

## Supporting Information

### Concise Copper-Catalyzed One-Pot Tandem Synthesis of Benzimidazo[1,2-*b*]isoquinolin-11-one Derivatives

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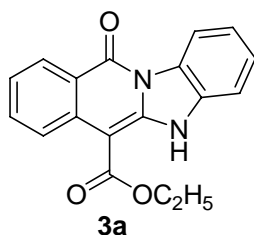
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## General experimental procedures

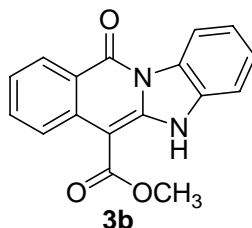
All reactions were carried out under nitrogen atmosphere. DMSO was dried over  $\text{MgSO}_4$ . Unless stated otherwise, all reagents were weighed and handled in air at room temperature. Flash chromatography was performed on silica gel (200 ~ 300 mesh). Proton and carbon magnetic resonance spectra ( $^1\text{H}$  NMR and  $^{13}\text{C}$  NMR) were recorded using tetramethylsilane (TMS) in the solvent of  $\text{DMSO-}d_6$  as the internal standard ( $^1\text{H}$  NMR: TMS at 0.00 ppm, DMSO at 2.50 ppm;  $^{13}\text{C}$  NMR: DMSO at 40.0 ppm).

**General procedure for synthesis of compounds 3a-q, 5 and 7.** DMSO (2 mL), substituted 2-halo-*N*-(2-halophenyl)benzamide (0.2 mmol), alkyl 2-cyanoacetates or malononitrile (0.24 mmol),  $\text{Na}_2\text{CO}_3$  (0.4 mmol, 43 mg) were added to a flask with a stir bar, and the mixture was stirred for 10 min under nitrogen atmosphere.  $\text{CuCl}$  (0.02 mmol, 2 mg) was added, and the reaction was performed at some shown temperature in Table 2 in text for 12 h under nitrogen atmosphere. The reaction was stopped when substituted 2-halo-*N*-(2-halophenyl)benzamide was consumed (TLC determination), and then the resulting solution was filtrated, the solid was washed with ethyl acetate ( $3 \times 5$  mL). The combined solution was concentrated by rotary evaporation, and the residue was purified by column chromatography on silica gel using petroleum ether/ethyl acetate as eluent to provide the desired product.

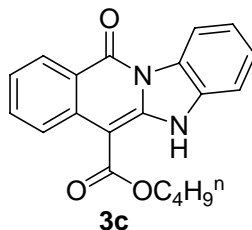


**11-Oxo-5,11-dihydro-benzo[4,5]imidazo[1,2-*b*]isoquinoline-6-carboxylic acid ethyl ester (3a).** Eluent: petroleum ether/ethyl acetate (5:1). Yield 90% (55 mg). Yellow solid, mp 317-319 °C.  $^1\text{H}$  NMR ( $\text{DMSO-}d_6$ , 300 MHz, ppm)  $\delta$  12.19 (s, br, 1H), 8.79 (d, 1H,  $J = 8.6$  Hz), 8.60 (d, 1H,  $J = 8.2$  Hz), 8.34 (d, 1H,  $J = 8.3$  Hz), 7.71-7.67 (m, 2H), 7.48 (t, 1H,  $J = 7.7$  Hz), 7.36-7.29 (m, 2H), 4.46 (q, 2H,  $J = 6.9$  Hz), 1.43 (t, 3H,  $J = 7.0$  Hz).  $^{13}\text{C}$  NMR ( $\text{DMSO-}d_6$ , 75 MHz, ppm)  $\delta$  166.5, 159.7, 146.2, 136.2, 133.5, 132.5, 127.8, 127.7, 126.7, 124.5, 123.1, 122.4, 118.8, 116.4,

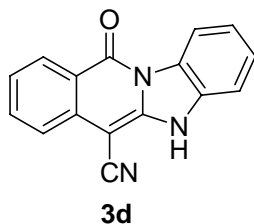
112.1, 82.3, 60.4, 15.2. HR-MS  $[M+H]^+$   $m/z$  Calcd for  $C_{18}H_{15}N_2O_3$ : 307.1083. Found: 307.1085.



