Supporting information for….

Moisture-Resistant Radical Anions of Quinoxalin-2(1H)-ones in Aerial Dioxygen Activation

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CONTENTS

EXPERIMENTAL SECTION

Chemicals: Chemicals like Potassium tert-butoxide, *o*-phenylenediamine, Ethyl glyoxylate & solvents were purchased commercially and used without further purification. Column chromatographic purifications of the compounds were performed using silica gel (mesh 100–200 or mesh 230–400) and hexane – ethyl acetate mixtures as eluent unless otherwise specified.

Instrumentation:

Absorption: UV-VIS absorption spectra of **1a** in the absence and presence of KO^{t}Bu in DMSO were recorded with JascoV-730 spectrophotometer (Sl. No. Ao33661798).

Nuclear magnetic resonance measurements: NMR spectra were recorded on a 700 MHz or 400 MHz instrument at 25 °C. The chemical shift values are reported in parts per million (ppm) with respect to residual trichloromethane (7.26 ppm for ^{1}H and 77.16 ppm for ^{13}C) and dimethyl sulfoxide (2.50 ppm for ^{1}H and 39.52 ppm for ^{13}C). The peak patterns are designated as follows: s: singlet; d: doublet; t: triplet; q: quartet; m: multiplet; dd: doublet of doublets; td: triplet of doublets; br s: broad singlet. The coupling constants (*J*) are reported in hertz (Hz).

High-resolution mass spectra (HR-MS): HR-MS were recorded on a TOF Q-II (Bruker) (time of flight) mass spectrometer. Clear solutions of samples were prepared after dissolving in MeCN.

Fourier-transform-Infrared spectra (FTIR): Infrared spectral data are reported in wave number (cm^{-1}). FT-IR spectra were recorded after making thin layer of the compounds on the surface of KBr crystal using dichloromethane.

Melting point measurements: Melting points of the compounds were determined using a digital melting point apparatus and are uncorrected.

Cyclic Voltammetry (CV): Cyclic voltammetric data were obtained from the CH Instruments Electrochemical Workstation (Model: 600E, SN: I1599) in dry and oxygen-free Dichloromethylene Chloride containing 0.1 M tetrabutylammonium hexafluorophosphate as a supporting electrolyte. The experiment was conducted using a three-electrode setup consisting platinum electrode as working electrode, Ag/AgCl electrode as reference electrode, and platinum wire as counter electrode. The deoxygenation of DCM solvent was done by purging Ar gas into the electrolytic solution with the help of a long needle syringe for 2 min.

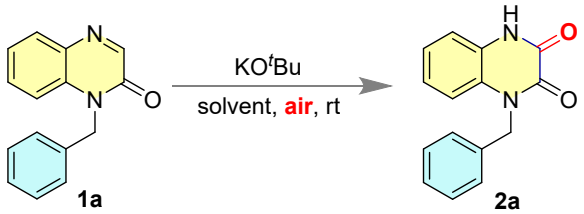


Table S1. Condition Optimization.[a]

Entry	Reagent (equiv)	Solvent	Time (h)	Yield (%)[b]
1	KO^{t}Bu (2.0)	DMSO	4	56
2	KO^{t}Bu (2.0)	DMSO	6	70
3	KO^{t}Bu (2.0)	DMSO	8	74
4	KO^{t}Bu (2.0)	DMSO	12	92
5	KO^{t}Bu (2.0)	DMSO	16	89
6	KO^{t}Bu (2.0)	ACN	12	61
7	KO^{t}Bu (2.0)	1,4-Dioxane	12	48
8	KO^{t}Bu (2.0)	DMF	12	34
9	KO^{t}Bu (2.0)	THF	12	NR[c]
10	KO^{t}Bu (2.0)	1,2-DCE	12	NR[c]
11	KO^{t}Bu (1.0)	DMSO	12	50

12	KO^{t}Bu (1.5)	DMSO	12	53
13	KO^{t}Bu (3.0)	DMSO	12	80
14	KOH (2.0)	DMSO	12	trace
15	Cs_2CO_3 (2.0)	DMSO	12	NR[b,c]
16	KO^{t}Bu (2.0)	DMSO	12	Trace[d]

[a]Standard Conditions **1a** (0.169 mmol), KO^{t}Bu (2.0 equiv.) in 2 mL of solvent at room temperature for 12 h in aerobic condition. [b] Isolated Yields. [c]No Reaction. [d]Ar-atmosphere.

Synthesis

Preparation of starting materials. Starting materials are known and were prepared by following the literature known procedure[1]

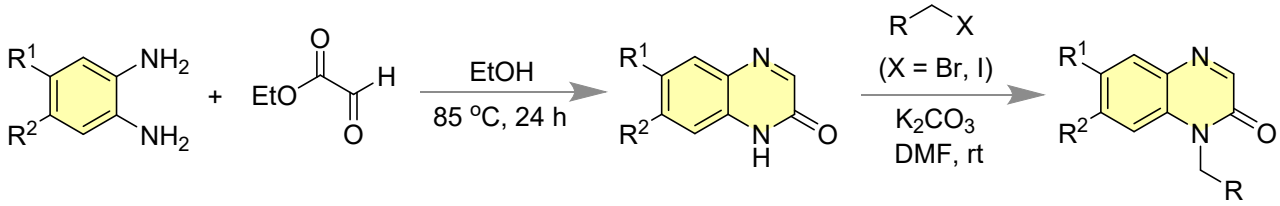


Figure S1. Procedure for the synthesis of 1-benzylquinoxaline-2-one (**1a**).

Synthetic procedure for 1-benzyl-1,4-dihydroquinoxaline-2,3-dione (2a). To an oven-dried 10 mL round bottom flask, 1-benzylquinoxalin-2(1*H*)-one (**1a**) (60 mg, 0.254 mmol, 1.0 equiv) and 2.0 mL DMSO were taken. Next, KO^{t}Bu (57.0 mg, 0.508 mmol, 2.0 equiv) was added to it and the reaction mixture was stirred at room temperature for 12 hours under an aerobic atmosphere. After completion of the reaction, it was diluted with water (10 mL) and extracted with ethyl acetate (3×5 mL). The combined organic phase was then dried over anhydrous sodium sulphate and evaporated under reduced pressure. Purification using column

chromatography on silica gel provided the product 1-benzyl-1,4-dihydroquinoxaline-2,3-dione (**2a**) as a yellow solid with 92% yield.

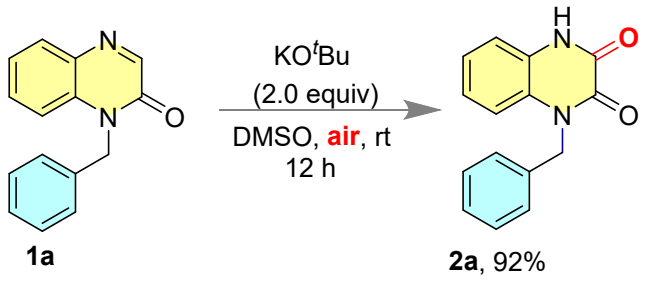


Figure S2. Procedure for the synthesis of 1-benzyl-1,4-dihydroquinoxaline-2,3-dione (**2a**).

A representative method for synthesizing 1-(4-(phenylethynyl)benzyl)-1,4-dihydroquinoxaline-2,3-dione (5a). [1a] To an oven-dried sealed tube charged with a magnetic stirring bar and 1-(4-bromobenzyl)-1,4-dihydroquinoxa-line-2,3-dione (**2h**) (60 mg, 0.181 mmol, 1.0 equiv), $PdCl_2(PPh3)_2$ (6 mg, 0.009 mmol, 5 mol %), and CuI (7 mg, 0.036 mmol, 20 mol %) in 2 mL of anhydrous DMF and 1 mL of Et_3N mixture was added phenylacetylene (30 µL, 0.271 mmol, 1.5 equiv) and it was stirred in a preheated oil bath of 80 °C temperature for 24 h under argon atmosphere. After completion, the reaction mixture was cooled to room temperature. The organic layer was extracted with ethyl acetate, dried over Na_2SO_4, and concentrated under reduced pressure. Column purification provided the desired product 1-(4-(phenylethynyl)benzyl)-1,4-dihydroquinoxaline-2,3-dione (**5a**) in 72% yield.

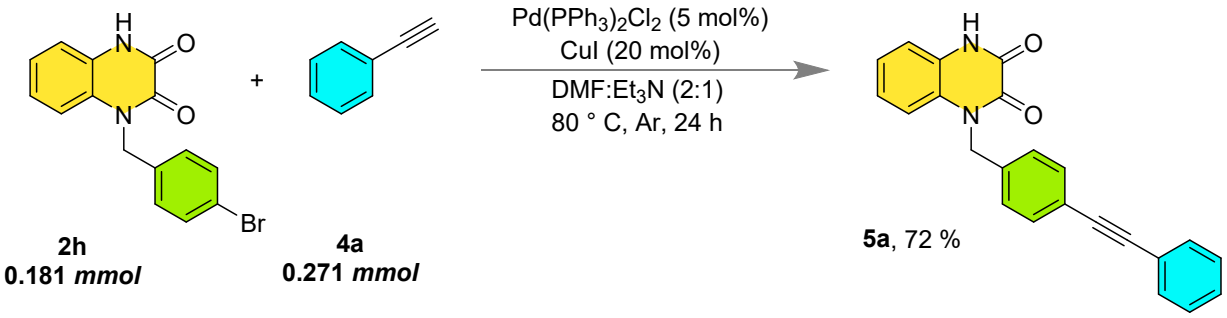


Figure S3. Procedure for the synthesis of 1-(4-(phenylethynyl)benzyl)-1,4-dihydroquinoxaline-2,3-dione **(5a)**.

A representative method for synthesizing 1-(3-(p-tolyl)prop-2-yn-1-yl)-1,4-dihydroquinoxaline-2,3-dione (5b). [2]To an oven-dried sealed tube charged with a magnetic stirring bar and 4-iodo toluene (40 mg, 0.180 mmol, 1.0 equiv), $PdCl_2(PPh_3)_2$ (6 mg, 0.009 mmol, 5 mol %), and CuI (7 mg, 0.036 mmol, 20 mol %) in 2 mL of anhydrous DMF and 1 mL of Et_3N mixture was added 1-(prop-2-yn-1yl)-1,4-dihydroquinoxaline-2,3-dione **2l** (54 mg, 0.270 mmol, 1.5 equiv) and it was stirred at 80 ºC for 24 h under argon atmosphere. After completion, the reaction mixture was cooled to room temperature and washed with brine solution. The organic layer was extracted with ethyl acetate, dried over Na_2SO_4, and concentrated under reduced pressure. Column purification provided the desired product 1-(3-(p-tolyl)prop-2-yn-1-yl)-1,4-dihydroquinoxaline-2,3-dione (**5b**) in 65% yield.

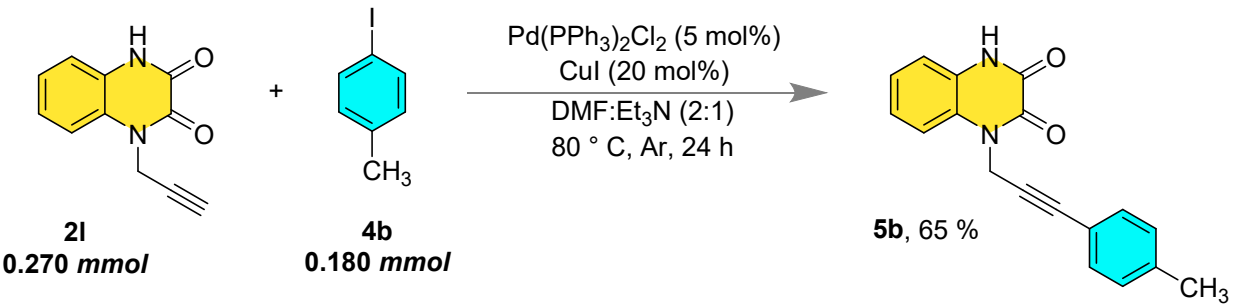


Figure S4. Procedure for the synthesis of 1-(3-(p-tolyl)prop-2-yn-1-yl)-1,4-dihydroquinoxaline-2,3-dione **(5b)**.

Gram-scale synthesis of 1-benzyl-1,4-dihydroquinoxaline-2,3-dione (2a). To an oven-dried 50 mL round bottom flask, 1-benzylquinoxalin-2(1*H*)-one (**1a**) (1.0 g, 4.23 mmol, 1.0 equiv) and 20 mL DMSO was taken. Next, KO^{t}Bu (949 mg, 8.46 mmol, 2.0 equiv) was added to it and the reaction mixture was stirred at room temperature for 24 hours under an aerobic atmosphere. After completion of the reaction, it was diluted with water and extracted with ethyl acetate. The combined organic phase was then dried over anhydrous sodium sulphate and

evaporated under reduced pressure. Purification using column chromatography on silica gel provided the product 1-benzyl-1,4-dihydroquinoxaline-2,3-dione (**2a**) as a yellow solid with 74% yield.

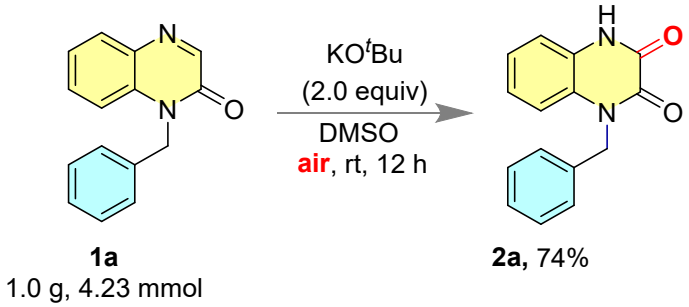
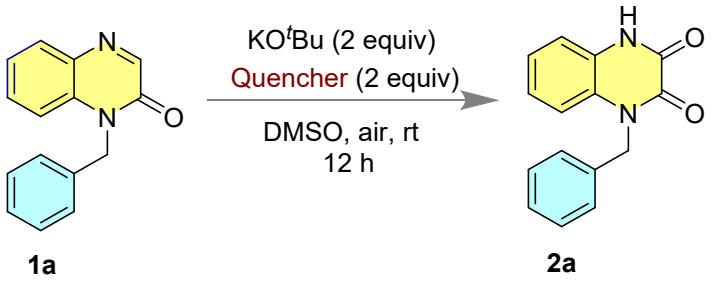


Figure S5. Gram-scale synthesis of 1-benzyl-1,4-dihydroquinoxaline-2,3-dione (**2a**).

Procedure for the radical quenching experiments.[1a] To an oven-dried 10 mL round bottom flask charged with a magnetic stirring bar, 1-benzylquinoxalin-2(1*H*)-one (60 mg, 0.254 mmol, 1.0 equiv) and quencher (2.0 equiv) were dissolved in 2.0 mL DMSO solvent. KO^{t}Bu (57.0 mg, 0.508 mmol, 2.0 equiv) was added to it and the reaction mixture was stirred at room temperature for 12 h under an aerobic atmosphere. After that, the reaction mixture was diluted with water (10 mL) and extracted with ethyl acetate (3×5 mL). The resulting organic solution was dried over anhydrous sodium Na_2SO_4 and concentrated under reduced pressure. Corresponding yields of the reactions were calculated after column chromatography.



Entry	Quencher	Yield (%)^b	Role
1	BHT	trace	radical scavenger
2	TEMPO	46	radical scavenger
3	$CuCl_2$	trace	electron scavenger
4	Sodium azide	79	Singlet oxygen scavenger

Figure S6. Control experiments in the presence of different quenchers (^{b}Isolated yield).

Procedure for the isotopic labelling experiments. To an oven-dried 10 mL round bottom flask charged with a magnetic stirring bar, 1-benzylquinoxalin-2(1*H*)-one (60 mg, 0.254 mmol, 1.0 equiv) and different isotopes of H_2O (D_2O and $H_2{}^{18}O$) (1.2 equiv) were dissolved in 2.0 mL dry DMSO solvent. KO^{t}Bu (57.0 mg, 0.508 mmol, 2.0 equiv) was added to it and the reaction mixture was stirred at room temperature for 12 hours under an aerobic atmosphere. After that, the reaction mixture was diluted with water (10 mL) and extracted with ethyl acetate (3×5 mL). The resulting organic solution was dried over anhydrous sodium Na_2SO_4 and concentrated under reduced pressure. The crude mixture was taken for HRMS analysis.

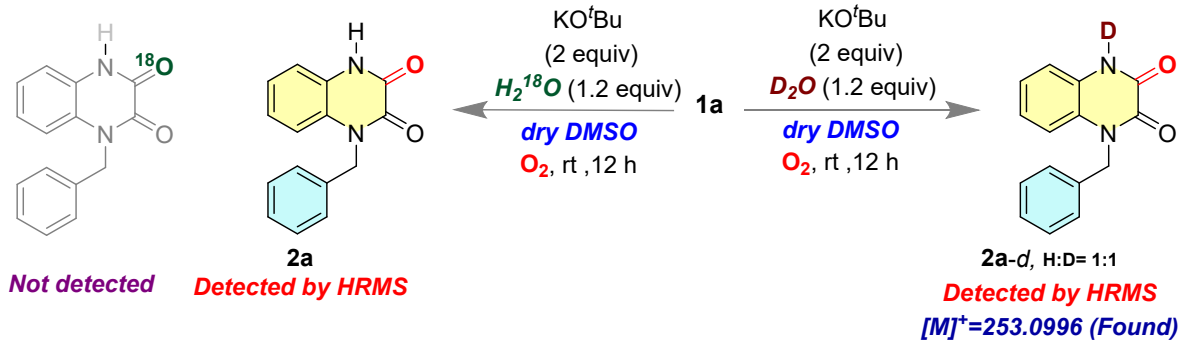


Figure S7. Isotopic labelling experiments with $H_2{}^{18}O$ and D_2O.

To investigate about the formation of the charge-transfer complex, we recorded UV-Visible spectra of **1a,** and the mixture of the starting compound **1a** with KO^{t}Bu in the 0.2 (M) DMSO and the corresponding UV-Visible spectra were plotted. In DMSO solution, substrate **1a** shows an absorption band at 347 nm but after the addition of KO^{t}Bu another absorption at 429 nm was observed with an intense purple color (Figure S6). When BHT was added to the mixture of **1a** and KO^{t}Bu a new absorption at 583 nm was observed whereas BHT itself do not show any absorption in presence of KO^{t}Bu which revealed the formation of trapped radical intermediate whereas the final compound **2a** shows an absorption at 313 nm in DMSO solvent.

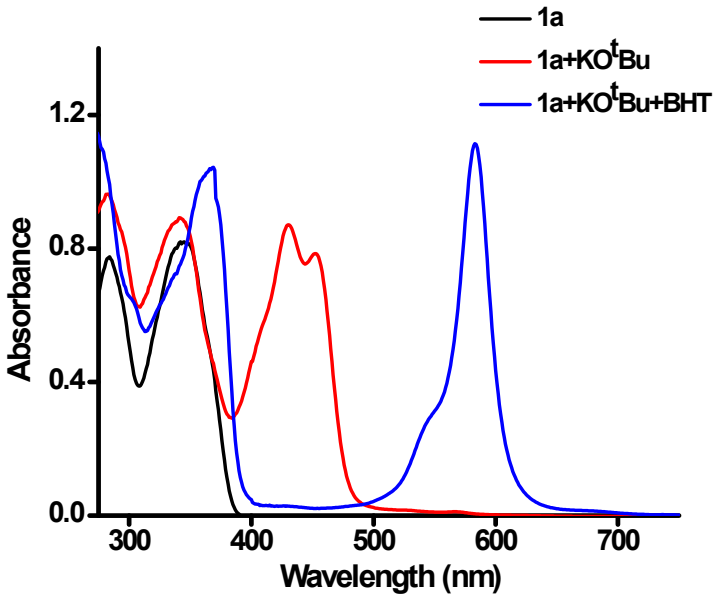


Figure S8. UV- visible spectra of **1a**, **1a**/KO^{t}Bu and **1a**/KO^{t}Bu/BHT in DMSO.

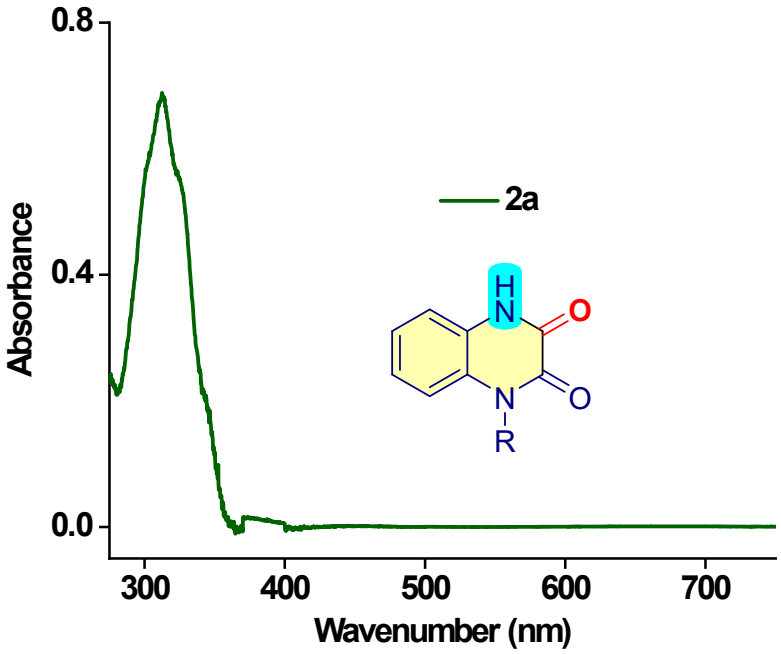


Figure S9. UV- visible spectra of **2a** in DMSO.

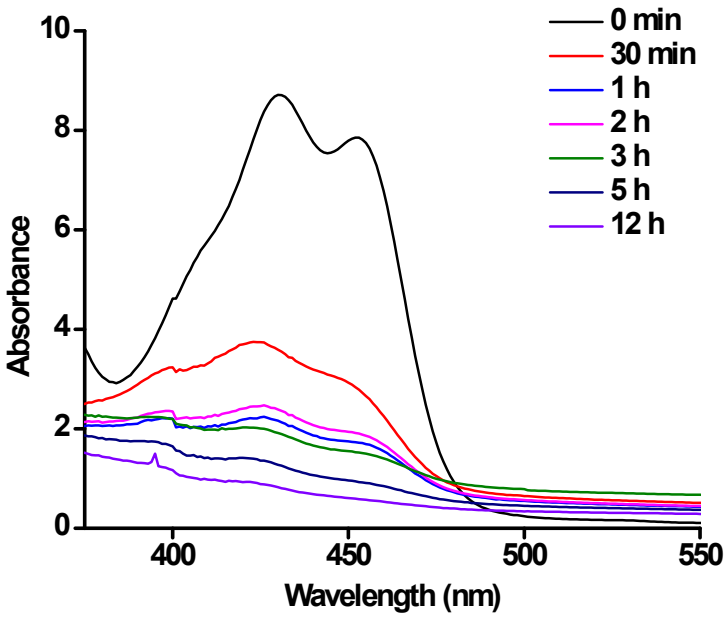


Figure S10. Time dependent UV- visible spectra of **1a** in presence of KO^{t}Bu in DMSO under aerobic condition.

Detection of hydrogen peroxide (H_2O_2).[3] The KI test was performed to detect the evolution of H_2O_2 as the by product during the reaction. In vial **A** the mixture of **1a** and potassium *tert*-butoxide shows the purple colour but in vial **B** after the addition of 2 equiv. of KI in the reaction mixture the colour turned into magenta colour from intense purple colour. In vial C in presence of strong acid like HCl the colour turned into green colouration which might be for the oxidation of iodide ion to I_3^- which further was confirmed by recording the absorption band of UV-Visible spectra of the mixture of **1a**, KO^{t}Bu, KI in presence of HCl at 368 nm. This band arises might be for the formed triiodide anion. This experiment confirmed the evolution of H_2O_2.

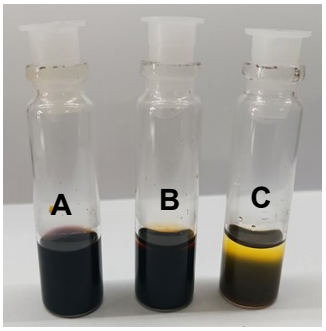


Figure S11. Control experiments to detect of H_2O_2 in presence of KI under acidic condition.

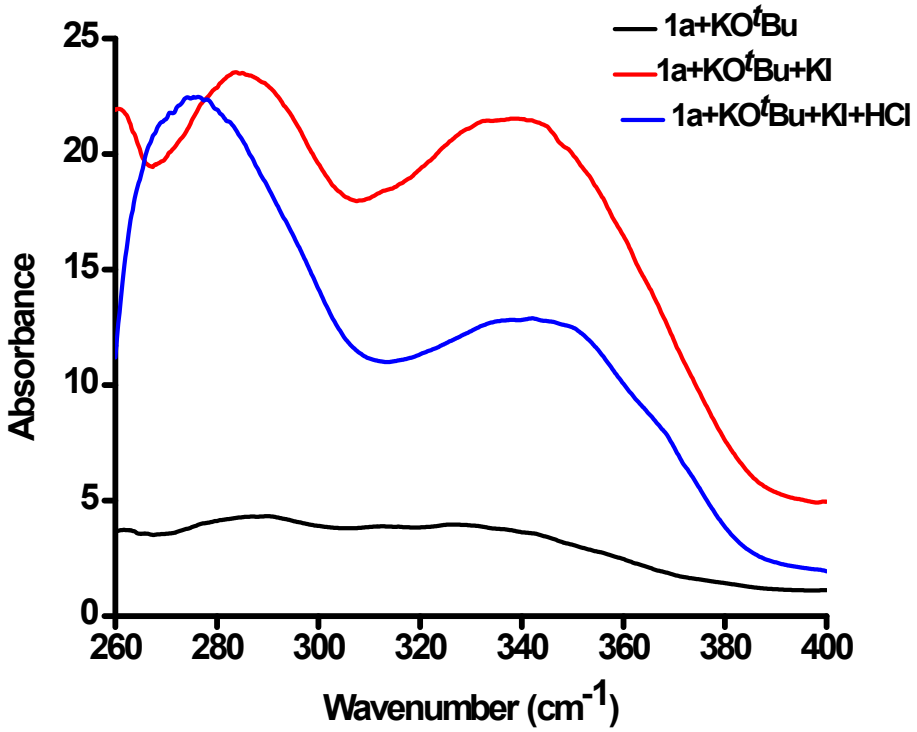


Figure S12. UV- visible spectra of **1a** in presence of KO^{t}Bu, KI and HCl separately in DMSO.

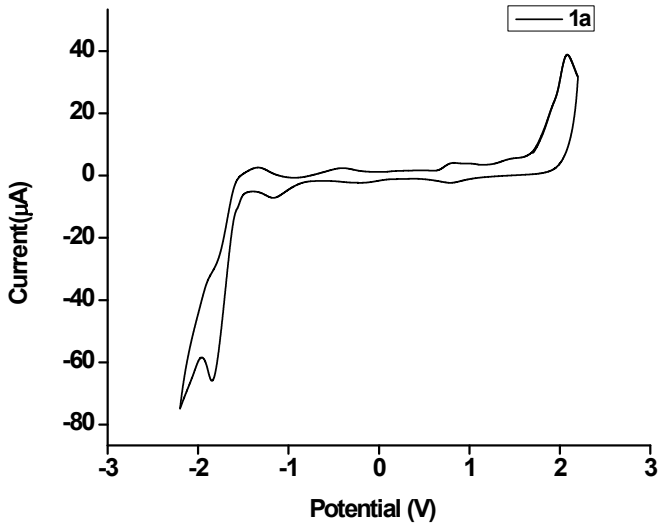


Figure S13. IUPAC-CV of 1-benzylquinoxalin-2(1*H*)-one **(1a)** using nBu$_4$NPF$_6$ as an electrolyte in dry degassed DCM.

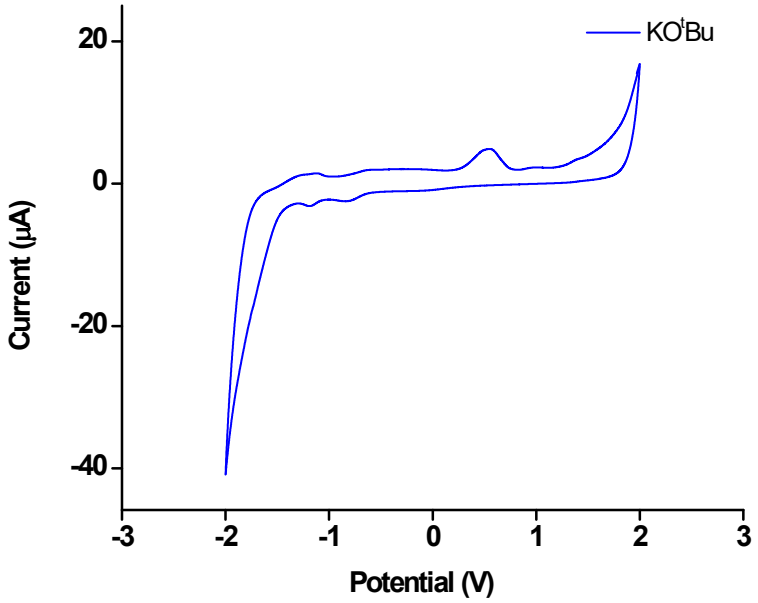


Figure S14. IUPAC-CV of Potassium *tert*-butoxide using nBu$_4$NPF$_6$ as an electrolyte in dry degassed DCM.

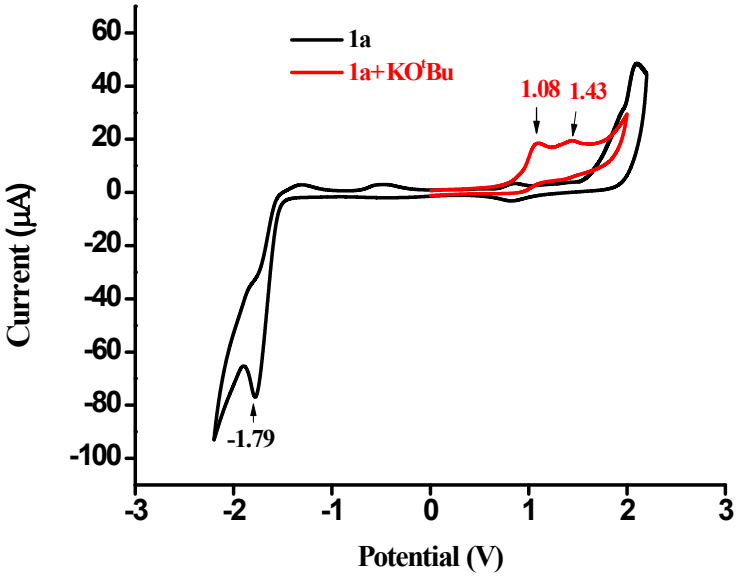


Figure S15. IUPAC-CV of 1-benzylquinoxalin-2(1*H*)-one **(1a)** and **1a** with KO^{t}Bu using nBu$_4$NPF$_6$ as an electrolyte in dry degassed DCM.

To get a detailed analysis about the formation of a stable radical anion intermediate we have performed the FT-IR study and it was observed that the two frequencies at 3007 cm^{-1} and 2914 cm^{-1} of **1a** disappeared after the addition of KO^{t}Bu while the C=O has retained it's stretching frequency at 1643 cm^{-1} in both the cases (Figure S14).

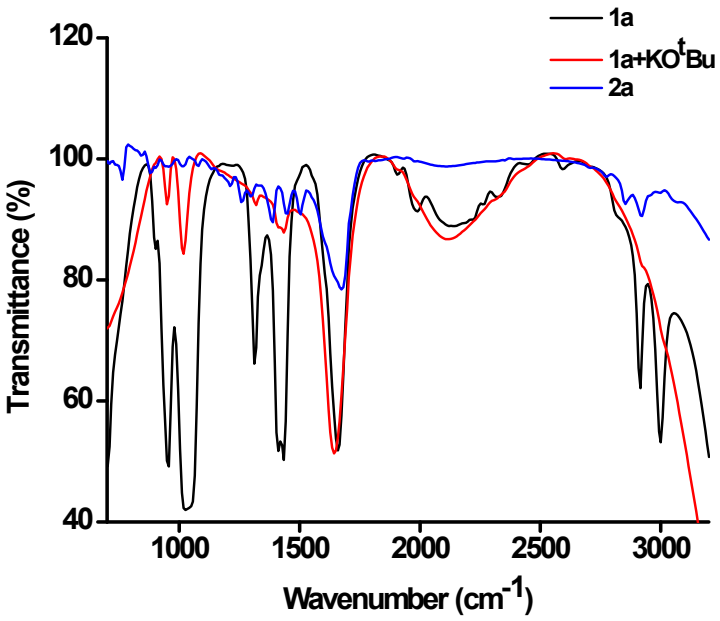
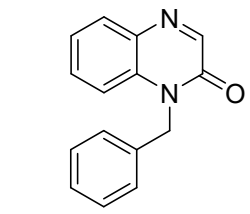


Figure S16. FT-IR Spectral analysis of **1a**, **1a** with KO^{t}Bu and **2a**.

Spin-trapping experiment with DMPO.[4] In a 10 mL quartz tube containing of 1-Benzylquinoxalin-2(1*H*)-one (**1a**) (60 mg, 0.25 mmol, 1.0 equiv), Potassium *tert*-butoxide (0.057 g, 0.51 mmol, 2 equiv) in 3.0 mL wet-DMSO, was charged and followed by DMPO (20 µL) was added. Then, the quartz tube was sealed by a septum and paraffin tape, and allowed for 2 h at room temperature. Afterward, 300 µL of the uncompleted reaction mixture was quickly taken out of the quartz tube and poured in an EPR tube and immediately around 200 µL of toluene was appended and EPR experiment was done.

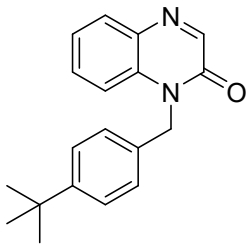
CHARACTERIZATION DATA

1-Benzylquinoxalin-2(1*H*)-one (1a).[5] R_f = 0.3 (20% ethyl acetate/hexane); pale yellow solid;

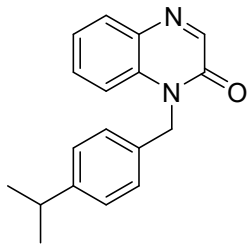


yield 131 mg (81%); mp: 120 ºC, ^{1}H NMR (700 MHz, DMSO-d_6) δ 8.36 (s, 1H), 7.86 (d, J = 7.7 Hz, 1H), 7.56 (t, J = 8.0 Hz, 1H), 7.47 (d, J = 8.4 Hz, 1H), 7.36 (t, J = 7.3 Hz, 1H), 7.32 (t, J = 7.3 Hz, 2H), 7.28 – 7.25 (m, 3H), 5.49 (s, 2H).

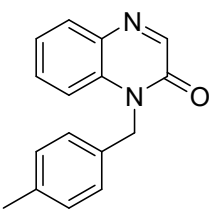
1-(4-(*tert*-Butyl)benzyl)quinoxalin-2(1*H*)-one (1b).[5] R_f = 0.3 (50% ethyl acetate/hexane); dark brown solid; yield 140 mg (70%); mp: 135-136 ºC, ^{1}H NMR (400 MHz, DMSO- d_6) δ 8.35 (s, 1H), 7.85 (d, J = 8.0 Hz, 1H), 7.57 (t, J = 7.8 Hz, 1H), 7.50 (d, J = 8.0 Hz, 1H), 7.36 (d, J = 7.6 Hz, 1H), 7.32 (d, J = 8.4 Hz, 2H), 7.20 (d, J = 8.0 Hz, 2H), 5.44 (s, 2H), 1.21 (s, 9H).



1-(4-Isopropylbenzyl)quinoxalin-2(1*H*)-one (1c).[5] R_f = 0.3 (20% ethyl acetate/hexane); dark brown solid; yield 137 mg (72%); mp: 131 ºC, ^{1}H NMR (400 MHz, DMSO- d_6) δ 8.35 (s, 1H), 7.85 (d, J = 7.6 Hz, 1H), 7.57 (t, J = 7.4 Hz, 1H), 7.50 (d, J = 8.0 Hz, 1H), 7.35 (d, J = 7.4 Hz, 1H), 7.20-7.16 (m, 4H), 2.84 – 2.79 (m, 1H), 1.14 (d, J = 6.8 Hz, 6H).



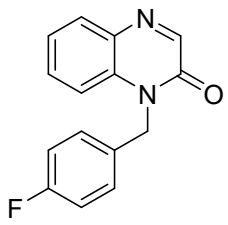
1-(4-Methylbenzyl)quinoxalin-2(1*H*)-one (1d).[5] R_f = 0.6 (20% ethyl acetate/hexane); pale yellow solid; yield 120 mg (70%); mp: 167-169 ºC, ^{1}H NMR (400 MHz, DMSO- d_6) δ 8.35 (s, 1H), 7.86 (d, J = 8.0 Hz, 1H), 7.57 (d, J = 7.2 Hz, 1H), 7.46 (d, J = 7.6 Hz, 1H), 7.35 (t, J = 7.0 Hz, 1H), 7.17 (d, J = 8.4 Hz, 2H), 7.11 (d, J = 8.0 Hz, 2H), 5.44 (s, 2H), 2.24 (s, 3H).



1-(4-(Trifluoromethyl)benzyl)quinoxalin-2(1*H*)-one (1e).[5] R_f = 0.2 (20% ethyl acetate/hexane); dark brown solid; yield 135 mg (65%); mp: 109-111 ºC, ^{1}H NMR (700 MHz, DMSO- d_6) δ 8.36 (s, 1H), 7.86 (d, J = 8.4 Hz, 1H),

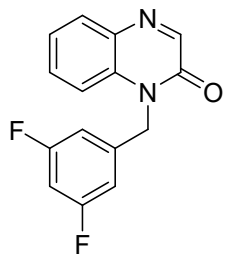
7.67 (d, *J* = 8.4 Hz, 2H), 7.57 – 7.54 (t, *J* = 8.0 Hz 1H), 7.48 (d, *J* = 8.4 Hz, 2H), 7.43 (d, *J* = 8.4 Hz, 1H), 7.36 (t, *J* = 7.3 Hz, 1H), 5.57 (s, 2H).

