Electro-oxidative C–H Azolation of Quinoxalin-2(1H)-ones

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1. General Information

Unless otherwise noted, Reagents were purchased from commercial sources and were used as received. $^1$H and $^{13}$C Nuclear Magnetic Resonance (NMR) spectra were recorded on Bruker Avance 400 Ultrashield NMR spectrometers. Chemical shifts ($\delta$) were given in parts per million (ppm) and were measured downfield from internal tetramethylsilane. High-resolution mass spectrometry (HRMS) data were obtained on an FTICR-MS instrument (Ionspec 7.0 T). The melting points were determined on an X-4 microscope melting point apparatus and are uncorrected. Conversion was monitored by thin layer chromatography (TLC). Flash column chromatography was performed over silica gel (100-200 mesh).

2. Preparation of quinoxalin-2(1H)-one

Quinoxalin-2(1H)-one was prepared from 1,2-phenylenediamines following the procedure of Cui and co-workers $^{[1]}$ on 5 mmol scale. To a solution of 1,2-phenylenediamines (5 mmol, 1.0 equiv.) in ethanol (40 mL) was added ethyl glyoxalate (6 mmol, 1.2 equiv.). The resultant reaction mixture was stirred at reflux until the raw material disappears. Then, the mixture was filtered and washed by ethanol. The solid was dried in vacuo. For alkylation, the corresponding halogenoalkane (1.6 equiv.) was added to a suspension of quinoxalinone (1.0 equiv.) and potassium carbonate (1.2 equiv.) in DMF (16 mL). The mixture was stirred at room temperature overnight. After complete reaction, brine was added, and then extracted three times with EtOAc. The combined organic layers were washed with a saturated solution of NH$_4$Cl then brine, dried over anhydrous Na$_2$SO$_4$, filtered and evaporated in vacuo. The residue was purified by column chromatography on silica gel to afford the desired product.

3. General procedure for the electrolysis

An oven-dried 10 mL undivided cell was equipped with two graphite sheet electrodes (10 mm × 10 mm × 3 mm). The corresponding quinoxalin-2(1H)-one (80.0 mg, 0.5 mmol, 1.0 equiv.), the pyrazole (68.1 mg, 1.0 mmol, 2.0 equiv.) and $^+$Bu$_4$NBF$_4$ (329.3 mg, 1.0 mmol, 2.0 equiv.) was added into the undivided cell. And then MeCN (5 mL) was added. The reaction mixture was stirred and electrolyzed at a constant current of 10.0 mA at room temperature for 8 h. The solvent was concentrated in vacuo. The pure product was obtained by flash column chromatography on silica gel (petroleum ether/ethyl acetate).

4. Use of 3-V battery as power source
An oven-dried 10 mL undivided cell was charged with quinoxalin-2(1H)-one (80.0 mg, 0.5 mmol, 1.0 equiv.), pyrazole (68.1 mg, 1.0 mmol, 2.0 equiv.), $^4$Bu$_4$NBF$_4$ (329.3 mg, 1.0 mmol, 2.0 equiv.) and MeCN (5 mL). Two pencil leads were first removed from the pencil and inserted into the mixture (30 mm × Φ A = 2 mm). Two 1.5 v NanFu batteries were connected by copper wires in series and were used as the power source. The reaction mixture was electrolyzed at room temperature for 24 h. After the reaction, the resulting mixture concentrated in vacuo and the crude material was purified by column chromatography (petroleum ether/ethyl acetate = 10:1) to furnish the desired product in 71% yield.

5. **Gram-scale Reaction**
A 200 mL bottle with a stir bar was charged with quinoxalin-2(1H)-one (0.80 g, 5.0 mmol, 1.0 equiv.), pyrazole (0.68 g, 10.0 mmol, 2.0 equiv.) and \( \text{Bu}_4\text{NBF}_4 \) (3.30 g, 1.0 mmol, 2.0 equiv.) and MeCN (100 mL). Two graphite sheet electrodes (300 mm × 500 mm × 3 mm) were inserted into the mixture. The reaction mixture was then pumped with a speed of 10 mL/min in the loop by peristaltic pump (Purchased from Taobao.com). Then, the reaction mixture was electrolyzed under a constant current of 60 mA at room temperature for 12 h. After the reaction, the electrodes were removed and rinsed with EtOAc. The solvent was concentrated in vacuo and the crude material was purified by column chromatography (petroleum ether/ethyl acetate = 1:1) to furnish the desired product in 84% yield as a white solid.

6. Control cell potential electrolysis

An oven-dried 10 mL undivided bottle was equipped with two graphite sheet electrodes (10 mm × 10 mm × 3 mm). The corresponding quinoxalin-2(1H)-one (80.0 mg, 0.5 mmol, 1.0 equiv.), the pyrazole (68.1 mg, 1.0 mmol, 2.0 equiv.) and \( \text{Bu}_4\text{NBF}_4 \) (329.3 mg, 1.0 mmol, 2.0 equiv.) was added.
into the undivided cell. And then MeCN (5 mL) was added. The reaction mixture was stirred and electrolyzed at a constant potential of 2.5 V at room temperature for 8 h. The solvent was concentrated in vacuo. The pure product was obtained by column chromatography (petroleum ether/ethyl acetate = 10:1) to furnish the desired product in 98% yield.

