

Electronic Supplementary Information for
Synthesis of 3-acylindoles via copper-mediated oxidative decarbethoxylation
of ethyl arylacetates

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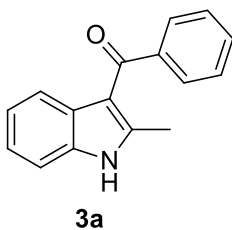
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- I. General Information:** All the reagents were purchased from Alfa Aesar or Merck, and were used as received. The reactions were monitored by thin layer chromatography (TLC) using Merck Kieselgel 60GF 254 plates (thickness 0.25 mm). Visualization of TLC was performed using UV light, and the product purification was done using Merck silica gel (100-200 mesh) column chromatography. NMR spectra were recorded with a 500 MHz spectrometer (JNM-ECZ500R/S1) for ^1H NMR, and 126 MHz for ^{13}C NMR spectroscopy using DMSO- d_6 solutions. Chemical shifts are given in δ ppm and are measured relative to tetramethylsilane (TMS) as internal standard. Mass spectra were recorded on SCIEX X500R QTOF (TOF-MS).
- II. General procedure for the synthesis of 3-acylindoles 3:** A mixture of indole **1** (1.0 mmol), ethyl arylacetate **2** (2.0 mmol), KOtBu (1.0 equiv.), Cu(OAc) $_2$ (40 mol %) and DMSO (1mL) was stirred in a glass vessel at 110 °C for 24 h under open atmosphere [Open atmosphere simply means the reaction without any special precautions to make it free from air]. After completion of reaction (as indicated by TLC), the mixture was quenched with aqueous NaHCO $_3$ saturated solution (5 mL), and then extracted with diethyl ether (3 $\times$ 5 mL). The combined organic phase was dried over anhydrous sodium sulfate, concentrated under reduced pressure, and then purified by silica gel column chromatography using a mixture of EtOAc and n-hexane (1:4) to give the pure product **3**.

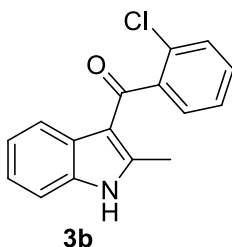
III. Spectral data of the products 3:

(2-Methyl-1H-indol-3-yl)(phenyl)methanone (3a).¹



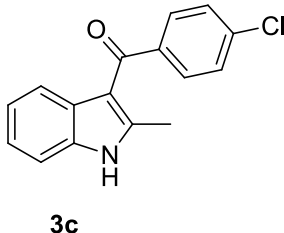
Yellow solid (78%, 183 mg); ¹H NMR (500 MHz, DMSO-d₆) δ_H = 2.37 (s, 3H), 6.99 (t, *J* = 7.5 Hz, 1H), 7.10 (t, *J* = 7.5 Hz, 1H), 7.31 (d, *J* = 8.0 Hz, 1H), 7.37 (d, *J* = 8.0 Hz, 1H), 7.49 (t, *J* = 7.5 Hz, 2H), 7.57 (t, *J* = 10.0 Hz, 3H), 11.95 (br s, 1H, NH); ¹³C NMR (126 MHz, DMSO-d₆) δ_C = 14.1, 111.2, 112.4, 120.0, 120.9, 121.8, 127.2, 128.0, 128.3, 131.0, 134.9, 141.6, 144.4, 191.7.

(2-Chlorophenyl)(2-methyl-1H-indol-3-yl)methanone (3b).



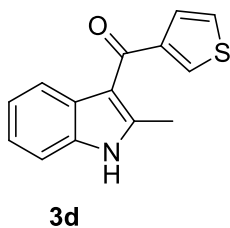
Yellow solid (67%, 180 mg); ¹H NMR (500 MHz, DMSO-d₆) δ_H = 2.26 (s, 3H), 7.03 (t, *J* = 7.5 Hz, 1H), 7.12 (t, *J* = 7.5 Hz, 1H), 7.35-7.39 (m, 3H), 7.46-7.53 (m, 2H), 7.57 (d, *J* = 8.0 Hz, 1H), 12.09 (s, 1H); ¹³C NMR (126 MHz, DMSO-d₆) δ_C = 13.8, 111.3, 112.4, 119.8, 121.6, 122.2, 126.9, 127.6, 127.7, 128.9, 129.6, 130.5, 135.0, 141.9, 146.2, 188.5; HRMS : (M+H)⁺ calcd. for C₁₆H₁₃³⁵ClNO: 270.0686; found: 270.0674.

