Catalytic Asymmetric Synthesis of Protected Tryptophan Regioisomers

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Analytical Data for compounds 4–13, and 22.

General procedure for synthesizing compound 4–13 are found in the main text.

N-Boc-2-formylindole (4a).¹ 2-formylindole **3a** (98 mg, 0.68 mmol) reacted to give *N*-Boc-2-formylindole **4a** (73 mg, 44%) as a yellow solid. mp: 70.4–72.6 °C; ¹H NMR (CDCl₃) δ 1.71 (s, 9H, CH₃), 7.30 (t, ³J_{HH} = 8.0 Hz, 1H, Ar), 7.44 (s, 1H, Ar), 7.48 (t, ³J_{HH} = 8.4 Hz, 1H, Ar), 7.68 (d, ³J_{HH} = 8.1 Hz, 1H, Ar), 8.17 (d, ³J_{HH} = 8.5 Hz, 1H, Ar), 10.44 (s, 1H, CHO); ¹³C NMR (CDCl₃) δ 28.22, 85.56, 115.99, 116.36, 123.11, 123.73, 127.44, 128.11, 137.74, 137.77, 149.72, 184.01; MS (CI) *m/z* 246 [M + H]⁺.

N-Boc-4-formylindole (4b). 4-formylindole **3b** (1.00 g, 6.9 mmol) reacted to give *N*-Boc-4-formylindole **4b** (1.54 g, 91%) as a yellow oil. ¹H NMR (CDCl₃) δ 1.69 (s, 9H, CH₃), 7.38 (dd, ³J_{HH} = 3.8 Hz, ⁵J_{HH} = 0.6 Hz, 1H, Ar), 7.47 (dd, ³J_{HH} = 8.1 Hz, ³J_{HH} = 7.6 Hz, 1H, Ar), 7.73 (dd, ³J_{HH} = 7.4 Hz, ⁴J_{HH} = 0.9 Hz, 1H, Ar), 7.77 (d, ³J_{HH} = 3.7 Hz, 1H, Ar), 8.47 (br d, ³J_{HH} = 8.3 Hz, 1H, Ar), 10.24 (s, 1H, CHO); ¹³C NMR (CDCl₃) δ 28.16, 84.41, 106.57, 120.93, 123.73, 128.25, 128.79, 128.92, 135.79, 149.21, 192.45. (11 C found); MS (CI) *m/z* 246 [M + H]⁺; HRMS (FAB) calcd for C₁₄H₁₆NO₃ [M + H]⁺ 246.1130, found 246.1123.

N-Boc-6-formylindole (4d).² 6-formylindole **3d** (1.9 g, 13 mmol) reacted in the same manner to give *N*-Boc-6-formylindole **4d** (3.3 g, 100%) as a yellow oil. ¹H NMR (CDCl₃) δ 1.71 (s, 9H, CH₃), 6.65 (dd, ³J_{HH} = 3.8 Hz, ⁵J_{HH} = 0.6 Hz, 1H, Ar), 7.67 (d, ³J_{HH} = 8.2 Hz, 1H, Ar), 7.78–7.81 (m, 2H, Ar), 8.68 (s, 1H, Ar), 10.08 (s, 1H, CHO); ¹³C

¹ Chinchilla, R.; Falvello, L. R.; Galindo, N.; Nájera, C. *J. Org. Chem.* **2000**, *65*, 3034–3041.

² Woolridge, E. M.; Rokita, S. E. *Tetrahedron Lett.* **1989**, *30*, 6117–6120.

NMR (CDCl₃) δ 28.16, 84.63, 107.28, 118.67, 121.31, 122.79, 129.56, 132.86, 134.78, 135.42, 149.08, 192.14; MS (CI) m/z 246 [M + H]⁺.

(Z)-N^α-acetyl-2,3-dehydro-3-(indol-2'-yl)-alanine, methyl ester (5a). Compound **5a** was isolated in 96% yield by recrystallization from ethyl acetate as a yellow solid. mp: 183.9–184.5 °C; ¹H NMR (CD₃OD) δ 2.21 (s, 3H, CH₃), 3.80 (s, 3H, OCH₃), 6.89 (s, 1H, Ar), 7.02 (td, ³J_{HH} = 7.5 Hz, ⁴J_{HH} = 0.7 Hz, 1H, Ar), 7.17 (td, ³J_{HH} = 7.6 Hz, ⁴J_{HH} = 1.0 Hz, 1H, Ar), 7.39 (dd, ³J_{HH} = 8.2 Hz, ⁴J_{HH} = 0.75 Hz, 1H, Ar), 7.50 (s, 1H, CH), 7.56 (br d, ³J_{HH} = 8.0 Hz, 1H, Ar); ¹³C NMR (CD₃OD) δ 22.81, 52.89, 108.74, 112.54, 121.15, 122.15, 124.16, 124.95, 126.93, 129.72, 132.48, 139.10, 167.03, 173.75; MS (CI) m/z 259 [M + H]⁺; Anal. Calcd for C₁₄H₁₄N₂O₃: C, 65.11; H, 5.46; N, 10.85. Found: C, 64.85; H, 5.45; N, 10.87.

(Z)-N^α-acetyl-2,3-dehydro-3-(indol-4'-yl)-alanine, methyl ester (5b). Compound **5b** was isolated in 58% yield by recrystallization from MeOH and flash chromatography (diethyl ether) of the remaining mother liquor as a white solid. mp: 183.1–183.5 °C; ¹H NMR (CD₃OD) δ 2.05 (s, 3H, CH₃), 3.83 (s, 3H, OCH₃), 6.52 (dd, ³J_{HH} = 3.1 Hz, ⁵J_{HH} = 0.7 Hz, 1H, Ar), 7.14 (t, ³J_{HH} = 7.8 Hz, 1H, Ar), 7.32 (d, ³J_{HH} = 3.2 Hz, 1H, Ar), 7.37 (d, ³J_{HH} = 7.5 Hz, 1H, Ar), 7.42 (d, ³J_{HH} = 8.1 Hz, 1H, Ar), 7.79 (s, 1H, CH); ¹³C NMR (CD₃OD) δ 22.48, 52.94, 100.83, 113.98, 121.04, 122.16, 125.81, 126.35, 126.93, 129.41, 133.21, 137.84, 167.54, 173.30; MS (CI) m/z 259 [M + H]⁺; Anal. Calcd for C₁₄H₁₄N₂O₃: C, 65.11; H, 5.46; N, 10.85. Found: C, 64.75; H, 5.53; N, 10.66.

(Z)-N^α-acetyl-2,3-dehydro-3-(indol-5'-yl)-alanine, methyl ester (5c). Compound **5c** was isolated in 55% yield by recrystallization from ethyl acetate as a white solid. mp: 187.0–187.9 °C; ¹H NMR (CD₃OD) δ 2.14 (s, 3H, CH₃), 3.79 (s, 3H, OCH₃), 6.49 (d, ³J_{HH}

= 3.1 Hz, 1H, Ar), 7.26 (d, $^3J_{\text{HH}} = 3.2$ Hz, 1H, Ar), 7.40–7.42 (m, 2H, Ar), 7.61 (s, 1H, CH), 7.85 (br s, 1H, Ar); ^{13}C NMR (CD_3OD) δ 22.59, 52.71, 103.30, 112.36, 123.01, 124.43, 124.51, 125.65, 126.88, 129.55, 138.42, 138.61, 167.73, 173.21; MS (CI) m/z 259 $[\text{M} + \text{H}]^+$; Anal. Calcd for $\text{C}_{14}\text{H}_{14}\text{N}_2\text{O}_3$: C, 65.11; H, 5.46; N, 10.85. Found: C, 64.83; H, 5.48; N, 10.67.

(Z)- N^α -acetyl-2,3-dehydro-3-(indol-6'-yl)-alanine, methyl ester (5d). Compound **5d** was isolated in 51% yield by recrystallization from ethyl acetate as a white solid. mp: 169.2–171.3 °C; ^1H NMR (CD_3OD) δ 2.15 (s, 3H, CH_3), 3.79 (s, 3H, OCH_3), 6.46 (s, 1H, Ar), 7.28 (d, $^3J_{\text{HH}} = 8.0$ Hz, 1H, Ar), 7.34 (d, $^3J_{\text{HH}} = 2.8$ Hz, 1H, Ar), 7.55 (d, $^3J_{\text{HH}} = 8.4$ Hz, 1H, Ar), 7.59 (s, 1H, CH), 7.71 (br s, 1H, Ar); ^{13}C NMR (CD_3OD) δ 22.61, 52.81, 102.62, 114.57, 121.14, 122.42, 123.43, 127.31, 128.33, 130.93, 137.37, 138.13, 167.45, 173.23; MS (CI) m/z 259 $[\text{M} + \text{H}]^+$; Anal. Calcd for $\text{C}_{14}\text{H}_{14}\text{N}_2\text{O}_3$: C, 65.11; H, 5.46; N, 10.85. Found: C, 64.82; H, 5.60; N, 10.94.

(Z)- N^α -acetyl- N^{in} -Boc-2,3-dehydro-3-(indol-4'-yl)-alanine, methyl ester (6b). Compound **6b** was isolated in 68% yield by recrystallization from ethyl acetate and flash chromatography of the remaining mother liquor as a yellow solid. mp: 150.5–151.8 °C; ^1H NMR (CDCl_3) δ 1.68 (s, 9H, CH_3), 2.05 (s, 3H, Ac), 3.88 (s, 3H, OCH_3), 6.62 (br s, 1H, Ar), 7.04 (br s, 1H, NH), 7.27–7.35 (m, 2H, Ar), 7.58 (s, 1H, Ar), 7.64 (d, $^3J_{\text{HH}} = 3.0$ Hz, 1H, Ar), 8.16 (d, $^3J_{\text{HH}} = 7.2$ Hz, 1H, Ar); ^{13}C NMR (CDCl_3) δ 23.22, 28.15, 52.68, 84.05, 105.47, 116.05, 122.63, 124.03, 125.70, 125.90, 126.53, 128.07, 129.76, 135.17, 149.31, 165.43, 168.76; MS (CI) m/z 359 $[\text{M} + \text{H}]^+$; HRMS (FAB) calcd for $\text{C}_{19}\text{H}_{23}\text{N}_2\text{O}_5$ $[\text{M} + \text{H}]^+$ 359.1607, found 359.1607.

(Z)-N^α-acetyl-Nⁱⁿ-Boc-2,3-dehydro-3-(indol-6'-yl)-alanine, methyl ester (6d).

Compound **6d** was isolated in 46% yield by flash chromatography (diethyl ether) as a yellow solid. mp: 119.5–121.2 °C; ¹H NMR (CDCl₃) δ 1.65 (s, 9H, CH₃), 2.21 (s, 3H, Ac), 3.86 (s, 3H, OCH₃), 6.54 (br d, ³J_{HH} = 3.6 Hz, 1H, Ar), 7.09 (br s, 1H, NH), 7.35 (d, ³J_{HH} = 8.1 Hz, 1H, Ar), 7.51–7.61 (m, 3H, Ar), 8.46 (br s, 1H, Ar); ¹³C NMR (CDCl₃) δ 23.49, 28.14, 52.58, 83.81, 107.10, 116.57, 120.67, 122.89, 124.79, 127.56, 129.53, 131.39, 133.52, 135.26, 149.17, 165.85, 168.78; MS (CI) *m/z* 359 [M + H]⁺; Anal. Calcd for C₁₉H₂₂N₂O₅: C, 63.68; H, 6.19; N, 7.82. Found: C, 63.83; H, 6.13; N, 7.60.

(Z)-N^α-Cbz-Nⁱⁿ-Boc-2,3-dehydro-3-(indol-4'-yl)-alanine, methyl ester (7b).

Compound **7b** was isolated in 83% yield by flash chromatography (20% ethyl acetate in hexane) as a yellow solid. mp: 83.4–84.7 °C; ¹H NMR (CD₃OD) δ 1.65 (s, 9H, CH₃), 3.80 (br s, 3H, OCH₃), 5.07 (br s, 2H, CH₂), 6.64 (d, ³J_{HH} = 3.8 Hz, 1H, Ar), 7.21–7.32 (m, 6H, Ph, Ar), 7.52 (br d, ³J_{HH} = 7.5 Hz, 1H, Ar), 7.57 (d, ³J_{HH} = 3.8 Hz, 1H, Ar), 7.64 (s, 1H, CH) 8.11 (d, ³J_{HH} = 8.3 Hz, 1H, Ar); ¹³C NMR (CD₃OD) δ 28.38, 53.04, 67.92, 85.16, 106.41, 116.98, 124.03, 125.03, 126.98, 127.20, 127.49, 128.78, 128.88, 129.16, 129.23, 130.67, 131.43, 136.47, 150.56, 156.68, 167.24; MS (CI) *m/z* 451 [M + H]⁺; Anal. Calcd for C₂₅H₂₆N₂O₆: C, 66.66; H, 5.82; N, 6.22. Found: C, 66.78; H, 5.94; N, 6.30.

(Z)-N^α-Cbz-Nⁱⁿ-Boc-2,3-dehydro-3-(indol-5'-yl)-alanine, methyl ester (7c).

