



Supporting Information

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Expanding the [1,2]-Aryl Migration to the Synthesis of Substituted Indoles

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Supporting Information

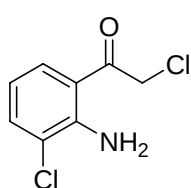
Experimental procedures, analytical and spectroscopic data for new compounds (30 pages).

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Experimental

General Methods. Reagents and solvents obtained from commercial suppliers were used without purification or drying unless otherwise noted. All reactions were conducted in standard RB-flasks under a nitrogen atmosphere. NMR spectra were obtained on Burkert DPX-400 and DPX-500 spectrometer. Flash column chromatography was performed employing 200-400 mesh silica gel (Aldrich) eluting with mixtures of hexanes and ethyl acetate. HPLC was performed on an Agilent 1100 series machine using a Agilent ZORBAX (Eclipse Plus C18) column (4.6 x 50 mm, 1.8 Micron, 600 Bar), 1.50 mL/min flowrate, 215 nm detection, 28 °C column temperature; mobile phase MeCN /0.1 wt% aqueous H₃PO₄ 10/90 ramp to 95/5 over 9 min and stay for 1 min.

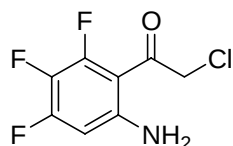
Acylation of anilines: A modified procedure of Sugasawa reaction ^[1] was used to react anilines with nitriles.



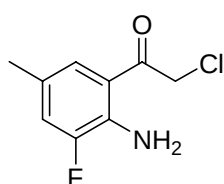
1-(2-Amino-3-chlorophenyl)-2-chloroethanone (3). 2-Chloroaniline (12.76 g, 100 mmol) and chloroacetonitrile (8.88 g, 250 mmol) were added sequentially to a mixture of AlCl₃ pellets (16.0 g, 120 mmol) and BCl₃ solution (1.0 M in dichloromethane, 120 mL, 120 mmol) with extra 60 mL dichloromethane cooled in ice bath. The cloudy solution was stirred for 0.5 h at room temperature before being heated at reflux for 14 h.

The reaction mixture was then cooled in ice bath, quenched with 2N HCl 150 mL, heated at reflux for 20 min, cooled, and extracted with dichloromethane (2 x 100 mL). The combined organic layers were dried over MgSO₄, concentrated, and chromatographed to give 1-(2-Amino-3-chlorophenyl)-2-chloroethanone (**3**, 13.05 g, 64%) as a bright yellow solid. mp 104-106 °C. ¹H NMR (500 MHz, CDCl₃): δ 7.61 (dd, *J* = 8.2, 1.2 Hz, 1H), 7.46 (dd, *J* = 7.8, 1.2 Hz, 1H), 6.85 (bs, 2H), 6.63 (m, 1H), 4.68 (s, 2H). ¹³C {¹H} NMR (125 MHz, CDCl₃): δ 192.3, 147.2, 134.8, 129.5, 121.0, 116.0, 115.5, 46.5. Anal. calcd (found) for C₈H₇Cl₂NO: C, 47.09 (46.95); H, 3.46 (3.29); N, 6.86 (6.78).

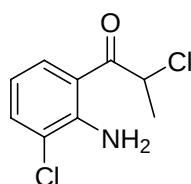
The remaining substituted 1-(2-aminophenyl)-2-chloroethanones were synthesized analogous to that employed in the synthesis of **3**.



1-(2-Amino-4,5,6-trifluorophenyl)-2-chloroethanone (6d): white solid, mp 105-106 °C. ¹H NMR (500 MHz, CDCl₃): δ 6.39 (bs, 2H), 6.28 (ddd, *J* = 11.6, 6.0, 2.3 Hz, 1H), 4.68 (d, *J* = 4.7 Hz, 2H). ¹³C {¹H} NMR (125 MHz, CDCl₃): δ 190.1 (m), 156.5 (dd, *J* = 11.1, 6.8 Hz), 154.5 (dd, *J* = 11.1, 3.2 Hz), 153.8 (dd, *J* = 10.8, 6.5 Hz), 151.8 (dd, *J* = 11.8, 6.5 Hz), 148.0 (dd, *J* = 7.4, 12.9 Hz), 132.4 (m), 130.5 (dd, *J* = 17.2, 16.0 Hz), 103.0 (dt, *J* = 14.2, 2.5 Hz), 99.4 (ddd, *J* = 20.3, 3.1, 1.2 Hz), 50.6 (d, *J* = 18.4 Hz). ¹⁹F {¹H} NMR (470 MHz, CDCl₃): δ -124.7 (dd, *J* = 22.9, 13.7 Hz), -128.9 (dd, *J* = 22.9, 15.3 Hz), -175.6 (m). Anal. calcd (found) for C₈H₅ClF₃NO: C, 42.98 (42.64); H, 2.25 (2.09); N, 6.26 (6.20).



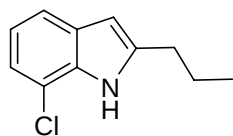
1-(2-Amino-3-fluoro-5-methylphenyl)-2-chloroethanone (6f): yellow solid, mp 98-91 °C. ¹H NMR (500 MHz, CDCl₃): δ 7.21 (s, 1H), 7.01 (dd, *J* = 11.9, 1.9 Hz, 1H), 5.99 (bs, 2H), 4.67 (s, 2H), 2.27 (s, 3H). ¹³C {¹H} NMR (100 MHz, CDCl₃): δ 192.2 (d, *J* = 2.4 Hz), 152.4, 150.5, 138.2 (d, *J* = 14.2 Hz), 125.2 (d, *J* = 3.0 Hz), 124.3 (d, *J* = 6.7 Hz), 120.5 (d, *J* = 17.8 Hz), 116.7 (d, *J* = 4.3 Hz), 46.6, 20.5 (d, *J* = 1.8 Hz). ¹⁹F {¹H} NMR (470 MHz, CDCl₃): δ -136.4. Anal. calcd (found) for C₉H₅ClFNO: C, 53.61 (53.80); H, 4.50 (4.37); N, 6.95 (6.83).



1-(2-Amino-3-chlorophenyl)-2-chloropropanone (8): yellow solid, mp 54-55 °C. ¹H NMR (500 MHz, CDCl₃): δ 7.75 (dd, *J* = 8.2, 1.2 Hz, 1H), 7.47 (dd, *J* = 7.7, 1.3 Hz, 1H), 6.89 (bs, 2H), 6.65 (m, 1H), 5.30 (q, *J* = 6.6 Hz, 1H), 1.74 (d, *J* = 6.6 Hz, 3H). ¹³C {¹H} NMR (125 MHz, CDCl₃): δ 192.3, 147.2, 134.8, 129.5, 121.0, 116.0, 115.5, 46.5.

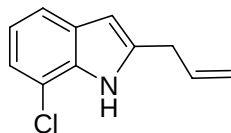
[1] T. Sugasawa, T. Toyoda, M. Adachi, K. Sasakura, *J. Am. Chem. Soc.* **1978**, *100*, 4842.

NMR (125 MHz, CDCl₃): δ 195.0, 147.7, 134.6, 129.8, 121.0, 115.7, 115.3, 53.0, 20.3. Anal. calcd (found) for C₉H₉Cl₂NO: C, 49.57 (49.35); H, 4.16 (4.07); N, 6.42 (6.35).

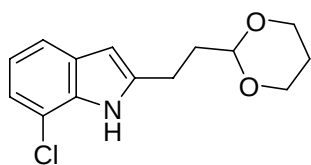


7-Chloro-2-propylindole (5a). To a solution of 1-(2-Amino-3-chlorophenyl)-2-chloroethanone (**3**) (204mg, 1.00 mmol) in 2.0 mL toluene at -10 °C was added dropwise a solution of propylmagnesium chloride (2.0M in diethyl ether, 1.25 mL, 2.50 mmol). The reaction was kept <10 °C during addition and stirred in cold bath for 15 min before removal of the bath. After 20 min at room temperature, the mixture was quenched with diluted aqueous NH₄Cl, extracted with MTBE, washed with brine, and dried over MgSO₄. After concentration, the crude residue was chromatographed to give 7-chloro-2-propylindole (**5**, 157 mg, 81%) as a yellow oil. ¹H NMR (500 MHz, CDCl₃): δ 8.08 (bs, 1H), 7.45 (d, *J* = 7.9 Hz, 1H), 7.14 (d, *J* = 7.6 Hz, 1H), 7.03 (m, 1H), 6.31 (s, 1H), 2.78 (t, *J* = 7.5 Hz, 2H), 1.80 (m, 2H), 1.05 (t, *J* = 7.4 Hz, 3H). ¹³C {¹H} NMR (125 MHz, CDCl₃): δ 140.7, 133.1, 130.3, 120.4, 120.3, 118.4, 115.8, 100.7, 30.3, 22.4, 13.9. HRMS calcd (found) for C₁₁H₁₃ClN (M+H)⁺: 194.0737 (194.0726).

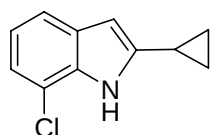
The remaining indoles were synthesized analogous to that employed in the synthesis of **5a**.



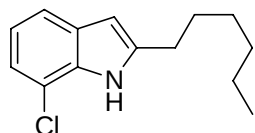
2-Allyl-7-chloroindole (5b): pale yellow oil. ¹H NMR (500 MHz, CDCl₃): δ 8.13 (bs, 1H), 7.49 (d, *J* = 7.7 Hz, 1H), 7.18 (dd, *J* = 7.6, 0.8 Hz, 1H), 7.06 (t, *J* = 7.8 Hz, 1H), 6.37 (m, 1H), 6.06 (ddt, *J* = 17.0, 10.1, 6.7 Hz, 1H), 5.28 (m, 2H), 3.58 (m, 2H). ¹³C {¹H} NMR (125 MHz, CDCl₃): δ 137.9, 134.4, 133.4, 130.3, 120.7, 120.5, 118.6, 117.7, 116.0, 101.4, 32.8. HRMS calcd (found) for C₁₁H₁₁ClN (M+H)⁺: 192.0580 (192.0573).



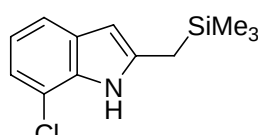
7-Chloro-2-(2-[1,3]-dioxan-2-ylethyl)indole (5c): pale yellow oil; ¹H NMR (400 MHz, CDCl₃): δ 1.41 (m, 1H), 2.05 (m, 2H), 2.20 (m, 1H), 2.95 (t, *J* = 7.1 Hz, 2H), 3.82 (m, 2H), 4.20 (m, 2H), 4.66 (t, *J* = 4.8 Hz, 1H), 6.27 (d, *J* = 1.8 Hz, 1H), 6.99 (t, *J* = 7.7 Hz, 1H), 7.11 (d, *J* = 7.5 Hz, 1H), 7.42 (d, *J* = 7.7 Hz, 1H), 8.72 (br s, 1H). ¹³C NMR (100 MHz, CDCl₃): δ 140.1, 133.2, 130.2, 120.2, 120.2, 118.4, 115.9, 100.2, 100.5, 67.0, 34.1, 25.7, 22.2. HRMS calcd (found) for C₁₄H₁₇ClNO₂ (M+H)⁺: 266.0948 (266.0954).



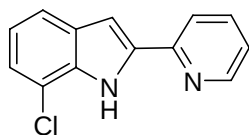
7-Chloro-2-cyclopropylindole (5d): pale yellow oil. ¹H NMR (400 MHz, CDCl₃): δ 8.16 (bs, 1H), 7.41 (d, *J* = 7.8 Hz, 1H), 7.12 (d, *J* = 7.4 Hz, 1H), 7.01 (t, *J* = 7.9 Hz, 1H), 6.20 (d, *J* = 2.3 Hz, 1H), 2.00 (tt, *J* = 5.1, 3.3 Hz, 1H), 1.02 (m, 2H), 0.82 (m, 2H). ¹³C {¹H} NMR (100 MHz, CDCl₃): δ 142.5, 132.9, 130.0, 120.4, 120.3, 118.2, 115.5, 98.6, 8.7, 7.4. Anal. calcd (found) for C₁₁H₁₀ClN: C, 68.93 (68.77); H, 5.26 (5.24); N, 7.31 (7.14).



7-Chloro-2-hexan-1-ylindole (5e): pale yellow oil. ¹H NMR (400 MHz, CDCl₃): δ 0.93 (m, 3H), 1.38 (m, 6H), 1.74 (m, 2H), 2.79 (t, *J* = 7.7 Hz, 2H), 6.30 (m, 1H), 7.01 (m, 1H), 7.12 (m, 1H), 7.44 (m, 1H), 8.06 (br s). ¹³C NMR (125 MHz, CDCl₃): δ 140.9, 133.1, 130.3, 120.4, 120.3, 118.3, 115.8, 100.5, 31.6, 29.1, 29.0, 28.3, 22.7, 14.1. HRMS calcd (found) for C₁₄H₁₉ClN (M+H)⁺: 236.1206 (236.1198).

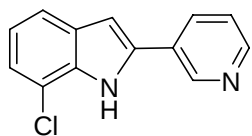


2-Trimethylsilylmethylindole (5f): pale yellow oil. ¹H NMR (400 MHz, CDCl₃): δ 0.11 (s, 9H), 2.21 (s, 2H), 6.11 (m, 1H), 6.98 (m, 1H), 7.06 (m, 1H), 7.37 (m, 1H), 7.85 (br s, 1H). ¹³C NMR (125 MHz, CDCl₃): δ 138.8, 132.9, 131.0, 120.3, 119.6, 117.6, 115.4, 99.7, 19.1, -1.8. HRMS calcd (found) for C₁₂H₁₈ClNSi (M+H)⁺: 238.0819 (238.0823).

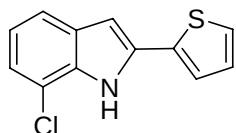


7-Chloro-2-pyridin-2-ylindole (5h): pale yellow solid, mp 118-120 °C. ¹H NMR (400 MHz, CDCl₃): δ 9.68 (bs, 1H), 8.62 (m, 1H), 7.79 (m, 1H), 7.73 (td, *J* = 7.3, 1.7 Hz, 1H), 7.55 (d, *J* = 7.9 Hz, 1H), 7.21 (m, 2H), 7.06 (t, *J* = 7.8 Hz, 1H), 7.04 (d,

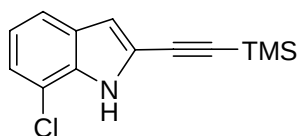
$J = 2.3$ Hz, 1H). ^{13}C $\{^1\text{H}\}$ NMR (100 MHz, CDCl_3): δ 149.7, 149.2, 137.3, 136.5, 133.8, 130.4, 122.4, 122.3, 120.8, 119.8, 119.6, 116.8, 101.1. HRMS calcd (found) for $\text{C}_{13}\text{H}_{10}\text{ClN}_2$ ($\text{M}+\text{H}$) $^+$: 229.0533 (229.0539).



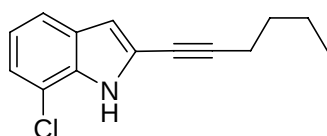
7-Chloro-2-pyridin-3-ylindole (5i): white solid, mp 207-209 °C. ^1H NMR (400 MHz, CDCl_3 & CD_3COD): δ 8.93 (dd, $J = 2.3, 0.7$ Hz, 1H), 8.40 (dd, $J = 5.0, 1.5$ Hz, 1H), 8.13 (dt, $J = 8.0, 2.0$ Hz, 1H), 7.43 (m, 1H), 7.40 (m, 1H), 7.10 (dd, $J = 7.6, 1.0$ Hz, 1H), 6.95 (t, $J = 7.7$ Hz, 1H), 6.84 (s, 1H). ^{13}C $\{^1\text{H}\}$ NMR (100 MHz, CDCl_3 & CD_3COD): δ 146.7, 145.3, 135.1, 135.0, 134.8, 130.5, 129.6, 124.7, 122.6, 121.1, 119.5, 117.0, 102.4. HRMS calcd (found) for $\text{C}_{13}\text{H}_{10}\text{ClN}_2$ ($\text{M}+\text{H}$) $^+$: 229.0533 (229.0528).



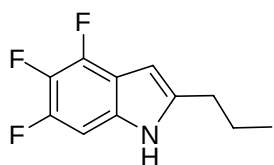
7-Chloro-2-thien-2-ylindole (5j): pale yellow solid, mp 86-88 °C. ^1H NMR (500 MHz, CDCl_3): δ 8.38 (bs, 1H), 7.52 (d, $J = 7.9$ Hz, 1H), 7.34 (m, 2H), 7.22 (dd, $J = 7.6, 0.6$ Hz, 1H), 7.12 (dd, $J = 5.0, 3.7$ Hz, 1H), 7.07 (t, $J = 7.8$ Hz, 1H), 6.77 (d, $J = 2.3$ Hz, 1H). ^{13}C $\{^1\text{H}\}$ NMR (125 MHz, CDCl_3): δ 134.9, 133.8, 133.1, 130.5, 128.0, 125.2, 123.6, 121.8, 121.2, 119.1, 116.2, 101.2. Anal. calcd (found) for $\text{C}_{12}\text{H}_8\text{ClNS}$: C, 61.67 (61.34); H, 3.45 (3.39); N, 5.99 (5.81).



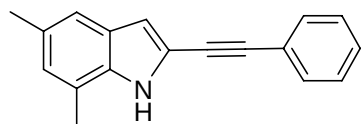
7-Chloro-2-(2-trimethylsilylacety-1-yl)indole (5k): white solid, mp 62-64 °C. ^1H NMR (400 MHz, CDCl_3): δ 8.39 (bs, 1H), 7.48 (dd, $J = 8.0, 0.5$ Hz, 1H), 7.24 (d, $J = 7.6$ Hz, 1H), 7.06 (t, $J = 7.9$ Hz, 1H), 6.81 (d, $J = 2.2$ Hz, 1H), 0.31 (s, 9H). ^{13}C $\{^1\text{H}\}$ NMR (100 MHz, CDCl_3): δ 133.1, 128.7, 122.7, 121.1, 119.4, 119.3, 116.1, 109.8, 99.2, 96.1, -0.3. Anal. calcd (found) for $\text{C}_{13}\text{H}_{14}\text{ClNSi}$: C, 63.01 (63.20); H, 5.69 (5.88); N, 5.65 (5.44).



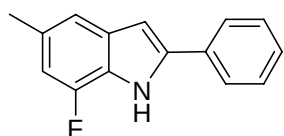
7-Chloro-2-hexyn-1-ylindole (5l): pale yellow oil. ^1H NMR (500 MHz, CDCl_3): δ 8.33, (bs, 1H), 7.48 (dd, $J = 8.0, 0.4$ Hz, 1H), 7.22 (dd, $J = 7.6, 0.7$ Hz, 1H), 7.06 (td, $J = 7.9, 1.1$ Hz, 1H), 6.71 (m, 1H), 2.50 (t, $J = 7.1$ Hz, 2H), 1.65 (m, 2H), 1.43 (m, 2H), 1.00 (t, $J = 7.3$ Hz, 3H). ^{13}C $\{^1\text{H}\}$ NMR (125 MHz, CDCl_3): δ 133.0, 129.2, 122.2, 121.0, 120.5, 119.2, 116.0, 108.2, 94.7, 72.5, 30.6, 22.1, 19.3, 13.6. HRMS calcd (found) for $\text{C}_{14}\text{H}_{15}\text{ClN}$ ($\text{M}+\text{H}$) $^+$: 232.0893 (232.0900).



