Supporting Information

Alkyl Carbazates for Electrochemical Deoxygenative Functionalization of Heteroarenes

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# Supporting Information

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1 General Considerations

All commercial reagents were used without additional purification unless otherwise specified. Solvents were purified and dried according to standard methods prior to use. All reactions were run under argon, unless otherwise noted. All experiments were monitored by thin layer chromatography (TLC) using UV light as visualizing agent. TLC was performed on pre-coated silica gel plated. Column chromatography was performed using silica gel 60 (300-400 mesh). The instrument for electrolysis is dual display potentiostat (DJS-292B) (made in China). The anode electrode is carbon anode (10 mm×10 mm×0.3 mm ) and the cathode electrode is platinum plate electrodes (10 mm×10 mm ×3mm). $^1$H NMR (400 MHz) and $^{13}$C NMR (101 MHz) were measured on a Bruker AVANCE III-400 spectrometer. Chemical shifts are reported in ppm (δ) relative to internal tetramethylsilane (TMS, δ 0.0 ppm) or with the solvent reference relative to TMS employed as the internal standard. Data are reported as follows: chemical shift (multiplicity [singlet (s), doublet (d), triplet (t), quartet (q), broad (br) and multiplet (m)], coupling constants [Hz, integration). Melting points are uncorrected. Infrared spectra were obtained on a Agilent Cary 630 instrument on a diamond plate by way of technology Attenuated Total Reflection (ATR). HRMS were conducted on an Agilent 6540Q-TOF LC/MS equipped with an electrospray ionization (ESI) probe operating in positive ion mode.
2. Graphical Guide for the set-up
3. General Procedure for Synthesis of the carbazates

A round-bottom flask was charged with isopropyl alcohol (1.0 ml, 10.0 mmol, 1 equiv), followed by the addition of dichloromethane (10 ml) and pyridine (1.5 equiv). The solution was cooled to 0 °C. A solution of phenyl chloroformate (1.38 mL, 11 mmol, 1.1 equiv) in dichloromethane (10 ml) was added, then cooled to room temperature and allowed to stir for overnight. The reaction was quenched with 1M hydrochloric acid. The aqueous layer was washed with methylene chloride, dried over Na₂SO₄ and concentrated in vacuo to afford the crude product carbonate. Next, hydrazine hydrate (2.0 equiv.) was added to the solution of the corresponding carbonate in EtOH (20ml) and then stirred for about 1 h at 80 °C. Once complete, the reaction was quenched with 1M Sodium hydroxide solution, and extracted with EtOAc (50 mL × 3), the organic solvent was dried over Na₂SO₄. The solvent was evaporated under reduced pressure. The corresponding carbazates was purified by silica gel column chromatography. (eluent: petroleum ether/ethyl acetate= 1:1).

3-methylpentan-3-yl hydrazinecarboxylate (Y1). White solid (1.52 g, 95% yield); mp 51-52 °C; \(^1\)H NMR (400 MHz, CDCl₃) δ 6.62 (s, 1H), 3.68 (s, 2H), 1.73 (m, 2H), 1.61 (m, 2H), 1.23 (s, 3H), 0.72 (t, \(J = 7.5\) Hz, 6H); \(^13\)C NMR (101 MHz, CDCl₃) δ 158.1, 85.0, 30.5, 22.8, 7.8. HRMS-ESI (m/z): calcd for [M + H]⁺ 161.1284, found 161.1282.
2-methylhexan-2-yl hydrazinecarboxylate (Y2). Colorless solid (1.64 g, 94% yield); \(^1\)H NMR (400 MHz, CDCl\(_3\)) \(\delta\) 6.23 (s, 1H), 3.70 (s, 2H), 1.80 – 1.67 (m, 2H), 1.40 (s, 6H), 1.30 – 1.18 (m, 4H), 0.87 (t, \(J = 6.7\) Hz, 3H); \(^13\)C NMR (101 MHz, CDCl\(_3\)) \(\delta\) 158.1, 82.6, 40.8, 26.2, 26.1, 23.0, 14.0. HRMS-ESI (m/z): calcd for [M + H]\(^+\) 175.1441, found 175.1440.

3,7-dimethyloctan-3-yl hydrazinecarboxylate (Y3). Colorless oil (1.99 g, 92% yield); \(^1\)H NMR (400 MHz, DMSO-\(d_6\)) \(\delta\) 7.82 (s, 1H), 3.89 (s, 2H), 1.78 (m, 2H), 1.73 – 1.61 (m, 2H), 1.56 – 1.47 (m, 1H), 1.31 (s, 3H), 1.28 – 1.21 (m, 2H), 1.17 – 1.08 (m, 2H), 0.85 (d, \(J = 6.6\) Hz, 6H), 0.81 (t, \(J = 7.5\) Hz, 3H). \(^13\)C NMR (101 MHz, DMSO-\(d_6\)) \(\delta\) 158.1, 82.8, 39.3, 38.5, 31.2, 27.8, 23.8, 22.9, 21.3, 8.3. HRMS-ESI (m/z): calcd for [M + H]\(^+\) 217.1910, found 217.1908.

2-methyl-1-phenylpropan-2-yl hydrazinecarboxylate (Y4). Colorless oil (1.96 g, 94% yield); \(^1\)H NMR (400 MHz, CDCl\(_3\)) \(\delta\) 7.27 – 7.15 (m, 5H), 6.55 (s, 1H), 3.75 (s, 2H), 3.06 (s, 2H), 1.42 (s, 6H). \(^13\)C NMR (101 MHz, CDCl\(_3\)) \(\delta\) 158.2, 137.3, 130.6, 128.0, 126.5, 82.1, 46.6, 26.3. HRMS-ESI (m/z): calcd for [M + H]\(^+\) 209.1285, found 209.1281.
methylcyclohexyl hydrazinecarboxylate (Y5). White solid (1.50 g, 87% yield); mp 61-62 °C; $^1$H NMR (400 MHz, CDCl$_3$) δ 6.61 (s, 1H), 3.75 (s, 2H), 2.07 (m, 2H), 1.60 – 1.37 (m, 10H), 1.35 – 1.22 (m, 1H). $^{13}$C NMR (101 MHz, CDCl$_3$) δ 158.1, 81.6, 37.0, 25.6, 25.3, 22.0. HRMS-ESI (m/z): calcd for [M + H]$^+$ 173.1285, found 173.1283.

(2r,5s)-2-methyladantan-2-yl hydrazinecarboxylate (Y6). White solid (2.06 g, 92% yield); mp 91-92 °C ; $^1$H NMR (400 MHz, DMSO-$_d$6) δ 7.92 (s, 1H), 3.93 (s, 2H), 2.15 (m, 2H), 2.04 (d, J = 11.8 Hz, 2H), 1.83 (d, J = 11.8 Hz, 2H), 1.74 (m, 2H), 1.67 (d, J = 12.2 Hz, 4H), 1.55 (s, 3H), 1.46 (d, J = 12.2 Hz, 2H). $^{13}$C NMR (101 MHz, DMSO-$_d$6) δ 157.9, 84.0, 38.1, 36.5, 34.4, 32.9, 27.3, 26.7, 23.0. HRMS-ESI (m/z): calcd for [M + H]$^+$ 225.1598, found 225.1595.

cyclohexyl hydrazinecarboxylate (Y7). White solid (1.50 g, 95% yield); mp 58-59 °C; $^1$H NMR (400 MHz, CDCl$_3$) δ 6.18 (s, 1H), 4.69 – 4.67 (m, 1H), 3.68 (s, 2H), 1.90 – 1.62 (m, 4H), 1.61 – 0.89 (m, 6H). $^{13}$C NMR (101 MHz, CDCl$_3$) δ 158.5, 74.0, 32.0, 25.3, 23.8. HRMS-ESI (m/z): calcd for [M + H]$^+$ 159.1128, found 159.1125.
cyclohexyl hydrazinecarboxylate (Y8). White solid (1.81 g, 97% yield); mp 62-63 °C; \(^1\)H NMR (400 MHz, DMSO-\(d_6\)) \(\delta\) 7.99 (s, 1H), 4.72 – 4.67 (m, 1H), 3.97 (s, 2H), 1.77 – 1.61 (m, 6H), 1.58 – 1.42 (m, 8H). \(^{13}\)C NMR (101 MHz, DMSO-\(d_6\)) \(\delta\) 158.5, 74.6, 31.8, 27.1, 25.3, 22.9. HRMS-ESI (m/z): calcd for [M + H]\(^+\) 187.1441, found 187.1439.

cyclododecyl hydrazinecarboxylate (Y9). White solid (2.25 g, 93% yield); mp 74-75 °C; \(^1\)H NMR (400 MHz, DMSO-\(d_6\)) \(\delta\) 8.01 (s, 1H), 4.81 – 4.79 (m, 1H), 4.00 (s, 2H), 1.65 – 1.60 (m, 2H), 1.42 – 1.13 (m, 20H). \(^{13}\)C NMR (101 MHz, DMSO-\(d_6\)) \(\delta\) 158.8, 71.2, 29.8, 23.8, 23.6, 23.3, 21.1. HRMS-ESI (m/z): calcd for [M + H]\(^+\) 243.2067, found 243.2066.

