SUPPLEMENTARY EXPERIMENTAL DATA

A Novel Route for the Synthesis of 3-(pyrrol-1-yl)-indolin-2-ones in Aqueous Micellar Medium

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Physical and chemical data for compounds 3a-3j

3-(Pyrrol-1-yl)-1,3-dihydroindol-2-one (3a): White needles, m.p. 150-152 °C (Lit.^[14] m.p. 148-150 °C); IR: 3298, 1721, 720 cm⁻¹; NMR (CDCl₃): δ_{H} 5.51 (1H, s), 6.25 (2H, m), 6.70 (2H, m), 6.93 (1H, d, $J = 7.5$ Hz), 7.07 (1H, t, $J = 7.5$ Hz, 15 Hz), 7.29 (2H, m), 8.98 (1H, s, -NH); δ_{C} 60.9 (CH), 109.5 (2xCH), 110.9 (2xCH), 120.3 (CH), 123.2 (CH), 125.1 (C), 125.3 (CH), 130.1 (CH), 141.4 (C), 175.5 (C); MS: (ESI-MS, positive mode) m/z 199 [M+H]⁺, 221 [M+Na]⁺; HRMS (ESI) calcd for C₁₂H₁₀N₂ONa: 221.0691, found 221.0695.

5-Iodo-3-(pyrrol-1-yl)-1,3-dihydroindol-2-one (3b): White needles, m.p. 206-208 °C (Lit.^[16] m.p. 204-206 °C); IR: 3294, 1723, 722 cm⁻¹; NMR (DMSO-*d*₆): δ_{H} 5.92 (1H, s), 6.08 (2H, m), 6.70 (2H, m), 6.94 (1H, d, $J = 8.1$ Hz), 7.12 (1H, s), 7.35 (1H, d, $J = 8.1$ Hz), 10.82 (1H, s, -NH); δ_{C} 60.2 (CH), 108.8 (2xCH), 111.6 (2xCH), 120.4 (CH), 124.6 (CH), 126.1 (C), 128.5 (C), 129.5 (CH), 141.6 (C), 173.8 (C); MS: (ESI-MS, positive mode) m/z 325 [M+H]⁺, 347 [M+Na]⁺; HRMS (ESI) calcd for C₁₂H₉IN₂ONa: 346.9657, found 346.9655.

5-Fluoro-3-(pyrrol-1-yl)-1,3-dihydroindol-2-one (3c): White needles, m.p. 145-147 °C (Lit.^[16] m.p. 143-145 °C); IR: 3196, 1719, 727 cm⁻¹; NMR (DMSO-*d*₆): δ_{H} 5.91 (1H, s), 6.08 (2H, m), 6.69 (2H, m), 6.92 (1H, m), 7.00 (1H, m), 7.14 (1H, t, $J = 9.0$ Hz),

10.70 (1H, s, -NH); δ_C 60.4 (CH), 108.7 (2xCH), 111.0 (CH), 111.1 (CH), 112.4 (CH, $^2J_{C-F}$ = 24.0 Hz), 116.1 (CH, $^2J_{C-F}$ = 23.25 Hz), 120.4 (CH), 128.1 (C, $^3J_{C-F}$ = 8.25 Hz), 138.6 (C), 158.1 (C, $^1J_{C-F}$ = 237), 174.0 (C); MS: (ESI-MS, positive mode) m/z 217 $[M+H]^+$, 249 $[M+Na]^+$; HRMS (ESI) calcd for $C_{12}H_9FN_2ONa$: 239.0597, found 239.0595.

5-Chloro-3-(pyrrol-1-yl)-1,3-dihydroindol-2-one (3d): White needles, m.p. 166-168 °C (Lit.^[16] m.p. 165-167 °C); IR: 3294, 1723, 722 cm^{-1} ; NMR (DMSO- d_6): δ_H 5.92 (1H, s), 6.08 (2H, m), 6.70 (2H, m), 6.94 (1H, d, J = 8.1 Hz), 7.12 (1H, s), 7.35 (1H, d, J = 8.1 Hz), 10.82 (1H, s, -NH); δ_C 60.2 (CH), 108.8 (2xCH), 111.6 (2xCH), 120.4 (CH), 124.6 (CH), 126.1 (C), 128.5 (C), 129.5 (CH), 141.6 (C), 173.8 (C); MS: (ESI-MS, positive mode) m/z 233 $[M+H]^+$, 235 $[M+2+H]^+$, 255 $[M+Na]^+$, 257 $[M+2+Na]^+$; HRMS (ESI) calcd for $C_{12}H_9ClN_2ONa$: 255.0301, found 255.0300.

5-Bromo-3-(pyrrol-1-yl)-1,3-dihydroindol-2-one (3e): White needles, m.p. 166-168 °C (Lit.^[14] m.p. 168-170 °C); IR: 3294, 1723, 722 cm^{-1} ; NMR (DMSO- d_6): δ_H 5.93 (1H, s), 6.08 (2H, m), 6.70 (2H, m), 6.89 (1H, d, J = 8.4 Hz), 7.22 (1H, s), 7.48 (1H, d, J = 8.1 Hz), 10.83 (1H, s, -NH); δ_C 60.1 (CH), 108.8 (2xCH), 112.1 (2xCH), 113.6 (C), 120.4 (CH), 127.3 (CH), 128.9 (C), 132.4 (CH), 141.6 (C), 173.6 (C); MS: (ESI-MS, positive mode) m/z 277 $[M+H]^+$, 279 $[M+2+H]^+$, 298 $[M+Na]^+$, 300 $[M+2+Na]^+$; HRMS (ESI) calcd for $C_{12}H_9BrN_2ONa$: 298.9796, found 298.9795.

