Palladium Catalyzed Suzuki-Miyaura Cross-Coupling Reactions of Potassium Aryl- and Heteroaryltrifluoroborates

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Table of contents

General.....	S2
Organotrifluoroborate Synthesis.....	S2
Representative Procedures for the Cross-Coupling Reactions of Potassium Aryl- and Heteroaryltrifluoroborates.....	S6
Mechanistic Studies.....	S18
References.....	S19
NMR spectra.....	S22

Experimental Section

General. ^1H , ^{13}C and ^{19}F NMR spectra were measured on spectrometers at 500.39, 125.77 and 470.53 MHz, respectively. ^{19}F NMR chemical shifts were referenced to external CFCl_3 (0.0 ppm). ^{11}B NMR spectra at 64.2 MHz were obtained on a spectrometer equipped with the appropriate decoupling accessories. 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 melting points were uncorrected. The mass spectra were obtained by ESI or CI (CH_4) with direct inlet for HRMS or LRMS, or by CI (CH_4) by GC-MS analysis. Methanol, ethanol, *n*-propanol, *i*-propanol and dioxane (HPLC quality) were kept over molecular sieves and used without further purification. THF was distilled from sodium benzophenone. The starting halides, boronic acids or esters and palladium catalysts were obtained from commercial sources and used without further purification. The amines were distilled from calcium hydride.

Potassium phenyltrifluoroborate (**1a**), potassium 4-methoxyphenyltrifluoroborate (**1b**), potassium 3-methoxyphenyltrifluoroborate (**1c**), potassium 4-fluorophenyltrifluoroborate (**1d**), potassium 1-naphthyltrifluoroborate (**1j**), potassium 2-methylphenyltrifluoroborate (**1k**), potassium 3-thiophenyltrifluoroborate (**1m**) and potassium 2-furyltrifluoroborate (**1p**) were prepared from the corresponding boronic acids according to the reported procedures.¹

Potassium 4-Acetylphenyltrifluoroborate (1e). To a solution of 4-acetylphenylboronic acid (10 g, 61 mmol) in 40 mL of methanol was added an aqueous solution of KHF_2 (41 mL, 4.5 M solution, 185 mmol) at room temperature. A heavy precipitate was deposited. The resulting suspension was stirred for 1 h at room temperature and then the precipitated product was collected and washed with methanol. Recrystallization from a minimum amount of acetone produced 12 g (87%) of potassium 4-acetylphenyltrifluoroborate. mp > 250 °C. ^1H NMR (acetone- d_6 , 500 MHz) δ 7.74 (d, J = 7.8 Hz, 2 H), 7.59 (d, J = 7.8 Hz, 2 H), 2.49 (s, 3 H). ^{13}C NMR (DMSO- d_6 , 125 MHz) δ 198.1, 134.2, 131.3 (d, J = 1.5 Hz), 126.2, 26.4. ^{11}B NMR (DMSO- d_6 , 64 MHz) δ 3.27 (br s). ^{19}F NMR (DMSO- d_6 , 471 MHz) δ -140.3 (br s). Anal. Calcd. for $\text{C}_9\text{H}_7\text{BF}_3\text{KO}$: C, 42.51, H, 3.12. Found: C, 39.30 H; 3.28.

Potassium 3-Nitrophenyltrifluoroborate (1f). To a solution of 3-nitrophenylboronic acid (15 g, 89.8 mmol) in 15 mL of methanol was added an aqueous solution of KHF_2 (66 mL, 4.5 M solution, 297 mmol) at room temperature. A heavy precipitate was deposited. The resulting suspension was stirred for 1 h at room temperature and then the precipitated product was collected and washed with methanol.

Recrystallization from a minimum amount of acetone produced 17.5 g (85%) of potassium 3-nitrophenyltrifluoroborate. mp 244-246 °C. ^1H NMR (acetone- d_6 , 500 MHz) δ 8.32 (s, 1 H), 7.96 (d, J = 7.5 Hz, 1 H), 7.89 (d, J = 7.0 Hz, 1 H), 7.38 (t, J = 7.5 Hz, 1 H). ^{13}C NMR (acetone- d_6 , 125 MHz) δ 148.4, 139.1, 128.4, 126.6, 121.3. ^{11}B NMR (acetone- d_6 , 64 MHz) δ 3.59 (br s). ^{19}F NMR (acetone- d_6 , 471 MHz) δ -143.8 (s). Anal. Calcd. for $\text{C}_6\text{H}_4\text{BF}_3\text{KNO}_2$: C, 31.47, H, 1.76, N, 6.12. Found: C, 31.31, H, 1.80, N, 5.67.

Potassium 3,5-Bis(trifluoromethyl)phenyltrifluoroborate (1g). To a solution of 3,5-bis(trifluoromethyl)phenylboronic acid (10 g, 38.8 mmol) in 15 mL of methanol was added an aqueous solution of KHF_2 (26 mL, 4.5 M solution, 117 mmol) at room temperature. A heavy precipitate was deposited. The resulting suspension was stirred for 1 h at room temperature and then the precipitated product was collected and washed with methanol. Recrystallization from a minimum amount of acetone produced 11 g (89%) of potassium 3,5-bis(trifluoromethyl)phenyltrifluoroborate. mp > 250 °C. ^1H NMR (DMSO- d_6 , 500 MHz) δ 7.87 (s, 2 H), 7.71 (s, 1 H). ^{13}C NMR (DMSO- d_6 , 125 MHz) δ 131.2, 128.1 (q, J = 31 Hz), 124.2 (q, J = 272 Hz), 118.6 (m). ^{11}B NMR (DMSO- d_6 , 64.2 MHz) δ 2.57 (br s). ^{19}F NMR (DMSO- d_6 , 471 MHz) δ -61.7, -141.6 (br d, J = 71 Hz). Anal. Calcd for $\text{C}_8\text{H}_3\text{BF}_9\text{K}$: C, 30.03, H, 0.94. Found: C, 29.72, H, 1.04.

Potassium 2,6-Difluorophenyltrifluoroborate (1h).² 2,6-Difluorophenylboronic acid (4.0686 g, 25.8 mmol) and potassium hydrogen fluoride (5.4820 g, 70.2 mmol) were combined in a Nalgene bottle and were vigorously stirred for 2 h in a mixture of water (10 mL) and methanol (20 mL) at room temperature. The resulting precipitate was allowed to stand overnight at 4 °C. The solid was then filtered off, washed with water and with ethyl ether. The crystalline material was dried on a high vacuum Schlenk line to give 5.1084 g (90%) of the desired material. mp > 250 °C. ^1H NMR (DMSO- d_6 , 500 MHz) δ 6.66 (m, 2 H), 7.10 (m, 1 H). ^{13}C NMR (DMSO- d_6 , 125 MHz) δ 168.7 (dd, J = 242, 18 Hz), 127.5 (t, J = 11 Hz), 110.0 (dd, J = 23, 8 Hz). ^{11}B NMR (DMSO- d_6 , 64.2 MHz) δ 2.17 (q, J = 44 Hz). ^{19}F NMR (DMSO- d_6 , 470.5 MHz) δ -103.7 (q, J = 9.4 Hz), -132.6 (qt, J = 43.9 Hz). Anal. Calcd for $\text{C}_6\text{H}_3\text{BF}_5\text{K}$: C, 32.76, H, 1.37. Found: C, 32.58, H, 1.30.

Potassium Pentafluorophenyltrifluoroborate (1i).² Pentafluorophenylboronic acid (1.9495 g, 9.2 mmol) and potassium hydrogen fluoride (2.1713 g, 27.8 mmol) were combined in a Nalgene bottle and were vigorously stirred overnight in a mixture of water (15 mL) and methanol (9 mL) at room temperature.

The resulting white precipitate was allowed to stand 1 h at 4 °C. The solid was then filtered off, washed with water and with ethyl ether. The crystalline material was dried on a high vacuum Schlenk line to give 4.9505 g (65%) of the desired material. mp > 250 °C. ^{11}B NMR (acetone- d_6 , 64.2 MHz) δ 1.68 (q, J = 40.8 Hz). ^{19}F NMR (DMSO- d_6 , 471 MHz) δ -132.9 (qt, J = 43, 11 Hz), -134.7 (m), -161.3 (t, J = 21 Hz), -165.7 (m).

Potassium 2,6-Dimethylphenyltrifluoroborate (1l). 2,6-Dimethylphenylboronic acid (2.6911 g, 17.94 mmol) and potassium hydrogen fluoride (4.2866 g, 54.88 mmol) were combined in a Nalgene bottle and were vigorously stirred for 1 h in a mixture of water (12 mL) and methanol (10 mL) at room temperature. The resulting precipitate was allowed to stand 1 h at 4 °C. The solid was then taken up in hot acetone and concentrated under reduced pressure. The solids were dissolved with hot acetone and then filtered. Ethyl ether was added to give a white solid, which was filtered and washed with cold ethyl ether. The resulting crystalline material was dried on a high vacuum Schlenk line to give 3.3345 g (88%) of potassium 2,6-dimethylphenyltrifluoroborate. mp > 250 °C. ^1H NMR (acetone- d_6 , 500 MHz) δ 6.83 (t, J = 7.4 Hz, 1 H), 6.75 (d, J = 7.4 Hz, 2 H), 2.40 (s, 6 H). ^{13}C NMR (acetone- d_6 , 125 MHz) δ 142.5, 127.7, 125.9, 23.8, 23.8. ^{11}B NMR (acetone- d_6 , 64.2 MHz) δ 4.94 (br d, J = 49 Hz). ^{19}F NMR (acetone- d_6 , 470.5 MHz) δ -132.5 (q, J = 48 Hz). Anal. Calcd for $\text{C}_8\text{H}_9\text{BF}_3\text{K}$: C, 45.31, H, 4.28. Found: C, 45.12, H, 4.23.

Potassium 3-Furyltrifluoroborate (1n). 3-Furylboronic acid (0.9320 g, 8.55 mmol) and potassium hydrogen fluoride (2.0907 g, 26.77 mmol) were combined in a Nalgene bottle and were vigorously stirred for 2 h in a mixture of water (6 mL) and methanol (8 mL) at room temperature. The resulting precipitate was allowed to stand overnight at 4 °C. The solid was then taken up in hot acetone and concentrated to dryness under reduced pressure. The solids were dissolved with hot acetone and then filtered. Ethyl ether was added to give a light yellow solid, which was filtered and washed with cold ethyl ether. The resulting crystalline material was dried on a high vacuum Schlenk line to give 1.2075 g (81%) of potassium 3-furantrifluoroborate mp 170 °C (decompose). ^1H NMR (acetone- d_6 , 500 MHz) δ 7.27 (br s, 1 H), 7.16 (s, 1 H), 6.30 (s, 1 H). ^{13}C NMR (acetone- d_6 , 125 MHz) δ 144.7, 141.6, 114.3. ^{11}B NMR (acetone- d_6 , 64.2 MHz) δ 4.25 (br s). ^{19}F NMR (acetone- d_6 , 471 MHz) δ -138.8 (q, J = 48 Hz). Anal. Calcd for $\text{C}_4\text{H}_3\text{BF}_3\text{KO}$: C, 27.62, H, 1.74. Found: C, 27.86 H, 1.51.

Potassium 3-Pyridyltrifluoroborate (1o). The preparation to arrive at 3-pyridylboronic acid has been adapted from a published procedure.³ A flask was charged with dry toluene (40 mL) and dry THF (10 mL)

under a nitrogen atmosphere. Then triisopropyl borate (6.1 mL, 26.4 mmol) and 3-bromopyridine (3.4563 g, 21.9 mmol) were added, and the mixture was cooled to -60 °C. *n*-BuLi (1.6 M solution in hexane, 39 mL, 62 mmol) was added dropwise, the mixture was stirred for 2 h and then the reaction was allowed to warm to room temperature overnight. The mixture was cooled to 0 °C and an aqueous solution of KHF₂ (4.5 M, 58 mmol) was added dropwise with vigorous stirring. After stirring for an additional 4 h, the reaction was completely evaporated under vacuum. The crude was then taken up in methanol and filtered. Attempts to crystallize using different solvent systems failed. Elimination of the solvent led to a viscous oil, which under high vacuum produced a solid product in approximately 90% yield. Although partial contamination with KBF₄ was observed, the product was used without further purification. ¹H NMR (methyl-*d*₃ alcohol-*d*, 500 MHz) δ 8.57 (br s, 1 H), 8.26 (br d, *J* = 4.6 Hz, 1 H), 7.90 (d, *J* = 7.3 Hz, 1 H), 7.23 (dd, *J* = 5.5, 6.6 Hz, 1 H). ¹³C NMR (DMSO-*d*₆, 125 MHz) δ 153.0, 145.7, 138.8, 122.0. ¹¹B NMR (methyl-*d*₃ alcohol-*d*, 64.2 MHz) δ 4.0 (br s). ¹⁹F NMR (DMSO-*d*₆, 471 MHz) δ -134.9 (s).

Potassium 2-Pyridyltrifluoroborate (1q). The preparation to arrive at methyl 2-pyridylboronate has been adapted from a published procedure.⁴ A flask was charged with dry ethyl ether (30 mL) under a nitrogen atmosphere. Then 2-bromopyridine (0.01 mol, 1.5777 g) was added and the resulting solution was cooled to -78 °C. *n*-BuLi (1.6M solution in hexane, 6.4 mL) was added dropwise and the mixture was stirred an additional hour at -78 °C. Trimethyl borate (2.4 mL, 0.021 mol) was added dropwise over 10 min, and the mixture was kept at -78 °C with stirring for an additional hour, then allowed to warm to room temperature overnight. The mixture was then cooled to 0 °C and an aqueous solution of KHF₂ (4.5 M, 6.7 mL, 0.03 mmol) was added dropwise with vigorous stirring. After stirring for an additional 3 h, the solvents were completely removed under vacuum. The crude was then taken up in methanol and filtered. Attempts to crystallize using different solvent systems failed. Elimination of the solvent led to a viscous oil, which under high vacuum produced a solid product in approximately 50% yield. The product decomposed quickly, even when kept under an inert atmosphere, and it was therefore used without further purification. ¹H NMR (methyl-*d*₃ alcohol-*d*, 500 MHz) δ 8.53 (dt, *J* = 6.0, 1.5 Hz, 1 H), 8.27 (t, *J* = 6.5 Hz, 1 H), 7.97 (d, *J* = 6.5 Hz, 1 H), 7.71 (t, *J* = 6.0 Hz, 1 H). ¹¹B NMR (methyl-*d*₃ alcohol-*d*, 64.2 MHz) δ 1.80 (br s). ¹⁹F NMR (methyl-*d*₃ alcohol-*d*, 471 MHz) δ -151.87 (br s).

Representative Procedures for the Cross-Coupling Reaction of Potassium Aryl- and Heteroaryltrifluoroborates.

Method A: To a suspension of potassium phenyltrifluoroborate (**1a**) (0.0923 g, 0.5 mmol), 1-bromonaphthalene (**2a**) (0.1035 g, 0.5 mmol), and K_2CO_3 (0.2045 g, 1.5 mmol) in 0.75 mL of methanol was added 1.25 mL of a 2×10^{-3} M solution of $Pd(OAc)_2$ in methanol, and then the reaction mixture was stirred and heated at reflux for 2 h, then cooled to room temperature and diluted with water (10 mL) followed by Work-up #1. Purification by chromatography on silica gel (elution with hexane) yielded 1-phenylnaphthalene (**3a**) (0.0761 mg, 0.37 mmol, 75%). The product was identical to authentic material by 1H -NMR, ^{13}C -NMR and by GC retention time.

Method B: To a mixture of potassium phenyltrifluoroborate (**1a**) (0.1834 g, 1.0 mmol), 4-hydroxyphenol (**2k**) (0.1764 g, 1.0 mmol), K_2CO_3 (0.4153 g, 3 mmol), and $Pd(OAc)_2$ (0.0011 g, 5×10^{-3} mmol), was added water (4 mL). The reaction was heated at 65-80 °C with stirring for 2 h. The reaction mixture was then cooled to room temperature and treated according to Work-up #3. The product **3k** was analyzed by NMR after recrystallization from dichloromethane/hexane. The spectral data obtained were in accordance with those described in the literature.¹

Method C: A mixture of 0.0088 g of $Pd(OAc)_2$ and 0.0263 g of Ph_3P was stirred in 10 mL of methanol for 30 min in order to obtain a 4×10^{-3} M solution of $Pd(OAc)_2/(Ph_3P)$. Then 1.25 mL of the solution (5×10^{-3} mmol) was added to a mixture of potassium phenyltrifluoroborate (**1a**) (0.0925 g, 0.5 mmol), 2,4-dimethoxy-1-bromobenzene (**2n**) (0.1080 g, 0.5 mmol), and K_2CO_3 (0.2127 g, 1.5 mmol) in 0.75 mL of methanol. The reaction mixture was stirred and heated at reflux in an open atmosphere for 18 h, then cooled to room temperature and diluted with 10 mL of water, followed by Work-up #1, to yield **3n** (0.0809 g, 75%).

Method D: To a mixture of potassium 3-nitrophenyltrifluoroborate (**1f**) (0.1150 g, 0.5 mmol), 4-bromobenzonitrile (**2e**) (0.0912 g, 0.5 mmol), Et_3N (0.21 mL, 1.5 mmol), and $PdCl_2(dppf) \cdot CH_2Cl_2$ (0.0020 g, 5×10^{-3} mmol), was added ethanol (2 mL). The reaction was heated at reflux with stirring for 12 h, then cooled to room temperature and treated according to Work-up #2. Purification by recrystallization with dichloromethane/hexane yielded 3'-nitrobiphenyl-4-carbonitrile (**3s**) (0.0999 g, 89%).

Work-up #1. The aqueous phase was extracted with dichloromethane (4 mL x 3). The organic solution was washed with brine (10 mL) and dried over $MgSO_4$. The solution was then filtered through a short pad of silica gel, using a sequence of pentane (to eliminate any nonpolar by-products), and

pentane/dichloromethane (to elute the product). Further addition of pure dichloromethane elutes polar by-products and the catalyst residue. The solvent was then removed under vacuum and the crude product was analyzed by NMR with or without further purification.

Work-up #2 (for water insoluble products). After the addition of water a precipitate was formed. The precipitate was filtered off, thoroughly washed with water, dissolved in dichloromethane, and dried over MgSO_4 . The solution was then filtered through a short pad of silica gel, using a sequence of pentane (to eliminate non polar by-products), and pentane/dichloromethane (to elute the product). Further addition of pure dichloromethane elutes polar by-products and the catalyst residue. The solvent was removed under vacuum and the crude product was analyzed by NMR with or without further purification.

Work-up #3 (for acidic products): The aqueous crude was treated with 1 N HCl until acidic to litmus. The formed precipitate was filtered off, thoroughly washed with water, dissolved with dichloromethane, and filtered to eliminate the palladium black formed during the reaction. The organic solution was dried over MgSO_4 and filtered. The solvent was removed under vacuum and the crude product was analyzed by NMR with or without further purification.

The synthesis of the following products has been previously reported:¹

4-(*N,N*-Dimethyl)phenylaniline (3m). This product was obtained as an off-white solid from **1a** and **2m** by Method C, Work-up #1 (Table 3, entry 4), after two recrystallizations with dichloromethane/pentane, in 65% yield when 1% catalyst was used. mp 115-116 °C (lit. 121-122).⁵ The spectral data obtained were in accordance with those described in the literature.⁶

2,4-Dimethoxybiphenyl (3n). This product was obtained as a colorless oil in 50% yield from **1a** and **2n** by Method A, Work-up #1 (Table 3, entry 5), after purification by chromatography on silica gel (elution with hexane/ethyl acetate 40:1 ~ 5:1), and in 75% yield by Method C, Work-up #1, without further purification. The spectral data obtained were in accordance with those described in the literature.⁷

4'-Acetylbiphenyl-4-carbonitrile (3r). This product was obtained as a white solid in 70% yield from **1e** and **2e** by Method C, Work-up #2 (Table 4, entry 4), after recrystallization with dichloromethane/hexane. mp 116 °C (lit. 117-120).⁸ The spectral data obtained were in accordance with those described in the literature.⁹

3'-Nitrobiphenyl-4-carbonitrile (3s). This product was obtained as an off-white solid in 89% yield from **1f** and **2e** by Method D, Work-up #2 (Table 4, entry 3), after recrystallization with dichloromethane/hexane. mp 162-164 °C. IR (neat): 2225, 1521, 1506, 1353 cm⁻¹. ¹H NMR (CDCl₃, 500 MHz) δ 8.46 (t, *J* = 1.9 Hz, 1 H), 8.29 (dd, *J* = 8.1, 1.3 Hz, 1 H), 7.93 (dd, *J* = 7.8, 1.3, 1 H), 7.81 (dd, *J* = 6.7, 1.7 Hz, 2 H), 7.75 (dd, *J* = 8.4, 1.9 Hz, 2 H), 7.69 (t, *J* = 8.0 Hz, 1 H), ¹³C NMR (CDCl₃, 125 MHz) δ 143.0, 140.8, 133.0, 132.9, 130.2, 127.9, 123.3, 122.1, 118.3, 112.4. HRMS (ESI): *m/z* calcd for C₁₃H₈N₂O₂ (M⁺) 224.0586, found 224.0579.

3',5'-Bis(trifluoromethyl)biphenyl-4-carbonitrile (3t). This product was obtained as a white solid in 70% yield from **1g** and **2e** by Method D, Work-up #2 (Table 4, entry 6), after recrystallization with dichloromethane/hexane. mp 125-126 °C. IR (neat): 2225, 1285, 1122 cm^{-1} . ^1H NMR (CDCl_3 , 500 MHz) δ 8.05 (s, 2 H), 7.95 (s, 1 H), 7.83 (d, $J = 8.3$ Hz, 2 H), 7.76 (d, $J = 8.3$ Hz, 2 H). ^{13}C NMR (CDCl_3 , 125 MHz) δ 142.4, 141.3, 133.0, 132.6 (q, $J = 34$ Hz), 128.0, 127.3 (d, $J = 3$ Hz), 125.3 (q, $J = 273$ Hz), 122.2 (q, $J = 4$ Hz), 118.2, 112.8. ^{19}F NMR (CDCl_3 , 470.5 MHz) δ -63.4 (s). HRMS (ESI): m/z calcd for $\text{C}_{15}\text{H}_7\text{F}_6\text{N}$ (M^+) 315.0483, found 315.0467.