4,4-difluorocyclohexyl hydrazinecarboxylate (Y10). White solid (1.67 g, 86% yield); mp 53-54 °C; \(^1\)H NMR (400 MHz, CDCl\(_3\)) \(\delta\) 12.90 (s, 1H), 9.48 (s, 1H), 8.78 (s, 2H), 6.73 – 6.43 (m, 9H). \(^{13}\)C NMR (101 MHz, CDCl\(_3\)) \(\delta\) 158.1, 122.5 (t, \(J = 241.1\) Hz), 69.8, 30.0 (t, \(J = 24.8\) Hz), 27.4 (t, \(J = 5.0\) Hz). HRMS-ESI (m/z): calcd for [M + H]\(^+\) 195.0940, found 195.0939.
tetrahydrofuran-3-yl hydrazinecarboxylate (Y11). White solid (1.26 g, 86% yield); mp 48-49 °C; $^1$H NMR (400 MHz, CDCl$_3$) δ 6.38 (s, 1H), 5.28 – 5.27 (m, 1H), 3.92 – 3.84 (m, 4H), 3.86 – 3.82 (s, 2H), 2.21 – 2.20 (m, 1H), 2.01 (m, 1H). $^{13}$C NMR (101 MHz, CDCl$_3$) δ 158.3, 75.9, 73.2, 66.9, 32.8. HRMS-ESI (m/z): calcd for [M + H]$^+$ 147.0764, found 147.0762.

tert-butyl 3-((hydrazinecarbonyloxy)pyrrolidine-1-carboxylate (Y12). Colorless oil (2.28 g, 93% yield); $^1$H NMR (400 MHz, CDCl$_3$) δ 5.24 (s, 1H), 3.57 – 3.37 (m, 7H), 2.05 (s, 2H), 1.46 (s, 9H). $^{13}$C NMR (101 MHz, CDCl$_3$) δ 158.1, 154.4, 79.5, 74.9, 52.0, 43.9, 30.8, 28.4. HRMS-ESI (m/z): calcd for [M + H]$^+$ 246.1448, found 246.1449.

2, 3-dihydro-1H-inden-2-yl hydrazinecarboxylate (Y13). White solid (1.82 g, 95% yield); mp 145-146 °C; $^1$H NMR (400 MHz, DMSO-d$_6$) δ 8.11 (s, 1H), 7.26 – 7.24 (m, 2H), 7.18 – 7.15 (m, 2H), 5.34 (m, 1H), 4.02 (s, 2H), 3.24 (dd, $J = 16.9$, 5.8 Hz, 2H), 2.88 (d, $J = 16.9$ Hz, 2H). $^{13}$C NMR (101 MHz, DMSO-d$_6$) δ 158.6, 141.1, 126.9, 119.5, 118.1, 117.0, 115.4, 114.6, 112.1, 107.2, 102.4, 99.2, 38.9, 30.7, 28.4.
125.0, 75.6, 39.9. HRMS-ESI (m/z): calcd for [M + H]$^+$ 193.0972, found 193.0970.

4-phenylbutan-2-yl hydrazinecarboxylate (Y14). Colorless oil (2.0 g, 96% yield); $^1$H NMR (400 MHz, DMSO-$d_6$) $\delta$ 8.12 (s, 1H), 7.28 (t, $J$ = 7.5 Hz, 2H), 7.23 – 7.11 (m, 3H), 4.71 – 4.66 (m, 1H), 4.05 (s, 2H), 2.63 – 2.57 (m, 2H), 1.82 – 1.77 (m, 2H), 1.18 (d, $J$ = 6.4 Hz, 3H). $^{13}$C NMR (101 MHz, DMSO-$d_6$) $\delta$ 170.8, 158.7, 142.0, 128.8, 126.2, 70.2, 38.0, 31.5, 20.7. HRMS-ESI (m/z): calcd for [M + H]$^+$ 209.1285, found 209.1282.

7-ethyl-2-methylundecan-4-yl hydrazinecarboxylate (Y15). Colorless oil (2.48 g, 91% yield); $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 5.93 (s, 1H), 4.90 – 4.85 (m, 1H), 3.76 (s, 2H), 1.69 – 1.59 (m, 1H), 1.51 (m, 3H), 1.35 – 1.16 (m, 12H), 0.95 – 0.88 (m, 9H), 0.84 (t, $J$ = 7.2 Hz, 3H). $^{13}$C NMR (101 MHz, CDCl$_3$) $\delta$ 158.9, 74.8, 43.6, 38.7, 32.8, 32.1, 28.9, 28.3, 25.7, 24.7, 23.1, 22.2, 14.1, 10.8. HRMS-ESI (m/z): calcd for [M + H]$^+$ 273.2537, found 273.2538.
naphthalen-2-ylmethyl hydrazinecarboxylate (Y16). White solid (1.99 g, 92% yield); mp 125-126 °C; $^1$H NMR (500 MHz, CDCl$_3$) $\delta$ 7.80 (d, $J$ = 8.7 Hz, 4H), 7.59 – 7.37 (m, 3H), 6.32 (s, 1H), 5.27 (s, 2H), 3.73 (s, 2H). $^{13}$C NMR (126 MHz, CDCl$_3$) $\delta$ 158.7, 133.5, 133.2, 133.2, 128.4, 128.0, 127.7, 127.4, 126.3, 126.3, 125.8, 67.5. HRMS-ESI (m/z): calcd for [M + Na]$^+$ 239.0791, found 239.0794.

![Y-17](image)

phenethyl hydrazinecarboxylate (Y17). White solid (1.67 g, 93% yield); mp 110-111 °C; $^1$H NMR (500 MHz, DMSO) $\delta$ 8.15 (s, 1H), 7.44 – 7.10 (m, 5H), 4.18 (t, $J$ = 6.9 Hz, 2H), 4.03 (s, 2H), 2.86 (t, $J$ = 6.8 Hz, 2H). $^{13}$C NMR (126 MHz, DMSO) $\delta$ 158.8, 138.6, 129.3, 128.8, 126.7, 65.0, 35.4. HRMS-ESI (m/z): calcd for [M + H]$^+$ 181.0972, found 181.0969.
4 Optimization for the reaction of quinoxalinone with t-butyl carbazate

![Diagram of the reaction]

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Table 1. Optimization of the reaction conditions. [a] Yields determined by 1H NMR spectroscopy using 1,3,5- trimethoxybenzene as internal standard; [b] 87% isolated yield; [c] 1:1 DMSO/MeCN; [d] 3:1 DMSO/MeCN. [e] 3mA for 16 h. [f] 12 mA for 4 h. [g] 80 °C. [h] r.t.
5 Optimization for the reaction of isoquinoline with cyclohexyl hydrazinecarboxylate

![Chemical Reaction Diagram]

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6 General experimental procedure for the electrochemical minisci reaction

An undivided three-necked bottle was equipped with a carbon anode (10 mm × 10 mm × 3 mm) and a platinum plate electrode (10 mm × 10 mm × 0.3 mm) and connected to a DC regulated power supply. To the bottle was added 2-quinoxalinone (29.2 mg, 0.2 mmol), tert-Butyl carbazate (79.3 mg, 0.6 mmol), tetrabutylammonium hexafluorophosphate (155.0 mg, 0.4 mmol) and 4 mL of DMSO/CH3CN. The reaction mixture was stirred and electrolyzed at constant current conditions 6 mA at 50 °C under argon atmosphere (The dual display potentiostat was operating in constant current mode) for 8 h.

Once complete, the reaction was quenched with aqueous NaHCO3 and extracted with EtOAc (50 mL × 3), the organic solvent was dried over Na2SO4. The solvent was evaporated under reduced pressure. The crude product was purified by silica gel column chromatography. (eluent : hexane/ethyl acetate= 3:1) or hexane/acetone (5:1, v/v).

3-(tert-butyl)quinoxalin-2(1H)-one (2)[1]. White solid (35.1 mg, 87% yield); mp 208-209 °C; 1H NMR (400 MHz,
CDCl₃ δ 12.56 (s, 1H), 7.90 – 7.85 (m, 1H), 7.52 – 7.48 (m, 1H), 7.36 – 7.32 (m, 2H), 1.58 (s, 9H). ¹³C NMR (101 MHz, CDCl₃) δ 165.8, 156.0, 132.4, 131.3, 129.6, 129.2, 123.7, 115.0, 39.3, 27.8. HRMS-ESI (m/z): calcd for [M + H]⁺ 203.8814, found 203.8813.

3-(3-methylpentan-3-yl)quinoxalin-2(1H)-one (3). White solid (37.7 mg, 82% yield); mp 215-216 °C; ¹H NMR (400 MHz, CDCl₃) δ 12.09 (s, 1H), 7.88 (d, J = 8.0 Hz, 1H), 7.50 (t, J = 7.8 Hz, 1H), 7.32 (m, 2H), 2.40 (m, 2H), 1.84 (m, 2H), 1.44 (s, 3H), 0.80 (t, J = 7.5 Hz, 6H). ¹³C NMR (101 MHz, CDCl₃) δ 164.8, 155.8, 132.4, 131.1, 129.5, 129.3, 123.7, 114.9, 46.6, 30.9, 21.9, 9.2. HRMS-ESI (m/z): calcd for [M + H]⁺ 231.1492, found 231.1490.