**11-Oxo-5,11-dihydro-benzo[4,5]imidazo[1,2-*b*]isoquinoline-6-carboxylic acid methyl ester (3b).** Eluent: petroleum ether/ethyl acetate (5:1). Yield 87% (51 mg). Brown solid, mp 322-324 °C.  $^1H$  NMR (DMSO- $d_6$ , 300 MHz, ppm)  $\delta$  12.06 (s, br, 1H), 8.80 (d, 1H,  $J = 8.3$  Hz), 8.58 (d, 1H,  $J = 7.9$  Hz), 8.30 (d, 1H,  $J = 7.9$  Hz), 7.66 (d, 2H,  $J = 7.2$  Hz), 7.47 (t, 1H,  $J = 7.6$  Hz), 7.34-7.26 (m, 2H), 3.93 (s, 3H).  $^{13}C$  NMR (DMSO- $d_6$ , 75 MHz, ppm)  $\delta$  166.5, 159.7, 145.9, 136.3, 133.5, 132.5, 127.7, 127.6, 126.7, 124.3, 123.0, 122.4, 118.7, 116.4, 111.9, 82.0, 51.7. HR-MS  $[M+H]^+$   $m/z$  Calcd for  $C_{17}H_{13}N_2O_3$ : 293.0921. Found: 293.0923.

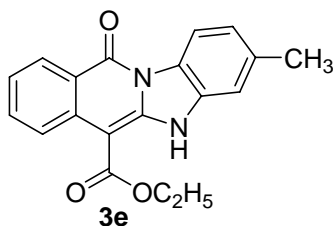


**6-Acetyl-5H-benzo[4,5]imidazo[1,2-*b*]isoquinolin-11-one (3c).** Eluent: petroleum ether/ethyl acetate (5:1). Yield 87% (58 mg). Brown solid.  $^1H$  NMR (DMSO- $d_6$ , 300 MHz, ppm)  $\delta$  12.20 (s, br, 1H), 8.70 (d, 1H,  $J = 8.6$  Hz), 8.58 (d, 1H,  $J = 7.9$  Hz), 8.31 (d, 1H,  $J = 7.6$  Hz), 7.71-7.63 (m, 2H), 7.47 (t, 1H,  $J = 7.4$  Hz), 7.34-7.26 (m, 2H), 4.39 (t, 2H,  $J = 6.3$  Hz), 1.82-1.77 (m, 2H), 1.51-1.44 (m, 2H), 0.99 (t, 3H,  $J = 7.2$  Hz).  $^{13}C$  NMR (DMSO- $d_6$ , 75 MHz, ppm)  $\delta$  166.2, 159.1, 145.7, 135.5, 132.9, 132.0, 127.3, 127.1, 126.1, 124.0, 122.5, 121.9, 118.2, 115.8, 111.6, 81.7, 63.6, 30.6, 18.9, 13.7. HR-MS  $[M+H]^+$   $m/z$  Calcd for  $C_{20}H_{19}N_2O_3$ : 335.1396. Found: 335.1398.



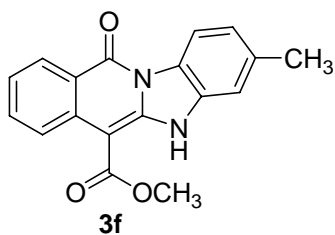
**11-Oxo-5,11-dihydro-benzo[4,5]imidazo[1,2-*b*]isoquinoline-6-carbonitrile (3d).**

Eluent: petroleum ether/ethyl acetate (5:1). Yield 85% (44 mg). Yellow solid, mp 284-287 °C. <sup>1</sup>H NMR (DMSO-*d*<sub>6</sub>, 300 MHz, ppm) δ 13.22 (s, br, 1H), 8.52 (d, 1H, *J* = 8.2 Hz), 8.28 (d, 1H, *J* = 7.9 Hz), 7.78 (t, 1H, *J* = 7.4 Hz), 7.62 (d, 1H, *J* = 7.9 Hz), 7.50-7.46 (m, 2H), 7.38-7.30 (m, 2H). <sup>13</sup>C NMR (DMSO-*d*<sub>6</sub>, 75 MHz, ppm) δ 159.2, 146.8, 136.1, 134.3, 132.7, 128.4, 128.2, 127.0, 123.7, 122.5, 122.1, 118.3, 117.3, 116.3, 111.2, 62.9. HR-MS [M+H]<sup>+</sup> *m/z* Calcd for C<sub>16</sub>H<sub>10</sub>N<sub>3</sub>O: 260.0824. Found: 260.0826.



