

Supporting Information

Facile diverted synthesis of pyrrolidinyl triazoles using organotrifluoroborate: Discovery of potential mPTP blockers

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I. Experimental Procedures for Table 2

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. ^1H and ^{13}C spectra were recorded on Bruker 300, Bruker 400 or Varian 300 NMR spectrometers. ^1H 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). ^1H NMR chemical shifts are reported relative to CDCl_3 (7.26 ppm). ^{13}C NMR was recorded relative to the central line of CDCl_3 (77.0 ppm).

Potassium (1-(3-hydroxypropyl)-1*H*-1,2,3-triazol-4-yl)trifluoroborate (**12a**)

To a solution of potassium ethynyltrifluoroborate **6** (41.0 mg, 0.31 mmol), CuBr (4.50 mg, 31.1 μmol), *N,N*-dimethylethylenediamine (6.70 μL , 62.2 μmol), Cs_2CO_3 (0.10 g, 0.31 mmol) in DMSO-d_6 (2 mL) was added 3-azidopropanol (34.6 mg, 0.34 mmol) at room temperature. The reaction mixture was carried out at 90 °C for 30 min (until the ^1H NMR indicated completion of the reaction). Then, the solvent was completely removed under high vacuum. The residual product was dissolved in dry acetone (3 x 7 mL) and the insoluble salts were removed by filtration through Celite and activated carbon. The solvent was concentrated and the crude solid was purified by dissolution in a minimal amount of dry acetone and precipitation with Et_2O to gave the title compound **12a** (51.5 mg, 72%) as a white solid; ^1H

NMR (DMSO-*d*₆, 400 MHz) δ 7.45 (s, 1H), 4.66 (t, *J* = 4.4 Hz, 1H), 4.30 (t, *J* = 7.1 Hz, 2H), 3.37 (t, *J* = 5.4 Hz, 2H), 2.50 (s, 1H), 1.89 (m, 2H); ¹³C NMR (DMSO-*d*₆, 100 MHz) δ 126.3, 58.0, 45.8, 33.7; ¹⁹F NMR (DMSO-*d*₆, 376 MHz) δ -134.7; ¹¹B NMR (DMSO-*d*₆, 128 MHz) δ 2.17.

Potassium (1-(2-ethoxy-2-oxoethyl)-1*H*-1,2,3-triazol-4-yl)trifluoroborate (12b)

Following the same procedure as that used for the synthesis of **12a**, potassium ethynyltrifluoroborate **6** (32.6 mg, 0.25 mmol), ethyl-2-azidoacetate (47.8 mg, 0.37 mmol), CuBr (3.54 mg, 24.7 μ mol), N,N-dimethylethylenediamine (5.30 μ L, 49.4 μ mol), Cs₂CO₃ (80.0 mg, 0.25 mmol) in DMSO-*d*₆ (1.5 mL) gave the title compound **12b** (40.2 mg, 62%) as a yellow solid; ¹H NMR (DMSO-*d*₆, 400 MHz) δ 7.45 (s, 1H), 5.22 (s, 2H), 4.15 (q, *J* = 7.1 Hz, 2H), 1.21 (t, *J* = 7.1 Hz, 3H); ¹³C NMR (DMSO-*d*₆, 100 MHz) δ 168.2, 127.7, 61.5, 49.8, 14.4; ¹⁹F NMR (DMSO-*d*₆, 376 MHz) δ -135.4; ¹¹B NMR (DMSO-*d*₆, 128 MHz) δ 2.17.

Potassium (1-cinnamyl-1*H*-1,2,3-triazol-4-yl)trifluoroborate (12c)

Following the same procedure as that used for the synthesis of **12a**, potassium ethynyltrifluoroborate **6** (20.0 mg, 0.15 mmol), (E)-(3-azidopropenyl)benzene (26.2 mg, 0.17 mmol), CuBr (2.20 mg, 15.1 μ mol), N,N-dimethylethylenediamine (3.26 μ L, 30.3 μ mol), Cs₂CO₃ (49.0 mg, 0.15 mmol) in DMSO-*d*₆ (1 mL) gave the title compound **12c** (38.1 mg, 87%) as a white solid; ¹H NMR (DMSO-*d*₆, 400 MHz) δ 7.50-7.42 (m, 3H), 7.34-7.23 (m, 3H), 5.06 (d, *J* = 6.0 Hz, 2H); ¹³C NMR (DMSO-*d*₆, 100 MHz) δ 136.4, 133.1, 129.1, 128.3, 126.9, 126.1, 125.2, 50.6; ¹⁹F NMR (DMSO-*d*₆, 376 MHz) δ -135.3; ¹¹B NMR (DMSO-*d*₆, 128 MHz) δ 2.14.

Potassium 1-(1-benzylpyrrolidin-3-yl)-1*H*-1,2,3-triazole-4-yl trifluoroborate (12d)

Following the same procedure as that used for the synthesis of **12a**, potassium ethynyltrifluoroborate **6** (29.0 mg, 0.22 mmol), 3-azido-1-benzylpyrrolidine (44.3 mg, 0.24 mmol), CuBr (3.20 mg, 21.9 μ mol), N,N-dimethylethylenediamine (4.10 μ L, 43.9 μ mol),

Cs₂CO₃ (72.0 mg, 0.22 mmol) in DMSO-*d*₆ (1.5 mL) gave the title compound **12d** (52.1 mg, 71%) as a white solid; ¹H NMR (MeOH-*d*₄, 400 MHz) δ 7.75 (s, 1H), 7.37-7.29 (m, 4H), 7.26-7.24 (m, 1H), 5.19 (m, 1H), 3.71 (q, *J* = 12.1 Hz, 2H), 2.98 (m, 2H), 2.89 (dd, *J* = 10.3, 4.3 Hz, 1H), 2.61 (m, 1H), 2.52 (m, 1H), 2.14 (m, 1H); ¹³C NMR (MeOH-*d*₄, 100 MHz) δ 138.1, 128.6, 128.0, 126.9, 124.6, 59.6, 59.3, 58.3, 52.4, 31.8; ¹⁹F NMR (DMSO-*d*₆, 376 MHz) δ -135.3; ¹¹B NMR (DMSO-*d*₆, 128 MHz) δ 2.19.

Potassium (1-(1-2-(*tert*-butoxy)-2-oxoethyl)piperidin-3-yl)-1*H*-1,2,3-triazole-4-yl)trifluoroborate (12e)

Following the same procedure as that used for the synthesis of **12a**, potassium ethynyltrifluoroborate **6** (24.0 mg, 0.18 mmol), *tert*-butyl 2-(3-azidopiperidin-1-yl)acetate (45.1 mg, 0.20 mmol), CuBr (2.60 mg, 18.1 μ mol), N,N-dimethylethylenediamine (3.90 μ L, 36.2 μ mol), Cs₂CO₃ (59.0 mg, 0.18 mmol) in DMSO-*d*₆ (1 mL) gave the title compound **12e** (31.9 mg, 45%) as a white solid; ¹H NMR (DMSO-*d*₆, 400 MHz) δ 7.50 (s, 1H), 4.39 (m, 1H), 4.03 (bs, 1H), 3.80 (d, *J* = 12.7 Hz, 1H), 3.15 (bs, 1H), 2.91 (td, *J* = 12.1, 4.6 Hz, 1H), 2.10-1.99 (m, 1H), 1.95 (m, 1H), 1.71 (m, 1H), 1.54-1.39 (m, 10H); ¹³C NMR (DMSO-*d*₆, 100 MHz) δ 154.2, 124.5, 79.5, 54.9, 48.8, 43.6, 30.8, 28.4, 23.8; ¹⁹F NMR (DMSO-*d*₆, 376 MHz) δ -135.6; ¹¹B NMR (DMSO-*d*₆, 128 MHz) δ 2.17.

Potassium (1-(4-methoxyphenyl)-1*H*-1,2,3-triazol-4-yl)trifluoroborate (12g)

Following the same procedure as that used for the synthesis of **12a**, potassium ethynyltrifluoroborate **6** (30.0 mg, 0.23 mmol), 1-azido-4-methoxybenzene (37.4 mg, 0.25 mmol), CuBr (3.30 mg, 22.8 μ mol), N,N-dimethylethylenediamine (4.90 μ L, 45.5 μ mol), Cs₂CO₃ (74.0 mg, 0.23 mmol) in DMSO-*d*₆ (1.5 mL) gave the title compound **12g** (57.7 mg, 90%) as a white solid; ¹H NMR (DMSO-*d*₆, 400 MHz) δ 8.03 (s, 1H), 7.76 (td, *J* = 6.2, 3.9 Hz, 2H), 7.07 (td, *J* = 6.2, 3.9 Hz, 2H), 3.80 (s, 3H); ¹³C NMR (DMSO-*d*₆, 100 MHz) δ 158.8, 131.4, 124.2, 121.6, 115.1, 55.9; ¹⁹F NMR (DMSO-*d*₆, 376 MHz) δ -134.9; ¹¹B NMR

(DMSO-*d*₆, 128 MHz) δ 2.15.

Potassium (1-(4-bromophenyl)-1*H*-1,2,3-triazol-4-yl)trifluoroborate (12h)

Following the same procedure as that used for the synthesis of **12a**, potassium ethynyltrifluoroborate **6** (22.6 mg, 0.17 mmol), 1-azido-4-bromobenzene (37.4 mg, 0.18 mmol), CuBr (2.46 mg, 17.2 μ mol), N,N-dimethylethylenediamine (3.68 μ L, 34.4 μ mol), Cs₂CO₃ (55.8 mg, 0.17 mmol) in DMSO-*d*₆ (1 mL) gave the title compound **12h** (40.6 mg, 72%) as a yellow solid; ¹H NMR (DMSO-*d*₆, 400 MHz) δ 8.17 (s, 1H), 7.85 (d, *J* = 8.8 Hz, 2H), 7.71 (d, *J* = 8.6 Hz, 2H); ¹³C NMR (DMSO-*d*₆, 100 MHz) δ 137.0, 132.9, 124.1, 121.9, 120.1; ¹⁹F NMR (DMSO-*d*₆, 376 MHz) δ -135.9; ¹¹B NMR (DMSO-*d*₆, 128 MHz) δ 2.15.

Potassium (1-(2,6-dimethylphenyl)-1*H*-1,2,3-triazol-4-yl)trifluoroborate (12i)

Following the same procedure as that used for the synthesis of **12a**, potassium ethynyltrifluoroborate **6** (34.4 mg, 0.26 mmol), 2-azido-1,3-dimethylbenzene (42.2 mg, 0.28 mmol), CuBr (3.70 mg, 26.1 μ mol), N,N-dimethylethylenediamine (5.60 μ L, 52.1 μ mol), Cs₂CO₃ (85.0 mg, 0.26 mmol) in DMSO-*d*₆ (1.5 mL) gave the title compound **12i** (50.1 mg, 69%) as a white solid; ¹H NMR (DMSO-*d*₆, 400 MHz) δ 7.56 (s, 1H), 7.31 (m, 1H), 7.22 (d, *J* = 7.5 Hz, 2H), 1.87 (s, 6H); ¹³C NMR (DMSO-*d*₆, 100 MHz) δ 137.3, 135.3, 129.4, 128.5, 127.6, 17.4; ¹⁹F NMR (DMSO-*d*₆, 376 MHz) δ -134.8; ¹¹B NMR (DMSO-*d*₆, 128 MHz) δ 2.20.

II. Experimental Procedure for compounds 2b

1-(1-Benzylpyrrolidin-3-yl)-4-(5-chloro-2-(3,4-dichlorobenzyloxy)phenyl)-1*H*-1,2,3-triazole (2ba)

Following the same procedure as that used for the synthesis of **2aa**, the reaction of 3-(4-(5-chloro-2-(3,4-dichlorobenzyloxy)phenyl)-1*H*-1,2,3-triazole-1-yl)pyrrolidinium 2,2,2-trifluoroacetate **18b** (23.4 mg, 43.5 μ mol), benzaldehyde (6.65 μ L, 65.3 μ mol), CH₃CO₂H (0.50 μ L, 8.70 μ mol), NaBH(OAc)₃ (27.6 mg, 131 μ mol) in THF (0.4 mL) gave the title compound **2ba** (19.7 mg, 88%) as a yellow solid; ¹H NMR (CDCl₃, 300 MHz) δ 8.33 (s, 1H), 8.14 (s, 1H), 7.54 (s, 1H), 7.35 (bs, 1H), 7.22 (m, 7H), 6.90 (d, *J* = 8.8 Hz, 1H), 5.24 (bs, 1H), 5.10 (s, 2H), 3.64 (bs, 2H), 2.91 (bs, 3H), 2.55 (bs, 2H), 2.03 (bs, 1H); ¹³C NMR (CDCl₃, 75 MHz) δ 152.9, 142.2, 136.5, 132.9, 132.5, 130.8, 129.6, 128.5, 128.4, 127.6, 127.3, 127.0, 126.9, 121.8, 121.7, 113.3, 69.6, 59.9, 59.4, 59.3, 52.6, 32.7; HRMS-ESI (*m/z*): [M+H]⁺ calcd for C₂₆H₂₄Cl₃N₄O 513.10102, Found 513.10048.

1-(1-(4-Fluorobenzyl)pyrrolidin-3-yl)-4-(2-(3,4-dichlorobenzyloxy)-5-chlorophenyl)-1*H*-1,2,3-triazole (2bb)

Following the same procedure as that used for the synthesis of **2aa**, the reaction of 3-(4-(5-chloro-2-(3,4-dichlorobenzyloxy)phenyl)-1*H*-1,2,3-triazole-1-yl)pyrrolidinium 2,2,2-trifluoroacetate **18b** (23.8 mg, 44.3 μ mol), 4-fluorobenzaldehyde (7.12 μ L, 66.4 μ mol), CH₃CO₂H (0.51 μ L, 8.85 μ mol), NaBH(OAc)₃ (28.1 mg, 133 μ mol) in THF (0.5 mL) gave the title compound **2bb** (14.8 mg, 63%) as a white solid; ¹H NMR (CDCl₃, 300 MHz) δ 8.34 (d, *J* = 2.6 Hz, 1H), 8.10 (s, 1H), 7.55 (d, *J* = 1.8 Hz, 1H), 7.40 (d, *J* = 8.2 Hz, 1H), 7.27-7.22 (m, 2H), 7.13 (bs, 2H), 6.95-6.89 (m, 3H), 5.24 (m, 1H), 5.10 (s, 2H), 3.61 (m, 2H), 2.87 (bs, 3H), 2.56 (m, 2H), 2.05 (m, 1H); ¹³C NMR (CDCl₃, 75 MHz) δ 162.0 (d, ¹*J* = 243.6 Hz), 152.9, 142.2, 136.5, 133.0, 132.6, 130.8, 129.9 (³d, *J* = 7.3 Hz), 129.6, 128.4, 127.6, 127.1, 127.0, 121.7 (⁴d, *J* = 6.2 Hz), 115.2 (²d, *J* = 21.2 Hz), 113.3, 69.6, 59.9, 59.2, 58.6, 52.5, 32.7;

HRMS-ESI (m/z): [M+H]⁺ calcd for C₂₆H₂₃Cl₃FN₄O 531.09160, Found 531.09110.

1-(1-(4-Chlorobenzyl)pyrrolidin-3-yl)-4-(2-(3,4-dichlorobenzyloxy)-5-chlorophenyl)-1H-1,2,3-triazole (2bc)

Following the same procedure as that used for the synthesis of **2aa**, the reaction of 3-(4-(5-chloro-2-(3,4-dichlorobenzyloxy)phenyl)-1H-1,2,3-triazole-1-yl)pyrrolidinium 2,2,2-trifluoroacetate **18b** (17.4 mg, 32.3 μmol), 4-chlorobenzaldehyde (6.82 mg, 48.5 μmol), CH₃CO₂H (0.37 μL, 6.47 μmol), NaBH(OAc)₃ (20.5 mg, 97.1 μmol) in THF (0.3 mL) gave the title compound **2bc** (11.1 mg, 63%) as a yellow solid; ¹H NMR (CDCl₃, 300 MHz) δ 8.34 (d, *J* = 2.6 Hz, 1H), 8.09 (s, 1H), 7.54 (d, *J* = 1.5 Hz, 1H), 7.41 (d, *J* = 8.2 Hz, 1H), 7.26-7.23 (m, 5H), 7.23 (bs, 1H), 6.92 (d, *J* = 8.8 Hz, 1H), 5.25 (bs, 1H), 5.10 (s, 2H), 3.58 (bs, 2H), 2.90 (bs, 2H), 2.57 (bs, 2H), 2.07 (bs, 1H); ¹³C NMR (CDCl₃, 75 MHz) δ 152.9, 142.3, 136.5, 133.0, 132.6, 130.8, 129.6, 128.9, 128.7, 128.5, 127.6, 127.1, 126.9, 121.9, 121.4, 113.3, 77.2, 69.6, 59.1, 58.5, 52.5, 32.7; HRMS-ESI (m/z): [M+H]⁺ calcd for C₂₆H₂₃Cl₄N₄O 547.06205, Found 547.06155.

1-(1-(2,3-Dichlorobenzyl)pyrrolidin-3-yl)-4-(2-(3,4-dichlorobenzyloxy)-5-chlorophenyl)-1H-1,2,3-triazole (2bd)

Following the same procedure as that used for the synthesis of **2aa**, the reaction of 3-(4-(5-chloro-2-(3,4-dichlorobenzyloxy)phenyl)-1H-1,2,3-triazole-1-yl)pyrrolidinium 2,2,2-trifluoroacetate **18b** (30.0 mg, 55.8 μmol), 2,3-dichlorobenzaldehyde (19.5 mg, 112 μmol), CH₃CO₂H (0.96 μL, 16.7 μmol), NaBH(OAc)₃ (47.3 mg, 223 μmol) in THF (0.6 mL) gave the title compound **2bd** (30.3 mg, 93%) as a yellow solid; ¹H NMR (CDCl₃, 300 MHz) δ 8.32 (d, *J* = 2.6 Hz, 1H), 8.18 (s, 1H), 7.47 (d, *J* = 1.7 Hz, 1H), 7.31 (t, *J* = 6.6 Hz, 2H), 7.20 (td, *J* = 2.4, 7.4 Hz, 2H), 7.13-7.03 (m, 2H), 6.88 (d, *J* = 8.8 Hz, 1H), 5.27 (m, 1H), 5.10 (s, 2H), 3.75 (q, *J* = 11.8 Hz, 2H), 2.99 (bs, 2H), 2.86 (bs, 1H), 2.60 (m, 2H), 2.04 (m, 1H); ¹³C NMR (CDCl₃, 75 MHz) δ 152.9, 142.3, 136.6, 133.2, 132.8, 132.4, 132.2, 130.7, 129.4,

128.4, 127.6, 127.1, 127.0, 126.8, 121.8, 121.6, 113.4, 69.5, 59.7, 59.1, 56.5, 52.5, 32.7;

HRMS-ESI (m/z): $[M+H]^+$ calcd for $C_{26}H_{22}Cl_5N_4O$ 581.02308, Found 581.02246.

1-(1-(2,4-Dichlorobenzyl)pyrrolidin-3-yl)-4-(2-(3,4-dichlorobenzyloxy)-5-chlorophenyl)-1H-1,2,3-triazole (2be)

Following the same procedure as that used for the synthesis of **2aa**, the reaction of 3-(4-(5-chloro-2-(3,4-dichlorobenzyloxy)phenyl)-1H-1,2,3-triazole-1-yl)pyrrolidinium 2,2,2-trifluoroacetate **18b** (29.2 mg, 54.3 μ mol), 2,4-dichlorobenzaldehyde (19.0 mg, 109 μ mol), CH_3CO_2H (0.93 μ L, 16.3 μ mol), $NaBH(OAc)_3$ (46.0 mg, 217 μ mol) in THF (0.5 mL) gave the title compound **2be** (27.1 mg, 86%) as a yellow solid; 1H NMR ($CDCl_3$, 300 MHz) δ 8.33 (d, J = 2.6 Hz, 1H), 8.16 (s, 1H), 7.50 (d, J = 1.7 Hz, 1H), 7.36 (d, J = 8.2 Hz, 1H), 7.29 (d, J = 1.2 Hz, 1H), 7.24-7.20 (m, 2H), 7.09 (bs, 2H), 6.89 (d, J = 8.8 Hz, 1H), 5.27 (bs, 1H), 5.09 (s, 2H), 3.68 (bs, 2H), 2.99 (bs, 2H), 2.83 (bs, 1H), 2.58 (m, 2H), 2.05 (m, 1H); ^{13}C NMR ($CDCl_3$, 75 MHz) δ 152.9, 142.3, 136.5, 134.5, 133.4, 132.9, 132.4, 130.9, 130.7, 129.4, 129.3, 128.3, 127.6, 127.0, 126.8, 121.6, 113.3, 69.5, 60.1, 59.3, 55.5, 52.5, 32.8.

(3-(4-(5-Chloro-2-(3,4-dichlorobenzyloxy)phenyl)-1H-1,2,3-triazole-1-yl)pyrrolidin-1-yl)(phenyl)methanone (2bf)

Following the same procedure as that used for the synthesis of **2af**, the reaction of 3-(4-(5-chloro-2-(3,4-dichlorobenzyloxy)phenyl)-1H-1,2,3-triazole-1-yl)pyrrolidinium 2,2,2-trifluoroacetate **18b** (20.4 mg, 37.9 μ mol), benzoyl chloride (4.39 μ L, 37.9 μ mol), TEA (5.34 μ L, 38.3 μ mol) in THF (0.4 mL) gave the title compound **2bf** (17.1 mg, 86%) as a yellow solid; 1H NMR ($CDCl_3$, 300 MHz) δ 8.35 (s, 1H), 7.94 (d, J = 32.5 Hz, 1H), 7.52-7.41 (m, 7H), 7.26-7.22 (m, 2H), 6.89 (d, J = 8.8 Hz, 1H), 5.29-5.12 (m, 3H), 4.19-3.66 (m, 4H), 2.52 (bs, 2H); ^{13}C NMR ($CDCl_3$, 75 MHz) δ 170.0, 152.8, 142.1, 136.4, 135.9, 133.0, 132.6, 131.0, 130.4, 129.4, 128.7, 128.5, 127.7, 127.2, 127.1, 126.7, 122.3, 122.0, 121.0, 113.3, 69.5, 59.3, 58.4, 54.3, 51.8, 47.7, 44.3, 32.7, 30.5; HRMS-ESI (m/z): $[M+H]^+$ calcd for

C₂₆H₂₂Cl₃N₄O₂ 527.08029, Found 527.07977.

(3-(4-(5-Chloro-2-(3,4-dichlorobenzyloxy)phenyl)-1*H*-1,2,3-triazole-1-yl)pyrrolidin-1-yl)(4-fluorophenyl)methanone (2bg)

Following the same procedure as that used for the synthesis of **2af**, the reaction of 3-(4-(5-chloro-2-(3,4-dichlorobenzyloxy)phenyl)-1*H*-1,2,3-triazole-1-yl)pyrrolidinium 2,2,2-trifluoroacetate **18b** (22.8 mg, 42.4 μmol), 4-fluorobenzoyl chloride (5.01 μL, 42.4 μmol), TEA (5.97 μL, 42.8 μmol) in THF (0.4 mL) gave the title compound **2bg** (19.0 mg, 83%) as a yellowish solid; ¹H NMR (CDCl₃, 300 MHz) δ 8.33 (bs, 1H), 7.94 (d, *J* = 29.7 Hz, 1H), 7.52-7.47 (m, 4H), 7.26-7.16 (m, 2H), 7.10-7.07 (bs, 2H), 6.89 (d, *J* = 8.8 Hz, 1H), 5.19 (bs, 1H), 5.11 (s, 2H), 4.14-4.01 (m, 2H), 3.86 (bs, 1H), 3.65 (bs, 1H), 2.51 (bs, 2H); ¹³C NMR (CDCl₃, 75 MHz) δ 169.0, 163.8 (d, ¹*J* = 249.4 Hz), 152.8, 142.1, 136.4, 133.0, 132.7, 131.9, 131.0, 129.7 (d, ⁴*J* = 6.2 Hz), 129.4, 128.7, 127.7, 127.1, 126.8, 122.3, 120.9, 115.5 (d, ²*J* = 21.7 Hz), 113.3, 69.6, 59.4, 58.4, 54.3, 52.1, 47.8, 44.5, 32.7, 30.5; HRMS-ESI (*m/z*): [M+H]⁺ calcd for C₂₆H₂₁Cl₃FN₄O₂ 545.07086, Found 545.07094.

(3-(4-(5-Chloro-2-(3,4-dichlorobenzyloxy)phenyl)-1*H*-1,2,3-triazole-1-yl)pyrrolidin-1-yl)(4-chlorophenyl)methanone (2bh)

Following the same procedure as that used for the synthesis of **2af**, the reaction of 3-(4-(5-chloro-2-(3,4-dichlorobenzyloxy)phenyl)-1*H*-1,2,3-triazole-1-yl)pyrrolidinium 2,2,2-trifluoroacetate **18b** (33.1 mg, 61.6 μmol), 4-chlorobenzoyl chloride (7.89 μL, 61.6 μmol), TEA (11.2 μL, 80.0 μmol) in THF (0.6 mL) gave the title compound **2bh** (34.4mg, 99%) as a white solid; ¹H NMR (CDCl₃, 300 MHz) δ 8.34 (s, 1H), 7.39 (d, *J* = 29.7 Hz, 1H), 7.52-7.38 (m, 6H), 7.26-7.22 (m, 2H), 6.89 (d, *J* = 8.7 Hz, 1H), 5.18 (bs, 1H), 5.10 (s, 2H), 4.11 (bs, 1H), 3.99 (bs, 1H), 3.87 (bs, 1H), 3.65 (bs, 1H), 2.51 (bs, 2H); ¹³C NMR (CDCl₃, 75 MHz) δ 168.9, 152.8, 142.1, 136.5, 136.4, 134.2, 133.0, 132.6, 131.0, 129.4, 128.7, 127.9, 127.6, 127.0, 126.8, 122.4, 120.9, 113.3, 69.5, 59.3, 58.4, 54.2, 51.9, 47.7, 44.4, 32.7, 30.5; HRMS-

ESI (m/z): [M+H]⁺ calcd for C₂₆H₂₁Cl₄N₄O₂ 561.04131, Found 561.04042.

4-(5-Chloro-2-(3,4-dichlorobenzyloxy)phenyl)-1-(1-(phenylsulfonyl)pyrrolidin-3-yl)-1H-1,2,3-triazole (2bi)

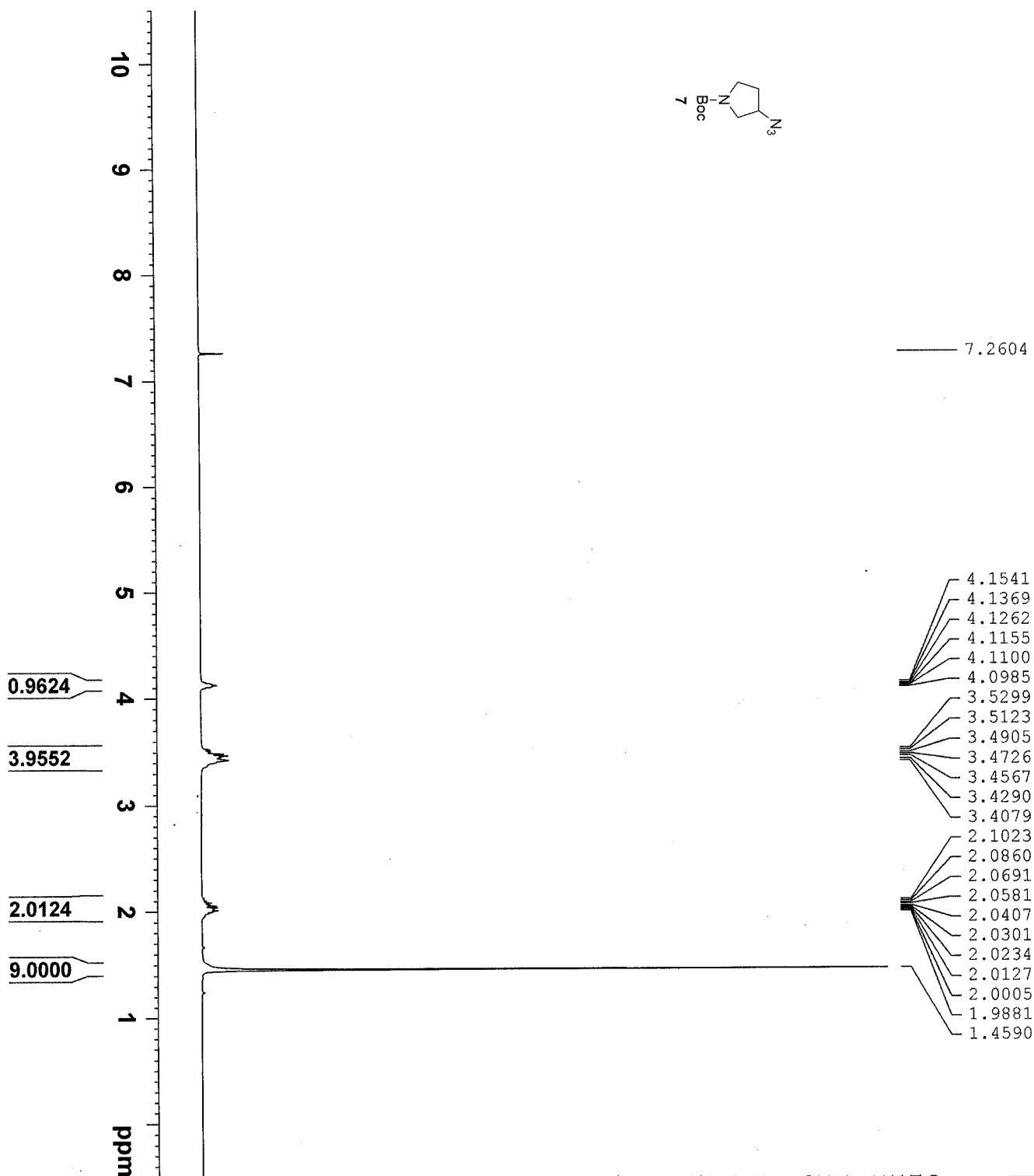
Following the same procedure as that used for the synthesis of **2af**, the reaction of 3-(4-(5-chloro-2-(3,4-dichlorobenzyloxy)phenyl)-1H-1,2,3-triazole-1-yl)pyrrolidinium 2,2,2-trifluoroacetate **18b** (20.3 mg, 37.7 μmol), benzenesulfonyl chloride (4.82 μL, 37.7 μmol), TEA (5.32 μL, 38.1 μmol) in THF (0.4 mL) gave the title compound **2bi** (8.70mg, 41%) as a white solid; ¹H NMR (CDCl₃, 300 MHz) δ 8.28 (d, *J* = 2.6 Hz, 1H), 7.89 (s, 1H), 7.79 (m, 2H), 7.57-7.48 (m, 6H), 7.26 (td, *J* = 8.2, 2.4 Hz, 1H), 6.90 (d, *J* = 8.8 Hz, 1H), 5.11 (s, 2H), 5.07 (m, 1H), 3.69 (m, 2H), 3.44 (m, 2H), 2.39 (m, 2H); ¹³C NMR (CDCl₃, 75 MHz) δ 152.8, 142.3, 136.4, 136.1, 133.1, 133.0, 132.7, 131.1, 129.5, 129.3, 128.7, 127.7, 127.4, 127.0, 126.9, 121.9, 121.0, 113.3, 69.6, 58.9, 53.4, 46.2, 31.6; HRMS-ESI (m/z): [M+H]⁺ calcd for C₂₅H₂₂Cl₃N₄O₃S 563.04727, Found 563.04863.

4-(5-Chloro-2-(3,4-dichlorobenzyloxy)phenyl)-1-(1-((4-fluorophenyl)sulfonyl)pyrrolidin-3-yl)-1H-1,2,3-triazole (2bj)

Following the same procedure as that used for the synthesis of **2af**, the reaction of 3-(4-(5-chloro-2-(3,4-dichlorobenzyloxy)phenyl)-1H-1,2,3-triazole-1-yl)pyrrolidinium 2,2,2-trifluoroacetate (**18b**) (23.2 mg, 43.1 μmol), 4-fluorobenzene-1-sulfonyl chloride (8.39 mg, 43.1 μmol), TEA (6.07 μL, 43.6 μmol) in THF (0.4 mL) gave the title compound **2bj** (10.0 mg, 40%) as a colorless oil; ¹H NMR (CDCl₃, 300 MHz) δ 8.30 (d, *J* = 2.7 Hz, 1H), 7.88 (s, 1H), 7.79 (m, 2H), 7.54 (d, *J* = 8.3 Hz, 2H), 7.26 (m, 2H), 7.18 (t, *J* = 8.6 Hz, 2H), 6.90 (d, *J* = 8.8 Hz, 1H), 5.10 (s, 2H), 5.06 (bs, 1H), 3.78-3.69 (m, 2H), 3.47 (t, *J* = 7.2 Hz, 2H), 2.43 (m, 2H); ¹³C NMR (CDCl₃, 75 MHz) δ 165.4 (d, ¹*J* = 254.1 Hz), 152.8, 136.4, 132.8 (²d, *J* = 23.3 Hz), 132.3, 131.1, 130.2 (³d, *J* = 9.3 Hz), 129.5, 128.7, 127.7, 127.1, 126.9, 121.8, 120.9, 116.6 (²d, *J* = 22.4 Hz), 113.3, 69.5, 58.9, 53.5, 46.2, 31.6; HRMS-ESI (m/z): [M+H]⁺ calcd

for $\text{C}_{25}\text{H}_{21}\text{Cl}_3\text{FN}_4\text{O}_3\text{S}$ 581.02308, Found 581.02247.

