Supporting information

Direct C-2 acylation of indoles with toluene derivatives via Pd(II)-catalyzed direct C-H activation

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General experimental procedure

NMR spectra were recorded on a 300 MHz instrument using CDCl₃ as solvent unless and otherwise stated (s = singlet, d = doublet, t = triplet, m = multiplet). The ¹H and ¹³C chemical shifts are reported in parts per million relative to tetramethylsilane as an internal standard. For the Mass spectrometry, ion source temperature was 150-250°C, as required. High-resolution EI-mass spectra were performed with a resolution of 10,000. For chromatography, analytical TLC plates and 70-230 mesh silica gel were used. All the solvents and chemicals were purchased and used as available.

Typical experimental procedure

1-(pyrimidin-2-yl)-1H-indole (1 equiv, 0.2 mmol), PdBr₂ (10 mol%, 0.02 mmol), PivOH (0.5 equiv), PhCl (0.5 mL), toluene (1.5 mL), TBHP (5 equiv, 1.0 mmol), were consecutively loaded to an oven dried 10 mL screw cap vial equipped with a magnetic stirring bar and then stirred at 120 °C for 24 h. The resulting reaction mixture was cooled to the ambient temperature and subjected to the column chromatography to afford desired 2-oxindole. The products were further identified by ¹H NMR, ¹³C NMR.

Removal of directing group

An oven-dried 10 mL screw-cap vial was charged with a mixture of 3c (65.8 mg, 0.3 mmol), DMSO (2.0 mL) and EtONa (61.2 mg, 0.90 mmol), and the reaction mixture was stirred at 100 °C under nitrogen atmosphere for 24 h. After cooling to ambient temperature, the reaction mixture was diluted with EtOAc and washed with H₂O. The aqueous phase was extracted with EtOAc, and the combined organic phase was dried over Na₂SO₄. After filtration and evaporation under reduced pressure, the residue was purified by flash column chromatography (petroleum ether/ethyl acetate) on silica gel to give the product 3cc.
Characterization of products

**phenyl(1-(pyrimidin-2-yl)-1H-indol-2-yl)methanone (3a)**

$^1$H NMR (300 MHz, CDCl$_3$) $\delta$ 8.64 (d, $J$ = 4.8 Hz, 2H), 8.40 (dd, $J$ = 8.5, 0.8 Hz, 1H), 7.97 (dd, $J$ = 8.3, 1.3 Hz, 2H), 7.71 (d, $J$ = 7.8 Hz, 1H), 7.59–7.52 (m, 1H), 7.48–7.41 (m, 3H), 7.32–7.27 (m, 1H), 7.13 (d, $J$ = 0.7 Hz, 1H), 7.07 (t, $J$ = 4.8 Hz, 1H).$^{13}$C NMR (101 MHz, CDCl$_3$) $\delta$ 187.6, 157.9, 157.3, 138.3, 138.0, 137.2, 132.7, 129.6, 128.3, 128.0, 126.5, 122.8, 122.5, 117.4, 115.4, 114.2. HRMS (ESI) for C$_{19}$H$_{14}$N$_3$O $[M+H]^+$ calculated 300.1131, found 300.1136.

**N,N,N(1-(pyrimidin-2-yl)-1H-indol-2-yl)(p-tolyl)methanone (3b)**

$^1$H NMR (300 MHz, CDCl$_3$) $\delta$ 8.64 (d, $J$ = 4.8 Hz, 2H), 8.40 (dd, $J$ = 8.5, 0.8 Hz, 1H), 7.89 (d, $J$ = 8.2 Hz, 2H), 7.70 (d, $J$ = 7.8 Hz, 1H), 7.44 (ddd, $J$ = 8.5, 7.1, 1.3 Hz, 1H), 7.32–7.27 (m, 1H), 7.25 (d, $J$ = 7.3 Hz, 2H), 7.10 (d, $J$ = 0.7 Hz, 1H), 7.06 (t, $J$ = 4.8 Hz, 1H), 2.42 (s, 3H). $^{13}$C NMR (101 MHz, CDCl$_3$) $\delta$ 187.4, 157.9, 157.4, 143.5, 138.2, 137.4, 135.4, 129.7, 129.1, 128.1, 126.3, 122.8, 122.4, 117.3, 115.0, 114.2, 21.7. HRMS (ESI) for C$_{20}$H$_{15}$N$_3$O $[M+H]^+$ calculated 314.1288, found 314.1291.