4,5,6-Trifluoro-2-propylindole (7d): light brown oil. ^1H NMR (400 MHz, CDCl_3): δ 7.91 (bs, 1H), 6.88 (m, 1H), 6.31 (m, 1H), 2.71 (t, $J = 7.5$ Hz, 2H), 1.75 (m, 2H), 1.02 (t, $J = 7.4$ Hz, 3H). ^{13}C $\{^1\text{H}\}$ NMR (100 MHz, CDCl_3): δ 148.9 (dd, $J = 12.8, 2.4$ Hz), 146.5 (dd, $J = 12.8, 2.4$ Hz), 144.2 (dd, $J = 11.2, 2.8$ Hz), 141.7 (dd, $J = 11.2, 5.6$ Hz), 141.2 (d, $J = 3.2$ Hz), 136.0 (dd, $J = 17.6, 14.4$ Hz), 133.6 (dd, $J = 17.6, 14.4$ Hz), 130.6 (t, $J = 12.8$ Hz), 114.2 (d, $J = 18.4$ Hz), 95.7 (d, $J = 4.8$ Hz), 93.6 (dd, $J = 21.7, 4.0$ Hz), 30.0, 22.1, 13.6. ^{19}F $\{^1\text{H}\}$ NMR (376 MHz, CDCl_3): δ -144.3 (d, $J = 20.7$ Hz), -146.3 (d, $J = 20.7$ Hz), -174.1 (m); HRMS calcd (found) for $\text{C}_{11}\text{H}_{11}\text{F}_3\text{N}$ ($\text{M}+\text{H}$) $^+$: 214.0844 (214.0837).

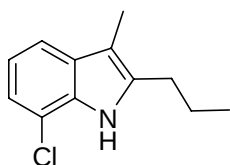


5,7-Dimethyl-2-phenylethynylindole (7e): light brown oil. ^1H NMR (500 MHz, CDCl_3): δ 8.15 (bs, 1H), 7.62 (m, 2H), 7.43 (m, 3H), 7.30 (s, 1H), 6.94 (s, 1H), 6.84 (d, $J = 2.0$ Hz, 1H), 2.49 (s, 3H), 2.48 (s, 3H). ^{13}C $\{^1\text{H}\}$ NMR (125 MHz, CDCl_3): δ 134.3, 131.5, 130.1, 128.6, 128.5, 127.7, 125.9, 122.8, 119.7, 118.5, 118.1, 109.0, 92.4, 82.3, 21.4, 16.6. HRMS calcd (found) for $\text{C}_{18}\text{H}_{16}\text{N}$ ($\text{M}+\text{H}$) $^+$: 246.1283 (246.1278).

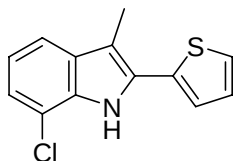


7-Fluoro-5-methyl-2-phenylindole (7f): white solid, mp 145-147 °C. ^1H NMR (500 MHz, CDCl_3): δ 8.37 (bs, 1H), 7.68 (d, $J = 7.2$ Hz, 2H), 7.47 (t, $J = 7.7$ Hz, 2H), 7.37 (t, $J = 7.4$ Hz, 1H), 7.21 (s, 1H), 6.79 (m, 2H), 2.47 (s, 3H). ^{13}C $\{^1\text{H}\}$

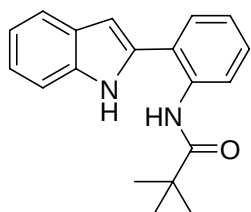
NMR (125 MHz, CDCl₃): δ 149.0 (d, J = 243.0 Hz), 138.8, 132.9 (d, J = 4.9 Hz), 132.0, 130.5 (d, J = 5.6 Hz), 129.1, 128.0, 125.2, 123.3 (d, J = 12.9 Hz), 115.9 (d, J = 3.1 Hz), 108.7 (d, J = 16.0 Hz), 100.1 (d, J = 2.4 Hz), 21.5. ¹⁹F {¹H} NMR (470 MHz, CDCl₃): δ -136.5. Anal. calcd (found) for C₁₅H₁₂FN: C, 79.98 (79.71); H, 5.37 (5.32); N, 6.22 (6.06).



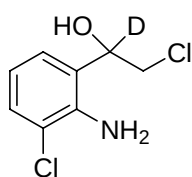
7-Chloro-3-methyl-2-propylindole (9a): pale yellow oil. ¹H NMR (500 MHz, CDCl₃): δ 7.95 (bs, 1H), 7.46 (d, J = 7.9 Hz, 1H), 7.20 (dd, J = 7.5, 0.6 Hz, 1H), 7.10 (t, J = 7.7 Hz, 1H), 2.77 (t, J = 7.5 Hz, 2H), 2.31 (s, 3H), 1.77 (m, 2H), 1.06 (t, J = 7.4 Hz, 3H). ¹³C {¹H} NMR (125 MHz, CDCl₃): δ 136.1, 132.4, 131.0, 120.4, 119.8, 116.8, 115.8, 108.2, 28.2, 23.0, 13.9, 8.7. HRMS calcd (found) for C₁₂H₁₅ClN (M+H)⁺: 208.0893 (208.0889).



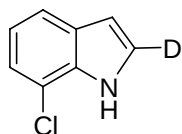
7-Chloro-3-methyl-2-thien-2-ylindole (9b): off-white solid; mp 111-112 °C; ¹H NMR (400 MHz, CDCl₃): δ 2.49 (s, 3H), 7.08 (m, 1H), 7.18 (m, 2H), 7.30 (m, 1H), 7.40 (m, 1H), 7.48 (d, J = 7.9 Hz, 1H), 8.17 (br s, 1H); ¹³C NMR (125 MHz, CDCl₃): δ 134.6, 133.0, 131.3, 129.2, 127.7, 125.4, 124.7, 121.9, 120.5, 117.6, 116.0, 110.4, 10.0. HRMS calcd (found) for C₁₃H₁₁ClNS (M+H)⁺: 248.0301 (248.0292).



2-(N-trimethylacetamido-2-aminophenyl)indole (15): pale brown oil; ¹H NMR (500 MHz, CDCl₃): δ 1.22 (s, 9H), 6.65 (s, 1H), 7.20 (m, 2H), 7.26 (m, 1H), 7.39 (m, 1H), 7.45 (m, 2H), 7.68 (d, J = 7.9 Hz, 1H), 8.22 (br s, 1H), 8.39 (d, J = 7.9 Hz, 1H), 8.44 (br s, 1H). ¹³C NMR (125 MHz, CDCl₃): δ 177.2, 136.6, 135.8, 134.2, 129.3, 128.7, 124.3, 123.7, 122.8, 121.7, 120.7, 120.6, 120.5, 111.1, 102.6, 39.9, 27.5. HRMS calcd (found) for C₁₉H₂₁N₂O (M+H)⁺: 293.1654 (293.1660).



1-(2-Amino-3-chlorophenyl)-2-chloro-1-D-ethan-1-ol (16). To a solution of 1-(2-amino-3-chlorophenyl)-2-chloroethanone (**3**, 1.02 g, 5.0 mmol) in 1,4-dioxane (9.0 mL) and water (1.0 mL) was added NaBD₄ (256 mg, 6.0 mmol) at room temperature, aged for 1 h, quenched with saturated NH₄Cl, extracted with MTBE, washed with brine, and dried over MgSO₄. After concentration, the crude residue was chromatographed to give alcohol **16** (0.78g, 75%) as a white solid. mp 61-63 °C. ¹H NMR (500 MHz, CDCl₃): δ 7.24 (dd, J = 7.9, 1.5 Hz, 1H), 6.97 (dd, J = 7.7, 1.4 Hz, 1H), 6.66 (m, 1H), 4.01 (d, J = 11.3 Hz, 1H), 3.74 (d, J = 11.3 Hz, 1H). ¹³C {¹H} NMR (125 MHz, CDCl₃): δ 142.0, 129.6, 126.8, 123.6, 120.9, 118.1, 74.6 (t, J = 22.5 Hz), 47.8. HRMS calcd (found) for C₈H₉DCl₂NO (M+H)⁺: 207.0202 (207.0201).



7-Chloro-2-D-indole (17). To a solution of 1-(2-amino-3-chlorophenyl)-2-chloro-1-D-ethan-1-ol (**16**, 207 mg, 1.0 mmol) in THF (2.0 mL) cooled at -10 °C was added *i*PrMgCl (2.0 M in THF, 1.25 mL, 2.5 mmol), warmed to room temperature, aged for 1 h, quenched with saturated NH₄Cl, extracted with MTBE, washed with brine, and dried over MgSO₄. After concentration, the crude residue was chromatographed to give indole **17** (105 mg, 69%) as a white solid. mp 52-54 °C. ¹H NMR (500 MHz, CDCl₃): δ 8.35, 7.61 (d, J = 7.9 Hz, 1H), 7.27 (dd, J = 7.6, 0.9 Hz, 1H), 7.12 (t, J = 7.8 Hz, 1H), 6.65 (d, J = 2.2 Hz, 1H). ¹³C {¹H} NMR (125 MHz, CDCl₃): δ 133.2, 129.4, 124.6 (t, J = 28.0 Hz), 121.4, 120.7, 119.4, 116.7, 103.6. HRMS calcd (found) for C₈H₆DCIN (M+H)⁺: 153.0330 (153.0325).

1-(2-Amino-3-chlorophenyl)-2-chloroethanone (3).

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Current Data Parameters
NAME          2372660265
EXPNO         1
PROCNO        1
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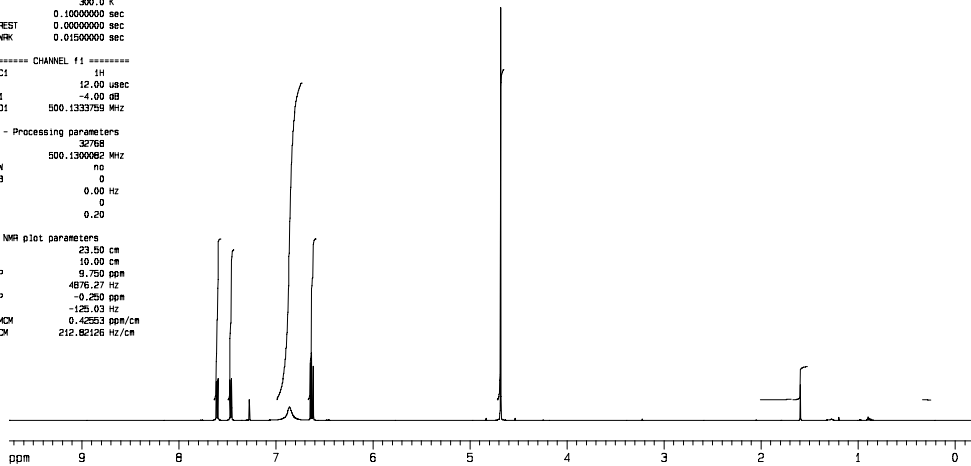
F2 - Acquisition Parameters
Date_          20070621
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INSTRUM       spect
PROBHD        5 mm QNP 1H/13
PULPROG       zg30
TD            65536
SOLVENT       CDCl3
NS            40
DS            4
SWH           13020.833 Hz
FIDRES       0.199682 Hz
AQ           2.5166323 sec
RG           181
DE           38.400 usec
DM           6.00 usec
TE           300.0 K
D1           0.10000000 sec
MCREST       0.00000000 sec
MCKRG       0.01500000 sec

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```
***** CHANNEL f1 *****
NUC1          1H
P1            12.00 usec
PL1           -4.00 dB
SF01         500.1333759 MHz
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F2 - Processing parameters
SI              32768
SF             500.1300082 MHz
WDW             no
SSB             0
LB             0.00 Hz
GB             0
PC             0.20
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1D NMR plot parameters	
CX	23.50 cm
CY	10.00 cm
F1P	9.750 ppm
F1	4876.27 Hz
F2P	-0.250 ppm
F2	-125.03 Hz
PPMCM	0.42553 ppm/cm
HZCM	212.82126 Hz/cm



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Current Data Parameters
NAME          237266026S
EXPNO         2
PROCNO        1
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F2 - Acquisition Parameters
Date_      20070621
Time       14.10
INSTRUM    spect
PROBHD     5 mm GNP 1H/13
PULPROG    zgpg
TD          131072
SOLVENT     CDCl3
NS          424
DS          4
SWH         40322.582 Hz
FIDRES     0.307637 Hz
AQ         1.6253428 sec
RG          8192
AW         12.400 usec
DE         6.00 usec
TE          300.0 K
d1          0.10000000 sec
d11         0.03000000 sec
MCREST     0.00000000 sec
MCKWAK     0.01500000 sec

```

```
***** CHANNEL f1 *****
NUC1          13C
P1             2.50 use
PL1            0.00 dB
SFQ1          125.7703643 MHz
```

```

===== CHANNEL f2 =====
CPOPRG2      waltz16
NUC2          1H
PCPD2        80.00 use
PL2          11.50 dB
PL12         11.50 dB
SF02         500.1325006 MHz

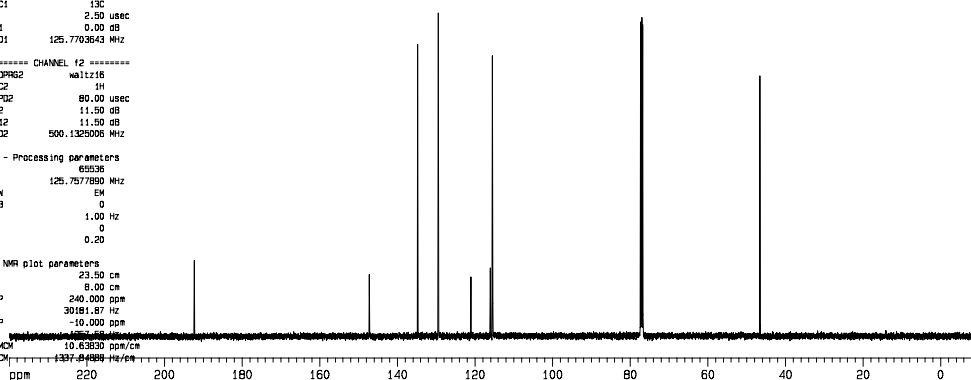
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F2 - Processing parameters
SI          65536
SF          125.7577890 MHz
WDW          EM
SSB          0
LB          1.00 Hz
GB          0
PC          0.20
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1D NMR plot parameters

CX	23.50 cm
CY	8.00 cm
F1P	240.000 ppm
F1	30181.87 Hz
F2P	-10.000 ppm
F2	-30181.87 Hz
PPMCM	10.63830 ppm/cm
HZCM	1337.84889 Hz/cm

ppm 220



7-Chloro-2-propylindole (5a).

Current Data Parameters
NAME 0270494002b
EXPNO 1
PROCNO 1

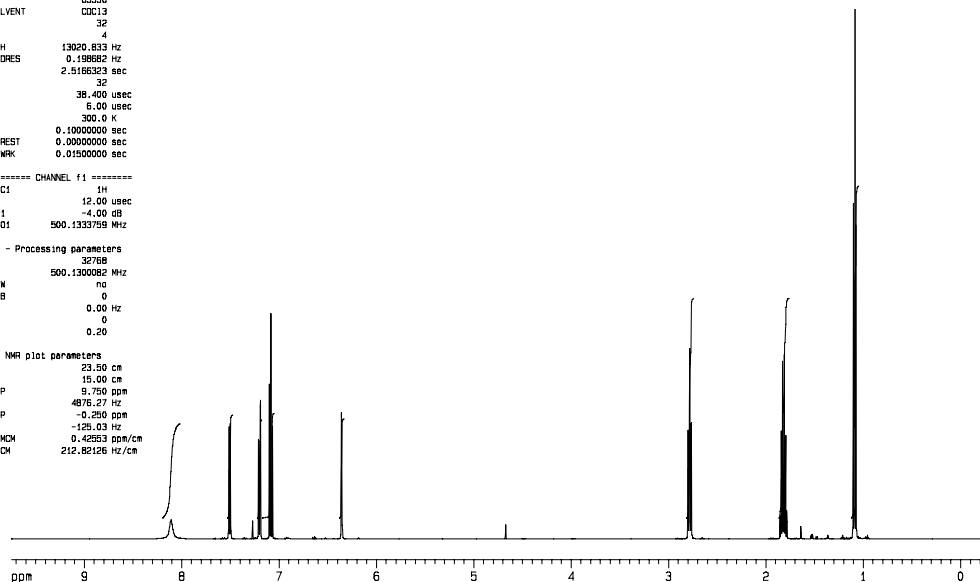
nmr500c h-1
02704940014F/CDC13

F2 - Acquisition Parameters
Date_ 20070725
Time 12.05
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 32
DS 4
SWH 13020.833 Hz
FIDRES 0.198682 Hz
AQ 2.5166323 sec
RG 32
DM 38.400 usec
DE 6.00 usec
TE 300.0 K
D1 0.10000000 sec
MCREST 0.00000000 sec
MCNRAK 0.01500000 sec

***** CHANNEL f1 *****
NUC1 1H
P1 12.00 usec
PL1 -4.00 dB
SFO1 500.133755 MHz

F2 - Processing parameters
SI 32768
SF 500.130082 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 0.20

1D NMR plot parameters
CX 23.50 cm
CY 15.00 cm
F1P 9.750 ppm
F1 4676.27 Hz
F2P -0.250 ppm
F2 -125.03 Hz
PRMDH 0.42653 ppm/cm
HZDM 212.62126 Hz/cm



Current Data Parameters
NAME 0270494002b
EXPNO 2
PROCNO 1

c-13 nmr500c
02704940014F/CDC13

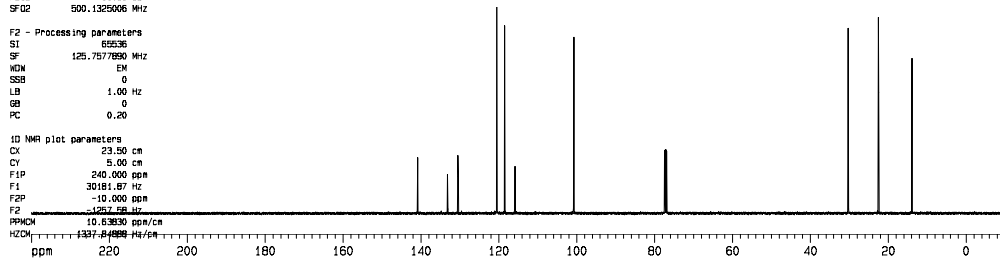
F2 - Acquisition Parameters
Date_ 20070725
Time 12.10
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 131072
SOLVENT CDC13
NS 169
DS 4
SWH 40322.582 Hz
FIDRES 0.307637 Hz
AQ 1.6253428 sec
RG 8192
DM 12.400 usec
DE 6.00 usec
TE 300.0 K
D1 0.15000000 sec
d11 0.03000000 sec
MCREST 0.00000000 sec
MCNRAK 0.01500000 sec

***** CHANNEL f1 *****
NUC1 13C
P1 2.50 usec
PL1 0.00 dB
SFO1 125.7703643 MHz

***** CHANNEL f2 *****
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 11.50 dB
PL12 11.50 dB
SFO2 500.1325006 MHz

F2 - Processing parameters
SI 65536
SF 125.7577890 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 0.20

1D NMR plot parameters
CX 23.50 cm
CY 5.00 cm
F1P 240.000 ppm
F1 30181.87 Hz
F2P -10.000 ppm
F2 -1257.58 Hz
PRMDH 10.63630 ppm/cm
HZDM 1337.84988 Hz/cm



2-Allyl-7-chloroindole (5b).