III. Spectral Data



Current Data Parameters
 NAME JSH-2-121-2-P
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20120203
 Time 19.50
 INSTRUM spect
 PROBD 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 456.1
 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
 PL -1.00 dB
 SFO1 300.1318534 MHz

F2 - Processing parameters
 SI 32768
 SF 300.1300119 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



Current Data Parameters
NAME JSH-2-121-2-p
EXPNO 2
PROCNO 1

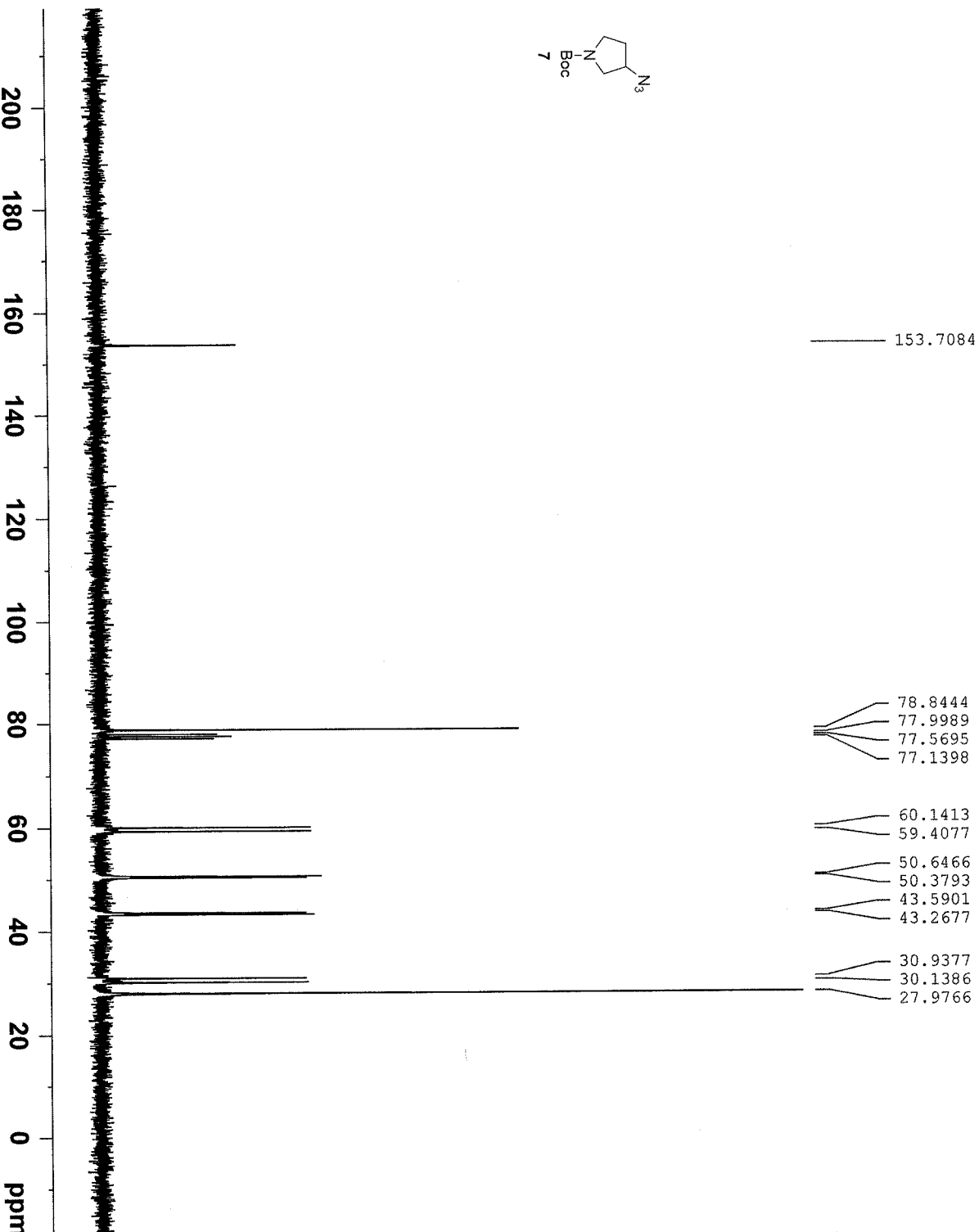
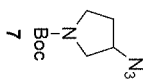
F2 - Acquisition Parameters

Date_ 20120207
Time_ 20.55
INSTRUM spect
PROBHD 5 mm DUL 1H-13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 10
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 11585.2
DM 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.0000000 sec
d11 0.0300000 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
PL2 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



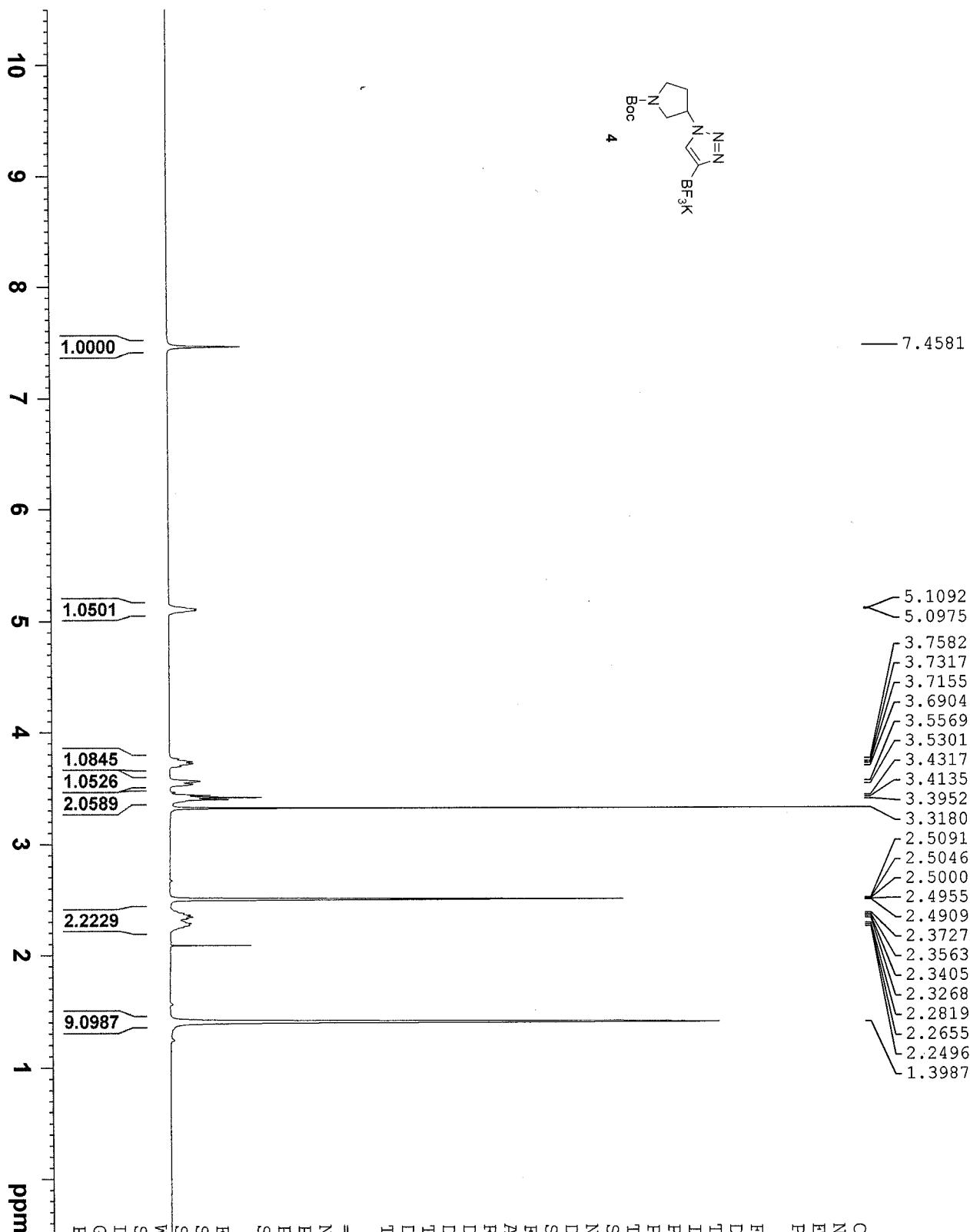
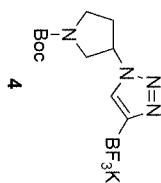


Current Data Parameters
NAME JSH-3-147-p
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20121010
Time 20.27
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 190.62
DW 60.800 usec
DE 6.50 usec
TE 298.9 K
D1 1.0000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 15.00 usec
PLW1 12.0000000 W
SFO1 400.2124715 MHz

F2 - Processing parameters
SI 65536
SF 400.2100063 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00





Current Data Parameters
NAME JSH-3-109-p
EXPNO 12
PROCNO 1

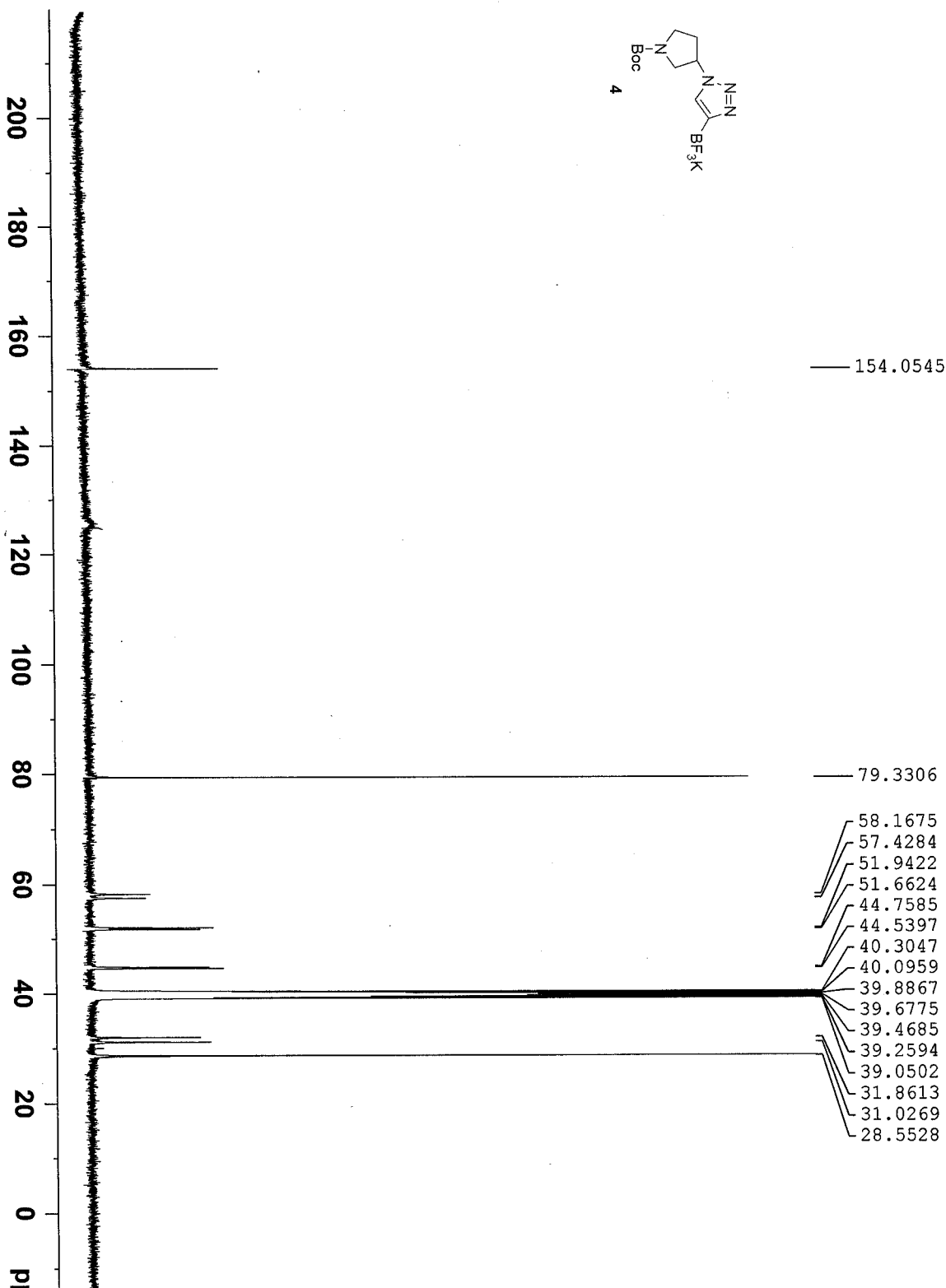
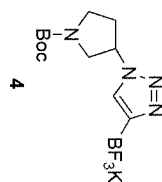
F2 - Acquisition Parameters

Date_ 20130306
Time 22.40
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 11194
DS 4
SWH 24038.461 H
FIDRES 0.366798 H
AQ 1.3631988 s
RG 190.62
DW 20.800 u
DE 6.50 u
TE 299.4 K
D1 2.0000000 s
D11 0.0300000 s
TDO 1

===== CHANNEL f1 =====
NUC1 13C
P1 10.00 u
PLW1 52.00000000 W
SFO1 100.6429474 N

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

F2 - Processing parameters
SI 32768
CT 1000000000 W





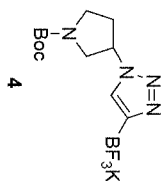
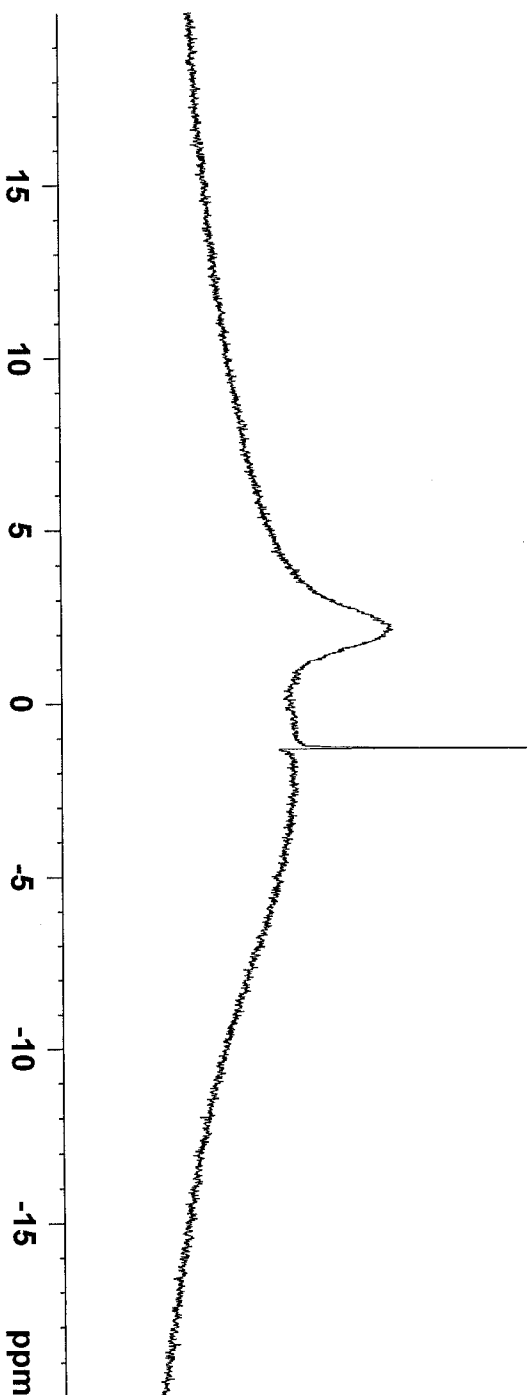
Current Data Parameters
NAME JSH-Boc pyrrolidine BF3K
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20130502
Time 16.44
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 66
DS 4
SWH 25510.203 Hz
FIDRES 0.389255 Hz
AQ 1.2845356 sec
RG 190.62
DE 19.600 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 11B
P1 15.00 usec
PLW1 34.20000076 W
SFO1 128.4032720 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 128.4032720 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40





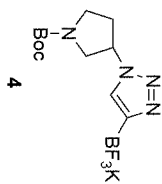
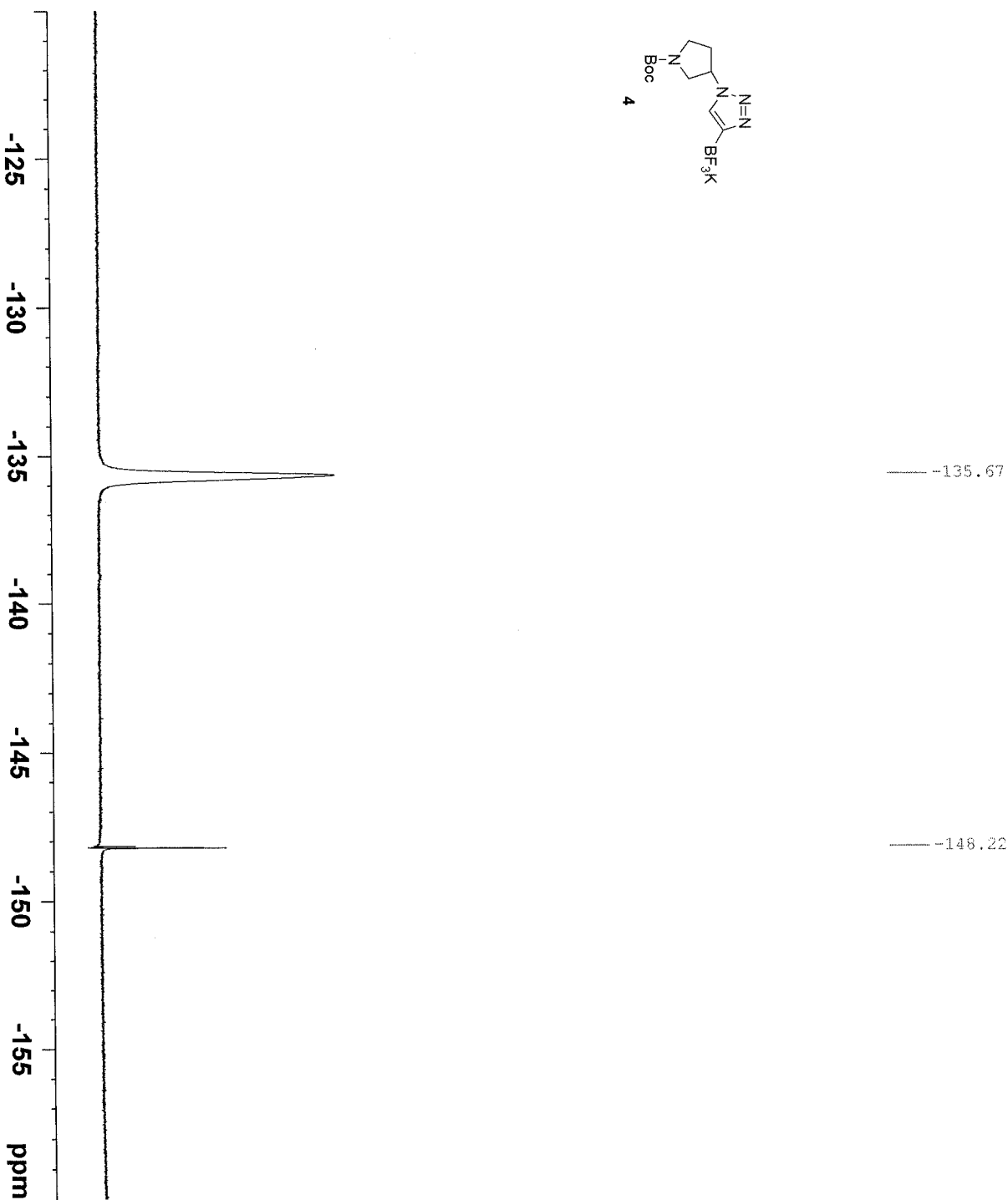
Current Data Parameters
 NAME JSH-Boc pyrrolidine BF3K
 EXNO 3
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20130502
 Time 16.48
 INSTRUM spect
 PROBD 5 mm PABBO BB/
 PULPROG zgfg
 TD 131072
 SOLVENT DMSO
 NS 16
 DS 4
 SWH 89285.711 Hz
 FIDRES 0.681196 Hz
 AQ 0.7340532 sec
 RG 190.62
 DW 5.600 usec
 DE 6.50 usec
 TE 299.7 K
 D1 1.00000000 sec
 D11 0.03000000 sec
 D12 0.00002000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 19F
 P1 15.00 usec
 PLW1 17.00000000 W
 SFO1 376.5359841 MHz

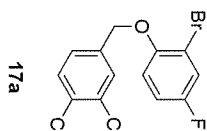
===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 90.00 usec
 PLW2 12.00000000 W
 PLW12 0.33333001 W
 SFO2 400.2116008 MHz

F2 - Processing parameters
 SI 65536
 SF 376.5736410 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



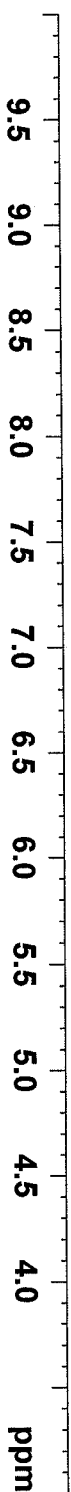
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7.2783
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6.9879
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6.8129

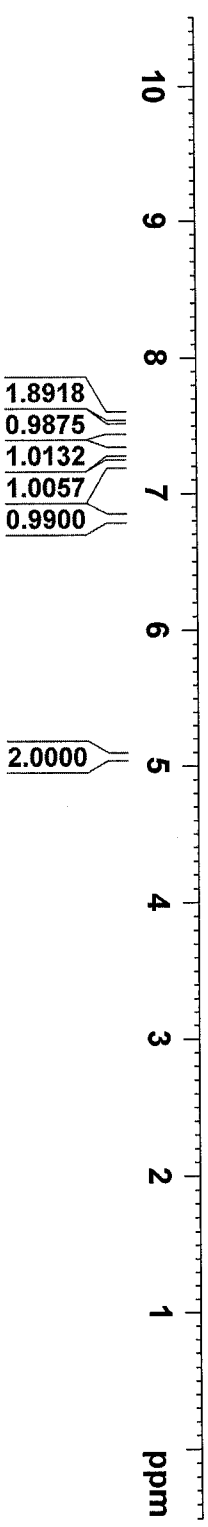
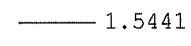
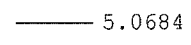
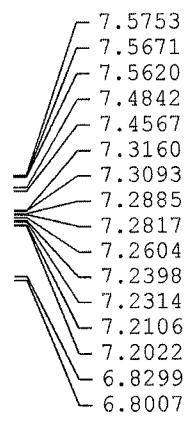
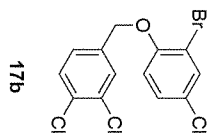
5.0257



NAME	ARI-5-product
EXPNO	1
PROCNO	1
Date_	20120202
Time	14.00
INSTRUM	spect
PROBHD	5 mm DUL
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	6172.839 Hz
FIDRES	0.094190 Hz
AQ	5.3084660 sec
RG	161.3
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
SI	32768
SF	300.1300121 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00





Current Data Parameters
 NAME JSH-2-49-P
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20121016
 Time_ 16.58
 INSTRUM spect
 PROBHD 5 mm DUL 1H-13
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 10
 DS 2
 SWH 6172.839 Hz
 FIDRES 0.094190 Hz
 AQ 5.3084660 sec
 RG 1824.6
 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 300.1300120 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



Current Data Parameters
NAME JSH-2-31-p
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters

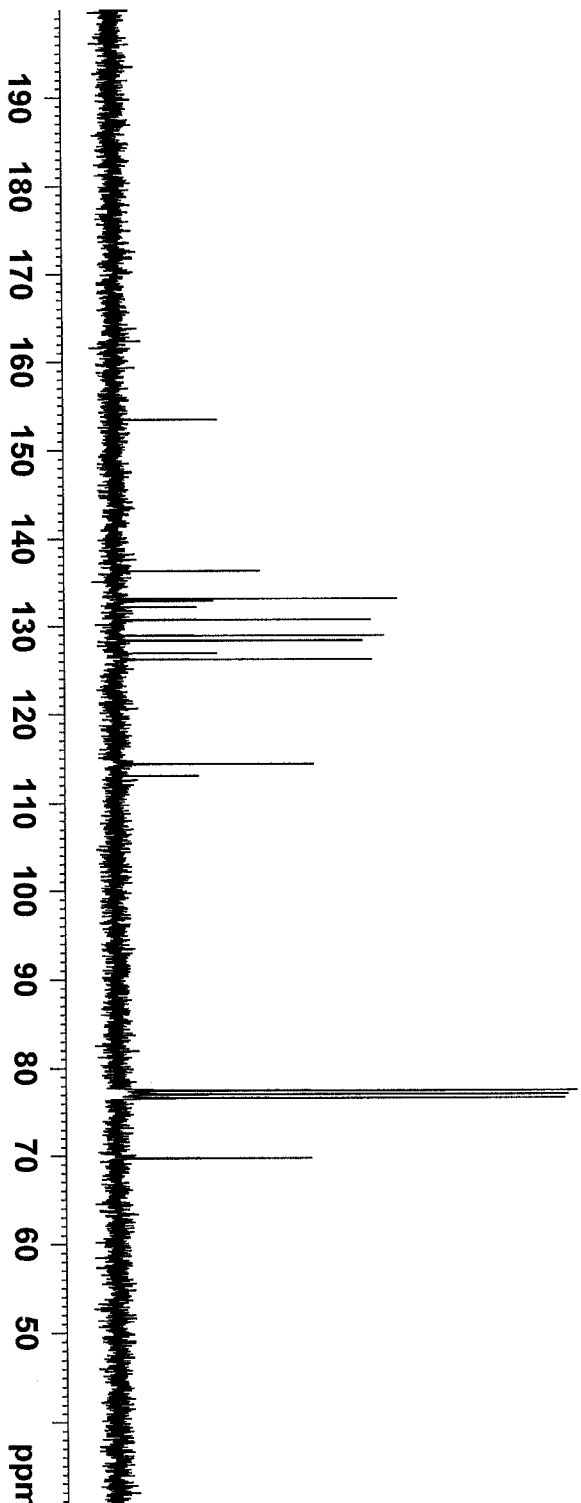
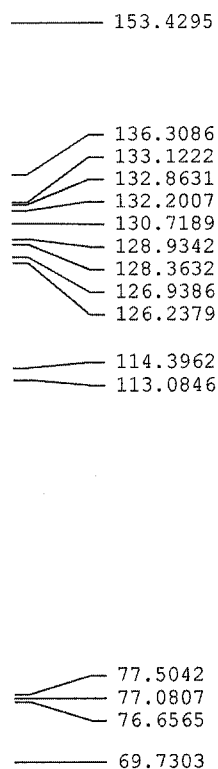
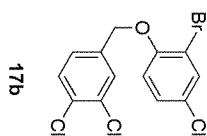
Date_ 20120201
Time 21.08
INSTRUM spect
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PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 65
DS 4
SWH 17985.611 Hz
FIDRES 0.27439 Hz
AQ 1.8219508 sec
RG 20642.5
DM 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.0000000 sec
d11 0.0300000 sec
DELTA 1.8999998 sec
TD0 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
PL2 0.00 dB
PL12 20.00 dB
PL13 22.00 dB
SFO2 300.1312005 MHz

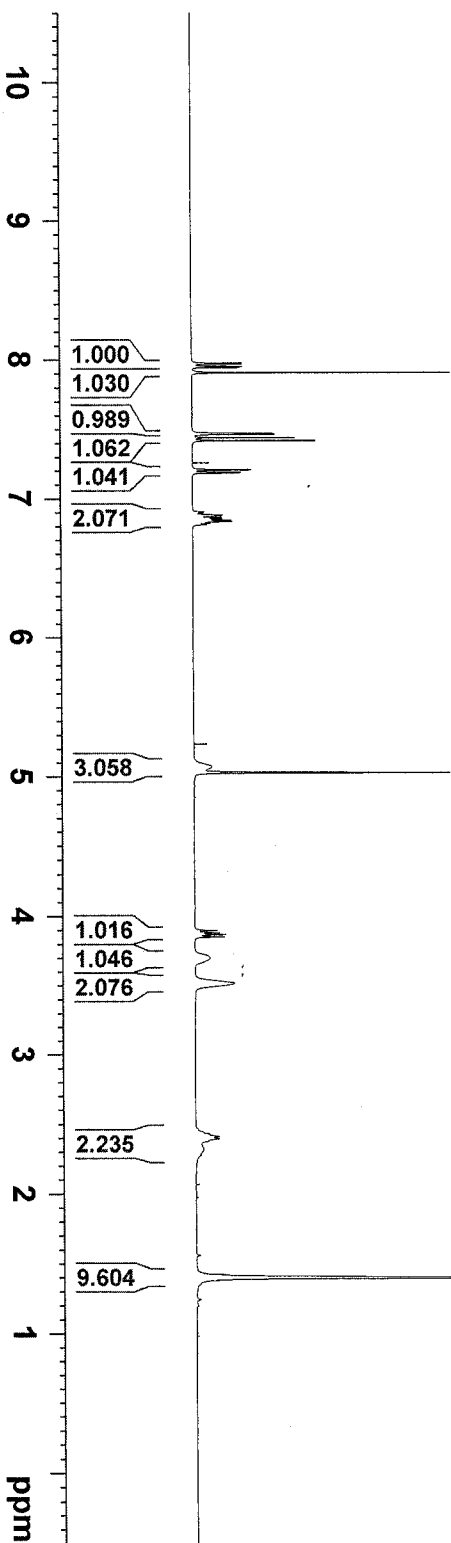
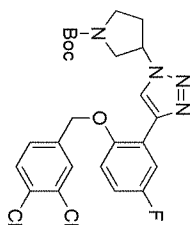
F2 - Processing parameters

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





7.977
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7.954
7.946
7.908
7.471
7.466
7.440
7.420
7.259
7.211
7.206
7.191
7.186
6.904
6.896
6.881
6.874
6.863
6.855
6.846
6.835
6.824
6.813
5.236
5.071
5.030
3.899
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1.401



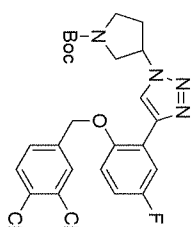
Current Data Parameters
NAME JSH-130625-P
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters

Date_ 20130625
Time_ 10.02
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 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 400.2100129 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



— 158.7074
 — 156.3332
 — 154.0902
 \ 150.5081
 / 150.4892

 — 142.1918
 / 136.7981
 / 132.8326
 / 132.3494
 / 130.8484
 — 129.3417
 — 126.7781
 / 121.8828
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 / 121.1071
 / 115.0905
 / 114.8574
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 / 114.1274
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 / 113.2980

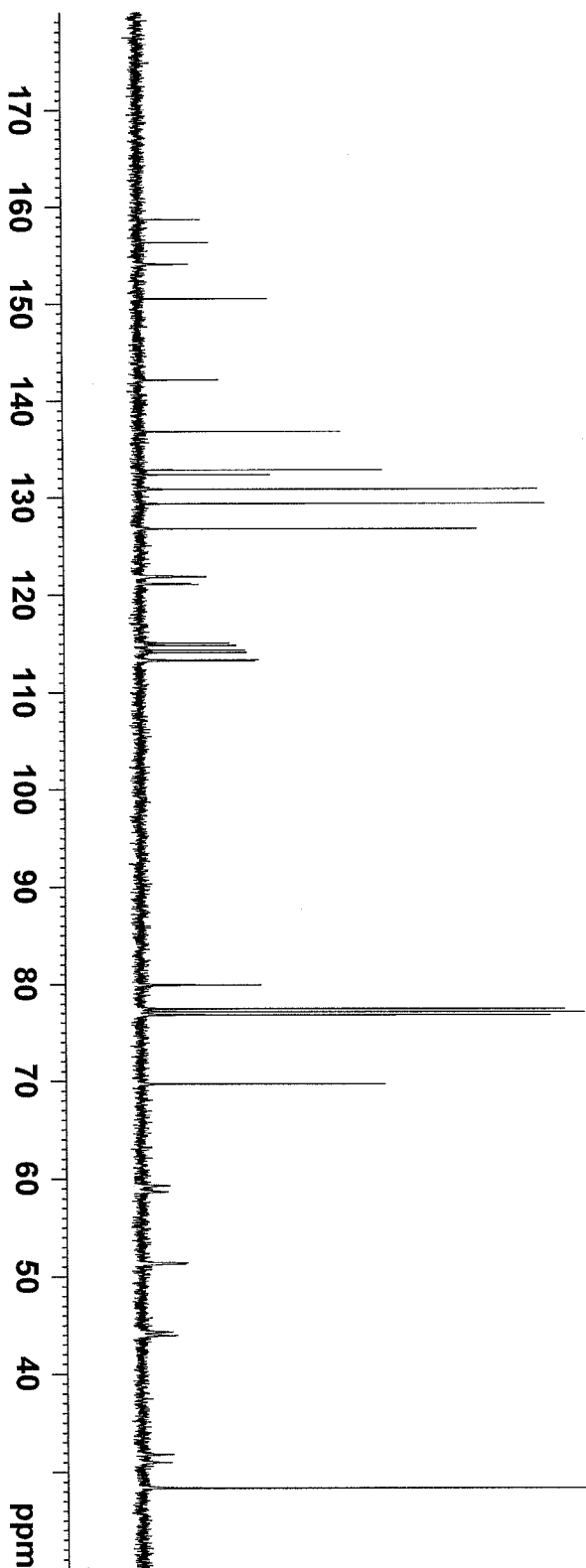
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 — 51.3987

 / 44.3277
 / 43.9743

 / 31.8399
 / 31.0204
 — 28.3866



1.40 PC

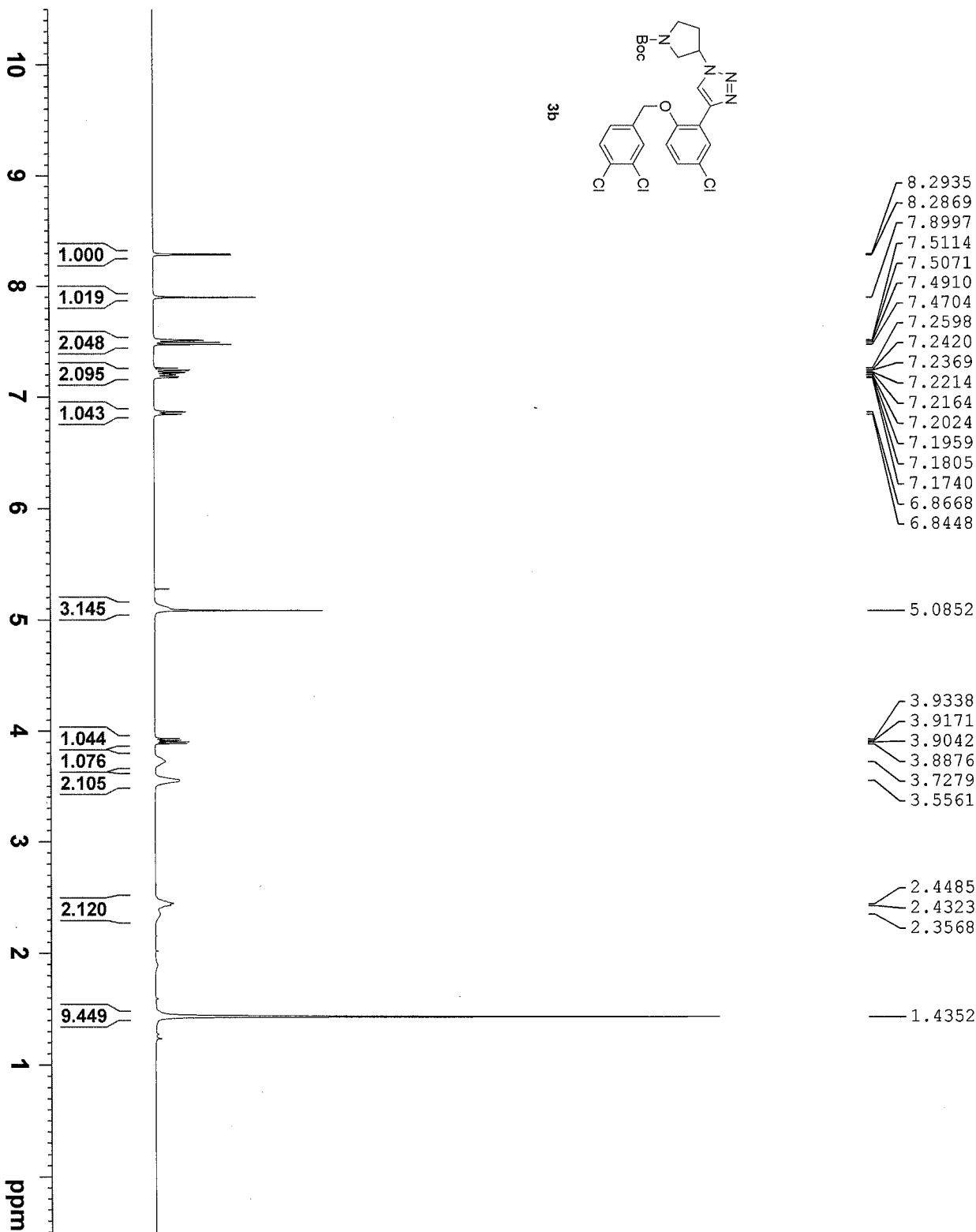


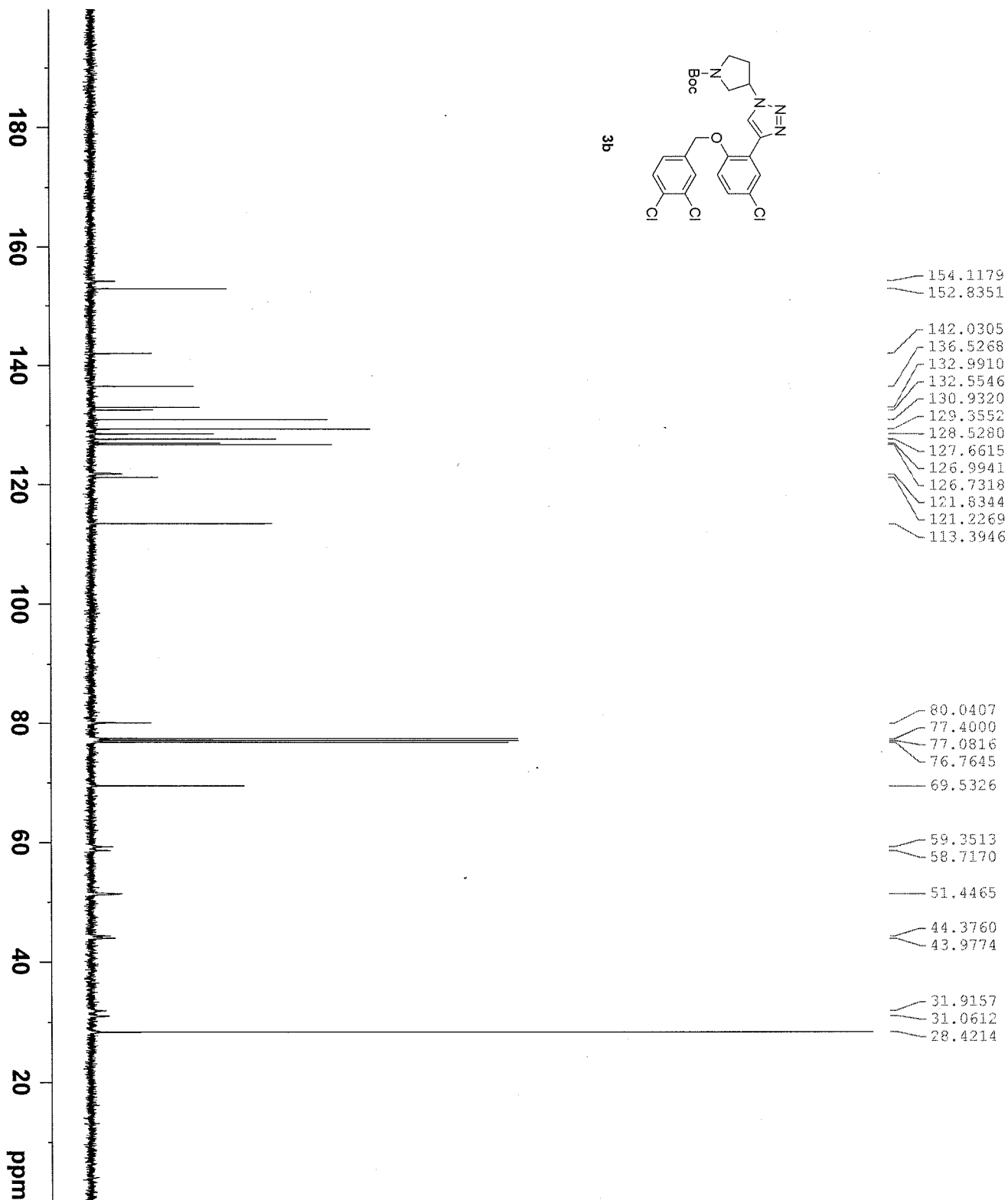
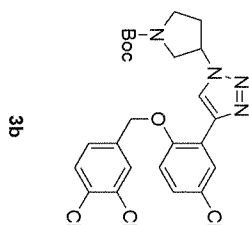
Current Data Parameters
NAME JSH-3-173-p
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20130617
Time 12.42
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 58.64
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 400.2100130 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00





Current Data Parameters

NAME JSH-3-173-p

EXPNO 3

PROCNO 1

F2 - Acquisition Parameters

Date_ 20130617

Time 12.46

INSTRUM spect

PROBHD 5 mm PABBO BB/

PULPROG zgpg30

TD 65536

SOLVENT CDCl3

NS 130

DS 4

SWH 24038.461 Hz

FIDRES 0.366798 Hz

AO 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

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

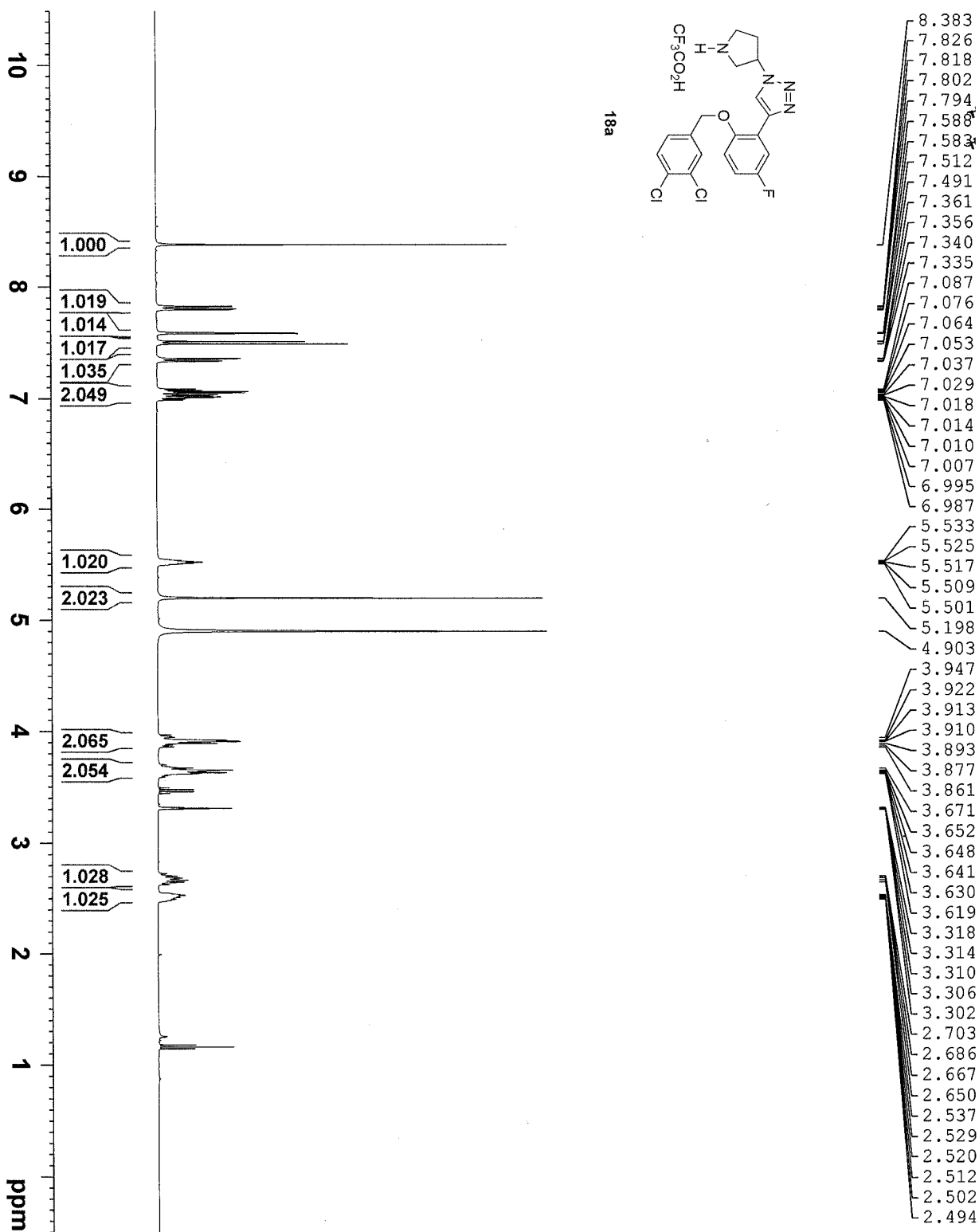
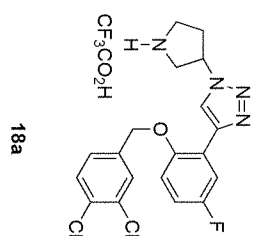
WDW EM

