

Visible light induced direct highly selective C-H functionalization of quinoxalin-2(1*H*)-one without orientating group

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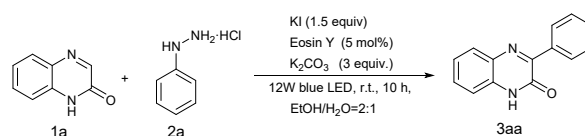
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1. General information

All reagents were purchased from commercial sources and used without further purification. All solvents were dried in a standard manner. Reactions were monitored by TLC on silica gel plates. Column chromatography was performed over silica gel (200-300 mesh) and a petroleum ether/ethyl. Shanghai chenhua CHI600E electrochemical workstation was used in the standard configuration as delivered, including proprietary software. All products were characterized by NMR. ^1H NMR spectra were recorded at 400 MHz and ^{13}C NMR spectra were recorded at 101 MHz (Bruker DPX) with DMSO- d_6 or CDCl_3 as solvent. Chemical shifts are reported in ppm using TMS as internal standard. NMR by the services provided at the Shandong Liaocheng University. HPLC were recorded on an SHIMDZU LC-20A instrument with a HP5-MS 30 m x 0.25 mm capillary apolar columns.

2. General procedure for the catalytic reactions



A dried 10 mL quartz tube equipped was charged with quinoxalin-2(1H)-one (0.2 mmol), phenylhydrazine (0.4 mmol), KI (0.3 mmol), Eosin Y (5 mol%), K_2CO_3 (0.3 mmol) and EtOH/ H_2O (v/v=2:1, 3 mL). The mixture was stirred at room temperature for 10 h under 12 W blue LED irradiation. After the reaction was completed the solution of the crude product was concentrated in vacuo, and the residue was purified by column chromatography on a silica gel (petroleum ether/ethyl acetate=3/1) to afford the target product as a white solid.

3. Optimization of the reaction conditions of quinoxalin-2(1H)-ones.

Table S1 Screening experiment of iodine, iodide and potassium salt^a

Entry	Variations from the standard Conditions	Yield(%) ^b
1	Standard Condition	88
2	NaI instead of KI	62
3	TBAI instead of KI	43
4	I_2 instead of KI	19
5	$\text{K}_2\text{S}_2\text{O}_8$ instead of KI	76
6	KBr instead of KI	42
7	0.1 mmol KI	56
8	0.6 mmol KI	88

^aStandard Conditions: **1a** (0.2 mmol), **2a** (0.4 mmol), catalyst (0.3 mmol), Eosin Y (5 mol%), K_2CO_3 (0.6 mmol), EtOH/ H_2O (v/v=2:1=3 mL), 12 W blue LED at room temperature for 10 h.

^bIsolated yield of **3aa** was determined by **1a**.

Table S2 Fluorescent dye screening experiment^a

Entry	Variations from the standard Conditions	Yield(%) ^b
1	Standard Condition	88
2	Eosin B instead of Eosin Y	72
3	Rose bengal instead of Eosin Y	43
4	Rhodamine B instead of Eosin Y	69
5	Erythrosin B instead of Eosin Y	46
6	10 mol% Eosin Y	83
7	12.5 mol% Eosin Y	83

^aStandard Conditions: **1a** (0.2 mmol), **2a** (0.4 mmol), KI (0.3 mmol), catalyst (5 mol%), K₂CO₃ (0.6 mmol), EtOH/H₂O (v/v=2:1=3 mL), 12 W blue LED at room temperature for 10 h. ^bIsolated yield of **3aa** was determined by **1a**.

Table S3 Base screening experiment^a

Entry	Variations from the standard Conditions	Yield(%) ^b
1	Standard Condition	88
2	NaOH instead of Blue LED	40
3	KOH instead of Blue LED	73
4	<i>t</i> -BuOK instead of Blue LED	13
5	K ₃ PO ₄ instead of 12 W Blue LED	72
6	1.0 mmol K ₂ CO ₃	87

^aStandard Conditions: **1a** (0.2 mmol), **2a** (0.4 mmol), KI (0.3 mmol), Eosin Y (5 mol%), base (0.6 mmol), EtOH/H₂O (v/v=2:1=3 mL), 12 W blue LED at room temperature for 10 h. ^bIsolated yield of **3aa** was determined by **1a**.

Table S4 Light source screening experiment^a

Entry	Variations from the standard Conditions	Yield(%) ^b
1	Standard Condition	88
2	Red LED instead of Blue LED	68
3	Green LED instead of Blue LED	Trace
4	Purple LED instead of Blue LED	43
5	32 W Blue LED instead of 12 W Blue LED	36
6	White LED instead of 12 W Blue LED	23
7	sunlight instead of 12 W Blue LED	Trace

^aStandard Conditions: **1a** (0.2 mmol), **2a** (0.4 mmol), KI (0.3 mmol), Eosin Y (5 mol%), K₂CO₃ (0.6 mmol), EtOH/H₂O (v/v=2:1=3 mL), 12 W LED lamp at room temperature for 10 h. ^bIsolated yield of **3aa** was determined by **1a**.

Table S5 Time control experiment^a

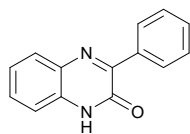
Entry	Variations from the standard Conditions	Yield(%) ^b
1	Standard Condition	88
2	5 h	48
3	8 h	62
4	12 h	88
5	24 h	16

^aStandard Conditions: **1a** (0.2 mmol), **2a** (0.4 mmol), KI (0.3 mmol), Eosin Y (5 mol%), K₂CO₃ (0.6 mmol), EtOH/H₂O (v/v=2:1=3 mL), 12 W blue LED lamp at room temperature, time (h).

^bIsolated yield of **3aa** was determined by **1a**.

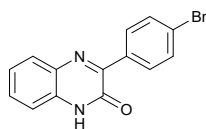
4. Experimental procedures and characterization data

(**3aa**) 3-Phenylquinoxalin-2(1H)-one^[1]



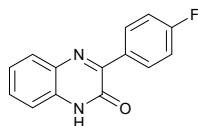
White solid. ¹H NMR (400 MHz, DMSO-*d*₆) δ 12.56 (s, 1H), 8.35-8.23 (m, 2H), 7.82 (dd, *J*=8.1, 1.3 Hz, 1H), 7.58-7.44 (m, 4H), 7.36-7.26 (m, 2H). ¹³C NMR (101 MHz, DMSO-*d*₆) δ 154.58, 154.13, 135.62, 132.05, 132.01, 130.30, 130.18, 129.21, 128.76, 127.84, 123.37, 115.09. MS [EI, *m/z*]: 223.10 [M+H]⁺.

(**3ab**) 3-(4-Bromophenyl)quinoxalin-2(1H)-one^[1]



White solid. ¹H NMR (400 MHz, DMSO-*d*₆+CDCl₃) δ 12.57 (s, 1H), 8.39 (d, *J*=8.7 Hz, 2H), 7.88 (dd, *J*=8.1, 1.4 Hz, 1H), 7.65 (dd, *J*=9.0, 2.2 Hz, 2H), 7.58-7.47 (m, 1H), 7.46-7.30(m, 2H). ¹³C NMR (101 MHz, DMSO-*d*₆+CDCl₃) δ 154.60, 152.60, 134.44, 132.01, 131.79, 130.71, 130.52, 129.90, 128.56, 124.04, 123.08, 114.98. MS [EI, *m/z*]: 301.00 [M+H]⁺.

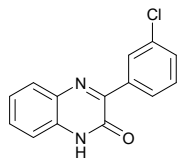
(**3ac**) 3-(4-Fluorophenyl)quinoxalin-2(1H)-one^[1]



White solid. ¹H NMR (400 MHz, DMSO-*d*₆+CDCl₃) δ 12.51 (s, 1H), 8.47-8.32 (m, 2H), 7.77-7.74(m, 1H), 7.45-7.42 (m, 1H), 7.35-7.21 (m, 2H), 7.17 (t, *J*=8.8 Hz, 2H). ¹³C NMR (101 MHz,

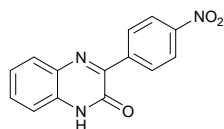
DMSO- d_6 +CDCl₃) δ 154.57, 152.59, 131.92(d, J =6.8 Hz), 131.45(d, J =8.6 Hz), 129.90, 128.55, 123.14, 115.01, 114.62, 114.41. **MS** [EI, m/z]: 241.10 [M+H]⁺.

(3ad) 3-(3-Chlorophenyl)quinoxalin-2(1H)-one^[4]



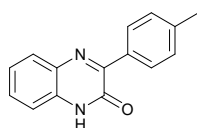
White solid. **¹H NMR** (400 MHz, DMSO- d_6) δ 12.59 (s, 1H), 8.32-8.31(m, 1H), 8.23-8.21(m, 1H), 7.78 (dd, J =8.1, 1.4 Hz, 1H), 7.5-7.42 (m, 3H), 7.29-7.24(m, 2H). **¹³C NMR** (101 MHz, DMSO- d_6) δ 154.51, 152.35, 137.53, 132.67, 132.20, 131.91, 130.77, 129.94, 129.85, 128.95, 128.80, 127.75, 123.55, 115.21. **MS** [EI, m/z]: 257.05 [M+H]⁺.

(3ae) 3-(4-Nitrophenyl)quinoxalin-2(1H)-one^[3]



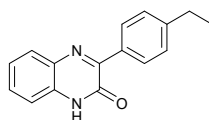
Pale yellow solid. **¹H NMR** (400 MHz, DMSO- d_6) δ 12.76 (s, 1H), 8.65-8.53 (m, 2H), 8.41-8.28 (m, 2H), 7.89 (dd, J =8.3, 1.4 Hz, 1H), 7.63-7.60(m, 1H), 7.39-7.35(m, 2H). **¹³C NMR** (101 MHz, DMSO- d_6) δ 154.53, 152.22, 148.09, 141.57, 132.46, 132.00, 131.36, 130.44, 129.19, 123.72, 123.04, 115.33. **ESI-MS** calcd for C₁₄H₁₀N₃O₃ [M+H]⁺: 268.0644; found: 268.0713.

(3af) 3-*p*-Tolylquinoxalin-2(1H)-one^[1]



White solid. **¹H NMR** (400 MHz, DMSO- d_6 +CDCl₃) δ 12.42 (s, 1H), 8.37 - 8.17 (m, 2H), 7.79 - 7.76 (m, 1H), 7.45-7.41(m, 1H), 7.32 (dd, J =8.2, 1.4 Hz, 1H), 7.29-7.21 (m, 3H), 2.39 (s, 3H). **¹³C NMR** (101 MHz, DMSO- d_6 +CDCl₃) δ 154.64, 153.69, 139.67, 132.75, 132.02, 131.68, 129.37, 128.93, 128.35, 128.11, 122.85, 114.81, 20.95. **MS** [EI, m/z]: 259.10. [M+Na]⁺.

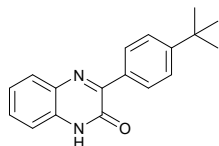
(3ag) 3-(4-Ethylphenyl)quinoxalin-2(1H)-one^[1]



White solid. **¹H NMR** (400 MHz, DMSO- d_6) δ 12.54 (s, 1H), 8.27 (d, J =8.1 Hz, 2H), 7.82 (dd, J =8.0, 1.4 Hz, 1H), 7.61-7.45 (m, 1H), 7.35-7.30(m, 4H), 2.68 (q, J =7.6 Hz, 2H), 1.22 (t, J =7.6

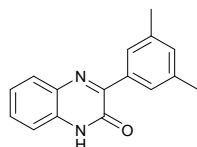
Hz, 3H). ^{13}C NMR (101 MHz, DMSO- d_6) δ 155.11, 154.38, 146.75, 133.63, 132.51, 132.41, 130.55, 129.77, 129.12, 127.76, 123.82, 115.51, 28.60, 15.90. MS [EI, m/z]: 251.12 [M+H] $^+$.

(3ah) 3-(4-*tert*-Butylphenyl)quinoxalin-2(1H)-one^[1]



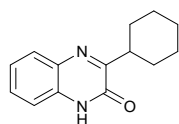
White solid. ^1H NMR (400 MHz, CDCl_3) δ 12.51 (s, 1H), 8.48-8.35 (m, 2H), 7.96 (dd, $J=8.2, 1.3$ Hz, 1H), 7.62-7.57 (m, 2H), 7.56-7.52 (m, 1H), 7.44-7.36 (m, 2H), 1.42 (s, 9H). ^{13}C NMR (101 MHz, CDCl_3) δ 156.68, 154.37, 153.89, 133.40, 132.90, 131.14, 130.15, 129.39, 129.28, 125.28, 124.32, 115.48, 34.94, 31.26. MS [EI, m/z]: 279.15 [M+H] $^+$.

(3ai) 3-(3,5-Dimethylphenyl)quinoxalin-2(1H)-one^[3]



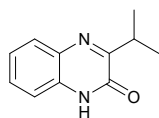
White solid. ^1H NMR (400 MHz, DMSO- d_6 + CDCl_3) δ 12.44 (s, 1H), 7.78-7.66 (m, 1H), 7.51-7.41 (m, 1H), 7.33-7.28 (m, 2H), 7.27-7.20 (m, 1H), 7.08-6.99 (m, 2H), 2.32 (d, $J=3.4$ Hz, 3H), 2.24 (d, $J=3.4$ Hz, 3H). ^{13}C NMR (101 MHz, DMSO- d_6 + CDCl_3) δ 158.68, 154.35, 138.08, 136.23, 133.00, 131.95, 131.85, 130.51, 129.68, 129.12, 128.37, 125.47, 122.83, 115.08, 20.76, 19.40. ESI-MS calcd for $\text{C}_{16}\text{H}_{15}\text{N}_2\text{O}$ [M+H] $^+$: 251.1106; found: 251.1175.

(3aj) 3-Cyclohexylquinoxalin-2(1H)-one^[2]



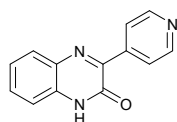
White solid. ^1H NMR (400 MHz, DMSO- d_6 + CDCl_3) δ 12.17 (s, 1H), 7.69-7.66 (m, 1H), 7.38-7.35 (m, 1H), 7.30-7.14 (m, 2H), 1.96 - 1.79 (m, 5H), 1.78-1.69 (m, 1H), 1.59-1.18 (m, 5H). ^{13}C NMR (101 MHz, DMSO- d_6 + CDCl_3) δ 164.51, 154.30, 131.75, 131.16, 128.58, 127.88, 122.47, 114.87, 29.87, 25.73, 25.59. MS [EI, m/z]: 229.15. [M+H] $^+$.

(3ak) 3-Isopropylquinoxalin-2(1H)-one^[2]



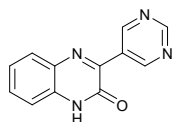
White solid. $^1\text{H NMR}$ (400 MHz, $\text{DMSO-}d_6+\text{CDCl}_3$) δ 12.21 (s, 1H), 7.69 (dd, $J=8.0, 1.4$ Hz, 1H), 7.42-7.36 (m, 1H), 7.29-7.19 (m, 2H), 3.48 (s, 1H), 1.23 (d, $J=6.9$ Hz, 6H). $^{13}\text{C NMR}$ (101 MHz, $\text{DMSO-}d_6+\text{CDCl}_3$) δ 165.27, 154.16, 131.57, 131.44, 128.80, 127.97, 122.56, 114.94, 29.73, 19.82. **ESI-MS** calcd for $\text{C}_{11}\text{H}_{13}\text{N}_2\text{O}$ $[\text{M}+\text{H}]^+$: 189.0950; found: 189.1019.

(3al) 3-(Pyridin-4-yl)quinoxalin-2(1H)-one^[4]



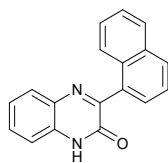
White solid. $^1\text{H NMR}$ (400 MHz, $\text{DMSO-}d_6+\text{CDCl}_3$) δ 12.66 (s, 1H), 8.67 (d, $J= 5.1$ Hz, 2H), 8.25 (d, $J=5.0$ Hz, 2H), 7.82 (d, $J=8.0$ Hz, 1H), 7.50 (t, $J=7.7$ Hz, 1H), 7.39-7.24 (m, 2H). $^{13}\text{C NMR}$ (101 MHz, $\text{DMSO-}d_6+\text{CDCl}_3$) δ 154.37, 151.54, 149.25, 142.31, 132.23, 131.85, 130.83, 128.96, 123.24, 122.69, 115.15. **MS** [EI, m/z]: 224.10. $[\text{M}+\text{H}]^+$.

(3am) 3-(Pyrimidin-5-yl)quinoxalin-2(1H)-one^[4]



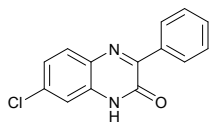
Brown solid. $^1\text{H NMR}$ (400 MHz, $\text{DMSO-}d_6$) δ 12.78 (s, 1H), 9.33 (d, $J=1.5$ Hz, 1H), 8.84 (dd, $J=2.5, 1.5$ Hz, 1H), 8.76 (d, $J=2.5$ Hz, 1H), 7.91-7.88(m, $J=8.1, 1.4$ Hz, 1H), 7.65-7.61(m, 1H), 7.49-7.23 (m, 2H). $^{13}\text{C NMR}$ (101 MHz, $\text{DMSO-}d_6$) δ 154.83, 153.46, 149.61, 146.34, 145.49, 145.01, 133.05, 132.58, 131.99, 129.80, 124.19, 115.96. **ESI-MS** calcd for $\text{C}_{12}\text{H}_9\text{N}_4\text{O}$ $[\text{M}+\text{H}]^+$: 225.0698; found: 225.0768.

(3an) 3-(Naphthalen-2-yl)-3,4-dihydroquinoxalin-2(1H)-one^[3]



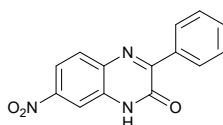
Lavender solid. $^1\text{H NMR}$ (400 MHz, $\text{DMSO-}d_6+\text{CDCl}_3$) δ 12.62 (s, 1H), 7.99-7.93(m, 2H), 7.88-7.86(m, 1H), 7.82-7.77(m, 1H), 7.73 - 7.67(m, 1H), 7.61-7.38 (m, 5H), 7.35-7.27(m, 1H). $^{13}\text{C NMR}$ (101 MHz, $\text{DMSO-}d_6+\text{CDCl}_3$) δ 158.4, 155.28, 134.18, 133.54, 132.78, 132.55, 131.48, 130.71, 129.71, 129.18, 128.52, 127.86, 126.58, 126.19, 125.88, 125.23, 123.60, 115.84. **MS** [EI, m/z]: 295.10 $[\text{M}+\text{Na}]^+$.

(3ao) 7-Chloro-3-phenylquinoxalin-2(1H)-one^[1]



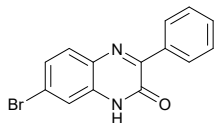
White solid. $^1\text{H NMR}$ (400 MHz, $\text{DMSO-}d_6+\text{CDCl}_3$) δ 12.53 (s, 1H), 8.38-8.19 (m, 2H), 7.72 (d, $J=8.6$ Hz, 1H), 7.50-7.34 (m, 3H), 7.29 (d, $J=2.2$ Hz, 1H), 7.20 (dd, $J=8.6, 2.3$ Hz, 1H). $^{13}\text{C NMR}$ (101 MHz, $\text{DMSO-}d_6+\text{CDCl}_3$) δ 154.35, 154.02, 135.17, 134.55, 132.75, 130.65, 129.95, 129.89, 128.99, 127.49, 123.20, 114.31. **MS** [EI, m/z]: 279.05 $[\text{M}+\text{Na}]^+$.

(3ap) 7-Nitro-3-phenylquinoxalin-2(1H)-one^[1]



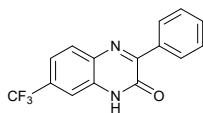
White solid. $^1\text{H NMR}$ (400 MHz, $\text{DMSO-}d_6+\text{CDCl}_3$) δ 12.88 (s, 1H), 8.43-8.35 (m, 2H), 8.18 (d, $J=2.5$ Hz, 1H), 8.11-8.04 (m, 2H), 7.55-7.46 (m, 3H). $^{13}\text{C NMR}$ (101 MHz, $\text{DMSO-}d_6+\text{CDCl}_3$) δ 157.29, 154.20, 146.90, 135.38, 134.70, 132.07, 130.78, 129.66, 129.40, 127.61, 117.17, 110.55. **MS** [EI, m/z]: 268.10 $[\text{M}+\text{H}]^+$.

(3aq) 7-Bromo-3-phenylquinoxalin-2(1H)-one^[1]



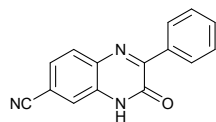
White solid. $^1\text{H NMR}$ (400 MHz, $\text{DMSO-}d_6+\text{CDCl}_3$) δ 12.59 (s, 1H), 8.31-8.28 (m, 3H), 7.91 (dd, $J=4.8, 2.2$ Hz, 1H), 7.55-7.52 (m, $J=8.7, 4.8, 2.2$ Hz, 1H), 7.46-7.43 (m, 2H), 7.26-7.22 (m, 1H). $^{13}\text{C NMR}$ (101 MHz, $\text{DMSO-}d_6+\text{CDCl}_3$) δ 155.04, 154.30, 135.09, 132.87, 132.24, 131.06, 130.55, 130.11, 129.10, 127.50, 116.67, 114.58. **MS** [EI, m/z]: 300.05 $[\text{M}+\text{H}]^+$.

(3ar) 3-Phenyl-7-(trifluoromethyl)quinoxalin-2(1H)-one^[1]



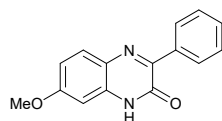
White solid. $^1\text{H NMR}$ (400 MHz, $\text{DMSO-}d_6$) δ 12.75 (s, 1H), 8.33 (d, $J=7.4$ Hz, 2H), 8.01 (d, $J=8.3$ Hz, 1H), 7.63-7.47 (m, 5H). $^{13}\text{C NMR}$ (101 MHz, $\text{DMSO-}d_6$) δ 157.25, 154.86, 135.58, 134.35, 132.66, 131.29, 130.40, 130.11, 129.94, 129.84, 129.79, 128.39, 125.59, 122.89, 119.79, 112.69. **MS** [EI, m/z]: 291.05 $[\text{M}+\text{H}]^+$.

(3as) 3-Oxo-2-phenyl-3,4-dihydroquinoxaline-6-carbonitrile^[1]



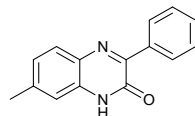
White solid. $^1\text{H NMR}$ (400 MHz, $\text{DMSO-}d_6$) δ 12.84 (s, 1H), 8.34-8.27 (m, 3H), 7.89 (dd, $J = 8.5, 1.8$ Hz, 1H), 7.57-7.48 (m, 3H), 7.43 (d, $J = 8.5$ Hz, 1H). $^{13}\text{C NMR}$ (101 MHz, $\text{DMSO-}d_6$) δ 156.55, 154.94, 136.16, 135.43, 133.77, 133.20, 131.95, 131.24, 129.85, 128.41, 118.96, 116.94, 105.93. **ESI-MS** calcd for $\text{C}_{15}\text{H}_{10}\text{N}_3\text{O}$ $[\text{M}+\text{H}]^+$: 300.00; found: 248.0850.

(3at) 7-Methoxy-3-phenylquinoxalin-2(1H)-one^[1]



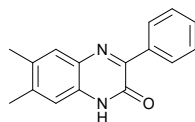
White solid. $^1\text{H NMR}$ (400 MHz, $\text{DMSO-}d_6+\text{CDCl}_3$) δ 12.34 (s, 1H), 8.33-8.22 (m, 2H), 7.66 (d, $J=8.9$ Hz, 1H), 7.42-7.33 (m, 3H), 6.83 (d, $J=8.9$ Hz, 1H), 6.76 (d, $J=2.7$ Hz, 1H), 3.83 (s, 3H). $^{13}\text{C NMR}$ (101 MHz, $\text{DMSO-}d_6+\text{CDCl}_3$) δ 160.60, 154.90, 150.30, 135.73, 133.39, 129.75, 129.14, 128.63, 127.37, 127.10, 111.95, 97.10, 55.21. **MS** [EI, m/z]: 275.10 $[\text{M}+\text{Na}]^+$.

(3au) 7-Methyl-3-phenylquinoxalin-2(1H)-one^[1]



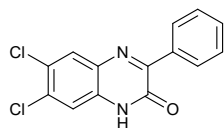
White solid. $^1\text{H NMR}$ (400 MHz, $\text{DMSO-}d_6$) δ 12.48 (s, 1H), 8.34-8.27 (m, 2H), 7.72-7.63 (m, 1H), 7.49 (dt, $J = 5.3, 2.5$ Hz, 3H), 7.38-7.10 (m, 2H), 2.40 (d, $J = 8.9$ Hz, 3H). $^{13}\text{C NMR}$ (101 MHz, $\text{DMSO-}d_6$) δ 155.20, 153.32, 141.09, 136.22, 132.46, 130.79, 130.43, 129.56, 128.98, 128.29, 125.28, 115.15, 21.80. **MS** [EI, m/z]: 237.10 $[\text{M}+\text{H}]^+$.

(3av) 6,7-Dimethyl-3-phenylquinoxalin-2(1H)-one^[4]



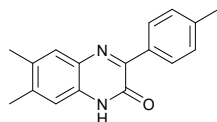
White solid. $^1\text{H NMR}$ (400 MHz, $\text{DMSO-}d_6+\text{CDCl}_3$) δ 12.30 (d, $J=3.8$ Hz, 1H), 8.53-8.20 (m, 2H), 7.57 (d, $J=4.2$ Hz, 1H), 7.46-7.40 (m, 3H), 7.12-7.06 (m, 1H), 2.36-2.32 (m, $J=8.2, 2.8$ Hz, 6H). $^{13}\text{C NMR}$ (101 MHz, $\text{DMSO-}d_6+\text{CDCl}_3$) δ 155.35, 153.21, 140.12, 136.33, 132.30, 131.25, 130.38, 129.90, 129.35, 128.96, 127.94, 115.56, 20.26, 19.50. **MS** [EI, m/z]: 273.10 $[\text{M}+\text{Na}]^+$.

