

## Supporting Information

### Efficient synthesis of mibefradil analogues: an insight into in vitro stability

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## I. Experimental Procedures for Scheme 4

### General Methods

All reactions were carried out under dry nitrogen unless otherwise indicated. Commercially available reagents were used without further purification. Solvents and gases were dried according to standard procedures. Organic solvents were evaporated with reduced pressure using a rotary evaporator. Analytical thin layer chromatography (TLC) was performed using glass plates precoated with silica gel (0.25 mm). TLC plates were visualized by exposure to UV light (UV), and then were visualized with a *p*-anisaldehyde stain followed by brief heating on hot plate. Flash column chromatography was performed using silica gel 60 (230-400 mesh, Merck) with the indicated solvents.  $^1\text{H}$  and  $^{13}\text{C}$  spectra were recorded on Bruker 300, Bruker 400 or Varian 300 NMR spectrometers.  $^1\text{H}$  NMR spectra are represented as follows: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet), integration, and coupling constant (*J*) in Hertz (Hz).  $^1\text{H}$  NMR chemical shifts are reported relative to  $\text{CDCl}_3$  (7.26 ppm).  $^{13}\text{C}$  NMR was recorded relative to the central line of  $\text{CDCl}_3$  (77.0 ppm). HPLC data were acquired from a Waters Alliance System with UV detector set to at 254 and 280 nm. Samples were injected (10  $\mu\text{L}$ ) onto a Waters Sunfire 4.6 x 150 mm, 5.0  $\mu\text{M}$ , C18 column maintained at 25.8  $^\circ\text{C}$ . A linear gradient from 30% to 100% **B** (MeCN) in 20 min was followed by pumping 100% **B** for another 10 minutes with **A** being  $\text{H}_2\text{O} + 0.1 \text{ M NH}_4\text{OAc}$  (or  $\text{NH}_4\text{HCO}_2$ ). The flow rate was 1.0 mL/min.

**Benzyl 4-(2-aminophenylamino)-4-oxobutyl(methyl)carbamate (17)** : To a solution of 4-(methylamino)butyric acid hydrochloride (1.00 g, 6.51 mmol) in 4 N NaOH (5 mL) was added benzyl chloroformate (1.02 mL, 7.16 mmol) at 0  $^\circ\text{C}$ . The reaction mixture was allowed to stir for 1 h at room temperature. The resulting solution was extracted with diethyl ether (3 x 20 mL). The organic layers were washed with brine, dried over anhydrous  $\text{MgSO}_4$  and

concentrated *in vacuo*. Concentration afforded the Cbz-protected amine (1.28 g, 78%), which was used for the next step without purification. The spectroscopic data were identical with those reported in the literature<sup>1</sup>; <sup>1</sup>H-NMR (300 MHz, CDCl<sub>3</sub>)  $\delta$  7.26-7.36 (m, 5H), 5.12 (s, 2H), 3.33-3.35 (m, 2H), 2.93 (s, 3H), 2.34-2.37 (m, 2H), 1.85-1.87 (m, 2H).

**Benzyl 4-(2-aminophenylamino)-4-oxobutyl(methyl)carbamate (19a):** To a solution of the Cbz protected amine **17** (1.28 g, 5.09 mmol) in distilled THF (4 mL) was added TEA (1.07 mL) and a solution of isobutyl chloroformate (0.67 mL, 5.09 mmol) in distilled THF (1 mL) at -15 °C. The reaction mixture was allowed to stir for 3 h at the same temperature. Then, a solution of 1,2-phenylene diamine **18a** (0.61 g, 5.60 mmol) in distilled THF (5 mL) was added to the reaction mixture at the same temperature. The reaction mixture was allowed to stir for 2 h at room temperature. The solvent was partially removed under reduced pressure. The resulting mixture was diluted aq NaHCO<sub>3</sub>/ethyl acetate and extracted with ethyl acetate (3 x 30 mL). The organic layers were washed with brine, dried over anhydrous MgSO<sub>4</sub> and concentrated *in vacuo*. The resulting residue was purified by flash column chromatography on silica gel (EtOAc:*n*-hexane = 4:1) to afford amide **19a** (1.40 g, 86%); <sup>1</sup>H-NMR (300 MHz, CDCl<sub>3</sub>)  $\delta$  7.34-7.40 (m, 6H), 7.00-7.04 (m, 1H), 6.74-6.79 (m, 2H), 5.13 (s, 2H), 3.41-3.45 (m, 2H), 2.94 (s, 3H), 2.31-2.35 (m, 2H), 1.90-1.97 (m, 2H).

**Benzyl 4-((2-amino-4-methylphenyl)amino)-4-oxobutyl)carbamate (19b):** The following the same procedure as that used for the synthesis of **19a**, the reaction of amine **17** (0.817 mg, 3.45 mmol), TEA (721  $\mu$ l, 5.17 mmol), iso-butyl chloroformate (451  $\mu$ l, 3.45 mmol), and 3,4-diaminotoluene **18b** (463 mg, 3.79 mmol) in dry THF gave amide **19b** (0.91 mg, 78%) as a

<sup>1</sup> M. Tegoni, L. Ferretti, F. Sansone, M. Remelli, V. Bertolasi, F. Dallavalle, *Chem. E ur. J.* **2007**, *13*, 1300.

white solid after purification by column chromatography on silica gel (EtOAc:*n*-hexane = 4:1);  $^1\text{H-NMR}$  (300 MHz,  $\text{CDCl}_3$ )  $\delta$  7.89 (s, 1H) 7.37-7.31 (m, 5H), 7.06 (d,  $J = 8.5$  Hz, 1H), 6.54 (s, 1H), 5.21 (s, 1H), 5.06 (s, 2H), 3.96 (s, 1H), 3.27-3.20 (m, 2H), 2.35 (t,  $J = 6.1$  Hz, 2H), 2.22 (s, 3H) 1.88-1.81 (m, 2H).  $^{13}\text{C-NMR}$  (100 MHz,  $\text{CDCl}_3$ )  $\delta$  171.5, 157.2, 140.7, 137.0, 136.4, 128.6, 128.1, 125.4, 121.5, 119.9, 118.2, 66.9, 40.1, 33.7, 26.6, 21.0. LRMS-EI ( $m/z$ ):  $[\text{M}]^+$  calcd for  $\text{C}_{19}\text{H}_{23}\text{N}_3\text{O}_3$  341.17, found 341.

**Benzyl (4-((2-amino-4-fluorophenyl)amino)-4-oxobutyl)carbamate (19c):** The following the same procedure as that used for the synthesis of **19a**, the reaction of amine **17** (799 mg, 3.36 mmol), TEA (702 ml, 5.04 mmol), iso-butyl chloroformate (439 ml, 3.36 mmol), and 4-fluoro-1,2-phenylenediamine **18c** (466 mg, 3.69 mmol) in dry THF gave the carbamate **19c** (899 mg, 78%) as a brown solid after purification by column chromatography on silica gel (EtOAc:*n*-hexane = 4:1);  $^1\text{H-NMR}$  (300 MHz,  $\text{CDCl}_3$ )  $\delta$  7.85 (s, 1H), 7.35 (s, 5H), 7.17 (t,  $J = 6.8$  Hz, 1H), 6.49-6.43 (m, 2H), 5.10 (s, 2H), 5.06 (s, 1H), 3.32 (m,  $J = 6.1$  Hz, 2H), 2.40 (t,  $J = 6.5$  Hz, 2H), 1.90 (m,  $J = 6.2$  Hz, 2H).  $^{13}\text{C-NMR}$  (100 MHz, MeOD)  $\delta$  173.4, 162.1 (d,  $^1J = 239.6$  Hz), 157.7 144.7, 137.0, 128.1, 127.8 (d,  $^3J = 10.5$  Hz), 127.5 (d,  $^3J = 13.9$  Hz), 118.9, 103.3 (d,  $^2J = 22.9$  Hz), 102.2 (d,  $^2J = 25.8$  Hz), 66.0, 39.8, 32.7, 25.7. LRMS-EI ( $m/z$ ):  $[\text{M}]^+$  calcd for  $\text{C}_{18}\text{H}_{20}\text{FN}_3\text{O}_3$  345.15, found 345.

**Benzyl (4-((2-amino-4-chlorophenyl)amino)-4-oxobutyl)carbamate (19d):** The following the same procedure as that used for the synthesis of **19a**, the reaction of amine **17** (1.51 g, 6.38 mmol), TEA (1.33 ml, 9.57 mmol), isobutyl chloroformate (910  $\mu\text{L}$ , 6.38 mmol), and 4-chloro-1,2-phenylenediamine (1.00 g, 7.02 mmol) in dry THF gave amide **19d** (1.67 g, 72%) as a yellow solid after purification by column chromatography on silica gel (EtOAc:*n*-hexane = 4:1);  $^1\text{H-NMR}$  (300 MHz,  $\text{CDCl}_3$ )  $\delta$  7.95 (s, 1H), 7.34 (s, 5H), 7.20 (d,  $J = 8.2$  Hz, 1H),

6.72-6.65 (m, 2H), 5.09 (s, 2H), 4.08 (s, 2H), 3.28 (t,  $J = 5.7$  Hz, 2H), 2.36 (t,  $J = 6.3$  Hz, 2H), 1.88 (m,  $J = 6.5$  Hz, 2H).  $^{13}\text{C}$ -NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  172.5, 157.3, 142.5, 136.5, 132.2, 128.6, 128.2, 128.0, 127.2, 122.0, 118.3, 116.6, 66.8, 40.1, 33.5, 26.3.

**Benzyl (4-((2-amino-4-bromophenyl)amino)-4-oxobutyl)carbamate (19e):** The following the same procedure as that used for the synthesis of **19a**, the reaction of amine **17** (1.43 g, 6.02 mmol), TEA (1.26 ml, 9.02 mmol), isobutyl chloroformate (786  $\mu\text{l}$ , 6.02 mmol), and 4-bromo-1,2-phenylenediamine **18e** (1.24 g, 6.62 mmol) in dry THF gave amide **19e** (1.64 g, 67 %) as a white solid after purification by column chromatography on silica gel (EtOAc:*n*-hexane = 4:1);  $^1\text{H}$ -NMR (400 MHz, MeOD)  $\delta$  7.33-7.25 (m, 5H), 6.99 (d,  $J = 8.4$  Hz, 1H), 6.95 (d,  $J = 2.2$  Hz, 1H), 6.73 (dd,  $J = 2.2, 8.4$  Hz, 1H), 5.05 (s, 2H), 3.19 (m,  $J = 3.7$  Hz, 2H), 2.41 (t,  $J = 7.4$  Hz, 2H), 1.86 (m,  $J = 6.9$  Hz, 2H).  $^{13}\text{C}$ -NMR (100 MHz, MeOD)  $\delta$  173.2, 157.6, 144.0, 136.9, 129.4, 128.2, 127.7, 127.5, 122.2, 120.0, 118.8, 118.0, 66.2, 39.9, 33.0, 25.8.

**Benzyl (4-((2-amino-4,5-dichlorophenyl)amino)-4-oxobutyl)carbamate (19f):** The following the same procedure as that used for the synthesis of **19a**, the reaction of amine **17** (1.62 g, 6.83 mmol), TEA (1.43 ml, 10.6 mmol), isobutyl chloroformate (893  $\mu\text{l}$ , 6.83 mmol), and 4,5-dichloro-1,2-phenylenediamine **18f** (1.33 g, 7.52 mmol) in dry THF gave amide **19f** (2.51 g, 93%) as a pale orange solid after purification by column chromatography on silica gel (EtOAc:*n*-hexane = 4:1);  $^1\text{H}$ -NMR (400 MHz, MeOD)  $\delta$  7.33-7.25 (m, 6H), 6.91 (s, 1H), 5.01 (s, 2H), 3.23-3.17 (m, 2H), 2.43 (t,  $J = 7.2$  Hz, 2H), 1.87 (m,  $J = 6.96$  Hz, 2H).  $^{13}\text{C}$ -NMR (100 MHz, MeOD)  $\delta$  173.1, 157.7, 142.3, 137.0, 129.4, 128.1, 127.6, 127.4, 126.9, 122.8, 118.6, 116.7, 66.1, 39.7, 32.8, 25.6

**Benzyl (4-((2-amino-4-nitrophenyl)amino)-4-oxobutyl)carbamate (19g):** The following the same procedure as that used for the synthesis of **19a**, the reaction of amine **17** (695 mg, 2.93 mmol), TEA (613 ml, 4.40 mmol), isobutyl chloroformate (383 ml, 2.93 mmol), and 4-nitro-1,2-phenylenediamine (494 mg, 3.22 mmol) in dry THF gave amide **19g** (0.26 g, 24%) as a orange solid after purification by column chromatography on silica gel (EtOAc:*n*-hexane = 4:1); <sup>1</sup>H-NMR (300 MHz, MeOD) δ 8.28 (d, *J* = 2.5 Hz, 1H), 8.06 (dd, *J* = 2.6, 9.1 Hz, 1H), 7.50-7.42 (m, 5H), 6.93 (d, *J* = 9.1 Hz, 1H), 5.22 (s, 2H), 3.31 (t, *J* = 7.2 Hz, 2H), 2.63 (t, *J* = 7.2 Hz, 2H), 2.04 (m, *J* = 6.9 Hz, 2H). <sup>13</sup>C-NMR (100 MHz, MeOD) δ 173.6, 157.7, 149.9, 137.0, 136.8, 128.1, 127.6, 127.4, 123.4, 123.1, 120.8, 113.7, 66.1, 39.7, 32.7, 25.5

**3-(1H-Benzo[d]imidazol-2-yl)-N-methylpropan-1-amine (19a'):** To a solution of the amide **19a** (1.40 g, 4.10 mmol) in toluene (30 mL) was added *p*-toluenesulfonic acid monohydrate (1.17 g, 6.15 mmol) at room temperature. The reaction mixture was treated under reflux condition with a Dean-Stark apparatus. The solvent was removed under reduced pressure. The resulting mixture was extracted with CH<sub>2</sub>Cl<sub>2</sub> (3 x 30 mL). The organic layers were dried over anhydrous MgSO<sub>4</sub> and concentrated *in vacuo*. The resulting residue was purified by flash column chromatography on silica gel (EtOAc only) to afford benzimidazole **19a'** (0.60 g, 45%). The spectroscopic data were identical with those reported in the literature<sup>13</sup>; <sup>1</sup>H-NMR (300 MHz, CDCl<sub>3</sub>) δ 7.57-7.58 (m, 2H), 7.33-7.38 (m, 5H), 7.19-7.22 (m, 2H), 5.23 (s, 2H), 3.40-3.44 (m, 2H), 2.96 (s, 3H), 2.86-2.90 (m, 2H), 1.99 (m, 2H).

**Benzyl (3-(1H-benzo[d]imidazol-2-yl)propyl)carbamate (19b'):** The following the same procedure as that used for the synthesis of **19a'**, the reaction of amide **19b** (798 g, 2.44 mmol) and *p*-toluenesulfonic acid monohydrate (695 mg, 3.65 mmol) in dry benzene (24 ml) gave benzimidazole **19b'** (0.32 g, 42%) as a yellow solid after purification by column

chromatography on silica gel (only EtOAc); <sup>1</sup>H-NMR (300 MHz, CDCl<sub>3</sub>) δ 7.46 (d, *J* = 8.1 Hz, 1H), 7.34 (s, 5H), 7.04 (d, *J* = 8.1 Hz, 1H), 5.36 (t, *J* = 6.4 Hz, 1H), 5.13 (s, 2H), 3.28 (q, *J* = 6.1 Hz, 2H), 2.92 (t, *J* = 6.5 Hz, 2H), 2.45 (s, 3H), 1.97-1.91 (m, 2H). <sup>13</sup>C-NMR (100 MHz, CDCl<sub>3</sub>) δ 157.6, 154.1, 138.3, 137.0, 136.4, 131.9, 129.1, 128.6, 128.2, 128.0, 123.6, 114.6, 114.2, 66.9, 39.7, 29.0, 25.7, 21.6. LRMS-EI (*m/z*): [M]<sup>+</sup> calcd for C<sub>19</sub>H<sub>21</sub>N<sub>3</sub>O<sub>2</sub> 323.16, found 323.

**Benzyl (3-(5-fluoro-1*H*-benzo[*d*]imidazol-2-yl)propyl)carbamate (19c')**: The following the same procedure as that used for the synthesis of **19a'**, the reaction of amide **19c** (975 mg, 2.82 mmol) and *p*-toluenesulfonic acid monohydrate (591 mg, 3.11 mmol) in dry toluene (25 ml) gave benzimidazole **19c'** (0.69 g, 75%) as a white solid after purification by column chromatography on silica gel (only EtOAc); <sup>1</sup>H-NMR (300 MHz, CDCl<sub>3</sub>) δ 7.45-7.41 (m, 1H), 7.35 (s, 5H), 7.21 (dd, *J* = 2.2, 9.0 Hz, 1H), 6.94 (td, *J* = 2.3, 9.2 Hz, 1H), 5.60 (t, *J* = 6.2 Hz, 1H), 5.04 (s, 2H), 3.25 (q, *J* = 6.2 Hz, 2H), 2.91 (t, *J* = 6.7 Hz, 2H), 1.97-1.89 (m, 2H). LRMS-EI (*m/z*): [M]<sup>+</sup> calcd for C<sub>18</sub>H<sub>18</sub>FN<sub>3</sub>O<sub>2</sub> 327.14, found 327.

**Benzyl (3-(5-chloro-1*H*-benzo[*d*]imidazol-2-yl)propyl)carbamate (19d')**: The following the same procedure as that used for the synthesis of **19a'**, the reaction of amide **19d** (1.67 g, 4.62 mmol) and *p*-toluenesulfonic acid monohydrate (958 mg, 5.08 mmol) in dry toluene (28 ml) gave benzimidazole **19d'** (573 mg, 36%) as a brown oil after purification by column chromatography on silica gel (only EtOAc); <sup>1</sup>H-NMR (300 MHz, CDCl<sub>3</sub>) δ 7.58 (s, 1H), 7.48 (d, *J* = 7.7 Hz, 1H), 7.37 (s, 5H), 7.21 (dd, *J* = 1.8, 8.5 Hz, 1H), 5.50 (t, *J* = 6.2 Hz, 1H), 5.17 (s, 2H), 3.31 (q, *J* = 6.2 Hz, 2H), 2.95 (t, *J* = 6.6 Hz, 2H), 1.97 (m, *J* = 6.2 Hz, 2H). <sup>13</sup>C-NMR (100 MHz, CDCl<sub>3</sub>) δ 157.9, 155.5, 139.2, 136.2, 131.0, 128.6, 128.3, 128.0, 127.8, 122.7, 115.5, 114.7, 67.1, 39.5, 29.0, 25.5. LRMS-EI (*m/z*): [M]<sup>+</sup> calcd for C<sub>18</sub>H<sub>18</sub>ClN<sub>3</sub>O<sub>2</sub> 343.11,

found 343.

**Benzyl (3-(5-bromo-1H-benzo[d]imidazol-2-yl)propyl)carbamate (19e')**: The following the same procedure as that used for the synthesis of **19a'**, the reaction of amide **19e** (1.64 g, 4.04 mmol) and *p*-toluenesulfonic acid monohydrate (923 mg, 4.85 mmol) in dry toluene (40 ml) gave benzimidazole **19e'** (651 mg, 41%) as a brown oil after purification by column chromatography on silica gel (only EtOAc); <sup>1</sup>H-NMR (400 MHz, MeOD) δ 7.58 (d, *J* = 0.8 Hz, 1H), 7.27 (d, *J* = 8.5 Hz, 1H), 7.19-7.13 (m, 6H), 3.16 (t, *J* = 6.4 Hz, 2H), 2.82 (t, *J* = 7.5 Hz, 2H), 1.96 (m, *J* = 7.1 Hz, 2H). <sup>13</sup>C-NMR (100 MHz, MeOD) δ 157.5, 156.0, 139.6, 136.8, 136.5, 128.1, 127.6, 127.4, 124.9, 117.2, 115.3, 114.8, 66.2, 39.9, 28.0, 25.8

**Benzyl (3-(5,6-dichloro-1H-benzo[d]imidazol-2-yl)propyl)carbamate (19f')**: The following the same procedure as that used for the synthesis of **19a'**, the reaction of amide **19f** (2.51 g, 6.33 mmol) and *p*-toluenesulfonic acid monohydrate (1.32 g, 6.96 mmol) in dry toluene (30 ml) gave benzimidazole **19f'** (624 mg, 26%) as a yellow solid after purification by column chromatography on silica gel (only EtOAc); <sup>1</sup>H-NMR (400 MHz, CDCl<sub>3</sub>) δ 11.43 (s, 1H), 7.74 (s, 1H), 7.57 (s, 1H), 7.36 (s, 5H), 5.20 (t, *J* = 6.3 Hz, 1H), 5.16 (s, 2H), 3.29 (q, *J* = 6.2 Hz, 2H), 2.92 (t, *J* = 6.3 Hz, 2H), 1.92 (m, *J* = 4.0, 2H)

**Benzyl (3-(5-nitro-1H-benzo[d]imidazol-2-yl)propyl)carbamate (19g')**: The following the same procedure as that used for the synthesis of **19a'**, the reaction of amide **19a** (358 mg, 962 μmol) and *p*-toluenesulfonic acid monohydrate (220 mg, 1.15 mmol) in dry benzene (10 ml) gave benzimidazole **19g'** (296 mg, 87%) as a yellow solid after purification by column chromatography on silica gel (only EtOAc); <sup>1</sup>H-NMR (400 MHz, MeOD) δ 8.24 (d, *J* = 1.7 Hz, 1H), 7.98 (dd, *J* = 2.2, 8.8 Hz, 1H), 7.46 (d, *J* = 8.9 Hz, 1H), 7.26-7.20 (m, 5H), 5.00 (s,



3H), 3.21 (t,  $J = 6.7$  Hz, 2H), 2.93 (t,  $J = 7.6$  Hz, 2H), 2.02 (m,  $J = 7.2$  Hz, 2H).  $^{13}\text{C}$ -NMR (100 MHz, MeOD)  $\delta$  159.7, 157.6, 143.1, 141.9, 138.2, 136.9, 128.0, 127.6, 127.3, 117.5, 113.4, 111.0, 66.1, 39.8, 27.7, 25.9. LRMS-EI ( $m/z$ ):  $[\text{M}]^+$  calcd for  $\text{C}_{18}\text{H}_{18}\text{N}_4\text{O}_4$  354.13, found 354.

**3-(1*H*-benzo[*d*]imidazol-2-yl)propan-1-amine (4a):** To a solution of the Cbz-protected amino benzimidazole **19a'** (600 mg, 1.86 mmol) in MeOH (8 mL) was added Pd/C (60 mg, 10 % (w/w)) at room temperature. The reaction mixture was stirred for 3 h under a hydrogen atmosphere (with the aid of a hydrogen balloon). It was filtered through a pad of Celite<sup>®</sup> and the solvent was removed under reduce pressure. Concentration afforded amine **5** (351 mg, quantitative) as a brown solid, which was used for the next step without further purification;  $^1\text{H}$ -NMR (300 MHz,  $\text{CDCl}_3$ )  $\delta$  7.51-7.54 (m, 2H), 7.17-7.24 (m, 2H), 3.07 (t,  $J = 6.5$  Hz, 2H), 2.78 (t,  $J = 5.9$  Hz, 2H), 2.49 (s, 3H), 1.98 (m, 2H).

**3-(5-Methyl-1*H*-benzo[*d*]imidazol-2-yl)propan-1-amine (4b):** The following the same procedure as that used for the synthesis of **4a**, the reaction of carbamate **19b'** (515 g, 1.59 mmol) and Pd/C (51 mg, 5 % (w/w) in dry MeOH (15 ml) gave amine **4b** (131 mg, 43%) as a brown oil after purification by column chromatography on silica gel ( $\text{CH}_2\text{Cl}_2:\text{MeOH}:\text{H}_2\text{O}:\text{NH}_4\text{Cl} = 80:4:1:1$ );  $^1\text{H}$ -NMR (300 MHz,  $\text{CDCl}_3$ )  $\delta$  7.38 (d,  $J = 8.1$  Hz, 1H), 7.28 (s, 1H), 6.97 (d,  $J = 8.1$ , 1H), 5.77 (s, 2H), 2.94 (t,  $J = 6.8$  Hz, 2H), 2.73 (t,  $J = 6.0$  Hz, 2H), 2.39 (s, 3H), 1.91 (t,  $J = 6.6$  Hz, 2H).  $^{13}\text{C}$ -NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  155.0, 138.7, 137.2, 131.6, 123.3, 114.4, 114.1, 41.3, 30.9, 27.1, 21.6. LRMS-EI ( $m/z$ ):  $[\text{M}]^+$  calcd for  $\text{C}_{11}\text{H}_{15}\text{N}_3$  189.13, found 189.

**3-(5-Fluoro-1*H*-benzo[*d*]imidazol-2-yl)propan-1-amine (4c):** The following the same

procedure as that used for the synthesis of **4a**, the reaction of carbamate **19c'** (699 mg, 2.01 mmol) and Pd/C (69 mg, 10 % (w/w) in dry MeOH (21 ml) gave amine **4c** (374 mg,  $\geq 99\%$ ) as a pale pink solid;  $^1\text{H-NMR}$  (300 MHz, MeOD)  $\delta$  7.41 (dd,  $J = 4.7, 8.7$  Hz, 1H), 7.16 (dd,  $J = 2.3, 9.1$  Hz, 1H), 6.92 (td,  $J = 3.4, 6.8$  Hz, 1H), 2.91 (t,  $J = 7.5$  Hz, 2H), 2.77 (t,  $J = 7.2$  Hz, 2H), 2.91 (q,  $J = 7.5$  Hz, 2H).  $^{13}\text{C-NMR}$  (100 MHz, MeOD)  $\delta$  159.3 (d,  $^1J = 235.0$  Hz), 156.0, 138.5 (d,  $^3J = 13.0$  Hz), 134.0, 114.6 (d,  $^3J = 10$  Hz), 109.7 (d,  $^2J = 25$  Hz), 100.1 (d,  $^2J = 26$  Hz), 40.3, 30.1, 25.8. LRMS-EI ( $m/z$ ):  $[\text{M}]^+$  calcd for  $\text{C}_{10}\text{H}_{12}\text{FN}_3$  193.10, found 193.

**3-(5-Chloro-1H-benzo[d]imidazol-2-yl)propan-1-amine (4d):** The following the same procedure as that used for the synthesis of **4a**, the reaction of carbamate **19d'** (573 mg, 1.67 mmol) and Pd/C (60 mg, 10% (w/w)) in dry MeOH (15 ml) gave amine **4c** (334 mg, 96%) as a yellow oil;  $^1\text{H-NMR}$  (400 MHz, MeOD)  $\delta$  7.51 (s, 1H), 7.43 (d,  $J = 6.4$  Hz, 1H), 7.15 (dd,  $J = 1.2, 6.6$  Hz, 1H), 3.08 (t,  $J = 6.5$  Hz, 2H), 2.94 (t,  $J = 5.8$  Hz, 2H), 1.96 (m,  $J = 6.2$  Hz, 2H).  $^{13}\text{C-NMR}$  (100 MHz, MeOD)  $\delta$  156.1, 139.2, 136.6, 127.4, 122.2, 114.8, 114.0, 40.0, 29.0, 25.7. LRMS-EI ( $m/z$ ):  $[\text{M}]^+$  calcd for  $\text{C}_{10}\text{H}_{12}\text{ClN}_3$  209.07, found 209.

**3-(5-Bromo-1H-benzo[d]imidazol-2-yl)propan-1-amine (4e):** The solution of the *N*-Cbz protected amine **19e'** (221 mg, 569  $\mu\text{mol}$ ) in 6N HCl (5 mL) was allowed to warm to reflux for 1 h. Concentration afforded isopropylchroman-3-ol **4e** (175 mg,  $\geq 99\%$ ) as a brown solid;  $^1\text{H-NMR}$  (400 MHz, MeOD)  $\delta$  7.94 (d,  $J = 1.2$  Hz, 1H), 7.70-7.65 (m, 2H), 3.39 (t,  $J = 8.0$  Hz, 2H), 3.17 (t,  $J = 7.4$  Hz, 2H), 2.37 (m,  $J = 7.9$  Hz, 2H).  $^{13}\text{C-NMR}$  (100 MHz, MeOD)  $\delta$  153.7, 132.1, 130.1, 129.3, 118.8, 116.5, 115.1, 38.4, 24.4, 23.6.

**3-(5,6-Dichloro-1H-benzo[d]imidazol-2-yl)propan-1-amine (4f):** The following the same procedure as that used for the synthesis of **4a**, the reaction of carbamate **19f'** (601 mg, 1.59

mmol) and Pd/C (60 mg, 10 % (w/w) in dry MeOH (15 ml) gave amine **4f** (354 mg, 91%) as a pale red brown solid; <sup>1</sup>H-NMR (400 MHz, MeOD)  $\delta$  7.45 (s, 2H), 2.87 (t,  $J = 7.5$  Hz, 2H), 2.75 (t,  $J = 7.2$  Hz, 2H), 1.95 (m,  $J = 7.3$  Hz, 2H). <sup>13</sup>C-NMR (100 MHz, MeOD)  $\delta$  157.5, 137.6, 125.3, 115.3, 40.1, 29.2, 25.8

**3-(5-Nitro-1H-benzo[d]imidazol-2-yl)propan-1-amine (4g):** The following the same procedure as that used for the synthesis of **4e**, the reaction of carbamate **19g'** (140 mg, 396  $\mu$ mol) in 6 N HCl (4 ml) gave amine **4g** (111 mg,  $\geq 99\%$ ) as a pale yellow solid; <sup>1</sup>H-NMR (300 MHz, MeOD)  $\delta$  8.69 (d,  $J = 1.9$  Hz, 1H), 8.47 (dd,  $J = 1.8, 9.0$  Hz, 1H), 7.98 (d,  $J = 9.0$  Hz, 1H), 3.40 (t,  $J = 7.0$  Hz, 2H), 3.36 (t,  $J = 7.5$  Hz, 2H), 2.34 (m,  $J = 7.7$  Hz, 2H). <sup>13</sup>C-NMR (100 MHz, MeOD)  $\delta$  157.2, 145.9, 135.0, 131.0, 121.2, 113.5, 110.3, 38.4, 24.3, 24.1.

**3-(1-Tosyl-1H-benzo[d]imidazol-2-yl)propan-1-ol (20a'):** To a solution of alcohol **20a** (35.7 mg, 188  $\mu$ mol) in dry CH<sub>2</sub>Cl<sub>2</sub>, THF (3 ml/3 ml) was added *p*-TsCl (119 mg, 624  $\mu$ mol), DMAP (3.50 mg, 28.4  $\mu$ mol) and TEA (57.4 mg, 568  $\mu$ mol) at 0 °C. The reaction mixture was allowed to stir for 4 h at room temperature. The resulting mixture was extracted with CH<sub>2</sub>Cl<sub>2</sub>. The organic layers were washed with brine, dried over anhydrous MgSO<sub>4</sub> and concentrated *in vacuo*. The resulting residue was purified by flash column chromatography on silica gel (EtOAc:*n*-hexane = 4:1) to afford the protected amine **20a'** (106 mg, 57%); <sup>1</sup>H-NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  8.04-8.01 (m, 1H), 7.80-7.78 (m, 2H), 7.64-7.61 (m, 1H), 7.36-7.24 (m, 4H), 3.78 (t,  $J = 5.8$  Hz, 2H), 3.55 (s, 1H), 3.32 (t,  $J = 7.1$  Hz, 2H), 2.35 (s, 3H), 2.21-2.15 (m, 2H). <sup>13</sup>C-NMR (100 MHz, CDCl<sub>3</sub>)  $\delta$  155.0, 146.1, 141.5, 135.4, 133.1, 130.3, 126.8, 124.9, 124.7, 119.7, 113.6, 61.9, 30.1, 27.1, 21.7.

**3-(1-Tosyl-1H-benzo[d]imidazol-2-yl)propanal (21a):** Dess-Martin periodinane (72.9 mg,

172  $\mu\text{mol}$ ) was added to a solution of alcohol **20a'** (51.6 mg, 156  $\mu\text{mol}$ ) in  $\text{CH}_2\text{Cl}_2$  (2 ml). After stirring for 2 h, the reaction mixture was quenched with  $\text{Na}_2\text{S}_2\text{O}_3$  and sat.  $\text{NaHCO}_3$ . The resulting mixture was extracted with  $\text{Et}_2\text{O}$ . The organic layers were washed with brine, dried over anhydrous  $\text{MgSO}_4$  and concentrated *in vacuo*. The resulting residue was purified by flash column chromatography on silica gel ( $\text{EtOAc}:\text{n-hexane} = 1:1$ ) to afford the aldehyde **21a** (38.4 mg, 75%) as a colorless oil;  $^1\text{H-NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  9.91 (s, 1H), 8.01-7.99 (m, 1H), 7.85 (dd,  $J = 1.7, 6.7$  Hz, 2H), 7.62-7.60 (m, 1H), 7.33-7.31 (m, 4H), 3.50 (t,  $J = 6.8$  Hz, 2H), 3.15 (t,  $J = 6.8$  Hz, 2H), 2.38 (s, 3H).  $^{13}\text{C-NMR}$  (100 MHz,  $\text{CDCl}_3$ )  $\delta$  200.2, 153.2, 146.1, 141.8, 135.3, 133.3, 130.3, 126.9, 124.9, 124.6, 119.9, 113.5, 40.3, 22.7, 21.7.

**3-(5-Methyl-1-tosyl-1H-benzo[d]imidazol-2-yl)propan-1-ol (20b')**: The following the same procedure as that used for the synthesis of **20a'**, the reaction of benzimidazole **20b** (35.7 mg, 188  $\mu\text{mol}$ ), *p*-TsCl (39.4 mg, 206  $\mu\text{mol}$ ), DMAP (1.15 mg, 9.38  $\mu\text{mol}$ ) and TEA (19.0 mg, 188  $\mu\text{mol}$ ) in dry  $\text{CH}_2\text{Cl}_2$ , THF (1:1) gave the N-protected benzimidazole **20b'** (34.2 mg, 53%) after purification by column chromatography on silica gel ( $\text{EtOAc}:\text{n-hexane} = 4:1$ );  $^1\text{H-NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.89-7.83 (m, 1H), 7.78-7.56 (m, 2H), 7.50-7.41 (m, 1H), 7.27-7.24 (m, 2H), 7.16-7.11 (m, 1H), 3.76 (t,  $J = 5.8$  Hz, 2H), 3.28 (q,  $J = 6.6$  Hz, 2H), 2.49 (s, 1H), 2.41 (s, 2H), 2.36 (d,  $J = 4.2$  Hz, 3H), 2.15 (m, 2H).

**3-(1-Tosyl-1H-benzo[d]imidazol-2-yl)propanal (21b)**: The following the same procedure as that used for the synthesis of **21a**, the reaction of alcohol **20b'** (34.2 mg, 100  $\mu\text{mol}$ ) and Dess-Martin periodinane (46.3 mg, 110  $\mu\text{mol}$ ) in dry  $\text{CH}_2\text{Cl}_2$  (1 ml) gave aldehyde **21b** (25.4 mg, 75%) as a brown oil after purification by column chromatography on silica gel ( $\text{EtOAc}:\text{n-hexane} = 1:1$ );  $^1\text{H-NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  9.90 (s, 1H), 7.87-7.81 (m, 3H), 7.45-7.40 (m, 1H), 7.30 (t,  $J = 7.2$  Hz, 2H), 7.14 (t,  $J = 9.0$  Hz, 1H), 3.49-3.44 (m, 2H), 3.14 (t,  $J = 6.8$  Hz,

2H), 2.49 (s, 1H), 2.42 (s, 2H), 2.39 (d,  $J = 4.4$  Hz, 3H).  $^{13}\text{C-NMR}$  (100 MHz,  $\text{CDCl}_3$ )  $\delta$  200.3, 153.2, 152.6, 145.9, 142.0, 139.8, 135.4, 135.3, 135.1, 134.6, 133.5, 131.3, 130.3, 130.3, 126.8, 126.2, 126.0, 119.8, 119.3, 113.5, 113.0, 40.4, 22.7, 22.0, 21.7, 21.3

**2-(1*H*-Benzo[*d*]imidazol-2-yl)ethanol (23a):** *o*-Phenylenediamine **22** (3.31 mL, 48.5 mmol) and 3-hydroxypropionitrile (4.20 g, 38.8 mmol) dissolved in conc. HCl (18 mL) were refluxed for 14h. The reaction mixture was neutralized with ammonia solution until pH 8 was reached at ice-bath. Neutralization gave brown powder which was filtered with water to give benzimidazole **23a**<sup>2</sup> (2.56 g, 41%);  $^1\text{H-NMR}$  (400 MHz, MeOD)  $\delta$  7.49-7.50 (m, 2H), 7.17-7.20 (m, 2H), 3.99 (t,  $J = 6.6$  Hz, 2H), 3.09 (t,  $J = 6.6$  Hz, 2H).  $^{13}\text{C-NMR}$  (100 MHz, MeOD)  $\delta$  153.0, 137.1, 122.3, 113.9, 59.5, 31.7.

**2-(5-Methyl-1*H*-benzo[*d*]imidazol-2-yl)ethanol (23b):** The following the same procedure as that used for the synthesis of **23a**, the reaction of 3,4-diaminotoluene (2.00 g, 16.37 mmol) and 3-hydroxypropionitrile (1.45 g, 20.46 mmol) dissolved in conc. HCl (10 mL) gave benzimidazole **23b**<sup>3</sup> (0.36 g, 13%) as a white solid after purification by column chromatography on silica gel (EtOAc:MeOH = 10:1);  $^1\text{H-NMR}$  (400 MHz, MeOD)  $\delta$  7.38 (d,  $J = 8.2$  Hz, 1H), 7.29 (s, 1H), 7.01 (dd,  $J = 1.0, 8.2$  Hz, 1H), 3.99 (t,  $J = 6.6$  Hz, 2H), 3.07 (t,  $J = 6.6$  Hz, 2H), 2.42 (s, 3H).  $^{13}\text{C-NMR}$  (100 MHz, MeOD)  $\delta$  152.7, 138.0, 136.6, 131.6, 123.2, 113.8, 113.6, 59.7, 32.0, 20.3.

**2-(5-Fluoro-1*H*-benzo[*d*]imidazol-2-yl)ethanol (23c):** The following the same procedure as that used for the synthesis of **23a**, the reaction of 4-fluoro-1,2-phenylenediamine (2.00 g,

<sup>2</sup> G. B. Bachman, L. V. Heisy, *J. Am. Chem. Soc.* **1949**, *71*, 1985-8.

<sup>3</sup> S. Akihama, M. Okude, K. Sato, S. Iwabauchi, *Yakugaku Zasshi* 1968, *88*, 684-689.

15.86 mmol) and 3-hydroxypropionitrile (1.24 g, 17.44 mmol) dissolved in conc. HCl (10 mL) gave benzimidazole **23c** (1.70 g, 59%) as a brown powder; <sup>1</sup>H-NMR (400 MHz, MeOD)  $\delta$  7.49-7.52 (m, 1H), 7.25 (dd,  $J$  = 1.7, 6.8 Hz, 1H), 7.01 (td,  $J$  = 1.8, 6.9 Hz, 1H), 4.02 (t,  $J$  = 4.8 Hz, 2H), 3.14 (t,  $J$  = 4.8 Hz, 2H). <sup>13</sup>C-NMR (100 MHz, MeOD)  $\delta$  159.4 (d,  $J$  = 236.0 Hz), 154.5, 137.6 (d,  $J$  = 13.0 Hz), 133.7, 114.6 (d,  $J$  = 11.0 Hz), 110.2 (d,  $J$  = 25.0 Hz), 100.1 (d,  $J$  = 27.0 Hz), 59.4, 31.7.

**2-(5-Chloro-1H-benzo[d]imidazol-2-yl)ethanol (23d):** The following the same procedure as that used for the synthesis of **23a**, the reaction of 4-chloro-1,2-phenylenediamine (5.00 g, 35.08 mmol) and 3-hydroxypropionitrile (3.12 g, 4.85 mmol) dissolved in conc. HCl (16 mL) gave benzimidazole **23d**<sup>3</sup> (1.53 g, 22%) as a pale-yellow solid after purification by column chromatography on silica gel (EtOAc:MeOH = 10:1); <sup>1</sup>H-NMR (400 MHz, MeOD)  $\delta$  7.48 (d,  $J$  = 1.7 Hz, 1H), 7.42 (d,  $J$  = 8.6 Hz, 1H), 7.15 (dd,  $J$  = 2.0, 8.6 Hz, 1H), 4.00 (t,  $J$  = 6.5 Hz, 2H), 3.09 (t,  $J$  = 6.5 Hz, 2H). <sup>13</sup>C-NMR (100 MHz, MeOD)  $\delta$  154.6, 139.1, 136.6, 127.3, 122.1, 114.8, 114.0, 59.5, 32.0.

**2-(2-(1H-Benzo[d]imidazol-2-yl)ethoxy)isoindoline-1,3-dione (23a'):** To a solution of *N*-hydroxyphthalimide (700 mg, 4.29 mmol), benzimidazole **23a** (580 mg, 3.58 mmol), and PPh<sub>3</sub> (1.31 g, 5.01 mmol) in distilled THF (17 mL) was added DIAD (0.97 mL, 5.01 mmol) at 0 °C. The reaction mixture was stirred for 1.5h at room temperature. The solvent of reaction mixture was removed under reduced pressure. The resulting mixture was extracted with EtOAc and washed with brine. The organic layer was dried over anhydrous MgSO<sub>4</sub> and concentrated *in vacuo*. The resulting residue was purified by flash column chromatography on silica-gel (EtOAc:*n*-hexane = 2:1) to give *N*-alkoxyphthalimide **23a'** (0.21 g, 19%); <sup>1</sup>H-NMR (300 MHz, CDCl<sub>3</sub>)  $\delta$  7.77-7.80 (m, 2H), 7.72-7.73 (m, 2H), 7.56-7.59 (m, 2H), 7.18-

7.21 (m, 2H), 4.59 (t,  $J = 5.3$  Hz, 2H), 3.34 (t,  $J = 5.4$  Hz, 2H).  $^{13}\text{C}$ -NMR (75 MHz,  $\text{CDCl}_3$ )  $\delta$  164.4 151.5 135.0 128.6 123.9 122.3 76.3 28.6.

**2-(2-(5-Methyl-1*H*-benzo[*d*]imidazol-2-yl)ethoxy)isoindoline-1,3-dione (23b')**: The following the same procedure as that used for the synthesis of **23a'**, the reaction of *N*-hydroxyphthalimide (330 mg, 2.02 mmol), methylbenzimidazole **23b** (356 mg, 2.02 mmol),  $\text{PPh}_3$  (583 mg, 2.22 mmol) and DIAD (0.43 mL, 2.22 mmol) in distilled THF (12 mL) gave the *N*-alkoxyphthalimide **23b'** (350 mg, 54%) as a white solid after purification by column chromatography on silica gel ( $\text{EtOAc}:\text{CHCl}_3=1:1$ );  $^1\text{H}$ -NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.80-7.81 (m, 2H), 7.72-7.75 (m, 2H), 7.44 (d,  $J = 8.0$  Hz, 1H) 7.34 (s, 1H), 7.01 (dd,  $J = 1.1, 8.2$  Hz, 1H) 4.56 (t,  $J = 5.4$  Hz, 2H), 3.29 (t,  $J = 5.4$  Hz, 2H).

**2-(2-(5-Fluoro-1*H*-benzo[*d*]imidazol-2-yl)ethoxy)isoindoline-1,3-dione (23c')**: The following the same procedure as that used for the synthesis of **23a'**, the reaction of *N*-hydroxyphthalimide (1.53 g, 9.38 mmol), fluorobenzimidazole **23c** (1.69 g, 9.38 mmol),  $\text{PPh}_3$  (2.71 g, 10.32 mmol) and DIAD (2.00 mL, 10.32 mmol) in distilled THF (60 mL) gave the *N*-alkoxyphthalimide **23c'** (0.17 g, 6%) as a white solid after purification by column chromatography on silica gel ( $\text{EtOAc}:\text{CHCl}_3 = 1:1$ );  $^1\text{H}$ -NMR (400 MHz, DMSO)  $\delta$  7.84 (s, 4H), 7.41-7.44 (m, 1H), 7.24 (dd,  $J = 2.2, 9.5$  Hz, 1H), 6.96 (t,  $J = 8.5$  Hz, 1H), 4.64 (t,  $J = 6.8$  Hz, 2H), 3.31 (t,  $J = 6.8$  Hz, 2H).  $^{13}\text{C}$ -NMR (100 MHz, DMSO)  $\delta$  163.7, [158.8 (d,  $J = 234.0$  Hz) and 158.5 (d,  $J = 232.0$  Hz)], [153.6 and 152.6], [144.0 (d,  $J = 12.0$  Hz) and 134.7 (d,  $J = 14.0$  Hz)], [140.2 and 131.3], 135.2, 129.1, 123.6, [119.3 (d,  $J = 10.0$  Hz) and 111.9 (d,  $J = 1.0$  Hz)], [109.9 (d,  $J = 25.0$  Hz) and 109.3 (d,  $J = 24.0$  Hz)], [104.1 (d,  $J = 23.0$  Hz) and 97.8 (d,  $J = 27.0$  Hz)], 75.3, 28.8.

**2-(2-(5-Chloro-1*H*-benzo[*d*]imidazol-2-yl)ethoxy)isoindoline-1,3-dione (23d')**: The following the same procedure as that used for the synthesis of **23a'**, the reaction of *N*-hydroxyphthalimide (292 mg, 1.79 mmol), chlorobenzimidazole **23d** (352 mg, 1.79 mmol), PPh<sub>3</sub> (516 mg, 1.97 mmol) and DIAD (0.38 mL, 1.97 mmol) in distilled THF (10 mL) gave the *N*-alkoxy phthalimide **23d'** (44 mg, 7%) as a white solid after purification by column chromatography on silica gel (EtOAc:CHCl<sub>3</sub> = 1:1); <sup>1</sup>H-NMR (400 MHz, DMSO) δ 7.84 (s, 4H), 7.44-7.50 (m, 2H), 7.11-7.16 (m, 1H), 4.64 (t, *J* = 6.6 Hz, 2H), 3.31 (t, *J* = 6.6 Hz, 2H). <sup>13</sup>C-NMR (100 MHz, DMSO) δ 163.7, [153.6 and 153.1], [144.6 and 142.4], 135.2, [135.4 and 133.5], 129.0, [126.5 and 125.8], 123.6, [122.2 and 121.7], [119.8 and 118.0], [112.6 and 111.2], 75.2, 28.8.

***O*-(2-(1*H*-Benzo[*d*]imidazol-2-yl)ethyl)hydroxylamine hydrochloride (5a)**: To a solution of *N*-alkoxyphthalimide **23a'** (120 mg, 0.39 mmol) in EtOH (3 mL) was added hydrazine monohydrate at room temperature. The reaction mixture was stirred for 3h at 80 °C. The resulting solution was filtered through a pad of silica gel and washed with EtOAc. The filtrate was solidified by treatment of 1M solution of HCl in Et<sub>2</sub>O (0.39 mL) to give *N*-alkoxyamine **5a** (45 mg, 54%); <sup>1</sup>H-NMR (300 MHz, MeOD) δ 7.81-7.85 (m, 2H), 7.61-7.65 (m, 2H), 4.62 (t, *J* = 5.8 Hz, 2H), 3.69 (t, *J* = 5.9 Hz, 2H).

***O*-(2-(5-Methyl-1*H*-benzo[*d*]imidazol-2-yl)ethyl)hydroxylamine hydrochloride (5b)**: The following the same procedure as that used for the synthesis of **5a**, the reaction of *N*-alkoxyphthalimide **23b'** (350 mg, 1.09 mmol), hydrazine monohydrate in EtOH (4 mL) gave the *N*-alkoxyamine **5b** (120 mg, 48 %); <sup>1</sup>H-NMR (400 MHz, MeOD) δ 7.70 (d, *J* = 8.4 Hz, 1H), 7.62 (d, *J* = 0.6 Hz, 1H), 7.45 (dd, *J* = 0.7, 8.5 Hz, 1H), 4.66 (t, *J* = 5.8 Hz, 2H), 3.70 (t, *J* = 5.8 Hz, 2H), 2.56 (s, 3H). <sup>13</sup>C-NMR (100 MHz, MeOD) δ 149.4, 137.1, 131.2, 128.9,



127.8, 113.0, 113.0, 70.7, 25.6, 20.3.

***O*-(2-(5-Fluoro-1*H*-benzo[*d*]imidazol-2-yl)ethyl)hydroxylamine hydrochloride (5c):** The following the same procedure as that used for the synthesis of **5a**, the reaction of *N*-alkoxyphthalimide **23c'** (167 mg, 0.51 mmol), hydrazine monohydrate in EtOH (2 mL) gave the *N*-alkoxyamine **5c** (101 mg, 85 %); <sup>1</sup>H-NMR (400 MHz, MeOD)  $\delta$  7.87 (dd, *J* = 4.3, 9.1 Hz, 1H), 7.63 (d, *J* = 2.2, 8.2 Hz, 1H), 7.44 (td, *J* = 2.4, 9.3 Hz, 1H), 4.67 (t, *J* = 5.8 Hz, 2H), 3.72 (t, *J* = 5.8 Hz, 2H). <sup>13</sup>C-NMR (100 MHz, MeOD)  $\delta$  161.1 (d, *J* = 243.0 Hz), 151.3, 131.5 (d, *J* = 13.0 Hz), 127.5, 115.2 (d, *J* = 10.0 Hz), 114.8 (d, *J* = 26.0 Hz), 100.2 (d, *J* = 28.0 Hz), 70.6, 25.7.

***O*-(2-(5-Chloro-1*H*-benzo[*d*]imidazol-2-yl)ethyl)hydroxylamine hydrochloride (5d):** The following the same procedure as that used for the synthesis of **5a**, the reaction of *N*-alkoxyphthalimide **23d'** (140 mg, 0.41 mmol), hydrazine monohydrate in EtOH (3 mL) gave the *N*-alkoxyamine **5d** (52 mg, 51%); <sup>1</sup>H-NMR (400 MHz, MeOD)  $\delta$  7.91 (s, 1H) 7.83-7.85 (m, 1H) 7.63-7.67 (m, 1H) 4.62-4.66 (m, 2H), 3.69-3.72 (m, 2H). <sup>13</sup>C-NMR (100 MHz, MeOD)  $\delta$  151.3, 132.0, 131.7, 129.7, 126.9, 114.9, 113.6, 70.5, 25.7.

## II. Experimental Procedures for 2ab-g, 2cb-g, 2db, and 2fb-d in Scheme 5

### (±)-(3*S*,4*S*)-7-Fluoro-4-isopropyl-3-(2-((3-(6-methyl-1*H*-benzo[*d*]imidazol-2-yl)propyl)amino)ethyl)chroman-3-ol (2ab)

The following the same procedure as that used for the synthesis of **2aa**, the reaction of amine **4b** (19.7 mg, 104  $\mu$ mol), sodium cyanoborohydride (6.53 mg, 104  $\mu$ mol), aldehyde **3** (26.2 mg, 104  $\mu$ mol) and acetic acid in MeOH (2 mL) gave amine **2ab** (13.5 mg, 31%) after purification by column chromatography on silica gel (CH<sub>2</sub>Cl<sub>2</sub>:MeOH:H<sub>2</sub>O:NH<sub>4</sub>OH = 80:20:1:1) as a brown oil; <sup>1</sup>H-NMR (300 MHz, CDCl<sub>3</sub>)  $\delta$  7.38 (d, *J* = 8.2 Hz, 1H), 7.26 (d, *J* = 6.9 Hz, 1H), 7.02 (d, *J* = 8.1 Hz, 1H), 6.94 (dd, *J* = 6.7, 8.3 Hz, 1H), 6.57 (td, *J* = 2.6, 8.3 Hz, 1H), 6.49 (dd, *J* = 2.5, 10.2 Hz, 1H) 4.11 (d, *J* = 11.0 Hz, 1H), 3.95 (dd, *J* = 1.6, 10.9 Hz, 1H), 3.00-2.92 (m, 4H), 2.76-2.65 (m, 2H) 2.57 (s, 1H), 2.44 (s, 3H), 2.02 (m, *J* = 6.1 Hz, 2H), 1.70 (m, *J* = 6.1 Hz, 2H), 1.18 (d, *J* = 6.9 Hz, 3H), 0.65 (d, *J* = 6.9 Hz, 3H). <sup>13</sup>C-NMR (100 MHz, CDCl<sub>3</sub>)  $\delta$  162.3 (d, <sup>1</sup>*J* = 242 Hz), 153.8, 153.6 (d, <sup>3</sup>*J* = 12 Hz), 138.0, 136.7, 132.2, 131.7 (d, <sup>3</sup>*J* = 10 Hz), 123.8, 118.8 (d, <sup>4</sup>*J* = 3 Hz), 114.6, 114.1, 107.1 (d, <sup>2</sup>*J* = 22 Hz), 103.1 (d, <sup>2</sup>*J* = 25 Hz), 71.0, 67.8, 51.6, 47.7, 44.8, 34.6, 27.8, 27.0, 26.6, 25.5, 21.6, 21.0. HPLC: 96.4%, RT 17.52 min. HRMS-ESI (*m/z*): [M+H]<sup>+</sup> calcd for C<sub>25</sub>H<sub>33</sub>FN<sub>3</sub>O<sub>2</sub> 426.2551, found 426.2555.

### (±)-(3*S*,4*S*)-7-Fluoro-3-(2-((3-(6-fluoro-1*H*-benzo[*d*]imidazol-2-yl)propyl)amino)ethyl)-4-isopropylchroman-3-ol (2ac)

The following the same procedure as that used for the synthesis of **2aa**, the reaction of amine **4c** (53.7 mg, 278  $\mu$ mol), sodium cyanoborohydride (8.46 mg, 139  $\mu$ mol), aldehyde **3** (35.9 mg, 139  $\mu$ mol) and acetic acid in MeOH (3 mL) gave amine **2ac** ((15.6 mg, 26%) after purification by column chromatography on silica gel (CH<sub>2</sub>Cl<sub>2</sub>:MeOH:H<sub>2</sub>O:NH<sub>4</sub>OH =

80:20:1:1) as a brown oil;  $^1\text{H-NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.36 (dd,  $J = 4.6, 8.7$  Hz, 1H), 7.16 (dd,  $J = 2.1, 8.9$  Hz, 1H), 6.95-6.89 (m, 2H), 6.57 (td,  $J = 2.5, 8.3$  Hz, 1H), 6.49 (dd,  $J = 2.5, 10.1$  Hz, 1H), 4.10 (d,  $J = 11.0$  Hz, 1H), 3.96 (dd,  $J = 1.5, 11.0$  Hz, 1H), 3.10-3.01 (m, 4H), 2.97 (t,  $J = 6.4$  Hz, 2H), 2.87-2.75 (m, 2H), 2.57 (s, 1H), 2.40-2.33 (m, 1H), 2.04 (t,  $J = 5.9$  Hz, 2H), 1.82 (m, 2H), 1.16 (d,  $J = 6.9$  Hz, 3H), 0.64 (d,  $J = 5.9$  Hz, 3H).  $^{13}\text{C-NMR}$  (100 MHz,  $\text{CDCl}_3$ )  $\delta$  162.3 (d,  $^1J = 243$  Hz), 159.3 (d,  $^1J = 237$  Hz), 155.3 (d,  $^4J = 2$  Hz), 153.5 (d,  $^3J = 11$  Hz), 138.3 (d,  $^3J = 12$  Hz), 134.5, 131.7 (d,  $^3J = 10$  Hz), 118.7 (d,  $^4J = 3$  Hz), 115.1 (d,  $^3J = 10$  Hz), 110.6 (d,  $^2J = 25$  Hz), 107.2 (d,  $^2J = 22$  Hz), 103.2 (d,  $^2J = 24$  Hz), 100.9 (d,  $^2J = 26$  Hz), 70.9, 67.8, 51.4, 47.9, 44.6, 34.8, 27.9, 26.8, 26.2, 25.4, 21.0. HPLC: 96.2%, RT 13.38 min. HRMS-ESI ( $m/z$ ):  $[\text{M}+\text{H}]^+$  calcd for  $\text{C}_{24}\text{H}_{30}\text{F}_2\text{N}_3\text{O}_2$  430.2301, found 430.2303.

**(±)-(3*S*,4*S*)-3-(2-((3-(6-Chloro-1*H*-benzo[*d*]imidazol-2-yl)propyl)amino)ethyl)-7-fluoro-4-isopropylchroman-3-ol (2ad)**

The following the same procedure as that used for the synthesis of **2aa**, the reaction of amine **4d** (31.7 mg, 151  $\mu\text{mol}$ ), sodium triacetoxyborohydride (48.0 mg, 227  $\mu\text{mol}$ ), aldehyde **3** (38.1 mg, 151  $\mu\text{mol}$ ) and acetic acid in MeOH (3 mL) gave the secondary amine **2ad** (17.4 mg, 26%) after purification by column chromatography on silica gel ( $\text{CH}_2\text{Cl}_2:\text{MeOH}:\text{H}_2\text{O}:\text{NH}_4\text{OH} = 80:20:1:1$ ) as a white oil;  $^1\text{H-NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.50 (d,  $J = 1.8$  Hz, 1H), 7.40 (d,  $J = 8.5$  Hz, 1H), 7.16 (dd,  $J = 1.9, 8.5$  Hz, 1H), 6.94 (dd,  $J = 6.6, 8.5$  Hz, 1H), 6.56 (td,  $J = 2.6, 8.3$  Hz, 1H), 6.49 (dd,  $J = 2.6, 10.2$  Hz, 1H) 4.10 (d,  $J = 11.0$  Hz, 1H), 3.94 (dd,  $J = 2.0, 11.0$  Hz, 1H), 2.97-2.94 (m, 4H), 2.73 (m,  $J = 6.1$  Hz, 1H), 2.65 (m,  $J = 6.1$  Hz, 1H), 2.56 (s, 1H), 2.42-2.34 (m, 1H), 2.03-1.99 (m, 2H), 1.74-1.56 (m, 2H), 1.17 (d,  $J = 7.0$  Hz, 3H), 0.66 (d,  $J = 6.9$  Hz, 3H).  $^{13}\text{C-NMR}$  (100 MHz,  $\text{CDCl}_3$ )  $\delta$  162.4 (d,  $^1J = 242$  Hz), 155.2, 153.6 (d,  $^3J = 11$  Hz), 139.2, 137.0, 131.7 (d,  $^3J = 9$  Hz), 127.9, 122.8, 118.8 (d,  $^4J = 3$  Hz), 115.3, 114.7, 107.1 (d,  $^2J = 21$  Hz), 103.2 (d,  $^2J = 24$  Hz), 71.3, 67.9,

51.7, 47.5, 45.1, 34.6, 27.9, 27.1, 26.5, 25.5, 21.0. HPLC: 93.0%, RT 16.65 min. HRMS-ESI ( $m/z$ ):  $[M+H]^+$  calcd for  $C_{24}H_{30}ClFN_3O_2$  446.2005, found 446.2008.

**(±)-(3*S*,4*S*)-3-(2-((3-(6-Bromo-1*H*-benzo[*d*]imidazol-2-yl)propyl)amino)ethyl)-7-fluoro-4-isopropylchroman-3-ol (2ae)**

The following the same procedure as that used for the synthesis of **2aa**, the reaction of amine **4e** (41.5 mg, 143  $\mu$ mol), sodium cyanoborohydride (5.99 mg, 95.2  $\mu$ mol) and aldehyde **3** (24.6 mg, 95.2  $\mu$ mol) in MeOH (2 mL) gave amine **2ae** (6.70 mg, 14%) after purification by column chromatography on silica gel ( $CH_2Cl_2$ :MeOH:H<sub>2</sub>O:NH<sub>4</sub>OH = 80:20:1:1) as a brown oil; <sup>1</sup>H-NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.64 (d,  $J$  = 1.5 Hz, 1H), 7.31-7.24 (m, 2H), 6.95 (dd,  $J$  = 6.5, 8.5 Hz, 1H), 6.58 (td,  $J$  = 2.6, 8.3 Hz, 1H), 6.50 (dd,  $J$  = 2.5, 10.1 Hz, 1H), 4.12 (d,  $J$  = 11.1 Hz, 1H), 3.99 (dd,  $J$  = 1.8, 11.1 Hz, 1H), 3.15-3.01 (m, 2H), 2.97 (t,  $J$  = 6.4 Hz, 2H), 2.92-2.91 (m, 2H), 2.59 (s, 1H), 2.41-2.32 (m, 1H), 2.04 (t,  $J$  = 6.0 Hz, 2H), 1.89 (t,  $J$  = 5.8 Hz, 2H), 1.18 (d,  $J$  = 7.0 Hz, 3H), 0.65 (d,  $J$  = 6.9 Hz, 3H). <sup>13</sup>C-NMR (100 MHz, CDCl<sub>3</sub>)  $\delta$  162.4 (d, <sup>1</sup> $J$  = 243 Hz), 154.3, 153.4 (d, <sup>3</sup> $J$  = 12 Hz), 138.3, 136.0, 131.7 (d, <sup>3</sup> $J$  = 10 Hz), 130.9, 126.0, 118.2 (d, <sup>4</sup> $J$  = 3 Hz), 117.6, 115.9, 107.6 (d, <sup>2</sup> $J$  = 21 Hz), 103.3 (d, <sup>2</sup> $J$  = 24 Hz), 70.2, 67.2, 50.9, 48.1, 43.9, 34.5, 28.1, 26.7, 25.4, 23.4, 21.0. HPLC: 95.2%, RT 13.72 min. HRMS-ESI ( $m/z$ ):  $[M+H]^+$  calcd for  $C_{24}H_{30}BrFN_3O_2$  490.1500, found 490.1501.

**(±)-(3*S*,4*S*)-3-(2-((3-(5,6-Dichloro-1*H*-benzo[*d*]imidazol-2-yl)propyl)amino)ethyl)-7-fluoro-4-isopropylchroman-3-ol (2af)**

The following the same procedure as that used for the synthesis of **2aa**, the reaction of amine **4f** (60.4 mg, 2.47 mmol), sodium cyanoborohydride (20.7 mg, 333  $\mu$ mol), aldehyde **3** (42.6 mg, 165  $\mu$ mol) and acetic acid in MeOH (3 mL) gave amine **2af** (36.6 mg, 46%) after purification by column chromatography on silica gel ( $CH_2Cl_2$ :MeOH:H<sub>2</sub>O:NH<sub>4</sub>OH =

80:20:1:1) as a brown oil;  $^1\text{H-NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.58 (s, 1H), 6.94 (dd,  $J = 6.6, 8.5$  Hz, 1H), 6.56 (td,  $J = 2.6, 8.3$  Hz, 1H), 6.48 (dd,  $J = 2.6, 10.2$  Hz, 1H) 4.08 (d,  $J = 10.9$  Hz, 1H), 3.91 (dd,  $J = 2.0, 11.0$  Hz, 1H), 2.97-2.93 (m, 4H), 2.71 (m,  $J = 6.1$  Hz, 1H), 2.63 (m,  $J = 6.1$  Hz, 1H), 2.54 (s, 1H), 2.38-2.29 (m, 1H), 2.00 (m,  $J = 6.5$  Hz, 2H), 1.68-1.51 (m, 2H), 1.16 (d,  $J = 7.0$  Hz, 3H), 0.64 (d,  $J = 6.9$  Hz, 3H).  $^{13}\text{C-NMR}$  (100 MHz,  $\text{CDCl}_3$ )  $\delta$  162.3 (d,  $^1J = 242$  Hz), 156.5, 153.5 (d,  $^3J = 12$  Hz), 137.8, 131.7 (d,  $^3J = 10$  Hz), 126.1, 118.7 (d,  $^4J = 3$  Hz), 115.9, 107.2 (d,  $^2J = 22$  Hz), 103.2 (d,  $^2J = 24$  Hz), 71.6, 67.9, 51.7, 47.6, 45.2, 34.6, 27.8, 27.4, 26.5, 25.5, 21.0. HPLC: 91.5%, RT 4.31 min. HRMS-ESI ( $m/z$ ):  $[\text{M}+\text{H}]^+$  calcd for  $\text{C}_{24}\text{H}_{29}\text{Cl}_2\text{FN}_3\text{O}_2$  480.1615, found 480.1617.

