Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supporting Information

Alkylsulfonium Salts for Photochemical Desulphurizative Functionalization of Heteroarenes

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I. General considerations

All reagents and solvents were obtained from commercial suppliers and used without further purification. The starting materials were synthesized according to literature procedures. Flash chromatography was performed on silica gel (200~300 mesh).

^{1}H and ^{13}C NMR data were recorded at 500 and 125 MHz on a BRUKER 500 spectrometer. Proton and carbon magnetic resonance spectra (^{1}H NMR and ^{13}C NMR) were recorded using tetramethylsilane (TMS) as the internal standard in DMSO-d_6 or in $CDCl_3$. Spectra were calibrated relative to solvent's residual proton and carbon chemical shift: $CHCl_3$ (δ = 7.26 for ^{1}H NMR and δ = 77.0 for ^{13}C NMR), DMSO-d_6 (δ = 2.50 and 3.30 for ^{1}H NMR and δ = 39.50 for ^{13}C NMR). Data are reported as follows: chemical shift δ/ppm, integration (^{1}H only), multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, dd = doublet of doublets, m = multiplet or combinations thereof; ^{13}C signals are singlets unless otherwise stated), coupling constants J in Hz, assignment.

High Resolution Mass Spectrometry (HRMS): All were recorded on an UPLC-Q/TOF Xevo G2-XS (Waters, MA, USA) with an ESI source.

UV-visible spectroscopy was recorded on a UV-2600 UV-visible spectrophotometer. The fluorescence emission intensity of reaction solution was recorded on a RF-6000 spectrofluorimeter. The reactor was 3.0 cm from 20W blue LED，the power density of the incident light was recorded on CEL-FZ-A radiometer.

Cyclic voltammetry was performed on a CH Instruments electrochemical workstation model CS300H.

The spectrum of our lamp and the visible-light irradiation instrument

All reactions have been studied in borosilicate glass vessels irradiated by a blue light LED manufactured by Xuzhou Ai Jia Electronic Technology Co., Ltd. without using filters.

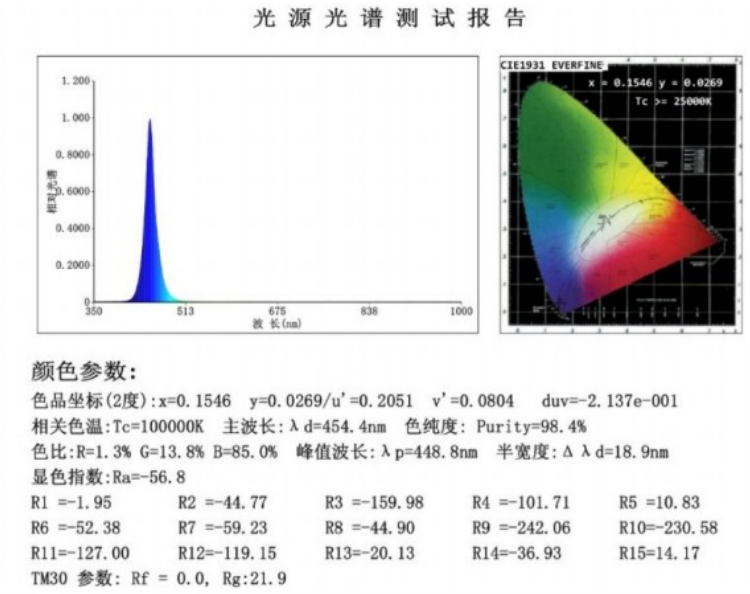


Figure S1. The spectrum of our lamp (blue LED)

Figure S2. The blue light LED

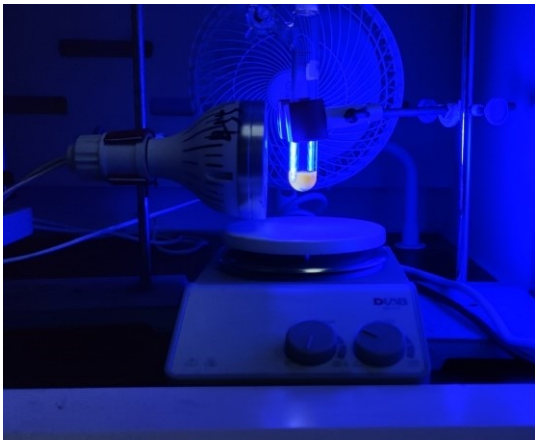
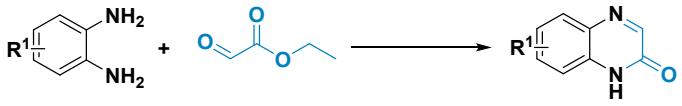


Figure S3. Photograph of the reaction setup

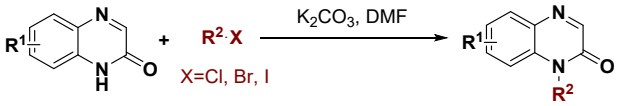
II. Experimental procedures

1. Preparation of quinoxalin-2 (1*H*)-one[1]



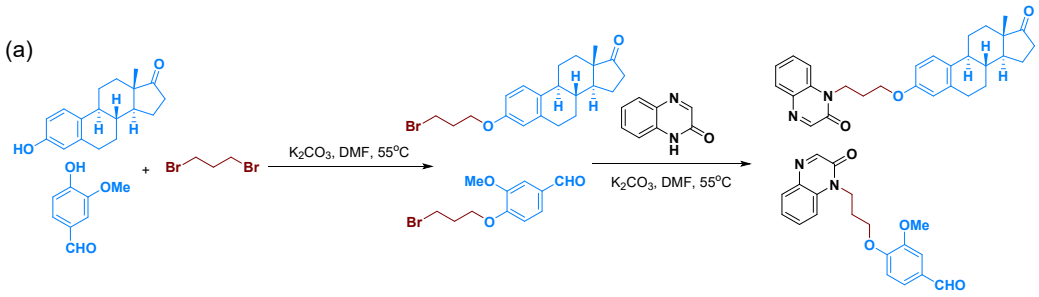
Ethyl-2-oxoacetate (22.1 mL, 111.11 mmol) was added to a solution of 1,2-diaminobenzene (10.0 g, 92.59 mmol) in ethanol (200 mL). The mixture was heated and maintained at 45 °C for 8 h. The resulting precipitate was filtered, thoroughly washed with water and dried under vacuum to afford quinoxalin-2 (1*H*) -ones.

Quinoxalin-2(1*H*)-one derivatives were prepared according to the reported methods[1]



General procedure: To a 100 mL round-bottomed flask with a stir bar was added quinoxalin-2(1*H*)-one (5.0 mmol), DMF (15.0 mL), then was added potassium carbonate (828 mg, 6.0 mmol), followed by the dropwise addition of R_2-X (8.0 mmol). The reaction mixture was then stirred for 1~12h at room temperature, poured into brine and extracted with EtOAc. The combined extracts were dried over Na_2SO_4, filtered, and evaporated. The residue was purified by column chromatography (petroleum ether/EtOAc) to afford the desired quinoxalin-2(1*H*)-ones.

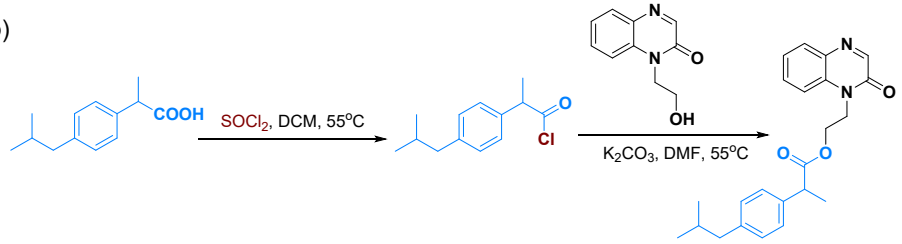
2. Modification of natural molecules and pharmaceutically relevant compounds are prepared from the following procedure:



General procedure: A mixture of phenol (4.0 mmol) and K_2CO_3 (1.1 g, 8.0 mmol) in DMF (6.4 mL) was stirred at 55 °C, and then 1, 3-dibromopropane (8.0 mmol) was

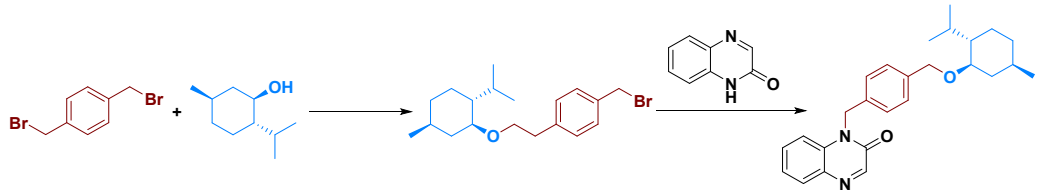
added. After stirring overnight, the mixture was added water and extracted with DCM. The organic phase was washed with water (40 mL x 2), then washed with brine (40 mL x 2), dried over Na_2SO_4, followed by concentrated and purification on silica gel column chromatography. The resulting compound (1.6 equiv.) was then dissolved anhydrous DMF (10 mL) and quinoxalin-2(1*H*)-one (1.0 equiv.) was added and the mixture stirred for 12 h at 55 °C. After the reaction was complete, reaction mixture was quenched with water and extracted with CH_2Cl_2. Combined organic layers were concentrated in vacuo and the residue obtained was purified by flash chromatography on silica gel to obtain the desired product.

(b)



General procedure: To a 25 mL round-bottomed flask with a stir bar was added ibuprofen (2.0 mmol), DCM (10 mL), then was added $SOCl_2$ (4.0 mmol). The reaction mixture was then refluxed for 4 h in oil bath. The solvent was then removed under reduced pressure with the aid of a rotary evaporator. The result mixture was added the quinoxalin-2(1*H*)-one (1.0 mmol), K_2CO_3 (1.5 mmol) and DMF (5.0 ml) , which was stirred at room temperature for 5 h, poured into brine and extracted with EtOAc. The combined extracts were dried over Na_2SO_4, filtered, and evaporated. The residue was purified by column chromatography to afford the desired product.

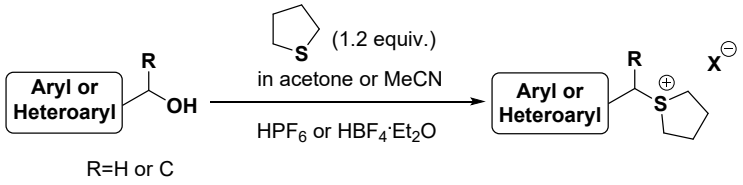
(c)



General procedure: Alcohol (1.0 mmol), alpha,alpha'-dibromo-p-xylene (1.2 mmol) and diisopropylethylamine (2.0 mmol) were charged in reaction vessel equipped with magnetic stirring bar under nitrogen atmosphere. The mixture was refluxed in 150 °C bath for 2 h. The resulting mixture typically showed two phases. Ethyl acetate (5.0 mL) and 10% aqueous sodium bisulphate (5.0 mL) were added to the mixture and the

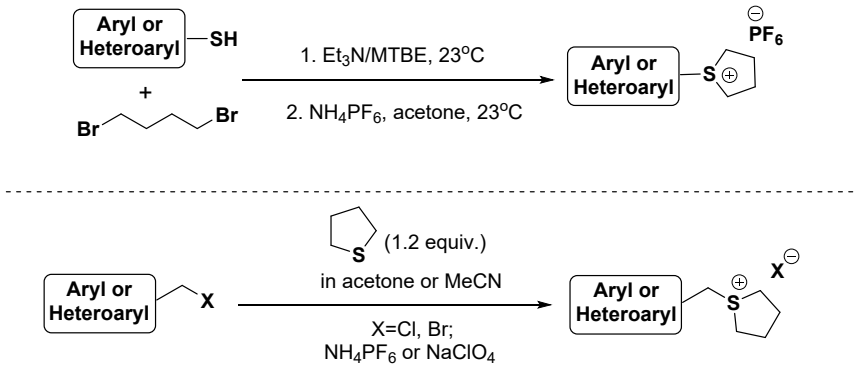
organic phase extracted by three potions of EtOAc. Combined organic layer was dried over magnesium sulfate and the solvent evaporated in vacuo. Further purification was carried out by silica gel column chromatography. The resulting compound (1.6 equiv.) was then dissolved anhydrous DMF (10 mL) and quinoxalin-2(1*H*)-one (1.0 equiv.) was added and the mixture stirred for 12 h at 55 °C. After the reaction was complete, reaction mixture was quenched with water and extracted with EA. Combined organic layers were concentrated in vacuo and the residue obtained was purified by flash chromatography on silica gel to obtain the desired product.

3. General method for sulfonium salt synthesis:[2][3][4]



Method A: Tetrahydrothiophene (441 mg, 816 µl, 5.00 mmol, 1.20 equiv.) and heteroaryl methanol (1.05 equiv.) was dissolved in diethyl ether (5 ml) and cooled to 0 °C using an ice bath. 60% HPF_6 in water (1.013 mg, 614 µl, 4.2 mmol, 1.00 equiv.) was added dropwise and the reaction was stirred for 30 minutes at 0 °C and then another hour at room temperature. The product was filtered and washed first with toluene (10 ml) then hexane (10 ml) finally with diethyl ether (15 ml) and dried in-vacuo.

Method B: A flame-dried round bottom flask (for 3 mmol: 50 mL flask, 5 mmol: 100 mL, 10 mmol: 250 mL) with a magnetic stirring bar was charged with the benzyl alcohol (1.1 equiv.), tetrahydrothiophene (THT) (1.2 equiv.), and acetonitrile (MeCN) ([1 M] with respect to (w.r.t.) the benzyl alcohol). Thereafter, tetrafluoroboric acid diethyl ether complex ($HBF_4 \cdot OEt_2$) (1.2 equiv.) was added dropwise and the reaction was left to stir until full consumption of the alcohol was observed by TLC (1:1 hexanes (Hex)/ethyl acetate (EtOAc)) or for a 12 h period. After the end of the reaction, the reaction liquid was concentrated, and then the desired product was obtained by adding ether to wash and removing the washing liquid.

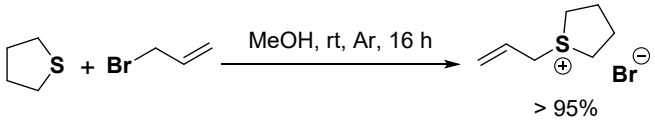


General procedure:

Method A: Tetrahydrothiophene (441 mg, 816 µl, 5.00 mmol, 1.10 equiv.), benzylbromide or benzylchloride (4.50 mmol, 1.00 equiv.) and NH_4PF_6 (815 mg, 5.00 mmol, 1.10 equiv.) was dissolved in acetone (5.0 ml) and stirred at 25 °C for 16 hours. The formed precipitate was filtered and washed with acetone. The filtrate was reduced to half its volume and excess diethyl ether was added. The formed precipitate was filtered and washed with diethyl ether then dried in-vacuo to get the product.

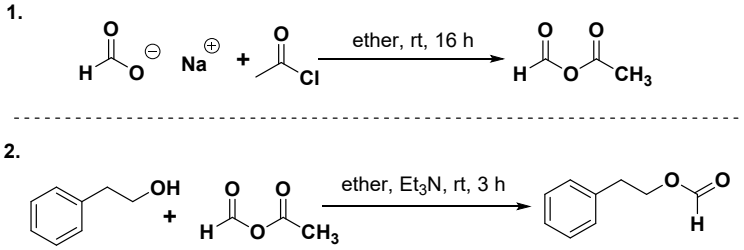
Method B: Triethylamine (27.5 g, 272.3 mmol, 1.5 equiv.) was slowly added to a 500 mL round-bottom flask containing thiophenol (20 g, 181.5 mmol), 1, 4-dibromobutane (78.4 g, 363 mmol, 2.0 equiv.) and Et_2O (200 mL). The reaction mixture was stirred for 30 min then diluted with Et_2O (200 mL) and washed with 1.2 N HCI (2 x 200 mL) and brine. The organic layer was dried ($MgSO_4$), the solvents were evaporated, and the crude material was dissolved in acetone (40 mL) and treated with NH_4PF_6 (44.4 g, 272.3 mmol). After stirring overnight at room temperature, the reaction mixture was filtered through a medium porosity fritted-glass funnel, the filtrate was concentrated under reduced pressure, and Et_2O (200 mL) was added producing colorless crystals. The crystals were collected on a coarse fritted-glass funnel and washed with water (200 mL), ethanol (200 mL), and Et_2O (200 mL). The product was purified by recrystallization from acetone/Et_2O to give 42.8 g (76 %) of analytically pure colorless crystals.

4. Preparation of 1-allyl-tetrahydrothiophenium bromide[5]



General procedure: To a 50 mL round bottom flask with stir bar was added 15 mL of MeOH (dried over anhydrous Na_2SO_4 and briefly dried over molecular sieves). Via syringe was added allyl bromide (6.05 g, 50 mmol, 4.32 35 mL, 1.0 equiv.) and tetrahydrothiophene (5.3 g, 5.3 mL, 60 mmol, 1.2 equiv.) and the reaction mixture stirred overnight at rt. The solvent was removed via rotary evaporator and the product dried under vacuum to give 1-allyl-tetrahydrothiophenium bromide as an off white solid (10.3 g / >95%). (**note:** tetrahydrothiophene has an extremely unpleasant and strong odor, the waste should be segregated and stored in a fume hood until disposal.)

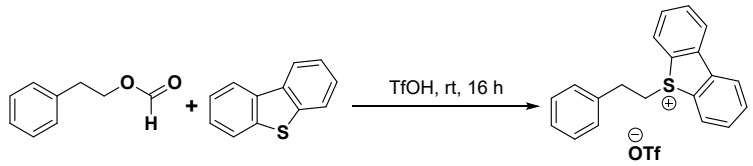
5. Preparation of 5-phenethyl-5*H*-dibenzo[*b,d*]thiophen-5-ium trifluoromethanesulfonate[6]



General procedure: 8.2 g (120 mmol, 1.2 equiv.) sodium formate was measured into a 100 mL round bottom flask. 8.8 mL abs. ether was added. Then 7.1 mL acetyl chloride (100 mmol, 1.0 equiv.) was added. The mixture was stirred at room temperature overnight. After 16 h, the sodium chloride was filtered off, washed with ether. The acetic formic anhydride was used as a solution in ether.

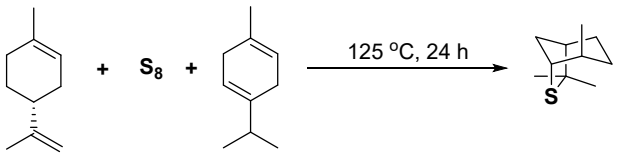
A 100 mL round bottom flask was charged with 7.2 mL 2-phenylethanol (60 mmol, 1.0 equiv.) and 25 mL abs. ether. 8.4 mL triethylamine (60 mmol, 1.0 equiv.) was added and finally acetic formic anhydride solution was added dropwise (29 mL solution, ca. 100 mmol, 1.6 equiv.). The mixture was stirred at room temperature for 3 hours. After the reaction was completed, the mixture was washed with sat. $NaHCO_3$ and water, dried over $MgSO_4$. Ether was evaporated, and the crude product was distilled at reduced pressure 65-70 °C. The product was obtained as a colourless liquid (6.3 g, yield: 70%), containing 18% phenylethyl acetate. The product was used without further purification.

3.



A 20 mL screw capped vial was charged with 3.68 g dibenzothiophene (20.0 mmol, 1 equiv.) and alkyl formate (40.0 mmol, 2 equiv.). The mixture was stirred vigorously on ice bath and then 10 mL trifluoromethanesulfonic acid (120 mmol, 6 equiv.) was added dropwise. The mixture was stirred over night at room temperature. After a night the mixture became a clear solution. The mixture was poured into water (200 mL) and extracted with dichloromethane (3 x 200 mL). The solution was concentrated under reduced pressure to 20 mL and poured into ether (370 mL). The product precipitated as white oil which crystallized easily after scratching and cooling in a refrigerator. The product was filtered and washed with ether, dried on air or under vacuum. The preparations were carried out in 2 mmol to 50 mmol scales.

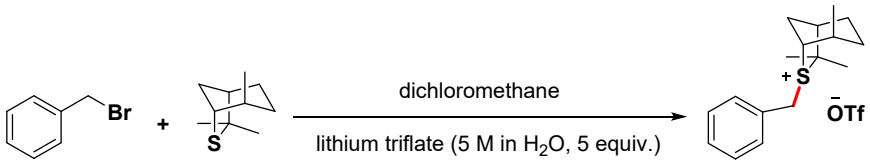
6. Synthesis of Sulfonium Salt 2a*



(*R*)-Limonene (161.8 mL, 1.0 mol, 99:1 e.r.) was placed in a 1.0 L three-necked round bottom flask equipped with a reflux condenser and a thermometer (to note the internal temperature). Elemental sulfur (32.0 g, 1.0 mol) and *γ*-terpinene (160.6 mL, 1.0 mol) were then added. The reaction mixture was heated to 125 ºC (internal temperature) for 8 h, (the oil bath temperature was set to a higher temperature of 130 ºC on this scale). After 8 h, more elemental sulfur (25.6 g, 0.8 mol) and *γ*-terpinene (176.7 mL, 1.1 mol) were added to the reaction mixture. It was then stirred at 125 ºC for another 16 h. From the ^{1}H-NMR spectrum of the crude reaction mixture after 24 h it was estimated that less than 5% (*R*)-Limonene was still left unreacted but the *γ*-terpinene was fully consumed. The reaction mixture was then cooled to room temperature, transferred to a 1.0 L one-necked round bottom flask and a vacuum distillation apparatus with a Vigreux column (18.0 cm long) was connected. The above compound 2 was distilled

at 40-46 °C/ approx. 0.64 mm Hg [79 °C/5 mm Hg]. Pure (*R*)-isothiocineole was obtained as a viscous yellow liquid (103.0 g, 61% yield, *e.r*. 99:1).

Detailed Description of the Distillation Procedure. The crude reaction mixture was transferred to a 1.0 L round bottom flask fitted with a 18.0 cm long Vigreux column. Under vacuum, at room temperature, the volatile by-products started distilling out. After the initial distillation of the volatile by-products, the oil bath temperature was increased every 5 ºC till 40 °C to make sure all the colourless volatiles (*p*-cymene and the other smelly by-products) were removed. From 40–45 °C, a yellow material started condensing in the Vigreux column. (*R*)-Isothiocineole was collected at 40–46 °C/approx. 0.64 mm Hg (the pressure was measured with a manometer directly from the vacuum pump without the manifold). The temperature of the oil bath was increased to 75 °C (internal temperature: 48 °C) to distil off the remaining isothiocineole from the viscous mixture. Pure fractions were analysed by ^{1}H-NMR for purity. A few mixed fractions containing both sulfide and *p*-cymene were also obtained. The mixed fractions were collected and redistilled to obtain the pure (*R*)-Isothiocineole to give a total yield of 61%.

