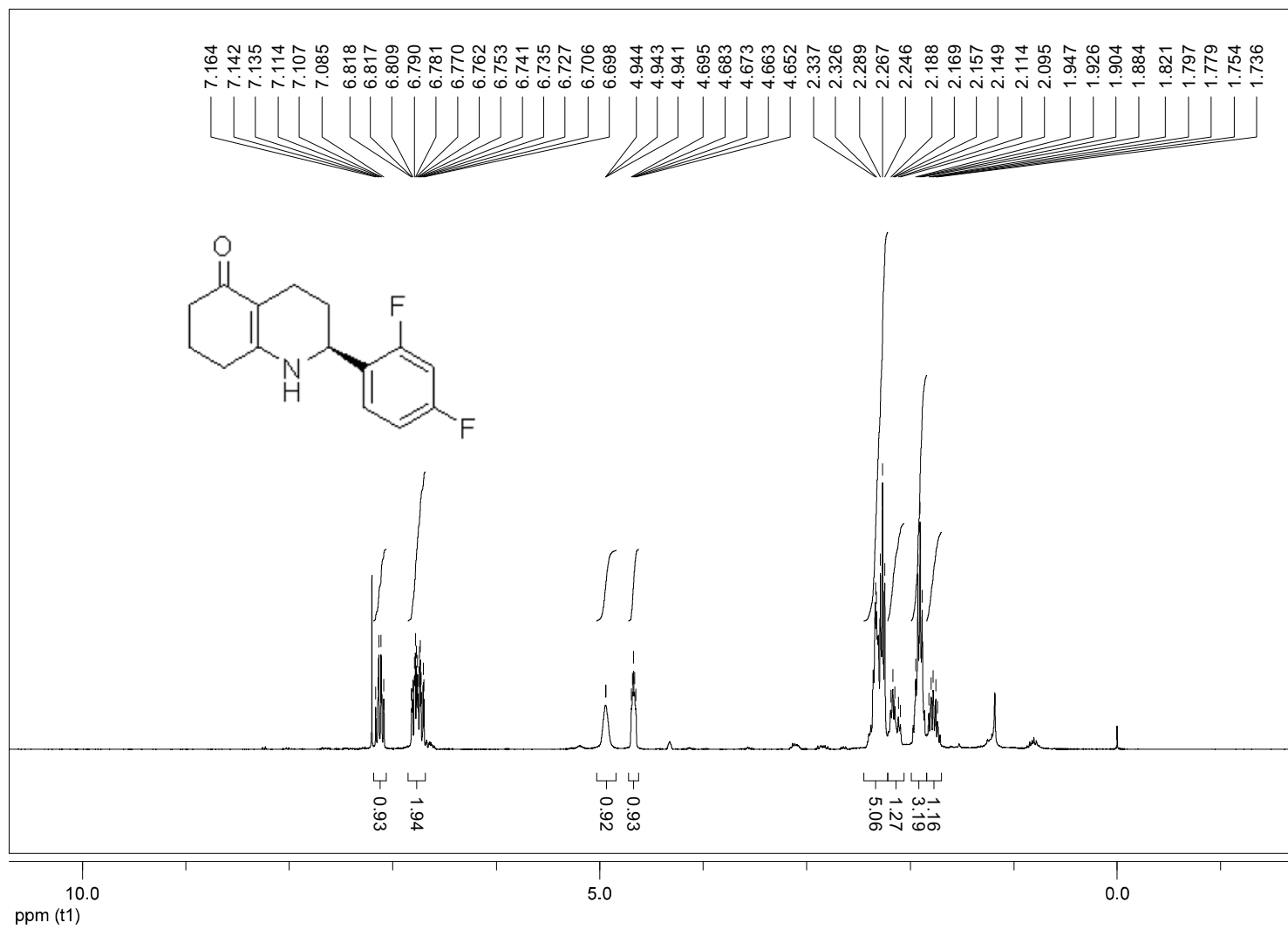


Chromatogram : AA849_2_ODH_8020_flow06_1

Data file: AA849_2_ODH_8020_flow06_1.DATA
Method: HPLC2_ODH_8020_flow06_acq90



Index	Start [Min]	Time [Min]	End [Min]	Area %
1	8,806	9,858	14,950	99,517
2	18,895	21,175	23,366	0,483
Total				100,000



Sample Information

Analyzed : 08.11.2007 10:28:55
 Sample Name : AA849_2

Method

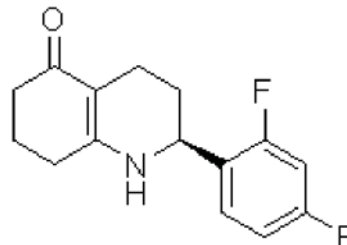
===== Analytical Line 1 =====

[GC-2010]

Column Oven Temp. : 60.0 °C
 Injection Temp. : 280.00 °C
 Injection Mode : Split
 Flow Control Mode : Linear Velocity
 Pressure : 29.2 kPa
 Total Flow : 17.2 mL/min
 Column Flow : 0.68 mL/min
 Linear Velocity : 30.0 cm/sec
 Purge Flow : 3.0 mL/min
 Split Ratio : 20.0

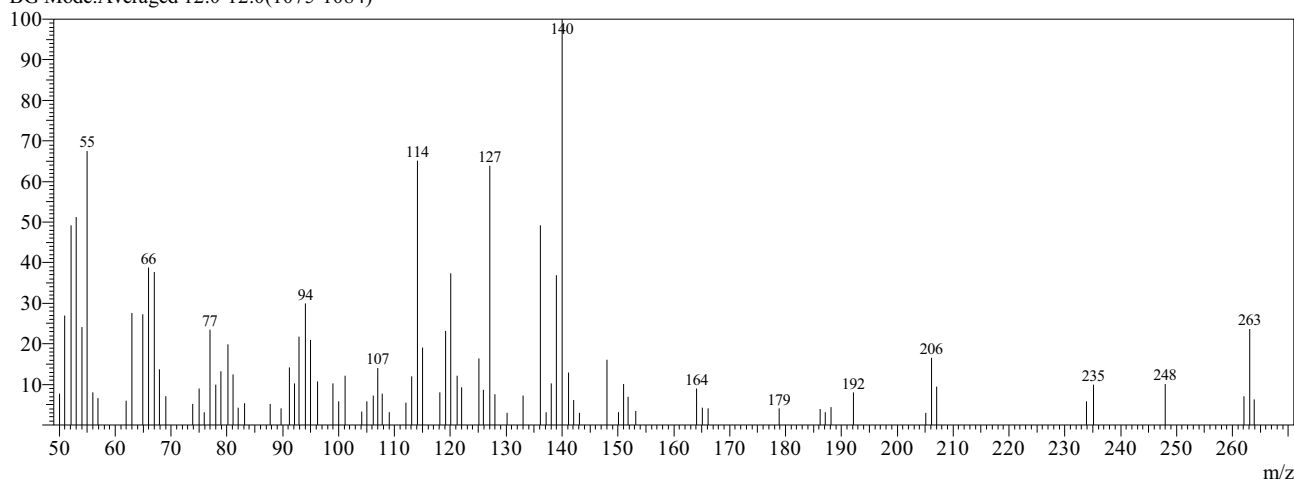
Oven Temp. Program

Rate	Temperature(°C)	Hold Time(min)
-	60.0	0.00
20.0	300.0	8.00



Spectrum

Line#:1 R.Time:11.8(Scan#:1059)
 MassPeaks:87 BasePeak:140(223066)
 RawMode:Averaged 11.8-11.8(1058-1060)
 BG Mode:Averaged 12.0-12.0(1075-1084)



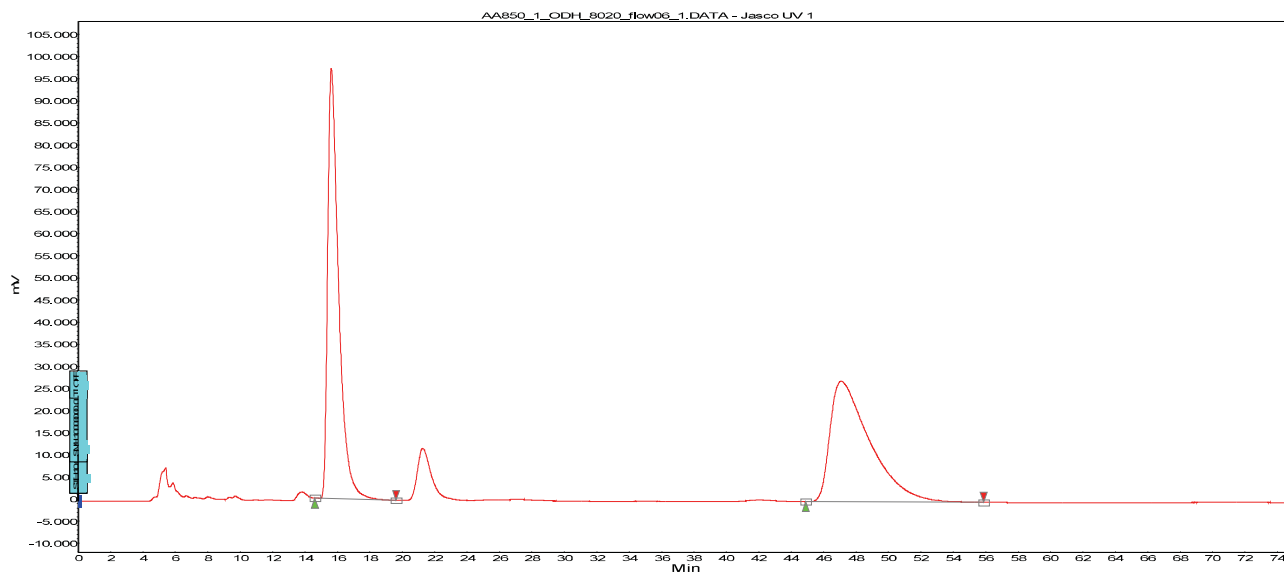
Mass Table

Line#:1 R.Time:11.8(Scan#:1059)
 MassPeaks:87 BasePeak:140(223066)
 RawMode:Averaged 11.8-11.8(1058-1060)
 BG Mode:Averaged 12.0-12.0(1075-1084)

#	m/z	Rel. Int.	#	m/z	Rel. Int.	#	m/z	Rel. Int.	#	m/z	Rel. Int.
1	50.00	7.71	23	81.05	12.39	45	114.05	65.15	67	150.05	3.15
2	51.00	27.03	24	82.00	4.27	46	115.00	19.02	68	151.05	10.02
3	52.05	49.17	25	83.10	5.41	47	118.15	8.00	69	151.80	6.92
4	53.05	51.19	26	87.75	5.15	48	119.10	23.14	70	153.15	3.49
5	54.00	24.07	27	89.70	4.04	49	120.05	37.39	71	164.05	9.02
6	55.00	67.53	28	91.15	14.17	50	121.15	12.18	72	165.05	4.27
7	56.00	8.06	29	92.10	10.25	51	122.05	9.33	73	166.10	4.16
8	56.95	6.64	30	92.95	21.80	52	125.05	16.45	74	178.90	4.07
9	61.95	6.01	31	94.05	30.02	53	125.95	8.63	75	186.15	3.93
10	63.00	27.58	32	94.95	21.02	54	127.10	63.88	76	187.15	3.19
11	64.90	27.24	33	96.20	10.66	55	127.95	7.56	77	188.10	4.40
12	66.00	38.86	34	99.00	10.26	56	130.10	3.04	78	192.10	8.10
13	67.05	37.65	35	100.05	5.88	57	133.05	7.21	79	205.10	3.03
14	67.90	13.73	36	101.10	12.10	58	136.15	49.22	80	206.10	16.54
15	69.05	7.16	37	104.15	3.29	59	137.10	3.19	81	207.10	9.52
16	73.90	5.13	38	105.00	5.80	60	138.00	10.20	82	233.90	5.91
17	75.00	8.94	39	106.15	7.18	61	138.95	36.83	83	235.10	9.95
18	75.95	3.10	40	107.05	14.07	62	140.00	100.00	84	248.00	10.09
19	77.00	23.56	41	107.80	7.65	63	141.10	12.95	85	262.10	7.12
20	78.00	9.95	42	109.05	3.19	64	142.10	6.23	86	263.05	23.69
21	78.90	13.20	43	112.00	5.48	65	143.05	3.07	87	263.95	6.38
22	80.15	19.81	44	113.05	11.94	66	148.00	16.07			

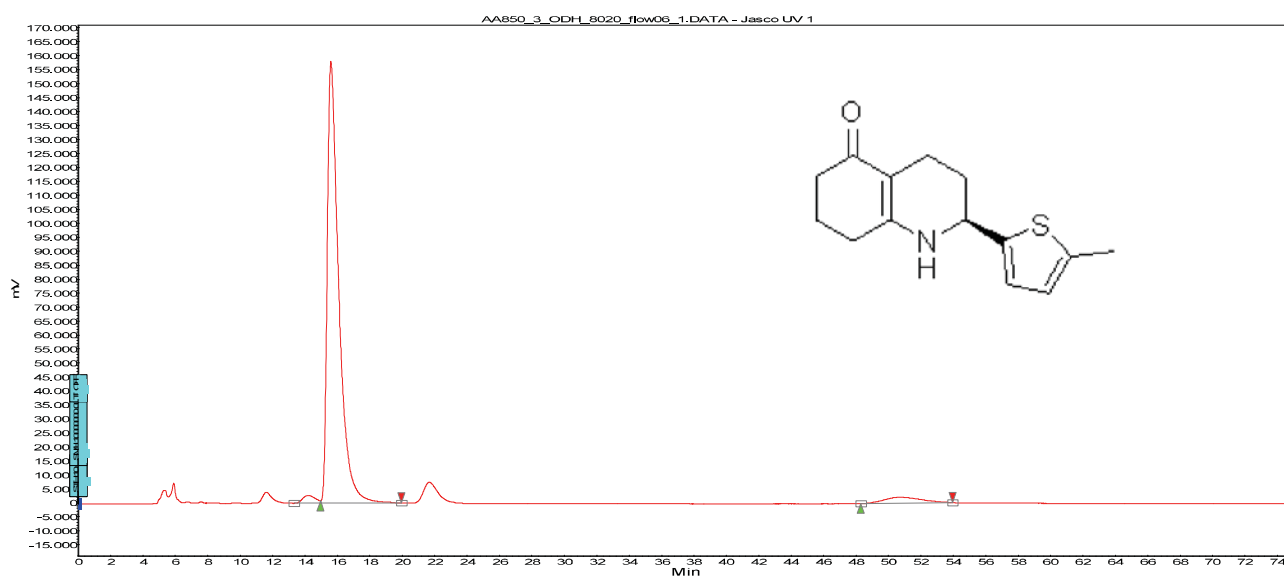
Chromatogram : AA850_1_ODH_8020_flow06_1

Data file: AA850_1_ODH_8020_flow06_1.DATA
Method: HPLC2_ODH_8020_flow06_acq90

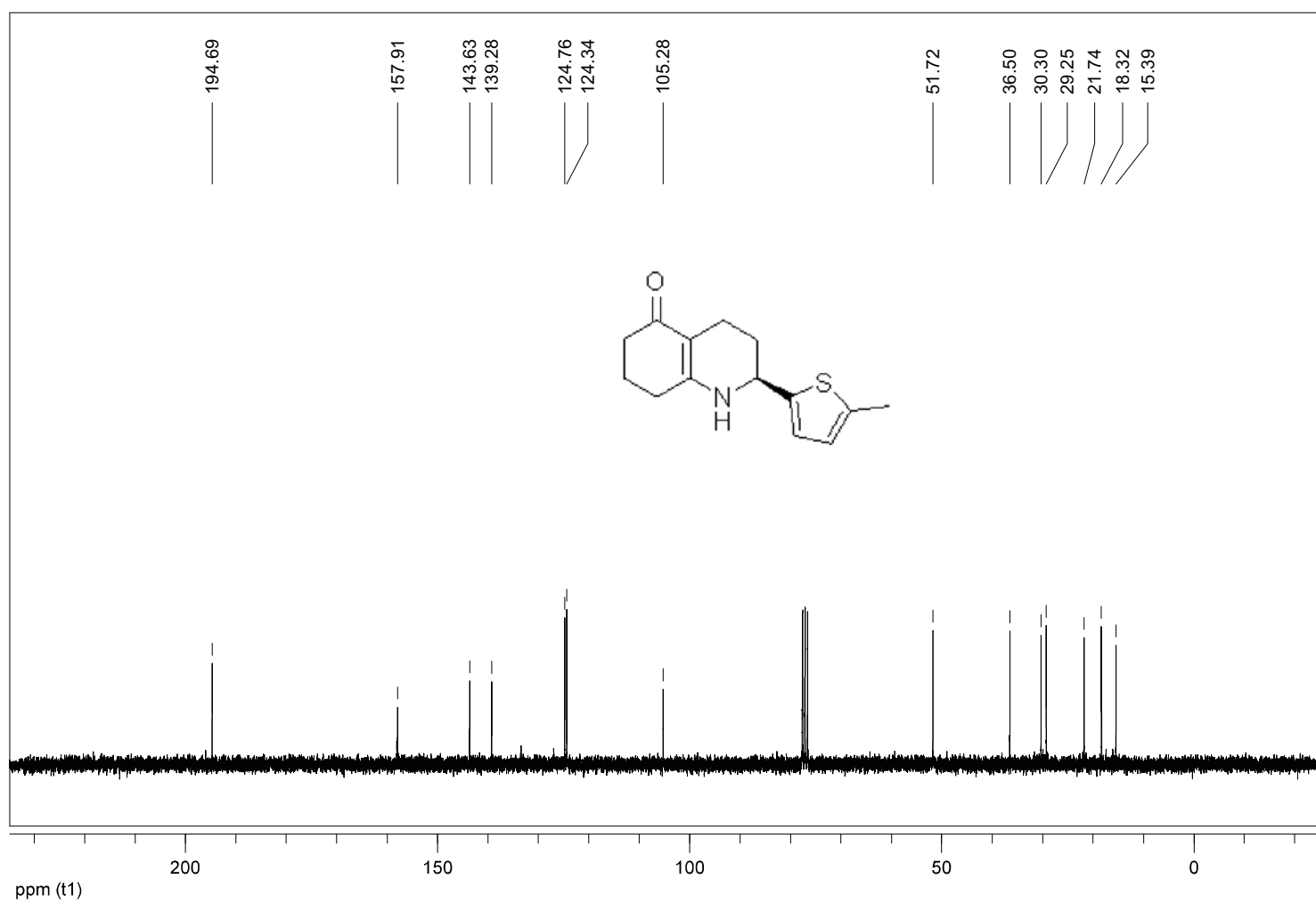
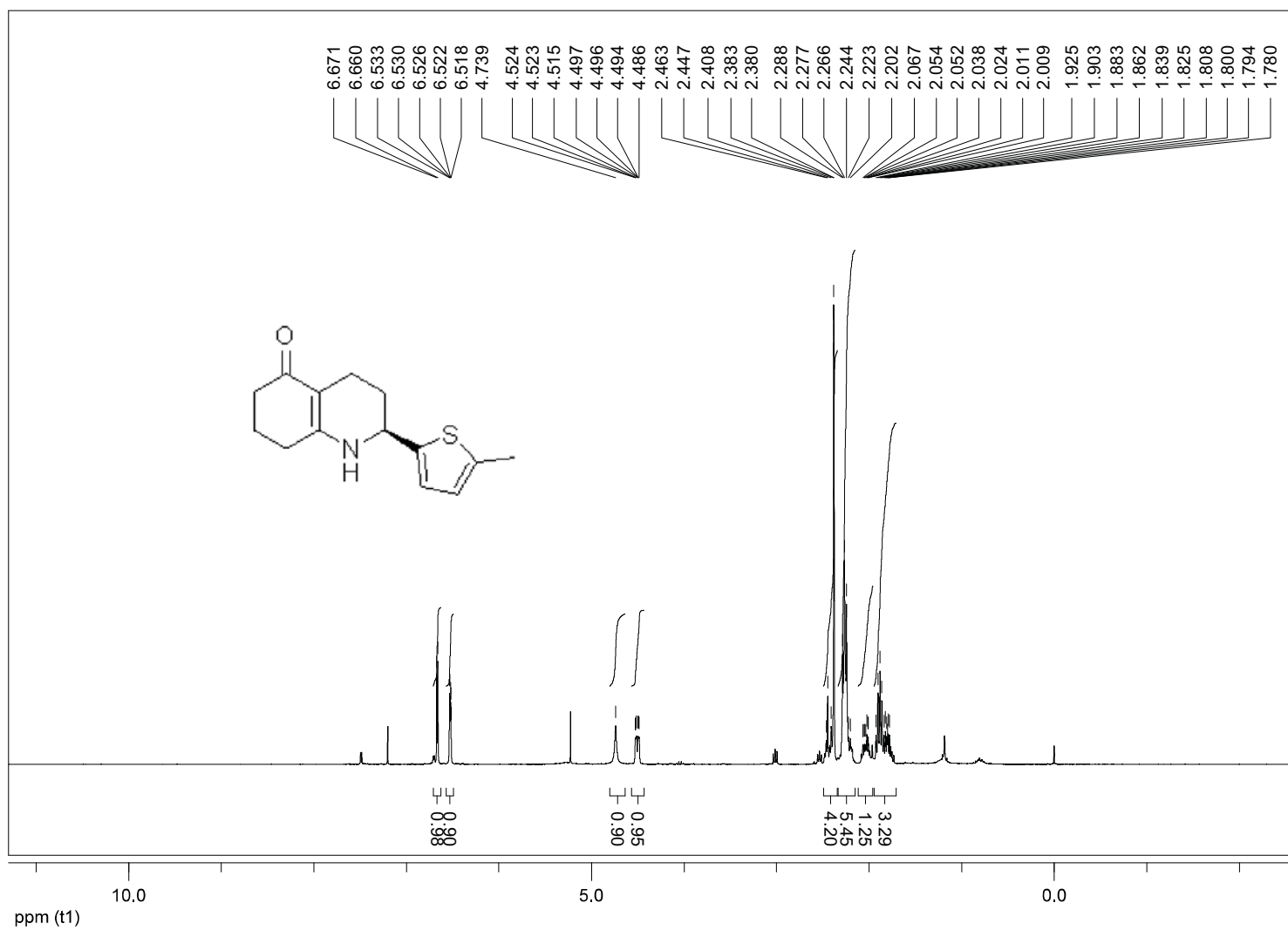


Chromatogram : AA850_3_ODH_8020_flow06_1

Data file: AA850_3_ODH_8020_flow06_1.DATA
Method: HPLC2_ODH_8020_flow06_acq90



Index	Start [Min]	Time [Min]	End [Min]	Area %
2	14,946	15,600	19,946	96,019
1	48,295	50,675	53,943	3,981
Total				100,000