SSB 0

LB 1.00 Hz

GB 0

PC 1.40



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Current Data Parameters
NAME          JSH-2-163-p
EXPNO         1
PROCNO        1
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F2 - Acquisition Parameters	
Date_	20130508
Time	22.14
INSTRUM	spect
PROBHD	5 mm PABBO BB/
PULPROG	zg30
TD	65536
SOLVENT	MeOD
NS	9
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	299.1 K
D1	1.00000000 sec
TDO	1

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

F2 - Processing parameters
SI                65536
SF                400.2100109 MHz
WDW               EM
SSB               0
LB                0.30 Hz
GB                0
PC                1.00

```





Current Data Parameters
NAME JSH-2-163-p
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters

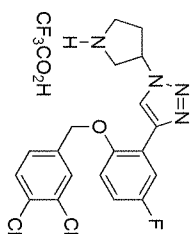
Date_ 20130508
Time_ 22.18
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT MeOD
NS 99
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 190.62
DW 20.800 usec
DE 6.50 usec
TE 299.8 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

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

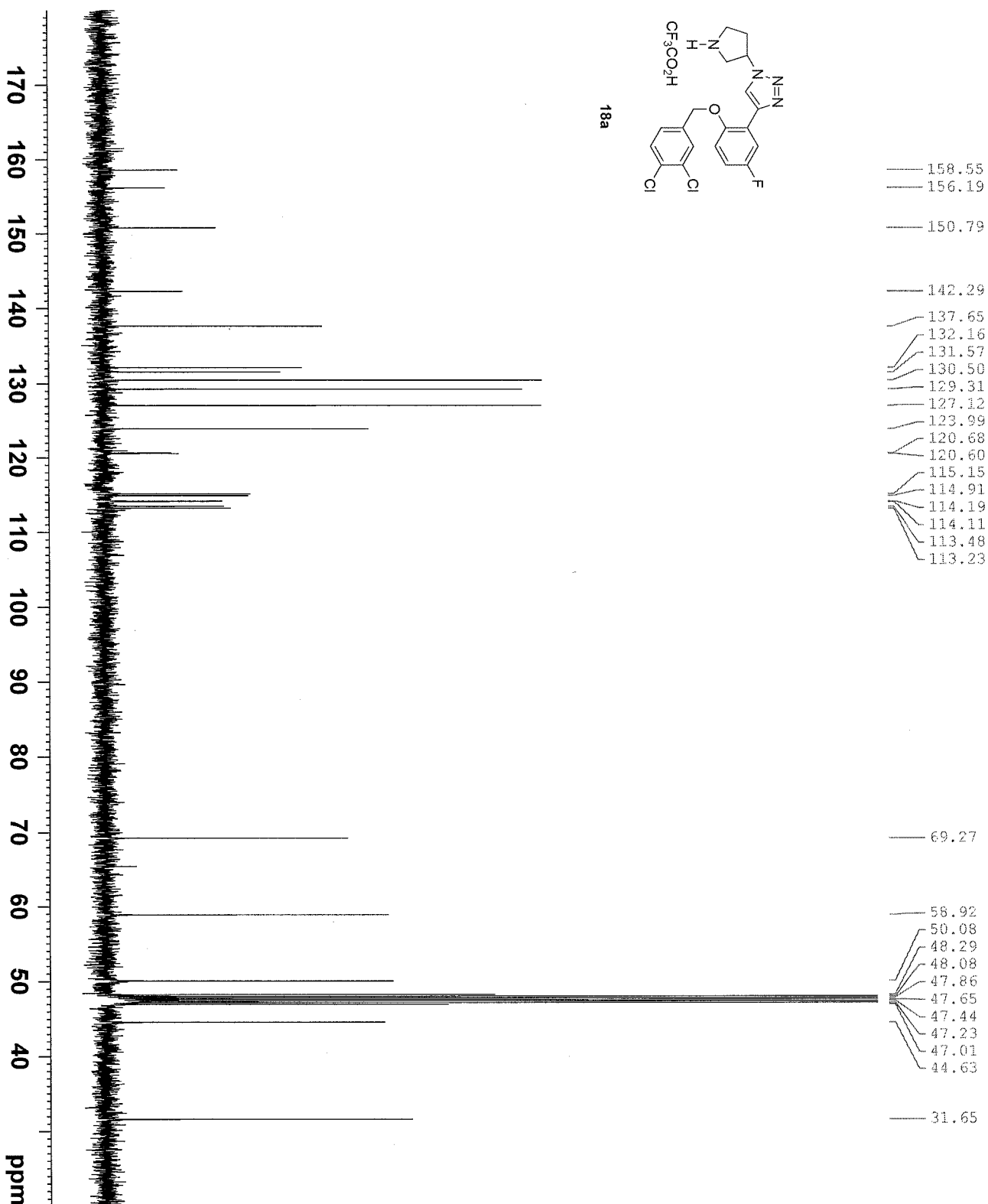
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 ¹H
PCPD2 90.00 usec
PLW2 12.00000000 W
PLW12 0.33333001 W
PLW13 0.27000001 W
SFO2 400.2116008 MHz

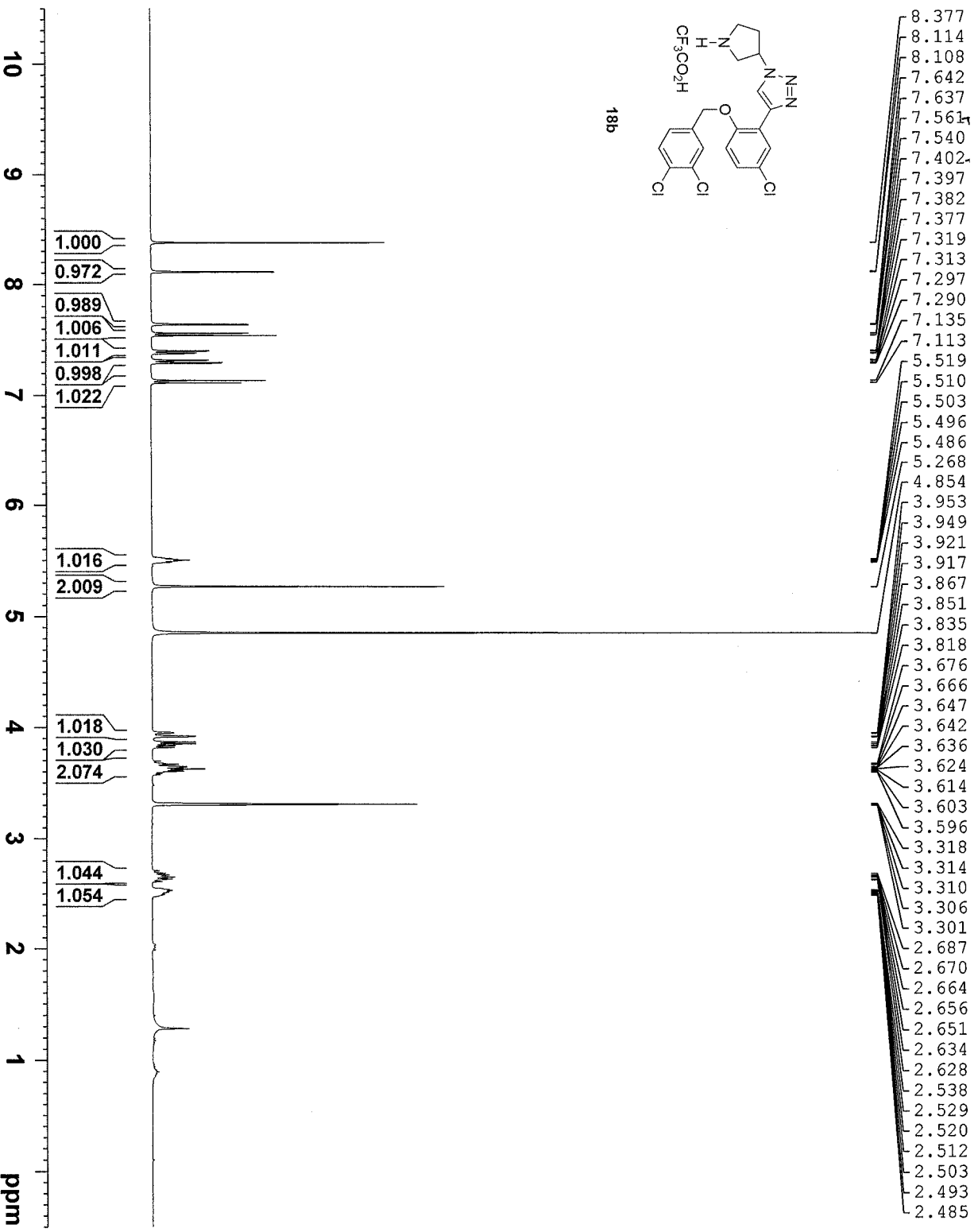
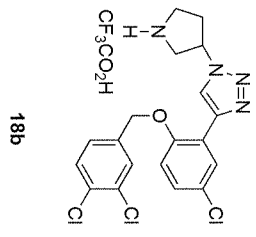
F2 - Processing parameters

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



18a





Current Data Parameters
 NAME JSH-2-131-p
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20130508
 Time_ 22.08
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT MeOD
 NS 8
 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 299.4 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 400.2100110 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



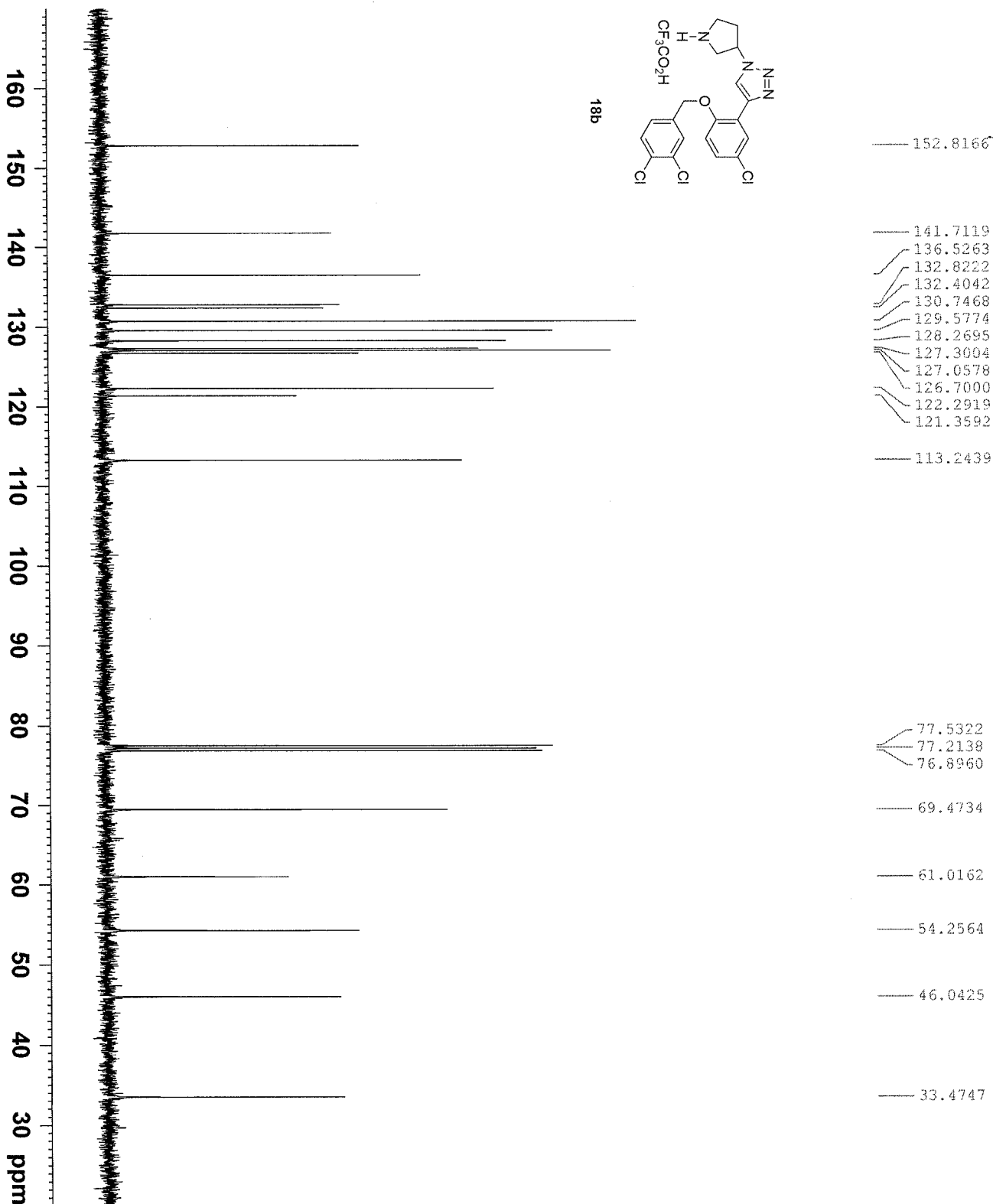
Current Data Parameters
NAME JSH-130702-p
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20130702
Time 20.36
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 1.3631988 sec
RG 190.62
DM 20.800 usec
DE 6.50 usec
TE 297.4 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1

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

===== CHANNEL f2 =====
CPDPRG2 waltz16
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
SE 100.632860 MHz
WDM EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40





Current Data Parameters
NAME JSH-2-167-p
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20120329
Time 21.30
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 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

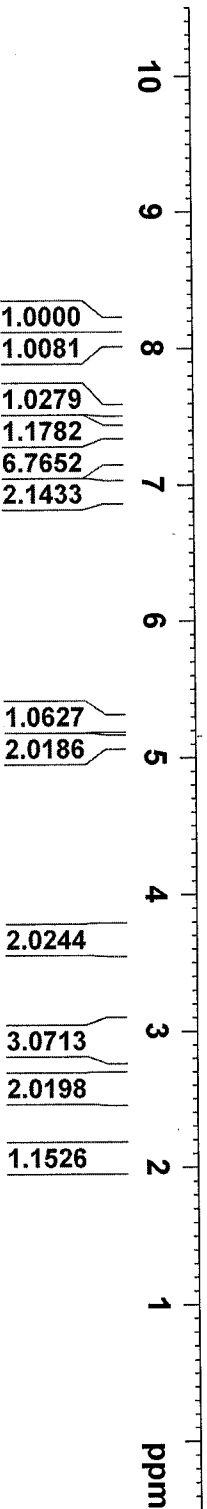
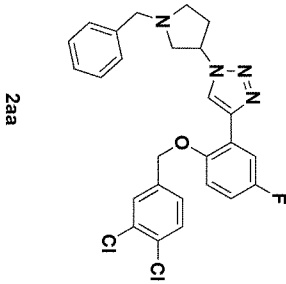
F2 - Processing parameters
SI 32768
SF 300.1300120 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

8.1689
8.0864
8.0764
8.0545
8.0447
7.5438
7.3872
7.3600
7.2582
7.2337
7.0066
6.9965
6.9766
6.9666
6.9519
6.9418
6.9314
6.9163
6.9014
6.8863
5.2929
5.2509
5.2389
5.0957
5.0563

3.7228
3.6819
3.6343
3.5915

2.9156
2.6054
2.5647

2.0730
2.0455



1.0000
1.0081
1.0279
1.1782
6.7652
2.1433

1.0627
2.0186

2.0244

3.0713
2.0198

1.1526



Current Data Parameters
NAME JSH-2-167-p
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters

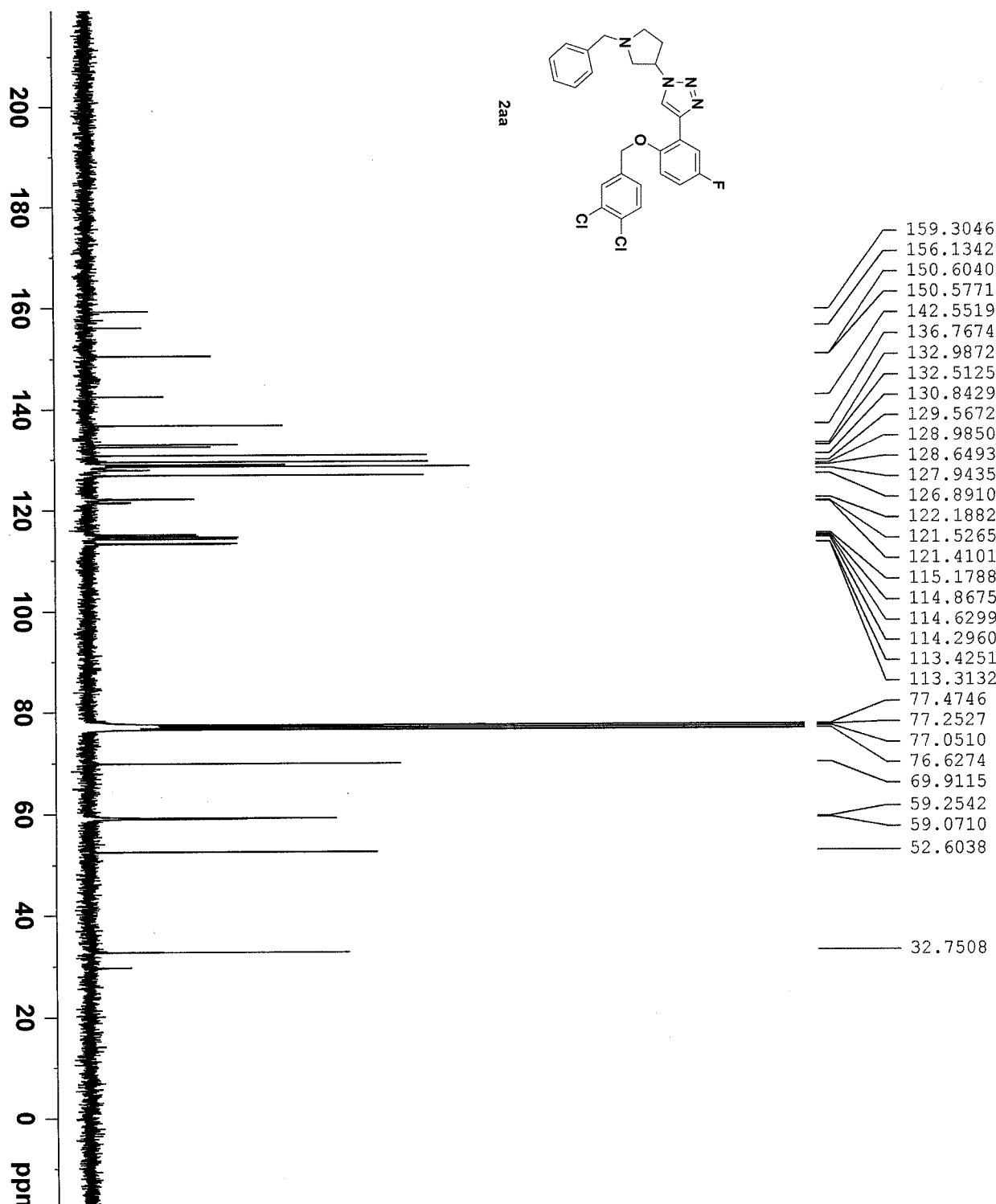
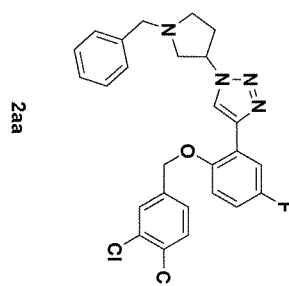
Date_ 20120617
Time 15.33
INSTRUM spect
PROBHD 5 mm DUL 1H-13
PULPROG zgpg30
TD 65336
SOLVENT CDCl3
NS 3959
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 18390.4
DW 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.0000000 sec
d11 0.0300000 sec
DELTA 1.8999998 sec
TD0 1

===== 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
PL2 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





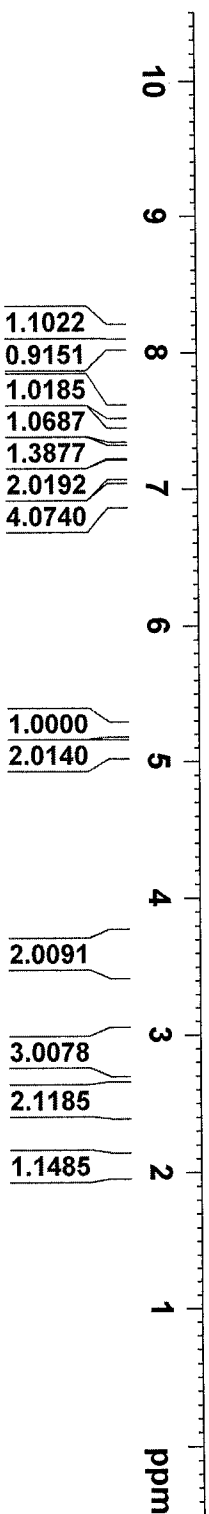
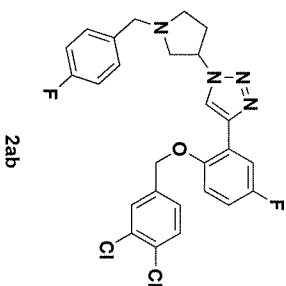
Current Data Parameters
NAME JSH-2-147-p
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20120327
Time_ 14.20
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 228.1
DE 81.000 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 300.1300122 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

8.1314
8.0864
8.0764
8.0543
8.0446
7.5530
7.5472
7.4042
7.3769
7.2740
7.2680
7.2600
7.2469
7.2409
7.1309
7.0118
7.0018
6.9818
6.9719
6.9569
6.9463
6.9262
6.9175
6.8958
6.8889
5.2578
5.2396
5.2277
5.1971
5.0821
3.6458
3.6044
3.5613
3.5195
2.8619
2.6215
2.5923
2.5769
2.5622
2.5478
2.5177
2.1100
2.0859
2.0545
2.0397
2.0280





Current Data Parameters
NAME JSH-2-147-p
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters

Date_ 20120712
Time_ 21.10
INSTRUM spect
PROBHD 5 mm DUL 1H-13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 11157
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 11585.2
DM 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

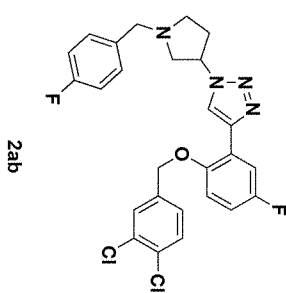
===== CHANNEL f1 =====
NUC1 13C
P1 10.00 usec
PL1 0.00 dB
SFO1 75.4752953 MHz

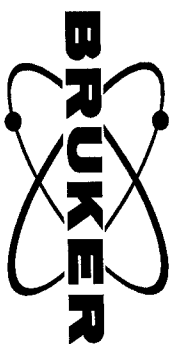
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 0.00 dB
PL12 20.00 dB
PL13 22.00 dB
SFO2 300.1312005 MHz

F2 - Processing parameters

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

- 163.8863
- 160.6246
- 159.3266
- 156.1554
- 150.6225
- 150.5961
- 142.5475
- 142.5201
- 136.7775
- 132.9936
- 132.5348
- 130.8033
- 130.3126
- 129.6340
- 126.9627
- 121.9648
- 121.5728
- 121.4613
- 115.5287
- 115.2456
- 115.1517
- 114.8406
- 114.6233
- 114.2890
- 113.3899
- 113.2784
- 78.1080
- 77.4730
- 77.2520
- 77.0494
- 76.6260
- 69.9441
- 59.4975
- 59.1588
- 58.5038
- 52.5308
- 32.7291
- 29.7145
- 25.9383



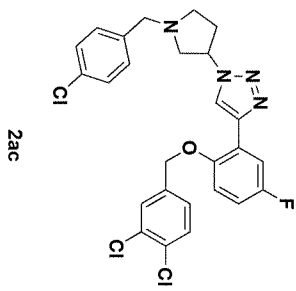


Current Data Parameters
NAME JSH-2-183-p
EXPNO 1
PROCNO 1

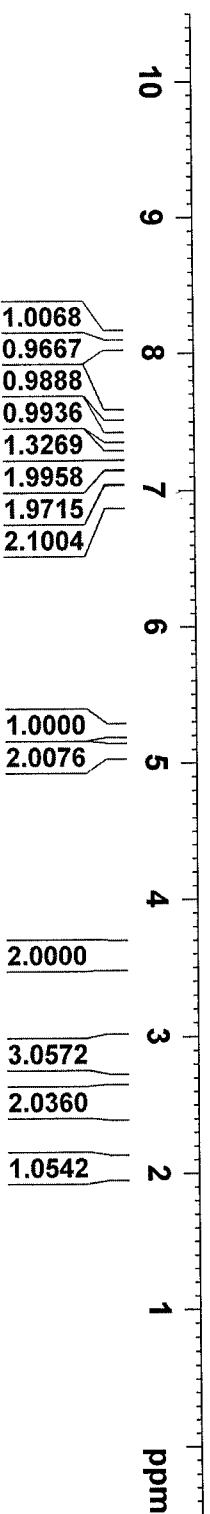
F2 - Acquisition Parameters
Date_ 20120402
Time 19.45
INSTRUM spect
PROBHD 5 mm DUL 1H-13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 203.2
DW 81.000 usec
DE 6.00 usec
TE 300.0 K
D1 1.0000000 sec
TD0 1

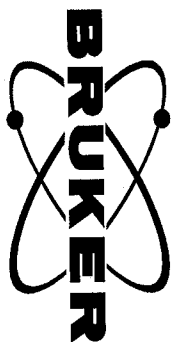
===== CHANNEL f1 =====
NUC1 1H
P1 10.50 usec
PL1 -1.00 dB
SFO1 300.1318534 MHz

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



8.1310
8.0857
8.0758
8.0535
8.0439
7.5503
7.5442
7.4009
7.3736
7.2704
7.2638
7.2603
7.2432
7.2367
7.2067
7.1789
7.1063
7.0789
7.0102
7.0001
6.9802
6.9702
6.9555
6.9450
6.9408
6.9253
6.9105
6.8953
5.2577
5.2469
5.2372
5.2273
5.2182
5.2074
5.0804
3.6476
3.6038
3.5505
3.5065
2.9250
2.9099
2.8971
2.8817
2.8661
2.8228
2.5907
2.5755
2.5611
2.5461
2.5338
2.5151
2.4693
2.0646
2.0538
2.0366
2.0287
2.0132
2.0015





Current Data Parameters
NAME JSH-2-183-p
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters

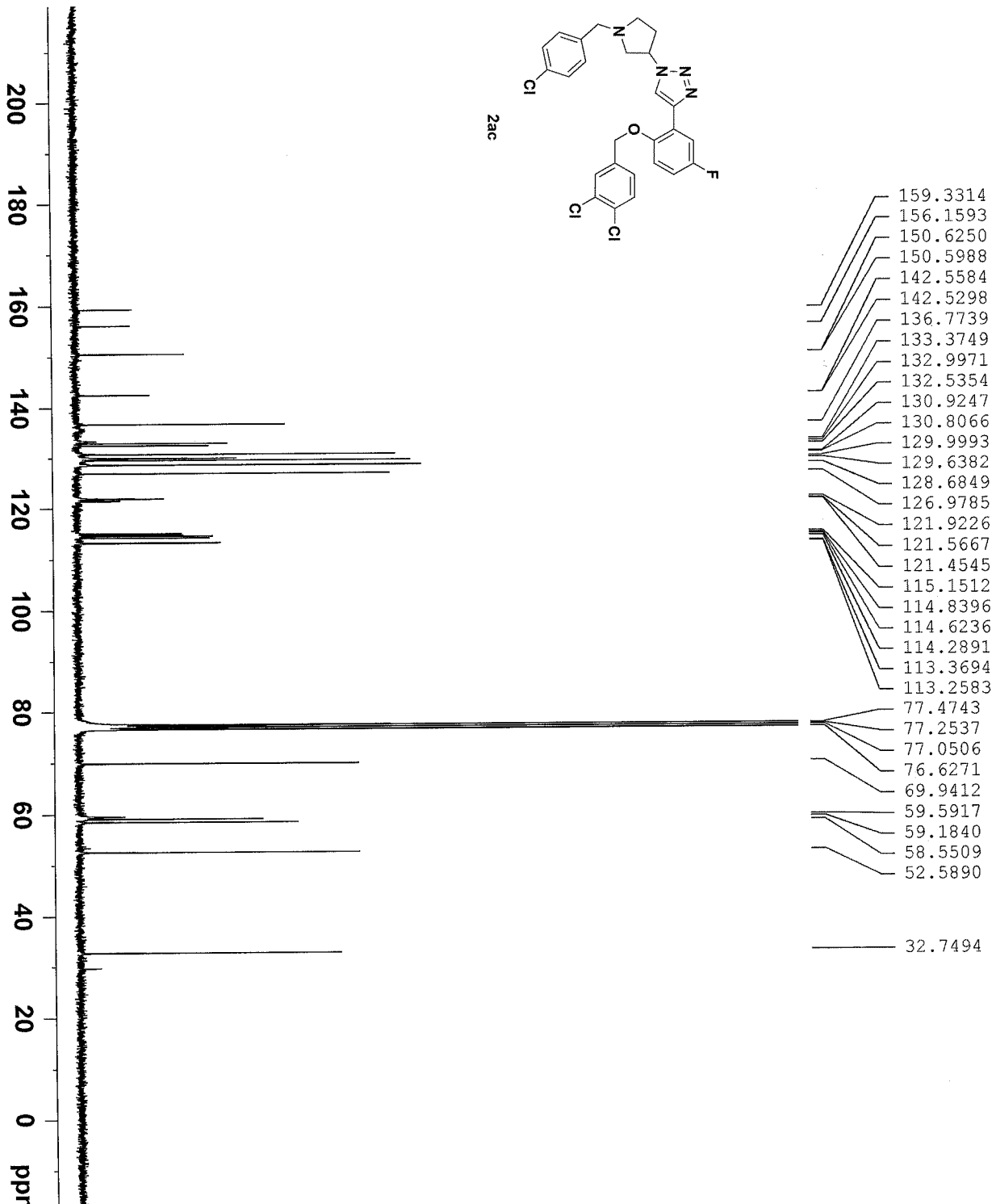
Date_ 20120719
Time 21.44
INSTRUM spect
PROBHD 5 mm DUL 1H-13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 9897
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 16384
DE 27.800 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

===== 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
PL2 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



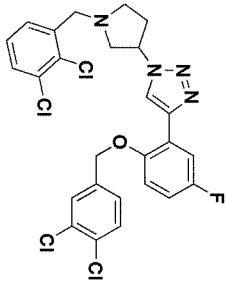


Current Data Parameters
NAME JSH-2-187-p
EXPNO 2
PROCNO 1

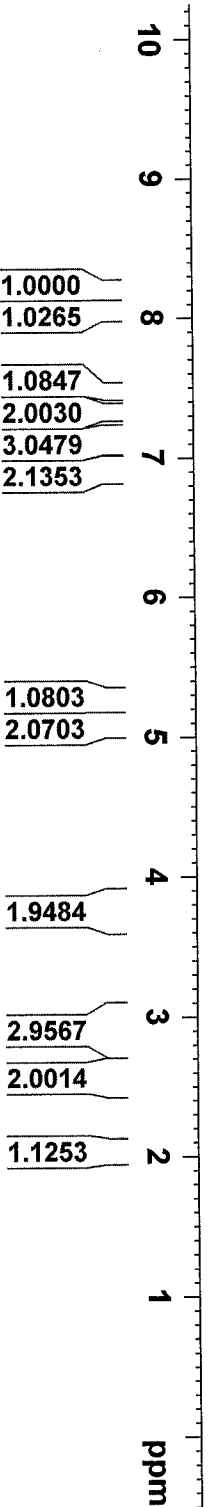
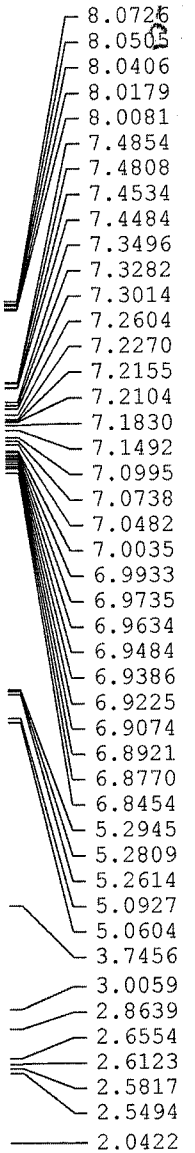
F2 - Acquisition Parameters
Date_ 20120409
Time 21.14
INSTRUM spect
PROBHD 5 mm DUL 1H-13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 287.4
DW 81.000 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

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

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



2ad





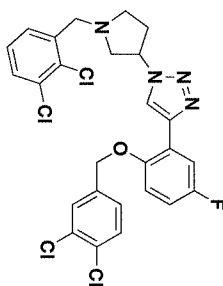
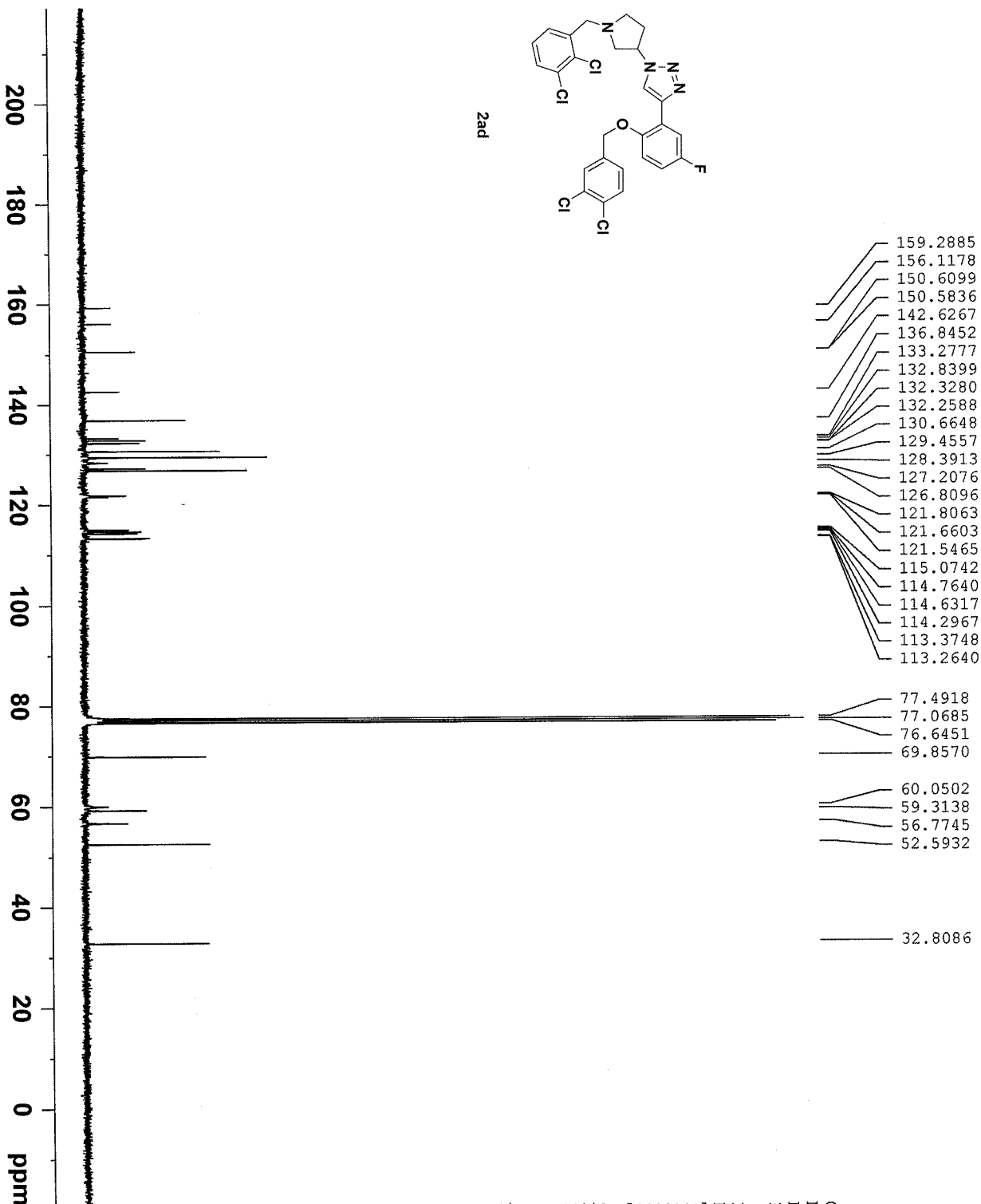
Current Data Parameters
 NAME JSH-2-187-P
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20120422
 Time_ 17.04
 INSTRUM spect
 PROBD 5 mm DUL 1H-13
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 1639
 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

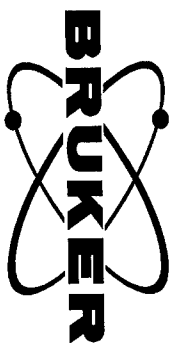
===== CHANNEL f1 =====
 NUC1 13C
