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DMSO/^{t}BuONa/O_2-Mediated Efficient Syntheses of Diverse Quinoxalines through α-imino Radicals

Chihong Zhang,[†] Zhen Zhang,*[,†] Deliang Wang,[†] Wenkun Wang,[†] Bo Jin,[†] Tao Wen,[†] Lihua Ye,[†] Zhong-Ning Chen,[†,‡] Hu Cai,*[,†]

[†] School of Chemistry and Chemical Engineering, Nanchang University, Jiangxi Province, Nanchang 330031, People's Republic of China; E-mail: caihu@ncu.edu.cn
[‡] Fujian Institute of Research on the Structure, Chinese Academy of Science. Fuzhou, Fujian 350001, People's Republic of China;

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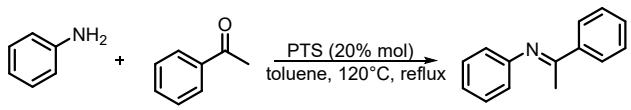
1. General Information

^{1}H NMR, ^{13}C NMR spectra were recorded in $CDCl_3$ or DMSO-d_6 solution on *Agilent ProPulse* AM-400 MHz instruments and the spectral data were reported in ppm relative to tetramethylsilane (0.00 ppm) or residual undeuterated solvent $CHCl_3$ (7.26 ppm) and DMSO (2.50 pm) as internal standard for ^{1}H NMR and deuterated solvent $CDCl_3$ (77.0 ppm) and DMSO-d_6 (39.5 ppm) as internal standard for ^{13}C NMR. High-resolution mass spectral analysis (HRMS) data were measured on an *Agilent* 7890-5975C spectrometer by means of the ESI technique. Electron paramagnetic resonance spectrometer (EPR) data were measured on a *EMXplus*-9.5/12 spectrometer. Coupling constants (J) are quoted in Hz. Multiplicities are reported as follows: singlet (s), doublet (d), doublet of doublets (dd), triplet (t), quartet (q), and multiplet (m).

Materials and Methods: Unless otherwise noted, all reactions were performed under an atmosphere of dry O_2 or Ar with oven-dried glassware. All solvents were purified and dried by standard techniques and distilled prior to use. Reactions were monitored by analytical thin layer chromatography on 0.20 mm Qingdao Haiyang silica gel plates. Silica gel (200-300 mesh) (from Qingdao Haiyang Chem. Company, Ltd.) was used for flash chromatography. The substrates were prepared according to the literature procedures. Other chemicals or reagents were obtained from commercial sources and used directly.

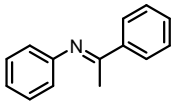
2. Synthetic Procedures

2.1. Preparation of *N*,1-diphenylethan-1-imine (4c)



In a three-neck flask (100 mL), PTS·H_2O (409 mg, 2.15 mmol, 20% mol), Toluene (50 mL), aniline **4e** (1.0 g, 10.75 mmol, 1.0 equiv.) and acetophenone **2a-1**

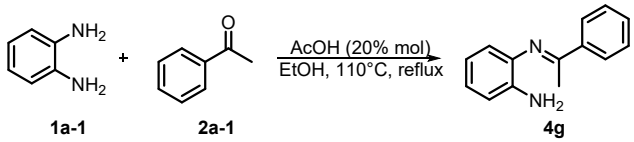
(1.55 g, 12.89 mmol, 1.2 equiv.) were added under Ar atmosphere. The reaction mixture was refluxed at 120℃ while progress of the reaction was monitored by TLC. After the reaction, the flask was cooled to room temperature, dried over Na_2SO_4 and concentrated in vacuo. Purification of the residue by neutral silica gel column chromatography afforded the desired compound **4c** (1.09 g, 52%)[1]



***N*,1-diphenylethan-1-imine (4c)**

Yellow liquid; yield: 52%; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.02-7.98 (m, 2H), 7.60-7.53 (m, 3H), 7.51-7.46 (m, 2H), 7.44-7.40 (m, 2H), 7.18 (d, J = 1.2 Hz, 1H), 2.61 (s, 3H); **^{13}C NMR** (101 MHz, $CDCl_3$): δ 191.9, 155.1, 142.8, 139.4, 132.5, 129.1, 128.6, 128.5, 128.3, 126.5, 122.1, 18.9; **HRMS**: m/z $[M + H]^+$ calcd for $C_{14}H_{13}N$: 196.1048 found 196.1052.

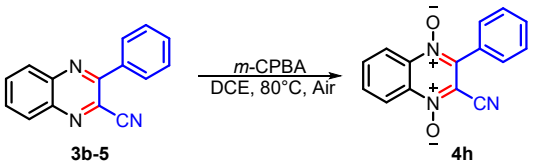
2.2. Preparation of 2-((1-phenylethylidene)amino)aniline (4g)



1a-1 2a-1 4g

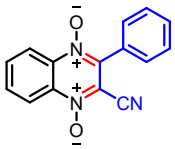
In a three-neck flask (100 ml), *o*-phenylenediamines **1a-1** (2.16 g, 20.0 mmol), EtOH (50 ml), AcOH (240 mg, 4.0 mmol, 20 mol%) and acetophenone **2a-1** (2.89 g, 24.0 mmol, 1.2 equiv.) were added under Ar atmosphere. The reaction mixture was refluxed at 110℃ for 5 h. After the reaction, the flask was cooled to room temperature, dried over Na_2SO_4 and concentrated in vacuo. Purification of the residue by neutral silica gel column chromatography quickly to afforded the desired compound **4g**. The resulting product is fed directly into the next reaction step[2].

2.3. Preparation of 2-cyano-3-phenylquinoxaline 1,4-dioxide (4h)



3b-5 4h

3-oxo-3-phenylpropanenitrile **3b-5** (69.3 mg, 0.3 mmol) and *m*-CPBA (75%) (414.2 mg, 1.8 mmol, 6.0 equiv.) were added to dry DCE (3 mL) solvent at room temperature. The reaction mixture was stirred at 80℃ and monitored by TLC. After 48h, the reaction mixture was cooled to room temperature and then quenched with 10% aqueous solution of Na_2SO_3, diluted with ethyl acetate, and extracted with ethyl acetate (25 mL × 3). The combined organic layer were washed with brine (5 mL), dried over Na_2SO_4 and concentrated in vacuo. Purify the residue to petroleum ether/ethyl acetate by column chromatography on silica gel. Compound **4h** (27.6 mg, 35%) was obtained as a yellow solid[3].



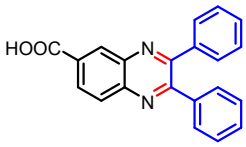
2-cyano-3-phenylquinoxaline 1,4-dioxide (4h)

Yellow solid; yield: 35%; (m.p.:203-205℃); **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.64-8.60 (m, 1H), 8.24-8.21 (m, 1H), 7.95-7.90 (m, 2H), 7.75-7.70 (m, 2H), 7.63-7.59 (m, 3H); **^{13}C NMR** (101 MHz, $CDCl_3$): δ 144.0, 142.7, 138.5, 133.2, 132.7, 131.9, 131.3, 130.8, 130.0, 129.0, 121.7, 119.4, 114.9; **HRMS**: m/z $[M + H]^+$ calcd for $C_{15}H_9N_3O_2$:264.0768 found: 264.0766.

2.4. Preparation of 2,3-diphenylquinoxaline-6-carboxylic acid (4i)

Ethyl 2,3-diphenylquinoxaline-6-carboxylate **3c-6** (106.2 mg, 0.3 mmol) and NaOH (24.0 mg, 0.6 mmol, 2.0 equiv.) were added to 90% ethanol aqueous solution (5 mL) solvent at room temperature. The reaction mixture was refluxed at 80℃ for 5 h. After the reaction, the mixture was cooled to room temperature and then acidified with 10% hydrochloric acid to pH=3, diluted with ethyl acetate, and extracted with ethyl acetate (25 mL × 3). The combined organic layer were washed with brine (5

mL), dried over Na_2SO_4 and concentrated in vacuo. Purify the residue to petroleum ether/ethyl acetate by column chromatography on silica gel. Compound **4i** (73.4 mg, 75%) was obtained as a white solid.



2,3-diphenylquinoxaline-6-carboxylic acid (4i)

White solid; yield: 75%; **^{1}H NMR** (400 MHz, DMSO-d_6): δ 13.46 (s, 1H), 8.66 (d, J = 1.6 Hz, 1H), 8.33-8.29 (m, 1H), 8.23 (d, J = 8.8 Hz, 1H), 7.50 (d, J = 7.2 Hz, 4H), 7.42-7.34 (m, 6H); **^{13}C NMR** (101 MHz, DMSO-d_6): δ 144.0, 142.7, 138.5, 133.2, 132.7, 131.9, 131.3, 130.8, 130.0, 129.0, 121.7, 119.4, 114.9; The spectroscopic properties of this compound were consistent with the data found in the literature[4].

3. General Experimental Procedure for Synthesis of Quinoxalines

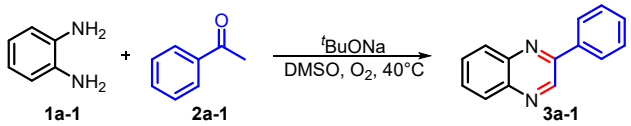
3.1. General Experimental Procedure

o-phenylenediamines **1a-1** (21.6 mg, 0.2 mmol) and ^{t}BuONa (67.3 mg, 0.7 mmol, 3.5 equiv.) were added to acetophenone (60.1 mg, 0.5 mmol, 2.5 equiv.) in dry DMSO (3.0 mL) solvent at room temperature under O_2 (1.0 atm) atmosphere. The reaction mixture was stirred at 40°C and monitored by TLC. After the complete consumption of **1**, the reaction mixture was cooled to room temperature and then quenched with water, diluted with ethyl acetate, and extracted with ethyl acetate (25 mL × 3). The combined organic phases were washed with brine (5 mL), dried over Na_2SO_4 and concentrated in vacuo. The residue was purified by neutral silica gel column chromatography. Compound **3a-1** (32.1 mg, 78%) was obtained as a white solid. Products **3a-1** to **3a-37, 3b-1** to **3b-5**, **3c-1** to **3c-5** were prepared by this

method.

3.2. Optimization of the Reaction Conditions

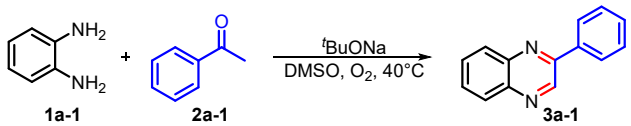
Table S1：Screening of alkali types



Entry[a]	Base (3.5 equiv.)	Yield%[b]
1	^{t}BuOK	59
2	CH_3OK	57
3	C_2H_5ONa	13
4	K_2CO_3	---.
5	NaOH	---
6	^{t}BuOLi	---.
7	**^{t}BuONa**	**78**

[a]Reaction conditions: **1a-1** (21.6 mg, 0.2 mmol), **2a-1** (60.1 mg, 0.5 mmol, 2.5 equiv.), Base (0.7 mmol, 3.5 equiv.) in DMSO (3 mL) and stirred for 1 h, 40°C, O_2 (1.0 atm); [b]Isolated yield.

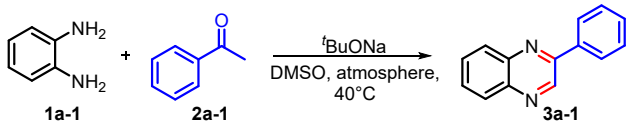
Table S2：Screening of reaction equivalent



Entry[a]	^{t}BuONa/equiv.	Acetophenone/equiv.	Yield/%[b]
1	0.5	1.0	27
2	1.0	1.0	47
3	1.5	1.0	50
4	2.0	1.0	59
5	2.5	1.0	56
6	3.0	1.0	59
7	3.5	1.0	64
8	4.0	1.0	58
9	3.5	1.5	66
10	3.5	2.0	71
11	**3.5**	**2.5**	**78**
12	3.5	3.0	77

[a]Reaction conditions: **1a-1** (21.6 mg, 0.2 mmol), **2a-1**, ^{t}BuONa in solvent (3 mL) and stirred for 1 h, 40°C, O_2 (1.0 atm); [b]Isolated yield.

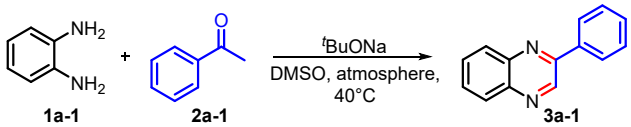
Table S3：Screening of reaction temperature



Entry[a]	T/°C	Yield%[b]
1	25	74
2	**40**	**78**
3	60	73
4	80	68

[a]Reaction conditions: **1a-1** (21.6 mg, 0.2 mmol), **2a-1** (60.1 mg, 0.5 mmol, 2.5 equiv.), ^{t}BuONa (67.3 mg, 0.7 mmol, 3.5 equiv.) in DMSO (3 mL) and stirred for 1 h, T°C, O_2 (1.0 atm); [b]Isolated yield.

Table S4：Screening of reaction atmosphere



Entry[a]	Atmosphere (1.0 atm)	Yield%[b]
1	Air	23
2	**O_2**	**78**
3	Ar	---.

[a]Reaction conditions: **1a-1** (21.6 mg, 0.2 mmol), **2a-1** (60.1 mg, 0.5 mmol, 2.5 equiv.), ^{t}BuONa (67.3 mg, 0.7 mmol, 3.5 equiv.) in DMSO (3 mL) and stirred for 1 h, 40°C, atmosphere (1.0 atm); [b]Isolated yield.

4. Gram-scale Synthesis

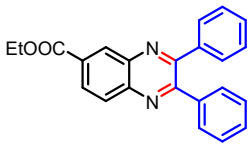
4.1. Gram-scale Synthesis of Compound 3b-5

o-phenylenediamines **1a-1** (1.32 g, 12.2 mmol) and 3-oxo-3-phenylpropanenitrile **2b-5** (4.42 g, 30.5 mmol, 2.5 equiv.) were added to ^{t}BuONa (4.10 g, 42.7 mmol, 3.5 equiv.) in dry DMSO (50.0 mL) solvent at room temperature in O_2 (1.0 atm) atmosphere. The reaction mixture was stirred at 40°C and monitored by TLC. After the complete consumption of **1a-1**, the reaction mixture was cooled to room temperature and then quenched with water, diluted with ethyl acetate, and extracted with ethyl acetate (100 mL × 3). The combined organic phases were washed with saturated NaCl aqueous solution, dried over Na_2SO_4 and concentrated in vacuo.

The residue was purified by neutral silica gel column chromatography. Compound **3b-5** (1.35 g, 48%) was obtained as a white solid.

4.2. Gram-scale Synthesis of Compound 3c-6

Ethyl 3,4-diaminobenzoate **1a-7** (1.08 g, 6.0 mmol) and 1,2-diphenylethan-1-one **2b-2** (2.35 g, 12.0 mmol, 2.0 equiv.) were added to ^{t}BuONa (2.01 g, 21.0 mmol, 3.5 equiv.) in dry DMSO (30.0 mL) solvent at room temperature in O_2 (1.0 atm) atmosphere. The reaction mixture was stirred at 60℃ while progress of the reaction was monitored by TLC. After the reaction, the flask was cooled to room temperature, The mixture was adjusted to pH=7 with 10% hydrochloric acid, diluted with ethyl acetate, and extracted with ethyl acetate (100 mL × 3) The combined organic phases were washed with saturated NaCl aqueous solution, dried over Na_2SO_4 and concentrated in vacuo. The residue was purified by neutral silica gel column chromatography. Compound **3c-6** (1.17 g, 55%) was obtained as a white solid.



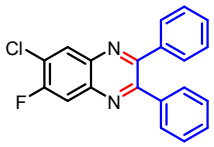
Ethyl 2,3-diphenylquinoxaline-6-carboxylate (3c-6)

White solid; yield: 55%; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.91 (d, J = 1.6 Hz, 1H), 8.39-8.35 (m, 1H), 8.21 (d, J = 8.4 Hz, 1H), 7.57-7.51 (m, 4H), 7.41-7.30 (m, 6H), 4.48 (q, J = 7.2 Hz, 2H), 1.46 (t, J = 7.2 Hz, 3H); **^{13}C NMR** (101 MHz, $CDCl_3$): δ 165.8, 155.0, 154.3, 143.1, 140.3, 138.6, 138.5, 131.7, 131.5, 129.8, 129.7, 129.5, 129.3, 129.2, 129.1, 128.3, 61.5, 14.3; The spectroscopic properties of this compound were consistent with the data found in the literature[5].

4.3. Gram-scale Synthesis of Compound 4j

4-chloro-5-fluorobenzene-1,2-diamine **1a-8** (1.12 g, 7.0 mmol) and 1,2-diphenylethan-1-one **2b-2** (2.74 g, 14.0 mmol, 2.0 equiv.) were added to ^{t}BuONa (2.35 g, 24.5 mmol, 3.5 equiv.) in dry DMSO (50.0 mL) solvent at room temperature

in O_2 (1.0 atm) atmosphere. The reaction mixture was stirred at 60℃ while progress of the reaction was monitored by TLC. After the reaction, the flask was cooled to room temperature, quenched with water, diluted with ethyl acetate, and extracted with ethyl acetate (100 mL × 3). The combined organic phases were washed with saturated NaCl aqueous solution, dried over Na_2SO_4 and concentrated in vacuo. The residue was purified by neutral silica gel column chromatography. Compound **4j** (1.21 g, 52%) was obtained as a white solid.



6-chloro-7-fluoro-2,3-diphenylquinoxaline (4j)

White solid; yield: 52%; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.07 (d, J = 7.6 Hz, 1H), 7.70 (d, J = 9.2 Hz, 1H), 7.38-7.34 (m, 4H), 7.23-7.16 (m, 6H); **^{13}C NMR** (101 MHz, $CDCl_3$): δ 157.9 (d, J = 253.0 Hz), 154.2, 153.5 (d, J = 3.0 Hz), 140.3 (d, J = 12.0 Hz), 138.3 (d, J = 2.0 Hz), 138.2 (d, J = 2.0 Hz), 130.2, 129.7 (d, J = 3.0 Hz), 129.0 (d, J = 9.0 Hz), 128.2, 113.6 (d, J = 22.0 Hz); The spectroscopic properties of this compound were consistent with the data found in the literature[6].

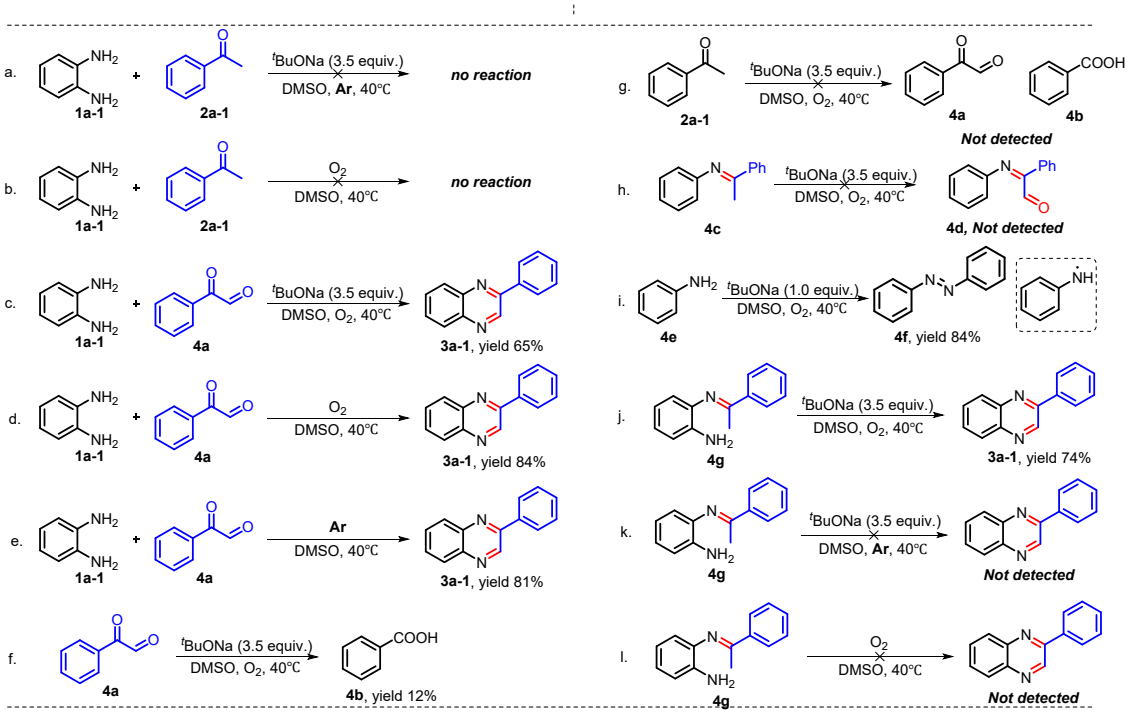
5. Mechanism Studies

5.1. Control experiments

To gain insight into the reaction mechanism, a series of control experiments were performed (Scheme S1). When there was no base in the reaction, no corresponding product was detected, indicating that the reaction was likely initiated by the nucleophilic attack of the -NH_2 on carbonyl group of **2a-1** under alkaline conditions (Scheme S1a). But it is worth noting that **2a-1** may be oxidized to 2-oxo-2-phenylacetaldehyde **4a** catalyzed by halogen (I_2, Br_2), thus undergoing nucleophilic attack of the adjacent amino groups of *o*-phenylenediamines **1a-1** on carbonyl groups of 2-oxo-2-phenylacetaldehyde **4a** to obtain the corresponding products[7]. Therefore,

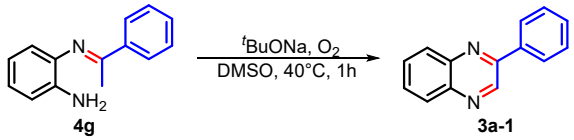
further studies were carried out to validate this possible reaction process. The reaction of 2-oxo-2-phenylacetaldehyde **4a** instead of **2a-1** was conducted, and **3a-1** was isolated in 65% yield (Scheme S1c). However, we observed that different from the standard reactions, neither O_2 nor base was essential for the reaction of 2-oxo-2-phenylacetaldehyde **4a** and **1a-1** (Scheme S1d, S1e). Furthermore, **2a-1** could not be oxidized to 2-oxo-2-phenylacetaldehyde under standard conditions (Scheme S1g). And there was no benzoic acid **4b**, the possible oxidation product of 2-oxo-2-phenylacetaldehyde **4a** under standard conditions (Scheme S1f), was detected even after further acidification. This was an indication that 2-oxo-2-phenylacetaldehyde **4a** was not an intermediate in the reaction. Hence, the possibility of this mechanism was eliminated by the above experimental results. Scheme 1h excluded the possibility of oxidation of imine to imino aldehyde. Surprisingly, aniline **4e** could form 1,2-diphenyldiazene **4f** in good yield under standard conditions, which could suggest that nitrogenous radicals could be generated under standard conditions (Scheme S1i)[8].

Combining the results of control experiments, we believe that the reaction starts with a nucleophilic attack of the $-NH_2$, followed by dehydration under alkaline conditions to give the intermediate (*E*)-2-((1-phenylethylidene)amino)aniline **4g**. To justify this mechanism, **4g** were carried out under standard conditions. Satisfactorily, **3a-1** was successfully acquired in 74% yield (Scheme S1j), with both the base and O_2 being required for the conversion process, indicating that the possible involvement of a radical process in this transformation of intermediate **4g** to product **3a-1** (Scheme S1k, S1l).

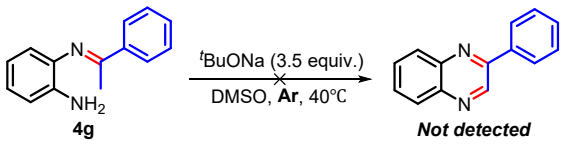


Scheme S1. Control experiments

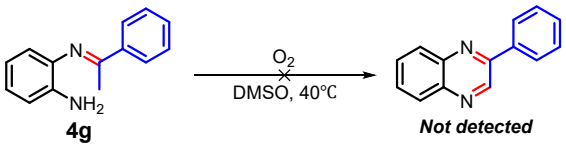
5.2. Reaction of 2-((1-phenylethylidene)amino)aniline (4g).



2-((1-phenylethylidene)amino)aniline **4g** (42.0 mg, 0.2 mmol) and ^{t}BuONa (67.3 mg, 0.7 mmol, 3.5 equiv.) were added to dry DMSO (3 mL) solvent at room temperature under O_2 (1.0 atm) atmosphere. The mixture was stirred for 1h while progress of the reaction was monitored by TLC. After the complete consumption of **4g**, the reaction mixture was cooled to room temperature and then quenched with water, diluted with ethyl acetate, and extracted with ethyl acetate (25 mL × 3). The combined organic phases were washed with brine (5 mL), dried over Na_2SO_4 and concentrated in vacuo. Purification of the residue by neutral silica gel column chromatography afforded the desired Compound **3a-1** (30.5 mg, 74%) was obtained as a white solid.

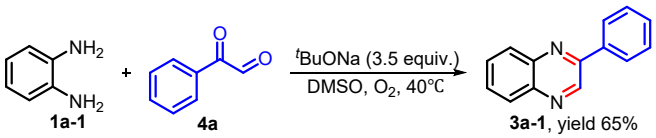


2-((1-phenylethylidene)amino)aniline **4g** (42.0 mg, 0.2 mmol) and ^{t}BuONa (67.3 mg, 0.7 mmol, 3.5 equiv.) were added to dry DMSO (3 mL) solvent at room temperature under Ar atmosphere. The reaction mixture was stirred at 40℃ for 1h and monitored by TLC. Then the reaction mixture was cooled to room temperature and then quenched with water, and extracted with ethyl acetate (25 mL × 3). The combined organic phases were washed with brine (5 mL), dried over Na_2SO_4 and concentrated in vacuo. No corresponding product was detected by TLC, NMR and HRMS.



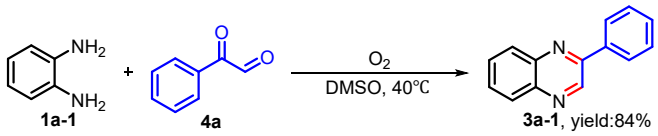
2-((1-phenylethylidene)amino)aniline **4g** (42.0 mg, 0.2 mmol) were added to dry DMSO (3 mL) solvent at room temperature under O_2 (1.0 atm) atmosphere. The reaction mixture was stirred at 40℃ for 1h and monitored by TLC. Then the reaction mixture was cooled to room temperature and then quenched with water, and extracted with ethyl acetate (25 mL × 3). The combined organic phases were washed with brine (5 mL), dried over Na_2SO_4 and concentrated in vacuo. No corresponding product was detected by TLC, NMR and HRMS.

5.3. Reaction of 2-oxo-2-phenylacetaldehyde (4a) with *o*-phenylenediamines (1a-1).

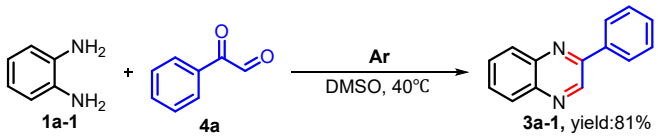


o-phenylenediamines **1a-1** (22.0 mg, 0.2 mmol), 2-oxo-2-phenylacetaldehyde **4a** (67.0 mg, 0.5 mmol, 2.5 equiv.) and ^{t}BuONa (67.3 mg, 0.7 mmol, 3.5 equiv.) were

added to dry DMSO (3.0 mL) solvent at room temperature under O_2 (1.0 atm) atmosphere. The reaction mixture was stirred at 40℃ for 1h and monitored by TLC. After the complete consumption of **1a-1**, the reaction mixture was cooled to room temperature and then quenched with water, and extracted with ethyl acetate (25 mL × 3). The combined organic phases were washed with brine (5 mL), dried over Na_2SO_4 and concentrated in vacuo. The residue was purified by neutral silica gel column chromatography. Product **3a-1** (26.7 mg, 65%) was obtained as a white solid.



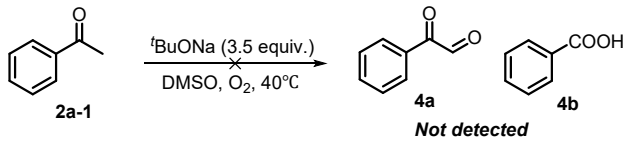
o-phenylenediamines **1a-1** (22.0 mg, 0.2 mmol) and 2-oxo-2-phenylacetaldehyde **4a** (67.0 mg, 0.5 mmol, 2.5 equiv.) were added to dry DMSO (3 mL) solvent at room temperature under O_2 (1.0 atm) atmosphere. The reaction mixture was stirred at 40℃ for 1h and monitored by TLC. After the complete consumption of **1a-1**, the reaction mixture was cooled to room temperature and then quenched with water, and extracted with ethyl acetate (25 mL × 3). The combined organic phases were washed with brine (5 mL), dried over Na_2SO_4 and concentrated in vacuo. The residue was purified by neutral silica gel column chromatography. Product **3a-1** (26.7 mg, 84%) was obtained as a white solid.



o-phenylenediamines **1a-1** (22.0 mg, 0.2 mmol) and 2-oxo-2-phenylacetaldehyde **4a** (67.0 mg, 0.5 mmol, 2.5 equiv.) were added to dry DMSO (3 mL) solvent at room temperature under Ar atmosphere. The reaction mixture was stirred at 40℃ for 1h and monitored by TLC. After the complete consumption of **1a-1**, the reaction mixture was cooled to room temperature and then quenched with water, and extracted with ethyl acetate (25 mL × 3). The combined organic phases were washed with brine (5 mL), dried over Na_2SO_4 and concentrated in vacuo. The residue was purified by neutral

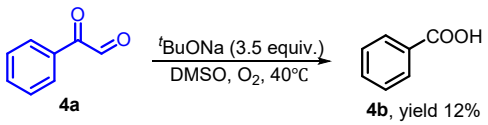
silica gel column chromatography. Product **3a-1** (26.7 mg, 81%) was obtained as a white solid.

5.4. Reaction of acetophenone (2a-1) under standard conditions.



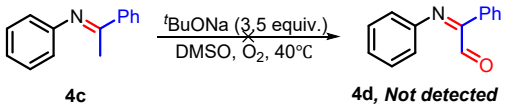
Acetophenone **2a-1** (67.0 mg, 0.5 mmol, 2.5 equiv.) and ^{t}BuONa (67.3 mg, 0.7 mmol, 3.5 equiv.) were added to dry DMSO (3.0 mL) solvent at room temperature under Ar atmosphere. The reaction mixture was stirred at 40℃ for 1h. Then the reaction mixture was cooled to room temperature and then quenched with water, and adjusted to pH=2~3 with 20% hydrochloric acid, extracted with ethyl acetate (25 mL × 3). The combined organic phases were washed with brine (5 mL), dried over Na_2SO_4 and concentrated in vacuo. No corresponding product 2-oxo-2-phenylacetaldehyde **4a** and benzoic acid **4b** was detected by TLC, NMR and HRMS.

5.5. Reaction of 2-oxo-2-phenylacetaldehyde (4a) under standard conditions.



2-oxo-2-phenylacetaldehyde **4a** (80.4 mg, 0.6 mmol) and ^{t}BuONa (67.3 mg, 0.7 mmol) were added to dry DMSO (3 mL) solvent at room temperature under O_2 (1.0 atm) atmosphere. The mixture was stirred for 1h at 40℃. Then the reaction mixture was cooled to room temperature, quenched with water, and adjusted to pH=2~3 with 20% hydrochloric acid, extracted with ethyl acetate (25 mL × 3). The combined organic phases were washed with brine (5 mL), dried over Na_2SO_4 and concentrated in vacuo. Benzoic acid **4b** (yield: 12%) was detected by NMR and HRMS. Yield determined by integration of the ^{1}H NMR spectrum.

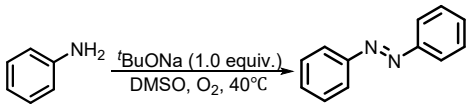
5.6. Reaction of *N*,1-diphenylethan-1-imine (4c) under standard conditions.



4c **4d, *Not detected***

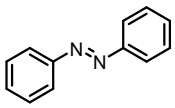
N,1-diphenylethan-1-imine **4c** (45.0 mg, 0.2 mmol) and ^{t}BuONa (67.3 mg, 0.7 mmol) were added to dry DMSO (3 mL) solvent at room temperature under O_2 (1.0 atm) atmosphere. The mixture was stirred for 1h at 40℃. Then the reaction mixture was cooled to room temperature, quenched with water, and extracted with ethyl acetate (25 mL × 3). The combined organic phases were washed with brine (5 mL), dried over Na_2SO_4 and concentrated in vacuo. No corresponding product 2-phenyl-2-(phenylimino)acetaldehyde **4d** was detected by TLC, NMR and HRMS.

5.7. Reaction of aniline (4e).



4e **4f**, yield 84%

Aniline **4e** (18.6 mg, 0.2 mmol) and ^{t}BuONa (19.2 mg, 0.2 mmol, 1.0 equiv.) were added to dry DMSO (2 mL) solvent at room temperature under O_2 atmosphere. The reaction mixture was stirred at 40℃ for 1h and monitored by TLC. After the complete consumption of aniline, the reaction mixture was cooled to room temperature and then quenched with water, and extracted with ethyl acetate (25 mL × 3). The combined organic phases were washed with brine (5 mL), dried over Na_2SO_4 and concentrated in vacuo. The residue was purified by neutral silica gel column chromatography. Product **4f** (15.3 mg, 84%) was obtained as a yellow solid.



1,2-diphenyldiazene (4f)

Yellow solid; yield: 84%; (m.p.: 65-67℃); **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.99-7.94 (m, 4H), 7.58-7.49 (m, 6H); **^{13}C NMR** (101 MHz, $CDCl_3$): δ 152.7, 131.0, 129.1, 122.8;

5.8. EPR experiments

In order to verify the reaction mechanism of this reaction, we conducted Electron Paramagnetic Resonance (EPR**)** experiments under standard conditions. Experimental details: 298 K, O_2 atmosphere, frequency 9.8660 GHz, microwave power 1 mW.

o-phenylenediamines **1a-1** (21.6 mg, 0.2 mmol) and ^{t}BuONa (67.3 mg, 0.7 mmol, 3.5 equiv.) were added to dry DMSO (3.0 mL) solvent at room temperature under O_2 atmosphere. The reaction mixture was stirred at 40℃ for 10 min, and samples were taken for testing. Under the standard conditions, a strong EPR signal was observed for *o*-phenylenediamine **1a-1** (g value = 2.0034 after fitting), implying the formation of a radical species. The radical signal obtained representing probably a nitrogen radical[9].

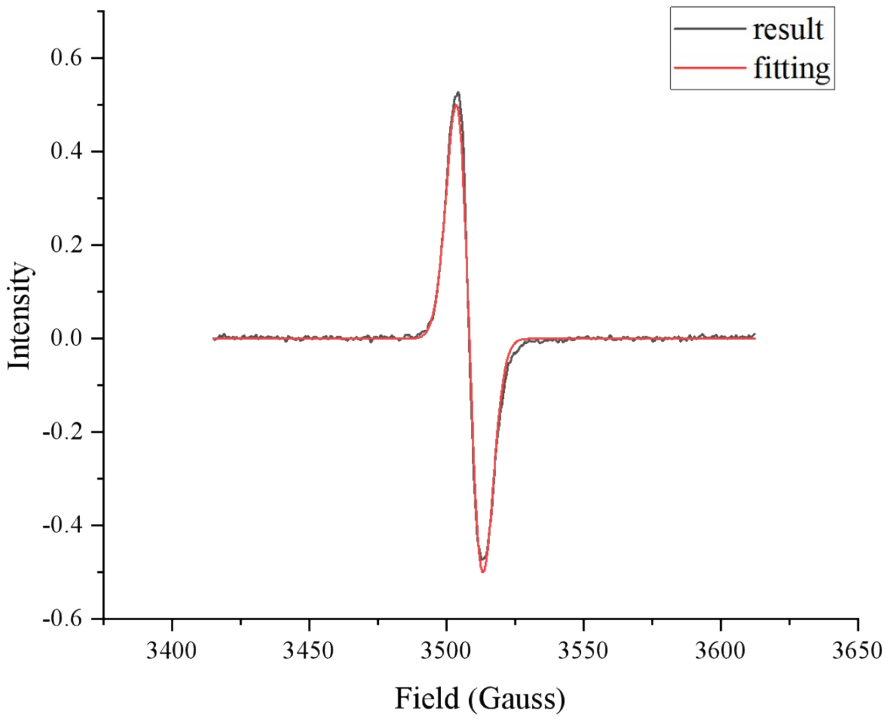


Fig S1. *o*-phenylenediamine **1a-1** (21.6 mg, 0.2 mmol), ^{t}BuONa (67.2 mg, 0.7 mmol, 3.5 equiv.), DMSO (3 mL), O_2 (1.0 atm), 40℃, reaction for 10 min.

5.9. Cyclic voltammetry measurement

Electrochemical experiments were carried out using a PalmSens4

Potentiostat/Galvanostat/Impedance Analyzer. Electrochemical experiments were performed at room temperature (25℃) under argon. Measurements employed a radium glassy carbon working electrode, platinum wire counter electrode, saturated KCl silver-silver chloride reference electrode. Samples were prepared with 0.01 mmol of aniline **4e**, 0.01 mmol of **4c** in 10 mL of 0.1 M tetrabutylammonium tetrafluoroborate in anhydrous acetonitrile. The blank samples were 10 ml of 0.1 M tetrabutylammonium tetrafluoroborate in anhydrous acetonitrile. The obtained value was referenced to Ag/AgCl. The scan rate was 100 mV/s.

During subsequent cyclic voltammetry (CV) measurements, the oxidation potentials of aniline (*Eox* = 1.27 V vs.Ag/AgCl) and *N*,1-diphenylethan-1-imine **4c** (*Eox* = 0.83 V vs. Ag/AgCl) were studied, which revealed both α-imino radicals and aniline radicals could be obtained under standard conditions.

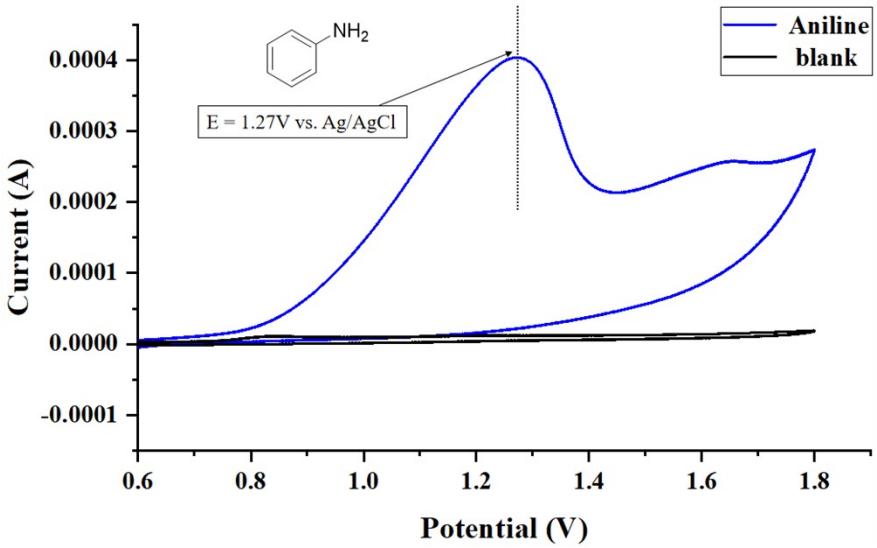


Fig S2. Cyclic voltammograms of Aniline **4e** (10 mM) in acetonitrile (MeCN) containing 0.1 M nBu$_4$NBF$_4$ as the electrolyte.