(4-Chlorophenyl)(2-methyl-1H-indol-3-yl)methanone (3c).²



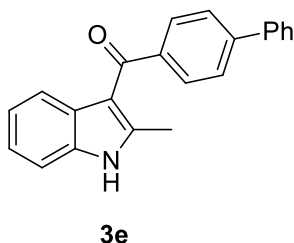
Brownish yellow solid (73%, 196 mg); ¹H NMR (500 MHz, DMSO-d₆) δ_H = 2.38 (s, 3H), 7.01 (t, *J* = 7.5 Hz, 1H), 7.10 (t, *J* = 7.5 Hz, 1H), 7.32 (d, *J* = 8.0 Hz, 1H), 7.38 (d, *J* = 8.0 Hz, 1H), 7.55 (dd, *J* = 8.0 Hz, *J* = 32.5 Hz, 4H), 11.97 (s, 1H); ¹³C NMR (126 MHz, DMSO-d₆) δ_C = 14.2, 111.3, 112.2, 119.9, 121.1, 121.9, 127.1, 128.5, 130.0, 135.0, 135.8, 140.2, 144.7, 190.3.

(2-Methyl-1H-indol-3-yl)(thiophen-3-yl)methanone (3d).



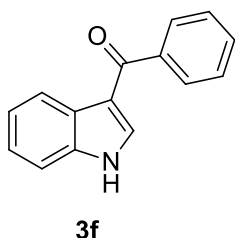
Reddish yellow solid (75%, 180 mg); ¹H NMR (500 MHz, DMSO-d₆) δ_H = 2.43 (s, 3H), 7.02 (t, *J* = 7.5 Hz, 1H), 7.10 (t, *J* = 7.5 Hz, 1H), 7.37 (d, *J* = 6.0 Hz, 2H), 7.47 (d, *J* = 8.0 Hz, 1H), 7.63 (t, *J* = 3.5, 1H), 7.99 (s, 1H), 11.87 (s, 1H); ¹³C NMR (126 MHz, DMSO-d₆) δ_C = 14.0, 111.1, 113.4, 119.9, 120.8, 121.7, 126.6, 127.1, 127.5, 130.8, 134.9, 143.4, 144.1, 185.5; HRMS : (M+H)⁺ calcd. for C₁₄H₁₂NOS: 242.0640; found: 242.0631.

[1,1'-Biphenyl]-4-yl(2-methyl-1H-indol-3-yl)methanone (3e).



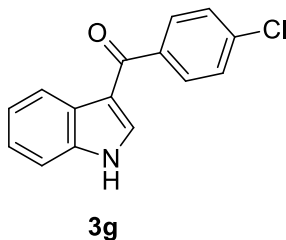
Reddish yellow solid (71%, 220 mg); **¹H NMR (500 MHz, DMSO-*d*₆)** δ_{H} = 1.98 (s, 3H), 7.32-7.37 (m, 2H), 7.43-7.46 (m, 3H), 7.64 (d, J = 7.5 Hz, 2H), 7.70-7.74 (m, 3H), 7.85 (t, J = 8.0 Hz, 1H), 8.10 (s, 1H), 8.62 (d, J = 8.5 Hz, 1H), 11.97 (s, 1H); **¹³C NMR (126 MHz, DMSO-*d*₆)** δ_{C} = 24.4, 90.0, 117.4, 119.9, 124.7, 124.8, 125.7, 126.7, 127.3, 127.7, 128.9, 136.1, 138.3, 139.3, 140.6, 152.5, 169.8, 196.0; **HRMS:** (M+H)⁺ calcd. for C₂₂H₁₈NO : 312.1388; found: 312.1378.

