Supplementary Information (SI) for Green Chemistry.

Supporting Information

Light-induced isomerization of quinoline-*N*-oxide derivatives through Zn-catalysis: a photochemical approach for synthesizing 2-quinolinone derivatives

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1. General Information.

All reactions were carried out under atmospheric pressure. Solvents were purified by standard techniques without special instructions. ^{1}H and ^{13}C NMR spectra were recorded on either a Varian Inova-400 spectrometer (400 MHz for ^{1}H, 100 MHz for ^{13}C) or a Bruker Avance II-400 spectrometer (400 MHz for ^{1}H, 100 MHz for ^{13}C); $CDCl_3$ (or DMSO-d_6) and TMS were used as a solvent and an internal standard, respectively. The chemical shifts are reported in ppm downfield (δ) from TMS, the coupling constants J are given in Hz. The peak patterns are indicated as follows: s, singlet; d, doublet; t, triplet; q, quartet; m, multiplet; bs, broad singlet. IR spectra were recorded on a NEXUS FT-IR spectrometer. High resolution mass spectra were recorded on either a Q-TOF mass spectrometry or a GC-TOF mass spectrometry. TLC was carried out on SiO_2 (silica gel 60 F_{254}, Merck), and the spots were located with UV light, iodoplatinate reagent or 1% aqueous $KMnO_4$. Flash chromatography was carried out on SiO_2 (silica gel 60, 200-300 mesh). UV-vis spectra were obtained on a Lambda 750S and Agilent 8453 UV-vis spectrophotometer.

2. Representative Procedure for Synthesis of Quinoline *N*-Oxides

Representative Procedure: To a mixture of quinoline (10.0 mmol, 1.29 g) in AcOH (20 mL) was added H_2O_2 (30 wt%, 1.4 mL) at room temperature. The reaction mixture was stirred at 70 °C for 36 h, and then was cooled to room temperature. The product was extracted with $CHCl_3$ (10 mL × 3), and the combined organic layers were dried over Na_2SO_4. The solvent was removed under reduced pressure, and the residue obtained was purified via silica gel chromatography (eluent: ethyl acetate/methanol = 8:1) to afford quinoline-*N*-oxide as a yellowish solid (1.31 g, 90% yield).

3. Representative Procedure for Synthesis of Quinolin-2(1*H*)-one Derivatives

Representative Procedure: A quartz reaction tube was charged with a mixture of quinoline-*N*-oxide (**1a**, 0.3 mmol, 43.5 mg), $ZnCl_2$ (10 mol%，4.0 mg) and CH_3CN (5.0 mL). The tube was capped. The reaction mixture was stirred under the irradiation of 300 W Xenon lamp for 2 h. The solvent was removed under reduced pressure, and the residue obtained was purified via silica gel chromatography (eluent: petroleum ether/ethyl acetate = 2:1) to afford quinolin-2(1*H*)-one (**2a**) as a white solid (37.0 mg, 85 % yield).

4. Synthesis of 2-*d*-Quinoline *N*-Oxide

Quinoline *N*-oxide (2.0 mmol, 258.0 mg), D_2O (1.5 mL), and NaOH (5 mmol, 200.1 mg) were weighed into a 30 mL pressure tube sealed with rubber plugs. The reaction mixture was stirred at 100 ℃ for overnight. After cooling to room temperature, the mixture was then extracted with chloroform (3 × 10 mL). The combined organic phase was washed with saturated NaCl solution (3 × 5 mL), dried over $NaSO_4$, and filtered. Chloroform was removed under reduced pressure to obtain the product. Deuterium incorporation was detected to be 96% by ^{1}H NMR in $CDCl_3$.

5. Zn-catalyzed NMR Tube Reaction of 2-*d*-Quinoline *N*-Oxide in CD_3CN

A NMR tube was charged with a mixture of 2-*d*-quinoline *N*-oxide (**1a-*d*$_1$,** D/H = 96/4, 0.03 mmol, 4.5 mg), $ZnCl_2$ (10 mol%, 0.4 mg) and anhydrous CD_3CN (0.55 mL). The tube was capped. The reaction mixture was stirred under the irradiation of 300 W Xenon lamp for 2 h.

6. Devices for the Photocatalytic Reactions

The photocatalytic reactions were performed under AM 1.5G light (100 mv Cm^{-2}, 300 W xenon lamp)

Figure S1. Light reactor

7. UV-vis Absorption Spectroscopic Measurements

UV-Visible analysis was performed on a Lambda 1050+ spectrophotometer. Experiments were recorded using a cuvette equipped with septa-lined screw cap. CH_3CN was chosen as the solvent.

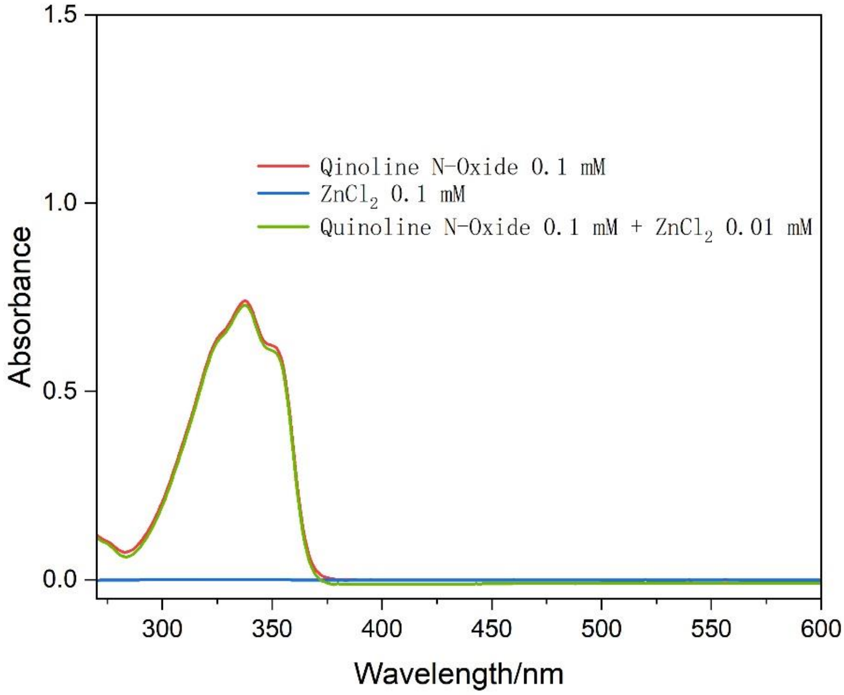


Figure S2 UV−vis absorption spectra of 2-quinoline *N*-oxide (0.1 mM), $ZnCl_2$ (1.0 mM), and the mixture (2-quinoline *N*-oxide (0.1 mM) + $ZnCl_2$ (0.01 mM)) in CH_3CN.

8. ESR Measurements

ESR spectra were recorded by X Band on a Bruker E500 spectrometer. EXR spectra was recorded at room temperature on ESR spectrometer operated at 9.415 GHz. Typical spectrometer parameters are shown as follows, Center field set: 3510 G; Sweep width: 100G; Number of Points: 1024; Attenuation:10 dB; Modulation frequency: 100 kHz; Modulation Amplitude: 1.0 G; Conver Time :20.00 ms; Sweep Time: 20.48 s.

Representative procedure for (**1a** + $ZnCl_2$) analysis: a ESR tube (pyrex, 170 mm) was charged with a mixture of 2-quinoline *N*-oxide (**1a**, 0.03 mmol, 4.5 mg), $ZnCl_2$ (10 mol%，0.4 mg) and anhydrous CH_3CN (0.4 mL). The tube was capped and analyzed by *in situ* ESR under the irradiation of 300 W Xenon lamp for 10 min. As shown in Figure S3, no signals were detected for b and c. A distinct peak with a *g*-value of approximately 2.004 was found in the mixture of **1a** with the $ZnCl_2$ in CH_3CN under irradiation (Figure S3a). The *g*-value is in good agreement with ESR data previously reported by Deng, Chen and Zhang, who reported that the Zn^+ exhibited an ESR signal around 1.998 [(a) *Angew. Chem. Int. Ed.* **2011**, *50*, 8299; (b) *J. Am. Chem. Soc.* **2013**, *135*, 6762; (c) *Chem. Sci.* **2012**, *3*, 2932; (d) *Adv. Mater.* **2015**, *27*, 7824; (e) *Adv. Sci.* **2016**, *3*, 15004240].

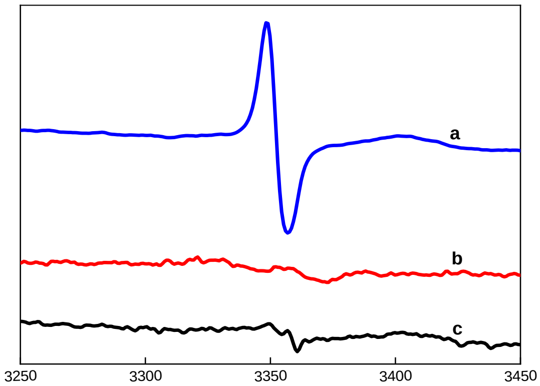


Figure S3. ESR spectra of (a) **1a** + $ZnCl_2$ in CH_3CN under irradiation, (b) **1a** + $ZnCl_2$ in CH_3CN without irradiation, and (c) **1a** in CH_3CN under irradiation.

9. Theoretical calculations

The molecular geometries were optimized using M06 exchange correlation functional with the Gaussian 09 package.[1] The cc-pvdz basis set was used for all atoms except for Zn, for which LANL2DZ is used.[2] Frequency calculations were carried out to confirm the characteristics of all of the optimized structures as minima or transition states. Transition state was further verified by intrinsic reaction coordinate (IRC) calculations by checking its connection to two respective minimum structures. The electronic energies were further refined with single point energy calculations with M06-2X functional and a higher basis set def2-TZVP[3] for all atoms. Solvent effects were taken into account using SMD model[4] for the single point energy calculations. All thermochemical data were obtained with the ideal gas-rigid rotor-simple harmonic oscillator approximations at 298.15 K and 1 atm. Zero point-energy corrections were included in the Gibbs free energy values along with a concentration correction for c = 1 mol/L condition in the solvent. The electron density difference analysis is performed by the Multiwfn program. [5]

The excitation energies in the n-th singlet (S_n) and n-th triplet (T_n) states were obtained using the TD-DFT method based on an optimized molecular structure at ground state (S_0) with the same functional and basis set as the single point energy calculations. Spin-orbit coupling (SOC) matrix elements between the singlet and triplet excited states are calculated using the ORCA 4.1.2 program[6] at the optimized geometry of the lowest singlet excited state (S_1).

The orbital transitions, excitation energies, the oscillator strengths and the corresponding absorption wavelengths of the three lowest excited singlet states of 2-*d*-quinoline *N*-oxide **1a-D** are given in Table S1. The excitation enery of the lowest singlet excited (S_1) state, which is $\pi\pi^*$ character and corresponds to the electronic transition from HOMO to LUMO, is calculated to be 3.97 eV. The S_1 has much higher oscillator strengths (0.192) than that of the other two singlet excitation states (Oscillator strength of S_2 and S_3 state is 0.016 and 0.002, respectively), indicating a significant possibility of ground state (S_0) to S_1 transition in **1a-D**.

Table S1. Orbital transition, excitation energies (in eV), oscillator strengths, and absorption wavelength (in nm) of the three lowest singlet excited states of **1a-D**.

Excited states	Orbital transitions	Excitation energies (eV)	Oscillator strengths	Absorption wavelengths (nm)
S_1 ($\pi\pi$*)	HOMO→LUMO	3.97	0.192	310
S_2 ($\pi\pi$*)	HOMO→LUMO+1	4.39	0.016	282
S_3 (nπ*)	HOMO-3→LUMO	4.48	0.002	276

By surveying the energy levels of the singlet and triplet excited states in Figure S1, it is found that intersystem crossing (ISC) can happen for **1a-D**. The energy level difference between S_1 and the lowest triplet excited (T_1) state is as large as 1.89 eV. Meanwhile, the calculated S_1 energy levels are considerably close (< 0.3 eV) to several triplet excited states (T_n), which are T_2, T_3 and T_4 states, demonstrating ISC can occur much more easily from S_1 to T_n than the S_1 to T_1 according to the energy gap law. Moreover, the considerable spin-orbit coupling (SOC) strengths between S_1 and T_n with similar electron density difference (EDD) isosurfaces further indicate the efficient ISC of S_1 to these T_n transition channels, especially S_1 to T_3.

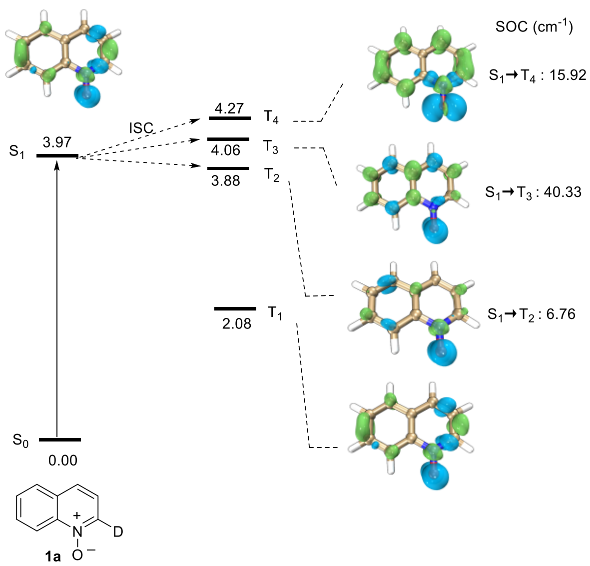
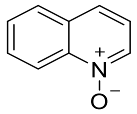


Figure S4. TD-DFT calculated energy levels (in eV), EDD isosurfaces, and SOC strengths (in cm^{-1}) of the singlet and triplet excited states of **1a-D**. The EDD isosurfaces of the excited states relative to the ground state, the green and blue respectively correspond to positive and negative values (isosurface is 0.003).

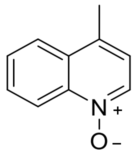
10. Characterization Data for All Products and Intermediate

Quinoline *N*-oxide (1a)[7]



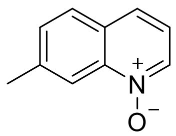
Yellowish solid. Mp 59-60 ºC (lit. 59-60 ºC). ^{1}H NMR ($CDCl_3$, 400 MHz) δ 8.74 (d, *J* = 8.8 Hz, 1H), 8.54 (d, *J* = 6.0 Hz, 1H), 7.87 (d, *J* = 8.2 Hz, 1H), 7.78–7.73 (m, 2H), 7.65–7.62 (m, 1H), 7.31–7.28 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 141.5, 135.6, 130.5, 130.4, 128.7, 128.1, 125.9, 121.0, 119.7.

4-Methylquinoline *N*-oxide (1b)[7]



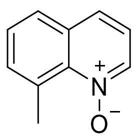
Yellowish solid. Mp 116-117 ºC (lit. 115-116 ºC).^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.77 (d, *J* = 8.8 Hz, 1H), 8.40 (d, *J* = 6.0 Hz, 1H), 7.94 (d, *J* = 8.4 Hz, 1H), 7.76–7.72 (m, 1H), 7.66–7.62 (m, 1H), 7.09 (d, *J* = 6.0 Hz, 1H), 2.63 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 141.1, 135.1, 134.8, 130.2, 130.0, 128.6, 124.9, 121.6, 120.5, 18.4.

7-Methylquinoline *N*-oxide (1c)[8]



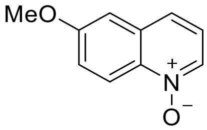
^{1}H NMR (400 MHz, DMSO-d_6) δ: 8.41 (s, 1H), 8.37 (d, J = 6.0 Hz, 1H), 7.61 (d, *J* = 8.4 Hz, 1H), 7.56 (d, *J* = 8.4 Hz, 1H), 7.31 (d, *J* = 8.8 Hz, 1H), 7.11–7.07 (m, 1H), 2.44 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 141.3, 141.2, 135.4, 130.4, 128.4, 127.7, 125.7, 119.8, 118.4, 21.8.

8-Methylquinoline *N*-oxide (1d)[7]



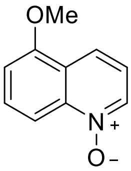
^{1}H NMR ($CDCl_3$, 400 MHz) δ 8.36 (d, *J* = 6.0 Hz, 1H), 7.62–7.59 (m, 2H), 7.41–7.37 (m, 2H), 7.16–7.12 (m, 1H), 3.15 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 141.4, 137.3, 133.6, 133.4, 132.5, 128.1, 126.8, 126.5, 120.7, 24.9.

6-Methoxyquinoline *N*-oxide (1e) [7]



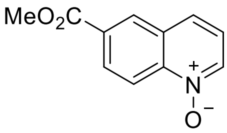
^{1}H NMR ($CDCl_3$, 400 MHz) δ 8.63 (d, J = 8.0 Hz, 1H), 8.39 (d, J = 6.0 Hz, 1H), 7.62 (d, J = 8.0 Hz, 1H), 7.37–7.34 (m, 1H), 7.26–7.22 (m, 1H), 7.09 (d, J = 2.3 Hz, 1H), 3.92 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.5, 137.2, 133.9, 132.0, 125.3, 122.9, 121.48, 121.42, 105.8, 55.7.

5-Methoxyquinoline *N*-oxide (1f)[9]



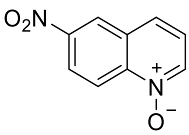
^{1}H NMR (400 MHz, DMSO-d_6) δ 8.58 (d, J = 7.6 Hz, 1H), 8.07 (d, J = 8.8 Hz, 1H), 8.00 (d, J = 8.4 Hz, 1H), 7.73–7.69 (m, 1H), 7.43–7.39 (m, 1H), 7.18 (d, J = 8.0 Hz, 1H), 4.00 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 155.8, 142.6, 136.2, 130.7, 123.5, 121.1, 119.9, 111.7, 106.7, 56.2.

1-Oxy-quinoline-6-carboxylic acid methyl ester (1g)[10]



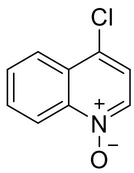
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.80 (d, J = 9.1 Hz, 1H), 8.62 (d, J = 1.7 Hz, 1H), 8.59 (dd, J = 6.1, 0.7 Hz, 1H), 8.33 (dd, J = 9.1, 1.8 Hz, 1H), 7.83 (d, J = 8.5 Hz, 1H), 7.37 (dd, J = 8.5, 6.1 Hz, 1H), 4.01 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 145.1, 141.8, 135.9, 131.1, 128.9, 128.0, 126.1, 120.2, 119.0, 31.0, 22.2.

6-Nitroquinoline *N*-oxide (1h) [10]



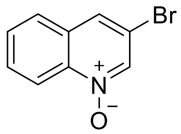
^{1}H NMR (500 MHz, $CDCl_3$) δ 8.93 (d, J = 9.5 Hz, 1H), 8.84 (d, J = 2.5 Hz, 1H), 8.65 (dd, J = 1.0, 6.0 Hz, 1H), 8.50 (dd, J = 2.5, 9.5 Hz, 1H), 7.91 (d, J = 8.5 Hz, 1H), 7.49 (dd, J = 6.5, 8.5 Hz, 1H); ^{13}C NMR (150 MHz, DMSO-d_6) δ 162.5, 143.8, 142.0, 140.6, 125.6, 124.8, 124.3, 119.0, 116.6.

4-Chloroquinoline *N*-oxide (1i) [11]



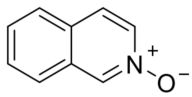
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.78 (d, J = 8.8 Hz, 1H), 8.44 (d, J = 6.4 Hz, 1H), 8.23 (d, J = 8.4 Hz, 1H), 7.86–7.82 (m, 1H), 7.79–7.75 (m, 1H), 7.38 (d, J = 6.4 Hz, 1H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 142.5, 136.2, 132.2, 131.0, 128.23, 128.17, 125.8, 123.0, 120.7.

3-Bromoquinoline *N*-oxide (1j)[11]



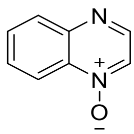
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.60 (d, J = 8.8 Hz, 1H), 8.55 (d, J = 1.6 Hz, 1H), 7.82 (s, 1H), 7.75–7.68 (m, 2H), 7.63–7.59 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 140.4, 136.8, 130.3, 130.1, 129.7, 127.3, 127.3, 119.6, 114.2.

Isoquinoline *N*-oxide(1k)[7]



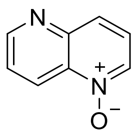
^{1}H NMR ($CDCl_3$, 400 MHz) δ 8.77 (s, 1H), 8.14 (dd, J = 1.2, 6.8 Hz, 1H), 7.80 (d, J = 7.6 Hz, 1H), 7.73 (d, J = 7.6 Hz, 1H), 7.68 (d, J = 7.2 Hz, 1H), 7.65–7.58 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 136.8, 136.1, 129.50, 129.47, 129.0, 128.8, 126.7, 124.9, 124.3.

Quinoxaline 1-oxide(1l)[12]



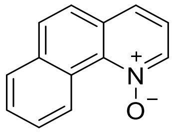
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.67 (d, J = 3.5 Hz, 1 H), 8.58 (dd, J = 8.6, 1.5 Hz, 1H), 8.35 (d, J = 3.6 Hz, 1 H), 8.14 (dd, J = 8.3, 1.4 Hz, 1H), 7.85-7.81 (m, 1H), 7.78-7.73 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 146.0, 137.5, 131.8, 130.3, 130.2, 129.3, 118.9.

1,5-Naphthyridine 1-oxide(1m)[13]



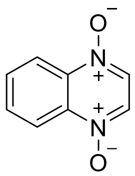
^{1}H NMR (400 MHz, $CDCl_3$) δ 9.03 (d, J = 5.7 Hz, 2H), 8.55 (d, J = 6.0 Hz, 1H), 8.01 (d, J = 8.8 Hz, 1H), 7.69–7.66 (m, 1H), 7.54–7.51 (m, 1 H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 153.0, 145.6, 138.6, 136.0, 128.5, 127.7, 124.8, 124.3.

Benzo[*h*]quinoline 1-oxide(1n) [11]



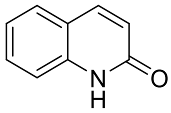
^{1}H NMR (400 MHz, $CDCl_3$) δ 10.87–10.85 (m, 1H), 8.68 (d, J = 6.2 Hz, 1H), 7.95–7.93 (m, 1 H), 7.87 (d, J = 8.8 Hz, 1H), 7.80–7.77 (m, 3H), 7.67 (d, J = 8.8 Hz, 1H), 7.44–7.40 (m, 1H); ^{13}C NMR (150 MHz, DMSO-d_6) δ 139.7, 137.5, 134.1, 131.4, 130.5, 129.4, 128.7, 127.9, 127.69, 127.66, 126.1, 125.9, 122.8.

Quinoxaline 1,4-dioxide(1o) [14]



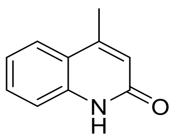
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.62–8.59 (m, 2H), 8.26 (s, 2H), 7.91–7.88 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 138.6, 132.2, 130.4, 120.5.

Quinolin-2(1*H*)-one (2a) [15]



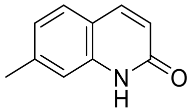
Pale yellow solid. Mp 192-193 ºC (lit. 198-199 ºC). ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.72 (s, 1H), 7.87 (d, J = 9.5 Hz, 1H), 7.62 (dd, J = 7.8, 1.1 Hz, 2H), 7.48–7.44 (m, 1H), 7.29 (d, J = 8.2 Hz, 1H), 7.16–7.12 (m, 1H), 6.47 (d, J = 9.5 Hz, 1H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 207.0, 162.4, 140.7, 139.3, 130.8, 128.3, 122.4, 122.2, 119.6, 115.6.

4-Methylquinolin-2(1*H*)-one (2b) [15]



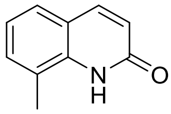
Pale yellow solid. Mp 219-220 ºC (lit. 218-220 ºC). ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.58 (s, 1 H), 7.69 (d, J = 8.0 Hz, 1 H), 7.50–7.46 (m, 1 H), 7.29 (d, J = 8.1 Hz, 1 H), 7.20–7.16 (m, 1 H), 6.38 (s, 1H), 2.40 (s, 3 H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 162.1, 148.4, 139.1, 130.7, 125.2, 122.1, 121.3, 120.0, 115.9, 18.9.

7-Methylquinolin-2(1*H*)-one (2c) [15]



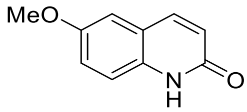
Pale yellow solid. Mp 194-195 ºC (lit. 195-196 ºC). ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.63 (s, 1H), 7.83 (d, J = 9.5 Hz, 1H), 7.52 (d, J = 8.0 Hz, 1H), 7.09 (s, 1H), 6.99 (d, J = 8.0 Hz, 1H), 6.40 (d, J = 9.5 Hz, 1H), 2.37 (s, 3H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 162.1, 140.4, 140.0, 139.0, 127.7, 123.1, 120.7, 117.0, 114.9, 21.3.

8-Methylquinolin-2(1*H*)-one (2d) [15]



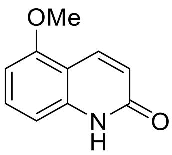
Light yellow solid. Mp 219-220 ºC (lit. 219-220 ºC). ^{1}H NMR (400 MHz, DMSO-d_6) δ 10.86 (s, 1H), 7.87 (d, J = 9.5 Hz, 1H), 7.47 (d, J = 7.4 Hz, 1H), 7.32 (d, J = 7.3 Hz, 1H), 7.08–7.05 (m, 1H), 6.48 (d, J = 9.5 Hz, 1H), 2.40 (s, 3H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 162.9, 141.3, 137.7, 132.1, 126.5, 123.9, 122.0, 119.6, 17.6.

6-Methoxyquinolin-2(1*H*)-one (2e) [15]



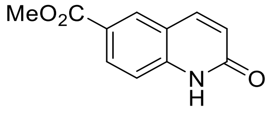
Pale yellow solid. Mp 220-221 ºC (lit. 220-221 ºC). ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.62 (s, 1H), 7.83 (d, J = 9.6 Hz, 1H), 7.22 (d, J = 8.9 Hz, 1H), 7.19 (d, J = 2.8 Hz, 1H), 7.13 (dd, J = 9.2, 2.8 Hz, 1H), 6.47 (d, J = 9.6 Hz, 1H), 3.76 (s, 3H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 155.2, 147.8, 133.5, 127.0, 116.0, 113.4, 113.2, 110.1, 103.0, 49.1.