**N,N,N(4-methoxyphenyl)(1-(pyrimidin-2-yl)-1H-indol-2-yl)methanone (3c)**

$^1$H NMR (300 MHz, CDCl$_3$) $\delta$ 8.65 (d, $J$ = 4.8 Hz, 2H), 8.40 (dq, $J$ = 8.4, 0.9 Hz, 1H), 8.04–7.94 (m, 2H), 7.71 (d, $J$ = 7.9 Hz, 1H), 7.46 (ddd, $J$ = 8.9, 5.2, 2.5 Hz, 2H), 7.34–7.26 (m, 1H), 7.17–7.06 (m, 4H). $^{13}$C NMR (75 MHz, CDCl$_3$) $\delta$ 186.5, 163.4, 157.9, 157.4, 138.1, 137.4, 131.9, 30.8, 128.1, 126.2, 122.7, 122.3, 117.3, 114.6, 114.2, 113.6, 55.5. HRMS (ESI) for C$_{20}$H$_{15}$N$_3$O$_2$ $[M+H]^+$ calculated 300.1237, found 330.1234.

**N,N,N(4-fluorophenyl)(1-(pyrimidin-2-yl)-1H-indol-2-yl)methanone (3d)**

$^1$H NMR (300 MHz, CDCl$_3$) $\delta$ 8.64 (d, $J$ = 4.8 Hz, 2H), 8.41 (dd, $J$ = 8.9, 5.2, 2.5 Hz, 2H), 7.71 (d, $J$ = 7.9 Hz, 1H), 7.46 (ddd, $J$ = 8.4, 7.2, 1.2 Hz, 1H), 7.34–7.27 (m, 1H), 7.17–7.06 (m, 4H). $^{13}$C NMR (75 MHz, CDCl$_3$) $\delta$ 186.2, 158.0, 157.2, 138.3, 136.9, 132.1, 132.0, 127.9, 126.6, 122.9, 122.5, 117.4, 115.7, 115.4, 115.3,
HRMS (ESI) for C19H12FN3O [M+H]+ calculated 318.1037, found 318.1042.

(4-bromophenyl)(1-(pyrimidin-2-yl)-1H-indol-2-yl)methanone (3e)

H NMR (300 MHz, CDCl₃) δ 8.64 (d, J = 4.8 Hz, 2H), 8.40 (dd, J = 8.5, 0.8 Hz, 1H), 7.97 (dd, J = 8.3, 1.3 Hz, 2H), 7.71 (d, J = 7.8 Hz, 1H), 7.59–7.52 (m, 2H), 7.48–7.41 (m, 1H), 7.32–7.27 (m, 1H), 7.13 (d, J = 0.7 Hz, 1H), 7.07 (t, J = 4.8 Hz, 1H). C NMR (101 MHz, CDCl₃) δ 186.6, 157.9, 157.2, 138.3, 136.9, 136.7, 131.7, 130.9, 128.0, 127.8, 126.7, 122.9, 122.5, 117.4, 115.3, 114.4. HRMS (ESI) for C19H12BrN3O [M+H]+ calculated 378.0237, found 378.0240.

(4-iodophenyl)(1-(pyrimidin-2-yl)-1H-indol-2-yl)methanone (3f)

H NMR (400 MHz, CDCl₃) δ 8.63 (s, 2H), 8.42 (d, J = 8.4 Hz, 1H), 7.80 (d, J = 8.0 Hz, 2H), 7.69 (t, J = 10.4 Hz, 3H), 7.46 (t, J = 7.3 Hz, 1H), 7.31 (d, J = 7.4 Hz, 1H), 7.09 (d, J = 11.6 Hz, 2H). C NMR (101 MHz, CDCl₃) δ 186.8, 157.9, 157.2, 138.3, 137.7, 137.4, 136.7, 130.9, 128.0, 126.7, 122.9, 122.5, 117.4, 115.3, 114.4, 100.5. HRMS (ESI) for C19H12IN3O [M+H]+ calculated 426.0100, found 426.0094.