 P1 10.00 usec
 PL1 0.00 dB
 SFO1 75.4752953 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 100.00 usec
 PL2 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
 IB 1.00 Hz
 GB 0
 PC 1.40



2ad

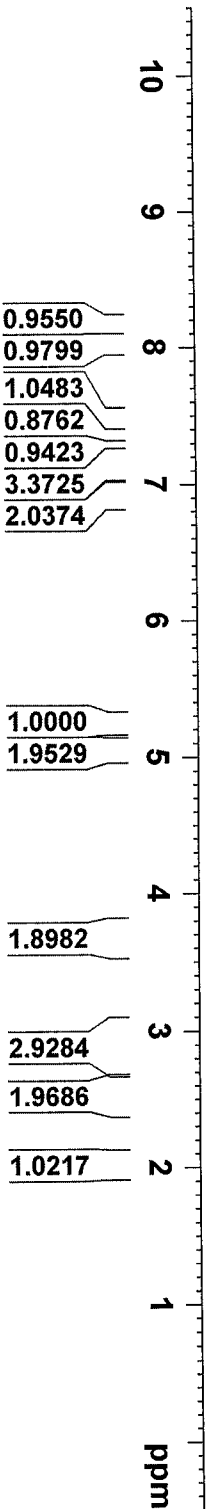
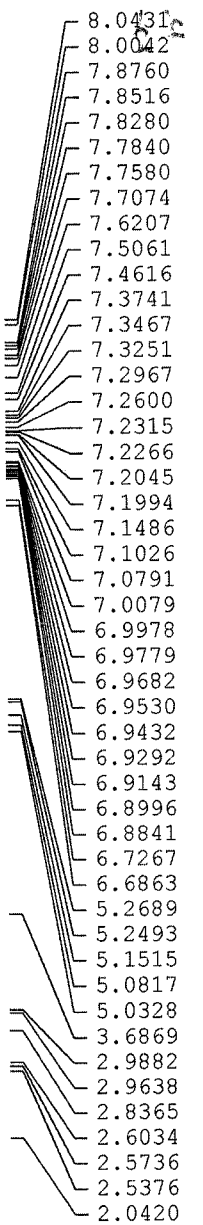
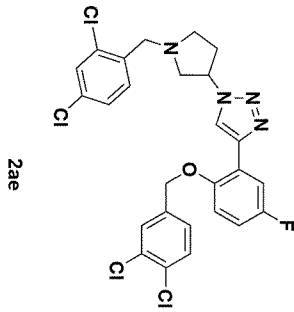


Current Data Parameters
NAME JSH-2-187-p
EXPNO 129
PROCNO 1

F2 - Acquisition Parameters
Date_ 20120409
Time 21.05
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 287.4
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 300.1300123 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00





Current Data Parameters
NAME JSH-2-189-p
EXPNO 1
PROCNO 1

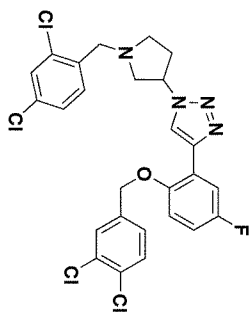
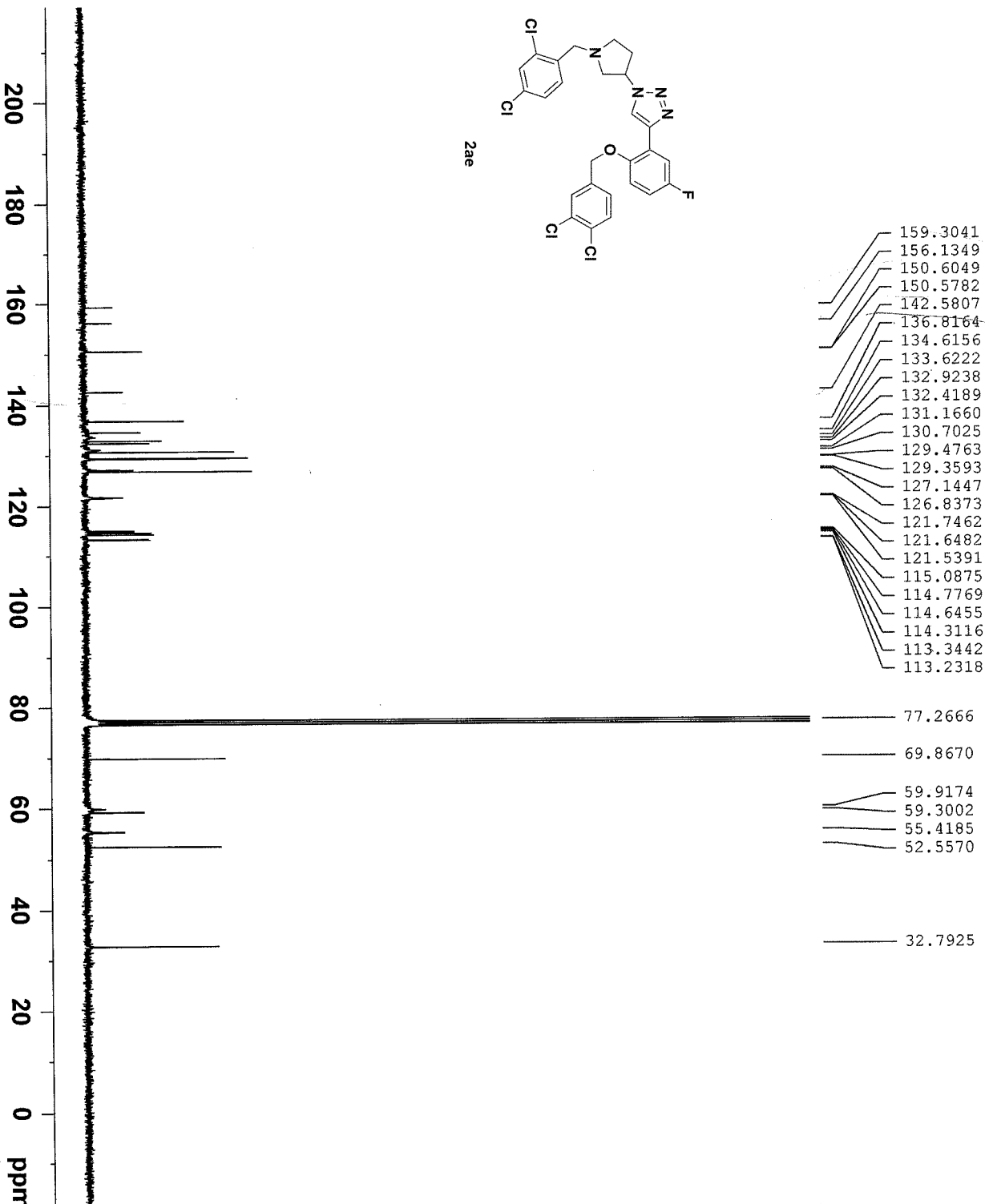
F2 - Acquisition Parameters
Date_ 20120422
Time 19.25
INSTRUM spect
PROBHD 5 mm DUL 1H-13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1624
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 16384
DM 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 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
PL2 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





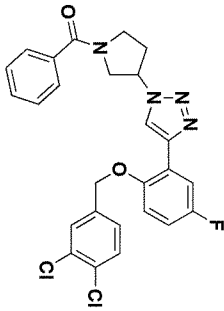
Current Data Parameters
NAME JSH-2-169-p
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20120329
Time 21.36
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 322.5
DM 81.000 usec
DE 6.00 usec
TE 300.0 K
D1 1.0000000 sec
TD0 1

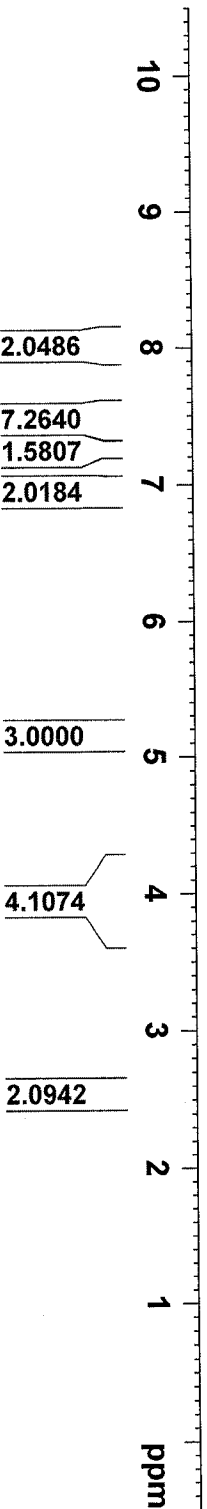
===== CHANNEL f1 =====
NUC1 1H
P1 10.50 usec
PL1 -1.00 dB
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1300121 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

8.0698
8.0482
8.0239
7.9094
7.5246
7.4895
7.4621
7.4104
7.3260
7.2600
7.0129
7.0028
6.9829
6.9733
6.9581
6.9482
6.9157
6.9013
6.8862
6.8715
5.2130
5.1056
4.1994
4.1317
4.0901
3.9925
3.8939
3.6597
2.5137



2af





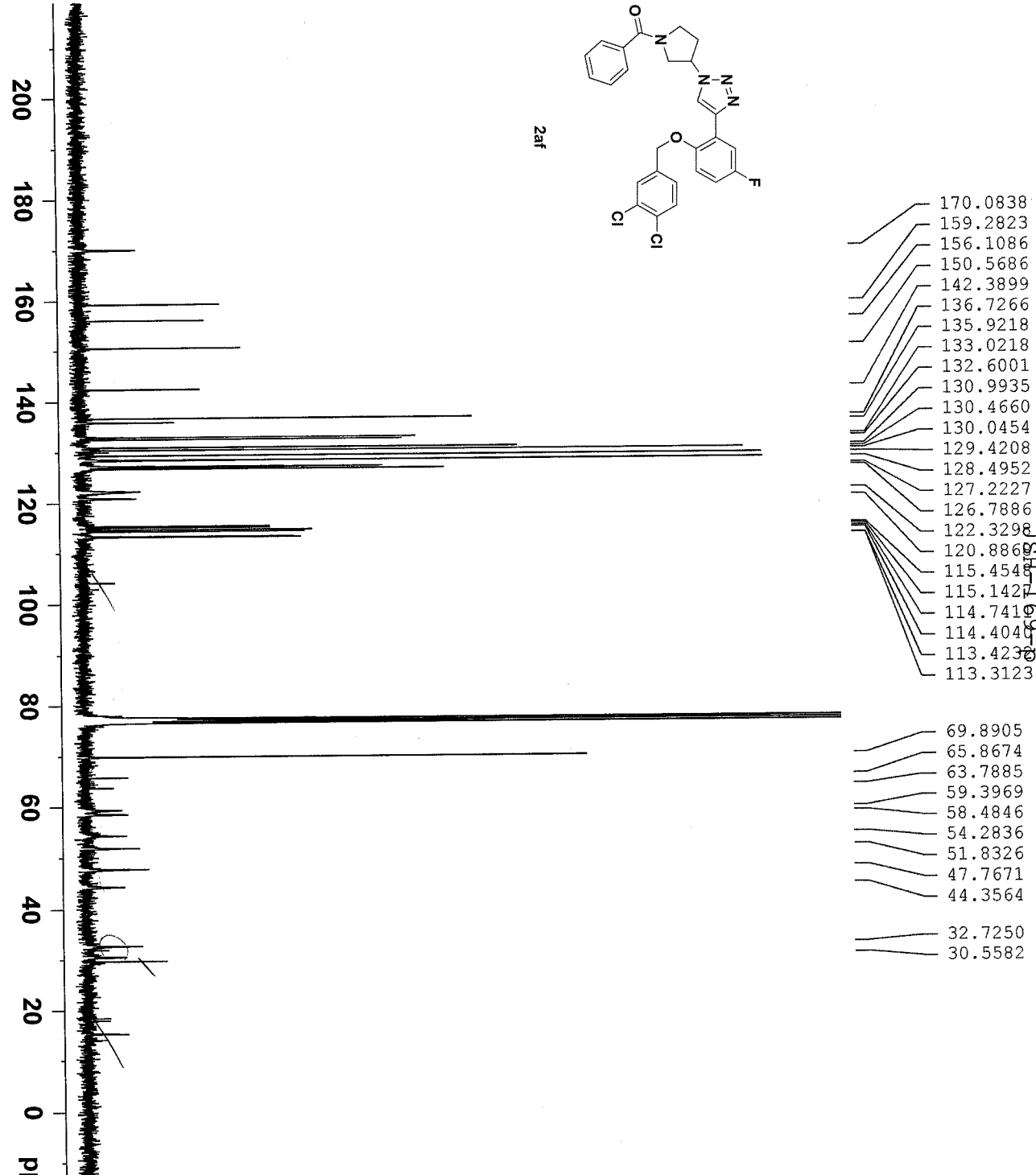
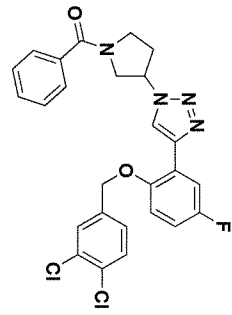
Current Data Parameters
NAME JSH-169-P
EXPNO 2
PROCNO 1

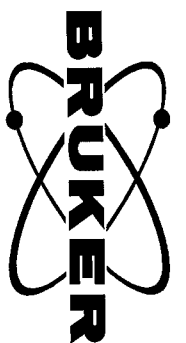
F2 - Acquisition Parameters
Date_ 20120617
Time 20.11
INSTRUM spect
PROBHD 5 mm DUL 1H-13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 11797
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 11585.2
DM 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89993998 sec
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
PL2 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



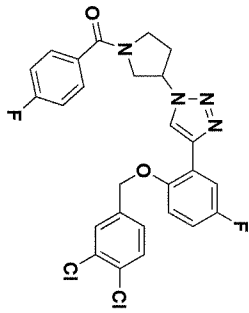


Current Data Parameters
NAME JSH-2-179-p
EXPNO 1
PROCNO 1

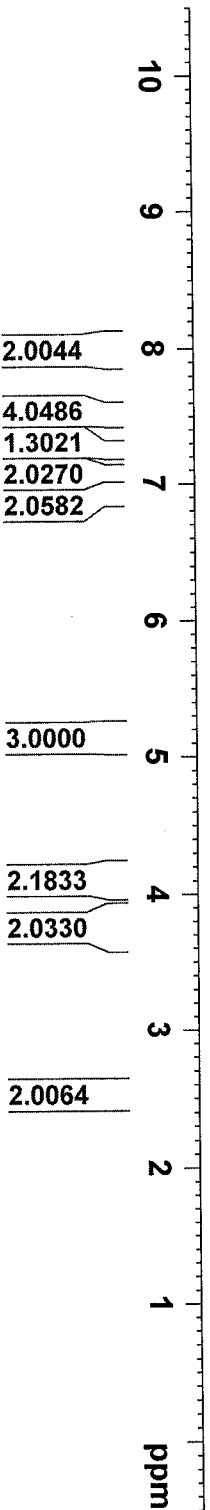
F2 - Acquisition Parameters
Date_ 20120402
Time 19.39
INSTRUM spect
PROBHD 5 mm DUL 1H-13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 10
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 228.1
DW 81.000 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

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

F2 - Processing parameters
SI 32768
SF 300.1300121 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



8.0476
8.0066
7.9090
7.5265
7.5218
7.4887
7.4613
7.2605
7.2285
7.0953
7.0693
7.0430
7.0065
6.9964
6.9765
6.9667
6.9516
6.9415
6.9134
6.8989
6.8837
6.8689
5.1910
5.0917
4.1630
4.1419
4.1178
4.0943
4.0704
4.0119
3.8590
3.6535
2.5109





Current Data Parameters
NAME JSH-2-179-p
EXPNO 2
PROCNO 1

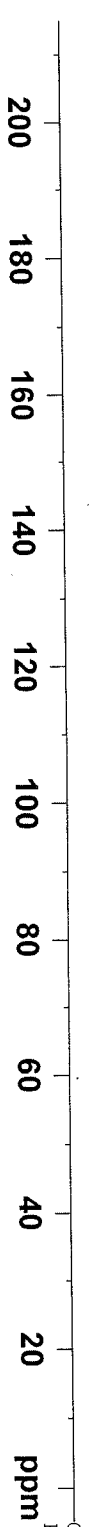
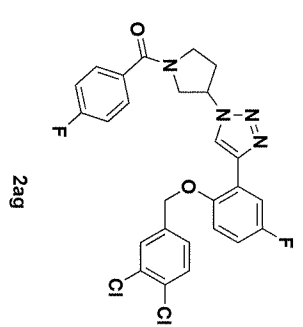
F2 - Acquisition Parameters
Date_ 20120718
Time_ 21.01
INSTRUM spect
PROBHD 5 mm DUL 1H-13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 11189
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 18390.4
DW 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
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
PL2 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

- 169.0196
- 165.5014
- 162.1765
- 159.2895
- 156.1135
- 150.5966
- 142.4426
- 136.7170
- 133.0207
- 132.6228
- 132.0009
- 130.9877
- 129.7164
- 129.6025
- 129.4546
- 126.8278
- 122.2429
- 121.0046
- 120.8929
- 115.7185
- 115.4532
- 115.1471
- 114.7127
- 114.3766
- 113.4034
- 113.2918
- 77.4860
- 77.2644
- 77.0627
- 76.6394
- 69.8997
- 59.3721
- 58.4870
- 54.3146
- 52.0200
- 47.8754
- 44.5167
- 32.7804
- 30.5492
- 29.7099



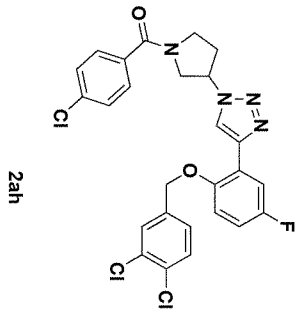


Current Data Parameters
 NAME JSH-2-185-p
 EXPNO 1
 PROCNO 1

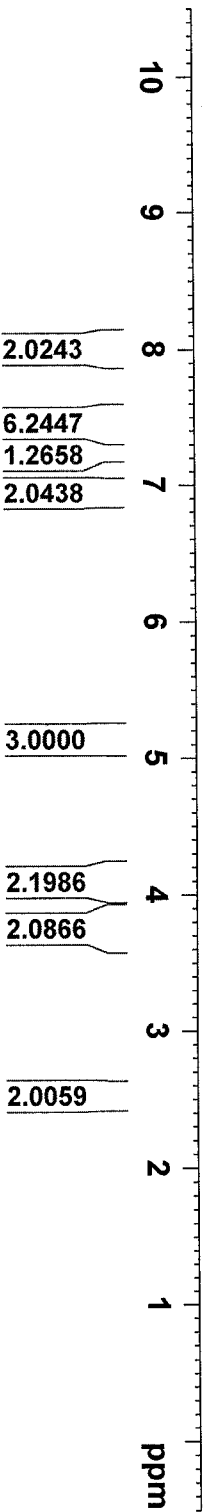
F2 - Acquisition Parameters
 Date_ 20120404
 Time_ 15.38
 INSTRUM spect
 PROBHD 5 mm DUL 1H-13
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 6172.839 Hz
 FIDRES 0.094190 Hz
 AQ 5.3084660 sec
 RG 203.2
 DW 81.000 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.00000000 sec
 TDO 1

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

F2 - Processing parameters
 SI 32768
 SF 300.1300121 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



8.0469
 7.9984
 7.9012
 7.5240
 7.5195
 7.4857
 7.4584
 7.4400
 7.3722
 7.2603
 7.2247
 7.0041
 6.9939
 6.9742
 6.9644
 6.9492
 6.9392
 6.9121
 6.8976
 6.8824
 6.8676
 5.2856
 5.1868
 5.0871
 4.1413
 4.1170
 4.0935
 4.0695
 3.9908
 3.8610
 3.8429
 3.6515
 2.5077





Current Data Parameters
NAME JSH-2-185-p
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters

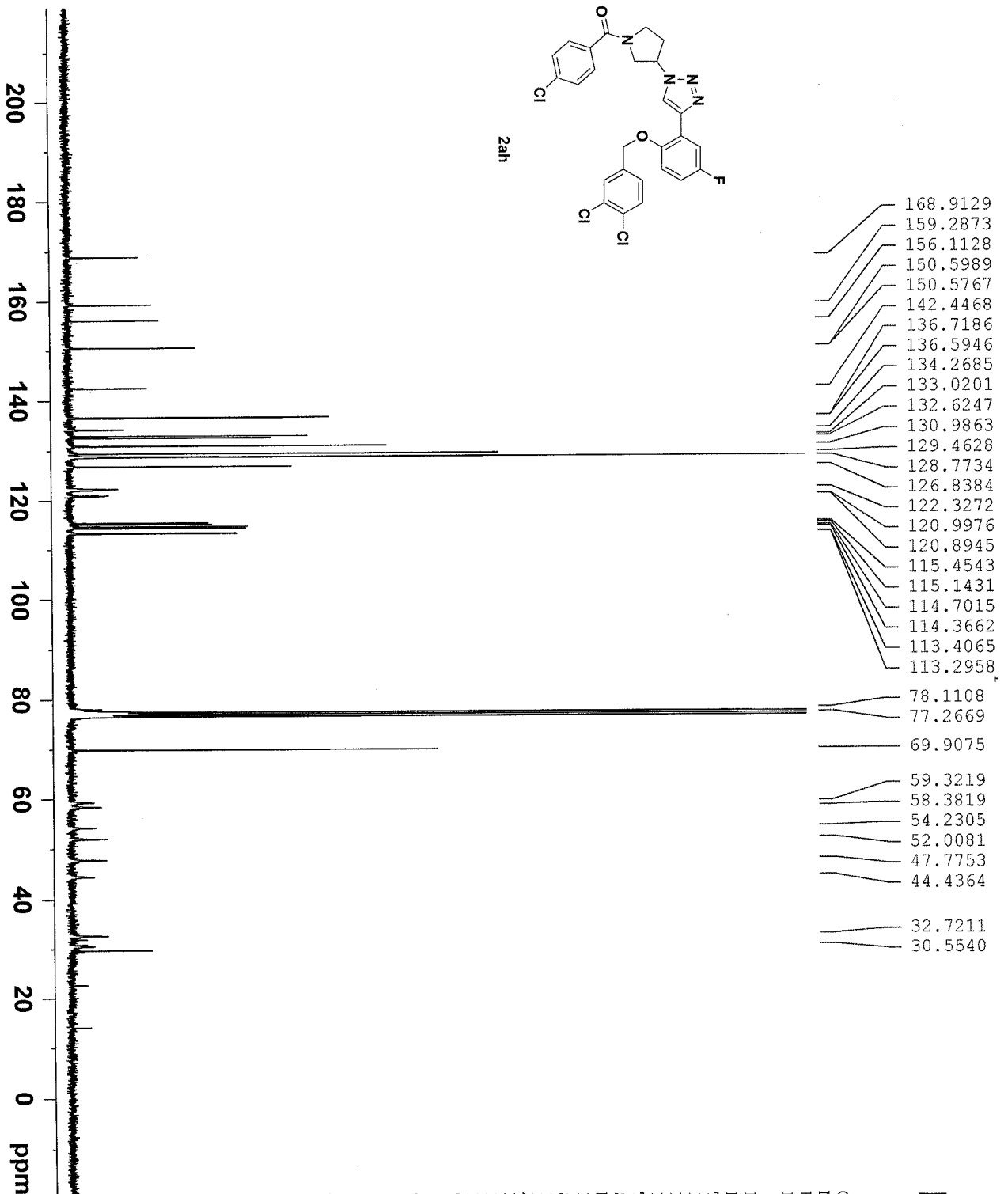
Date_ 20120726
Time 20.53
INSTRUM spect
PROBHD 5 mm DUL 1H-13
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 10941
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 18390.4
DW 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TDO 1

===== 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
PL2 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



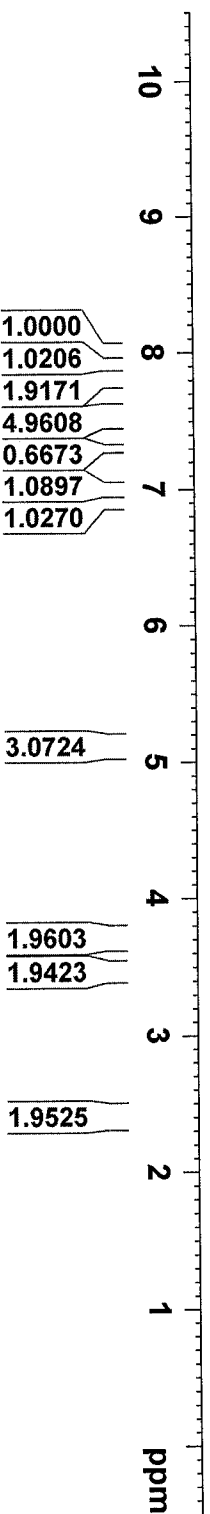
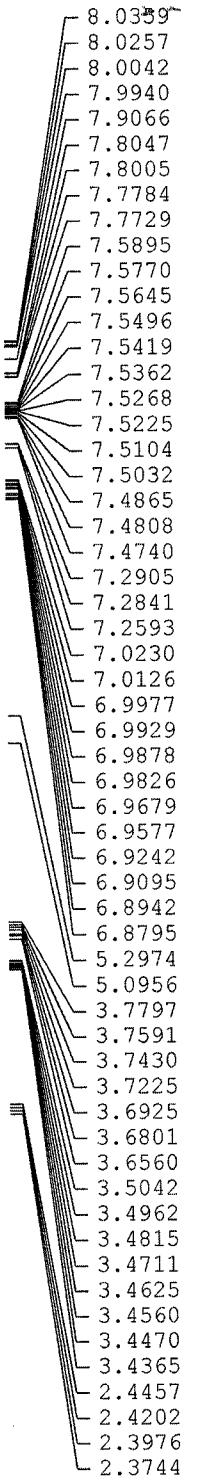
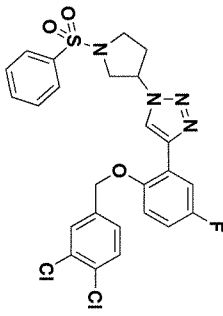


Current Data Parameters
NAME JSB-2-171-p (UP)
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20120410
Time 18.09
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 1149.4
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 300.1300124 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00





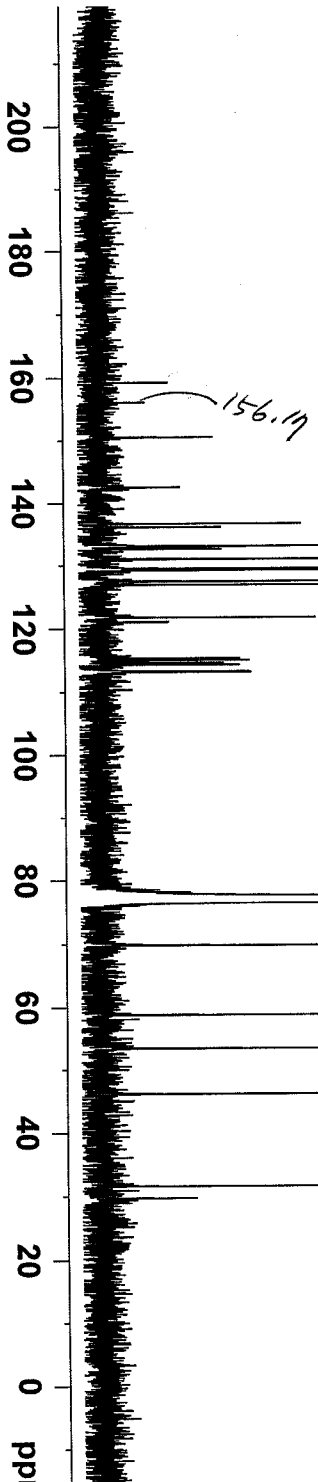
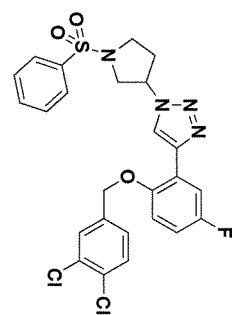
Current Data Parameters
NAME JSH-171-p
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20120419
Time_ 21.25
INSTRUM spect
PROBHD 5 mm DUL 1H-13
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 10870
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 14596.5
DM 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
PL2 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



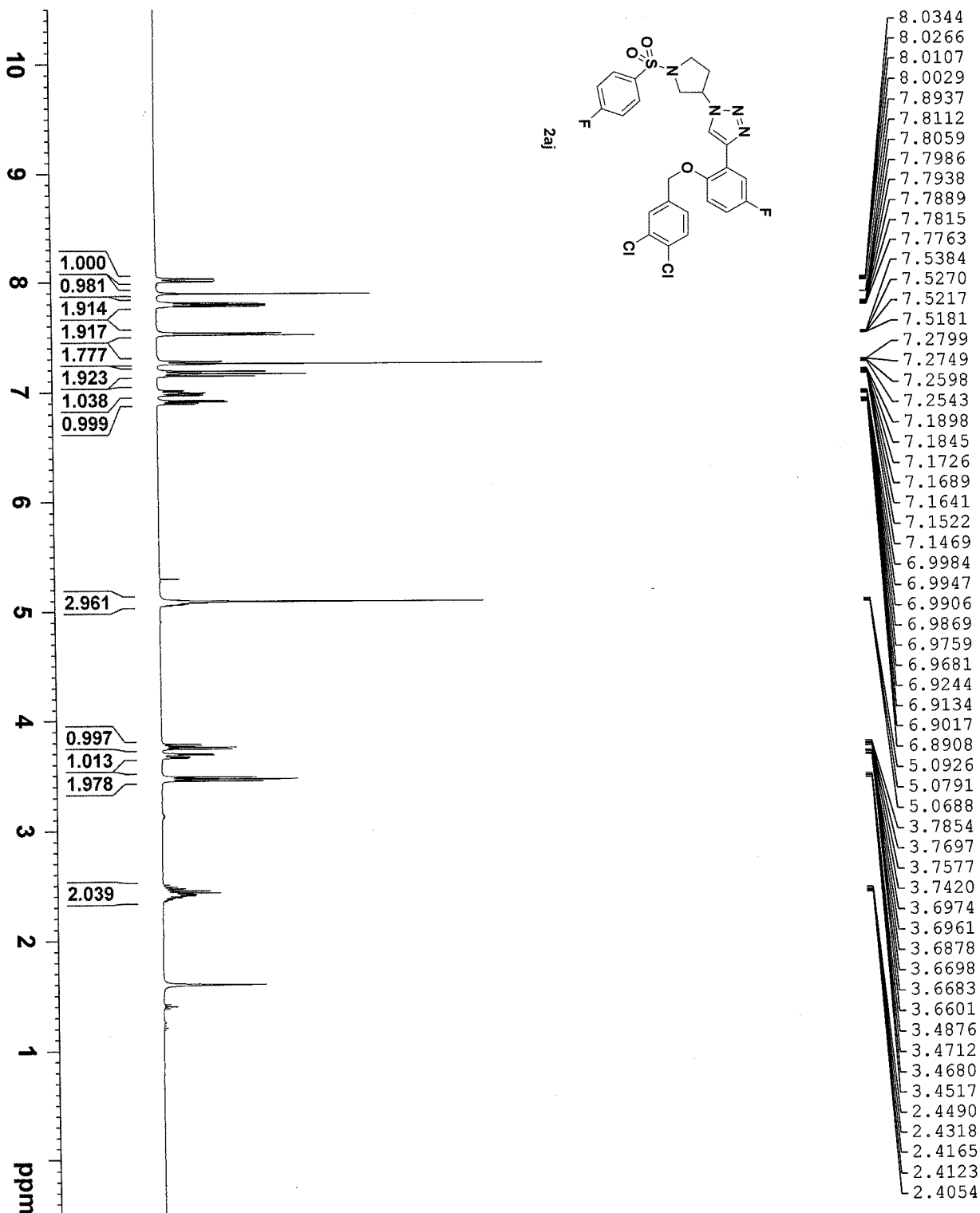
- 159.2748
- 150.5480
- 142.5407
- 136.7016
- 136.1570
- 133.1571
- 133.0054
- 132.6494
- 131.0597
- 129.5451
- 129.2838
- 127.4878
- 126.9557
- 121.7859
- 121.1456
- 121.0336
- 115.3779
- 115.0691
- 114.6956
- 114.3599
- 113.3678
- 113.2566
- 77.4601
- 77.0362
- 76.6131
- 69.9088
- 58.8666
- 53.4542
- 46.2092
- 31.5821
- 29.7205



Current Data Parameters
 NAME JSH-130626-p
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20130626
 Time 17.36
 INSTRUM spect
 PROBD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 12
 DS 2
 SWH 8223.685 Hz
 FIDRES 0.125483 Hz
 AQ 3.9846387 sec
 RG 190.62
 DW 60.800 usec
 DE 6.50 usec
 TE 298.3 K
 D1 1.0000000 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 400.2100131 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00





Current Data Parameters
NAME JSH-2-181-p
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters

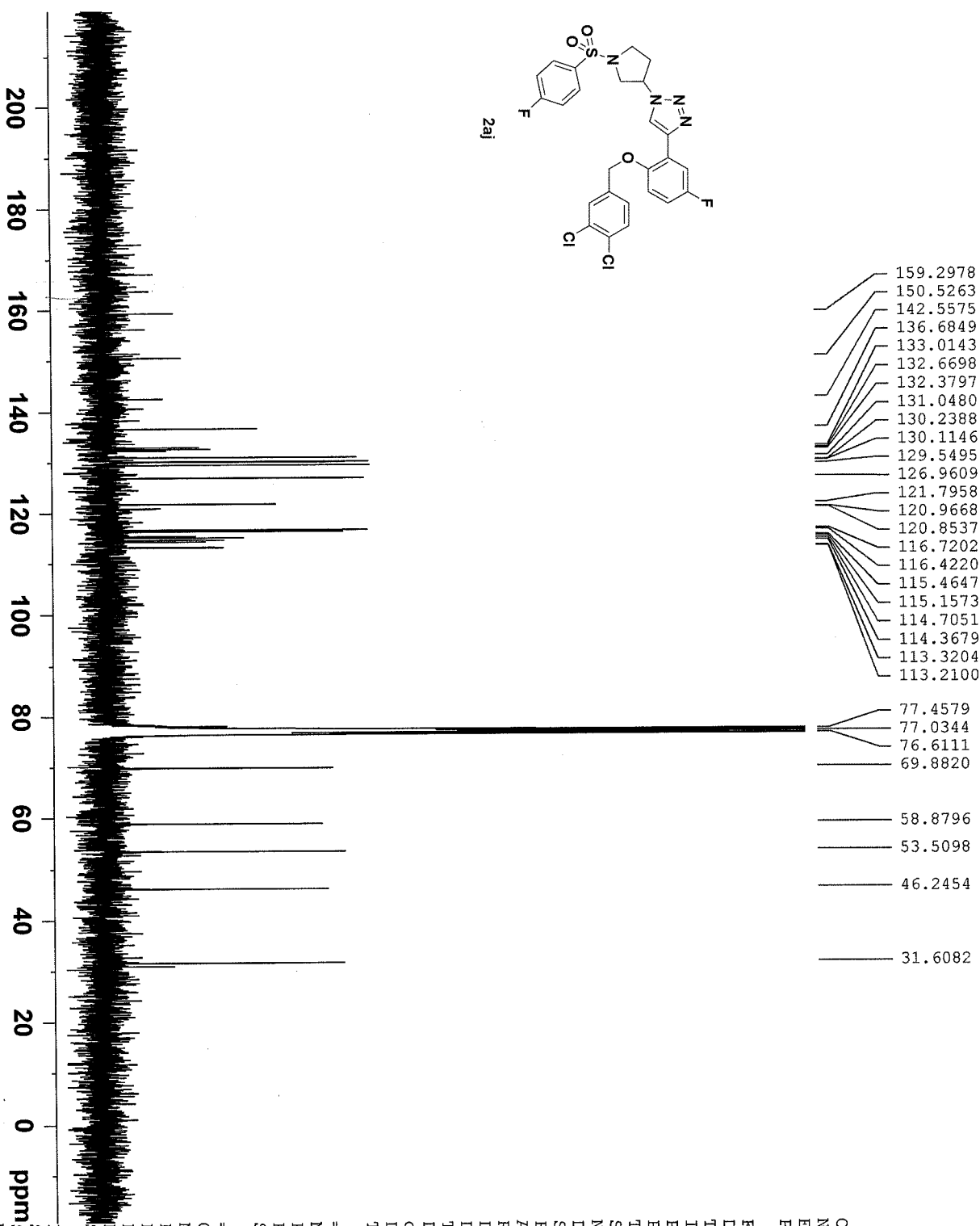
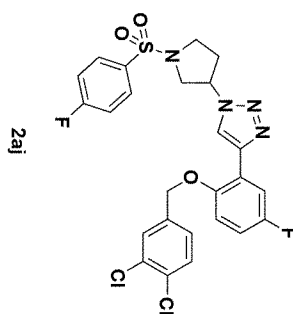
Date_ 20120422
Time_ 21.26
INSTRUM spect
PROBHD 5 mm DUL 1H-13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 10534
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 20642.5
DM 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

===== 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
PL2 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 1.00



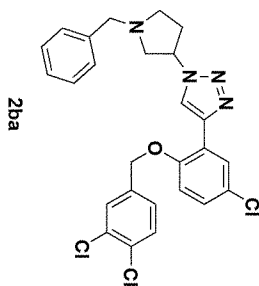


Current Data Parameters
NAME JSH-2-133-p
EXPNO 2
PROCNO 1

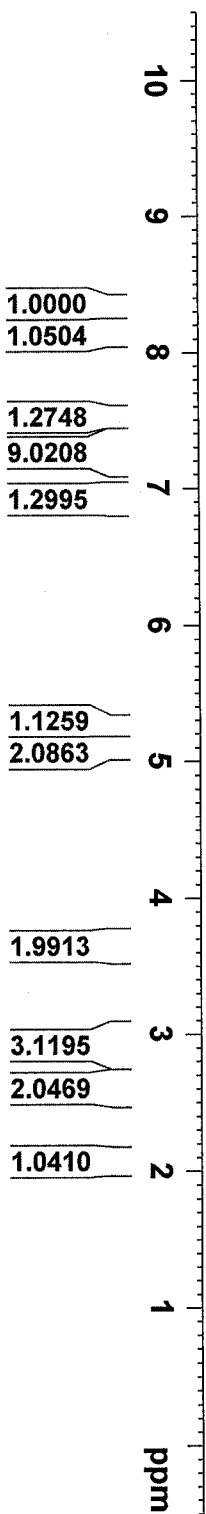