(1H-Indol-3-yl)(phenyl)methanone (3f).¹



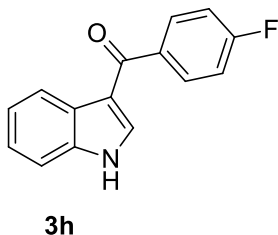
Yellow solid (68%, 150 mg); **¹H NMR (500 MHz, DMSO-*d*₆)** δ_{H} = 7.22-7.28 (m, 2H), 7.51-7.55 (m, 3H), 7.59-7.62 (m, 1H), 7.77 (d, J = 7.5 Hz, 2H), 7.92 (d, J = 3.0 Hz, 1H), 8.24 (d, J = 7.5 Hz, 1H), 12.06 (s, 1H); **¹³C NMR (126 MHz, DMSO-*d*₆)** δ_{C} = 112.2, 115.0, 121.4, 121.9, 123.1, 126.2, 128.3, 128.4, 131.0, 135.8, 136.7, 140.5, 190.0.

(4-Chlorophenyl)(1H-indol-3-yl)methanone (3g).¹



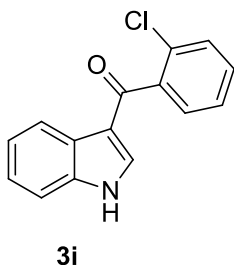
Yellow solid (72%, 183 mg); **¹H NMR (500 MHz, DMSO-*d*₆)** δ_{H} = 7.17-7.22 (m, 2H), 7.46 (d, J = 7.5 Hz, 1H), 7.52 (d, J = 8.5 Hz, 2H), 7.73 (d, J = 8.5, 2H), 7.90 (d, J = 3.0 Hz, 1H), 8.17 (d, J = 7.5, 1H), 12.06 (s, 1H); **¹³C NMR (126 MHz, DMSO-*d*₆)** δ_{C} = 112.3, 114.8, 121.4, 122.1, 123.3, 126.2, 128.5, 130.3, 135.9, 136.0, 136.8, 139.1, 188.7.

(4-Fluorophenyl)(1H-indol-3-yl)methanone (3h).²



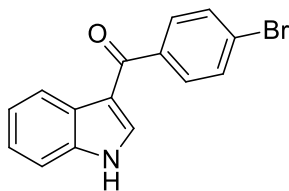
Reddish yellow solid (56%, 133 mg); **¹H NMR (500 MHz, DMSO-*d*₆)** δ_{H} = 7.22-7.26 (m, 2H), 7.34-7.37 (m, 2H), 7.51 (d, J = 8.0 Hz, 1H), 7.85-7.88 (m, 2H), 7.95 (d, J = 3.0 Hz, 1H), 8.22 (d, J = 7.5 Hz, 1H), 12.09 (s, 1H); **¹³C NMR (126 MHz, DMSO-*d*₆)** δ_{C} = 112.7, 115.3, 115.7, 115.9, 121.9, 122.4, 123.7, 126.7, 131.5, 131.6, 136.3, 137.2, 137.5, 189.0; **¹⁹F (470 MHz, DMSO-*d*₆)** δ_{F} = -109.31.

(2-Chlorophenyl)(1H-indol-3-yl)methanone (3i).³



Reddish brown solid (55%, 140 mg); **¹H NMR (500 MHz, DMSO-*d*₆)** δ_{H} = 7.23-7.28 (m, 2H), 7.45-7.58 (m, 5H), 7.64 (s, 1H), 8.14 (d, J = 7.0 Hz, 1H), 12.12 (s, 1H); **¹³C NMR (126 MHz, DMSO-*d*₆)** δ_{C} = 112.5, 116.0, 121.1, 122.2, 123.3, 125.3, 127.0, 128.6, 129.6, 129.7, 130.6, 136.9, 137.0, 140.2, 188.2.

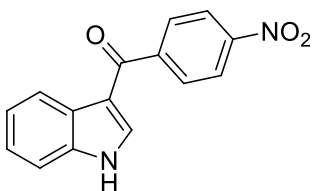
(4-Bromophenyl)(1H-indol-3-yl)methanone (3j).¹



3j

Reddish yellow solid (68%, 202 mg); ¹H NMR (500 MHz, DMSO-d₆) δ_H = 7.22-7.28 (m, 2H), 7.51 (d, *J* = 7.5 Hz, 1H), 7.73 (s, 4H), 7.96 (d, *J* = 2.5 Hz, 1H), 8.23 (d, *J* = 7.5 Hz, 1H), 12.12 (s, 1H), ¹³C NMR (126 MHz, DMSO-d₆) δ_C = 112.2, 114.7, 121.4, 122.0, 123.2, 124.7, 126.1, 130.4, 131.4, 136.0, 136.7, 139.4, 188.7.

