

**Spectroscopic data:**

**Indole (3a):** Yellow solid; Mp: 51-52 °C (lit.<sup>11a</sup> 51 °C); IR (KBr): 3402, 3097, 3043, 1616, 1496, 1454, 1338, 744 cm<sup>-1</sup>; <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>): δ = 8.12 (br s, 1 H), 7.72 (d, *J* = 7.8 Hz, 1 H), 7.43 (d, *J* = 8.1 Hz, 1 H), 7.26 (t, *J* = 8.1 Hz, 1 H), 7.23 (t, *J* = 2.8 Hz, 1 H), 7.19 (t, *J* = 7.9 Hz, 1 H), 6.62 (t, *J* = 2.1 Hz, 1 H); <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>): δ = 135.80, 127.87, 124.13, 122.00, 120.75, 119.83, 111.02, 102.65; MS: *m/z* 117 [M<sup>+</sup>], 89, 63.

**6-Chloroindole (3b):** White solid; Mp: 88-89 °C (lit.<sup>11c</sup> 88-89 °C); IR (KBr): 3394, 3097, 3039, 1616, 1566, 1496, 1446, 1334, 806, 733 cm<sup>-1</sup>; <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>): δ = 8.12 (br s, 1 H), 7.56 (d, *J* = 8.4 Hz, 1 H), 7.39 (br s, 1 H), 7.20 (t, *J* = 2.8 Hz, 1 H), 7.11 (dd, *J* = 8.4, 1.8 Hz, 1 H), 6.55 (br s, 1 H); <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>): δ = 136.15, 127.89, 126.46, 124.83, 121.57, 120.61, 110.96, 102.83; MS: *m/z* 153, 151 [M<sup>+</sup>], 124, 116 [M<sup>+</sup>-Cl], 89, 63.

**6-Bromoindole (3c):** Off-white solid; Mp: 93-94 °C (lit.<sup>11d</sup> 95-97 °C); IR (KBr): 3398, 3093, 3035, 1604, 1570, 1493, 1450, 1331, 810, 729 cm<sup>-1</sup>; <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>): δ = 8.16 (br s, 1 H), 7.57 (br s, 1 H), 7.53 (d, *J* = 8.4 Hz, 1 H), 7.26 (dd, *J* = 8.4, 1.7 Hz, 1 H), 7.20 (dd, *J* = 3.1, 2.5 Hz, 1 H), 6.57-6.56 (m, 1 H); <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>): δ = 136.60, 126.77, 124.78, 123.17, 121.95, 115.49, 113.96, 102.87; MS: *m/z* 197, 195 [M<sup>+</sup>], 116 [M<sup>+</sup>-Br], 89, 63.

**6-Aminoindole (3d):** Light grey solid; Mp: 63-64 °C (lit.<sup>11f</sup> 64-67 °C); IR (KBr): 3394, 3359, 3294, 3101, 3020, 1624, 1512, 1454, 1342, 849, 795, 729 cm<sup>-1</sup>; <sup>1</sup>H NMR (500 MHz, CD<sub>3</sub>OD): δ = 7.30 (d, *J* = 8.3 Hz, 1 H), 6.99 (d, *J* = 3.15 Hz, 1 H), 6.78 (d, *J* = 1.0 Hz, 1 H), 6.57 (dd, *J* = 8.4, 2.0 Hz, 1 H), 6.28 (d, *J* = 3.1 Hz, 1 H); <sup>13</sup>C NMR (125 MHz, CD<sub>3</sub>OD): δ = 141.25, 137.40, 122.14, 121.94, 120.13, 110.57, 100.73, 97.44; MS: *m/z* 132 [M<sup>+</sup>], 104, 77.

