

# A new rapid multicomponent domino reaction for the formation of functionalized benzo[*h*]pyrazolo[3,4-*b*]quinolines

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## 1. General information

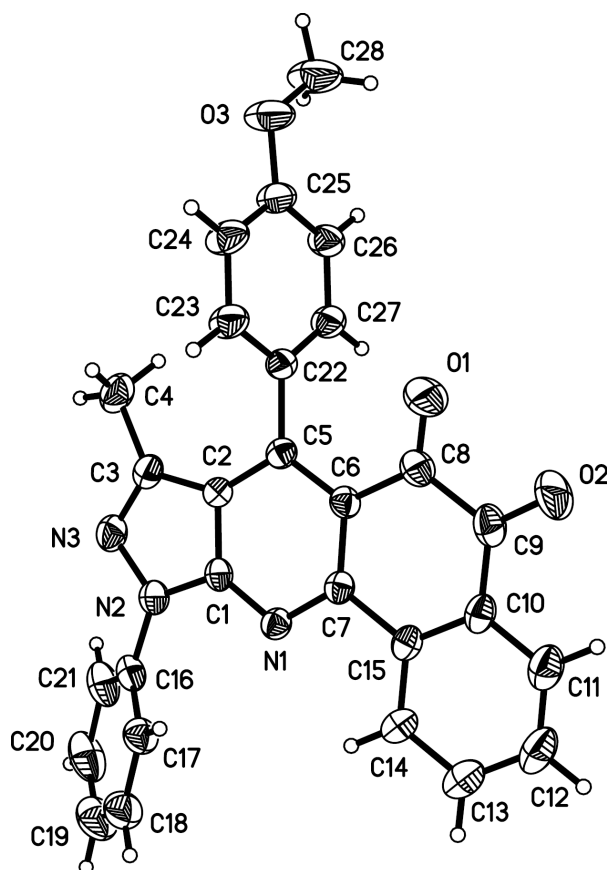
Microwave irradiation was carried out with microwave oven Emrys Creator from Personal Chemistry, Uppsala, Sweden.

## 2. General procedure for the synthesis of compounds **4a**, **5a**, and **6a**

**Preparation of compounds **4a** or **5a****, Microwave Heating: 4-Fluorobenzaldehyde **1a** (1.0 mmol) was introduced in a 10-mL Emrys reaction vial, and 2-hydroxy-1,4-naphthoquinone **2** (1.0 mmol), 3-methyl-1-phenyl-1*H*-pyrazol-5-amine **3a** or (3-methyl-isoxazol-5-amine **3b**) (1.1 mmol) and HOAc (1.5 mL) were then successively added. Subsequently, the reaction vial was capped and then stirred for 20 s. The mixture was irradiated (initial power 100 W and maximum power 200 W) at 120 °C until TLC (petroleum ether/acetone, 4:1 v/v) revealed that conversion of the starting material **1a** was complete (10 min or 12 min). The reaction mixture was then cooled to room temperature and diluted with cold water (40 mL). The solid product was collected by Büchner filtration and was purified by flash column chromatography (silica gel, mixtures of petroleum ether/ethyl acetate, 5:1 v/v) to afford the desired pure products **4a** (or **5a**) as a red solid.

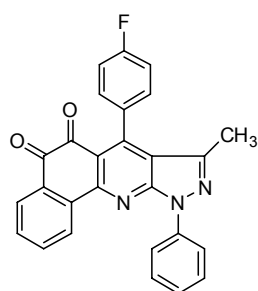
**Preparation of compounds **6a****: In a 10-mL Emrys<sup>TM</sup> reaction vial, quinoxaline-fused benzo[*h*]isoxazolo[5,4-*b*]quinolines **5a** and benzene-1,2-diamine (**7**, 1.1 mmol) and DMF (2.5 mL) were mixed and capped, and then stirred for 20 s. The mixture was irradiated for a given time at 120 °C under microwave irradiation (initial power 100 W and maximum power 250 W). When the reaction was completed (monitored by TLC). The reaction mixture was then cooled to room temperature and diluted with cold water (40 mL). The solid product was collected by

Büchner filtration and was purified by recrystallization from 95% EtOH to afford the desired pure products **6a** as a pale yellow solid.



**X-ray Crystallographic Structure of Compound 4h**

**7-(4-Fluorophenyl)-8-methyl-10-phenyl-5H-benzo[h]pyrazolo[3,4-b]quinoline-5,6(10H)-dione (4a)**



Red solid, mp: >300 °C

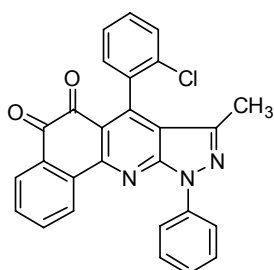
$^1\text{H}$  NMR (400 MHz, DMSO- $d_6$ ) ( $\delta$ , ppm): 8.76 (d,  $J$  = 8.0 Hz, 1H, ArH), 8.30 (d,  $J$  = 7.6 Hz, 2H, ArH), 8.05 (d,  $J$  = 7.2 Hz, 1H, ArH), 7.95 (t,  $J$  = 7.6 Hz, 1H, ArH), 7.72 (d,  $J$  = 7.6 Hz, 1H, ArH), 7.67 (t,  $J$  = 8.0 Hz, 2H, ArH), 7.46-7.36 (m, 5H, ArH), 1.89 (s, 3H, CH<sub>3</sub>).

$^{13}\text{C}$  NMR (100 MHz, DMSO- $d_6$ , 25 °C) ( $\delta$ , ppm): 179.19, 153.28, 145.50, 138.23, 136.57, 135.62, 132.50, 131.94, 131.42, 129.64, 129.57, 129.45, 128.15, 128.13, 127.12, 126.56, 126.48, 120.79, 116.25, 115.12, 114.90, 14.23.

IR (KBr,  $\nu$ , cm<sup>-1</sup>): 3073, 1680, 1559, 1509, 1419, 1382, 1286, 1217, 1159, 1087, 947, 840, 773, 693, 647.

HRMS (ESI)  $m/z$ : calc. for C<sub>27</sub>H<sub>16</sub>FN<sub>3</sub>O<sub>2</sub>Na: 456.1119, found: 456.1119.

**7-(2-Chlorophenyl)-8-methyl-10-phenyl-5H-benzo[h]pyrazolo[3,4-b]quinoline-5,6(10H)-dione (4b)**



Red solid, mp: 262-263 °C

$^1\text{H}$  NMR (400 MHz, DMSO- $d_6$ ) ( $\delta$ , ppm): 8.79 (d,  $J$  = 8.0 Hz, 1H, ArH), 8.31 (d,  $J$  = 7.6 Hz, 2H, ArH), 8.06 (d,  $J$  = 8.0 Hz, 1H, ArH), 7.97 (t,  $J$  = 7.6 Hz, 1H, ArH), 7.75-7.66 (m, 4H, ArH), 7.58 (t,  $J$  = 7.0 Hz, 1H, ArH), 7.52 (t,  $J$  = 7.8 Hz, 1H, ArH), 7.45 (t,  $J$  = 7.6 Hz, 1H, ArH), 7.37 (dd,  $J_1$  = 7.6 Hz,  $J_2$  = 1.2 Hz, 1H, ArH), 1.87 (s, 3H, CH<sub>3</sub>).