Sample Information

Analyzed : 13.11.2007 19:28:28
 Sample Name : AA850_3

Method

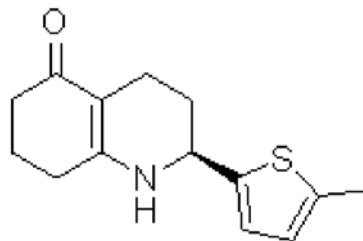
===== Analytical Line 1 =====

[GC-2010]

Column Oven Temp. : 60.0 °C
 Injection Temp. : 280.00 °C
 Injection Mode : Split
 Flow Control Mode : Linear Velocity
 Pressure : 29.2 kPa
 Total Flow : 17.2 mL/min
 Column Flow : 0.68 mL/min
 Linear Velocity : 30.0 cm/sec
 Purge Flow : 3.0 mL/min
 Split Ratio : 20.0

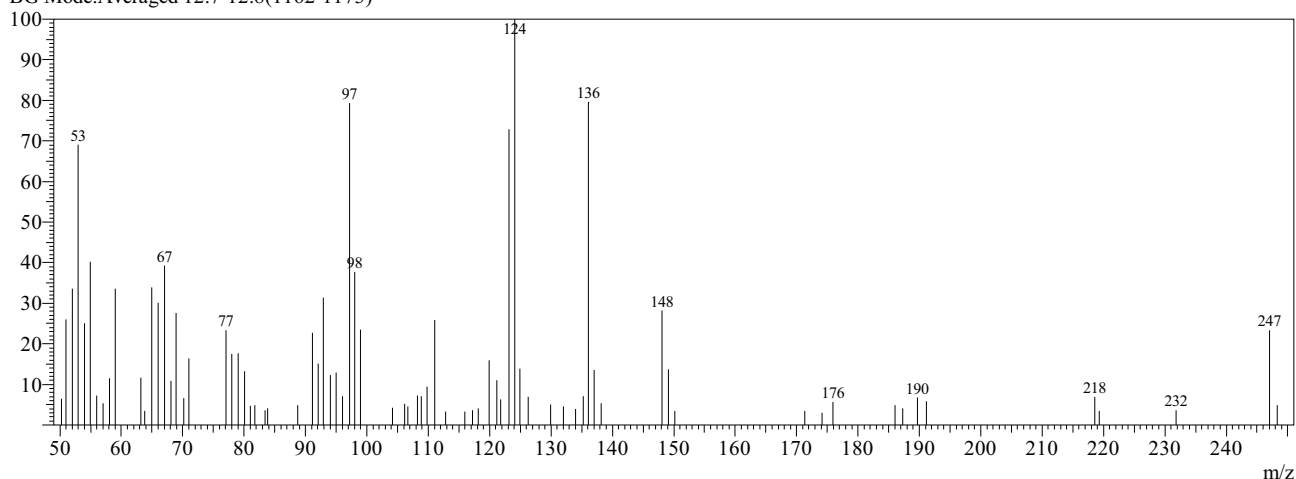
Oven Temp. Program

Rate	Temperature(°C)	Hold Time(min)
-	60.0	0.00
20.0	300.0	8.00



Spectrum

Line#:1 R.Time:12.5(Scan#:1142)
 MassPeaks:77 BasePeak:124(84013)
 RawMode:Averaged 12.5-12.5(1140-1143)
 BG Mode:Averaged 12.7-12.8(1162-1173)



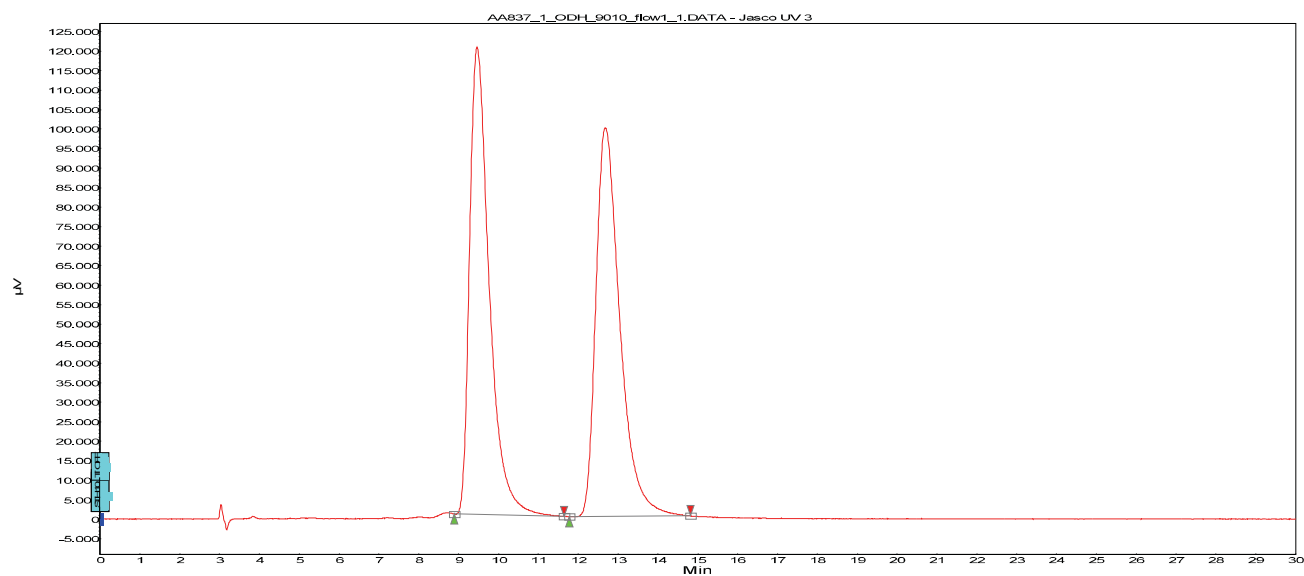
Mass Table

Line#:1 R.Time:12.5(Scan#:1142)
 MassPeaks:77 BasePeak:124(84013)
 RawMode:Averaged 12.5-12.5(1140-1143)
 BG Mode:Averaged 12.7-12.8(1162-1173)

#	m/z	Rel. Int.	#	m/z	Rel. Int.	#	m/z	Rel. Int.	#	m/z	Rel. Int.
1	50.20	6.50	21	77.95	17.51	41	108.25	7.33	61	137.05	13.62
2	51.00	26.00	22	79.05	17.64	42	108.90	7.16	62	138.15	5.32
3	52.05	33.63	23	80.05	13.30	43	109.85	9.49	63	148.10	28.22
4	53.00	69.05	24	81.00	4.75	44	111.05	25.92	64	149.10	13.72
5	54.05	25.04	25	81.75	4.83	45	112.85	3.35	65	150.15	3.47
6	54.90	40.24	26	83.40	3.65	46	116.00	3.32	66	171.35	3.48
7	56.00	7.30	27	83.80	4.07	47	117.25	3.61	67	174.10	3.03
8	57.05	5.37	28	88.75	4.84	48	118.15	4.08	68	175.95	5.64
9	58.10	11.57	29	91.10	22.71	49	119.90	15.88	69	186.00	4.83
10	59.00	33.53	30	92.10	15.18	50	121.15	11.08	70	187.25	4.13
11	63.15	11.73	31	92.95	31.46	51	121.80	6.26	71	189.65	6.76
12	63.85	3.44	32	94.10	12.23	52	123.10	72.93	72	191.15	5.86
13	65.00	33.90	33	94.95	12.98	53	124.05	100.00	73	218.55	6.94
14	66.05	30.16	34	96.05	7.02	54	124.95	13.92	74	219.25	3.47
15	67.05	39.26	35	97.15	79.38	55	126.25	6.88	75	231.85	3.55
16	68.05	10.88	36	98.05	37.66	56	129.90	4.97	76	247.00	23.33
17	68.95	27.63	37	99.00	23.55	57	132.05	4.65	77	248.25	4.85
18	70.15	6.61	38	104.15	4.18	58	133.95	3.98			
19	71.00	16.41	39	106.10	5.22	59	135.20	7.08			
20	77.10	23.37	40	106.70	4.65	60	136.10	79.63			

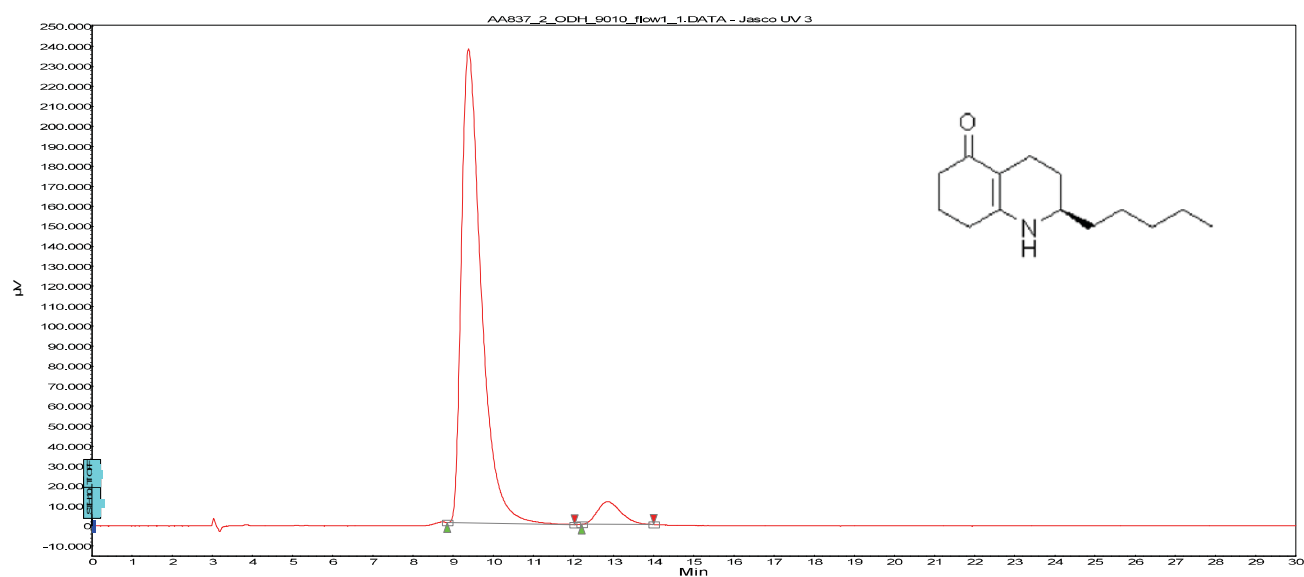
Chromatogram : AA837_1_ODH_9010_flow1_1

Data file: AA837_1_ODH_9010_flow1_1.DATA
Method: HPLC1_ODH_9010_flow1_acq_30



Chromatogram : AA837_2_ODH_9010_flow1_1

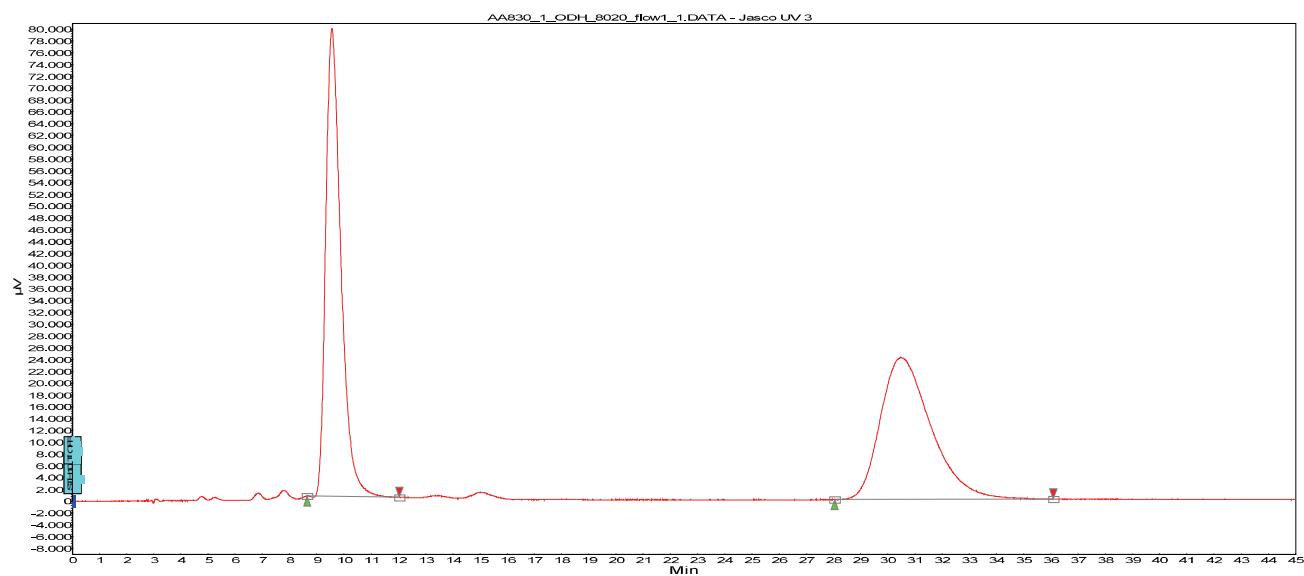
Data file: AA837_2_ODH_9010_flow1_1.DATA
Method: HPLC1_ODH_9010_flow1_acq_30



Index	Start [Min]	Time [Min]	End [Min]	Area %
1	8,851	9,383	12,033	94,501
2	12,200	12,850	13,998	5,499
Total				100,000

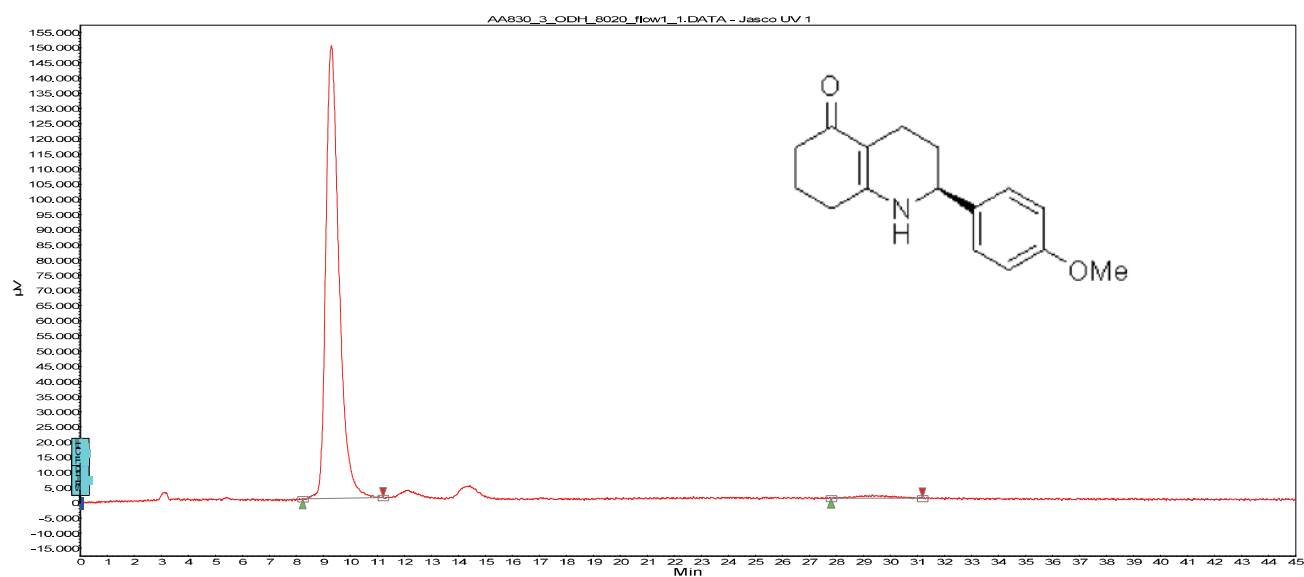
Chromatogram : AA830_1_ODH_8020_flow1_1

Data file: AA830_1_ODH_8020_flow1_1.DATA
Method: HPLC1_ODH_8020_flow1_acq_60

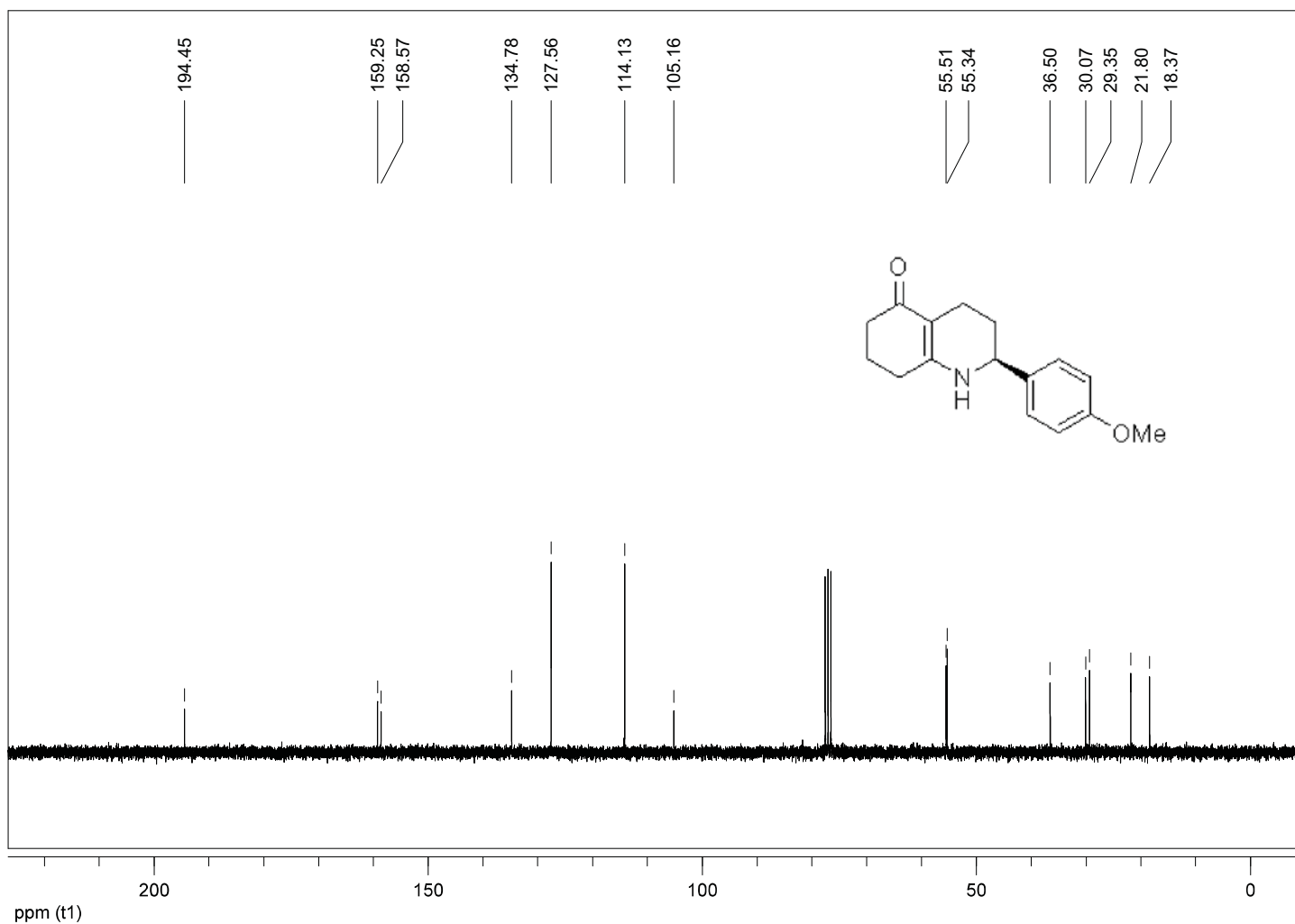
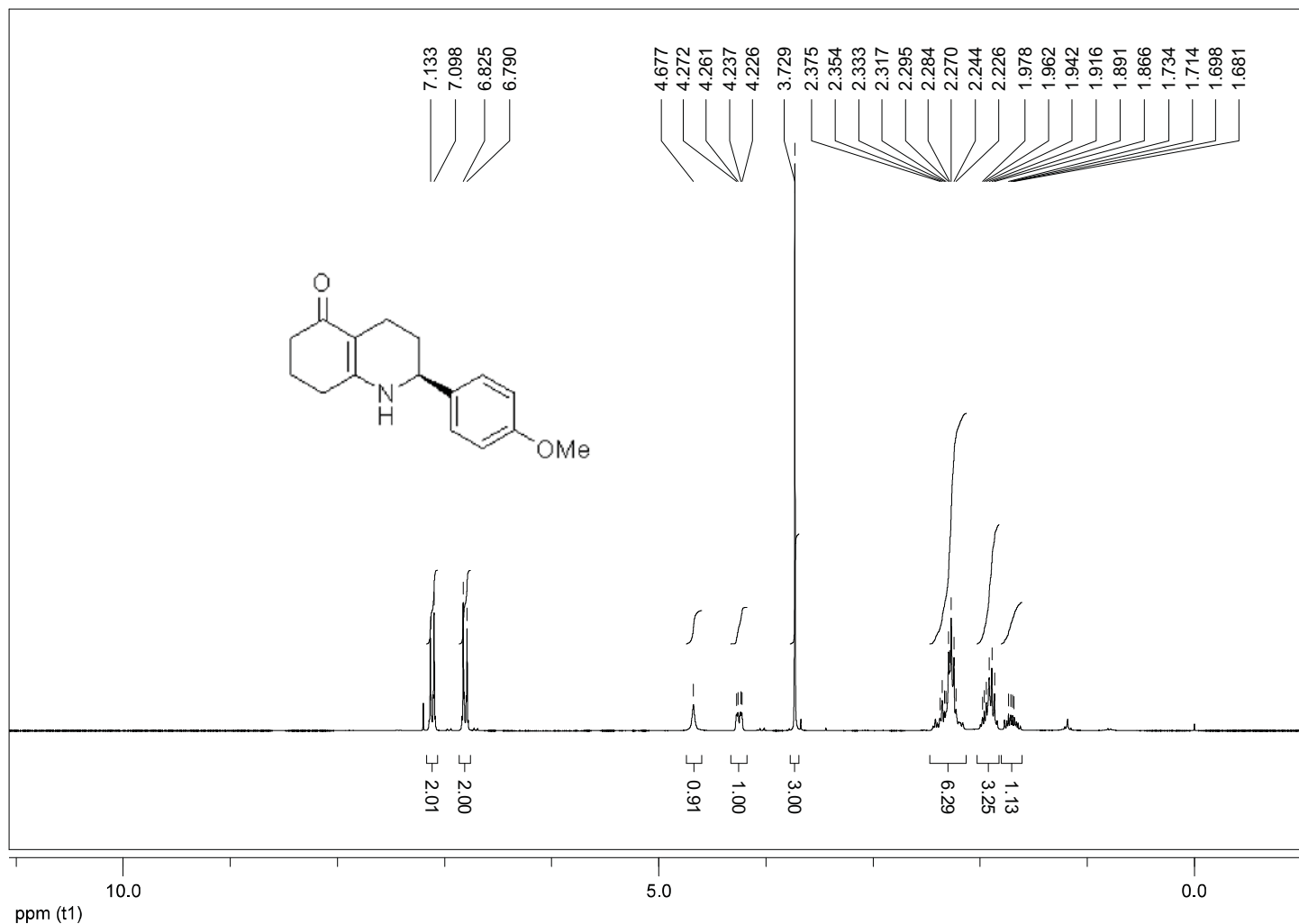