7. Mechanistic Studies

To a 10 mL oven-dried undivided bottle was added quinoxalin-2(1H)-one (80.0 mg, 0.5 mmol, 1.0 equiv.), pyrazole (68.1 mg, 1.0 mmol, 2.0 equiv.), "Bu4NBF4 (329.3 mg, 1.0 mmol, 2.0 equiv.), TEMPO (156.3 mg, 1.0 mmol, 2.0 equiv.) and MeCN (5 mL). The reaction mixture was stirred and electrolyzed at a constant current of 10.0 mA at room temperature for 8 h. The reaction was completely suppressed. A similar procedure was conducted with BHT (220.4 mg, 1.0 mmol, 2.0 equiv.). The radical trapping product 3ad can be observed by HR-MS (positive mode ESI).
To a 10 mL oven-dried undivided bottle was added 1,1’-(1,2-ethenediyl)dibenzene (88 μL, 0.5 mmol, 1.0 equiv.), pyrazole (68.1 mg, 1.0 mmol, 2.0 equiv.), "Bu4NBF4 (329.3 mg, 1.0 mmol, 2.0 equiv.), TEMPO (156.3 mg, 1.0 mmol, 2.0 equiv.) and MeCN (5 mL). The reaction mixture was stirred and electrolyzed at a constant current of 10.0 mA at room temperature for 8 h. The product 3ae was observed by HR-MS (positive mode ESI).

To a 10 mL oven-dried undivided bottle was added N-methyl-N-phenyl methacrylamide (87.6 mg, 0.5 mmol, 1.0 equiv.), pyrazole (68.1 mg, 1.0 mmol, 2.0 equiv.), "Bu4NBF4 (329.3 mg, 1.0 mmol, 2.0 equiv.), TEMPO (156.3 mg, 1.0 mmol, 2.0 equiv.) and MeCN (5 mL). The reaction mixture was
stirred and electrolyzed at a constant current of 10.0 mA at room temperature for 8 h. The product 3af was observed by HR-MS (positive mode ESI).
8. Characterization Data for Electrolysis Products

1-methyl-3-(1H-pyrazol-1-yl)quinoxalin-2(1H)-one 3a

On 0.5 mmol scale. Electrolysis was conducted following the general procedure. The crude material was purified by flash column chromatography (silica gel, 50% EtOAc in petroleum ether) to give 3a as a white solid (107.8 mg, 95% yield).

M. p. = 145 – 146 °C;

R<sub>f</sub> = 0.3 (Petroleum ether/EtOAc = 1:1);

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 9.07 (d, J = 2.7 Hz, 1H), 8.01 (dd, J = 8.0, 1.3 Hz, 1H), 7.87 (d, J = 1.2 Hz, 1H), 7.58 – 7.52 (m, 1H), 7.42 – 7.31 (m, 2H), 6.49 (dd, J = 2.6, 1.7 Hz, 1H), 3.80 (s, 3H).

<sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>) δ 150.6, 143.3, 142.5, 133.2, 132.5, 131.2, 130.1, 124.5, 113.6, 108.2, 29.9.

HRMS (ESI): Calcd for C<sub>12</sub>H<sub>11</sub>N<sub>4</sub>O [M+H]<sup>+</sup>: 227.0927; found: 227.0924

6-fluoro-1-methyl-3-(1H-pyrazol-1-yl)quinoxalin-2(1H)-one 3b

On 0.5 mmol scale. Electrolysis was conducted following the general procedure. The crude material was purified by flash column chromatography (silica gel, 50% EtOAc in petroleum ether) to give 3b as a yellow solid (70.1 mg, 57% yield).

M. p. = 188 – 189 °C;

R<sub>f</sub> = 0.2 (Petroleum ether/EtOAc = 1:1);

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 9.13 (s, 1H), 7.91 (s, 1H), 7.71 (d, J = 8.5 Hz, 1H), 7.41 – 7.26 (m, 2H), 6.53 (s, 1H), 3.81 (s, 3H).

<sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>) δ 150.6, 143.3, 142.5, 133.2, 132.5, 131.2, 130.1, 124.5, 113.6, 108.6, 30.2.

<sup>19</sup>F NMR (376 MHz, CDCl<sub>3</sub>) δ -117.2 (s).

HRMS (ESI): Calcd for C<sub>12</sub>H<sub>10</sub>FN<sub>4</sub>O [M+H]<sup>+</sup>: 245.0833; found: 245.0831

6-chloro-1-methyl-3-(1H-pyrazol-1-yl)quinoxalin-2(1H)-one 3c

On 0.5 mmol scale. Electrolysis was conducted following the general procedure. The crude material was purified by flash column chromatography (silica gel, 50% EtOAc in petroleum ether) to give 3c as a
yellow solid (116.0 mg, 89% yield).

**M. p.** = 183 – 184 °C;

**Rf** = 0.6 (Petroleum ether /EtOAc = 1:1);

1\textsuperscript{H} NMR (400 MHz, CDCl\textsubscript{3}) δ 9.08 (s, 1H), 7.94 (d, \textit{J} = 29.9 Hz, 2H), 7.49 (s, 1H), 7.30 – 7.21 (m, 1H), 6.52 (s, 1H), 3.78 (s, 3H).

13\textsuperscript{C} NMR (101 MHz, CDCl\textsubscript{3}) δ 150.2, 143.8, 143.2, 133.3, 131.8, 131.0, 129.9, 129.2, 114.8, 108.6, 30.0.

**HRMS** (ESI): Calcd for C\textsubscript{12}H\textsubscript{10}ClN\textsubscript{4}O \[\text{[M+H]}\]^+: 261.0538; found: 261.0537

6-bromo-1-methyl-3-(1H-pyrazol-1-yl)quinoxalin-2(1H)-one 3d

On 0.5 mmol scale. Electrolysis was conducted following the general procedure. The crude material was purified by flash column chromatography (silica gel, 50% EtOAc in petroleum ether) to give 3d as a yellow solid (133.3 mg, 87% yield).

**M. p.** = 186 – 187 °C;

**Rf** = 0.6 (Petroleum ether /EtOAc = 1:1);

1\textsuperscript{H} NMR (400 MHz, CDCl\textsubscript{3}) δ 9.08 (d, \textit{J} = 1.7 Hz, 1H), 8.12 (s, 1H), 7.89 (s, 1H), 7.61 (d, \textit{J} = 8.0 Hz, 1H), 7.19 (d, \textit{J} = 8.9 Hz, 1H), 6.51 (s, 1H), 3.76 (s, 3H).

