Supporting Information

Synthesis of Functionalized Organotrifluoroborates via Halomethyltrifluoroborates

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General Considerations: ^1H -, ^{13}C -, and ^{19}F -NMR spectra were recorded on 500.39 or 360.13, 125.75, and 470.55 MHz, respectively. ^{19}F -NMR chemical shifts were referenced to external CFCl_3 (0.0 ppm). ^{11}B -NMR spectra at 128.4 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. Mass spectra of potassium organotrifluoroborates were performed using negative ion electrospray at the mass spectrometry facilities at the University of Pennsylvania. Elemental analyses were performed by MHW Laboratories. THF was distilled from sodium. Commercially obtained anhydrous DMSO, DMF, and reagents were used without further purification.

Preparation of Potassium Halomethyltrifluoroborates **1** and **2**.

Potassium Bromomethyltrifluoroborate (1). To a soln of dibromomethane (1.76 mL, 25 mmol) and triisopropyl borate (5.2 mL, 23 mmol) in THF (35 mL) was slowly added *n*-BuLi (2.5 M soln in hexanes, 8.5 mL, 21 mmol) at -78 °C for 1 h under N_2 . The soln was vigorously stirred for 1 h. Then, KHF_2 (4.9 g, 63 mmol) was added in one portion, followed by the dropwise addition of H_2O (15 mL). The reaction mixture was warmed to rt. After stirring at rt for 30 min, the suspension was concentrated on a rotary evaporator. The resulting white solids were subjected to high vacuum for 3 h. The crude compound was purified by dissolving in acetone and precipitating with Et_2O to obtain the desired compound **1** as a white solid (3.75 g, 89% yield). mp = 220 °C. ^1H NMR (500 MHz, Acetone- d_6) δ 2.21 (br s, 2H). ^{13}C NMR (125.8 MHz, Acetone- d_6) δ no peaks. ^{19}F (470.8 MHz, Acetone- d_6) δ -146.2. ^{11}B NMR (128.4 MHz, Acetone- d_6) δ 2.95. IR (neat): 3435, 1696, 1256, 1096, 980, 952 cm^{-1} . HRMS (m/z): calcd. for $\text{C}_1\text{H}_2\text{BBrF}_3$, 160.9385 [M-K^+]; found, 160.9383.

Potassium Iodomethyltrifluoroborate (2). The compound was prepared using diiodomethane by the procedure used for potassium bromomethyltrifluoroborate (4.6 g, 89% yield). mp = 242 °C. ^1H NMR (500 MHz, Acetone- d_6) δ 1.80 (br s, 2H). ^{13}C NMR (125.8 MHz, Acetone- d_6) δ no peaks. ^{19}F (470.8 MHz, Acetone- d_6) δ -145.0. ^{11}B NMR (128.4 MHz, Acetone- d_6) δ 2.97. IR (neat): 3435, 1398, 1165, 1073, 953, 931 cm^{-1} . HRMS (m/z): calcd. for $\text{C}_1\text{H}_2\text{BF}_3\text{I}$, 208.9246 [M-K^+]; found, 208.9254.

Potassium Iodomethyltrifluoroborate (2). To a soln of potassium bromomethyltrifluoroborate (2.0 g, 10 mmol) in acetone (150 mL) was added NaI (1.5 g, 10 mmol) in one portion. After stirring at rt for 2 h, the suspension was filtered through Celite and then the solvent was evaporated under reduced pressure to give the crude product. The crude compound was purified by dissolving in a minimal amount of dry acetone

and precipitating with Et₂O to obtain the pure compound **2** as a white solid (2.38 g 96% yield).

Reaction Condition A for Preparing Compounds 3–5.

To a soln of an organolithium or Grignard reagent (1.2 mmol) in anhydrous THF (2 mL) was slowly added a soln of potassium iodomethyltrifluoroborate (99.1 mg, 0.4 mmol) in THF (3 mL) at -25 °C for 10 min under N₂ and then the reaction mixture was slowly warmed to 0 °C during the reaction time (see Table 2). After the reaction was complete, it was quenched with 1.5 N KHF₂ (2 mL) followed by removal of all the solvent under high vacuum. The residual solid was dissolved in dry acetone (15 mL), the insoluble salts were filtered off and then the product was concentrated. The crude solid was purified by dissolving in a minimal amount of dry acetone (4 mL) and precipitating with Et₂O (10 mL) to obtain the desired pure compound.

Potassium (2-Thiophenyl)methyltrifluoroborate (3). The title compound was isolated as a yellow solid (70 mg, 86% yield) using 2-thienyllithium (1.0 M soln in THF). mp = 172-173 °C (dec.). ¹H NMR (500 MHz, Acetone-*d*₆) δ 6.85 (dd, 1H, *J* = 5.2, 1.2 Hz), 6.72 (dd, 1H, *J* = 5.2, 3.3 Hz), 6.59 (dd, 1H, *J* = 3.3, 0.9 Hz), 1.78 (br s, 2H). ¹³C NMR (125.8 MHz, Acetone-*d*₆) δ 125.8, 122.2, 119.5, 110.3. ¹⁹F (470.8 MHz, Acetone-*d*₆) δ -141.8. ¹¹B NMR (128.4 MHz, Acetone-*d*₆) δ 4.18. IR (neat): 3531, 2886, 1609, 1532, 1443, 1234, 1077, 1034, 977, 945 cm⁻¹. HRMS (*m/z*): calcd. for C₅H₅BF₃S, 165.0157 [M-K⁺]; found, 165.0161.

Potassium Pentyltrifluoroborate (4). The title compound was isolated as a white solid (59 mg, 83% yield) using *n*-BuLi (2.5 M soln in hexanes). mp > 250 °C. ¹H NMR (500 MHz, Acetone-*d*₆) δ 1.25 (m, 6H), 0.84 (t, 3H, *J* = 6.8 Hz), 0.13 (br s, 2H). ¹³C NMR (125.8 MHz, Acetone-*d*₆) δ 36.3, 25.6, 23.1, 14.0. ¹⁹F (470.8 MHz, Acetone-*d*₆) δ -141.6. ¹¹B NMR (128.4 MHz, Acetone-*d*₆) δ 5.85. IR (neat): 3391, 2916, 1460, 1070, 971, 890 cm⁻¹. HRMS (*m/z*): calcd. for C₅H₁₁BF₃, 139.0906 [M-K⁺]; found, 139.0905.