Chromatogram : AA830_3_ODH_8020_flow1_1

Data file: AA830_3_ODH_8020_flow1_1.DATA
Method: HPLC1_ODH_8020_flow1_acq_60



Index	Start [Min]	Time [Min]	End [Min]	Area %
1	8,244	9,300	11,219	98,519
2	27,801	29,333	31,178	1,481
Total				100,000



Sample Information

Analyzed : 23.10.2007 11:58:34
 Sample Name : AA830_1

Method

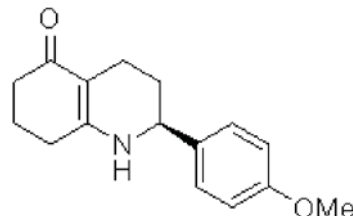
===== Analytical Line 1 =====

[GC-2010]

Column Oven Temp. : 60.0 °C
 Injection Temp. : 280.00 °C
 Injection Mode : Split
 Flow Control Mode : Linear Velocity
 Pressure : 29.2 kPa
 Total Flow : 17.2 mL/min
 Column Flow : 0.68 mL/min
 Linear Velocity : 30.0 cm/sec
 Purge Flow : 3.0 mL/min
 Split Ratio : 20.0

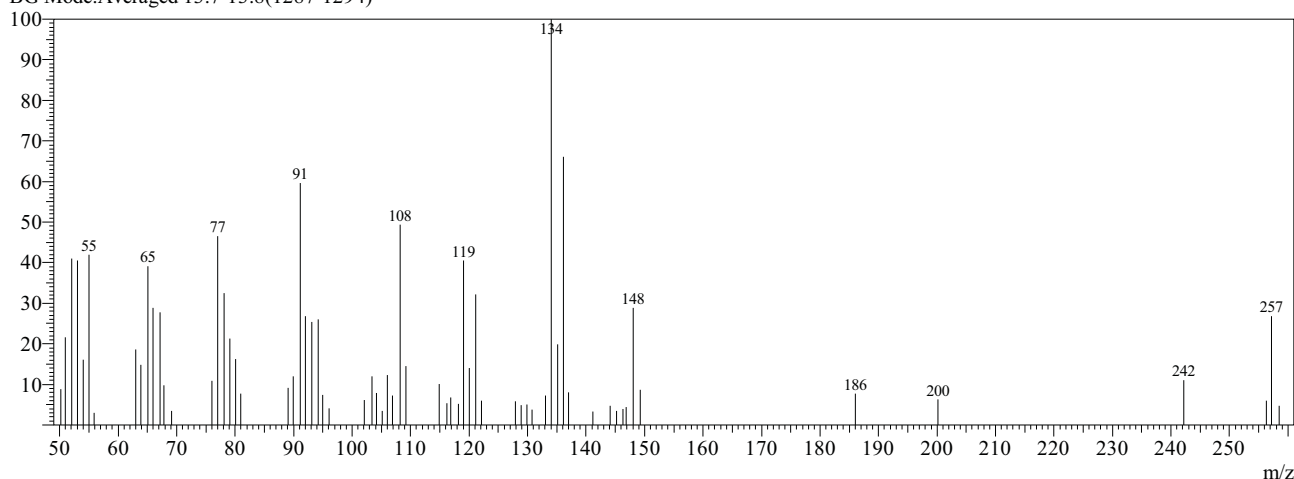
Oven Temp. Program

Rate	Temperature(°C)	Hold Time(min)
-	60.0	0.00
20.0	300.0	15.00



Spectrum

Line#:1 R.Time:13.5(Scan#:1264)
 MassPeaks:66 BasePeak:134(100072)
 RawMode:Averaged 13.5-13.5(1261-1266)
 BG Mode:Averaged 13.7-13.8(1287-1294)



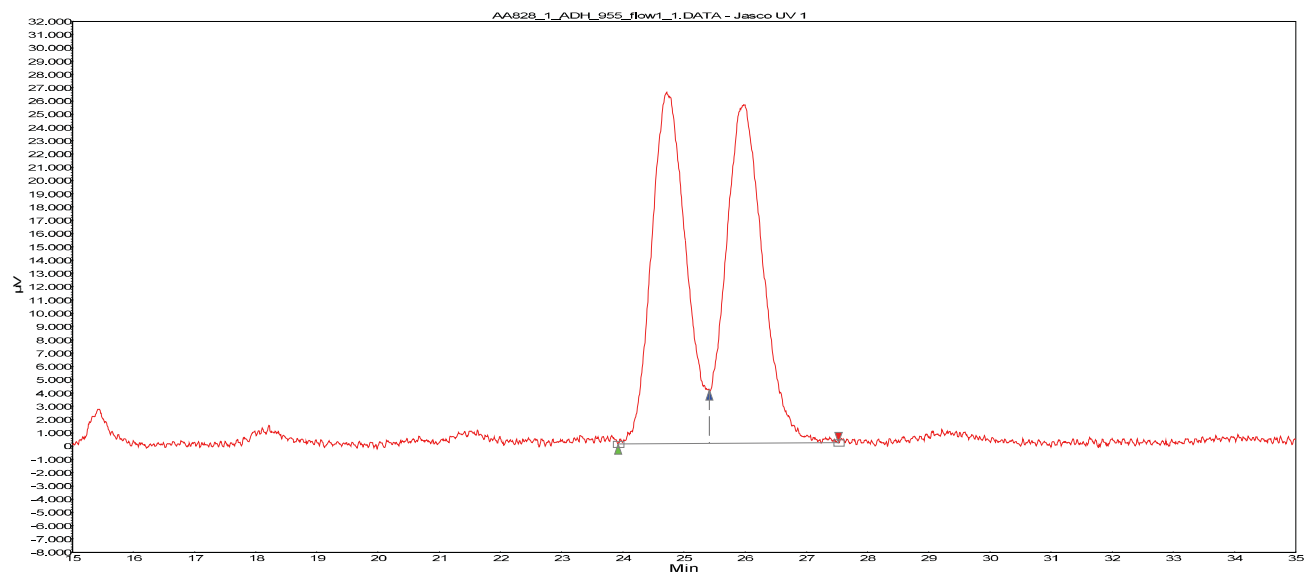
Mass Table

Line#:1 R.Time:13.5(Scan#:1264)
 MassPeaks:66 BasePeak:134(100072)
 RawMode:Averaged 13.5-13.5(1261-1266)
 BG Mode:Averaged 13.7-13.8(1287-1294)

#	m/z	Rel. Int.	#	m/z	Rel. Int.	#	m/z	Rel. Int.	#	m/z	Rel. Int.
1	50.15	8.91	18	79.05	21.30	35	108.20	49.30	52	136.10	66.03
2	50.95	21.61	19	80.05	16.18	36	109.15	14.55	53	137.05	8.12
3	52.05	41.02	20	80.95	7.67	37	114.90	10.14	54	141.15	3.33
4	53.00	40.61	21	89.10	9.18	38	116.15	5.38	55	144.10	4.71
5	54.05	16.08	22	89.95	11.92	39	116.90	6.77	56	145.15	3.40
6	55.00	41.92	23	91.10	59.65	40	118.15	5.27	57	146.25	3.98
7	55.90	3.01	24	92.05	26.88	41	119.10	40.59	58	146.90	4.41
8	63.05	18.64	25	93.10	25.47	42	120.05	14.05	59	148.10	28.79
9	63.90	14.84	26	94.20	25.98	43	121.15	32.19	60	149.20	8.60
10	65.10	39.10	27	95.00	7.48	44	122.10	6.07	61	186.05	7.73
11	66.00	28.94	28	96.05	4.04	45	127.95	5.78	62	200.20	6.33
12	67.20	27.73	29	102.05	6.13	46	128.90	4.96	63	242.15	10.98
13	67.85	9.80	30	103.40	11.92	47	129.90	5.03	64	256.25	6.02
14	69.15	3.47	31	104.20	7.96	48	130.80	3.85	65	257.15	26.75
15	76.00	10.83	32	105.10	3.42	49	133.05	7.31	66	258.45	4.66
16	77.00	46.58	33	106.00	12.30	50	134.00	100.00			
17	78.10	32.43	34	106.95	7.24	51	135.10	19.86			

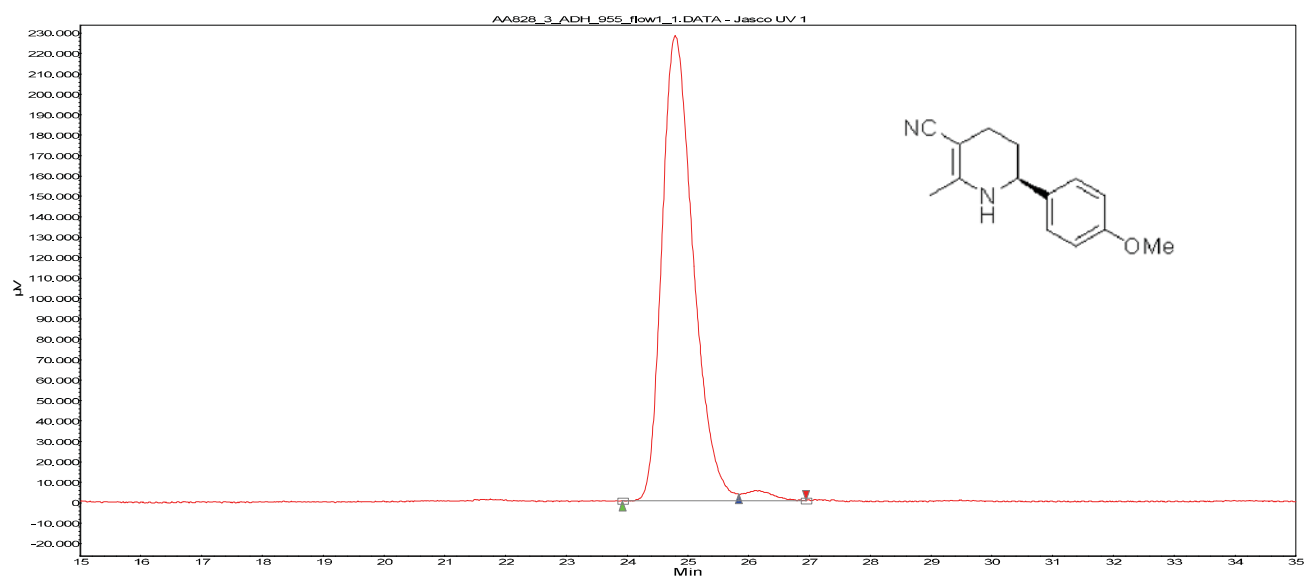
Chromatogram : AA828_1_ADH_955_flow1_1

Data file: AA828_1_ADH_955_flow1_1.DATA
Method: HPLC1_ADH_955_flow1_acq_90

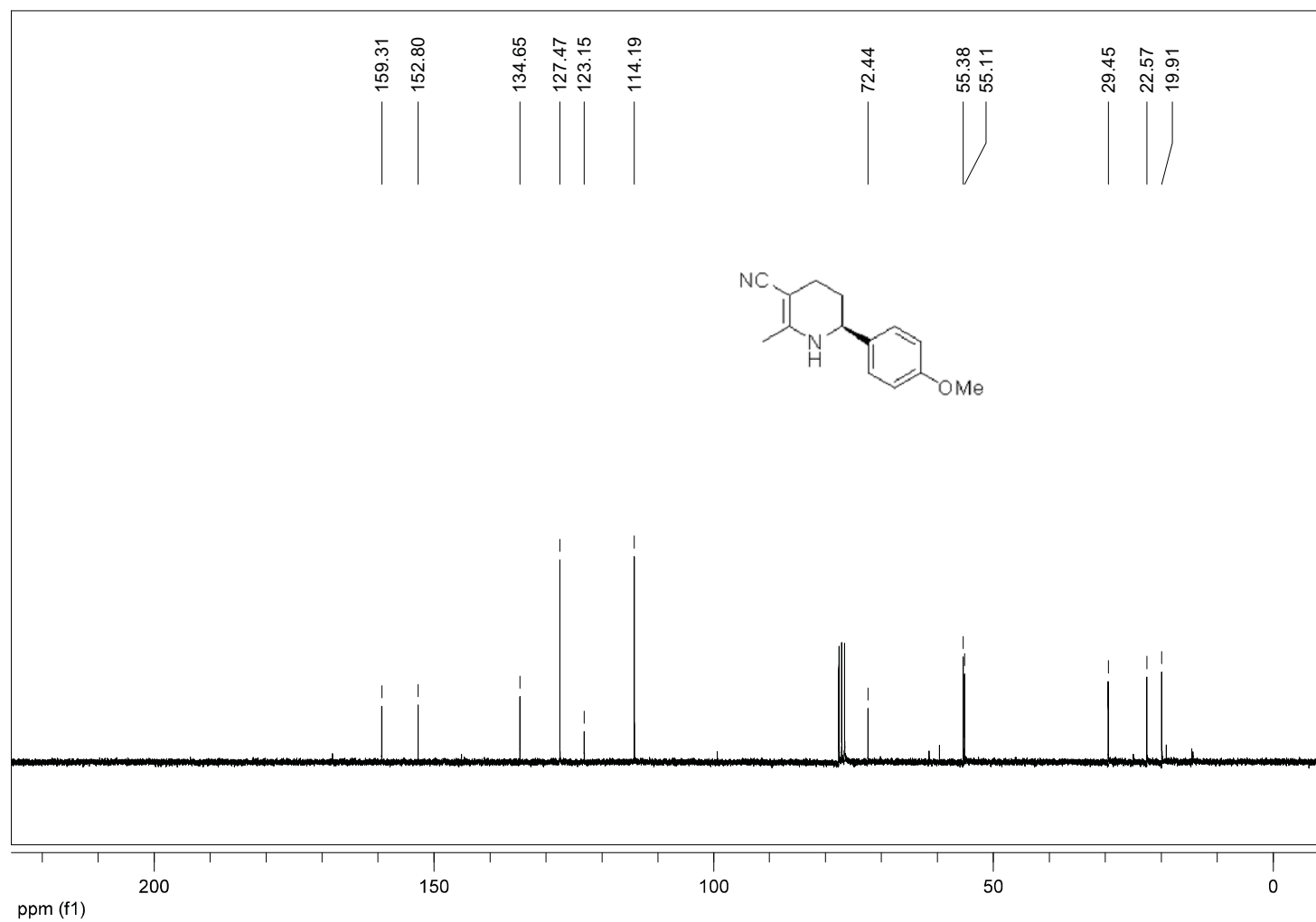
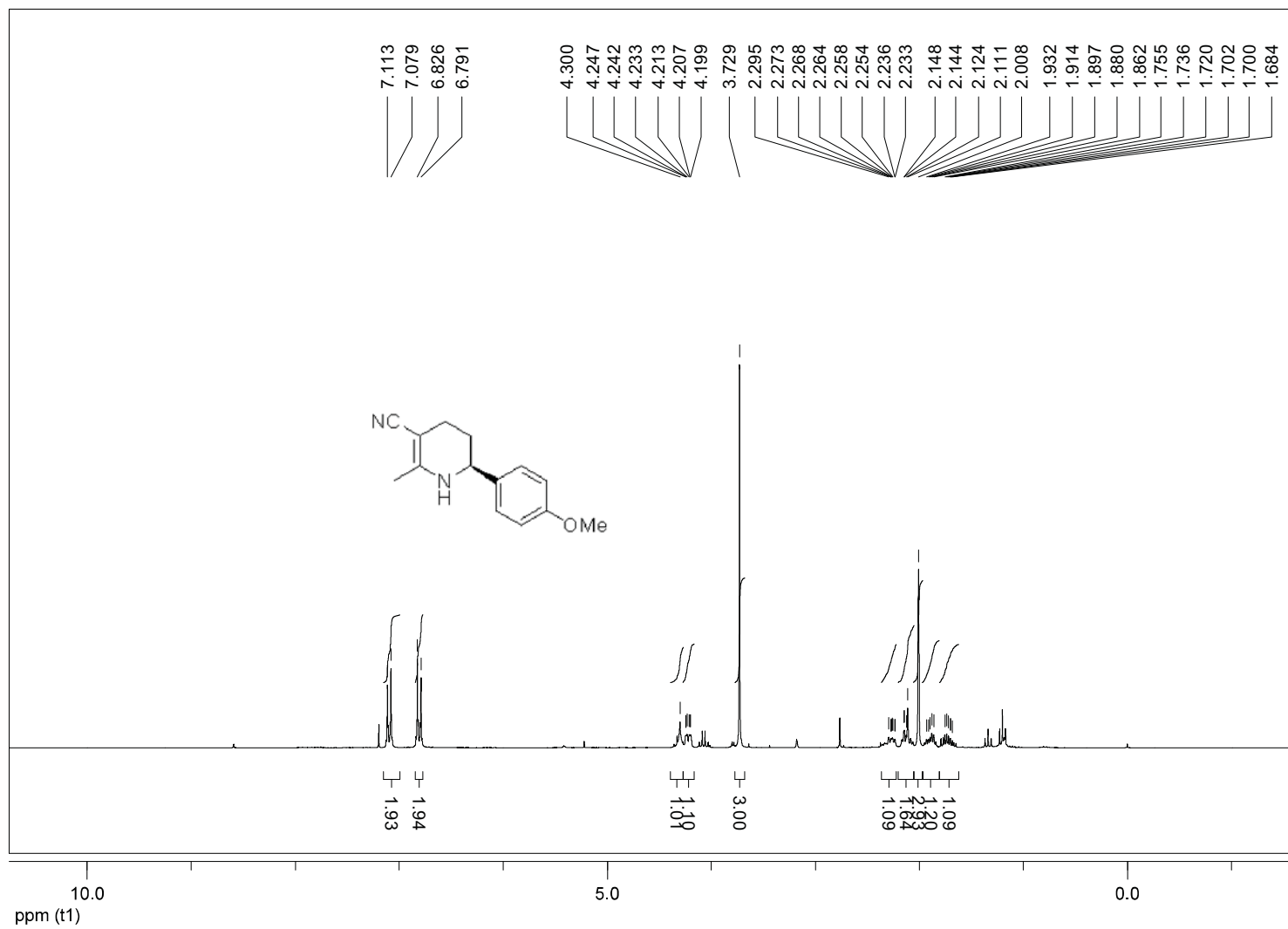


Chromatogram : AA828_3_ADH_955_flow1_1

Data file: AA828_3_ADH_955_flow1_1.DATA
Method: HPLC1_ADH_955_flow1_acq_90



Index	Start	Time	End	Area %
	[Min]	[Min]	[Min]	[%]
1	23,927	24,792	25,838	98,060
2	25,838	26,108	26,941	1,940
Total				100,000



Sample Information

Analyzed : 31.10.2007 11:16:33
 Sample Name : AA828_3

Method

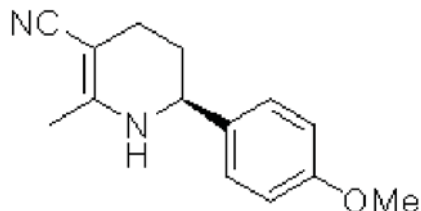
===== Analytical Line 1 =====

[GC-2010]

Column Oven Temp. : 60.0 °C
 Injection Temp. : 280.00 °C
 Injection Mode : Split
 Flow Control Mode : Linear Velocity
 Pressure : 29.2 kPa
 Total Flow : 17.2 mL/min
 Column Flow : 0.68 mL/min
 Linear Velocity : 30.0 cm/sec
 Purge Flow : 3.0 mL/min
 Split Ratio : 20.0

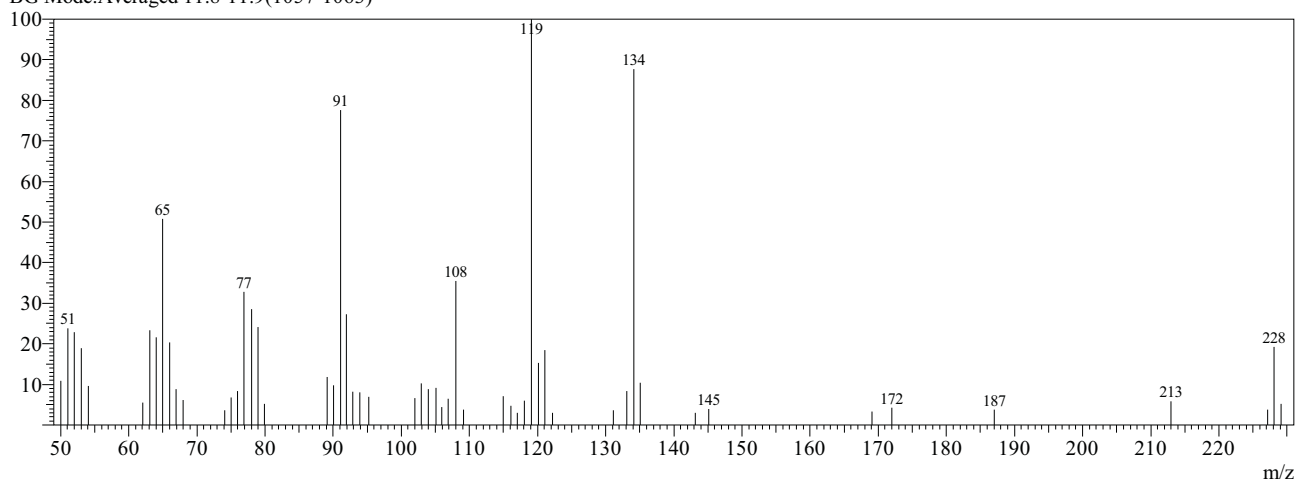
Oven Temp. Program

Rate	Temperature(°C)	Hold Time(min)
-	60.0	0.00
20.0	300.0	8.00



Spectrum

Line#:1 R.Time:11.7(Scan#:1045)
 MassPeaks:55 BasePeak:119(342922)
 RawMode:Averaged 11.7-11.7(1043-1047)
 BG Mode:Averaged 11.8-11.9(1057-1063)