F2 - Acquisition Parameters
Date_ 20120217
Time 21.49
INSTRUM spect
PROBHD 5 mm DUL 1H-13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 256
DW 81.000 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

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

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



8.3333
8.1473
7.5349
7.3548
7.2267
6.9096
6.8844
5.2408
5.1064
3.6675
3.6272
2.9127
2.5532
2.0396





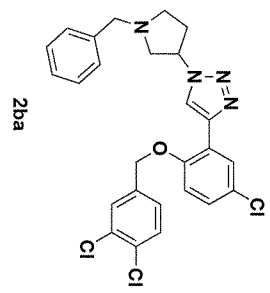
Current Data Parameters
NAME JSH-2-133-p
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20120217
Time 21.53
INSTRUM spect
PROBHD 5 mm DUL 1H-13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 18390.4
DM 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.0000000 sec
d11 0.0300000 sec
DELTA 1.8999998 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
PL2 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 0.80

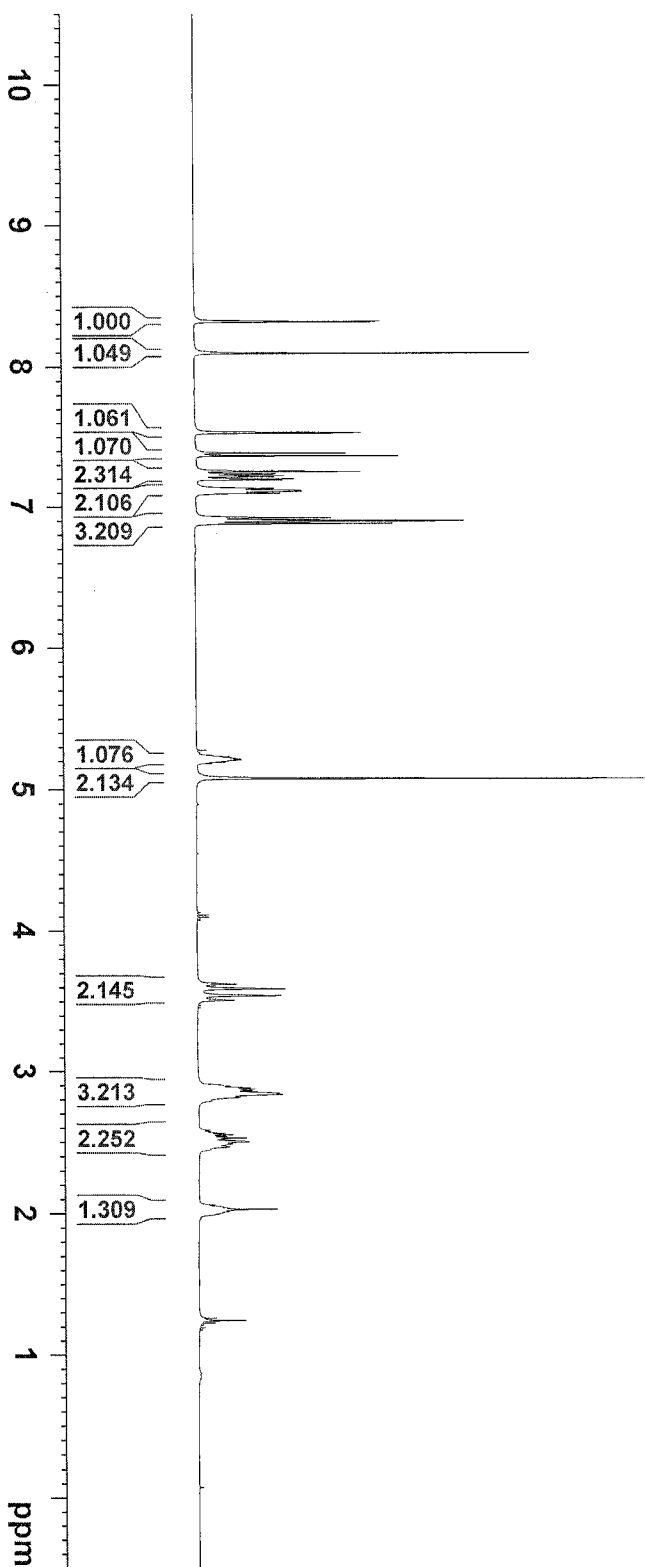
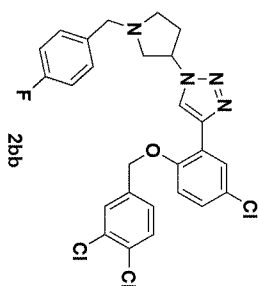
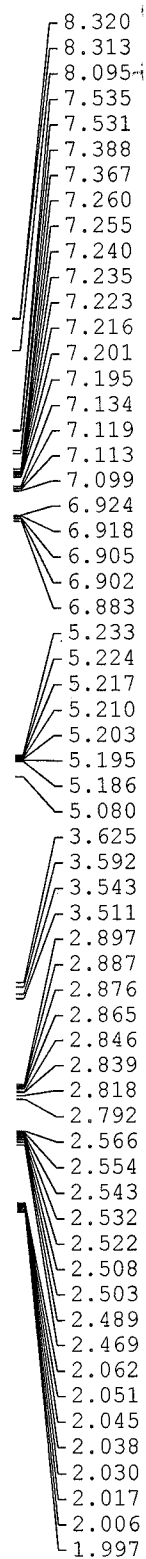


152.9045
142.2010
136.5799
132.9976
132.5510
130.8346
129.6234
128.5399
128.4082
127.6686
127.5506
127.3304
127.0794
126.9643
121.8059
121.7019
113.3606

77.4883
77.0649
76.6410
69.6200
59.9937
59.4221
59.3344
52.6143

32.7717

200 180 160 140 120 100 80 60 40 20 0 ppm



Current Data Parameters
NAME JSH-130714-p
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20130714
Time 15.48
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 10
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 297.6 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 400.2100151 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



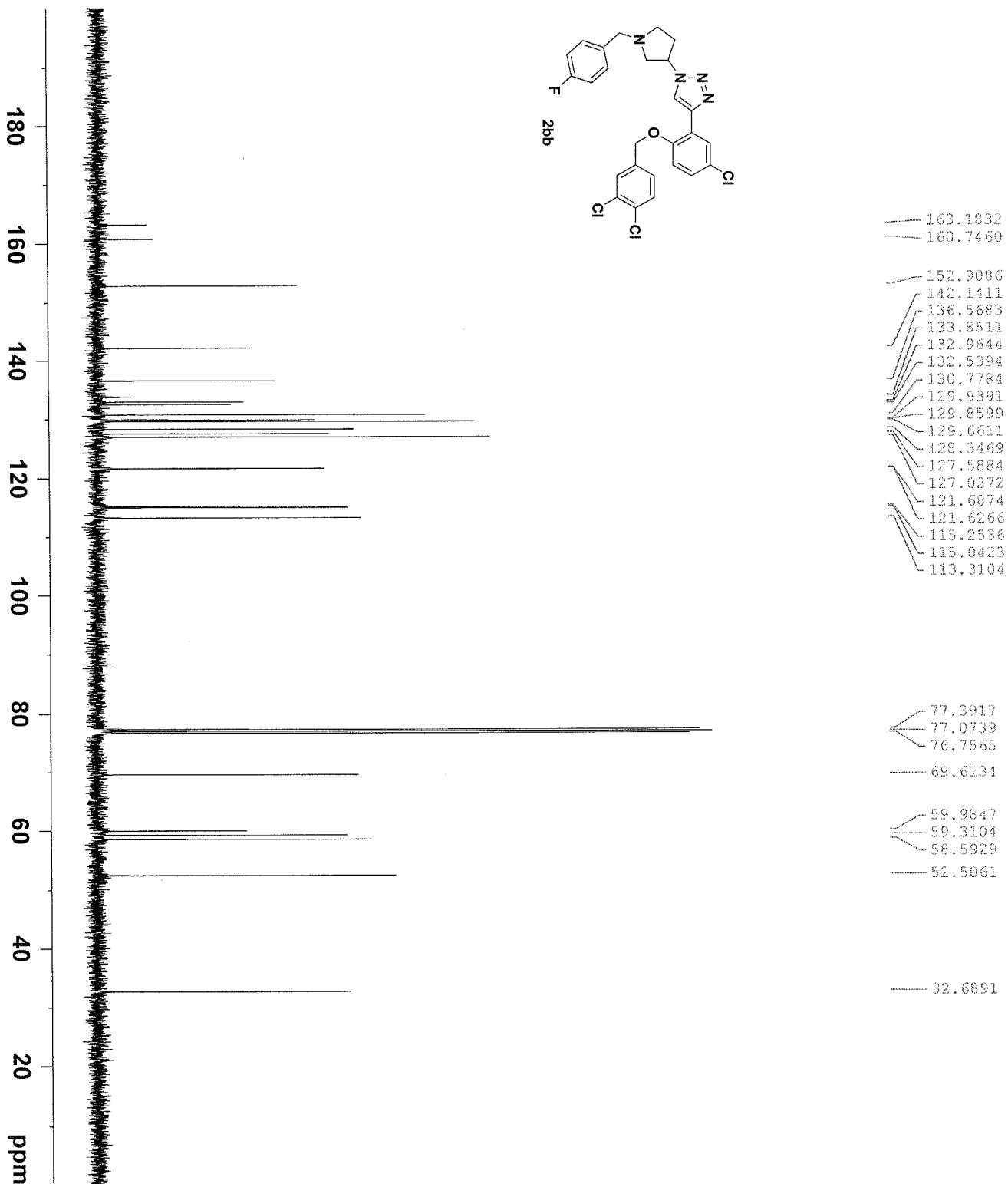
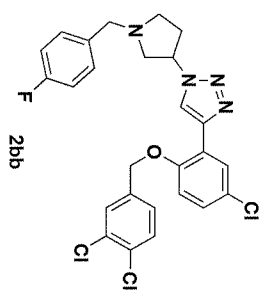
Current Data Parameters
NAME JSH-130714-P
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20130714
Time 15.55
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 104
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 190.62
DE 20.800 usec
TE 298.4 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



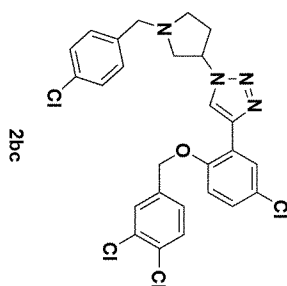


Current Data Parameters
NAME JSH-2-145-p
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20120316
Time_ 11.14
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 1024
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 300.1300120 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



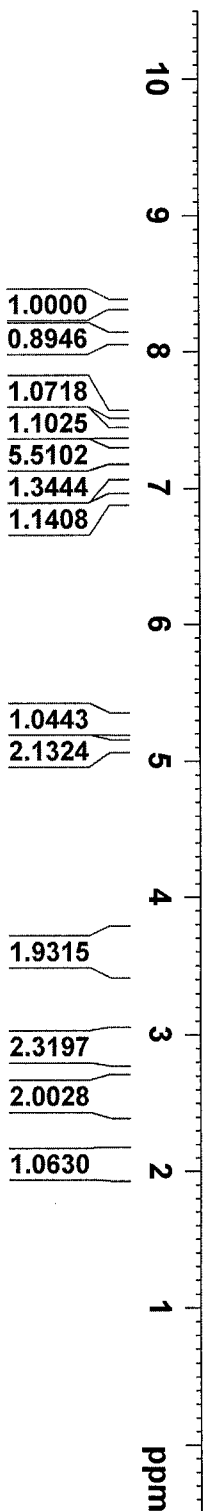
8.3483
8.3397
8.0993
7.5470
7.5420
7.4204
7.3930
7.3268
7.2604
7.2406
7.2326
7.1297
6.9337
6.9043

5.2589
5.2471
5.1093

3.5863

2.9071
2.6860
2.5778

2.0753



1.0000
0.8946
1.0718
1.1025
5.5102
1.3444
1.1408

1.0443
2.1324

1.9315

2.3197
2.0028

1.0630



Current Data Parameters
NAME JSH-2-145-p
EXPNO 2
PROCNO 1

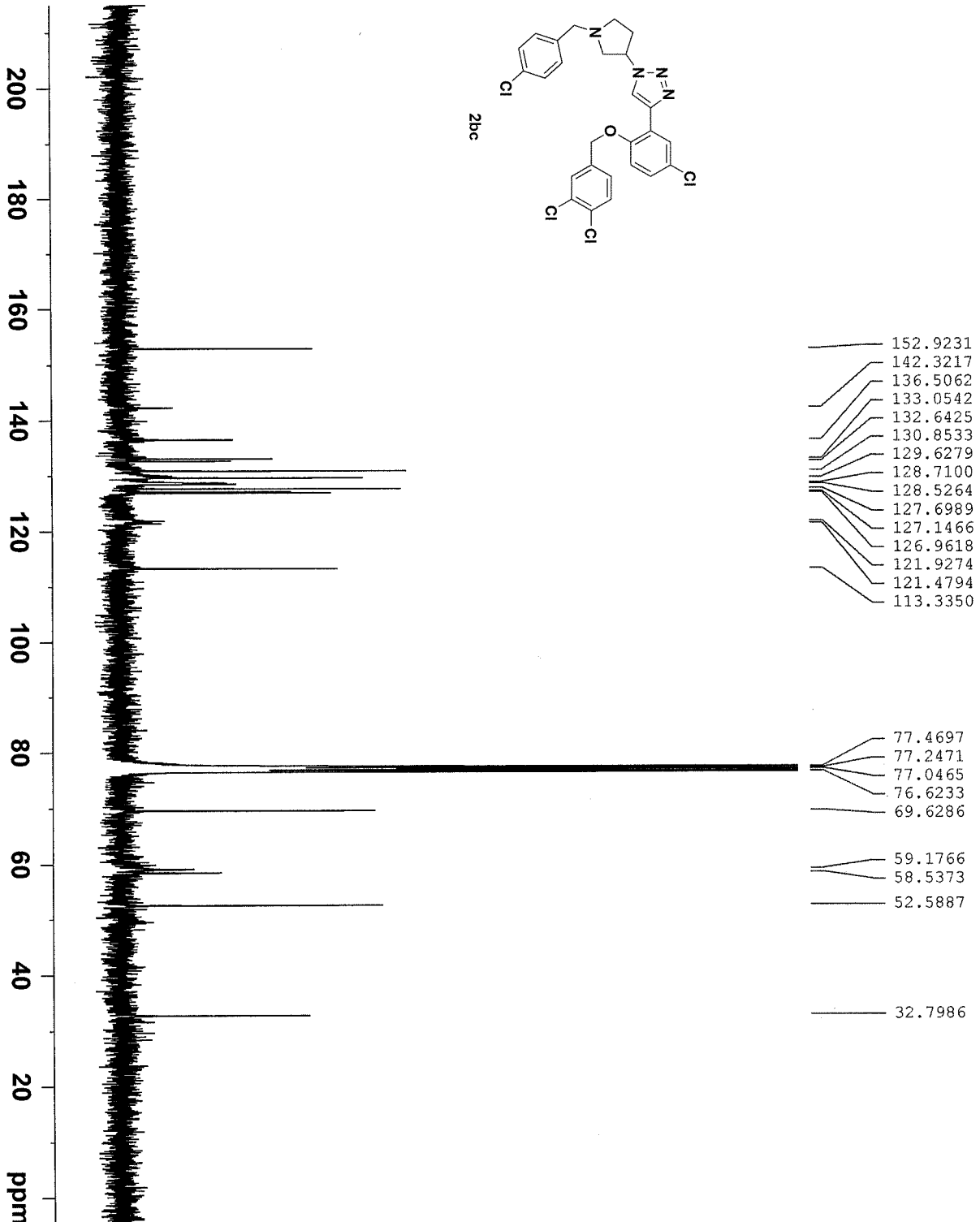
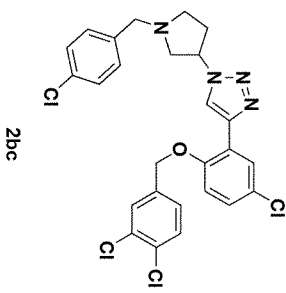
F2 - Acquisition Parameters

Date_ 20120320
Time 22.17
INSTRUM spect
PROBHD 5 mm DUL 1H-13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 10019
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 14596.5
DM 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.0000000 sec
d11 0.0300000 sec
DELTA 1.8999998 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
PL2 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



152.9231
142.3217
136.5062
133.0542
132.6425
130.8533
129.6279
128.7100
128.5264
127.6989
127.1466
126.9618
121.9274
121.4794
113.3350

77.4697
77.2471
77.0465
76.6233
69.6286

59.1766
58.5373
52.5887

32.7986



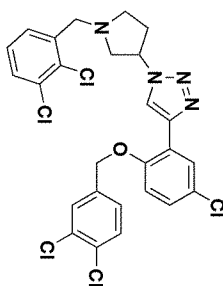
Current Data Parameters
NAME JSH-2-175-p
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20120316
Time 14.54
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 203.2
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 300.1300122 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

8.3235
8.3148
8.1840
7.4740
7.4684
7.3377
7.3206
7.3126
7.2939
7.2602
7.2315
7.2227
7.2023
7.1937
7.1811
7.1749
7.1303
7.0899
7.0643
7.0387
6.8981
6.8687
5.2891
5.2795
5.2715
5.2515
5.0998
5.0608
3.9438
3.8071
3.7610
3.7362
3.6893
3.4771
2.9988
2.8637
2.6466
2.6176
2.6041
2.5885
2.5737
2.5416
2.0556
2.0373



2bd

10
9
8
7
6
5
4
3
2
1
ppm

1.0000
0.9816
1.0577
2.0861
2.1600
1.9876
1.0312

1.0804
2.0481

2.0025

2.0946
0.9376
1.9700

1.0772



Current Data Parameters
NAME JSH-2-175-P
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20120424
Time 20.18

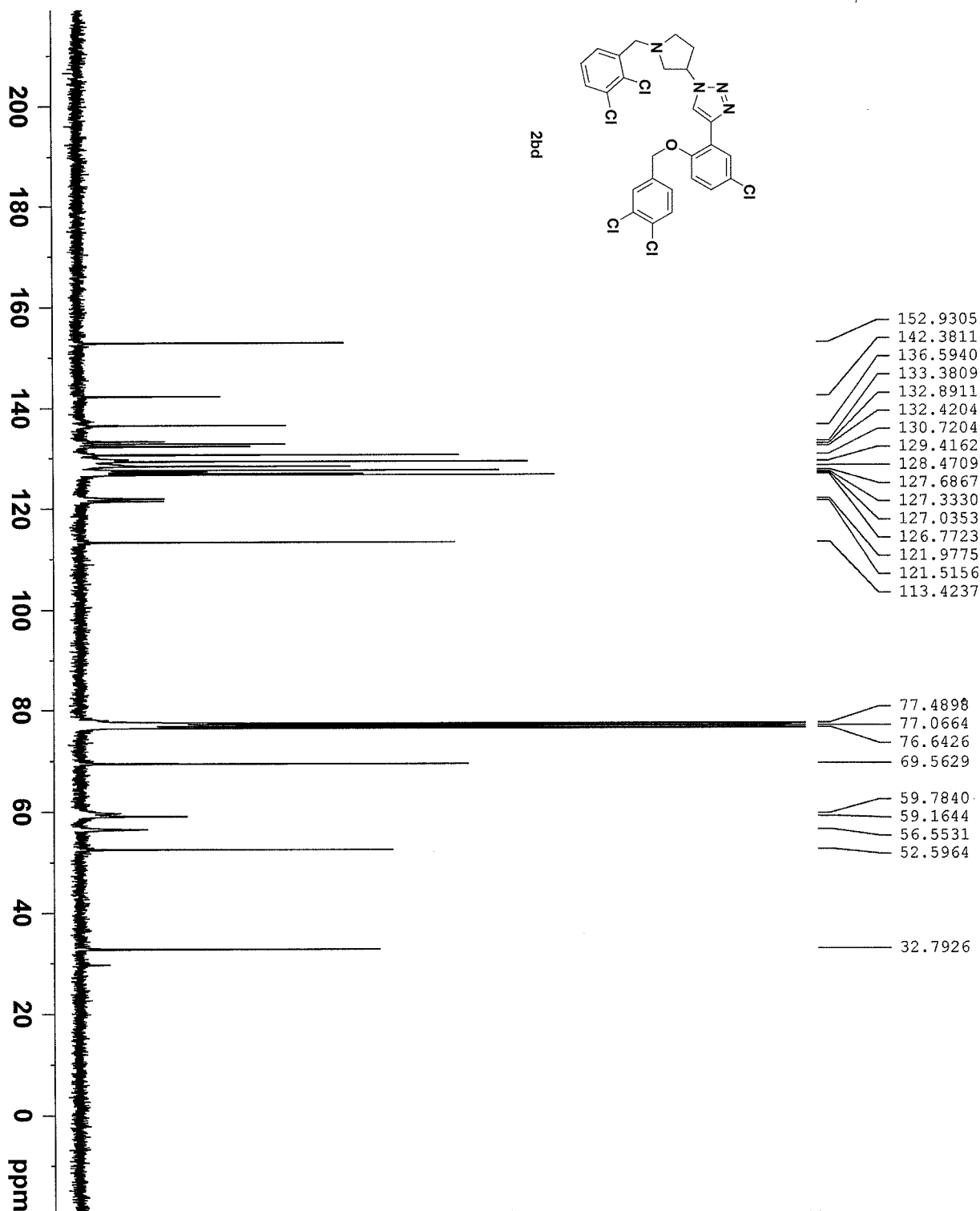
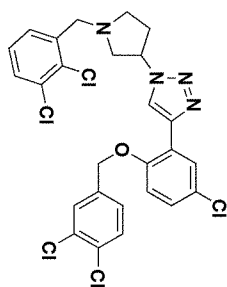
INSTRUM spect
PROBHD 5 mm DUL 1H-13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 11603
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 9195.2
DM 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.0000000 sec
d11 0.0300000 sec
DELTA 1.8999998 sec
TD0 1

===== 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
PL2 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



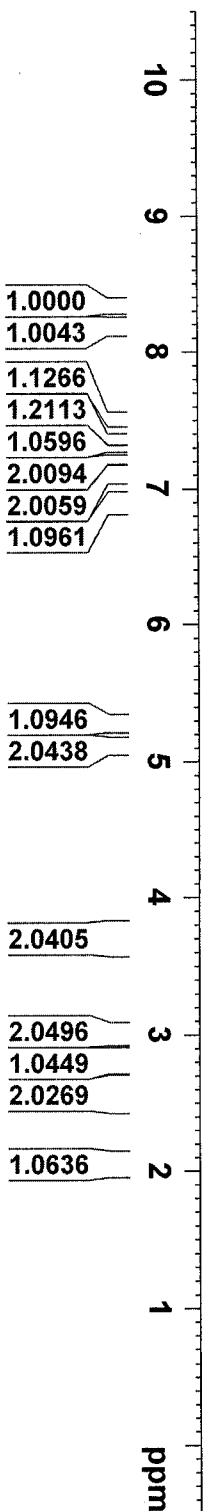
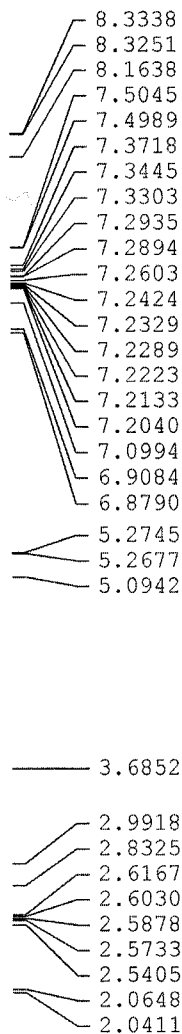
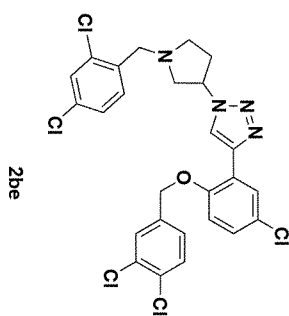


Current Data Parameters
 NAME JSH-2-177-p
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20120320
 Time 21.02
 INSTRUM spect
 PROBD 5 mm DUL
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 6172.839 Hz
 FIDRES 0.094190 Hz
 AQ 5.3084660 sec
 RG 256
 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 300.1300120 MHz
 WDM EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00





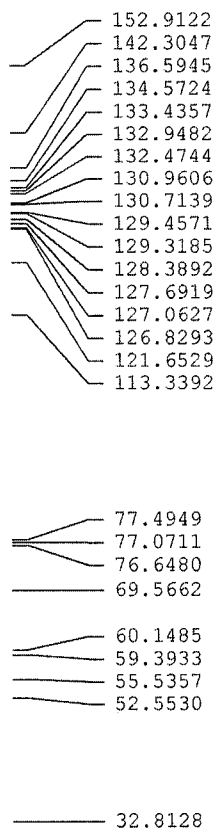
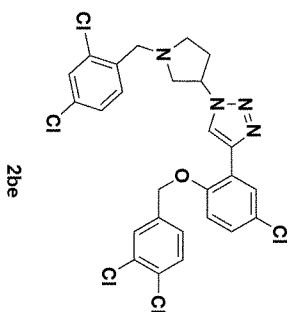
Current Data Parameters
NAME JSH-2-177-p
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20120320
Time_ 21.08
INSTRUM spect
PROBHD 5 mm DUL 1H-13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
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 2.0000000 sec
d11 0.0300000 sec
DELTA 1.8999998 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
PL2 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



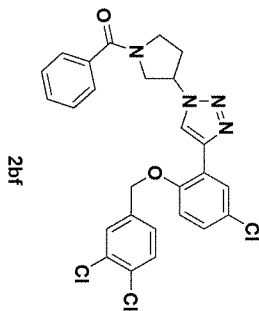


Current Data Parameters
NAME JSH-2-135-P
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20120308
Time 11.18
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 5.308460 sec
RG 512
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
PL -1.00 dB
SFO1 300.1318534 MHz

F2 - Processing Parameters
SI 32768
SF 300.1300116 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

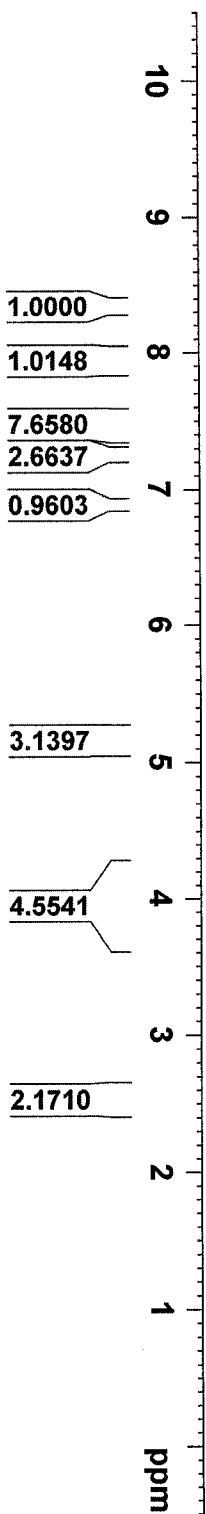


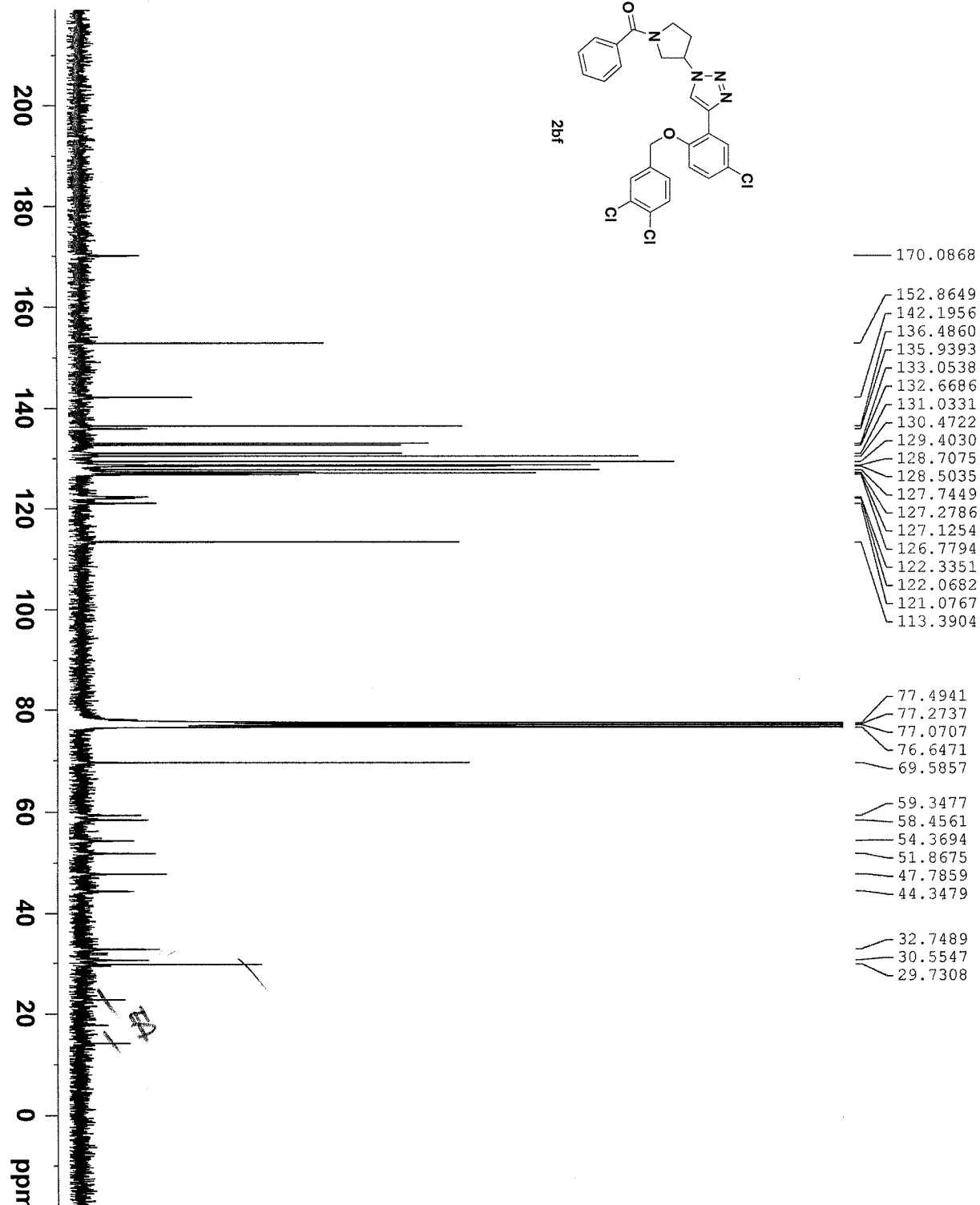
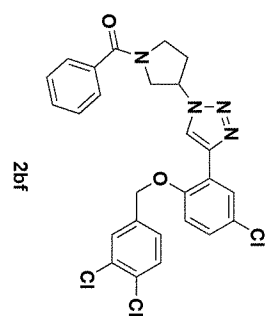
8.3523
7.9966
7.9414
7.8882
7.5250
7.4934
7.4667
7.4109
7.2606
7.2274
6.9032
6.8739

5.2933
5.1217

4.1979
4.1315
3.9939
3.8922
3.6616

2.5202





NAME JSH-2-135-P
EXPNO 3
PROCNO 1
Date_ 20120313
Time 8.59
INSTRUM spect
PROBHD 5 mm DUL 1H-13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 10839
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 13004
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
PL2 0.00 dB
PL12 20.00 dB
PL13 22.00 dB
SFO2 300.1312005 MHz
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
GB 1.00 Hz
PC 1.40

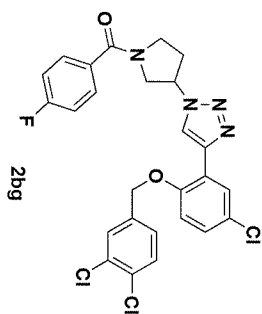


Current Data Parameters
NAME JSH-2-141-P
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20120321
Time 20.11
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 362
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 300.1300127 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

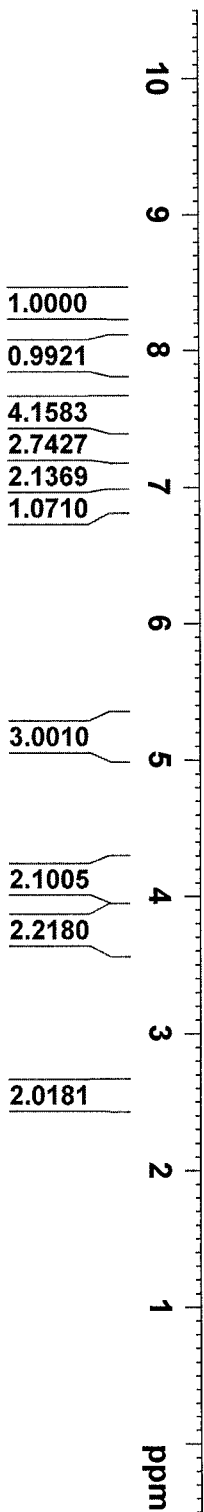


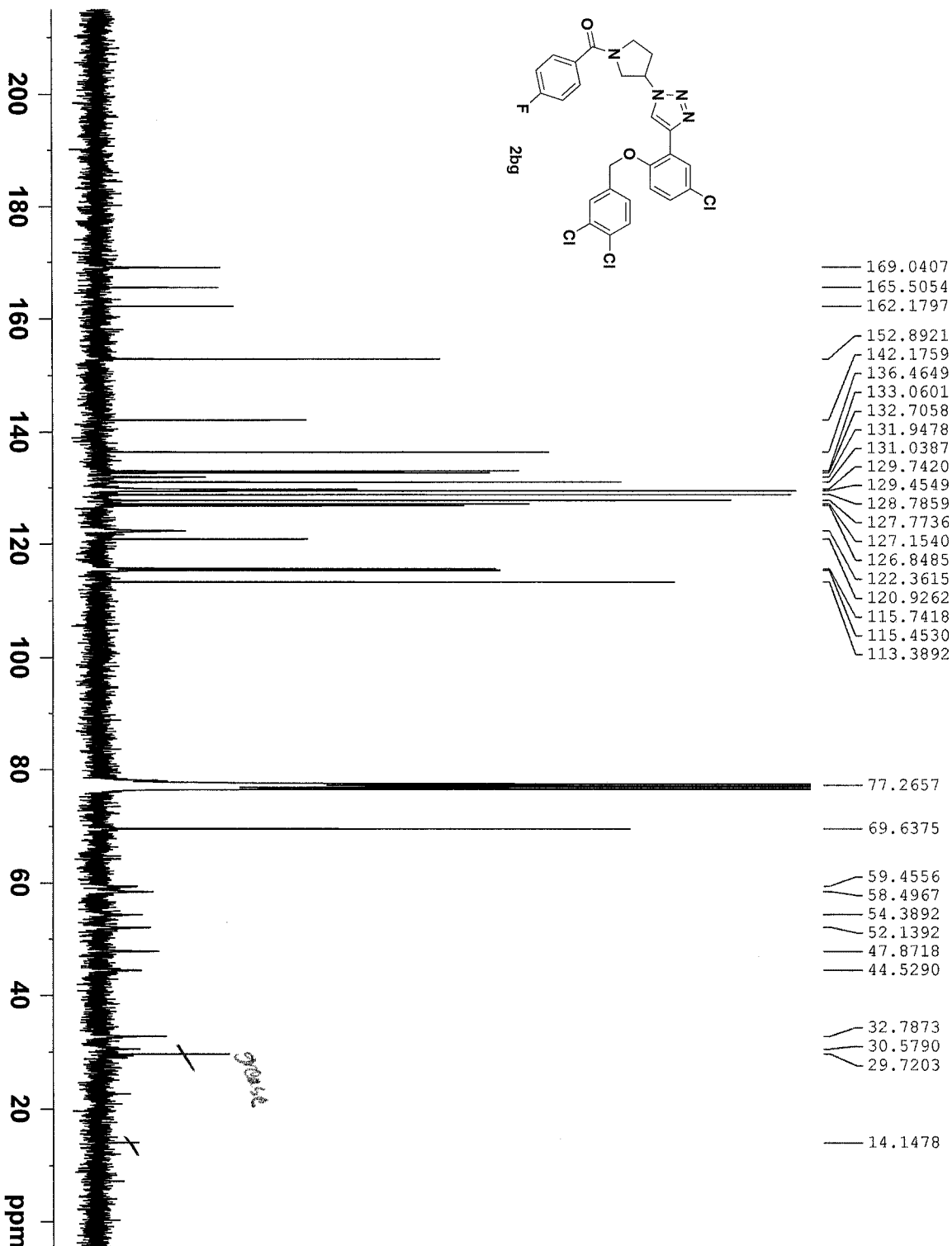
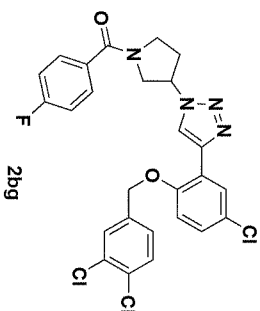
8.3396
7.9796
7.8924
7.5274
7.5008
7.4740
7.3773
7.2571
7.2289
7.0774
6.9043
6.8756

5.2902
5.1136

4.1018
4.0201
3.8645
3.6579

2.5170





NAME JSH-2-141-P
EXPNO 3
PROCNO 1
Date_ 20120322
Time 22.02
INSTRUM spect
PROBHD 5 mm DUL 1H-13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 10219
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
PL2 0.00 dB
PL12 20.00 dB
PL13 22.00 dB
SFO2 300.1312005 MHz
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

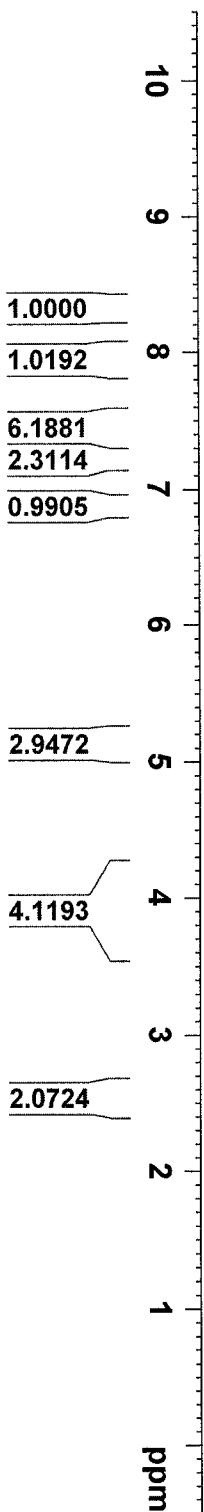
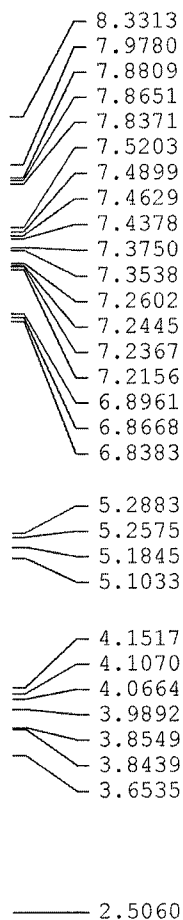
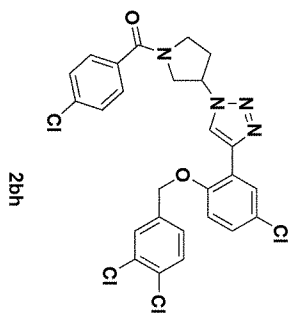