Current Data Parameters
NAME 02704940025F
EXPNO 1
PROCNO 1

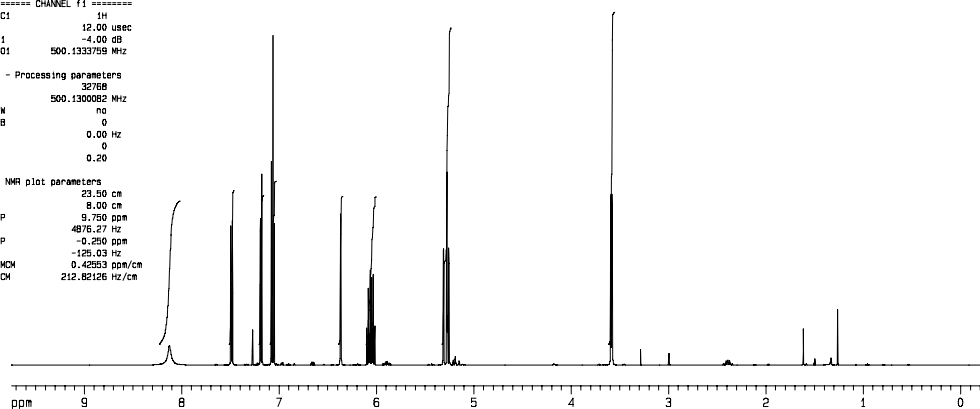
nmr500c h-1
02704940014F/CDC13

F2 - Acquisition Parameters
Date_ 20070817
Time 17.47
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 32
DS 4
SWH 13020.833 Hz
FIDRES 0.198682 Hz
AQ 2.5166323 sec
RG 80.6
DW 38.400 usec
DE 6.00 usec
TE 300.0 K
D1 0.10000000 sec
MCREST 0.00000000 sec
MCWPK 0.01500000 sec

***** CHANNEL f1 *****
NUC1 1H
P1 12.00 usec
PL1 -4.00 dB
SFO1 500.1333759 MHz

F2 - Processing parameters
SI 32768
SF 500.1300082 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 0.20

1D NMR plot parameters
CX 23.50 cm
CY 8.00 cm
F1P 9.750 ppm
F1 4876.27 Hz
F2P -0.250 ppm
F2 -125.03 Hz
PCHM 0.42553 ppm/cm
HZCM 212.82126 Hz/cm



Current Data Parameters
NAME 02704940025F
EXPNO 2
PROCNO 1

c-13 nmr500c
02704940014F/CDC13

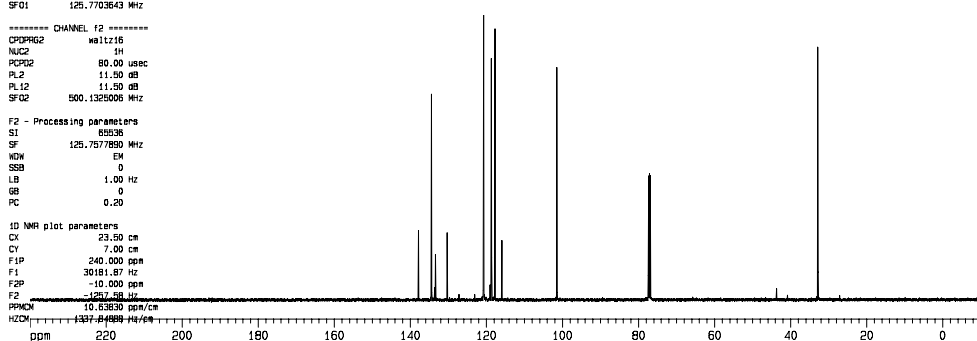
F2 - Acquisition Parameters
Date_ 20070817
Time 17.56
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 131072
SOLVENT CDC13
NS 363
DS 4
SWH 40322.582 Hz
FIDRES 0.307637 Hz
AQ 1.6253428 sec
RG 8192
DW 12.400 usec
DE 6.00 usec
TE 300.0 K
D1 0.10000000 sec
d11 0.03000000 sec
MCREST 0.00000000 sec
MCWPK 0.01500000 sec

***** CHANNEL f1 *****
NUC1 13C
P1 2.50 usec
PL1 0.00 dB
SFO1 125.7703643 MHz

***** CHANNEL f2 *****
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 11.50 dB
PL12 11.50 dB
SFO2 500.1350005 MHz

F2 - Processing parameters
SI 83536
SF 125.7577890 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 0.20

1D NMR plot parameters
CX 23.50 cm
CY 7.00 cm
F1P 240.000 ppm
F1 30181.87 Hz
F2P -10.000 ppm
F2 -125.750 Hz
PCHM 10.63530 ppm/cm
HZCM 1337.84888 Hz/cm



2-Chloro-2-(2-[1,3]-dioxan-2-ylethyl)indole (5c).

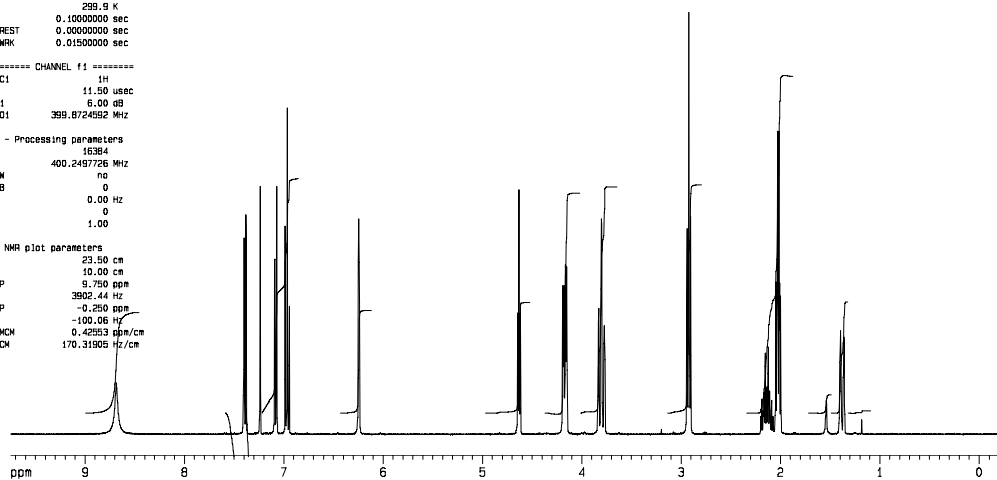
Current Data Parameters
NAME 66806-221-1
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20071002
Time 12.50
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 32
DS 2
SWH 6578.947 Hz
FIDRES 0.200774 Hz
AQ 2.4904180 sec
RG 322.5
DM 76.000 usec
DE 6.00 usec
TE 299.9 K
D1 0.10000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 11.50 usec
PL1 6.00 dB
SFO1 399.8724952 MHz

F2 - Processing parameters
SI 16384
SF 400.2457726 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 23.50 cm
CY 10.00 cm
F1P 9.750 ppm
F1 3902.44 Hz
F2P -0.250 ppm
F2 -100.00 Hz
PCHM 0.42951 ppm/cm
HZCM 170.31905 Hz/cm



Current Data Parameters
NAME 66806-221-1
EXPNO 1
PROCNO 1

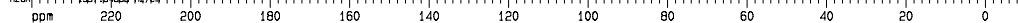
F2 - Acquisition Parameters
Date_ 20071002
Time 14.08
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 131072
SOLVENT CDCl3
NS 2014
DS 4
SWH 40322.582 Hz
FIDRES 0.307637 Hz
AQ 1.6293428 sec
RG 8192
DM 12.400 usec
DE 6.00 usec
TE 300.1 K
D1 0.10000000 sec
d11 0.03000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 2.50 usec
PL1 0.00 dB
SFO1 125.7703643 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 11.50 dB
PL12 11.50 dB
SFO2 500.1325006 MHz

F2 - Processing parameters
SI 65536
SF 125.7577690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 0.20

1D NMR plot parameters
CX 23.50 cm
CY 10.00 cm
F1P 240.000 ppm
F1 30181.87 Hz
F2P -10.000 ppm
F2 -125.758 Hz
PCHM 10.83530 ppm/cm
HZCM 1337.81888 Hz/cm



7-Chloro-2-cyclopropylindole (5d).

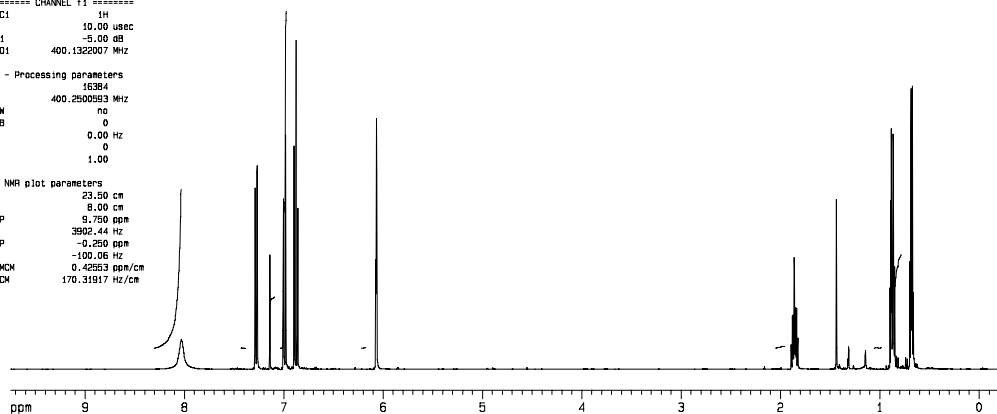
Current Data Parameters
NAME 02704940044F
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20070825
Time 15.55
INSTRUM spect
PROBHD 5 mm GNP 1H/1
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 32
DS 2
SWH 6561.680 Hz
FIDRES 0.200247 Hz
AQ 2.4969716 sec
RG 328.1
DM 76.200 usec
DE 6.00 usec
TE 300.2 K
D1 0.10000000 sec
MCREST 0.00000000 sec
MCNRK 0.01500000 sec

***** CHANNEL f1 *****
NUC1 1H
P1 10.00 usec
PL1 -5.00 dB
SFO1 400.1322007 MHz

F2 - Processing parameters
SI 16384
SF 400.2500553 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 23.50 cm
CY 8.00 cm
FIP 9.750 ppm
F1 3992.44 Hz
F2P -0.250 ppm
F2 -100.06 Hz
PPMCM 0.42553 ppm/cm
HZCM 170.31917 Hz/cm



Current Data Parameters
NAME 02704940044F
EXPNO 2
PROCNO 1

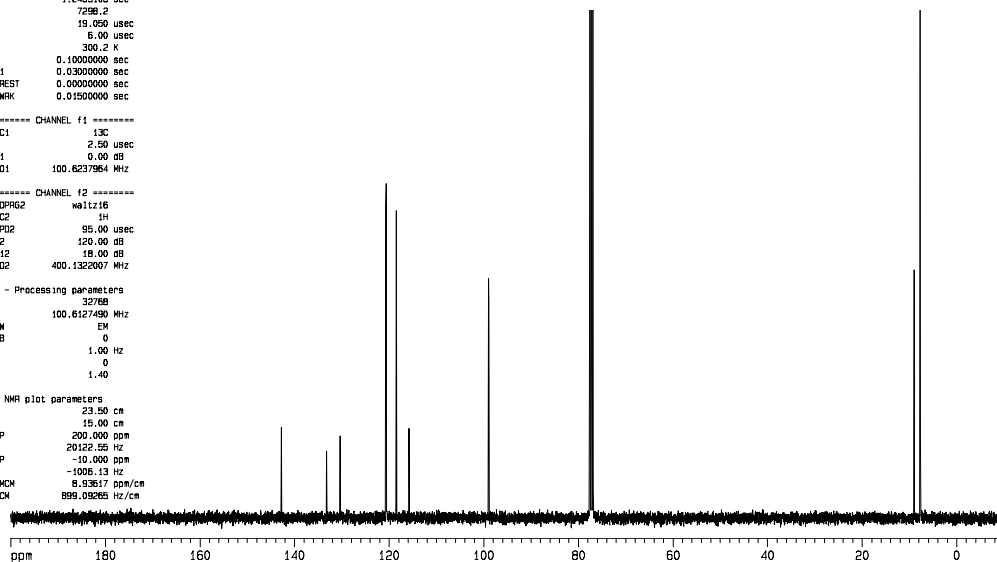
F2 - Acquisition Parameters
Date_ 20070825
Time 17.02
INSTRUM spect
PROBHD 5 mm GNP 1H/1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 778
DS 0
SWH 26246.719 Hz
FIDRES 0.400493 Hz
AQ 1.2481098 sec
RG 7286.2
DM 19.050 usec
DE 6.00 usec
TE 300.2 K
D1 0.10000000 sec
d11 0.03000000 sec
MCREST 0.00000000 sec
MCNRK 0.01500000 sec

***** CHANNEL f1 *****
NUC1 13C
P1 2.50 usec
PL1 0.00 dB
SFO1 100.6237964 MHz

***** CHANNEL f2 *****
CPDPRG2 waltz16
NUC2 1H
PCPD2 95.00 usec
PL2 120.00 dB
PL12 18.00 dB
SFO2 400.1322007 MHz

F2 - Processing parameters
SI 32768
SF 100.6127490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 23.50 cm
CY 15.00 cm
FIP 200.000 ppm
F1 20122.55 Hz
F2P -10.000 ppm
F2 -1006.13 Hz
PPMCM 8.93617 ppm/cm
HZCM 899.09265 Hz/cm



7-Chloro-2-hexan-1-ylindole (5e):

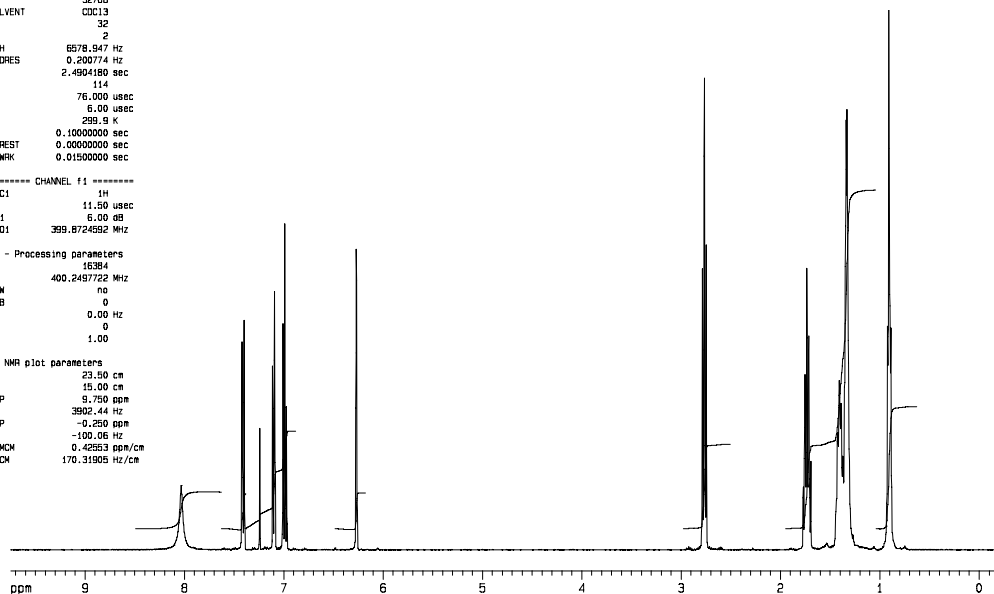
Current Data Parameters
NAME 66806-220-2
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20071002
Time 12.46
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 32
DS 2
SWH 6578.947 Hz
FIDRES 0.200774 Hz
AQ 2.4904180 sec
RG 114
DM 76.000 usec
DE 6.00 usec
TE 299.9 K
D1 0.10000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 11.50 usec
PL1 6.00 dB
SFO1 399.8724582 MHz

F2 - Processing parameters
SI 16384
SF 400.2497722 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 23.50 cm
CY 15.00 cm
FIP 9.750 ppm
F1 3902.44 Hz
F2P -0.250 ppm
F2 -100.00 Hz
PPMCM 0.42553 ppm/cm
HZCM 170.31905 Hz/cm



Current Data Parameters
NAME 66806-220-2
EXPNO 1
PROCNO 1

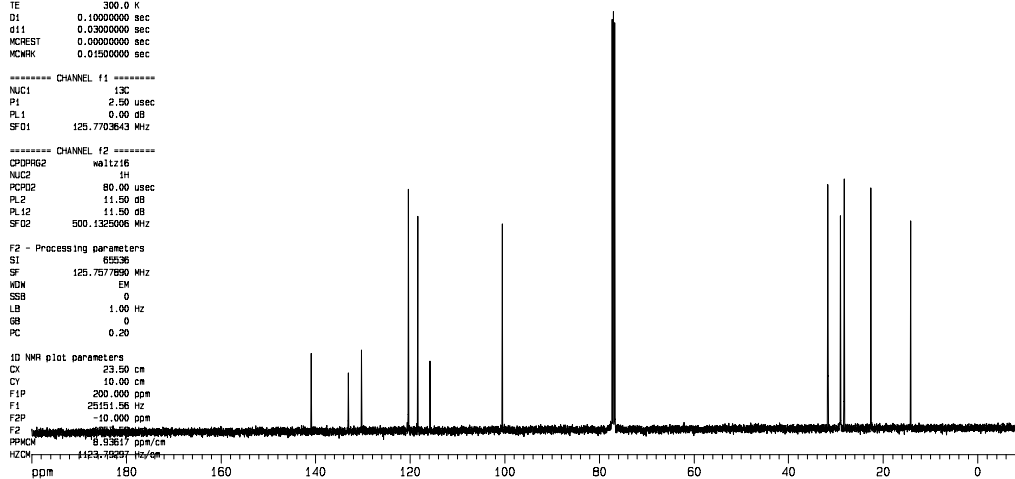
F2 - Acquisition Parameters
Date_ 20071002
Time 15.12
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 131072
SOLVENT CDCl3
NS 348
DS 4
SWH 40322.562 Hz
FIDRES 0.307637 Hz
AQ 1.6253428 sec
RG 8192
DM 12.400 usec
DE 6.00 usec
TE 300.0 K
D1 0.10000000 sec
d11 0.03000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 2.50 usec
PL1 0.00 dB
SFO1 125.7703643 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 11.50 dB
PL12 11.50 dB
SFO2 500.1325006 MHz

F2 - Processing parameters
SI 65536
SF 125.7577690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 0.20

1D NMR plot parameters
CX 23.50 cm
CY 10.00 cm
FIP 200.000 ppm
F1 25151.56 Hz
F2P -10.000 ppm
F2 -1923.19097 Hz/cm
PPMCM 16.53617 ppm/cm
HZCM 1923.19097 Hz/cm



2-Trimethylsilylmethylindole (5f):

Current Data Parameters

NAME 225042-225-3
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters

Date_ 20070703
Time 15.30
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 32
DS 2
SWH 6578.947 Hz
FIDRES 0.200774 Hz
AQ 2.4904180 sec
RG 405.4
DM 76.000 usec
DE 6.00 usec
TE 300.0 K
D1 0.10000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