5-Methoxyquinolin-2(1*H*)-one(2f) [15]



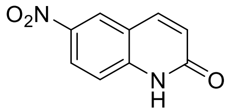
Pale yellow solid. Mp 180-181 ºC (lit. 170-175 ºC). ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.62 (s, 1H), 7.83 (d, J = 9.6 Hz, 1H), 7.23–7.18 (m, 2H), 7.14–7.11 (m, 1H), 6.47 (d, J = 9.5 Hz, 1H), 3.76 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 161.9, 155.5, 140.1, 134.1, 131.4, 120.4, 109.3, 107.8, 102.7, 55.8.

1-Oxo-1,2-dihydroquinoline-6-carboxylic acid methyl ester (2g) [15]



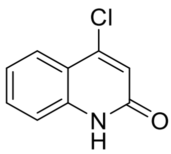
Pale yellow solid. Mp 250-251 °C (lit. 252-253 ºC). ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.04 (s, 1H), 8.33 (s, 1H), 8.07–8.02 (m, 2H), 7.37 (d, J = 8.6 Hz, 1H), 6.57 (dd, J = 1.5, 8.6 Hz, 1H), 3.86 (s, 3H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 165.7, 162.0, 142.1, 140.4, 130.6, 129.9, 122.9, 122.8, 118.7, 115.4, 52.0.

6-Nitroquinolin-2(1*H*)-one(2h) [15]



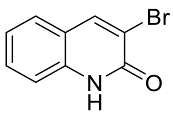
Light yellow solid, Mp 279-280 ºC (lit. 279-281 ºC). ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.23 (s, 1H), 8.47 (s, 1H), 7.65–7.63 (m, 1H), 7.53–7.49 (m, 1H), 7.29 (d, J = 8.3 Hz, 1H), 7.20–7.16 (m, 1H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 162.5, 143.8, 142.0, 140.6, 125.6, 124.8, 124.3, 119.0, 116.6.

4-Chloroquinolin-2(1*H*)-one (2i) [16]



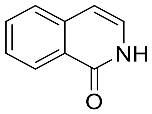
White solid, Mp 248-249 ºC (lit. 249-250℃) ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.00 (s, 1H), 7.83 (d, J = 8.1 Hz, 1H), 7.62–7.58 (m, 1H), 7.36 (d, J = 8.2 Hz, 1H), 7.30–7.26 (m, 1H), 6.80 (s, 1H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 160.9, 144.5, 139.1, 132.4, 125.1, 123.1, 121.8, 117.6, 116.2.

3-Bromoquinolin-2(1*H*)-one (2j) [17]



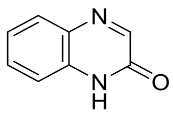
White solid, Mp 263-265 ºC (lit. 266-267℃). ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.28 (s, 1H), 8.68 (d, J = 2.6 Hz, 1H), 8.31 (dd, J = 2.6, 9.1 Hz, 1H), 8.11 (d, J = 9.6 Hz, 1H), 7.41 (d, J = 9.1 Hz, 1H), 6.65 (dd, J = 1.5, 9.6 Hz, 1H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 158.2, 142.2, 138.6, 131.2, 127.8, 122.8, 119.9, 117.5, 115.7.

Isoquinolin-1(2*H*)-one(2k) [18]



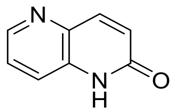
White solid, Mp 207-208 ºC (lit. 208-211 ºC). ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.68 (s, 1H), 7.83 (d, J = 9.5 Hz, 1H), 7.59 (dd, J = 1.0, 7.8 Hz, 2H), 7.45–7.41 (m, 1H), 7.25 (d, J = 8.2, 1H), 7.09–7.13 (m, 1H), 6.44 (d, J = 9.5 Hz, 1H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 162.3, 138.4, 132.8, 129.4, 127.1, 126.8, 126.7, 105.1.

Quinoxalin-2(1*H*)-one (2l) [19]



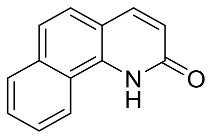
White solid, Mp 237-238 ºC (lit. 239-240 ºC). ^{1}H NMR (400 MHz, DMSO-*d*6) δ 12.41 (s, 1H), 8.16 (s, 1H), 7.77 (d, *J* = 7.8 Hz, 1H), 7.56–7.53 (m, 1H), 7.32–7.28 (m, 2H); ^{13}C NMR (100 MHz, DMSO-*d*6) δ 155.4, 152.1, 132.5, 132.3, 131.2, 129.3, 123.7, 116.2.

1,5-Naphthyridin-2(1*H*)-one (2m) [20]



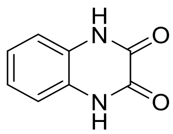
Pale yellow solid, Mp 259-260 ºC (lit. 261-263 ºC). ^{1}H NMR (400 MHz, DMSO-*d*6) δ 11.87 (s, 1H), 8.47 (dd, *J* = 1.4, 4.4 Hz, 1H), 7.92 (d, *J* = 9.8 Hz, 1H), 7.67 (d, *J* = 7.6 Hz, 1H), 7.50 (dd, *J* = 4.4, 8.4 Hz, 1H), 6.74 (d, *J* = 9.8 Hz, 1H); ^{13}C NMR (100 MHz, DMSO-*d*6) δ 161.8, 145.0, 141.7, 137.1, 135.5, 126.4, 125.3, 123.3.

Benzo[h]quinolin-2(1H)-one(2n) [21]



White solid, Mp 250-251 ºC (lit. 250-251 ºC). ^{1}H NMR (400 MHz, DMSO-*d*6) δ 8.83 (d, *J* = 8.1 Hz, 1H), 7.96–7.91 (m, 2H), 7.63–7.55 (m, 4H), 6.57 (d, *J* = 9.4 Hz, 1H); ^{13}C NMR (100 MHz, DMSO-*d*6) δ 163.1, 150.2, 141.7, 136.3, 134.2, 128.9, 128.3, 126.9, 125.7, 122.8, 122.7, 121.9, 116.0.

1,4-Dihydroquinoxaline-2,3-dione (2o) [22]



White solid, Mp > 300 ºC (lit 360-362 ºC). ^{1}H NMR (400 MHz, DMSO-*d*6) δ 11.90 (s, 2H), 7.15–7.07 (m, 4H); ^{13}C NMR (100 MHz, DMSO-*d*6) δ 155.6, 126.1, 123.5, 115.6.

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12. Copies of ^{1}H and ^{13}C NMR Spectra of Products and Intermediate

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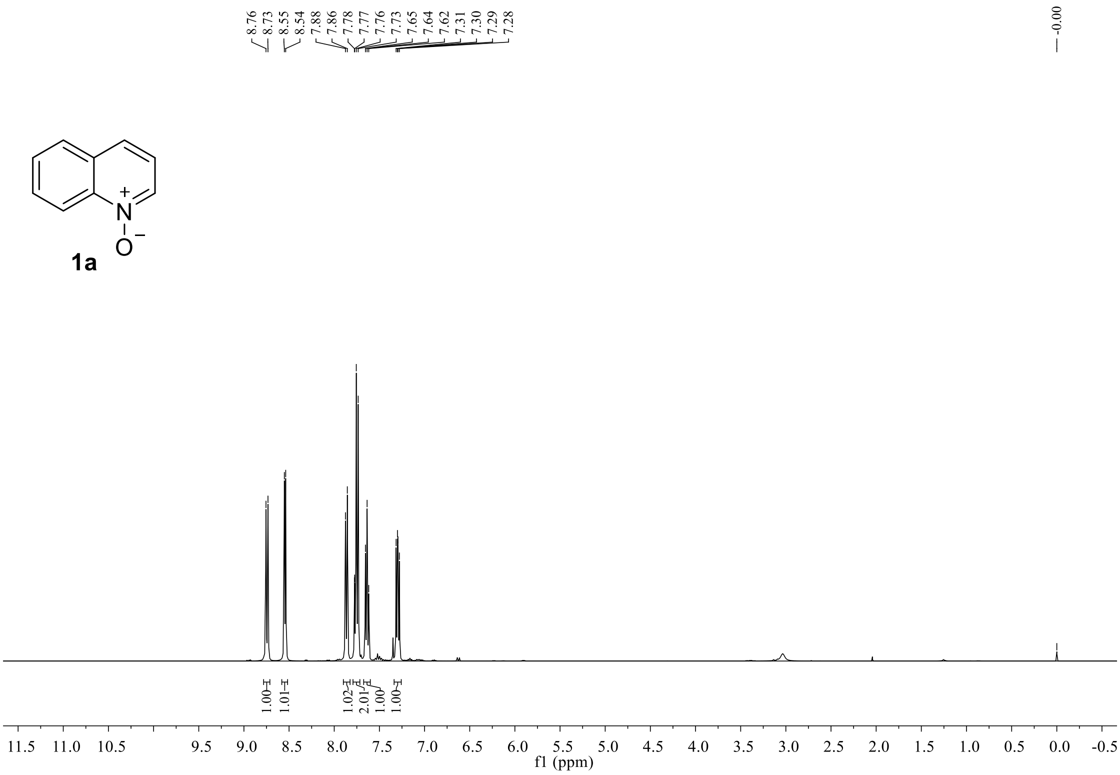
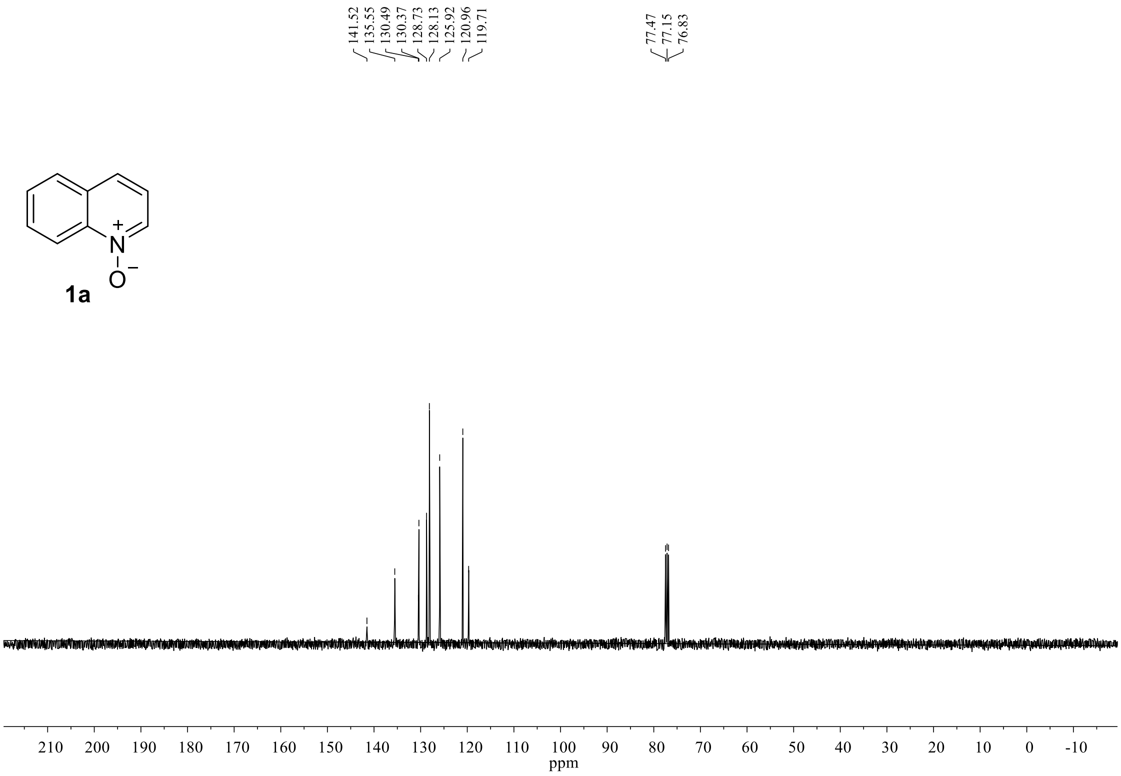


^{13}C NMR, 100 MHz, $CDCl_3$



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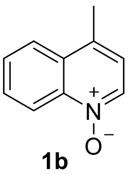
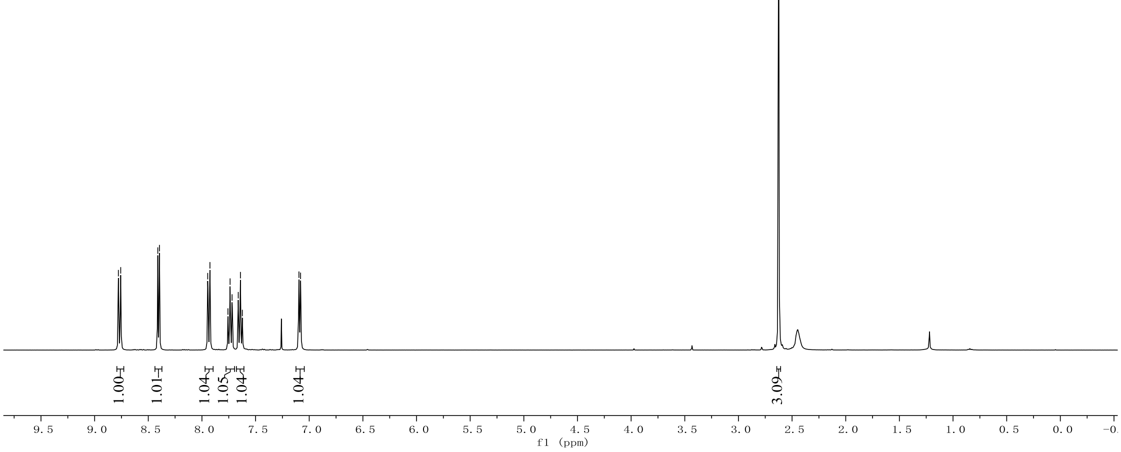


1b



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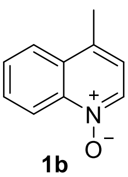
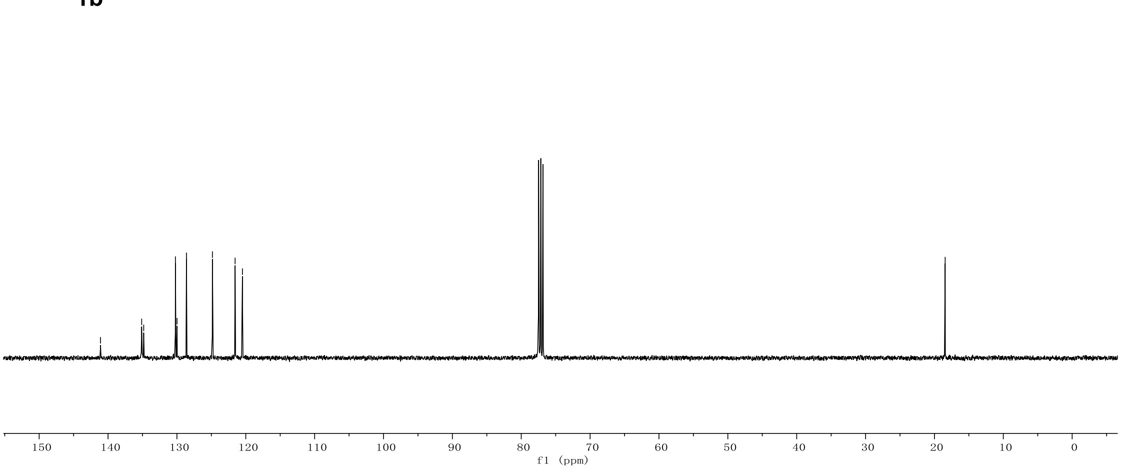


1b



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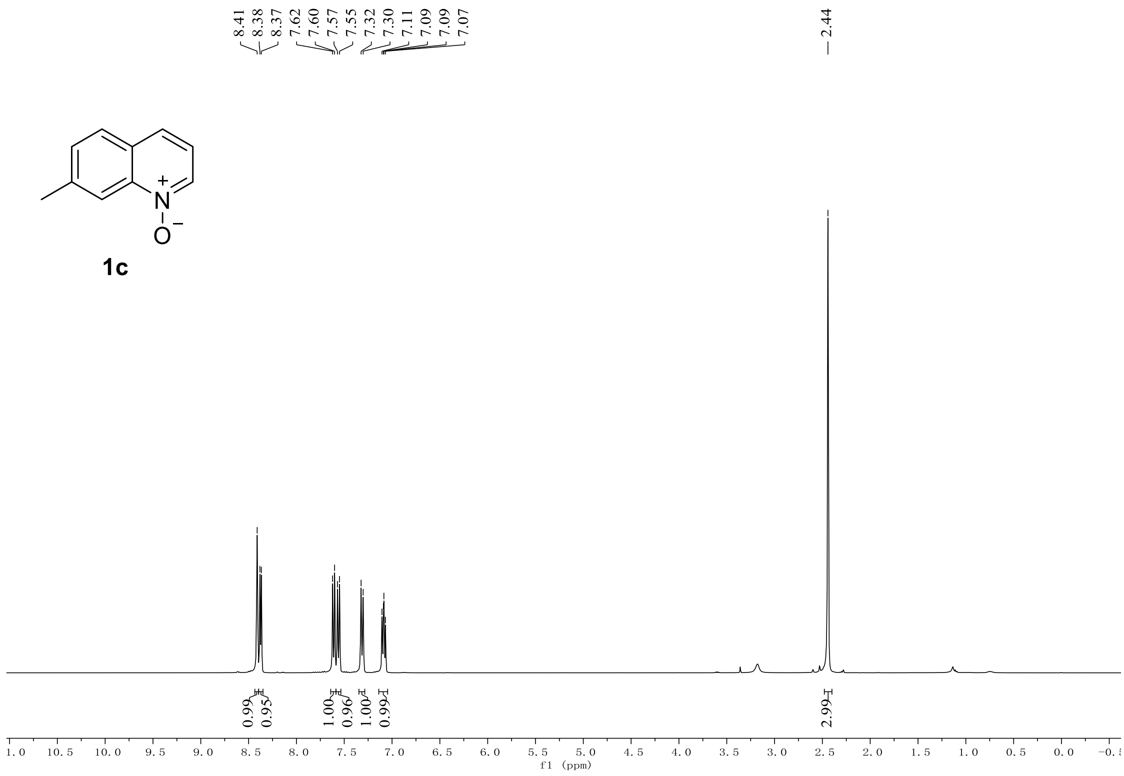

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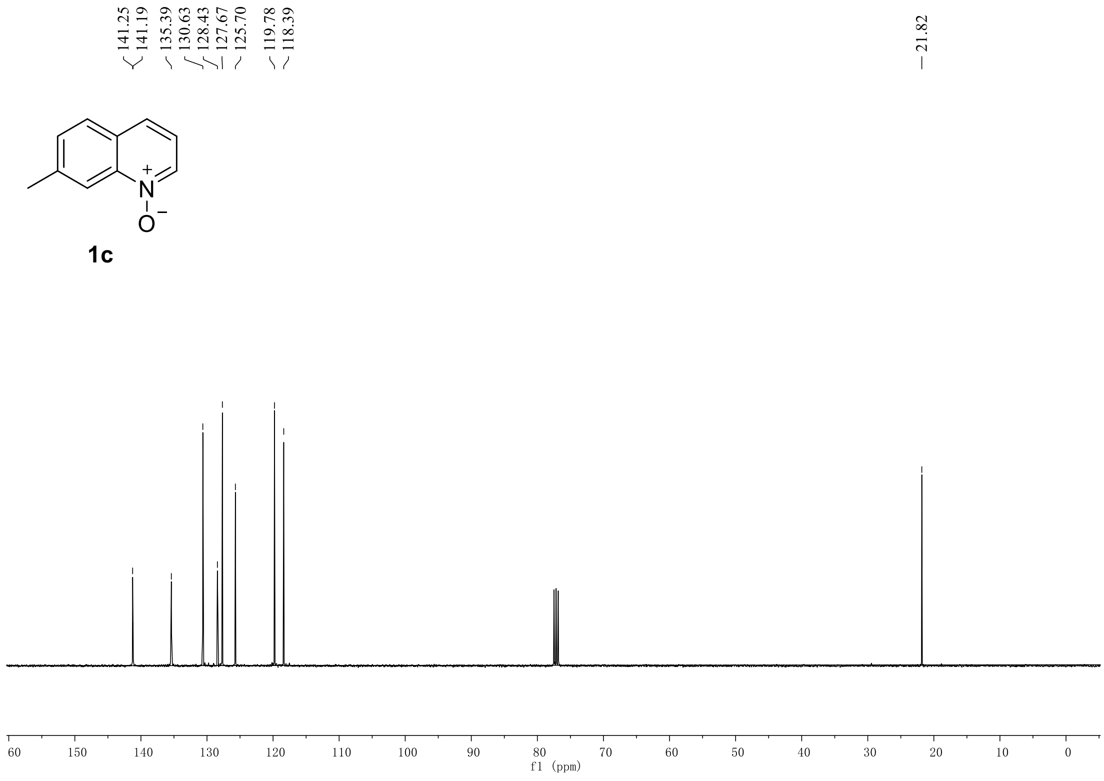

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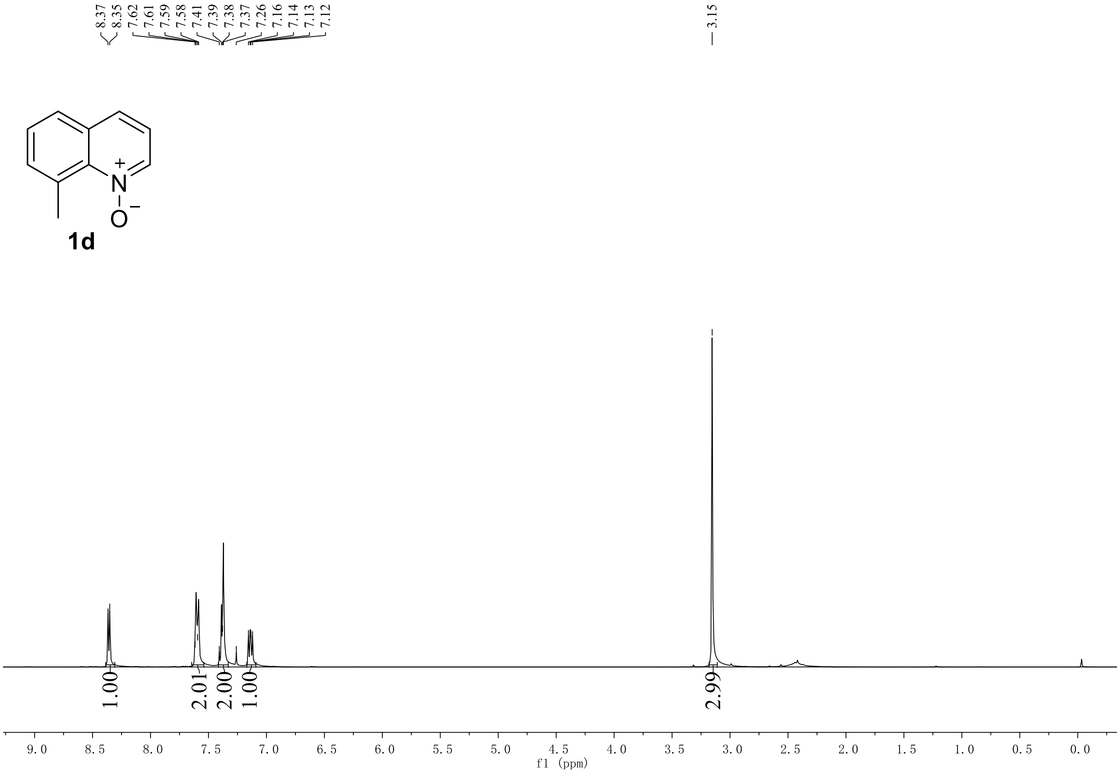

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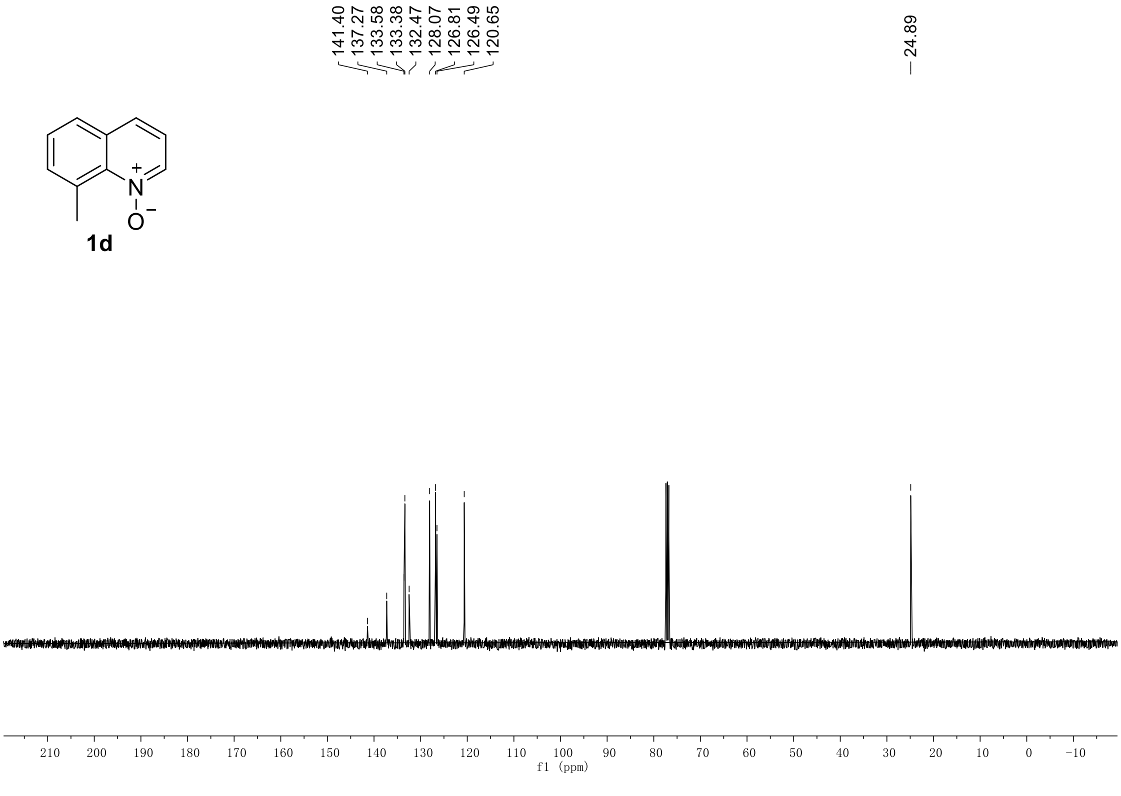