13\textsuperscript{C} NMR (101 MHz, CDCl\textsubscript{3}) δ 150.2, 143.8, 143.1, 133.3, 132.6, 132.0, 131.6, 117.2, 115.1, 108.6, 30.1.

**HRMS** (ESI): Calcd for C\textsubscript{12}H\textsubscript{10}BrN\textsubscript{4}O \[\text{[M+H]}\]^+: 305.0032; found: 305.0031

6-methoxy-1-methyl-3-(1H-pyrazol-1-yl)quinoxalin-2(1H)-one 3e

On 0.5 mmol scale. Electrolysis was conducted following the general procedure. The crude material was purified by flash column chromatography (silica gel, 50% EtOAc in petroleum ether) to give 3e as a white solid (90.2 mg, 70% yield).

**M. p.** = 193 – 194 °C;

**Rf** = 0.3 (Petroleum ether /EtOAc = 1:1);

1\textsuperscript{H} NMR (400 MHz, CDCl\textsubscript{3}) δ 9.18 (s, 1H), 7.91 (s, 1H), 7.54 (d, \textit{J} = 2.0 Hz, 1H), 7.30 (d, \textit{J} = 9.4 Hz, 1H), 7.22 (d, \textit{J} = 2.1 Hz, 1H), 6.53 (s, 1H), 3.89 (s, 3H), 3.83 (s, 3H).

13\textsuperscript{C} NMR (101 MHz, CDCl\textsubscript{3}) δ 156.7, 150.2, 142.9, 142.4, 142.9, 133.3, 132.2, 126.8, 119.7, 114.6, 111.3, 108.3, 55.8, 30.0.

**HRMS** (ESI): Calcd for C\textsubscript{13}H\textsubscript{13}N\textsubscript{2}O\textsubscript{2} [M+H]^+: 257.1033; found: 257.1030

1-methyl-3-(1H-pyrazol-1-yl)-6-(trifluoromethyl)quinoxalin-2(1H)-one 3f
On 0.5 mmol scale. Electrolysis was conducted following the general procedure. The crude material was purified by flash column chromatography (silica gel, 50% EtOAc in petroleum ether) to give 3f as a white solid (120.4 mg, 82% yield).

**M. p. = 218 – 219 °C;**

**Rf = 0.4 (Petroleum ether /EtOAc = 1:1);**

**1H NMR (400 MHz, CDCl3) δ 9.09 (d, J = 2.5 Hz, 1H), 8.31 (s, 1H), 7.91 (s, 1H), 7.77 (d, J = 8.7 Hz, 1H), 7.46 (d, J = 8.7 Hz, 1H), 6.53 (s, 1H), 3.84 (s, 3H).**

**13C NMR (101 MHz, CDCl3) δ 150.5, 144.0, 143.4, 134.6, 133.3, 130.7, 127.1, 126.7, 126.5 – 126.0 (m), 124.9, 122.2, 119.5, 114.4, 110.1 – 109.9 (m), 108.8, 30.2.**

**19F NMR (376 MHz, CDCl3) δ -62.2 (s).**


1,6,7-trimethyl-3-(1H-pyrazol-1-yl)quinoxalin-2(1H)-one 3g

On 0.5 mmol scale. Electrolysis was conducted following the general procedure. The crude material was purified by flash column chromatography (silica gel, 50% EtOAc in petroleum ether) to give 3g as a white solid (96.1 mg, 76% yield).

**M. p. = 205 – 206 °C;**

**Rf = 0.4 (Petroleum ether /EtOAc = 1:1);**

**1H NMR (400 MHz, CDCl3) δ 9.06 (d, J = 2.0 Hz, 1H), 7.87 (s, 1H), 7.73 (s, 1H), 7.06 (s, 1H), 6.49 (s, 1H), 3.75 (s, 3H), 2.37 (s, 3H), 2.32 (s, 3H).**

**13C NMR (101 MHz, CDCl3) δ 150.5, 142.9, 141.7, 140.2, 133.6, 132.9, 130.5, 130.0, 129.4, 114.1, 107.9, 29.7, 20.5, 19.3.**

**HRMS (ESI): Calcd for C14H15F2N4O [M+H]+: 255.1240; found: 255.1236**

6,7-difluoro-1-methyl-3-(1H-pyrazol-1-yl)quinoxalin-2(1H)-one 3h

On 0.5 mmol scale. Electrolysis was conducted following the general procedure. The crude material was purified by flash column chromatography (silica gel, 50% EtOAc in petroleum ether) to give 3h as a white solid (71.8 mg, 55% yield).

**M. p. = 203 – 204 °C;**

**Rf = 0.4 (Petroleum ether /EtOAc = 1:1);**

**1H NMR (400 MHz, CDCl3) δ 9.10 (d, J = 2.5 Hz, 1H), 7.92 (s, 1H), 7.87 (dd, J = 10.0, 8.4 Hz, 1H),**
7.20 (dd, J = 11.0, 7.0 Hz, 1H), 6.55 (s, 1H), 3.81 (s, 3H).

$^{13}$C NMR (101 MHz, CDCl$_3$) $\delta$ 148.6 (d, $J = 13.7$ Hz), 146.2 (d, $J = 13.9$ Hz), 143.8 (s), 142.8 (s), 133.3 (s), 129.7 (d, $J = 7.8$ Hz), 127.7 (dd, $J = 10.0, 2.6$ Hz), 117.7 (d, $J = 19.5$ Hz), 108.7, 102.6, 102.4, 30.5.

$^{19}$F NMR (376 MHz, CDCl$_3$) $\delta$ -130.2 (d, $J = 22.5$ Hz), -140.0 (d, $J = 22.4$ Hz).