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

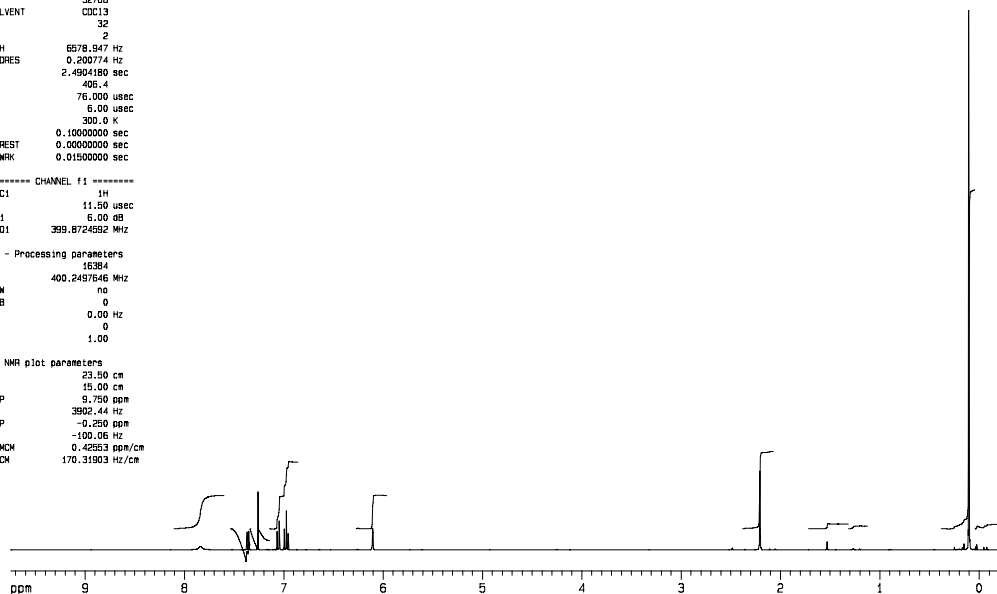
NUC1 1H
P1 11.50 usec
PL1 6.00 dB
SFO1 399.8724582 MHz

F2 - Processing parameters

SI 16384
SF 400.2497546 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

1D NMR plot parameters

CX 23.50 cm
CY 15.00 cm
FIP 9.750 ppm
F1 3902.44 Hz
F2P -0.250 ppm
F2 -100.00 Hz
PPMCM 0.42553 ppm/cm
HZCM 170.31903 Hz/cm



Current Data Parameters

NAME 225042-225-3
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters

Date_ 20070703
Time 15.10
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 131072
SOLVENT CDCl3
NS 966
DS 4
SWH 40322.562 Hz
FIDRES 0.307637 Hz
AQ 1.6253428 sec
RG 8192
DM 12.400 usec
DE 6.00 usec
TE 300.1 K
D1 0.10000000 sec
d11 0.03000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

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

NUC1 13C
P1 2.50 usec
PL1 0.00 dB
SFO1 125.7703643 MHz

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

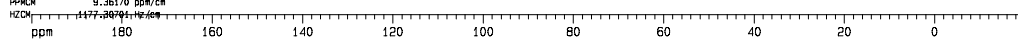
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 11.50 dB
PL12 11.50 dB
SFO2 500.1325006 MHz

F2 - Processing parameters

SI 65536
SF 125.7577690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 0.20

1D NMR plot parameters

CX 23.50 cm
CY 15.00 cm
FIP 200.000 ppm
F1 25151.56 Hz
F2P -20.000 ppm
F2 -2515.16 Hz
PPMCM 9.36170 ppm/cm
HZCM 1177.30741 Hz/cm



7-Chloro-2-pyridin-2-ylindole (5h).

Current Data Parameters
NAME 02704940041F
EXPNO 1
PROCNO 1

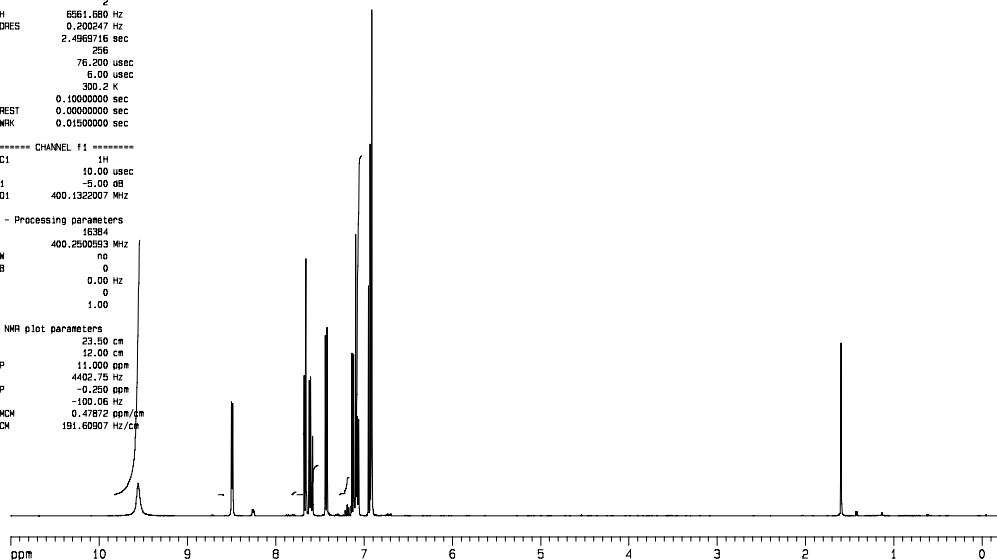
F2 - Acquisition Parameters

Date_ 20070629
Time 12.47
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 32
DS 2
SWH 6561.680 Hz
FIDRES 0.200247 Hz
AQ 2.4969716 sec
RG 256
DM 76.200 usec
DE 6.00 usec
TE 300.2 K
D1 0.10000000 sec
MCREST 0.00000000 sec
MCNPRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 10.00 usec
PL1 -5.00 dB
SFO1 400.1322007 MHz

F2 - Processing parameters
SI 16384
SF 400.250053 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 23.50 cm
CY 15.00 cm
FIP 11.000 ppm
F1 4402.75 Hz
F2P -0.250 ppm
F2 -100.05 Hz
PPHMC 0.47872 ppm/cm
HZCM 191.60907 Hz/cm



Current Data Parameters
NAME 02704940041F
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters

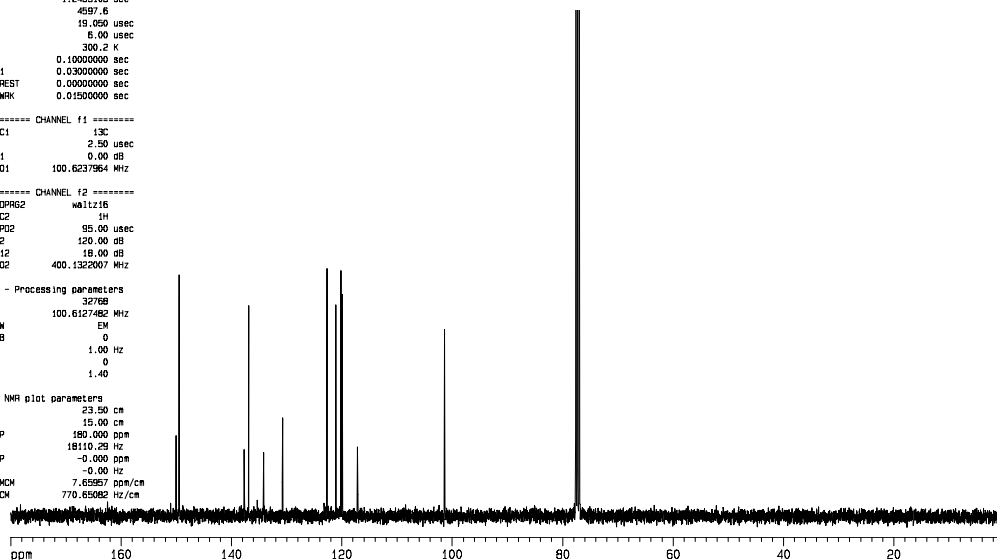
Date_ 20070629
Time 12.57
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 516
DS 0
SWH 26246.719 Hz
FIDRES 0.400493 Hz
AQ 1.2485108 sec
RG 4697.6
DM 19.050 usec
DE 6.00 usec
TE 300.2 K
D1 0.10000000 sec
d11 0.03000000 sec
MCREST 0.00000000 sec
MCNPRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 2.50 usec
PL1 0.00 dB
SFO1 100.6237964 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 95.00 usec
PL2 120.00 dB
PL12 18.00 dB
SFO2 400.1322007 MHz

F2 - Processing parameters
SI 32768
SF 100.6127482 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 23.50 cm
CY 15.00 cm
FIP 180.000 ppm
F1 18110.28 Hz
F2P -0.000 ppm
F2 -7.65957 ppm/cm
PPHMC 770.65082 Hz/cm
HZCM



7-Chloro-2-pyridin-3-ylindole (5i).

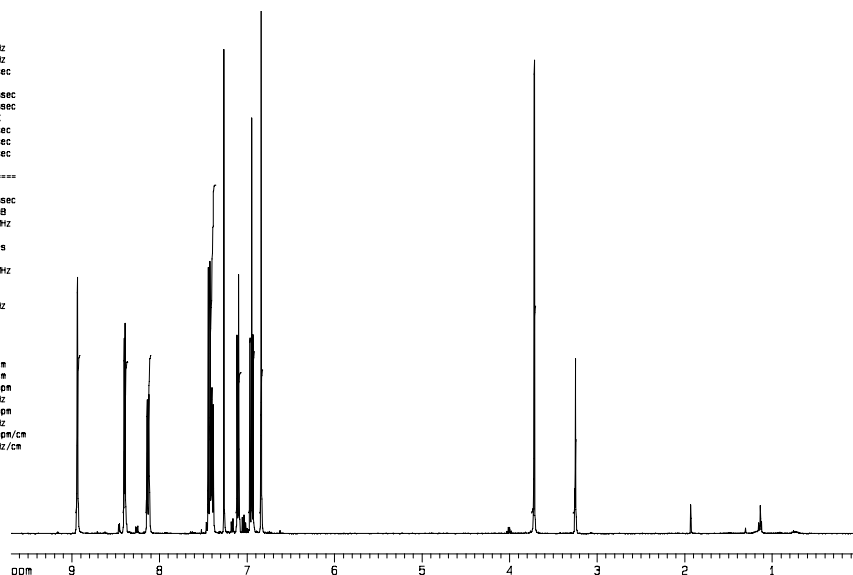
Current Data Parameters
NAME 02704940052F2
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20071010
Time 18.25
INSTRUM spect
PROBHD 5 mm GNP 1H/1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 256
DS 2
SWH 6561.680 Hz
FIDRES 0.200247 Hz
AQ 2.4869716 sec
RG 456.1
DM 76.200 usec
DE 6.00 usec
TE 300.2 K
D1 0.10000000 sec
MCREST 0.00000000 sec
MCWRR 0.01500000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 10.00 usec
PL1 -5.00 dB
SFO1 400.1322007 MHz

F2 - Processing parameters
SI 16384
SF 400.2516117 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 23.50 cm
CY 15.00 cm
F1P 11.000 ppm
F1 4402.77 Hz
F2P -0.000 ppm
F2 -0.00 Hz
PPMCM 0.46809 ppm/cm
HZCM 187.35181 Hz/cm



Current Data Parameters
NAME 02704940052F2
EXPNO 2
PROCNO 1

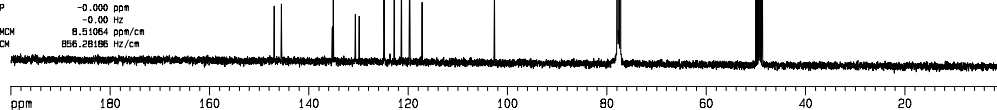
F2 - Acquisition Parameters
Date_ 20071010
Time 18.37
INSTRUM spect
PROBHD 5 mm GNP 1H/1
PULPROG zgpgc
TD 65536
SOLVENT CDCl3
NS 20000
DS 0
SWH 26248.719 Hz
FIDRES 0.400493 Hz
AQ 1.2485108 sec
RG 5160.6
DM 19.050 usec
DE 6.00 usec
TE 300.2 K
D1 0.10000000 sec
d11 0.03000000 sec
MCREST 0.00000000 sec
MCWRR 0.01500000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 2.50 usec
PL1 0.00 dB
SFO1 100.6237964 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 95.00 usec
PL2 120.00 dB
PL12 15.00 dB
SFO2 400.1322007 MHz

F2 - Processing parameters
SI 32768
SF 100.6131197 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 23.50 cm
CY 30.00 cm
F1P 200.000 ppm
F1 20122.62 Hz
F2P -0.000 ppm
F2 8.51084 ppm/cm
PPMCM 856.28186 ppm/cm
HZCM 856.28186 Hz/cm



7-Chloro-2-thien-2-ylindole (5j).

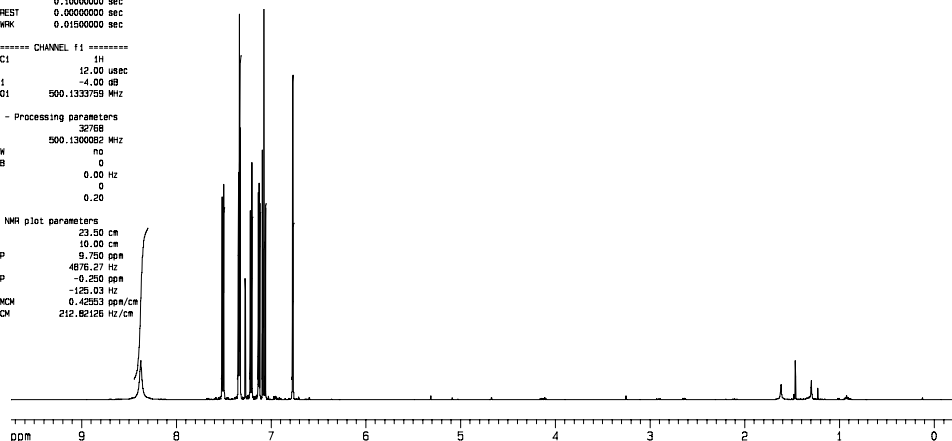
Current Data Parameters
NAME 02704940049F
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20070829
Time 12.17
INSTRUM spect
PROBHD 5 mm GNP 1H/13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 32
DS 4
SWH 13020.833 Hz
FIDRES 0.188582 Hz
AQ 2.5166323 sec
RG 203.2
DM 38.400 usec
DE 6.00 usec
TE 300.0 K
D1 0.10000000 sec
WCHST 0.00000000 sec
MCWK 0.01500000 sec

***** CHANNEL f1 *****
NUC1 1H
P1 12.00 usec
PL1 -4.00 dB
SFO1 500.133759 MHz

F2 - Processing parameters
SI 32768
SF 500.1350000 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 0.20

1D NMR plot parameters
CX 23.50 cm
CY 10.00 cm
F1P 9.750 ppm
F1 4876.27 Hz
F2P -0.250 ppm
F2 -125.03 Hz
PPMCK 0.42553 ppm/cm
HZCM 212.82126 Hz/cm



Current Data Parameters
NAME 02704940049F
EXPNO 2
PROCNO 1

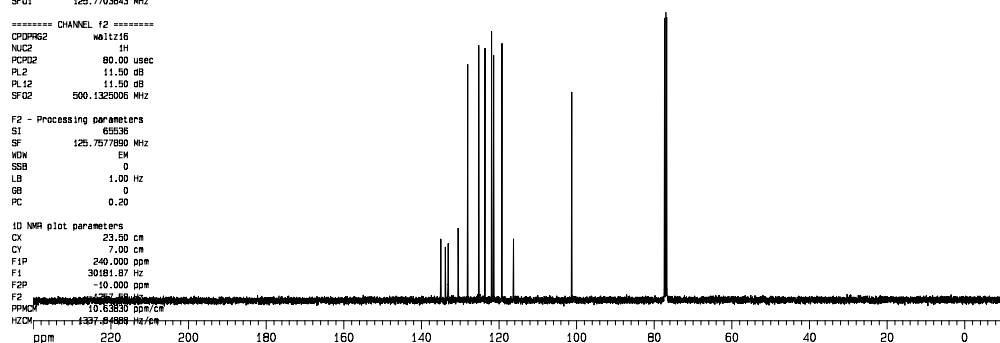
F2 - Acquisition Parameters
Date_ 20070829
Time 12.24
INSTRUM spect
PROBHD 5 mm GNP 1H/13
PULPROG zgpg
TD 131072
SOLVENT CDCl3
NS 256
DS 4
SWH 40322.582 Hz
FIDRES 0.307637 Hz
AQ 1.6253428 sec
RG 8192
DM 12.400 usec
DE 8.00 usec
TE 300.0 K
D1 0.10000000 sec
d11 0.03000000 sec
WCHST 0.00000000 sec
MCWK 0.01500000 sec

***** CHANNEL f1 *****
NUC1 13C
P1 2.50 usec
PL1 0.00 dB
SFO1 125.7703643 MHz

***** CHANNEL f2 *****
CPDPRG2 mltz16
NUC2 1H
PCPD2 80.00 usec
PL2 11.50 dB
PL12 11.50 dB
SFO2 500.1320006 MHz

F2 - Processing parameters
SI 65536
SF 125.7577690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 0.20

1D NMR plot parameters
CX 23.50 cm
CY 7.00 cm
F1P 240.000 ppm
F1 30181.87 Hz
F2P -10.000 ppm
F2 -250.135 Hz
PPMCK 10.63830 ppm/cm
HZCM 1337.84998 Hz/cm



7-Chloro-2-(2-trimethylsilylacety-1-yl)indole (5k).