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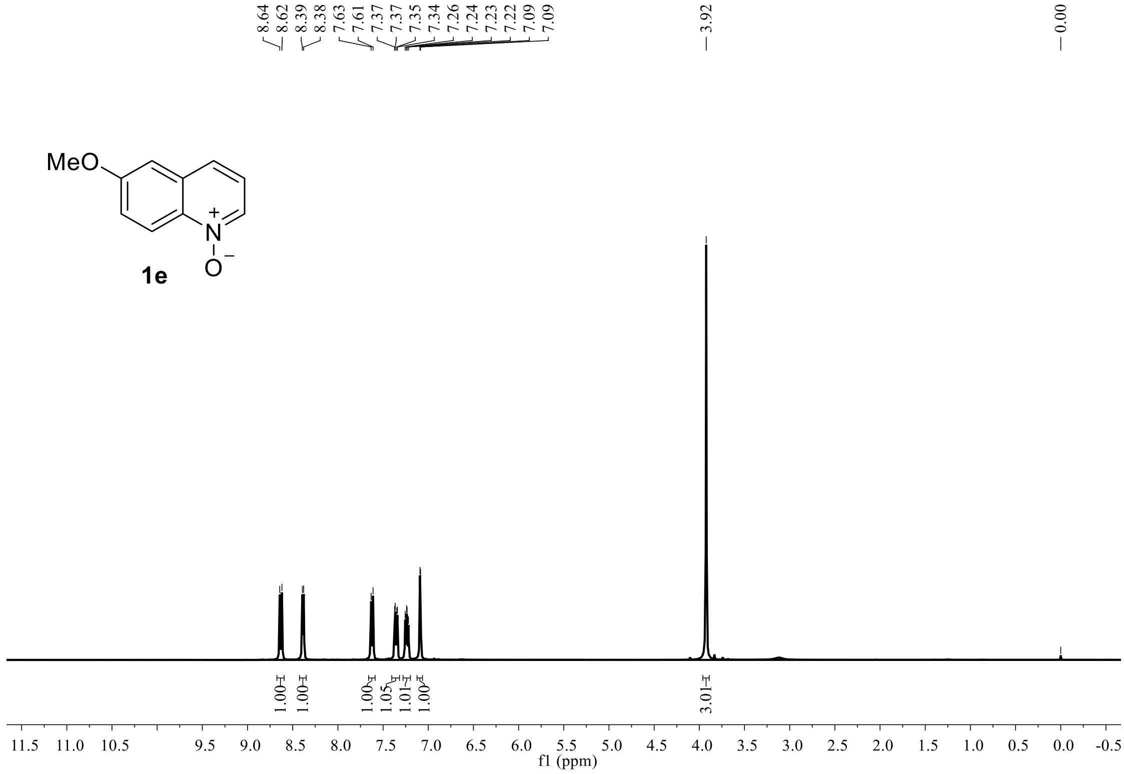

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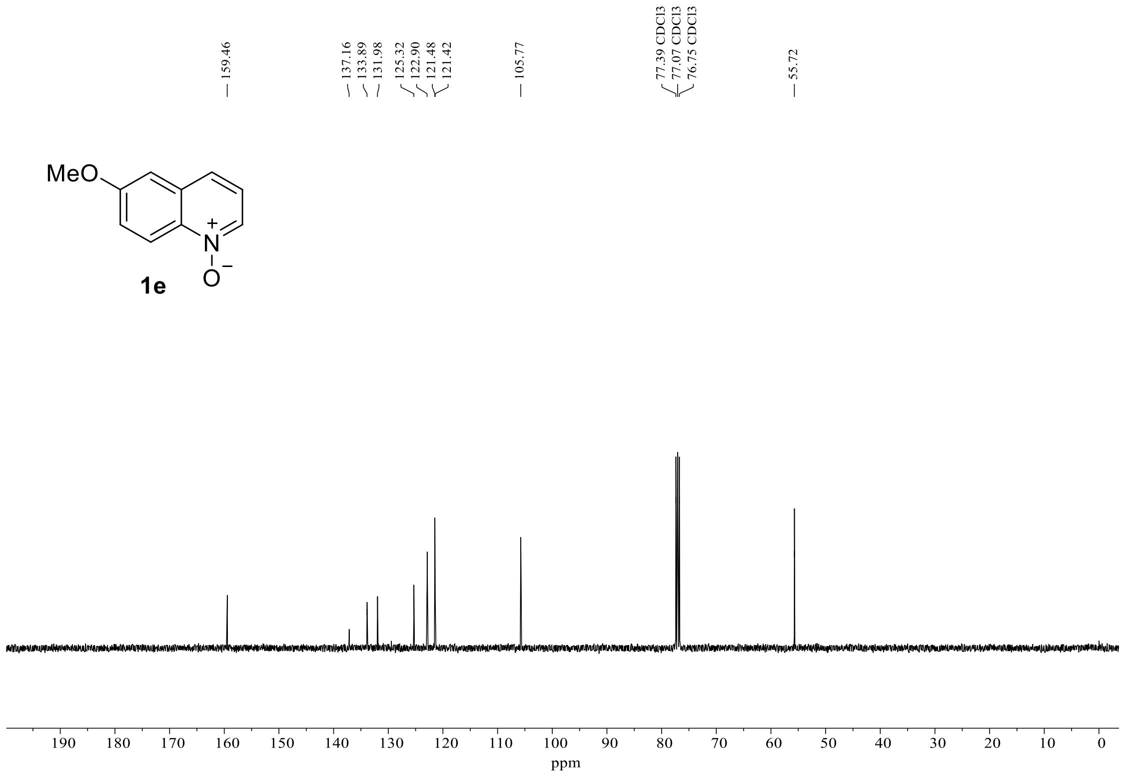

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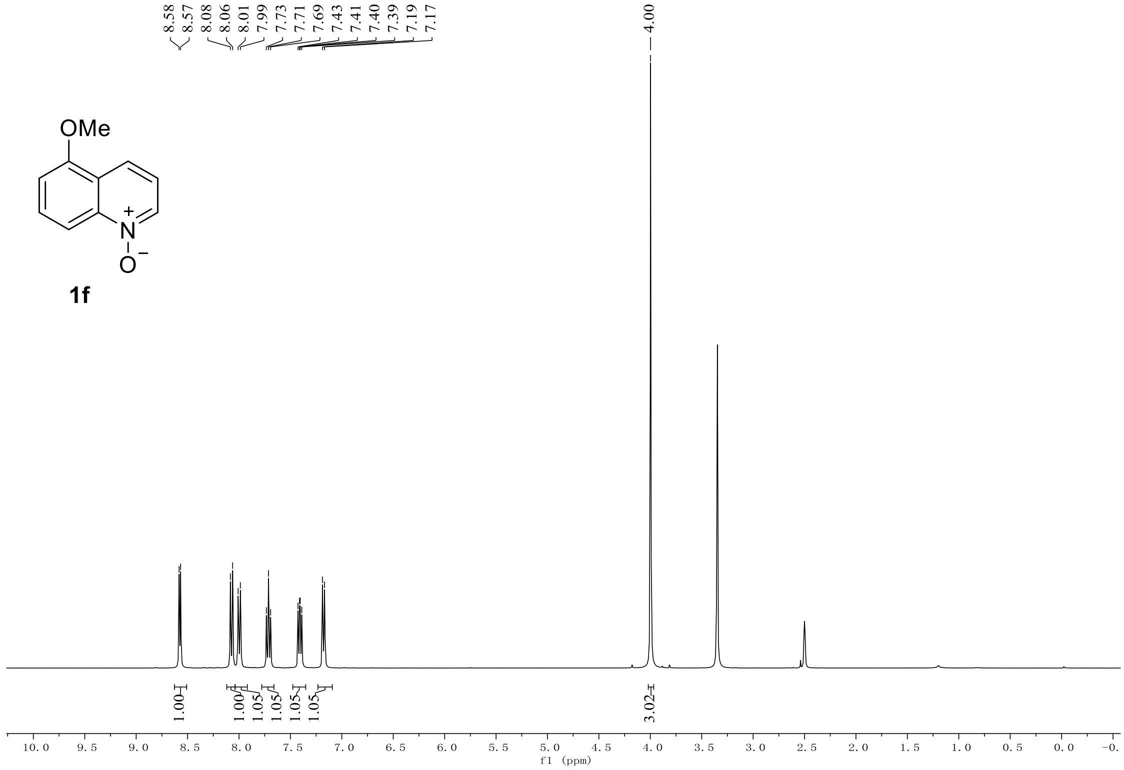

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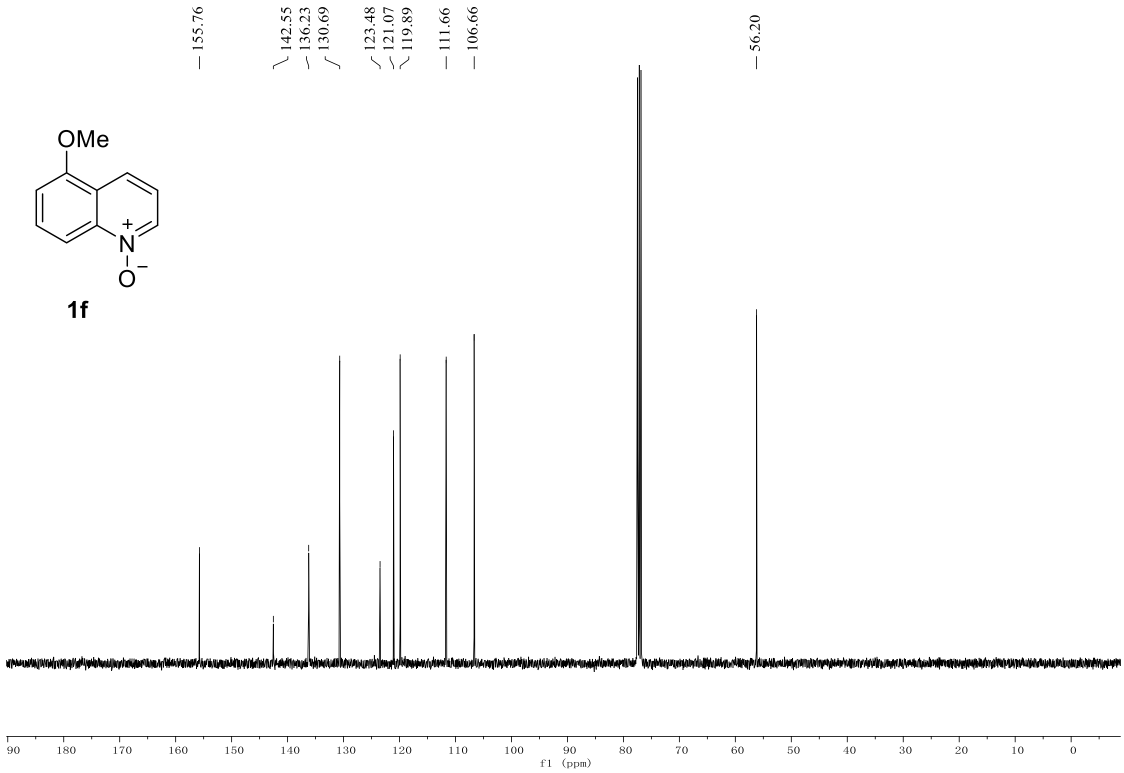

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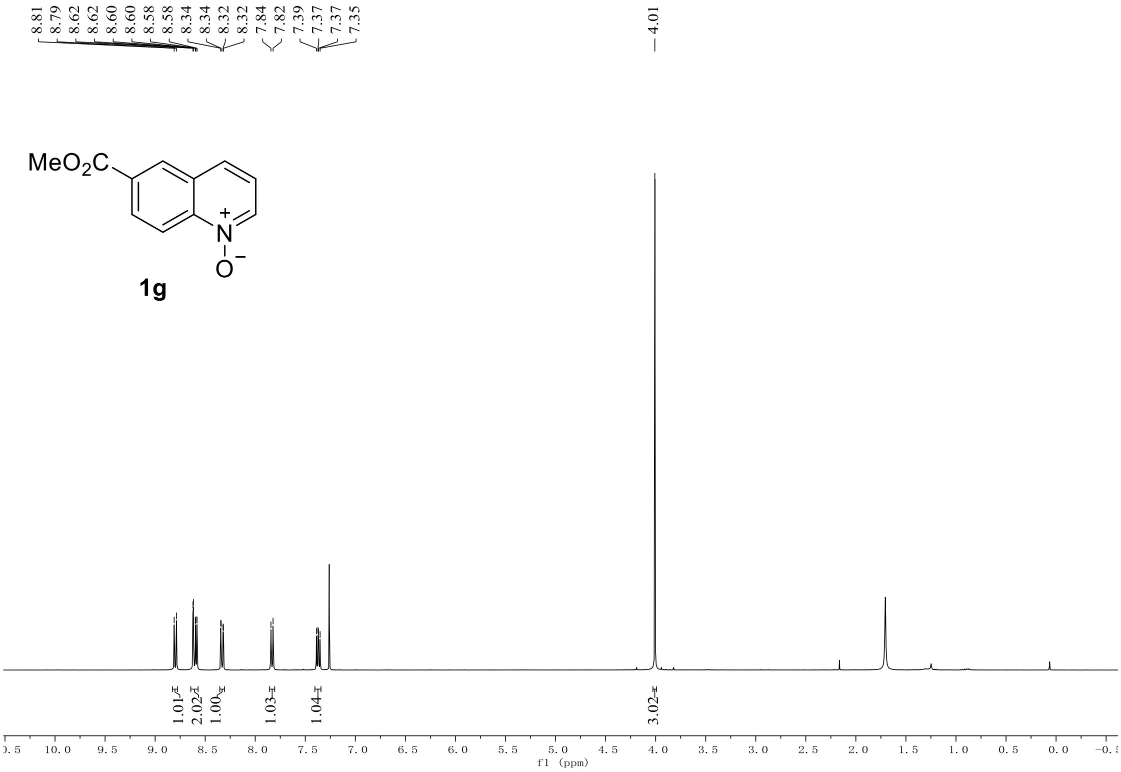

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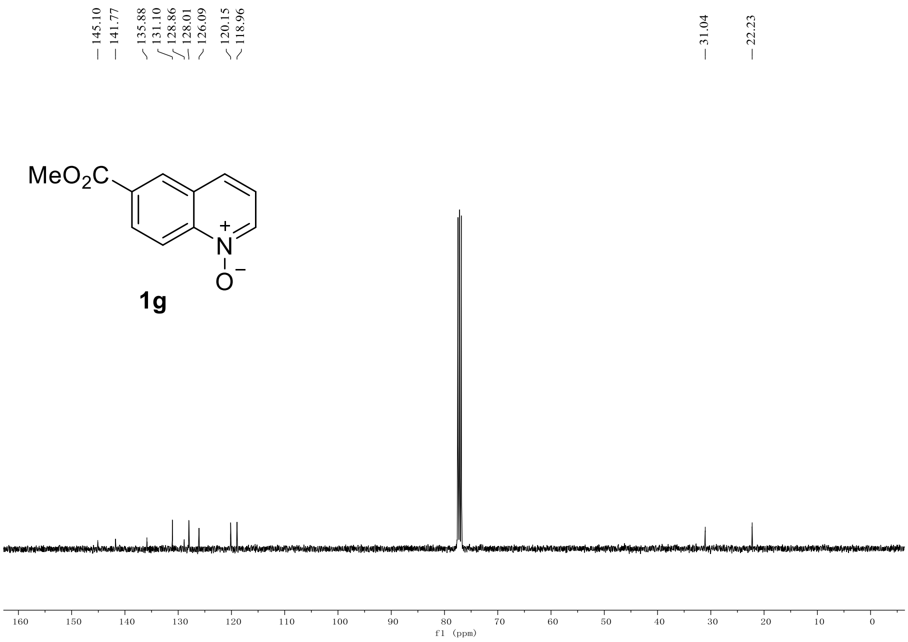

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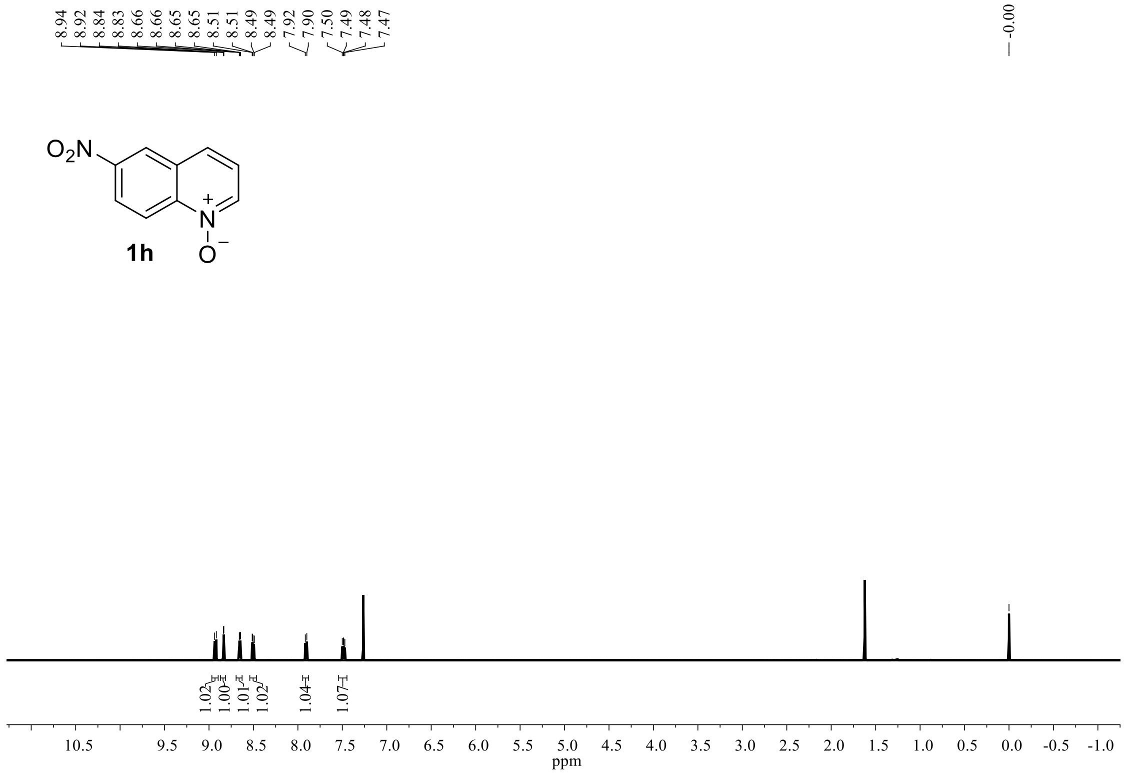

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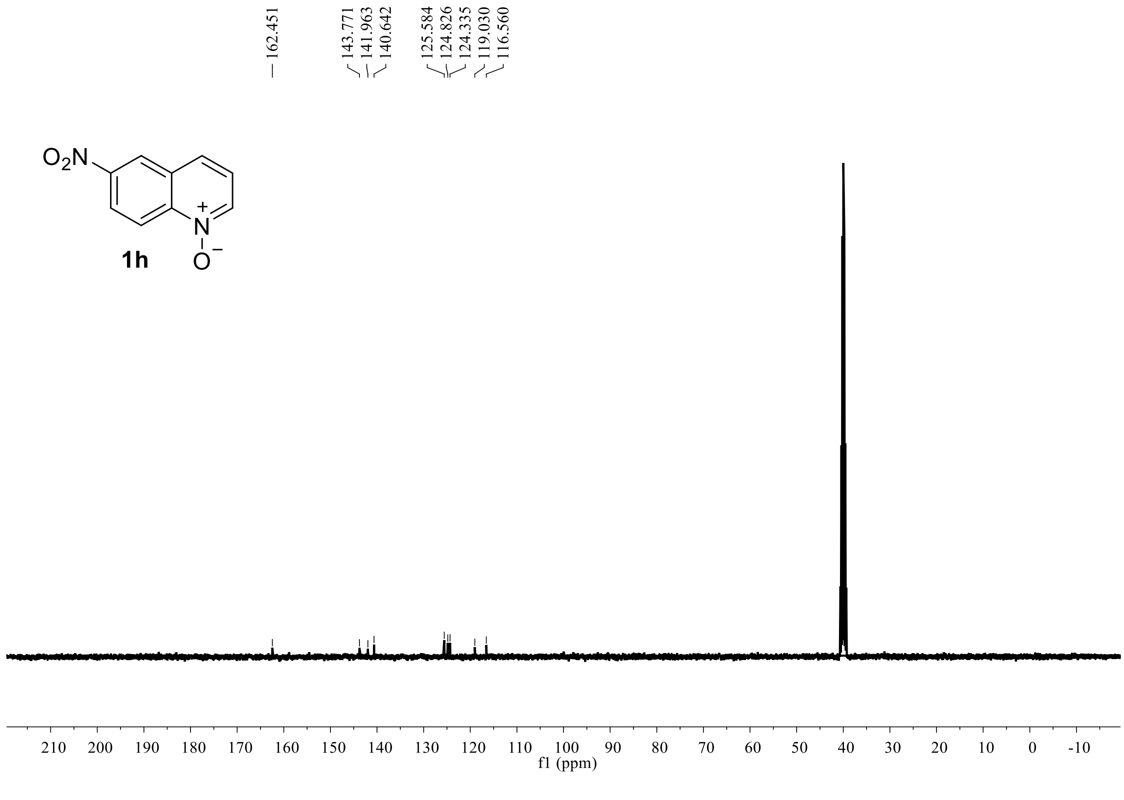

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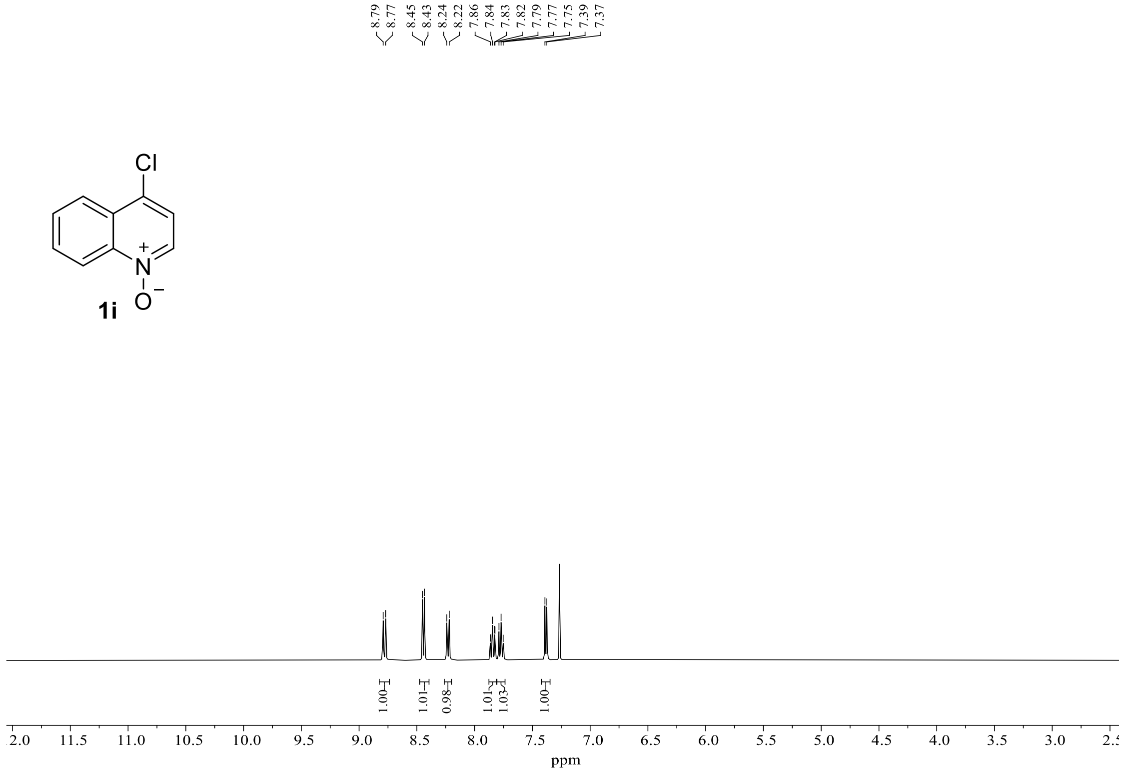
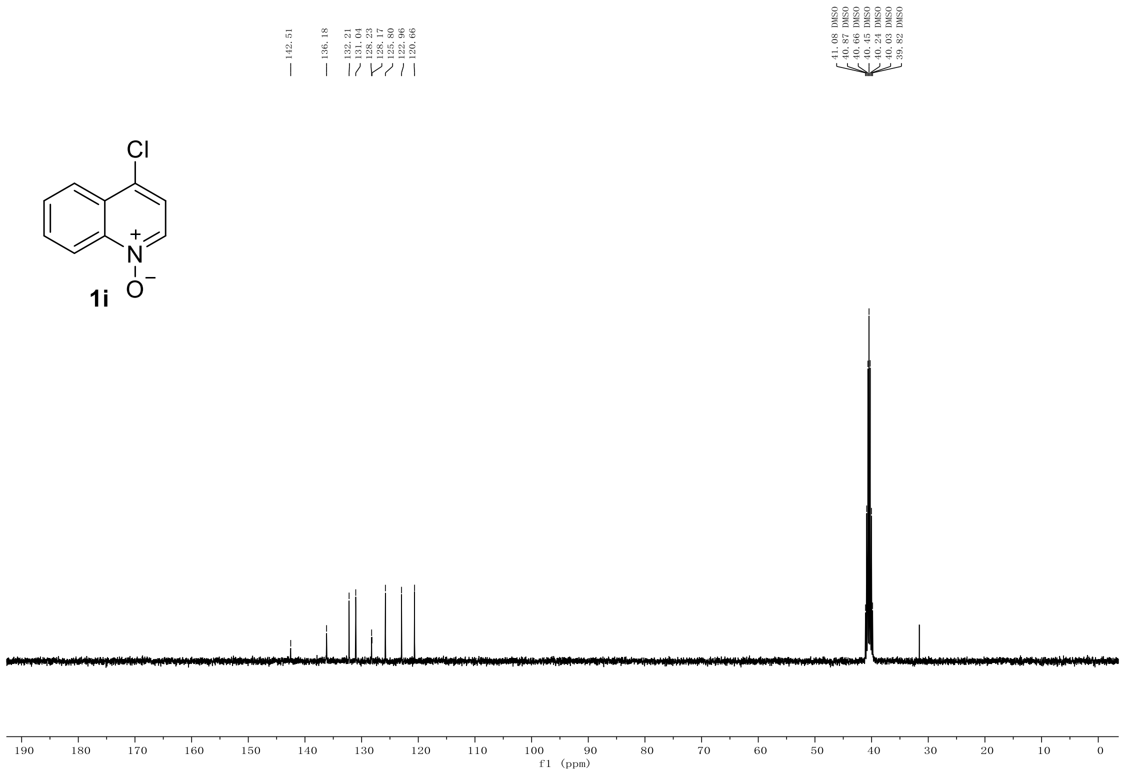


