Supplementary Information

Visible-light photoredox-catalyzed four component reaction for the construction of sulfone-containing quinoxalin-2(1H)-ones

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1. General information

All commercially available reagent grade chemicals were purchased from Adamas, Strem, MERYER, Alfa Aesar and Energy Chemical Company and used as received without further purification unless otherwise stated. $^1$H NMR and $^{13}$C NMR were recorded in CDCl$_3$ on a Bruker Avance III 500MHz or 400 MHz spectrometer with TMS as internal standard at room temperature, the chemical shifts ($\delta$) were expressed in ppm and $J$ values were given in Hz. The following abbreviations are used to indicate the multiplicity: singlet (s), doublet (d), triplet (t), quartet (q), doublet of doublets (dd), doublet of triplets (dt), and multiplet (m). All first order splitting patterns were assigned on the basis of the appearance of the multiplet. Splitting patterns that could not be easily interpreted were designated as multiplet (m). High-resolution mass spectra (HRMS) were obtained on an LTQ Orbitrap XL mass spectrometry equipped with an ESI source. Column chromatography was performed on silica gel (200-300 mesh).
2. General procedure for visible-light photoredox-catalyzed four component reaction leading to sulfone-containing quinoxalin-2(1H)-ones.

\[
\begin{align*}
\text{R}_1^1 & \text{N} & + \text{R}_2^2 & \rightarrow & \text{ArN}_2\text{BF}_4^4 + \text{Na}_2\text{S}_2\text{O}_5^5 & \text{Rose Bengal (1 mol\%)} \\
& & & & & 3\text{W Blue LEDs}, \\
& & & & & \text{DCE, rt, N}_2, 12\text{h} &
\end{align*}
\]

A mixture of quinoxalin-2(1H)-ones 1 (0.1 mmol), arylazidoniumtetrafluoroborate 3 (0.2 mmol), Na\textsubscript{2}S\textsubscript{2}O\textsubscript{5} 4 (0.3 mmol), and Rose Bengal (1 mol\%), and DCE(2 mL) in a tube (20 mL). Then, the tube was filled with N\textsubscript{2}. Alkene 2 (0.2 mmol) and DCE (2 mL) was added in tube under nitrogen atmosphere. The reaction mixture was stirred and irradiated by 3 W blue LEDs at room temperature for 12h. After completion of the reaction, the reaction mixture was concentrated in vacuum. The residue was purified by flash column chromatography using a mixture of petroleum ether and ethyl acetate as eluent to give the desired product 5.

3. Preliminary mechanistic studies

3.1 The addition of TEMPO in the model reaction system.

A mixture of 1-methylquinoxalin-2(1H)-one (1a), phenylazidoniumtetrafluoroborate (3a), Na\textsubscript{2}S\textsubscript{2}O\textsubscript{5} (4), Rose Bengal (1 mol\%), and TEMPO (0.2 mmol) in a 20mL tube. Then, the tube was filled with N\textsubscript{2}. Styrene 2a (0.2 mmol) and DCE (2 mL) were added in tube under nitrogen atmosphere. The reaction mixture was stirred and irradiated by 3 W blue LEDs at room temperature for
12h. After completion of the reaction, the reaction mixture was concentrated in vacuum. None of the desired product 5a was detected and TEMPO trapped complexes A and B were detected by LC-MS. The above result indicated that a radical process should be involved in this reaction.

2. On/off experiments.

A mixture of 1-methylquinoxalin-2(1H)-one (1a),
phenyldiazoniumtetrafluoroborate (3a), Na₂S₂O₅ (4), and Rose Bengal (1 mol%) in a 20mL tube. Then, the tube was filled with N₂. Styrene 2a and DCE (2 mL) were added in tube under nitrogen atmosphere. The reaction mixture was stirred and irradiated by 3 W blue LEDs at room temperature under nitrogen atmosphere for 3h, the corresponding product was isolated in 36% yield. The reaction mixture was stirred and irradiated by 3 W blue LEDs at room temperature under nitrogen atmosphere for 3h, then the reaction mixture was continuously stirred in the dark for 3h, the desired product was obtained in 36.1% yield. Furthermore, when the reaction mixture was stirred and irradiated by 3 W blue LEDs at room temperature under nitrogen atmosphere for 6h, the desired product was isolated in 57% yield. Moreover, the reaction mixture was stirred and irradiated by 3 W blue LEDs at room temperature under nitrogen atmosphere for 6h, then the reaction mixture was continuously stirred in the dark for 3h, the desired product was obtained in 57% yield. The above results indicated that the continuous visible light irradiation is essential for promoting this transformation (Fig. S1).

![Fig. S1 On/off experiments](image)

4. Characterization data of products
1,6-dimethyl-3-(1-phenyl-2-(phenylsulfonyl)ethyl)-5-vinylpyrazin-2(1H)-one (5a). \(^1\)H NMR (500 MHz, CDCl\(_3\)): \(\delta\) 7.82 (d, \(J = 8.0\) Hz, 2H), 7.77 (d, \(J = 8.0\) Hz, 1H), 7.53 - 7.49 (m, 1H), 7.38 - 7.30 (m, 6H), 7.21 (t, \(J = 7.9\) Hz, 3H), 7.17 - 7.14 (m, 1H), 5.28 (dd, \(J_1 = 3.4\) Hz, \(J_2 = 10.0\) Hz, 1H), 4.79 (dd, \(J_1 = 10.0\) Hz, \(J_2 = 14.4\) Hz, 1H), 3.64 (dd, \(J_1 = 3.4\) Hz, \(J_2 = 14.4\) Hz, 1H), 3.57 (s, 3H); \(^{13}\)C NMR (125 MHz, CDCl\(_3\)): \(\delta\) 157.4, 153.9, 144.2, 139.6, 139.0, 138.5, 133.8, 133.0, 132.1, 130.2, 130.0, 129.4, 128.8, 128.4, 128.3, 127.5, 123.5, 113.4, 59.4, 42.1, 29.1; ESI HRMS: calculated for C\(_{23}\)H\(_{21}\)N\(_2\)O\(_3\)S [M+H]\(^+\) 405.1273, found 405.1261.

