Suzuki-Miyaura Cross-Coupling Reaction of Potassium Alkenyltrifluoroborates

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Table of contents

Supporting Information

General: All of the experiments were carried out under nitrogen atmosphere. ^1H , ^{13}C and ^{19}F NMR spectra were measured on spectrometers at 500.13, 125.77 and 470.53 MHz, respectively. ^{19}F NMR chemical shifts were referenced to external CFCl_3 (0.0 ppm). All ^{11}B chemical shifts were referenced to external $\text{BF}_3\cdot\text{OEt}_2$ (0.0 ppm) with a negative sign indicating an upfield shift. The triflates, halides and palladium catalyst were obtained from commercial sources. $t\text{-BuNH}_2$ was distilled from calcium hydride and Et_3N was distilled from calcium hydroxide. The $i\text{-PrOH}/\text{H}_2\text{O}$ mixture was degassed using nitrogen.

Potassium *trans*-1-Dec-1-enyl Trifluoroborate (1a). To a solution of *trans*-2-(decenyl) vinylboronic acid¹ (1.83 g, 10 mmol) in diethyl ether (20 mL) was added KHF_2 (2.18 g, 28 mmol), followed by water (9 mL) during 30 min. After stirring at rt for 3 h, the solution was concentrated and the crude material was dissolved in acetone, filtered and concentrated. The resulting white solid was purified by dissolving in hot acetone and precipitating with Et_2O , resulting in a white solid (2.04 g, 8.30 mmol, 83%): mp > 260 °C; ^1H NMR (500 MHz, $\text{DMSO}-d^6$) δ 5.44 (dt, $J = 17.5$ Hz, 6.2 Hz, 1H), 5.16-5.21 (m, 1H), 1.85 (t, $J = 6.0$ Hz, 2H), 1.19-1.27 (m, 12H), 0.85 (t, $J = 7.1$ Hz, 3H). ^{13}C NMR (125.8 MHz, $\text{DMSO}-d^6$) δ 133.49, 133.45, 35.37, 31.31, 29.25, 29.03, 28.81, 28.74, 22.09, 13.94; ^{19}F NMR (471 MHz, $\text{DMSO}-d^6$) δ -137.68 Hz; ^{11}B NMR (64.2 Mz, $\text{DMSO}-d^6$) δ 3.55. Anal. Calcd for $\text{C}_{10}\text{H}_{19}\text{BF}_3\text{K}$: C, 48.79; H, 7.78. found: C, 48.63; H, 7.62. IR (neat): 1636, 922 cm^{-1} .

Potassium Isopropenyl trifluoroborate (1b).² To a solution of 2-bromopropene (1.09 g, 9.0 mmol) in THF (15 mL) was added dropwise $t\text{-BuLi}$ (1.7 M in pentane, 6.4 mL 18.81 mmol) at 78 °C. After stirring at that temperature for 30 min, trimethyl borate (1.40 g, 13.5 mmol) was added. The resulting suspension was stirred for 20 min at -78 °C and then allowed to warm to rt for 1 h. The mixture was then cooled to 0 °C and KHF_2 (4.22 g, 78.1 mmol) was added followed by water (9 mL) over 30 min. After stirring at room temperature for 20 min, the solution was concentrated and the crude material was dissolved in acetone, filtered, and concentrated. The resulting white solid was purified by dissolving in hot acetone

and precipitating with ethyl ether obtaining a white solid (332 mg, 25%) mp > 260 °C. The spectral data obtained were in accordance with those described in the literature.³

Potassium Vinyl Trifluoroborate (1c). To a solution of trimethyl borate (2.32 g, 22.3 mmol) in THF (15 mL) was added dropwise vinylmagnesium bromide (1.0 M THF solution, 18.0 mL, 18.0 mmol) at -78 °C. The resulting suspension was stirred for 20 min at -78 °C and then allowed to warm to rt for 1 h. The mixture was then cooled to 0 °C and KHF₂ (6.97 g, 89.2 mmol) was added followed by water (12 mL) over 30 min. After stirring at rt for 20 min, the solution was concentrated and the crude material was dissolved in acetone, filtered, and concentrated. The resulting white solid was purified by dissolving in hot acetone and precipitating with Et₂O, obtaining a white solid (2.25 g, 16.8 mmol, 93%). mp 224 °C [lit.² mp 225 °C (dec.)]. The spectral data obtained were in accordance with those described in the literature.³

Potassium *trans*-Styryl Trifluoroborate (1d).⁴ To a solution of *trans*-2-phenylethenyl boronic acid (1.48 g, 10 mmol) in diethyl ether (20 mL) was added KHF₂ (2.18 g, 28 mmol), followed by water (9 mL) during 30 min. After stirring at rt for 3 h, the solution was concentrated and the crude material was dissolved in acetone, filtered, and concentrated. The resulting white solid was purified by dissolving in hot acetone and precipitating with Et₂O, resulting in a white solid (1.89 g, 9.0 mmol, 90%): mp > 260 °C. The spectral data obtained were in accordance with those described in the literature.

Potassium *trans*-7-Chlorohept-1-enyl Trifluoroborate (1e). To a solution of *trans*-7-chlorohept-1-enyl boronic acid (0.91 g, 6.11 mmol) in ethyl ether (12 mL) was added KHF₂ (1.44 g, 18.4 mmol), followed by water (9 mL) during 30 min. After stirring at rt for 3 h, the solution was concentrated and the crude material was dissolved in acetone, filtered, and concentrated. The resulting white solid was purified by dissolving in hot acetone and precipitating with Et₂O, resulting in a white solid (0.88 g, 68%), mp > 260 °C. ¹H NMR (500 MHz, acetone-d₆) δ 5.71 (dt, *J* = 17.6, 5.5 Hz, 1 H), 5.42 (d, *J* = 17.6 Hz, 1H), 3.56 (t, *J* = 7.0 Hz), 2.09-2.04 (m, 2H), 1.79 (m, 2H); ¹³C NMR (125.8 MHz, acetone-d₆) δ 134.88, 134.81, 45.61, 33.42, 33.29; ¹⁹F NMR (471 MHz, acetone-d₆): δ -141.58. ¹¹B NMR (64.2 MHz, acetone-d₆) δ 3.99.

Anal. Calcd for $C_5H_8ClBF_3K$: C, 28.53; H, 3.83. found: C, 28.68; H, 3.84. IR (neat): 2843, 1708, 1645, 954 cm^{-1} .

Potassium *trans*-1-Ethylbut-1-enyl Trifluoroborate (1f). To a solution of 1-ethenylbut-1-enyl boronic acid¹ (1.28 g, 10 mmol) in ethyl ether (20 mL) was added KHF_2 (2.18 g, 28 mmol), followed by water (9 mL) during 30 min. After stirring at rt for 3 h, the solution was concentrated and the crude material was dissolved in acetone, filtered, and concentrated. The resulting white solid was purified by dissolving in hot acetone and precipitating with Et_2O , resulting in a white solid (1.19 g, 6.3 mmol, 63%), mp 230-232 °C. 1H NMR (500 MHz, acetone- d^6) δ 5.18 (t, J = 6.7 Hz, 1H), 1.89-1.83 (m, 4H), 0.86-0.77 (m, 6H); ^{13}C NMR (125.8 MHz, acetone- d^6) δ 130.47, 130.45, 22.92, 21.24, 15.39, 15.36; ^{19}F NMR (471 MHz, acetone d^6) δ -143.00. ^{11}B NMR (64.2 MHz, acetone- d^6) δ 4.68 (d, J = 52.9 Hz). Anal. Calcd for $C_6H_{11}BF_3K$: C, 37.92; H, 5.83. Found: C, 38.08; H, 5.86. IR (neat, cm^{-1}): 1707, 1635, 939.

Potassium *trans*-4-Fluorostyryl Trifluoroborate (1g). To a solution of *trans*-2-(4-fluorophenyl) vinyl boronic acid (1.84 g, 10 mmol) in diethyl ether (20 mL) was added KHF_2 (2.18 g, 28 mmol), followed by water (9 mL) during 30 min. After stirring at rt for 3 h, the solution was concentrated and the crude material was dissolved in acetone, filtered, and concentrated. The resulting white solid was purified by dissolving in hot acetone and precipitating with Et_2O , resulting in a white solid (1.85 g, 8.1 mmol, 81%), mp >280 °C. 1H NMR (500 MHz, DMSO- d^6) δ 7.33-7.30 (m, 2H), 7.06-7.02 (m, 2H), 6.43 (d, J = 18.2 Hz, 1H), 6.12-6.07 (m, 2H); ^{13}C NMR (125.8 MHz, DMSO- d^6) δ 162.52, 132.60, 132.56, 127.78, 127.72, 115.58, 115.48; ^{19}F NMR (471 MHz, DMSO- d^6) δ -117.01, -138.33. ^{11}B NMR (64.2 MHz, acetone- d^6) δ 7.02. Anal. Calcd for $C_8H_6BF_4K$: C, 42.14; H, 2.65. Found: C, 42.23; H, 2.59. IR (neat): 2995, 1636, 921 cm^{-1} .

Potassium *trans*-1-Hex-5-enoic Acid, Methyl Ester Trifluoroborate (1h). To a solution of *trans*-1-hex-5-enoic methyl ester boronic acid,¹ (1.72 g, 10 mmol) in ethyl ether (20 mL) was added KHF_2 (2.18 g, 28 mmol), followed by water (9 mL) during 30 min. After stirring at rt for 3 h, the solution was

concentrated and the crude material was dissolved in acetone, filtered, and concentrated. The resulting white solid was purified by dissolving in hot acetone and precipitating with Et₂O, resulting in a white solid (1.09 g, 4.7 mmol, 47%), mp > 260 °C. ¹H NMR (500 MHz, acetone-*d*⁶), δ 5.65 (m, 1H), 5.39 (m, 1H), 3.61 (s, 3H), 2.27(t, *J* = 7.4 Hz, 2H), 1.95 (m, 2H), 1.62 (m, 2H); ¹³C NMR (125.8 MHz, acetone-*d*⁶) δ 174.07, 134.11, 134.08, 50.90, 35.32, 33.47, 25.10; ¹¹B NMR (64.2 MHz, acetone-*d*) δ 6.62; ¹⁹F NMR (471 MHz, acetone-*d*⁶) δ -141.71 Anal. Calcd for C₇H₁₁BF₃KO₂: C, 35.92; H, 4.74. Found: C, 35.75; H, 4.90. IR (neat): 1731, 1643, 1098 cm⁻¹.

Potassium *cis*-Styryl Trifluoroborate (1j). To a solution of *cis*-2-phenylethenyl boronic acid (0.29 g, 2 mmol, obtained from commercial sources, 95% purity) in diethyl ether (4 mL) was added KHF₂ (0.62 g, 8 mmol), followed by water (1.8 mL) during 30 min. After stirring at rt for 3 h, the solution was concentrated and the crude material was dissolved in acetone, filtered, and concentrated. The resulting white solid was purified by dissolving in hot acetone and precipitating with Et₂O, resulting in a white solid (0.33 g, 1.59 mmol, 78%) mp > 260 °C. ¹H NMR (500 MHz, acetone-*d*⁶), δ 7.64-7.62 (m, 2H), 7.19-7.16 (m, 2H), 7.06-7.03 (m, 1H), 6.60-6.74 (m, 1H), 5.69 (m, 1H); ¹³C NMR (125.8 MHz, acetone-*d*⁶) δ 141.69, 136.24, 136.20, 128.97, 128.95, 127.64 (2C), 125.66; ¹⁹F NMR (471 MHz, acetone-*d*⁶) δ -136.46 (q, *J* = 45.2 Hz); ¹¹B NMR (64.2 MHz, solvent) δ 6.19 (q, *J* = 54.31 Hz); IR (neat): 2990, 1600, 925, cm⁻¹.

Representative Procedure for the Cross-coupling Reaction with Potassium Alkenyltrifluoroborates. *trans*-1-Dec-1-enyl-naphthalene (3a). A solution of potassium *trans*-1-dec-1-enyl trifluoroborate (**1a**) (123.4 mg, 0.5 mmol), PdCl₂(dppf)•CH₂Cl₂ (8.1 mg, 0.01 mmol), 1-bromonaphthalene (**2a**) (103.5 mg, 0.5 mmol) and *t*-BuNH₂ (109.7 mg, 1.5 mmol), in *i*-PrOH/H₂O (2:1, 5 mL) was heated at reflux under nitrogen atmosphere. The reaction mixture was stirred at reflux for 10 h, then cooled to rt and diluted with water (10 mL), followed by extraction with ethyl ether. The organic layers were combined and washed with 1 N HCl and brine, dried over MgSO₄ and then filtered. The solvent was removed under vacuum and the crude product was purified by silica gel chromatography (eluting with hexane/ ethyl acetate) to afford a colorless oil (103.7 mg, 78%): ¹H NMR (500 MHz, CDCl₃) δ 8.12 (dd, *J* = 8.0, 1.0 Hz, 1H), 7.83 (dd, *J* = 8.5, 1.7 Hz, 1H), 7.73 (d, *J* = 8.1 Hz, 1H), 7.55 (d, *J* = 7.1 Hz, 1H), 7.40-
S5

7.51 (m, 3H), 7.10 (d, $J = 15.5$ Hz, 1H), 6.23 (dd, $J = 15.5, 6.9$ Hz, 1H), 2.33 (m, 2H), 1.25-1.41 (m, 13 H), 0.89 (t, $J = 7.0$ Hz, 3H); ^{13}C NMR (125.8 MHz, CDCl_3) δ 135.79, 134.58, 133.60, 131.12, 128.42, 127.14, 126.83, 125.72, 125.64, 125.58, 123.96, 123.46, 33.45, 31.90, 29.50, 29.41, 29.31, 29.26, 22.68, 14.11. HRMS (CI): m/z calcd. for $\text{C}_{20}\text{H}_{26}$ 266.2034, found 266.2043. IR (neat): 1502, 1377 cm^{-1} .