(3aw) 6,7-Dichloro-3-phenylquinoxalin-2(1H)-one^[4]



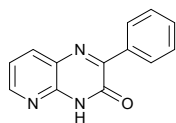
White solid. $^1\text{H NMR}$ (400 MHz, $\text{DMSO-}d_6$) δ 12.64 (s, 1H), 8.28 (dt, $J = 6.8, 1.6$ Hz, 2H), 8.03 (s, 1H), 7.56-7.44 (m, 4H). $^{13}\text{C NMR}$ (101 MHz, $\text{DMSO-}d_6$) δ 160.84, 159.38, 140.23, 137.40, 137.08, 136.66, 135.93, 134.79, 134.59, 133.13, 130.32, 121.30. **MS** [EI, m/z]: 291.10 $[\text{M}+\text{H}]^+$.

(3ax) 6,7-Dimethyl-3-*p*-tolylquinoxalin-2(1H)-one^[4]



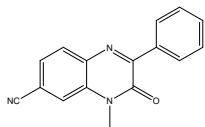
White solid. $^1\text{H NMR}$ (400 MHz, $\text{DMSO-}d_6$) δ 12.40 (s, 1H), 8.24 (d, $J=7.9$ Hz, 2H), 7.59 (s, 1H), 7.28 (d, $J=7.9$ Hz, 2H), 7.08 (s, 1H), 2.37 (s, 3H), 2.30 (d, $J=8.3$ Hz, 6H). $^{13}\text{C NMR}$ (101 MHz, $\text{DMSO-}d_6$) δ 154.72, 152.45, 139.74, 139.70, 133.15, 132.04, 130.59, 129.99, 129.03, 128.47 (d, $J=3.3$ Hz), 115.03, 21.04, 19.82, 18.96. **MS** [EI, m/z]: 287.15. $[\text{M}+\text{Na}]^+$.

(3ay) 2-Phenylpyrido[3,2-*b*]pyrazin-3(4H)-one^[2]



White solid. $^1\text{H NMR}$ (400 MHz, $\text{DMSO-}d_6+\text{CDCl}_3$) δ 12.87 (s, 1H), 8.22-8.16 (m, 2H), 8.07 (dd, $J = 8.0, 1.7$ Hz, 1H), 7.40-7.30 (m, 4H), 7.22 (dd, $J = 7.9, 4.7$ Hz, 1H). $^{13}\text{C NMR}$ (101 MHz, $\text{DMSO-}d_6+\text{CDCl}_3$) δ 155.77, 155.19, 149.83, 143.61, 136.36, 135.00, 132.33, 130.22, 129.21, 129.08, 128.03, 127.58, 119.45. **ESI-MS** calcd for $\text{C}_{13}\text{H}_{10}\text{N}_3\text{O}$ $[\text{M}+\text{H}]^+$: 224.0746; found: 224.0818.

(3az) 4-methyl-3-oxo-2-phenyl-3,4-dihydroquinoxaline-6-carbonitrile^[1]



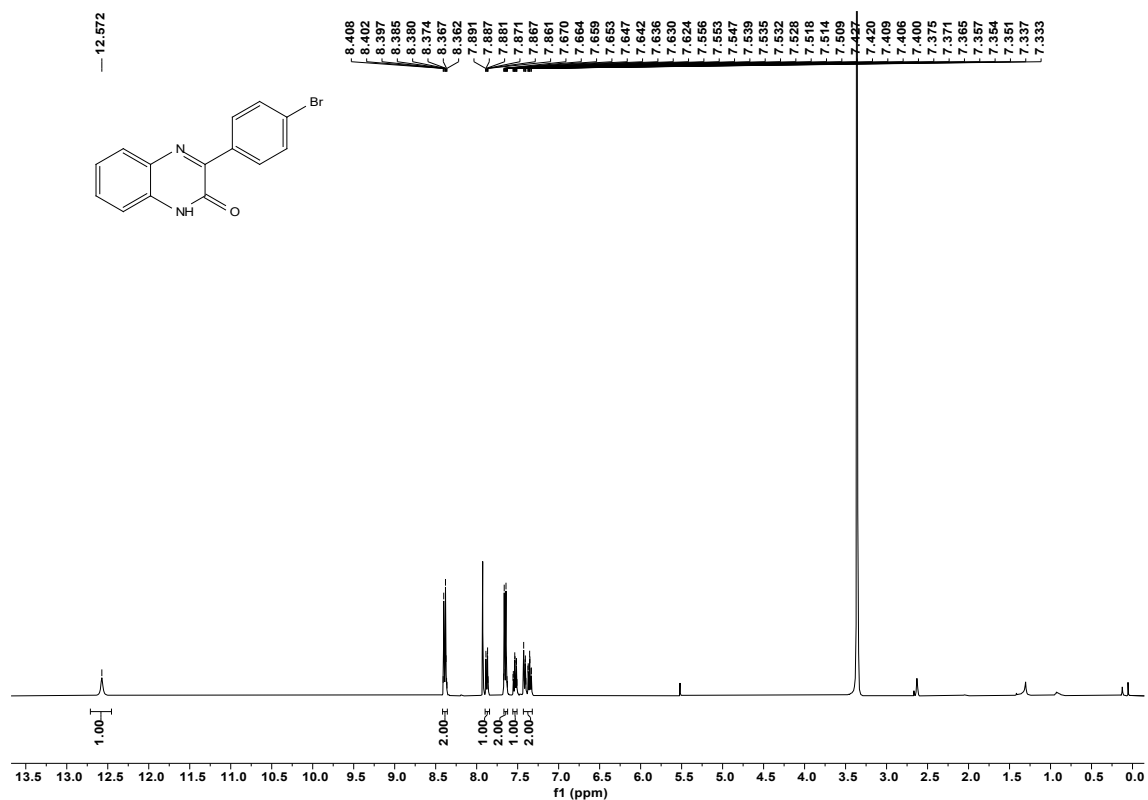
White solid. $^1\text{H NMR}$ (400 MHz, $\text{DMSO-}d_6$) δ 8.36 (d, $J = 1.9$ Hz, 1H), 8.23 (s, 1H), 8.04 (d, $J = 2.0$ Hz, 1H), 7.74 (d, $J = 8.7$ Hz, 1H), 7.53 (s, 2H), 3.69 (s, 5H). $^{13}\text{C NMR}$ (101 MHz, $\text{DMSO-}d_6$) δ 175.00, 155.44, 154.39, 137.23, 135.73, 134.24, 133.42, 132.31, 131.21, 130.12, 129.94, 128.41, 116.78, 106.21, 30.08. **MS** [EI, m/z]: 262.10 $[\text{M}+\text{H}]^+$.

References

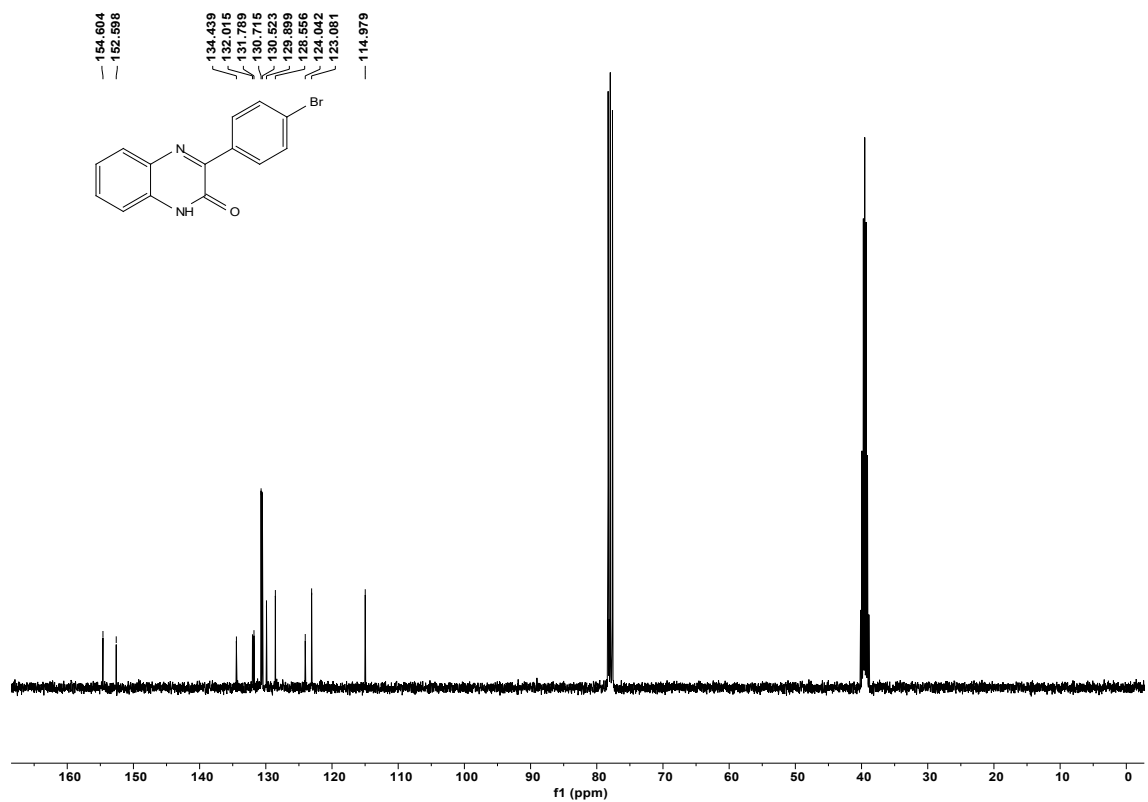
- [1] Ebersol C, Rocha N, Penteadó F, *et al.* A niobium-catalyzed coupling reaction of α -keto acids with ortho-phenylenediamines: synthesis of 3-arylquinoxalin-2(1H)-ones[J]. Green

Chemistry, 2019, 21: 6154-6160.

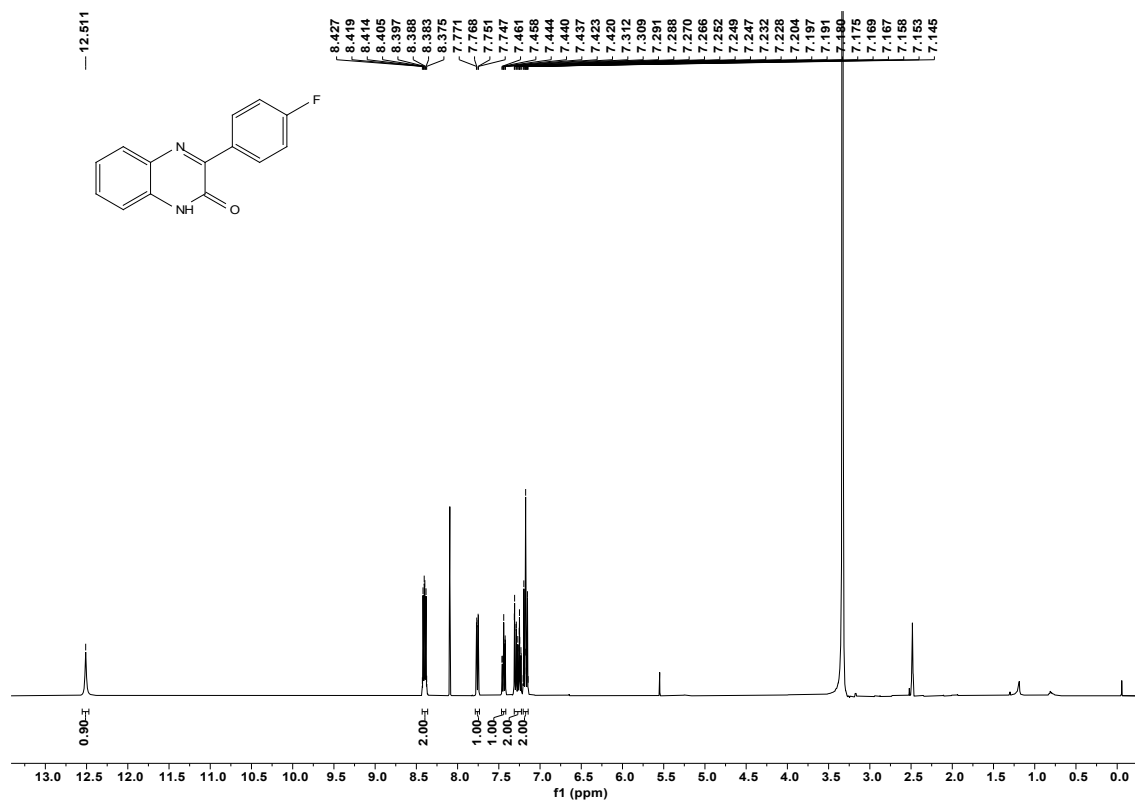
- [2] Lian F, Wang W, Zhang H, *et al.* Nickel-catalyzed electrochemical reductive decarboxylative coupling of *N*-hydroxyphthalimide esters with quinoxalinones[J]. Chemical Communications, 2019, 55, 14685-14688.
- [3] Kristoffersen T, Elumalai V, Starck E, *et al.* Microwave-assisted synthesis of heterocycles from aryldiazoacetates[J]. European Journal of Organic Chemistry, 2020, 2020 (45): 7069-7078.
- [4] Wen J W, Yang X T, Yan K L, *et al.* Electroreductive C3 pyridylation of quinoxalin-2(1*H*)-ones: an effective way to access bidentate nitrogen ligands[J]. Organic Letters, 2021, 23, 1081-1085.



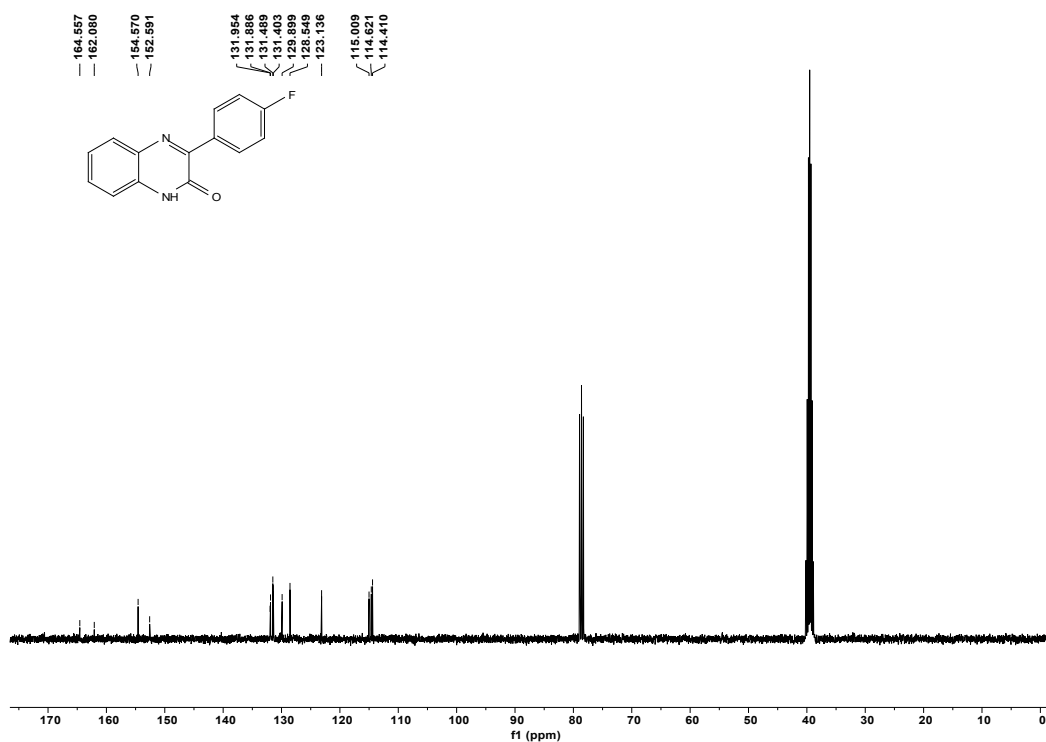
¹H NMR Spectrum of 3-(4-Bromophenyl)quinoxalin-2(1H)-one (Solvent: DMSO-*d*₆+CDCl₃)



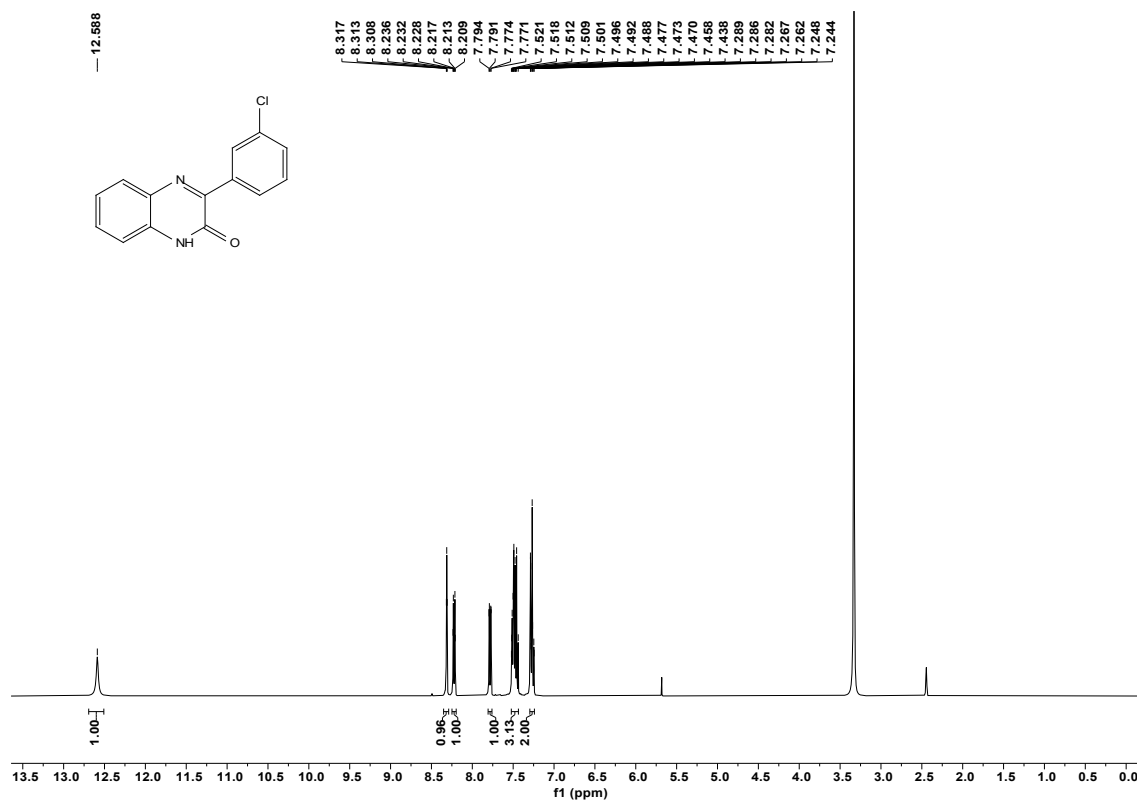
¹³C NMR Spectrum of 3-(4-Bromophenyl)quinoxalin-2(1H)-one (Solvent: DMSO-*d*₆+CDCl₃)



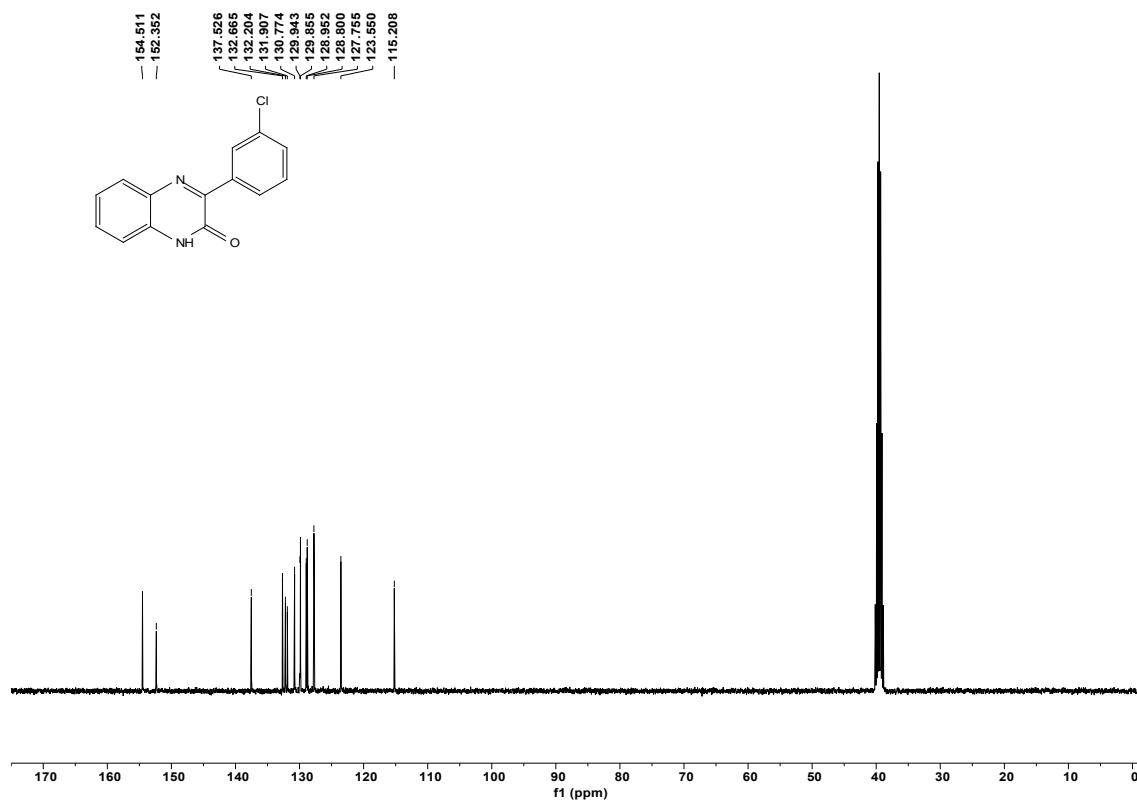
¹H NMR Spectrum of 3-(4-Fluorophenyl)quinoxalin-2(1H)-one (Solvent: DMSO-*d*₆+CDCl₃)



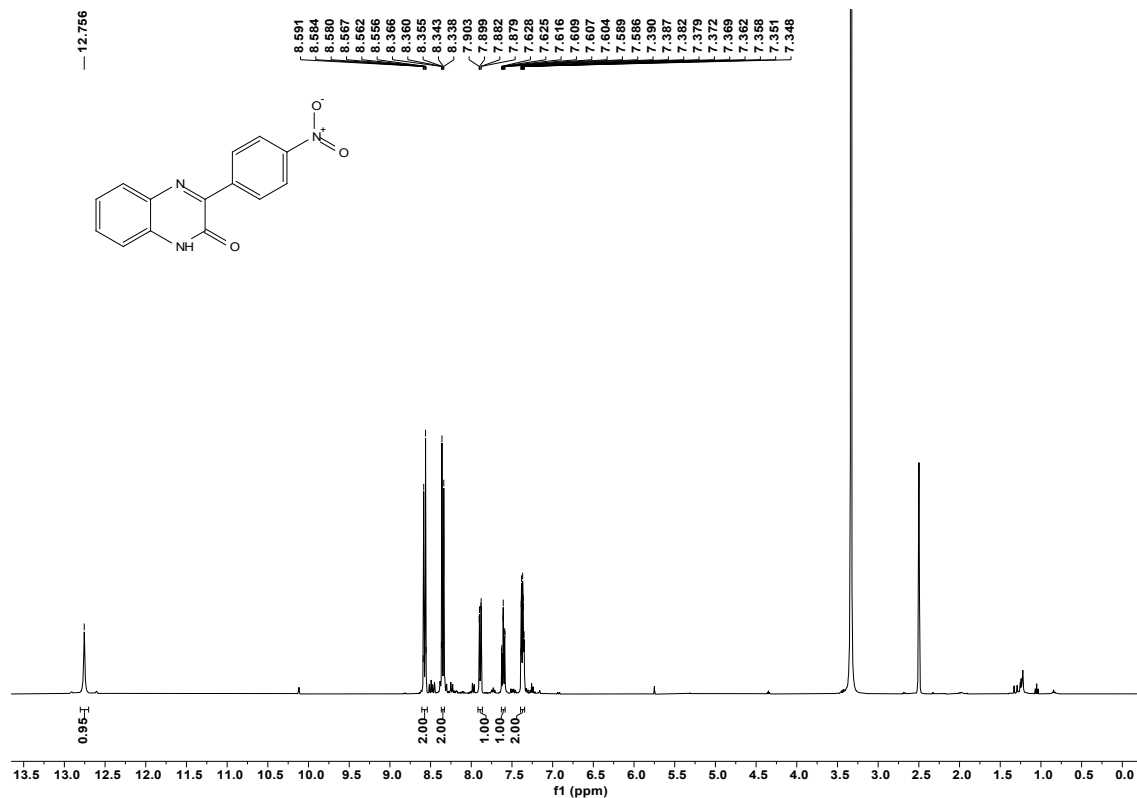
¹³C NMR Spectrum of 3-(4-Fluorophenyl)quinoxalin-2(1H)-one (Solvent: DMSO-*d*₆+CDCl₃)