Potassium 1-Propenyltrifluoroborate (5).¹ The title compound was isolated as a white solid (55 mg, 85% yield) using allylmagnesium chloride (2.0 M soln in THF). mp = 243-245 °C (dec.). ¹H NMR (500 MHz, Acetone-*d*₆) δ 5.89 (m, 1H), 4.83 (m, 1H), 4.67 (m, 1H), 1.96 (m, 2H), 0.21 (q, 2H, *J* = 7.1 Hz). ¹³C NMR (125.8 MHz, Acetone-*d*₆) δ 144.8, 109.8, 30.1. ¹⁹F (470.8 MHz, Acetone-*d*₆) δ -141.9. ¹¹B NMR (128.4 MHz, Acetone-*d*₆) δ 5.36. IR (neat): 3468, 2911, 1701, 1638, 1445, 1253, 1081, 1006, 962, 902, 863 cm⁻¹. HRMS (*m/z*): calcd. for C₄H₇BF₃, 123.0592 [M-K⁺], found, 123.0584.

Reaction Condition B for Preparing Compounds 6–9.

Potassium bromomethyltrifluoroborate (100 mg, 0.5 mmol) was added to neat alkylamine (2 mL) at rt. The reaction mixture was heated at 80 °C for 30 min and concentrated under high vacuum. The residual product was dissolved in a soln of KHCO₃ (69.1 mg, 0.5 mmol) and dry acetone (15 mL), followed by stirring the mixture at rt. After 20 min, the insoluble salts were filtered off, and then the product was concentrated. The crude solid was purified by dissolving in a minimal amount of dry acetone and precipitating with Et₂O to obtain the desired pure compound.

Potassium *N*-Butyl-aminomethyltrifluoroborate (6). The title compound was isolated as a yellow solid (85 mg, 88% yield) using *n*-butylamine. mp = 118-120 °C. ¹H NMR (500 MHz, Acetone-*d*₆) δ 6.08 (br s, 1H, NH), 3.13 (m, 2H), 2.00 (br s, 2H, -CH₂-B), 1.80 (m, 2H), 1.44 (m, 2H), 0.95 (t, 3H, *J* = 7.4 Hz). ¹³C NMR (125.8 MHz, Acetone-*d*₆) δ 50.0, 27.9, 19.5, 13.0. ¹⁹F (470.8 MHz, Acetone-*d*₆) δ -145.7. ¹¹B NMR (128.4 MHz, Acetone-*d*₆) δ 2.31. IR (neat): 3400, 3003, 2821, 2443, 1471, 1103, 1024, 1010, 958, 868 cm⁻¹. HRMS (*m/z*): calcd. for C₅H₁₂BF₃N, 154.1015 [M-K⁺]; found, 154.1019.

Potassium *N*-Cyclohexyl-aminomethyltrifluoroborate (7). The title compound was isolated as a white solid (107 mg, 98% yield) using cyclohexylamine. mp = 228 °C. ¹H NMR (500 MHz, Acetone-*d*₆) δ 6.74 (br s, 1H, NH), 3.12 (tt, 1H, *J* = 11.5, 3.8 Hz), 2.25 (ddd, 2H, *J* = 11.2, 2.4, 1.4 Hz), 1.97 (br s, 2H, -CH₂-B), 1.87 (dt, 2H, *J* = 14.0, 3.5 Hz), 1.69 (m, 1H), 1.48 (qd, 2H, *J* = 12.5, 3.4 Hz), 1.36 (qt, 2H, *J* = 12.7, 3.2 Hz), 1.20 (qt, 1H, *J* = 12.8, 3.5 Hz). ¹³C NMR (125.8 MHz, DMSO-*d*₆) δ 58.0, 29.0, 25.7, 24.9. ¹⁹F (470.8 MHz, Acetone-*d*₆) δ -145.7. ¹¹B NMR (128.4 MHz, Acetone-*d*₆) δ 2.11. IR (neat): 3229, 2927, 2856, 1585, 1445, 1298, 1067, 1023, 900, 826 cm⁻¹. HRMS (*m/z*): calcd. for C₇H₁₄BF₃N, 180.1171 [M-K⁺]; found, 180.1174.

Potassium Pyrrolidine-1-methyltrifluoroborate (8). The title compound was isolated as a yellow solid (88 mg, 92% yield) using pyrrolidine. mp = 85-87 °C. ¹H NMR (500 MHz, Acetone-*d*₆) δ 3.40 (br s, 4H, -(CH₂)₂-N), 2.17 (br s, 2H, -CH₂-B), 2.09 (m, 4H). ¹³C NMR (125.8 MHz, Acetone-*d*₆) δ 56.1, 22.7. ¹⁹F (470.8 MHz, Acetone-*d*₆) δ -144.3. ¹¹B NMR (128.4 MHz, Acetone-*d*₆) δ 1.98. IR (neat): 3413, 3208, 2974, 2761, 1631, 1460, 1309, 1178, 1005 cm⁻¹. HRMS (*m/z*): calcd. for C₅H₁₀BF₃N, 152.0858 [M-K⁺]; found, 152.0848.

Potassium Piperidinyl-1-methyltrifluoroborate (9). The title compound was isolated as a white solid (97 mg, 95% yield) using piperidine. mp = 146-148 °C. ¹H NMR (500 MHz, Acetone-*d*₆) δ 3.28 (br s, 4H, -(CH₂)₂-N), 2.06 (br s, 2H, -CH₂-B), 1.89 (m, 4H), 1.67, (br s, 2H, -CH₂-). ¹³C NMR (125.8 MHz, Acetone-*d*₆) δ 56.4, 24.0, 22.4. ¹⁹F (470.8 MHz, Acetone-*d*₆) δ -142.6. ¹¹B NMR (128.4 MHz, Acetone-*d*₆) δ 1.94 (q, *J* = 50.5 Hz). IR (neat): 3401, 3180, 2951, 2774, 1458, 1306, 1227, 1043, 1004, 950 cm⁻¹. HRMS (*m/z*): calcd. for C₆H₁₂BF₃N, 166.1015 [M-K⁺]; found, 166.1016.

Reaction Condition C for Preparing Compounds 10 and 11.

To a soln of the nucleophile (1.2 mmol), which was prepared from substrate (1.2 mmol) and NaH (1.2 mmol, 60% dispersion in mineral oil) in dry solvent (3.5 mL), was slowly added a soln of potassium iodomethyltrifluoroborate (99.1 mg, 0.4 mmol) in dry solvent (2 mL) at 0 °C for 0.5 h under N₂. The reaction mixture was stirred at rt for 8 h. After the reaction was completed, it was quenched with 1.5 N KHF₂ (2 mL) followed by removal of all the solvent under high vacuum. The residual solid was dissolved in dry acetone (15 mL), the insoluble salts were filtered off, and then the product was concentrated. The crude solid was purified by dissolving in a minimal amount of dry acetone (4 mL) and precipitating with Et₂O (10 mL) to obtain the desired pure compound.