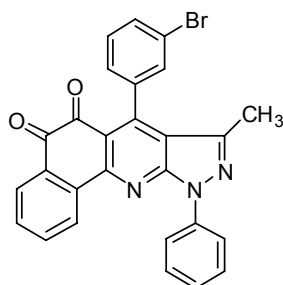
$^{13}\text{C}$  NMR (100 MHz, DMSO- $d_6$ , 25 °C) ( $\delta$ , ppm): 178.72, 153.51, 145.21, 138.15,

136.36, 135.64, 135.36, 132.04, 131.57, 130.87, 130.01, 129.48, 128.97, 128.90, 128.29, 127.23, 126.60, 126.52, 120.87, 120.35, 115.68, 13.09.

IR (KBr,  $\nu$ , cm<sup>-1</sup>): 3066, 1681, 1595, 1557, 1488, 1383, 1288, 1216, 1133, 1030, 948, 745, 689, 639.

HRMS (ESI)  $m/z$ : calc. for C<sub>27</sub>H<sub>16</sub>ClN<sub>3</sub>O<sub>2</sub>Na: 472.0824, found: 472.0801.

**7-(3-Bromophenyl)-8-methyl-10-phenyl-5H-benzo[h]pyrazolo[3,4-b]quinoline-5,6(10H)-dione (4c)**



Red solid, mp: >300 °C

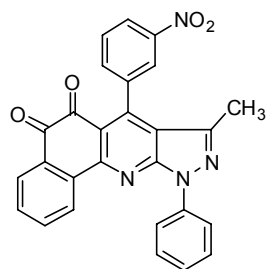
$^1\text{H}$  NMR (400 MHz, DMSO- $d_6$ ) ( $\delta$ , ppm): 8.77 (d,  $J$  = 8.0 Hz, 1H, ArH), 8.30 (d,  $J$  = 8.0 Hz, 2H, ArH), 8.06 (d,  $J$  = 7.6 Hz, 1H, ArH), 7.96 (t,  $J$  = 7.6 Hz, 1H, ArH), 7.75-7.63 (m, 5H, ArH), 7.52 (t,  $J$  = 7.8 Hz, 1H, ArH), 7.44 (t,  $J$  = 7.2 Hz, 2H, ArH), 1.90 (s, 3H, CH<sub>3</sub>).

$^{13}\text{C}$  NMR (100 MHz, DMSO- $d_6$ , 25 °C) ( $\delta$ , ppm): 178.44, 153.23, 149.74, 148.47, 145.34, 138.66, 138.19, 135.62, 131.96, 131.47, 130.87, 130.21, 129.84, 129.47, 129.37, 128.20, 126.58, 126.52, 121.24, 120.80, 120.48, 110.62, 14.20.

IR (KBr,  $\nu$ , cm<sup>-1</sup>): 3075, 1678, 1666, 1555, 1487, 1420, 1381, 1287, 1215, 1129, 1087, 949, 752, 688, 646.

HRMS (ESI)  $m/z$ : calc. for C<sub>27</sub>H<sub>16</sub>BrN<sub>3</sub>O<sub>2</sub>Na: 516.0319, found: 516.0287.

**8-Methyl-7-(3-nitrophenyl)-10-phenyl-5H-benzo[h]pyrazolo[3,4-b]quinoline-5,6(10H)-dione (4d)**



Red solid, mp: >300 °C

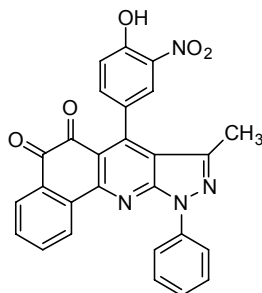
$^1\text{H}$  NMR (400 MHz, DMSO- $d_6$ ) ( $\delta$ , ppm): 8.78 (d,  $J$  = 7.6 Hz, 1H, ArH), 8.43-8.40 (m, 1H, ArH), 8.31-8.29 (m, 3H, ArH), 8.07 (d,  $J$  = 7.2 Hz, 1H, ArH), 7.99-7.85 (m, 3H, ArH), 7.75-7.66 (m, 3H, ArH), 7.44 (t,  $J$  = 7.4 Hz, 1H, ArH), 1.88 (s, 3H, CH<sub>3</sub>).

$^{13}\text{C}$  NMR (100 MHz, DMSO- $d_6$ , 25 °C) ( $\delta$ , ppm): 178.79, 178.35, 153.23, 147.53, 147.39, 145.21, 138.16, 138.09, 136.37, 135.59, 134.29, 132.02, 131.52, 129.81, 129.50, 128.21, 126.53, 122.99, 122.48, 120.81, 120.66, 115.85, 14.44.

IR (KBr,  $\nu$ , cm<sup>-1</sup>): 3074, 1680, 1558, 1527, 1419, 1347, 1287, 1216, 1087, 953, 757, 690, 640.

HRMS (ESI)  $m/z$ : calc. for  $C_{27}H_{16}N_4O_4Na$ : 483.1064, found: 483.1058.

**7-(4-Hydroxy-3-nitrophenyl)-8-methyl-10-phenyl-5H-benzo[h]pyrazolo[3,4-b]quinoline-5,6(10H)-dione (4e)**



Red solid, mp: >300 °C

$^1H$  NMR (400 MHz,  $DMSO-d_6$ ) ( $\delta$ , ppm): 11.36 (s, 1H, OH), 8.76 (d,  $J = 7.6$  Hz, 1H, ArH), 8.29 (d,  $J = 7.6$  Hz, 2H, ArH), 8.06 (d,  $J = 7.6$  Hz, 1H, ArH), 7.96-7.93 (m, 2H, ArH), 7.73-7.65 (m, 3H, ArH), 7.60 (dd,  $J_1 = 8.8$  Hz,  $J_2 = 2.4$  Hz, 1H, ArH), 7.43 (t,  $J = 7.4$  Hz, 1H, ArH), 7.30 (d,  $J = 8.4$  Hz, 1H, ArH), 2.00 (s, 3H,  $CH_3$ ).

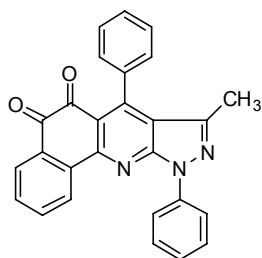
$^{13}C$  NMR (100 MHz,  $DMSO-d_6$ , 25 °C) ( $\delta$ , ppm): 178.99, 178.58, 153.17, 151.99, 149.74, 147.92, 145.31, 138.17, 136.50, 136.42, 135.57, 134.66, 131.80, 131.42, 129.38, 128.13, 126.91, 126.51, 126.40, 124.35, 120.77, 120.61, 118.87, 116.22,

112.71, 14.58.

IR (KBr,  $\nu$ ,  $cm^{-1}$ ): 3241, 3077, 1680, 1629, 1583, 1489, 1419, 1325, 1289, 1215, 1177, 1085, 954, 836, 759, 689, 630.