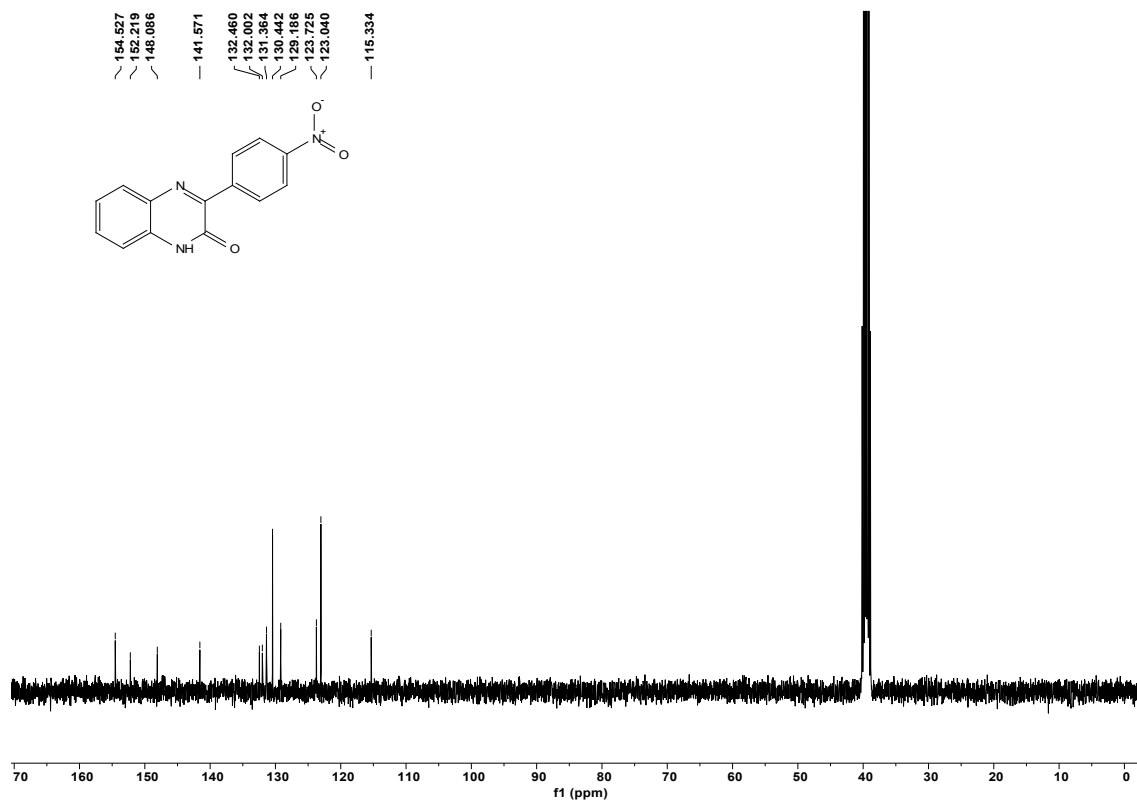
¹H NMR Spectrum of 3-(3-Chlorophenyl)quinoxalin-2(1H)-one (Solvent: DMSO-*d*₆)



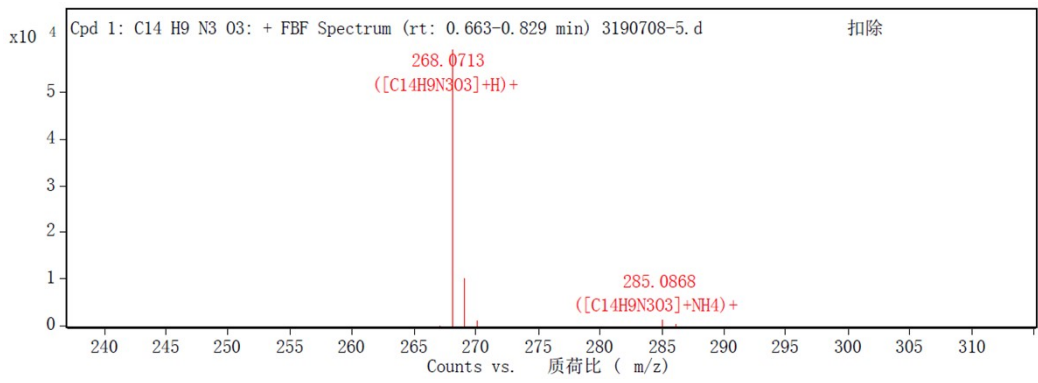
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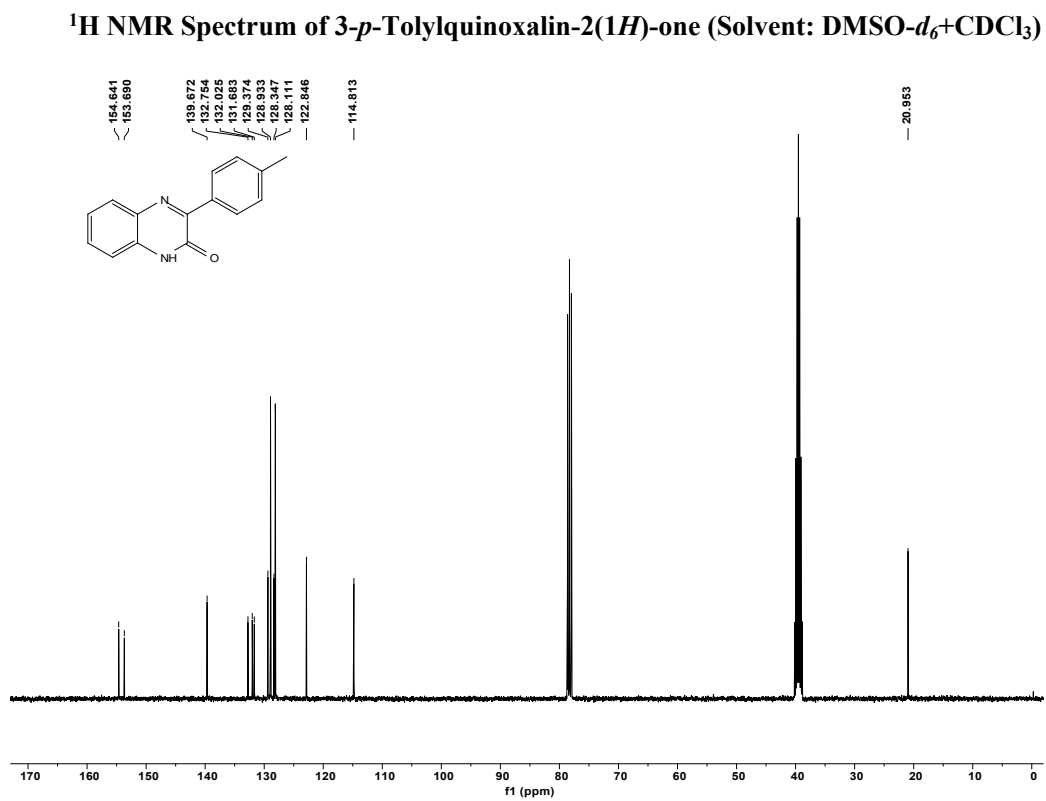
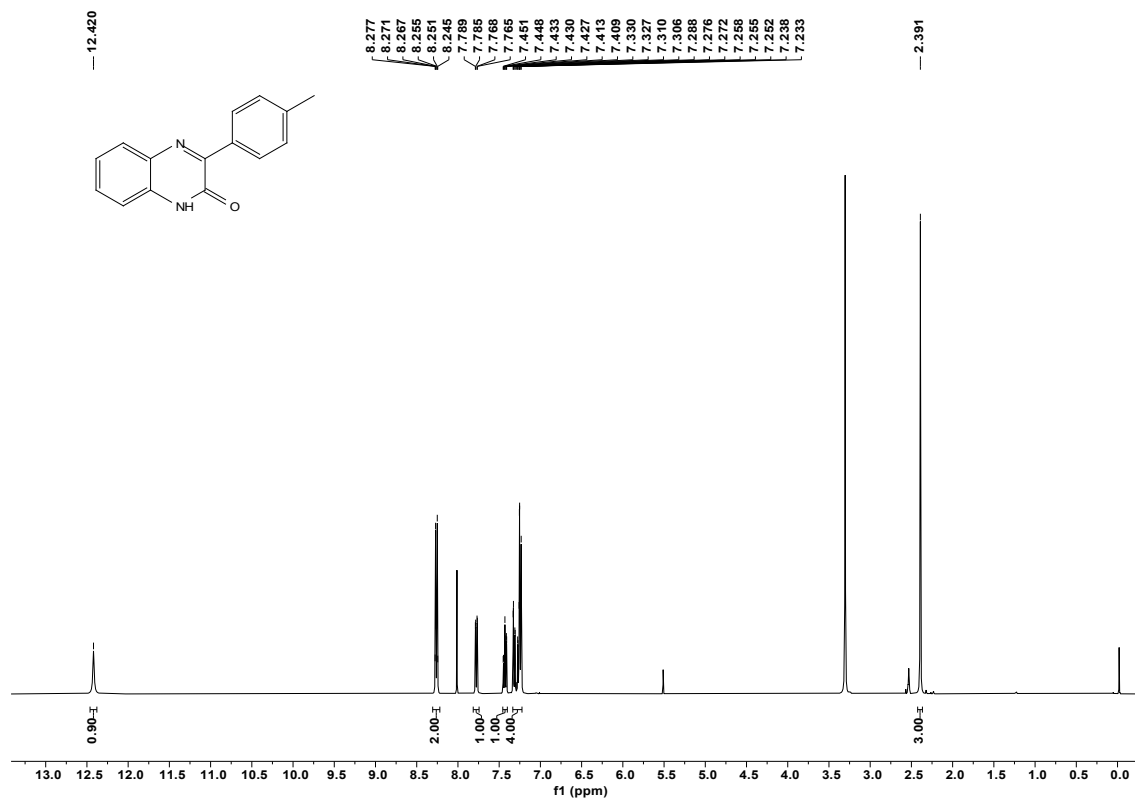
¹H NMR Spectrum of 3-(4-Nitrophenyl)quinoxalin-2(1H)-one (Solvent: DMSO-*d*₆)

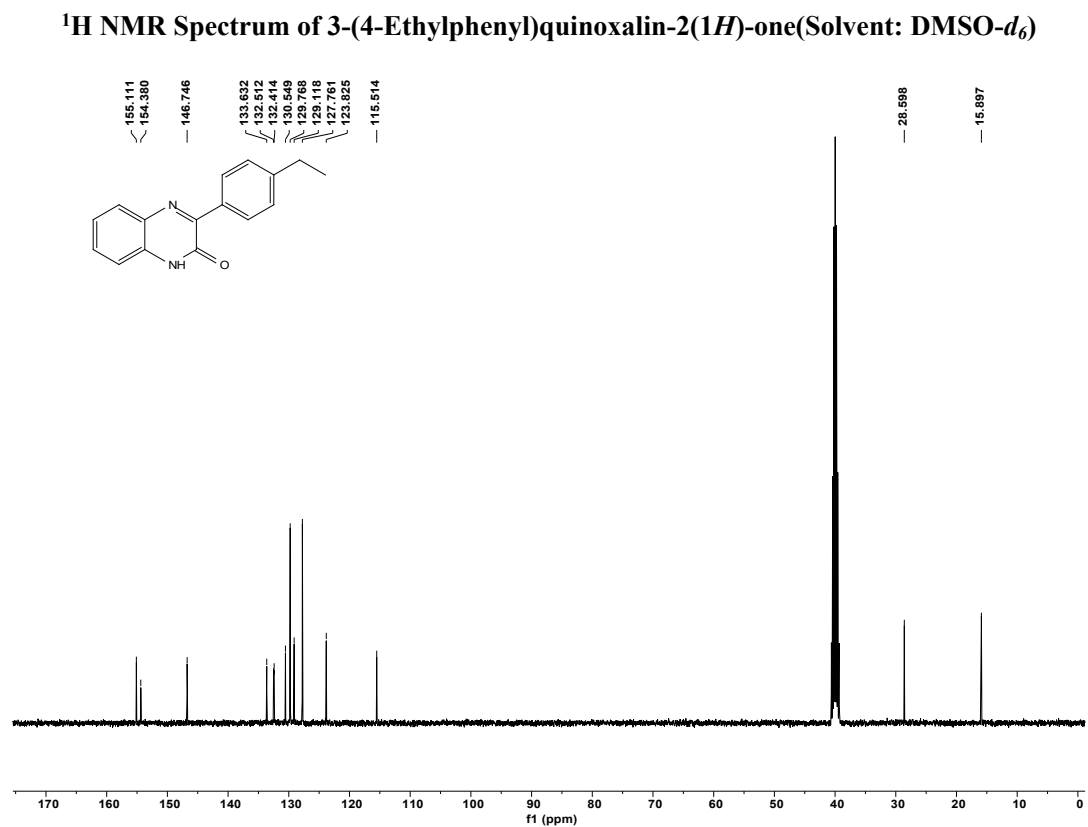
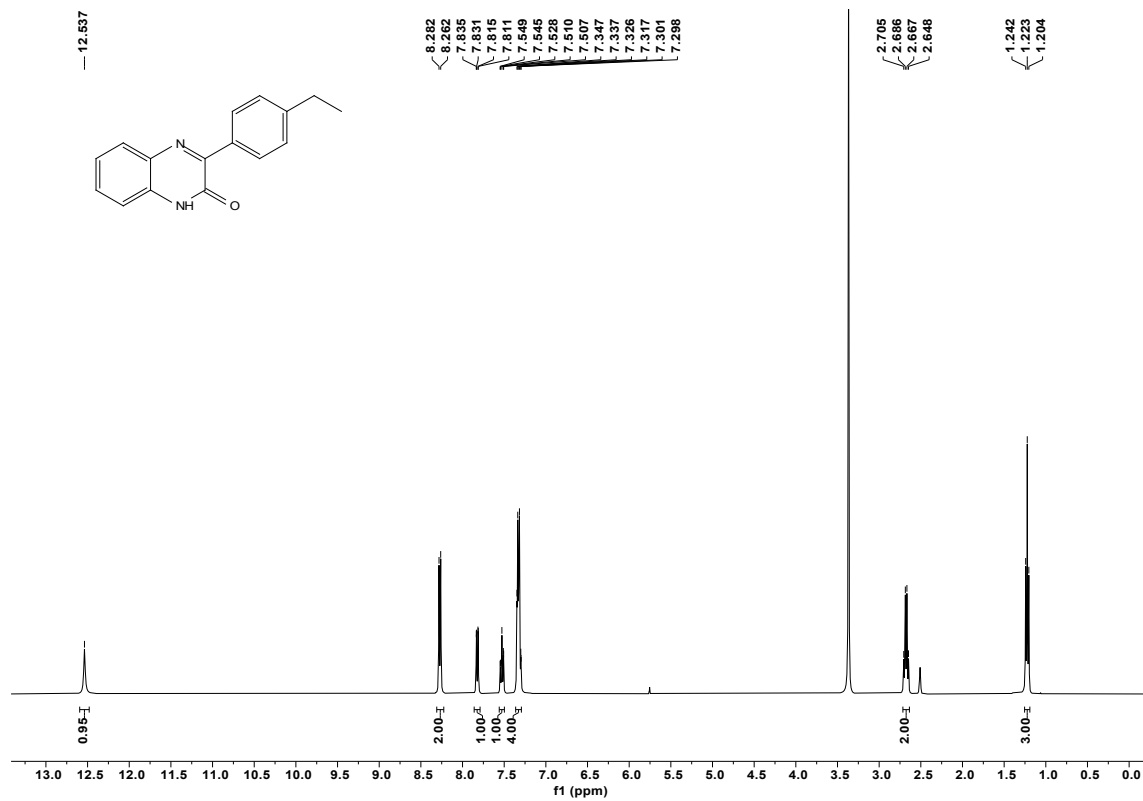


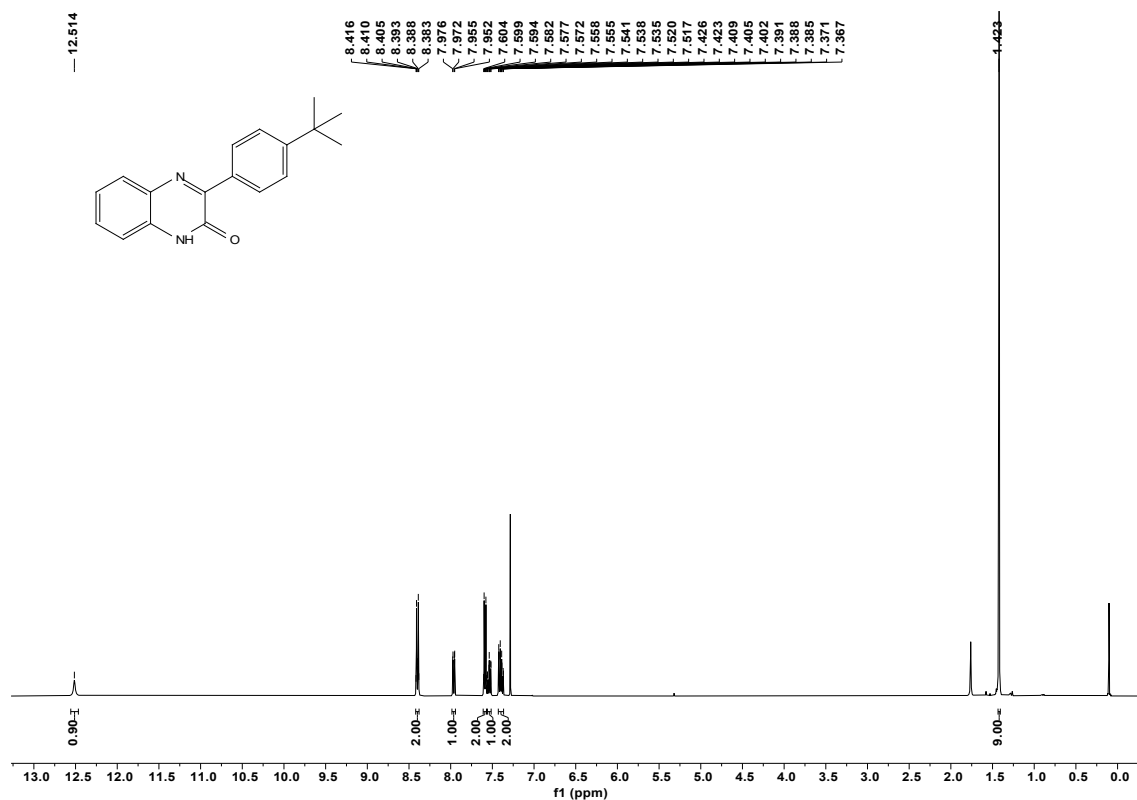
¹³C NMR Spectrum of 3-(4-Nitrophenyl)quinoxalin-2(1H)-one (Solvent: DMSO-*d*₆)



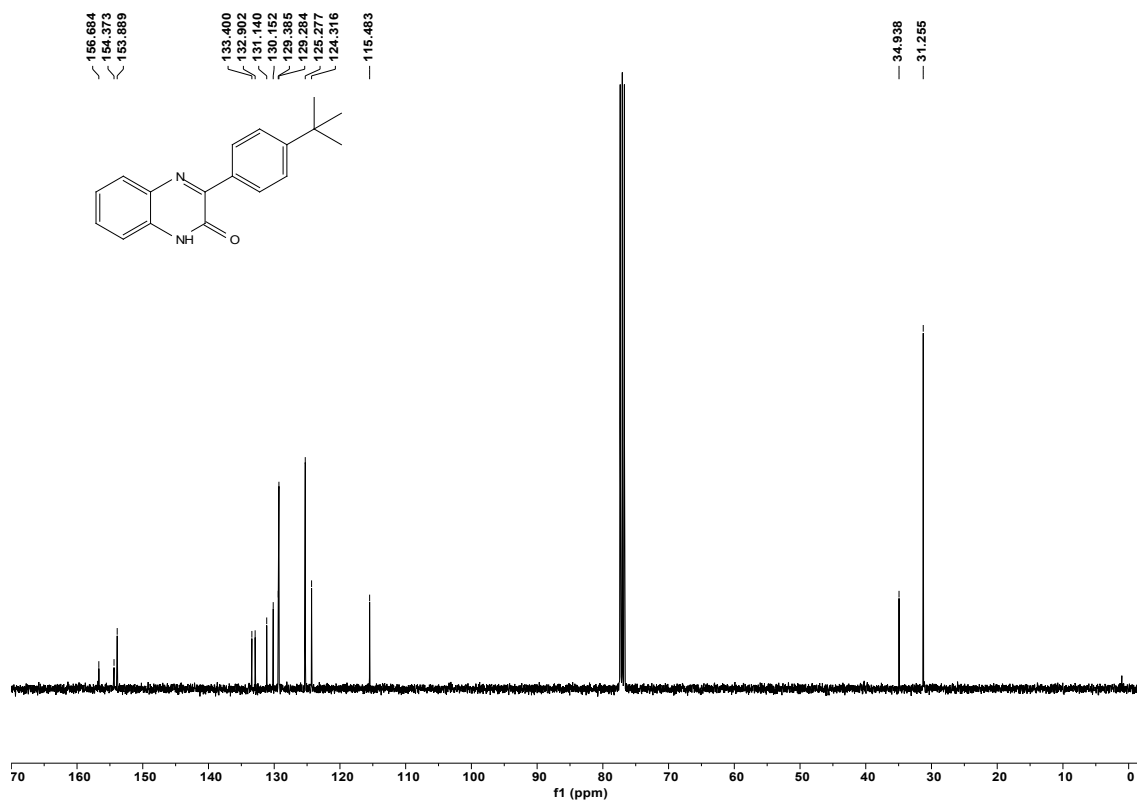
ESI-MS Spectrum of 3-(4-Nitrophenyl)quinoxalin-2(1H)-one



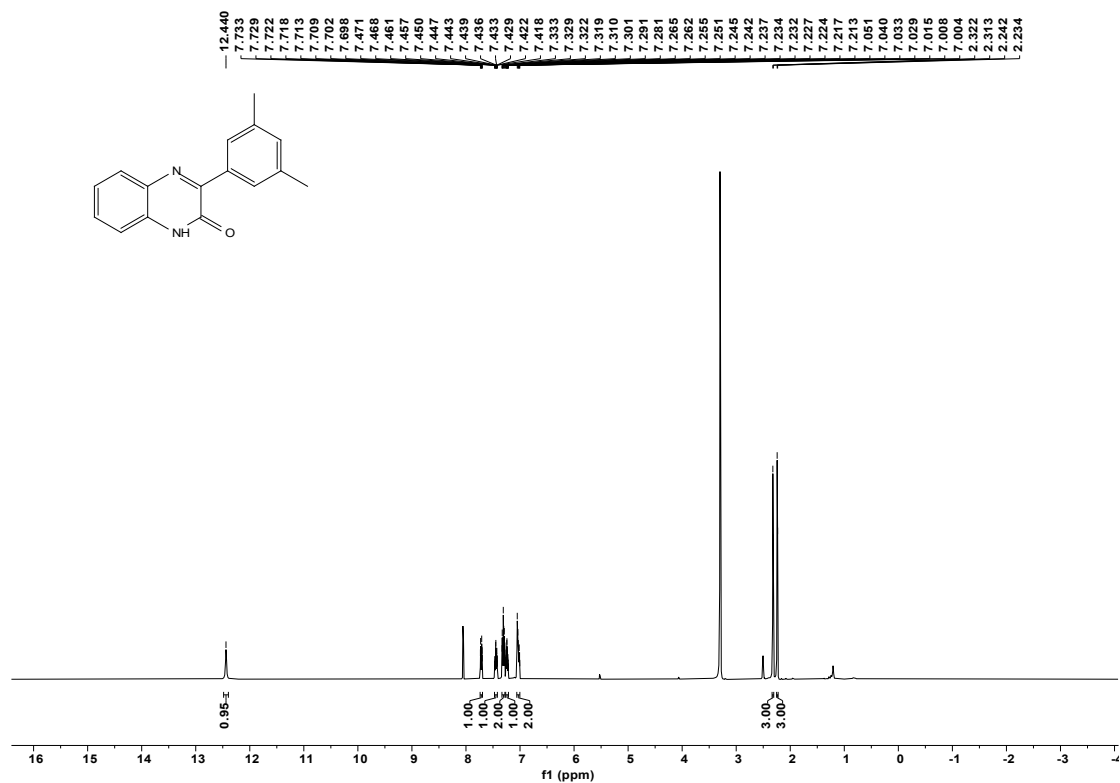




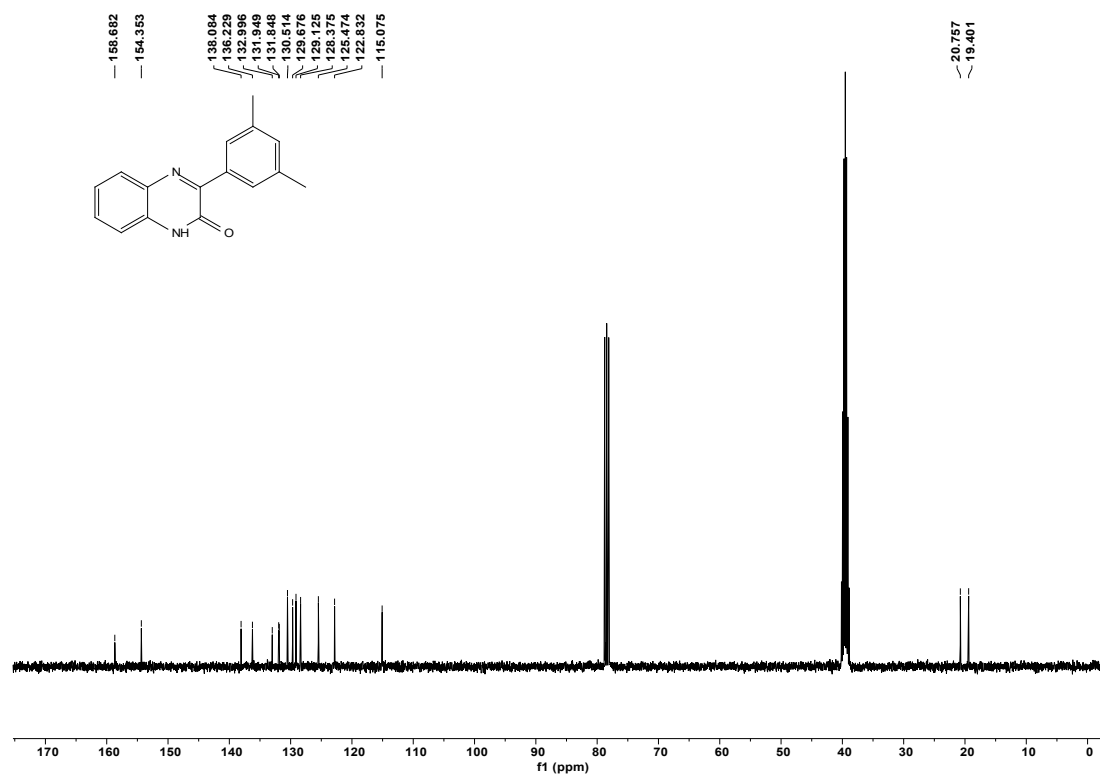
¹H NMR Spectrum of 3-(4-*tert*-Butylphenyl)quinoxalin-2(1*H*)-one (Solvent: CDCl₃)