**5-Metylindole (3e):** White solid; Mp: 58-59 °C (lit.<sup>11b</sup> 58-60 °C); IR (KBr): 3390, 3097, 3027, 2912, 2858, 1631, 1573, 1465, 1326, 798, 763, 717 cm<sup>-1</sup>; <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>): δ = 7.98 (br s, 1 H), 7.42 (s, 1 H), 7.25 (d, *J* = 8.2 Hz, 1 H), 7.13 (t, *J* = 2.8 Hz, 1 H), 7.01 (dd, *J* = 8.2, 1.4 Hz, 1 H), 6.47-6.45 (m, 1 H), 2.44 (s, 3 H); <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>): δ = 134.13, 129.02, 128.16, 124.24, 123.63, 120.36, 110.67, 102.13, 21.45; MS: *m/z* 131 [M<sup>+</sup>], 130, 103, 77.

**5-Cyanoindole (3f):** White solid; Mp: 105-106 °C (lit.<sup>11e</sup> 104.5-106.5 °C); IR

(KBr): 3321, 3070, 3035, 2214, 1608, 1508, 1466, 1342, 802, 768, 733  $\text{cm}^{-1}$ ;  $^1\text{H}$  NMR (500 MHz,  $\text{CD}_3\text{COCD}_3$ ):  $\delta$  = 10.83 (br s, 1 H), 8.06 (s, 1 H), 7.63 (d,  $J$  = 8.3 Hz, 1 H), 7.56 (t,  $J$  = 2.7 Hz, 1 H), 7.43 (dd,  $J$  = 8.6, 1.5 Hz, 1 H), 6.66 (d,  $J$  = 2.4 Hz, 1 H);  $^{13}\text{C}$  NMR (125 MHz,  $\text{CD}_3\text{COCD}_3$ ):  $\delta$  = 137.98, 128.02, 127.55, 125.74, 123.93, 120.35, 112.53, 102.46, 102.21; MS:  $m/z$  142 [ $\text{M}^+$ ], 115, 88, 62.

**5-Chloroindole (3g):** White solid; Mp: 72-73  $^\circ\text{C}$  (lit.<sup>11b</sup> 69-71  $^\circ\text{C}$ ); IR (KBr): 3386, 3100, 3035, 1624, 1566, 1450, 1315, 802, 760  $\text{cm}^{-1}$ ;  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ):  $\delta$  = 8.20 (br s, 1 H), 7.65 (d,  $J$  = 2.0 Hz, 1 H), 7.33 (d,  $J$  = 8.6 Hz, 1 H), 7.25 (t,  $J$  = 2.8 Hz, 1 H), 7.19 (dd,  $J$  = 8.6, 2.0 Hz, 1 H), 6.55-6.54 (m, 1 H);  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ ):  $\delta$  = 134.16, 128.97, 125.54, 125.49, 122.33, 120.13, 112.00, 102.43; MS:  $m/z$  153, 151 [ $\text{M}^+$ ], 124, 116 [ $\text{M}^+\text{-Cl}$ ], 89, 63.

**5,6-Dichloroindole (3h):** Light brown solid; Mp: 152-153  $^\circ\text{C}$  (lit.<sup>11h</sup> 148-151  $^\circ\text{C}$ ); IR (KBr): 3402, 3086, 3039, 1628, 1558, 1496, 1446, 1288, 760, 725  $\text{cm}^{-1}$ ;  $^1\text{H}$  NMR (500 MHz,  $\text{CD}_3\text{COCD}_3$ ):  $\delta$  = 10.53 (s, 1 H), 7.76 (s, 1 H), 7.65 (s, 1 H), 7.45 (t,  $J$  = 2.4 Hz, 1 H), 6.50 (d,  $J$  = 2.2 Hz, 1 H);  $^{13}\text{C}$  NMR (125 MHz,  $\text{CD}_3\text{COCD}_3$ ):  $\delta$  = 136.49, 129.42, 128.85, 125.45, 123.60, 122.45, 114.13, 102.63; MS:  $m/z$  189, 187, 185 [ $\text{M}^+$ ], 150 [ $\text{M}^+\text{-Cl}$ ], 152, 123, 114, 87, 62.