HRMS (ESI)  $m/z$ : calc. for  $C_{27}H_{16}N_4O_5Na$ : 499.1013, found: 499.0989.

**8-Methyl-7,10-diphenyl-5H-benzo[h]pyrazolo[3,4-b]quinoline-5,6(10H)-dione (4f)**



Red solid, mp: 278-279 °C

$^1H$  NMR (400 MHz,  $DMSO-d_6$ ) ( $\delta$ , ppm): 8.76 (d,  $J = 7.6$  Hz, 1H, ArH), 8.29 (d,  $J = 7.6$  Hz, 2H, ArH), 8.04 (dd,  $J_1 = 7.6$  Hz,  $J_2 = 1.2$  Hz, 1H, ArH), 7.96-7.92 (m, 1H, ArH), 7.72-7.64 (m, 3H, ArH), 7.54-7.52 (m, 3H, ArH), 7.42 (t,  $J = 7.4$  Hz, 1H, ArH), 7.38-7.36 (m, 2H, ArH), 1.82 (s, 3H,  $CH_3$ ).

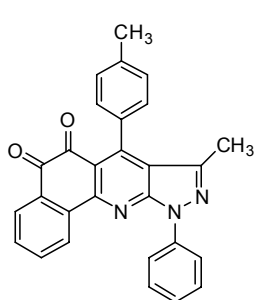
$^{13}C$  NMR (100 MHz,  $DMSO-d_6$ , 25 °C) ( $\delta$ , ppm): 179.23, 178.63, 153.27, 150.69, 145.58, 138.26, 136.62, 136.31, 135.59, 131.95, 131.38, 129.43, 128.14, 127.97,

127.25, 126.55, 126.43, 120.76, 120.52, 116.18, 13.99.

IR (KBr,  $\nu$ ,  $cm^{-1}$ ): 3065, 2924, 1679, 1666, 1555, 1490, 1417, 1382, 1287, 1216, 1164, 1086, 947, 864, 756, 690, 640, 579.

HRMS (ESI)  $m/z$ : calc. for  $C_{27}H_{17}N_3O_2Na$ : 438.1213, found: 438.1203.

**8-Methyl-10-phenyl-7-p-tolyl-5H-benzo[h]pyrazolo[3,4-b]quinoline-5,6(10H)-dione (4g)**



Red solid, mp: >300 °C

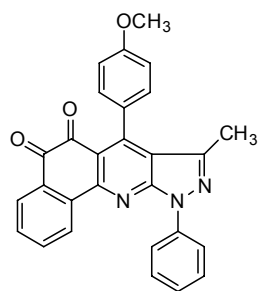
$^1H$  NMR (400 MHz,  $DMSO-d_6$ ) ( $\delta$ , ppm): 8.72 (d,  $J = 8.0$  Hz, 1H, ArH), 8.28 (d,  $J = 8.4$  Hz, 2H, ArH), 8.01 (d,  $J = 7.6$  Hz, 1H, ArH), 7.92 (t,  $J = 7.8$  Hz, 1H, ArH), 7.70-7.62 (m, 3H, ArH), 7.41 (t,  $J = 7.4$  Hz, 1H, ArH), 7.33 (d,  $J = 7.6$  Hz, 2H, ArH), 7.24 (d,  $J = 8.0$  Hz, 2H, ArH), 2.45 (s, 3H,  $CH_3$ ), 1.84 (s, 3H,  $CH_3$ ).

$^{13}C$  NMR (100 MHz,  $DMSO-d_6$ , 25 °C) ( $\delta$ , ppm): 179.30, 178.74, 153.24, 149.67, 145.63, 144.76, 138.26, 137.20, 136.62, 135.56, 133.29, 131.90, 131.34, 129.42, 128.53, 128.09, 127.26, 126.54, 126.38, 120.70, 116.27, 21.00, 14.19.

IR (KBr,  $\nu$ ,  $cm^{-1}$ ): 3028, 2918, 1682, 1642, 1555, 1447, 1382, 1286, 1218, 1154, 1021, 922, 821, 768, 692, 645.

HRMS (ESI)  $m/z$ : calc. for  $C_{28}H_{19}N_3O_2Na$ : 452.1369, found: 452.1354.

**7-(4-Methoxyphenyl)-8-methyl-10-phenyl-5H-benzo[h]pyrazolo[3,4-b]quinoline-5,6(10H)-dione (4h)**



Red solid, mp: 283-284 °C

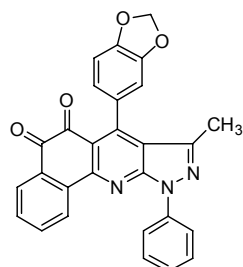
$^1\text{H}$  NMR (400 MHz, DMSO- $d_6$ ) ( $\delta$ , ppm): 8.74 (d,  $J$  = 8.0 Hz, 1H, ArH), 8.29 (d,  $J$  = 8.0 Hz, 2H, ArH), 8.01 (d,  $J$  = 7.6 Hz, 1H, ArH), 7.93 (t,  $J$  = 7.8 Hz, 1H, ArH), 7.71-7.63 (m, 3H, ArH), 7.42 (t,  $J$  = 7.4 Hz, 1H, ArH), 7.31 (d,  $J$  = 8.4 Hz, 2H, ArH), 7.08 (d,  $J$  = 8.8 Hz, 2H, ArH), 3.87 (s, 3H, OCH<sub>3</sub>), 1.90 (s, 3H, CH<sub>3</sub>).

$^{13}\text{C}$  NMR (100 MHz, DMSO- $d_6$ , 25 °C) ( $\delta$ , ppm): 179.43, 178.92, 159.15, 153.26, 149.72, 145.68, 138.29, 136.68, 131.88, 131.33, 129.42, 128.90, 128.10, 126.56, 126.39, 120.89, 120.73, 116.48, 113.42, 111.72, 55.16, 14.38.

IR (KBr,  $\nu$ ,  $\text{cm}^{-1}$ ): 3063, 2935, 2838, 1681, 1642, 1608, 1555, 1442, 1382, 1289, 1248, 1176, 1029, 947, 829, 766, 691, 646.

HRMS (ESI)  $m/z$ : calc. for C<sub>28</sub>H<sub>19</sub>N<sub>3</sub>O<sub>3</sub>Na: 468.1319, found: 468.1327.

#### 7-(Benzo[d][1,3]dioxol-5-yl)-8-methyl-10-phenyl-5H-benzo[h]pyrazolo[3,4-b]quinoline-5,6(10H)-dione (4i)



Red solid, mp: >300 °C

$^1\text{H}$  NMR (400 MHz, DMSO- $d_6$ ) ( $\delta$ , ppm): 8.76 (d,  $J$  = 7.6 Hz, 1H, ArH), 8.30 (d,  $J$  = 7.6 Hz, 2H, ArH), 8.05 (d,  $J$  = 7.2 Hz, 1H, ArH), 7.97-7.93 (m, 1H, ArH), 7.73-7.65 (m, 3H, ArH), 7.43 (t,  $J$  = 7.6 Hz, 1H, ArH), 7.08 (d,  $J$  = 7.6 Hz, 1H, ArH), 6.98 (s, 1H, ArH), 6.85 (dd,  $J_1$  = 8.0 Hz,  $J_2$  = 1.6 Hz, 1H, ArH), 6.16 (d,  $J$  = 10.0 Hz, 2H, CH<sub>2</sub>), 2.01 (s, 3H, CH<sub>3</sub>).