3-(2-methylhexan-2-yl)quinoxalin-2(1H)-one (4). White solid (31.3 mg, 64% yield); mp 218-219 °C; ¹H NMR (400 MHz, CDCl₃) δ 11.90 (s, 1H), 7.87 – 7.85 (m, 1H), 7.49 (t, J = 7.6 Hz, 1H), 7.33 (t, J = 7.7 Hz, 1H), 7.29 (m, 1H), 2.11 – 2.06 (m, 2H), 1.51 (s, 6H), 1.33 – 1.27 (m, 2H), 1.14 (m, 2H), 0.86 (t, J = 7.3 Hz, 3H). ¹³C NMR (101 MHz, CDCl₃) δ 165.5, 155.7, 132.3, 131.2, 129.5, 129.2, 123.7, 114.8, 42.6, 39.6, 27.5, 26.3, 23.5, 14.1. HRMS-ESI (m/z): calcd for [M + H]⁺ 245.1648, found 245.1648.

3-(3,7-dimethyloctan-3-yl)quinoxalin-2(1H)-one (5). Yellow oil (38.9 mg, 68% yield); ¹H NMR (400 MHz, S13
CDCl$_3$ $\delta$ 12.67 (s, 1H), 7.86 – 7.84 (m, 1H), 7.50 – 7.45 (m, 1H), 7.33 – 7.29 (m, 2H), 2.45 – 2.26 (m, 2H), 1.90 – 1.68 (m, 3H), 1.45 (s, 3H), 1.33 – 1.22 (m, 2H), 1.19 – 1.11 (m, 2H), 1.09 – 0.95 (m, 1H), 0.88 – 0.82 (m, 2H), 0.79 – 0.75 (m, 6H). $^{13}$C NMR (101 MHz, CDCl$_3$) $\delta$ 164.8, 156.2, 132.5, 131.2, 129.5, 129.2, 123.7, 115.1, 46.3, 39.8, 38.7, 31.4, 27.7, 22.7, 22.6, 22.5, 9.2. HRMS-ESI (m/z): calcd for [M + H]$^+$ 287.2118, found 287.2117.

3-(2-methyl-1-phenylpropan-2-yl)quinoxalin-2(1H)-one (6). White solid (42.8 mg, 77% yield); mp 255-256 °C; $^1$H NMR (400 MHz, DMSO-$d_6$) $\delta$ 12.39 (s, 1H), 7.64 – 7.57 (m, 1H), 7.50 – 7.42 (m, 1H), 7.34 – 7.27 (m, 1H), 7.26 – 7.18 (m, 1H), 7.14 m, 2H), 7.10 – 7.04 (m, 1H), 7.02 – 6.95 (m, 2H), 3.36 (s, 2H), 1.38 (s, 6H). $^{13}$C NMR (101 MHz, DMSO-$d_6$) $\delta$ 164.9, 154.6, 139.4, 132.3, 131.4, 130.3, 130.1, 129.0, 128.2, 126.3, 123.4, 115.3, 44.7, 43.7, 26.4. HRMS-ESI (m/z): calcd for [M + H]$^+$ 279.1491, found 279.1492.

3-(1-methylcyclohexyl)quinoxalin-2(1H)-one (7). White solid (42.1 mg, 87% yield); mp 235-236 °C; $^1$H NMR (400 MHz, DMSO-$d_6$) $\delta$ 12.22 (s, 1H), 7.71 (d, $J = 7.9$ Hz, 1H), 7.47 (t, $J = 7.6$ Hz, 1H), 7.26 (t, $J = 8.6$ Hz, 2H), 2.42 (m, 2H), 1.61 – 1.47 (m, 4H), 1.47 – 1.36 (m, 4H), 1.34 (s, 3H). $^{13}$C NMR (101 MHz, DMSO-$d_6$) $\delta$ 165.6, 154.2, 132.2, 131.5, 130.0, 128.9, 123.3, 115.2, 42.5, 35.5, 26.5, 24.8, 22.8. HRMS-ESI (m/z): calcd for [M + H]$^+$ 243.1492, found 243.1489.
3-((2r,5s)-2-methyladamantan-2-yl)quinoxalin-2(1H)-one (8). White solid (42.4 mg, 72% yield); mp 285-286 °C; 
$^1$H NMR (400 MHz, DMSO-$d_6$) $\delta$ 12.19 (s, 1H), 7.68 (d, $J = 7.8$ Hz, 1H), 7.47 (t, $J = 7.4$ Hz, 1H), 7.26 (dd, $J = 11.8$, 7.7 Hz, 2H), 2.15 (d, $J = 12.0$ Hz, 3H), 1.78 (m, 2H), 1.57 (m, 8H), 1.40 (m, 3H), 1.19 (m, 1H). $^{13}$C NMR (101 MHz, DMSO-$d_6$) $\delta$ 166.4, 154.2, 132.1, 131.6, 130.0, 128.6, 123.3, 115.2, 113.8, 38.8, 32.9, 27.9, 27.4, 23.4. 

3-((4-phenylbutan-2-yl)quinoxalin-2(1H)-one (9). White solid (17.8 mg, 32% yield); mp 251-252 °C; 
$^1$H NMR (400 MHz, DMSO-$d_6$) $\delta$ 12.32 (s, 1H), 7.74 (dd, $J = 8.6$, 1.3 Hz, 1H), 7.48 (m 1H), 7.40 – 7.02 (m, 7H), 3.54 – 3.33 (m, 1H), 2.71 – 2.54 (m, 2H), 2.14 (m, 1H), 1.80 (m, 1H), 1.23 (d, $J = 6.8$ Hz, 3H). $^{13}$C NMR (101 MHz, DMSO-$d_6$) $\delta$ 165.3, 154.8, 142.6, 132.1, 132.0, 129.9, 128.7, 128.7, 126.1, 123.5, 115.6, 36.2, 35.0, 33.5, 18.7. 
HRMS-ESI (m/z): calcd for [M + H]$^+$ 279.1492, found 279.1491.

3-(7-ethyl-2-methylundecan-4-yl)quinoxalin-2(1H)-one (10). Yellow oil (39.7 mg, 58% yield); 
$^1$H NMR (400 MHz, DMSO-$d_6$) $\delta$ 12.29 (s, 1H), 7.69 (dd, $J = 8.0$, 0.8 Hz, 1H), 7.54 – 7.37 (m, 1H), 7.34 – 7.02 (m, 2H), 3.48 – 3.39 (m, 1H), 1.77 – 1.67 (m, 2H), 1.53 – 1.39 (m, 2H), 1.39 – 1.32 (m, 1H), 1.20 – 1.08 (m, 12H), 0.86 – 0.83 (m,
3H), 0.82 – 0.78 (m, 4H), 0.77 – 0.75 (m, 1H), 0.74 – 0.69 (m, 3H). $^{13}$C NMR (101 MHz, DMSO-$d_6$) δ 165.4, 155.1, 132.2, 131.8, 129.8, 128.5, 123.4, 115.6, 43.2, 38.4, 32.7, 30.8, 30.4, 28.9, 26.1, 25.9, 23.5, 22.8, 14.4, 11.2, 10.9.

HRMS-ESI (m/z): calcd for [M + H]$^+$ 343.2744, found 343.2743.

3-cyclohexylquinoxalin-2(1H)-one (11). White solid (39.2 mg, 86% yield); mp 252-253 °C; $^1$H NMR (400 MHz, DMSO-$d_6$) δ 12.31 (s, 1H), 7.70 (d, $J$ = 7.7 Hz, 1H), 7.53 – 7.35 (m, 1H), 7.27 (d, $J$ = 7.6 Hz, 2H), 3.17 (m, 1H), 1.83 (m, 4H), 1.71 (m, 1H), 1.39 (m, 4H), 1.23 (m, 1H). $^{13}$C NMR (101 MHz, DMSO-$d_6$) δ 165.3, 154.6, 132.1, 131.9, 129.8, 128.6, 123.5, 115.6, 39.9, 30.5, 26.3, 26.2. HRMS-ESI (m/z): calcd for [M + H]$^+$ 229.1335, found 229.1335.

3-cyclooctylquinoxalin-2(1H)-one (12). White solid (46.6 mg, 91% yield); mp 278-279 °C; $^1$H NMR (400 MHz, DMSO-$d_6$) δ 12.30 (s, 1H), 7.69 (d, $J$ = 7.8 Hz, 1H), 7.44 (m, 1H), 7.24 (m, 2H), 3.40 (m, 1H), 1.86 – 1.65 (m, 6H), 1.55 (m, 8H). $^{13}$C NMR (101 MHz, DMSO-$d_6$) δ 166.6, 154.5, 132.0, 129.6, 128.6, 123.4, 115.5, 39.3, 30.4, 26.7, 26.5, 25.8. HRMS-ESI (m/z): calcd for [M + H]$^+$ 257.1648, found 257.1649.