Potassium (4-Phenylpropoxy)methyltrifluoroborate (10). The title compound was isolated as a white solid (88 mg, 86% yield) using 4-phenylpropanoxide. mp = 220 °C (dec.). ¹H NMR (500 MHz, Acetone-*d*₆) δ 7.25 (m, 2H), 7.20 (m, 2H), 7.14 (m, 1H), 3.34 (t, 2H, *J* = 6.9 Hz), 2.71 (q, 2H, *J* = 5.6 Hz), 2.61 (t, 2H, *J* = 7.7 Hz), 1.85 (m, 2H). ¹³C NMR (125.8 MHz, Acetone-*d*₆) δ 142.4, 128.3, 128.1, 125.5, 73.5, 32.2, 31.4. ¹⁹F (470.8 MHz, Acetone-*d*₆) δ -146.2. ¹¹B NMR (128.4 MHz, Acetone-*d*₆) δ 3.26 (q, *J* = 54.9 Hz). IR (neat): 3400, 2941, 2859, 1611, 1453, 1083, 996 cm⁻¹. HRMS (*m/z*): calcd. for C₁₀H₁₃BF₃O, 217.1012 [M-K⁺]; found, 217.1014.

Potassium 2,2-Dicyanoethyltrifluoroborate (11). The title compound was isolated as a pink solid (68 mg, 91% yield) using malononitrile. mp = 223 °C. ¹H NMR (500 MHz, Acetone-*d*₆) δ 4.13 (t, 1H, *J* = 7.4 Hz), 0.64 (br s, 2H). ¹³C NMR (125.8 MHz, Acetone-*d*₆) δ 108.9, 48.4. ¹⁹F (470.8 MHz, Acetone-*d*₆) δ -138.9. ¹¹B NMR (128.4 MHz, Acetone-*d*₆) δ 3.13 (q, *J* = 54.9 Hz). IR (neat): 2924, 2259, 2194, 1450,

1250, 1034, 1014, 987, 967 cm^{-1} . HRMS (m/z): calcd. for $\text{C}_4\text{H}_3\text{BF}_3\text{N}_2$, 147.0341 [M-K^+]; found, 147.0341.

Reaction Condition D for Preparing Compound 12.

Potassium Ethyl 3-Oxo-5-(trifluoroborato) pentanoate (12). A soln of ethyl acetoacetate dianion (1.2 mmol) was prepared by addition of ethyl acetoacetate (0.15 mL, 1.2 mmol) to a soln of NaH (52 mg, 1.3 mmol, 60% dispersion in mineral oil) in THF (2 mL) at 0 °C for 20 min followed by addition of *n*-BuLi (2.5 M soln in hexanes, 0.48 mL, 1.2 mmol) at the same temperature under N_2 . The orange soln was stirred at 0 °C for an additional 15 min. To this mixture was added a soln of potassium iodomethyltrifluoroborate (99.1 mg, 0.4 mmol) in THF (3 mL) at 0 °C. After 3 h, it was quenched with 1.5 N KHF_2 (2 mL) followed by removal of all the solvent under high vacuum. The residual solid was dissolved in hot EtOAc (25 mL), the insoluble salts were filtered off, and then the product was concentrated. The crude solid was purified by dissolution in a minimal amount of dry acetone and precipitation with Et_2O to obtain the desired pure compound **12** as a yellow viscous solid (88 mg, 88% yield). ^1H NMR (500 MHz, Acetone- d_6) δ 4.10 (q, 2H, $J = 7.1$ Hz, - CH_2CH_3), 3.45 (s, 2H, -CO- CH_2 -CO-), 2.33 (t, 2H, $J = 8.3$ Hz, -CO- CH_2 -), 1.21 (t, 3H, $J = 7.1$ Hz, - CH_2CH_3), 0.36 (m, 2H, - CH_2 -B). ^{13}C NMR (125.8 MHz, Acetone- d_6) δ 206.9, 167.9, 60.3, 47.7, 40.0, 13.5. ^{19}F (470.8 MHz, Acetone- d_6) δ -142.3. ^{11}B NMR (128.4 MHz, Acetone- d_6) δ 5.26. IR (neat): 3436, 2914, 1731, 1370, 1312, 1234, 1072, 1024 cm^{-1} . HRMS (m/z): calcd. for $\text{C}_7\text{H}_{10}\text{BF}_3\text{O}_3$, 191.0691 [M-KHF^+] 2 ; found, 191.0705.

Reaction Condition E for Preparing Compound 13.

Potassium Cyanomethyltrifluoroborate (13). Potassium bromomethyltrifluoroborate (100 mg, 0.5 mmol) and potassium cyanide (39.1 mg, 0.6 mmol) were dissolved in DMSO (3.5 mL). The reaction mixture was heated at 80 °C for 10 h and concentrated under high vacuum. The residual product was dissolved in dry acetone (15 mL), the insoluble salts were filtered off, and then the product was concentrated. The crude solid was purified by dissolving in a minimal amount of dry acetone and precipitating with Et_2O to obtain the desired pure compound **13** as a white solid (72 mg, 98% yield). mp = 146-147 °C. ^1H NMR (500 MHz, Acetone- d_6) δ 0.99 (m, 2H). ^{13}C NMR (125.8 MHz, Acetone- d_6) δ 124.6. ^{19}F (470.8 MHz, Acetone- d_6) δ -141.2. ^{11}B NMR (128.4 MHz, Acetone- d_6) δ 2.83. IR (neat): 2238, 1197, 1004, 947 cm^{-1} .

Anal. Calc for $\text{C}_2\text{H}_2\text{BF}_3\text{KN}$: C, 16.35; H, 1.37; N, 9.53. Found: C, 16.50; H, 1.46; N, 9.81.

Reaction Condition F for Preparing Compounds 14–16.

To a soln of aryl bromide (1.2 mmole) in anhydrous THF (3 mL) was added a soln of *t*-BuLi (1.5 M soln in pentane, 2.4 mmole) at $-78\text{ }^{\circ}\text{C}$ for 15 min under N_2 . Sulfur powder (38.4 mg, 1.2 mmole) was added in one portion. After the reaction mixture changed to a yellow clear soln, a soln of potassium iodomethyltrifluoroborate (99.1 mg, 0.4 mmol) in THF (3 mL) was slowly added and then the reaction mixture was slowly warmed to rt for 2 h. After the reaction was completed, it was quenched with 1.5 N KHF_2 (2 mL) followed by removal of all the solvent under high vacuum. The residual solid was dissolved in dry acetone (10 mL), the insoluble salts were filtered off, and then the product was concentrated. The crude solid was purified by dissolving in a minimal amount of dry acetone and precipitating with Et_2O to obtain the desired pure compound.