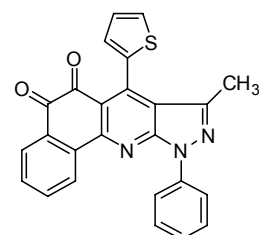
$^{13}\text{C}$  NMR (100 MHz, DMSO- $d_6$ , 25 °C) ( $\delta$ , ppm): 179.34, 178.77, 153.21, 150.39,

147.17, 147.05, 145.64, 138.26, 136.63, 135.61, 131.84, 131.37, 129.57, 129.41, 128.11, 126.55, 126.39, 121.03, 120.91, 120.71, 116.37, 108.39, 108.04, 101.21, 14.34.

IR (KBr,  $\nu$ ,  $\text{cm}^{-1}$ ): 3070, 2928, 1681, 1556, 1491, 1440, 1337, 1239, 1214, 1037, 935, 807, 770, 694.

HRMS (ESI)  $m/z$ : calc. for C<sub>28</sub>H<sub>17</sub>N<sub>3</sub>O<sub>4</sub>Na: 482.1112, found: 482.1075.

#### 8-Methyl-10-phenyl-7-(thiophen-2-yl)-5H-benzo[h]pyrazolo[3,4-b]quinoline-5,6(10H)-dione (4j)



Red solid, mp: 271-273 °C

$^1\text{H}$  NMR (400 MHz, DMSO- $d_6$ ) ( $\delta$ , ppm): 8.71 (d,  $J$  = 7.6 Hz, 1H, ArH), 8.27 (d,  $J$  = 7.6 Hz, 2H, ArH), 8.03 (dd,  $J_1$  = 8.0 Hz,  $J_2$  = 1.2 Hz, 1H, ArH), 7.93-7.89 (m, 1H, ArH), 7.84 (dd,  $J_1$  = 5.2 Hz,  $J_2$  = 1.2 Hz, 1H, ArH), 7.67-7.63 (m, 3H, ArH), 7.42 (t,  $J$  = 7.4 Hz, 1H, Thienyl-H), 7.26-7.24 (m, 1H, Thienyl-H), 7.15 (dd,  $J_1$  = 3.6 Hz,  $J_2$  = 1.2 Hz, 1H, Thienyl-H), 1.99 (s, 3H, CH<sub>3</sub>).

$^{13}\text{C}$  NMR (100 MHz, DMSO- $d_6$ , 25 °C) ( $\delta$ , ppm): 179.04, 178.28, 153.30, 145.50, 138.19, 136.45, 135.53, 135.30, 131.93, 131.40, 129.41, 129.25, 128.11, 127.49, 127.35, 126.97, 126.55, 126.50, 120.86, 120.73, 119.54, 117.48, 13.38.

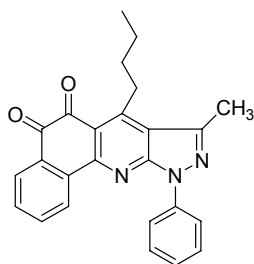
IR (KBr,  $\nu$ ,  $\text{cm}^{-1}$ ): 3046, 2919, 1678, 1635, 1569, 1491, 1378, 1283, 1158, 1084, 925, 816, 756, 690, 640.

HRMS (ESI)  $m/z$ : calc. for C<sub>25</sub>H<sub>15</sub>N<sub>3</sub>O<sub>2</sub>SNa: 444.0778, found: 444.0763.

#### 7-Butyl-8-methyl-10-phenyl-5H-benzo[h]pyrazolo[3,4-b]quinoline-5,6(10H)-dione (4k)

Red solid, mp: 192-194 °C

$^1\text{H}$  NMR (400 MHz, DMSO- $d_6$ ) ( $\delta$ , ppm): 8.60 (d,  $J$  = 8.0 Hz, 1H, ArH), 8.23 (d,  $J$  = 7.6 Hz, 2H, ArH), 7.99 (d,  $J$  = 7.6 Hz, 1H, ArH), 7.86 (t,  $J$  = 7.6 Hz, 1H, ArH), 7.67-7.60 (m, 3H, ArH), 7.40 (t,  $J$  = 7.4 Hz, 1H, ArH),



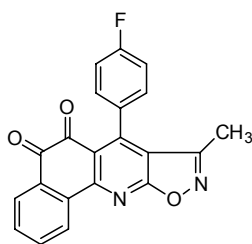
2.72 (s, 3H, CH<sub>3</sub>), 1.62-1.55 (m, 4H, 2CH<sub>2</sub>), 1.00 (t, *J* = 7.0 Hz, 3H, CH<sub>3</sub>).

<sup>13</sup>C NMR (100 MHz, DMSO-*d*<sub>6</sub>, 25 °C) ( $\delta$ , ppm): 179.82, 178.99, 155.95, 153.69, 149.76, 145.23, 138.23, 136.71, 135.49, 131.52, 131.21, 129.32, 127.97, 126.50, 126.31, 120.68, 116.19, 112.71, 31.96, 29.83, 22.83, 15.52, 13.61.

IR (KBr,  $\nu$ , cm<sup>-1</sup>): 3080, 2961, 2928, 2854, 1696, 1672, 1660, 1564, 1490, 1417, 1378, 1289, 1216, 1165, 1089, 965, 762, 693, 636.

HRMS (ESI) *m/z*: calc. for C<sub>25</sub>H<sub>21</sub>N<sub>3</sub>O<sub>2</sub>Na: 418.1526, found: 418.1497.

#### 7-(4-Fluorophenyl)-8-methylbenzo[h]isoxazolo[5,4-b]quinoline-5,6-dione (5a)



Red solid, mp: 262-264 °C

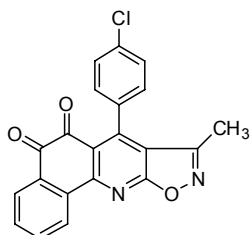
<sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>) ( $\delta$ , ppm): 8.72 (d, *J* = 8.0 Hz, 1H, ArH), 8.06 (d, *J* = 7.6 Hz, 1H, ArH), 7.93 (t, *J* = 7.2 Hz, 1H, ArH), 7.74 (t, *J* = 7.6 Hz, 1H, ArH), 7.48-7.44 (m, 2H, ArH), 7.18 (t, *J* = 9.2 Hz, 2H, ArH), 1.89 (s, 3H, CH<sub>3</sub>).

IR (KBr,  $\nu$ , cm<sup>-1</sup>): 3069, 1692, 1672, 1573, 1510, 1442, 1341, 1219, 1162, 1076, 936, 842, 774, 611.

<sup>13</sup>C NMR (100 MHz, DMSO-*d*<sub>6</sub>, 25 °C) ( $\delta$ , ppm): 178.44, 178.11, 169.04, 163.45, 161.01, 157.21, 155.32, 151.12, 135.56, 132.18, 131.99, 129.78, 129.70, 128.27, 126.83, 123.32, 115.17, 114.96, 113.33, 11.98.