HRMS (ESI): Calcd for C$_{12}$H$_9$F$_2$N$_4$O $[M+H]^+$: 263.0739; found: 263.0739

6,7-dichloro-1-methyl-3-(1H-pyrazol-1-yl)quinoxalin-2(1H)-one 3i

On 0.5 mmol scale. Electrolysis was conducted following the general procedure. The crude material was purified by flash column chromatography (silica gel, 50% EtOAc in petroleum ether) to give 3i as a white solid (122.1 mg, 83% yield).

M. p. = 178 – 179 °C;
$R_f$ = 0.3 (Petroleum ether /EtOAc = 1:1);

$^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 9.09 (s, 1H), 8.10 (s, 1H), 7.91 (s, 1H), 7.46 (s, 1H), 6.54 (s, 1H), 3.78 (s, 3H).

$^{13}$C NMR (101 MHz, CDCl$_3$) $\delta$ 150.1, 144.0, 143.2, 134.1, 133.4, 131.8, 130.7, 130.4, 128.5, 115.2, 108.9, 30.2.

HRMS (ESI): Calcd for C$_{12}$H$_9$Cl$_2$N$_4$O $[M+H]^+$: 295.0148; found: 295.1047

6,7-dibromo-1-methyl-3-(1H-pyrazol-1-yl)quinoxalin-2(1H)-one 3j

On 0.5 mmol scale. Electrolysis was conducted following the general procedure. The crude material was purified by flash column chromatography (silica gel, 50% EtOAc in petroleum ether) to give 3j as a white solid (179.7 mg, 94% yield).

M. p. = 182 – 183 °C;
$R_f$ = 0.3 (Petroleum ether /EtOAc = 1:1);

$^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 9.09 (d, $J = 2.1$ Hz, 1H), 8.26 (s, 1H), 7.91 (s, 1H), 7.63 (s, 1H), 7.46 (s, 1H), 6.54 (s, 1H), 3.78 (s, 3H).

$^{13}$C NMR (101 MHz, CDCl$_3$) $\delta$ 151.6, 150.2, 144.1, 143.3, 133.9, 133.4, 131.1, 126.3, 120.0, 118.6, 118.3, 108.9, 77.4, 77.1, 76.7, 30.2.

HRMS (ESI): Calcd for C$_{12}$H$_9$Br$_2$N$_4$O $[M+H]^+$: 382.9138; found: 382.9135

1-ethyl-3-(1H-pyrazol-1-yl)quinoxalin-2(1H)-one 3k

On 0.5 mmol scale. Electrolysis was conducted following the general procedure. The crude material was
purified by flash column chromatography (silica gel, 50% EtOAc in petroleum ether) to give 3k as a white solid (108.8 mg, 91% yield).

M. p. = 114 – 115 °C;

$R_f = 0.3$ (Petroleum ether /EtOAc = 1:1);

$^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 9.10 (d, $J = 2.3$ Hz, 1H), 8.02 (d, $J = 7.9$ Hz, 1H), 7.89 (s, 1H), 7.53 (t, $J = 7.6$ Hz, 1H), 7.36 (t, $J = 9.0$ Hz, 2H), 6.51 (s, 1H), 4.40 (q, $J = 7.1$ Hz, 2H), 1.41 (t, $J = 7.2$ Hz, 3H).

$^{13}$C NMR (101 MHz, CDCl$_3$) $\delta$ 150.0, 143.2, 142.5, 133.2, 131.5, 131.4, 130.3, 130.0, 124.3, 113.5, 108.1, 38.2, 12.3.

HRMS (ESI): Calcd for C$_{13}$H$_{13}$N$_4$O [M+H]$^+$: 241.1084; found: 241.1080

1-butyl-3-(1H-pyrazol-1-yl)quinoxalin-2(1H)-one 3l

On 0.5 mmol scale. Electrolysis was conducted following the general procedure. The crude material was purified by flash column chromatography (silica gel, 50% EtOAc in petroleum ether) to give 3l as a yellow oil (68.0 mg, 51% yield).

$R_f = 0.6$ (Petroleum ether /EtOAc = 1:1);

$^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 9.11 (d, $J = 2.3$ Hz, 1H), 8.04 (d, $J = 8.0$ Hz, 1H), 7.90 (s, 1H), 7.56 (t, $J = 7.8$ Hz, 1H), 7.44 – 7.33 (m, 2H), 6.52 (s, 1H), 4.43 – 4.28 (m, 2H), 1.85 – 1.74 (m, 2H), 1.58 – 1.42 (m, 2H), 1.02 (t, $J = 7.3$ Hz, 3H).

$^{13}$C NMR (101 MHz, CDCl$_3$) $\delta$ 150.3, 143.3, 142.5, 133.1, 131.7, 131.5, 130.3, 129.9, 124.3, 113.6, 108.1, 43.0, 29.2, 20.2, 13.7.

HRMS (ESI): Calcd for C$_{15}$H$_{17}$N$_4$O [M+H]$^+$: 269.1397; found: 269.1396

1-benzyl-3-(1H-pyrazol-1-yl)quinoxalin-2(1H)-one 3m

On 0.5 mmol scale. Electrolysis was conducted following the general procedure. The crude material was purified by flash column chromatography (silica gel, 50% EtOAc in petroleum ether) to give 3m as a white solid (127.8 mg, 85% yield).

M. p. = 138 – 139 °C;

$R_f = 0.5$ (Petroleum ether /EtOAc = 1:1);

$^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 9.13 (s, 1H), 8.03 (d, $J = 7.9$ Hz, 1H), 7.92 (s, 1H), 7.49 – 7.40 (m, 1H), 7.35 – 7.20 (m, 7H), 6.51 (s, 1H), 5.58 (s, 2H).

$^{13}$C NMR (101 MHz, CDCl$_3$) $\delta$ 150.6, 143.4, 142.5, 134.5, 133.2, 131.8, 131.3, 130.1, 130.0, 128.9, 127.8, 126.6, 124.5, 114.3, 108.2, 46.52.