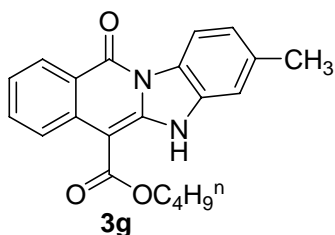
**3-Methyl-11-oxo-5,11-dihydro-benzo[4,5]imidazo[1,2-*b*]isoquinoline-6-carboxylic acid ethyl ester (3e).**

Eluent: petroleum ether/ethyl acetate (5:1). Yield 91% (58 mg). Brown solid, mp 202-204 °C. <sup>1</sup>H NMR (DMSO-*d*<sub>6</sub>, 300 MHz, ppm) δ 12.02 (s, br, 1H), 8.75 (d, 1H, *J* = 8.6 Hz), 8.39 (d, 1H, *J* = 8.2 Hz), 8.31 (d, 1H, *J* = 7.9 Hz), 7.66 (t, 1H, *J* = 7.7 Hz), 7.42 (s, 1H), 7.30 (t, 1H, *J* = 7.4 Hz), 7.06 (d, 1H, *J* = 8.3 Hz), 4.45 (q, 2H, *J* = 6.9 Hz), 2.40 (s, 3H), 1.43 (t, 3H, *J* = 7.0 Hz). <sup>13</sup>C NMR (DMSO-*d*<sub>6</sub>, 75 MHz, ppm) δ 166.5, 159.4, 146.1, 136.3, 136.0, 133.3, 132.6, 127.7, 125.6, 124.5, 123.2, 122.9, 118.7, 115.9, 112.1, 82.3, 60.4, 21.9, 15.1. HR-MS [M+H]<sup>+</sup> *m/z* Calcd for C<sub>19</sub>H<sub>17</sub>N<sub>2</sub>O<sub>3</sub>: 321.1239. Found: 321.1240.

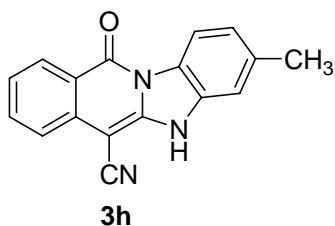


**3-Methyl-11-oxo-5,11-dihydro-benzo[4,5]imidazo[1,2-*b*]isoquinoline-6-carboxylic**

**acid methyl ester (3f).** Eluent: petroleum ether/ethyl acetate (5:1). Yield 89% (54 mg). Yellow solid, mp 213-215 °C. <sup>1</sup>H NMR (DMSO-*d*<sub>6</sub>, 300 MHz, ppm) δ 11.94 (s, br, 1H), 8.81 (d, 1H, *J* = 7.9 Hz), 8.37 (d, 1H, *J* = 7.9 Hz), 8.30 (d, 1H, *J* = 7.2 Hz), 7.66 (s, 1H), 7.39 (s, 1H), 7.31 (d, 1H, *J* = 6.5 Hz), 7.06 (d, 1H, *J* = 7.6 Hz), 3.93 (s, 3H), 2.41 (s, 3H). <sup>13</sup>C NMR (DMSO-*d*<sub>6</sub>, 75 MHz, ppm) δ 166.5, 159.5, 145.9, 136.4, 136.2, 133.4, 132.6, 127.6, 125.6, 124.3, 123.2, 123.0, 118.7, 115.9, 111.9, 82.0, 51.7, 21.9. HR-MS [M+H]<sup>+</sup> m/z Calcd for C<sub>18</sub>H<sub>15</sub>N<sub>2</sub>O<sub>3</sub>: 307.1083. Found: 307.1086.

