

SUPPLEMENTARY MATERIAL TO
**A novel approach toward the synthesis of some new
tridentate Schiff bases from anil-like compounds**

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CHARACTERIZATION DATA FOR **1b** AND **1c**

1-((Pyrimidin-2-ylimino)methyl)naphthalen-2-ol (1b). Yield: 88 %; yellow crystalline solid; m.p.: 150–151 °C; Anal. Calcd. for C₁₅H₁₁N₃O: C, 72.29; H, 4.41; N, 16.86 %. Found: C, 72.34; H, 4.38; N, 16.94 %; IR (KBr, cm⁻¹): 3421, 3059, 1627, 1587, 1538, 1480, 1402, 1317, 1285; ¹H-NMR (300 MHz, DMSO-*d*₆, δ / ppm): 6.66 (1H, *d*, *J* = 9.6 Hz, Ar-H), 7.28–7.35 (2H, *m*, pyrimidine-H5, Ar-H), 7.49 (1H, *t*, *J* = 8.4 Hz, Ar-H), 7.64 (1H, *d*, *J* = 7.5 Hz, Ar-H), 7.84 (1H, *d*, *J* = 9.6 Hz, Ar-H), 8.04 (1H, *d*, *J* = 8.1 Hz, Ar-H), 8.78 (2H, *d*, *J* = 4.8 Hz, pyrimidine-H4 & H6), 9.52 (1H, *d*, *J* = 10.5 Hz, =CH), 14.53 (1H, *d*, *J* = 10.5 Hz, OH); ¹³C-NMR (75 MHz, DMSO-*d*₆, δ / ppm): 108.83, 118.56, 119.96, 125.10, 126.56, 126.87, 129.70, 129.96, 134.01, 141.93, 146.41, 157.54, 159.72, 184.19; MS (*m/z*, (relative abundance, %)): 249 (M)⁺ (100), 248 (80), 232 (13), 220 (70), 170 (21), 140 (8), 115 (20), 80 (50).

2-((Pyrimidin-2-ylimino)methyl)naphthalen-1-ol (1c). Yield: 82 %; orange crystalline solid; m.p.: 167–169 °C; Anal. Calcd. for C₁₅H₁₁N₃O: C, 72.29; H, 4.41; N, 16.86 %. Found: C, 72.23; H, 4.37; N, 16.89 %; IR (KBr, cm⁻¹): 3437, 3049, 1630, 1600, 1530, 1407, 1279, 1132; ¹H-NMR (300 MHz, DMSO-*d*₆, δ / ppm): 6.78 (1H, *d*, *J* = 9.0 Hz, Ar-H), 7.20 (1H, *d*, *J* = 9.0 Hz, Ar-H), 7.31 (1H, *t*, *J* = 4.8 Hz, pyrimidine-H5), 7.46 (1H, *t*, *J* = 7.8 Hz, Ar-H), 7.58–7.67 (2H, *m*, Ar-H), 8.27 (1H, *d*, *J* = 7.8 Hz, Ar-H), 8.76 (2H, *d*, *J* = 4.8 Hz, pyrimidine-H4 & H6), 8.89 (1H, *d*, *J* = 11.4 Hz, =CH), 13.90 (1H, *d*, *J* = 11.4 Hz, OH); ¹³C-NMR (75 MHz, DMSO-*d*₆, δ / ppm): 111.28, 117.46, 118.46, 126.38, 127.01, 127.99, 129.56, 130.57, 132.93, 138.47, 149.85, 157.04, 159.70, 183.55; MS (*m/z*, (relative abundance, %)): 249 (M)⁺ (100), 220 (76), 169 (10), 140 (12), 127 (6), 115 (18), 80 (68).