1-(4-Fluorobenzyl)quinoxalin-2(1H)-one (1f).[5] R_f = 0.5 (20% ethyl acetate/hexane); pale



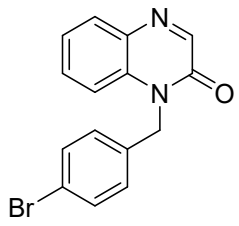
yellow solid; yield 96 mg (55%); mp: 115 ºC, ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.35 (s, 1H), 7.85 (d, *J* = 7.6 Hz, 1H), 7.57 (t, *J* = 8.4 Hz, 1H), 7.48 (d, *J* = 7.6 Hz, 1H), 7.37 (d, *J* = 8.0 Hz, 1H), 7.34 (d, *J* = 5.6 Hz, 2H), 7.15 (t, *J* = 8.8 Hz, 2H), 5.47 (s, 2H).

1-(3,5-Difluorobenzyl)quinoxalin-2(1*H*)-one (1g).[5] R_f = 0.2 (20% ethyl acetate/hexane);



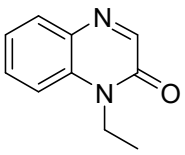
light brown solid; yield 123 mg (66%); mp: 142-144 ºC, ^{1}H NMR (400 MHz, DMSO- d_6) δ 8.34 (s, 1H), 7.86 (d, *J* = 8.0 Hz, 1H), 7.59 (t, *J* = 7.8 Hz, 1H), 7.41 (d, *J* = 8.0 Hz, 1H), 7.38 (t, *J* = 7.6 Hz, 1H), 7.14 (t, *J* = 9.4 Hz, 1H), 7.06 (d, *J* = 6.4 Hz, 2H), 5.48 (s, 2H).

1-(4-Bromobenzyl)quinoxalin-2(1*H*)-one (1h).[5] R_f = 0.4 (20% ethyl acetate/hexane); light



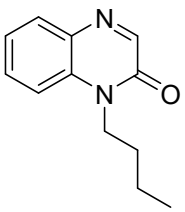
yellow solid; yield 147 mg (68%); mp: 170-173 ºC, ^{1}H NMR (700 MHz, DMSO- d_6) δ 8.35 (s, 1H), 7.86 (d, *J* = 7.7 Hz, 1H), 7.57 (t, *J* = 8.1 Hz, 1H), 7.51 (d, *J* = 8.3 Hz, 2H), 7.45 (d, *J* = 8.4 Hz, 1H), 7.37 (t, *J* = 7.3 Hz, 1H), 7.25 (d, *J* = 8.4 Hz, 2H), 5.46 (s, 2H).

1-Ethylquinoxalin-2(1*H*)-one (1i).[5] R_f = 0.4 (20% ethyl acetate/hexane); pinkish white solid;



yield 85 mg (70%); mp: 81-83 ºC, ^{1}H NMR (400 MHz, DMSO- d_6) δ 8.23 (s, 1H), 7.84 (d, *J* = 7.6 Hz, 1H), 7.70 – 7.67 (m, 1H), 7.65 (d, *J* = 5.8 Hz, 1H), 7.41 – 7.37 (m, 1H), 4.25 (q, *J* = 7.1 Hz, 2H), 1.23 (t, *J* = 7.1 Hz, 3H).

1-Butylquinoxalin-2(1*H*)-one (1j).[5] R_f = 0.3 (20% ethyl acetate/hexane); pale yellow



liquid; yield 97 mg (70%); ^{1}H NMR (700 MHz, DMSO- d_6) δ 8.22 (s, 1H), 7.83 (d, *J* = 7.7 Hz, 1H), 7.66 (t, *J* = 7.7 Hz, 1H), 7.62 (d, *J* = 8.4 Hz, 1H),

7.38 (t, *J* = 7.7 Hz, 1H), 4.20 (t, *J* = 7.7 Hz, 2H), 1.64 – 1.58 (m, 2H), 1.41 – 1.35 (m, 2H), 0.92 (t, *J* = 7.4 Hz, 3H).

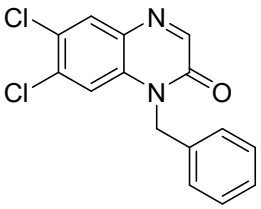
1-Phenethylquinoxalin-2(1*H*)-one (1k).[5] R_f = 0.5 (20% ethyl acetate/hexane); yellow solid; yield 111 mg (65%); mp: 132-134 ºC, ^{1}H NMR (700 MHz, DMSO- d_6) δ 8.24 (s, 1H), 7.85 (d, *J* = 7.7 Hz, 1H), 7.69 (d, *J* = 8.4 Hz, 1H), 7.66 (d, *J* = 7.0 Hz, 1H), 7.39 (t, *J* = 7.0 Hz, 1H), 7.30 (d, *J* = 4.2 Hz, 4H), 7.24 – 7.22 (m, 1H), 4.44 – 4.41 (t, *J* = 7.7 Hz, 2H), 2.96 – 2.93 (t, *J* = 8.1 Hz, 2H).

1-(Prop-2-yn-1-yl)quinoxalin-2(1*H*)-one (1l).[5] R_f = 0.2 (20% ethyl acetate/hexane); light brown solid; yield 92 mg (73%); mp: 177-179 ºC, ^{1}H NMR (400 MHz, DMSO- d_6) δ 8.29 (s, 1H), 7.87 (d, *J* = 7.6 Hz, 1H), 7.72 (t, *J* = 7.8 Hz, 1H), 7.65 (d, *J* = 8.0 Hz, 1H), 7.43 (t, *J* = 7.4 Hz, 1H), 5.07 (d, *J* = 2.4 Hz, 2H), 3.36 (t, *J* = 2.5 Hz, 1H).

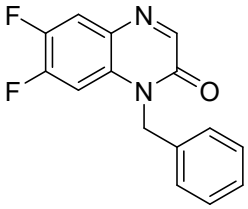
1-Benzylbenzo[g]quinoxalin-2(1*H*)-one (1m).[5] R_f = 0.4 (20% ethyl acetate/hexane); dark brown solid; yield 147 mg (75%); mp: 194-196 ºC, ^{1}H NMR (700 MHz, DMSO- d_6) δ 8.51 (s, 1H), 8.40 (s, 1H), 8.10 (d, *J* = 8.4 Hz, 1H), 7.92 (t, *J* = 7.0 Hz, 2H), 7.58(t, *J* = 7.4 Hz 1H), 7.51 (t, *J* = 7.3 Hz, 1H), 7.37 (d, *J* = 7.7 Hz, 2H), 7.32 (t, *J* = 7.7 Hz, 2H), 7.25 (t, *J* = 7.0 Hz, 1H), 5.55 (s, 2H).

1-Benzyl-6,7-dimethylquinoxalin-2(1*H*)-one (1n).[5] R_f = 0.3 (20% ethyl acetate/hexane); white solid; yield 118 mg (65%); mp: 179-182 ºC, ^{1}H NMR (400 MHz, DMSO- d_6) δ 8.25 (s, 1H), 7.63 (s, 1H), 7.33 (s, 1H), 7.31 (d, *J* = 6.4 Hz, 2H), 7.25 (d, *J* = 7.3 Hz, 3H), 5.46 (s, 2H), 2.28 (s, 3H), 2.27 (s, 3H).

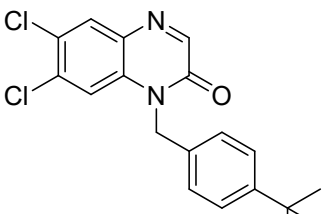
1-Benzyl-6,7-dichloroquinoxalin-2(1*H*)-one (1o).[5] R_f = 0.4 (20% ethyl acetate/hexane); pink solid; yield 115 mg (55%); mp: 179 ºC, ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.40 (s, 1H), 8.14 (s, 1H), 7.76 (s, 1H), 7.35 – 7.31 (m, 2H), 7.28-7.26 (m, 3H), 5.48 (s, 2H).



1-Benzyl-6,7-difluoroquinoxalin-2(1*H*)-one (1p).[5] R_f = 0.7 (20% ethyl acetate/hexane); light pink solid; yield 121 mg (65%); mp: 146 ºC, ^{1}H NMR (700 MHz, DMSO-d_6) δ 8.37 (s, 1H), 8.03 – 7.98 (m, 1H), 7.63 (dd, *J* = 12.3, 7.3 Hz, 1H), 7.33 (t, *J* = 7.7 Hz, 2H), 7.29 (d, *J* = 7.7 Hz, 2H), 7.26 (d, *J* = 7.0 Hz, 1H), 5.46 (s, 2H).

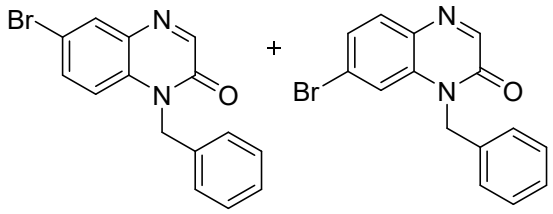


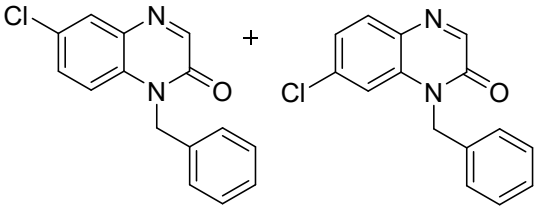
1-(4-(*tert*-Butyl)benzyl)-6,7-dichloroquinoxalin-2(1*H*)-one (1q).[5] R_f = 0.3 (20% ethyl acetate/hexane); light yellowish brown solid; yield 173 mg (70%); mp: 160-162 ºC, ^{1}H NMR (400 MHz, DMSO- d_6) δ 8.39 (s, 1H), 8.14 (s, 1H), 7.83 (s, 1H), 7.34 (d, *J* = 8.4 Hz, 2H), 7.20 (d, *J* = 8.3 Hz, 2H), 5.44 (s, 2H), 1.23 (s, 9H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 154.0, 152.1, 149.9, 133.3, 132.4, 132.4, 132.2, 130.6, 126.6, 126.3, 125.5, 116.8, 44.3, 34.2, 31.0; ῡ = 2960,1667,1593,841cm^{-1}; HRMS (ESI/QTOF) m/z: [M + H]$^+$ calcd for $C_{19}H_{19}Cl_2N_2O$ 361.0874; Found 361.0868.

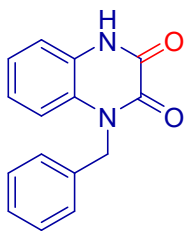


1-Benzyl-6-methylquinoxalin-2(1*H*)-one and 1-Benzyl-7-methylquinoxalin-2(1*H*)-one (1r).[5] R_f = 0.3 (20% ethyl acetate/hexane); gray solid; yield 154 mg (75%); mp: 110 ºC, two regio-isomers with 62:38 ratio; ^{1}H NMR (700 MHz, DMSO- d_6) δ 8.33 (s, 1H), 8.27 (s, 0.6H), 7.74 (d,

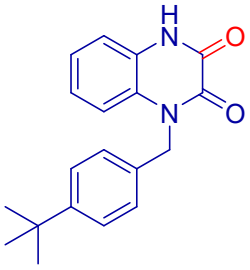
J = 8.0 Hz, 0.6H), 7.67 (s, 1H), 7.39-7.35 (m, 2H), 7.33-7.30 (m, 3H), 7.27-7.24 (m, 5H), 7.19 (d, *J* = 7.9 Hz, 0.6H), 5.47 (s, 4H), 2.37 (s, 6H).

1-Benzyl-6-bromoquinoxalin-2(1*H*)-one and 1-Benzyl-7-bromoquinoxalin-2(1*H*)-one (1s).[5]  R_f = 0.4 (20% ethyl acetate/hexane); light pink solid; yield 259 mg (60%); mp: 152 ºC, two regio-isomers with 59:41 ratio; ^{1}H NMR (400 MHz, DMSO- d_6) δ 8.39 (s, 1H), 8.37 (s, 0.6H), 8.05 (d, *J* = 2.2 Hz, 1H), 7.78 (d, *J* = 8.5 Hz, 1H), 7.74 – 7.71 (m, 1H), 7.67 (d, *J* = 1.8 Hz, 1H), 7.53 (dd, *J* = 8.5, 1.9 Hz, 1H), 7.41 (d, *J* = 9.0 Hz, 1H), 7.35-7.30 (m,5H), 7.28 – 7.24 (m, 5H), 5.48 (d, *J* = 8.7 Hz, 4H).

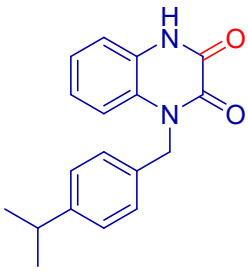
1-Benzyl-6-chloroquinoxalin-2(1*H*)-one and 1-Benzyl-7-chloroquinoxalin-2(1*H*)-one (1t).[5]  R_f = 0.5 (20% ethyl acetate/hexane); brown solid; yield 230 mg (62%); mp: 140-142 ºC, two regio-isomers with 75:25 ratio; ^{1}H NMR (400 MHz, DMSO- d_6) δ 8.40 (s, 1H), 8.36 (s, 0.4H), 7.92 (d, *J* = 2.4 Hz, 1H), 7.86 (d, *J* = 8.5 Hz, 0.5H), 7.60-7.62 (m, 1H), 7.54 (d, *J* = 2.0 Hz, 0.6H), 7.46 (d, *J* = 8.8 Hz,1H), 7.38-7.41 (m, 0.6H), 7.30 – 7.33 (m, 4H), 7.26 (d, *J* = 6.3 Hz, 5H), 5.48 (d, *J* = 6.0 Hz, 4H).

1-Benzyl-1,4-dihydroquinoxaline-2,3-dione (2a).[1a]  R_f = 0.3 (50% ethyl acetate/hexane); yellow solid; yield 59 mg (92%); mp: 295-297 ºC, ^{1}H NMR (700 MHz, DMSO-d_6) δ 12.11 (s, 1H), 7.34 – 7.29 (m, 4H), 7.25 (d, *J* = 6.3 Hz, 1H), 7.19 (dd, *J* = 16.0, 7.7 Hz, 2H), 7.13 (t, *J* = 7.7 Hz, 1H), 7.06 (t, *J* = 7.7 Hz, 1H), 5.38 (s, 2H); ^{13}C{^{1}H} NMR (175 MHz, DMSO-d_6) δ 155.7, 153.7, 135.8, 128.6, 127.2, 126.7, 126.3, 125.9, 123.6, 123.1, 115.7, 115.4, 45.6.

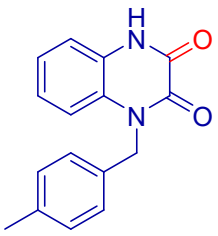
1-(4-(*tert*-Butyl)benzyl)-1,4-dihydroquinoxaline-2,3-dione (2b).[1a] R_f = 0.2 (50% ethyl acetate/hexane); yellow solid; yield 56 mg (89%); mp: >300 ºC; ^{1}H NMR (700 MHz, DMSO-d_6) δ 12.11 (s, 1H), 7.33 (d, J = 7.7 Hz, 2H), 7.22 (d, J = 7.7 Hz, 1H), 7.20 (d, J = 7.7 Hz, 1H), 7.13 (t, J = 7.7 Hz, 1H), 7.08 (t, J = 8.4 Hz, 1H), 5.33 (s, 2H), 1.23 (s, 9H); ^{13}C{^{1}H} NMR (175 MHz, DMSO-d_6) δ 155.5, 153.6, 149.5, 132.6, 126.4, 126.2, 125.8, 125.3, 123.6, 123.1, 115.6, 115.4, 45.1, 34.1, 31.0.



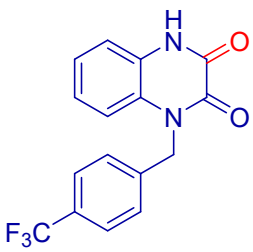
1-(4-Isopropylbenzyl)-1,4-dihydroquinoxaline-2,3-dione (2c).[1a] R_f = 0.3 (50% ethyl acetate/hexane); yellow solid; yield 53 mg (84%); mp: 271-273 ºC; ^{1}H NMR (700 MHz, DMSO-d_6) δ 12.11 (s, 1H), 7.22-7.17 (m, 6H), 7.13 (t, J = 7.7 Hz, 1H), 7.07 (t, J = 7.7 Hz, 1H), 5.33 (s, 2H), 2.85-2.81 (m, 1H), 1.15 (d, J = 7.0 Hz, 6H); ^{13}C{^{1}H} NMR (175 MHz, DMSO-d_6) δ 155.7, 153.7, 147.4, 133.1, 126.8, 126.6, 126.3, 125.9, 123.7, 123.2, 115.7, 115.5, 45.4, 33.1, 23.9.



1-(4-Methylbenzyl)-1,4-dihydroquinoxaline-2,3-dione (2d).[1a] R_f = 0.3 (50% ethyl acetate/hexane); yellow solid; yield 49 mg (77%); mp: >300 ºC; ^{1}H NMR (700 MHz, DMSO-d_6) δ 12.10 (s, 1H), 7.19-7.16 (m, 4H), 7.12 (t, J = 7.7 Hz, 3H), 7.06 (t, J = 7.7 Hz, 1H), 5.33 (s, 2H), 2.25 (s, 3H); ^{13}C{^{1}H} NMR (175 MHz, DMSO- d_6) δ 155.6, 153.6, 136.3, 132.6, 129.1, 126.6, 126.1, 125.8, 123.5, 123.0, 115.6, 115.4, 45.3, 20.5.

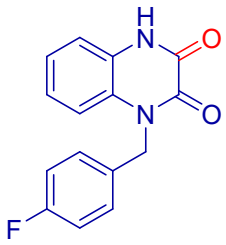


1-(4-(Trifluoromethyl)benzyl)-1,4-dihydroquinoxaline-2,3-dione (2e).[1a] R_f = 0.3 (50% ethyl acetate/hexane); pale yellow solid; yield 54 mg (84%); mp: 266-268 ºC; ^{1}H NMR (700 MHz, DMSO-d_6) δ 12.12 (s, 1H), 7.68 (d, J = 8.4 Hz, 2H), 7.55 (d, J = 7.7 Hz, 2H), 7.21 (d, J = 7.7 Hz, 1H), 7.14 (t, J =

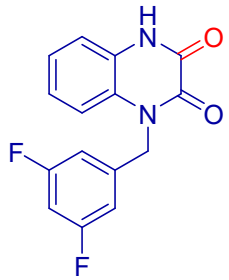


7.7 Hz, 2H), 7.06 (t, J = 7.7 Hz, 1H), 5.47 (s, 2H); $^{13}C\{^{1}H\}$ NMR (175 MHz, DMSO-d_6) δ 155.8, 153.7, 140.7, 127.9 (q, $^{2}J_{C\text{-}F}$ = 31.5 Hz) 127.5, 126.2, 126.0, 125.6 (q, $^{3}J_{C\text{-}F}$ = 3.7 Hz), 124.3 (q, $^{1}J_{C\text{-}F}$ = 270.2 Hz), 123.8, 123.2, 115.8, 115.3, 45.4.

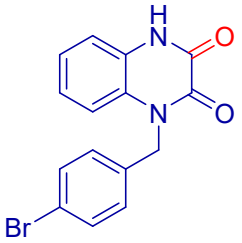
4-(4-Fluorobenzyl)-3,4-dihydroquinoxalin-2(1H)-one (2f).[1a] R_f = 0.2 (50% ethyl acetate/hexane); pale yellow solid; yield 53 mg (82%); mp: >300 ºC; ^{1}H NMR (700 MHz, DMSO-d_6) δ 12.09 (s, 1H), 7.40 – 7.34 (m, 2H), 7.19 (t, J = 7.7 Hz, 2H), 7.16 – 7.12 (m, 3H), 7.07 (t, J = 7.7 Hz, 1H), 5.35 (s, 2H); $^{13}C\{^{1}H\}$ NMR (175 MHz, DMSO-d_6) δ 161.5 (d, $^{1}J_{C\text{-}F}$ = 241.5 Hz), 155.9, 153.8, 132.07 (d, $^{4}J_{C\text{-}F}$ = 2.6 Hz), 129.0 (d, $^{3}J_{C\text{-}F}$ = 8.2 Hz), 126.3, 126.1, 123.8, 123.2, 115.8, 115.6 (d, $^{2}J_{C\text{-}F}$ = 21.3 Hz), 115.5 45.1.



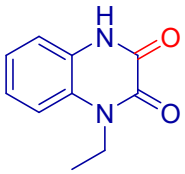
1-(3,5-Difluorobenzyl)-1,4-dihydroquinoxaline-2,3-dione (2g).[1a] R_f = 0.2 (50% ethyl acetate/hexane); pale yellow solid; yield 52 mg (82%); mp: 274-276 ºC; ^{1}H NMR (700 MHz, DMSO-d_6) δ 12.04 (s, 1H), 7.20 (d, J = 7.7 Hz, 1H), 7.15 – 7.11 (m, 4H), 7.09-7.07 (m, 2H), 5.37 (s, 2H); $^{13}C\{^{1}H\}$ NMR (175 MHz, DMSO-d_6) δ 162.6 (dd, J = 246.2, 12.6 Hz), 155.9, 153.8, 140.7 (t, J = 9.3 Hz), 126.3, 126.2, 123.6, 123.0, 115.7, 115.1, 110.01 (dd, J = 21.0, 4.5 Hz), 102.70 (t, J = 25.7 Hz), 45.2



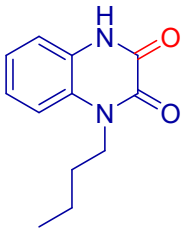
4-(4-Bromobenzyl)-3,4-dihydroquinoxalin-2(1H)-one (2h).[1a] R_f = 0.2 (50% ethyl acetate/hexane); yellow solid; yield 55 mg (87%); mp: 281-283 ºC; ^{1}H NMR (700 MHz, DMSO-d_6) δ 12.10 (s, 1H), 7.50 (d, J = 8.4 Hz, 2H), 7.28 (d, J = 8.4 Hz, 2H), 7.22 – 7.18 (m, 1H), 7.14 (t, J = 7.7 Hz, 2H), 7.10 – 7.04 (m, 1H), 5.34 (s, 2H); $^{13}C\{^{1}H\}$ NMR (175 MHz, DMSO-d_6) δ 155.8, 153.7, 135.3, 131.6, 129.1, 126.2, 126.0, 123.8, 123.2, 120.4, 115.8, 115.4, 45.1.



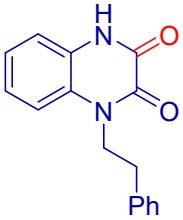
1-Ethyl-1,4-dihydroquinoxaline-2,3-dione (2i).[1a] R_f = 0.1 (50% ethyl acetate/hexane); pale yellow solid; yield 54 mg (84%); mp: 282-284 ºC; ^{1}H NMR (700 MHz, DMSO- d_6) δ 12.02 (s, 1H), 7.40 (d, J = 7.7 Hz, 1H), 7.20-7.16 (m, 3H), 4.16-4.13 (m, 2H), 1.21 (t, J = 7.0 Hz, 3H); ^{13}C{^{1}H} NMR (175 MHz, DMSO- d_6) δ 154.8, 153.6, 125.9, 125.8, 123.5, 123.4, 115.8, 114.8, 37.3, 12.0.



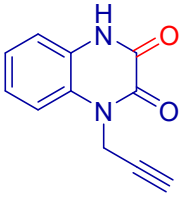
1-Butyl-1,4-dihydroquinoxaline-2,3-dione (2j).[1a] R_f = 0.2 (50% ethyl acetate/hexane); yellow solid; yield 55 mg (85%); mp: 183-185 ºC; ^{1}H NMR (700 MHz, DMSO-d_6) δ 12.02 (s, 1H), 7.37 (d, J = 8.4 Hz, 1H), 7.19-7.15 (m, 3H), 4.12 – 4.06 (m, 2H), 1.62-1.57 (m, 2H), 1.41-1.35 (m, 2H), 0.92 (t, J = 7.7 Hz, 3H); ^{13}C{^{1}H} NMR (175 MHz, DMSO-d_6) δ 155.0, 153.6, 126.1, 125.8, 123.5, 123.3, 115.8, 114.9, 41.9, 28.6, 19.6, 13.7.



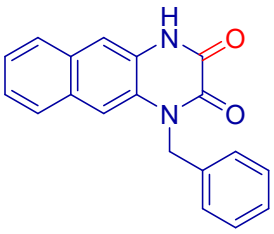
1-Phenethyl-1,4-dihydroquinoxaline-2,3-dione (2k).[1a] R_f = 0.1 (50% ethyl acetate/hexane); pale yellow solid; yield 49 mg (72%); mp: 228-230 ºC; ^{1}H NMR (700 MHz, DMSO-d_6) δ 12.04 (s, 1H), 7.45 (d, J = 7.7 Hz, 1H), 7.31 (d, J = 4.2 Hz, 4H), 7.25 – 7.16 (m, 4H), 4.32 – 4.27 (m, 2H), 2.93 – 2.89 (m, 2H); ^{13}C{^{1}H} NMR (175 MHz, DMSO-d_6) δ 155.1, 153.6, 138.2, 128.9, 128.6, 126.6, 126.1, 125.8, 123.7, 123.5, 115.9, 115.0, 43.6, 32.5.



1-(Prop-2-yn-1-yl)-1,4-dihydroquinoxaline-2,3-dione (2l).[1a] R_f = 0.2 (50% ethyl acetate/hexane); yellow solid; yield 45 mg (70%); mp 279-281 ºC; ^{1}H NMR (700 MHz, DMSO-d_6) δ 12.11 (s, 1H), 7.42 (d, J = 7.0 Hz, 1H), 7.21 (s, 3H), 4.95 (s, 2H), 3.31 (s, 1H); ^{13}C{^{1}H} NMR (175 MHz, DMSO-d_6) δ 154.7, 153.4, 125.8, 125.6, 124.0, 123.3, 115.8, 115.4, 78.1, 75.1, 32.0.

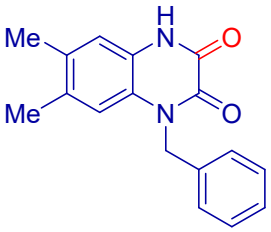


4-Benzyl-3,4-dihydrobenzo[g]quinoxalin-2(1H)-one (2m).[5] R_f = 0.4 (50% ethyl



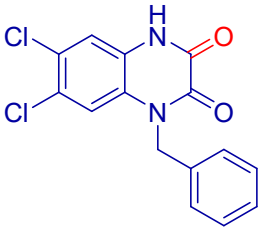
acetate/hexane); yellow solid; yield 58 mg (92%); mp: >300 ºC; ^{1}H NMR (700 MHz, DMSO-d_6) δ 12.28 (s, 1H), 7.82 (d, J = 8.4 Hz, 1H), 7.77 (d, J = 8.4 Hz, 1H), 7.69 (s, 1H), 7.60 (s, 1H), 7.41-7.38 (m, 3H), 7.36 (d, J = 7.0 Hz, 1H), 7.33 (t, J = 7.7 Hz, 2H), 7.25 (t, J = 7.0 Hz, 1H), 5.48 (s, 2H); ^{13}C{^{1}H} NMR (175 MHz, DMSO-d_6) δ 155.4, 153.5, 135.7, 129.3, 129.2, 128.6, 127.3, 127.2, 126.9, 126.8, 126.4, 126.2, 125.7, 125.1, 112.1, 111.4, 45.8.

1-Benzyl-6,7-dimethyl-1,4-dihydroquinoxaline-2,3-dione (3a).[1a] R_f = 0.2 (50% ethyl



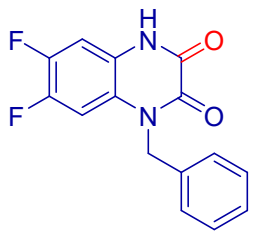
acetate/hexane); yellow solid; yield 50 mg (80%); mp: >300 ºC; ^{1}H NMR (700 MHz, DMSO-d_6) δ 12.00 (s, 1H), 7.34 – 7.22 (m, 6H), 7.01 (s, 1H), 6.95 (s, 1H), 5.34 (s, 2H), 2.15 (s, 3H), 2.12 (s, 3H); ^{13}C{^{1}H} NMR (175 MHz, DMSO-d_6) δ 155.7, 153.8, 136.0, 132.0, 131.4, 128.7, 127.3, 126.7, 124.2, 123.5, 116.4, 116.2, 45.5, 19.3, 18.8.

1-Benzyl-6,7-dichloro-1,4-dihydroquinoxaline-2,3-dione (3b).[1a] R_f = 0.4 (50% ethyl



acetate/hexane); yellow solid; yield 55 mg (87%); mp: >300 ºC; ^{1}H NMR (700 MHz, DMSO-d_6) δ 12.23 (s, 1H), 7.37 (s, 1H), 7.35 – 7.29 (m, 5H), 7.26 (t, J = 7.0 Hz, 1H), 5.36 (s, 2H); ^{13}C{^{1}H} NMR (175 MHz, DMSO-d_6) δ 155.4, 153.5, 135.2, 128.8, 127.5, 126.8, 126.7, 126.4, 125.3, 124.7, 116.9, 116.5, 45.8.

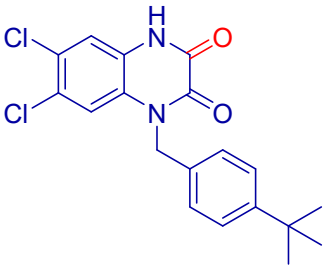
1-Benzyl-6,7-difluoro-1,4-dihydroquinoxaline-2,3-dione (3c).[1a] R_f = 0.3 (50% ethyl



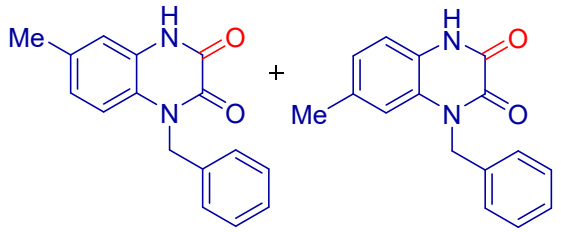
acetate/hexane); pale yellow solid; yield 53 mg (84%); mp 269-271 ºC; ^{1}H NMR (700 MHz, DMSO-d_6) δ 12.17 (s, 1H), 7.36 – 7.28 (m, 5H), 7.28 – 7.23 (m, 2H), 7.17-7.15 (m, 1H), 5.33 (s, 2H); ^{13}C{^{1}H} NMR (175 MHz, DMSO-d_6) δ 155.6, 153.6, 145.4 (dd, J = 237.1, 9.8 Hz),

145.1 (dd, J = 237.3, 12.2 Hz), 135.3, 128.9, 127.6, 126.9, 123.3 (d, J = 8.4 Hz), 122.8 (d, J = 9.5 Hz), 105.1 (d, J = 23.5 Hz), 104.4 (d, J = 21.9 Hz), 46.2.

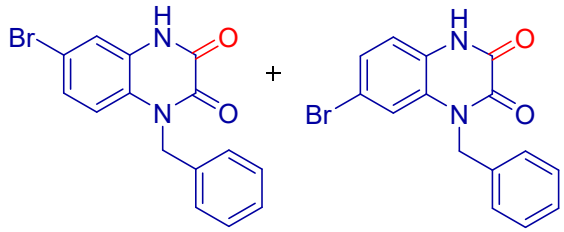
1-(4-(*tert*-Butyl)benzyl)-6,7-dichloro-1,4-dihydroquinoxaline-2,3-dione (3d).[5] R_f = 0.8 (50% ethyl acetate/hexane); reddish brown solid; yield 59 mg (82%); mp 283-285 ºC; ^{1}H NMR (700 MHz, DMSO-d_6) δ 12.23 (s, 1H), 7.46 (s, 1H), 7.34-7.24 (m, 5H), 5.32 (s, 2H), 1.24 (s, 9H); ^{13}C{^{1}H} NMR (175 MHz, DMSO-d_6) δ 155.2, 153.3, 149.8, 132.2, 126.8, 126.5, 126.3, 125.4, 125.2, 124.6, 116.8, 116.4, 45.4, 34.2, 31.1.



1-Benzyl-6-methyl-1,4-dihydroquinoxaline-2,3-dione and 1-Benzyl-7-methyl-1,4-dihydroquinoxaline-2,3-dione (3e).[1a] R_f = 0.4 (50% ethyl acetate/hexane); pale yellow solid; yield 53 mg (83%); mp 259-261 ºC; Two regioisomers with 63:37 Ratio; ^{1}H NMR (700 MHz, DMSO-d_6) δ 12.07 (s, 1.6H), 7.33-7.29 (m, 4H), 7.28-7.23 (m, 5H), 7.09 (d, J = 7.7 Hz, 0.6H), 7.04 (d, J = 8.4 Hz, 1H), 7.01 (s, 0.6H), 6.99 (s, 1H), 6.96 (d, J = 7.7 Hz, 0.6H), 6.87 (d, J = 8.4 Hz, 1H), 5.34 (d, J = 6.4 Hz, 3.2H), 2.23 (s, 3H), 2.20 (s, 1.8H); ^{13}C{^{1}H} NMR (175 MHz, DMSO-d_6) δ 156.0, 155.8, 154.1, 153.8, 136.0, 135.9, 133.5, 132.9, 128.9, 128.9, 127.5, 126.9, 126.8, 126.4, 125.8, 124.7, 124.3, 124.2, 123.7, 116.1, 115.9, 115.8, 115.6, 45.8, 45.8, 21.0, 20.5.

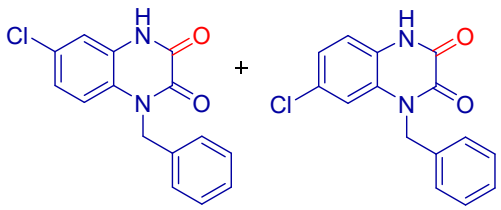


1-Benzyl-6-bromo-1,4-dihydroquinoxaline-2,3-dione and 1-Benzyl-7-bromo-1,4-dihydroquinoxaline-2,3-dione (3f).[1a] R_f = 0.4 (50% ethyl acetate/hexane); pale yellow solid; yield 48 mg (76%); mp 256-258 ºC; Two regioisomers with 67:33 Ratio; ^{1}H NMR (700 MHz, DMSO-d_6) δ 12.19 (s, 1.5H), 7.34 – 7.28



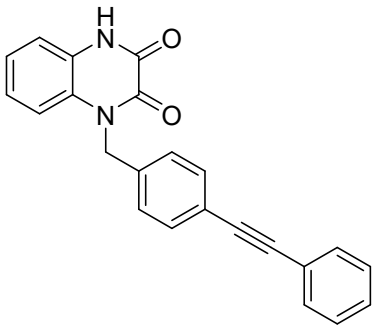
(m, 5H), 7.27 – 7.23 (m, 5H), 7.20 (dd, J = 9.1, 1.4 Hz, 1H), 7.12 (d, J = 8.4 Hz, 0.5H), 7.07 (d, J = 9.1 Hz, 1H), 5.34 (s, 1H), 5.32 (s, 2H); $^{13}C\{^1H\}$ NMR (175 MHz, DMSO-d_6) δ 156.0, 155.8, 154.0, 153.9, 135.6, 135.6, 129.2, 129.1, 128.1, 127.8, 127.8, 127.7, 126.9, 126.9, 126.7, 126.1, 126.0, 125.7, 118.2, 118.2, 117.9, 117.7, 46.2, 46.1.

1-Benzyl-6-chloro-1,4-dihydroquinoxaline-2,3-dione and 1-Benzyl-7-chloro-1,4-dihydroquinoxaline-2,3-dione (3g).[1a] R_f = 0.3 (50% ethyl aetate/hexane); play yellow solid;



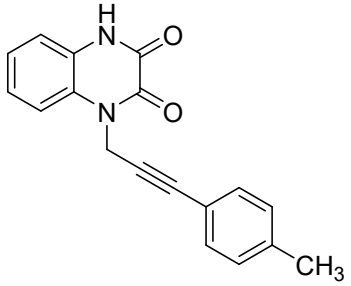
yield 53 mg (84%); mp: 248-250 ºC; Two regio isomers with 75:25 Ratio; ^1H NMR (400 MHz, DMSO-d_6) δ 12.17 (s, 1.3H), 7.37 – 7.22 (m, 7.6H), 7.21-7.17 (m, 2.5H), 7.16 – 7.07 (m, 2H), 5.38 (s, 0.7H), 5.35 (s, 2H); $^{13}C\{^1H\}$ NMR (100 MHz, DMSO-d_6) δ 155.6, 155.4, 153.6, 153.4, 135.4, 135.4, 128.7, 128.6, 127.6, 127.4, 127.3, 127.3, 126.9, 126.6, 125.5, 125.1, 123.4, 122.6, 117.1, 115.1, 114.9, 45.8, 45.6.

1-(4-(phenylethynyl)benzyl)-1,4-dihydroquinoxaline-2,3-dione (5a). [1a] R_f = 0.3 (50% ethyl



acetate/hexane); pale yellow solid; yield 46 mg (72%); mp: > 300 ºC, ^1H NMR (400 MHz, DMSO-d_6) δ 12.14 (s, 1H), 7.52 (dd, J = 12.0, 6.4 Hz, 4H), 7.41-7.36 (m, 5H), 7.21 (d, J = 8.0 Hz, 1H), 7.14 (t, J = 7.6 Hz, 2H), 7.08 (d, J = 7.6 Hz, 1H), 5.41 (s, 2H).

1-(3-(p-tolyl)prop-2-yn-1-yl)-1,4-dihydroquinoxaline-2,3-dione (5b). [5] R_f = 0.3 (50% ethyl acetate/hexane); pale yellow solid; yield 57 mg (65%); mp: 293 ºC, ^1H NMR (400 MHz,



DMSO-d_6) δ 12.12 (s, 1H), 7.52 (d, J = 8.0 Hz, 1H), 7.29 - 7.21 (m, 5H), 7.16 (d, J = 7.6 Hz, 2H), 5.19 (s, 2H), 2.28 (s, 3H).