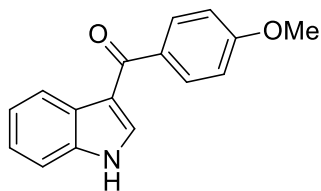
(1H-Indol-3-yl)(4-nitrophenyl)methanone (3k).¹



3k

Reddish yellow solid (62%, 165 mg); ¹H NMR (500 MHz, DMSO-d₆) δ_H = 7.28 (d, *J* = 4.5 Hz, 2H), 7.53 (d, *J* = 6.0 Hz, 1H), 7.99 (d, *J* = 7.5, 3H), 8.26 (d, *J* = 6.5, 1H), 8.35 (d, *J* = 7.5 Hz, 2H), 12.25 (s, 1H), ¹³C NMR (126 MHz DMSO-d₆) δ_C = 112.4, 114.8, 121.4, 122.2, 123.5, 123.6, 125.9, 129.6, 136.8, 136.9, 145.9, 148.6, 188.1.

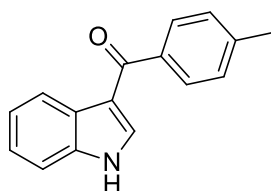
(1H-Indol-3-yl)(4-methoxyphenyl)methanone (3l).⁴



3l

Reddish yellow solid (65%, 163 mg); ¹H NMR (500 MHz, DMSO-d₆) δ_H = 3.85 (s, 3H), 7.06 (d, *J* = 8.5 Hz, 2H), 7.20-7.26 (m, 2H), 7.51 (d, *J* = 7.5 Hz, 1H), 7.80 (d, *J* = 8.5 Hz, 2H), 7.94 (d, *J* = 2.5 Hz, 1H), 8.22 (d, *J* = 7.5 Hz, 1H), 12.01 (s, 1H); ¹³C NMR (126 MHz, DMSO-d₆) δ_C = 55.3, 112.1, 113.6, 115.0, 121.4, 121.6, 122.9, 126.4, 130.5, 132.9, 134.8, 136.6, 161.7, 188.7.

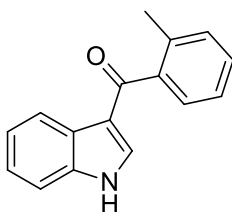
(1H-Indol-3-yl)(p-tolyl)methanone (3m).²



3m

Reddish yellow solid (66%, 146 mg); ¹H NMR (500 MHz, DMSO-d₆) δ_H = 2.40 (s, 3H), 7.20 (quin, *J* = 7.0 Hz, 2H), 7.33 (d, *J* = 7.5 Hz, 2H), 7.50 (d, *J* = 7.5 Hz, 1H), 7.69 (d, *J* = 7.5 Hz, 2H), 7.92 (d, *J* = 2.5, 1H), 8.22 (d, *J* = 7.5 Hz, 1H), 12.03 (s, 1H); ¹³C NMR (126 MHz, DMSO-d₆) δ_C = 21.0, 112.2, 115.0, 121.4, 121.8, 123.0, 126.3, 128.5, 128.9, 135.4, 136.6, 137.8, 141.0, 190.4.

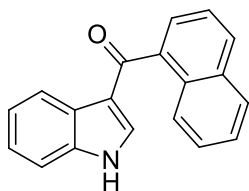
(1H-Indol-3-yl)(o-tolyl)methanone (3n).²



3n

Reddish yellow solid (63%, 148 mg); ¹H NMR (500 MHz, DMSO-d₆) δ_H = 2.27 (s, 3H), 7.21-7.27 (m, 4H), 7.37-7.41 (m, 2H), 7.50 (d, *J* = 8.0 Hz, 1H), 7.59 (d, *J* = 3.0, 1H), 8.18 (d, *J* = 7.5 Hz, 1H), 12.01 (s, 1H); ¹³C NMR (126 MHz, DMSO-d₆) δ_C = 19.1, 112.3, 116.5, 121.2, 122.0, 123.1, 125.2, 125.6, 127.1, 129.1, 130.5, 134.7, 136.2, 136.9, 141.0, 192.1.