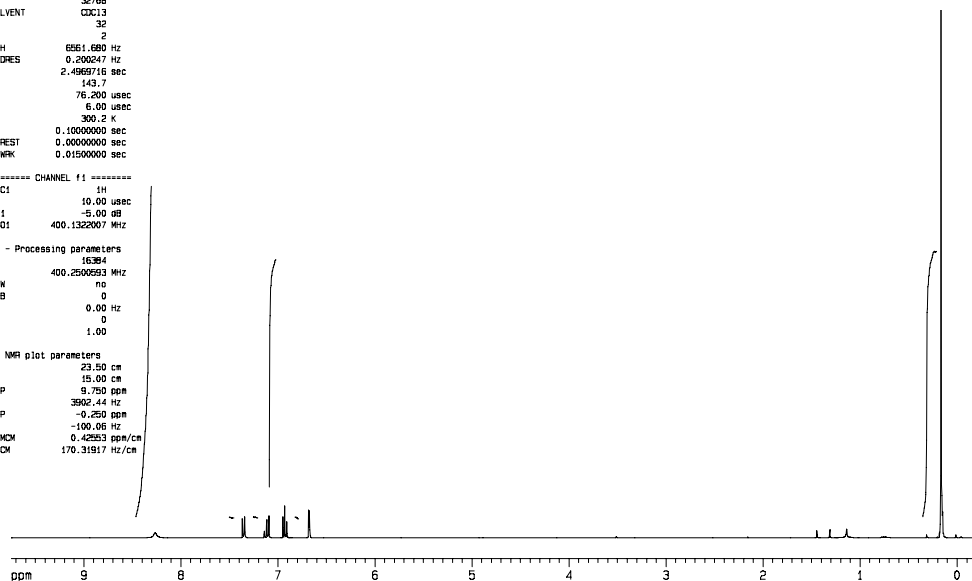
Current Data Parameters
NAME 0270494003BP
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20070824
Time 8.00
INSTRUM spect
PROBHD 5 mm GNP 1H/1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 32
DS 2
SWH 6561.680 Hz
FIDRES 0.206247 Hz
AQ 2.4969716 sec
RG 143.7
DM 76.200 usec
DE 6.00 usec
TE 300.2 K
D1 0.10000000 sec
MCHST 0.00000000 sec
MCHWK 0.01500000 sec

***** CHANNEL f1 *****
NUC1 1H
P1 10.00 usec
PL1 -5.00 dB
SFO1 400.132007 MHz

F2 - Processing parameters
SI 16384
SF 400.2500593 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 23.50 cm
CY 15.00 cm
FIP 9.750 ppm
F1 3902.44 Hz
F2P -0.250 ppm
F2 -100.06 Hz
PPMCM 0.42633 ppm/cm
HZCM 170.31917 Hz/cm



Current Data Parameters
NAME 0270494003BP
EXPNO 2
PROCNO 1

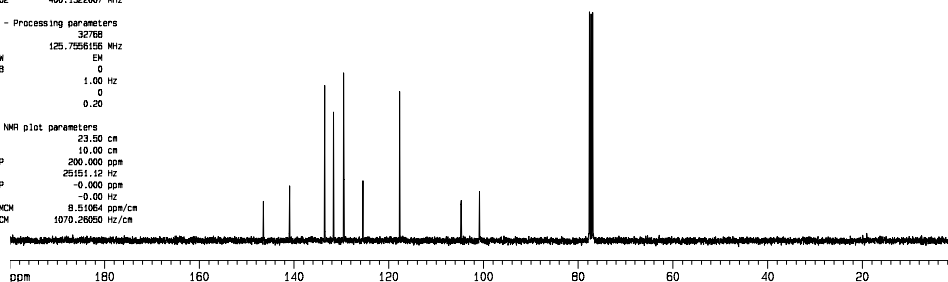
F2 - Acquisition Parameters
Date_ 20070824
Time 8.08
INSTRUM spect
PROBHD 5 mm GNP 1H/1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 654
DS 0
SWH 26246.719 Hz
FIDRES 0.404053 Hz
AQ 1.2485106 sec
RG 14586.5
DM 19.050 usec
DE 6.00 usec
TE 300.2 K
D1 0.10000000 sec
d11 0.03000000 sec
MCHST 0.00000000 sec
MCHWK 0.01500000 sec

***** CHANNEL f1 *****
NUC1 13C
P1 2.50 usec
PL1 0.00 dB
SFO1 100.6237864 MHz

***** CHANNEL f2 *****
CPDPRG2 waltz16
NUC2 1H
PCPD2 95.00 usec
PL2 120.00 dB
PL12 18.00 dB
SFO2 400.132007 MHz

F2 - Processing parameters
SI 32768
SF 125.7556156 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 0.20

1D NMR plot parameters
CX 23.50 cm
CY 10.00 cm
FIP 200.000 ppm
F1 25151.12 Hz
F2P -0.000 ppm
F2 -0.00 Hz
PPMCM 8.51064 ppm/cm
HZCM 1070.26050 Hz/cm



7-Chloro-2-hexyn-1-ylindole (5l).

Current Data Parameters
NAME 02704940040F
EXPNO 1
PROCNO 1

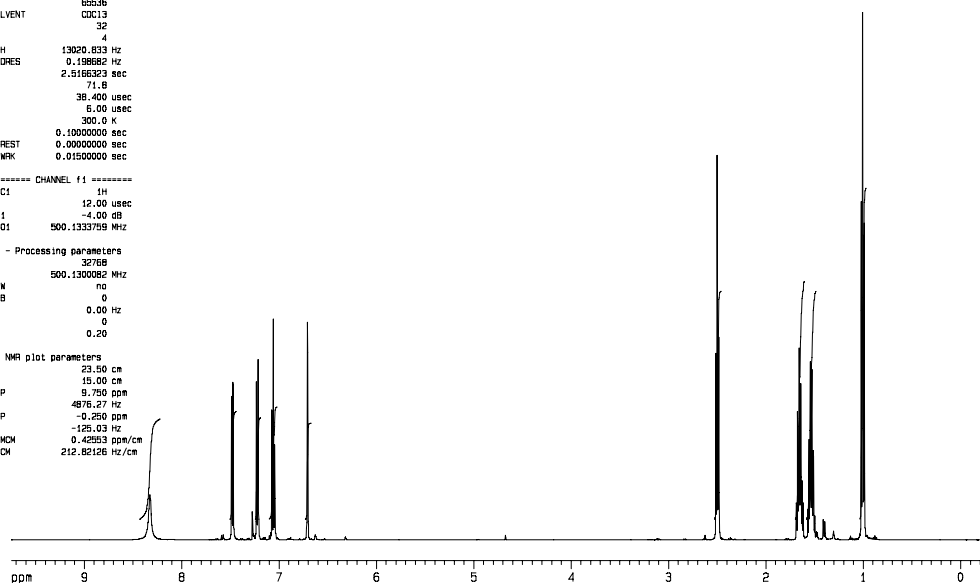
nmr500c h-1
02704940014F/CDC13

F2 - Acquisition Parameters
Date_ 20070824
Time 8.50
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 32
DS 4
SWH 13020.833 Hz
FIDRES 0.198682 Hz
AQ 2.5165323 sec
RG 71.8
DW 38.400 usec
DE 5.00 usec
TE 300.0 K
D1 0.10000000 sec
MCREST 0.00000000 sec
MCNPK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 12.00 usec
PL1 -4.00 dB
SF01 500.1333759 MHz

F2 - Processing parameters
SI 32768
SF 500.1300082 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 0.20

1D NMR plot parameters
CX 23.50 cm
CY 15.00 cm
F1P 9.750 ppm
F1 4876.27 Hz
F2P -0.250 ppm
F2 -125.03 Hz
PPHM 0.42553 ppm/cm
HZCM 212.82126 Hz/cm



Current Data Parameters
NAME 02704940040F
EXPNO 2
PROCNO 1

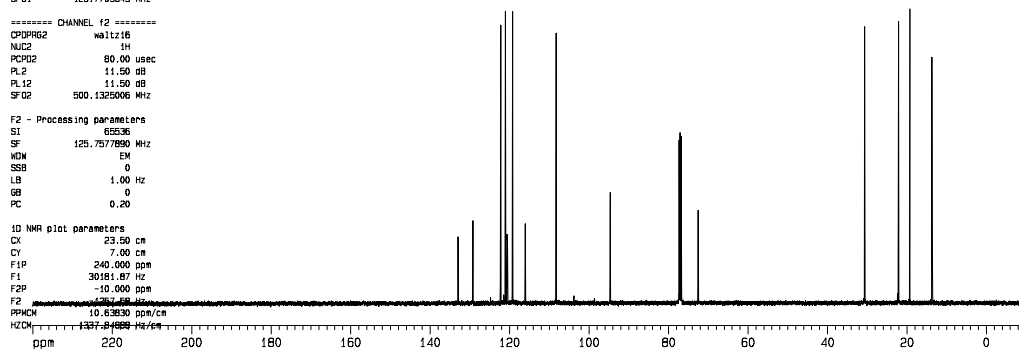
F2 - Acquisition Parameters
Date_ 20070824
Time 8.57
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 131072
SOLVENT CDCl3
NS 377
DS 4
SWH 40322.582 Hz
FIDRES 0.307637 Hz
AQ 1.6253428 sec
RG 8192
DW 12.400 usec
DE 5.00 usec
TE 300.0 K
D1 0.10000000 sec
D11 0.03000000 sec
MCREST 0.00000000 sec
MCNPK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 2.50 usec
PL1 0.00 dB
SF01 125.7703643 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 11.50 dB
PL12 11.50 dB
SF02 500.1325006 MHz

F2 - Processing parameters
SI 65536
SF 125.7577890 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 0.20

1D NMR plot parameters
CX 23.50 cm
CY 7.00 cm
F1P 240.000 ppm
F1 30181.87 Hz
F2P -10.000 ppm
F2 -125.03 Hz
PPHM 10.83630 ppm/cm
HZCM 1337.81888 Hz/cm



1-(2-Amino-4,5,6-trifluorophenyl)-2-chloroethanone (6d).

Current Data Parameters
NAME 027049400245
EXPNO 1
PROCNO 1

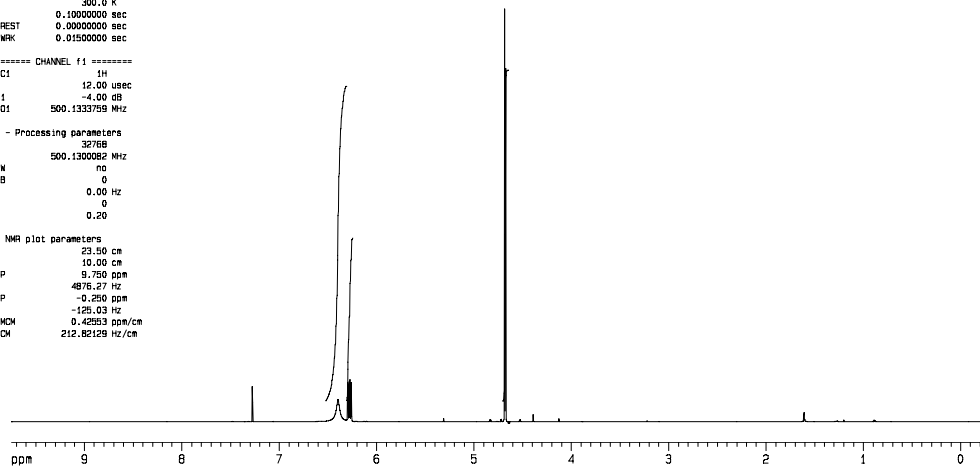
nmr500c h-1
02704940014F/CDC13

F2 - Acquisition Parameters
Date_ 20070817
Time 16.55
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 32
DS 4
SWH 13020.833 Hz
FIDRES 0.198662 Hz
AQ 2.3166323 sec
RG 256
DM 38.400 usec
DE 6.00 usec
TE 300.0 K
D1 0.10000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

***** CHANNEL f1 *****
NUC1 1H
P1 12.00 usec
PL1 -4.00 dB
SFO1 500.133759 MHz

F2 - Processing parameters
SI 32768
SF 500.130082 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 0.20

1D NMR plot parameters
CX 23.50 cm
CY 10.00 cm
F1P 9.750 ppm
F1 4876.27 Hz
F2P -0.250 ppm
F2 -125.032 Hz
PPOH 0.42953 ppm/cm
H2OH 212.82129 Hz/cm



Current Data Parameters
NAME 027049400245
EXPNO 3
PROCNO 1

nmr500c f-19

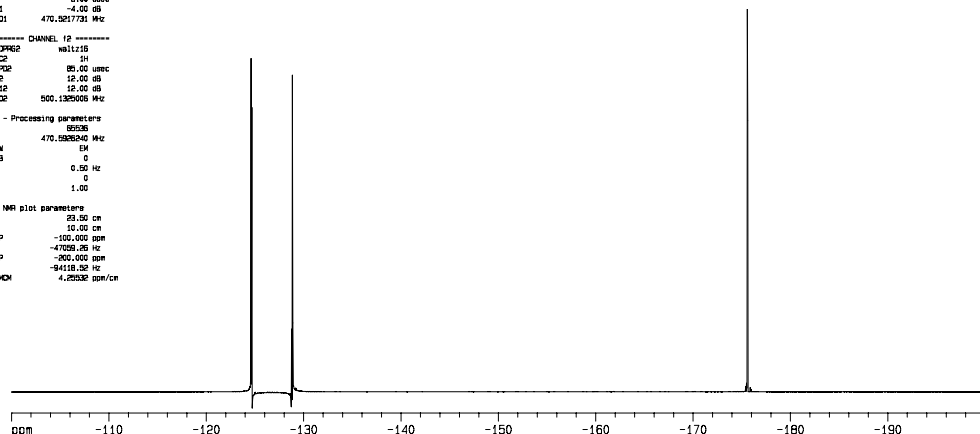
F2 - Acquisition Parameters
Date_ 20070817
Time 17.33
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 131072
SOLVENT CDC13
NS 64
DS 4
SWH 100000.000 Hz
FIDRES 0.765939 Hz
AQ 0.064100 sec
RG 64
DM 5.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
d12 0.00000000 sec

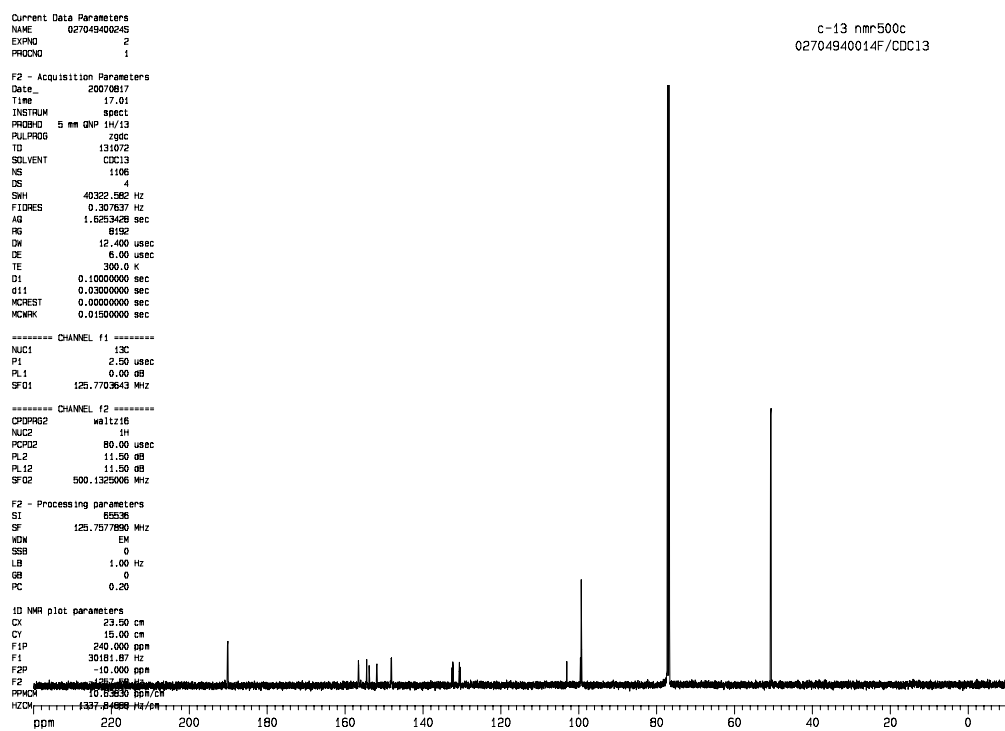
***** CHANNEL f1 *****
NUC1 19F
P1 5.00 usec
PL1 -4.00 dB
SFO1 470.321731 MHz

***** CHANNEL f2 *****
OPRG22 hllz15
NUC2 1H
PCPD 85.00 usec
PL2 12.00 dB
PL12 12.00 dB
SFO2 500.130082 MHz

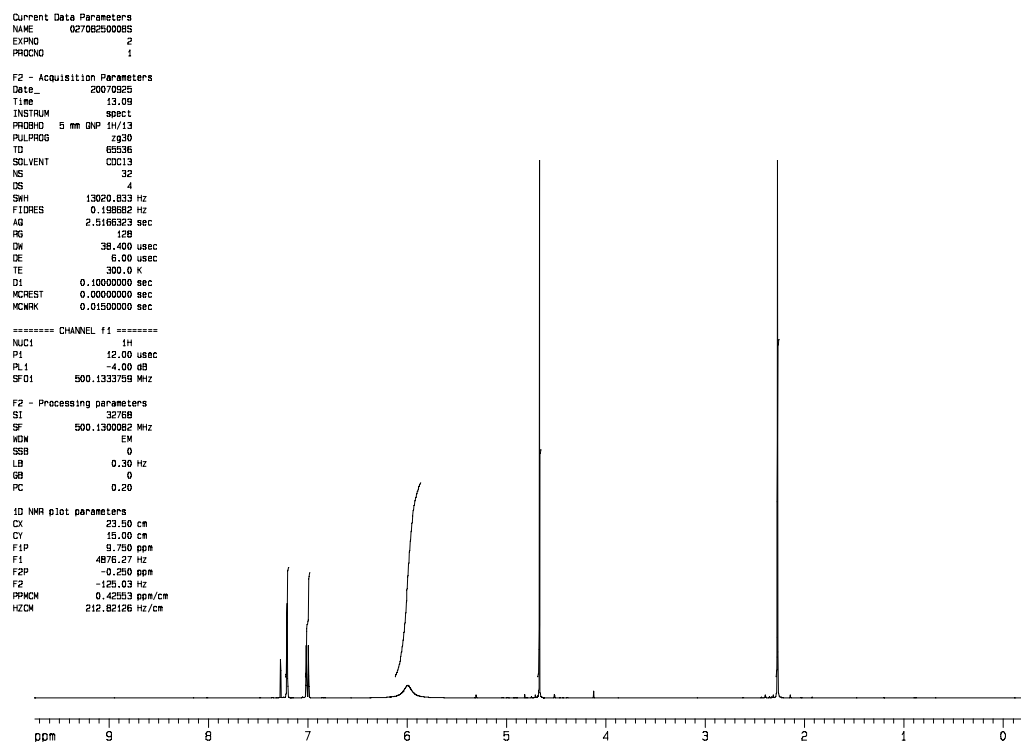
F2 - Processing parameters
SI 85536
SF 470.5926240 MHz
WDW EM
SSB 0
LB 0.50 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 25.50 cm
CY 10.00 cm
F1P -100.000 ppm
F1 -47009.26 Hz
F2P -900.000 ppm
F2 -94118.32 Hz
PPOH 4.25532 ppm/cm





1-(2-Amino-3-fluoro-5-methylphenyl)-2-chloroethanone (6f).