***trans*-1-Dec-1-enyl-4-trifluoromethyl-benzene (3b).** This product was obtained from the reaction of potassium *trans*-1-dec-1-enyl trifluoroborate (**1a**) and 4-bromobenzotrifluoride (**2b**) to afford the title compound in 65% yield. ^1H NMR (500 MHz, CDCl_3) δ 7.52 (dd, $J = 8.0, 1.0$ Hz, 2H), 7.41 (d, $J = 8.1$ Hz, 2H), 6.39 (d, $J = 16.0$ Hz, 1H), 6.29-6.35 (m, 1H), 2.22 (q, $J = 7.0$ Hz, 2H), 1.47 (m, 2H), 1.25-1.30 (m, 10H), 0.88 (t, $J = 6.7$ Hz, 3H). ^{13}C NMR (125.8 MHz, CDCl_3) δ 141.41, 134.14, 128.53, 125.99 (3C), 125.41, 125.38, 33.07, 31.86, 29.69, 29.45, 29.25, 29.22, 29.14, 22.66, 14.09. HRMS (CI): m/z calcd. for $\text{C}_{17}\text{H}_{23}\text{F}_3$ 284.1751, found 284.1737; IR (neat): 1325, 1265, 1167, 1128, 1067 cm^{-1} .

***trans*-4-Dec-1-enyl-benzonitrile (3c)** This product was obtained from reaction of potassium *trans*-1-dec-1-enyl trifluoroborate (**1a**) and 4-bromobenzonitrile (**2c**) to afford the title compound in 87% yield. ^1H NMR (500 MHz, CDCl_3) δ 7.56 (d, $J = 8.2$ Hz, 2H), 7.39 (d, $J = 8.3$ Hz, 2H), 6.36-6.37 (m, 2H), 2.22 (m, 2H), 1.47 (m, 2H), 1.28-1.35 (m, 10H), 0.88 (t, $J = 7.0$ Hz, 3H); ^{13}C NMR (125.8 MHz, CDCl_3) δ 142.44, 135.63, 132.31 (2C), 128.38, 126.34 (2C), 119.16, 109.89, 33.12, 31.85, 29.43, 29.22 (2C), 29.03, 22.65, 14.08; HRMS (CI): m/z calcd. for $\text{C}_{17}\text{H}_{23}\text{N}$ 241.183, found 241.1833; IR (neat): 2225, 1604 cm^{-1} .

***trans*-2-Dec-1-enyl-acetophenone (3d).** This product was obtained from potassium *trans*-1-dec-1-enyl trifluoroborate (**1a**) and 2-bromoacetophenone (**2d**) to afford the title compound in 63% yield. ^1H NMR (500 MHz, CDCl_3) δ 7.56 (dt, $J = 7.5, 1.5$ Hz, 1H), 7.50 (d, $J = 7.5$ Hz, 1H), 7.40 (t, $J = 8.0$ Hz, 1H), 7.28-7.25 (m, 1H), 6.83 (d, $J = 15.5$ Hz, 1H), 6.11 (dt, $J = 15.5, 1.8$ Hz, 1H), 2.56 (s, 3H), 2.22 (m, 2H), 1.46 (m, 2H), 1.35-1.28 (m, 10H), 0.88 (t, $J = 6.2$ Hz, 3H); ^{13}C NMR (125.8 MHz, CDCl_3) δ 202.76, 137.59, 137.40, 134.60, 131.25, 128.42, 128.19, 127.45, 126.48, 32.21, 31.87, 30.11, 29.46, 29.27 (2C),

29.21, 22.66, 14.09; HRMS (CI): m/z calcd. for $C_{18}H_{26}O$ 258.1983, found 258.1979; IR (neat): 1682, 1466, 1354, 1244 cm^{-1} .

***trans*-4-Dec-1-enyl-anisole (3e).**⁵ This product was obtained from potassium *trans*-1-dec-1-enyl trifluoroborate (**1a**) and 4-iodoanisole (**2e**) to afford the title compound in 60% yield. 1H NMR (500 MHz, $CDCl_3$) δ 7.27 (d, J = 9.3 Hz, 2H), 6.28 (d, J = 9.2 Hz, 2H), 6.31 (d, J = 15.7 Hz, 1H), 6.07 (dt, J = 15.8, 6.9 Hz, 1H), 2.17 (q, J = 6.8 Hz, 2H), 1.44 (m, 2H), 1.24-1.34 (m, 10H), 0.88 (t, J = 6.8 Hz, 3H); ^{13}C NMR (125.8 MHz, $CDCl_3$) δ 158.57, 131.00, 129.11, 128.96, 126.93 (2C), 113.88 (2C), 55.27, 33.02, 31.89, 29.53, 29.50, 29.29, 29.24, 22.67, 14.10; HRMS (CI): m/z calcd for $C_{17}H_{26}O$ 246.1983, found 246.1986; IR (neat) 1605, 1513, 1463, 1302, 1250, 1173 cm^{-1} .

***trans*-4-Dec-1-enyl-nitrobenzene (3f).** This product was obtained by the general method from potassium *trans*-1-dec-1-enyl trifluoroborate (**1a**) and 4-nitrophenyl bromide (**2f**) (71% yield), and also from 4-nitrophenyl trifluoromethanesulfonate (**2m**) by the following procedure: To a solution of potassium *trans*-1-dec-1-enyl trifluoroborate (**1a**) (123.4 mg, 0.5 mmol), $PdCl_2(dppf) \cdot CH_2Cl_2$ (8.1 mg, 0.01 mmol), 4-nitrophenyl trifluoromethanesulfonate (135.6 mg, 0.5 mmol) in *i*-PrOH/ H_2O (2:1, 5 mL), was added *t*-BuNH₂ (109.7 mg, 1.5 mmol). The reaction mixture was stirred under argon at reflux for 3 h, then cooled to rt and diluted with water, followed by extraction of ethyl ether. The organic layers were combined and washed with 1 N HCl and brine, dried over $MgSO_4$ and then filtered. The solvent was removed under vacuum and the crude product was purified by silica gel chromatography (eluting with hexane/ ethyl acetate) to afford **3f** in a yellow oil (99 mg, 76% yield). 1H NMR (500 MHz, $CDCl_3$) δ 8.14 (d, J = 8.8 Hz, 2H), 7.44 (d, J = 8.8 Hz, 2H), 6.43-6.44 (m, 2H), 2.25 (m, 2H), 1.49 (m, 2H), 1.27-1.34 (m, 10H), 0.88 (t, J = 6.6 Hz, 3H); ^{13}C NMR (125.8 MHz, $CDCl_3$) δ 146.36, 144.44, 128.03, 126.27 (2C), 123.92 (2C), 33.20, 31.83, 29.41, 29.22, 28.96, 22.63, 14.07; HRMS (CI): m/z calcd. for $C_{16}H_{21}NO_2$ 261.1723, found 261.1720; IR (neat): 1596, 1514, 1341 cm^{-1} .

***trans*-4-Dec-1-enyl-acetophenone (3g).** This product was obtained by the general method from potassium *trans*-1-dec-1-enyl trifluoroborate (**1a**) and 4-bromoacetophenone (**2g**) to afford the title compound in 69% yield, and from 4-acetylphenyl trifluoromethanesulfonate (**2n**) according to the procedure for the preparation of **3f** from **2m**, to afford a colorless solid (78 mg, 60% yield). mp 35-36 ° C; ¹H NMR (500 MHz, CDCl₃) δ 7.86 (d, *J* = 8.4 Hz, 2H), 7.40 (d, *J* = 8.4 Hz, 2H), 6.37-6.39 (m, 2H), 2.57(s, 3H), 2.23 (q, *J* = 7.2 Hz, 2H), 1.46-1.49 (m, 2H), 1.28-1.33 (m, 10H), 0.88 (d, *J* = 6.8 Hz, 3H); ¹³C NMR (125.8 MHz, CDCl₃) δ 197.49, 142.64, 135.34, 134.54, 128.86, 128.69 (2C), 125.85 (2C), 33.15, 31.83, 29.42, 29.22 (2C), 29.10, 26.47, 22.63, 14.06; mp 35-36 °C; HRMS (CI): *m/z* calcd. for C₁₈H₂₆O 258.1970, found 258.1992; IR (bromoform): 2924, 1673, 1600 cm⁻¹.

***trans*-2-Dec-1-enyl-benzonitrile (3h).** This product was obtained from potassium *trans*-1-dec-1-enyl trifluoroborate (**1a**) and 2-bromobenzonitrile (**2h**) to afford the title compound in 75% yield. ¹H NMR (500 MHz, CDCl₃) δ 7.57-7.60 (m, 2H), 7.51-7.49 (m, 1H), 7.25-7.27 (m, 1H), 6.74 (d, *J* = 15.7 Hz, 1H), 6.43 (dt, *J* = 15.7, 7.0 Hz, 1H), 2.27 (q, *J* = 7.1 Hz, 2H), 1.49 (m, 1H), 1.25-1.35 (m, 10H), 0.88 (t, *J* = 7.1 Hz, 3H); ¹³C NMR (125.8 MHz, CDCl₃) δ 141.22, 136.88, 132.85, 132.56, 126.83, 125.83, 125.29, 118.13, 110.25, 33.20, 31.85, 29.42, 29.24, 29.23, 29.03, 22.65, 14.08; HRMS (CI): *m/z* calcd. for C₁₇H₂₃N 241.1930, found 241.1822; IR (neat): 2225 cm⁻¹.

***trans*-3-Dec-1-enyl-anisole (3i).**⁶ This product was obtained from potassium *trans*-1-dec-1-enyl trifluoroborate (**1a**) and 3-bromoanisole (**2i**) to afford the title compound in 61% yield. ¹H NMR (500 MHz, CDCl₃) δ 7.19 (t, *J* = 7.8 Hz, 1H), 6.93 (d, *J* = 7.6 Hz, 1H), 6.87 (s, 1H), 6.73 (dd, *J* = 8.2, 2.5 Hz, 1H), 6.34 (d, *J* = 15.8 Hz, 1H), 6.22 (dt, *J* = 15.8, 6.8 Hz, 1H), 2.19 (q, *J* = 7.6 Hz, 2H), 1.45 (m, 2H), 1.27-1.34 (m, 10H), 0.88 (t, *J* = 7.1 Hz, 3H); ¹³C NMR (125.8 MHz, CDCl₃) δ 159.78, 139.46, 131.62, 129.57, 129.40, 118.60, 112.37, 111.25, 55.16, 33.03, 31.90, 29.51, 29.36, 29.30, 22.69, 14.16; HRMS (CI): *m/z* calcd. for C₁₇H₂₇O (M+H⁺) 247.198, found 247.2051; IR (neat): 1598, 1465, 1264, 1049 cm⁻¹.

***trans*-2-Dec-1-enyl-mesitylene (3j).** This product was obtained from potassium *trans*-1-dec-1-enyl trifluoroborate (**1a**) and 2-bromo-bromomesitylene (**2j**) to afford the title compound in 38% yield when Et₃N was used as base. ¹H NMR (500 MHz, CDCl₃) δ 6.84 (s, 2H), 6.26 (d, *J* = 17.5 Hz, 1H), 6.62 (dt, *J* = 15.8, 2.8 Hz, 1H), 2.25 (s, 9H), 2.23-2.21 (m, 2H), 1.46-1.43 (m, 2H), 1.36-1.27 (m, 10H), 0.88 (t, *J* = 5.0 Hz, 3H); ¹³C NMR (125.8 MHz, CDCl₃) δ 135.82, 135.69, 135.50, 134.82, 128.31 (3C), 127.06, 33.41, 31.88, 29.50, 29.58 (2C), 29.32, 29.14, 22.67, 20.87 (2C), 14.10; HRMS (CI): *m/z* calcd. for C₁₉H₃₀ 258.234, found 258.233; IR (neat): 1455 cm⁻¹.

***trans*-1-Dec-1-enyl-4-fluoro-benzene (3l).** This product was obtained from potassium *trans*-1-dec-1-enyl trifluoroborate (**1a**) and 1-bromo-4-fluorobenzene (**2l**) to afford the title compound in 59% yield using Et₃N as base. ¹H NMR (500 MHz, CDCl₃) δ 7.24-7.29 (m, 2H), 6.94-6.98 (m, 2H), 6.33 (d, *J* = 15.8 Hz, 1H), 6.13 (dt, *J* = 15.8, 6.9 Hz, 1H), 2.18 (m, 2H), 1.44 (m, 2H), 1.27-1.34 (m, 10H), 0.88 (t, *J* = 7.1 Hz, 3H); ¹³C NMR (125.8 MHz, CDCl₃): δ 162.8, 134.2, 130.97, 128.47, 127.28, 127.22, 115.34, 115.17, 32.98, 31.89, 29.48, 29.37, 29.28, 29.24, 22.67, 14.09; HRMS (CI): *m/z* calcd. for C₁₆H₂₃F 234.1778, found 234.1772; IR (neat) 1602, 1510, 1465, 1229, 1156 cm⁻¹.

4-Isopropenyl-benzonitrile (4b).⁷ This product was obtained from potassium isopropenyl trifluoroborate (**1b**) and 4-bromobenzonitrile (**2c**) to afford the title compound in 70% yield. The spectral data were in accordance with those described in the literature.

4-Cyano-styrene (4c).⁸ This compound was obtained from potassium vinyl trifluoroborate (**1d**) and 4-bromobenzonitrile (**2c**) to afford the title compound in 76% yield using Et₃N as base. The spectral data obtained were in accordance with those described in the literature.

***trans*-4-Cyanostilbene (4d).**⁹ This compound was obtained from potassium *trans*-styryl trifluoroborate (**1c**) and 4-bromobenzonitrile (**2c**), to afford the title compound in 80% yield. The spectral data obtained were in accordance with those described in the literature. mp 113.5-114.5 °C (lit.⁹ 115 °C)

***trans*-4-(5-Chloro-pent-1-enyl)-benzonitrile (4e).**¹⁰ This compound was obtained from potassium *trans*-7-chloro-hept-1-enyl trifluoroborate (**1e**) and 4-bromobenzonitrile (**2c**) (52% yield). The spectral data obtained were in accordance with those described in the literature.