Compound **7c** was isolated in 85% yield by flash chromatography (20% ethyl acetate in hexane) as a yellow solid. mp: 125.3–126.5 °C; ¹H NMR (CD₃OD) δ 1.67 (s, 9H, CH₃), 3.79 (br s, 3H, OCH₃), 5.15 (br s, 2H, CH₂), 6.59 (d, ³J_{HH} = 3.7 Hz, 1H, Ar), 7.21–7.45 (m, 5H, Ph), 7.52 (s, 1H, Ar), 7.57 (dd, ³J_{HH} = 8.9 Hz, ⁴J_{HH} = 1.5 Hz, 1H, Ar), 7.64 (d,

$^3J_{\text{HH}} = 3.7$ Hz, 1H, Ar), 7.85 (s, 1H, CH), 8.08 (d, $^3J_{\text{HH}} = 8.7$ Hz, 1H, Ar); ^{13}C NMR (CD_3OD) δ 28.38, 52.90, 67.97, 85.33, 108.56, 115.95, 124.31, 124.94, 127.29, 127.78, 128.63, 128.75, 128.93, 129.30, 132.04, 136.14, 136.85, 138.02, 150.58, 157.10, 167.55; MS (CI) m/z 451 $[\text{M} + \text{H}]^+$; Anal. Calcd for $\text{C}_{25}\text{H}_{26}\text{N}_2\text{O}_6$: C, 66.66; H, 5.82; N, 6.22. Found: C, 66.32; H, 5.74; N, 6.13.

Ring-closed olefination product of 2a (8). Compound **8** was isolated in 59 % yield by flash chromatography (CH_2Cl_2), and then purified further by recrystallization (CH_2Cl_2) as a yellow solid. mp: 220.7–221.8 °C; ^1H NMR (CDCl_3) δ 3.98 (s, 3H, OCH_3), 6.88 (s, 1H, Ar), 7.30 (d, $^4J_{\text{HH}} = 1.9$ Hz, 1H, CH), 7.40 (td, $^3J_{\text{HH}} = 7.4$ Hz, $^4J_{\text{HH}} = 1.0$ Hz, 1H, Ar), 7.44 (td, $^3J_{\text{HH}} = 8.1$ Hz, $^4J_{\text{HH}} = 1.2$ Hz, 1H, Ar), 7.70 (d, $^3J_{\text{HH}} = 7.6$ Hz, 1H, Ar), 8.23 (br s, 1H, NH), 8.67 (d, $^3J_{\text{HH}} = 8.3$ Hz, 1H, Ar); ^{13}C NMR (CDCl_3) δ 53.16, 104.18, 104.87, 116.24, 120.55, 124.26, 124.46, 130.24, 133.34, 133.88, 147.10, 161.89 (12 C found); MS (CI) m/z 243 $[\text{M} + \text{H}]^+$; HRMS (FAB) calcd for $\text{C}_{13}\text{H}_{11}\text{N}_2\text{O}_3$ $[\text{M} + \text{H}]^+$ 243.0770, found 243.0772.

N-Me Ring-closed olefination product of 2a (9). Compound **9** was isolated in 35 % yield by flash chromatography (CH_2Cl_2), and purified further by recrystallization (CH_2Cl_2) as a yellow solid. mp: 203.0–204.1 °C; ^1H NMR (CDCl_3) δ 3.73 (s, 3H, NCH_3), 3.92 (s, 3H, OCH_3), 6.75 (s, 1H, Ar), 7.27 (s, 1H, CH), 7.37 (td, $^3J_{\text{HH}} = 7.2$ Hz, $^4J_{\text{HH}} = 1.5$ Hz, 1H, Ar), 7.42 (td, $^3J_{\text{HH}} = 7.2$ Hz, $^4J_{\text{HH}} = 1.7$ Hz, 1H, Ar), 7.67 (d, $^3J_{\text{HH}} = 7.1$ Hz, 1H, Ar), 8.69 (d, $^3J_{\text{HH}} = 8.5$ Hz, 1H, Ar); ^{13}C NMR (CDCl_3) δ 33.51, 52.79, 102.46, 107.15, 116.32, 120.29, 124.02, 124.06, 129.01, 130.23, 131.94, 133.79, 148.83, 162.59; MS (CI) m/z 257 $[\text{M} + \text{H}]^+$; Anal. Calcd for $\text{C}_{14}\text{H}_{12}\text{N}_2\text{O}_3$: C, 65.62; H, 4.72; N, 10.93. Found: C, 65.35; H, 4.82; N, 10.85.

Ring-closed olefination product of 2e (10). Compound **10** was isolated in 76 % yield by recrystallization (CH₂Cl₂) as a yellow solid. mp: 134.5–136.0 °C; ¹H NMR (CDCl₃) δ 3.89 (s, 3H, OCH₃), 6.49 (d, ³J_{HH} = 3.4 Hz, 1H, Ar), 6.69 (d, ⁴J_{HH} = 1.2 Hz, 1H, CH), 6.79 (d, ³J_{HH} = 7.2 Hz, 1H, Ar), 7.01 (t, ³J_{HH} = 7.6 Hz, 1H, Ar), 7.31 (d, ³J_{HH} = 8.0 Hz, 1H, Ar), 7.34 (br s, 1H, NH), 7.74 (d, ³J_{HH} = 3.6 Hz, 1H, Ar); ¹³C NMR (CDCl₃) δ 53.50, 107.38, 117.13, 120.59, 122.47, 123.17, 123.48, 124.67, 126.65, 131.34, 133.03, 148.93, 163.16; MS (CI) *m/z* 243 [M + H]⁺; Anal. Calcd for C₁₃H₁₀N₂O₃: C, 64.46; H, 4.16; N, 11.56. Found: C, 64.48; H, 4.25; N, 11.34.

(S)-N^α-acetyl-3-(indol-2'-yl)-alanine, methyl ester [(S)-11a]. Hydrogenation was performed in ethyl acetate. HPLC analysis (AD column) indicated 98.6 %ee and 92% conversion. [α]_D²⁵ = +34.3° (c 0.755, MeOH); ¹H NMR (CD₃OD) δ 1.92 (s, 3H, CH₃), 3.14 (dd, ²J_{HH} = 15.1 Hz, ³J_{HH} = 8.5 Hz, 1H, CH₂), 3.27 (dd, ²J_{HH} = 15.0 Hz, ³J_{HH} = 5.8 Hz, 1H, CH₂), 3.68 (s, 3H, OCH₃), 4.79 (dd, ³J_{HH} = 8.6 Hz, 5.6 Hz, 1H, CH), 6.19 (d, ⁵J_{HH} = 0.5 Hz, 1H, Ar), 6.93 (td, ³J_{HH} = 7.0 Hz, ⁴J_{HH} = 1.1 Hz, 1H, Ar), 7.02 (td, ³J_{HH} = 7.1 Hz, ⁴J_{HH} = 1.2 Hz, 1H, Ar), 7.27 (dd, ³J_{HH} = 8.0 Hz, ⁴J_{HH} = 0.7 Hz, 1H, Ar), 7.41 (dd, ³J_{HH} = 7.6 Hz, ⁴J_{HH} = 0.8 Hz, 1H, Ar); ¹³C NMR (CD₃OD) δ 22.31, 31.33, 52.80, 53.98, 101.51, 111.57, 119.93, 120.49, 121.82, 129.86, 135.27, 137.93, 173.11, 173.23; MS (CI) *m/z* 261 [M + H]⁺; HRMS (FAB) calcd for C₁₄H₁₇N₂O₃ [M + H]⁺ 261.1239, found 261.1239.

(S)-N^α-acetyl-3-(indol-4'-yl)-alanine, methyl ester [(S)-11b]. HPLC analysis (OD column) indicated 99.1 %ee. [α]_D²⁵ = -1.93° (c 0.88, MeOH); ¹H NMR (CD₃OD) δ 1.87 (s, 3H, CH₃), 3.20 (dd, ²J_{HH} = 13.7 Hz, ³J_{HH} = 8.3 Hz, 1H, CH₂), 3.40 (dd, ²J_{HH} = 13.7 Hz, ³J_{HH} = 6.0 Hz, 1H, CH₂), 3.62 (s, 3H, OCH₃), 4.78 (dd, ³J_{HH} = 8.0 Hz, 6.2 Hz, 1H, CH), 6.51 (dd, ³J_{HH} = 3.2 Hz, ⁵J_{HH} = 0.7 Hz, 1H, Ar), 6.81 (d, ³J_{HH} = 7.2 Hz, 1H, Ar), 7.01 (td

$^3J_{\text{HH}} = 7.2$ Hz, 1H, Ar), 7.22 (d, $^3J_{\text{HH}} = 3.2$ Hz, 1H, Ar), 7.26 (d, $^3J_{\text{HH}} = 8.2$ Hz, 1H, Ar); ^{13}C NMR (CD_3OD) δ 22.34, 36.47, 52.61, 54.93, 100.20, 111.10, 120.40, 122.06, 125.37, 128.78, 129.10, 137.48, 172.92, 173.77; MS (CI) m/z 261 $[\text{M} + \text{H}]^+$; HRMS (FAB) calcd for $\text{C}_{14}\text{H}_{17}\text{N}_2\text{O}_3$ $[\text{M} + \text{H}]^+$ 261.1239, found 261.1236.

(S)-N α -acetyl-3-(indol-5'-yl)-alanine, methyl ester [(S)-11c]. HPLC analysis (OD column) indicated 98.0 %ee. $[\alpha]_{\text{D}}^{25} = +38.7^\circ$ (c 0.82, MeOH); ^1H NMR (CD_3OD) δ 1.88 (s, 3H, CH_3), 3.00 (dd, $^2J_{\text{HH}} = 13.8$ Hz, $^3J_{\text{HH}} = 8.6$ Hz, 1H, CH_2), 3.18 (dd, $^2J_{\text{HH}} = 13.8$ Hz, $^3J_{\text{HH}} = 5.9$ Hz, 1H, CH_2), 3.65 (s, 3H, OCH_3), 4.65 (dd, $^3J_{\text{HH}} = 8.5$ Hz, 5.9 Hz, 1H, CH), 6.37 (dd, $^3J_{\text{HH}} = 3.2$ Hz, $^5J_{\text{HH}} = 0.9$ Hz, 1H, Ar), 6.93 (dd, $^3J_{\text{HH}} = 8.3$ Hz, $^4J_{\text{HH}} = 1.6$ Hz, 1H, Ar), 7.18 (d, $^3J_{\text{HH}} = 2.9$ Hz, 1H, Ar), 7.29 (d, $^3J_{\text{HH}} = 8.3$ Hz, 1H, Ar), 7.35 (d, $^4J_{\text{HH}} = 0.8$ Hz, 1H, Ar); ^{13}C NMR (CD_3OD) δ 22.28, 38.79, 52.56, 56.11, 101.99, 111.99, 121.39, 123.28, 125.78, 128.02, 129.47, 136.58, 172.94, 173.76; MS (CI) m/z 261 $[\text{M} + \text{H}]^+$; HRMS (FAB) calcd for $\text{C}_{14}\text{H}_{17}\text{N}_2\text{O}_3$ $[\text{M} + \text{H}]^+$ 261.1239, found 261.1236.

(S)-N α -acetyl-3-(indol-6'-yl)-alanine, methyl ester [(S)-11d]. HPLC analysis (AD column) indicated 96.7 %ee. $[\alpha]_{\text{D}}^{25} = +28.6^\circ$ (c 1.13, MeOH); ^1H NMR (CD_3OD) δ 1.89 (s, 3H, CH_3), 3.03 (dd, $^2J_{\text{HH}} = 13.8$ Hz, $^3J_{\text{HH}} = 8.4$ Hz, 1H, CH_2), 3.19 (dd, $^2J_{\text{HH}} = 13.8$ Hz, $^3J_{\text{HH}} = 5.9$ Hz, 1H, CH_2), 3.65 (s, 3H, OCH_3), 4.67 (dd, $^3J_{\text{HH}} = 8.4$ Hz, 5.9 Hz, 1H, CH), 6.37 (d, $^3J_{\text{HH}} = 3.1$ Hz, $^5J_{\text{HH}} = 0.9$ Hz, 1H, Ar), 6.84 (dd, $^3J_{\text{HH}} = 8.1$ Hz, $^4J_{\text{HH}} = 1.4$ Hz, 1H, Ar), 7.16 (d, $^3J_{\text{HH}} = 3.2$ Hz, 1H, Ar), 7.20 (br s, 1H, Ar), 7.44 (d, $^3J_{\text{HH}} = 8.1$ Hz, 1H, Ar); ^{13}C NMR (CD_3OD) δ 22.30, 38.88, 52.27, 55.94, 102.02, 112.36, 120.97, 121.29, 125.48, 128.26, 130.57, 137.66, 172.92, 173.65; MS (CI) m/z 261 $[\text{M} + \text{H}]^+$; HRMS (FAB) calcd for $\text{C}_{14}\text{H}_{17}\text{N}_2\text{O}_3$ $[\text{M} + \text{H}]^+$ 261.1239, found 261.1237.

(S)-N^α-acetyl-NⁱⁿBoc-3-(indol-4'-yl)-alanine, methyl ester [(S)-12b]. HPLC analysis (OD column) indicated 98.9 %ee. $[\alpha]^{25}_D = +11.0^\circ$ (*c* 0.89, MeOH); ¹H NMR (CD₃OD) δ 1.66 (s, 9H, CH₃), 1.87 (s, 3H, CH₃), 3.20 (dd, ²*J*_{HH} = 13.8 Hz, ³*J*_{HH} = 8.3 Hz, 1H, CH₂), 3.38 (dd, ²*J*_{HH} = 13.9 Hz, 6.2 Hz, 1H, CH₂), 3.64 (s, 3H, OCH₃), 4.60 (dd, ³*J*_{HH} = 8.2 Hz, 6.2 Hz, 1H, CH), 6.70 (d, ³*J*_{HH} = 3.8 Hz, 1H, Ar), 7.03 (d, ³*J*_{HH} = 7.3 Hz, 1H, Ar), 7.21 (t, ³*J*_{HH} = 7.9 Hz, 1H, Ar), 7.62 (d, ³*J*_{HH} = 3.8 Hz, 1H, Ar), 8.02 (d, ³*J*_{HH} = 8.3 Hz, 1H, Ar); ¹³C NMR (CD₃OD) δ 22.32, 28.40, 35.86, 52.70, 54.91, 84.92, 106.18, 114.76, 124.28, 125.09, 126.67, 130.29, 131.29, 136.44, 150.80, 172.86, 173.29; MS (CI) *m/z* 361 [M + H]⁺; HRMS (FAB) calcd for C₁₉H₂₅N₂O₅ [M + H]⁺ 361.1763, found 361.1768.

