



SUPPLEMENTARY MATERIAL TO
**Facile synthesis of bis(indolyl)methanes
using iron(III) phosphate**

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PHYSICAL AND SPECTRAL DATA OF THE SYNTHESIZED COMPOUNDS

3-[(1H-Indol-3-yl)(phenyl)methyl]-1H-indole (1). Yield: 90 %; m.p. 125 °C; IR (KBr, cm^{-1}): 3412 (–N–H stretching of amine), 3055 (–C–H stretching of aromatic ring), 1492, 1455 (–C=C stretching), 1092 (–C–N stretching); $^1\text{H-NMR}$ (300 MHz, $\text{DMSO-}d_6$, δ / ppm): 7.85 (2H, *s*, –NH), 7.43 (2H, *d*, $J = 8.1$ Hz, aromatic), 7.21–7.43 (7H, *m*, aromatic), 7.01 (2H, *t*, $J = 7.5$ Hz, aromatic), 6.6 (2H, *d*, $J = 1.8$ Hz, aromatic), 6.68 (2H, *s*, H–C–N), 5.58 (1H, *s*, –CH); $^{13}\text{C-NMR}$ (300 MHz, CDCl_3 , δ / ppm): 32.6 (CH), 110.9–145.2 (aromatic); MS (m/z , (relative abundance, %)): 322 (M^+ , 3.5) 116, 77 (BP, 100).

3-[(2-Chlorophenyl)(1H-indol-3-yl)methyl]-1H-indole (2). Yield: 80 %; m.p. 72 °C; IR (KBr, cm^{-1}): 3409 (–NH stretching of amine), 3054 (–C–H stretching of aromatic ring), 1416–1455 (–C=C stretching), 1092 (–C–N stretching); $^1\text{H-NMR}$ (300 MHz, $\text{DMSO-}d_6$, δ / ppm): 7.83 (2H, *brs*, –NH), 7.38–7.5 (4H, *m*, aromatic), 7.1–7.22 (6H, *m*, aromatic), 7.0 (2H, *t*, $J = 7.8$ Hz, aromatic), 6.58 (2H, *s*, H–C–N), 6.31 (1H, *s*, –C–H); $^{13}\text{C-NMR}$ (300 MHz, CDCl_3 , δ / ppm): 37.1 (CH), 110.4–141.5 (aromatic); MS (m/z , (relative abundance, %)): 356 (M^+ , 5.7), 358 ($\text{M}+2$, 2) 116, 111, 113, 76 (BP, 100).

3-[(4-Chlorophenyl)(1H-indol-3-yl)methyl]-1H-indole (3). Yield: 85 %; m.p. 75 °C; IR (KBr, cm^{-1}): 3407 (–NH stretching of amine), 3052 (–C–H stretching of aromatic ring), 1415–1453 (–C=C stretching), 1037 (–C–N stretching); $^1\text{H-NMR}$ (300 MHz, $\text{DMSO-}d_6$, δ / ppm): 10.85 (2H, *s*, –NH), 7.94 (2H, *d*, $J = 7.8$ Hz, aromatic), 7.01–7.95 (8H, *m*, aromatic), 6.87–6.94 (2H, *m*, aromatic), 6.84 (2H, *s*, H–C–N), 5.85 (1H, *s*, –C–H); $^{13}\text{C-NMR}$ (100 MHz, CDCl_3 , δ / ppm): 38.5 (CH), 111.1–143.6 (aromatic); MS (m/z , (relative abundance, %)): 356 (M^+ , 5.5), 358 ($\text{M}+2$, 1.8) 116, 111, 113, 76 (BP, 100).

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(E)-3-[1-(1H-Indol-3-yl)-3-phenylallyl]-1H-indole (**4**). Yield: 85 %; m.p. 100 °C; IR (KBr, cm^{-1}): 3449 (–NH stretching of amine), 3042 (–C–H stretching of aromatic ring), 1434, 1455 (–C=C stretching), 1090 (–C–N stretching); $^1\text{H-NMR}$ (300 MHz, $\text{DMSO-}d_6$, δ / ppm): 8.01 (2H, *s*, –NH), 7.30–7.12 (13H, *m*, aromatic), 6.96 (1H, *d*, $J = 15.9$, Ph-CH=CH), 6.07 (1H, *t*, $J = 7.9$ Hz, Ph-CH=CH), 6.50 (2H, *s*, H–C–N), 4.14 (1H, *d*, $J = 7.9$ Hz, –C–H); $^{13}\text{C-NMR}$ (300 MHz, CDCl_3 , δ / ppm): 39.5 (CH), 111.1–136.6 (aromatic); MS (m/z , (relative abundance, %)): 348 (M^+ , 4.2), 116, 77 (BP, 100).