Potassium 2-Methoxy-phenylsulfanylmethyltrifluoroborate (14). The title compound was isolated as an ivory solid (94 mg, 90% yield) starting with 2-bromoanisole. mp = $154\text{ }^{\circ}\text{C}$ (dec.). ^1H NMR (500 MHz, $\text{DMSO}-d_6$) δ 7.07 (dd, 1H, J = 7.6, 1.6 Hz), 6.95 (td, 1H, J = 7.7, 1.7 Hz), 6.88 (td, 1H, J = 7.5, 1.3 Hz), 6.81 (dd, 1H, J = 8.0, 1.2 Hz), 3.74 (s, 3H), 1.44 (q, 2H, J = 5.4 Hz). ^{13}C NMR (125.8 MHz, $\text{DMSO}-d_6$) δ 155.5, 124.3, 123.6, 121.3, 110.1, 55.8, 30.8. ^{19}F (470.8 MHz, Acetone- d_6) δ -141.7. ^{11}B NMR (128.4 MHz, $\text{DMSO}-d_6$) δ 2.90. IR (neat): 3401, 2951, 2235, 1573, 1476, 1236, 1192, 1016, 982 cm^{-1} . HRMS (m/z): calcd. for $\text{C}_8\text{H}_9\text{BF}_3\text{OS}$. 221.0419 [$\text{M}-\text{K}^+$]; found, 221.0423.

Potassium 3-Methoxy-phenylsulfanylmethyltrifluoroborate (15). The title compound was isolated as a white solid (96 mg, 92% yield) starting with 3-bromoanisole. mp = $223\text{ }^{\circ}\text{C}$ (dec.). ^1H NMR (500 MHz, Acetone- d_6) δ 7.07 (t, 1H, J = 8.3 Hz), 6.76 (m, 2H), 6.53 (dd, 1H, J = 9.1, 7.2 Hz), 3.74 (s, 3H), 1.80 (m, 2H). ^{13}C NMR (125.8 MHz, Acetone- d_6) δ 159.9, 128.8, 117.4, 110.3, 108.3, 54.4, 29.9. ^{19}F (470.8 MHz, Acetone- d_6) δ -141.8. ^{11}B NMR (128.4 MHz, Acetone- d_6) δ 3.81 (q, J = 49.6 Hz). IR (neat): 3595, 3467, 2938, 2902, 1589, 1574, 1479, 1423, 1248, 1115, 1036, 969, 773 cm^{-1} . HRMS (m/z): calcd. for $\text{C}_8\text{H}_9\text{BF}_3\text{OS}$. 221.0419 [$\text{M}-\text{K}^+$]; found, 221.0422.

Potassium 4-Bromo-phenylsulfanylmethyltrifluoroborate (16). The title compound was isolated as a white solid (116 mg, 94% yield) starting with 1,4-dibromoanisole. mp $> 250\text{ }^{\circ}\text{C}$.

^1H NMR (500 MHz, Acetone- d_6) δ 7.32 (d, 2H, J = 8.8 Hz), 7.13 (d, 2H, J = 8.7 Hz), 1.78 (m, 2H). ^{13}C NMR (125.8 MHz, Acetone- d_6) δ 133.7, 130.9, 126.8, 115.2. ^{19}F (470.8 MHz, Acetone- d_6) δ -140.5. ^{11}B NMR (128.4 MHz, Acetone- d_6) δ 3.48 (q, J = 51.4 Hz). IR (neat): 2899, 1474, 1385, 1212, 1068, 978, 949, 809 cm^{-1} . 1 . HRMS (m/z): calcd. for $\text{C}_7\text{H}_6\text{BBrF}_3\text{S}$. 268.9419 [M-K^+]; found, 268.9431.

Reaction Condition for Preparing Compounds 17 and 18.

Potassium 5-Bromopentyltrifluoroborate (17).³ To a soln of 5-bromo-1-pentene (1.0 mL, 10 mmol) in CH_2Cl_2 (5 mL) in the presence of 1 mol% $\text{Rh}(\text{PPh}_3)_3\text{Cl}$ catalyst was added pinacolborane (1.0 M THF solution, 10 mL, 10 mmol) at 0 °C. The reaction mixture was stirred for 2 h at rt, and then extracted with Et_2O (80 mL), washed with H_2O (30 mL), dried (Mg_2SO_4), and filtered. After the removal of solvent, the crude product was obtained. The crude compound was purified by column chromatography on silica gel with eluting with hexane/ether (20:1 to 10:1, v/v) to obtain the hydroborated intermediate (1.33 g, 48% yield). A part (500 mg, 1.8 mmol) of the hydroborated intermediate was dissolved in Et_2O (5 mL). To the solution was added KHF_2 (0.84 g, 11 mmol) at 0 °C followed by the addition of H_2O (2 mL). After the mixture was stirred for 1 h, acetone (50 mL) was added and the suspension was concentrated on a rotary evaporator. The resulting white solids were subjected to high vacuum for 2 h. The crude compound was purified by dissolving in acetone and precipitating with Et_2O to obtain the desired compound **17** as a white solid (253 mg, 55% yield). mp > 250 °C. ^1H NMR (500 MHz, DMSO- d_6) δ 3.46 (t, 2H, J = 6.9 Hz), 1.73 (m, 2H), 1.27 (m, 2H), 1.13 (m, 2H), -0.07 (m, 2H, $-\text{CH}_2\text{-B}$). ^{13}C NMR (125.8 MHz, DMSO- d_6) δ 36.1, 33.3, 31.8, 25.2. ^{19}F (470.8 MHz, DMSO- d_6) δ -137.2. ^{11}B NMR (128.4 MHz, DMSO- d_6) δ 4.58. IR (neat): 3435, 2925, 2910, 2841, 1463, 1340, 1298, 1239, 1098, 1077, 1036, 935, 862 cm^{-1} . HRMS (m/z): calcd. for $\text{C}_5\text{H}_{10}\text{BBrF}_3$, 217.0011 [M-K^+]; found, 217.0003.

Potassium 5-Cyanopentyltrifluoroborate (18).³ Potassium 5-bromopentyltrifluoroborate **17**³ (51.4 mg, 0.2 mmol) and KCN (13 mg, 0.20 mmol) were dissolved in DMSO (1.0 mL). The reaction mixture was heated at 80 °C for 1 h and concentrated under high vacuum. The residual product was dissolved in dry acetone (2.0 mL), the insoluble salts were filtered off, and then the product was concentrated. The crude solid was purified by dissolving in a minimal amount of dry acetone and precipitating with Et_2O to obtain the desired pure compound **18** as a white solid (37.4 mg, 92% yield). mp = 177-180 °C. ^1H NMR (360.13 MHz, DMSO- d_6) δ 2.39 (t, 2H, J = 7.1 Hz), 1.45 (q, 2H, J = 7.3 Hz), 1.24 (m, 2H), 1.11 (m, 2H), -0.07 (m, 2H, $-\text{CH}_2\text{-B}$). ^{13}C NMR (90.6 MHz, DMSO- d_6) δ 121.3, 32.3, 25.5, 25.2, 25.1, 16.6. ^{19}F (470.8 MHz, DMSO- d_6) δ -137.2. ^{11}B NMR (128.4 MHz, DMSO- d_6) δ 4.41. IR (neat): 2937, 2907, 2843, 2260,

1459, 1420, 1057, 961, 870 cm^{-1} . HRMS (m/z): calcd. for $\text{C}_6\text{H}_{10}\text{BF}_3\text{N}$. 164.0858 $[\text{M-K}^+]$; found, 164.0856.