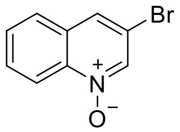
1i

^{13}C NMR, 100 MHz, DMSO-d_6

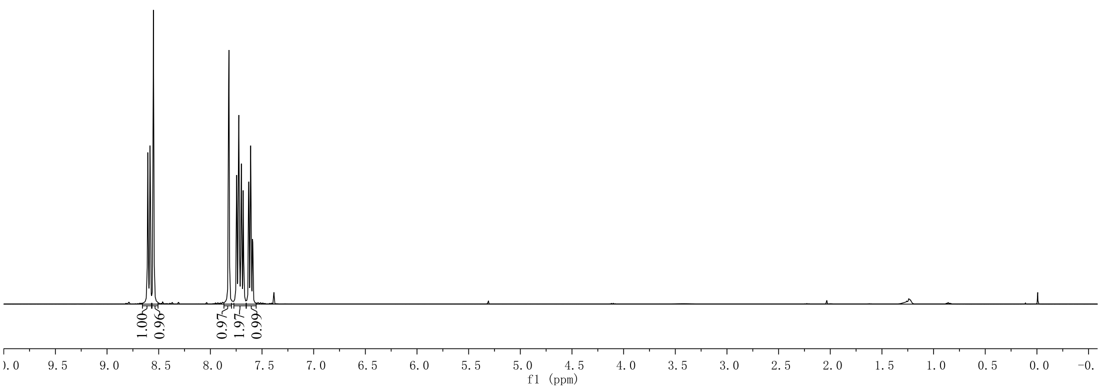


1i

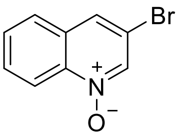
^{1}H NMR, 400 MHz, $CDCl_3$



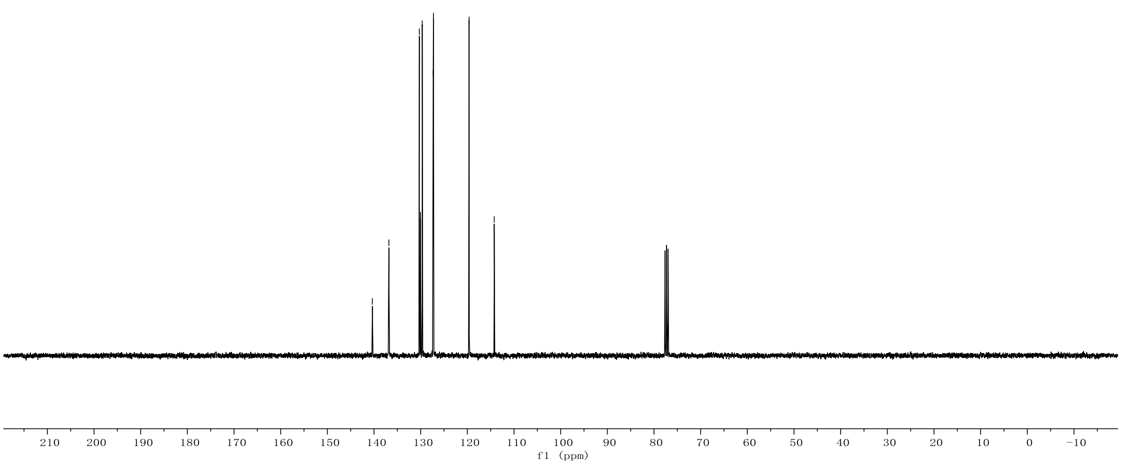
1j



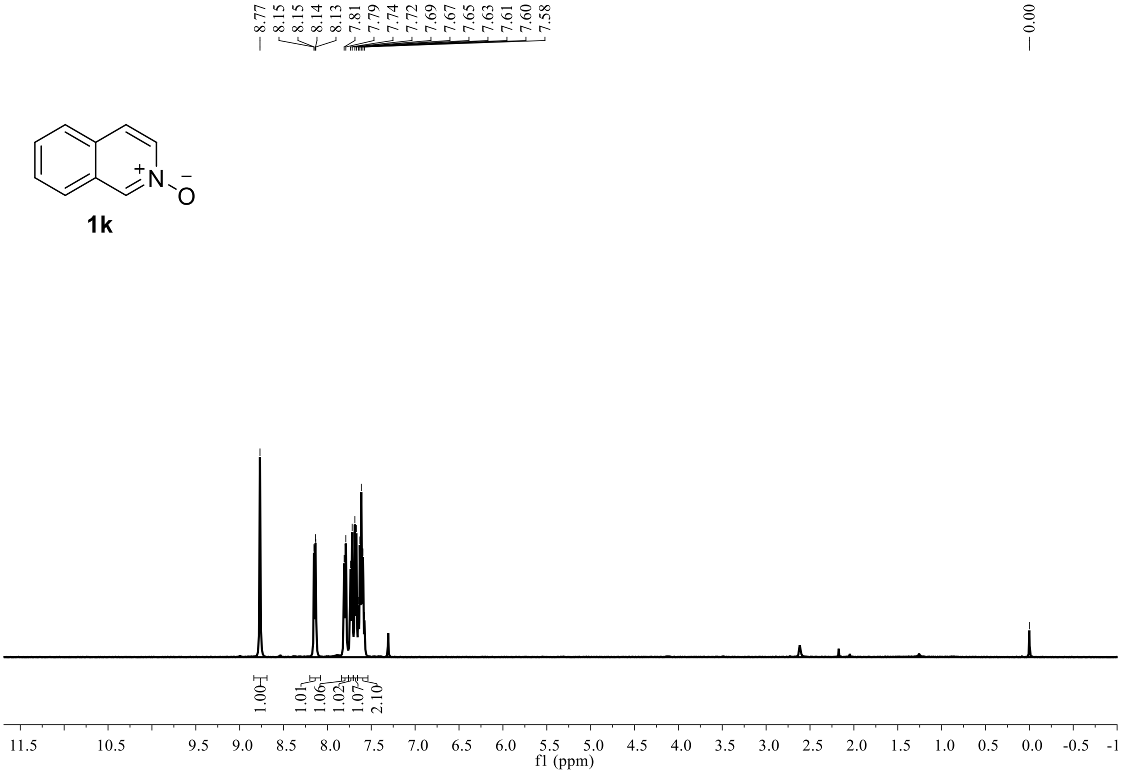
^{13}C NMR, 100 MHz, $CDCl_3$



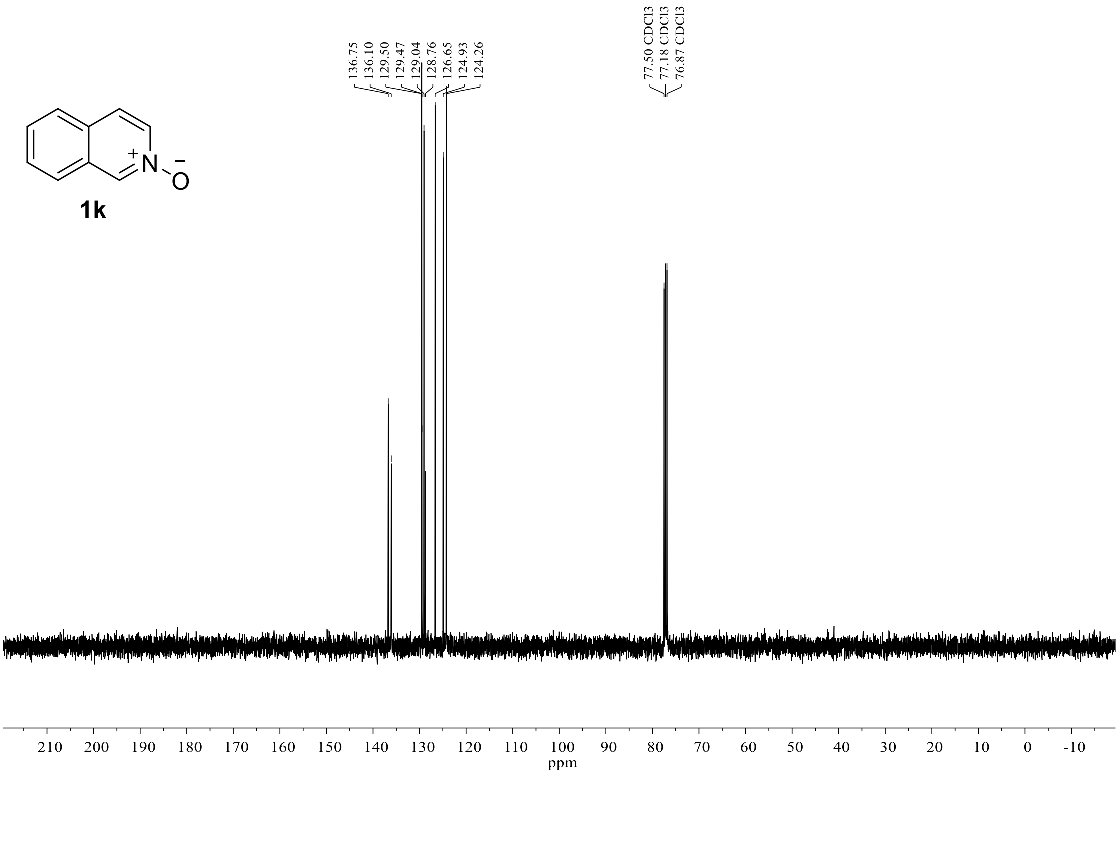
1j



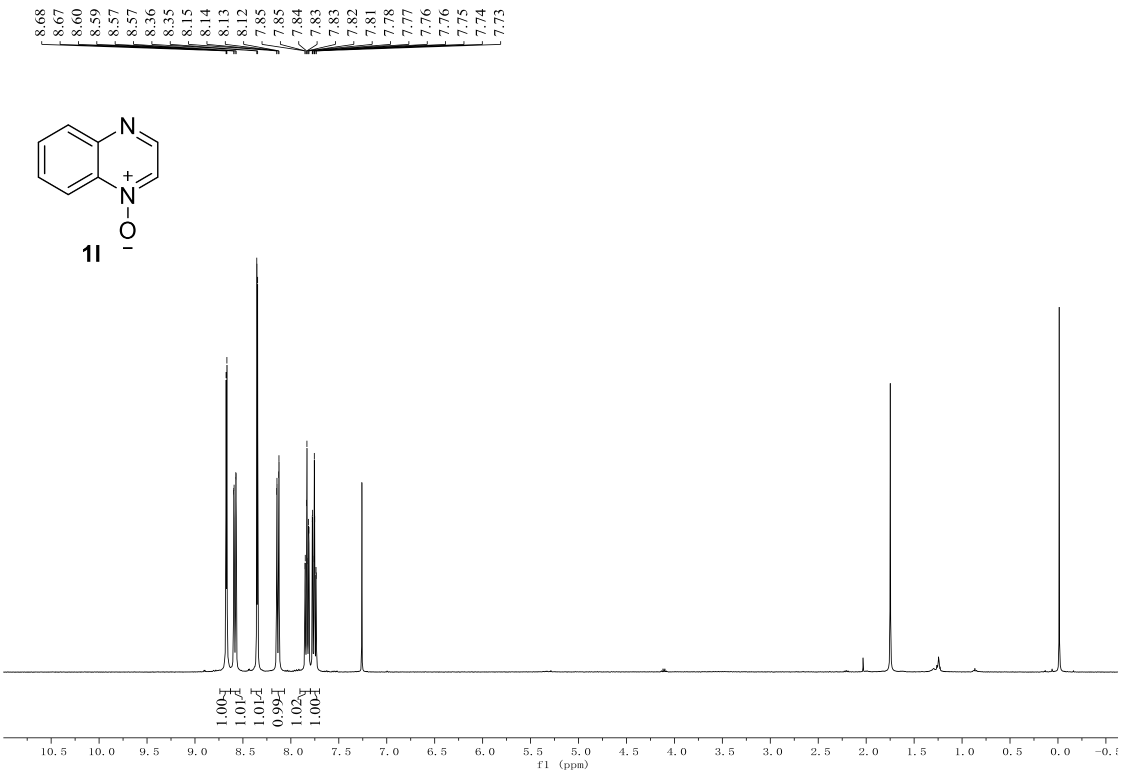
^{1}H NMR, 400 MHz, $CDCl_3$



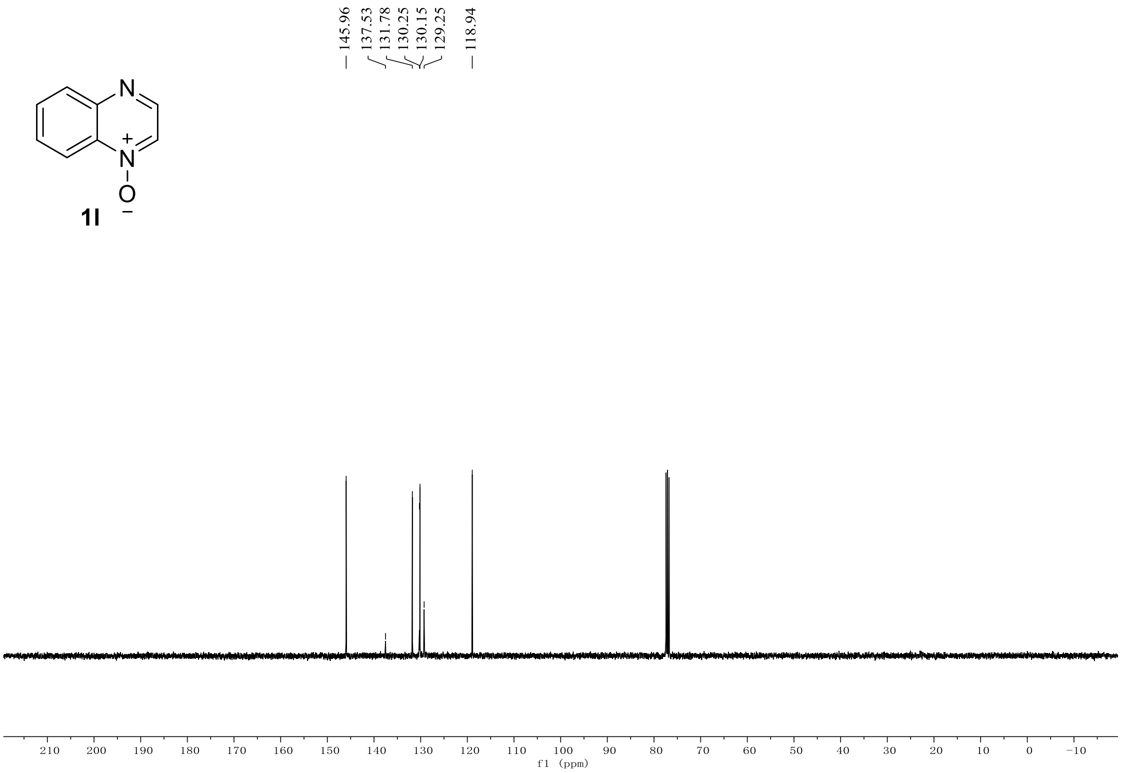
^{13}C NMR, 100 MHz, $CDCl_3$



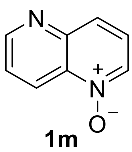
^{1}H NMR, 400 MHz, $CDCl_3$



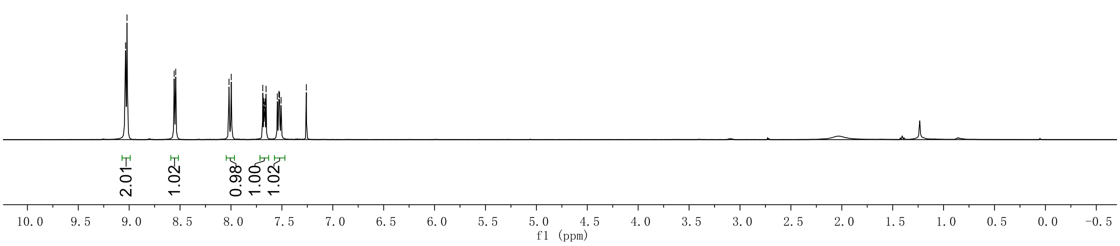
^{13}C NMR, 100 MHz, $CDCl_3$



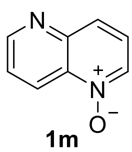
^{1}H NMR, 400 MHz, $CDCl_3$



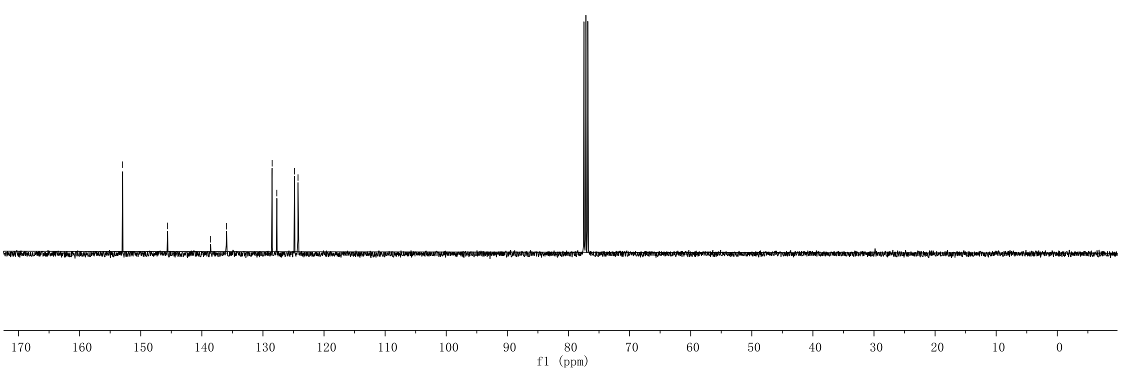
1m



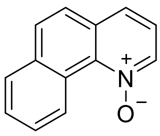
^{13}C NMR, 100 MHz, $CDCl_3$



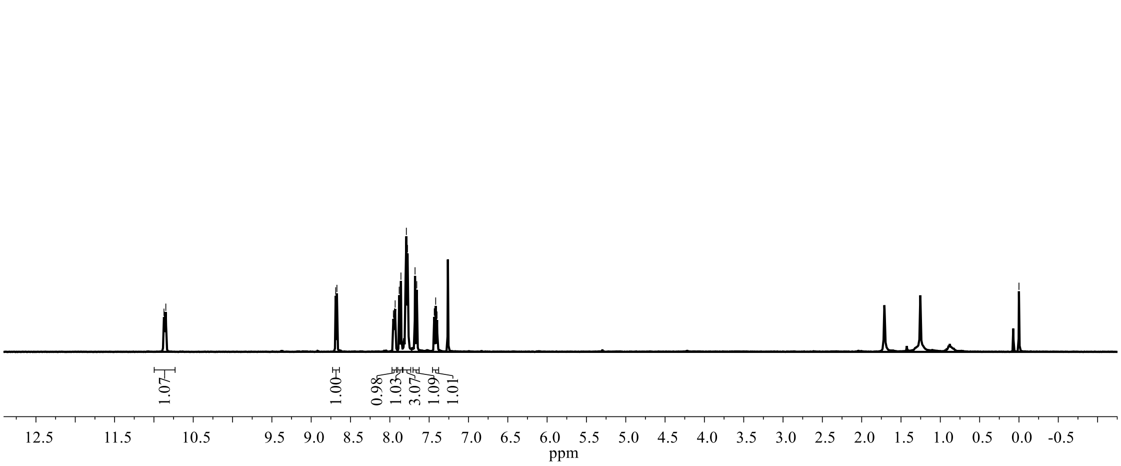
1m



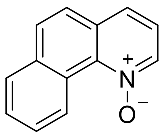
^{1}H NMR, 400 MHz, $CDCl_3$



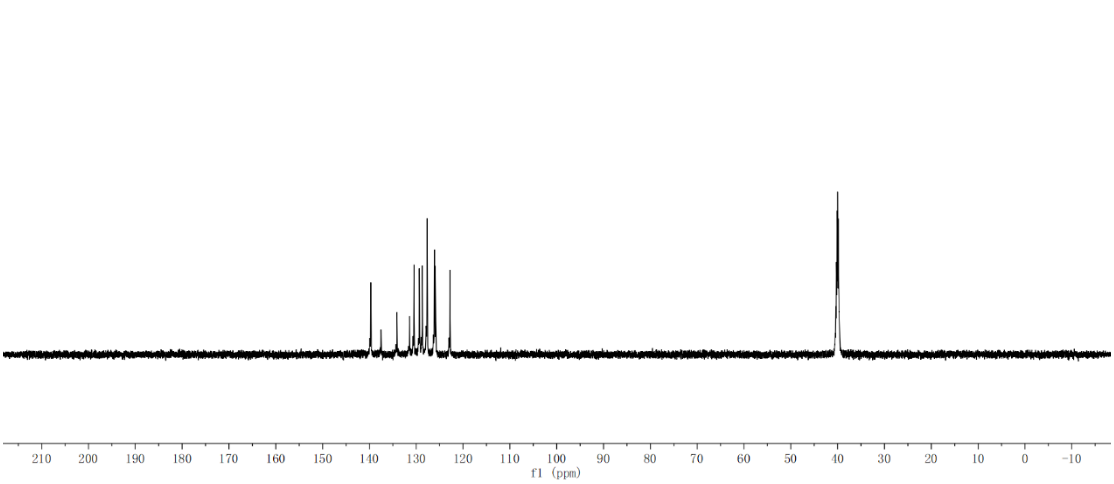
1n



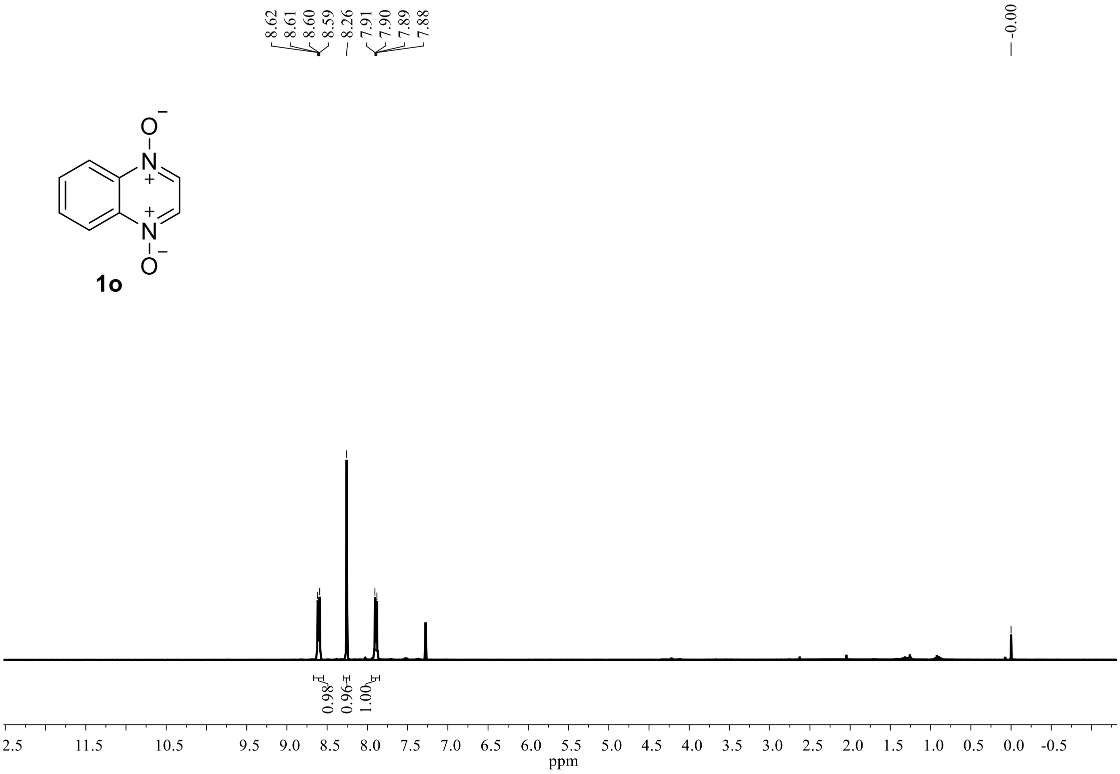
^{1}H NMR, 150 MHz, DMSO-d_6



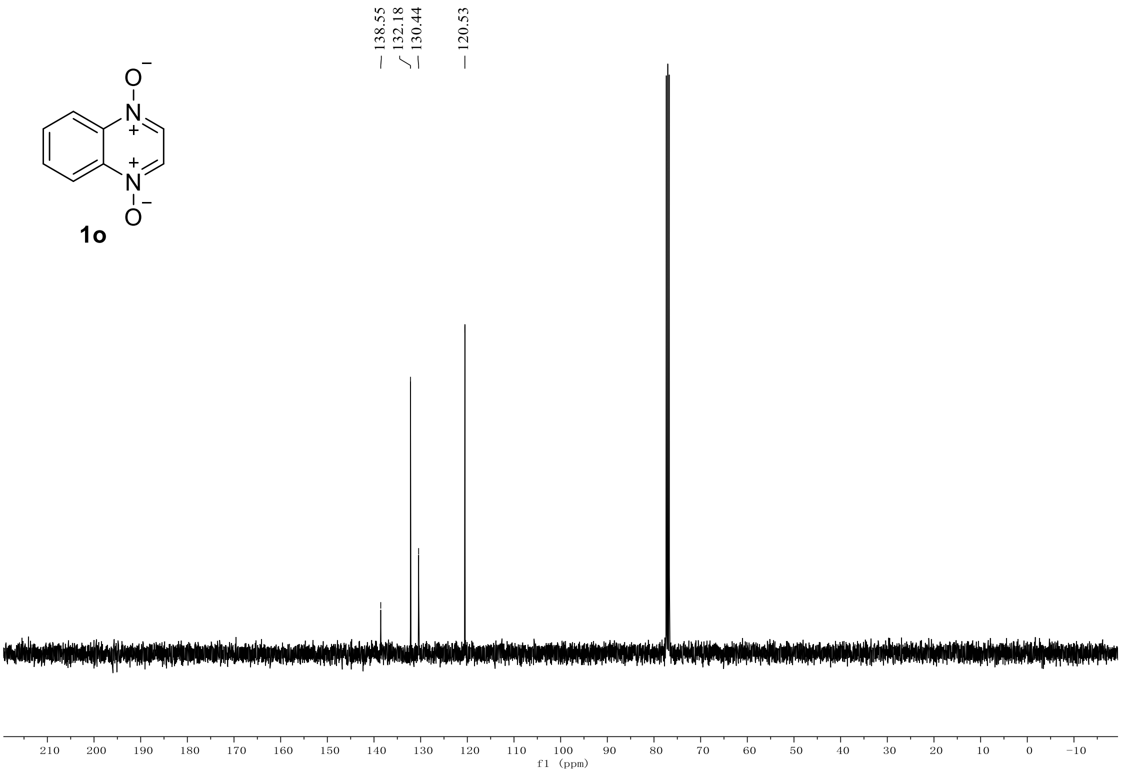
1n



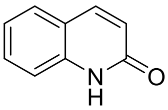
^{1}H NMR, 400 MHz, $CDCl_3$



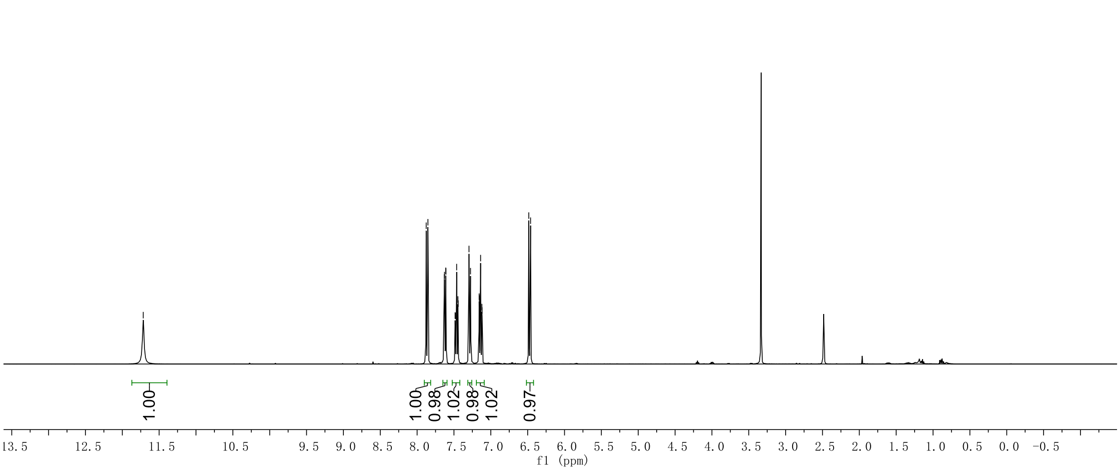
^{13}C NMR, 100 MHz, $CDCl_3$



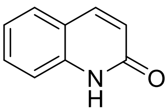
^{1}H NMR, 400 MHz, DMSO-d_6



2a



^{13}C NMR, 100 MHz, DMSO-d_6



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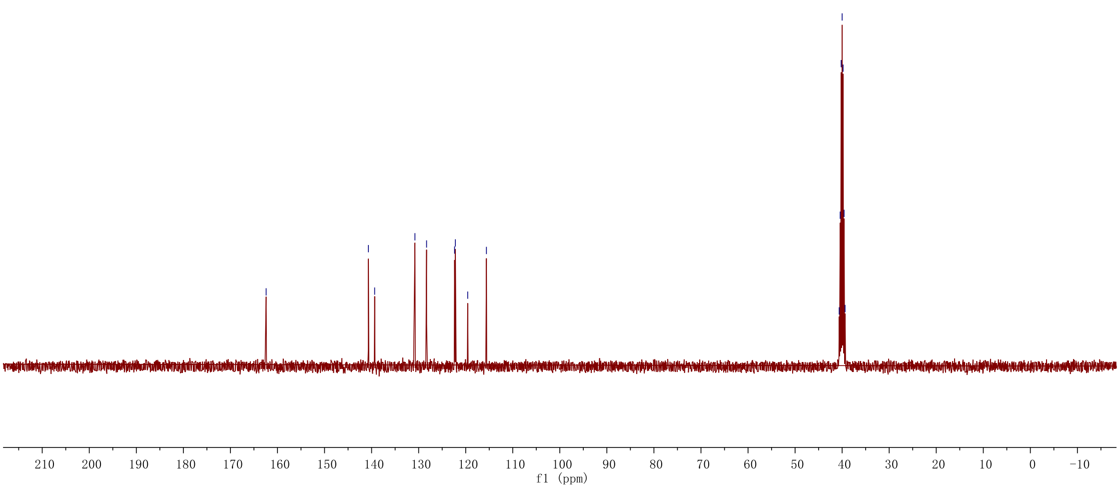
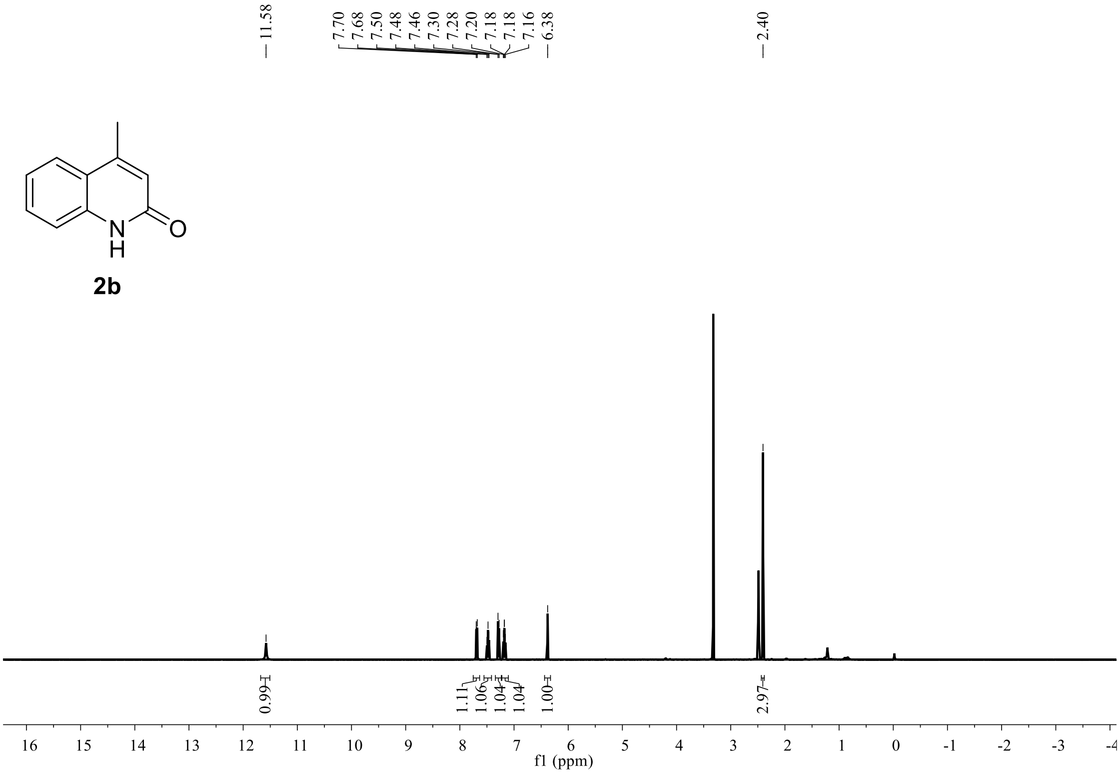
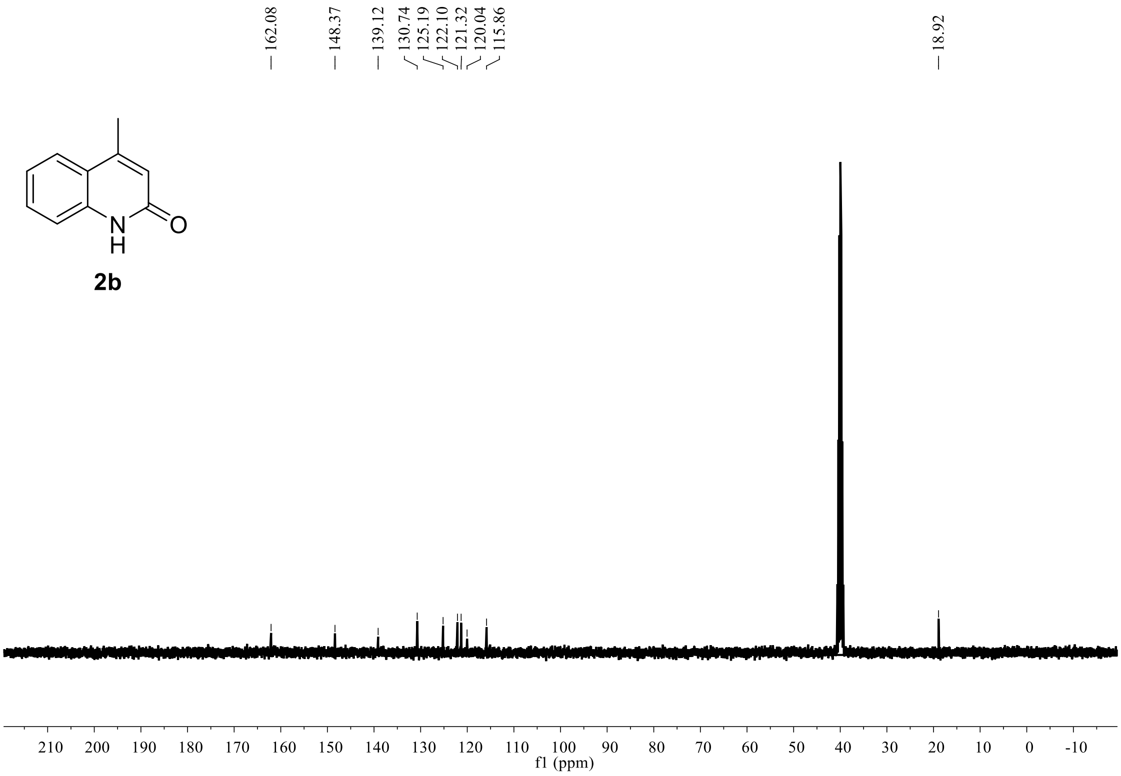