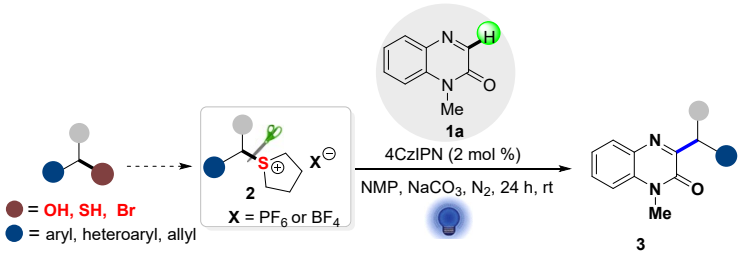


2a*

Sulfide (1-2 equiv.) was dissolved in dichloromethane (1 mL for each 2.4 mmol of sulfide) and then the appropriate bromide (2 equiv.) and a solution of lithium triflate (5 M in H_2O, 5 equiv) were added. The resulting biphasic mixture was stirred at rt for 24 h. Water (same amount as starting volume) and dichloromethane (same amount as starting volume) were added and the layers were separated. The aqueous organic layer was extracted with dichloromethane (3 × half the amount of starting volume). The combined organic layers were dried over $MgSO_4$ and the solvent was removed under reduced pressure. The crude product was dissolved in the minimum amount of dichloromethane and added dropwise to rapidly stirring diethyl ether (at least 10 times the volume of dichloromethane used to dissolve the crude). The precipitate was

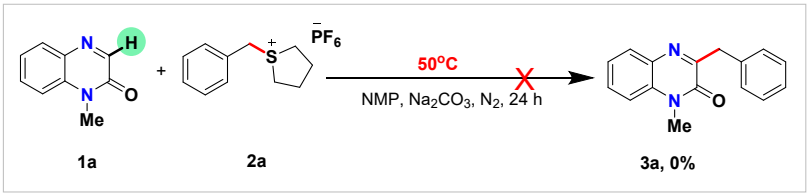
filtered and washed several times with diethyl ether (same amount as used to precipitate the salt).

7. General procedure for synthesis of quinoxalin-2(1*H*)-ones

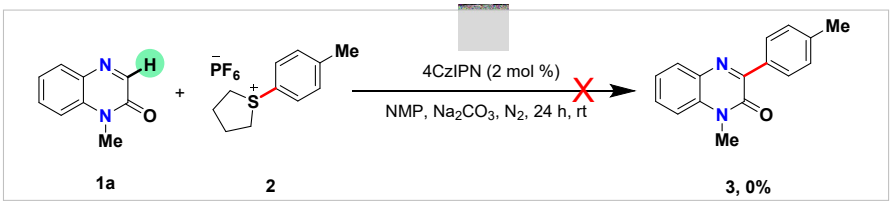


General procedure: To a 25 mL Schlenk tube equipped with a magnetic stir bar, added quinoxalin-2(1*H*)-ones **1** (0.2 mmol), sulfonium salt **2** (0.3 mmol), Na_2CO_3 (2.0 equiv.) and 4CzIPN (0.004 mmol, 2 mol%) in NMP (2.0 mL). The tube was evacuated and backfilled with nitrogen (three times), Then the mixture was stirred and irradiated by the two 20W blue LEDs at room temperature for 24 h. The residue was added water (10 mL) and extracted with ethyl acetate (5 mL × 3). The combined organic phase was dried over Na_2SO_4. The resulting crude residue was purified via column chromatography on silica gel to afford the desired products.

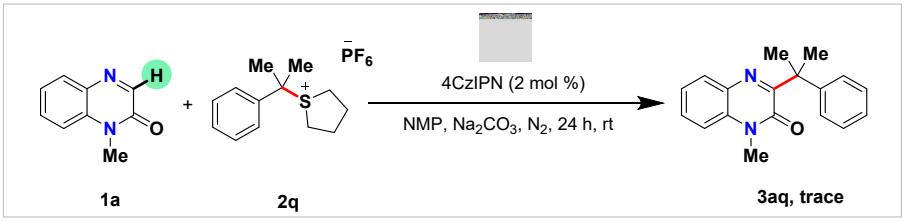
General procedure: To a 25 mL Schlenk tube equipped with a magnetic stir bar, added quinoxalin-2(1*H*)-ones **1** (0.2 mmol), sulfonium salt **2** (0.3 mmol), Na_2CO_3 (2.0 equiv.) and 4CzIPN (0.004 mmol, 2 mol%) in H_2O (2.0 mL). The tube was evacuated and backfilled with nitrogen (three times), Then the mixture was stirred and irradiated by the two 20W blue LEDs at room temperature for 24 h. The residue was extracted with ethyl acetate (5 mL × 3). The combined organic phase was dried over Na_2SO_4. The resulting crude residue was purified via column chromatography on silica gel to afford the desired products.



General procedure: To a 25 mL Schlenk tube equipped with a magnetic stir bar, added quinoxalin-2(1*H*)-ones **1** (0.2 mmol), sulfonium salt **2** (0.3 mmol), Na_2CO_3 (2.0 equiv.) in NMP (2.0 mL). The tube was evacuated and backfilled with nitrogen (three times), Then the mixture was stirred at 50℃ for 24 h. The residue was extracted with ethyl acetate (5 mL × 3). The combined organic phase was dried over Na_2SO_4. The resulting crude residue was purified via column chromatography on silica gel to afford the desired products.

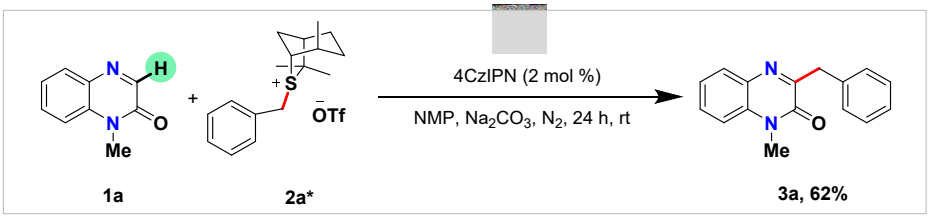


General procedure: To a 25 mL Schlenk tube equipped with a magnetic stir bar, added quinoxalin-2(1*H*)-ones **1** (0.2 mmol), sulfonium salt **2** (0.3 mmol), Na_2CO_3 (2.0 equiv.) and 4CzIPN (0.004 mmol, 2 mol%) in NMP (2.0 mL). The tube was evacuated and backfilled with nitrogen (three times), Then the mixture was stirred and irradiated by the two 20W blue LEDs at room temperature for 24 h. The residue was added water (10 mL) and extracted with ethyl acetate (5 mL × 3). The combined organic phase was dried over Na_2SO_4. The resulting crude residue was purified via column chromatography on silica gel to afford the desired products.



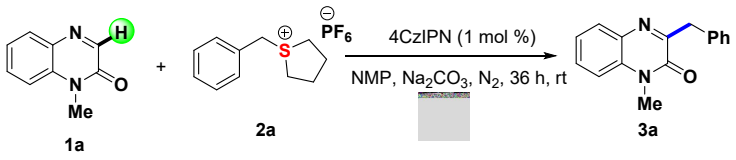
General procedure: To a 25 mL Schlenk tube equipped with a magnetic stir bar, added quinoxalin-2(1*H*)-ones **1** (0.2 mmol), sulfonium salt **2q** (0.3 mmol), Na_2CO_3 (2.0 equiv.) and 4CzIPN (0.004 mmol, 2 mol%) in NMP (2.0 mL). The tube was evacuated and backfilled with nitrogen (three times), Then the mixture was stirred and

irradiated by the two 20W blue LEDs at room temperature for 24 h. The residue was added water (10 mL) and extracted with ethyl acetate (5 mL × 3). The combined organic phase was dried over Na_2SO_4. The resulting crude residue was purified via column chromatography on silica gel to afford the desired products.



General procedure: To a 25 mL Schlenk tube equipped with a magnetic stir bar, added quinoxalin-2(1*H*)-ones **1** (0.2 mmol), sulfonium salt **2a*** (0.3 mmol), Na_2CO_3 (2.0 equiv.) and 4CzIPN (0.004 mmol, 2 mol%) in NMP (2.0 mL). The tube was evacuated and backfilled with nitrogen (three times), Then the mixture was stirred and irradiated by the two 20W blue LEDs at room temperature for 24 h. The residue was added water (10 mL) and extracted with ethyl acetate (5 mL × 3). The combined organic phase was dried over Na_2SO_4. The resulting crude residue was purified via column chromatography on silica gel to afford the desired products.

8. Gram scale

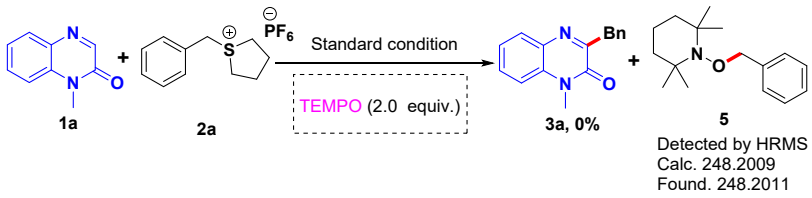


General procedure: To an oven-dried 50 mL Schlenk Tube with a stirring bar was added quinoxalin-2(1*H*)-ones **1a** (5.5 mmol), followed by the addition of sulfonium salt **2a** (8.25 mmol), Na_2CO_3 (2.0 equiv.) and 4CzIPN (0.11 mmol, 2 mol%) Then, air was withdrawn and backfilled with N_2 (three times). NMP (25 mL) was added and the mixture was irradiated under 20W blue LEDs for 36 h. When the reaction is completed, The residue was added water and extracted with CH_2Cl_2, washed with brine, dried over anhydrous sodium sulfate, concentrated in vacuo, and purified by column chromatography (hexane/ethyl acetate = 5/1, v/v) to afford the product **3a**.

III. Mechanistic studies

1. Investigation on the effect of TEMPO and 1,1-diphenylethylene

(a)



Reaction conditions: a mixture of **1a** (0.2 mmol), **2a** (0.3 mmol), 4CzIPN (2 mol %) and 2, 2, 6, 6-tetramethyl-1-piperidinyloxy (TEMPO, 0.4 mmol) in NMP (2 mL) irradiated with two 20W blue LEDs for 24 hours at room temperature in N_2.

The radical trapping experiments were conducted with **1a** and **2a** under the standard conditions with a trapping agent 2, 2, 6, 6-tetramethyl-1-piperidinyloxy (TEMPO, 0.4 mmol) to capture the radical intermediate expected in our system, and the products were detected by HRMS techniques. Supplementary Figure S4 showed that TEMPO, the most common trapping agent, captured benzyl radical with TEMPO-trapped compound **5** observed. HRMS (ESI): compound **5**, HRMS (ESI) calcd for $C_{16}H_{26}NO^+$ $[M+H]^+$: 248.2009, found: 248.2011.

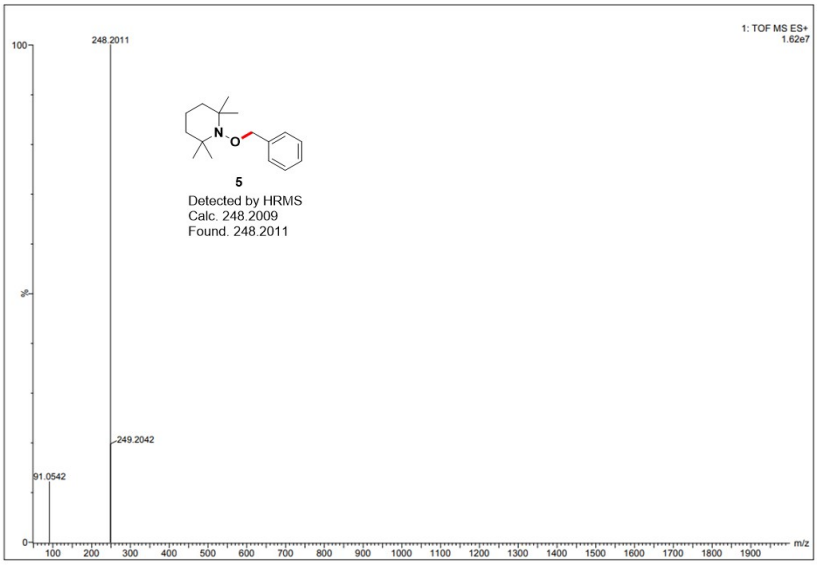
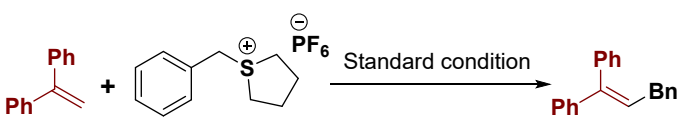


Figure S4. HRMS of TEMPO and the Benzylic Radical Adduct

(b)



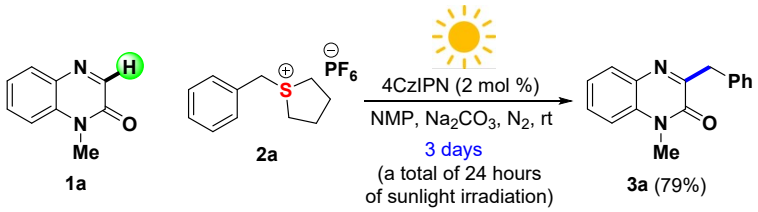
8 **2a** **9, 64% isolated yield**

Reaction conditions: a mixture of **1a** (0.2 mmol), **2a** (0.3 mmol), 4CzIPN (2 mol %)

and 1, 1-diphenylethylene (0.4 mmol) in NMP (2 mL) irradiated with two 20W blue LEDs for 24 hours at room temperature in N_2.

The radical trapping experiments were conducted with **1a** and **2a** under the standard conditions with a trapping agent 1,1-diphenylethylene (0.4 mmol) to capture the radical intermediate expected in our system, and the product **10** was detected by ^{1}H NMR and ^{13}C NMR techniques.

2. Sunlight-driven experiment



1a (0.20 mmol), **2a** (0.30 mmol), 4CzIPN (2 mol %), Na_2CO_3（2.0 equiv.） and a magnetic stir bar were added to an oven dried 25 mL Schlenk tube. The tube was evacuated twice and backfilled with nitrogen. 2.0 mL NMP was then added to the mixture in the presence of a flow of nitrogen. The solution was stirred under solar light for three days (A total of 24 hours of sunlight irradiation, Location: 36°8′54″ N, 120°23′3″ E). Afterward, the residue was added water (10 mL) and extracted with ethyl acetate (5 mL × 3). The combined organic phase was dried over Na_2SO_4, The resulting crude residue was purified via column chromatography on silica gel to afford **3a** in 79% yield.

Figure S5. Sunlight-driven experiment

3. Light on/ off

A standard reaction mixtures in 25 mL schlenk tube were equipped with a magnetic stir bar, added **1a** (0.20 mmol, 1.0 equiv.), **2a** (0.30 mmol, 1.5 equiv.), Na_2CO_3 (0.40 mmol, 2.0 equiv.), 1, 3, 5-trimethoxybenzene (0.20 mmol, as the internal standard) and 4CzIPN (0.004 mmol, 2 mol %) in NMP (2.0 mL). The tube was evacuated twice

and backfilled with nitrogen. Then the mixture was stirred and irradiated by two 20W blue LEDs at room temperature. After 2.0 h, the blue LEDs were turned off, and the schlenk tube was taken from the irradiation device and 0.2 ml of the mixture was taken out for analysis. The remaining mixture was stirred in the absence of light for an additional 2.0 h. Then, the schlenk tube was taken from the irradiation device and 0.2 ml of the mixture was taken out for analysis, and the blue LEDs were turned back on to irradiate the residual mixture. After an additional 2.0 h of irradiation, the blue LEDs were turned off, and the schlenk tube was taken from the irradiation device and 0.2 ml of the mixture was taken out for analysis. The remaining mixture was stirred in the absence of light for an additional 2.0 h. Then, schlenk tube was removed for analysis, and the blue LEDs were turned back on to irradiate the residual mixture. After 2.0 h, the blue LEDs were turned off, and the schlenk tube was taken from the irradiation device and 0.2 ml of the mixture was taken out for analysis. The remaining mixture was stirred in the absence of light for an additional 2.0 h, and then it was analyzed. The yield was determined by ^{1}H NMR spectroscopy using 1, 3, 5-trimethoxybenzene as the internal standard.

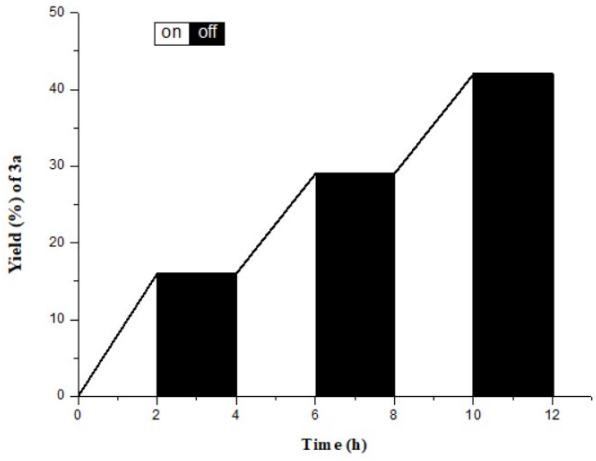


Figure S6. Light on/ off experiment

4. Calculation of apparent quantum efficiency (A. Q. E)

Experimental procedure

A standard reaction mixtures in 25 mL schlenk tube were equipped with a magnetic stir bar, added **1a** (0.20 mmol, 1.0 equiv.), **2a** (0.30 mmol, 1.5 equiv.), Na_2CO_3 (0.40 mmol, 2.0 equiv.), 1, 3, 5-trimethoxybenzene (0.20 mmol, as the internal standard)

and 4CzIPN (0.004 mmol, 2 mol %) in NMP (2.0 mL). The tube was evacuated twice and backfilled with nitrogen. Then the mixture was stirred and irradiated by two 20W blue LEDs at room temperature. After 2.0 h, the blue LEDs were turned off, and the schlenk tube was taken from the irradiation device and 0.2 ml of the mixture was taken out for analysis.

The photon flux of the light source was determined by an optical power meter to be 82.30 mW (average of three experiments)

$$E_{photon} = \frac{hc}{\lambda_{inc\ (455\ nm)}} = \frac{6.63 \times 10^{-34} J \cdot S \times 3 \times 10^{8} m \cdot x \cdot s^{-1}}{455 \times 10^{-9} m} = 4.37 \times 10^{-19} J$$

$$E_{total} = \text{PSt} = 82.30 \times 10^{-3}\ W \cdot cm^{-2} \times 2.57\ cm^{2} \times 2.0 \times 3600\ s = 1.52 \times 10^{3} J$$

$$\text{Number of incident photons} = \frac{E_{total}}{E_{photon}} = 3.48 \times 10^{21} = 5.78\ mmol$$

$$\text{A. Q. Y (\%)} = \frac{Number\ of\ product}{Number\ of\ incident\ photons} = \frac{0.032\ mmol}{5.78\ mmol} = 0.55\% < 1$$

Where h (J·s) is Planck's constant, c ($m \cdot s^{-1}$) is the speed of light and λ_{inc} (m) is the wavelength of the incident light. P ($W \cdot cm^{-2}$) is the power density of the incident light, S (cm^2) is the irradiation area and t (s) is the photoreaction time.

5. EPR experiments

Free radical trapping investigation by Electron Paramagnetic Resonance Spectroscopy (EPR):

To an oven-dried Schlenk tube equipped with a stir bar was loaded with 4CzIPN (0.002 mmol), Sulfonium salt **2a** (0.3 mmol), and 5,5-dimethyl-1-pyrroline *N*-oxide (DMPO, 2.0 equiv.) in NMP (2.0 mL) under N_2, the solution sample was taken out into a capillary tube, then the capillary tube was transferred to a EPR tube and measured. Subsequently, the reaction solution was irradiated with 20W blue LED (455 nm) for 5 min, then analyzed by EPR again, as is shown by the orange line. EPR spectrum was recorded at 123 K on EPR spectrometer operated at 9.045GHz, scan width 1.57 mT, center field 2.32 mT, time constant 0.1s, scan time 1min, modulation width 0.1 mT, gain 500, power 1mW.

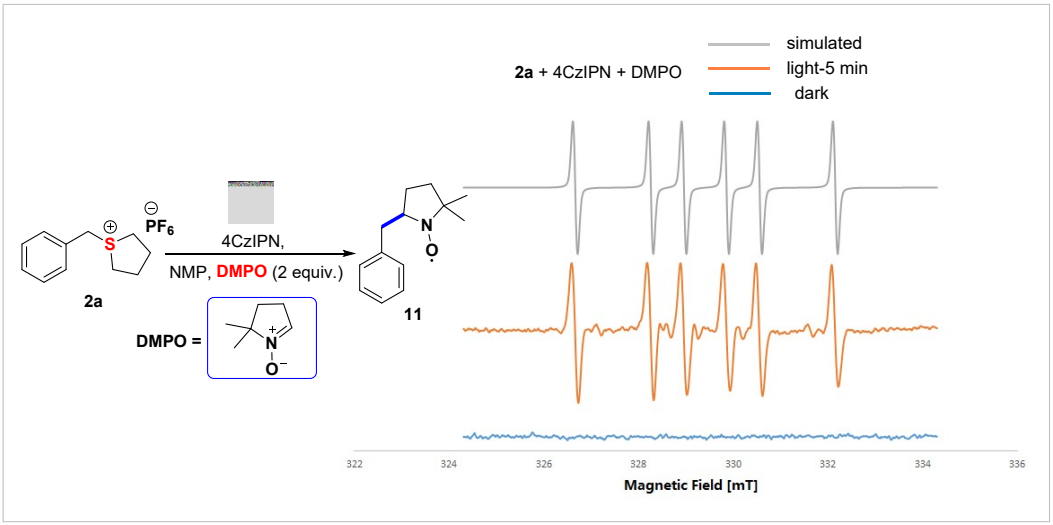


Figure S7. EPR Spectra of the DMPO-Radical Adduct

6. The UV–vis spectra of Sulfonium salt 2a

UV-visible spectroscopy of reaction solution was recorded on a UV-2600 UV-visible spectrophotometer. The sample was prepared by mixing Sulfonium salt **2a** with NMP ($C = 5.0\times10^{-3}$ M), in a light path quartz UV cuvette. The absorption was collected and the result was listed in Figure S8

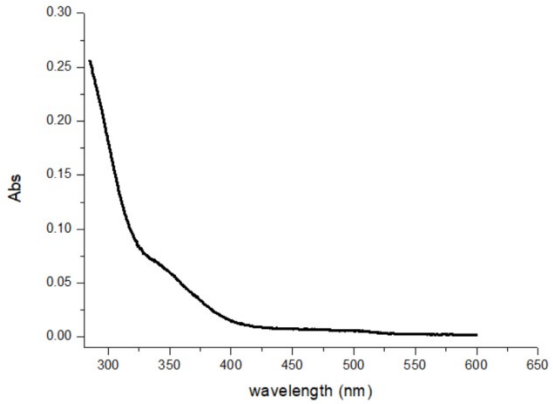


Figure S8. UV–vis spectra of Sulfonium salt **2a**

7. Emission spectrum of Sulfonium salt 2a

The fluorescence emission intensities were recorded on a HITACHI F-2700 spectrofluorimeter. The excitation wavelength was fixed at 338 nm. The sample is the NMP solution of **2a** in the optical path quartz fluorescence cuvette. Then the emission intensity was collected and the results were presented in Figure S8.

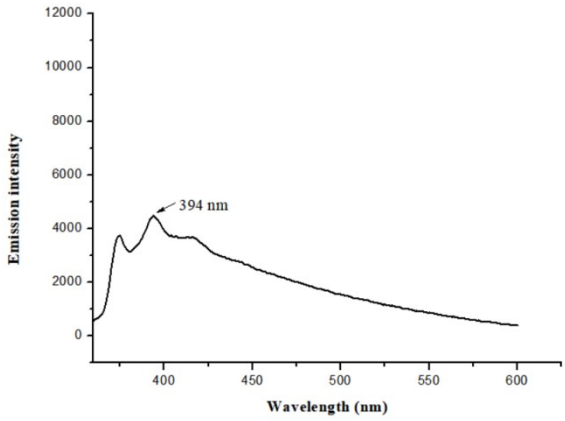


Figure S9. Emission spectrum of Sulfonium salt **2a**

8. Fluorescence quenching experiments

The fluorescence emission intensities were recorded on a RF-6000 spectrofluorimeter. The excitation wavelength was fixed at 475 nm. The samples were prepared by mixing 4CzIPN (2×10^{-3} mol/L) and different amount of quencher in NMP in a light path quartz fluorescence cuvette. The concentration of quencher is 5M in NMP. For each quenching experiment, 0.003 ml of quencher solution was titrated to a mixed solution of 4CzIPN (0.003 mL, in a total volume = 3.0 mL). Then the emission intensity was collected and the results were presented in Figure S10 or Figure S11.