3-[(1H-Indol-3-yl)(2-methoxyphenyl)methyl]-1H-indole (**5**). Yield: 93 %; m.p. 138 °C; IR (KBr, cm^{-1}): 3412 (–NH stretching of amine), 3055 (–C–H stretching of aromatic ring), 1417–1455 (–C=C stretching), 1092 (–C–N stretching); $^1\text{H-NMR}$ (300 MHz, $\text{DMSO-}d_6$, δ / ppm): 7.80 (2H, *brs*, –NH), 6.81–7.40 (12H, *m*, aromatic), 6.61 (2H, *s*, H–C–N), 6.32 (1H, *s*, –C–H), 3.83 (3H, *s*, –OCH₃); $^{13}\text{C-NMR}$ (300 MHz, CDCl_3 , δ / ppm): 32.3 (CH), 56.2 (O–CH₃), 110–157.1 (aromatic); MS (m/z , (relative abundance, %)): 352 (M^+ , 3.1), 107, 76 (BP, 100).

3-[(1H-indol-3-yl)(4-methoxyphenyl)methyl]-1H-indole (**6**). Yield: 92 %; m.p. 176 °C; IR (KBr, cm^{-1}): 3395 (–NH stretching of amine), 3045 (–C–H stretching of aromatic ring), 1418, 1455 (–C=C stretching), 1171 (–C–N stretching); $^1\text{H-NMR}$ (300 MHz, $\text{DMSO-}d_6$, δ / ppm): 7.86 (2H, *brs*, –NH), 7.38 (4H, *dd*, aromatic), 7.28 (2H, *d*, $J = 8.43$, aromatic), 7.14 (2H, *t*, $J = 7.36$, aromatic), 7.05 (2H, *t*, $J = 7.29$, aromatic), 6.81 (2H, *d*, $J = 8.63$, aromatic), 6.63 (2H, *s*, H–C–N), 5.85 (1H, *s*, –C–H), 3.79 (3H, *s*, –OCH₃); $^{13}\text{C-NMR}$ (300 MHz, CDCl_3 , δ / ppm): 37.6 (CH), 54.8 (O–CH₃), 110.4–157.2 (aromatic); MS (m/z , (relative abundance, %)): 352 (M^+ , 3.6), 107, 76 (BP, 100).

3-[(3,4-Dimethoxyphenyl)(1H-indol-3-yl)methyl]-1H-indole (**7**). Yield: 84 %; m.p. 195–198 °C; IR (KBr, cm^{-1}): 3415 (–NH stretching of amine), 3056 (–C–H stretching of aromatic ring), 1418–1456 (–C=C stretching), 1094 (–C–N stretching); $^1\text{H-NMR}$ (300 MHz, $\text{DMSO-}d_6$, δ / ppm): 7.86 (2H, *brs*, –NH), 7.38 (1H, *s*, aromatic), 7.28 (1H, *d*, $J = 8.5$ Hz, aromatic), 7.14 (1H, *dd*, $J = 7.35$, 2.3 Hz, aromatic), 6.81–7.05 (8H, *m*, aromatic), 6.63 (2H, *s*, H–C–N), 5.85 (1H, *s*, –C–H), 3.79 (6H, *s*, OCH₃); $^{13}\text{C-NMR}$ (100 MHz, CDCl_3 , δ / ppm): 38.2 (CH), 55.1 (O–CH₃), 111.1–149.7 (aromatic); MS (m/z , (relative abundance, %)): 382 (M^+ , 4.1), 137, 106, 75 (BP, 100).

3-[(1H-Indol-3-yl)(*p*-tolyl)methyl]-1H-indole (**8**). Yield: 84 %; m.p. 64–98 °C; IR (KBr, cm^{-1}): 3408 (–NH stretching of amine), 3048 (–C–H stretching of aromatic ring), 1485, 1508 (–C=C stretching), 1453, 1336, 1182, 1039 (–C–N stretching); $^1\text{H-NMR}$ (300 MHz, $\text{DMSO-}d_6$, δ / ppm): 10.77 (2H, *s*, NH), 7.33–7.65 (8H, *m*, aromatic), 7.54 (2H, *d*, $J = 8.1$, aromatic), 7.9 (2H, *d*, $J = 8.1$ Hz, aromatic), 6.77 (2H, *s*, H–C–N), 5.75 (1H, *s*, –C–H), 2.21 (3H, *s*, CH₃); $^{13}\text{C-NMR}$ (300 MHz, CDCl_3 , δ / ppm): 21.0 (CH₃), 39.0 (CH), 111.8–142.3 (aromatic); MS (m/z , (relative abundance, %)): 336 (M^+ , 5.1), 116, 91, 76 (BP, 100).