2',6'-Difluorobiphenyl-4-carbonitrile (3u). This product was obtained as a white solid in 86% yield from **1h** and **2e** by Method D (using 1% catalyst loading), Work-up #2 (Table 4, entry 7), after recrystallization with dichloromethane/hexane. mp 87-88 °C. IR (neat): 2233, 1464, 1227, 994 cm^{-1} . ^1H NMR (CDCl_3 , 500 MHz) δ 7.72 (d, $J = 8.0$ Hz, 2 H), 7.58 (d, $J = 7.9$ Hz, 2 H), 7.38-7.33 (m, 1 H), 7.04-6.99 (m, 2 H). ^{13}C NMR (CDCl_3 , 125 MHz) δ 159.7 (dd, $J = 250, 7$ Hz), 134.0, 131.9, 131.0 (t, $J = 1.5$ Hz), 130.2 (t, $J = 10$ Hz), 118.5, 116.7, 111.8 (dd, $J = 21, 5$ Hz). ^{19}F NMR (CDCl_3 , 470.5) δ -114.8 (s). HRMS (ESI): m/z calcd for $\text{C}_{13}\text{H}_7\text{F}_2\text{N}$ (M^+) 215.0547, found 215.0547.

2',3',4',5',6'-Pentafluorobiphenyl-4-carbonitrile (3v). This product was obtained as a white solid in 38% yield from **1i** and **2e** by Method D (using 5% catalyst loading, dry THF as a solvent and 3 equiv of Hünig's base, under inert atmosphere), Work-up #1 (Table 4, entry 8), after purification by chromatography on silica gel (elution with hexane/ethyl acetate 15:1 ~ 1:1). mp 122-124 °C (112-113 lit. °C). The spectral data obtained were in accordance with those described in the literature.¹⁰

4-[1]Naphthylbenzonitrile (3w). This product was obtained as a white solid in 60% yield from **1j** and **2e** by Method D, Work-up #1 (Table 5, entry 1), after recrystallization with dichloromethane/hexane. mp 82-83 °C (lit 76-77).¹¹ IR (neat): 2227, 1606, 1503, 1396 cm⁻¹. ¹H NMR (CDCl₃, 500 MHz) δ 7.90 (t, *J* = 8.3 Hz, 2 H), 7.76-7.74 (m, 3 H), 7.58 (d, *J* = 8.3 Hz, 2 H), 7.53-7.50 (m, 2 H), 7.44 (t, *J* = 7.0 Hz, 1 H), 7.37 (dd, *J* = 7.0, 1.1 Hz, 1 H). ¹³C NMR (CDCl₃, 125 MHz) δ 145.6, 138.2, 133.8, 132.1, 130.9, 130.7, 128.7, 128.5, 127.0, 126.6, 126.1, 125.3, 125.1, 118.8, 111.2. The spectral data obtained were in accordance with those described in the literature.¹¹

2',6'-Dimethylbiphenyl-4-carbonitrile (3aa). This product was obtained as an off-white solid in 82% yield from **1l** and **2e** by Method D, Work-up #1 (Table 5, entry 5), after recrystallization with dichloromethane/hexane. mp 118-119 °C. IR (neat): 2226, 1606, 1467 cm⁻¹. ¹H NMR (CDCl₃, 500 MHz) δ 7.71 (d, *J* = 8.0 Hz, 2 H), 7.27 (d, *J* = 8.0 Hz, 2 H), 7.19 (t, *J* = 7.4 Hz, 1 H), 7.12 (d, *J* = 7.4 Hz, 2 H), 2.0 (s, 6 H). ¹³C NMR (CDCl₃, 125 MHz) δ 146.2, 139.8, 135.3, 132.3, 130.0, 127.8, 127.5, 118.8, 110.7, 20.6. HRMS (ESI): *m/z* calcd for C₁₅H₁₃N (M⁺) 207.1048, found 207.1040.

4'-Methoxy-2,6-dimethylbiphenyl (3ab). This product was obtained as an off-white solid in 50% yield from **1l** and **2j** by Method D, Work-up #1 (Table 5, entry 6), after purification by chromatography on silica gel (elution with hexane/ethyl acetate 40-1 ~ 5-1), recovering 40% of unreacted **2j**. mp 50-51 °C. ¹H NMR (CDCl₃, 500 MHz) δ 7.14 (t, *J* = 6.1 Hz, 1 H), 7.09 (d, *J* = 7.4 Hz, 2 H), 7.05 (dd, *J* = 6.6, 2.1 Hz, 2 H), 6.96 (dd, *J* = 6.5, 2.0 Hz, 2 H), 3.85 (s, 3 H), 2.04 (s, 6 H). ¹³C NMR (CDCl₃, 125 MHz) δ 158.2, 141.5, 136.5, 133.3, 130.0, 127.2, 126.9, 113.8, 55.2, 20.9. HRMS (CI): *m/z* calcd for C₁₅H₁₆O (M⁺) 212.1201, found 212.1192. The spectral data obtained were in accordance with those described in the literature.¹²

4-Methoxy-2',4',6'-trimethylbiphenyl (3ad) This product was obtained as a bright white solid in 52% yield from **1b** and **2o** by Method C (2% catalyst loading), Work-up #1 (Table 5, entry 8), after purification by recrystallization with pentane. mp 70-71 °C (lit 71-73 °C).¹³ ¹H NMR (CDCl₃, 500 MHz) δ 7.03 (m, 2 H), 6.95-6.92 (m, 4 H), 3.83 (s, 3 H), 2.31 (s, 3 H), 2.01 (s, 6 H). ¹³C NMR (CDCl₃, 125 MHz) δ 158.2, 138.6, 136.4, 133.3, 130., 128.0, 113.7, 55.1, 20.9, 20.7. The spectral data obtained were in accordance with those described in the literature.¹⁴

2-Phenylpyridine (3af). This product was obtained as a colorless liquid in 70% yield from **1a** and **2p** by Method A, Work-up #1 (Table 6, entry 1) . The spectral data obtained were in accordance with those described in the literature.¹⁵

3-Phenylpyridine (3ag). This product was obtained as a colorless liquid in 90% yield from **1a** and **2q** by Method A, Work-up #1 (Table 6, entry 2). The spectral data obtained were in accordance with those described in the literature.¹⁶

5-Phenylpyrimidine (3ah). This product was obtained as an off-white solid in 92% yield from **1a** and **2r** by Method A, Work-up #1 (Table 6, entry 3). mp 39-40 °C (lit. 38 °C).¹⁷ The spectral data obtained were in accordance with those described in the literature.¹⁷

5-Phenylfuran-2-carboxylic acid (3aj). This product was obtained as a pale yellow solid in 49% yield from **1a** and **2t** by Method A, Work-up #3, and in 67% by Method B, Work-up #3 (Table 6, entry 5). mp 129-132 °C (lit. 146-148 °C).¹⁸ The spectral data obtained were in accordance with those described in the literature.¹⁹

7-Phenyl-1H-indole (3ak). This product was obtained as a pale red solid in 44% yield from **1a** and **2u** by Method A, Work-up #1 (Table 6, entry 6), after purification by chromatography on silica gel (elution with hexane/ethyl acetate 10:1 ~ 1:1), with the recovery of 22% of starting bromide **2u**. mp 60-61 °C. IR (neat): 3432, 1420, 1338 cm⁻¹. ¹H NMR (CDCl₃, 500 MHz) δ 8.37 (br s, NH), 7.59 (t, *J* = 4.7 Hz, 1 H), 7.52 (d, *J* = 7.7 Hz, 2 H), 7.41 (t, *J* = 7.6 Hz, 2 H), 7.32 (t, *J* = 7.2 Hz, 1 H), 7.15 (d, *J* = 4.2 Hz, 2 H), 6.97 (s, 1 H), 6.53 (d, *J* = 3.0 Hz, 1 H). ¹³C NMR (CDCl₃, 125 MHz) δ 139.2, 133.6, 129.0, 128.2, 128.1, 127.3, 125.5, 124.3, 121.8, 120.2, 120.0, 102.9. HRMS (ESI): *m/z* calcd for C₁₄H₁₁N (M⁺) 193.0892, found 193.0887.

2-[1]Naphthylthiophene (3al). This product was obtained as a colorless liquid in 83% yield from **1j** and **2v** by Method D (2% catalyst loading, K₂CO₃ used as base), Work-up #1 (Table 7, entry 1), after purification by chromatography on silica gel (elution with pentane) ¹H NMR (CDCl₃, 500 MHz) δ 8.23-8.20 (m, 1 H), 7.88-7.84 (m, 1 H), 7.81 (d, *J* = 8.1 Hz, 1 H), 7.55 (dd, *J* = 7.0, 0.9 Hz, 1 H), 7.48-7.43 (m, 3 H), 7.38 (dd, *J* = 5.0, 0.9 Hz, 1 H), 7.22 (dd, *J* = 3.5, 1.1 Hz, 1 H), 7.14 (dd, *J* = 5.1, 3.5 Hz, 1 H). ¹³C NMR (CDCl₃, 125 MHz) δ 141.7, 133.8, 132.4, 131.8, 128.4, 128.3, 128.2, 127.3, 127.2, 126.4, 126.0, 125.7, 125.6, 125.2. The spectral data obtained were in accordance with those described in the literature.²⁰

3-[1]Naphthylthiophene (3am). This product was obtained as a colorless liquid in 72% yield from **1j** and **2w** by Method D (2% catalyst loading, K₂CO₃ used as base), Work-up #1 (Table 7, entry 2), after purification by chromatography on silica gel (elution with pentane). ¹H NMR (CDCl₃, 500 MHz) δ 8.02 (d, *J* = 8.4 Hz, 1 H), 7.85 (d, *J* = 8.4 Hz, 1 H), 7.79 (t, *J* = 4.7 Hz, 1 H), 7.48-7.39 (m, 4 H), 7.38 (dd, *J* = 4.7, 2.9 Hz, 1 H), 7.33 (dd, *J* = 2.9, 1.3 Hz, 1 H), 7.26 (dd, *J* = 5.0, 1.3 Hz, 1 H). ¹³C NMR (CDCl₃, 125

MHz) δ 141.1, 134.9, 133.8, 131.8, 129.6, 128.3, 127.7, 126.9, 126.1, 125.8, 125.7, 125.3, 125.2, 123.4.

The spectral data obtained were in accordance with those described in the literature.²¹

3-[1]Naphthylfuran (3an). This product was obtained as a pale yellow liquid in 68% yield from **1j** and **2x** by Method D (2% catalyst loading, K_2CO_3 used as base), Work-up #1 (Table 7, entry 3). IR (neat): 1500, 1158, 784 cm^{-1} . 1H NMR ($CDCl_3$, 500 MHz) δ 8.21 (dd, $J = 6.0, 2.6$ Hz, 1 H), 7.94 (dd, $J = 6.0, 2.6$ Hz, 1 H), 7.88 (dd, $J = 6.2, 2.6$ Hz, 1 H), 7.72 (dd, $J = 1.5, 0.9$ Hz, 1 H), 7.64 (t, $J = 1.7$ Hz, 1 H), 7.58-7.52 (m, 4 H), 6.77 (dd, $J = 1.8, 0.9$ Hz, 1 H). ^{13}C NMR ($CDCl_3$, 125 MHz) δ 143.4, 142.8, 140.4, 133.8, 131.7, 130.7, 128.4, 127.8, 126.8, 126.8, 126.1, 125.8, 125.6, 125.4, 112.4. HRMS (CI): m/z calcd for $C_{14}H_{10}O$ (M^+) 194.0732, found 194.0730.

2-[1]Naphthylthiazole (3ao). This product was obtained as a pale yellow liquid in 80% yield from **1j** and **2y** by Method D (2% catalyst loading, K_2CO_3 used as base), Work-up #1 (Table 7, entry 4), without further purification. 1H NMR ($CDCl_3$, 500 MHz) δ 8.78 (d, $J = 8.7$ Hz, 1 H), 8.00 (d, $J = 3.4$ Hz, 1 H), 7.90 (d, $J = 8.2$ Hz, 1 H), 7.87 (d, $J = 8.1$ Hz, 1 H), 7.79 (dd, $J = 7.2, 1.2$ Hz, 1 H), 7.58-7.46 (m, 3 H), 7.39 (d, $J = 3.4$ Hz, 1 H). ^{13}C NMR ($CDCl_3$, 125 MHz) δ 167.6, 143.3, 134.0, 130.8, 130.6, 130.3, 128.5, 128.3, 127.2, 126.3, 125.8, 124.9, 119.6. The spectral data obtained were in accordance with those described in the literature.²²

2-[1]Naphthylpyrazine (3ap). This product was obtained as a pale yellow liquid in 85% yield from **1j** and **2z** by Method D (1% catalyst loading), Work-up #1 (Table 7, entry 5), without further purification. IR (neat): 1473, 1387, 1144, 1015 cm^{-1} . 1H NMR ($CDCl_3$, 500 MHz) δ 8.87 (d, $J = 1.5$ Hz, 1 H), 8.72 (dd, $J = 2.5, 1.6$ Hz, 1 H), 8.58 (d, $J = 2.5$ Hz, 1 H), 8.10-8.00 (m, 1 H), 7.93 (d, $J = 8.2$ Hz, 1 H), 7.92-7.88 (m,

1 H), 7.61 (dd, $J = 7.1, 1.2$ Hz, 1 H), 7.55 (dd, $J = 8.1, 7.1$ Hz, 1 H), 7.53-7.47 (m, 2 H). ^{13}C NMR (CDCl_3 , 125 MHz) δ 154.9, 145.8, 143.9, 142.8, 134.6, 133.9, 130.9, 129.8, 128.4, 128.0, 126.9, 126.1, 125.2, 124.9. HRMS (ESI): m/z calcd for $\text{C}_{14}\text{H}_{10}\text{N}_2$ (M^+) 206.0844, found 206.0836.

2-(3'-Thienyl)pyridine (3aq). This product was obtained as a colorless liquid in 60% yield from **1m** and **2p** by Method A (1% catalyst loading), Work-up #1 (Table 8, entry 1), without further purification. The spectral data obtained were in accordance with those described in the literature.²³

3-(3'-Thienyl)pyridine (3ar). This product was obtained as an off-white solid in 68% yield from **1m** and **2q** by Method A, Work-up #1 (Table 8, entry 2), without further purification. mp 75-76 °C (lit. 73-74 °C).²⁴ The spectral data obtained were in accordance with those described in the literature.²³

5-(3'-Thienyl)pyrimidine (3as). This product was obtained as a bright off-white solid in 64% yield from **1m** and **2r** by Method A, Work-up #1 (Table 8, entry 3), along with 30% unreacted **2r**, and in 75% yield from **1m** and **2r** by Method D, Work-up #1 (Table 8, entry 3), without further purification. mp 97-98 °C (lit. 101-102 °C).¹⁷ IR (neat): 1563, 1427 cm^{-1} . ^1H NMR (CDCl_3 , 500 MHz) δ 9.13 (s, 1 H), 8.94 (s, 2 H), 7.60 (dd, $J = 2.8, 1.2$ Hz, 1 H), 7.49 (dd, $J = 5.0, 2.9$ Hz, 1 H), 7.39 (dd, $J = 5.0, 1.2$ Hz, 1 H). ^{13}C NMR (CDCl_3 , 125 MHz) δ 156.9, 153.9, 134.8, 129.2, 127.5, 125.1, 122.3. HRMS (ESI): m/z calcd for $\text{C}_8\text{H}_6\text{N}_2\text{S}$ (M^+) 162.0252, found 162.0253. The spectral data obtained were in accordance with those described in the literature.²⁵

[2,3']-Bithiophenyl (3at). This product was obtained as a bright off-white solid in 63% yield from **1m** and **2v** by Method D, Work-up #1 (Table 8, entry 4), after purification by chromatography on silica gel (elution with pentane). mp 62-64 °C (61.5-63 °C).²⁷ ^1H NMR (CDCl_3 , 500 MHz) δ 7.34 (dd, $J = 2.8, 1.4$ Hz, 1 H), 7.28-7.30 (m, 2 H), 7.17-7.16 (m, 2 H), 7.00 (t, $J = 4.8$ Hz, 1 H). ^{13}C NMR (CDCl_3 , 125 MHz) δ 139.1, 135.6, 127.6, 126.2, 126.1, 123.7, 123.1, 119.5. The spectral data obtained were in accordance with those described in the literature.^{26,27}

5-Acetyl-2,3'-bithiophene (3au). This product was obtained as a pale yellow solid in 84% yield from **1m** and **2s** by Method A (2% catalyst loading), Work-up #2 (Table 8, entry 5), without further purification. mp 119-120 °C (lit 125 °C). IR (neat): 1659, 1455 cm⁻¹. ¹H NMR (CDCl₃, 500 MHz) δ 7.60 (d, *J* = 3.9 Hz, 1 H), 7.52 (dd, *J* = 2.9, 1.3 Hz, 1 H), 7.37 (dd, *J* = 5.0, 2.9 Hz, 1 H), 7.32 (dd, *J* = 5.0, 1.2 Hz, 1 H), 7.18 (d, *J* = 3.9 Hz, 1 H), 2.53 (s, 3 H). ¹³C NMR (CDCl₃, 125 MHz) δ 190.3, 147.3, 142.2, 134.7, 133.3, 126.9, 125.9, 123.8, 121.9, 26.4. The spectral data obtained were in accordance with those described in the literature.²⁶

3-(3'-Thienyl)furan (3av). This product was obtained as a yellow solid, mixture with [3,3']-bithiophenyl **3aw**, in 24% and 17% respectively (by GC-MS) from the reaction between **1m** and **2x**, by Method D (1% catalyst loading), Work-up #1 (Table 8, entry 6), without further purification.²⁷

5-(3'-Thienyl)furan-2-carboxylic Acid (3ax). This product was obtained as a pale red solid in 80% yield from **1m** and **2t** by Method D, Work-up #3 (Table 8, entry 7). mp 158 °C. IR (neat): 1682, 1556, 1538, 1485, 1301, 1161, 776 cm⁻¹. ¹H NMR (CDCl₃, 500 MHz) δ 8.6 (br s, 1 H), 7.76 (dd, *J* = 2.9, 1.1 Hz, 1 H), 7.43 (dd, *J* = 5.1, 1.2 Hz, 1 H), 7.39 (m, 2 H), 6.62 (d, *J* = 3.6 Hz, 1 H). ¹³C NMR (CDCl₃, 125 MHz) δ 163.3, 155.4, 142.1, 131.1, 126.8, 125.0, 122.6, 122.1, 107.0. HRMS (ESI): *m/z* calcd for C₉H₆O₃S (M⁺) 194.008, found 194.0033.

2-(3'-Thienyl)thiazole (3ay). This product was obtained as a pale yellow liquid in 80% yield from **1m** and **2y** by Method D (2% catalyst loading), Work-up #1 (Table 8, entry 8), without further purification. The spectral data obtained were in accordance with those described in the literature.²⁶

7-(3'-Thienyl)-1H-indole (3az). This product was obtained as a pale red oil in 77% yield from **1m** and **2u** by Method D (1% catalyst loading), Work-up #1 (Table 8, entry 9), after purification by chromatography on silica gel (elution with hexane/ethyl acetate 20:1 ~ 5:1). IR (neat): 3437, 1429, 1411, 1326, 782, 729 cm^{-1} . ^1H NMR (CDCl_3 , 500 MHz) δ 8.27 (br s, NH), 7.59 (d, $J = 7.9$ Hz, 1 H), 7.42-7.40 (dd, $J = 4.8, 3.0$ Hz, 2 H), 7.40 (dd, $J = 3.0, 1.5$ Hz, 1 H), 7.34 (dd, $J = 4.8, 1.5$ Hz, 1 H), 7.22 (dd, $J = 7.2, 1.0$ Hz, 1 H), 7.14 (dd, $J = 7.7, 7.2$ Hz, 1 H), 6.57 (dd, $J = 3.1, 2.1$ Hz, 1 H). ^{13}C NMR (CDCl_3 , 125 MHz) δ 139.8, 133.7, 128.3, 127.5, 126.6, 124.3, 121.5, 121.3, 120.4, 120.1, 120.0, 103.1. HRMS (ESI): m/z calcd for $\text{C}_{12}\text{H}_9\text{NS}$ (M^+) 199.0456, found 199.0444.

2-(3'-Thienyl)pyrazine (3ba). This product was obtained as an off-white solid in 83% yield from **1m** and **2z** by Method D, Work-up #1 (Table 8, entry 10), without further purification. mp 79-80 $^{\circ}\text{C}$ (lit. 81 $^{\circ}\text{C}$).²⁸ IR (neat): 1726, 1516, 1422, 1298, 1260 cm^{-1} . ^1H NMR (CDCl_3 , 500 MHz) δ 8.92 (d, $J = 1.4$ Hz, 1 H), 8.55 (d, $J = 1.7$ Hz, 1 H), 8.43 (d, $J = 2.5$ Hz, 1 H), 7.99 (dd, $J = 3.0, 1.2$ Hz, 1 H), 7.69 (dd, $J = 5.1, 1.2$ Hz, 1 H), 7.44 (dd, $J = 5.1, 3.0$ Hz, 1 H). ^{13}C NMR (CDCl_3 , 125 MHz) δ 149.1, 144.2, 142.5, 141.9, 139.0, 127.0, 125.8, 124.8. HRMS (ESI): m/z calcd for $\text{C}_8\text{H}_6\text{N}_2\text{S}$ (M^+) 162.0252, found 162.0252.