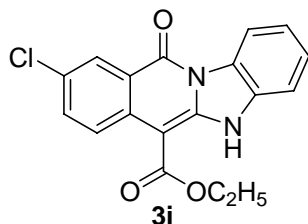


**6-Acetyl-3-methyl-5H-benzo[4,5]imidazo[1,2-*b*]isoquinolin-11-one (3g).** Eluent: petroleum ether/ethyl acetate (5:1). Yield 63% (44 mg). Brown solid, mp 204-206 °C. <sup>1</sup>H NMR (DMSO-*d*<sub>6</sub>, 300 MHz, ppm) δ 12.17 (s, br, 1H), 8.77 (d, 1H, *J* = 8.3 Hz), 8.44 (d, 1H, *J* = 8.3 Hz), 8.36 (d, 1H, *J* = 7.9 Hz), 7.72 (t, 1H, *J* = 7.6 Hz), 7.48 (s, 1H), 7.34 (t, 1H, *J* = 7.4 Hz), 7.13 (d, 1H, *J* = 8.3 Hz), 4.43 (t, 2H, *J* = 6.4 Hz), 2.44 (s, 3H), 1.81 (m, 2H), 1.48 (m, 2H), 0.98 (t, 3H, *J* = 7.2 Hz). <sup>13</sup>C NMR (DMSO-*d*<sub>6</sub>, 75 MHz, ppm) δ 166.8, 159.5, 146.3, 136.5, 136.1, 133.5, 132.67, 127.9, 125.7, 124.5, 123.4, 123.1, 118.8, 115.9, 112.2, 82.3, 64.2, 31.1, 21.9, 19.5, 14.2. HR-MS [M+H]<sup>+</sup> m/z Calcd for C<sub>21</sub>H<sub>21</sub>N<sub>2</sub>O<sub>3</sub>: 349.1552. Found: 349.1553.

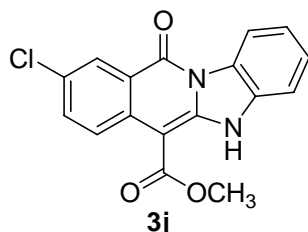


**3-Methyl-11-oxo-5,11-dihydro-benzo[4,5]imidazo[1,2-*b*]isoquinoline-6-carbonitril e (3h).** Eluent: petroleum ether/ethyl acetate (2:1). Yield 91% (58 mg). Yellow solid, mp >350 °C. <sup>1</sup>H NMR (DMSO-*d*<sub>6</sub>, 300 MHz, ppm) δ 13.09 (s, br, 1H), 8.33 (d, 1H, *J* = 7.9 Hz), 8.27 (d, 1H, *J* = 7.9 Hz), 7.77 (m, 1H), 7.61 (d, 1H, *J* = 8.3 Hz), 7.35 (m, 1H), 7.19 (s, 1H), 7.07 (d, 1H, *J* = 7.9 Hz), 2.40 (s, 3H). <sup>13</sup>C NMR (DMSO-*d*<sub>6</sub>, 75 MHz, ppm) δ 158.9, 146.6, 136.8, 136.1, 134.1, 132.8, 128.1, 126.2, 123.7, 123.3,

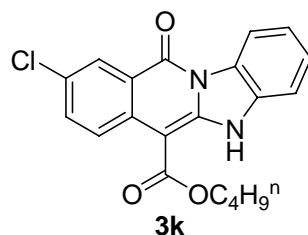
122.1, 118.3, 117.3, 115.8, 111.2, 62.9, 21.7. HR-MS  $[M+H]^+$   $m/z$  Calcd for  $C_{17}H_{12}N_3O$ : 274.0975. Found: 274.0974.



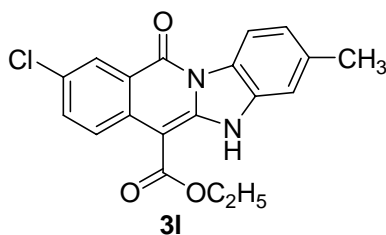
**9-Chloro-11-oxo-5,11-dihydro-benzo[4,5]imidazo[1,2-*b*]isoquinoline-6-carboxylic acid ethyl ester (3i).** Eluent: petroleum ether/ethyl acetate (6:1). Yield 81% (55 mg). Yellow solid, mp 246-248 °C.  $^1H$  NMR (DMSO- $d_6$ , 600 MHz, ppm)  $\delta$  12.02 (s, br, 1H), 8.76 (d, 1H,  $J = 8.9$  Hz), 8.56 (d, 1H,  $J = 8.2$  Hz), 8.22 (s, 1H), 7.69 (d, 1H,  $J = 8.3$  Hz), 7.64 (d, 1H,  $J = 8.9$  Hz), 7.47 (t, 1H,  $J = 7.6$  Hz), 7.32 (t, 1H,  $J = 7.6$  Hz), 4.48 (q, 2H,  $J = 6.9$  Hz), 1.44 (t, 3H,  $J = 7.2$  Hz).  $^{13}C$  NMR (DMSO- $d_6$ , 150 MHz, ppm)  $\delta$  166.2, 158.6, 146.2, 134.9, 133.3, 132.6, 127.7, 127.6, 126.9, 126.8, 126.4, 122.6, 119.9, 116.4, 112.2, 82.4, 60.5, 15.1. HR-MS  $[M+H]^+$   $m/z$  Calcd for  $C_{18}H_{14}ClN_2O_3$ : 341.0693. Found: 341.0695.