HRMS (ESI) *m/z*: calc. for C<sub>21</sub>H<sub>11</sub>FN<sub>2</sub>O<sub>3</sub>Na: 381.0646, found: 381.0640.

#### 7-(4-Chlorophenyl)-8-methylbenzo[h]isoxazolo[5,4-b]quinoline-5,6-dione (5b)



Red solid, mp: 260-262 °C

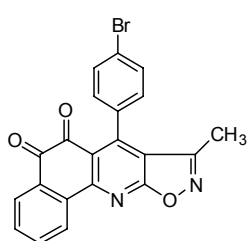
<sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>) ( $\delta$ , ppm): 8.73 (d, *J* = 8.0 Hz, 1H, ArH), 8.07 (d, *J* = 7.2 Hz, 1H, ArH), 7.93 (t, *J* = 8.0 Hz, 1H, ArH), 7.74 (t, *J* = 7.6 Hz, 1H, ArH), 7.61 (d, *J* = 8.4 Hz, 2H, ArH), 7.44 (d, *J* = 8.4 Hz, 2H, ArH), 1.90 (s, 3H, CH<sub>3</sub>).

IR (KBr,  $\nu$ , cm<sup>-1</sup>): 3072, 1684, 1671, 1571, 1492, 1346, 1274, 1089, 1020, 937, 829, 771, 631, 595.

<sup>13</sup>C NMR (100 MHz, DMSO-*d*<sub>6</sub>, 25 °C) ( $\delta$ , ppm): 178.29, 177.97, 169.02, 157.15, 155.31, 150.67, 135.54, 133.94, 133.28, 132.19, 132.01, 129.38, 128.28, 128.15, 126.80, 123.16, 113.09, 12.02.

HRMS (ESI) *m/z*: calc. for C<sub>21</sub>H<sub>11</sub>ClN<sub>2</sub>O<sub>3</sub>Na: 397.0350, found: 397.0323.

#### 7-(4-Bromophenyl)-8-methylbenzo[h]isoxazolo[5,4-b]quinoline-5,6-dione (5c)



Red solid, mp: 264-265 °C

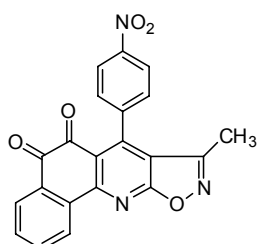
<sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>) ( $\delta$ , ppm): 8.73 (d, *J* = 8.0 Hz, 1H, ArH), 8.07 (d, *J* = 8.0 Hz, 1H, ArH), 7.93 (t, *J* = 7.6 Hz, 1H, ArH), 7.76-7.73 (m, 3H, ArH), 7.37 (d, *J* = 8.4 Hz, 2H, ArH), 1.90 (s, 3H, CH<sub>3</sub>).

IR (KBr,  $\nu$ , cm<sup>-1</sup>): 3070, 2925, 1706, 1682, 1673, 1569, 1489, 1392, 1294, 1217, 1012, 936, 875, 770, 629.

<sup>13</sup>C NMR (100 MHz, DMSO-*d*<sub>6</sub>, 25 °C) ( $\delta$ , ppm): 178.29, 177.96, 169.03, 157.16, 155.34, 150.65, 135.53, 134.36, 132.02, 131.04, 129.62, 128.28, 126.81, 123.13, 121.87, 113.02, 12.05.

HRMS (ESI) *m/z*: calc. for C<sub>21</sub>H<sub>11</sub>BrN<sub>2</sub>O<sub>3</sub>Na: 440.9846, found: 440.9832.

#### 8-Methyl-7-(4-nitrophenyl)benzo[h]isoxazolo[5,4-b]quinoline-5,6-dione (5d)



Red solid, mp: 268-269 °C

<sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>) ( $\delta$ , ppm): 8.74 (d, *J* = 8.0 Hz, 1H, ArH), 8.41 (d, *J* = 8.8 Hz, 2H, ArH), 8.08 (d, *J* = 7.6 Hz, 1H, ArH), 7.94 (t, *J* = 8.0 Hz, 1H, ArH), 7.76 (t, *J* = 7.2 Hz, 1H, ArH), 7.71 (d, *J* = 8.8 Hz, 2H, ArH), 1.87 (s, 3H, CH<sub>3</sub>).

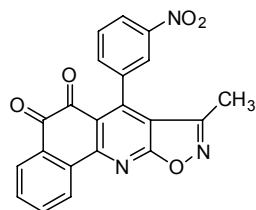
<sup>13</sup>C NMR (100 MHz, DMSO-*d*<sub>6</sub>, 25 °C) ( $\delta$ , ppm): 178.05, 177.72, 169.08, 157.01, 155.37, 149.39, 147.50, 142.30, 135.55, 135.41, 132.31, 132.11, 129.01, 128.34,

126.80, 123.28, 122.98, 112.77, 12.00.

IR (KBr,  $\nu$ ,  $\text{cm}^{-1}$ ): 1683, 1569, 1522, 1442, 1353, 1297, 1220, 1206, 1056, 976, 844, 777, 630, 591.

HRMS (ESI)  $m/z$ : calc. for  $\text{C}_{21}\text{H}_{11}\text{N}_3\text{O}_5\text{Na}$ : 408.0591, found: 408.0564.

### 8-Methyl-7-(3-nitrophenyl)benzo[*h*]isoxazolo[5,4-*b*]quinoline-5,6-dione (5e)



Red solid, mp: 236-237 °C

$^1\text{H}$  NMR (400 MHz,  $\text{DMSO-}d_6$ ) ( $\delta$ , ppm): 8.74 (d,  $J = 8.0$  Hz, 1H, ArH), 8.42-8.40 (m, 1H, ArH), 8.34-8.33 (m, 1H, ArH), 8.09 (d,  $J = 8.8$  Hz, 1H, ArH), 7.95-7.92 (m, 2H, ArH), 7.86 (t,  $J = 8.0$  Hz, 1H, ArH), 7.75 (t,  $J = 8.0$  Hz, 1H, ArH), 1.88 (s, 3H,  $\text{CH}_3$ ).

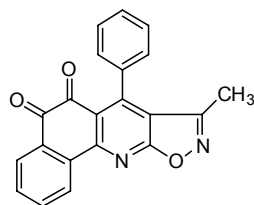
$^{13}\text{C}$  NMR (100 MHz,  $\text{DMSO-}d_6$ , 25 °C) ( $\delta$ , ppm): 178.09, 177.73, 169.04, 157.09, 155.26, 148.87, 147.50, 136.77, 135.54, 135.40, 134.21, 132.24, 132.08, 129.80,

128.32, 126.78, 123.32, 122.67, 113.16, 12.14.

IR (KBr,  $\nu$ ,  $\text{cm}^{-1}$ ): 3178, 3082, 1685, 1672, 1529, 1433, 1349, 1281, 1164, 974, 876, 731, 630.

HRMS (ESI)  $m/z$ : calc. for  $\text{C}_{21}\text{H}_{11}\text{N}_3\text{O}_5\text{Na}$ : 408.0591, found: 408.0569.