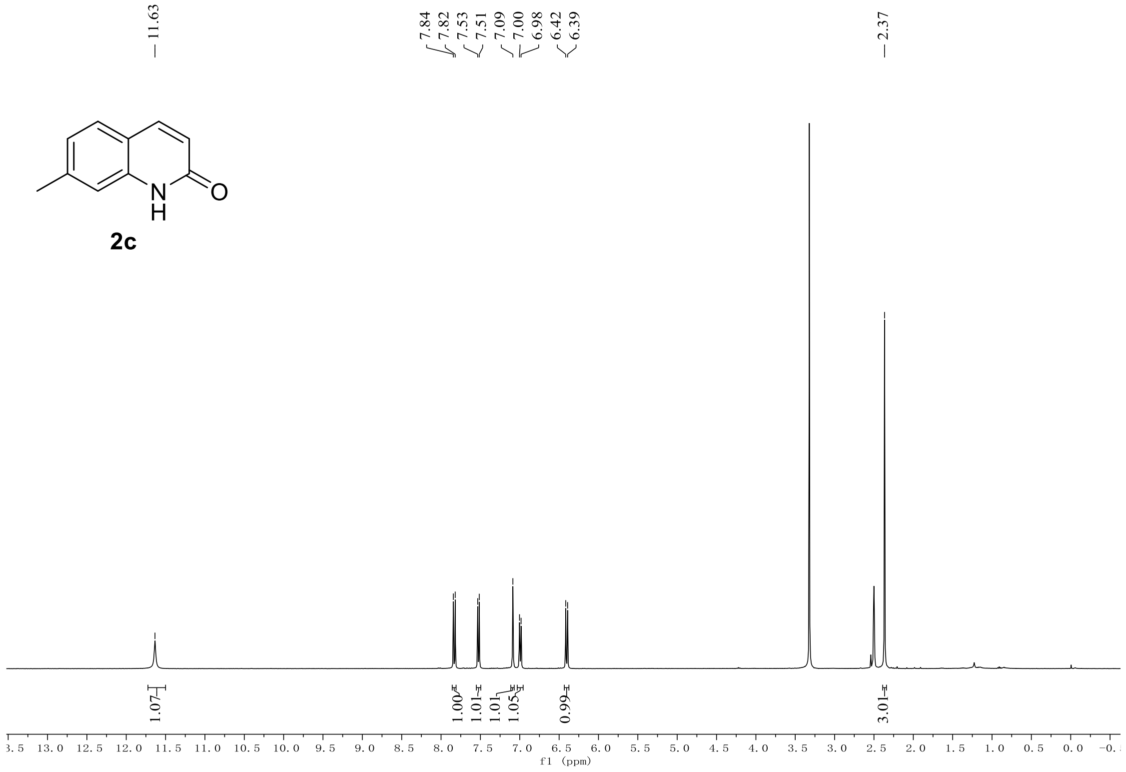
^{1}H NMR, 400 MHz, DMSO-d_6



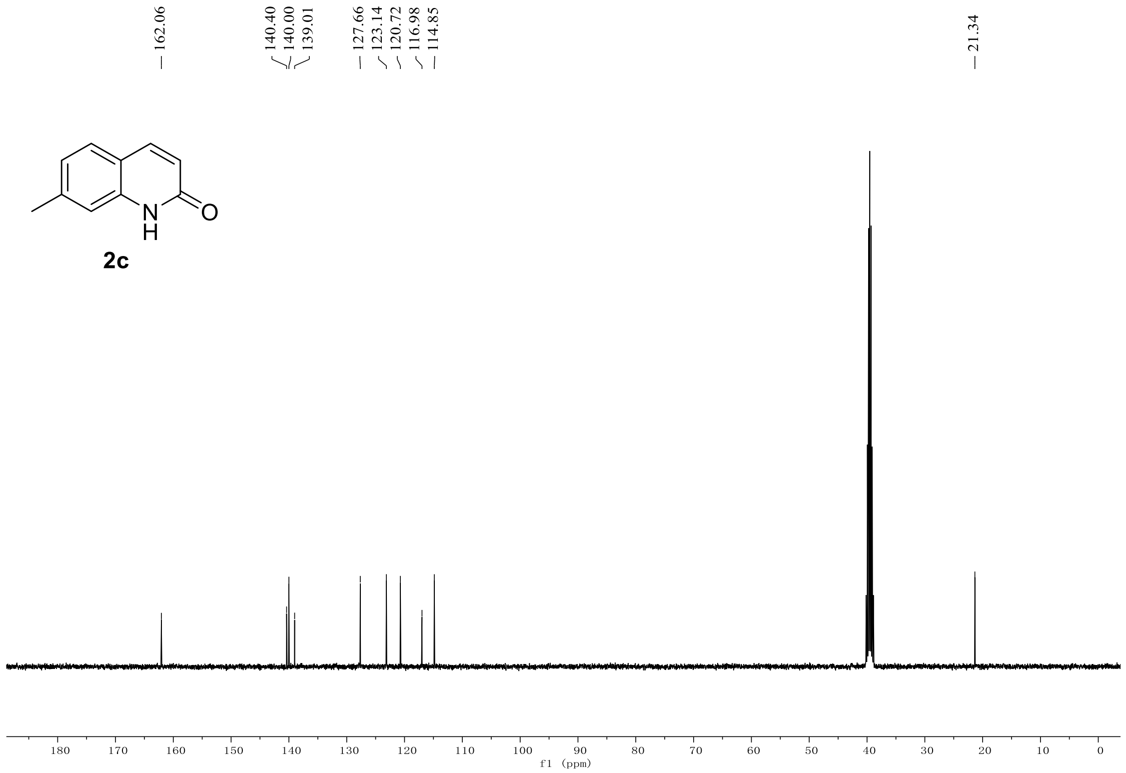
^{13}C NMR, 100 MHz, DMSO-d_6



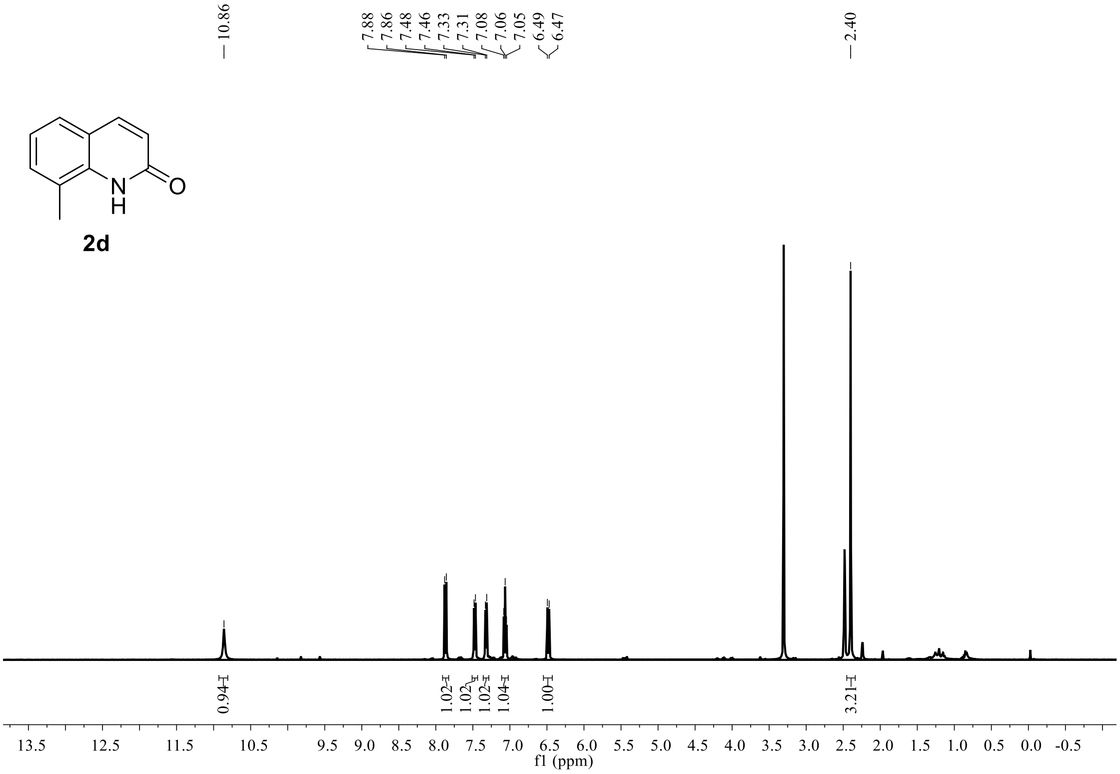
^{1}H NMR, 400 MHz, DMSO-d_6



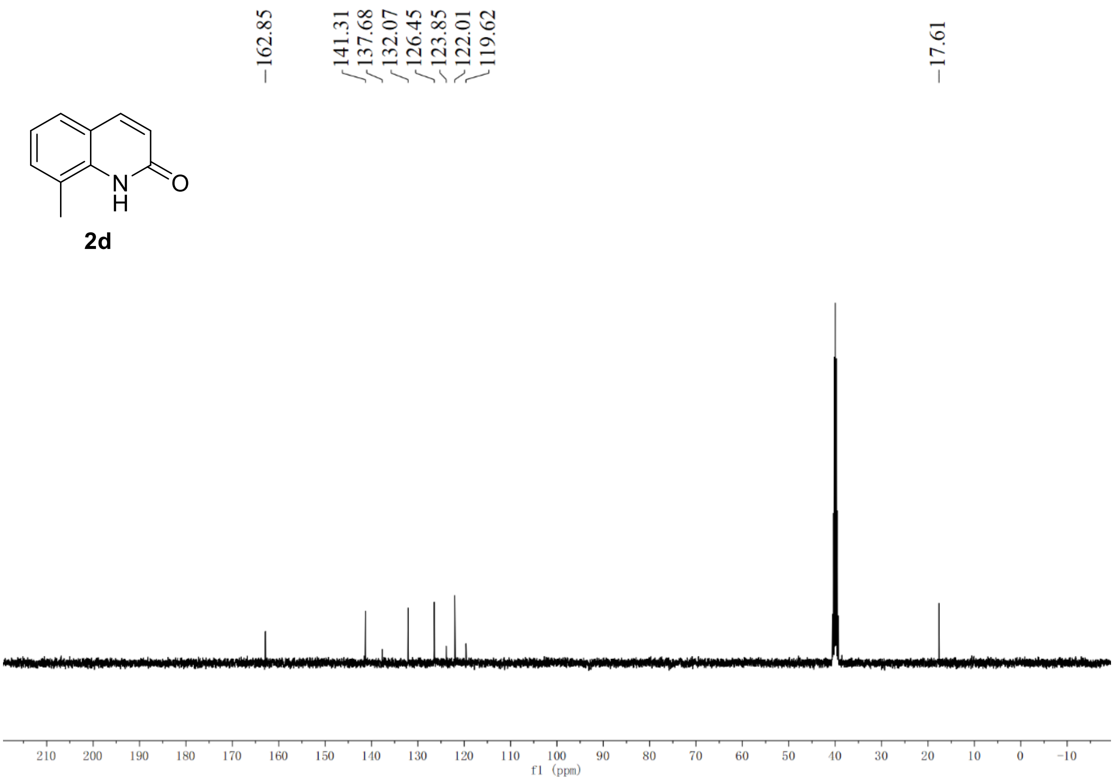
^{13}C NMR, 100 MHz, DMSO-d_6



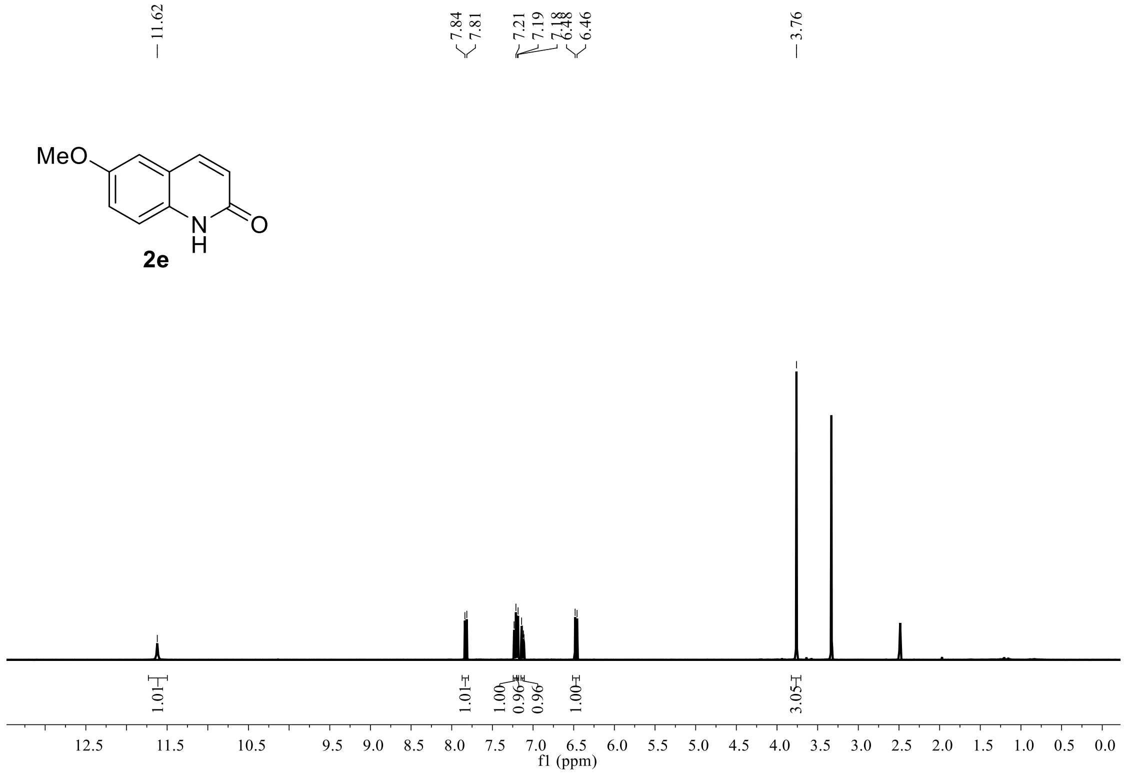
^{1}H NMR, 400 MHz, DMSO-d_6



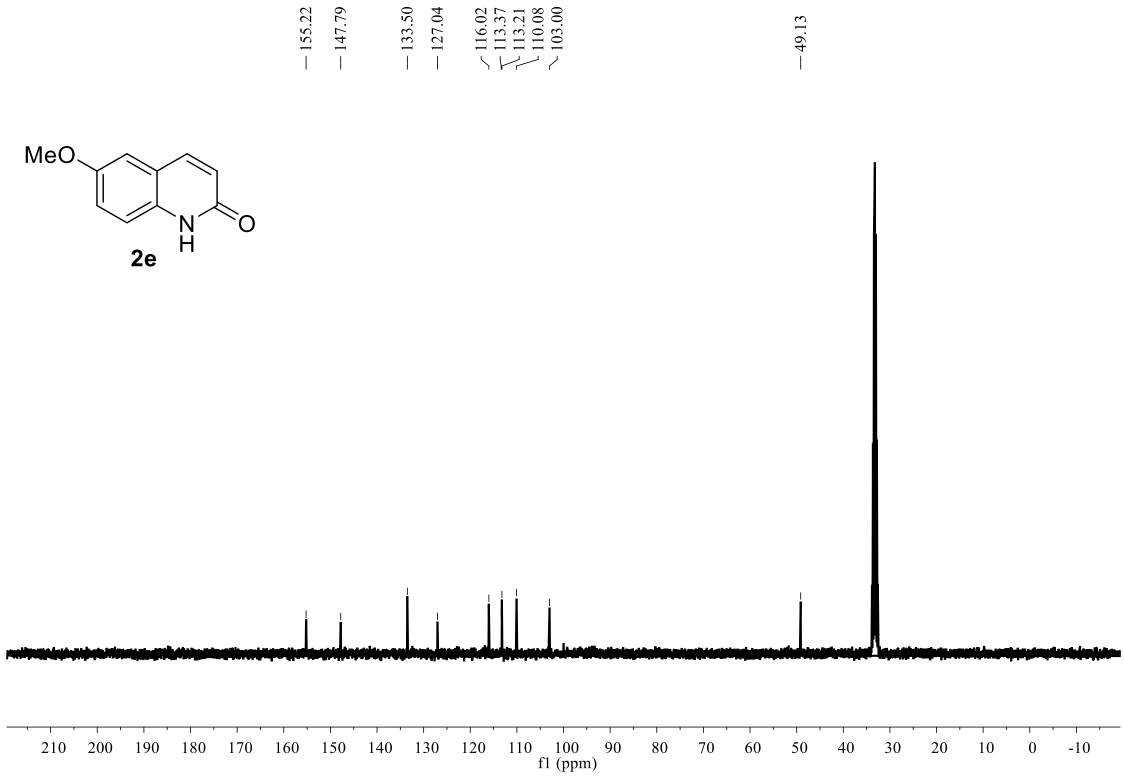
^{13}C NMR, 100 MHz, DMSO-d_6



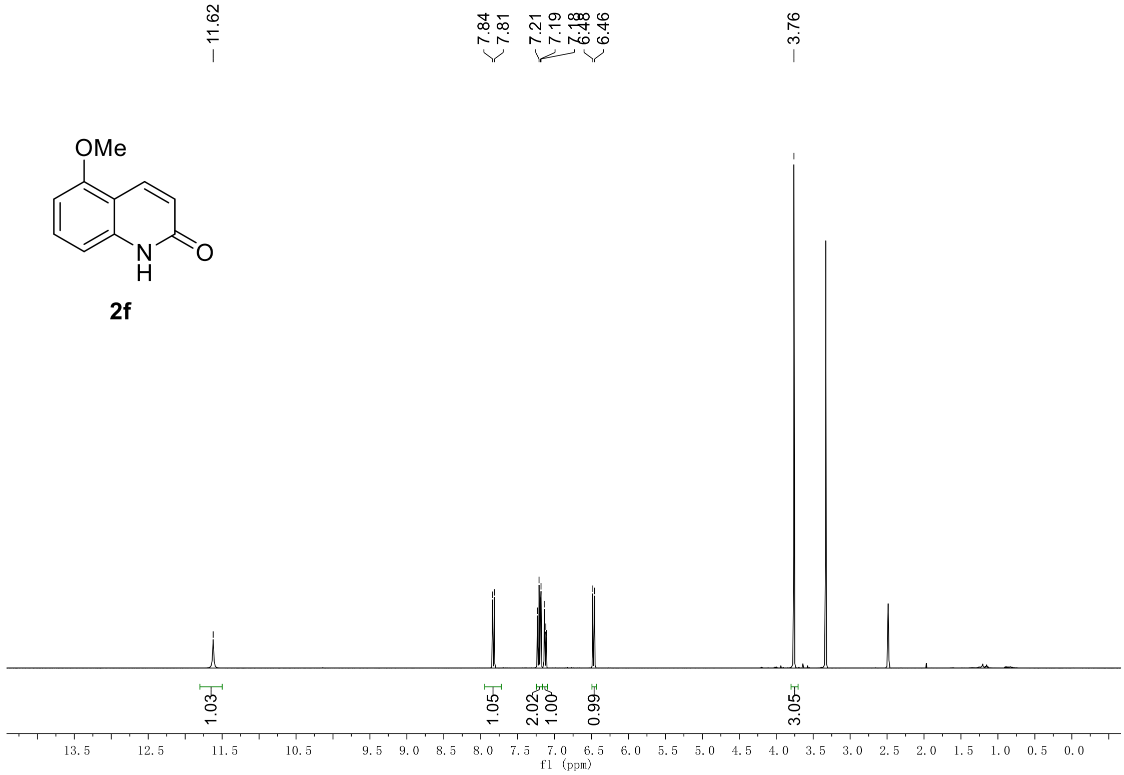
^{1}H NMR, 400 MHz, DMSO-d_6



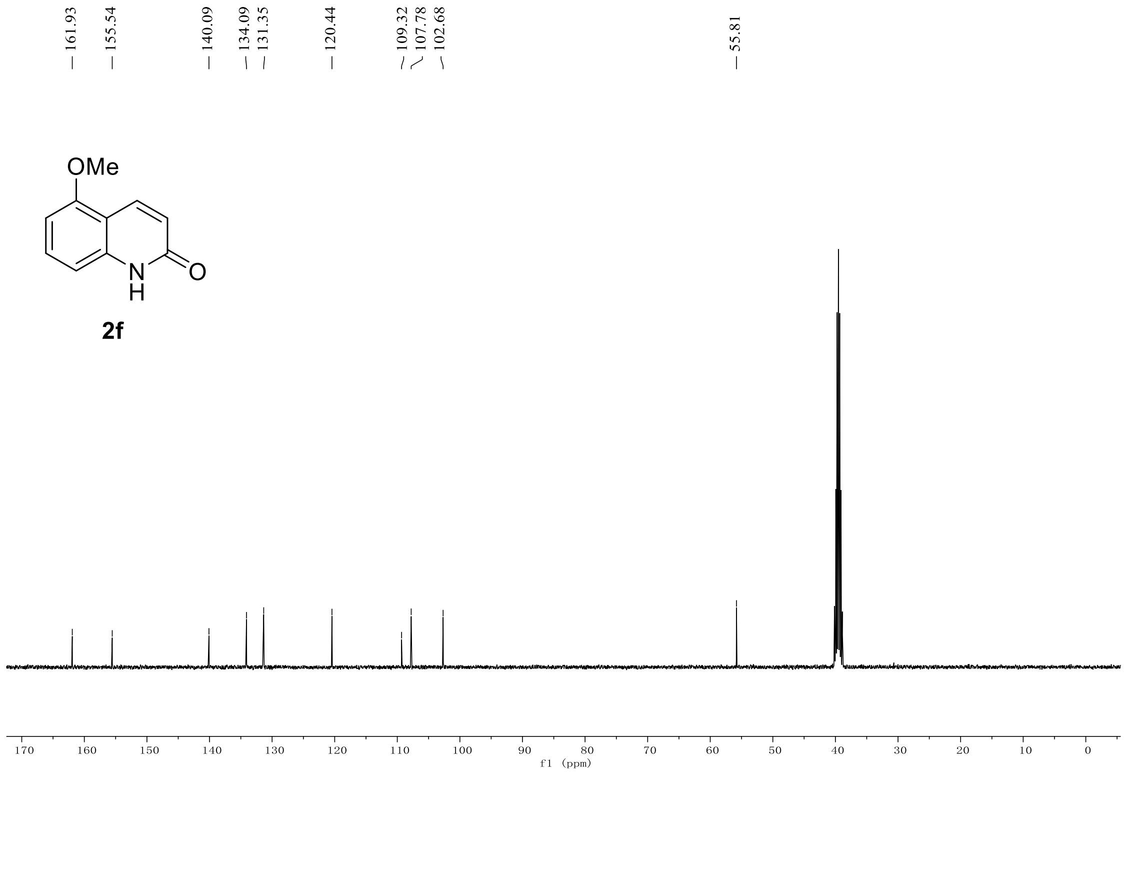
^{13}C NMR, 100 MHz, DMSO-d_6



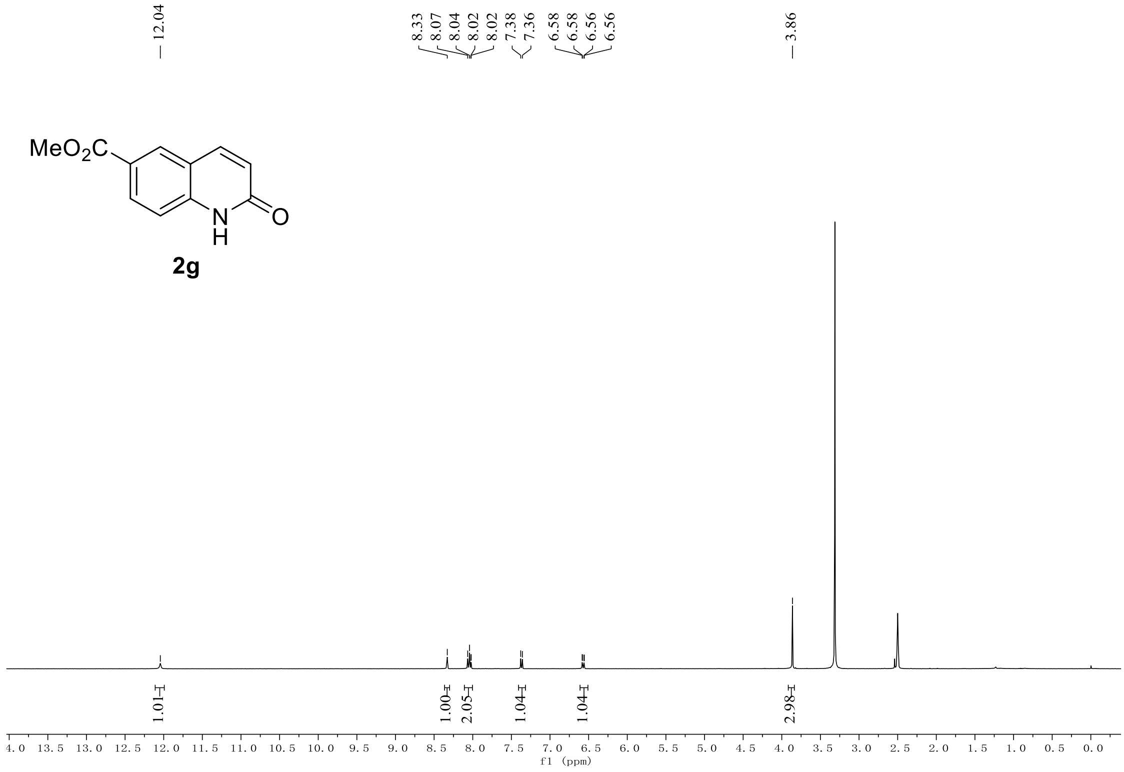
^1H NMR, 400 MHz, DMSO-d_6



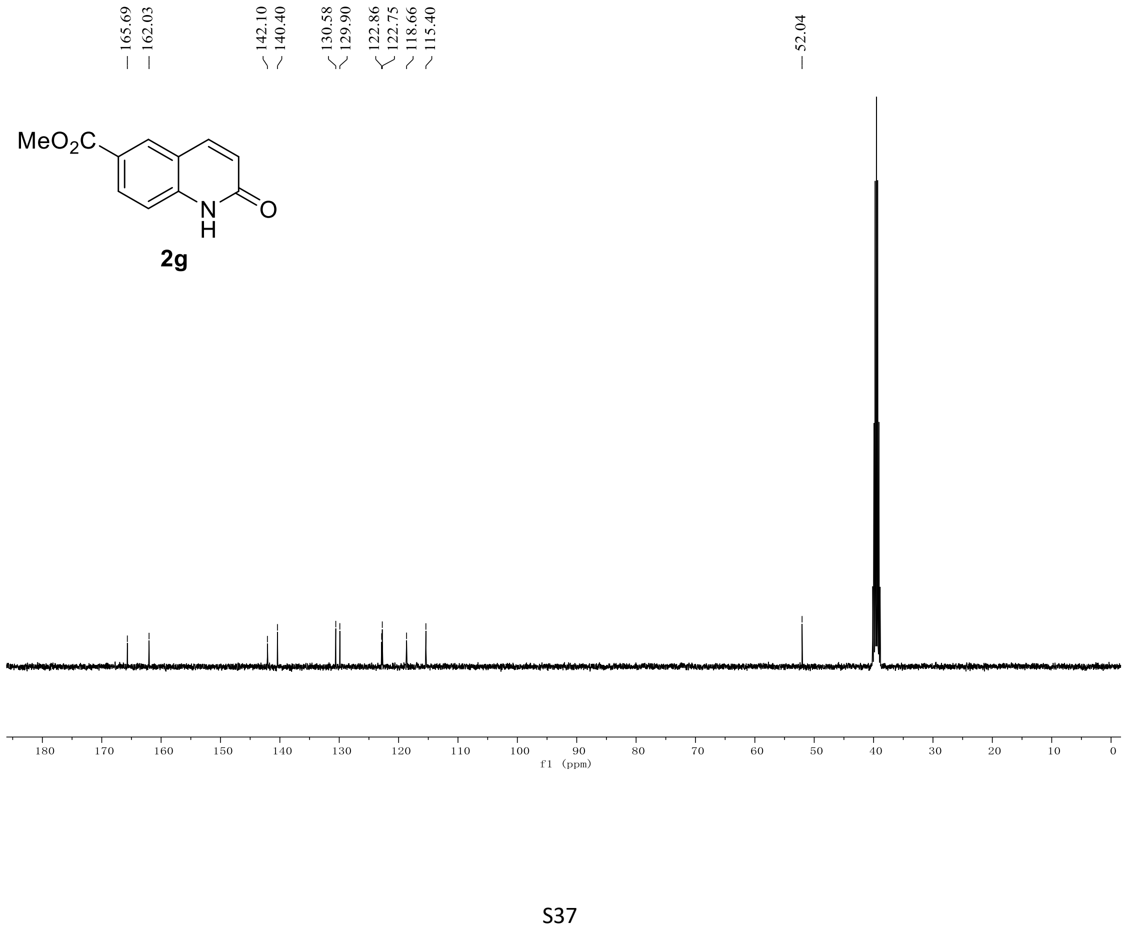
^{13}C NMR, 100 MHz, DMSO-d_6



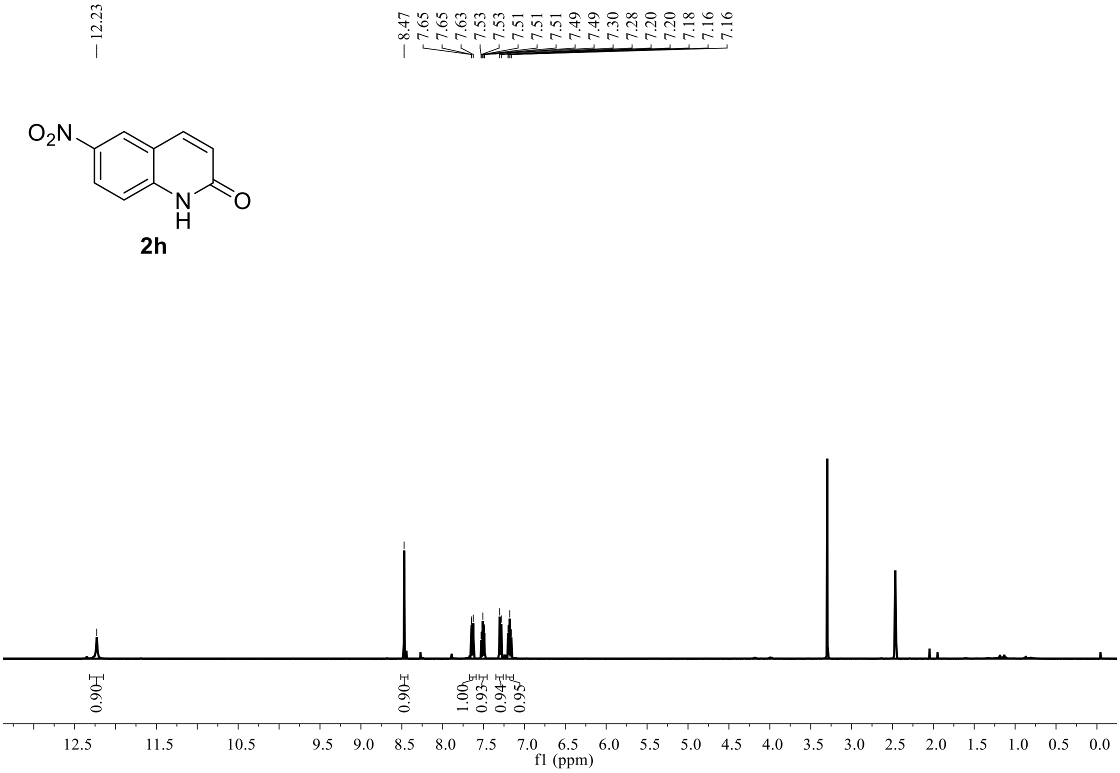
[1]H NMR, 400 MHz, DMSO-d_6



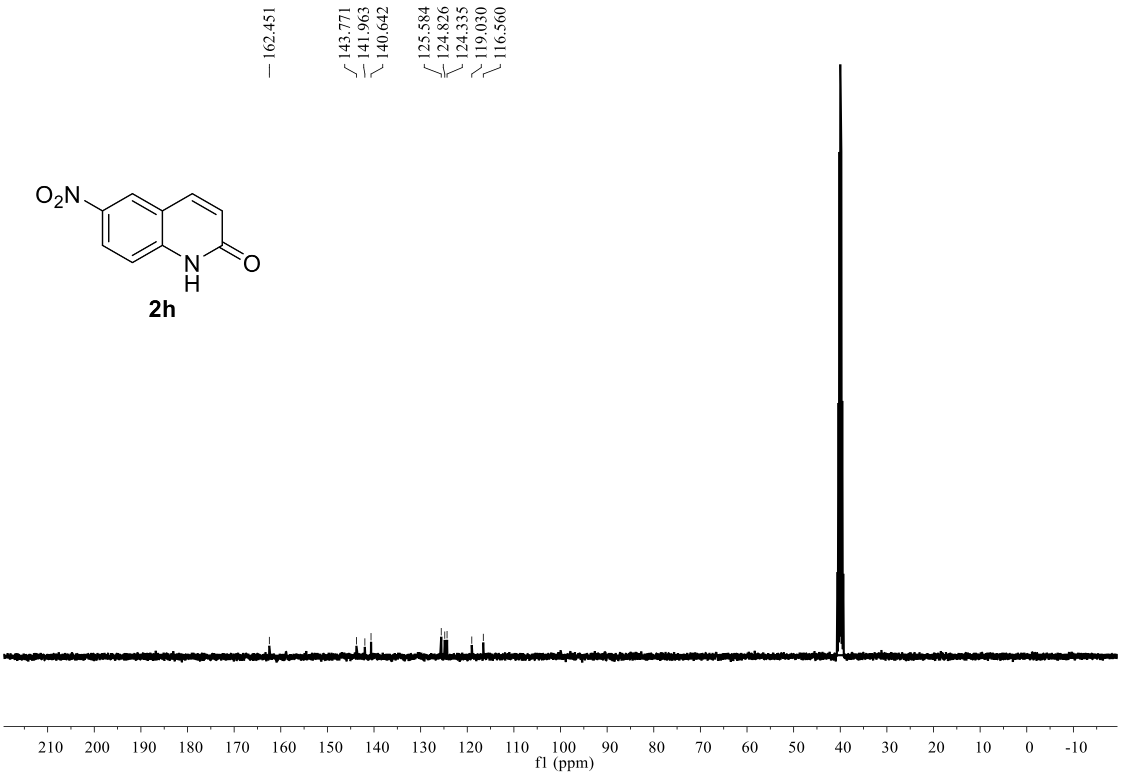
[13]C NMR, 100 MHz, DMSO-d_6



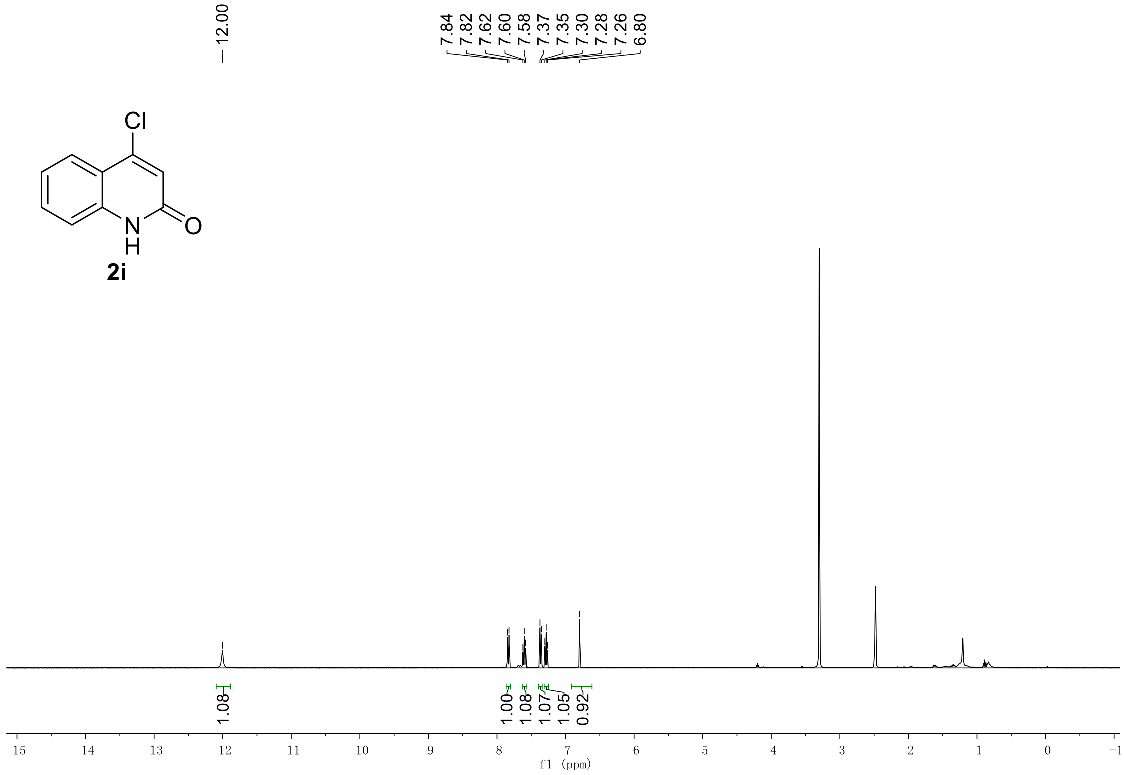
^{1}H NMR, 400 MHz, DMSO-d_6



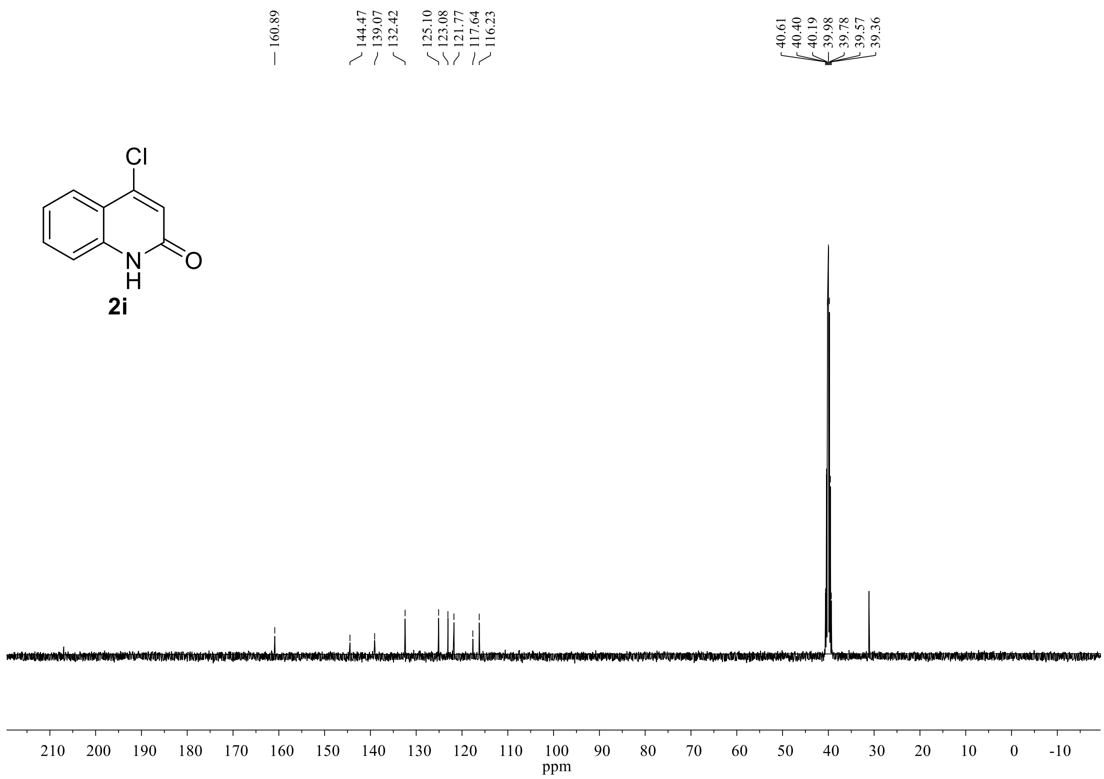
^{13}C NMR, 100 MHz, DMSO-d_6



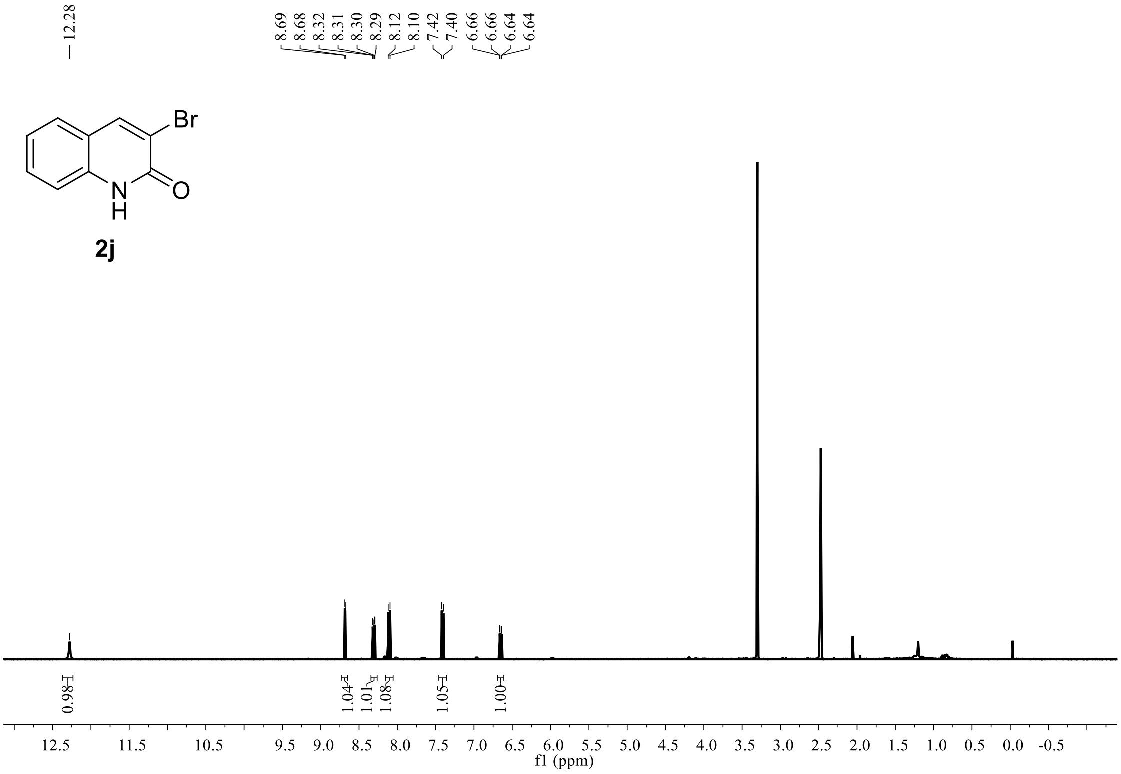
^{1}H NMR, 400 MHz, DMSO-d_6



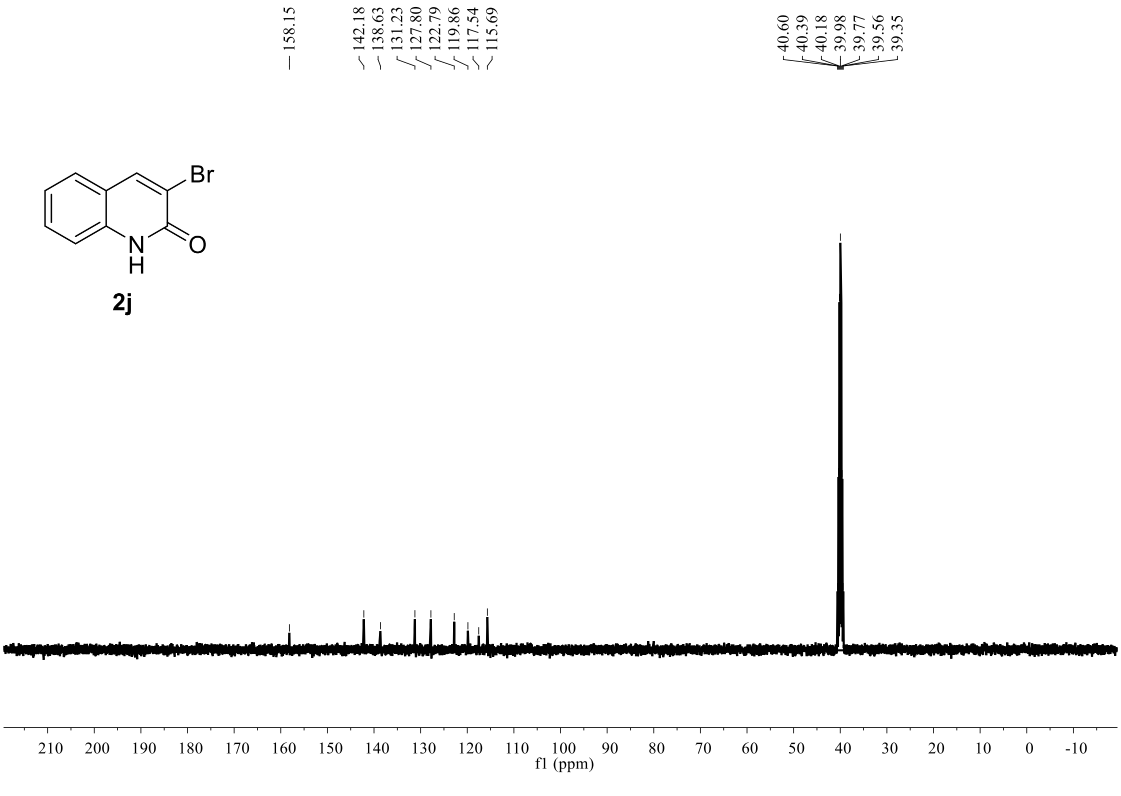
^{13}C NMR, 100 MHz, DMSO-d_6



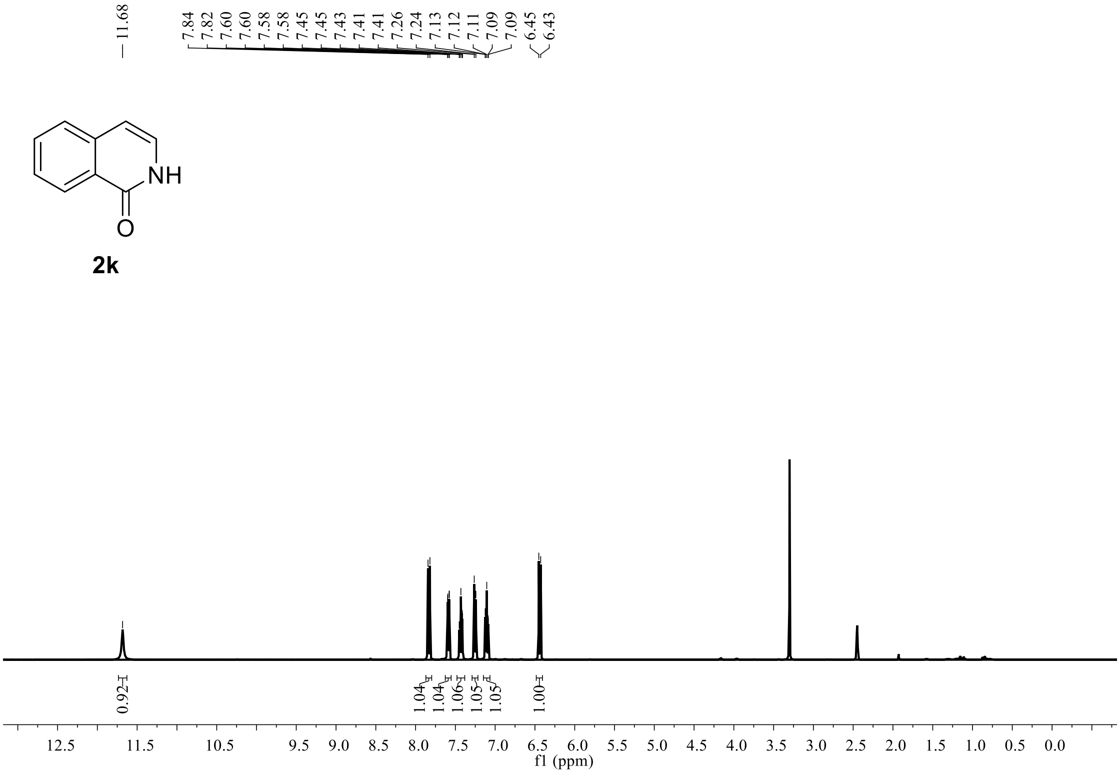
^{1}H NMR, 400 MHz, DMSO-d_6



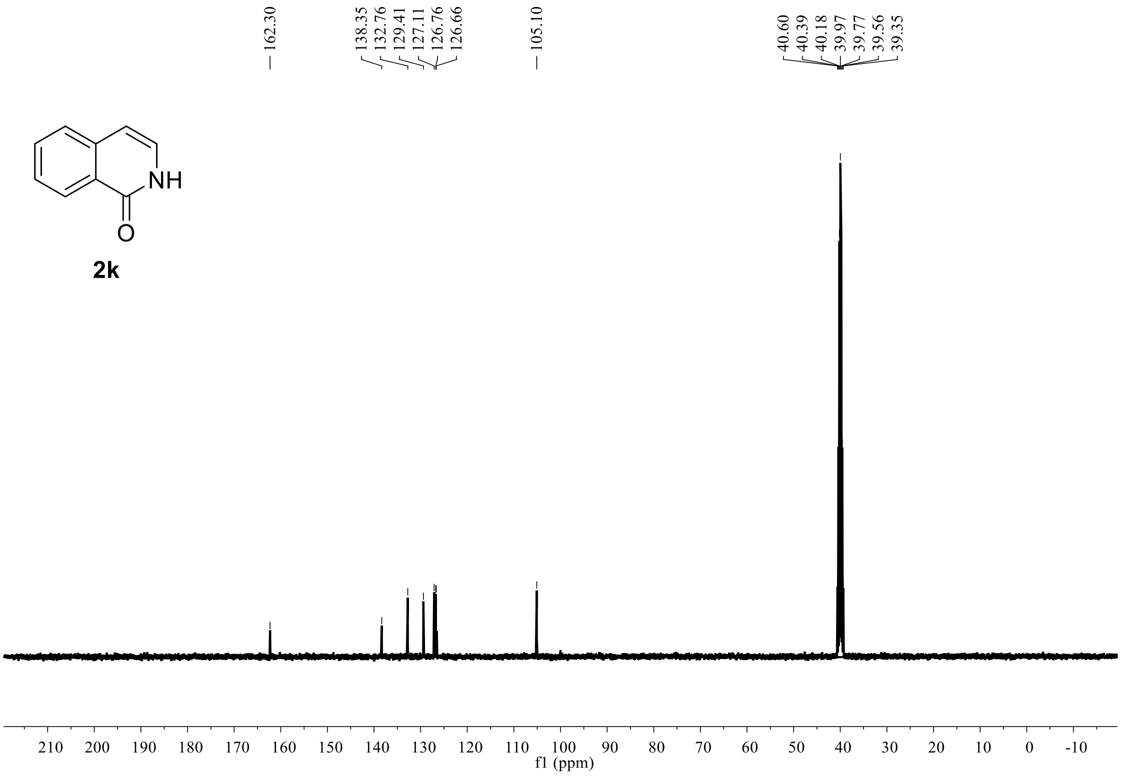
^{13}C NMR, 100 MHz, DMSO-d_6



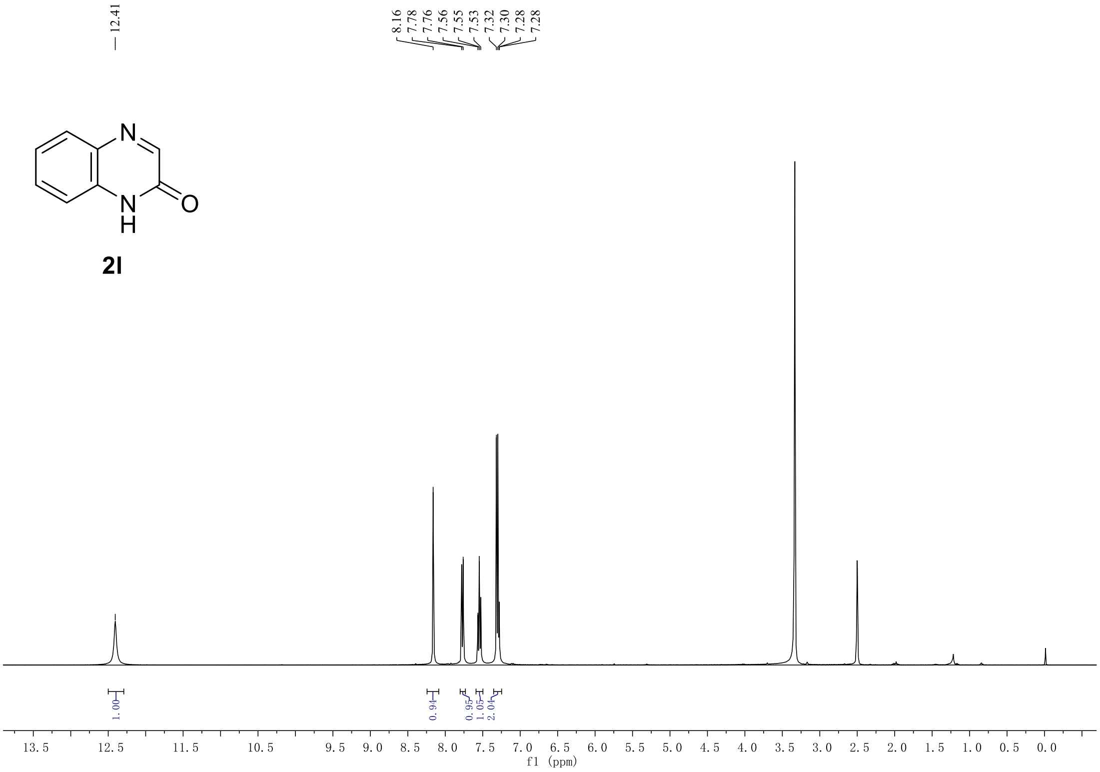
^{1}H NMR, 400 MHz, DMSO-d_6



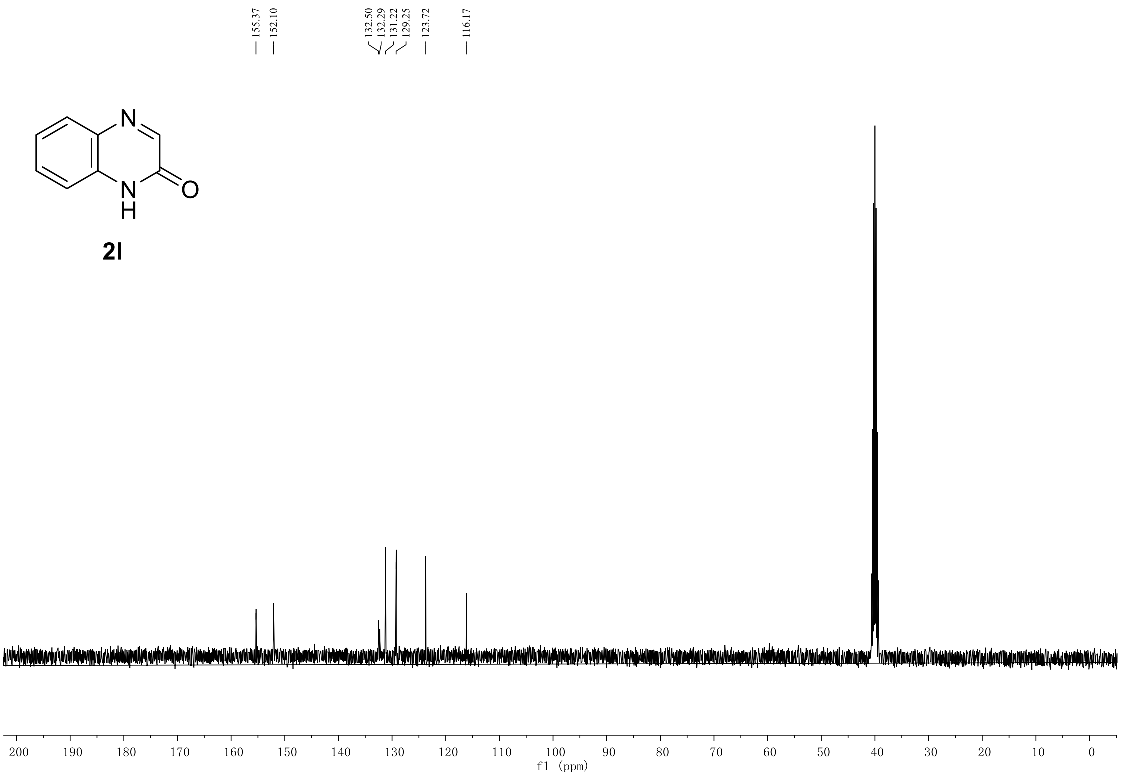
^{13}C NMR, 100 MHz, DMSO-d_6



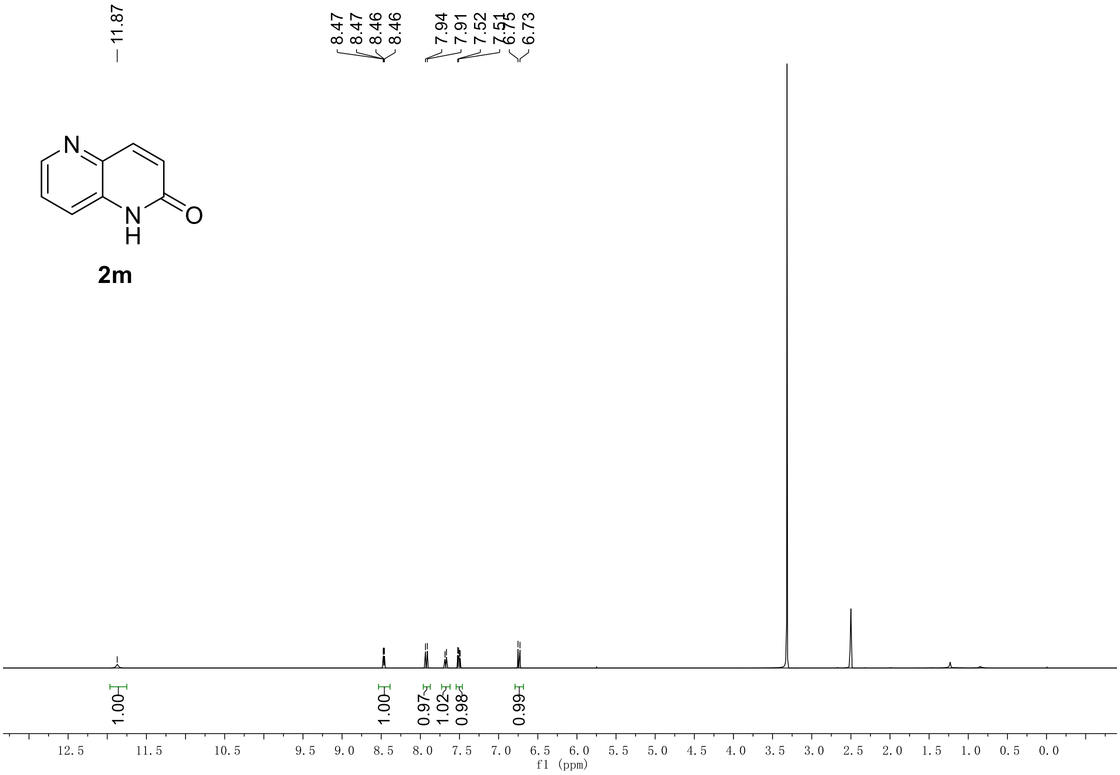
^{1}H NMR, 400 MHz, DMSO-d_6



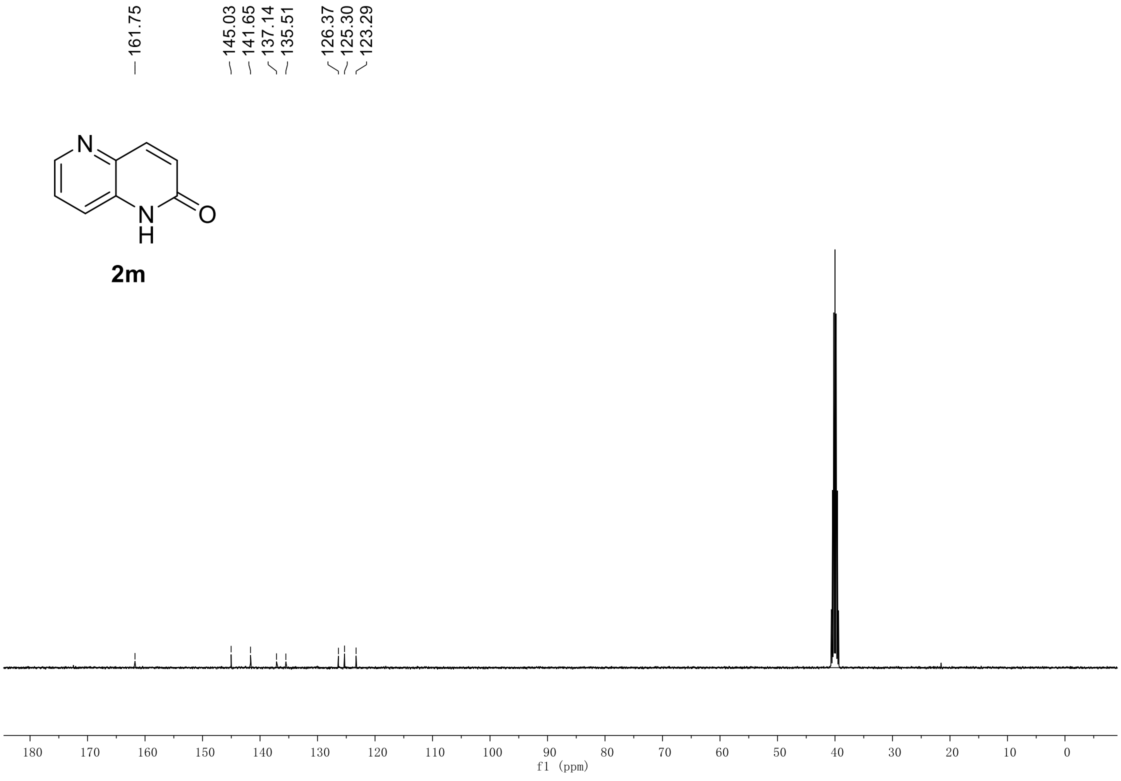
^{13}C NMR, 100 MHz, DMSO-d_6



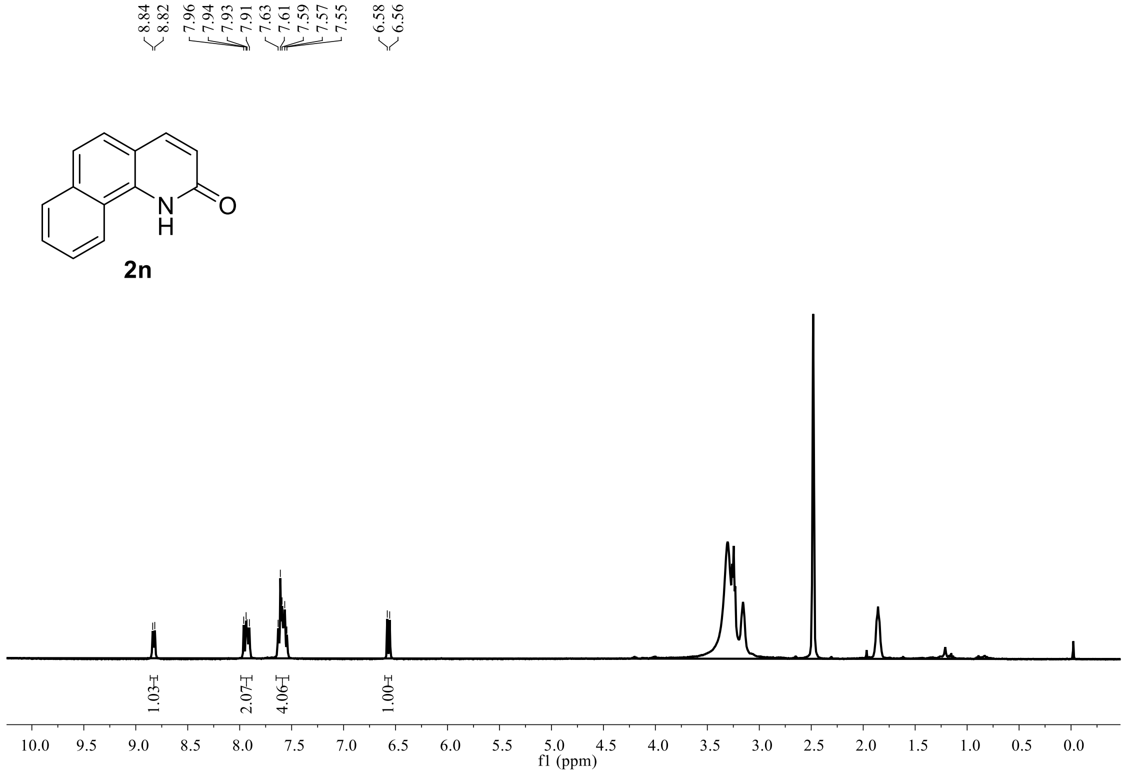
^{1}H NMR, 400 MHz, DMSO-d_6



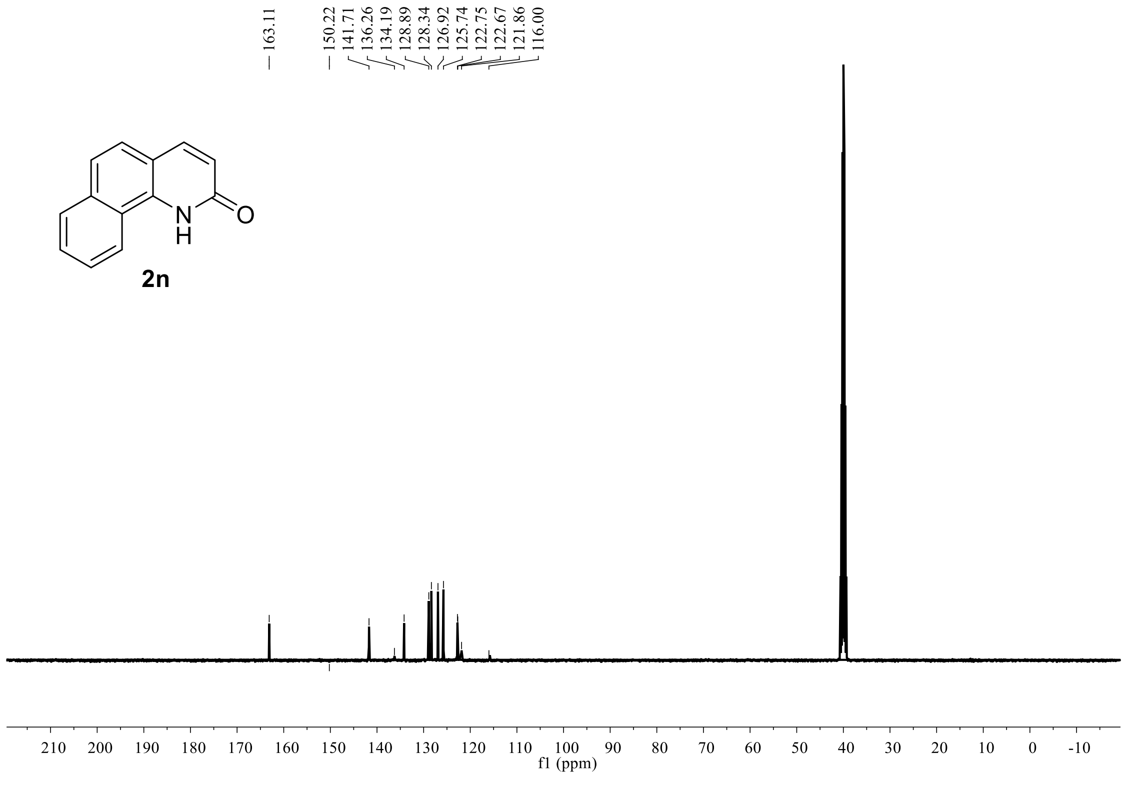
^{13}C NMR, 100 MHz, DMSO-d_6



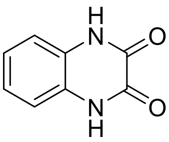
^{1}H NMR, 400 MHz, DMSO-d_6



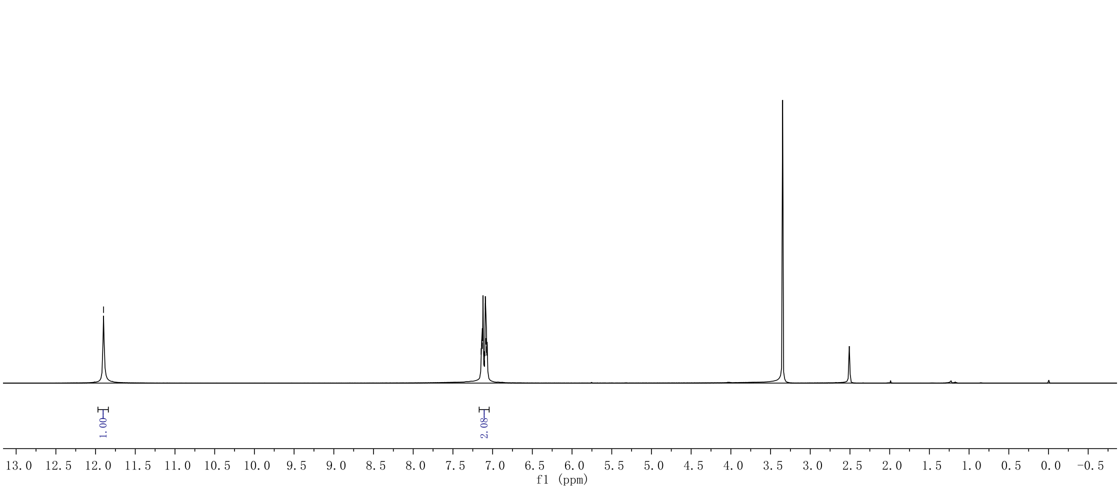
^{13}C NMR, 100 MHz, DMSO-d_6



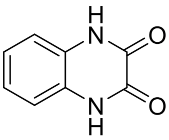
^{1}H NMR, 400 MHz, DMSO-d_6



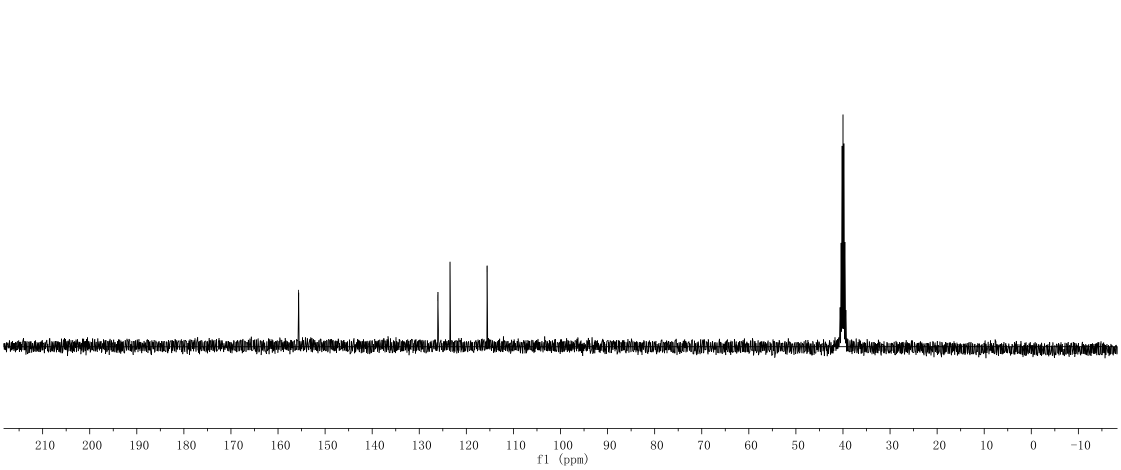
2o



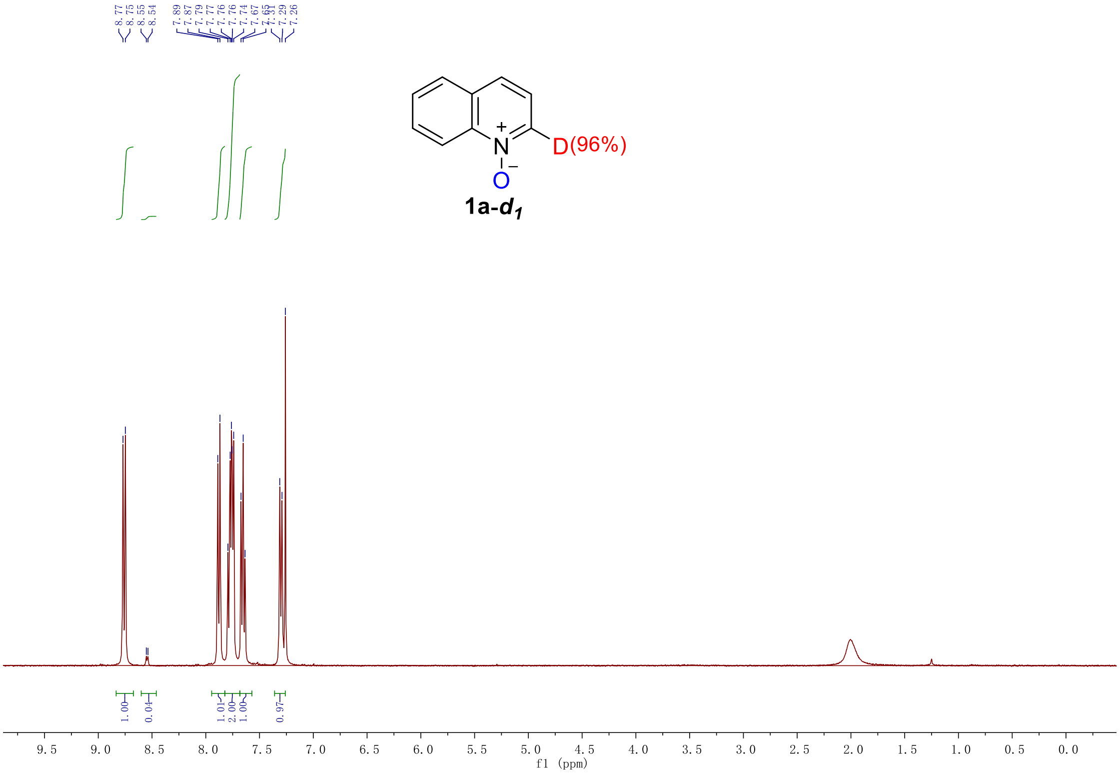
^{13}C NMR, 100 MHz, DMSO-d_6



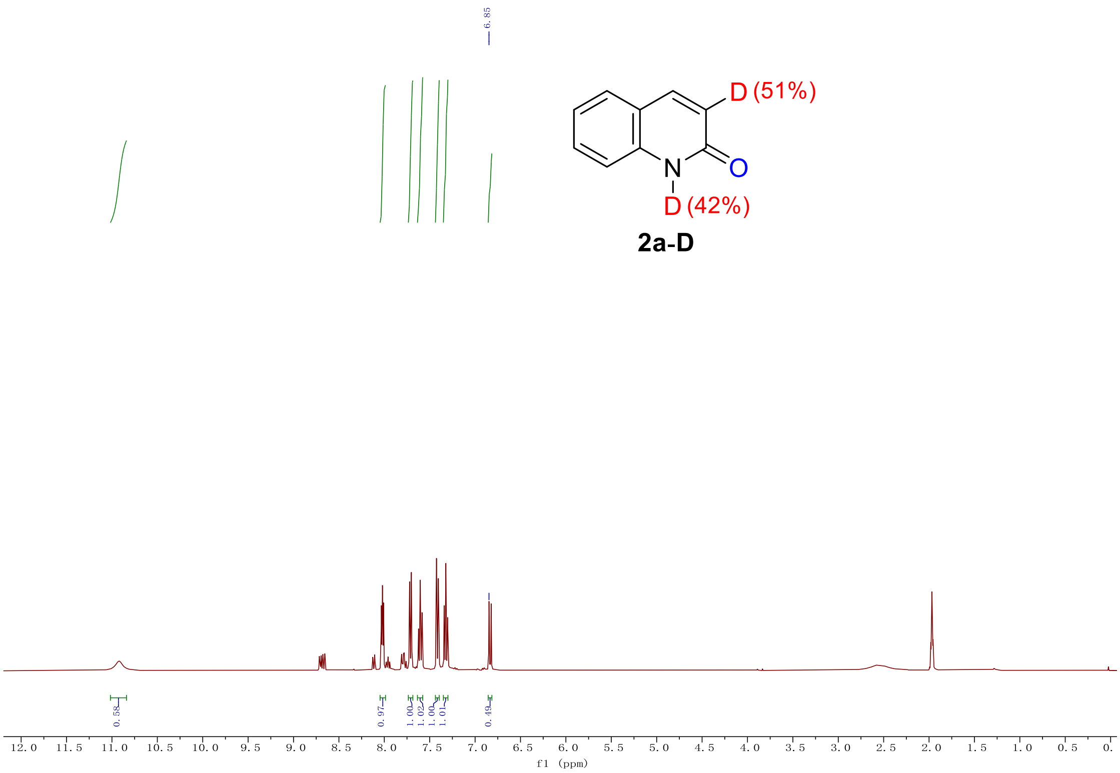
2o



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



^{1}H NMR, 400 MHz, CD_3CN



13. Cartesian coordinates for all of the calculated structures

1a-D （S0）

C	2.36583200	-0.99184400	0.00002500
C	1.05136500	-1.39810700	-0.00005200
C	0.03261200	-0.43086900	-0.00010300
C	0.32701500	0.95495400	-0.00003700
C	1.69339400	1.33147100	0.00002500
C	2.68760800	0.38283000	0.00005500
H	3.16482900	-1.73671400	0.00004900
H	0.75122400	-2.44616700	-0.00010700
C	-0.73200100	1.89446400	-0.00002400
H	1.93728500	2.39768100	0.00006800
H	3.73567400	0.69226200	0.00011200
C	-2.02246600	1.42661400	0.00005400
C	-2.28916600	0.05314700	0.00000000
H	-0.50923700	2.96377900	0.00002600
H	-2.87272600	2.11160300	0.00017500
H(Iso=2)	-3.28948700	-0.37929800	0.00012800
N	-1.30503100	-0.87307500	-0.00022100
O	-1.55843800	-2.10344800	0.00018000

A

C	2.51712400	-0.92076100	-0.03487700
C	1.21965200	-1.41944300	-0.19243300
C	0.13223900	-0.56775900	-0.21864000
C	0.30957500	0.86300000	-0.04071600
C	1.66092700	1.33853000	0.11937200
C	2.72101900	0.47278800	0.12130300
H	3.37019900	-1.60267700	-0.03960500
H	1.03317300	-2.49020600	-0.30696900
C	-0.78896700	1.68495400	0.01923300
H	1.81575500	2.41596800	0.23052500
H	3.73703300	0.85799200	0.24015300
C	-2.12562600	1.13203500	-0.19968400