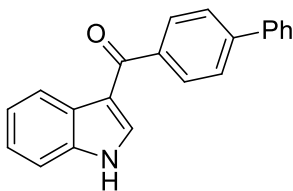
(1H-Indol-3-yl)(naphthalen-1-yl)methanone (3o).⁵



3o

Reddish yellow solid (67%, 181 mg); ¹H NMR (500 MHz, DMSO-d₆) δ_H = 7.27 (t, *J* = 3.5 Hz, 2H), 7.49-7.57 (m, 3H), 7.60 (t, *J* = 7.0 Hz, 1H), 7.67-7.70 (m, 2H), 8.0 (t, *J* = 8.0 Hz, 2H), 8.07 (d, *J* = 8.5 Hz, 1H), 8.29 (d, *J* = 6.0 Hz, 1H), 12.06 (s, 1H); ¹³C NMR (126 MHz, DMSO-d₆) δ_C = 112.4, 117.1, 121.4, 122.2, 123.3, 124.9, 125.3, 125.7, 125.8, 126.2, 126.7, 128.3, 129.6, 130.1, 133.3, 136.7, 137.0, 138.6, 191.3.

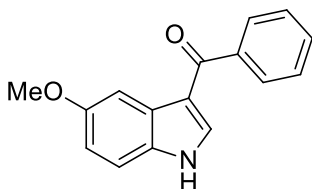
[1,1'-Biphenyl]-4-yl(1H-indol-3-yl)methanone (3p).⁴



3p

Reddish yellow solid (52%, 154 mg); ¹H NMR (500 MHz, DMSO-d₆) δ_H = 7.23-7.29 (m, 2H), 7.41 (t, *J* = 7.5 Hz, 1H), 7.50-7.54 (m, 3H), 7.54 (d, *J* = 7.5 Hz, 2H), 7.82 (d, *J* = 8.5 Hz, 2H), 7.88 (d, *J* = 8.0 Hz, 2H), 8.01 (d, *J* = 3.5 Hz, 1H), 8.27 (d, *J* = 7.5 Hz, 1H), 12.01 (s, 1H); ¹³C NMR (126 MHz, DMSO-d₆) δ_C = 112.7, 115.5, 122.0, 122.4, 123.6, 126.8, 127.1, 127.4, 128.5, 129.4, 129.6, 129.7, 136.2, 137.2, 139.8, 143.1, 189.9.

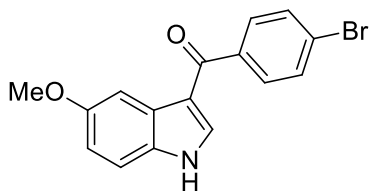
(5-Methoxy-1H-indol-3-yl)(phenyl)methanone (3q).¹



3q

Light yellow solid (46%, 115 mg); ¹H NMR (500 MHz, DMSO-d₆) δ_H = 3.80 (s, 3H), 6.88-6.90 (m, 1H), 7.40, (d, *J* = 9.0 MHz, 1H), 7.52 (t, *J* = 8.0 Hz, 2H), 7.58 (t, *J* = 7.5 Hz, 1H), 7.76 (q, *J* = 7.0 Hz, 3H), 7.86 (d, *J* = 2.0 Hz, 1H), 11.98 (s, 1H); ¹³C NMR (126 MHz, DMSO-d₆) δ_C = 55.2, 103.1, 112.9, 113.0, 114.8, 127.0, 128.2, 128.3, 130.9, 131.5, 135.9, 140.6, 155.5, 189.9.