2,6-Dimethoxy-4-(3'-thienyl)pyrimidine (3bb). This product was obtained a clear oil in 40% yield from **1m** and **2ac** by Method A (2% catalyst loading), Work-up #1 (Table 9, entry 1), after purification by chromatography on silica gel (elution with hexane/ethyl acetate 30:1). IR (neat, cm^{-1}): 1592, 1360, 1340. ^1H NMR (CDCl_3 , 500 MHz) δ 8.07 (dd, $J = 3.1, 1.1$ Hz, 1 H), 7.59 (dd, $J = 5.0, 1.1$ Hz, 1 H), 7.35 (dd, $J = 5.0, 3.1$ Hz, 1 H), 6.60 (s, 1 H), 4.04 (s, 3 H), 3.98 (s, 3 H). ^{13}C NMR (CDCl_3 , 125 MHz) δ 172.5, 165.5, 161.6, 140.0, 126.4, 126.3, 125.9, 96.7, 54.6, 53.9. HRMS (ESI): m/z calcd for $\text{C}_{10}\text{H}_{10}\text{N}_2\text{O}_2\text{S}$ (M^+) 222.0463, ($\text{M}+\text{H}$) $^+$ 223.0541, found 223.0535.

2,6-Dichloro-4-(3'-thienyl)pyrimidine (3bc). This product was obtained as a bright white solid in 70% yield from **1m** and **2ac** by Method D (1% catalyst loading), Work-up #1 (Table 9, entry 2), after purification by chromatography on silica gel (elution with hexane/ethyl acetate 30:1). mp 60-61 °C. IR (neat): 1579, 1556, 1497, 1428 cm^{-1} . ^1H NMR (CDCl_3 , 500 MHz) δ 8.22 (dd, $J = 3.0, 1.2$ Hz, 1 H), 7.63 (dd, $J = 5.1, 1.2$ Hz, 1 H), 7.47 (s, 1 H), 7.44 (dd, $J = 5.1, 3.0$ Hz, 1 H). ^{13}C NMR (CDCl_3 , 125 MHz) δ 163.3, 162.7, 160.9, 137.4, 129.5, 127.6, 125.8, 114.9. HRMS (CI): m/z calcd for $\text{C}_8\text{H}_4\text{Cl}_2\text{N}_2\text{S}$ (M^+) 229.9472, found 229.9465.

2-Chloro-4,6-di(3'-thienyl)pyrimidine (3bd). This product was obtained as a bright white solid from **1m** and **2ac** by Method D (1% catalyst loading), Work-up #1, in 10% yield (Table 9, entry 2), in 50% yield (Table 9, entry 3), and in 5% yield (Table 9, entry 4) after purification by chromatography on silica gel (elution with hexane/ethyl acetate 30:1). mp 137-138 °C (lit. 143-144 °C) IR (neat): 1580, 1531, 1496, 836, 795, 756, 711 cm^{-1} . ^1H NMR (CDCl_3 , 500 MHz) δ 8.17 (dd, $J = 3.0, 1.2$ Hz, 2 H), 7.67 (dd, $J = 5.1, 1.2$ Hz, 2H), 7.60 (s, 1 H), 7.40 (dd, $J = 5.1, 3.0$ Hz, 2 H). ^{13}C NMR (CDCl_3 , 125 MHz) δ 162.8, 161.9, 138.7, 128.1, 127.1, 125.8, 110.3. HRMS (CI): m/z calcd for $\text{C}_{12}\text{H}_7\text{ClN}_2\text{S}_2$ (M^+) 277.9739, found 277.9750. The spectral data obtained were in accordance with those described in the literature.²⁹

2,4,6-Tri(3'-thienyl)pyrimidine (3be). This product was obtained as a bright white solid from **1m** and **2ac** by Method D (1% catalyst loading), Work-up #1, in 25% yield (Table 9, entry 3), and in 70% yield (Table 9, entry 4), after purification by chromatography on silica gel (elution with hexane/ethyl acetate 30:1). mp 157-158 °C. IR (neat): 1578, 1506, 1428, 1310, 816 cm^{-1} . ^1H NMR (CDCl_3 , 500 MHz) δ 8.39 (dd, $J = 3.1, 1.1$ Hz, 1 H), 8.19 (dd, $J = 3.0, 1.2$ Hz, 2 H), 8.03 (dd, $J = 5.0, 1.1$ Hz, 1 H), 7.78 (dd, $J = 5.1,$

1.2 Hz, 2 H), 7.56 (s, 1H), 7.42 (dd, $J = 5.0, 3.0$ Hz, 2 H), 7.37 (dd, $J = 5.0, 3.5$ Hz, 1 H). ^{13}C NMR (CDCl_3 , 125 MHz) δ 161.9, 160.4, 142.2, 140.6, 127.9, 127.8, 126.6, 126.5, 126.1, 125.6, 109.4. HRMS (ESI): m/z calcd for $\text{C}_{16}\text{H}_{10}\text{N}_2\text{S}_3$ (M^+) 326.0006 ($\text{M}+\text{H}^+$) 327.0084, found ($\text{M}+\text{H}^+$) 327.0085.

5-(3'-Furyl)pyrimidine (3bf). This product was obtained as a bright off-white solid in 72% yield from **1n** and **2r** by Method D, Work-up #1 (Table 10, entry 1), without further purification. mp 82-83 °C. IR (neat): 1414, 1186, 1161 cm^{-1} . ^1H NMR (CDCl_3 , 500 MHz) δ 9.12 (s, 1 H), 8.85 (s, 2 H) 7.84 (t, $J = 1.2$ Hz, 1 H), 7.57 (t, $J = 1.7$ Hz, 1 H), 6.73 (dd, $J = 1.9, 0.9$ Hz, 1 H). ^{13}C NMR (CDCl_3 , 125 MHz) δ 157.2, 153.7, 144.7, 139.4, 126.7, 120.0, 108.0. HRMS (ESI): m/z calcd for $\text{C}_8\text{H}_6\text{N}_2\text{O}$ (M^+) 146.0480, found 146.0473.

5-(3'-Pyridyl)pyrimidine or 5-Pyridin-3-yl-pyrimidine (3bg) This product was obtained as a bright off-white solid in 64% yield from **1o** and **2r** by Method D, Work-up #1 (Table 10, entry 2), without further purification. mp 105-106 °C (lit. 107-108 °C).³⁰ IR (neat): 1579, 1557, 1417, 1402, 811, 725, 711 cm^{-1} . ^1H NMR (CDCl_3 , 500 MHz) δ 9.28 (s, 1 H), 9.0 (s, 2 H), 8.88 (d, $J = 1.9$ Hz, 1 H), 8.74 (dd, $J = 4.8, 1.2$ Hz, 1H), 7.93 (dt, $J = 7.9, 1.9$ Hz, 1 H), 7.49 (dd, $J = 7.8, 4.8$ Hz, 1 H). ^{13}C NMR (CDCl_3 , 125 MHz) δ 158.0, 154.8, 150.1, 147.8, 134.2, 131.3, 130.0, 123.9. HRMS (ESI): m/z calcd for $\text{C}_9\text{H}_7\text{N}_3$ (M^+) 157.0640, found 157.0634. The spectral data obtained were in accordance with those described in the literature.³⁰

Mechanistic studies

Analysis of the Effect of the Amount of Base Added to the Cross-Coupling Reaction.

To a suspension of 2% of $\text{Pd}(\text{OAc})_2$, potassium phenyltrifluoroborate (**1a**) (0.5 mmol), 1-bromonaphthalene (**2a**) (0.5 mmol) and two (Experiment 1) or three (Experiment 2) equivalents of K_2CO_3 in 2 mL of methanol, hexadecane was added as internal standard (0.5 mmol) and the reaction mixture was stirred and heated at reflux. Every 1 h a sample was taken, diluted with ethyl ether and hexane, then filtered through a short pad of silica gel to eliminate the palladium residues, and the conversion of 1-bromonaphthalene (**2a**) and the yield of 1-phenylnaphthalene (**3a**) was analyzed by GC. The reaction was

worked up when no further increase in the conversion of **2a** or yield of **3a** was observed after two consecutive analyses. Experiment 1 showed 85% conversion of **2a**, with 80% yield of **3a** after 7 h of reaction. Experiment 2 showed 99% conversion of **2a**, with 90% yield of **3a** after 5 h of reaction.

Analysis of the Effect of the Amount Base Added to the Arylboron Compound.

Reactions of Potassium Phenyltrifluoroborate (1a) in Wet Methanol. A suspension of potassium phenyltrifluoroborate (**1a**) (0.25 mmol) and 0, 1, 2 or 3 equivalents of K_2CO_3 in 2 mL of methanol were heated at reflux for 2 h. The reaction mixture was cooled down (the reaction with no addition of base precipitated), 2 mL of deuterated acetone was added to each one, the reaction was filtered, and the resulting solutions were analyzed using ^{11}B - and ^{19}F -NMR. The results are summarized in Table 11, entries 1-4.

Reactions of Potassium Phenyltrifluoroborate (1a) and Phenylboronic acid in Wet Deuterated Methanol. A suspension of potassium phenyltrifluoroborate or phenylboronic acid in 2 mL of wet deuterated methanol was heated at reflux in the presence of 3 equivalents of K_2CO_3 . After 45 minutes, both reactions were filtered and analyzed by 1H , ^{13}C , ^{19}F and ^{11}B NMR. The results are summarized in Table 11, entries 6-7.

Reactions of Potassium Pentafluorophenyltrifluoroborate (1i) and Pentafluorophenylboronic Acid in Dry Tetrahydrofuran. A suspension of potassium pentafluorophenyltrifluoroborate (0.25 mmol) or pentafluorophenylboronic acid (0.25 mmol) in 2 mL of dry THF was heated at reflux in the presence of 3 equivalents of diisopropylethylamine under an inert atmosphere. After 12 h each reaction was allowed to cool down, 2 mL of deuterated acetone were added, and each reaction was filtered and analyzed by ^{19}F and ^{11}B NMR.

References

1. (a) Vedejs, E.; Chapman, R. W.; Fields, S. C.; Lin, S.; Schrimpf, M. R. *J. Org. Chem.* **1995**, *60*, 3020-3027. (b) Darses, S.; Michaud, G.; Genêt, J.-P. *Eur. J. Org. Chem.* **1999**, 1875-1883. (c) Molander, G. A.; Biolatto, B. *Org. Lett.* **2002**, *4*, 1867-1870.
2. (a) Frohn, H. -J.; Adonin, N. Y.; Bardin, V. V. *J. Fluorine Chem.* **2002**, *117*, 115-120. (b) Frohn, H. -J.; Franke, H.; Fritzen, P.; Bardin, V. V. *J. Organometallic Chem.* **2000**, *598*, 127-135.
3. Li, W.; Neson, D. P.; Jensen, M. S.; Hoerrner, R. S.; Cai, D.; Larse, R. D.; Reider, P. J. *J. Org. Chem.* **2002**, *67*, 5396-5397.

4. Fernando, S. R. L.; Maharoof, U. S. M.; Deshayes, K. D.; Kinstle, T. H.; Ogawa, M. Y. *J. Am. Chem. Soc.* **1996**, *118*, 5783-5790.
5. Shudo, K.; Ohta, T.; Okamoto, T. *J. Am. Chem. Soc.* **1981**, *103*, 645-653.
6. Badone, D.; Baroni, M.; Cardamone, R.; Ielmini, A.; Guzzi, U. *J. Org. Chem.* **1997**, *62*, 7170-7173.
7. Darses, S.; Brayer, J.-L.; Demoute, J.-P.; Genêt, J.-P. *Tetrahedron Lett.* **1997**, *38*, 4393-4396.
8. Tsuno, Y.; Chong, W.-Y.; Tairaka, Y.; Sawada, M.; Yukawa, Y. *Bull. Chem. Soc. Jpn.* **1978**, *51*, 596-600.
9. Ueda, M.; Daitoh, A.; Oh-tani, S.; Miyaura, N. *Tetrahedron* **1998**, *54*, 13079-13086.
10. (a) Frohn, H. J.; Klose, A.; Bardin, V. V. *J. Fluorine Chem.* **1993**, *64*, 201-216. (b) Kamigata, N.; Yoshikawa, M.; Shimizu, T. *J. Fluorine Chem.* **1998**, *87*, 91-96.
11. Hassan, J.; Hathroubi, C.; Gozzi, C.; Lemaire, M. *Tetrahedron* **2001**, *57*, 7845 - 7856.
12. Shaughnessy, K. H.; Booth, R. S. *Org. Lett.* **2001**, *3*, 2757 - 2760.
13. Bell, H. C.; Kalman, J. R.; May, G. L.; Pinhey, J. T.; Sternhell, S. *Aust. J. Chem.* **1979**, *32*, 1531-1550.
14. Kang, S.-K.; Lee, H.-W.; Jang, S.-B.; Ho, P.-S. *J. Org. Chem.* **1996**, *61*, 4720-4724.
15. Ellames, G. J.; Gibson, J. S.; Herbert, J. M.; McNeill, A. H. *Tetrahedron* **2001**, *57*, 9487 - 9498.
16. Sakamoto, T.; Kondo, Y.; Murata, N.; Yamanaka, H. *Tetrahedron* **1993**, *49*, 9713-9720.
17. Allen, D.W.; Buckland, D. J.; Hutley, B. G.; Oades, A. C.; Turner, J. B. *J. Chem. Soc. Perkin Trans. I* **1977**, 621-624.
18. Chadwick, D. J.; Chambers, J.; Meakins, G. D. Snowden, R. L. *J. Chem. Soc. Perkin Trans. I* **1973**, 1766-1770.
19. Guillard, J.; Lamazzi, C.; Meth-Cohn, O.; Rees, C. W.; White, A. J. P.; Williams, D. J. *J. Chem. Soc. Perkin Trans. I* **2001**, 1304-1313.
20. Kuroda, M.; Nakayama, J.; Hoshino, M.; Furusho, N.; Kawata, T.; Ohba, S. *Tetrahedron* **1993**, *49*, 3735-3748.
21. MacDowell, D. W. H.; Jourdenais, R. A.; Naylor, R.; Paulovicks, G. E. *J. Org. Chem.* **1971**, *36*, 2683.
22. Jensen, J.; Skjaerbaek, N.; Vedsoe, P. *Synthesis* **2001**; 128 - 134.
23. Novak, I.; Ng, S.-C.; Mok, C.-Y.; Huang, H.-H.; Fang, J.; Wang, K. K.-T. *J. Chem. Soc. Perkin Trans.2* **1994**, *8*, 1771-1776.
24. Ryang, H.-S.A.; Sakurai, H. *J. Chem. Soc. Chem. Commun.* **1972**, 594.
25. Gronowitz, S.; Liljefors, S. *Chemica Scripta* **1979**, *13*, 39-45.

26. Al-Taweel, S. A.; Al-Saraierh, H. F. *Phosphorus, Sulfur, Silicon Relat. Elem.* **1999**, *155*, 47-58.
27. (a) Wynberg, H.; Bantjes, A. *J. Org. Chem.* **1959**, *24*, 1421-1423. (b) Wynberg, H.; Sinnige, H. J. M.; Creemers, H. M. J. C. *J. Org. Chem.* **1971**, *36*, 1011-1013.
28. Bourguignon, J.; Boucly, J. M.; Clinet, J. C.; Queguiner, G. *C. R. Hebd. Seances Acad. Sci. Ser. C* **1975**, *281*, 1019-1022.
29. Streckowski, L.; Harden, D. B.; Grubb, W. B.; Patterson, S. E.; Czarny, A. *J. Heterocycl. Chem.* **1990**, *27*, 1393-1400.
30. van der Stoel, R. E.; van der Plas, H. C. *J. Chem. Soc. Perkin Trans. I* **1979**, 2393-2396.

7.744
7.729
7.728
7.604
7.588

2.750
2.715
2.490
2.071
2.067
2.063
2.059
2.054
2.050
2.046
2.041

2.000
1.914

2.997

Current Data Parameters
F2 - Acquisition Parameters
Date_ 20071115
Time 11:15
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 32768
SOLVENT dms
NS 1
DS 2
SWH 6000.415 Hz
FIDRES 0.112355 Hz
AQ 2.1212477 sec
RG 327.144
DN 63.300 us
DE 1.70 us
TE 300.2 K
D1 1.00000000 sec
===== CHANNEL f1 =====
NUC1 13C
P1 7.14 us
PL1 0.00 dB
SFO1 100.626150 MHz
F2 - Processing parameters
SI 32768
SF 100.626150 MHz
WDW 64
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
===== CHANNEL f2 =====
1D NMR plot parameters
SI 32768
SF 100.626150 MHz
WDW 64
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
F1 100.626150 MHz
F2 100.626150 MHz
FREQH 100.626150 MHz
P1 7.14 us

Current Data Parameters
 EXPNO 2
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 20030120
 Time 20.09
 INSTRUM spect
 PROBHD 5 mm QNP 1H/1
 PULPROG zgpg30
 TD 65536
 CHANVT 201
 NS 201
 DS 31445.514
 SWH 31445.514
 FIDRES 0.479131
 AQ 1.0420724
 RG 14598.5
 DW 15.500
 DE 6.00
 TE 300.0
 D1 2.00000000
 D11 0.00000000
 D12 0.00000000
 ===== CHANNEL f1 =====
 NUCL1 13C
 P1 7.50
 PL1 3.00
 SFO1 125.8369536
 ===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUCL2 1H
 P2 100.00
 PL2 0.00
 PL12 28.00
 PL13 28.00
 SFO2 500.3152016
 F2 - Processing parameters
 SI 32768
 SF 125.8232169
 WDW EM
 SSB 0
 LB 1.00
 GB 0
 PC 1.40
 ID INE Plot parameters
 CX 22.00
 F1F 235.000
 F1 29568.46
 F2 -1887.35
 PPMON 11.38364
 HZCON 1429.80945

-140.299

```

Current Data Parameters
NAME      bbtb021-d
EXPNO     1
PROCNO    1

F2 - Acquisition Parameters
Date_     20030120
Time      20.20
PULPROG   zgpg30
TD         131072
SOLVENT    CHL
DE         4
DS         4
SWH        10000.000 Hz
FIDRES     0.774339 Hz
AQ         0.000000 sec
RG          919.2
WDW         5.000 usec
SSB         0.00 usec
LB          0.00 Hz
GB          0.00 usec
PC          1.00
D11        1.0000000 sec
D12        0.0300000 sec
D13        0.0000000 sec

===== CHANNEL f1 =====
NUC1       19F
P1         10.60 usec
PL1        -3.00 dB
SFO1       470.790443 MHz

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

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

ID MR plot parameters
CX         20.00 cm
F1         0.0000000 Hz
F2         -200.000 ppm
F3         -943.9745 Hz/cm
PC         2.0000000 Hz/cm
MECH       4788.37207 Hz/cm
  
```

Mdd

B115MM.500

DATE 14-2-2

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

AG 0.205

RG 160

NS 803

TE 297

FW 12500

O2 3300.000

DP 26H BB

LB 20.000

GB 0.0

CX 25.00

CY 0.0

F1 50.037P

F2 -59.961P

HZ/CM 282.520

PPM/CM 4.400

SR 10422.36

3.27211

Current Data Parameters
NAME CSY-600
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20011119
Time 16.00
INSTRUM spect
PULPROG 5 mm gpc 1H/1
TD 65536
FIDRES 0.183399 Hz
AQ 2.7933477 sec
RG 80.6
DM 83.200 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 1.00 usec
PL1 0.00 dB
SFO1 500.1320008 MHz

F2 - Processing parameters
SI 32768
SF 500.1300103 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

10 MHz plot parameters
CL 27.00 cm
F1 16.0000000 MHz
F2 500.1300103 MHz
F3 -314.43 MHz
PNUC 0.54618 usec/
NUC2 273.16434 MHz

0.00660

Current Data Parameters
NAME C3H-648
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20011119
Time 16.34
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1448
DS 4
SWH 31446.541 Hz
FIDRES 0.478836 Hz
AQ 1.6420724 sec
RG 7298.2
DM 15.900 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.00000000 sec
D12 0.00000000 sec

***** CHANNEL f1 *****
NUC1 13C
P1 12.00 usec
PL1 0.00 dB
SFO1 125.7718719 MHz

***** CHANNEL f2 *****
CPDPRG2 waltz16
NUC2 1H
P2 12.00 usec
PL2 0.00 dB
PL12 28.00 dB
PL13 28.00 dB
SFO2 500.1320000 MHz

F2 - Processing parameters
SI 32768
SF 125.7579700 MHz
WDW 16.0
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 22.00 cm
F1P 235.465600 MHz
F2P 29815.26 MHz
ZP -14.562000 MHz
FREQ 11.36621000 MHz
WID 1428.36831 MHz

ppm

143.79

Current Data Parameters
NAME TEST2
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20011207
Time 13.13
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg30
TD 131072
SOLVENT CSO6
NS 86
DS 4
SWH 10000.000 Hz
FIDRES 0.762939 Hz
AQ 0.6554100 sec
RG 362
DM 5.000 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
d11 0.03000000 sec
d12 0.00000000 sec

CHANNEL f1
NUC1 19F
P1 10.60 usec
PL1 -3.00 dB
SF01 470.545277 MHz

CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 95.00 usec
PL2 0.00 dB
PL12 26.00 dB
SF02 500.1320005 MHz

F2 - Processing parameters
SI 65536
SF 470.5923870 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
FIP 0.000 ppm
F1 0.00 Hz
F2 -210.000 ppm
F2 -98824.45 Hz
PPMCM 10.50000 ppm/cm
HZCM 4941.22217 Hz/cm

PPM

-15.9333

-13.9050

-4.0633

3.5863

PPM

2.504
2.500
2.496

3.288

5.735

7.870
7.712

Current Data Parameters
NAME 190003-0000
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 2003120
Time 21:15
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 1
DS 2
SWH 600.13500 MHz
FIDRES 2.7103177 Hz
AQ 0.011
RG 327.500
DE 1.0000000
TE 300.2 K
D1 1.00000000 sec
===== CHANNEL f1 =====
NUC1 1H
P1 7.00 usec
PL1 0.00 dB
PR1 500.1350515 MHz
F2 - Processing parameters
SI 32768
SF 500.1350501 MHz
WDW EM
SSB 0
LB 0.3 Hz
GB 0
PC 1.00
F2 - 1D NMR Plot Parameters
CX 32.00 cm
CY 13.00 cm
F1 190.1350515 MHz
F2 500.1350515 MHz
P2 12.00 usec
PL2 0.00 dB
PR2 500.1350515 MHz
FREQ 330.432508 MHz/c
WDW 330.432508 Hz/c