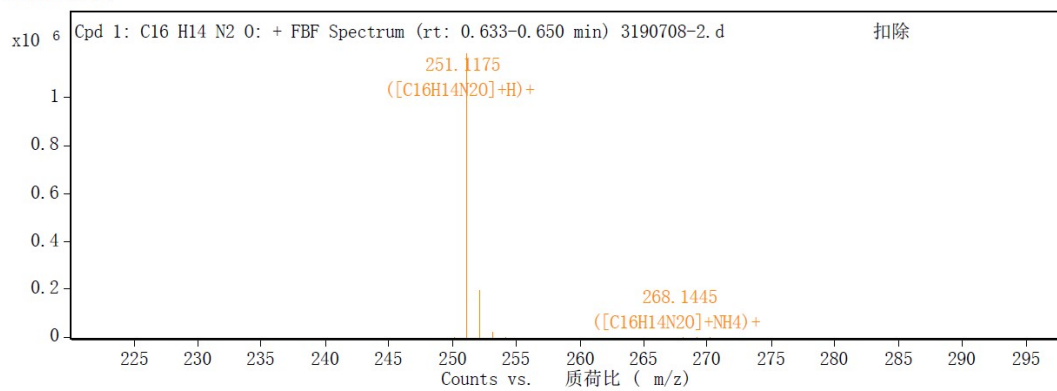
¹³C NMR Spectrum of 3-(4-*tert*-Butylphenyl)quinoxalin-2(1*H*)-one (Solvent: CDCl₃)



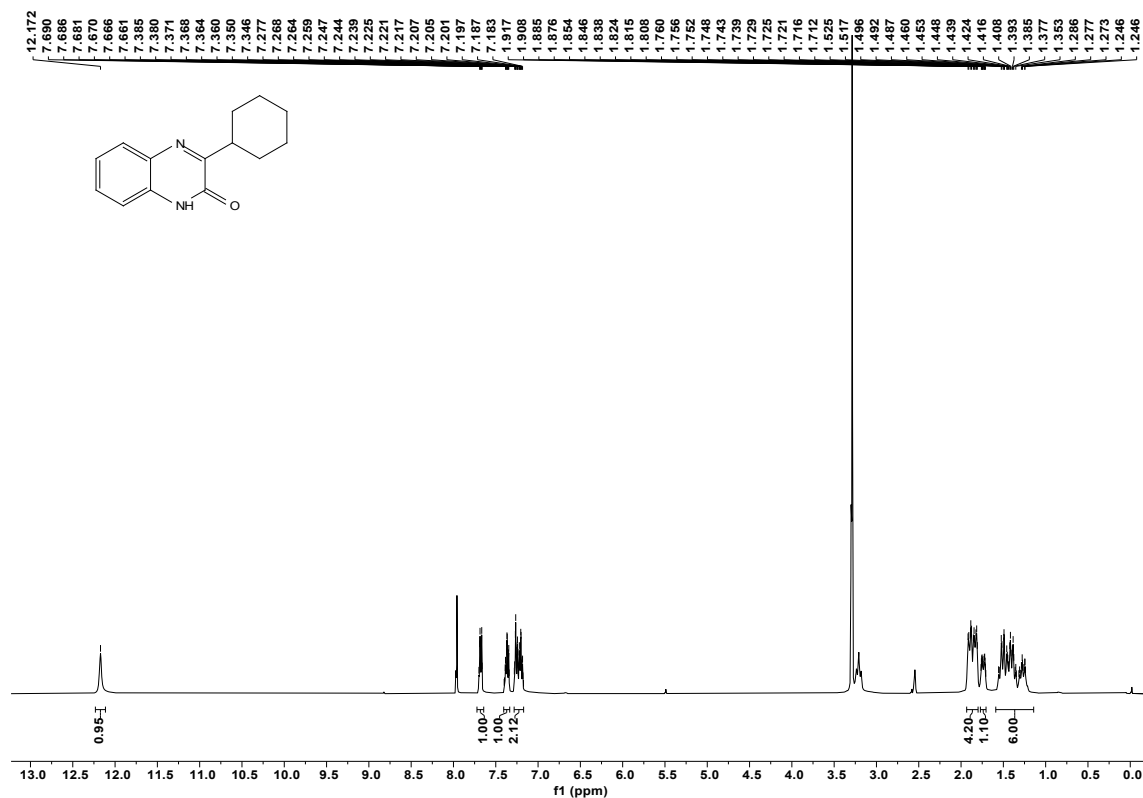
¹H NMR Spectrum of 3-(3,5-Dimethylphenyl)quinoxalin-2(1H)-one (Solvent: DMSO-*d*₆+CDCl₃)



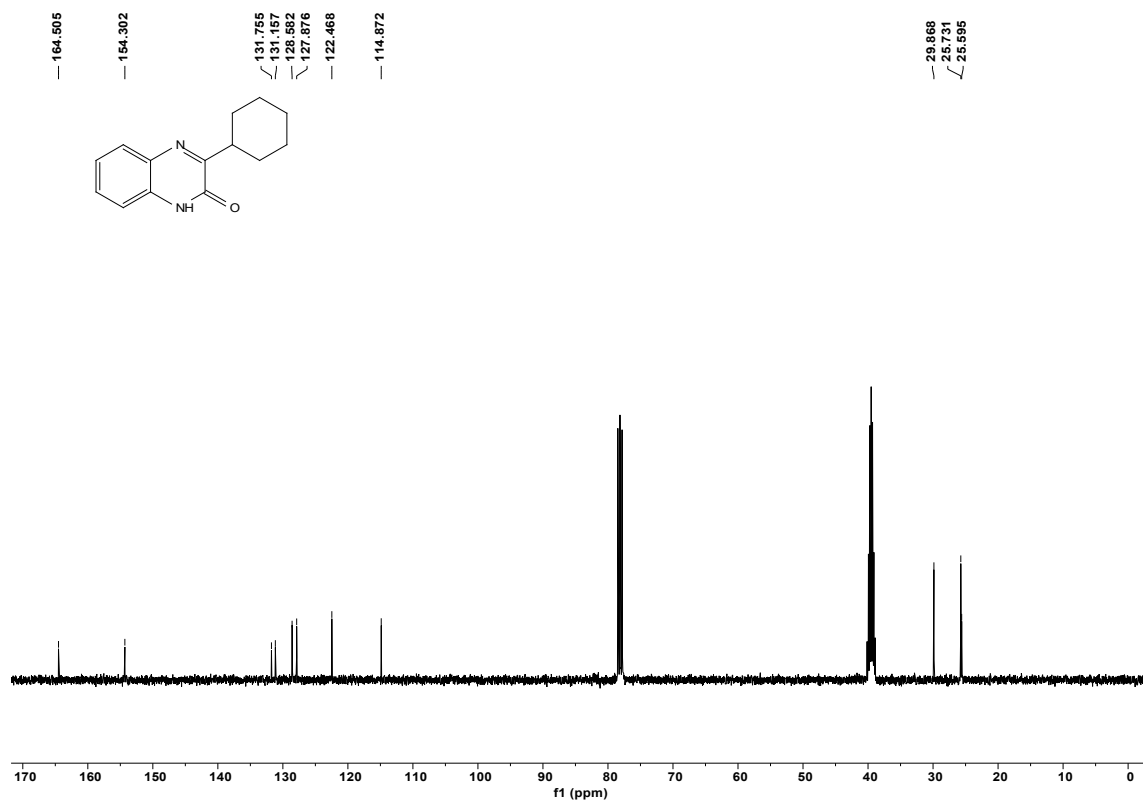
¹³C NMR Spectrum of 3-(3,5-Dimethylphenyl)quinoxalin-2(1H)-one (Solvent: DMSO-*d*₆+CDCl₃)



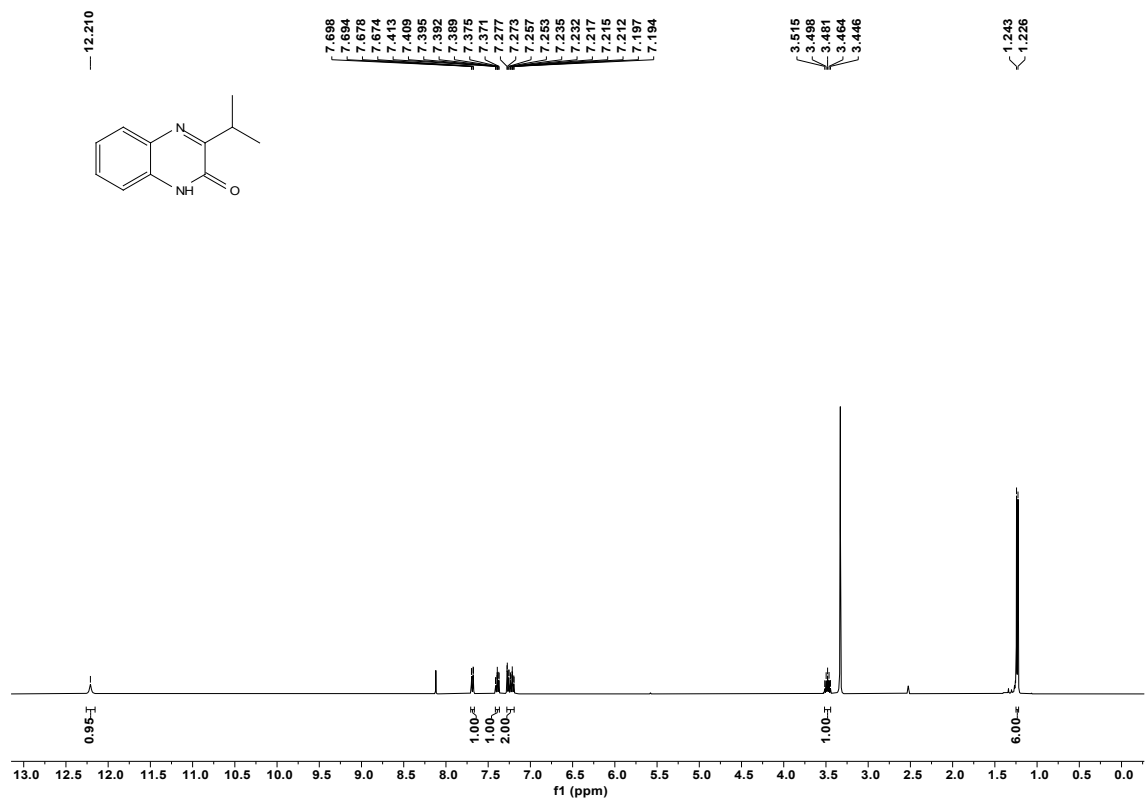
ESI-MS Spectrum of 3-(3,5-Dimethylphenyl)quinoxalin-2(1H)-one



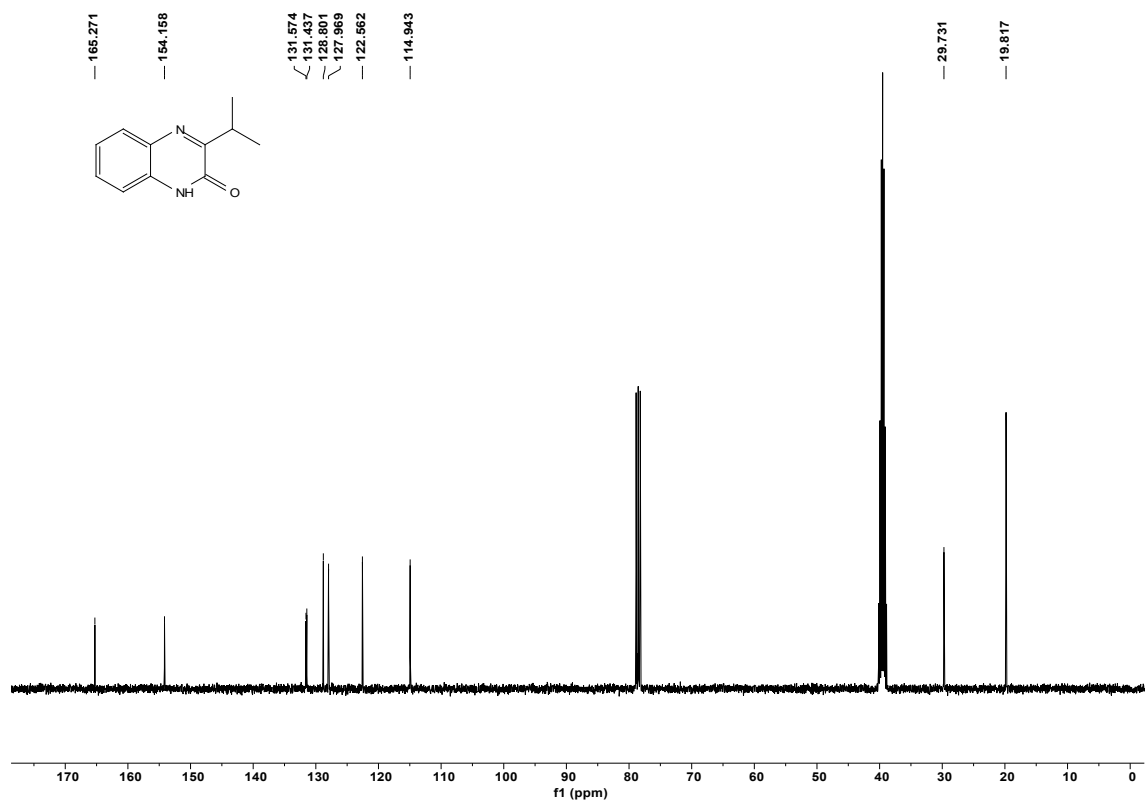
¹H NMR Spectrum of 3-Cyclohexylquinoxalin-2(1H)-one (Solvent: DMSO-*d*₆+CDCl₃)



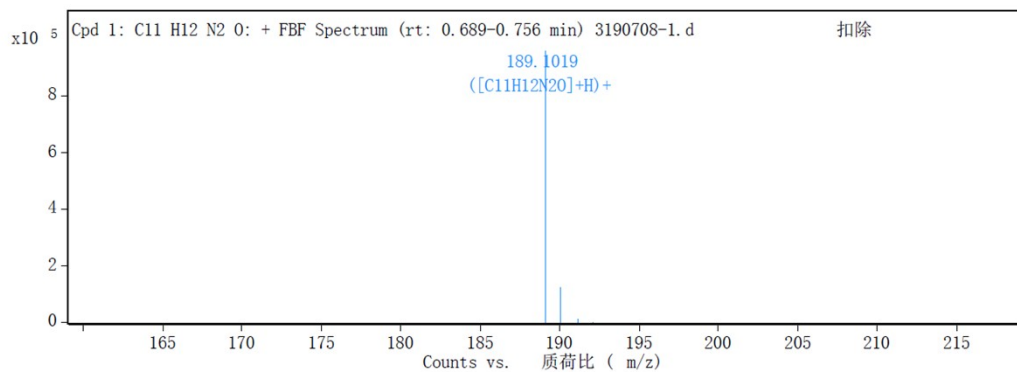
¹³C NMR Spectrum of 3-Cyclohexylquinoxalin-2(1H)-one (Solvent: DMSO-*d*₆+CDCl₃)



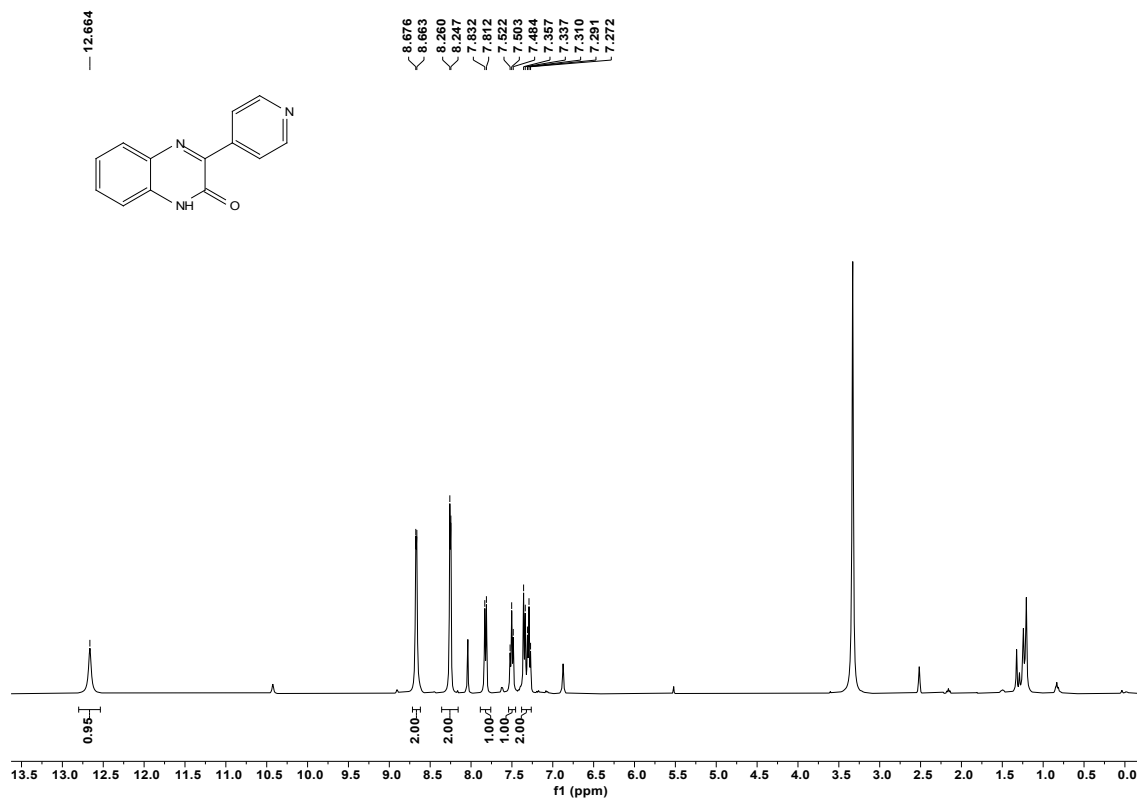
¹H NMR Spectrum of 3-Isopropylquinoxalin-2(1H)-one (Solvent: DMSO-*d*₆+CDCl₃)



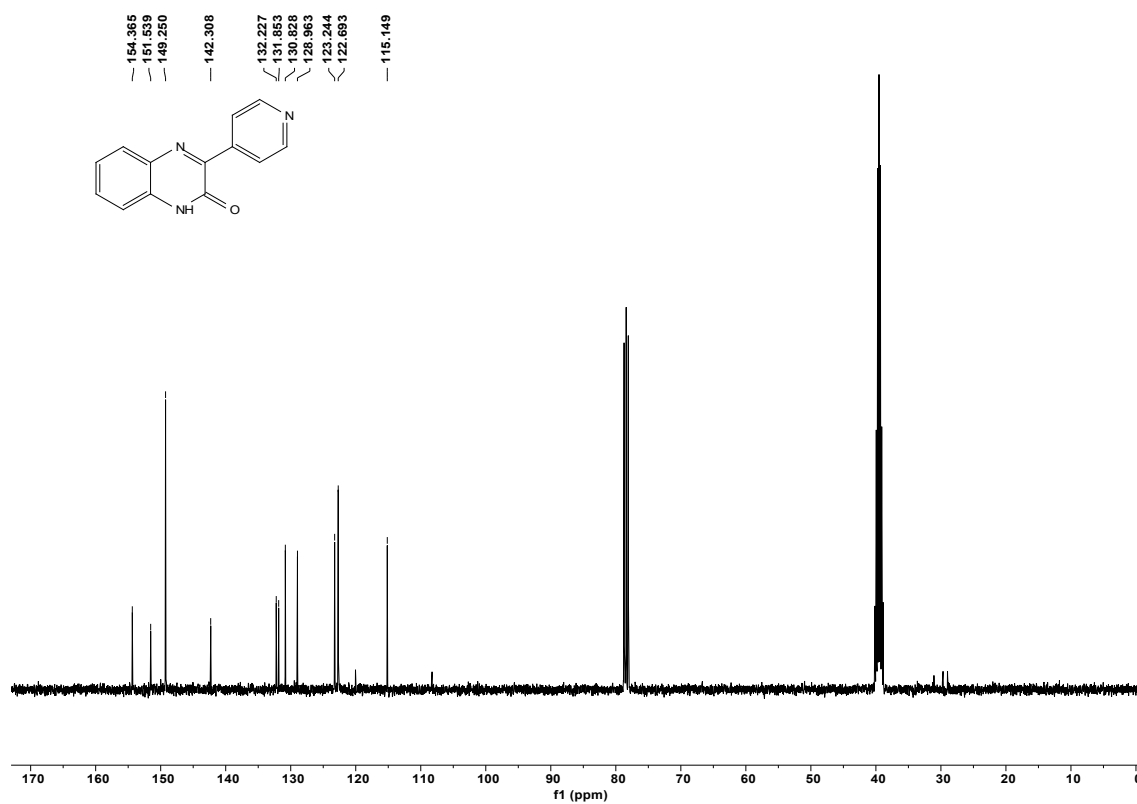
¹³C NMR Spectrum of 3-Isopropylquinoxalin-2(1H)-one (Solvent: DMSO-*d*₆+CDCl₃)



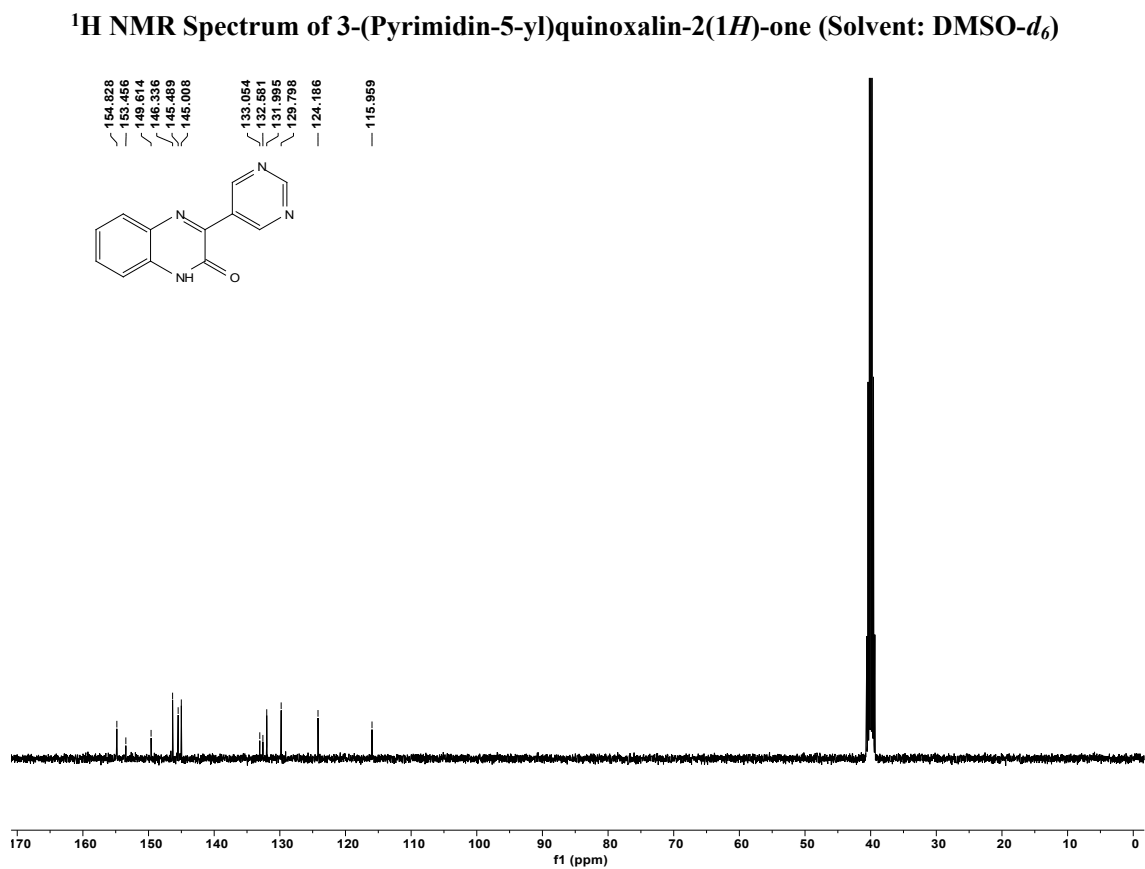
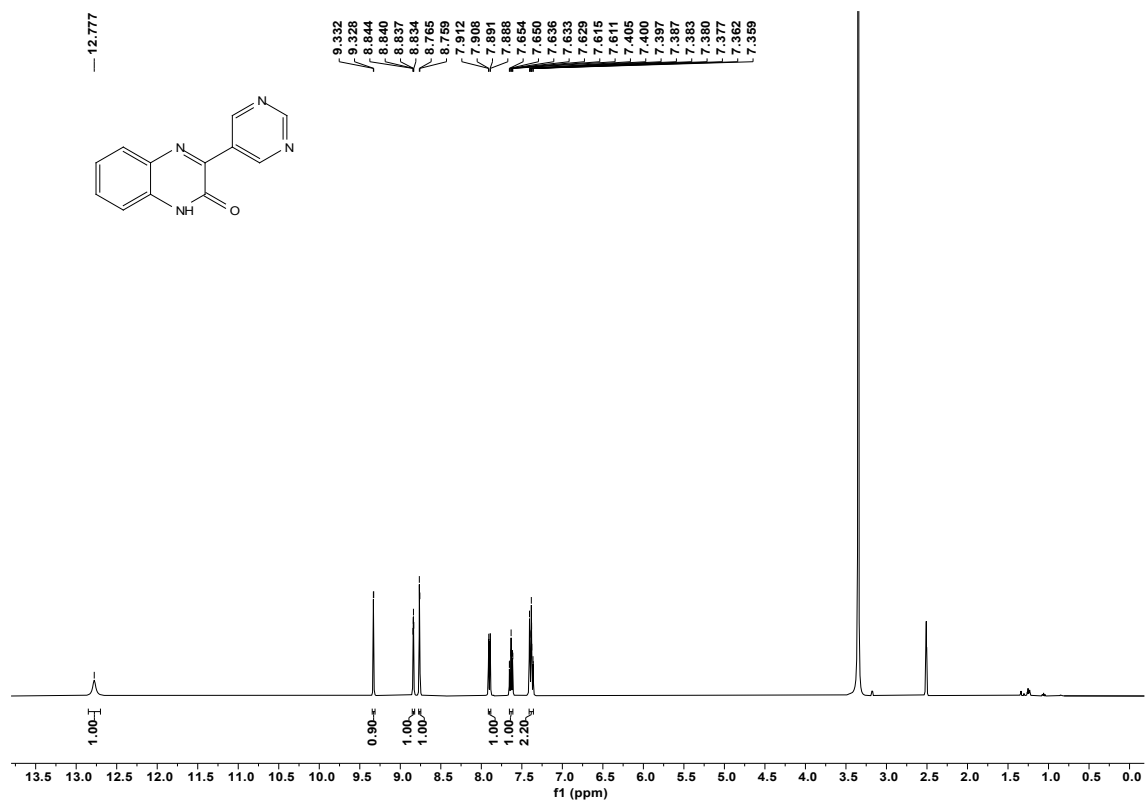
ESI-MS Spectrum of 3-Isopropylquinoxalin-2(1H)-one