### 8-Methyl-7-phenylbenzo[*h*]isoxazolo[5,4-*b*]quinoline-5,6-dione (5f)



Red solid, mp: 270-271 °C

$^1\text{H}$  NMR (400 MHz,  $\text{DMSO-}d_6$ ) ( $\delta$ , ppm): 8.72 (d,  $J = 8.0$  Hz, 1H, ArH), 8.06 (d,  $J = 7.6$  Hz, 1H, ArH), 7.92 (t,  $J = 7.2$  Hz, 1H, ArH), 7.73 (t,  $J = 7.2$  Hz, 1H, ArH), 7.54-7.52 (m, 3H, ArH), 7.40-7.39 (m, 2H, ArH), 1.83 (s, 3H,  $\text{CH}_3$ ).

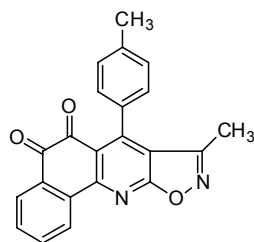
$^{13}\text{C}$  NMR (100 MHz,  $\text{DMSO-}d_6$ , 25 °C) ( $\delta$ , ppm): 178.49, 178.08, 169.05, 157.24, 155.34, 152.16, 135.66, 135.53, 135.07, 132.21, 131.95, 128.38, 128.26, 127.99,

127.30, 126.83, 123.11, 113.20, 11.74.

IR (KBr,  $\nu$ ,  $\text{cm}^{-1}$ ): 3058, 1685, 1672, 1570, 1445, 1345, 1274, 1219, 1057, 979, 879, 770, 697, 629.

HRMS (ESI)  $m/z$ : calc. for  $\text{C}_{21}\text{H}_{12}\text{N}_2\text{O}_3\text{Na}$ : 393.0741, found: 363.0750.

### 8-Methyl-7-*p*-tolylbenzo[*h*]isoxazolo[5,4-*b*]quinoline-5,6-dione (5g)



Red solid, mp: 250-251 °C

$^1\text{H}$  NMR (400 MHz,  $\text{DMSO-}d_6$ ) ( $\delta$ , ppm): 8.73 (d,  $J = 8.0$  Hz, 1H, ArH), 8.06 (d,  $J = 8.0$  Hz, 1H, ArH), 7.93 (t,  $J = 8.0$  Hz, 1H, ArH), 7.74 (t,  $J = 7.6$  Hz, 1H, ArH), 7.33 (d,  $J = 8.0$  Hz, 2H, ArH), 7.28 (d,  $J = 8.0$  Hz, 2H, ArH), 2.44 (s, 3H,  $\text{CH}_3$ ), 1.87 (s, 3H,  $\text{CH}_3$ ).

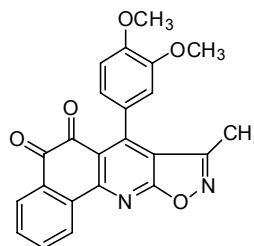
$^{13}\text{C}$  NMR (100 MHz,  $\text{DMSO-}d_6$ , 25 °C) ( $\delta$ , ppm): 178.64, 178.27, 169.07, 157.28,

155.34, 152.48, 137.76, 135.72, 135.54, 132.17, 132.07, 131.92, 128.55, 128.23, 127.35, 126.84, 123.28, 30.65, 20.98, 11.93.

IR (KBr,  $\nu$ ,  $\text{cm}^{-1}$ ): 1686, 1672, 1575, 1457, 1390, 1218, 1076, 825, 772, 611.

HRMS (ESI)  $m/z$ : calc. for  $\text{C}_{22}\text{H}_{14}\text{N}_2\text{O}_3\text{Na}$ : 377.0897, found: 377.0902.

### 7-(3,4-Dimethoxyphenyl)-8-methylbenzo[*h*]isoxazolo[5,4-*b*]quinoline-5,6-dione (5h)



Red solid, mp: 246-248 °C

$^1\text{H}$  NMR (400 MHz,  $\text{DMSO-}d_6$ ) ( $\delta$ , ppm): 8.72 (d,  $J = 8.0$  Hz, 1H, ArH), 8.06 (d,  $J = 7.6$  Hz, 1H, ArH), 7.92 (t,  $J = 7.6$  Hz, 1H, ArH), 7.73 (t,  $J = 7.2$  Hz, 1H, ArH), 7.09 (d,  $J = 8.0$  Hz, 1H, ArH), 7.04 (s, 1H, ArH), 6.94 (dd,  $J_1 = 8.0$  Hz,  $J_2 = 1.6$  Hz, 1H, ArH), 3.86 (s, 3H,  $\text{OCH}_3$ ), 3.73 (s, 3H,  $\text{OCH}_3$ ), 1.96 (s, 3H,  $\text{CH}_3$ ).

$^{13}\text{C}$  NMR (100 MHz,  $\text{DMSO-}d_6$ , 25 °C) ( $\delta$ , ppm): 178.68, 178.28, 169.07, 157.44, 155.25, 152.34, 149.07, 148.41, 135.72, 135.55, 132.09, 131.91, 128.22, 127.12,

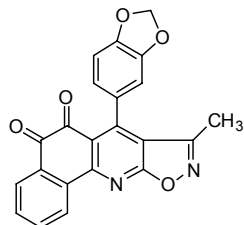


126.83, 123.46, 120.07, 113.37, 111.81, 111.31, 55.67, 55.58, 12.08.

IR (KBr,  $\nu$ ,  $\text{cm}^{-1}$ ): 3000, 2934, 2837, 1685, 1570, 1516, 1463, 1344, 1260, 1042, 874, 763, 636.

HRMS (ESI)  $m/z$ : calc. for  $\text{C}_{23}\text{H}_{16}\text{N}_2\text{O}_5\text{Na}$ : 423.0952, found: 423.0952.

#### 7-(Benzo[d][1,3]dioxol-5-yl)-8-methylbenzo[h]isoxazolo[5,4-b]quinoline-5,6-dione (5i)



Red solid, mp: 284-285 °C

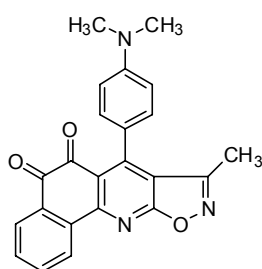
$^1\text{H}$  NMR (400 MHz,  $\text{DMSO-}d_6$ ) ( $\delta$ , ppm): 8.72 (d,  $J$  = 8.0 Hz, 1H, ArH), 8.06 (d,  $J$  = 8.0 Hz, 1H, ArH), 7.92 (t,  $J$  = 7.6 Hz, 1H, ArH), 7.74 (t,  $J$  = 6.8 Hz, 1H, ArH), 7.07 (d,  $J$  = 8.0 Hz, 1H, ArH), 6.99 (s, 1H, ArH), 6.89 (dd,  $J_1$  = 8.0 Hz,  $J_2$  = 1.6 Hz, 1H, ArH), 6.15 (d,  $J$  = 10.4 Hz, 2H,  $\text{CH}_2$ ), 2.00 (s, 3H,  $\text{CH}_3$ ).