(S)-N^α-acetyl-NⁱⁿBoc-3-(indol-6'-yl)-alanine, methyl ester [(S)-12d]. HPLC analysis (OD column) indicated 98.5 %ee. $[\alpha]^{25}_D = +23.7^\circ$ (*c* 1.10, MeOH); ¹H NMR (CD₃OD) δ 1.66 (s, 9H, CH₃), 1.91 (s, 3H, CH₃), 3.07 (dd, ²*J*_{HH} = 13.8 Hz, ³*J*_{HH} = 8.6 Hz, 1H, CH₂), 3.23 (dd, ²*J*_{HH} = 13.5 Hz, 6.0 Hz, 1H, CH₂), 3.68 (s, 3H, OCH₃), 4.69 (dd, ³*J*_{HH} = 8.2 Hz, 6.2 Hz, 1H, CH), 6.55 (d, ³*J*_{HH} = 3.6 Hz, 1H, Ar), 7.05 (dd, ³*J*_{HH} = 8.0 Hz, ⁴*J*_{HH} = 1.2 Hz, 1H, Ar), 7.46 (d, ³*J*_{HH} = 8.0 Hz, 1H, Ar), 7.54 (d, ³*J*_{HH} = 4.0 Hz, 1H, Ar), 8.00 (br s, 1H, Ar); ¹³C NMR (CD₃OD) δ 22.33, 28.41, 39.00, 52.66, 55.78, 84.83, 108.10, 116.48, 121.71, 124.90, 126.72, 130.74, 134.05, 136.63, 150.81, 172.89, 173.33; MS (CI) *m/z* 361 [M + H]⁺; HRMS (FAB) calcd for C₁₉H₂₅N₂O₅ [M + H]⁺ 361.1763, found 361.1754.

(S)-N^α-Cbz-NⁱⁿBoc-3-(indol-4'-yl)-alanine, methyl ester [(S)-13b]. The (S,S)-MeDuPhos catalyst was used. HPLC analysis (OD column) indicated 98.9 %ee. $[\alpha]^{25}_D = -13.4^\circ$ (*c* 0.685, MeOH); ¹H NMR (CD₃OD) δ 1.66 (s, 9H, CH₃), 3.18 (dd, ²*J*_{HH} = 13.9 Hz, ³*J*_{HH} = 8.7 Hz, 1H, CH₂), 3.38 (dd, ²*J*_{HH} = 13.8 Hz, ³*J*_{HH} = 5.7 Hz, 1H, CH₂), 3.65 (s, 3H, OCH₃), 4.54 (dd, ³*J*_{HH} = 8.8 Hz, 5.7 Hz, 1H, CH), 4.95 (d, ²*J*_{HH} = 12.6 Hz, 1H, CH₂),

5.01 (d, $^2J_{\text{HH}} = 12.5$ Hz, 1H, CH₂), 6.68 (d, $^3J_{\text{HH}} = 3.8$ Hz, 1H, Ar), 7.02 (d, $^3J_{\text{HH}} = 7.3$ Hz, 1H, Ar), 7.19 (t, $^3J_{\text{HH}} = 7.9$ Hz, 1H, Ar), 7.20-7.33 (m, 5H, Ph), 7.57 (d, $^3J_{\text{HH}} = 3.8$ Hz, 1H, Ar), 8.01 (d, $^3J_{\text{HH}} = 8.3$ Hz, 1H, Ar); ¹³C NMR (CD₃OD) δ 28.41, 36.05, 52.73, 56.54, 84.88, 106.23, 114.71, 124.43, 125.09, 126.64, 128.47, 128.73, 129.21, 130.41, 131.21, 136.42, 137.97, 150.81, 158.02, 173.62; MS (CI) m/z 453 [M + H]⁺; HRMS (FAB) calcd for C₂₅H₂₉N₂O₆ [M + H]⁺ 453.2026, found 453.2033.

(R)-N α -Cbz-NⁱⁿBoc-3-(indol-5'-yl)-alanine, methyl ester [(R)-13c]. The (R,R)-MeDuPhos catalyst and CH₂Cl₂ solvent were used. HPLC analysis (AD column) indicated 97.5 %ee. $[\alpha]_{\text{D}}^{25} = +6.98^\circ$ (c 0.86, MeOH); ¹H NMR (CD₃OD) δ 1.65 (s, 9H, CH₃), 2.99 (dd, $^2J_{\text{HH}} = 13.7$ Hz, $^3J_{\text{HH}} = 9.3$ Hz, 1H, CH₂), 3.22 (dd, $^2J_{\text{HH}} = 13.8$ Hz, $^3J_{\text{HH}} = 5.4$ Hz, 1H, CH₂), 3.68 (s, 3H, OCH₃), 4.48 (dd, $^3J_{\text{HH}} = 9.1$ Hz, 5.5 Hz, 1H, CH), 4.95 (d, $^2J_{\text{HH}} = 12.6$ Hz, 1H, CH₂), 5.02 (d, $^2J_{\text{HH}} = 12.6$ Hz, 1H, CH₂), 6.52 (d, $^3J_{\text{HH}} = 3.8$ Hz, 1H, Ar), 7.12 (dd, $^3J_{\text{HH}} = 8.6$ Hz, $^4J_{\text{HH}} = 1.4$ Hz, 1H, Ar), 7.19–7.28 (m, 5H, Ph), 7.38 (br s, 1H, Ar), 7.57 (d, $^3J_{\text{HH}} = 3.7$ Hz, 1H, Ar), 8.00 (d, $^3J_{\text{HH}} = 8.5$ Hz, 1H, Ar); ¹³C NMR (CD₃OD) δ 28.41, 38.60, 52.68, 57.27, 67.42, 84.81, 108.21, 115.76, 122.36, 126.34, 126.96, 128.38, 128.68, 129.19, 132.07, 132.43, 135.38, 138.00, 150.85, 158.10, 173.77; MS (CI) m/z 453 [M + H]⁺; HRMS (FAB) calcd for C₂₅H₂₉N₂O₆ [M + H]⁺ 453.2026, found 453.2034.

The enantiomers of **13d** could not be resolved with any of the chiral stationary phases tried. Thus **13d** was transformed to the N α -Ac-Nⁱⁿ-Boc-2',3'-dihydro-derivative **22** as follows:

(R)-N α -Ac-NⁱⁿBoc-3-(2',3'-dihydroindol-6'-yl)-alanine, methyl ester (22). A 10 mL round bottomed flask was charged with (R)-**13d** (5 mg, 0.01 mmol), Pd/C (10 mg). MeOH (4 mL) and acetic anhydride (1 mL) was then added. It was then charged with H₂

at 1 atm, and stirred at room temperature overnight. The mixture was then filtered, concentrated in vacuo, dissolved in ethyl acetate, and passed through a short plug of SiO₂ before HPLC analysis (OD column), which indicated 96.9 %ee. ¹H NMR (CD₃OD) δ 1.55 (br s, 9H, CH₃), 1.91 (s, 3H, CH₃), 2.91 (dd, ²*J*_{HH} = 13.6 Hz, ³*J*_{HH} = 8.4 Hz, 1H, CH₂), 3.01 (t, ³*J*_{HH} = 8.6 Hz, 2H, CH₂), 3.07 (dd, ²*J*_{HH} = 13.8 Hz, ³*J*_{HH} = 6.0 Hz, 1H, CH₂), 3.26 (s, 3H, OCH₃), 3.92 (t, ³*J*_{HH} = 8.6 Hz, 2H, CH₂), 4.62 (dd, ³*J*_{HH} = 8.5 Hz, 5.7 Hz, 1H, CH), 6.76 (dd, ³*J*_{HH} = 7.6 Hz, ⁴*J*_{HH} = 1.6 Hz, 1H, Ar), 7.06 (d, ³*J*_{HH} = 7.6 Hz, 1H, Ar), 7.62 (br s, 1H, Ar); ¹³C NMR (CDCl₃) δ 23.11, 27.03, 28.37, 37.91, 47.77, 52.30, 53.21, 80.34, 115.52, 122.80, 124.51, 129.85, 135.04, 143.37, 152.36, 169.55, 172.07; MS (CI) *m/z* 363 [M + H]⁺; HRMS (FAB) calcd for C₁₉H₂₇N₂O₅ [M + H]⁺ 363.1920, found 363.1914.

Table S1. Summary of Experimental Details for HPLC Enantiomeric Excess Determination.

amino acid	Daicel column used	eluent (% <i>i</i> -PrOH in hexane) ^a	retention time of major ^b (<i>S</i>) enantiomer (min)	retention time of minor ^b (<i>R</i>) enantiomer (min)	retention times of overhydrogenation products (min) ^c
11a	AD	gradient ^d	15.0	12.6	11.7
11b	OD	20	23.6	14.0	nd
11c	OD	15	26.0	18.7	nd
11d	AD	20	10.1	7.6	nd
11e	OD	10	16.5	12.9	21.6
12b	OD	5	22.7	17.6	30.7, 42.4
12c	OD	10	13.9	11.1	10.1, 13.8
12d	OD	5	17.4	14.3	20.2

13b	OD	5	21.8	24.0	36.1
13c	AD	10	18.8	23.3	26.8
13d	OD	5	30.4 ^e	20.3 ^e	na

^a Flow rate: 1 mL/min. ^b In reactions using (*S,S*)-DuPhos ligands. ^c Overhydrogenation products were observed at elevated pressures, or in the case of **12** and **13**, when methanol was used as the hydrogenation solvent. nd: not detected; na: not applicable (see procedure). ^d Gradient conditions: 0 min: 10%; 15 min: 15%; 20 min: 50%; 30 min: 50%. ^e *N*^α-Ac-*N*ⁱⁿ-Boc-2',3'-dihydro derivative of **13d**.

Table S2. List of ligands and complexes in calculations.

	Ligand	η ⁶ Complex	η ⁵ Complex
Indole	14a	14b	14c
<i>N</i> -Me indole	15a	15b	15c
2-Me indole	16a	16b	16c
3-Me indole	17a	17b	17c
4-Me indole	18a	18b	18c
5-Me indole	19a	19b	19c
6-Me indole	20a	20b	20c
7-Me indole	21a	21b	21c

Table S3. Energies for compounds **14–21**.

	6-31G** Absolute Energy (a.u.) ^a	Zero Point Vibrational Energy (ZPVE) (kcal/mol) ^b	ZPVE Corrected Absolute Energy (a.u.)
Na⁺	-161.6592884	N/A	-161.6592884
14a	-361.4829178	78.3815	-361.3579991
14b	-523.1941831	79.2969	-523.0678056
14c	-523.1884604	79.1629	-523.0622964
15a	-400.5146122	95.1479	-400.3629723

15b	-562.2275917	95.9716	-562.0746391
15c	-562.2216668	95.7873	-562.0690080
16a	-400.5276780	94.8350	-400.3765368
16b	-562.2415446	95.7351	-562.0889689
16c	-562.2351562	95.6002	-562.0827955
17a	-400.5242550	94.9196	-400.3729791
17b	-562.2364210	95.8421	-562.0836748
17c	-562.2312926	95.7846	-562.0786381
18a	-400.5239258	94.9231	-400.3726442
18b	-562.2366583	95.8430	-562.0839107
18c	-562.2306768	95.6713	-562.0782029
19a	-400.5221746	94.7919	-400.3711022
19b	-562.2346701	95.7342	-562.0820959
19c	-562.2296737	95.5975	-562.0773173
20a	-400.5228110	94.8027	-400.3717214
20b	-562.2353168	95.7396	-562.0827340
20c	-562.2304897	95.6002	-562.0781290
21a	-400.5236713	94.9240	-400.3723883
21b	-562.2365291	95.8385	-562.0837886
21c	-562.2304208	95.6650	-562.0779569

^a HF/6-31G**//HF/6-31G**;^b Scaled by 0.8992.

PDB files for compounds 14–21.