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CHARACTERIZATION DATA FOR **2a–d**

1-(((2-Aminophenyl)imino)methyl)naphthalene-2,7-diol (2a). Yield: 84 %; yellow powder; m.p. 223–225 °C; Anal. Calcd. for C₁₇H₁₄N₂O₂: C, 73.38; H, 5.03; N, 10.07. Found: C, 73.45; H, 5.07; N, 10.12; IR (KBr, cm⁻¹): 3400, 3344, 3283, 3062, 1600, 1557, 1514, 1331, 1217, 1142; ¹H-NMR (300 MHz, DMSO-*d*₆, δ / ppm): 5.07 (2H, *s*, NH₂), 6.68 (1H, *t*, *J* = 7.5 Hz, Ar-H), 6.81–6.92 (3H, *m*, Ar-H), 7.02 (1H, *t*, *J* = 7.5 Hz, Ar-H), 7.39 (1H, *d*, *J* = 7.8 Hz, Ar-H), 7.64–7.67 (2H, *m*, Ar-H), 7.80 (1H, *d*, *J* = 9.0 Hz, Ar-H), 9.36 (1H, *d*, *J* = 1.8 Hz, =CH), 9.84 (1H, *s*, OH), 15.40 (1H, *d*, *J* = 1.80 Hz, OH); ¹³C-NMR (75 MHz, DMSO-*d*₆, δ / ppm): 103.76, 108.88, 115.14, 116.15, 117.53, 117.65, 119.41, 121.72, 127.87, 131.15, 132.79, 135.35, 135.98, 142.25, 156.26, 158.02, 167.21; MS (*m/z*, (relative abundance, %)): 278 (M⁺) (87), 277 (90), 185 (9), 160 (19), 139 (9), 131 (12), 119 (100), 108 (22), 93 (12).

1-(((2-Aminophenyl)imino)methyl)naphthalen-2-ol (2b). Yield: 80 %; yellow powder; m.p.: 168–169 °C; Anal. Calcd. for C₁₇H₁₄N₂O: C, 77.86; H, 5.34; N, 10.68 %. Found: C, 77.84; H, 5.39; N, 10.70 %; IR (KBr, cm⁻¹): 3471, 3374, 3042, 1611, 1560, 1492, 1320, 1160; ¹H-NMR (300 MHz, DMSO-*d*₆, δ / ppm): 5.11 (2H, *s*, NH₂), 6.70 (1H, *t*, *J* = 7.2 Hz, Ar-H), 6.85 (1H, *d*, *J* = 7.8 Hz, Ar-H), 7.02–7.10 (3H, *m*, Ar-H & NH), 7.35 (1H, *t*, *J* = 7.2 Hz, Ar-H), 7.46 (1H, *d*, *J* = 7.8 Hz, Ar-H), 7.54 (1H, *t*, *J* = 7.2 Hz, Ar-H), 7.81 (1H, *d*, *J* = 7.8 Hz, Ar-H), 7.93 (1H, *d*, *J* = 9.0 Hz, Ar-H), 8.49 (1H, *d*, *J* = 8.4 Hz, Ar-H), 9.60 (1H, *s*, =CH), 15.66 (1H, *s*, OH); ¹³C-NMR (75 MHz, DMSO-*d*₆, δ / ppm): 109.73, 116.32, 117.69, 119.62, 120.89, 121.62, 123.80, 127.29, 128.06, 128.40, 129.40, 132.11, 133.32, 136.09, 142.26, 156.13, 167.56; MS (*m/z*, (relative abundance, %)): 262 (M⁺) (70), 261 (60), 233 (7), 144 (16), 131 (5), 119 (100), 108 (64), 92 (9).

1-(((2-Amino-4-nitrophenyl)imino)methyl)naphthalene-2,7-diol (2c). Yield: 78 %; orange powder; m.p.: 252–254 °C; Anal. Calcd. for C₁₇H₁₃N₃O₄: C, 63.15; H, 4.02; N, 13.00 %. Found: C, 63.17; H, 3.95; N, 13.02 %; IR (KBr, cm⁻¹): 3431, 3338, 3230, 3049, 1629, 1605, 1580, 1481, 1297, 1218, 1135; ¹H-NMR (300 MHz, DMSO-*d*₆, δ / ppm): 6.65 (2H, *s*, NH₂), 6.82 (1H, *d*, *J* = 9.0 Hz, Ar-H), 6.95 (2H, *m*, Ar-H), 7.71 (1H, *d*, *J* = 8.7 Hz, Ar-H), 7.82 (1H, *s*, Ar-H), 7.87 (1H, *d*, *J* = 9.0 Hz, Ar-H), 7.97 (1H, *d*, *J* = 9.0 Hz, Ar-H), 8.14 (1H, *s*, Ar-H), 9.50 (1H, *s*, =CH), 9.93 (1H, *s*, OH), 14.33 (1H, *s*, OH); ¹³C-NMR (75 MHz, DMSO-*d*₆, δ / ppm): 104.24, 109.44, 113.76, 115.80, 116.02, 122.35, 124.50, 131.19, 133.69, 135.17, 136.03, 136.94, 150.02, 158.12, 160.86, 163.84; MS (*m/z*, (relative abundance, %)): 323 (M⁺) (47), 322 (49), 276 (45), 164 (57), 160 (100), 153 (17), 131 (28), 115 (53), 91 (19).