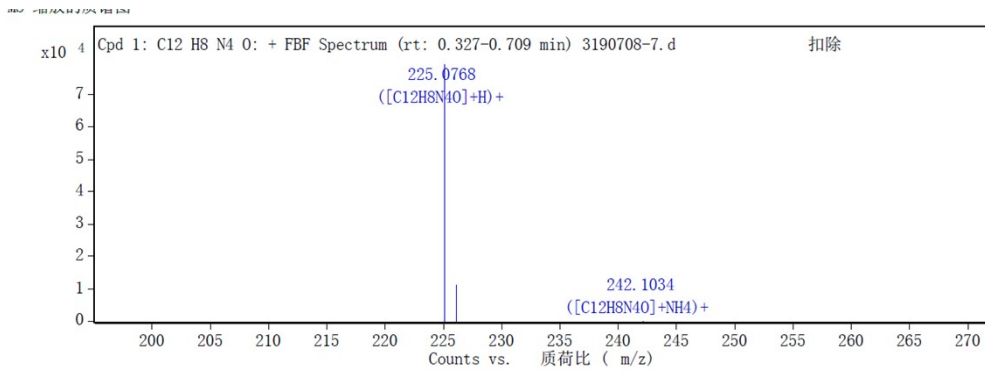
^1H NMR Spectrum of 3-(Pyridin-4-yl)quinoxalin-2(1H)-one (Solvent: $\text{DMSO-}d_6+\text{CDCl}_3$)



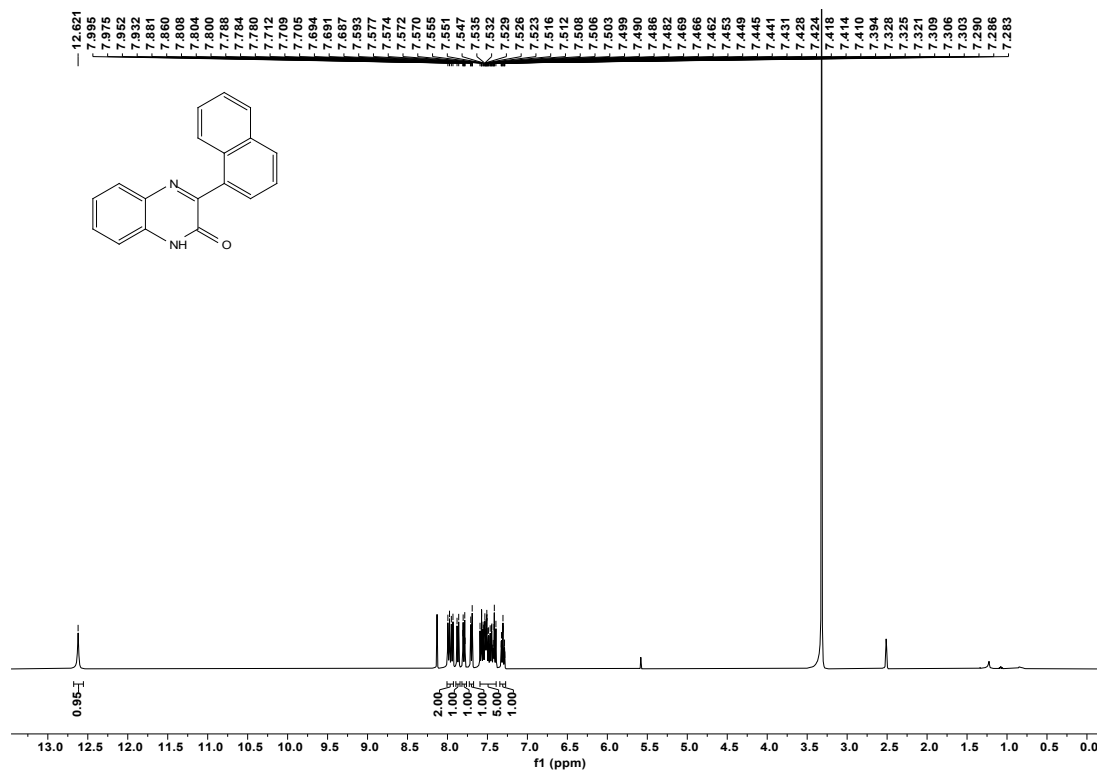
^{13}C NMR Spectrum of 3-(Pyridin-4-yl)quinoxalin-2(1H)-one (Solvent: $\text{DMSO-}d_6+\text{CDCl}_3$)



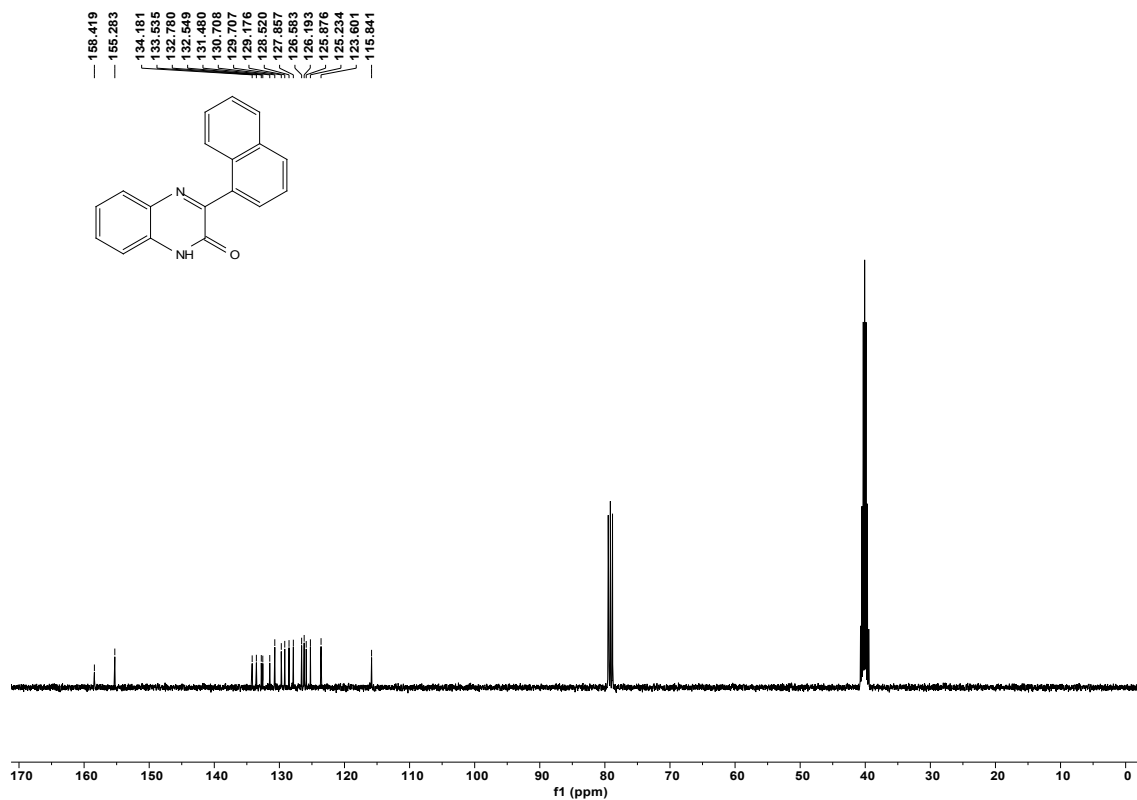
¹³C NMR Spectrum of 3-(Pyrimidin-5-yl)quinoxalin-2(1H)-one (Solvent: DMSO-*d*₆)



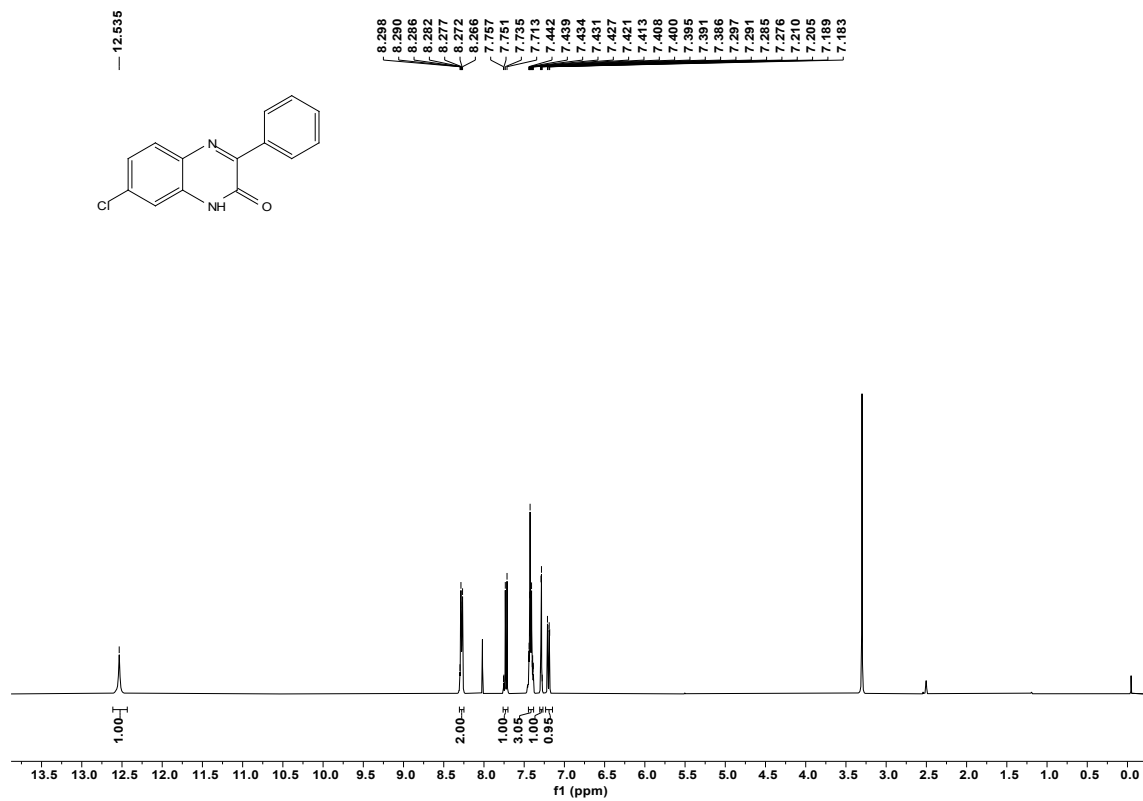
ESI Spectrum of 3-(Pyrimidin-5-yl)quinoxalin-2(1H)-one



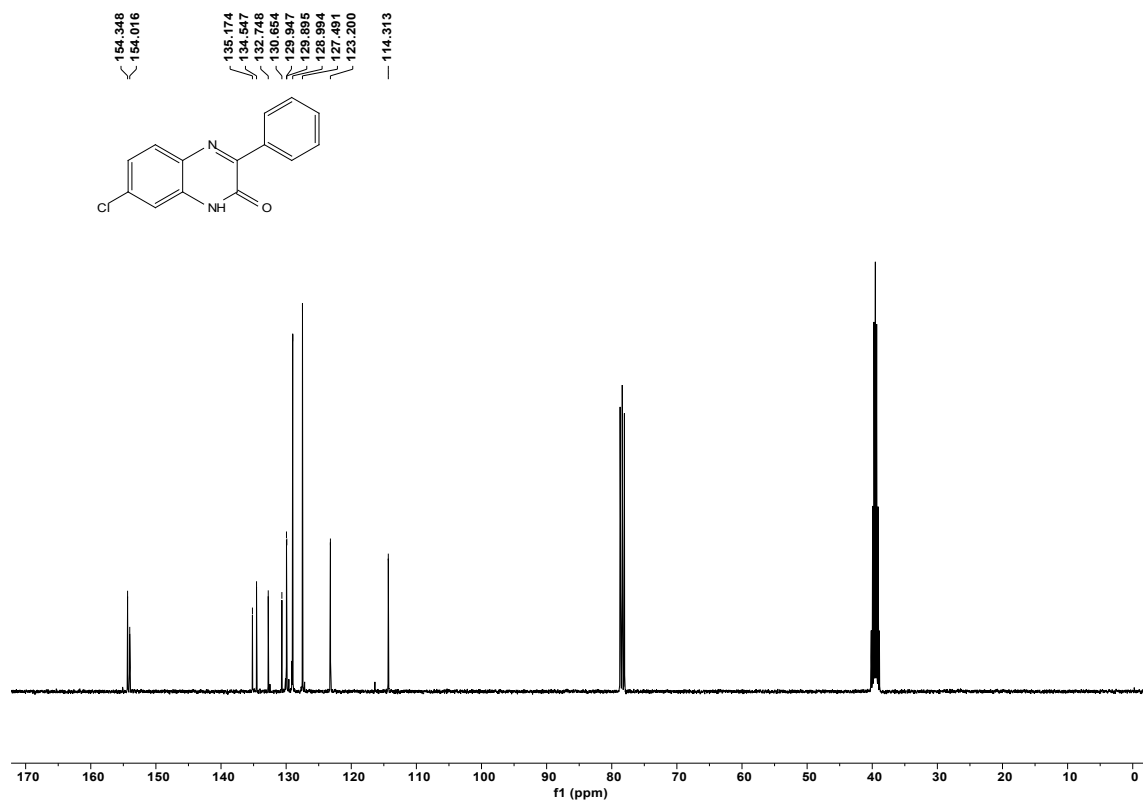
¹H NMR Spectrum of 3-(Naphthalen-3-yl)quinoxalin-2(1H)-one (Solvent: DMSO-*d*₆+CDCl₃)



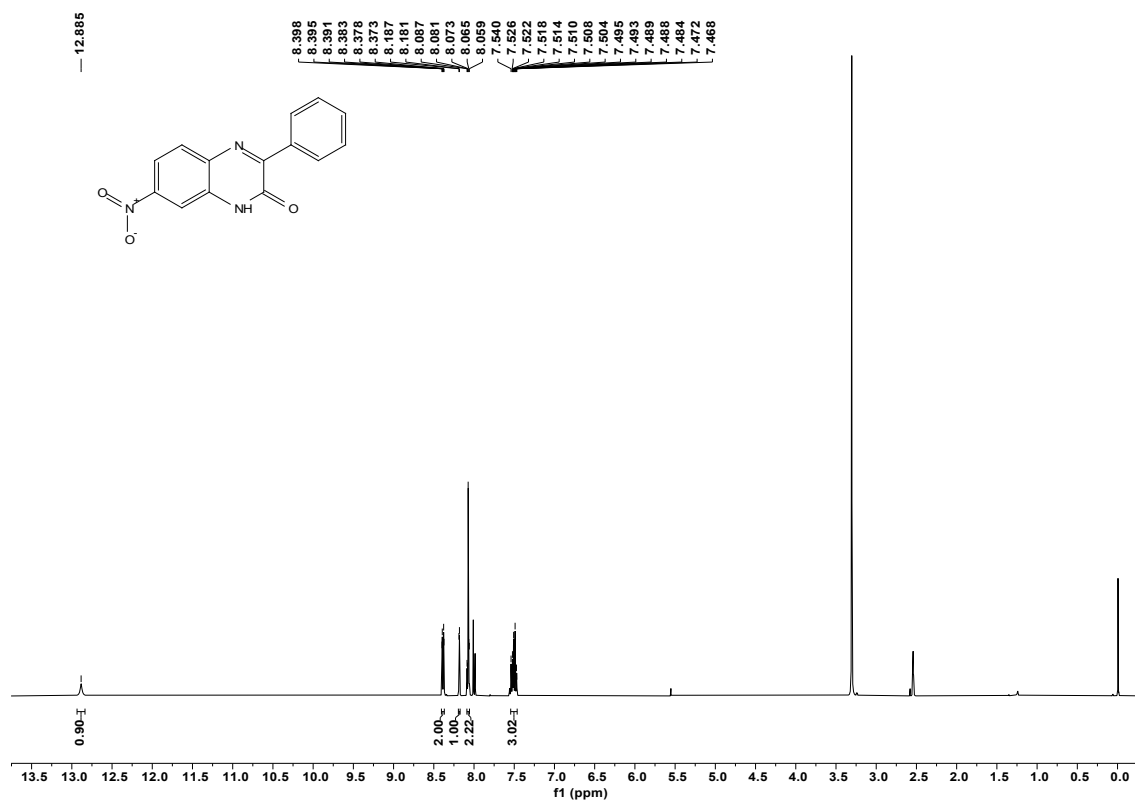
¹³C NMR Spectrum of 3-(Naphthalen-3-yl)quinoxalin-2(1H)-one (Solvent: DMSO-*d*₆+CDCl₃)



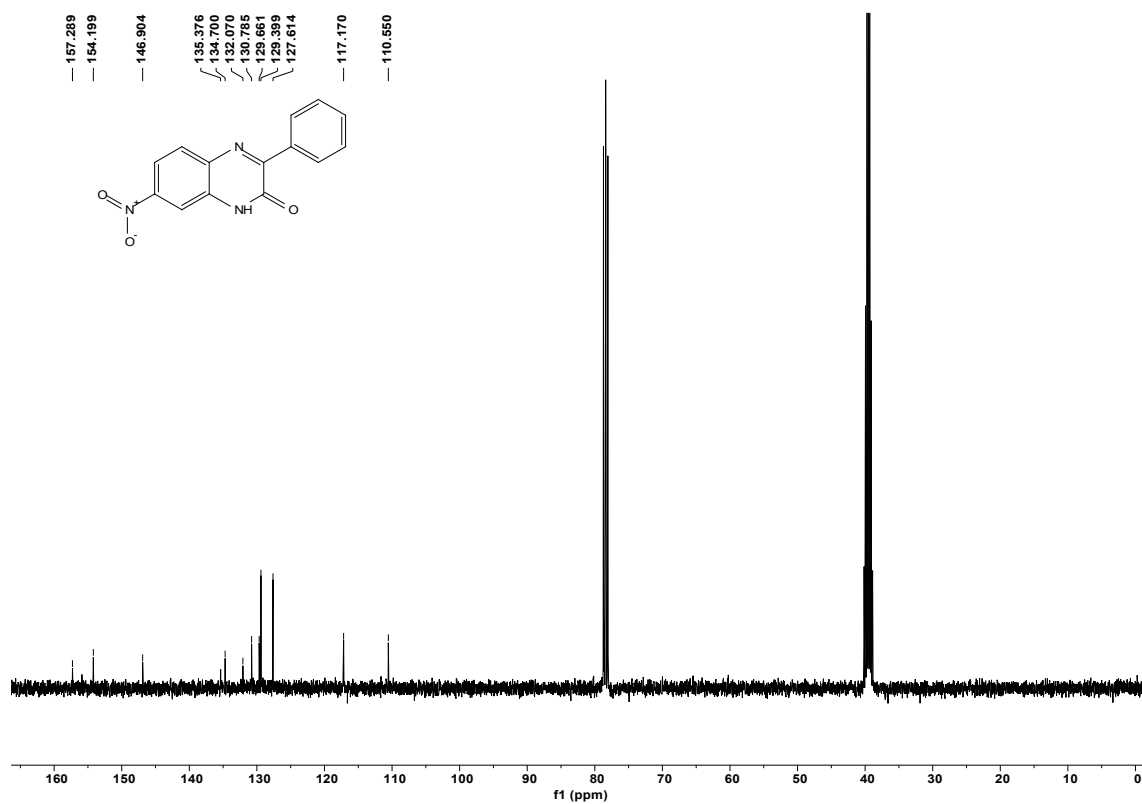
¹H NMR Spectrum of 7-Chloro-3-phenylquinoxalin-2(1H)-one(Solvent: DMSO-*d*₆+CDCl₃)



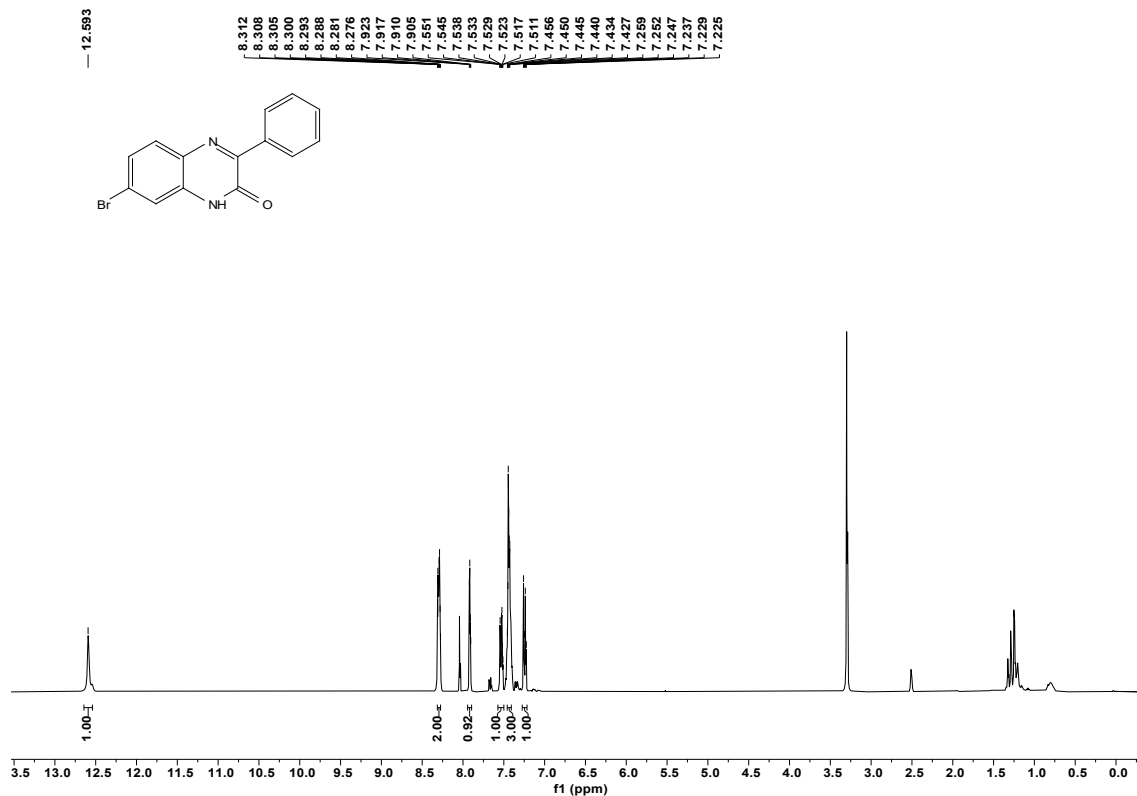
¹³C NMR Spectrum of 7-Chloro-3-phenylquinoxalin-2(1H)-one(Solvent: DMSO-*d*₆+CDCl₃)



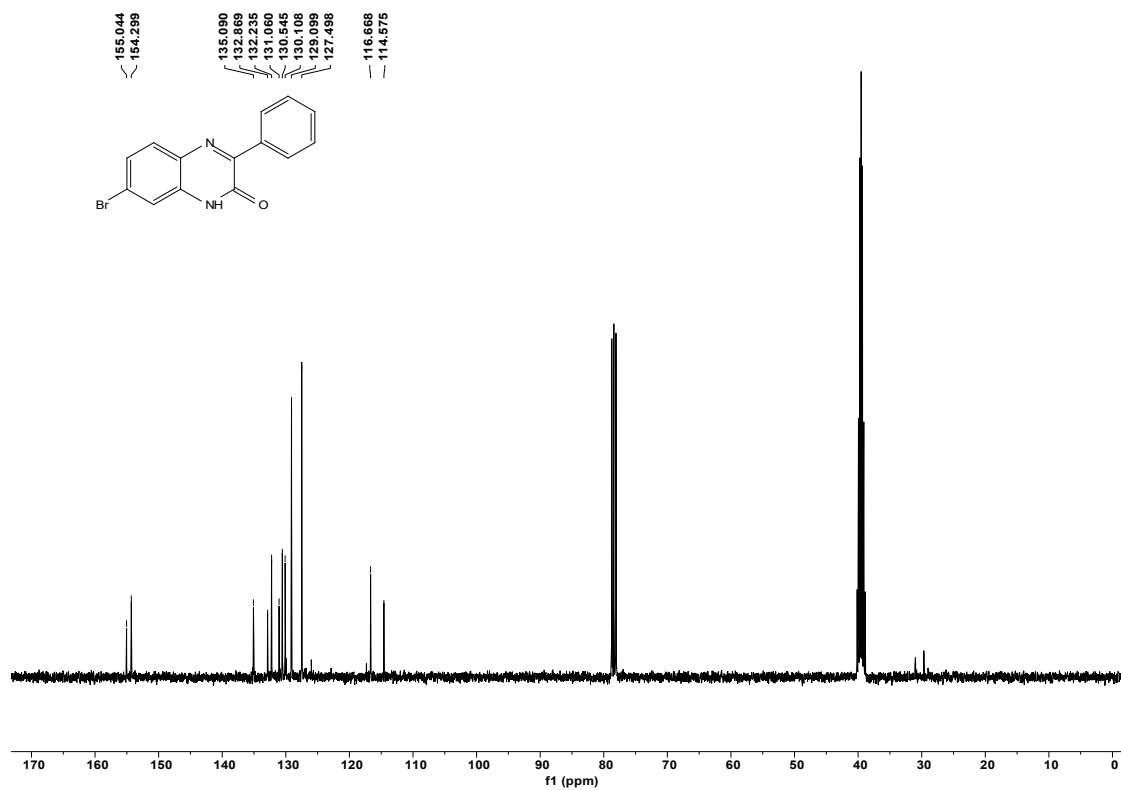
¹H NMR Spectrum of 7-Nitro-3-phenylquinoxalin-2(1H)-one (Solvent: DMSO-*d*₆+CDCl₃)