NMR SPECTRA

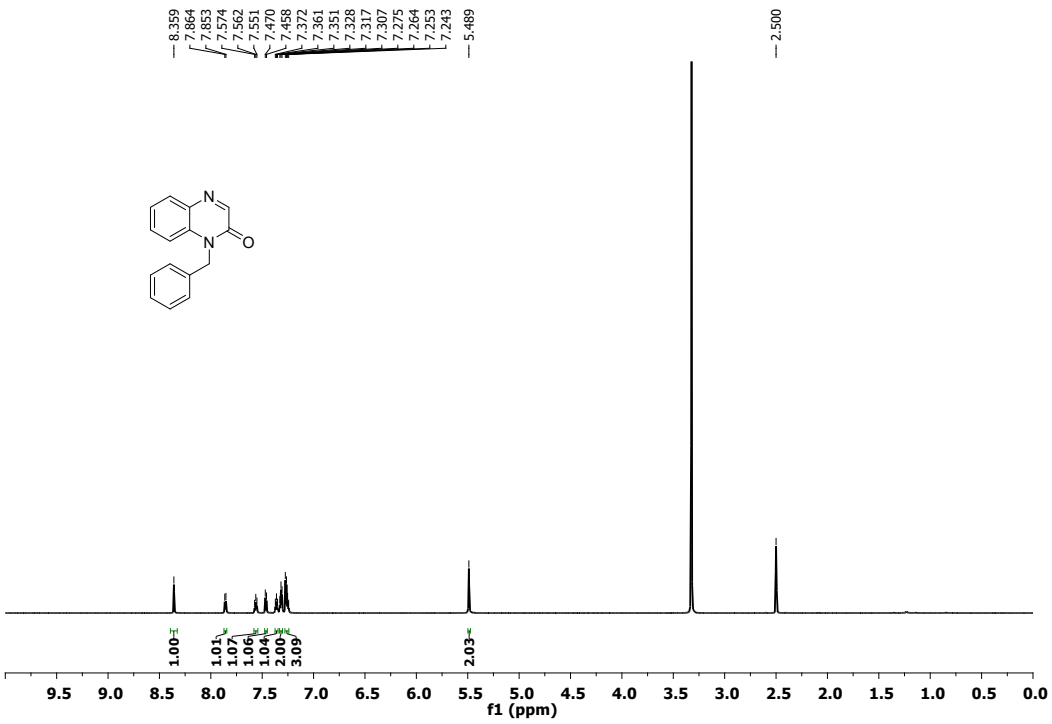


Figure S17. ^{1}H NMR (700 MHz, DMSO-d_6) spectrum of 1-benzyl-quinoxalin-2(1H)-one (**1a**).

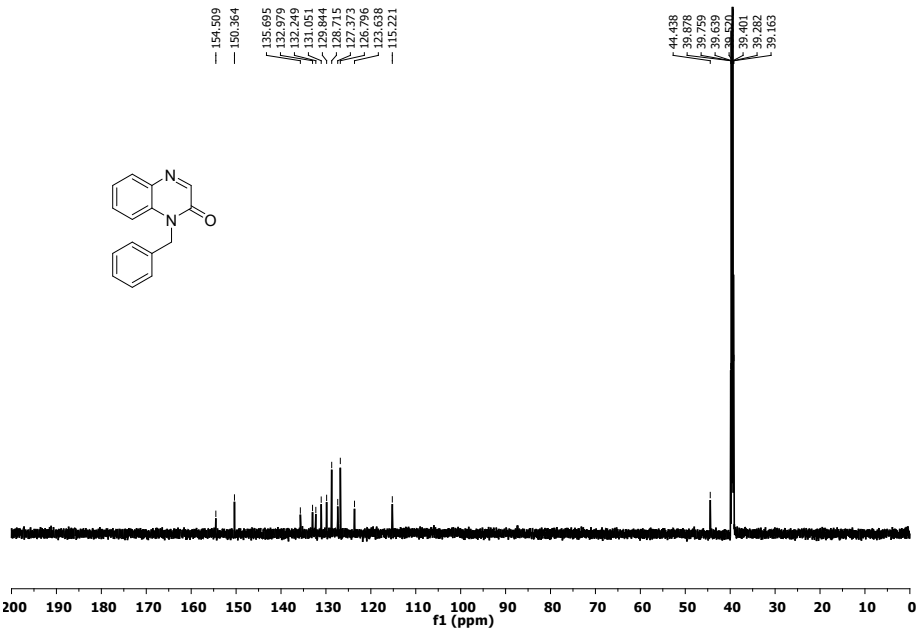


Figure S18. ^{13}C{^{1}H} NMR (175 MHz, DMSO-d_6) spectrum of 1-benzylquinoxalin-2(1*H*)-one (**1a**)

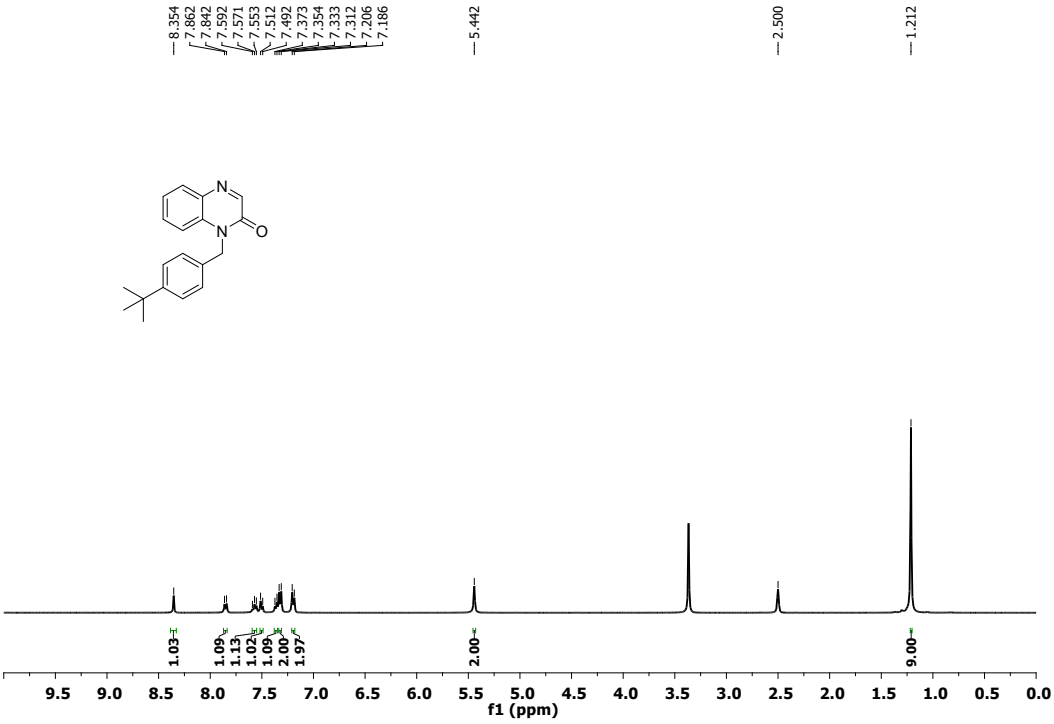


Figure S19. ^{1}H NMR (400 MHz, DMSO-d_6) spectrum of 1-(4-(*tert*-butyl)benzyl)quinoxalin-2(1*H*)-one (**1b**).

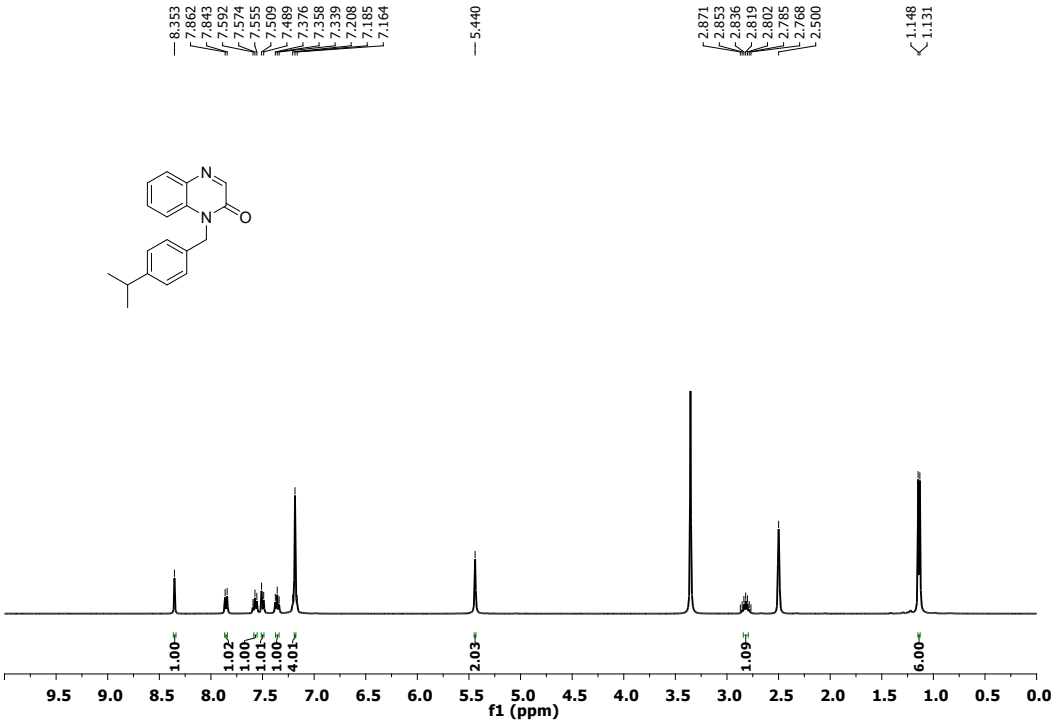


Figure S20. ^{1}H NMR (400 MHz, DMSO-d_6) spectrum of 1-(4-isopropylbenzyl)quinoxalin-2(1*H*)-one (**1c**).

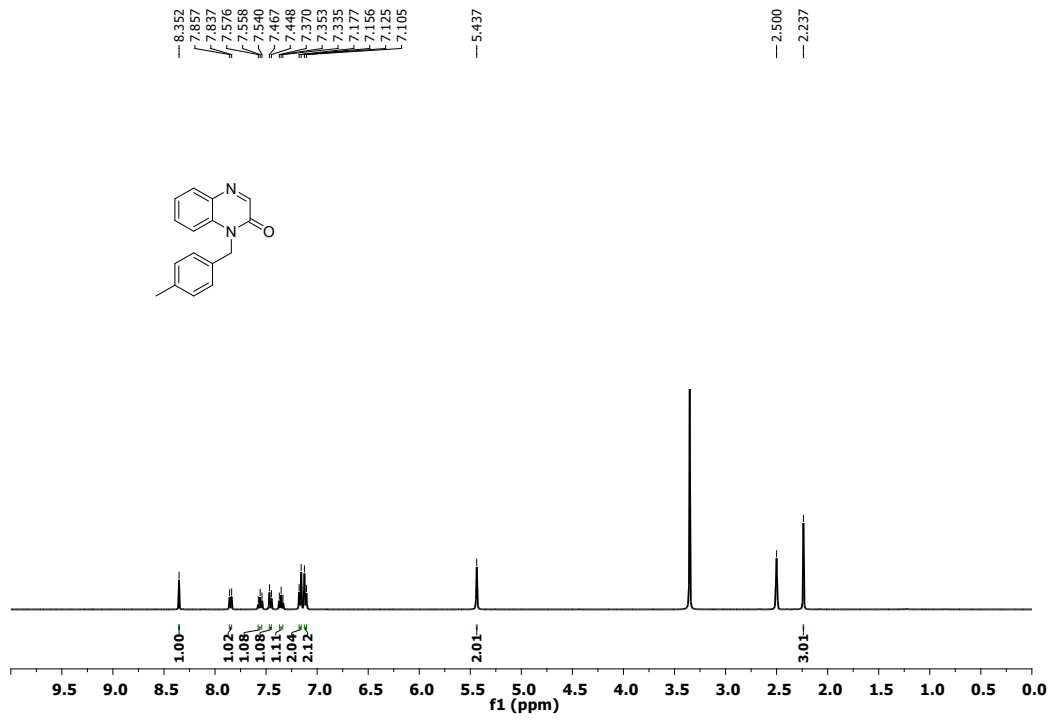


Figure S21. ^{1}H NMR (400 MHz, DMSO-d_6) spectrum of 1-(4-methylbenzyl)quinoxalin-2(1*H*)-one (**1d**).

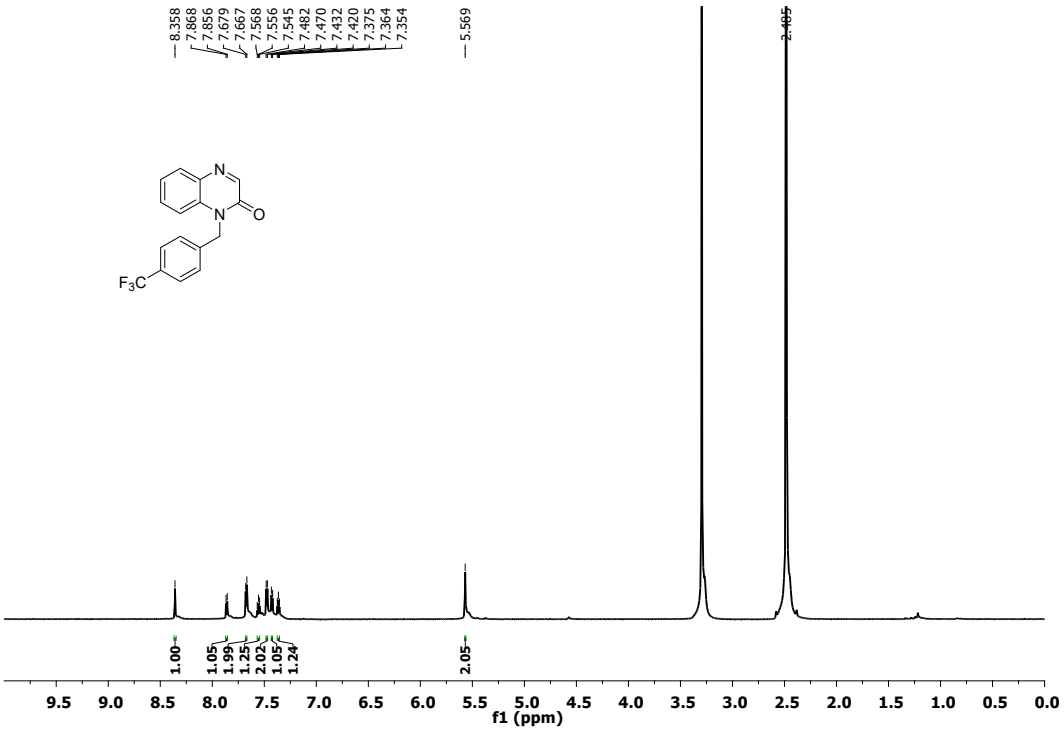


Figure S22. ^{1}H NMR (700 MHz, DMSO-d_6) spectrum of 1-(4-(trifluoromethyl)benzyl)quinoxalin-2(1*H*)-one (**1e**).

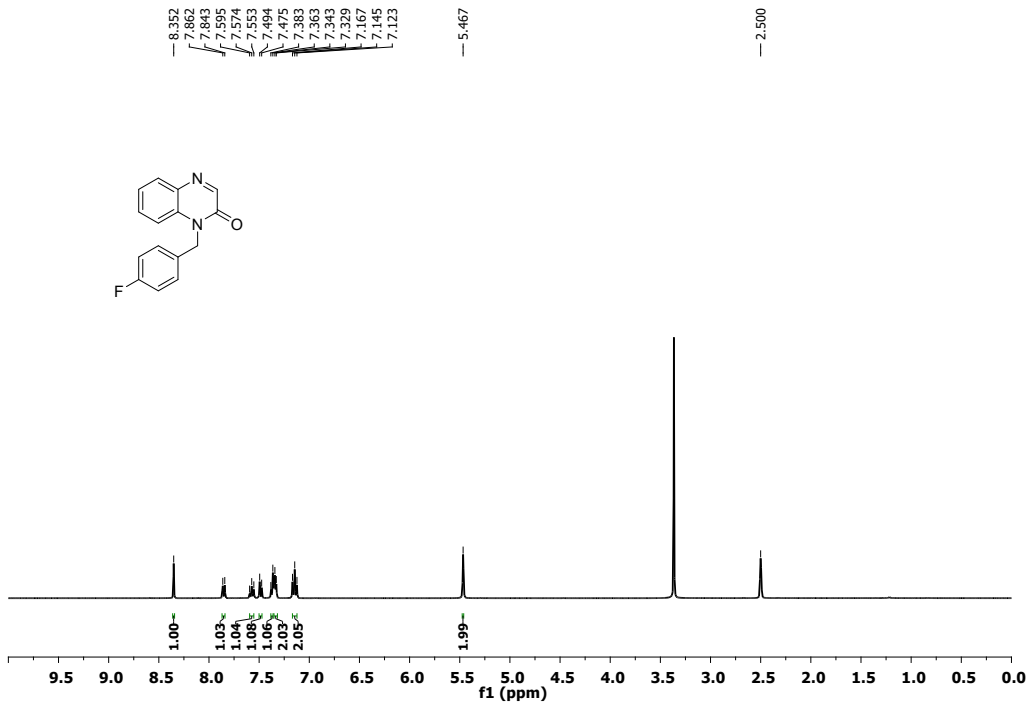


Figure S23. ^{1}H NMR (400 MHz, DMSO-d_6) spectrum of 1-(4-fluorobenzyl)quinoxalin-2(1***H***)-one (**1f**).

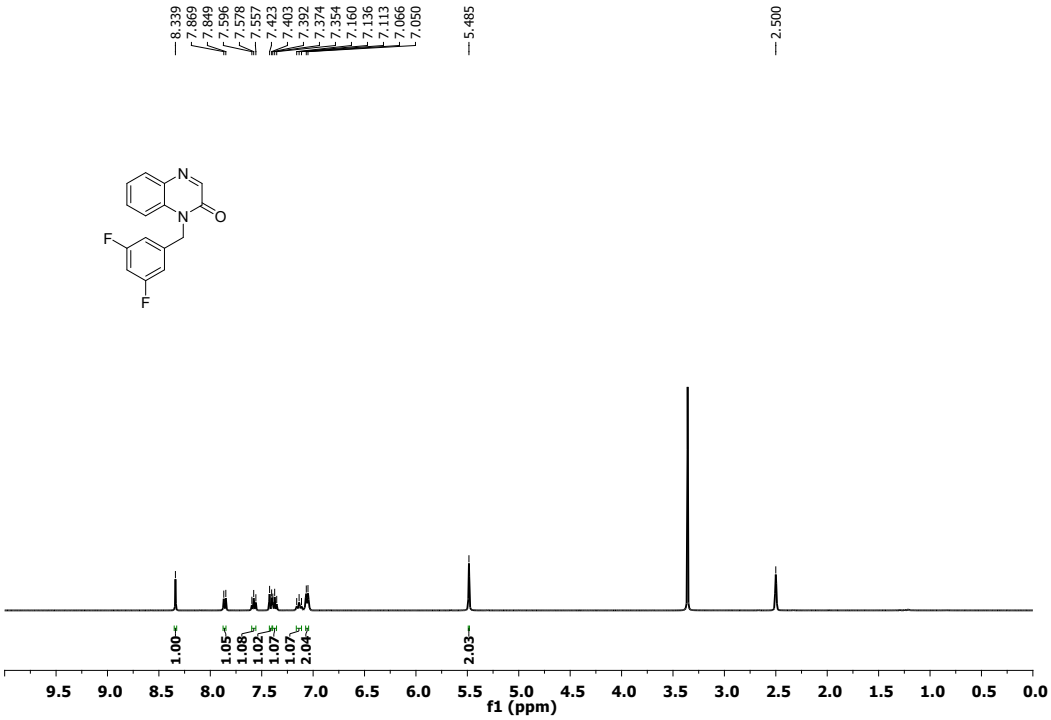


Figure S24. ^{1}H NMR (700 MHz, DMSO-d_6) spectrum of 1-(3,5-difluorobenzyl)quinoxalin-2(1*H*)-one (**1g**).

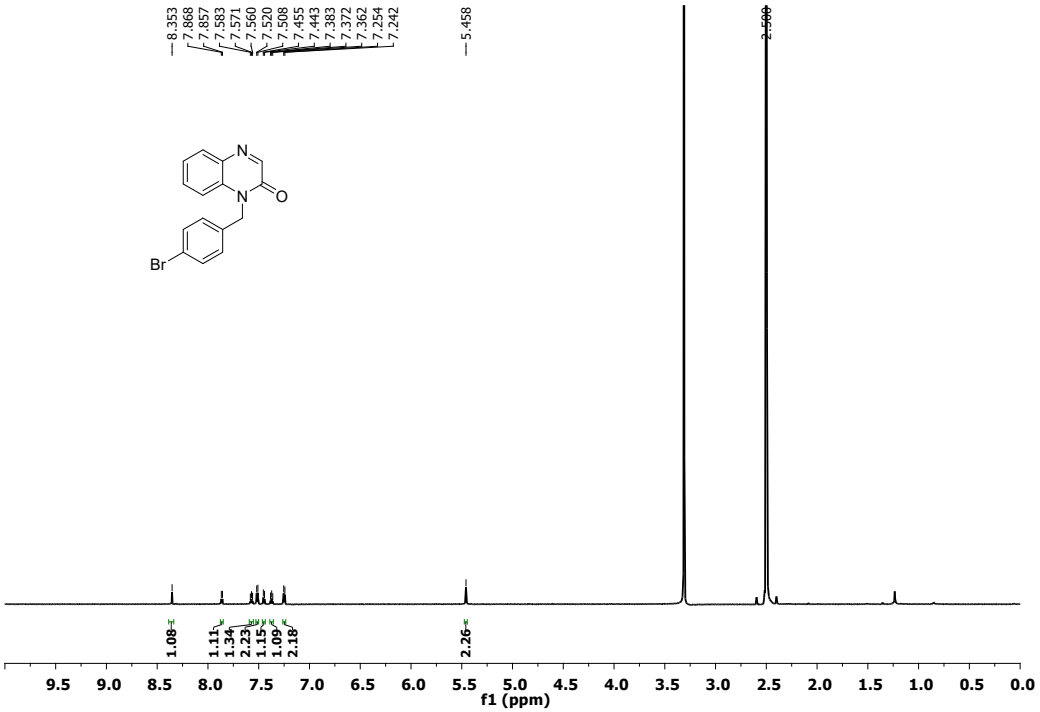


Figure S25. ^{1}H NMR (700 MHz, DMSO-d_6) spectrum of 1-(4-bromobenzyl)quinoxalin-2(1*H*)-one (**1h**).

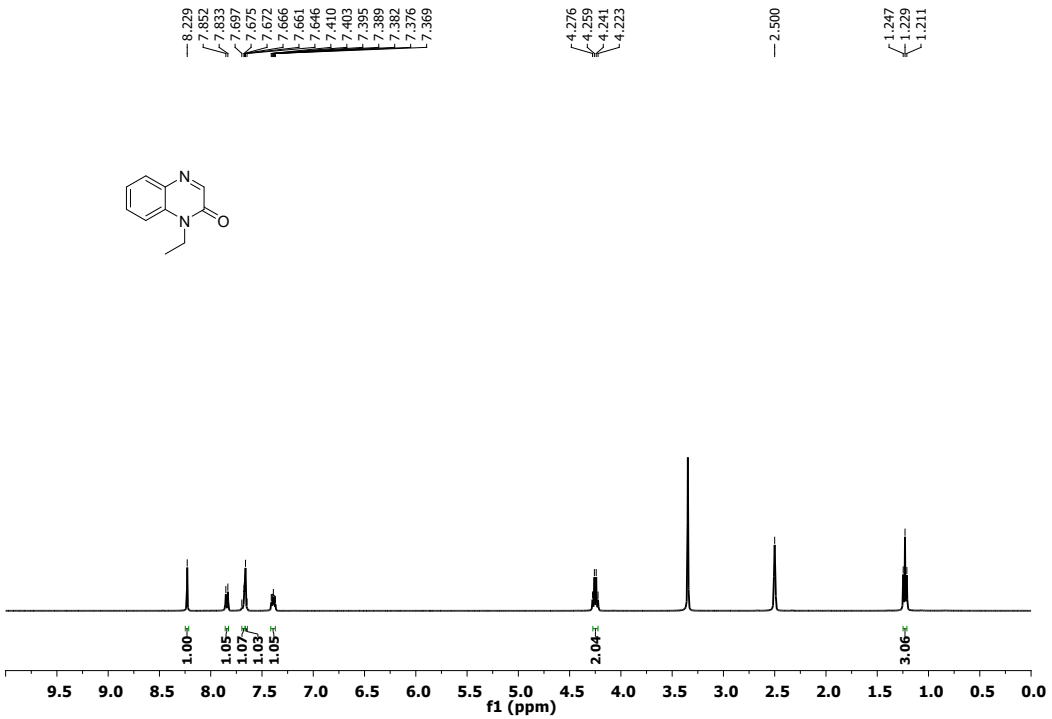


Figure S26. ^{1}H NMR (400 MHz, DMSO-d_6) spectrum of 1-ethylquinoxalin-2(1*H*)-one (**1i**).

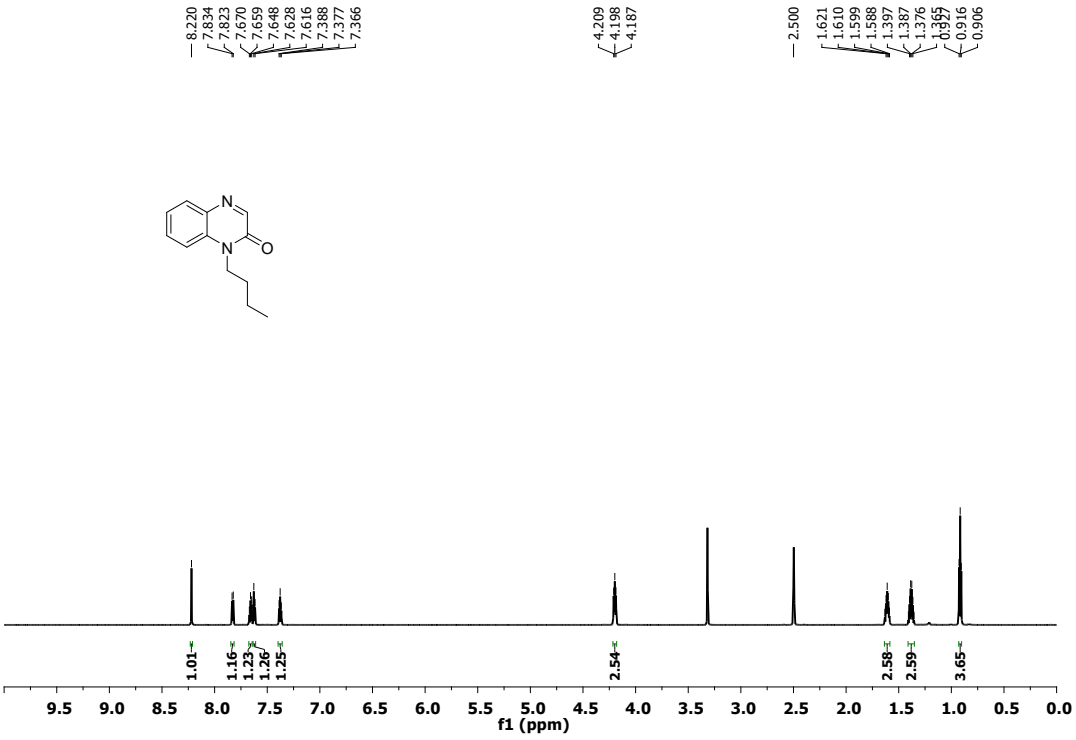


Figure S27. ^{1}H NMR (700 MHz, DMSO-d_6) spectrum of 1-butylquinoxalin-2(1*H*)-one (**1j**).

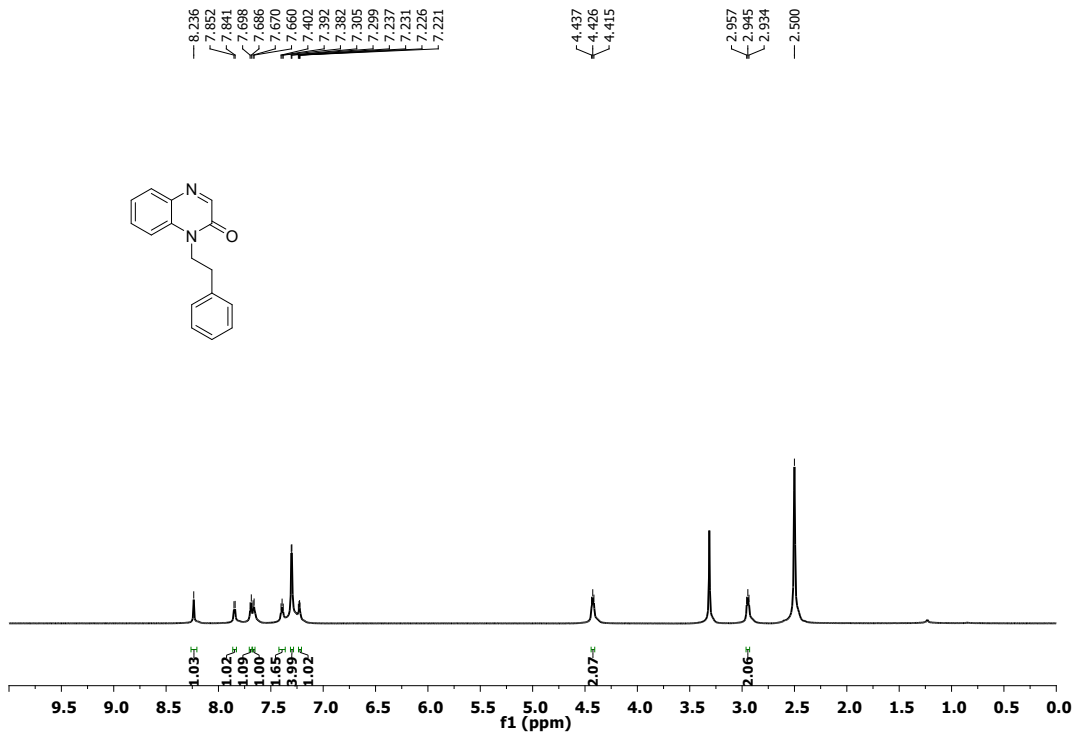


Figure S28. ^{1}H NMR (700 MHz, DMSO-d_6) spectrum of 1-phenethylquinoxalin-2(1*H*)-one (**1k**).

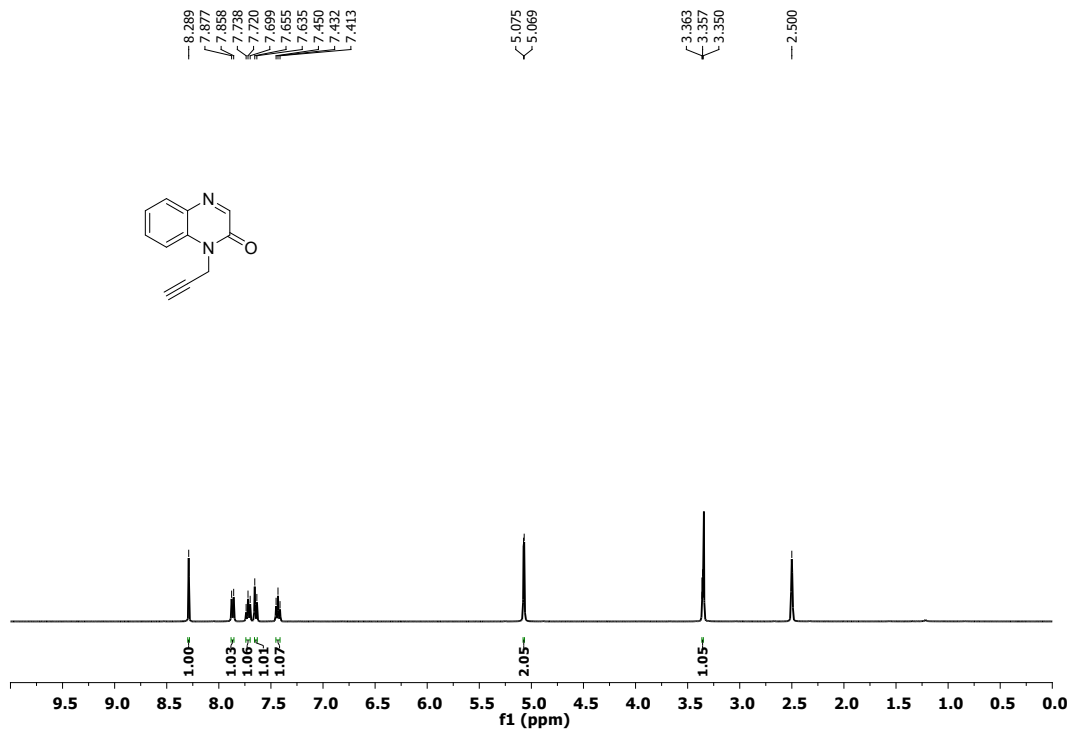


Figure S29. ^{1}H NMR (400 MHz, DMSO-d_6) spectrum of 1-(prop-2-yn-1-yl)quinoxalin-2(1*H*)-one (**1l**).

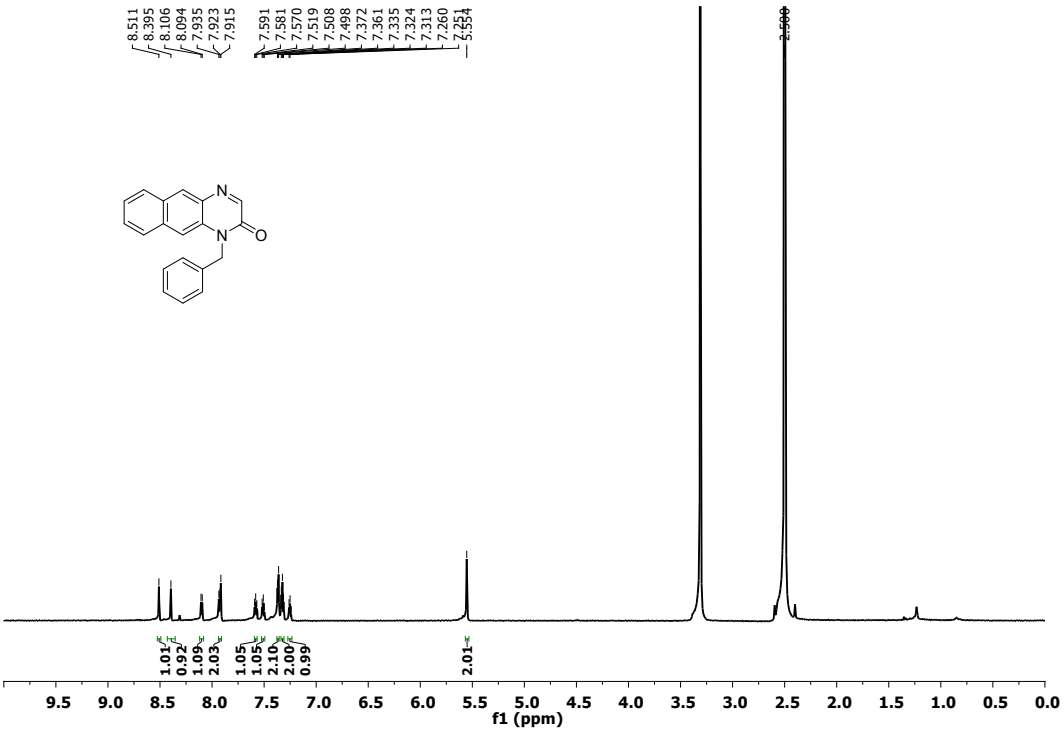


Figure S30. ^{1}H NMR (700 MHz, DMSO-d_6) spectrum of 1-benzylbenzo[g]quinoxalin-2(1*H*)-one (**1m**).

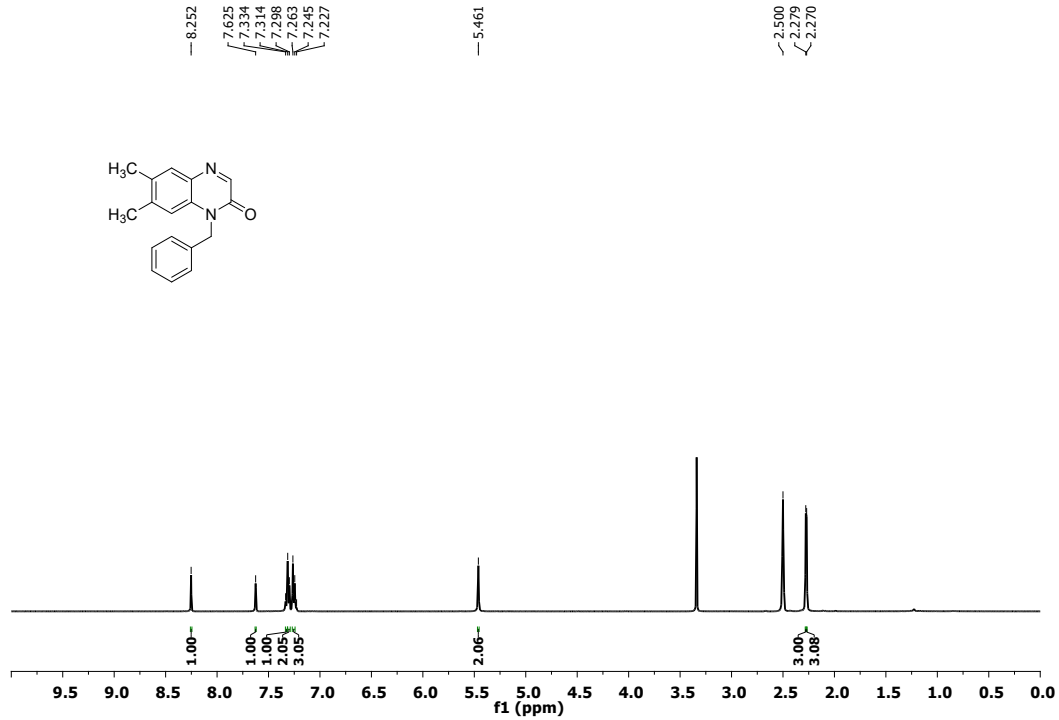


Figure S31. ^{1}H NMR (400 MHz, DMSO-d_6) spectrum of 1-benzyl-6,7-dimethylquinoxalin-2(1*H*)-one (**1n**).