HRMS (ESI): Calcd for C$_{18}$H$_{15}$N$_4$O [M+H]$^+$: 303.1240; found: 303.1237

1-(2-oxo-2-phenylethyl)-3-(1H-pyrazol-1-yl)quinoxalin-2(1H)-one 3n
On 0.5 mmol scale. Electrolysis was conducted following the general procedure. The crude material was purified by flash column chromatography (silica gel, 50% EtOAc in petroleum ether) to give 3o as a white solid (143.0 mg, 87% yield).

\[ Rf = 0.5 \text{ (Petroleum ether /EtOAc = 1:1)}; \]

\[ \text{H NMR (400 MHz, CDCl}_3\text{)} \delta 9.02 (d, J = 2.5 Hz, 1H), 8.13 – 8.00 (m, 3H), 7.90 (s, 1H), 7.67 (d, J = 7.4 Hz, 1H), 7.55 (t, J = 7.7 Hz, 2H), 7.43 (d, J = 7.4 Hz, 1H), 7.37 (d, J = 7.6 Hz, 1H), 6.99 (d, J = 8.2 Hz, 1H), 6.49 (s, 1H), 5.82 (s, 2H). \]

\[ \text{C NMR (101 MHz, CDCl}_3\text{)} \delta 190.5, 150.5, 143.5, 134.6, 134.3, 133.2, 132.0, 131.4, 130.4, 130.2, 129.1, 128.2, 124.7, 113.5, 108.4, 49.2. \]

HRMS (ESI): Calcd for C_{19}H_{15}N_{4}O_{2} [M+H]^+: 331.1190; found: 331.1185

1-(prop-2-yn-1-yl)-3-(1H-pyrazol-1-yl)quinoxalin-2(1H)-one 3o

On 0.5 mmol scale. Electrolysis was conducted following the general procedure. The crude material was purified by flash column chromatography (silica gel, 50% EtOAc in petroleum ether) to give 3o as a yellow solid (103.6 mg, 83% yield).

\[ Rf = 0.4 \text{ (Petroleum ether /EtOAc = 1:1)}; \]

\[ \text{H NMR (400 MHz, CDCl}_3\text{)} \delta 9.10 (s, 1H), 8.06 (d, J = 7.3 Hz, 1H), 7.91 (s, 1H), 7.61 (d, J = 7.0 Hz, 1H), 7.53 (d, J = 7.8 Hz, 1H), 7.46 (d, J = 7.0 Hz, 1H), 6.53 (s, 1H), 5.18 (s, 2H), 2.36 (s, 1H). \]

\[ \text{C NMR (101 MHz, CDCl}_3\text{)} \delta 149.8, 143.6, 142.4, 133.2, 131.5, 131.1, 130.3, 130.2, 125.0, 114.1, 108.4, 77.4, 73.7, 32.3. \]

HRMS (ESI): Calcd for C_{14}H_{11}N_{4}O [M+H]^+: 251.0927; found: 251.0924

1-allyl-3-(1H-pyrazol-1-yl)quinoxalin-2(1H)-one 3p

On 0.5 mmol scale. Electrolysis was conducted following the general procedure. The crude material was purified by flash column chromatography (silica gel, 50% EtOAc in petroleum ether) to give 3p as a white solid (102.6 mg, 81% yield).
M. p. = 84 – 85 °C;

\( Rf = 0.4 \) (Petroleum ether /EtOAc = 1:1);

\(^1\)H NMR (400 MHz, CDCl\(_3\)) \( \delta \) 9.10 (s, 1H), 8.03 (d, \( J = 8.0 \) Hz, 1H), 7.91 (s, 1H), 7.52 (t, \( J = 7.8 \) Hz, 1H), 7.39 (d, \( J = 7.6 \) Hz, 1H), 7.32 (d, \( J = 7.5 \) Hz, 1H), 6.51 (s, 1H), 6.03 – 5.89 (m, 1H), 5.30 (d, \( J = 10.4 \) Hz, 1H), 5.19 (d, \( J = 17.2 \) Hz, 1H), 5.00 (d, \( J = 3.5 \) Hz, 2H).

\(^{13}\)C NMR (101 MHz, CDCl\(_3\)) \( \delta \) 150.1, 143.3, 142.3, 133.1, 131.6, 131.2, 130.1, 129.9, 124.5, 118.3, 114.1, 108.2, 45.1.

HRMS (ESI): Calcd for C\(_{14}\)H\(_{13}\)N\(_4\)O \([\text{M+H}]^+\): 253.1084; found: 253.1080.

ethyl 2-(2-oxo-3-(1H-pyrazol-1-yl)quinoxalin-1(2H)-yl)acetate 3q

On 0.5 mmol scale. Electrolysis was conducted following the general procedure. The crude material was purified by flash column chromatography (silica gel, 50% EtOAc in petroleum ether) to give 3q as a yellow solid (100.2 mg, 67% yield).

M. p. = 150 – 151 °C;

\( Rf = 0.5 \) (Petroleum ether /EtOAc = 1:1);

\(^1\)H NMR (400 MHz, CDCl\(_3\)) \( \delta \) 9.06 (d, \( J = 2.2 \) Hz, 1H), 8.06 (d, \( J = 8.0 \) Hz, 1H), 7.91 (s, 1H), 7.54 (t, \( J = 7.7 \) Hz, 1H), 7.41 (t, \( J = 7.6 \) Hz, 1H), 7.14 (d, \( J = 8.4 \) Hz, 1H), 6.52 (s, 1H), 5.13 (2H), 4.27 (q, \( J = 7.1 \) Hz, 2H), 1.28 (t, \( J = 7.1 \) Hz, 3H).

\(^{13}\)C NMR (101 MHz, CDCl\(_3\)) \( \delta \) 166.7, 150.5, 143.6, 142.4, 133.2, 131.7, 131.3, 130.5, 130.3, 124.9, 113.1, 108.5, 62.3, 44.2, 14.1.