Current Data Parameters
NAME JSH-2-173-P
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20120322
Time 17.36
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 256
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 300.1300123 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00





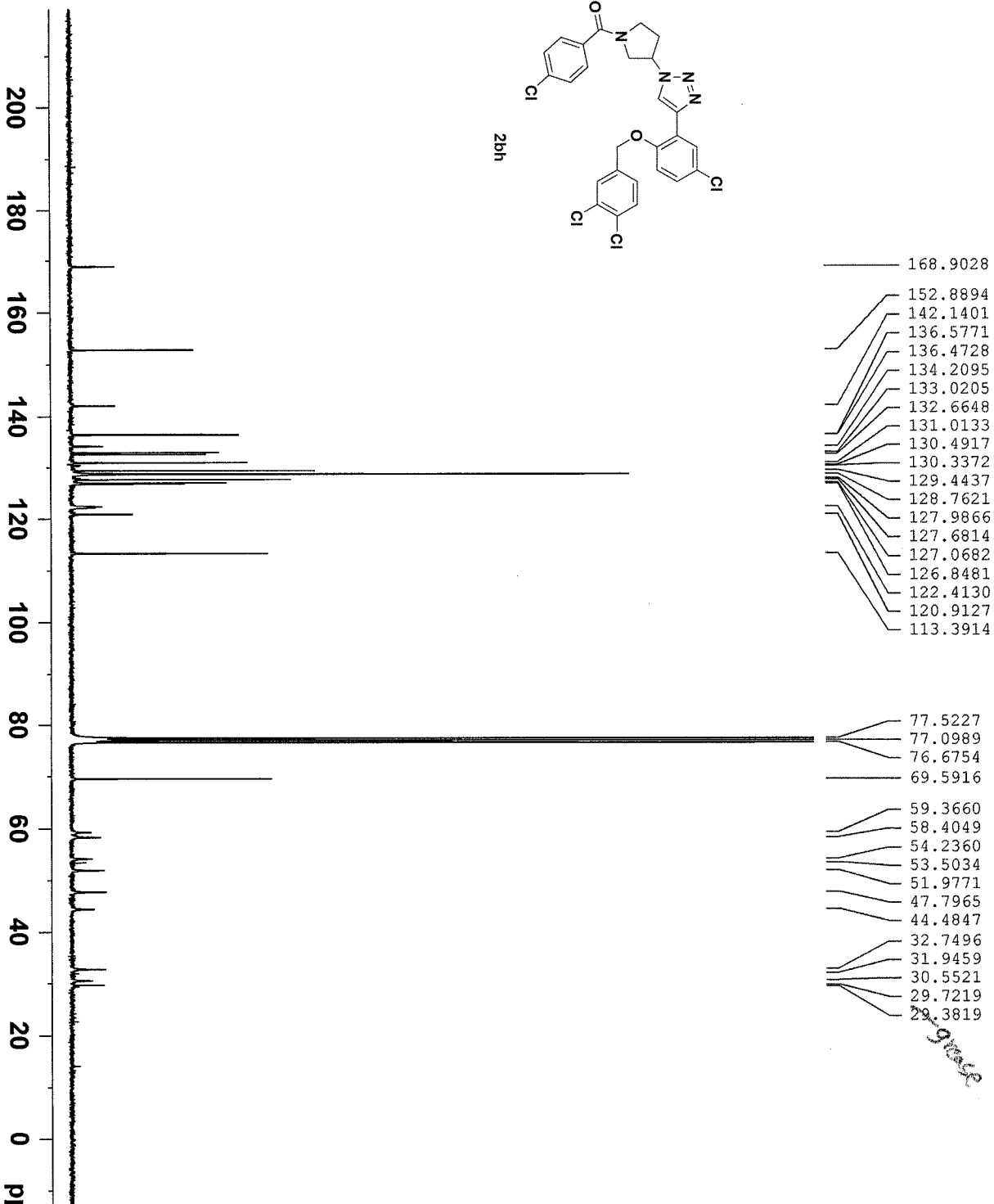
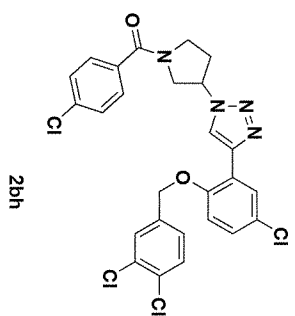
Current Data Parameters
NAME JSH-2-173-p
EXPNO 3
PROCNO 1

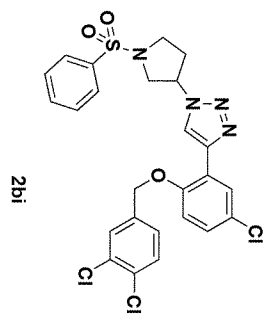
F2 - Acquisition Parameters
Date_ 20120403
Time 9.11
INSTRUM spect
PROBHD 5 mm DUL 1H-13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 10615
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 8192
DW 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 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
PL2 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





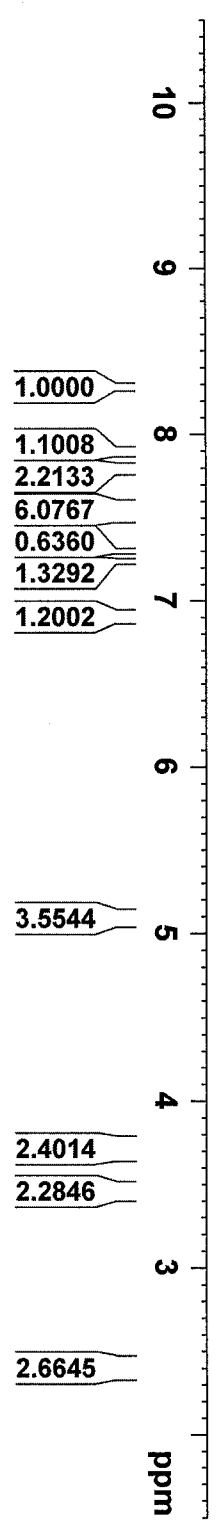
- 8.2881
- 8.2793
- 7.8931
- 7.8068
- 7.8029
- 7.7975
- 7.7806
- 7.7751
- 7.5729
- 7.5643
- 7.5563
- 7.5502
- 7.5445
- 7.5337
- 7.5292
- 7.5171
- 7.5094
- 7.4860
- 7.2936
- 7.2869
- 7.2689
- 7.2604
- 7.2401
- 7.2312
- 6.9122
- 6.8828
- 5.1139
- 5.0893
- 5.0826
- 5.0678
- 5.0611
- 3.7707
- 3.7500
- 3.7338
- 3.7131
- 3.6954
- 3.6818
- 3.6583
- 3.6447
- 3.5025
- 3.4941
- 3.4754
- 3.4691
- 3.4562
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- 3.4157
- 3.3963
- 2.4477
- 2.4226
- 2.3988

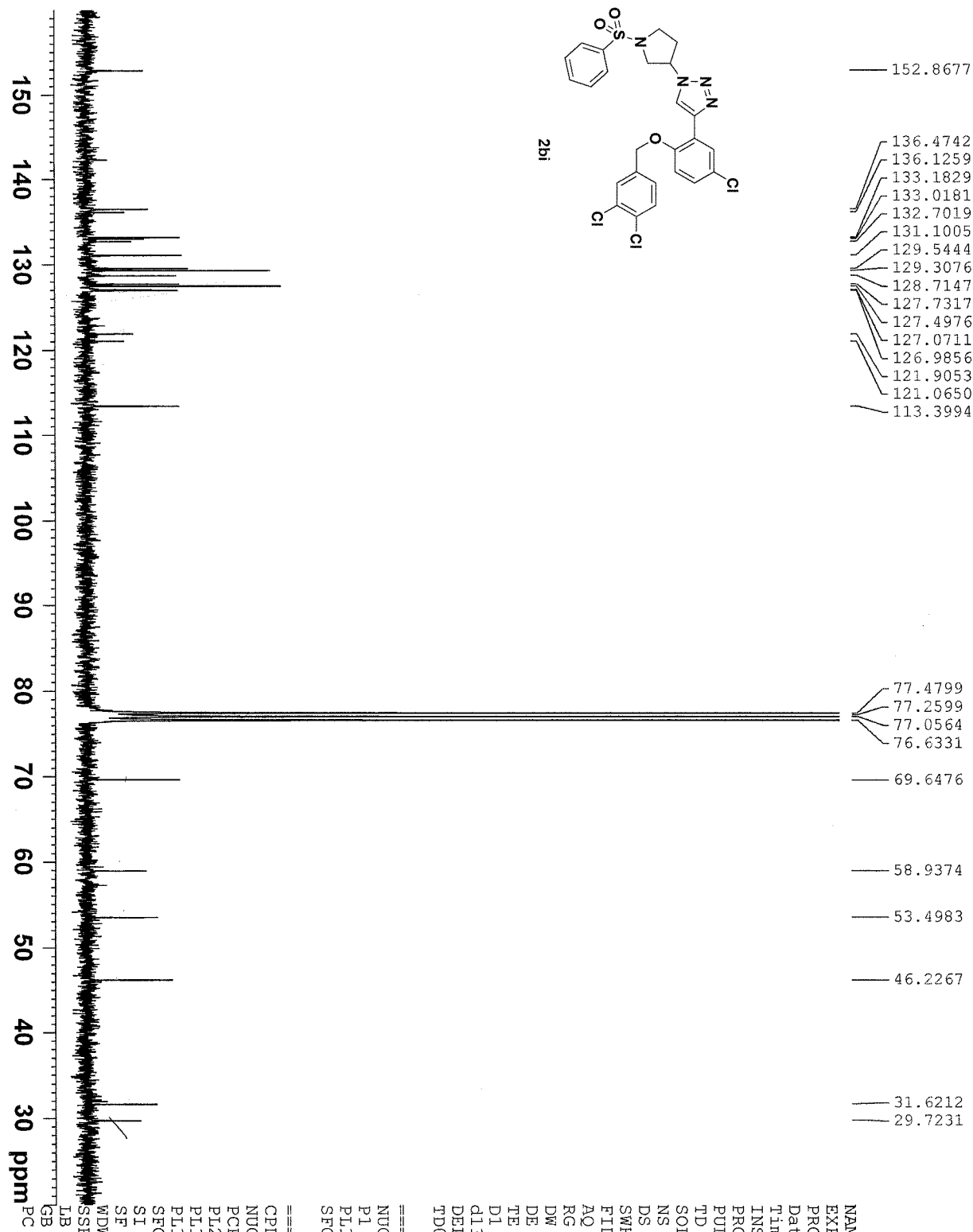
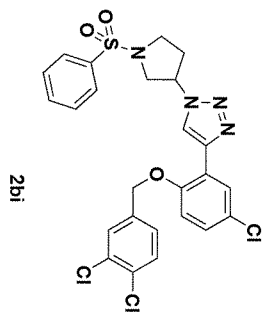
Current Data Parameters
 NAME JSH-2-137-p
 EXPNO 1
 PROCNO 5

F2 - Acquisition Parameters
 Date_ 20121121
 Time 17.06
 INSTRUM spect
 PROBHD 5 mm DUL 1H-13
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 12
 DS 2
 SWH 6172.839 Hz
 FIDRES 0.094190 Hz
 AQ 5.3084660 sec
 RG 574.7
 DE 81.000 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 300.1300121 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

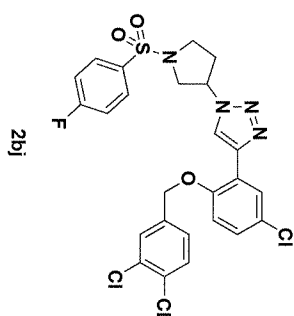




NAME JSH-2-137-p
EXPNO 3
PROCNO 1
Date_ 20120313
Time_ 14.32
INSTRUM spect
PROBHD 5 mm DUL 1H-13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 567
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 13004
DW 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.83999998 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
PL2 0.00 dB
PL12 20.00 dB
PL13 22.00 dB
SFO2 300.1312005 MHz
SI 32768
SEF 75.4677490 MHz
WDM EM
LB 0
SSB 1.00 Hz
GB 0
PC 1.40



8.2997
8.2908
7.8853
7.8224
7.8055
7.7992
7.7927
7.7760
7.5511
7.5235
7.2883
7.2814
7.2760
7.2667
7.2601
7.2466
7.2378
7.2069
7.1787
7.1499
6.9172
6.8878

5.1129
5.0928
5.0744

3.7848
3.7640
3.7477
3.7274
3.7040
3.6910
3.4904
3.4679
3.4424

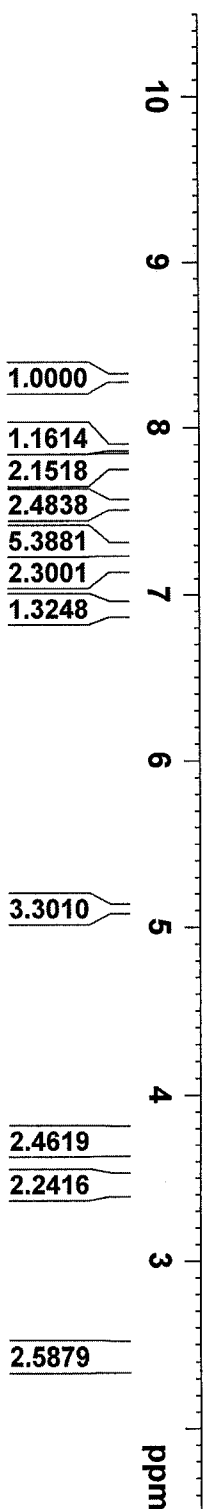
2.4529
2.4429
2.4295
2.4053

Current Data Parameters
NAME JSH-2-143-p
EXPNO 1
PROCNO 5

F2 - Acquisition Parameters
Date_ 20121121
Time 17.15
INSTRUM spect
PROBHD 5 mm DUL 1H-13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 13
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 512
DE 81.000 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

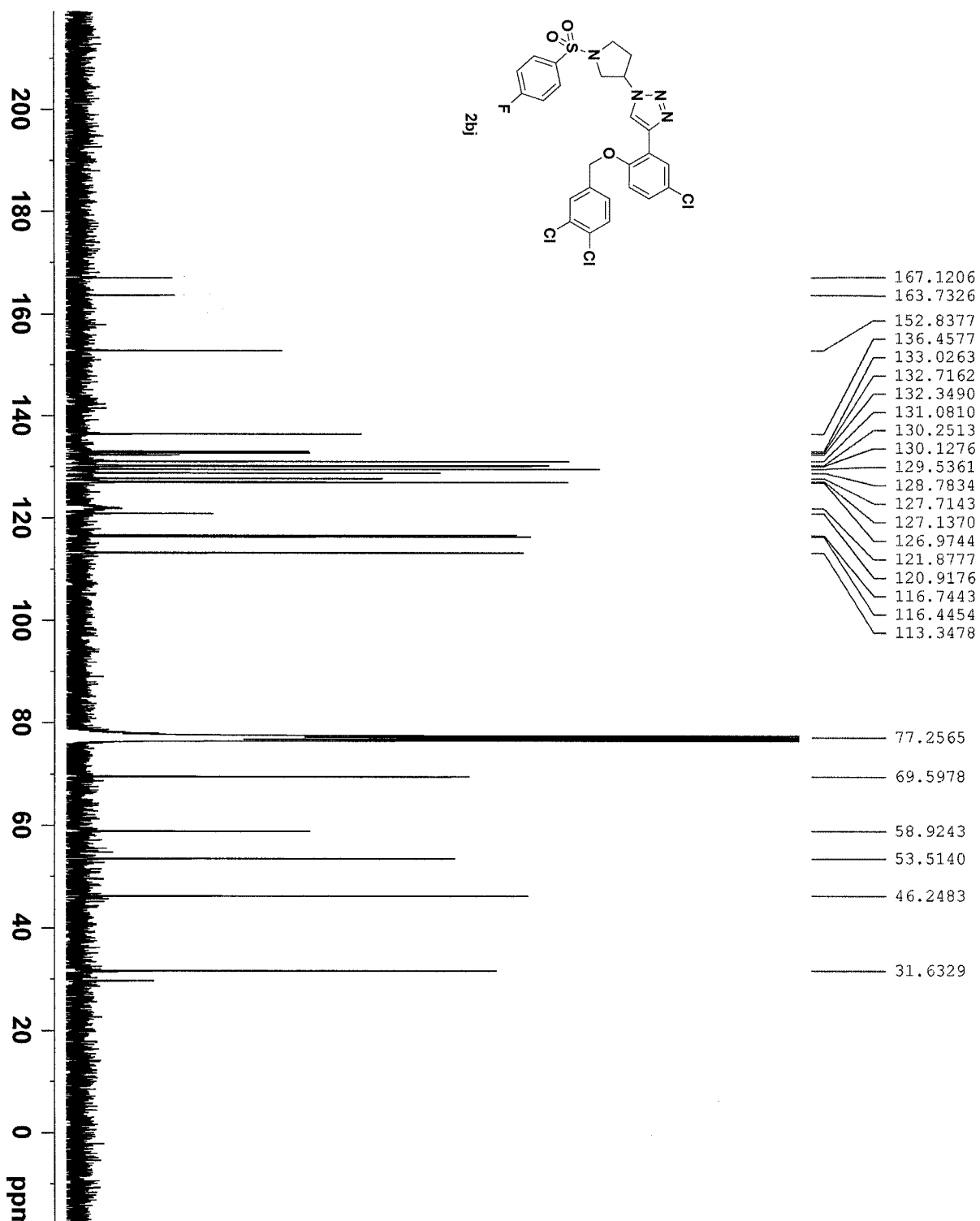
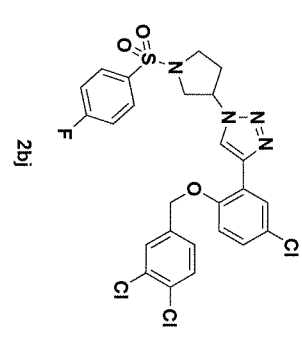
===== CHANNEL f1 =====
NUC1 1H
P1 10.50 usec
PL1 -1.00 dB
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1300122 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00





Current Data Parameters
NAME JSH-2-143-P
EXPNO 3
PROCNO 1



F2 - Acquisition Parameters
Date_ 20120326
Time_ 21.22
INSTRUM spect
PROBHD 5 mm DUL 1H-13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 10979
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 9195.2
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
PL2 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 JSH-3-159-p
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters

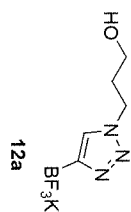
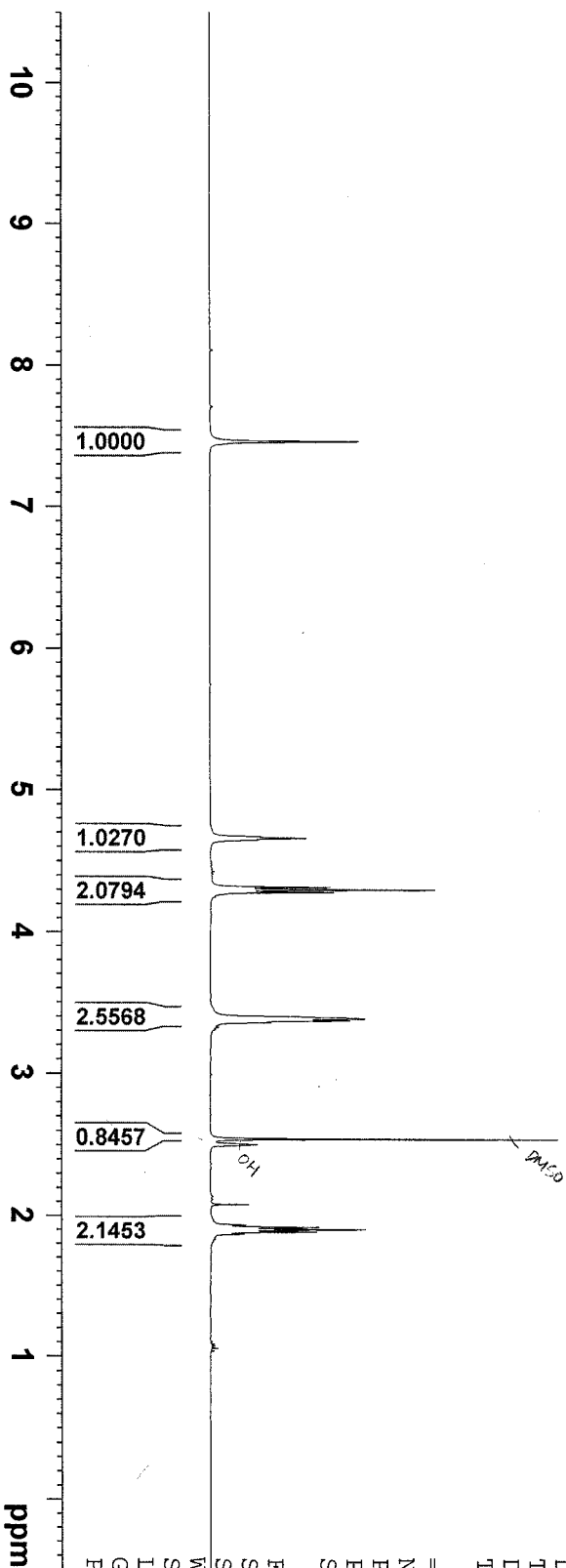
Date_ 20121016
Time 13.40
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 9
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 76.56
DW 60.800 usec
DE 6.50 usec
TE 299.2 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====

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

F2 - Processing parameters

SI 65536
SF 400.2100051 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



7.4551

4.6670
4.6561
4.6449
4.3147
4.2971
4.2794

3.3819
3.3690
3.3547

2.5390
2.5000
2.0778
1.9309
1.9146
1.8979
1.8812
1.8649



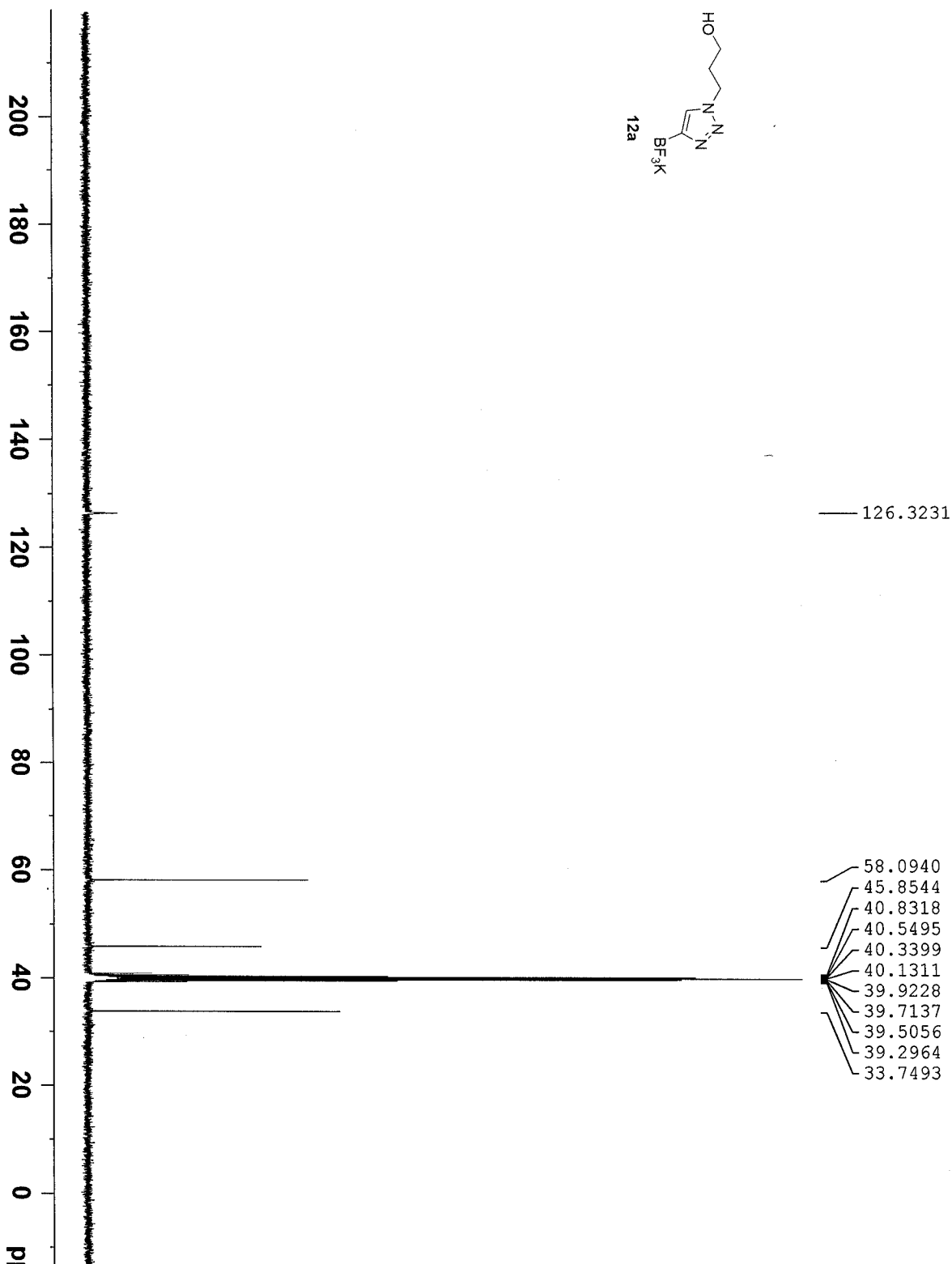
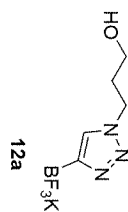
Current Data Parameters
NAME JSH-3-159-p
EXPNO 6
PROCNO 1

F2 - Acquisition Parameters
Date_ 20121016
Time_ 18.59
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 108
DS 4
SWH 24038.461 H
FIDRES 0.366798 H
AQ 1.3631988 s
RG 190.62
DW 20.800 u
DE 6.50 u
TE 299.6 K
D1 2.0000000 s
D11 0.0300000 s
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 10.00 u
PLW1 52.00000000 W
SFO1 100.6429474 M

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

F2 - Processing parameter
SI 32768
CF 100 6000000 M





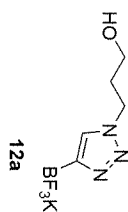
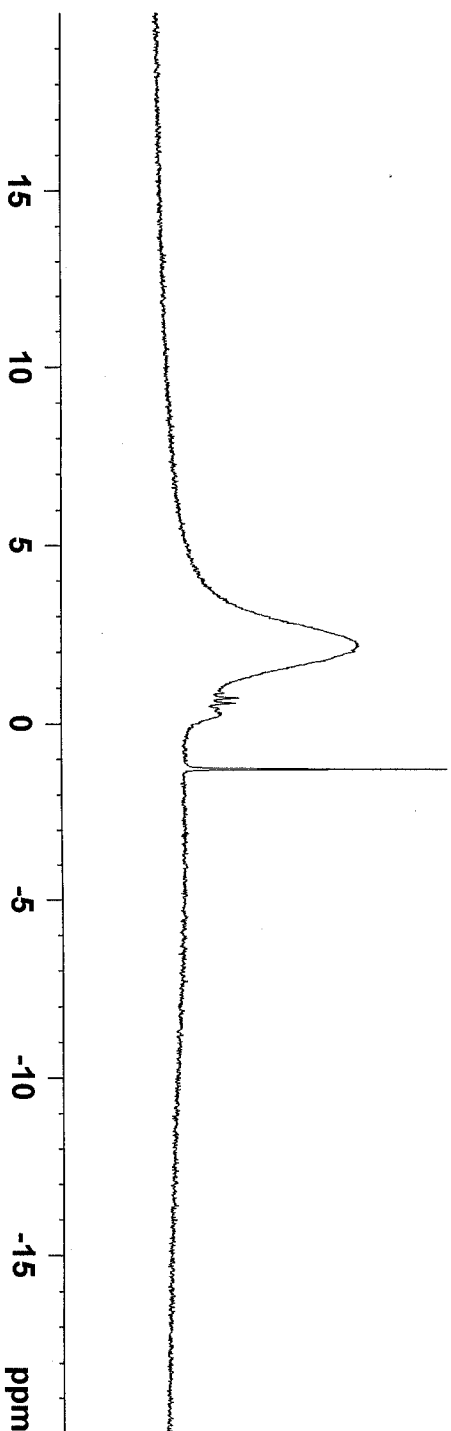
Current Data Parameters
NAME JSH-propanol BF3K
EXPNO 6
PROCNO 1

F2 - Acquisition Parameters
Date_ 20130507
Time 13.30
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 17
DS 4
SWH 25510.203 Hz
FIDRES 0.389255 Hz
AQ 1.2845556 sec
RG 190.62
DW 19.600 usec
DE 6.50 usec
TE 299.4 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 11B
P1 15.00 usec
PLW1 34.20000076 W
SFO1 128.4032720 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 128.4032720 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



2.17
-1.27



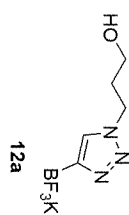
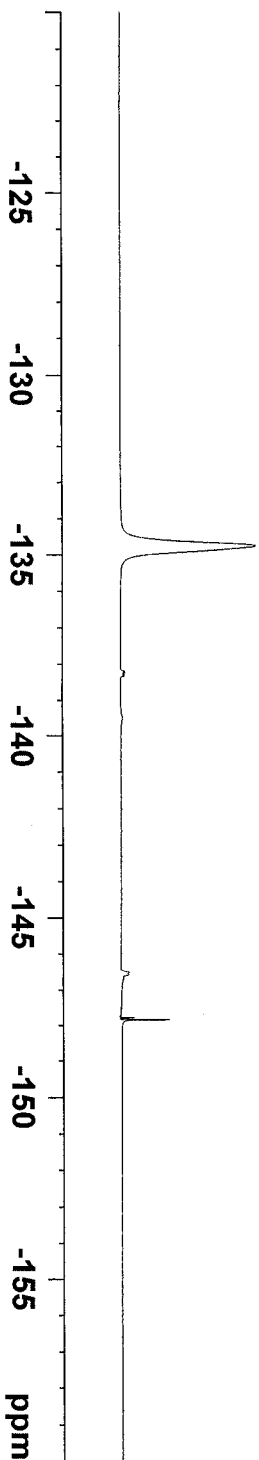
Current Data Parameters
NAME JSH-propanol BF3K
EXPNO 7
PROCNO 1

F2 - Acquisition Parameters
Date_ 20130507
Time 13.33
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgfg
TD 131072
SOLVENT DMSO
NS 16
DS 4
SWH 89285.711 Hz
FIDRES 0.681196 Hz
AQ 0.7340532 sec
RG 190.62
DW 5.600 usec
DE 6.50 usec
TE 299.2 K
D1 1.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 19F
P1 15.00 usec
PLW1 17.00000000 W
SFO1 376.5359841 MHz

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

F2 - Processing parameters
SI 65536
SF 376.5736410 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00





Current Data Parameters
NAME JSH-4-26-p
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters

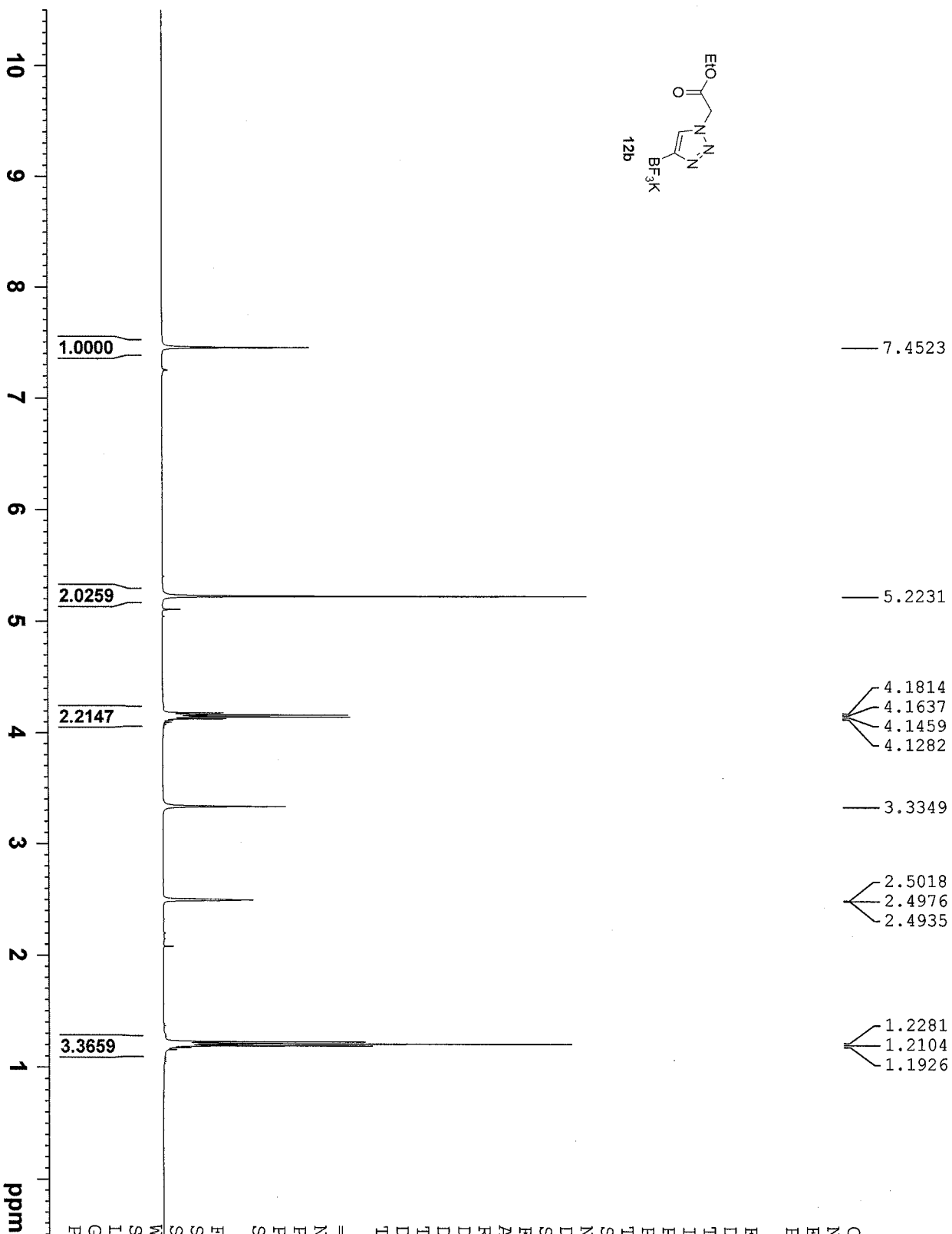
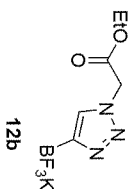
Date_ 20130320
Time 19.52
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 133.17
DW 60.800 usec
DE 6.50 usec
TE 298.6 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====

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

F2 - Processing parameters

SI 65536
SF 400.2100071 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00





Current Data Parameters
NAME JSH-4-26-P
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date_ 20130320

Time 19.54

INSTRUM spect

PROBHD 5 mm PABBO BB/

PULPROG zgpg30

TD 65536

SOLVENT DMSO

NS 489

DS 4

SWH 24038.461 H

FIDRES 0.366798 H

AQ 1.3631988 s

RG 190.62

DW 20.800 u

DE 6.50 u

TE 299.1 K

D1 2.00000000 s

D11 0.03000000 s

TD0 1

===== CHANNEL f1 =====

NUC1 13C

P1 10.00 u

PLW1 52.00000000 W

SFO1 100.6429474 N

===== CHANNEL f2 =====

CPDPRG2 waltz16

NUC2 1H

PCPD2 90.00 u

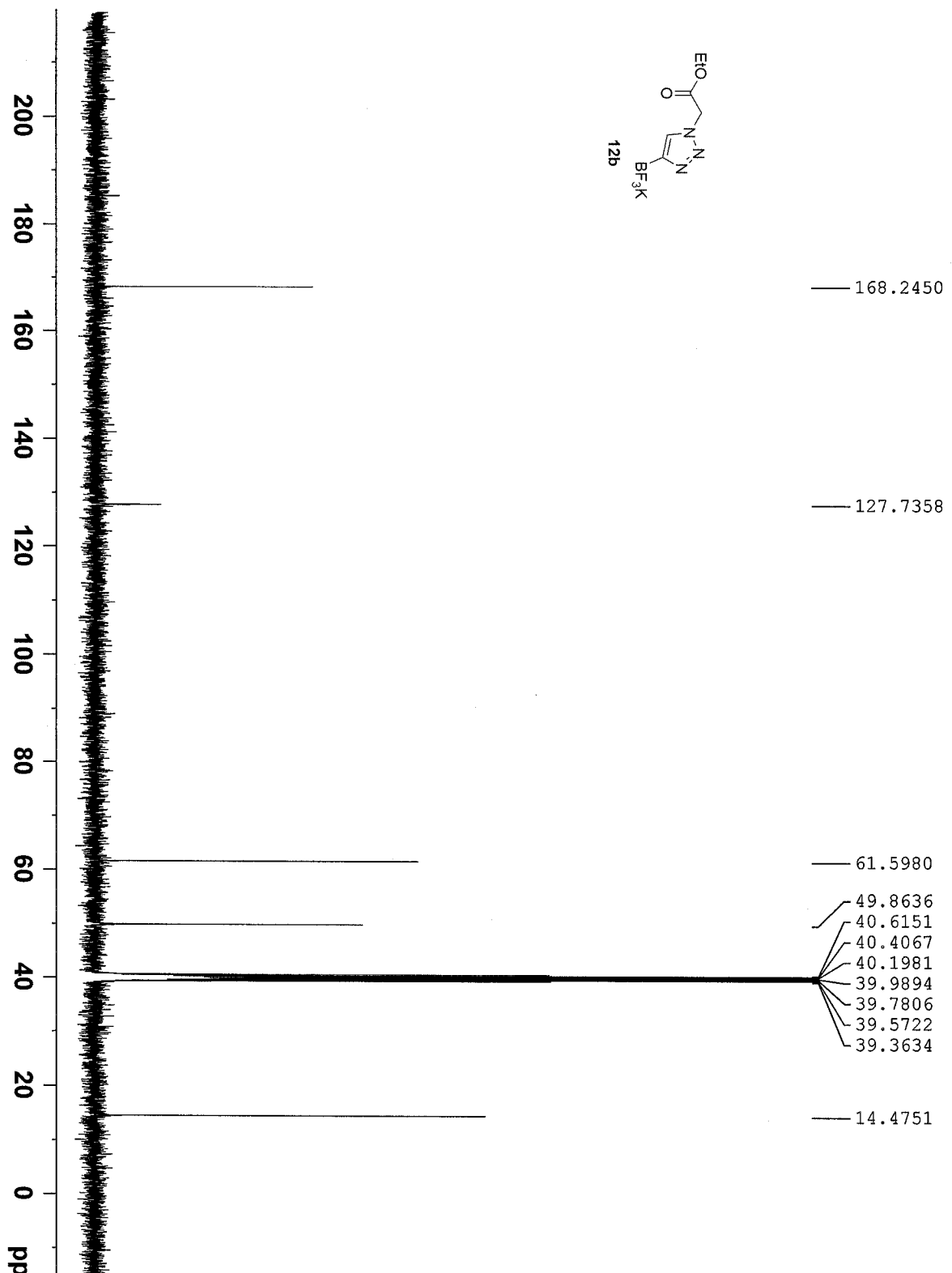
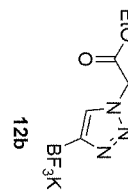
PLW2 12.00000000 W

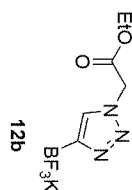
PLW12 0.33333001 W

PLW13 0.27000001 W

SFO2 400.2116008 N

F2 - Processing parameter
SI 32768
FF 100 65536000 N





2.17
-1.28

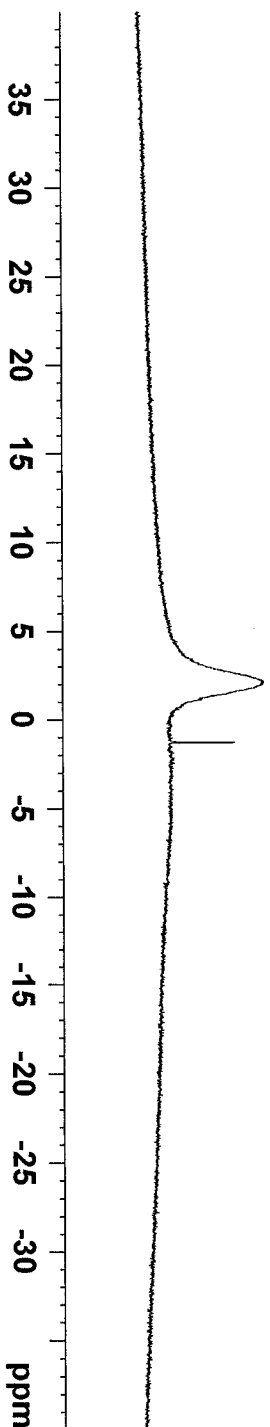
Current Data Parameters
NAME JSH-ethyl acetate BF3K
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20130501
Time 22.11
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 21
DS 4
SWH 25510.203 Hz
FIDRES 0.389255 Hz
AQ 1.2845556 sec
RG 190.62
DW 19.600 usec
DE 6.50 usec
TE 299.7 K
D1 2.00000000 sec
D11 0.03000000 sec
TDO 1

===== CHANNEL f1 =====
NUC1 11B
P1 15.00 usec