***trans*-4-(1-Ethylbut-1-enyl)-benzonitrile (4f):** This compound was obtained from potassium 1-ethyl-but-1-enyl trifluoroborate (**1f**) and bromobenzonitrile (**2c**) to afford the title compound in 70% yield. ¹H NMR (500 MHz, CDCl₃) δ 7.58-7.56 (m, 2H), 7.49-7.42 (m, 2H), 5.74 (t, *J* = 7.2 Hz, 1H), 2.53-2.48 (m, 2H), 2.23 (t, *J* = 7.4 Hz, 2H), 1.07 (t, *J* = 7.5 Hz, 3H), 0.97 (t, *J* = 7.4 Hz, 3H); ¹³C NMR (125.8 MHz, CDCl₃) δ 147.67, 139.74, 133.12, 132.00 (2C), 126.76 (2C), 119.15, 109.82; HRMS (CI): *m/z* calcd. for C₁₃H₁₅N 185.1204; found 185.1201; IR (neat) 1461, 1393 cm⁻¹.

4-[2-(4-Fluorophenyl) vinyl] benzonitrile (4g). This compound was obtained from potassium *trans*-4-fluoro-styryl trifluoroborate (**1g**) and 4-bromobenzonitrile (**2c**) to afford the title compound in 73% yield. mp 118-120 °C; ¹H NMR (500 MHz, CDCl₃) 7.61 (d, *J* = 7.9 Hz, 2H), 7.54 (d, *J* = 7.9 Hz, 2H), 7.50-7.47 (m, 2H), 7.15 (d, *J* = 16.2, 1H), 7.08-7.05 (m, 2H), 6.98 (d, *J* = 16.2 Hz, 1H); ¹³C NMR (125.8 MHz, CDCl₃) δ 163.79, 161.82, 141.60, 132.47 (2C), 131.06, 128.49, 128.43, 126.73 (2C), 126.44, 118.91, 115.89, 157.72, 110.53; HRMS (CI): *m/z* calcd. for C₁₅H₁₀NF 223.0795, found, 223.0782; IR (bromoform): 2256, 1598, 1509 cm⁻¹; Anal. Calcd for C₁₅H₁₀NF: C, 80.70; H, 4.51, found: C, 80.88; H, 4.65.

6-(4-Cyanophenyl)-hex-5-enoic Acid, Methyl Ester (4h). This compound was obtained from potassium *trans*-1-hex-5-enoic acid methyl ester trifluoroborate (**1h**) and 4-bromobenzonitrile (**2c**) to

afford the title compound in 33% yield. ^1H NMR (500 MHz, CDCl_3) δ 7.56 (d, J = 8.3 Hz, 2H), 7.40 (d, J = 8.3 Hz, 2H), 6.40 (d, J = 15.9, 1H), 6.35-6.30 (m, 1H), 3.66 (s, 3H), 2.37 (t, J = 7.4 Hz, 2H), 2.35-2.27 (m, 2H), 1.83 (m, 2H); ^{13}C NMR (125.8 MHz, CDCl_3) δ 174.18, 142.45, 134.30, 132.76 (2C), 129.80, 126.86 (2C), 119.45, 110.62, 51.97, 33.72, 32.78, 24.56; HRMS (CI): m/z calcd. for $\text{C}_{14}\text{H}_{15}\text{NO}_2$ 229.1102, found 229.1102; IR (neat) 2225, 1731, 1435 cm^{-1} .

***cis*-4-Cyanostilbene (4j).** This compound was obtained from potassium *cis*-styryl trifluoroborate (**1j**) and 4-bromobenzonitrile (**2c**), to afford the title compound in 86% yield. ^1H NMR (500 MHz, CDCl_3) δ 7.50 (d, J = 8.3 Hz, 2H), 7.32 (d, J = 8.3 Hz, 2H), 7.24-7.26 (m, 3H), 7.20-7.19 (m, 2 H), 6.77 (d, J = 12.1 Hz, 1H), 6.57 (d, J = 12.2 Hz, 1H); ^{13}C NMR (125.8 MHz, CDCl_3) δ 142.04, 136.20, 133.36, 131.97 (2C), 129.47 (2C), 128.72 (2C), 128.47 (2C), 128.33, 127.78, 118.89, 110.44. HRMS (CI): m/z calcd. for $\text{C}_{15}\text{H}_{11}\text{N}$ 205.0891, found 205.0888. IR (neat) 2226, 1603, 1503 cm^{-1} .

***trans*-1-(β -Phenylvinyl)thiazole (6a).**¹¹ This compound was obtained from potassium styryltrifluoroborate (**1d**) and 2-bromothiazole (**5a**) by the general procedure. After extraction, the ethereal solution was washed with 1 N NaHCO_3 and brine, filtered and then dried over MgSO_4 to afford the title product in 47% when *t*- BuNH_2 was used as base, and 83% yield using Et_3N as base. The spectral data obtained were in accordance with those described in the literature. mp 57-58 $^\circ\text{C}$ (lit.¹¹ 57-59 $^\circ\text{C}$).

***trans*-2-Acetyl-5-(β -phenylvinyl)thiophene (6b).**¹² This compound was obtained from potassium styryltrifluoroborate (**1d**) and 2-bromo-5-acetylthiophene (**5b**) to afford the title compound in 91% yield, using 3 equiv of *t*- BuNH_2 as base. The spectral data obtained were in accordance with those described in the literature. mp 128-130 $^\circ\text{C}$.

***trans*-2-(β -Phenylvinyl)thiophene (6c).**¹³ This compound was obtained from potassium styryltrifluoroborate (**1d**) and 2-bromothiophene (**5c**) to afford the title compound in 69% yield using 3

equiv of *t*-BuNH₂ as base. The spectral data obtained were in accordance with those described in the literature. mp 110-111 °C (lit.^{13b} 111-112 °C).

***trans*-3-(β -Phenylvinyl)thiophene (6d).**¹⁴ This compound was obtained from potassium styryltrifluoroborate (**1d**) and 3-bromothiophene (**5d**) to afford the title compound in 80% yield using 3 equiv of *t*-BuNH₂ as base. The spectral data obtained were in accordance with those described in the literature. mp 117-118 °C. (lit.¹⁴ 117-118 °C)

***trans*-7-(β -Phenylvinyl)indole (6e).** This compound was obtained from potassium styryltrifluoroborate (**1d**) and 7-bromoindole (**5e**) to afford the title compound in 70% yield using 3 equiv of *t*-BuNH₂ as base. mp: 214-216 °C. ¹H NMR (500 MHz, CDCl₃): δ 8.43 (s, 1H), 7.58 (d, *J* = 8.0 Hz, 1H), 7.54 (d, *J* = 8.0 Hz, 2H), 7.39-7.33 (m, 4H), 7.27 (t, *J* = 7.3Hz, 1H), 7.22-7.21 (m, 1H), 7.17-7.12(m, 2H), 6.59 (t, *J* = 3Hz, 1H); ¹³C NMR (125.8 MHz, CDCl₃): δ 137.46, 133.73, 129.59, 128.75 (2C), 128.49, 127.69, 126.38 (2C), 125.08, 124.24, 121.37, 120.48, 120.46, 120.20, 103.25; HRMS (CI): *m/z* calcd. for C₁₆H₁₃N 219.1048, found 219.1048; IR (bromoform): 2256, 1444, 1296 cm⁻¹.

***trans*-2-(β -Phenylvinyl)pyridine (6f).**¹⁵ This compound was obtained from potassium styryltrifluoroborate (**1d**) and 2-bromopyridine (**5f**) to afford the title compound in 70% yield using 3 equiv of *t*-BuNH₂ as base, and from 2-trifluoromethanesulfonate pyridine (**5g**) (41% yield using 3 equiv of *t*-BuNH₂ as base). The spectral data obtained were in accordance with those described in the literature. mp 86-87.5 °C.

***trans*-5-(β -Phenylvinyl)pyrimidine (6h).**¹⁶ This compound was obtained from potassium styryltrifluoroborate (**1d**) and 5-bromopyrimidine (**5h**) to afford the title compound in 73% yield using 3 equiv of *t*-BuNH₂ as base. The spectral data obtained were in accordance with those described in the literature. mp 71-72 °C.

***trans*-3-(β -Phenylvinyl)pyridine (6i).**¹⁷ This compound was obtained from potassium styryltrifluoroborate (**1d**) and 3-bromopyridine (**5i**) to afford the title compound in 57% yield using 3 equiv of *t*-BuNH₂ as base and 31% yield, using 3 equiv of Et₃N as base. The spectral data obtained were in accordance with those described in the literature. mp 80-81 °C. (lit³⁵: 81.4-82 °C).

***trans*-2-(β -Phenylvinyl)-4,6-dichloro Pyrimidine (6j).** This compound was obtained from 1 equiv of potassium styryltrifluoroborate (**1d**) and 1 equiv of 2,4,6-trichloropyrimidine (**5j**) to afford the title compound in 55% yield, using 3 equiv of Et₃N as base. mp 108-109 °C; ¹H NMR (500 MHz, CDCl₃): δ 7.95 (d, *J* = 15.8 Hz, 1H), 7.59-7.57 (m, 2H), 7.31-7.49 (m, 3H), 7.21 (s, 1H), 6.94 (d, *J* = 15.8 Hz, 1H); ¹³C NMR (125.8 MHz, CDCl₃): δ 166.45, 162.60, 161.30, 140.74, 134.72, 130.33, 128.99 (2C), 128.05 (2C), 122.92, 116.88; mp: 108-109 °C; HRMS (CI): *m/z* calcd. for C₁₂H₈N₂Cl₂ 250.0064, found 250.0050. Anal. Calcd for C₁₂H₈Cl₂N₂: C, 57.40; H, 3.31. Found: C, 57.57; H, 3.39. IR (bromoform): 2256, 1551, 1522 cm⁻¹.

2,4,6-Tristyrylpyrimidine (6j'). This compound was obtained from 3.5 equiv of potassium styryltrifluoroborate (**1d**) and 1 equiv of 2,4,6-trichloropyrimidine (**5j**) to afford the title compound in 72% yield, using 6 equiv of Et₃N as base. mp 185-186 °C; ¹H NMR (500 MHz, CDCl₃): δ 8.12 (d, *J* = 15.9 Hz, 1H), 7.94 (d, *J* = 15.9 Hz, 2H), 7.69 (d, *J* = 7.7 Hz, 1H), 7.64 (d, *J* = 7.6 Hz, 2H), 7.42-7.39 (m, 6H), 7.36-7.30 (m, 4H), 7.15 (s, 1H), 7.12 (d, *J* = 15.9, 2H); ¹³C NMR (125.8 MHz, CDCl₃): δ 164.52, 162.82 (2C), 137.77, 136.61 (2C), 136.35, 135.92 (2C), 129.20 (2C), 128.84 (5C), 128.72 (2C), 128.19, 127.66 (2C), 127.62 (4C), 126.41 (2C), 113.54; HRMS (CI): *m/z* calcd. for C₂₈H₂₂N₂ 387.1683, found 387.1857; IR (bromoform): 1564, 1446, 1296 cm⁻¹.

2,4,6-Tristyryl[1,3,5]triazine (6k). This compound was obtained from 3.5 equiv of potassium styryltrifluoroborate (**1d**) and 1 equiv of 2,4,6-trichlorotriazine (**5k**) (64% yield using 6 equiv of Et₃N as base); mp 149-151 °C. ¹H NMR (500 MHz, CDCl₃): δ 7.78 (d, *J* = 18 Hz, 3H), 7.71 (m, 6H),

7.74-7.35 (m, 9H), 6.35 (d, $J = 18.1$ Hz, 3H). ^{13}C NMR (125.8 MHz, CDCl_3): δ 152.27, 137.17, 129.45, 129.01, 128.63, 127.56, 127.07. IR (bromoform): 1616, 1446, 1374 cm^{-1} .

2-Nitro-6-styrylpyridine (6l). This compound was obtained from potassium styryltrifluoroborate (**1d**) and 2-nitro-6-bromo-pyridine (**5l**) to afford the title compound in 51% yield, using 3 equiv of Et_3N as base. mp 101-102 $^\circ\text{C}$ ^1H NMR (500 MHz, CDCl_3): δ 8.77 (dd, $J = 4.49, 1.3$ Hz, 1H), 8.21 (dd, $J = 7.8, 1.5$ Hz, 1H), 8.05 (d, $J = 15.5$ Hz, 1H), 7.74 (d, $J = 15.5$ Hz, 1H), 7.62 (d, $J = 7.3$ Hz, 2H), 7.41-7.38 (m, 2H), 7.36-7.33 (m, 1H), 7.30-7.27 (m, 1H); ^{13}C NMR (125.8 MHz, CDCl_3): δ 153.20, 149.66, 144.68, 139.50, 136.38, 133.24, 129.86, 129.40, 129.26, 128.33, 122.29, 121.67; HRMS (CI): m/z calcd. for $\text{C}_{13}\text{H}_{10}\text{N}_2\text{O}_2$ 226.0741, found 226.0752. Anal. Calcd for $\text{C}_{13}\text{H}_{10}\text{N}_2\text{O}_2$: C, 69.02; H, 4.46. Found: C, 69.12; H, 4.36. IR (bromoform): 1587, 1520, 1158 cm^{-1} .