3-cyclododecylquinoxalin-2(1H)-one (13). White solid (35.0 mg, 56% yield); mp 284-285 °C; $^1$H NMR (500 MHz, DMSO-$d_6$) δ 12.31 (s, 1H), 7.70 (d, $J$ = 7.7 Hz, 1H), 7.53 – 7.35 (m, 1H), 7.27 (d, $J$ = 7.6 Hz, 2H), 3.17 (m, 1H), 1.83 (m, 4H), 1.71 (m, 1H), 1.39 (m, 4H), 1.23 (m, 1H). $^{13}$C NMR (101 MHz, DMSO-$d_6$) δ 165.4, 155.1, 132.2, 131.8, 129.8, 128.5, 123.4, 115.6, 43.2, 38.4, 32.7, 30.8, 30.4, 28.9, 26.1, 25.9, 23.5, 22.8, 14.4, 11.2, 10.9.

HRMS-ESI (m/z): calcd for [M + H]$^+$ 343.2744, found 343.2743.
MHz, DMSO) δ 12.29 (s, 1H), 7.72 (d, J = 7.7 Hz, 1H), 7.46 (t, J = 7.3 Hz, 1H), 7.37 – 7.03 (m, 2H), 3.56 (d, J = 5.5 Hz, 1H), 1.67 (s, 4H), 1.59 – 1.12 (m, 22H). 13C NMR (101 MHz, DMSO-d6) δ 165.4, 154.5, 132.0, 130.0, 128.6, 123.4, 115.5, 35.0, 28.1, 23.9, 23.7, 23.4, 23.1, 22.9. HRMS-ESI (m/z): calcd for [M + H]+ 313.2274, found 313.2273.

3-(tetrahydrofuran-3-yl)quinoxalin-2(1H)-one (14). White solid (31.6 mg, 73% yield); mp 122-123 °C; 1H NMR (500 MHz, DMSO-d6) δ 12.40 (s, 1H), 7.73 (dd, J = 8.0, 1.0 Hz, 1H), 7.52 – 7.47 (m, 1H), 7.29 (m, 2H), 4.05 (t, J = 7.5 Hz, 1H), 3.90 – 3.72 (m, 4H), 2.31 (m, 1H), 2.23 – 2.12 (m, 1H). 13C NMR (126 MHz, DMSO-d6) δ 161.8, 155.1, 132.2, 131.7, 130.1, 128.7, 123.6, 115.7, 70.9, 68.1, 41.7, 29.85. HRMS-ESI (m/z): calcd for [M + H]+ 217.0972, found 217.0967.

tert-butyl 3-(3-oxo-3,4-dihydroquinoxalin-2-yl)pyrrolidine-1-carboxylate (15). White solid (52.3 mg, 83% yield); mp 171-172 °C; 1H NMR (500 MHz, DMSO-d6) δ 12.41 (s, 1H), 7.71 (d, J = 7.9 Hz, 1H), 7.61 – 7.43 (m, 1H), 7.41 – 7.19 (m, 2H), 3.82 (m, 1H), 3.70 – 3.59 (m, 1H), 3.53 (m, 1H), 3.48 – 3.40 (m, 1H), 3.35 – 3.28 (m, 1H), 2.32 – 2.19 (m, 1H), 2.16 – 2.05 (m, 1H), 1.41 (s, 9H). 13C NMR (126 MHz, DMSO) δ 161.2, 161.0, 154.9, 154.0, 132.3, 131.8, 130.2, 128.8, 123.6, 115.7, 78.7, 49.1, 49.0, 45.9, 45.7, 41.0, 29.7, 28.7. HRMS-ESI (m/z): calcd for [M + H]+ 316.1656, found 316.1654.
3-(2,3-dihydro-1H-inden-2-yl)quinoxalin-2(1H)-one (16). White solid (44.6 mg, 85% yield); mp 272-273 °C; $^1$H NMR (400 MHz, DMSO-$d_6$) δ 12.41 (s, 1H), 7.70 (dd, $J = 8.0, 1.1$ Hz, 1H), 7.60 – 7.41 (m, 1H), 7.41 – 7.23 (m, 4H), 7.19 – 7.08 (m, 2H), 4.31 – 3.97 (m, 1H), 3.30 (dd, $J = 9.6, 7.4$ Hz, 4H). $^{13}$C NMR (101 MHz, DMSO-$d_6$) δ 163.3, 155.1, 142.6, 132.3, 131.8, 130.0, 128.7, 126.7, 124.7, 123.6, 115.6, 41.9, 36.8. HRMS-ESI (m/z): calcd for [M + H]$^+$ 263.1179, found 263.1180.

3-(4,4-difluorocyclohexyl)quinoxalin-2(1H)-one (17). White solid (26.9 mg, 51% yield); mp 272-273 °C; $^1$H NMR (400 MHz, DMSO-$d_6$) δ 12.38 (s, 1H), 7.73 (d, $J = 7.8$ Hz, 1H), 7.50 – 7.46 (m, 1H), 7.27 (t, $J = 7.6$ Hz, 2H), 3.33 – 3.30 (m, 1H), 2.14 – 2.10 (m, 2H), 2.05 – 1.93 (m, 4H), 1.90 – 1.73 (m, 2H). $^{13}$C NMR (101 MHz, DMSO-$d_6$) δ 163.4, 154.5, 132.0, 132.0, 130.1, 128.7, 126.9, 124.5, (t, $J = 240.4$ Hz), 115.7, 37.4, 33.2 (t, $J = 22.7$ Hz), 26.7 (d, $J = 9.7$ Hz). HRMS-ESI (m/z): calcd for [M + H]$^+$ 265.1147, found 265.1145.

3-((1R,4R)-1,7,7-trimethylbicyclo[2.2.1]heptan-2-yl)quinoxalin-2(1H)-one (18). White solid (40.1 mg, 71% yield); mp 272-276 °C; dr = 1:1.3; $^1$H NMR (400 MHz, DMSO-$d_6$) δ 12.28 (s, 1H), 7.71 (dd, $J = 22.9, 7.8$ Hz, 1H), 7.47 (t, $J = 7.5$ Hz, 1H), 7.27 (d, $J = 7.7$ Hz, 2H), 3.47 (dd, $J = 21.7, 13.5$ Hz, 1H), 2.62 (s, 1H), 2.06 – 1.62 (m, 3H).
1.49 (m, 2H), 1.35 – 1.16 (m, 1H), 1.08 – 0.80 (m, 6H), 0.79 (s, 3H). $^{13}$C NMR (101 MHz, DMSO-$d_6$) δ 163.6, 163.4, 155.9, 155.8, 132.0, 131.8, 131.8, 131.6, 130.0, 129.9, 128.8, 128.5, 123.4, 115.5, 51.9, 51.4, 51.2, 48.7, 47.7, 45.5, 45.4, 44.0, 33.0, 32.7, 29.0, 28.2, 27.7, 21.5, 19.8, 19.2, 15.9, 13.1. HRMS-ESI (m/z): calcd for [M + H]$^+$ 283.1805, found 283.1802.

![3-benzylquinoxalin-2(1H)-one](image)

3-benzylquinoxalin-2(1H)-one (19). White solid (21.2 mg, 45% yield); mp 187-188 °C; $^1$H NMR (400 MHz, CDCl$_3$) δ 12.02 (s, 1H), 7.87 (d, $J = 8.1$ Hz, 1H), 7.49 (t, $J = 15.9$ Hz, 3H), 7.39 – 7.15 (m, 5H), 4.32 (s, 2H). $^{13}$C NMR (101 MHz, CDCl$_3$) δ 159.8, 156.3, 137.0, 132.9, 131.2, 129.9, 129.5, 128.4, 126.6, 124.1, 115.5, 40.0. HRMS-ESI (m/z): calcd for [M + Na]$^+$ 259.0847, found 259.0846.

![3-(thiophen-2-ylmethyl)quinoxalin-2(1H)-one](image)

3-(thiophen-2-ylmethyl)quinoxalin-2(1H)-one (20). White solid (27.6 mg, 57% yield); mp 104-105 °C; $^1$H NMR (400 MHz, DMSO-$d_6$) δ 11.10 (s, 1H), 8.05 (s, 1H), 7.80 (dd, $J = 2.9$, 1.1 Hz, 1H), 7.70 – 7.49 (m, 3H), 7.38 (d, $J = 4.9$ Hz, 1H), 7.15 (dd, $J = 4.7$, 1.5 Hz, 1H), 5.14 (s, 2H). $^{13}$C NMR (101 MHz, DMSO-$d_6$) δ 153.7, 140.6, 137.9, 137.8, 128.4, 128.0, 127.6, 127.2, 125.3, 125.0, 61.3. HRMS-ESI (m/z): calcd for [M + H]$^+$ 243.0592, found 243.0591.

![3-(naphthalen-2-ylmethyl)quinoxalin-2(1H)-one](image)

3-(naphthalen-2-ylmethyl)quinoxalin-2(1H)-one (21). White solid (29.2 mg, 51% yield); mp 219-220 °C; $^1$H NMR (500 MHz, DMSO) δ 12.40 (s, 1H), 7.94 – 7.77 (m, 4H), 7.73 (d, $J = 8.0$ Hz, 1H), 7.58 – 7.41 (m, 4H), 7.37
– 7.19 (m, 2H), 4.31 (s, 2H). $^{13}$C NMR (126 MHz, DMSO) $\delta$ 160.7, 155.0, 135.6, 133.5, 132.5, 132.2, 132.1, 130.2, 128.7, 128.3, 128.2, 127.9, 127.9, 127.7, 126.5, 126.0, 123.6, 115.8, 64.6.