**4-Chloroindole (3i):** Yellow Oil; IR (KBr): 3425, 3116, 3070, 1616, 1574, 1485, 1427, 1338, 806, 748  $\text{cm}^{-1}$ ;  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ):  $\delta$  = 8.27 (br s, 1 H), 7.29 (ddd,  $J$  = 7.0, 1.8, 0.9 Hz, 1 H), 7.24 (dd,  $J$  = 5.6, 2.9 Hz, 1 H), 7.14-7.09 (m, 2 H), 6.67-6.66 (m, 1 H);  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ ):  $\delta$  = 136.49, 126.81, 126.14, 124.66, 122.61, 119.61, 109.65, 101.40; MS:  $m/z$  153, 151 [ $\text{M}^+$ ], 124, 116 [ $\text{M}^+\text{-Cl}$ ], 89, 63.

**4-Aminoindole (3j):** Dark grey solid; Mp: 106-107  $^\circ\text{C}$  (lit.<sup>11g</sup> 106-108.5  $^\circ\text{C}$ ); IR (KBr): 3394, 3325, 3178, 3008, 1592, 1511, 1442, 1361, 775, 744  $\text{cm}^{-1}$ ;  $^1\text{H}$  NMR (500 MHz,  $\text{CD}_3\text{COCD}_3$ ):  $\delta$  = 9.96 (br s, 1 H), 7.11 (t,  $J$  = 2.8 Hz, 1 H), 6.83 (t,  $J$  = 7.9 Hz, 1 H), 6.72 (d,  $J$  = 8.1 Hz, 1 H), 6.53-6.52 (m, 1 H), 6.26 (d,  $J$  = 7.5 Hz, 1 H), 4.66 (br s, 2 H);  $^{13}\text{C}$  NMR (125 MHz,  $\text{CD}_3\text{COCD}_3$ ):  $\delta$  = 146.14, 142.62, 127.66, 126.97, 122.62, 107.68, 105.99, 103.83; MS:  $m/z$  132 [ $\text{M}^+$ ], 104, 77.

**7-Chloroindole (3k):** White solid; Mp: 59-60  $^\circ\text{C}$  (lit.<sup>11a</sup> 58  $^\circ\text{C}$ ); IR (KBr): 3398, 3108, 3023, 1619, 1562, 1485, 1431, 1331, 783, 721  $\text{cm}^{-1}$ ;  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ):  $\delta$  = 8.35 (br s, 1 H), 7.54 (d,  $J$  = 8.0 Hz, 1 H), 7.24 (t,  $J$  = 2.8 Hz, 1 H), 7.19 (d,  $J$  = 7.6 Hz, 1 H), 7.05 (t,  $J$  = 7.8 Hz, 1 H), 6.59 (t,  $J$  = 2.7 Hz, 1 H);  $^{13}\text{C}$  NMR (125

MHz, CDCl<sub>3</sub>):  $\delta$  = 133.19, 129.32, 124.77, 121.36, 120.60, 119.37, 116.60, 103.72;  
MS:  $m/z$  153, 151 [M<sup>+</sup>], 124, 116 [M<sup>+</sup>-Cl], 89, 63.

**7-Methylindole (3l):** White solid; Mp: 81-82 °C (lit.<sup>11a</sup> 81 °C); IR (KBr): 3398, 3100, 3050, 2923, 2854, 1619, 1592, 1492, 1454, 1338, 782, 721 cm<sup>-1</sup>; <sup>1</sup>H NMR (500 MHz, CD<sub>3</sub>COCD<sub>3</sub>):  $\delta$  = 10.15 (br s, 1 H), 7.40 (d,  $J$  = 7.2 Hz, 1 H), 7.29 (t,  $J$  = 2.7 Hz, 1 H), 6.94-6.89 (m, 2 H), 6.46 (t,  $J$  = 2.2 Hz, 1 H), 2.49 (s, 3 H); <sup>13</sup>C NMR (125 MHz, CD<sub>3</sub>COCD<sub>3</sub>):  $\delta$  = 136.80, 128.81, 125.25, 122.67, 121.33, 120.22, 118.87, 102.88, 17.09; MS:  $m/z$  131 [M<sup>+</sup>], 130, 103, 77.