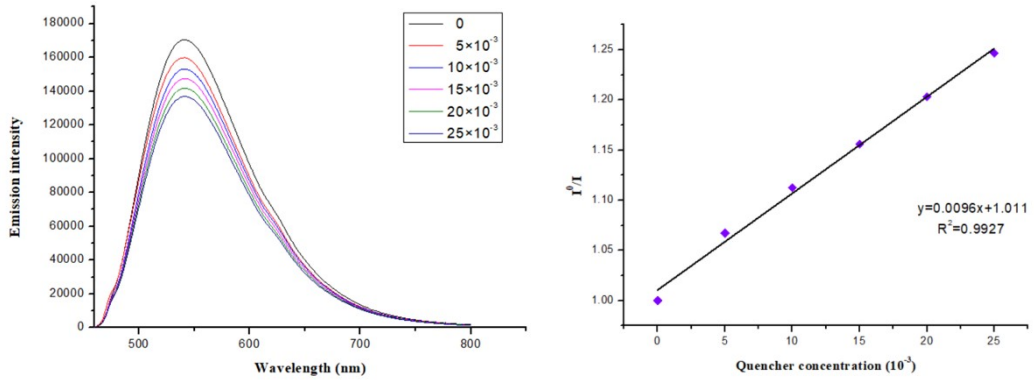


Figure S10. The emission spectra of a solution of 4CzIPN in NMP upon irradiation at 475 nm in the presence of varying amounts of quinoxalin-2(1*H*)-one **1a**

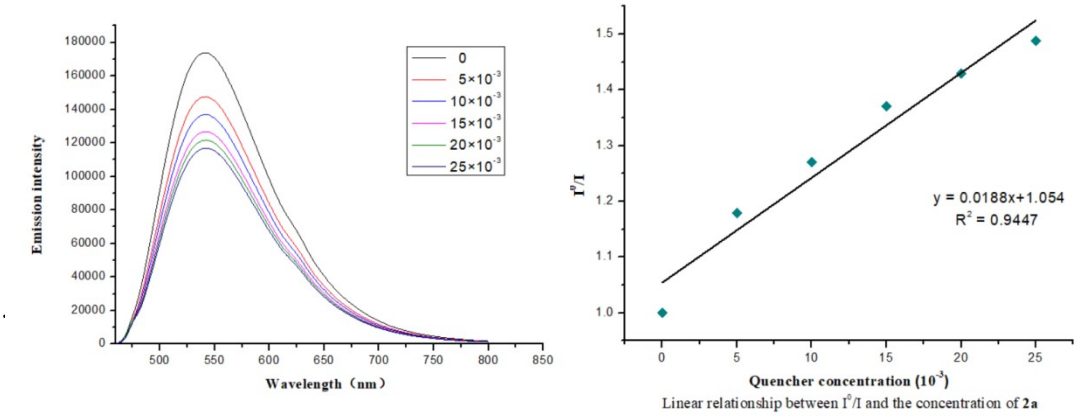


Figure S11. The emission spectra of a solution of 4CzIPN in NMP upon irradiation at 475 nm in the presence of varying amounts of sulfonium salt **2a**

9. Cyclic Voltammetry Experiments

Cyclic Voltammetry was performed on a CH Instruments Electrochemical Workstation model CS300H. A solution of the sample in CH_2Cl_2 (0.2 M) was tested with 0.3 M Bu_4NBr as the supporting electrolyte, using a glassy carbon as the working electrode, a Pt as the counter electrode, and Ag/AgCl as reference electrode. Scan rate = 100 mV/s.

Reductive potential of 2a

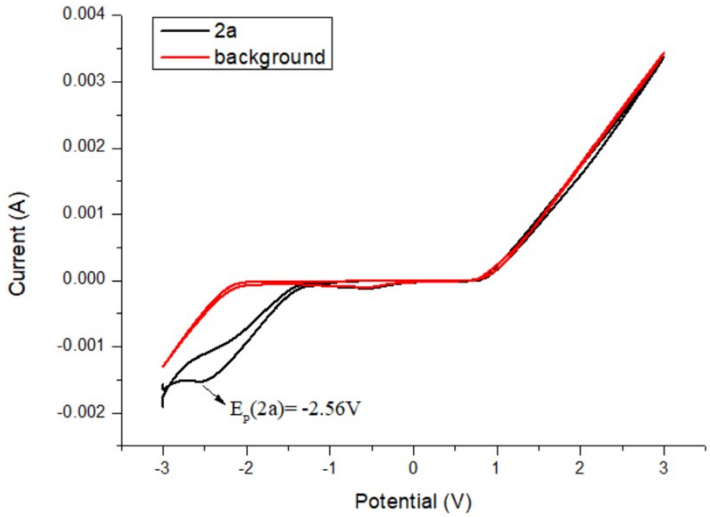
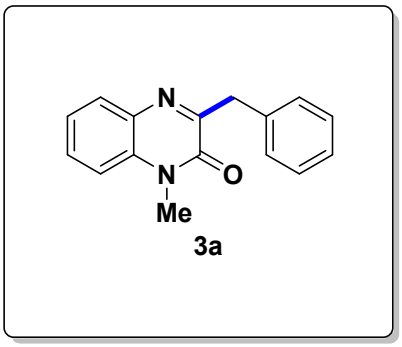


Figure S12. Cyclic Voltammogram of **2a,** $E_p^{0/-1}$(**2a**) = -2.56 V (vs Ag/AgCl), $E_p^{0/-1}$(**2a**) = -2.607 V (vs SCE)

According to the emission spectra of **2a**, which was excited at 338 nm, the maximum emission wavelength is 394 nm, After calculation, the E_{00} (**2a***/**2a**) = 3.15 V, E^*(**2a***/**2a**$^-$) = E_{00} (**2a***/**2a**) + E(**2a** /**2a**$^-$), $E^*_p{}^{0/-1}$(**2a**) = 0.543V (vs SCE).

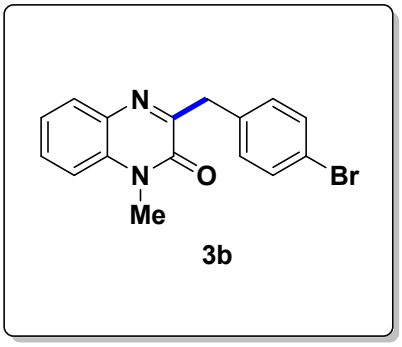
IV. Characterization of products

Characterization data of compounds 3a-10



3a

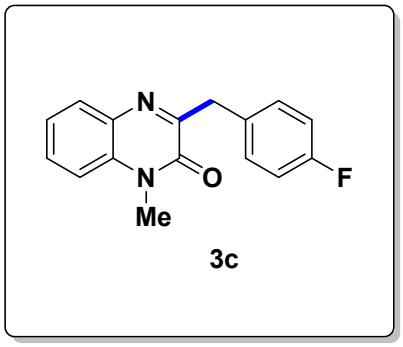
3-Benzyl-1-methylquinoxalin-2(1*H*)-one (3a)[8]. Eluent petroleum ether/ethyl acetate (5:1). White solid, 43 mg, 86% yield. ^{1}H NMR ($CDCl_3$, 500 MHz, ppm) δ 7.87 (d, *J* = 8.0 Hz, 1H), 7.52 (t, *J* = 7.8 Hz, 1H), 7.48 (d, *J* = 7.6 Hz, 2H), 7.37 – 7.27 (m, 4H), 7.22 (t, *J* = 7.3 Hz, 1H), 4.28 (s, 2H), 3.67 (s, 3H). ^{13}C NMR ($CDCl_3$, 125 MHz, ppm) δ 159.3, 154.7, 137.0, 133.3, 132.7, 130.0, 129.9, 129.5, 128.4, 126.6, 123.5, 113.5, 40.7, 29.1. HRMS calcd for $C_{16}H_{15}N_2O^+$ $[M+H]^+$: 251.1179; found 251.1183.



3b

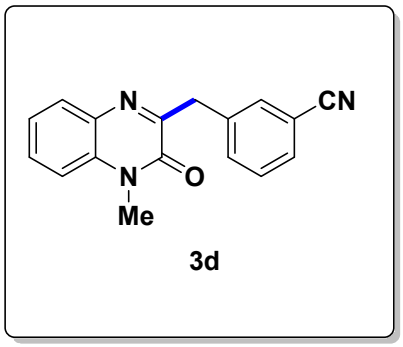
3-(4-Bromobenzyl)-1-methylquinoxalin-2(1*H*)-one (3b)[9]. Eluent petroleum ether/ethyl acetate (5:1). Yellow solid, 51 mg, 78% yield. ^{1}H NMR ($CDCl_3$, 500 MHz, ppm) δ 7.84 (d, *J* = 7.9 Hz, 1H), 7.54 (t, *J* = 7.7 Hz, 1H), 7.40 (d, *J* = 8.3 Hz, 2H), 7.34 (t, *J* = 7.9 Hz, 3H), 7.28 (d, *J* = 8.4 Hz, 1H), 4.21 (s, 2H), 3.67 (s, 3H). ^{13}C NMR ($CDCl_3$, 125 MHz, ppm) δ 158.7, 154.6, 136.0, 133.3, 132.7, 131.5, 131.3, 130.1,

130.0, 123.7, 120.6, 113.6, 40.2, 29.1. HRMS calcd for $C_{16}H_{14}BrN_2O^+$ $[M+H]^+$: 329.0284; found 329.0286.



3c

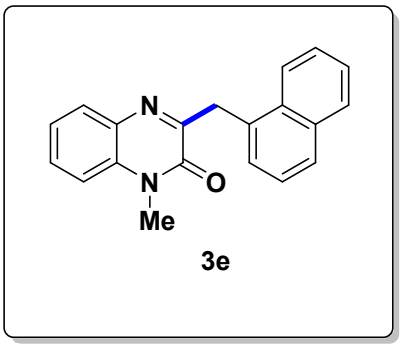
3-(4-Fluorobenzyl)-1-methylquinoxalin-2(1*H*)-one (3c)[9]. Eluent petroleum ether/ethyl acetate (5:1). White solid, 49 mg, 91% yield. ^{1}H NMR ($CDCl_3$, 500 MHz, ppm) δ 7.85 (dd, *J* = 8.1, 0.9 Hz, 1H), 7.55-7.51 (m, 1H), 7.44-7.41 (m, 2H), 7.34 (t, *J* = 7.5 Hz, 1H), 7.28 (d, *J* = 8.4 Hz, 1H), 6.97 (t, *J* = 8.7 Hz, 2H), 4.23 (s, 2H), 3.67 (s, 3H). ^{13}C NMR ($CDCl_3$, 125 MHz, ppm) δ 162.7, 160.8, 159.0, 154.7, 133.3, 132.7, 132.6, 131.0, 130.9, 130.0, 129.9, 123.6, 115.2, 115.1, 113.6, 39.9, 29.1. HRMS calcd for $C_{16}H_{14}FN_2O^+$ $[M+H]^+$: 269.1085; found 269.1089.



3d

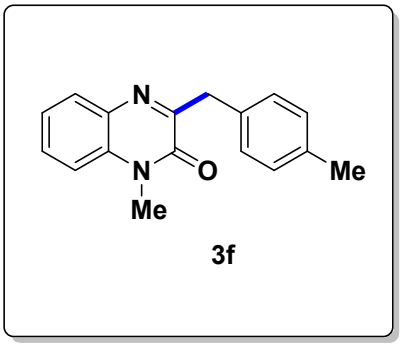
3-((4-methyl-3-oxo-3,4-dihydroquinoxalin-2-yl)methyl)benzonitrile (3d). Eluent petroleum ether/ethyl acetate (5:1). White solid, 22 mg, 40% yield. ^{1}H NMR ($CDCl_3$, 500 MHz, ppm) δ 7.85 (d, *J* = 8.0 Hz, 1H), 7.74 (s, 1H), 7.70 (d, *J* = 7.8 Hz, 1H), 7.58 – 7.54 (m, 1H), 7.51 (d, *J* = 7.8 Hz, 1H), 7.41 – 7.35 (m, 2H), 7.30 (d, *J* = 8.3 Hz, 1H),

4.28 (s, 2H), 3.68 (s, 3H). ^{13}C NMR ($CDCl_3$, 125 MHz, ppm) δ 157.9, 154.6, 138.6, 134.2, 133.3, 133.0, 132.6, 130.4, 130.3, 130.1, 129.1, 123.8, 118.9, 113.7, 112.4, 40.1, 29.2. HRMS calcd for $C_{17}H_{14}N_3O^+$ $[M+H]^+$: 276.1131; found 276.1137.



3e

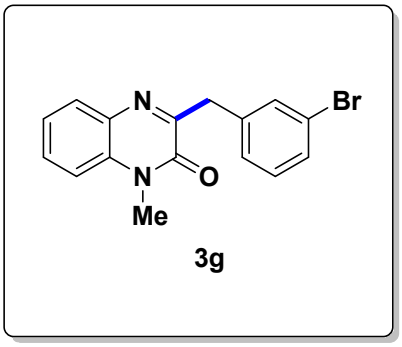
1-Methyl-3-(naphthalen-1-ylmethyl)quinoxalin-2(1*H*)-one (3e)[9]. Eluent petroleum ether/ethyl acetate (5:1). yellow oil, 35 mg, 58% yield. ^{1}H NMR ($CDCl_3$, 500 MHz, ppm) δ 8.40 (d, *J* = 8.5 Hz, 1H), 7.83 (d, *J* = 8.1 Hz, 1H), 7.79-7.74 (m, 2H), 7.63 (d, *J* = 7.0 Hz, 1H), 7.52 – 7.42 (m, 4H), 7.28 (t, *J* = 7.6 Hz, 1H), 7.24 (d, *J* = 8.4 Hz, 1H), 4.75 (s, 2H), 3.67 (s, 3H). ^{13}C NMR ($CDCl_3$, 125 MHz, ppm) δ 158.9, 154.8, 133.9, 133.3, 133.2, 132.7, 132.5, 130.0, 129.9, 128.5, 128.3, 127.4, 125.9, 125.5, 125.4, 124.8, 123.5, 113.5, 37.7, 29.1. HRMS calcd for $C_{20}H_{17}N_2O^+$ $[M+H]^+$: 301.1335; found 301.1344.



3f

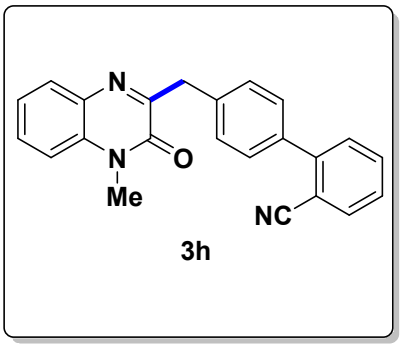
1-Methyl-3-(4-methylbenzyl)quinoxalin-2(1*H*)-one (3f)[8]. Eluent petroleum ether/ethyl acetate (5:1). Red solid, 46 mg, 86% yield. ^{1}H NMR ($CDCl_3$, 500 MHz,

ppm) δ 7.82 – 7.79 (m, 1H), 7.48 – 7.44 (m, 1H), 7.32 – 7.28 (m, 3H), 7.20 (d, J = 8.8 Hz, 1H), 7.05 (d, J = 7.8 Hz, 2H), 4.18 (s, 2H), 3.60 (s, 3H), 2.25 (s, 3H). ^{13}C NMR ($CDCl_3$, 125 MHz, ppm) δ 159.5, 154.7, 136.1, 133.9, 133.3, 132.7, 129.9, 129.8, 129.4, 129.1, 123.5, 113.5, 40.4, 29.1, 21.0. HRMS calcd for $C_{17}H_{17}N_2O^+$ $[M+H]^+$: 265.1335; found 265.1340.



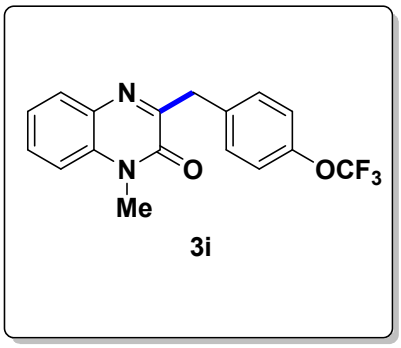
3g

3-(3-Bromobenzyl)-1-methylquinoxalin-2(1*H*)-one (3g). Eluent petroleum ether/ethyl acetate (5:1). White solid, 44 mg, 67% yield. ^{1}H NMR ($CDCl_3$, 500 MHz, ppm) δ 7.84 (d, J = 7.8 Hz, 1H), 7.59 (s, 1H), 7.52 (t, J = 7.7 Hz, 1H), 7.39 (d, J = 7.5 Hz, 1H), 7.33 (t, J = 6.7 Hz, 2H), 7.26 (d, J = 8.6 Hz, 1H), 7.15 (t, J = 7.8 Hz, 1H), 4.21 (s, 2H), 3.66 (s, 3H). ^{13}C NMR ($CDCl_3$, 125 MHz, ppm) δ 158.5, 154.6, 139.3, 133.3, 132.7, 132.3, 130.1, 130.0, 129.9, 129.7, 128.3, 123.6, 122.4, 113.6, 40.2, 29.1. HRMS calcd for $C_{16}H_{14}BrN_2O^+$ $[M+H]^+$: 329.0284; found 329.0287.



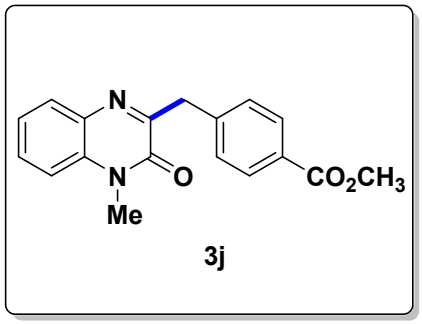
3h

4'-((4-Methyl-3-oxo-3,4-dihydroquinoxalin-2-yl)methyl)-[1,1'-biphenyl]-2-carbonitrile (3h). Eluent petroleum ether/ethyl acetate (5:1). White solid, 37 mg, 52% yield. ^{1}H NMR ($CDCl_3$, 500 MHz, ppm) δ 7.87 – 7.81 (m, 1H), 7.70 (d, *J* = 7.8 Hz, 1H), 7.59 – 7.55 (m, 3H), 7.51 – 7.43 (m, 4H), 7.37 (t, *J* = 7.6 Hz, 1H), 7.31 (t, *J* = 7.6 Hz, 1H), 7.26 – 7.23 (m, 1H), 4.29 (s, 2H), 3.65 (s, 3H). ^{13}C NMR ($CDCl_3$, 125 MHz, ppm) δ 158.8, 154.7, 145.3, 137.8, 136.4, 133.7, 133.3, 132.7, 130.1, 130.0, 129.9, 128.7, 127.3, 123.6, 118.8, 113.6, 111.1, 40.4, 29.1. HRMS calcd for $C_{23}H_{18}N_3O^+$ $[M+H]^+$: 352.1444; found 352.1446.



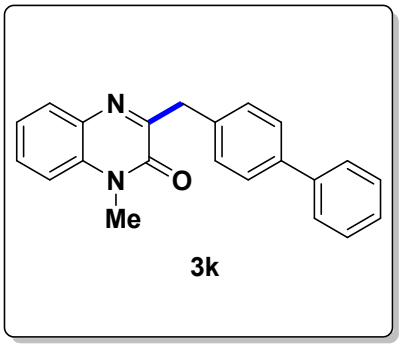
3i

1-Methyl-3-(4-(trifluoromethoxy)benzyl)quinoxalin-2(1*H*)-one (3i).[12] Eluent petroleum ether/ethyl acetate (5:1). White solid, 40 mg, 60% yield. ^{1}H NMR ($CDCl_3$, 500 MHz, ppm) δ 7.82 (d, *J* = 8.1 Hz, 1H), 7.51 (t, *J* = 7.5 Hz, 1H), 7.46 (d, *J* = 8.5 Hz, 2H), 7.32 (t, *J* = 7.5 Hz, 1H), 7.24 (d, *J* = 6.0 Hz, 1H), 7.10 (d, *J* = 8.1 Hz, 2H), 4.23 (s, 2H), 3.64 (s, 3H). ^{13}C NMR ($CDCl_3$, 125 MHz, ppm) δ 158.7, 154.7, 148.0, 135.7, 133.3, 132.7, 130.8, 130.1, 130.0, 123.7, 120.9, 113.6, 40.0, 29.1. HRMS calcd for $C_{17}H_{14}F_3N_2O_2^+$ $[M+H]^+$: 335.1002; found 335.1005.



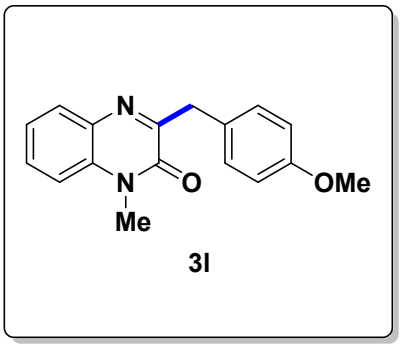
3j

Methyl 4-((4-methyl-3-oxo-3,4-dihydroquinoxalin-2-yl)methyl)benzoate (3j). Eluent petroleum ether/ethyl acetate (5:1). White solid, 43 mg, 69% yield. ^{1}H NMR ($CDCl_3$, 500 MHz, ppm) δ 7.96 (d, *J* = 8.1 Hz, 2H), 7.84 (d, *J* = 8.0 Hz, 1H), 7.55-7.51 (m, 3H), 7.34 (t, *J* = 7.6 Hz, 1H), 7.28 (d, *J* = 8.3 Hz, 1H), 4.31 (s, 2H), 3.88 (s, 3H), 3.67 (s, 3H). ^{13}C NMR ($CDCl_3$, 125 MHz, ppm) δ 167.0, 158.5, 154.6, 142.4, 133.3, 132.7, 130.1, 130.0, 129.7, 129.5, 128.5, 123.7, 113.6, 52.0, 40.7, 29.1. HRMS calcd for $C_{18}H_{17}N_2O_3^+$ $[M+H]^+$: 309.1234; found 309.1233.



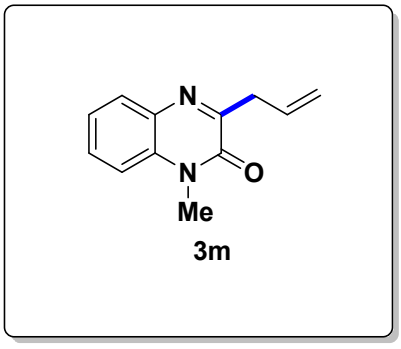
3k

3-([1,1'-Biphenyl]-4-ylmethyl)-1-methylquinoxalin-2(1*H*)-one (3k). Eluent petroleum ether/ethyl acetate (5:1). White solid, 56 mg, 85% yield. ^{1}H NMR ($CDCl_3$, 500 MHz, ppm) δ 7.86 (d, *J* = 8.0 Hz, 1H), 7.55 – 7.47 (m, 7H), 7.38 (t, *J* = 7.7 Hz, 2H), 7.33 – 7.27 (m, 2H), 7.23 (d, *J* = 8.2 Hz, 1H), 4.30 (s, 2H), 3.64 (s, 3H). ^{13}C NMR ($CDCl_3$, 125 MHz, ppm) δ 159.1, 154.7, 141.0, 139.5, 136.1, 133.3, 132.7, 129.9, 128.6, 127.1, 127.0, 127.0, 123.5, 113.5, 40.4, 29.1. HRMS calcd for $C_{22}H_{19}N_2O^+$ $[M+H]^+$: 327.1492; found 327.1490.