14a. Indole (LCH0004)

HEADER

REMARK Spartan `02 exported Molecule001

HETATM	1	C	UNK	0001	0.293	-0.678	0.000
HETATM	2	C	UNK	0001	-2.078	0.709	0.000
HETATM	3	C	UNK	0001	0.312	0.722	0.000

HETATM	4	C	UNK	0001	-0.897	-1.404	0.000
HETATM	5	C	UNK	0001	-2.074	-0.695	0.000
HETATM	6	C	UNK	0001	-0.901	1.418	0.000
HETATM	7	H	UNK	0001	-0.896	-2.481	0.000
HETATM	8	H	UNK	0001	-3.011	-1.224	0.000
HETATM	9	H	UNK	0001	-0.911	2.495	0.000
HETATM	10	H	UNK	0001	-3.019	1.232	0.000
HETATM	11	C	UNK	0001	1.698	1.118	0.000
HETATM	12	H	UNK	0001	2.086	2.116	0.000
HETATM	13	C	UNK	0001	2.425	-0.017	0.000
HETATM	14	H	UNK	0001	3.489	-0.146	0.000
HETATM	15	N	UNK	0001	1.594	-1.109	0.000
HETATM	16	H	UNK	0001	1.890	-2.055	0.000
CONNECT	1	4	3	15			
CONNECT	2	5	6	10			
CONNECT	3	6	1	11			
CONNECT	4	1	5	7			
CONNECT	5	4	2	8			
CONNECT	6	2	3	9			
CONNECT	7	4					
CONNECT	8	5					
CONNECT	9	6					
CONNECT	10	2					
CONNECT	11	12	3	13			
CONNECT	12	11					
CONNECT	13	14	11	15			
CONNECT	14	13					
CONNECT	15	16	13	1			
CONNECT	16	15					

END

14b. η^6 -Indole•Na⁺ (LCH0005)

HEADER

REMARK Spartan `02 exported Molecule001

HETATM	1	Na	UNK	0001	1.071	-0.136	2.248
HETATM	2	H	UNK	0001	2.957	-1.213	-0.332
HETATM	3	C	UNK	0001	2.020	-0.695	-0.231
HETATM	4	C	UNK	0001	-0.368	0.693	-0.087
HETATM	5	C	UNK	0001	2.011	0.714	-0.204
HETATM	6	C	UNK	0001	0.838	-1.413	-0.177
HETATM	7	C	UNK	0001	-0.380	-0.719	-0.095
HETATM	8	C	UNK	0001	0.825	1.423	-0.127
HETATM	9	H	UNK	0001	2.942	1.248	-0.275
HETATM	10	H	UNK	0001	0.851	-2.487	-0.228
HETATM	11	H	UNK	0001	0.824	2.498	-0.140
HETATM	12	C	UNK	0001	-1.763	-1.120	-0.058

HETATM	13	H	UNK	0001	-2.147	-2.119	-0.071
HETATM	14	C	UNK	0001	-2.490	0.016	-0.041
HETATM	15	H	UNK	0001	-3.554	0.141	-0.031
HETATM	16	N	UNK	0001	-1.665	1.113	-0.039
HETATM	17	H	UNK	0001	-1.972	2.055	-0.112
HETATM	18	Lig	UNK	0001	0.824	0.001	-0.153
CONECT	1	18					
CONECT	2	3					
CONECT	3	2	6	5			
CONECT	4	7	8	16			
CONECT	5	8	3	9			
CONECT	6	3	7	10			
CONECT	7	6	4	12			
CONECT	8	4	5	11			
CONECT	9	5					
CONECT	10	6					
CONECT	11	8					
CONECT	12	13	7	14			
CONECT	13	12					
CONECT	14	15	12	16			
CONECT	15	14					
CONECT	16	17	14	4			
CONECT	17	16					
CONECT	18	1					

END

14c. η^5 -Indole•Na⁺ (LCH0006)

HEADER

REMARK Spartan `02 exported Molecule001

HETATM	1	Na	UNK	0001	-1.126	-0.028	-2.285
HETATM	2	H	UNK	0001	-2.020	-2.111	0.272
HETATM	3	C	UNK	0001	-1.634	-1.114	0.197
HETATM	4	C	UNK	0001	-2.365	0.024	0.220
HETATM	5	H	UNK	0001	-3.424	0.153	0.315
HETATM	6	N	UNK	0001	-1.533	1.123	0.108
HETATM	7	H	UNK	0001	-1.812	2.044	0.365
HETATM	8	C	UNK	0001	-0.219	0.683	0.126
HETATM	9	C	UNK	0001	-0.239	-0.718	0.139
HETATM	10	C	UNK	0001	0.975	-1.424	0.100
HETATM	11	H	UNK	0001	0.984	-2.499	0.123
HETATM	12	C	UNK	0001	2.148	-0.713	0.057
HETATM	13	H	UNK	0001	3.088	-1.233	0.040
HETATM	14	C	UNK	0001	2.145	0.695	0.047
HETATM	15	H	UNK	0001	3.083	1.220	0.024
HETATM	16	C	UNK	0001	0.973	1.412	0.074
HETATM	17	H	UNK	0001	0.976	2.487	0.078

HETATM	18	Lig	UNK	0001	-1.198	-0.001	0.158
CONNECT	1	18					
CONNECT	2	3					
CONNECT	3	2	9	4			
CONNECT	4	6	3	5			
CONNECT	5	4					
CONNECT	6	8	4	7			
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CONNECT	8	9	6	16			
CONNECT	9	3	8	10			
CONNECT	10	11	9	12			
CONNECT	11	10					
CONNECT	12	13	10	14			
CONNECT	13	12					
CONNECT	14	15	12	16			
CONNECT	15	14					
CONNECT	16	17	14	8			
CONNECT	17	16					
CONNECT	18	1					

END

15a. *N*-Methylindole (LCH0008)

HEADER

REMARK Spartan `02 exported Molecule001

HETATM	1	C	UNK	0001	0.058	-0.201	0.002
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HETATM	3	C	UNK	0001	-0.608	1.033	0.000
HETATM	4	C	UNK	0001	-0.634	-1.413	0.002
HETATM	5	C	UNK	0001	-2.008	-1.362	0.001
HETATM	6	C	UNK	0001	-2.006	1.054	-0.001
HETATM	7	H	UNK	0001	-0.117	-2.356	0.002
HETATM	8	H	UNK	0001	-2.571	-2.279	0.000
HETATM	9	H	UNK	0001	-2.536	1.991	-0.002
HETATM	10	H	UNK	0001	-3.768	-0.136	-0.001
HETATM	11	C	UNK	0001	0.412	2.049	-0.000
HETATM	12	C	UNK	0001	1.595	1.403	0.002
HETATM	13	H	UNK	0001	2.588	1.805	0.002
HETATM	14	N	UNK	0001	1.408	0.042	0.004
HETATM	15	H	UNK	0001	0.271	3.110	-0.000
HETATM	16	C	UNK	0001	2.443	-0.959	-0.002
HETATM	17	H	UNK	0001	2.383	-1.579	-0.890
HETATM	18	H	UNK	0001	2.374	-1.596	0.874
HETATM	19	H	UNK	0001	3.407	-0.469	0.008

CONNECT	1	4	3	14
CONNECT	2	5	6	10
CONNECT	3	6	1	11


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CONNECT      4      1      5      7
CONNECT      5      4      2      8
CONNECT      6      2      3      9
CONNECT      7      4
CONNECT      8      5
CONNECT      9      6
CONNECT     10      2
CONNECT     11      3     12     15
CONNECT     12     13     11     14
CONNECT     13     12
CONNECT     14     12      1     16
CONNECT     15     11
CONNECT     16     17     18     19     14
CONNECT     17     16
CONNECT     18     16
CONNECT     19     16
END

```

15b. η^6 -(N-Methylindole)•Na⁺ (LCH0009)

```

HEADER
REMARK MacSpartan exported Tue, May 21, 2002 1:49:56 PM
HETATM      1 Na   UNK  0001      0.175   1.043   2.248
HETATM      2 ?   UNK  0001      0.119   0.766  -0.154
HETATM      3 C   UNK  0001      1.520   0.529  -0.225
HETATM      4 H   UNK  0001      2.576   0.352  -0.314
HETATM      5 C   UNK  0001      0.606  -0.529  -0.130
HETATM      6 C   UNK  0001     -0.787  -0.301  -0.041
HETATM      7 C   UNK  0001     -1.270   1.017  -0.082
HETATM      8 C   UNK  0001     -0.370   2.063  -0.190
HETATM      9 C   UNK  0001      1.016   1.817  -0.257
HETATM     10 H   UNK  0001      1.693   2.646  -0.369
HETATM     11 H   UNK  0001     -0.729   3.073  -0.260
HETATM     12 H   UNK  0001     -2.328   1.210  -0.060
HETATM     13 C   UNK  0001     -1.408  -1.594   0.031
HETATM     14 C   UNK  0001     -0.405  -2.497  -0.032
HETATM     15 N   UNK  0001      0.815  -1.877  -0.116
HETATM     16 C   UNK  0001      2.096  -2.540  -0.279
HETATM     17 H   UNK  0001      2.791  -2.226   0.491
HETATM     18 H   UNK  0001      2.521  -2.326  -1.252
HETATM     19 H   UNK  0001      1.950  -3.606  -0.192
HETATM     20 H   UNK  0001     -0.461  -3.566  -0.026
HETATM     21 H   UNK  0001     -2.454  -1.810   0.088
CONNECT      1      2
CONNECT      2      3      5      6      7
CONNECT      2      8      9      1
CONNECT      3      4      5      9      2

```

```

CONNECT      4      3
CONNECT      5      3      6      15      2
CONNECT      6      5      7      13      2
CONNECT      7      6      8      12      2
CONNECT      8      7      9      11      2
CONNECT      9      8      3      10      2
CONNECT     10      9
CONNECT     11      8
CONNECT     12      7
CONNECT     13      6      14      21
CONNECT     14     13      15      20
CONNECT     15     14      5      16
CONNECT     16     15      17      18      19
CONNECT     17     16
CONNECT     18     16
CONNECT     19     16
CONNECT     20     14
CONNECT     21     13
END

```

15c. η^5 -(*N*-Methylindole)•Na⁺ (LCH0010)

```

HEADER
REMARK Spartan `02 exported Molecule001
HETATM      1 Na   UNK   0001      0.033      1.064      2.325
HETATM      2 N   UNK   0001      1.411     -0.012      0.000
HETATM      3 C   UNK   0001      1.606      1.340     -0.129
HETATM      4 H   UNK   0001      2.599      1.739     -0.173
HETATM      5 C   UNK   0001      0.418      1.993     -0.204
HETATM      6 H   UNK   0001      0.285      3.047     -0.342
HETATM      7 C   UNK   0001     -0.610      0.975     -0.170
HETATM      8 C   UNK   0001      0.054     -0.257     -0.057
HETATM      9 C   UNK   0001     -0.645     -1.469      0.020
HETATM     10 H   UNK   0001     -0.135     -2.413      0.085
HETATM     11 C   UNK   0001     -2.017     -1.410     -0.018
HETATM     12 H   UNK   0001     -2.584     -2.322      0.026
HETATM     13 C   UNK   0001     -2.700     -0.184     -0.126
HETATM     14 H   UNK   0001     -3.774     -0.185     -0.163
HETATM     15 C   UNK   0001     -2.016      1.004     -0.202
HETATM     16 H   UNK   0001     -2.542      1.936     -0.306
HETATM     17 C   UNK   0001      2.452     -1.022     -0.122
HETATM     18 H   UNK   0001      3.412     -0.558      0.049
HETATM     19 H   UNK   0001      2.444     -1.465     -1.110
HETATM     20 H   UNK   0001      2.308     -1.800      0.617
HETATM     21 Lig  UNK   0001      0.576      0.808     -0.112
CONNECT      1     21
CONNECT      2      8      3      17

```

```

CONNECT      3      5      2      4
CONNECT      4      3
CONNECT      5      7      3      6
CONNECT      6      5
CONNECT      7      8      5     15
CONNECT      8      2      7      9
CONNECT      9     10      8     11
CONNECT     10      9
CONNECT     11     12      9     13
CONNECT     12     11
CONNECT     13     14     11     15
CONNECT     14     13
CONNECT     15     16     13      7
CONNECT     16     15
CONNECT     17     18     19     20      2
CONNECT     18     17
CONNECT     19     17
CONNECT     20     17
CONNECT     21      1
END

```

16a. 2-Methylindole (LCH0012)

```

HEADER
REMARK Spartan `02 exported Molecule001
HETATM      1  C   UNK   0001      -0.388  -0.650  -0.001
HETATM      2  C   UNK   0001      -2.808   0.650   0.001
HETATM      3  C   UNK   0001      -0.419   0.750  -0.001
HETATM      4  C   UNK   0001      -1.549  -1.418   0.000
HETATM      5  C   UNK   0001      -2.754  -0.750   0.001
HETATM      6  C   UNK   0001      -1.654   1.401  -0.000
HETATM      7  H   UNK   0001      -1.510  -2.493   0.000
HETATM      8  H   UNK   0001      -3.670  -1.313   0.002
HETATM      9  H   UNK   0001      -1.703   2.477  -0.001
HETATM     10  H   UNK   0001      -3.765   1.140   0.001
HETATM     11  C   UNK   0001       0.954   1.191  -0.002
HETATM     12  H   UNK   0001       1.306   2.203  -0.002
HETATM     13  C   UNK   0001       1.732   0.087   0.000
HETATM     14  N   UNK   0001       0.930  -1.032  -0.003
HETATM     15  H   UNK   0001       1.259  -1.967  -0.004
HETATM     16  C   UNK   0001       3.221  -0.044   0.002
HETATM     17  H   UNK   0001       3.569  -0.588  -0.872
HETATM     18  H   UNK   0001       3.567  -0.577   0.883
HETATM     19  H   UNK   0001       3.682   0.934  -0.004
CONNECT      1      4      3     14
CONNECT      2      5      6     10
CONNECT      3      6      1     11

```

```

CONNECT    4    1    5    7
CONNECT    5    4    2    8
CONNECT    6    2    3    9
CONNECT    7    4
CONNECT    8    5
CONNECT    9    6
CONNECT   10    2
CONNECT   11   12    3   13
CONNECT   12   11
CONNECT   13   11   14   16
CONNECT   14   15   13    1
CONNECT   15   14
CONNECT   16   17   18   19   13
CONNECT   17   16
CONNECT   18   16
CONNECT   19   16
END

```

16b. η^6 -(2-Methylindole)•Na⁺ (LCH0013)