1-methyl-3-(1-phenyl-2-tosylethyl)quinoxalin-2(1H)-one (5b). \(^1\)H NMR(500 MHz, CDCl\(_3\)): \(\delta\) 7.74 (d, \(J = 8.0\) Hz, 1H), 7.68 (d, \(J = 8.0\) Hz, 2H), 7.47 (t, \(J = 7.8\) Hz, 1H), 7.34 - 7.30 (m, 3H), 7.23 - 7.19 (m, 4H), 7.05 (d, \(J = 8.2\) Hz, 2H), 5.26 (dd, \(J_1 = 3.0\) Hz, \(J_2 = 10.2\) Hz, 1H), 4.78 (dd, \(J_1 = 10.0\) Hz, \(J_2 = 14.4\) Hz, 1H), 3.60 (dd, \(J_1 = 3.0\) Hz, \(J_2 = 14.4\) Hz, 1H), 3.56 (s, 3H), 2.17 (s, 3H); \(^{13}\)C NMR (125 MHz, CDCl\(_3\)): \(\delta\) 157.4, 153.9, 144.2, 139.6, 139.0, 138.5, 133.8, 133.0, 132.1, 130.2, 130.0, 129.4, 128.8, 128.4, 128.3, 127.5, 123.5, 113.4, 59.4, 42.1, 29.1, 21.4; ESI HRMS: calculated for C\(_{24}\)H\(_{23}\)N\(_2\)O\(_3\)S [M+H]\(^+\) 419.1429, found 419.1438.

1-methyl-3-(1-phenyl-2-(m-tolylsulfonyl)ethyl)quinoxalin-2(1H)-one (5c). \(^1\)H NMR(500 MHz, CDCl\(_3\)): \(\delta\) 7.76 - 7.74 (m, 1H), 7.62 (d, \(J = 8.0\) Hz, 1H), 7.68 (d, \(J = 8.0\) Hz, 2H), 7.47 (t, \(J = 7.8\) Hz, 1H), 7.34 - 7.30 (m, 3H), 7.23 - 7.19 (m, 3H), 7.17 - 7.15 (m, 2H), 7.08 (d, \(J = 7.6\) Hz, 1H), 5.27 (dd, \(J_1 = 3.4\) Hz, \(J_2 = 10.0\) Hz, 1H), 4.78 (dd, \(J_1 = 10.2\) Hz, \(J_2 = 14.4\) Hz, 1H), 3.62 (dd, \(J_1 = 3.0\) Hz, \(J_2 = 14.4\) Hz, 1H), 3.55 (s, 3H), 2.18 (s, 3H); \(^{13}\)C NMR (125 MHz, CDCl\(_3\)): \(\delta\) 157.4, 153.8, 139.2, 139.0, 138.5, 133.8, 133.0, 132.1, 130.3, 130.0, 128.8, 128.7, 128.6, 128.3, 127.5, 125.5, 123.5, 113.4, 59.4, 42.2, 29.1, 21.0; ESI HRMS: calculated for C\(_{24}\)H\(_{23}\)N\(_2\)O\(_3\)S [M+H]\(^+\) 419.1429, found 419.1464.
1-methyl-3-(1-phenyl-2-(o-tolylsulfonyl)ethyl)quinoxalin-2(1H)-one (5d), 
$^{1}$HNMR (500 MHz, CDCl$_3$): $\delta$ 7.89 - 7.87 (m, 1H), 7.76 (d, $J = 7.9$ Hz, 1H), 7.50 (t, $J = 7.8$ Hz, 1H), 7.36 (d, $J = 7.4$ Hz, 2H), 7.31 (t, $J = 7.6$ Hz, 1H), 7.22 (t, $J = 7.6$ Hz, 2H), 7.16 (t, $J = 7.8$ Hz, 2H), 7.13 - 7.10 (m, 2H), 6.89 - 6.88 (m, 1H), 5.28 (dd, $J_1 = 3.4$ Hz, $J_2 = 10.0$ Hz, 1H), 4.88 (dd, $J_1 = 10.0$ Hz, $J_2 = 14.4$ Hz, 1H), 3.62 (dd, $J_1 = 3.0$ Hz, $J_2 = 14.4$ Hz, 1H), 3.59 (s, 3H), 2.67 (s, 3H); $^{13}$C NMR (125 MHz, CDCl$_3$): $\delta$ 157.4, 153.7, 138.6, 138.5, 137.1, 133.1, 132.9, 132.2, 131.9, 130.5, 130.3, 129.8, 128.8, 128.3, 127.5, 126.0, 123.5, 113.5, 58.3, 42.0, 29.0, 20.5; ESI HRMS: calculated for C$_{24}$H$_{22}$N$_2$NaO$_3$S [M+Na]$^+$ 441.1249, found 441.1283.

3-(2-((4-methoxyphenyl)sulfonyl)-1-phenylethyl)-1-methylquinoxalin-2(1H)-one (5e), $^1$H NMR (400 MHz, CDCl$_3$): $\delta$ 7.78 - 7.76 (m, 1H), 7.71 (d, $J = 8.8$ Hz, 2H), 7.53 - 7.49 (m, 1H), 7.35 - 7.30 (m, 3H), 7.24 - 7.14 (m, 4H), 6.69 (d, $J = 8.8$ Hz, 2H), 5.27 (dd, $J_1 = 3.4$ Hz, $J_2 = 10.0$ Hz, 1H), 4.78 (dd, $J_1 = 10.2$ Hz, $J_2 = 14.4$ Hz, 1H), 3.64 (s, 3H), 3.62 (dd, $J_1 = 3.0$ Hz, $J_2 = 14.4$ Hz, 1H), 3.56 (s, 3H); $^{13}$C NMR (100 MHz, CDCl$_3$): $\delta$ 163.2, 157.5, 153.8, 138.6, 133.0, 132.2, 130.7, 130.6, 130.1, 130.0, 128.8, 128.3, 127.5, 123.5, 113.9, 113.4, 59.6, 55.4, 42.2, 29.0; ESI HRMS: calculated for C$_{24}$H$_{23}$N$_2$O$_4$S [M+H]$^+$ 435.1379, found 435.1415.