(1-(pyrimidin-2-yl)-1H-indol-2-yl)(o-tolyl)methanone (3i)

H NMR (300 MHz, CDCl₃) δ 8.68 (d, J = 4.8 Hz, 2H), 8.29 (dq, J = 8.5, 0.9 Hz, 1H), 7.68 (dt, J = 7.9, 1.0 Hz, 1H), 7.56 (dd, J = 7.6, 1.4 Hz, 1H), 7.43 (ddd, J = 8.5, 7.1, 1.3 Hz, 1H), 7.34 (td, J = 7.5, 1.5 Hz, 1H), 7.31–7.26 (m, 1H), 7.26–7.22 (m, 1H), 7.20–7.14 (m, 1H), 7.12–7.05 (m, 2H), 2.56 (s, 3H). C NMR (101 MHz, CDCl₃) δ 189.2, 157.9, 157.5, 138.7, 138.1, 131.2, 131.1, 130.3, 129.9, 127.8, 127.6, 126.7, 126.1, 125.1, 122.8, 122.7, 117.6, 116.3, 113.9, 20.4. HRMS (ESI) for C20H15N3O [M+H]+ calculated 314.1288, found 314.1293.

(3,5-dimethylphenyl)(1-(pyrimidin-2-yl)-1H-indol-2-yl)methanone (3j)

H NMR (300 MHz, CDCl₃) δ 8.66 (d, J = 4.8 Hz, 2H), 8.37 (dd, J = 8.5, 0.7 Hz, 1H), 7.71 (d, J = 7.8 Hz, 1H), 7.62 (s, 2H), 7.44 (ddd, J = 8.4, 7.2, 1.2 Hz, 1H), 7.34–7.26 (m, 1H), 7.21 (s, 1H), 7.12–7.05 (m, 2H), 2.36 (s, 6H). C NMR (101 MHz, CDCl₃) δ 187.9, 157.9, 157.4, 138.3, 138.0, 137.9, 137.4, 134.5, 127.9, 127.5, 126.4, 122.7, 122.5, 117.4, 115.3, 114.1, 21.2. HRMS (ESI) for C21H17N3O [M+H]+ calculated 328.1444, found 328.1449.
naphthalen-1-yl(1-(pyrimidin-2-yl)-1H-indol-2-yl)methanone (3k)

$^1$H NMR (300 MHz, CDCl$_3$) δ 8.74–8.67 (m, 1H), 8.54 (d, $J = 4.8$ Hz, 2H), 8.37 (dq, $J = 8.5$, 0.9 Hz, 1H), 7.97–7.83 (m, 2H), 7.79–7.66 (m, 2H), 7.65–7.50 (m, 2H), 7.49–7.35 (m, 2H), 7.29 (ddd, $J = 8.1$, 7.1, 1.0 Hz, 1H), 7.16 (d, $J = 0.9$ Hz, 1H), 6.96 (t, $J = 4.8$ Hz, 1H).

$^{13}$C NMR (101 MHz, CDCl$_3$) δ 188.8, 157.8, 157.3, 138.9, 138.5, 136.0, 133.7, 132.3, 131.1, 129.0, 128.2, 127.9, 127.6, 126.7, 126.4, 126.1, 124.2, 122.8, 122.6, 117.3, 116.2, 114.2.

HRMS (ESI) for C$_{23}$H$_{15}$N$_3$O [M+H]$^+$ calculated 350.1288, found 350.1284.

(1-(pyrimidin-2-yl)-1H-indol-2-yl)(m-tolyl)methanone (3l)

$^1$H NMR (300 MHz, CDCl$_3$) δ 8.65 (d, $J = 4.8$ Hz, 2H), 8.38 (dd, $J = 8.5$, 0.9 Hz, 1H), 7.81 (dq, $J = 1.7$, 0.8 Hz, 1H), 7.78 (dd, $J = 7.2$, 1.8 Hz, 1H), 7.71 (dt, $J = 7.9$, 1.0 Hz, 1H), 7.44 (ddd, $J = 8.5$, 7.1, 1.3 Hz, 1H), 7.40–7.26 (m, 3H), 7.12 (d, $J = 0.8$ Hz, 1H), 7.08 (t, $J = 4.8$ Hz, 1H), 2.40 (s, 3H).