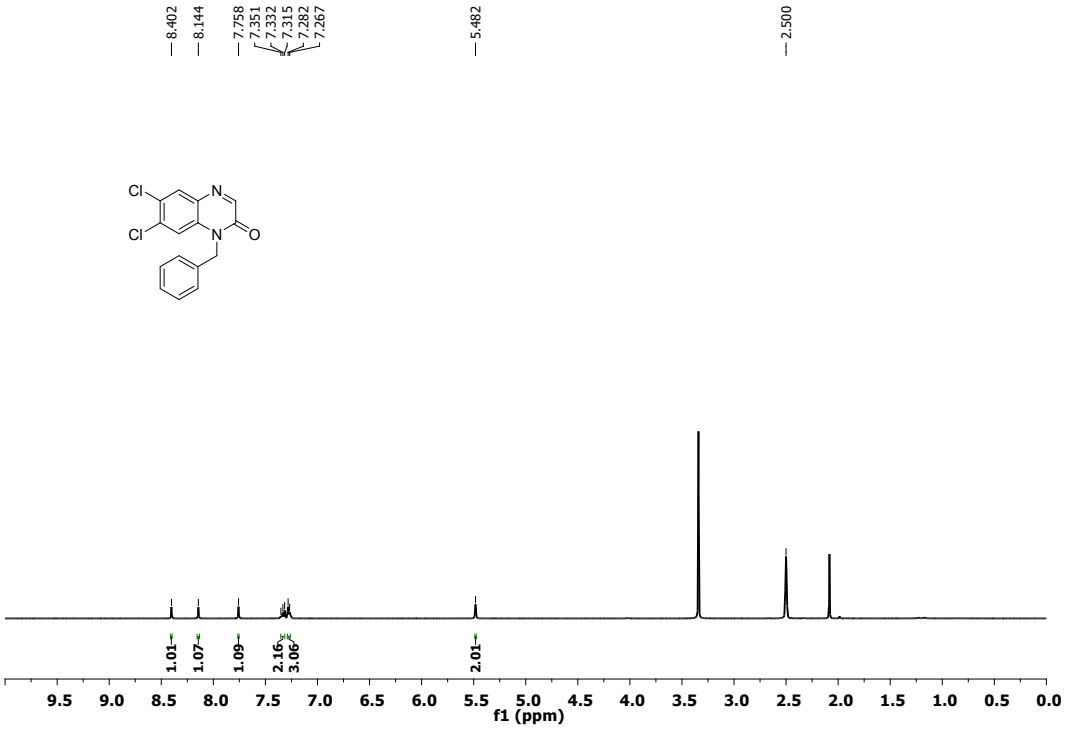


Fig. S32. ^{1}H NMR (400 MHz, DMSO-d_6) spectrum of 1-benzyl-6,7-dichloroquinoxalin-2(1*H*)-one (**1o**).

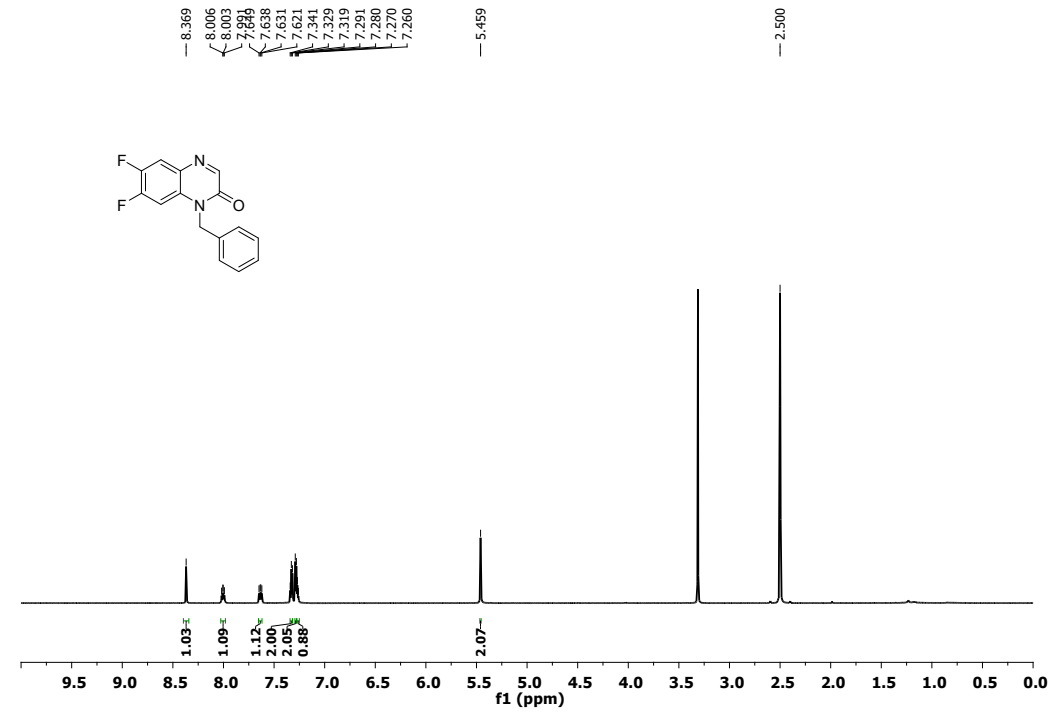


Figure S33. ^{1}H NMR (700 MHz, DMSO-d_6) spectrum of 1-benzyl-6,7-difluoroquinoxalin-2(1*H*)-one (**1p**).

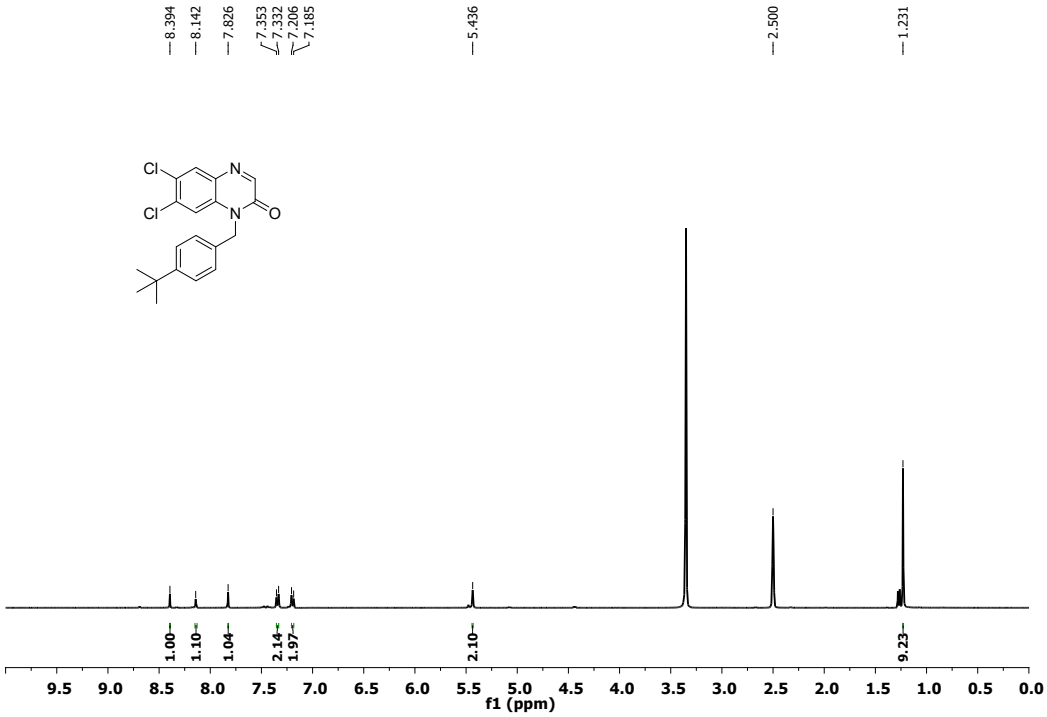


Figure S34. ^{1}H NMR (400 MHz, DMSO-d_6) spectrum of 1-(4-(*tert*-butyl)benzyl)-6,7-dichloroquinoxalin-2(1*H*)-one (**1q**).

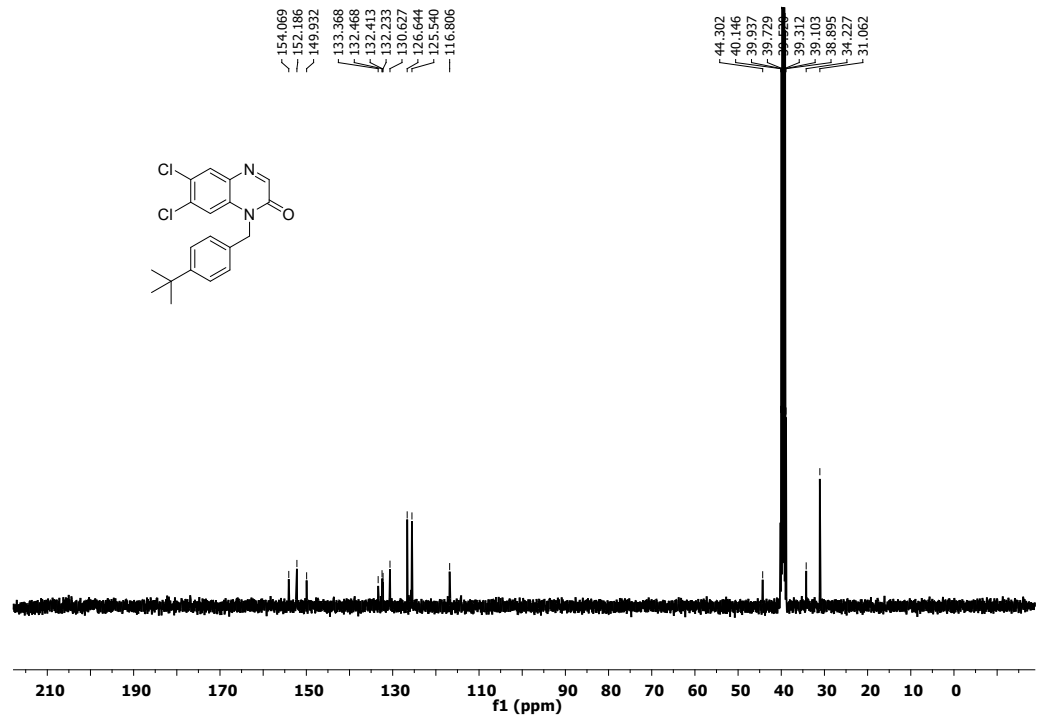


Figure S35. $^{13}C\{^{1}H\}$ NMR (100 MHz, DMSO-d_6) spectrum of 1-(4-(*tert*-butyl)benzyl)-6,7-dichloroquinoxalin-2(1*H*)-one (**1q**).

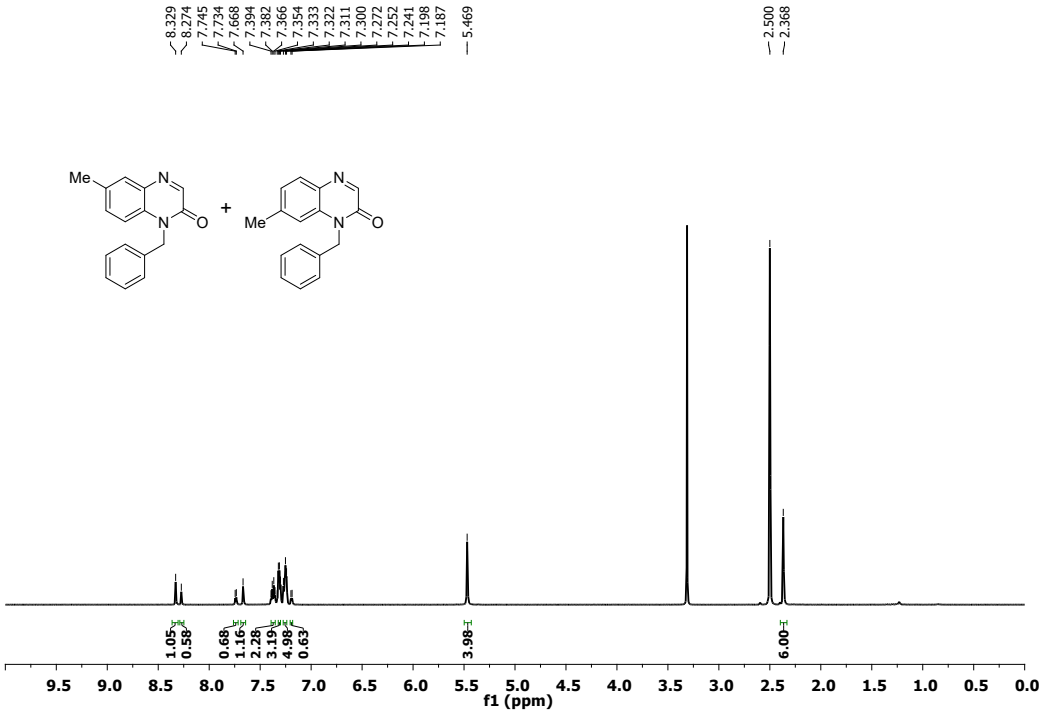


Figure S36. ^{1}H NMR (700 MHz, DMSO-d_6) spectrum of 1-benzyl-6-methylquinoxalin-2(1*H*)-one and 1-benzyl-7-methylquinoxalin-2(1*H*)-one (**1r**).

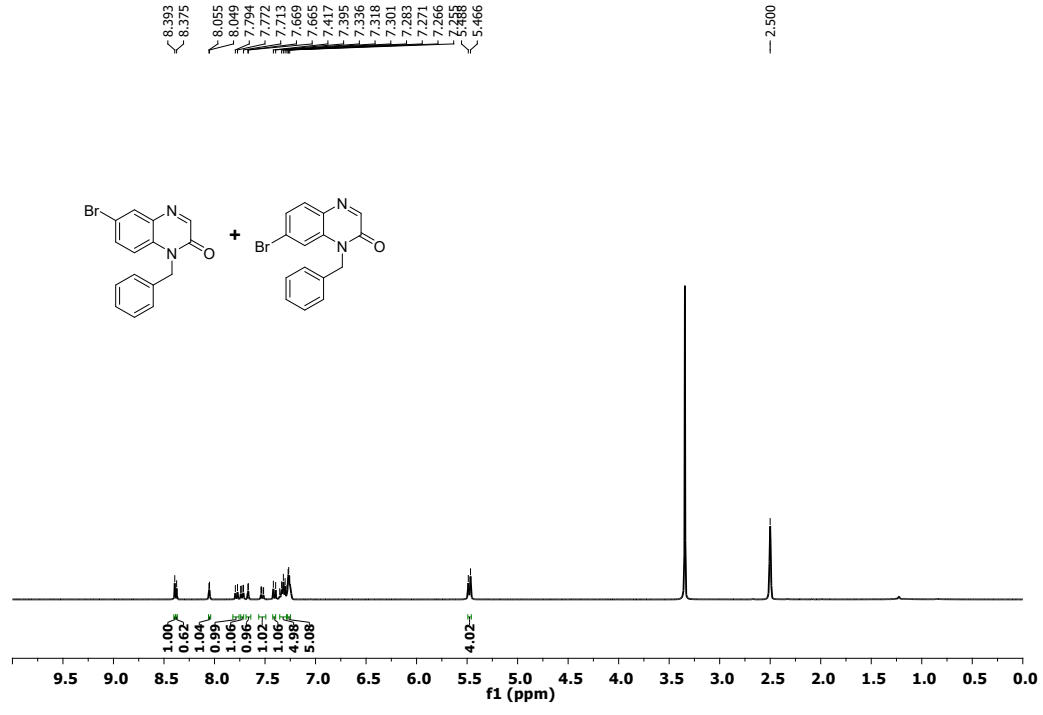


Figure S37. ^{1}H NMR (400 MHz, DMSO-d_6) spectrum of 1-benzyl-6-bromoquinoxalin-2(1*H*)-one and1-benzyl-7-bromoquinoxalin-2(1*H*)-one (**1s**).

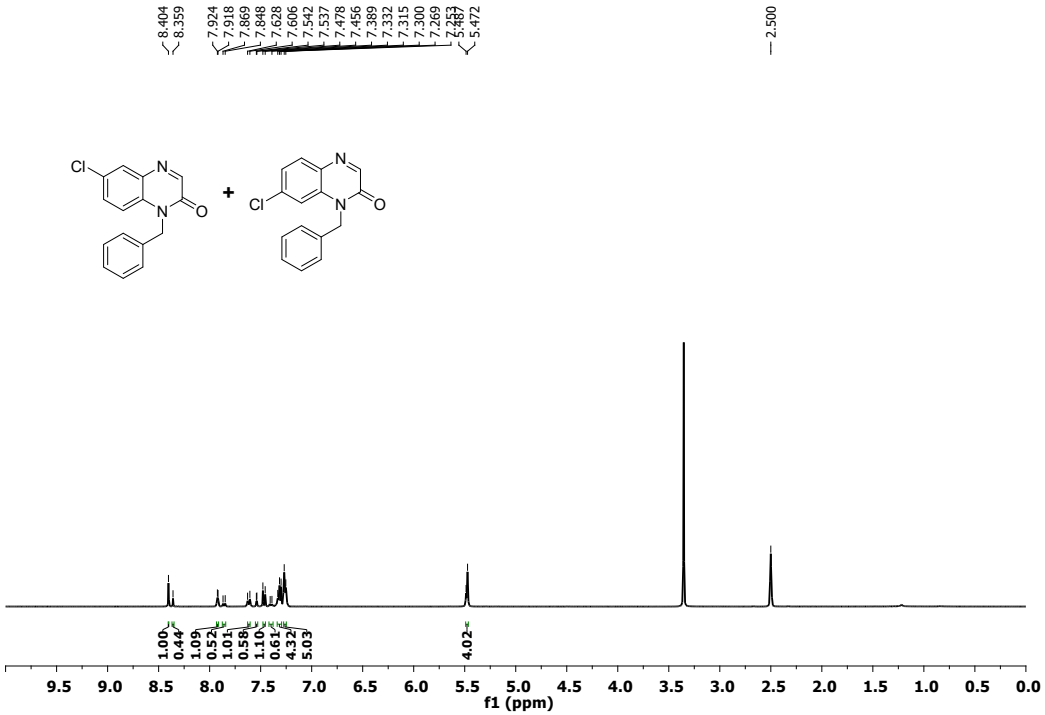


Figure S38. ^{1}H NMR (400 MHz, DMSO-d_6) spectrum of 1-benzyl-6-chloroquinoxalin-2(1*H*)-one and1-benzyl-7-chloroquinoxalin-2(1*H*)-one (**1t**).

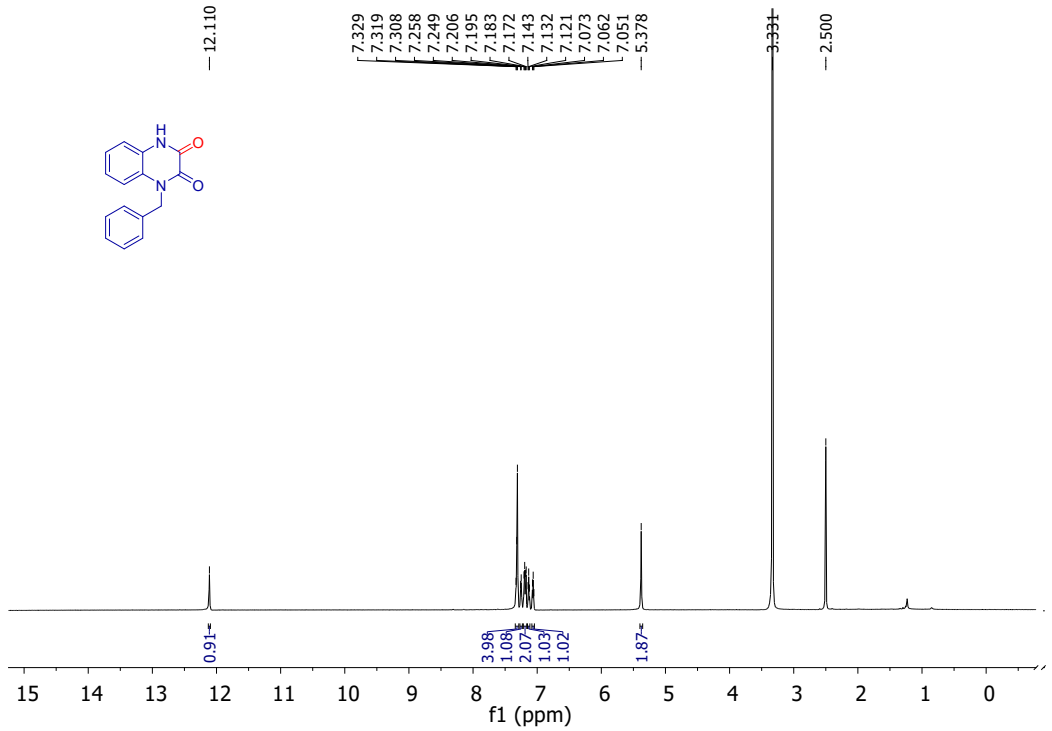


Figure S39. ^{1}H NMR (700 MHz, DMSO-d_6) spectrum of 1-benzyl-1,4-dihydroquinoxaline-2,3-dione (**2a**).

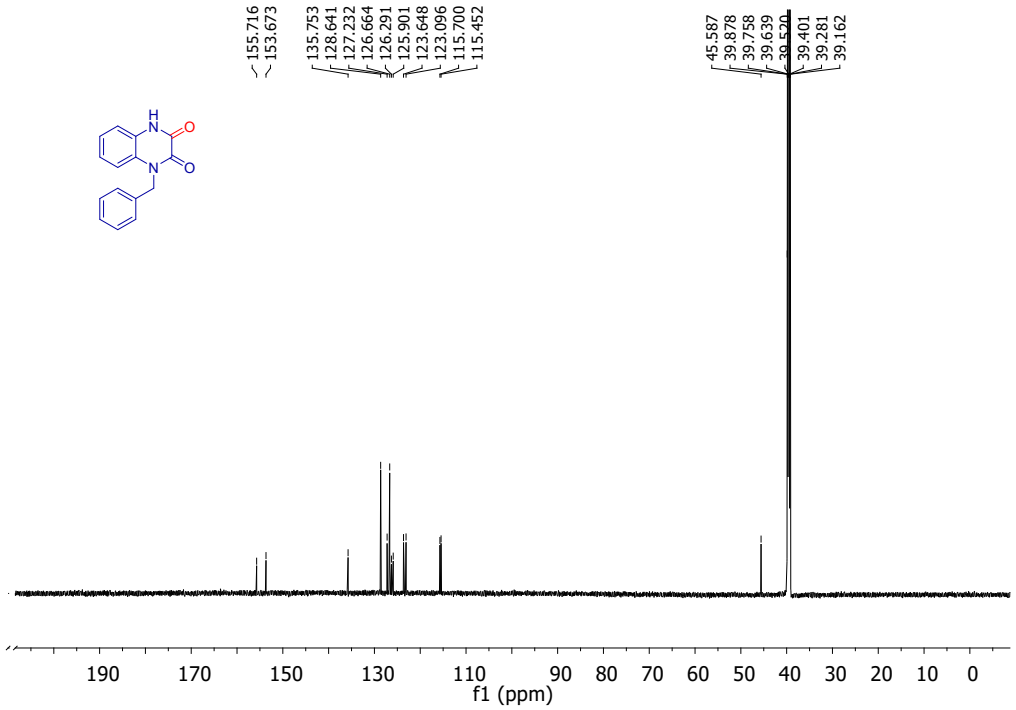


Figure S40. $^{13}C\{^{1}H\}$ NMR (175 MHz, DMSO-d_6) spectrum of 1-benzyl-1,4-dihydroquinoxaline-2,3-dione (**2a**)

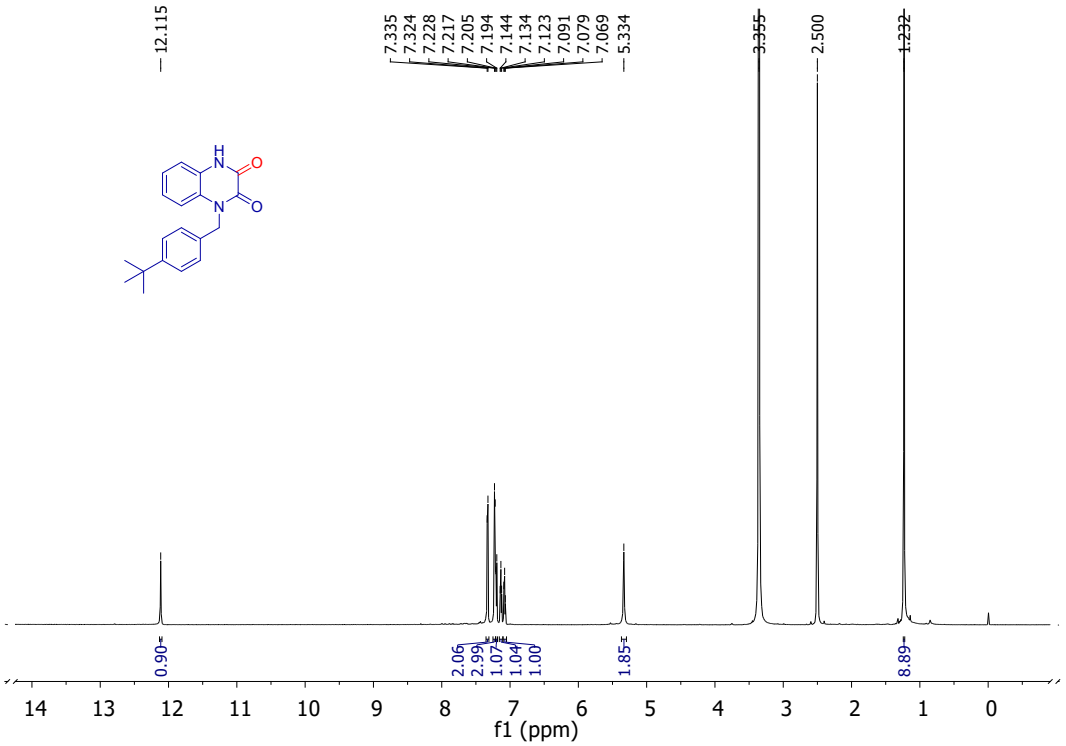


Figure S41. ^{1}H NMR (700 MHz, DMSO-d_6) spectrum of 1-(4-(*tert*-butyl)benzyl)-1,4-dihydroquinoxaline-2,3-dione (**2b**).

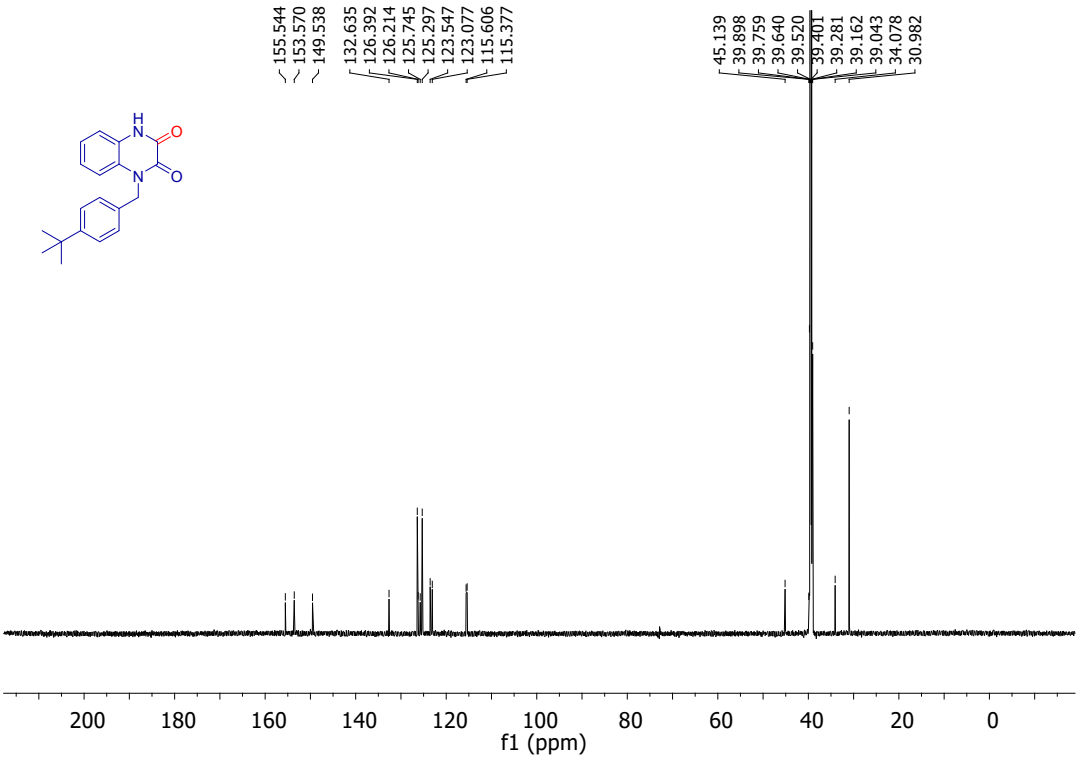


Figure S42. $^{13}C\{^{1}H\}$ NMR (175 MHz, DMSO-d_6) spectrum of 1-(4-(*tert*-butyl)benzyl)-1,4-dihydroquinoxaline-2,3-dione (**2b**).

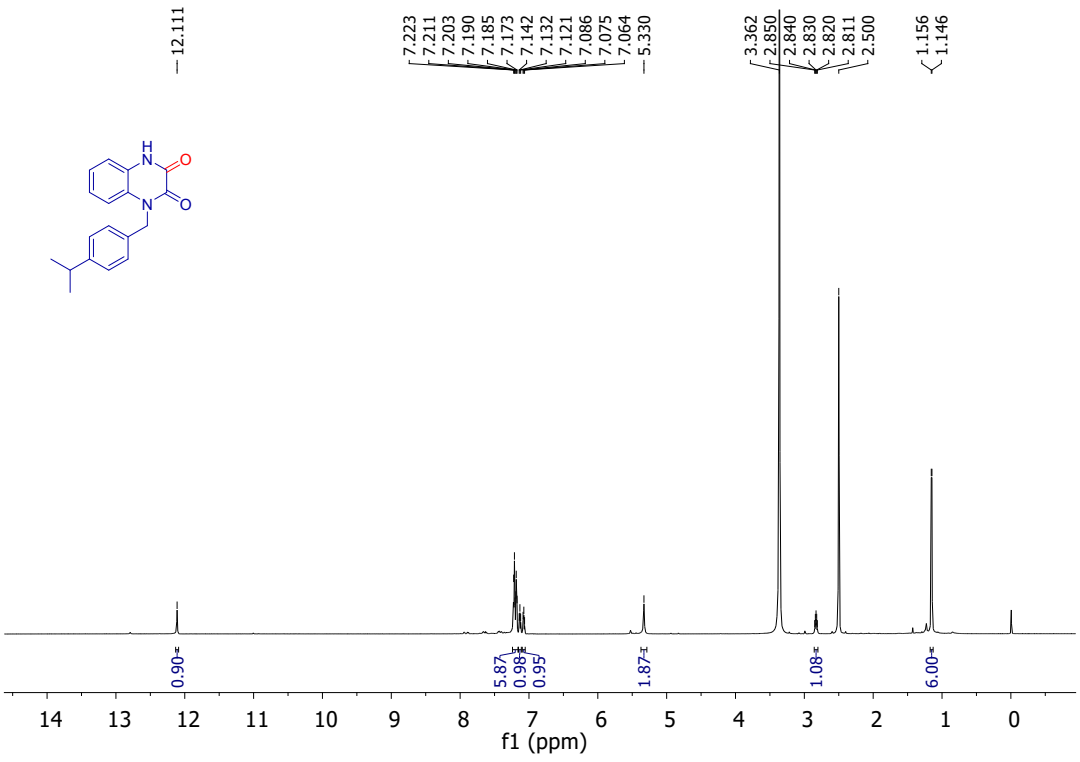


Figure S43. ^{1}H NMR (700 MHz, DMSO-d_6) spectrum of 1-(4-Isopropylbenzyl)-1,4-dihydroquinoxaline-2,3-dione (**2c**).

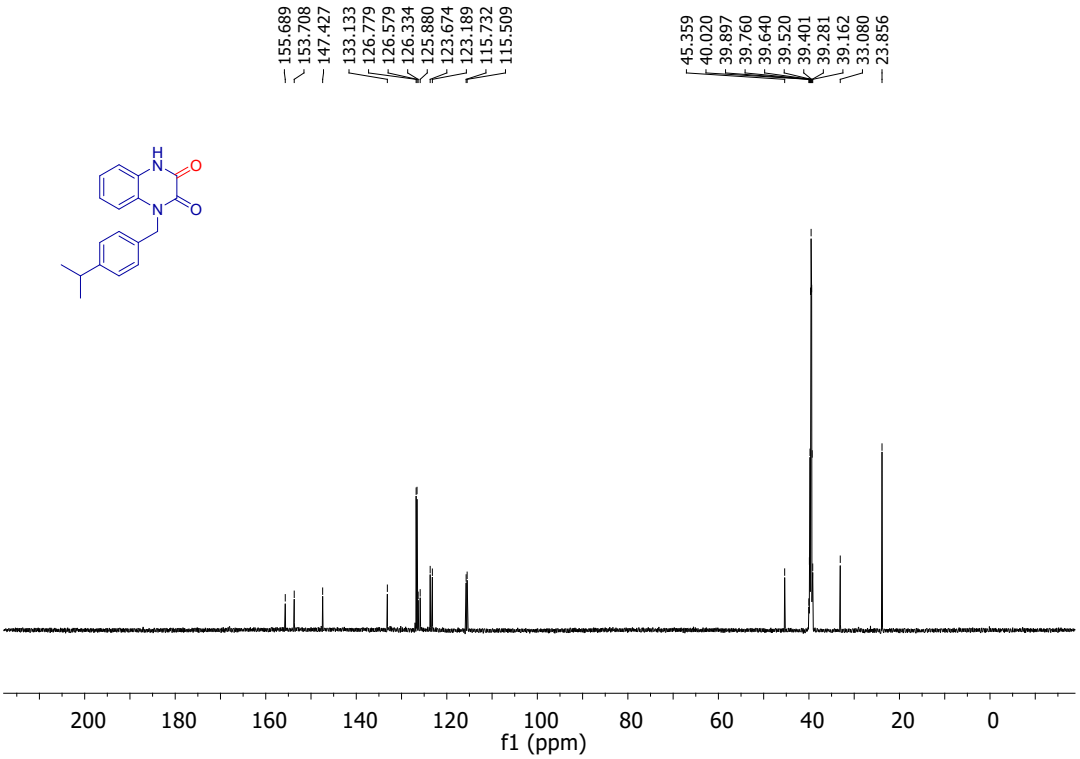


Figure S44. ^{13}C{^{1}H} NMR (175 MHz, DMSO-d_6) spectrum of 1-(4-isopropylbenzyl)-1,4-dihydroquinoxaline-2,3-dione (**2c**).

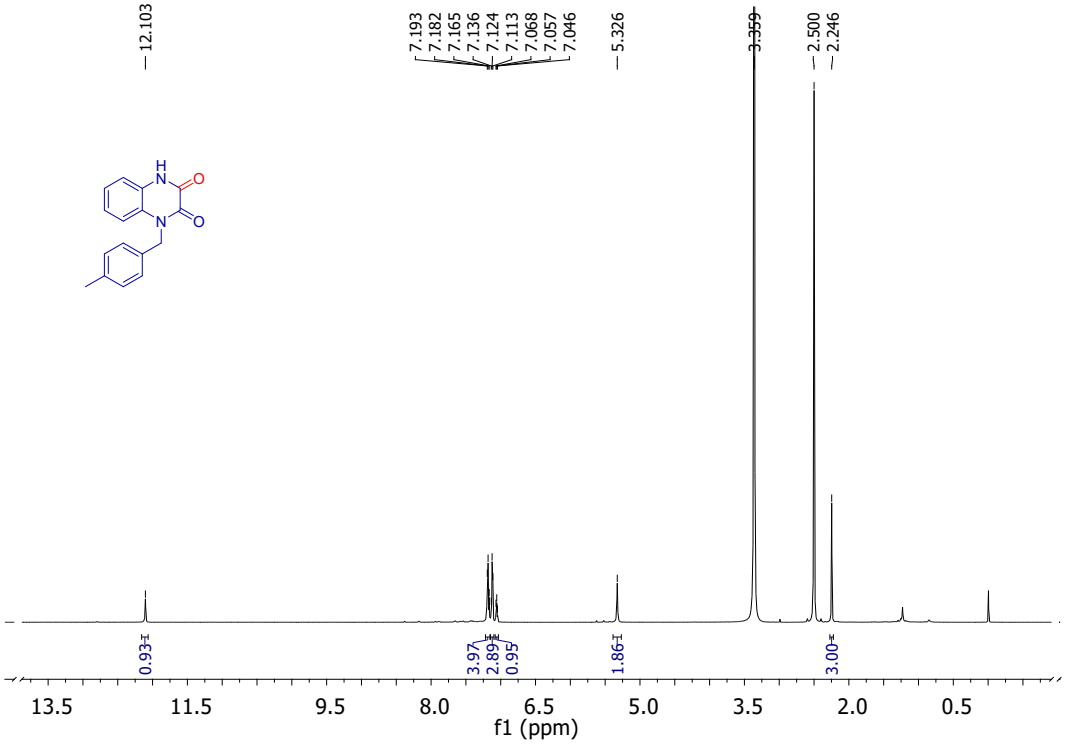


Figure S45. ^{1}H NMR (700 MHz, DMSO-d_6) spectrum of 1-(4-methylbenzyl)-1,4-dihydroquinoxaline-2,3-dione (**2d**).