**(±)-(3S,4S)-7-Fluoro-4-isopropyl-3-(2-((3-(6-nitro-1H-benzo[d]imidazol-2-yl)propyl)amino)ethyl)chroman-3-ol (2ag)**

Acetic acid was added to a solution of amine **4g** (44.3 mg, 171  $\mu\text{mol}$ ) in anhydrous MeOH (3 mL) until pH 6 was reached. To this solution was added sodium cyanoborohydride (10.8 mg, 171  $\mu\text{mol}$ ), aldehyde **3** (43.5 mg, 171  $\mu\text{mol}$ ). After stirring for 3.5 h at room temperature, the reaction mixture was stirred for an additional 5 h at 45 °C. The reaction was monitored by TLC, quenched with saturated aqueous  $\text{NaHCO}_3$  (15 mL) after completion of the reaction and extracted with  $\text{CH}_2\text{Cl}_2$  (3 x 20 mL). The organic layers were washed with brine, dried over anhydrous  $\text{MgSO}_4$  and concentrated under reduced pressure. The resulting residue was purified by flash column chromatography on silica gel ( $\text{CH}_2\text{Cl}_2:\text{MeOH}:\text{H}_2\text{O}:\text{NH}_4\text{OH} = 80:20:1:1$ ) to afford amine **2ag** (17.6 mg, 24%) as a yellow oil;  $^1\text{H-NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.47 (d,  $J = 2.1$  Hz, 1H), 8.13 (dd,  $J = 2.2, 8.9$  Hz, 1H), 7.55 (d,  $J = 8.9$  Hz, 1H), 6.96 (dd,  $J = 6.5, 8.5$  Hz, 1H), 6.57 (td,  $J = 2.6, 8.3$  Hz, 1H), 6.50 (dd,  $J = 2.6, 10.1$  Hz, 1H) 4.13 (d,  $J = 11.0$  Hz, 1H), 3.96 (dd,  $J = 2.0, 11.0$  Hz, 1H), 3.06 (t,  $J = 6.7$  Hz, 2H), 3.03-2.95 (m, 2H) 2.79-2.73 (m, 1H), 2.70-2.64 (m, 1H), 2.59 (d,  $J = 2.1$  Hz, 1H), 2.45-2.37 (m, 1H), 2.09 (m,  $J$

= 6.3 Hz, 2H), 1.70-1.63 (m, 2H), 1.21 (d,  $J = 7.0$  Hz, 3H), 0.69 (d,  $J = 6.9$  Hz, 3H).  $^{13}\text{C}$ -NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  162.4 (d,  $^1J = 243$  Hz), 158.57, 153.5 (d,  $^3J = 12$  Hz), 143.2, 142.4, 138.0, 131.7 (d,  $^3J = 10$  Hz), 118.5 (d,  $^4J = 3$  Hz), 118.2, 114.1, 111.7, 107.4 (d,  $^2J = 21$  Hz), 103.3 (d,  $^2J = 24$  Hz), 71.4, 67.6, 51.5, 47.7, 44.9, 34.5, 28.0, 26.8, 26.1, 25.5, 21.0. HPLC: 98.2%, RT 12.66 min. HRMS-ESI ( $m/z$ ):  $[\text{M}+\text{H}]^+$  calcd for  $\text{C}_{24}\text{H}_{30}\text{FN}_4\text{O}_4$  457.2246, found 457.2246.

**(±)-(3*S*,4*S*)-7-Fluoro-4-isopropyl-3-(2-(isopropyl(3-(6-methyl-1*H*-benzo[*d*]imidazol-2-yl)propyl)amino)ethyl)chroman-3-ol (2cb)**

The following the same procedure as that used for the synthesis of **2ca**, the reaction of amine **2ab** (33.3 mg, 78.3  $\mu\text{mol}$ ), acetic acid (8.96  $\mu\text{L}$ , 156  $\mu\text{mol}$ ), sodium cyanoborohydride (9.84 mg, 156  $\mu\text{mol}$ ) and acetone (23.0  $\mu\text{L}$ , 313  $\mu\text{mol}$ ) in MeOH (1 mL) gave amine **2cb** (36.6 mg, 46%) after purification by column chromatography on silica gel ( $\text{CH}_2\text{Cl}_2:\text{MeOH} = 10:1$ ) as a pale brown oil;  $^1\text{H}$ -NMR (300 MHz,  $\text{CDCl}_3$ )  $\delta$  7.41 (d,  $J = 10.9$  Hz, 1H), 7.30 (s, 1H), 7.03 (d,  $J = 10.9$  Hz, 1H), 6.92 (dd,  $J = 8.9, 11.0$  Hz, 1H), 6.55 (td,  $J = 3.4, 11.1$  Hz, 1H), 6.48 (dd,  $J = 3.3, 13.6$  Hz, 1H), 4.12 (d,  $J = 14.5$  Hz, 1H), 3.93 (dd,  $J = 2.2, 14.6$  Hz, 1H), 3.20 (m, 1H), 2.96-2.89 (m, 2H), 2.75 (t,  $J = 7.6$  Hz, 2H), 2.56-2.45 (m, 2H), 2.45-2.34 (m, 4H), 2.15-2.01 (m, 2H), 1.66-1.60 (m, 2H), 1.16 (d,  $J = 9.3$  Hz, 3H), 1.07 (d,  $J = 8.8$  Hz, 6H), 0.64 (d,  $J = 9.2$  Hz, 3H).  $^{13}\text{C}$ -NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  162.4 (d,  $^1J = 242$  Hz), 154.1, 153.6 (d,  $^3J = 12$  Hz), 138.1, 136.8, 132.1, 131.6 (d,  $^3J = 10$  Hz), 123.7, 118.8 (d,  $^4J = 3$  Hz), 114.5, 114.1, 107.0 (d,  $^2J = 21$  Hz), 103.1 (d,  $^2J = 24$  Hz), 71.1, 68.4, 51.4, 49.8, 48.7, 45.5, 32.2, 27.7, 26.5, 25.6, 25.5, 21.6, 20.9, 17.3, 16.6. HPLC: 95.9%, RT 16.91 min. HRMS-ESI ( $m/z$ ):  $[\text{M}+\text{H}]^+$  calcd for  $\text{C}_{28}\text{H}_{39}\text{FN}_3\text{O}_2$  468.2021, found 468.3024.

**(±)-(3*S*,4*S*)-7-Fluoro-3-(2-((3-(6-fluoro-1*H*-benzo[*d*]imidazol-2-yl)propyl)(isopropyl)amino)ethyl)-4-isopropylchroman-3-ol (2cc)**

The following the same procedure as that used for the synthesis of **2ca**, the reaction of amine **2ac** (46.7 mg, 109  $\mu$ mol), acetic acid (12.5  $\mu$ L, 217  $\mu$ mol), sodium cyanoborohydride (13.7 mg, 217  $\mu$ mol) and acetone (31.9  $\mu$ L, 435  $\mu$ mol) in MeOH (1 mL) gave amine **2cc** (12.7 mg, 25%) after purification by column chromatography on silica gel (CH<sub>2</sub>Cl<sub>2</sub>:MeOH = 10:1) as a pale brown oil; <sup>1</sup>H-NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.45 (s, 1H), 7.22 (d, *J* = 8.12 Hz, 2H), 7.00-6.93 (m, 2H), 6.57 (td, *J* = 2.6, 8.3 Hz, 1H), 6.50 (dd, *J* = 2.5, 10.2 Hz, 1H), 4.15 (d, *J* = 10.9 Hz, 1H), 3.95 (dd, *J* = 1.9, 10.8 Hz, 1H), 3.20 (m, 1H), 2.99-2.85 (m, 2H), 2.72 (t, *J* = 5.6 Hz, 2H), 2.60 (s, 1H), 2.57-2.44 (m, 3H), 2.13-2.00 (m, 2H), 1.66-1.55 (m, 2H), 1.18 (d, *J* = 7.0 Hz, 3H), 1.07 (dd, *J* = 4.3, 6.5 Hz, 6H), 0.67 (d, *J* = 6.9 Hz, 3H). <sup>13</sup>C-NMR (100 MHz, CDCl<sub>3</sub>)  $\delta$  162.4 (d, <sup>1</sup>*J* = 242 Hz), 159.3 (d, <sup>1</sup>*J* = 236 Hz), 155.7, 153.6 (d, <sup>3</sup>*J* = 12 Hz), 138.5, 135.2, 131.5 (d, <sup>3</sup>*J* = 9 Hz), 118.7 (d, <sup>4</sup>*J* = 3 Hz), 114.9, 110.3 (d, <sup>2</sup>*J* = 25 Hz), 107.1 (d, <sup>2</sup>*J* = 22 Hz), 103.1 (d, <sup>2</sup>*J* = 25 Hz), 100.8, 71.6, 68.5, 51.5, 49.2, 48.2, 45.6, 32.1, 27.7, 26.3, 26.1, 25.5, 20.8, 17.4, 16.6. HPLC: 95.5%, RT 15.93 min. HRMS-ESI (*m/z*): [M+H]<sup>+</sup> calcd for C<sub>27</sub>H<sub>36</sub>F<sub>2</sub>N<sub>3</sub>O<sub>2</sub> 472.2770, found 472.2771.

**(±)-(3*S*,4*S*)-3-(2-((3-(6-Chloro-1*H*-benzo[*d*]imidazol-2-yl)propyl)(isopropyl)amino)ethyl)-7-fluoro-4-isopropylchroman-3-ol (2cd)**

The following the same procedure as that used for the synthesis of **2ca**, the reaction of amine **2ad** (29.7 mg, 66.6  $\mu$ mol), acetic acid (7.63  $\mu$ L, 133  $\mu$ mol), sodium cyanoborohydride (8.37 mg, 133  $\mu$ mol) and acetone (19.6  $\mu$ L, 266  $\mu$ mol) in MeOH (1 mL) gave amine **2cd** (4.50 mg, 14%) after purification by column chromatography on silica gel (CH<sub>2</sub>Cl<sub>2</sub>:MeOH = 10:1) as a pale brown oil; <sup>1</sup>H-NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.53 (s, 1H), 7.45 (dd, *J* = 7.2 Hz, 1H), 7.19 (dd, *J* = 1.8, 8.5 Hz, 1H), 6.95 (d, *J* = 6.6, 8.3 Hz, 1H), 6.57 (td, *J* = 2.6, 8.3 Hz, 1H), 6.50

(dd,  $J = 2.6, 10.2$  Hz, 1H), 4.15 (d,  $J = 10.8$  Hz, 1H), 3.95 (dd,  $J = 1.8, 10.9$  Hz, 1H), 3.21 (m, 1H), 2.99-2.86 (m, 2H), 2.73 (t,  $J = 5.5$  Hz, 2H), 2.60 (s, 1H), 2.57-2.40 (m, 3H), 2.15-2.00 (m, 2H), 1.65-1.55(m, 2H), 1.18 (d,  $J = 7.0$  Hz, 3H), 1.07 (dd,  $J = 4.3, 6.5$  Hz, 6H), 0.68 (d,  $J = 6.9$  Hz, 3H).  $^{13}\text{C}$ -NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  162.4 (d,  $^1J = 242$  Hz), 155.5, 153.6 (d,  $^3J = 12$  Hz), 139.4, 137.0, 131.5 (d,  $^3J = 9$  Hz), 127.8, 122.7, 118.6 (d,  $^4J = 2$  Hz), 115.3, 114.7, 107.1 (d,  $^2J = 21$  Hz), 103.1 (d,  $^2J = 24$  Hz), 71.4, 68.4, 51.4, 49.7, 48.4, 45.6, 32.1, 27.7, 26.3, 25.7, 25.5, 20.8, 17.4, 16.6. HPLC: 94.8%, RT 16.74 min. HRMS-ESI ( $m/z$ ):  $[\text{M}+\text{H}]^+$  calcd for  $\text{C}_{27}\text{H}_{36}\text{ClFN}_3\text{O}_2$  488.2475, found 488.2477.

**(±)-(3*S*,4*S*)-3-(2-((3-(6-Bromo-1*H*-benzo[*d*]imidazol-2-yl)propyl)(isopropyl)amino)ethyl)-7-fluoro-4-isopropylchroman-3-ol (2ce)**

The following the same procedure as that used for the synthesis of **2ca**, the reaction of amine **2ae** (63.4 mg, 129  $\mu\text{mol}$ ), acetic acid (14.4  $\mu\text{L}$ , 259  $\mu\text{mol}$ ), sodium cyanoborohydride (16.2 mg, 259  $\mu\text{mol}$ ) and acetone (38.0  $\mu\text{L}$ , 517  $\mu\text{mol}$ ) in MeOH (1.3 mL) gave amine **2ce** (20.2 mg, 29%) after purification by column chromatography on silica gel ( $\text{CH}_2\text{Cl}_2:\text{MeOH} = 10:1$ ) as a brown oil;  $^1\text{H}$ -NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.67 (s, 1H), 7.39 (d,  $J = 8.6$  Hz, 1H), 6.94 (dd,  $J = 6.6, 8.5$  Hz, 1H), 6.56 (td,  $J = 2.6, 8.3$  Hz, 1H), 6.50 (dd,  $J = 2.6, 10.2$  Hz, 1H), 4.13 (d,  $J = 10.8$  Hz, 1H), 3.93 (dd,  $J = 2.0, 10.9$  Hz, 1H), 3.22-3.14 (m, 1H), 2.99-2.86 (m, 2H), 2.72 (t,  $J = 5.6$  Hz, 2H), 2.58-2.48 (m, 3H), 2.45-2.38 (m, 1H), 2.13-1.99 (m, 2H), 1.62-1.58 (m, 2H), 1.16 (d,  $J = 7.0$  Hz, 3H), 1.06 (dd,  $J = 3.9, 6.6$  Hz, 6H), 0.66 (d,  $J = 6.9$  Hz, 3H).  $^{13}\text{C}$ -NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  162.4 (d,  $^1J = 243$  Hz), 155.6, 153.6 (d,  $^3J = 12$  Hz), 140.4, 137.7, 131.5 (d,  $^3J = 10$  Hz), 125.3, 118.7 (d,  $^4J = 3$  Hz), 117.8, 115.7, 115.1, 107.1 (d,  $^2J = 21$  Hz), 103.1 (d,  $^2J = 24$  Hz), 71.7, 68.5, 51.5, 49.0, 48.1, 45.6, 32.1, 27.6, 26.2, 26.1 25.5, 20.8, 17.5, 16.6. HPLC: 95.5%, RT 16.91 min. HRMS-ESI ( $m/z$ ):  $[\text{M}+\text{H}]^+$  calcd for  $\text{C}_{27}\text{H}_{36}\text{BrFN}_3\text{O}_2$  532.1969, found 532.1971.



**(±)-(3*S*,4*S*)-3-(2-((3-(5,6-Dichloro-1*H*-benzo[*d*]imidazol-2-**

**yl)propyl)(isopropylamino)ethyl)-7-fluoro-4-isopropylchroman-3-ol (2cf)**

The following the same procedure as that used for the synthesis of **2ca**, the reaction of amine **2af** (7.20 mg, 15.0  $\mu$ mol), acetic acid (1.72  $\mu$ L, 30.0  $\mu$ mol), sodium cyanoborohydride (1.88 mg, 30.0  $\mu$ mol) and acetone (4.40  $\mu$ L, 60.0  $\mu$ mol) in MeOH (150  $\mu$ L) gave amine **2cf** (3.70 mg, 47%) after purification by column chromatography on silica gel (CH<sub>2</sub>Cl<sub>2</sub> : MeOH = 10 : 1) as a colorless oil; <sup>1</sup>H-NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.60 (s, 1H), 6.94 (dd, *J* = 6.5, 8.4 Hz, 1H), 6.58 (td, *J* = 2.6, 8.3 Hz, 1H), 6.50 (dd, *J* = 2.5, 10.1 Hz, 1H), 4.12 (d, *J* = 10.9 Hz, 1H), 3.91 (dd, *J* = 1.9, 10.9 Hz, 1H), 3.30 (m, *J* = 6.64 Hz, 1H), 3.04-2.92 (m, 2H), 2.84 (t, *J* = 5.7 Hz, 2H), 2.66 (m, 2H), 2.47 (s, 1H), 2.43-2.35 (m, 1H), 2.22-2.07 (m, 2H), 1.70-1.67 (m, 1H), 1.18-1.12 (m, 9H), 0.66 (d, *J* = 6.9 Hz, 3H). <sup>13</sup>C-NMR (150 MHz, CDCl<sub>3</sub>)  $\delta$  162.4 (d, *J* = 243 Hz), 156.8, 153.6 (d, *J* = 12 Hz), 138.0, 131.5 (d, *J* = 9 Hz), 126.0, 118.6 (d, *J* = 3 Hz), 115.9, 107.1 (d, *J* = 22 Hz), 103.1 (d, *J* = 25 Hz), 71.6, 68.4, 51.4, 49.2, 48.2, 45.6, 32.1, 27.7, 26.2, 25.9, 25.4, 20.8, 17.5, 16.5. HPLC: 88.9%, RT 4.97 min. HRMS-ESI (*m/z*): [M+H]<sup>+</sup> calcd for C<sub>27</sub>H<sub>35</sub>Cl<sub>2</sub>FN<sub>3</sub>O<sub>2</sub> 522.2085, found 522.2086.

**(±)-(3*S*,4*S*)-7-Fluoro-4-isopropyl-3-(2-(isopropyl(3-(6-nitro-1*H*-benzo[*d*]imidazol-2-**

**yl)propyl)amino)ethyl)chroman-3-ol (2cg)**

The following the same procedure as that used for the synthesis of **2ca**, the reaction of amine **2ag** (40.2 mg, 88.0  $\mu$ mol), acetic acid (10.1  $\mu$ L, 176  $\mu$ mol), sodium cyanoborohydride (11.7 mg, 176  $\mu$ mol) and acetone (25.9  $\mu$ L, 352  $\mu$ mol) in MeOH (1 mL) gave amine **2cg** (17.1 mg, 39%) after purification by column chromatography on silica gel (CH<sub>2</sub>Cl<sub>2</sub>:MeOH = 10:1) as a yellow oil; <sup>1</sup>H-NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  8.48 (s, 1H), 8.17 (dd, *J* = 2.1, 8.8 Hz, 1H), 7.56 (d, *J* = 8.76 Hz, 1H), 6.96 (d, *J* = 6.7, 8.3 Hz, 1H), 6.57 (td, *J* = 2.5, 8.3 Hz, 1H), 6.51 (dd, *J* =

2.5, 10.1 Hz, 1H), 4.17 (d,  $J = 10.8$  Hz, 1H), 3.95 (dd,  $J = 1.5, 10.8$  Hz, 1H), 3.22 (m, 1H), 3.06-2.92 (m, 2H), 2.75 (t,  $J = 5.3$  Hz, 2H), 2.62-2.49 (m, 3H), 2.47-2.40 (m, 1H), 2.19-2.02 (m, 2H), 1.63 (t,  $J = 4.9$  Hz, 2H), 1.18 (d,  $J = 7.0$  Hz, 3H), 1.08 (dd,  $J = 6.7, 9.1$  Hz, 6H), 0.69 (d,  $J = 6.9$  Hz, 3H).  $^{13}\text{C}$ -NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  162.4 (d,  $^1J = 243$  Hz), 159.3, 153.6 (d,  $^3J = 11$  Hz), 143.4, 142.9, 138.4, 131.5 (d,  $^3J = 9$  Hz), 118.6 (d,  $^4J = 3$  Hz), 118.2, 114.0, 111.9, 107.2 (d,  $^2J = 21$  Hz), 103.2 (d,  $^2J = 24$  Hz), 71.9, 68.6, 51.4, 49.0, 48.1, 45.7, 32.0, 27.7, 26.5, 26.2, 25.5, 20.8, 17.7, 16.4. HPLC: 96.7%, RT 14.98 min. HRMS-ESI ( $m/z$ ):  $[\text{M}+\text{H}]^+$  calcd for  $\text{C}_{27}\text{H}_{36}\text{FN}_4\text{O}_4$  499.2715, found 499.2716.

**( $\pm$ )-(3*S*,4*S*)-7-Fluoro-4-isopropyl-3-(2-((2,2,2-trifluoroethyl)amino)ethyl)chroman-3-ol (24b)**

To a solution of the aldehyde **3** (31.8 mg, 126  $\mu\text{mol}$ ) in dry MeOH (1.5 mL) was sequentially added trifluoroethylamine (28.5 mg, 288  $\mu\text{mol}$ ) and sodium cyanoborohydride (13.6 mg, 216  $\mu\text{mol}$ ) at room temperature. The reaction was allowed to stir for 18 h at the same temperature. The reaction mixture was quenched with  $\text{NaHCO}_3$  (10 mL), extracted with  $\text{CH}_2\text{Cl}_2$  (3 x 15 mL) and washed with brine. The organic layers were dried over anhydrous  $\text{MgSO}_4$  and concentrated *in vacuo*. The resulting residue was purified by flash column chromatography on silica gel ( $\text{CH}_2\text{Cl}_2$ :MeOH = 10:1) to afford amine **24b** (38.8 mg, 80%) as a colorless oil.;  $^1\text{H}$ -NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  6.92 (dd,  $J = 6.6, 8.5$  Hz, 1H), 6.54 (td,  $J = 2.6, 8.4$  Hz, 1H), 6.47 (dd,  $J = 2.6, 10.2$  Hz, 1H), 4.04 (d,  $J = 11.0$  Hz, 1H), 3.87 (dd,  $J = 2.2, 11.1$  Hz, 2H), 3.25-3.12 (m, 2H), 3.05-2.95 (m, 2H), 2.52-2.50 (m, 1H), 2.36-2.27 (m, 1H), 1.68-1.58 (m, 2H), 1.13 (d,  $J = 6.9$  Hz, 3H), 0.61 (d,  $J = 7.0$  Hz, 3H).  $^{13}\text{C}$ -NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  162.3 (d,  $^1J = 242$  Hz), 153.6 (d,  $^3J = 12$  Hz), 131.7 (d,  $^3J = 10$  Hz), 125.0 (q,  $^1J = 277$  Hz), 119.1 (d,  $^4J = 3$  Hz), 107.0 (d,  $^2J = 21$  Hz), 103.1 (d,  $^2J = 24$  Hz), 70.6, 68.0, 51.5, 50.2 (q,  $^2J = 31$  Hz), 45.4, 35.9, 27.9, 25.4, 21.3.

**(±)-(3*S*,4*S*)-3-(2-(Cyclopropyl(3-(5-methyl-1*H*-benzo[*d*]imidazol-2-yl)propyl)amino)ethyl)-7-fluoro-4-isopropylchroman-3-ol (2db)**

The following the same procedure as that used for the synthesis of **2da**, the reaction of amine **24a** (22.9 mg, 78.1  $\mu\text{mol}$ ), acetic acid (8.49  $\mu\text{L}$ , 148  $\mu\text{mol}$ ), sodium cyanoborohydride (9.32 mg, 148  $\mu\text{mol}$ ) and aldehyde **21b** (25.4 mg, 74.2  $\mu\text{mol}$ ) in MeOH (1 mL) gave tertiary amine intermediate;  $^1\text{H-NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.80-7.77 (m, 2H), 7.51 (d,  $J = 8.2$  Hz, 1H), 7.43 (t,  $J = 0.8$  Hz, 1H), 7.29-7.25 (m, 2H), 7.17-7.13 (m, 1H), 6.92 (dd,  $J = 6.6, 8.4$  Hz, 1H), 6.54 (td,  $J = 2.6, 8.3$  Hz, 1H), 6.48 (dd,  $J = 2.6, 10.3$  Hz, 1H), 4.00 (d,  $J = 11.0$  Hz, 1H), 3.90 (dd,  $J = 1.8, 11.0$  Hz, 1H), 3.12(m,  $J = 7.0$  Hz, 1H), 3.00-2.94 (m, 1H), 2.91-2.77 (m, 3H), 2.51 (s, 2H), 2.50 (s, 2H), 2.38 (d,  $J = 4.4$  Hz, 3H), 2.35-2.26 (m, 1H), 2.22-2.12 (m, 2H), 1.83-1.78 (m, 1H), 1.64 (t,  $J = 4.9$  Hz, 2H), 1.11 (d,  $J = 7.0$  Hz, 3H), 0.59 (d,  $J = 7.0$  Hz, 7H).

The reaction of the above tertiary amine (37.6 mg, 61.0  $\mu\text{mol}$ ) and tetrabutylammonium fluoride (607  $\mu\text{mol}$ , 1.0 M solution in THF) in THF (1 mL) gave amine **2db** (16.0 mg, 57%) after purification by column chromatography on silica gel ( $\text{CH}_2\text{Cl}_2:\text{MeOH} = 10:1$ ) as a brown oil;  $^1\text{H-NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.45 (d,  $J = 8.2$  Hz, 1H), 7.33 (s, 1H), 7.02 (dd,  $J = 1.0, 8.2$  Hz, 1H), 6.94 (dd,  $J = 6.6, 8.5$  Hz, 1H), 6.57 (td,  $J = 3.6, 6.9$  Hz, 1H), 6.49 (dd,  $J = 2.6, 10.2$  Hz, 1H), 4.11 (d,  $J = 10.8$  Hz, 1H), 3.93 (dd,  $J = 2.1, 10.8$  Hz, 1H), 2.93-2.83 (m, 4H), 2.65-2.58 (m, 3H), 2.47 (s, 3H), 2.43-2.34 (m, 1H), 2.24-2.11 (m, 2H), 1.68 (m, 1H), 1.57 (t,  $J = 5.7$  Hz, 2H), 1.19 (d,  $J = 7.0$  Hz, 3H), 0.66-0.55 (m, 7H).  $^{13}\text{C-NMR}$  (100 MHz,  $\text{CDCl}_3$ )  $\delta$  162.4 (d,  $^1J = 242$  Hz), 154.1, 153.5 (d,  $^3J = 14$  Hz), 138.2, 137.0, 132.0, 131.6 (d,  $^3J = 10$  Hz), 123.7, 118.8 (d,  $^4J = 3$  Hz), 114.8, 114.3, 107.0 (d,  $^2J = 22$  Hz), 103.1 (d,  $^2J = 25$  Hz), 71.6, 68.3, 54.2, 53.1 51.4, 37.9, 32.2, 27.8, 26.6, 25.5, 25.3, 21.6, 21.0, 6.7, 6.3.

HPLC: 96.1%, RT 19.07 min. HRMS-ESI ( $m/z$ ):  $[M+H]^+$  calcd for  $C_{28}H_{37}FN_3O_2$  466.2864, found 466.2868.

**(±)-(3*S*,4*S*)-2-(7-Fluoro-3-hydroxy-4-isopropylchroman-3-yl)acetaldehyde**      ***O*-(2-(6-methyl-1*H*-benzo[*d*]imidazol-2-yl)ethyl) oxime (2fb)**

The following the same procedure as that used for the synthesis of **2fa**, the reaction of aldehyde **3** (41 mg, 0.16 mmol),  $K_2CO_3$  (34 mg, 0.24 mmol) and *N*-alkoxyamine **5b** (41 mg, 0.18 mmol) in MeOH (1 mL) gave an inseparable mixture of oximes **2fb** (17 mg, 25%, *E/Z* = 1:1) after purification by column chromatography on silica gel (EtOAc:*n*-hexane = 1:1); **isomer A**:  $^1H$ -NMR (400 MHz,  $CDCl_3$ )  $\delta$  7.48 (t,  $J$  = 6.0 Hz, 1H), 7.41-7.45 (m, 1H), 7.30-7.32 (m, 1H), 7.02-7.08 (m, 1H), 6.93-6.98 (m, 1H), 6.49-6.62 (m, 2H), 4.38-4.42 (m, 2H), 4.06 (d,  $J$  = 11.0 Hz, 1H), 3.87 (dd,  $J$  = 2.0, 11.0 Hz, 1H), 3.18-3.30 (m, 2H), 2.58-2.63 (m, 1H), 2.36-2.44 (m, 6H), 1.14 (d,  $J$  = 7.0 Hz, 3H), 0.66 (d,  $J$  = 6.6 Hz, 3H).  $^{13}C$ -NMR (100 MHz,  $CDCl_3$ )  $\delta$  162.4 (d,  $J$  = 243.0 Hz), 153.6, 151.9 149.0, 138.0 (broad), 136.7 (broad), 132.3, 131.7, 123.9, 118.5, 114.6 (broad), 114.2 (broad), 107.5 (d,  $J$  = 21.0 Hz), 103.4 (d,  $J$  = 24.0 Hz), 71.1, 70.4, 68.2, 50.8, 38.5, 29.3, 28.3, 25.1, 21.0. HRMS-ESI ( $m/z$ ):  $[M+H]^+$  calcd for  $C_{24}H_{29}FN_3O_3$  426.2188, found 426.2186; **isomer B**:  $^1H$ -NMR (400 MHz,  $CDCl_3$ )  $\delta$  7.41-7.45 (m, 1H), 7.30-7.32 (m, 1H), 6.93-7.08 (m, 3H), 6.49-6.62 (m, 2H), 4.38-4.42 (m, 2H), 4.13 (d,  $J$  = 11.2 Hz, 1H), 3.92 (dd,  $J$  = 2.0, 11.0 Hz, 1H), 3.18-3.30 (m, 2H), 2.58-2.63 (m, 2H), 2.36-2.44 (m, 5H), 1.17 (d,  $J$  = 7.0 Hz, 3H), 0.68 (d,  $J$  = 6.4 Hz, 3H).  $^{13}C$ -NMR (100 MHz,  $CDCl_3$ )  $\delta$  162.4 (d,  $J$  = 243.0 Hz), 153.5, 152.1, 148.8 138.0 (broad), 136.7 (broad), 132.3, 131.6, 123.9, 118.5, 114.6 (broad), 114.2 (broad), 107.5 (d,  $J$  = 21.0 Hz), 103.3 (d,  $J$  = 24.0 Hz), 71.4, 70.6, 68.7, 51.0, 35.4, 29.3, 28.1, 25.2, 21.0. HPLC (mixture): 88.2%, RT 5.83 min.

**(±)-(3S,4S)-2-(7-Fluoro-3-hydroxy-4-isopropylchroman-3-yl)acetaldehyde**      **O-(2-(6-fluoro-1H-benzo[d]imidazol-2-yl)ethyl) oxime (2fc)**

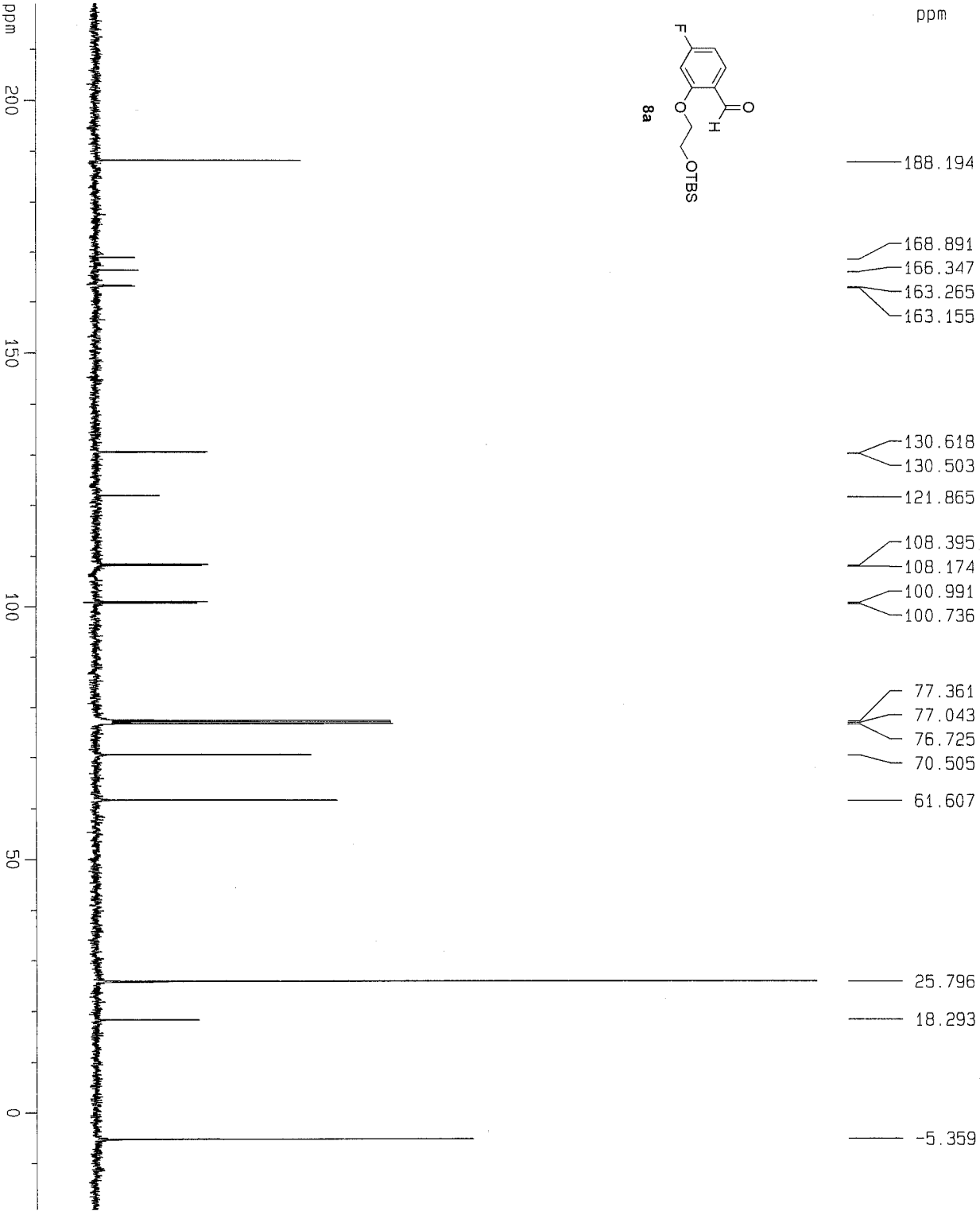
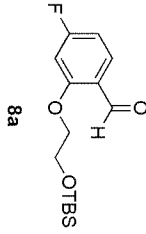
The following the same procedure as that used for the synthesis of **2fa**, the reaction of aldehyde **3** (48 mg, 0.19 mmol), K<sub>2</sub>CO<sub>3</sub> (39 mg, 0.29 mmol) and *N*-alkoxyamine **5c** (52 mg, 0.21 mmol) in MeOH (1 mL) gave an inseparable mixture of oximes **2fc** (17 mg, 21%, *E/Z* = 2:1) after purification by column chromatography on silica gel (EtOAc:*n*-hexane = 1:1); **major isomer**: <sup>1</sup>H-NMR (400 MHz, CDCl<sub>3</sub>) δ 7.46-7.53 (m, 2H), 7.23-7.25 (m, 1H), 6.93-7.02 (m, 2H), 6.51-6.62 (m, 2H), 4.42-4.46 (m, 2H), 4.05 (d, *J* = 11.0 Hz, 1H), 3.88 (dd, *J* = 1.9, 11.0 Hz, 1H), 3.25-3.34 (m, 2H), 2.59-2.63 (m, 1H), 2.31-2.42 (m, 3H), 1.13 (d, *J* = 7.0 Hz, 3H), 0.66 (d, *J* = 7.0 Hz, 3H). <sup>13</sup>C-NMR (100 MHz, CDCl<sub>3</sub>) δ 163.4 (d, *J* = 243.0 Hz), 159.6 (d, *J* = 237.0 Hz), 153.4 (broad), 149.2, 137.5 (broad), 133.8 (broad), 131.7, 131.6, 118.4, 115.2 (broad), 111.3 (d, *J* = 25.0 Hz), 107.6 (d, *J* = 21.0 Hz), 103.4 (d, *J* = 24.0 Hz), 101.0 (d, *J* = 26.0 Hz), 70.8, 70.5, 68.2, 50.8, 38.5, 29.1, 28.3, 25.1, 21.0. HRMS-ESI (*m/z*): [M+H]<sup>+</sup> calcd for C<sub>23</sub>H<sub>26</sub>F<sub>2</sub>N<sub>3</sub>O<sub>3</sub> 430.1937, found 430.1933; **minor isomer**: <sup>1</sup>H-NMR (400 MHz, CDCl<sub>3</sub>) δ 7.46-7.53 (m, 1H), 7.23-7.25 (m, 1H), 6.93-7.02 (m, 3H), 6.51-6.62 (m, 2H), 4.42-4.46 (m, 2H), 4.12 (d, *J* = 9.8 Hz, 1H), 3.90-3.93 (m, 1H), 3.25-3.34 (m, 2H), 2.59-2.63 (m, 3H), 2.31-2.42 (m, 1H), 1.16 (d, *J* = 7.0 Hz, 3H), 0.67 (d, *J* = 7.0 Hz, 3H). <sup>13</sup>C-NMR (100 MHz, CDCl<sub>3</sub>) δ 163.5 (d, *J* = 243.0 Hz), 159.6 (d, *J* = 237.0 Hz), 153.4 (broad), 148.7, 137.5 (broad), 133.8 (broad), 131.7, 131.6, 118.4, 115.2 (broad), 111.23 (d, *J* = 26.0 Hz), 107.6 (d, *J* = 19.0 Hz), 103.4 (d, *J* = 24.0 Hz), 101.0 (d, *J* = 26.0 Hz), 71.1, 70.9, 68.5, 51.0, 35.4, 29.4, 28.2, 25.2, 21.0. HPLC (mixture): 86.9%, RT 3.52 min.

**(±)-(3S,4S)-2-(7-Fluoro-3-hydroxy-4-isopropylchroman-3-yl)acetaldehyde**      **O-(2-(6-chloro-1H-benzo[d]imidazol-2-yl)ethyl) oxime (2fd)**

The following the same procedure as that used for the synthesis of **2fa**, the reaction of

aldehyde **3** (48 mg, 0.19 mmol), K<sub>2</sub>CO<sub>3</sub> and *N*-alkoxyamine **5d** (52 mg, 0.21 mmol) in MeOH (1 mL) gave the inseparable mixture of oximes **2fd** (18 mg, 21%, *E/Z* = 2:1) after purification by column chromatography on silica gel (EtOAc:*n*-hexane = 1:1); *major isomer*: <sup>1</sup>H-NMR (400 MHz, CDCl<sub>3</sub>) δ 7.4-7.53 (m, 2H), 7.41-7.43 (m, 1H), 7.16-7.19 (m, 1H), 6.93-6.97 (m, 1H), 6.52-6.63 (m, 2H), 4.40-4.44 (m, 2H), 4.07 (d, *J* = 11.4 Hz, 1H), 3.86 (dd, *J* = 1.9, 10.9 Hz, 1H), 3.22-3.32 (m, 2H), 2.58 (s, 1H), 2.04-2.41 (m, 3H), 1.11 (d, *J* = 5.0 Hz, 3H), 0.66 (d, *J* = 6.5 Hz, 3H). <sup>13</sup>C-NMR (100 MHz, CDCl<sub>3</sub>) δ 162.4 (d, *J* = 243.0 Hz), 153.5 (broad), 149.0, 139.0 (broad), 137.0 (broad), 131.7 (d, *J* = 100.0 Hz), 128.1, 122.0, 118.4, 115.6 (broad), 114.7 (broad), 107.6 (d, *J* = 21.0 Hz), 103.4 (d, *J* = 24.0 Hz), 70.9, 70.6, 68.2, 50.8, 38.5, 29.4, 28.3, 25.1, 21.0. HRMS-ESI (*m/z*): [M+H]<sup>+</sup> calcd for C<sub>23</sub>H<sub>26</sub>ClFN<sub>3</sub>O<sub>3</sub> 446.1641, found 446.1638; *minor isomer*: <sup>1</sup>H-NMR (400 MHz, CDCl<sub>3</sub>) δ 7.4-7.53 (m, 2H), 7.41-7.43 (m, 1H), 7.16-7.19 (m, 1H), 6.93-6.97 (m, 1H), 6.52-6.63 (m, 2H), 4.40-4.44 (m, 2H), 4.12 (d, *J* = 9.9 Hz, 1H), 3.91 (dd, *J* = 1.9, 10.9 Hz, 1H), 3.22-3.32 (m, 2H), 2.60-2.62 (m, 3H), 2.04-2.41 (m, 1H), 1.15 (d, *J* = 5.9 Hz, 3H), 0.68 (d, *J* = 6.8 Hz, 3H). <sup>13</sup>C-NMR (100 MHz, CDCl<sub>3</sub>) δ 163.4 (d, *J* = 242.0 Hz), 153.5 (broad), 148.6, 139.0 (broad), 137.0 (broad), 131.7 (d, *J* = 100.0 Hz), 128.0, 122.0, 118.4, 115.6 (broad), 114.7 (broad), 107.7 (d, *J* = 21.0 Hz), 103.4 (d, *J* = 24.0 Hz), 71.2, 70.9, 68.5, 51.0, 35.4, 29.3, 28.2, 25.2, 20.9. HPLC (mixture): 86.3%, RT 6.40 min.





Current Data Parameters  
 NAME KTH-m-56  
 EXPNO 2  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20110519  
 Time 13.51

INSTRUM spect  
 PROBHD 5 mm Dual 13C/  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3

DS 0  
 SMH 23980.814 Hz  
 FIDRES 0.365918 Hz  
 AQ 1.3664756 sec

RG 128  
 DW 20.850 usec  
 DE 6.00 usec  
 TE 297.4 K

D1 2.00000000 sec  
 d11 0.03000000 sec  
 DELTA 1.89999998 sec  
 MCREST 0.00000000 sec  
 MCMRK 0.01500000 sec

==== CHANNEL f1 =====  
 NUC1 13C  
 P1 8.60 usec  
 PL1 4.00 dB  
 SFO1 100.628298 MHz

==== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUC2 1H  
 PCPD2 80.00 usec  
 PL2 1.40 dB  
 PL12 18.90 dB  
 PL13 22.63 dB  
 SFO2 400.1316005 MHz

F2 - Processing parameters  
 SI 32768  
 SF 100.6127690 MHz  
 WDM EM  
 SSB 0  
 LB 3.00 Hz  
 GB 0  
 PC 1.40

1D NMR plot parameters  
 CX 20.00 cm  
 CY 12.00 cm  
 F1P 220.000 ppm  
 F1 22134.81 Hz  
 F2P -20.000 ppm  
 F2 -2012.26 Hz  
 PPMQCM 12.00000 ppm/cm  
 HZCM 1207.35327 Hz/cm

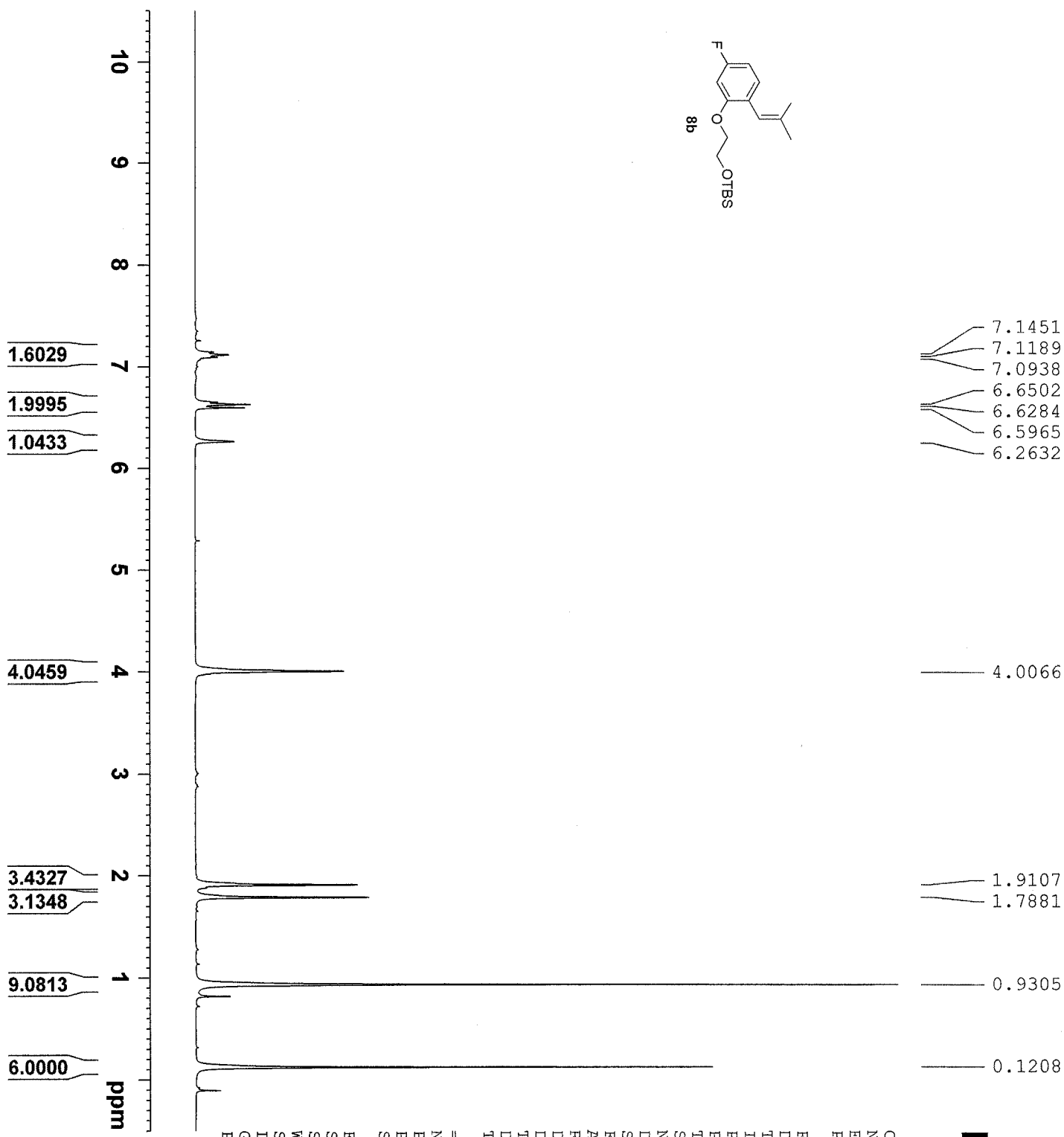
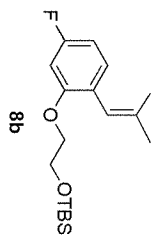


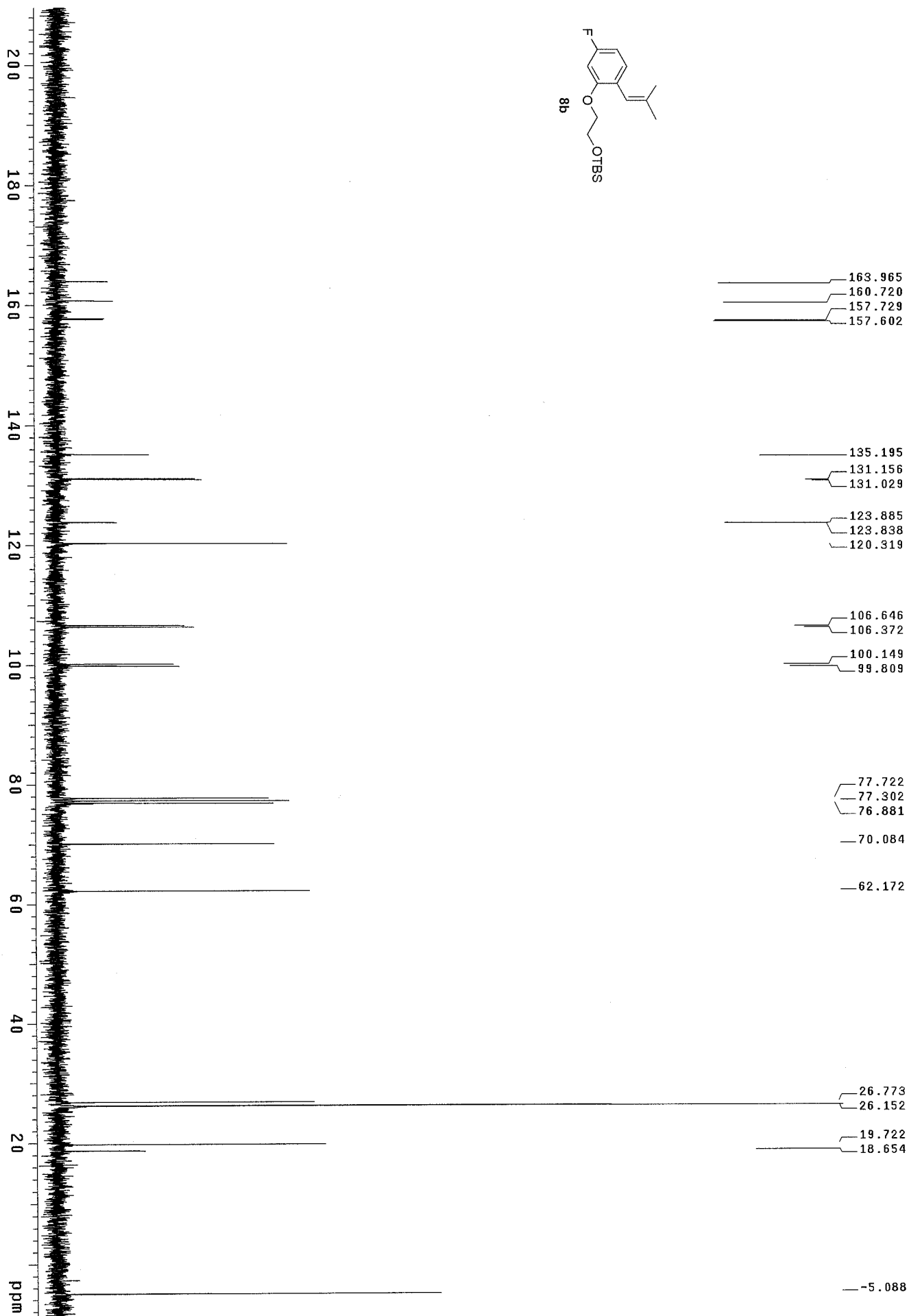


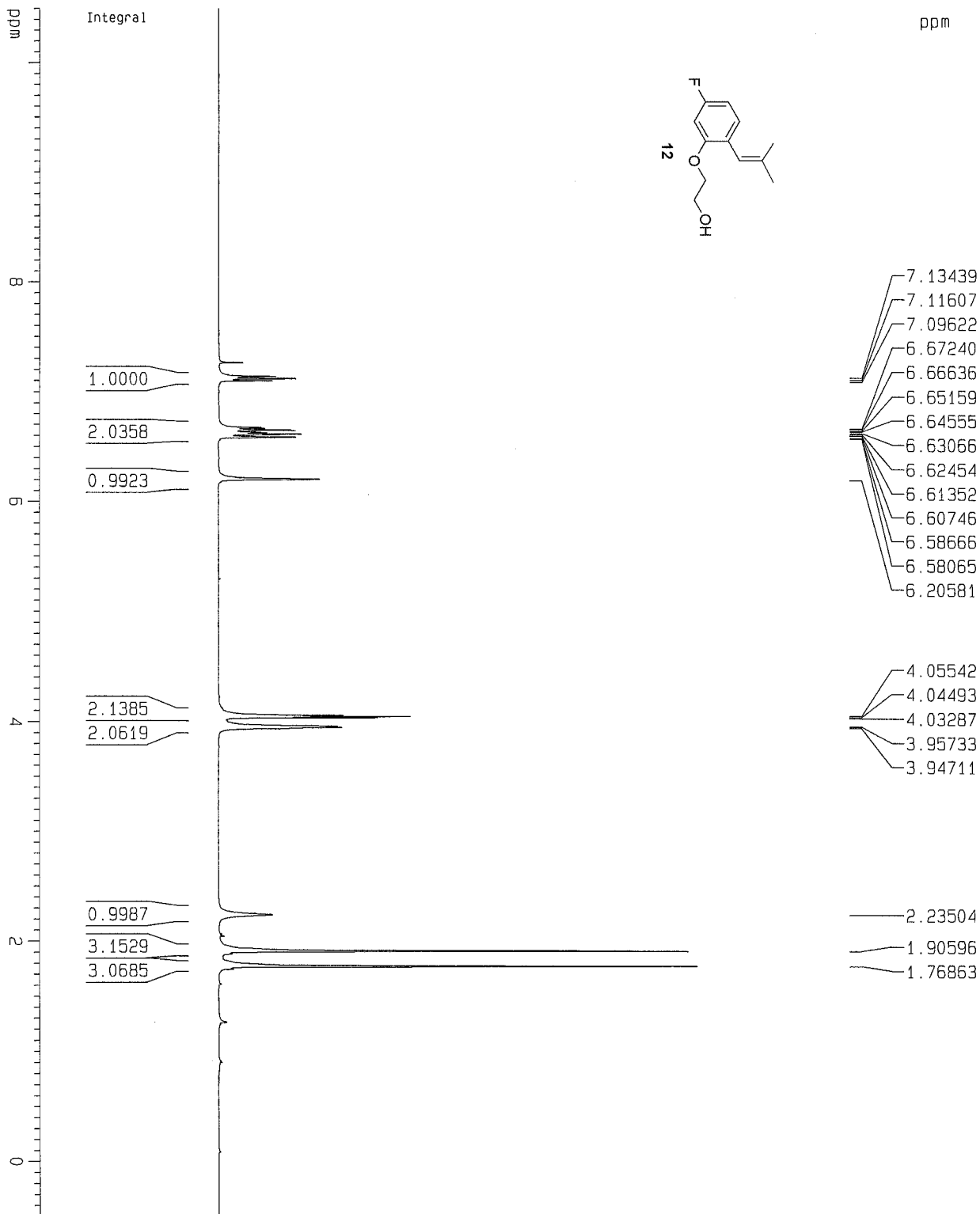
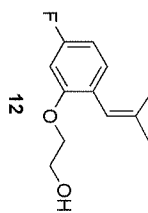
Current Data Parameters  
 NAME KTH-m-11  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20110307  
 Time 22.01  
 INSTRUM spect  
 PROBHD 5 mm DUL 1H-13  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 8  
 DS 1  
 SWH 6172.839 Hz  
 FIDRES 0.094190 Hz  
 AQ 5.3084660 sec  
 RG 50.8  
 DW 81.000 usec  
 DE 6.00 usec  
 TE 300.0 K  
 D1 1.00000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 NUC1 1H  
 P1 10.50 usec  
 PL1 -1.00 dB  
 SFO1 300.1318534 MHz  
 F2 - Processing parameters  
 SI 32768  
 SF 300.1300074 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00







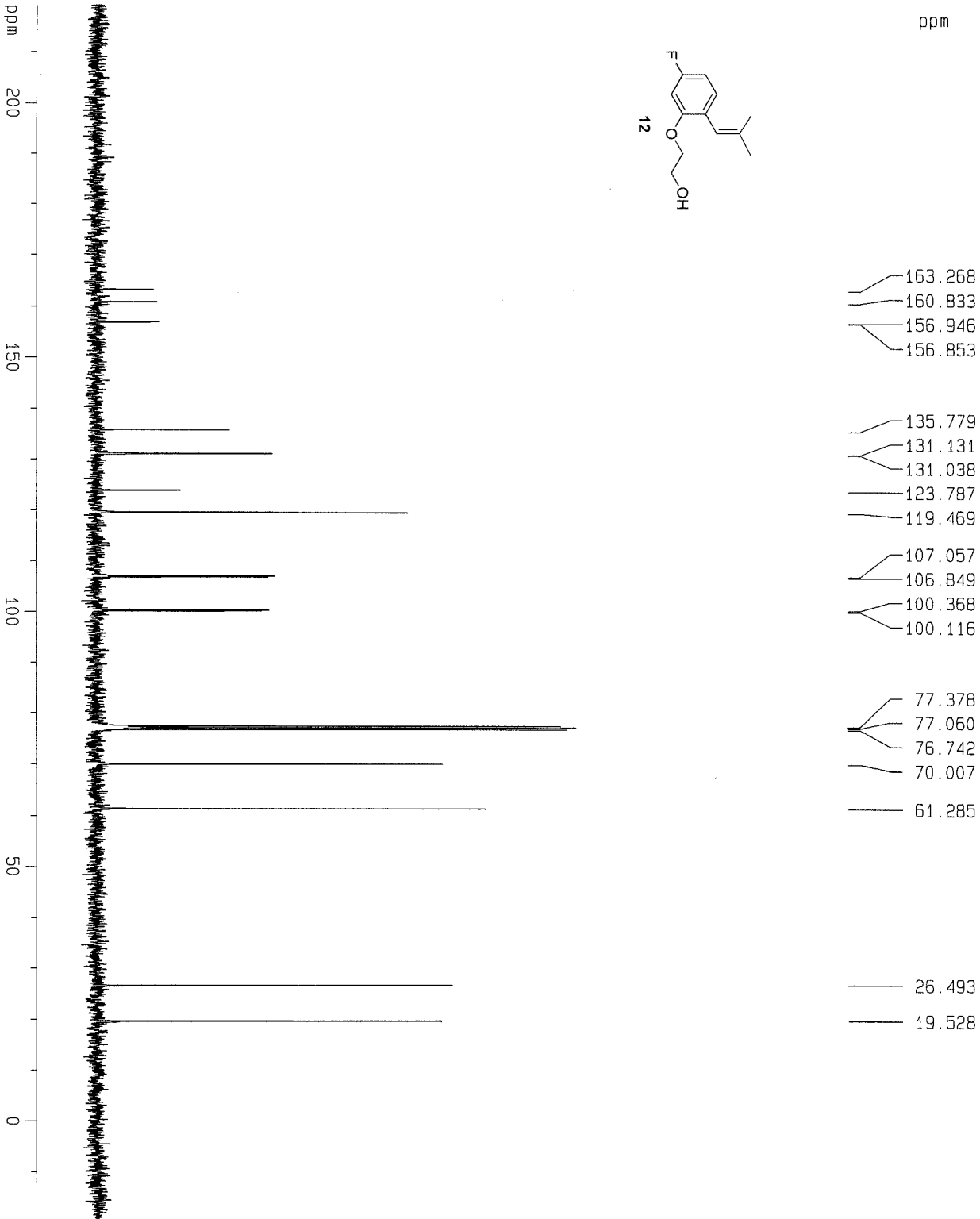
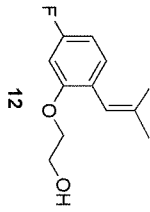
Current Data Parameters  
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 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20110308  
 Time 21.58  
 INSTRUM spect  
 PROBHD 5 mm Dual 13C/  
 PULPROG zg30  
 TD 65536  
 SOLVENT MeOD  
 NS 16  
 DS 0  
 SMH 8278.146 Hz  
 FIDRES 0.126314 Hz  
 AQ 3.9584243 sec  
 RG 45.3  
 DW 50.400 usec  
 DE 6.00 usec  
 TE 296.7 K  
 D1 1.00000000 sec  
 MCREST 0.00000000 sec  
 MCWRR 0.01500000 sec

==== CHANNEL f1 =====  
 NUC1 1H  
 P1 11.50 usec  
 PL1 1.40 dB  
 SF01 400.1324710 MHz

F2 - Processing parameters  
 SI 32768  
 SF 400.1300094 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

1D NMR plot parameters  
 CX 20.00 cm  
 CY 8.00 cm  
 F1P 10.500 ppm  
 F1 4201.37 Hz  
 F2P -0.500 ppm  
 F2 -200.06 Hz  
 PPMCM 0.55000 ppm/cm  
 HZCM 220.07150 Hz/cm



- 163.268
- 160.833
- 156.946
- 156.853
- 135.779
- 131.131
- 131.038
- 123.787
- 119.469
- 107.057
- 106.849
- 100.368
- 100.116
- 77.378
- 77.060
- 76.742
- 70.007
- 61.285
- 26.493
- 19.528

Current Data Parameters  
 NAME KTH-m-11  
 EXPNO 2  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20110308  
 Time 22.02

INSTRUM spect  
 PROBD 5 mm Dui1 13C/  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT DMS  
 NS 68  
 DS 0  
 SMH 23980.814 Hz  
 FIDRES 0.365918 Hz  
 AQ 1.3664756 sec  
 RG 128  
 DW 20.850 usec  
 DE 6.00 usec  
 TE 297.3 K

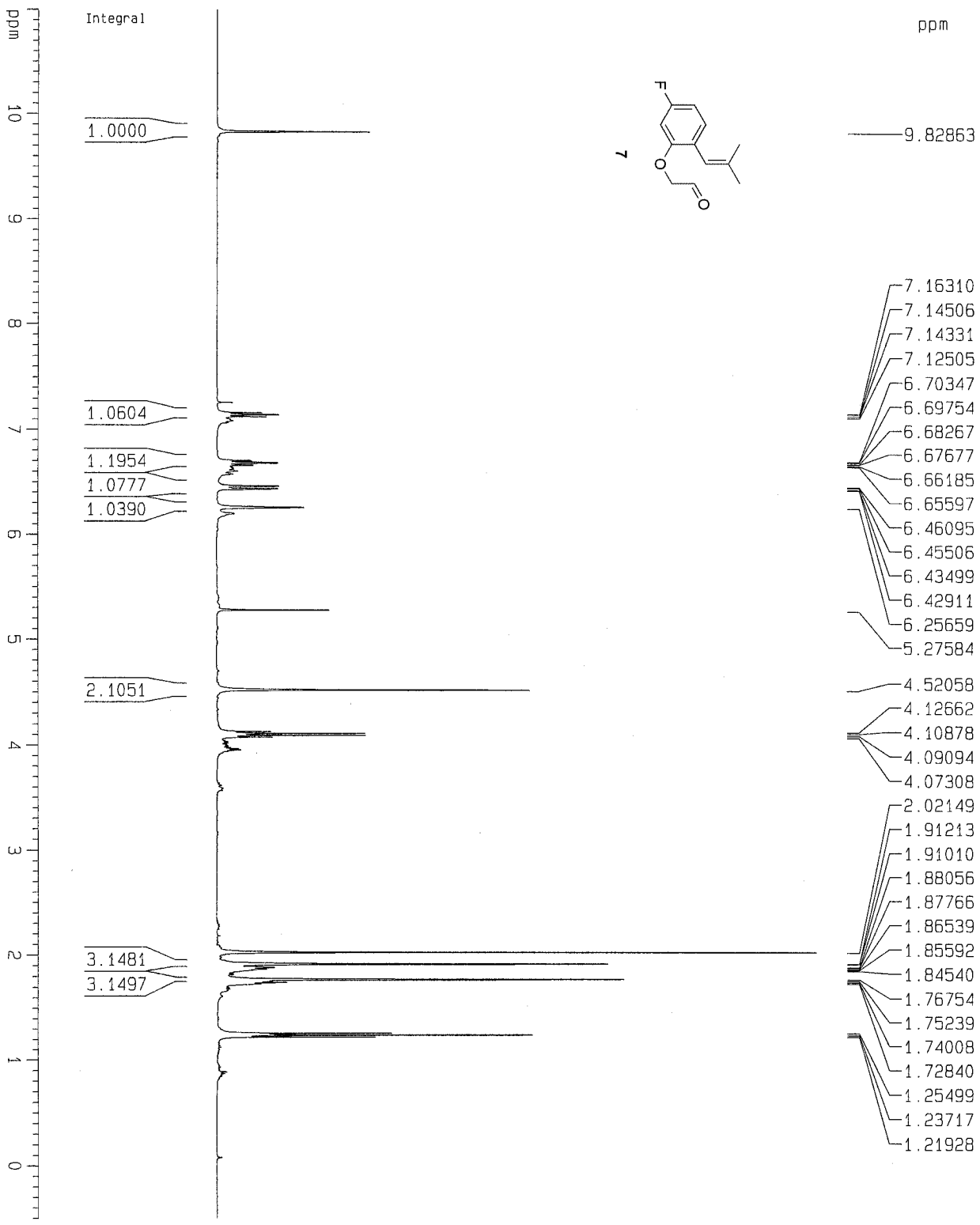
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 d11 0.03000000 sec  
 DELTA 1.89999998 sec  
 MCREST 0.00000000 sec  
 MCMRK 0.01500000 sec

==== CHANNEL f1 =====  
 NUC1 13C  
 P1 8.60 usec  
 PL1 4.00 dB  
 SF01 100.6282828 MHz

==== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUC2 1H  
 PCPD2 80.00 usec  
 PL2 1.40 dB  
 PL12 18.90 dB  
 PL13 22.63 dB  
 SF02 400.1316005 MHz