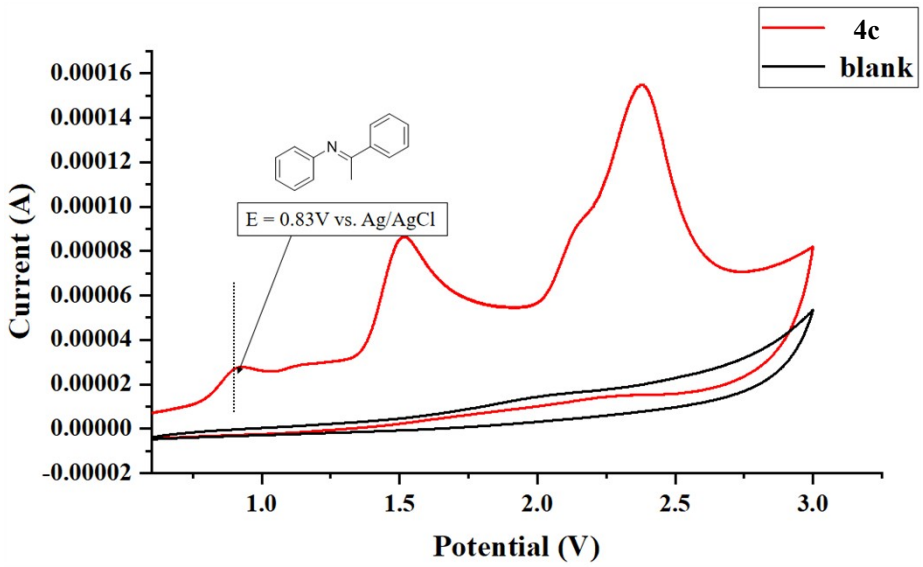


Fig S3. Cyclic voltammograms of **4c** (10 mM) in acetonitrile (MeCN) containing 0.1 M nBu$_4$NBF$_4$ as the electrolyte.

6. Theoretical Calculations

6.1. Computational Details

Geometry optimizations of all reactants, intermediates, transition states and products were carried out using Gaussian 16 C.01 software package[10] at B3LYP[11,12]-D3[13](BJ[14-16])/Def2-SVP[17]/SMD[18](DMSO) level of theory. Vibrational frequency calculations were carried out at the same level of theory to verify that each transition state structure has only one imaginary frequency, and the other structures have no imaginary frequency. Intrinsic reaction coordinate[19, 20] (IRC) calculations were also performed to verify each transition state connected to corresponding reactant and product. Spin densities of all radicals and triplet state molecules were analyzed using Multiwfn 3.8 (dev) software[21] to investigate the radical distributions. Optimized structures were drawn using CYLview software[22]。

DFT calculations were done to understand the reaction mechanism further. Intermediate **4g** has a calculated Gibbs free energy of 9.3 kcal/mol. Due to the formation of dimsyl radicals in the ^{t}BuONa/DMSO/O_2 system, intermediate **4g** tends to experience N-H bond cleavage to produce the nitrogen radical intermediate **A** of -4.0 kcal/mol via the transition state **TS1** of 17.0 kcal/mol through Hydrogen Atom

Transfer (HAT). A similar HAT process subsequently occurred in the α-C of imine, forming the triplet state specie **B(T^1)** of -14.0 kcal/mol via transition state **TS2** of 6.4 kcal/mol. The Π3 3 system in **B(T^1)** can be easily attacked by the lone-pair electron on nitrogen to produce another triplet state species **C(T^1)** of -35.5 kcal/mol through transition state **TS3** of 0.5 kcal/mol. **C(T1)** then transitioned to intermediate **C** of -74.0 kcal/mol.

6.2. Reaction Potential Energy Surface and Spin Density Calculations

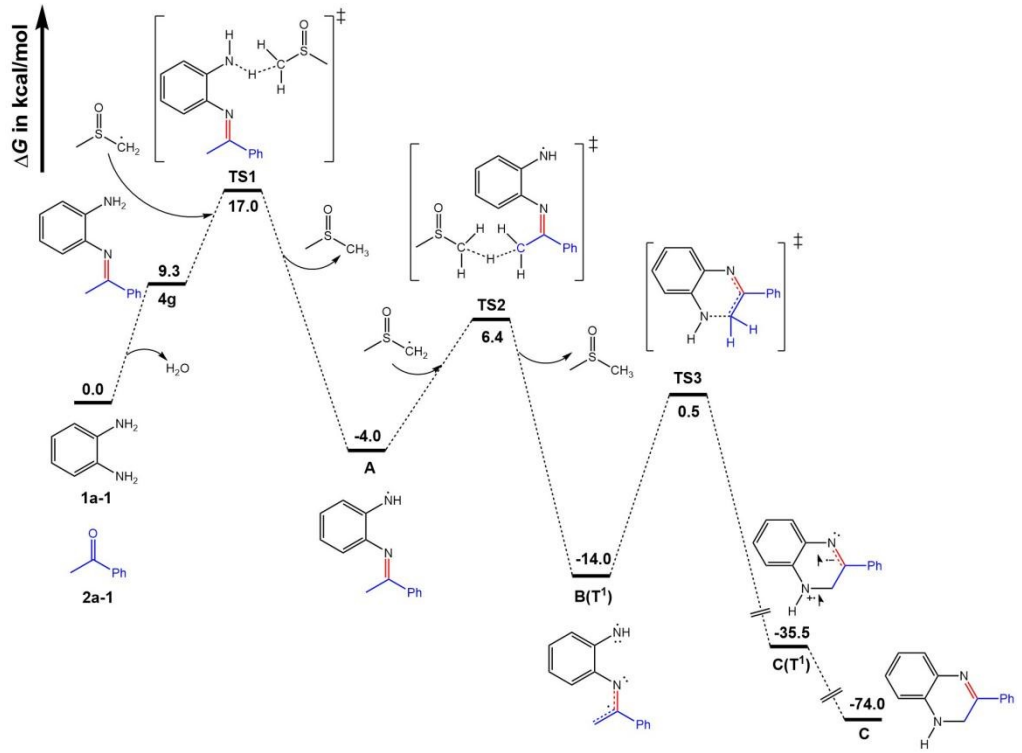


Fig. S4. Potential energy surface of proposed reaction mechanism. The Gibbs free energies of **1a-1**, **2a-1**, **H_2O** and **DMSO-radical** were set to 0.0 kcal/mol as references.

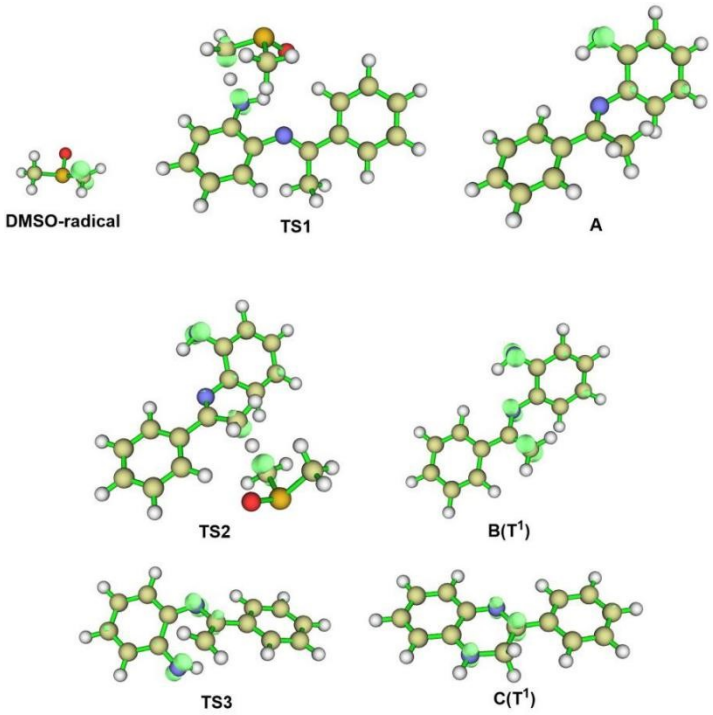


Fig. S5. Spin densities of all radicals and triplet state molecules. Green and blue clouds represent for alpha- and beta-electron distribution, respectively. Isovalues were set to 0.03 a.u..

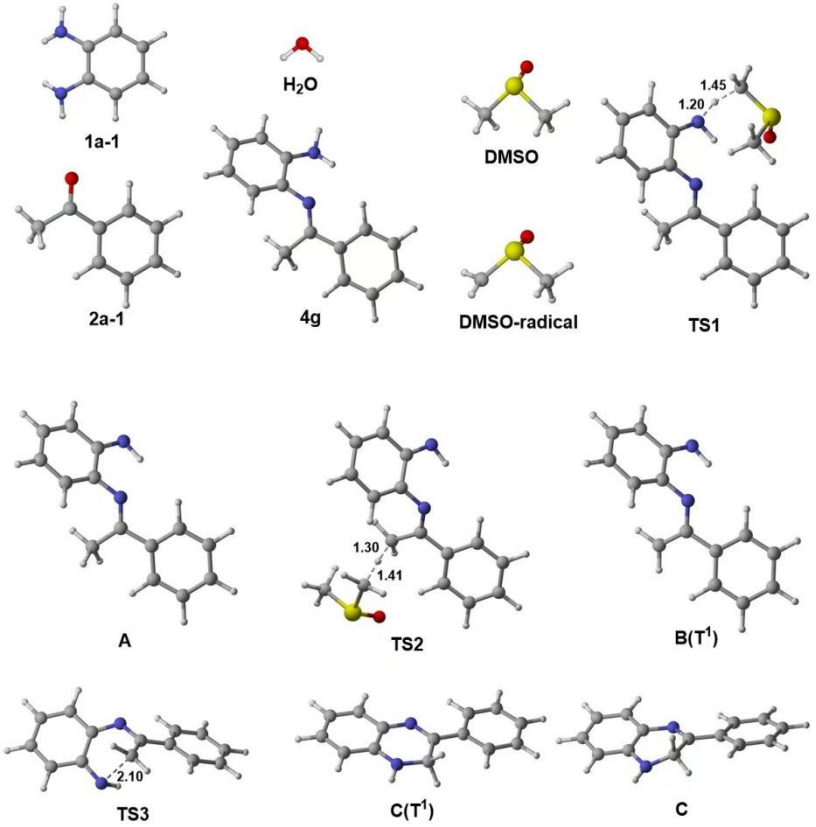


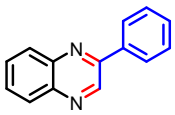
Fig. S6. Optimized structures of all reactants, intermediates, transition states and products. Some inter- and intramolecular interactions were omitted for clarity. Distances are in Å.

6.3. Calculated Original Data

Table S5. Calculated Gibbs free energies (in a.u.) of all optimized structures, and imaginary frequency (v_i, in cm^{-1}) of each transition state structure.

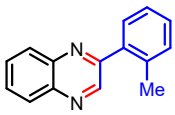
optimized structure	Gibbs free energy	v_i
DMSO	-552.928947	
DMSO-radical	-552.268732	
1a-1	-342.654136	
2a-1	-384.553332	
H_2O	-76.362593	
4g	-650.830037	
TS1	-1203.086468	-1644.7
A	-650.191040	
TS2	-1202.443156	-1595.1
B(T^1)	-649.546714	
TS3	-649.523719	-460.8
C(T^1)	-649.581007	
C	-649.642292	

7. Characterization Data



2-Phenylquinoxaline (3a-1)

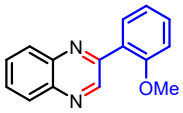
White solid; yield: 78%; (m.p.: 68-70°C); **^{1}H NMR** (400 MHz, $CDCl_3$): δ 9.28 (s, 1H), 8.18-8.06 (m, 4H), 7.75-7.65 (m, 2H), 7.55-7.45 (m, 3H); **^{13}C NMR** (101 MHz, $CDCl_3$): δ 151.5, 143.1, 142.0, 141.3, 136.5, 130.0, 129.9, 129.4, 129.3, 129.0, 128.9, 127.3; **HRMS**: m/z $[M + H]^+$ calcd for $C_{14}H_{10}N_2$: 207.0917; found: 207.0925.



2-(*o*-tolyl)quinoxaline (3a-2)

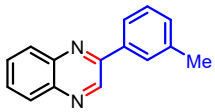
White solid; yield: 67%; (m.p.: 78-80°C); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 9.01 (s, 1H), 8.19-8.14 (m, 2H), 7.84-7.77 (m, 2H), 7.58-7.53 (m, 1H), 7.43- 7.34 (m, 4H), 2.48 (s, 3H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 155.0, 145.9, 142.0, 140.1, 137.1, 136.6, 131.2, 130.3, 130.0, 129.8, 129.5, 129.4, 129.1, 126.3, 20.3; **HRMS**: *m/z* $[M + H]^+$ calcd for

$C_{15}H_{12}N_2$: 221.1073 found: 221.1076.



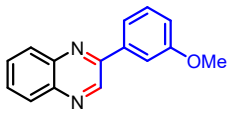
2-(2-methoxyphenyl)quinoxaline (3a-3)

Yellow solid; yield: 64%; (m.p.: 100-102℃) ; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 9.34 (s, 1H), 8.17-8.11 (m, 2H), 7.90 (dd, J = 1.6 ,0.4 Hz, 1H), 7.78-7.71 (m, 2H), 7.50-7.44 (m, 1H), 7.16 (t, J = 7.4 Hz, 1H), 7.05 (d, J = 8.4 Hz, 1H), 3.89 (s, 3H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 157.3, 152.1, 147.2, 142.6, 140.9, 131.5, 131.4, 129.7, 129.4, 129.3, 128.9, 126.4, 121.4, 111.3, 55.5; **HRMS**: *m/z* $[M + H]^+$ calcd for $C_{15}H_{12}N_2O$: 237.1022 found: 237.1024.



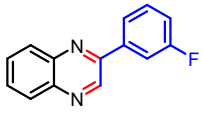
2-(m-tolyl)quinoxaline (3a-4)

Yellow liquid; yield: 67%; (m.p.: 86-88 ℃); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 9.30 (s, 1H), 8.17-8.08 (m, 2H), 8.01 (s, 1H), 7.95 (d, J = 7.6 Hz, 1H), 7.78-7.69 (m, 2H), 7.43 (t, J = 7.6 Hz, 1H), 7.31 (d, J =7.6 Hz, 1H), 2.48 (s, 3H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 151.9, 143.4, 142.1, 141.4, 138.8, 136.6, 130.9, 130.1, 129.4, 129.3, 129.0, 128.9, 128.1, 124.6, 21.5. **HRMS**: *m/z* $[M + H]^+$ calcd for $C_{15}H_{12}N_2$: 221.1073 found: 221.1076.



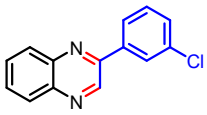
2-(3-methoxyphenyl)quinoxaline (3a-5)

White solid; yield: 73%; (m.p.: 85-87℃); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 9.30 (s, 1H), 8.13 (dd, J = 15.8, 8.2 Hz, 2H), 7.80-7.71 (m, 4H), 7.46 (t, J = 7.8 Hz, 1H), 7.06 (d, J = 8.0 Hz, 1H), 3.93 (s, 3H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 160.2, 151.5, 143.4, 142.2, 141.6, 138.1, 130.2, 130.1, 129.6, 129.5, 129.0, 119.8, 116.1, 112.6, 55.4; **HRMS**: m/z [M + H]+ calcd for $C_{15}H_{12}N_2O$: 237.1022 found: 237.1025.



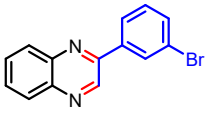
2-(3-fluorophenyl)quinoxaline (3a-6)

White solid; yield: 71%; (m.p.: 103-105°C); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 9.22 (s, 1H), 8.06 (t, J = 8.6 Hz, 2H), 7.88 (d, J = 7.6 Hz, 2H), 7.74-7.66 (m, 2H), 7.47-7.42 (m, 1H), 7.13 (t, J = 8.0 Hz, 1H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 164.6, 162.1, 158.7, 150.3 (d, J = 2.0 Hz), 142.9, 142.1, 138.9 (d, J = 8.0 Hz), 130.7 (d, J = 8.0 Hz), 130.5, 129.9, 129.6 (d, J = 50.0 Hz), 123.0 (d, J = 2.0 Hz), 117.2 (d, J = 22.0 Hz), 114.6 (d, J = 22.0 Hz); **HRMS**: *m/z* $[M + H]^+$ calcd for $C_{14}H_9FN_2$: 225.0823 found: 225.0825.



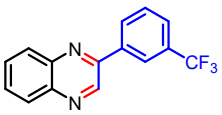
2-(3-chlorophenyl)quinoxaline (3a-7)

White solid; yield: 68%; (m.p.: 109-111°C); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 9.28 (s, 1H), 8.21 (s, 1H), 8.13 (t, J = 8.4 Hz, 2H), 8.04 (t, J = 4.2 Hz, 1H), 7.82-7.73 (m, 2H), 7.48 (d, J = 4.4 Hz, 2H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 150.2, 142.9, 142.1, 141.7, 138.4, 135.3, 130.5, 130.3, 130.1, 129.9, 129.6, 129.1, 127.6, 125.4; **HRMS**: *m/z* $[M + H]^+$ calcd for $C_{14}H_9ClN_2$: 241.0527 found: 241.0528.



2-(3-bromophenyl)quinoxaline (3a-8)

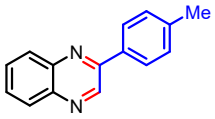
White solid; yield: 72%; (m.p.: 120-122°C); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 9.27 (s, 1H), 8.37 (s, 1H), 8.16-8.06 (m, 3H), 7.82-7.73 (m, 2H), 7.63 (d, J = 7.6 Hz, 1H), 7.42 (t, J = 7.8 Hz, 1H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 158.7, 150.1, 142.8, 142.1, 141.7, 138.6, 133.0, 130.5, 130.1 129.9, 129.6, 129.1, 125.9, 123.4; **HRMS**: *m/z* $[M + H]^+$ calcd for $C_{14}H_9BrN_2$: 285.0022 found: 285.0020.



2-(3-(trifluoromethyl)phenyl)quinoxaline (3a-9)

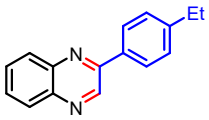
White solid; yield: 50%; (m.p.: 105-107°C); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 9.34 (s, 1H), 8.50 (s, 1H), 8.37 (d, J = 7.6 Hz, 1H), 8.19-8.11 (m, 2H), 7.84-7.76 (m, 3H), 7.69 (t, J = 7.8 Hz, 1H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 150.1, 142.8, 142.1 (d, J = 30.0 Hz), 137.5, 131.8 (d, J = 33.0 Hz), 130.6, 130.5 (d, J = 1.0 Hz), 130.1, 129.7, 129.6, 129.2, 126.7 (q, J = 4.0 Hz), 125.3, 124.4 (q, J = 4.0 Hz), 122.6; **HRMS**: *m/z*

$[M + H]^+$ calcd for $C_{15}H_9F_3N_2$: 275.0791 found: 275.0788.



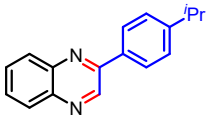
2-(*p*-tolyl)quinoxaline (3a-10)

White solid; yield: 67%; (m.p.: 83-85°C); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 9.30 (s, 1H), 8.16-8.05 (m, 4H), 7.81-7.67 (m, 2H), 7.35 (d, J = 7.6 Hz, 2H), 2.44 (s, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 151.8, 143.2, 142.2, 141.3, 140.4, 133.9, 130.1, 129.8, 129.5, 129.2, 129.0, 127.4, 21.4; **HRMS**: *m/z* $[M + H]^+$ calcd for $C_{15}H_{12}N_2$: 221.1073; found: 221.1076.



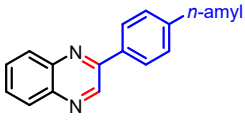
2-(4-ethylphenyl)quinoxaline (3a-11)

Yellow solid; yield: 64%; (m.p.: 60-62°C); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 9.30 (s, 1H), 8.15-8.08 (m, 4H), 7.78-7.68 (m, 2H), 7.38 (d, J = 8.0 Hz, 2H), 2.73 (q, J =7.6 Hz, 2H), 1.29 (t, J = 7.6 Hz, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 151.8, 146.7, 143.2, 142.2, 141.3, 134.1, 130.1, 129.5, 129.2, 129.0, 128.6, 127.5, 28.7, 15.4; **HRMS**: *m/z* $[M + H]^+$ calcd for $C_{16}H_{14}N_2$: 235.1230; found: 235.1231.



2-(4-isopropylphenyl)quinoxaline (3a-12)

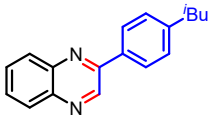
Yellow liquid; yield: 76%; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 9.30 (s, 1H), 8.16-8.08 (m, 4H), 7.77-7.68 (m, 2H), 7.41 (d, J = 8.0 Hz, 2H), 3.04-2.94 (m, 1H), 1.31 (d, J = 7.2 Hz, 6H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 151.8, 151.2, 143.2, 142.2, 141.3, 134.3, 130.1, 129.4, 129.2, 129.0, 127.5, 127.2, 34.0, 23.8; **HRMS**: *m/z* [M + H]+ calcd for $C_{17}H_{16}N_2$: 249.1386 found: 249.1384.



2-(4-pentylphenyl)quinoxaline (3a-13)

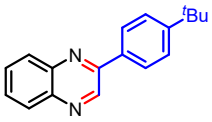
Yellow liqiud; yield: 72%; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 9.31 (s, 1H), 8.17-8.08 (m , 4H), 7.79-7.69 (m, 2H), 7.37 (d, J = 8.0 Hz, 2H), 2.69 (t, J = 7.8 Hz, 2H), 1.71-1.63

(m, 2H), 1.39-1.31 (m, 4H), 0.90 (t, J = 6.6 Hz, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 151.9, 145.5, 143.3, 142.3, 141.3, 134.1, 130.2, 129.5,129.3 129.2, 129.0, 127.4, 35.7, 31.4, 31.0, 22.5, 14.0; **HRMS**: *m/z* $[M + H]^+$ calcd for $C_{19}H_{20}N_2$: 277.1699 found: 277.1702.



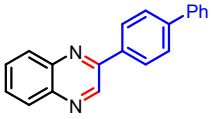
2-(4-isobutylphenyl)quinoxaline (3a-14)

Yellow liquid; yield: 71%; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 9.32 (s, 1H), 8.17-8.06 (m, 4H), 7.81-7.68 (m, 2H), 7.34 (d, J = 8.0 Hz, 2H), 2.57 (d, J = 7.2 Hz, 2H), 1.97-1.90 (m, 1H), 0.94 (d, J = 6.4 Hz, 6H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 151.9, 144.2, 143.4, 142.3, 141.4, 134.2, 130.2, 129.9, 129.5, 129.3, 129.0, 127.3, 45.2, 30.2, 22.3; **HRMS**: *m/z* $[M + H]^+$ calcd for $C_{18}H_{18}N_2$: 263.1543 found: 263.1545.



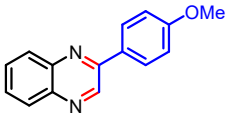
2-(4-(tert-butyl)phenyl)quinoxaline (3a-15)

Yellow liquid; yield: 70%; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 9.32 (s, 1H), 8.18-8.08 (m, 4H), 7.80-7.68 (m, 2H), 7.59 (d, J = 8.4 Hz, 2H), 1.39 (s, 9H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 153.6, 151.8, 143.3, 142.3, 141.4, 133.9, 130.1, 129.5, 129.3, 129.0, 127.3, 126.1, 34.8, 31.2; **HRMS**: *m/z* $[M + H]^+$ calcd for $C_{18}H_{18}N_2$: 263.1543 found: 263.1545.



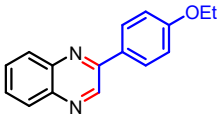
2-([1,1'-biphenyl]-4-yl)quinoxaline (3a-16)

White solid; yield: 79%; (m.p.: 157-159°C); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 9.38 (s, 1H), 8.29 (d, J = 8.4 Hz, 2H), 8.15 (dd, J = 15.2, 8.0 Hz, 2H), 7.83-7.73 (m, 4H), 7.69 (d, J = 8.8 Hz, 2H), 7.49 (t, J = 7.6 Hz, 2H), 7.41 (t, J = 7.4 Hz, 1H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 151.4, 143.2, 142.9, 142.3, 141.5, 140.1, 135.5, 130.3, 129.6, 129.5, 129.1, 128.9, 127.9, 127.8, 127,7, 127.1; **HRMS**: *m/z* $[M + H]^+$ calcd for $C_{20}H_{14}N_2$: 283.1230 found: 283.1233.



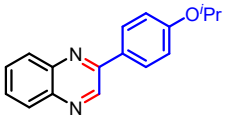
2-(4-methoxyphenyl)quinoxaline (3a-17)

Yellow solid; yield: 85%; (m.p.: 91-93°C); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 9.27 (s, 1H), 8.15 (d, J = 8.8 Hz, 2H), 8.09 (t, J = 8.8 Hz, 2H), 7.77-7.66 (m, 1H), 7.06 (d, J = 8.4 Hz, 2H), 3.87 (s, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 161.3, 151.3, 143.0, 142.2, 141.1, 130.1, 129.3, 129.2, 129.0, 128.9, 114.5, 55.4; **HRMS**: *m/z* $[M + H]^+$ calcd for $C_{15}H_{12}N_2O$: 237.1022; found: 237.1025.



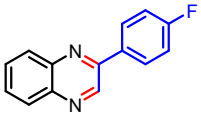
2-(4-ethoxyphenyl)quinoxaline (3a-18)

Yellow solid; yield: 86%; (m.p.: 115-117°C); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 9.27 (s, 1H), 8.15 (d, J = 8.8 Hz, 2H), 8.08 (t, J = 8.4 Hz, 2H), 7.77-7.66 (m, 2H), 7.04 (d, J = 8.4 Hz, 2H), 4.10 (q, J = 6.8 Hz, 2H), 1.45 (t, J = 7.0 Hz, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 160.8, 151.4, 143.0, 142.2, 141.1, 130.1, 129.3, 129.0, 128.9, 128.8, 115.0, 63.6, 14.7; **HRMS**: *m/z* $[M + H]^+$ calcd for $C_{16}H_{14}N_2O$: 251.1179 found: 251.1180.



2-(4-isopropoxyphenyl)quinoxaline (3a-19)

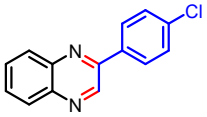
Yellow solid; yield: 79%; (m.p.: 85-87°C); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 9.28 (s, 1H), 8.18-8.05 (m, 4H), 7.78-7.66 (m, 2H), 7.04 (d, J = 8.4 Hz, 2H), 4.70-4.61 (m, 1H), 1.38 (d, J = 6.0 Hz, 6H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 159.8, 151.4, 143.0, 142.2, 141.1, 130.1, 129.3, 129.0, 128.9, 128.8, 128.8, 116.2, 69.9, 21.9; **HRMS**: *m/z* $[M + H]^+$ calcd for $C_{17}H_{16}N_2O$: 265.1335 found: 265.1339.



2-(4-fluorophenyl)quinoxaline (3a-20)

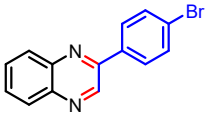
White solid; yield: 70%; (m.p.: 115-117°C); **^{1}H NMR** (400 MHz, $CDCl_3$): δ 9.27 (s, 1H), 8.18 (q, J = 5.6 Hz, 2H), 8.11 (t, J = 7.2 Hz , 2H), 7.80-7.71 (m, 2H), 7.24 (t，J = 8.4 Hz, 2H); **^{13}C NMR** (101 MHz, $CDCl_3$): δ 165.4, 162.9, 150.7, 142.9, 142.1 (d, J

= 70.0 Hz), 132.9 (d, *J* = 3.0 Hz), 130.4, 129.6, 129.5 (d, *J* = 3.0 Hz), 129.4, 129.1, 116.3 (d, *J* = 22.0 Hz) ; **HRMS**: *m/z* $[M + H]^+$ calcd for $C_{14}H_9FN_2$: 225.0823; found: 225.0824.



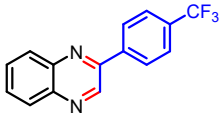
2-(4-chlorophenyl)quinoxaline (3a-21)

Yellow solid; yield: 71%; (m.p.: 125-127°C); **^{1}H NMR** (400 MHz, $CDCl_3$): *δ* 9.29 (s, 1H), 8.17-8.09 (m, 4H), 7.81-7.73 (m, 2H), 7.53 (d, *J* = 8.4 Hz, 2H); **^{13}C NMR** (101 MHz, $CDCl_3$): *δ* 150.5, 142.8, 142.2, 141.6, 136.5, 135.1, 130.4, 129.8, 129.5, 129.4, 129.1, 128.7; **HRMS**: *m/z* $[M + H]^+$ calcd for $C_{14}H_9ClN_2$: 241.0527; found: 241.0528.



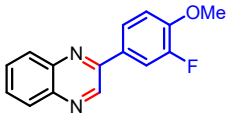
2-(4-bromophenyl)quinoxaline (3a-22)

Yellow solid; yield: 69%; (m.p.: 129-131°C); **^{1}H NMR** (400 MHz, $CDCl_3$): *δ* 9.28 (s, 1H), 8.15-8.04 (m, 4H), 7.82-7.72 (m, 2H), 7.68 (d, *J* = 8.0 Hz, 2H). **^{13}C NMR** (101 MHz, $CDCl_3$): *δ* 150.6, 142.8, 142.1, 141.6, 135.5, 132.3, 130.4, 129.8, 129.5, 129.1, 128.9, 124.9; **HRMS**: *m/z* $[M + H]^+$ calcd for $C_{14}H_9BrN_2$: 285.0022; found: 285.0024.



2-(4-(trifluoromethyl)phenyl)quinoxaline (3a-23)

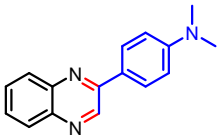
White solid; yield: 43%; (m.p.: 120-122°C); **^{1}H NMR** (400 MHz, $CDCl_3$) *δ* 9.35 (s, 1H), 8.33 (d, *J* = 8.0 Hz, 2H), 8.16 (t, *J* = 9.2 Hz, 2H), 7.86-7.77 (m, 4H). **^{13}C NMR** (101 MHz, $CDCl_3$) *δ* 150.2, 143.0, 142.2 (d, *J* = 30.0 Hz), 140.0, 132.0, 131.7, 130.6, 130.2, 129.7, 129.2, 127.8, 126.1 (q, *J* = 4.0 Hz), 125.3; **HRMS**: *m/z* $[M + H]^+$ calcd for $C_{15}H_9F_3N_2$: 275.0791 found: 275.0791.



2-(3-fluoro-4-methoxyphenyl)quinoxaline (3a-24)

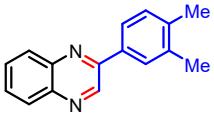
White solid; yield: 78%; (m.p.: 160-162°C); **^{1}H NMR** (400 MHz, $CDCl_3$) *δ* 9.26 (s, 1H), 8.10 (t, *J* = 7.2 Hz, 2H), 8.03 (dd, *J* = 12.4 Hz, 2,0 Hz, 1H), 7.94 (d, *J* = 8.4 Hz,

1H), 7.79-7.70 (m, 2H), 7.12 (t, J = 8.6 Hz, 1H), 3.98 (s, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 154.1, 151.6, 150.2, 149.7 (d, J = 11.0 Hz), 142.5, 142.2, 141.3, 130.4, 129.4 (d, J = 5.0 Hz), 129.0, 123.5 (d, J = 3.0 Hz), 115.3, 115.1, 113.4 (d, J = 2.0 Hz), 56.3; **HRMS**: *m/z* $[M + H]^+$ calcd for $C_{15}H_{11}FN_2O$: 255.0928 found: 255.0929.



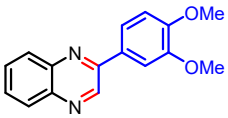
***N,N*-dimethyl-4-(quinoxalin-2-yl)aniline (3a-25)**

White solid; yield: 65%; (m.p.: 95-97°C); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 9.27 (s, 1H), 8.15-8.04 (m, 4H), 7.75-7.63 (m, 2H), 6.83 (d, J = 8.8 Hz, 2H), 3.05 (s, 6H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 151.8, 151.7, 143.1, 142.4, 140.8, 129.9, 129.1, 129.0, 128.6, 128.3, 124.1, 112.3, 40.2; **HRMS**: *m/z* $[M + H]^+$ calcd for $C_{16}H_{15}N_3$: 250.1339 found: 250.1340.



2-(3,4-dimethylphenyl)quinoxaline (3a-26)

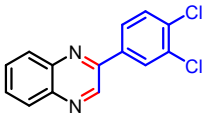
Yellow solid; yield: 71%; (m.p.: 100-102°C); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 9.30 (s, 1H), 8.16-8.08 (m, 2H), 7.99 (s, 1H), 7.90 (d, J = 7.6 Hz, 1H), 7.80-7.70 (m, 2H), 7.31 (d, J = 8.0 Hz, 1H), 2.39 (s, 3H), 2.34 (s, 3H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 151.9, 143.4, 142.2, 141.3, 139.1, 137.5, 134.2, 130.3, 130.1, 129.4, 129.1, 129.0, 128.5, 124.9, 19.9, 19.7; **HRMS**: *m/z* $[M + H]^+$ calcd for $C_{16}H_{14}N_2$: 235.1230 found: 235.1231.



2-(3,4-dimethoxyphenyl)quinoxaline (3a-27)

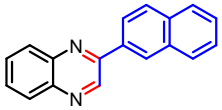
White solid; yield: 76%; (m.p.: 115-117°C); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 9.28 (s, 1H), 8.09 (dd, J = 14.4, 8.0 Hz, 2H), 7.84 (d, J = 1.6 Hz, 1H), 7.77-7.66 (m, 3H), 6.99 (d, J = 8.4 Hz, 1H), 4.04 (s, 3H), 3.95 (s, 3H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 151.2, 151.0, 149.6, 143.0, 142.1, 141.1, 130.1, 129.4, 129.3, 129.0, 128.9, 120.3, 111.0, 110.0, 56.0, 55.9; **HRMS**: *m/z* $[M + H]^+$ calcd for $C_{16}H_{14}N_2O_2$: 267.1128 found:

267.1131.



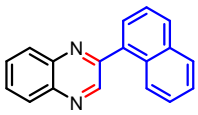
2-(3,4-dichlorophenyl)quinoxaline (3a-28)

Yellow solid; yield: 47%; (m.p.: 176-178°C); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 9.28 (s, 1H), 8.35 (s, 1H), 8.13 (t, J = 6.8 Hz, 2H), 8.03 (d, J = 8.4 Hz, 1H), 7.84-7.76 (m, 2H), 7.63 (d, J = 8.4 Hz, 1H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 149.2, 142.5, 142.1, 141.8, 136.5, 134.6, 133.6, 131.1, 130.7, 130.1, 129.6, 129.3, 129.2, 126.4; **HRMS**: *m/z* [M + H]$^+$ calcd for $C_{14}H_8Cl_2N_2$: 275.0137 found: 275.0139.



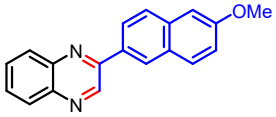
2-(naphthalen-2-yl)quinoxaline (3a-29)

Yellow solid; yield: 83%; (m.p.: 125-127°C); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 9.48 (s, 1H), 8.66 (s, 1H), 8.36 (d, J = 8.4 Hz, 1H), 8.17 (dd, J = 22.0, 8.0 Hz, 2H), 8.06-8.00 (m, 2H), 7.94-7.88 (m, 1H), 7.83-7.74 (m, 2H), 7.60-7.54 (m, 2H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 151.6, 143.5, 142.3, 141.5, 134.1, 134.0, 133.3, 130.3, 129.6, 129.5, 129.1, 129.0, 128.9, 127.8, 127.4, 127.3, 126.7, 124.4; **HRMS**: *m/z* [M + H]$^+$ calcd for $C_{18}H_{12}N_2$: 257.1073 found: 257.1075.



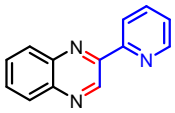
2-(naphthalen-1-yl)quinoxaline (3a-30)

Yellow solid; yield: 61%; (m.p.: 100-102°C); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 9.17 (s, 1H), 8.27-8.15 (m, 3H), 8.02 (d, J = 8.0 Hz, 1H), 7.97 (d, J = 7.2 Hz, 1H), 7.88-7.81 (m, 2H), 7.78 (d, J = 7.2 Hz, 1H), 7.65 (t, J = 7.6 Hz, 1H), 7.60-7.50 (m, 2H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 154.2, 146.6, 142.1, 141.3, 135.0, 134.0, 131.1, 130.4, 130.1, 129.9, 129.6, 129.2, 128.6, 128.5, 127.2, 126.3, 125.4, 125.0; **HRMS**: m/z [M + H]$^+$ calcd for $C_{18}H_{12}N_2$: 257.1073 found: 257.1070.



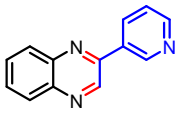
2-(6-methoxynaphthalen-2-yl)quinoxaline (3a-31)

Yellow solid; yield: 80%; (m.p.: 155-157°C); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 9.44 (s, 1H), 8.58 (s, 1H), 8.33 (d, J = 8.8 Hz, 1H), 8.15 (dd, J = 20.0, 8.2 Hz, 2H), 7.90 (d, J = 8.4 Hz, 2H), 7.81-7.70 (m, 2H), 7.24-7.17 (m, 2H), 3.95 (s, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 158.7, 151.7, 143.3, 142.3, 141.3, 135.5, 131.8, 130.4, 130.3, 129.4, 129.3, 129.0, 128.8, 127.8, 127.2, 124.9, 119.6, 105.6, 55.3; **HRMS**: *m/z* $[M + H]^+$ calcd for $C_{19}H_{14}N_2O$: 287.1179 found: 287.1182.



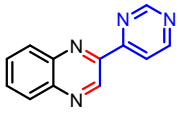
2-(pyridin-2-yl)quinoxaline (3a-32)

White solid; yield: 65%; (m.p.: 110-112°C); **^{1}H NMR** (400 MHz, DMSO-d_6) δ 9.88 (s, 1H), 8.81 (d, J = 4.0 Hz, 1H), 8.55 (d, J = 8.0 Hz, 1H), 8.20-8.14 (m, 2H), 8.09-8.03 (m, 1H), 7.93-7.88 (m, 2H), 7.62-7.57 (m, 1H); **^{13}C NMR** (101 MHz, d_6-DMSO) δ 153.9, 150.1, 150.0, 144.0, 142.4, 141.4, 138.3, 131.3, 131.1, 129.8, 129.4, 125.8, 122.1; **HRMS**: *m/z* $[M + H]^+$ calcd for $C_{13}H_9N_2$: 208.0869 found: 208.0868.



2-(pyridin-3-yl)quinoxaline (3a-33)

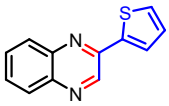
White solid; yield: 67%; (m.p.: 109-111°C); **^{1}H NMR** (400 MHz, DMSO-d_6) δ 9.66 (s, 1H), 9.51 (d, J = 2.0 Hz, 1H), 8.76 (dd, J = 4.8, 1.6 Hz, 1H), 8.71-8.67 (m, 1H), 8.20-8.14 (m, 2H), 7.95-7.86 (m, 2H), 7.65 (dd, J =8.0, 4.8 Hz, 1H); **^{13}C NMR** (101 MHz, DMSO-d_6) δ 151.9, 149.6, 149.0, 144.2, 141.8, 141.7, 135.4, 132.2, 131.3, 130.8, 129.7, 129.4, 124.5. **HRMS**: *m/z* $[M + H]^+$ calcd for $C_{13}H_9N_3$: 208.0869 found 208.0872.