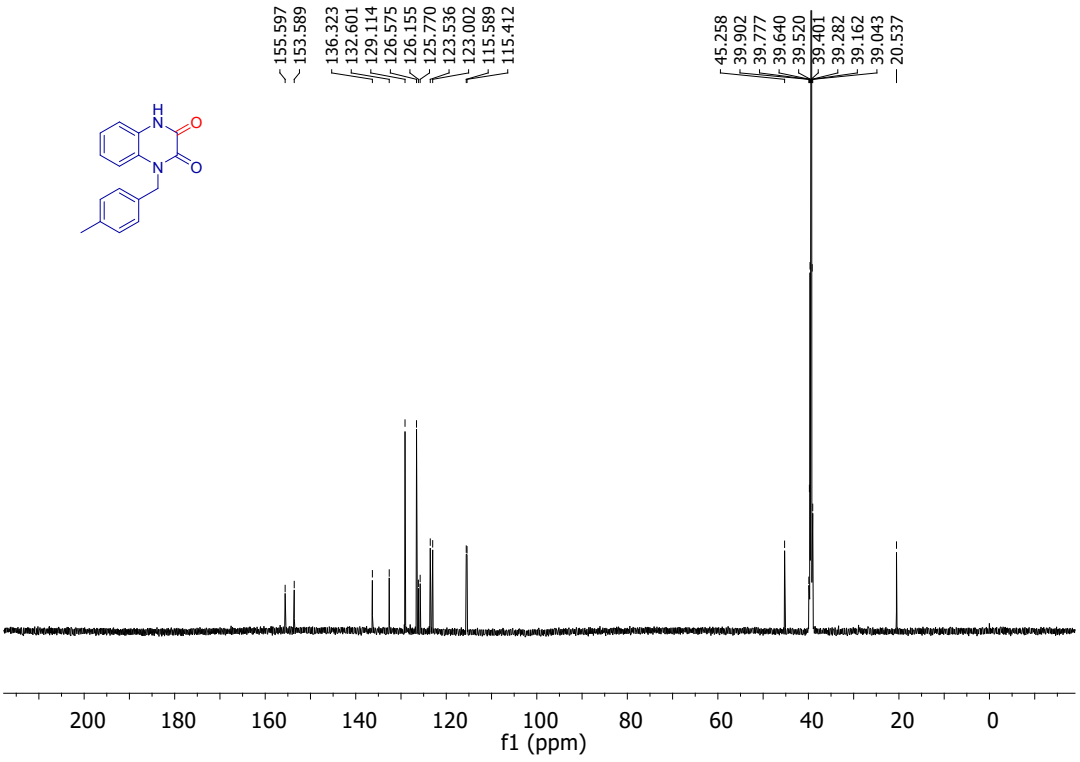


Figure S46. $^{13}C\{^{1}H\}$ NMR (175 MHz, DMSO-d_6) spectrum of 1-(4-methylbenzyl)-1,4-dihydroquinoxaline-2,3-dione (**2d**).

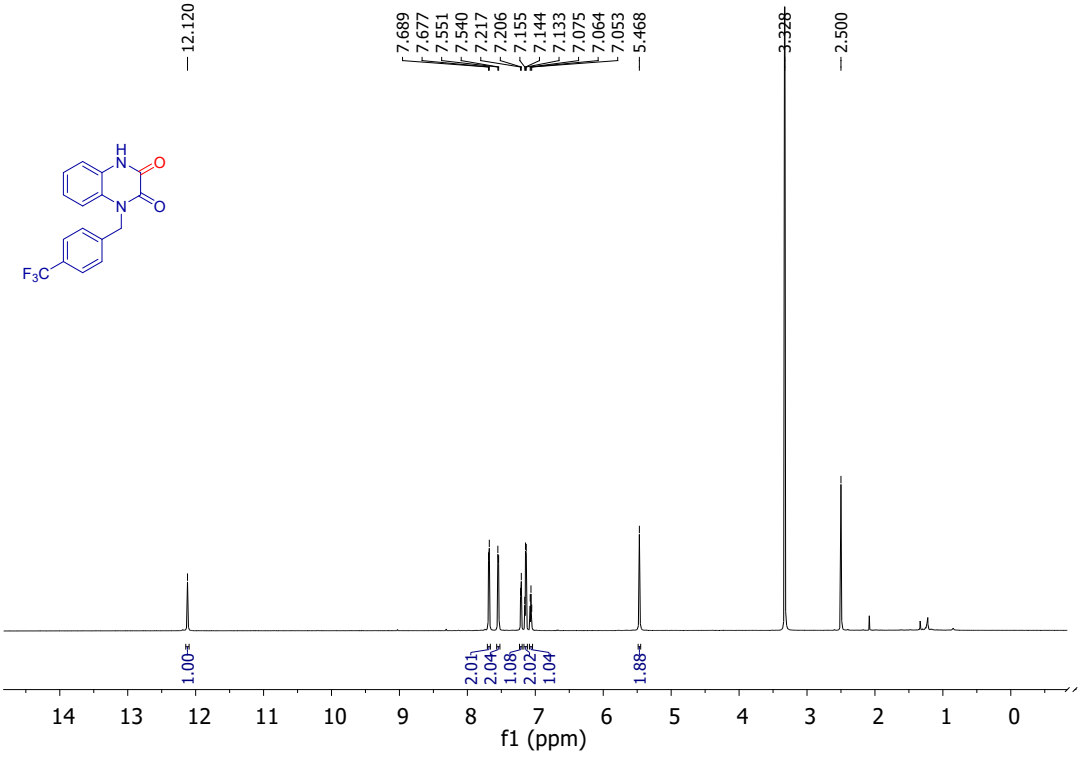


Figure S47. ^{1}H NMR (700 MHz, DMSO-d_6) spectrum of 1-(4-trifluoromethylbenzyl)-1,4-dihydroquinoxaline-2,3-dione (**2e**).

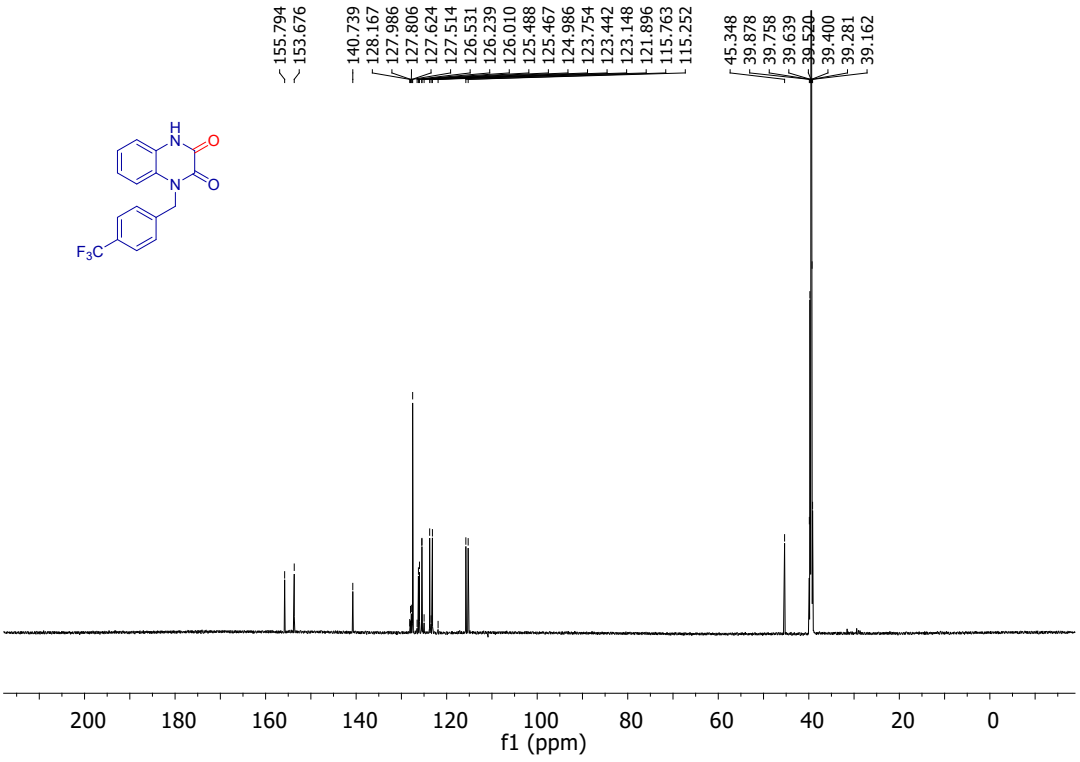


Figure S48.^{13}C{^{1}H} NMR (175 MHz, DMSO-d_6) spectrum of 1-(4-trifluoromethylbenzyl)-1,4-dihydroquinoxaline-2,3-dione (**2e**).

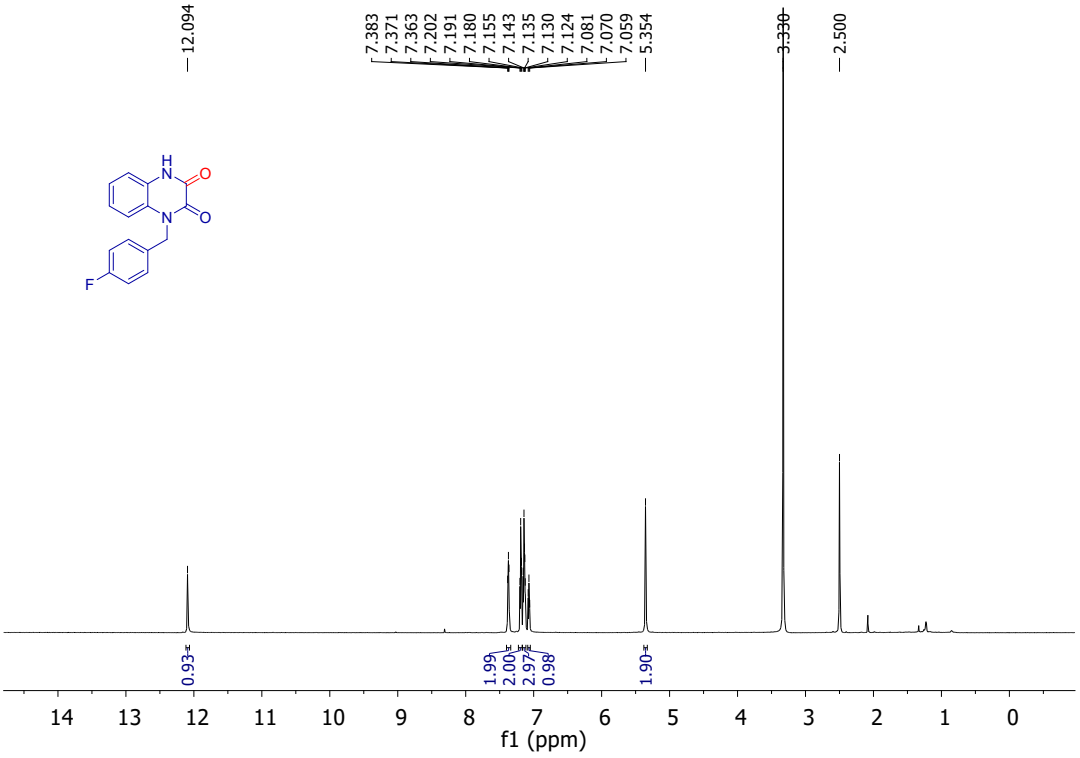


Figure S49. ^{1}H NMR (700 MHz, DMSO-d_6) spectrum of 1-(4-fluorobenzyl)-1,4-dihydroquinoxaline-2,3-dione (**2f**).

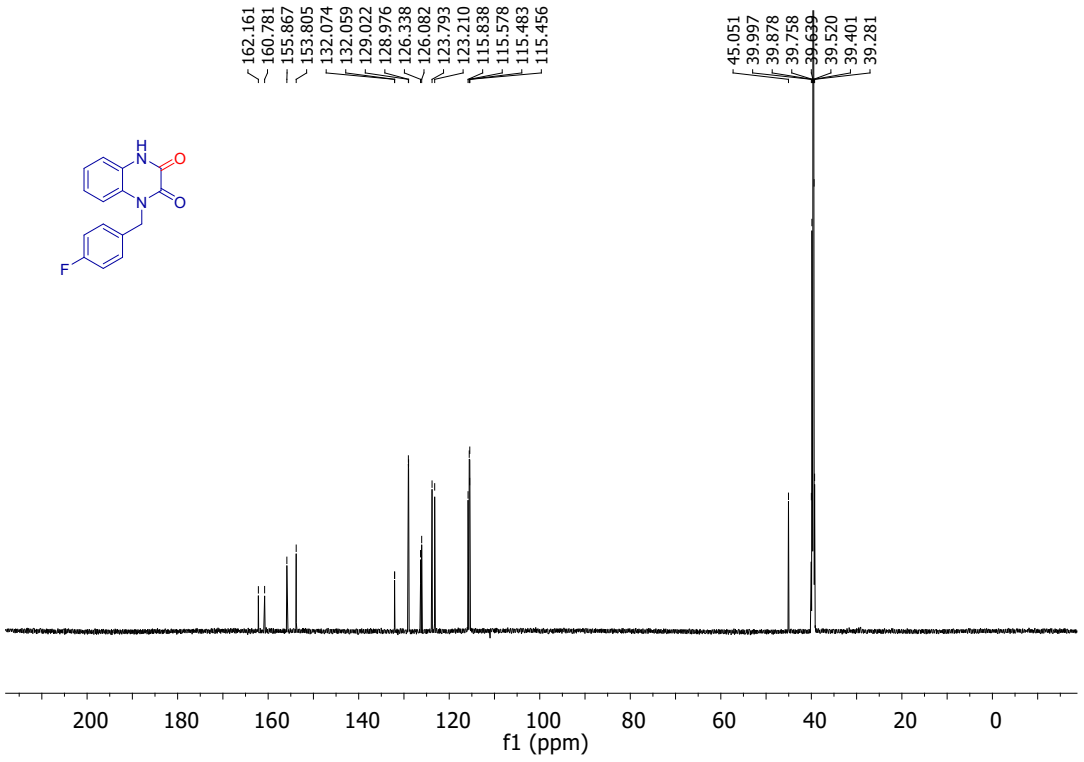


Figure S50. ^{13}C{^{1}H} NMR (175 MHz, DMSO-d_6) spectrum of 1-(4-fluorobenzyl)-1,4-dihydroquinoxaline-2,3-dione (**2f**).

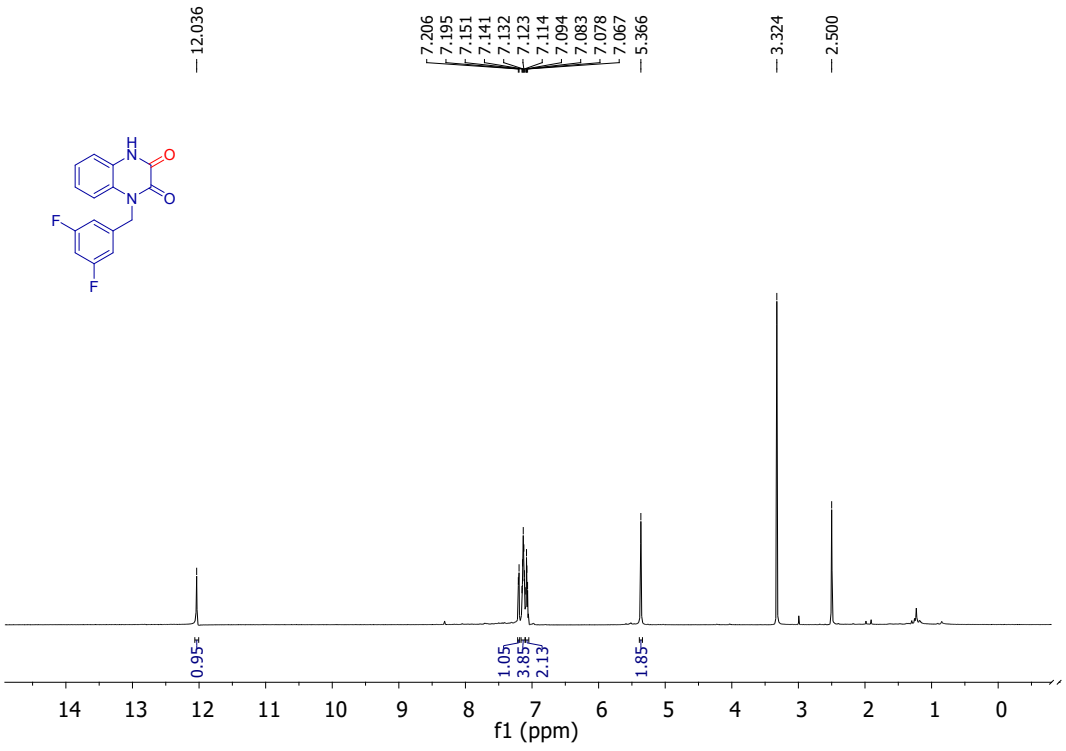


Figure S51. ^{1}H NMR (700 MHz, DMSO-d_6) spectrum of 1-(3,5-difluorobenzyl)-1,4-dihydroquinoxaline-2,3-dione (**2g**).

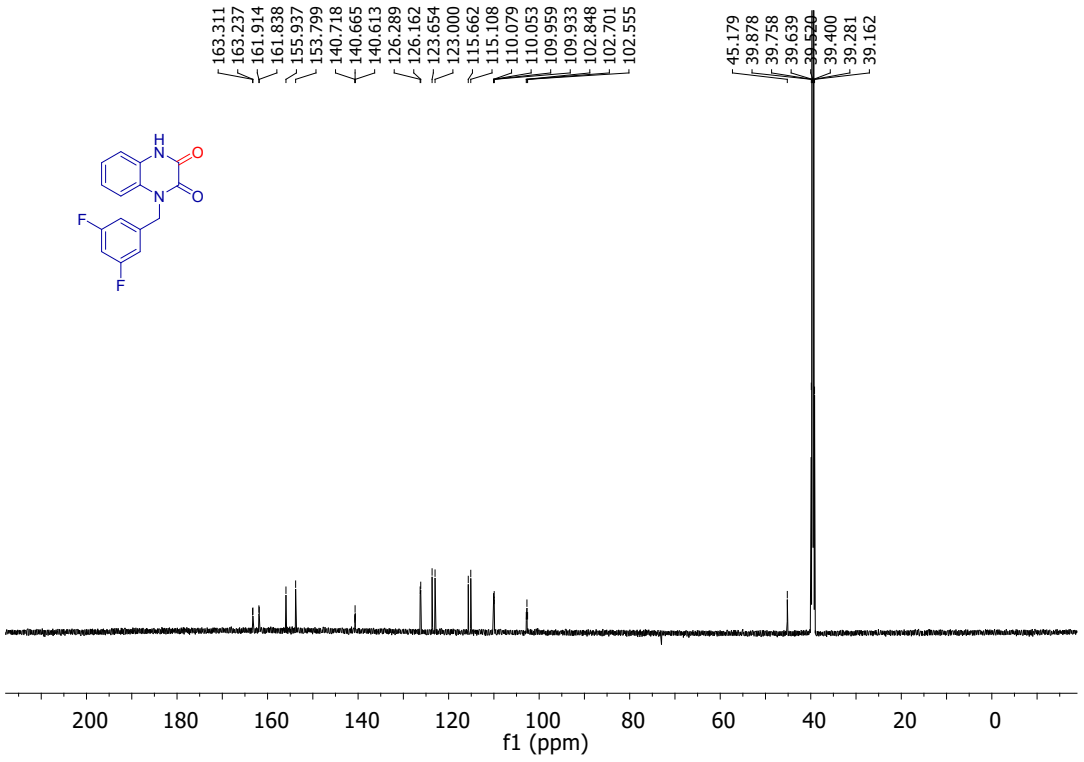


Figure S52.^{13}C{^{1}H} NMR (175 MHz, DMSO-d_6) spectrum of 1-(3,5-difluorobenzyl)-1,4-dihydroquinoxaline-2,3-dione (**2g**).

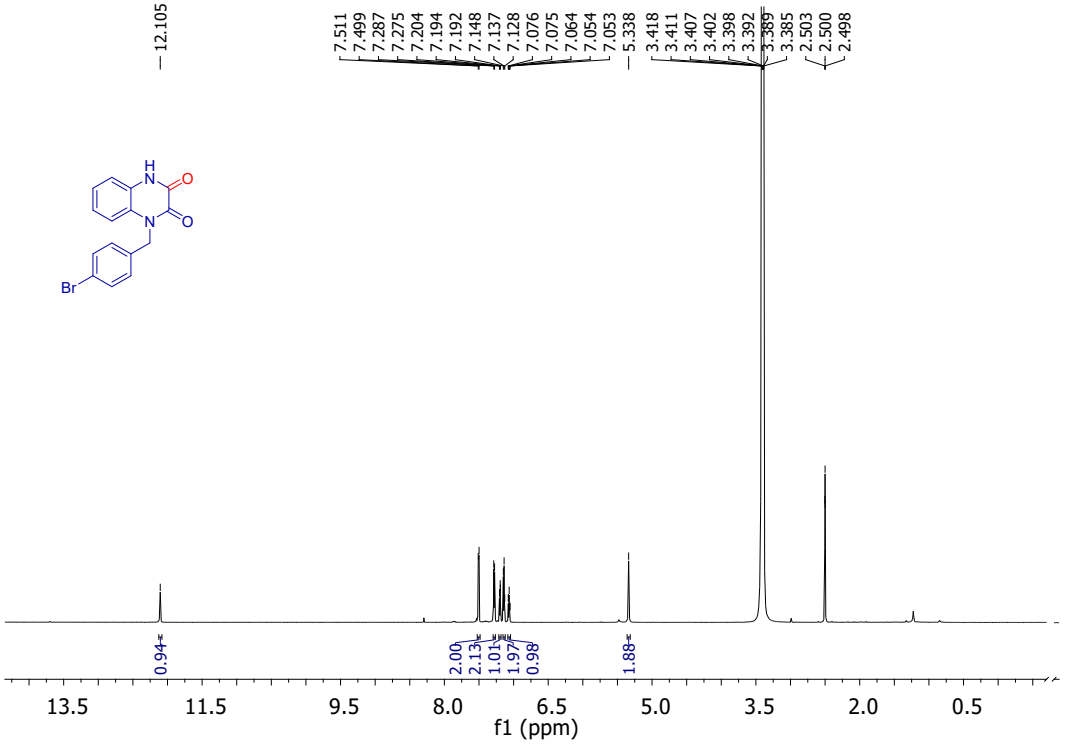


Figure S53. ^{1}H NMR (700 MHz, DMSO-d_6) spectrum of 1-(4-bromobenzyl)-1,4-dihydroquinoxaline-2,3-dione (**2h**).

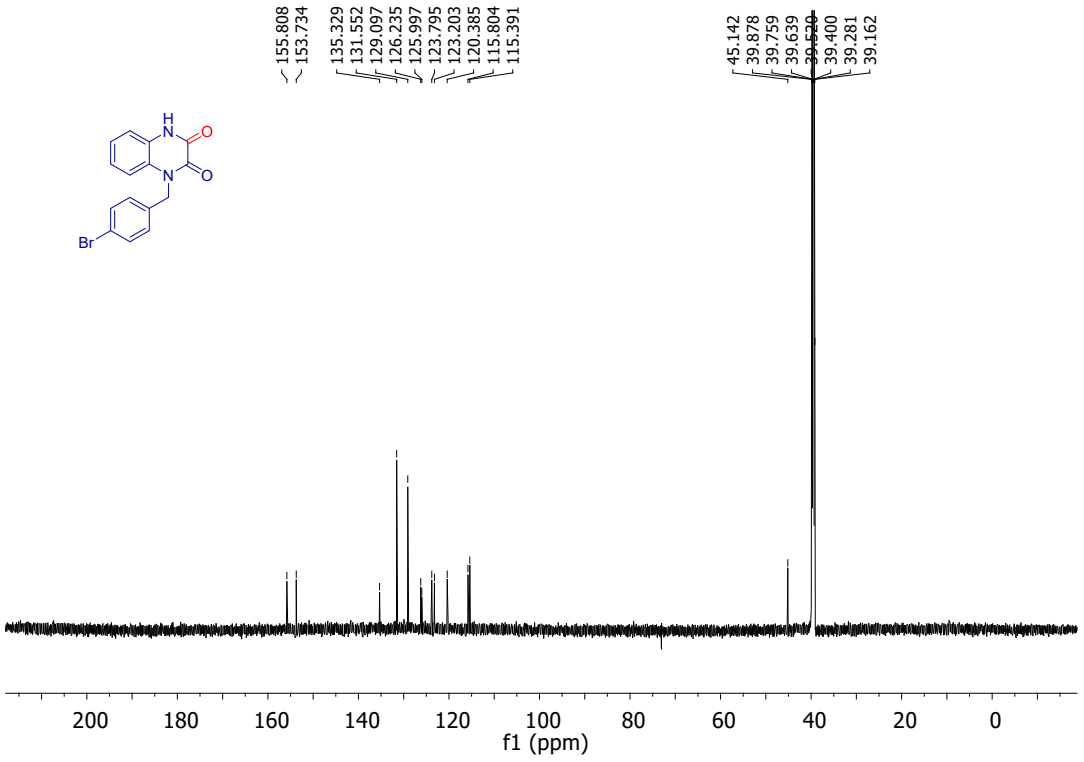


Figure S54. $^{13}C\{^{1}H\}$ NMR (175 MHz, DMSO-d_6) spectrum of 1-(4-bromobenzyl)-1,4-dihydroquinoxaline-2,3-dione (**2h**).

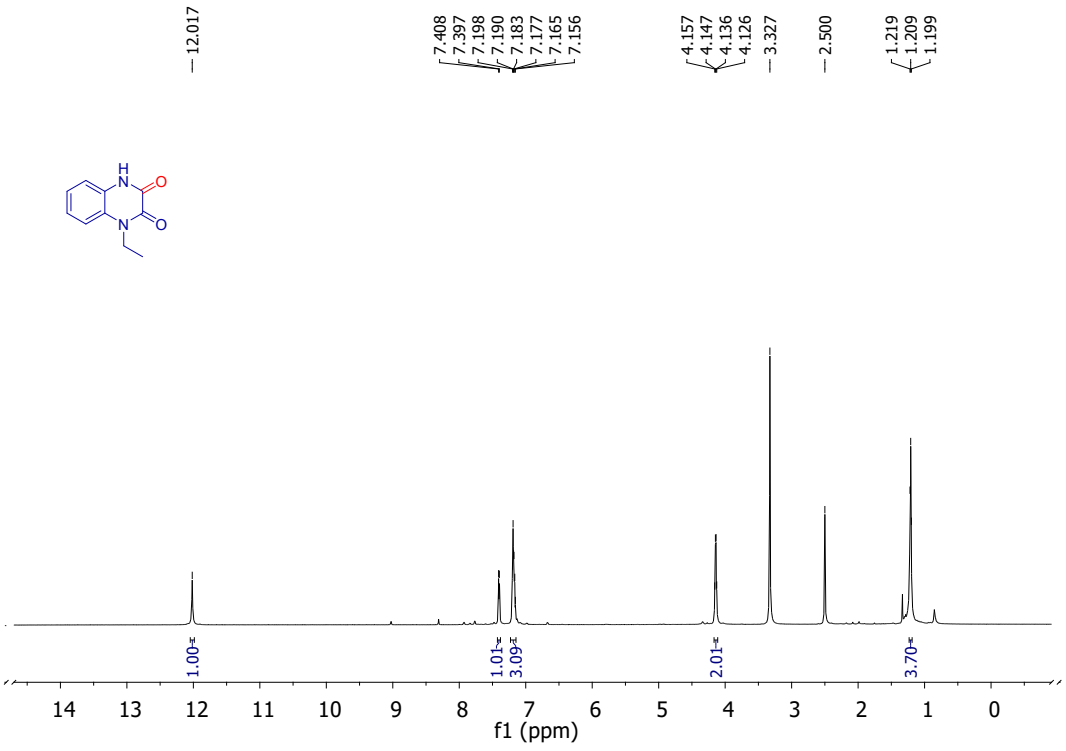


Figure S55. ^{1}H NMR (700 MHz, DMSO-d_6) spectrum of 1-ethyl-1,4-dihydroquinoxaline-2,3-dione (**2i**).

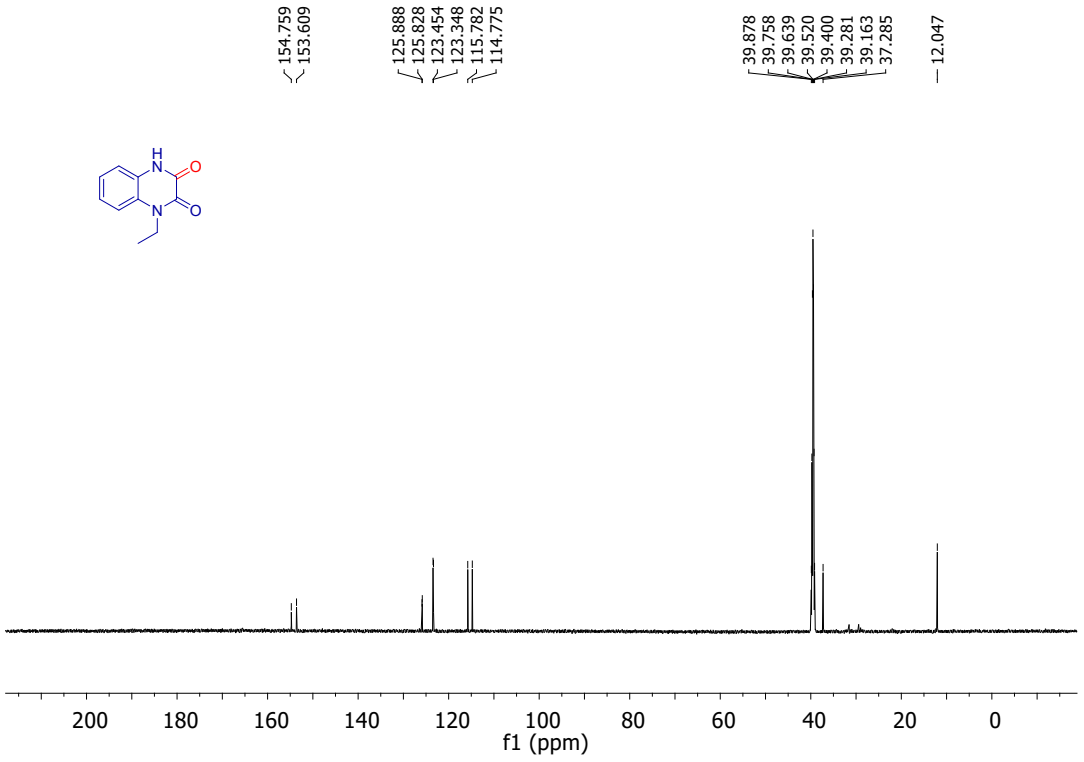


Figure S56. $^{13}C\{^{1}H\}$ NMR (175 MHz, DMSO-d_6) spectrum of 1-ethyl-1,4-dihydroquinoxaline-2,3-dione (**2i**).

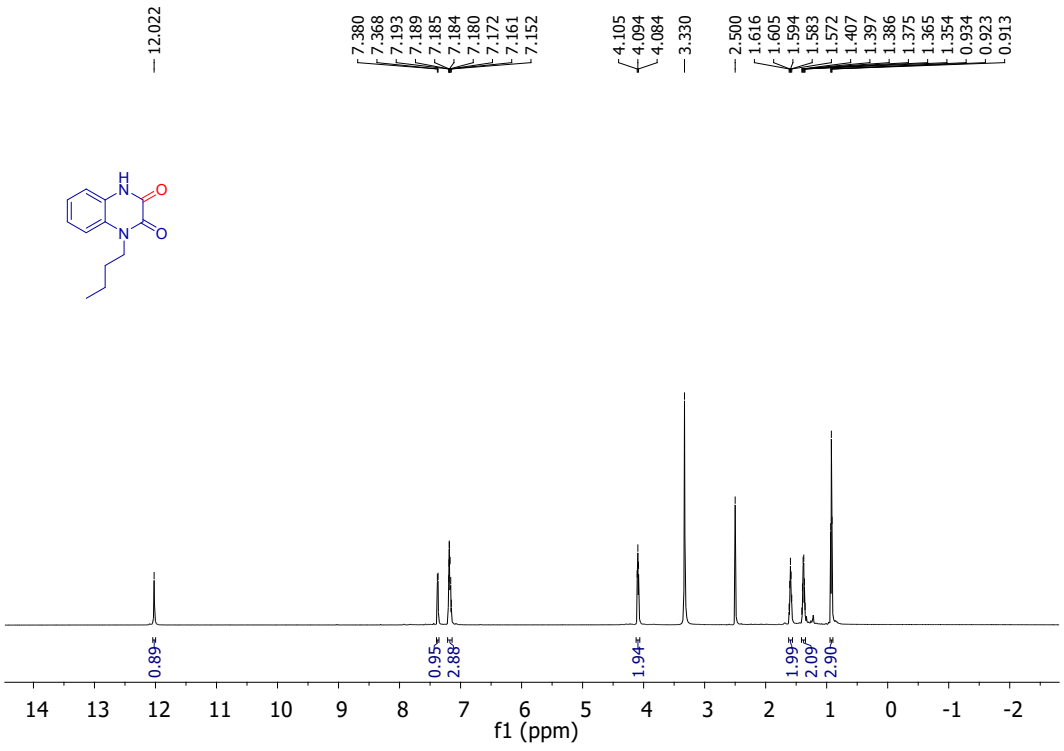


Figure S57. ^{1}H NMR (700 MHz, DMSO-d_6) spectrum of 1-butyl-1,4-dihydroquinoxaline-2,3-dione (**2j**).

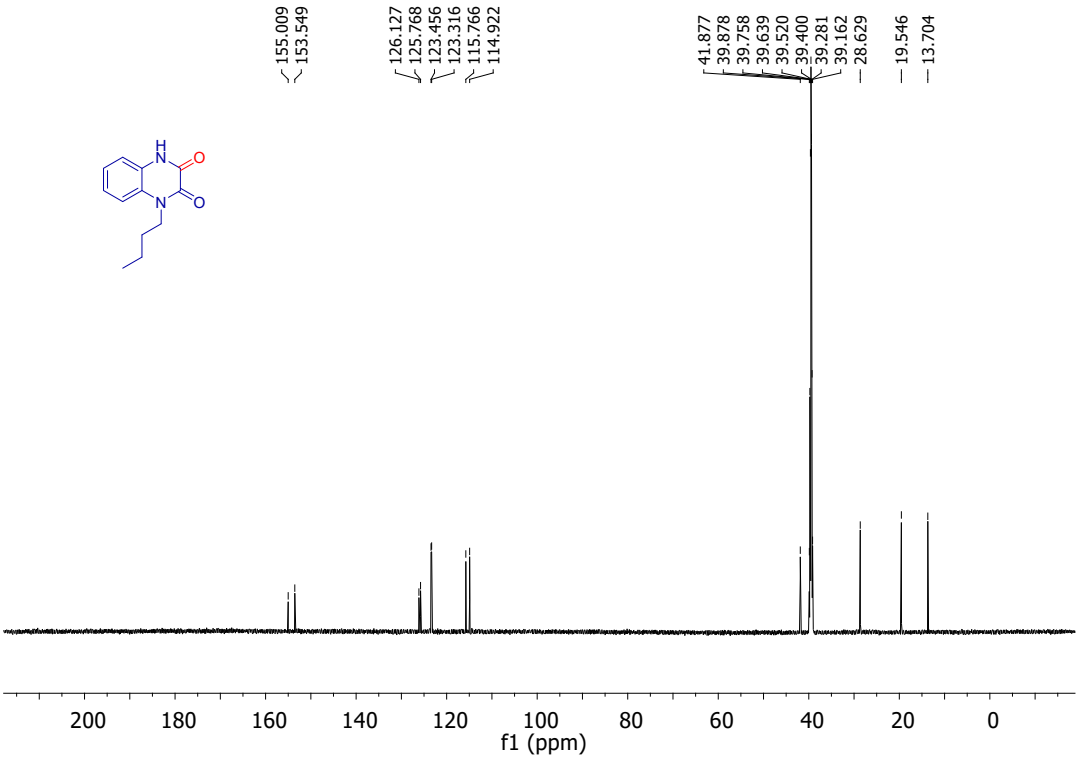


Figure S58. ^{13}C{^{1}H} NMR (175 MHz, DMSO-d_6) spectrum of 1-butyl-1,4-dihydroquinoxaline-2,3-dione (**2j**).

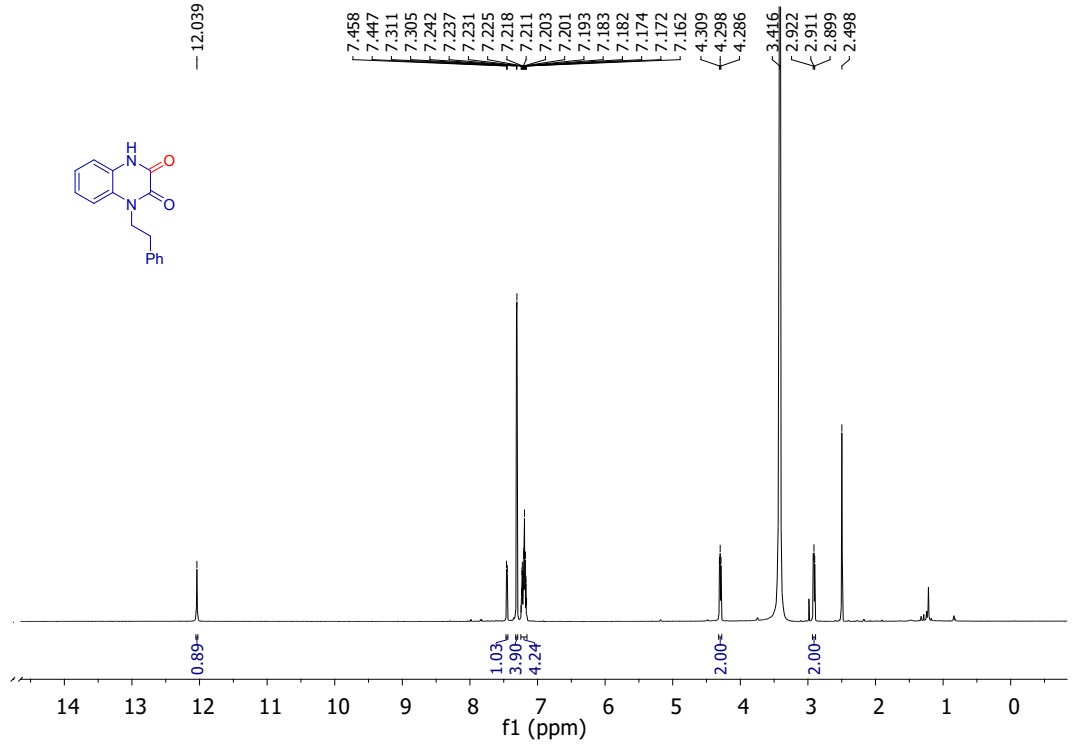


Figure S59. ^{1}H NMR (700 MHz, DMSO-d_6) spectrum of 1-phenethyl-1,4-dihydroquinoxaline-2,3-dione (**2k**).