3-(2-((4-fluorophenyl)sulfonyl)-1-phenylethyl)-1-methylquinoxalin-2(1H)-one (5f), $^1$H NMR (400 MHz, CDCl$_3$): $\delta$ 7.82 - 7.77 (m, 3H), 7.55 - 7.51 (m, 1H), 7.36 - 7.32 (m, 3H), 7.23 - 7.16 (m, 4H), 6.96 (t, $J = 8.6$ Hz, 2H), 6.69 (d, $J = 8.8$ Hz, 2H), 5.27 (dd, $J_1 = 3.8$ Hz, $J_2 = 10.0$ Hz, 1H), 4.75 (dd, $J_1 = 10.0$ Hz, $J_2 = 14.4$ Hz, 1H), 3.67 (dd, $J_1 = 3.8$ Hz, $J_2 = 14.4$ Hz, 1H), 3.58 (s, 3H); $^{13}$C NMR (100 MHz, CDCl$_3$): $\delta$ 165.4 (d, $J = 254.6$ Hz), 157.4, 153.8, 138.2, 135.4 (d, $J = 3.2$ Hz), 133.0, 132.1, 131.2 (d, $J = 9.5$ Hz), 130.5, 130.0, 128.8, 128.3, 127.6, 123.7, 116.0 (d, $J = 22.5$ Hz), 113.6, 59.5, 42.1, 29.1; ESI HRMS: calculated for C$_{23}$H$_{20}$FN$_2$O$_3$S [M+H]$^+$ 423.1179, found 423.1202.
3-(2-((4-chlorophenyl)sulfonyl)-1-phenylethyl)-1-methylquinoxalin-2(1H)-one (5g). $^1$H NMR (400 MHz, CDCl$_3$): $\delta$ 7.76 - 7.74 (m, 1H), 7.70 (d, $J = 8.6$ Hz, 2H), 7.55 - 7.50 (m, 1H), 7.36 - 7.33 (m, 3H), 7.23 - 7.15 (m, 6H), 6.69 (d, $J = 8.8$ Hz, 2H), 5.24 (dd, $J_1 = 3.4$ Hz, $J_2 = 10.0$ Hz, 1H), 4.76 (dd, $J_1 = 10.2$ Hz, $J_2 = 14.4$ Hz, 1H), 3.66 (dd, $J_1 = 3.4$ Hz, $J_2 = 14.4$ Hz, 1H), 3.57 (s, 3H); $^{13}$C NMR (100 MHz, CDCl$_3$): $\delta$ 157.2, 153.7, 140.0, 138.2, 137.7, 133.0, 132.0, 129.9, 129.0, 128.8, 128.3, 127.6, 123.7, 113.6, 59.5, 42.2, 29.1; ESI HRMS: calculated for C$_{23}$H$_{20}$ClN$_2$O$_3$S [M+H]$^+$ 439.0883, found 439.0901.

3-(2-((4-bromophenyl)sulfonyl)-1-phenylethyl)-1-methylquinoxalin-2(1H)-one (5h). $^1$H NMR (400MHz, CDCl$_3$): $\delta$ 7.76 - 7.74 (m, 1H), 7.63 (d, $J = 8.6$ Hz, 2H), 7.56 - 7.51 (m, 1H), 7.38 - 7.33 (m, 5H), 7.24 - 7.17 (m, 4H), 6.69 (d, $J = 8.8$ Hz, 2H), 5.24 (dd, $J_1 = 3.4$ Hz, $J_2 = 10.0$ Hz, 1H), 4.77 (dd, $J_1 = 10.0$ Hz, $J_2 = 14.4$ Hz, 1H), 3.64 (dd, $J_1 = 3.4$ Hz, $J_2 = 14.4$ Hz, 1H), 3.58 (s, 3H); $^{13}$C NMR (100 MHz, CDCl$_3$): $\delta$ 157.2, 153.7, 138.2, 138.1, 132.9, 132.0, 130.5, 130.0, 129.9, 128.8, 128.3, 127.6, 123.8, 113.7, 59.4, 42.2, 29.1; ESI HRMS: calculated for C$_{23}$H$_{20}$BrN$_2$O$_3$S [M+H]$^+$ 483.0378, found 483.0412.

Methyl4-((2-(4-methyl-3-oxo-3,4-dihydroquinoxalin-2-yl)-2-phenylethyl)sulfonyl)benzoate (5i). $^1$H NMR(400MHz, CDCl$_3$): $\delta$ 7.91 - 7.84 (m, 4H), 7.71 - 7.69 (m, 1), 7.51 - 7.47 (m, 1H), 7.34 - 7.29 (m, 3H), 7.23 - 7.14 (m, 4H), 5.28 (dd, $J_1 = 3.4$ Hz, $J_2 = 10.0$ Hz, 1H), 4.77 (dd, $J_1 = 10.1$ Hz, $J_2 = 14.4$ Hz, 1H), 3.89 (s, 3H), 3.67 (dd, $J_1 = 3.4$ Hz, $J_2 = 14.4$ Hz, 1H), 3.57 (s, 3H); $^{13}$C NMR (100 MHz, CDCl$_3$): $\delta$ 165.2, 157.1, 153.8, 143.1, 138.1, 134.1, 132.9, 131.9, 130.3, 129.9, 129.9, 128.9, 128.4, 128.3, 127.7, 123.6, 113.5, 59.4, 52.5, 42.1, 29.1; ESI HRMS: calculated for C$_{25}$H$_{23}$N$_2$O$_5$S [M+H]$^+$ 463.1328, found 463.1306.
1-methyl-3-(1-phenyl-2-((4-(trifluoromethyl)phenyl)sulfonyl)ethyl)quinoxalin-2(1H)-one (5j). $^1$H NMR (400 MHz, CDCl$_3$): $\delta$ 7.90 (d, $J = 8.2$ Hz, 2H), 7.72 - 7.70 (m, 1H), 7.54 - 7.49 (m, 3H), 7.34 - 7.31 (m, 3H), 7.22 - 7.16 (m, 4H), 5.28 (dd, $J_1 = 3.4$ Hz, $J_2 = 10.0$ Hz, 1H), 4.77 (dd, $J_1 = 10.1$ Hz, $J_2 = 14.4$ Hz, 1H), 3.73 (dd, $J_1 = 3.4$ Hz, $J_2 = 14.4$ Hz, 1H), 3.55 (s, 3H); $^{13}$C NMR (100 MHz, CDCl$_3$): $\delta$ 157.0, 153.7, 142.8, 137.9, 134.7 (q, $J = 33.9$ Hz), 132.9, 131.8, 130.6, 129.8, 129.0, 128.8, 128.3, 127.7, 125.8(q, $J = 3.6$ Hz), 123.8, 113.6, 59.3, 42.2, 29.0; ESI HRMS: calculated for C$_{24}$H$_{23}$F$_3$N$_2$O$_3$S [M+H]$^+$ 473.1147, found 473.1150.