5.466
5.431
5.211
5.207
5.204
5.201
5.176
5.172
5.169

2.507
2.503
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2.496
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PROCNO 1

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DATE 24-8-1

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CY 0.0
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39.163
38.998
22.901

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BOOK R

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DATE 26-8-1

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CY 0.0
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1b

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1D NMR plot parameters
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119.112

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39.166
38.999

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RG          0.6534100 sec
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1D NMR plot parameters
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 -139.639
 -139.752

1c

Chemical shift values (ppm) for the aromatic region:

- 7.313
- 7.298
- 7.260
- 7.245
- 7.229
- 7.117
- 7.103
- 7.089
- 6.488
- 6.451
- 6.204
- 6.201
- 6.197
- 6.168
- 6.164
- 6.161

3.319

2.500
2.497

Current Data Parameters
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PROCNO: 1
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INSTRUM: spect
PROBHD: 5 mm QNP 290
PULPROG: zgpg30
TD: 32768
SOLVENT: CDCl₃
NS: 16
DS: 2
SWH: 6008.62 Hz
FIDRES: 0.183399 Hz
AQ: 2.7263477 sec
RG: 327.500
DM: 83.200 usec
DE: 6.00 usec
TE: 300.2 K
D1: 1.0000000 sec
----- CHANNEL f1 -----
NUC1: ¹H
P1: 7.50 usec
PL1: 0.00 dB
SFO1: 500.3920019 MHz
F2 - Processing parameters
SI: 32768
SF: 500.3900084 MHz
WDW: EM
SSB: 0
LB: 0.30 Hz
GB: 0
PC: 1.00
ID: NMR plot parameters
CX: 20.00 cm
FIP: 10.000 ppm
FIDRES: 0.183399 Hz
F2P: -10.000 ppm
F2: -500.39 Hz
FREQ0: 500.3900084 MHz
HETCON: 270.21451 Hz/cm

140.294
133.088
133.052
128.228
125.807
125.354

40.004
39.837
39.670
39.504
39.337
39.170
39.004

Current Data Parameters
NAME: crb004
PROCNO: 1
F2 - Acquisition Parameters
Time: 2.002400
Date_ : 11/11/2011
Time: 4.06
INSTRUM: spect
PROBHD: 5 mm QNP 1H/1
PULPROG: zgpg30
TD: 65536
SOLVENT: CDCl3
NS: 149
DS: 4
SWH: 31446.541 Hz
FIDRES: 0.477836 Hz
AQ: 1.0420724 sec
RG: 327.68
DQ: 1.155900 us
DE: 6.00 us
TE: 300.00 K
D1: 2.00000000 sec
d11: 0.03000000 sec
d12: 0.00020000 sec
===== CHANNEL f1 =====
NUC1: 13C
P1: 7.50 us
PL1: 0.00 dB
SFO1: 125.7715719 MHz
===== CHANNEL f2 =====
PULPROG: zgpg30
TD: 65536
SOLVENT: CDCl3
P1: 7.50 us
PL1: 0.00 dB
SFO2: 500.1320005 MHz
F2 - Processing parameters
SI: 32768
SF: 125.7578493 MHz
WDW: EM
SSB: 0
LB: 1.00 Hz
GB: 0
PC: 1.40
1D NMR plot parameters
CX: 21.00 ct
FIP: 177.986 DE
F1P: 220.000000 MHz
F2P: 20.797 DE
F2: 2615.36 Hz
FENCH: 7.48518 DE
H2CH: 941.52068 Hz

```

Current Data Parameters
NAME      ctb026
EXPNO     1
PROCNO    1

F2 - Acquisition Parameters
Date_     20020202
Time      14.40
INSTRUM   spect
PROBHD    5 mm QNP 1H/1
PULPROG   zgpg30
TD         131072
SOLVENT   CDCl3
NS         63
DS         4
SWH        10000.000 Hz
AQ          0.7255810 sec
RG          2048
DM          5.000 usec
DE          6.00 usec
TE          300.2 K
D1          1.00000000 sec
d11         0.03000000 sec
d12         0.00002000 sec

===== CHANNEL f1 =====
NUC1       19F
P1          10.60 usec
PL1         -3.00 dB
SFO1        470.545277 MHz

===== CHANNEL f2 =====
CPDPRG2    waltz16
NUC2        1H
P2          95.00 usec
PL2         0.00 dB
PL12        26.00 dB
SFO2        500.1320005 MHz

F2 - Processing parameters
SI          65536
SF          470.5925870 MHz
WDW         EM
SSB         0
LB          0.30 Hz
GB          0
PC          1.00

1D NMR plot parameters
CX          20.00 cm
F1P         -100.000 ppm
F1          -47059.26 Hz
F2P         -200.000 ppm
F2          -94118.52 Hz
PPMCM       5.00000 ppm/cm
HZCM        2352.96289 Hz/cm

```

-141.583

1d

BK-R

B115MM-500
DATE 26-8-1

SF 64.210
SY 64.2
O1 10000.000
SI 8192
TD 4096
SW 10000.000
HZ/PT 2.441

PW 4.5
RD 0.0
AQ .205
RG 160
NS 390
TE 297

FW 12500
O2 3300.000
DP 26H BB

LB 10.000
GB 0.0
CX 25.00
CY 0.0
F1 59.991P
F2 -60.006P
HZ/CM 308.203
PPM/CM 4.800
SR 10493.65

2.25

206.327

130.226

Current Data Parameters
 NAME: cbl07
 EXPNO: 2
 PROCNO: 1
 F2 - Acquisition Parameters
 Date_ : 20081119
 Time: 11.39
 INSTRUM: spect
 PROBHD: 5 mm QNP 1H/1
 PULPROG: zgpg30
 TD: 65536
 SOLVENT: CDCl3
 NS: 190
 DS: 4
 SWH: 31446.541 Hz
 FIDRES: 0.478936 Hz
 AQ: 1.0420754 sec
 RG: 327.671
 DW: 15.900 us
 DE: 6.00 us
 TE: 300.2 K
 D1: 2.00000000 sec
 D11: 0.03000000 sec
 D12: 0.00020000 sec
 CHANNEL f1 ==
 NUC1: 13C
 P1: 7.50 us
 PL1: 0.00 dB
 SFO1: 125.8369556 MHz
 =====
 CHANNEL f2 ==
 CPDPRG2: waltz16
 NUC2: 1H
 P2: 100.00 us
 PL2: 0.00 dB
 PL12: 19.00 dB
 PL13: 26.00 dB
 SFO2: 500.3920016 MHz
 F2 - Processing parameters
 SI: 32768
 SF: 125.8230443 MHz
 WDW: EM
 SSB: 0
 LB: 1.00 Hz
 GB: 0
 PC: 1.40
 1D NMR plot parameters
 CX: 21.00 ct
 FIP: 220.000 DE
 ZF: 270.000 MHz
 F2p: -5.000 DE
 F2: -629.12 Hz
 PENCH: 10.71429 DE
 HZCH: 1349.10400 Hz

```

Current Data Parameters
NAME      criB026
EXPNO     5
PROCNO    1

F2 - Acquisition Parameters
Date_     20020202
Time      4.47
INSTRUM   spect
PROBHD    5 mm QNP 1H/1
PULPROG   zgpg30
TD         131072
SOLVENT   CDCl3
NS         63
DS         4
SWH        100000.000 Hz
FIDRES     0.762939 Hz
AQ         0.6554100 sec
RG         3.2048
DE         5.000 usec
TE         300.0 K
D1         1.00000000 sec
d11        0.03000000 sec
d12        0.00002000 sec

===== CHANNEL f1 =====
NUC1       13C
P1         10.60 usec
PL1        0.00 dB
SFO1       470.5455277 MHz

===== CHANNEL f2 =====
CPDPRG2    waltz16
NUC2       1H
PCPD2      95.00 usec
PL2        0.00 dB
PL12       26.00 dB
SFO2       500.1320005 MHz

F2 - Processing parameters
SI         65536
SF         470.5925870 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00

1D NMR plot parameters
CX         20.00 cm
F1P        -100.000 ppm
F1         -47059.26 Hz
F2P        -200.000 ppm
F2         -91885.42 Hz
PPMCM      5.00000 Hz/cm
HZCM       2352.96289 Hz/cm

```

-141.583

B115MM.500
DATE 24-8-1

SF 64.210
SY 64.2
O1 10000.000
SI 8192
TD 4096
SW 10000.000
HZ/PT 2.441

PW 4.5
RD 0.0
AQ .205
RG 160
NS 581
TE 297

FW 12500
O2 3300.000
DP 26H 88

LB 10.000
GB 0.0
CX 25.00
CY 0.0
F1 59.999P
F2 -69.998P
HZ/CM 333.887
PPM/CM 5.200
SR 10378.42

PPM

3.991

5.441
5.428
5.415

2.061
2.057
2.053
2.048
2.044
2.025
2.010
1.994
1.979
1.965
1.950
1.938
0.919
0.908
0.904
0.893
0.889
0.878
0.840

Current Data Parameters
NAME ccd167
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20010513
Time 11:53
INSTRUM spect
PROBHD 5 mm QNP 290
PULPROG zgpg30
TD 32768
SOLVENT CDCl₃
NS 16
DS 2
SWH 600.62 Hz
FIDRES 0.185399 Hz
AQ 2.7263477 sec
RG 327.68
DM 83.200 usec
DE 6.00 usec
TE 300.2 K
D1 1.0000000 sec
----- CHANNEL f1 -----
NUC1 ¹H
P1 7.50 usec
PL1 0.00 dB
SFO1 500.3922019 MHz
F2 - Processing Parameters
SF 500.3900115 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
ID NOE plot parameters
CD 20.00 cm
FIP 10.000 ppm
FIDRES 0.185399 Hz
F2P 10.000 ppm
F2 -500.39 Hz
FREQ 500.3900115 MHz
HETCON 270.21451 Hz/cm

30.383
30.226
30.073
29.919
29.766
29.613
29.459
23.005
21.274
15.439
15.375

Current Data Parameters
NAME: crb107
PROCNO: 1
F2 - Acquisition Parameters
Time: 200.13
Date_ : 11.19
INSTRUM: spect
PROBHD: 5 mm QNP 1H/1
PULPROG: zgpg30
TD: 65536
SOLVENT: CDCl3
NS: 130
DS: 4
SWH: 31446.541 Hz
FIDRES: 0.477836 Hz
AQ: 1.0420754 sec
RG: 327.67
WDW: EM
SS: 30.000 us
LB: 15.900 us
GB: 0
PC: 1.40
DE: 6.00 us
TE: 300.00 K
D1: 2.00000000 sec
D11: 0.03000000 sec
D12: 0.00020000 sec
===== CHANNEL f1 =====
NUC1: 13C
P1: 7.50 us
PL1: 0.00 dB
SFO1: 125.8365556 MHz
===== CHANNEL f2 =====
CPDPRG2: waltz16
NUC2: 1H
P2: 100.00 us
PL2: 0.00 dB
PL3: 0.00 dB
PL13: 28.00 dB
SFO2: 500.3920016 MHz
F2 - Processing parameters
SI: 32768
SF: 125.8230443 MHz
WDW: EM
SS: 30.000 us
LB: 15.900 us
GB: 0
PC: 1.40
1D NMR plot parameters
CX: 21.00 ct
FIP: 220.000 DE
Z: 2768.000 DE
F2p: -5.000 DE
F2: -629.12 Hz
PENCH: 10.71429 DE
HECH: 1348.10400 Hz

206.327

Current Data Parameters
NAME ctb102
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20070605
Time 14.53
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg30
TD 131072
SOLVENT CDCl3
NS 63
DS 4
SWH 100000.000 Hz
FIDRES 0.725358 Hz
AQ 0.6584100 sec
RG 1024
DM 5.000 usec
DE 6.00 usec
TE 300.2 K
D1 1.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec

===== CHANNEL f1 =====
NUC1 19F
P1 10.60 usec
PL1 -3.00 dB
SFO1 470.7901483 MHz
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
P2 100.00 usec
PL2 0.00 dB
PL12 26.00 dB
SFO2 500.3920016 MHz
F2 - Processing parameters
SI 65536
SF 470.8372320 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
F1P -100.000 ppm
F1 -47083.72 Hz
F2P -200.000 ppm
F2 -94167.44 Hz
PPMCM 5.00000 ppm/cm
HZCM 2354.18604 Hz/cm

1f

-143.003

S37

Kdd

B115MM.500
DATE 23-8-1

SF 64.210
SY 64.2
OI 10000.000
SI 8192
TD 4096
SW 10000.000
HZ/PT 2.441

PW 4.5
RD 0.0
AQ .205
RG 160
NS 3240
TE 297

FW 12500
O2 3300.000
DP 26H BB

LB 10.000
GB 0.0
CX 25.00
CY 0.0
F1 59.999P
F2 -69.998P
HZ/CM 333.887
PPM/CM 5.200
SR 10378.42

5.0963
4.2697

7.335
7.322
7.318
7.307
7.064
7.046
7.029
6.453
6.417
6.124
6.117
6.110
6.087
6.080

1g

Current Data Parameters
NAME C20070
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20071114
Time 11.14
INSTRUM spect
PROBHD 5 mm QNP 2930
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 16
DS 2
SWH 600.62 Hz
FIDRES 0.18339 Hz
AQ 2.723977 sec
RG 327.68
W 63.200 usec
DE 6.00 usec
TE 300.2 K
D1 1.0000000 sec
----- CHANNEL f1 -----
NUC1 1H
P1 7.50 usec
PL1 0.00 dB
SFO1 500.3922019 MHz
F2 - Processing parameters
SF 500.3900115 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
ID Non plot parameters
CD 20.00 cm
FIP 10.000 ppm
F2 500.3900115 MHz
F2P -10.000 ppm
F2 -500.39 Hz
PCLOCK 125.000 MHz
RECN 275.21451 Hz/G

3.302

2.494
2.491

0.617

0.467

1.023

1.000

1.965

2.044

ppm

1g

Current Data Parameters
NAME: crb070
PROCNO: 1
F2 - Acquisition Parameters
Time: 20.00
Time: 11.50
INSTRUM: spect
PROBHD: 5 mm QNP 1H/1
PULPROG: zgpg30
TD: 65536
SOLVENT: CDCl3
NS: 80
DS: 4
SWH: 31446.541 Hz
FIDRES: 0.478936 Hz
AQ: 1.0420724 sec
RG: 327.68
WDW: EM
SS: 30.000000
LB: 3.000000
GB: 0
PC: 1.40
F2 - Processing parameters
SI: 32768
SF: 125.8231160 MHz
WDW: EM
SS: 30.000000
LB: 3.000000
GB: 0
PC: 1.40
1D NMR plot parameters
CX: 21.00 ct
FIP: 177.986 DE
ZGPG: 22.000000 DE
F2P: 20.797 DE
F2: 2616.71 Hz
FENCH: 7.48518 DE
HECH: 941.69520 DE