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Current Data Parameters

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INSTRUM	spect
PROBHD	5 mm QNP 1H/1
PULPROG	zgpg30
TD	131072
SOLVENT	Aceton
NS	48
DS	4
SWH	100000.000 Hz
FIDRES	0.762939 Hz
AQ	0.6554100 sec
RG	11980.2
DW	5.000 usec
DE	6.00 usec
TE	300.0 K
D1	1.00000000 sec
D11	0.03000000 sec
D12	0.00002000 sec

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

NUC1	19F
P1	10.60 usec
PL1	-3.00 dB
SFO1	470.7801483 MHz

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

CPDPRG2	waltz16
NUC2	1H
PCPD2	95.00 usec
PL2	0.00 dB
PL12	26.00 dB
SFO2	500.3920016 MHz

F2 - Processing parameters

SI	65536
SF	470.8372320 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.00

1D NMR plot parameters

CX	20.00 cm
F1P	-80.000 ppm
F2P	-180.000 ppm

Current Data Parameters

NAME	ham-Br-OL
EXPNO	4
PROCNO	1

F2 - Acquisition Parameters

Date_	20060120
Time	20.55
INSTRUM	spect
PROBHD	5 mm BBO
PULPROG	zgpg30
TD	65536
SOLVENT	C6D6
NS	107
DS	2
SWH	25641.025 Hz
FIDRES	0.391251 Hz
AQ	1.2780020 sec
RG	8192
DW	19.500 usec
DE	6.00 usec
TE	300.0 K
D1	1.00000000 sec
d11	0.03000000 sec
d12	0.00002000 sec

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

NUC1	11B
P1	7.00 usec
PL1	2.00 dB
SFO1	128.3772130 MHz

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

CPDPRG2	waltz16
NUC2	1H
PCPD2	100.00 usec
PL2	120.00 dB
PL12	26.00 dB
PL13	28.00 dB
SFO2	400.1320007 MHz

F2 - Processing parameters

SI	32768
SF	128.377075 MHz
WDW	EM
SSB	0
LB	5.00 Hz
GB	0
PC	1.40

1D NMR plot parameters

CX	20.00 cm
F1P	40.000 ppm
F1	5135.11 Hz
F2P	-40.000 ppm
F2	-5135.11 Hz
PPMCM	4.00000 ppm/cm
HZCM	513.51080 Hz/cm

Current Data Parameters
DU /y
USER gam
NAME ham-1-DL
EXPRO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20060120
Time 20.21
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg30
TD 131072
SOLVENT Aceton
NS 25
DS 4
SWH 100000.000 Hz
FIDRES 0.762939 Hz
AQ 0.6554100 sec
RG 1280.2
DW 5.000 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec

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

***** CHANNEL f2 *****
CPOPRG2 waltz16
NUC2 1H
PCPD2 95.00 usec
PL2 0.00 dB
PL12 26.00 dB
SFO2 500.3920016 MHz

F2 - Processing parameters
SI 65536
SF 470.8372320 MHz
RGW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
F1P -80.000 ppm
F2P -180.000 ppm

Current Data Parameters
NAME ham-1-DL
EXPRO 4
PROCNO 1

F2 - Acquisition Parameters
Date_ 20060120
Time 21.05
INSTRUM spect
PROBHD 5 mm BBO
PULPROG zgpg
TD 65536
SOLVENT CDCl3
NS 118
DS 2
SWH 25641.025 Hz
FIDRES 0.391251 Hz
AQ 1.2780020 sec
RG 8192
DW 19.500 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
d11 0.03000000 sec
d12 0.00002000 sec

***** CHANNEL f1 *****
NUC1 11B
P1 7.00 usec
PL1 2.00 dB
SFO1 128.3772130 MHz

***** CHANNEL f2 *****
CPOPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 120.00 dB
PL12 26.00 dB
PL13 28.00 dB
SFO2 400.1320007 MHz

F2 - Processing parameters
SI 32768
SF 128.3777075 MHz
RGW BM
SSB 0
LB 5.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 20.00 cm
F1P 40.000 ppm
F1 5135.11 Hz
F2P -40.000 ppm
F2 -5135.11 Hz
PPMCH 4.00000 ppm/cm
NUC1 513.51080 Hz/cm

Current Data Parameters
DU /y
USER gam
NAME han-77-01.2
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20060112
Time 16.34
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpgnqn
TD 131072
SOLVENT Aceton
NS 40
DS 4
SWH 100000.000 Hz
FIDRES 0.762939 Hz
AQ 0.6554100 sec
RG 11585.2
DM 5.000 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec

***** CHANNEL f1 *****
NUC1 19F
P1 10.50 usec
PL1 -3.00 dB
SFO1 470.7901483 MHz

***** CHANNEL f2 *****
CPDPRG2 waltz16
NUC2 1H
PCPD2 95.00 usec
PL2 0.00 dB
PL12 26.00 dB
SFO2 500.3920016 MHz

F2 - Processing parameters
SI 65536
SF 470.8372320 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
F1P -80.000 ppm
F2P -180.000 ppm

Current Data Parameters
NAME han-124-01
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date_ 20060111
Time 15.06
INSTRUM spect
PROBHD 5 mm BBO

PULPROG zgpg
TD 65536
SOLVENT Tol
NS 100
DS 2
SWH 25641.025 Hz
FIDRES 0.391351 Hz
AQ 1.2780020 sec
RG 8192
DM 19.500 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
d11 0.03000000 sec
d12 0.00002000 sec

***** CHANNEL f1 *****
NUC1 11B
P1 7.00 usec
PL1 2.00 dB
SFO1 128.3772130 MHz

***** CHANNEL f2 *****
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 120.00 dB
PL12 26.00 dB
PL13 28.00 dB
SFO2 400.1320007 MHz

F2 - Processing parameters
SI 32768
SF 128.3777775 MHz
WDW EM
SSB 0
LB 5.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 20.00 cm
F1P 40.000 ppm
F1 5135.11 Hz
F2P -40.000 ppm
F2 -5135.11 Hz
PPMCM 4.00000 ppm/cm
HDCM 513.51080 Hz/cm

Current Data Parameters
NAME ham-16
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20050921
Time 12.12
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg30
TD 131072
SOLVENT C6D6
NS 201
DS 4
SWH 100000.000 Hz
FIDRES 0.762939 Hz
AQ 0.6554100 sec
RG 2048
DM 5.000 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec

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

***** CHANNEL f2 *****
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 0.00 dB
PL12 26.00 dB
SFO2 500.3920016 MHz

F2 - Processing parameters
SI 65536
SF 470.8372120 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
FIP -80.000 ppm
F1 -37666.98 Hz
F2P -180.000 ppm
F2 -84750.70 Hz
PPMCM 5.00000 ppm/cm
HZCM 2354.18604 Hz/cm