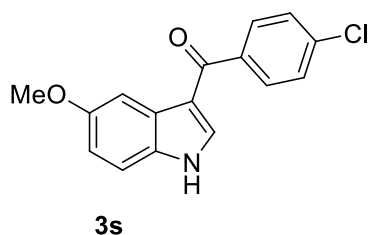
(4-Bromophenyl)(5-methoxy-1H-indol-3-yl)methanone (3r).¹



3r

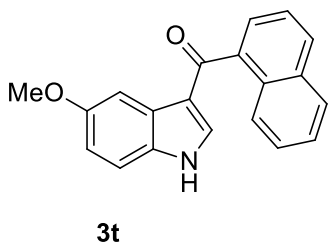
Yellow solid (72%, 237 mg); ¹H NMR (500 MHz, DMSO-d₆) δ_H = 3.80 (s, 3H), 6.89-6.91 (m, 1H), 7.41 (d, *J* = 8.5 Hz, 1H), 7.70-7.77 (m, 5H), 7.90 (d, *J* = 3.5 Hz, 1H), 12.01 (s, 1H); ¹³C NMR (126 MHz, DMSO-d₆) δ_C = 55.3, 103.1, 113.0, 113.1, 114.6, 124.6, 126.9, 130.3, 131.4, 131.5, 136.1, 139.6, 155.6, 188.6.

(4-Chlorophenyl)(5-methoxy-1H-indol-3-yl)methanone (3s).¹



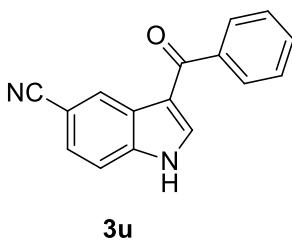
Yellow solid (68%, 194 mg); ¹H NMR (500 MHz, DMSO-d₆) δ_H = 3.80 (s, 3H), 6.89 (d, *J* = 7.5 Hz, 1H), 7.40 (d, *J* = 9.0 Hz, 1H), 7.58 (d, *J* = 8.0 Hz, 2H), 7.77-7.79 (m, 3H), 7.90 (d, *J* = 2.5 Hz, 1H), 12.02 (s, 1H); ¹³C NMR (126 MHz, DMSO-d₆) δ_C = 55.3, 103.2, 113.0, 113.1, 114.6, 127.0, 128.5, 130.2, 131.5, 135.7, 136.1, 139.2, 155.6, 188.6.

(5-Methoxy-1H-indol-3-yl)(naphthalen-1-yl)methanone (3t).



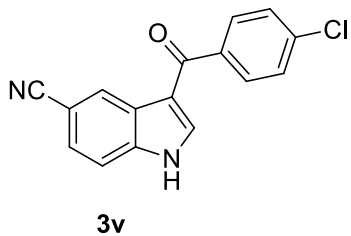
Reddish brown solid (66%, 198 mg); ¹H NMR (500 MHz, DMSO-d₆) δ_H = 3.85 (s, 3H), 6.91 (d, *J* = 9.0 Hz, 1H), 7.41 (d, *J* = 8.5 Hz, 1H), 7.50-7.62 (m, 4H), 7.66 (d, *J* = 7.0 Hz, 1H), 7.82 (s, 1H), 7.99 (t, *J* = 9.5 Hz, 2H), 8.06 (d, *J* = 8.0 Hz, 1H), 11.94 (s, 1H); ¹³C NMR (126 MHz, DMSO-d₆) δ_C = 55.2, 103.2, 113.0, 113.1, 117.1, 124.9, 125.3, 125.5, 126.2, 126.6, 126.7, 128.2, 129.5, 130.0, 132.0, 133.6, 136.7, 138.4, 155.9, 191.4; **HRMS:** (M+H)⁺ calcd. for C₂₀H₁₆NO₂: 302.1181; found: 302.1172.

3-Benzoyl-1H-indole-5-carbonitrile (3u).³



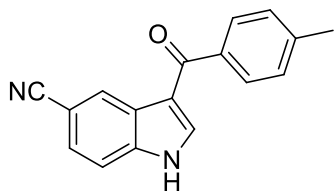
Greenish yellow (81%, 199 mg); ¹H NMR (500 MHz, DMSO-d₆) δ_H = 7.56 (d, *J* = 6.0 Hz, 2H), 7.63 (d, *J* = 6.5 Hz, 2H), 7.69 (d, *J* = 7.5 Hz, 1H), 7.82 (d, *J* = 6.0 Hz, 2H), 8.18 (s, 1H), 8.61 (s, 1H), 12.54 (s, 1H); ¹³C NMR (126 MHz, DMSO-d₆) δ_C = 104.1, 113.7, 115.0, 120.1, 126.0, 126.5, 128.4, 128.5, 131.5, 137.8, 138.5, 139.6, 141.5, 189.8.