$^{13}\text{C}$  NMR (100 MHz,  $\text{DMSO-}d_6$ , 25 °C) ( $\delta$ , ppm): 178.62, 178.26, 169.09, 157.33, 155.27, 151.89, 147.54, 147.07, 135.68, 135.57, 132.11, 131.94, 128.33, 128.24, 128.83, 123.51, 121.29, 113.36, 108.44, 108.03, 101.33, 12.11.

IR (KBr,  $\nu$ ,  $\text{cm}^{-1}$ ): 3073, 2894, 1684, 1673, 1591, 1571, 1436, 1345, 1237, 1117, 1037, 930, 874, 770, 632.

HRMS (ESI)  $m/z$ : calc. for  $\text{C}_{22}\text{H}_{12}\text{N}_2\text{O}_5\text{Na}$ : 407.0639, found: 407.0619.

#### 7-(4-(Dimethylamino)phenyl)-8-methylbenzo[h]isoxazolo[5,4-b]quinoline-5,6-dione (5j)



Red solid, mp: 270-271 °C

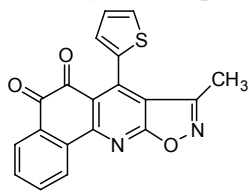
$^1\text{H}$  NMR (400 MHz,  $\text{DMSO-}d_6$ ) ( $\delta$ , ppm): 8.70 (d,  $J$  = 8.0 Hz, 1H, ArH), 8.04 (d,  $J$  = 7.6 Hz, 1H, ArH), 7.91 (t,  $J$  = 7.6 Hz, 1H, ArH), 7.72 (t,  $J$  = 7.6 Hz, 1H, ArH), 7.25 (d,  $J$  = 8.4 Hz, 2H, ArH), 6.82 (d,  $J$  = 8.8 Hz, 2H, ArH), 3.01 (d,  $J$  = 4.0 Hz, 6H, 2 $\text{CH}_3$ ), 2.00 (s, 3H,  $\text{CH}_3$ ).

$^{13}\text{C}$  NMR (100 MHz,  $\text{DMSO-}d_6$ , 25 °C) ( $\delta$ , ppm): 179.13, 178.89, 169.24, 157.42, 155.32, 153.53, 150.49, 135.89, 135.55, 132.00, 131.82, 129.18, 128.11, 126.86, 123.40, 121.53, 113.28, 111.13, 30.65, 12.51.

IR (KBr,  $\nu$ ,  $\text{cm}^{-1}$ ): 2890, 1687, 1572, 1529, 1435, 1354, 1271, 1199, 975, 811, 772, 633.

HRMS (ESI)  $m/z$ : calc. for  $\text{C}_{23}\text{H}_{18}\text{N}_3\text{O}_3$ : 384.1343, found: 384.1340.

#### 8-Methyl-7-(thiophen-2-yl)benzo[h]isoxazolo[5,4-b]quinoline-5,6-dione (5k)



Red solid, mp: 207-208 °C

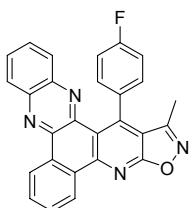
$^1\text{H}$  NMR (400 MHz,  $\text{DMSO-}d_6$ ) ( $\delta$ , ppm): 8.72 (d,  $J$  = 8.0 Hz, 1H, ArH), 8.07 (d,  $J$  = 7.6 Hz, 1H, ArH), 7.93 (t,  $J$  = 8.0 Hz, 1H, ArH), 7.85 (dd,  $J_1$  = 4.8 Hz,  $J_2$  = 1.2 Hz, 1H, Thienyl-H), 7.74 (t,  $J$  = 7.6 Hz, 1H, ArH), 7.25-7.23 (m, 1H, Thienyl-H), 7.21-7.20 (m, 1H, Thienyl-H), 2.00 (s, 3H,  $\text{CH}_3$ ).

$^{13}\text{C}$  NMR (100 MHz,  $\text{DMSO-}d_6$ , 25 °C) ( $\delta$ , ppm): 178.31, 177.66, 168.83, 157.25, 155.40, 145.12, 135.48, 133.93, 132.20, 132.00, 128.24, 128.18, 127.99, 126.98, 126.84, 124.32, 122.52, 114.16, 11.25

IR (KBr,  $\nu$ ,  $\text{cm}^{-1}$ ): 3074, 2927, 1686, 1573, 1432, 1389, 1295, 1205, 1076, 969, 772, 724.

HRMS (ESI)  $m/z$ : calc. for  $\text{C}_{19}\text{H}_{10}\text{N}_2\text{NaO}_3\text{S}$ : 369.0304, found: 369.0319.

#### Hexacyclic quinoxaline-fused benzo[h]pyrazolo[3,4-b]quinolines (6a)



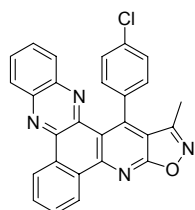
Pale yellow solid, mp: > 300 °C

$^1\text{H}$  NMR (400MHz,  $\text{DCCl}_3$ , 25 °C):  $\delta$  = 9.30-9.25 (m, 2H, ArH), 8.22 (d,  $J$  = 7.6 Hz, 1H, ArH), 7.85-7.77 (m, 3H, ArH), 7.71-7.67 (m, 1H, ArH), 7.39-7.28 (m, 5H, ArH), 2.04 (s, 3H,  $\text{CH}_3$ );

IR (KBr,  $\nu$ ,  $\text{cm}^{-1}$ ): 1590, 1569, 1509, 1419, 1383, 1322, 1221, 1126, 998, 810.

HRMS (ESI):  $m/z$  calcd for  $C_{27}H_{16}FN_4O$ : 431.1303, found: 431.1301.

#### Hexacyclic quinoxaline-fused benzo[*h*]pyrazolo[3,4-*b*]quinolines (6b)



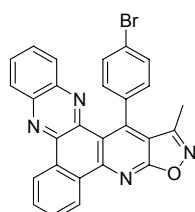
Pale yellow solid, mp: > 300 °C

$^1H$  NMR (400MHz,  $DCCl_3$ , 25 °C):  $\delta$  = 9.26 (d,  $J$  = 7.6 Hz, 2H, ArH), 8.22 (d,  $J$  = 8.4 Hz, 1H, ArH), 7.84-7.76 (m, 3H, ArH), 7.72-7.68 (m, 1H, ArH), 7.62-7.59 (m, 2H, ArH), 7.37-7.34 (m, 2H, ArH), 7.28-7.26 (m, 1H, ArH), 2.05 (s, 3H,  $CH_3$ );

IR (KBr,  $\nu$ ,  $cm^{-1}$ ): 1599, 1580, 1506, 1396, 1296, 1240, 1123, 1013, 767.

HRMS (ESI):  $m/z$  calcd for  $C_{27}H_{16}ClN_4O$ : 447.1007, found: 447.1013.