Current Data Parameters
NAME ham-130-GL
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date_ 20060112
Time 14.56
INSTRUM spect
PROBHD 5 mm BBO

PULPROG zgpg
TD 65536
SOLVENT Acetone
NS 200
DS 2
SWH 25641.025 Hz
FIDRES 0.391251 Hz
AQ 1.2780020 sec
RG 8192
DM 19.500 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
d11 0.03000000 sec
d12 0.00002000 sec

***** CHANNEL f1 *****
NUC1 11B
P1 8.00 usec
PL1 6.00 dB
SFO1 128.3772130 MHz

***** CHANNEL f2 *****
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 6.00 dB
PL12 21.00 dB
PL13 21.00 dB
SFO2 400.1320007 MHz

F2 - Processing parameters
SI 32768
SF 128.377075 MHz
WDW EM
SSB 0
LB 5.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 20.00 cm
FIP 40.000 ppm
F1 5135.11 Hz
F2P -40.000 ppm
F2 -5135.11 Hz
PPMCM 4.00000 ppm/cm
HZCM 513.51080 Hz/cm

Current Data Parameters
 DU /y
 USER gam
 NAME ham-68-OL
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20060119
 Time 11:46
 INSTRUM spect
 PROBHD 5 mm QNP 1H/1
 PULPROG zgpg30
 TD 131072
 SOLVENT Aceton
 NS 128
 DS 4
 SWH 100000.000 Hz
 FIDRES 0.762939 Hz
 AQ 0.6554100 sec
 RG 1290.2
 DM 5.000 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.00000000 sec
 D11 0.03000000 sec
 D12 0.00002000 sec

***** CHANNEL f1 *****
 NUC1 19F
 P1 10.00 usec
 PL1 -3.00 dB
 SFO1 470.7901483 MHz

***** CHANNEL f2 *****
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 95.00 usec
 PL2 0.00 dB
 PL12 26.00 dB
 SFO2 500.3920016 MHz

F2 - Processing parameters
 SI 65536
 SF 470.8372320 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 F1P -80.000 ppm
 F2P -180.000 ppm

Current Data Parameters
 NAME ham-68-OL
 EXPNO 4
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20060120
 Time 21:09
 INSTRUM spect
 PROBHD 5 mm BBO

PULPROG zgpg30
 TD 65536
 SOLVENT C6D6
 NS 107
 DS 2
 SWH 25641.025 Hz
 FIDRES 0.391251 Hz
 AQ 1.2780020 sec
 RG 8192
 DM 19.500 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.00000000 sec
 d11 0.03000000 sec
 d12 0.00002000 sec

***** CHANNEL f1 *****
 NUC1 11B
 P1 7.00 usec
 PL1 2.00 dB
 SFO1 128.3772130 MHz

***** CHANNEL f2 *****
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 100.00 usec
 PL2 120.00 dB
 PL12 26.00 dB
 PL13 28.00 dB
 SFO2 400.1320007 MHz

F2 - Processing parameters
 SI 32768
 SF 128.3777075 MHz
 WDW EM
 SSB 0
 LB 5.00 Hz
 GB 0
 PC 1.40

1D NMR plot parameters
 CX 20.00 cm
 F1P 40.000 ppm
 F1 5135.11 Hz
 F2P -40.000 ppm
 F2 -5135.11 Hz
 FPMCM 4.00000 ppm/cm
 HZCM 513.51080 Hz/cm

Current Data Parameters
 DU /y
 USER gam
 NAME han-85-KHC033
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20060128
 Time 12.25
 INSTRUM spect
 PROBHD 5 mm QNP 1H/1
 PULPROG zgpg30
 TD 131072
 SOLVENT Aceton
 NS 90
 DS 4
 SWH 100000.000 Hz
 FIDRES 0.762938 Hz
 AQ 0.6554100 sec
 RG 1290.2
 DW 5.000 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.00000000 sec
 D11 0.03000000 sec
 D12 0.00002000 sec

===== CHANNEL f1 =====
 NUC1 19F
 P1 10.60 usec
 PL1 -3.00 dB
 SF01 470.7901483 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 95.00 usec
 PL2 0.00 dB
 PL12 26.00 dB
 SF02 500.3920016 MHz

F2 - Processing parameters
 SI 65536
 SF 470.8372320 MHz
 WDM no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 F1P -90.000 ppm
 F2P -180.000 ppm

Current Data Parameters
 NAME han-84-OL
 EXPNO 5
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20060128
 Time 17.44
 INSTRUM spect
 PROBHD 5 mm BBO

PULPROG zgpg30
 TD 4096
 SOLVENT Tol
 NS 502
 DS 2
 SWH 25641.025 Hz
 FIDRES 6.260016 Hz
 AQ 0.0799220 sec
 RG 16384
 DW 19.500 usec
 DE 6.00 usec
 TE 300.0 K
 D1 0.20000000 sec
 d11 0.03000000 sec
 d12 0.00002000 sec

===== CHANNEL f1 =====
 NUC1 11B
 P1 7.00 usec
 PL1 2.00 dB
 SF01 128.3772130 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 100.00 usec
 PL2 120.00 dB
 PL12 26.00 dB
 PL13 28.00 dB
 SF02 400.1320007 MHz

F2 - Processing parameters
 SI 2048
 SF 128.3777068 MHz
 WDM RM
 SSB 0
 LB 5.00 Hz
 GB 0
 PC 1.40

1D NMR plot parameters
 CX 20.00 cm
 F1P 40.000 ppm
 F1 5135.11 Hz
 F2P -40.000 ppm
 F2 -5135.11 Hz
 PPMCH 4.00000 ppm/cm
 HZCH 513.51080 Hz/cm

Current Data Parameters
 DU /y
 USER gam
 NAME ham-106-1
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20051120
 Time 19.48
 INSTRUM spect
 PROBHD 5 mm QNP 1H/1
 PULPROG zgpg30
 TD 131072
 SOLVENT C6D6
 NS 101
 DS 4
 SWH 100000.000 Hz
 FIDRES 0.762539 Hz
 AQ 0.6554100 sec
 RG 1290.2
 DM 5.000 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.00000000 sec
 D11 0.03000000 sec
 D12 0.00020000 sec

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

***** CHANNEL f2 *****
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 100.00 usec
 PL2 0.00 dB
 PL12 26.00 dB
 SFO2 500.3820016 MHz

F2 - Processing parameters
 SI 65536
 SF 470.8372320 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 F1P -80.000 ppm
 F2P -180.000 ppm

Current Data Parameters
 NAME ham-106-GL
 EXPNO 4
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20060113
 Time 22.03
 INSTRUM spect
 PROBHD 5 mm BBO