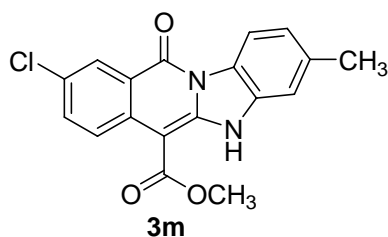
**9-Chloro-11-oxo-5,11-dihydro-benzo[4,5]imidazo[1,2-*b*]isoquinoline-6-carboxylic acid methyl ester (3j).** Eluent: petroleum ether/ethyl acetate (5:1). Yield 65% (43 mg). Yellow solid, mp 258-260 °C.  $^1H$  NMR (DMSO- $d_6$ , 600 MHz, ppm)  $\delta$  12.01 (s, br, 1H), 8.83 (d, 1H,  $J = 8.9$  Hz), 8.57 (d, 1H,  $J = 8.2$  Hz), 8.23 (s, 1H), 7.67 (m, 2H), 7.48 (t, 1H,  $J = 7.5$  Hz), 7.33 (t, 1H,  $J = 7.6$  Hz), 3.96 (s, 3H).  $^{13}C$  NMR (DMSO- $d_6$ , 150 MHz, ppm)  $\delta$  166.3, 158.7, 146.0, 135.1, 133.4, 132.6, 127.7, 127.6, 127.0, 126.8, 126.4, 122.6, 119.9, 116.5, 112.1, 82.2, 51.7. HR-MS  $[M+H]^+$   $m/z$  Calcd for  $C_{17}H_{12}ClN_2O_3$ : 327.0536. Found: 327.0538.



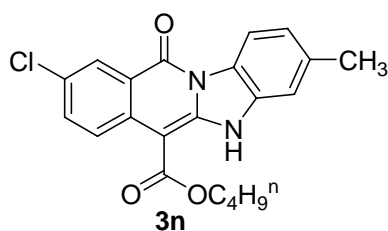
**6-Acetyl-9-chloro-5H-benzo[4,5]imidazo[1,2-*b*]isoquinolin-11-one (3k).** Eluent: petroleum ether/ethyl acetate (5:1). Yield 65% (48 mg). Yellow solid, mp 212-214 °C. <sup>1</sup>H NMR (DMSO-*d*<sub>6</sub>, 600 MHz, ppm) δ 12.12 (s, br, 1H), 8.78 (d, 1H, *J* = 8.9 Hz), 8.59 (d, 1H, *J* = 7.6 Hz), 8.27 (s, 1H), 7.70 (m, 2H), 7.49 (t, 1H, *J* = 7.9 Hz), 7.34 (t, 1H, *J* = 7.6 Hz), 4.44 (q, 2H, *J* = 6.5 Hz), 1.82 (m, 2H), 1.48 (m, 2H), 0.98 (t, 3H, *J* = 7.2 Hz). <sup>13</sup>C NMR (DMSO-*d*<sub>6</sub>, 150 MHz, ppm) δ 166.4, 158.7, 146.3, 134.9, 133.4, 132.6, 127.7, 127.6, 126.9, 126.8, 126.5, 122.6, 112.0, 116.4, 112.3, 82.4, 60.4, 31.1, 19.4, 14.1. HR-MS [M+H]<sup>+</sup> *m/z* Calcd for C<sub>20</sub>H<sub>17</sub>ClN<sub>2</sub>O<sub>3</sub>: 369.1006. Found: 369.1008.