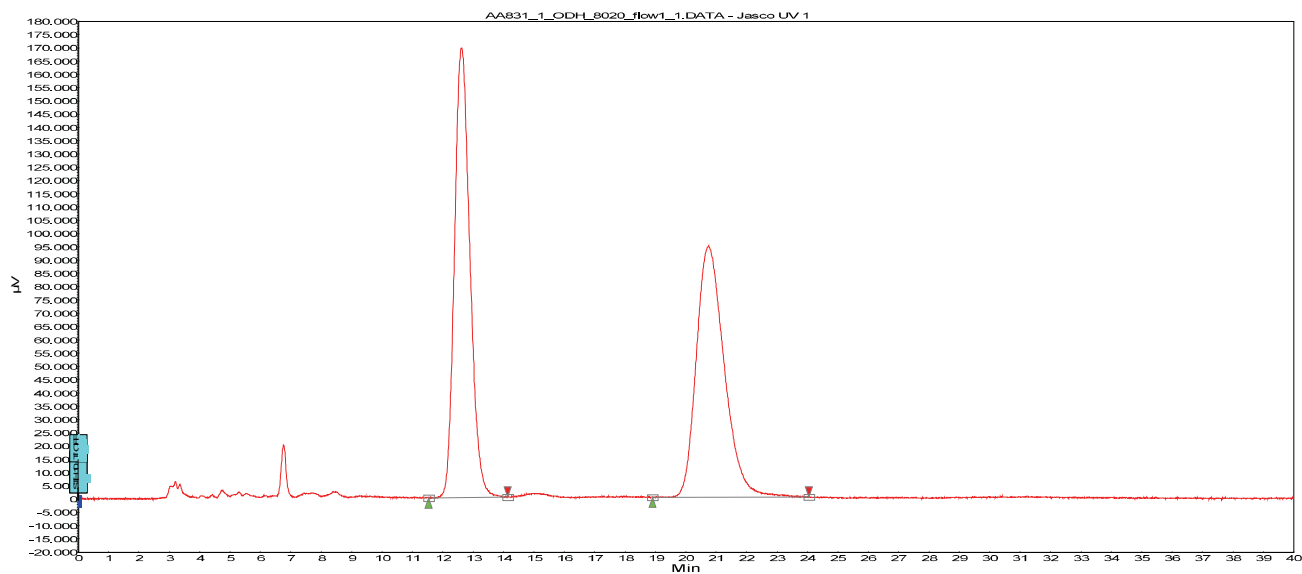
Mass Table

Line#:1 R.Time:11.7(Scan#:1045)
 MassPeaks:55 BasePeak:119(342922)
 RawMode:Averaged 11.7-11.7(1043-1047)
 BG Mode:Averaged 11.8-11.9(1057-1063)

#	m/z	Rel. Int.	#	m/z	Rel. Int.	#	m/z	Rel. Int.	#	m/z	Rel. Int.
1	50.00	10.93	15	75.95	8.34	29	103.95	8.90	43	131.10	3.58
2	51.05	23.81	16	76.95	32.82	30	105.10	9.15	44	133.05	8.43
3	52.00	22.92	17	78.00	28.48	31	105.95	4.41	45	134.10	87.67
4	53.00	18.86	18	79.00	24.19	32	106.90	6.54	46	135.10	10.37
5	54.10	9.67	19	79.90	5.22	33	108.05	35.46	47	143.15	3.05
6	62.05	5.50	20	89.10	11.91	34	109.10	3.79	48	145.10	3.94
7	63.05	23.29	21	90.05	9.84	35	114.95	7.10	49	169.10	3.37
8	64.00	21.58	22	91.10	77.66	36	116.05	4.70	50	172.00	4.34
9	65.00	50.78	23	91.95	27.29	37	117.05	3.04	51	187.00	3.84
10	66.00	20.41	24	92.90	8.23	38	118.05	6.03	52	213.00	5.86
11	66.90	8.81	25	93.95	8.01	39	119.10	100.00	53	227.15	3.76
12	68.00	6.08	26	95.25	7.01	40	120.15	15.23	54	228.10	19.28
13	74.10	3.66	27	101.95	6.67	41	121.10	18.40	55	229.15	5.16
14	75.00	6.73	28	102.90	10.28	42	122.20	3.07			

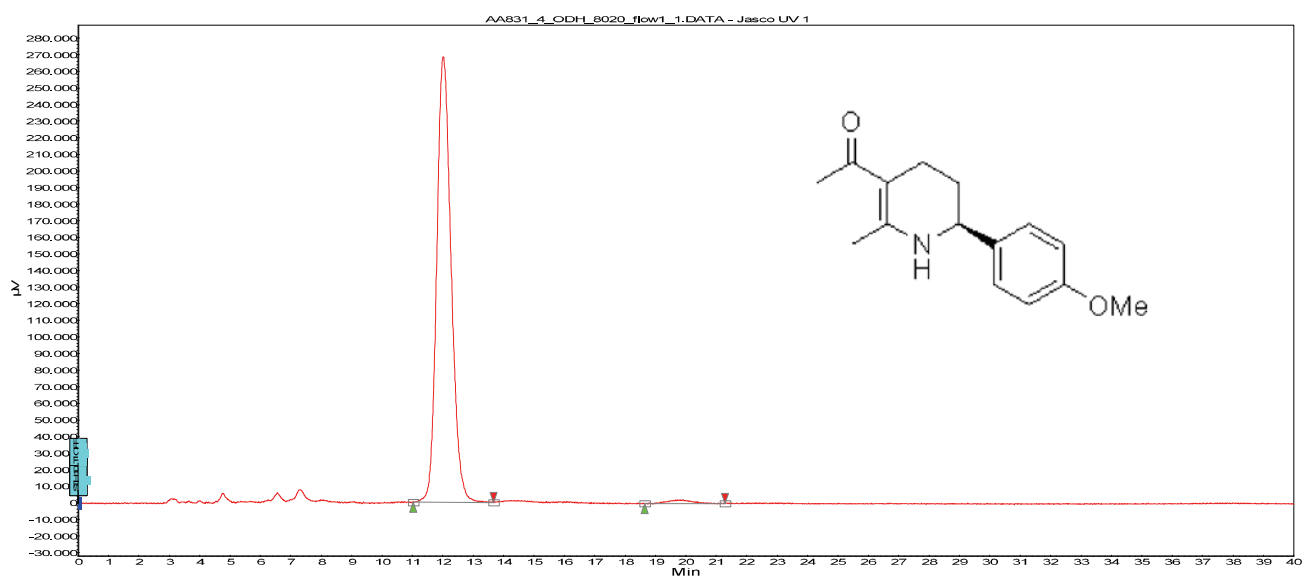
Chromatogram : AA831_1_ODH_8020_flow1_1

Data file: AA831_1_ODH_8020_flow1_1.DATA
Method: HPLC1_ODH_8020_flow1_acq_60

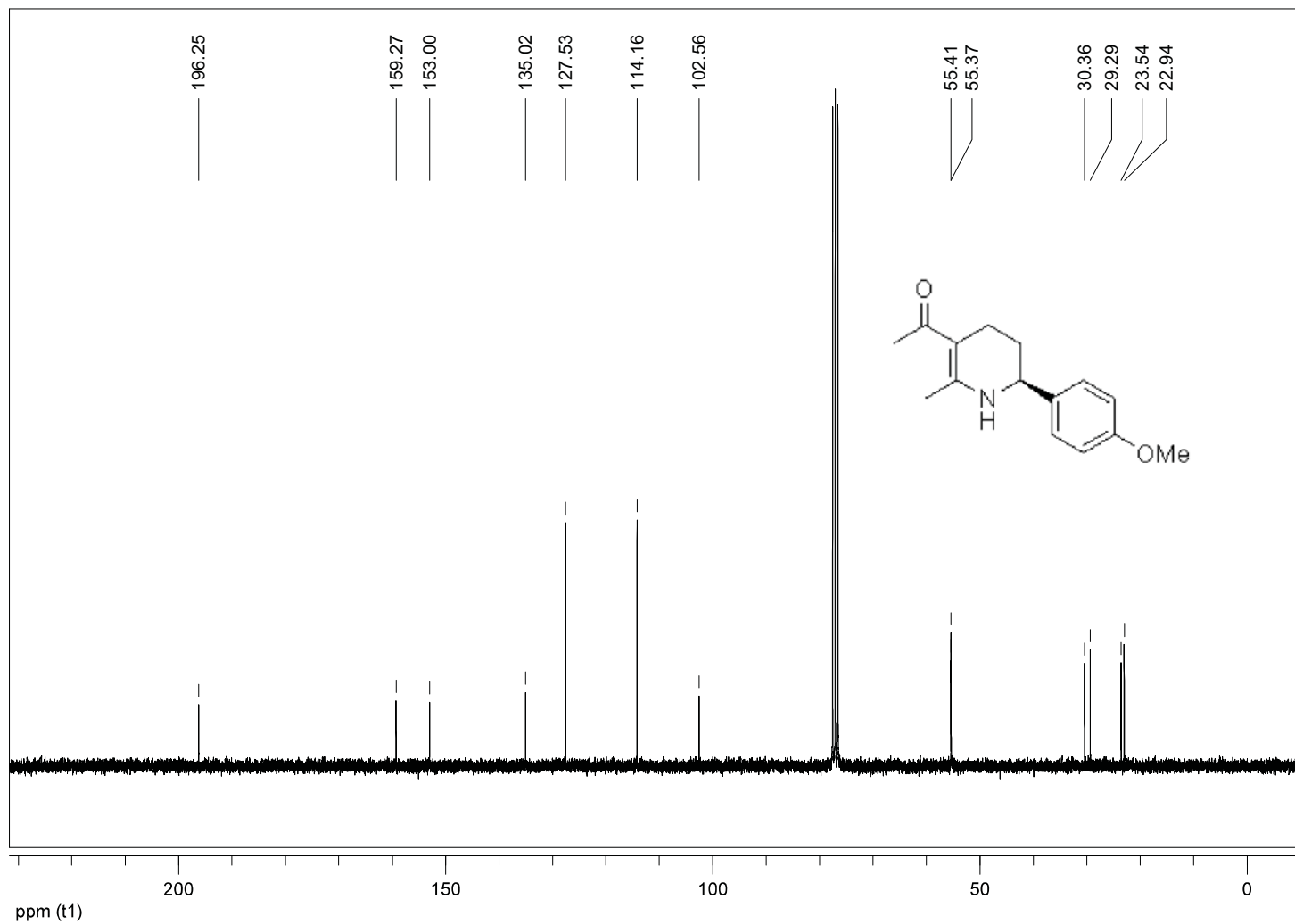
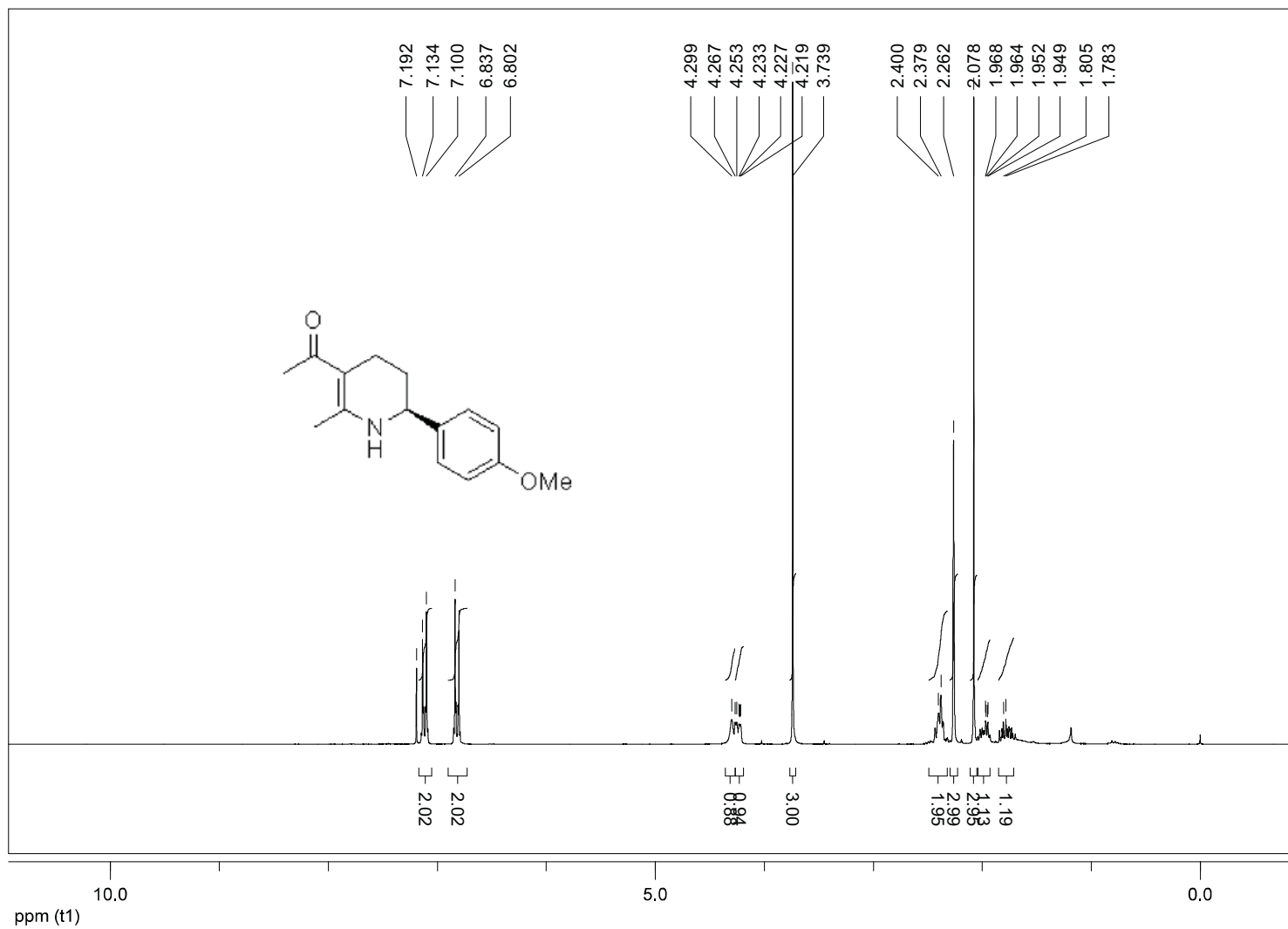


Chromatogram : AA831_4_ODH_8020_flow1_1

Data file: AA831_4_ODH_8020_flow1_1.DATA
Method: HPLC1_ODH_8020_flow1_acq_40



Index	Start [Min]	Time [Min]	End [Min]	Area % [%]
1	11,033	12,017	13,678	98,690
2	18,636	19,808	21,281	1,310
Total				100,000



Sample Information

Analyzed : 28.10.2007 17:59:08
 Sample Name : AA831_2

Method

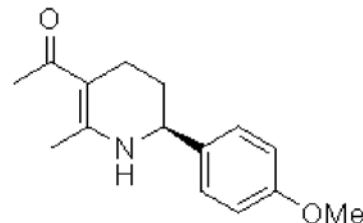
===== Analytical Line 1 =====

[GC-2010]

Column Oven Temp. : 60.0 °C
 Injection Temp. : 280.00 °C
 Injection Mode : Split
 Flow Control Mode : Linear Velocity
 Pressure : 29.2 kPa
 Total Flow : 17.2 mL/min
 Column Flow : 0.68 mL/min
 Linear Velocity : 30.0 cm/sec
 Purge Flow : 3.0 mL/min
 Split Ratio : 20.0

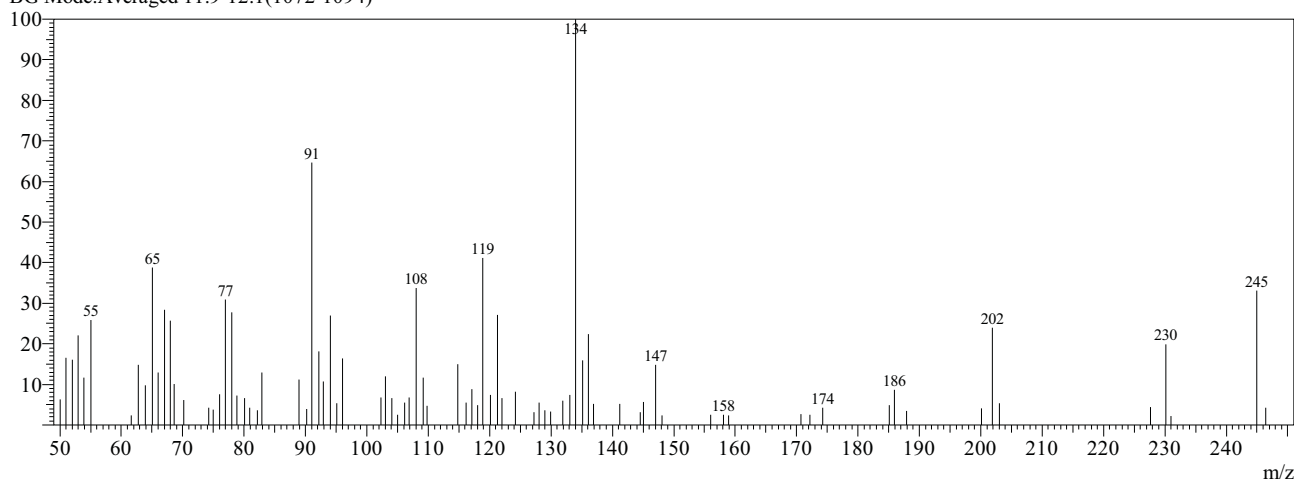
Oven Temp. Program

Rate	Temperature(°C)	Hold Time(min)
-	60.0	0.00
20.0	300.0	8.00



Spectrum

Line#:1 R.Time:11.7(Scan#:1043)
 MassPeaks:83 BasePeak:134(61204)
 RawMode:Averaged 11.7-11.7(1040-1046)
 BG Mode:Averaged 11.9-12.1(1072-1094)



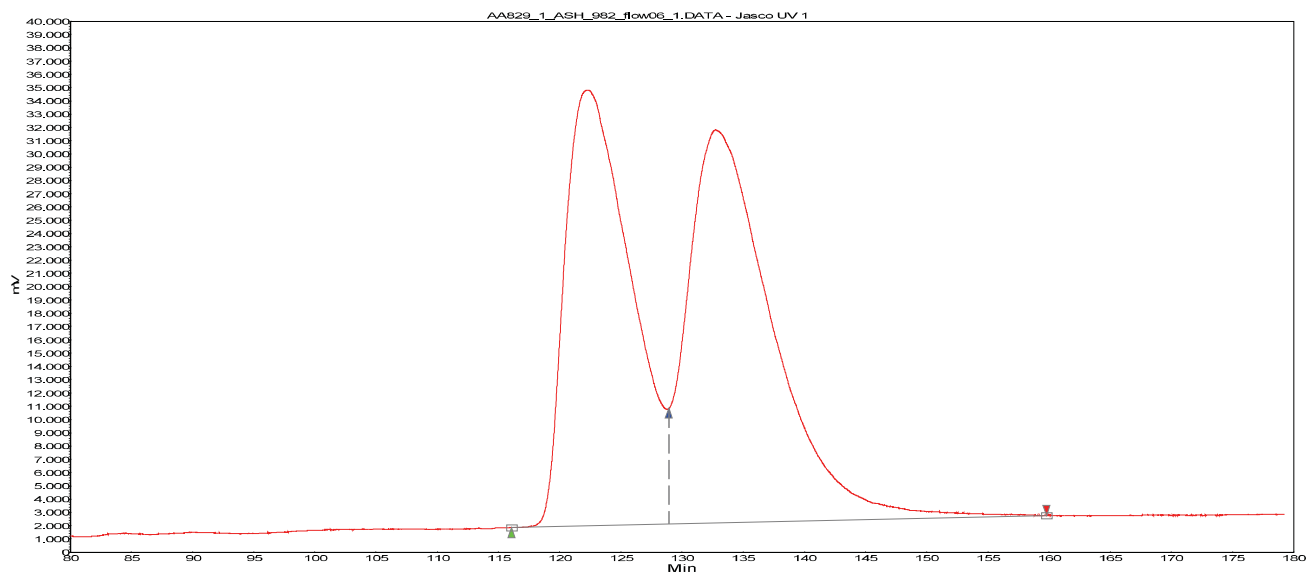
Mass Table

Line#:1 R.Time:11.7(Scan#:1043)
 MassPeaks:83 BasePeak:134(61204)
 RawMode:Averaged 11.7-11.7(1040-1046)
 BG Mode:Averaged 11.9-12.1(1072-1094)

#	m/z	Rel. Int.	#	m/z	Rel. Int.	#	m/z	Rel. Int.	#	m/z	Rel. Int.
1	50.05	6.36	22	80.05	6.67	43	114.80	14.94	64	145.00	5.65
2	51.00	16.51	23	80.90	4.32	44	116.15	5.52	65	147.00	14.82
3	52.05	16.08	24	82.15	3.63	45	117.05	8.91	66	148.05	2.33
4	53.00	22.07	25	82.90	12.88	46	118.00	4.85	67	156.00	2.53
5	53.85	11.61	26	88.95	11.21	47	118.90	41.15	68	158.05	2.59
6	55.10	25.80	27	90.15	4.01	48	120.15	7.47	69	158.90	2.39
7	61.65	2.36	28	91.05	64.65	49	121.25	27.15	70	170.75	2.68
8	62.75	14.81	29	92.15	18.19	50	122.05	6.56	71	172.15	2.56
9	63.90	9.77	30	92.95	10.76	51	124.20	8.20	72	174.25	4.21
10	65.10	38.82	31	94.10	26.96	52	127.20	3.15	73	185.10	4.90
11	66.00	12.98	32	95.10	5.32	53	128.00	5.56	74	185.95	8.61
12	67.00	28.40	33	96.00	16.47	54	128.95	3.63	75	187.95	3.40
13	68.00	25.72	34	102.25	6.77	55	129.90	3.36	76	200.15	4.08
14	68.60	10.06	35	103.05	11.99	56	131.90	5.98	77	201.90	23.93
15	70.15	6.19	36	104.05	6.60	57	133.10	7.35	78	203.00	5.41
16	74.25	4.30	37	105.00	2.58	58	134.00	100.00	79	227.65	4.48
17	74.95	3.78	38	106.10	5.60	59	135.15	15.95	80	230.10	19.90
18	76.00	7.62	39	106.85	6.86	60	136.10	22.42	81	231.00	2.29
19	77.00	30.95	40	108.05	33.68	61	136.95	5.27	82	244.95	33.13
20	78.00	27.76	41	109.15	11.75	62	141.15	5.27	83	246.45	4.25
21	78.85	7.21	42	109.85	4.79	63	144.50	3.09			