PULPROG zgpg
 TD 65536
 SOLVENT Aceton
 NS 100
 DS 2
 SWH 25641.025 Hz
 FIDRES 0.391251 Hz
 AQ 1.2780020 sec
 RG 8192
 DM 19.500 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.00000000 sec
 d11 0.03000000 sec
 d12 0.00020000 sec

***** CHANNEL f1 *****
 NUC1 11B
 P1 7.00 usec
 PL1 2.00 dB
 SFO1 128.3772130 MHz

***** CHANNEL f2 *****
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 100.00 usec
 PL2 120.00 dB
 PL12 26.00 dB
 PL13 28.00 dB
 SFO2 400.1320007 MHz

F2 - Processing parameters
 SI 32768
 SF 128.377075 MHz
 WDW EM
 SSB 0
 LB 5.00 Hz
 GB 0
 PC 1.40

1D NMR plot parameters
 CX 20.00 cm
 F1P 40.000 ppm
 F1 5135.11 Hz
 F2P -40.000 ppm
 F2 -5135.11 Hz
 PPMCM 4.00000 ppm/cm
 HZCM 513.51080 Hz/cm

Current Data Parameters
 DU /y
 USER gam
 NAME ham-135-OL
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20051229
 Time 12.15
 INSTRUM spect
 PROBHD 5 mm QNP 1H/1
 PULPROG zgpg30
 TO 131072
 SOLVENT Aceton
 NS 56
 DS 4
 SWH 100000.000 Hz
 FIDRES 0.762939 Hz
 AQ 0.6554100 sec
 RG 1250.2
 DW 5.000 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.00000000 sec
 D11 0.03000000 sec
 D12 0.00020000 sec

===== CHANNEL f1 =====
 NUC1 19F
 P1 10.00 usec
 PL1 -3.00 dB
 SF01 470.7901483 MHz

===== CHANNEL f2 =====
 CPOPRG2 waltz16
 NUC2 1H
 PCPD2 95.00 usec
 PL2 0.00 dB
 PL12 26.00 dB
 SF02 500.3920016 MHz

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

1D NMR plot parameters
 CX 20.00 cm
 F1P -80.000 ppm
 F2P -180.000 ppm

Current Data Parameters
 NAME ham-135-OL
 EXPNO 4
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20051112
 Time 14.37
 INSTRUM spect
 PROBHD 5 mm BBO

PULPROG zgpg
 TO 65536
 SOLVENT Aceton
 NS 200
 DS 2
 SWH 25641.025 Hz
 FIDRES 0.391251 Hz
 AQ 1.2780020 sec
 RG 8192
 DW 19.500 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.00000000 sec
 d11 0.03000000 sec
 d12 0.00020000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 8.00 usec
 PL1 6.00 dB
 SF01 128.3772130 MHz

===== CHANNEL f2 =====
 CPOPRG2 waltz16
 NUC2 1H
 PCPD2 100.00 usec
 PL2 6.00 dB
 PL12 21.00 dB
 PL13 21.00 dB
 SF02 400.1320007 MHz

F2 - Processing parameters
 SI 32768
 SF 128.3777075 MHz
 WDM DM
 SSB 0
 LB 5.00 Hz
 GB 0
 PC 1.40

1D NMR plot parameters
 CX 20.00 cm
 F1P 40.000 ppm
 F1 5135.11 Hz
 F2P -40.000 ppm
 F2 -5135.11 Hz
 PPMCH 4.00000 ppm/cm
 HZCH 513.51080 Hz/cm

Current Data Parameters
 DU /y
 USER gam
 NAME han-38-OL
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20060111
 Time 11.14
 INSTRUM spect
 PROBHD 5 mm QNP 1H/1
 PULPROG zgpg30
 TD 131072
 SOLVENT C6D6
 NS 21
 DS 4
 SWH 100000.000 Hz
 FIDRES 0.762939 Hz
 AQ 0.6554100 sec
 RG 1290.2
 DM 5.000 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.00000000 sec
 D11 0.03000000 sec
 D12 0.00002000 sec

***** CHANNEL f1 *****
 NUC1 19F
 P1 10.60 usec
 PL1 -3.00 dB
 SFO1 470.7961463 MHz

***** CHANNEL f2 *****
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 100.00 usec
 PL2 0.00 dB
 PL12 26.00 dB
 SFO2 500.3920016 MHz

F2 - Processing parameters
 SI 65536
 SF 470.8372320 MHz
 MDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 F1P -80.000 ppm
 F2P -180.000 ppm

Current Data Parameters
 NAME han-38-OL
 EXPNO 4
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20060111
 Time 14.55
 INSTRUM spect
 PROBHD 5 mm BBO
 PULPROG zgpg30
 TD 65536
 SOLVENT Tol
 NS 200
 DS 2
 SWH 25641.025 Hz
 FIDRES 0.391251 Hz
 AQ 1.2780020 sec
 RG 8192
 DM 19.500 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.00000000 sec
 d11 0.03000000 sec
 d12 0.00002000 sec

***** CHANNEL f1 *****
 NUC1 13C
 P1 7.00 usec
 PL1 2.00 dB
 SFO1 125.7712130 MHz

***** CHANNEL f2 *****
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 100.00 usec
 PL2 120.00 dB
 PL12 26.00 dB
 PL13 28.00 dB
 SFO2 400.1320007 MHz

F2 - Processing parameters
 SI 32768
 SF 125.7777775 MHz
 MDW RM
 SSB 0
 LB 5.00 Hz
 GB 0
 PC 1.40

1D NMR plot parameters
 CX 20.00 cm
 F1P 40.000 ppm
 F1 5135.11 Hz
 F2P -40.000 ppm
 F2 -5135.11 Hz
 PPMCH 4.00000 ppm/cm
 HZCH 513.51080 Hz/cm

Current Data Parameters
DU /y
USER gm
NAME ham-101-0
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20051119
Time 19.01
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg30
TD 131072
SOLVENT C6D6
NS 110
DS 4
SWH 10000.000 Hz
FIDRES 0.762539 Hz
AQ 0.6554100 sec
RG 1024
OW 5.000 usec
DE 5.00 usec
TE 300.0 K
D1 1.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec

***** CHANNEL f1 *****
NUC1 13C
P1 10.50 usec
PL1 -3.00 dB
SFO1 470.7901483 MHz

***** CHANNEL f2 *****
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 0.00 dB
PL12 26.00 dB
SFO2 500.3520015 MHz

F2 - Processing parameters
SI 65536
SF 470.8372320 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
F1P -80.000 ppm
F2P -180.000 ppm

Current Data Parameters
NAME ham-101-OL
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date_ 20060113
Time 21.48
INSTRUM spect
PROBHD 5 mm BBO

PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 100
DS 2
SWH 25641.025 Hz
FIDRES 0.391251 Hz
AQ 1.2780020 sec
RG 8192
OW 19.500 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
d11 0.03000000 sec
d12 0.00002000 sec