3-(4-Chlorobenzoyl)-1H-indole-5-carbonitrile (3v).



Yellow solid (66%, 185 mg); ¹H NMR (500 MHz, DMSO-d₆) δ_H = 7.60 (d, *J* = 8.0 Hz, 2H), 7.63 (d, *J* = 8.5 Hz, 1H), 7.70 (d, *J* = 8.5 Hz, 1H), 7.83 (d, *J* = 8.0 Hz, 2H), 8.20 (s, 1H), 8.60 (s, 1H), 12.58 (s, 1H); ¹³C NMR (126 MHz, DMSO-d₆) δ_C = 104.3, 113.8, 114.9, 120.1, 126.0, 126.2, 126.5, 128.6, 130.4, 136.4, 138.0, 138.3, 138.6, 188.6; **HRMS:** (M+H)⁺ calcd. for C₁₆H₁₀³⁵ClN₂O: 281.0482; found: 281.0472.

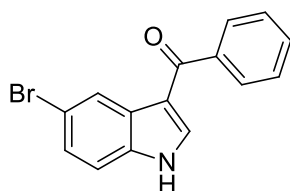
3-(4-Methylbenzoyl)-1H-indole-5-carbonitrile (3w).



3w

Light yellow solid (75%, 195 mg); **¹H NMR (500 MHz, DMSO-*d*₆)** δ_{H} = 2.37 (s, 3H), 7.31 (d, *J* = 8.0 Hz, 2H), 7.58 (d, *J* = 8.5 Hz, 1H), 7.65 (d, *J* = 8.5 Hz, 1H), 7.69 (d, *J* = 7.5, 2H), 8.14 (s, 1H), 8.56 (s, 1H), 12.47 (s, 1H); **¹³C NMR (126 MHz, DMSO-*d*₆)** δ_{C} = 21.0, 104.0, 113.7, 115.1, 120.1, 125.9, 126.1, 126.5, 128.6, 129.0, 136.9, 137.4, 138.5, 141.7, 189.4; **HRMS:** (M+H)⁺ calcd. for C₁₇H₁₃N₂O: 261.1028; found: 261.1015.

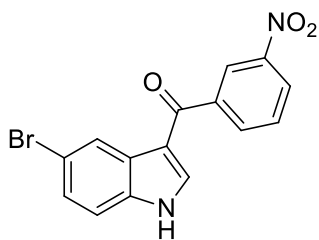
(5-Bromo-1H-indol-3-yl)(phenyl)methanone (3x).⁴



3x

Yellow solid (71%, 211 mg); **¹H NMR (500 MHz, DMSO-*d*₆)** δ_{H} = 7.39 (d, *J* = 8.5 Hz, 1H), 7.49 (d, *J* = 9.0 Hz, 1H), 7.53 (t, *J* = 7.5 Hz, 2H), 7.60 (t, *J* = 7.5 Hz, 1H), 7.78 (d, *J* = 7.0 Hz, 2H), 8.01 (d, *J* = 2.0 Hz, 1H), 8.39 (s, 1H), 12.25 (s, 1H); **¹³C NMR (126 MHz, DMSO-*d*₆)** δ_{C} = 114.3, 114.4, 114.7, 123.6, 125.7, 128.0, 128.4, 128.5, 131.3, 135.4, 136.8, 140.0, 189.8.

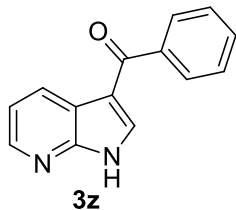
(5-Bromo-1H-indol-3-yl)(3-nitrophenyl)methanone (3y).