3-phenethylquinoxalin-2(1H)-one (22). White solid (21.0 mg, 42% yield); mp 212-213 °C; $^1$H NMR (500 MHz, DMSO) $\delta$ 12.36 (s, 1H), 7.84 – 7.66 (m, 1H), 7.64 – 7.44 (m, 1H), 7.36 – 7.23 (m, 6H), 7.19 (m, 1H), 3.10 (m, 2H), 3.07 – 3.00 (m, 2H). $^{13}$C NMR (126 MHz, DMSO) $\delta$ 161.3, 155.1, 142.0, 132.2, 132.0, 123.0, 128.8, 128.8, 128.6, 126.3, 123.6, 115.7, 35.0, 32.2.

3-(tert-butyl)-6,7-dimethylquinoxalin-2(1H)-one (23). White solid (42.3 mg, 92% yield); mp 225-226 °C; $^1$H NMR (DMSO-$d_6$, 400 MHz): $\delta$ (ppm) 12.07 (s, 1H), 7.49 (s, 1H), 7.03 (s, 1H), 2.29 (s, 3H), 2.27 (s, 3H), 1.39 (s, 9H); $^{13}$C NMR (DMSO-$d_6$, 101 MHz): $\delta$ (ppm) 164.4, 153.8, 138.8, 131.5, 130.0, 129.4, 128.4, 114.8, 38.6, 27.6, 19.7, 18.8. HRMS-ESI (m/z): calcd for [M + Na]$^+$ 253.1317, found 253.1319.

3-(tert-butyl)-6,7-difluoroquinoxalin-2(1H)-one (24). White solid (38.5 mg, 81% yield); $^1$H mp 221-222 °C; $^1$H NMR (DMSO-$d_6$, 400 MHz): $\delta$ (ppm) 12.32 (s, 1H), 7.74 (dd, $J = 11.1, 8.2$ Hz, 1H), 7.16 (dd, $J = 11.1, 7.6$ Hz, 1H), 1.38 (s, 9H); $^{13}$C NMR (DMSO-$d_6$, 101 MHz): $\delta$ (ppm) 166.5, 153.2, 149.9 (dd, $J = 249.2, 14.7$ Hz), 145.5 (dd, $J = 242.0, 14.1$ Hz), 129.3 (d, $J = 10.0$ Hz), 127.2 (d, $J = 9.1$ Hz), 116.1 (d, $J = 17.8$ Hz), 102.5 (d, $J = 21.8$ Hz), 38.8, 27.3; HRMS-ESI (m/z): calcd for [M + H]$^+$ 239.0996, found 239.0994.
3-(tert-butyl)-6,7-dichloroquinoxalin-2(1H)-one (25). White solid (46.4 mg, 86% yield); mp 242-243 °C; \(^1\)H NMR (DMSO-\(d_6\), 400 MHz): \(\delta\) (ppm) 12.38 (s, 1H), 7.88 (s, 1H), 7.39 (s, 1H), 1.39 (s, 9H); \(^{13}\)C NMR (DMSO-\(d_6\), 101 MHz): \(\delta\) (ppm) 167.7, 153.1, 131.8, 131.5, 130.4, 129.3, 124.6, 115.8, 39.0, 27.4; HRMS-ESI (m/z): calcd for [M + H\(^+\)]\(^+\) 271.0405, found 271.0400.

6,7-dibromo-3-(tert-butyl)quinoxalin-2(1H)-one (26). White solid (48.7 mg, 68% yield); mp 272-273 °C; \(^1\)H NMR (DMSO-\(d_6\), 400 MHz): \(\delta\) (ppm) 12.34 (s, 1H), 8.00 (s, 1H), 7.56 (s, 1H), 1.38 (s, 9H); \(^{13}\)C NMR (DMSO-\(d_6\), 101 MHz): \(\delta\) (ppm) 167.8, 153.1, 132.4, 132.3, 131.0, 124.2, 118.9, 116.4, 39.0, 27.4. HRMS-ESI (m/z): calcd for [M + H\(^+\)]\(^+\) 358.9395, found 358.9393.

3-(tert-butyl)-6-chloroquinoxalin-2(1H)-one (27). White solid (40.6 mg, 86% yield); mp 228-229 °C; \(^1\)H NMR (DMSO-\(d_6\), 400 MHz): \(\delta\) (ppm) 12.34 (s, 1H), 7.72 (d, \(J = 1.8\) Hz, 1H), 7.55 (dd, \(J = 8.7, 2.1\) Hz, 1H), 7.27 (d, \(J = 8.7\) Hz, 1H), 1.39 (s, 9H); \(^{13}\)C NMR (DMSO-\(d_6\), 101 MHz): \(\delta\) (ppm) 167.3, 153.4, 131.5, 130.9, 129.4, 127.4, 126.5, 116.4, 38.9, 27.4. HRMS-ESI (m/z): calcd for [M + H\(^+\)]\(^+\) 237.0795, found 237.0796.

6-bromo-3-(tert-butyl)quinoxalin-2(1H)-one (28). White solid (34.7 mg, 62% yield); mp 230-231 °C; \(^1\)H NMR (400 MHz, DMSO-\(d_6\)) \(\delta\) 12.34 (s, 1H), 7.86 (d, \(J = 2.2\) Hz, 1H), 7.62 (dd, \(J = 8.7, 2.2\) Hz, 1H), 7.22 (d, \(J = 8.7\) Hz,
$^1$H, 1.39 (s, 9H); $^{13}$C NMR (101 MHz, DMSO-d$_6$) δ 167.3, 153.4, 132.1, 131.9, 131.3, 130.4, 116.7, 114.1, 38.9, 27.4. HRMS-ESI (m/z): calcd for [M + H]$^+$ 281.0290, found 281.0289.

![3-(tert-butyl)-7-methoxyquinoxalin-2(1H)-one (29).](image)

White solid (34.4 mg, 74% yield); mp 260-261 °C; $^1$H NMR (400 MHz, DMSO-d$_6$) δ 12.09 (s, 1H), 7.59 (d, $J = 8.9$ Hz, 1H), 6.84 (dd, $J = 8.9$, 2.7 Hz, 1H), 6.73 (d, $J = 2.7$ Hz, 1H), 3.80 (s, 3H), 1.38 (s, 9H). $^{13}$C NMR (101 MHz, DMSO-d$_6$) δ 162.1, 160.0, 153.9, 133.4, 129.7, 125.8, 97.2, 55.5, 38.3, 27.6. HRMS-ESI (m/z): calcd for [M + H]$^+$ 233.1290, found 233.1291.

![7-bromo-3-(tert-butyl)quinoxalin-2(1H)-one (30).](image)

White solid (34.2 mg, 61% yield); mp 220-221 °C; $^1$H NMR (400 MHz, DMSO-d$_6$) δ 12.27 (s, 1H), 7.62 (d, $J = 8.5$ Hz, 1H), 7.41 (t, $J = 2.0$ Hz, 1H), 7.38 (dd, $J = 8.5$, 2.0 Hz, 1H), 1.39 (s, 9H). $^{13}$C NMR (101 MHz, DMSO-d$_6$) δ 166.4, 153.3, 133.2, 130.3, 129.9, 125.8, 122.1, 117.0, 38.8, 27.4. HRMS-ESI (m/z): calcd for [M + H]$^+$ 281.0290, found 281.0287.

![3-(tert-butyl)-1-methylquinoxalin-2(1H)-one (31).](image)

White solid (30.7 mg, 71% yield); mp 108-109 °C; $^1$H NMR (400 MHz, CDCl$_3$) δ 7.84 – 7.82 (m, 1H), 7.53 – 7.48 (m, 1H), 7.33 – 7.31 (m, 1H), 7.29 – 7.26 (m, 1H), 3.68 (s, 3H), 1.49 (s, 9H). $^{13}$C NMR (101 MHz, CDCl$_3$) δ 165.3, 153.8, 133.4, 132.2, 130.1, 129.5, 123.2, 113.3, 39.5, 28.8, 27.9. HRMS-ESI (m/z): calcd for [M + Na]$^+$ 239.1160, found 239.1158.
3-(tert-butyl)-1-(cyclopropylmethyl)quinoxalin-2(1H)-one (32). Yellow solid (34.8 mg, 68% yield); mp 155-156 °C; \(^1\)H NMR (CDCl\(_3\), 400 MHz): \(\delta\) (ppm) 7.75 (d, \(J = 8.2\), 1H), 7.76 – 7.74 (m, 1H), 7.32 (d, \(J = 8.2\) Hz, 1H), 7.20 (m, 1H), 4.11 (s, 1H), 4.09 (s, 1H), 1.40 (s, 9H), 1.20 – 1.17 (m, 1H), 0.47 (m, 4H); \(^{13}\)C NMR (CDCl\(_3\), 100 MHz): \(\delta\) (ppm) 164.4, 152.6, 131.7, 131.3, 129.3, 128.3, 121.9, 112.5, 44.5, 38.4, 26.9, 8.7, 3.0. HRMS-ESI (m/z): calcd for [M + H]\(^+\) 257.1654, found 257.1655.

ethyl 3-(3-(tert-butyl)-2-oxoquinoxalin-1(2H)-yl)propanoate (33). White solid (25.9 mg, 45% yield); mp 88-89 °C; \(^1\)H NMR (CDCl\(_3\), 400 MHz): \(\delta\) (ppm) 7.86 – 7.84 (m, 1H), 7.48 – 7.44 (m, 1H), 7.33 – 7.26 (m, 1H), 7.03 (d, \(J = 8.3\) Hz, 1H), 4.99 (s, 2H), 4.24 (q, \(J = 7.1\) Hz, 2H), 1.49 (s, 9H), 1.26 (t, \(J = 7.1\) Hz, 3H); \(^{13}\)C NMR (CDCl\(_3\), 100 MHz): \(\delta\) (ppm) 167.4, 165.1, 153.2, 132.5, 132.3, 130.4, 129.7, 123.5, 112.7, 61.92, 43.33, 39.5, 27.9, 14.1. HRMS-ESI (m/z): calcd for [M + Na]\(^+\) 311.1372, found 311.1370.