F2 - Processing parameters  
 SI 32768  
 SF 100.6127690 MHz  
 WDM EM  
 SSB 0  
 LB 3.00 Hz  
 GB 0  
 PC 1.40

1D NMR plot parameters  
 CX 20.00 cm  
 CY 8.00 cm  
 F1p 219.169 ppm  
 F1 23051.21 Hz  
 F2p -19.179 ppm  
 F2 -1929.61 Hz  
 PPMCM 11.91738 ppm/cm  
 HZCM 1199.04077 Hz/cm



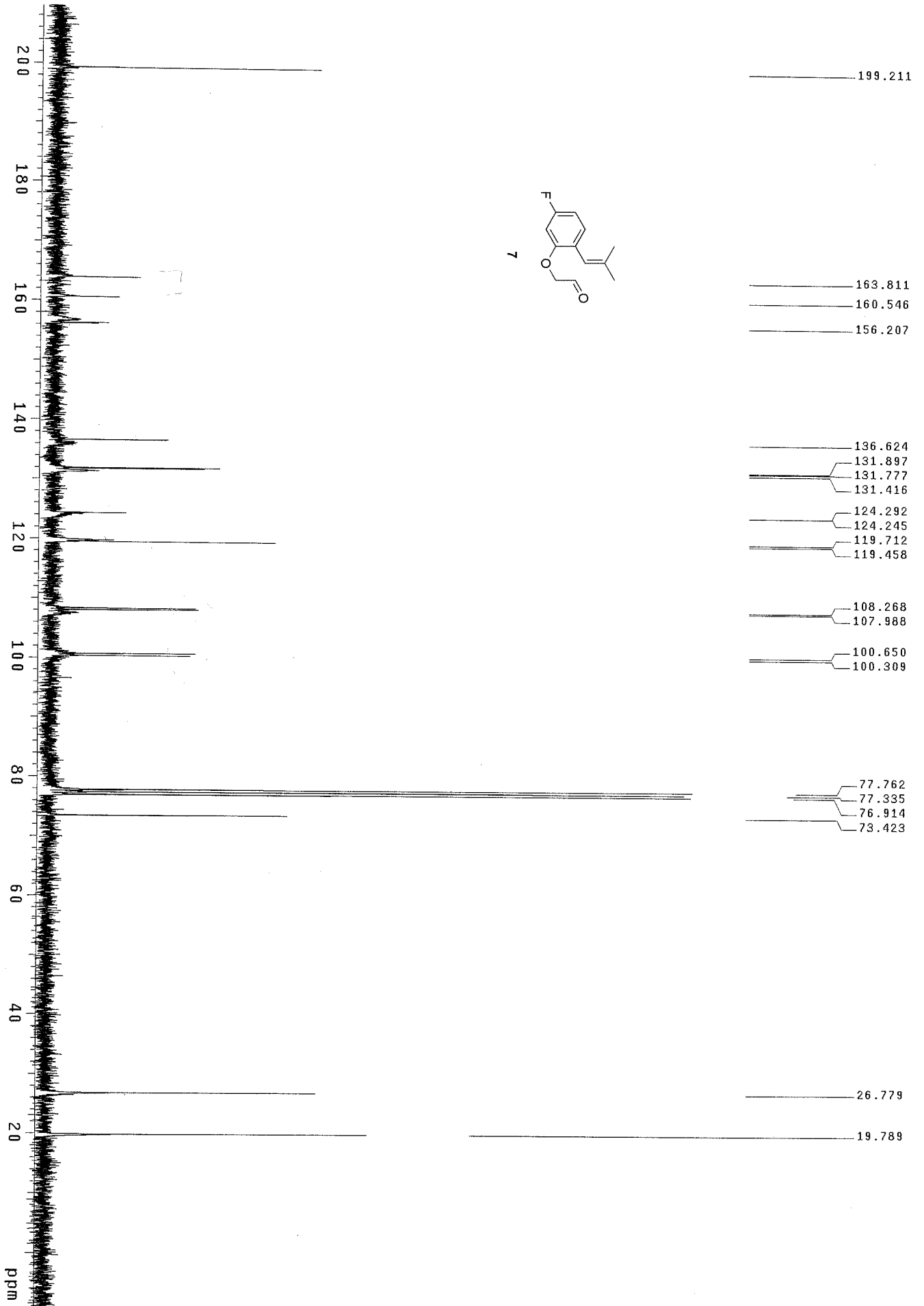
Current Data Parameters  
 NAME KTH-m-16  
 EXPNO 1  
 PROCNO 1

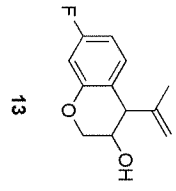
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 Date\_ 20110315  
 Time 21.31  
 INSTRUM spect  
 PROBD 5 mm Dual 13C/  
 PULPROG zg30  
 TD 65536  
 SOLVENT MeOD  
 NS 8  
 DS 0  
 SWH 8278.145 Hz  
 FIDRES 0.126314 Hz  
 AQ 3.9584243 sec  
 RG 45.3  
 DW 60.400 usec  
 DE 6.00 usec  
 TE 296.9 K  
 D1 1.00000000 sec  
 MCREST 0.00000000 sec  
 MCMRK 0.01500000 sec

==== CHANNEL f1 =====  
 NUC1 1H  
 P1 11.50 usec  
 PL1 1.40 dB  
 SF01 400.1324710 MHz

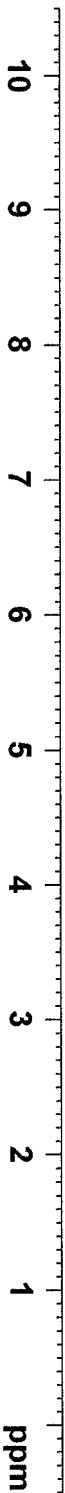
F2 - Processing parameters  
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 SF 400.1300094 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

1D NMR plot parameters  
 CX 20.00 cm  
 CY 10.00 cm  
 F1P 11.000 ppm  
 F1 4401.43 Hz  
 F2P -0.500 ppm  
 F2 -200.07 Hz  
 PPMCM 0.57500 ppm/cm  
 HZCM 230.07475 Hz/cm





- 7.2588
- 7.0637
- 7.0396
- 7.0372
- 7.0137
- 6.9865
- 6.9641
- 6.9609
- 6.9364
- 6.6594
- 6.6507
- 6.6445
- 6.6324
- 6.6227
- 6.6171
- 6.6072
- 6.5936
- 6.5847
- 6.5809
- 6.5740
- 6.5655
- 6.5596
- 6.5511
- 5.2977
- 5.2958
- 5.2260
- 5.2215
- 5.1299
- 5.1255
- 4.8564
- 4.8544
- 4.8292
- 4.8269
- 4.3071
- 4.2914
- 4.2861
- 4.2770
- 4.2707
- 4.2514
- 4.2424
- 4.1276
- 4.1223
- 4.1065
- 4.1024
- 4.0956
- 4.0637
- 4.0608
- 4.0581
- 4.0492
- 4.0403
- 4.0256
- 4.0165
- 4.0032
- 3.9947
- 3.9571
- 3.9332
- 3.9224
- 3.8984
- 3.7281
- 3.7145
- 3.4272
- 3.4060
- 1.8835
- 1.7012



Current Data Parameters  
 NAME KTH-m-36  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20110402  
 Time 19.29  
 INSTRUM spect  
 PROBHD 5 mm DUL 1H-13  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 16  
 DS 2  
 SWH 6172.839 Hz  
 FIDRES 0.094190 Hz  
 AQ 5.3084660 sec  
 RG 724.1  
 DW 81.000 usec  
 DE 6.00 usec  
 TE 300.0 K  
 D1 1.00000000 sec  
 TD0 1

==== CHANNEL f1 =====  
 NUC1 1H  
 P1 10.50 usec  
 PL1 -1.00 dB  
 SFO1 300.1318534 MHz  
 F2 - Processing parameters  
 SI 32768  
 SF 300.1300128 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



Current Data Parameters  
 NAME 2011-03-17  
 EXXNO 2  
 PROCNO 1

F2 - Acquisition Parameters

Date\_ 20110317  
 Time\_ 12.44  
 INSTRUM spect  
 PROBHD 5 mm QNP 1H/1  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDC13  
 NS 420  
 DS 4  
 SMH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3632196 sec  
 RG 32768  
 DW 20.800 usec  
 DE 6.00 usec  
 TE 298.2 K  
 D1 2.00000000 sec  
 d11 0.03000000 sec  
 DELTA 1.89999998 sec  
 TDO 1

==== CHANNEL F1 =====

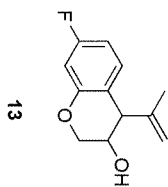
NUC1 13C  
 P1 7.50 usec  
 PL1 1.00 dB  
 SFO1 100.6228298 MHz

==== CHANNEL F2 =====

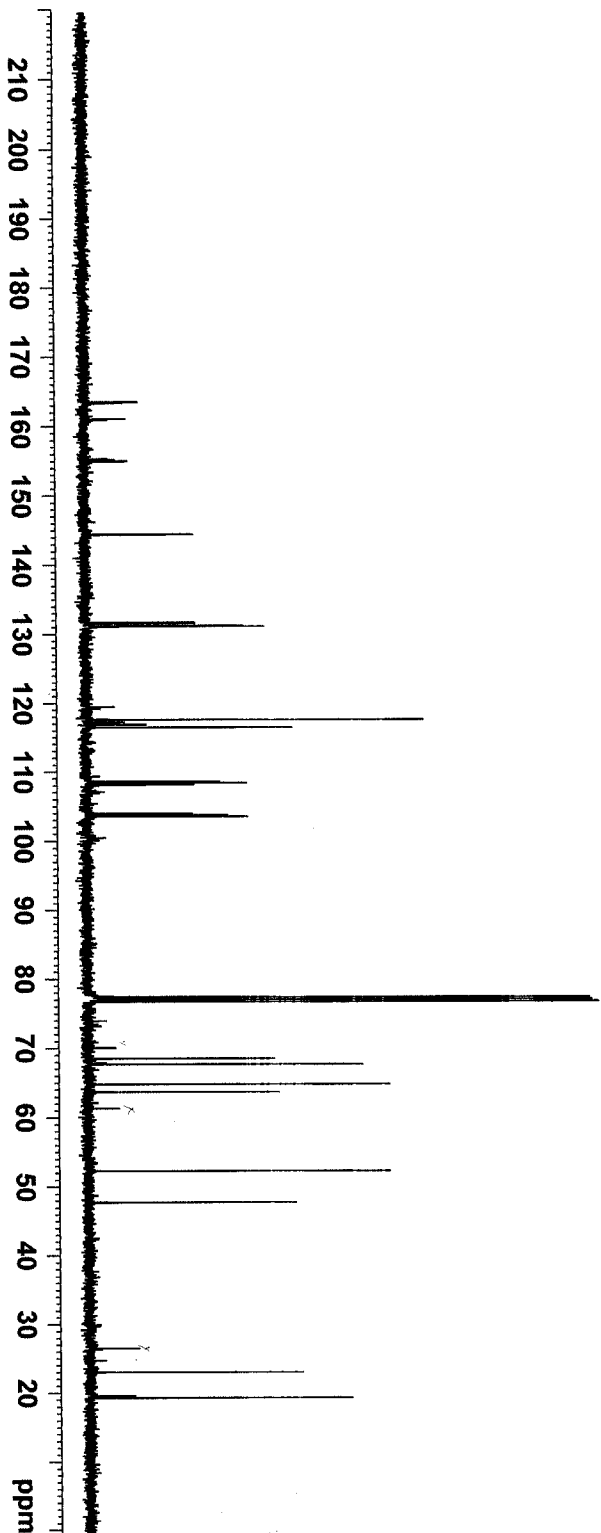
CPDPRG2 waltz16  
 NUC2 1H  
 PCPD2 100.00 usec  
 PL2 -2.00 dB  
 PL12 17.41 dB  
 PL13 21.00 dB  
 SFO2 400.1316005 MHz

F2 - Processing parameters

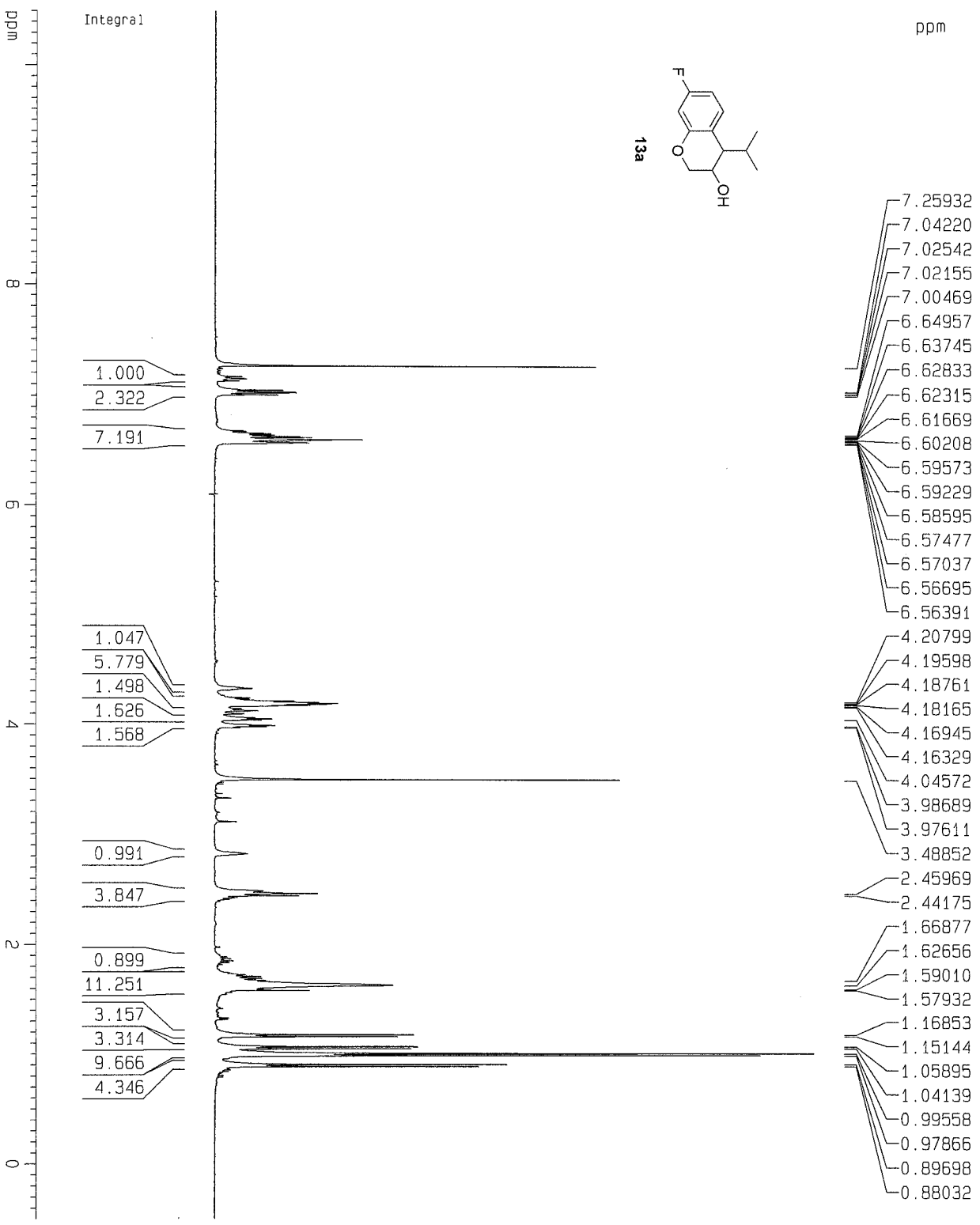
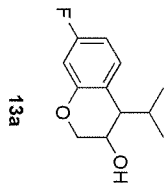
SI 32768  
 SF 100.6127690 MHz  
 WDM EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40



163.502
163.342
161.070
160.912
155.364
155.242
155.074
154.956
144.455
144.371
131.683
131.588
131.232
131.136
119.453
117.596
117.208
116.904
116.875
116.461
108.581
108.366
108.324
108.110
103.962
103.747
103.722
103.503
77.357
77.040
76.722
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67.661
64.754
63.672
52.259
47.746
26.471
22.963
19.515
19.261







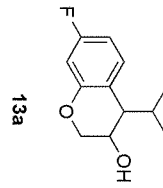
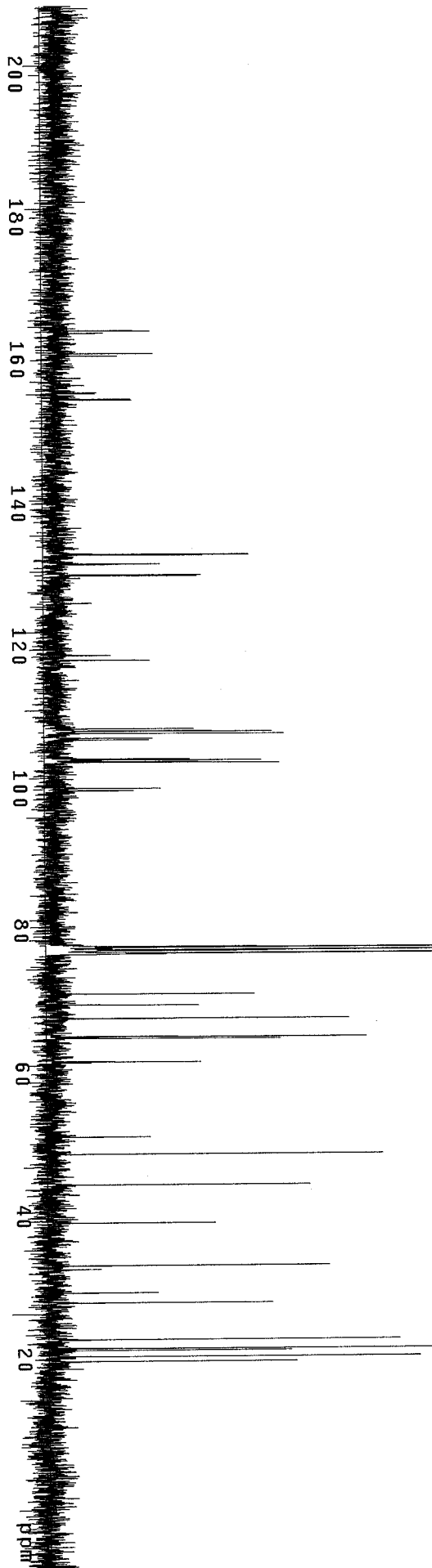
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 EXPNO 2  
 PROCNO 1

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 Date\_ 20110604  
 Time 16.07  
 INSTRUM spect  
 PROBHD 5 mm Dual 13C/  
 PULPROG zg30  
 TD 65536  
 SOLVENT MeOD  
 NS 16  
 DS 0  
 SWH 8278.146 Hz  
 FIDRES 0.126314 Hz  
 AQ 3.9584243 sec  
 RG 322.5  
 DW 60.400 usec  
 DE 6.00 usec  
 TE 296.7 K  
 D1 1.00000000 sec  
 MCREST 0.00000000 sec  
 MCWPRK 0.01500000 sec

===== CHANNEL f1 =====  
 NUC1 1H  
 P1 11.50 usec  
 PL1 1.40 dB  
 SF01 400.1324710 MHz

F2 - Processing parameters  
 SI 32768  
 SF 400.1300096 MHz  
 MDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

1D NMR plot parameters  
 CX 20.00 cm  
 CY 10.00 cm  
 F1P 10.500 ppm  
 F1 4201.37 Hz  
 F2P -0.500 ppm  
 F2 -200.06 Hz  
 PPMTCM 0.55000 ppm/cm  
 HZCM 220.07150 Hz/cm



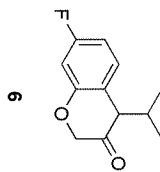
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129.900
118.016
117.976
111.005
108.455
108.175
108.101
107.814
107.153
106.879
104.202
104.068
103.881
103.748
100.082
99.749
77.742
77.315
76.894
74.658
71.213
69.684
67.781
65.237
65.010
61.752
51.156
48.732
46.869
44.439
39.298
39.111
35.272
33.069
31.974
29.283
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26.319
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22.213
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20.416
19.722
14.321
-1.009



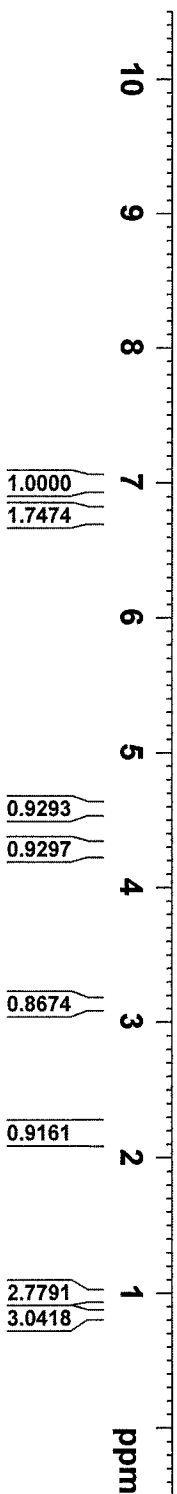
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 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20110318  
 Time 20.15  
 INSTRUM spect  
 PROBHD 5 mm DUL IH-13  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 16  
 DS 2  
 SWH 6172.839 Hz  
 FIDRES 0.094190 Hz  
 AQ 5.3084660 sec  
 RG 287.4  
 DW 81.000 usec  
 DE 6.00 usec  
 TE 300.0 K  
 D1 1.00000000 sec  
 TD0 1

==== CHANNEL f1 =====  
 NUC1 1H  
 P1 10.50 usec  
 PL1 -1.00 dB  
 SFO1 300.1318534 MHz  
 F2 - Processing parameters  
 SI 32768  
 SF 300.1300142 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



- 7.2534
- 7.0222
- 7.0013
- 6.9918
- 6.9710
- 6.7966
- 6.7881
- 6.7804
- 6.7726
- 6.7663
- 6.7599
- 6.7489
- 6.7410
- 6.7383
- 4.6081
- 4.5478
- 4.3051
- 4.3009
- 4.2449
- 4.2406
- 3.1470
- 3.1222
- 2.2617
- 2.2445
- 2.2217
- 2.1987
- 2.1754
- 2.1523
- 2.1295
- 0.9942
- 0.9715
- 0.8479
- 0.8254





Current Data Parameters  
 NAME KTH-m-23  
 EXPNO 2  
 PROCNO 1

F2 - Acquisition Parameters

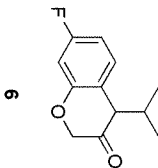
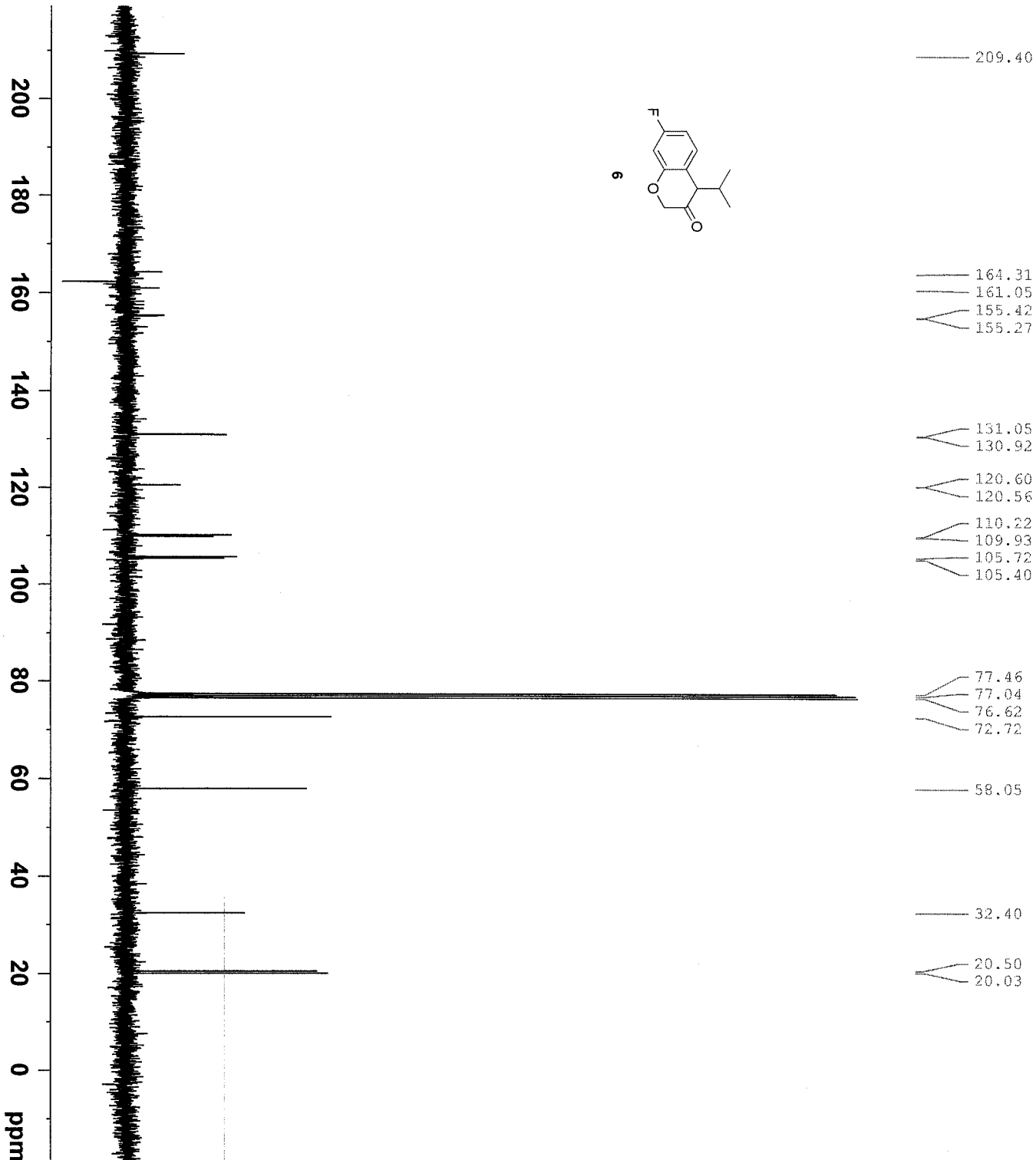
Date\_ 20110318  
 Time 20.20  
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 PROBHD 5 mm DUL 1H-13  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 130  
 DS 4  
 SWH 17985.611 Hz  
 FIDRES 0.274439 Hz  
 AQ 1.8219508 sec  
 RG 32768  
 DW 27.800 usec  
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 TE 300.0 K  
 D1 2.00000000 sec  
 d11 0.03000000 sec  
 DELTA 1.89999998 sec  
 TD0 1

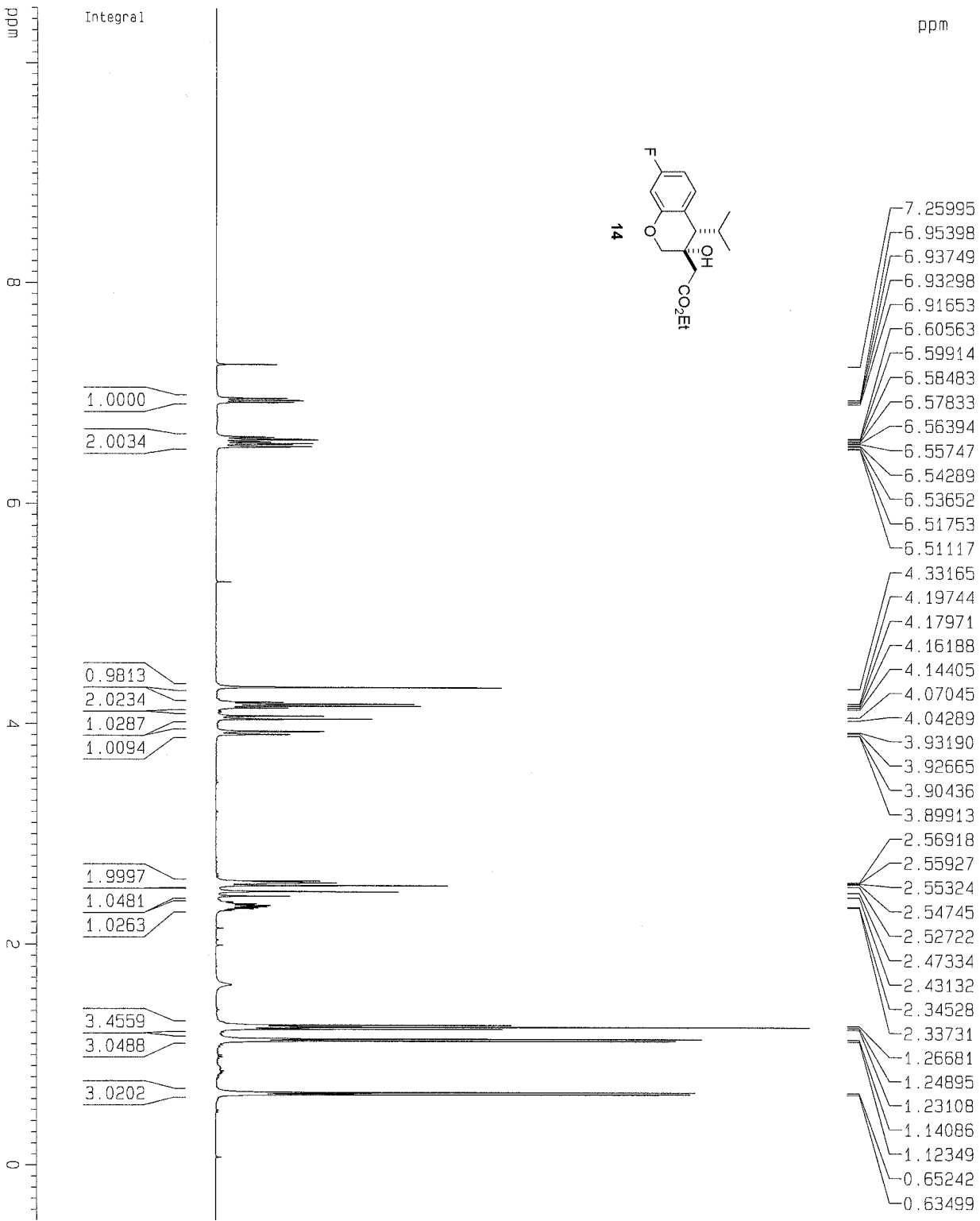
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 P1 10.00 usec  
 PL1 0.00 dB  
 SFO1 75.4752953 MHz

==== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUC2 1H  
 PCPD2 100.00 usec  
 PI2 0.00 dB  
 PL12 20.00 dB  
 PL13 22.00 dB  
 SFO2 300.1312005 MHz

F2 - Processing parameters

SI 32768  
 SF 75.4677490 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40





Current Data Parameters  
NAME KTH-m-105  
EXPNO 1  
PROCNO 1

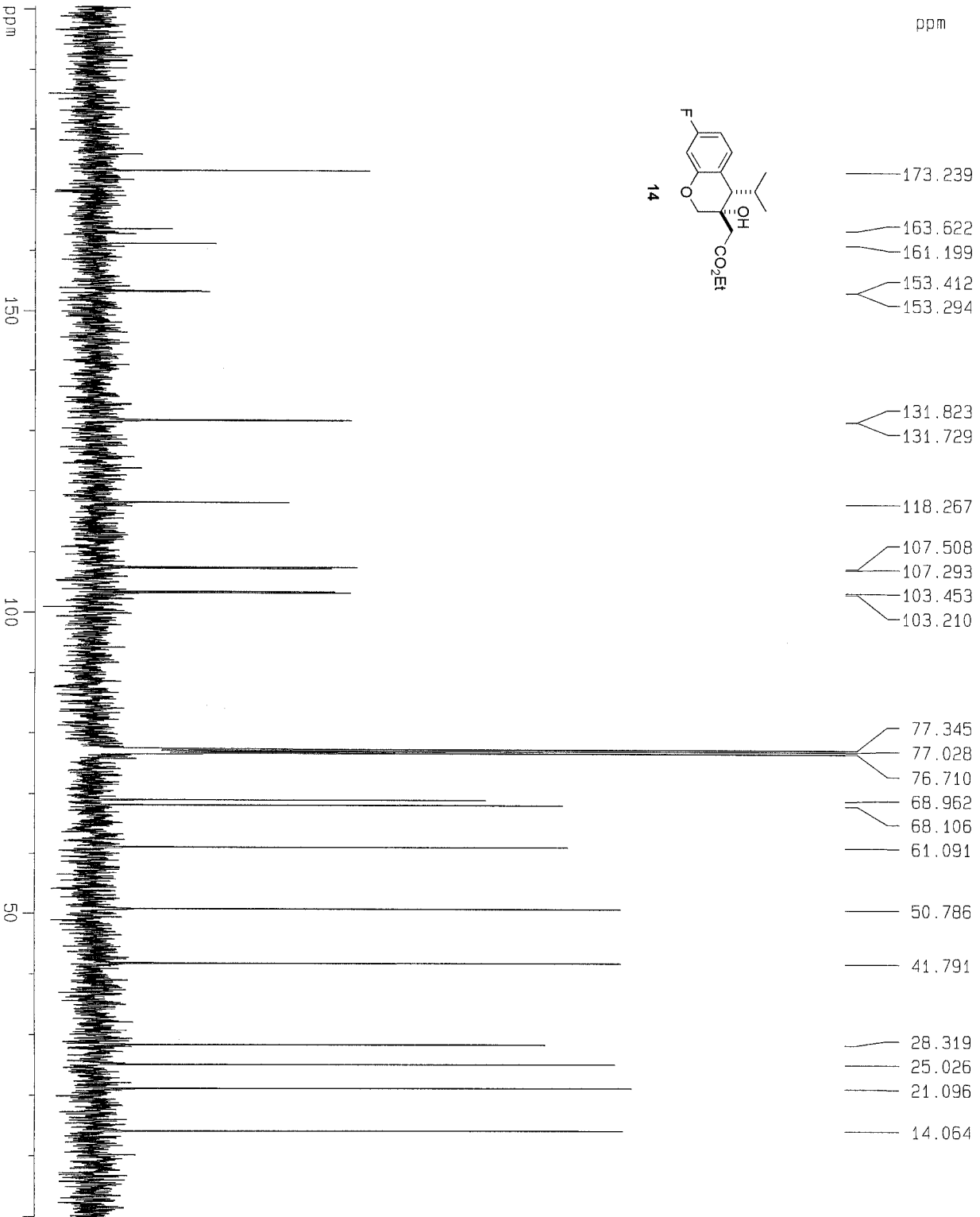
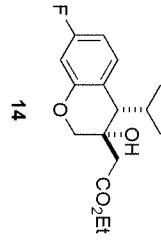
F2 - Acquisition Parameters  
Date\_ 20110903  
Time 15:28  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zg30  
ID 65536  
SOLVENT MeOD  
NS 16  
DS 0  
SWH 8278.146 Hz  
FIDRES 0.126314 Hz  
AQ 3.9584243 sec  
RG 71.8  
DM 60.400 usec  
DE 6.00 usec  
TE 297.3 K  
D1 1.00000000 sec  
d11 0.03000000 sec  
DELTA 0.89999998 sec  
MGREST 0.00000000 sec  
MCRRK 0.01500000 sec

==== CHANNEL f1 =====  
NUC1 1H  
P1 11.50 usec  
PL1 1.40 dB  
SF01 400.1324710 MHz

==== CHANNEL f2 =====  
CPDPRG2 off  
NUC2  
PCPD2 80.00 usec  
PL2 120.00 dB  
PL12 120.00 dB  
PL13 120.00 dB  
SF02 400.1324710 MHz

F2 - Processing parameters  
SI 32768  
SF 400.1300094 MHz  
NDM EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

1D NMR Plot Parameters  
CX 20.00 cm  
CY 10.00 cm  
F1P 10.500 ppm  
F1 4201.37 Hz  
F2P -0.500 ppm  
F2 -200.06 Hz  
PPMCM 0.55000 ppm/cm  
HZCM 220.07150 Hz/cm



Current Data Parameters  
 NAME KTH-m-105  
 EXPNO 1  
 PROCNO 2

F2 - Acquisition Parameters  
 Date\_ 20110903  
 Time 15.28

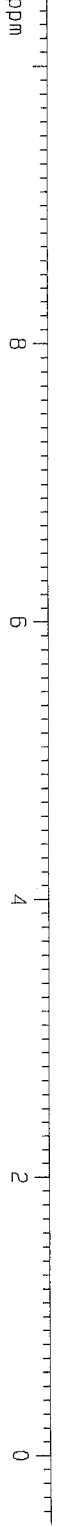
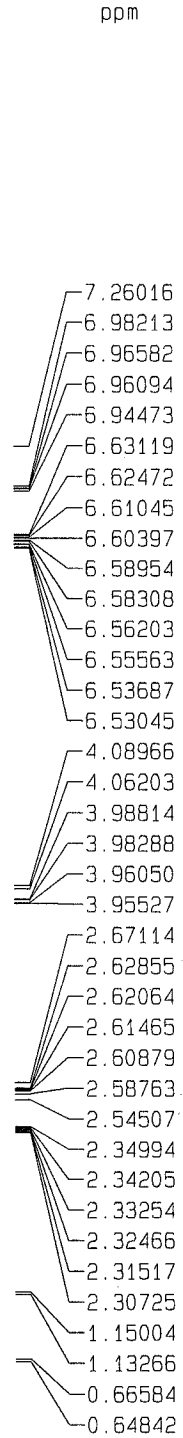
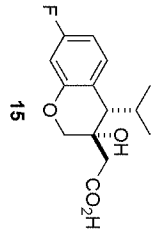
INSTRUM spect  
 PROBHD 5 mm DUL 13C-1  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 84  
 DS 0  
 SWH 23980.814 Hz  
 FIDRES 0.365918 Hz  
 AQ 1.3664756 sec  
 RG 128  
 DW 20.850 usec  
 DE 6.00 usec  
 TE 297.6 K  
 D1 2.00000000 sec  
 d11 0.03000000 sec  
 DELTA 1.89999998 sec  
 MCREST 0.00000000 sec  
 MCPRK 0.01500000 sec

==== CHANNEL f1 =====  
 NUC1 13C  
 P1 8.60 usec  
 PL1 4.00 dB  
 SFO1 100.628298 MHz

==== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUC2 1H  
 PCPD2 80.00 usec  
 PL2 1.40 dB  
 PL12 18.90 dB  
 PL13 22.63 dB  
 SFO2 400.1316005 MHz

F2 - Processing parameters  
 SI 32768  
 SF 100.6127690 MHz  
 WDW EM  
 SSB 0  
 LB 3.00 Hz  
 GB 0  
 PC 1.40

1D NMR Plot Parameters  
 CX 20.00 cm  
 CY 30.00 cm  
 F1P 200.500 ppm  
 F1 20172.86 Hz  
 F2P -0.500 ppm  
 F2 -50.31 Hz  
 PPMCM 10.05000 ppm/cm  
 HZCM 1011.15833 Hz/cm



```

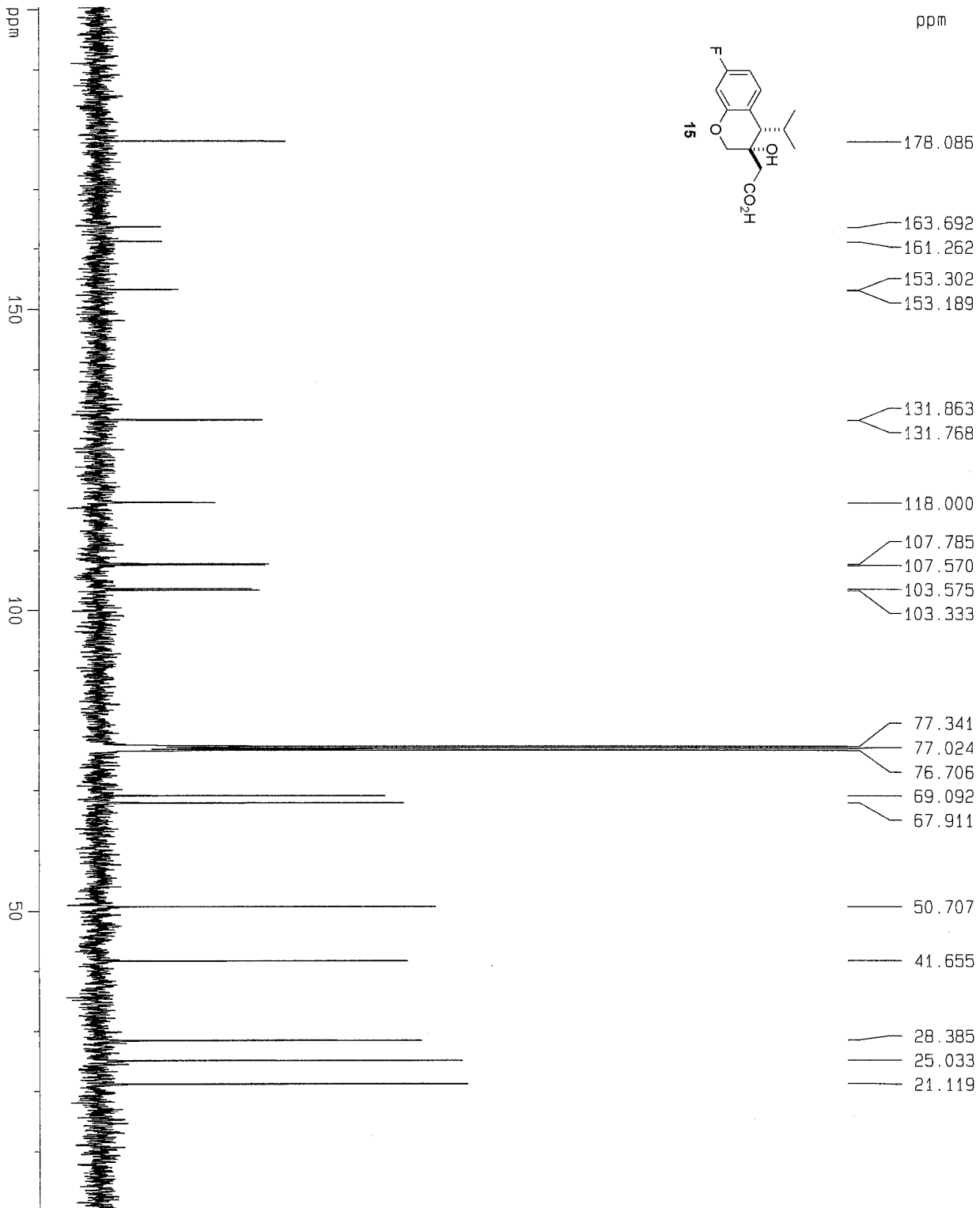
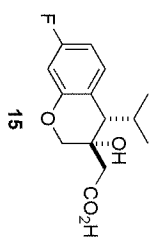
Current Data Parameters
NAME          KTH-m-57
EXPNO        1
PROCNO       1

F2 - Acquisition Parameters
Date_        20110519
Time         17.11
INSTRUM     spect
PROBHD      5 mm Dual 13C/
PULPROG     zg30
TD          65536
SOLVENT     MeOD
NS          16
DS          0
SMH         8278.146 Hz
FIDRES      0.126314 Hz
AQ          3.9584243 sec
RG          161.3
DM          60.400 usec
DE          5.00 usec
TE          297.2 K
D1          1.00000000 sec
MCREST      0.00000000 sec
MCMRK       0.01500000 sec

===== CHANNEL f1 =====
NUC1        1H
P1          11.50 usec
PL1         1.40 dB
SFO1        400.1382710 MHz

F2 - Processing parameters
SI          32768
SF          400.1300094 MHz
WDW         EM
SSB         0
LB          0.30 Hz
GB          0
PC          1.00

1D NMR plot parameters
CX          20.00 cm
CY          6.00 cm
F1P        10.500 ppm
F1         4201.37 Hz
F2P        -0.500 ppm
F2         -200.05 Hz
PPMCM      0.55000 ppm/cm
HZCM       220.07150 Hz/cm
  
```



- 178.086
- 163.692
- 161.262
- 153.302
- 153.189
- 131.863
- 131.768
- 118.000
- 107.785
- 107.570
- 103.575
- 103.333
- 77.341
- 77.024
- 76.706
- 69.092
- 67.911
- 50.707
- 41.655
- 28.385
- 25.033
- 21.119

```

Current Data Parameters
NAME          KTH-m-57
EXPNO        2
PROCNO       1

F2 - Acquisition Parameters
Date_        20110519
Time         17.13
INSTRUM     spect
PROBHD      5 mm Dual 13C/
PULPROG     zgpg30
TD          65536
SOLVENT     CDCl3
NS          149
DS          0
SMH         23980.814 Hz
FIDRES      0.365918 Hz
AQ          1.3664756 sec
RG          128
DE          20.850 usec
TE          297.5 K
D1          2.00000000 sec
d11         0.03000000 sec
DELTA       1.89999998 sec
MCREST      0.00000000 sec
MCMRK       0.01500000 sec

===== CHANNEL f1 =====
NUC1         13C
P1           8.60 usec
PL1          4.00 dB
SF01        100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG2     waltz16
NUC2         1H
PCPD2       80.00 usec
PL2         1.40 dB
PL12        18.90 dB
PL13        22.63 dB
SF02        400.1316005 MHz

F2 - Processing parameters
SI           32768
SF          100.6127690 MHz
WDW          EK
SSB          0
LB           3.00 Hz
GB           0
PC           1.40

1D NMR plot parameters
CX          20.00 cm
CY          20.00 cm
F1P         200.500 ppm
F1          20172.86 Hz
F2P         -0.500 ppm
F2          -50.31 Hz
PWCMD      10.05000 ppm/cm
HZCMD      1011.15833 Hz/cm
  
```

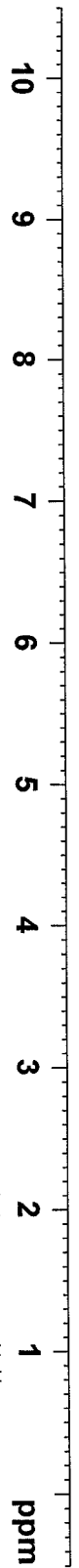
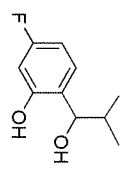




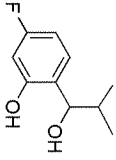
Current Data Parameters  
 NAME LJE-201  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20120713  
 Time\_ 19.30  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDC13  
 NS 16  
 DS 2  
 SWH 8223.685 Hz  
 FIDRES 0.125483 Hz  
 AQ 3.9846387 sec  
 RG 33.2  
 DW 60.800 usec  
 DE 6.50 usec  
 TE 298.0 K  
 D1 1.00000000 sec  
 TD0 1

==== CHANNEL F1 =====  
 NUC1 1H  
 P1 15.00 usec  
 PL1 12.00000000 W  
 SFO1 400.2124715 MHz  
 F2 - Processing parameters  
 SI 65536  
 SF 400.2100129 MHz  
 WDM EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



- 8.4480
- 6.8387
- 6.8223
- 6.8179
- 6.8016
- 6.5573
- 6.5511
- 6.5352
- 6.5314
- 6.5291
- 6.5253
- 6.5145
- 6.5081
- 6.4938
- 6.4874
- 4.4857
- 4.4682
- 3.0768
- 2.1008
- 2.0837
- 2.0667
- 2.0497
- 2.0327
- 2.0158
- 1.9988
- 1.9819
- 1.0270
- 1.0103
- 0.8393
- 0.8223



164.16  
161.73  
157.08  
156.96

129.14  
129.04  
121.99  
121.96

106.32  
106.11  
104.52  
104.28

81.46  
77.37  
77.05  
76.73

34.46

19.08  
18.10



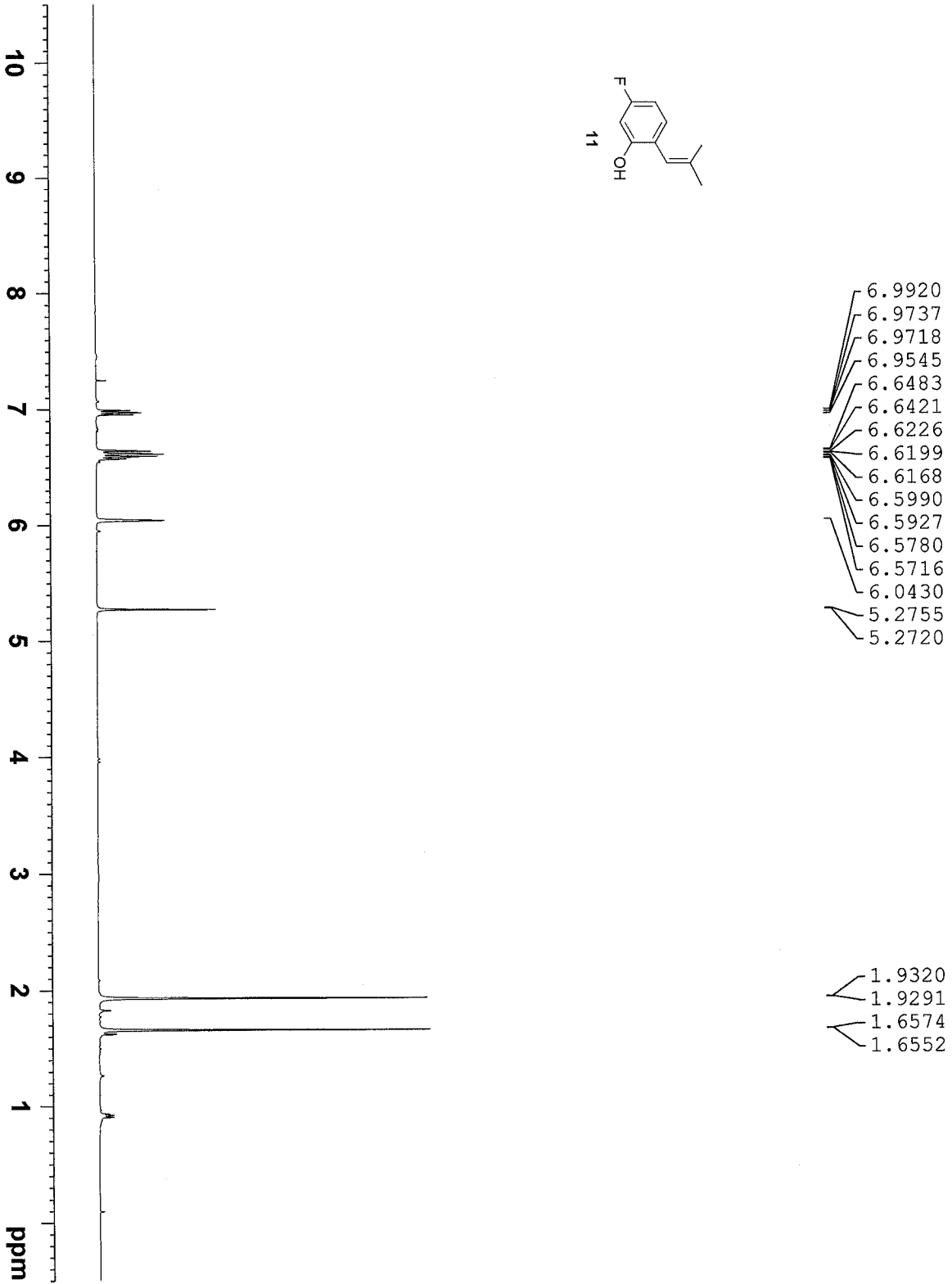
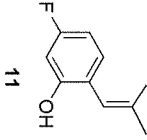
Current Data Parameters  
NAME LJE-201  
EXPNO 2  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20120713  
Time 19.31  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 35  
DS 4  
SWH 24038.461 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631988 sec  
RG 190.62  
DW 20.800 usec  
DE 6.50 usec  
TE 298.3 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

==== CHANNEL f1 =====  
NUC1 13C  
P1 10.00 usec  
PLW1 52.00000000 W  
SFO1 100.6429474 MHz

==== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 90.00 usec  
PLW2 12.00000000 W  
PLW12 0.33333001 W  
PLW13 0.27000001 W  
SFO2 400.2116008 MHz

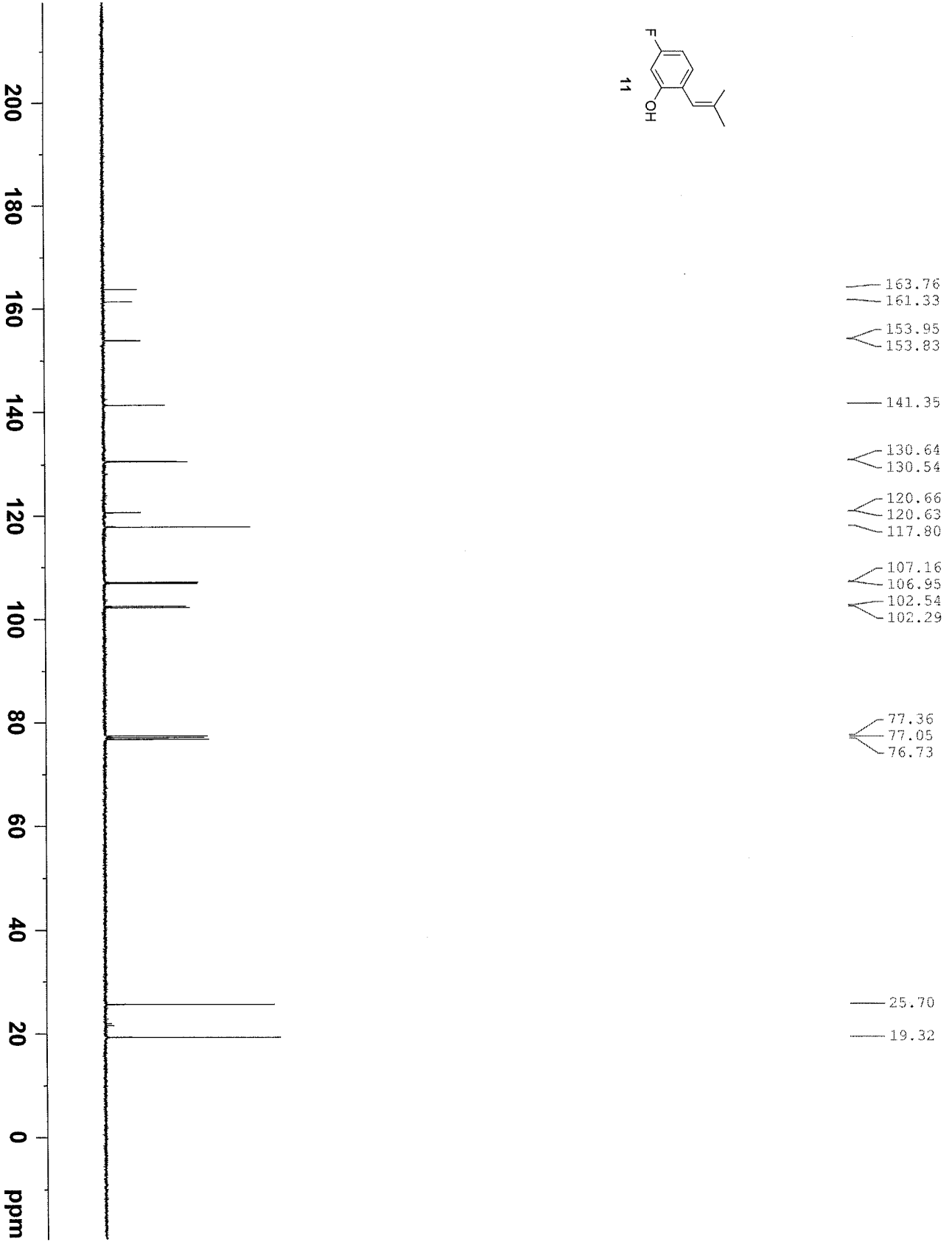
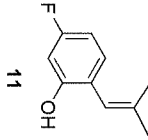
F2 - Processing parameters  
SI 32768  
SF 100.6328860 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



Current Data Parameters  
 NAME LJE-200  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20120719  
 Time\_ 20.00  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 16  
 DS 2  
 SWH 8223.685 Hz  
 FIDRES 0.125483 Hz  
 AQ 3.9846387 sec  
 RG 33.2  
 DW 60.800 usec  
 DE 6.50 usec  
 TE 298.1 K  
 D1 1.00000000 sec  
 TDO 1

==== CHANNEL f1 =====  
 NUC1 1H  
 P1 15.00 usec  
 PLM1 12.00000000 W  
 SFO1 400.2124715 MHz  
 F2 - Processing parameters  
 SI 65536  
 SF 400.2100165 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



Current Data Parameters  
NAME LUF-200  
EXPNO 2  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20120719  
Time 20.05  
INSTRUM spect  
PROBHD 5 mm PABBO BBI  
PULPROG zgpg30  
TD 65536  
SOLVENT CHCl3  
NS 4  
DS 4  
SFO1 24038.461 Hz  
FIDRES 0.366728 Hz  
AQ 1.3631988 sec  
RG 190.62  
DW 20.800 usec  
DE 6.50 usec  
TE 298.7 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TDO 1

CHANNEL f1  
NUC1 13C  
P1 10.00 usec  
PLW1 52.00000000 W  
SFO1 100.6429474 MHz

CHANNEL f2  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 90.00 usec  
PLW2 12.00000000 W  
PLW12 0.3333001 W  
PLW13 0.27000001 W  
SFO2 400.2116008 MHz

F2 - Processing parameters  
SI 32768  
SF 100.6328860 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



Current Data Parameters  
 NAME LJE-260  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters

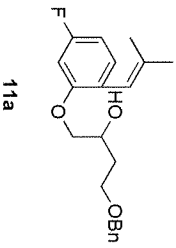
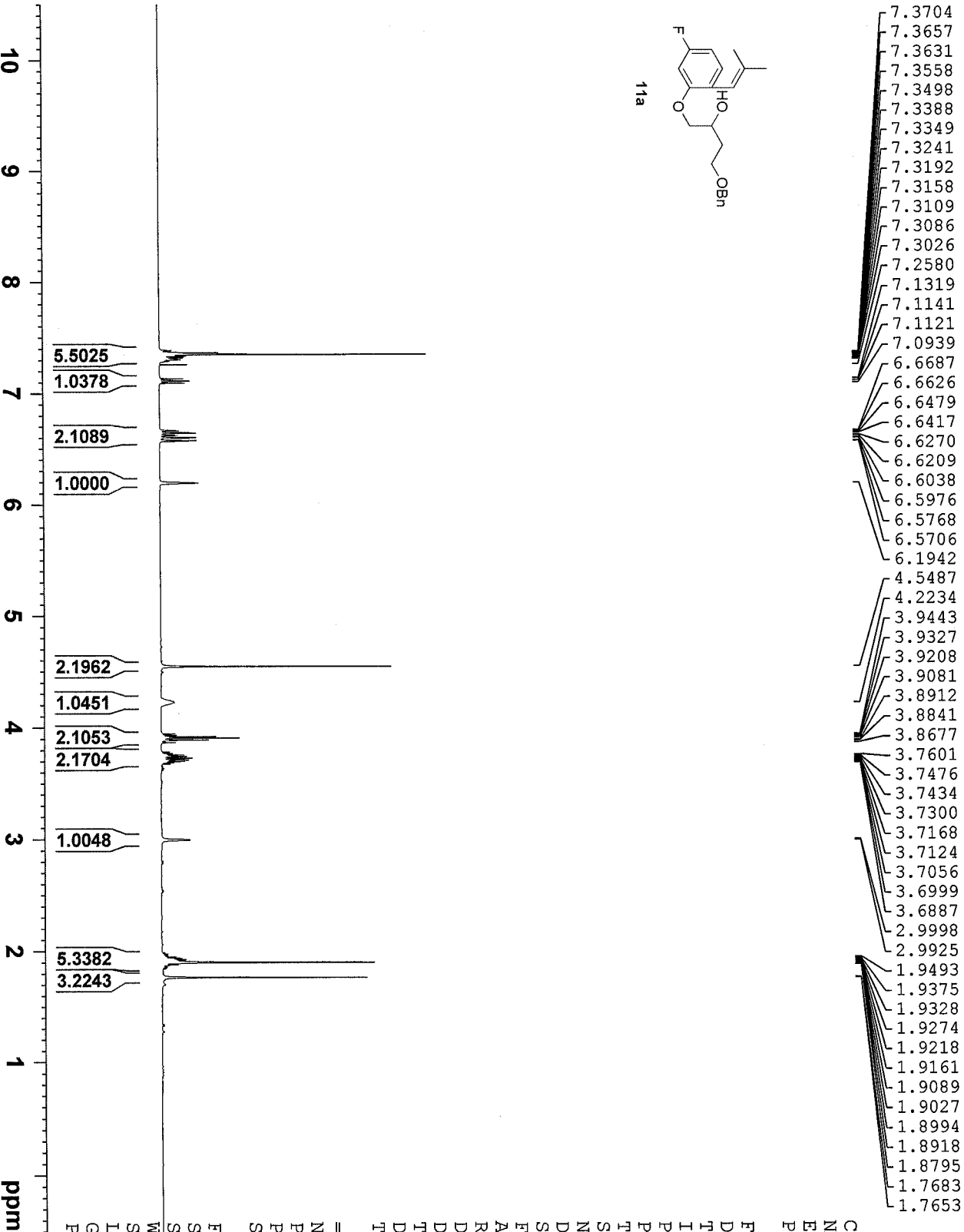
Date\_ 20121114  
 Time 14.37  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 16  
 DS 2  
 SWH 8223.685 Hz  
 FIDRES 0.125483 Hz  
 AQ 3.9846387 sec  
 RG 56.34  
 DW 60.800 usec  
 DE 6.50 usec  
 TE 297.2 K  
 D1 1.00000000 sec  
 TD0 1

==== CHANNEL f1 =====

NUC1 1H  
 P1 15.00 usec  
 PLW1 12.00000000 W  
 SFO1 400.2124715 MHz

F2 - Processing parameters

SI 65536  
 SF 400.2100136 MHz  
 WDM EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00





Current Data Parameters  
 NAME LJE-212  
 EXPNO 8  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20120807  
 Time 10.34

INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zgpg30

TD 65536  
 FIDRES 0.36198 Hz  
 AQ 1.352162 sec

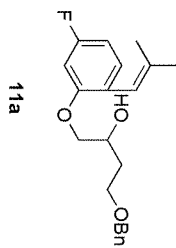
RG 20.802 usec  
 DM 5.50 usec  
 DE 299.0 K

TE 300.2 K  
 D1 2.0000000 sec  
 D11 0.0300000 sec  
 D12 1.0000000 sec

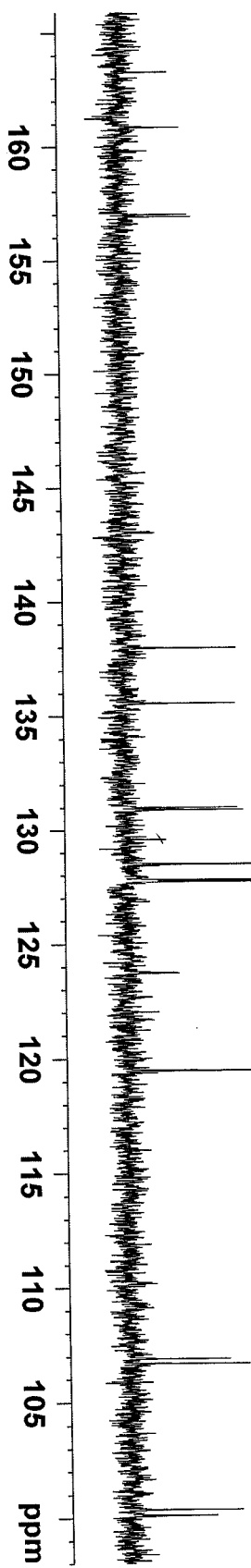
CHANNEL F1  
 NUC1 13C  
 P1 10.00 usec  
 PL1 52.0000000 W  
 SFO1 100.6429474 MHz

CHANNEL F2  
 NUC2 1H  
 P2 90.00 usec  
 PL2 12.0000000 W  
 PL12 0.3333001 W  
 PLM12 0.27000001 W  
 SFO2 400.2116008 MHz

Processing parameters  
 SI 32768  
 SF 100.6328860 MHz  
 WDW EM  
 SSB 0  
 IB 1.00 Hz  
 GB 0  
 PC 1.40