2-(pyrimidin-4-yl)quinoxaline (3a-34)

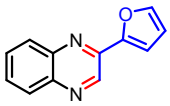
White solid; yield: 48%; (m.p.: 163-165°C); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 9.99 (s, 1H), 9.42 (s, 1H), 8.98 (d, J = 5.2 Hz, 1H), 8.57 (d, J = 5.2 Hz, 1H), 8.24-8.17 (m, 2H), 7.88-7.83 (m, 2H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 158.9, 158.2, 149.1, 147.9, 143.7, 131.2, 130.6, 130.0, 129.5, 118.2. **HRMS**: *m/z* $[M + H]^+$ calcd for $C_{12}H_8N_4$:

209.0822 found 209.0821.



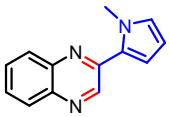
2-(thiophen-2-yl)quinoxaline (3a-35)

Yellow solid; yield: 65%; (m.p.: 103-105°C); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 9.20 (s, 1H), 8.04 (d, J = 8.0 Hz, 2H), 7.82 (d, J = 3.2 Hz, 1H), 7.75-7.63 (m, 2H), 7.52 (d, J = 5.2 Hz, 1H), 7.17 (t, J =4.2 Hz, 1H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 147.3, 142.1, 142.0, 141.9, 141.2, 130.3, 129.7, 129.1, 129.0, 128.9, 128.4, 126.9; **HRMS**: *m/z* [M + H]$^+$ calcd for $C_{12}H_8N_2S$: 213.0481 found: 213.0475.



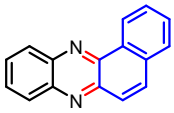
2-(furan-2-yl)quinoxaline (3a-36)

Yellow solid; yield: 50%; (m.p.: 95-97°C); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 9.14 (s, 1H), 8.02-7.94 (m, 2H), 7.68-7.57 (m, 3H), 7.22 (d, J = 3.2 Hz, 1H), 6.55-6.50 (m, 1H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 151.5, 145.0, 143.7, 142.0, 141.9, 141.2, 130.8, 130.4, 129.2, 129.1, 112.4, 111.8; **HRMS**: *m/z* [M + H]$^+$ calcd for $C_{12}H_8N_2O$: 197.0175 found: 197.0180.



2-(1-methyl-1H-pyrrol-2-yl)quinoxaline (3a-37)

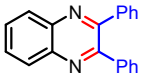
Yellow solid; yield: 49%; (m.p.: 123-125°C); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 9.12 (s, 1H), 8.05-7.94 (m, 2H), 7.71-7.59 (m, 2H), 6.98-6.93 (m 1H), 6.85 (s, 1H), 6.29-6.24 (m, 1H), 4.17 (s, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 147.0, 144.4, 141.5, 139.7, 129.9, 129.3, 128.9, 128.8, 128.2, 113.5, 108.4, 37.8; HRMS: m/z [M + H]$^+$ calcd for $C_{13}H_{11}N_3$: 210.1022 found: 210.1025.



Benzo[a]phenazine (3b-1)

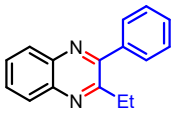
Yellow solid; yield: 74%; (m.p.: 142-143°C); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 9.39 (d, J = 4.0 Hz, 1H), 8.39-8.33 (m, 1H), 8.31-8.26 (m, 1H), 8.00 (q, J = 8.0 Hz, 2H), 7.92-

7.84 (m, 3H), 7.82-7.74 (m, 2H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 143.4, 142.6, 142.5, 141.9, 133.4, 133.2, 131.0, 130.1, 129.9, 129.8, 129.7, 129.0, 128.2, 128.0, 127.0, 125.3; The spectroscopic properties of this compound were consistent with the data found in the literature[23].



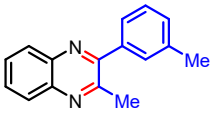
2,3-diphenylquinoxaline (3b-2)

White solid; yield: 73%; (m.p.: 119-121 °C); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.19 (dd, J = 6.4, 3.2 Hz, 2H), 7.78 (dd, J = 6.4, 3.2 Hz, 2H), 7.54-7.50 (m, 4H), 7.38-7.32 (m, 6H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 153.5, 141.2, 139.0, 130.0, 129.8, 129.2, 128.8, 128.3; **HRMS**: *m/z* $[M + Na]^+$ calcd for $C_{20}H_{14}N_2$: 305.1049 found 305.1047.



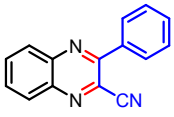
2-ethyl-3-phenylquinoxaline (3b-3)

White solid; yield: 34%; (m.p.: 46-48°C); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.13-8.08 (m, 2H), 7.78-7.69 (m, 2H), 7.63-7.59 (m, 2H), 7.54-7.50 (m, 3H), 3.07 (q, J = 14.8, 7.2 Hz, 2H), 1.30 (t, J = 7.6 Hz, 3H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 157.1, 155.0, 141.4, 140.7, 139.1, 129.7, 129.3, 129.2, 128.9, 128.8, 128.6, 128.5, 29.4, 13.1; **HRMS**: *m/z* $[M + H]^+$ calcd for $C_{16}H_{14}N_2$: 235.1230 found 235.1231.



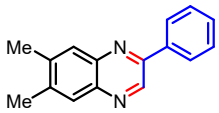
2-methyl-3-(m-tolyl)quinoxaline (3b-4)

Yellow liquid; yield: 32%; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.15-8.06 (m, 2H), 7.78-7.70 (m, 2H), 7.48-7.38 (m, 3H), 7.33-7.29 (m, 1H), 2.80 (s, 3H), 2.46 (s, 3H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 155.2, 152.5, 138.4, 129.8, 129.6, 129.3, 129.2, 128.4, 128.1, 125.9, 24.2, 21.5; **HRMS**: *m/z* $[M + H]^+$ calcd for $C_{16}H_{14}N_2$: 235.1230 found 235.1235.



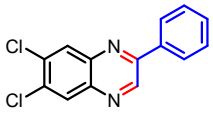
3-phenylquinoxaline-2-carbonitrile (3b-5)

White solid; yield: 62%; (m.p.: 163-165 ℃); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.23-8.18 (m, 2H), 8.08-8.03 (m, 2H), 7.98-7.93 (m, 1H), 7.92-7.86 (m, 1H), 7.63-7.58 (m, 3H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 154.3, 142.4, 140.7, 135.1, 133.5, 131.4, 130.8, 129.6, 129.5, 129.3, 129.0, 128.4, 116.6; The spectroscopic properties of this compound were consistent with the data found in the literature[24].



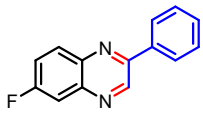
6,7-dimethyl-2-phenylquinoxaline (3c-1)

Yellow solid; yield: 40%; (m.p.: 63-65℃); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 9.22 (s, 1H), 8.17 (d, J =7.2 Hz, 2H), 7.93 (s, 1H), 7.88 (s, 1H), 7.59-7.50 (m, 3H), 2.52 (s, 6H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 151.0, 141.8, 141.3, 141.1, 140.5, 140.0, 136.9, 130.0, 129.1, 128.6, 127.8, 127.4, 20.4, 20.3; **HRMS**: *m/z* $[M + H]^+$ calcd for $C_{16}H_{14}N_2$: 235.1230 found: 235.1233.



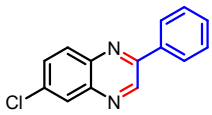
6,7-dichloro-2-phenylquinoxaline (3c-2)

Yellow solid; yield: 70%; (m.p.: 135-137℃); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 9.32 (s, 1H), 8.27 (s, 1H), 8.23 (s, 1H), 8.20-8.17 (m, 2H), 7.60-7.56 (m, 3H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 152.6, 144.3, 141.1, 140.3, 136.0, 134.9, 134.0, 130.8, 130.2, 129.8, 129.3, 127.6; **HRMS**: *m/z* $[M + H]^+$ calcd for $C_{14}H_8Cl_2N_2$: 275.0137 found: 275.0129.



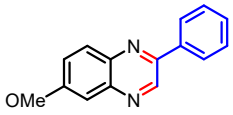
6-fluoro-2-phenylquinoxaline (3c-3)

Yellow solid; yield: 50%; (m.p.: 95-97℃); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 9.28 (s, 1H), 8.18 (d, J = 7.2 Hz, 2H), 8.13-8.05 (m, 1H), 7.76 (d, J = 9.2 Hz, 1H), 7.59-7.48 (m, 4H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 164.2, 161.7, 152.4, 142.6 (d, J = 3.0 Hz), 138.7, 136.3, 131.1 (d, J = 11.0 Hz), 130.4, 129.1, 127.6, 119.8 (d, J = 25.0 Hz), 113.0 (d, J = 21.0 Hz) ; **HRMS**: *m/z* $[M + H]^+$ calcd for $C_{14}H_9FN_2$: 225.0823 found: 225.0826.



6-chloro-2-phenylquinoxaline (3c-4)

Yellow solid; yield: 50%; (m.p.: 107-109℃); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 9.30 (s, 1H), 8.20-8.17 (m, 2H), 8.14 (d, J = 2.4 Hz, 1H), 8.04 (d, J = 9.2 Hz, 1H), 7.67 (dd, J = 8.8, 2.4 Hz, 1H), 7.59-7.53 (m, 3H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 152.5, 143.4, 142.6, 140.0, 136.3, 136.1, 130.5, 130.4, 130.3, 129.2, 128.5, 127.6; **HRMS**: *m/z* $[M + H]^+$ calcd for $C_{14}H_9ClN_2$: 241.0527 found: 241.0525.



6-methoxy-2-phenylquinoxaline (3c-5)

Yellow solid; yield: 66%; (m.p.: 70-72℃); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 9.16 (s, 1H), 8.16 (d, J = 7.2 Hz, 2H), 7.98 (d, J = 8.8 Hz, 1H), 7.58-7.49 (m, 3H), 7.44-7.36 (m, 2H), 3.98 (s, 3H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 161.0, 151.9, 143.9, 140.7, 137.7, 136.9, 130.0, 129.9, 129.1, 127.5, 122.9, 106.8, 55.8; **HRMS**: *m/z* $[M + H]^+$ calcd for $C_{15}H_{12}N_2O$: 237.1022 found: 237.1026.

8. Reference

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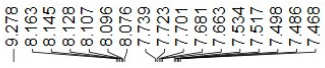
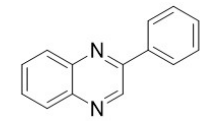
9. NMR Spectra of Substrates and Products

3-Phenylquinoxaline (3a-1)





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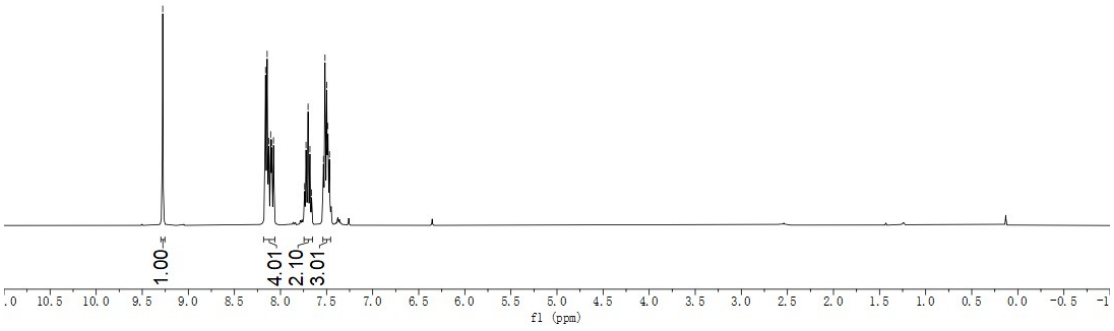

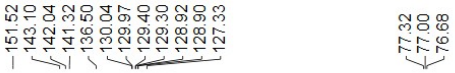

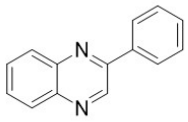

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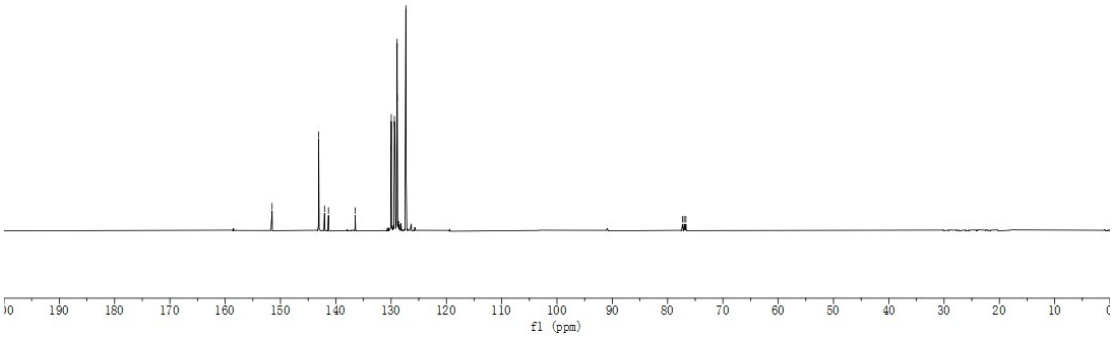

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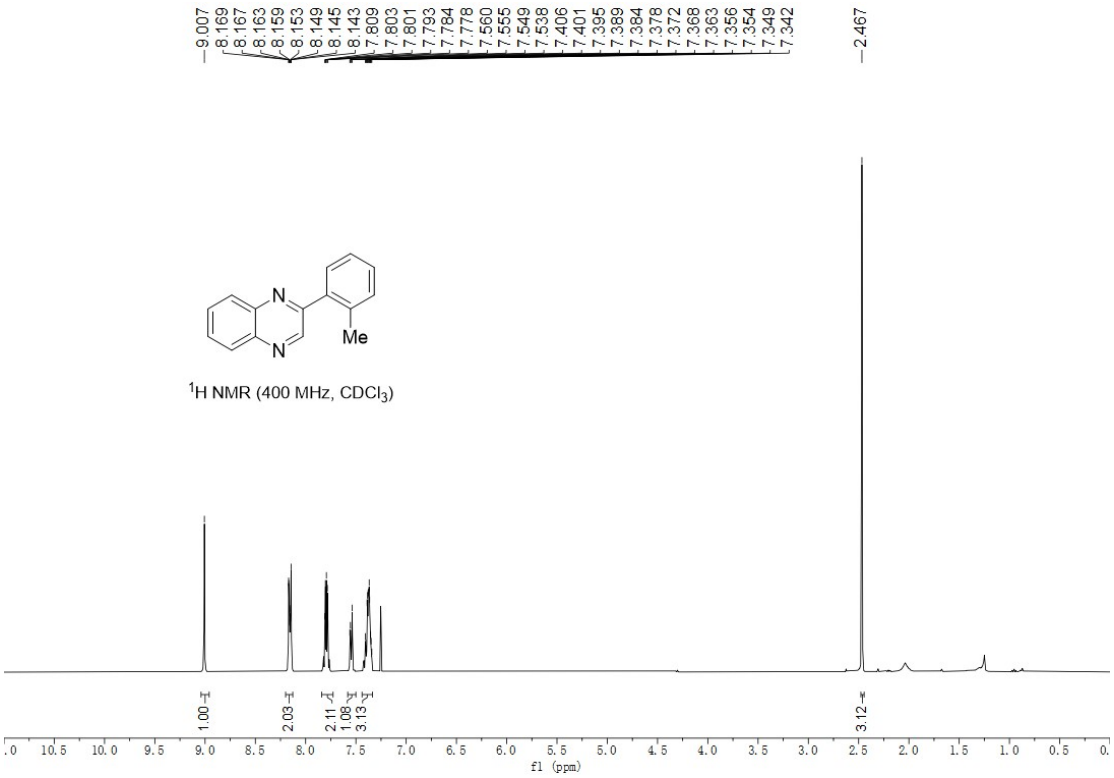

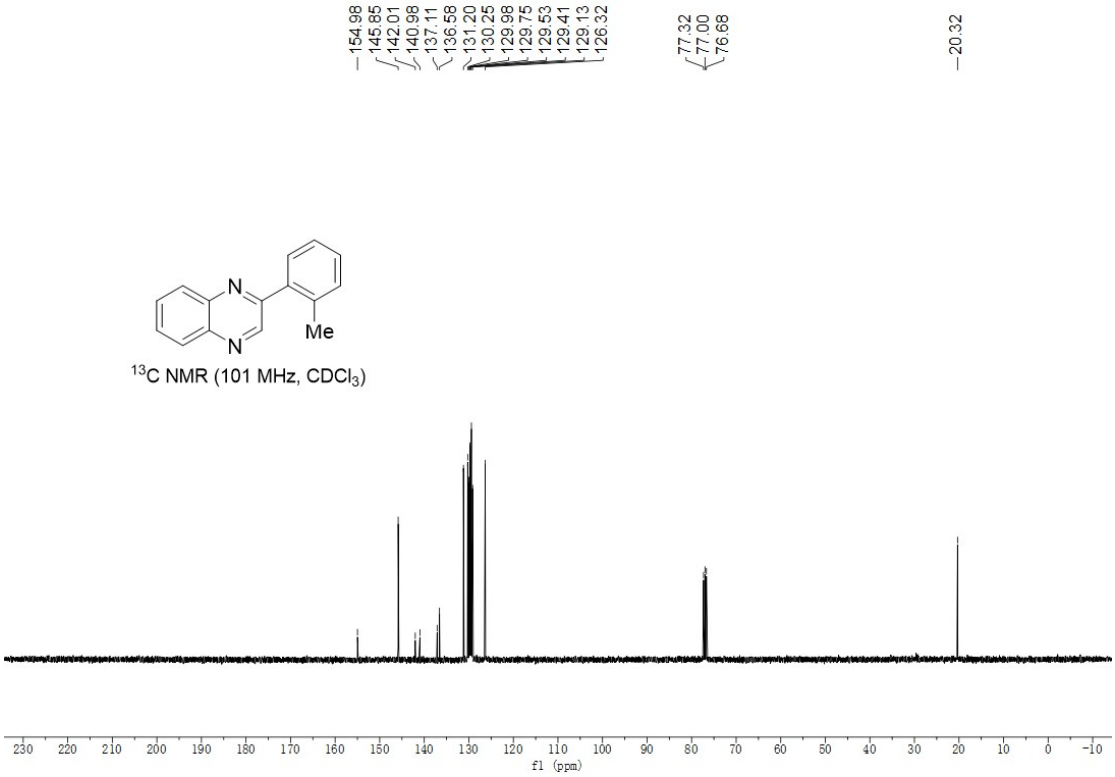

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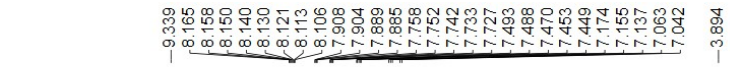

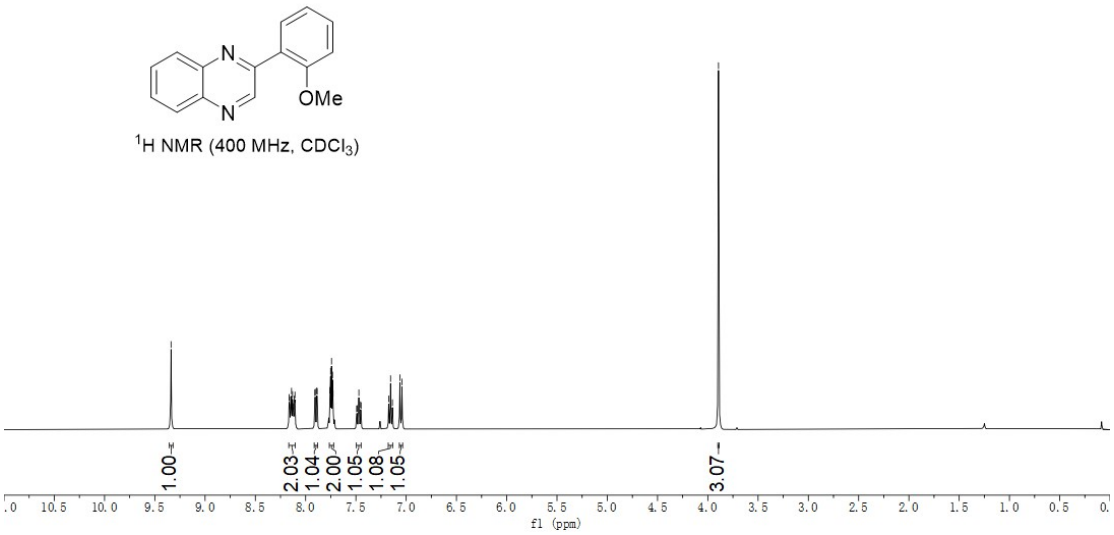

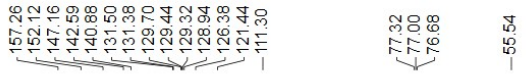

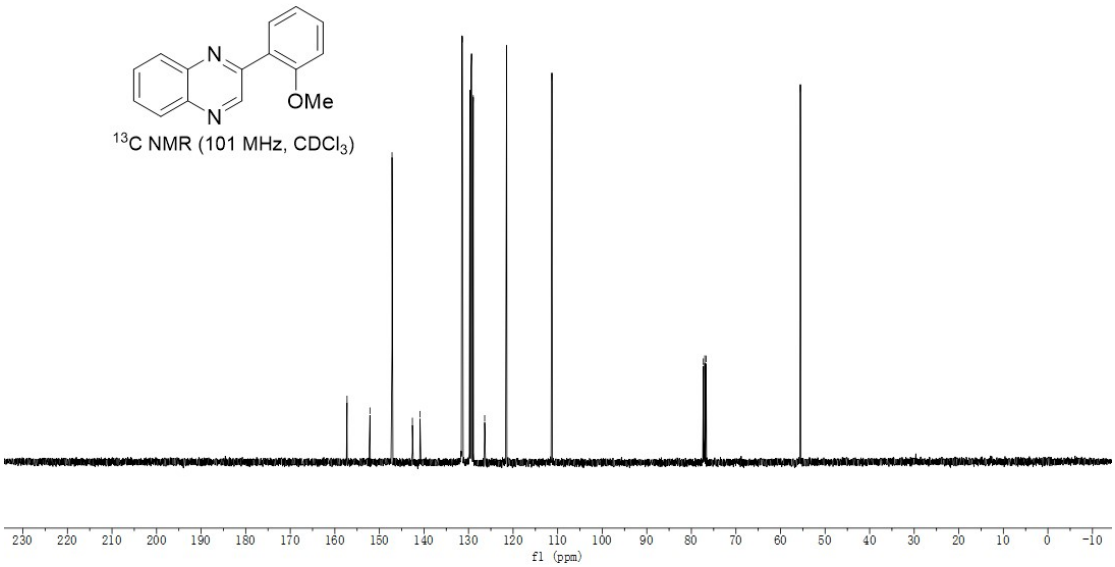

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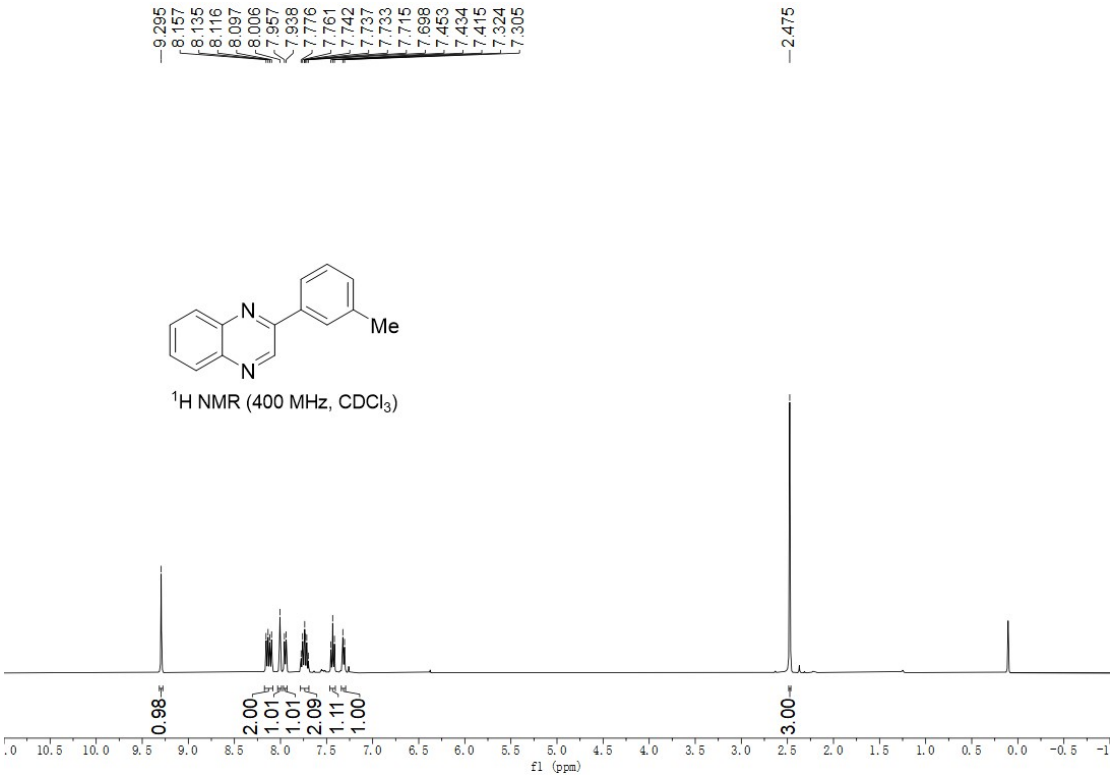

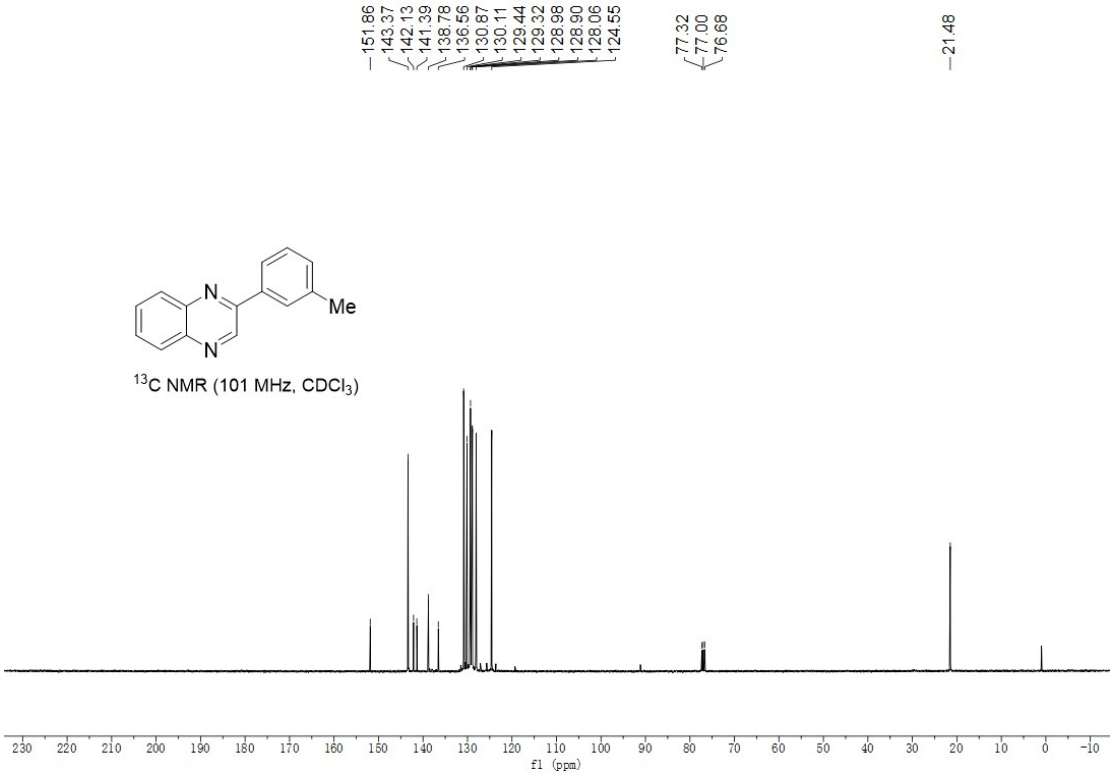

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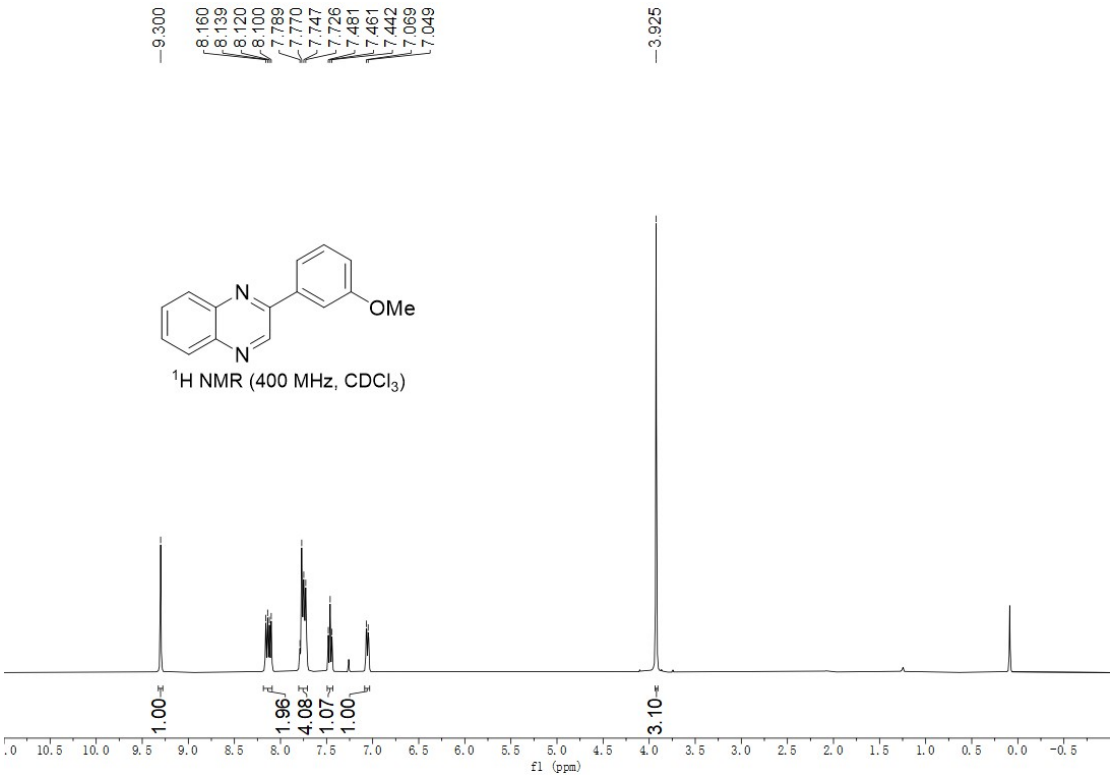

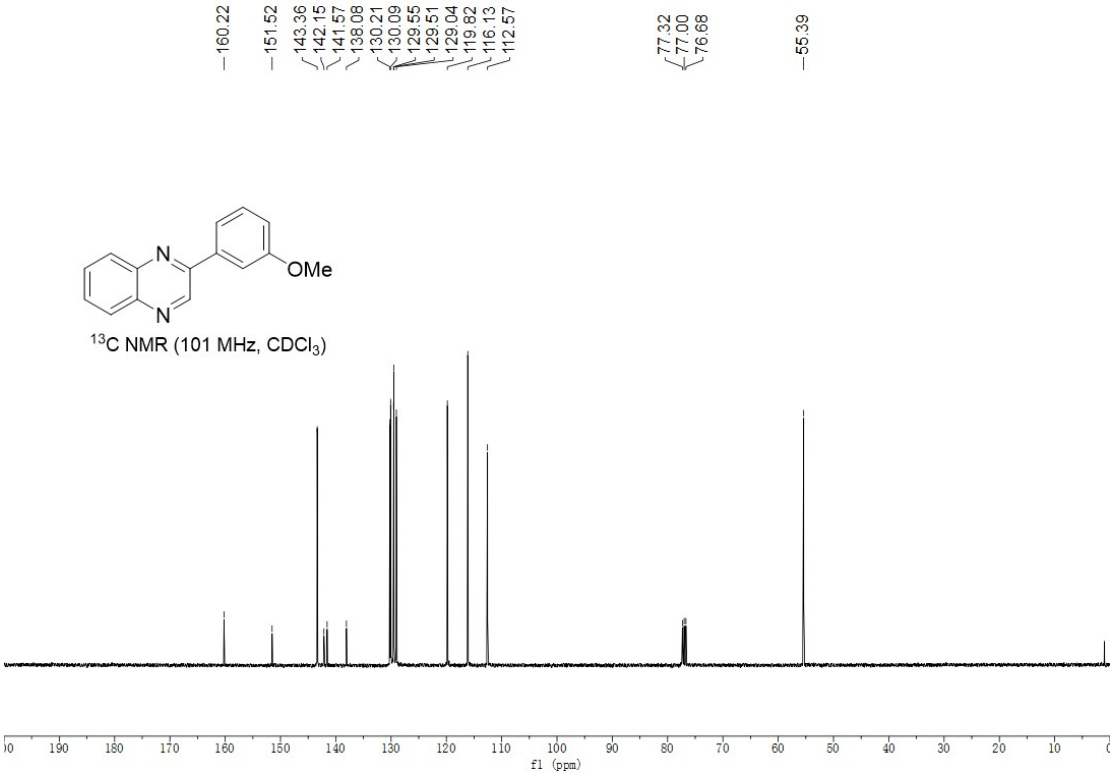

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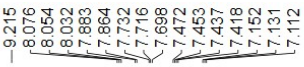

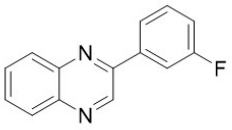

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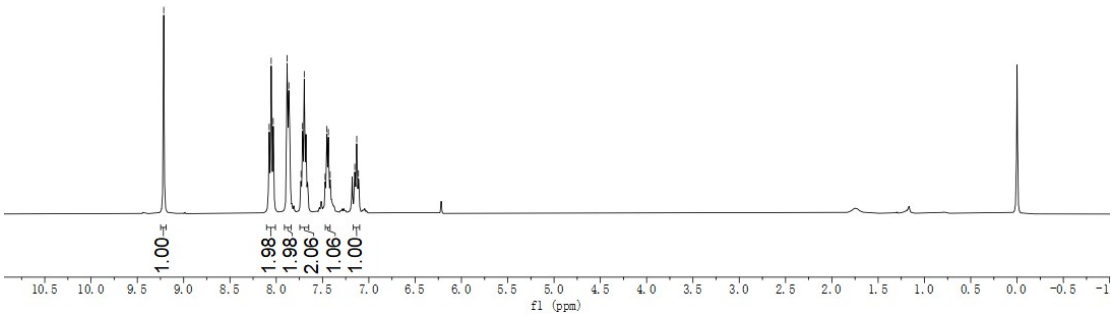

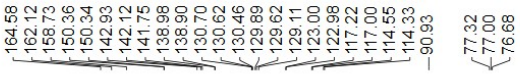

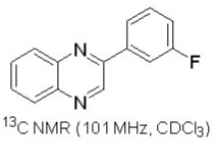

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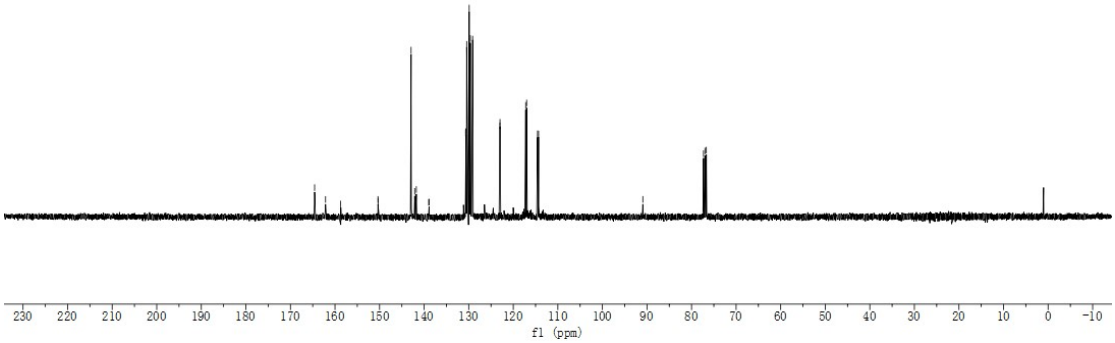

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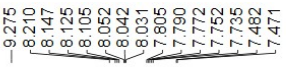

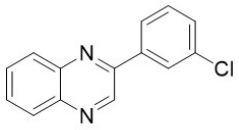

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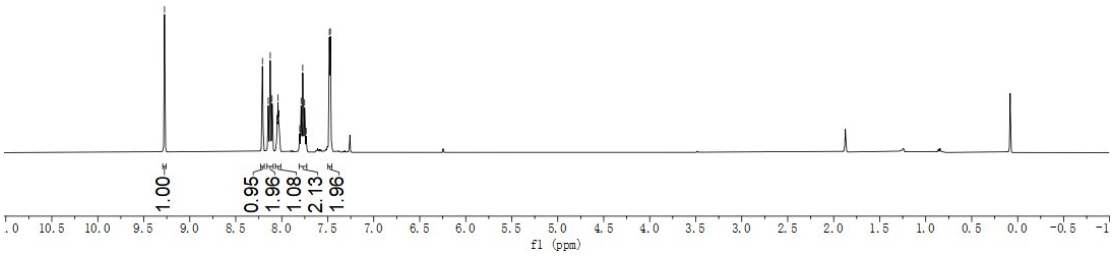

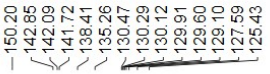

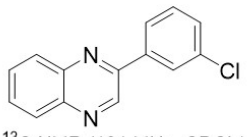

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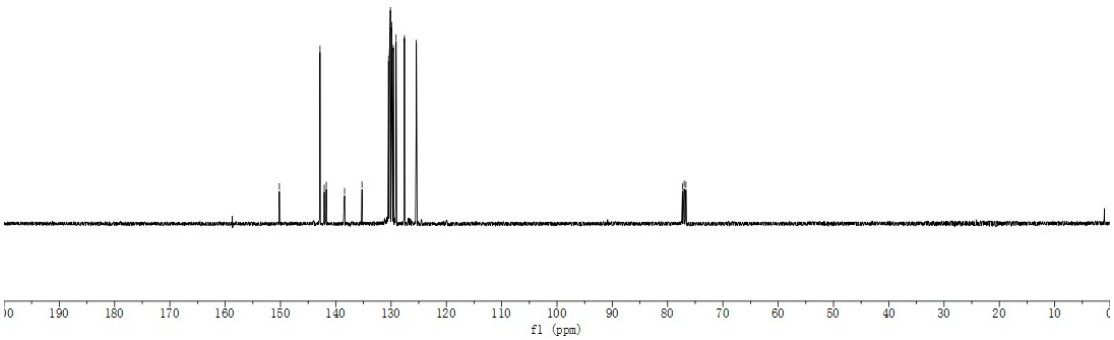

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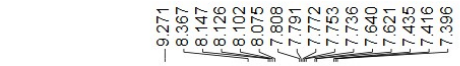