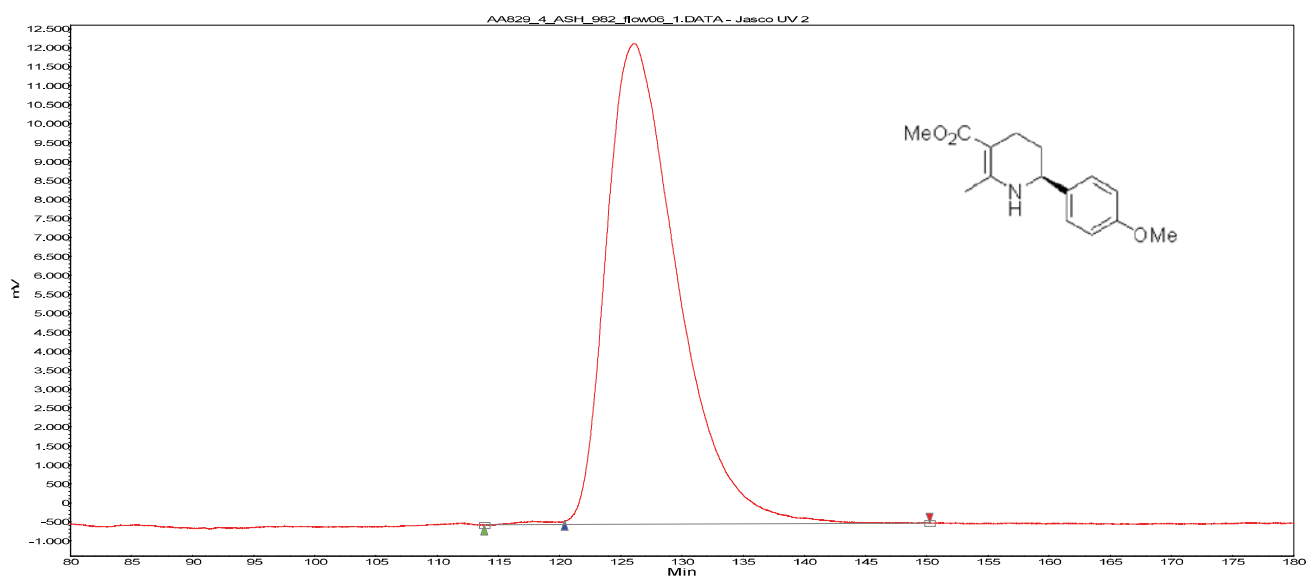
Chromatogram : AA829_1_ASH_982_flow06_1

Data file: AA829_1_ASH_982_flow06_1.DATA
Method: HPLC2_ASH_982_flow06_acq210

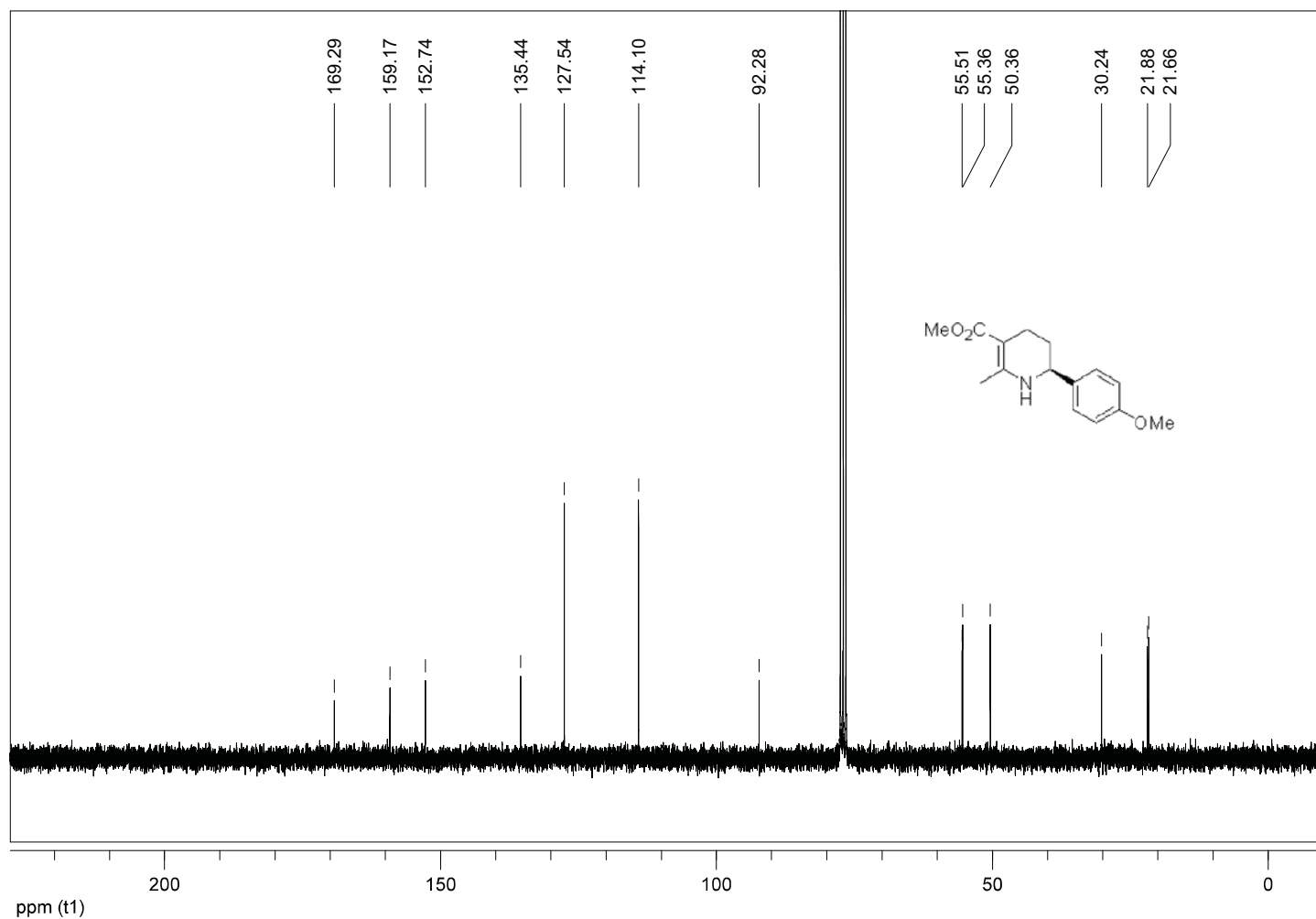
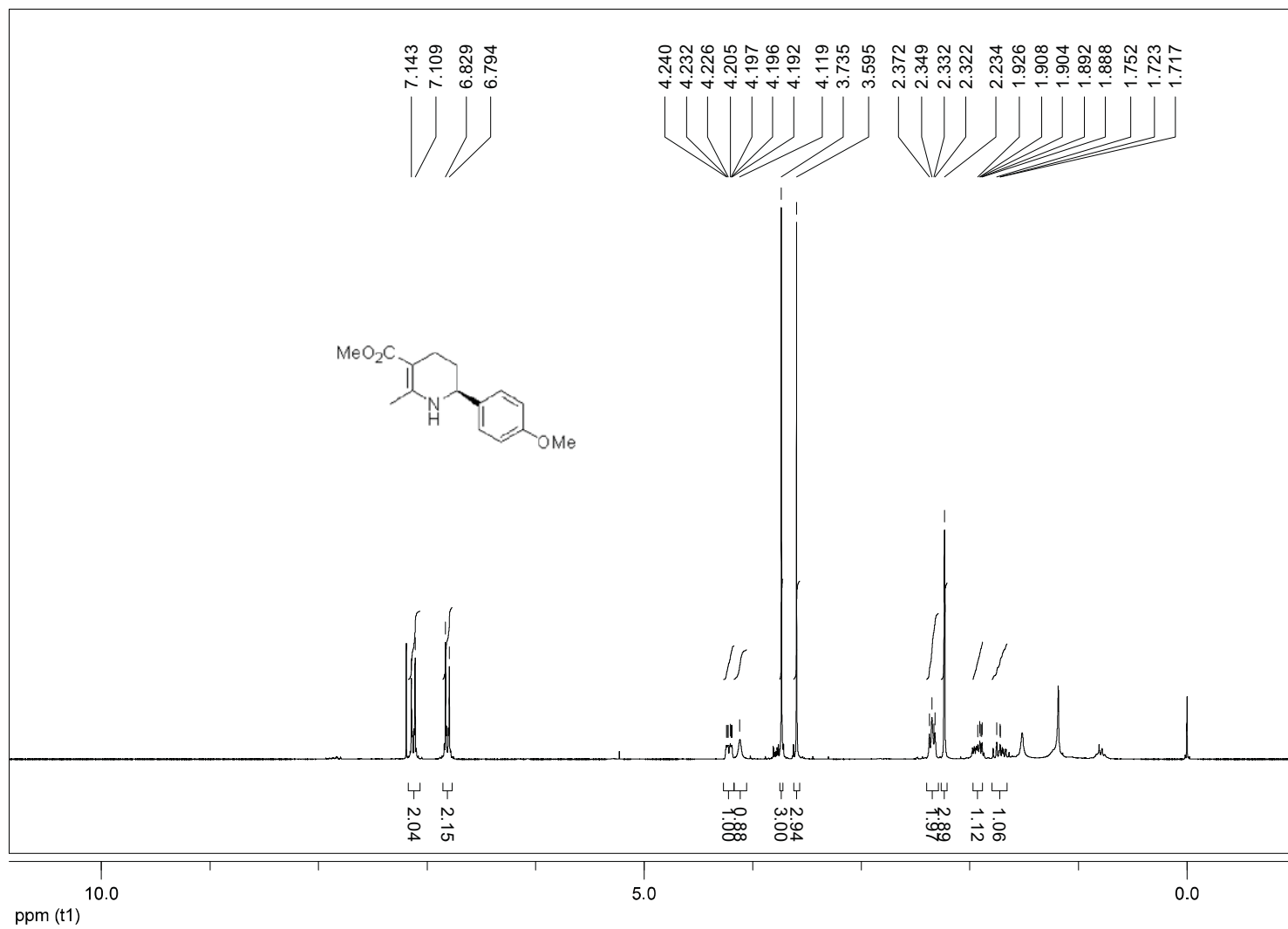


Chromatogram : AA829_4_ASH_982_flow06_1

Data file: AA829_4_ASH_982_flow06_1.DATA
Method: HPLC2_ASH_982_flow06_acq210



Index	Start	Time	End	Area %
	[Min]	[Min]	[Min]	[%]
1	113,858	117,708	120,425	0,414
2	120,425	126,100	150,252	99,586
Total				100,000



Sample Information

Analyzed : 23.10.2007 11:35:16
 Sample Name : AA829_1

Method

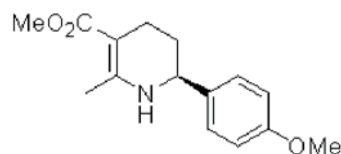
===== Analytical Line 1 =====

[GC-2010]

Column Oven Temp. : 60.0 °C
 Injection Temp. : 280.00 °C
 Injection Mode : Split
 Flow Control Mode : Linear Velocity
 Pressure : 29.2 kPa
 Total Flow : 17.2 mL/min
 Column Flow : 0.68 mL/min
 Linear Velocity : 30.0 cm/sec
 Purge Flow : 3.0 mL/min
 Split Ratio : 20.0

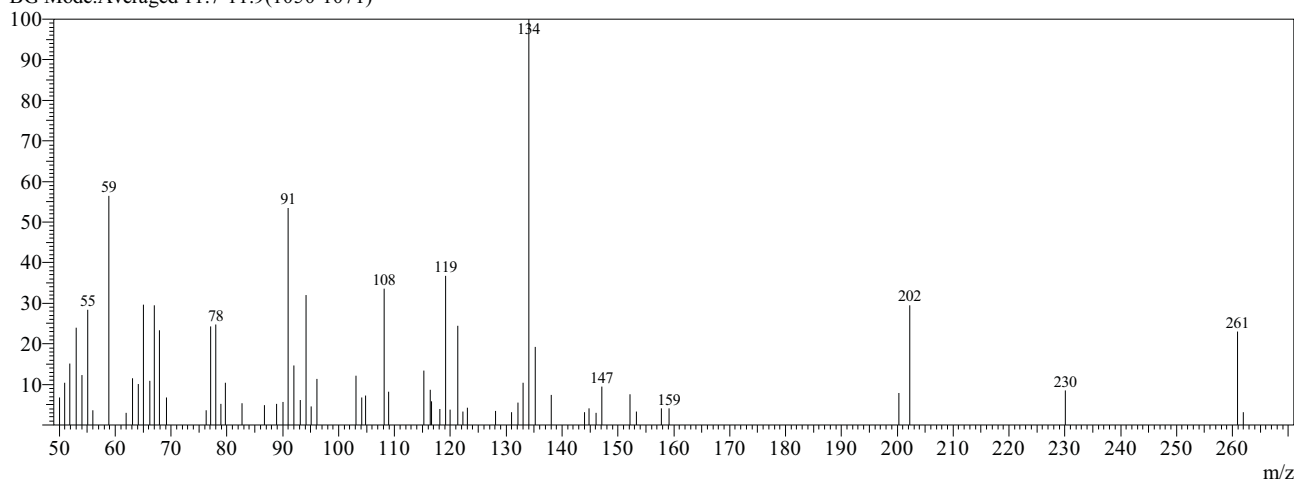
Oven Temp. Program

Rate	Temperature(°C)	Hold Time(min)
-	60.0	0.00
20.0	300.0	15.00



Spectrum

Line#:1 R.Time:11.6(Scan#:1034)
 MassPeaks:65 BasePeak:134(43941)
 RawMode:Averaged 11.6-11.6(1029-1037)
 BG Mode:Averaged 11.7-11.9(1050-1071)



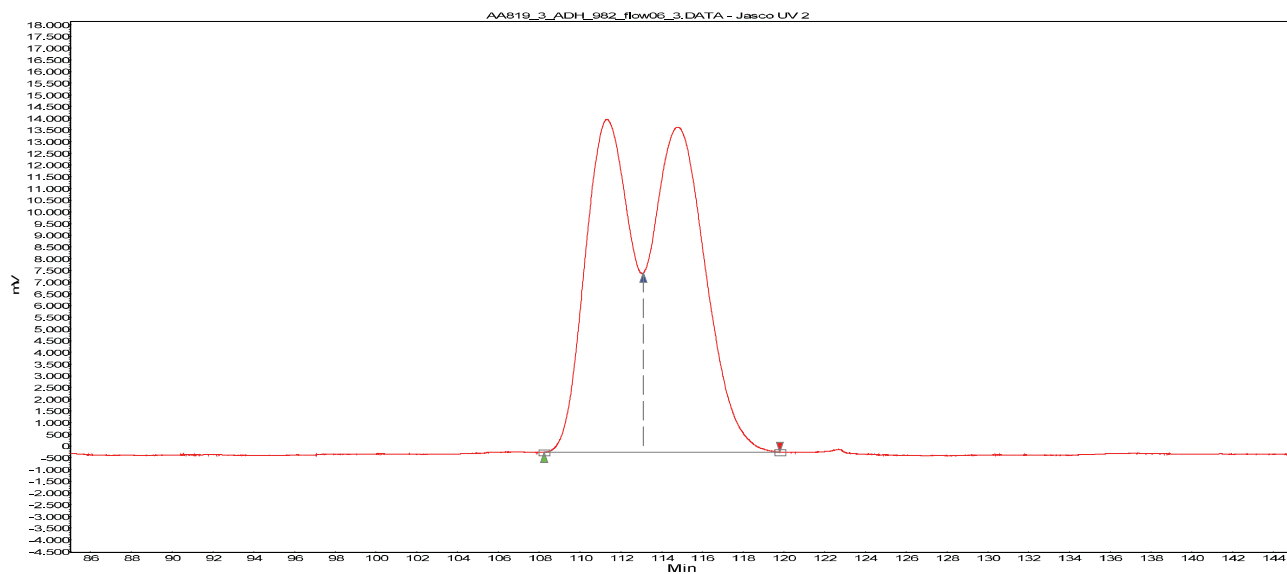
Mass Table

Line#:1 R.Time:11.6(Scan#:1034)
 MassPeaks:65 BasePeak:134(43941)
 RawMode:Averaged 11.6-11.6(1029-1037)
 BG Mode:Averaged 11.7-11.9(1050-1071)

#	m/z	Rel. Int.	#	m/z	Rel. Int.	#	m/z	Rel. Int.	#	m/z	Rel. Int.
1	50.00	6.73	18	77.10	24.31	35	108.10	33.62	52	138.05	7.38
2	50.90	10.42	19	78.00	24.80	36	108.95	8.15	53	144.00	3.22
3	51.90	15.11	20	78.90	5.28	37	115.30	13.43	54	144.85	4.07
4	53.00	24.03	21	79.70	10.40	38	116.40	8.64	55	146.05	3.01
5	54.10	12.23	22	82.75	5.43	39	116.65	5.79	56	147.15	9.53
6	55.10	28.44	23	86.65	4.95	40	118.15	3.93	57	152.15	7.62
7	56.00	3.56	24	88.90	5.28	41	119.10	36.70	58	153.25	3.25
8	58.85	56.48	25	90.05	5.67	42	119.95	3.78	59	157.80	4.05
9	61.95	3.05	26	91.00	53.44	43	121.30	24.44	60	159.15	4.07
10	63.05	11.52	27	91.95	14.67	44	122.25	3.29	61	200.30	7.88
11	64.10	10.14	28	93.15	6.13	45	123.05	4.18	62	202.20	29.46
12	65.10	29.63	29	94.10	32.05	46	128.05	3.42	63	230.05	8.51
13	66.15	10.82	30	95.05	4.64	47	131.00	3.16	64	260.90	23.11
14	67.05	29.48	31	96.05	11.38	48	132.10	5.47	65	261.90	3.19
15	67.95	23.32	32	103.05	12.21	49	133.05	10.45			
16	69.15	6.81	33	104.10	6.73	50	134.00	100.00			
17	76.25	3.67	34	104.85	7.22	51	135.20	19.31			

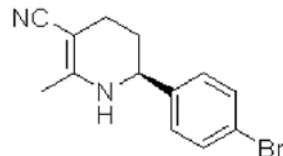
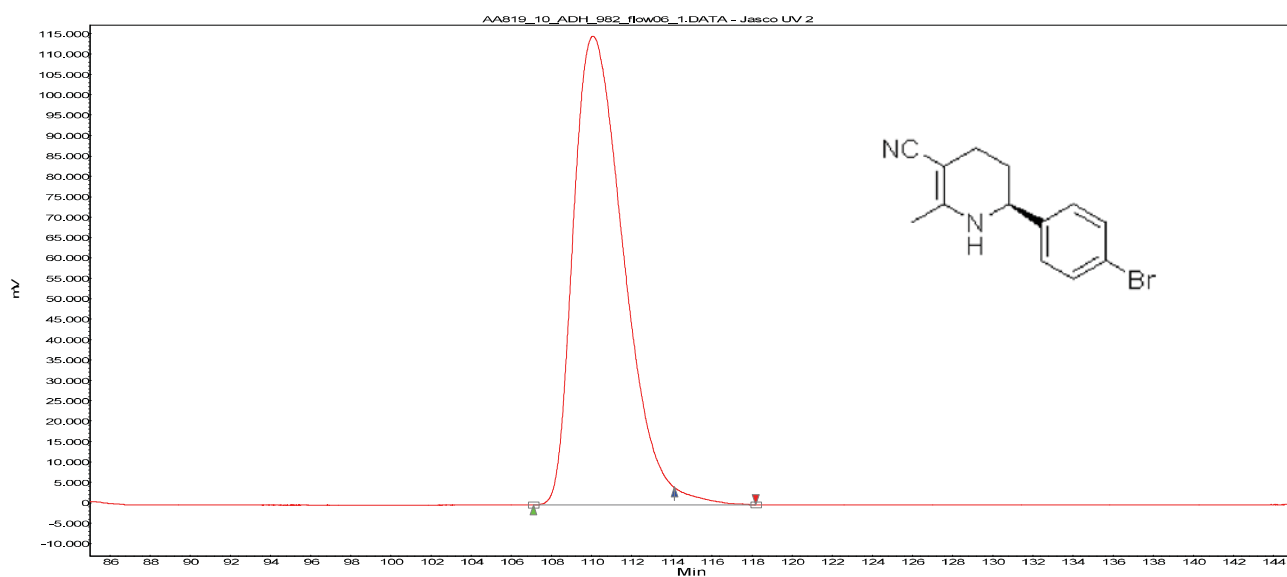
Chromatogram : AA819_3_ADH_982_flow06_3