- 163.27
- 160.84
- 156.99
- 156.90
- 137.98
- 135.56
- 131.00
- 130.91
- 128.49
- 127.80
- 127.72
- 123.76
- 123.72
- 119.49
- 106.91
- 106.71
- 100.36
- 100.10





Current Data Parameters  
 NAME LJE-261  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters

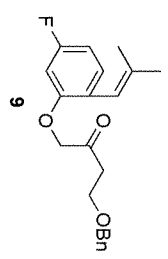
Date\_ 20121114  
 Time 20.15  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 2  
 DS 2  
 SWH 8223.685 Hz  
 FIDRES 0.125483 Hz  
 AQ 3.9846387 sec  
 RG 76.56  
 DW 60.800 usec  
 DE 6.50 usec  
 TE 297.9 K  
 D1 1.00000000 sec  
 TD0 1

==== CHANNEL f1 =====

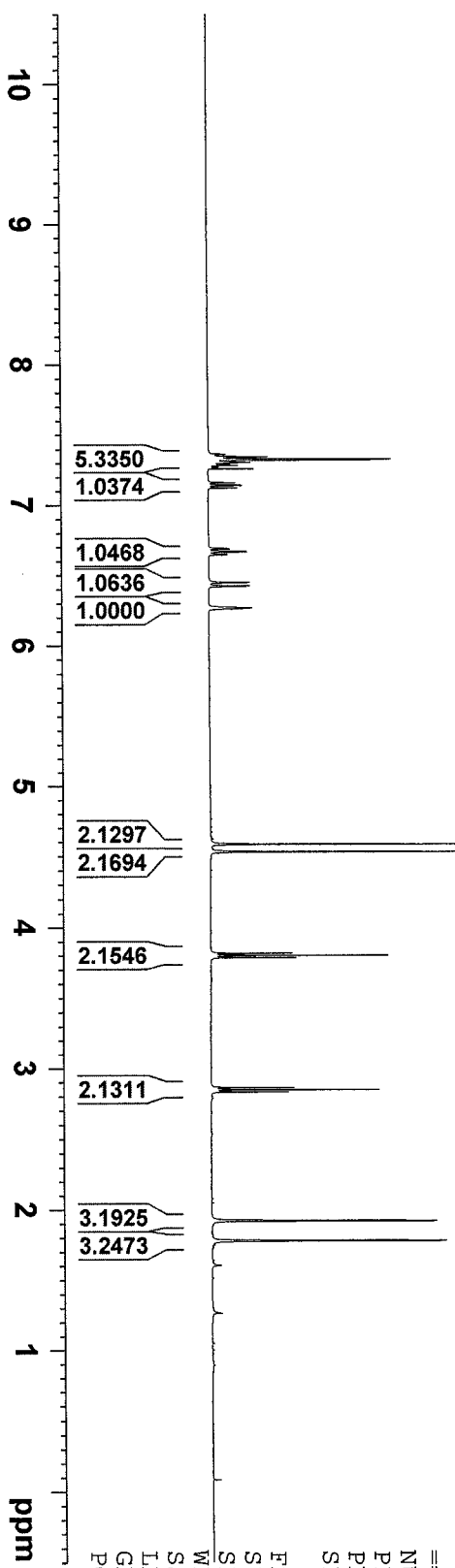
NUC1 1H  
 P1 15.00 usec  
 PLW1 12.00000000 W  
 SFO1 400.2124715 MHz

F2 - Processing parameters

SI 65536  
 SF 400.2100134 MHz  
 WDM EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



- 7.3625
- 7.3586
- 7.3486
- 7.3445
- 7.3419
- 7.3363
- 7.3285
- 7.3276
- 7.3239
- 7.3122
- 7.3085
- 7.3061
- 7.3018
- 7.2984
- 7.2925
- 7.2845
- 7.2753
- 7.2688
- 7.2585
- 7.1601
- 7.1420
- 7.1394
- 7.1221
- 6.6923
- 6.6862
- 6.6715
- 6.6654
- 6.6506
- 6.6446
- 6.4527
- 6.4466
- 6.4263
- 6.4202
- 6.2686
- 4.5857
- 4.5326
- 3.8162
- 3.8009
- 3.7857
- 2.8629
- 2.8477
- 2.8325
- 1.9225
- 1.9191
- 1.7804
- 1.7773



ppm



Current Data Parameters  
 NAME LJE-219  
 EXPNO 2  
 PROCNO 1

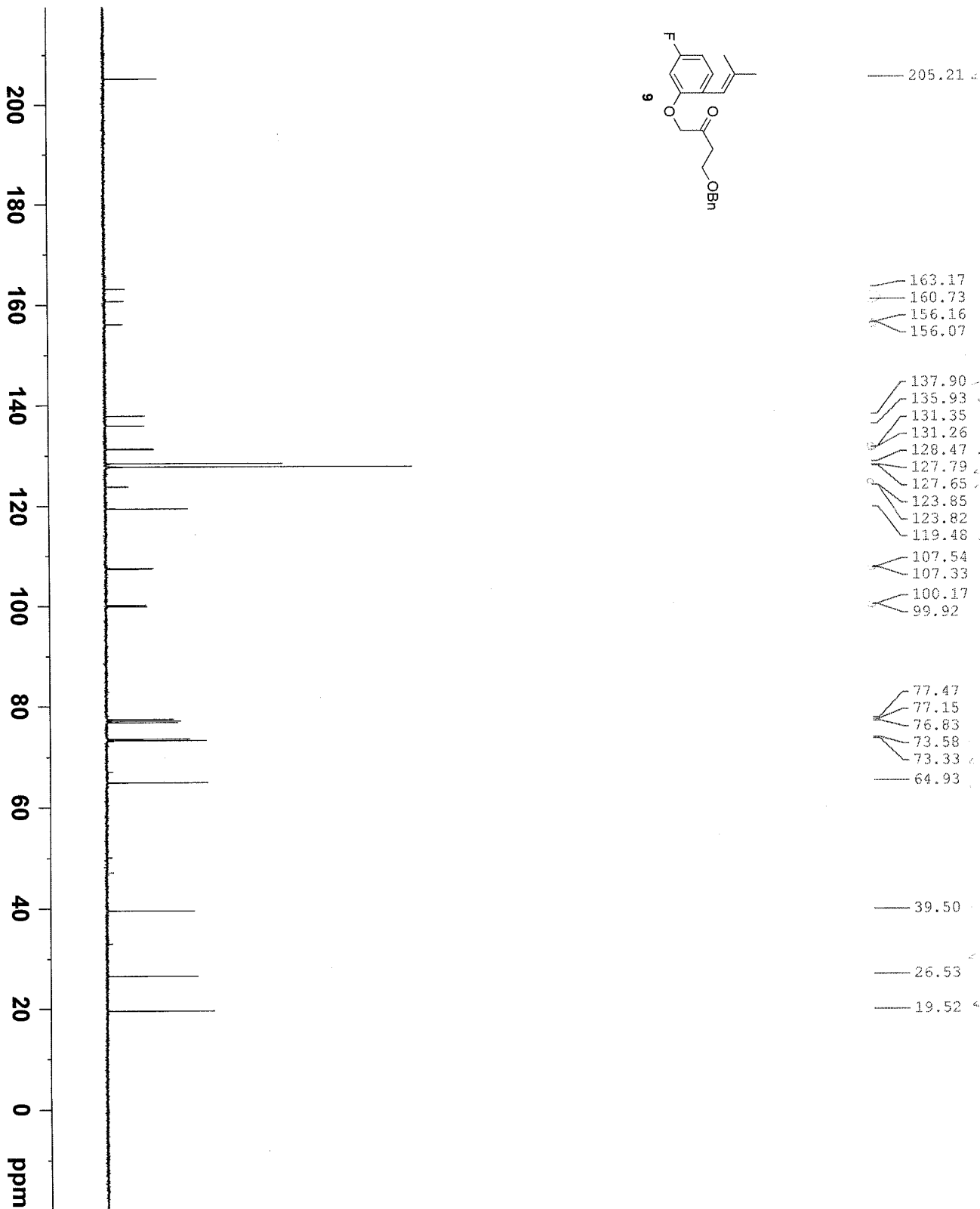
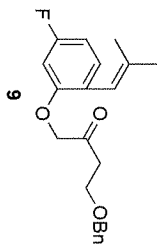
F2 - Acquisition Parameters

Date\_ 20120823  
 Time 20.53  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 57  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3631988 sec  
 RG 190.62  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 298.9 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TDO 1

==== CHANNEL f1 =====  
 NUC1 13C  
 P1 10.00 usec  
 PLW1 52.00000000 W  
 SFO1 100.6429474 MHz

==== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUC2 1H  
 PCPD2 90.00 usec  
 PLW2 12.00000000 W  
 PLWI2 0.33333001 W  
 PLWI3 0.27000001 W  
 SFO2 400.2116008 MHz

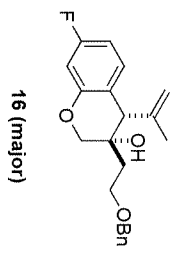
F2 - Processing parameters  
 SI 32768  
 SF 100.6328860 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40







Current Data Parameters  
 NAME LJE-265  
 EXPNO 1  
 PROCNO 1



- 7.3836
- 7.3663
- 7.3615
- 7.3564
- 7.3489
- 7.3352
- 7.3223
- 7.3188
- 7.3124
- 7.2594
- 6.9628
- 6.9615
- 6.9464
- 6.9449
- 6.9416
- 6.9251
- 6.9238
- 6.6254
- 6.6189
- 6.6046
- 6.5980
- 6.5836
- 6.5771
- 6.5648
- 6.5584
- 6.5396
- 6.5332
- 5.1347
- 5.1308
- 5.1268
- 4.6637
- 4.6617
- 4.6596
- 4.5404
- 4.5345
- 4.1203
- 4.0928
- 3.9147
- 3.9113
- 3.8871
- 3.8837
- 3.8025
- 3.7932
- 3.7806
- 3.7713
- 3.7595
- 3.7575
- 3.7461
- 3.4288
- 2.0583
- 2.0511
- 2.0425
- 2.0323
- 2.0208
- 1.8438
- 1.8425
- 1.8282
- 1.8238
- 1.8143
- 1.7998
- 1.7905
- 1.7858

F2 - Acquisition Parameters

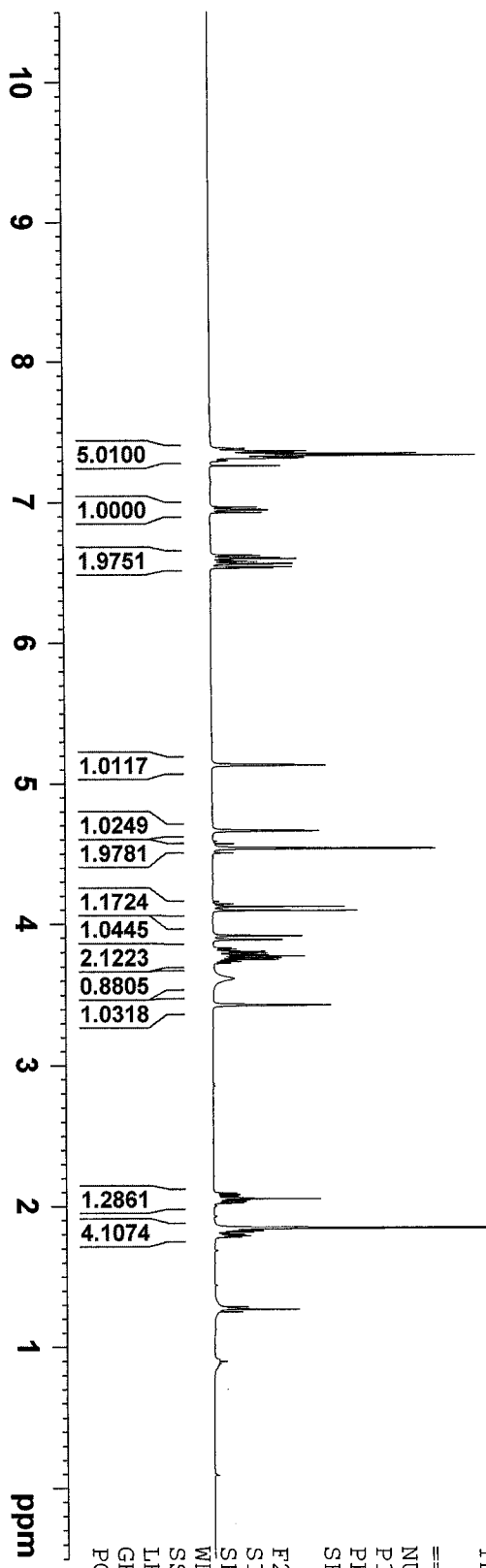
Date\_ 20121119  
 Time 13.44  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 16  
 DS 2  
 SWH 8223.685 Hz  
 FIDRES 0.125483 Hz  
 AQ 3.9846387 sec  
 RG 58.64  
 DW 60.800 usec  
 DE 6.50 usec  
 TE 297.1 K  
 D1 1.00000000 sec  
 TD0 1

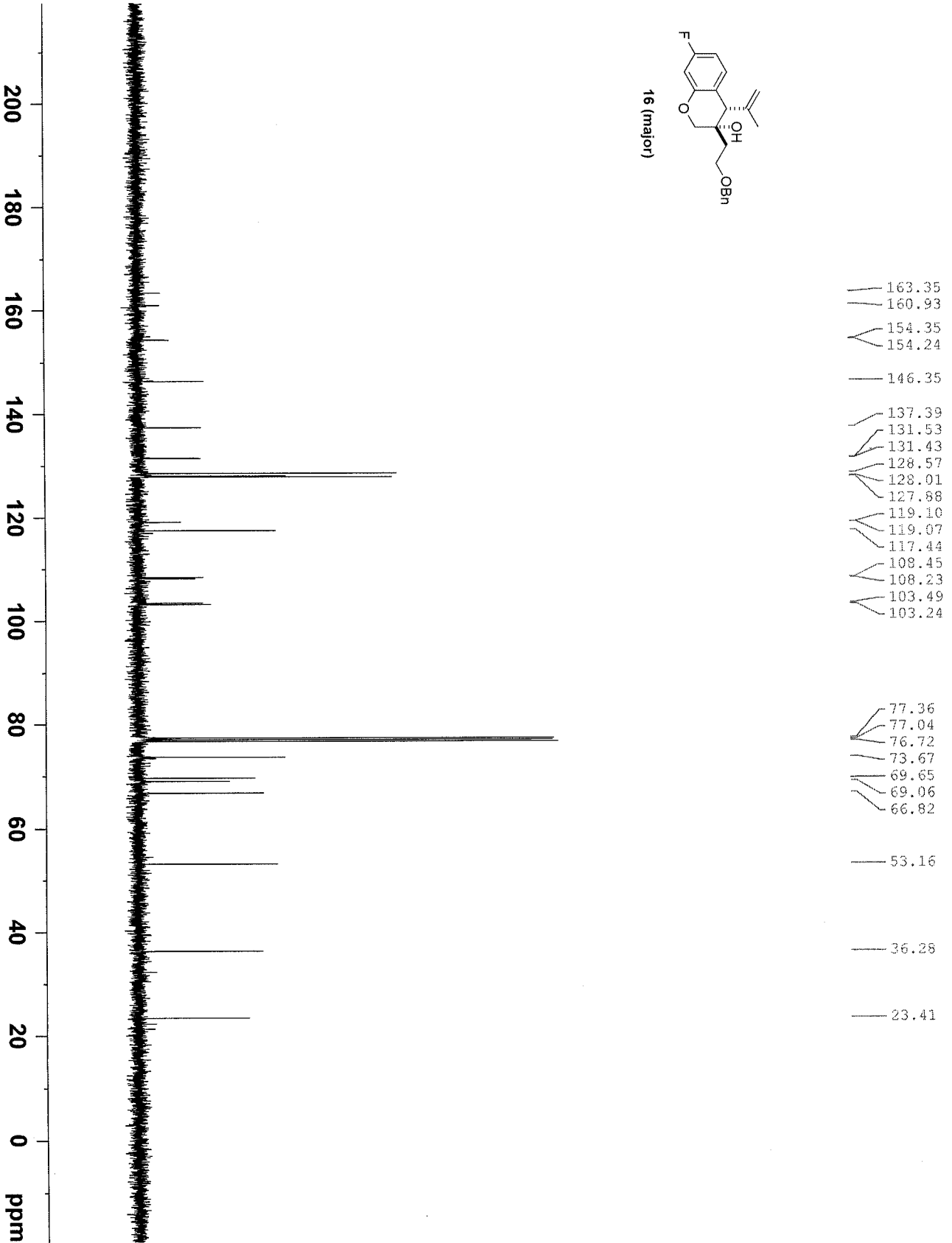
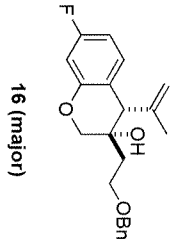
==== CHANNEL f1 =====

NUC1 1H  
 P1 15.00 usec  
 PLW1 12.00000000 W  
 SFO1 400.2124715 MHz

F2 - Processing parameters

SI 65536  
 SF 400.2100130 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00





- 163.35
- 160.93
- 154.35
- 154.24
- 146.35
- 137.39
- 131.53
- 131.43
- 128.57
- 128.01
- 127.88
- 119.10
- 119.07
- 117.44
- 108.45
- 108.23
- 103.49
- 103.24
- 77.36
- 77.04
- 76.72
- 73.67
- 69.65
- 69.06
- 66.82
- 53.16
- 36.28
- 23.41

Current Data Parameters  
NAME LJE-242  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20121004  
Time\_ 15.09  
INSTRUM spect  
PROBHD 5 mm PABBO-BB/  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 35  
DS 4  
SWH 24038.461 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631988 sec  
RG 190.62  
DW 20.800 usec  
DE 6.50 usec  
TE 299.4 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TDO 1

CHANNEL F1  
NUC1 13C  
P1 10.00 usec  
PLM1 52.00000000 W  
SFO1 100.629474 MHz

CHANNEL F2  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 90.00 usec  
PLM2 12.00000000 W  
PLM12 0.33333001 W  
PLM13 0.27000001 W  
SFO2 400.2116008 MHz

F2 - Processing parameters  
SI 32768  
SF 100.628860 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



Current Data Parameters  
 NAME LJE-265  
 EXPNO 3  
 PROCNO 1

F2 - Acquisition Parameters

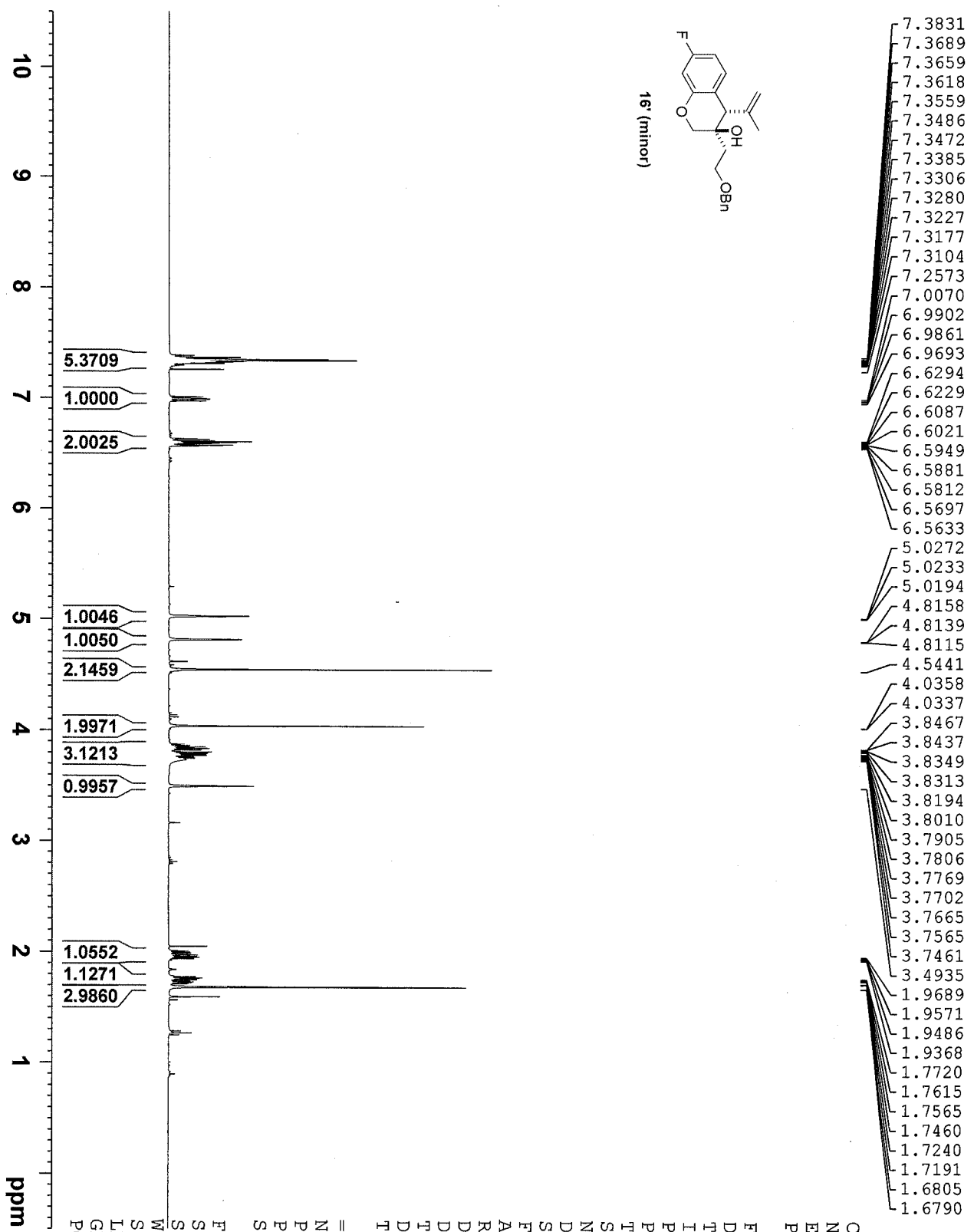
Date\_ 20121119  
 Time 13.52  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 5  
 DS 2  
 SWH 8223.685 Hz  
 FIDRES 0.125483 Hz  
 AQ 3.9846387 sec  
 RG 69.69  
 DW 60.800 usec  
 DE 6.50 usec  
 TE 297.3 K  
 D1 1.00000000 sec  
 TD0 1

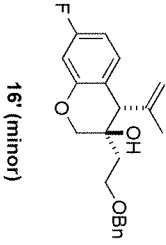
==== CHANNEL f1 =====

NUC1 1H  
 P1 15.00 usec  
 PLW1 12.00000000 W  
 SFO1 400.2124715 MHz

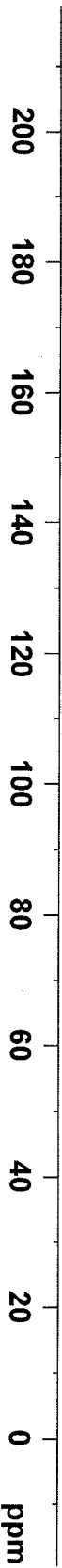
F2 - Processing parameters

SI 65536  
 SF 400.2100138 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00





- 163.29
- 160.86
- 154.36
- 154.24
- 144.53
- 137.41
- 131.60
- 131.50
- 128.56
- 128.01
- 127.89
- 118.53
- 118.50
- 117.21
- 108.39
- 108.18
- 103.56
- 103.31
- 77.34
- 77.02
- 76.70
- 73.62
- 70.28
- 69.80
- 66.48
- 54.56
- 33.49
- 22.29



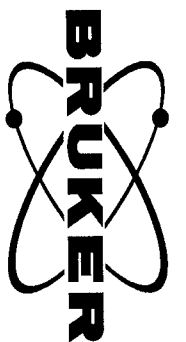
Current Data Parameters  
 NAME LJE-265  
 EXNO 7  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20121120  
 Time\_ 15.40  
 INSTRUM spect  
 PROBD 5 mm PABBO BB/  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 557  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3631988 sec  
 RG 190.62  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 297.4 K  
 D1 2.0000000 sec  
 D11 0.0300000 sec  
 TDO 1

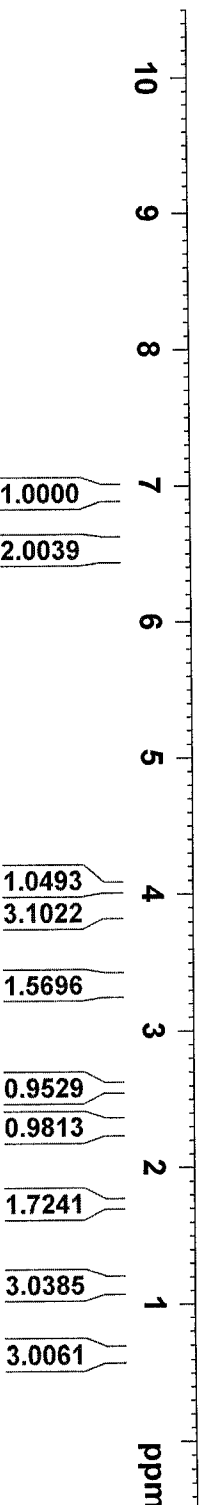
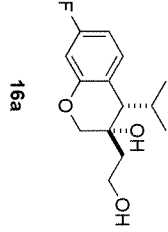
CHANNEL F1  
 NUCL 13C  
 P1 10.00 usec  
 PL1 52.0000000 W  
 SFO1 100.6429474 MHz

CHANNEL F2  
 CPDPRG2 waltz16  
 NUCL2 1H  
 PCPD2 90.00 usec  
 FREQ2 12.0000000 M  
 P1M1 0.2320001 W  
 P1M2 0.2700001 W  
 P1M3 0.2700001 W  
 SFO2 400.2116008 MHz

F2 - Processing parameters  
 SI 32768  
 SF 100.6328860 MHz  
 XDM RM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40



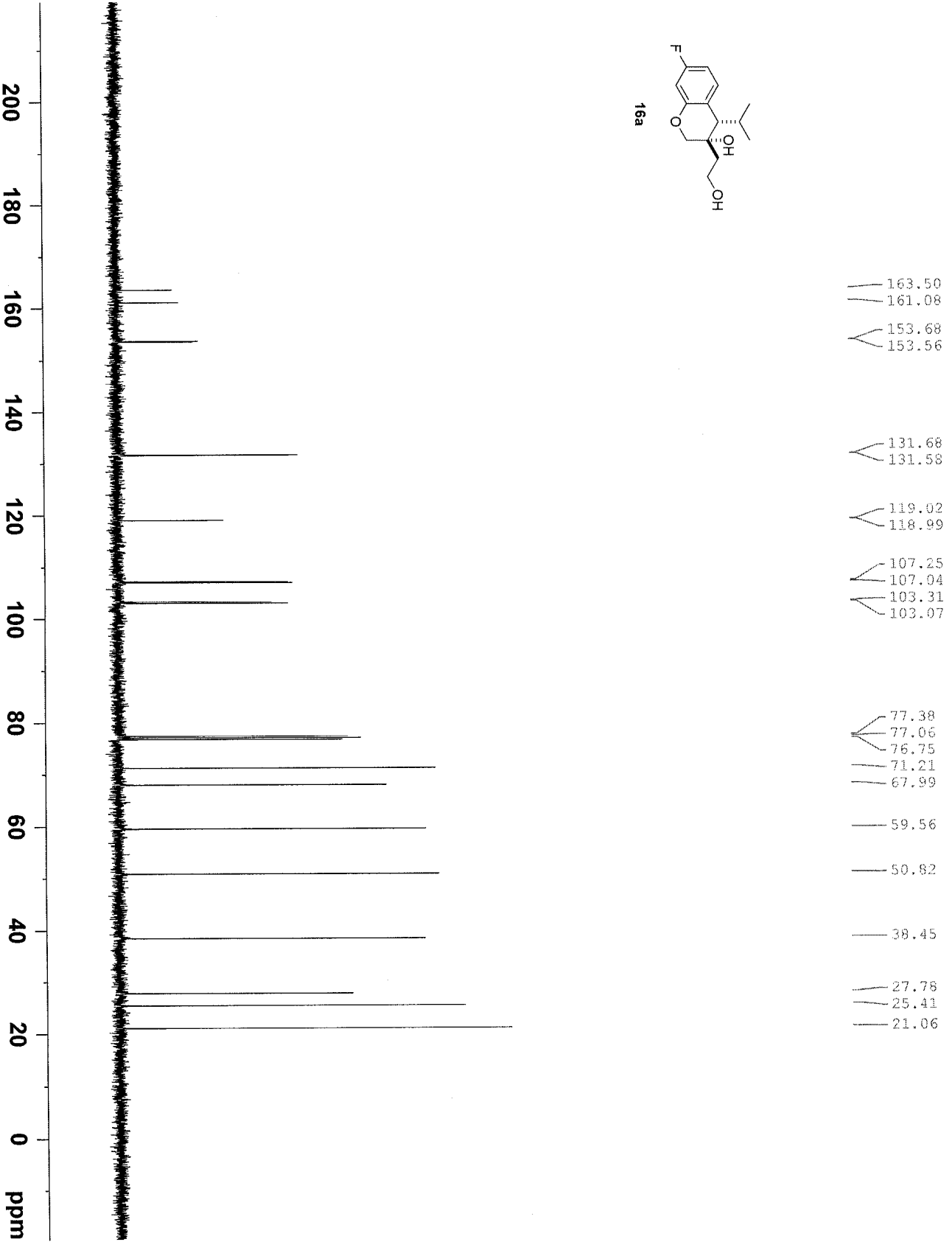
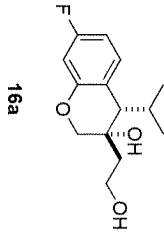
7.2521
7.2501
6.9678
6.9454
6.9400
6.9178
6.5847
6.5762
6.5570
6.5488
6.5290
6.5205
6.5087
6.5004
6.4747
6.4664
4.0742
4.0376
3.9954
3.9806
3.9694
3.9621
3.9443
3.9337
3.9265
3.9182
3.8986
3.8812
3.8612
3.3432
2.6349
2.5934
2.3622
2.3492
2.3394
2.3261
2.3166
2.3029
2.2935
2.2799
2.2704
2.2570
2.2473
1.8147
1.8003
1.7899
1.7640
1.7472
1.7401
1.7272
1.7127
1.6960
1.6766
1.6617
1.1534
1.1302
0.6365
0.6133



Current Data Parameters  
 NAME LJE-163  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20120320  
 Time 20.52  
 INSTRUM spect  
 PROBHD 5 mm DUL 1H-13  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 16  
 DS 2  
 SWH 6172.839 Hz  
 FIDRES 0.094190 Hz  
 AQ 5.3084660 sec  
 RG 90.5  
 DW 81.000 usec  
 DE 6.00 usec  
 TE 300.0 K  
 D1 1.0000000 sec  
 TD0 1

==== CHANNEL f1 =====  
 NUC1 1H  
 P1 10.50 usec  
 PL1 -1.00 dB  
 SFO1 300.1318534 MHz  
 F2 - Processing parameters  
 SI 32768  
 SF 300.1300147 MHz  
 WDM EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



Current Data Parameters  
 NAME LJF-d11  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20130416  
 Time 10.03  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 13  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.36798 Hz  
 AQ 1.3631988 sec  
 RG 190.62  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 300.7 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TDO 1

CHANNEL F1  
 NUC1 13C  
 P1 10.00 usec  
 PLW1 52.00000000 W  
 SFO1 100.629474 MHz

CHANNEL F2  
 walz16  
 NUC2 1H  
 PCPD2 90.00 usec  
 PLW2 12.00000000 W  
 PLW12 0.3333001 W  
 PLW13 0.2700001 W  
 SFO2 400.2116008 MHz  
 SFO3 400.2116008 MHz

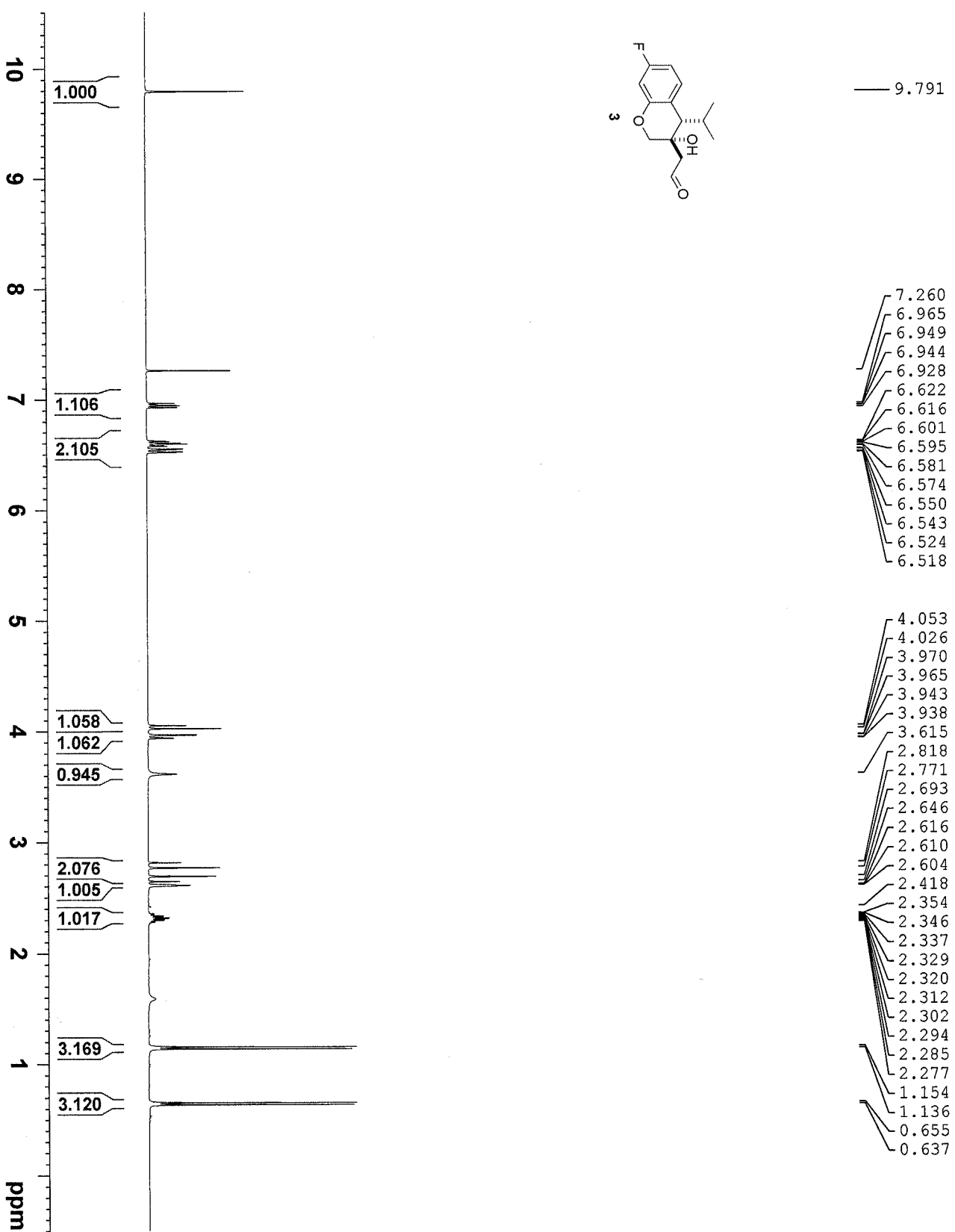
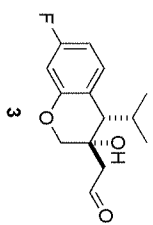
F2 - Processing parameters  
 SI 32768  
 SF 100.628650 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

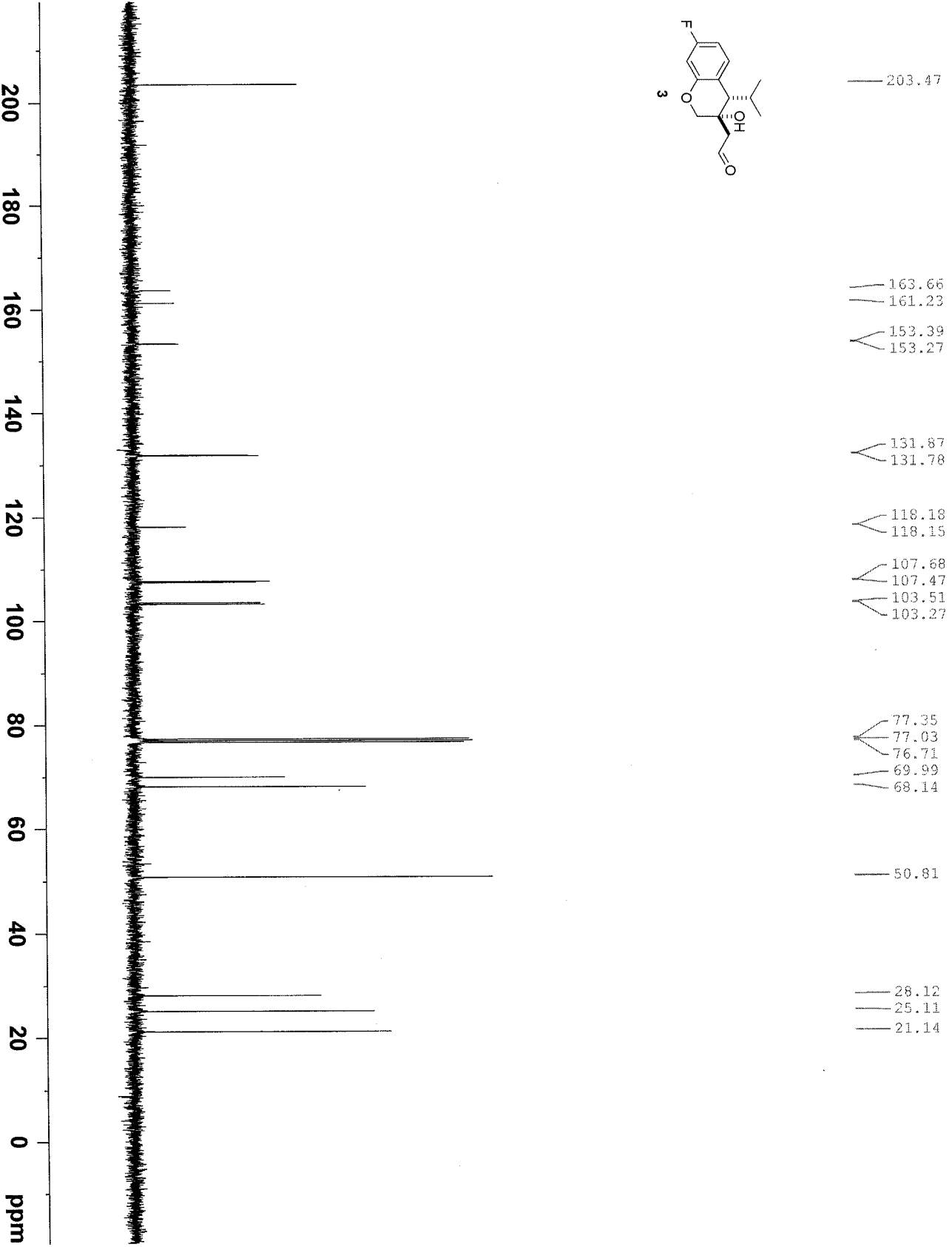
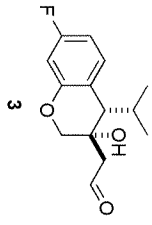


Current Data Parameters  
 NAME LJE-189  
 EXPNO 2  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20120622  
 Time\_ 14.12  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 16  
 DS 2  
 SWH 8223.685 Hz  
 FIDRES 0.125483 Hz  
 AQ 3.9846387 sec  
 RG 133.17  
 DW 60.800 usec  
 DE 6.50 usec  
 TE 298.0 K  
 DL 1.00000000 sec  
 TPO 1

==== CHANNEL f1 =====  
 NUCL 1H  
 P1 15.00 usec  
 P1M1 12.00000000 W  
 SFO1 400.2124715 MHz  
 F2 - Processing parameters  
 SI 65536  
 SF 400.2100130 MHz  
 WDM EM  
 SSB 0  
 TB 0.30 Hz  
 GB 0  
 PC 1.00





Current Data Parameters  
 NAME LJE-333  
 EKXNO 3  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20130416  
 Time\_ 21.43  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 39  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3631988 sec  
 RG 190.62  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 299.6 K  
 D1 2.0000000 sec  
 D11 0.0300000 sec  
 TDO 1

CHANNEL F1  
 NUCL 13C  
 P1 10.00 usec  
 PLM1 52.0000000 W  
 SF01 100.6429174 MHz

CHANNEL F2  
 CPDPRG2 waltz16  
 NUC2 1H  
 POC2 90.00 usec  
 FMC2 12.00000000 W  
 PLM2 0.33333001 W  
 PLM13 0.27000001 W  
 SF02 400.2116008 MHz

F2 - Processing Parameters  
 SI 32768  
 SF 100.6328850 MHz  
 WDW EM  
 SSB 0  
 GB 0  
 PC 1.40





Current Data Parameters  
 NAME LJE-2nd-15  
 EXPNO 1  
 PROCNO 1

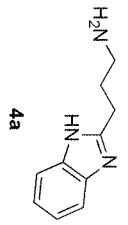
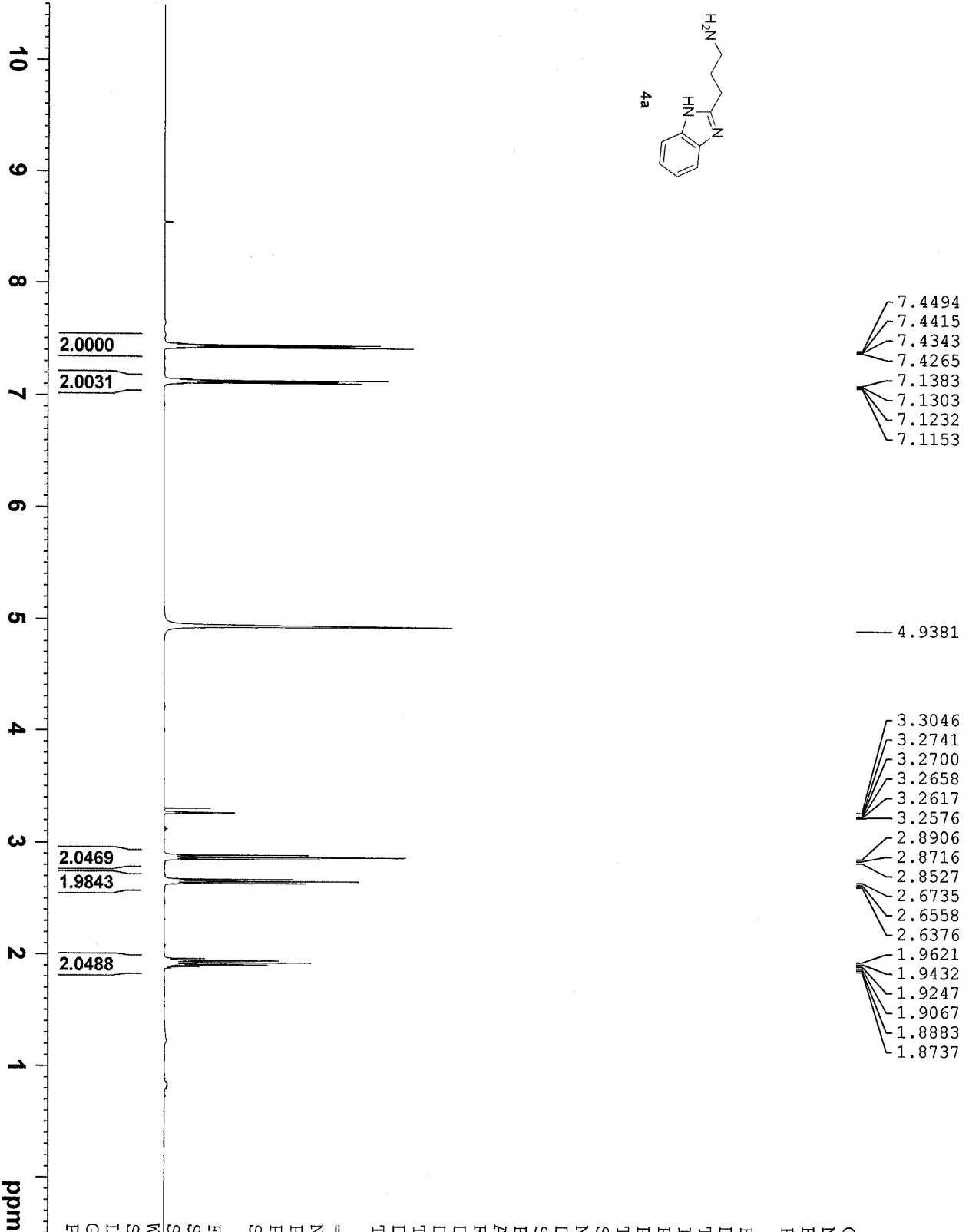
F2 - Acquisition Parameters

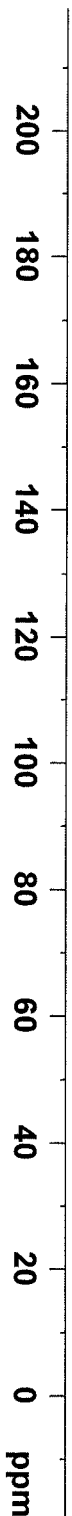
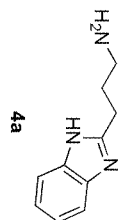
Date\_ 20121113  
 Time\_ 15.57  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zg30  
 TD 65536  
 SOLVENT MeOD  
 NS 16  
 DS 2  
 SWH 8223.685 Hz  
 FIDRES 0.125483 Hz  
 AQ 3.9846387 sec  
 RG 69.69  
 DW 60.800 usec  
 DE 6.50 usec  
 TE 298.2 K  
 D1 1.00000000 sec  
 TD0 1

==== CHANNEL F1 =====  
 NUC1 1H  
 P1 15.00 usec  
 PLW1 12.00000000 W  
 SFO1 400.2124715 MHz

F2 - Processing parameters

SI 65536  
 SF 400.2100286 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00





Current Data Parameters  
 NAME LJE-2nd-33  
 EXPNO 4  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20120521  
 Time 14.35  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT MeOD  
 NS 56  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3631988 sec  
 RG 190.62  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 298.8 K  
 D1 2.0000000 sec  
 D11 0.0300000 sec  
 TD0 1

==== CHANNEL F1 =====  
 NUC1 13C  
 P1 10.00 usec  
 PLW1 52.00000000 W  
 SFO1 100.6429474 MHz

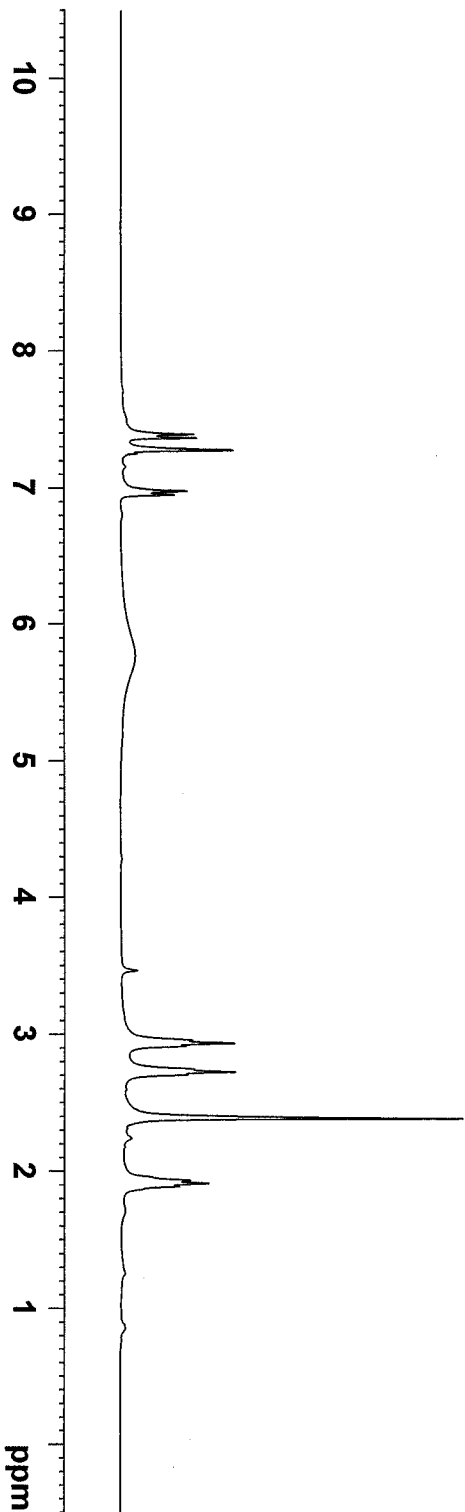
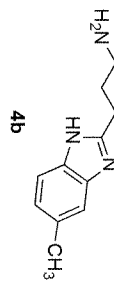
==== CHANNEL F2 =====  
 CPDPRG2 waltz16  
 NUC2 1H  
 PCPD2 90.00 usec  
 PLM2 12.00000000 W  
 PLW2 0.33333001 W  
 PLM13 0.270000001 W  
 SFO2 400.2116008 MHz

F2 - Processing parameters  
 SI 32768  
 SF 100.6328860 MHz  
 WDM EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40



Current Data Parameters  
 NAME LJE-2nd-21  
 EXPNO 1  
 PROCNO 1

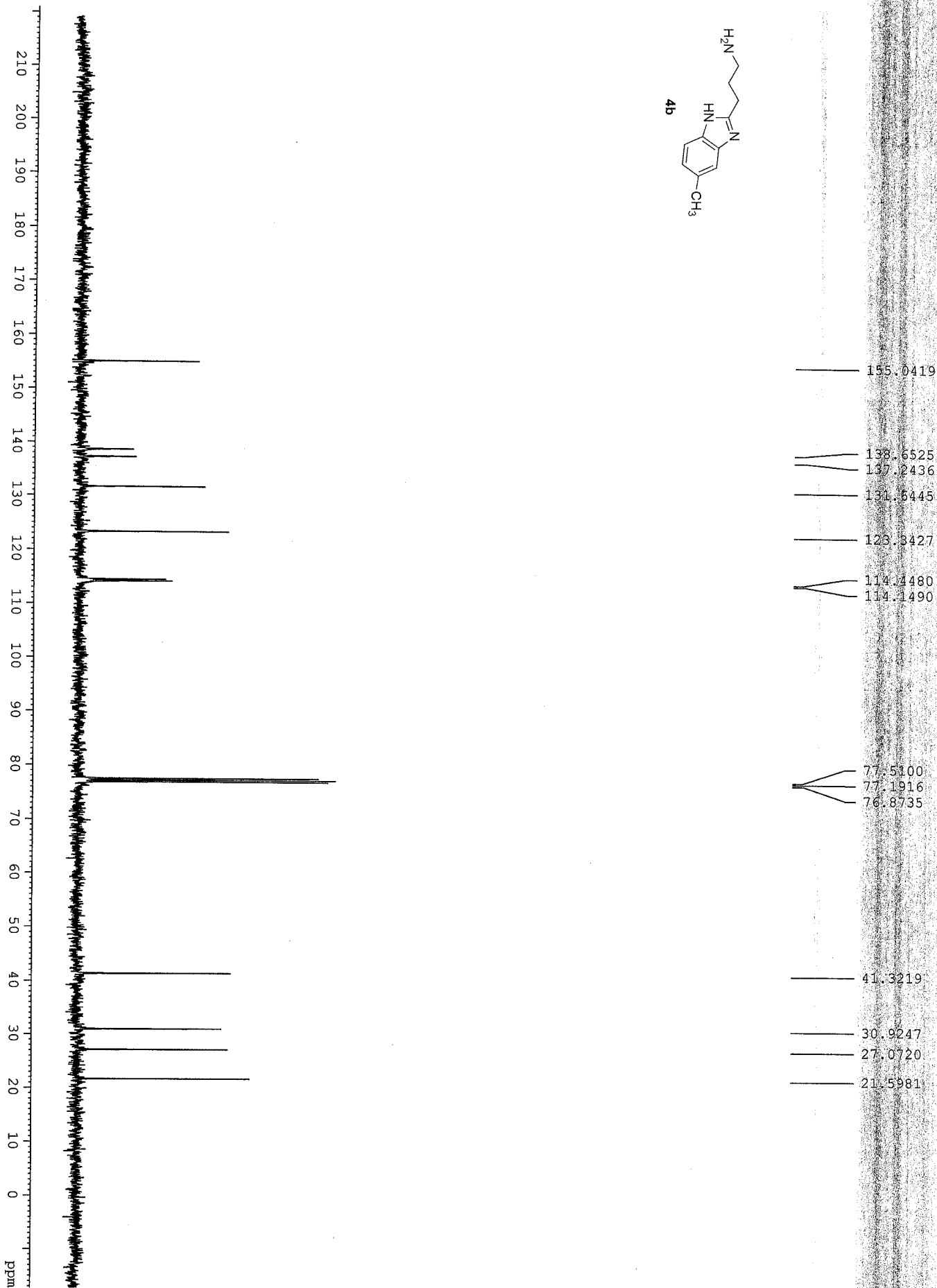
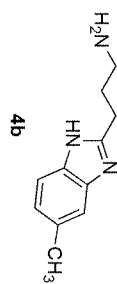
7.3943  
 7.3673  
 7.2796  
 6.9805  
 6.9536  
 5.7715  
 2.9593  
 2.9370  
 2.9142  
 2.7462  
 2.7265  
 2.7062  
 2.3891  
 1.9331  
 1.9112  
 1.8891

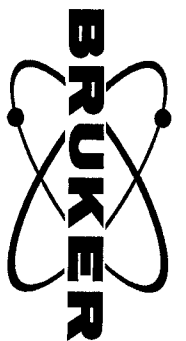


F2 - Acquisition Parameters  
 Date\_ 20120202  
 Time\_ 10.59  
 INSTRUM spect  
 PROBHD 5 mm DUL 1H-13  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 16  
 DS 2  
 SWH 6172.839 Hz  
 FIDRES 0.094190 Hz  
 AQ 5.3084660 sec  
 RG 71.8  
 DW 81.000 usec  
 DE 6.00 usec  
 TE 300.0 K  
 D1 1.00000000 sec  
 TDO 1

==== CHANNEL f1 =====  
 NUC1 1H  
 P1 10.50 usec  
 PL1 -1.00 dB  
 SFO1 300.1318534 MHz

F2 - Processing parameters  
 SI 32768  
 SF 300.1300139 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



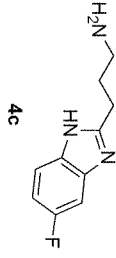


Current Data Parameters  
 NAME LJE-2nd-31  
 EXPNO 1  
 PROCNO 1

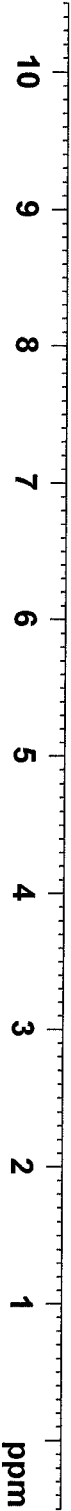
F2 - Acquisition Parameters  
 Date\_ 20120303  
 Time\_ 16.35  
 INSTRUM spect  
 PROBHD 5 mm DUL 1H-13  
 PULPROG zg30  
 TD 65536  
 SOLVENT MeOD  
 NS 16  
 DS 2  
 SWH 6172.839 Hz  
 FIDRES 0.094190 Hz  
 AQ 5.3084660 sec  
 RG 80.6  
 DW 81.000 usec  
 DE 6.00 usec  
 TE 300.0 K  
 D1 1.00000000 sec  
 TD0 1

==== CHANNEL f1 =====  
 NUC1 1H  
 P1 10.50 usec  
 PL1 -1.00 dB  
 SFO1 300.1318534 MHz

F2 - Processing parameters  
 SI 32768  
 SF 300.1300101 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



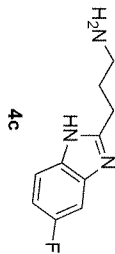
- 8.5930
- 7.4284
- 7.4127
- 7.3992
- 7.3836
- 7.1821
- 7.1744
- 7.1516
- 7.1439
- 6.9506
- 6.9426
- 6.9204
- 6.9183
- 6.9131
- 6.8888
- 6.8809
- 5.1990
- 3.3299
- 3.2966
- 3.2913
- 2.9326
- 2.9076
- 2.8823
- 2.7895
- 2.7661
- 2.7411
- 2.0470
- 2.0222
- 1.9979
- 1.9734
- 1.9483



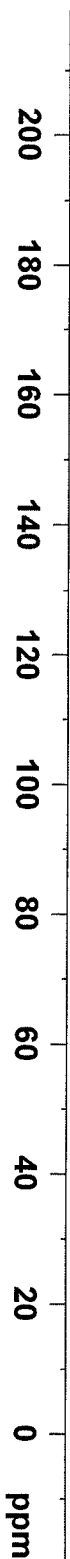
- 1.0491
- 1.0596
- 1.0673

- 2.1631
- 2.0000

- 2.0581



- 169.13
- 160.44
- 158.09
- 156.53
- 138.58
- 138.45
- 134.62
- 114.60
- 114.50
- 109.81
- 109.56
- 100.20
- 99.94
- 48.46
- 48.25
- 48.04
- 47.83
- 47.61
- 47.40
- 47.19
- 46.97
- 40.32
- 30.11
- 25.82



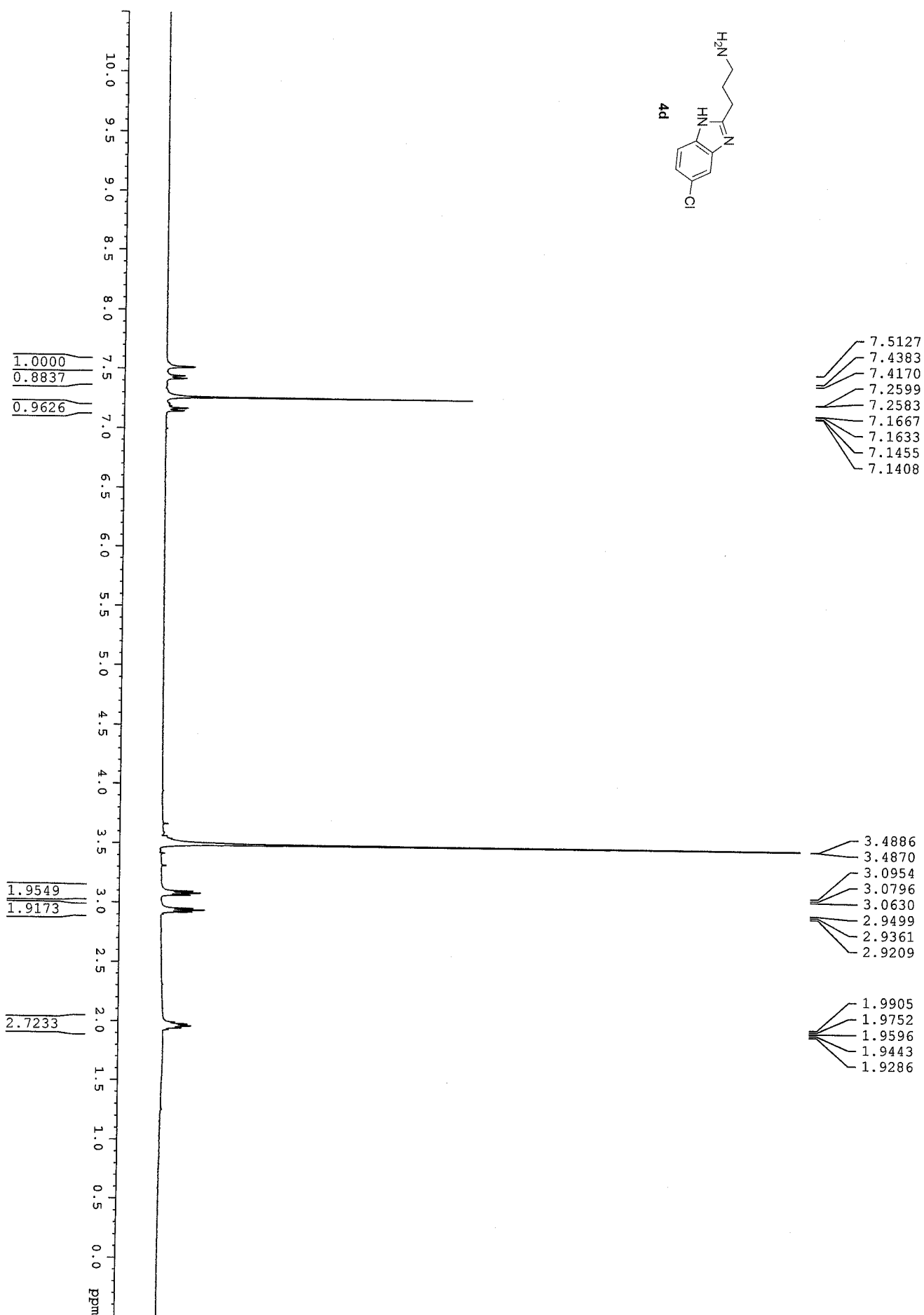
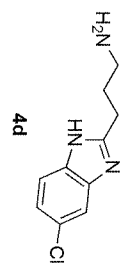
Current Data Parameters  
 NAME IJE-2nd-23  
 EXPNO 2  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20120518  
 Time\_ 20.54  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT MeOD  
 NS 89  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3631988 sec  
 RG 190.62  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 298.7 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TD0 1

==== CHANNEL F1 =====  
 NUC1 13C  
 P1 10.00 usec  
 PLW1 52.00000000 W  
 SFO1 100.6429474 MHz

==== CHANNEL F2 =====  
 CPDPRG2 waltz16  
 NUC2 1H  
 PCPD2 90.00 usec  
 PLW2 12.00000000 W  
 PLW12 0.33333001 W  
 PLW13 0.27000001 W  
 SFO2 400.2116008 MHz

F2 - Processing parameters  
 SI 32768  
 SF 100.6328860 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40





Current Data Parameters  
 NAME IJE-2nd-44  
 EXPNO 2  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20120518  
 Time 20.47

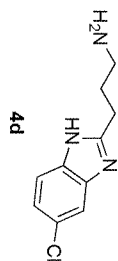
INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT MeOD  
 NS 47  
 DS 4

SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3631988 sec  
 RG 190.62  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 298.8 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TD0 1

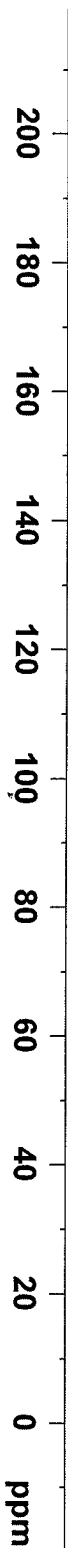
==== CHANNEL f1 =====  
 NUC1 13C  
 P1 10.00 usec  
 PLW1 52.00000000 W  
 SFO1 100.6429474 MHz

==== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUC2 1H  
 PCPBD2 90.00 usec  
 PLW2 12.00000000 W  
 PLW12 0.33333001 W  
 PLW13 0.27000001 W  
 SFO2 400.2116008 MHz

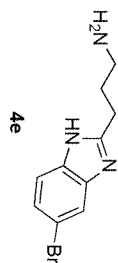
F2 - Processing parameters  
 SI 32768  
 SF 100.6328860 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40



- 156.12
- 139.15
- 136.62
- 127.36
- 122.20
- 114.84
- 114.01
- 48.49
- 48.27
- 48.06
- 47.85
- 47.64
- 47.42
- 47.21
- 47.00
- 39.97
- 29.00
- 25.72