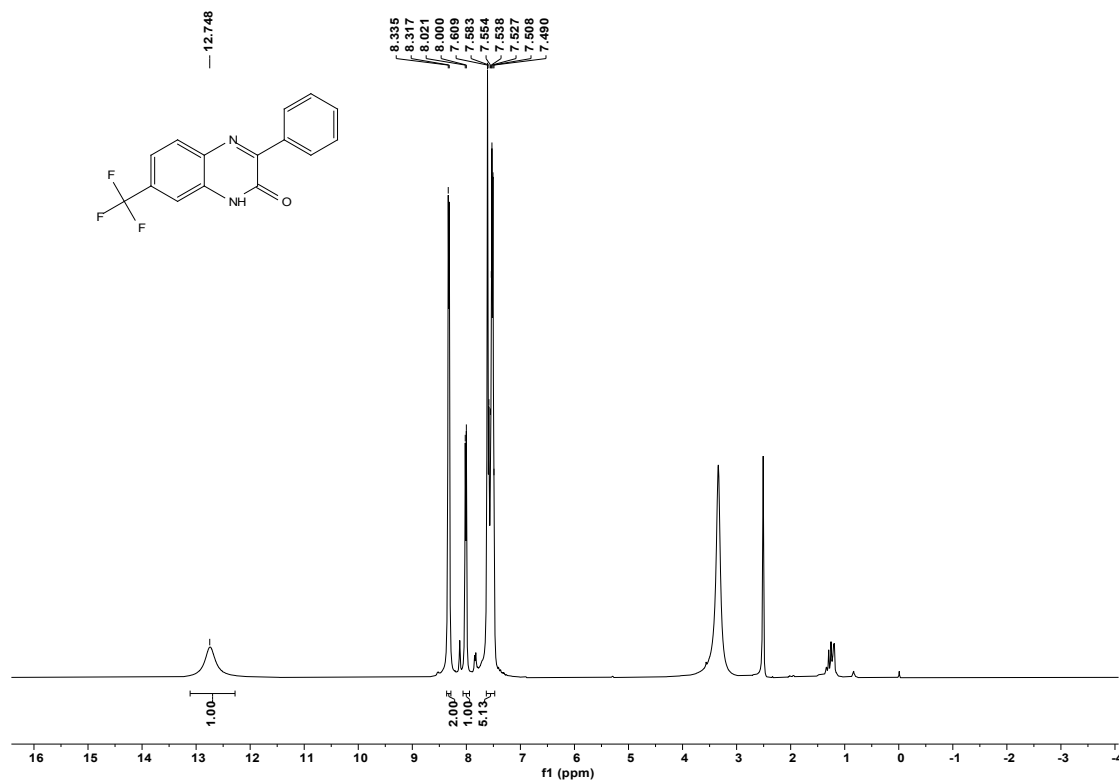
¹³C NMR Spectrum of 7-Nitro-3-phenylquinoxalin-2(1H)-one (Solvent: DMSO-*d*₆+CDCl₃)



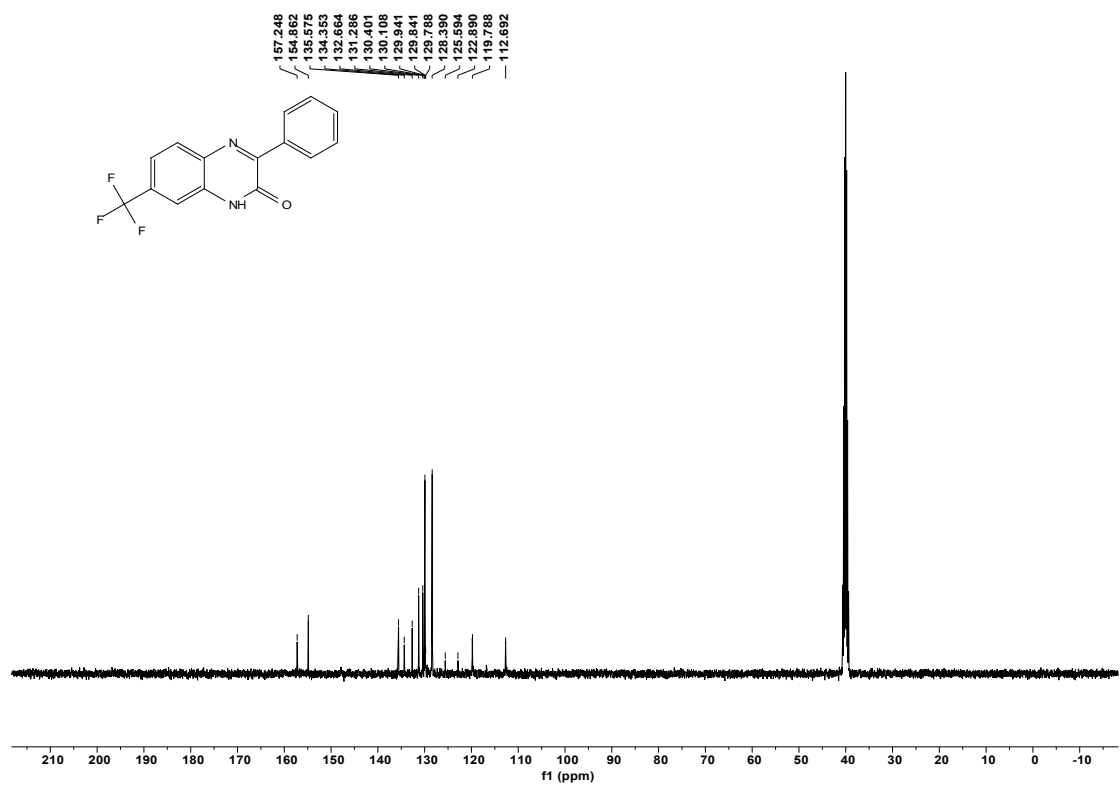
¹H NMR Spectrum of 7-Bromo-3-phenylquinoxalin-2(1H)-one (Solvent: DMSO-*d*₆+CDCl₃)



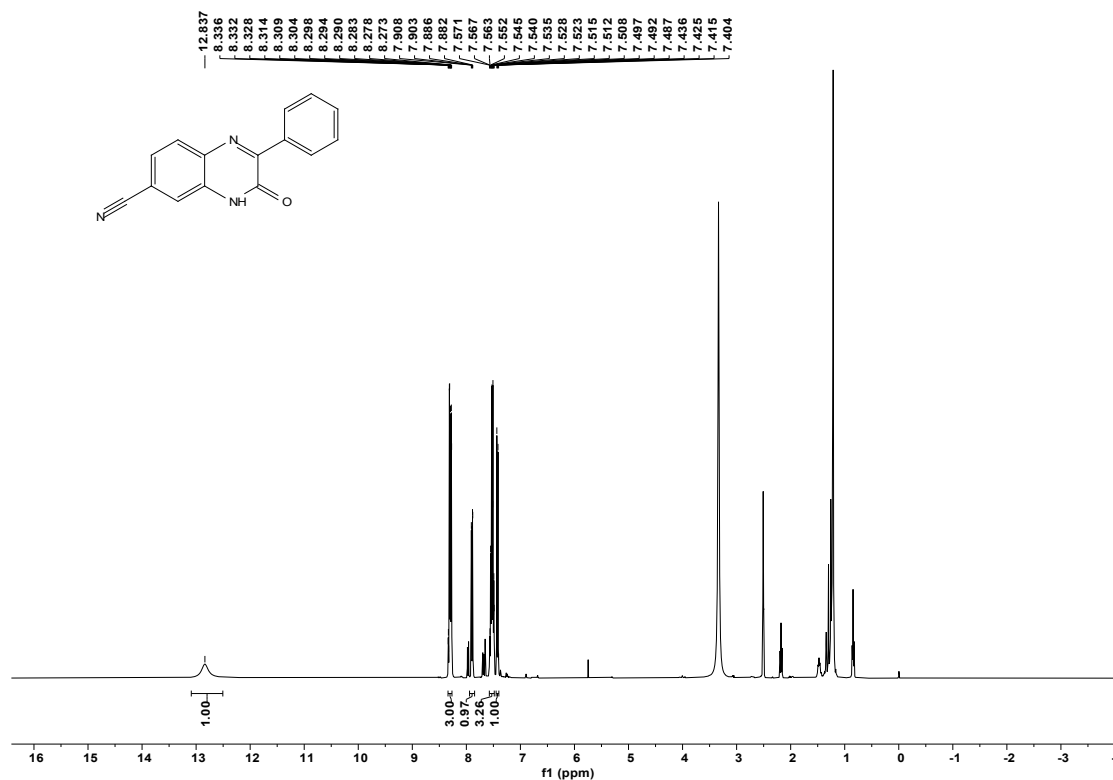
¹³C NMR Spectrum of 7-Bromo-3-phenylquinoxalin-2(1H)-one (Solvent: DMSO-*d*₆+CDCl₃)



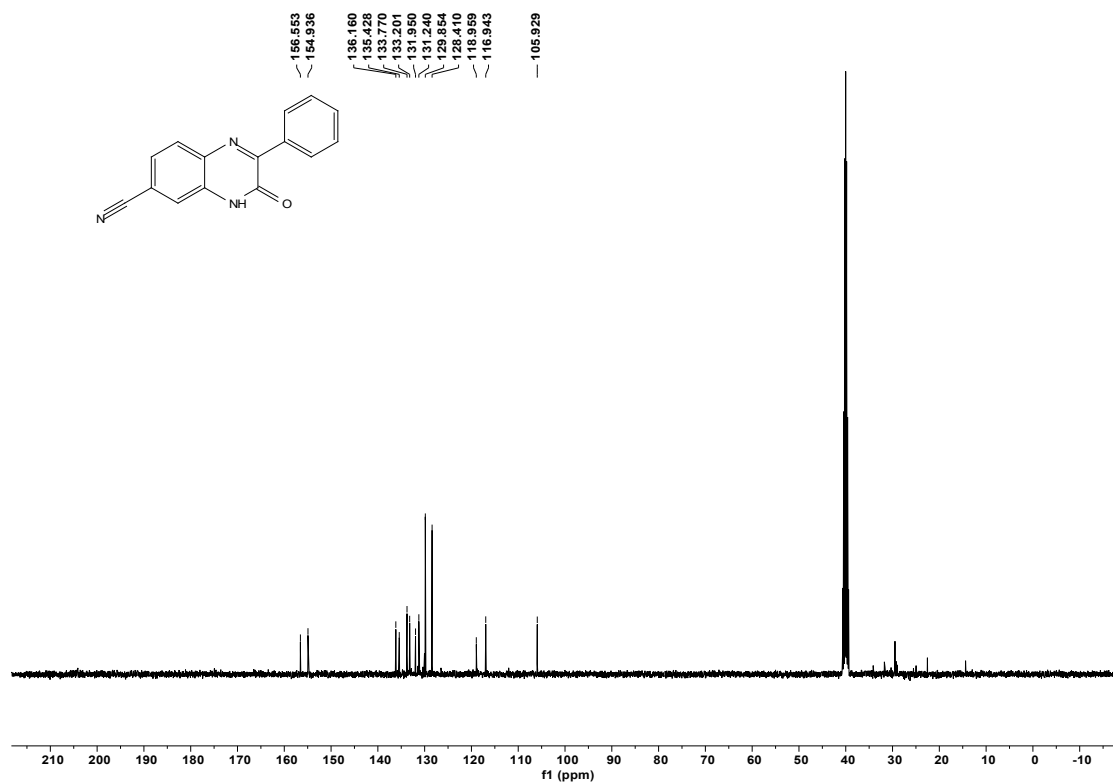
¹H NMR Spectrum of 3-Phenyl-7-(trifluoromethyl)quinoxalin-2(1H)-one (Solvent: DMSO-*d*₆)



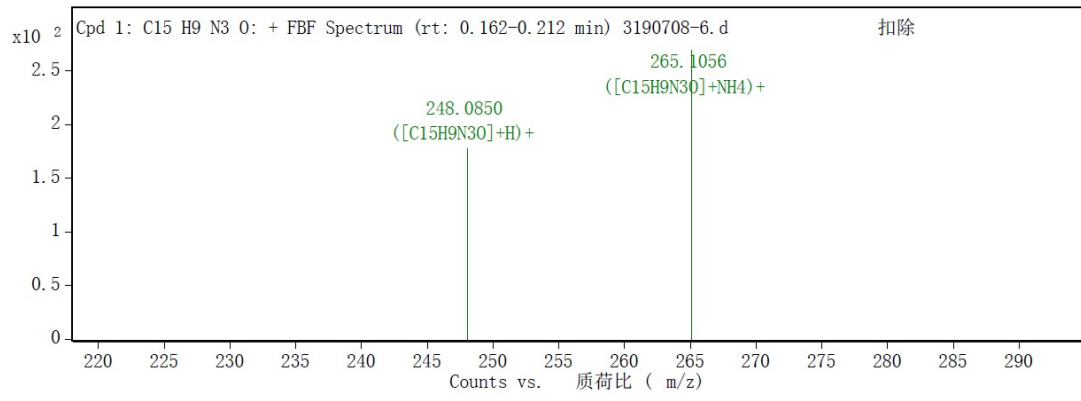
¹³C NMR Spectrum of 3-Phenyl-7-(trifluoromethyl)quinoxalin-2(1H)-one (Solvent: DMSO-*d*₆)



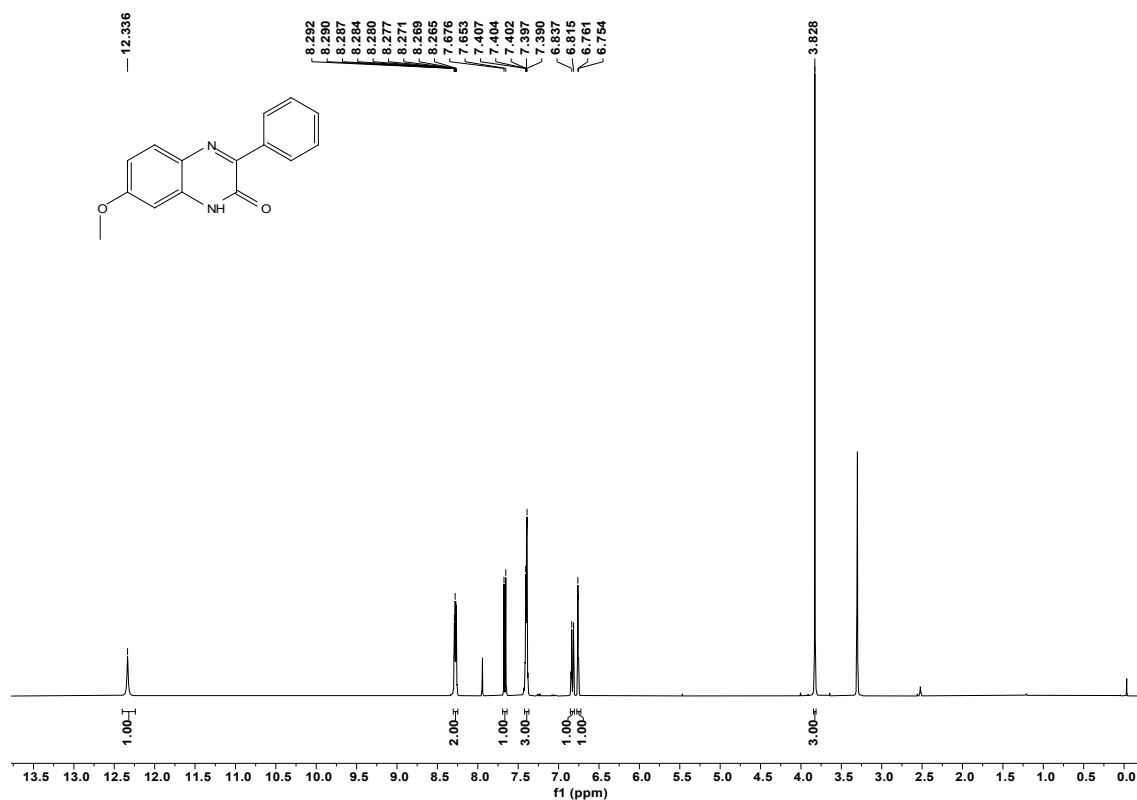
¹H NMR Spectrum of 3-Oxo-2-phenyl-3,4-dihydroquinoxaline-6-carbonitrile (Solvent: DMSO-*d*₆)



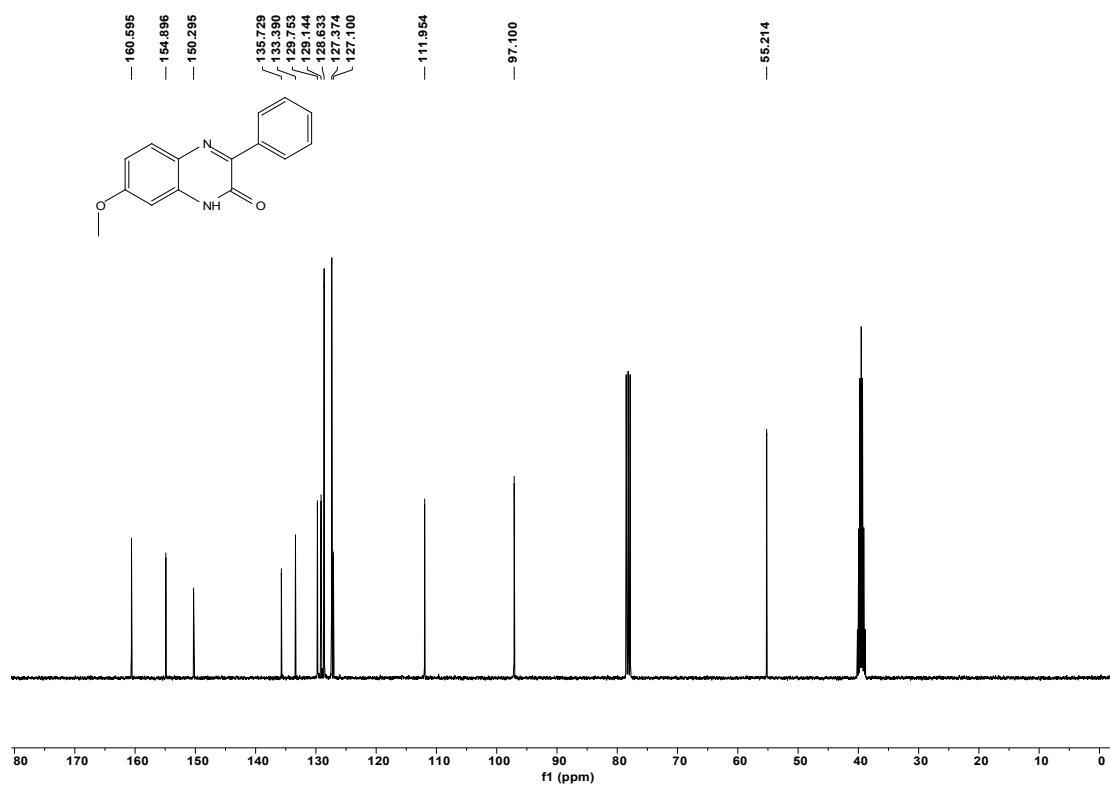
¹³C NMR Spectrum of 3-Oxo-2-phenyl-3,4-dihydroquinoxaline-6-carbonitrile (Solvent: DMSO-*d*₆)



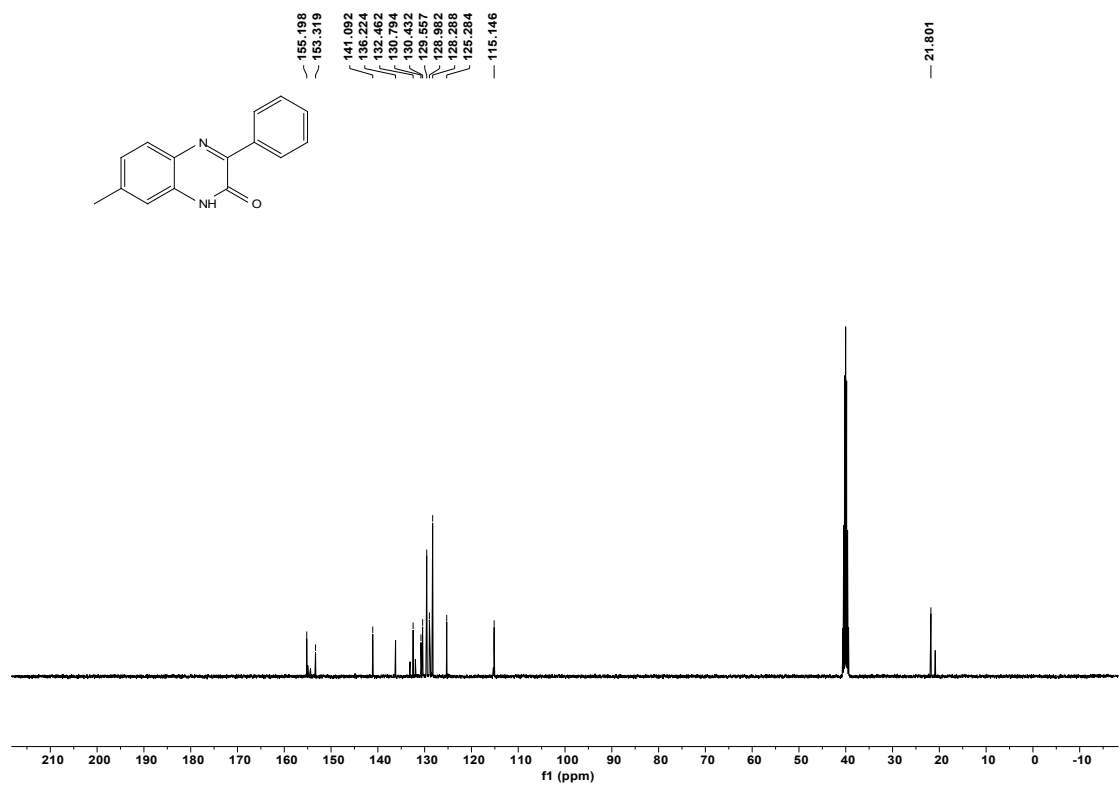
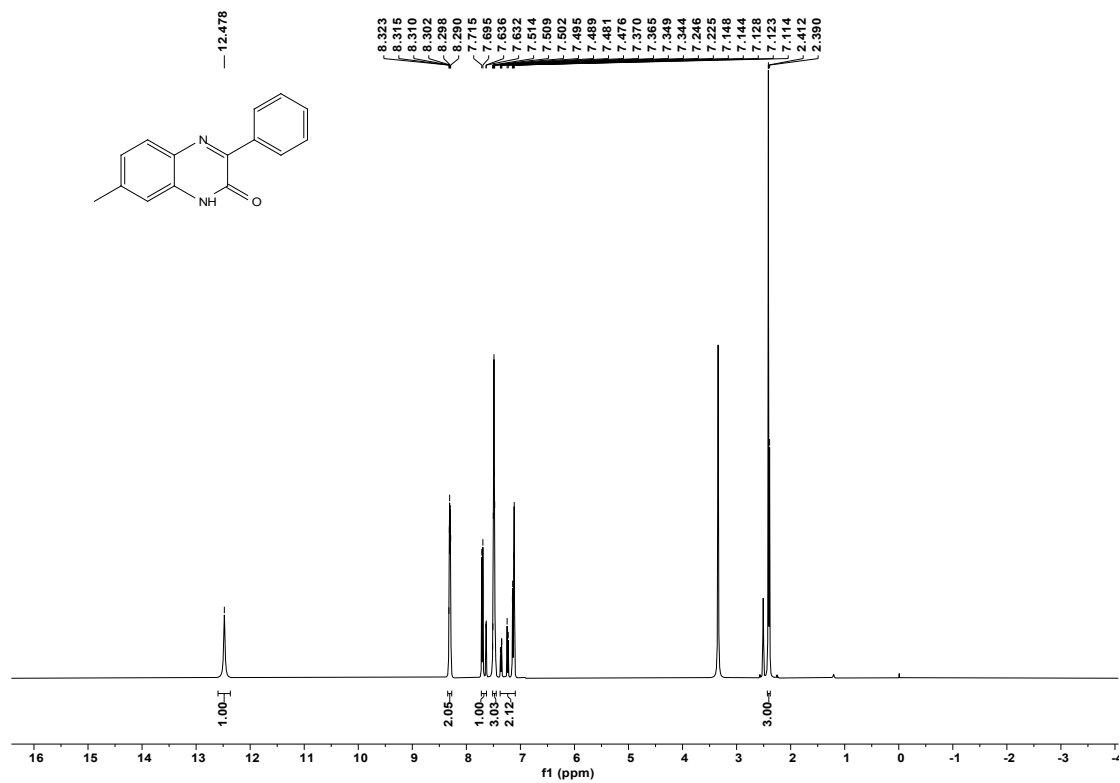
ESI-MS Spectrum of 3-Oxo-2-phenyl-3,4-dihydroquinoxaline-6-carbonitrile