Current Data Parameters
NAME ctb070
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20020417
Time 14.04
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg30
TD 131072
SOLVENT CDCl3
NS 120
DS 4
SWH 100000.000 Hz
AQ 0.0225589 sec
RG 0.6534100 sec
RG 1625.5
DM 5.000 usec
DE 6.00 usec
TE 300.2 K
D1 1.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec

===== CHANNEL f1 =====
NUC1 19F
P1 10.60 usec
PL1 -3.00 dB
SFO1 470.7901483 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
P2 100.00 usec
PL2 0.00 dB
PL12 26.00 dB
SFO2 500.3920016 MHz

F2 - Processing parameters
SI 65536
SF 470.8372320 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
F1P -100.000 ppm
F1 -47083.72 Hz
F2P -200.000 ppm
F2 -94167.44 Hz
PPMCM 5.00000 ppm/cm
HZCM 2354.18604 Hz/cm

B115MM.500
DATE 24-8-1

SF 64.210
SY 64.2
O1 10000.000
SI 8192
TO 4096
SW 10000.000
HZ/PT 2.441

PW 4.5
RD 0.0
AQ .205
RG 160
NS 420
TE 297

FW 12500
O2 3300.000
DP 26H BB

LB 10.000
GB 0.0
CX 25.00
CY 0.0
F1 59.999P
F2 -69.998P
HZ/CM 333.887
PPM/CM 5.200
SR 10378.42

Current Data Parameters
 NAME: cbl04
 PROCNO: 1
 F2 - Acquisition Parameters
 Time: 20.00
 INSTRUM: spect
 PROBD: 5 mm QNP 1H/1
 PULPROG: zgpg30
 TD: 65536
 SOLVENT: Aceton
 NS: 476
 DS: 4
 SWH: 31446.541 Hz
 FIDRES: 0.479936 Hz
 AQ: 1.0420724 sec
 RG: 327.68
 DW: 15.900 us
 DE: 6.00 us
 TE: 300.2 K
 D1: 2.00000000 sec
 D11: 0.03000000 sec
 D12: 0.00020000 sec
 CHANNEL f1 ==
 NUC1: 13C
 P1: 7.50 us
 PL1: 0.00 dB
 SFO1: 125.836556 MHz
 =====
 CHANNEL f2 ==
 NUC2: 1H
 PULPROG: zgpg30
 P1: 95.00 us
 PL2: 0.00 dB
 PL12: 0.00 dB
 PL13: 28.00 dB
 SFO2: 500.3920016 MHz
 F2 - Processing parameters
 SI: 32768
 SF: 125.8231160 MHz
 WDW: EM
 SS: 0
 LB: 1.00 Hz
 GB: 0
 PC: 1.40
 =====
 1D NMR plot parameters
 CX: 21.00 cr
 FIP: 220.000 DE
 ZF: 270.000 DE
 F2: -5.000 DE
 F2: -629.12 Hz
 PENCH: 10.71429 DE
 HECH: 1346.10474 Hz

Current Data Parameters
NAME ctb104
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20070606
Time 14:08
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg30
TD 131072
SOLVENT CDCl3
NS 122
DS 4

SWH 100000.000 Hz
FIDRES 0.725358 Hz
AQ 0.6584100 sec
RG 4096
DM 5.000 usec
DE 6.00 usec
TE 300.2 K
D1 1.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec

===== CHANNEL f1 =====
NUC1 ¹⁹F
P1 10.60 usec
PL1 -3.00 dB
SFO1 470.7901483 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 ¹H
P2 100.00 usec
PL2 0.00 dB
PL12 26.00 dB
SFO2 500.3920016 MHz

F2 - Processing parameters
SI 65536
SF 470.8372320 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
F1P -100.000 ppm
F1 -47083.72 Hz
F2P -200.000 ppm
F2 -94167.44 Hz
PPMCM 5.00000 ppm/cm
HZCM 2354.18604 Hz/cm

-141.650
-141.708

1h

B115MM.500
DATE 24-8-1

SF 64.210
SY 64.2
O1 10000.000
SI 8192
TD 4096
SW 10000.000
HZ/PT 2.441

PW 4.5
RD 0.0
AQ .205
RG 160
NS 581
TE 297

FW 12500
O2 3300.000
DP 26H BB

LB 10.000
GB 0.0
CX 25.00
CY 0.0
F1 59.999P
F2 -69.998P
HZ/CM 333.887
PPM/CM 5.200
SR 10378.42

PPM

5.6225

7.643
7.629
7.627
7.195
7.192
7.180
7.168
7.164
7.072
7.069
7.067
7.054
7.042
7.040
7.038
6.570
5.707
5.694
5.690
5.680
5.677
5.663
5.650

1j

2.862
2.830
2.828
2.057
2.052
2.048
2.044

Current Data Parameters
NAME ccd168
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20070707
Time 12.01
INSTRUM spect
PROBHD 5 mm QNP 293D
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 16
DS 2
SWH 600.62 Hz
FIDRES 0.18339 Hz
AQ 2.7263477 sec
RG 327.68
DM 83.200 usec
DE 6.00 usec
TE 300.2 K
D1 1.0000000 sec
----- CHANNEL f1 -----
NUC1 1H
P1 7.20 usec
PL1 0.00 dB
SFO1 500.3920019 MHz
F2 - Processing Parameters
SF 500.3900115 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
ID NOE plot parameters
CD 20.00 cm
FIP 10.000 ppm
SFO2 500.3900115 MHz
F2P -0.500 ppm
F2 -250.20 Hz
FREQM 0.500 MHz/G
RECN 262.70477 Hz/G

Current Data Parameters
NAME: crbl09
PROCNO: 1
F2 - Acquisition Parameters
Time: 20.01
Date_: 21.35
INSTRUM: spect
PROBHD: 5 mm QNP 1H/1
PULPROG: zgpg30
TD: 65536
SOLVENT: CDCl3
NS: 391
DS: 4
SWH: 31446.541 Hz
FIDRES: 0.478936 Hz
AQ: 1.042072 sec
RG: 327.68
DW: 15.900 us
DE: 6.00 us
TE: 300.0 K
T1: 2.00000000 sec
D11: 0.03000000 sec
D12: 0.0002000 sec
===== CHANNEL f1 =====
NUC1: 13C
P1: 7.50 us
PL1: 0.00 dB
SFO1: 125.8365556 MHz
===== CHANNEL f2 =====
CPDPRG2: waltz16
NUC2: 1H
PCPD2: 100.00 us
PL2: 0.00 dB
PL3: 0.00 dB
PL13: 28.00 dB
SFO2: 500.3920016 MHz
F2 - Processing parameters
SI: 32768
SF: 125.8231160 MHz
WDW: EM
SSB: 0
LB: 1.00 Hz
GB: 0
PC: 1.40
1D NMR plot parameters
CX: 21.00 ct
FIP: 234.956 DE
ZGPG: 23.00 DE
F2p: -14.91 DE
F2: -1883.68 Hz
PENCH: 11.90127 DE
HECH: 1497.45435 DE

Current Data Parameters
NAME ctb108
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20020612
Time 14.15
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg30
TD 131072
SOLVENT CDCl3
NS 111
DS 4
SWH 100000.000 Hz
FIDRES 0.72535 Hz
AQ 0.653400 sec
RG 1625.5
DN 5.000 usec
DE 6.00 usec
TE 300.2 K
D1 1.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec

===== CHANNEL f1 =====
NUC1 ¹⁹F
P1 10.60 usec
PL1 -3.00 dB
SFO1 470.7901483 MHz
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 ¹H
P2 100.00 usec
PL2 0.00 dB
PL12 26.00 dB
SFO2 500.3920016 MHz
F2 - Processing parameters
SI 65536
SF 470.8372320 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
F1P -100.000 ppm
F1 -47083.72 Hz
F2P -200.000 ppm
F2 -94167.44 Hz
PPMCM 5.00000 ppm/cm
HZCM 2354.18604 Hz/cm

-136.309
-136.405
-136.528
-136.635

-152.578

1j

B115MM.500
DATE 24-8-1

SF 64.210
SY 64.2
O1 10000.000
SI 8192
TD 4096
SW 10000.000
HZ/PT 2.441

PW 4.5
RD 0.0
AQ .205
RG 160
NS 556
TE 297

FW 12500
O2 3300.000
DP 25H 88

LB 10.000
GB 0.0
CX 25.00
CY 0.0
F1 59.999P
F2 -69.998P
HZ/CM 333.887
PPM/CM 5.200
SR 10378.42

PPM

7.4561
6.6209
5.7789

3c

Current Data Parameters
 NAME: 2CEN063
 EXPNO: 1
 PROCNO: 1
 F2 - Acquisition Parameters
 Date_ 20071221
 Time 21.12
 INSTRUM spect
 PULPROG zgpg30
 TD 32768
 ID 837
 NS 837
 DS 2
 SWH 600.62 Hz
 FIDRES 0.183399 Hz
 AQ 2.7263477 sec
 SFO1 500.132006 MHz
 DM 83200 usec
 DE 6.00 usec
 TE 300.2 K
 D1 1.0000000 sec
 CHANNEL f1
 NUC1 1H
 P1 7.50 usec
 PL1 0.00 dB
 SFO1 500.132006 MHz
 F2 - Processing Parameters
 SF 500.130025 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00
 ID NOE plot parameters
 CD 20.00 cm
 FIP 10.000 ppm
 FID 10.000 ppm
 F2P -1.000 ppm
 F2 -500.13 Hz
 FREQ 500.130025 MHz
 RECN 275.07150 Hz/G

8.153
 8.136
 8.131
 7.454
 7.436
 7.262
 6.447
 6.438
 6.432

3f

Current Data Parameters
 NAME CEN007
 EXPNO 1
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 20070907
 Time 10.07
 INSTRUM spect
 PULPROG zgpg30
 TD 32768
 ID 32768
 NS 832
 DS 2
 FIDRES 0.183399 Hz
 AQ 2.7263477 sec
 SFO1 500.1320006 MHz
 DM 83200 usec
 DE 6.00 usec
 TE 300.2 K
 D1 1.0000000 sec
 CHANNEL f1
 NUC1 1H
 P1 7.50 usec
 PL 0.00 dB
 SFO1 500.1320006 MHz
 F2 - Processing Parameters
 SF 500.1300127 MHz
 DS 2
 SFO1 500.1300127 MHz
 LB 0
 GB 0
 RB 0
 PC 1.00
 ID NMR plot parameters
 CD 20.00 cm
 F1 10.000 ppm
 F2 0.000 ppm
 F3 -0.500 ppm
 F4 -250.07 Hz
 F5 0.500 Hz/G
 HZCN 262.56824 Hz/G

7.890
7.887
7.877
7.873
7.409
7.392
7.260
6.430
6.398
6.385
6.373
6.353

2.603
2.591
2.572
2.252
2.238
2.227
2.212
1.508
1.494
1.480
1.466
1.450
1.338
1.318
1.306
1.290
1.282
0.897
0.884
0.870
0.000

Current Data Parameters
 NAME: crb007
 PROCNO: 1
 F2 - Acquisition Parameters
 Time: 20051113 10.13
 INSTRUM: spect
 PROBD: 5 mm QNP 1H/1
 PULPROG: zgpg30
 TD: 65536
 SOLVENT: CDCl3
 NS: 118
 DS: 4
 SWH: 31446.541 Hz
 FIDRES: 0.477936 Hz
 AQ: 1.042524 sec
 RG: 327.680
 DW: 15.940 us
 DE: 6.00 us
 TE: 300.2 K
 D1: 2.00000000 sec
 d11: 0.03000000 sec
 d12: 0.00020000 sec
 CHANNEL f1 ==
 NUC1: 13C
 P1: 7.50 us
 PL1: 0.00 dB
 SFO1: 125.7713719 MHz
 CHANNEL f2 ==
 NUC2: 1H
 P2: 95.00 us
 PL2: 0.00 dB
 PL3: 28.00 dB
 PL13: 28.00 dB
 SFO2: 500.1320005 MHz
 F2 - Processing parameters
 SI: 32768
 SF: 125.7577955 MHz
 WDW: EM
 SS: 0
 LB: 1.00 Hz
 GB: 0
 PC: 1.40
 1D NMR plot parameters
 CX: 21.00 cr
 FIP: 220.000 DE
 ZF: 270.000 MHz
 F2p: -5.000 DE
 F2: -628.79 Hz
 FENCH: 10.71429 DE
 HZCH: 1347.4535 Hz

Current Data Parameters
 NAME: 20020601
 EXPNO: 1
 PROCNO: 1
 F2 - Acquisition Parameters
 Date_: 20020601
 Time: 12.00
 INSTRUM: spect
 PULPROG: zgpg30
 TD: 32768
 NS: 400
 DS: 2
 SWH: 6000.62 Hz
 FIDRES: 0.183399 Hz
 AQ: 2.7263477 sec
 RG: 327.68
 DW: 83.200 usec
 DE: 6.00 usec
 TE: 300.2 K
 D1: 1.0000000 sec
 CHANNEL: f1
 NUC1: 1H
 P1: 7.50 usec
 PL1: 0.00 dB
 SFO1: 500.1320006 MHz
 F2 - Processing Parameters
 SF: 500.1300238 MHz
 WDW: EM
 SSB: 0
 LB: 0.30 Hz
 GB: 0
 PC: 1.00
 ID: NMR plot parameters
 CX: 20.00 cm
 FIP: 10.000 ppm
 FID: 0.000 Hz
 F2P: -0.500 ppm
 F2: -250.07 Hz
 FREQ0: 0.500 MHz/G
 RECN: 262.56827 Hz/G