Data file: AA819_3_ADH_982_flow06_3.DATA
Method: HPLC2_ADH_982_flow06_acq180

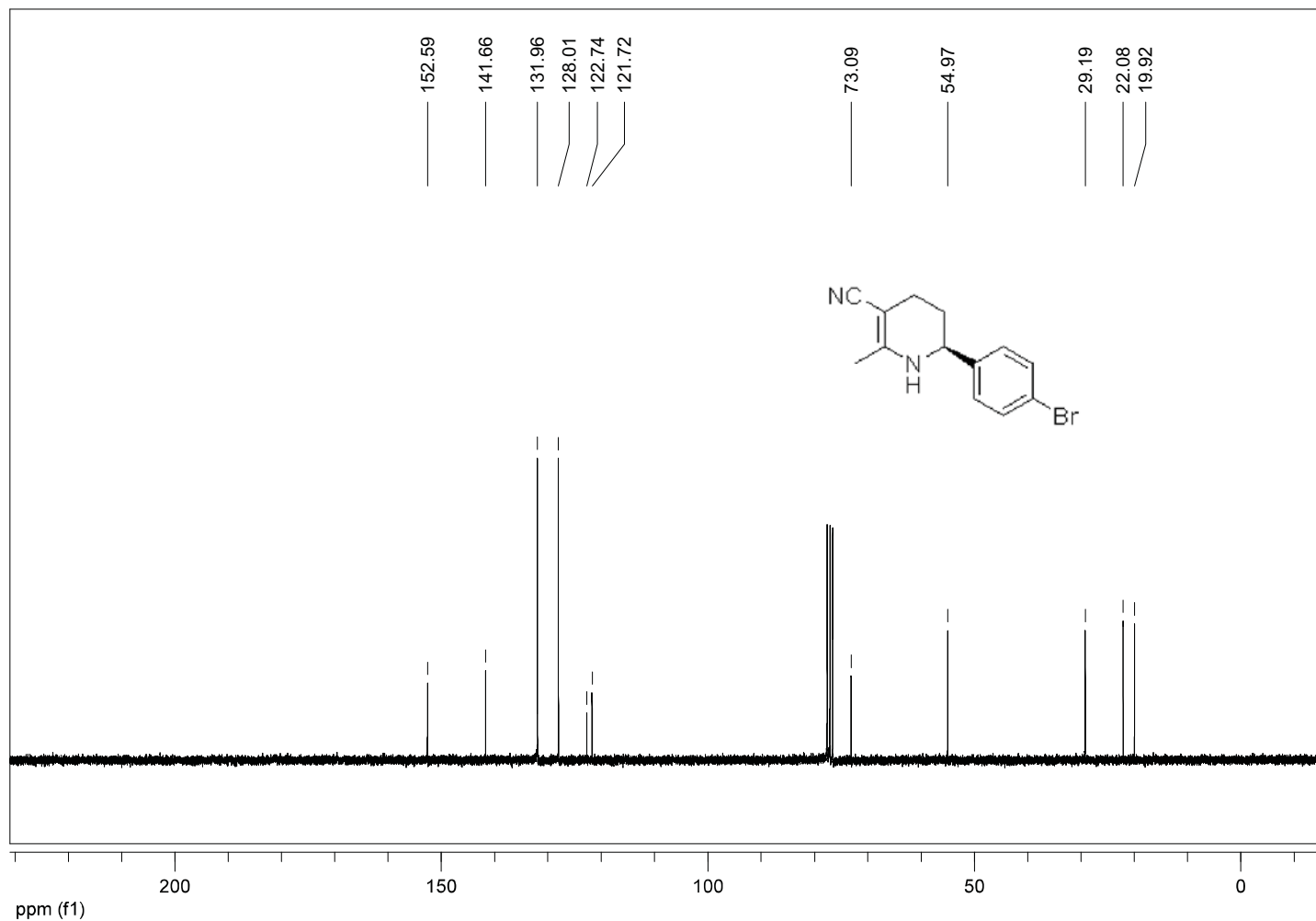
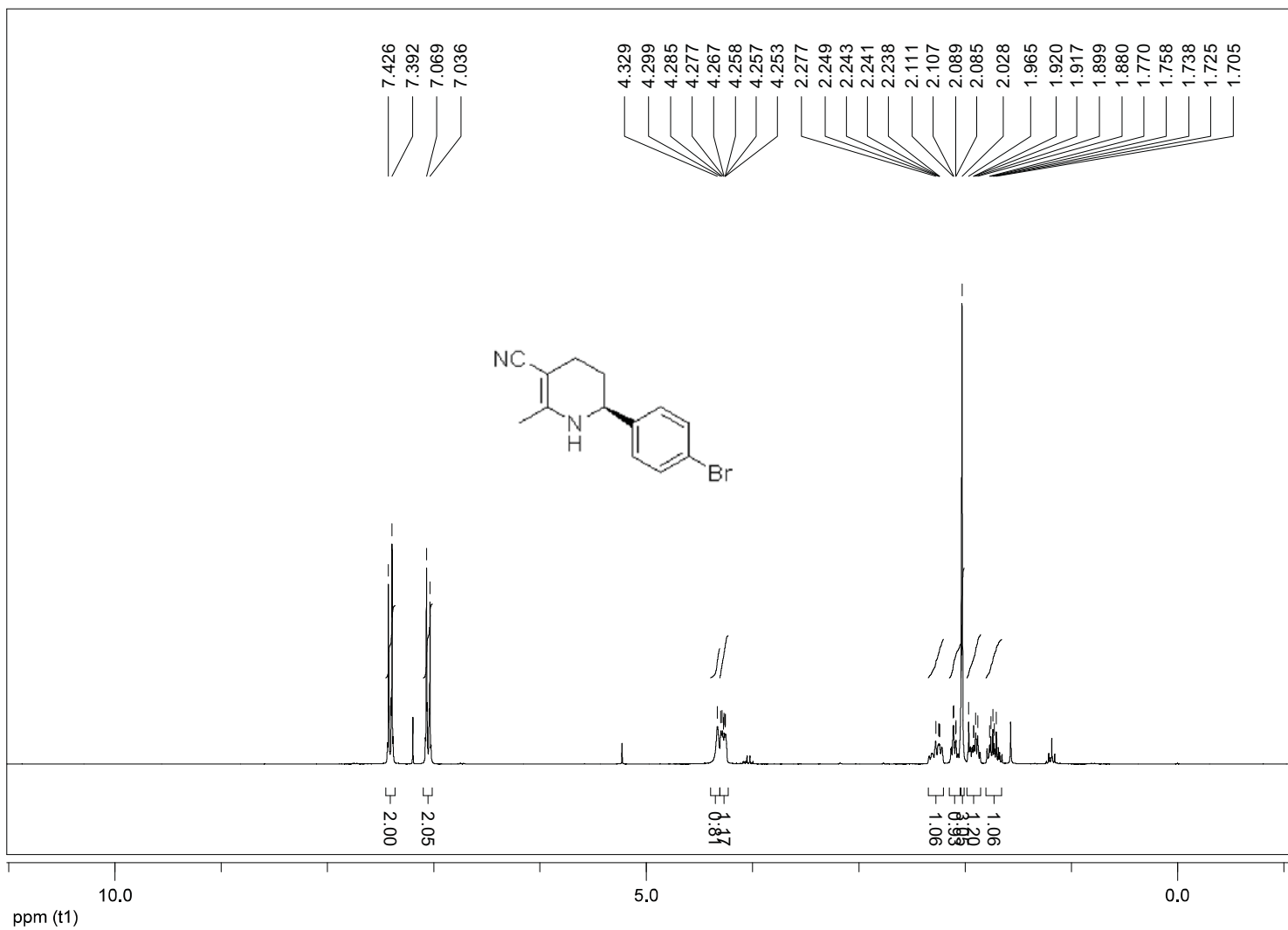


Chromatogram : AA819_10_ADH_982_flow06_1

Data file: AA819_10_ADH_982_flow06_1.DATA
Method: HPLC2_ADH_982_flow06_acq180



Index	Start	Time	End	Area %
	[Min]	[Min]	[Min]	[%]
1	107,101	110,075	114,127	98,541
2	114,127	114,127	118,184	1,459
Total				100,000



Sample Information

Analyzed : 17.10.2007 14:07:16
 Sample Name : AA819_4

Method

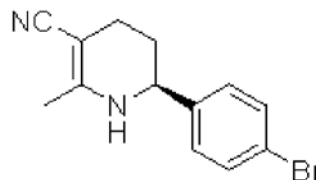
===== Analytical Line 1 =====

[GC-2010]

Column Oven Temp. : 60.0 °C
 Injection Temp. : 280.00 °C
 Injection Mode : Split
 Flow Control Mode : Linear Velocity
 Pressure : 29.2 kPa
 Total Flow : 17.2 mL/min
 Column Flow : 0.68 mL/min
 Linear Velocity : 30.0 cm/sec
 Purge Flow : 3.0 mL/min
 Split Ratio : 20.0

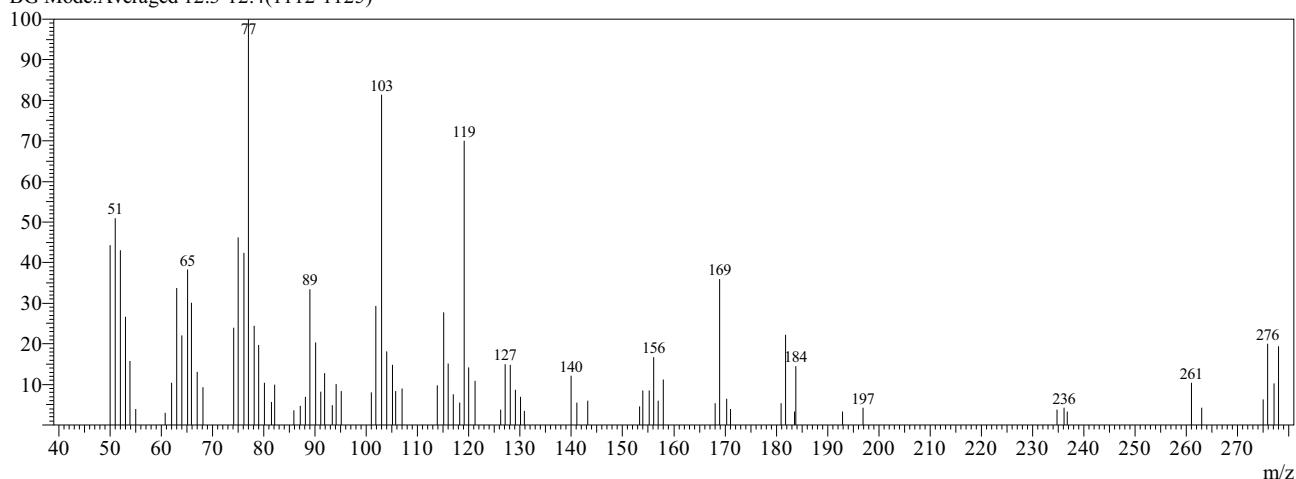
Oven Temp. Program

Rate	Temperature(°C)	Hold Time(min)
-	60.0	0.00
20.0	300.0	8.00



Spectrum

Line#:1 R.Time:12.1(Scan#:1092)
 MassPeaks:82 BasePeak:77(103400)
 RawMode:Averaged 12.1-12.1(1090-1093)
 BG Mode:Averaged 12.3-12.4(1112-1125)



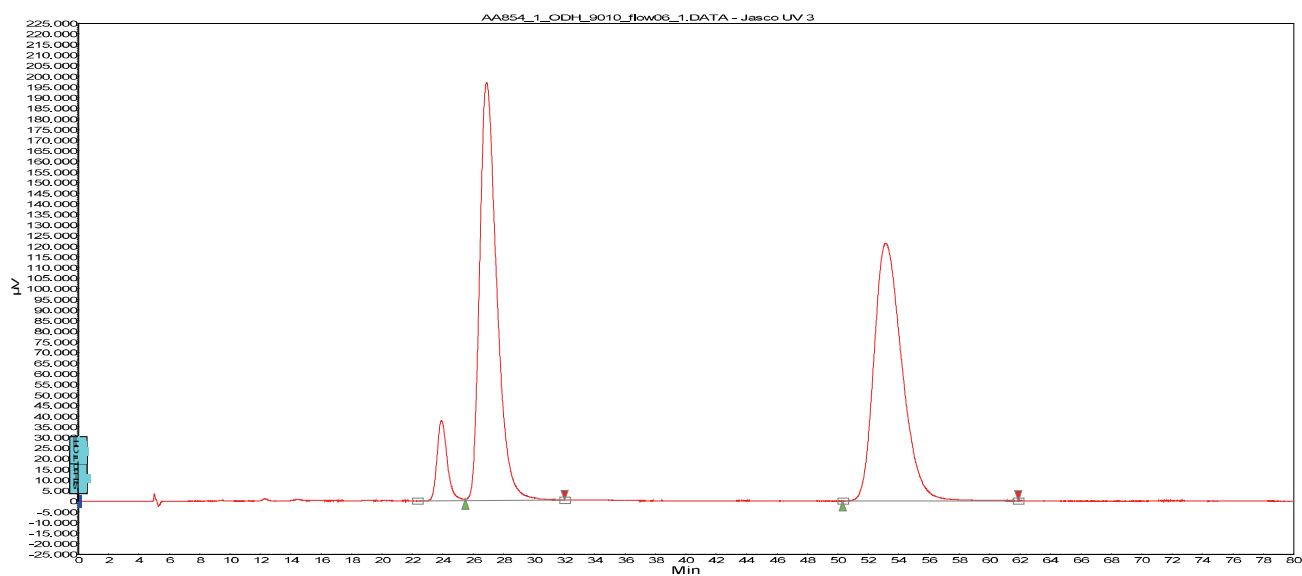
Mass Table

Line#:1 R.Time:12.1(Scan#:1092)
 MassPeaks:82 BasePeak:77(103400)
 RawMode:Averaged 12.1-12.1(1090-1093)
 BG Mode:Averaged 12.3-12.4(1112-1125)

#	m/z	Rel. Int.	#	m/z	Rel. Int.	#	m/z	Rel. Int.	#	m/z	Rel. Int.
1	49.95	44.35	22	81.50	5.69	43	115.95	15.19	64	168.05	5.39
2	51.05	50.93	23	82.15	10.00	44	116.95	7.55	65	168.95	36.02
3	52.00	43.02	24	85.85	3.68	45	118.15	5.47	66	170.25	6.40
4	53.00	26.72	25	87.05	4.80	46	119.10	70.01	67	171.05	3.92
5	53.85	15.77	26	88.15	7.01	47	120.00	14.17	68	180.95	5.38
6	55.05	3.93	27	89.00	33.46	48	121.15	10.82	69	181.80	22.19
7	60.80	3.00	28	90.10	20.35	49	126.20	3.81	70	183.50	3.27
8	62.00	10.42	29	91.10	8.28	50	127.10	15.03	71	183.80	14.50
9	63.05	33.69	30	91.90	12.85	51	128.05	14.88	72	192.95	3.27
10	64.00	22.03	31	93.30	4.89	52	129.05	8.67	73	196.95	4.29
11	65.05	38.38	32	94.10	10.08	53	130.05	6.92	74	234.80	3.75
12	65.90	30.10	33	95.05	8.40	54	130.85	3.43	75	236.15	4.24
13	67.00	13.07	34	101.00	7.98	55	140.00	12.07	76	236.75	3.30
14	68.10	9.38	35	101.90	29.26	56	141.05	5.46	77	261.00	10.41
15	74.05	23.90	36	103.00	81.37	57	143.15	5.94	78	263.05	4.18
16	75.00	46.21	37	103.95	18.18	58	153.35	4.55	79	275.00	6.33
17	76.05	42.49	38	105.05	14.84	59	153.90	8.51	80	275.90	19.98
18	77.00	100.00	39	105.70	8.30	60	155.15	8.50	81	277.15	10.29
19	78.10	24.48	40	106.95	9.00	61	156.05	16.69	82	278.05	19.44
20	79.00	19.68	41	113.80	9.82	62	156.90	6.07			
21	80.10	10.39	42	115.05	27.79	63	158.00	11.21			

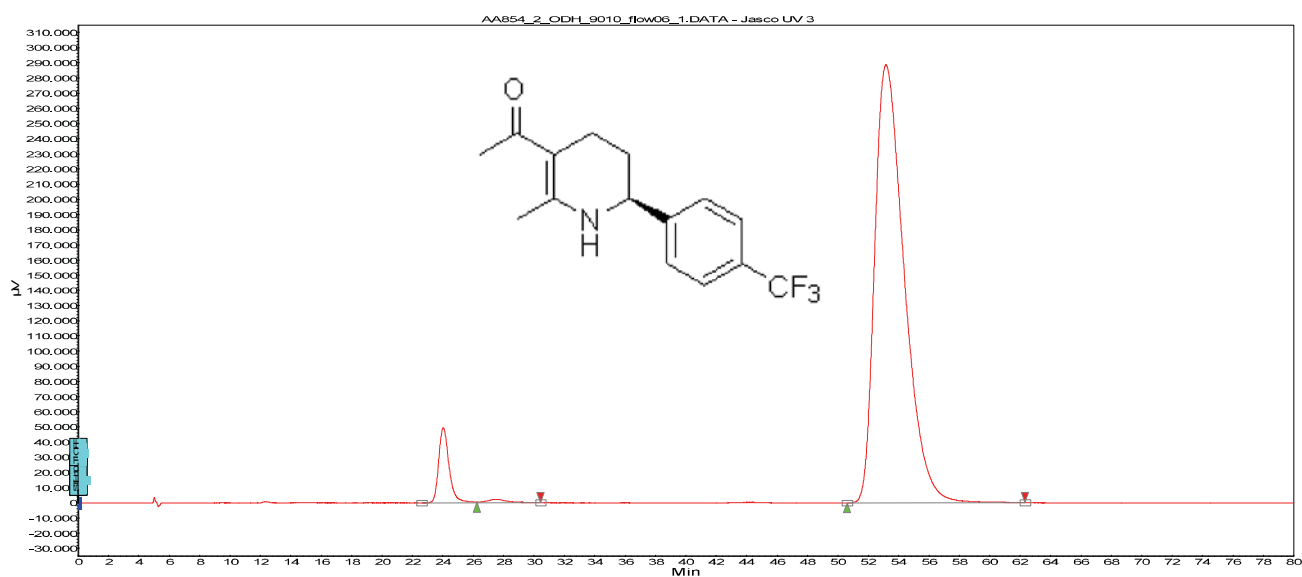
Chromatogram : AA854_1_ODH_9010_flow06_1

Data file: AA854_1_ODH_9010_flow06_1.DATA
Method: HPLC1_ODH_9010_flow06_acq_90

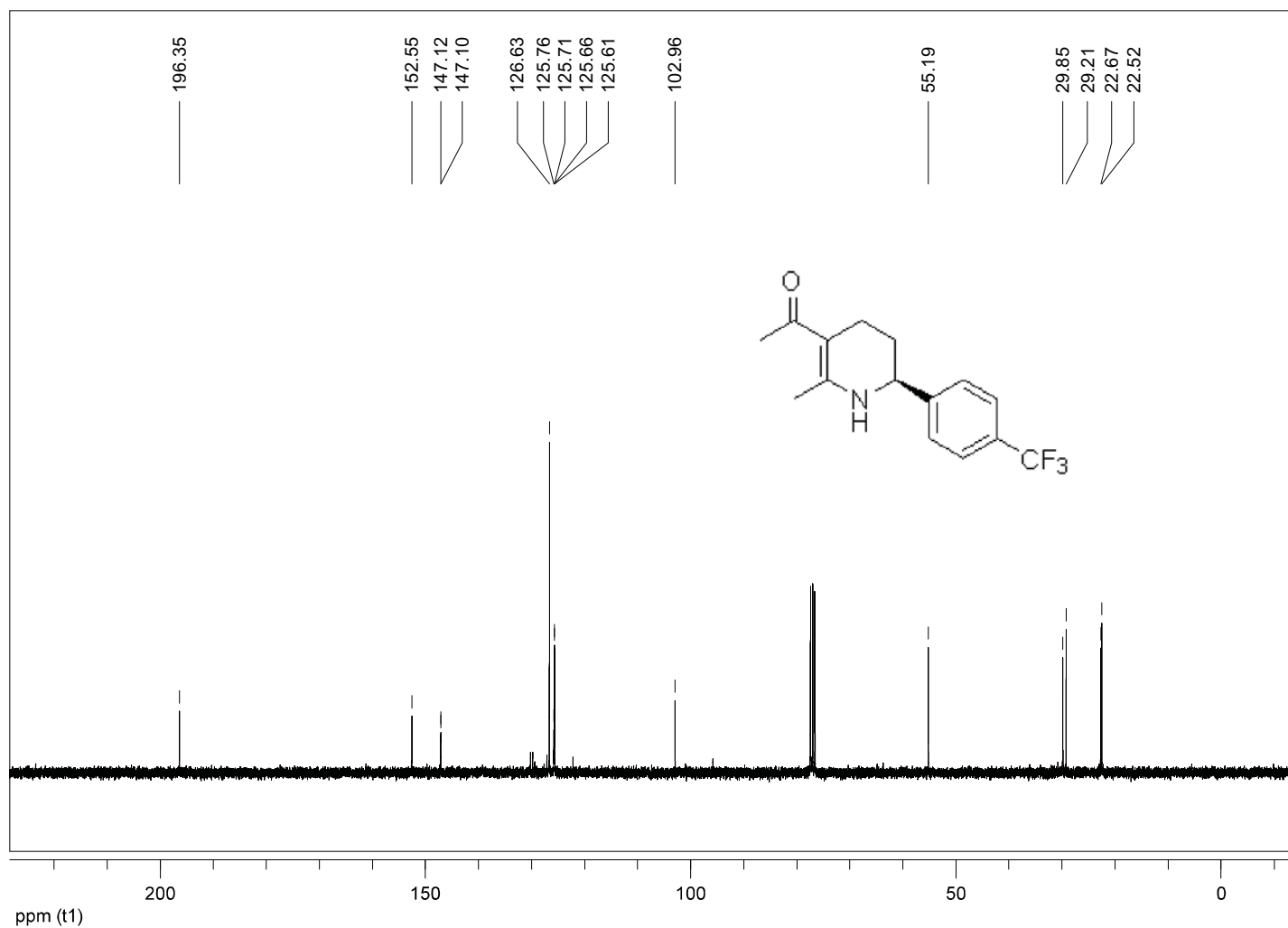
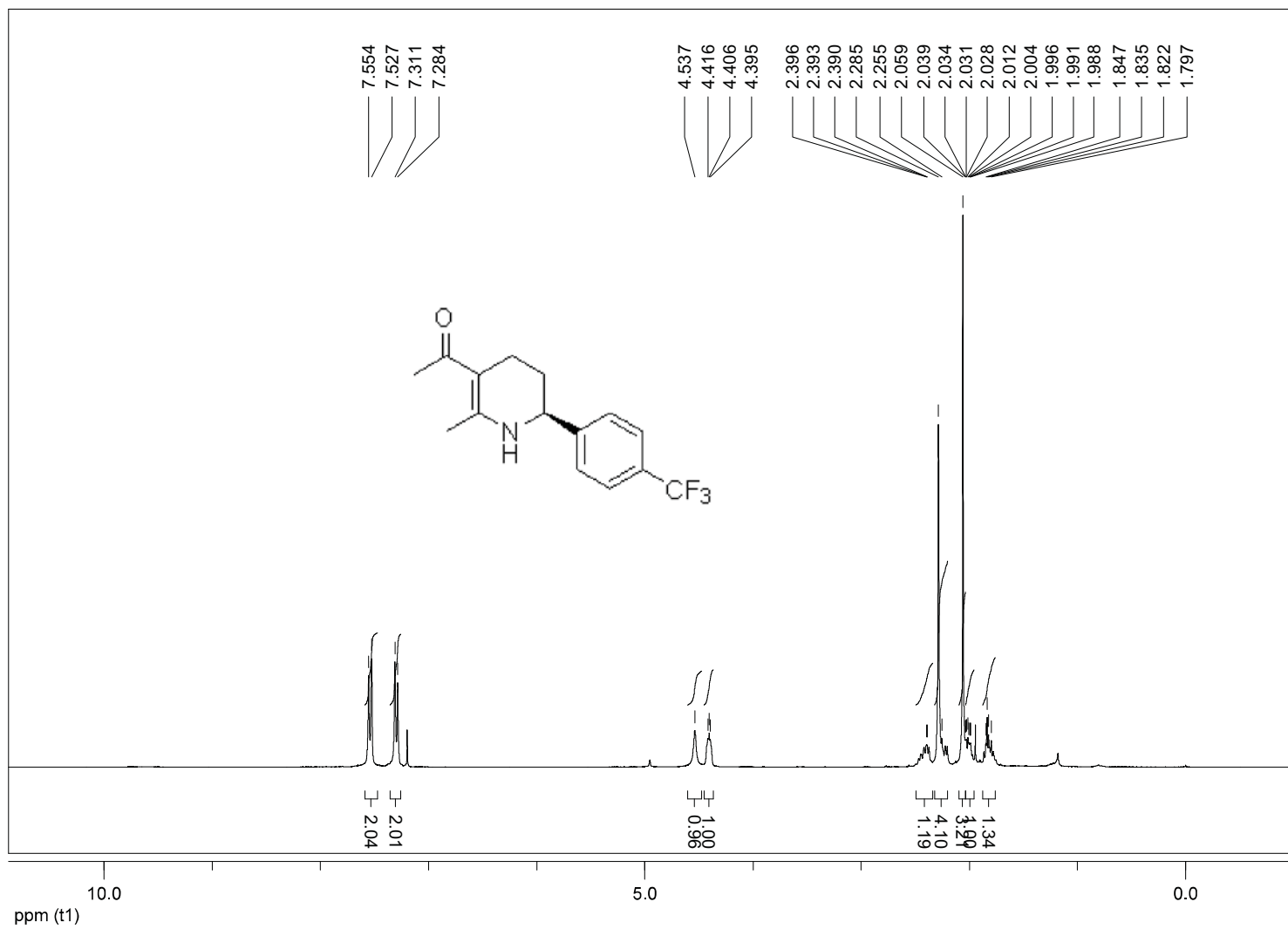