C	-2.29310800	-0.30793300	-0.22279900
H	-0.66500900	2.75435700	0.21075200
H	-2.96822800	1.77610900	-0.45675600
H(Iso=2)	3.19351600	-0.68591700	-0.72540800
N	-1.15045800	-1.16776100	-0.36205200
O	-1.89915200	-1.06297100	0.90963900

A1

C	2.52374400	-0.88656800	-0.04034000
C	1.24233100	-1.43277100	-0.19304900
C	0.15358100	-0.58875600	-0.19009600
C	0.31881100	0.82400000	-0.03141200
C	1.62702100	1.34667700	0.12441600
C	2.71354400	0.49926700	0.12126300
H	3.39135400	-1.55072600	-0.04583800
H	1.08896300	-2.50763700	-0.30415900
C	-0.82843800	1.65267900	-0.01165500
H	1.75518300	2.42747200	0.22473700
H	3.72292400	0.89765500	0.23725700
C	-2.09074400	1.12896800	-0.18332900
C	-2.29532500	-0.31322700	-0.27087700
H	-0.69953100	2.73219400	0.10732300
H	-2.95680500	1.78774400	-0.28343400
H(Iso=2)	-3.17889400	-0.69166200	-0.79481000
N	-1.14092200	-1.16485000	-0.30778300
O	-1.91548600	-1.04033800	0.88298500

B

C	-2.63833100	-1.00002400	-0.03374900
C	-1.37843600	-1.51020000	0.02331800
C	-0.23395300	-0.61958900	0.05607100
C	-0.45342100	0.83583200	0.01617300
C	-1.76414600	1.30883400	-0.03894300
C	-2.82361500	0.41195100	-0.06153300
H	-3.50976400	-1.65617800	-0.05542000
H	-1.16760900	-2.58133000	0.05032400
C	0.68323600	1.69258800	-0.00218100
H	-1.95052400	2.38454500	-0.07222200
H	-3.84347700	0.80440500	-0.10791000
C	1.92509700	1.15061900	0.04346100
C	2.09275900	-0.32526400	0.18439800
H	0.54002400	2.77339100	-0.07933700
H	2.84102600	1.74693900	0.03252900
H(Iso=2)	2.26902800	-0.38666400	1.31357100
N	0.94286900	-1.16788200	0.06936000
O	3.22076000	-0.82230200	-0.33614300

TSBC

C	-2.62783000	-1.00889700	-0.01235500
C	-1.36217900	-1.51332900	0.01556600
C	-0.22958000	-0.62007900	0.02720600
C	-0.46343700	0.82774100	0.00348100
C	-1.78274300	1.29900400	-0.02062100
C	-2.83451200	0.40029900	-0.02894100
H	-3.49179900	-1.67568400	-0.02058700

H	-1.14817500	-2.58386200	0.03078600
C	0.65981800	1.68468300	-0.01852500
H	-1.97024600	2.37501500	-0.03933100
H	-3.85871800	0.78162700	-0.05324600
C	1.92211800	1.15371700	-0.00119200
C	2.08459000	-0.33260800	0.08325900
N	0.96210800	-1.15999200	0.01121200
O	3.25848700	-0.83319000	-0.17796600
H	2.84224700	1.74333900	0.01835900
H(Iso=2)	2.10604000	0.03491400	1.21128100
H	0.52053100	2.76692000	-0.08928300

TSBE

C	-2.62469600	-1.00827700	-0.01867700
C	-1.35384400	-1.50926200	0.02012600
C	-0.23943700	-0.61125700	0.02633100
C	-0.46636200	0.82686700	0.00579400
C	-1.78398900	1.29711800	-0.02185600
C	-2.83644800	0.39752300	-0.03613700
H	-3.48492500	-1.67983700	-0.02985100
H	-1.13964800	-2.57970400	0.03600600
C	0.66395500	1.69087000	0.00968400
H	-1.97093500	2.37321900	-0.03600700
H	-3.86136100	0.77649200	-0.06096600
C	1.91934300	1.16569000	0.02627300
C	2.10108300	-0.28443100	0.05203700
H	0.50907300	2.77279200	-0.01642600
H	2.82506800	1.77625600	0.02288700
H(Iso=2)	1.84106000	-0.71523100	1.15840800
N	0.97399400	-1.15851800	-0.01759500
O	3.27326100	-0.80042600	-0.16654300

C

C	-2.63159200	-0.96652800	-0.00356000
C	-1.36020300	-1.49118300	0.15286000
C	-0.21393800	-0.63395300	0.12855700
C	-0.43952000	0.80879000	-0.01078200
C	-1.75930900	1.29623400	-0.16139800
C	-2.83618000	0.41998200	-0.16830400
H	-3.49546200	-1.63521800	0.01024500
H	-1.18191800	-2.56289100	0.26702500
C	0.65708800	1.64320600	0.04560700
H	-1.92206000	2.37469300	-0.24473900
H	-3.85086700	0.80705100	-0.28205800
C	1.98591900	1.09407900	0.29679800
C	2.11184700	-0.39042400	-0.03933700
H	0.52968600	2.72283200	-0.10067200