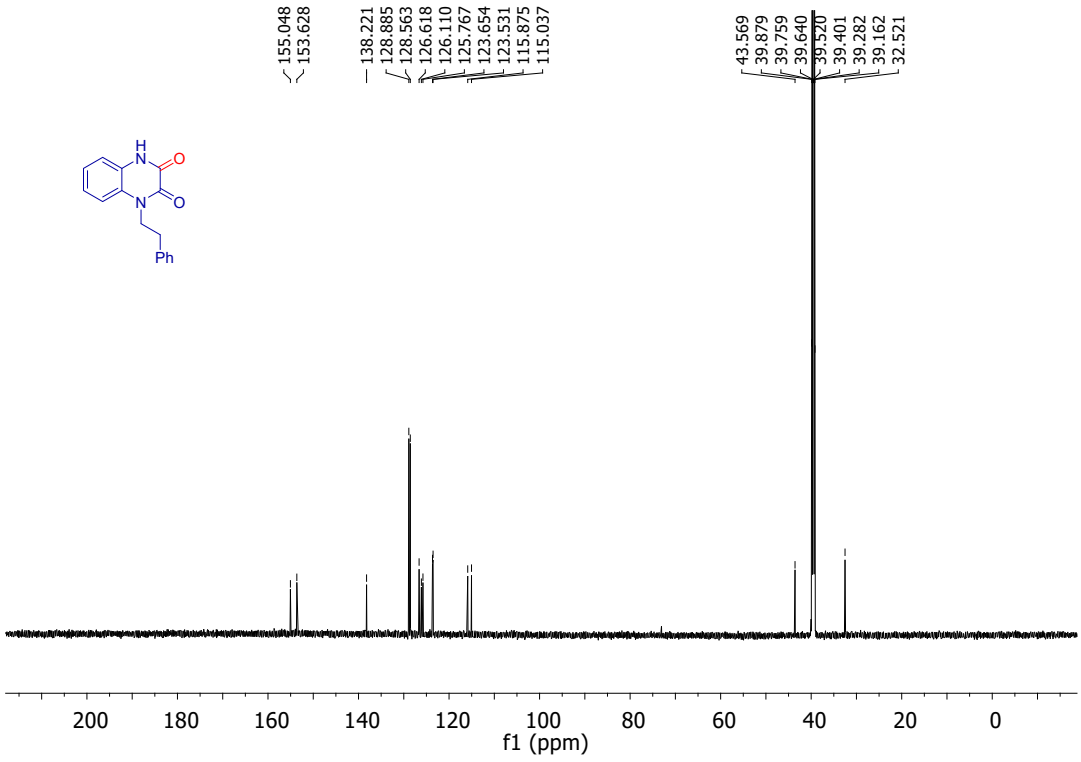


Figure S60. ^{13}C{^{1}H} NMR (175 MHz, DMSO-d_6) spectrum of 1-phenethyl-1,4-dihydroquinoxaline-2,3-dione (**2k**).

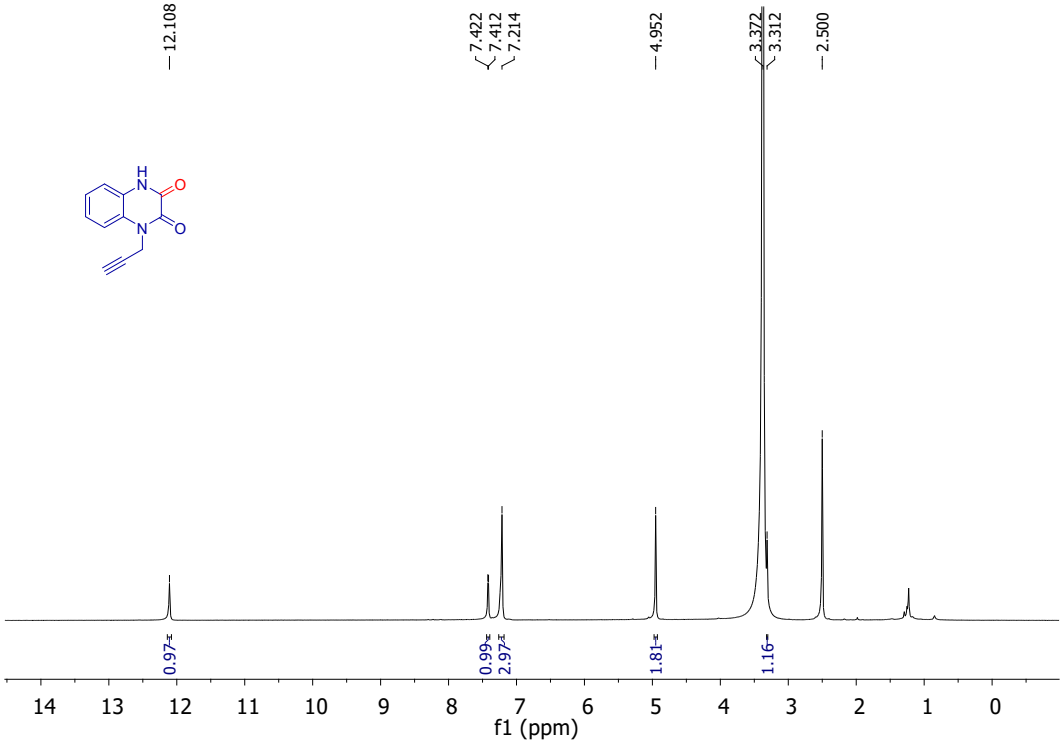


Figure S61. ^{1}H NMR (700 MHz, DMSO-d_6) spectrum of 1-(prop-2-yn-1-yl)-1,4-dihydroquinoxaline-2,3-dione (**2l**).

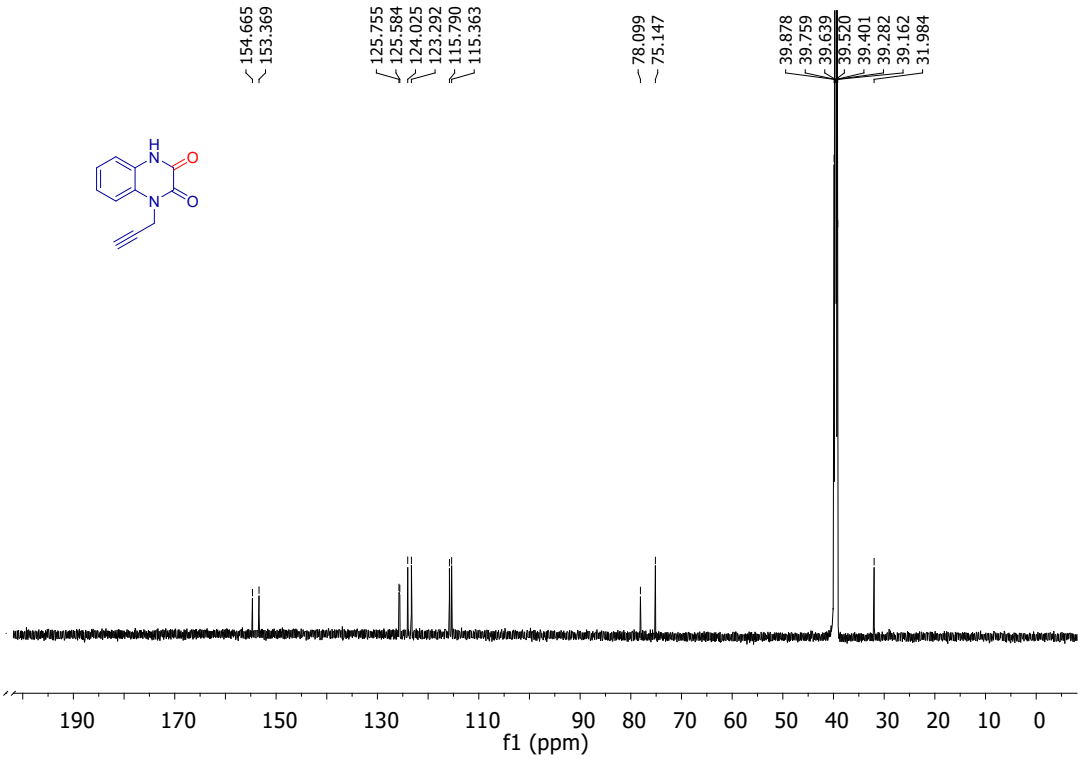


Figure S62. $^{13}C\{^{1}H\}$ NMR (175 MHz, DMSO-d_6) spectrum of 1-(prop-2-yn-1-yl)-1,4-dihydroquinoxaline-2,3-dione (**2l**).

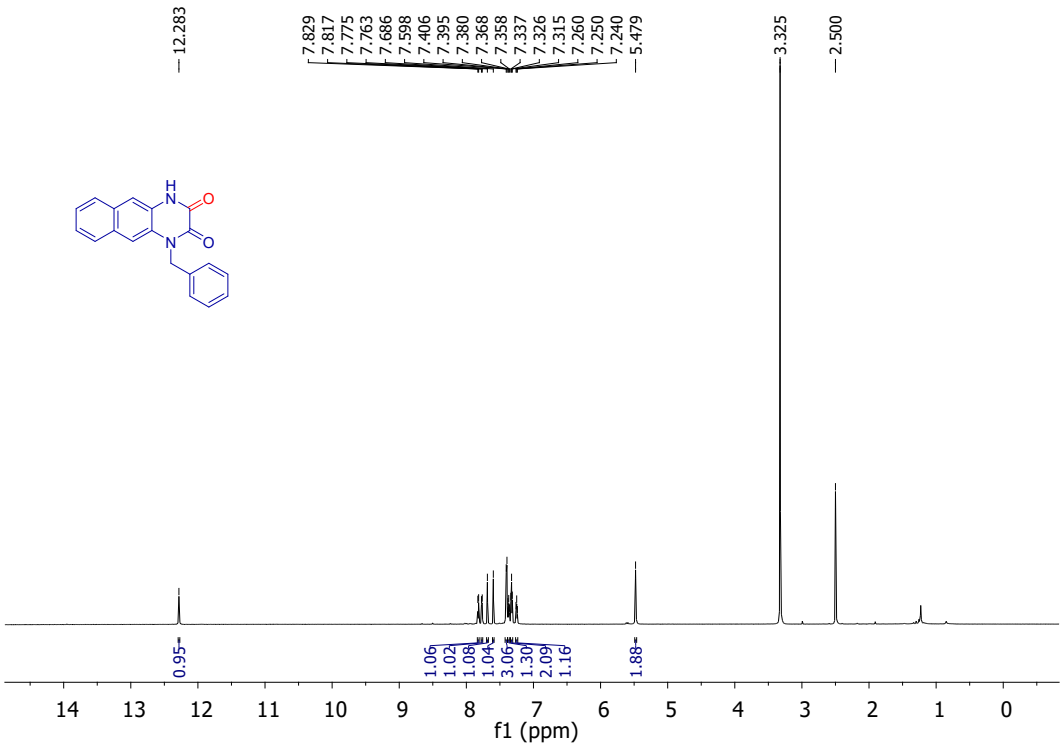


Figure S63. ^{1}H NMR (700 MHz, DMSO-d_6) spectrum of 1-benzyl-1,4-dihydrobenzo[g]quinoxaline-2,3-dione (**2m**).

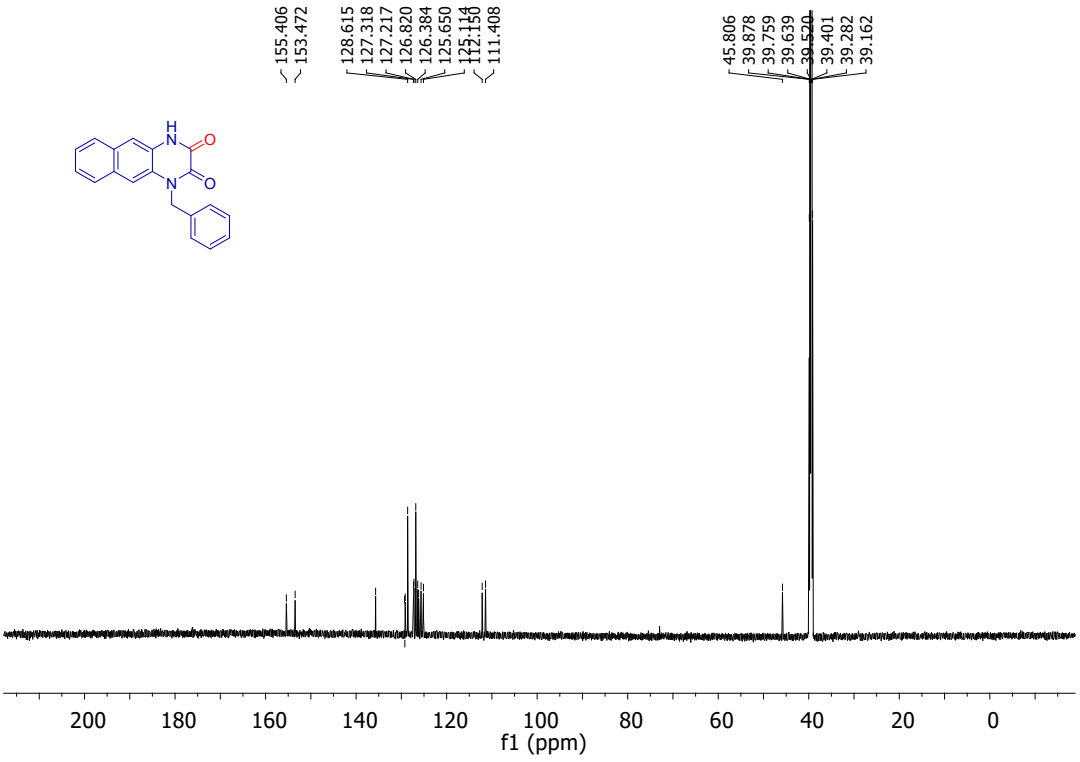


Figure S64. $^{13}C\{^{1}H\}$ NMR (175 MHz, DMSO-d_6) spectrum of 1-benzyl-1,4-dihydrobenzo[g]quinoxaline-2,3-dione (**2m**).

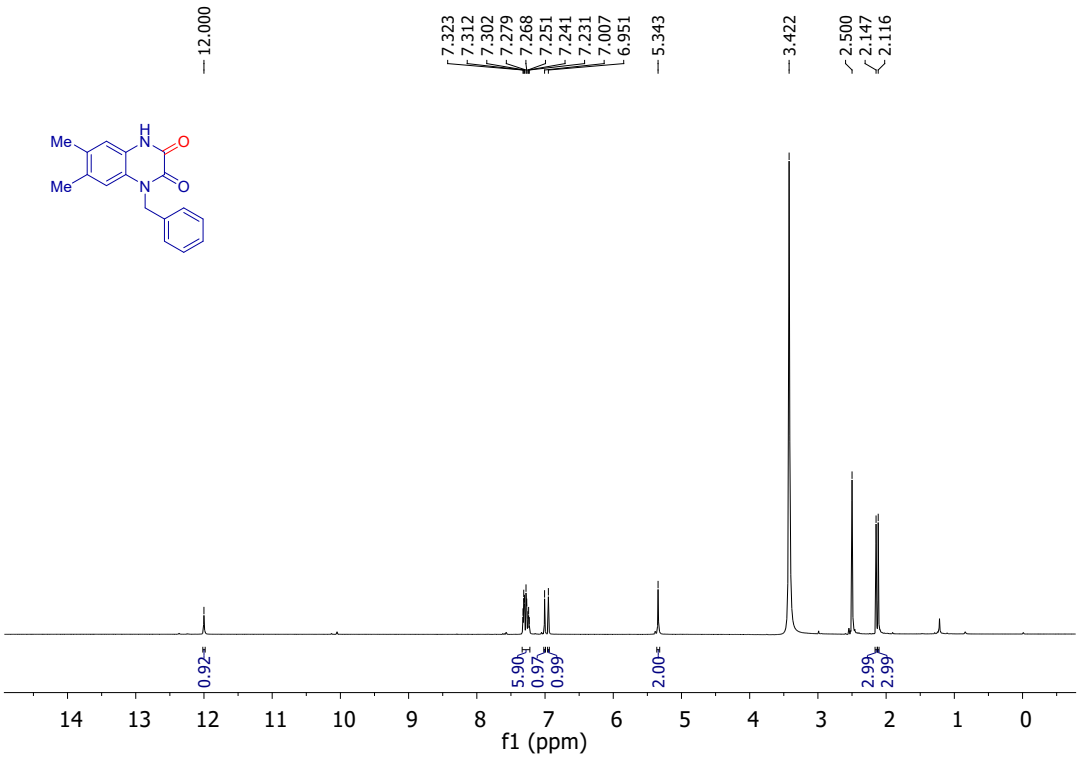


Figure S65. ^{1}H NMR (700 MHz, DMSO-d_6) spectrum of 1-benzyl-6,7-dimethyl-1,4-dihydroquinoxaline-2,3-dione **3a).**

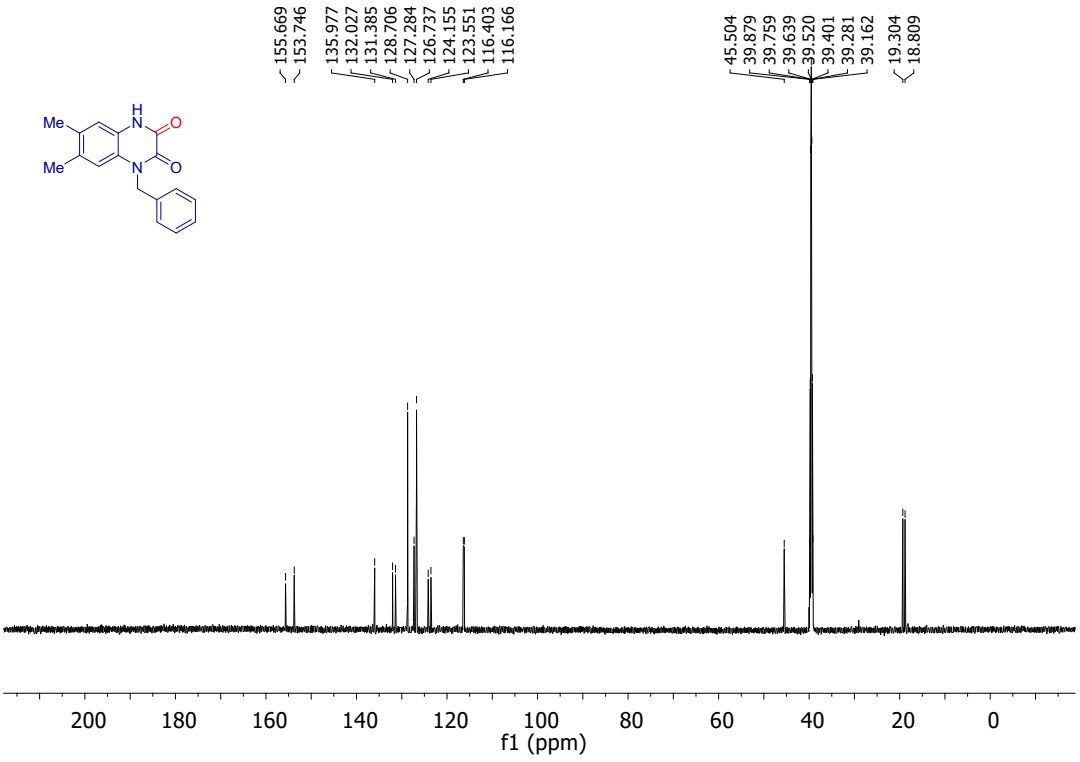


Figure S66. $^{13}C\{^{1}H\}$ NMR (175 MHz, DMSO-d_6) spectrum of 1-benzyl-6,7-dimethyl-1,4-dihydroquinoxaline-2,3-dione **(3a).**

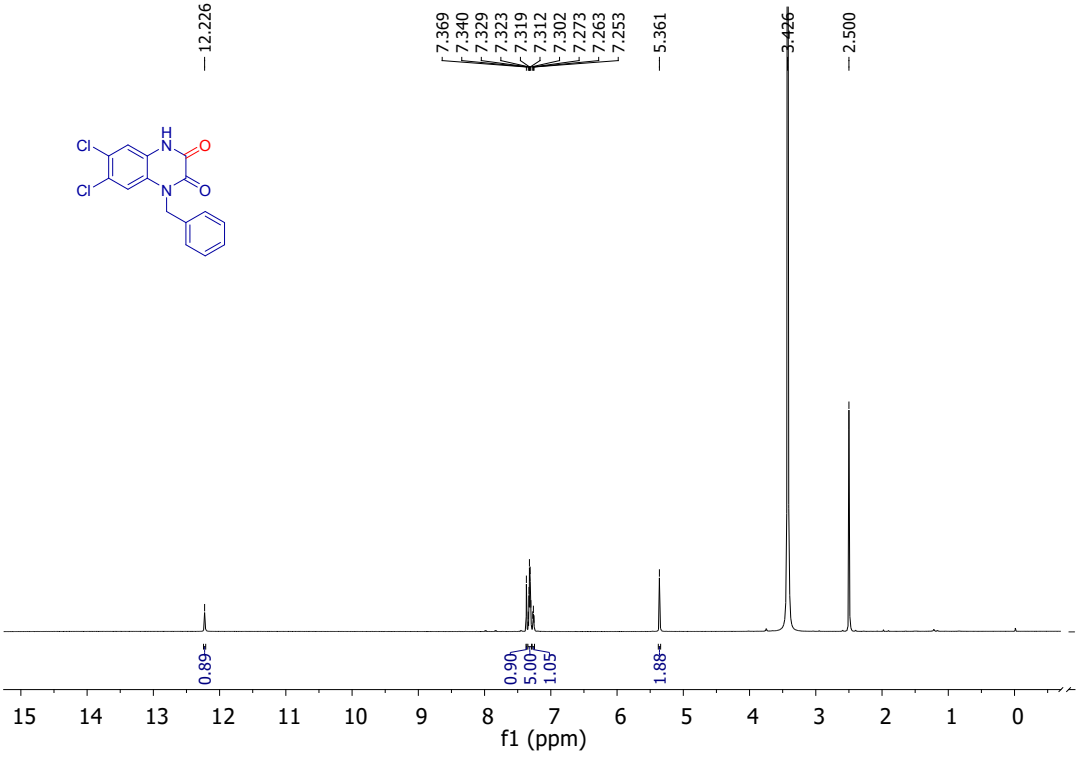


Figure S67. ^{1}H NMR (700 MHz, DMSO-d_6) spectrum of 1-benzyl-6,7-dichloro-1,4-dihydroquinoxaline-2,3-dione (**3b**).

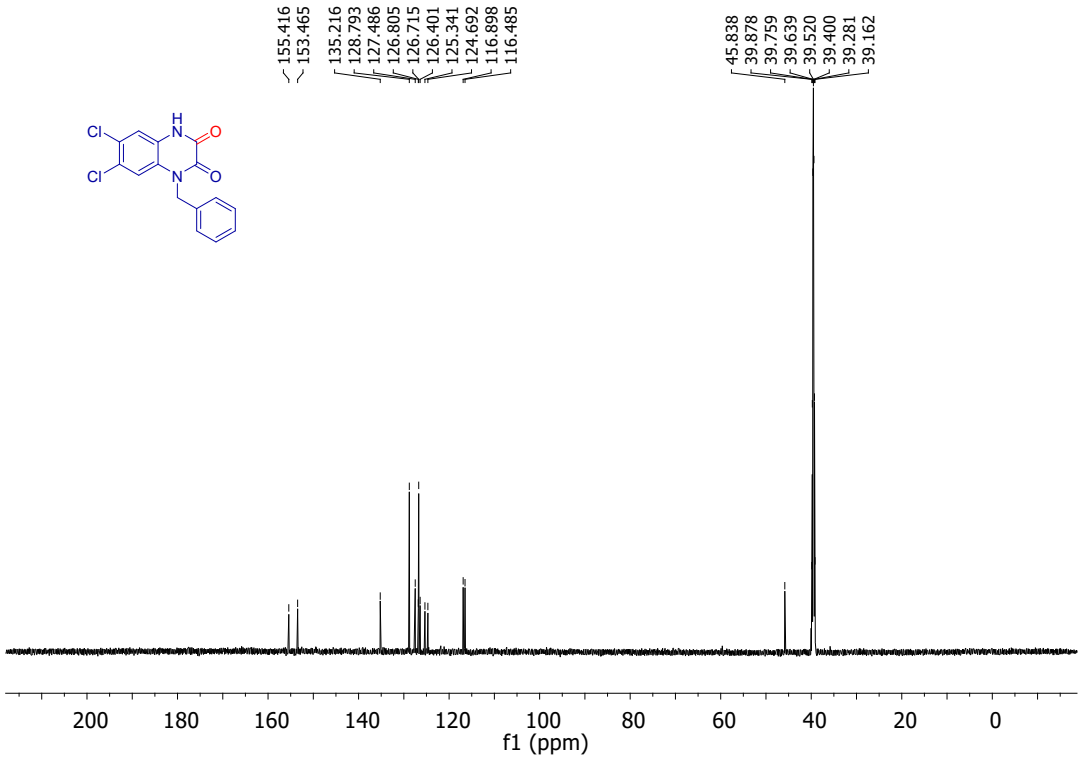


Figure S68. $^{13}C\{^{1}H\}$ NMR (175 MHz, DMSO-d_6) spectrum of 1-benzyl-6,7-dichloro-1,4-dihydroquinoxaline-2,3-dione (**3b**).

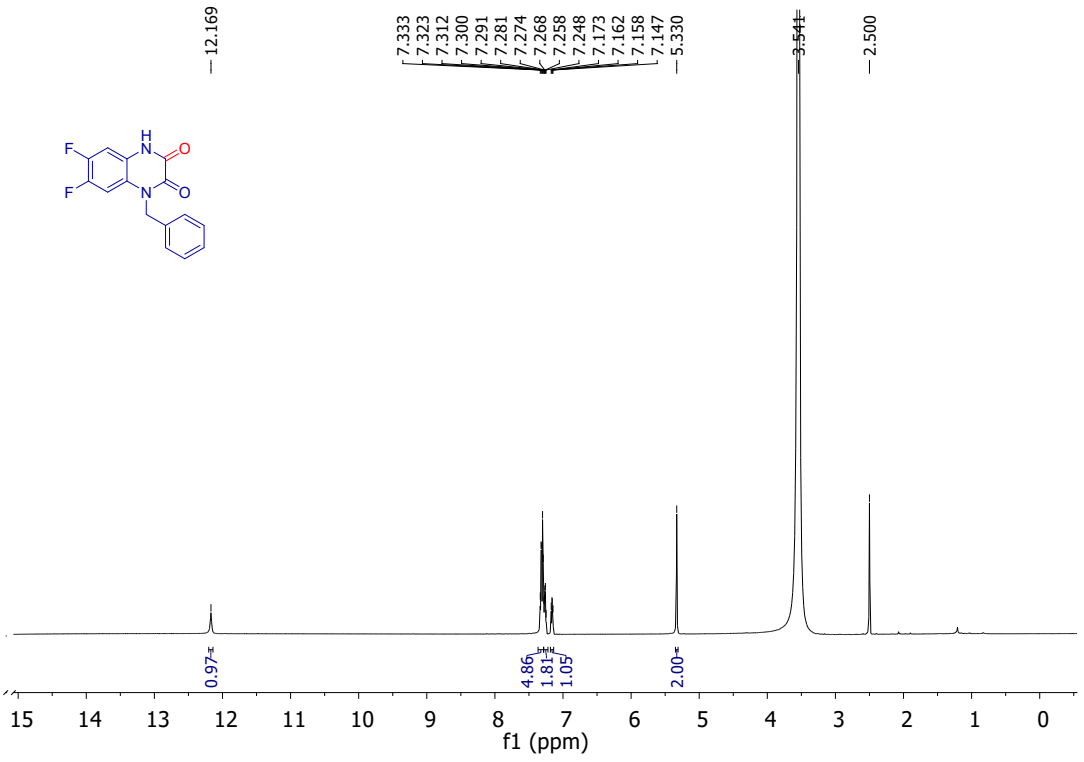


Figure S69. ^{1}H NMR (700 MHz, DMSO-d_6) spectrum of 1-benzyl-6,7-difluoro-1,4-dihydroquinoxaline-2,3-dione (**3c**).

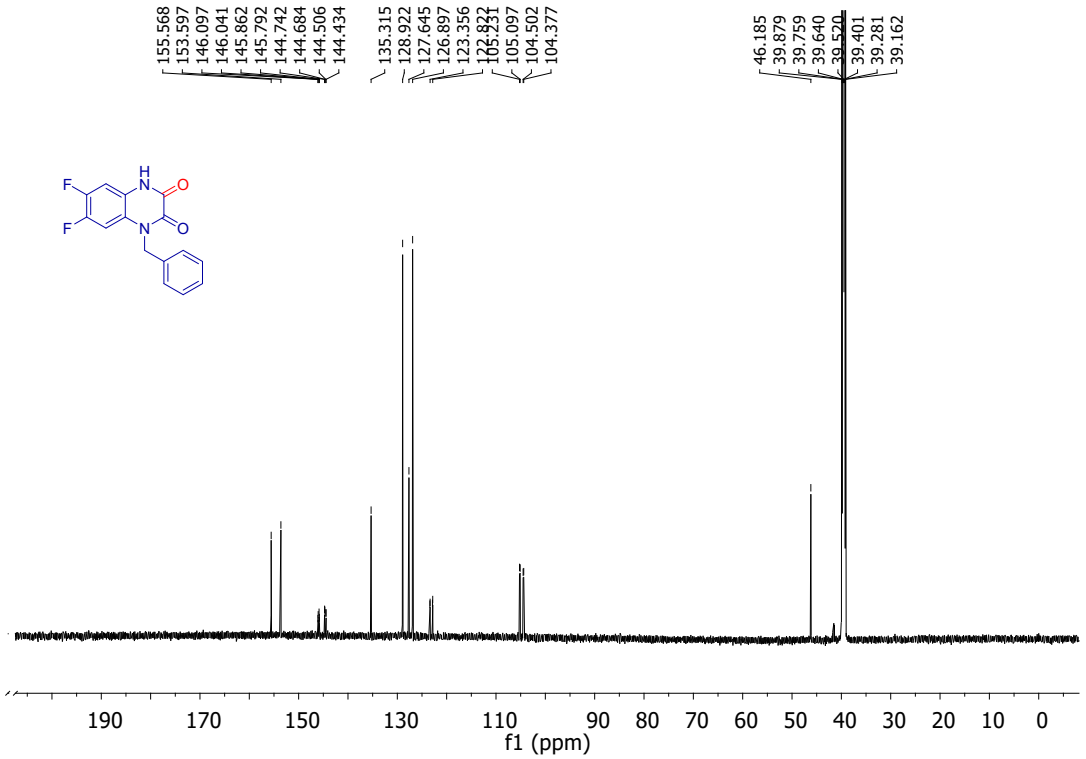


Figure S70. ^{13}C{^{1}H} NMR (175 MHz, DMSO-d_6) spectrum of 1-benzyl-6,7-difluoro-1,4-dihydroquinoxaline-2,3-dione (**3c**).

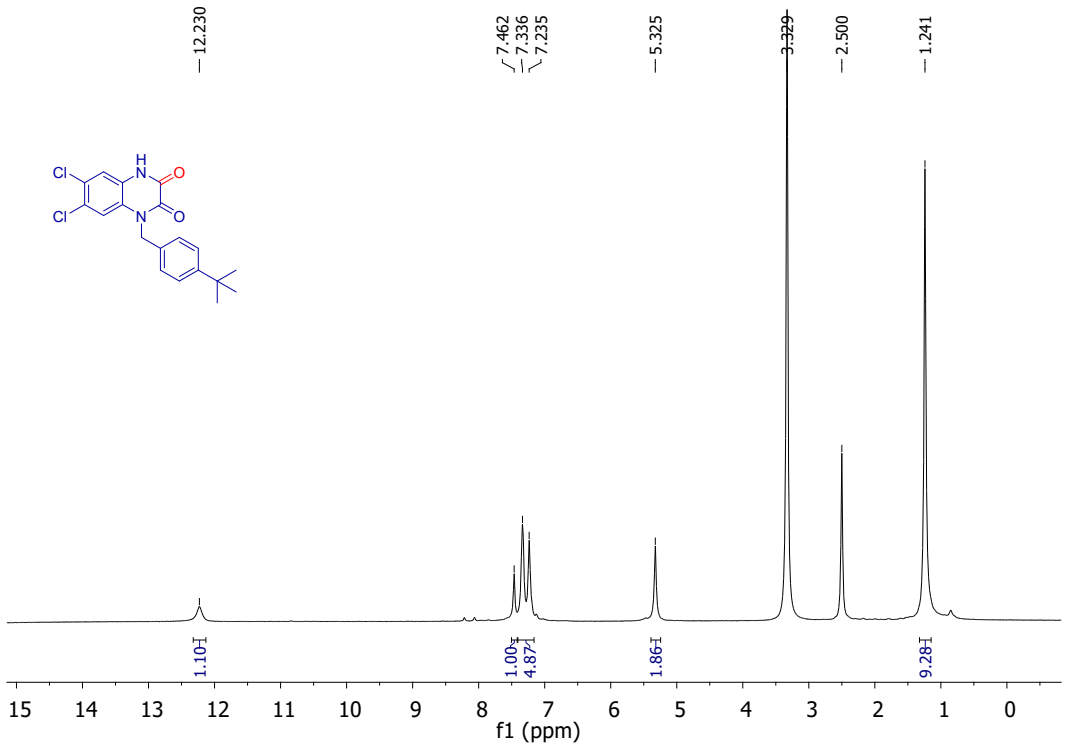


Figure S71. ^{1}H NMR (700 MHz, DMSO-d_6) spectrum of 1-(4-(*tert*-butyl)benzyl)-6,7-dichloro-1,4-dihydroquinoxaline-2,3-dione (**3d**).

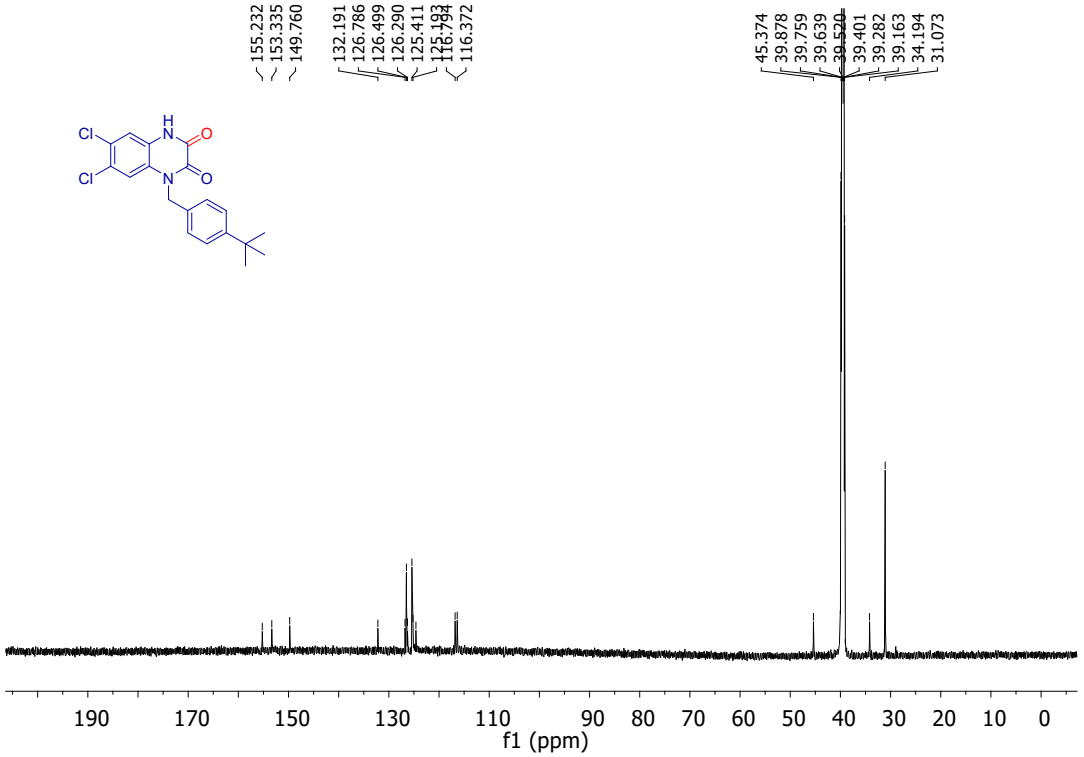


Figure S72. ^{13}C{^{1}H} NMR (175 MHz, DMSO-d_6) spectrum of 1-(4-(*tert*-butyl)benzyl)-6,7-dichloro-1,4-dihydroquinoxaline-2,3-dione (**3d**).

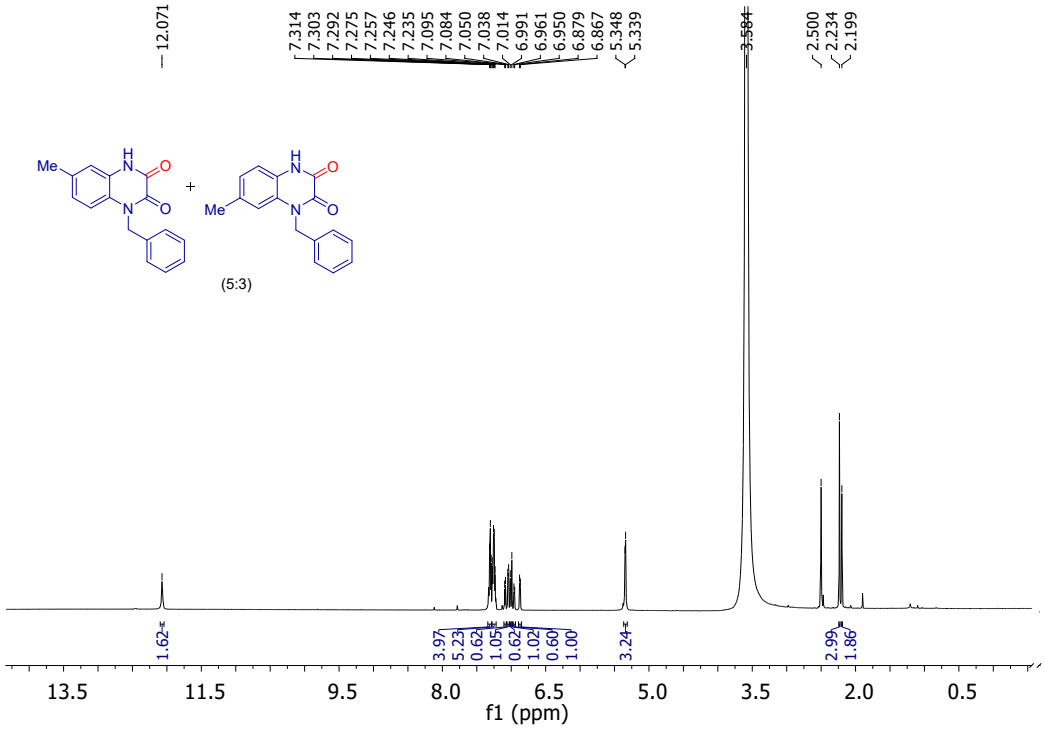


Figure S73. ^{1}H NMR (700 MHz, DMSO-d_6) spectrum of 1-benzyl-6-methyl-1,4-dihydroquinoxaline-2,3-dione and 1-benzyl-7-methyl-1,4-dihydroquinoxaline-2,3-dione (**3e**).