#### Hexacyclic quinoxaline-fused benzo[*h*]pyrazolo[3,4-*b*]quinolines (6c)



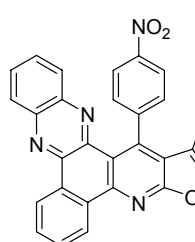
Pale yellow solid, mp: > 300 °C

$^1H$  NMR (400MHz,  $DCCl_3$ , 25 °C):  $\delta$  = 9.24 (d,  $J$  = 8.4 Hz, 2H, ArH), 8.21 (d,  $J$  = 7.6 Hz, 1H, ArH), 7.83-7.69 (m, 6H, ArH), 7.32-7.25 (m, 3H, ArH), 2.05 (s, 3H,  $CH_3$ ).

IR (KBr,  $\nu$ ,  $cm^{-1}$ ): 1602, 1579, 1485, 1394, 1350, 1312, 1223, 1125, 1014, 896.

HRMS (ESI):  $m/z$  calcd for  $C_{27}H_{16}BrN_4O$ : 491.0502, found: 491.0505.

#### Hexacyclic quinoxaline-fused benzo[*h*]pyrazolo[3,4-*b*]quinolines (6d)



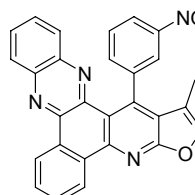
Pale yellow solid, mp: > 300 °C

$^1H$  NMR (400MHz,  $DCCl_3$ , 25 °C):  $\delta$  = 9.33-9.29 (m, 2H, ArH), 8.52 (d,  $J$  = 8.8 Hz, 2H, ArH), 8.24 (d,  $J$  = 8.4 Hz, 1H, ArH), 7.90-7.77 (m, 3H, ArH), 7.69-7.63 (m, 3H, ArH), 7.09 (d,  $J$  = 8.4 Hz, 1H, ArH), 2.02 (s, 3H,  $CH_3$ );

IR (KBr,  $\nu$ ,  $cm^{-1}$ ): 1673, 1596, 1579, 1519, 1483, 1392, 1341, 1222, 1076, 843.

HRMS (ESI):  $m/z$  calcd for  $C_{27}H_{16}N_5O_3$ : 458.1248, found: 458.1247.

#### Hexacyclic quinoxaline-fused benzo[*h*]pyrazolo[3,4-*b*]quinolines (6e)



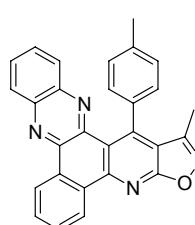
Pale yellow solid, mp: > 300 °C

$^1H$  NMR (400MHz,  $DCCl_3$ , 25 °C):  $\delta$  = 9.29-9.27 (m, 2H, ArH), 8.56 (d,  $J$  = 8.0 Hz, 1H, ArH), 8.37 (s, 1H, ArH), 8.23 (d,  $J$  = 8.4 Hz, 1H, ArH), 7.86-7.77 (m, 5H, ArH), 7.65 (t,  $J$  = 7.6 Hz, 1H, ArH), 7.08 (d,  $J$  = 8.4 Hz, 1H, ArH), 2.02 (s, 3H,  $CH_3$ );

IR (KBr,  $\nu$ ,  $cm^{-1}$ ): 1601, 1583, 1531, 1483, 1432, 1349, 1313, 1285, 1223, 1076, 771.

HRMS (ESI):  $m/z$  calcd for  $C_{27}H_{16}N_5O_3$ : 458.1248  $[M+H]^+$ , found: 458.1242.

#### Hexacyclic quinoxaline-fused benzo[*h*]pyrazolo[3,4-*b*]quinolines (6f)



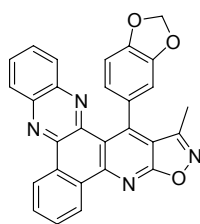
Pale yellow solid, mp: > 300 °C

$^1H$  NMR (400MHz,  $DCCl_3$ , 25 °C):  $\delta$  = 9.39-9.32 (m, 2H, ArH), 8.24 (d,  $J$  = 8.4 Hz, 1H, ArH), 7.90-7.86 (m, 2H, ArH), 7.78 (t,  $J$  = 7.6 Hz, 1H, ArH), 7.68-7.65 (m, 1H, ArH), 7.52-7.38 (m, 3H, ArH), 7.25-7.23 (m, 2H, ArH), 2.62 (s, 3H,  $CH_3$ ), 2.05 (s, 3H,  $CH_3$ );

IR (KBr,  $\nu$ ,  $cm^{-1}$ ): 1601, 1581, 1515, 1483, 1393, 1359, 1348, 1313, 1222, 1074, 824, 768.

HRMS (ESI):  $m/z$  calcd for  $C_{28}H_{19}N_4O$ : 427.1553, found: 427.1550.

#### Hexacyclic quinoxaline-fused benzo[*h*]pyrazolo[3,4-*b*]quinolines (6g)



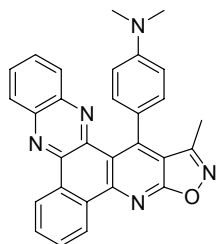
Pale yellow solid, mp: > 300 °C

$^1\text{H NMR}$  (400MHz,  $\text{DCCl}_3$ , 25 °C):  $\delta$  = 9.31-9.26 (m, 2H, ArH), 8.23 (d,  $J$  = 8.0 Hz, 1H, ArH), 7.85-7.77 (m, 3H, ArH), 7.72-7.69 (m, 1H, ArH), 7.41 (d,  $J$  = 7.6 Hz, 1H, ArH), 7.05 (d,  $J$  = 7.6 Hz, 1H, ArH), 6.88-6.81 (m, 2H, ArH), 6.17 (d,  $J$  = 13.6 Hz, 1H,  $\text{CH}_2$ ), 2.15 (s, 3H,  $\text{CH}_3$ );

IR (KBr,  $\nu$ ,  $\text{cm}^{-1}$ ): 1603, 1581, 1498, 1484, 1439, 1360, 1350, 1236, 1039, 922, 762.

HRMS (ESI):  $m/z$  calcd for  $\text{C}_{28}\text{H}_{17}\text{N}_4\text{O}_3$ : 457.1295  $[\text{M}+\text{H}]^+$ , found: 457.1280.

#### Hexacyclic quinoxaline-fused benzo[*h*]pyrazolo[3,4-*b*]quinolines (6h)



Pale yellow solid, mp: > 300 °C

$^1\text{H NMR}$  (400MHz,  $\text{DCCl}_3$ , 25 °C):  $\delta$  = 9.37-9.29 (m, 2H, ArH), 8.22 (d,  $J$  = 8.4 Hz, 1H, ArH), 7.89-7.85 (m, 2H, ArH), 7.79-7.75 (m, 1H, ArH), 7.68-7.64 (m, 1H, ArH), 7.37 (d,  $J$  = 8.4 Hz, 1H, ArH), 7.23 (d,  $J$  = 8.4 Hz, 2H, ArH), 6.96-6.95 (m, 2H, ArH), 3.15 (s, 6H,  $\text{CH}_3$ ), 2.11 (s, 3H,  $\text{CH}_3$ );

IR (KBr,  $\nu$ ,  $\text{cm}^{-1}$ ): 1612, 1602, 1578, 1523, 1481, 1439, 1389, 1359, 1348, 1225, 757.

HRMS (ESI):  $m/z$  calcd for  $\text{C}_{29}\text{H}_{22}\text{N}_5\text{O}$ : 456.1819, found: 456.1820.