Chromatogram : AA854_2_ODH_9010_flow06_1

Data file: AA854_2_ODH_9010_flow06_1.DATA
Method: HPLC1_ODH_9010_flow06_acq_90



Index	Start [Min]	Time [Min]	End [Min]	Area %
2	26,229	27,492	30,427	0,475
1	50,599	53,167	62,318	99,525
Total				100,000



Sample Information

Analyzed : 14.11.2007 10:40:41
 Sample Name : AA854_2

Method

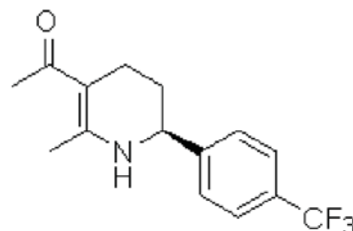
===== Analytical Line 1 =====

[GC-2010]

Column Oven Temp. : 60.0 °C
 Injection Temp. : 280.00 °C
 Injection Mode : Split
 Flow Control Mode : Linear Velocity
 Pressure : 29.2 kPa
 Total Flow : 17.2 mL/min
 Column Flow : 0.68 mL/min
 Linear Velocity : 30.0 cm/sec
 Purge Flow : 3.0 mL/min
 Split Ratio : 20.0

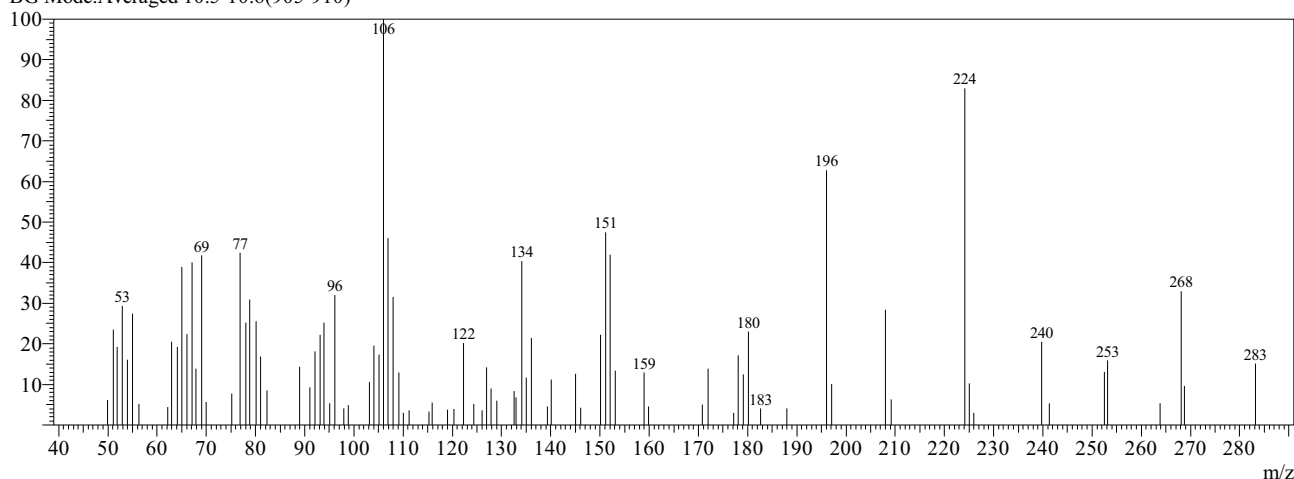
Oven Temp. Program

Rate	Temperature(°C)	Hold Time(min)
-	60.0	0.00
20.0	300.0	8.00



Spectrum

Line#:1 R.Time:10.4(Scan#:884)
 MassPeaks:89 BasePeak:106(61016)
 RawMode:Averaged 10.3-10.4(882-885)
 BG Mode:Averaged 10.5-10.6(905-910)



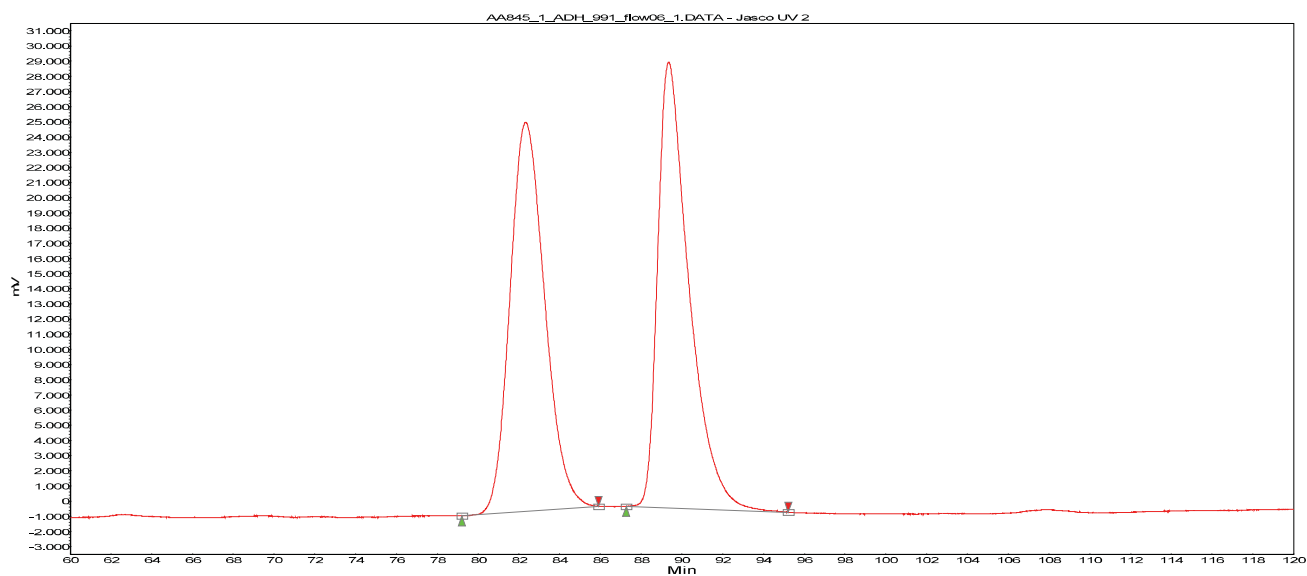
Mass Table

Line#:1 R.Time:10.4(Scan#:884)
 MassPeaks:89 BasePeak:106(61016)
 RawMode:Averaged 10.3-10.4(882-885)
 BG Mode:Averaged 10.5-10.6(905-910)

#	m/z	Rel. Int.	#	m/z	Rel. Int.	#	m/z	Rel. Int.	#	m/z	Rel. Int.
1	49.95	6.22	24	88.90	14.39	47	124.30	5.13	70	178.10	17.22
2	51.05	23.53	25	91.05	9.34	48	126.00	3.62	71	179.10	12.44
3	51.90	19.28	26	92.10	18.17	49	127.00	14.15	72	180.10	23.07
4	52.90	29.42	27	93.10	22.16	50	127.85	8.97	73	182.65	4.11
5	54.00	16.07	28	93.95	25.17	51	129.05	6.03	74	187.95	4.08
6	54.95	27.50	29	95.05	5.43	52	132.50	8.34	75	196.05	62.71
7	56.25	5.23	30	96.05	31.94	53	132.90	6.72	76	197.10	10.17
8	62.15	4.46	31	97.95	4.10	54	134.10	40.41	77	208.05	28.31
9	63.00	20.48	32	98.90	4.91	55	134.95	11.64	78	209.15	6.24
10	64.10	19.27	33	103.15	10.59	56	136.00	21.47	79	224.10	83.01
11	65.05	38.95	34	104.10	19.58	57	139.25	4.54	80	225.10	10.18
12	66.00	22.36	35	105.05	17.35	58	140.15	11.22	81	226.00	3.07
13	67.05	40.06	36	106.00	100.00	59	145.05	12.64	82	239.80	20.45
14	67.90	13.85	37	106.90	46.10	60	146.10	4.22	83	241.25	5.42
15	69.10	41.74	38	108.00	31.62	61	150.15	22.29	84	252.45	13.06
16	70.00	5.64	39	109.10	12.91	62	151.10	47.40	85	253.10	15.88
17	75.15	7.70	40	110.05	3.01	63	152.05	41.93	86	263.75	5.33
18	76.90	42.49	41	111.20	3.61	64	153.05	13.37	87	268.15	33.00
19	78.00	25.23	42	115.30	3.38	65	159.00	12.90	88	268.75	9.59
20	78.80	30.87	43	115.85	5.49	66	159.85	4.61	89	283.15	15.09
21	80.15	25.56	44	119.05	3.79	67	170.80	5.10			
22	81.05	16.93	45	120.25	4.01	68	171.95	13.87			
23	82.35	8.45	46	122.30	20.22	69	177.15	3.02			

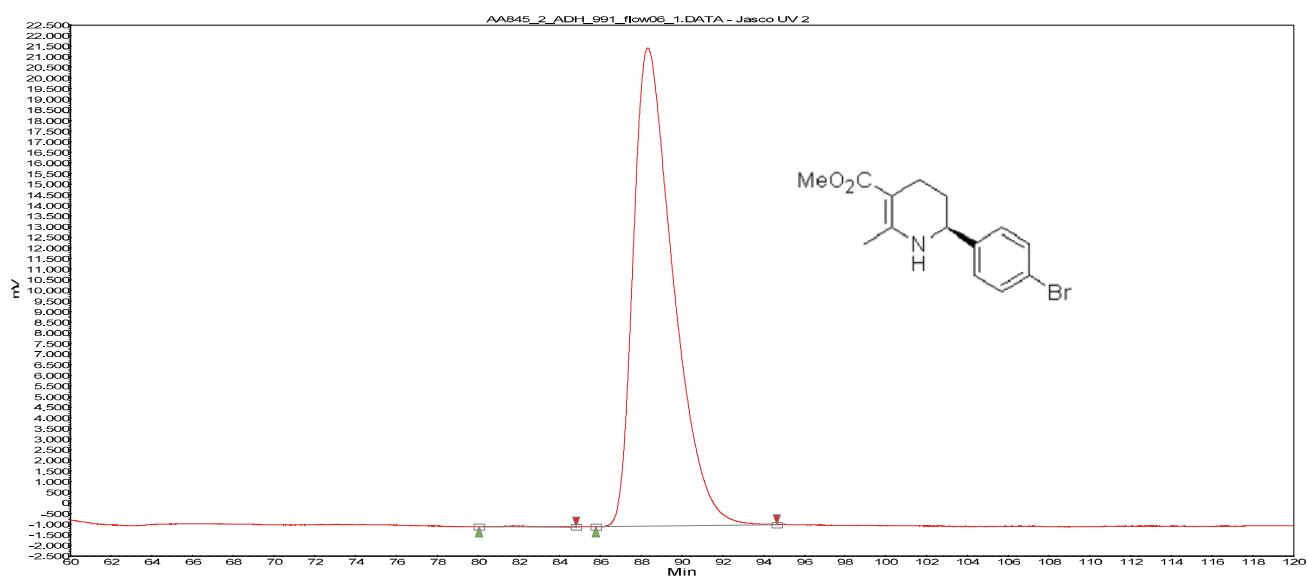
Chromatogram : AA845_1_ADH_991_flow06_1

Data file: AA845_1_ADH_991_flow06_1.DATA
Method: HPLC2_ADH_991_flow06_acq120

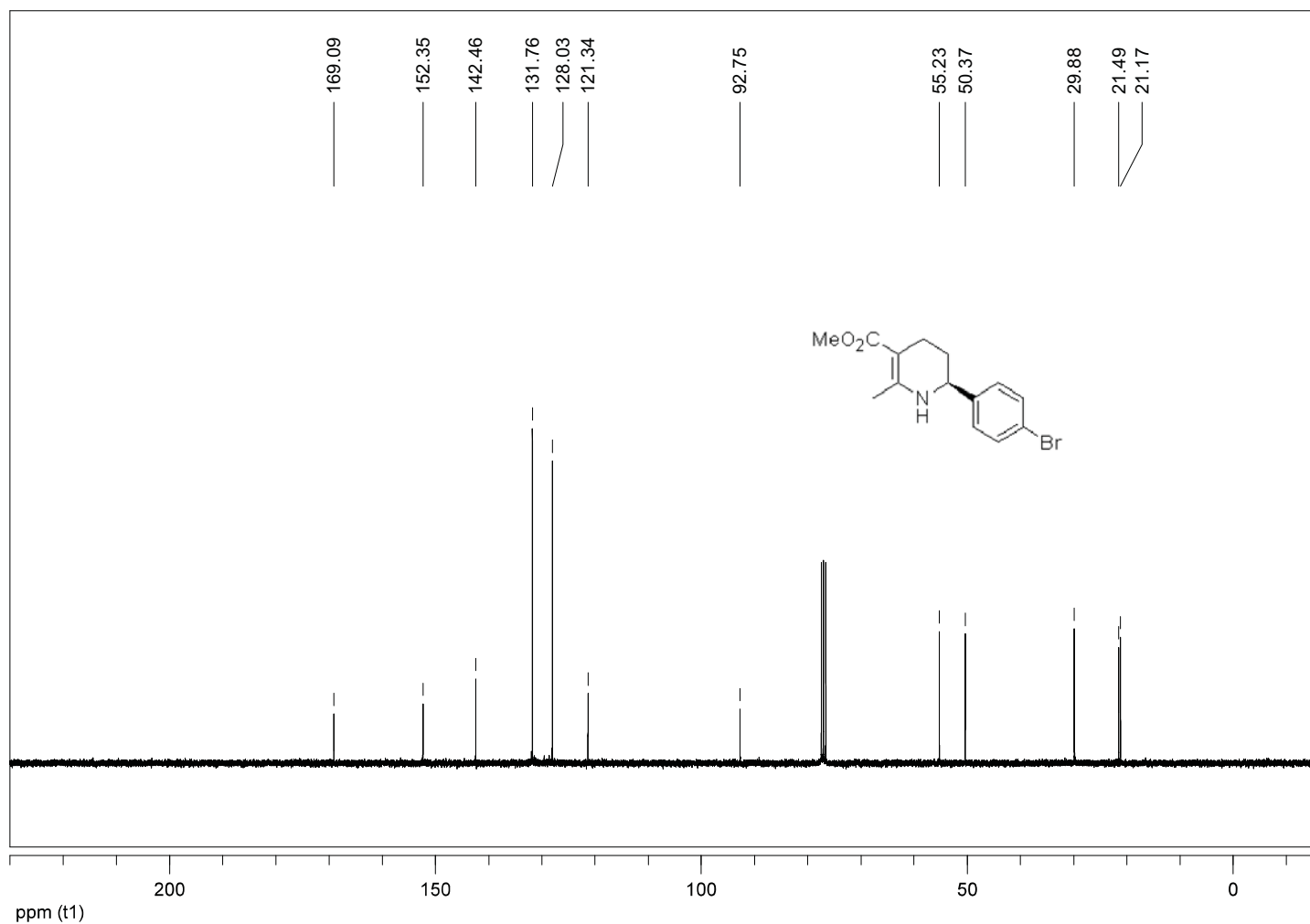
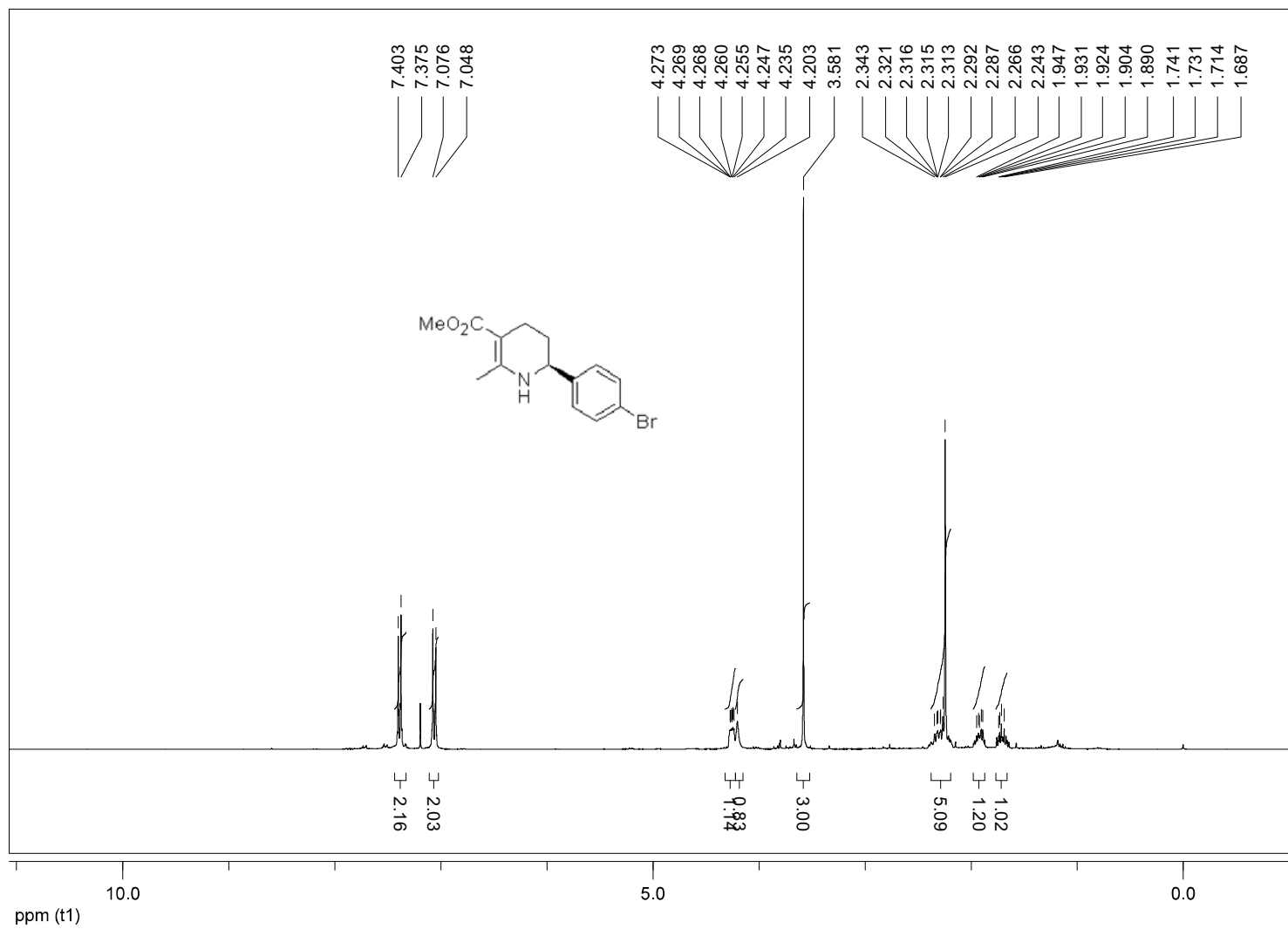


Chromatogram : AA845_2_ADH_991_flow06_1

Data file: AA845_2_ADH_991_flow06_1.DATA
Method: HPLC2_ADH_991_flow06_acq120



Index	Start	Time	End	Area
	[Min]	[Min]	[Min]	[%]
2	80,059	81,842	84,806	0,117
1	85,787	88,317	94,654	99,883
Total				100,000



Sample Information

Analyzed : 06.11.2007 11:45:19
 Sample Name : AA845_2

Method

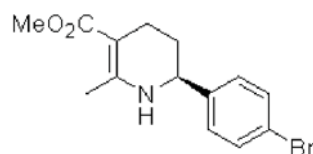
===== Analytical Line 1 =====

[GC-2010]

Column Oven Temp. : 60.0 °C
 Injection Temp. : 280.00 °C
 Injection Mode : Split
 Flow Control Mode : Linear Velocity
 Pressure : 29.2 kPa
 Total Flow : 17.2 mL/min
 Column Flow : 0.68 mL/min
 Linear Velocity : 30.0 cm/sec
 Purge Flow : 3.0 mL/min
 Split Ratio : 20.0