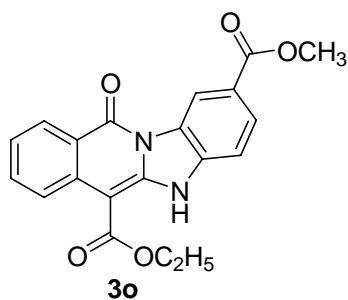
**9-Chloro-3-methyl-11-oxo-5,11-dihydro-benzo[4,5]imidazo[1,2-*b*]isoquinoline-6-carboxylic acid ethyl ester (3l).** Eluent: petroleum ether/ethyl acetate (6:1). Yield 78% (55 mg). Yellow solid, mp 248-250 °C. <sup>1</sup>H NMR (DMSO-*d*<sub>6</sub>, 600 MHz, ppm) δ 11.90 (s, br, 1H), 8.80 (d, 1H, *J* = 8.9 Hz), 8.42 (d, 1H, *J* = 8.2 Hz), 8.24 (s, 1H), 7.66 (d, 1H, *J* = 8.9 Hz), 7.48 (s, 1H), 7.13 (d, 1H, *J* = 8.2 Hz), 4.48 (q, 2H, *J* = 6.9 Hz), 2.45 (s, 3H), 1.44 (t, 3H, *J* = 7.2 Hz). <sup>13</sup>C NMR (DMSO-*d*<sub>6</sub>, 150 MHz, ppm) δ 166.2, 158.4, 146.2, 136.8, 134.9, 133.2, 132.7, 127.6, 126.9, 126.4, 125.6, 123.5, 120.0, 116.0, 112.2, 82.4, 60.5, 21.8, 15.0. HR-MS [M+H]<sup>+</sup> *m/z* Calcd for C<sub>19</sub>H<sub>16</sub>ClN<sub>2</sub>O<sub>3</sub>: 355.0850. Found: 355.0851.



**9-Chloro-3-methyl-11-oxo-5,11-dihydro-benzo[4,5]imidazo[1,2-*b*]isoquinoline-6-carboxylic acid methyl ester (3m).** Eluent: petroleum ether/ethyl acetate (6:1). Yield 83% (57 mg). Brown solid, mp 234-236 °C. <sup>1</sup>H NMR (DMSO-*d*<sub>6</sub>, 600 MHz, ppm) δ 11.88 (s, br, 1H), 8.83 (d, 1H, *J* = 8.9 Hz), 8.42 (d, 1H, *J* = 8.2 Hz), 8.23 (s, 1H), 7.67 (d, 1H, *J* = 8.9 Hz), 7.46 (s, 1H), 7.14 (d, 1H, *J* = 7.6 Hz), 3.98 (s, 3H), 2.47 (s, 3H). <sup>13</sup>C NMR (DMSO-*d*<sub>6</sub>, 150 MHz, ppm) δ 166.3, 158.4, 146.0, 136.8, 135.0, 133.2, 132.7, 127.6, 126.7, 126.3, 125.6, 123.5, 119.9, 116.0, 112.1, 82.2, 51.6, 21.8. HR-MS [M+H]<sup>+</sup> *m/z* Calcd for C<sub>18</sub>H<sub>14</sub>ClN<sub>2</sub>O<sub>3</sub>: 341.0693. Found: 341.0696.