1-methyl-3-(2-(phenylsulfonyl)-1-(p-tolyl)ethyl)quinoxalin-2(1H)-one (5k). $^1$H NMR (400 MHz, CDCl$_3$): $\delta$ 7.82 - 7.80 (m, 2H), 7.77 - 7.75 (m, 1H), 7.52 - 7.48 (m, 1H), 7.38 - 7.29 (m, 4H), 7.20 (t, $J = 8.3$ Hz, 3H), 7.01 (d, $J = 8.0$ Hz, 2H), 5.24 (dd, $J_1 = 3.4$ Hz, $J_2 = 10.0$ Hz, 1H), 4.77 (dd, $J_1 = 10.0$ Hz, $J_2 = 14.4$ Hz, 1H), 3.63 (dd, $J_1 = 3.4$ Hz, $J_2 = 14.4$ Hz, 1H), 3.56 (s, 3H), 2.23 (s, 3H); $^{13}$C NMR (100 MHz, CDCl$_3$): $\delta$ 157.5, 153.9, 139.4, 137.3, 135.4, 133.0, 132.1, 130.2, 130.0, 129.5, 128.8, 128.3, 128.2, 123.5, 113.5, 59.4, 41.8, 29.1, 21.0; ESI HRMS: calculated for C$_{24}$H$_{23}$N$_2$O$_3$S [M+H]$^+$ 419.1429, found 419.1436.

1-methyl-3-(2-(phenylsulfonyl)-1-(m-tolyl)ethyl)quinoxalin-2(1H)-one (5l). $^1$H NMR (400 MHz, CDCl$_3$): $\delta$ 7.82 - 7.76 (m, 3H), 7.53 - 7.49 (m, 1H), 7.38 - 7.29 (m, 4H), 7.20 (d, $J = 8.2$ Hz, 1H), 7.13 - 7.07 (m, 3H) 6.96 (d, $J = 7.0$ Hz, 1H), 5.24 (dd, $J_1 = 3.4$ Hz, $J_2 = 10.0$ Hz, 1H), 4.78 (dd, $J_1 = 10.0$ Hz, $J_2 = 14.4$ Hz, 1H), 3.63 (dd, $J_1 = 3.4$ Hz, $J_2 = 14.4$ Hz, 1H), 3.57 (s, 3H), 2.23 (s, 3H); $^{13}$C NMR (100 MHz, CDCl$_3$): $\delta$ 157.5, 153.9, 139.4, 138.4, 138.3, 133.0, 132.1, 130.2, 130.1, 129.0, 128.8, 128.6, 128.3, 125.3, 123.5, 113.5, 59.4, 42.0, 29.1, 21.4. ESI HRMS: calculated for C$_{24}$H$_{23}$N$_2$O$_3$S [M+H]$^+$ 419.1429, found 419.1416.

3-(1-(4-(tert-butyl)phenyl)-2-(phenylsulfonyl)ethyl)-1,6-dimethyl-5-vinylpyrazin-2(1H)-one (5m). $^1$H NMR (400 MHz, CDCl$_3$): $\delta$ 7.82 - 7.76 (m, 3H), 7.52 -7.48 (m, 1H), 7.35 - 7.28 (m, 4H), 7.24 - 7.18 (m, 5H), 5.26 (dd, $J_1 = 3.4$ Hz, $J_2 = 10.0$ Hz, 1H), 4.78 (dd, $J_1 = 10.0$ Hz, $J_2 = 14.4$ Hz, 1H), 3.66 (dd, $J_1 = 3.4$ Hz, $J_2 = 14.4$ Hz, 1H), 3.57 (s, 3H), 1.22 (s, 9H); $^{13}$C NMR (100 MHz, CDCl$_3$): $\delta$ 157.6, 153.9, 150.3, 139.4,
135.3, 133.0, 132.2, 130.2, 128.8, 128.3, 127.9, 125.7, 123.5, 113.4, 59.3, 41.6, 34.4, 31.2, 29.1; ESI HRMS: calculated for C_{27}H_{29}N_{2}O_{3}S \ [M+H]^+ 461.1899, found 461.1967.

3-(1-(4-fluorophenyl)-2-(phenylsulfonyl)ethyl)-1-methylquinoxalin-2(1H)-one (5n), \(^1\)H NMR (400 MHz, CDCl\(_3\)): \(\delta\) 7.81 - 7.76 (m, 3H), 7.55 - 7.51 (m, 1H), 7.40 - 7.28 (m, 6H), 7.22 (d, \(J = 8.3\) Hz, 1H), 6.88 (t, \(J = 8.7\) Hz, 2H), 5.27 (dd, \(J_1 = 4.1\) Hz, \(J_2 = 10.0\) Hz, 1H), 4.69 (dd, \(J_1 = 10.0\) Hz, \(J_2 = 14.4\) Hz, 1H), 3.65 (dd, \(J_1 = 4.1\) Hz, \(J_2 = 14.4\) Hz, 1H), 3.58 (s, 3H); \(^{13}\)C NMR (100 MHz, CDCl\(_3\)): \(\delta\) 162.1 (d, \(J = 245.1\) Hz), 157.3, 153.8, 139.3, 134.0 (d, \(J = 3.2\) Hz), 133.1, 133.0, 132.1, 130.4, 130.0 (d, \(J = 9.3\) Hz), 128.9, 128.3, 123.6, 115.6 (d, \(J = 21.4\) Hz), 113.5, 59.3, 41.4, 29.1; ESI HRMS: calculated for C_{23}H_{20}FN_{2}O_{3}S \ [M+H]^+ 423.1179, found 423.1196.