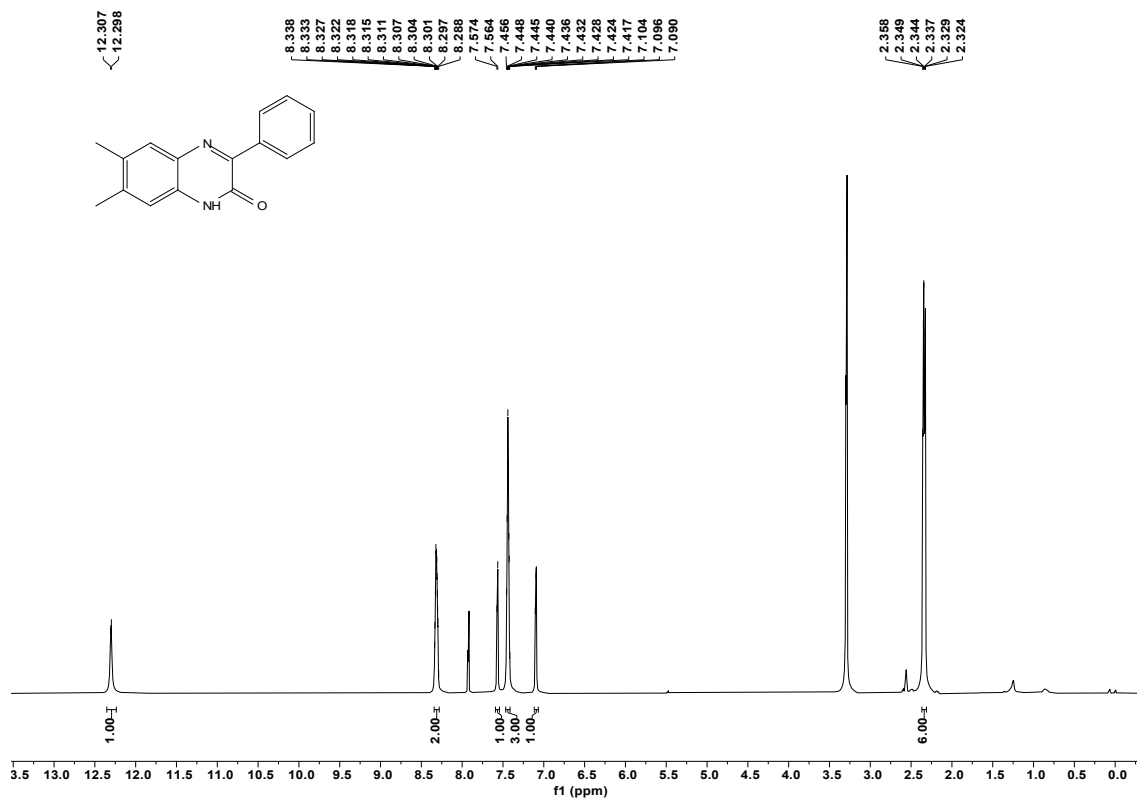


¹H NMR Spectrum of 7-Methoxy-3-phenylquinoxalin-2(1H)-one (Solvent: DMSO-*d*₆+CDCl₃)

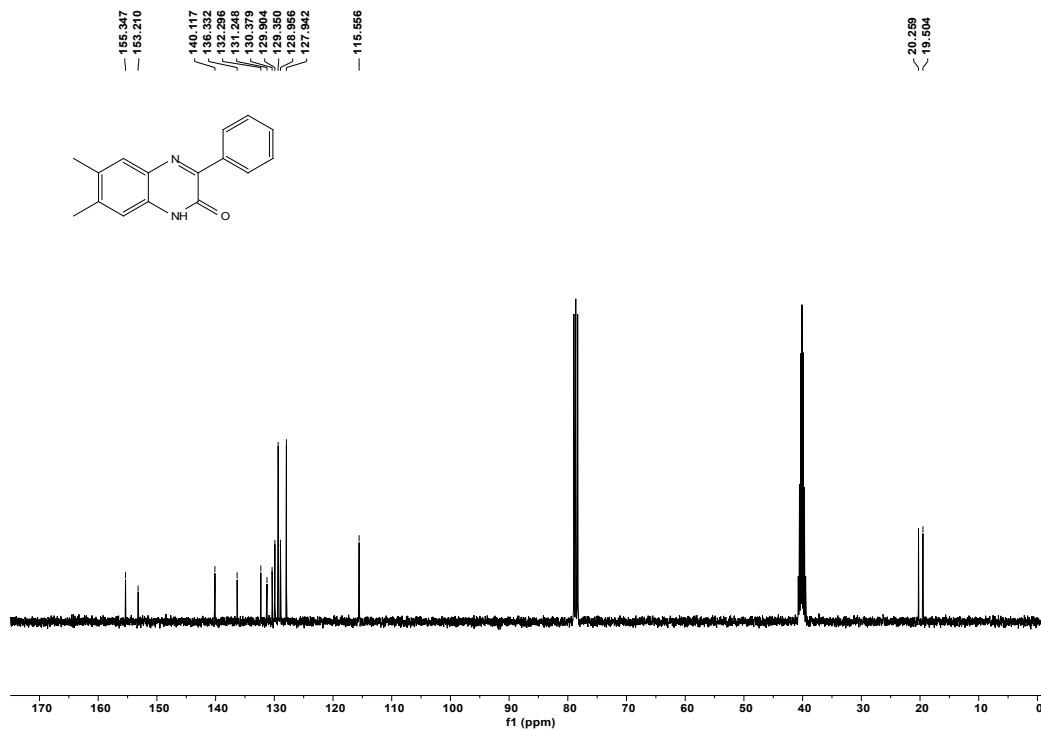


¹³C NMR Spectrum of 7-Methoxy-3-phenylquinoxalin-2(1H)-one (Solvent: DMSO-*d*₆+CDCl₃)

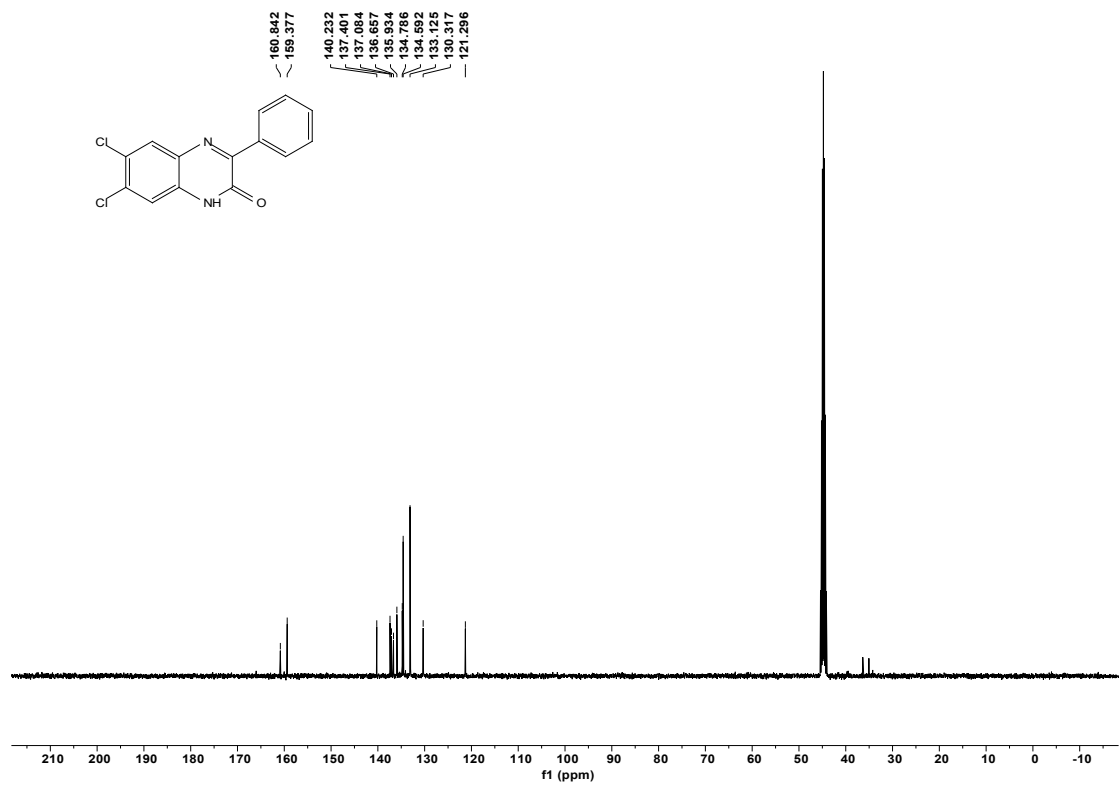
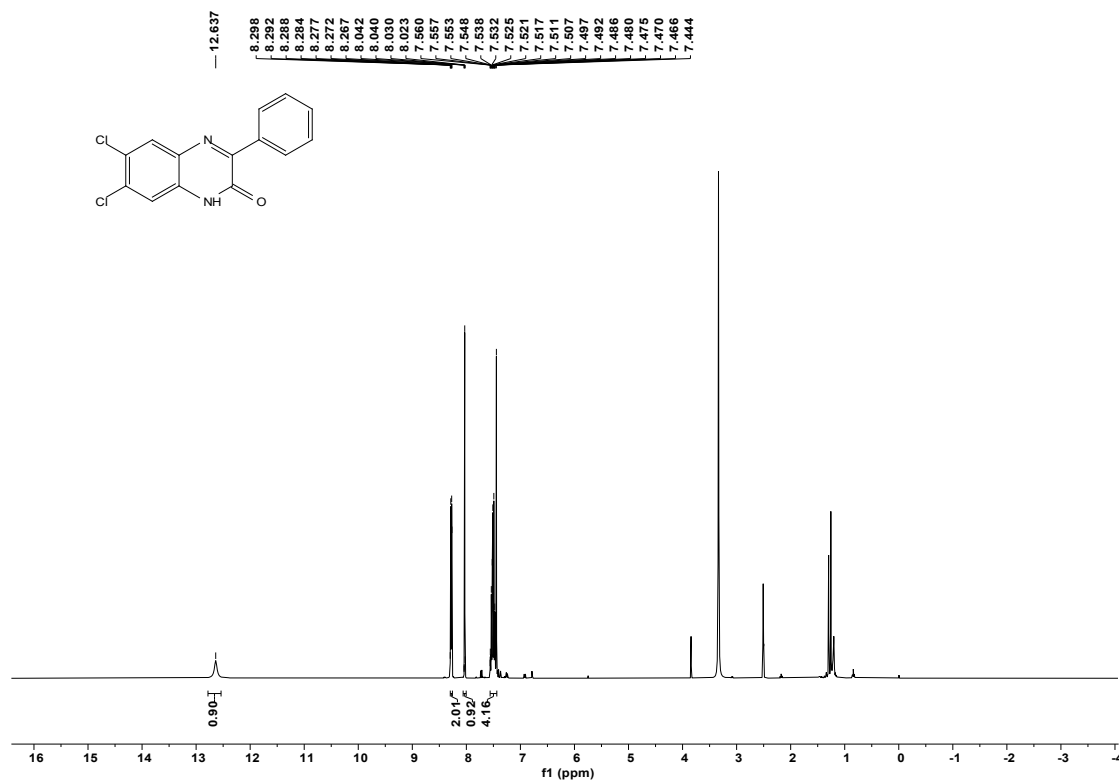


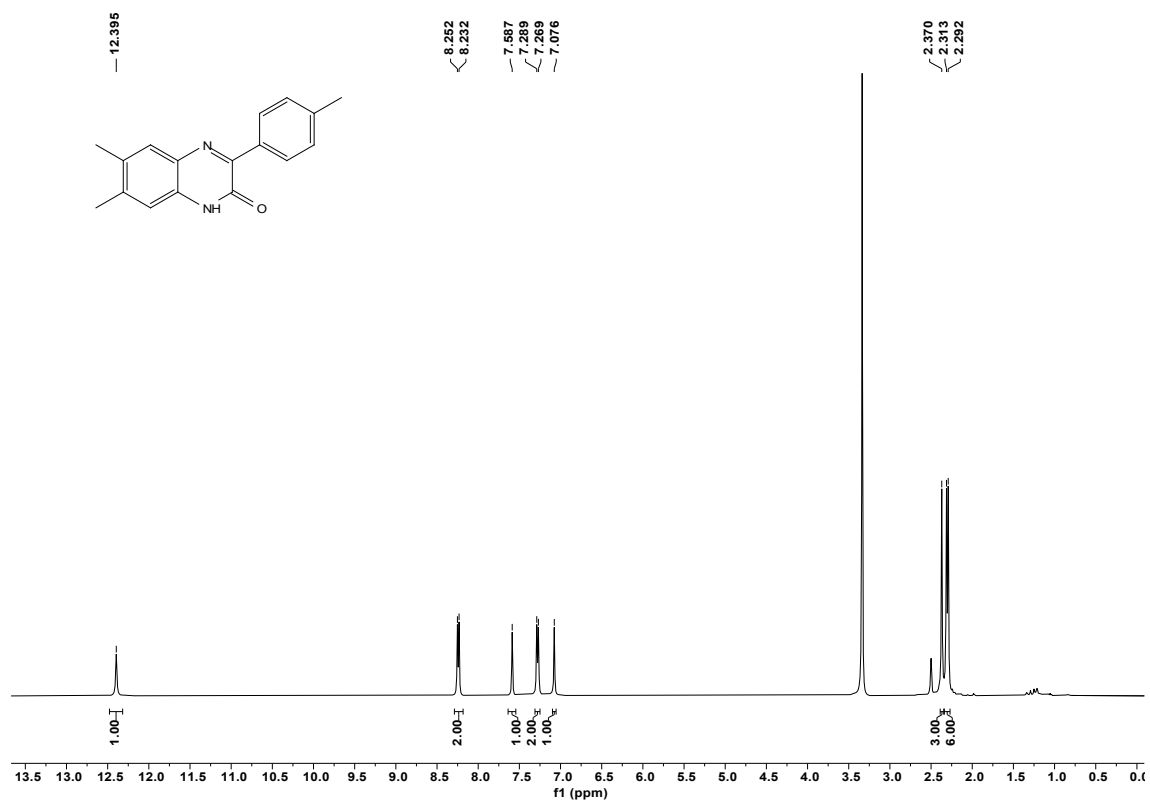


¹H NMR Spectrum of 6,7-Dimethyl-3-phenylquinoxalin-2(1H)-one (Solvent: DMSO-*d*₆+CDCl₃)

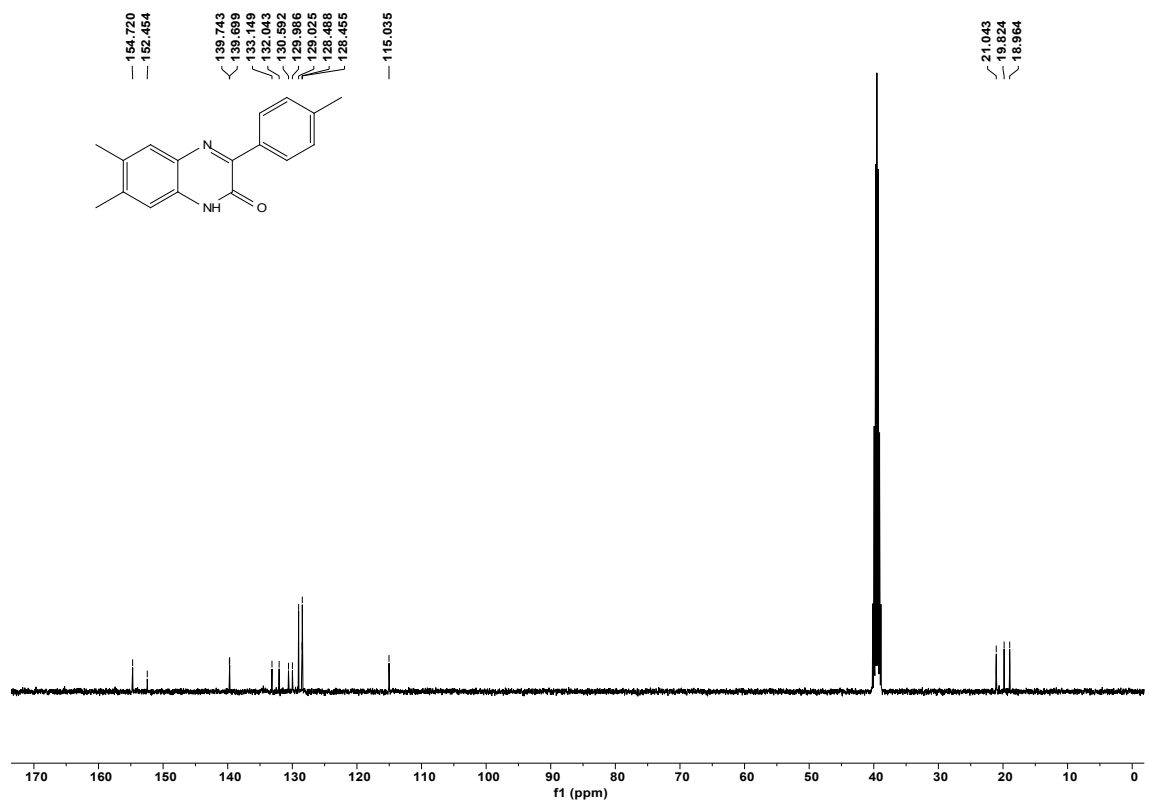


¹³C NMR Spectrum of 6,7-Dimethyl-3-phenylquinoxalin-2(1H)-one (Solvent: DMSO-*d*₆+CDCl₃)

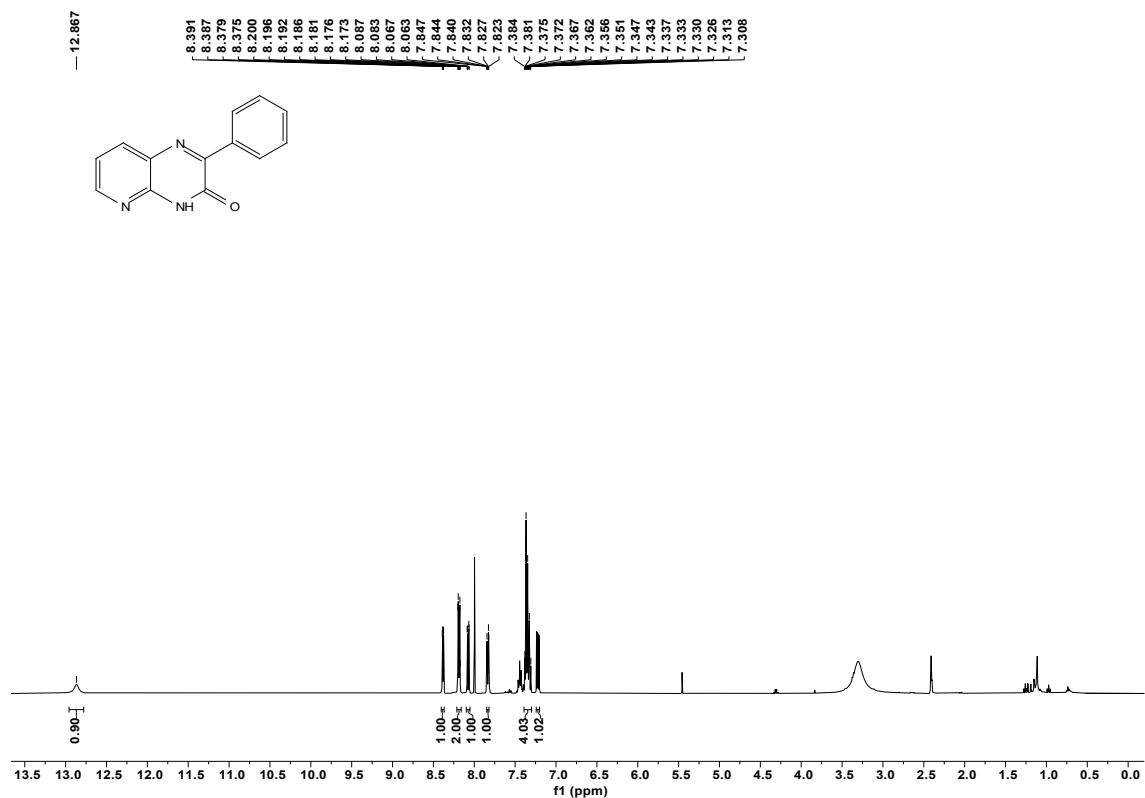




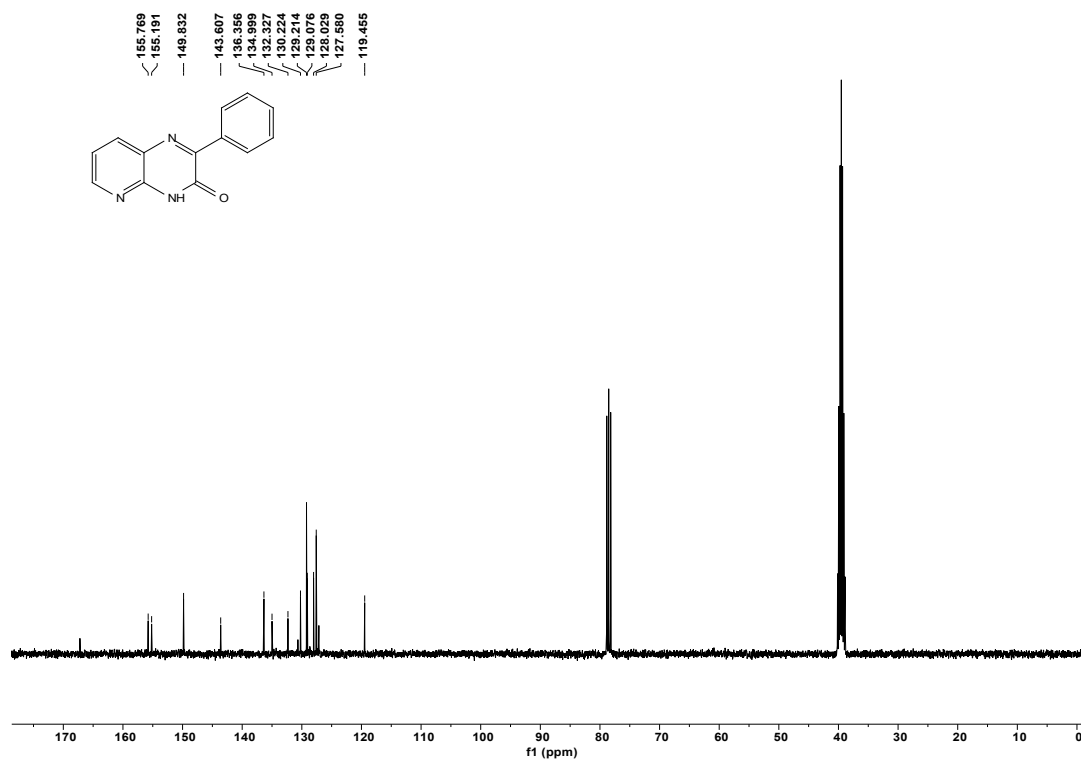
¹H NMR Spectrum of 6,7-Dimethyl-3-*p*-tolylquinoxalin-2(1H)-one (Solvent: DMSO-*d*₆)



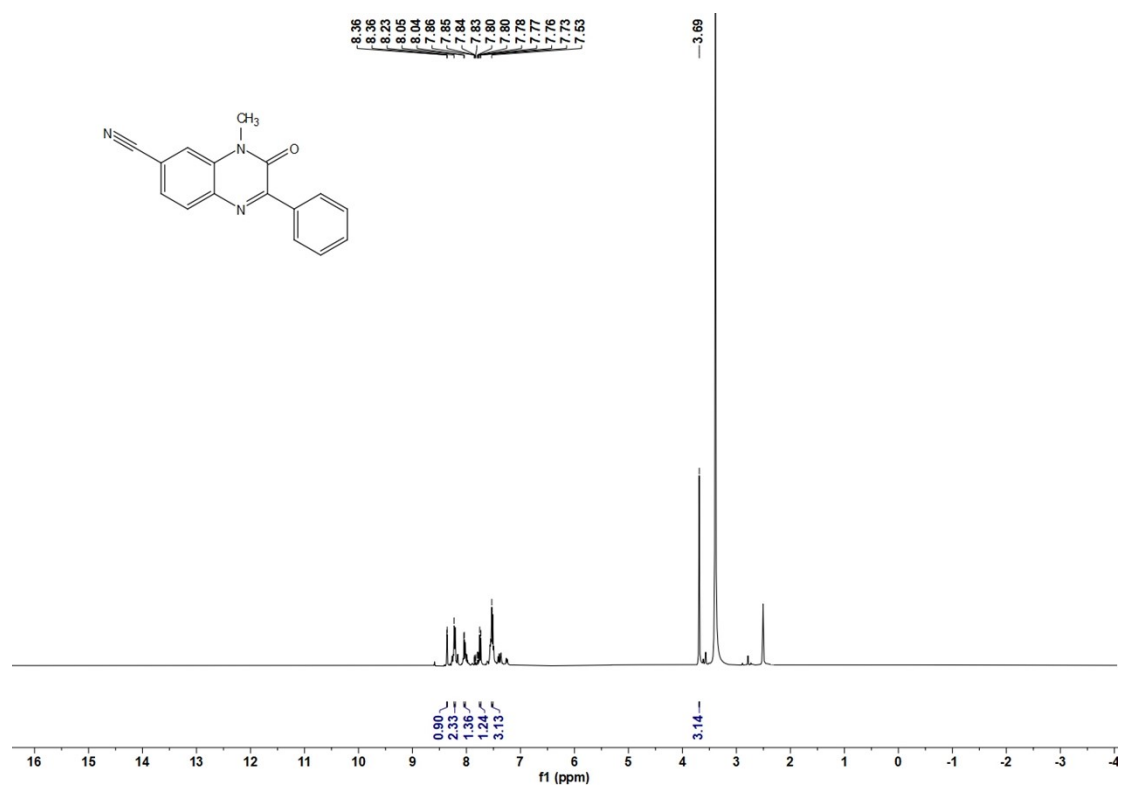
¹³C NMR Spectrum of 6,7-Dimethyl-3-*p*-tolylquinoxalin-2(1H)-one (Solvent: DMSO-*d*₆)