4-[Di(1H-indol-3-yl)methyl]-N,N-dimethylbenzenamine (**9**). Yield: 75 %; m.p. 208–220 °C; IR (KBr, cm^{-1}): 3396 (–NH stretching of amine), 3047 (–C–H stretching of aromatic ring), 2891, 1597, 1465, 1515 (–C=C stretching), 1374, 1166 (–C–N stretching); $^1\text{H-NMR}$ (300 MHz, $\text{DMSO-}d_6$, δ / ppm): 7.86 (2H, *brs*, –NH), 7.38 (2H, *d*, $J = 7.9$ Hz, aromatic), 7.14 (2H, *dd*, $J = 7.23, 2.35$ Hz, aromatic), 6.81–7.05 (8H, *m*, aromatic ring), 6.63 (2H, *s*, H–C–N), 5.85 (1H, *s*, –C–H), 3.79 (6H, *s*, $\text{N}(\text{CH}_3)_2$); $^{13}\text{C-NMR}$ (300 MHz, CDCl_3 , δ / ppm): 35.3 (CH), 22.6 (N–CH₃), 117.3–148.6 (aromatic); MS (m/z , (relative abundance, %)): 365 (M^+ , 3.1), 76 (BP, 100).

2-[Di(1H-indol-3-yl)methyl]phenol (**10**). Yield: 75 %; m.p. 350 °C; IR (KBr, cm^{-1}): 3445 (–NH stretching of amine), 3044 (–C–H stretching of aromatic ring), 1480–1616 (–C=C stretching), 1256, 1173, 1082 (–C–N stretching); 7.90–7.48 (aromatic ring); $^1\text{H-NMR}$ (300 MHz, $\text{DMSO-}d_6$, δ / ppm): 7.93 (2H, *brs*, –NH), 7.94 (1H, *s*, OH), 7.66 (2H, *d*, $J = 7.36, 3.2$ Hz, aromatic), 7.35 (2H, *t*, $J = 7.35$, aromatic), 7.19–7.29 (8H, *m*, aromatic), 6.72 (2H, *s*, H–C–N), 5.93 (1H, *s*, –C–H); $^{13}\text{C-NMR}$ (300 MHz, CDCl_3 , δ / ppm): 38.8(CH), 136.3–111.5 (aromatic), 155.2 (O–Ar); MS (m/z , (relative abundance, %)): 338 (M^+ , 3.2), 116, 93, 76 (BP, 100).

4-[Di(1H-indol-3-yl)methyl]phenol (**11**). Yield: 87 %; m.p. 150 °C; IR (KBr, cm^{-1}): 3445 (–NH stretching of amine), 3052 (–C–H stretching of aromatic ring), 1424, 1613 (–C=C stretching), 1173, 1132, 1082 (–C–N stretching), 742, 796 (aromatic ring); $^1\text{H-NMR}$ (300 MHz, $\text{DMSO-}d_6$, δ / ppm): 7.93 (2H, *brs*, –NH), 7.64 (1H, *s*, OH), 7.56 (2H, *d*, $J = 8.2$ Hz, aromatic), 7.45 (2H, *d*, $J = 8.2$ Hz, aromatic), 7.19–7.29 (8H, *m*, aromatic), 6.75 (2H, *s*, H–C–N), 5.53 (1H, *s*, –C–H); $^{13}\text{C-NMR}$ (300 MHz, CDCl_3 , δ / ppm): 38.8 (CH), 136.3–111.5 (aromatic), 155.2 (O–Ar); MS (m/z , (relative abundance, %)): 338 (M^+ , 3.4), 116, 93, 76 (BP, 100).