$^{13}$C NMR (101 MHz, CDCl$_3$) δ 187.7, 157.9, 157.4, 138.3, 138.2, 137.9, 137.3, 133.6, 130.1, 128.2, 128.0, 126.9, 126.5, 122.8, 122.5, 117.4, 115.4, 114.2, 21.3.

HRMS (ESI) for C$_{20}$H$_{15}$N$_3$O [M+H]$^+$ calculated 314.1288, found 314.1284.

(3-fluorophenyl)(1-(pyrimidin-2-yl)-1H-indol-2-yl)methanone (3m)

$^1$H NMR (300 MHz, CDCl$_3$) δ 8.65 (d, $J = 4.9$ Hz, 2H), 8.42 (dq, $J = 8.5$, 0.9 Hz, 1H), 7.87–7.63 (m, 3H), 7.51–7.36 (m, 2H), 7.31 (ddd, $J = 8.1$, 7.1, 1.0 Hz, 1H), 7.27–7.21 (m, 1H), 7.15 (d, $J = 0.8$ Hz, 1H), 7.08 (t, $J = 4.8$ Hz, 1H).

$^{13}$C NMR (101 MHz, CDCl$_3$) δ 186.2, 163.9, 161.4, 157.9, 157.2, 140.2, 140.1, 138.3, 136.7, 136.0, 129.9, 127.9, 126.7, 125.3, 125.2, 122.9, 122.6, 119.8, 119.5, 117.4, 116.2, 115.9, 115.6, 114.4.

HRMS (ESI) for C$_{19}$H$_{12}$FN$_3$O [M+H]$^+$ calculated 318.1037, found 318.1035.

(3-bromophenyl)(1-(pyrimidin-2-yl)-1H-indol-2-yl)methanone (3n)

$^1$H NMR (300 MHz, CDCl$_3$) δ 8.65 (d, $J = 4.8$ Hz, 2H), 8.42 (dq, $J = 8.5$, 0.9 Hz, 1H), 8.13 (t, $J = 1.8$ Hz, 1H), 7.87 (ddd, $J = 7.7$, 1.6, 1.1 Hz, 1H), 7.76–7.65 (m, 2H), 7.47 (ddd, $J = 8.5$, 7.2, 1.3 Hz, 1H), 7.36–7.28 (m, 2H), 7.14 (d, $J = 0.8$ Hz, 1H), 7.09 (t, $J = 4.9$ Hz, 1H).

$^{13}$C NMR (101 MHz, CDCl$_3$) δ 185.9, 157.9, 157.2, 139.9, 138.4, 136.5, 135.5, 132.6, 129.9, 128.0, 127.9, 126.8, 122.9, 122.6, 117.4, 115.7, 114.4.

HRMS (ESI) for C$_{19}$H$_{12}$BrN$_3$O [M+H]$^+$ calculated
(3-iodophenyl)(1-(pyrimidin-2-yl)-1H-indol-2-yl)methanone (3o)

1H NMR (300 MHz, CDCl₃) δ 8.66 (d, J = 4.8 Hz, 2H), 8.41 (dq, J = 8.5, 0.9 Hz, 1H), 8.33 (t, J = 1.7 Hz, 1H), 7.95–7.83 (m, 2H), 7.72 (dt, J = 7.9, 1.0 Hz, 1H), 7.46 (ddd, J = 8.5, 7.1, 1.3 Hz, 1H), 7.31 (ddd, J = 8.0, 7.1, 1.0 Hz, 1H), 7.18 (t, J = 7.8 Hz, 1H), 7.13 (d, J = 0.8 Hz, 1H), 7.10 (t, J = 4.8 Hz, 1H).

13C NMR (101 MHz, CDCl₃) δ 185.9, 157.9, 157.2, 141.4, 139.8, 138.4, 138.2, 136.5, 130.0, 128.7, 127.9, 126.8, 122.9, 122.6, 117.5, 115.8, 114.3, 94.1.

HRMS (ESI) for C₁₉H₁₂IN₃O [M+H]+ calculated 426.0100, found 426.0097.