Current Data Parameters
NAME 027062500085
EXPNO 3
PROCNO 1

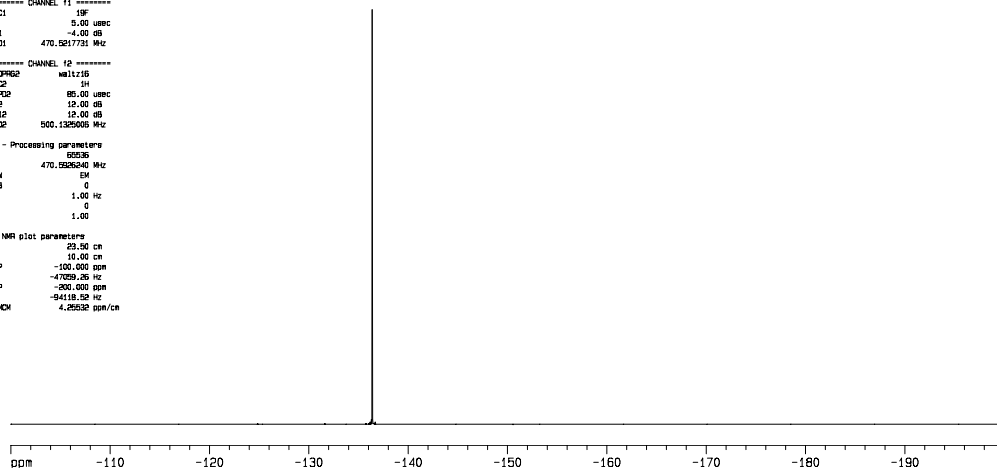
F2 - Acquisition Parameters
Date_ 20070925
Time 13.14
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 131072
SOLVENT CDCl3
NS 64
DS 4
SWH 10000.000 Hz
FIDRES 0.765939 Hz
AQ 0.0554100 sec
RG 64
DM 5.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
d12 0.00000000 sec

***** CHANNEL f1 *****
NUC1 13C
P1 5.00 usec
PL1 -4.00 dB
SFO1 470.5217731 MHz

***** CHANNEL f2 *****
CPDPRG2 meltz16
NUC2 1H
PCPD2 85.00 usec
PL2 12.00 dB
PL12 12.00 dB
SFO2 500.1325000 MHz

F2 - Processing parameters
SI 65536
SF 470.5206240 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 23.50 cm
CY 15.00 cm
F1P -100.000 ppm
F1 -47059.36 Hz
F2P -300.000 ppm
F2 -9418.58 Hz
PPMCH 4.25532 ppm/cm



Current Data Parameters
NAME 027062500085
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date_ 20070925
Time 13.18
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 131072
SOLVENT CDCl3
NS 441
DS 4
SWH 40322.582 Hz
FIDRES 0.307637 Hz
AQ 1.6253428 sec
RG 8192
DM 12.400 usec
DE 16.00 usec
TE 300.0 K
D1 0.10000000 sec
d11 0.03000000 sec
WCREST 0.00000000 sec
WCHWK 0.01500000 sec

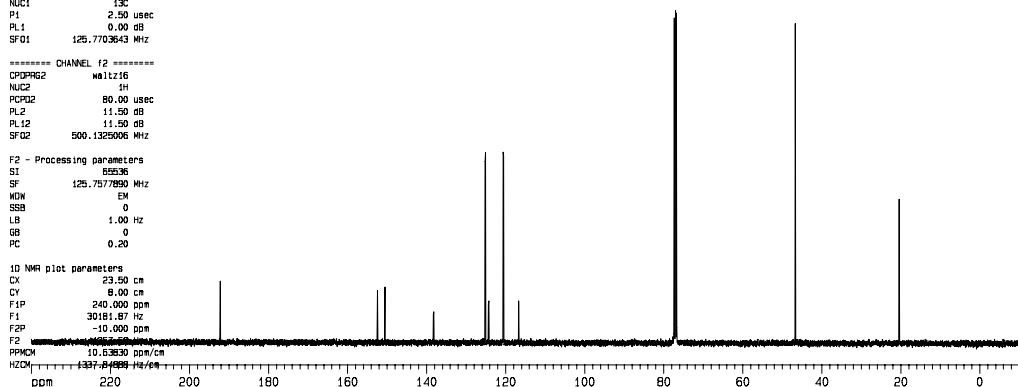
***** CHANNEL f1 *****
NUC1 13C
P1 2.50 usec
PL1 0.00 dB
SFO1 125.7703643 MHz

***** CHANNEL f2 *****
CPDPRG2 meltz16
NUC2 1H
PCPD2 80.00 usec
PL2 11.50 dB
PL12 11.50 dB
SFO2 500.1325006 MHz

F2 - Processing parameters
SI 65536
SF 125.7577890 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 0.20

1D NMR plot parameters
CX 23.50 cm
CY 8.00 cm
F1P 240.000 ppm
F1 30181.87 Hz
F2P -10.000 ppm
F2 -10.00000000 Hz
PPMCH 10.53530 ppm/cm

HZCM 1337.8488 Hz/cm



4,5,6-Trifluoro-2-propylindole (7d).

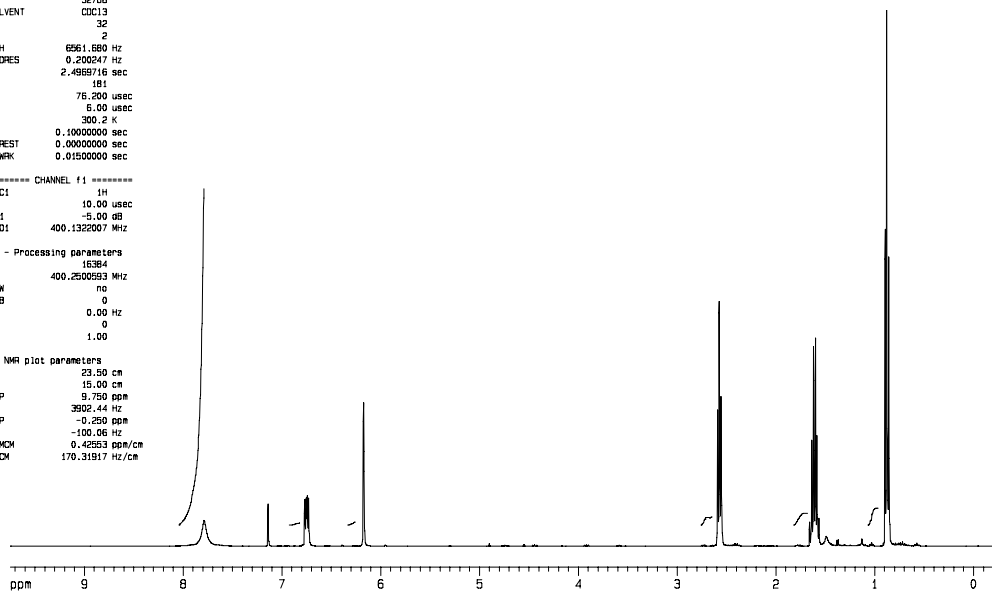
Current Data Parameters
NAME 02704940033F
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20070802
Time 17.40
INSTRUM spect
PROBHD 5 mm QNP
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 32
DS 2
SWH 6561.680 Hz
FIDRES 0.200247 Hz
AQ 2.4968716 sec
RG 181
DM 75.200 usec
DE 6.00 usec
TE 300.2 K
D1 0.10000000 sec
MCREST 0.00000000 sec
MCWFK 0.01500000 sec

***** CHANNEL f1 *****
NUC1 1H
P1 10.00 usec
PL1 -5.00 dB
SFO1 400.132007 MHz

F2 - Processing parameters
SI 16384
SF 400.2500593 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 23.50 cm
CY 15.00 cm
FIP 9.750 ppm
F1 3502.44 Hz
F2 -0.250 ppm
F2 -100.06 Hz
PPMCM 0.42553 ppm/cm
HZCM 170.31917 Hz/cm



Current Data Parameters
NAME 02704940033F
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20070802
Time 17.46
INSTRUM spect
PROBHD 5 mm QNP
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 455
DS 4
SWH 112994.302 Hz
FIDRES 0.862078 Hz
AQ 0.5800436 sec
RG 184.6
DM 4.420 usec
DE 8.30 usec
TE 300.2 K
D1 0.10000000 sec
d11 0.03000000 sec
d12 0.00000000 sec

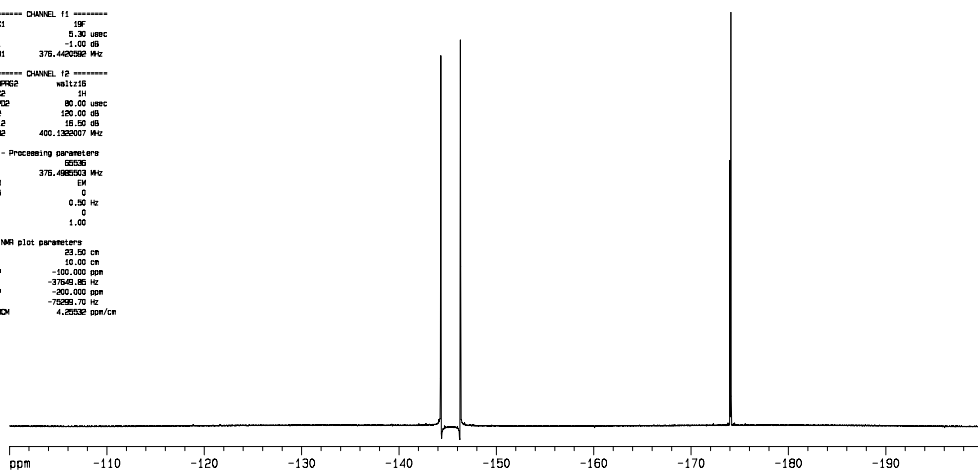
***** CHANNEL f1 *****
NUC1 13C
P1 8.30 usec
PL1 -1.00 dB
SFO1 375.4620980 MHz

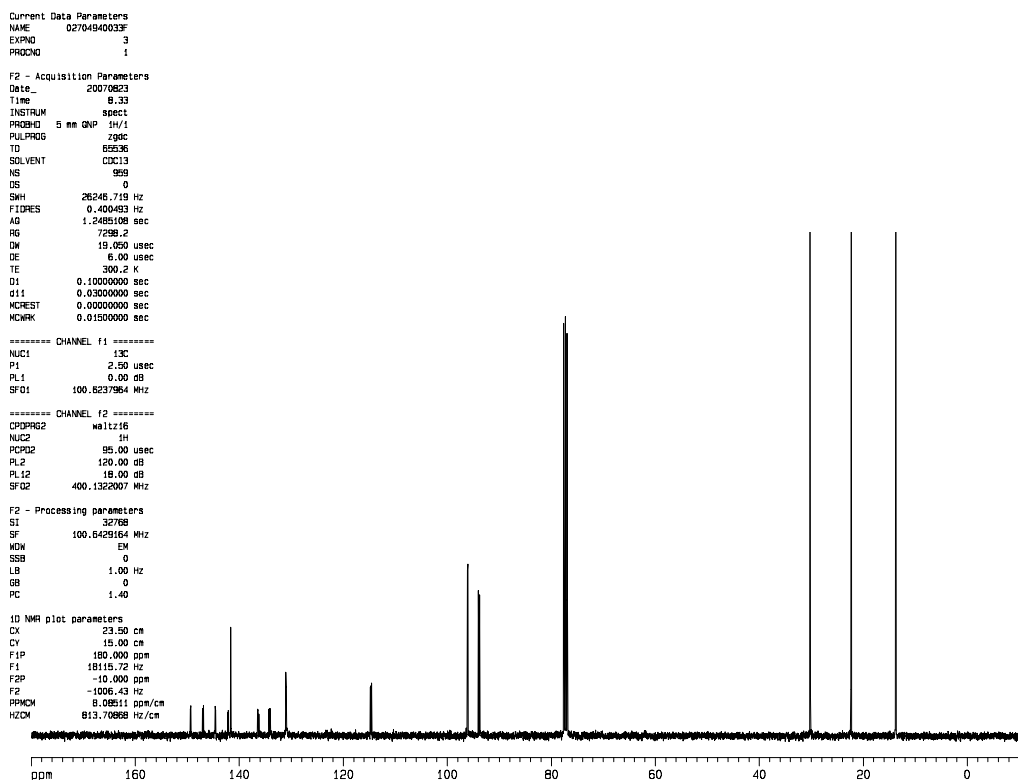
***** CHANNEL f2 *****
OPRG2 waltz16
NUC2 1H
PCPD 80.00 usec
PL2 190.00 dB
PL12 19.00 dB
SFO2 400.132007 MHz

F2 - Processing parameters
SI 65536
SF 375.4685953 MHz
WDW EM
SSB 0
LB 0.50 Hz
GB 0
PC 1.00

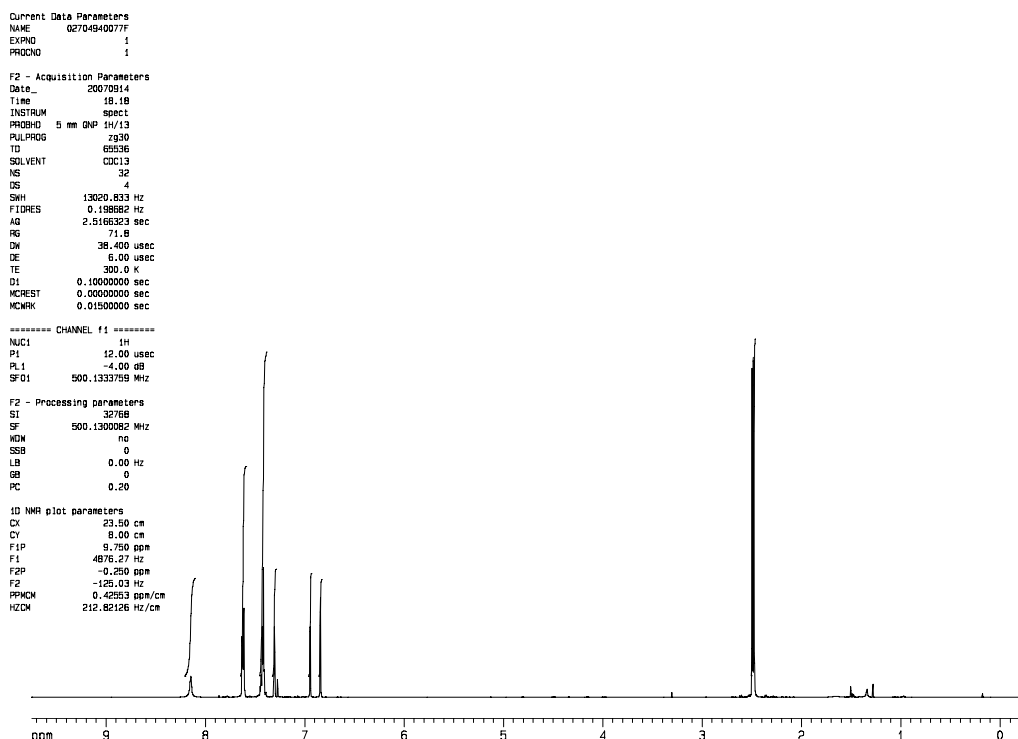
1D NMR plot parameters
CX 23.50 cm
CY 10.00 cm
FIP -100.000 ppm
F1 -37546.85 Hz
F2 -260.000 ppm
F2 -70599.70 Hz
PPMCM 4.25533 ppm/cm

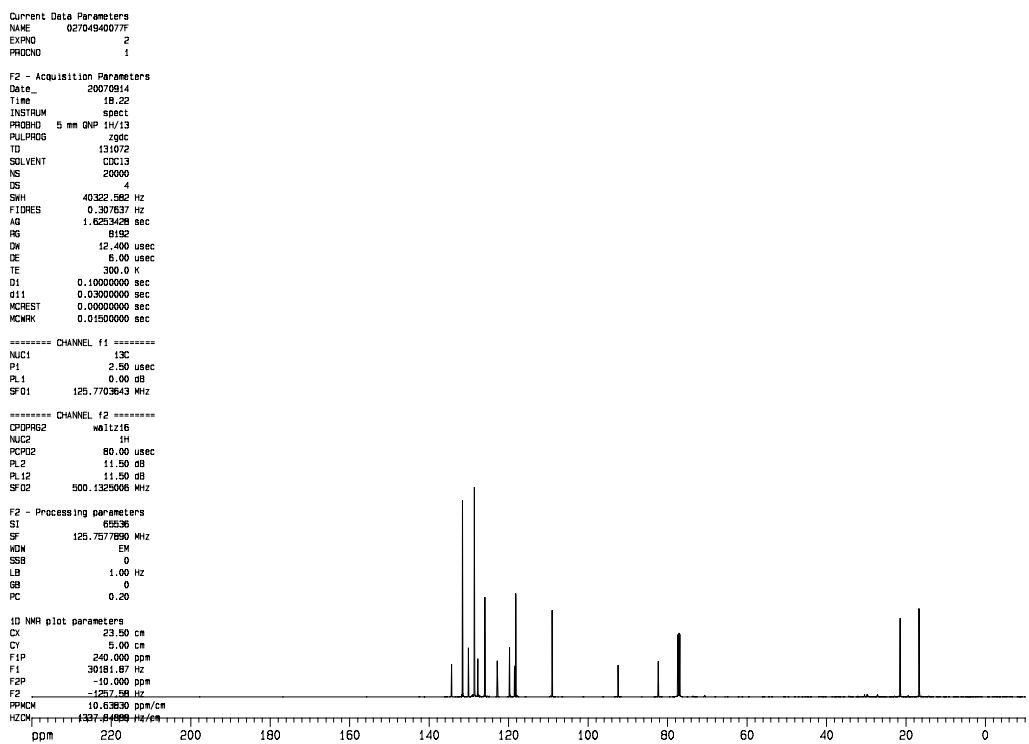
nmr400c h-1 decoupled f-19



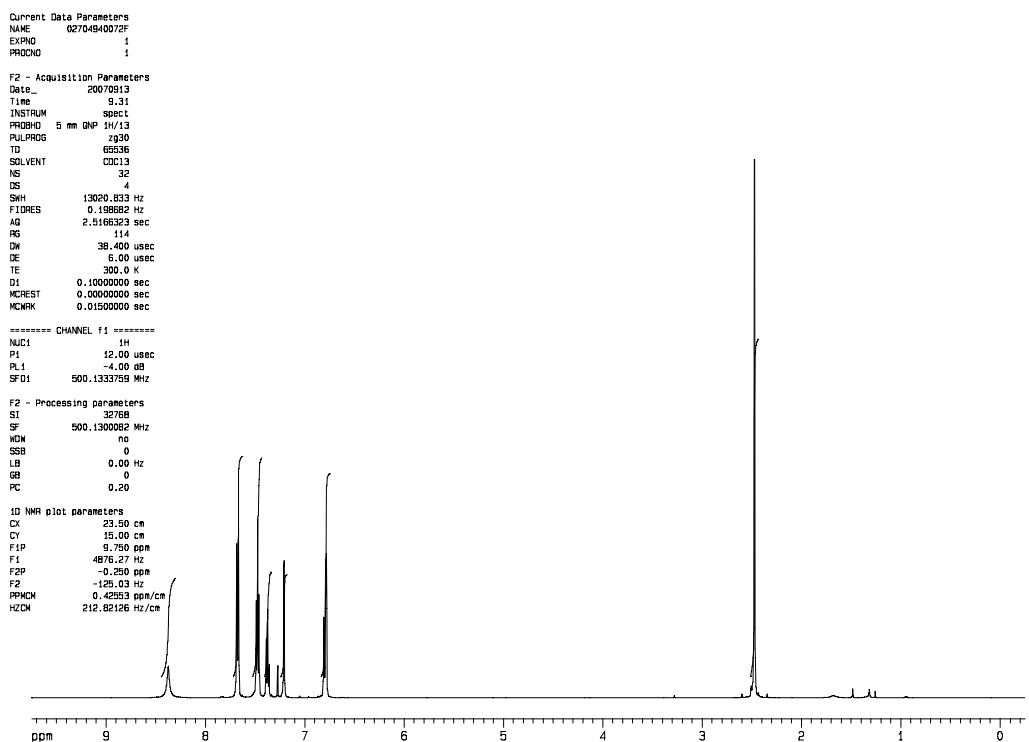


5,7-Dimethyl-2-phenylethynylindole (7e).





7-Fluoro-5-methyl-2-phenylindole (7f).