3-(1-(4-bromophenyl)-2-(phenylsulfonyl)ethyl)-1-methylquinoxalin-2(1H)-one (5o), \(^1\)H NMR (400 MHz, CDCl\(_3\)): \(\delta\) 7.80 - 7.76 (m, 3H), 7.55 - 7.51 (m, 1H), 7.41 - 7.38 (m, 1H), 7.35 - 7.30 (m, 5H), 7.21 (t, \(J = 8.1\) Hz, 3H), 5.24 (dd, \(J_1 = 4.3\) Hz, \(J_2 = 9.2\) Hz, 1H), 4.67 (dd, \(J_1 = 9.2\) Hz, \(J_2 = 14.4\) Hz, 1H), 3.66 (dd, \(J_1 = 4.3\) Hz, \(J_2 = 14.4\) Hz, 1H), 3.58 (s, 3H); \(^{13}\)C NMR (100 MHz, CDCl\(_3\)): \(\delta\) 157.0, 153.8, 139.3, 137.3, 133.2, 133.0, 132.1, 131.8, 130.5, 130.1, 130.1, 128.9, 128.2, 123.7, 121.7, 113.6, 59.1, 41.7, 29.1; ESI HRMS: calculated for C_{23}H_{20}BrN_{2}O_{3}S \ [M+H]^+ 483.0378, found 483.0392.

3-(1-(3-fluorophenyl)-2-(phenylsulfonyl)ethyl)-1-methylquinoxalin-2(1H)-one (5p), \(^1\)H NMR (500 MHz, CDCl\(_3\)): \(\delta\) 7.81 (d, \(J = 7.3\) Hz, 2H), 7.77 (d, \(J = 7.9\) Hz, 1H), 7.53 (t, \(J = 7.8\) Hz, 1H), 7.39 - 7.37 (m, 1H), 7.34 - 7.32 (m, 3H), 7.22 (d, \(J = 8.4\) Hz, 1H), 7.19 - 7.13 (m, 2H), 7.08 (d, \(J = 9.8\) Hz, 1H), 6.87 - 6.83 (m, 1H), 5.28 (dd, \(J_1 = 3.8\) Hz, \(J_2 = 10.0\) Hz, 1H), 4.71 (dd, \(J_1 = 10.0\) Hz, \(J_2 = 14.4\) Hz, 1H), 3.66 (dd, \(J_1 = 3.8\) Hz, \(J_2 = 14.4\) Hz, 1H), 3.58 (s, 3H); \(^{13}\)C NMR (125 MHz, CDCl\(_3\)): \(\delta\) 162.8 (d, \(J = 245.3\) Hz), 156.9, 153.8, 140.8 (d, \(J = 7.2\) Hz), 139.2, 133.2, 133.1, 132.1, 130.6, 130.3 (d, \(J = 8.2\) Hz), 130.1, 128.9, 128.3, 124.2 (d, \(J = 2.8\) Hz), 123.7, 115.2 (d, \(J = 21.9\) Hz), 114.6 (d, \(J = 20.9\) Hz), 113.6, 59.2, 41.8, 29.2; ESI HRMS: calculated for C_{23}H_{20}F2N_{2}O_{3}S \ [M+H]^+ 423.1179, found 423.1222.
3-(1-(3-chlorophenyl)-2-(phenylsulfonyl)ethyl)-1-methylquinoxalin-2(1H)-one (5q), $^1$H NMR (400 Hz, CDCl$_3$): $\delta$ 7.81 - 7.78 (m, 3H), 7.53 (t, $J = 7.3$ Hz, 2H), 7.39 - 7.32 (m, 4H), 7.26 - 7.21 (m, 3H), 7.17 - 7.11 (m, 2H), 5.25 (ddd, $J_1 = 4.1$ Hz, $J_2 = 10.0$ Hz, 1H), 4.69 (ddd, $J_1 = 10.0$ Hz, $J_2 = 14.4$ Hz, 1H), 3.65 (ddd, $J_1 = 4.1$ Hz, $J_2 = 14.4$ Hz, 1H), 3.59 (s, 3H); 13C NMR (100 MHz, CDCl$_3$): $\delta$ 156.9, 153.8, 140.3, 139.3, 134.5, 133.2, 132.1, 130.6, 130.2, 130.0, 128.9, 128.3, 128.3, 127.8, 126.8, 123.7, 113.6, 59.1, 41.8, 29.2; ESI HRMS: calculated for C$_{23}$H$_{20}$ClN$_2$O$_3$S [M+H]$^+$ 439.0883, found 439.0920.

3-(1-(4-chlorophenyl)-2-(phenylsulfonyl)ethyl)-1-methylquinoxalin-2(1H)-one (5r), $^1$H NMR (500 Hz, CDCl$_3$): $\delta$ 7.79 - 7.75 (m, 3H), 7.54 - 7.51 (m, 2H), 7.40 - 7.37 (m, 1H), 7.34 - 7.31 (m, 3H), 7.26 (d, $J = 8.5$ Hz, 2H), 7.21 (d, $J = 8.4$ Hz, 1H), 7.16 (d, $J = 8.5$ Hz, 2H), 5.25 (ddd, $J_1 = 4.3$ Hz, $J_2 = 9.2$ Hz, 1H), 4.67 (ddd, $J_1 = 9.2$ Hz, $J_2 = 14.4$ Hz, 1H), 3.66 (ddd, $J_1 = 4.3$ Hz, $J_2 = 14.4$ Hz, 1H), 3.57 (s, 3H); 13C NMR (125 MHz, CDCl$_3$): $\delta$ 157.1, 153.8, 139.3, 136.8, 133.5, 133.2, 133.0, 132.1, 130.5, 130.1, 129.8, 128.9, 128.3, 128.3, 123.7, 113.6, 59.2, 41.6, 29.2; ESI HRMS: calculated for C$_{23}$H$_{20}$ClN$_2$O$_3$S [M+H]$^+$ 439.0883, found 439.0854.