Current Data Parameters
 NAME: crb016
 PROCNO: 1
 F2 - Acquisition Parameters
 Time: 2.002803
 Date_: 8.37
 INSTRUM: spect
 PROBD: 5 mm QNP 1H/1
 PULPROG: zgpg30
 TD: 65536
 SOLVENT: CDCl3
 NS: 171
 DS: 4
 SWH: 31446.541 Hz
 FIDRES: 0.478936 Hz
 AQ: 1.042524 sec
 RG: 327.68
 DW: 15.940 us
 DE: 6.00 us
 TE: 300.2 K
 D1: 2.00000000 sec
 d11: 0.03000000 sec
 d12: 0.00020000 sec
 CHANNEL f1 ==
 NUC1: 13C
 P1: 7.50 us
 PL1: 0.00 dB
 SFO1: 125.7713719 MHz
 =====
 CHANNEL f2 ==
 PULPROG: zgpg30
 NUC2: 1H
 WALTZ16
 PCPD2: 95.00 us
 PL2: 0.00 dB
 PL3: 0.00 dB
 PL13: 28.00 dB
 SFO2: 500.1320005 MHz
 F2 - Processing parameters
 SI: 32768
 SF: 125.7577917 MHz
 WDW: EM
 SSF: 0
 LB: 1.00 Hz
 GB: 0
 PC: 1.40
 1D NMR plot parameters
 CX: 21.00 ct
 FIP: 220.000 DE
 ZF: 270.000 MHz
 F2p: -5.000 DE
 F2: -628.79 Hz
 FENCH: 10.71429 DE
 HZCH: 1347.40491 Hz

31

Current Data Parameters	
NAME	crs002
PRGNO	1
Data Acquisition Parameters	
Time	24.12.12
Time	14.53
INSTRUM	SP1
PROBHD	5 mm QNP 1H/13
PULPROG	zg30
PROBHD	5 mm QNP 1H/13
SOLVENT	CDCl3
NS	66
DS	4
SWH	6093.615 Hz
FIDRES	0.163339 Hz
WDW	EM
SSB	0
LB	2.76277 Hz
GB	0
PC	83.200 sec
DC	0
WDW	EM
SSB	0
LB	300.0 Hz
GB	0
PC	1.000000 sec
DC	0
CHANNEL F2	
NUC1	13C
NUC2	1H
PCPD1	7.00 sec
PL1	0.0000 MHz
PL2	500.132000 MHz
F2 - Processing parameters	
F2	32768
WDW	EM
SSB	0
LB	500.130000 MHz
GB	0
PC	0.26207 sec
DC	0
PC	1.00
1D NMR plot parameters	
CD	20.00 cm
CP	0
PL1	500.1300 MHz
F2	32768
F2	-1.000 ppm
F2	0.500000 MHz
PC	0.26207 sec
PC	275.07153 Hz/cm

Current Data Parameters	
NAME	etbol4
EXPNO	1
PROCNO	1
F2 - Acquisition Parameters	
Time	17.24
INSTRUM	gpc30
PULPROG	zgpg30
SOLVENT	DMSO
NS	42
DS	4
SWH	6099.61 Hz
FIDRES	0.183599 Hz
AQ	2.76263372 sec
RG	32
RG2	83.2000 usec
RG3	30.0000 usec
DE	1.00000000 sec
DE2	
DE3	
CHANNEL f1	
NUC1	¹ H
P1	7.50 usec
PL1	0.00 dB
RF1	500.1320000 MHz
F2 - Processing parameters	
SF	32768
WDW	EM
SSB	500.1300490 MHz
GB	0
PC	0.30 Hz
LB	1.00 Hz
GB2	
PC2	
LB2	
GB3	
PC3	
LB3	
DC NMR plot parameters	
IND	20.00 cm
PRP	50.000 ppm
F1P	-1.000 ppm
F2P	-500.113 Hz
F3P	275.07155 Hz/cm
HZCM

5.396 —
5.171 —

210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

7.637
7.620
7.583
7.567
7.537
7.522
7.402
7.387
7.372
7.331
7.316
7.302
7.253
7.226
7.194
7.100
7.068

0.075
0.000

4d

Current Data Parameters
NAME: 20022006
EXPNO: 1
PROCNO: 1
F2 - Acquisition Parameters
Date_ : 20022006
Time : 9.07
INSTRUM: spect
PROBHD: 5 mm QNP 2930
PULPROG: zgpg30
TD: 32768
SOLVENT: CDCl3
NS: 63
DS: 2
SWH: 6008.62 Hz
FIDRES: 0.185399 Hz
AQ: 2.7263477 sec
RG: 327.68
DM: 83.200 usec
DE: 6.00 usec
TE: 300.2 K
D1: 1.0000000 sec
----- CHANNEL f1 -----
NUC1: 1H
P1: 7.50 usec
PL1: 0.00 dB
SFO1: 500.1320006 MHz
F2 - Processing parameters
SF: 500.1300169 MHz
WDW: EM
SSB: 0
LB: 0.30 Hz
GB: 0
PC: 1.00
ID: NMR plot parameters
CX: 20.00 cm
FIP: 10.000 ppm
SFO2: 500.1300169 MHz
F2P: -1.000 ppm
FZ: -500.13 Hz
GPCPM: 0.0000000 Hz/G
HSCN: 273.07150 Hz/C

1.935
2.004
1.993
1.984
0.992
1.030
1.003

141.804
136.256
132.463
132.380
128.832
128.618
126.887
126.836
126.695
119.003
110.554

4d

77.252
76.999
76.745

Current Data Parameters
NAME crb006
PROCNO 1
F2 - Acquisition Parameters
Time 2.003119
Time 9.12
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg30
TD 65536
SOLVENT CDCl₃
NS 156
DS 4
SWH 31446.541 Hz
FIDRES 0.477836 Hz
AQ 1.042524 sec
RG 327.680
WDW EM
SS 15.940 us
DE 6.00 us
TE 300.00 K
D1 2.00000000 sec
d11 0.03000000 sec
d12 0.00020000 sec
===== CHANNEL f1 =====
NUC1 13C
P1 7.50 us
PL1 0.00 dB
SFO1 125.7713719 MHz
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
P2 95.00 us
PL2 0.00 dB
PL3 0.00 dB
PL13 26.00 dB
SFO2 500.1320005 MHz
F2 - Processing Parameters
SI 32768
SF 125.7577955 MHz
WDW EM
SS 15.940 us
LB 1.00 Hz
GB 0
PC 1.40
F2 - 1D NMR plot parameters
CX 21.00 ct
FIP 220.000 DE
Z 2768.000 DE
F2p -5.000 DE
F2 -628.79 Hz
FENCH 10.71429 DE
HECH 1347.40505 Hz

Current Data Parameters
 NAME: crb020
 PROCNO: 1
 F2 - Acquisition Parameters
 Time: 2.002114
 INSTRUM: spect
 PROBD: 5 mm QNP 1H/1
 PULPROG: zgpg30
 ID: 6556
 SOLVENT: CDCl3
 NS: 217
 DS: 4
 SWH: 31446.541 Hz
 FIDRES: 0.478936 Hz
 AQ: 1.042524 sec
 RG: 327.680
 DW: 15.900 us
 DE: 6.00 us
 TE: 300.0 K
 D1: 2.00000000 sec
 d11: 0.03000000 sec
 d12: 0.00020000 sec
 CHANNEL f1 ==
 NUC1: 13C
 P1: 7.50 us
 PL1: 0.00 dB
 SFO1: 125.7713719 MHz
 CHANNEL f2 ==
 NUC2: 1H
 PULPROG: zgpg30
 WALTZ16
 PCPD2: 95.00 us
 PL2: 0.00 dB
 PL3: 0.00 dB
 PL13: 28.00 dB
 SFO2: 500.1320005 MHz
 F2 - Processing parameters
 SI: 327.68
 SF: 125.7577955 MHz
 WDW: EM
 SSB: 0
 LB: 1.00 Hz
 GB: 0
 PC: 1.40
 1D NMR plot parameters
 CX: 21.00 cr
 FIP: 220.000 DE
 ZF: 270.000 MHz
 F2p: -5.000 DE
 F2: -628.79 Hz
 PENCH: 10.71429 DE
 HZCH: 1347.40505 Hz

4e

7.622
7.605
7.555
7.539
7.506
7.502
7.495
7.489
7.482
7.478
7.171
7.139
7.085
7.081
7.068
7.054
7.051
7.002
6.969

4g

Current Data Parameters
NAME: CEN072
EXPNO: 1
PROCNO: 1
F2 - Acquisition Parameters
Date_ : 20080515
Time : 18.45
INSTRUM : spect
PROBHD : 5 mm QNP 2930
PULPROG : zgpg30
TD : 32768
SOLVENT : CDCl3
NS : 16
DS : 2
SWH : 600.62 Hz
FIDRES : 0.185399 Hz
AQ : 2.7263477 sec
RG : 327.68
DM : 83.200 usec
DE : 6.00 usec
TE : 300.2 K
D1 : 1.0000000 sec
----- CHANNEL f1 -----
NUC1 : 1H
P1 : 7.50 usec
PL1 : 0.00 dB
SFO1 : 500.3920019 MHz
F2 - Processing Parameters
SF : 500.3900189 MHz
WDW : EM
SSB : 0
LB : 0.30 Hz
GB : 0
PC : 1.00
ID: NMR plot parameters
SI : 32768
SF : 500.3900189 MHz
WDW : EM
SSB : 0
LB : 0.30 Hz
GB : 0
PC : 1.00
CD : 20.00 cm
FIP : 10.000 ppm
SFO2 : 500.3900189 MHz
F2P : -0.500 ppm
F2 : -250.20 Hz
NUC2 : 13C
P2 : 6.00 usec
PL2 : 0.00 dB
SFO3 : 262.14477 Hz

Current Data Parameters
NAME: crb073
PROCNO: 1
F2 - Acquisition Parameters
Time: 20.0313
Time: 20.13
INSTRUM: spect
PROBHD: 5 mm QNP 1H/1
PULPROG: zgpg30
TD: 65536
SOLVENT: CDCl3
NS: 173
DS: 1
SWH: 31446.541 Hz
FIDRES: 0.478936 Hz
AQ: 1.0420724 sec
RG: 327.67
WDW: EM
SSB: 0
LB: 1.00 Hz
GB: 0
PC: 1.40
F2 - Processing Parameters
SI: 32768
SF: 125.8231160 MHz
WDW: EM
SSB: 0
LB: 1.00 Hz
GB: 0
PC: 1.40
1D NMR plot parameters
CX: 21.00 cr
FIP: 220.000 DE
Z: 2768.000 DE
F2p: -5.000 DE
F2: -629.12 Hz
PENCH: 10.71429 DE
HECH: 1348.10474 Hz

7.493
7.479
7.476
7.319
7.303
7.261
7.251
7.240
7.237
7.231
7.194
7.188
7.183
7.178
6.773
6.748
6.579
6.554

Current Data Parameters
NAME csbl30
EXPNO 1
PROCNO 1
PP2 Acquisition Parameters
Date_ 20080903
Time 18.50
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 16
DS 4
SWH 6009.635 Hz
FIDRES 0.183399 Hz
AQ 2.726477 sec
RG 327.5
DM 83.200 usec
DE 3.00 usec
TE 300.2 K
D1 1.0000000 sec
===== CHANNEL f1 =====
NUC1 1H
P1 7.00 usec
PL1 0.00 dB
SFO1 500.13625019 MHz
F2 - Processing parameters
SI 32768
SF 500.1360156 MHz
WDW EM
SSB 0
GB 0.50 Hz
PC 1.00
1D NMR plot parameters
CX 20.00 cm
F1P 10.000 ppm
F2P 500.1360156 MHz
F2P -1.000 ppm
F2 500.139 Hz
F2ACQ 1.0000000 Hz/GS
HSCN 275.21451 Hz/cm

1.579

1.986
2.030
2.957
1.904
0.993
1.000

142.035
136.200
133.279
131.965
129.491
128.720
128.461
128.330
127.781
118.887
110.439

77.254
77.000
76.746

Current Data Parameters
NAME: 4j
EXPNO: 2
PROCNO: 1
F2 - Acquisition Parameters
Date_: 20020623
Time: 18.53
INSTRUM: spect
PROBHD: 5 mm QNP 400P
PULPROG: zgpg
TD: 65536
SOLVENT: CDCl3
NS: 208
DS: 4
SWH: 31445.541 Hz
FIDRES: 0.77953 Hz
RG: 1.042974
RG: 9195.2
DW: 15.900 us
DE: 360.00 us
TE: 300.0 K
D1: 2.00000000 se
D11: 0.03000000 se
D12: 0.00002000 se
===== CHANNEL f1 =====
NUC1: 13C
P1: 1.50 us
PL1: 0.00 dB
SFO1: 125.8369556 MHz
===== CHANNEL f2 =====
CPDPRG2: waltz16
NUC2: 1H
PCPD2: 100.00 us
PL2: 0.00 dB
PL12: 0.00 dB
PL13: 26.00 dB
SFO2: 500.3920016 MHz
F2 - Processing parameters
SI: 32768
SF: 125.8231742 MHz
WDW: EM
SSB: 0
LB: 1.00 Hz
GB: 0
PC: 1.40
1D NMR plot parameters
CX: 22.00 C°
F1P: 1.400000 Hz
F1R: 18758.03 Hz
F2P: 95.897 Hz
F2R: 12569.33 Hz
GAMMA: 125.69 Hz
HETCON: 283.12292 Hz

7.796
7.790
7.532
7.516
7.440
7.407
7.383
7.369
7.353
7.327
7.323
7.308
7.304
7.295
7.249
7.232
7.225