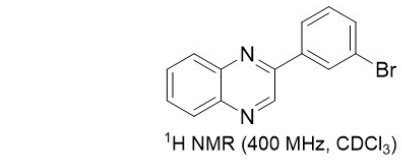

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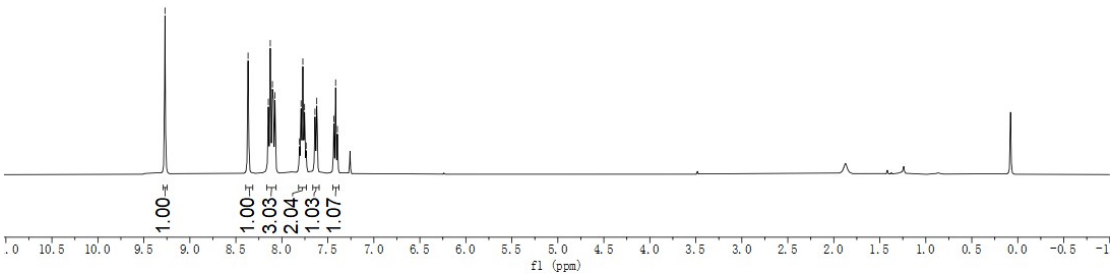

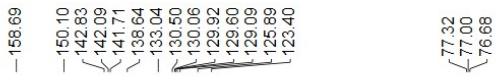

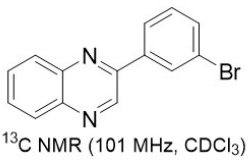

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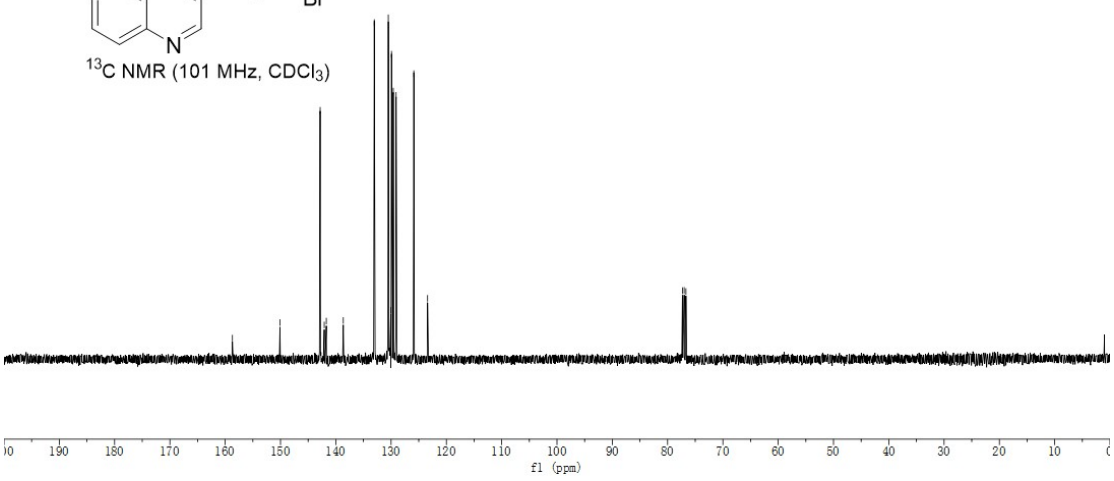

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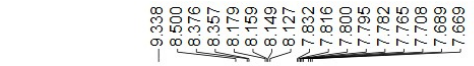

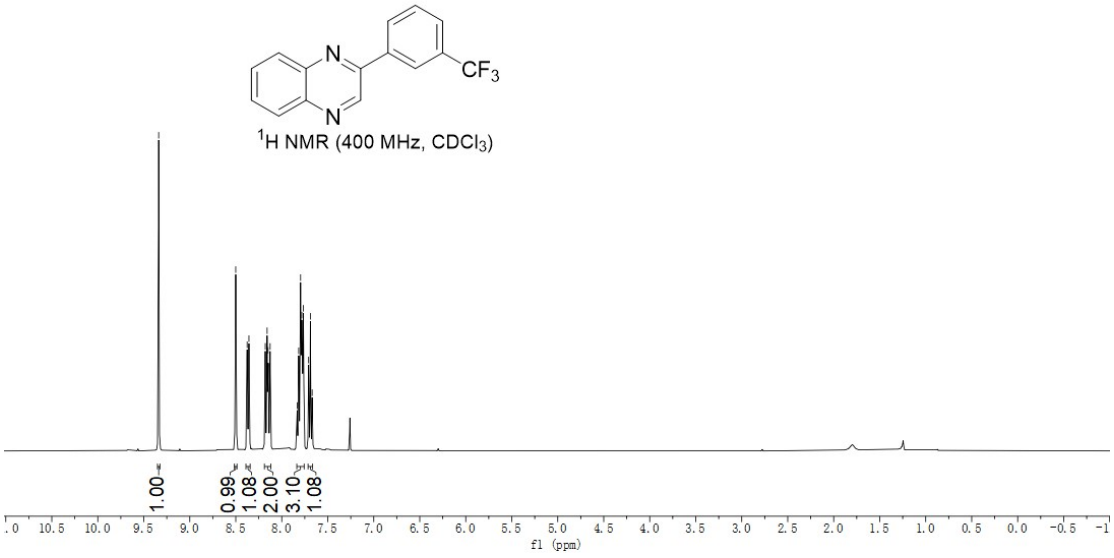

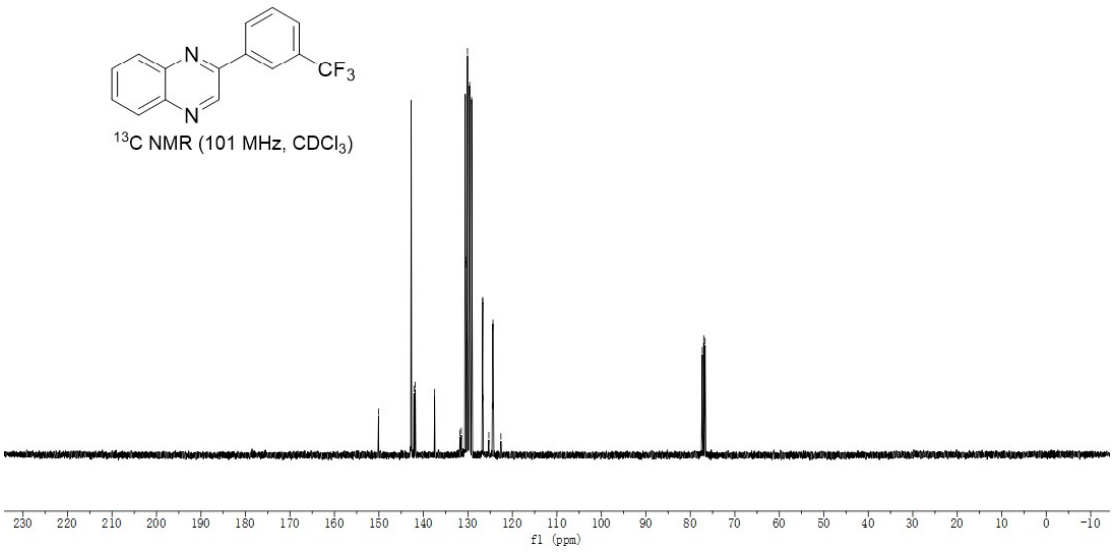

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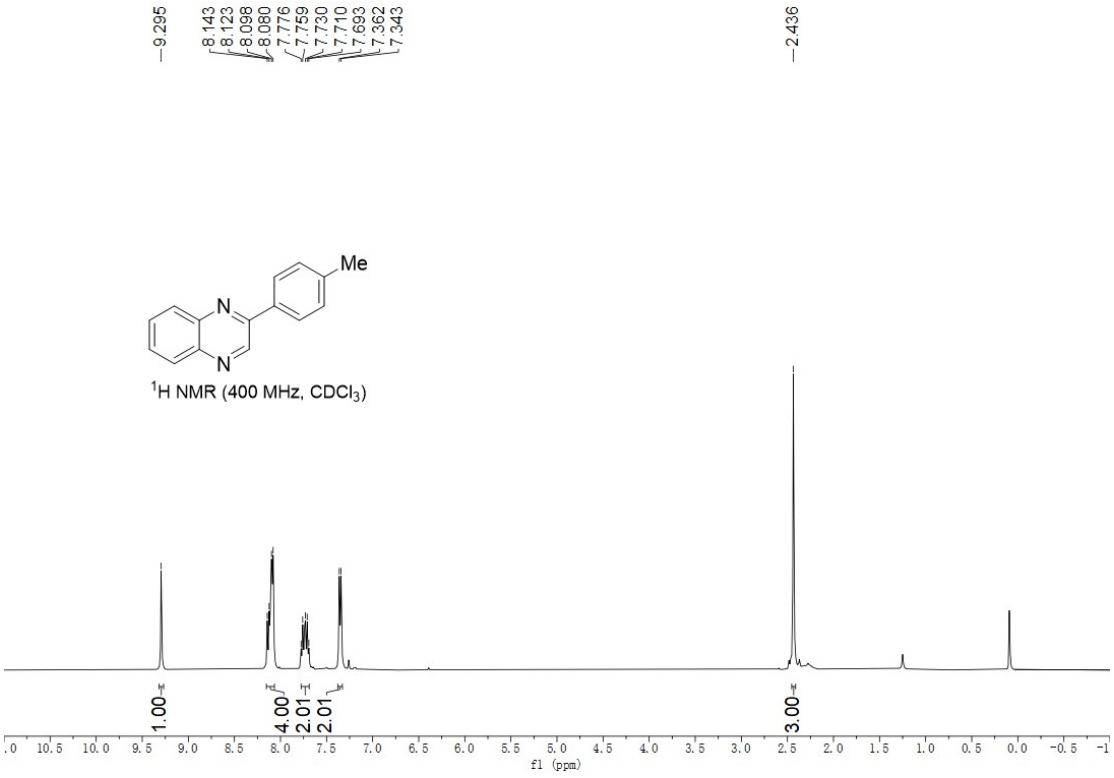

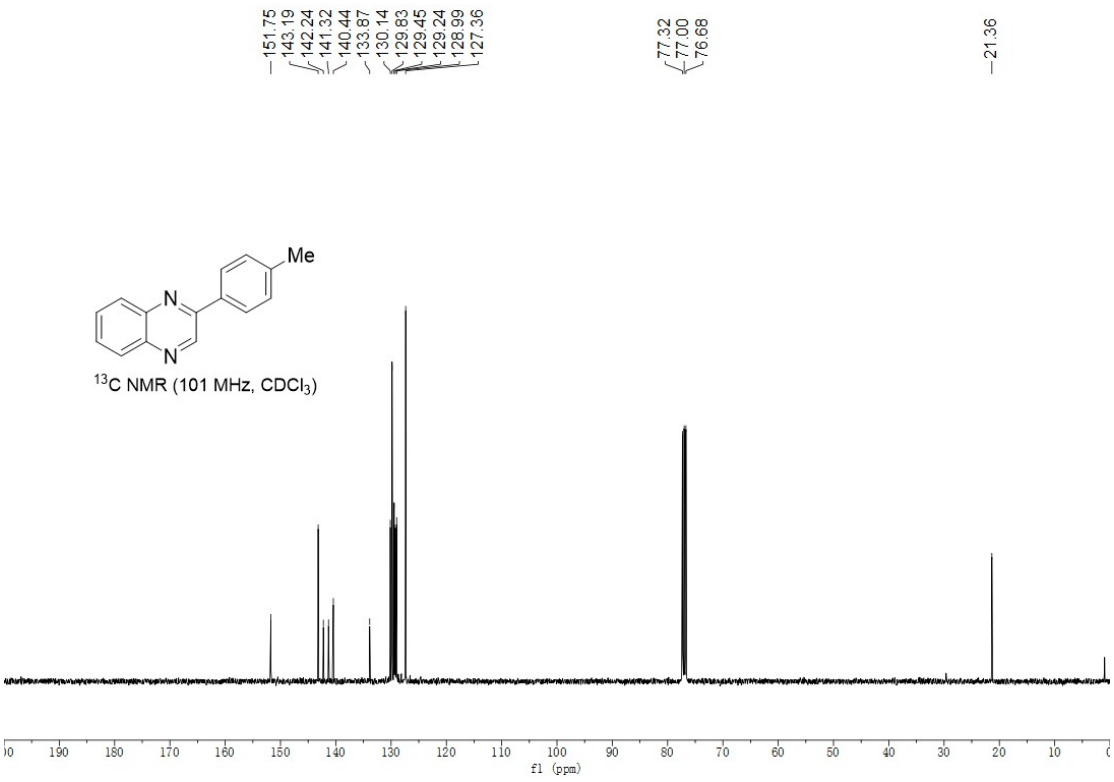

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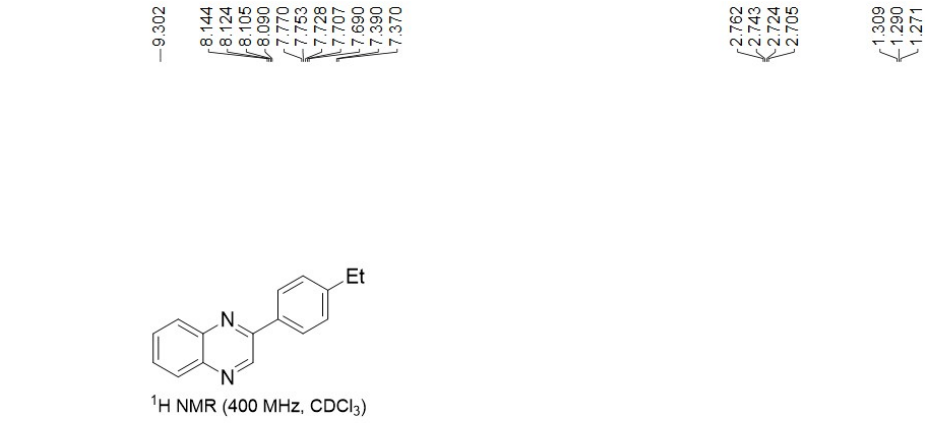
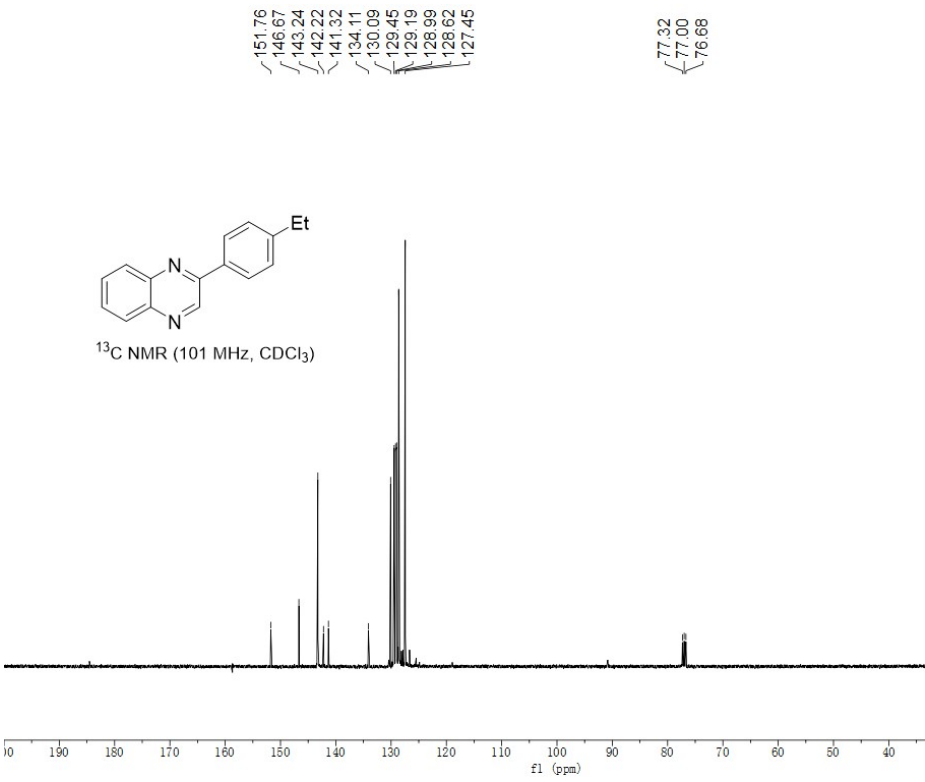
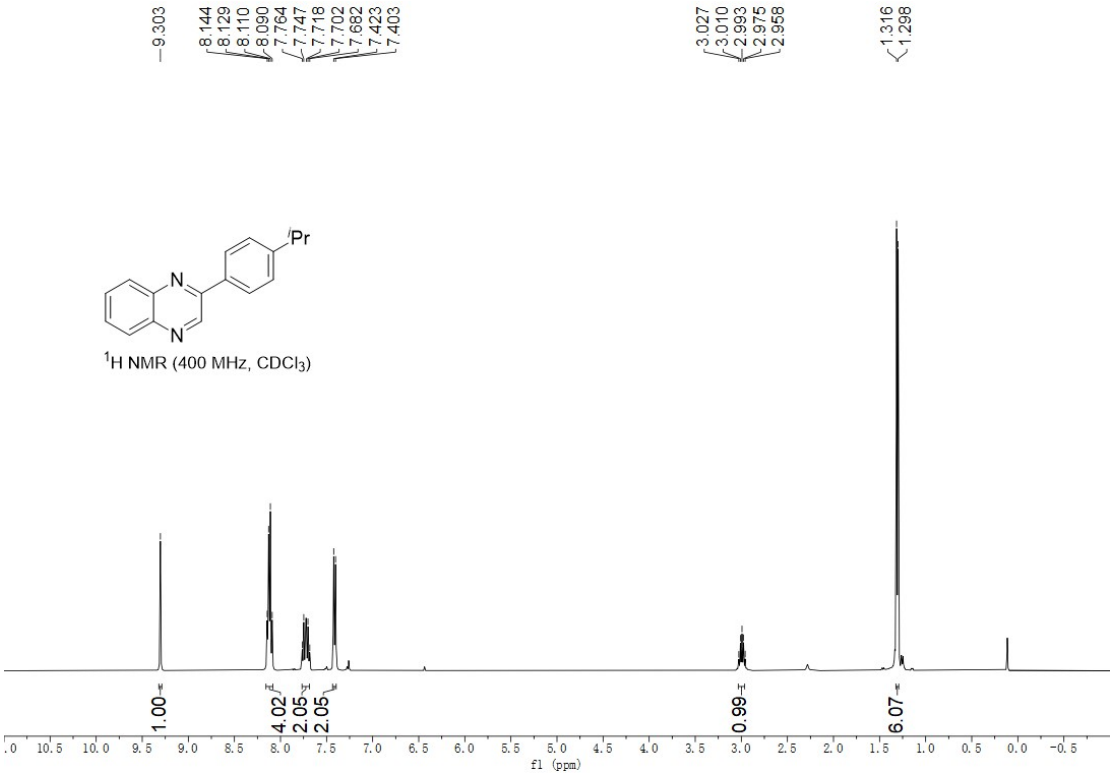
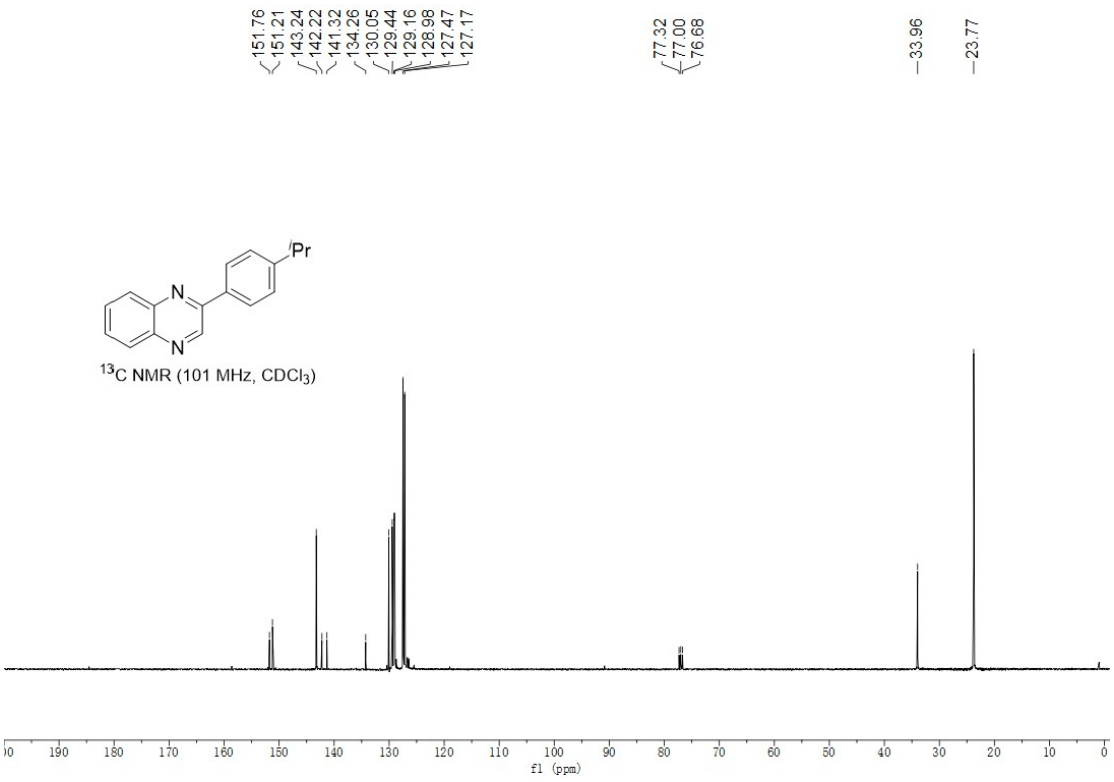


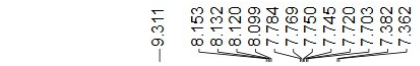


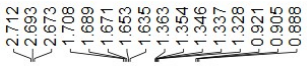
2-(4-isopropylphenyl)quinoxaline (3a-12)

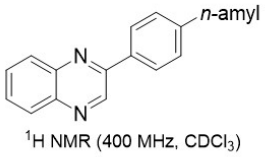




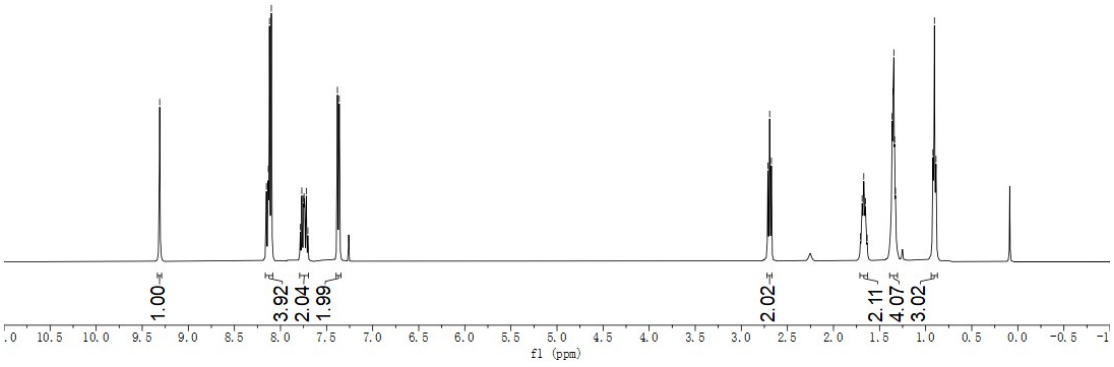
2-(4-pentylphenyl)quinoxaline (3a-13)

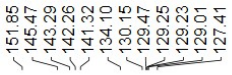


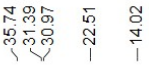


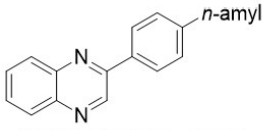


^{1}H NMR (400 MHz, $CDCl_3$)

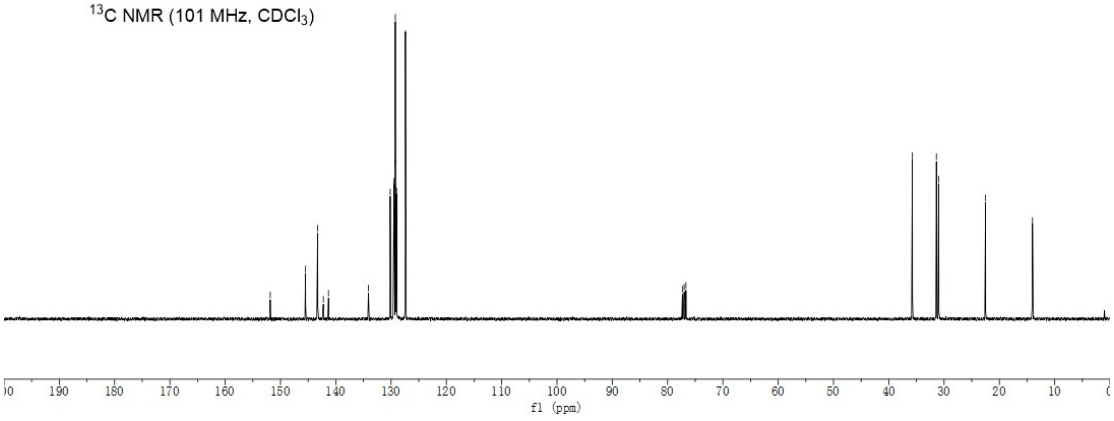




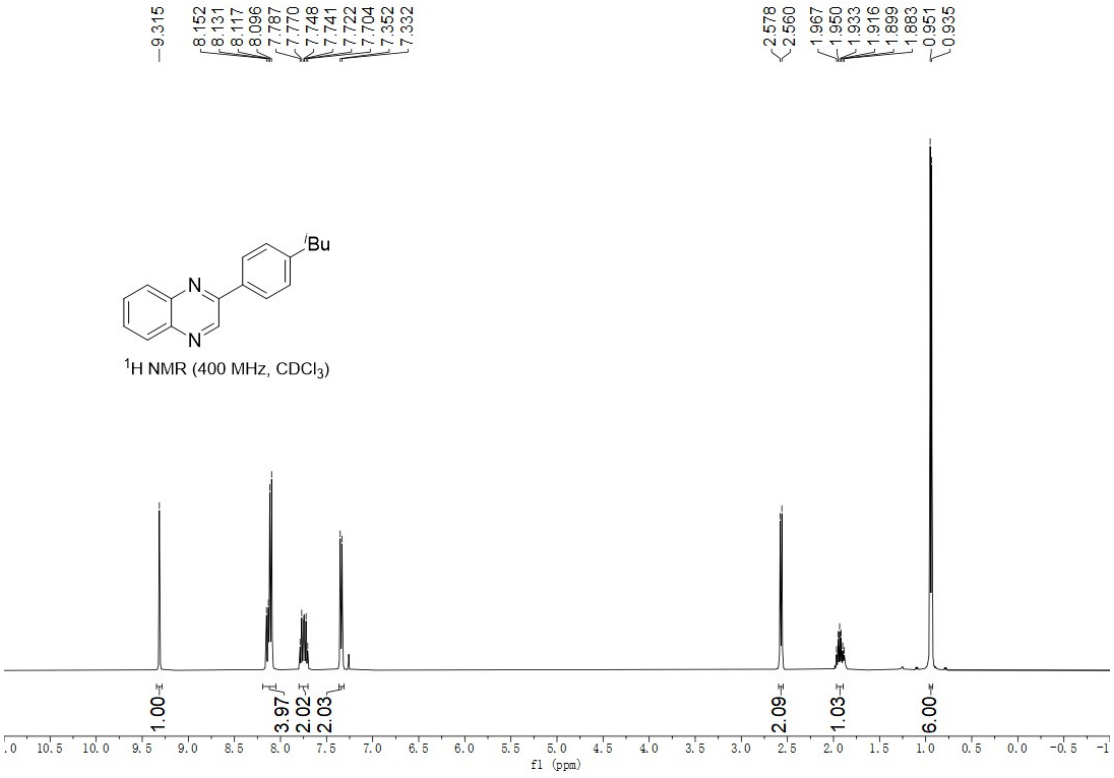


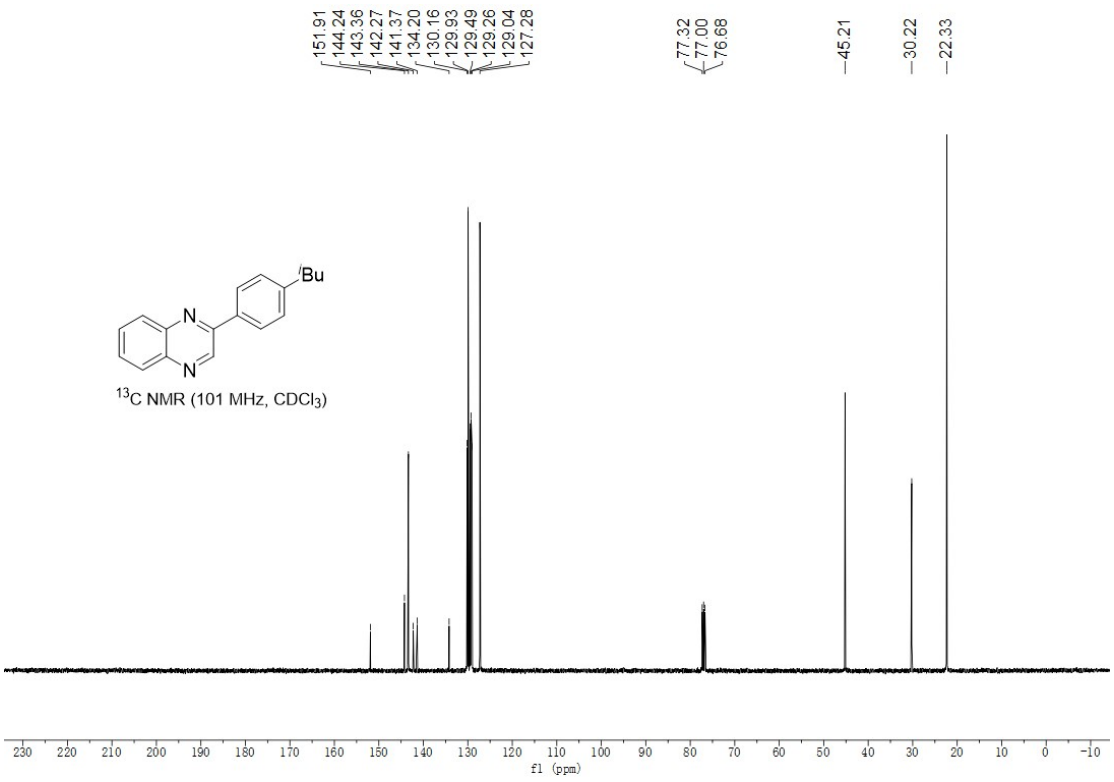


^{13}C NMR (101 MHz, $CDCl_3$)

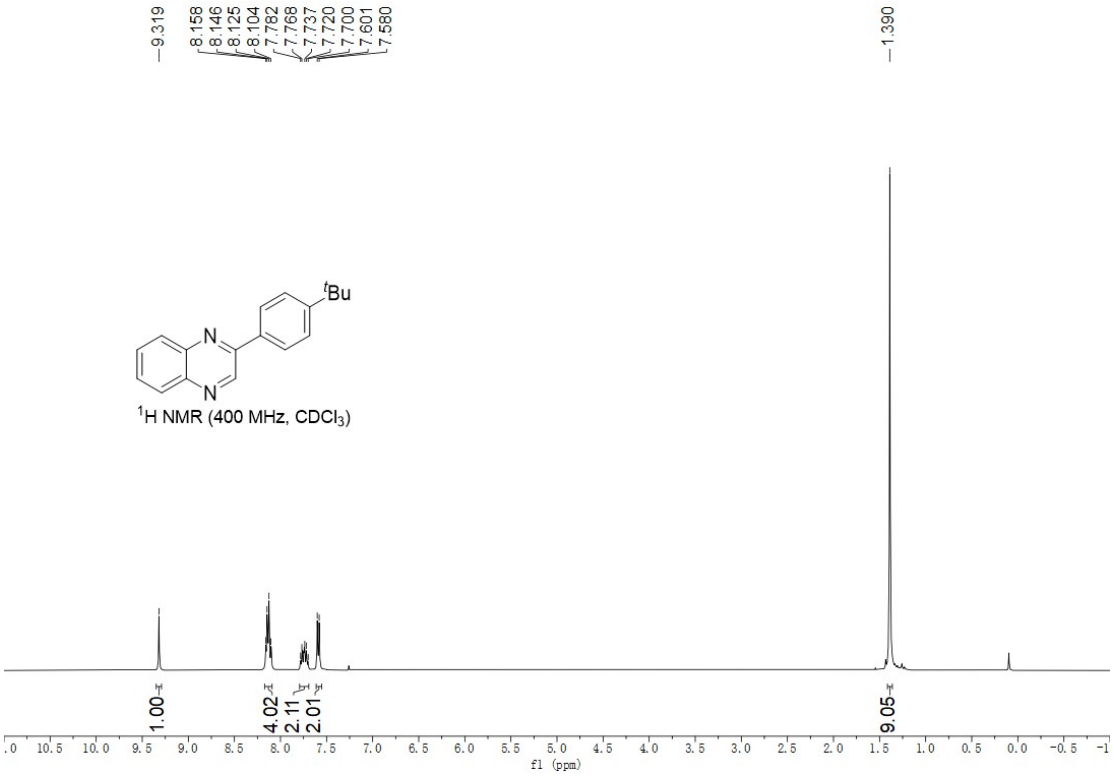


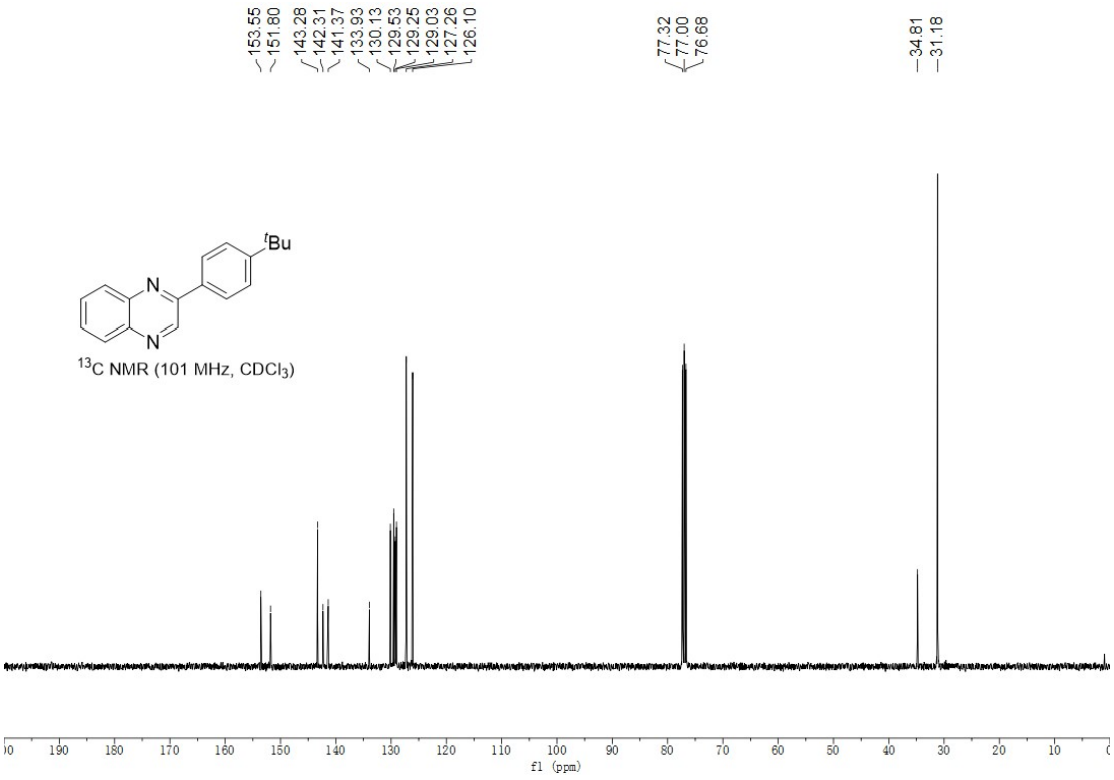
2-(4-isobutylphenyl)quinoxaline (3a-14)



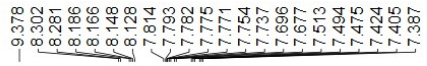


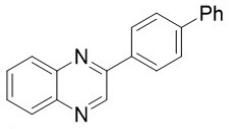
2-(4-(tert-butyl)phenyl)quinoxaline (3a-15)



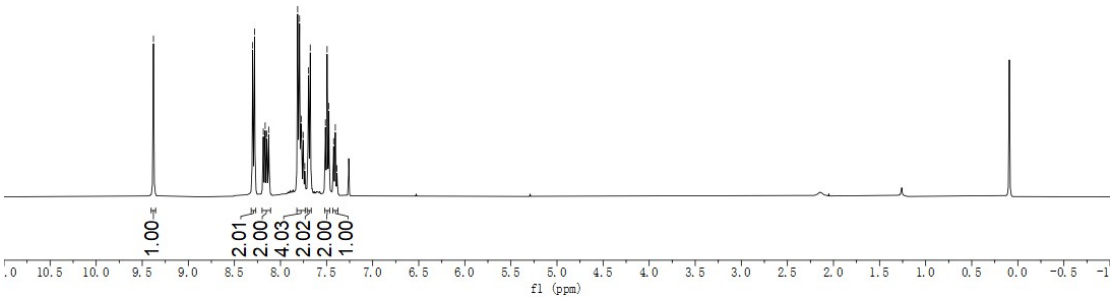


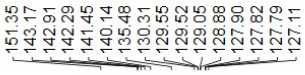
2-([1,1'-biphenyl]-4-yl)quinoxaline (3a-16)

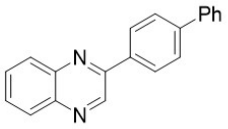




^{1}H NMR (400 MHz, $CDCl_3$)