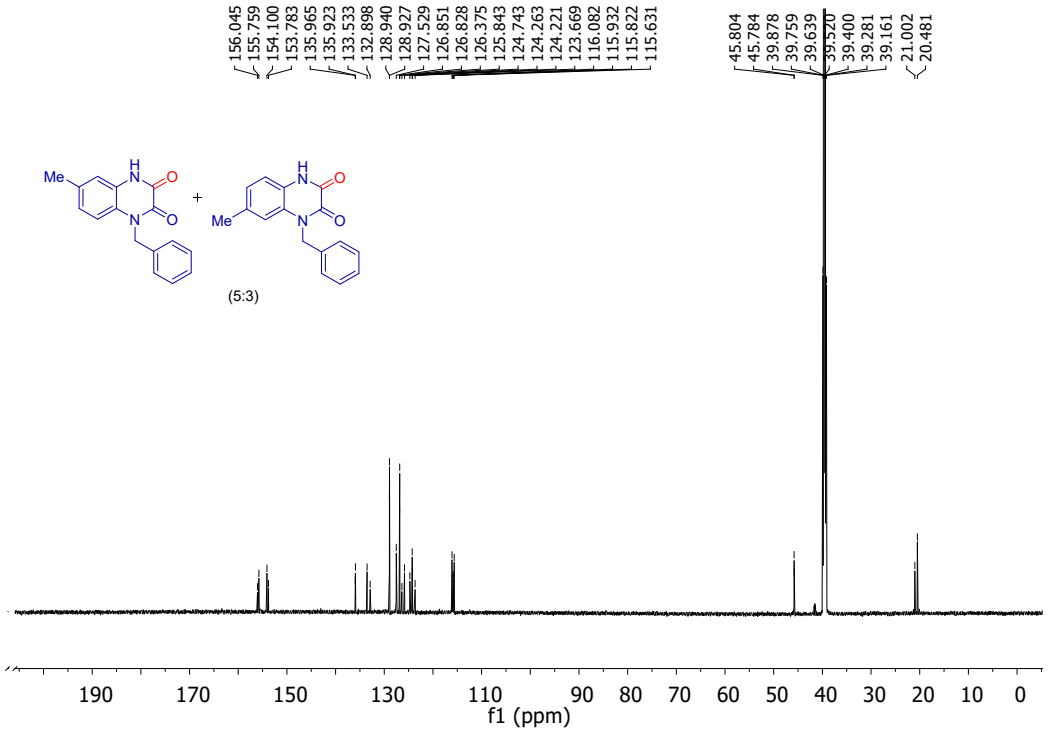


Figure S74. ^{13}C{^{1}H} NMR (175 MHz, DMSO-d_6) spectrum of 1-benzyl-6-methyl-1,4-dihydroquinoxaline-2,3-dione and 1-benzyl-7-methyl-1,4-dihydroquinoxaline-2,3-dione (**3e**).

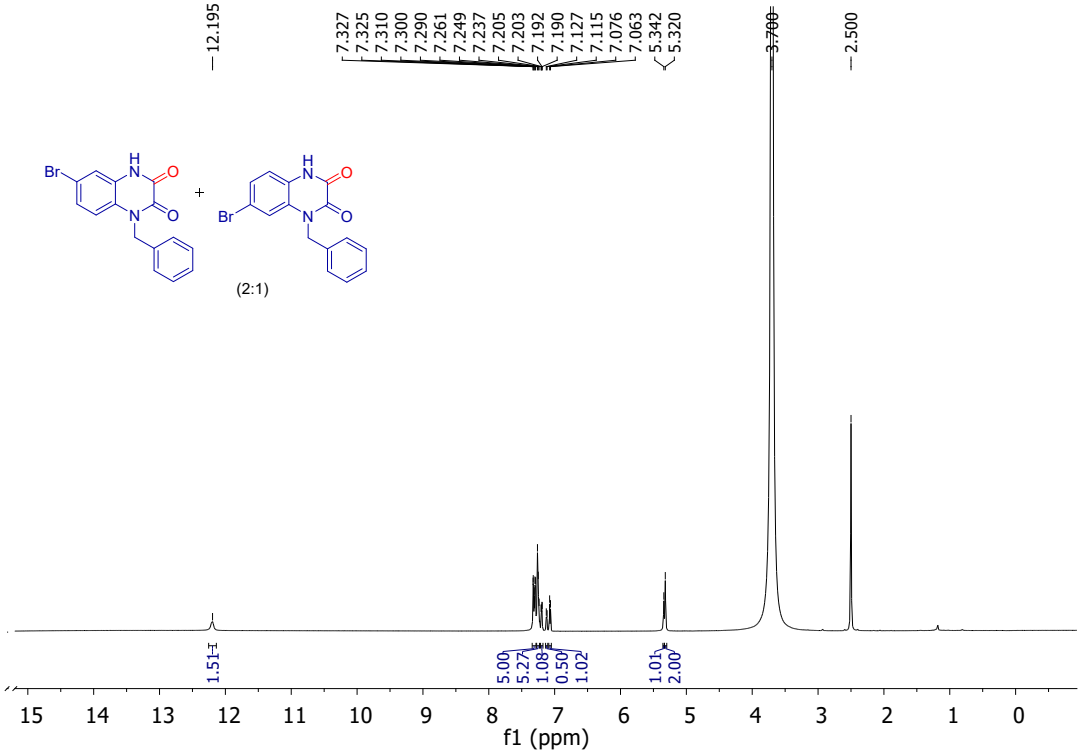


Figure S75. ^{1}H NMR (700 MHz, DMSO-d_6) spectrum of 1-benzyl-6-bromo-1,4-dihydroquinoxaline-2,3-dione and 1-benzyl-7-bromo-1,4-dihydroquinoxaline-2,3- (**3f**).

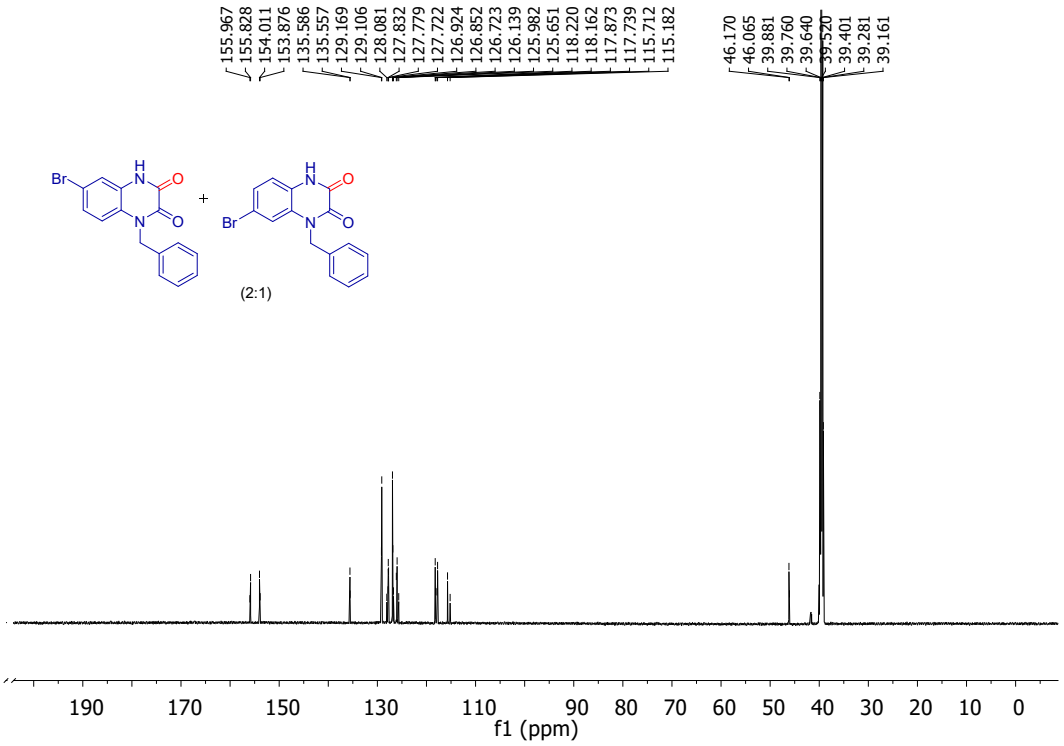


Figure S76. ^{13}C{^{1}H} NMR (175 MHz, DMSO-d_6) spectrum of 1-benzyl-6-bromo-1,4-dihydroquinoxaline-2,3-dione and 1-benzyl-7-bromo-1,4-dihydroquinoxaline-2,3-dione (**3f**).

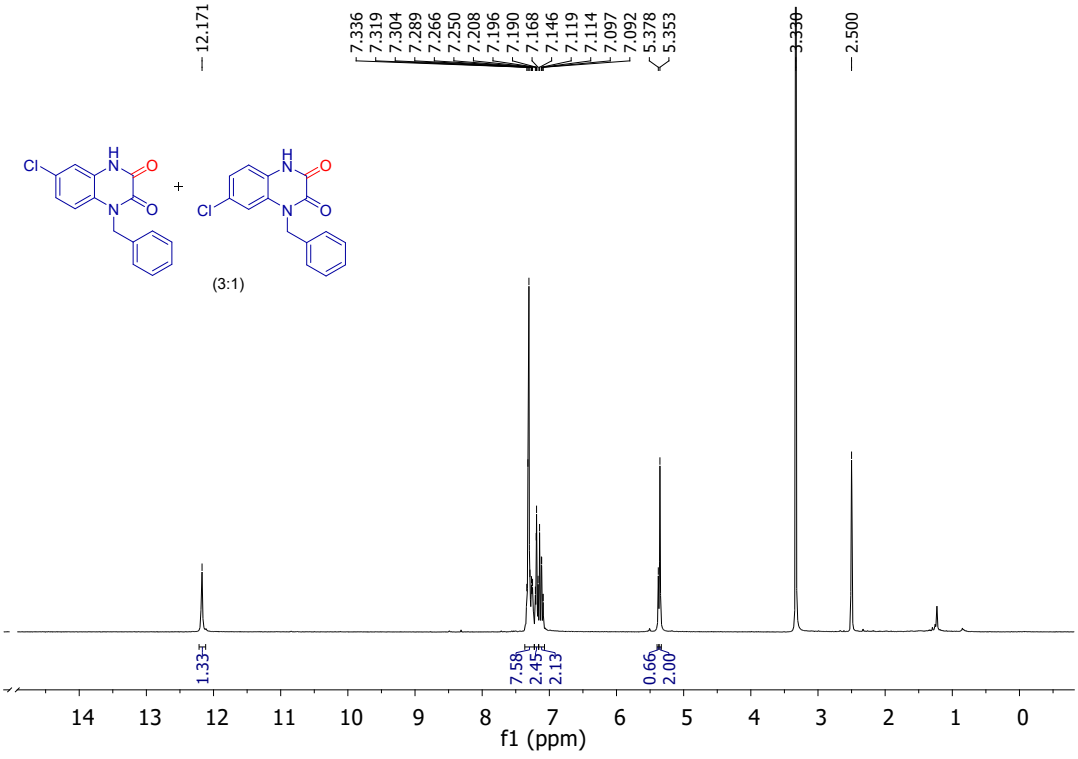


Figure S77. ^{1}H NMR (400 MHz, DMSO-d_6) spectrum of 1-benzyl-6-chloro-1,4-dihydroquinoxaline-2,3-dione and 1-benzyl-7-chloro-1,4-dihydroquinoxaline-2,3-dione (**3g**).

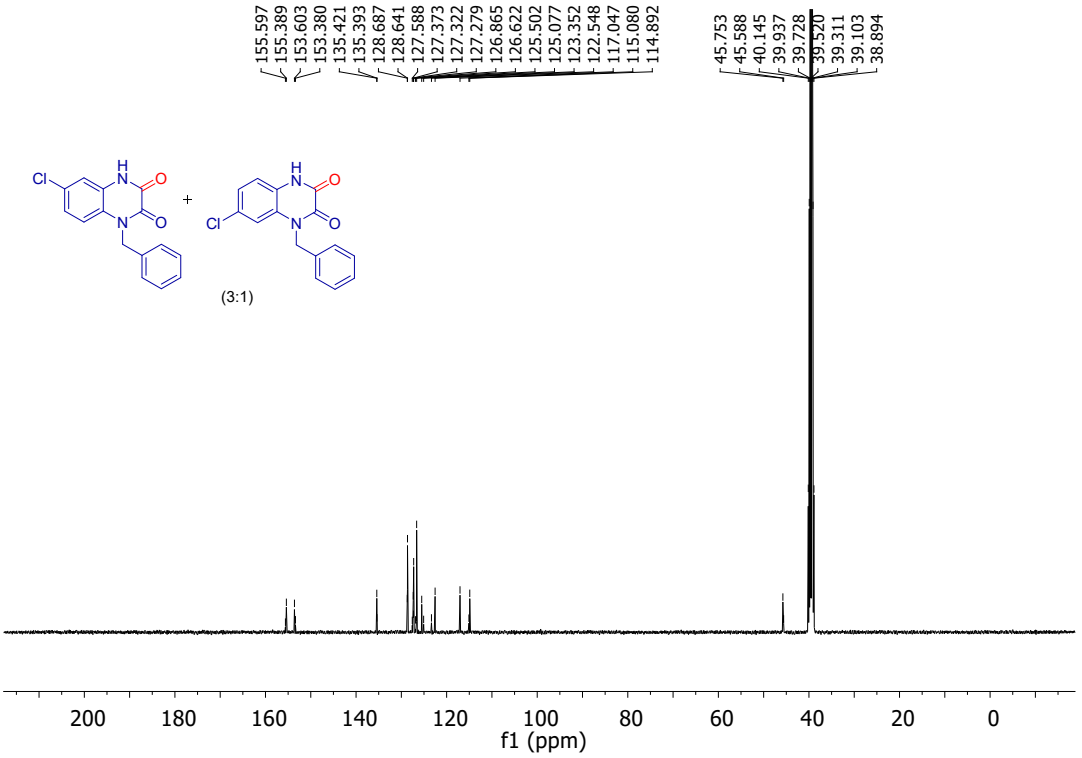


Figure S78. ^{13}C{^{1}H} NMR (100 MHz, DMSO-d_6) spectrum of 1-benzyl-6-chloro-1,4-dihydroquinoxaline-2,3-dione and 1-benzyl-7-chloro-1,4-dihydroquinoxaline-2,3-dione(**3g**).

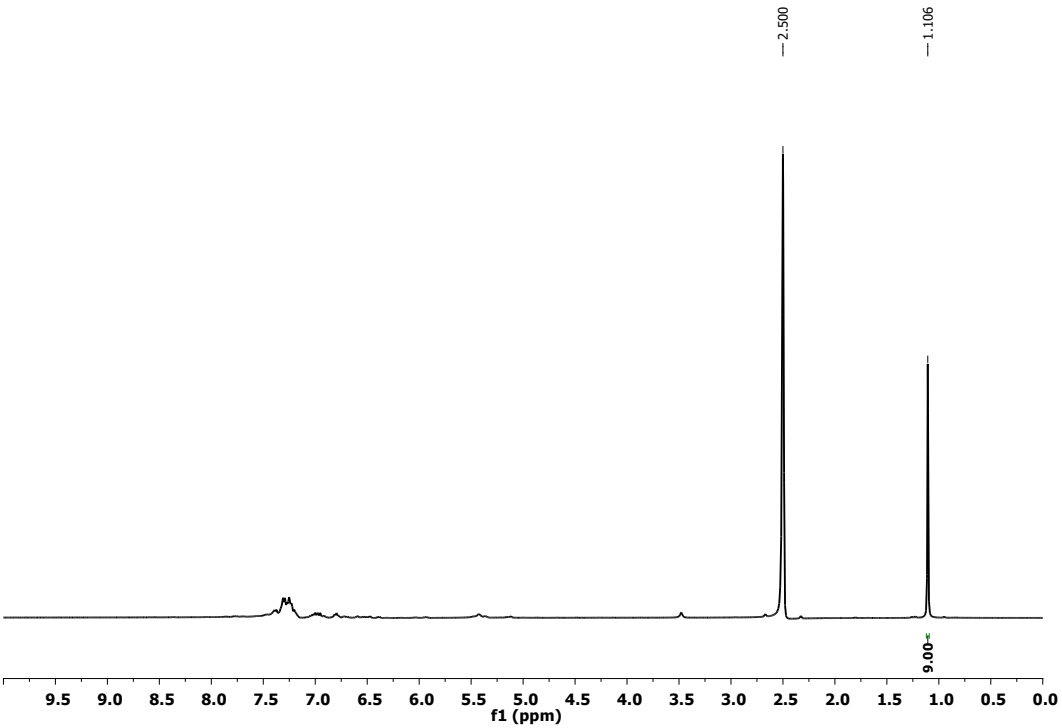


Figure S79. ^{1}H NMR (400 MHz, DMSO-d_6) spectrum of 1-benzylquinoxalin-2(1*H*)-one (**1a**) in presence of potassium *tert*-butoxide.

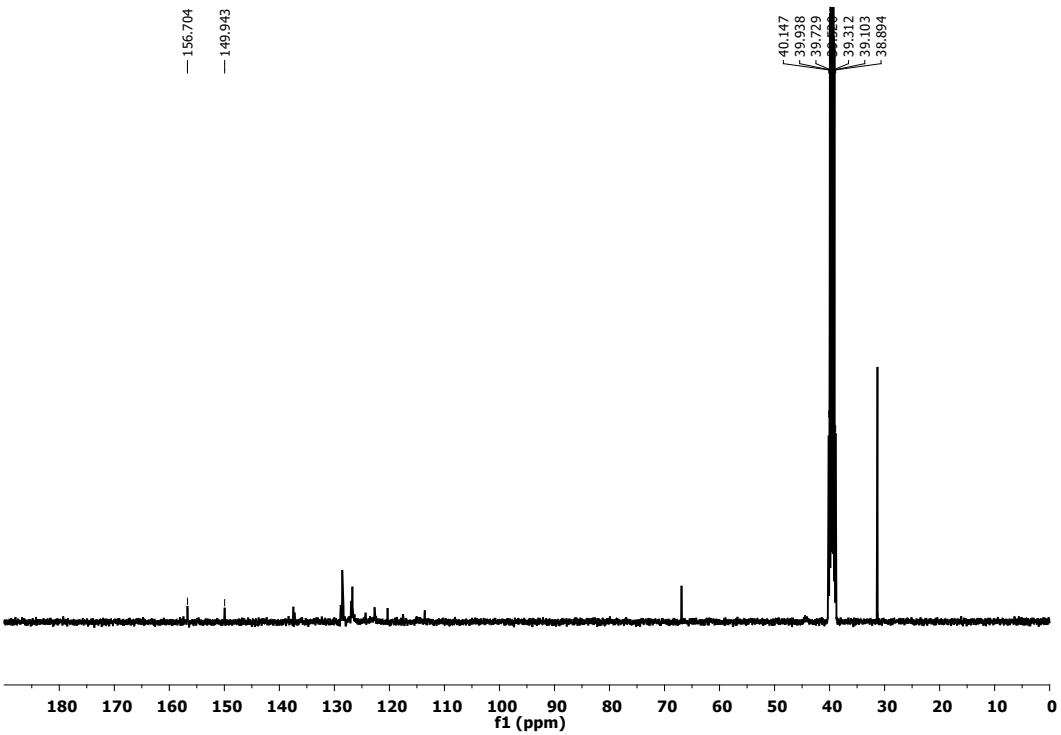


Figure S80. ^{13}C{^{1}H} NMR (100 MHz, DMSO-d_6) spectrum of 1-benzylquinoxalin-2(1*H*)-one (**1a**) in presence of potassium *tert*-butoxide.

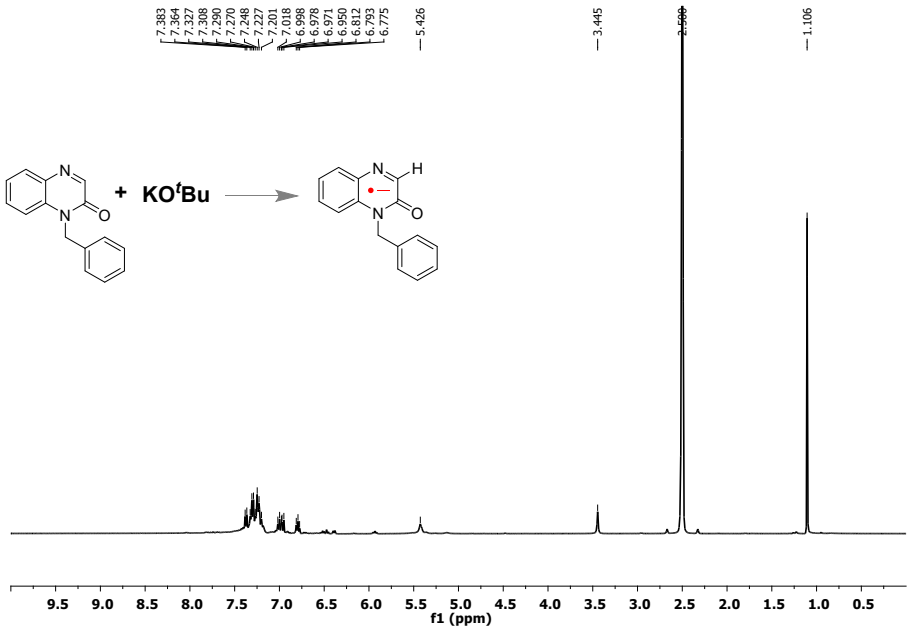


Figure S81. ^{1}H NMR (400 MHz, DMSO-d_6) spectrum of 1-benzylquinoxalin-2(1*H*)-one radical anion after 12 h under Ar atmosphere.

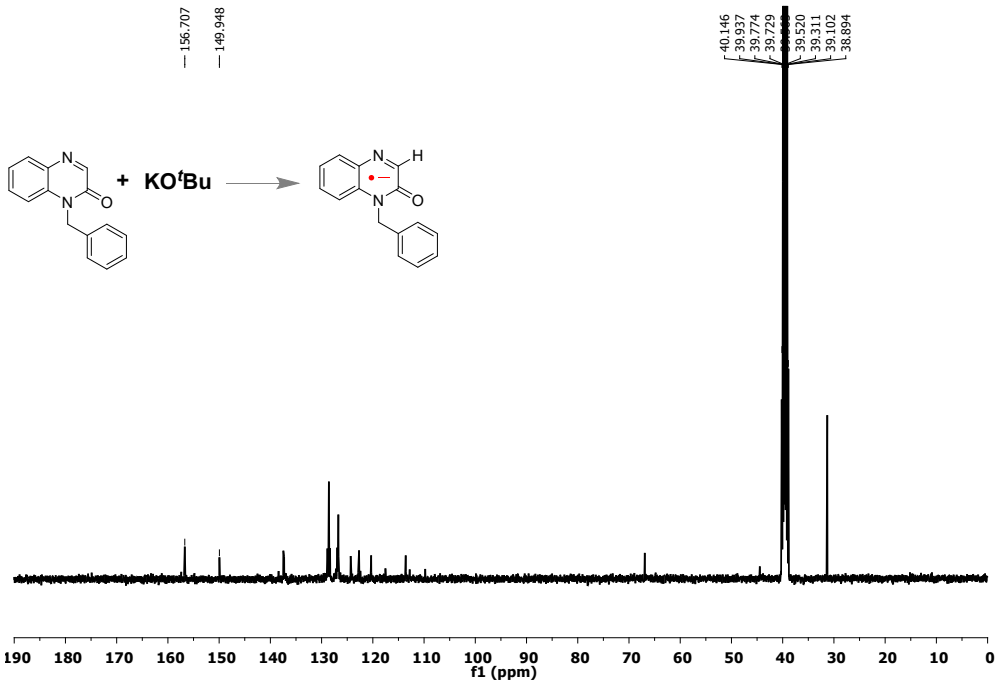


Figure S82. ^{13}C{^{1}H} NMR (100 MHz, DMSO-d_6) spectrum of 1-benzylquinoxalin-2(1*H*)-one radical anion after 12 h under Ar atmosphere.

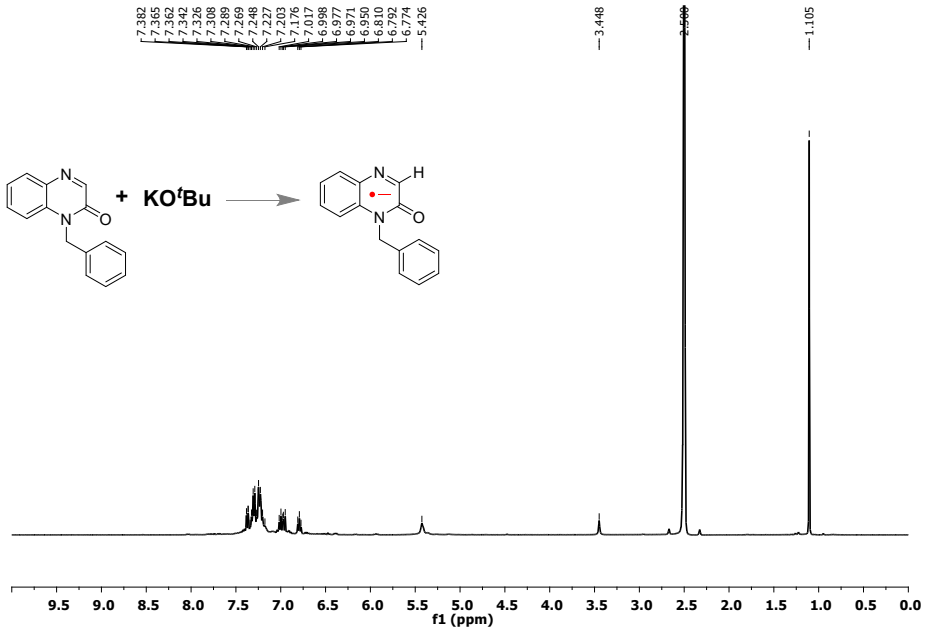


Figure S83. ^{1}H NMR (400 MHz, DMSO-d_6) spectrum of 1-benzylquinoxalin-2(1*H*)-one radical anion after 24 h under Ar atmosphere.

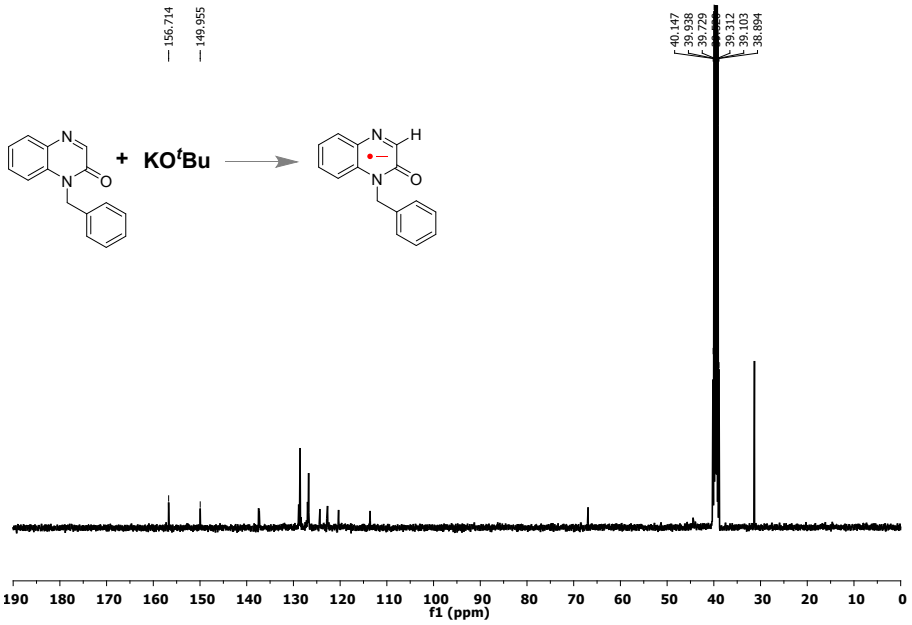


Figure S84. ^{13}C{^{1}H} NMR (100 MHz, DMSO-d_6) spectrum of 1-benzylquinoxalin-2(1*H*)-one radical anion after 24 h under Ar atmosphere.

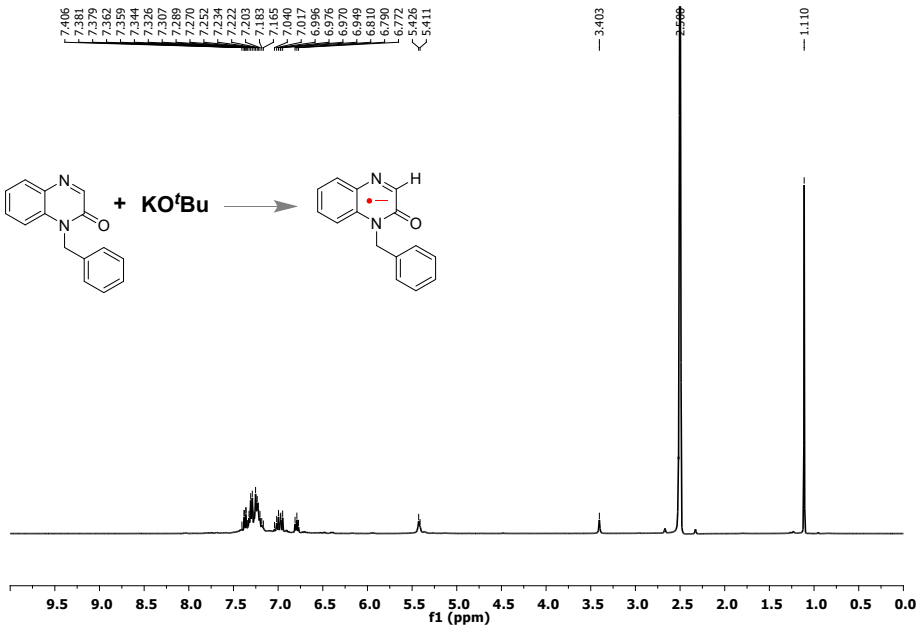


Figure S85. ^{1}H NMR (400 MHz, DMSO-d_6) spectrum of 1-benzylquinoxalin-2(1*H*)-one radical anion after 36 h under Ar atmosphere.

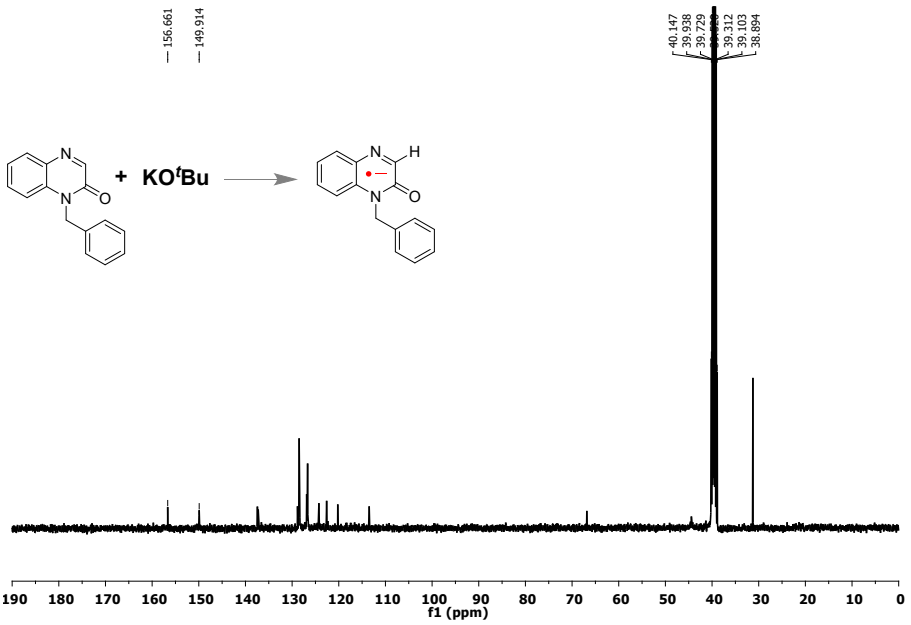


Figure S86. ^{13}C{^{1}H} NMR (100 MHz, DMSO-d_6) spectrum of 1-benzylquinoxalin-2(1*H*)-one radical anion after 36 h under Ar atmosphere.

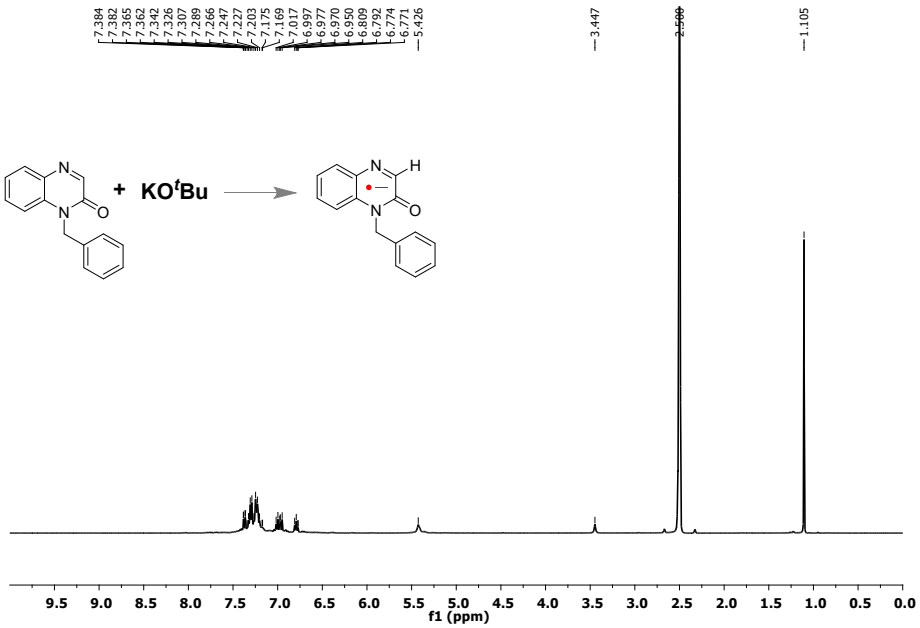


Figure S87. ^{1}H NMR (400 MHz, DMSO-d_6) spectrum of 1-benzylquinoxalin-2(1*H*)-one radical anion after 48 h under Ar atmosphere.

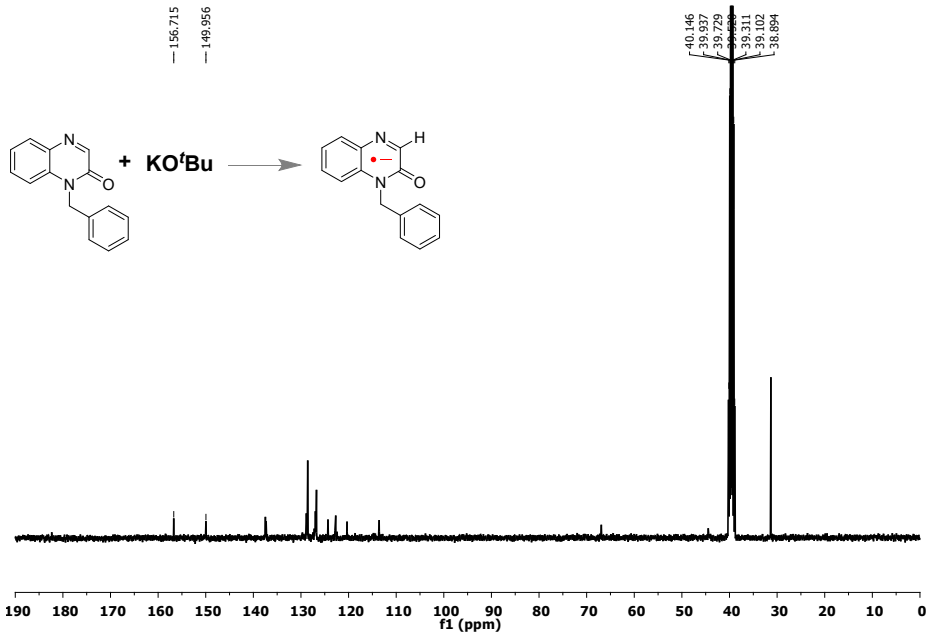


Figure S88. ^{13}C{^{1}H} NMR (100 MHz, DMSO-d_6) spectrum of 1-benzylquinoxalin-2(1*H*)-one radical anion after 48 h under Ar atmosphere.

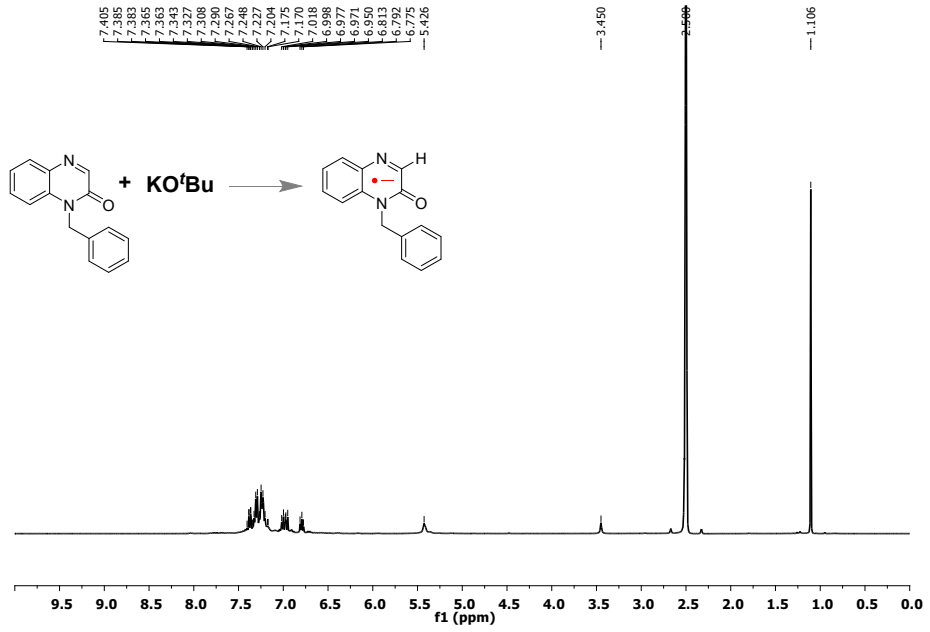


Figure S89. ^{1}H NMR (400 MHz, DMSO-d_6) spectrum of 1-benzylquinoxalin-2(1*H*)-one radical anion after 60 h under Ar atmosphere.