(1g)

C(F)(F)Fc1cc(B(F)(F)F)cc(C(F)(F)F)c1

Current Data Parameters		Acquisition Parameters		Processing Parameters		IDMR Plot Parameters	
NAME	VALUE	NAME	VALUE	NAME	VALUE	NAME	VALUE
EXPNO	1	DATA_	2030322	CPROG1	waitile	CT	22.00
PROCNO	2	INSTRUM	ppvst	CPROG2		CP	23.00
NAME	hbc031-040	PHOSD	5 mm QNP 1H/1	CPFL2	100.50	FP	2586.44
		TD	65536	FL1	28.00	F2	15.00
		DELTA	0.00000000	FL2	28.00	F3	-15.00
		TD0	32768	FL3	28.00	F4	1187.22
		TD1	32768	FL4	28.00	F5	1187.22
		TD2	32768	FL5	28.00	F6	1187.22
		TD3	32768	FL6	28.00	F7	1187.22
		TD4	32768	FL7	28.00	F8	1187.22
		TD5	32768	FL8	28.00	F9	1187.22
		TD6	32768	FL9	28.00	F10	1187.22
		TD7	32768	FL10	28.00	F11	1187.22
		TD8	32768	FL11	28.00	F12	1187.22
		TD9	32768	FL12	28.00	F13	1187.22
		TD10	32768	FL13	28.00	F14	1187.22
		TD11	32768	FL14	28.00	F15	1187.22
		TD12	32768	FL15	28.00	F16	1187.22
		TD13	32768	FL16	28.00	F17	1187.22
		TD14	32768	FL17	28.00	F18	1187.22
		TD15	32768	FL18	28.00	F19	1187.22
		TD16	32768	FL19	28.00	F20	1187.22
		TD17	32768	FL20	28.00	F21	1187.22
		TD18	32768	FL21	28.00	F22	1187.22
		TD19	32768	FL22	28.00	F23	1187.22
		TD20	32768	FL23	28.00	F24	1187.22
		TD21	32768	FL24	28.00	F25	1187.22
		TD22	32768	FL25	28.00	F26	1187.22
		TD23	32768	FL26	28.00	F27	1187.22
		TD24	32768	FL27	28.00	F28	1187.22
		TD25	32768	FL28	28.00	F29	1187.22
		TD26	32768	FL29	28.00	F30	1187.22
		TD27	32768	FL30	28.00	F31	1187.22
		TD28	32768	FL31	28.00	F32	1187.22
		TD29	32768	FL32	28.00	F33	1187.22
		TD30	32768	FL33	28.00	F34	1187.22
		TD31	32768	FL34	28.00	F35	1187.22
		TD32	32768	FL35	28.00	F36	1187.22
		TD33	32768	FL36	28.00	F37	1187.22
		TD34	32768	FL37	28.00	F38	1187.22
		TD35	32768	FL38	28.00	F39	1187.22
		TD36	32768	FL39	28.00	F40	1187.22
		TD37	32768	FL40	28.00	F41	1187.22
		TD38	32768	FL41	28.00	F42	1187.22
		TD39	32768	FL42	28.00	F43	1187.22
		TD40	32768	FL43	28.00	F44	1187.22
		TD41	32768	FL44	28.00	F45	1187.22
		TD42	32768	FL45	28.00	F46	1187.22
		TD43	32768	FL46	28.00	F47	1187.22
		TD44	32768	FL47	28.00	F48	1187.22
		TD45	32768	FL48	28.00	F49	1187.22

-141.498

-61.675
-61.700

Current Data Parameters
NAME: 141023-000
PROCNO: 1

F2 - Acquisition Parameters
Date_: 20030120
Time: 21.15
INSTRUM: spect
PROBHD: 5 mm QNP 1H/1
PULPROG: zgpg30
TD: 131072
SOLVENT: CDCl3
NS: 4
DS: 4
SWH: 100000.000 Hz
FIDRES: 0.762199 Hz
AQ: 0.0355116 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: 13C
P1: 10.00 usec
PL1: -3.00 dB
SFO1: 470.7901493 MHz

===== CHANNEL f2 =====
CROSSP2: waltz16
NUC2: 1H
P2: 100.00 usec
PL2: 0.00 dB
PL12: 24.00 dB
SFO2: 500.3920016 MHz

F2 - Processing parameters
SI: 65536
SF: 470.8373230 MHz
WDW: EM
SSB: 0
LB: 0.30 Hz
GB: 0
PC: 1.00

1D NMR plot parameters
CX: 20.00 cm
F1: 10.00000000 MHz
F2: 500.3920016 MHz
F3: 470.8373230 MHz
F4: 200.0000000 MHz
F5: 941.6745 Hz
F6: 5.00000000 Hz/cm
NUC1: 13C
NUC2: 1H

ppm

PPM

B115MM.500
DATE 14-2-2

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 316
TE 297

FW 12500
O2 3300.000
DP 26H BB

LB 20.000
GB 0.0
CX 25.00
CY 0.0
F1 50.037P
F2 -59.961P
HZ/CM 282.520
PPM/CM 4.400
SR 10422.36

2.56792

PPM
-50
-40
-30
-20
-10
0
10
20
30
40

Fc1cc(ccc1BF3K)F

-103.735
 -103.758
 -103.781
 -103.804
 -132.526
 -132.615

Current Data Parameters
 NAME hbb022-dmso
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20031210
 Time_ 15:02:00
 INSTRUM spect
 PROCD 5 mm QNP 1H/1
 PULPROG zgpg30
 PRGNAME zgpg30
 SOLVENT DMSO
 NS 50
 DS 4
 SWH 10000.000 Hz
 FIDRES 0.743039 Hz
 AQ 0.655100 sec
 RG 2048
 IN 5.000 usec
 DE 1.000 usec
 TE 300.0 K
 D1 1.00000000 sec
 D11 0.03000000 sec
 D12 0.00000000 sec

===== CHANNEL F1 =====
 NUCL1 19F
 P1 15.00 usec
 PL1 -3.00 dB
 SFO1 470.7901483 MHz

===== CHANNEL F2 =====
 CPDPRG2 waltz16
 NUCL2 1H
 P2 100.00 usec
 PL2 0.00 dB
 PL12 20.00 dB
 SFO2 500.3250016 MHz

F2 - Processing parameters
 SI 32768
 SF 470.7901483 MHz
 DF 470.8373330 MHz
 BM 0
 GB 0
 CB 0
 SC 0
 AS 0
 PC 1.00

1D NMR plot parameters
 CZ 20.00 cm
 F1P 0.000 ppm
 P1 0.00 Hz
 ZF -200.000 MHz
 F2 -94157.45 Hz
 FREQM 10.00000 ppm/cm
 NSCM 4708.37287 Hz/cm

PPM

B115MM.500

DATE 14-2-2

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 80

NS 454

TE 297

FW 12500

O2 3300.000

DP 26H BB

LB 20.000

GB 0.0

CX 25.00

CY 0.0

F1 50.037P

F2 -59.961P

HZ/CM 282.520

PPM/CM 4.400

SR 10422.36

2.51602
1.82940

```

Current Data Parameters
=====
NAME          bb6021-usno
PROBNO        1
PROCNO        1

Data - Acquisition Parameters
=====
Date         20101020
Time         21:39
INSTRUM      VLA
PROBNO       5 mm QIP 1H/1
PROCNO       1978nm
TD           13102
FREQ         430 MHz
NCHANS       123
NPTS         5000 user
DWS          10000.000 Hz
RES          0.6551100 sec
DM            8132
RG            5.000 user
WDW           300.0 K
SSB           1.00000000 sec
D1            0.03000000 sec
D11           0.00020000 sec
D12           0.00020000 sec

===== CHANNEL f1 =====
P1          19f
PL1         10. user
SF01        470.791483 MHz

===== CHANNEL f2 =====
P2          19f
PL2         100.00 user
SF02        470.837200 MHz

===== Processing parameters =====
SI          0
SN          0
NMN         0 dB
SSB         0 dB
PC          300.1920016 Mhz
FREQ        470.837200 MHz
DM           8132
RES          0.30 Hz
PC          1.00

===== NMR plot parameters =====
RTP         -100.000 ppm
F1P         -47083.72 Hz
F2P         -200.00 Hz
F3P         -200.00 Hz
F4P         3.000000 MHz
FANCH       2351.18604 Hz/

```

PPM

B115MM.500
DATE 14-2-2

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 719
TE 297

FW 12500
O2 3300.000
DP 26H BB

LB 20.000
GB 0.0
CX 25.00
CY 0.0
F1 50.037P
F2 -59.961P
HZ/CM 282.520
PPM/CM 4.400
SR 10422.36

2.00173
1.35454

Current Data Parameters
 EXPNO 1
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 200805
 Time 14.00
 INSTRUM spect
 PROCNM 1
 PULPROG zgpg30
 TD 32768
 SFO 300.135060
 AQ 32768
 FIDRES 0.000150
 AQ 32768
 RG 32768
 DQ 32768
 PR 1.0000000
 CHANDEL 1
 SFO 300.135060
 P1 7.00
 PL1 0.00
 SFO 300.135060
 F2 - Processing parameters
 SI 32768
 SF 300.135060
 DS 0.0
 CB 1.00
 PC

Current Data Parameters
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20020808
Time 11.35
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg30
OBSFREQ 499.9
SOLVENT CDCl3
NS 44
DS 4
SWH 31646.564 Hz
FIDRES 0.478836 Hz
AQ 1.0420724 sec
RG 1159.42
AQ 15.960 us
DE 6.00 us
TE 300.0 K
ZG 2.0000000 sec
D1 1.00000000 sec
D11 0.03000000 sec
D12 0.00020000 sec
===== CHANNEL f1 =====
NUC1 13C
P1 13C
PL1 7.50 us
PT1 2.00 us
SFO1 125.836156 MHz
===== CHANNEL f2 =====
NUC2 1H
P2 1H
PL2 100.00 us
PT2 0.00 us
SFO2 500.332015 MHz
F2 - Processing parameters
SI 32768
SF 125.8320462 MHz
WDW 0
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

-132.441
 -132.508
 -132.642

Current Data Parameters
 NAME: Met015-1
 EXPNO: 1
 PROCNO: 1
 F2 - Acquisition Parameters
 Date_: 20020808
 Time: 11.57
 INSTRUM: spect
 PULPROG: zgpg30
 TD: 131072
 SOLVENT: CDCl3
 NS: 400
 DS: 4
 SWH: 100000.000 Hz
 FIDRES: 0.763739 Hz
 AQ: 0.0891000 sec
 RG: 1024
 DW: 5.000 usec
 DE: 2.00 usec
 TE: 300.2 K
 D1: 1.00000000 sec
 D11: 0.03000000 sec
 D12: 0.00000000 sec
 CHANNEL F1
 NUC1: 13C
 P1: 10.00 usec
 PL1: -1.00 dB
 SFO1: 470.790103 MHz
 CHANNEL F2
 CPDPRG2: waltz16
 NUC2: 1H
 PCPD2: 100.00 usec
 PL2: 0.00 dB
 PL12: 26.00 dB
 SFO2: 500.325015 MHz
 F2 - Processing parameters
 SI: 32768
 SF: 500.385959 MHz
 WDM: 1
 SSF: 0
 LA: 0.30 Hz
 GB: 0
 PC: 1.00

PPM

B115MM.500
DATE 3-10-1

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 80
NS 405
TE 297

FW 12500
O2 3300.000
DP 26H BB

LB 20.000
GB 0.0
CX 25.00
CY 0.0
F1 59.999P
F2 -59.999P
HZ/CM 308.203
PPM/CM 4.800
SR 10419.92

5 32638
4 55850

7.274
7.273
7.162
6.302

Current Data Parameters
NAME: 1n1b20-2
EXPNO: 1
PROCNO: 1

F2 - Acquisition Parameters
Date_: 20021011
Time: 10.10
INSTRUM: spect
PROBHD: 5 mm QNP 1H/1
PULPROG: zgpg30
TD: 65536
SOLVENT: CDCl3
NS: 15
DS: 4
SWH: 6000.415 Hz
FIDRES: 0.113397 Hz
AQ: 0.021441 sec
RG: 327.000
DM: 819.000 umsc
DE: 2.0000000
TE: 300.2 K
D1: 1.0000000 sec

===== CHANNEL f1 =====
NUC1: 13C
P1: 7.10 umsc
PL1: 0.00 dB
SFO1: 500.3925015 MHz

F2 - Processing parameters
SI: 32768
SF: 500.3900121 MHz
WDW: EM
SSB: 0
LB: 0.30 Hz
GB: 0
PC: 1.00

1D NMR Plot Parameters
SI: 32768
SF: 500.3900121 MHz
WDW: EM
SSB: 0
LB: 0.30 Hz
GB: 0
PC: 1.00
FIDRES: 0.113397 Hz
AQ: 0.021441 sec
RG: 327.000
DM: 819.000 umsc
DE: 2.0000000
TE: 300.2 K
D1: 1.0000000 sec

30.253
30.101
29.947
29.790
29.636

114.308

144.717
141.586

Current Data Parameters
NAME bbb020-1
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20081111
Time_ 14.47
INSTRUM spect
PROBHD 5 mm QNP 1H/1
TD 65536
SOLVENT CDCl3
DS 14
SWH 31446.541 Hz
FIDRES 0.478976 Hz
AQ 1.046025 sec
RG 6502
DM 15.800 us
DE 600.0 us
D1 300.0 us
D11 2.00000000 sec
D12 0.00020000 sec
===== CHANNEL f1 =====
NUC1 13C
P1 130.00 us
PL1 3.00 dB
SFO1 125.8236556 MHz
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
P2 100.00 us
PL2 0.00 dB
F2 500.1362016 MHz
SFO2 500.1362016 MHz
F2 - Processing parameters
SI 32768
SF 125.8236556 MHz
WDW EM
SSB 0
GB 0.30 Hz
PC 1.00

-139.001
 -138.899
 -138.785
 -138.688

Current Data Parameters
 NAME bbf020-2
 EXPNO 2
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 20021011
 Time 20:32
 INSTRUM spect
 PROBM 5 mm QNP 1H/1
 PULPROG zgpg30
 TD 131072
 SFO1 500.1360016 MHz
 NS 512
 DS 4
 SWH 10000.000 Hz
 F2 500.1360016 MHz
 AQ 0.655100 sec
 RG 10321.3
 DM 5.000 usec
 DE 60.000 usec
 TE 300.0 K
 D1 1.00000000 sec
 D11 0.03000000 sec
 D12 0.00020000 sec
 CHANNEL F1
 NUCL1 139F
 P1 10.00 usec
 PL1 0.00 dB
 SFO1 470.7801483 MHz
 CHANNEL F2
 NUCL2 1H
 P2 100.00 usec
 PL2 0.00 dB
 SFO2 500.1360016 MHz
 F2 - Processing parameters
 SI 32768
 SF 470.8173200 MHz
 EM 0
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00
 ID MR plot parameters
 SI 32768
 SF 470.8173200 MHz
 EM 0
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00
 F1 0.000 ppm
 F2 -200.000 ppm
 F2 10.000000 Hz/cm
 F2 10.000000 Hz/cm
 MICH 4788.37207 Hz/cm

PPM

B115MM.500
DATE 2-11-1

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 80
NS 282
TE 297

FW 12500
O2 3300.000
DP 26H BB

LB 20.000
GB 0.0
CX 25.00
CY 10.00
F1 49.999P
F2 -49.999P
HZ/CM 256.836
PPM/CM 4.000
SR 10432.13

4.25157

from deuterated methanol

4.813

7.247
7.236
7.233
7.222

8.567 —
8.261 > 8.251
7.911 > 7.896

[illegible]

[illegible]

-134.924

Current Data Parameters
 NAME: bbf005dmo
 INSTRUM: spect
 PROCNO: 2
 F2 - Acquisition Parameters
 Date_ : 20031215
 Time : 21.57
 INSTRUM: spect
 PROBNM: 5 mm QNP 1H/1
 PULPROG: zgpg30
 TOUPROG: zgpg30
 SOLVENT: CDCl3
 NS: 73
 DS: 4
 SWH: 100000.000 Hz
 FIDRES: 0.742833 Hz
 AQ: 0.4554100 sec
 RG: 1024
 DW: 5.000 usec
 DE: 6.000 usec
 TE: 300.0 K
 D1: 1.00000000 sec
 D11: 0.03000000 sec
 D12: 0.00000000 sec
 CHANNEL f1
 NUC1: 13F
 P1: 10.00 usec
 PL1: -1.00 dB
 SFO1: 470.7901483 MHz
 CHANNEL f2
 NUC2: 1H
 P2: 100.00 usec
 PL2: 0.00 dB
 SFO2: 500.392016 MHz
 F2 - Processing parameters
 SI: 65536
 SF: 470.8372150 MHz
 WDW: EM
 SSB: 0
 LB: 0.30 Hz
 GB: 0
 PC: 1.00
 ID MHz plot parameters
 CX: 20.00 cm
 CY: 10.00 cm
 F1: -47083.72 Hz
 F2: -47083.72 Hz
 F2: -200.000 ppm
 F2: -94167.45 Hz
 F2: -5.000 Hz/cm
 F2: 235.18604 Hz/cm

~~SECRET~~

PPM

B115MM.500
DATE 18-9-1

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
AG .205
RG 80
NS 121
TE 297

FW 12500
O2 3300.000
DP 26H BB

LB 20.000
GB 0.0
CX 25.00
CY 0.0
F1 59.999P
F2 -59.999P
HZ/CM 308.203
PPM/CM 4.800
SR 10478.52

3.99795

8.534
8.531
8.524
8.522
8.268
8.255
7.983
7.970
7.727
7.715
7.702

[illegible]

-155.598
-155.572
-155.547
-152.043

Current Data Parameters
NAME: bbb006-2s
EXPNO: 3
PROCNO: 1
Date_ Acquisition Parameters:
Date_: 20020717
Time: 14.57
INSTRUM: spect
PROBHD: 5 mm QNP 1H/1
PULPROG: zgpg30
TD: 65536
SOLVENT: CDCl3
NS: 37
DS: 4
SWH: 100000.000 Hz
FIDRES: 0.742339 Hz
AQ: 0.00000000 Hz
RG: 1821.4
DM: 5.000 u
TE: 300.2 K
D1: 1.00000000 Hz
D11: 0.00000000 Hz
D12: 0.00000000 Hz
----- CHANNEL f1 -----
NUC1: 13C
P1: 19.00 u
PL1: 0.00 dB
SFO1: 470.7901483 MHz
----- CHANNEL f2 -----
CPDPRG2: waltz16
NUC2: 1H
P2: 100.00 u
PL2: 0.00 dB
PL12: 0.00 dB
SFO2: 500.3920015 MHz
P2 - Processing parameters:
SI: 32768
SF: 470.8372210 MHz
WDW: EM
SSB: 0
LB: 0.30 Hz
GB: 0
PC: 1.00

~~BUKRA~~

PPM

B115MM.500
DATE 13-9-1

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 573
TE 297

FW 12500
O2 3300.000
DP 26H 88

LB 20.000
GB 0.0
CX 25.00
CY 0.0
F1 59.999P
F2 -59.999P
HZ/CM 308.203
PPM/CM 4.800
SR 10478.52

1.80491

50 40 30 20 10 0 -10 -20 -30 -40 -50
PPM

Current	Parameter	Value	Unit
DATE	DATE	20031113	
NAME	NAME	bk00000000	
EXPNO	EXPNO	2	
PROCNO	PROCNO	1	
F2 - Acquisition Parameters			
DATE_	DATE_	20031113	
TIME	TIME	12.00	hh:mm
INSTRUM	INSTRUM	SPARK	
PROBHD	PROBHD	5 mm QNP 1H/1	
PULPROG	PULPROG	zgpg30	
TD	TD	65536	
SOLVENT	SOLVENT	CDCl3	
NS	NS	129	
DS	DS	4	
SWH	SWH	31466.361	Hz
FIDRES	FIDRES	0.479936	Hz
AQ	AQ	1.4459675	s
RG	RG	1.4459675	s
DELTA	DELTA	135.000	us
DE	DE	35.000	us
TE	TE	300.2	K
D1	D1	4.000000000	ss
D11	D11	0.030000000	ss
D2	D2	0.000200000	ss
D12	D12	0.000200000	ss
CHANNEL f1 ==			
NUC1	NUC1	13C	
P1	P1	7.00	us
PL1	PL1	3.00	dB
SFO1	SFO1	125.1369556	MHz
CHANNEL f2 ==			
NUC2	NUC2	1H	
P2	P2	100.00	us
PL2	PL2	0.00	dB
PL12	PL12	28.00	dB
PL13	PL13	28.00	dB
SFO2	SFO2	500.3520015	MHz
F2 - Processing parameters			
SI	SI	32768	
WDW	WDW	EM	
SSB	SSB	0	
GB	GB	1.00	Hz
PC	PC	1.40	
10 NMR plot parameters			
CT	CT	3.00	cr
RG	RG	170.00	cr
FI	FI	23394.72	Hz
F2	F2	20.797	ppm
F3	F3	20.797	ppm
F4	F4	24.833	ppm
F5	F5	24.833	ppm
F6	F6	48.161	ppm
F7	F7	941.48063	Hz

Current Data Parameters
 NAME: 20000422
 EXPNO: 1
 PROCNO: 1
 F2 - Acquisition Parameters
 Date_: 20000422
 Time: 11.34
 INSTRUM: spect
 PULPROG: 5 mm gcp 1h/1
 TO: 32768
 SOLVENT: CDCl₃
 NS: 16
 DS: 4
 SWH: 6000.615 Hz
 FIDRES: 0.181389 Hz
 AQ: 2.7263177 sec
 RG: 32
 DM: 63.200 usec
 DE: 6.00 usec
 TE: 300.0 K
 D1: 1.00000000 sec
 ***** CHANNEL f1 *****
 NUC1: 1H
 P1: 7.50 usec
 PL1: 0.00 dB
 SFO1: 500.3625018 MHz
 F2 - Processing parameters
 SI: 32768
 SF: 500.3603776 MHz
 MDW: 0
 EN: 0
 SSB: 0
 LB: 0.30 Hz
 GB: 0
 PC: 1.00
 10 MHz plot parameters
 CX: 22.00 cm
 FIP: 10.000 ppm
 F1: 5003.80 Hz
 F2: -50.500 ppm
 F3: 2501.9 Hz
 GRCH: 0.1777 sec/pt
 -ZCN: 230.82251 Hz/c

ppm

160.238
157.378
138.322
131.174
129.375
127.872
126.384
123.528
104.565
98.937
77.260
77.004
76.750
55.402
55.265