4-(1-(4-methyl-3-oxo-3,4-dihydroquinoxalin-2-yl)-2-(phenylsulfonyl)ethyl)benzonitrile (5s), $^1$H NMR (400 Hz, CDCl$_3$): $\delta$ 7.81 - 7.77 (m, 3H), 7.58 - 7.54 (m, 1H), 7.51 - 7.45 (m, 4H), 7.44 - 7.40 (m, 1H), 7.37 - 7.33 (m, 3H), 7.24 (d, $J = 8.5$ Hz, 1H), 5.33 (ddd, $J_1 = 4.7$ Hz, $J_2 = 8.8$ Hz, 1H), 4.64 (ddd, $J_1 = 8.8$ Hz, $J_2 = 14.4$ Hz, 1H), 3.69 (ddd, $J_1 = 4.7$ Hz, $J_2 = 14.4$ Hz, 1H), 3.59 (s, 3H); 13C NMR (100 MHz, CDCl$_3$): $\delta$ 156.4, 153.7, 143.6, 139.2, 133.4, 133.1, 132.5, 132.0, 130.9, 130.1, 129.3, 129.0, 128.2, 123.9, 118.5, 113.7, 111.5, 58.8, 42.3, 29.2; ESI HRMS: calculated for C$_{24}$H$_{20}$N$_3$O$_3$S [M+H]$^+$ 430.1225, found 430.1237.
1-methyl-3-(2-(phenylsulfonyl)-1-(4-trifluoromethyl)phenyl)ethyl)quinoxalin-2(1H)-one (5t), \(^1\)H NMR (400Hz, CDCl\(_3\)): \(\delta\) 7.80 - 7.77 (m, 3H), 7.56 - 7.52 (m, 1H), 7.47 - 7.43 (m, 4H), 7.41 - 7.30 (m, 4H), 7.23 (d, \(J = 8.3\) Hz, 1H), 5.35 (dd, \(J_1 = 4.6\) Hz, \(J_2 = 8.9\) Hz, 1H), 4.68 (dd, \(J_1 = 8.9\) Hz, \(J_2 = 14.4\) Hz, 1H), 3.72 (dd, \(J_1 = 4.6\) Hz, \(J_2 = 14.4\) Hz, 1H), 3.59 (s, 3H); \(^{13}\)C NMR (100 MHz, CDCl\(_3\)): \(\delta\) 156.8, 153.8, 142.2, 139.2, 133.3, 133.1, 132.1, 130.7, 130.1, 129.8 (d, \(J = 32.3\) Hz), 128.9, 128.8, 128.2, 125.6 (q, \(J = 3.7\) Hz), 123.9 (d, \(J = 270.5\) Hz), 123.8, 113.6, 59.0, 42.1, 29.2; ESI HRMS: calculated for C\(_{24}\)H\(_{23}\)F\(_3\)N\(_2\)O\(_3\)S [M+H\(^+\)] 473.1147, found 473.1121.

1-methyl-3-(2-(phenylsulfonyl)-1-(o-tolyl)ethyl)quinoxalin-2(1H)-one (5u), \(^1\)H NMR (400 Hz, CDCl\(_3\)): \(\delta\) 7.87 - 7.81 (m, 3H), 7.55 - 7.51 (m, 1H), 7.41 - 7.32 (m, 4H), 7.22 (d, \(J = 8.3\) Hz, 1H), 7.08 - 7.03 (m, 2H), 6.96 (t, \(J = 7.4\) Hz, 1H), 5.48 (dd, \(J_1 = 2.6\) Hz, \(J_2 = 10.3\) Hz, 1H), 4.79 (dd, \(J_1 = 10.3\) Hz, \(J_2 = 14.4\) Hz, 1H), 3.58 (s, 3H), 3.41 (dd, \(J_1 = 2.6\) Hz, \(J_2 = 14.4\) Hz, 1H), 2.48 (s, 3H); \(^{13}\)C NMR (100 MHz, CDCl\(_3\)): \(\delta\) 157.6, 154.1, 139.1, 136.9, 136.8, 133.1, 133.0, 132.0, 131.0, 130.3, 128.9, 128.4, 127.4, 127.1, 126.1, 123.6, 113.5, 59.2, 37.4, 29.1, 19.5; ESI HRMS: calculated for C\(_{24}\)H\(_{23}\)N\(_2\)O\(_3\)S [M+H\(^+\)] 419.1429, found 419.1413.

1-methyl-3-(1-phenyl-3-(phenylsulfonyl)propan-2-yl)quinoxalin-2(1H)-one (5v), \(^1\)H NMR (400 Hz, CDCl\(_3\)): \(\delta\) 7.77 - 7.74 (m, 1H), 7.70 - 7.74 (m, 1H), 7.55 - 7.51 (m, 1H), 7.39 - 7.31 (m, 2H), 7.30 - 7.24 (m, 3H), 7.19 - 7.15 (m, 3H), 7.08 - 7.06 (m, 2H), 4.33 - 4.27 (m, 1H), 4.25 - 4.21 (m, 1H), 3.64 (s, 3H), 3.28 (dd, \(J_1 = 1.8\) Hz, \(J_2 = 13.9\) Hz, 1H), 3.13 (dd, \(J_1 = 5.1\) Hz, \(J_2 = 13.9\) Hz, 1H), 2.69 (t, \(J = 9.7\) Hz, \(J_2 = 13.9\) Hz, 1H); \(^{13}\)C NMR (100 MHz, CDCl\(_3\)): \(\delta\) 158.9, 154.1, 133.0, 132.9, 132.3, 130.3, 129.9, 129.1, 128.7, 128.6, 128.3, 126.7, 123.6, 113.5, 56.1, 39.0, 38.9, 29.1; ESI HRMS: calculated for C\(_{24}\)H\(_{23}\)N\(_2\)O\(_3\)S [M+H\(^+\)] 419.1429, found 419.1397.