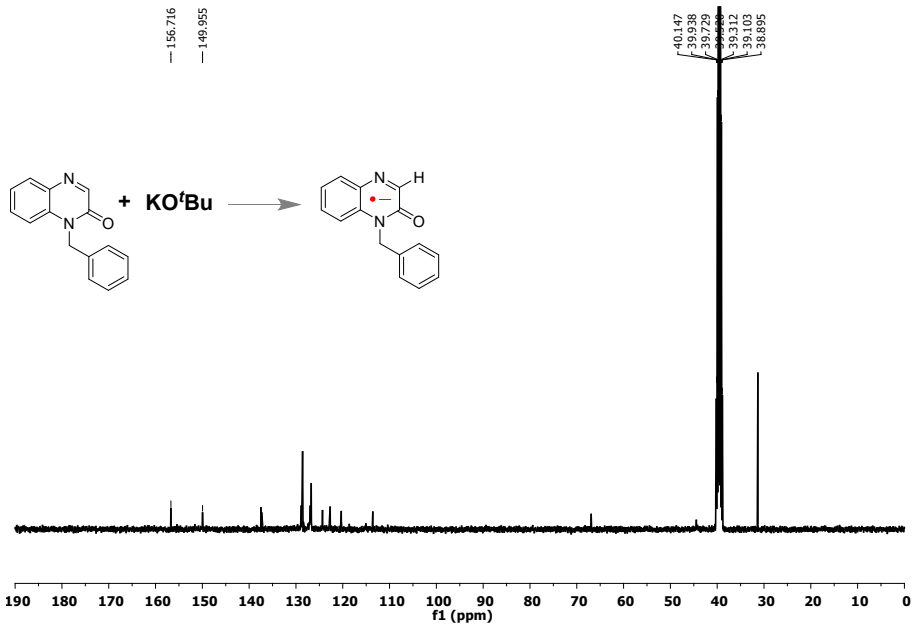


Figure S90. ^{13}C{^{1}H} NMR (100 MHz, DMSO-d_6) spectrum of 1-benzylquinoxalin-2(1*H*)-one radical anion after 60 h under Ar atmosphere.

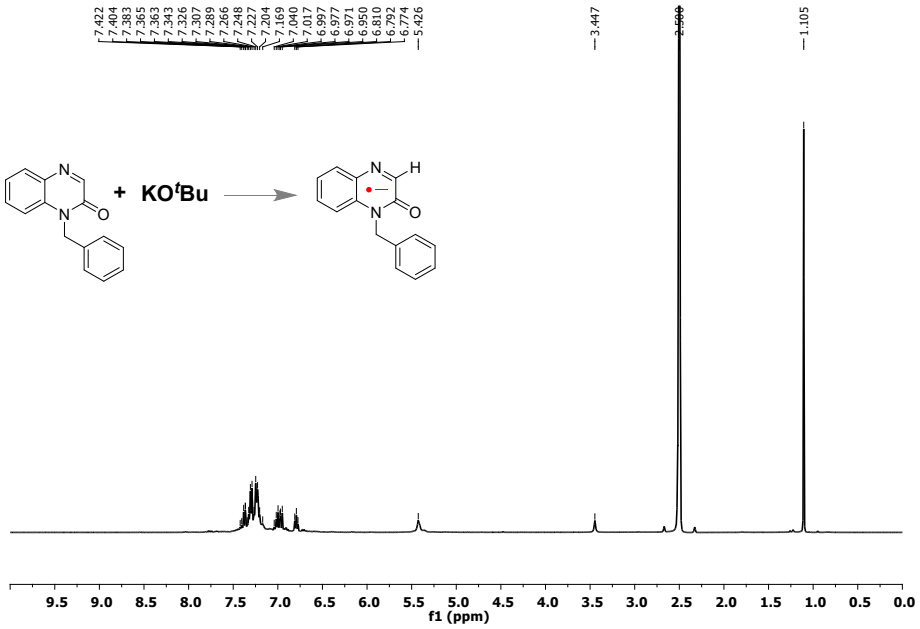


Figure S91. ^{1}H NMR (100 MHz, DMSO-d_6) spectrum of 1-benzylquinoxalin-2(1*H*)-one radical anion after 72 h under Ar atmosphere.

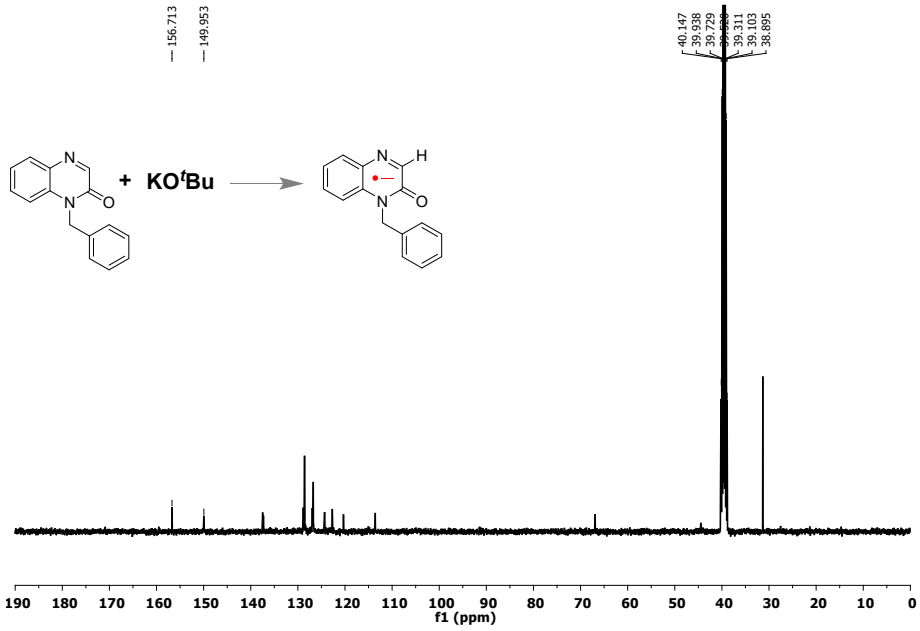


Figure S92. ^{13}C{^{1}H} NMR (100 MHz, DMSO-d_6) spectrum of 1-benzylquinoxalin-2(1*H*)-one radical anion after 72 h under Ar atmosphere.

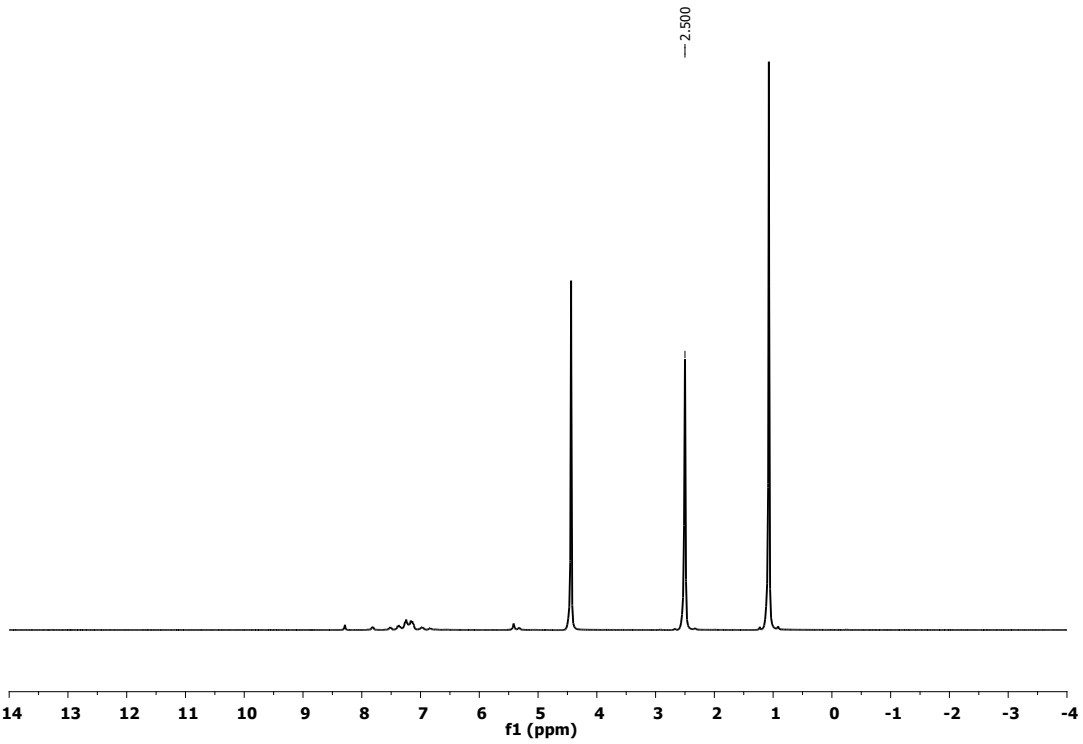


Figure S93. [1]H NMR (100 MHz, DMSO-d_6) spectrum of the reaction under standard condition after the completion of reaction in presence of D_2O.

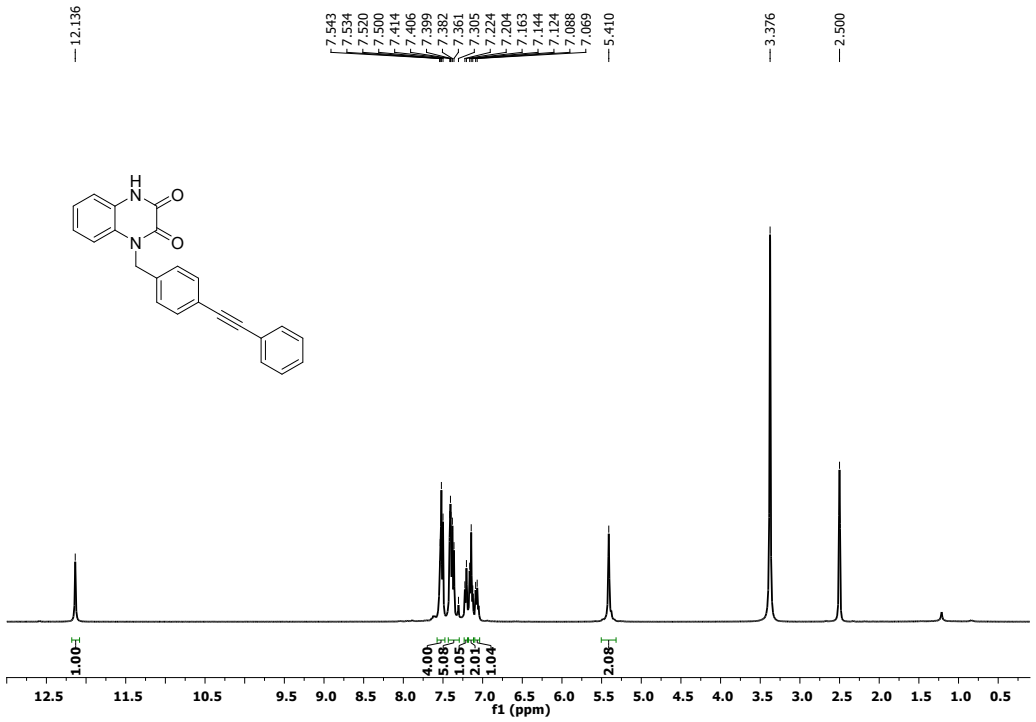


Figure S94. [1]H NMR (100 MHz, DMSO-d_6) spectrum of 1-(4-(phenylethynyl)benzyl)-1,4-dihydroquinoxaline-2,3-dione.

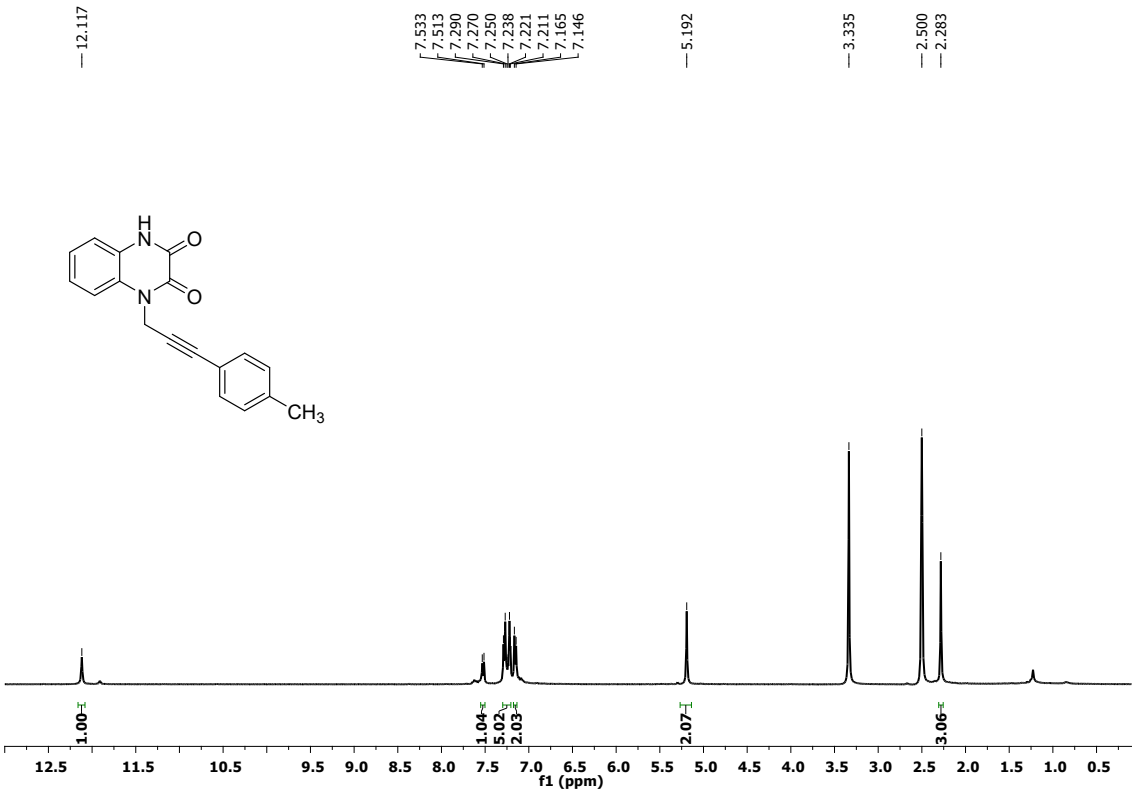


Figure S95. ^{1}H NMR (100 MHz, DMSO-d_6) spectrum of 1-(3-(p-tolyl)prop-2-yn-1-yl)-1,4-dihydroquinoxaline-2,3-dione.

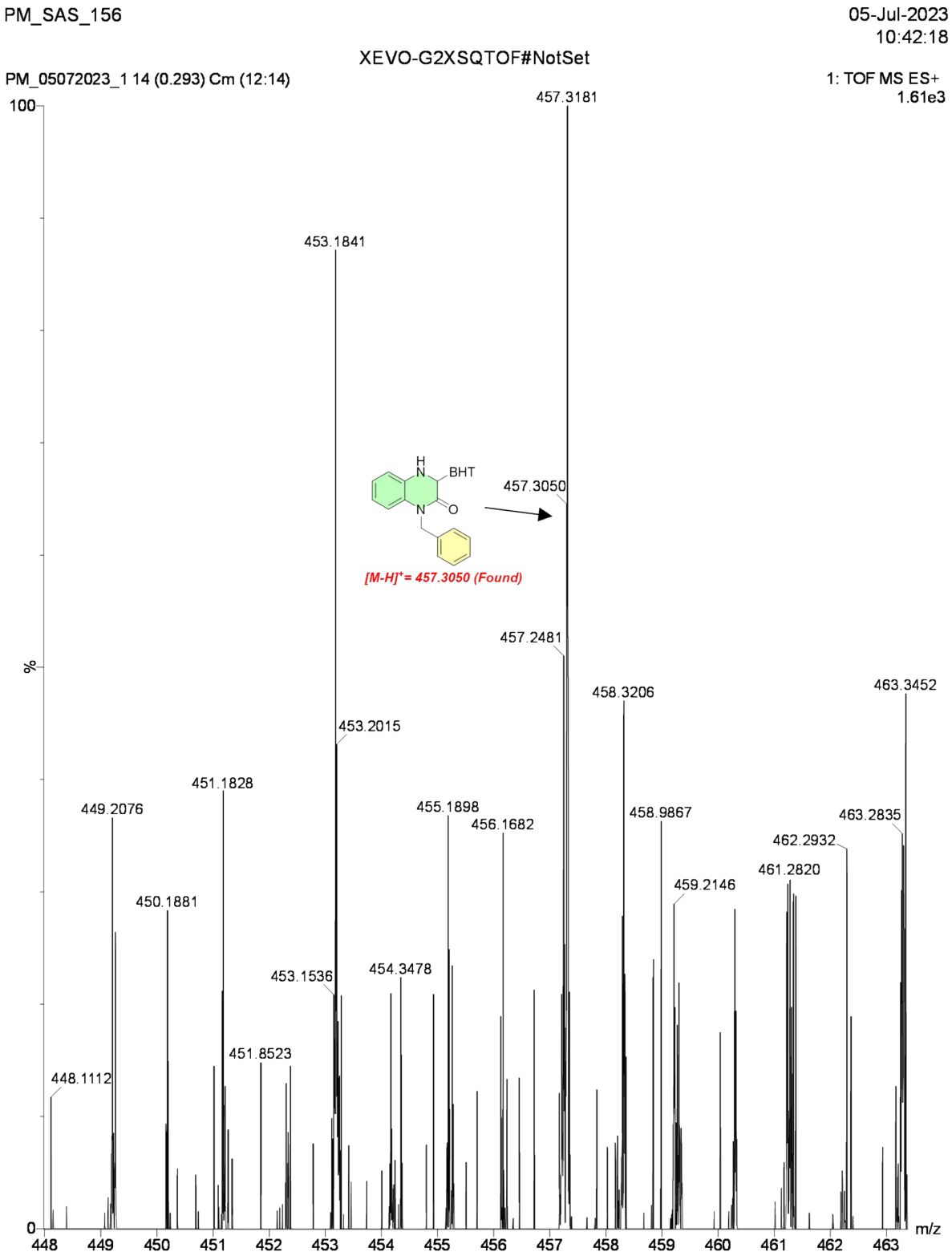


Figure S96. ESI-MS analysis with radical intermediate trapping experiment with BHT.

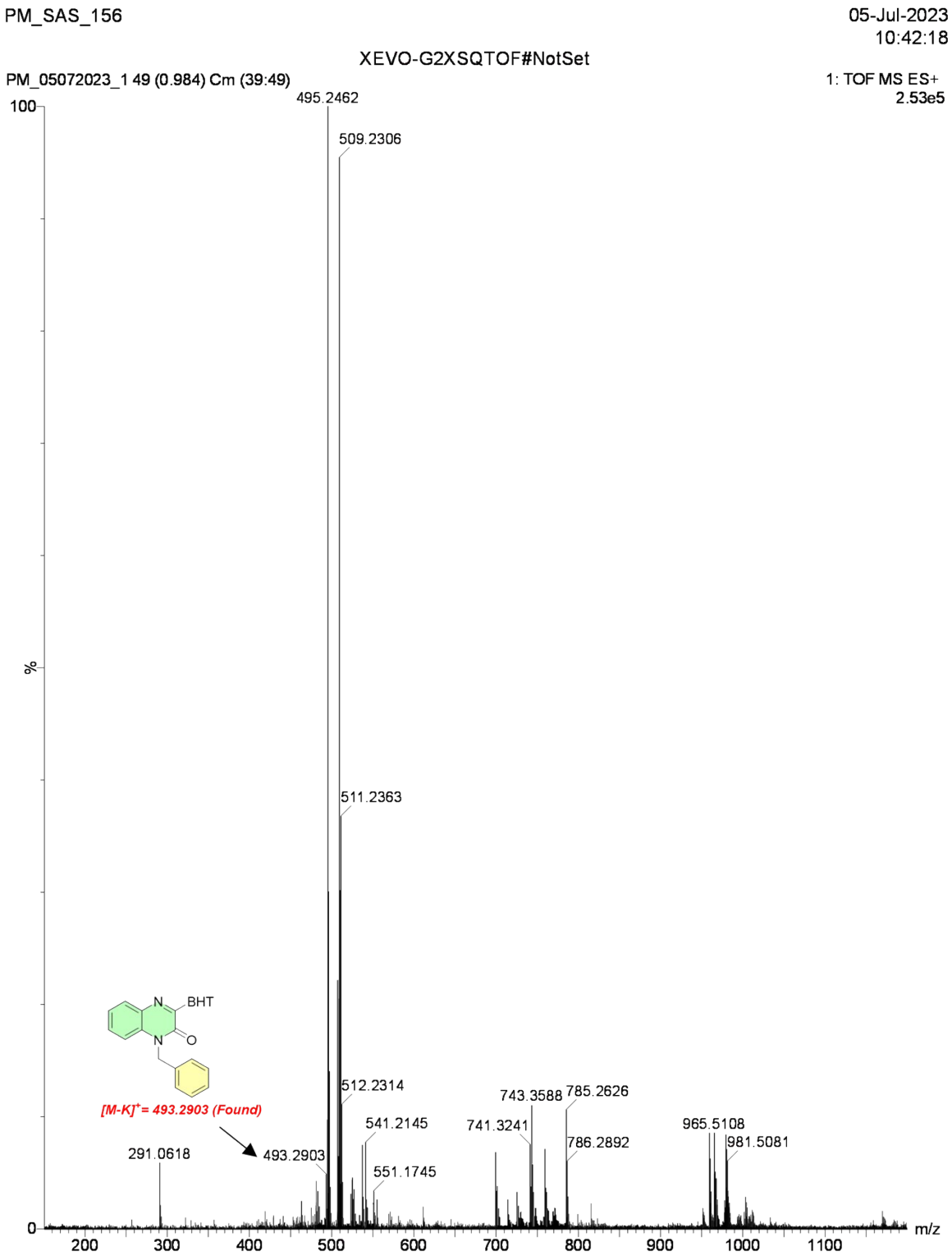


Figure S97. ESI-MS analysis with radical trapping experiment with BHT.

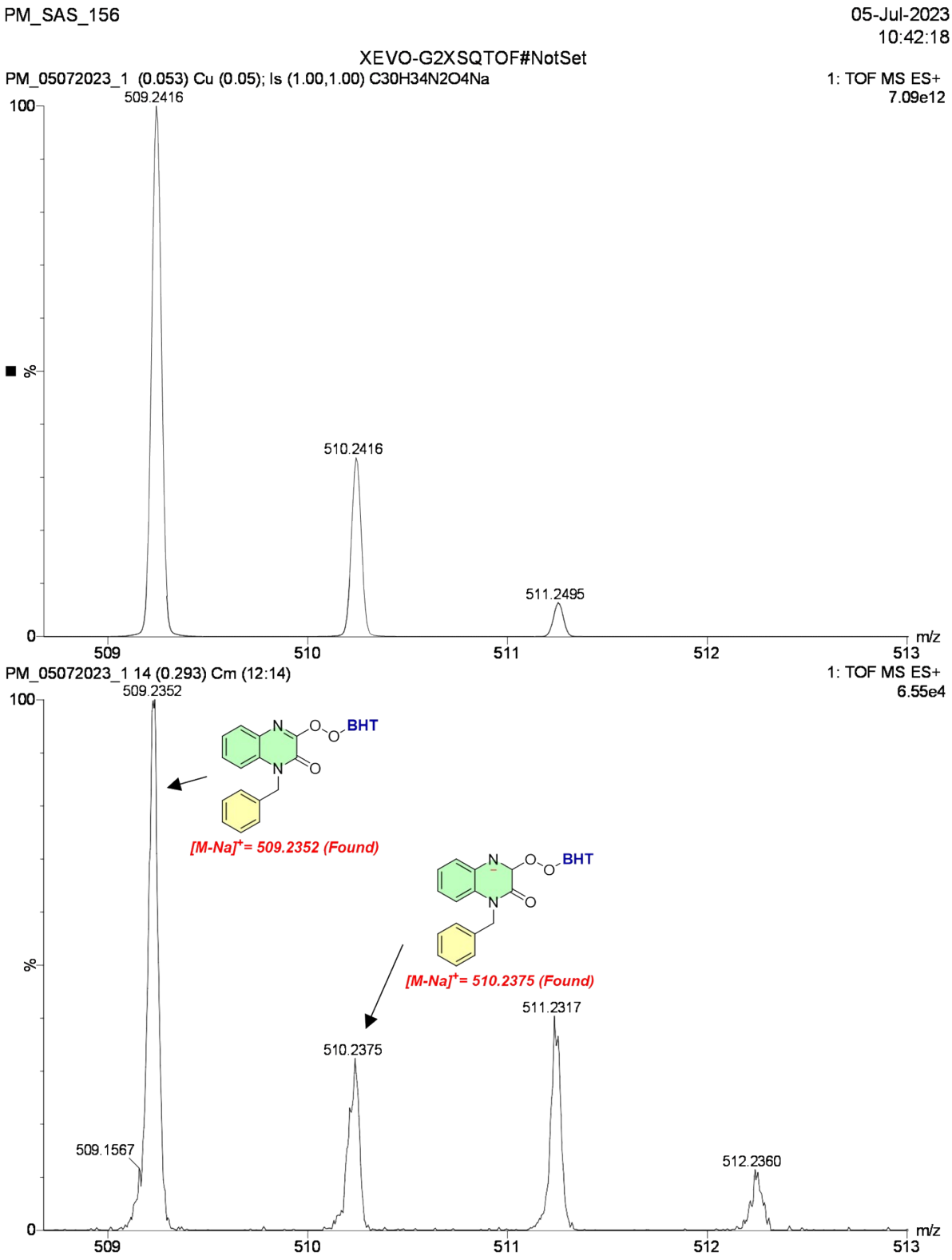


Figure S98. ESI-MS analysis with radical trapping experiment with BHT.

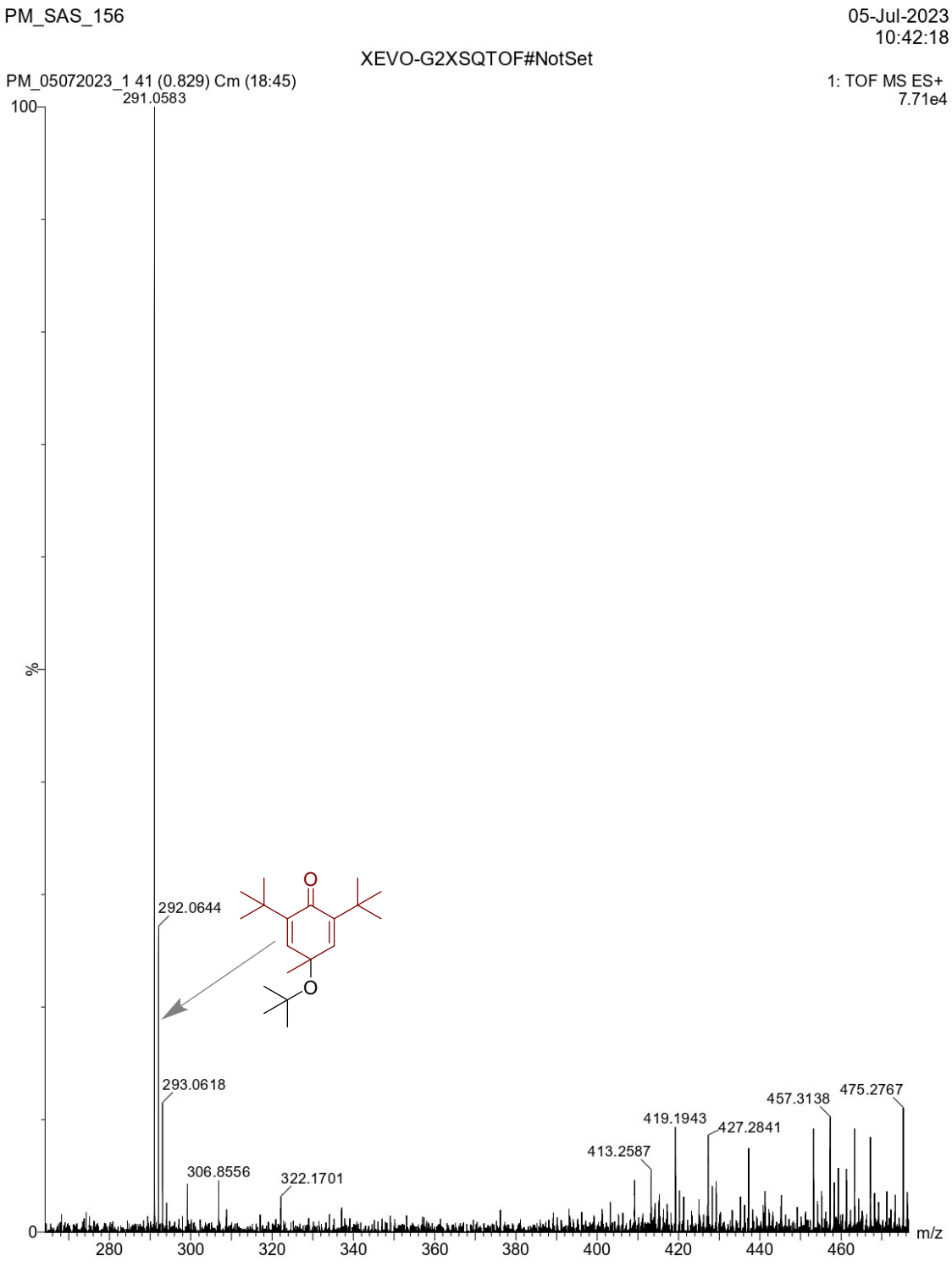


Figure S99. ESI-MS analysis with radical trapping experiment with BHT.

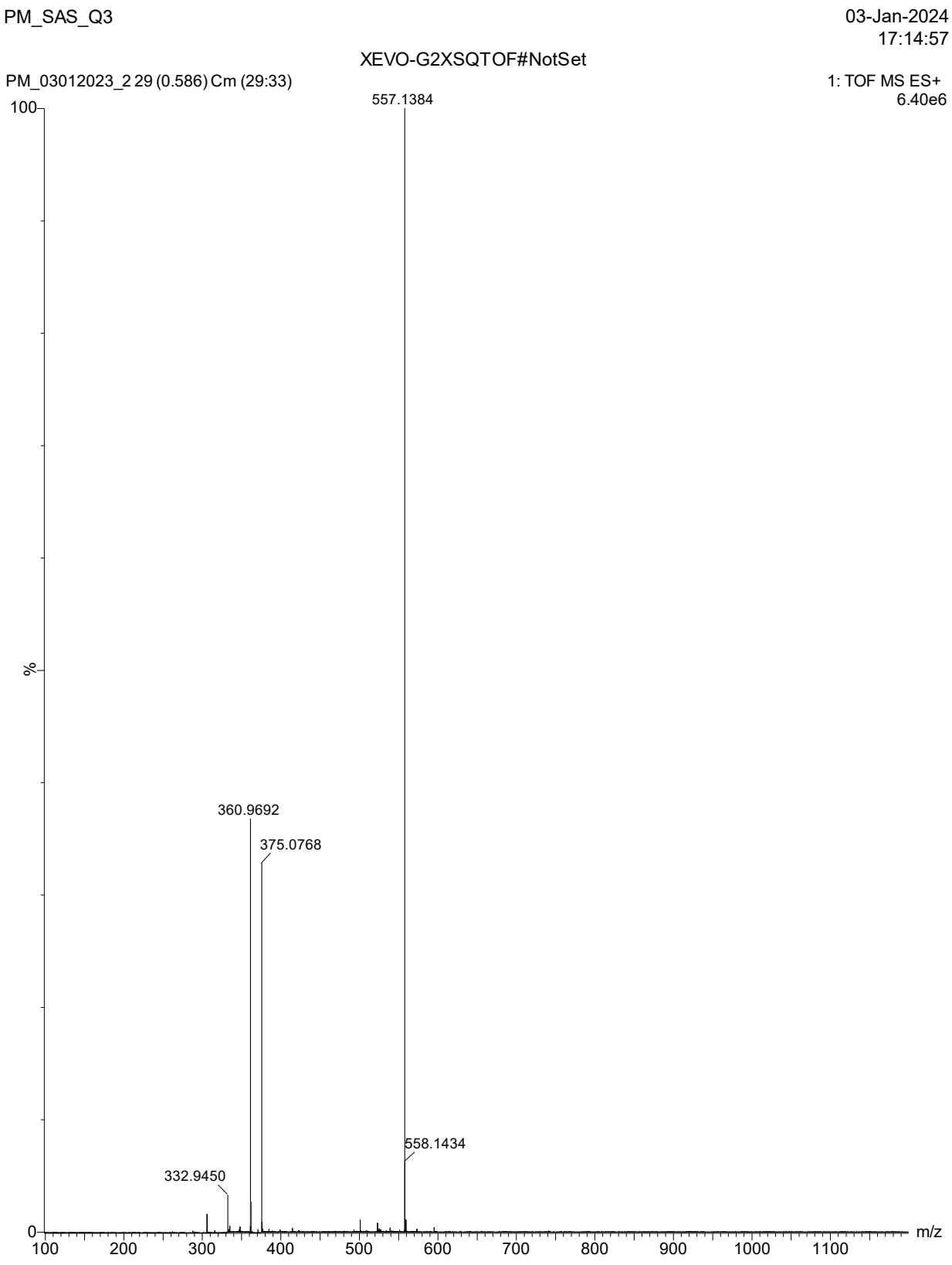


Figure S100. ESI-MS analysis of KO^{t}Bu with BHT in DMSO.

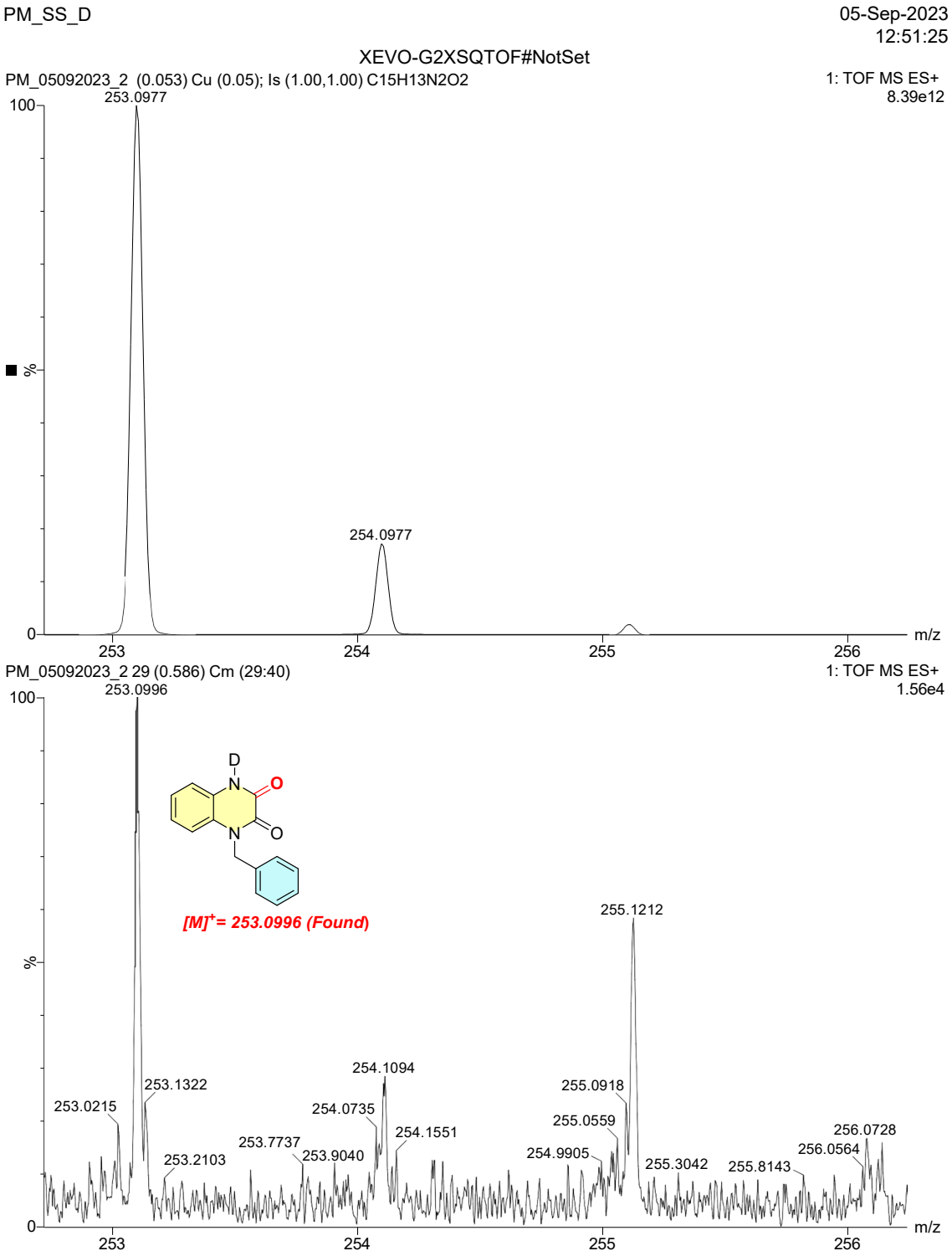


Figure S101. HRMS analysis of isotopic labeling experiment in presence of D_2O.

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2. S. Sau and P. Mal, *European Journal of Organic Chemistry*, 2022, **2022**.
3. S.-H. Jung, J.-W. Yeon, Y. Kang and K. Song, *Asian J. Chem.*, 2014, **26**, 4084.
4. A. Manna, T. K. Dinda, S. Ghosh and P. Mal, *Chem. Mater.*, 2023, **35**, 628.
5. S. Sau and P. Mal, *Eur. J. Org. Chem.*, 2022, e202200425.