(3-methyl-1-(pyrimidin-2-yl)-1H-indol-2-yl)(phenyl)methanone(3p)

1H NMR (400 MHz, CDCl₃) δ 8.64 (d, J = 8.4 Hz, 1H), 8.46 (d, J = 4.8 Hz, 2H), 7.78 (d, J = 7.4 Hz, 2H), 7.69 (d, J = 7.8 Hz, 1H), 7.51 – 7.39 (m, 2H), 7.33 (q, J = 7.4 Hz, 3H), 6.85 (t, J = 4.8 Hz, 1H), 2.37 (s, 3H).

13C NMR (101 MHz, CDCl₃) δ 189.47, 157.6, 157.1, 139.3, 136.4, 133.3, 132.3, 130.3, 128.6, 128.3, 126.1, 122.6, 121.7, 120.2, 116.1, 115.2, 9.4.

HRMS (ESI) for C₂₀H₁₅N₃O [M+H]+ calculated 314.1288, found 314.1284.

(5-methoxy-1-(pyrimidin-2-yl)-1H-indol-2-yl)(phenyl)methanone(3q)

1H NMR (300 MHz, CDCl₃) δ 8.59 (d, J = 4.8 Hz, 2H), 8.34 (d, J = 9.0 Hz, 1H), 7.98–7.91 (m, 2H), 7.57–7.49 (m, 1H), 7.46–7.39 (m, 2H), 7.13–7.06 (m, 2H), 7.05 (d, J = 0.6 Hz, 1H), 7.02 (t, J = 4.8 Hz, 1H), 3.88 (s, 3H).

13C NMR (101 MHz, CDCl₃) δ 187.6, 157.9, 157.2, 156.0, 138.1, 137.7, 133.2, 132.6, 129.5, 128.7, 128.3, 117.1, 116.5, 115.5, 114.9, 103.5, 55.7.

HRMS (ESI) for C₂₀H₁₅N₃O₂ [M+H]+ calculated 330.1237, found 330.1237.

(5-fluoro-1-(pyrimidin-2-yl)-1H-indol-2-yl)(phenyl)methanone(3r)

1H NMR (400 MHz, CDCl₃) δ 8.60 (s, 2H), 8.46–8.37 (m, 1H), 7.94 (d, J = 6.9 Hz, 2H), 7.55 (s, 1H), 7.44 (d, J = 6.8 Hz, 2H), 7.34 (d, J = 9.0 Hz, 1H), 7.17 (t, J = 9.0 Hz, 1H), 7.05 (s, 2H).

13C NMR (101 MHz, CDCl₃) δ 187.6, 158.0, 157.9, 157.0, 138.5, 137.8, 134.5, 132.8, 129.5, 128.6, 128.6, 128.4, 127.6, 126.9, 117.4, 115.8, 115.7, 114.7, 114.5, 114.2, 114.2, 107.3, 107.1.

HRMS (ESI) for C₁₉H₁₂FN₃O [M+H]+ calculated 318.1037, found 318.1036.
(5-bromo-1-(pyrimidin-2-yl)-1H-indol-2-yl)(phenyl)methanone (3s)

$^1$H NMR (400 MHz, CDCl$_3$) δ 8.60 (s, 2H), 8.33 (d, $J$ = 8.8 Hz, 1H), 7.94 (d, $J$ = 6.5 Hz, 2H), 7.82 (s, 1H), 7.60–7.48 (m, 2H), 7.48–7.26 (m, 2H), 7.06 (s, 1H), 7.02 (s, 1H).$^{13}$C NMR (101 MHz, CDCl$_3$) δ 187.4, 157.9, 156.9, 138.1, 137.7, 136.6, 132.9, 129.7, 129.5, 129.1, 128.4, 124.7, 117.6, 116.1, 115.9, 113.6. HRMS (ESI) for C19H12BrN3O [M+H]$^+$ calculated 378.0237, found 378.0230.