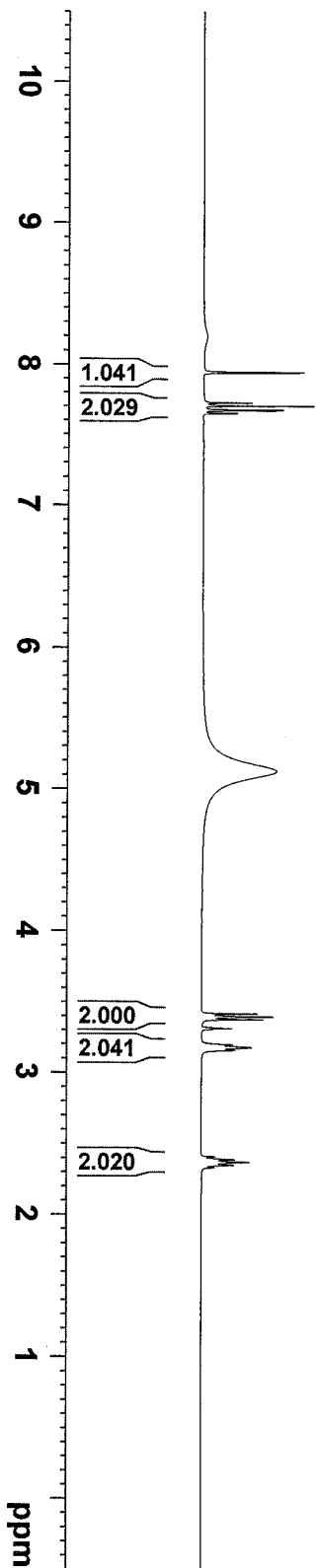




7.942  
7.939  
7.722  
7.700  
7.672  
7.668  
7.650  
7.646

5.125

3.413  
3.394  
3.373  
3.318  
3.314  
3.310  
3.306  
3.302  
3.193  
3.175  
3.156  
2.405  
2.385  
2.366  
2.346  
2.327



Current Data Parameters  
NAME LJE-2nd-54  
EXPNO 2  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20120619  
Time 14.47  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zg30  
TD 65536  
SOLVENT MeOD  
NS 16  
DS 2  
SWH 8223.685 Hz  
FIDRES 0.125483 Hz  
AQ 3.9846387 sec  
RG 33.2  
DW 60.800 usec  
DE 6.50 usec  
TE 298.3 K  
D1 1.00000000 sec  
TD0 1

==== CHANNEL f1 =====  
NUC1 1H  
P1 15.00 usec  
PLW1 12.00000000 W  
SFO1 400.2124715 MHz  
F2 - Processing parameters  
SI 65536  
SF 400.2100108 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



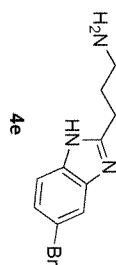
Current Data Parameters  
 NAME LJE-2nd-54  
 EXPNO 4  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20120619  
 Time 14.54  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT MeOD  
 NS 53  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3631988 sec  
 RG 190.62  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 299.0 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TD0 1

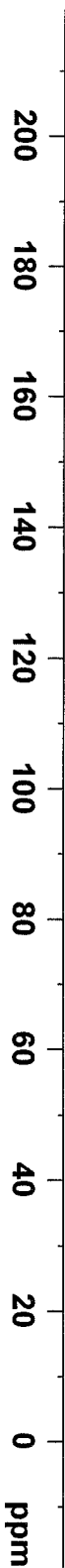
===== CHANNEL f1 =====  
 NUC1 13C  
 P1 10.00 usec  
 PLW1 52.00000000 W  
 SFO1 100.6429474 MHz

===== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUC2 1H  
 PCPD2 90.00 usec  
 PLW2 12.00000000 W  
 PLW12 0.33333001 W  
 PLW13 0.27000001 W  
 SFO2 400.2116008 MHz

F2 - Processing parameters  
 SI 32768  
 SF 100.6328860 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40



153.69  
 132.01  
 130.05  
 129.25  
 118.81  
 116.46  
 115.14  
 48.37  
 48.15  
 47.94  
 47.73  
 47.52  
 47.30  
 47.09  
 38.41  
 24.40  
 23.61

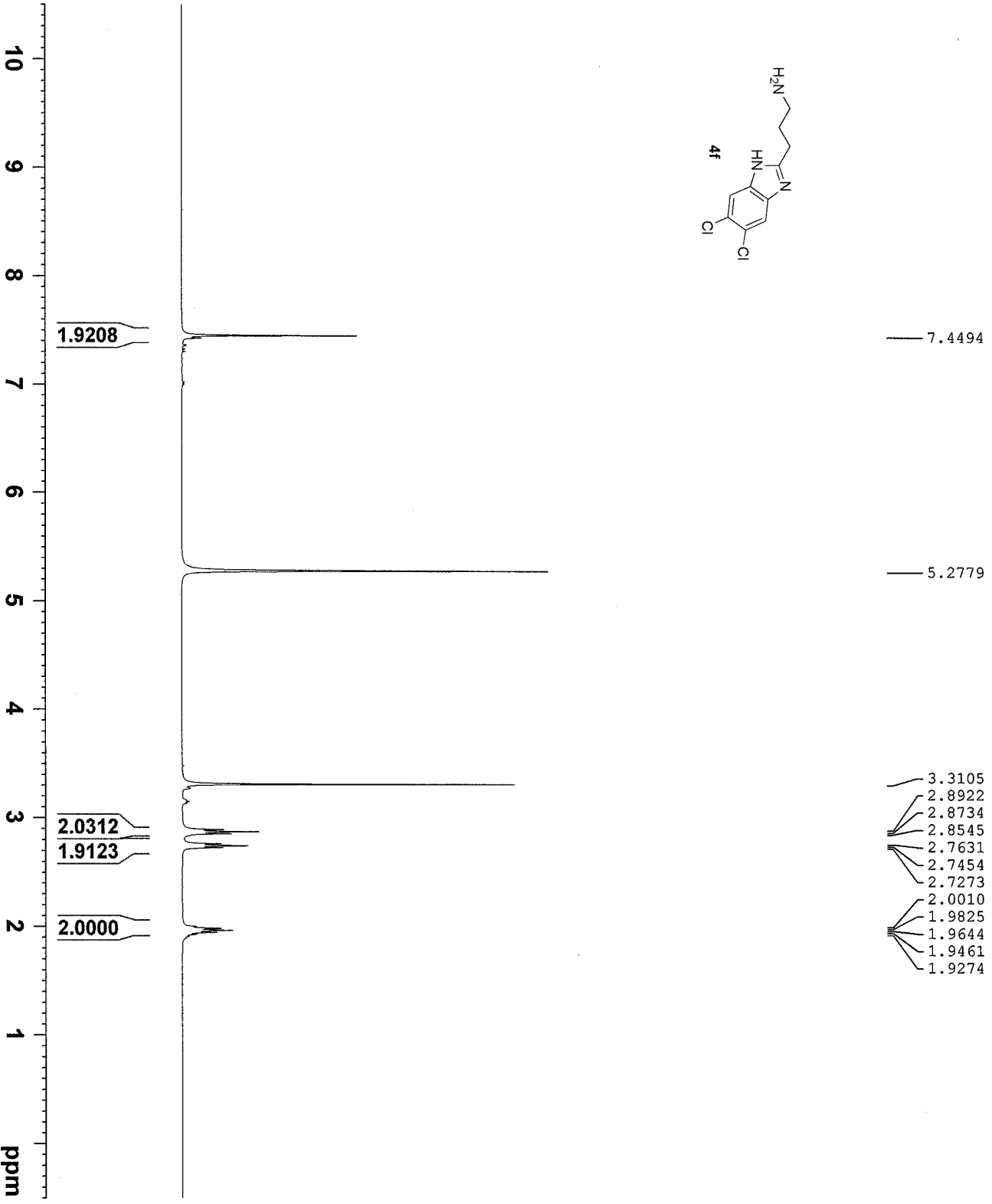
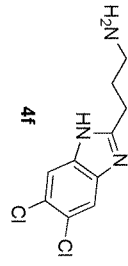


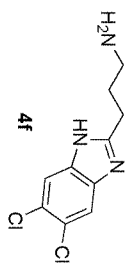


Current Data Parameters  
 NAME LJE-2nd-48  
 EXPNO 1  
 PROCNO 1

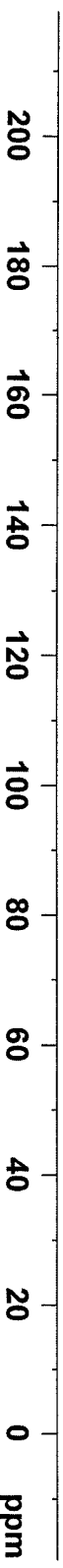
F2 - Acquisition Parameters  
 Date\_ 20120530  
 Time 20.34  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zg30  
 TD 65536  
 SOLVENT MeOD  
 NS 16  
 DS 2  
 SWH 8223.685 Hz  
 FIDRES 0.125483 Hz  
 AQ 3.9846387 sec  
 RG 33.2  
 DW 60.800 usec  
 DE 6.50 usec  
 TE 298.5 K  
 D1 1.00000000 sec  
 TD0 1

==== CHANNEL f1 =====  
 NUCL1 1H  
 P1 15.00 usec  
 PLMW1 12.00000000 W  
 SFO1 400.2124715 MHz  
 F2 - Processing parameters  
 SI 65536  
 SF 400.2100261 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00





- 157.46
- 137.61
- 125.28
- 115.25
- 48.53
- 48.32
- 48.11
- 47.90
- 47.69
- 47.47
- 47.26
- 47.05
- 40.14
- 29.22
- 25.83



Current Data Parameters  
 NAME LUF-2nd-48  
 EXPNO 2  
 PROCNO 1

F2 - Acquisition Parameters

Date\_ 20120530  
 Time\_ 20.38  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT MeOD  
 NS 64  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3631988 sec  
 RG 190.62  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 299.1 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TD0 1

==== CHANNEL f1 =====

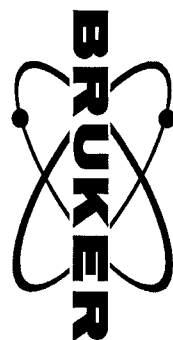
NUC1 13C  
 P1 10.00 usec  
 PLW1 52.00000000 W  
 SFO1 100.6429474 MHz

==== CHANNEL f2 =====

CPDPRG2 waltz16  
 NUC2 1H  
 PCPD2 90.00 usec  
 PLW2 12.00000000 W  
 PLW12 0.33333001 W  
 PLW13 0.27000001 W  
 SFO2 400.2116008 MHz

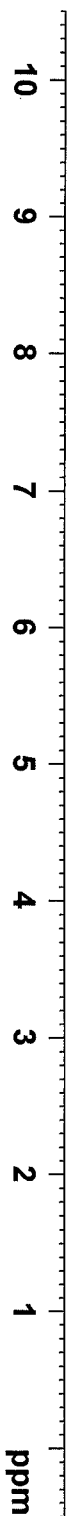
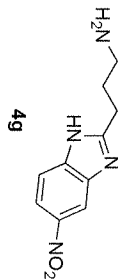
F2 - Processing parameters

SI 32768  
 SF 100.6328860 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40



Current Data Parameters  
 NAME LJE-2nd-40  
 EXPNO 1  
 PROCNO 1

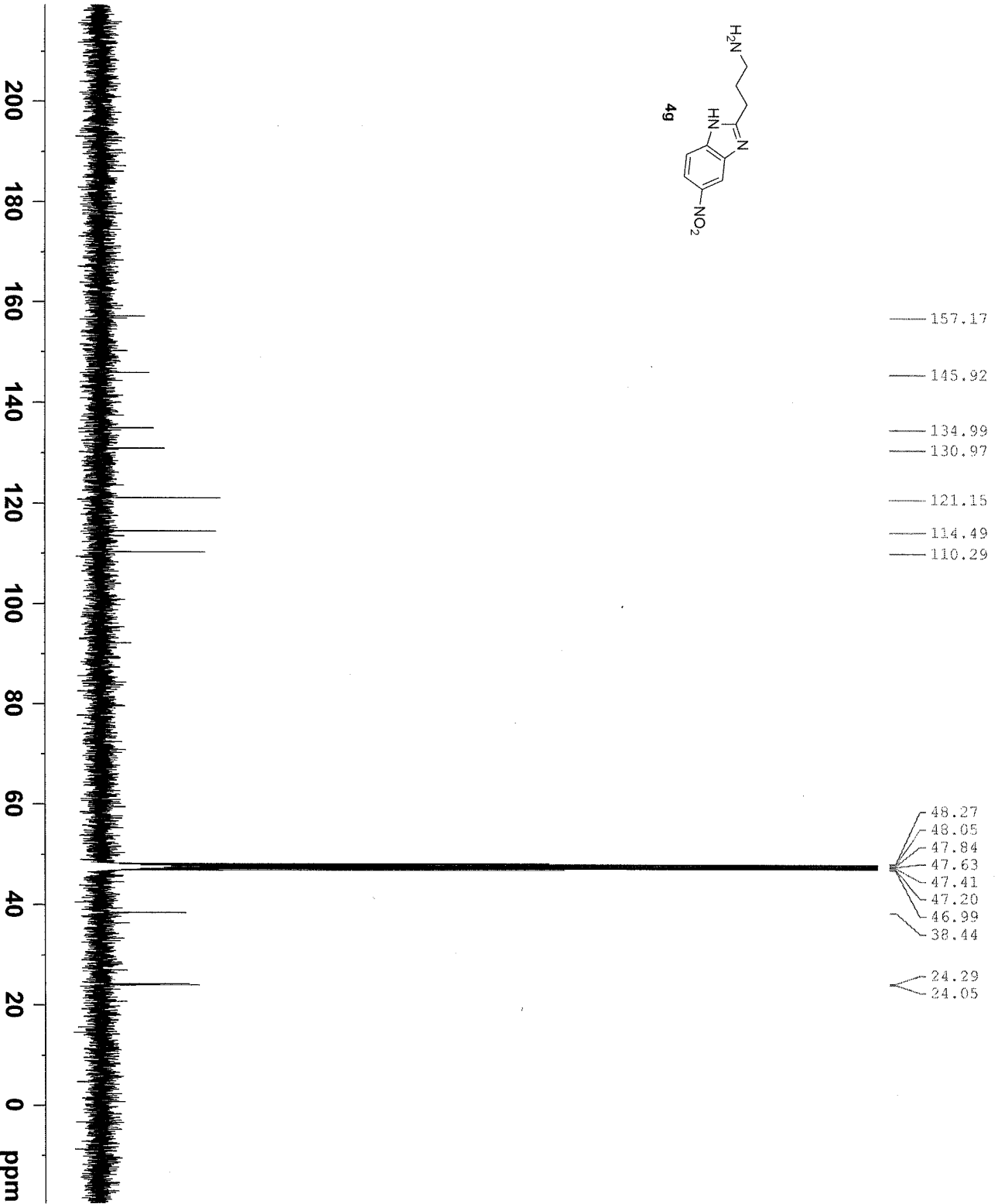
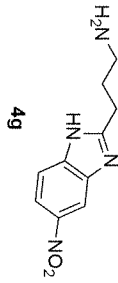
- 8.6893
- 8.6831
- 8.4550
- 7.9904
- 7.9603
- 4.8960
- 3.4255
- 3.3990
- 3.3731
- 3.3083
- 3.3037
- 3.2986
- 3.2935
- 3.1844
- 3.1595
- 3.1341
- 2.3930
- 2.3656
- 2.3410
- 2.3161
- 2.2909



F2 - Acquisition Parameters  
 Date\_ 20120411  
 Time\_ 20.44  
 INSTRUM spect  
 PROBHD 5 mm DUL 1H-13  
 PULPROG zg30  
 TD 65536  
 SOLVENT MeOD  
 NS 16  
 DS 2  
 SWH 6172.839 Hz  
 FIDRES 0.094190 Hz  
 AQ 5.3084660 sec  
 RG 912.3  
 DW 81.000 usec  
 DE 6.00 usec  
 TE 300.0 K  
 D1 1.00000000 sec  
 TD0 1

==== CHANNEL f1 =====  
 NUC1 1H  
 P1 10.50 usec  
 PL1 -1.00 dB  
 SFO1 300.1318534 MHz

F2 - Processing parameters  
 SI 32768  
 SF 300.1300067 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



Current Data Parameters  
 NAME LJE-2nd-37  
 EXPNO 2  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20120520  
 Time\_ 18.08

INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT MeOD  
 NS 213  
 DS 4

SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3631988 sec  
 RG 190.62  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 298.9 K  
 D1 2.0000000 sec  
 D11 0.0300000 sec  
 TD0 1

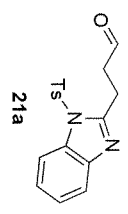
==== CHANNEL f1 =====  
 NUCL1 13C  
 P1 10.00 usec  
 PLM1 52.00000000 W  
 SFO1 100.6429474 MHz

==== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUCC2 1H  
 PCDP2 90.00 usec  
 PLM2 12.00000000 W  
 PLM12 0.33333001 W  
 PLM13 0.27000001 W  
 SFO2 400.2116008 MHz

F2 - Processing parameters  
 SI 32768  
 SF 100.6328860 MHz  
 WDM EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

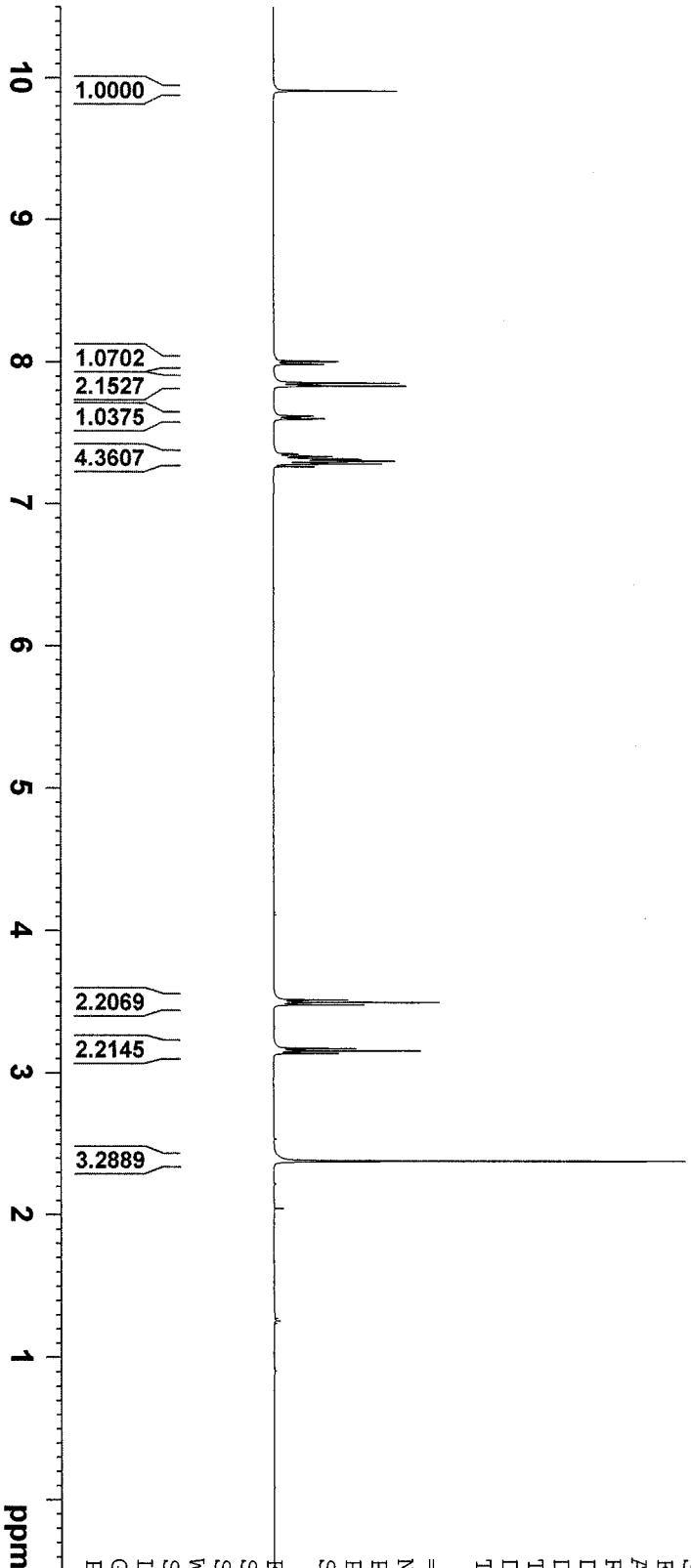


Current Data Parameters  
 NAME LJE-296  
 EXPNO 5  
 PROCNO 1



- 9.9084
- 8.0127
- 8.0112
- 8.0077
- 7.9945
- 7.9912
- 7.9893
- 7.9878
- 7.8576
- 7.8534
- 7.8408
- 7.8366
- 7.6242
- 7.6223
- 7.6189
- 7.6065
- 7.6025
- 7.3528
- 7.3382
- 7.3343
- 7.3210
- 7.3201
- 7.3161
- 7.3066
- 7.3052
- 7.3028
- 7.2986
- 7.2852
- 7.2839
- 7.2636

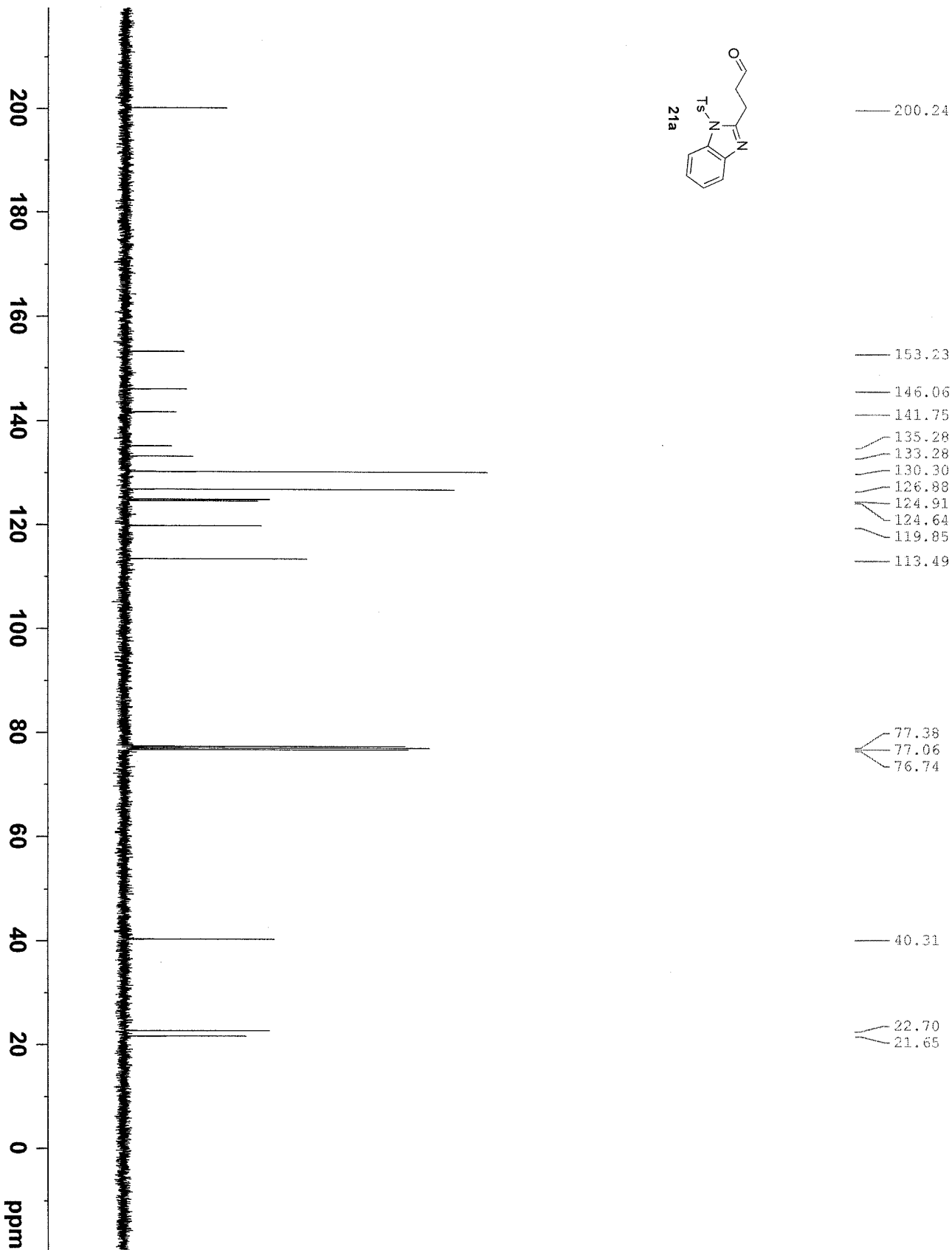
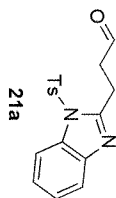
- 3.5126
- 3.4956
- 3.4787
- 3.1719
- 3.1552
- 3.1539
- 3.1378
- 2.3773



F2 - Acquisition Parameters  
 Date\_ 20130205  
 Time 15.10  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 16  
 DS 2  
 SWH 8223.685 Hz  
 FIDRES 0.125483 Hz  
 AQ 3.9846387 sec  
 RG 76.56  
 DW 60.800 usec  
 DE 6.50 usec  
 TE 299.6 K  
 D1 1.00000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 NUCL 1H  
 P1 15.00 usec  
 PLM1 12.00000000 W  
 SFO1 400.2124715 MHz

F2 - Processing parameters  
 SI 65536  
 SF 400.2100112 MHz  
 WDM EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



Current Data Parameters  
 NAME LJD-296  
 EXPNO 6  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20130205  
 Time 13.13

INSTRUM spect  
 F2PROB 5 mm PABBO BBI  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 34  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.366728 Hz  
 AQ 1.3631268 sec  
 RG 130  
 TM 190.62  
 DE 20.60 usec  
 TE 301.2 K usec  
 DI 2.00000000 sec  
 D11 0.03000000 sec  
 TDO 1

CHANNEL f1

NUC1 13C  
 P1 10.00 usec  
 PL1 52.00000000 W  
 SFO1 100.6429474 MHz

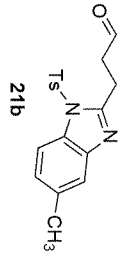
CHANNEL f2

CPDPRG2 walz216  
 NUC2 1H  
 PCPD2 90.00 usec  
 PLW2 12.00000000 W  
 PLW12 0.33333001 W  
 PLW13 0.27000001 W  
 SFO2 400.2116008 MHz

F2 - Processing Parameters

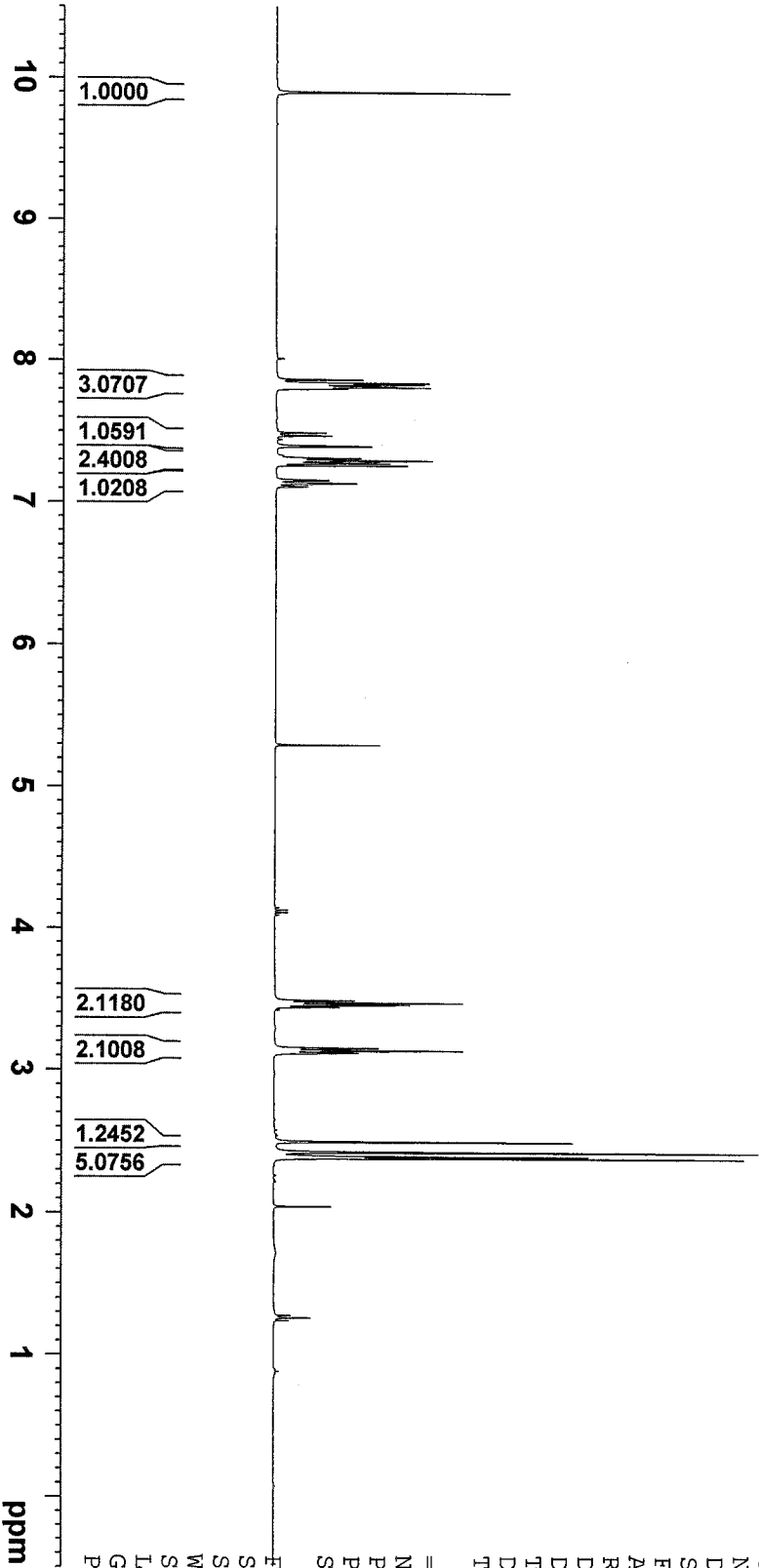
SI 32768  
 SF 100.6328860 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40





- 9.9006
- 7.8677
- 7.8451
- 7.8360
- 7.8229
- 7.8150
- 7.8071
- 7.8056
- 7.4915
- 7.4711
- 7.3968
- 7.3141
- 7.2979
- 7.2779
- 7.2608
- 7.1593
- 7.1355
- 7.1140

- 3.4863
- 3.4692
- 3.4561
- 3.4525
- 3.4393
- 3.1527
- 3.1355
- 3.1187
- 2.4922
- 2.4211
- 2.3909
- 2.3796



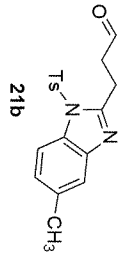
Current Data Parameters  
 NAME LJF-326  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters

Date\_ 20130327  
 Time\_ 19.49  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 16  
 DS 2  
 SWH 8223.685 Hz  
 FIDRES 0.125483 Hz  
 AQ 3.9846387 sec  
 RG 119.61  
 DW 60.800 usec  
 DE 6.50 usec  
 TE 298.8 K  
 D1 1.00000000 sec  
 TD0 1

==== CHANNEL f1 =====  
 NUC1 1H  
 P1 15.00 usec  
 PLW1 12.00000000 W  
 SF01 400.2124715 MHz

F2 - Processing parameters  
 SI 65536  
 SF 400.2100119 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

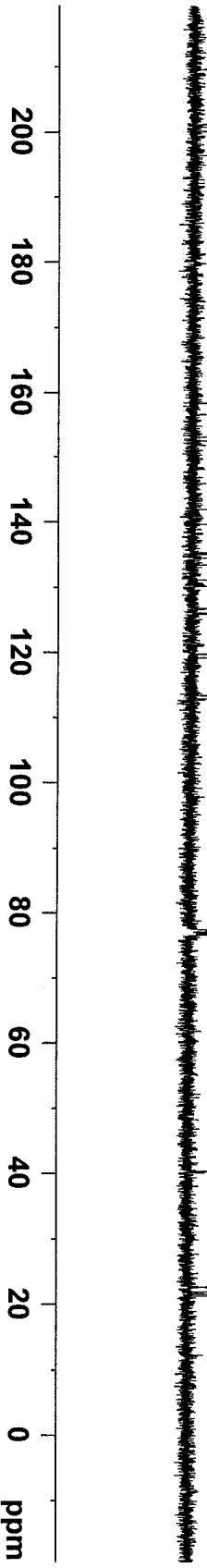


- 200.27
- 153.22
- 152.60
- 145.93
- 142.03
- 139.76
- 135.43
- 135.36
- 135.13
- 134.57
- 133.52
- 131.26
- 130.28
- 130.26
- 126.82
- 126.15
- 125.99
- 119.82
- 119.29
- 113.52
- 113.00

- 77.35
- 77.03
- 76.71

40.39

- 22.70
- 21.97
- 21.65
- 21.33



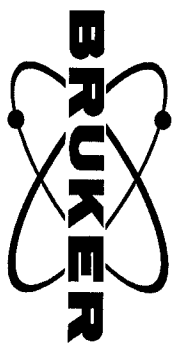
Current Data Parameters  
 NAME LTE-326  
 EXPNO 2  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20130327  
 Time\_ 19.52  
 INSTRUM spect  
 PROBD 5 mm PABBO BB/  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 73  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3631988 sec  
 RG 190.62  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 299.3 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TDO 1

===== CHANNEL f1 =====  
 NUCL1 13C  
 P1 10.00 usec  
 PLW1 52.00000000 W  
 SFO1 100.6429474 MHz

===== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUCL2 1H  
 P2 90.00 usec  
 PLW2 12.00000000 W  
 PLW2 0.3323001 W  
 P1M13 0.2720001 W  
 SFO2 400.2116008 MHz

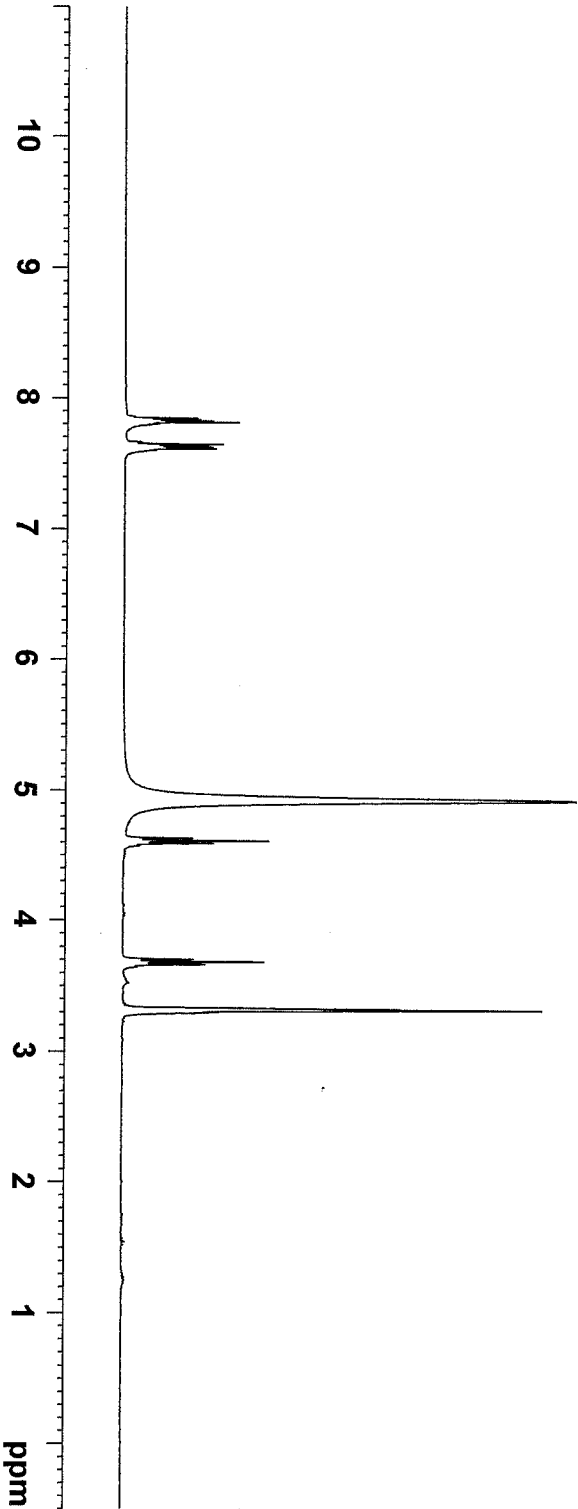
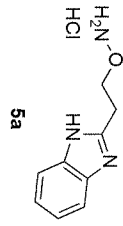
F2 - Processing parameters  
 SI 32768  
 SF 100.6328660 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40



Current Data Parameters  
 NAME KTH-m-138  
 EXPNO 1  
 PROCNO 1

7.8460  
 7.8354  
 7.8248  
 7.8147  
 7.6479  
 7.6370  
 7.6270  
 7.6168

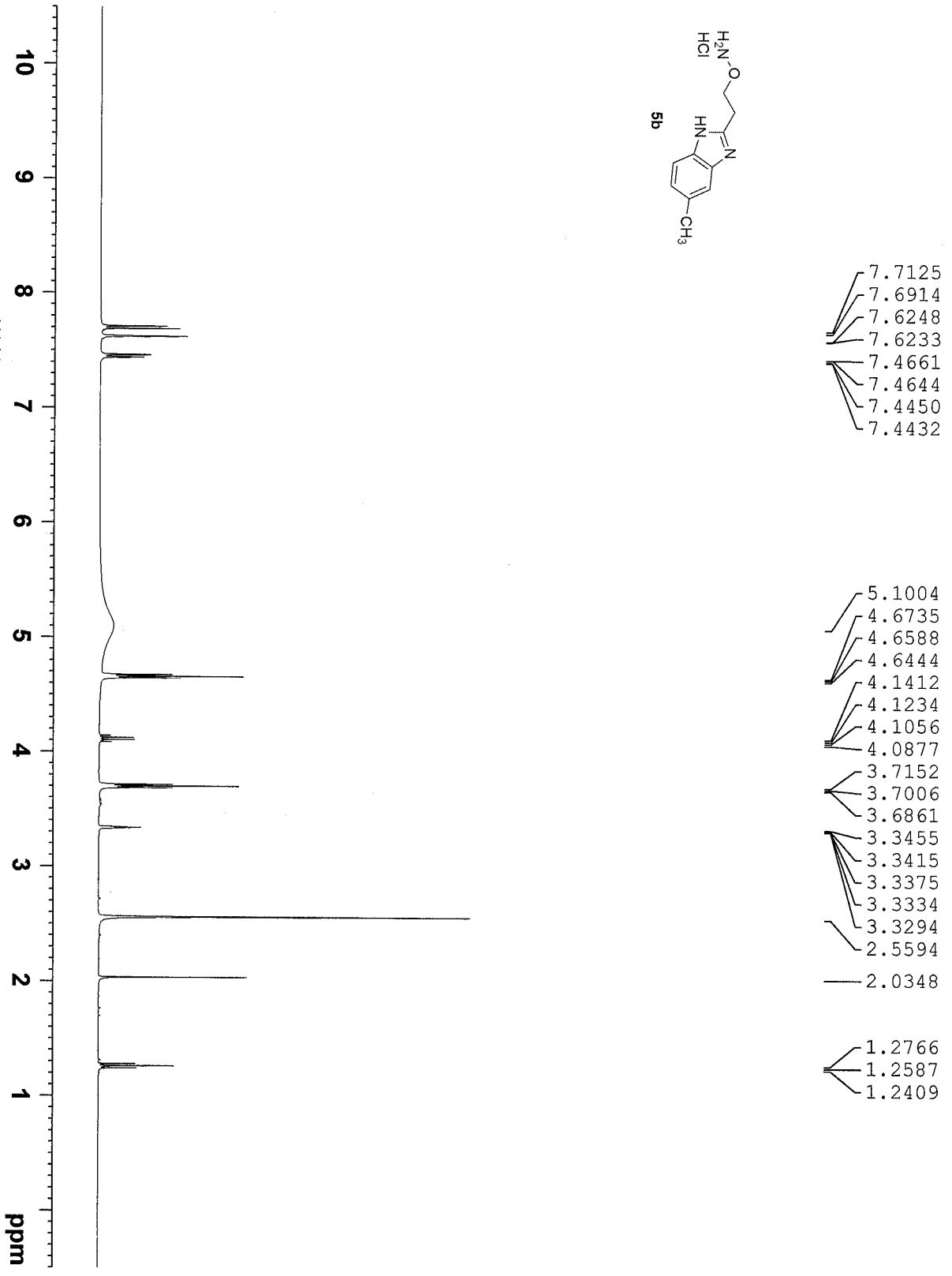
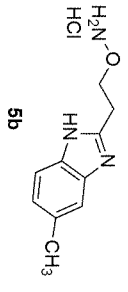
4.9329  
 4.6346  
 4.6148  
 4.5956  
 3.7078  
 3.6882  
 3.6688  
 3.3318  
 3.3263  
 3.3211  
 3.3158  
 3.3089  
 3.3030  
 3.2977



F2 - Acquisition Parameters  
 Date\_ 20120422  
 Time 19.17  
 INSTRUM spect  
 PROBHD 5 mm DUL 1H-13  
 PULPROG zg30  
 TD 65536  
 SOLVENT MeOD  
 NS 16  
 DS 2  
 SWH 6172.839 Hz  
 FIDRES 0.094190 Hz  
 AQ 5.3084660 sec  
 RG 812.7  
 DW 81.000 usec  
 DE 6.00 usec  
 TE 300.0 K  
 D1 1.00000000 sec  
 TD0 1

==== CHANNEL f1 =====  
 NUCL1 1H  
 P1 10.50 usec  
 PL1 -1.00 dB  
 SFO1 300.1318534 MHz

F2 - Processing parameters  
 SI 32768  
 SF 300.1300000 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

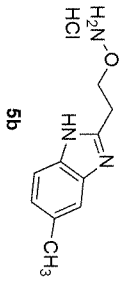


Current Data Parameters  
 NAME KTH-m-155  
 EXPNO 1  
 PROCNO 1

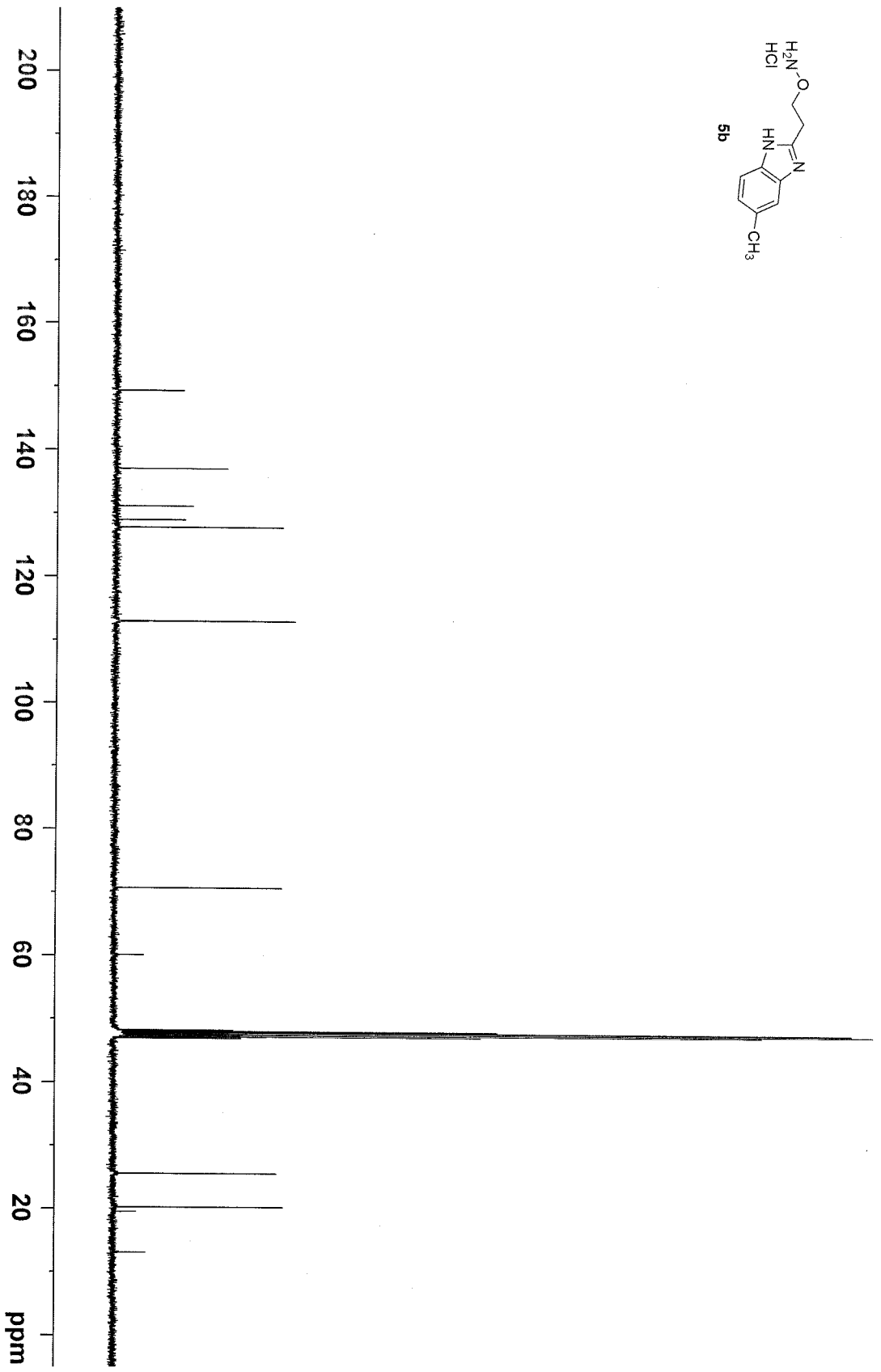
F2 - Acquisition Parameters  
 Date\_ 20120614  
 Time 10.07  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zg30  
 TD 65536  
 SOLVENT MeOD  
 NS 16  
 DS 2  
 SWH 8223.685 Hz  
 FIDRES 0.125483 Hz  
 AQ 3.9846387 sec  
 RG 58.64  
 DW 60.800 usec  
 DE 6.50 usec  
 TE 296.0 K  
 D1 1.00000000 sec  
 TD0 1

==== CHANNEL f1 =====  
 NUC1 1H  
 P1 15.00 usec  
 PLM1 12.00000000 W  
 SFO1 400.2124715 MHz

F2 - Processing parameters  
 SI 65536  
 SF 400.2100000 MHz  
 WDM EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



- 149.37
- 137.10
- 131.16
- 128.94
- 127.75
- 113.03
- 112.98
- 70.67
- 48.28
- 48.07
- 47.85
- 47.64
- 47.43
- 47.21
- 47.00
- 25.59
- 20.26



Current Data Parameters  
 NAME KTH-m-152  
 EXNO 2  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20120614  
 Time\_ 10.11  
 INSTRUM spect  
 PROBD 5 mm PABBO BB/  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT MeOD  
 NS 127  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.363198 sec  
 RG 190.62  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 296.8 K  
 D1 2.0000000 sec  
 D11 0.0300000 sec  
 TDO 1

CHANNEL F1  
 NUC1 13C  
 P1 10.00 usec  
 PLM1 52.00000000 W  
 SFO1 100.6429474 MHz

CHANNEL F2  
 CPDPRG2 waltz16  
 NUC2 1H  
 PCPD2 90.00 usec  
 PLW2 12.00000000 W  
 PLM2 0.33333001 W  
 PLW3 0.27000001 W  
 SFO2 400.2116008 MHz

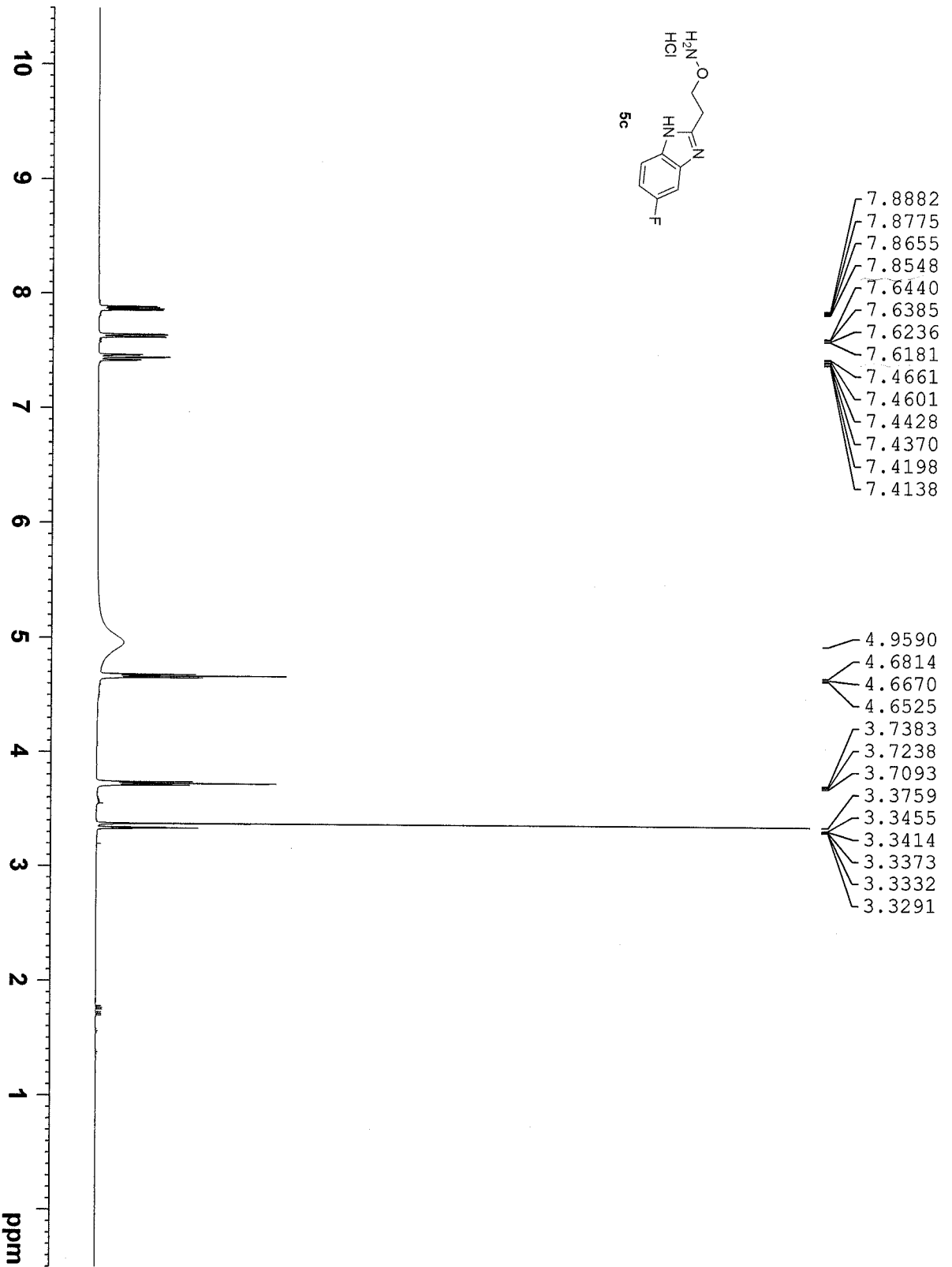
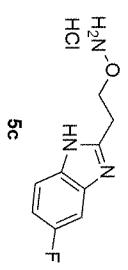
F2 - Processing parameters  
 SI 32768  
 SF 100.6328860 MHz  
 WDM EM  
 SSB 0  
 GB 1.00 Hz  
 LB 0  
 FC 1.40

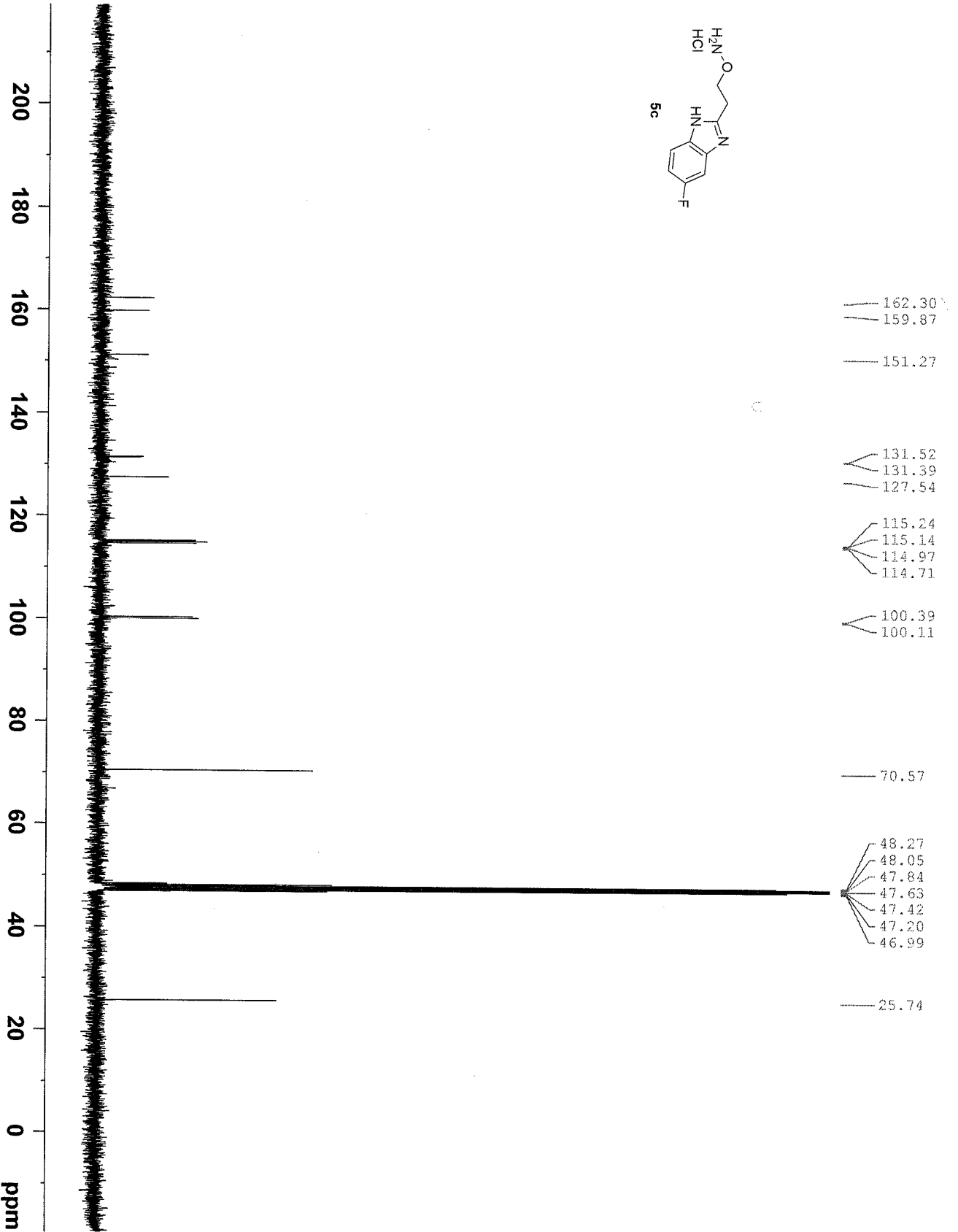
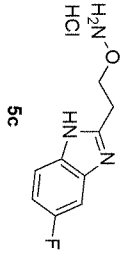


Current Data Parameters  
 NAME KTH-m-162  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20120624  
 Time\_ 23.58  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zg30  
 TD 65536  
 SOLVENT MeOD  
 NS 16  
 DS 2  
 SWH 8223.685 Hz  
 FIDRES 0.125483 Hz  
 AQ 3.9846387 sec  
 RG 84.76  
 DW 60.800 usec  
 DE 6.50 usec  
 TE 297.9 K  
 D1 1.00000000 sec  
 TD0 1

==== CHANNEL f1 =====  
 NUC1 1H  
 P1 15.00 usec  
 P1M1 12.00000000 W  
 SFO1 400.2124715 MHz  
 F2 - Processing parameters  
 SI 65536  
 SF 400.2100000 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00





Current Data Parameters  
 NAME K1H-M-162  
 EXNO 2  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20120629  
 Time\_ 0.03  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT MeOD  
 NS 78  
 DS 4  
 SSW 24038.461 Hz  
 FTIDRES 0.366798 Hz  
 AQ 1.3631988 sec  
 RG 190.62  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 298.6 K  
 D1 2.0000000 sec  
 D11 0.0300000 sec  
 TDO 1

===== CHANNEL f1 =====  
 NUC1 13C  
 P1 10.00 usec  
 PLW1 52.0000000 W  
 SFO1 100.6429474 MHz

===== CHANNEL f2 =====  
 CPDPRG2 waitz16  
 NUC2 1H  
 PCPD2 90.00 usec  
 PLW2 12.0000000 W  
 PLW12 0.33333001 W  
 PLW13 0.27000001 W  
 SFO2 400.2116008 MHz

F2 - Processing parameters  
 SI 32768  
 SF 100.6388860 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40



Current Data Parameters  
NAME KTH-m-153  
EXPNO 2  
PROCNO 1

F2 - Acquisition Parameters

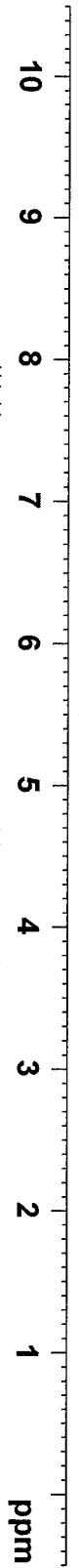
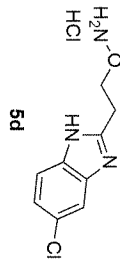
Date\_ 20120612  
Time 21.58  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zg30  
TD 65536  
SOLVENT MeOD  
NS 16  
DS 2  
SWH 8223.685 Hz  
FIDRES 0.125483 Hz  
AQ 3.9846387 sec  
RG 171.62  
DW 60.800 usec  
DE 6.50 usec  
TE 296.2 K  
D1 1.00000000 sec  
TD0 1

==== CHANNEL f1 =====

NUC1 1H  
P1 15.00 usec  
PLW1 12.00000000 W  
SFO1 400.2124715 MHz

F2 - Processing parameters

SI 65536  
SF 400.2100000 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



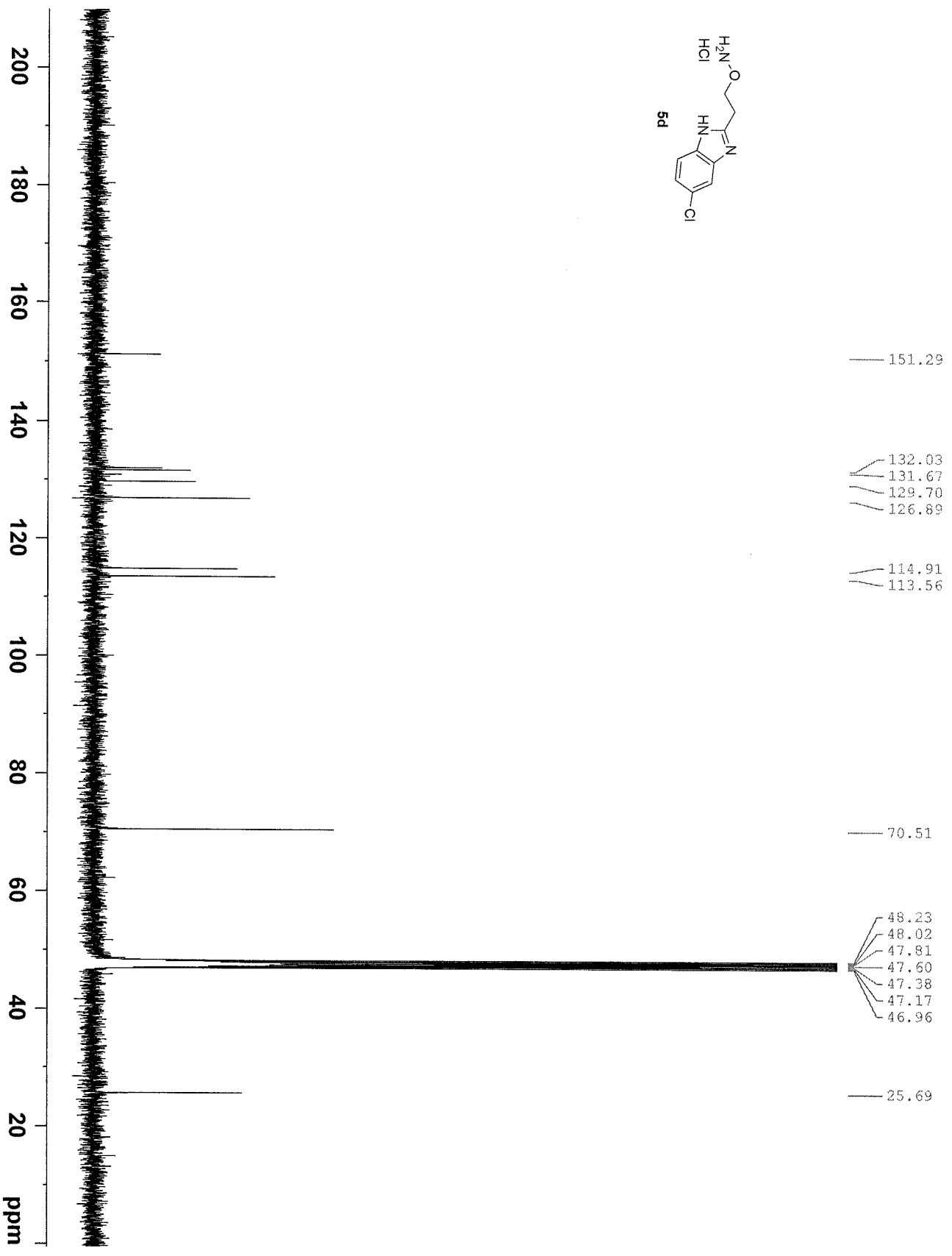
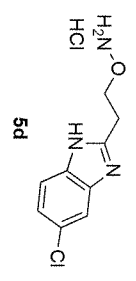
- 7.9094
- 7.8538
- 7.8471
- 7.8318
- 7.8251
- 7.6672
- 7.6624
- 7.6549
- 7.6452
- 7.6404
- 7.6330
- 5.0252
- 4.9312
- 4.6569
- 4.6426
- 4.6282
- 4.6188
- 3.7219
- 3.7073
- 3.6924
- 3.3372

- 1.0000
- 1.1433
- 1.1462

- 2.0777

- 2.0612





Current Data Parameters  
 NAME KTH-m-153  
 EXPNO 3  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20120613  
 Time 8.55

INSTRUM spect  
 PROBHD 5 mm PABBO BH/  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT MeOD  
 NS 11477  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3631988 sec  
 RG 190.62  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 297.3 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TDO 1

CHANNEL f1  
 NUCL 13C  
 P1 10.00 usec  
 PLM1 52.00000000 W  
 SF01 100.6429474 MHz

CHANNEL f2  
 CPDPRG2 waltz16  
 NUC2 1H  
 PCPD2 90.00 usec  
 PLM2 12.00000000 W  
 PLM12 0.33333001 M  
 PLM13 0.27000001 M  
 SF02 400.2116008 MHz