```

HEADER
REMARK MacSpartan exported Tue, May 21, 2002 1:50:27 PM
HETATM    1 Na  UNK  0001    0.373    2.281   -1.619
HETATM    2 ?  UNK  0001    0.191   -0.113   -1.421
HETATM    3 C  UNK  0001    1.585   -0.255   -1.182
HETATM    4 H  UNK  0001    2.636   -0.396   -1.002
HETATM    5 C  UNK  0001    0.674   -0.145   -0.129
HETATM    6 C  UNK  0001   -0.711    0.014   -0.351
HETATM    7 C  UNK  0001   -1.193    0.031   -1.669
HETATM    8 C  UNK  0001   -0.295   -0.094   -2.717
HETATM    9 C  UNK  0001    1.084   -0.232   -2.475
HETATM   10 H  UNK  0001    1.756   -0.356   -3.304
HETATM   11 H  UNK  0001   -0.657   -0.121   -3.730
HETATM   12 H  UNK  0001   -2.248    0.108   -1.862
HETATM   13 C  UNK  0001   -1.330    0.079    0.947
HETATM   14 C  UNK  0001   -0.345   -0.054    1.866
HETATM   15 N  UNK  0001    0.867   -0.167    1.223
HETATM   16 H  UNK  0001    1.730   -0.359    1.677
HETATM   17 C  UNK  0001   -0.420   -0.095    3.358
HETATM   18 H  UNK  0001    0.180    0.694    3.801
HETATM   19 H  UNK  0001   -0.058   -1.046    3.736
HETATM   20 H  UNK  0001   -1.444    0.031    3.684
HETATM   21 H  UNK  0001   -2.375    0.178    1.156
CONNECT    1    2
CONNECT    2    3    5    6    7
CONNECT    2    8    9    1
CONNECT    3    4    5    9    2

```

```

CONNECT      4      3
CONNECT      5      3      6      15      2
CONNECT      6      5      7      13      2
CONNECT      7      6      8      12      2
CONNECT      8      7      9      11      2
CONNECT      9      8      3      10      2
CONNECT     10      9
CONNECT     11      8
CONNECT     12      7
CONNECT     13      6      14      21
CONNECT     14     13      15      17
CONNECT     15     14      5      16
CONNECT     16     15
CONNECT     17     14      18      19      20
CONNECT     18     17
CONNECT     19     17
CONNECT     20     17
CONNECT     21     13
END

```

16c. η^5 -(2-Methylindole)•Na⁺ (LCH0014)

```

HEADER
REMARK Spartan `02 exported Molecule001
HETATM      1 Na UNK 0001      0.166      0.190     -2.364
HETATM      2 C UNK 0001     -0.402     -0.660      0.083
HETATM      3 C UNK 0001     -0.432      0.740      0.113
HETATM      4 H UNK 0001      1.252     -1.964      0.200
HETATM      5 C UNK 0001      0.950      1.184      0.089
HETATM      6 H UNK 0001      1.301      2.194      0.160
HETATM      7 C UNK 0001      1.734      0.076      0.069
HETATM      8 N UNK 0001      0.927     -1.046     -0.009
HETATM      9 C UNK 0001     -1.565     -1.433      0.073
HETATM     10 H UNK 0001     -1.527     -2.508      0.062
HETATM     11 C UNK 0001     -2.766     -0.762      0.108
HETATM     12 H UNK 0001     -3.683     -1.322      0.120
HETATM     13 C UNK 0001     -2.820      0.642      0.136
HETATM     14 H UNK 0001     -3.778      1.128      0.168
HETATM     15 C UNK 0001     -1.672      1.398      0.135
HETATM     16 H UNK 0001     -1.721      2.472      0.172
HETATM     17 C UNK 0001      3.223     -0.057      0.150
HETATM     18 H UNK 0001      3.612     -0.696     -0.636
HETATM     19 H UNK 0001      3.510     -0.492      1.103
HETATM     20 H UNK 0001      3.692      0.914      0.070
HETATM     21 Lig UNK 0001      0.555      0.059      0.069
CONNECT      1     21
CONNECT      2      8      3      9

```

```

CONNECT      3      5      2     15
CONNECT      4      8
CONNECT      5      7      3      6
CONNECT      6      5
CONNECT      7      8      5     17
CONNECT      8      2      7      4
CONNECT      9     10      2     11
CONNECT     10      9
CONNECT     11     12      9     13
CONNECT     12     11
CONNECT     13     14     11     15
CONNECT     14     13
CONNECT     15     16     13      3
CONNECT     16     15
CONNECT     17     18     19     20      7
CONNECT     18     17
CONNECT     19     17
CONNECT     20     17
CONNECT     21      1
END

```

17a. 3-Methylindole (LCH0016)

```

HEADER
REMARK Spartan `02 exported Molecule001
HETATM      1  C   UNK   0001      -0.642  -0.973   0.000
HETATM      2  C   UNK   0001      -2.033   1.399  -0.000
HETATM      3  C   UNK   0001       0.058   0.240   0.000
HETATM      4  C   UNK   0001      -2.035  -1.023   0.000
HETATM      5  C   UNK   0001      -2.714   0.172  -0.000
HETATM      6  C   UNK   0001      -0.659   1.441   0.000
HETATM      7  H   UNK   0001      -2.561  -1.962   0.000
HETATM      8  H   UNK   0001      -3.790   0.168  -0.000
HETATM      9  H   UNK   0001      -0.143   2.385   0.000
HETATM     10  H   UNK   0001      -2.598   2.315  -0.000
HETATM     11  C   UNK   0001       1.469  -0.082  -0.000
HETATM     12  C   UNK   0001       1.542  -1.428   0.000
HETATM     13  H   UNK   0001       2.410  -2.057   0.000
HETATM     14  N   UNK   0001       0.282  -1.982   0.001
HETATM     15  H   UNK   0001       0.081  -2.952  -0.001
HETATM     16  C   UNK   0001       2.609   0.892  -0.000
HETATM     17  H   UNK   0001       2.581   1.535  -0.876
HETATM     18  H   UNK   0001       3.562   0.375   0.000
HETATM     19  H   UNK   0001       2.581   1.536   0.876
CONNECT      1      4      3     14
CONNECT      2      5      6     10
CONNECT      3      6      1     11

```

```

CONNECT      4      1      5      7
CONNECT      5      4      2      8
CONNECT      6      2      3      9
CONNECT      7      4
CONNECT      8      5
CONNECT      9      6
CONNECT     10      2
CONNECT     11      3     12     16
CONNECT     12     13     11     14
CONNECT     13     12
CONNECT     14     15     12      1
CONNECT     15     14
CONNECT     16     17     18     19     11
CONNECT     17     16
CONNECT     18     16
CONNECT     19     16
END

```

17b. η^6 -(3-Methylindole)•Na⁺ (LCH0017)

```

HEADER
REMARK MacSpartan exported Tue, May 21, 2002 1:50:59 PM
HETATM      1 Na   UNK   0001      -0.630  -2.274  -1.266
HETATM      2 ?   UNK   0001      -0.616   0.129  -1.052
HETATM      3 C   UNK   0001      -2.018   0.162  -0.817
HETATM      4 H   UNK   0001      -3.077   0.221  -0.640
HETATM      5 C   UNK   0001      -1.104   0.110   0.240
HETATM      6 C   UNK   0001       0.290   0.061   0.019
HETATM      7 C   UNK   0001       0.775   0.094  -1.298
HETATM      8 C   UNK   0001      -0.126   0.158  -2.348
HETATM      9 C   UNK   0001      -1.513   0.191  -2.106
HETATM     10 H   UNK   0001      -2.191   0.271  -2.936
HETATM     11 H   UNK   0001       0.234   0.222  -3.359
HETATM     12 H   UNK   0001       1.833   0.099  -1.490
HETATM     13 C   UNK   0001       0.928   0.037   1.317
HETATM     14 C   UNK   0001      -0.077   0.076   2.216
HETATM     15 N   UNK   0001      -1.302   0.098   1.587
HETATM     16 H   UNK   0001      -2.174   0.228   2.045
HETATM     17 H   UNK   0001      -0.024   0.090   3.286
HETATM     18 C   UNK   0001       2.404   0.014   1.589
HETATM     19 H   UNK   0001       2.597   0.003   2.655
HETATM     20 H   UNK   0001       2.893   0.889   1.173
HETATM     21 H   UNK   0001       2.878  -0.863   1.159
CONNECT      1      2
CONNECT      2      3      5      6      7
CONNECT      2      8      9      1
CONNECT      3      4      5      9      2

```

```

CONNECT      4      3
CONNECT      5      3      6      15      2
CONNECT      6      5      7      13      2
CONNECT      7      6      8      12      2
CONNECT      8      7      9      11      2
CONNECT      9      8      3      10      2
CONNECT     10      9
CONNECT     11      8
CONNECT     12      7
CONNECT     13      6      14      18
CONNECT     14     13      15      17
CONNECT     15     14      5      16
CONNECT     16     15
CONNECT     17     14
CONNECT     18     13      19      20      21
CONNECT     19     18
CONNECT     20     18
CONNECT     21     18
END

```

17c. η^5 -(3-Methylindole)•Na⁺ (LCH0018)

```

HEADER
REMARK Spartan `02 exported Molecule001
HETATM      1 Na   UNK   0001      0.330  -1.099  -2.296
HETATM      2  C   UNK   0001     -0.656  -0.923   0.131
HETATM      3  C   UNK   0001      0.034   0.291   0.058
HETATM      4  H   UNK   0001      0.106  -2.844   0.501
HETATM      5  C   UNK   0001      1.460  -0.017   0.084
HETATM      6  C   UNK   0001      1.551  -1.363   0.155
HETATM      7  N   UNK   0001      0.283  -1.948   0.100
HETATM      8  C   UNK   0001     -2.050  -0.989   0.144
HETATM      9  H   UNK   0001     -2.569  -1.929   0.214
HETATM     10  C   UNK   0001     -2.735   0.203   0.096
HETATM     11  H   UNK   0001     -3.810   0.194   0.122
HETATM     12  C   UNK   0001     -2.063   1.434   0.018
HETATM     13  H   UNK   0001     -2.636   2.342  -0.015
HETATM     14  C   UNK   0001     -0.690   1.492  -0.004
HETATM     15  H   UNK   0001     -0.182   2.438  -0.050
HETATM     16  H   UNK   0001      2.423  -1.979   0.245
HETATM     17  C   UNK   0001      2.584   0.979   0.114
HETATM     18  H   UNK   0001      2.546   1.656  -0.734
HETATM     19  H   UNK   0001      3.546   0.480   0.103
HETATM     20  H   UNK   0001      2.529   1.582   1.014
HETATM     21 Lig  UNK   0001      0.535  -0.792   0.106
CONNECT      1     21
CONNECT      2      7      3      8

```



```

CONNECT      3      5      2      14
CONNECT      4      7
CONNECT      5      6      3      17
CONNECT      6      7      5      16
CONNECT      7      2      6      4
CONNECT      8      9      2      10
CONNECT      9      8
CONNECT     10     11      8      12
CONNECT     11     10
CONNECT     12     13     10     14
CONNECT     13     12
CONNECT     14     15     12      3
CONNECT     15     14
CONNECT     16      6
CONNECT     17     18     19     20      5
CONNECT     18     17
CONNECT     19     17
CONNECT     20     17
CONNECT     21      1
END

```

18a. 4-Methylindole (LCH0020)

```

HEADER
REMARK Spartan `02 exported Molecule001
HETATM      1  C  UNK  0001      1.128      0.649     -0.000
HETATM      2  C  UNK  0001     -1.567      1.137      0.000
HETATM      3  C  UNK  0001      0.229     -0.422      0.000
HETATM      4  C  UNK  0001      0.705      1.979     -0.000
HETATM      5  C  UNK  0001     -0.649      2.202     -0.000
HETATM      6  C  UNK  0001     -1.155     -0.176      0.000
HETATM      7  H  UNK  0001      1.408      2.794     -0.000
HETATM      8  H  UNK  0001     -1.020      3.212     -0.000
HETATM      9  H  UNK  0001     -2.619      1.362      0.000
HETATM     10  C  UNK  0001      1.023     -1.627     -0.000
HETATM     11  C  UNK  0001      2.315     -1.241      0.000
HETATM     12  H  UNK  0001      3.205     -1.837      0.000
HETATM     13  N  UNK  0001      2.395      0.128      0.000
HETATM     14  H  UNK  0001      3.235      0.654      0.001
HETATM     15  H  UNK  0001      0.671     -2.638     -0.000
HETATM     16  C  UNK  0001     -2.137     -1.320      0.000
HETATM     17  H  UNK  0001     -3.159     -0.958      0.001
HETATM     18  H  UNK  0001     -2.004     -1.950      0.875
HETATM     19  H  UNK  0001     -2.005     -1.949     -0.876
CONNECT      1      4      3      13
CONNECT      2      5      6      9
CONNECT      3      6      1      10

```

```

CONNECT    4    1    5    7
CONNECT    5    4    2    8
CONNECT    6    2    3   16
CONNECT    7    4
CONNECT    8    5
CONNECT    9    2
CONNECT   10    3   11   15
CONNECT   11   12   10   13
CONNECT   12   11
CONNECT   13   14   11    1
CONNECT   14   13
CONNECT   15   10
CONNECT   16   17   18   19    6
CONNECT   17   16
CONNECT   18   16
CONNECT   19   16
END

```

18b. η^6 -(4-Methylindole)•Na⁺ (LCH0021)