H	2.79984300	1.66947800	-0.17103100
H(Iso=2)	2.17533900	1.17059600	1.39238600
N	0.97271800	-1.19775700	0.19283600
O	3.13146800	-0.85543300	-0.45795700

E

C	2.62043200	-0.99753600	0.00019800
C	1.35251800	-1.50608600	0.00015100
C	0.24995400	-0.60836500	-0.00015200
C	0.46501100	0.82519100	-0.00003900
C	1.78347700	1.29968100	-0.00009100
C	2.84408200	0.41242600	0.00009300
H	3.47795200	-1.67315500	0.00046200
H	1.16805700	-2.58290600	0.00022100
C	-0.67117100	1.68763100	0.00013400
H	1.95811100	2.37782300	-0.00022400
H	3.86927000	0.78892000	0.00034000
C	-1.93577600	1.18684600	-0.00011200
C	-2.17650900	-0.24814100	-0.00026100
H	-0.50280500	2.76784800	0.00038300
H	-2.82553800	1.81904800	-0.00022200
H(Iso=2)	-1.19872200	-2.06586700	-0.00064100
N	-1.00990900	-1.05999000	-0.00077800
O	-3.25863400	-0.79020900	0.00069900

C1

C	2.65427100	-1.01683600	0.00007800
C	1.35930400	-1.49775500	0.00000500
C	0.23902500	-0.58796300	0.00004400
C	0.48612500	0.82830900	-0.00008800
C	1.79570500	1.28120900	-0.00000600
C	2.87686200	0.36468900	0.00004500
H	3.49951800	-1.70661200	0.00010400
H	1.12921900	-2.56605700	0.00001800
C	-0.65355200	1.69122500	-0.00025200
H	1.99927500	2.35576900	-0.00004900
H	3.89852100	0.75199700	0.00007200
C	-1.90495100	1.15159000	0.00011500
C	-2.02227400	-0.26813900	-0.00013600
H	-0.50944400	2.77483000	0.00031000
H	-3.92126000	-0.24663900	0.00082700
H(Iso=2)	-2.80012200	1.77822400	0.00077000
N	-0.97610400	-1.11484700	-0.00005900
O	-3.18075800	-0.87694500	-0.00005800

D

C	-2.62030700	-0.99757400	-0.00000900
C	-1.35240200	-1.50607000	0.00013400
C	-0.24989400	-0.60828300	0.00006100
C	-0.46500500	0.82525600	0.00010300
C	-1.78349800	1.29962600	-0.00004500
C	-2.84409700	0.41239900	-0.00015800
H	-3.47769500	-1.67336300	0.00011400
H	-1.16784000	-2.58288800	0.00032900
C	0.67122900	1.68776800	0.00008900
H	-1.95805400	2.37780400	-0.00010500
H	-3.86926900	0.78893000	-0.00023800
C	1.93570500	1.18683300	0.00002600
C	2.17638300	-0.24818700	-0.00004900
H	0.50297700	2.76800200	0.00023100
H(Iso=2)	2.82576100	1.81868500	-0.00001000
N	1.00981200	-1.05997600	-0.00009400
O	3.25855800	-0.79024500	-0.00005700
H	1.19829000	-2.06598500	-0.00012200

2a-D3

C	-2.63248500	-0.99096600	0.00012600
C	-1.33737800	-1.48228400	0.00002800
C	-0.25488300	-0.59244500	-0.00000600
C	-0.48681500	0.80017700	0.00005700
C	-1.80980100	1.26909000	0.00015500
C	-2.87732700	0.38853200	0.00019000
H	-3.47110500	-1.69170900	0.00015200
H	-1.14819000	-2.55984700	-0.00002200
C	0.65919300	1.66961300	0.00001500
H	-1.97943100	2.35019400	0.00020200
H	-3.90271300	0.76413700	0.00026600
C	1.92088900	1.18399900	-0.00007800
C	2.19489900	-0.25035800	-0.00013900
H	0.48380700	2.75072800	0.00006200
H(Iso=2)	2.79913600	1.83223600	-0.00011000
N	1.04624300	-1.04189700	-0.00009900
O	3.30118100	-0.76025500	-0.00022500
H	1.22759900	-2.04256300	-0.00014300

2a-D1

C	-2.63248500	-0.99096600	0.00012600
C	-1.33737800	-1.48228400	0.00002800
C	-0.25488300	-0.59244500	-0.00000600
C	-0.48681500	0.80017700	0.00005700
C	-1.80980100	1.26909000	0.00015500
C	-2.87732700	0.38853200	0.00019000
H	-3.47110500	-1.69170900	0.00015200
H	-1.14819000	-2.55984700	-0.00002200
C	0.65919300	1.66961300	0.00001500
H	-1.97943100	2.35019400	0.00020200
H	-3.90271300	0.76413700	0.00026600
C	1.92088900	1.18399900	-0.00007800
C	2.19489900	-0.25035800	-0.00013900
H	0.48380700	2.75072800	0.00006200
H	2.79913600	1.83223600	-0.00011000
N	1.04624300	-1.04189700	-0.00009900