3y

Yellow solid (58%, 200 mg); **¹H NMR (500 MHz, DMSO-*d*₆)** δ_{H} = 7.42 (d, *J* = 8.5 Hz, 1H), 7.52 (d, *J* = 8.5 Hz, 1H), 7.82 (t, *J* = 7.5 Hz, 1H), 8.16 (d, *J* = 2.5 Hz, 1H), 8.22 (d, *J* = 7.5 Hz, 1H), 8.41-8.48 (m, 3H), 12.41 (s, 1H); **¹³C NMR (126 MHz, DMSO-*d*₆)** δ_{C} = 114.0, 114.5, 115.0, 123.0, 123.5, 125.7, 126.1, 127.8, 130.3, 134.6, 135.6, 137.7, 141.1, 147.7, 187.3; **HRMS:** (M-H)⁻ calcd. for C₁₅H₈⁷⁹BrN₂O₃: 342.9718; found: 342.9721.

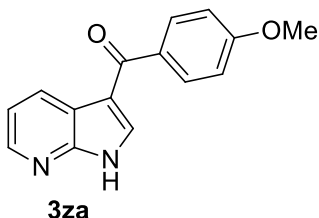
Phenyl(1H-pyrrolo[2,3-*b*]pyridin-3-yl)methanone (3z).⁶



3z

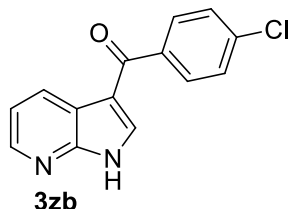
Yellow solid (71%, 157 mg); **¹H NMR (500 MHz, DMSO-*d*₆)** δ_{H} = 7.26 (s, 2H), 7.49 (t, *J* = 7.5 Hz, 2H), 7.56 (t, *J* = 6.5 Hz, 1H), 7.77 (d, *J* = 7.5 Hz, 2H), 8.04 (s, 1H), 8.49 (d, *J* = 7.5 Hz, 1H), 12.60 (s, 1H); **¹³C NMR (126 MHz, DMSO-*d*₆)** δ_{C} = 113.6, 118.2, 118.7, 128.2, 128.5, 129.8, 131.4, 135.8, 139.6, 144.5, 149.0, 189.2.

(4-Methoxyphenyl)(1H-pyrrolo[2,3-b]pyridin-3-yl)methanone (3za).



Yellow solid (62%, 156 mg); **¹H NMR (500 MHz, DMSO-*d*₆)** δ_{H} = 3.83 (s, 3H), 7.05 (d, *J* = 9.0 Hz, 2H), 7.25 (q, *J* = 4.5 Hz, 1H), 7.80 (d, *J* = 9.0 Hz, 2H), 8.06 (s, 1H), 8.34 (d, *J* = 3.0 Hz, 1H), 8.47 (m, 1H), 12.56 (s, 1H); **¹³C NMR (126 MHz, DMSO-*d*₆)** δ_{C} = 55.4, 113.7, 113.8, 118.0, 129.9, 130.8, 132.0, 134.9, 141.3, 144.3, 148.8, 162.0, 188.5; **HRMS:** (M+H)⁺ calcd. for C₁₅H₁₃N₂O₂: 253.0977; found: 253.0946.

(4-Chlorophenyl)(1H-pyrrolo[2,3-b]pyridin-3-yl)methanone(3zb).



Yellow solid (73%, 187 mg); **¹H NMR (500 MHz, DMSO-*d*₆)** δ_{H} = 7.29 (q, *J* = 4.5 Hz, 1H), 7.59 (d, *J* = 8.0 Hz, 2H), 7.82 (d, *J* = 8.0 Hz, 2H), 8.13 (s, 1H), 8.39 (s, 1H), 8.52 (d, *J* = 7.5 Hz, 1H), 12.71 (s, 1H); **¹³C NMR (126 MHz, DMSO-*d*₆)** δ_{C} = 113.4, 118.3, 118.7, 128.6, 129.8, 130.4, 136.1, 136.2, 138.2, 144.5, 149.0, 188.6; **HRMS:** (M+H)⁺ calcd. for C₁₄H₁₀³⁵ClN₂O: 257.0482; Found: 257.0447.

IV. References:

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