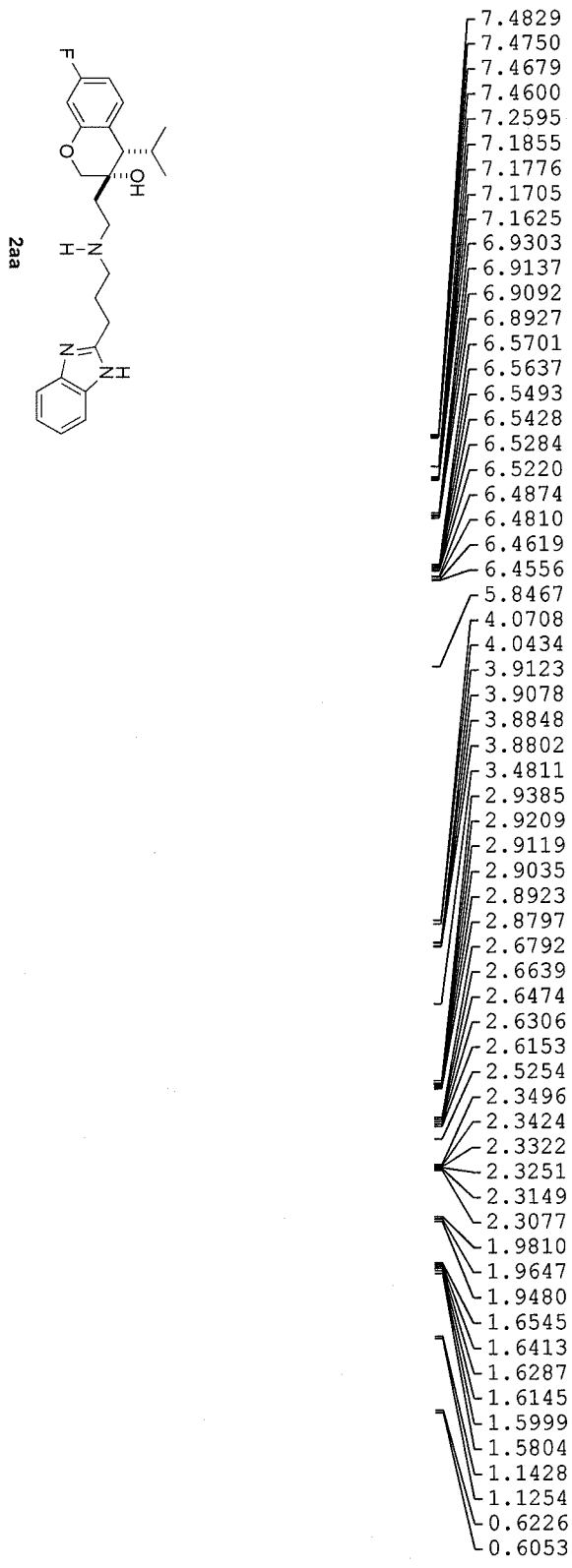
F2 - Processing Parameters  
 SI 32768  
 SF 100.6328960 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40



Current Data Parameters  
 NAME LTJ-182  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20120531  
 Time\_ 20.35  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 16  
 DS 2  
 SWH 8223.685 Hz  
 FIDRES 0.125483 Hz  
 AQ 3.9846387 sec  
 RG 33.2  
 DW 60.800 usec  
 DE 6.50 usec  
 TE 298.4 K  
 D1 1.00000000 sec  
 TDO 1

==== CHANNEL f1 =====  
 NUC1 1H  
 P1 15.00 usec  
 PL1 12.00000000 W  
 SFO1 400.2124715 MHz  
 F2 - Processing parameters  
 S1 65536  
 SF 400.2100130 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00





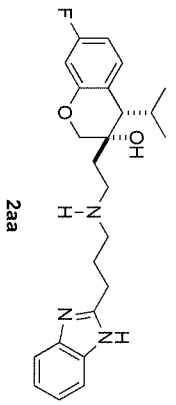
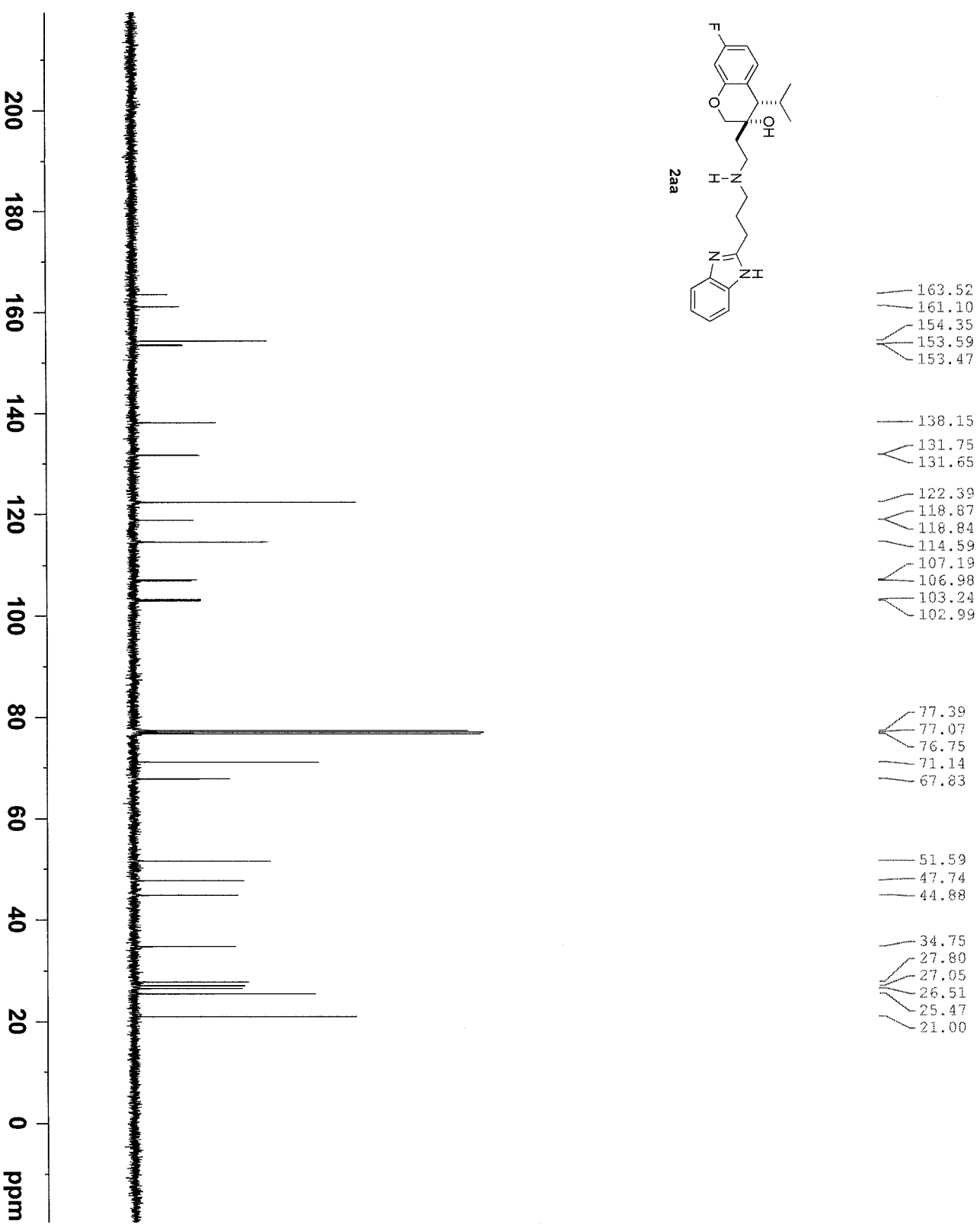
Current Data Parameters  
 NAME LJE-182  
 EXPNO 2  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20120531  
 Time 20.42  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 100  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3631988 sec  
 RG 190.62  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 299.2 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TD0 1

==== CHANNEL f1 =====  
 NUC1 13C  
 P1 10.00 usec  
 PLW1 52.00000000 W  
 SFO1 100.6429474 MHZ

==== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUC2 1H  
 PCPD2 90.00 usec  
 PLW2 12.00000000 W  
 PLW12 0.33333001 W  
 PLW13 0.27000001 W  
 SFO2 400.2116008 MHZ

F2 - Processing parameters  
 SI 32768  
 SF 100.6328860 MHZ  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40





Current Data Parameters  
 NAME LJE-285  
 EXPNO 4  
 PROCNO 1

F2 - Acquisition Parameters

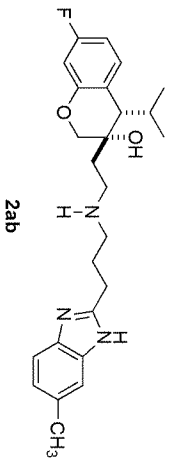
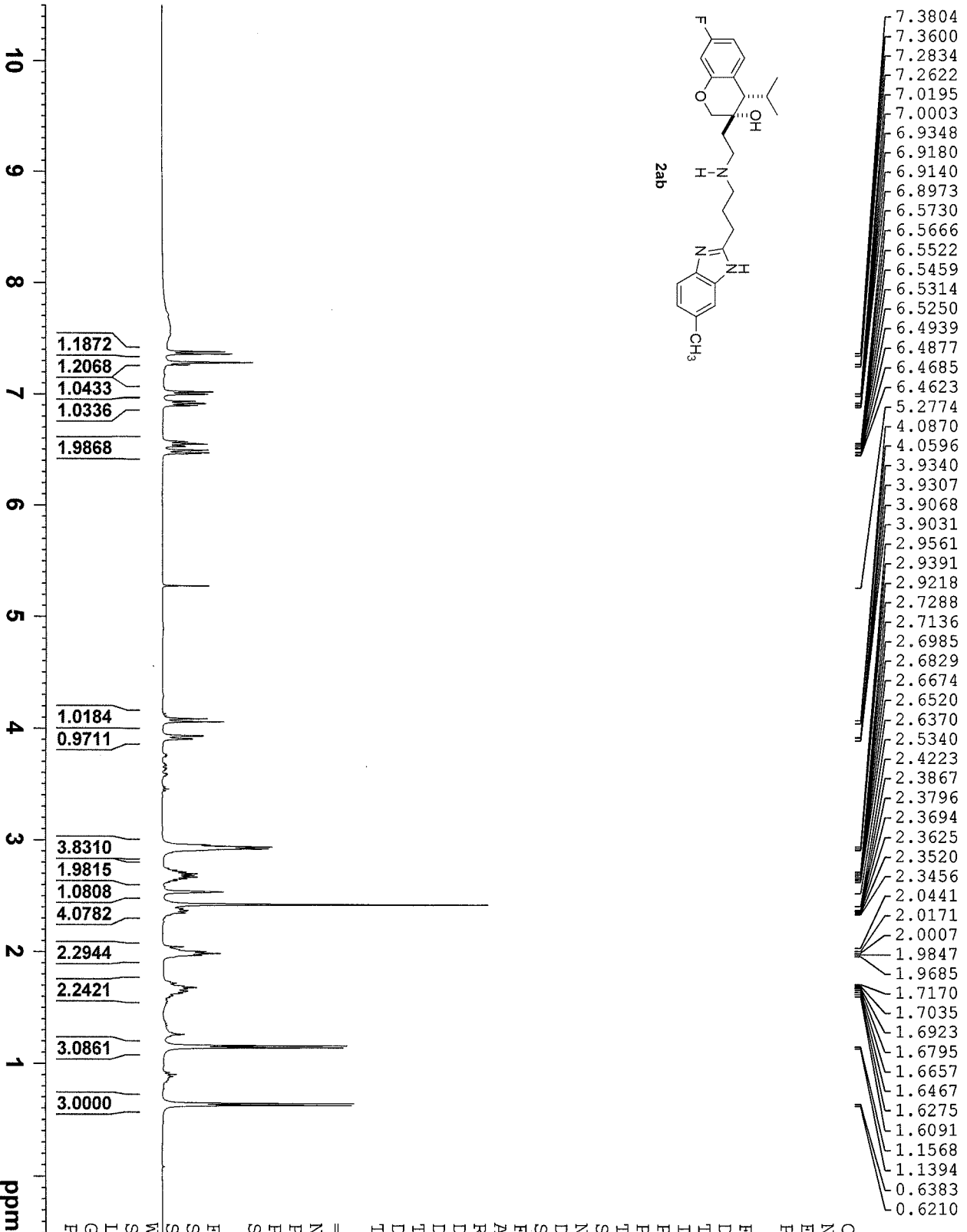
Date\_ 20130102  
 Time 15.44  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 7  
 DS 2  
 SWH 8223.685 Hz  
 FIDRES 0.125483 Hz  
 AQ 3.9846387 sec  
 RG 33.2  
 DW 60.800 usec  
 DE 6.50 usec  
 TE 298.4 K  
 D1 1.00000000 sec  
 TD0 1

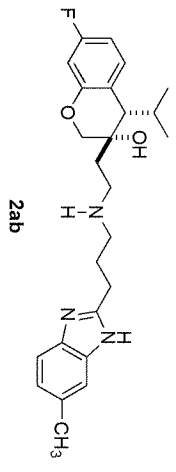
==== CHANNEL f1 =====

NUC1 1H  
 P1 15.00 usec  
 PLW1 12.00000000 W  
 SFO1 400.2124715 MHz

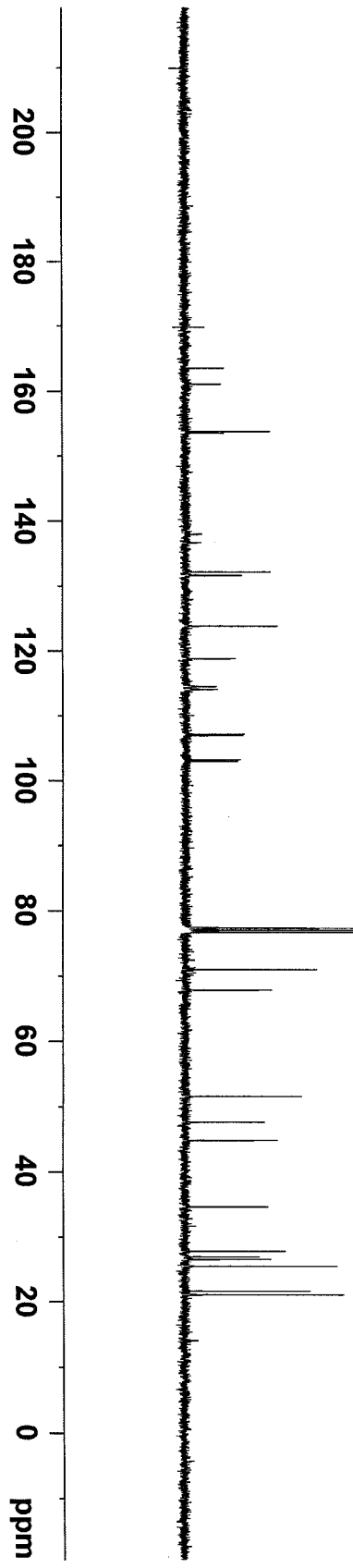
F2 - Processing parameters

SI 65536  
 SF 400.2100118 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00





- 163.53
- 161.11
- 153.77
- 153.63
- 153.51
- 138.01
- 136.73
- 132.20
- 131.73
- 131.63
- 123.81
- 118.85
- 118.82
- 114.57
- 114.13
- 107.19
- 106.97
- 103.26
- 103.01
- 77.38
- 77.06
- 76.74
- 71.02
- 67.84
- 51.60
- 47.66
- 44.83
- 34.60
- 27.82
- 26.96
- 26.56
- 25.49
- 21.61
- 21.02



Current Data Parameters  
 NAME LJE-285  
 EXPNO 6  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20130113  
 Time 14.18  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 214  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.356798 Hz  
 AQ 1.363198 sec  
 RG 190.62  
 DW 20.890 usec  
 DE 6.90 usec  
 TE 295.6 K  
 D1 2.0000000 sec  
 D11 0.0500000 sec  
 TDO 1

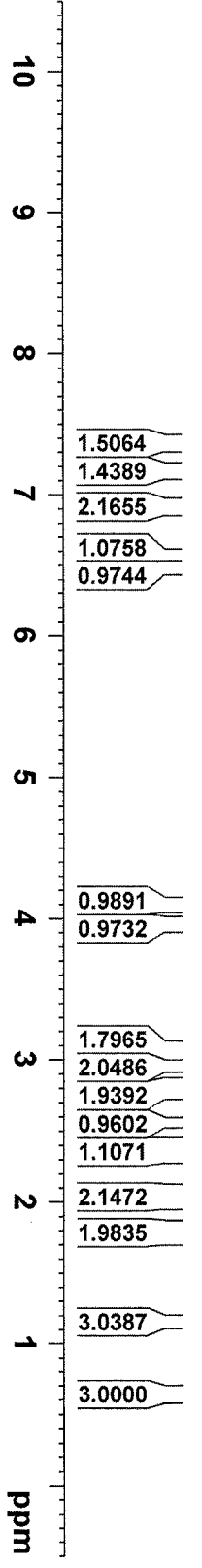
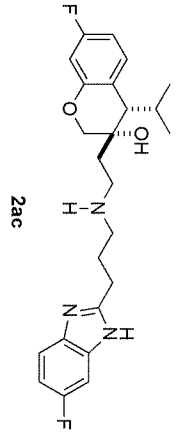
CHANNEL F1  
 NUC1 13C  
 P1 10.00 usec  
 PL1 52.00000000 W  
 SFO1 100.6229474 MHz

CHANNEL F2  
 waltz16  
 NUC2 1H  
 P2 90.00 usec  
 PL2 12.00000000 W  
 PLM12 0.3333001 W  
 PLM13 0.27000001 W  
 SFO2 400.2116008 MHz

F2 - Processing parameters  
 SI 32768  
 SF 100.6228660 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40



- 7.3809
- 7.3693
- 7.3591
- 7.3475
- 7.2599
- 7.1773
- 7.1720
- 7.1552
- 7.1498
- 6.9523
- 6.9449
- 6.9364
- 6.9315
- 6.9215
- 6.9156
- 6.8993
- 6.8935
- 6.5930
- 6.5867
- 6.5723
- 6.5659
- 6.5515
- 6.5451
- 6.5056
- 6.4994
- 6.4803
- 6.4741
- 5.2929
- 4.1154
- 4.0879
- 3.9732
- 3.9695
- 3.9457
- 3.9418
- 3.0721
- 3.0539
- 3.0395
- 3.0257
- 3.0117
- 2.9818
- 2.9661
- 2.9497
- 2.8529
- 2.8368
- 2.8215
- 2.8024
- 2.7870
- 2.5678
- 2.3844
- 2.3774
- 2.3671
- 2.3602
- 2.3499
- 2.3430
- 2.0517
- 2.0367
- 2.0223
- 1.8150
- 1.1714
- 1.1541
- 0.6526
- 0.6354



```

Current Data Parameters
NAME      LJE-161
EXPNO    4
PROCNO   1

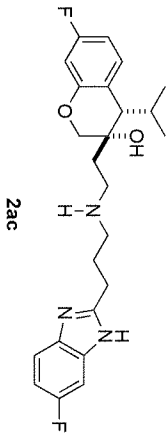
F2 - Acquisition Parameters
Date_    20120623
Time_    17.06
INSTRUM  spect
PROBHD   5 mm PABBO BB/
PULPROG  zg30
TD       65536
SOLVENT  CDCl3
NS       16
DS       2
SMH      8223.685 Hz
FIDRES   0.125483 Hz
AQ       3.9846387 sec
RG       119.61
DW       60.800 usec
DE       6.50 usec
TE       300.4 K
D1       1.00000000 sec
TD0      1

===== CHANNEL f1 =====
NUC1     1H
P1       15.00 usec
PLW1     12.00000000 W
SFO1     400.2124715 MHz

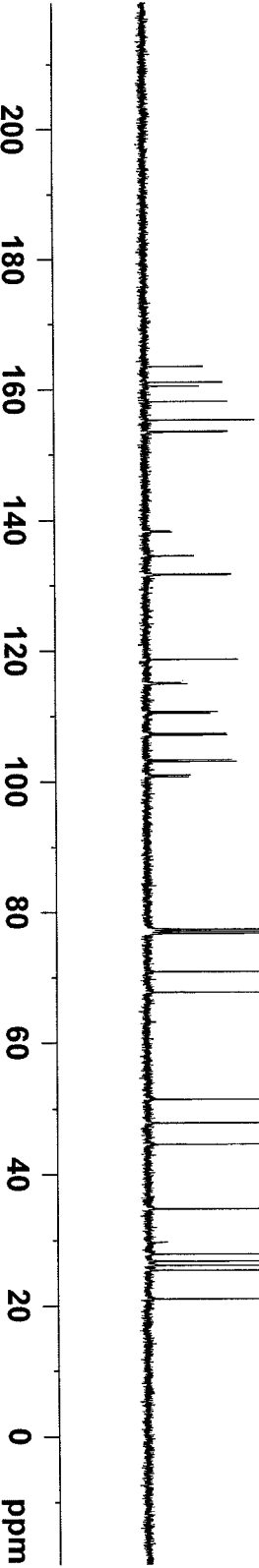
F2 - Processing parameters
SI       65536
SF       400.2100130 MHz
WDW      EM
SSB      0
LB       0.30 Hz
GB       0
PC       1.00
  
```



Current Data Parameters  
 NAME LJE-196  
 EXPNO 3  
 PROCNO 1



- 163.53
- 161.10
- 160.51
- 158.14
- 155.31
- 155.29
- 153.56
- 153.45
- 138.36
- 138.24
- 134.54
- 131.72
- 131.62
- 118.71
- 118.68
- 115.10
- 115.00
- 110.73
- 110.48
- 107.32
- 107.10
- 103.28
- 103.04
- 100.98
- 100.72
- 77.40
- 77.08
- 76.77
- 70.88
- 67.75
- 51.43
- 47.86
- 44.60
- 34.75
- 27.88
- 26.79
- 26.15
- 25.42
- 20.99



F2 - Acquisition Parameters

Date\_ 20120709  
 Time 15.30  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 325  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3631988 sec  
 RG 190.62  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 298.9 K  
 D1 2.0000000 sec  
 D11 0.03000000 sec  
 TD0 1

==== CHANNEL f1 =====

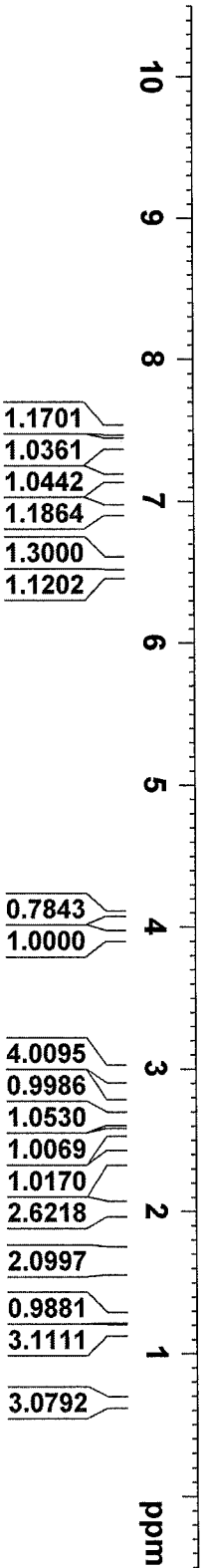
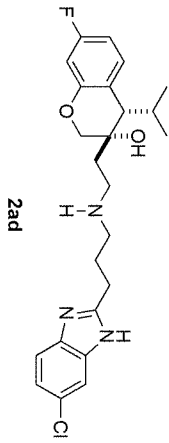
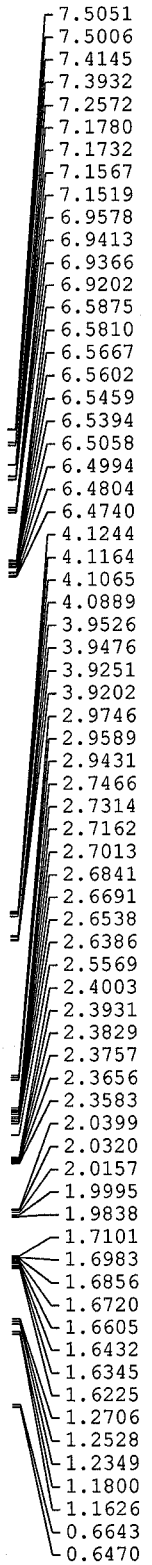
NUC1 13C  
 P1 10.00 usec  
 PLW1 52.00000000 W  
 SFO1 100.6429474 MHz

==== CHANNEL f2 =====

CPDPRG2 waltz16  
 NUC2 1H  
 PCPD2 90.00 usec  
 PLW2 12.00000000 W  
 PLW12 0.33333001 W  
 PLW13 0.27000001 W  
 SFO2 400.2116008 MHz

F2 - Processing parameters

SI 32768  
 SF 100.6328860 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40



Current Data Parameters  
NAME LJTE-175  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20120514  
Time 16.54  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SMH 8223.685 Hz  
FIDRES 0.125483 Hz  
AQ 3.9846387 sec  
RG 91.91  
DE 60.800 usec  
TE 298.4 K  
D1 1.00000000 sec  
TD0 1

==== CHANNEL f1 =====  
NUC1 1H  
P1 15.00 usec  
PLM1 12.00000000 W  
SFO1 400.2124715 MHz  
F2 - Processing parameters  
SI 65536  
SF 400.2100141 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00





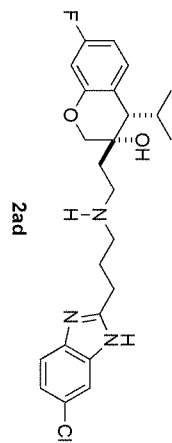
Current Data Parameters  
 NAME LJE-175  
 EXPNO 5  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20120623  
 Time 16.31  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 495  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3631988 sec  
 RG 190.62  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 304.3 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TD0 1

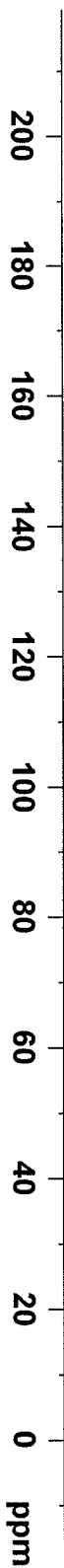
==== CHANNEL F1 =====  
 NUC1 13C  
 P1 10.00 usec  
 PLW1 52.00000000 W  
 SFO1 100.6429474 MHz

==== CHANNEL F2 =====  
 CPDPRG2 waltz16  
 NUC2 1H  
 PCPD2 90.00 usec  
 PLW2 12.00000000 W  
 PLW12 0.33333001 W  
 PLW13 0.27000001 W  
 SFO2 400.2116008 MHz

F2 - Processing parameters  
 SI 32768  
 SF 100.6328860 MHz  
 WDW EM  
 SSB 0  
 GB 1.00 Hz  
 PC 1.40

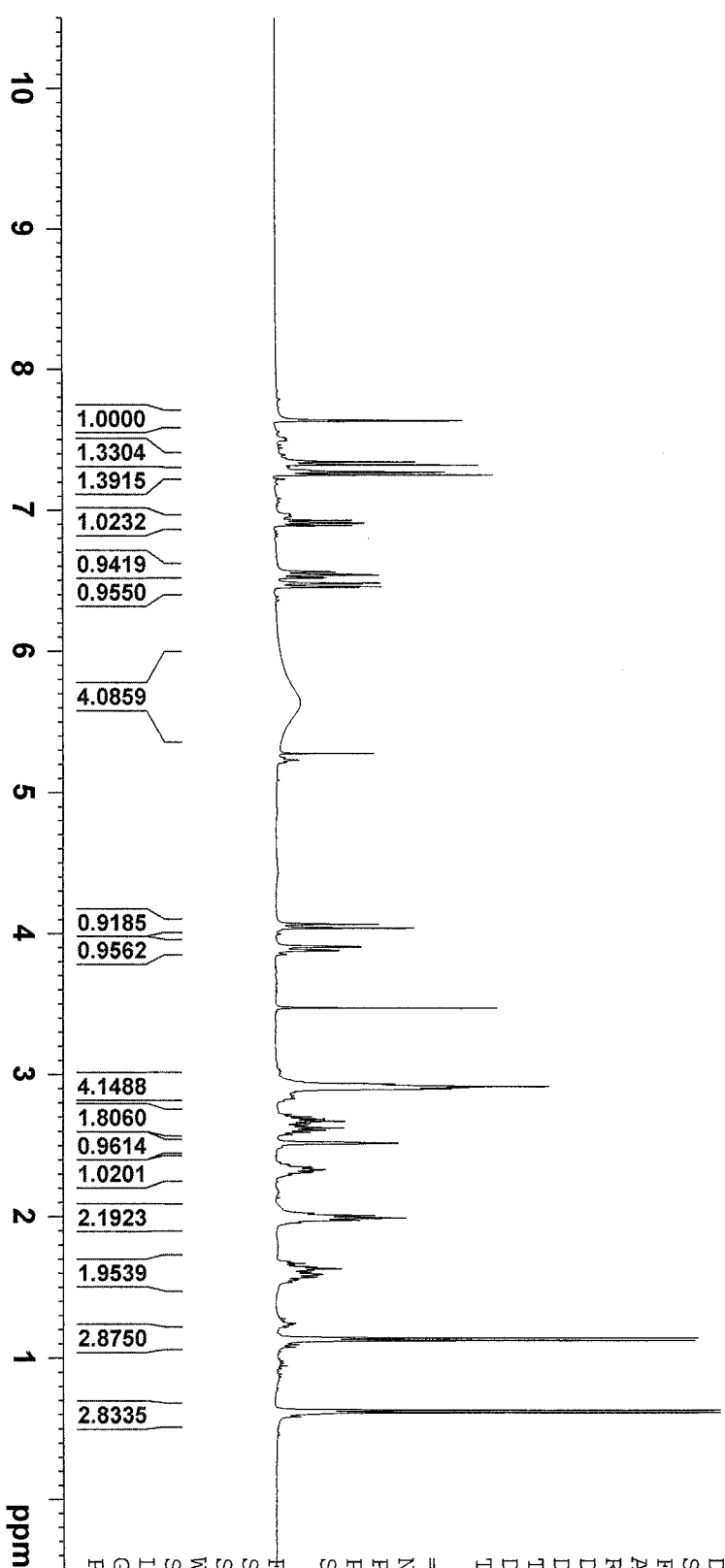
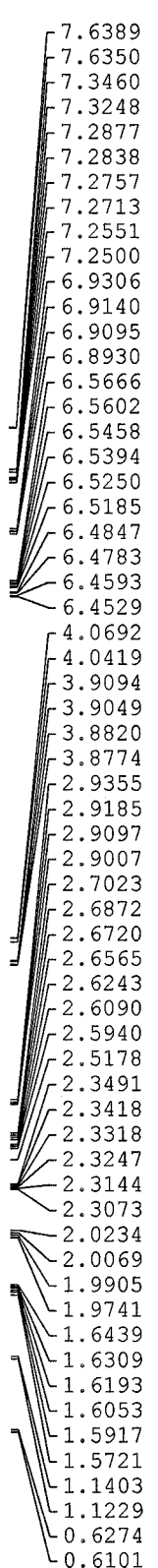
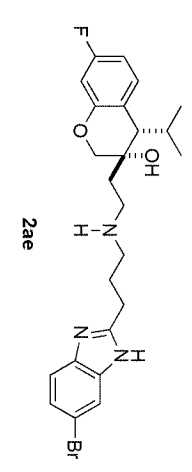


- 163.57
- 161.15
- 155.17
- 153.62
- 153.51
- 139.18
- 136.99
- 131.71
- 131.62
- 127.93
- 122.84
- 122.48
- 118.79
- 118.76
- 115.34
- 114.66
- 107.25
- 107.04
- 103.29
- 103.05
- 77.33
- 77.01
- 76.69
- 71.34
- 67.85
- 51.70
- 47.54
- 45.06
- 34.60
- 27.89
- 27.14
- 26.46
- 25.47
- 21.01





Current Data Parameters  
 NAME IJE-325  
 EXPNO 3  
 PROCNO 1



F2 - Acquisition Parameters  
 Date\_ 20130329  
 Time\_ 15.24  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 4  
 DS 2  
 SWH 8223.685 Hz  
 FIDRES 0.125483 Hz  
 AO 3.9846387 sec  
 RG 69.69  
 DW 60.800 usec  
 DE 6.50 usec  
 TE 298.5 K  
 D1 1.00000000 sec  
 TD0 1

==== CHANNEL f1 =====  
 NUC1 1H  
 P1 15.00 usec  
 PLW1 12.00000000 W  
 SFO1 400.2124715 MHz

F2 - Processing parameters  
 SI 65536  
 SF 400.2100148 MHz  
 MDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

ppm



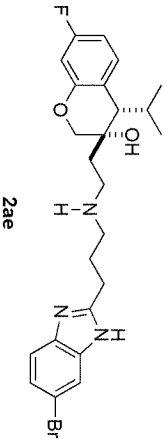
Current Data Parameters  
 NAME IJE-195  
 EXPNO 5  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20120715  
 Time\_ 16.35  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDC13  
 NS 2803  
 DS 4  
 SWSH 24038.461 Hz  
 FTDRS 0.366798 Hz  
 AQ 1.3631988 sec  
 RG 190.62  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 298.9 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TDO 1

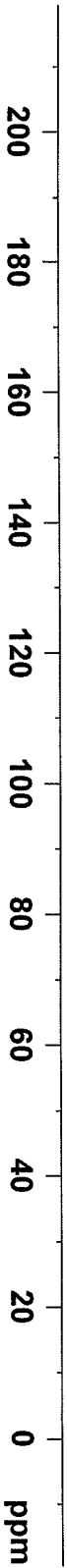
==== CHANNEL f1 =====  
 NUC1 13C  
 P1 10.00 usec  
 PLW1 52.00000000 W  
 SFO1 100.6429474 MHz

==== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUC2 1H  
 PCPD2 90.00 usec  
 PLM2 12.00000000 W  
 PLM12 0.33333001 W  
 PLM13 0.27000001 W  
 SFO2 400.2116008 MHz

F2 - Processing parameters  
 SI 32768  
 SF 100.6328860 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40



- 163.60
- 161.17
- 154.32
- 153.45
- 153.33
- 138.34
- 135.97
- 131.72
- 131.62
- 130.93
- 128.84
- 126.01
- 118.22
- 118.19
- 117.61
- 115.88
- 107.70
- 107.49
- 103.48
- 103.24
- 77.34
- 77.02
- 76.70
- 70.23
- 67.16
- 50.92
- 48.07
- 43.87
- 34.45
- 29.70
- 28.07
- 26.73
- 25.35
- 23.39
- 21.02





Current Data Parameters  
 NAME LJE-325  
 EXPNO 4  
 PROCNO 1

F2 - Acquisition Parameters

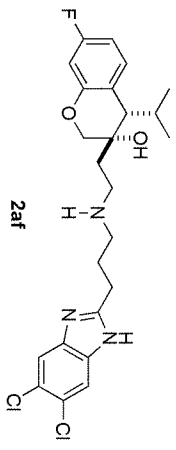
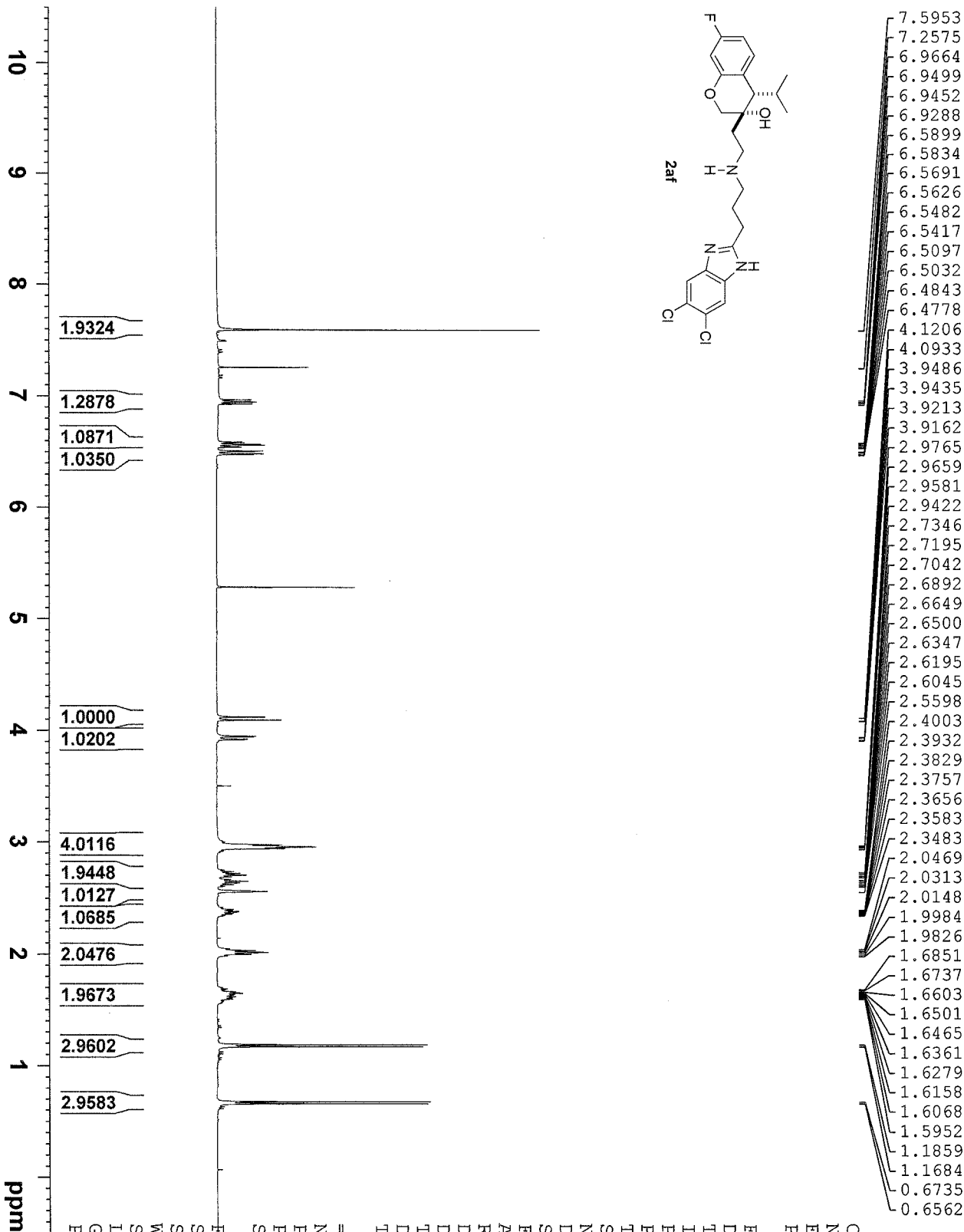
Date\_ 20130329  
 Time\_ 15.31  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 3  
 DS 2  
 SWH 8223.685 Hz  
 FIDRES 0.125483 Hz  
 AO 3.9846387 sec  
 RG 84.76  
 DW 60.800 usec  
 DE 6.50 usec  
 TE 298.4 K  
 D1 1.00000000 sec  
 TD0 1

==== CHANNEL F1 =====

NUC1 1H  
 P1 15.00 usec  
 PLW1 12.00000000 W  
 SFO1 400.2124715 MHz

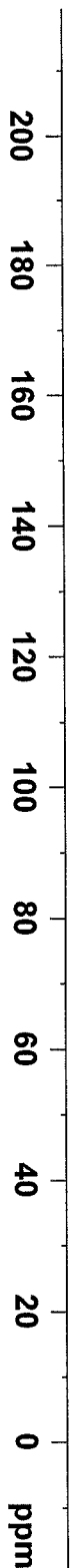
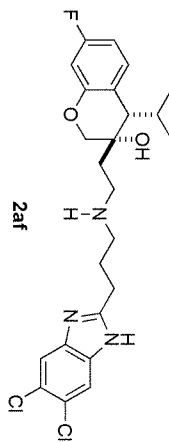
F2 - Processing parameters

SI 65536  
 SF 400.2100138 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00





- 163.54
- 161.12
- 156.54
- 153.59
- 153.47
  
- 137.79
- 131.73
- 131.63
- 126.14
- 118.75
- 118.72
- 115.88
- 107.27
- 107.05
- 103.28
- 103.04
  
- 77.37
- 77.05
- 76.73
- 71.58
- 67.90
  
- 51.69
- 47.55
- 45.21
  
- 34.62
- 27.84
- 27.43
- 26.46
- 25.50
- 20.97



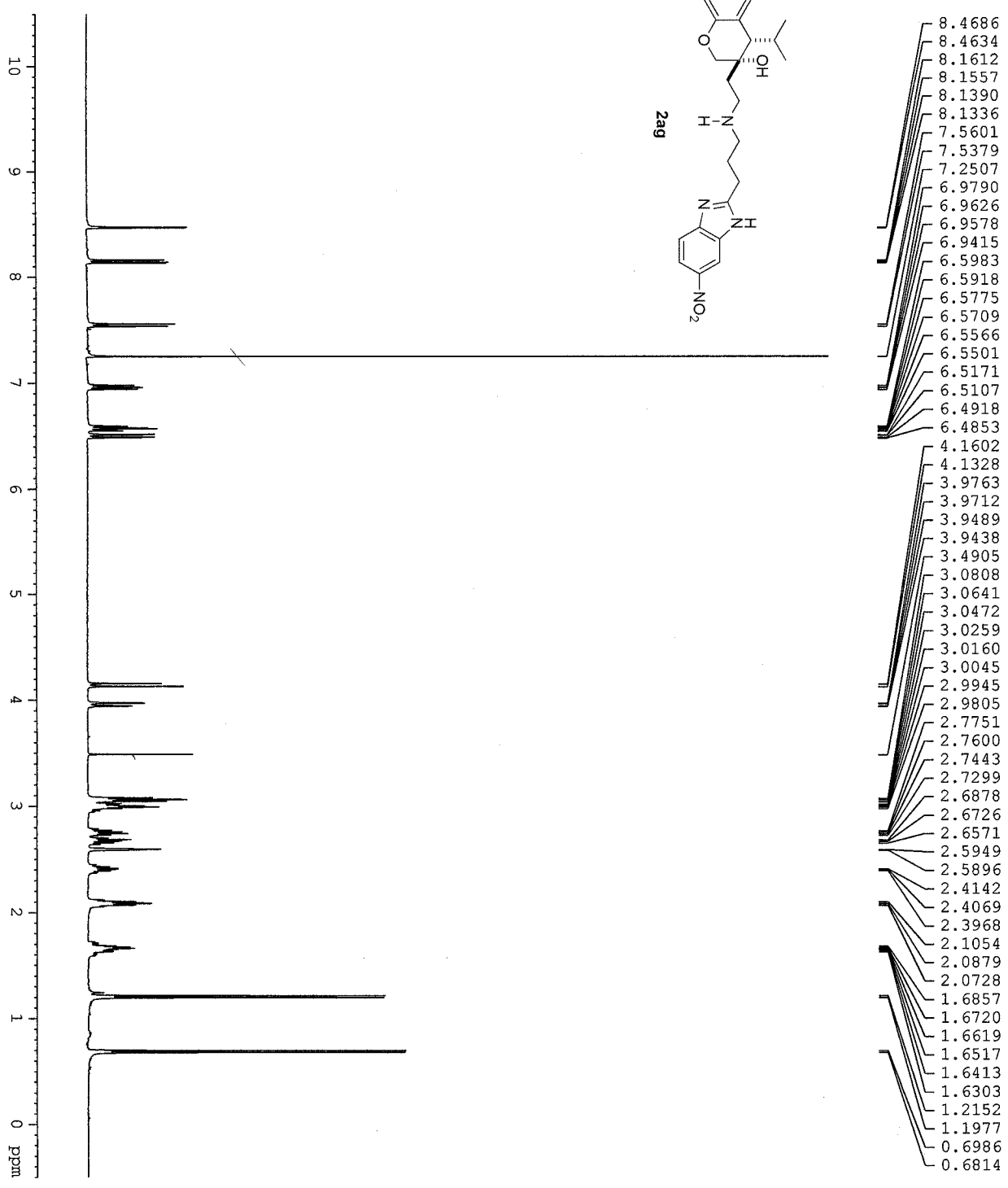
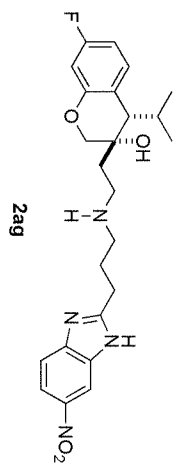
Current Data Parameters  
 NAME LJE-183  
 EXPNO 2  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20120601  
 Time 17.14  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 75  
 DS 4  
 SMH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AO 1.3631988 sec  
 RG 190.62  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 299.2 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TD0 1

==== CHANNEL f1 =====  
 NUC1 13C  
 P1 10.00 usec  
 PLW1 52.00000000 W  
 SFO1 100.6429474 MHz

==== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUC2 1H  
 PCPD2 90.00 usec  
 PLW2 12.00000000 W  
 PLW12 0.33333001 W  
 PLW13 0.27000001 W  
 SFO2 400.2116008 MHz

F2 - Processing parameters  
 SI 32768  
 SF 100.6328860 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40



Current Data Parameters  
 NAME LJE-173  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20120420  
 Time 21.14

INSTRUM spect  
 PROBHD 5 mm DUL 13C-1  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 16  
 DS 2  
 SWH 8278.146 Hz  
 FIDRES 0.126314 Hz  
 AQ 3.9584243 sec  
 RG 645.1  
 DW 60.400 usec  
 DE 6.00 usec  
 TE 298.0 K  
 D1 1.00000000 sec  
 TD0 1

CHANNEL f1  
 NUC1 1H  
 P1 8.60 usec  
 PL1 4.00 dB  
 SFO1 400.1324710 MHz

F2 - Processing parameters  
 SI 32768  
 SF 400.1300136 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



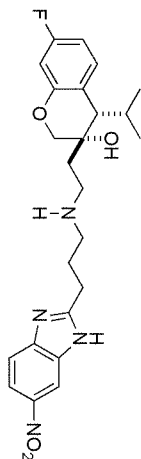
Current Data Parameters  
 NAME LJE-173  
 EXPNO 2  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20120521  
 Time\_ 14.45  
 INSTRUM spect  
 PROBHD 5 mm PABBO BR/  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 1024  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3631988 sec  
 RG 190.62  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 298.9 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TD0 1

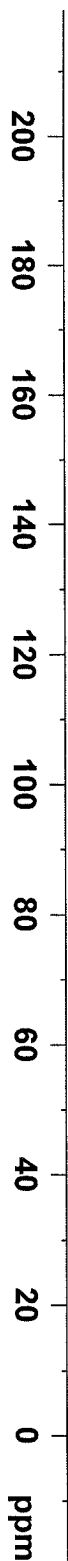
==== CHANNEL f1 =====  
 NUC1 13C  
 P1 10.00 usec  
 P1M1 52.00000000 W  
 SFO1 100.6429474 MHz

==== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUC2 1H  
 PCPD2 90.00 usec  
 P1M2 12.00000000 W  
 P1M12 0.33333001 W  
 P1M13 0.27000001 W  
 SFO2 400.2116008 MHz

F2 - Processing parameters  
 SI 32768  
 SF 100.6328860 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40



- 163.59
- 161.16
- 158.57
- 153.54
- 153.42
- 143.24
- 142.35
- 137.99
- 131.73
- 131.63
- 118.51
- 118.48
- 118.21
- 114.12
- 111.73
- 107.46
- 107.25
- 103.38
- 103.14
- 77.34
- 77.02
- 76.70
- 71.37
- 67.64
- 51.47
- 50.70
- 47.68
- 44.90
- 34.50
- 27.96
- 26.78
- 26.07
- 25.46
- 20.99



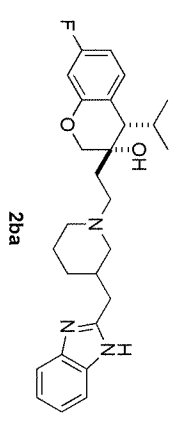
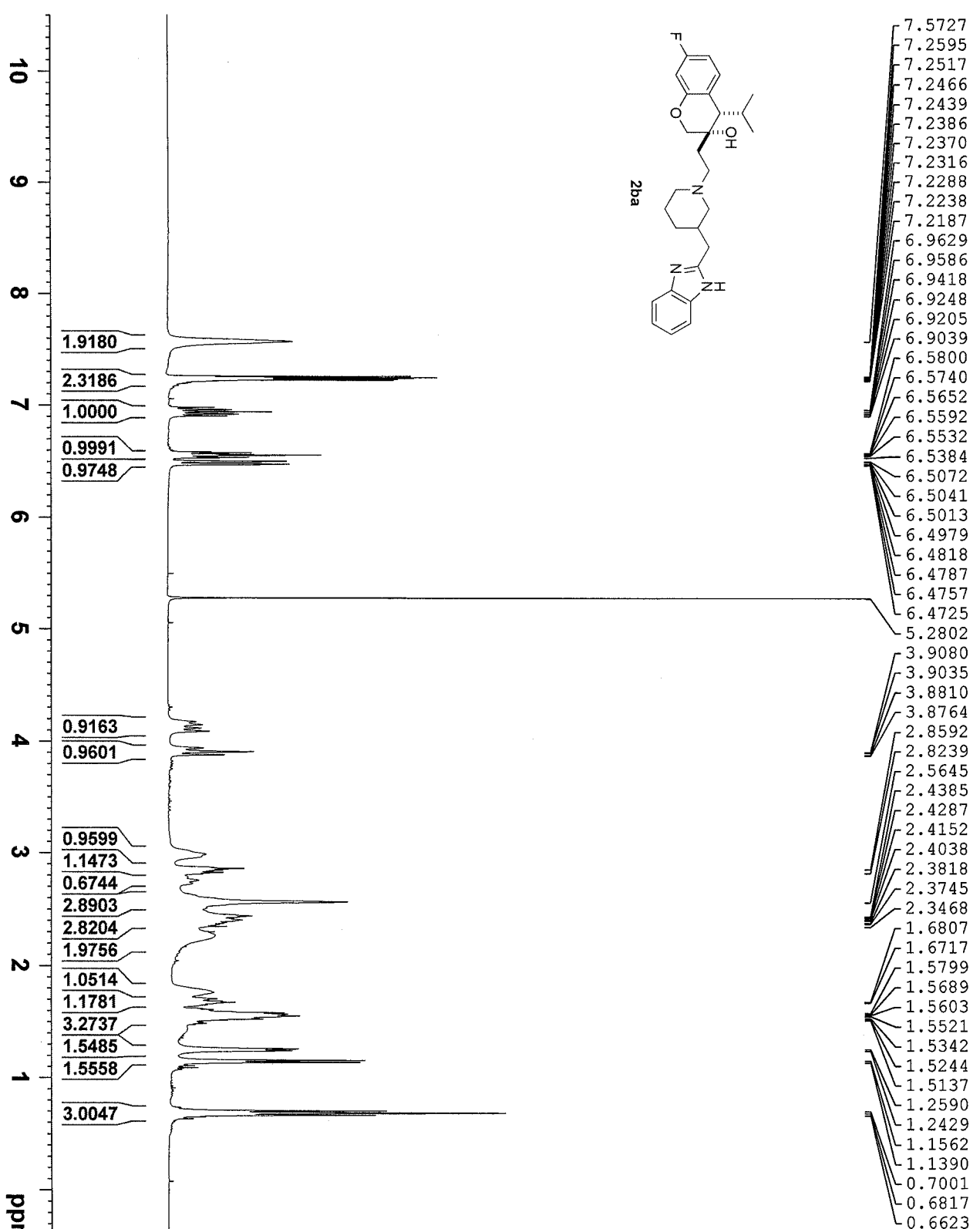


Current Data Parameters  
 NAME KTH-m-198  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20121221  
 Time 15.46

INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 16  
 DS 2  
 SWH 8223.685 Hz  
 FIDRES 0.125483 Hz  
 AO 3.9846387 sec  
 RG 58.64  
 DW 60.800 usec  
 DE 6.50 usec  
 TE 298.9 K  
 D1 1.00000000 sec  
 TD0 1

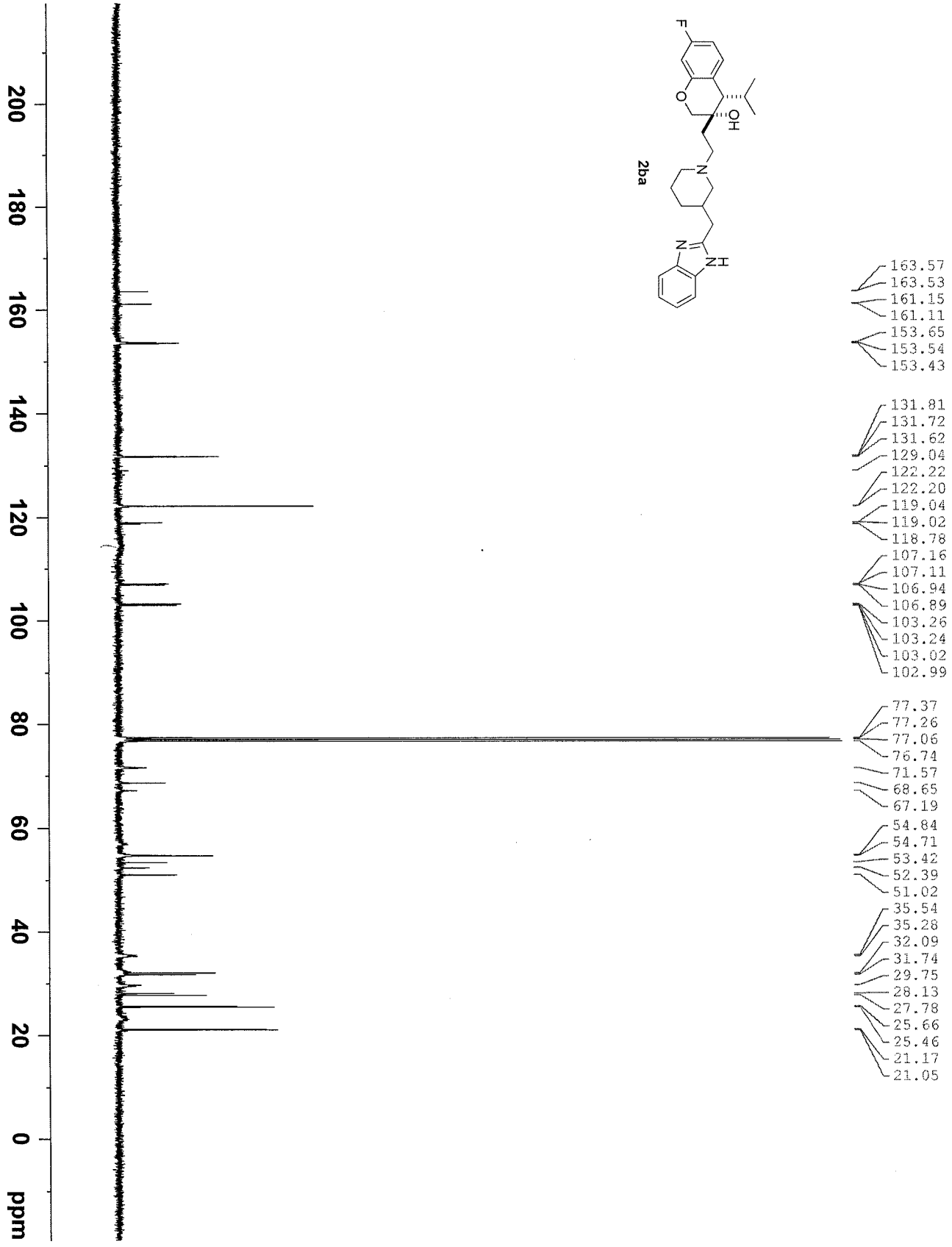
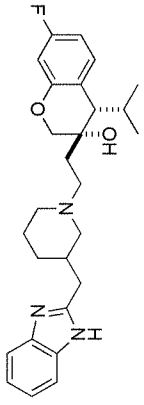
==== CHANNEL f1 =====  
 NUC1 1H  
 P1 15.00 usec  
 PLW1 12.00000000 W  
 SFO1 400.2124715 MHz  
 F2 - Processing parameters  
 SI 65536  
 SF 400.2100132 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00







Current Data Parameters  
 NAME KTH-n-198  
 EXPNO 7  
 PROCNO 1



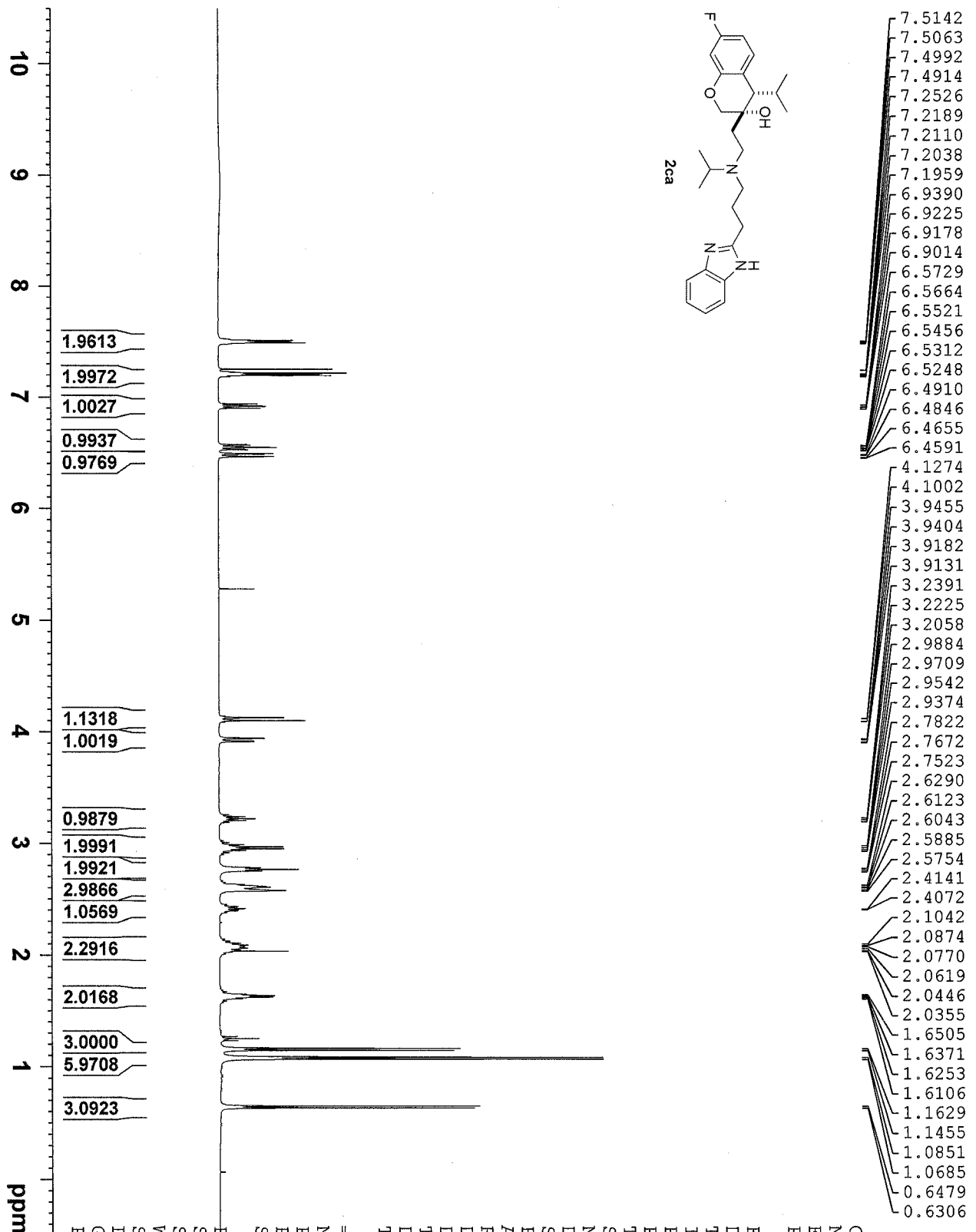
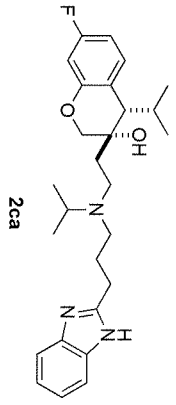
- 163.57
- 163.53
- 161.15
- 161.11
- 153.65
- 153.54
- 153.43
- 131.81
- 131.72
- 131.62
- 129.04
- 122.22
- 122.20
- 119.04
- 119.02
- 118.78
- 107.16
- 107.11
- 106.94
- 106.89
- 103.26
- 103.24
- 103.02
- 102.99
- 77.37
- 77.26
- 77.06
- 76.74
- 71.57
- 68.65
- 67.19
- 54.84
- 54.71
- 53.42
- 52.39
- 51.02
- 35.54
- 35.28
- 32.09
- 31.74
- 29.75
- 28.13
- 27.78
- 25.66
- 25.46
- 21.17
- 21.05

F2 - Acquisition Parameters  
 Date\_ 20121221  
 Time 19.51  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 592  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.36798 Hz  
 AQ 1.3631988 sec  
 RG 180.62  
 DW 20.890 usec  
 DE 6.30 usec  
 TE 339.3 K  
 D1 2.0000000 sec  
 D11 0.0300000 sec  
 D10 1

CHANNEL F1  
 NUC1 13C  
 P1 10.00 usec  
 PL1 52.0000000 W  
 SFO1 100.6429474 MHz

CHANNEL F2  
 waltr216  
 NUC2 1H  
 POC2 90.00 usec  
 PLM2 12.0000000 W  
 PLM12 0.3333001 W  
 PLM13 0.27000001 W  
 SFO2 400.2116098 MHz

F2 - Processing Parameters  
 SI 32768  
 SF 100.6328660 MHz  
 MDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40



Current Data Parameters  
 NAME LJE-328  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20130328  
 Time 19.03  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 16  
 DS 2  
 SWH 8223.685 Hz  
 FIDRES 0.125483 Hz  
 AQ 3.9846387 sec  
 RG 84.76  
 DW 60.800 usec  
 DE 6.50 usec  
 TE 298.7 K  
 D1 1.00000000 sec  
 TD0 1

==== CHANNEL F1 =====  
 NUC1 1H  
 P1 15.00 usec  
 P1M1 12.00000000 W  
 SFO1 400.2124715 MHz  
 F2 - Processing parameters  
 SI 65536  
 SF 400.2100157 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



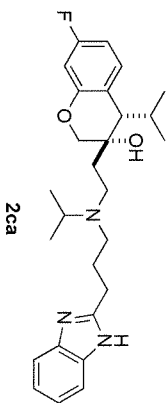
Current Data Parameters  
 NAME LJE-328  
 EXPNO 2  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20130328  
 Time 19.07  
 INSTRUM 5 mm PABBO B8/  
 PROBDI zpg30  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 133  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.366788 Hz  
 AQ 1.3631928 sec  
 RG 120.602  
 KE 120.602  
 DM 2.0000000 usec  
 DE 6.50 usec  
 TE 299.1 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TDO 1

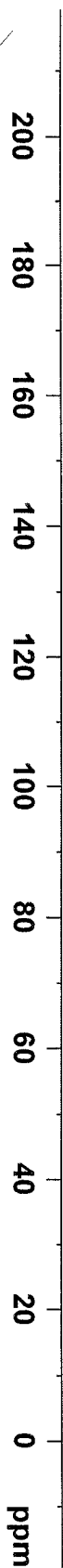
===== CHANNEL f1 =====  
 NUC1 13C  
 P1 10.00 usec  
 PLW1 52.00000000 W  
 SFO1 100.6429474 MHz

===== CHANNEL f2 =====  
 CDPDRG2 waltz16  
 NUC2 1H  
 PCPD2 90.00 usec  
 PLW2 12.00000000 W  
 PLM12 0.33333001 W  
 PLM13 0.27000001 W  
 SFO2 400.2116008 MHz

F2 - Processing parameters  
 SI 32768  
 SF 100.6328860 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40



- 163.58
- 161.16
- 154.52
- 153.64
- 153.53
- 138.33
- 131.60
- 131.51
- 122.30
- 118.76
- 118.73
- 114.62
- 107.15
- 106.93
- 103.23
- 102.99
- 77.35
- 77.03
- 76.71
- 71.29
- 68.39
- 51.43
- 49.49
- 48.63
- 45.49
- 32.20
- 27.67
- 26.47
- 25.77
- 25.48
- 20.86
- 17.34
- 16.62