O	3.30118100	-0.76025500	-0.00022500
H(Iso=2)	1.22759900	-2.04256300	-0.00014300

B'

C	-2.64677300	-0.97073000	-0.04982800
C	-1.34135200	-1.47521800	0.05398900
C	-0.23124900	-0.62126400	0.10252400
C	-0.45744600	0.80479400	0.02307600
C	-1.75979300	1.29095100	-0.08634200
C	-2.84768000	0.42355500	-0.11884200
H	-3.50781100	-1.64306800	-0.07791900
H	-1.18182900	-2.55715300	0.10481100
C	0.69898200	1.66438600	0.03560800
H	-1.91639700	2.37251900	-0.14906700
H	-3.86103400	0.82446700	-0.20156800
C	1.93115500	1.14095400	0.14457600
C	2.12850500	-0.35016000	0.25960100
H	0.55186200	2.74573000	-0.05375600
H	2.83830700	1.75023500	0.14124900
H(Iso=2)	2.60271400	-0.52564500	1.27491300
N	0.96196700	-1.18748000	0.20646600
O	3.11179100	-0.76229200	-0.58376500

TSBF

C	2.12491100	0.80898000	0.35932200
C	0.93017500	1.49344600	0.22391200
C	-0.30146400	0.75389900	0.08038000
C	-0.25203600	-0.68566500	0.14820000
C	2.11646200	-0.67414900	0.24486600
H	-1.55747600	2.47314400	-0.14529800
H	3.06818700	1.31142100	0.57326700
H	0.89637200	2.58632600	0.25855200
C	-1.52579200	1.38093200	-0.08121900
C	-1.47072200	-1.40167800	0.07421600
H(Iso=2)	2.88404400	-1.20757700	0.83559100
C	-2.68989800	-0.74556400	-0.07418200

C	-2.72128300	0.64206000	-0.15955300
H	-1.40488000	-2.49088500	0.13305100
H	-3.61638300	-1.32153400	-0.13126800
H	-3.67248200	1.16488900	-0.28551100
N	0.88116900	-1.39607600	0.27513400
O	2.49654000	-0.27210300	-1.00749900

F

C	-2.19676000	0.71070500	-0.23328700
C	-0.94457700	1.46020700	-0.24126000
C	0.27956600	0.74891000	-0.10544900
C	0.25744000	-0.69961500	-0.12189000
C	-2.09675400	-0.76530500	-0.25428800
H	1.53024500	2.48544800	0.01575000
H	-3.09292300	1.18943500	-0.64591900
H	-0.94183000	2.55247100	-0.29737600
C	1.50754400	1.39108300	0.01125200
C	1.47775100	-1.38919000	-0.01882100
H(Iso=2)	-2.91374200	-1.35026600	-0.69409900
C	2.70579400	-0.71211600	0.10926200
C	2.71993400	0.66652200	0.12330100
H	1.42698600	-2.48067800	-0.04442500
H	3.63493800	-1.28010300	0.19094400
H	3.66321300	1.21042800	0.21524300
N	-0.86032000	-1.44489800	-0.26581000
O	-2.44303400	-0.08495700	0.93845300

G

C	-2.21232500	1.16794600	0.00025000
C	-0.85939500	1.53059300	-0.00006600
C	0.28830900	0.74633300	-0.00006800
C	0.27228800	-0.72877800	0.00002800
C	-2.07792600	-1.23918500	-0.00017000
H	1.57896700	2.49292900	-0.00034100
H	-2.99392900	1.92931500	0.00078900
H	-0.70856900	2.61572200	-0.00015700
C	1.56885400	1.39849700	-0.00019100
C	1.52718700	-1.40533800	0.00016400
H(Iso=2)	-2.81726500	-2.04359100	-0.00033900
C	2.71859200	-0.73611400	0.00016800
C	2.73725700	0.70223000	-0.00004100
H	1.48255700	-2.49700300	0.00026400
H	3.66051900	-1.28995000	0.00030000
H	3.69334600	1.23095000	-0.00006700
N	-0.81451400	-1.51713600	-0.00019900
O	-2.74638400	-0.05444100	0.00006300

2a'

C	-2.17753100	1.15480700	0.04158500
C	-0.92026000	1.51922600	-0.21654900
C	0.29818400	0.71913200	-0.11096300
C	0.28908100	-0.69182100	-0.11028900
C	-2.04917100	-1.21773300	-0.04794800
H	1.53337000	2.47324800	-0.04558400
H	-3.00689500	1.86244100	-0.03766300
H	-0.78935200	2.56861000	-0.49916600
C	1.52691600	1.37914200	-0.01769800
C	1.49590400	-1.38277300	0.00848200
H(Iso=2)	-2.82778600	-1.97839000	-0.19533700
C	2.70706500	-0.70892400	0.14227700
C	2.72372100	0.68107500	0.11986400
H	1.45259500	-2.47401100	-0.02026400
H	3.63732500	-1.27345800	0.24056500
H	3.66721500	1.22624500	0.20048100
N	-0.84860100	-1.49925400	-0.29092500
O	-2.63621400	-0.07783800	0.44261000