Current Data Parameters
NAME: 101000449h
EXPNO: 2
PROCNO: 1

F2 - Acquisition Parameters
Date_: 20030422
Time: 11.36
INSTRUM: spect
PROBHD: 5 mm QNP
PULPROG: zgpg30
TO: 1.00
SOLVENT: CDCl3
NS: 66
DS: 4
SWH: 31446.341 Hz
FIDRES: 0.478638 Hz
AQ: 1.0420724 sec
RG: 7288.2
DM: 15.900 usec
DE: 6.00 usec
TE: 300.0 K
D1: 2.00000000 sec
D11: 0.03000000 sec
D12: 0.00000000 sec

***** CHANNEL f1 *****
NUC1: 13C
P1: 7.50 usec
PL1: 3.00 dB
SFO1: 125.8300000 MHz

***** CHANNEL f2 *****
CPDPRG2: waltz16
NUC2: 1H
PCPD2: 100.00 usec
PL2: 0.00 dB
PL12: 28.00 dB
PL13: 28.00 dB
SFO2: 500.3620018 MHz

F2 - Processing parameters
SI: 32768
SF: 125.8231884 MHz
WDW: EM
SSB: 0
LB: 1.00 Hz
GB: 0
PC: 1.40

1D NMR plot parameters
CA: 22.00 cm
F1: 225.000 ppm
F2: 225.000 Hz
F3: 115.000 ppm
F4: 115.000 Hz
P1: 11.36384 sec
P2: 1425.80888 Hz

S58

77.252
76.999
76.745

111.778
118.566
127.368
127.843
129.032
132.653
132.798
136.798
143.409
144.193

197.381

Current Data Parameters		Channel #1		Channel #2	
NAME	bbt005f1f	NAME	CH1001	NAME	CH2002
DEPTH	2	DEPTH	1	DEPTH	1
PROG	2	PROG	1	PROG	1
TIME	200.126	TIME	1.00	TIME	1.00
TIME	200.126	TIME	1.00	TIME	1.00
INSTRUM	spec	INSTRUM	15.000 us	INSTRUM	15.000 us
PROBHD	5 mm QNP 1H/1	PROBHD	15.000 us	PROBHD	15.000 us
PROCPRG	zgpg30	PROCPRG	15.000 us	PROCPRG	15.000 us
TD	65536	TD	2.00000000	TD	2.00000000
TO SOLVENT	CDCl3	TO SOLVENT	0.03000000	TO SOLVENT	0.03000000
NUC1	1H	NUC1	13C	NUC1	13C
NUC2	1H	NUC2	13C	NUC2	13C
CH1001	125.8349554 MHz	CH2002	125.8349554 MHz	CH2002	125.8349554 MHz
CH1002	125.8349554 MHz	CH2003	125.8349554 MHz	CH2003	125.8349554 MHz
CH1003	125.8349554 MHz	CH2004	125.8349554 MHz	CH2004	125.8349554 MHz
CH1004	125.8349554 MHz	CH2005	125.8349554 MHz	CH2005	125.8349554 MHz
CH1005	125.8349554 MHz	CH2006	125.8349554 MHz	CH2006	125.8349554 MHz
CH1006	125.8349554 MHz	CH2007	125.8349554 MHz	CH2007	125.8349554 MHz
CH1007	125.8349554 MHz	CH2008	125.8349554 MHz	CH2008	125.8349554 MHz
CH1008	125.8349554 MHz	CH2009	125.8349554 MHz	CH2009	125.8349554 MHz
CH1009	125.8349554 MHz	CH2010	125.8349554 MHz	CH2010	125.8349554 MHz
CH1010	125.8349554 MHz	CH2011	125.8349554 MHz	CH2011	125.8349554 MHz
CH1011	125.8349554 MHz	CH2012	125.8349554 MHz	CH2012	125.8349554 MHz
CH1012	125.8349554 MHz	CH2013	125.8349554 MHz	CH2013	125.8349554 MHz
CH1013	125.8349554 MHz	CH2014	125.8349554 MHz	CH2014	125.8349554 MHz
CH1014	125.8349554 MHz	CH2015	125.8349554 MHz	CH2015	125.8349554 MHz
CH1015	125.8349554 MHz	CH2016	125.8349554 MHz	CH2016	125.8349554 MHz
CH1016	125.8349554 MHz	CH2017	125.8349554 MHz	CH2017	125.8349554 MHz
CH1017	125.8349554 MHz	CH2018	125.8349554 MHz	CH2018	125.8349554 MHz
CH1018	125.8349554 MHz	CH2019	125.8349554 MHz	CH2019	125.8349554 MHz
CH1019	125.8349554 MHz	CH2020	125.8349554 MHz	CH2020	125.8349554 MHz
CH1020	125.8349554 MHz	CH2021	125.8349554 MHz	CH2021	125.8349554 MHz
CH1021	125.8349554 MHz	CH2022	125.8349554 MHz	CH2022	125.8349554 MHz
CH1022	125.8349554 MHz	CH2023	125.8349554 MHz	CH2023	125.8349554 MHz
CH1023	125.8349554 MHz	CH2024	125.8349554 MHz	CH2024	125.8349554 MHz
CH1024	125.8349554 MHz	CH2025	125.8349554 MHz	CH2025	125.8349554 MHz
CH1025	125.8349554 MHz	CH2026	125.8349554 MHz	CH2026	125.8349554 MHz
CH1026	125.8349554 MHz	CH2027	125.8349554 MHz	CH2027	125.8349554 MHz
CH1027	125.8349554 MHz	CH2028	125.8349554 MHz	CH2028	125.8349554 MHz
CH1028	125.8349554 MHz	CH2029	125.8349554 MHz	CH2029	125.8349554 MHz
CH1029	125.8349554 MHz	CH2030	125.8349554 MHz	CH2030	125.8349554 MHz
CH1030	125.8349554 MHz	CH2031	125.8349554 MHz	CH2031	125.8349554 MHz
CH1031	125.8349554 MHz	CH2032	125.8349554 MHz	CH2032	125.8349554 MHz
CH1032	125.8349554 MHz	CH2033	125.8349554 MHz	CH2033	125.8349554 MHz
CH1033	125.8349554 MHz	CH2034	125.8349554 MHz	CH2034	125.8349554 MHz
CH1034	125.8349554 MHz	CH2035	125.8349554 MHz	CH2035	125.8349554 MHz
CH1035	125.8349554 MHz	CH2036	125.8349554 MHz	CH2036	12

8.463
8.459
8.300
8.298
8.296
8.294
8.283
8.282
8.279
7.942
7.939
7.929
7.927
7.926
7.814
7.811
7.801
7.797
7.758
7.754
7.741
7.707
7.691
7.676
7.268

0.000

Current Data Parameters
 Date_ 28/06/93
 Time_ 11:11
 Operator_ J.S.
 Instrument_ 5 mm QNP 300
 P1_ 12.00
 PR_ 27.00
 TO_ 327.60
 FIDUCIAL_ CDM
 NS_ 2
 DS_ 4
 SWH_ 6000.451 Hz
 FWHZ_ 0.163359 Hz
 AQ_ 2.7525477 sec
 RG_ 327.60
 DM_ 32.258 msec
 DE_ 1.0000000
 TE_ 300.2 K
 D1_ 1.00000000 sec
 ===== CHANNEL f1 =====
 NUC1_ 13C
 P1_ 12.00 sec
 PL1_ 0.00 dB
 SFO1_ 100.332619 MHz
 ===== CHANNEL f2 =====
 P2_ Processing parameters
 S1_ 327.60
 SFO2_ 500.336021 MHz
 WDP_ 0.00 Hz
 SSB_ 0.00 Hz
 GB_ 0.00 Hz
 PC_ 1.00

142.967
140.787
133.029
132.923
130.179
127.858
123.297
122.100
118.347
112.383

77.252
76.999
76.744

Current Data Parameters
NAME hbec004-mp
PROCNO 1
F2 - Acquisition Parameters
Date_ 20020403
Time 11:57
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
DS 4
SWH 31446.541 Hz
FIDRES 0.420000 Hz
AQ 1.0425724 sec
RG 8192
DW 15.000000 usec
DE 6.000000 usec
TE 300.0 K
D1 2.00000000 sec
d11 1.10000000 sec
D12 0.05000000 sec
D13 0.00000000 sec
===== CHANNEL f1 =====
NUC1 13
P1 7.50 usec
PL1 2.00 dB
SFO1 125.8369556 MHz
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
P2 100.00 usec
PL2 0.00 dB
PL12 0.00 dB
PL13 26.00 dB
PL14 19.00 dB
SFO2 500.3250316 MHz
F2 - Processing parameters
SI 32768
SF 125.8231788 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

8.048
7.947
7.839
7.822
7.770
7.753

Current Data Parameters
 EXPNO 1
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 20150801
 Time 11.32
 INSTRUM spect
 PULPROG zgpg30
 TD 32768
 SFO 500.136199 MHz
 F2 - Processing parameters
 SI 32768
 SF 500.136199 MHz
 DS 4
 SS 0.20 Hz
 CB 1.00
 PC 1.00

142.430
 141.329
 132.994
 132.720
 132.453
 132.186
 127.969
 127.343
 126.350
 124.183
 122.209
 122.179
 122.153
 122.014
 119.846
 118.167
 112.834

77.254
 77.000
 76.746

Current Data Parameters
 NAME: bcc006
 EXPNO: 1
 PROCNO: 1
 F2 - Acquisition Parameters
 Date_: 200212
 Time: 16.
 INSTRUM: spect
 PROBHD: 5 mm Data
 PULPROG: zgpg30
 TO: 655
 SOLVENT: CDC
 NS: 33333.3
 DS: 0.5086
 FIDRES: 0.93333
 AQ: 1.80
 RG: 150
 DE: 18.
 TE: 300
 ML1: 4.000000
 D1: 4.000000
 CPOPRG: waltz
 P31: 107.
 S4: 0.03000
 S2: 5.
 SFO1: 125.83821
 NUCLEUS: 1
 F2 - Processing Parameters
 SI: 327
 SF: 125.82317
 HW: 1.
 HB: 1.
 GB: 1.
 PC: 1.
 1D NMR plot parameters
 CK: 21.
 FIP: 235.0
 FI: 235.86
 F2: -1847.0
 F3: 11.904
 PPMCH: 1497.894

-63.406

Current Data Parameters
NAME: 100000000 Hz
EXPNO: 3
PROCNO: 1
F2 - Acquisition Parameters
Date_: 20020804
Time: 11.40
INSTRUM: spect
PROBHD: 5 mm QNP 1H/13
PULPROG: zgpg30
TO: 131.672
SOLVENT: CDCl3
NS: 4
DS: 4
SWH: 100000.000 Hz
FIDRES: 0.742939 Hz
AQ: 0.65546100 sec
RG: 312
DM: 5.000 usec
DE: 6.00 usec
TE: 300.2 K
D1: 1.0000000 sec
D11: 0.0300000 sec
D12: 0.0002000 sec
===== CHANNEL f1 =====
NUC1: 13C
P1: 10.00 usec
PL1: -3.00 dB
SFO1: 470.7961805 MHz
===== CHANNEL f2 =====
CPDPRG2: waltz16
NUC2: 1H
P2: 100.00 usec
PL2: 0.00 dB
PL12: 24.00 dB
SFO2: 500.3920016 MHz
F2 - Processing parameters
SI: 16384
SF: 470.8373324 MHz
WDW: EM
SSB: 0
LB: 0.30 Hz
GB: 0
PC: 1.00

ppm

-180

-160

-140

-120

-100

-80

-60

-40

-20

Current Data Parameters
 Name: 3u
 ExpNo: 1
 PROCNO: 1
 F2 - Acquisition Parameters
 Date_: 20011109
 Time: 11.15
 Instrument: spect
 Progam: 1d
 Preampl: 5 mm qnp 1h1
 TO: 22748
 FIDRES: 0.0001
 AQCNT: 1
 DS: 2
 SWH: 6000.2
 FWHM: 0.00118 Hz
 AQ: 2.7255477 sec
 RG: 327.5
 RW: 93.380 sec
 DB: 1.00 sec
 DD: 0.00 sec
 DT: 1.0000000 sec
 ===== CHANNEL f1 =====
 NUC1: 1H
 P1: 7.50 sec
 PL: 0.00
 SFO1: 500.1325619 MHz
 F2 - Processing parameters
 SI: 32768
 SF: 500.1306771 MHz
 WDW: 0
 SSF: 0.90 Hz
 LB: 1.00
 GB: 0
 PC: 1.00
 10 mm plot parameters
 CL: 22.00 cm
 CY: 10.00 cm
 FI: 1601.50 Hz
 SFO: 500.1306771 MHz
 ZF9: -20.000 Hz
 ZF7: 0.0000000 Hz
 FREQH: 0.47177 ppm/c
 NSCH: 230.02250 Hz/c

160.802
 160.751
 158.816
 158.763
 134.069
 131.943
 131.092
 130.299
 130.216
 130.133
 118.537
 116.692
 112.070
 112.019
 111.976
 111.856
 111.811
 77.260
 77.005
 76.751

Current Data Parameters
 NAME bat007b10c
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 20021109
 Time_ 21.09
 INSTRUM spect
 PULPROG zgpg30
 TD 65536
 SFO1 125.834554 MHz
 SOLVENT CDCl3
 DS 4
 SWH 3146.341 Hz
 FIDRES 0.000000 Hz
 AQ 1.640724 sec
 RG 13004
 DW 15.500 usec
 DE 2.000 usec
 TE 300.2 K
 D1 4.0000000 sec
 d11 0.0000000 sec
 D12 0.0000000 sec
 D13 0.0000000 sec
 CHANNEL f1
 NUC1 13C
 P1 7.15 usec
 PL1 3.00 dB
 SFO1 125.834554 MHz
 CHANNEL f2
 NUC2 1H
 P2 100.00 usec
 PL2 0.00 dB
 PCPD2 0.00 dB
 PL3 24.00 dB
 PL4 19.00 dB
 SFO2 500.3620014 MHz
 F2 - Processing parameters
 SF 125.834554 MHz
 SF2 500.3620014 MHz
 EQ 1.00 Hz
 LB 0.30 Hz
 GB 1.0
 PC 1.40
 ID 100% plot parameters
 CT 22.00 sec
 FI 232.000000 Hz
 F1 29248.45 Hz
 F2P -15.000 PP
 F2 -1187.15 Hz
 FIDRES 1.185134 Hz
 RESOL 1433.80884 Hz

-114.768

```

Current Data Parameters
NAME          hsc007k-2
EXPNO         1
PROCNO        1
F2 - Acquisition Parameters
Date_         20020606
Time          11.43
INSTRUM       spect
PROBHD        5 mm QNP 1H/1
PULPROG       zgpg30
TD            131072
AQ            0.0400000
RG            1024
DS            4
SOLVENT       CDCl3
NS            11
DS            4
SWH            10000.000 Hz
FIDRES        0.000100 Hz
AQRES         0.634100 sec
RG            1024
DM            5.000 usec
DE            16.00 usec
TE            300.2 usec
D1            1.0000000 sec
D11           0.0300000 sec
D12           0.0002000 sec
===== CHANNEL f1 =====
NUC1          13C
P1            10.00 usec
PL1           -2.00 dB
SFO1          470.7501483 MHz
===== CHANNEL f2 =====
CPDPRG2       waltz16
NUC2          1H
PCPD2         100.00 usec
PL2           0.00 dB
PL12          0.00 dB
SFO2          500.362016 MHz
F2 - Processing parameters
SI            32768
SF            470.8372515 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.40
  
```

ppm

-180

-160

-140

-120

-100

-80

-60

-40

-20

(3v)

Year	Number of people (millions)
1970	7.813
1975	7.809
1980	7.800

Current Data Parameters		Acquisition Parameters		Processing Parameters		10 Mark Plot Parameters	
NAME	VALUE	NAME	VALUE	NAME	VALUE	NAME	VALUE
NAME	bbcc0595pro	PS - Acquisition Rate	22.5	MC1	1.0000000	CK	32.0
PRNO	1	Time	22.5	MC2	0.0	FL1	503.9
PRACHO	1	Time	22.5	FL1	500.32501	FL2	503.9
		Time	22.5	FL2	500.32501	FL3	503.9
		Time	22.5	FL3	500.32501	FL4	503.9
		Time	22.5	FL4	500.32501	FL5	503.9
		Time	22.5	FL5	500.32501	FL6	503.9
		Time	22.5	FL6	500.32501	FL7	503.9
		Time	22.5	FL7	500.32501	FL8	503.9
		Time	22.5	FL8	500.32501	FL9	503.9
		Time	22.5	FL9	500.32501	FL10	503.9
		Time	22.5	FL10	500.32501	FL11	503.9
		Time	22.5	FL11	500.32501	FL12	503.9
		Time	22.5	FL12	500.32501	FL13	503.9
		Time	22.5	FL13	500.32501	FL14	503.9
		Time	22.5	FL14	500.32501	FL15	503.9
		Time	22.5	FL15	500.32501	FL16	503.9
		Time	22.5	FL16	500.32501	FL17	503.9
		Time	22.5	FL17	500.32501	FL18	503.9
		Time	22.5	FL18	500.32501	FL19	503.9
		Time	22.5	FL19	500.32501	FL20	503.9
		Time	22.5	FL20	500.32501	FL21	503.9
		Time	22.5	FL21	500.32501	FL22	503.9
		Time	22.5	FL22	500.32501	FL23	503.9
		Time	22.5	FL23	500.32501	FL24	503.9
		Time	22.5	FL24	500.32501	FL25	503.9
		Time	22.5	FL25	500.32501	FL26	503.9
		Time	22.5	FL26	500.32501	FL27	503.9
		Time	22.5	FL27	500.32501	FL28	503.9
		Time	22.5	FL28	500.32501	FL29	503.9
		Time	22.5	FL29	500.32501	FL30	503.9
		Time	22.5	FL30	500.32501	FL31	503.9
		Time	22.5	FL31	500.32501	FL32	503.9
		Time	22.5	FL32	500.32501	FL33	503.9
		Time	22.5	FL33	500.32501	FL34	503.9
		Time	22.5	FL34	500.32501	FL35	503.9
		Time	22.5	FL35	500.32501	FL36	503.9
		Time	22.5	FL36	500.32501	FL37	503.9
		Time	22.5	FL37	500.32501	FL38	503.9
		Time	22.5	FL38	500.32501	FL39	503.9
		Time	22.5	FL39	500.32501	FL40	503.9
		Time	22.5	FL40	500.32501	FL41	503.9
		Time	22.5	FL41	500.32501	FL42	503.9
		Time	22.5	FL42	500.32501	FL43	503.9
		Time	22.5	FL43	500.32501	FL44	503.9
		Time	22.5	FL44	500.32501	FL45	503.9
		Time	22.5	FL45	500.32501	FL46	503.9
		Time	22.5	FL46	500.32501	FL47	503.9
		Time	22.5	FL47	500.32501	FL48	503.9
		Time	22.5	FL48	500.32501	FL49	503.9
		Time	22.5	FL49	500.32501	FL50	5

Current Data File
 Name: 13C
 EXNO: 1
 PROCNO: 1
 F2 - Acquisition 2
 Date_ Time
 INSTRUM 5 mm
 PROBHD
 PULPROG
 TO
 SOLVENT
 NS
 DS
 SMH 33
 FIDRES 0
 AQ 0.
 RG
 DW
 DE
 TE
 AL1 7.0
 C11
 CPDPRG
 P31
 S4
 D11 0.
 S2
 F1
 SFO1 125.
 NUCLEUS
 F2 - Processing
 S2
 SF 125.
 WDM
 SSB
 LB
 GB
 PC
 1D NMR plot para
 CW
 F1P 2
 F2P
 F2
 PPMCM 1
 HZCM 149

76.745
 76.999
 77.252

113.415
 118.059

130.975
 132.461

-143.160
 -143.177
 -143.208
 -143.225
 -153.291
 -153.335
 -153.379
 -161.373
 -161.390
 -161.419
 -161.435
 -161.464
 -161.481

(3v)

Current Data Parameters
 NAME btc9302
 PROCNO 1
 PRGCHO 1
 F2 - Acquisition Parameters
 Date_ 2002124
 Time_ 14:00
 INSTRUM spect
 PROBRD 5 mm QNP 1H/1
 PULPROG zgpg30
 SOLVENT CDCl3
 NS 53
 DS 4
 SWH 10000.000 Hz
 FIDRES 0.651100 sec
 AQ 0.651100 sec
 RG 4096
 NG 5.000 usec
 DW 2.000 usec
 DE 300.0 V
 TE 1.00000000 sec
 D1 0.03000000 sec
 D11 0.03000000 sec
 D12 0.00000000 sec
 CHANNEL F1
 NUC1 19F
 P1 10.40 usec
 PL 0.00 dB
 SFO1 470.7901483 MHz
 CHANNEL F2
 NUC2 1H
 P2 10.00 usec
 PL2 0.00 dB
 SFO2 500.392016 MHz
 F2 - Processing parameters
 SI 65536
 SF 470.8372320 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00
 ID MRB plot parameters
 CX 20.00 cm
 F1 0.00 ppm
 F2 -200.000 ppm
 F2 -94167.45 Hz
 GAMMA 10.00000 ppm/cm
 HZCN 4708.37207 Hz/cm

[illegible]