HRMS (ESI): Calcd for C\(_{15}\)H\(_{15}\)N\(_4\)O \([\text{M+H}]^+\): 299.1139; found: 299.1136.

1-methyl-3-(4-methyl-1H-pyrazol-1-yl)quinoxalin-2(1H)-one 3r

On 0.5 mmol scale. Electrolysis was conducted following the general procedure. The crude material was purified by flash column chromatography (silica gel, 50% EtOAc in petroleum ether) to give 3r as a white solid (100.0 mg, 82% yield).

M. p. = 155 – 156 °C;

\( Rf = 0.4 \) (Petroleum ether /EtOAc = 1:1);

\(^1\)H NMR (400 MHz, CDCl\(_3\)) \( \delta \) 8.83 (s, 1H), 7.98 (d, \( J = 7.9 \) Hz, 1H), 7.71 (s, 1H), 7.50 (d, \( J = 7.4 \) Hz, 1H), 7.39 – 7.25 (m, 2H), 3.77 (s, 3H), 2.17 (s, 3H).

\(^{13}\)C NMR (101 MHz, CDCl\(_3\)) \( \delta \) 150.5, 144.6, 142.4, 132.3, 131.2, 131.1, 129.8, 129.6, 124.3, 118.7, 113.5, 29.7, 8.8.

HRMS (ESI): Calcd for C\(_{13}\)H\(_{13}\)N\(_4\)O \([\text{M+H}]^+\): 241.1084; found: 241.1082.

1-methyl-3-(5-methyl-1H-pyrazol-1-yl)quinoxalin-2(1H)-one 3s
On 0.5 mmol scale. Electrolysis was conducted following the general procedure. The crude material was purified by flash column chromatography (silica gel, 50% EtOAc in petroleum ether) to give 3s as a white solid (120.1 mg, 98% yield).

M. p. = 130 – 131 °C;

Rf = 0.3 (Petroleum ether /EtOAc = 1:1);

$^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 9.04 (d, $J = 1.9$ Hz, 1H), 8.04 (d, $J = 8.0$ Hz, 1H), 7.55 (t, $J = 7.7$ Hz, 1H), 7.43 – 7.30 (m, 2H), 6.32 (d, $J = 2.0$ Hz, 1H), 3.81 (s, 3H), 2.46 (s, 3H).

$^{13}$C NMR (101 MHz, CDCl$_3$) $\delta$ 153.4, 150.6, 142.3, 134.1, 132.3, 131.3, 130.1, 129.6, 124.4, 113.6, 109.0, 29.9, 14.1.

HRMS (ESI): Calcd for C$_{13}$H$_{13}$N$_4$O [M+H]$^+$: 241.1084; found: 241.1082

1-methyl-3-(3-methyl-1H-pyrazol-1-yl)quinoxalin-2(1H)-one 3t

On 0.5 mmol scale. Electrolysis was conducted following the general procedure. The crude material was purified by flash column chromatography (silica gel, 50% EtOAc in petroleum ether) to give 3t as a yellow solid (105.8 mg, 88% yield).

M. p. = 145 – 146 °C;

Rf = 0.3 (Petroleum ether /EtOAc = 1:1);

$^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 9.03 (d, $J = 2.2$ Hz, 1H), 8.03 (d, $J = 7.9$ Hz, 1H), 7.53 (t, $J = 7.6$ Hz, 1H), 7.42 – 7.28 (m, 2H), 6.31 (d, $J = 2.3$ Hz, 1H), 3.79 (s, 3H), 2.46 (s, 3H).

$^{13}$C NMR (101 MHz, CDCl$_3$) $\delta$ 153.4, 150.6, 142.3, 134.1, 132.3, 131.3, 130.1, 129.6, 124.4, 113.6, 109.0, 29.9, 14.1.

HRMS (ESI): Calcd for C$_{13}$H$_{13}$N$_4$O [M+H]$^+$: 241.1084; found: 241.1079

3-(4-fluoro-1H-pyrazol-1-yl)-1-methylquinoxalin-2(1H)-one 3u

On 0.5 mmol scale. Electrolysis was conducted following the general procedure. The crude material was purified by flash column chromatography (silica gel, 50% EtOAc in petroleum ether) to give 3u as a yellow solid (85.6 mg, 70% yield).

M. p. = 178 – 179 °C;

Rf = 0.4 (Petroleum ether /EtOAc = 1:1);

$^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 9.00 (s, 1H), 8.02 (d, $J = 6.1$ Hz, 1H), 7.80 (s, 1H), 7.59 (d, $J = 7.2$ Hz,
1H), 7.47 – 7.34 (m, 2H), 3.82 (s, 3H).

$^{13}$C NMR (101 MHz, CDCl$_3$) δ 150.4, 142.0, 132.7, 132.1 (d, $J = 15.8$ Hz), 131.1, 130.3 (d, $J = 17.4$ Hz), 124.7, 118.9 (d, $J = 31.5$ Hz), 113.8, 29.9.

$^{19}$F NMR (376 MHz, CDCl$_3$) δ -173.5 (s).

HRMS (ESI): Calcd for C$_{12}$H$_{10}$FN$_4$O [M+H]$^+$: 245.0833; found: 245.0829

3-(4-chloro-1H-pyrazol-1-yl)-1-methylquinoxalin-2(1H)-one 3v

On 0.5 mmol scale. Electrolysis was conducted following the general procedure. The crude material was purified by flash column chromatography (silica gel, 50% EtOAc in petroleum ether) to give 3v as a yellow solid (92.4 mg, 71% yield).

M. p. = 197 – 198 °C;

$R_f$ = 0.6 (Petroleum ether /EtOAc = 1:1);

$^1$H NMR (400 MHz, CDCl$_3$) δ 9.12 (s, 1H), 8.09 – 7.99 (m, 1H), 7.83 (d, $J = 5.2$ Hz, 1H), 7.66 – 7.58 (m, 1H), 7.48 – 7.35 (m, 2H), 3.84 (s, 3H).