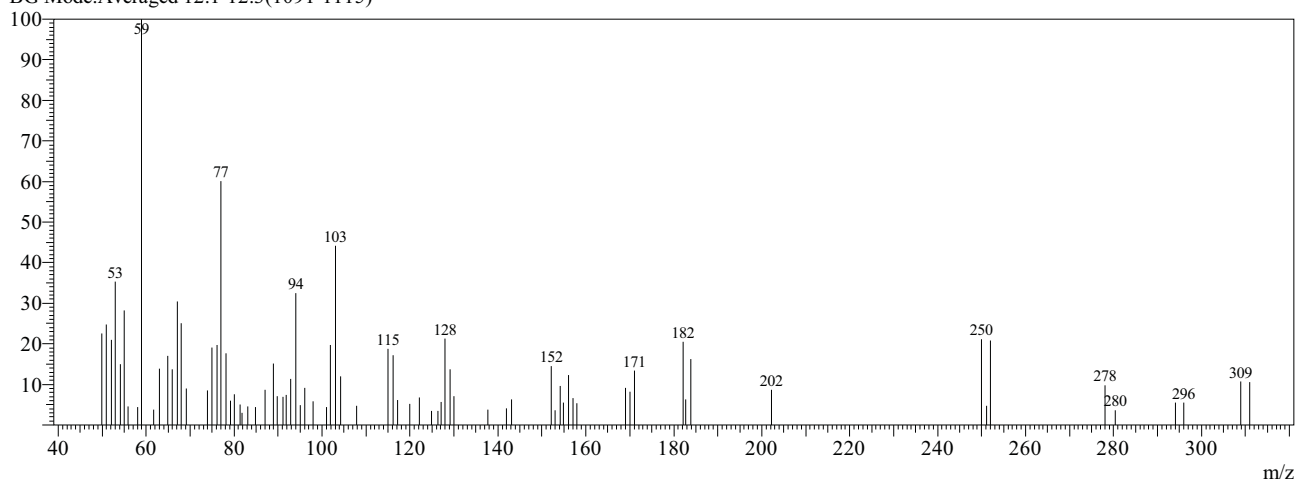
Oven Temp. Program

Rate	Temperature(°C)	Hold Time(min)
-	60.0	0.00
20.0	300.0	8.00



Spectrum

Line#:1 R.Time:11.9(Scan#:1069)
 MassPeaks:79 BasePeak:59(79573)
 RawMode:Averaged 11.9-11.9(1065-1072)
 BG Mode:Averaged 12.1-12.3(1091-1115)



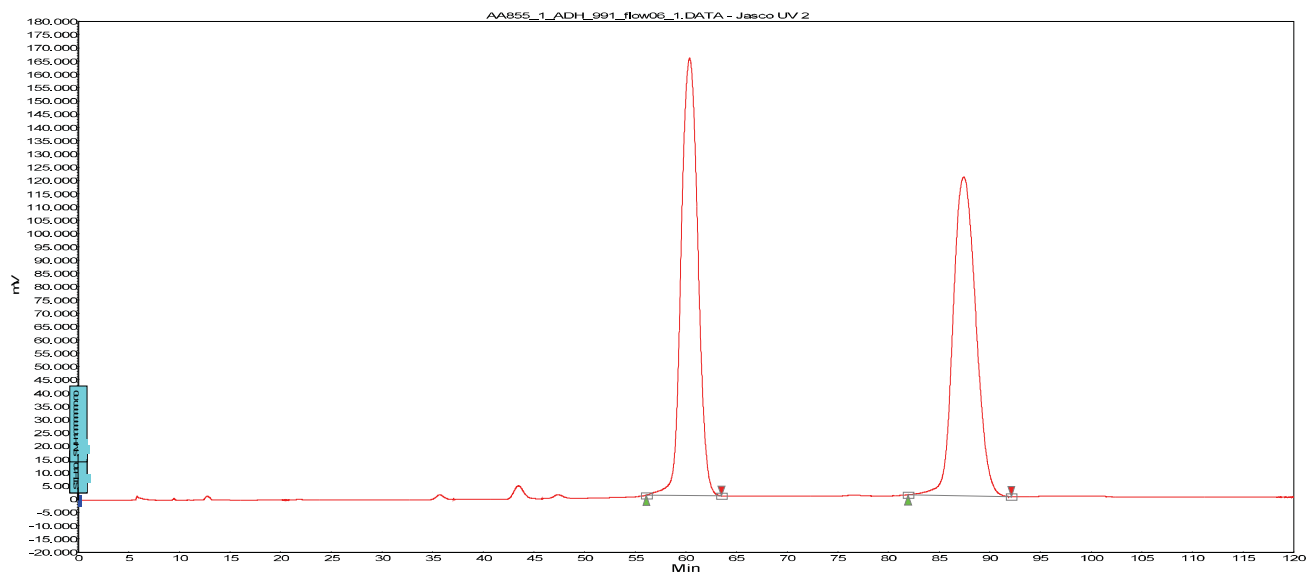
Mass Table

Line#:1 R.Time:11.9(Scan#:1069)
 MassPeaks:79 BasePeak:59(79573)
 RawMode:Averaged 11.9-11.9(1065-1072)
 BG Mode:Averaged 12.1-12.3(1091-1115)

#	m/z	Rel. Int.	#	m/z	Rel. Int.	#	m/z	Rel. Int.	#	m/z	Rel. Int.
1	49.85	22.59	21	78.10	17.74	41	104.20	12.00	61	156.10	12.31
2	50.95	24.77	22	79.25	5.99	42	107.80	4.74	62	157.05	6.68
3	52.05	20.94	23	80.10	7.53	43	114.95	18.82	63	157.90	5.36
4	53.00	35.30	24	81.35	5.09	44	116.10	17.26	64	168.95	9.09
5	54.15	14.95	25	81.80	3.07	45	117.20	6.16	65	170.05	8.14
6	54.95	28.31	26	83.10	4.62	46	119.95	5.27	66	171.10	13.33
7	55.85	4.51	27	84.85	4.42	47	122.15	6.74	67	182.10	20.57
8	58.05	4.42	28	87.10	8.71	48	124.85	3.46	68	182.75	6.37
9	58.90	100.00	29	89.00	15.11	49	126.35	3.39	69	183.90	16.25
10	61.75	3.78	30	89.85	7.12	50	127.10	5.61	70	202.15	8.72
11	63.05	13.93	31	91.15	6.98	51	128.00	21.22	71	249.90	21.21
12	64.95	17.10	32	91.85	7.46	52	129.15	13.75	72	251.10	4.72
13	65.95	13.75	33	92.90	11.40	53	129.95	7.08	73	252.05	20.78
14	67.05	30.40	34	94.00	32.44	54	137.75	3.74	74	278.10	9.74
15	67.90	25.11	35	95.00	4.93	55	141.90	4.14	75	280.40	3.69
16	69.10	8.91	36	96.10	9.12	56	143.05	6.36	76	294.05	5.53
17	73.95	8.44	37	97.95	5.87	57	152.05	14.47	77	295.95	5.56
18	75.00	19.04	38	100.95	4.43	58	152.95	3.58	78	308.90	10.76
19	76.10	19.69	39	101.90	19.66	59	154.20	9.55	79	311.00	10.58
20	77.00	60.14	40	103.05	44.09	60	154.90	5.46			

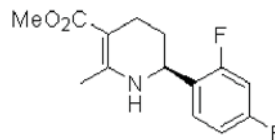
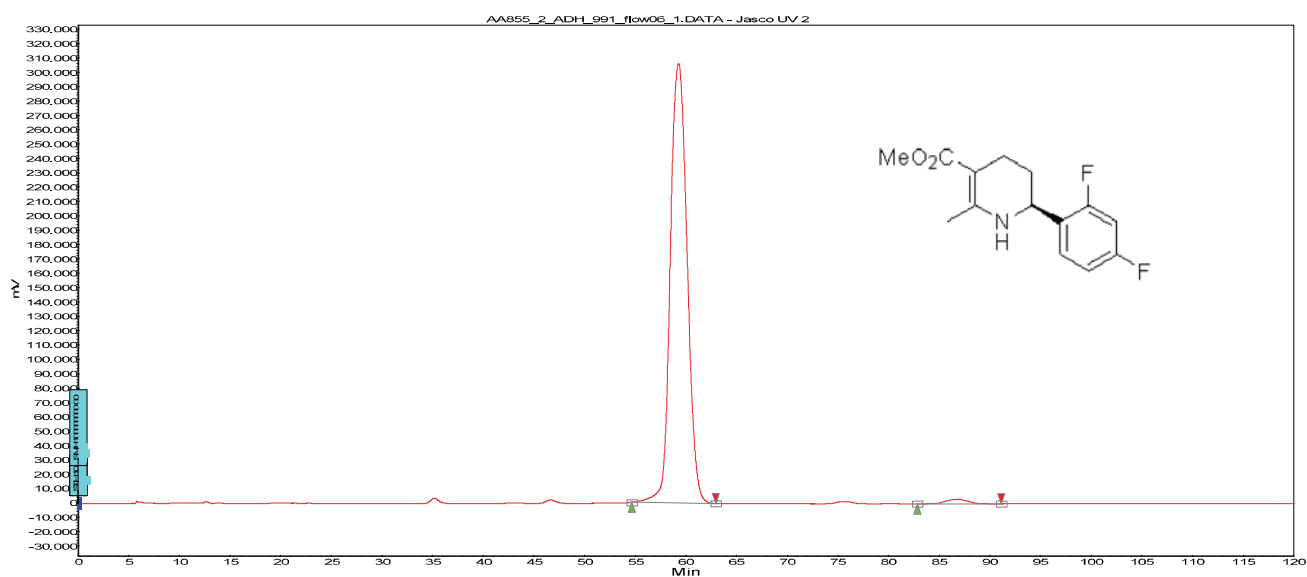
Chromatogram : AA855_1_ADH_991_flow06_1

Data file: AA855_1_ADH_991_flow06_1.DATA
Method: HPLC2_ADH_991_flow06_acq180

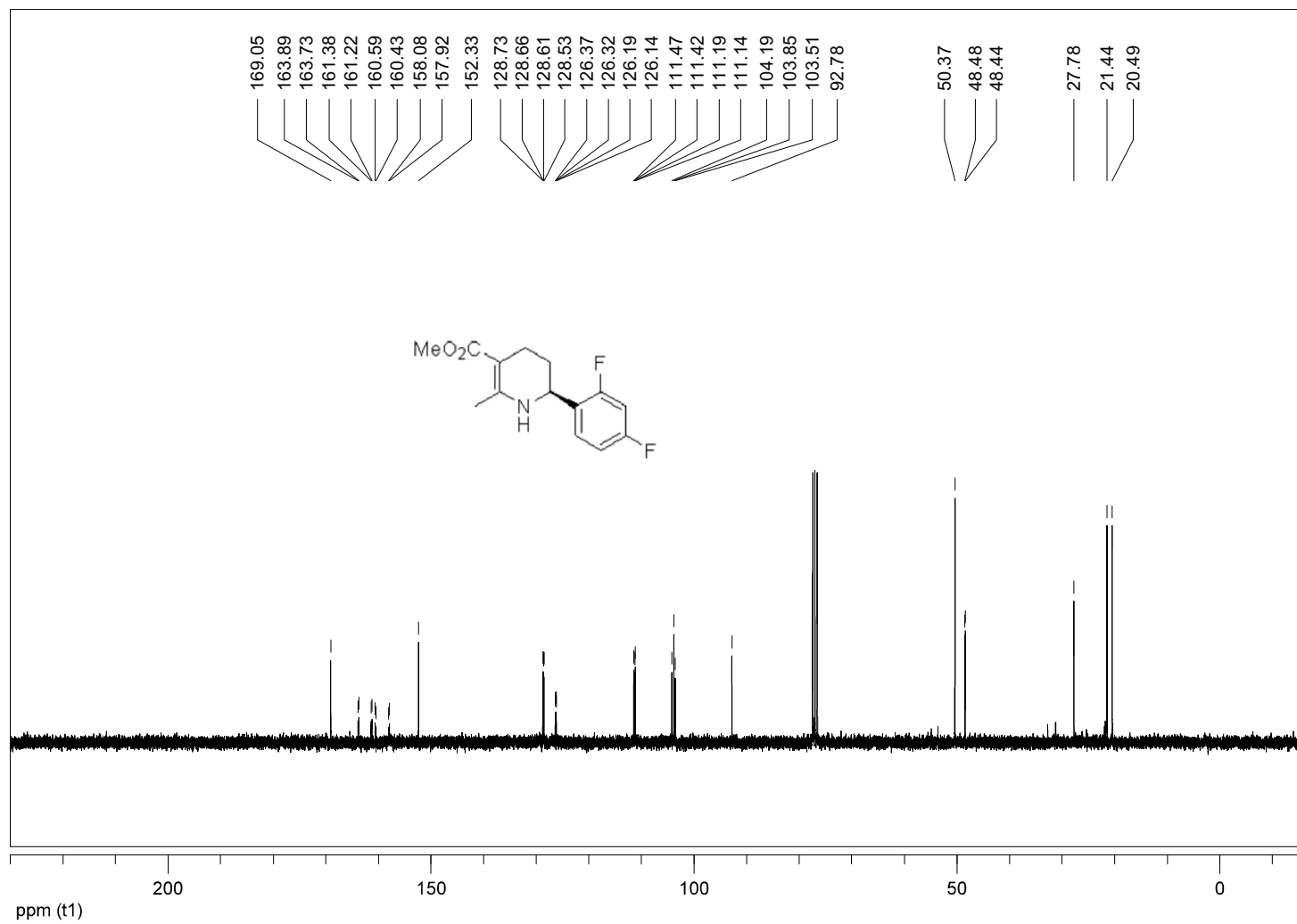
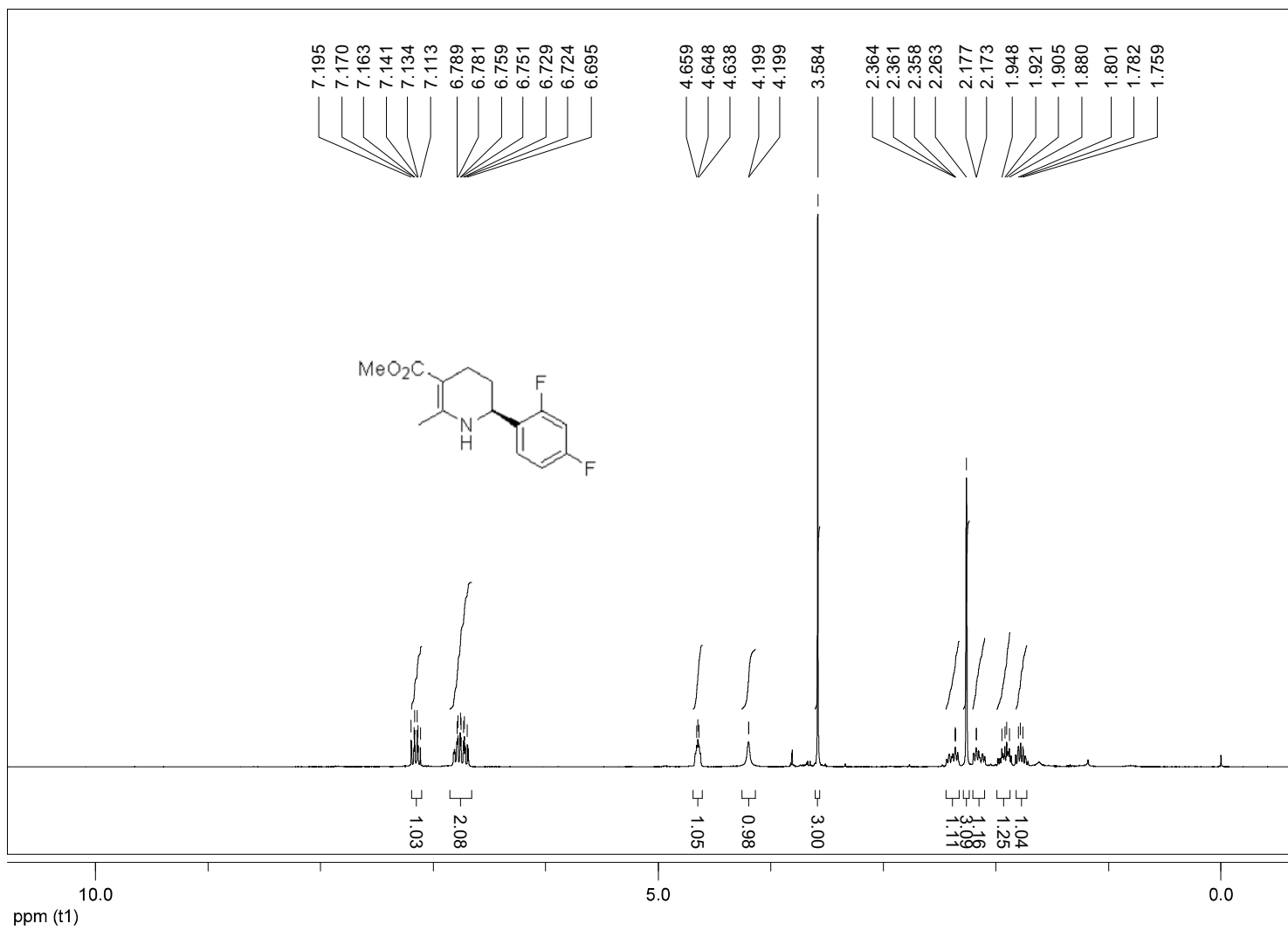


Chromatogram : AA855_2_ADH_991_flow06_1

Data file: AA855_2_ADH_991_flow06_1.DATA
Method: HPLC2_ADH_991_flow06_acq180



Index	Start	Time	End	Area
	[Min]	[Min]	[Min]	[%]
1	54,670	59,267	62,954	98,781
2	82,834	86,775	91,117	1,219
Total				100,000



Sample Information

Analyzed : 14.11.2007 16:03:33
 Sample Name : AA855_2

Method

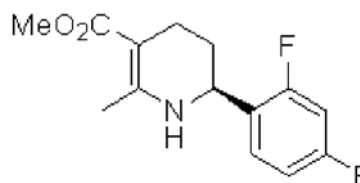
===== Analytical Line 1 =====

[GC-2010]

Column Oven Temp. : 60.0 °C
 Injection Temp. : 280.00 °C
 Injection Mode : Split
 Flow Control Mode : Linear Velocity
 Pressure : 29.2 kPa
 Total Flow : 17.2 mL/min
 Column Flow : 0.68 mL/min
 Linear Velocity : 30.0 cm/sec
 Purge Flow : 3.0 mL/min
 Split Ratio : 20.0

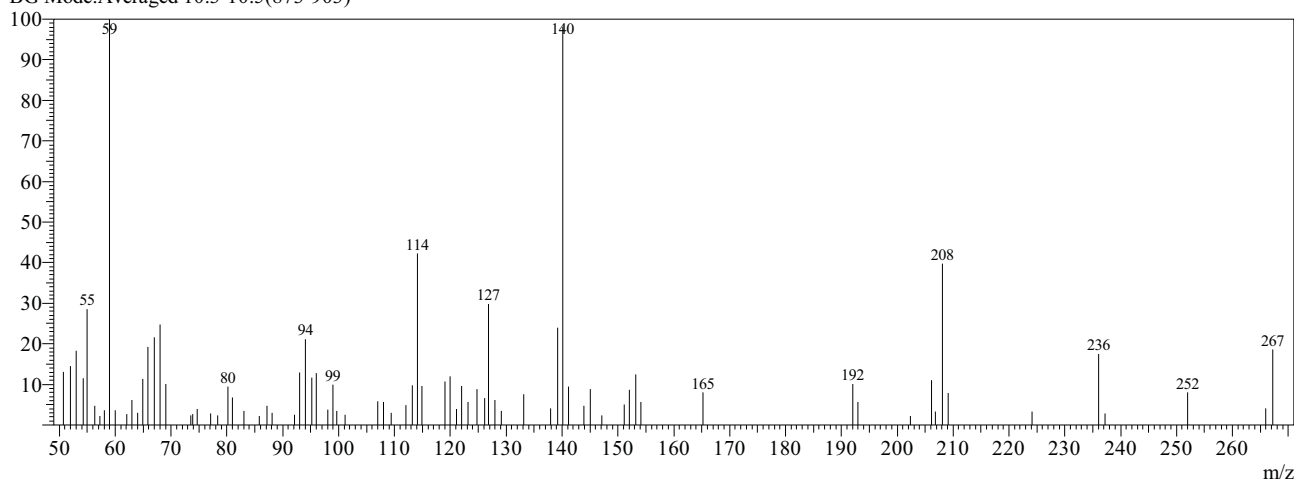
Oven Temp. Program

Rate	Temperature(°C)	Hold Time(min)
-	60.0	0.00
20.0	300.0	8.00



Spectrum

Line#:1 R.Time:10.1(Scan#:853)
 MassPeaks:81 BasePeak:59(68730)
 RawMode:Averaged 10.1-10.1(851-855)
 BG Mode:Averaged 10.3-10.5(873-903)



Mass Table

Line#:1 R.Time:10.1(Scan#:853)
 MassPeaks:81 BasePeak:59(68730)
 RawMode:Averaged 10.1-10.1(851-855)
 BG Mode:Averaged 10.3-10.5(873-903)

#	m/z	Rel. Int.	#	m/z	Rel. Int.	#	m/z	Rel. Int.	#	m/z	Rel. Int.
1	50.70	13.16	22	77.05	2.87	43	113.15	9.70	64	151.15	5.07
2	52.00	14.58	23	78.35	2.39	44	114.10	42.31	65	152.05	8.63
3	53.00	18.22	24	80.15	9.43	45	114.90	9.61	66	153.15	12.43
4	54.30	11.54	25	81.00	6.77	46	119.05	10.76	67	154.15	5.67
5	55.00	28.56	26	83.00	3.42	47	119.95	12.00	68	165.25	7.99
6	56.35	4.71	27	85.80	2.20	48	121.05	3.94	69	192.00	10.14
7	57.20	2.14	28	87.15	4.68	49	122.05	9.63	70	192.95	5.72
8	58.05	3.67	29	88.10	3.01	50	123.10	5.65	71	202.30	2.13
9	59.00	100.00	30	92.05	2.53	51	124.80	8.85	72	206.15	11.07
10	59.95	3.59	31	93.00	12.94	52	126.10	6.70	73	206.85	3.30
11	62.05	2.67	32	94.00	21.09	53	126.85	29.75	74	208.10	39.70
12	63.00	6.12	33	95.20	11.60	54	128.00	6.18	75	209.15	7.81
13	64.00	2.99	34	95.95	12.78	55	129.15	3.44	76	224.10	3.33
14	64.95	11.31	35	98.05	3.77	56	133.10	7.61	77	236.10	17.44
15	65.80	19.31	36	98.95	9.92	57	137.90	4.04	78	237.20	2.82
16	67.00	21.59	37	99.65	3.51	58	139.15	24.03	79	251.95	8.11
17	68.00	24.72	38	101.10	2.54	59	140.10	98.05	80	266.00	4.04
18	69.00	10.03	39	107.05	5.86	60	141.20	9.43	81	267.25	18.55
19	73.50	2.30	40	108.00	5.65	61	143.95	4.69			
20	73.85	2.75	41	109.35	2.96	62	145.10	8.75			
21	74.70	3.94	42	112.05	4.87	63	147.15	2.42			