1-benzyl-3-(tert-butyl)quinoxalin-2(1H)-one (34). Yellow oil (33.3 mg, 57% yield); \(^1\)H NMR (CDCl\(_3\), 400 MHz): \(\delta\) (ppm) 7.83 (dd, \(J = 7.9, 1.5\) Hz, 1H), 7.38 – 7.32 (m, 1H), 7.32 – 7.16 (m, 7H), 5.47 (s, 2H), 1.53 (s, 9H); \(^{13}\)C NMR (CDCl\(_3\), 100 MHz): \(\delta\) (ppm) 165.5, 153.7, 135.7, 132.7, 132.5, 130.2, 129.5, 128.9, 127.5, 126.8, 123.2,
2-(3-(tert-butyl)-2-oxoquinoxalin-1(2H)-yl)acetonitrile (35). White solid (29.9 mg, 62% yield); mp 155-156 °C; 
$^1$H NMR (CDCl$_3$, 400 MHz): $\delta$ (ppm) 7.88 (dd, $J = 8.0, 1.3$ Hz, 1H), 7.63 – 7.53 (m, 1H), 7.47 – 7.34 (m, 1H), 7.27 (d, $J = 8.9$ Hz, 1H), 5.17 (s, 2H), 1.48 (s, 9H); $^{13}$C NMR (CDCl$_3$, 100 MHz): $\delta$ (ppm) 165.0, 152.2, 132.3, 131.2, 130.8, 130.3, 124.4, 114.0, 112.6, 39.7, 29.1, 27.8. HRMS-ESI (m/z): calcd for [M + Na]$^+$ 264.1113, found 264.1114.

3-(tert-butyl)-1-((tetrahydrofuran-2-yl)methyl)quinoxalin-2(1H)-one (36). White solid; (41.2 mg, 72% yield); mp 165-166 °C; $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.71 (m, 1H), 7.44 – 7.29 (m, 2H), 7.24 – 7.06 (m, 1H), 4.43 (dd, $J = 13.9, 4.4$ Hz, 1H), 4.23 (qd, $J = 6.9, 4.4$ Hz, 1H), 4.07 (dd, $J = 13.9, 7.0$ Hz, 1H), 3.88 – 3.76 (m, 1H), 3.63 (m, 1H), 2.05 – 1.94 (m, 1H), 1.94 – 1.75 (m, 2H), 1.68 (m, 1H), 1.39 (s, 9H); $^{13}$C NMR (101 MHz, CDCl$_3$) $\delta$ 164.0, 152.8, 132.1, 131.3, 129.1, 128.2, 122.0, 113.2, 75.9, 67.2, 45.0, 38.3, 28.6, 26.9, 24.4. HRMS-ESI (m/z): calcd for [M + H]$^+$ 287.17540, found 287.17538.

3-(tert-butyl)benzo[g]quinoxalin-2(1H)-one (37). White solid (43.9 mg, 87% yield); mp 241-242 °C; $^1$H NMR
(DMSO-$d_6$, 400 MHz): $\delta$ (ppm) 12.22 (s, 1H), 8.36 (s, 1H), 8.04 (d, $J = 8.2$ Hz, 1H), 7.92 (d, $J = 8.2$ Hz, 1H), 7.63
(s, 1H), 7.59 – 7.49 (m, 1H), 7.49 – 7.35 (m, 1H), 1.45 (s, 9H); $^{13}$C NMR (DMSO-$d_6$, 100 MHz): $\delta$ (ppm) 166.7,
153.6, 132.9, 130.8, 130.5, 129.3, 128.5, 127.5, 127.4, 126.6, 124.4, 109.8, 39.0, 27.7. HRMS-ESI (m/z): calcd for
[M + Na]$^+$ 275.1160, found 275.1161.

3-(tert-butyl)-5,6-diphenylpyrazin-2(1H)-one (38). Yellow solid (43.2 mg, 71% yield); mp 101-102 °C; $^1$H NMR
(400 MHz, DMSO-$d_6$) $\delta$ 12.21 (s, 1H), 7.40 – 7.31 (m, 5H), 7.24 – 7.16 (m, 5H), 1.42 (s, 9H). $^{13}$C NMR (101 MHz,
DMSO-$d_6$) $\delta$ 154.8, 138.4, 130.1, 129.6, 129.5, 128.9, 128.2, 127.2, 38.4, 27.9. HRMS-ESI (m/z): calcd for [M +
H]$^+$ 305.1648, found 305.1647.

2-cyclohexylquinazolin-4(3H)-one (39). White solid (24.2 mg, 53% yield); mp 214-215 °C; $^1$H NMR
(400 MHz, DMSO-$d_6$) $\delta$ 12.13 (s, 1H), 8.12 (dd, $J = 7.9$, 1.3 Hz, 1H), 7.80 (m, 1H), 7.64 (d, $J = 7.9$ Hz, 1H), 7.52 – 7.28 (m,
1H), 2.66 – 2.57 (m, 1H), 2.00 – 1.90 (m, 2H), 1.89 – 1.80 (m, 2H), 1.66 (m, 3H), 1.40 – 1.23 (m, 3H). $^{13}$C NMR
(101 MHz, DMSO-$d_6$) $\delta$ 162.4, 161.2, 149.4, 134.7, 127.4, 126.4, 126.1, 121.4, 43.3, 30.7, 26.0, 25.8.

Cyclohexylisoquinoline (40). White solid (17.7 mg, 42% yield); mp 45-46 °C; $^1$H NMR (400 MHz, CDCl$_3$) $\delta$
8.47 (d, J = 5.6 Hz, 1H), 8.20 (d, J = 8.3 Hz, 1H), 7.77 (d, J = 8.2 Hz, 1H), 7.61 – 7.55 (m, 2H), 7.53 – 7.44 (m, 1H), 3.55 (t, J = 11.5 Hz, 1H), 2.00 – 1.88 (m, 4H), 1.85 – 1.79 (m, 3H), 1.57 – 1.51 (m, 2H), 1.48 – 1.26 (m, 1H).

$^{13}$C NMR (101 MHz, CDCl₃) $\delta$ 165.7, 141.9, 136.4, 129.5, 127.5, 126.8, 126.3, 124.7, 118.9, 41.6, 32.6, 26.9, 26.3.

1,4-dicyclohexylphthalazine (41). White solid (16.5 mg, 28% yield); mp 107-108 °C; $^1$H NMR (400 MHz, CDCl₃) $\delta$ 8.16 (dd, J = 6.3, 3.3 Hz, 2H), 7.84 (dd, J = 6.3, 3.3 Hz, 2H), 3.50 – 3.43 (m, 2H), 2.04 – 1.91 (m, 12H), 1.87 – 1.76 (m, 2H), 1.55 – 1.45 (m, 4H), 1.44 – 1.35 (m, 2H).

$^{13}$C NMR (101 MHz, CDCl₃) $\delta$ 161.8, 131.1, 125.0, 124.2, 40.5, 32.3, 26.9, 26.3.

4-cyclohexyl-2-phenylquinazoline (42). White solid (39.2 mg, 68% yield); mp 103-104 °C; $^1$H NMR (400 MHz, CDCl₃) $\delta$ 8.68 – 8.66 (m, 2H), 8.15 – 8.06 (m, 2H), 7.82 (m, 1H), 7.60 – 7.48 (m, 4H), 3.57 (tt, J = 10.9, 3.6 Hz, 1H), 2.09 – 1.90 (m, 7H), 1.62 – 1.48 (m, 2H), 1.48 – 1.38 (m, 1H).

$^{13}$C NMR (101 MHz, CDCl₃) $\delta$ 174.7, 160.1, 151.0, 138.7, 133.1, 130.3, 129.6, 128.6, 128.5, 126.6, 124.1, 121.8, 41.5, 32.1, 26.6, 26.2.