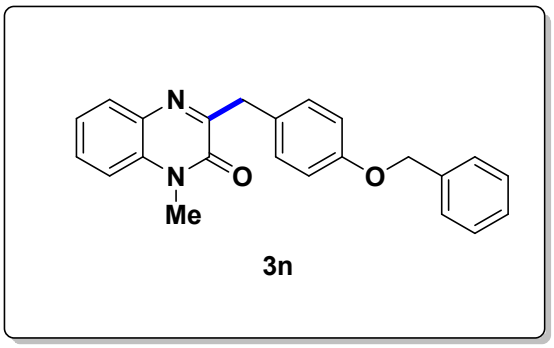
3l

3-(4-Methoxybenzyl)-1-methylquinoxalin-2(1*H*)-one (3l)[10]. Eluent petroleum ether/ethyl acetate (5:1). White solid, 51 mg, 90% yield. ^{1}H NMR ($CDCl_3$, 500 MHz, ppm) δ 7.84 – 7.79 (m, 1H), 7.50 – 7.45 (m, 1H), 7.36 (d, *J* = 8.6 Hz, 2H), 7.29 (t, *J* = 7.7 Hz, 1H), 7.23 – 7.21 (m, 1H), 6.79 (d, *J* = 8.6 Hz, 2H), 4.16 (s, 2H), 3.72 (s, 3H), 3.62 (s, 3H). ^{13}C NMR ($CDCl_3$, 500 MHz, ppm) δ 159.5, 158.4, 154.7, 133.3, 132.7, 130.5, 129.9, 129.8, 129.0, 123.5, 113.8, 113.5, 55.2, 39.9, 29.1. HRMS calcd for $C_{17}H_{17}N_2O_2^+$ $[M+H]^+$: 281.1285; found 281.1285.



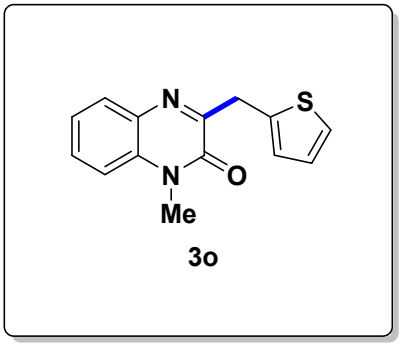
3m

3-Allyl-1-methylquinoxalin-2(1*H*)-one (3m). Eluent petroleum ether/ethyl acetate (6:1). Yellow solid, 18 mg, 45% yield. ^{1}H NMR ($CDCl_3$, 500 MHz, ppm) δ 7.85 (d, *J* = 8.0 Hz, 1H), 7.53 (t, *J* = 7.8 Hz, 1H), 7.33 (t, *J* = 7.6 Hz, 1H), 7.29 (d, *J* = 8.4 Hz, 1H), 6.23-6.15 (m, 1H), 5.27 (dd, *J* = 17.1, 1.1 Hz, 1H), 5.19 (d, *J* = 10.1 Hz, 1H), 3.73 (d, *J* = 6.7 Hz, 2H), 3.70 (s, 3H). ^{13}C NMR ($CDCl_3$, 500 MHz, ppm) δ 159.0, 154.7, 133.2, 133.1, 132.7, 129.9, 129.8, 123.6, 117.7, 113.6, 38.8, 29.1. HRMS calcd for $C_{12}H_{13}N_2O^+$ $[M+H]^+$: 201.1022; found 201.1020.



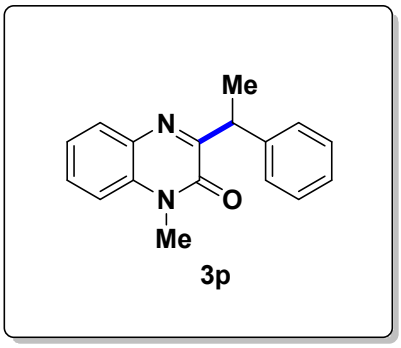
3n

3-(4-(Benzyloxy)benzyl)-1-methylquinoxalin-2(1*H*)-one (3n). Eluent petroleum ether/ethyl acetate (5:1). White solid, 62 mg, 87% yield. ^{1}H NMR ($CDCl_3$, 500 MHz, ppm) δ 7.85 (d, *J* = 8.1 Hz, 1H), 7.54 – 7.48 (m, 1H), 7.42 – 7.29 (m, 8H), 7.25 (d, *J* = 7.5 Hz, 1H), 6.91 (d, *J* = 8.6 Hz, 2H), 5.02 (s, 2H), 4.21 (s, 2H), 3.65 (s, 3H). ^{13}C NMR ($CDCl_3$, 125 MHz, ppm) δ 159.5, 157.6, 154.7, 137.1, 133.3, 132.7, 130.5, 129.9, 129.8, 129.3, 128.5, 127.8, 127.4, 123.5, 114.8, 113.5, 70.0, 39.9, 29.1. HRMS calcd for $C_{23}H_{21}N_2O_2^+$ $[M+H]^+$: 357.1598; found 357.1593.



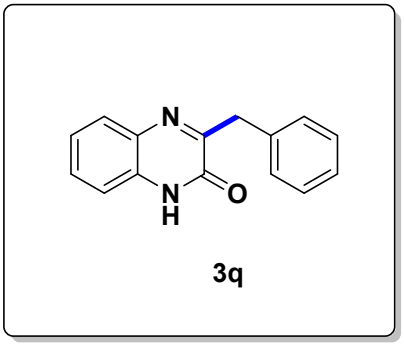
3o

1-Methyl-3-(thiophen-2-ylmethyl)quinoxalin-2(1*H*)-one (3o)[9]. Eluent petroleum ether/ethyl acetate (5:1). Yellow solid, 32 mg, 63% yield. ^{1}H NMR ($CDCl_3$, 500 MHz, ppm) δ 7.86 (d, *J* = 8.0 Hz, 1H), 7.53 (t, *J* = 7.8 Hz, 1H), 7.34 (t, *J* = 7.6 Hz, 1H), 7.28 (d, *J* = 8.4 Hz, 1H), 7.16 (d, *J* = 5.0 Hz, 1H), 7.06 (d, *J* = 2.6 Hz, 1H), 6.96 – 6.89 (m, 1H), 4.47 (s, 2H), 3.70 (s, 3H). ^{13}C NMR ($CDCl_3$, 125 MHz, ppm) δ 158.0, 154.6, 138.6, 133.4, 132.7, 130.1, 130.0, 126.8, 126.6, 124.6, 123.7, 113.6, 34.8, 29.2. HRMS calcd for $C_{14}H_{13}N_2OS^+$ $[M+H]^+$: 257.0743; found 257.0745.



3p

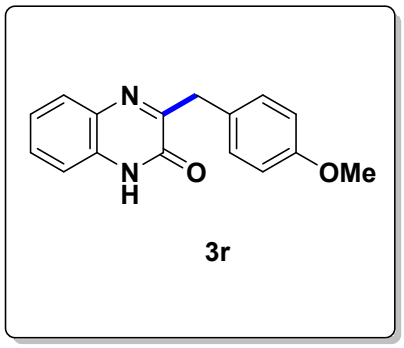
(*S*)-1-Methyl-3-(1-phenylethyl)quinoxalin-2(1*H*)-one (3p)[8]. Eluent petroleum ether/ethyl acetate (5:1). White solid, 46 mg, 86% yield. ^{1}H NMR ($CDCl_3$, 500 MHz, ppm) δ 7.92 (d, *J* = 8.0 Hz, 1H), 7.49 (t, *J* = 7.7 Hz, 1H), 7.45 (d, *J* = 7.5 Hz, 2H), 7.33 (t, *J* = 7.6 Hz, 1H), 7.29-7.22 (m, 3H), 7.17 (t, *J* = 7.3 Hz, 1H), 4.83 (q, *J* = 7.1 Hz, 1H), 3.61 (s, 3H), 1.69 (d, *J* = 7.1 Hz, 3H). ^{13}C NMR ($CDCl_3$, 500 MHz, ppm) δ 161.8, 154.4, 143.1, 133.0, 132.7, 130.1, 129.6, 128.3, 128.1, 126.4, 123.4, 113.4, 41.8, 29.0, 19.6. HRMS calcd for $C_{17}H_{17}N_2O^+$ $[M+H]^+$: 265.1355; found 265.1340.



3q

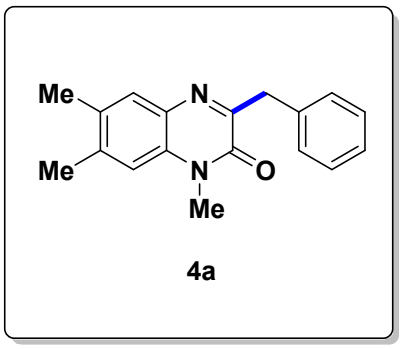
3-Benzylquinoxalin-2(1*H*)-one (3q)[8]. Eluent petroleum ether/ethyl acetate (5:1). Yellow solid, 37 mg, 79% yield. ^{1}H NMR (DMSO-d_6, 500 MHz, ppm) δ 12.40 (s, 1H), 7.72 (d, *J* = 7.9 Hz, 1H), 7.48 (t, *J* = 7.6 Hz, 1H), 7.33 (d, *J* = 7.5 Hz, 2H), 7.28 (t, *J* = 7.2 Hz, 4H), 7.20 (t, *J* = 7.1 Hz, 1H), 4.12 (s, 2H). ^{13}C NMR (DMSO-d_6, 125 MHz,

ppm) δ 160.4, 154.6, 137.5, 132.0, 131.7, 129.9, 129.2, 128.4, 128.3, 126.4, 123.3, 115.4, 39.0. HRMS calcd for $C_{15}H_{13}N_2O^+$ $[M+H]^+$: 237.1022; found 237.1023.



3r

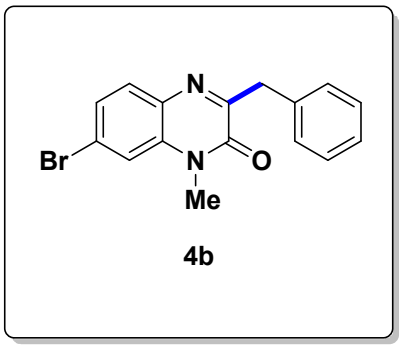
3-(4-Methoxybenzyl)quinoxalin-2(1*H*)-one (3r)[13]. Eluent petroleum ether/ethyl acetate (4:1). White solid, 38 mg, 71% yield. ^{1}H NMR ($CDCl_3$, 500 MHz, ppm) δ 12.17 (s, 1H), 7.84 (d, *J* = 7.9 Hz, 1H), 7.50 – 7.46 (m, 1H), 7.40 (d, *J* = 8.6 Hz, 2H), 7.32 (t, *J* = 7.6 Hz, 1H), 7.25 (d, *J* = 9.6 Hz, 1H), 6.83 (d, *J* = 8.6 Hz, 2H), 4.23 (s, 2H), 3.75 (s, 3H). ^{13}C NMR ($CDCl_3$, 500 MHz, ppm) δ 160.0, 158.4, 156.3, 132.9, 131.1, 130.5, 129.8, 129.1, 129.0, 124.1, 115.6, 113.9, 55.2, 39.1. HRMS calcd for $C_{16}H_{15}N_2O_2^+$ $[M+H]^+$: 267.1128; found 267.1131.



4a

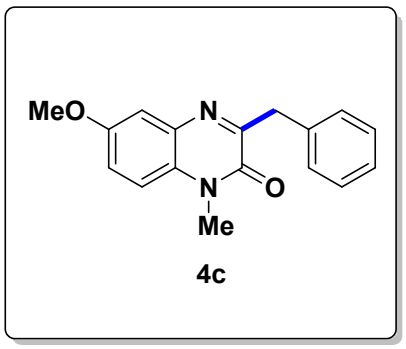
3-Benzyl-1,6,7-trimethylquinoxalin-2(1*H*)-one (4a)[8]. Eluent petroleum ether/ethyl acetate (5:1). White solid, 52 mg, 93% yield. ^{1}H NMR ($CDCl_3$, 500 MHz, ppm) δ 7.58 (s, 1H), 7.44 (d, *J* = 7.5 Hz, 2H), 7.26 (t, *J* = 7.5 Hz, 2H), 7.18 (t, *J* = 7.2 Hz, 1H), 6.99 (s, 1H), 4.22 (s, 2H), 3.60 (s, 3H), 2.37 (s, 3H), 2.32 (s, 3H). ^{13}C NMR ($CDCl_3$, 125 MHz, ppm) δ 157.9, 154.7, 139.5, 137.3, 132.3, 131.3, 131.1, 129.9, 129.4, 128.3,

126.4, 114.1, 40.6, 28.9, 20.4, 19.1. HRMS calcd for $C_{18}H_{19}N_2O^+$ $[M+H]^+$: 279.1492; found 279.1496.



4b

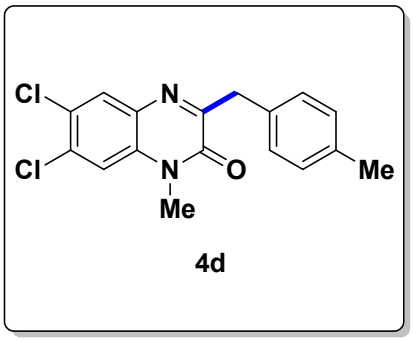
3-Benzyl-7-bromo-1-methylquinoxalin-2(1*H*)-one (4b)[9]. Eluent petroleum ether/ethyl acetate (5:1). White solid, 53 mg, 80% yield. ^{1}H NMR ($CDCl_3$, 500 MHz, ppm) δ 7.99 (d, *J* = 1.2 Hz, 1H), 7.64-7.54 (m, 1H), 7.43 (d, *J* = 7.1 Hz, 2H), 7.31-7.19 (m, 3H), 7.12 (d, *J* = 8.8 Hz, 1H), 4.24 (s, 2H), 3.62 (s, 3H). ^{13}C NMR ($CDCl_3$, 125 MHz, ppm) δ 160.7, 154.4, 136.6, 133.6, 132.6, 132.5, 132.4, 129.6, 128.4, 126.7, 116.1, 115.0, 40.7, 29.2. HRMS calcd for $C_{16}H_{14}BrN_2O^+$ $[M+H]^+$: 329.0284; found 329.0286.



4c

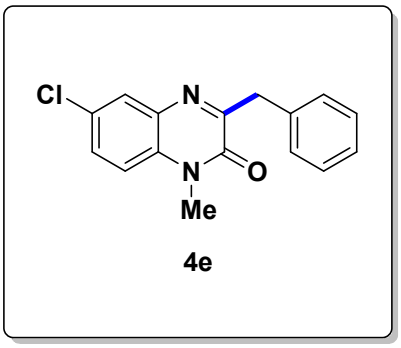
3-Benzyl-6-methoxy-1-methylquinoxalin-2(1*H*)-one (4c). Eluent petroleum ether/ethyl acetate (5:1). Yellow solid, 51 mg, 90% yield. ^{1}H NMR ($CDCl_3$, 500 MHz, ppm) δ 7.47 (d, *J* = 7.5 Hz, 2H), 7.34 – 7.27 (m, 3H), 7.21 (t, *J* = 7.3 Hz, 1H), 7.17 (d, *J* = 9.1 Hz, 1H), 7.14-7.11 (m, 1H), 4.26 (s, 2H), 3.87 (s, 3H), 3.64 (s, 3H). ^{13}C NMR

($CDCl_3$, 125 MHz, ppm) δ 159.8, 155.9, 154.3, 137.1, 133.4, 129.5, 128.4, 127.5, 126.5, 119.0, 114.4, 111.4, 55.7, 40.8, 29.2. HRMS calcd for $C_{17}H_{17}N_2O_2^+$ $[M+H]^+$: 281.1285; found 281.1286.



4d

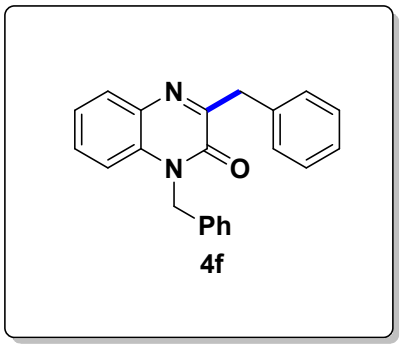
6, 7-Dichloro-1-methyl-3-(4-methylbenzyl)quinoxalin-2(1*H*)-one (4d). Eluent petroleum ether/ethyl acetate (5:1). White solid, 32 mg, 48% yield. ^1H NMR ($CDCl_3$, 500 MHz, ppm) δ 7.92 (s, 1H), 7.36 – 7.29 (m, 3H), 7.11 (d, *J* = 7.8 Hz, 2H), 4.19 (s, 2H), 3.60 (s, 3H), 2.30 (s, 3H). ^{13}C NMR ($CDCl_3$, 125 MHz, ppm) δ 161.0, 154.1, 136.4, 133.8, 133.2, 132.7, 131.8, 130.8, 129.4, 129.2, 127.3, 115.0, 40.3, 29.3, 21.1. HRMS calcd for $C_{17}H_{15}C_{l2}N_2O^+$ $[M+H]^+$: 333.0556; found 333.0551.



4e

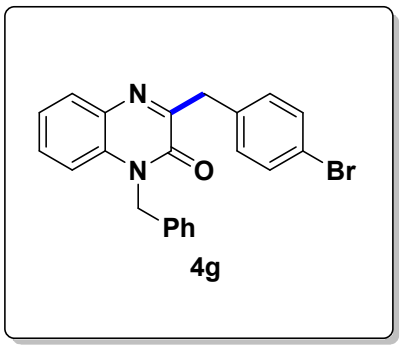
3-Benzyl-6-chloro-1-methylquinoxalin-2(1*H*)-one (4e)[8]. Eluent petroleum ether/ethyl acetate (5:1). White solid, 44 mg, 76% yield. ^1H NMR ($CDCl_3$, 500 MHz, ppm) δ 7.83 (d, *J* = 2.3 Hz, 1H), 7.49 – 7.43 (m, 3H), 7.29 (t, *J* = 7.6 Hz, 2H), 7.21 (t, *J* = 7.3 Hz, 1H), 7.17 (d, *J* = 8.9 Hz, 1H), 4.24 (s, 2H), 3.63 (s, 3H). ^{13}C NMR ($CDCl_3$,

125 MHz, ppm) δ 160.7, 154.4, 136.6, 133.3, 132.0, 129.8, 129.6, 129.3, 128.9, 128.4, 126.7, 114.7, 40.7, 29.3. HRMS calcd for $C_{16}H_{14}ClN_2O^+$ $[M+H]^+$: 285.0789; found 285.0793.



4f

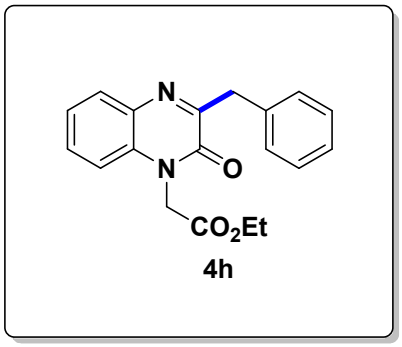
1, 3-Dibenzylquinoxalin-2(1*H*)-one (4f)[8]. Eluent petroleum ether/ethyl acetate (5:1). White solid, 59 mg, 90% yield. ^{1}H NMR ($CDCl_3$, 500 MHz, ppm) δ 7.84 (d, *J* = 8.0 Hz, 1H), 7.48 (d, *J* = 7.6 Hz, 2H), 7.36 (t, *J* = 7.8 Hz, 1H), 7.31 – 7.25 (m, 4H), 7.23-7.21 (m, 2H), 7.19 (s, 1H), 7.17 (d, *J* = 7.0 Hz, 3H), 5.43 (s, 2H), 4.32 (s, 2H). ^{13}C NMR ($CDCl_3$, 125 MHz, ppm) δ 159.4, 154.8, 137.1, 135.2, 133.0, 132.6, 130.0, 129.8, 129.5, 128.9, 128.4, 127.6, 126.8, 126.6, 123.6, 114.3, 45.9, 40.7. HRMS calcd for $C_{22}H_{19}N_2O^+$ $[M+H]^+$: 327.1492; found 327.1493.



4g

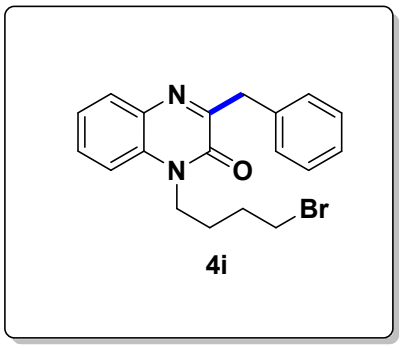
1-Benzyl-3-(4-bromobenzyl)quinoxalin-2(1*H*)-one (4g). Eluent petroleum ether/ethyl acetate (5:1). Yellow solid, 50 mg, 62% yield. ^{1}H NMR ($CDCl_3$, 500 MHz, ppm) δ 7.84 (d, *J* = 7.9 Hz, 1H), 7.44-7.35 (m, 5H), 7.30 (t, *J* = 6.9 Hz, 3H), 7.25 (d, *J*

= 5.3 Hz, 1H), 7.22 (d, *J* = 8.4 Hz, 1H), 7.19 (d, *J* = 7.3 Hz, 2H), 5.46 (s, 2H), 4.27 (s, 2H). ^{13}C NMR ($CDCl_3$, 125 MHz, ppm) δ158.8, 154.7, 136.0, 135.1, 133.0, 132.6, 131.5, 131.3, 130.1, 130.0, 128.9, 127.7, 126.8, 123.7, 120.6, 114.4, 46.0, 40.1. HRMS calcd for $C_{22}H_{18}BrN_2O^+$ $[M+H]^+$: 405.0597; found 405.0589.



4h

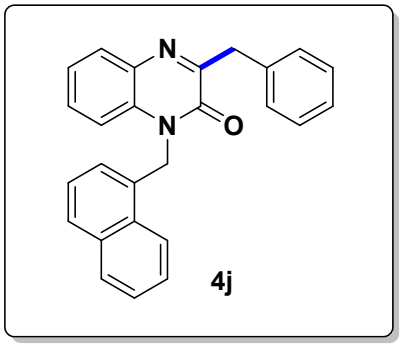
Ethyl 2-(3-benzyl-2-oxoquinoxalin-1(2*H*)-yl)acetate (4h)[8]. Eluent petroleum ether/ethyl acetate (5:1). White solid, 48 mg, 75% yield. ^{1}H NMR ($CDCl_3$, 500 MHz, ppm) δ 7.87 (d, *J* = 8.0 Hz, 1H), 7.50-7.44 (m, 3H), 7.35-7.28 (m, 3H), 7.21 (t, *J* = 7.3 Hz, 1H), 7.03 (d, *J* = 8.3 Hz, 1H), 4.98 (s, 2H), 4.28 (s, 2H), 4.22 (q, *J* = 7.1 Hz, 2H), 1.24 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR ($CDCl_3$, 125 MHz, ppm) δ 167.0, 159.1, 154.3, 136.8, 132.8, 132.4, 130.3, 130.0, 129.5, 128.4, 126.6, 123.8, 113.0, 62.0, 43.6, 40.6, 14.0. HRMS calcd for $C_{19}H_{19}N_2O_3^+$ $[M+H]^+$: 323.1390; found 323.1399.