```

HEADER
REMARK MacSpartan exported Tue, May 21, 2002 1:51:29 PM
HETATM    1 Na   UNK   0001    0.679    2.282   -0.706
HETATM    2 ?   UNK   0001    0.594   -0.111   -0.578
HETATM    3 C   UNK   0001    2.003   -0.155   -0.335
HETATM    4 H   UNK   0001    3.060   -0.227   -0.148
HETATM    5 C   UNK   0001    1.074   -0.096    0.713
HETATM    6 C   UNK   0001   -0.314   -0.034    0.482
HETATM    7 C   UNK   0001   -0.815   -0.073   -0.838
HETATM    8 C   UNK   0001    0.112   -0.130   -1.868
HETATM    9 C   UNK   0001    1.501   -0.176   -1.620
HETATM   10 H   UNK   0001    2.177   -0.256   -2.452
HETATM   11 H   UNK   0001   -0.232   -0.188   -2.886
HETATM   12 C   UNK   0001   -2.301   -0.106   -1.100
HETATM   13 H   UNK   0001   -2.516   -0.017   -2.157
HETATM   14 H   UNK   0001   -2.819    0.691   -0.576
HETATM   15 H   UNK   0001   -2.717   -1.046   -0.751
HETATM   16 C   UNK   0001   -0.945    0.002    1.778
HETATM   17 C   UNK   0001    0.048   -0.046    2.691
HETATM   18 N   UNK   0001    1.267   -0.085    2.064
HETATM   19 H   UNK   0001    2.139   -0.218    2.523
HETATM   20 H   UNK   0001   -0.011   -0.056    3.760
HETATM   21 H   UNK   0001   -1.993    0.034    1.990
CONNECT    1    2
CONNECT    2    3    5    6    7
CONNECT    2    8    9    1
CONNECT    3    4    5    9    2

```

```

CONNECT      4      3
CONNECT      5      3      6      18      2
CONNECT      6      5      7      16      2
CONNECT      7      6      8      12      2
CONNECT      8      7      9      11      2
CONNECT      9      8      3      10      2
CONNECT     10      9
CONNECT     11      8
CONNECT     12      7      13      14      15
CONNECT     13      12
CONNECT     14      12
CONNECT     15      12
CONNECT     16      6      17      21
CONNECT     17      16      18      20
CONNECT     18      17      5      19
CONNECT     19      18
CONNECT     20      17
CONNECT     21      16
END

```

18c. η^5 -(4-Methylindole)•Na⁺ (LCH0022)

```

HEADER
REMARK Spartan `02 exported Molecule001
HETATM      1 Na UNK 0001      1.385 -0.318  2.281
HETATM      2 C UNK 0001      1.036  0.704 -0.137
HETATM      3 C UNK 0001      0.169 -0.394 -0.104
HETATM      4 H UNK 0001      3.123  0.751 -0.427
HETATM      5 C UNK 0001      1.003 -1.583 -0.153
HETATM      6 C UNK 0001      2.287 -1.163 -0.215
HETATM      7 N UNK 0001      2.334  0.217 -0.136
HETATM      8 C UNK 0001      0.579  2.025 -0.099
HETATM      9 H UNK 0001      1.254  2.861 -0.137
HETATM     10 C UNK 0001     -0.781  2.200 -0.045
HETATM     11 H UNK 0001     -1.185  3.196 -0.031
HETATM     12 C UNK 0001     -1.669  1.108 -0.017
HETATM     13 H UNK 0001     -2.725  1.306  0.017
HETATM     14 C UNK 0001     -1.229 -0.195 -0.047
HETATM     15 H UNK 0001      3.189 -1.732 -0.316
HETATM     16 H UNK 0001      0.677 -2.603 -0.194
HETATM     17 C UNK 0001     -2.179 -1.366 -0.055
HETATM     18 H UNK 0001     -3.203 -1.037  0.055
HETATM     19 H UNK 0001     -1.963 -2.063  0.750
HETATM     20 H UNK 0001     -2.102 -1.915 -0.989
HETATM     21 Lig UNK 0001      1.366 -0.444 -0.149
CONNECT      1     21
CONNECT      2      7      3      8

```

```

CONNECT 3 5 2 14
CONNECT 4 7
CONNECT 5 6 3 16
CONNECT 6 7 5 15
CONNECT 7 2 6 4
CONNECT 8 9 2 10
CONNECT 9 8
CONNECT 10 11 8 12
CONNECT 11 10
CONNECT 12 13 10 14
CONNECT 13 12
CONNECT 14 12 3 17
CONNECT 15 6
CONNECT 16 5
CONNECT 17 18 19 20 14
CONNECT 18 17
CONNECT 19 17
CONNECT 20 17
CONNECT 21 1
END

```

19a. 5-Methylindole (LCH0024)

```

HEADER
REMARK Spartan `02 exported Molecule001
HETATM 1 C UNK 0001 1.118 0.698 -0.000
HETATM 2 C UNK 0001 -1.543 -0.079 0.000
HETATM 3 C UNK 0001 0.790 -0.660 -0.000
HETATM 4 C UNK 0001 0.135 1.688 0.000
HETATM 5 C UNK 0001 -1.176 1.283 0.000
HETATM 6 C UNK 0001 -0.559 -1.039 -0.000
HETATM 7 H UNK 0001 0.392 2.733 -0.000
HETATM 8 H UNK 0001 -1.953 2.029 0.001
HETATM 9 C UNK 0001 2.035 -1.386 -0.000
HETATM 10 C UNK 0001 3.021 -0.465 0.001
HETATM 11 H UNK 0001 4.083 -0.604 0.002
HETATM 12 N UNK 0001 2.486 0.797 -0.001
HETATM 13 H UNK 0001 3.005 1.641 -0.001
HETATM 14 H UNK 0001 2.165 -2.449 -0.000
HETATM 15 H UNK 0001 -0.822 -2.084 -0.000
HETATM 16 C UNK 0001 -3.007 -0.454 -0.000
HETATM 17 H UNK 0001 -3.516 -0.060 0.876
HETATM 18 H UNK 0001 -3.137 -1.530 -0.001
HETATM 19 H UNK 0001 -3.516 -0.059 -0.875
CONNECT 1 4 3 12
CONNECT 2 5 6 16
CONNECT 3 6 1 9

```

```

CONNECT    4    1    5    7
CONNECT    5    4    2    8
CONNECT    6    2    3   15
CONNECT    7    4
CONNECT    8    5
CONNECT    9    3   10   14
CONNECT   10   11    9   12
CONNECT   11   10
CONNECT   12   13   10    1
CONNECT   13   12
CONNECT   14    9
CONNECT   15    6
CONNECT   16   17   18   19    2
CONNECT   17   16
CONNECT   18   16
CONNECT   19   16
END

```

19b. η^6 -(5-Methylindole)•Na⁺ (LCH0025)

```

HEADER
REMARK Spartan `02 exported Molecule001
HETATM    1 Na   UNK   0001   -0.254   0.292  -2.324
HETATM    2 H   UNK   0001   -0.808  -2.101   0.043
HETATM    3 C   UNK   0001   -0.546  -1.057   0.038
HETATM    4 C   UNK   0001    0.152   1.680   0.105
HETATM    5 C   UNK   0001   -1.540  -0.092   0.076
HETATM    6 C   UNK   0001    0.809  -0.676   0.045
HETATM    7 C   UNK   0001    1.140   0.691   0.094
HETATM    8 C   UNK   0001   -1.170   1.275   0.095
HETATM    9 H   UNK   0001   -1.943   2.021   0.139
HETATM   10 H   UNK   0001    0.403   2.725   0.156
HETATM   11 C   UNK   0001    2.052  -1.403   0.050
HETATM   12 H   UNK   0001    2.181  -2.465   0.038
HETATM   13 C   UNK   0001    3.035  -0.479   0.115
HETATM   14 H   UNK   0001    4.095  -0.620   0.158
HETATM   15 N   UNK   0001    2.504   0.784   0.121
HETATM   16 H   UNK   0001    3.026   1.619   0.253
HETATM   17 C   UNK   0001   -3.001  -0.476   0.173
HETATM   18 H   UNK   0001   -3.164  -1.498  -0.148
HETATM   19 H   UNK   0001   -3.628   0.173  -0.428
HETATM   20 H   UNK   0001   -3.342  -0.395   1.200
HETATM   21 Lig  UNK   0001   -0.193   0.303   0.076
CONNECT    1   21
CONNECT    2    3
CONNECT    3    2    6    5
CONNECT    4    7    8   10

```

```

CONNECT    5      8      3      17
CONNECT    6      3      7      11
CONNECT    7      6      4      15
CONNECT    8      4      5       9
CONNECT    9      8
CONNECT   10      4
CONNECT   11     12      6      13
CONNECT   12     11
CONNECT   13     14     11      15
CONNECT   14     13
CONNECT   15     16     13       7
CONNECT   16     15
CONNECT   17     18     19     20     5
CONNECT   18     17
CONNECT   19     17
CONNECT   20     17
CONNECT   21      1
END

```

19c. η^5 -(5-Methylindole)•Na⁺ (LCH0026)

```

HEADER
REMARK  Spartan `02 exported Molecule001
HETATM    1 Na    UNK    0001      1.759  -0.170   2.274
HETATM    2  C    UNK    0001      1.018   0.716  -0.124
HETATM    3  C    UNK    0001      0.699  -0.644  -0.131
HETATM    4  H    UNK    0001      2.891   1.652  -0.387
HETATM    5  C    UNK    0001      1.956  -1.366  -0.194
HETATM    6  C    UNK    0001      2.942  -0.439  -0.228
HETATM    7  N    UNK    0001      2.402   0.828  -0.115
HETATM    8  C    UNK    0001      0.029   1.704  -0.071
HETATM    9  H    UNK    0001      0.276   2.751  -0.078
HETATM   10  C    UNK    0001     -1.275   1.284  -0.037
HETATM   11  H    UNK    0001     -2.057   2.023  -0.013
HETATM   12  C    UNK    0001     -1.638  -0.085  -0.041
HETATM   13  C    UNK    0001     -0.651  -1.040  -0.081
HETATM   14  H    UNK    0001      4.000  -0.571  -0.331
HETATM   15  H    UNK    0001      2.089  -2.427  -0.265
HETATM   16  H    UNK    0001     -0.904  -2.086  -0.098
HETATM   17  C    UNK    0001     -3.100  -0.462  -0.022
HETATM   18  H    UNK    0001     -3.607  -0.022   0.831
HETATM   19  H    UNK    0001     -3.230  -1.536   0.029
HETATM   20  H    UNK    0001     -3.600  -0.108  -0.918
HETATM   21 Lig   UNK    0001      1.803  -0.181  -0.158
CONNECT    1     21
CONNECT    2      7      3      8
CONNECT    3      5      2     13

```

```

CONNECT      4      7
CONNECT      5      6      3      15
CONNECT      6      7      5      14
CONNECT      7      2      6      4
CONNECT      8      9      2      10
CONNECT      9      8
CONNECT     10     11      8      12
CONNECT     11     10
CONNECT     12     10     13     17
CONNECT     13     12      3     16
CONNECT     14      6
CONNECT     15      5
CONNECT     16     13
CONNECT     17     18     19     20     12
CONNECT     18     17
CONNECT     19     17
CONNECT     20     17
CONNECT     21      1
END

```

20a. 6-Methylindole (LCH0028)

```

HEADER
REMARK Spartan `02 exported Molecule001
HETATM      1  C   UNK   0001      0.782  -0.612  -0.000
HETATM      2  C   UNK   0001     -1.180   1.297  -0.000
HETATM      3  C   UNK   0001      1.144   0.737  -0.000
HETATM      4  C   UNK   0001     -0.551  -1.028  -0.000
HETATM      5  C   UNK   0001     -1.537  -0.068   0.000
HETATM      6  C   UNK   0001      0.130   1.702  -0.000
HETATM      7  H   UNK   0001     -0.802  -2.075  -0.000
HETATM      8  C   UNK   0001      2.585   0.782   0.000
HETATM      9  C   UNK   0001      3.012  -0.497   0.000
HETATM     10  H   UNK   0001      4.010  -0.884   0.000
HETATM     11  N   UNK   0001      1.935  -1.351  -0.001
HETATM     12  H   UNK   0001      1.988  -2.340   0.000
HETATM     13  H   UNK   0001      3.206   1.654   0.000
HETATM     14  H   UNK   0001      0.375   2.751  -0.000
HETATM     15  H   UNK   0001     -1.963   2.037   0.000
HETATM     16  C   UNK   0001     -2.998  -0.454   0.000
HETATM     17  H   UNK   0001     -3.123  -1.531  -0.000
HETATM     18  H   UNK   0001     -3.507  -0.059  -0.875
HETATM     19  H   UNK   0001     -3.506  -0.060   0.876
CONNECT      1      4      3      11
CONNECT      2      5      6      15
CONNECT      3      6      1      8
CONNECT      4      1      5      7

```

```

CONNECT    5    4    2    16
CONNECT    6    2    3    14
CONNECT    7    4
CONNECT    8    3    9    13
CONNECT    9   10    8    11
CONNECT   10    9
CONNECT   11   12    9    1
CONNECT   12   11
CONNECT   13    8
CONNECT   14    6
CONNECT   15    2
CONNECT   16   17   18   19    5
CONNECT   17   16
CONNECT   18   16
CONNECT   19   16
END

```

20b. η^6 -(6-Methylindole)•Na⁺ (LCH0029)