2-(((2-Aminophenyl)imino)methyl)naphthalen-1-ol (2d). Yield: 88 %; orange powder; m.p.: 157–159 °C; Anal. Calcd. for C₁₇H₁₄N₂O: C, 77.86; H, 5.34; N, 10.68 %. Found: C, 77.89; H, 5.31; N, 10.74 %; IR (KBr, cm⁻¹): 3366, 3240, 3039, 1649, 1598, 1545, 1450, 1309, 1263, 1131; ¹H-NMR (300 MHz, DMSO-

$-d_6$, δ / ppm): 5.16 (2H, *s*, NH₂), 6.71 (1H, *t*, $J = 7.5$ Hz, Ar-H), 6.86 (1H, *d*, $J = 7.8$ Hz, Ar-H), 7.02 (1H, *d*, $J = 7.5$ Hz, Ar-H), 7.06 (1H, *s*, NH), 7.10 (1H, *d*, $J = 8.7$ Hz, Ar-H), 7.35 (1H, *d*, $J = 7.8$ Hz, Ar-H), 7.43 (1H, *d*, $J = 8.7$ Hz, Ar-H), 7.50 (1H, *d*, $J = 8.1$ Hz, Ar-H), 7.61 (1H, *t*, $J = 8.1$ Hz, Ar-H), 7.76 (1H, *d*, $J = 8.1$ Hz, Ar-H), 8.33 (1H, *d*, $J = 8.1$ Hz, Ar-H), 8.89 (1H, *d*, $J = 5.4$ Hz, =CH), 14.90 (1H, *d*, $J = 5.4$ Hz, OH); ¹H-NMR (300 MHz, DMSO-*d*₆ + D₂O, δ / ppm): 6.72 (1H, *t*, $J = 7.2$ Hz, Ar-H), 6.86 (1H, *d*, $J = 7.2$ Hz, Ar-H), 7.02 (1H, *d*, $J = 8.2$ Hz, Ar-H), 7.09 (1H, *d*, $J = 9.0$ Hz, Ar-H), 7.35 (1H, *d*, $J = 7.5$ Hz, Ar-H), 7.40–7.50 (2H, *m*, Ar-H), 7.60 (1H, *t*, $J = 7.8$ Hz, Ar-H), 7.75 (1H, *d*, $J = 8.1$ Hz, Ar-H), 8.31 (1H, *d*, $J = 8.1$ Hz, Ar-H), 8.84 (1H, *s*, =CH); ¹³C-NMR (75 MHz, DMSO-*d*₆, δ / ppm): 111.84, 116.45, 116.94, 117.99, 118.83, 124.58, 125.75, 127.75, 127.84, 127.96, 128.88, 130.16, 130.45, 136.85, 141.66, 158.32, 169.24; MS (*m/z*, (relative abundance, %)): 262 (M⁺) (70), 261 (89), 144 (7), 127 (5), 119 (100), 115 (21), 92 (11).