6-cyclohexylphenanthridine (43). White solid (32.4 mg, 62% yield); mp 102-103 °C; $^1$H NMR (400 MHz, CDCl₃) $\delta$ 8.43 (d, J = 8.2 Hz, 1H), 8.33 (dd, J = 8.1, 0.8 Hz, 1H), 8.13 (d, J = 8.2 Hz, 1H), 8.02 (d, J = 8.1 Hz, 1H).
7.62 – 7.57 (m, 1H), 7.57 – 7.51 (m, 1H), 7.51 – 7.46 (m, 1H), 7.45 – 7.39 (m, 1H), 3.55 – 3.35 (m, 1H), 1.95 (d, J = 11.0 Hz, 2H), 1.89 – 1.75 (m, 4H), 1.71 (dd, J = 9.2, 4.3 Hz, 1H), 1.42 (m, 2H), 1.36 – 1.26 (m, 1H). 13C NMR (101 MHz, CDCl3) δ 164.1, 142.8, 131.9, 128.8, 128.8, 127.3, 125.9, 125.0, 124.5, 123.6, 122.2, 121.4, 120.7, 40.9, 31.2, 25.8, 25.3.

8-cyclohexyl-1,3,7-trimethyl-3,7-dihydro-1H-purine-2,6-dione (46). White solid (17.1 mg, 31% yield); mp 215-216 °C; 1H NMR (400 MHz, DMSO-d6) δ 3.87 (s, 3H), 3.38 (s, H), 3.20 (s, 3H), 2.88 (t, J = 11.3 Hz, 1H), 1.89 – 1.75 (m, 4H), 1.70 (d, J = 11.6 Hz, 1H), 1.53 (dd, J = 23.5, 11.3 Hz, 2H), 1.39 (dd, J = 25.0, 12.5 Hz, 2H), 1.31 – 1.24 (m, 1H). 13C NMR (101 MHz, DMSO-d6) δ 158.2, 155.0, 151.4, 147.9, 130.1, 106.6, 34.9, 31.6, 31.0, 29.8, 27.9, 25.8.

2-(2-(1-chlorocyclopropyl)-3-(2-chlorophenyl)-2-hydroxypropyl)-5-cyclohexyl-1,2-dihydro-3H-1,2,4-triazole-3-thione (47). Yellow oil (52.7 mg, 62% yield); 1H NMR (400 MHz, CDCl3) δ 7.89 (s, 1H), 7.53 (dd, J = 7.2, 2.1 Hz, 1H), 7.35 (dd, J = 7.3, 2.2 Hz, 1H), 7.24 – 7.14 (m, 2H), 4.91 – 4.80 (m, 1H), 4.77 (d, J = 0.9 Hz, 1H), 3.99 – 3.87 (m, 1H), 3.75 – 3.63 (m, 1H), 3.58 (dd, J = 14.1, 1.1 Hz, 1H), 3.08 (d, J = 14.1 Hz, 1H), 2.17 – 1.97 (m, 2H), 1.83 – 1.70 (m, 2H), 1.67 – 1.56 (m, 1H), 1.57 – 1.35 (m, 4H), 1.30 (m, 1H), 0.96 (m, 1H), 0.78 (m, 1H), 0.65 – 0.53 (m, 2H). 13C NMR (101 MHz, CDCl3) δ 153.9, 151.3, 135.1, 134.0, 133.8, 129.3, 128.2, 126.4, 75.8, 51.9, 47.8, 45.5, 38.1, 33.6, 33.3, 25.9, 25.9, 25.5, 10.9, 10.4. HRMS-ESI (m/z): calcd for [M + H]+ 426.1168, found
3-(2,2-dimethyl-propyl)-1,3-dimethylindolin-2-one (48). White solid (10.8 mg, 31% yield); mp 81-82 °C; $^1$H NMR (CDCl$_3$, 400 MHz): $\delta$ (ppm) 7.26 (t, $J = 7.7$ Hz, 1H), 7.20 (d, $J = 7.3$ Hz, 1H), 7.03 (t, $J = 7.5$ Hz, 1H), 6.85 (d, $J = 7.8$ Hz, 1H), 3.22 (s, 3H), 2.16 (d, $J = 14.4$ Hz, 1H), 1.86 (d, $J = 14.4$ Hz, 1H), 1.30 (s, 3H), 0.61 (s, 9H); $^{13}$C NMR (CDCl$_3$, 100 MHz): $\delta$ (ppm) 181.1, 142.9, 134.2, 127.5, 123.9, 122.0, 108.0, 50.8, 47.4, 31.8, 30.8, 28.3, 26.2.

3-oxo-3,4-dihydro-quinoxaline-2-carboxylic acid methyl ester (49). White solid (22.4 mg, 55% yield); mp 218-219 °C; $^1$H NMR (DMSO-$d_6$, 400 MHz): $\delta$ (ppm) 12.90 (s, 1H), 7.84 (d, $J = 8.0$ Hz, 1H), 7.66 (t, $J = 7.7$ Hz, 1H), 7.37 (t, $J = 8.8$ Hz, 2H), 3.91 (s, 3H); $^{13}$C NMR (DMSO-$d_6$, 101 MHz): $\delta$ (ppm) 164.0, 152.3, 150.1, 132.7, 132.4, 130.6, 129.2, 124.0, 115.8, 52.7. HRMS-ESI (m/z): calcd for [M + Na]$^+$ 227.0433, found 227.0435.

References:

7 General experimental procedure for the gram scale experiment

In glovebox, an undivided bottle was equipped with a carbon anode (20 mm×20 mm×3 mm) and a platinum plate electrode (20 mm×20 mm×0.3 mm) and connected to a DC regulated power supply. To the bottle was added 2-quinoxalinone (1000.0 mg, 6.8 mmol), tert-Butyl carbazate (2712.8 mg, 20.5 mmol), tetrabutylammonium hexafluorophosphate (5301.8 mg, 13.7 mmol) and 137 mL of DMSO/CH₃CN (3:1). The reaction mixture was stirred and electrolyzed at constant current conditions (32 mA) at 50 °C under argon atmosphere (The dual display potentiostat was operating in constant current mode) for 36 h. Once complete, the reaction was quenched with aqueous NaHCO₃ and extracted with EtOAc (50 mL × 3), the organic solvent was dried over Na₂SO₄. The solvent was evaporated under reduced pressure. The crude product was purified by silica gel column chromatography.

(eluent: hexane /ethyl acetate= 3:1)
**8 Radical Trapping Experiments**

**Electrochemical conditions:** An undivided three-necked bottle was equipped with a carbon anode (10 mm×10 mm×3 mm) and a platinum plate electrode (10mm×10mm×0.3mm) and connected to a DC regulated power supply. To the bottle was added 2-quinoxalinone (29.2 mg, 0.2 mmol), tert-butyl carbazate (79.3 mg, 0.6 mmol), tetrabutylammonium hexafluorophosphate (155.0 mg, 0.4 mmol), 2,2,6,6-tetramethylpiperidine-1-oxyl (93.8 mg, 0.6 mmol) and 4 mL of DMSO/CH₃CN. The reaction mixture was stirred and electrolyzed at constant current of 6 mA at 50 °C under argon atmosphere (The dual display potentiostat was operating in constant current mode) for 8 h. No product was detected on LC-MS.

**Chemical oxidant conditions:** A mixture of tert-butyl carbazate (26.4 mg, 0.2 mmol), 2,2,6,6-tetramethylpiperidine-1-oxyl (93.8 mg, 0.6 mmol) and Na₂S₂O₆ (95.2 mg, 0.4 mmol) in CH₃CN (2 mL) was stirred at 50 °C under Ar for 1 h. LC-MS showed peaks for TMEPO-OCO-tBu and TEMPO-tBu species. This is clean evidence for the fragmentation of carbazate that follows the proposed pathway from tBuOCO radical to t-butyl radical.
An undivided three-necked bottle was equipped with a carbon anode (10 mm×10 mm×3 mm) and a platinum plate electrode (10mm×10mm×0.3mm) and connected to a DC regulated power supply. To the bottle was added N-methyl-N-phenylmethacrylamide (35.0 mg, 0.2 mmol), tert-butyl carbazate (79.3 mg, 0.6 mmol), tetrabutylammonium hexafluorophosphate (155.0 mg, 0.4 mmol), and 4 mL of CH₃CN. The reaction mixture was stirred and electrolyzed at constant current conditions (6 mA) at 80 °C under argon atmosphere (The dual display potentiostat was operating in constant current mode) for 8 h. Once complete, the reaction was quenched with 1M Sodium hydroxide solution. and extracted with EtOAc (50 mL × 3), the organic solvent was dried over Na₂SO₄. The solvent was evaporated under reduced pressure. The crude product was purified by silica gel column chromatography. (eluent: petroleum ether/ethyl acetate = 5:1).
An undivided three-necked bottle was equipped with a carbon anode (10 mm×10 mm×3 mm) and a platinum plate electrode (10 mm×10 mm×0.3 mm) and connected to a DC regulated power supply. To the bottle was added 2-quinoxalinone (29.2 mg, 0.2 mmol), methyl hydrazinecarboxylate (54.0 mg, 0.6 mmol), tetrabutylammonium hexafluorophosphate (155.0 mg, 0.4 mmol), and 4 mL of DMSO/CH₃CN. The reaction mixture was stirred and electrolyzed at constant current conditions (6 mA) at 50 °C under argon atmosphere (The dual display potentiostat was operating in constant current mode) for 8 h. Once complete, the reaction was quenched with 1M Sodium hydroxide solution and extracted with EtOAc (50 mL × 3), the organic solvent was dried over Na₂SO₄. The solvent was evaporated under reduced pressure. The crude product was purified by silica gel column chromatography (eluent: petroleum ether/ethyl acetate= 5:1).
9 NMR Spectra