```

HEADER
REMARK Spartan `02 exported Molecule001
HETATM    1 Na    UNK    0001    -0.208  -0.554  -2.303
HETATM    2  H    UNK    0001     0.390  -2.725   0.243
HETATM    3  C    UNK    0001     0.146  -1.680   0.160
HETATM    4  C    UNK    0001    -0.542   1.056   0.008
HETATM    5  C    UNK    0001    -1.175  -1.275   0.138
HETATM    6  C    UNK    0001     1.163  -0.714   0.104
HETATM    7  C    UNK    0001     0.797   0.645   0.044
HETATM    8  C    UNK    0001    -1.537   0.093   0.072
HETATM    9  H    UNK    0001    -0.796   2.102  -0.016
HETATM   10  C    UNK    0001     2.604  -0.755   0.133
HETATM   11  H    UNK    0001     3.225  -1.624   0.198
HETATM   12  C    UNK    0001     3.023   0.526   0.102
HETATM   13  H    UNK    0001     4.020   0.916   0.128
HETATM   14  N    UNK    0001     1.948   1.378   0.027
HETATM   15  H    UNK    0001     2.003   2.369   0.082
HETATM   16  H    UNK    0001    -1.954  -2.013   0.215
HETATM   17  C    UNK    0001    -2.995   0.489   0.144
HETATM   18  H    UNK    0001    -3.621  -0.184  -0.430
HETATM   19  H    UNK    0001    -3.152   1.496  -0.222
HETATM   20  H    UNK    0001    -3.339   0.454   1.173
HETATM   21 Lig   UNK    0001    -0.191  -0.312   0.088
CONNECT    1   21
CONNECT    2    3
CONNECT    3    2    6    5
CONNECT    4    7    8    9
CONNECT    5    8    3   16

```



```

CONNECT    6    3    7    10
CONNECT    7    6    4    14
CONNECT    8    4    5    17
CONNECT    9    4
CONNECT   10   11    6    12
CONNECT   11   10
CONNECT   12   13   10   14
CONNECT   13   12
CONNECT   14   15   12    7
CONNECT   15   14
CONNECT   16    5
CONNECT   17   18   19   20    8
CONNECT   18   17
CONNECT   19   17
CONNECT   20   17
CONNECT   21    1
END

```

20c. η^5 -(6-Methylindole)•Na⁺ (LCH0030)

```

HEADER
REMARK Spartan `02 exported Molecule001
HETATM    1 Na   UNK   0001      1.776   0.143   2.272
HETATM    2  C   UNK   0001      0.688   0.603  -0.120
HETATM    3  C   UNK   0001      1.043  -0.748  -0.135
HETATM    4  H   UNK   0001      1.906   2.306  -0.364
HETATM    5  C   UNK   0001      2.492  -0.802  -0.204
HETATM    6  C   UNK   0001      2.931   0.478  -0.228
HETATM    7  N   UNK   0001      1.858   1.345  -0.107
HETATM    8  C   UNK   0001     -0.643   1.031  -0.062
HETATM    9  H   UNK   0001     -0.888   2.079  -0.064
HETATM   10  C   UNK   0001     -1.632   0.074  -0.037
HETATM   11  C   UNK   0001     -1.280  -1.298  -0.048
HETATM   12  C   UNK   0001      0.022  -1.717  -0.094
HETATM   13  H   UNK   0001      3.927   0.857  -0.329
HETATM   14  H   UNK   0001      3.104  -1.678  -0.283
HETATM   15  H   UNK   0001      0.260  -2.765  -0.118
HETATM   16  H   UNK   0001     -2.067  -2.030  -0.030
HETATM   17  C   UNK   0001     -3.091   0.461  -0.014
HETATM   18  H   UNK   0001     -3.602  -0.000   0.825
HETATM   19  H   UNK   0001     -3.586   0.128  -0.921
HETATM   20  H   UNK   0001     -3.217   1.533   0.061
HETATM   21 Lig  UNK   0001      1.802   0.175  -0.159
CONNECT    1    21
CONNECT    2    7    3    8
CONNECT    3    5    2   12
CONNECT    4    7

```

```

CONNECT    5    6    3    14
CONNECT    6    7    5    13
CONNECT    7    2    6    4
CONNECT    8    9    2    10
CONNECT    9    8
CONNECT   10    8   11   17
CONNECT   11   10   12   16
CONNECT   12   11    3   15
CONNECT   13    6
CONNECT   14    5
CONNECT   15   12
CONNECT   16   11
CONNECT   17   18   19   20   10
CONNECT   18   17
CONNECT   19   17
CONNECT   20   17
CONNECT   21    1
END

```

21a. 7-Methylindole (LCH0032)

```

HEADER
REMARK Spartan `02 exported Molecule001
HETATM    1  C  UNK  0001    -0.241  -0.371  -0.000
HETATM    2  C  UNK  0001     0.660   2.215   0.000
HETATM    3  C  UNK  0001    -1.163   0.680   0.000
HETATM    4  C  UNK  0001     1.145  -0.171  -0.000
HETATM    5  C  UNK  0001     1.565   1.139   0.000
HETATM    6  C  UNK  0001    -0.694   1.999   0.000
HETATM    7  C  UNK  0001    -2.474   0.082  -0.000
HETATM    8  C  UNK  0001    -2.292  -1.254  -0.000
HETATM    9  H  UNK  0001    -3.018  -2.042  -0.001
HETATM   10  N  UNK  0001    -0.952  -1.546  -0.002
HETATM   11  H  UNK  0001    -0.566  -2.458   0.006
HETATM   12  H  UNK  0001    -3.416   0.590  -0.001
HETATM   13  H  UNK  0001    -1.384   2.826  -0.000
HETATM   14  H  UNK  0001     1.045   3.220   0.001
HETATM   15  H  UNK  0001     2.621   1.349   0.000
HETATM   16  C  UNK  0001     2.103  -1.336  -0.001
HETATM   17  H  UNK  0001     1.966  -1.963   0.877
HETATM   18  H  UNK  0001     3.130  -0.993  -0.002
HETATM   19  H  UNK  0001     1.963  -1.964  -0.877
CONNECT    1    4    3   10
CONNECT    2    5    6   14
CONNECT    3    6    1    7
CONNECT    4    1    5   16
CONNECT    5    4    2   15

```

```

CONNECT    6    2    3   13
CONNECT    7    3    8   12
CONNECT    8    9    7   10
CONNECT    9    8
CONNECT   10   11    8    1
CONNECT   11   10
CONNECT   12    7
CONNECT   13    6
CONNECT   14    2
CONNECT   15    5
CONNECT   16   17   18   19    4
CONNECT   17   16
CONNECT   18   16
CONNECT   19   16
END

```

21b. η^6 -(7-Methylindole)•Na⁺ (LCH0033)

```

HEADER
REMARK Spartan `02 exported Molecule001
HETATM    1 Na   UNK   0001   -0.208  -1.210  -2.248
HETATM    2 H   UNK   0001   -1.072  -3.141   0.343
HETATM    3 C   UNK   0001   -0.677  -2.147   0.231
HETATM    4 C   UNK   0001    0.257   0.438   0.051
HETATM    5 C   UNK   0001   -1.574  -1.059   0.152
HETATM    6 C   UNK   0001    0.688  -1.947   0.209
HETATM    7 C   UNK   0001    1.174  -0.631   0.107
HETATM    8 C   UNK   0001   -1.137   0.253   0.068
HETATM    9 H   UNK   0001   -2.631  -1.255   0.201
HETATM   10 H   UNK   0001    1.367  -2.777   0.301
HETATM   11 C   UNK   0001    2.490  -0.050   0.086
HETATM   12 H   UNK   0001    3.426  -0.567   0.133
HETATM   13 C   UNK   0001    2.318   1.288   0.034
HETATM   14 H   UNK   0001    3.053   2.067   0.022
HETATM   15 N   UNK   0001    0.983   1.595  -0.005
HETATM   16 H   UNK   0001    0.614   2.516   0.036
HETATM   17 C   UNK   0001   -2.085   1.428   0.065
HETATM   18 H   UNK   0001   -3.112   1.099  -0.025
HETATM   19 H   UNK   0001   -1.878   2.111  -0.753
HETATM   20 H   UNK   0001   -1.997   1.987   0.992
HETATM   21 Lig UNK   0001   -0.211  -0.849   0.136
CONNECT    1   21
CONNECT    2    3
CONNECT    3    2    6    5
CONNECT    4    7    8   15
CONNECT    5    8    3    9
CONNECT    6    3    7   10

```

```

CONNECT 7 6 4 11
CONNECT 8 4 5 17
CONNECT 9 5
CONNECT 10 6
CONNECT 11 12 7 13
CONNECT 12 11
CONNECT 13 14 11 15
CONNECT 14 13
CONNECT 15 16 13 4
CONNECT 16 15
CONNECT 17 18 19 20 8
CONNECT 18 17
CONNECT 19 17
CONNECT 20 17
CONNECT 21 1
END

```

21c. η^5 -(7-Methylindole)•Na⁺ (LCH0034)