(4-bromo-1-(pyrimidin-2-yl)-1H-indol-2-yl)(phenyl)methanone(3t)

$^1$H NMR (400 MHz, CDCl$_3$) δ 8.64 (s, 2H), 8.35 (d, $J$ = 8.4 Hz, 1H), 7.98 (d, $J$ = 7.0 Hz, 1H), 7.10 (s, 1H).$^{13}$C NMR (101 MHz, CDCl$_3$) δ 187.3, 158.1, 157.1, 138.3, 137.6, 137.5, 132.9, 129.6, 128.8, 128.5, 127.2, 125.7, 117.8, 116.1, 114.5, 113.4. HRMS (ESI) for C19H12BrN3O [M+H]$^+$ calculated 378.0237, found 378.0240.

2-benzoyl-1-(pyrimidin-2-yl)-1H-indole-4-carbonitrile (3u)

$^1$H NMR (300 MHz, CDCl$_3$) δ 8.72–8.63 (m, 3H), 8.04–7.95 (m, 2H), 7.68–7.59 (m, 2H), 7.50 (ddd, $J$ = 8.5, 7.2, 1.1 Hz, 3H), 7.27 (d, $J$ = 0.9 Hz, 1H), 7.16 (t, $J$ = 4.9 Hz, 1H).$^{13}$C NMR (101 MHz, CDCl$_3$) δ 187.20, 158.19, 156.69, 139.00, 137.48, 137.14, 133.35, 129.70, 129.41, 128.59, 127.77, 125.79, 119.35, 118.19, 117.66, 111.76, 105.08. HRMS (ESI) for C20H12N4O [M+H]$^+$ calculated 325.1084, found 325.1085.

(6-bromo-1-(pyrimidin-2-yl)-1H-indol-2-yl)(phenyl)methanone (3v)

$^1$H NMR (300 MHz, CDCl$_3$) δ 8.67–8.59 (m, 3H), 7.99–7.91 (m, 2H), 7.49–7.37 (m, 3H), 7.10–7.05 (m, 2H).$^{13}$C NMR (101 MHz, CDCl$_3$) δ 187.3, 158.0, 156.9, 138.6, 137.7, 137.6, 132.8, 129.5, 128.4, 126.8, 126.3, 123.5, 120.3, 117.6, 117.5, 114.6. HRMS (ESI) for C19H12BrN3O [M+H]$^+$ calculated 378.0237, found 378.0238.

(7-methyl-1-(pyrimidin-2-yl)-1H-indol-2-yl)(phenyl)methanone(3w)
\textbf{H NMR} (300 MHz, CDCl$_3$) \(\delta\) 8.88 (d, \(J = 4.9\) Hz, 2H), 7.95–7.90 (m, 2H), 7.62–7.56 (m, 2H), 7.52–7.45 (m, 2H), 7.43 (t, \(J = 4.9\) Hz, 1H), 7.21 (s, 1H), 7.15–7.11 (m, 2H), 1.97 (s, 3H).\textbf{C NMR} (101 MHz, CDCl$_3$) \(\delta\) 187.1, 159.8, 158.2, 138.4, 138.3, 136.1, 132.4, 129.7, 129.3, 128.3, 127.3, 122.5, 121.9, 121.1, 120.2, 116.5, 19.4. HRMS (ESI) for C$_{20}$H$_{15}$N$_3$O \([\text{M+H}]^+\) calculated 314.1288, found 314.1288.

(1H-indol-2-yl)(4-methoxyphenyl)methanone (3cc)

\textbf{H NMR} (400 MHz, Chloroform-d) \(\delta\) 9.32 (s, 1H), 8.04 (d, \(J = 8.8\) Hz, 2H), 7.72 (d, \(J = 8.0\) Hz, 1H), 7.48 (d, \(J = 8.3\) Hz, 1H), 7.37 (t, \(J = 7.7\) Hz, 1H), 7.21–7.12 (m, 2H), 7.03 (d, \(J = 8.8\) Hz, 2H), 3.91 (s, 3H). \textbf{C NMR} (101 MHz, CDCl$_3$) \(\delta\) 185.9, 163.4, 137.4, 134.6, 131.7, 130.8, 127.9, 126.3, 123.2, 121.1, 113.9, 112.2, 111.9, 77.2, 55.7.
\( ^1H \) and \( ^{13}C \)-NMR Spectra of the Products

3a
\[ \text{N} \quad \text{N} \quad \text{N} \\
\text{O} \quad \text{I} \]
3r