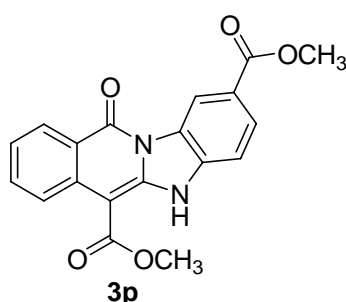


**6-Acetyl-9-chloro-3-methyl-5H-benzo[4,5]imidazo[1,2-*b*]isoquinolin-11-one (3n).** Eluent: petroleum ether/ethyl acetate (6:1). Yield 69% (53 mg). Brown solid, mp 172-174 °C. <sup>1</sup>H NMR (DMSO-*d*<sub>6</sub>, 600 MHz, ppm) δ 11.93 (s, br, 1H), 8.75 (s, 1H), 8.41 (s, 1H), 8.23 (s, 1H), 7.66 (d, 1H, *J* = 8.2 Hz), 7.48 (s, 1H), 7.12 (d, 1H, *J* = 7.6 Hz), 4.43 (s, 2H), 2.45 (s, 3H), 1.82 (s, 2H), 1.49 (m, 2H), 0.99 (m, 3H). <sup>13</sup>C NMR (DMSO-*d*<sub>6</sub>, 150 MHz, ppm) δ 166.0, 158.1, 145.9, 136.5, 134.5, 132.8, 132.4, 127.2, 126.5, 126.1, 125.3, 123.2, 119.6, 115.6, 111.9, 82.1, 64.0, 30.8, 21.5, 19.0, 13.6. HR-MS [M+H]<sup>+</sup> *m/z* Calcd for C<sub>21</sub>H<sub>20</sub>ClN<sub>2</sub>O<sub>3</sub>: 383.1157. Found: 383.1160.

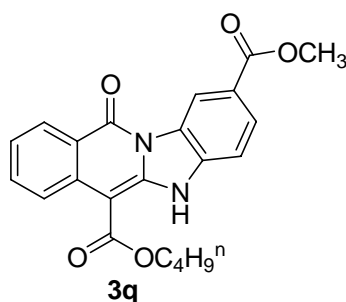




**11-Oxo-5,11-dihydro-benzo[4,5]imidazo[1,2-*b*]isoquinoline-2,6-dicarboxylic acid 6-ethyl ester 2-methyl ester (3o).** Eluent: petroleum ether/ethyl acetate (5:1). Yield 72% (52 mg). Yellow solid, mp 238-240 °C. <sup>1</sup>H NMR (DMSO-*d*<sub>6</sub>, 600 MHz, ppm) δ 12.22 (s, br, 1H), 9.12 (s, 1H), 8.81 (d, 1H, *J* = 7.6 Hz), 8.38 (d, 1H, *J* = 6.9 Hz), 8.07 (d, 1H, *J* = 7.6 Hz), 7.73 (m, 2H), 7.38 (m, 1H), 4.51 (m, 2H), 3.93 (s, 3H), 1.47 (t, 3H, *J* = 6.9 Hz). <sup>13</sup>C NMR (DMSO-*d*<sub>6</sub>, 150 MHz, ppm) δ 166.4, 166.3, 159.5, 146.6, 136.3, 136.0, 133.6, 128.3, 127.8, 124.7, 123.7, 123.6, 119.2, 117.3, 111.7, 83.5, 60.6, 52.5, 15.0. HR-MS [M+H]<sup>+</sup> *m/z* Calcd for C<sub>20</sub>H<sub>17</sub>N<sub>2</sub>O<sub>5</sub>: 365.1132. Found: 365.1133.

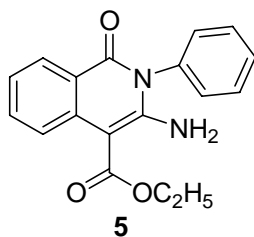


**11-Oxo-5,11-dihydro-benzo[4,5]imidazo[1,2-*b*]isoquinoline-2,6-dicarboxylic acid dimethyl ester (3p).** Eluent: petroleum ether/ethyl acetate (5:1). Yield 81% (57 mg). Brown solid, mp 256-258 °C. <sup>1</sup>H NMR (DMSO-*d*<sub>6</sub>, 600 MHz, ppm) δ 12.16 (s, br, 1H), 9.15 (s, 1H), 8.85 (d, 1H, *J* = 8.3 Hz), 8.39 (d, 1H, *J* = 7.6 Hz), 8.09 (d, 1H, *J* = 8.3 Hz), 7.76 (t, 1H, *J* = 7.2 Hz), 7.71 (d, 1H, *J* = 8.2 Hz), 7.40 (t, 1H, *J* = 6.9 Hz), 4.00 (s, 3H), 3.94 (s, 3H). <sup>13</sup>C NMR (DMSO-*d*<sub>6</sub>, 150 MHz, ppm) δ 166.4, 166.3, 159.6, 146.6, 136.4, 136.2, 133.7, 128.4, 127.9, 127.8, 124.7, 123.8, 123.7, 119.2, 117.4, 111.6, 83.3, 52.5, 51.7. HR-MS [M+H]<sup>+</sup> *m/z* Calcd for C<sub>19</sub>H<sub>15</sub>N<sub>2</sub>O<sub>5</sub>: 351.0981. Found: 351.0983.