Current Data Parameters  
 NAME LJE-328  
 EXPNO 5  
 PROCNO 1

F2 - Acquisition Parameters

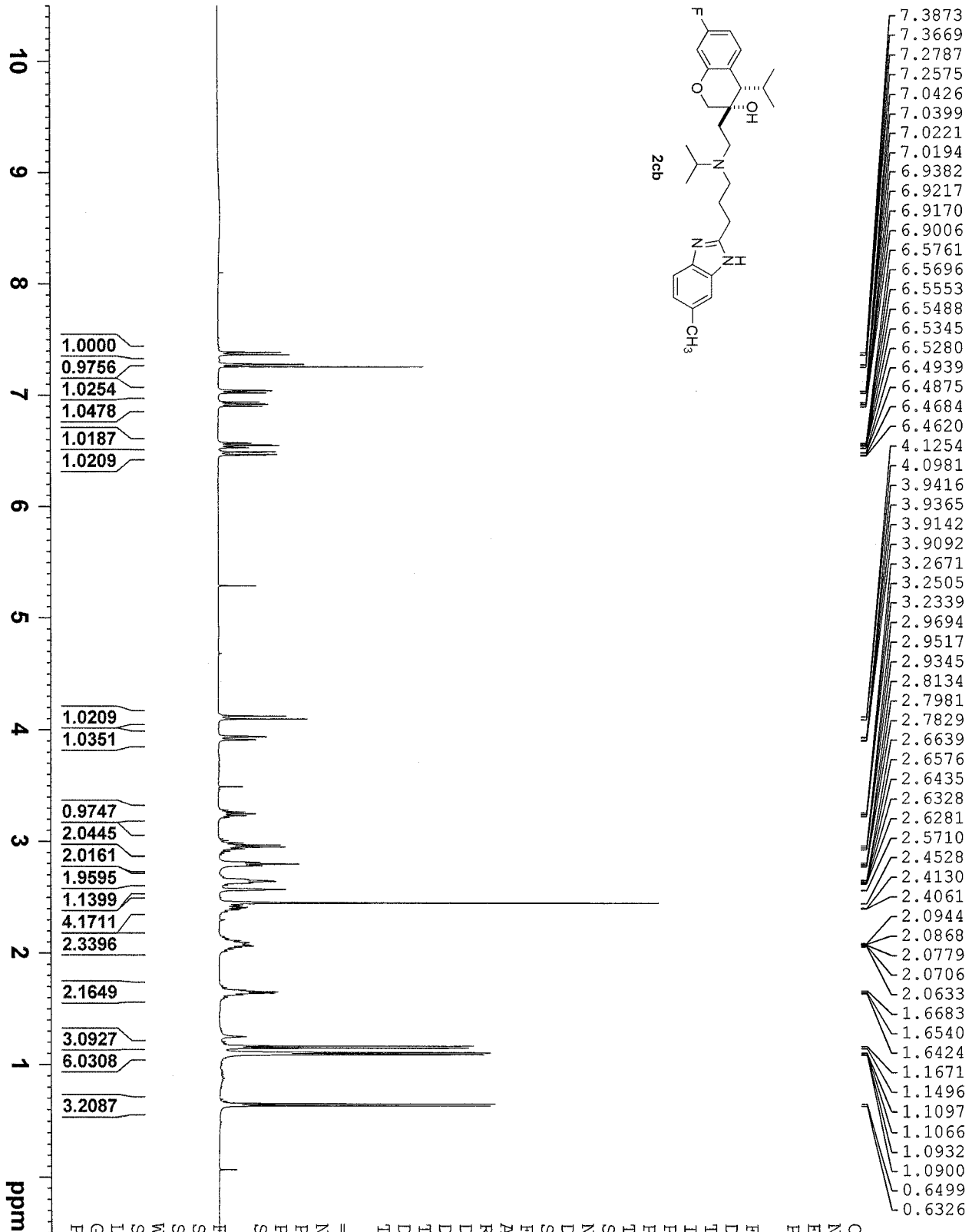
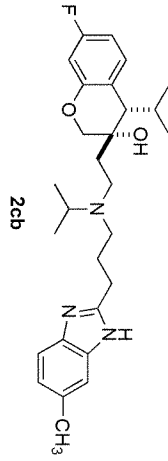
Date\_ 20130329  
 Time 15.28  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 3  
 DS 2  
 SWH 8223.685 Hz  
 FIDRES 0.125483 Hz  
 AQ 3.9846387 sec  
 RG 103.95  
 DW 60.800 usec  
 DE 6.50 usec  
 TE 298.6 K  
 D1 1.00000000 sec  
 TD0 1

==== CHANNEL F1 =====

NUC1 1H  
 P1 15.00 usec  
 PLM1 12.00000000 W  
 SFO1 400.2124715 MHz

F2 - Processing parameters

SI 65536  
 SF 400.2100138 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



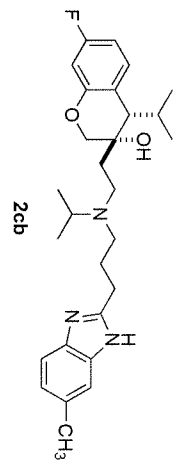
- 7.3873
- 7.3669
- 7.2787
- 7.2575
- 7.0426
- 7.0399
- 7.0221
- 7.0194
- 6.9382
- 6.9217
- 6.9170
- 6.9006
- 6.5761
- 6.5696
- 6.5553
- 6.5488
- 6.5345
- 6.5280
- 6.4939
- 6.4875
- 6.4684
- 6.4620
- 4.1254
- 4.0981
- 3.9416
- 3.9365
- 3.9142
- 3.9092
- 3.2671
- 3.2505
- 3.2339
- 2.9694
- 2.9517
- 2.9345
- 2.8134
- 2.7981
- 2.7829
- 2.6639
- 2.6576
- 2.6435
- 2.6328
- 2.6281
- 2.5710
- 2.4528
- 2.4130
- 2.4061
- 2.0944
- 2.0868
- 2.0779
- 2.0706
- 2.0633
- 1.6683
- 1.6540
- 1.6424
- 1.1671
- 1.1496
- 1.1097
- 1.1066
- 1.0932
- 1.0900
- 0.6499
- 0.6326



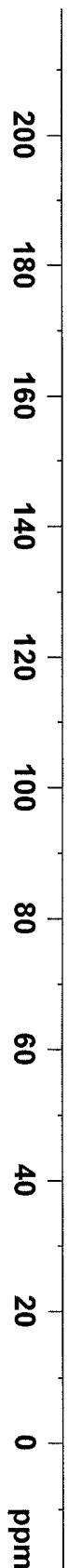
Current Data Parameters  
 NAME LJE-328  
 EXPNO 7  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20130401  
 Time 16.56  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 1308  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.36798 Hz  
 AQ 1.3631988 sec  
 RG 196.62  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 299.4 K  
 D1 2.0000000 sec  
 D11 0.0300000 sec  
 TDO 1

===== CHANNEL f1 =====  
 NUCL 13C  
 P1 10.00 usec  
 PLM1 52.0000000 W  
 SF01 100.629474 MHz  
 ===== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUC2 1H  
 P2 90.00 usec  
 PLM2 12.0000000 W  
 SF02 400.2116008 MHz  
 =====  
 F2 - Processing parameters  
 SI 32768  
 SF 100.6328860 MHz  
 MDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

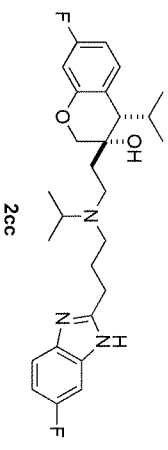


- 163.57
- 161.15
- 154.09
- 153.67
- 153.55
- 138.11
- 136.78
- 132.09
- 131.61
- 131.51
- 123.72
- 118.79
- 118.76
- 114.52
- 114.10
- 107.12
- 106.91
- 103.21
- 102.97
- 77.35
- 77.04
- 76.72
- 71.08
- 68.36
- 51.38
- 49.80
- 48.72
- 45.45
- 32.21
- 27.68
- 26.47
- 25.58
- 25.47
- 21.61
- 20.88
- 17.30
- 16.63





Current Data Parameters  
 NAME LJE-289  
 EXPNO 5  
 PROCNO 1



- 7.2618
- 7.0021
- 6.9961
- 6.9785
- 6.9726
- 6.9679
- 6.9560
- 6.9505
- 6.9471
- 6.9302
- 6.5959
- 6.5894
- 6.5751
- 6.5686
- 6.5542
- 6.5478
- 6.5197
- 6.5133
- 6.4942
- 6.4879
- 4.1598
- 4.1325
- 3.9668
- 3.9620
- 3.9397
- 3.9349
- 3.2143
- 3.1976
- 3.1811
- 2.9491
- 2.9308
- 2.9084
- 2.8903
- 2.7352
- 2.7072
- 2.6048
- 2.5538
- 2.5387
- 2.5272
- 2.5122
- 2.4632
- 2.4458
- 2.4392
- 2.4284
- 2.1072
- 2.0901
- 2.0717
- 2.0542
- 2.0449
- 2.0372
- 1.6241
- 1.6126
- 1.5988
- 1.5858
- 1.1880
- 1.1706
- 1.0790
- 1.0681
- 1.0626
- 1.0518
- 0.6816
- 0.6644

F2 - Acquisition Parameters

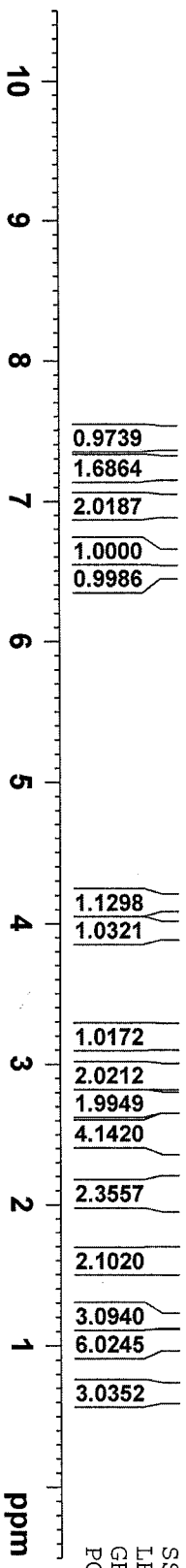
Date\_ 20130313  
 Time 19.36  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 16  
 DS 2  
 SWH 8223.685 Hz  
 FIDRES 0.125483 Hz  
 AQ 3.9846387 sec  
 RG 133.17  
 DW 60.800 usec  
 DE 6.50 usec  
 TE 298.7 K  
 D1 1.00000000 sec  
 TD0 1

==== CHANNEL f1 =====

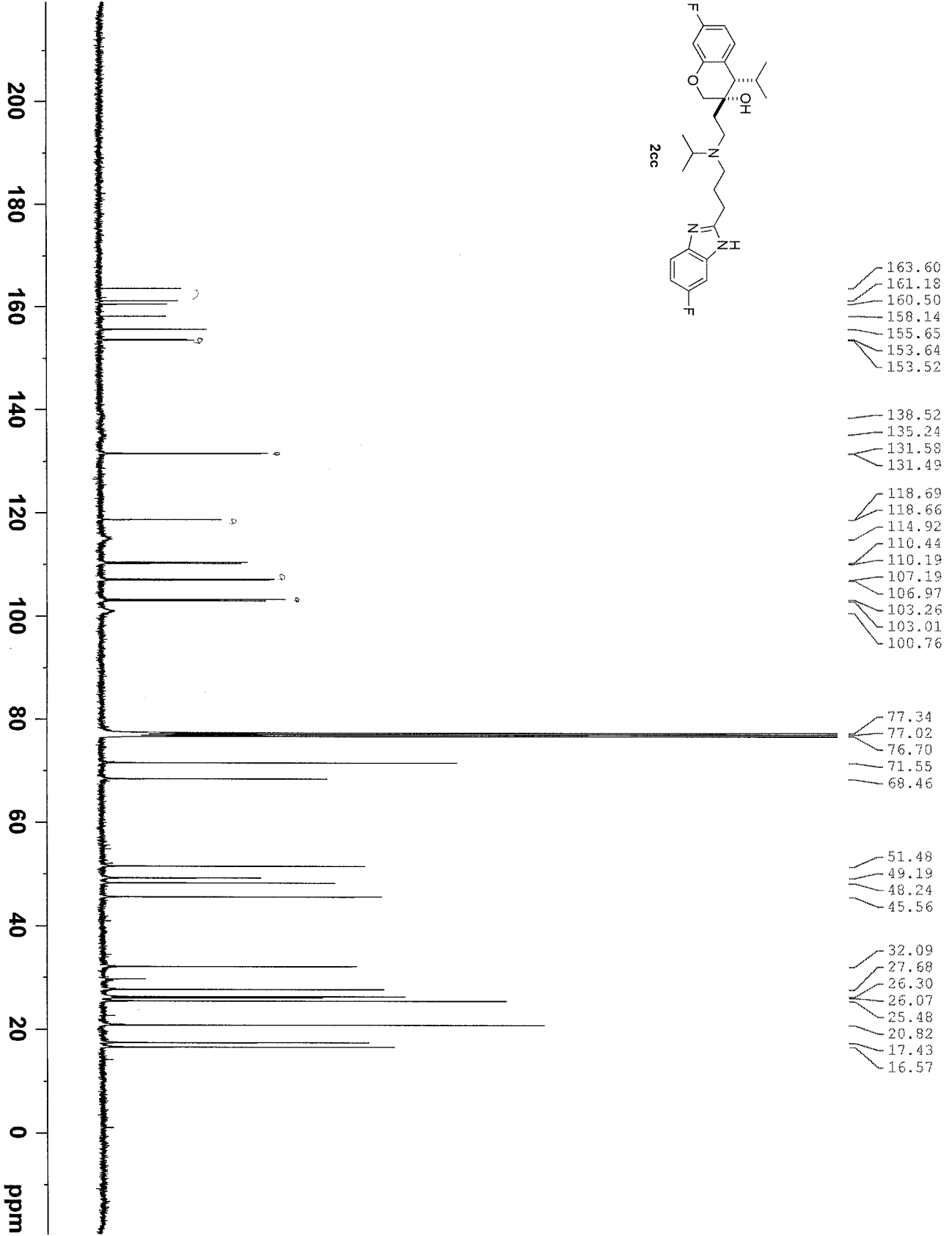
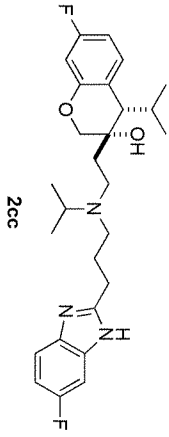
NUC1 1H  
 P1 15.00 usec  
 PLW1 12.00000000 W  
 SFO1 400.2124715 MHz

F2 - Processing parameters

SI 65536  
 SF 400.2100124 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



ppm



- 163.60
- 161.18
- 160.50
- 158.14
- 155.65
- 153.64
- 153.52
- 138.52
- 135.24
- 131.58
- 131.49
- 118.69
- 118.66
- 114.92
- 110.44
- 110.19
- 107.19
- 106.97
- 103.26
- 103.01
- 100.76
- 77.34
- 77.02
- 76.70
- 71.55
- 68.46
- 51.48
- 49.19
- 48.24
- 45.56
- 32.09
- 27.68
- 26.30
- 26.07
- 25.48
- 20.82
- 17.43
- 16.57

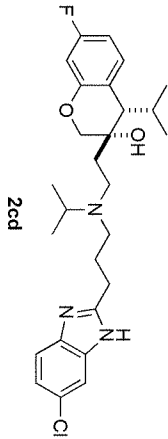
Current Data Parameters  
NAME LJE-289  
EXPNO 8  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20130409  
Time 21.59  
INSTRUM spect  
PROBHD 5 mm PABBO BH/  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 11638  
DS 4  
SWH 24038.461 Hz  
FIDRES 0.366788 Hz  
AQ 1.3631988 sec  
RG 190.62  
DE 20.90 usec  
DM 6.90 usec  
TE 28.5 K  
D1 2.0000000 sec  
D11 0.0300000 sec  
TD0 1

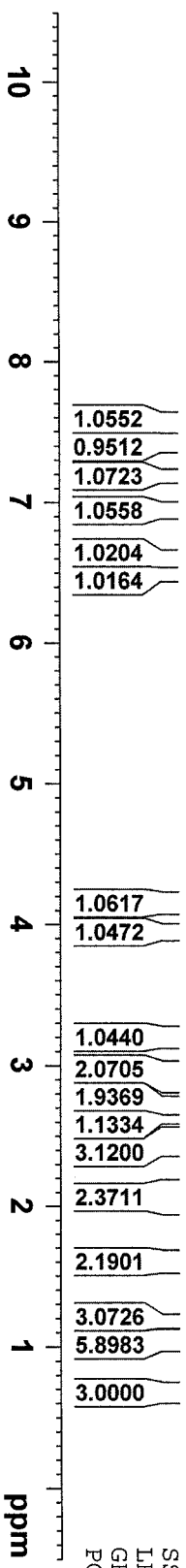
CHANNEL F1  
NUC1 13C  
P1 10.00 usec  
PL1 52.00000000 W  
SFO1 100.6429474 MHz

CHANNEL F2  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 90.00 usec  
PLM2 12.00000000 W  
PLM12 0.33333001 W  
PLM13 0.27000001 W  
SFO2 400.2116008 MHz

F2 - Processing parameters  
SI 32768  
SF 100.6328860 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



- 7.5293
- 7.2576
- 7.2065
- 7.2019
- 7.1852
- 7.1806
- 6.9672
- 6.9505
- 6.9463
- 6.9298
- 6.5964
- 6.5900
- 6.5756
- 6.5692
- 6.5547
- 6.5483
- 6.5202
- 6.5138
- 6.4948
- 6.4884
- 4.1645
- 4.1374
- 3.9645
- 3.9601
- 3.9374
- 3.9329
- 3.2227
- 3.2060
- 3.1895
- 2.9560
- 2.9380
- 2.9288
- 2.9198
- 2.9112
- 2.8936
- 2.7408
- 2.7269
- 2.7135
- 2.6043
- 2.5538
- 2.5383
- 2.5288
- 2.5146
- 2.4450
- 2.4385
- 2.1137
- 2.0961
- 2.0739
- 2.0555
- 2.0388
- 1.6269
- 1.6160
- 1.6025
- 1.5900
- 1.1896
- 1.1721
- 1.0839
- 1.0732
- 1.0677
- 1.0571
- 0.6848
- 0.6676



Current Data Parameters  
 NAME LJE-289  
 EXPNO 6  
 PROCNO 1

F2 - Acquisition Parameters

Date\_ 20130314  
 Time 15.54  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 16  
 DS 2  
 SWH 8223.685 Hz  
 FIDRES 0.125483 Hz  
 AQ 3.9846387 sec  
 RG 171.62  
 DW 60.800 usec  
 DE 6.50 usec  
 TE 299.1 K  
 D1 1.00000000 sec  
 TD0 1

==== CHANNEL F1 =====

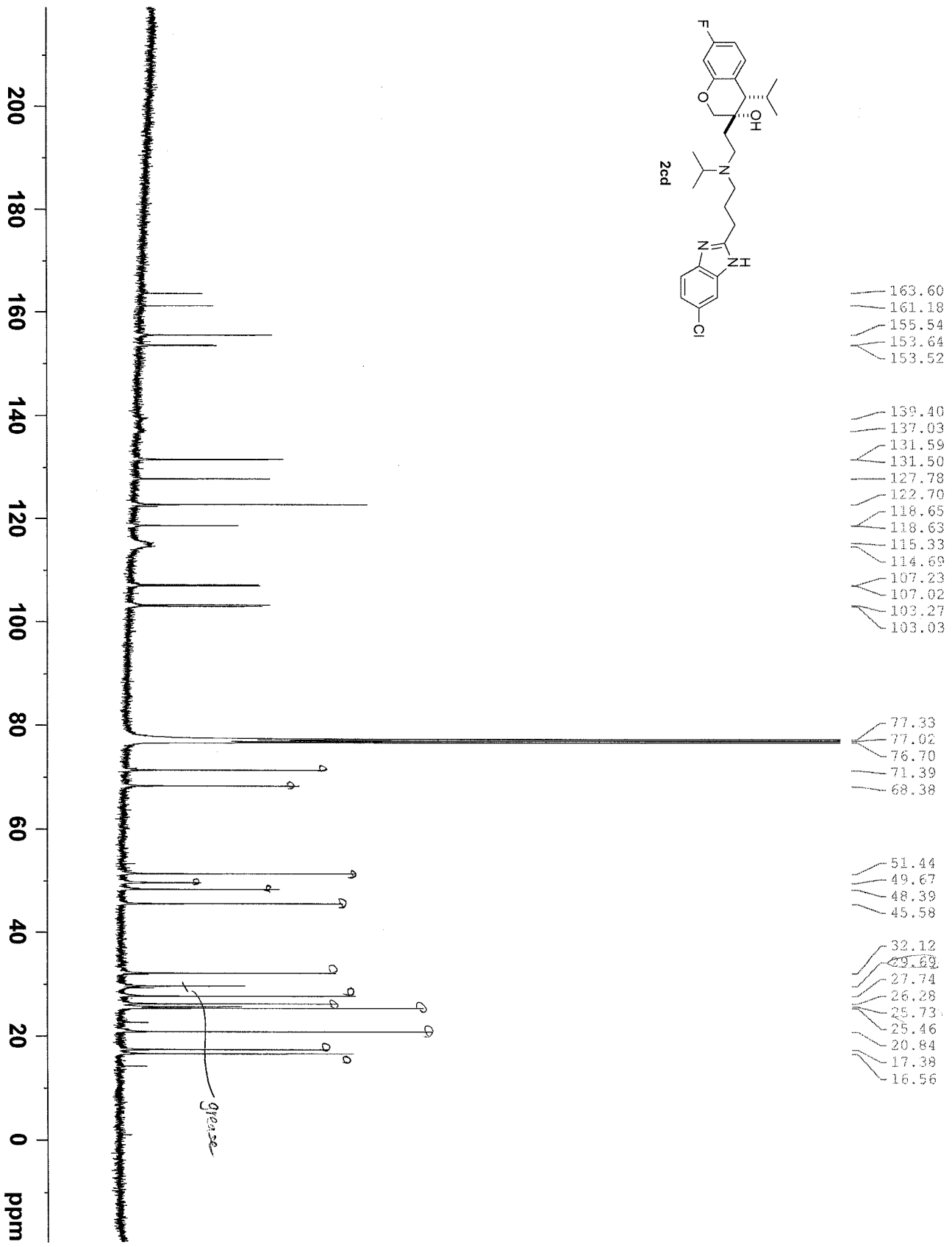
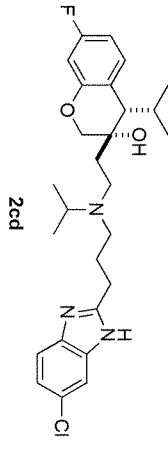
NUC1 1H  
 P1 15.00 usec  
 PLW1 12.00000000 W  
 SFO1 400.2124715 MHz

F2 - Processing parameters

SI 65536  
 SF 400.2100138 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

ppm





- 163.60
- 161.18
- 155.54
- 153.64
- 153.52
- 139.40
- 137.03
- 131.59
- 131.50
- 127.78
- 122.70
- 118.65
- 118.63
- 115.33
- 114.69
- 107.23
- 107.02
- 103.27
- 103.03
- 77.33
- 77.02
- 76.70
- 71.39
- 68.38
- 51.44
- 49.67
- 48.39
- 45.58
- 32.12
- 29.69
- 27.74
- 26.28
- 25.73
- 25.46
- 20.84
- 17.38
- 16.56

Current Data Parameters  
 NAME KRCB01012  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20130422  
 Time 8:39  
 INSTRUM spect  
 PROBHD 5 mm PABBO 5HT  
 PULPROG zgpg30  
 ID C013  
 SOLVENT DMSO  
 NS 12351  
 DS 4

===== CHANNEL f1 =====  
 NUC1 13C  
 P1 10.00 usec  
 PLW1 52.00000000 W  
 SFO1 100.629474 MHz  
 ===== CHANNEL f2 =====  
 CPDPRG2 waitz16  
 NUC2 1H  
 PCPD2 90.00 usec  
 PLW2 12.00000000 W  
 PLW12 0.33333001 W  
 PLW13 0.27000001 W  
 SFO2 400.2116008 MHz

F2 - Processing parameters  
 SI 32768  
 SF 100.6328660 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40



Current Data Parameters  
 NAME LJE-331  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters

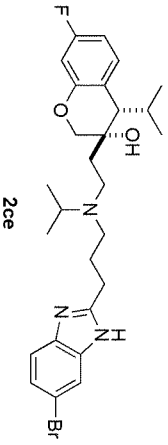
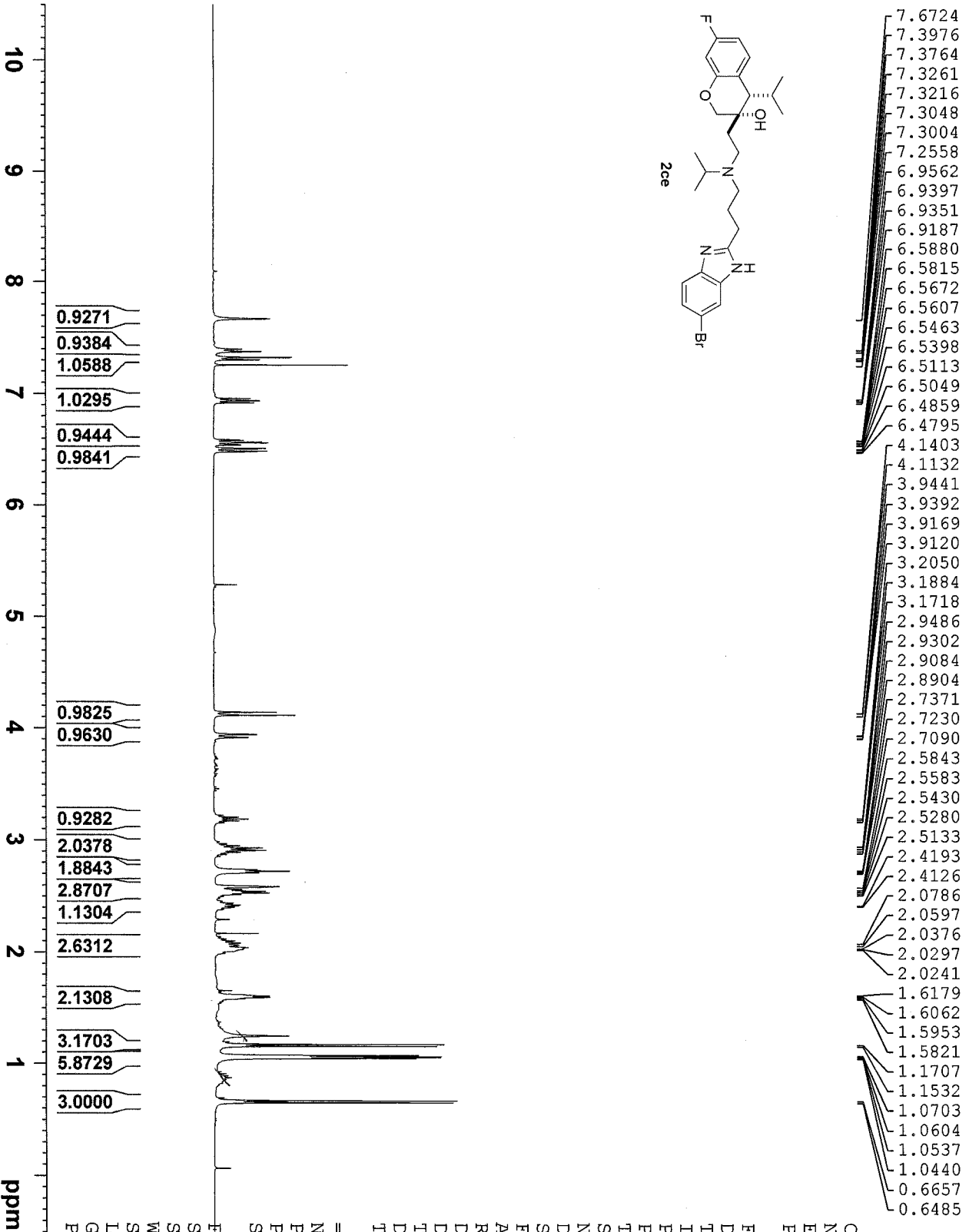
Date\_ 20130403  
 Time 17.48  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 16  
 DS 2  
 SWH 8223.685 Hz  
 FIDRES 0.125483 Hz  
 AQ 3.9846387 sec  
 RG 84.76  
 DW 60.800 usec  
 DE 6.50 usec  
 TE 298.3 K  
 D1 1.00000000 sec  
 TD0 1

==== CHANNEL f1 =====

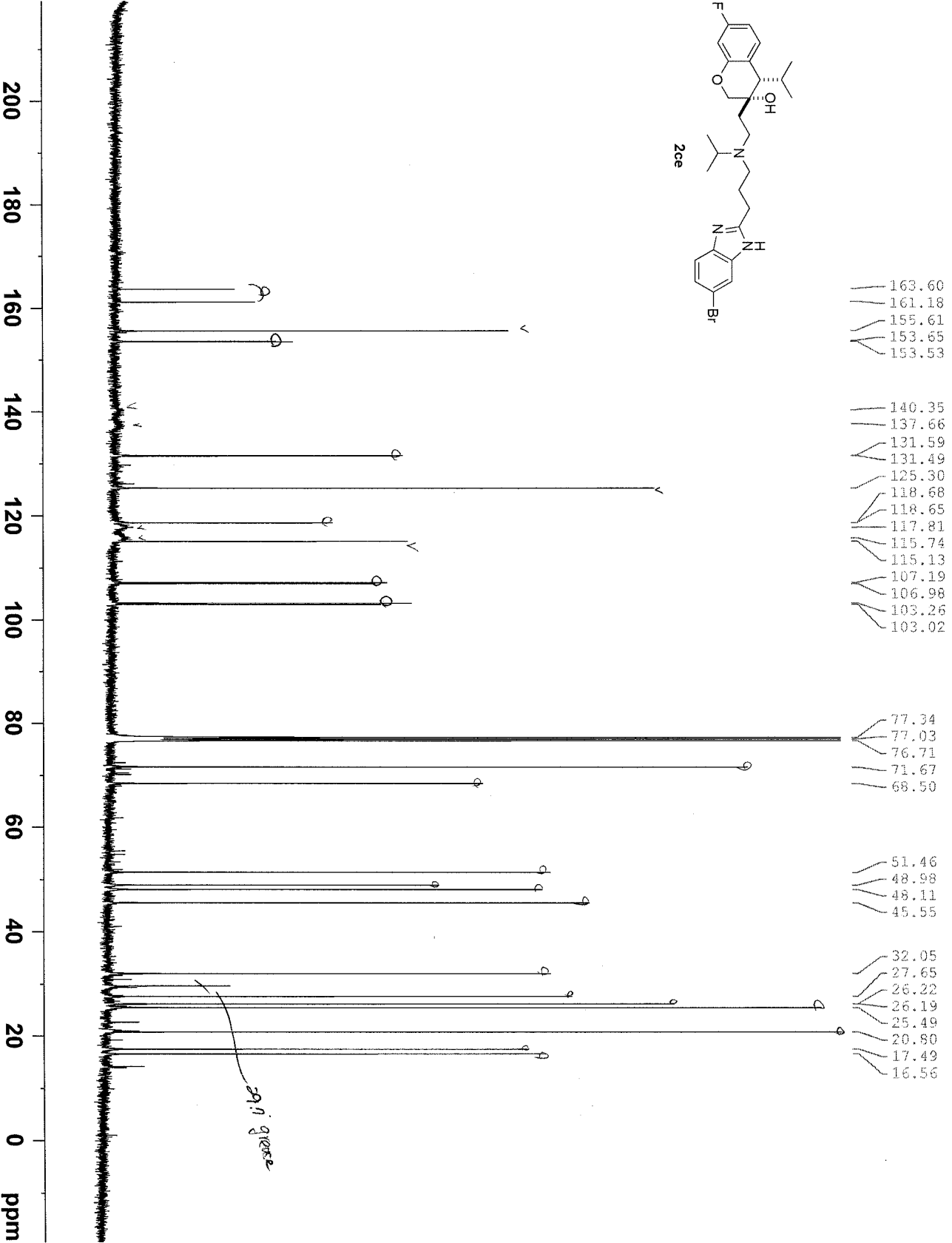
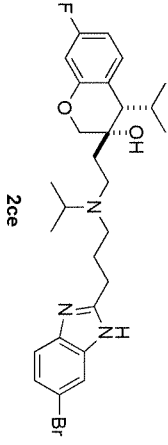
NUC1 1H  
 P1 15.00 usec  
 PLW1 12.00000000 W  
 SFO1 400.2124715 MHz

F2 - Processing parameters

SI 65536  
 SF 400.2100145 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



10  
9  
8  
7  
6  
5  
4  
3  
2  
1  
ppm



- 163.60
- 161.18
- 155.61
- 153.65
- 153.53
- 140.35
- 137.66
- 131.59
- 131.49
- 125.30
- 118.68
- 118.65
- 117.81
- 115.74
- 115.13
- 107.19
- 106.98
- 103.26
- 103.02
- 77.34
- 77.03
- 76.71
- 71.67
- 68.50
- 51.46
- 48.98
- 48.11
- 45.55
- 32.05
- 27.65
- 26.22
- 26.19
- 25.49
- 20.80
- 17.49
- 16.56

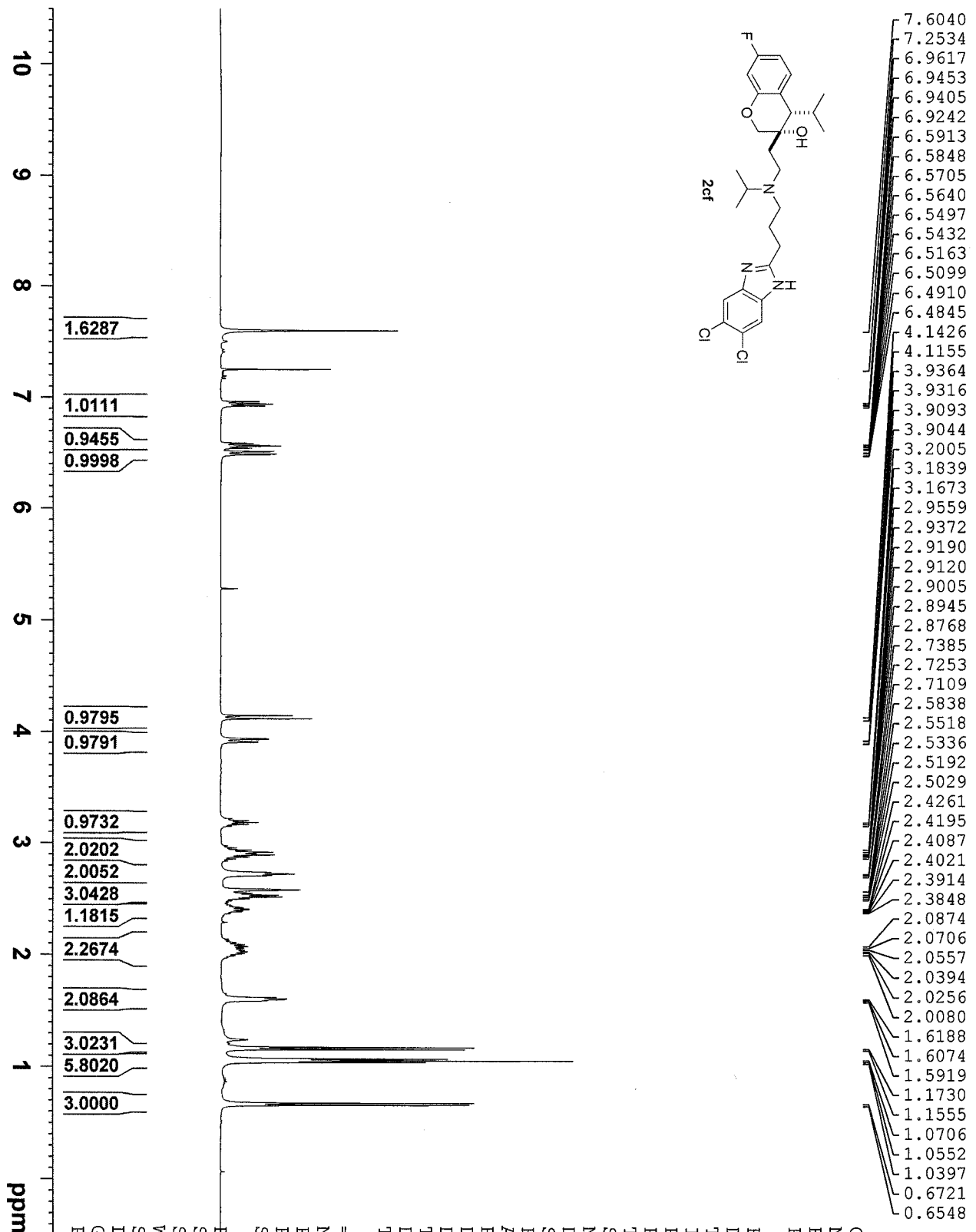
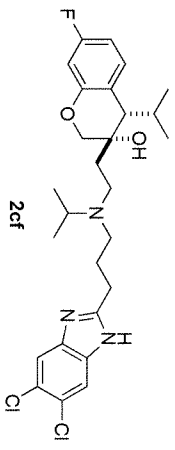
Current Data Parameters  
NAME LJP-331  
EXPNO 8  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20130404  
Time 21:55  
INSTRUM spect  
PROBHD 5 mm PABBO-BB/  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 11344  
DS 4  
SWH 24038.461 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631988 sec  
RG 190.62  
DW 20.800 usec  
DE 6.50 usec  
TE 298.6 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TDO 1

CHANNEL F1 =====  
NUC1 13C  
P1 10.00 usec  
PLW1 52.00000000 W  
SFO1 100.6429474 MHz

CHANNEL F2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 90.00 usec  
PLW2 12.00000000 W  
PLM12 0.3333001 W  
PLM13 0.27000001 W  
SFO2 400.2116008 MHz

F2 - Processing parameters  
SI 32768  
SF 100.6328860 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



Current Data Parameters  
 NAME LJE-331  
 EXPNO 2  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20130403  
 Time 17.54

INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 16  
 DS 2

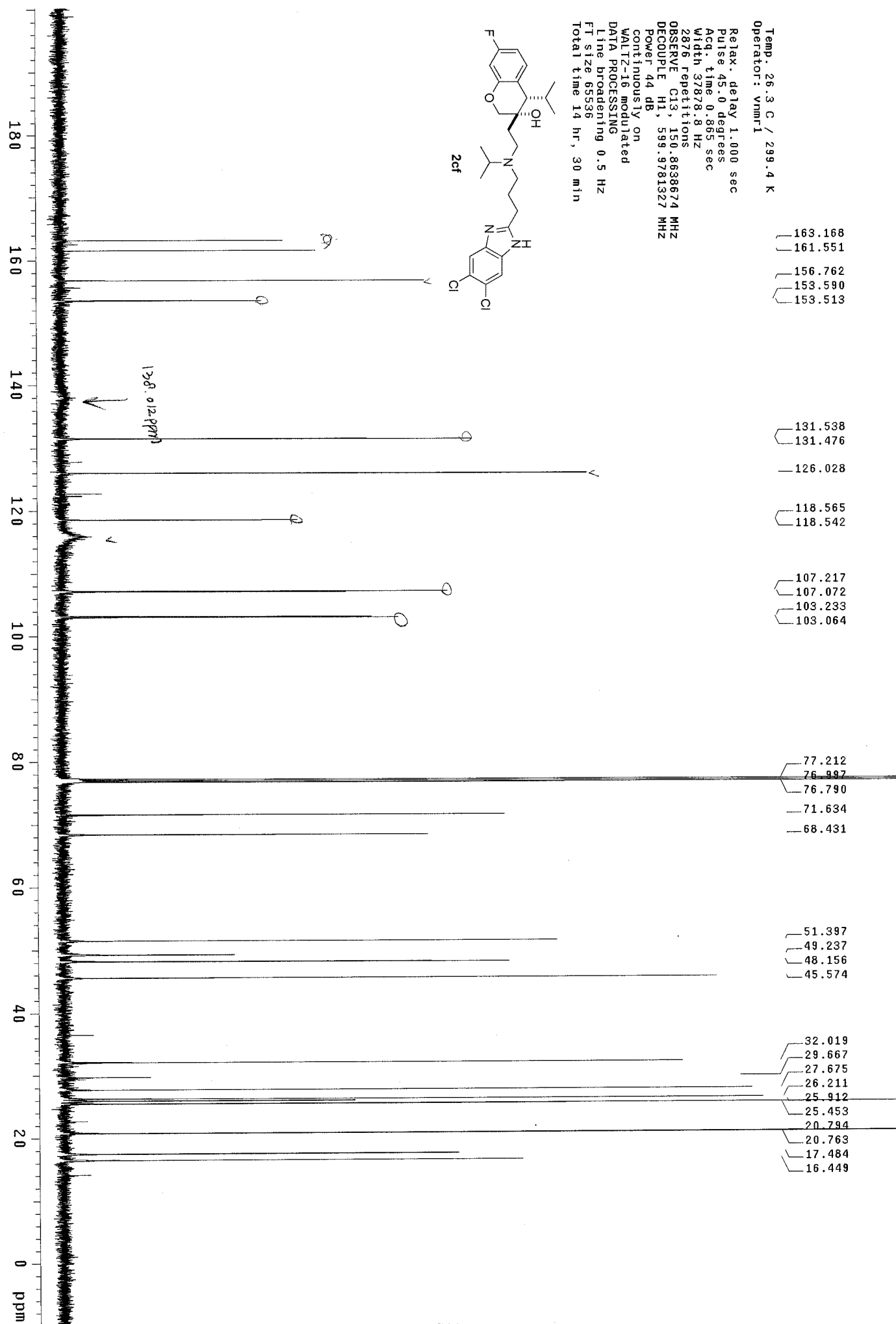
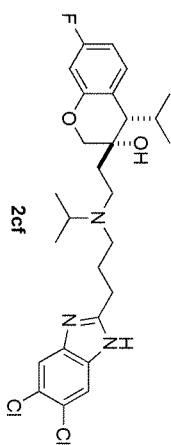
SWH 8223.685 Hz  
 FIDRES 0.125483 Hz  
 AQ 3.9846387 sec  
 RG 84.76  
 DW 60.800 usec  
 DE 6.50 usec  
 TE 298.2 K  
 D1 1.00000000 sec  
 TD0 1

==== CHANNEL f1 =====  
 NUC1 1H  
 P1 15.00 usec  
 PLW1 12.00000000 W  
 SFO1 400.2124715 MHz

F2 - Processing parameters  
 SI 65536  
 SF 400.2100155 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

ppm

Temp. 26.3 C / 299.4 K  
 Operator: vnmr1  
 Relax. delay 1.000 sec  
 Pulse 45.0 degrees  
 Acq. time 0.865 sec  
 Width 37878.8 Hz  
 2876 repetitions  
 OBSERVE C13, 150.8638674 MHz  
 DECOUPLE H1, 599.9781327 MHz  
 Power 44 dB  
 continuously on  
 WALTZ-16 modulated  
 DATA PROCESSING  
 Line broadening 0.5 Hz  
 FI size 65536  
 Total time 14 hr, 30 min





Current Data Parameters  
 NAME LJE-302  
 EXPNO 4  
 PROCNO 1

F2 - Acquisition Parameters

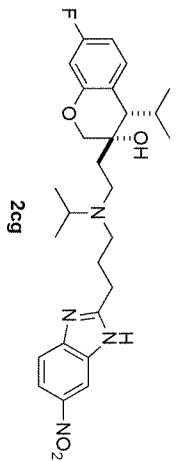
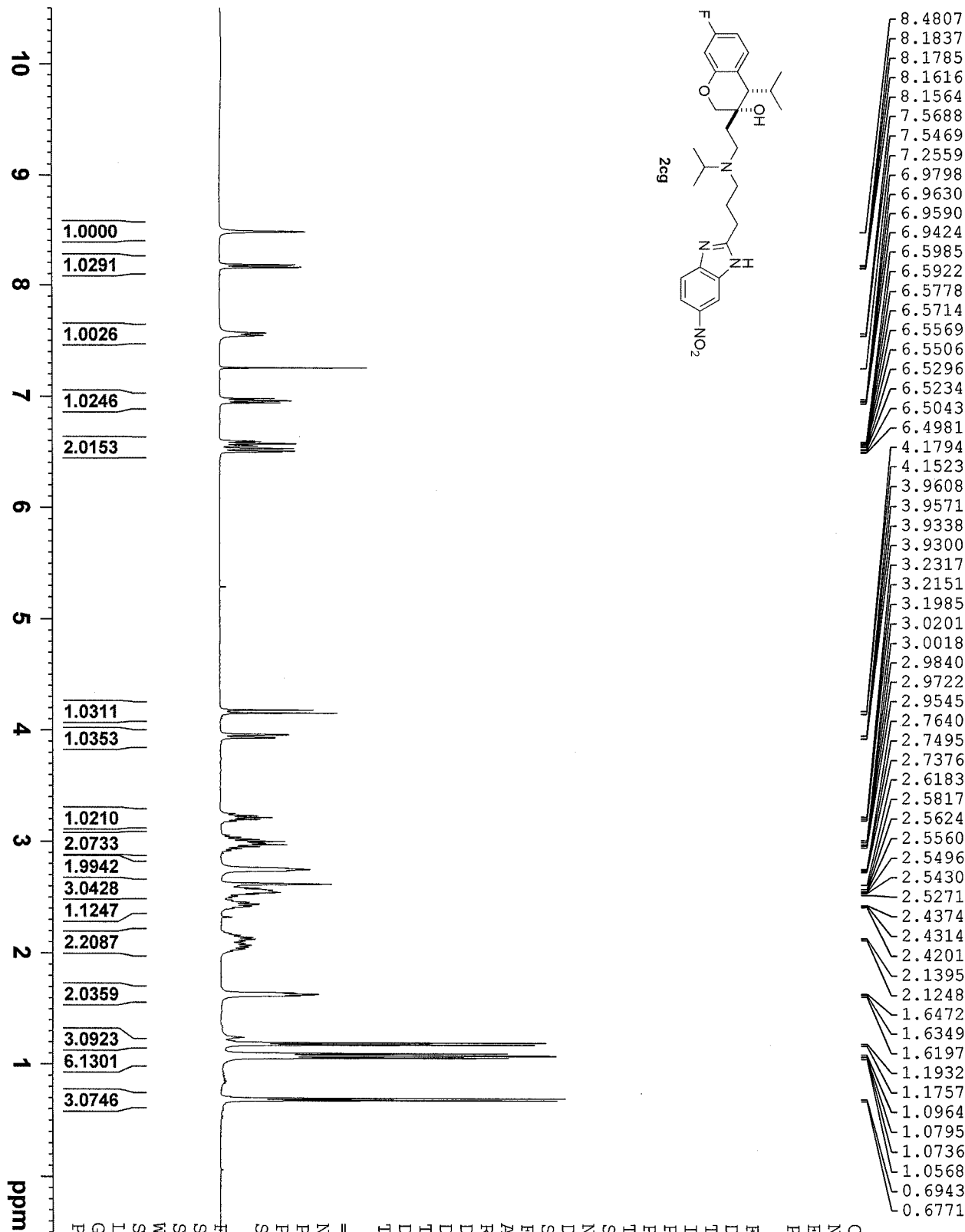
Date\_ 20130318  
 Time 13.12  
 INSTRUM spect  
 PROHD 5 mm PABBO BB/  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 16  
 DS 2  
 SWH 8223.685 Hz  
 FIDRES 0.125483 Hz  
 AQ 3.9846387 sec  
 RG 91.91  
 DW 60.800 usec  
 DE 6.50 usec  
 TE 296.0 K  
 D1 1.00000000 sec  
 TDO 1

==== CHANNEL f1 =====

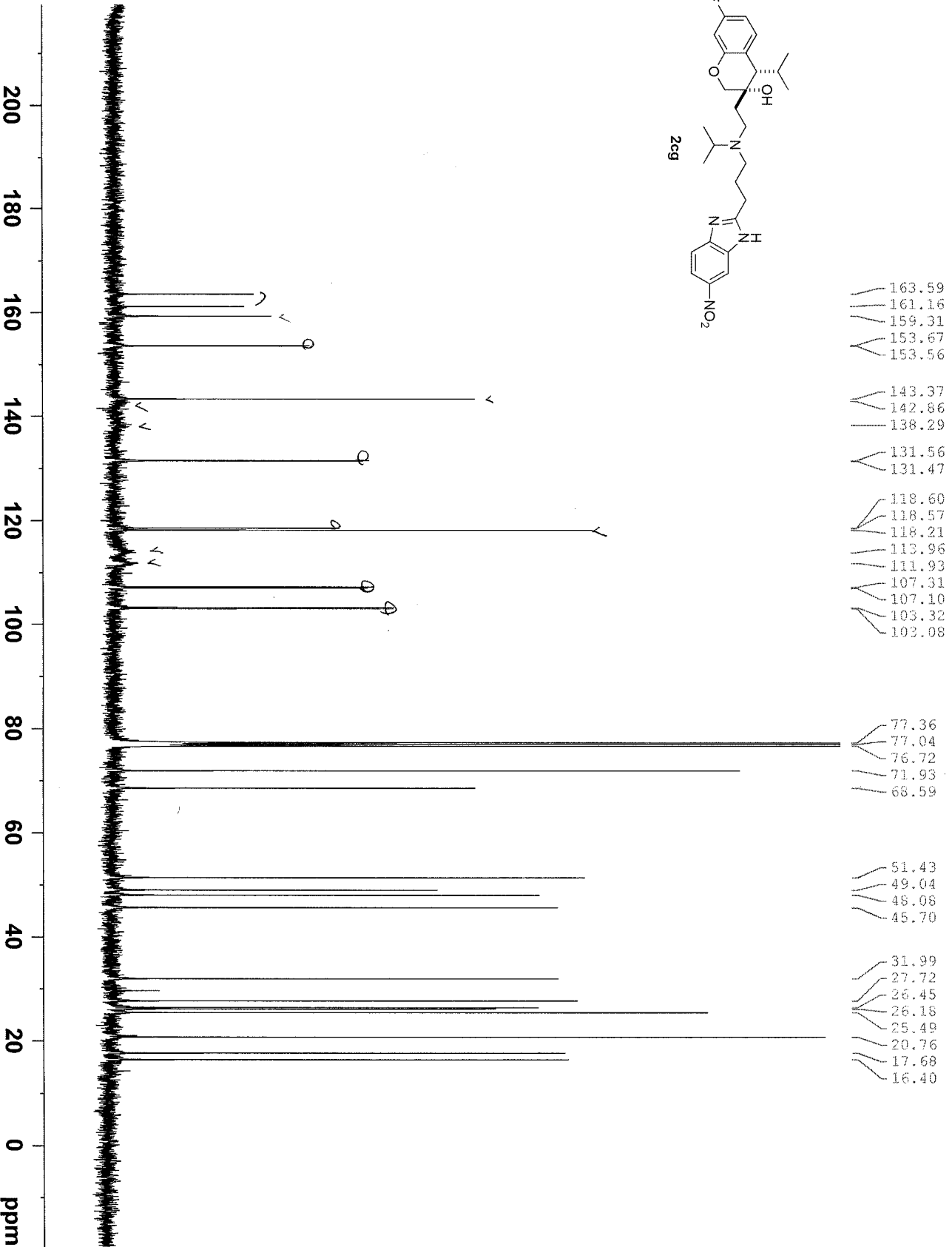
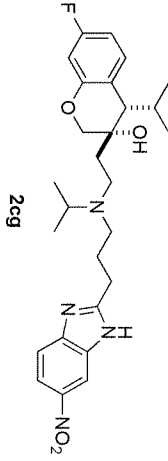
NUC1 1H  
 P1 15.00 usec  
 PLW1 12.00000000 W  
 SFO1 400.2124715 MHz

F2 - Processing parameters

SI 65536  
 SF 400.2100138 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



- 8.4807
- 8.1837
- 8.1785
- 8.1616
- 8.1564
- 7.5688
- 7.5469
- 7.2559
- 6.9798
- 6.9630
- 6.9590
- 6.9424
- 6.5985
- 6.5922
- 6.5778
- 6.5714
- 6.5569
- 6.5506
- 6.5296
- 6.5234
- 6.5043
- 6.4981
- 4.1794
- 4.1523
- 3.9608
- 3.9571
- 3.9338
- 3.9300
- 3.2317
- 3.2151
- 3.1985
- 3.0201
- 3.0018
- 2.9840
- 2.9722
- 2.9545
- 2.7640
- 2.7495
- 2.7376
- 2.6183
- 2.5817
- 2.5624
- 2.5560
- 2.5496
- 2.5430
- 2.5271
- 2.4374
- 2.4314
- 2.4201
- 2.1395
- 2.1248
- 1.6472
- 1.6349
- 1.6197
- 1.1932
- 1.1757
- 1.0964
- 1.0795
- 1.0736
- 1.0568
- 0.6943
- 0.6771



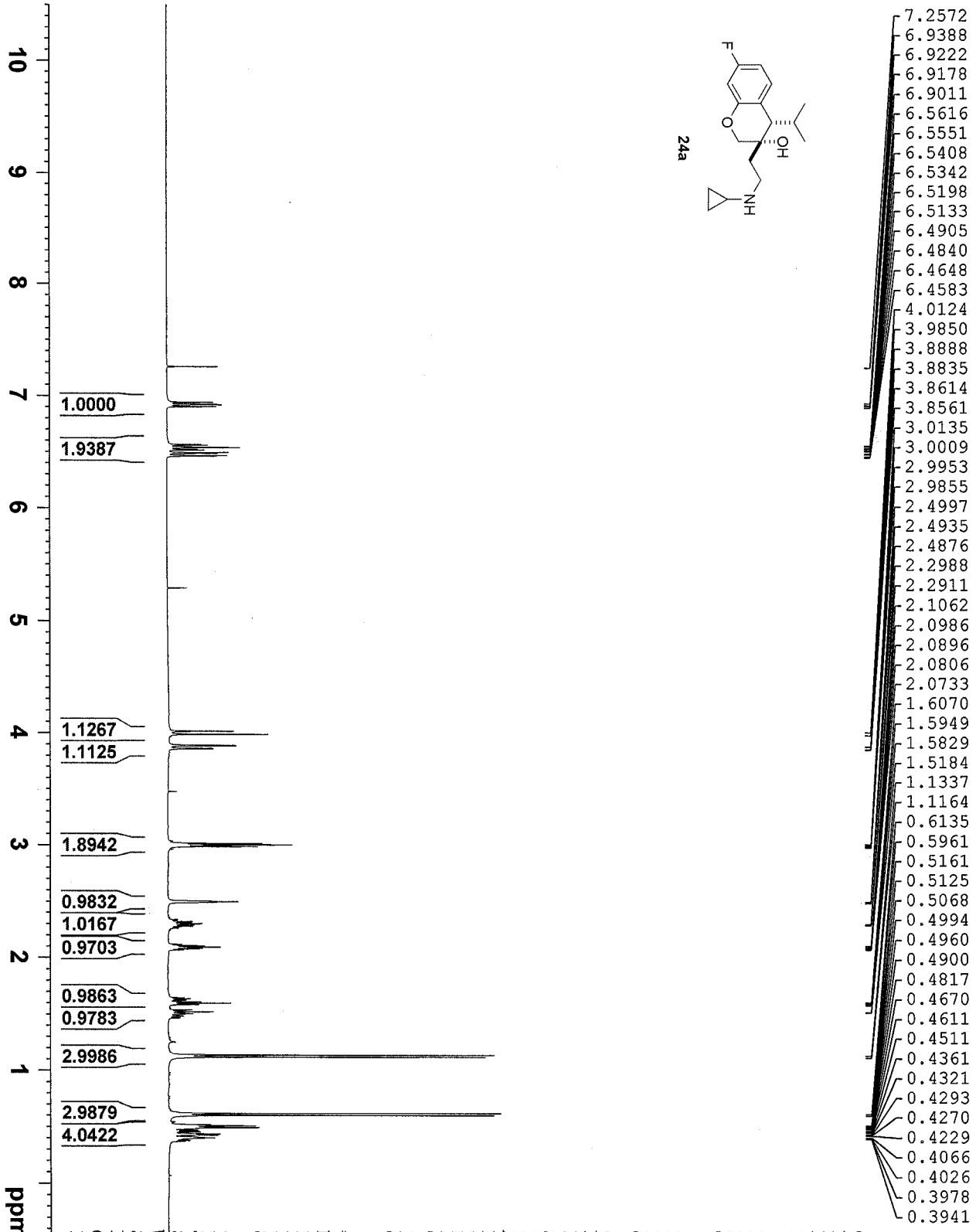
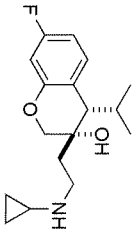
```

Current Data Parameters
NAME          Job-332
EXPNO         3
PROCNO        1
F2 - Acquisition Parameters
Date_         20130405
Time          19.20
INSTRUM      spect
PROBHD       5 mm PABBO/BB/
PULPROG      zgpg30
TD            65536
SOLVENT      CDCl3
NS            2048
DS            4
SWH           24038.461 Hz
FIDRES       0.366798 Hz
AQ            1.3631988 sec
RG            190.62
DE            20.800 usec
TE            299.5 K
D1            6.50 usec
D11           0.03000000 sec
TD0           1

===== CHANNEL f1 =====
NUC1          13C
P1            10.00 usec
PLM1          52.00000000 W
SFO1          100.6429474 MHz

===== CHANNEL f2 =====
CPDPRG2      waltz16
NUC2          1H
PCPD2        90.00 usec
PLM2          12.00000000 W
PLM12         0.33333001 W
PLM13         0.27000001 W
SFO2          400.2116008 MHz

F2 - Processing parameters
SI            32768
SF            100.6328860 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.40
  
```



Current Data Parameters  
 NAME LJE-285  
 EXPNO 2  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20121227  
 Time\_ 17.53  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 16  
 DS 2  
 SWH 8223.685 Hz  
 FIDRES 0.125483 Hz  
 AQ 3.9846387 sec  
 RG 69.69  
 DW 60.800 usec  
 DE 6.50 usec  
 TE 299.0 K  
 D1 1.00000000 sec  
 TD0 1

==== CHANNEL F1 =====  
 NUC1 1H  
 P1 15.00 usec  
 PLW1 12.00000000 W  
 SFO1 400.2124715 MHz  
 F2 - Processing parameters  
 SI 65536  
 SF 400.2100138 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00





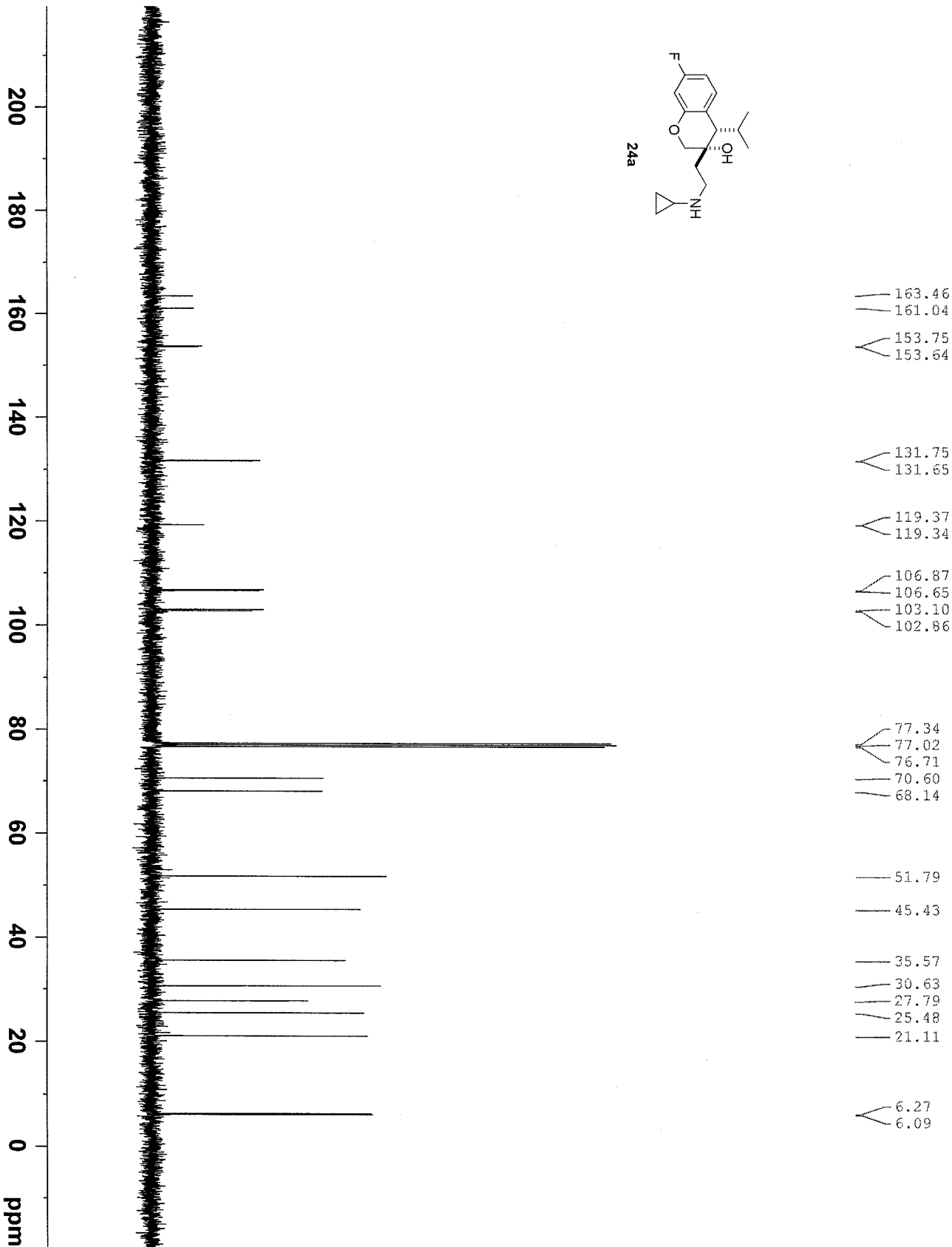
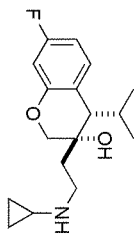
Current Data Parameters  
NAME LJE-285  
EXPNO 3  
PROCNO 1

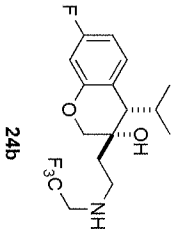
F2 - Acquisition Parameters  
Date\_ 20121227  
Time 17.56  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 31  
DS 4  
SWH 24038.461 Hz  
FIDRES 0.366798 Hz  
AQ 1.363198 sec  
RG 130.62  
DW 20.800 usec  
DE 6.30 usec  
TE 293.7 K  
D1 2.0000000 sec  
D11 0.0300000 sec  
TD0 1

CHANNEL f1  
NUC1 13C 13C  
P1 10.00 usec  
PL1 52.00000000 W  
SFO1 100.629474 MHz

CHANNEL f2  
CPDPRG2 waltz16  
NUC2 1H 1H  
PCPD2 90.00 usec  
PUM2 12.00000000 W  
PLM12 0.3333001 W  
PLM13 0.27000001 W  
SFO2 400.2116008 MHz

F2 - Processing parameters  
SI 32768  
SF 100.6328860 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40





7.2446  
6.9381  
6.9215  
6.9169  
6.9004  
6.5631  
6.5566  
6.5422  
6.5357  
6.5213  
6.5148  
6.4862  
6.4797  
6.4606  
6.4541  
4.0490  
4.0213  
3.8895  
3.8841  
3.8618  
3.8564  
3.2333  
3.2267  
3.2240  
3.2104  
3.2037  
3.1875  
3.1807  
3.1647  
3.1577  
3.0168  
3.0016  
2.9900  
2.9801  
2.5172  
2.5109  
2.5049  
2.3474  
2.3126  
2.3030  
2.2952  
2.2856  
1.6827  
1.6737  
1.6672  
1.6580  
1.6446  
1.6345  
1.6301  
1.6200  
1.5873  
1.5756  
1.5675  
1.5558  
1.5497  
1.5386  
1.5283  
1.5178  
1.1342  
1.1169  
0.6198  
0.6024

Current Data Parameters  
NAME LJE-309  
EXPNO 2  
PROCNO 1

F2 - Acquisition Parameters

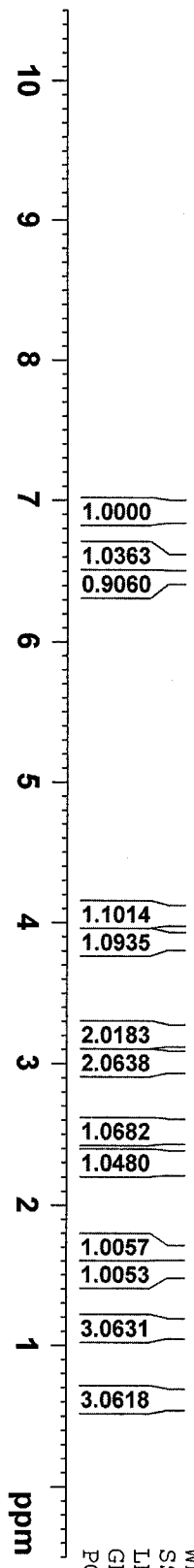
Date\_ 20130227  
Time 15.45  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 8223.685 Hz  
FIDRES 0.125483 Hz  
AQ 3.9846387 sec  
RG 58.64  
DW 60.800 usec  
DE 6.50 usec  
TE 298.8 K  
D1 1.00000000 sec  
TD0 1