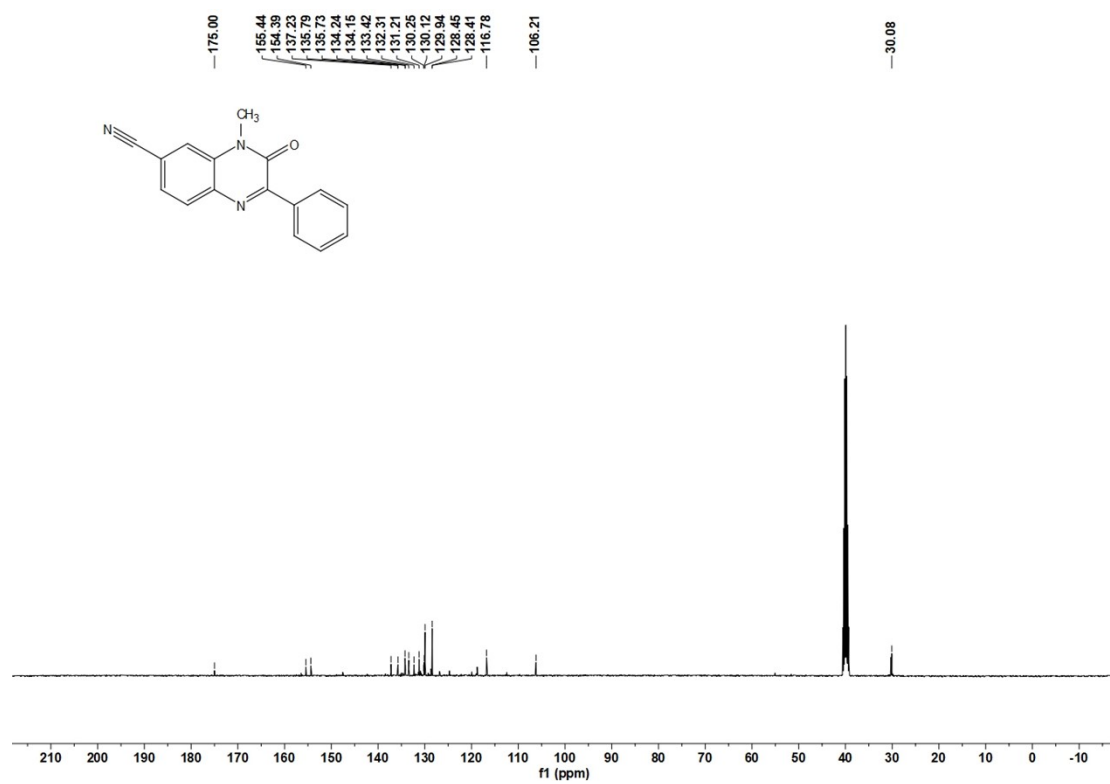
¹H NMR Spectrum of 2-Phenylpyrido[3,2-b]pyrazin-3(4H)-one (Solvent: DMSO-*d*₆+CDCl₃)



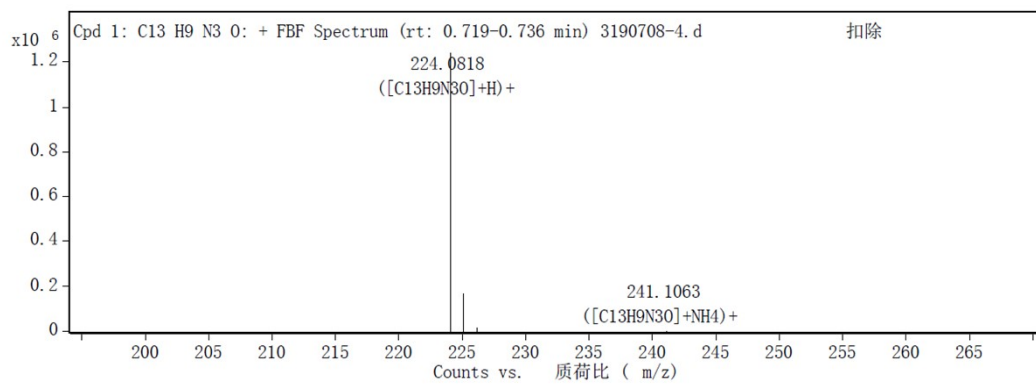
¹³C NMR Spectrum of 2-Phenylpyrido[3,2-b]pyrazin-3(4H)-one (Solvent: DMSO-*d*₆+CDCl₃)



¹H NMR Spectrum of 4-methyl-3-oxo-2-phenyl-3,4-dihydroquinoxaline-6-carbonitrile (Solvent: DMSO-*d*₆)

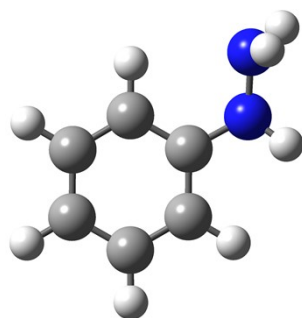


¹³C NMR Spectrum of 4-methyl-3-oxo-2-phenyl-3,4-dihydroquinoxaline-6-carbonitrile (Solvent: DMSO-*d*₆)



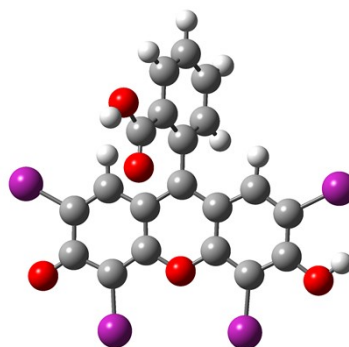
ESI-MS Spectrum of 2-Phenylpyrido[3,2-b]pyrazin-3(4H)-one

6. Optimized Structures and Cartesian Coordinates



A

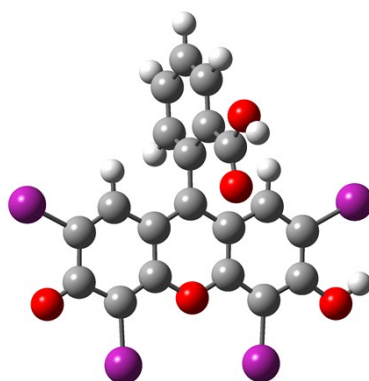
C	-0.45018300	-0.24612200	0.08316800
C	0.48592000	-1.29121800	0.00260200
C	1.84900500	-1.01365200	-0.06178600
C	2.30668300	0.30597300	-0.05546600
C	1.37463000	1.34305200	0.01856700
C	0.00711500	1.08022900	0.08700600
H	0.13960100	-2.32353400	-0.00320500
H	2.55650500	-1.83696300	-0.12331700
H	3.36999200	0.52100700	-0.10994500
H	1.71319900	2.37648700	0.02182700
H	-0.71773600	1.88376400	0.14229100
N	-1.81355100	-0.56420600	0.21257400
H	-2.03082800	-1.49568000	-0.13441500
N	-2.74071200	0.43832400	-0.14825300
H	-3.02549200	0.35065200	-1.12583800
H	-3.56442600	0.33586900	0.43781200



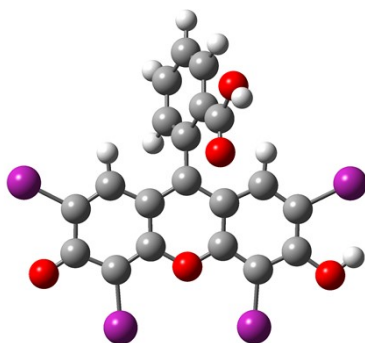
EY*

C	-0.02619300	1.17292200	-0.24840600
C	-1.06802300	-1.06128500	-0.09549300
C	-1.22597500	0.33351300	-0.21403200
C	-2.53737000	0.85118300	-0.32436600

H	-2.67206200	1.92002500	-0.43447500
C	-3.64076800	0.02925500	-0.29650600
C	-3.53396000	-1.41449400	-0.15910900
C	-2.16414700	-1.91947400	-0.06360500
C	-0.13289600	2.64508000	-0.41377800
C	-0.58641100	3.52341800	0.60334700
C	0.22092000	3.19972100	-1.65484800
C	-0.69146400	4.89904000	0.34471000
C	0.11851900	4.56856700	-1.89882100
H	0.56533300	2.53529600	-2.44206600
C	-0.34533800	5.42223100	-0.89747400
H	-1.04057300	5.55456800	1.13379700
H	0.39241000	4.96376100	-2.87313500
H	-0.43429900	6.48890800	-1.08071700
C	-0.90615300	3.00128800	1.96159200
O	-0.81318800	1.84266800	2.31599300
O	-1.31981600	3.97326900	2.81454800
H	-1.49526200	3.52160300	3.66088500
Br	-5.37678600	0.76277600	-0.44229300
O	-4.52174200	-2.17886800	-0.12895800
O	0.16516300	-1.64355700	-0.01562700
Br	-1.91665600	-3.76740800	0.09803800
C	3.72264000	-0.88054900	-0.04578300
C	3.66770700	0.52557700	-0.14799000
C	2.47795900	1.21827300	-0.21559900
C	1.23418400	0.53024900	-0.19352800
C	1.29659500	-0.89165200	-0.07463900
C	2.50298600	-1.57892200	-0.00655000
H	2.48792600	2.29837900	-0.28164100
Br	5.32948500	1.47815900	-0.18336700
Br	2.51306800	-3.46516600	0.14284700
O	4.87249700	-1.57742000	0.01931200
H	5.61745200	-0.94753800	-0.01242700



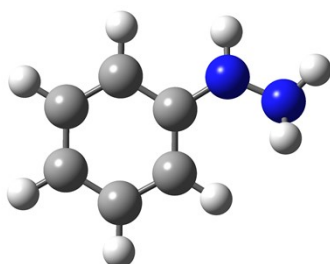
	EY		
C	-0.06987900	1.13250500	-0.25508000
C	-1.21967900	-1.01824900	-0.08523100
C	-1.25288100	0.42573400	-0.20792000
C	-2.55318800	1.04776200	-0.25579200
H	-2.60827300	2.12618800	-0.34039400
C	-3.68491800	0.31025500	-0.19717300
C	-3.69333000	-1.17305100	-0.07971300
C	-2.35399200	-1.77223400	-0.02697300
C	-0.06296200	2.61709500	-0.44533300
C	0.05465800	3.54312600	0.61642100
C	-0.17853900	3.10463100	-1.75366400
C	0.05002100	4.91896400	0.34153100
C	-0.17776000	4.47506400	-2.01550800
H	-0.27348100	2.39683200	-2.57187800
C	-0.06260900	5.38536500	-0.96528800
H	0.13355100	5.61740400	1.16579800
H	-0.27061900	4.82667600	-3.03905000
H	-0.06400100	6.45343600	-1.16105200
C	0.17474400	3.06122700	2.02236500
O	0.25532700	1.89791700	2.36087200
O	0.19070100	4.07368000	2.92371300
H	0.27000200	3.64916200	3.79827300
Br	-5.38433500	1.14692700	-0.26355100
O	-4.72924400	-1.82456500	-0.03243300
O	-0.01652500	-1.66205200	-0.02758300
Br	-2.25753200	-3.65314500	0.12684000
C	3.57142000	-1.11531900	-0.11606300
C	3.59846700	0.29106300	-0.24088700
C	2.44287500	1.04295000	-0.29081700
C	1.18495000	0.41749100	-0.21640600
C	1.15302800	-0.98804100	-0.09552200
C	2.32385300	-1.74885000	-0.04540200
H	2.50494400	2.11970900	-0.38702100
Br	5.30822300	1.14664400	-0.34241400
Br	2.22870800	-3.62819000	0.11533700
O	4.68159900	-1.86985100	-0.06617700
H	5.46008900	-1.28361400	-0.12451800



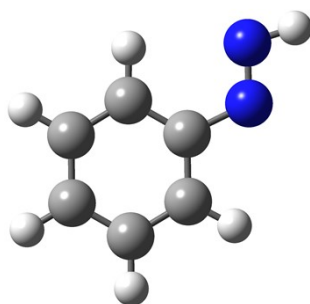
EY⁻

C	-0.03358300	1.17754300	-0.16664100
C	-1.37323600	-0.89796600	-0.04498800
C	-1.30300000	0.52711300	-0.11208900
C	-2.55442700	1.20449600	-0.06675100
H	-2.56434900	2.28749400	-0.05841500
C	-3.74328500	0.52457400	-0.02073400
C	-3.87193200	-0.92889100	0.00479900
C	-2.56593200	-1.58163000	0.00295300
C	0.04874900	2.62797000	-0.41982700
C	0.73226200	3.58536000	0.39266000
C	-0.57321200	3.11474000	-1.59290800
C	0.82013900	4.92989900	-0.03030500
C	-0.48636300	4.44158000	-1.98807300
H	-1.10323400	2.40255100	-2.21750800
C	0.22903100	5.36080500	-1.20628800
H	1.35370100	5.63413100	0.59734000
H	-0.95784900	4.75881500	-2.91516400
H	0.31479400	6.40005300	-1.51277900
C	1.25671000	3.23089600	1.72841300
O	1.21865900	2.14207500	2.27011600
O	1.81824400	4.30120700	2.38668500
H	2.09554700	3.92510900	3.24138300
Br	-5.38555900	1.51925400	0.03339900
O	-4.95449400	-1.53629800	0.03720400
O	-0.21791500	-1.64917300	-0.02314700
Br	-2.56485600	-3.48797900	0.07542400
C	3.41172500	-1.41892200	-0.13075100
C	3.55180000	-0.02963200	-0.22503500
C	2.47134300	0.83653400	-0.22777300
C	1.15068800	0.35216500	-0.13061300
C	1.00178600	-1.05797800	-0.06229300
C	2.10241700	-1.91707100	-0.05629800
H	2.64787100	1.90012700	-0.31729800
Br	5.34181400	0.68359000	-0.35092100

Br	1.82912800	-3.79551700	0.04297800
O	4.45944000	-2.28556000	-0.11560600
H	5.27350100	-1.75294800	-0.17512000

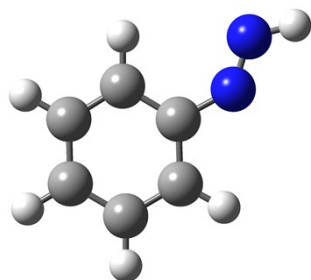


B			
C	1.83445700	1.04107000	-0.02746100
C	0.47706700	1.30827200	-0.00072800
C	-0.44158200	0.22775600	0.02513300
C	0.01314300	-1.11260000	0.04147500
C	1.37630500	-1.35321100	0.01449000
C	2.29053800	-0.28615700	-0.02487300
H	2.54346400	1.86183000	-0.05086300
H	0.11365400	2.33267400	-0.01239700
H	-0.68227300	-1.94145900	0.11928900
H	1.73855100	-2.37568000	0.03894900
H	3.35611500	-0.49099200	-0.04305000
N	-1.77755000	0.54055100	0.01396100
H	-2.05447000	1.50319600	0.18889800
N	-2.79261400	-0.36107400	0.02802600
H	-3.69828100	0.07027400	-0.13331300
H	-2.62518800	-1.16696700	-0.56963500



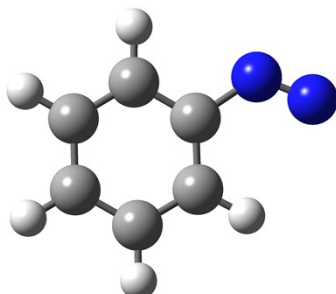
C			
C	1.30524300	1.32921700	0.00000000
C	-0.06649500	1.10305300	0.00000000
C	-0.54741800	-0.21519100	0.00000000
C	0.34497000	-1.29193500	0.00000000
C	1.72054900	-1.05896500	0.00000000
C	2.20051500	0.25128300	0.00000000

H	1.68473700	2.34764900	0.00000000
H	-0.77811200	1.92160400	0.00000000
H	-0.06159800	-2.29872300	0.00000000
H	2.41386800	-1.89540600	0.00000000
H	3.27127800	0.43735300	0.00000000
N	-1.93330400	-0.57265200	0.00000000
N	-2.72373400	0.39996100	0.00000000
H	-3.67508700	-0.00841300	0.00000000



D

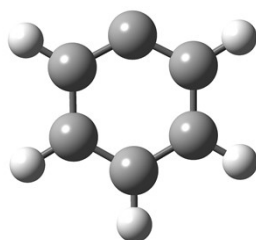
C	1.35840600	1.32255300	0.00000000
C	-0.01332000	1.15807800	0.00000000
C	-0.52144600	-0.16773400	0.00000000
C	0.32121500	-1.30283400	0.00000000
C	1.69327800	-1.10440200	0.00000000
C	2.20700300	0.19938800	0.00000000
H	1.78045500	2.32234800	0.00000000
H	-0.69511000	2.00226000	0.00000100
H	-0.11285200	-2.29706200	0.00000000
H	2.36424600	-1.95651600	-0.00000100
H	3.28263700	0.34860800	-0.00000100
N	-1.87068500	-0.40329000	0.00000100
N	-2.85696200	0.27505300	-0.00000200
H	-3.79665900	-0.15228100	0.00000200



E

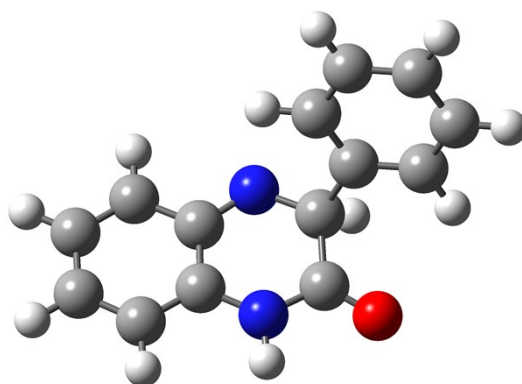
C	-1.27829700	1.31975900	0.00000000
C	0.09853200	1.11634900	0.00000000
C	0.59001000	-0.19317800	0.00000000

C	-0.27046400	-1.28967500	0.00000000
C	-1.64919100	-1.07593100	0.00000000
C	-2.15224400	0.22645300	0.00000000
H	-1.67329200	2.33203100	0.00000000
H	0.79657000	1.94785900	0.00000000
H	0.15029300	-2.29051000	0.00000000
H	-2.32779700	-1.92408400	0.00000000
H	-3.22589300	0.39290500	0.00000000
N	2.01634700	-0.48555500	0.00000000
N	2.87651700	0.33114600	0.00000000



F

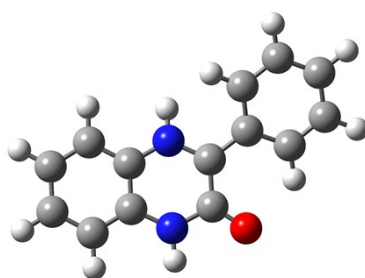
C	-1.21419800	0.63260900	-0.00000600
C	-1.22640100	-0.77179400	0.00002200
C	-0.00001200	-1.40013100	-0.00001000
C	1.22640400	-0.77178500	-0.00000800
C	1.21421200	0.63258300	0.00001800
C	-0.00000300	1.32471600	-0.00000500
H	-2.15467600	1.17909500	-0.00002800
H	-2.16291000	-1.32331500	-0.00000900
H	2.16288300	-1.32336000	-0.00002600
H	2.15466800	1.17910700	0.00001100
H	0.00002700	2.41128500	-0.00002200



G

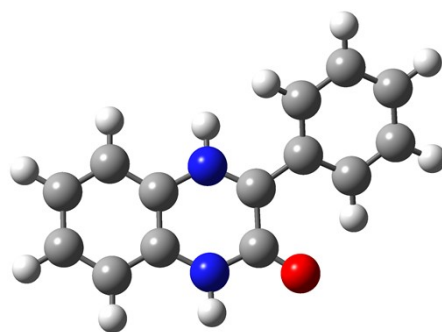
C	-4.13468300	-0.47772700	-0.77696300
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C	-3.23542800	0.56255000	-1.01751900
C	-2.01548200	0.59782200	-0.34682900
C	-1.65744900	-0.43647000	0.59119700
C	-2.61638900	-1.47558600	0.81467000
C	-3.82262900	-1.49617900	0.14549400
H	-5.08302100	-0.49504800	-1.30571200
H	-3.48350400	1.35132800	-1.72392100
H	-2.34298300	-2.24490000	1.52975600
H	-4.53336500	-2.29704700	0.32632300
C	0.50465500	0.53323700	0.98361800
C	0.08735100	1.75578200	0.14784300
H	0.80304500	0.94892600	1.95773000
N	-0.49881900	-0.47879900	1.25104600
N	-1.11071000	1.63481000	-0.52590200
H	-1.36924700	2.43549100	-1.09300300
O	0.75877200	2.77041300	0.06632000
C	1.77354700	-0.09162800	0.37176500
C	2.97091900	0.63629100	0.36933600
C	1.75117900	-1.37386000	-0.18431200
C	4.12566600	0.08793000	-0.18661100
H	2.98812700	1.63817800	0.78601900
C	2.91087700	-1.92202000	-0.73710900
H	0.83139000	-1.94846200	-0.16809300
C	4.10027900	-1.19404200	-0.74100800
H	5.04799700	0.66292400	-0.18337800
H	2.88113200	-2.92142700	-1.16358000
H	5.00248600	-1.62195200	-1.17014400



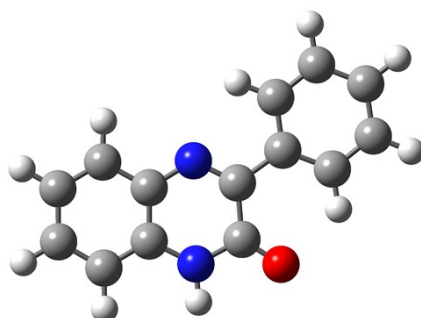
	H		
C	4.55952500	-0.30239900	0.02092700
C	3.70977200	0.80126000	0.11249100
C	2.32519800	0.62768000	0.05670400
C	1.79040200	-0.66975700	-0.08396400
C	2.64887100	-1.77048300	-0.17901200
C	4.02969100	-1.58636300	-0.12774200

H	5.63436900	-0.15528400	0.06346000
H	4.11556000	1.80388400	0.22126200
H	2.22744800	-2.76685800	-0.29020400
H	4.68842300	-2.44616500	-0.20200300
C	-0.50360700	0.24505400	-0.02765100
C	0.02856500	1.59569500	0.07601100
N	0.41008900	-0.79842800	-0.12624300
N	1.42638500	1.68524800	0.11850800
H	1.77083500	2.63359800	0.20187400
O	-0.63390800	2.63252200	0.13854600
C	-1.91749300	-0.08161700	0.00477200
C	-2.91532500	0.87991900	-0.29207900
C	-2.34919900	-1.39580800	0.31429000
C	-4.25994000	0.52812400	-0.29836000
H	-2.61163200	1.89421700	-0.51200500
C	-3.69802700	-1.73596000	0.30203800
H	-1.63210900	-2.15148900	0.62533700
C	-4.66553400	-0.77896500	-0.01049500
H	-5.00254100	1.28556600	-0.53594400
H	-3.99449000	-2.75099500	0.55399600
H	-5.71894700	-1.04452400	-0.01915500
H	0.04161700	-1.70814300	-0.36841900



I			
C	4.53124300	-0.30439800	-0.00553100
C	3.70767700	0.80535800	0.12419300
C	2.31784700	0.63506300	0.07517300
C	1.78668300	-0.65689500	-0.10107000
C	2.62286300	-1.77457900	-0.23681000
C	3.99478000	-1.59307100	-0.18720800
H	5.60768900	-0.17276600	0.03287300
H	4.12653900	1.79775700	0.26085200
H	2.19371900	-2.76336800	-0.37510000

H	4.65606800	-2.44666000	-0.28784200
C	-0.49262000	0.20699600	-0.01424200
C	0.04182400	1.60563300	0.12632200
N	0.39842000	-0.77313200	-0.14239400
N	1.42316300	1.68327700	0.18349900
H	1.77719600	2.62880700	0.30544100
O	-0.66492200	2.59265900	0.20080900
C	-1.90852500	-0.09671000	0.00680600
C	-2.86589600	0.85294000	-0.42362500
C	-2.35072100	-1.37407900	0.43670000
C	-4.21395800	0.51285400	-0.44950700
H	-2.54482000	1.83400900	-0.74398000
C	-3.69880200	-1.69330400	0.41916800
H	-1.65053100	-2.09424500	0.85395800
C	-4.63394500	-0.75212400	-0.03280900
H	-4.94032700	1.24140800	-0.79485000
H	-4.02892600	-2.66424400	0.77411500
H	-5.68990200	-1.00479600	-0.04532200
H	0.03088600	-1.71029800	-0.29971500



3aa			
C	4.52149900	-0.35162900	0.00001400
C	3.71628200	0.78021800	-0.00005600
C	2.32309300	0.62633300	-0.00004500
C	1.73596100	-0.65941000	0.00003500
C	2.57740200	-1.78891200	0.00010100
C	3.95525900	-1.63853000	0.00008600
H	5.60160900	-0.23624400	-0.00001300
H	4.15239100	1.77612700	-0.00012800
H	2.10824300	-2.76768000	0.00016100
H	4.59919800	-2.51266200	0.00015200
C	-0.44854900	0.19376100	-0.00000100
C	0.06328100	1.60655300	-0.00004200
N	0.37085000	-0.82342700	0.00004000

N	1.44813700	1.69228900	-0.00007800
H	1.80315100	2.64282700	-0.00010700
O	-0.60473100	2.63577100	-0.00005700
C	-1.90530900	-0.09607100	-0.00001300
C	-2.89701000	0.90353800	0.00015700
C	-2.31577500	-1.44573300	-0.00015500
C	-4.24865900	0.55644800	0.00016700
H	-2.60311200	1.94348300	0.00027800
C	-3.66325900	-1.78273100	-0.00015100
H	-1.55533800	-2.21780600	-0.00026300
C	-4.63971900	-0.78130400	0.00000600
H	-4.99841300	1.34323100	0.00029900
H	-3.95555500	-2.82962400	-0.00026400
H	-5.69422700	-1.04504300	-0.00000800