4i

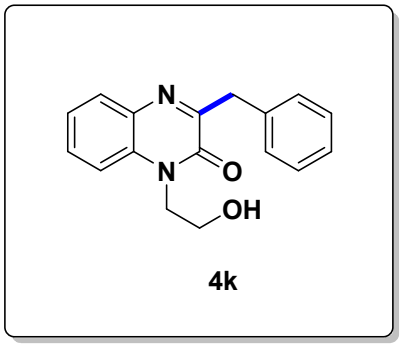
3-Benzyl-1-(4-bromobutyl)quinoxalin-2(1*H*)-one. (4i) Eluent petroleum ether/ethyl acetate (5:1). Yellow oil, 62 mg, 83% yield. ^{1}H NMR ($CDCl_3$, 500 MHz, ppm) δ 7.78

(d, J = 8.0 Hz, 1H), 7.46 – 7.41 (m, 1H), 7.38 (d, J = 7.5 Hz, 2H), 7.27 – 7.19 (m, 4H), 7.13 (t, J = 7.4 Hz, 1H), 4.20 – 4.15 (m, 4H), 3.37 (t, J = 6.2 Hz, 2H), 1.94 – 1.81 (m, 4H). ^{13}C NMR ($CDCl_3$, 125 MHz, ppm) δ 159.2, 154.4, 137.0, 133.0, 132.3, 130.3, 129.9, 129.5, 128.4, 126.5, 123.5, 113.4, 41.2, 40.6, 32.8, 29.7, 25.8. HRMS calcd for $C_{19}H_{20}BrN_2O^+$ $[M+H]^+$: 371.0754; found 371.0752.



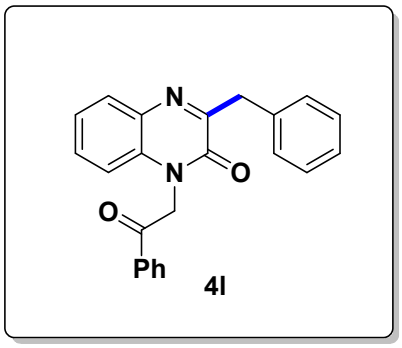
4j

3-Benzyl-1-(naphthalen-1-ylmethyl)quinoxalin-2(1*H*)-one (4j). Eluent petroleum ether/ethyl acetate (4:1). White oil, 55 mg, 80% yield. ^{1}H NMR ($CDCl_3$, 500 MHz, ppm) δ 8.05 (d, J = 8.3 Hz, 1H), 7.90-7.88 (m, 2H), 7.73 (d, J = 8.2 Hz, 1H), 7.60-7.57 (m, 1H), 7.54 (t, J = 7.3 Hz, 1H), 7.49 (d, J = 7.4 Hz, 2H), 7.33 – 7.25 (m, 4H), 7.23 – 7.20 (m, 2H), 6.97-6.94 (m, 1H), 6.71 (d, J = 7.1 Hz, 1H), 5.89 (s, 2H), 4.34 (s, 2H). ^{13}C NMR ($CDCl_3$, 125 MHz, ppm) δ 159.4, 154.9, 137.0, 133.8, 133.0, 132.8, 130.5, 130.0, 129.9, 129.6, 129.3, 129.1, 128.4, 128.0, 126.7, 126.6, 126.0, 125.4, 123.7, 122.4, 122.1, 114.6, 43.8, 40.8. HRMS calcd for $C_{26}H_{21}N_2O^+$ $[M+H]^+$: 377.1648; found 377.1647.



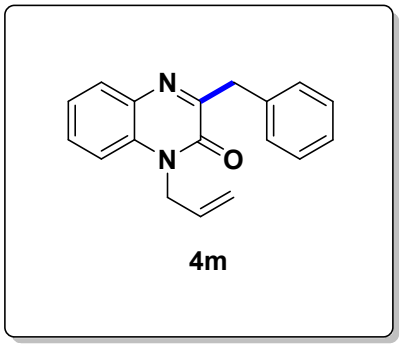
4k

3-Benzyl-1-(2-hydroxyethyl)quinoxalin-2(1*H*)-one (4k)[8]. Eluent petroleum ether/ethyl acetate (3:1). White solid, 48 mg, 85% yield. ^{1}H NMR ($CDCl_3$, 500 MHz, ppm) δ 7.82 (d, *J* = 7.9 Hz, 1H), 7.47 (t, *J* = 7.7 Hz, 1H), 7.40 (d, *J* = 7.5 Hz, 2H), 7.36 (d, *J* = 8.4 Hz, 1H), 7.29 (t, *J* = 7.6 Hz, 1H), 7.25 (t, *J* = 7.3 Hz, 2H), 7.16 (t, *J* = 7.3 Hz, 1H), 4.39 (t, *J* = 5.4 Hz, 2H), 4.20 (s, 2H), 3.95 (t, *J* = 5.3 Hz, 2H), 2.75 (s, 1H). ^{13}C NMR ($CDCl_3$, 125 MHz, ppm) δ 159.0, 155.5, 136.9, 133.0, 132.7, 130.2, 129.9, 129.5, 128.4, 126.6, 123.8, 113.8, 60.3, 44.9, 40.5. HRMS calcd for $C_{17}H_{17}N_2O_2^+$ $[M+H]^+$: 281.1285; found 281.1289.



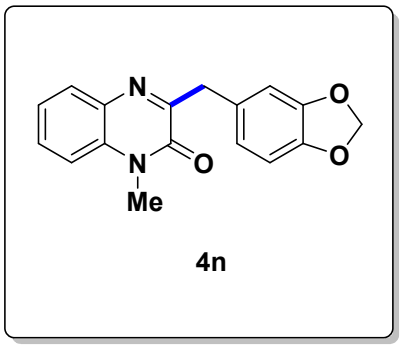
4l

3-Benzyl-1-(2-oxo-2-phenylethyl)quinoxalin-2(1*H*)-one (4l)[8]. Eluent petroleum ether/ethyl acetate (5:1). White solid, 62 mg, 88% yield. ^{1}H NMR ($CDCl_3$, 500 MHz, ppm) δ 8.03 (d, *J* = 7.5 Hz, 2H), 7.88 (d, *J* = 7.7 Hz, 1H), 7.65 (t, *J* = 7.4 Hz, 1H), 7.52 (t, *J* = 7.7 Hz, 2H), 7.46 (d, *J* = 7.4 Hz, 2H), 7.42-7.39 (m, 1H), 7.32-7.26 (m, 3H), 7.22 (t, *J* = 7.3 Hz, 1H), 6.91 (d, *J* = 8.3 Hz, 1H), 5.68 (s, 2H), 4.29 (s, 2H). ^{13}C NMR ($CDCl_3$, 125 MHz, ppm) δ 191.1, 158.9, 154.5, 136.9, 134.5, 134.2, 132.9, 132.7, 130.2, 129.9, 129.5, 129.0, 128.4, 128.1, 126.6, 123.7, 113.4, 48.5, 40.6. HRMS calcd for $C_{23}H_{19}N_2O_2^+$ $[M+H]^+$: 355.1441; found 355.1442.



4m

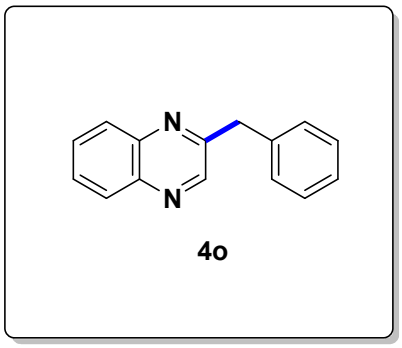
1-Allyl-3-benzylquinoxalin-2(1*H*)-one (4m)[8]. Eluent petroleum ether/ethyl acetate (5:1). White solid, 38 mg, 68% yield. ^{1}H NMR ($CDCl_3$, 500 MHz, ppm) δ 7.84 (d, *J* = 8.3 Hz, 1H), 7.47-7.44 (m, 3H), 7.31-7.26 (m, 3H), 7.23-7.18 (m, 2H), 5.92-5.85 (m, 1H), 5.22 (d, *J* = 10.4 Hz, 1H), 5.12 (d, *J* = 17.3 Hz, 1H), 4.84 (d, *J* = 5.0 Hz, 2H), 4.26 (s, 2H). ^{13}C NMR ($CDCl_3$, 125 MHz, ppm) δ 159.3, 154.3, 137.0, 132.9, 132.5, 130.6, 130.0, 129.7, 129.5, 128.4, 126.5, 123.5, 118.1, 114.1, 44.5, 40.6. HRMS calcd for $C_{18}H_{17}N_2O^+$ $[M+H]^+$: 277.1335; found 277.1340.



4n

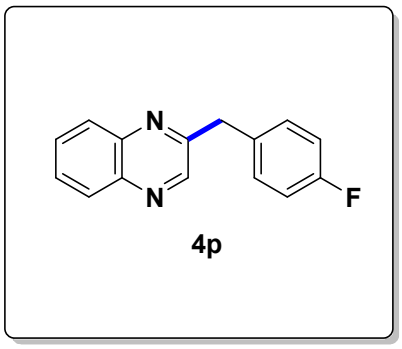
3-(Benzo[*d*][1,3]dioxol-5-ylmethyl)-1-methylquinoxalin-2(1*H*)-one (4n). Eluent petroleum ether/ethyl acetate (5:1). White solid, 48 mg, 82% yield. ^{1}H NMR ($CDCl_3$, 500 MHz, ppm) δ 7.85 (d, *J* = 7.6 Hz, 1H), 7.51 (d, *J* = 7.6 Hz, 1H), 7.33 (t, *J* = 7.6 Hz, 1H), 7.27 (d, *J* = 7.5 Hz, 1H), 6.96 (d, *J* = 0.9 Hz, 1H), 6.92 (d, *J* = 7.8 Hz, 1H), 6.73 (d, *J* = 8.0 Hz, 1H), 5.89 (s, 2H), 4.17 (s, 2H), 3.66 (s, 3H). ^{13}C NMR ($CDCl_3$, 125 MHz, ppm) δ 159.2, 154.7, 147.5, 146.3, 133.3, 132.7, 130.6, 129.9, 129.9, 123.6,

122.5, 113.5, 110.0, 108.2, 100.8, 40.3, 29.1. HRMS calcd for $C_{17}H_{15}N_2O_3^+$ $[M+H]^+$: 295.1077; found 298.1082.



4o

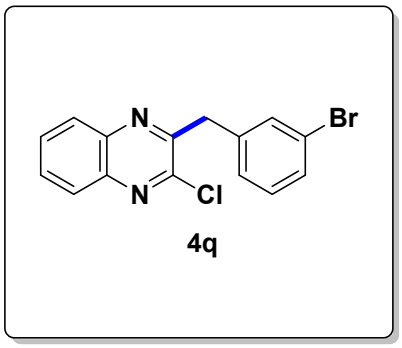
2-Benzylquinoxaline (4o)[11]. Eluent petroleum ether/ethyl acetate (20:1). Yellow oil, 27 mg, 61% yield. ^{1}H NMR ($CDCl_3$, 500 MHz, ppm) δ 8.72 (s, 1H), 8.10 – 8.04 (m, 2H), 7.77-7.70 (m, 2H), 7.35 – 7.30 (m, 4H), 7.26 – 7.21 (m, 1H), 4.38 (s, 2H). ^{13}C NMR ($CDCl_3$, 500 MHz, ppm) δ 155.8, 145.9, 142.1, 141.2, 137.9, 130.1, 129.3, 129.2, 129.1, 129.0, 128.9, 126.9, 43.0. HRMS calcd for $C_{15}H_{13}N_2^+$ $[M+H]^+$: 221.1073; found 221.1081.



4p

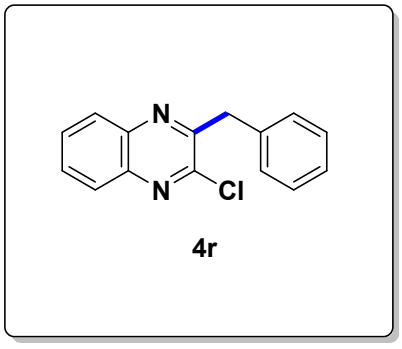
2-(4-Fluorobenzyl)quinoxaline (4p). Eluent petroleum ether/ethyl acetate (20:1). White solid, 31 mg, 65% yield. ($CDCl_3$, 500 MHz, ppm) δ 8.70 (s, 1H), 8.07 (d, J = 8.2 Hz, 2H), 7.77-7.70 (m, 2H), 7.30-7.27 (m, 2H), 7.03 – 6.98 (m, 2H), 4.34 (s, 2H). ^{13}C NMR ($CDCl_3$, 500 MHz, ppm) δ 162.8, 160.9, 155.5, 145.7, 142.0, 141.2, 133.6,

133.5, 130.6, 130.5, 130.1, 129.3, 129.2, 129.0, 115.7, 115.6, 42.1. HRMS calcd for $C_{15}H_{12}FN_2^+$ $[M+H]^+$: 239.0979; found 239.0990.



4q

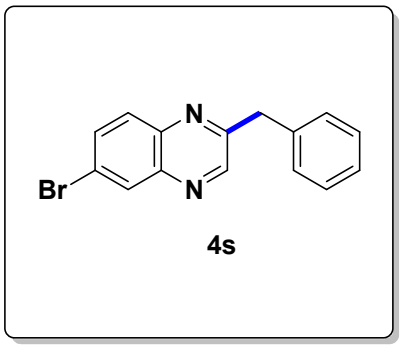
2-(3-Bromobenzyl)-3-chloroquinoxaline (4q). Eluent petroleum ether/ethyl acetate (15:1). Yellow solid, 30 mg, 45% yield. ^{1}H NMR ($CDCl_3$, 500 MHz, ppm) δ 8.14 – 8.12 (m, 1H), 8.06 – 7.99 (m, 1H), 7.82 – 7.78(m, 2H), 7.54 (s, 1H), 7.41 (d, *J* = 7.8 Hz, 1H), 7.31 (d, *J* = 7.7 Hz, 1H), 7.20 (t, *J* = 7.8 Hz, 1H), 4.50 (s, 2H). ^{13}C NMR ($CDCl_3$, 500 MHz, ppm) δ 153.3, 147.4, 141.2, 141.0, 138.9, 132.2, 130.6, 130.3, 130.1, 130.0, 128.9, 128.1, 127.9, 122.6, 41.5. HRMS calcd for $C_{15}H_{11}BrClN_2^+$ $[M+H]^+$: 332.9789; found 332.9796.



4r

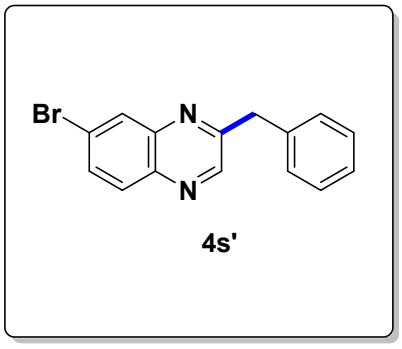
2-Benzyl-3-chloroquinoxaline (4r)[12]. Eluent petroleum ether/ethyl acetate (15:1). Brown solid, 30 mg, 58% yield. ^{1}H NMR ($CDCl_3$, 500 MHz, ppm) δ 8.10 – 8.08 (m, 1H), 7.80 – 7.98 (m, 1H), 7.78 – 7.72 (m, 2H), 7.36 (d, *J* = 7.5 Hz, 2H), 7.30 (t, *J* = 7.5 Hz, 2H), 7.23 (t, *J* = 7.3 Hz, 1H), 4.51 (s, 2H). ^{13}C NMR ($CDCl_3$, 500 MHz, ppm)

δ 154.1, 147.7, 141.1, 141.0, 136.6, 130.3, 130.1, 129.2, 128.9, 128.5, 128.1, 126.8, 42.0. HRMS calcd for $C_{15}H_{12}ClN_2^+$ $[M+H]^+$: 255.0684; found 255.0695.



4s

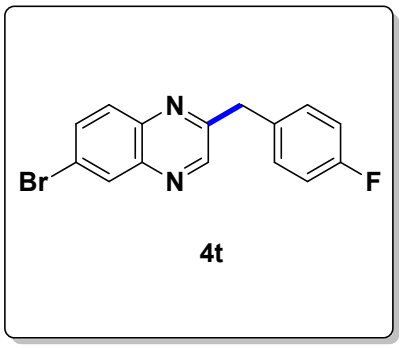
2-Benzyl-6-bromoquinoxaline (4s). Eluent petroleum ether/ethyl acetate (15:1). White solid, 26 mg, 44% yield. ^{1}H NMR ($CDCl_3$, 500 MHz, ppm) δ 8.70 (s, 1H), 8.24 (d, *J* = 2.0 Hz, 1H), 7.94 (d, *J* = 8.9 Hz, 1H), 7.83 – 7.81 (m, 1H), 7.39 – 7.30 (m, 4H), 7.27 – 7.23 (m, 1H), 4.35 (s, 2H). ^{13}C NMR ($CDCl_3$, 500 MHz, ppm) δ 156.2, 146.7, 141.8, 140.8, 137.5, 133.6, 131.5, 130.4, 129.1, 128.9, 127.0, 123.1, 42.9. HRMS calcd for $C_{15}H_{12}BrN_2^+$ $[M+H]^+$: 299.0178; found 299.0186.



4s'

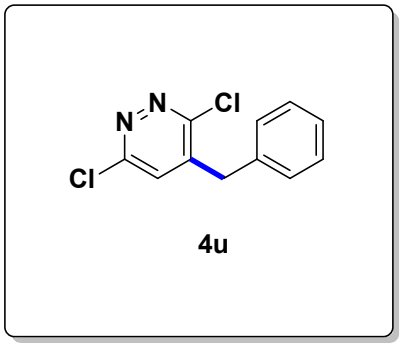
2-Benzyl-7-bromoquinoxaline (4s'). Eluent petroleum ether/ethyl acetate (20:1). White solid, 22 mg, 36% yield. ^{1}H NMR ($CDCl_3$, 500 MHz, ppm) δ 8.71 (s, 1H), 8.26 (d, *J* = 1.9 Hz, 1H), 7.92 (d, *J* = 8.9 Hz, 1H), 7.80 – 7.77 (m, 1H), 7.33 – 7.29 (m, 4H), 7.27 – 7.24 (m, 1H), 4.36 (s, 2H). ^{13}C NMR ($CDCl_3$, 125 MHz, ppm) δ 156.8, 146.2,

142.7, 140.0, 137.5, 132.8, 131.5, 130.5, 129.1, 128.9, 127.0, 124.1, 43.0. HRMS calcd for $C_{15}H_{12}BrN_2^+$ $[M+H]^+$: 299.0178; found 299.0187.



4t

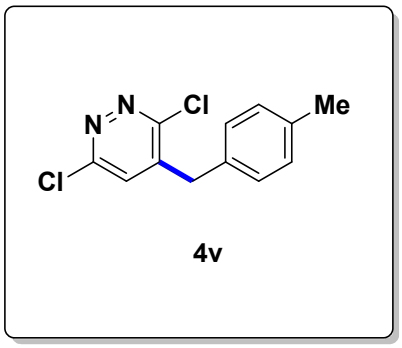
6-Bromo-2-(4-fluorobenzyl)quinoxaline (4t). Eluent petroleum ether/ethyl acetate (2:1). White solid, 24 mg, 38% yield. ^{1}H NMR ($CDCl_3$, 500 MHz, ppm) δ 8.69 (s, 1H), 8.25 (d, *J* = 2.1 Hz, 1H), 7.93 (d, *J* = 8.9 Hz, 1H), 7.84 – 7.82 (m, 1H), 7.29 – 7.26 (m, 2H), 7.01 (t, *J* = 8.6 Hz, 2H), 4.32 (s, 2H). ^{13}C NMR ($CDCl_3$, 125 MHz, ppm) δ 162.9, 161.0, 155.9, 146.5, 141.8, 140.8, 133.7, 133.3, 133.2, 131.5, 130.7, 130.6, 130.4, 123.2, 115.9, 115.7, 42.0. HRMS calcd for $C_{15}H_{11}BrFN_2^+$ $[M+H]^+$: 317.0084; found 317.0089.



4u

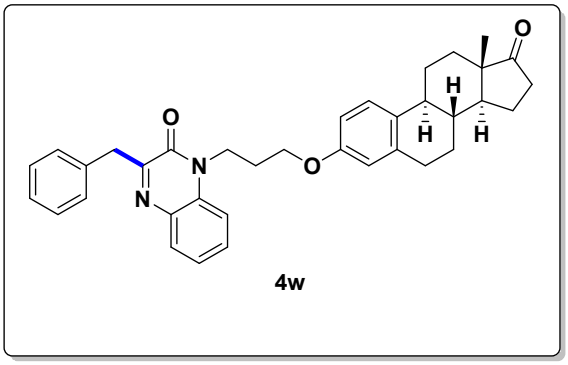
4-Benzyl-3,6-dichloropyridazine (4u)[11]. Eluent petroleum ether/ethyl acetate (8:1). Yellow oil, 16 mg, 33% yield. ^{1}H NMR ($CDCl_3$, 500 MHz, ppm) δ 7.40 (t, *J* = 7.3 Hz, 2H), 7.35 (d, *J* = 7.2 Hz, 1H), 7.19 (d, *J* = 7.3 Hz, 2H), 7.08 (s, 1H), 4.05 (s, 2H). ^{13}C

NMR ($CDCl_3$, 500 MHz, ppm) δ 156.8, 156.1, 143.6, 134.5, 129.5, 129.3, 127.8, 38.2. HRMS calcd for $C_{11}H_9C_{l2}N_2^+$ $[M+H]^+$: 239.0137; found 239.0148.



4v

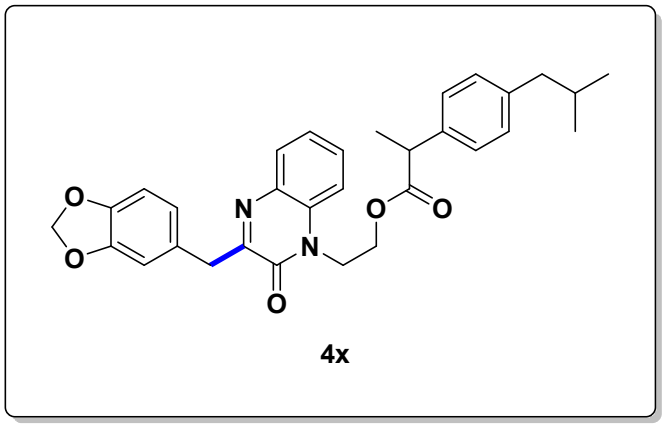
3,6-Dichloro-4-(4-methylbenzyl)pyridazine (4v). Eluent petroleum ether/ethyl acetate (8:1). Colorless oil, 18 mg, 35% yield. ^1H NMR ($CDCl_3$, 500 MHz, ppm) δ 7.20 (d, J = 7.8 Hz, 2H), 7.07 (d, J = 7.5 Hz, 3H), 4.01 (s, 2H), 2.37 (s, 3H). ^{13}C NMR ($CDCl_3$, 500 MHz, ppm) δ 156.8, 156.1, 143.9, 137.6, 131.4, 130.0, 129.5, 129.2, 37.8, 21.1. HRMS calcd for $C_{12}H_{11}C_{l2}N_2^+$ $[M+H]^+$: 253.0294; found 253.0302.