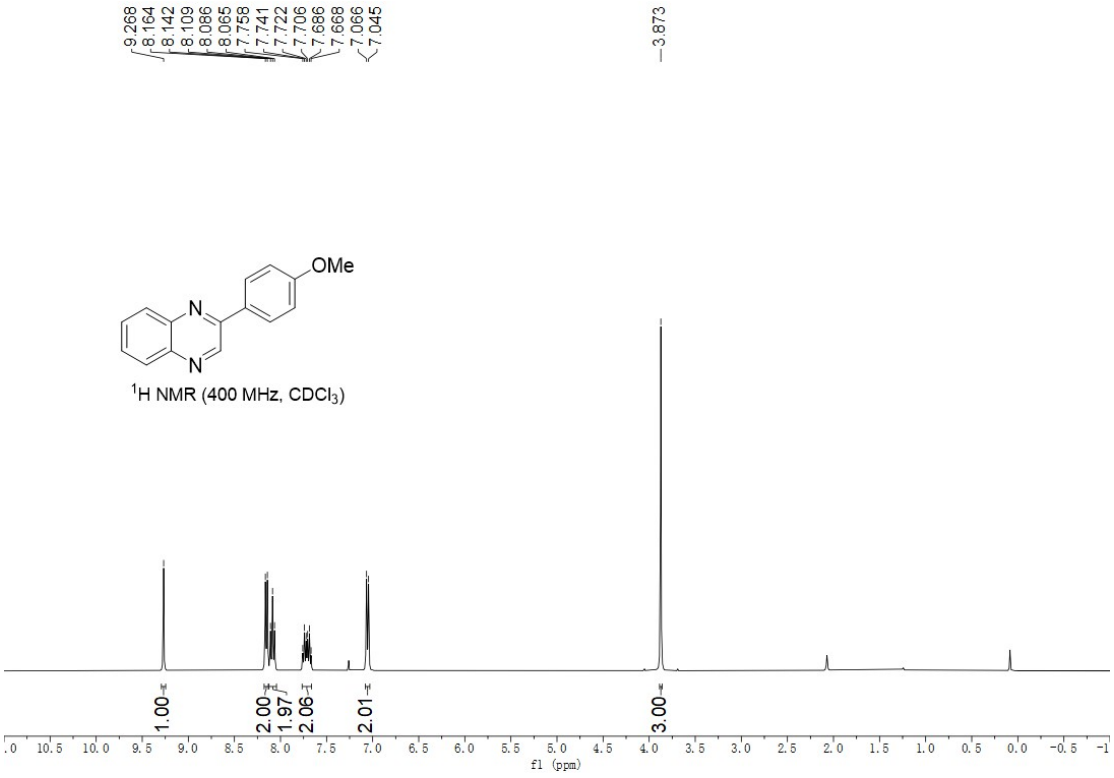


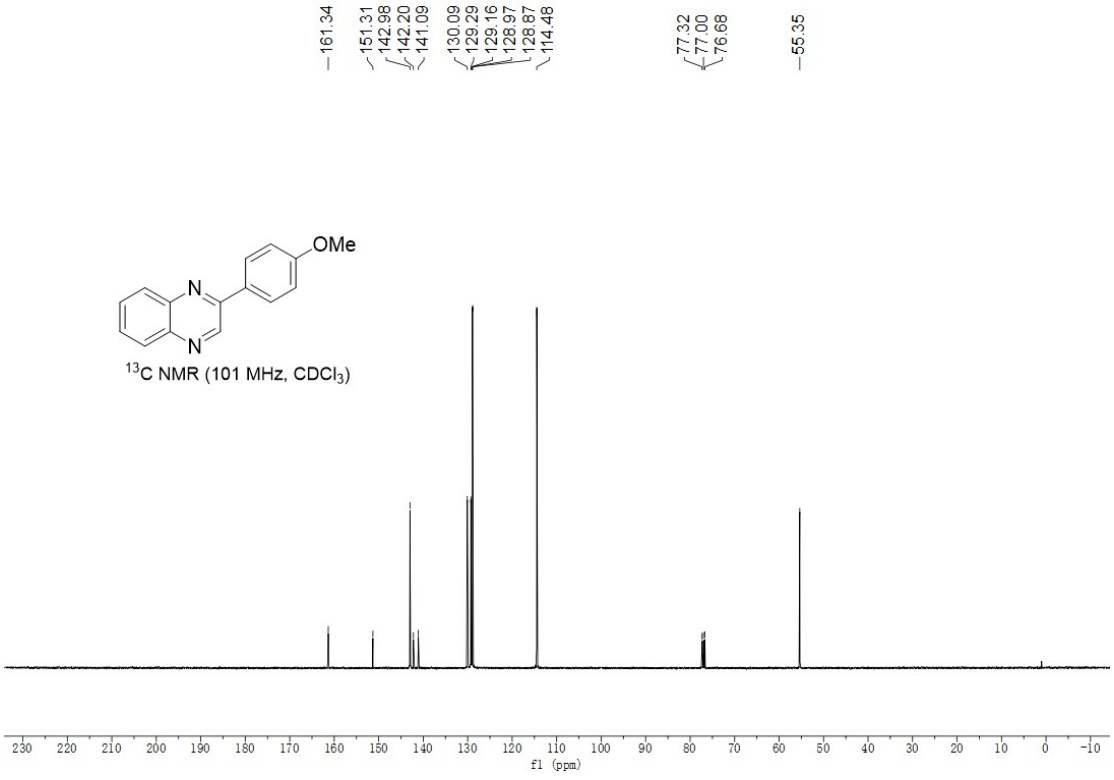




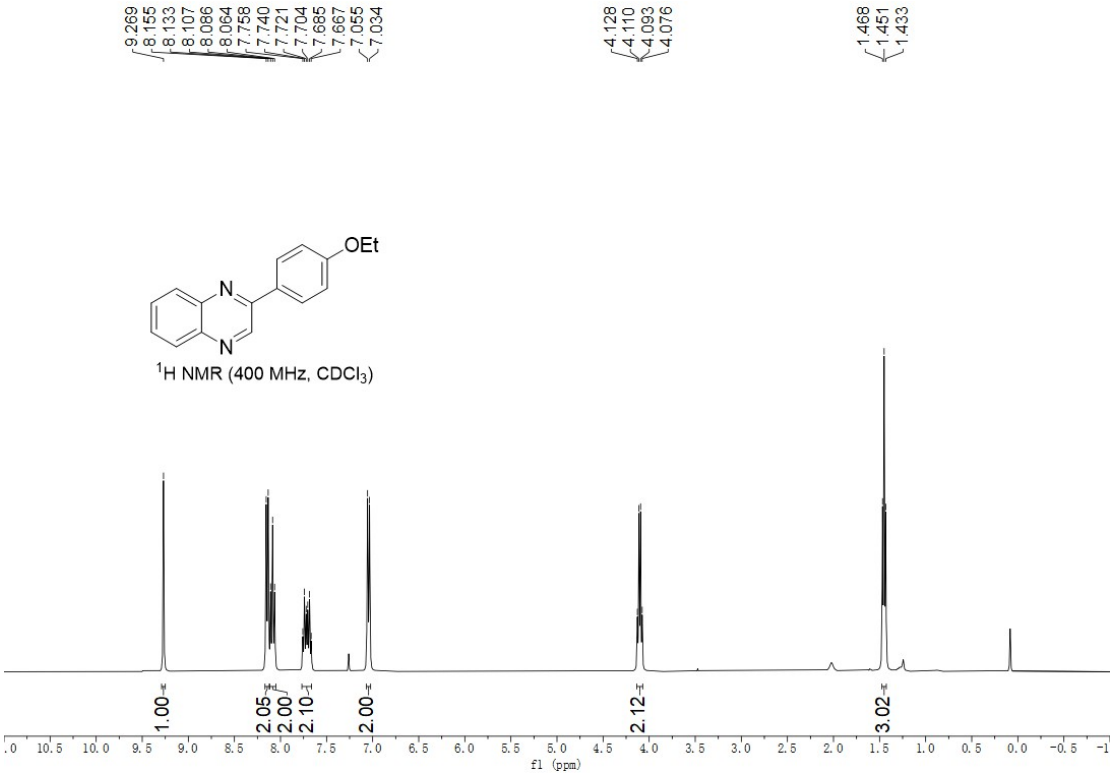
^{13}C NMR (101 MHz, $CDCl_3$)

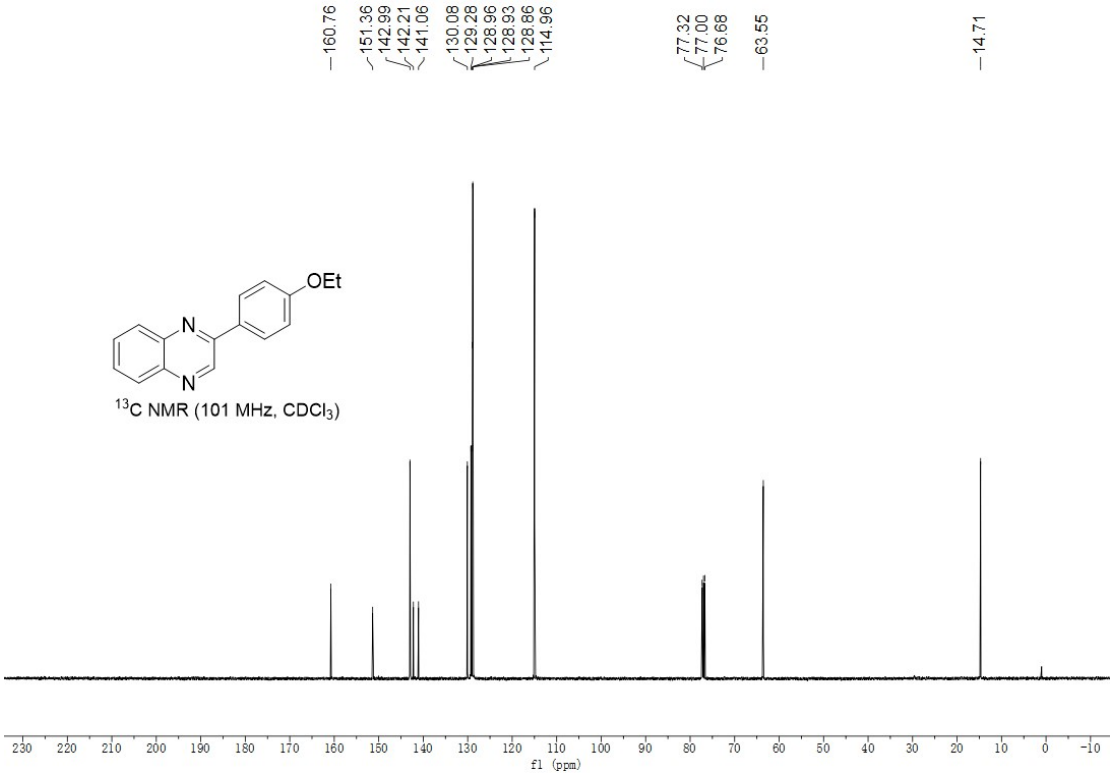
2-(4-methoxyphenyl)quinoxaline (3a-17)



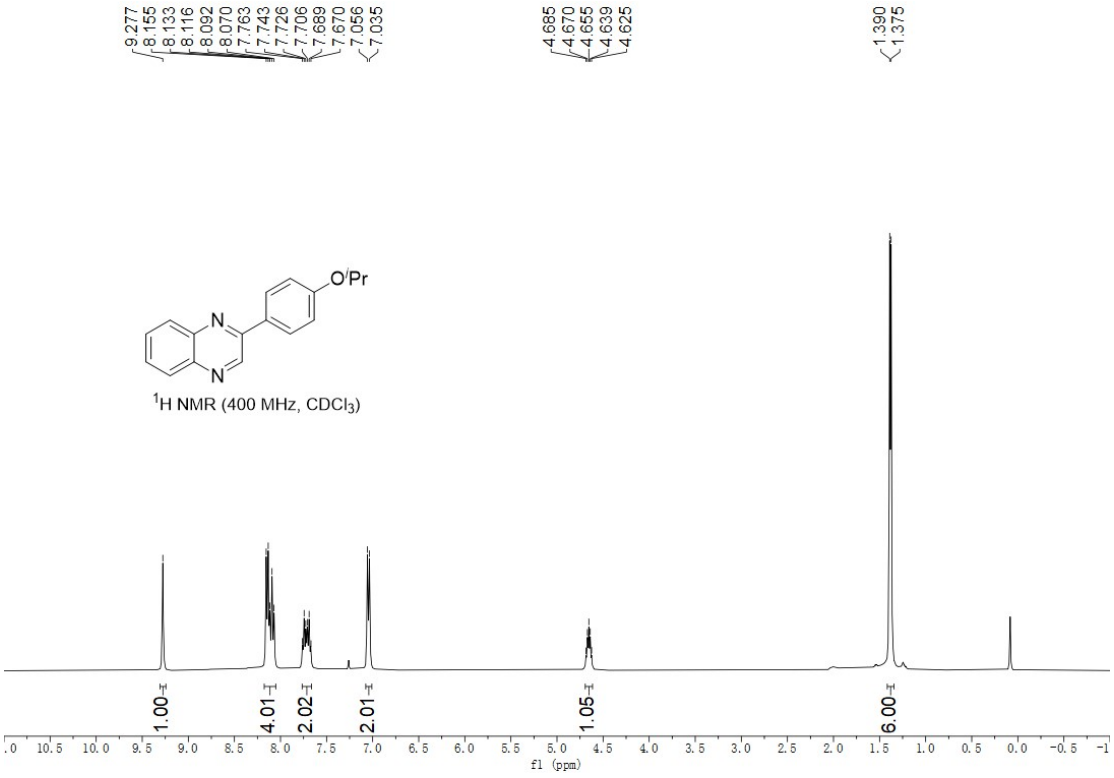


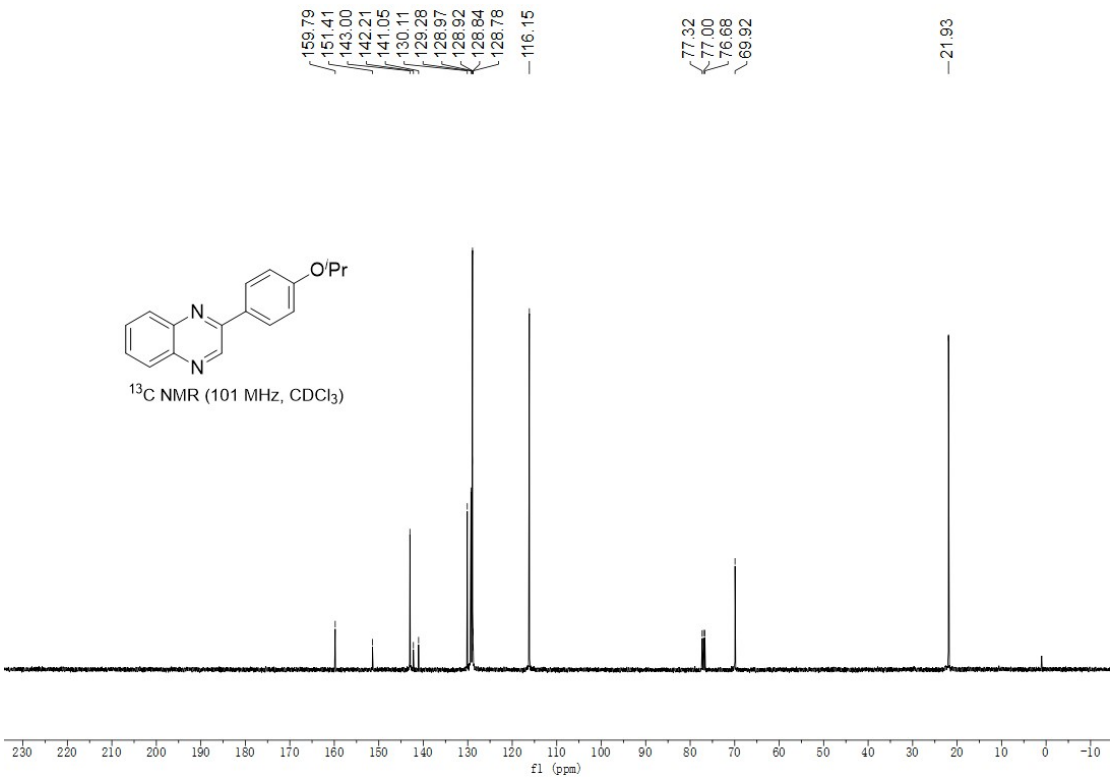
2-(4-ethoxyphenyl)quinoxaline (3a-18)



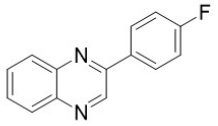


2-(4-isopropoxyphenyl)quinoxaline (3a-19)

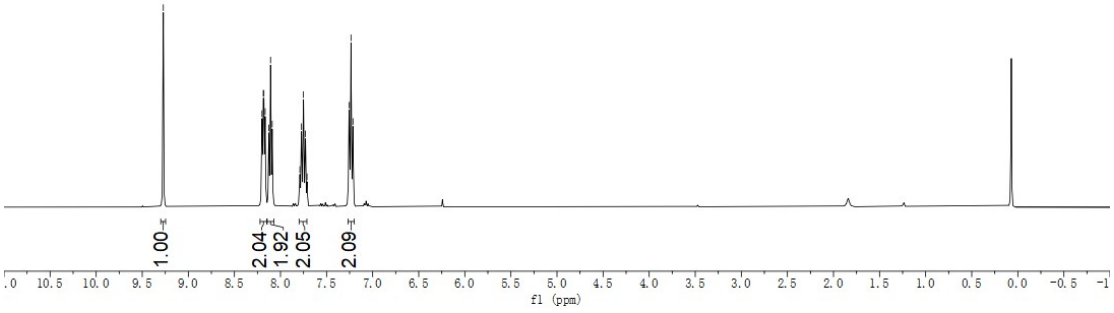


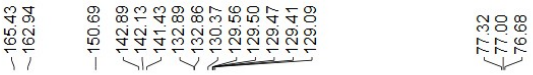


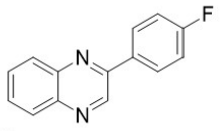
2-(4-fluorophenyl)quinoxaline (3a-20)



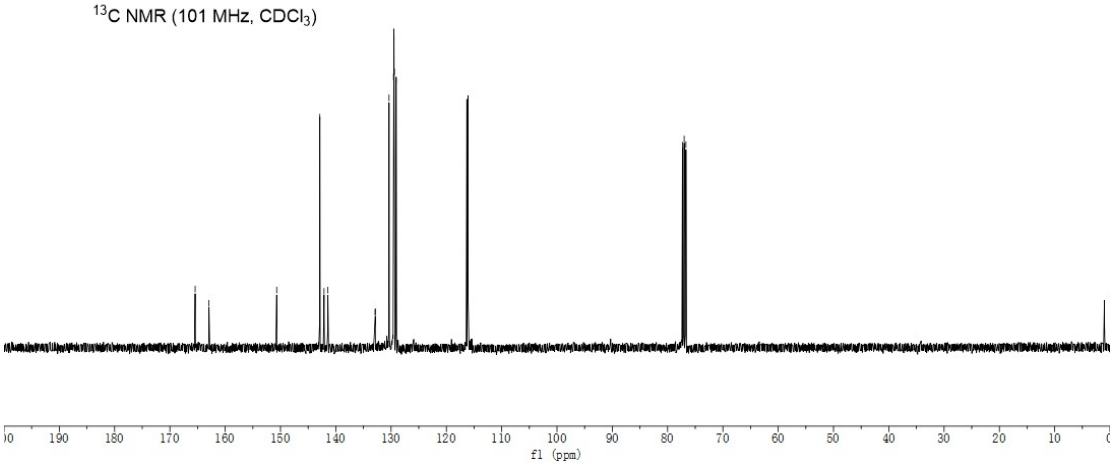
^{1}H NMR (400 MHz, $CDCl_3$)



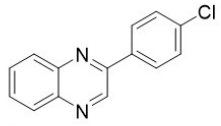




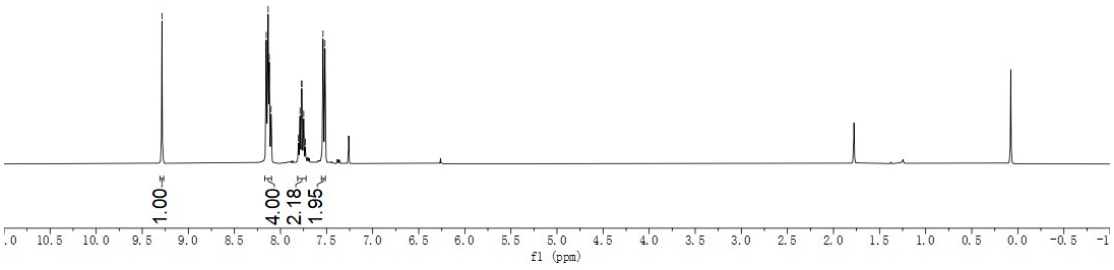
^{13}C NMR (101 MHz, $CDCl_3$)

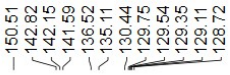


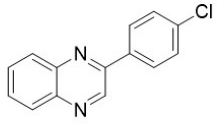
2-(4-chlorophenyl)quinoxaline (3a-21)



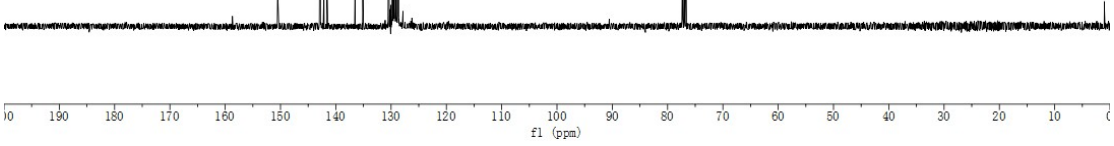
^{1}H NMR (400 MHz, $CDCl_3$)



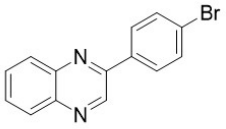




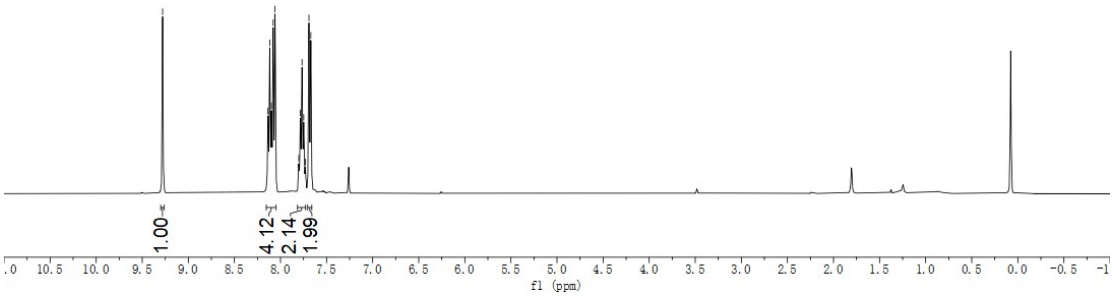
^{13}C NMR (101 MHz, $CDCl_3$)

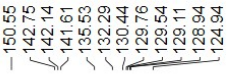


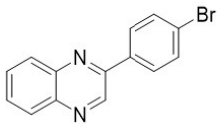
2-(4-bromophenyl)quinoxaline (3a-22)



^{1}H NMR (400 MHz, $CDCl_3$)

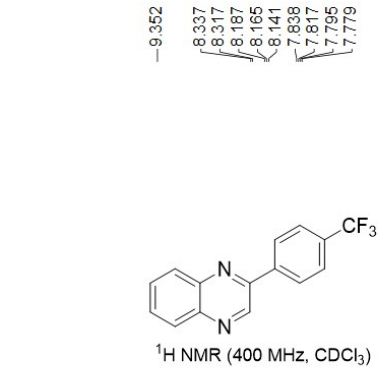




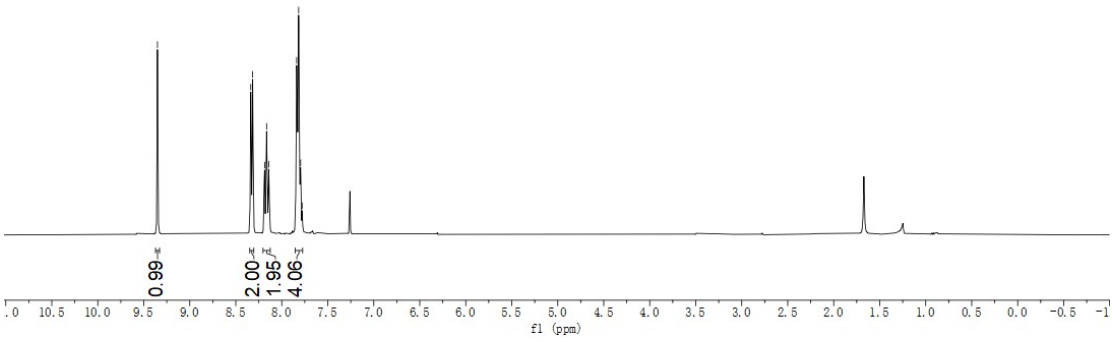


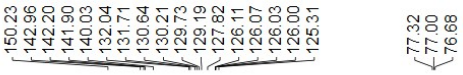
^{13}C NMR (101 MHz, $CDCl_3$)

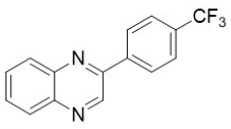
2-(4-(trifluoromethyl)phenyl)quinoxaline (3a-23)



^{1}H NMR (400 MHz, $CDCl_3$)

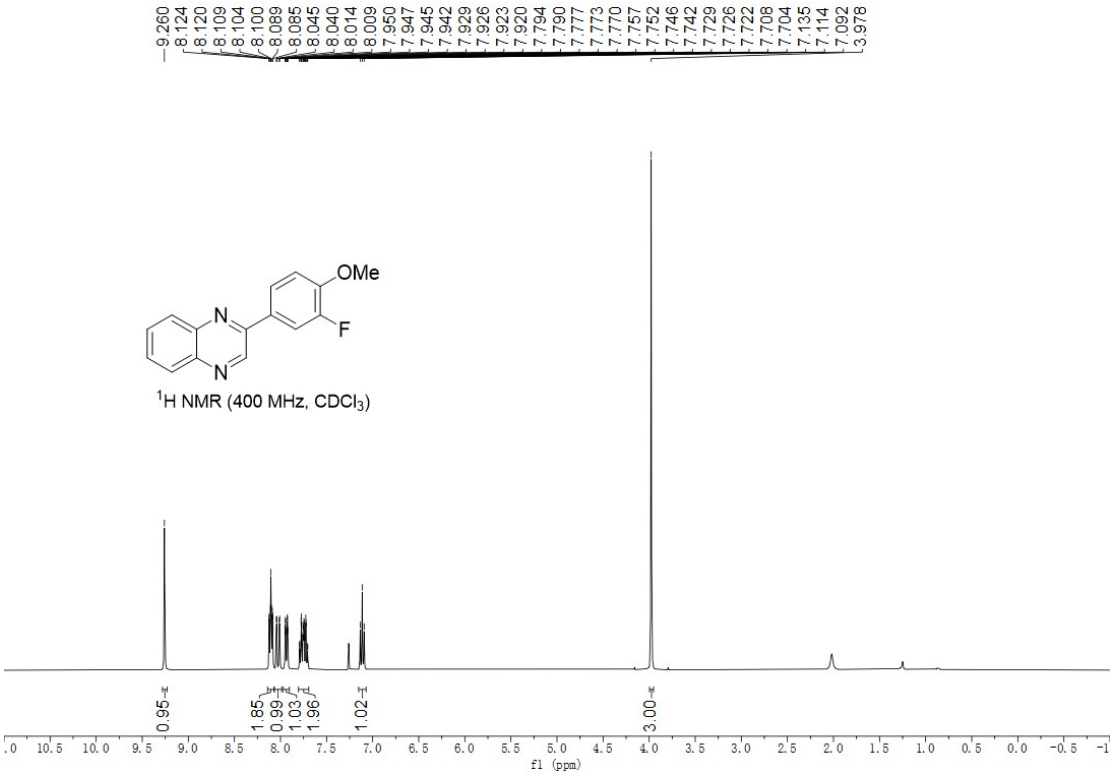


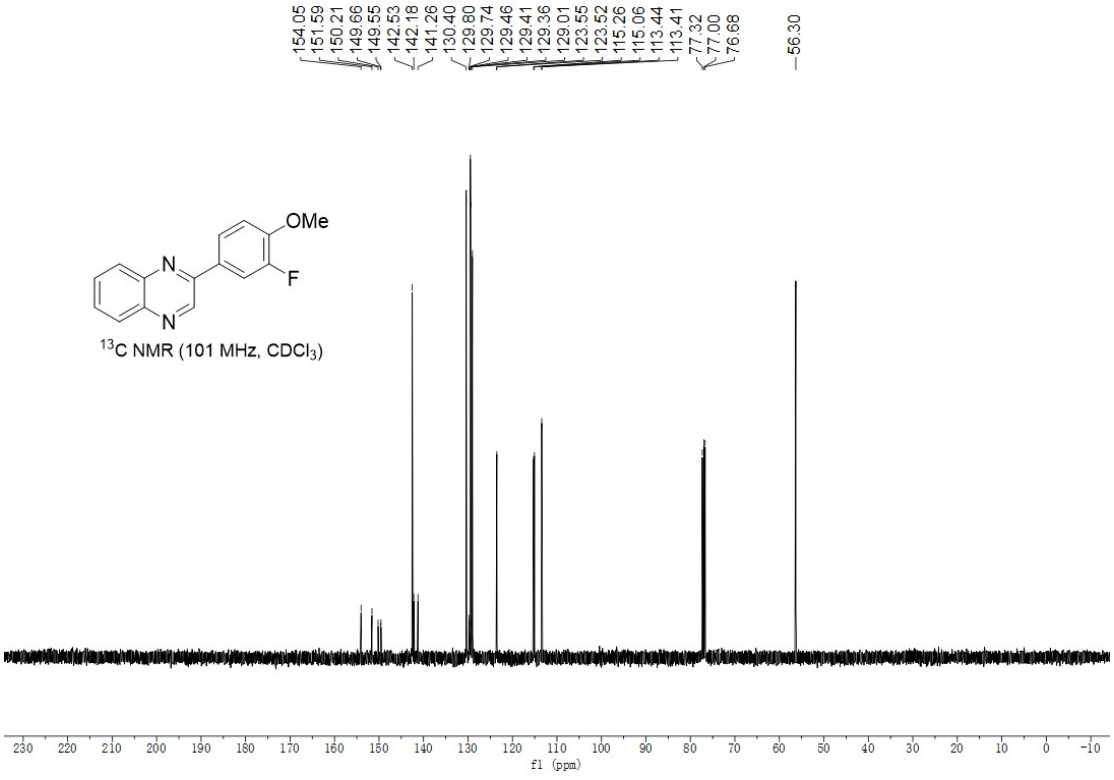




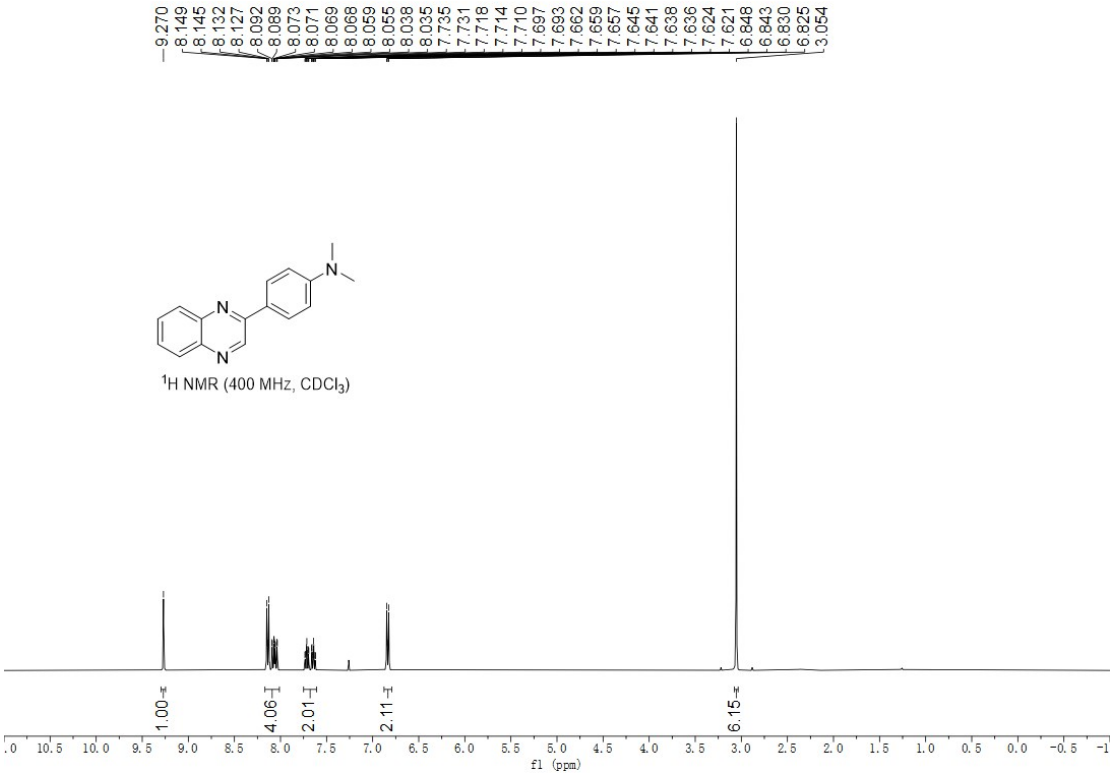
^{13}C NMR (101 MHz, $CDCl_3$)

2-(3-fluoro-4-methoxyphenyl)quinoxaline (3a-24)

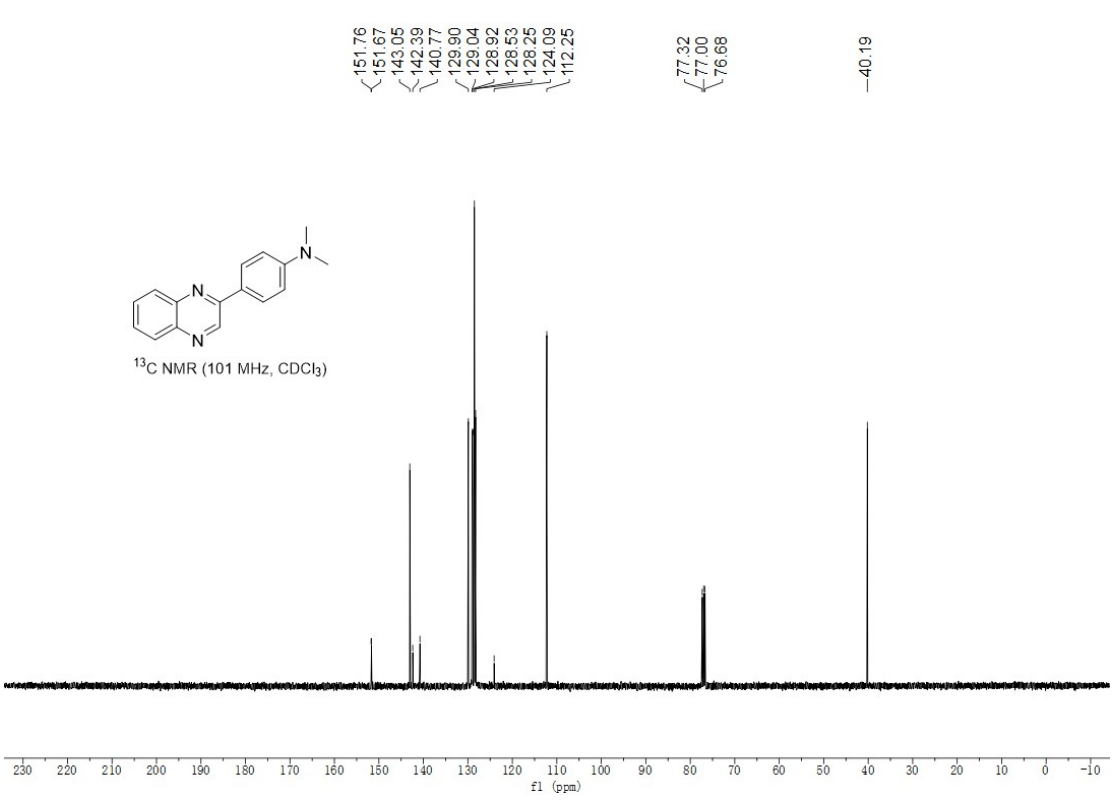




N,N-dimethyl-4-(quinoxalin-2-yl)aniline (3a-25)

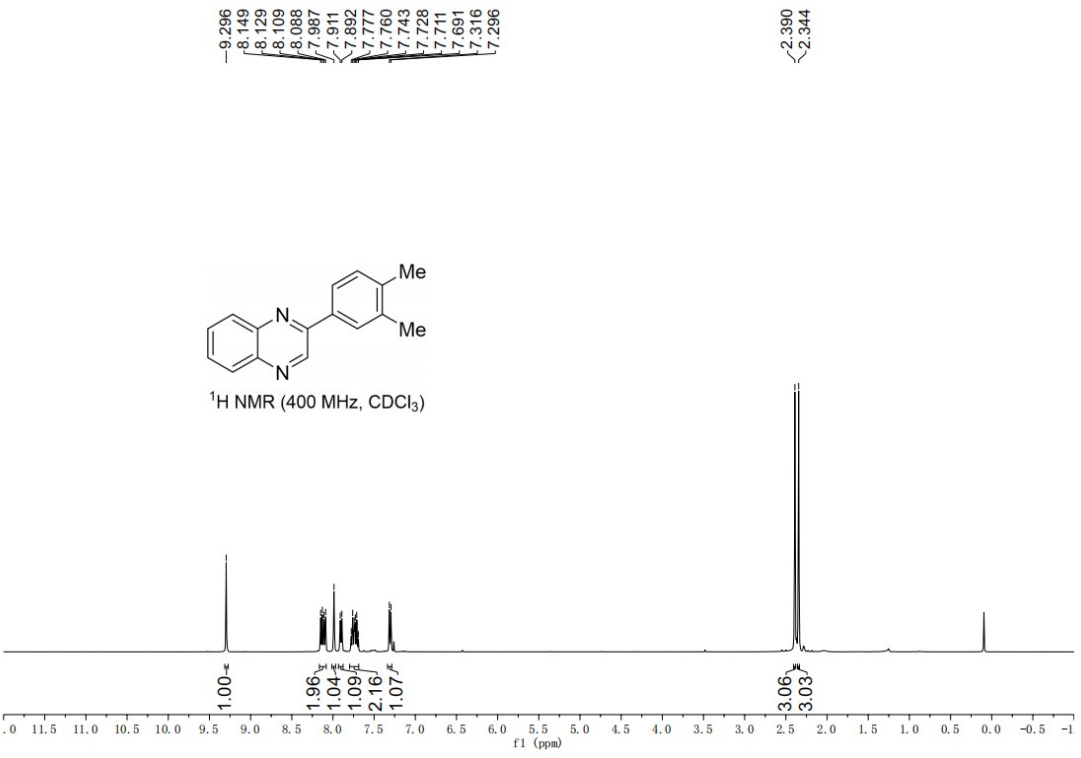


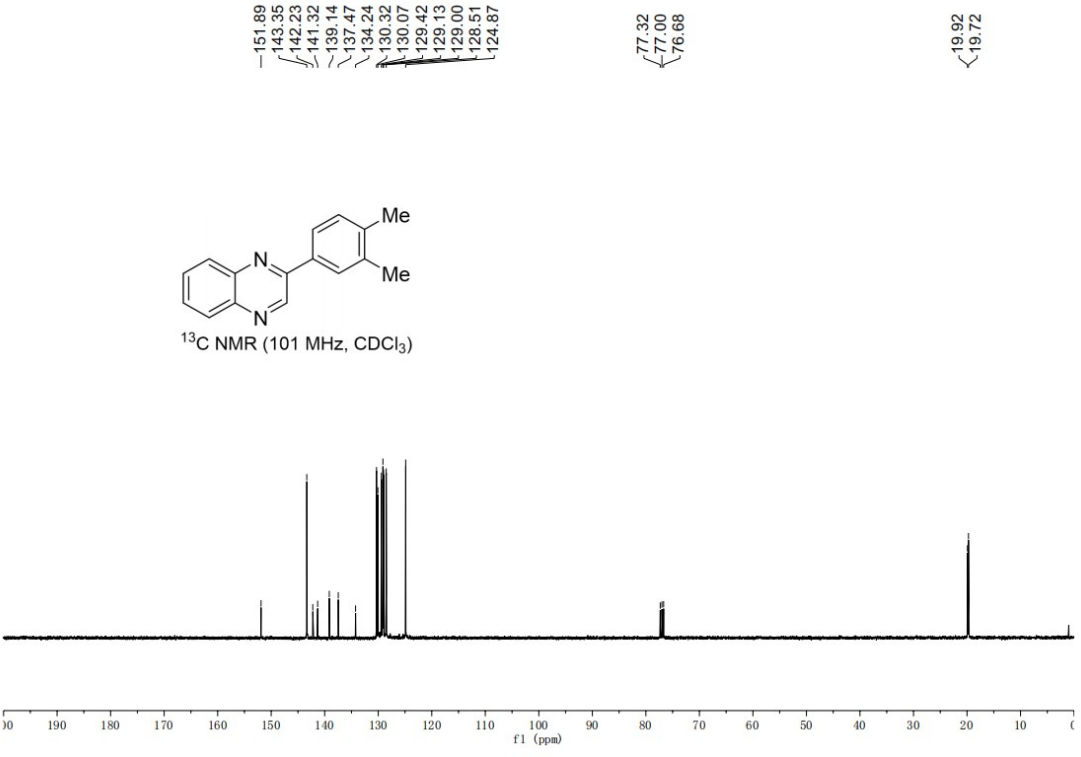
^{1}H NMR (400 MHz, $CDCl_3$)