Current Data Parameters
NAME 0270494007F
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20070913
Time 9.36
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 131072
SOLVENT CDCl3
NS 84
DS 4
SWH 100000.000 Hz
FIDRES 0.762908 Hz
AQ 0.0054100 sec
RG 64
DM 5.000 usec
DE 5.00 usec
TE 300.0 K
D1 2.0000000 sec
d11 0.2000000 sec
d12 0.0000000 sec

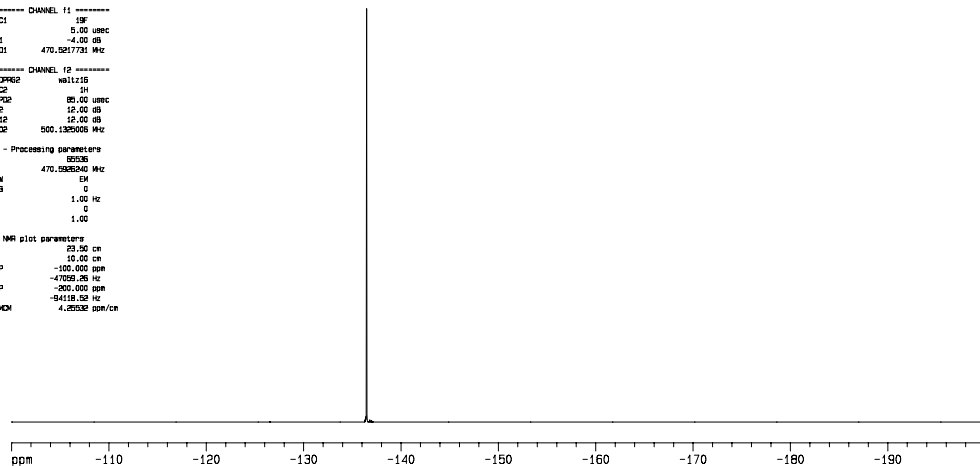
===== CHANNEL f1 =====
NUC1 13C
P1 5.00 usec
PL1 -4.00 dB
SFO1 470.5217731 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 85.00 usec
PL2 12.00 dB
PL12 12.00 dB
SFO2 500.1325008 MHz

F2 - Processing parameters
SI 65536
SF 470.526240 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 23.50 cm
CY 15.00 cm
F1P -100.000 ppm
F1 -47059.26 Hz
F2P -94118.52 Hz
F2 -184118.52 Hz
PPMCM 4.25532 ppm/cm

nmr500c f-19



Current Data Parameters
NAME 0270494007F
EXPNO 3
PROCNO 1

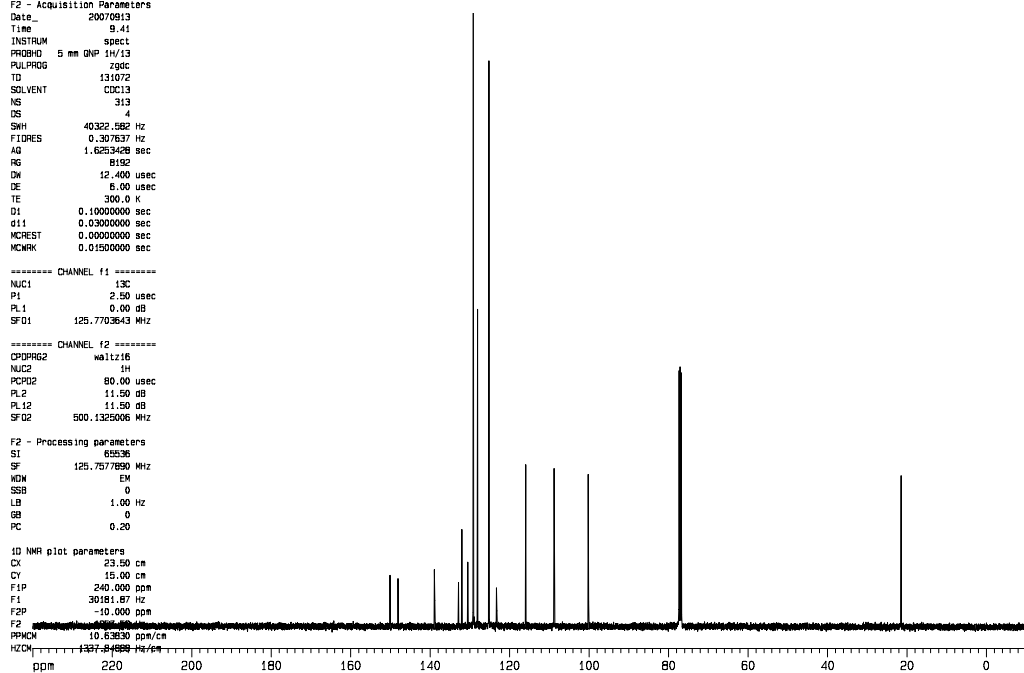
F2 - Acquisition Parameters
Date_ 20070913
Time 9.41
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 131072
SOLVENT CDCl3
NS 313
DS 4
SWH 40322.282 Hz
FIDRES 0.307637 Hz
AQ 1.6253428 sec
RG 8192
DM 12.400 usec
DE 5.00 usec
TE 300.0 K
D1 0.1000000 sec
d11 0.0300000 sec
MCREST 0.0000000 sec
MCWRK 0.0150000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 2.50 usec
PL1 0.00 dB
SFO1 125.7703643 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 11.50 dB
PL12 11.50 dB
SFO2 500.1325006 MHz

F2 - Processing parameters
SI 65536
SF 125.7577890 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 0.20

1D NMR plot parameters
CX 23.50 cm
CY 15.00 cm
F1P 240.000 ppm
F1 30181.87 Hz
F2P -10.000 ppm
F2 -101818.52 Hz
PPMCM 10.18333 ppm/cm
HZCM 1337.8488 Hz/cm



1-(2-Amino-3-chlorophenyl)-2-chloropropan-1-one (8).

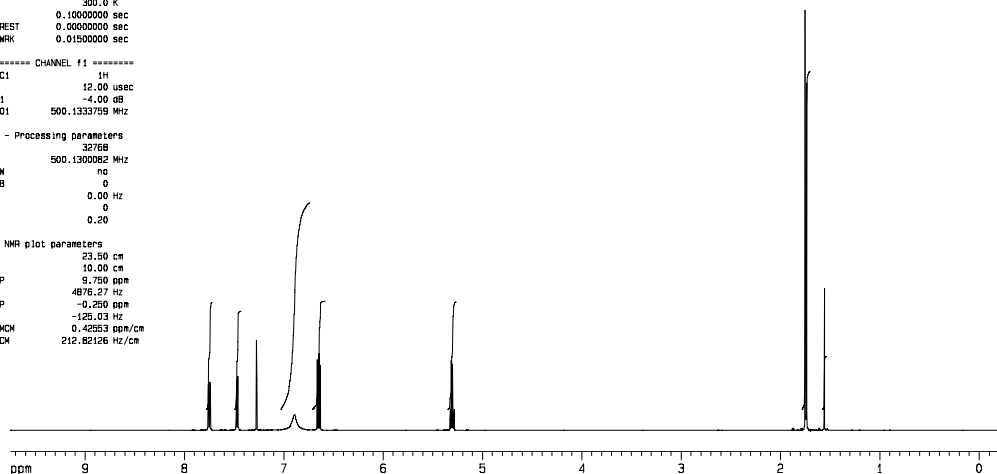
Current Data Parameters
NAME 2372661155
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20070719
Time 15.16
INSTRUM spect
PROBHD 5 mm GNP 1H/13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 32
DS 4
SWH 13020.833 Hz
FIDRES 0.198682 Hz
AQ 2.5166323 sec
RG 362
DM 38.400 usec
DE 6.00 usec
TE 300.0 K
D1 0.10000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

***** CHANNEL f1 *****
NUC1 1H
P1 12.00 usec
PL1 -4.00 dB
SFO1 500.1333759 MHz

F2 - Processing parameters
SI 32768
SF 500.1300082 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 0.20

1D NMR plot parameters
CX 23.50 cm
CY 10.00 cm
FIP 9.750 ppm
F1 4876.27 Hz
F2 -0.250 ppm
F2 -125.03 Hz
PPHMCN 0.42553 ppm/cm
HZCM 212.82126 Hz/cm



Current Data Parameters
NAME 2372661155
EXPNO 2
PROCNO 1

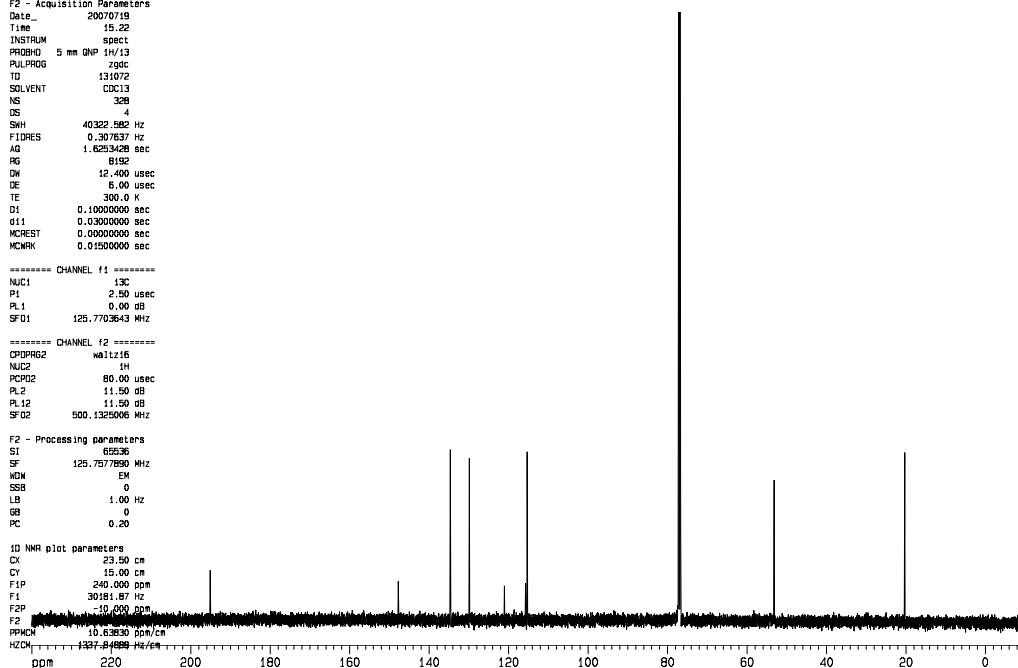
F2 - Acquisition Parameters
Date_ 20070719
Time 15.22
INSTRUM spect
PROBHD 5 mm GNP 1H/13
PULPROG zgpg30
TD 131072
SOLVENT CDCl3
NS 328
DS 4
SWH 40322.582 Hz
FIDRES 0.307637 Hz
AQ 1.6253428 sec
RG 8152
DM 12.400 usec
DE 6.00 usec
TE 300.0 K
D1 0.10000000 sec
d11 0.03000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

***** CHANNEL f1 *****
NUC1 13C
P1 2.50 usec
PL1 0.00 dB
SFO1 125.7703643 MHz

***** CHANNEL f2 *****
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 11.50 dB
PL12 11.50 dB
SFO2 500.1325006 MHz

F2 - Processing parameters
SI 65536
SF 125.7577890 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 0.20

1D NMR plot parameters
CX 23.50 cm
CY 15.00 cm
FIP 240.000 ppm
F1 30181.87 Hz
F2 -10.000 ppm
F2 10.63830 ppm/cm
HZCM 1337.89888 Hz/cm



7-Chloro-3-methyl-2-propylindole (9a).

Current Data Parameters
NAME 0270494004b
EXPNO 1
PROCNO 1

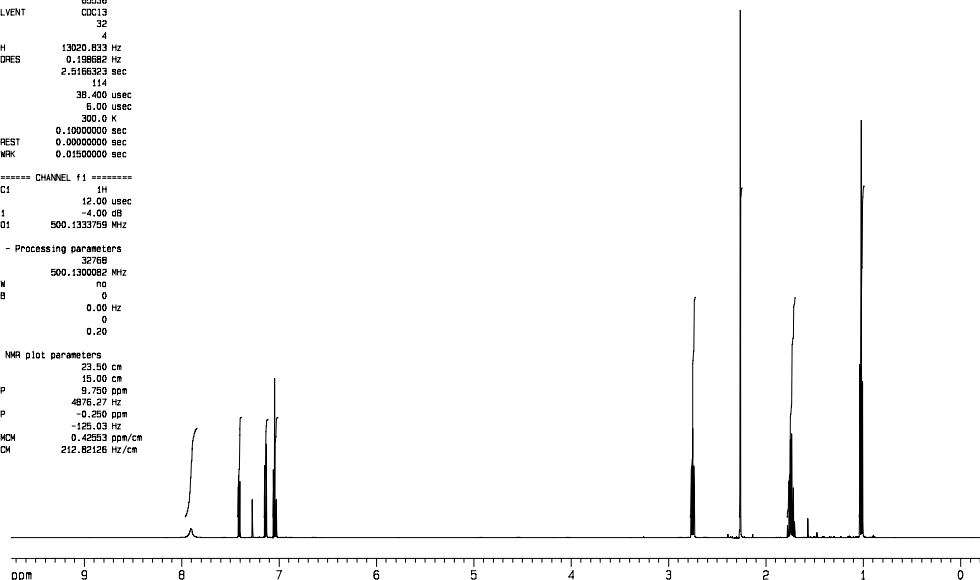
nmr500c h-1
02704940014F/CDC13

F2 - Acquisition Parameters
Date_ 20070726
Time 14.14
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 32
DS 4
SWH 13020.833 Hz
FIDRES 0.198682 Hz
AQ 2.5166323 sec
RG 114
DM 38.400 usec
DE 6.00 usec
TE 300.0 K
D1 0.10000000 sec
MCREST 0.00000000 sec
MCNRA 0.01500000 sec

***** CHANNEL f1 *****
NUC1 1H
P1 12.00 usec
PL1 -4.00 dB
SF01 500.133759 MHz

F2 - Processing parameters
SI 32768
SF 500.130082 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 0.20

1D NMR plot parameters
CX 23.50 cm
CY 15.00 cm
F1P 9.750 ppm
F1 4876.27 Hz
F2P -0.250 ppm
F2 -125.03 Hz
PRCHM 0.42553 ppm/cm
HZCM 212.82126 Hz/cm



Current Data Parameters
NAME 0270494001d
EXPNO 2
PROCNO 1

c-13 nmr500c
02704940014F/CDC13

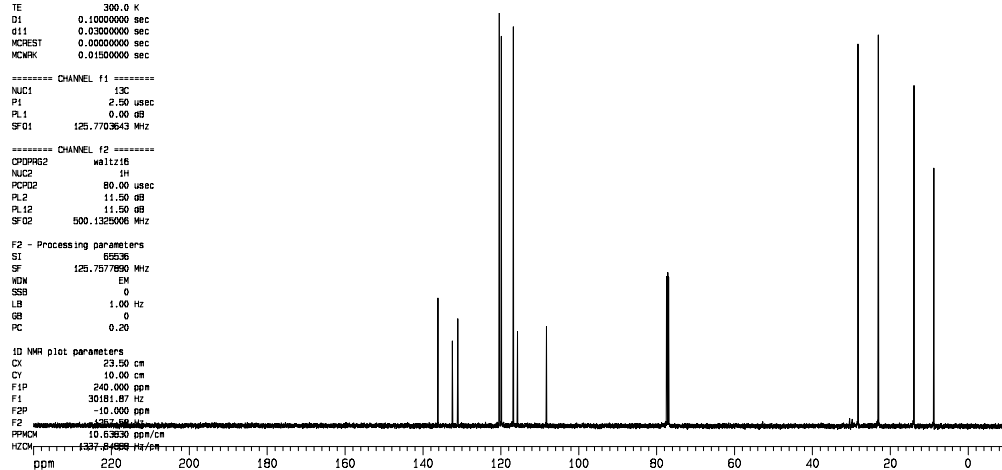
F2 - Acquisition Parameters
Date_ 20070726
Time 9.20
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 131072
SOLVENT CDC13
NS 179
DS 4
SWH 40322.580 Hz
FIDRES 0.307637 Hz
AQ 1.6253428 sec
RG 8192
DM 12.400 usec
DE 6.00 usec
TE 300.0 K
D1 0.10000000 sec
g11 0.03000000 sec
MCREST 0.00000000 sec
MCNRA 0.01500000 sec

***** CHANNEL f1 *****
NUC1 13C
P1 2.50 usec
PL1 0.00 dB
SF01 125.7703643 MHz

***** CHANNEL f2 *****
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 11.50 dB
PL12 11.50 dB
SF02 500.1326006 MHz

F2 - Processing parameters
SI 65536
SF 125.7577890 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 0.20

1D NMR plot parameters
CX 23.50 cm
CY 10.00 cm
F1P 240.000 ppm
F1 30181.87 Hz
F2P -10.000 ppm
F2 -10.63530 ppm/cm
PRCHM 1337.84888 Hz/cm
HZCM 1337.84888 Hz/cm



7-Chloro-3-methyl-2-thien-2-ylindole (9b).