***** CHANNEL f1 *****
NUC1 13C
P1 7.00 usec
PL1 2.00 dB
SFO1 128.3772130 MHz

***** CHANNEL f2 *****
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 120.00 dB
PL12 26.00 dB
PL13 28.00 dB
SFO2 400.1320007 MHz

F2 - Processing parameters
SI 32768
SF 128.3777775 MHz
WDW EM
SSB 0
LB 5.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 20.00 cm
F1P 40.000 ppm
F1 5135.11 Hz
F2P -40.000 ppm
F2 -5135.11 Hz
PPHCH 4.00000 ppm/cm
HZCM 513.51080 Hz/cm

Current Data Parameters

DU	/y
USER	gam
NAME	ham-000-DL
EXPNO	3
PROCNO	1

F2 - Acquisition Parameters

Date_	20051220
Time	9.59
INSTRUM	spect
PROBHD	5 mm QNP 1H/1
PULPROG	zgpg30gn
TD	131072
SOLVENT	Aceton
NS	128
DS	4
SWH	100000.000 Hz
FIDRES	0.762939 Hz
AQ	0.6554100 sec
RG	1250.2
DM	5.000 usec
DE	6.00 usec
TE	300.0 K
D1	1.00000000 sec
D11	0.03000000 sec
D12	0.00002000 sec

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

NUC1	13C
P1	19.60 usec
PL1	-3.00 dB
SFO1	470.7901483 MHz

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

CPDPRG2	waltz16
NUC2	1H
PCPD2	95.00 usec
PL2	0.00 dB
PL12	26.00 dB
SFO2	500.3920016 MHz

F2 - Processing parameters

SI	65536
SF	470.8372320 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.00

1D NMR plot parameters

CX	20.00 cm
F1P	-80.000 ppm
F2P	-180.000 ppm

Current Data Parameters

NAME	ham-102-OL
EXPNO	4
PROCNO	1

F2 - Acquisition Parameters

Date_	20060113
Time	21.42
INSTRUM	spect
PROBHD	5 mm BBO
PULPROG	zgpg30
TD	65536
SOLVENT	Aceton
NS	100
DS	2
SWH	25641.025 Hz
FIDRES	0.391251 Hz
AQ	1.2780020 sec
RG	8192
DM	19.500 usec
DE	6.00 usec
TE	300.0 K
D1	1.00000000 sec
d11	0.03000000 sec
d12	0.00002000 sec

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

NUC1	13C
P1	7.00 usec
PL1	2.00 dB
SFO1	128.3772139 MHz

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

CPDPRG2	waltz16
NUC2	1H
PCPD2	100.00 usec
PL2	120.00 dB
PL12	26.00 dB
PL13	28.00 dB
SFO2	400.1320007 MHz

F2 - Processing parameters

SI	32768
SF	128.3771075 MHz
WDW	EM
SSB	0
LB	5.00 Hz
GB	0
PC	1.40

1D NMR plot parameters

CX	20.00 cm
F1P	40.000 ppm
F1	5135.11 Hz
F2P	-40.000 ppm
F2	-5135.11 Hz
PPMCM	4.00000 ppm/cm
HZCM	513.51080 Hz/cm

Current Data Parameters
DU /y
USER gam
NAME ham-115-0
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20051127
Time 22.27
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg30
TD 131072
SOLVENT DMSO
NS 102
DS 4
SWH 100000.000 Hz
FIDRES 0.762939 Hz
AQ 0.6554100 sec
RG 1290.2
DM 5.000 usec
DE 5.00 usec
TE 300.0 K
D1 1.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec

===== CHANNEL f1 =====
NUC1 19F
P1 10.50 usec
PL1 -3.00 dB
SFO1 470.7901463 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 95.00 usec
PL2 0.00 dB
PL12 26.00 dB
SFO2 500.3520016 MHz

F2 - Processing parameters
SI 65536
SF 470.8372320 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
F1P -80.000 ppm
F2P -180.000 ppm

Current Data Parameters
NAME ham-142-0
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date_ 20060114
Time 12.18
INSTRUM spect
PROBHD 5 mm BBO

PULPROG zgpg
TD 65536
SOLVENT DMSO
NS 111
DS 2
SWH 25641.025 Hz
FIDRES 0.391251 Hz
AQ 1.2780020 sec
RG 8192
DM 19.500 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
d11 0.03000000 sec
d12 0.00002000 sec

===== CHANNEL f1 =====
NUC1 11B
P1 7.00 usec
PL1 2.00 dB
SFO1 128.3772130 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 120.00 dB
PL12 26.00 dB
PL13 28.00 dB
SFO2 400.1320007 MHz

F2 - Processing parameters
SI 32768
SF 128.3777075 MHz
WDW RM
SSB 0
LB 5.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 20.00 cm
F1P 40.000 ppm
F1 5135.11 Hz
F2P -40.000 ppm
F2 -5135.11 Hz
FPMCH 4.00000 ppm/cm
HSCN 513.51000 Hz/cm

Current Data Parameters
 DU /y
 USER gam
 NAME ham-142-OL
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20060130
 Time 9.46
 INSTRUM spect
 PROBHD 5 mm QNP 1H/1
 PULPROG zgpg30
 TD 131072
 SOLVENT DMSO
 NS 360
 DS 4
 SWH 100000.000 Hz
 FIDRES 0.762939 Hz
 AQ 0.6554100 sec
 RG 1250.2
 DM 5.000 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.00000000 sec
 D11 0.03000000 sec
 D12 0.00002000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 10.60 usec
 PL1 -3.00 dB
 SFO1 470.7901483 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 100.00 usec
 PL2 0.00 dB
 PL12 26.00 dB
 SFO2 500.3520016 MHz

F2 - Processing parameters
 SI 65536
 SF 470.8372320 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 F1P -80.000 ppm
 F2P -180.000 ppm

Current Data Parameters
 NAME ham-142-1
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20060114
 Time 17.14
 INSTRUM spect
 PROBHD 5 mm BBO

PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 50
 DS 2
 SWH 25641.025 Hz
 FIDRES 0.391251 Hz
 AQ 1.2780000 sec
 RG 8192
 DM 19.500 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.00000000 sec
 d11 0.03000000 sec
 d12 0.00002000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 7.00 usec
 PL1 2.00 dB
 SFO1 128.3772130 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 100.00 usec
 PL2 120.00 dB
 PL12 26.00 dB
 PL13 28.00 dB
 SFO2 400.1320007 MHz

F2 - Processing parameters
 SI 32768
 SF 128.3777075 MHz
 WDW DM
 SSB 0
 LB 5.00 Hz
 GB 0
 PC 1.40

1D NMR plot parameters
 CX 20.00 cm
 F1P 40.000 ppm
 F1 5135.11 Hz
 F2P -40.000 ppm
 F2 -5135.11 Hz
 PPMCN 4.00000 ppm/cm
 HSCN 513.51080 Hz/cm