4w

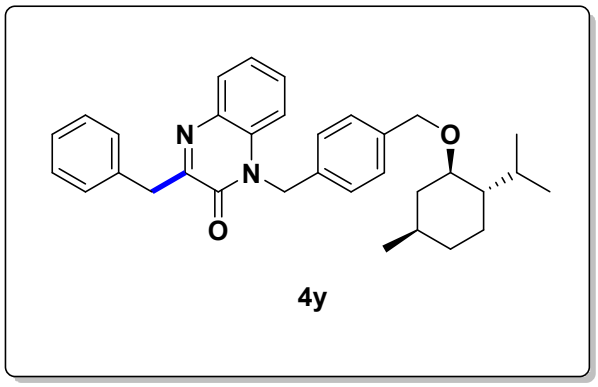
3-Benzyl-1-(3-(((8*R*,9*S*,13*S*,14*S*)-13-methyl-17-oxo-7,8,9,11,12,13,14,15,16,17-decahydro-6*H*-cyclopenta[*a*]phenanthren-2-yl)oxy)propyl)quinoxalin-2(1*H*)-one (4w). Eluent petroleum ether/ethyl acetate (5:1). White soild, 82 mg, 75% yield. ^1H NMR ($CDCl_3$, 500 MHz, ppm) δ 7.87 (dd, J = 8.1, 0.8 Hz, 1H), 7.51 – 7.41 (m, 4H), 7.33-7.28 (m, 3H), 7.23-7.20 (m, 2H), 6.71 (dd, J = 8.5, 2.4 Hz, 1H), 6.65 (d, J = 2.2 Hz, 1H), 4.45 – 4.39 (m, 2H), 4.27 (s, 2H), 4.04 (t, J = 5.7 Hz, 2H), 2.92-2.88 (m, 2H),

2.54-2.48 (m, 1H), 2.40 (d, J = 10.4 Hz, 1H), 2.28-2.22 (m, 2H), 2.14 (d, J = 9.8 Hz, 1H), 2.09 – 1.95 (m, 3H), 1.69 – 1.39 (m, 7H), 0.92 (s, 3H). ^{13}C NMR ($CDCl_3$, 125 MHz, ppm) δ 220.8, 159.2, 156.6, 154.5, 137.8, 137.1, 133.0, 132.5, 132.4, 130.1, 129.9, 129.5, 128.4, 126.5, 126.4, 123.5, 114.6, 113.6, 112.2, 65.2, 50.4, 48.0, 44.0, 40.6, 39.8, 38.3, 35.8, 31.6, 29.7, 29.6, 27.2, 26.5, 25.9, 21.6, 13.8. HRMS calcd for $C_{36}H_{39}N_2O_3^+$ $[M+H]^+$: 547.2955; found 547.2960.



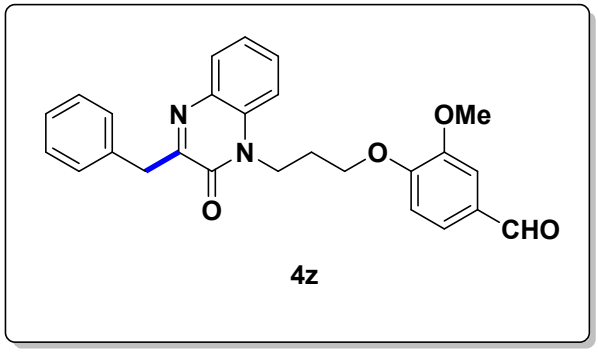
4x

2-(3-(Benzo[*d*][1,3]dioxol-5-ylmethyl)-2-oxoquinoxalin-1(2*H*)-yl)ethyl 2-(4-isobutylphenyl)propanoate. (4x). Eluent petroleum ether/ethyl acetate (3:1). yellow oil, 80 mg, 78% yield. ^{1}H NMR ($CDCl_3$, 500 MHz, ppm) δ 7.84 (d, J = 8.1 Hz, 1H), 7.46-7.43 (m, 1H), 7.32 (t, J = 7.9 Hz, 2H), 7.05 (q, J = 8.1 Hz, 4H), 6.96 (s, 1H), 6.93 – 6.88 (m, 1H), 6.73 (d, J = 8.0 Hz, 1H), 5.88 (s, 2H), 4.52 – 4.32 (m, 4H), 4.16 (d, J = 8.2 Hz, 2H), 3.53 (q, J = 7.1 Hz, 1H), 2.43 (d, J = 7.2 Hz, 2H), 1.88 – 1.79 (m, 1H), 1.39 (d, J = 7.2 Hz, 3H), 0.89 (d, J = 6.5 Hz, 6H). ^{13}C NMR ($CDCl_3$, 125 MHz, ppm) δ 174.7, 159.0, 154.5, 147.5, 146.3, 140.6, 137.2, 132.9, 132.8, 130.5, 130.1, 129.9, 129.3, 127.0, 123.6, 122.5, 113.7, 110.0, 108.2, 100.8, 60.9, 45.0, 44.9, 40.8, 40.2, 30.1, 22.4, 18.3. HRMS calcd for $C_{31}H_{33}N_2O_5^+$ $[M+H]^+$: 513.2384; found 513.2388.



4y

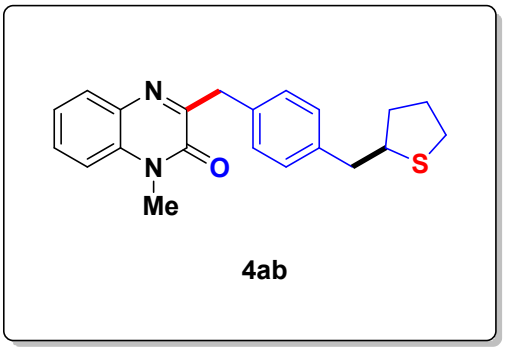
3-Benzyl-1-(4-((((1*R*,2*S*,5*R*)-2-isopropyl-5-methylcyclohexyl)oxy)methyl)benzyl)quinoxalin-2(1*H*)-one (4y). Eluent petroleum ether/ethyl acetate (5:1). Yellow oil, 84 mg, 85% yield. ^{1}H NMR ($CDCl_3$, 500 MHz, ppm) δ 7.82 (d, *J* = 7.9 Hz, 1H), 7.47 (d, *J* = 7.4 Hz, 2H), 7.35 – 7.20 (m, 7H), 7.15 (t, *J* = 8.7 Hz, 3H), 5.42 (s, 2H), 4.58 (d, *J* = 11.5 Hz, 1H), 4.32 (d, *J* = 8.0 Hz, 3H), 3.14-3.09 (m, 1H), 2.24-2.21 (m, 1H), 2.13 (d, *J* = 11.9 Hz, 1H), 1.64-1.57 (m, 2H), 1.27-1.22 (m, 2H), 0.97-0.79 (m, 9H), 0.65 (d, *J* = 6.8 Hz, 3H). ^{13}C NMR ($CDCl_3$, 125 MHz, ppm) δ 159.4, 154.8, 138.6, 137.1, 134.3, 133.0, 132.6, 130.0, 129.8, 129.5, 128.4, 128.3, 126.8, 126.5, 123.5, 114.4, 78.8, 69.9, 48.2, 45.7, 40.7, 40.2, 34.5, 31.5, 25.5, 23.2, 22.3, 21.0, 16.00.HRMS calcd for $C_{33}H_{39}N_2O_2^+$ $[M+H]^+$: 495.3006; found 495.3008.



4z

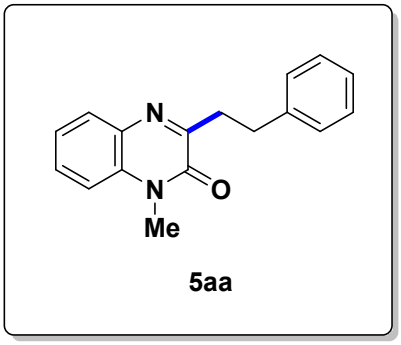
4-(3-(3-Benzyl-2-oxoquinoxalin-1(2*H*)-yl)propoxy)-3-methoxybenzaldehyde (4z)[8]. Eluent petroleum ether/ethyl acetate (5:1). White solid, 75 mg, 88% yield. ^{1}H NMR

($CDCl_3$, 500 MHz, ppm) δ 9.84 (s, 1H), 8.00 (d, *J* = 8.0 Hz, 1H), 7.76 (d, *J* = 8.1 Hz, 1H), 7.60 (t, *J* = 7.4 Hz, 1H), 7.54 (t, *J* = 7.4 Hz, 1H), 7.40 (d, *J* = 7.2 Hz, 2H), 7.29 (d, *J* = 7.4 Hz, 2H), 7.21 (t, *J* = 7.4 Hz, 2H), 7.15 (t, *J* = 7.1 Hz, 1H), 6.80 (d, *J* = 8.4 Hz, 1H), 4.65 (t, *J* = 5.9 Hz, 2H), 4.31 (s, 2H), 4.05 (t, *J* = 6.4 Hz, 2H), 3.90 (s, 3H), 2.39-2.34 (m, 2H). ^{13}C NMR ($CDCl_3$, 125 MHz, ppm) δ 190.8, 155.8, 153.8, 149.8, 149.1, 140.0, 138.6, 137.6, 130.1, 129.2, 128.9, 128.5, 128.4, 126.7, 126.5, 126.5, 111.6, 109.3, 65.7, 63.0, 55.9, 40.3, 28.5. HRMS calcd for $C_{26}H_{25}N_2O_4^+$ $[M+H]^+$: 429.1809; found 429.1809.



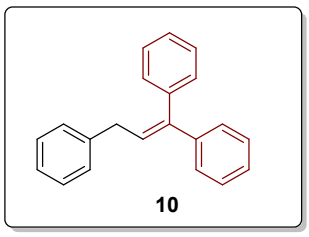
4ab

(*R*)-1-Methyl-3-(4-((tetrahydrothiophen-2-yl)methyl)benzyl)quinoxalin-2(1*H*)-one (4ab). Eluent petroleum ether/ethyl acetate (5:1). White solid, 62 mg, 88% yield. ^1H NMR ($CDCl_3$, 500 MHz, ppm) δ 7.84 (dd, *J* = 7.7, 0.8 Hz, 1H), 7.53 – 7.49 (m, 1H), 7.41 (d, *J* = 8.0 Hz, 2H), 7.32 (t, *J* = 7.5 Hz, 1H), 7.27 – 7.24 (m, 3H), 4.23 (s, 2H), 3.80 (dd, *J* = 11.6, 2.1 Hz, 1H), 3.65 (s, 3H), 2.87 – 2.81 (m, 1H), 2.63 (d, *J* = 13.3 Hz, 1H), 2.10 – 1.86 (m, 4H), 1.67 – 1.61 (m, 1H), 1.49 – 1.41 (m, 1H). ^{13}C NMR ($CDCl_3$, 125 MHz, ppm) δ 159.2, 154.7, 141.1, 135.9, 133.3, 132.8, 129.9, 129.8, 129.7, 127.5, 123.54, 113.5, 47.1, 40.4, 35.1, 30.8, 29.1, 27.0, 26.7. HRMS calcd for $C_{21}H_{23}N_2OS^+$ $[M+H]^+$: 351.1526; found 351.1524.



5aa

1-Methyl-3-phenethylquinoxalin-2(1*H*)-one (5aa)[8]. Eluent petroleum ether/ethyl acetate (5:1). White solid, 25 mg, 57% yield. ^{1}H NMR ($CDCl_3$, 500 MHz, ppm) δ 7.86 (d, *J* = 7.9 Hz, 1H), 7.54 (t, *J* = 7.8 Hz, 1H), 7.37 – 7.28 (m, 6H), 7.18 (d, *J* = 7.2 Hz, 1H), 3.71 (s, 3H), 3.30 – 3.25 (m, 2H), 3.16 – 3.11 (m, 2H). ^{13}C NMR ($CDCl_3$, 500 MHz, ppm) δ 160.1, 154.9, 141.6, 133.1, 132.7, 129.7, 129.7, 128.6, 128.3, 125.9, 123.57, 113.6, 35.9, 32.5, 29.0. HRMS calcd for $C_{17}H_{17}N_2O^+$ $[M+H]^+$: 265.1335; found 265.1349.



10

Prop-1-ene-1, 1, 3-triyltribenzene (10)[7]. Eluent petroleum ether. Colorless oil, 35 mg, 64% yield. ^{1}H NMR ($CDCl_3$, 500 MHz, ppm) δ 7.42 (t, *J* = 7.4 Hz, 2H), 7.39-7.24 (m, 10H), 7.25-7.21(m, 3H), 6.30 (t, *J* = 7.6 Hz, 1H), 3.50 (d, *J* = 7.6 Hz, 2H). ^{13}C NMR ($CDCl_3$, 125 MHz, ppm) δ 142.5, 142.4, 141.0, 139.8, 129.9, 128.5, 128.4, 128.3, 128.1, 127.8, 127.3, 127.1, 127.0, 126.0, 35.9. HRMS (ESI) calcd for $C_{21}H_{19}^+$ $[M+H]^+$: 271.1481, found: 271.1478.

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VI. X-ray Crystallography Data of 4k.

Crystal preparation of compound 4k.

Compound **4k** (20 mg) was dissolved in $CHCl_3$ (3 mL), and it was crystallized to give crystal as colorless prisms after the solvent was slowly volatilized in 3 days at room temperature (~ 25 °C). All diffraction data were obtained on a Bruker Smart Apex CCD diffractometer equipped with graphite-monochromated Mo Kα radiation. X-ray crystallographic data for **4k** is available as Figure S12. X-ray crystallographic data in CIF format are available from the Cambridge Crystallographic Data Centre (http://www.ccdc.cam.ac.uk/).

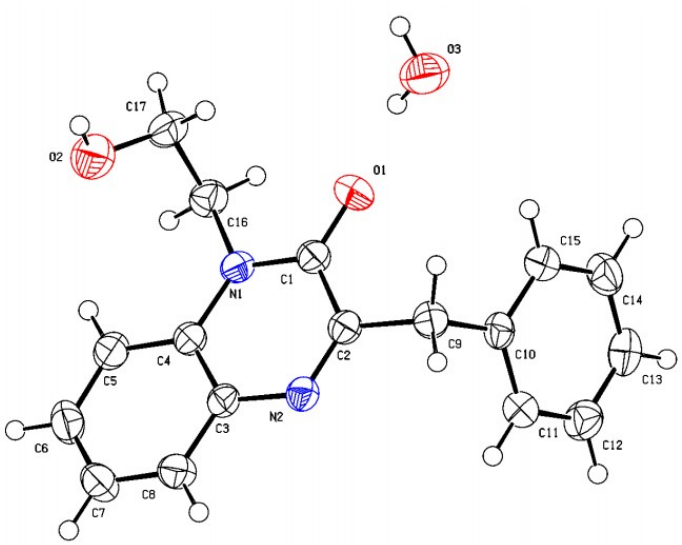


Figure S12 X-ray crystallography of **4k**.

Table 1. Crystal data and structure refinement for 210830c.

CCDC number	2107239
Empirical formula	C17 H18 N2 O3
Formula weight	298.33
Temperature	298(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P2(1)/n
Unit cell dimensions	a = 9.5217(9) A alpha = 90 deg. b = 16.1081(16) A beta = 104.665(4) deg. c = 9.6233(8) A gamma = 90 deg.
Volume	1427.9(2) A^3
Z, Calculated density	4, 1.388 Mg/m^3
Absorption coefficient	0.096 mm^-1
F(000)	632
Crystal size	0.30 x 0.21 x 0.18 mm
Theta range for data collection	2.53 to 25.01 deg.
Limiting indices	-11<=h<=11, -19<=k<=10, -11<=l<=11
Reflections collected / unique	7006 / 2519 [R(int) = 0.0359]
Completeness to theta = 25.01	99.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9829 and 0.9717
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2519 / 0 / 200
Goodness-of-fit on F^2	1.016
Final R indices [I>2sigma(I)]	R1 = 0.0407, wR2 = 0.0985
R indices (all data)	R1 = 0.0626, wR2 = 0.1080
Largest diff. peak and hole	0.174 and -0.166 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for 210830c. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
N(1)	5848(1)	885(1)	3605(1)	31(1)
N(2)	5194(1)	1813(1)	5781(1)	31(1)
O(1)	8059(1)	1473(1)	4162(1)	45(1)
O(2)	4682(1)	1005(1)	474(2)	56(1)
O(3)	9691(2)	2784(1)	3530(2)	61(1)
C(1)	6860(2)	1407(1)	4395(2)	32(1)
C(2)	6454(2)	1862(1)	5548(2)	30(1)
C(3)	4163(2)	1310(1)	4911(2)	30(1)
C(4)	4466(2)	827(1)	3829(2)	30(1)
C(5)	3389(2)	319(1)	3031(2)	37(1)
C(6)	2050(2)	305(1)	3295(2)	43(1)
C(7)	1735(2)	801(1)	4336(2)	45(1)
C(8)	2784(2)	1296(1)	5134(2)	39(1)
C(9)	7577(2)	2403(1)	6491(2)	35(1)
C(10)	8715(2)	1921(1)	7549(2)	32(1)
C(11)	8421(2)	1604(1)	8770(2)	38(1)
C(12)	9453(2)	1164(1)	9747(2)	44(1)
C(13)	10790(2)	1033(1)	9507(2)	44(1)
C(14)	11094(2)	1348(1)	8315(2)	46(1)
C(15)	10070(2)	1793(1)	7337(2)	40(1)
C(16)	6287(2)	398(1)	2507(2)	38(1)
C(17)	6138(2)	860(1)	1137(2)	43(1)

Table 3. Bond lengths [A] and angles [deg] for 210830c.

N(1)-C(1)	1.358(2)
N(1)-C(4)	1.389(2)
N(1)-C(16)	1.459(2)
N(2)-C(2)	1.2773(19)
N(2)-C(3)	1.380(2)
O(1)-C(1)	1.2220(19)
O(2)-C(17)	1.391(2)
O(2)-H(2)	0.8200
O(3)-H(3C)	0.8501
O(3)-H(3D)	0.8500
C(1)-C(2)	1.462(2)
C(2)-C(9)	1.495(2)
C(3)-C(8)	1.383(2)
C(3)-C(4)	1.387(2)
C(4)-C(5)	1.383(2)
C(5)-C(6)	1.362(2)
C(5)-H(5)	0.9300
C(6)-C(7)	1.372(3)
C(6)-H(6)	0.9300
C(7)-C(8)	1.355(3)
C(7)-H(7)	0.9300
C(8)-H(8)	0.9300
C(9)-C(10)	1.501(2)
C(9)-H(9A)	0.9700
C(9)-H(9B)	0.9700
C(10)-C(15)	1.372(2)
C(10)-C(11)	1.374(2)
C(11)-C(12)	1.372(2)
C(11)-H(11)	0.9300
C(12)-C(13)	1.366(3)
C(12)-H(12)	0.9300
C(13)-C(14)	1.351(3)
C(13)-H(13)	0.9300
C(14)-C(15)	1.374(3)
C(14)-H(14)	0.9300
C(15)-H(15)	0.9300
C(16)-C(17)	1.489(2)
C(16)-H(16A)	0.9700
C(16)-H(16B)	0.9700

C(17)-H(17A)	0.9700
C(17)-H(17B)	0.9700
C(1)-N(1)-C(4)	121.41(14)
C(1)-N(1)-C(16)	116.42(14)
C(4)-N(1)-C(16)	122.17(14)
C(2)-N(2)-C(3)	119.02(14)
C(17)-O(2)-H(2)	109.5
H(3C)-O(3)-H(3D)	108.7
O(1)-C(1)-N(1)	121.02(16)
O(1)-C(1)-C(2)	122.33(15)
N(1)-C(1)-C(2)	116.62(14)
N(2)-C(2)-C(1)	122.91(15)
N(2)-C(2)-C(9)	119.26(15)
C(1)-C(2)-C(9)	117.83(14)
N(2)-C(3)-C(8)	118.19(16)
N(2)-C(3)-C(4)	122.25(15)
C(8)-C(3)-C(4)	119.55(15)
C(5)-C(4)-C(3)	118.88(15)
C(5)-C(4)-N(1)	123.50(15)
C(3)-C(4)-N(1)	117.62(14)
C(6)-C(5)-C(4)	120.25(17)
C(6)-C(5)-H(5)	119.9
C(4)-C(5)-H(5)	119.9
C(5)-C(6)-C(7)	120.97(17)
C(5)-C(6)-H(6)	119.5
C(7)-C(6)-H(6)	119.5
C(8)-C(7)-C(6)	119.35(17)
C(8)-C(7)-H(7)	120.3
C(6)-C(7)-H(7)	120.3
C(7)-C(8)-C(3)	120.96(18)
C(7)-C(8)-H(8)	119.5
C(3)-C(8)-H(8)	119.5
C(2)-C(9)-C(10)	113.11(14)
C(2)-C(9)-H(9A)	109.0
C(10)-C(9)-H(9A)	109.0
C(2)-C(9)-H(9B)	109.0
C(10)-C(9)-H(9B)	109.0
H(9A)-C(9)-H(9B)	107.8
C(15)-C(10)-C(11)	118.31(16)
C(15)-C(10)-C(9)	121.38(16)
C(11)-C(10)-C(9)	120.31(15)
C(12)-C(11)-C(10)	120.86(17)
C(12)-C(11)-H(11)	119.6

C(10)-C(11)-H(11)	119.6
C(13)-C(12)-C(11)	120.03(18)
C(13)-C(12)-H(12)	120.0
C(11)-C(12)-H(12)	120.0
C(14)-C(13)-C(12)	119.60(17)
C(14)-C(13)-H(13)	120.2
C(12)-C(13)-H(13)	120.2
C(13)-C(14)-C(15)	120.72(18)
C(13)-C(14)-H(14)	119.6
C(15)-C(14)-H(14)	119.6
C(10)-C(15)-C(14)	120.47(18)
C(10)-C(15)-H(15)	119.8
C(14)-C(15)-H(15)	119.8
N(1)-C(16)-C(17)	113.13(15)
N(1)-C(16)-H(16A)	109.0
C(17)-C(16)-H(16A)	109.0
N(1)-C(16)-H(16B)	109.0
C(17)-C(16)-H(16B)	109.0
H(16A)-C(16)-H(16B)	107.8
O(2)-C(17)-C(16)	110.52(15)
O(2)-C(17)-H(17A)	109.5
C(16)-C(17)-H(17A)	109.5
O(2)-C(17)-H(17B)	109.5
C(16)-C(17)-H(17B)	109.5
H(17A)-C(17)-H(17B)	108.1

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for 210830c. The anisotropic displacement factor exponent takes the form: -2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
N(1)	32(1)	36(1)	26(1)	0(1)	9(1)	1(1)
N(2)	30(1)	35(1)	28(1)	2(1)	5(1)	2(1)
O(1)	32(1)	60(1)	47(1)	-4(1)	17(1)	-5(1)
O(2)	51(1)	68(1)	47(1)	11(1)	8(1)	7(1)
O(3)	76(1)	64(1)	50(1)	-8(1)	27(1)	-21(1)
C(1)	30(1)	37(1)	29(1)	6(1)	7(1)	0(1)
C(2)	30(1)	31(1)	28(1)	6(1)	6(1)	3(1)
C(3)	31(1)	33(1)	26(1)	4(1)	5(1)	-1(1)
C(4)	29(1)	32(1)	27(1)	7(1)	5(1)	1(1)
C(5)	41(1)	40(1)	31(1)	-1(1)	6(1)	-3(1)
C(6)	34(1)	47(1)	44(1)	3(1)	0(1)	-9(1)
C(7)	30(1)	55(1)	49(1)	4(1)	10(1)	-5(1)
C(8)	36(1)	47(1)	38(1)	2(1)	13(1)	2(1)
C(9)	33(1)	36(1)	36(1)	1(1)	7(1)	-1(1)
C(10)	31(1)	31(1)	31(1)	-6(1)	4(1)	-6(1)
C(11)	33(1)	45(1)	37(1)	-2(1)	10(1)	-3(1)
C(12)	49(1)	46(1)	36(1)	7(1)	7(1)	-6(1)
C(13)	41(1)	42(1)	39(1)	0(1)	-5(1)	2(1)
C(14)	29(1)	58(1)	49(1)	-5(1)	6(1)	3(1)
C(15)	34(1)	52(1)	34(1)	2(1)	9(1)	-4(1)
C(16)	39(1)	40(1)	36(1)	-4(1)	11(1)	5(1)
C(17)	46(1)	55(1)	32(1)	-5(1)	13(1)	2(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for 210830c.

	x	y	z	U(eq)
H(2)	4616	1387	-102	84
H(3C)	9168	2363	3581	74
H(3D)	9754	2834	2668	74
H(5)	3580	-14	2311	45
H(6)	1338	-45	2762	52
H(7)	810	797	4493	53
H(8)	2574	1632	5841	47
H(9A)	7103	2782	7012	42
H(9B)	8044	2733	5894	42
H(11)	7512	1688	8937	46
H(12)	9242	955	10572	53
H(13)	11486	728	10161	52
H(14)	12006	1262	8155	55
H(15)	10297	2010	6524	48
H(16A)	5699	-101	2316	45
H(16B)	7290	229	2872	45
H(17A)	6649	1384	1330	52
H(17B)	6572	540	500	52

Table 6. Torsion angles [deg] for 210830c.