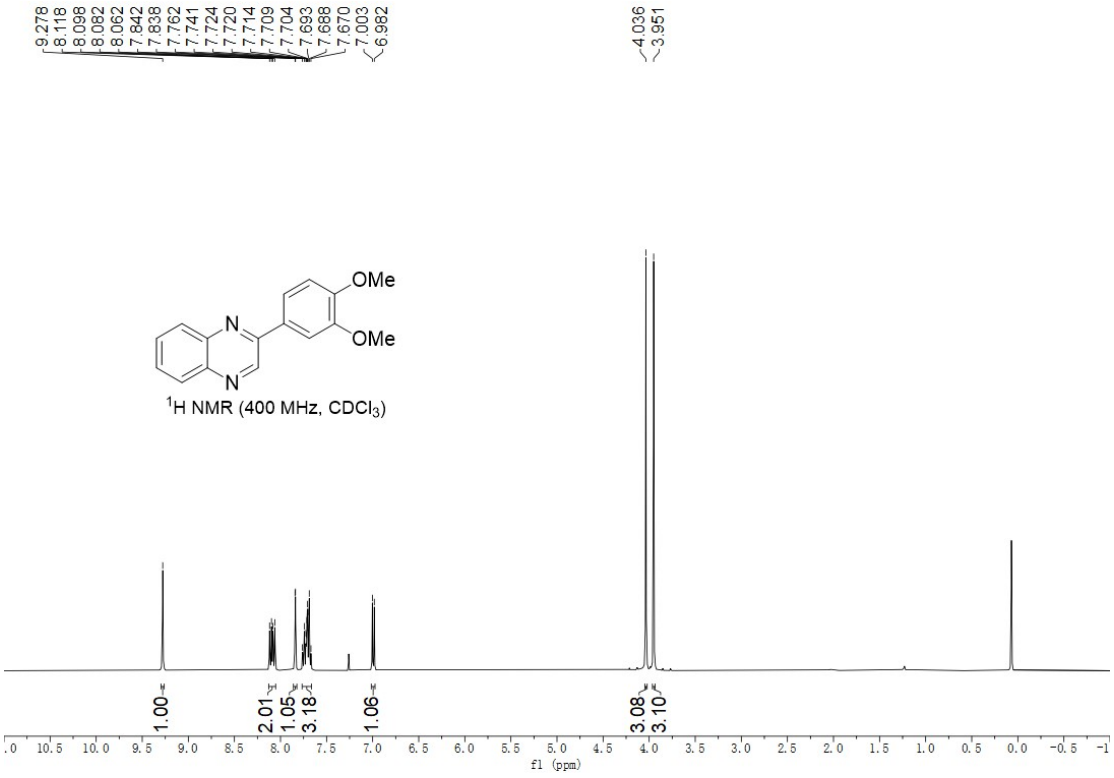
^{13}C NMR (101 MHz, $CDCl_3$)

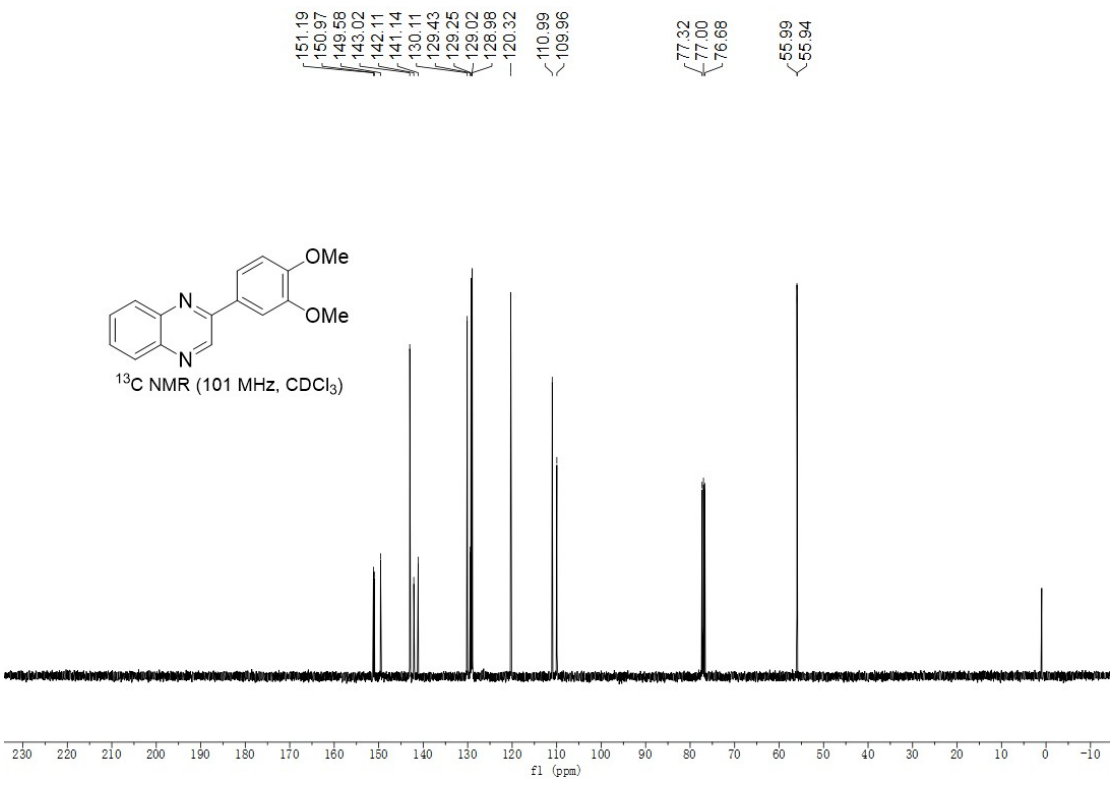
2-(3,4-dimethylphenyl)quinoxaline (3a-26)



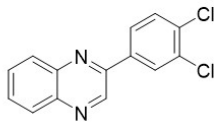


2-(3,4-dimethoxyphenyl)quinoxaline (3a-27)

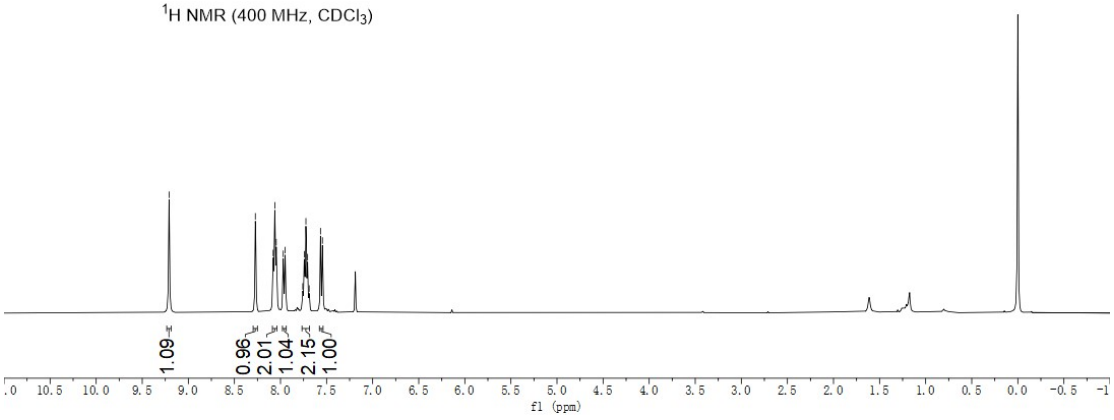


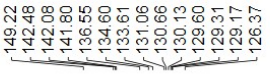


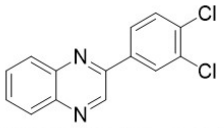
2-(3,4-dichlorophenyl)quinoxaline (3a-28)



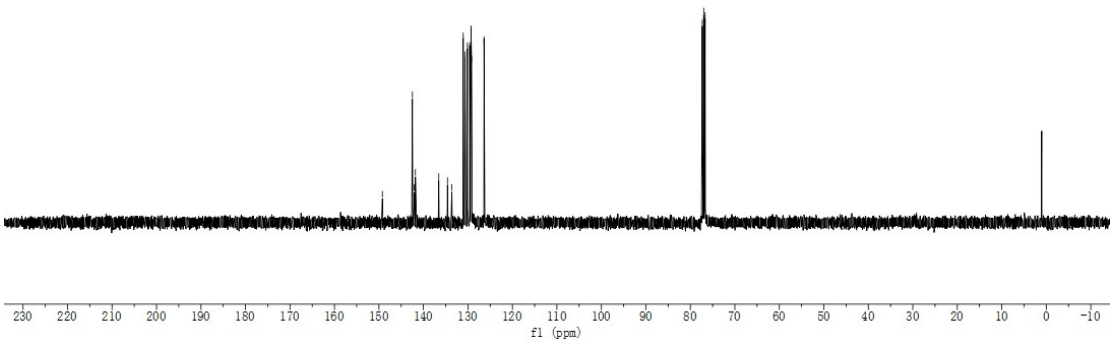
^{1}H NMR (400 MHz, $CDCl_3$)



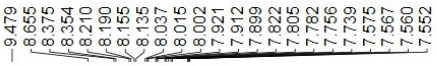


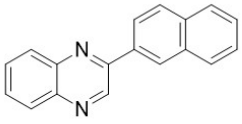


^{13}C NMR (101 MHz, $CDCl_3$)

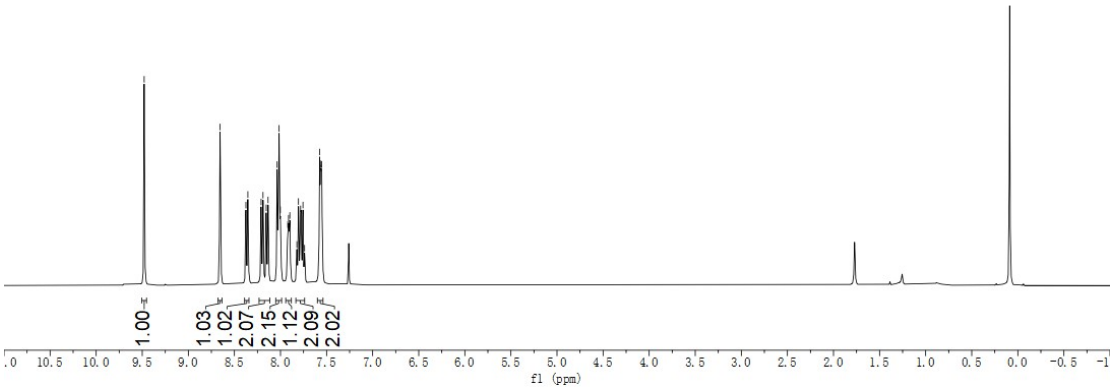


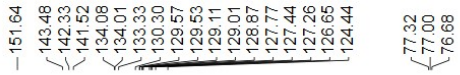
2-(naphthalen-2-yl)quinoxaline (3a-29)

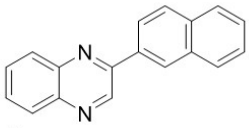




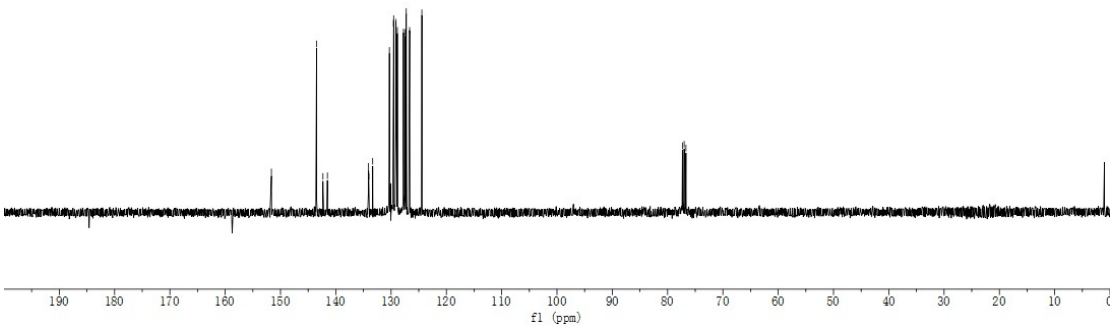
^{1}H NMR (400 MHz, $CDCl_3$)



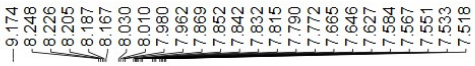


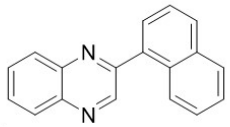


^{13}C NMR (101 MHz, $CDCl_3$)

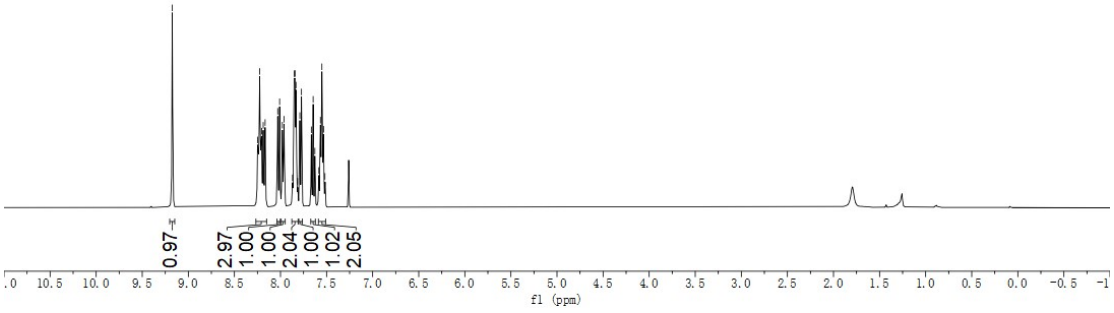


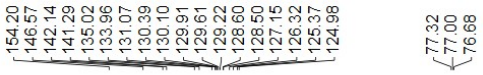
2-(naphthalen-1-yl)quinoxaline (3a-30)

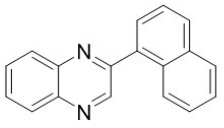




^{1}H NMR (400 MHz, $CDCl_3$)

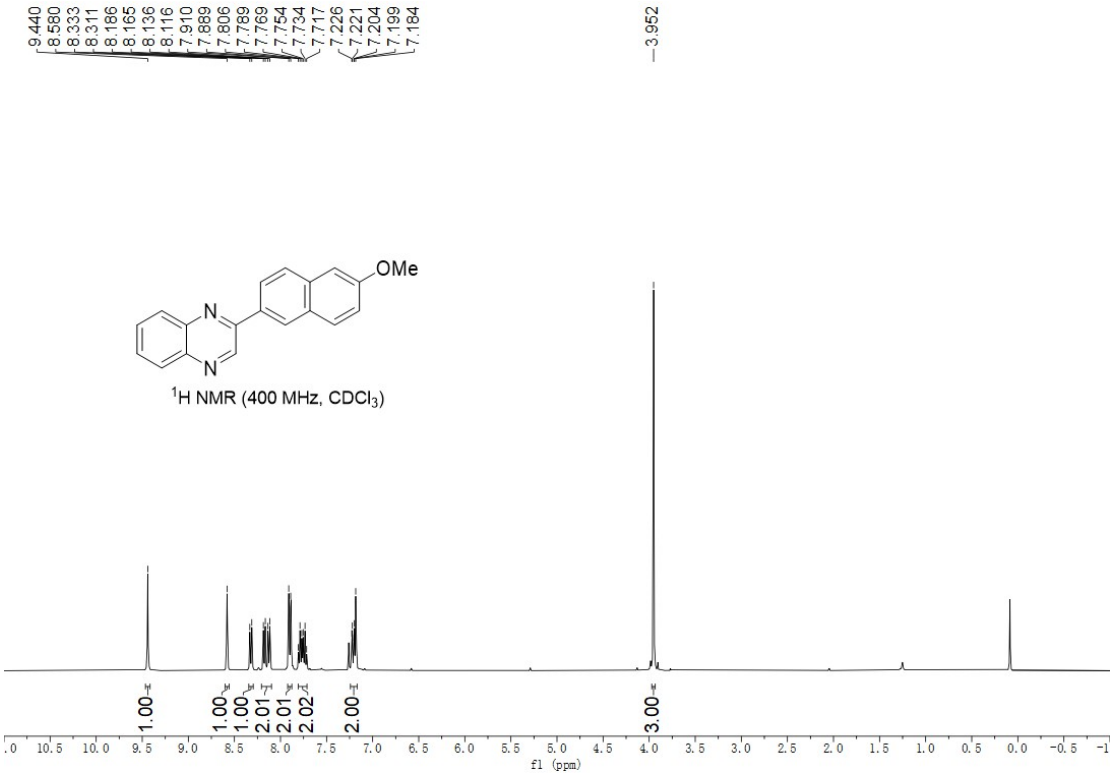


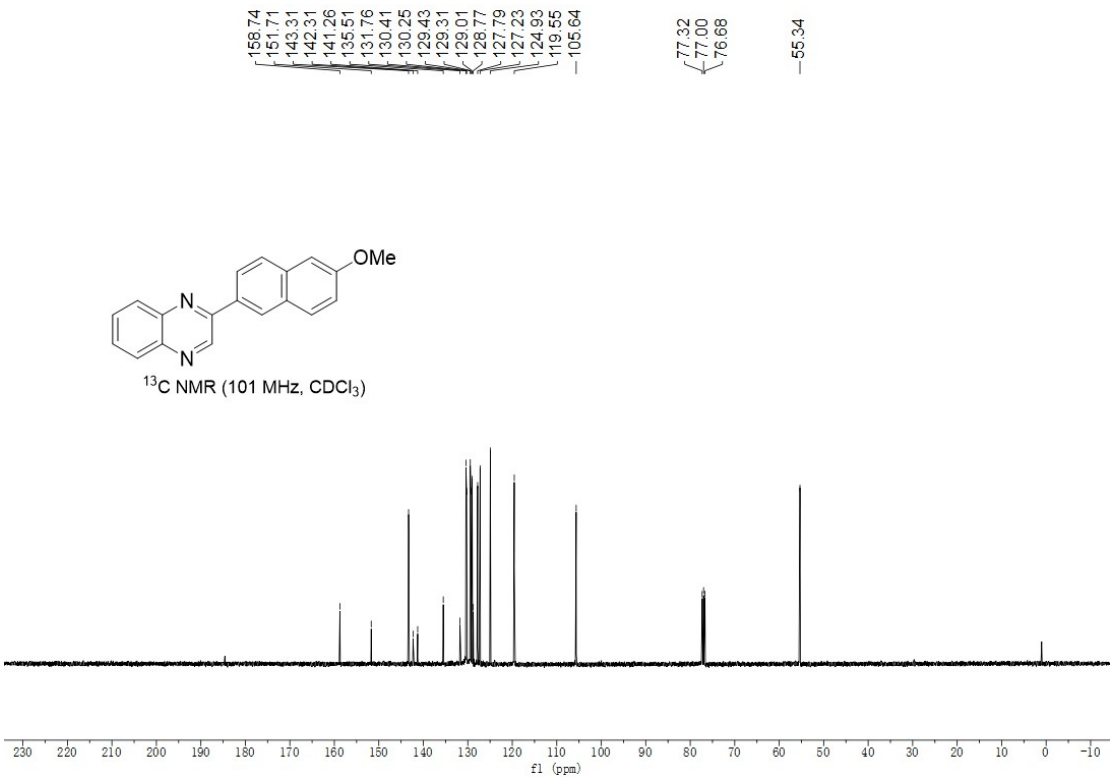




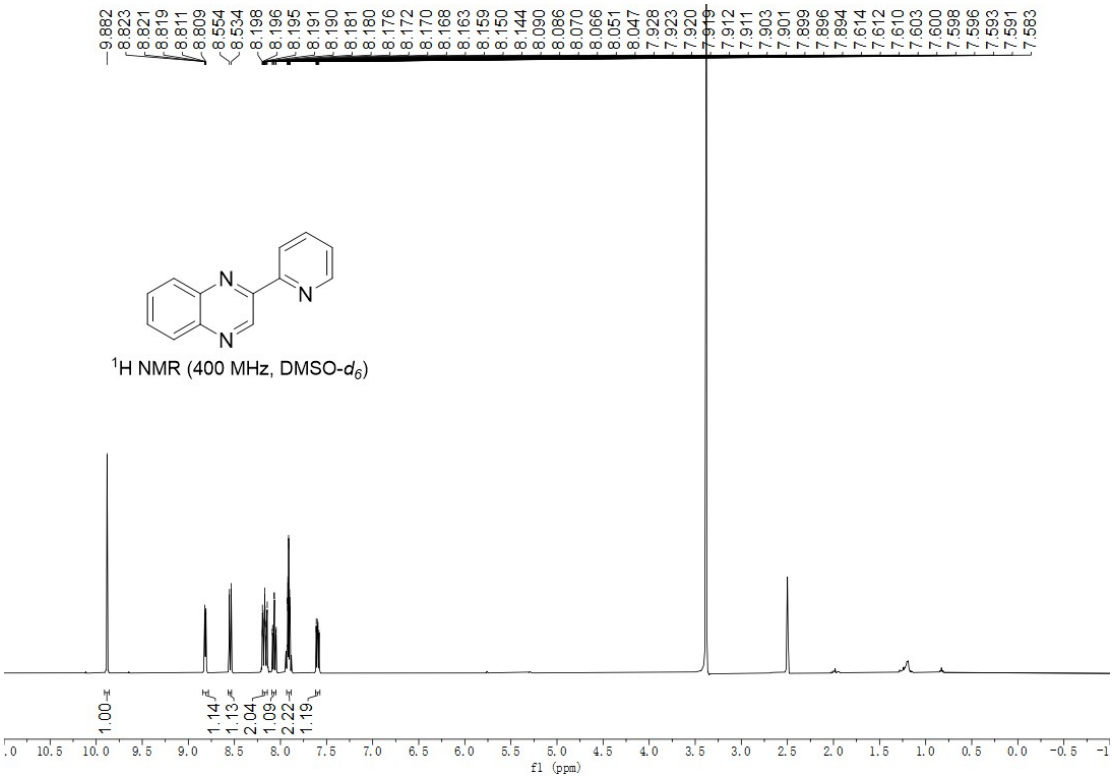
^{13}C NMR (101 MHz, $CDCl_3$)

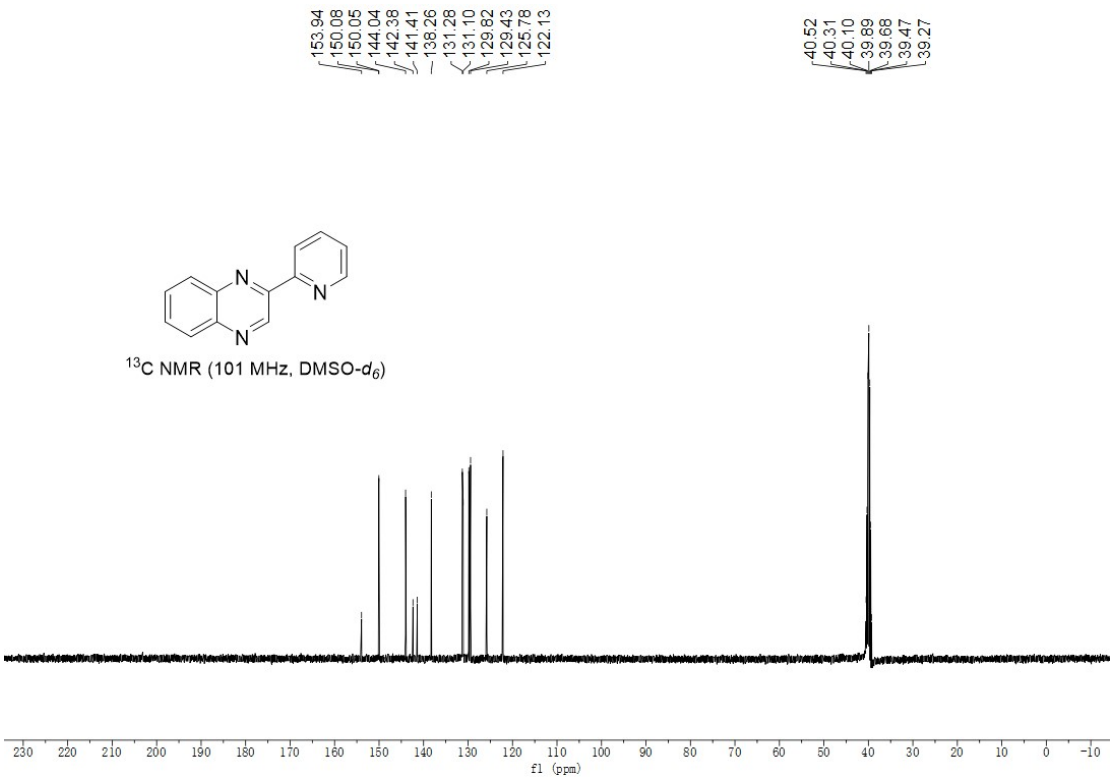
2-(6-methoxynaphthalen-2-yl)quinoxaline (3a-31)



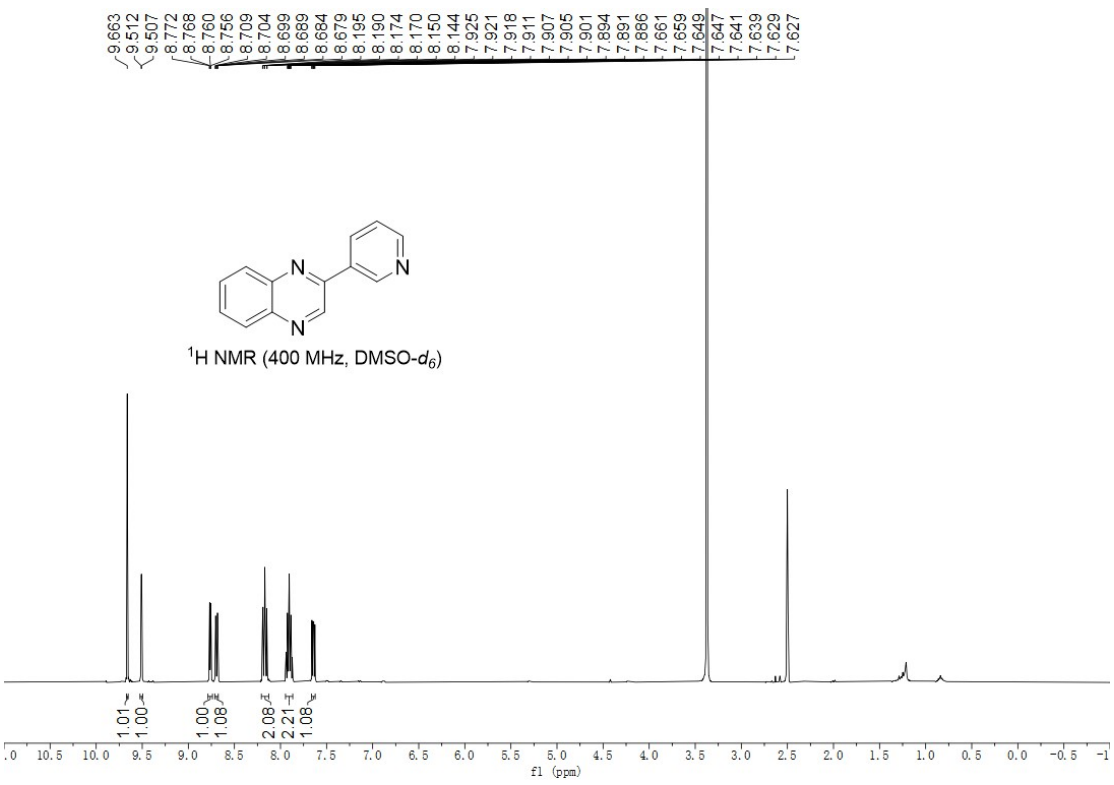


2-(pyridin-2-yl)quinoxaline (3a-32)

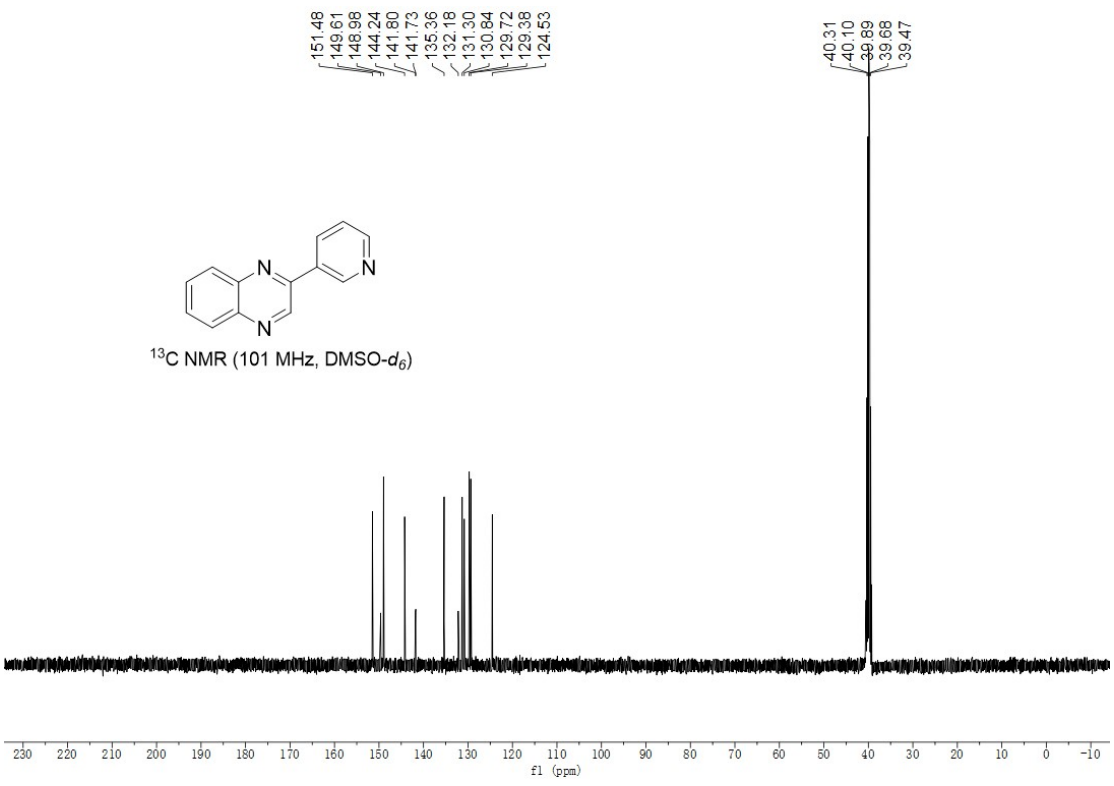




2-(pyridin-3-yl)quinoxaline (3a-33)

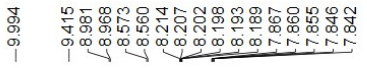


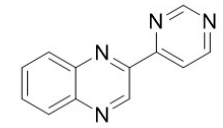
^{1}H NMR (400 MHz, DMSO-d_6)



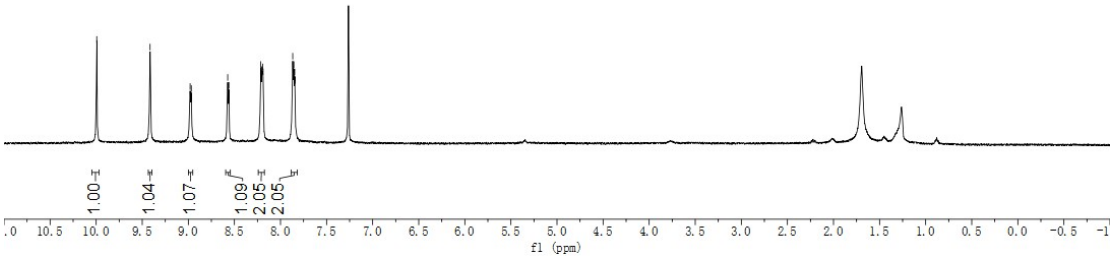
^{13}C NMR (101 MHz, DMSO-d_6)

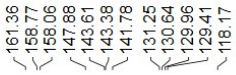
2-(pyrimidin-4-yl)quinoxaline (3a-34)

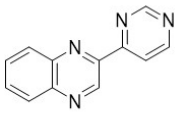




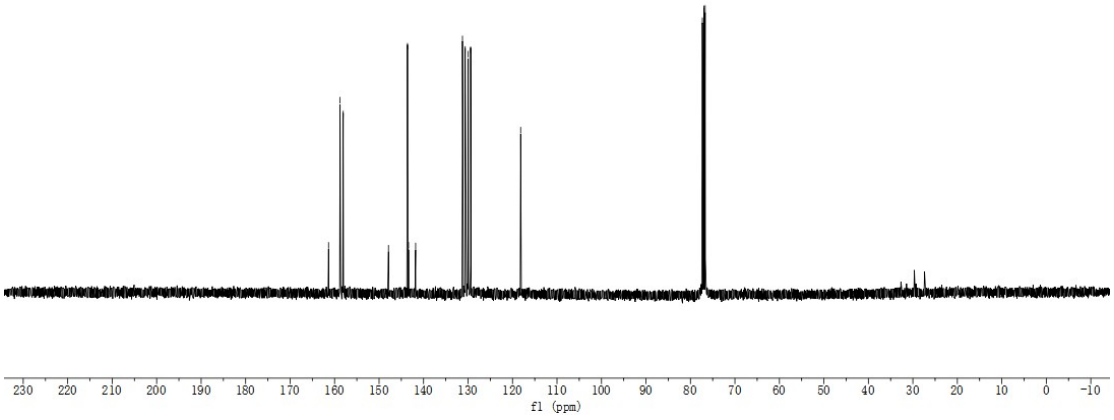
^{1}H NMR (400 MHz, $CDCl_3$)



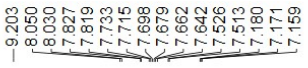


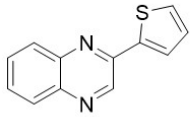


^{13}C NMR (101 Mhz, $CDCl_3$)

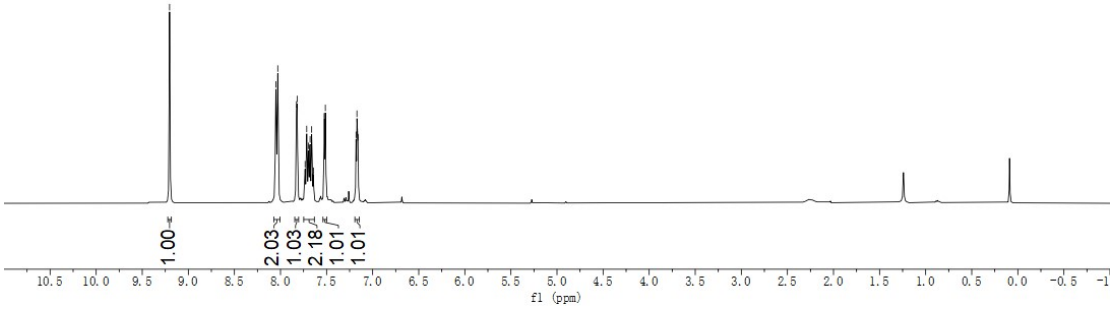


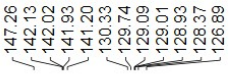
2-(thiophen-2-yl)quinoxaline (3a-35)

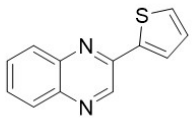




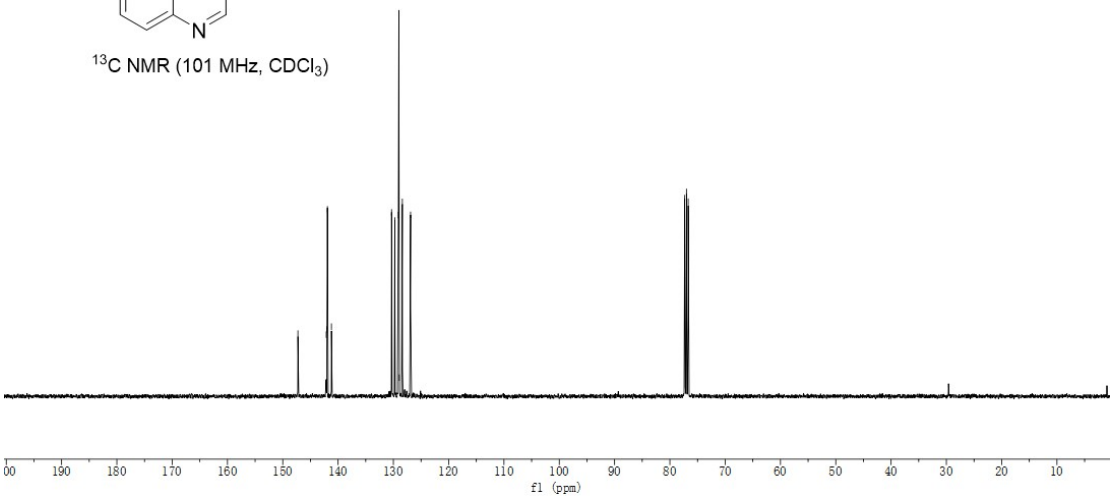
^{1}H NMR (400 MHz, $CDCl_3$)



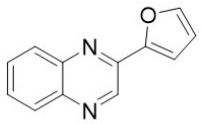




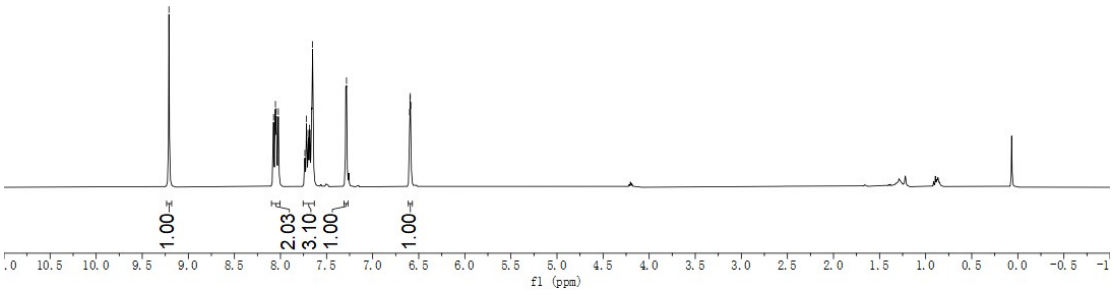
^{13}C NMR (101 MHz, $CDCl_3$)

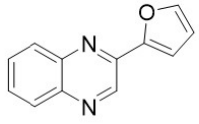


2-(furan-2-yl)quinoxaline (3a-36)

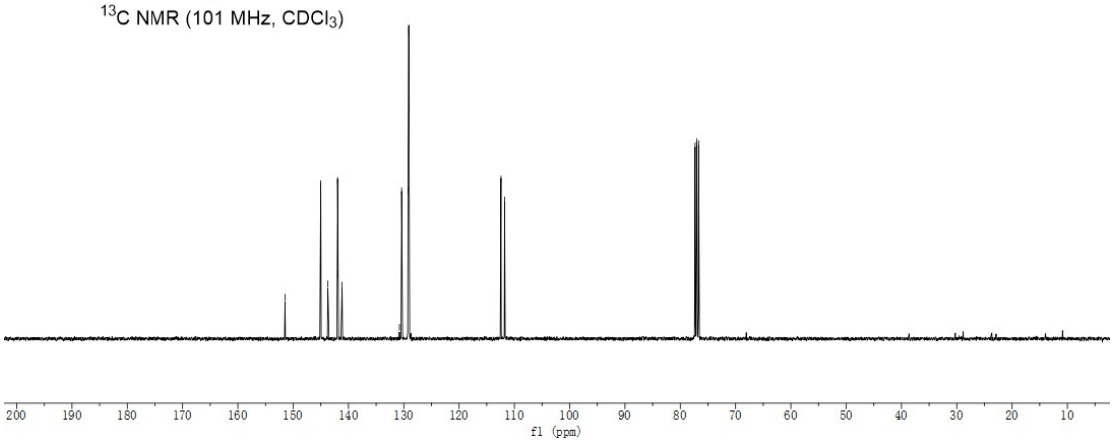


^{1}H NMR (400 MHz, $CDCl_3$)