1.947

0.000

Current Data Parameters
NAME CEB041
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20090901
Time 11:54
INSTRUM spect
PROBHD 5 mm QNP 293D
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 639
DS 2
SWH 6008.62 Hz
FIDRES 0.183399 Hz
AQ 2.726347 sec
RG 327.5
DM 83.200 usec
DE 6.00 usec
TE 300.2 K
D1 1.0000000 sec
----- CHANNEL f1 -----
NUC1 1H
P1 7.50 usec
PL1 0.00 dB
SFO1 500.3920019 MHz
F2 - Processing Parameters
SF 500.3900217 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
ID NOE plot parameters
CD 20.00 cm
FIP 10.000 ppm
SFO2 500.3900217 MHz
F2P -0.500 ppm
F2 -230.20 Hz
NUC2 13C
P2 0.500 usec
PL2 0.00 dB
SFO3 262.14477 Hz

167.037
143.474
135.682
134.285
128.819
128.790
127.013
121.345
118.081
77.253
76.999
76.745

Current Data Parameters
 Name: 125-8369556
 EXPNO: 2
 PROCNO: 1
 F2 - Acquisition Parameters
 Date_: 20020320
 Time: 17.47
 INSTRUM: spect
 PULPROG: 5 mm QNP
 TD: 65536
 NUC1: 13C
 NUC2: 1H
 SOLVENT: DMSO
 DS: 4
 SWH: 31446.541 Hz
 FIDRES: 0.447755 Hz
 AQ: 0.0429734 sec
 RG: 4096
 DW: 15.900 us
 DE: 380.00 us
 TE: 300.2 K
 D1: 2.00000000 sec
 D11: 0.03000000 sec
 D12: 0.00002000 sec
 CHANNEL f1
 NUC1: 13C
 P1: 1.50 us
 PL1: 0.00 dB
 SFO1: 125.8369556 MHz
 CHANNEL f2
 NUC2: 1H
 P2: 100.00 us
 PL2: 0.00 dB
 PL12: 26.00 dB
 PL13: 26.00 dB
 SFO2: 500.3920016 MHz
 F2 - Processing parameters
 SI: 32768
 SF: 125.8231790 MHz
 WDW: EM
 SSB: 0
 LB: 1.00 Hz
 GB: 0
 PC: 1.40
 ID inner plot parameters
 CX: 21.00 CF
 F1P: 244.559 Hz
 F1Q: 244.559 Hz
 F2P: -15.472 DF
 F2Q: -15.472 DF
 GAMMA: 180.00 DF
 HZCN: 1497.8447 Hz

Current Data Parameters
 NAME: 6b
 EXPNO: 1
 PROCNO: 1
 F2 - Acquisition Parameters
 Date_ : 20020612
 Time : 12.06
 INSTRUM: spect
 PULPROG: zgpg30
 TD: 32768
 SFO1: 500.136099 MHz
 FIDRES: 0.183399 Hz
 AQ: 2.7263477 sec
 RG: 327.68
 DW: 83.200 usec
 DE: 6.00 usec
 TE: 300.2 K
 D1: 1.0000000 sec
 CHANNEL: f1
 NUC1: ¹H
 P1: 7.50 usec
 PL1: 0.00 dB
 SFO1: 500.136099 MHz
 F2 - Processing Parameters
 SF: 500.136099 MHz
 DS: 2
 AS: 0
 LB: 0.30 Hz
 GB: 0
 PC: 1.00
 ID: NMR plot parameters
 CD: 20.00 cm
 FIP: 10.000 ppm
 FID: 10.000 ppm
 F2P: 10.000 ppm
 F2: -500.39 Hz
 FREQ: 500.136099 MHz
 RECN: 273.21454 Hz/G

Current Data Parameters
 NAME: crb039
 PROCNO: 1
 F2 - Acquisition Parameters
 Time: 20051110
 Date_Time: 12.11
 INSTRUM: spect
 PROBD: 5 mm QNP 1H/1
 PULPROG: zgpg30
 ID: 6556
 SOLVENT: CDCl3
 NS: 107
 DS: 4
 SWH: 31446.541 Hz
 FIDRES: 0.478936 Hz
 AQ: 1.042072 s
 RG: 327.67
 DW: 15.900 us
 DE: 6.00 us
 TE: 300.0 K
 D1: 2.00000000 s
 D11: 0.03000000 s
 D12: 0.00020000 s
 CHANNEL f1 ==
 NUC1: 13C
 P1: 7.50 us
 PL1: 0.00 dB
 SFO1: 125.836556 MHz
 =====
 CHANNEL f2 ==
 PULPROG: waltz16
 INOC: 1H
 PCPD2: 100.00 us
 PL2: 0.00 dB
 PL3: 0.00 dB
 PL13: 26.00 dB
 SFO2: 500.3920016 MHz
 F2 - Processing parameters
 SI: 32768
 SF: 125.8231848 MHz
 WDW: EM
 SS: 0
 LB: 1.00 Hz
 GB: 0
 PC: 1.40
 1D NMR plot parameters
 CX: 21.00 ct
 FIP: 234.409 DE
 F1P: 250.131 MHz
 F2P: -15.517 DE
 F2: -1952.43 Hz
 PENCH: 11.90156 DE
 HZC4: 1497.45455 Hz

7.446
7.430
7.334
7.319
7.304
7.239
7.236
7.223
7.212
7.209
7.207
7.190
7.164
7.154
7.045
7.039
6.985
6.978
6.975
6.968
6.930
6.898

1.454
0.000

Current Data Parameters
NAME C2D060
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20060601
Time 16.10
INSTRUM spect
PROBHD 5 mm QNP 2930
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 16
DS 2
SWH 6000.62 Hz
FIDRES 0.185399 Hz
AQ 2.7263477 sec
RG 327.5
DM 83.200 usec
DE 6.00 usec
TE 300.2 K
D1 1.0000000 sec
----- CHANNEL f1 -----
NUC1 13
P1 7.50 usec
PL1 0.00 dB
SFO1 500.3920019 MHz
F2 - Processing Parameters
SF 500.3900495 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
ID NMR plot parameters
CD 20.00 cm
FIP 10.906 ppm
SFO 500.3900495 MHz
F2P -1.104 ppm
F2 -552.40 Hz
PCLOCK 0.0000000 Hz/G
HPCON 300.00077 Hz/G

565

142.839
136.925
128.649
128.300
127.543
126.257
126.041
124.286
121.740

77.250
76.996
76.741

39

Current Data Parameters
NAME: crb060
PROCNO: 1
F2 - Acquisition Parameters
Time: 2005.00
Time: 18.22
INSTRUM: spect
PROBHD: 5 mm QNP 1H/1
PULPROG: zgpg30
TD: 65536
SOLVENT: CDCl3
NS: 288
DS: 4
SWH: 31446.541 Hz
FIDRES: 0.477936 Hz
AQ: 1.0420754 sec
RG: 327.68
WDW: EM
SS: 0
LB: 1.00 Hz
GB: 0
PC: 1.40
F2 - Processing Parameters
SI: 327.68
SF: 125.8231809 MHz
WDW: EM
SS: 0
LB: 1.00 Hz
GB: 0
PC: 1.40
1D NMR plot parameters
CX: 21.00 cr
FIP: 234.440 DE
F1P: 249.870 DE
F2P: -15.487 DE
F2: -1348.59 Hz
F2: 11.90156 DE
H2CH: 1497.45455 Hz

6.983
6.965
7.103
7.135
7.239
7.241
7.253
7.256
7.300
7.306
7.310
7.316
7.323
7.336
7.339
7.346
7.349
7.354
7.461
7.476

0.000

Current Data Parameters
NAME: C2B071
EXPNO: 1
PROCNO: 1
F2 - Acquisition Parameters
Date_ : 20070111
Time : 17.44
INSTRUM : spect
PROBHD : 5 mm QNP 293D
PULPROG : zgpg30
TD : 32768
SOLVENT : CDCl3
NS : 1638
DS : 2
SWH : 6000.62 Hz
FIDRES : 0.183399 Hz
AQ : 2.7263477 sec
RG : 327.68
DM : 83.200 usec
DE : 5.00 usec
TE : 300.2 K
D1 : 1.0000000 sec
----- CHANNEL f1 -----
NUC1 : 1H
P1 : 7.50 usec
PL1 : 0.00 dB
SFO1 : 500.3920019 MHz
F2 - Processing Parameters
SF : 500.3900257 MHz
WDW : EM
SSB : 0
LB : 0.30 Hz
GB : 0
PC : 1.00
ID: NMR plot parameters
CX : 20.00 cm
FIP : 10.94 ppm
SFO : 500.3900257 MHz
F2P : -1.056 ppm
F2 : -528.55 Hz
NUC2 : 13C
P2 : 12.00 usec
PL2 : 0.00 dB
SFO2 : 300.40077 Hz

8.485
7.622
7.606
7.584
7.569
7.425
7.421
7.415
7.410
7.394
7.382
7.321
7.307
7.292
7.288
7.283
7.277
7.269
7.217
7.185
7.169
7.154
6.634
6.630
6.628
6.624

1.549

Current Data Parameters
NAME: cbl27
EXPNO: 1
PROCNO: 1
Date_ Acquisition: 20020626
Time: 16.57
INSTRUM: spect
PULPROG: zgpg30
TD: 65536
SOLVENT: CDCl3
NS: 16
DS: 4
SWH: 6019.615 Hz
FIDRES: 0.183399 Hz
AQ: 2.78577 sec
RG: 327.2
DM: 83.200 usec
DE: 3.00 usec
TE: 300.2 K
D1: 1.0000000 sec
===== CHANNEL f1 =====
NUC1: 1H
P1: 7.50 usec
PL1: 0.00 dB
SF01: 500.3925019 MHz
F2 - Processing Parameters
SI: 32768
SF: 500.3900115 MHz
WDW: EM
SSB: 0
LB: 0.30 Hz
GB: 0
PC: 1.00
===== 1D NMR plot parameters =====
CX: 22.00 cm
F1P: 8.82 ppm
F2P: 4.00 ppm
F3P: 5.80 ppm
F4P: 2902.28 Hz
F5P: 2902.28 Hz
F6P: 68.72978 Hz/C
HSCN: 68.72978 Hz/C

Current Data Parameters		Channel #1		Channel #2		Channel #3		Channel #4		Channel #5		Channel #6		Channel #7		Channel #8		Channel #9		Channel #10		Channel #11		Channel #12		Channel #13		Channel #14		Channel #15		Channel #16		Channel #17		Channel #18		Channel #19		Channel #20		Channel #21		Channel #22		Channel #23		Channel #24		Channel #25		Channel #26		Channel #27		Channel #28		Channel #29		Channel #30		Channel #31		Channel #32		Channel #33		Channel #34		Channel #35		Channel #36		Channel #37		Channel #38		Channel #39		Channel #40		Channel #41		Channel #42		Channel #43		Channel #44		Channel #45		Channel #46		Channel #47		Channel #48		Channel #49		Channel #50		Channel #51		Channel #52		Channel #53		Channel #54		Channel #55		Channel #56		Channel #57		Channel #58		Channel #59		Channel #60		Channel #61		Channel #62		Channel #63		Channel #64		Channel #65		Channel #66		Channel #67		Channel #68		Channel #69		Channel #70		Channel #71		Channel #72		Channel #73		Channel #74		Channel #75		Channel #76		Channel #77		Channel #78		Channel #79		Channel #80		Channel #81		Channel #82		Channel #83		Channel #84		Channel #85		Channel #86		Channel #87		Channel #88		Channel #89		Channel #90		Channel #91		Channel #92		Channel #93		Channel #94		Channel #95		Channel #96		Channel #97		Channel #98		Channel #99		Channel #100		Channel #101		Channel #102		Channel #103		Channel #104		Channel #105		Channel #106		Channel #107		Channel #108		Channel #109		Channel #110		Channel #111		Channel #112		Channel #113		Channel #114		Channel #115		Channel #116		Channel #117		Channel #118		Channel #119		Channel #120		Channel #121		Channel #122		Channel #123		Channel #124		Channel #125		Channel #126		Channel #127		Channel #128		Channel #129		Channel #130		Channel #131		Channel #132		Channel #133		Channel #134		Channel #135		Channel #136		Channel #137		Channel #138		Channel #139		Channel #140		Channel #141		Channel #142		Channel #143		Channel #144		Channel #145		Channel #146		Channel #147		Channel #148		Channel #149		Channel #150		Channel #151		Channel #152		Channel #153		Channel #154		Channel #155		Channel #156		Channel #157		Channel #158		Channel #159		Channel #160		Channel #161		Channel #162		Channel #163		Channel #164		Channel #165		Channel #166		Channel #167		Channel #168		Channel #169		Channel #170		Channel #171		Channel #172		Channel #173		Channel #174		Channel #175		Channel #176		Channel #177		Channel #178		Channel #179		Channel #180		Channel #181		Channel #182		Channel #183		Channel #184		Channel #185		Channel #186		Channel #187		Channel #188		Channel #189		Channel #190		Channel #191		Channel #192		Channel #193		Channel #194		Channel #195		Channel #196		Channel #197		Channel #198		Channel #199		Channel #200		Channel #201		Channel #202		Channel #203		Channel #204		Channel #205		Channel #206		Channel #207		Channel #208		Channel #209		Channel #210		Channel #211		Channel #212		Channel #213		Channel #214		Channel #215		Channel #216		Channel #217		Channel #218		Channel #219		Channel #220		Channel #221		Channel #222		Channel #223		Channel #224		Channel #225		Channel #226		Channel #227		Channel #228		Channel #229		Channel #230		Channel #231		Channel #232		Channel #233		Channel #234		Channel #235		Channel #236		Channel #237		Channel #238		Channel #239		Channel #240		Channel #241		Channel #242		Channel #243		Channel #244		Channel #245		Channel #246		Channel #247		Channel #248		Channel #249		Channel #250		Channel #251		Channel #252		Channel #253		Channel #254		Channel #255		Channel #256		Channel #257		Channel #258		Channel #259		Channel #260		Channel #261		Channel #262		Channel #263		Channel #264		Channel #265		Channel #266		Channel #267		Channel #268		Channel #269		Channel #270		Channel #271		Channel #272		Channel #273		Channel #274		Channel #275		Channel #276		Channel #277		Channel #278		Channel #279		Channel #280		Channel #281		Channel #282		Channel #283		Channel #284		Channel #285		Channel #286		Channel #287		Channel #288		Channel #289		Channel #290		Channel #291		Channel #292		Channel #293		Channel #294		Channel #295		Channel #296		Channel #297		Channel #298		Channel #2	
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Current Data Parameters
NAME: 6f
EXPNO: 1
PROCNO: 1
F2 - Acquisition Parameters
Date_ : 20070717
Time : 14.59
INSTRUM: spect
PROBHD: 5 mm QNP 1H/13
PULPROG: zgpg30
TD: 32768
SOLVENT: CDCl3
NS: 2048
DS: 2
SWH: 600.62 Hz
FIDRES: 0.185399 Hz
AQ: 2.7263477 sec
RG: 327.68
INW: 83.200 usec
DE: 6.00 usec
TE: 300.2 K
D1: 1.0000000 sec
===== CHANNEL f1 =====
NUC1: 13C
P1: 7.50 usec
PL1: 0.00 dB
SFO1: 500.3920019 MHz
F2 - Processing parameters
SF: 500.3900237 MHz
WDW: EM
SSB: 0
LB: 0.30 Hz
GB: 0
PC: 1.00
ID: NMR plot parameters
CX: 20.00 cm
FIP: 10.98 ppm
SFO2: 500.3900237 MHz
F2P: -1.032 ppm
F2: -526.54 Hz
FREQ: 600.618399 MHz
HETCON: 300.90077 Hz/cm