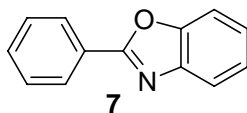
**6-Acetyl-11-oxo-5,11-dihydro-benzo[4,5]imidazo[1,2-*b*]isoquinoline-2-carboxylic acid methyl ester (3q).** Eluent: petroleum ether/ethyl acetate (5:1). Yield 70% (55

mg). Yellow solid, mp 203-205 °C.  $^1\text{H}$  NMR (DMSO- $d_6$ , 600 MHz, ppm)  $\delta$  12.18 (s, br, 1H), 9.07 (m, 1H), 8.71 (d, 1H,  $J = 6.2$  Hz), 8.33 (d, 1H,  $J = 6.8$  Hz), 8.02 (d, 1H,  $J = 5.5$  Hz), 7.68 (d, 2H,  $J = 7.6$  Hz), 7.33 (d, 1H,  $J = 6.8$  Hz), 4.42 (d, 2H,  $J = 5.5$  Hz), 3.90 (s, 3H), 1.82 (m, 2H), 1.50 (m, 2H), 0.99 (t, 3H,  $J = 7.6$  Hz).  $^{13}\text{C}$  NMR (DMSO- $d_6$ , 150 MHz, ppm)  $\delta$  166.5, 166.4, 159.4, 146.7, 136.3, 135.8, 133.5, 128.3, 127.8, 127.7, 124.7, 123.7, 123.5, 119.2, 117.3, 111.7, 83.5, 64.4, 52.5, 31.1, 19.4, 14.0. HR-MS  $[\text{M}+\text{H}]^+$   $m/z$  Calcd for  $\text{C}_{22}\text{H}_{21}\text{N}_2\text{O}_5$ : 393.1451. Found: 393.1452.



**3-Amino-1-oxo-2-phenyl-1,2-dihydro-isoquinoline-4-carboxylic acid ethyl ester**

**(5).** Eluent: petroleum ether/ethyl acetate (5:1). Yield 87% (54 mg). Yellow solid, mp 196-197 °C.  $^1\text{H}$  NMR (DMSO- $d_6$ , 600 MHz, ppm)  $\delta$  8.43 (m, 1H), 8.07 (s, 1H), 7.62-7.57 (m, 4H), 7.39 (s, 4H), 7.19 (m, 1H), 4.35 (q, 2H,  $J = 6.2$  Hz), 1.37 (t, 3H,  $J = 4.1$  Hz).  $^{13}\text{C}$  NMR (DMSO- $d_6$ , 150 MHz, ppm)  $\delta$  168.9, 161.7, 154.4, 137.2, 135.7, 133.7, 130.7, 129.9, 129.7, 128.0, 124.8, 122.8, 119.9, 82.7, 60.4, 14.9. HR-MS  $[\text{M}+\text{H}]^+$   $m/z$  Calcd for  $\text{C}_{18}\text{H}_{17}\text{N}_2\text{O}_3$ : 309.1239. Found: 309.1241.



**2-Phenyl-benzoxazole (7).**<sup>1</sup> Eluent: petroleum ether/ethyl acetate (5:1). Yield 81% (32 mg). Yellow solid.  $^1\text{H}$  NMR (DMSO- $d_6$ , 600 MHz, ppm)  $\delta$  8.22 (d, 2H,  $J = 6.2$  Hz), 7.82 (q, 2H,  $J = 7.6$  Hz), 7.63 (m, 3H), 7.44 (m, 2H).  $^{13}\text{C}$  NMR (DMSO- $d_6$ , 150 MHz, ppm)  $\delta$  162.7, 150.7, 142.0, 132.4, 129.8, 127.8, 126.9, 126.0, 125.4, 120.3, 111.4. HR-MS  $[\text{M}+\text{H}]^+$   $m/z$  Calcd for  $\text{C}_{13}\text{H}_{10}\text{NO}$ : 196.0762. Found: 196.0766.

Reference

- 1 A. J. Blacker, M. M. Farah, M. I. Hall, S. P. Marsden, O. Saidi, *Org. Lett.*, 2009, **11**, 2039.