PLW1 34.20000076 W
SFO1 128.4032720 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 128.4032720 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40





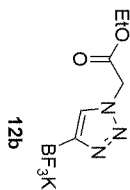
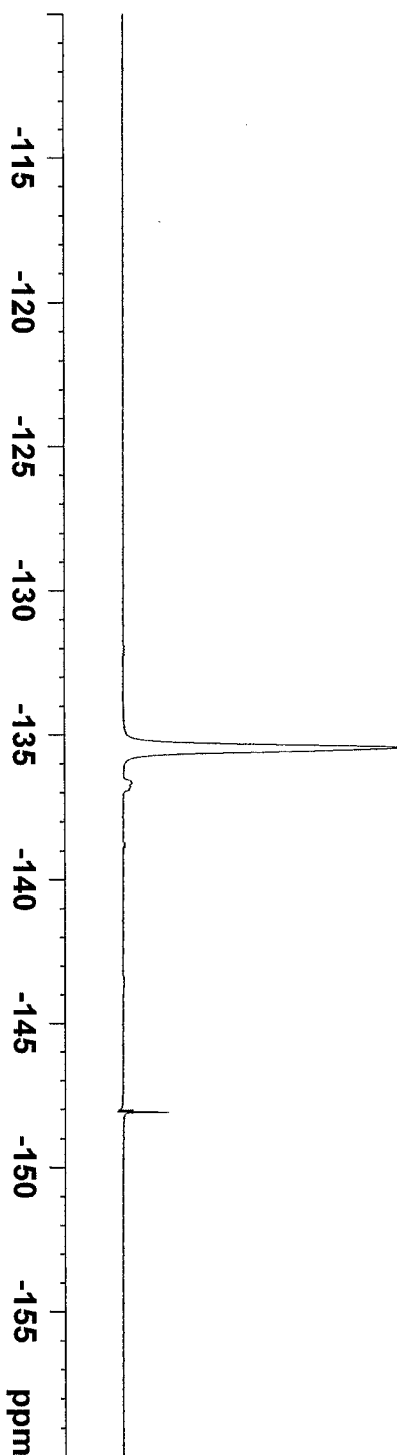
Current Data Parameters
 NAME JSH-ethyl acetate BF3K
 EXPNO 3
 PROCNO 1

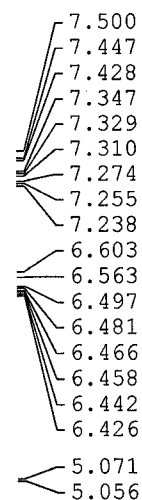
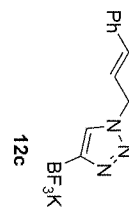
F2 - Acquisition Parameters
 Date_ 20130501
 Time 22.15
 INSTRUM spect
 PROBD 5 mm PABBO BB/
 PULPROG zgfg
 TD 131072
 SOLVENT DMSO
 NS 16
 DS 4
 SWH 89285.711 Hz
 FIDRES 0.681196 Hz
 AQ 0.7340532 sec
 RG 190.62
 DW 5.600 usec
 DE 6.50 usec
 TE 299.5 K
 D1 1.00000000 sec
 D11 0.03000000 sec
 D12 0.00002000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 19F
 P1 15.00 usec
 PLW1 17.00000000 W
 SFO1 376.5359841 MHz

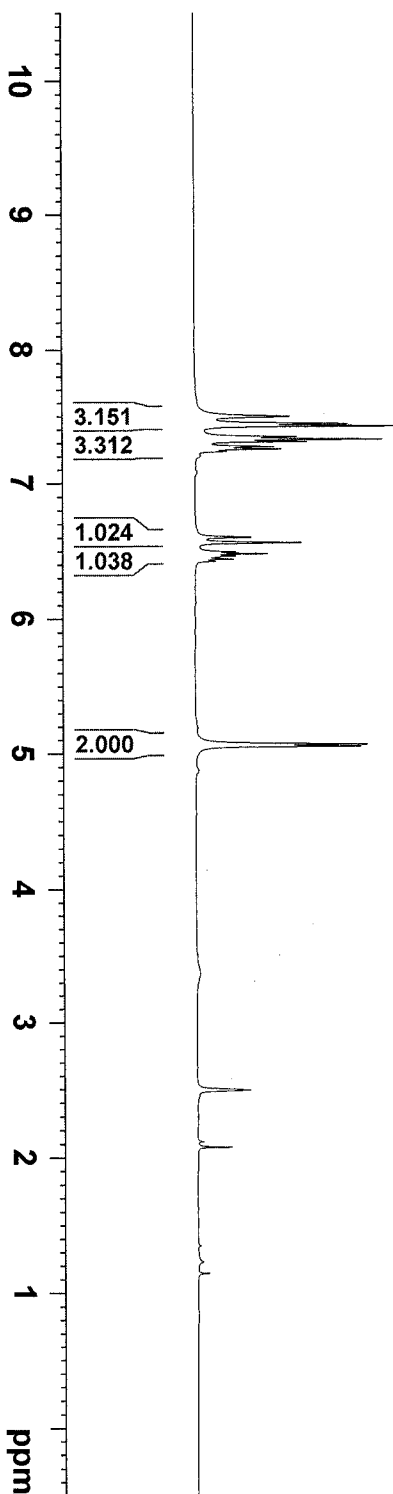
===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 90.00 usec
 PLW2 12.00000000 W
 PLW12 0.33333001 W
 SFO2 400.2116008 MHz

F2 - Processing parameters
 SI 65536
 SF 376.5736410 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00





— 2.498
— 2.079

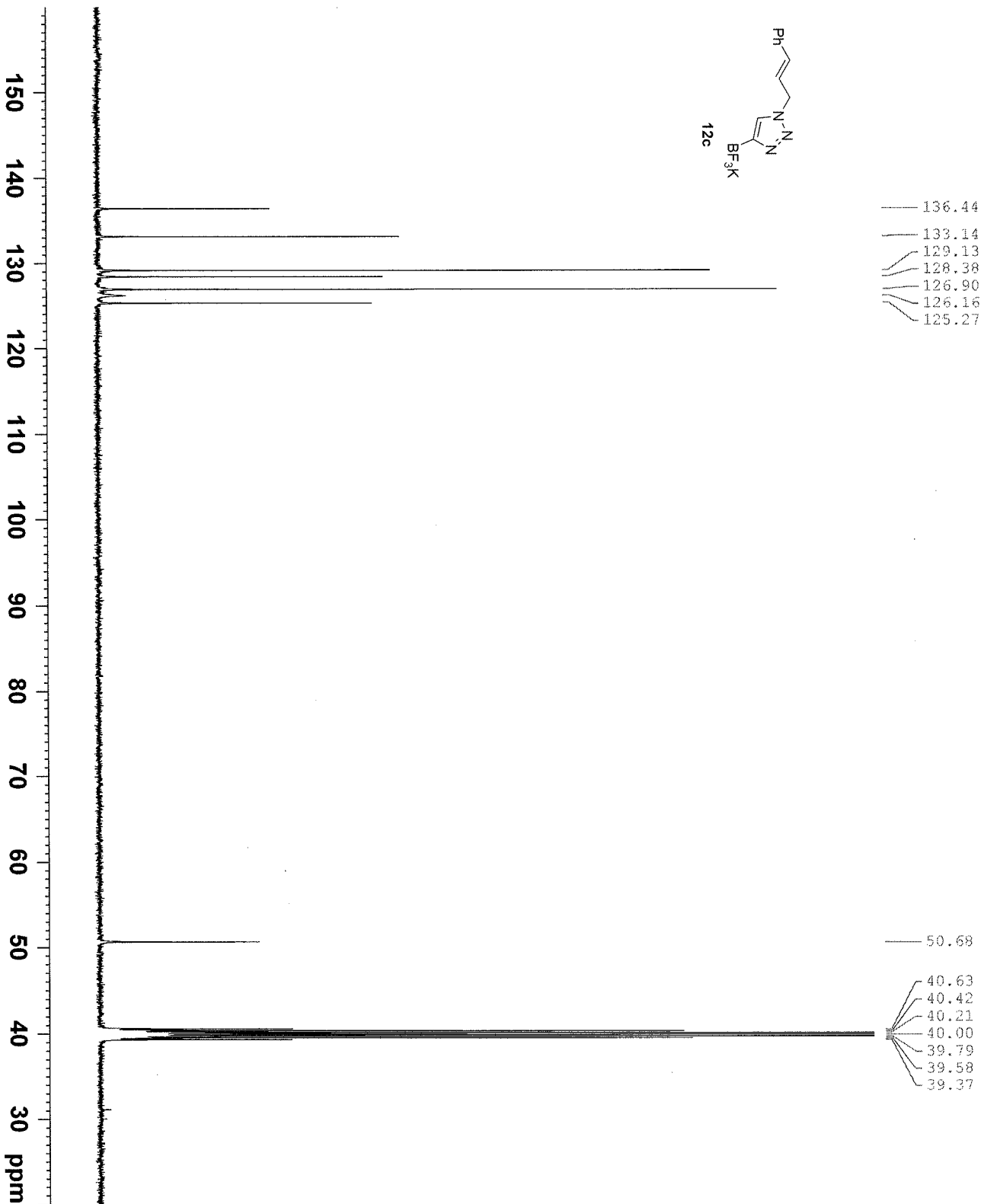
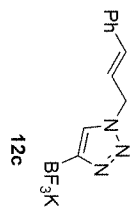


Current Data Parameters
NAME JSH-cinamy1 BF3K
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20130505
Time_ 22.05
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
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 300.1 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 400.2100065 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



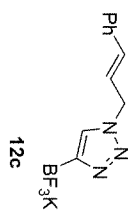
Current Data Parameters
NAME JSH-cinamyl BF3K
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date_ 20130505
Time_ 22.12
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 907
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 300.3 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1

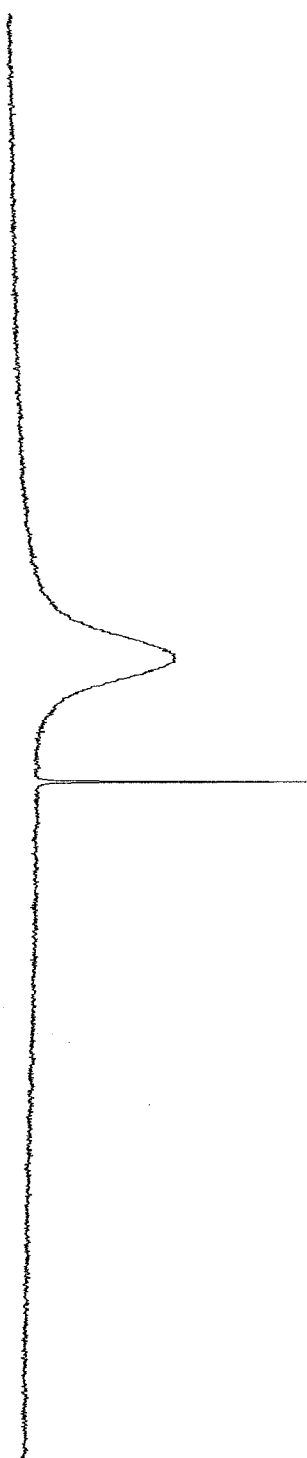
===== CHANNEL f1 =====
NUC1 13C
P1 10.00 usec
PLW1 52.0000000 W
SFO1 100.6429474 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
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 100.6328860 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



2.14
-1.25



Current Data Parameters
NAME JSH-cinamyl BF3K
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20130505
Time 22.01
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 14
DS 4
SWH 25510.203 Hz
FIDRES 0.389255 Hz
AQ 1.2845556 sec
RG 190.62
DW 19.600 usec
DE 6.50 usec
TE 300.6 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 11B
P1 15.00 usec
PLM1 34.20000076 W
SFO1 128.4032720 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 128.4032720 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



Current Data Parameters
NAME JSH-clnamyl BF3K
EXPNO 1
PROCNO 1

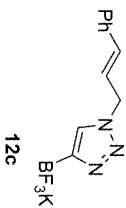
F2 - Acquisition Parameters
Date_ 20130505
Time_ 21.58
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgfg
TD 131072
SOLVENT DMSO
NS 16
DS 4
SWH 89285.711 Hz
FIDRES 0.681196 Hz
AQ 0.7340532 sec
RG 190.62
DW 5.600 usec
DE 6.50 usec
TE 300.3 K
D1 1.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 19F
P1 15.00 usec
PLW1 17.00000000 W
SFO1 376.5359841 MHz

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

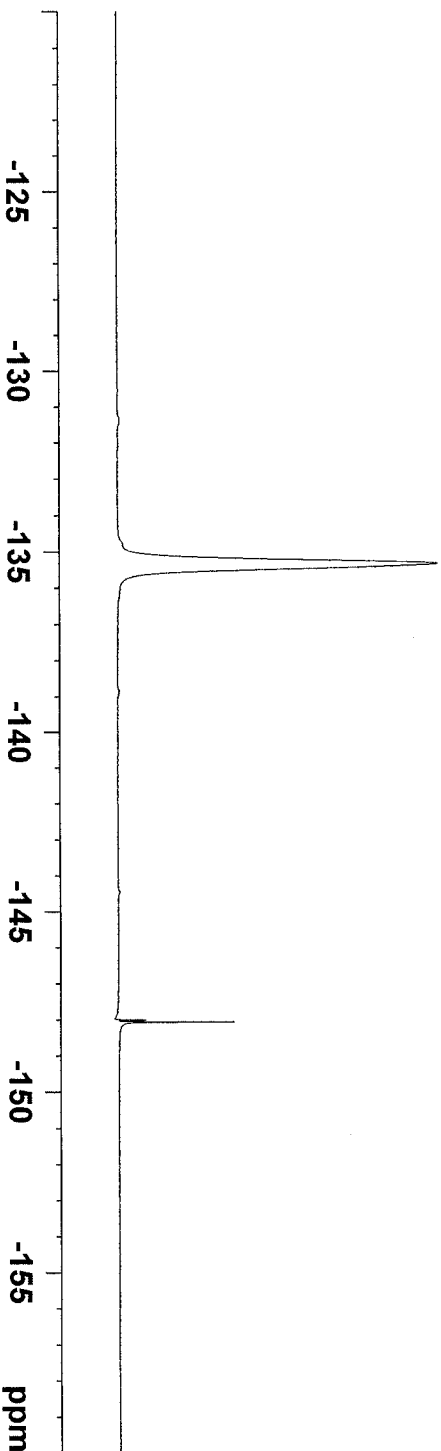
F2 - Processing parameters

SI 65536
SF 376.5736410 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



135.31

148.06



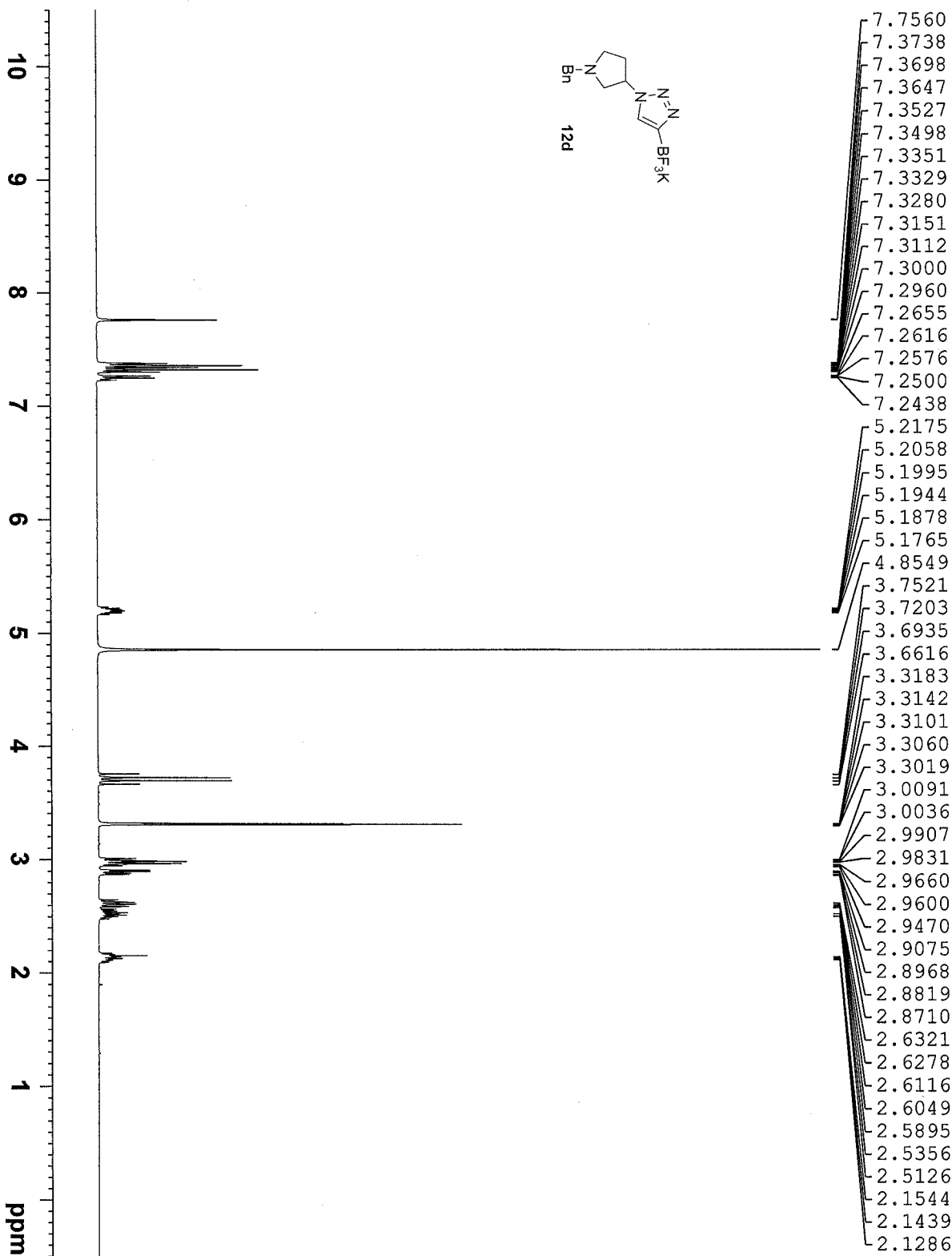
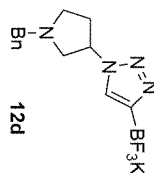


Current Data Parameters
NAME JSH-3-95-P
EXPNO 6
PROCNO 1

F2 - Acquisition Parameters
Date_ 20120725
Time 16.10
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 146.31
DW 60.800 usec
DE 6.50 usec
TE 298.3 K
D1 1.0000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 15.00 usec
PLW1 12.0000000 W
SFO1 400.2124715 MHz

F2 - Processing parameters
SI 65536
SF 400.2100110 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00





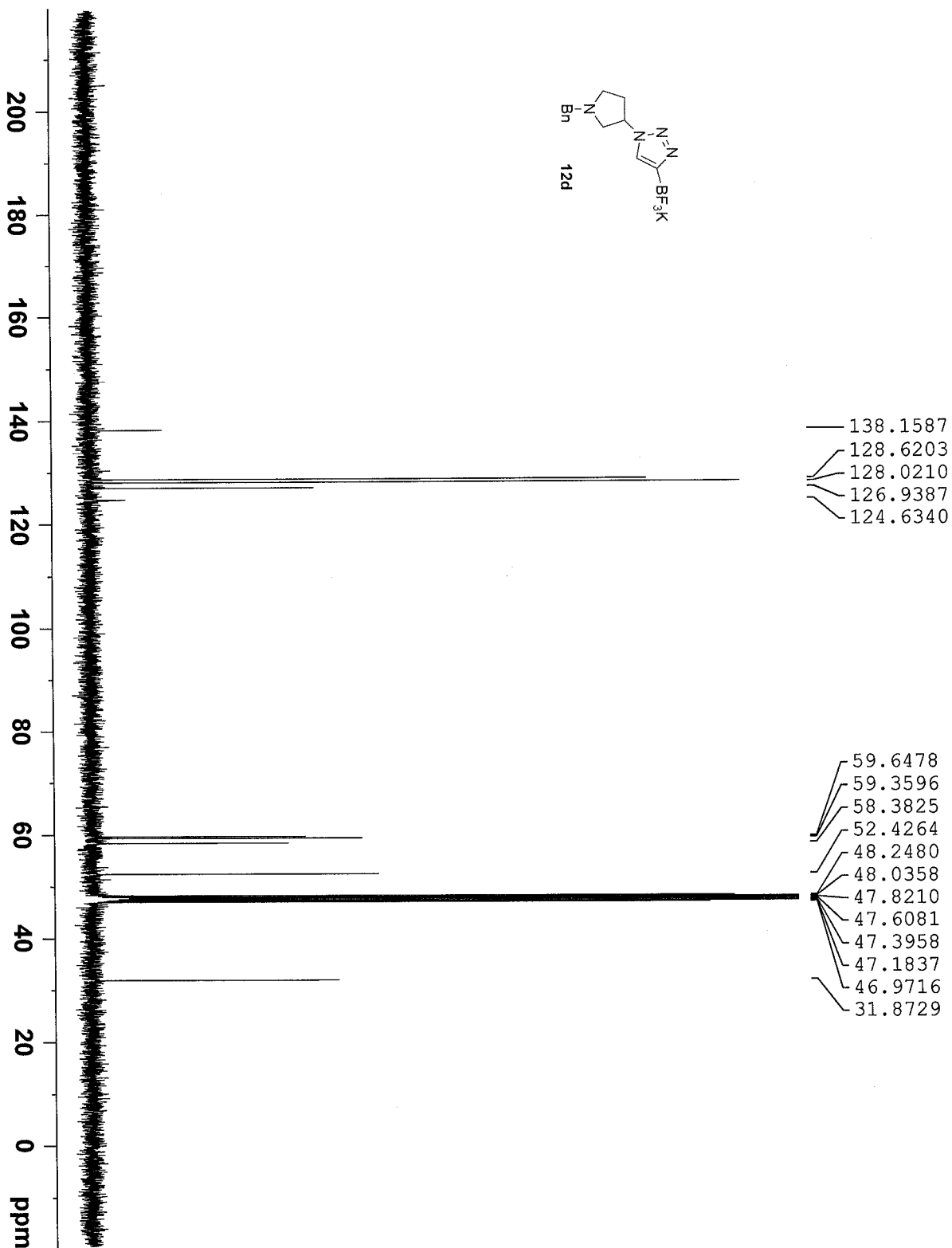
Current Data Parameters
NAME JSH-3-101-p
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date_ 20120731
Time 14.38
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT MeOD
NS 516
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 2.0000000 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
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





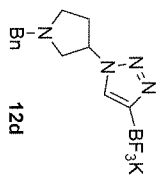
Current Data Parameters
NAME USH-benzylpyrrolidine BF3K
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20130502
Time_ 16.36
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 30
DS 4
SWH 25510.203 Hz
FIDRES 0.389255 Hz
AQ 1.2845536 sec
RG 190.62
DW 19.600 usec
DE 6.50 usec
TE 299.5 K
D1 2.0000000 sec
D11 0.03000000 sec
TD0 1

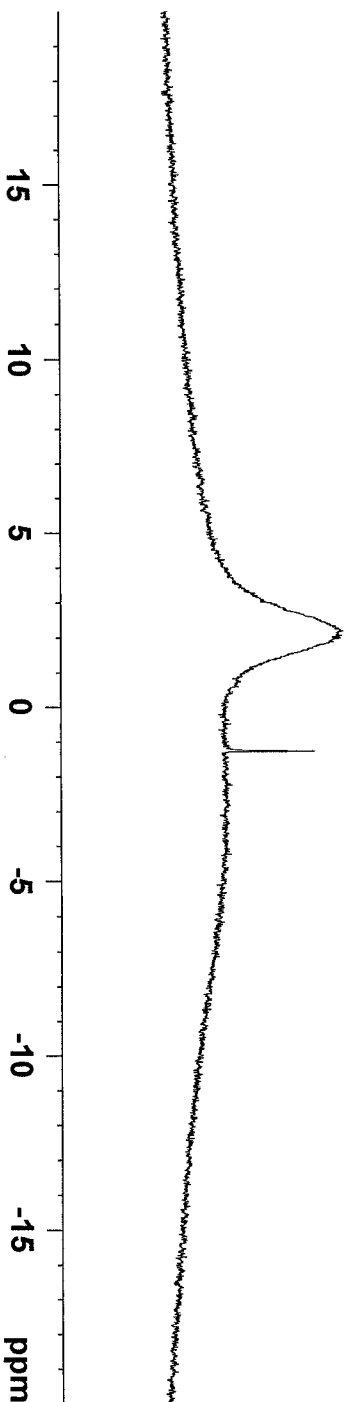
===== CHANNEL f1 =====
NUC1 11B
P1 15.00 usec
PLW1 34.20000076 W
SFO1 128.4032720 MHz

===== 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 128.4032720 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



2.19
-1.27





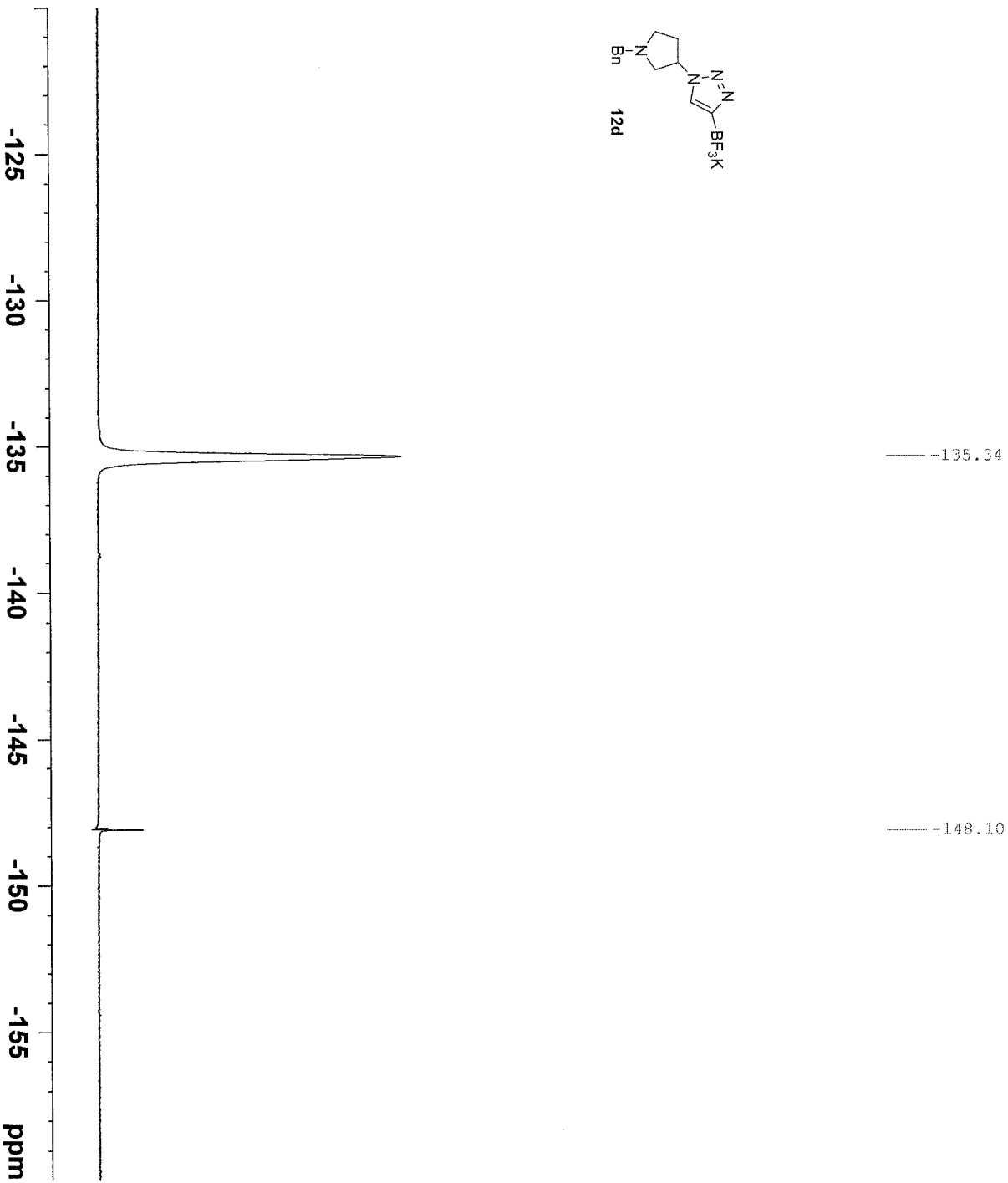
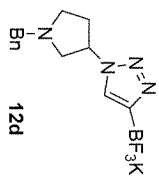
Current Data Parameters
NAME JSH-benzylpyrrolidine BF3K
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20130502
Time_ 16.33
INSTRUM spect
PROBHD 5 mm PABO BB/
PULPROG zgpg30
TD 131072
SOLVENT DMSO
NS 16
DS 4
SWH 89285.711 Hz
FIDRES 0.681196 Hz
AQ 0.7340532 sec
RG 190.62
DW 5.600 usec
DE 6.50 usec
TE 299.6 K
D1 1.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 19F
P1 15.00 usec
PLW1 17.00000000 W
SFO1 376.5359841 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 12.00000000 W
PLM12 0.33333001 W
SFO2 400.2116008 MHz

F2 - Processing parameters
SI 65536
SF 376.5736410 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



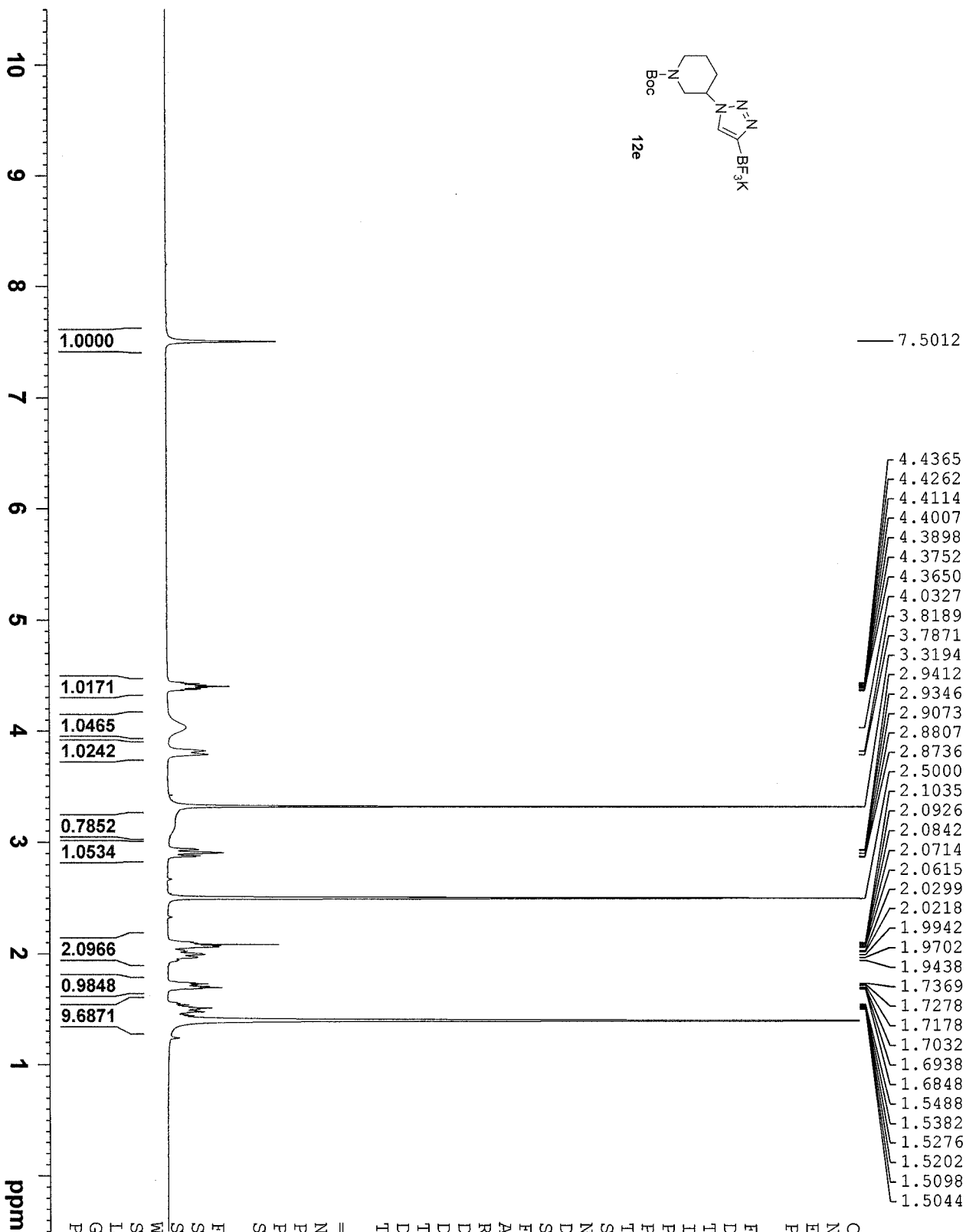


Current Data Parameters
NAME JSH-3-149-p
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20121010
Time 20.35
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
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 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 400.210063 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00





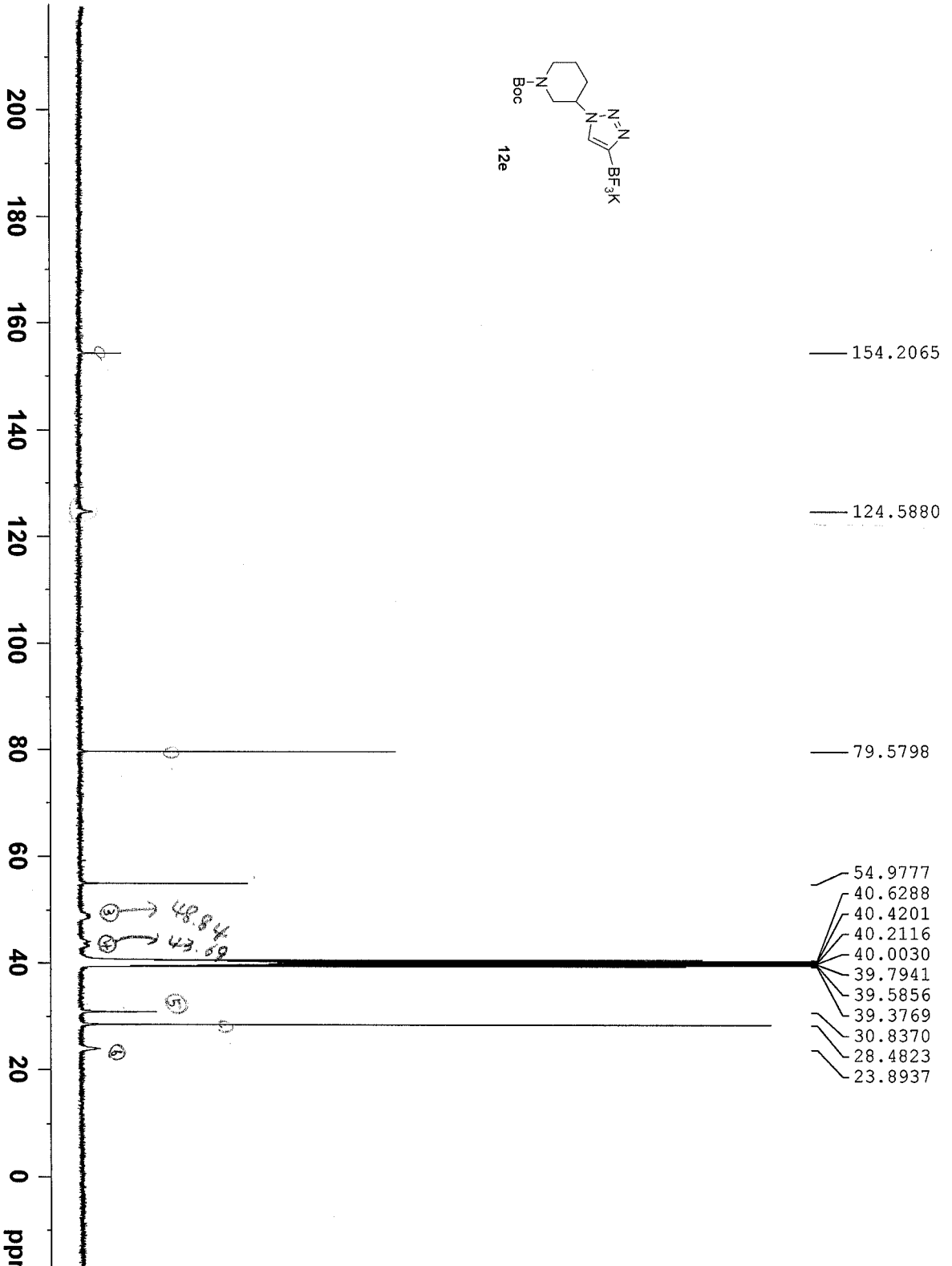
Current Data Parameters
NAME JSH-3-149-p
EXPNO 6
PROCNO 1

F2 - Acquisition Parameters
Date_ 20121010
Time 21.13
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 12477
DS 4
SWH 24038.461 H
FIDRES 0.366798 H
AQ 1.3631988 s
RG 190.62
DW 20.800 u
DE 6.50 u
TE 299.9 K
D1 2.0000000 s
D11 0.0300000 s
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 10.00 u
PLW1 52.00000000 W
SFO1 100.6429474 N

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

F2 - Processing parameter
SI 32768
SF 100.6260600 N





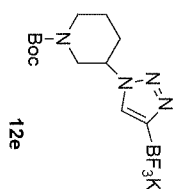
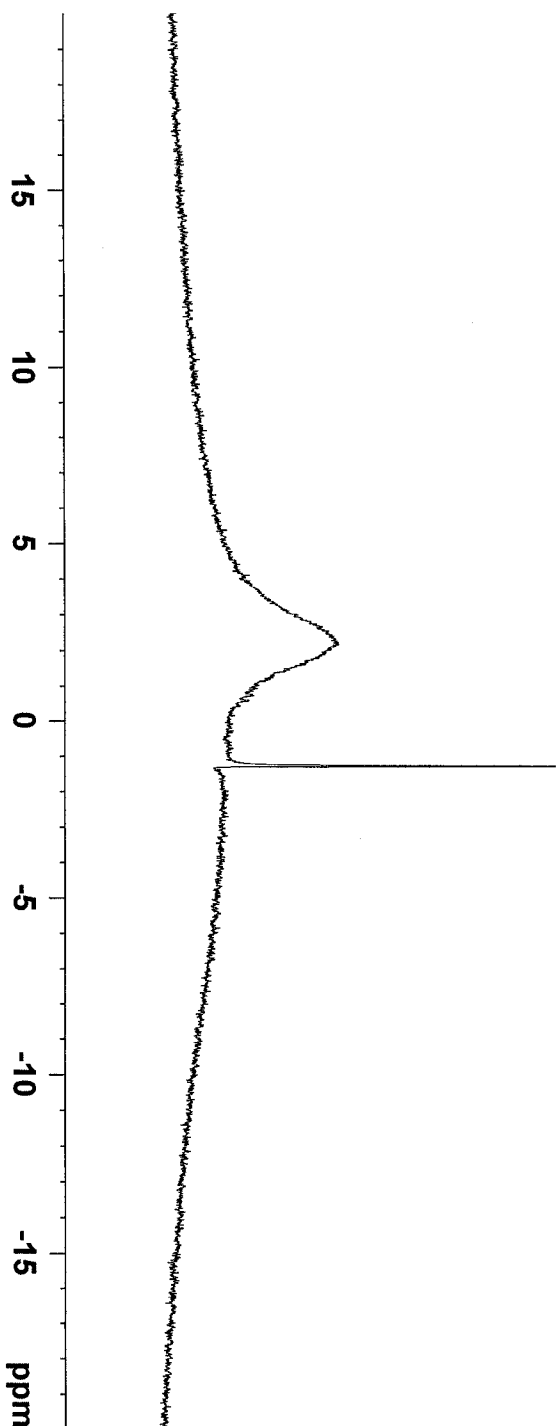
Current Data Parameters
NAME JSH-Boc piperidine BF3K
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20130502
Time 16.55
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 22
DS 4
SWH 25510.203 Hz
FIDRES 0.389255 Hz
AQ 1.2845556 sec
RG 190.62
DW 19.600 usec
DE 6.50 usec
TE 299.4 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 11B
P1 15.00 usec
PLW1 34.20000076 W
SFO1 128.4032720 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 128.4032720 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



2.17
-1.28



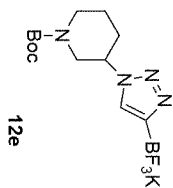
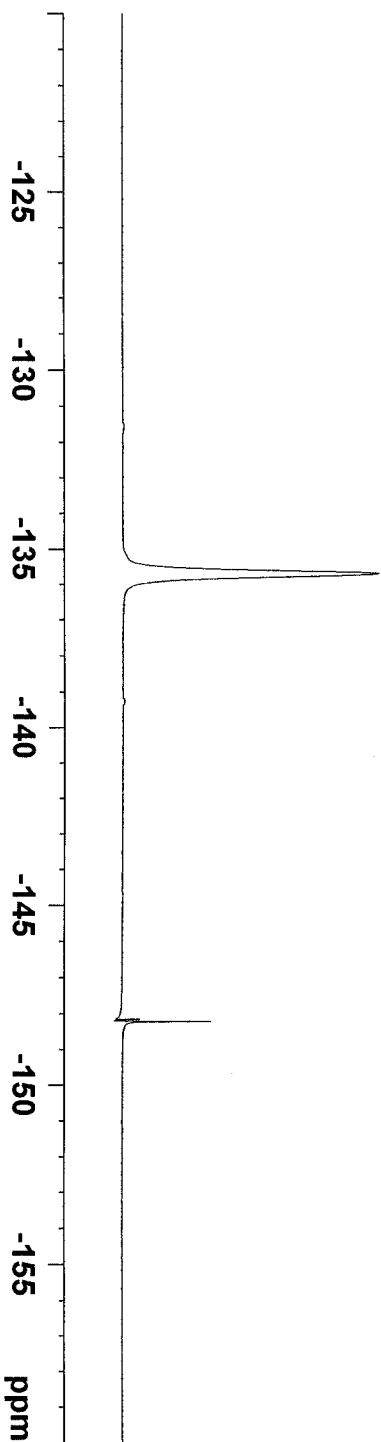
Current Data Parameters
NAME JSH-Boc piperidine BF3K
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20130502
Time 16.52
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgfh1gqn.2
TD 131072
SOLVENT DMSO
NS 16
DS 4
SWH 89285.711 Hz
FIDRES 0.681196 Hz
AQ 0.7340532 sec
RG 190.62
DM 5.600 usec
DE 6.50 usec
TE 299.5 K
D1 1.00000000 sec
D11 0.03000000 sec
D12 0.0002000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 19F
P1 15.00 usec
PLW1 17.00000000 W
SFO1 376.5359841 MHz

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

F2 - Processing parameters
SI 65536
SF 376.5736410 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00