3-[(1H-Indol-3-yl)(4-nitrophenyl)methyl]-1H-indole (**12**). Yield: 84 %; m.p. 220 °C; IR (KBr, cm^{-1}): 3448 (–NH stretching of amine), 3055 (–C–H stretching of aromatic ring), 1417, 1594 (–C=C stretching), 1342, 1218, 1012 (–C–N stretching), 735, 598 (aromatic ring); $^1\text{H-NMR}$ (300 MHz, $\text{DMSO-}d_6$, δ / ppm): 8.15 (2H, *s*, –NH), 7.01–7.08 (4H, *m*, aromatic), 7.36 (2H, *d*, $J = 8.1$ Hz, aromatic), 7.41 (2H, *d*, $J = 8.1$ Hz, aromatic), 7.49 (2H, *d*, $J = 8.6$ Hz, aromatic), 7.5 (2H, *d*, $J = 8.6$ Hz, aromatic), 6.68 (2H, *s*, H–C–N), 6 (1H, *s*, –C–H); $^{13}\text{C-NMR}$ (300 MHz, CDCl_3 , δ / ppm): 41.6 (CH), 112.4–147.5 (aromatic), 153.6 (O₂N–Ar); MS (m/z , (relative abundance, %)): 367 (M^+ , 4.5), 116, 76 (BP, 100).

3-[1-(1H-Indol-3-yl)hexyl]-1H-indole (**13**). Yield: 76 % ; m.p. 65 °C; IR (KBr, cm^{-1}): 3350 (–NH stretching of amine), 3065 (–C–H stretching of aromatic ring), 1585–1615 (–C=C stretching), 1062 (–C–N stretching); $^1\text{H-NMR}$ (300 MHz, $\text{DMSO-}d_6$, δ / ppm): 7.87 (2H, *brs*, –NH), 7.52 (2H, *d*, $J = 8.5$ Hz, aromatic), 7.36 (2H, *d*, $J = 8.5$ Hz, aromatic), 7.02–7.18 (4H, *m*, aromatic), 6.66 (2H, *s*, H–C–N), 4.60 (1H, *t*, $J = 6.9$ Hz, CH), 4.24–1.24 (6H, *m*, CH₂), 0.8 (3H,

t, $J = 7.3$ Hz, CH₃); ¹³C-NMR (300 MHz, CDCl₃, δ / ppm): 12.1 (CH₃), 20.8 (CH₂), 24.4 (CH₂), 30.2 (CH₂), 36.9 (CH₂), 40.5 (CH), 111.2–136.5 (aromatic); MS (m/z , (relative abundance, %)): 316 (M⁺, 2.5), 116, 43 (BP, 100).

3-[1-(1H-Indol-3-yl)butyl]-1H-indole (14). Yield: 75 %; m.p. 80 °C; IR (KBr, cm⁻¹): 3465 (–NH stretching of amine), 3028 (–C–H stretching of aromatic ring), 1495–1618 (–C=C stretching), 1009 (–C–N stretching), 782 (aromatic ring); ¹H-NMR (300 MHz, DMSO-*d*₆, δ / ppm): 7.92 (2H, *brs*, –NH), 7.53 (2H, *d*, $J = 8.1$ Hz, aromatic), 7.26 (2H, *d*, $J = 8.1$ Hz, aromatic), 7.06 (4H, *m*, aromatic), 4.47 (1H, *t*, $J = 7.5$ Hz, CH), 1.77–2.56 (4H, *m*, CH₂), 0.86 (3H, *t*, $J = 6.9$ Hz, CH₃); ¹³C-NMR (300 MHz, CDCl₃, δ / ppm): 17.4 (CH₃), 31.2 (CH₂), 36.9 (CH₂), 40.5 (CH), 111.1–138.5 (aromatic); MS (m/z , (relative abundance, %)): 288 (M⁺, 2.3), 116, 43 (BP, 100).

3-[Furan-2-yl(1H-indol-3-yl)methyl]-1H-indole (15). Yield: 90 % ; m.p. 340–345 °C; IR (KBr, cm⁻¹): 3409 (–NH stretching of amine), 3053 (–C–H stretching of aromatic ring), 1418, 1600 (–C=C stretching), 1093 (–C–N stretching); ¹H-NMR (300 MHz, DMSO-*d*₆, δ / ppm): 7.71 (2H, *brs*, –NH), 7.12–7.42 (8H, *m*, aromatic), 6.98 (1H, *t*, $J = 6.8$ Hz, furanyl), 6.72 (1H, *d*, $J = 2.4$ Hz, aromatic), 6.28 (1H, *d*, $J = 2.2$ Hz, aromatic), 5.95 (2H, *d*, $J = 3.4$ Hz, aromatic), 5.82 (1H, *s*, –CH).); ¹³C-NMR (300 MHz, CDCl₃, δ / ppm): 34.6 (CH), 106.2–136.2 (aromatic), 141.2 (O–C–CH). MS (m/z , (relative abundance, %)): 312 (M⁺, 2.8), 116 (BP, 100).