CHARACTERIZATION DATA FOR 4a–c

1-(((2-Hydroxyphenyl)imino)methyl)naphthalen-2-ol (4a). Yield: 88 %; orange powder; m.p.: 252–253 °C; Anal. Calcd. for C₁₇H₁₃NO₂: C, 77.56; H, 4.94; N, 5.32 %. Found: C, 77.51; H, 4.98; N, 5.39 %; IR (KBr, cm⁻¹): 3431, 3047, 1628, 1592, 1544, 1460, 1354, 1212, 1139; ¹H-NMR (300 MHz, DMSO-*d*₆, δ / ppm): 6.77 (1H, *d*, $J = 9.3$ Hz, Ar-H), 6.91–7.00 (2H, *m*, Ar-H), 7.10 (1H, *t*, $J = 7.2$ Hz, Ar-H), 7.26 (1H, *t*, $J = 7.2$ Hz, Ar-H), 7.46 (1H, *t*, $J = 8.1$ Hz, Ar-H), 7.67 (1H, *d*, $J = 7.8$ Hz, Ar-H), 7.79 (1H, *d*, $J = 9.3$ Hz, Ar-H), 7.94 (1H, *d*, $J = 7.8$ Hz, Ar-H), 8.39 (1H, *d*, $J = 8.1$ Hz, Ar-H), 9.49 (1H, *d*, $J = 9.9$ Hz, =CH), 10.34 (1H, *s*, OH), 15.71 (1H, *d*, $J = 9.9$ Hz, OH); ¹³C-NMR (75 MHz, DMSO-*d*₆, δ / ppm): 108.11, 116.37, 117.99, 120.19, 120.26, 123.48, 125.62, 126.26, 127.19, 128.56, 128.92, 129.45, 134.39, 138.43, 148.84, 149.77, 178.23; MS (*m/z*, (relative abundance, %)): 263 (M⁺) (100), 262 (89), 246 (13), 234 (6), 220 (3), 170 (6), 144 (15), 127 (10), 115 (25), 93 (7).

2-(((2-Hydroxyphenyl)imino)methyl)naphthalen-1-ol (4b). Yield: 85 %; brown powder; m.p.: 243–244 °C; Anal. Calcd. for C₁₇H₁₃NO₂: C, 77.56; H, 4.94; N, 5.32 %. Found: C, 77.62; H, 4.90; N, 5.29 %; IR (KBr, cm⁻¹): 3411, 3153, 3044, 1634, 1608, 1540, 1451, 1308, 1237, 1135; ¹H-NMR (300 MHz, DMSO-*d*₆, δ / ppm): 6.79 (1H, *d*, $J = 9.0$ Hz, Ar-H), 6.90–7.11 (4H, *m*, Ar-H, NH), 7.19 (1H, *d*, $J = 9.0$ Hz, Ar-H), 7.38–7.64 (3H, *m*, Ar-H), 7.70 (1H, *d*, $J = 7.2$ Hz, Ar-H), 8.31 (1H, *d*, $J = 7.8$ Hz, Ar-H), 8.86 (1H, *d*, $J = 11.7$ Hz, =CH), 10.52 (1H, *s*, OH), 14.59 (1H, *d*, $J = 11.7$ Hz, Ar-H); ¹³C-NMR (75 MHz, DMSO-*d*₆, δ / ppm): 110.21, 114.68, 116.44, 116.63, 120.35, 125.46, 125.76, 126.88, 127.63, 127.77, 129.60, 130.56, 131.28, 138.00, 148.15, 152.38, 179.17; MS (*m/z*, (relative abundance, %)): 263 (M⁺) (100), 262 (72), 246 (17), 234 (12), 218 (3), 169 (7), 144 (18), 128 (15), 115 (27), 93 (10).

2-(((1-Hydroxynaphthalen-2-yl)methylene)amino)pyridin-3-ol (**4c**). Yield: 81 %; orange powder; m.p.: 267–269 °C; Anal. Calcd. for C₁₆H₁₂N₂O₂: C, 72.72; H, 4.54; N, 10.60 %. Found: C, 72.65; H, 4.56; N, 10.67 %; IR (KBr, cm⁻¹): 3437, 3049, 1620, 1605, 1576, 1540, 1479, 1312, 1180, 1132; ¹H-NMR (300 MHz, DMSO-*d*₆, δ / ppm): 6.78 (1H, *d*, *J* = 9.0 Hz, Ar-H), 7.11–7.62 (7H, *m*, Ar-H), 7.93 (1H, *d*, *J* = 4.5 Hz, Ar-H), 8.30 (1H, *d*, *J* = 7.8 Hz, Ar-H), 9.00 (1H, *d*, *J* = 11.4 Hz, =CH), 11.02 (1H, *s*, OH), 14.38 (1H, *d*, *J* = 11.4 Hz, OH); ¹³C-NMR (75 MHz, DMSO-*d*₆, δ / ppm): 110.75, 115.86, 122.18, 123.47, 125.87, 126.09, 127.87, 129.96, 130.67, 132.05, 138.29, 138.97, 140.26, 143.30, 149.27, 181.53; MS (*m/z*, (relative abundance, %)): 264 (M⁺) (100), 247 (32), 235 (36), 169 (22), 140 (14), 127 (18), 115 (27), 95 (53).