Current Data Parameters
NAME JSH-3-157-p
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters

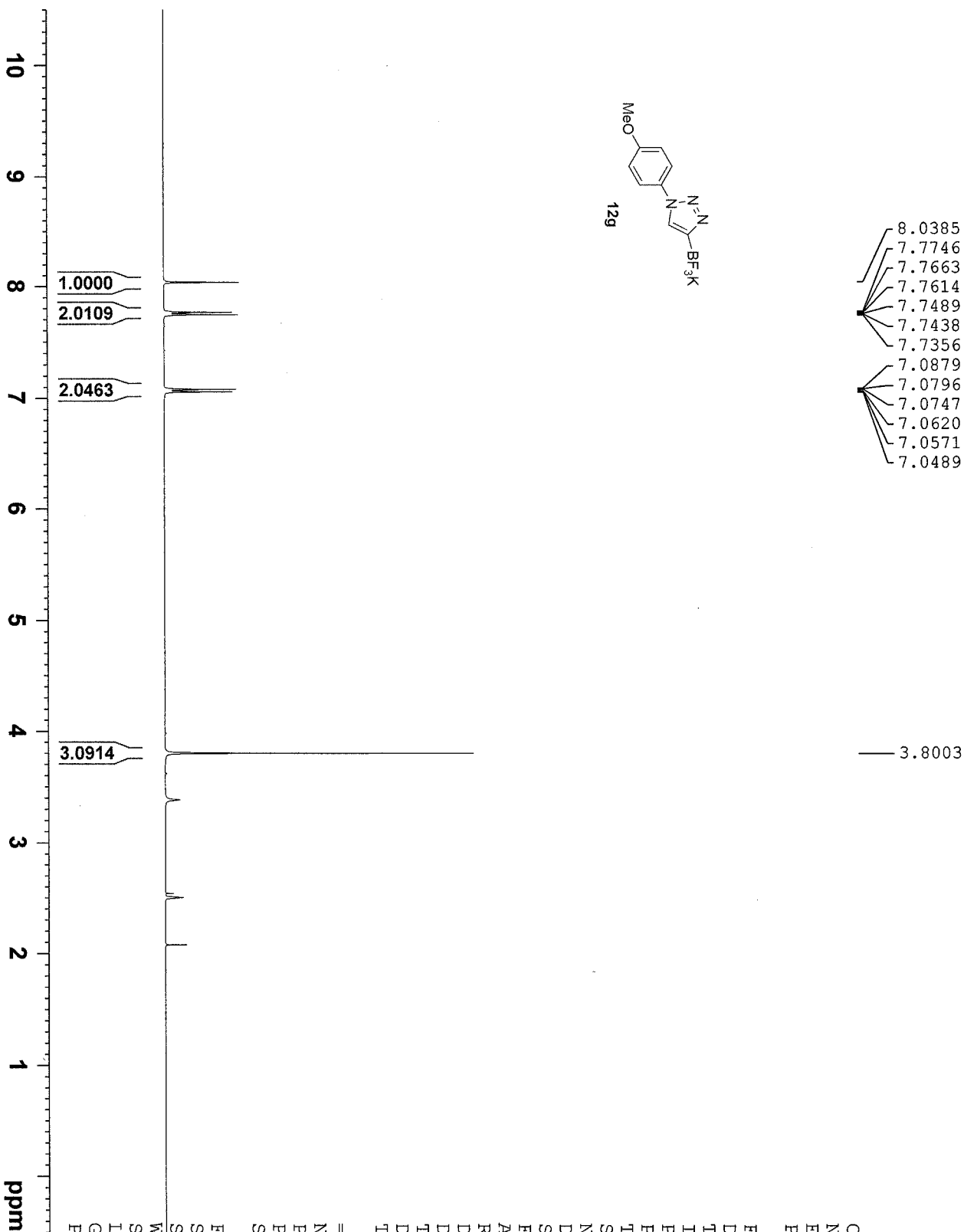
Date_ 20121016
Time_ 13.22
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 5
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 91.91
DW 60.800 usec
DE 6.50 usec
TE 299.2 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====

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

F2 - Processing parameters

SI 65536
SF 400.2100062 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00





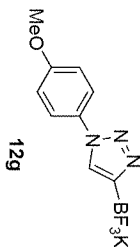
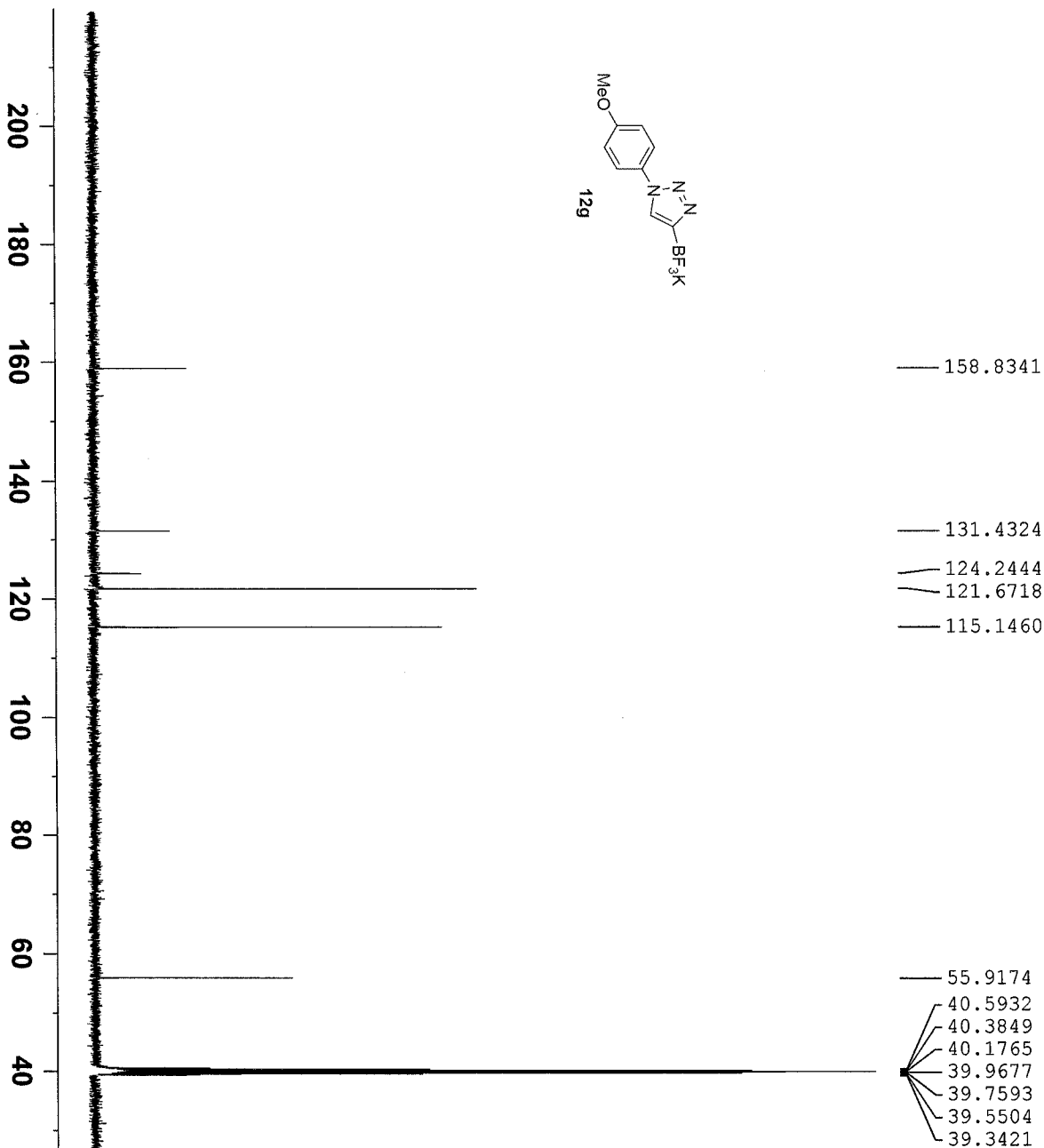
Current Data Parameters
NAME JSH-3-157-p
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date_ 20121016
Time_ 13.25
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 70
DS 4
SWH 24038.461 H
FIDRES 0.366798 H
AQ 1.3631988 s
RG 190.62
DW 20.800 u
DE 6.50 u
TE 299.9 K
D1 2.00000000 s
D11 0.03000000 s
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 10.00 u
PLW1 52.00000000 W
SFO1 100.6429474 M

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 u
PLW2 12.00000000 W
PLM12 0.33333001 W
PLM13 0.270000001 W
SFO2 400.2116008 M

F2 - Processing parameter
SI 32768
SF 100.6260600 M





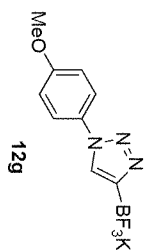
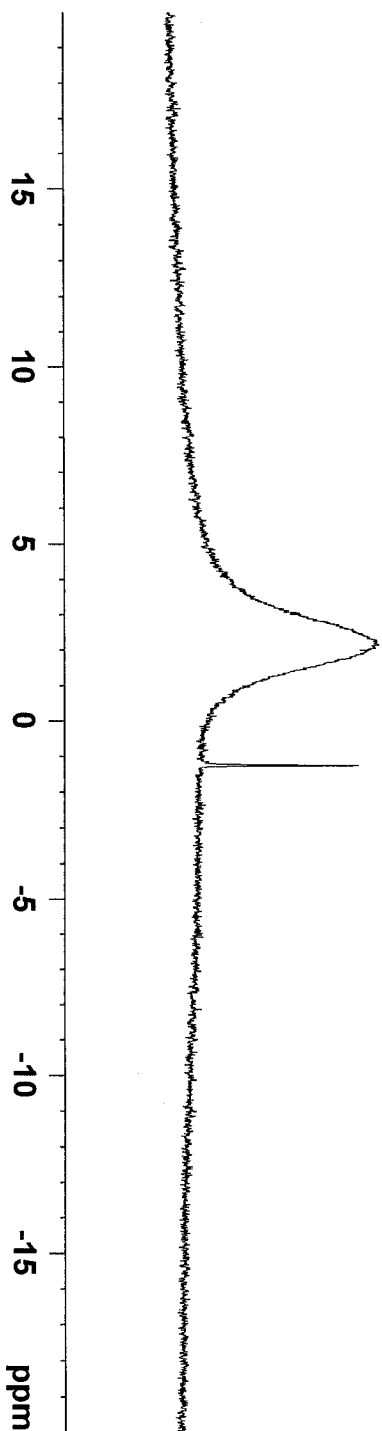
Current Data Parameters
NAME JSH-methoxybenzene BF3K
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20130505
Time 21.51
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 11
DS 4
SWH 25510.203 Hz
FIDRES 0.389255 Hz
AQ 1.2845556 sec
RG 190.62
DW 19.600 usec
DE 6.50 usec
TE 300.4 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

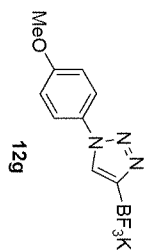
===== CHANNEL f1 =====
NUC1 11B
P1 15.00 usec
PLW1 34.20000076 W
SFO1 128.4032720 MHz

===== 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 128.4032720 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



2.15
-1.25



-134.99

-147.83

Current Data Parameters
NAME JSH-methoxybenzene BF3K
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters

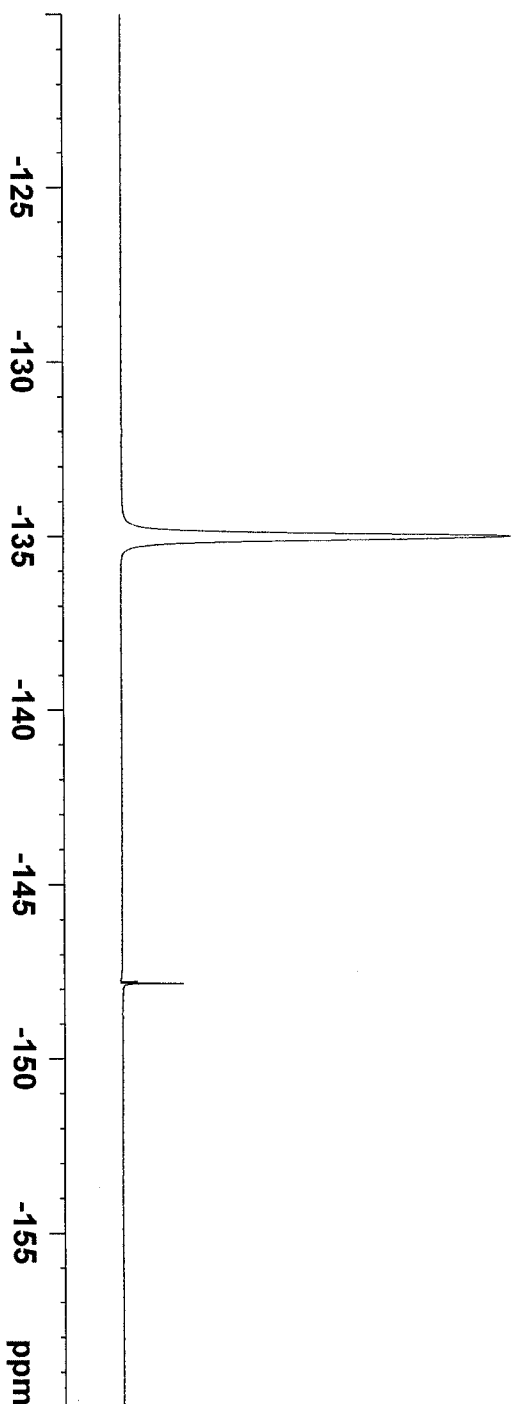
Date_ 20130505
Time_ 21.54
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgfhgpn.2
TD 131072
SOLVENT DMSO
NS 16
DS 4
SWH 89285.711 Hz
FIDRES 0.681196 Hz
AQ 0.7340532 sec
RG 190.62
DE 5.600 usec
TE 300.4 K
D1 1.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 19F
P1 15.00 usec
PLW1 17.00000000 W
SFO1 376.5359841 MHz

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

F2 - Processing parameters

SI 65536
SF 376.5736410 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00





Current Data Parameters
NAME JSB-4-1-p
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date_ 20130305
Time 11.15
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 9
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 146.31
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

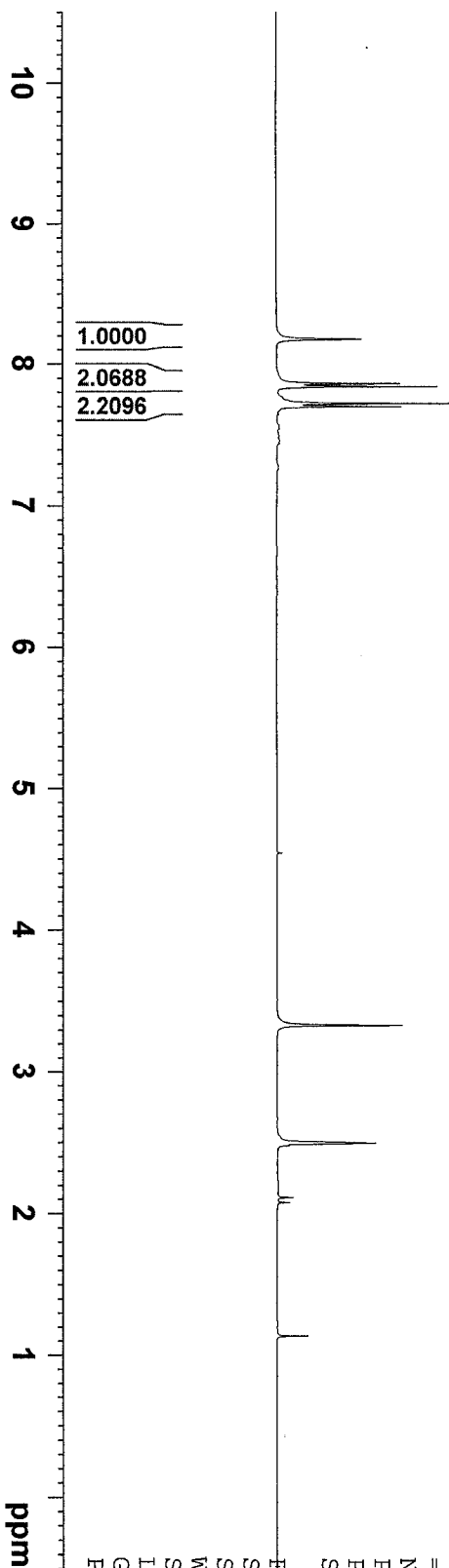
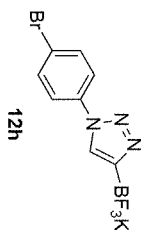
F2 - Processing parameters
SI 65536
SF 400.2100063 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

8.1766
7.8623
7.8403
7.7237
7.7016

3.3365

2.5034
2.4993
2.4953
2.4804
2.1146
2.0795

1.1388





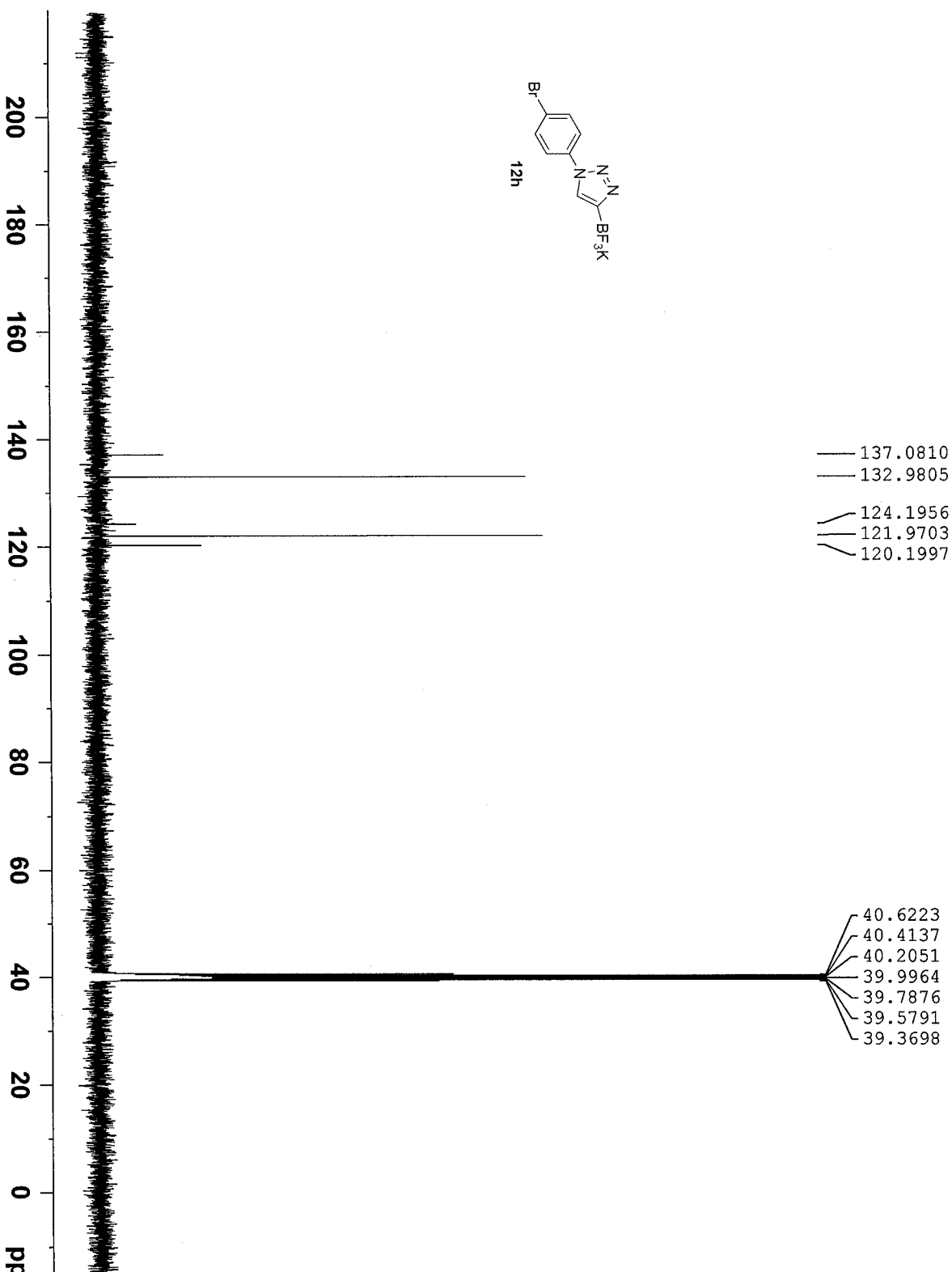
Current Data Parameters
NAME JSH-4-1-P
EXPNO 5
PROCNO 1

F2 - Acquisition Parameters
Date_ 20130305
Time 11.16
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 249
DS 4
SWH 24038.461 H
FIDRES 0.366798 H
AQ 1.3631988 s
RG 190.62
DW 20.800 u
DE 6.50 u
TE 299.2 K
D1 2.0000000 s
D11 0.0300000 s
TD0 1

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

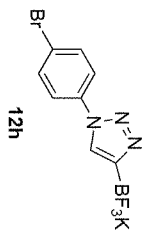
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 u
PLW2 12.00000000 W
PLW12 0.33333001 W
PLW13 0.27000001 W
SFO2 400.2116008 W

F2 - Processing parameter
SI 32768
CT 100000000 W



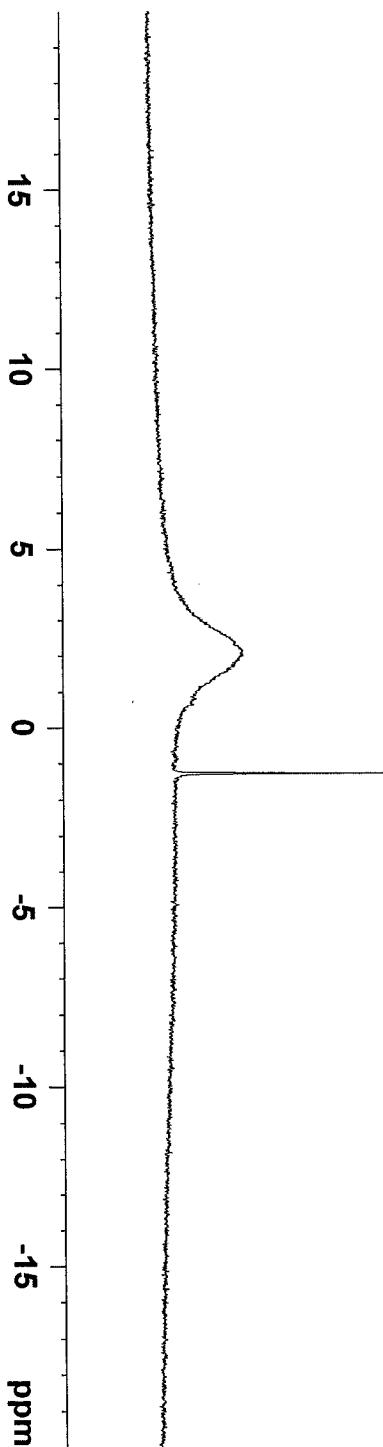
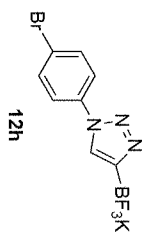
137.0810
132.9805
124.1956
121.9703
120.1997

40.6223
40.4137
40.2051
39.9964
39.7876
39.5791
39.3698





2.15
-1.27



Current Data Parameters
NAME JSH-4-bromophenyl BF3K
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20130501
Time 22.30
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 15
DS 4
SWH 25510.203 Hz
FIDRES 0.389255 Hz
AQ 1.2845556 sec
RG 190.62
DW 19.600 usec
DE 6.50 usec
TE 299.7 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 11B
P1 15.00 usec
PLW1 34.20000076 W
SFO1 128.4032720 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 128.4032720 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



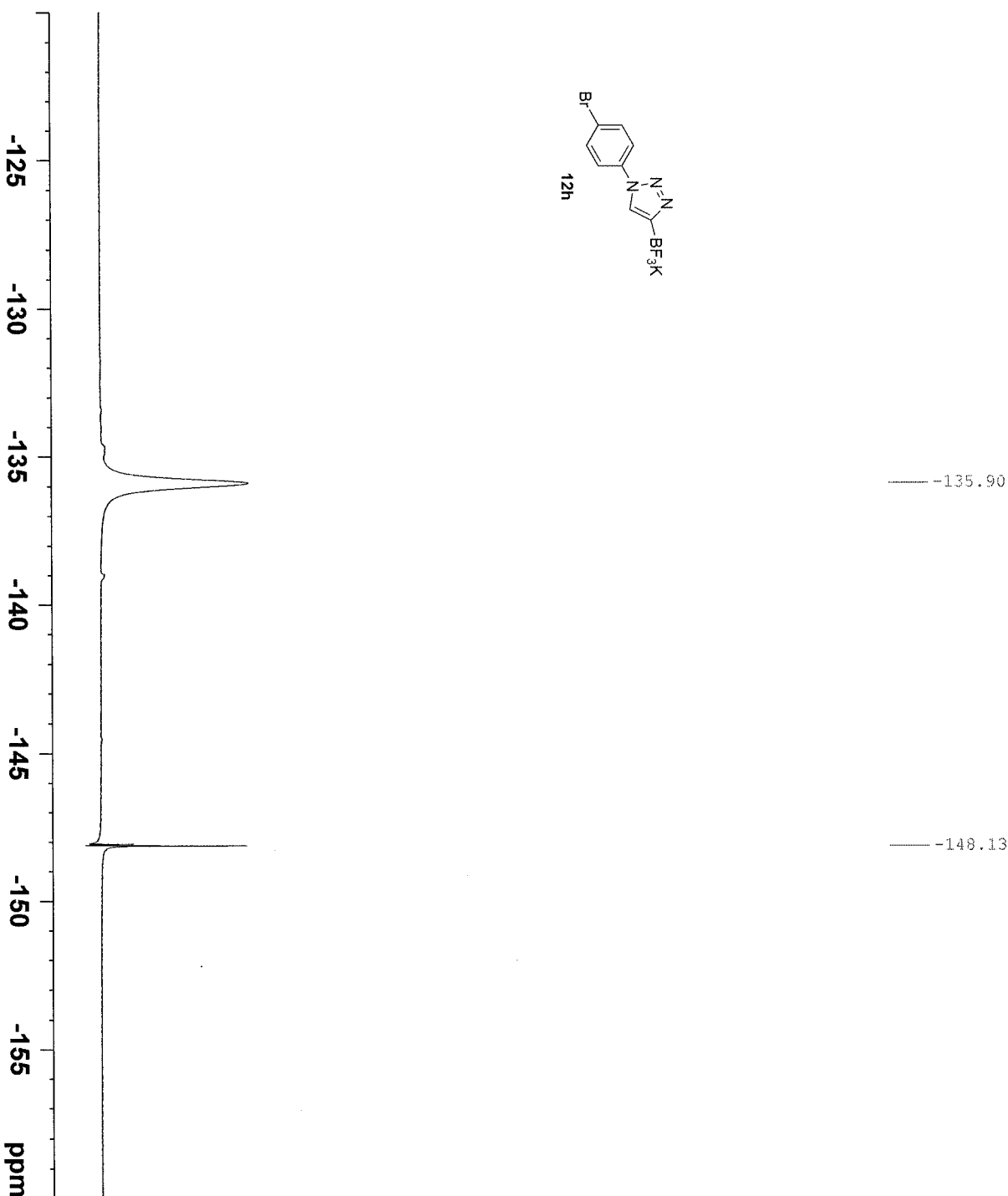
Current Data Parameters
NAME JSH-4-bromophenyl BF3K
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20130501
Time 22.33
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 131072
SOLVENT DMSO
NS 16
DS 4
SWH 89285.711 Hz
FIDRES 0.681196 Hz
AQ 0.7340532 sec
RG 190.62
DW 5.600 usec
DE 6.50 usec
TE 299.6 K
D1 1.00000000 sec
D11 0.03000000 sec
D12 0.0002000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 19F
P1 15.00 usec
PLW1 17.00000000 W
SFO1 376.5359841 MHz

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

F2 - Processing parameters
SI 65536
SF 376.5736410 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00





Current Data Parameters
NAME JSH-4-18-P
EXPNO 6
PROCNO 1

F2 - Acquisition Parameters

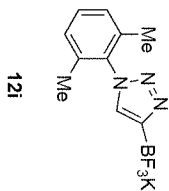
Date_ 20130308
Time 12.54
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 11
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 103.95
DW 60.800 usec
DE 6.50 usec
TE 297.9 K
D1 1.0000000 sec
TD0 1

===== CHANNEL f1 =====

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

F2 - Processing parameters

SI 65536
SF 400.2100061 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



7.5622
7.3374
7.3180
7.2998
7.2329
7.2141

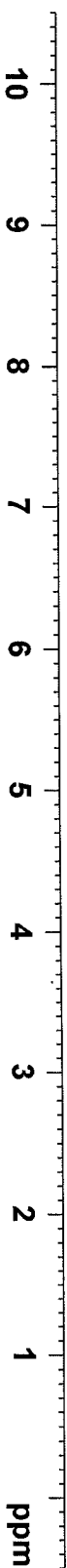
3.3440

2.4997

1.8750

1.0000
1.0473
2.0772

6.2539





Current Data Parameters
NAME JSH-4-18-P
EXPNO 7
PROCNO 1

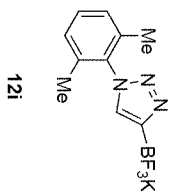
F2 - Acquisition Parameters

Date_ 20130308
Time 12.55
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 112
DS 4
SWH 24038.461 H
FIDRES 0.366798 H
AQ 1.3631988 s
RG 190.62
DW 20.800 u
DE 6.50 u
TE 298.3 K
D1 2.0000000 s
D11 0.0300000 s
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 10.00 u
PLW1 52.00000000 W
SFO1 100.6429474 N

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

F2 - Processing parameter
SI 32768
CF 100000000 W



200 180 160 140 120 100 80 60 40 20 0 ppm

137.3380
135.3320
129.4953
128.5373
127.6639

40.6046
40.3966
40.1878
39.9793
39.7707
39.5621
39.3538

17.4631



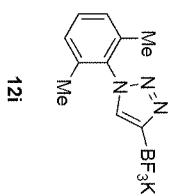
Current Data Parameters
NAME JSH-2,6-dimethylphenyl BF3K
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20130504
Time 21.26
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 30
DS 4
SWH 25510.203 Hz
FIDRES 0.389255 Hz
AQ 1.2845556 sec
RG 190.62
DM 19.600 usec
DE 6.50 usec
TE 300.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 11B
P1 15.00 usec
PLM1 34.20000076 W
SFO1 128.4032720 MHz

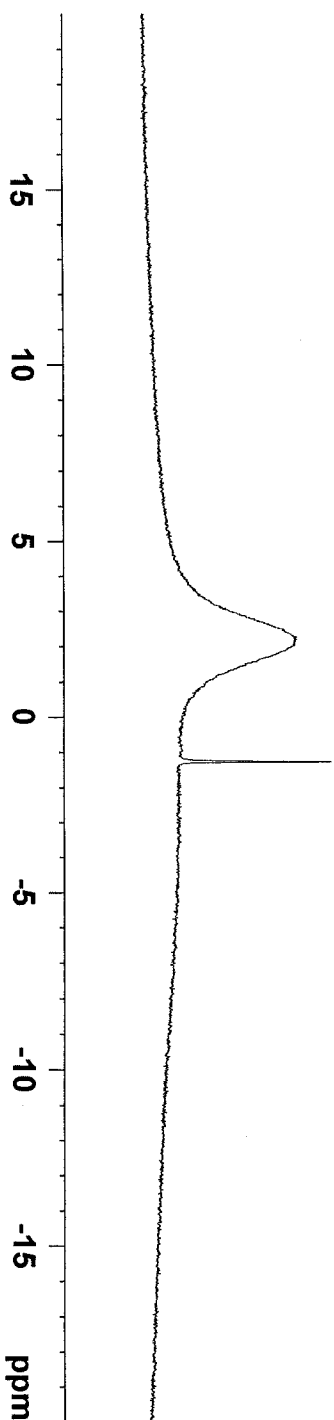
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PLM2 12.00000000 W
PLM12 0.333333001 W
PLM13 0.270000001 W
SFO2 400.2116008 MHz

F2 - Processing parameters
SI 32768
SF 128.4032720 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



2.20

-1.26





Current Data Parameters
 NAME JSH-2,6-dimethylphenyl BF3K
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20130504
 Time_ 21.29
 INSTRUM spect
 PROBD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 131072
 SOLVENT DMSO
 NS 16
 DS 4
 SWH 89285.711 Hz
 FIDRES 0.681196 Hz
 AQ 0.7340532 sec
 RG 190.62
 DW 5.600 usec
 DE 6.50 usec
 TE 299.7 K
 D1 1.00000000 sec
 D11 0.03000000 sec
 D12 0.0002000 sec
 TDO 1

===== CHANNEL f1 =====
 NUC1 19F
 P1 15.00 usec
 PLW1 17.00000000 W
 SFO1 376.5359841 MHz

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

F2 - Processing parameters
 SI 65536
 SF 376.5736410 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