0.000

155.537
149.583
136.576
136.430
132.641
128.643
128.246
127.882
127.026
122.007
121.961

77.252
76.999
76.744

Current Data Parameters
NAME crb051
PROCNO 1

F2 - Acquisition Parameters
Time 2.005000
Time 15.04
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 72
DS 4
SWH 31446.541 Hz
FIDRES 0.478936 Hz
AQ 1.0420754 se
RG 327.68
WDW EM
SS 0
LB 1.00 Hz
GB 0
PC 1.40

===== CHANNEL f1 =====
NUC1 13C
P1 7.50 us
PL1 0.00 dB
SFO1 125.836556 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
P2 100.00 us
PL2 0.00 dB
PL3 0.00 dB
PL13 26.00 dB
SFO2 500.3920016 MHz

F2 - Processing Parameters
SI 32768
SF 125.8231809 MHz
WDW EM
SS 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 21.00 cr
FIP 234.440 DE
F1P 234.440 DE
F2P -15.487 DE
F2 -1348.59 Hz
F2 11.90156 DE
PENCH 1497.45455 Hz
H2CH

Current Data Parameters	
NAME	csb04
EXPNO	1
PROCNO	1
F2 - Acquisition Parameters	
Time	20.29
INSTRUM	zgpg30
PULPROG	zgpg30
PCPDPRG2	zgpg30
SOLVENT	CDCl3
NS	107
DS	4
SWH	6095.615 Hz
FIDRES	0.15339 Hz
AQ	2.7254377 sec
RG	327.5
ADQ	83.200 usec
DELTA	6.00 usec
TE	300.2 K
DE	1.00000000 sec
===== CHANNEL f1 =====	
NUC1	13C
NUC2	13C
PCPDPRG1	zgpg30
RF1	500.995019 MHz
F2 - Processing parameters	
F1	500.995019 MHz
SE	32768
SS	0
SC	0
SI	0
PC	1.00
D1 NMR plot parameters	
CD	20.00 cm
IX	10.985 ppm
F1P	5.1024 ppm
F2P	-5.2624 ppm
PCPDPRG3	zgpg30
PCPDPRG4	zgpg30
PCPDPRG5	300.480777 Hz/cm

7.032
7.065
7.128
7.161
7.244
7.253
7.260
7.269
7.284
7.298
7.351
7.367
7.378
7.381
7.504
7.519
7.788
7.792
7.795
7.804
7.808
7.811
8.474
8.481
8.713

Current Data Parameters
NAME: C20045
EXPNO: 1
PROCNO: 1
F2 - Acquisition Parameters
Date_ 20070727
Time 20.42
INSTRUM spect
PROBHD 5 mm QNP 2930
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 2
DS 2
SWH 6000.62 Hz
FIDRES 0.185399 Hz
AQ 2.7263477 sec
RG 327.68
DWDW 83.200 usec
DE 6.00 usec
TE 300.2 K
D1 1.0000000 sec
===== CHANNEL f1 =====
NUC1 13
P1 7.50 usec
PL1 0.00 dB
SFO1 500.3920019 MHz
F2 - Processing Parameters
SF 500.3900204 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
ID NOE plot parameters
AQ 20.00 cm
FIP 10.000 ppm
FIDRES 0.185399 Hz
F2P 10.000 ppm
F2 -500.39 Hz
NUC2 13
NUC2FREQ 270.21451 MHz

0.000

1.205
1.189
1.199
2.432
2.401
2.462
1.270
1.243

148.989
137.073
133.403
133.050
131.234
129.212
128.641
127.093
125.314
123.949

77.764
77.509
77.256

Current Data Parameters
NAME: crb045
PROCNO: 1
F2 - Acquisition Parameters
Time: 2.008115
Time: 19.15
INSTRUM: spect
PROBHD: 5 mm QNP 1H/1
PULPROG: zgpg30
TD: 65536
SOLVENT: CDCl3
NS: 204
DS: 2
SWH: 31446.541 Hz
FIDRES: 0.478936 Hz
AQ: 1.0420721 se
RG: 327.67
WDW: EM
SS: 0.000000 se
LB: 0.000000 Hz
GB: 0
PC: 1.40
F2 - Processing Parameters
SI: 32768
SF: 125.823160 MHz
WDW: EM
SS: 0.000000 se
LB: 0.000000 Hz
GB: 0
PC: 1.40
1D NMR plot parameters
CX: 21.00 cr
FIP: 234.956 DE
F1P: 234.956 DE
F2P: -14.971 DE
F2: -1883.69 Hz
PENCH: 11.90127 DE
HECH: 1497.45435 Hz

Current Data Parameters
NAME: CDB58
EXPNO: 1
PROCNO: 1
F2 - Acquisition Parameters
Date_ : 20070616
Time : 17.59
INSTRUM: spect
PROBHD: 5 mm QNP 290
PULPROG: zgpg30
TD: 32768
SOLVENT: CDCl3
NS: 600
DS: 2
SWH: 600.62 Hz
FIDRES: 0.185399 Hz
AQ: 2.726347 sec
RG: 327.68
DM: 83.200 usec
DE: 6.00 usec
TE: 300.2 K
D1: 1.0000000 sec
----- CHANNEL f1 -----
NUC1: 1H
P1: 7.50 usec
PL1: 0.00 dB
SFO1: 500.3920019 MHz
F2 - Processing parameters
SF: 500.3900167 MHz
WDW: EM
SSB: 0
LB: 0.30 Hz
GB: 0
PC: 1.00
ID: NMR plot parameters
CX: 20.00 cm
FIP: 10.000 ppm
ZG: 0.000 ppm
FZP: -10.000 ppm
F2: -500.39 Hz
PCPROG: nmr2
HETCN: 270.21451 Hz/cm

Current Data Parameters
 Name: 6j
 EXPNO: 2
 PROCNO: 1
 F2 - Acquisition Parameters
 Date_: 20020404
 Time: 18.04
 INSTRUM: spect
 PROBHD: 5 mm QNP
 PULPROG: zgpg30
 TD: 65536
 SOLVENT: CDCl3
 NS: 511
 DS: 4
 SWH: 31446.541 Hz
 FIDRES: 0.478936 Hz
 AQ: 0.0422724 sec
 RG: 8152
 DW: 15.900 us
 DE: 6.00 us
 TE: 300.2 K
 D1: 2.00000000 sec
 D11: 0.03000000 sec
 D12: 0.00002000 sec
 CHANNEL f1
 NUC1: ¹³C
 P1: 7.50 us
 PL1: 0.00 dB
 SFO1: 125.8369556 MHz
 CHANNEL f2
 CPDPRG2: waltz16
 NUC2:
 PCPD2: 100.00 us
 PL2: 0.00 dB
 PL12: 26.00 dB
 PL13: 26.00 dB
 SFO2: 500.3920016 MHz
 F2 - Processing parameters
 SI: 32768
 SF: 125.8231742 MHz
 WDW: EM
 SSF: 0
 LB: 1.00 Hz
 GB: 0
 PC: 1.40
 1D NMR plot parameters
 CX: 21.00 cm
 F1P: 177.052 PP
 F2P: 223.692 PP
 F2P: 20.737 PP
 F2: 2616.72 Hz
 PPGN: 7.46513 PP
 HPGN: 941.8953 Hz

Current Data Parameters
 NAME: 5k129
 EXPNO: 1
 PROCNO: 1
 F2 - Acquisition Parameters
 Date_Time: 20160318 18:13
 Time: 18:13
 INSTRUM: spect
 PULPROG: zgpg30
 TD: 32768
 SFO1: 500.1360519 MHz
 FIDRES: 0.163339 Hz
 AQ: 2.7263477 sec
 RG: 327.68
 DM: 83.200 usec
 DE: 6.00 usec
 TE: 300.2 K
 D1: 1.0000000 sec
 ===== CHANNEL f1 =====
 NUC1: 1H
 P1: 7.50 usec
 PL1: 0.00 dB
 SFO1: 500.1360519 MHz
 F2 - Processing parameters
 SI: 32768
 SF: 500.1360519 MHz
 DS: 4
 SSF: 128.000 MHz
 LB: 0.30 Hz
 GB: 0.00 Hz
 PC: 1.00
 ID NMR plot parameters
 CX: 20.00 cm
 F1P: 10.959 ppm
 F1Q: 0.000 ppm
 F2P: -1.051 ppm
 F2Q: 0.000 ppm
 FIDRES: 0.163339 Hz
 HZCX: 300.48074 Hz/cm

0.000

Current Data Parameters
 Name: 5k
 EXPNO: 2
 PROCNO: 1
 F2 - Acquisition Parameters
 Date_: 20020623
 Time: 18.07
 INSTRUM: spect
 PROBHD: 5 mm QNP
 PULPROG: zgpg30
 TD: 65536
 SOLVENT: CDCl3
 NS: 700
 DS: 4
 SWH: 31446.541 Hz
 FIDRES: 0.478936 Hz
 AQ: 1.0422744 s
 RG: 8152
 DW: 15.900 us
 DE: 6.00 us
 TE: 300.2 K
 D1: 2.00000000 s
 D11: 0.03000000 s
 D12: 0.00002000 s
 CHANNEL f1
 NUC1 13C
 P1 7.50 us
 PL1 0.00 dB
 SFO1 125.8369556 MHz
 CHANNEL f2
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 100.00 us
 PL2 0.00 dB
 PL12 26.00 dB
 PL13 26.00 dB
 SFO2 500.3920016 MHz
 F2 - Processing parameters
 SI 32768
 SF 125.8321704 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40
 1D NMR plot parameters
 CX 22.00 cr
 F1P 2281.00 PP
 F2P -5.000 PP
 F2 -629.12 Hz
 PPM0 0.2777 PP
 HSCN 128.632788 Hz

Current Data Parameters
NAME: 1
EXPNO: 1
PROCNO: 1
F2 - Acquisition Parameters
Date_ : 20080912
Time : 12.29
INSTRUM : spect
PROBHD : 5 mm QNP 290
PULPROG : zgpg30
TD : 32768
SOLVENT : CDCl₃
NS : 1024
DS : 2
SWH : 6008.62 Hz
FIDRES : 0.185399 Hz
AQ : 2.7263477 sec
RG : 327.68
DM : 83.200 usec
DE : 6.00 usec
TE : 300.2 K
D1 : 1.0000000 sec
----- CHANNEL f1 -----
NUC1 : ¹H
P1 : 7.50 usec
PL1 : 0.00 dB
SFO1 : 500.3920019 MHz
F2 - Processing parameters
SF : 500.3900198 MHz
WDW : EM
SSB : 0
LB : 0.30 Hz
GB : 0
PC : 1.00
ID: NMR plot parameters
CX : 20.00 cm
FIP : 10.000 ppm
FIDRES : 0.185399 Hz
F2P : -10.000 ppm
FZ : -500.39 Hz
GPCPM : 0.5000000 Hz/G
HSCN : 270.21451 Hz/C

Current Data Parameters
 NAME: crb080
 PROCNO: 1
 F2 - Acquisition Parameters
 Time: 2.00133
 INSTRUM: spect
 PROBD: 5 mm QNP 1H/1
 PULPROG: zgpg30
 TD: 65536
 SOLVENT: CDCl₃
 NS: 360
 DS: 4
 SWH: 31446.541 Hz
 FIDRES: 0.478936 Hz
 AQ: 1.0420754 sec
 RG: 327.68
 DW: 15.900 us
 DE: 6.00 us
 TE: 300.2 K
 D1: 2.00000000 sec
 D11: 0.03000000 sec
 D12: 0.00020000 sec
 CHANNEL f1 ==
 NUC1: ¹³C
 P1: 7.50 us
 PL1: 0 dB
 SFO1: 125.8365556 MHz
 =====
 CHANNEL f2 ==
 NUC2: ¹H
 PULPROG: waltz16
 PCPD2: 100.00 us
 PL2: 0.00 dB
 PL3: 0.00 dB
 PL13: 28.00 dB
 SFO2: 500.3920016 MHz
 F2 - Processing parameters
 SI: 32768
 SF: 125.8231160 MHz
 WDW: EM
 SS: 0
 LB: 1.00 Hz
 GB: 0
 PC: 1.40
 1D NMR plot parameters
 CX: 21.00 ct
 FIP: 234.956 DF
 ZFPC: 230.000 MHz
 F2P: -14.971 DE
 F2: -1883.69 Hz
 PENCH: 11.90127 DF
 HZCH: 1497.45435 Hz

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