THE CHARACTERIZATION DATA FOR **6** AND **7**

1-(3H-Imidazo[4,5-*c*]pyridin-2-yl)naphthalen-2-ol (**6**). Yellow powder; m.p.: 223–225 °C; Anal. Calcd. for C₁₆H₁₁N₃O: C, 73.56; H, 4.21; N, 16.09 %. Found: C, 73.60; H, 4.23; N, 16.15 %; IR (KBr, cm⁻¹): 3462, 3329, 3037, 1618, 1588, 1469, 1328, 1174; ¹H-NMR (300 MHz, DMSO-*d*₆, δ / ppm): 7.16 (1H, *d*, *J* = 9.0 Hz, Ar-H), 7.29 (1H, *t*, *J* = 7.5 Hz, Ar-H), 7.37–7.64 (4H, *m*, Ar-H, NH), 7.81 (1H, *d*, *J* = 8.1 Hz, Ar-H), 7.89 (1H, *d*, *J* = 8.1 Hz, Ar-H), 8.05 (1H, *d*, *J* = 9.0 Hz, Ar-H), 8.61 (1H, *d*, *J* = 8.7 Hz, Ar-H), 9.77 (1H, *s*, NH), 15.03 (1H, *s*, OH); ¹³C-NMR (75 MHz, DMSO-*d*₆, δ / ppm): 110.02, 119.71, 120.55, 121.45, 124.30, 127.79, 128.02, 128.26, 128.62, 129.26, 129.49, 129.94, 133.18, 136.77, 145.73, 159.39, 165.38; MS (*m/z*, (relative abundance, %)): 263 (M+2)⁺ (100), 262 (M+1)⁺ (95), 261 (M⁺) (84), 246 (7), 234 (10), 170 (8), 144 (30), 127 (18), 120 (94), 115 (33), 93 (14).

2-(2,3-Dihydro-1H-perimidin-2-yl)naphthalen-1-ol (**7**). Yellowish powder; m.p.: 181–183 °C; Anal. Calcd. for C₂₁H₁₆N₂O: C, 80.76; H, 5.12; N, 8.97 %. Found: C, 80.70; H, 5.16; N, 8.99 %; IR (KBr, cm⁻¹): 3367, 3272, 3042, 2913, 1605, 1576, 1412, 1381, 1300, 1098; ¹H-NMR (300 MHz, DMSO-*d*₆, δ / ppm): 5.80 (1H, *s*, CH), 6.58 (2H, *d*, *J* = 7.20 Hz, Ar-H), 6.82 (2H, *s*, NH), 7.07 (2H, *d*, *J* = 8.4 Hz, Ar-H), 7.19 (2H, *m*, Ar-H), 7.45–7.55 (3H, *m*, Ar-H), 7.60 (1H, *d*, *J* = 8.4 Hz, Ar-H), 7.86–7.88 (1H, *m*, Ar-H), 8.24–8.27 (1H, *m*, Ar-H), 9.76 (1H, *s*, OH); ¹³C-NMR (75 MHz, DMSO-*d*₆, δ / ppm): 63.86, 105.69, 113.33, 116.47, 119.28, 120.26, 122.63, 125.52, 126.95, 127.20, 127.27, 127.92, 132.22, 134.63, 134.82, 143.67, 151.88; MS (*m/z*, (relative abundance, %)): 312 (M⁺) (100), 311 (66), 295 (8), 169 (84), 168 (54), 156 (8), 140 (10), 115 (32).