C(4)-N(1)-C(1)-O(1)	-177.74(15)
C(16)-N(1)-C(1)-O(1)	1.6(2)
C(4)-N(1)-C(1)-C(2)	3.9(2)
C(16)-N(1)-C(1)-C(2)	-176.74(14)
C(3)-N(2)-C(2)-C(1)	0.0(2)
C(3)-N(2)-C(2)-C(9)	-179.74(14)
O(1)-C(1)-C(2)-N(2)	178.39(16)
N(1)-C(1)-C(2)-N(2)	-3.3(2)
O(1)-C(1)-C(2)-C(9)	-1.9(2)
N(1)-C(1)-C(2)-C(9)	176.41(14)
C(2)-N(2)-C(3)-C(8)	-176.81(15)
C(2)-N(2)-C(3)-C(4)	2.8(2)
N(2)-C(3)-C(4)-C(5)	178.00(15)
C(8)-C(3)-C(4)-C(5)	-2.3(2)
N(2)-C(3)-C(4)-N(1)	-2.2(2)
C(8)-C(3)-C(4)-N(1)	177.49(15)
C(1)-N(1)-C(4)-C(5)	178.42(15)
C(16)-N(1)-C(4)-C(5)	-0.9(2)
C(1)-N(1)-C(4)-C(3)	-1.4(2)
C(16)-N(1)-C(4)-C(3)	179.31(15)
C(3)-C(4)-C(5)-C(6)	1.0(2)
N(1)-C(4)-C(5)-C(6)	-178.88(16)
C(4)-C(5)-C(6)-C(7)	1.0(3)
C(5)-C(6)-C(7)-C(8)	-1.5(3)
C(6)-C(7)-C(8)-C(3)	0.1(3)
N(2)-C(3)-C(8)-C(7)	-178.49(16)
C(4)-C(3)-C(8)-C(7)	1.8(3)
N(2)-C(2)-C(9)-C(10)	104.81(18)
C(1)-C(2)-C(9)-C(10)	-74.91(19)
C(2)-C(9)-C(10)-C(15)	102.70(19)
C(2)-C(9)-C(10)-C(11)	-78.0(2)
C(15)-C(10)-C(11)-C(12)	-0.5(3)
C(9)-C(10)-C(11)-C(12)	-179.85(16)
C(10)-C(11)-C(12)-C(13)	-0.4(3)
C(11)-C(12)-C(13)-C(14)	0.9(3)
C(12)-C(13)-C(14)-C(15)	-0.5(3)
C(11)-C(10)-C(15)-C(14)	1.0(3)
C(9)-C(10)-C(15)-C(14)	-179.74(17)
C(13)-C(14)-C(15)-C(10)	-0.5(3)
C(1)-N(1)-C(16)-C(17)	-83.44(18)
C(4)-N(1)-C(16)-C(17)	95.88(18)

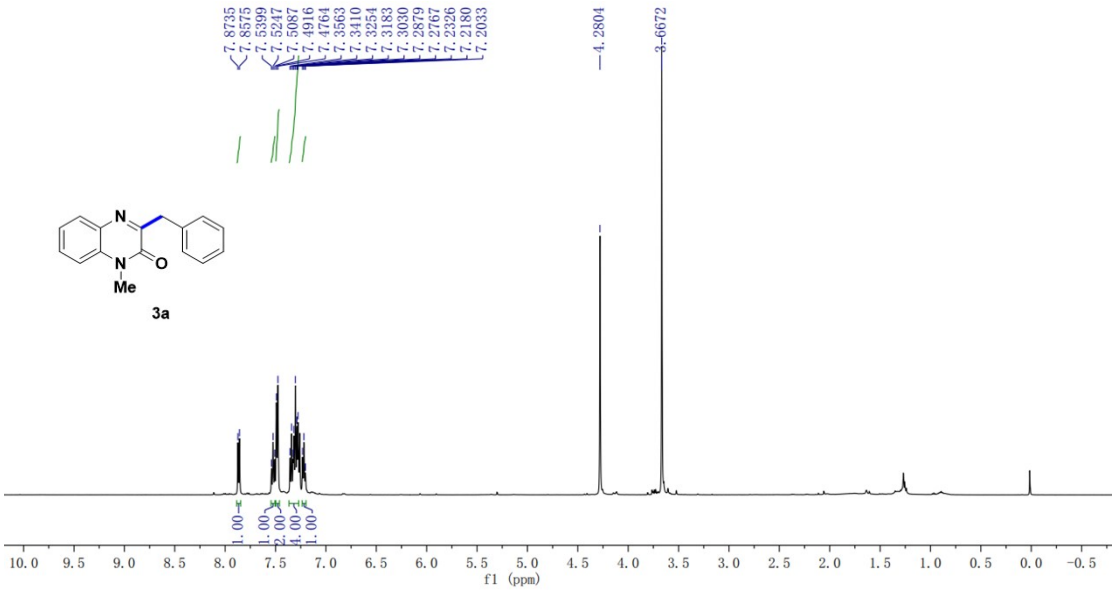
N(1)-C(16)-C(17)-O(2)	-67.4(2)

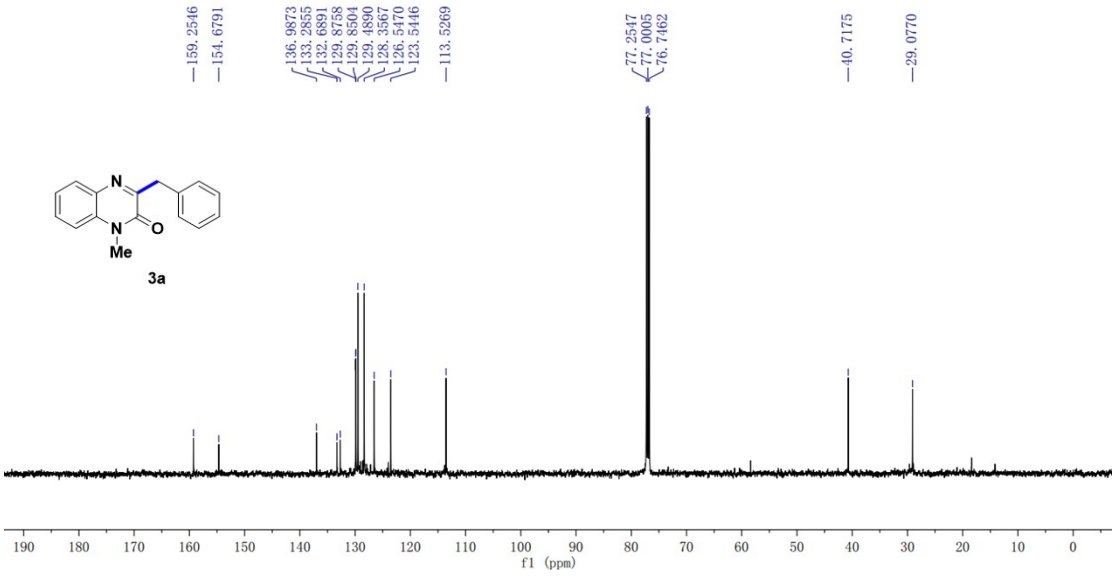
Symmetry transformations used to generate equivalent atoms:

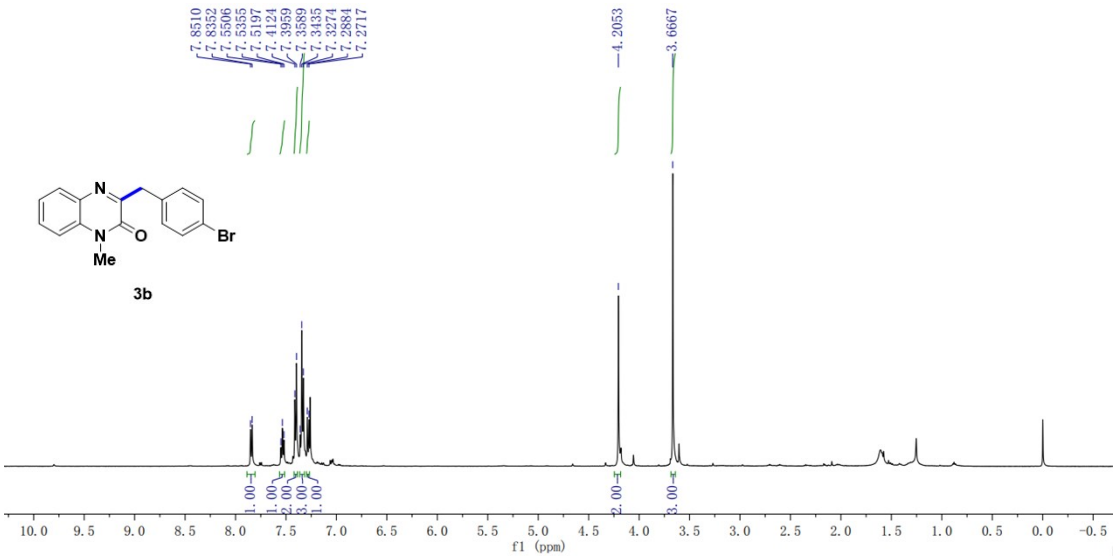
Table 7. Hydrogen bonds for 210830c [A and deg.].

D-H	d(D-H)	d(H..A)	<DHA	d(D..A)	A
O2-H2	0.820	1.890	172.62	2.705	O3 [x-1/2, -y+1/2, z-1/2]
O3-H3C	0.850	1.944	166.74	2.778	O1
O3-H3D	0.850	2.045	166.81	2.879	N2 [x+1/2, -y+1/2, z-1/2]