5-Methyl-3-(pyrrol-1-yl)-1,3-dihydroindol-2-one (3f): White needles, m.p. 170-172 °C (Lit.^[14] m.p. 168-170 °C); IR: 3298, 1721, 720 cm^{-1} ; NMR (CDCl₃): δ_H 2.22 (3H, s), 5.82 (1H, s), 6.06 (2H, m), 6.67 (2H, m), 6.81 (1H, d, J = 7.8 Hz), 6.92 (1H, s), 7.09 (1H, d, J = 7.5 Hz), 10.55 (1H, s, -NH); δ_C 20.5 (CH₃), 60.3 (CH), 108.5 (2xCH),

109.8 (2xCH), 120.3 (CH), 125.2 (CH), 126.5 (C), 129.8 (CH), 131.1 (C), 139.8 (C), 174.0 (C); MS: (ESI-MS, positive mode) m/z 213 $[M+H]^+$, 235 $[M+Na]^+$; HRMS (ESI) calcd for $C_{13}H_{12}N_2ONa$: 235.0847, found 235.0844.

5-Nitro-3-(pyrrol-1-yl)-1,3-dihydroindol-2-one (3g): Yellow needles, m.p. 163-165 °C (Lit.^[14] m.p. 162-164 °C); IR: 3285, 1725, 722 cm^{-1} ; NMR (DMSO- d_6): δ_H 6.05 (1H, s), 6.10 (2H, m), 6.76 (2H, m), 7.12 (1H, d, $J = 8.7$ Hz), 7.88 (1H, s), 8.26 (1H, dd, $J = 8.7$ Hz, 1.5 Hz), 11.38 (1H, s, -NH); δ_C 59.8 (CH), 109.0 (2xCH), 110.4 (2xCH), 120.1 (CH), 120.6 (CH), 126.8 (CH), 127.6 (C), 142.4 (C), 148.8 (C), 174.5 (C); MS: (ESI-MS, positive mode) m/z 244 $[M+H]^+$, 266 $[M+Na]^+$; HRMS (ESI) calcd for $C_{12}H_9N_3O_3Na$: 266.0542, found 266.0540.

5,7-Dimethyl-3-(pyrrol-1-yl)-1,3-dihydroindol-2-one (3h): White needles, m.p. 153-155 °C (Lit.^[16] m.p. 155-157 °C); IR: 3174, 1711, 722 cm^{-1} ; NMR (CDCl₃): δ_H 2.22 (3H, s), 2.25 (3H, s), 5.47 (1H, s), 6.23 (2H, m), 6.70 (2H, m), 6.91 (2H, d, $J = 9.6$ Hz), 9.39 (1H, s, -NH); δ_C 16.2 (CH₃), 20.9 (CH₃), 61.3 (CH), 109.2 (2xCH), 119.8 (2xCH), 120.3 (CH), 123.3 (C), 124.9 (CH), 131.9 (C), 132.8 (C), 137.6 (C), 175.4 (C); MS: (ESI-MS, positive mode) m/z 227 $[M+H]^+$, 249 $[M+Na]^+$; HRMS (ESI) calcd for $C_{14}H_{14}N_2ONa$: 249.1004, found 249.1007.

4,7-Dichloro-3-(pyrrol-1-yl)-1,3-dihydroindol-2-one (3i): White needles, m.p. 188-190 °C (Lit.^[16] m.p. 188-190 °C); IR: 3423, 1705, 727 cm^{-1} ; NMR (DMSO- d_6): δ_H 6.06 (1H, s), 6.07 (2H, m), 6.70 (2H, m), 7.05 (1H, d, $J = 8.7$ Hz), 7.43 (1H, d, $J = 8.7$ Hz), 11.31 (1H, s, -NH); δ_C 60.6 (CH), 108.6 (2xCH), 113.2 (2xCH), 120.6 (CH), 123.5 (CH), 124.9 (C), 129.4 (C), 131.2 (CH), 142.0 (C), 173.3 (C); MS: (ESI-MS, positive mode) m/z 267 $[M+H]^+$, 269 $[M+2+H]^+$, 271 $[M+4+H]^+$, 289 $[M+Na]^+$, 291

$[M+2+Na]^+$, 293 $[M+4+Na]^+$; HRMS (ESI) calcd for $C_{12}H_8Cl_2N_2ONa$: 288.9911, found 288.9914.

1-Benzyl-3-(pyrrol-1-yl)-1,3-dihydroindol-2-one (3j): White needles, m.p. 124-126 °C (Lit.^[15] m.p. 125-127 °C); IR: 3066, 1721, 736 cm^{-1} ; NMR ($CDCl_3$): δ_H 4.91 (2H, dd, $J = 15$ Hz, 21 Hz), 5.57 (1H, s), 6.25 (2H, m), 6.70 (2H, m), 6.79 (1H, d, $J = 7.8$ Hz), 7.05 (1H, t, $J = 7.5$ Hz, 15 Hz), 7.30 (7H, m); δ_C 44.0 (CH_2), 60.2 (CH), 109.4 (2xCH), 109.6 (2xCH), 120.2 (CH), 123.2 (CH), 124.5 (C), 125.3 (CH), 127.3 (CH), 127.8 (2xCH), 128.8 (2xCH), 130.0 (CH), 135.2 (C), 143.2 (C), 172.5 (C); MS: (ESI-MS, positive mode) m/z 289 $[M+H]^+$, 311 $[M+Na]^+$; HRMS (ESI) calcd for $C_{19}H_{16}N_2ONa$: 311.1160, found 311.1156