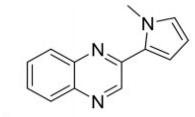




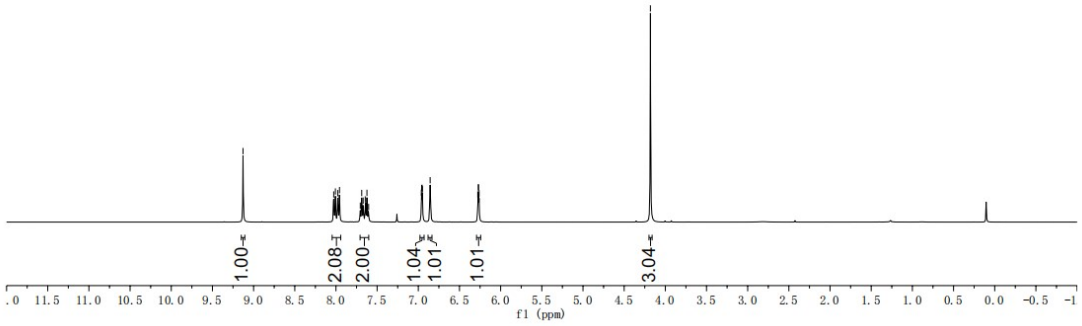
^{13}C NMR (101 MHz, $CDCl_3$)

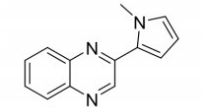


2-(1-methyl-1H-pyrrol-2-yl)quinoxaline (3a-37)

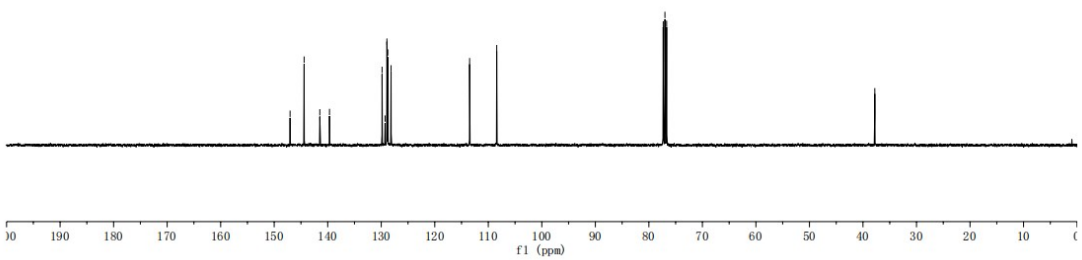


^{1}H NMR (400 MHz, $CDCl_3$)

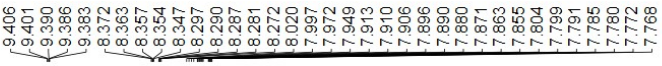


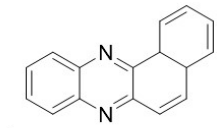


^{13}C NMR (101 MHz, $CDCl_3$)

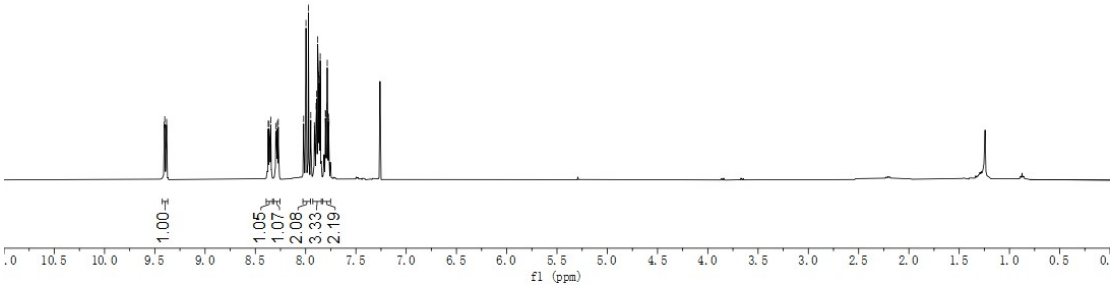


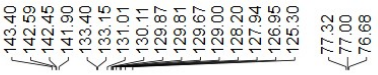
Benzo[a]phenazine (3b-1)

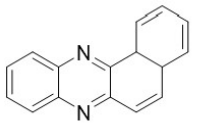




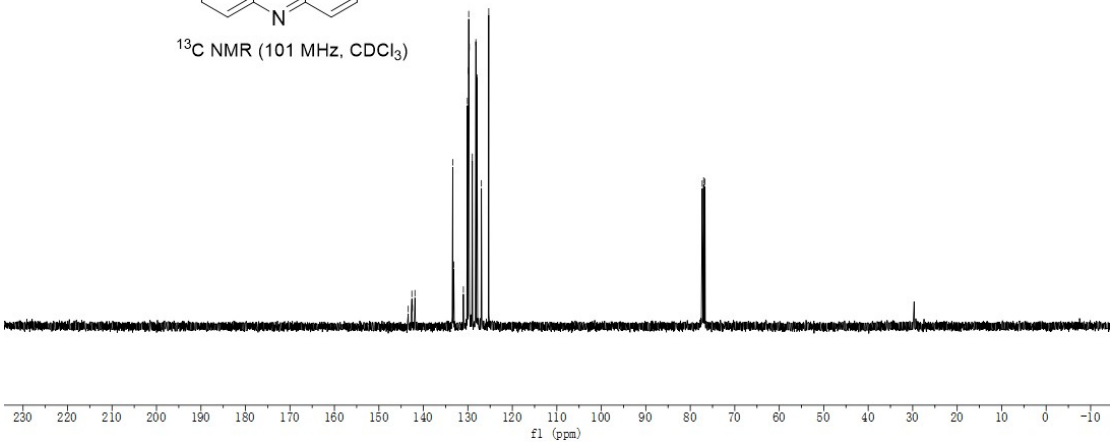
^{1}H NMR (400 MHz, $CDCl_3$)



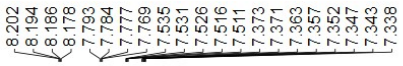


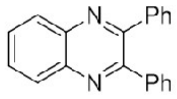


^{13}C NMR (101 MHz, $CDCl_3$)

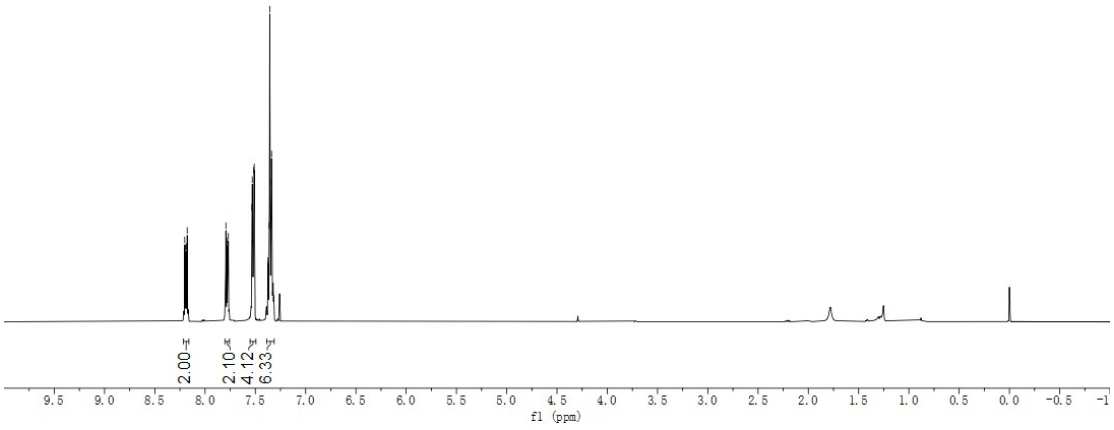


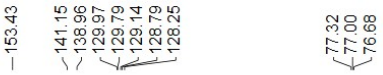
2,3-diphenylquinoxaline (3b-2)

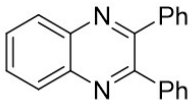




^{1}H NMR (400 MHz, $CDCl_3$)

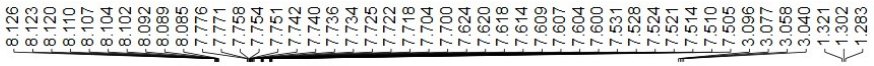


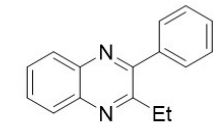




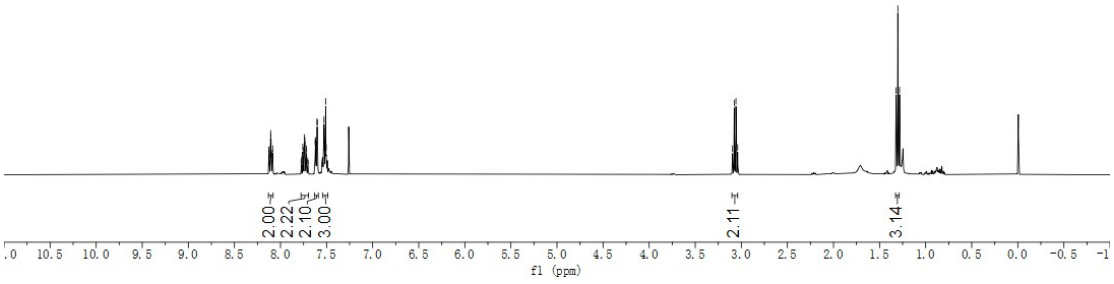
^{13}C NMR (101 MHz, $CDCl_3$)

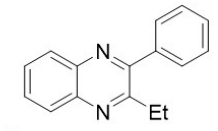
2-ethyl-3-phenylquinoxaline (3b-3)





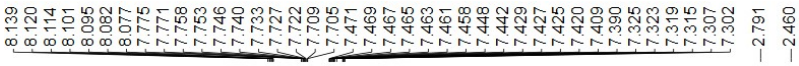
^{1}H NMR (400 MHz, $CDCl_3$)

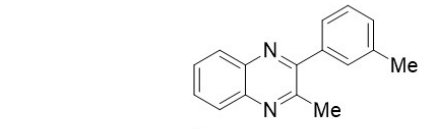




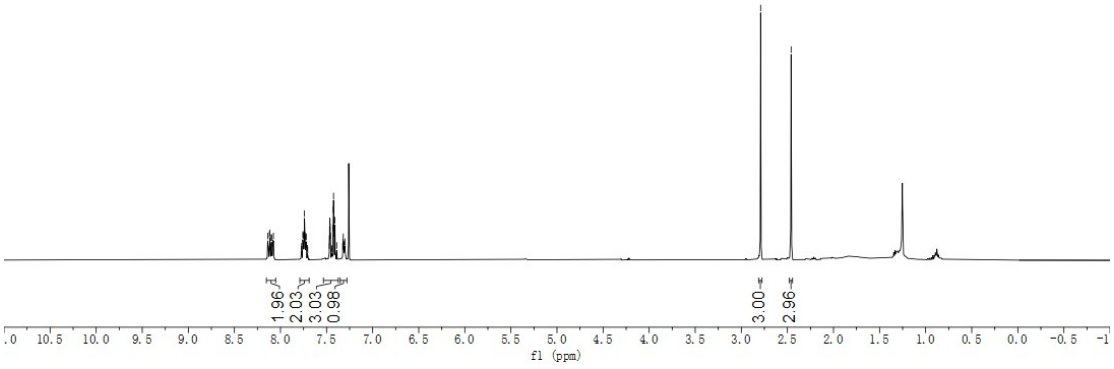
^{13}C NMR (101 MHz, $CDCl_3$)

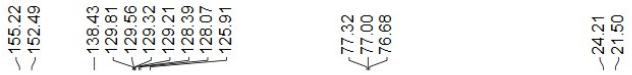
2-methyl-3-(m-tolyl)quinoxaline (3b-4)

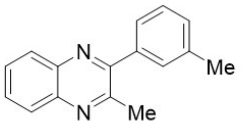




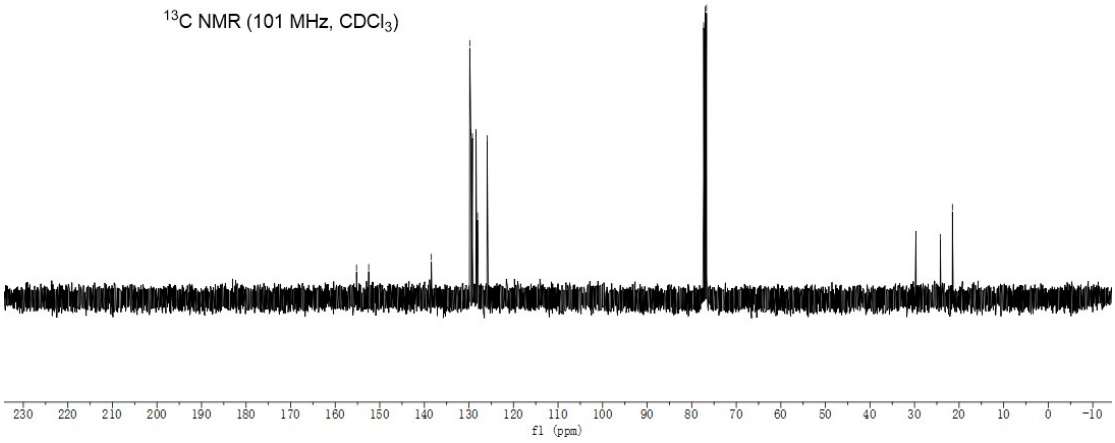
^{1}H NMR (400 MHz, $CDCl_3$)



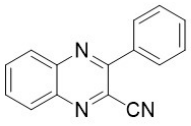




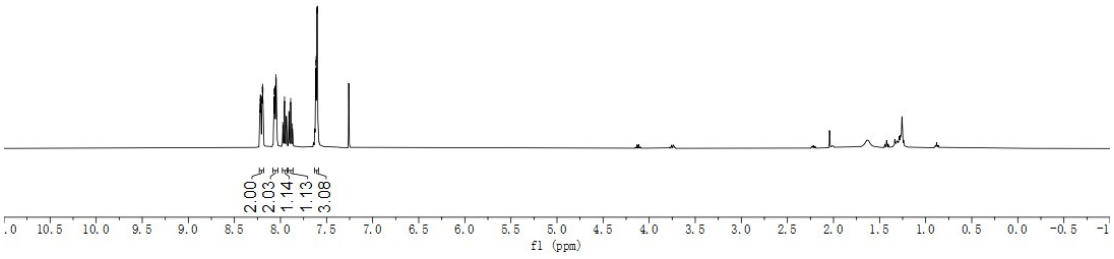
^{13}C NMR (101 MHz, $CDCl_3$)

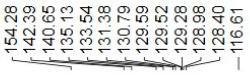


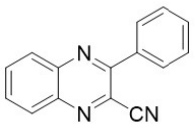
2-phenylquinoxaline-2-carbonitrile (3b-5)



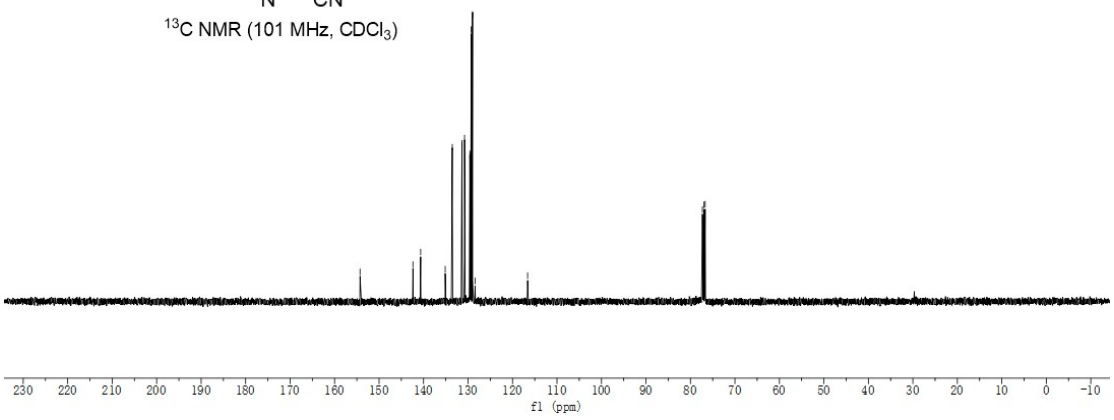
^{1}H NMR (400 MHz, $CDCl_3$)



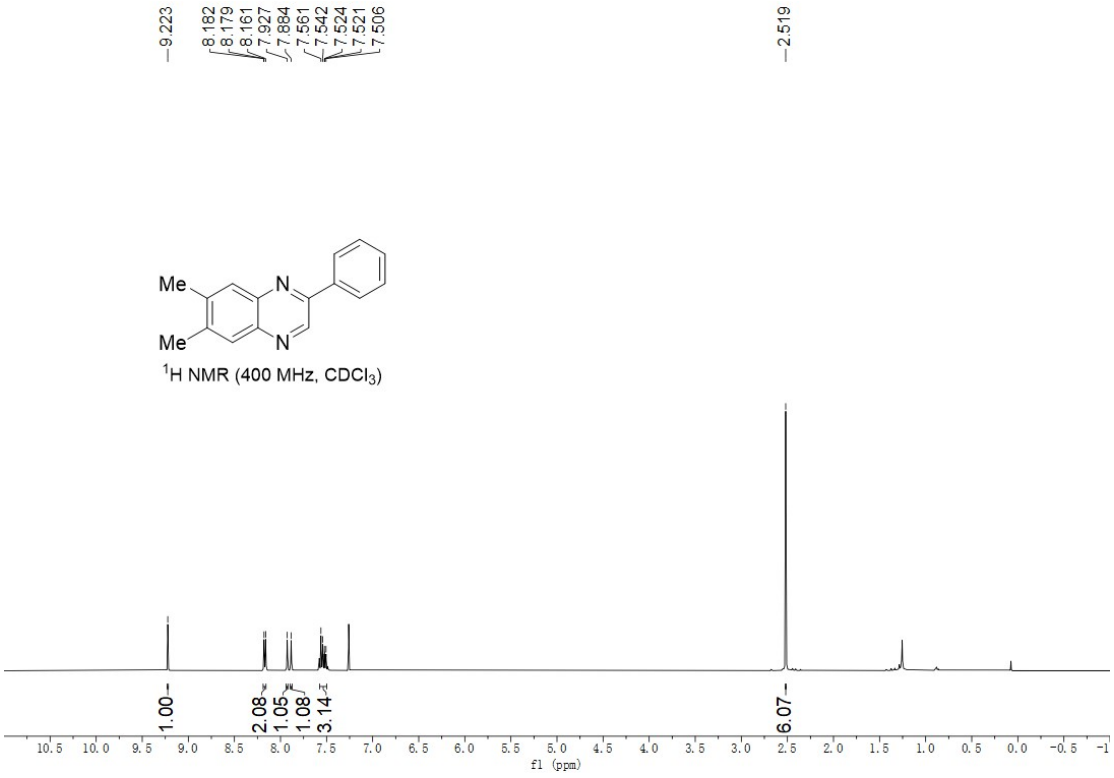


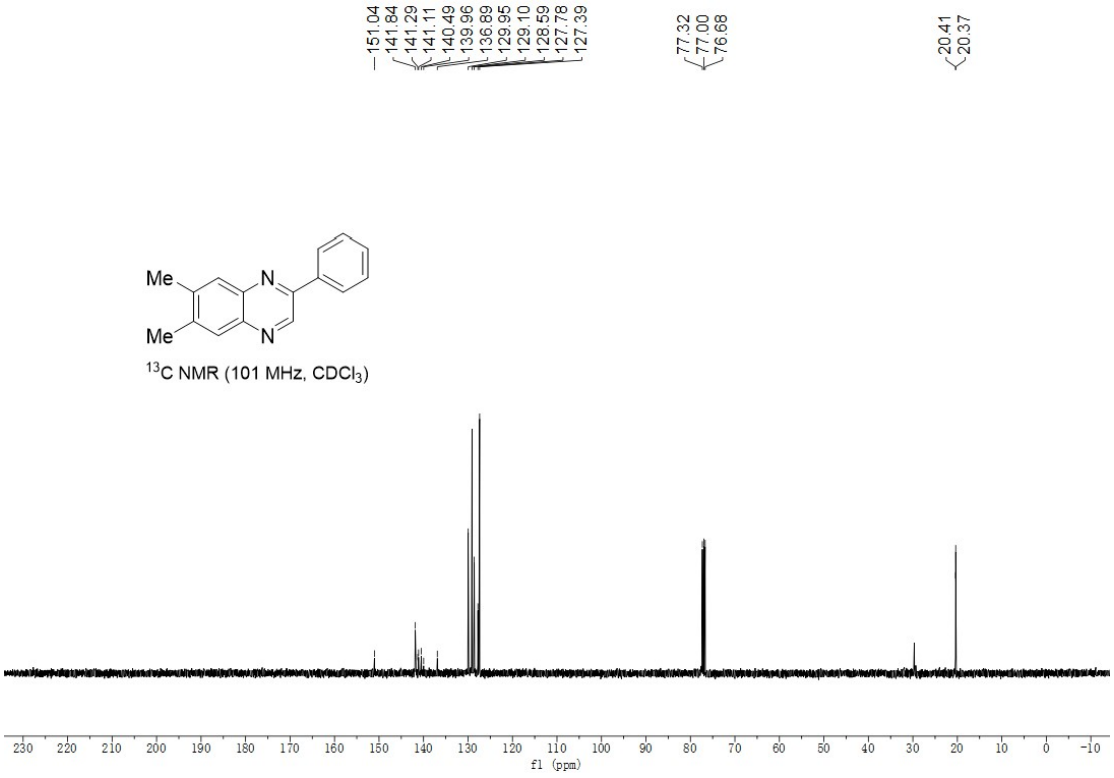


^{13}C NMR (101 MHz, $CDCl_3$)

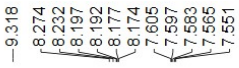


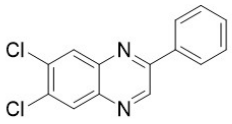
6,7-dimethyl-2-phenylquinoxaline (3c-1)



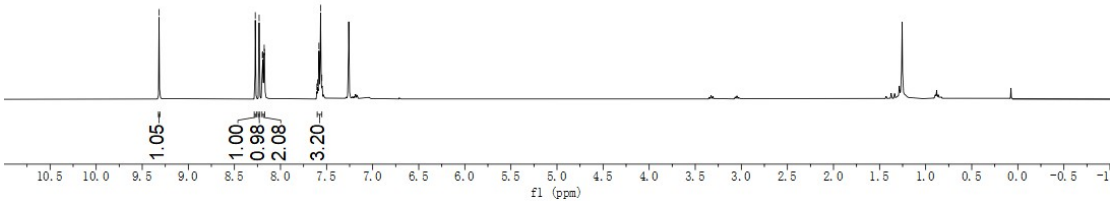


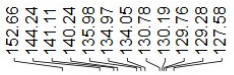
6,7-dichloro-2-phenylquinoxaline (3c-2)

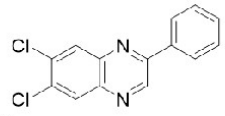




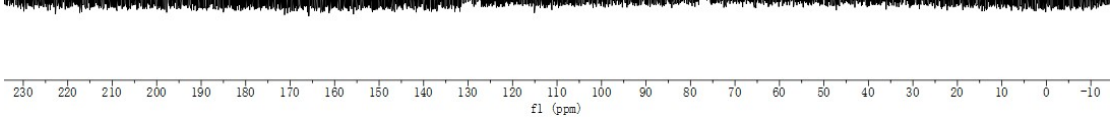
^{1}H NMR (400 MHz, $CDCl_3$)



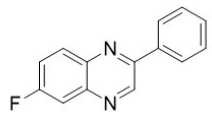




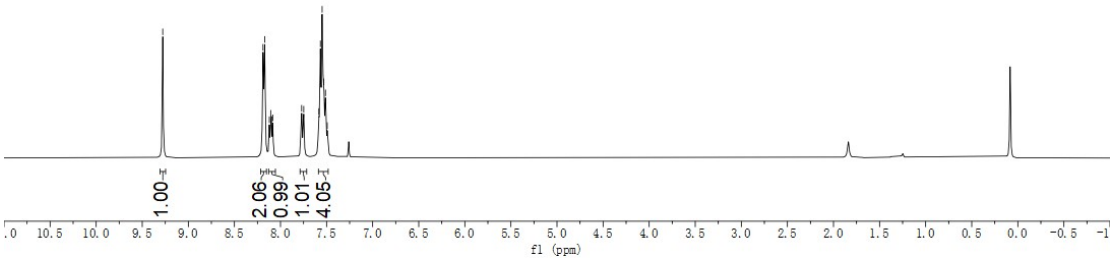
^{13}C NMR (101 MHz, $CDCl_3$)

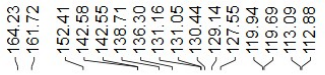


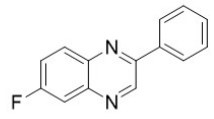
6-fluoro-2-phenylquinoxaline (3c-3)



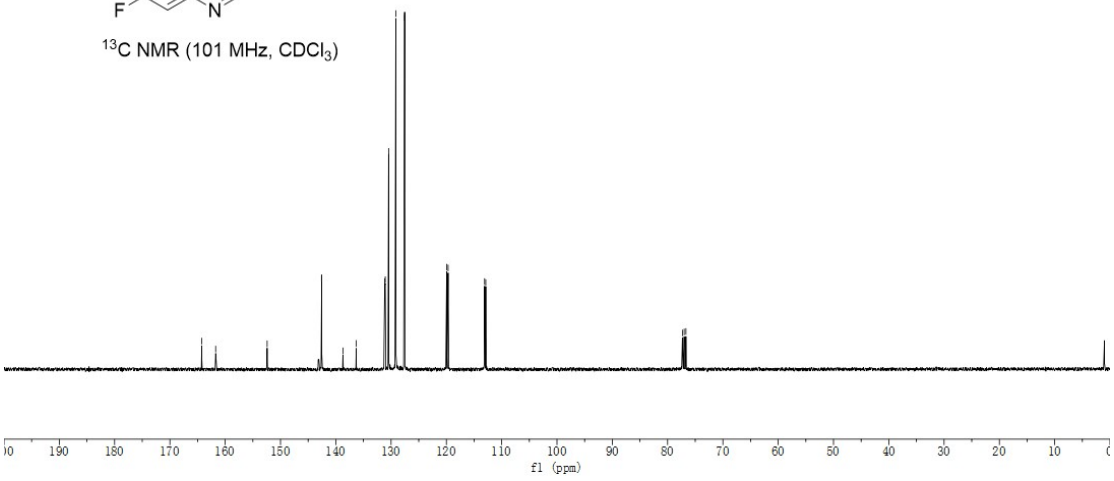
^{1}H NMR (400 MHz, $CDCl_3$)



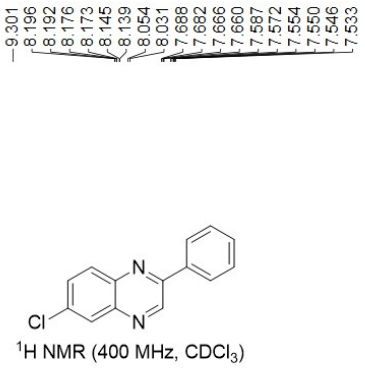


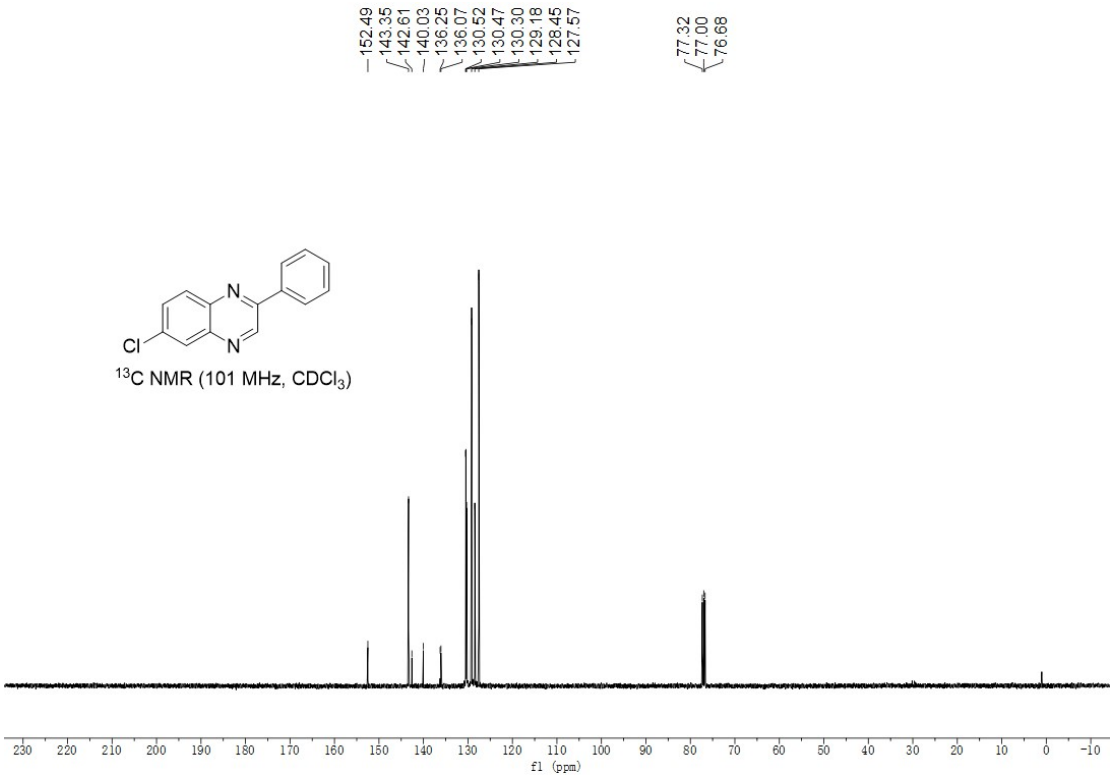


^{13}C NMR (101 MHz, $CDCl_3$)

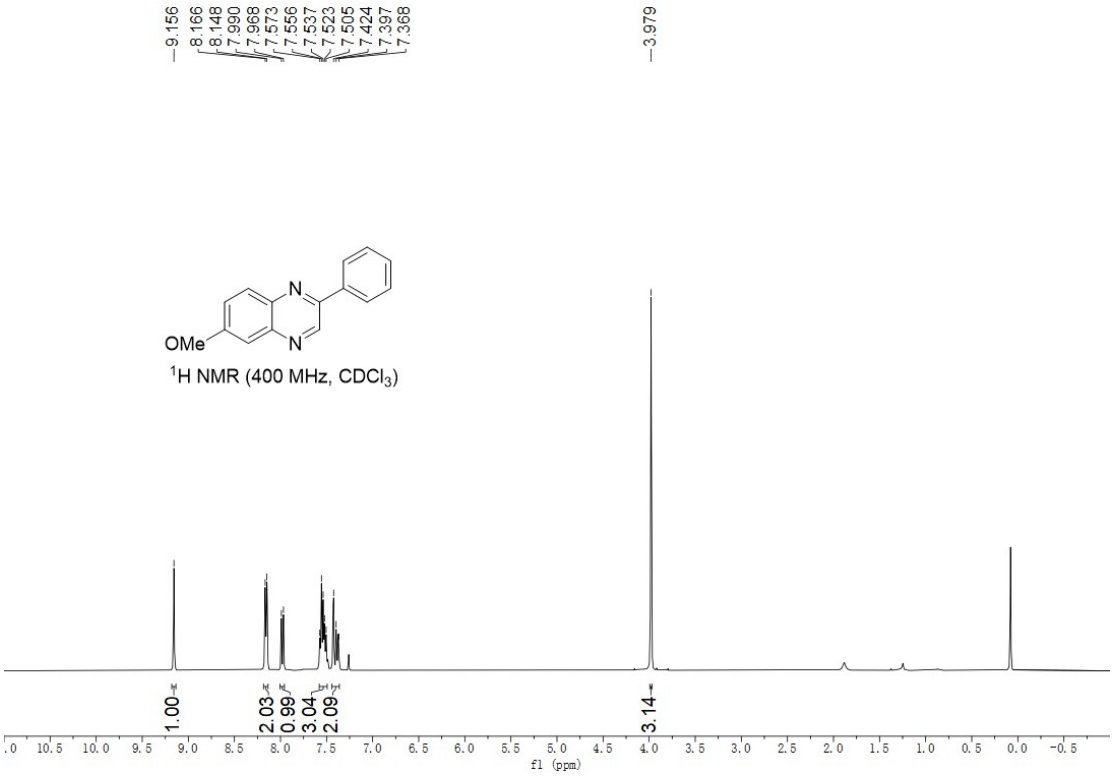


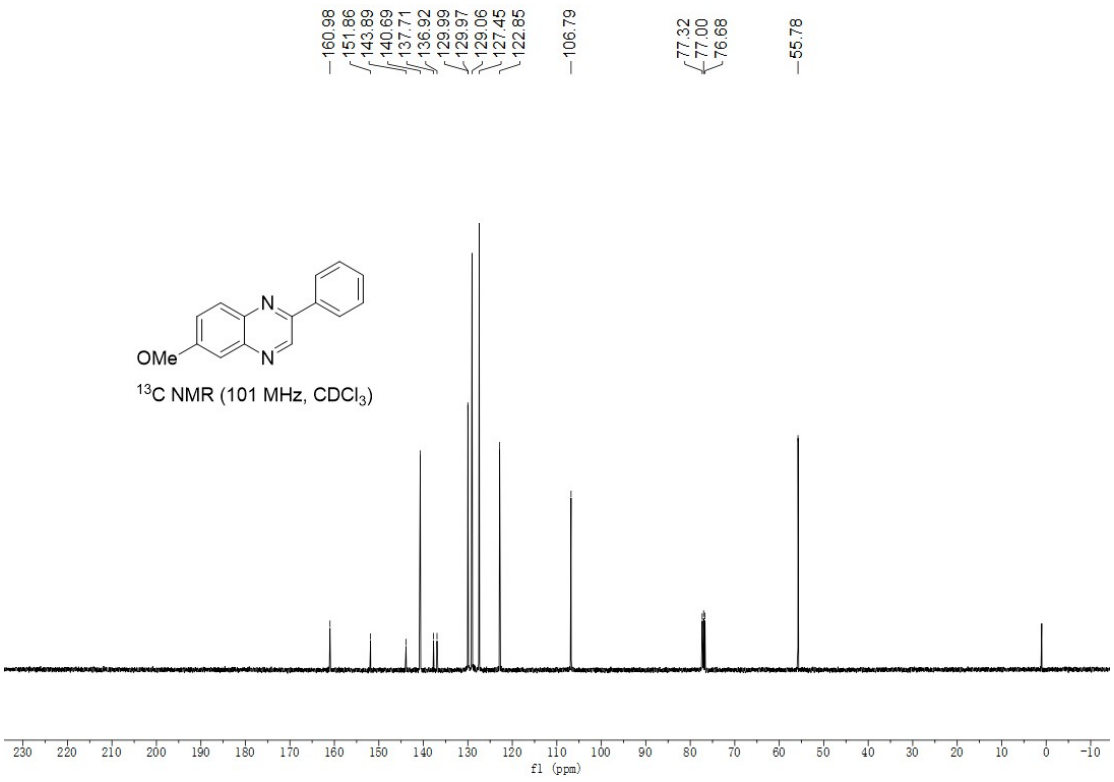
6-chloro-2-phenylquinoxaline (3c-4)



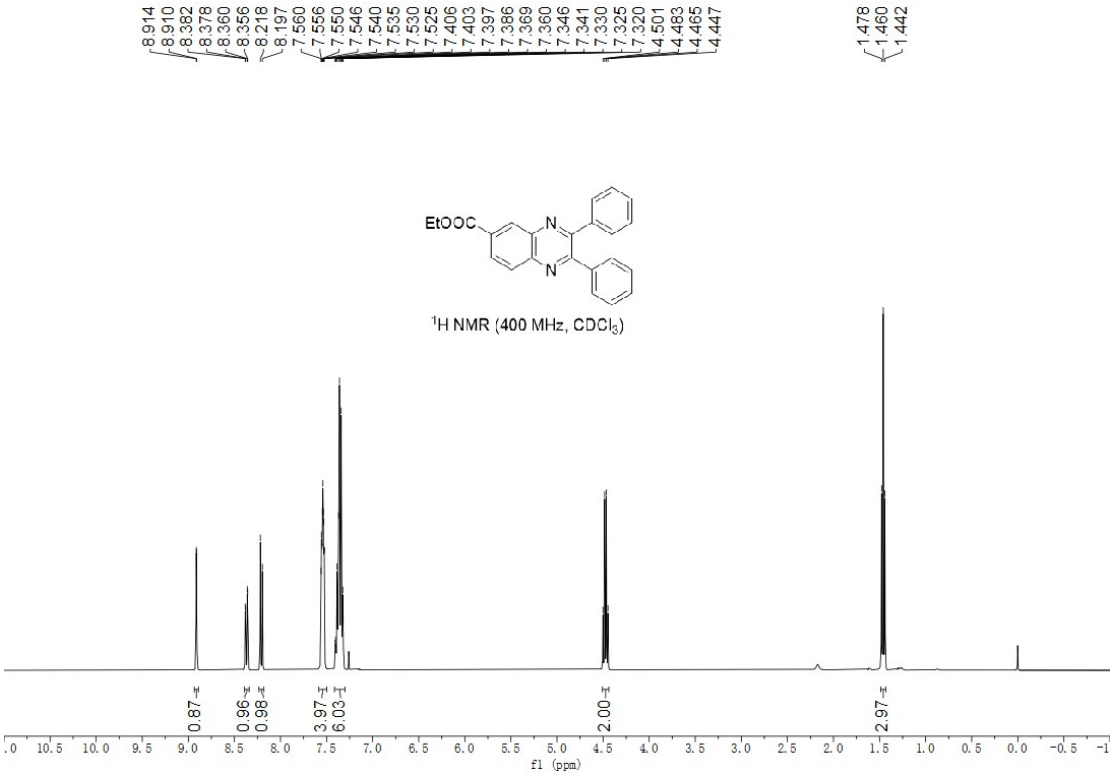


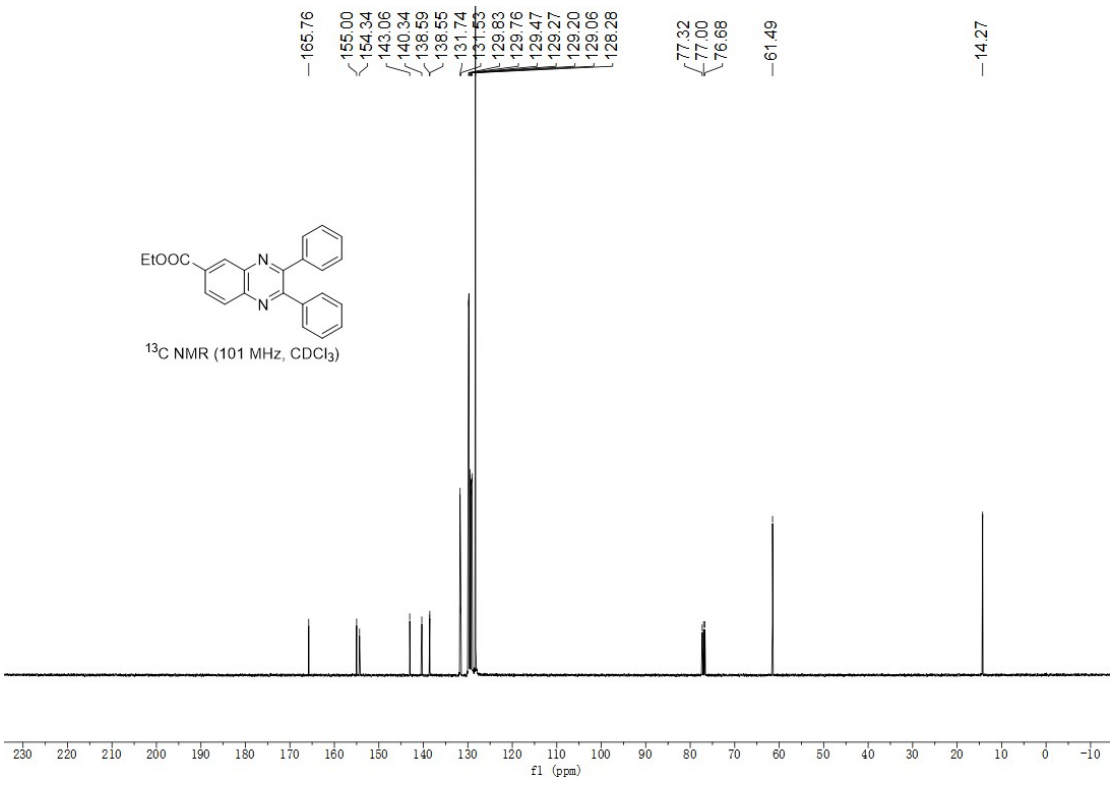
6-methoxy-2-phenylquinoxaline (3c-5)