146.214
139.831
135.269
132.266
129.995
127.803
127.512
118.802
110.732

77.252
76.999
76.744

Current Data Parameters
NAME: 3aa
EXPNO: 1
PROCNO: 1
F2 - Acquisition Parameters
Date_ Time: 20020111
INSTRUM: spect
PROBHD: 5 mm BBO
PULPROG: zgpg30
TD: 65536
SOLVENT: CDCl3
NS: 2048
DS: 4
SWH: 33333.33
FIDRES: 0.500000
AQ: 0.983333
RG: 1.00
DW: 15.00
DE: 1.00
TE: 300.2
RL1: 2.000000
CDPRG: zgpg30
SFO1: 125.838
NUC1: 13C
F2 - Processing parameters
SI: 32768
SF: 125.823
WDW: EM
SSB: 0
LB: 0.3
GB: 0
PC: 0

Current Data Parameters
NAME: Micro-1011
PROCNO: 1
F2 - Acquisition Parameters
Date_ Time: 01/05/2012 12:37
INSTRUM: spect
PROBHD: 5 mm QNP 1H/1
PULPROG: zgpg30
AQ: 2.213
RG: 327.1
SD/CMET: 5
RG: 5
FIDRES: 0.009415 Hz
AQRES: 0.143359 Hz
F2 - Processing parameters
Date_ Time: 01/05/2012 12:37
PRG: 1
F2: 500.1325001 MHz
WDW: EM
SSB: 0
LB: 0.30 Hz
GB: 0
PC: 1.00
F2 - 10 MHz plot parameters
Date_ Time: 01/05/2012 12:37
F2: 500.1325001 MHz
WDW: EM
SSB: 0
LB: 0.30 Hz
GB: 0
PC: 1.00
F2 - 10 MHz plot parameters
Date_ Time: 01/05/2012 12:37
F2: 500.1325001 MHz
WDW: EM
SSB: 0
LB: 0.30 Hz
GB: 0
PC: 1.00

Current Data Parameters
NAME: 3ad
EXPNO: 1
PROCNO: 1
F2 - Acquisition Parameters
Date_: 20020412
Time: 22.37
INSTRUM: spect
PROBHD: 5 mm QNP 1H/1
PULPROG: zgpg30
SOLVENT: CDCl3
NS: 12
DS: 2
SWH: 6002.615 Hz
FIDRES: 0.0933 Hz
AQ: 2.7182377 sec
RG: 48.3
DQ: 93.00 usec
DE: 5.00 usec
TE: 300.2 K
D1: 1.0000000 sec
===== CHANNEL f1 =====
NUC1: 13C
P1: 7.10 usec
PL1: 0.00 dB
F1: 500.3925017 MHz
===== CHANNEL f2 =====
F2 - Processing parameters
NUC2: 1H
P2: 19.00 usec
PL2: 0.00 dB
F2: 500.390486 MHz
SFO: 500
AQ: 9.30 Hz
RG: 1.00
DE: 1.00

Current Data Parameters
 Name: 3af
 ExpNO: 1
 F2 - Acquisition Parameters
 Date_: 20021122
 Time: 12.12
 Instrument: spect
 PROBHD: 5 mm QNP 1H/1
 PULPROG: zgpg30
 TO: 32748
 SOLVENT: CDCl₃
 DS: 1
 SC: 2
 FWHM: 0.001315 Hz
 FIDRES: 2.7243177 Hz
 AQ: 0.10000000 sec
 RG: 655.5
 PE: 0.00000000 sec
 DE: 16.00 usec
 TE: 300.2 K
 D1: 1.00000000 sec
 CHANNEL: f1
 NUC1: ¹H
 P1: 7.50 usec
 PL: 0.00 dB
 RFPO: 500.1325019 MHz
 F2 - Processing parameters
 SI: 32768
 SF: 500.1360988 MHz
 WDW: EM
 SSF: 0
 LB: 0.30 Hz
 GB: 0
 PC: 1.00

157.398
149.571
139.337
136.606
128.849
128.641
126.835
121.970
120.430

77.263
77.009
76.754

Current Data Parameters
NAME hbcollipz
PROCNO 1

F2 - Acquisition Parameters
Date_ 2001.12
Time 20.25
INSTRUM spect
PROBHD 5 mm QNP
PULPROG zgpg
TD 65536
SOLVENT CDCl3
NS 37
DS 4
SWH 3146.341 Hz
FIDRES 0.00232 Hz
AQ 1.0420724 sec
RG 8193.2
DW 15.000 usec
DE 6.000 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.00000000 sec
D12 0.00000000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 1.50 usec
PL1 3.00 dB
SFO1 125.8249556 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
P2 100.00 usec
PL2 0.00 dB
PL12 26.00 dB
PL13 26.00 dB
SFO2 500.3522016 MHz

F2 - Processing parameters
SI 32768
SF 125.8231819 MHz
WDW EM
SS 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 22.00 cm
F1 25.000 MHz
F2 25.000 MHz
F3 -15.000 MHz
F4 -1887.35 MHz
NUC1 13C
NUC2 1H
1433.80884 Hz

[illegible]

Current Data Parameters
 Name: 3ag
 ExpNO: 2
 PROCNO: 1
 F2 - Acquisition Parameters
 Date_: 20020412
 Time: 23.12
 INSTRUM: spect
 PULPROG: zgpg30
 TO: 6536
 SOLVENT: CDCl3
 NS: 45
 DS: 4
 SWH: 31465.51 Hz
 FIDRES: 0.1461916 Hz
 AQ: 1.0420724 sec
 RG: 13004
 DD: 13.900000 sec
 DE: 6.000000 sec
 TE: 300.0 K
 D1: 2.00000000 sec
 d11: 0.10000000 sec
 D12: 0.00000000 sec
 ===== CHANNEL f1 =====
 NUC1: 13C
 P1: 7.50 usec
 PL1: 3.00 dB
 SFO1: 125.8345358 MHz
 ===== CHANNEL f2 =====
 CPDPRG2: waltz16
 NUC2: 1H
 P2: 100.00 usec
 PL2: 0.00 dB
 PCPD2: 28.00 usec
 PL3: 28.00 dB
 PL15: 28.00 dB
 SFO2: 500.3620016 MHz
 F2 - Processing parameters
 SF: 125.8223601 MHz
 DSF: 3127468
 SWH: 31465.51 Hz
 FWH: 0.30 Hz
 LB: 0
 GB: 0
 PC: 1.00

9.189
8.921
7.567
7.554
7.550
7.542
7.540
7.538
7.534
7.502
7.500
7.496
7.486
7.483
7.473
7.471
7.449
7.447
7.444
7.437
7.433

Current Data Parameters
Date_ 20111111
Time_ 11:13
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 32768
AQ 3.15
RG 31
WDW EM
SSB 0
GB 0
PC 1.00
FIDRES 600.613 Hz
AQ 0.163333 Hz
RG 31
WDW EM
SSB 0
GB 0
PC 1.00
F2 - Acquisition Parameters
Date_ 20111111
Time_ 11:13
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 32768
AQ 3.15
RG 31
WDW EM
SSB 0
GB 0
PC 1.00
FIDRES 600.613 Hz
AQ 0.163333 Hz
RG 31
WDW EM
SSB 0
GB 0
PC 1.00
F2 - Processing parameters
SI 32768
SF 500.136000 MHz
WDW EM
SSB 0
GB 0
PC 1.00
F2 - 1H NMR parameters
Date_ 20111111
Time_ 11:13
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 32768
AQ 3.15
RG 31
WDW EM
SSB 0
GB 0
PC 1.00
FIDRES 600.613 Hz
AQ 0.163333 Hz
RG 31
WDW EM
SSB 0
GB 0
PC 1.00
F2 - Processing parameters
SI 32768
SF 500.136000 MHz
WDW EM
SSB 0
GB 0
PC 1.00
F2 - 1H NMR parameters
Date_ 20111111
Time_ 11:13
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 32768
AQ 3.15
RG 31
WDW EM
SSB 0
GB 0
PC 1.00
FIDRES 600.613 Hz
AQ 0.163333 Hz
RG 31
WDW EM
SSB 0
GB 0
PC 1.00

157.062
154.431
133.830
133.790
128.994
128.582
126.553

Current Data Parameters
NAME Maccomp49
PROCNO 1
P2 - Acquisition Parameters
Date_ 20030322
Time 11:35
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg30
PCPDPRG 4500
SOLVENT CDCl3
NS 47
DS 47
DE 31446.541 Hz
FIDRES 0.479836 Hz
AQ 1.0480724 sec
RG 655.36
WDW EM
SS 15.800 us
DE 6.00 us
TE 300.2 K
D1 2.0000000 sec
D11 0.03000000 sec
D12 0.00002000 sec
===== CHANNEL f1 =====
NUC1 13C
P1 7.50 us
PL1 0.00 dB
SFO1 125.8241516 MHz
===== CHANNEL f2 =====
NUC2 1H
P2 100.00 us
PL2 0.00 dB
SFO2 500.3320015 MHz
P2 - Processing parameters
SI 32768
SF 125.8225984 MHz
WDW EM
SS 0
LB 0.30 Hz
GB 0
PC 1.00

Current Data Parameters
 Name: 3aI
 P1: 1.0000000 sec
 P2: 1.0000000 sec
 P3: 1.0000000 sec
 P4: 1.0000000 sec
 P5: 1.0000000 sec
 P6: 1.0000000 sec
 P7: 1.0000000 sec
 P8: 1.0000000 sec
 P9: 1.0000000 sec
 P10: 1.0000000 sec
 P11: 1.0000000 sec
 P12: 1.0000000 sec
 P13: 1.0000000 sec
 P14: 1.0000000 sec
 P15: 1.0000000 sec
 P16: 1.0000000 sec
 P17: 1.0000000 sec
 P18: 1.0000000 sec
 P19: 1.0000000 sec
 P20: 1.0000000 sec
 P21: 1.0000000 sec
 P22: 1.0000000 sec
 P23: 1.0000000 sec
 P24: 1.0000000 sec
 P25: 1.0000000 sec
 P26: 1.0000000 sec
 P27: 1.0000000 sec
 P28: 1.0000000 sec
 P29: 1.0000000 sec
 P30: 1.0000000 sec
 P31: 1.0000000 sec
 P32: 1.0000000 sec
 P33: 1.0000000 sec
 P34: 1.0000000 sec
 P35: 1.0000000 sec
 P36: 1.0000000 sec
 P37: 1.0000000 sec
 P38: 1.0000000 sec
 P39: 1.0000000 sec
 P40: 1.0000000 sec
 P41: 1.0000000 sec
 P42: 1.0000000 sec
 P43: 1.0000000 sec
 P44: 1.0000000 sec
 P45: 1.0000000 sec
 P46: 1.0000000 sec
 P47: 1.0000000 sec
 P48: 1.0000000 sec
 P49: 1.0000000 sec
 P50: 1.0000000 sec
 P51: 1.0000000 sec
 P52: 1.0000000 sec
 P53: 1.0000000 sec
 P54: 1.0000000 sec
 P55: 1.0000000 sec
 P56: 1.0000000 sec
 P57: 1.0000000 sec
 P58: 1.0000000 sec
 P59: 1.0000000 sec
 P60: 1.0000000 sec
 P61: 1.0000000 sec
 P62: 1.0000000 sec
 P63: 1.0000000 sec
 P64: 1.0000000 sec
 P65: 1.0000000 sec
 P66: 1.0000000 sec
 P67: 1.0000000 sec
 P68: 1.0000000 sec
 P69: 1.0000000 sec
 P70: 1.0000000 sec
 P71: 1.0000000 sec
 P72: 1.0000000 sec
 P73: 1.0000000 sec
 P74: 1.0000000 sec
 P75: 1.0000000 sec
 P76: 1.0000000 sec
 P77: 1.0000000 sec
 P78: 1.0000000 sec
 P79: 1.0000000 sec
 P80: 1.0000000 sec
 P81: 1.0000000 sec
 P82: 1.0000000 sec
 P83: 1.0000000 sec
 P84: 1.0000000 sec
 P85: 1.0000000 sec
 P86: 1.0000000 sec
 P87: 1.0000000 sec
 P88: 1.0000000 sec
 P89: 1.0000000 sec
 P90: 1.0000000 sec
 P91: 1.0000000 sec
 P92: 1.0000000 sec
 P93: 1.0000000 sec
 P94: 1.0000000 sec
 P95: 1.0000000 sec
 P96: 1.0000000 sec
 P97: 1.0000000 sec
 P98: 1.0000000 sec
 P99: 1.0000000 sec
 P100: 1.0000000 sec

Current Data Parameters
 NAME: bbec03bpf
 EXPNO: 1
 PROCNO: 1
 F2 - Acquisition Parameters
 Date_ : 2008.01.11
 Time : 20.35
 INSTRUM : spect
 PULPROG : 5 mm QNP 1H/1
 TD : 65536
 TO : 0.00000000
 SOLVENT : CDCl3
 DS : 4
 SWH : 31646.561 Hz
 FZRES : 0.49926 Hz
 AQ : 1.0207724 sec
 RG : 3288.2
 DN : 15.900 us
 DE : 6.000 us
 TE : 300.0 K
 D1 : 2.00000000 sec
 D11 : 0.03000000 sec
 D12 : 0.00000000 sec
 ===== CHANNEL f1 =====
 NUC1 : 13C
 P1 : 1.50 us
 PL1 : 3.00 dB
 SFO1 : 125.8369556 MHz
 ===== CHANNEL f2 =====
 CPDPRG2 : waltz16
 NUC2 : 1H
 P2 : 100.00 us
 PL2 : 0.00 dB
 PL12 : 26.00 dB
 PL13 : 19.00 dB
 SFO2 : 500.3260016 MHz
 F2 - Processing parameters
 SI : 32768
 SF : 125.8369556 MHz
 WDW : EM
 SSB : 0
 GB : 0
 PC : 1.40
 LO MHz plot parameters
 CK : 22.00 cm
 F1P : 225.000 MHz
 F2P : 500.3260016 MHz
 F3P : -15.000 MHz
 F2 : -1887.35 Hz
 F1 : 125.8369556 MHz
 FREQ : 1433.80884 MHz

163.640
 158.718
 142.797
 129.251
 129.223
 128.827
 125.004
 122.200
 107.183
 77.257
 77.002
 76.748

230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

8.140
7.598
7.588
7.580
7.532
7.517
7.421
7.406
7.391
7.327
7.312
7.297
7.156
7.147
6.965
6.535
6.530
6.526

Current Data Parameters
NAME 3ak
PROCNO 1
F2 - Acquisition Parameters
Date_ 20021115
Time 11:15
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg30
TD 32768
SOLVENT cdcl3
NS 2
DS 2
AQ 6000.412 Hz
FIDRES 0.113159 Hz
AQ 2.790473 sec
RG 32.380 msec
DE 1.5000000
TE 300.2 K
SI 320.0 M
O1 1.00000000 sec
===== CHANNEL f1 =====
NUC1 1H
P1 7.10 sec
PL1 0.00 dB
SFO1 500.135519 MHz
F2 - Processing parameters
SI 32768
SF 500.135519 MHz
WDW EM
SSB 0
GB 0.0 Hz
CB 0
PC 1.00
LD MM plot parameters
CH 1
FID 15.000 cm
P1 1.00000000 sec
F1 500.135519 MHz
F2 500.135519 MHz
F3 500.135519 MHz
PPHM 0.35000 ppm/c
FREQH 275.31411 MHz/c

Current Data Parameters
NAME hbcoup-3f
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20080525
Time 21.23
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
D1 1.00
D2 4.00
D3 0.00
SFR 31446.341 Hz
FIDRES 0.478834 Hz
AQ 0.02000000 sec
RG 4096
DM 15.900 us
DE 2.000 us
TE 300.2 K
B1 2.00000000 sec
D11 0.03000000 sec
D12 0.00000000 sec
===== CHANNEL f1 =====
NUC1 13C
P1 7.00 us
PL1 3.00 dB
SFO1 125.8369556 MHz
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
P2 100.00 us
PL2 0.00 dB
PL3 26.00 dB
PL13 26.00 dB
SFO2 500.3380019 MHz
F2 - Processing parameters
SI 32768
SF 125.832074 MHz
WDW EM
SSB 0
GB 0
PC 1.00

Current Data Parameters
 EXPNO 1
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 20021111
 Time 22:10
 INSTRUM spect
 PULPROG zgpg30
 TD 32768
 SFO 500.1362619 MHz
 FIDRES 0.1000000 sec
 AQ 0.1000000 sec
 RG 327.68
 DQ 0.1000000 sec
 DE 0.1000000 sec
 TE 300.2 K
 DI 1.0000000 sec
 ===== CHANNEL f1 =====
 NUC1 13C
 P1 1.00 usec
 PL1 0.00 dB
 SFO1 500.1362619 MHz
 F2 - Processing parameters
 SI 32768
 SF 500.1362619 MHz
 WDW EM
 SS 0.30 Hz
 LB 0.30 Hz
 GB 0
 PC 1.00
 1D NMR plot parameters
 SI 32768
 SF 500.1362619 MHz
 FIDRES 0.1000000 sec
 AQ 0.1000000 sec
 RG 327.68
 DQ 0.1000000 sec
 DE 0.1000000 sec
 TE 300.2 K
 DI 1.0000000 sec
 ===== CHANNEL f1 =====
 NUC1 13C
 P1 1.00 usec
 PL1 0.00 dB
 SFO1 500.1362619 MHz
 F2 - Processing parameters
 SI 32768
 SF 500.1362619 MHz
 WDW EM
 SS 0.30 Hz
 LB 0.30 Hz
 GB 0
 PC 1.00
 1D NMR plot parameters
 SI 32768
 SF 500.1362619 MHz
 FIDRES 0.1000000 sec
 AQ 0.1000000 sec
 RG 327.68
 DQ 0.1000000 sec
 DE 0.1000000 sec
 TE 300.2 K
 DI 1.0000000 sec

0.875

(3a1)

Year	Average number of children
1960	1.45
1975	1.35
1980	1.30
1985	1.28
1990	1.27
1995	1.26
2000	1.255
2005	1.252
2010	1.25

Current Data Parameters		Acquisition Parameters		Processing Parameters		10 MHz plot parameters	
NAME	VALUE	NAME	VALUE	NAME	VALUE	NAME	VALUE
EXPNO	2	DATE_	20030128	PROCNO	10	DATA	22.00 CM
PROCNO	1	TIME	10.00	PROCPS	235.000 PS	RG	2.00
NAME	NOIC010EXP	INSTRUM	SPECT	CHOP	1	WIDTH	21.500 PS
		PROBHD	5 mm QNP 1H/1	DELTA	0.00	PD	2.1500 PD
		PULPROG	zgpg30	DE	26.00 DE	PC	1.00
		PCPGM2	zgpg30	TE	300.2 K	W2H	10.000 PS
		TO SOLVENT	CDCl3	RG2	500.392000 CM	W2H2	10.000 PS
		DS	37			W2H3	10.000 PS
		SWH	31445.541 Hz			W2H4	10.000 PS
		FIDRES	0.79391 Hz			W2H5	10.000 PS
		DELTA	1.401000 s			W2H6	10.000 PS
		NUC1	13C			W2H7	10.000 PS
		NUC2	1H			W2H8	10.000 PS
		NUC3	13C			W2H9	10.000 PS
		RF1	125.819554 MM			W2H10	10.000 PS
		RF2	500.136000 MM			W2H11	10.000 PS
		RF3	125.819554 MM			W2H12	10.000 PS
		RF4	500.136000 MM			W2H13	10.000 PS
		RF5	125.819554 MM			W2H14	10.000 PS
		RF6	500.136000 MM			W2H15	10.000 PS
		RF7	125.819554 MM			W2H16	10.000 PS
		RF8	500.136000 MM			W2H17	10.000 PS
		RF9	125.819554 MM			W2H18	10.000 PS
		RF10	500.136000 MM			W2H19	10.000 PS
		RF11	125.819554 MM			W2H20	10.000 PS
		RF12	500.136000 MM			W2H21	10.000 PS
		RF13	125.819554 MM			W2H22	10.000 PS
		RF14	500.136000 MM			W2H23	10.000 PS
		RF15	125.819554 MM			W2H24	10.000 PS
		RF16	500.136000 MM			W2H25	10.000 PS
		RF17	125.819554 MM			W2H26	10.000 PS
		RF18	500.136000 MM			W2H27	10.000 PS
		RF19	125.819554 MM			W2H28	10.000 PS
		RF20	500.136000 MM			W2H29	10.000 PS
		RF21	125.819554 MM			W2H30	10.000 PS
		RF22	500.136000 MM			W2H31	10.000 PS
		RF23	125.819554 MM			W2H32	10.000 PS
		RF24	500.136000 MM			W2H33	10.000 PS
		RF25	125.819554 MM			W2H34	10.000 PS
		RF26	500.136000 MM			W2H35	10.000 PS
		RF27	125.819554 MM			W2H36	10.000 PS
		RF28	500.136000 MM			W2H37	10.000 PS
		RF29	125.819554 MM			W2H38	10.000 PS
		RF30	500.136000 MM			W2H39	10.000 PS
		RF31	125.819554 MM			W2H40	10.000 PS
		RF32	500.136000 MM			W2H41	10.000 PS
		RF33	125.819554 MM			W2H42	10.000 PS
		RF34	500.136000 MM			W2H43	10.000 PS
		RF35	125.819554 MM			W2H44	10.000 PS
		RF36	500.136000 MM			W2H45	10.000 PS
		RF37	125.819554 MM			W2H46	10.000 PS
		RF38	500.136000 MM			W2H47	10.000 PS

7.256
7.258
7.265
7.268
7.329
7.331
7.335
7.337
7.374
7.380
7.384
7.390
7.406
7.409
7.422
7.425
7.429
7.434
7.442
7.446
7.791
7.838
7.851
7.854
8.008
8.025