```

HEADER
REMARK Spartan `02 exported Molecule001
HETATM 1 Na UNK 0001 1.370 0.255 2.287
HETATM 2 H UNK 0001 3.331 -0.677 -0.315
HETATM 3 C UNK 0001 2.405 -0.148 -0.217
HETATM 4 C UNK 0001 2.254 1.197 -0.211
HETATM 5 H UNK 0001 2.995 1.967 -0.299
HETATM 6 N UNK 0001 0.920 1.522 -0.079
HETATM 7 H UNK 0001 0.555 2.420 -0.303
HETATM 8 C UNK 0001 0.175 0.351 -0.106
HETATM 9 C UNK 0001 1.073 -0.721 -0.153
HETATM 10 C UNK 0001 0.580 -2.037 -0.122
HETATM 11 H UNK 0001 1.248 -2.878 -0.168
HETATM 12 C UNK 0001 -0.778 -2.215 -0.059
HETATM 13 H UNK 0001 -1.187 -3.208 -0.048
HETATM 14 C UNK 0001 -1.659 -1.117 -0.025
HETATM 15 H UNK 0001 -2.717 -1.308 0.010
HETATM 16 C UNK 0001 -1.219 0.187 -0.044
HETATM 17 C UNK 0001 -2.153 1.372 -0.036
HETATM 18 H UNK 0001 -2.085 1.928 -0.967
HETATM 19 H UNK 0001 -1.928 2.059 0.776
HETATM 20 H UNK 0001 -3.180 1.052 0.080
HETATM 21 Lig UNK 0001 1.365 0.440 -0.153
CONNECT 1 21
CONNECT 2 3
CONNECT 3 2 9 4
CONNECT 4 6 3 5
CONNECT 5 4

```

CONECT	6	8	4	7	
CONECT	7	6			
CONECT	8	9	6	16	
CONECT	9	3	8	10	
CONECT	10	11	9	12	
CONECT	11	10			
CONECT	12	13	10	14	
CONECT	13	12			
CONECT	14	15	12	16	
CONECT	15	14			
CONECT	16	14	8	17	
CONECT	17	18	19	20	16
CONECT	18	17			
CONECT	19	17			
CONECT	20	17			
CONECT	21	1			
END

DFILE C:\WINNMR95\Data\polo\ST
 COMNT LCH-IV-82-1-C
 DATIM Wed Oct 06 12:58:32 199
 OBNUC 13C
 EXMOD BCM
 OBFRQ 100.40 MHz
 OBSET 125.00 KHz
 OBFIN 10500.0 Hz
 POINT 32768
 FREQU 27173.9 Hz
 SCANS 497
 ACQTM 1.206 sec
 PD 1.794 sec
 PW1 5.1 us
 1H
 CDCL3 22.6 c
 SLVNT
 EXREF 77.00 ppm
 BF 1.00 Hz
 RGAIN 26

C:\WINMR95\COMMON\
 LCH-V-17-1-C
 DATIM Wed Oct 06 13: 57: 27
 OBNUC 13C
 EXMOD BCM
 OBFRQ 100.40 MHz
 OBSET 125.00 KHz
 OBFIN 10500.0 Hz
 POINT 32768
 FREQ 27173.9 Hz
 SCANS 279
 ACQTM 1.206 sec
 PD 1.794 sec
 PW1 5.1 us
 1H
 CDCL3 22.5 c
 SLVNT 77.00 ppm
 EXREF 1.00 Hz
 BF 24
 RGAIN

----- ACQUISITION PARAMETERS -----
 File Name - LCH-VII-55-4-H-11-9-00
 Author - Carlier@va Tech
 Sample ID - S8434396
 Content - Single Pulse Experiment
 Creation Date - 9-NOV-2000 12:07:38
 Revision Date - 9-NOV-2000 12:10:41
 Spec Site - Eclipse+ 500

Spec Type - DELTA_NMR
 Data Format - 1D REAL
 Dimensions - 1H
 Dim Title - 32768
 Dim Size - [ppm]
 Dim Units - 0.1314[ms]
 Acq_delay - 0
 Changer_sample - single_pulse.exp
 Experiment - 11.7473579[T]
 Field_strength - 10.8[us]
 Irr90 - 22.9[us]
 Irr90_lo - 50[us]
 Irr90_hi - 50[us]
 Lock_status - IDLE
 Recvr_gain - 21
 Relaxation_delay - 1[s]
 Scans - 32
 Solvent - CHLOROFORM-D
 Spin_get - 16[Hz]
 Spin_lock_90 - 0.1[ms]
 Spin_lock_attn - 21[db]
 Spin_set - 15[Hz]
 Spin_status - SPIN ON
 Spin_status - SPIN ON
 Temp_set - 25[dc]
 Temp_status - TEMP OFF
 Temp_status - TEMP OFF
 X90 - 10.8[us]
 X90_lo - 22.9[us]
 X90_hi - 50[us]
 X_acq_duration - 4.3646976[s]
 X_domain - 1H
 X_freq - 500.16241602[MHz]
 X_offset - 5[ppm]
 X_points - 32768
 X_prescans - 0
 X_pulse - 3.6[us]
 X_resolution - 0.22911794[Hz]
 X_sweep - 7.50750751[KHz]

(Millions)

120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0

X : parts per Million : 13C

----- ACQUISITION PARAMETERS -----
File Name - LCH-VII-55-4-C-11-9-00
Author - carlier@va Tech
Sample ID - S#437093
Content - Single Pulse with Broc
Creation Date - 9-NOV-2000 12:33:17
Revision Date - 9-NOV-2000 12:34:05
Spec Site - Eclipse+ 500
Spec Type - DELTA_NMR
Data Format - 1D REAL
Dimensions - X
Dim Title - 13C
Dim Size - 32768
Dim Units - [ppm]
Acq_delay - 33.8[us]
Changer_sample - 0
Experiment - single_pulse_dec
Field_strength - 11.7473579[T]
Irr90_hi - 10.8[us]
Irr90_lo - 22.9[us]
Irr_domain - 1H
Irr_width - 50[us]
Lock_status - IDLE
Recvr_gain - 25
Relaxation_delay - 1[s]
Scans - 720
Solvent - CHLOROFORM-D
Spin_get - 13[Hz]
Spin_lock_90 - 0.1[ms]
Spin_lock_atn - 21[db]
Spin_set - 15[Hz]
Spin_status - SPIN ON
Temp_get - 26.2[dc]
Temp_set - 25[dc]
Temp_status - TEMP OFF
X90 - 9.4[us]
X90_lo - 10[us]
X90_hi - 35[us]
X_acq_duration - 1.0420234[s]
X_domain - 13C
X_freq - 125.77787547[MHz]
X_offset - 100[ppm]
X_points - 32768
X_prescans - 4
X_pulse - 4.7[us]
X_resolution - 0.95970156[Hz]
X_sweep - 31.46654088[kHz]

C:\WINNMR95\DATA\POLEV
LCH-V-85-1-C
Fr1 Oct 15 13:39:10 199

COMNT
DATIM
OBNUC 13C
EXMOD BCM
OBFRQ 100.40 MHz
OBSET 125.00 KHz
OBFIN 10500.0 Hz
POINT 32768
FREQU 27173.9 Hz
SCANS 571
ACQTM 1.206 sec
PD 1.794 sec
PW1 5.1 us
IRNUC 1H
CTEMP 22.9 C
SLVNT CD3OD
EXREF 49.00 ppm
BF 2.00 Hz
RGAIN 26

Current Data Parameters
 NAME LCH-VI-80-1
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20000124
 Time 13.07
 INSTRUM apx300
 PROBO 5 mm QNP 1H
 PULPROG zg30
 TD 32768
 SOLVENT MeOH
 NS 16
 DS 2
 SWH 6250.000 Hz
 FIDRES 0.190735 Hz
 AQ 2.6214900 sec
 RG 512
 DW 80.000 usec
 DE 114.29 usec
 TE 300.0 K
 D1 3.0000000 sec
 P1 10.00 usec
 DE 114.29 usec
 SF01 300.1318383 MHz
 NUCLEUS 1H

F2 - Processing parameters

SI 16384
 SF 300.1300678 MHz
 WDW EM
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

1D NMR plot parameters

CA 23.00 cm
 F1P 7.822 ppb
 F1 2347.60 Hz
 F2P 0.005 ppb
 F2 1.49 Hz
 PPMCM 0.33987 ppb/Hz
 HZCM 102.00499 Hz/Hz

DFILE C:\WINMR95\Data\po1o\spect;
 CONIT LCH-VI-80-1-C
 DATIM Sat Apr 08 08:47:54 2000
 OBNUC 13C
 EXMCD BCM
 OFRG 100.40 MHz
 OBSET 125.00 KHz
 OFIN 10500.0 Hz
 POINT 32768
 FREGU 27247.9 Hz
 SCANS 149
 ACQTM 1.203 sec
 PD 1.794 sec
 PW1 5.1 us
 1H
 IRNUC 23.3 c
 CTEMP CD30D
 SLVNT 49.30 ppm
 EXREF 1.00 Hz
 BF
 RGAIN 26

Current Data Parameters
 NAME LCH-VII-S-1
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20000131
 Time 12.02
 INSTRUM arx300
 PROBHD 5 mm QNP 1H
 PULPROG zg30
 TD 32768
 SOLVENT MeOH
 NS 16
 DS 2
 SWH 6250.000 Hz
 FIDRES 0.190735 Hz
 AQ 2.6214500 sec
 RG 715
 DM 80.000 USEC
 DE 114.29 USEC
 TE 300.0 K
 D1 3.00000000 sec
 P1 10.00 USEC
 DE 114.29 USEC
 SF01 300.1318383 MHz
 NUCLEUS 1H

F2 - Processing parameters
 SI 16384
 SF 300.1300678 MHz
 MDW EM
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 23.00 cm
 FIP 8.409 ppm
 F1 2523.88 Hz
 F2 0.277 ppm
 F2 83.17 Hz
 PPMCM 0.35357 ppm/c
 HZCM 106.11813 Hz/c

C:\WINNMR95\Data\polo\spec
 LCH-VII-5-1-C
 Sat Apr 08 12: 15: 25 2000
 13C
 EXMOD BCM
 OBFRQ 100.40 MHz
 OBSET 125.00 KHz
 OBFIN 10500.0 Hz
 POINT 32768
 FREQU 27247.9 Hz
 SCANS 144
 ACQTM 1.203 sec
 PD 1.794 sec
 PW1 5.1 us
 1H
 IRNUC 23.3 c
 CD30D
 SLVNT
 EXREF 49.30 ppm
 BF 2.00 Hz
 RGAIN 26

DFILE
CLINT
CLATIM
CLRNG
EXVAL
GBFBS
GBFBI
GBFBN
POINT
PFREQ
SCANS
ACQTM
PD
PW1
IRNUC
CTEMP
SLVNT
EXREF
BF
RGAIN

0.8205
0.8272
0.8418
0.8556
0.8645
0.8774
0.8885
0.8998
0.9044
0.9242
1.1954
1.2194
1.2434
1.2728
1.3467
1.3909
1.8891
1.9922
2.0726
3.2152
3.2416
3.2625
3.2888
3.2937
3.2999
3.3049
3.3277
3.3382
3.3520
3.3749
3.5911
4.0441
4.0678
4.0917
4.1156
4.2495
4.7515
4.7749
4.8007
4.8480
6.4304
6.4408
6.8673
6.8870
6.8909
6.9036
6.9286
6.9528
7.2169
7.2274
7.4143
7.4190
7.4395
7.4441
7.5840
7.5952
ppm

DFILE C:\WINMR95\Data\po1o\spect
 LCH-VII-8-1-C
 CONNT Wed Apr 12 14:13:05 2000
 DATIM
 OBNUC 13C
 EXMOD BCM
 OBFRQ 100.40 MHz
 OBSET 125.00 KHz
 OBFIN 10500.0 Hz
 POINT 32768
 FREQU 27247.9 Hz
 SCANS 219
 ACQTM 1.203 sec
 PD 1.794 sec
 PM1 5.1 us
 IRNUC 1H
 CTEMP 23.2 c
 SLVNT CD3OD
 EXREF 49.30 ppm
 BF 2.00 Hz
 RGAIN 26

```

DFILE  COMNT  DATIM  OBNUC  EXMOD  OBFRQ  OBSET  OBFIN  POINT  FREQU  SCANS  ACQTM  PD      PW1      IRNUC  CTEMP  SLVNT  EXREF  BF      RGAIN

```

OBFRQ	100.40 MHz			
OBSET	125.00 KHz			
OBFNZ	10500.0 Hz			
POINT	32768			
FREQU	27247.9 Hz			
SCANS	425			
ACQTM	1.203 sec			
PD	1.794 sec			
PW1	5.1 us			
		1H		
IRNUC			23.5 c	
CTEMP				
SLVNT		CD30D		
EXREF			49.30 ppm	
BF			2.00 Hz	
RGAIN				26

```

DFILE
COMNT
DATIM
OBNUC
EXMOD
OBFRQ
OBSET
OBFIN
POINT
FREQU
SCANS
ACQTM
PD
PW1
IRNUC
CTEMP
SLVNT
EXREF
BF
RGAIN

```

300.0

200.0

100.0

(Millions)

0

----- ACQUISITION PARAMETERS -----
 File Name - LCH-VII-37-1-C-12-7-00
 Author - carlier@va Tech
 Sample ID - S#475464
 Content - Single Pulse with Broa
 Creation Date - 7-DEC-2000 13:56:44
 Revision Date - 7-DEC-2000 13:57:43
 Spec Site - Eclipse+ 500

Spec Type - DELTA_NMR
 Data Format - 1D REAL
 Dimensions - x
 Dim Title - 13C
 Dim Size - 32768
 Dim Units - [ppm]
 Acq_delay - 33.5[us]
 Changer_sample - 0
 Experiment - single_pulse_dec
 Field_strength - 11.7473579[T]
 Irr90 - 11.5[us]
 Irr90_hi - 22.9[us]
 Irr90_lo - 55[us]
 Irr_domain - 1H
 Irr_width - 55[us]
 Lock_status - IDLE
 Recvr_gain - 25
 Relaxation_delay - 1[s]
 Scans - 1293
 Solvent - CHLOROFORM-D
 Spin_get - 16[Hz]
 Spin_lock_90 - 0.1[ms]
 Spin_lock_attn - 21[dB]
 Spin_set - 15[Hz]
 Spin_state - SPIN ON
 Spin_status - SPIN ON
 Temp_get - 25.5[dc]
 Temp_set - 25[dc]
 Temp_status - TEMP OFF
 X90 - 11[us]
 X90_hi - 10[us]
 X90_lo - 35[us]
 X_acq_duration - 1.0420224[s]
 X_domain - 13C
 X_freq - 125.77787547 [MHz]
 X_offset - 100[ppm]
 X_points - 32768
 X_prescans - 4
 X_pulse - 5.5[us]
 X_resolution - 0.95970155[Hz]
 X_sweep - 31.44654088[kHz]

(Millions)

---- ACQUISITION PARAMETERS ----
 File Name - LCH-VIII-89-1-H-12-15-
 Author - CarliserVa Tech
 Sample ID - S#469815
 Content - Single Pulse Experiment
 Creation Date - 15-DEC-2000 13:06:59
 Revision Date - 15-DEC-2000 13:16:19
 Spec Site - Eclipse+ 500
 Spec Type - DELTA NMR
 Data Format - 1D COMPLEX
 Dimensions - X
 Dim Title - 1H
 Dim Size - 32768
 Dim Units - [ppm]
 Acq_delay - 0.1313[ms]
 Changer_sample - 0
 Experiment - single pulse.exp
 Field_strength - 11.7473579[T]
 Irr90 - 11.5[us]
 Irr90_lo - 22.9[us]
 Irr90_hi - 55[us]
 Irr_width - 55[us]
 Lock_status - IDLE
 Recvr_gain - 13
 Relaxation_delay - 1[s]
 Scans - 32
 Solvent - METHANOL-D3
 Spin_get - 17[Hz]
 Spin_lock_90 - 0.1[ms]
 Spin_lock_attn - 21[dB]
 Spin_set - 15[Hz]
 Spin_status - SPIN ON
 Spin_on - SPIN ON
 Temp_get - 24.1[dc]
 Temp_set - 25[dc]
 Temp_status - TEMP OFF
 X90 - 11.5[us]
 X90_lo - 22.9[us]
 X90_hi - 55[us]
 X_acq_duration - 4.3646976[s]
 X_domain - 1H
 X_freq - 500.16241602[MHz]
 X_offset - 5[ppm]
 X_points - 32768
 X_prescans - 0
 X_pulse - 3.83333333[us]
 X_resolution - 0.22911794[Hz]
 X_sweep - 7.50750751[kHz]

----- ACQUISITION PARAMETERS -----
 File Name - LCH-VIII-89-1-C-CDC13-
 Author - carliar@va Tech
 Sample ID - S#560359
 Content - Single Pulse with Broa
 Creation Date - 15-DEC-2000 16:29:02
 Revision Date - 15-DEC-2000 16:30:15
 Spec Site - Eclipse+ 500

Spec Type - DELTA_NMR
 Data Format - 1D COMPLEX
 Dimensions - X
 Dim Title - 13C
 Dim Size - 32768
 Dim Units - [ppm]
 Acq_Delay - 33.5[us]
 Changer_sample - 0
 Experiment - single pulse dec
 Field_strength - 11.7473579[T]
 Irr90_hi - 11.5[us]
 Irr90_lo - 22.9[us]
 Irr_domain - 55[us]
 Irr_width - 1H
 Lock_status - 55[us]
 Lock_gain - IDLZ
 Recvz_gain - 25
 Relaxation_delay - 1[s]
 Scans - 1437
 Solvent - CHLOROFORM-D
 Spin_get - 15[Hz]
 Spin_lock_90 - 0.1[ms]
 Spin_lock_attn - 21[dB]
 Spin_set - 15[Hz]
 Spin_status - SPIN ON
 Temp_get - 25.1[dc]
 Temp_set - 25[dc]
 Temp_status - TEMP OFF
 X90 - 11[us]
 X90_hi - 10[us]
 X90_lo - 35[us]
 X_acq_duration - 1.0420224[s]
 X_domain - 13C
 X_freq - 125.77787547 [MHz]
 X_offset - 100[ppm]
 X_points - 32768
 X_prescans - 4
 X_pulse - 5.5[us]
 X_resolution - 0.95970156[Hz]
 X_sweep - 31.44654088[kHz]