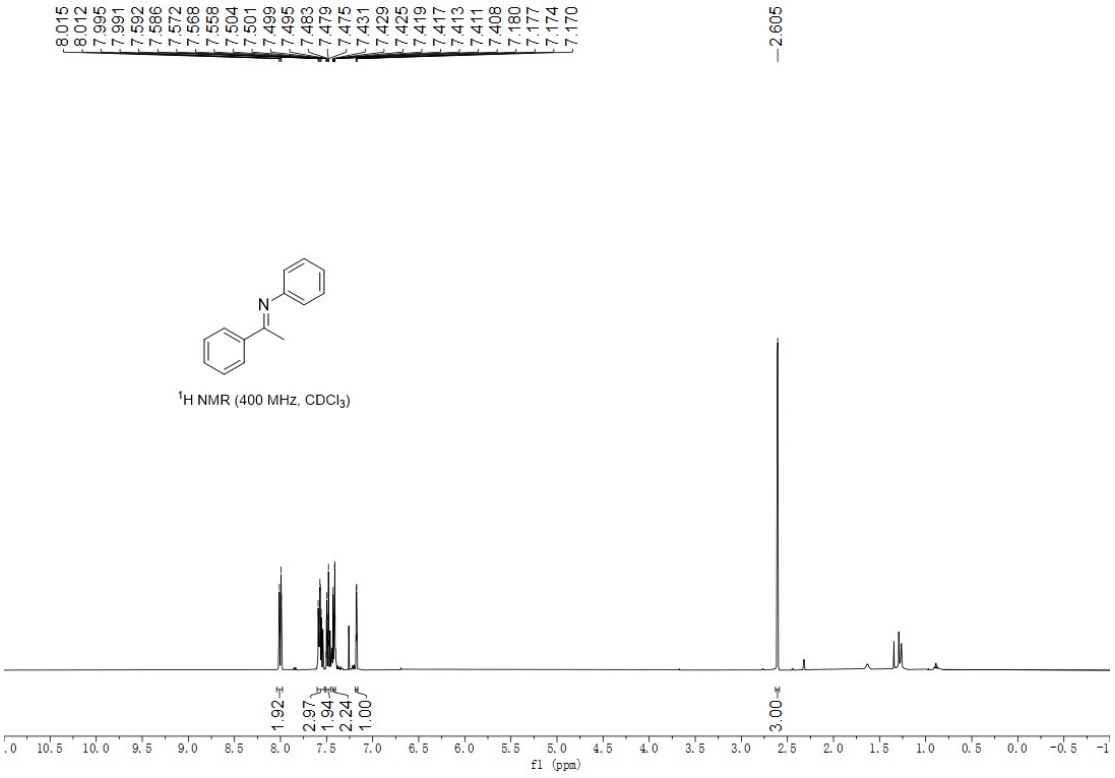


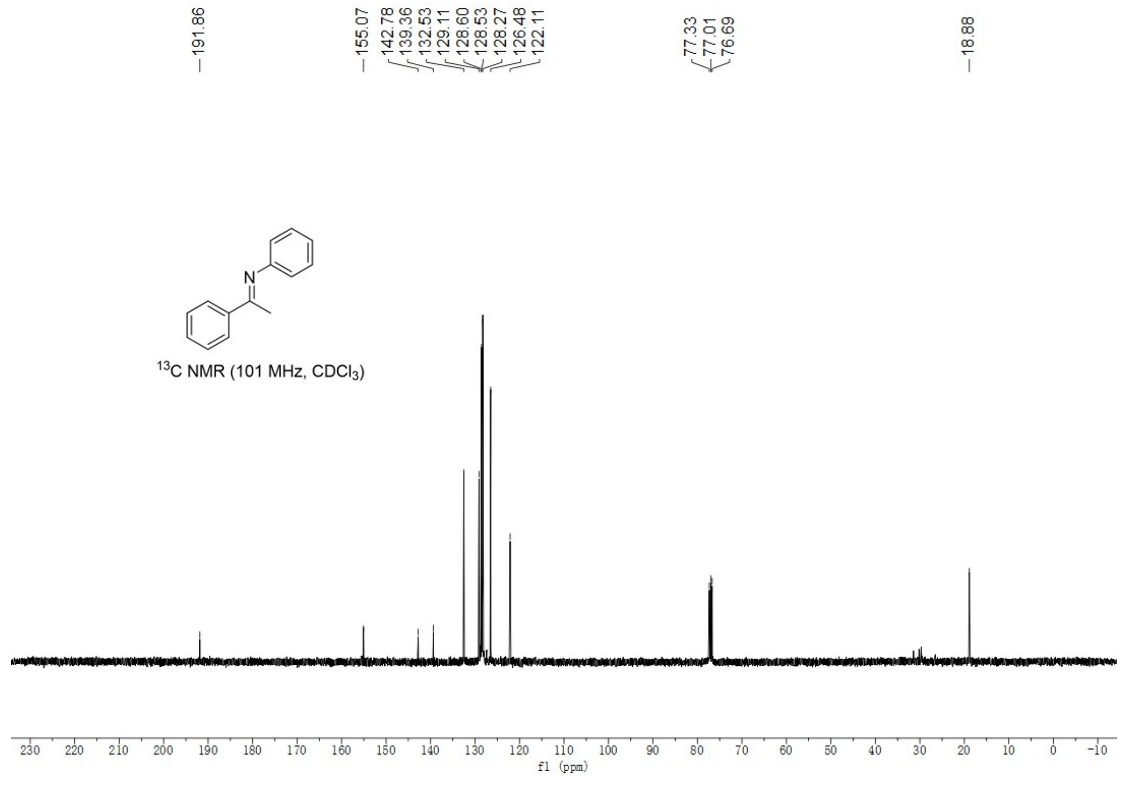
Ethyl 2,3-diphenylquinoxaline-6-carboxylate (3c-6)



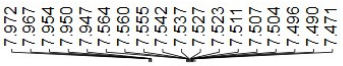


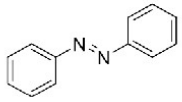
N,1-diphenylethan-1-imine (4c)



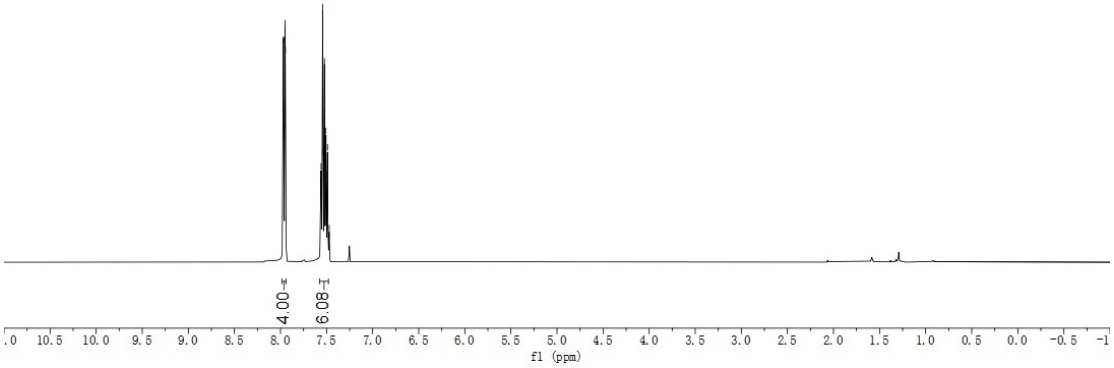


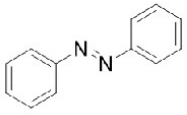
1,2-diphenyldiazene (4f)



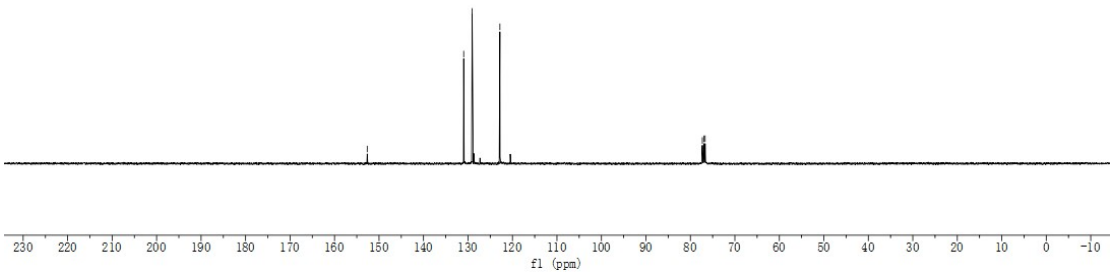


^{1}H NMR (400 MHz, $CDCl_3$)

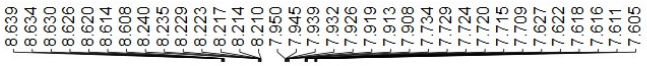


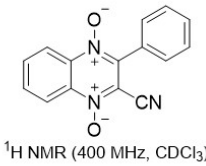


^{13}C NMR (101 MHz, $CDCl_3$)

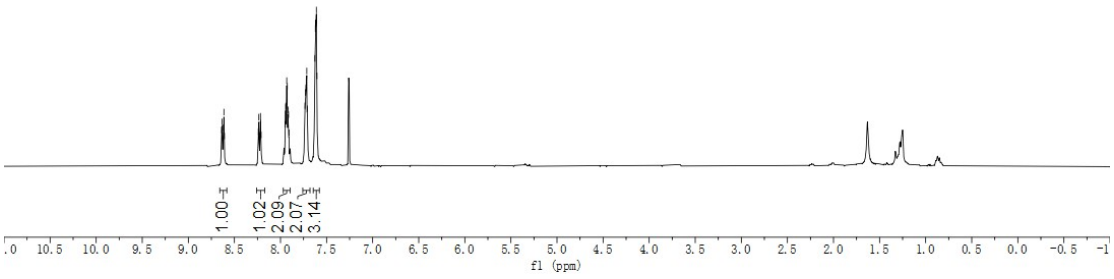


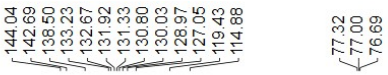
2-cyano-3-phenylquinoxaline 1,4-dioxide (4h)

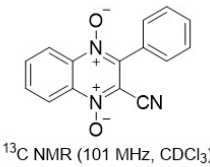




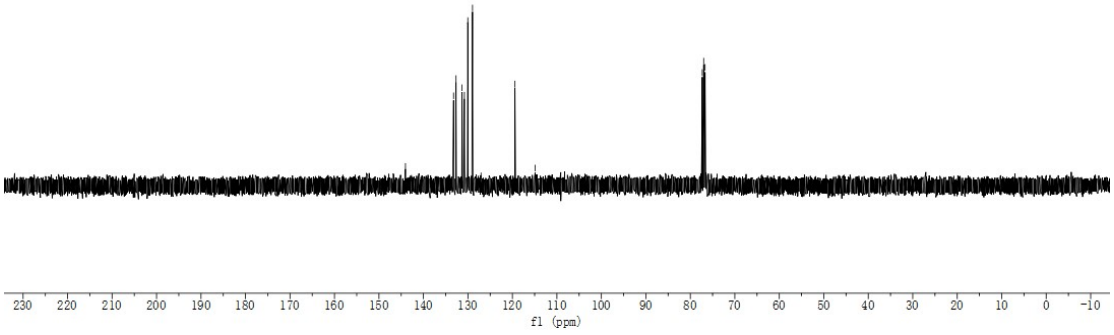
^{1}H NMR (400 MHz, $CDCl_3$)



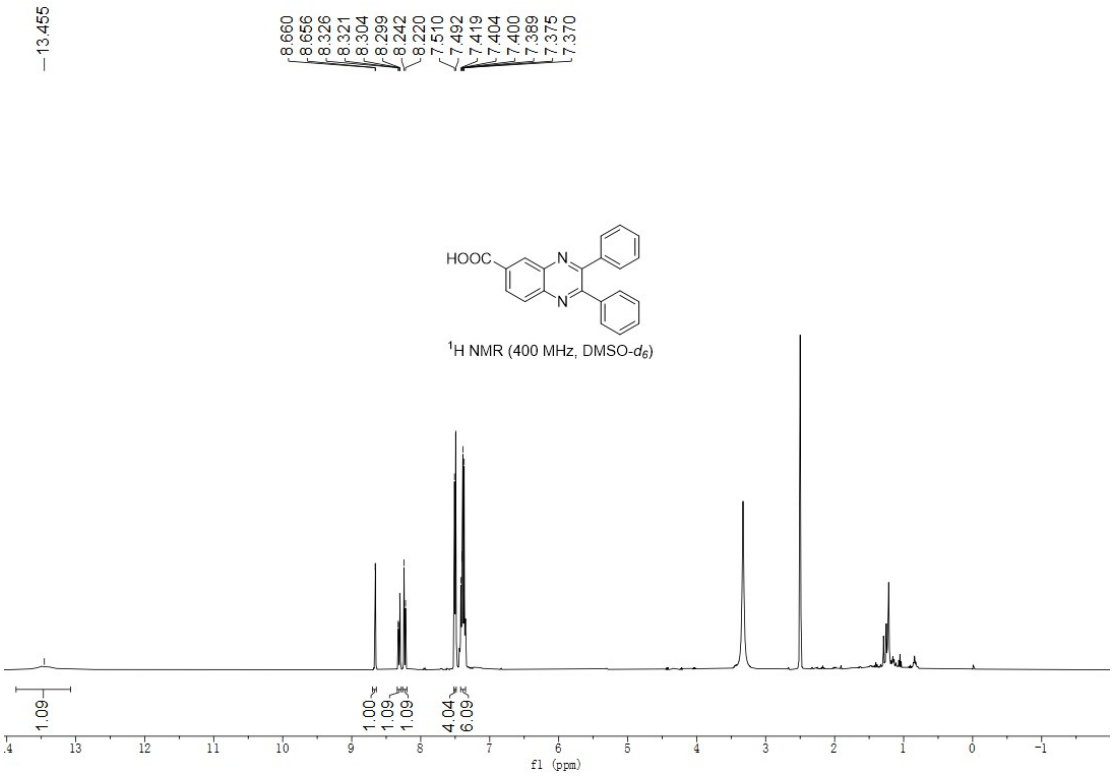


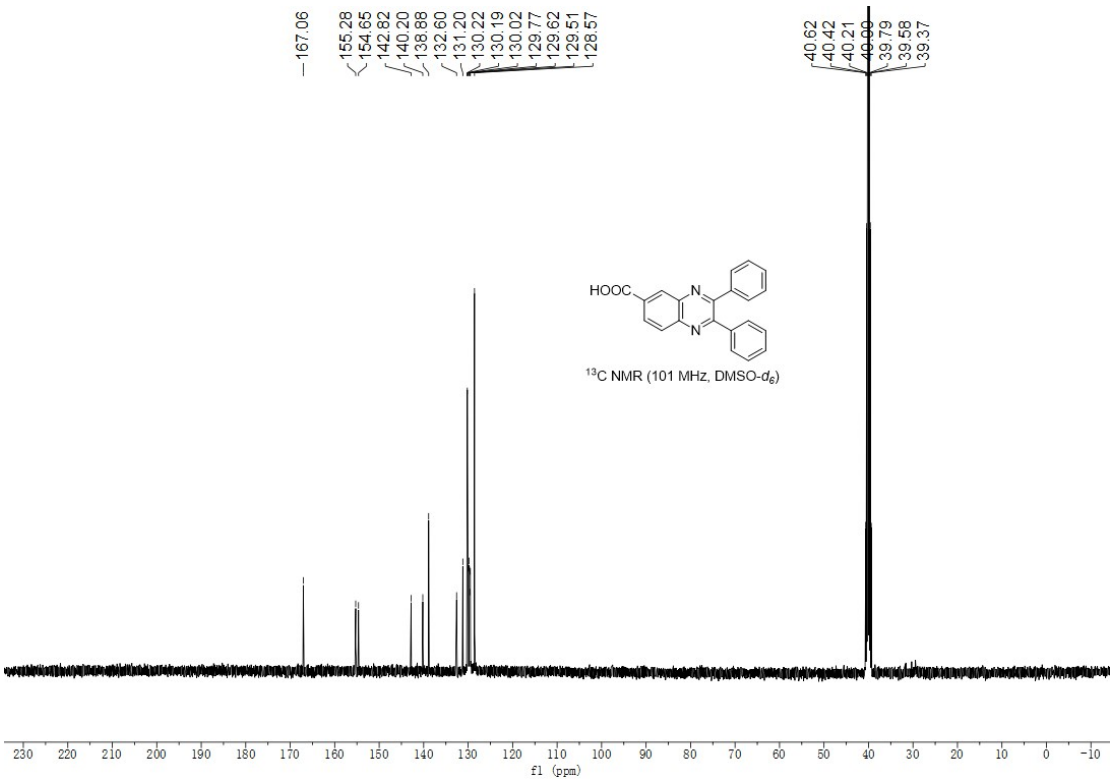


^{13}C NMR (101 MHz, $CDCl_3$)

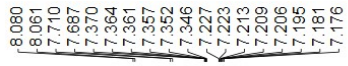


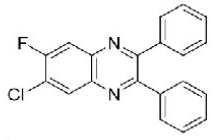
2,3-diphenylquinoxaline-6-carboxylic acid (4i)



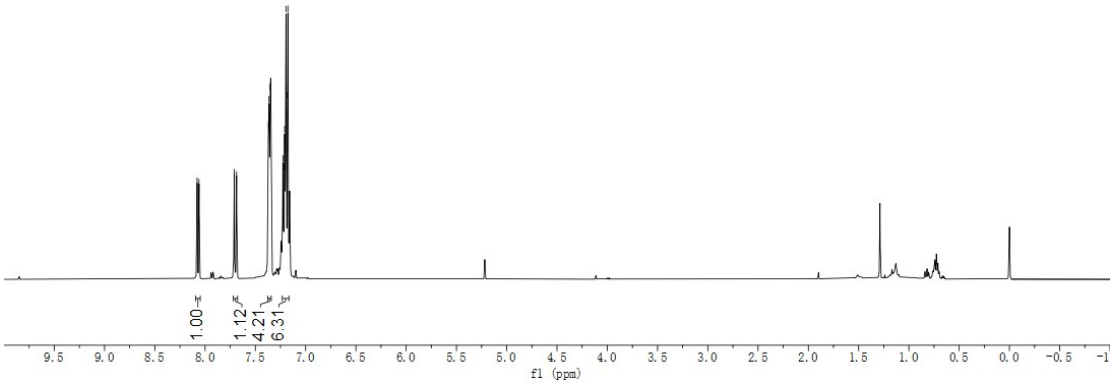


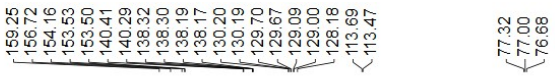
2,3-diphenylquinoxaline-6-carboxylic acid (4j)

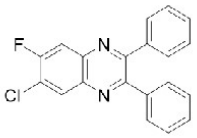




^{1}H NMR (400 MHz, $CDCl_3$)

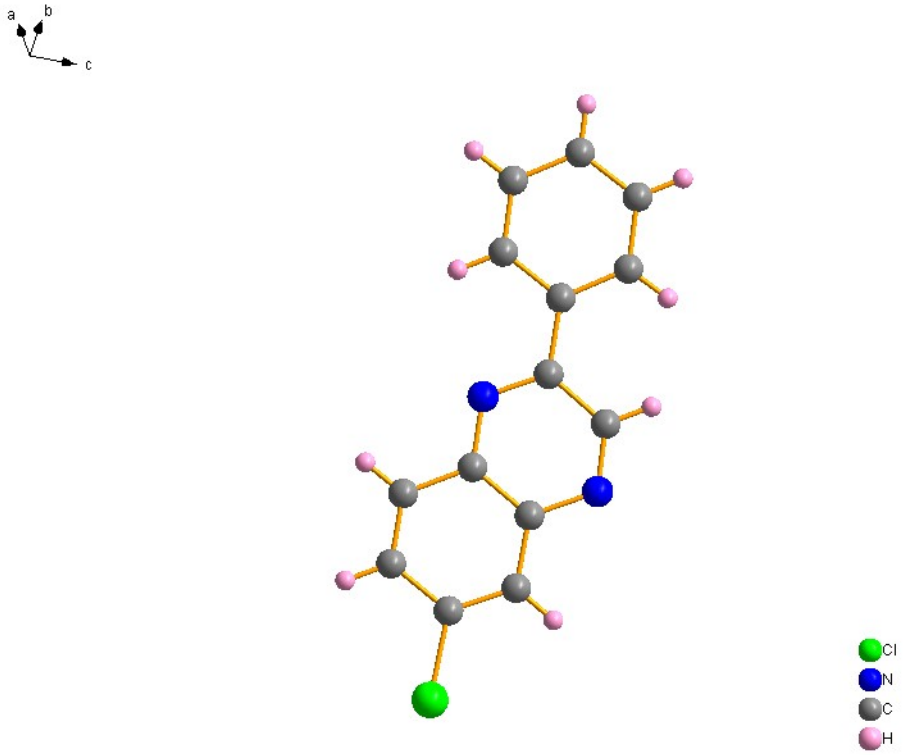






^{13}C NMR (101 Mhz, $CDCl_3$)

10. X-Ray Ellipsoid Plots of 3c-4.



Compound	6-chloro-2-phenylquinoxaline
CCDC Name	CCDC 2234240
Chemical Formula	$C_{14}H_9ClN_2$
Formula Weight	240.05
Temperature(K)	296
Crystal System	Monoclinic
Space Group	*P 21*
a(Å)	9.5545(14)
b(Å)	4.7731(7)
c(Å)	12.5151(18)
α(°)	90
β(°)	103.509(2)
γ(°)	90
Volume[Å]^3	554.96(14)
Z	2
D_{calc}(g/cm^3)	1.440
F(000)	248
GOF, S	1.065
R_1, wR_2 (obsd data)	0.0356, 0.0868
R_1, wR_2 (all data)	0.1989, 0.2250

11. Cartesian Coordinates

DMSO

O	0.00281700	1.49785700	0.38655700
C	1.36209900	-0.80849800	0.18795600
H	1.24764400	-0.90731400	1.27783900
H	1.34948100	-1.79129800	-0.30680200
H	2.29583200	-0.27866300	-0.04911400
C	-1.36610400	-0.80349200	0.18761800
H	-1.35882400	-1.78597700	-0.30779300
H	-1.25093600	-0.90356500	1.27729000
H	-2.29694800	-0.26833400	-0.04873900
S	0.00095300	0.22651500	-0.44928600

DMSO-radical

O	0.52324300	1.41819100	0.30881400
C	1.01497600	-1.21373500	0.23570200
H	2.05125000	-1.00309000	0.51889000
H	0.72194300	-2.21519200	-0.09779700
C	-1.55616000	-0.31926900	0.19217500
H	-1.83837900	-1.29193200	-0.23639300
H	-1.53614300	-0.35065900	1.29037800
H	-2.23189600	0.46979500	-0.16646000
S	0.11839900	0.14022300	-0.39664900

1a-1

C	0.71156100	-1.39236100	0.02243800
C	-0.51347400	-0.71206400	0.00269500
C	-0.51342300	0.71210700	-0.00268500
C	0.71160300	1.39234000	-0.02248800
C	1.92848800	0.69783000	-0.01644200
C	1.92849500	-0.69792100	0.01648400
H	0.70129600	-2.48644600	0.03027500
H	0.70137800	2.48642600	-0.03029700
H	2.86951100	1.25369000	-0.02890500
H	2.86950200	-1.25380300	0.02893200
N	-1.74212500	1.37472200	-0.04848900
H	-2.45684300	0.94951000	0.54184600
H	-1.67815100	2.37235000	0.13969000
N	-1.74220200	-1.37471900	0.04845400
H	-2.45738600	-0.94906900	-0.54099700
H	-1.67852400	-2.37226200	-0.14031000

2a-1

C	1.82136100	1.27822000	-0.00019200
C	0.42681000	1.19633000	-0.00025100
C	-0.20962400	-0.05680000	-0.00003600
C	0.57602400	-1.22281800	0.00020600
C	1.96707800	-1.14072200	0.00022500
C	2.59290900	0.11211900	0.00003200
H	2.30769000	2.25667500	-0.00033400
H	-0.16020600	2.11587500	-0.00041700
H	0.07040500	-2.19011400	0.00038000
H	2.56875200	-2.05301600	0.00040000
H	3.68383900	0.17874200	0.00004300
C	-1.70375000	-0.20320000	-0.00005600
O	-2.21724000	-1.30992200	-0.00047700
C	-2.54807800	1.04847700	0.00042400
H	-3.60986900	0.76999100	0.00022800
H	-2.32961000	1.66541700	0.88692700
H	-2.32945900	1.66616600	-0.88552400

H_2O

O	0.00000000	0.00000000	0.12140200
H	0.00000000	0.75542700	-0.48560800
H	0.00000000	-0.75542700	-0.48560800

4g

C	2.28712000	-1.15721600	-0.73130600
C	1.68808900	-0.02094300	-0.16254800
C	2.51496600	1.03140200	0.33276900
C	3.91247500	0.88819700	0.25178100
C	4.48655300	-0.25269300	-0.31270300
C	3.67737800	-1.27932300	-0.81200900
H	1.64381700	-1.93616100	-1.14592500
H	4.54564900	1.69337200	0.63485000
H	5.57533100	-0.33382500	-0.36949100
H	4.12234900	-2.16588200	-1.26988100
N	1.92331100	2.12605900	0.92786600
H	0.94664200	2.26440300	0.67733700
C	-0.58783800	-0.61044400	0.23910600
N	0.31263600	0.21521900	-0.16289600
C	-0.30647300	-1.92990500	0.91129400
H	-0.57446200	-2.77465200	0.25572200
H	0.75231400	-2.02546400	1.17956100
H	-0.91166200	-2.02697400	1.82501400
C	-2.01503700	-0.21309100	0.05108500
C	-2.33078100	1.03562700	-0.52046200

C	-3.07249100	-1.06648600	0.41555500
C	-3.65551700	1.42174800	-0.70979900
H	-1.51301700	1.69516400	-0.81394600
C	-4.40182900	-0.68053000	0.22081000
H	-2.86819400	-2.04435100	0.85233400
C	-4.69929700	0.56400000	-0.33912400
H	-3.87910000	2.39629200	-1.15140700
H	-5.20848300	-1.35893000	0.50946900
H	-5.73898100	0.86544800	-0.48956700
H	2.47226600	2.98056100	0.94444700

TS1

C	-1.69913100	-2.50280600	0.75407800
C	-1.29728600	-1.37540800	0.01446200
C	-2.29377400	-0.56298400	-0.61988400
C	-3.65521900	-0.91857000	-0.47703400
C	-4.03006000	-2.03043900	0.26716800
C	-3.05017300	-2.82580200	0.88467100
H	-0.94298900	-3.10138000	1.26451900
H	-4.40646600	-0.29252700	-0.96488000
H	-5.08745900	-2.28533400	0.37185300
H	-3.34294800	-3.69746600	1.47496500
N	-1.94018800	0.52895600	-1.37524100
H	-0.92875900	0.70448100	-1.31131300
C	1.07024600	-1.58371300	-0.25045600
N	0.00343000	-0.90058300	-0.02865500
C	1.09112700	-3.03543300	-0.65250600
H	1.38332100	-3.67221700	0.19889400
H	0.10548100	-3.36814800	-1.00182300
H	1.83071100	-3.20142600	-1.44928700
C	2.37226700	-0.87224800	-0.12001800
C	2.41383600	0.53687700	-0.12246700
C	3.57672000	-1.58540500	0.02326000
C	3.62870800	1.20541800	0.02192500
H	1.49630800	1.11242600	-0.26375400
C	4.78960900	-0.90975300	0.18070300
H	3.57329400	-2.67641100	0.02955700
C	4.82064900	0.48743000	0.18021000
H	3.64481500	2.29848100	0.00583900
H	5.71424700	-1.47929600	0.30289300
H	5.77040100	1.01559100	0.29735400
H	-2.38272600	1.56467500	-0.95714300
O	0.11154100	2.77062700	-0.83660100
C	-2.49445800	2.81909300	-0.24784200

H	-2.82870600	3.50072100	-1.04366800
H	-3.20249800	2.73262400	0.58838700
C	-0.65315100	2.09626300	1.66146500
H	-1.43663600	2.29597000	2.40664800
H	-0.69686800	1.06865600	1.27707100
H	0.33766600	2.29430500	2.09376000
S	-0.84216700	3.24797100	0.26336100

A

C	2.28258400	-1.07834300	-0.80386400
C	1.68639100	0.02100600	-0.16840400
C	2.53101100	1.07009900	0.40019300
C	3.95635600	0.89443500	0.30833000
C	4.50969600	-0.20280700	-0.31783100
C	3.67231500	-1.19124400	-0.88323500
H	1.64422000	-1.84046000	-1.25521800
H	4.58107700	1.67516600	0.74872600
H	5.59507700	-0.31067300	-0.38231200
H	4.11386500	-2.05561800	-1.38503300
N	2.04098400	2.14964500	0.99376500
H	1.01433500	2.11253500	0.92582500
C	-0.57708100	-0.58870100	0.26182600
N	0.32775800	0.23456700	-0.13869000
C	-0.28492500	-1.89892300	0.94301700
H	-0.57753500	-2.74504100	0.30014500
H	0.77993600	-1.99894300	1.18423800
H	-0.86906800	-1.98245700	1.87166500
C	-1.99994000	-0.19744800	0.06235400
C	-2.31301400	1.05691300	-0.49800800
C	-3.05492300	-1.06208900	0.40684800
C	-3.63731400	1.43604100	-0.70180100
H	-1.49573300	1.72746400	-0.76750100
C	-4.38312200	-0.68210000	0.19776000
H	-2.84863900	-2.04237600	0.83724900
C	-4.67934600	0.56654400	-0.35441200
H	-3.86204500	2.41436100	-1.13394300
H	-5.19001200	-1.36712500	0.46899600
H	-5.71880100	0.86338400	-0.51499400

TS2

C	2.41867600	-0.98210000	-0.89020100
C	2.40952300	0.22946600	-0.18551300
C	3.63420700	0.69646400	0.45869300
C	4.79420300	-0.14759000	0.36560400

C	4.76787700	-1.33978300	-0.33064900
C	3.57908300	-1.75848400	-0.96636300
H	1.50580100	-1.30939200	-1.39177100
H	5.70148900	0.20052600	0.86519200
H	5.66464600	-1.96093100	-0.39227800
H	3.55977000	-2.70078500	-1.51924000
N	3.70992500	1.84528700	1.12062500
H	2.79858900	2.31787300	1.04335900
C	0.13219000	0.75008100	0.25678200
N	1.31945600	1.07098000	-0.15116400
C	-0.20166700	-0.54357400	0.87103700
H	-0.72823300	-1.28097700	-0.06068900
H	0.65554000	-1.14072900	1.19778100
H	-1.01859900	-0.51894300	1.59841600
C	-0.95303800	1.75374800	0.07264900
C	-0.62714500	3.09125400	-0.22297100
C	-2.30909300	1.38671900	0.15977900
C	-1.62804300	4.04134300	-0.41480300
H	0.42487000	3.37216700	-0.29304400
C	-3.30912000	2.34188500	-0.04593800
H	-2.60484700	0.35390100	0.36234000
C	-2.97561000	3.66918200	-0.32764300
H	-1.35911100	5.07803000	-0.63261500
H	-4.35837900	2.04158600	0.01426700
H	-3.76142300	4.41348000	-0.47982900
O	-3.47794200	-1.64554900	0.56255300
C	-1.37129900	-2.04598200	-1.05365100
H	-1.65828400	-1.29209700	-1.79816700
H	-0.66161300	-2.80134100	-1.41673200
C	-1.92880000	-3.81785400	0.93751500
H	-1.39104500	-4.60230700	0.38511100
H	-1.24082200	-3.21162100	1.54355800
H	-2.70685900	-4.26580300	1.57109100
S	-2.79970500	-2.74317300	-0.24933500

B(T^1)

C	2.26776300	-1.12699600	-0.80110400
C	1.68283800	0.00296700	-0.21910300
C	2.53008700	1.05522700	0.32963700
C	3.94977100	0.84624800	0.28699600
C	4.50023500	-0.28465000	-0.28801900
C	3.66056200	-1.27314300	-0.83782400
H	1.62187100	-1.89408700	-1.23331200
H	4.57849100	1.62517300	0.72497600

H	5.58446700	-0.41612000	-0.31384000
H	4.09406300	-2.17008600	-1.28658600
N	2.04685300	2.17596100	0.85889700
H	1.02234200	2.16372700	0.76035600
C	-0.57274900	-0.55650600	0.34178900
N	0.32153700	0.22773000	-0.23355800
C	-0.22086300	-1.63412600	1.18341100
H	0.82778400	-1.85371400	1.38829800
H	-0.97587900	-2.24083300	1.68268200
C	-2.00981700	-0.21568000	0.10481300
C	-2.35071700	1.05654800	-0.38784700
C	-3.03863400	-1.14182800	0.34793500
C	-3.68298000	1.39681300	-0.62122800
H	-1.55449000	1.77689100	-0.58067100
C	-4.37217500	-0.80272600	0.10709700
H	-2.80449200	-2.14408300	0.70992500
C	-4.70003800	0.46773200	-0.37462800
H	-3.93019900	2.39298500	-0.99664000
H	-5.15833300	-1.53816500	0.29452300
H	-5.74405500	0.73318600	-0.55865100

TS3

C	-2.63737400	1.53393500	0.44154200
C	-1.65023700	0.52026700	0.21148700
C	-2.06633300	-0.73108900	-0.44520100
C	-3.44202300	-0.92355200	-0.67344600
C	-4.37116900	0.08024700	-0.41512800
C	-3.96226400	1.32175900	0.13263800
H	-2.29898100	2.46778500	0.89571600
H	-3.75590000	-1.87430400	-1.10992600
H	-5.42576200	-0.08760700	-0.64662500
H	-4.70338000	2.10155400	0.32216200
N	-1.17809700	-1.74305400	-0.73982300
H	-0.37811100	-1.36805700	-1.25981300
C	0.48733300	-0.32614100	0.67917500
N	-0.40430500	0.72135000	0.64017400
C	0.00771300	-1.60775100	0.99204700
H	-0.87420500	-1.70962300	1.62558100
H	0.66787100	-2.47485600	0.96040500
C	1.87286700	-0.04700500	0.27929300
C	2.22601300	1.24877700	-0.15961700
C	2.88162800	-1.03548500	0.31428900
C	3.53116200	1.54126000	-0.55197100
H	1.45725300	2.02233500	-0.18286600

C	4.18321600	-0.73954600	-0.08519100
H	2.65071500	-2.04398000	0.65998300
C	4.51752500	0.54926600	-0.52008200
H	3.78132500	2.55142700	-0.88624700
H	4.94697000	-1.52062200	-0.05187400
H	5.54066700	0.77821000	-0.82795500

C(T^1)

C	-2.57955400	1.68676600	0.00005300
C	-1.66672700	0.57669200	-0.00004500
C	-2.26894800	-0.76154200	0.00013800
C	-3.67333600	-0.92146200	0.00008900
C	-4.50340300	0.18538800	-0.00009300
C	-3.94155700	1.49767000	0.00005400
H	-2.14277200	2.68784400	0.00035900
H	-4.08310000	-1.93508400	-0.00000500
H	-5.58775600	0.05775400	-0.00024900
H	-4.60902300	2.36329800	0.00028400
N	-1.43293800	-1.81716300	0.00014100
H	-1.83021100	-2.75358800	0.00011000
C	0.50792000	-0.29740700	-0.00020600
N	-0.35805600	0.78034400	-0.00004300
C	0.00496600	-1.71216500	-0.00013100
H	0.39703500	-2.26235500	0.87775600
H	0.39659600	-2.26213800	-0.87833600
C	1.91353900	-0.04813900	-0.00009100
C	2.41249600	1.29180100	-0.00012300
C	2.88052700	-1.10112900	-0.00001800
C	3.77657600	1.55166700	0.00000700
H	1.69002200	2.10816200	-0.00029700
C	4.24187800	-0.82417500	0.00012100
H	2.55718000	-2.14354100	-0.00007800
C	4.70968900	0.50121300	0.00014500
H	4.12611700	2.58818400	-0.00007400
H	4.95643100	-1.65212900	0.00023000
H	5.78204600	0.71026700	0.00022600

C

C	-2.56629100	1.64359800	0.21341300
C	-1.70989000	0.54488400	0.05350600
C	-2.26038800	-0.75316600	-0.14102700
C	-3.65772200	-0.90362500	-0.19329100
C	-4.48967900	0.20530500	-0.02804200
C	-3.95278900	1.48320600	0.18463100

H	-2.11173400	2.62753200	0.35400500
H	-4.08051600	-1.89858900	-0.35678800
H	-5.57378700	0.06804500	-0.06255700
H	-4.61097300	2.34466500	0.31710300
N	-1.38065200	-1.78771700	-0.33300400
H	-1.77578800	-2.72135200	-0.37853200
C	0.47138400	-0.27041000	0.05354300
N	-0.32987100	0.73941900	0.01849400
C	-0.04149000	-1.69273400	0.21585300
H	0.00516000	-1.96275200	1.29500300
H	0.60645000	-2.40332500	-0.31406400
C	1.93200500	-0.03124500	0.00916800
C	2.42189200	1.27369600	-0.20575300
C	2.86058100	-1.07222900	0.19897600
C	3.79030100	1.52597700	-0.23775400
H	1.70261700	2.08140800	-0.34706600
C	4.23427700	-0.81562600	0.17212300
H	2.52118400	-2.09371500	0.37498600
C	4.70475800	0.48075000	-0.04872100
H	4.15083800	2.54316800	-0.41089700
H	4.93936100	-1.63648700	0.32425400
H	5.77915400	0.67920500	-0.07362600