$^{13}$C NMR (101 MHz, CDCl$_3$) δ 150.4, 142.0, 141.8, 132.7, 131.1, 130.3, 124.8, 113.8, 113.1, 30.0.

HRMS (ESI): Calcd for C$_{12}$H$_{10}$ClN$_4$O [M+H]$^+$: 261.0538; found: 261.0533

3-(4-bromo-1H-pyrazol-1-yl)-1-methylquinoxalin-2(1H)-one 3w

On 0.5 mmol scale. Electrolysis was conducted following the general procedure. The crude material was purified by flash column chromatography (silica gel, 50% EtOAc in petroleum ether) to give 3w as a yellow solid (141.7 mg, 93% yield).

M. p. = 154 – 155 °C;

$R_f$ = 0.6 (Petroleum ether /EtOAc = 1:1);

$^1$H NMR (400 MHz, CDCl$_3$) δ 9.18 (s, 1H), 8.00 (d, $J = 7.9$ Hz, 1H), 7.87 (s, 1H), 7.66 – 7.58 (m, 1H), 7.44 – 7.32 (m, 2H), 3.81 (s, 3H).

$^{13}$C NMR (101 MHz, CDCl$_3$) δ 150.3, 142.0, 141.5, 137.3, 132.6, 130.9, 130.5, 130.2, 124.7, 113.7, 60.4, 30.0.

HRMS (ESI): Calcd for C$_{12}$H$_{10}$BrN$_4$O [M+H]$^+$: 305.0032; found: 305.0041

3-(4-iodo-1H-pyrazol-1-yl)-1-methylquinoxalin-2(1H)-one 3x

On 0.5 mmol scale. Electrolysis was conducted following the general procedure. The crude material was
purified by flash column chromatography (silica gel, 50% EtOAc in petroleum ether) to give 3x as a yellow solid (114.8 mg, 65% yield).

M. p. = 130 – 131 °C;

Rf = 0.6 (Petroleum ether /EtOAc = 1:1);

1H NMR (400 MHz, CDCl3) δ 8.90 (d, J = 2.6 Hz, 1H), 8.02 (d, J = 8.0 Hz, 1H), 7.58 (d, J = 8.6 Hz, 1H), 7.45 – 7.34 (m, 2H), 6.66 (d, J = 2.6 Hz, 1H), 3.81 (s, 3H).

13C NMR (101 MHz, CDCl3) δ 150.2, 141.3, 135.1, 132.6, 131.0, 130.5, 124.7, 117.5, 113.7, 102.3, 30.0.

HRMS (ESI): Calcd for C12H10IN4O [M+H]+: 352.9894; found: 352.9890

ethyl 1-(4-methyl-3-oxo-3,4-dihydroquinoxalin-2-yl)-1H-pyrazole-4-carboxylate 3y

\[
\text{On 0.5 mmol scale. Electrolysis was conducted following the general procedure. The crude material was purified by flash column chromatography (silica gel, 50% EtOAc in petroleum ether) to give 3y as a yellow solid (145.2 mg, 71% yield).}
\]

M. p. = 104 – 105 °C;

Rf = 0.3 (Petroleum ether /EtOAc = 1:1);

1H NMR (400 MHz, CDCl3) δ 9.59 (s, 1H), 8.28 (s, 1H), 8.08 – 8.04 (m, 1H), 7.70 – 7.57 (m, 1H), 7.46 (s, 1H), 7.44 – 7.39 (m, 1H), 4.37 (q, J = 7.2 Hz, 2H), 3.87 (s, 3H), 1.40 (t, J = 6.2 Hz, 3H).

13C NMR (101 MHz, CDCl3) δ 162.5, 150.4, 143.7, 141.9, 136.5, 132.8, 131.0, 130.5, 124.9, 117.5, 113.8, 60.7, 30.1, 14.4.

HRMS (ESI): Calcd for C15H15N4O3 [M+H]+: 299.1139; found: 299.1136

3-(3-iodo-1H-pyrazol-1-yl)-1-methylquinoxalin-2(1H)-one 3z

\[
\text{On 0.5 mmol scale. Electrolysis was conducted following the general procedure. The crude material was purified by flash column chromatography (silica gel, 50% EtOAc in petroleum ether) to give 3z as a yellow solid (157.8 mg, 90% yield).}
\]

M. p. = 139 – 140 °C;

Rf = 0.6 (Petroleum ether /EtOAc = 1:1);

1H NMR (400 MHz, CDCl3) δ 8.88 (d, J = 2.3 Hz, 1H), 8.00 (d, J = 7.9 Hz, 1H), 7.57 (t, J = 7.6 Hz, 1H), 7.44 – 7.34 (m, 2H), 6.65 (d, J = 2.3 Hz, 1H), 3.80 (s, 3H).

13C NMR (101 MHz, CDCl3) δ 150.2, 141.2, 135.1, 132.6, 130.9, 130.4, 130.3, 124.6, 123.7, 117.4, 113.7, 102.3, 30.0.

HRMS (ESI): Calcd for C13H10IN3O[M+H]+: 352.9894; found: 352.9889

3-(3,4-dimethyl-1H-pyrazol-1-yl)-1-methylquinoxalin-2(1H)-one 3aa
On 0.5 mmol scale. Electrolysis was conducted following the general procedure. The crude material was purified by flash column chromatography (silica gel, 50% EtOAc in petroleum ether) to give 3aa as a white solid (90.5 mg, 71% yield).

**M. p.** = 132 – 133 °C;

**Rf** = 0.4 (Petroleum ether /EtOAc = 1:1);

**1H NMR** (400 MHz, CDCl$_3$) $\delta$ 8.83 (s, 1H), 8.03 (d, $J = 7.9$ Hz, 1H), 7.53 (t, $J = 7.6$ Hz, 1H), 7.45 – 7.32 (m, 2H), 3.81 (s, 3H), 2.37 (s, 3H), 2.09 (s, 3H).