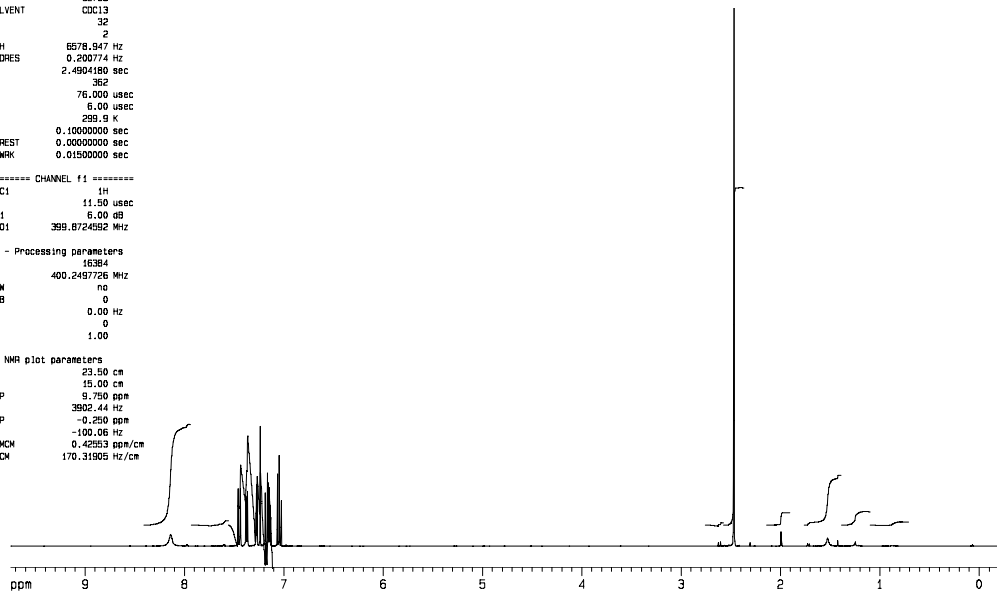
Current Data Parameters
NAME 66806-224-1
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20070926
Time 13.51
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 32
DS 2
SWH 6578.947 Hz
FIDRES 0.200774 Hz
AQ 2.4904180 sec
RG 362
DM 76.000 usec
DE 6.00 usec
TE 299.9 K
D1 0.10000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 11.50 usec
PL1 6.00 dB
SF01 399.8724952 MHz

F2 - Processing parameters
SI 16384
SF 400.2457726 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 23.50 cm
CY 15.00 cm
F1P 9.750 ppm
F1 3902.44 Hz
F2P -0.250 ppm
F2 -100.06 Hz
PCPM 0.42953 ppm/cm
HZCM 170.31905 Hz/cm



Current Data Parameters
NAME 66806-224-2
EXPNO 1
PROCNO 1

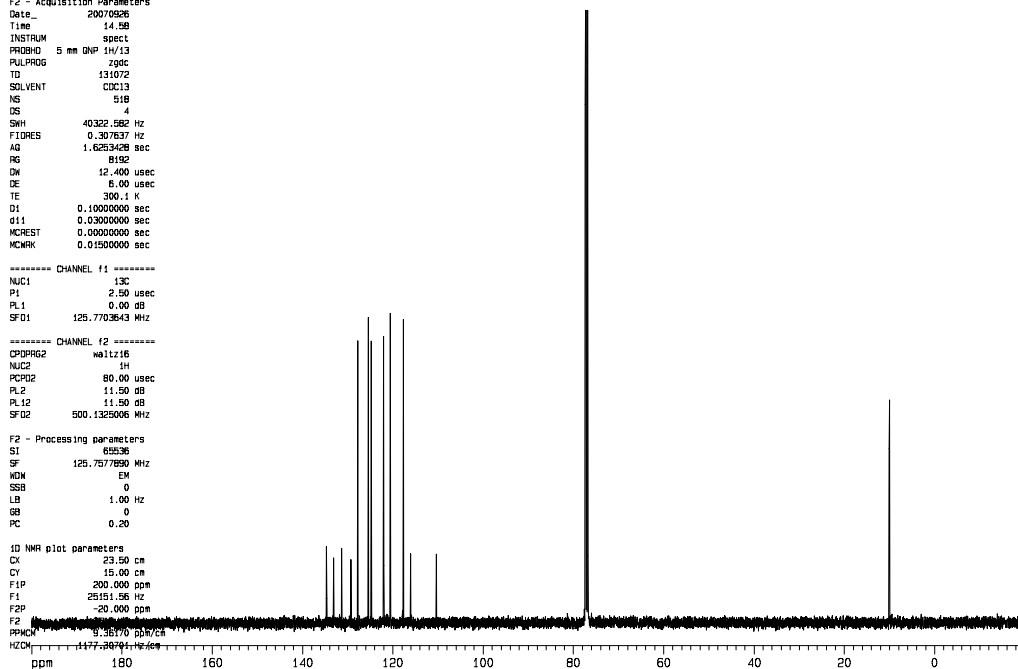
F2 - Acquisition Parameters
Date_ 20070926
Time 14.58
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 131072
SOLVENT CDCl3
NS 518
DS 4
SWH 40322.582 Hz
FIDRES 0.307637 Hz
AQ 1.6253428 sec
RG 8192
DM 12.400 usec
DE 6.00 usec
TE 300.1 K
D1 0.10000000 sec
D11 0.03000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 2.50 usec
PL1 0.00 dB
SF01 125.7703643 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 11.50 dB
PL12 11.50 dB
SF02 500.1325006 MHz

F2 - Processing parameters
SI 65536
SF 125.7577890 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 0.20

1D NMR plot parameters
CX 23.50 cm
CY 15.00 cm
F1P 200.000 ppm
F1 25151.56 Hz
F2P -20.000 ppm
F2 -117.30710 ppm/cm
HZCM 1177.30710 Hz/cm



2-(*N*-trimethylacetyl-2-aminophenyl)indole (15):

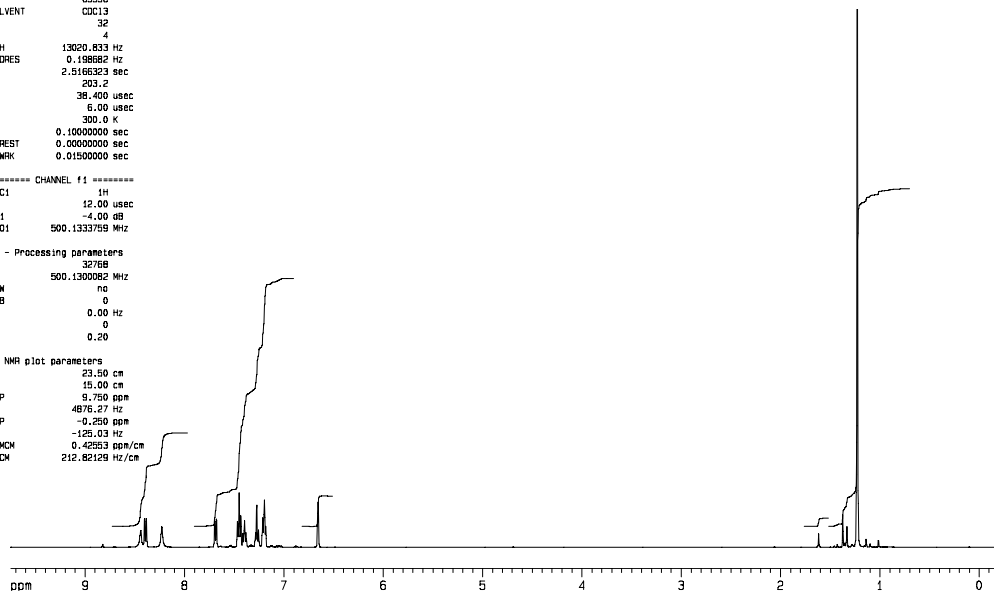
Current Data Parameters
NAME 66806-250-1
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20071004
Time 11.18
INSTRUM spect
PROBHD 5 mm GNP 1H/13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 32
DS 4
SWH 13020.833 Hz
FIDRES 0.198682 Hz
AQ 2.5166323 sec
RG 293.2
DM 38.400 usec
DE 6.00 usec
TE 300.0 K
D1 0.10000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

***** CHANNEL f1 *****
NUC1 1H
P1 12.00 usec
PL1 -4.00 dB
SFO1 500.1333759 MHz

F2 - Processing parameters
SI 32768
SF 500.1300082 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 0.20

1D NMR plot parameters
CX 23.50 cm
CY 15.00 cm
FIP 9.750 ppm
F1 4876.27 Hz
F2P -0.250 ppm
F2 -125.03 Hz
PPHMC 0.42553 ppm/cm
HZCM 212.82129 Hz/cm



Current Data Parameters
NAME 66806-250-1
EXPNO 2
PROCNO 1

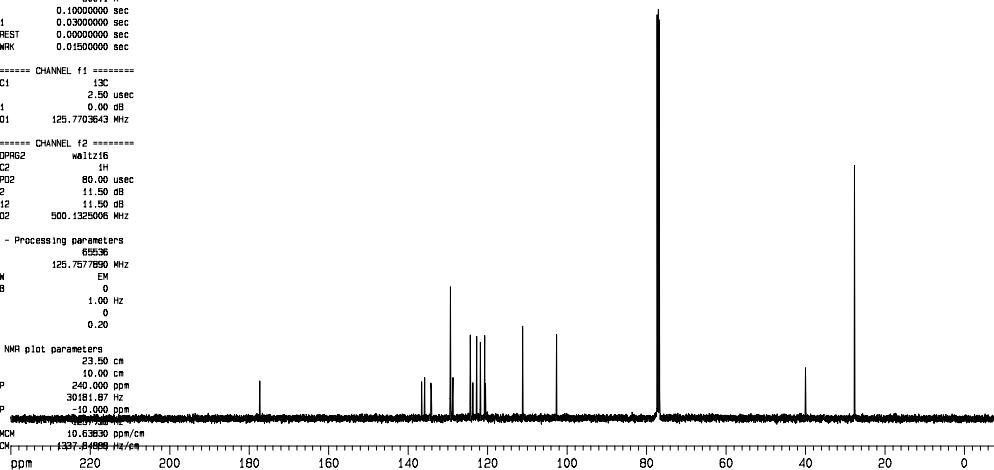
F2 - Acquisition Parameters
Date_ 20071004
Time 11.27
INSTRUM spect
PROBHD 5 mm GNP 1H/13
PULPROG zgpg30
TD 131072
SOLVENT CDCl3
NS 472
DS 4
SWH 40322.582 Hz
FIDRES 0.307637 Hz
AQ 1.6293428 sec
RG 8192
DM 12.400 usec
DE 6.00 usec
TE 300.1 K
D1 0.10000000 sec
d11 0.03000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

***** CHANNEL f1 *****
NUC1 13C
P1 2.50 usec
PL1 0.00 dB
SFO1 125.7703643 MHz

***** CHANNEL f2 *****
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 11.50 dB
PL12 11.50 dB
SFO2 500.1325006 MHz

F2 - Processing parameters
SI 65536
SF 125.7577990 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 0.20

1D NMR plot parameters
CX 23.50 cm
CY 19.00 cm
FIP 240.000 ppm
F1 30181.87 Hz
F2P -10.000 ppm
F2 1337.81888 Hz/cm
PPHMC 10.63830 ppm/cm
HZCM 1337.81888 Hz/cm



1-(2-Amino-3-chlorophenyl)-2-chloro-1-D-ethan-1-ol (16).

Current Data Parameters
NAME 02704940014F
EXPNO 3
PROCNO 1

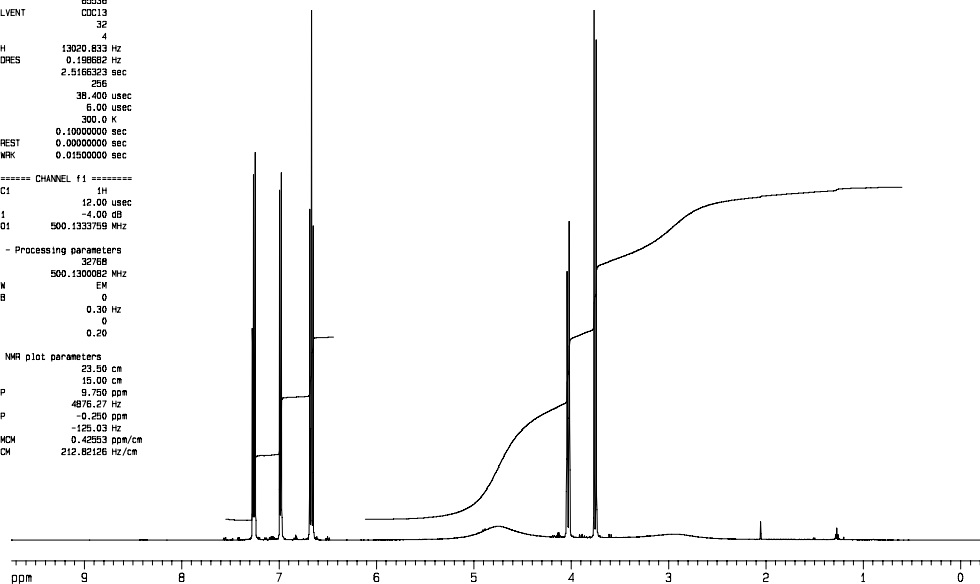
nmr500c h-1
02704940014F/CDC13

F2 - Acquisition Parameters
Date_ 20070816
Time 18.03
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 32
DS 4
SWH 13020.833 Hz
FIDRES 0.198682 Hz
AQ 2.5166323 sec
RG 256
DW 38.400 usec
DE 6.00 usec
TE 300.0 K
D1 0.10000000 sec
MCREST 0.00000000 sec
MCNRA 0.01500000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 12.00 usec
PL1 -4.00 dB
SFO1 500.1333758 MHz

F2 - Processing parameters
SI 32768
SF 500.1300082 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 0.20

1D NMR plot parameters
CX 23.50 cm
CY 15.00 cm
F1P 9.750 ppm
F1 4876.27 Hz
F2P -0.250 ppm
F2 -125.03 Hz
PRHCH 0.42553 ppm/cm
HZCH 212.82126 Hz/cm



Current Data Parameters
NAME 02704940014F
EXPNO 4
PROCNO 1

c-13 nmr500c
02704940014F/CDC13

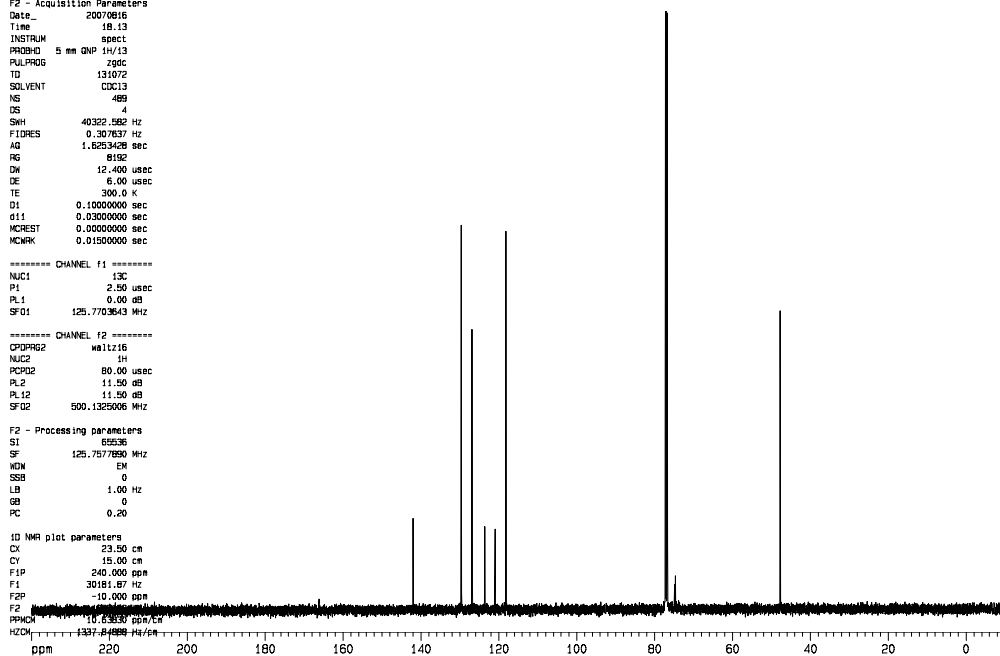
F2 - Acquisition Parameters
Date_ 20070816
Time 18.13
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 131072
SOLVENT CDC13
NS 489
DS 4
SWH 40322.582 Hz
FIDRES 0.307637 Hz
AQ 1.6253428 sec
RG 8192
DW 12.400 usec
DE 6.00 usec
TE 300.0 K
D1 0.10000000 sec
d11 0.03000000 sec
MCREST 0.00000000 sec
MCNRA 0.01500000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 2.50 usec
PL1 0.00 dB
SFO1 125.7703643 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 11.50 dB
PL12 11.50 dB
SFO2 500.1325006 MHz

F2 - Processing parameters
SI 65536
SF 125.7577890 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 0.20

1D NMR plot parameters
CX 23.50 cm
CY 15.00 cm
F1P 240.000 ppm
F1 30181.87 Hz
F2P -10.000 ppm
F2 -116.25533 ppm/cm
PRHCH 1337.84988 Hz/cm
HZCH 1337.84988 Hz/cm



7-Chloro-2-D-indole (17).

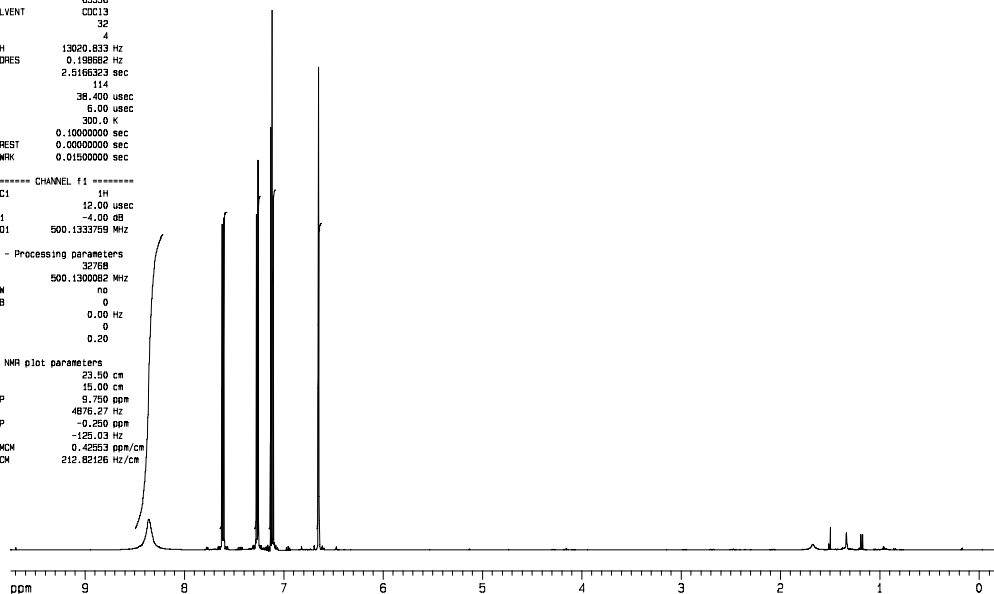
Current Data Parameters
NAME 02704940063F
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20070910
Time 14.19
INSTRUM spect
PROBHD 5 mm GNP 1H/13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 32
DS 4
SWH 13020.833 Hz
FIDRES 0.198682 Hz
AQ 2.5166323 sec
RG 114
DM 38.400 usec
DE 6.00 usec
TE 300.0 K
D1 0.10000000 sec
MCREST 0.00000000 sec
MCWPK 0.01500000 sec

***** CHANNEL f1 *****
NUC1 1H
P1 12.00 usec
PL1 -4.00 dB
SFO1 500.1333759 MHz

F2 - Processing parameters
SI 32768
SF 500.1300682 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 0.20

1D NMR plot parameters
CX 23.50 cm
CY 15.00 cm
F1P 9.750 ppm
F1 4876.27 Hz
F2P -0.250 ppm
F2 125.013 Hz
PPHCH 0.42553 ppm/cm
HZCM 212.82126 Hz/cm



Current Data Parameters
NAME 02704940063F
EXPNO 2
PROCNO 1

c-13 nmr500c
02704940014F/CDCl3

F2 - Acquisition Parameters
Date_ 20070910
Time 14.26
INSTRUM spect
PROBHD 5 mm GNP 1H/13
PULPROG zgpg30
TD 131072
SOLVENT CDCl3
NS 274
DS 4
SWH 40322.582 Hz
FIDRES 0.307637 Hz
AQ 1.6253426 sec
RG 8130
DM 12.400 usec
DE 6.00 usec
TE 300.0 K
D1 0.10000000 sec
d11 0.03000000 sec
MCREST 0.00000000 sec
MCWPK 0.01500000 sec

***** CHANNEL f1 *****
NUC1 13C
P1 2.50 usec
PL1 0.00 dB
SFO1 125.7703643 MHz

***** CHANNEL f2 *****
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 11.50 dB
PL12 11.50 dB
SFO2 500.1325006 MHz

F2 - Processing parameters
SI 65536
SF 125.7577890 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 0.20

1D NMR plot parameters
CX 23.50 cm
CY 10.00 cm
F1P 240.000 ppm
F1 30181.87 Hz
F2P -10.000 ppm
F2 125.013 Hz
PPHCH 10.63630 ppm/cm
HZCM 1337.84888 Hz/cm