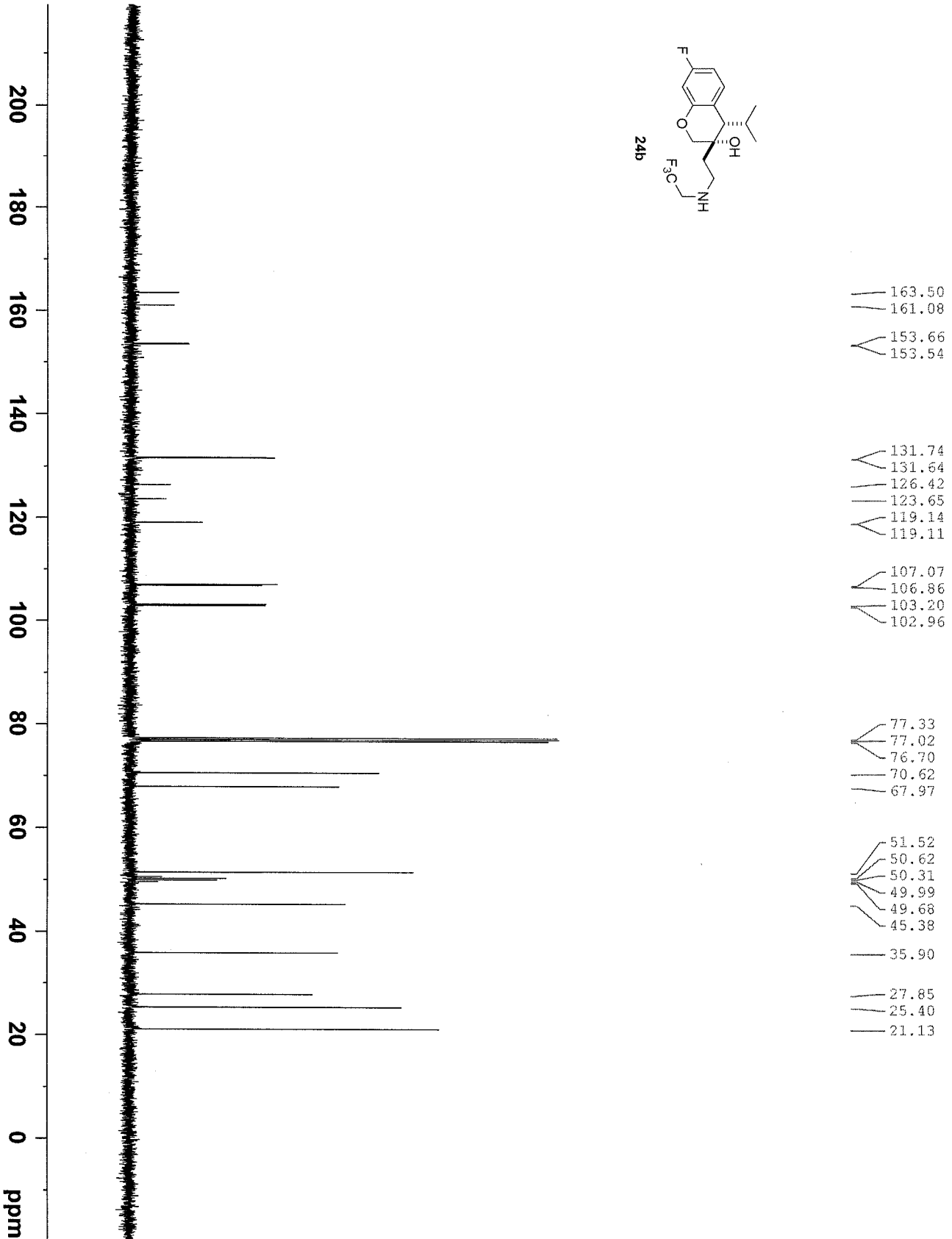
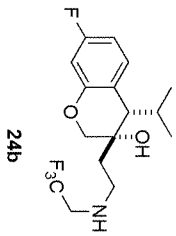
==== CHANNEL f1 =====  
NUC1 1H

P1 15.00 usec  
PLW1 12.00000000 W  
SFO1 400.2124715 MHz

F2 - Processing parameters

SI 65536  
SF 400.2100190 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00





Current Data Parameters  
 NAME LJE-309  
 EXPNO 3  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20130227  
 Time 15.52

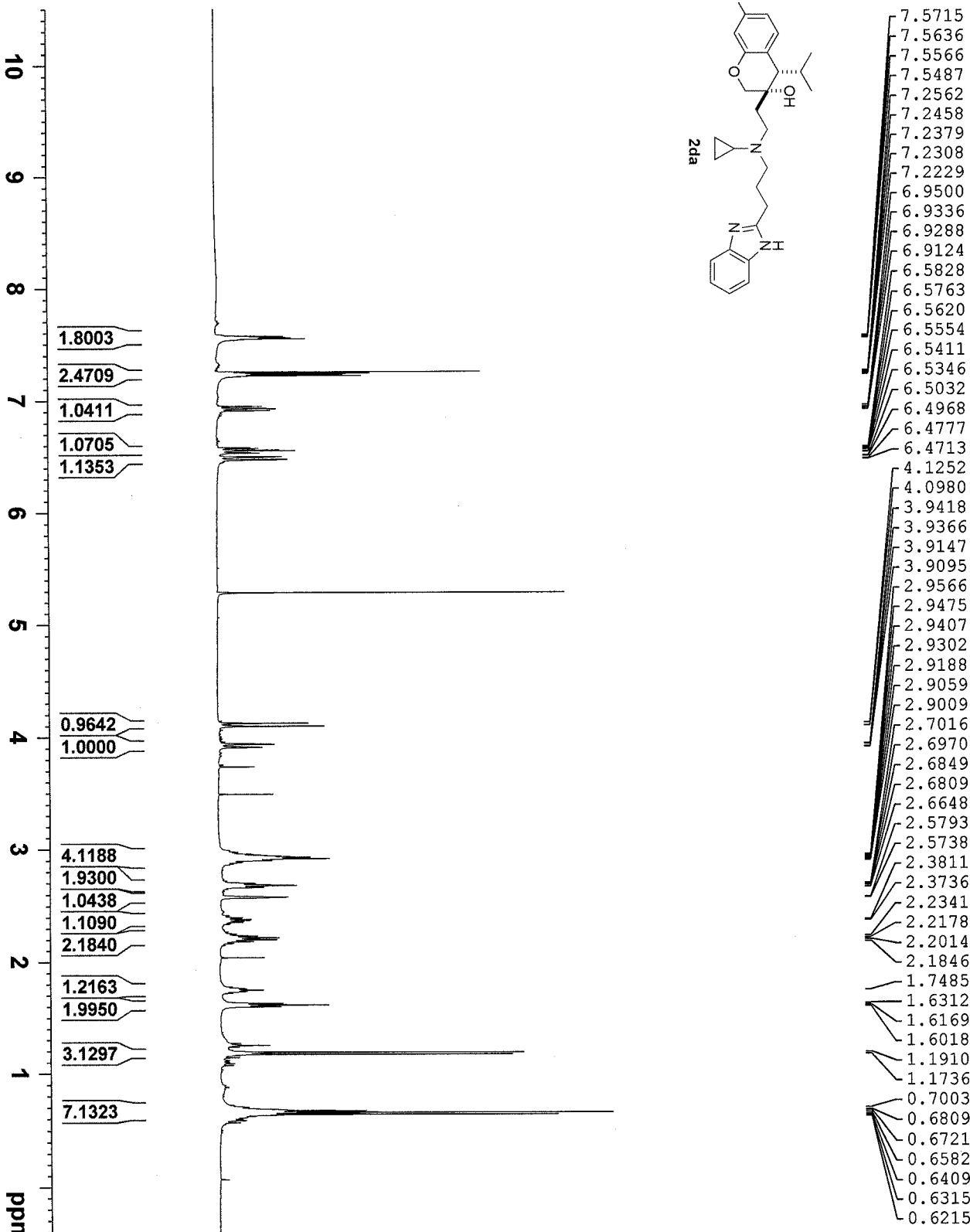
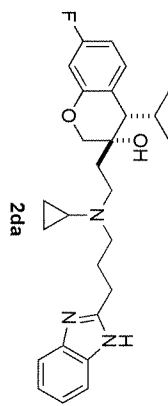
INSTRUM spect  
 PROBHD 5 mm PABBO BH/  
 PULPROG zgpg30  
 TD 65536  
 FIDRES 0.36798 Hz  
 AQ 1.961398 sec  
 RG 130.82  
 DW 20.890 usec  
 DE 29.32 usec  
 TE 293.2 K  
 D11 2.0000000 sec  
 D1 0.03000000 sec  
 TDO 1

NS 85  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.36798 Hz  
 AQ 1.961398 sec  
 RG 130.82  
 DW 20.890 usec  
 DE 29.32 usec  
 TE 293.2 K  
 D11 2.0000000 sec  
 D1 0.03000000 sec  
 TDO 1

==== CHANNEL f1 =====  
 NUC1 13C  
 P1 10.00 usec  
 P1M1 52.00000000 W  
 SFO1 100.6429474 MHz

==== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUC2 1H  
 PCPD2 90.00 usec  
 P1M2 12.00000000 W  
 P1M12 0.33333001 W  
 P1M13 0.27000001 W  
 SFO2 400.2116008 MHz

F2 - Processing parameters  
 SI 32768  
 SF 100.6328860 MHz  
 WDM EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40



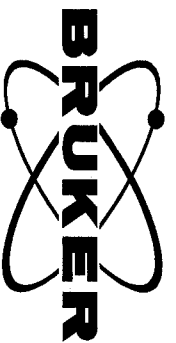
Current Data Parameters  
 NAME LJE-306  
 EXPNO 2  
 PROCNO 1

F2 - Acquisition Parameters

Date 20130222  
 Time 17.20  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 16  
 DS 2  
 SMH 8223.685 Hz  
 FIDRES 0.125483 Hz  
 AQ 3.9846387 sec  
 RG 103.95  
 DW 60.800 usec  
 DE 6.50 usec  
 TE 300.3 K  
 D1 1.00000000 sec  
 TD0 1

==== CHANNEL F1 =====  
 NUC1 1H  
 P1 15.00 usec  
 PLW1 12.00000000 W  
 SFO1 400.2124715 MHz

F2 - Processing parameters  
 SI 65536  
 SF 400.2100144 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



Current Data Parameters  
NAME LJF-Final  
EXPNO 8  
PROCNO 1

F2 - Acquisition Parameters

Date\_ 20130328  
Time\_ 13.05  
INSTRUM spect  
PROBHD 5 mm DUL 1H-13  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 882  
DS 4  
SWH 17985.611 Hz  
FIDRES 0.274439 Hz  
AQ 1.8219508 sec  
RG 18390.4  
DW 27.800 usec  
DE 6.00 usec  
TE 300.0 K  
D1 2.00000000 sec  
d11 0.03000000 sec  
DELTA 1.89999998 sec  
TD0 1

==== CHANNEL f1 =====

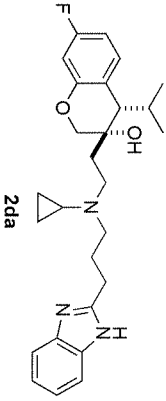
NUC1 13C  
P1 10.00 usec  
PL1 0.00 dB  
SFO1 75.4752953 MHz

==== CHANNEL f2 =====

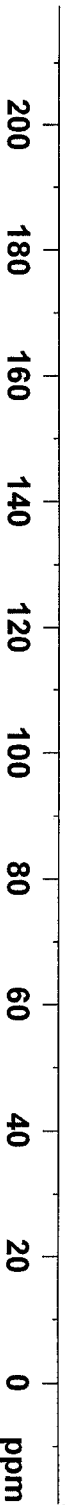
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 100.00 usec  
PI2 0.00 dB  
PL12 20.00 dB  
PL13 22.00 dB  
SFO2 300.1312005 MHz

F2 - Processing parameters

SI 32768  
SF 75.4677490 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

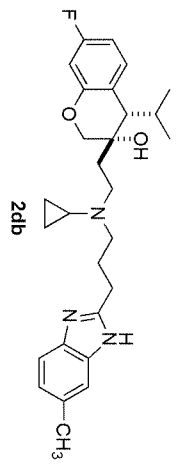


- 164.00
- 160.79
- 154.39
- 153.62
- 153.46
- 138.55
- 131.71
- 131.58
- 122.32
- 118.79
- 118.75
- 114.68
- 107.16
- 106.87
- 103.28
- 102.96
- 77.47
- 77.05
- 76.62
- 71.56
- 68.25
- 54.28
- 53.01
- 51.44
- 37.90
- 32.16
- 27.84
- 26.55
- 25.56
- 25.24
- 20.96
- 6.66
- 6.24





- 7.4597
- 7.4393
- 7.3320
- 7.2628
- 7.0655
- 7.0629
- 7.0451
- 7.0425
- 6.9573
- 6.9408
- 6.9361
- 6.9197
- 6.5885
- 6.5820
- 6.5676
- 6.5611
- 6.5468
- 6.5403
- 6.5101
- 6.5037
- 6.4846
- 6.4782
- 4.1252
- 4.0981
- 3.9457
- 3.9406
- 3.9187
- 3.9135
- 2.8985
- 2.8859
- 2.8806
- 2.8672
- 2.8512
- 2.6500
- 2.6455
- 2.6332
- 2.6292
- 2.6162
- 2.6131
- 2.5888
- 2.5831
- 2.4707
- 2.3840
- 2.3765
- 2.2028
- 2.1854
- 2.1648
- 2.1472
- 1.6969
- 1.6847
- 1.6717
- 1.5874
- 1.5737
- 1.5588
- 1.1940
- 1.1766
- 0.6627
- 0.6454
- 0.6368
- 0.6276
- 0.6138
- 0.6043

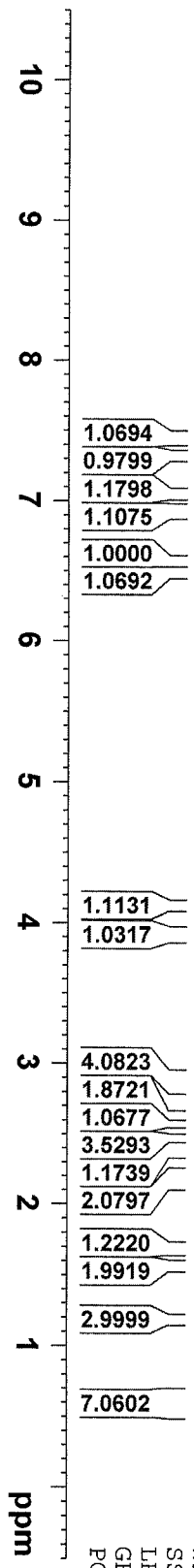


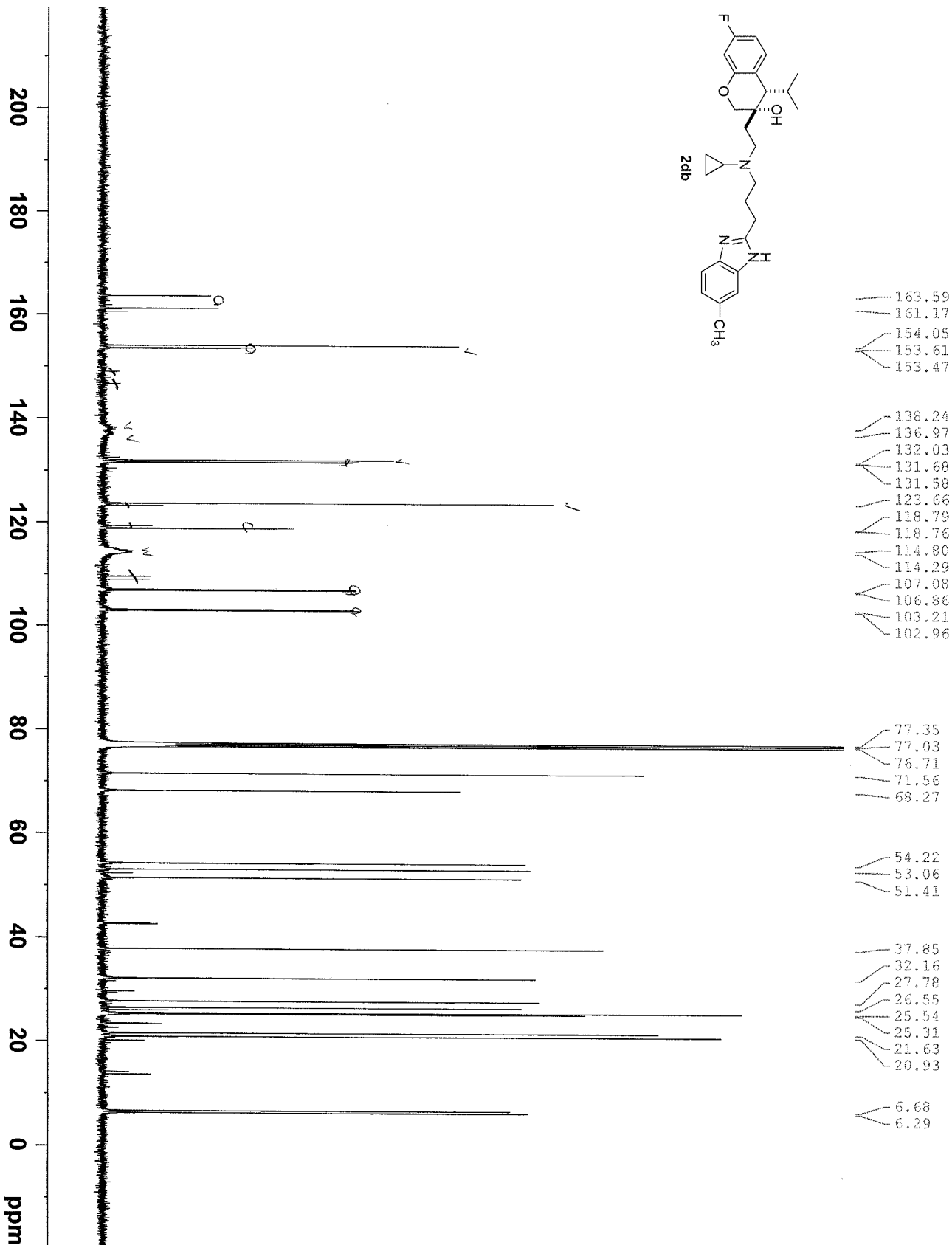
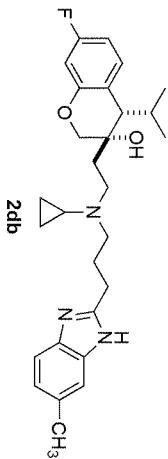
Current Data Parameters  
 NAME LJF-333  
 EXPNO 2  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20130411  
 Time\_ 17.43  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 16  
 DS 2  
 SWH 8223.685 Hz  
 FIDRES 0.125483 Hz  
 AQ 3.9846387 sec  
 RG 103.95  
 DW 60.800 usec  
 DE 6.50 usec  
 TE 298.4 K  
 D1 1.00000000 sec  
 TD0 1

==== CHANNEL f1 =====  
 NUC1 1H  
 P1 15.00 usec  
 P1M1 12.00000000 W  
 SFO1 400.2124715 MHz

F2 - Processing parameters  
 SI 65536  
 SF 400.2100118 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00





Current Data Parameters  
 NAME LJE-final  
 EXPNO 5  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20130417  
 Time 21.54  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 1115  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3631988 sec  
 RG 190.62  
 DW 20.800 usec  
 DE 6.30 usec  
 TE 300.4 K  
 D1 2.0000000 sec  
 D11 0.0300000 sec  
 TDO 1

===== CHANNEL f1 =====  
 NUC1 13C 13C  
 P1 10.00 usec  
 PL1 52.0000000 W  
 SFO1 100.629474 MHz

===== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUC2 1H 1H  
 P1 90.00 usec  
 PL1 12.0000000 W  
 PL12 0.33333001 W  
 PL13 0.27000001 W  
 SFO2 400.2116008 MHz

F2 - Processing parameters  
 SI 32768  
 SF 100.6328860 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40



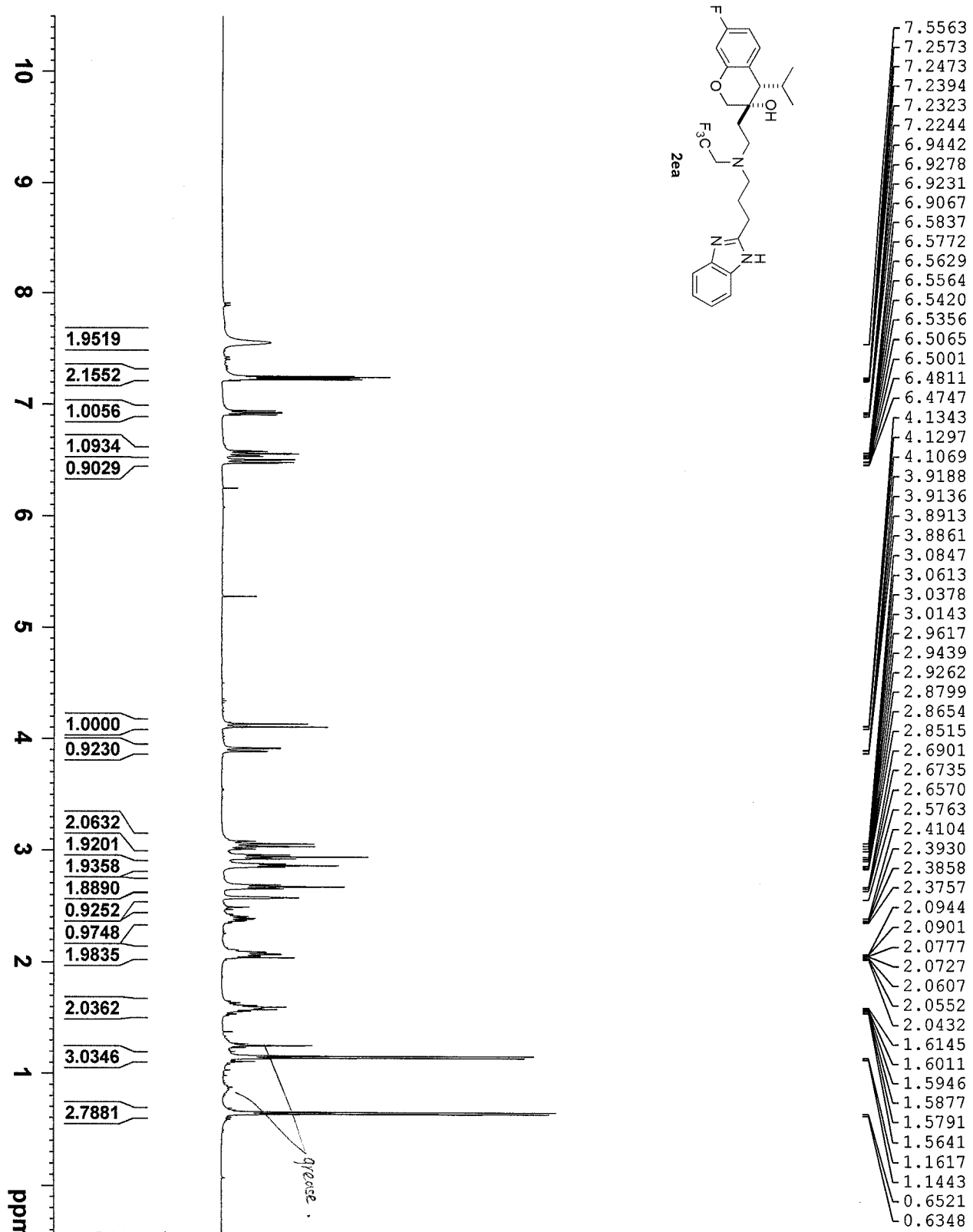
Current Data Parameters  
 NAME LJE-312  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters

Date\_ 20130305  
 Time 17.01  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 16  
 DS 2  
 SWH 8223.685 Hz  
 FIDRES 0.125483 Hz  
 AQ 3.9846387 sec  
 RG 69.69  
 DW 60.800 usec  
 DE 6.50 usec  
 TE 299.7 K  
 D1 1.00000000 sec  
 TD0 1

==== CHANNEL F1 =====  
 NUC1 1H  
 P1 15.00 usec  
 PLW1 12.00000000 W  
 SFO1 400.2124715 MHz

F2 - Processing parameters  
 SI 65536  
 SF 400.2100138 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00







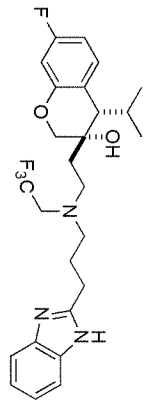
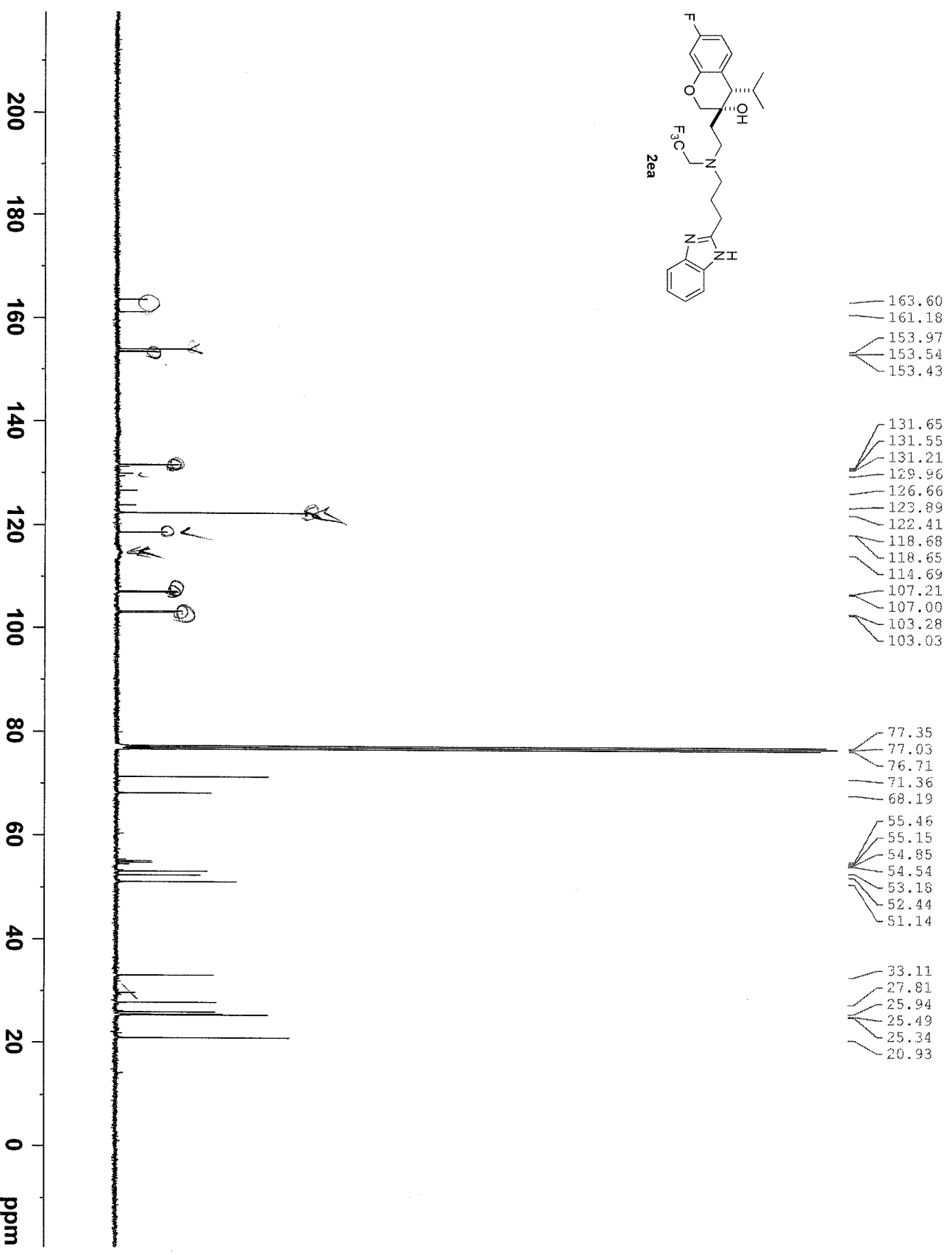
Current Data Parameters  
 NAME LJE-312  
 EXPNO 6  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20130327  
 Time 20.49  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 1024  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3631988 sec  
 RG 190.62  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 299.9 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TDO 1

CHANNEL f1  
 NUCL1 13C  
 P1 10.00 usec  
 ELEM1 52.00000000 W  
 SFO1 100.6429474 MHz

CHANNEL f2  
 CPDPRG2 waltz16  
 NUCL2 1H  
 P2 90.00 usec  
 ELEM2 12.00000000 M  
 SFO2 400.2116008 MHz

F2 - Processing parameters  
 SI 32768  
 SF 100.6328660 MHz  
 RDXW EM  
 SSB 0  
 GB 0  
 PC 1.40





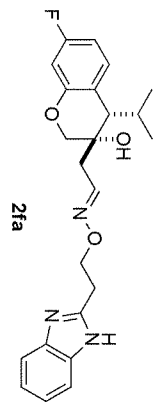
Current Data Parameters  
 NAME KTH-m-140  
 EXPNO 5  
 PROCNO 1

F2 - Acquisition Parameters

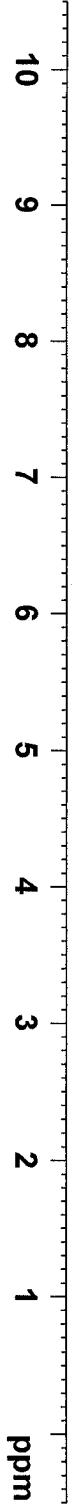
Date\_ 20120507  
 Time 14.04  
 INSTRUM spect  
 PROBHD 5 mm DUL 1H-13  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 16  
 DS 2  
 SWH 6172.839 Hz  
 FIDRES 0.094190 Hz  
 AQ 5.3084660 sec  
 RG 181  
 DE 81.000 usec  
 TE 300.0 K  
 D1 1.00000000 sec  
 TD0 1

==== CHANNEL f1 =====  
 NUC1 1H  
 P1 10.50 usec  
 PL1 -1.00 dB  
 SFO1 300.1318534 MHz

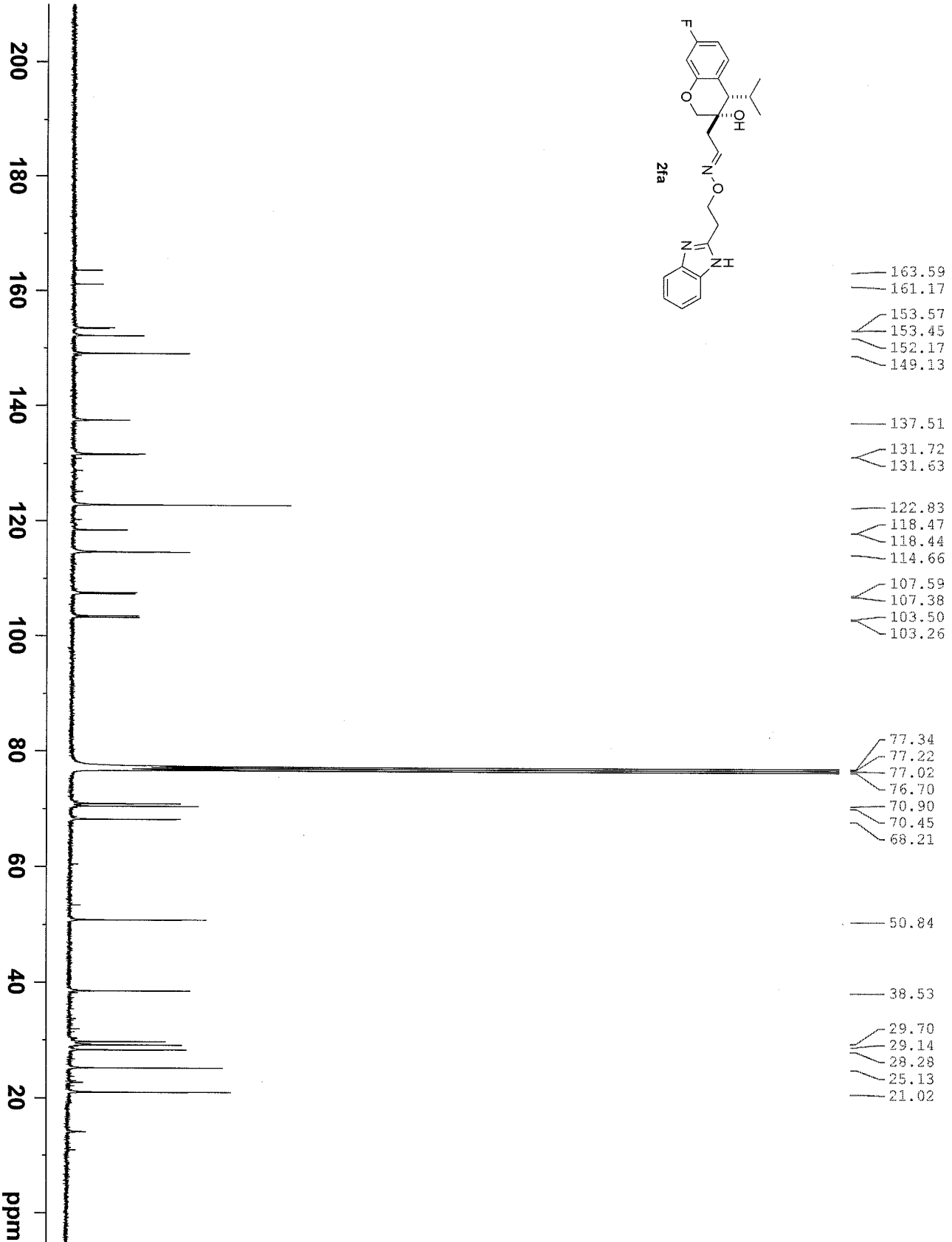
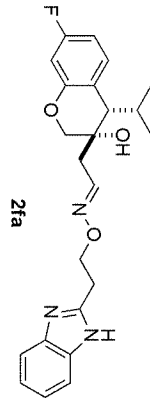
F2 - Processing Parameters  
 SI 32768  
 SF 300.1300123 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



- 7.5416
- 7.5321
- 7.5036
- 7.4833
- 7.4635
- 7.2586
- 7.2468
- 7.2333
- 7.2227
- 7.2133
- 7.2027
- 6.9744
- 6.9521
- 6.9465
- 6.9246
- 6.6098
- 6.5908
- 6.5821
- 6.5545
- 6.5463
- 6.5210
- 6.5126
- 4.4528
- 4.4354
- 4.4202
- 4.4148
- 4.3982
- 4.1326
- 4.1088
- 4.0804
- 4.0439
- 3.8949
- 3.8888
- 3.8584
- 3.8522
- 3.3248
- 3.3059
- 3.3020
- 3.2844
- 3.2670
- 2.5854
- 2.4063
- 2.3860
- 2.3625
- 2.3484
- 2.3342
- 2.0466
- 1.2808
- 1.2761
- 1.2567
- 1.2333
- 1.1450
- 1.1218
- 0.8904
- 0.8780
- 0.8550
- 0.6732
- 0.6502



- 1.6711
- 1.2657
- 2.6581
- 1.0000
- 1.9488
- 1.9698
- 1.6380
- 1.0460
- 2.0708
- 1.0012
- 3.0406
- 0.8922
- 3.9029
- 3.3605



Current Data Parameters  
 NAME KTH-m-140  
 EXEMO 3  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20120718  
 Time\_ 9.02  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 12288  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3631988 sec  
 RG 190.62  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 299.7 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TDO 1

==== CHANNEL f1 =====  
 NUCL1 13C  
 P1 10.00 usec  
 PLW1 52.00000000 W  
 SFO1 100.6429474 MHz

==== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUCC2 1H  
 EPCPD2 90.00 usec  
 FLMW2 12.00000000 W  
 ELMW2 0.3333001 W  
 ELMW12 0.27000001 W  
 SFO2 400.2118008 MHz

F2 - Processing parameters  
 SI 32768  
 SF 100.632850 MHz  
 NAW 6M  
 MSB 0  
 LGB 0  
 GB 0  
 PC 1.40



Current Data Parameters  
 NAME KPH-m-166  
 EXPNO 3  
 PROCNO 1

F2 - Acquisition Parameters

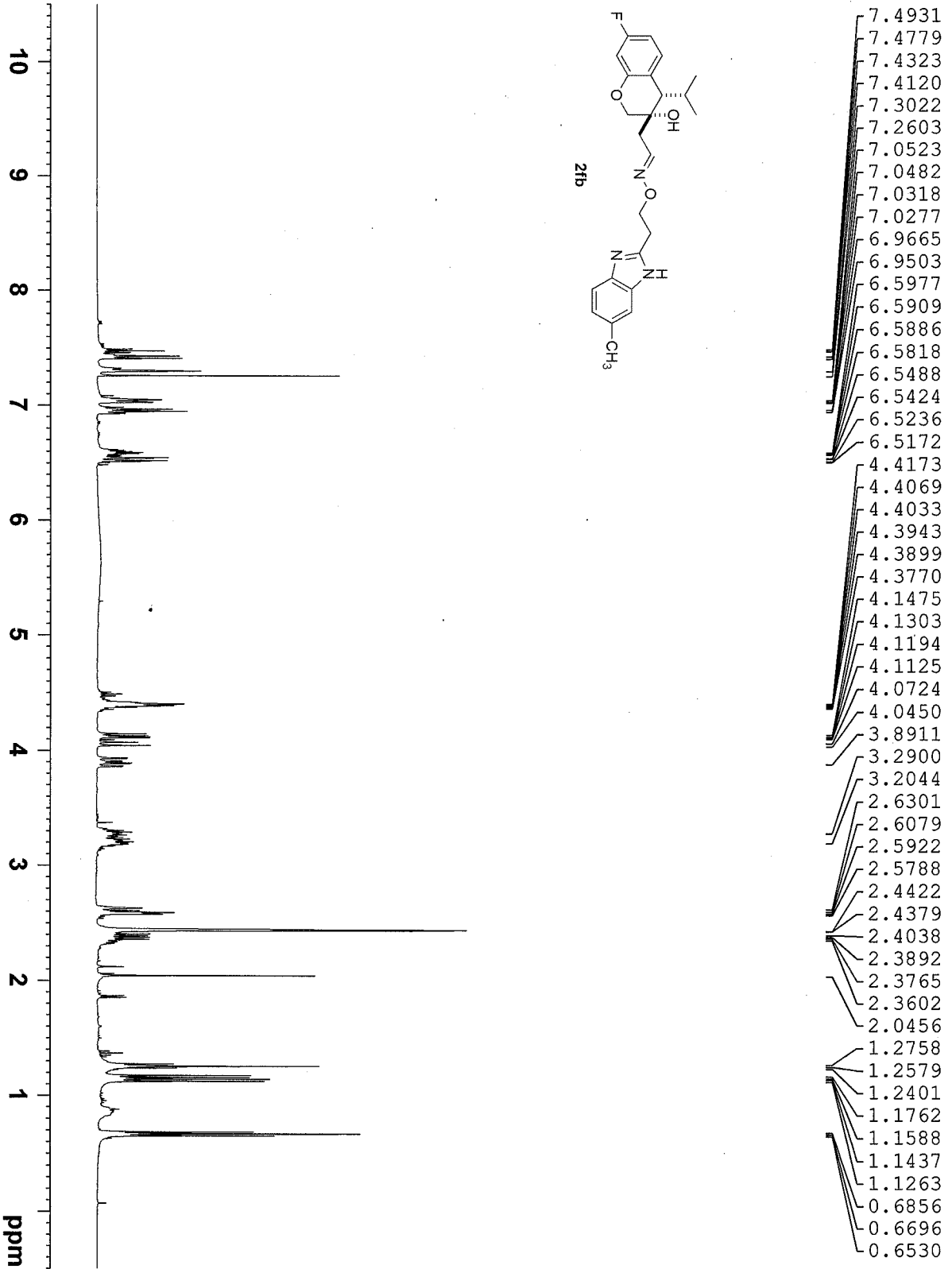
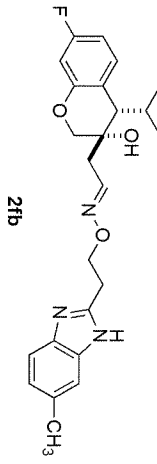
Date\_ 20120708  
 Time 21.13  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDC13  
 NS 16  
 DS 2  
 SWH 8223.685 Hz  
 FIDRES 0.125483 Hz  
 AQ 3.9846387 sec  
 RG 91.91  
 DW 60.800 usec  
 DE 6.50 usec  
 TE 297.9 K  
 D1 1.00000000 sec  
 TD0 1

==== CHANNEL f1 =====

NUC1 1H  
 P1 15.00 usec  
 PL1 12.00000000 W  
 SFO1 400.2124715 MHz

F2 - Processing parameters

SI 65536  
 SF 400.2100128 MHz  
 WDM EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00





Current Data Parameters  
 NAME KTH-m-156  
 EXPNO 4  
 PROCNO 1

F2 - Acquisition Parameters

Date\_ 20120708  
 Time\_ 22.12  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 1024  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3631988 sec  
 RG 190.62  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 298.9 K  
 D1 2.0000000 sec  
 D11 0.0300000 sec  
 TDO 1

CHANNEL f1

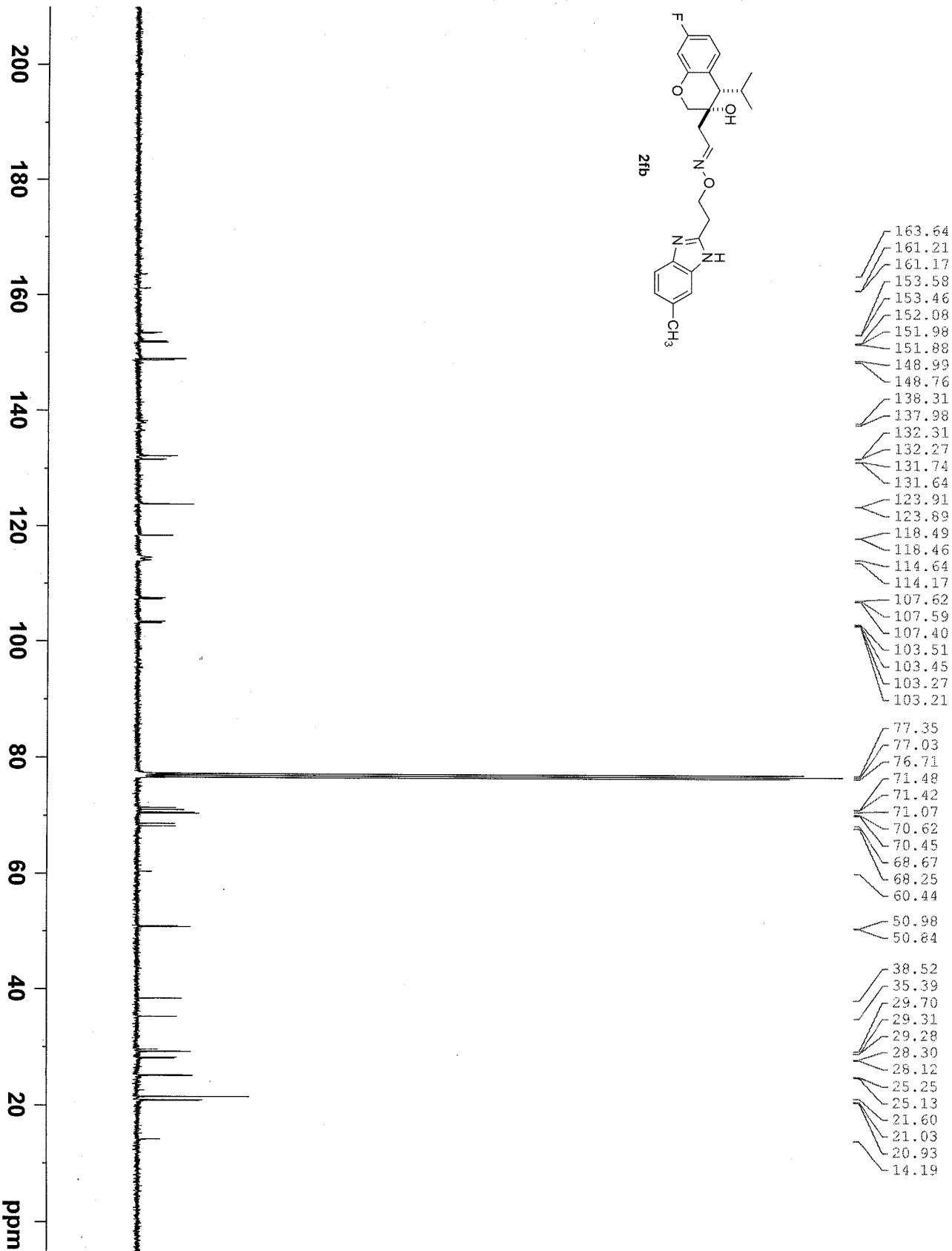
NUC1 13C  
 P1 10.00 usec  
 PL1 52.0000000 W  
 SF01 100.629474 MHz

CHANNEL f2

wait216  
 NOE2 90.0 H  
 FOC2 12.0000000 W  
 PL12 3333001 W  
 PL13 0.27000001 W  
 SF02 400.2116008 MHz

F2 - Processing parameters

SI 32768  
 SF 100.6328960 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40



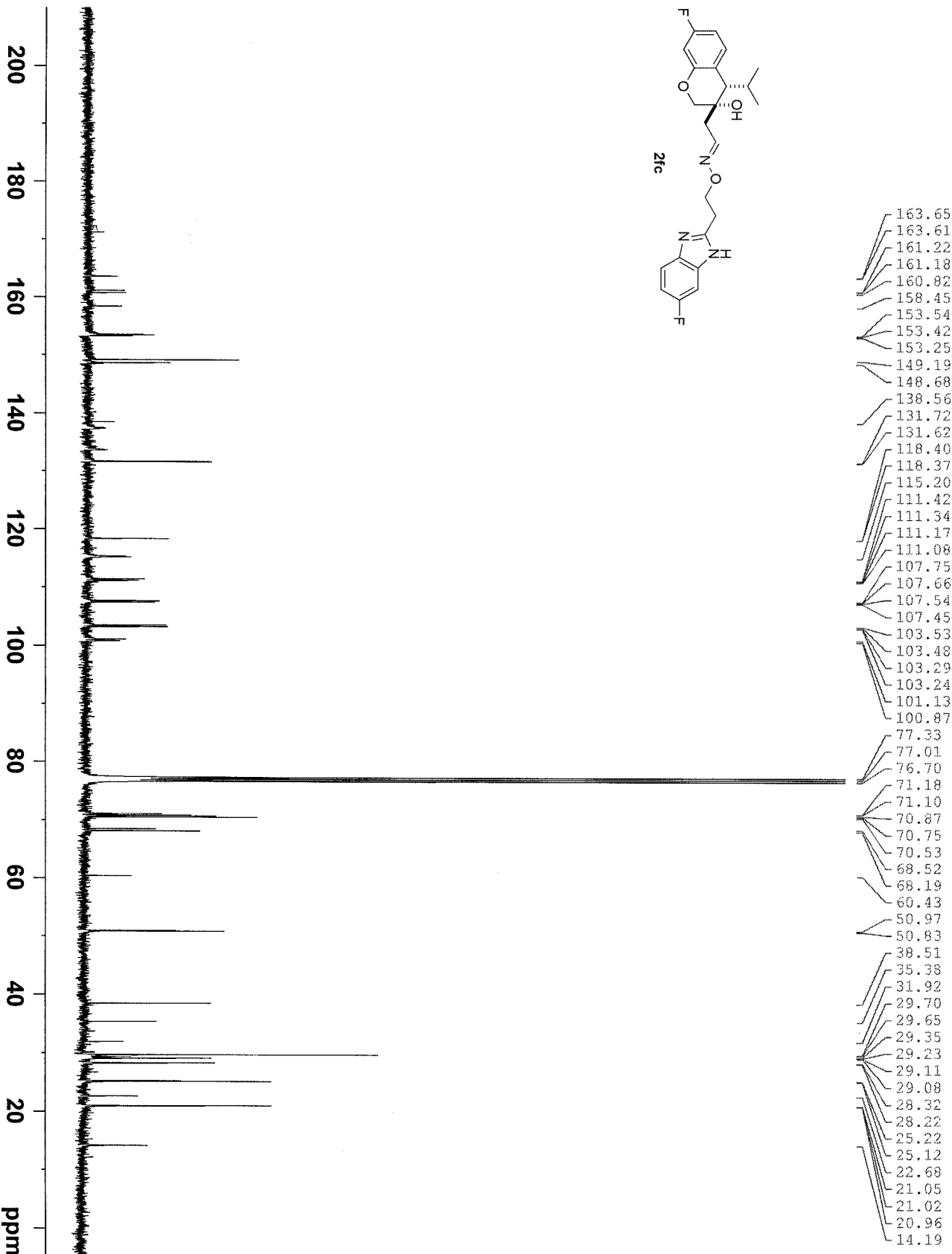


Current Data Parameters  
NAME KTH-m-155  
EXPNO 5  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20120709  
Time\_ 21.34  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 12170  
DS 4  
SWH 24038.461 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631988 sec  
RG 190.62  
DW 20.800 usec  
DE 6.50 usec  
TE 298.9 K  
D1 2.0000000 sec  
D11 0.0300000 sec  
TD0 1

==== CHANNEL f1 =====  
NUC1 13C  
P1 10.00 usec  
PLM1 52.0000000 W  
SFO1 100.6429474 MHz  
===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
FOC2 90.0H  
PUL2 12.0000000 M  
PLM2 0.3333001 M  
PLM13 0.2700001 M  
SFO2 400.2116008 MHz

F2 - Processing parameters  
SI 37768  
SF 100.6328660 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

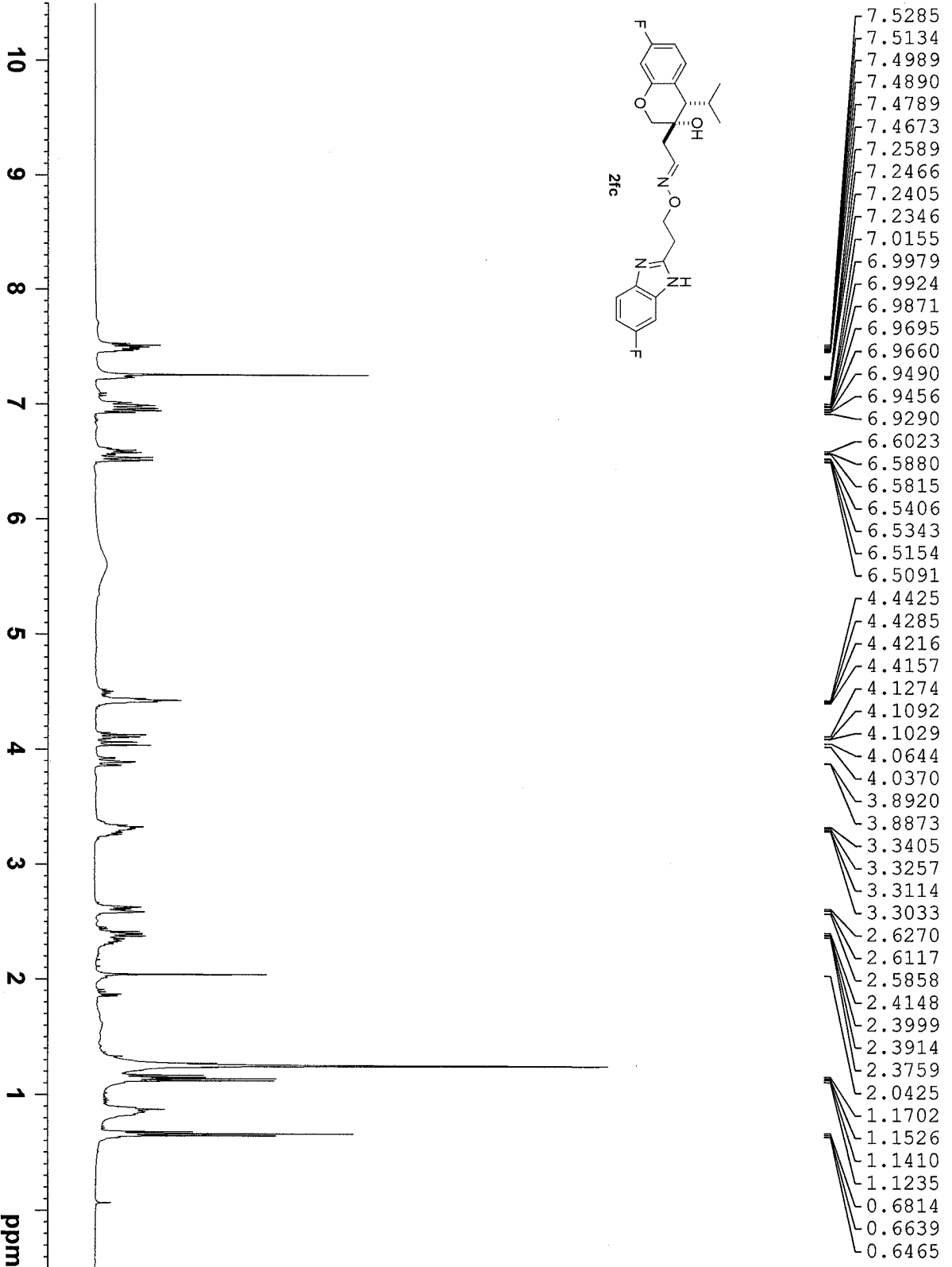
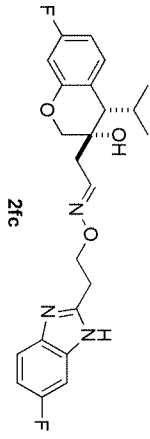




Current Data Parameters  
 NAME KTH-m-165  
 EXPNO 4  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20120709  
 Time 21.28  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 16  
 DS 2  
 SWH 8223.685 Hz  
 FIDRES 0.125483 Hz  
 AQ 3.9846387 sec  
 RG 119.61  
 DW 60.800 usec  
 DE 6.50 usec  
 TE 298.2 K  
 D1 1.00000000 sec  
 TD0 1

==== CHANNEL f1 =====  
 NUC1 1H  
 P1 15.00 usec  
 P1M1 12.00000000 W  
 SF01 400.2124715 MHz  
 F2 - Processing parameters  
 SI 65536  
 SF 400.2100135 MHz  
 WDM EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

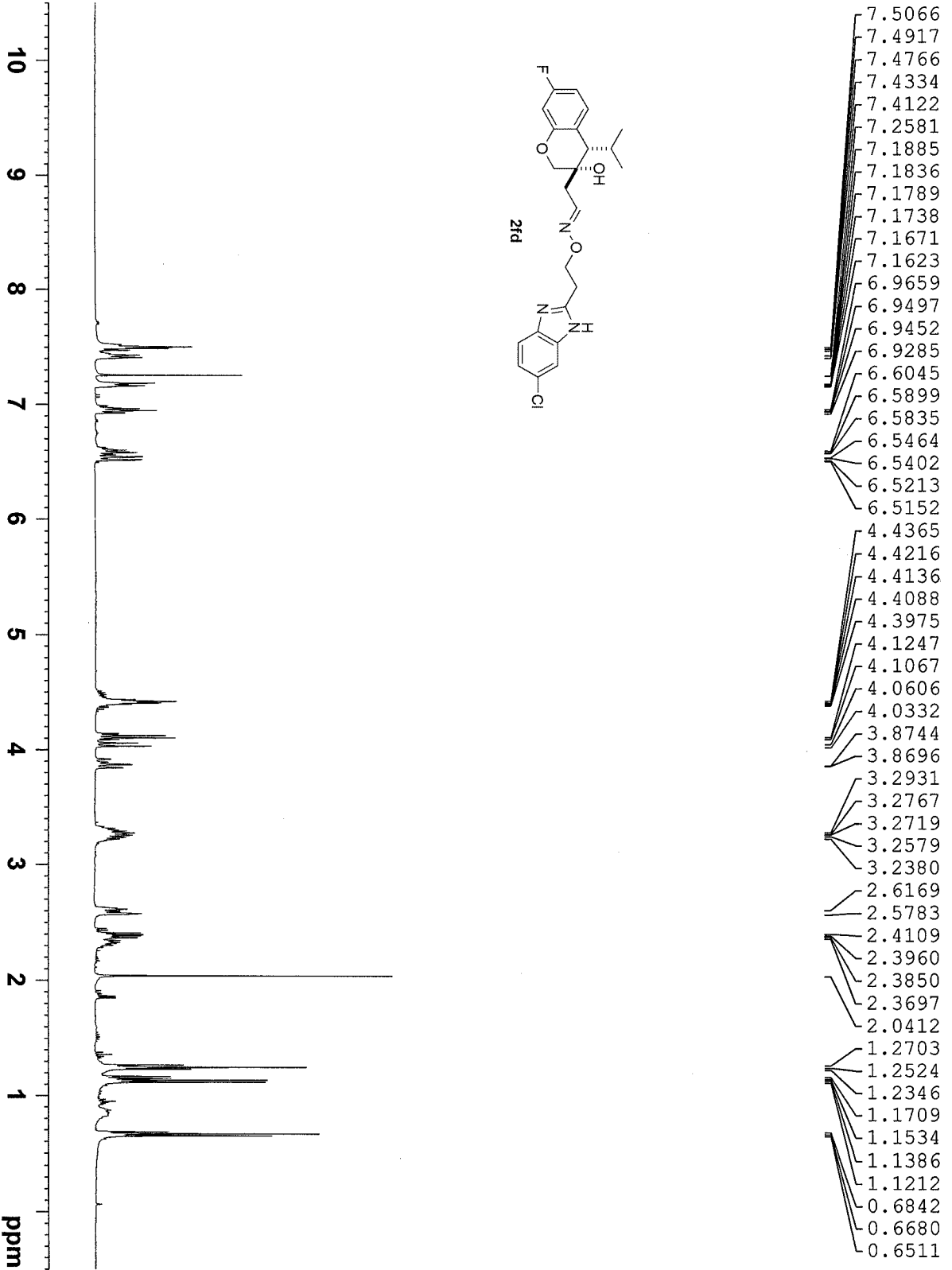
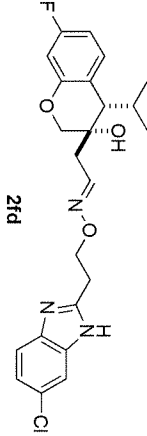




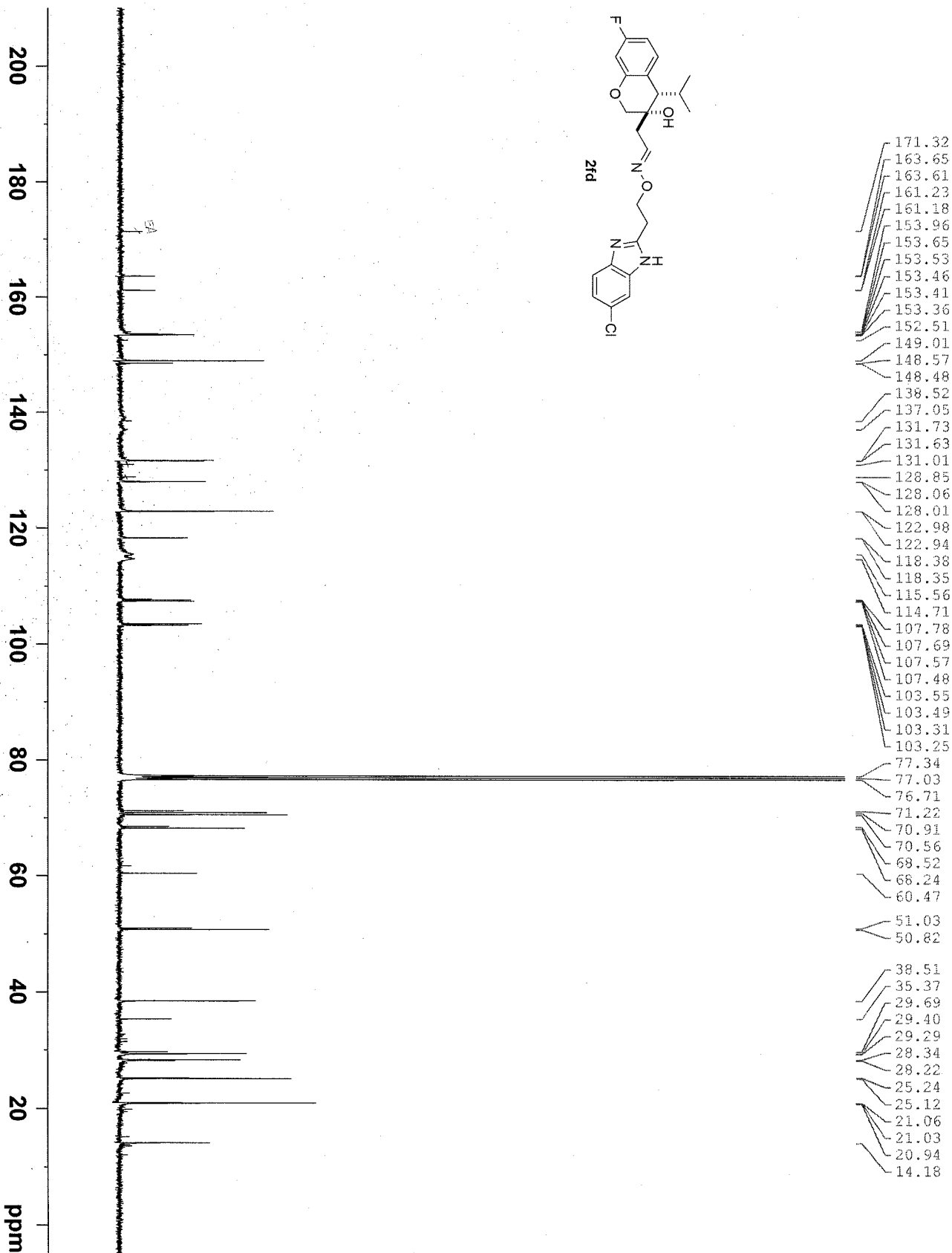
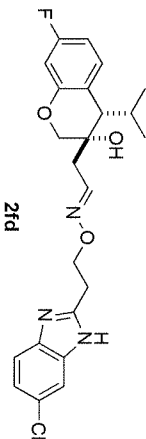
Current Data Parameters  
 NAME KTH-m-164  
 EXPNO 3  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20120708  
 Time 23.43  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 16  
 DS 2  
 SWH 8223.685 Hz  
 FIDRES 0.125483 Hz  
 AQ 3.9846387 sec  
 RG 91.91  
 DW 60.800 usec  
 DE 6.50 usec  
 TE 297.9 K  
 D1 1.00000000 sec  
 TD0 1

==== CHANNEL f1 =====  
 NUC1 1H  
 P1 15.00 usec  
 PL1 12.00000000 W  
 SFO1 400.2124715 MHz  
 F2 - Processing parameters  
 SI 65536  
 SF 400.2100138 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00







Current Data Parameters  
 NAME KTH-m-164  
 EXPNO 4  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20120709  
 Time 4.21

INSTRUM spect  
 PROBHD 5 mm PABBO BH/  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 4848

DS 4  
 SMH 24038.461 Hz  
 FIDRES 0.366788 Hz  
 AQ 1.363198 sec  
 RG 190.62  
 DE 20.90 usec  
 DM 26.90 usec  
 TE 29.30 Ksec  
 D1 2.00060000 sec  
 D11 0.03000000 sec  
 TDO 1

CHANNEL F1  
 NUC1 13C  
 P1 10.00 usec  
 PLM1 52.00000000 W  
 SFO1 100.6429474 MHz

CHANNEL F2  
 CPDPRG2 waltz16  
 NUC2 1H  
 PCPD2 90.00 usec  
 PLM2 12.00000000 W  
 PLM12 0.3333001 W  
 PLM13 0.27000001 W  
 SFO2 400.2116008 MHz

F2 - Processing parameters  
 SI 32768  
 SF 100.6328860 MHz  
 MDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40