**13C NMR** (101 MHz, CDCl$_3$) $\delta$ 153.4, 150.3, 142.3, 132.2, 131.8, 131.6, 130.0, 129.3, 124.4, 118.0, 113.5, 29.8, 12.2, 8.6.

**HRMS** (ESI): Calcd for C$_{14}$H$_{15}$N$_4$O [M+H]$^+$: 255.1240; found: 255.1238

1-methyl-3-(1H-1,2,3-triazol-1-yl)quinoxalin-2(1H)-one 3ab

On 0.5 mmol scale. Electrolysis was conducted following the general procedure. The crude material was purified by flash column chromatography (silica gel, 50% EtOAc in petroleum ether) to give 3ab as a yellow solid (106.6 mg, 94% yield).

**M. p.** = 148 – 149 °C;

**Rf** = 0.1 (Petroleum ether /EtOAc = 1:1);

**1H NMR** (400 MHz, CDCl$_3$) $\delta$ 8.99 (s, 1H), 8.09 (d, $J = 7.9$ Hz, 1H), 7.88 (s, 1H), 7.71 (t, $J = 7.5$ Hz, 1H), 7.54 – 7.43 (m, 2H), 3.88 (s, 3H).

**13C NMR** (101 MHz, CDCl$_3$) $\delta$ 150.3, 141.2, 133.6, 133.4, 131.8, 131.0, 130.9, 125.9, 125.0, 114.0, 30.16.

**HRMS** (ESI): Calcd for C$_{11}$H$_{10}$N$_5$O [M+H]$^+$: 228.0880; found: 228.0878

3-(1H-benzo[d][1,2,3]triazol-1-yl)-1-methylquinoxalin-2(1H)-one 3ac

On 0.5 mmol scale. Electrolysis was conducted following the general procedure. The crude material was purified by flash column chromatography (silica gel, 50% EtOAc in petroleum ether) to give 3ac as a yellow solid (123.2 mg, 89% yield).

**M. p.** = 200 – 201 °C;

**Rf** = 0.3 (Petroleum ether /EtOAc = 1:1);

**1H NMR** (400 MHz, CDCl$_3$) $\delta$ 8.17 (d, $J = 8.0$ Hz, 1H), 8.02 (d, $J = 8.0$ Hz, 1H), 7.97 (d, $J = 7.7$ Hz, 1H), 7.68 (t, $J = 7.4$ Hz, 1H), 7.61 (t, $J = 7.1$ Hz, 1H), 7.45 (d, $J = 7.5$ Hz, 3H), 3.88 (s, 3H).
$^{13}$C NMR (101 MHz, CDCl$_3$) δ 150.8, 145.9, 143.5, 133.6, 132.8, 131.7, 130.9, 130.4, 128.8, 125.0, 124.7, 120.2, 114.1, 113.3, 30.2.

HRMS (ESI): Calcd for C$_{15}$H$_{12}$N$_3$O [M+H]$^+$: 278.1036; found: 278.103
## 9. X-ray Crystallography

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10. Spectra of prepared compounds

$^1$H NMR spectrum of compound 3a

$^{13}$C NMR spectrum of compound 3a
$^1$H NMR spectrum of compound 3b

$^{13}$C NMR spectrum of compound 3b
$^{19}$F NMR spectrum of compound 3b
$^1$H NMR spectrum of compound 3c

$^{13}$C NMR spectrum of compound 3c
$^1$H NMR spectrum of compound 3d

$^{13}$C NMR spectrum of compound 3d
$^1$H NMR spectrum of compound 3e

$^{13}$C NMR spectrum of compound 3e
$^{1}H$ NMR spectrum of compound 3f

$^{13}C$ NMR spectrum of compound 3f
$^{19}$F NMR spectrum of compound 3f
$^1$H NMR spectrum of compound 3g

$^{13}$C NMR spectrum of compound 3g
$^1$H NMR spectrum of compound $3h$

$^{13}$C NMR spectrum of compound $3h$
$^{19}$F NMR spectrum of compound 3h
$^{1}H$ NMR spectrum of compound 3i

$^{13}C$ NMR spectrum of compound 3i
$^1$H NMR spectrum of compound 3j

$^{13}$C NMR spectrum of compound 3j
$^1$H NMR spectrum of compound 3k

$^{13}$C NMR spectrum of compound 3k
$^1$H NMR spectrum of compound 3l

$^{13}$C NMR spectrum of compound 3l
$^1$H NMR spectrum of compound 3m

$^{13}$C NMR spectrum of compound 3m
$^1$H NMR spectrum of compound 3n

$^{13}$C NMR spectrum of compound 3n
$^1$H NMR spectrum of compound 3o

$^{13}$C NMR spectrum of compound 3o
$^1$H NMR spectrum of compound 3p

$^{13}$C NMR spectrum of compound 3p
$^1$H NMR spectrum of compound 3q

$^{13}$C NMR spectrum of compound 3q
$^1$H NMR spectrum of compound 3r

$^{13}$C NMR spectrum of compound 3r
$^{1}H$ NMR spectrum of compound 3s

$^{13}C$ NMR spectrum of compound 3s
$^1$H NMR spectrum of compound 3t

$^{13}$C NMR spectrum of compound 3t
$^1$H NMR spectrum of compound 3u

$^{13}$C NMR spectrum of compound 3u
$^{19}$F NMR spectrum of compound 3u
$^{1}$H NMR spectrum of compound 3v

$^{13}$C NMR spectrum of compound 3v
$^1$H NMR spectrum of compound 3w

$^{13}$C NMR spectrum of compound 3w
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$^{13}$C NMR spectrum of compound 3aa
\textsuperscript{1}H NMR spectrum of compound 3ab

\textsuperscript{13}C NMR spectrum of compound 3ab
$^1$H NMR spectrum of compound 3ac

$^{13}$C NMR spectrum of compound 3ac
11. References