1-methyl-3-(4-phenyl-1-(phenylsulfonyl)butan-2-yl)quinoxalin-2(1H)-one (5w), \(^1\)H NMR (400 Hz, CDCl\(_3\)): \(\delta\) 7.81 - 7.79 (m, 2H), 7.76 - 7.74 (m, 1H), 7.70 - 7.68 (m, 2H), 7.56 - 7.52 (m, 1H), 7.41 - 7.37 (m, 1H), 7.32 (t, \(J = 7.4\) Hz, 3H), 7.21 (d, \(J = 8.4\) Hz, 1H), 7.15 (t, \(J = 7.2\) Hz, 2H), 7.09 - 7.07 (m, 1H), 7.04 (d, \(J = 8.2\) Hz, 2H), 4.31 (dd, \(J_1 = 10.0\) Hz, \(J_2 = 14.4\) Hz, 1H), 4.06 - 4.02 (m, 1H), 3.58 (s, 3H), 3.40 (dd, \(J_1 = 3.1\) Hz, \(J_2 = 14.4\) Hz, 1H), 2.68 - 2.60 (m, 1H), 2.53 - 2.46 (m, 1H), 2.23 - 2.15 (m, 1H), 2.02 - 1.93 (m, 1H);
$^{13}$C NMR (100 MHz, CDCl$_3$): $\delta$ 159.2, 154.2, 140.9, 139.1, 133.1, 133.0, 132.2, 130.2, 129.9, 128.8, 128.4, 128.3, 128.2, 125.9, 123.5, 113.4, 58.3, 37.5, 35.2, 33.1, 29.0; ESI HRMS: calculated for C$_{25}$H$_{25}$N$_2$O$_3$S [M+H]$^+$ 433.1586, found 433.1580.

![Structural Diagram]

1-ethyl-3-(1-phenyl-2-(phenylsulfonyl)ethyl)quinoxalin-2(1H)-one (5x), $^1$H NMR (500 Hz, CDCl$_3$): $\delta$ 7.81 - 7.80 (m, 2H), 7.77 - 7.75 (m, 1H), 7.52 - 7.48 (m, 1H), 7.34 - 7.26 (m, 6H), 7.21 (t, $J$ = 7.3 Hz, 3H), 7.16 (t, $J$ = 7.2 Hz, 1H), 5.30 - 5.27 (m, 1H), 4.82 - 4.77 (m, 1H), 4.26 - 4.18 (m, 1H), 4.16 - 4.08 (m, 1H), 1.29 (t, $J$ = 7.2 Hz, 3H); $^{13}$C NMR (125 MHz, CDCl$_3$): $\delta$ 157.4, 153.3, 139.3, 138.6, 133.1, 132.4, 131.9, 130.3, 130.3, 128.9, 128.8, 128.3, 127.5, 123.3, 113.3, 59.4, 42.0, 37.5, 12.3; ESI HRMS: calculated for C$_{24}$H$_{23}$N$_2$O$_3$S [M+H]$^+$ 419.1429, found 429.1426.

1-butyl-3-(1-phenyl-2-(phenylsulfonyl)ethyl)quinoxalin-2(1H)-one (5y), $^1$H NMR (400 Hz, CDCl$_3$): 67.95-7.89 (m, 1H), 7.82-7.79 (m, 2H), 7.76 (dd, $J_1$ = 1.3 Hz, $J_2$ = 8.0 Hz, 1H), 7.52-7.46 (m, 1H), 7.34 - 7.26 (m, 6H), 7.22-7.15 (m, 3H), 5.28 (dd, $J_1$ = 3.4 Hz, $J_2$ = 10.0 Hz, 1H), 4.78 (dd, $J_1$ = 10.0 Hz, $J_2$ = 14.4 Hz, 1H), 4.20-4.12 (m, 1H), 4.07-3.99 (m, 1H), 3.64 (dd, $J_1$ = 3.4 Hz, $J_2$ = 14.4 Hz, 1H), 1.69-1.61 (m, 2H), 1.47-1.40 (m, 2H), 0.97 (s, 3H); $^{13}$C NMR (100 MHz, CDCl$_3$): $\delta$ 157.4, 153.6, 139.4, 138.6, 133.0, 132.4, 132.2, 130.3, 130.2, 128.9, 128.8, 128.3, 127.4, 123.3, 113.5, 59.4, 42.3, 42.0, 29.2, 20.3, 13.8. ESI HRMS: calculated for C$_{26}$H$_{27}$N$_2$O$_3$S [M+H]$^+$ 447.1742, found 447.1750.

1-benzyl-3-(1-phenyl-2-(phenylsulfonyl)ethyl)quinoxalin-2(1H)-one (5z), $^1$H NMR (400 Hz, CDCl$_3$): $\delta$ 7.82 (d, $J$ = 7.1 Hz, 2H), 7.74 (dd, $J_1$ = 1.4 Hz, $J_2$ = 8.0 Hz, 1H), 7.38-7.33 (m, 3H), 7.26 - 7.23 (m, 9H), 7.18-7.15 (m, 4H), 5.46 (d, $J$ = 15.6 Hz, 1H), 5.35 (dd, $J_1$ = 3.4 Hz, $J_2$ = 10.0 Hz, 1H), 5.22 (d, $J$ = 15.6 Hz, 1H), 4.81 (dd, $J_1$ = 10.0 Hz, $J_2$ = 14.4 Hz, 1H), 3.66 (dd, $J_1$ = 3.4 Hz, $J_2$ = 14.4 Hz, 1H); $^{13}$C NMR (100 MHz, CDCl$_3$): $\delta$ 157.6, 154.1, 139.4, 138.5, 135.1, 133.2, 132.4, 132.3, 130.3, 130.2, 128.9, 128.8, 128.3, 128.3, 127.8, 127.6, 127.0, 123.6, 114.3, 59.4, 46.0, 42.2. ESI HRMS: calculated for C$_{29}$H$_{25}$N$_2$O$_3$S [M+H]$^+$ 481.1586, found 481.1595.
1,6,7-trimethyl-3-(1-phenyl-2-(phenylsulfonyl)ethyl)quinoxalin-2(1H)-one(5a’),
$^1$H NMR (400 Hz, CDCl$_3$): $\delta$ 7.82 - 7.80 (m, 2H), 7.54 (s, 1H), 7.39 - 7.36 (m, 1H), 7.34 - 7.30 (m, 4H), 7.21 - 7.14 (m, 3H), 6.96 (s, 1H), 5.24 (dd, $J_1$ = 3.7 Hz, $J_2$ = 9.8 Hz, 1H), 4.75 (dd, $J_1$ = 10.0 Hz, $J_2$ = 14.4 Hz, 1H), 3.64 (dd, $J_1$ = 3.7 Hz, $J_2$ = 14.4 Hz, 1H), 3.54 (s, 3H), 2.40 (s, 3H), 2.34 (s, 3H); $^{13}$C NMR (100 MHz, CDCl$_3$): $\delta$ 156.1, 153.9, 140.1, 139.4, 138.7, 133.0, 132.4, 131.1, 130.6, 130.1, 128.8, 128.7, 128.3, 128.3, 127.4, 114.0, 59.4, 42.0, 29.0, 20.6, 19.1; ESI HRMS: calculated for C$_{25}$H$_{25}$N$_2$O$_3$S [M+H]$^+$ 433.1586, found 433.1596.