Current Data Parameters
NAME: 3am
EXPNO: 1
PROCNO: 1
F2 - Acquisition Parameters
Date_ : 20010101
Time : 22.44
INSTRUM : spect
PROBHD : 5 mm QNP 1H/1
PULPROG : zgpg30
D1 : 1.00000000
SOLVENT : CDCl3
NS : 16
DS : 4
SWH : 4005.415 Hz
FIDRES : 0.103399 Hz
AQ : 2.7246111 sec
RG : 40.13 sec
DE : 0.1300 usec
TE : 300.2 K
D1 : 1.00000000 sec
===== CHANNEL f1 =====
NUC1 : 1H
P1 : 1.00 usec
PL1 : 0.00 dB
SFO1 : 500.1362519 MHz
F2 - Processing parameters
SI : 32768
SF : 500.1362519 MHz
WDW : EM
SSB : 0.00 Hz
LB : 0.00 Hz
GB : 0.00 Hz
PC : 1.00
F2 - sub plot parameters
SI : 32768
SF : 500.1362519 MHz
WDW : EM
SSB : 0.00 Hz
LB : 0.00 Hz
GB : 0.00 Hz
PC : 1.00
F2 - sub plot parameters
SI : 32768
SF : 500.1362519 MHz
WDW : EM
SSB : 0.00 Hz
LB : 0.00 Hz
GB : 0.00 Hz
PC : 1.00

(3am)

(3am)

141.081
134.887
133.761
131.762
129.556
128.265
127.713
126.901
126.094
125.812
125.790
125.342
125.231
123.421

77.255
77.000
76.747

Current Data Parameters
NAME: 3am
PROCNO: 1
PROCNO: 1
F2 - Acquisition Parameters
Date_: 20021111
Time: 22.20
INSTRUM: spect
PROBHD: 5 mm QNP 1H/1
PULPROG: zgpg30
TD: 65536
SOLVENT: CDCl3
NS: 400
DS: 4
SWH: 31646.341 Hz
FIDRES: 0.479934 Hz
AQ: 1.049171 sec
RG: 512.16
DM: 15.900 us
DE: 2.00 us
TE: 300.2 K
D1: 0.00000000 sec
D11: 0.03000000 sec
D12: 0.00001000 sec
----- CHANNEL f1 -----
NUC1: 13C
P1: 12.00 us
PL1: 0.00 dB
SFO1: 125.0165556 MHz
----- CHANNEL f2 -----
CPDPRG2: waltz16
NUC2: 1H
P2: 100.00 us
PL2: 0.00 dB
PL12: 26.00 dB
PL13: 26.00 dB
SFO2: 500.1320016 MHz
F2 - Processing parameters
SI: 32768
SF: 125.031815 MHz
WDW: EM
SSB: 0
LB: 1.00 Hz
GB: 0
PC: 1.40
IDWDW Plot Parameters
CX: 22.00 us
FIP: 235.000 PF
F1P: 250.000 MHz
F2P: -100.000 MHz
F2: -100.000 MHz
FPHCH: 11.26366 PF
RGCH: 1.025.00056 Hz

Current Data Parameters
 Date_ 2005.11.11
 Time_ 11.11
 InstName_ spect
 Sample_ 3an
 PULPROG_ zgpg30
 TD_ 32768
 SOLVENT_ CDCl3
 NS_ 1024
 DS_ 4
 FIDRES_ 0.243170 Hz
 AQ_ 2.031660 sec
 RG_ 327.68
 DW_ 42.000 nsec
 DE_ 65.57 usec
 TE_ 300.2 K
 HL1_ 1.00
 B1_ 1.0000000 sec
 B2_ 1.0000000 sec
 B3_ 1.0000000 sec
 SFO1_ 500.1362318 MHz
 NUCLEUS_ 1H
 P2 - Processing parameters
 SI_ 32768
 SF_ 500.1362318 MHz
 EQ_ 1.00
 AS_ 1.50 Hz
 CA_ 0
 PC_ 1.00
 10 mm plot parameters
 SI_ 32768
 SF_ 500.1362318 MHz
 EQ_ 1.00
 AS_ 1.50 Hz
 CA_ 0
 PC_ 1.00
 PPM2H_ 0.47157 ppm/c
 NUCN_ 210.62245 Hz/c

Current Data Parameters
NAME bblec031
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 200301
Time 17
INSTRUM 5 mm Dual
PROBHD 5 mm Dual
PULPROG zgpg30
SOLVENT CDCl3
NS 655
DS 33333.3
SWH 0.5086
FIDRES 0.98309
AQ 163
RG 15.0
DE 1.0
TE 300
H1 2.000000
D1 125.83821
CPDPRG waltz
P31 107.
S4 0.03000
D11 5.
S2 1
STO1 125.83821
NUCLEUS 1
F2 - Processing parameters
SI 327
SF 125.82317
WDW 1.
SSB 1.
LB 1.
GB 1.
PC 1.
1D NMR plot parameters
CX 21.
CY 235.0
F1 29568.
F2 -15.0
F2 -1887.
PPMCK 11.904
HZCK 1497.894

Current Data Parameters
 Name: 380
 Date: 20081122
 Time: 14:00
 Instrument: spect
 P1: 5.00 sec
 P2: 0.10 sec
 P3: 0.10 sec
 P4: 0.10 sec
 P5: 0.10 sec
 P6: 0.10 sec
 P7: 0.10 sec
 P8: 0.10 sec
 P9: 0.10 sec
 P10: 0.10 sec
 P11: 0.10 sec
 P12: 0.10 sec
 P13: 0.10 sec
 P14: 0.10 sec
 P15: 0.10 sec
 P16: 0.10 sec
 P17: 0.10 sec
 P18: 0.10 sec
 P19: 0.10 sec
 P20: 0.10 sec
 P21: 0.10 sec
 P22: 0.10 sec
 P23: 0.10 sec
 P24: 0.10 sec
 P25: 0.10 sec
 P26: 0.10 sec
 P27: 0.10 sec
 P28: 0.10 sec
 P29: 0.10 sec
 P30: 0.10 sec
 P31: 0.10 sec
 P32: 0.10 sec
 P33: 0.10 sec
 P34: 0.10 sec
 P35: 0.10 sec
 P36: 0.10 sec
 P37: 0.10 sec
 P38: 0.10 sec
 P39: 0.10 sec
 P40: 0.10 sec
 P41: 0.10 sec
 P42: 0.10 sec
 P43: 0.10 sec
 P44: 0.10 sec
 P45: 0.10 sec
 P46: 0.10 sec
 P47: 0.10 sec
 P48: 0.10 sec
 P49: 0.10 sec
 P50: 0.10 sec
 P51: 0.10 sec
 P52: 0.10 sec
 P53: 0.10 sec
 P54: 0.10 sec
 P55: 0.10 sec
 P56: 0.10 sec
 P57: 0.10 sec
 P58: 0.10 sec
 P59: 0.10 sec
 P60: 0.10 sec
 P61: 0.10 sec
 P62: 0.10 sec
 P63: 0.10 sec
 P64: 0.10 sec
 P65: 0.10 sec
 P66: 0.10 sec
 P67: 0.10 sec
 P68: 0.10 sec
 P69: 0.10 sec
 P70: 0.10 sec
 P71: 0.10 sec
 P72: 0.10 sec
 P73: 0.10 sec
 P74: 0.10 sec
 P75: 0.10 sec
 P76: 0.10 sec
 P77: 0.10 sec
 P78: 0.10 sec
 P79: 0.10 sec
 P80: 0.10 sec
 P81: 0.10 sec
 P82: 0.10 sec
 P83: 0.10 sec
 P84: 0.10 sec
 P85: 0.10 sec
 P86: 0.10 sec
 P87: 0.10 sec
 P88: 0.10 sec
 P89: 0.10 sec
 P90: 0.10 sec
 P91: 0.10 sec
 P92: 0.10 sec
 P93: 0.10 sec
 P94: 0.10 sec
 P95: 0.10 sec
 P96: 0.10 sec
 P97: 0.10 sec
 P98: 0.10 sec
 P99: 0.10 sec
 P100: 0.10 sec

Current Data Parameters
 NAME: Meca035f
 EXPNO: 2
 PROCNO: 1
 F2 - Acquisition Parameters
 Date_: 20021122
 Time: 20:42
 INSTRUM: spect
 PROBHD: 5 mm QNP 1H/1
 PULPROG: zgpg30
 CPDPRG2: zgpg30
 SOLVENT: CDCl3
 NS: 36
 DS: 4
 SWH: 31446.346 Hz
 FIDRES: 0.475836 Hz
 AQ: 1.0420724 sec
 RG: 13004
 DE: 1.00000000
 TE: 300.0 K
 D1: 0.00000000 sec
 d11: 0.00000000 sec
 d12: 0.00000000 sec
 d13: 0.00000000 sec
 ===== CHANNEL f1 =====
 NUC1: 13C
 P1: 1.00
 PL1: 7.50 dB
 SFO1: 125.8345534 MHz
 ===== CHANNEL f2 =====
 CPDPRG2: zgpg30
 NUC2: 1H
 P2: 100.00
 PL2: 0.00 dB
 PL12: 19.00 dB
 PL13: 19.00 dB
 SFO2: 500.3320016 MHz
 F2 - Processing parameters
 SI: 32768
 SF: 125.831803 MHz
 WDW: EM
 SS: 0
 LB: 1.00 Hz
 GB: 0
 PC: 1.40
 LO MHz plot parameters
 CE: 22.00 dB
 F1: 255.000000 MHz
 F2: 255.000000 MHz
 F3: 255.000000 MHz
 F4: 255.000000 MHz
 F5: 255.000000 MHz
 F6: 255.000000 MHz
 F7: 255.000000 MHz
 F8: 255.000000 MHz
 F9: 255.000000 MHz
 F10: 255.000000 MHz
 F11: 255.000000 MHz
 F12: 255.000000 MHz
 F13: 255.000000 MHz
 F14: 255.000000 MHz
 F15: 255.000000 MHz
 F16: 255.000000 MHz
 F17: 255.000000 MHz
 F18: 255.000000 MHz
 F19: 255.000000 MHz
 F20: 255.000000 MHz
 F21: 255.000000 MHz
 F22: 255.000000 MHz
 F23: 255.000000 MHz
 F24: 255.000000 MHz
 F25: 255.000000 MHz
 F26: 255.000000 MHz
 F27: 255.000000 MHz
 F28: 255.000000 MHz
 F29: 255.000000 MHz
 F30: 255.000000 MHz
 F31: 255.000000 MHz
 F32: 255.000000 MHz
 F33: 255.000000 MHz
 F34: 255.000000 MHz
 F35: 255.000000 MHz
 F36: 255.000000 MHz
 F37: 255.000000 MHz
 F38: 255.000000 MHz
 F39: 255.000000 MHz
 F40: 255.000000 MHz
 F41: 255.000000 MHz
 F42: 255.000000 MHz
 F43: 255.000000 MHz
 F44: 255.000000 MHz
 F45: 255.000000 MHz
 F46: 255.000000 MHz
 F47: 255.000000 MHz
 F48: 255.000000 MHz
 F49: 255.000000 MHz
 F50: 255.000000 MHz
 F51: 255.000000 MHz
 F52: 255.000000 MHz
 F53: 255.000000 MHz
 F54: 255.000000 MHz
 F55: 255.000000 MHz
 F56: 255.000000 MHz
 F57: 255.000000 MHz
 F58: 255.000000 MHz
 F59: 255.000000 MHz
 F60: 255.000000 MHz
 F61: 255.000000 MHz
 F62: 255.000000 MHz
 F63: 255.000000 MHz
 F64: 255.000000 MHz
 F65: 255.000000 MHz
 F66: 255.000000 MHz
 F67: 255.000000 MHz
 F68: 255.000000 MHz
 F69: 255.000000 MHz
 F70: 255.000000 MHz
 F71: 255.000000 MHz
 F72: 255.000000 MHz
 F73: 255.000000 MHz
 F74: 255.000000 MHz
 F75: 255.000000 MHz
 F76: 255.000000 MHz
 F77: 255.000000 MHz
 F78: 255.000000 MHz
 F79: 255.000000 MHz
 F80: 255.000000 MHz
 F81: 255.000000 MHz
 F82: 255.000000 MHz
 F83: 255.000000 MHz
 F84: 255.000000 MHz
 F85: 255.000000 MHz
 F86: 255.000000 MHz
 F87: 255.000000 MHz
 F88: 255.000000 MHz
 F89: 255.000000 MHz
 F90: 255.000000 MHz
 F91: 255.000000 MHz
 F92: 255.000000 MHz
 F93: 255.000000 MHz
 F94: 255.000000 MHz
 F95: 255.000000 MHz
 F96: 255.000000 MHz
 F97: 255.000000 MHz
 F98: 255.000000 MHz
 F99: 255.000000 MHz
 F100: 255.000000 MHz

(3a0)

76.747
 77.001
 77.254

119.581
 124.950
 125.791
 126.288
 127.232
 128.267
 128.541
 130.300
 130.596
 130.784
 133.984
 143.449

167.584

Current Data Parameters		Acquisition Parameters		Processing Parameters		10 MHz plot parameters	
NAME	VALUE	NAME	VALUE	NAME	VALUE	NAME	VALUE
IMAGE	1	TIME	30.00	CH1	1	CH	20.00
PROG	1	TIME	21.18	F1	160.325181 MeV	F1	160.325181 MeV
INSTR	1	TIME	21.18	F2	377.68	F2	377.68
ACQ	1	TIME	21.18	F3	500.3960248 MeV	F3	500.3960248 MeV
NAME	1	TIME	21.18	F4	0.00	F4	0.00
NAME	1	TIME	21.18	F5	0.00	F5	0.00
NAME	1	TIME	21.18	F6	0.00	F6	0.00
NAME	1	TIME	21.18	F7	0.00	F7	0.00
NAME	1	TIME	21.18	F8	0.00	F8	0.00
NAME	1	TIME	21.18	F9	0.00	F9	0.00
NAME	1	TIME	21.18	F10	0.00	F10	0.00
NAME	1	TIME	21.18	F11	0.00	F11	0.00
NAME	1	TIME	21.18	F12	0.00	F12	0.00
NAME	1	TIME	21.18	F13	0.00	F13	0.00
NAME	1	TIME	21.18	F14	0.00	F14	0.00
NAME	1	TIME	21.18	F15	0.00	F15	0.00
NAME	1	TIME	21.18	F16	0.00	F16	0.00
NAME	1	TIME	21.18	F17	0.00	F17	0.00
NAME	1	TIME	21.18	F18	0.00	F18	0.00
NAME	1	TIME	21.18	F19	0.00	F19	0.00
NAME	1	TIME	21.18	F20	0.00	F20	0.00
NAME	1	TIME	21.18	F21	0.00	F21	0.00
NAME	1	TIME	21.18	F22	0.00	F22	0.00
NAME	1	TIME	21.18	F23	0.00	F23	0.00
NAME	1	TIME	21.18	F24	0.00	F24	0.00
NAME	1	TIME	21.18	F25	0.00	F25	0.00
NAME	1	TIME	21.18	F26	0.00	F26	0.00
NAME	1	TIME	21.18	F27	0.00	F27	0.00
NAME	1	TIME	21.18	F28	0.00	F28	0.00
NAME	1	TIME	21.18	F29	0.00	F29	0.00
NAME	1	TIME	21.18	F30	0.00	F30	0.00
NAME	1	TIME	21.18	F31	0.00	F31	0.00
NAME	1	TIME	21.18	F32	0.00	F32	0.00
NAME	1	TIME	21.18	F33	0.00	F33	0.00
NAME	1	TIME	21.18	F34	0.00	F34	0.00
NAME	1	TIME	21.18	F35	0.00	F35	0.00
NAME	1	TIME	21.18	F36	0.00	F36	0.00
NAME	1	TIME	21.18	F37	0.00	F37	0.00
NAME	1	TIME	21.18	F38	0.00	F38	0.00
NAME	1	TIME	21.18	F39	0.00	F39	0.00
NAME	1	TIME	21.18	F40	0.00	F40	0.00
NAME	1	TIME	21.18	F41	0.00	F41	0.00
NAME	1	TIME	21.18	F42	0.00	F42	0.00
NAME	1	TIME	21.18	F43	0.00	F43	0.00
NAME	1	TIME	21.18	F44	0.00	F44	0.00
NAME	1	TIME	21.18	F45	0.00	F45	0.00
NAME	1	TIME	21.18	F46	0.00	F46	0.00
NAME	1	TIME	21.18	F47	0.00	F47	0.00
NAME	1	TIME	21.18	F48	0.00	F48	0.00
NAME	1	TIME	21.18	F49	0.00	F49	0.00
NAME	1	TIME	21.18	F50	0.00	F50	0.00
NAME	1	TIME	21.18	F51	0.00	F51	0.00
NAME	1	TIME	21.18	F52

230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

(3ap)

77.252
76.999
76.744

154.901
145.791
143.936
142.768
134.638
133.877
130.929
129.810
128.453
128.012
126.874
126.118
125.168
124.866

Current Data Parameters
NAME: 3ap
EXPNO: 1
PROCNO: 1
F2 - Acquisition Parameters
Date_ : 20021111
Time : 20:23:11
INSTRUM : spect
PROBHD : 5 mm QNP
PULPROG : zgpg30
TD : 65536
SOLVENT : CDCl3
NS : 4
DS : 4
SWH : 31446.341 Hz
FIDRES : 0.479816 Hz
AQ : 1.10000000 sec
RG : 3298.2
DE : 15.800 us
TE : 300.2 K
D1 : 1.00000000 sec
D11 : 0.53000000 sec
D12 : 0.00020000 sec
===== CHANNEL f1 =====
NUC1 : 13C
P1 : 13.00 us
PL1 : 3.00 dB
SFO1 : 125.834556 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 : 500.3920016 MHz
WDW : 125.834556 MHz
SSB : 0
LB : 1.00 Hz
GB : 0
PC : 1.40
F2 - 1D NMR plot parameters
SI : 32768
SF : 500.3920016 MHz
WDW : 125.834556 MHz
SSB : 0
LB : 1.00 Hz
GB : 0
PC : 1.40
F1P : 235.000 MHz
F1 : 235.000 MHz
F2P : 500.3920016 MHz
F2 : 500.3920016 MHz
PPMCH : 11.36364 PPM
NUCCH : 1039.80864 Hz

(3aq)

Current Data Parameters
 NAME: 3aq
 PROCNO: 1
 P2 - Acquisition Parameters
 Date_: 20080515
 Time: 14.15
 INSTRUM: spect
 PULPROG: zgpg30
 FIDRES: 0.090
 AQ: 1.00000000 sec
 SFO: 500.1360610 MHz
 P2 - Processing parameters
 F1: 12164
 SFO: 500.1360610 MHz
 P2: 0.10 sec
 SFO: 0.10 Hz
 SFO: 1.00

Current Data Parameters
NAME: 14230004
EXPNO: 1
PROCNO: 1
F2 - Acquisition Parameters
Date_ : 20080624
Time : 14.00
INSTRUM : spect
PROBHD : 5 mm QNP 1H/1
PULPROG : zgpg30
TD : 65536
SOLVENT : CDCl3
NS : 61
DS : 4
SWH : 31946.544
FIDRES : 0.479814
AQ : 1.0420724
RG : 327.5
DM : 149.912
DE : 4.00
TE : 300.2
D1 : 2.00000000
D11 : 0.03000000
D12 : 0.00020000
===== CHANNEL f1 =====
NUC1 : 13C
P1 : 7.50
PL1 : 3.00
SFO1 : 125.8349554
===== CHANNEL f2 =====
CHUPROG : waltz16
NUC2 : 1H
PCPD2 : 100.00
PL2 : 0.00
PL12 : 24.00
PL13 : 24.00
SFO2 : 500.13620012
F2 - Processing parameters
SI : 32768
SF : 125.8231761
WDW : EM
SSB : 0
GB : 0
PC : 1.40
ID: non plot parameters
CK : 22.00
FIP : 235.000
F1P : 251.4845
F2P : -1087.19
PPHMCN : 11.36344
HCCN : 1425.80884

[illegible]

148.307
 148.102
 147.580
 138.679
 133.302
 131.381
 126.813
 125.746
 123.433
 121.274

77.251
 76.998
 76.742

Current Data Parameters
 NAME hmc00391f
 EXPNO 2
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 20021123
 Time_ 08:11
 INSTRUM spect
 PROBHD 5 mm QNP 1H/1
 PULPROG zgpg
 SOLVENT cdcl3
 NS 49
 DS 4
 SWH 31446.341 Hz
 FIDRES 0.478834 Hz
 AQ 1.0420724 sec
 RG 327.500
 DW 15.800 usec
 DE 6.00 usec
 TE 300.2 K
 D1 4.00000000 sec
 D11 0.03000000 sec
 D12 0.00000000 sec
 D13 0.00000000 sec
 ===== CHANNEL f1 =====
 NUC1 13C
 P1 7.50 usec
 PL 0.00 dB
 SFO1 125.836554 MHz
 ===== CHANNEL f2 =====
 NUC2 1H
 P2 100.00 usec
 PL2 0.00 dB
 PL12 24.00 dB
 PL13 24.00 dB
 SFO2 500.3320016 MHz
 F2 - Processing parameters
 SI 32768
 SF 125.8231868 MHz
 DSF 31.2500000 MHz
 SSB 0
 LA 1.00 Hz
 GB 0
 PC 1.40
 LO MHz plot parameters
 CR 22.00 usec
 F1 2346.43 Hz
 F2 -15.000 usec
 F2 187.15 Hz
 FREQH 111.34344 Hz
 FREQV 1423.80884 Hz

7.601
7.598
7.500
7.495
7.491
7.485
7.396
7.386

9.132
8.943

1.255

Current Data Parameters
NAME: 3as
EXPNO: 1
PROCNO: 1
F2 - Acquisition Parameters
Date_: 20020311
Time: 15.31
PROBHD: 5 mm QNP 1H/1
PULPROG: zgpg30
AQPROG: zgpg30
SOLVENT: CDCl3
NS: 17
DS: 4
SWH: 6000.615 Hz
F2: 200.130 MHz
AQ: 2.7201171 sec
RG: 327.500
GB: 16.000
WB: 1.000 MHz
TE: 300.2 K
D1: 1.00000000 sec
===== CHANNEL f1 =====
NUC1: 13C
P1: 1.50 usec
PL1: 0.00 dB
SFO1: 100.628155 MHz
F2 - Processing parameters
SI: 32768
SF: 100.628155 MHz
WDW: EM
SSB: 0
LB: 1.00 Hz
GB: 0
PC: 1.40