Y1 (¹H NMR)
Solvent: CDCl₃

Y1 (¹³C NMR)
Solvent: CDCl₃
Y2 (1H NMR)
Solvent: CDCl₃

Y2 (13C NMR)
Solvent: CDCl₃
Y3 (1H NMR)
Solvent: DMSO-δ6

Y3 (13C NMR)
Solvent: DMSO-δ6
Y4 (³¹H NMR)
Solvent: CDCl₃

Y4 (³¹C NMR)
Solvent: CDCl₃
Y5 (¹H NMR)
Solvent: CDCl₃

Y5 (¹³C NMR)
Solvent: CDCl₃
Y6 ($^1$H NMR)
Solvent: DMSO-d$_6$

Y6 ($^{13}$C NMR)
Solvent: DMSO-d$_6$
Y7 ($^1$H NMR)
Solvent: CDCl$_3$

Y7 ($^{13}$C NMR)
Solvent: CDCl$_3$
Y8 (1H NMR)
Solvent: DMSO-d$_6$

H$_2$N
\[
\begin{array}{c}
\text{O} \\
\text{C} \\
\text{O} \\
\text{H}
\end{array}
\]

Y8 (13C NMR)
Solvent: DMSO-d$_6$
Y9 (¹H NMR)
Solvent: DMSO-d₆

Y9 (¹³C NMR)
Solvent: DMSO-d₆
Y10 (¹H NMR)
Solvent: CDCl₃

Y10 (¹³C NMR)
Solvent: CDCl₃
Y11 (¹H NMR)
Solvent: CDCl₃

Y11 (¹³C NMR)
Solvent: CDCl₃
Y12 (1H NMR)
Solvent: CDCl₃

Y12 (13C NMR)
Solvent: CDCl₃
Y13 (¹H NMR)
Solvent: DMSO-d$_6$

Y13 (¹³C NMR)
Solvent: DMSO-d$_6$
Y14 ($^1$H NMR)
Solvent: DMSO-$d_6$

Y14 ($^{13}$C NMR)
Solvent: DMSO-$d_6$
Y15 (\(^1\)H NMR)
Solvent: CDCl\(_3\)

Y15 (\(^13\)C NMR)
Solvent: CDCl\(_3\)
Y16 (¹H NMR)
Solvent: CDCl₃

Y16 (¹³C NMR)
Solvent: CDCl₃
Y17 (¹H NMR)
Solvent: DMSO-d₆

Y17 (¹³C NMR)
Solvent: DMSO-d₆
$2 \left(^{1}H \text{ NMR}\right)$

Solvent: CDCl$_3$

$2 \left(^{13}C \text{ NMR}\right)$

Solvent: CDCl$_3$
3 (¹H NMR)
Solvent: CDCl₃

3 (¹³C NMR)
Solvent: CDCl₃
4 (\textsuperscript{1}H NMR)
Solvent: CDCl\textsubscript{3}

4 (\textsuperscript{13}C NMR)
Solvent: CDCl\textsubscript{3}
5 ($^1$H NMR)
Solvent: CDCl$_3$

5 ($^{13}$C NMR)
Solvent: CDCl$_3$
6 (1H NMR)
Solvent: DMSO-d6

6 (13C NMR)
Solvent: DMSO-d6
7 (\textsuperscript{1}H NMR)
 Solvent: DMSO-d\textsubscript{6}

7 (\textsuperscript{13}C NMR)
 Solvent: DMSO-d\textsubscript{6}
8 (\textsuperscript{1}H NMR)
Solvent: DMSO-d\textsubscript{6}

8 (\textsuperscript{13}C NMR)
Solvent: DMSO-d\textsubscript{6}
10 (¹H NMR)
Solvent: DMSO-d₆

10 (¹³C NMR)
Solvent: DMSO-d₆
11 (¹H NMR)  
Solvent: DMSO-d$_6$

11 (¹³C NMR)  
Solvent: DMSO-d$_6$
S60

12 (¹H NMR)
Solvent: DMSO-d₆

12 (¹³C NMR)
Solvent: DMSO-d₆
13 (¹H NMR)
Solvent: DMSO-d₆

13 (¹³C NMR)
Solvent: DMSO-d₆ with a drop of conc. HCl
14(\(^1\)H NMR)
Solvent: DMSO-\(d_6\)

14(\(^{13}\)C NMR)
Solvent: DMSO-\(d_6\)
$^{1}H$ NMR
Solvent: DMSO-$d_6$

$^{13}C$ NMR
Solvent: DMSO-$d_6$
16 ($^1$H NMR)
Solvent: DMSO-d$_6$

16 ($^{13}$C NMR)
Solvent: DMSO-d$_6$
17 (^1H NMR)
Solvent: DMSO-d6

17 (^13C NMR)
Solvent: DMSO-d6
18 \text{ dr} = 1:1.3 \text{ (}^1\text{H NMR)}
Solvent: \text{ DMSO-d}_6

18 \text{ dr} = 1:1.3 \text{ (}^{13}\text{C NMR)}
Solvent: \text{ DMSO-d}_6
19 (1H NMR)
Solvent: DMSO-d$_6$

19 (13C NMR)
Solvent: DMSO-d$_6$
20 (\textsuperscript{1}H NMR)  
Solvent: DMSO-\textsubscript{d$_6$}
21 ($^1$H NMR)
Solvent: DMSO-$d_6$

21 ($^{13}$C NMR)
Solvent: DMSO-$d_6$
22 $^1$H NMR
Solvent: DMSO-$_d_6$

22 $^{13}$C NMR
Solvent: DMSO-$_d_6$
23 (\(^1\)H NMR)
Solvent: DMSO-\(d_6\)

21 (\(^13\)C NMR)
Solvent: DMSO-\(d_6\)
24 (¹H NMR)
Solvent: DMSO-d₆

24 (¹³C NMR)
Solvent: DMSO-d₆
25 ($^1$H NMR)
Solvent: DMSO-$d_6$

25 ($^{13}$C NMR)
Solvent: DMSO-$d_6$
26 ($^1$H NMR)
Solvent: DMSO-$d_6$

26 ($^{13}$C NMR)
Solvent: DMSO-$d_6$
27 ($^1$H NMR)
Solvent: DMSO-d$_6$

27 ($^{13}$C NMR)
Solvent: DMSO-d$_6$
28 (¹H NMR)
Solvent: DMSO-d₆

28 (¹³C NMR)
Solvent: DMSO-d₆
29 (¹H NMR)
Solvent: DMSO-d₆

29 (¹³C NMR)
Solvent: DMSO-d₆
30 ($^1$H NMR)
Solvent: DMSO-$d_6$

30 ($^{13}$C NMR)
Solvent: DMSO-$d_6$
$^{1}H$ NMR
Solvent: CDCl$_3$

$^{13}C$ NMR
Solvent: CDCl$_3$
32 (\(^1\)H NMR)
Solvent: CDCl\(_3\)

32 (\(^{13}\)C NMR)
Solvent: CDCl\(_3\)
33 (\textsuperscript{1}H NMR)
Solvent: CDCl\textsubscript{3}

33 (\textsuperscript{13}C NMR)
Solvent: CDCl\textsubscript{3}
34 (\textsuperscript{1}H NMR)
Solvent: CDCl\textsubscript{3}

34 (\textsuperscript{13}C NMR)
Solvent: CDCl\textsubscript{3}
$^{1}H$ NMR
Solvent: CDCl$_3$

$^{13}C$ NMR
Solvent: CDCl$_3$
36 (\textsuperscript{1}H NMR)
Solvent: CDCl\textsubscript{3}

36 (\textsuperscript{13}C NMR)
Solvent: CDCl\textsubscript{3}
37 ($^1$H NMR)
Solvent: DMSO-$d_6$
38 (\(^1\)H NMR)
Solvent: DMSO-d\(_6\)

38 (\(^{13}\)C NMR)
Solvent: DMSO-d\(_6\)
39 ($^1$H NMR)
Solvent: DMSO-$d_6$

39 ($^{13}$C NMR)
Solvent: DMSO-$d_6$
40 (1H NMR)
Solvent: CDCl$_3$

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40 (1H NMR)
Solvent: CDCl$_3$
41 \(^1\text{H NMR}\)
Solvent: CDCl\(_3\)

41 \(^{13}\text{C NMR}\)
Solvent: CDCl\(_3\)
42 ($^1$H NMR)  
Solvent: CDCl$_3$

42 ($^{13}$C NMR)  
Solvent: CDCl$_3$
43 (¹H NMR)
Solvent: CDCl₃

43 (¹³C NMR)
Solvent: CDCl₃
46 (1H NMR)
Solvent: DMSO-d$_6$

46 (13C NMR)
Solvent: DMSO-d$_6$
47 (1H NMR)
Solvent: CDCl₃

47 (1³C NMR)
Solvent: CDCl₃
48 ($^1$H NMR)
Solvent: CDCl$_3$

48 ($^{13}$C NMR)
Solvent: CDCl$_3$
49 (1H NMR)
Solvent: DMSO-d$_6$

49 (13C NMR)
Solvent: DMSO-d$_6$