1-methyl-3-(1-phenyl-2-(phenylsulfonyl)ethyl)-6-(trifluoromethyl)quinoxalin-2(1H)-one(5b’), $^1$H NMR (400 Hz, CDCl$_3$): $\delta$ 8.04 (s, 1H), 7.84 - 7.82 (m, 2H), 7.75 - 7.72 (m, 1H), 7.44 - 7.30 (m, 6H), 7.25 - 7.15 (m, 4H), 5.31 (dd, $J_1$ = 3.2 Hz, $J_2$ = 10.4 Hz, 1H), 4.75 (dd, $J_1$ = 10.4 Hz, $J_2$ = 14.4 Hz, 1H), 3.64(dd, $J_1$ = 3.2 Hz, $J_2$ = 14.4 Hz, 1H), 3.62 (s, 3H); $^{13}$C NMR (100 MHz, CDCl$_3$): $\delta$ 159.4, 153.8, 139.5, 137.8, 135.4, 133.3, 131.4, 128.9 (q, $J$ = 9.9 Hz), 128.3, 128.3, 127.8, 127.5, 127.4 (q, $J$ = 3.8 Hz), 126.6 (q, $J$ = 3.4 Hz), 125.8 (q, $J$ = 45.6 Hz), 122.3, 114.2, 59.2, 42.1, 29.4; ESI HRMS: calculated for C$_{24}$H$_{23}$F$_3$N$_2$O$_3$S [M+H]$^+$ 473.1147, found 473.1177.

6-chloro-1-methyl-3-(1-phenyl-2-(phenylsulfonyl)ethyl)quinoxalin-2(1H)-one(5c’), $^1$H NMR (400 Hz, CDCl$_3$): $\delta$ 7.81 (d, $J$ = 7.4 Hz, 2H), 7.68 (d, $J$ = 8.4 Hz, 1H), 7.46 - 7.28 (m, 6H), 7.23 - 7.15 (m, 4H), 5.25 (d, $J$ = 9.9 Hz, 1H), 4.77 - 4.71 (dd, $J_1$ = 10.5Hz, $J_2$ =14.4Hz, 1H), 3.62 (d, $J$ = 14.4 Hz, 1H), 3.53 (s, 3H); $^{13}$C NMR (100 MHz, CDCl$_3$): $\delta$ 157.6, 153.6, 139.3, 138.2, 136.3, 133.9, 133.2, 131.1, 130.6, 128.9, 128.8, 128.3, 128.3, 127.7, 124.0, 113.6, 59.2, 42.0, 29.3. ESI HRMS: calculated for C$_{23}$H$_{20}$ClN$_2$O$_3$S [M+H]$^+$ 439.0883, found 439.0883.

6-fluoro-1-methyl-3-(1-phenyl-2-(phenylsulfonyl)ethyl)quinoxalin-2(1H)-one(5d’), $^1$H NMR (400Hz, CDCl$_3$): $\delta$ 7.84 - 7.82 (m, 2H), 7.49 - 7.46 (m, 1H), 7.41 - 7.31 (m, 5H), 7.27 - 7.15 (m, 5H), 5.29 (dd, $J_1$ = 3.3 Hz, $J_2$ = 10.2 Hz, 1H), 4.75 (dd, $J_1$ =10.2
Hz, $J_2 = 14.4$ Hz, 1H), 3.63 (dd, $J_1 = 3.3$ Hz, $J_2 = 14.4$ Hz, 1H), 3.58 (s, 3H); $^{13}$C NMR (100 MHz, CDCl$_3$): $\delta$ 159.1, 158.6 (d, $J = 242.5$ Hz), 153.6, 139.4, 138.1, 133.2, 132.6 (d, $J = 11.2$ Hz), 129.7 (d, $J = 2.0$ Hz), 128.9, 128.8, 128.3, 128.3, 127.7, 118.0 (d, $J = 23.8$ Hz), 115.4 (d, $J = 22.3$ Hz), 114.6 (d, $J = 8.7$ Hz), 59.2, 42.1, 29.4; ESI HRMS: calculated for C$_{23}$H$_{20}$FN$_2$O$_3$S [M+H]$^+$ 423.1179, found 423.1186.
5. Copies of NMR and HRMS spectra
4-Me-Ph S
O
O
Ph
N
N
O
M+H

Scan (0.164-0.663 min, 31 Scans) L-18-POS.d Subtract (2)

* 419.1438

M+H

 Counts vs. Mass-to-Charge (m/z)
4-Cl-Ph

+ Scan (0.176-0.509 min, 21 Scans) L-19-POS.d Subtract (2)

M+H

439.0901  441.1267  443.1276
Scan (0.151-0.683 min, 33 Scans) L-26-POS.d Subtract (2)

M+H

439.0920

461.1947

477.1886
ESI 扫描 (rt: 0.490 min) Frag=175.8V WorklistData-0063.d
Scan (0.145-0.544 min, 25 Scans) L-28-POS.d Subtract (2)

M+H

423.1186

467.1444

489.1252