77.263
77.008
76.754

156.917
153.883
134.845
129.230
127.554
125.129
122.336

Current Data Parameters
NAME Metc013-ef
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20020531
Time 11:11:11
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg30
SOLVENT CDCl3
NS 15
DS 4
SWH 31646.541 Hz
FIDRES 0.478816 Hz
AQ 1.0420724 sec
RG 327.500
DE 15.900 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 125.836954 MHz
===== CHANNEL f2 =====
NUC2 1H
P2 100.00 us
PL2 0.00 dB
PL3 0.00 dB
PL4 26.00 dB
PL5 26.00 dB
SFO2 500.3920015 MHz
F2 - Processing parameters
SI 32768
SF 125.8331970 MHz
WDW EM
SSB 0
LA 1.00 Hz
GB 0
PC 1.40

[illegible]

Current Data Parameters
NAME b0tc008pp
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters

Date_ 20030131

Time 16.37

INSTRUM amx500

PROBHD 5 mm Dual 13

PULPROG zgpg

TD 65536

SOLVENT CDCl3

NS 55

DS 2

SWH 33333.332

FIDRES 0.50826

AD 0.9830900

RG 16384

DM 15.000

DE 18.75

TE 300.0

HL1 40

D1 2.00000000

CPDPRG waltz16

P31 107.00

S4 24

D11 0.0300000

S2 18

P1 5.00

SF01 125.8382148

NUCLEUS 13C

F2 - Processing parameters

S1 32768

SF 125.8231767

WDW EM

SSB 0

L8 1.50

G8 0

PC 1.40

10 NMR plot parameters

CX 21.00

F1P 235.000

F1 29568.45

F2P -15.000

F2 -1887.35

PPMCH 11.90476

HZCN 1497.89490

(3au)

7.650
7.430
7.426
7.423
7.361
7.358
7.355
7.353
7.333
7.327
7.321
7.318
7.261
7.259
7.255
7.253
7.204
7.201
7.194
7.191
6.614
6.612
6.611

3w

===== CHANNEL f1 =====
Date_ 11-11-11
Time_ 11:18
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 16
DS 4
SWH 600.613 MHz
FIDRES 0.181559 Hz
AQ 2.1218333 sec
RG 327.68
DE 3.00
TE 300.2 K
D1 1.00000000 sec
===== CHANNEL f2 =====
NUC1 13C
P1 1.20 sec
PL 0.00 dB
SFO1 500.132519 MHz
===== CHANNEL f3 =====
P2 - Processing parameters
F1 327.68 MHz
SFO2 500.132519 MHz
WDW EM
SSB 0
GB 0
PC 1.00

— 0.077

230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

143.387 { 3av
138.360
137.216
133.271 { 3av
126.325 3av
126.121
126.029
125.936 { 3av
121.763
119.742
119.376 { 3av
109.209

77.254
77.000
76.748

50.145

Current Data Parameters
NAME 1
PROCNO 2
Date_ 20020603
Time_ 11:40
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 45
DS 4
DE 3144.514 Hz
FIDRES 0.475814 Hz
AQ 1.0428734 sec
RG 118.72
RM 15.50 us
OR 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 2.00 dB
SFO1 125.0130516 MHz
===== CHANNEL f2 ==
NUC2 1H
P2 100.00 us
PL2 0.00 dB
SFO2 500.1320016 MHz
P2 - Processing parameters
SI 32768
SF 125.0231846 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

0.01316

Current Data Parameters
NAME 160301132
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 16031132
Time 22.33
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 2
AQ 6009.615 Hz
RG 327.68
AQ 2.7268157 sec
RG 356
DS 81.200 usec
DE 6.80 usec
TE 300.2 K
D1 1.00000000 sec

***** CHANNEL f1 ****
NUC1 1H
P1 7.50 usec
PL1 0.00 dB
SFO1 500.1325019 MHz

F2 - Processing parameters
SI 32768
SF 500.13500115 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 22.00 cm
F1 10.000 ppm
F2 5003.90 Hz
F3 -6.500 ppm
F4 -256.15 Hz
F5 0.47727 ppm/c
F6 238.82248 Hz/c

7.846
7.844
7.840
7.838
7.798
7.791
7.573
7.571
7.563
7.561
7.381
7.375
7.370
7.364
7.251
7.244

Current Data Parameters
 Name: 3ay
 Date: 10/12/10
 Time: 10:10
 File: 3ay
 Path: C:\Program Files\Agilent\ChemStation\1D\1D\3ay
 Solvent: CDCl3
 NS: 1
 DS: 1
 SWH: 100.000
 FID: 100.000
 AC: 100.000
 PC: 100.000
 TE: 100.000
 DI: 1.0000000
 ===== CHANNEL f1 =====
 NUC1: 13C
 P1: 1.00
 PL1: 0.0
 RF1: 100.335001
 F2 - Processing parameters
 SI: 32768
 SF: 100.335001
 MD: 100.335001
 WD: 100.335001
 ZG: 0.0
 ZF: 0.0
 CA: 1.0

163.222
143.234
135.668
126.668
126.149
123.724
117.962
77.257
76.999
76.742

Current Data Parameters
NAME: 123.724-48p
EXPNO: 1
PROCNO: 1
F2 - Acquisition Parameters
Date_: 20020311
Time: 15.19
PROBHD: 5 mm QNP 1H/1
PULPROG: zgpg
TO: 45334
SOLVENT: CDCl3
DS: 4
SWH: 3144.541
AQ: 0.020724
RG: 8192
DM: 15.900
DE: 0.001
TE: 300.0
D1: 2.00000000
D11: 0.03000000
D12: 0.00000000
===== CHANNEL f1
NUC1: 13C
P1: 1.00
PL1: 3.00
SF01: 125.834556
===== CHANNEL f2
CPDPRG2: waltz16
NUC2: 1H
P2: 1.00
PL2: 0.00
PL12: 24.00
PL13: 24.00
SF02: 500.3920016
F2 - Processing parameters
SI: 16384
SF: 125.834556
WDW: EM
SSB: 0
LB: 0.30
GB: 0
PC: 1.00

139.847
133.732
128.331
127.512
126.569
124.323
121.504
121.292
120.445
120.141
120.000
119.904
103.145

77.251
76.997
76.742

Current Data Parameters
NAME hmc0191f1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20021122
Time 20:33
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 4
DS 4
SWH 31446.341 Hz
FIDRES 0.4718834 Hz
AQ 1.0420724 sec
RG 655
DM 15.000 usec
DE 6.000 usec
TE 300.0 K
D1 0.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec
----- CHANNEL f1 -----
NUC1 13C
P1 7.50 usec
PL1 0.00 dB
SFO1 125.834554 MHz
----- CHANNEL f2 -----
CPDPR2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 0.00 dB
PL3 2.00 dB
PL13 26.00 dB
SFO2 500.3920016 MHz
F2 - Processing parameters
SI 32768
SF 125.8321648 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
10 MHz plot parameters
CE 32.00 cm
F1 255.000 MHz
F2 500.136 MHz
F3 -15.000 MHz
F4 -1007.33 MHz
F5 1.000000 MHz
F6 1.000000 MHz
F7 1.000000 MHz
F8 1.000000 MHz
F9 1.000000 MHz
F10 1.000000 MHz
F11 1.000000 MHz
F12 1.000000 MHz
F13 1.000000 MHz
F14 1.000000 MHz
F15 1.000000 MHz
F16 1.000000 MHz
F17 1.000000 MHz
F18 1.000000 MHz
F19 1.000000 MHz
F20 1.000000 MHz
F21 1.000000 MHz
F22 1.000000 MHz
F23 1.000000 MHz
F24 1.000000 MHz
F25 1.000000 MHz
F26 1.000000 MHz
F27 1.000000 MHz
F28 1.000000 MHz
F29 1.000000 MHz
F30 1.000000 MHz
F31 1.000000 MHz
F32 1.000000 MHz
F33 1.000000 MHz
F34 1.000000 MHz
F35 1.000000 MHz
F36 1.000000 MHz
F37 1.000000 MHz
F38 1.000000 MHz
F39 1.000000 MHz
F40 1.000000 MHz
F41 1.000000 MHz
F42 1.000000 MHz
F43 1.000000 MHz
F44 1.000000 MHz
F45 1.000000 MHz
F46 1.000000 MHz
F47 1.000000 MHz
F48 1.000000 MHz
F49 1.000000 MHz
F50 1.000000 MHz
F51 1.000000 MHz
F52 1.000000 MHz
F53 1.000000 MHz
F54 1.000000 MHz
F55 1.000000 MHz
F56 1.000000 MHz
F57 1.000000 MHz
F58 1.000000 MHz
F59 1.000000 MHz
F60 1.000000 MHz
F61 1.000000 MHz
F62 1.000000 MHz
F63 1.000000 MHz
F64 1.000000 MHz
F65 1.000000 MHz
F66 1.000000 MHz
F67 1.000000 MHz
F68 1.000000 MHz
F69 1.000000 MHz
F70 1.000000 MHz
F71 1.000000 MHz
F72 1.000000 MHz
F73 1.000000 MHz
F74 1.000000 MHz
F75 1.000000 MHz
F76 1.000000 MHz
F77 1.000000 MHz
F78 1.000000 MHz
F79 1.000000 MHz
F80 1.000000 MHz
F81 1.000000 MHz
F82 1.000000 MHz
F83 1.000000 MHz
F84 1.000000 MHz
F85 1.000000 MHz
F86 1.000000 MHz
F87 1.000000 MHz
F88 1.000000 MHz
F89 1.000000 MHz
F90 1.000000 MHz
F91 1.000000 MHz
F92 1.000000 MHz
F93 1.000000 MHz
F94 1.000000 MHz
F95 1.000000 MHz
F96 1.000000 MHz
F97 1.000000 MHz
F98 1.000000 MHz
F99 1.000000 MHz
F100 1.000000 MHz

Current Data Parameters
NAME 3ba
EXPNO 1
PROCNO 1
Date_ Acquired 20021008
Time 21.04
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg30
SOLVENT CDCl3
NS 32
DS 4
SWH 8009.415 MHz
FIDRES 0.183359 Hz
AQ 2.748731 sec
RG 320
DE 93.200 usec
TE 300.2 K
D1 1.0000000 sec
===== CHANNEL f1 =====
NUC1 13C
P1 1.00 usec
PL1 0.00 dB
SFO1 100.625019 MHz
F2 - Processing parameters
SI 32768
SF 500.130014 MHz
WDW EM
SSB 0
GB 0.70 Hz
CB 1.00
PC 1.00
===== CHANNEL f2 =====
NUC2 1H
P2 0.00 usec
PL2 0.00 dB
SFO2 500.130014 MHz
F2 - Processing parameters
SI 32768
SF 500.130014 MHz
WDW EM
SSB 0
GB 0.70 Hz
CB 1.00
PC 1.00
===== 1D NMR plot parameters =====
SI 32768
SF 500.130014 MHz
WDW EM
SSB 0
GB 0.70 Hz
CB 1.00
PC 1.00
===== 2D NMR plot parameters =====
SI 32768
SF 500.130014 MHz
WDW EM
SSB 0
GB 0.70 Hz
CB 1.00
PC 1.00

Current Data Parameters
NAME: hacc55p
EXPNO: 2
PROCNO: 1
F2 - Acquisition Parameters
Date_: 2002108
Time: 15.22
INSTRUM: spect
PROBHD: 5 mm QNP 1H/1
PULPROG: zgpg30
SOLVENT: CDCl3
NS: 129
DS: 4
SWH: 31646.344 Hz
FIDRES: 0.479816 Hz
AQ: 1.0220724 sec
RG: 327.500
DE: 15.500 us
TE: 300.2 K
D1: 0.0000000 sec
D11: 0.0300000 sec
D12: 0.0000000 sec
===== CHANNEL f1 =====
NUC1: 13C
P1: 7.50 us
PL1: 0.00 dB
SFO1: 125.8136556 MHz
===== CHANNEL f2 =====
NUC2: 1H
P2: 100.00 us
PL2: 0.00 dB
SFO2: 500.1320016 MHz
F2 - Processing parameters
SI: 32768
SF: 125.8231694 MHz
WDW: EM
SSB: 0
LB: 1.00 Hz
GB: 0
PC: 1.40
LO MHz plot parameters
CF: 22.00 MHz
CFCW: 22.00 MHz
F1: 25569.44 MHz
F2: -15.000 MHz
F3: 25569.44 MHz
FREQH: 11.93472 Hz
NECH: 1425.80872 Hz

Current Data Parameters
 NAME: 3bb
 EXPNO: 1
 PROCNO: 1
 F2 - Acquisition Parameters
 Date_Time: 10/10/2010 15:14
 Time: 15:14
 Date: 10/10/2010
 Time: 15:14
 PULPROG: zgpg30
 PCV: zgpg30
 SOLVENT: CDCl3
 NS: 512
 DS: 4
 SWH: 8044.314 Hz
 FIDRES: 0.000110 Hz
 AQ: 2.0116400 sec
 RG: 316
 GB: 0
 PR: 0.000000 sec
 TE: 300.2 K
 DE: 1.0000000 dB
 B1: 12.00 uV
 B2: 12.00 uV
 B3: 12.00 uV
 B4: 12.00 uV
 F1 - Processing parameters
 SI: 32768
 SF: 100.6261314 MHz
 DF: 327.68 MHz
 AS: 0.000000 sec
 L3: 1.50 Hz
 L4: 1.50 Hz
 PC: 1.40
 F2 - MMS plot parameters
 SI: 32768
 SF: 100.6261314 MHz
 DF: 327.68 MHz
 AS: 0.000000 sec
 L3: 1.50 Hz
 L4: 1.50 Hz
 PC: 1.40
 F2 - MMS plot parameters
 SI: 32768
 SF: 100.6261314 MHz
 DF: 327.68 MHz
 AS: 0.000000 sec
 L3: 1.50 Hz
 L4: 1.50 Hz
 PC: 1.40

172.514
 165.481
 161.617
 139.998
 126.365
 126.320
 125.905
 96.745
 77.256
 77.001
 76.748
 54.613
 53.961
 53.812

Current Data Parameter
 NAME bbt061p
 EXPNO
 PROCNO
 F2 - Acquisition Para
 Date_ 200102
 Time 19
 INSTRUM amx5
 PROBHD 5 mm Dual
 PULPROG zg
 TD 655
 SOLVENT CDC
 NS
 DS 11311.3
 SWH 0.5046
 FIDRES 0.98109
 RG 163
 DW 15.0
 DE 18
 TE 300
 HL1
 DI 4.000000
 CDPRG waltz
 S1 107
 D11
 S2 0.03000
 P1 5
 SF01 125.81821
 NUCLEUS 1
 F2 - Processing param
 SI 327
 SF 125.82317
 GAM 1
 SSB 1
 LB 1
 GB 1
 PC 1
 1D NMR plot parameter
 CX 21
 FIP 235.0
 F1 29568
 F2 -188.0
 F3 -188.0
 PPMCH 11.904
 HZCN 1497.894

8.223
8.220
8.217
8.214
7.635
7.632
7.624
7.622
7.469
7.450
7.444
7.439
7.434

[illegible]

163.301
162.706
160.914

137.384
129.495
127.575
125.762
114.878

77.252
76.998
76.743

Current Data Parameters
NAME: 3bc
EXPNO: 2
PROCNO: 1
F2 - Acquisition Parameters
Date_ Time: 20021108 20:28
INSTRUM: spect
PROBHD: 5 mm QNP
PULPROG: zgpg30
TD: 65536
SOLVENT: CDCl3
DS: 4
SWH: 31414.341 Hz
FIDRES: 0.400000 Hz
AQ: 1.0120214 sec
RG: 11585.2
DF: 15.900 us
DE: 800.0 us
TE: 300.0 K
D1: 2.00000000 sec
D11: 0.00000000 sec
D12: 0.00000000 sec
----- CHANNEL f1 -----
NUC1: 13C
P1: 1.00 us
PL1: 1.00 dB
SFO1: 125.6369556 MHz
----- CHANNEL f2 -----
CTDPRG2: waltz16
NUC2: 1H
PCPD2: 100.00 us
PL2: 0.00 dB
PL12: 26.00 dB
PL13: 26.00 dB
SFO2: 500.1320016 MHz
F2 - Processing parameters
SI: 32768
SF: 125.6369556 MHz
WDW: EM
SSB: 0
GB: 0
PC: 1.40
ID: HHG plot parameters
CH: 22.00 dB
FIP: 235.000 PE
F1: 29566.45 Hz
F2: -1889.35 Hz
PPMCH: 11.36344 PE
MCHN: 1429.60884 Hz

Current Data Parameters
 NAME hbc2282
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20021104
 Time 23:28
 INSTRUM spect
 PROBHD 5 mm QNP 1H/1
 PULPROG zgpg
 TO 65516
 SOLVENT CDCl₃
 NS 129
 DS 4
 SW 31446.541 Hz
 FIDRES 0.474816 Hz
 AQ 1.0420724 sec
 RG 4096
 DQ 15.900 usec
 DE 6.00 usec
 TE 300.0 K
 D1 2.00000000 sec
 D11 0.01000000 sec
 D12 0.00002000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 7.50 usec
 PL1 1.00 dB
 SFO1 125.0109556 MHz

===== CHANNEL f2 =====
 NUC2 1H
 P2 100.00 usec
 PL2 0.00 dB
 SFO2 500.13020016 MHz

F2 - Processing parameters
 SI 32768
 SF 125.0231780 MHz
 WDW EM
 LB 1.00 Hz
 GB 0
 PC 1.40

1D NMR plot parameters
 CI 25.00 cm
 FI 215.000 ppm
 F1 20640.45 Hz
 F2 -15.000 ppm
 F3 -1007.35 Hz
 FWHM 11.36344 ppm/
 RMSC 1429.00000 Hz/c

[illegible]

Current Data Parameters
 Date_ 20021104
 Time_ 12.11
 Sample 12-11
 PULPROG 5 mm QNP 1H/13
 TO 65318
 AC SOLVENT CDCl3
 NS 1
 DS 4
 SWH 31461.561 Hz
 FID 1
 AQ 1.012724 sec
 RG 11583.2
 DW 15.960 us
 DE 0.000000 us
 TE 300.0 K
 D1 2.00000000 sec
 D11 0.15000000 sec
 D12 0.00000000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 12.00 dB
 PL1 3.00 dB
 SFO1 125.8369536 MHz

===== CHANNEL f2 =====
 CDPRG2 waltz16
 NUC2 1H
 P2 100.00 dB
 PL2 0.00 dB
 PL3 0.00 dB
 PL12 25.00 dB
 PL13 15.00 dB
 SFO2 500.3750161 MHz

F2 - Processing parameters
 SI 32768
 SF 125.8231732 MHz
 MD 0
 WD 0
 SS 0
 GB 0
 PC 1.40

1D NMR Plot Parameters
 CX 22.00 cm
 FIP 235.000 PE
 FI 29548.45 Hz
 F1 -1887.35 Hz
 F2 -1887.35 Hz
 PRNCH 11.76344 PE
 RECN 1.429.0084 Hz

Current Data Parameters
NAME: 20021106
EXPNO: 1
PROCNO: 1

F2 - Acquisition Parameters
Date_: 20021106
Time: 16.24
INSTRUM: spect
PROBHD: 5 mm QNP 1H/1
PULPROG: zg30
TD: 32768
SOLVENT: CDCl3
NS: 16
DS: 2
SWH: 6091.615 Hz
FIDRES: 0.181359 Hz
AQ: 2.7261877 sec
RG: 384
ACQ: 81.200 usec
PC: 1.00 usec
RE: 300.0 K
F2: 1.00000000 sec
DI: 1.00000000 sec

***** CHANNEL f1 ***
NUC1: 1H
P1: 7.50 usec
PL1: 0.00 dB
SFO1: 500.3725019 MHz

F2 - Processing parameters
SI: 32768
SF: 500.3700136 MHz
WDW: EM
SSB: 0
LB: 0.30 Hz
GB: 0
PC: 1.00

1D NMR plot parameters
CF: 22.00 cm
F1P: 10.000 ppm
F1: 500.3700136 MHz
F2P: -0.500 ppm
F2: -250.15 Hz
FREQM: 0.47727 ppm
NUC2: 13C

Current Data Parameters
NAME batc057kp
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20021109
Time 21 04
INSTRUM amx500
PROBHD 5 mm Dual 13
PULPROG zgpg
TD 65536
SOLVENT CDCl3
NS 232
DS 2
SWH 3333.332
FIDRES 0.508626
AQ 0.9830900
RG 16384
DM 15 000
DE 18.75
TE 300.0
HL1 40
D1 5.0000000
CPOPRG waltz16
P31 107.00
S4 24
D11 0.0300000
S2 18
P1 5.00
SF01 125.8382148
NUCLEUS 13C

F2 - Processing parameters
SI 32768
SF 125.8231695
WDW EM
SSB 0
LB 1.50
GB 0
PC 1.40

1D NMR plot parameters
CX 21.00
FIP 235.000
F1 29568.44
F2p -15.000
F2 -1887.35
PPMCM 11.90476
HZCM 1497.89478

7.941
7.925
7.504
7.494
7.488
7.479

9.282
8.995
8.885
8.745
8.736

77.251
76.996
76.742

158.047
154.763
150.052
147.768
134.175
131.283
130.019
123.859

Current Data Parameters
NAME: 20020331
EXPNO: 1
PROCNO: 1
F2 - Acquisition Parameters
Date_ 20020331
Time 18.41
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
D1 0.00100000
SOLVENT CDCl3
NS 65
DS 4
SWH 31445.344 Hz
FIDRES 0.1718236 Hz
AQ 1.0420724 s
RG 655
PC 15.800 us
DE 4.00 us
TE 300.2 K
T1 1.00000000 s
D11 0.03000000 s
D12 0.00020000 s
===== CHANNEL f1 =====
NUC1 13C
P1 7.50 us
PL1 0.00 dB
SFO1 125.831724 MHz
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 us
PL2 0.00 dB
PL3 0.00 dB
PL4 0.00 dB
PL5 24.00 dB
SFO2 500.3920014 MHz
F2 - Processing parameters
SI 32768
SF 125.831724 MHz
WDW EM
SS 0
LB 1.50 Hz
GB 0
PC 1.40