VII. NMR spectra of the products



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7.2884
7.2717
4.2053
3.6667
N
N
O
Me
Br
3b
1.00
1.00
1.00
2.00
3.00
1.00
2.00
3.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
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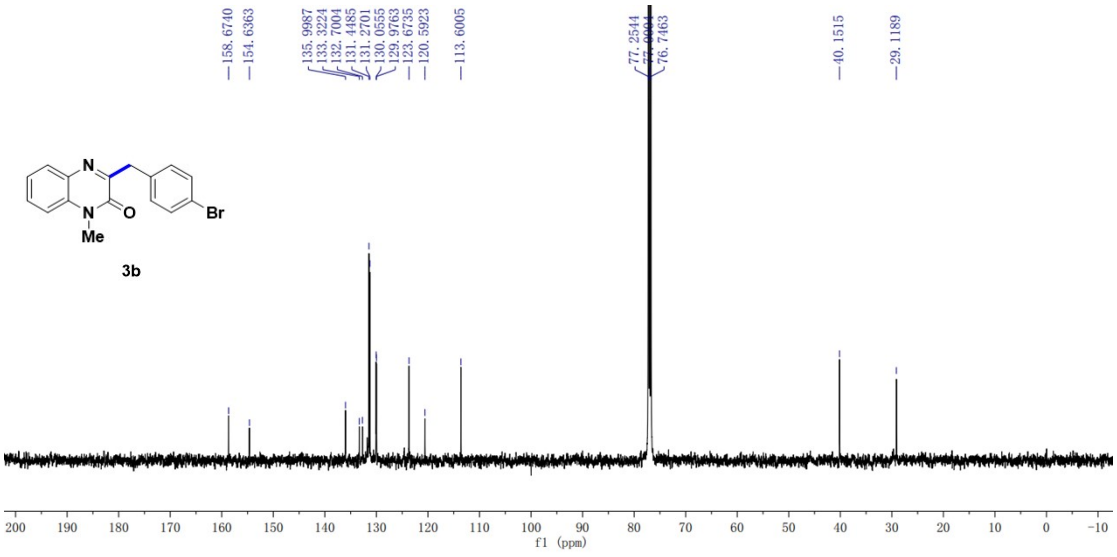
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77.0044
76.7463
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O
Me
Br
3b
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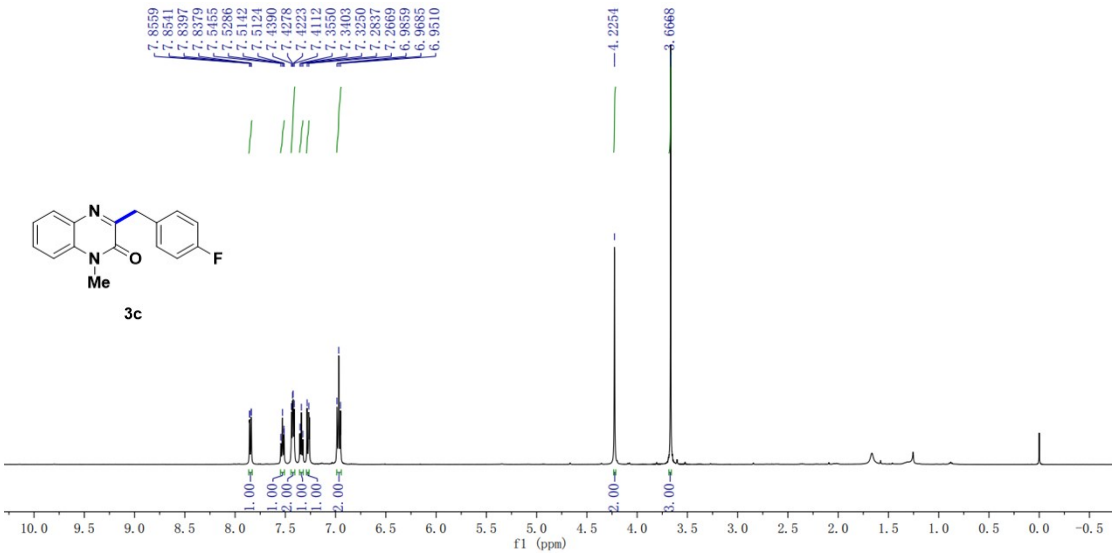
f1 (ppm)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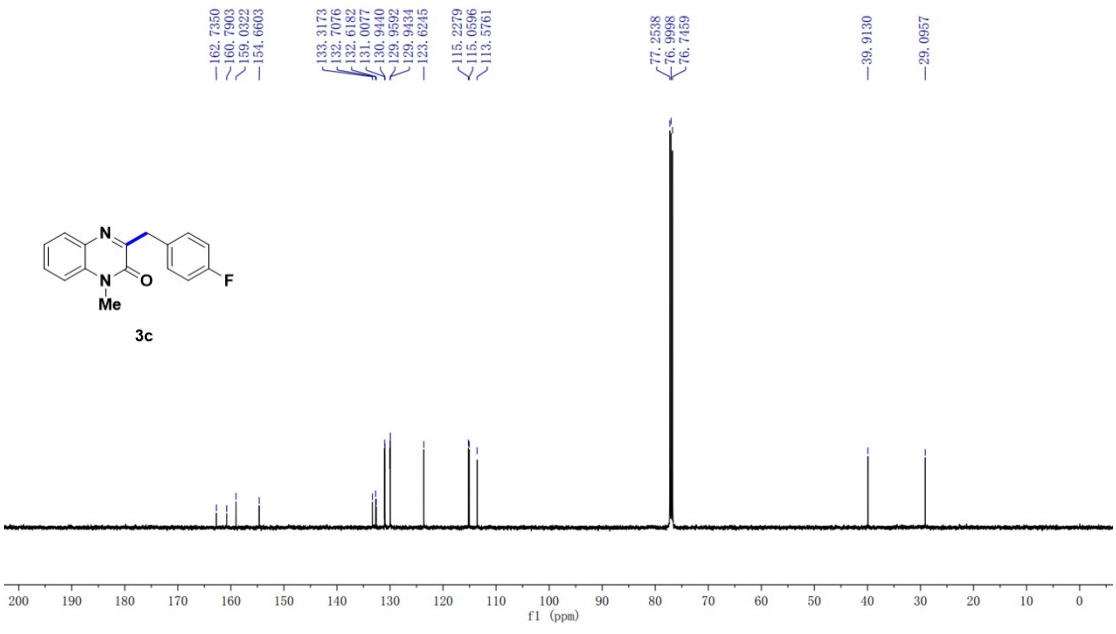
F
3c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129.9434
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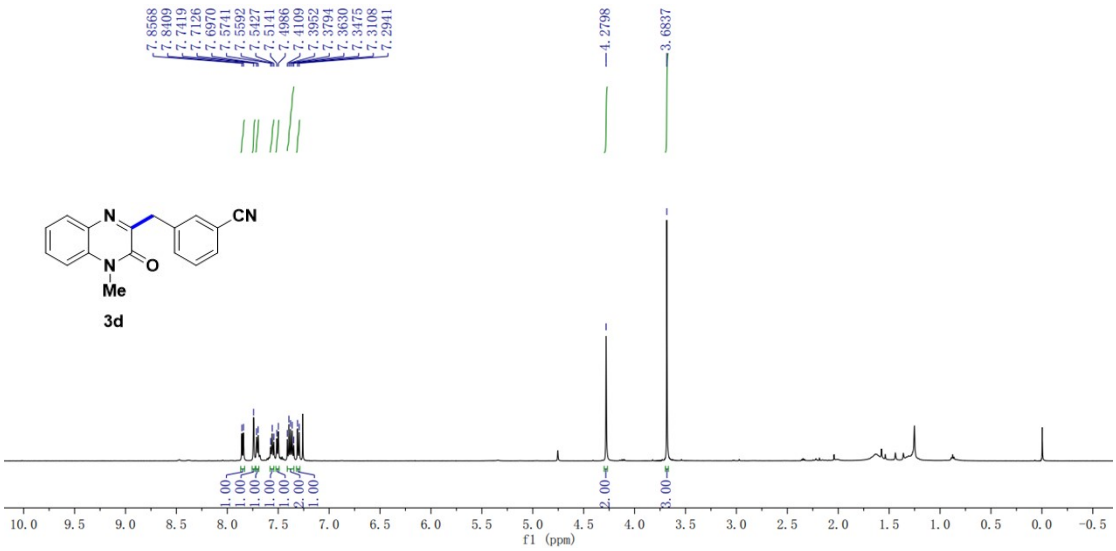
Me
F
3c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O
Me
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1.00
1.00
1.00
2.00
1.00
2.00
3.00
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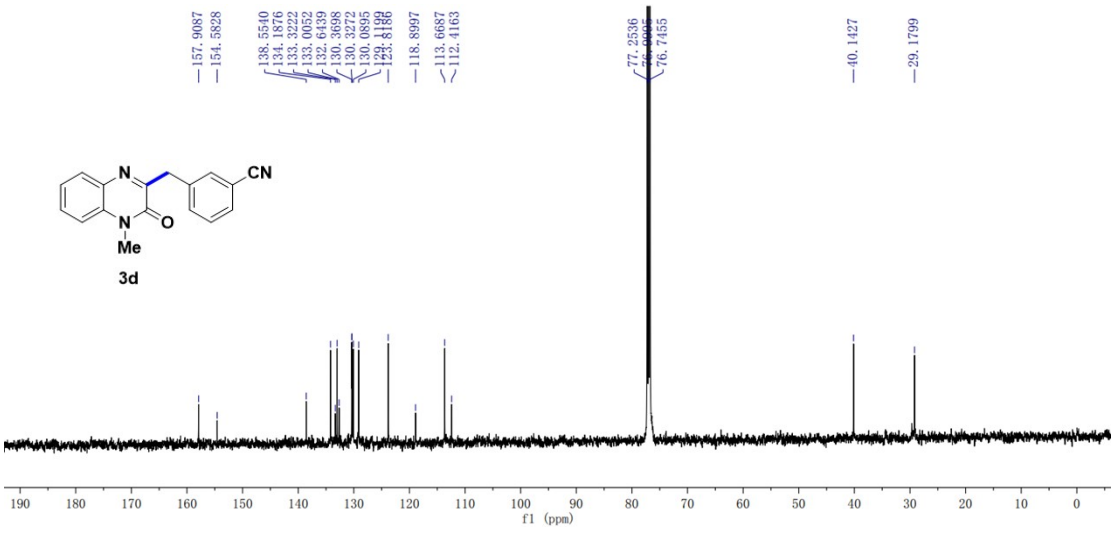
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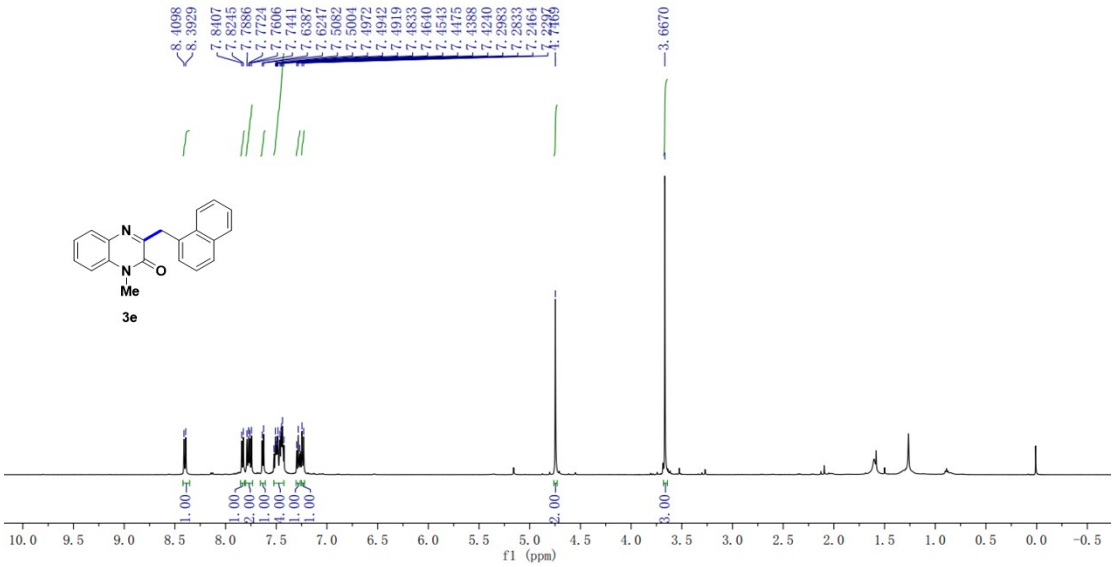
f1 (ppm)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1.00
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2.00
1.00
4.00
1.00
1.00
2.00
3.00
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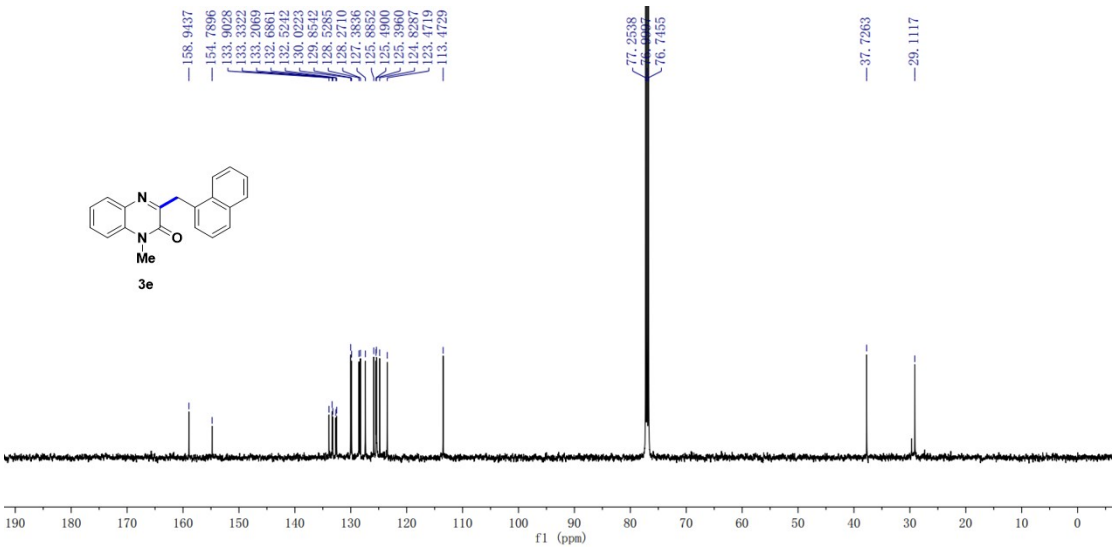
f1 (ppm)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125.3960
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123.4719
113.4729
77.2538
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Me
3e
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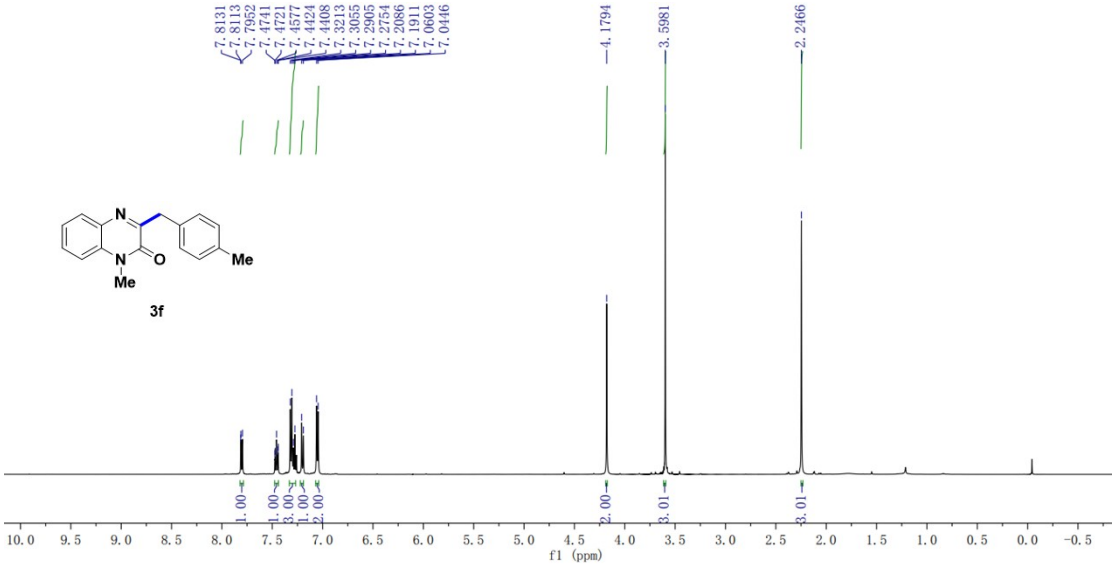
f1 (ppm)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7.2754
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7.0603
7.0446
4.1794
3.5981
2.2466
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N
O
Me
Me
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1.00
3.00
1.00
2.00
2.00
3.01
3.01
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 −0.5
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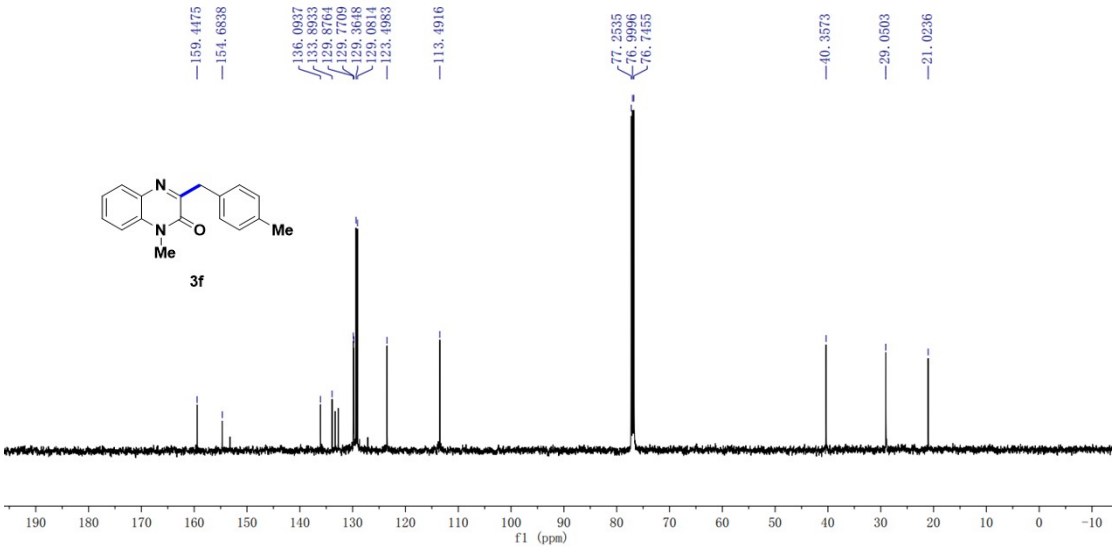
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Me
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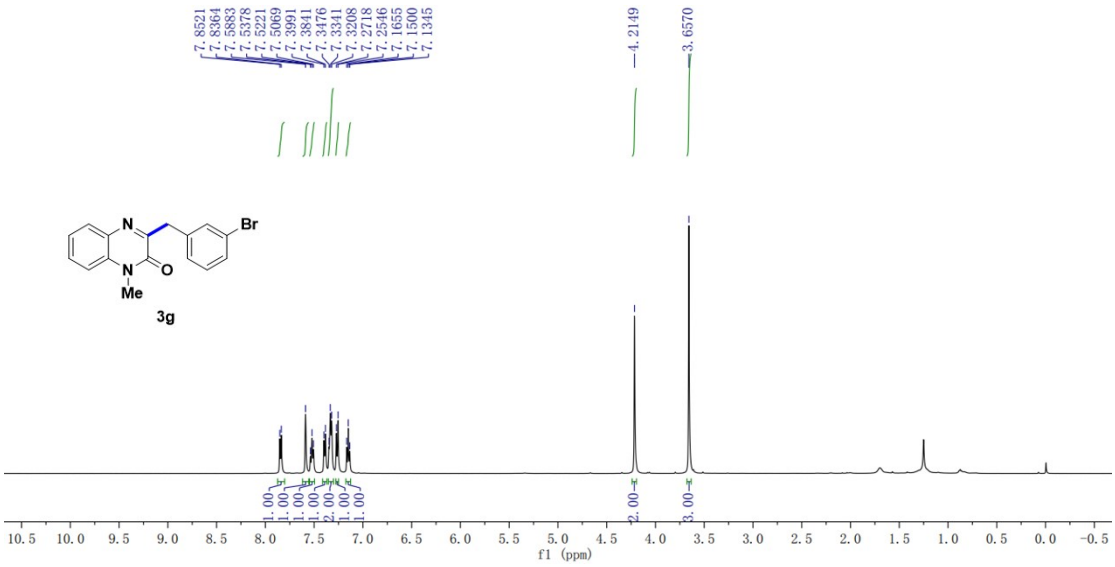
f1 (ppm)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O
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2.00
3.00
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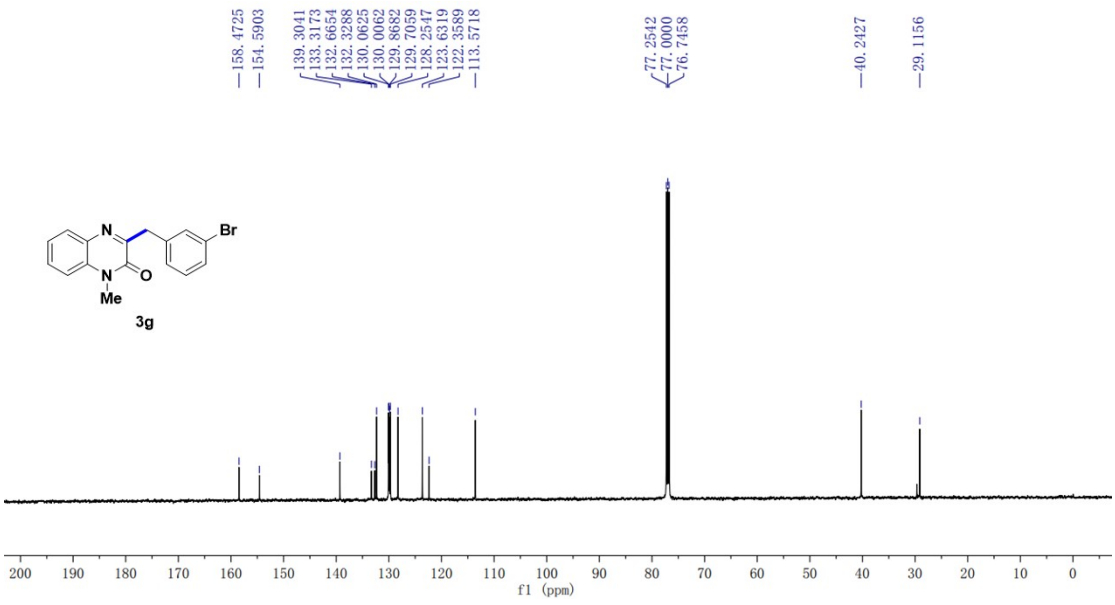
f1 (ppm)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122.3589
113.5718
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N
Me
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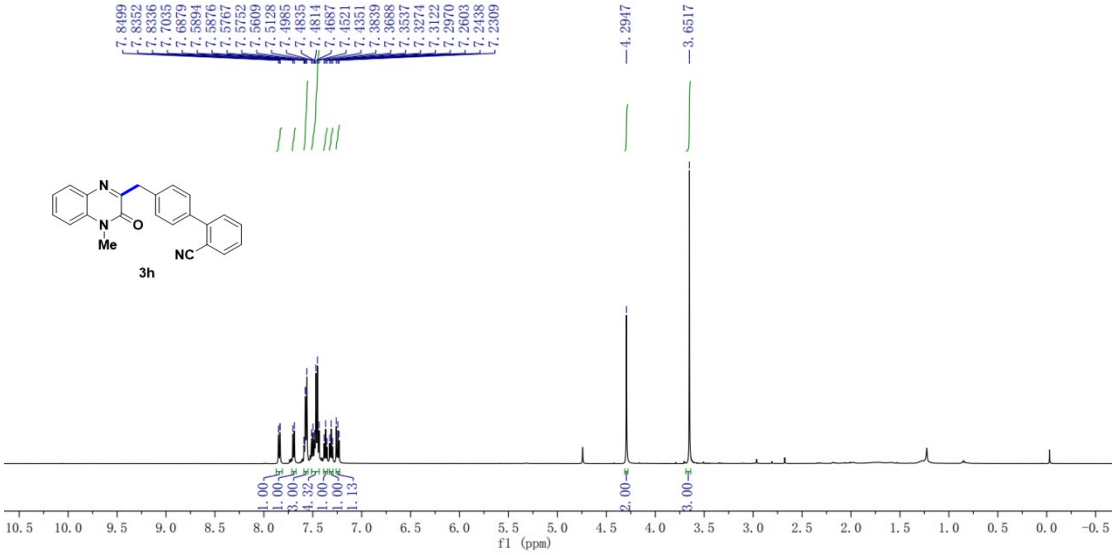
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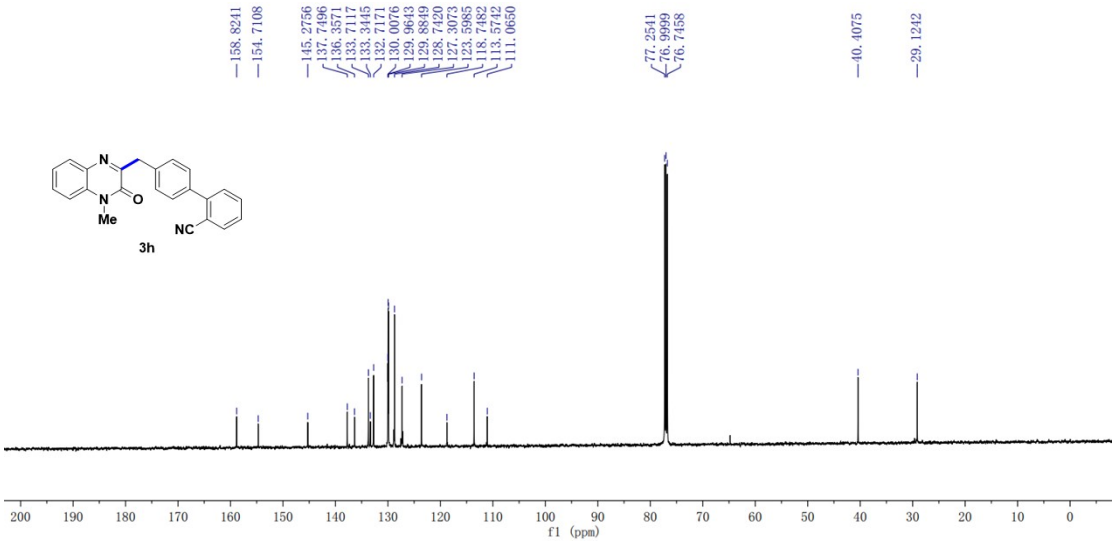
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NC
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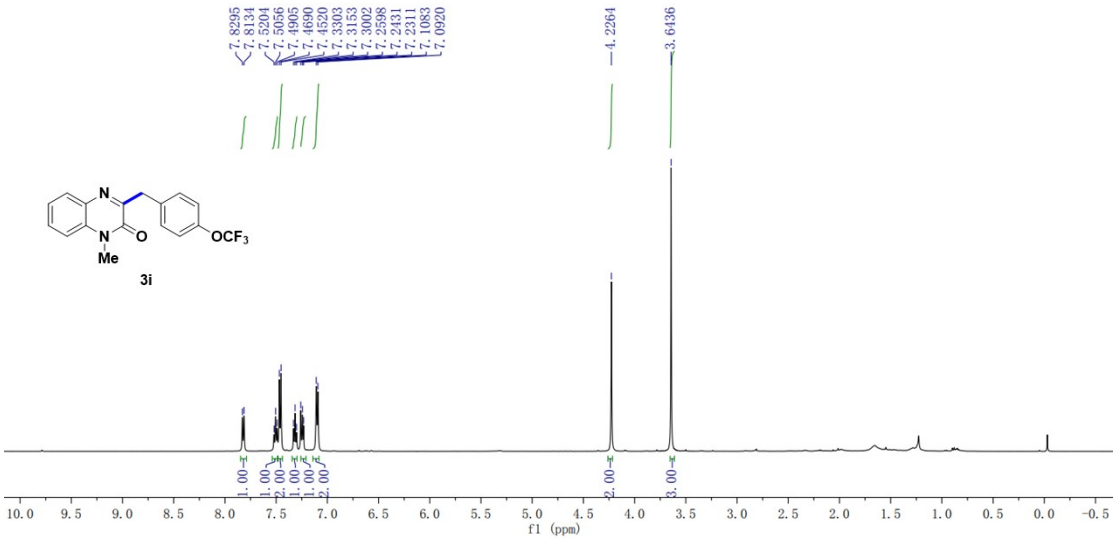
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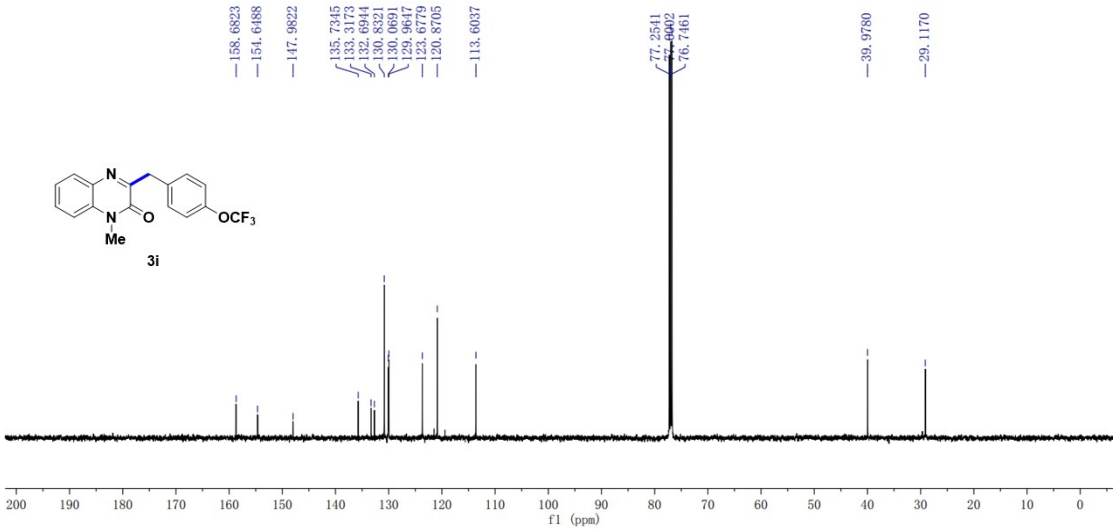
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OCF3
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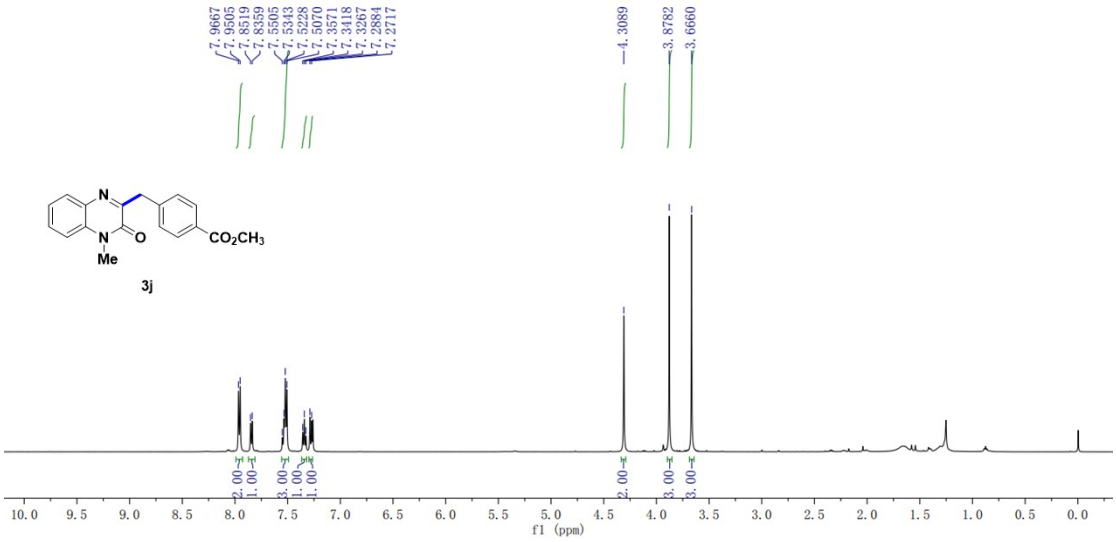
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O
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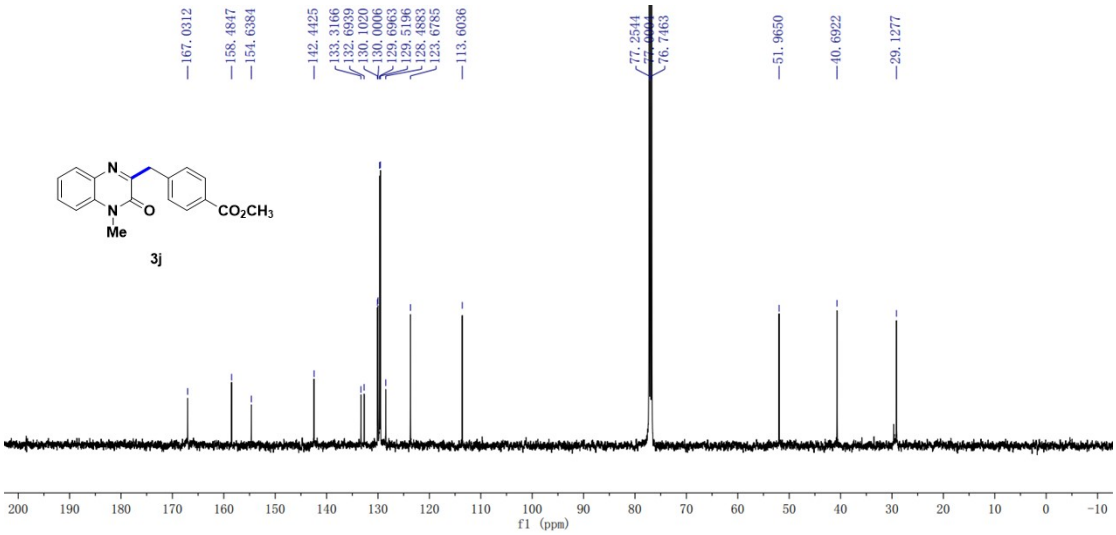
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CO2CH3
3j
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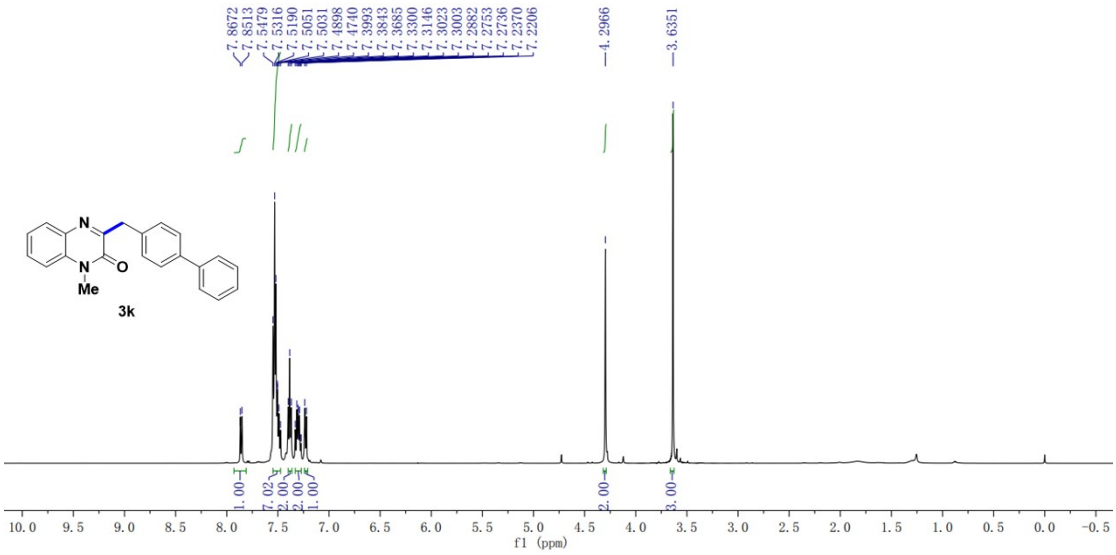
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7.3146
7.3023
7.3003
7.2882
7.2753
7.2736
7.2370
7.2206
4.2966
3.6351
N
O
N
Me
3k
1.00
7.02
2.00
2.00
1.00
2.00
3.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
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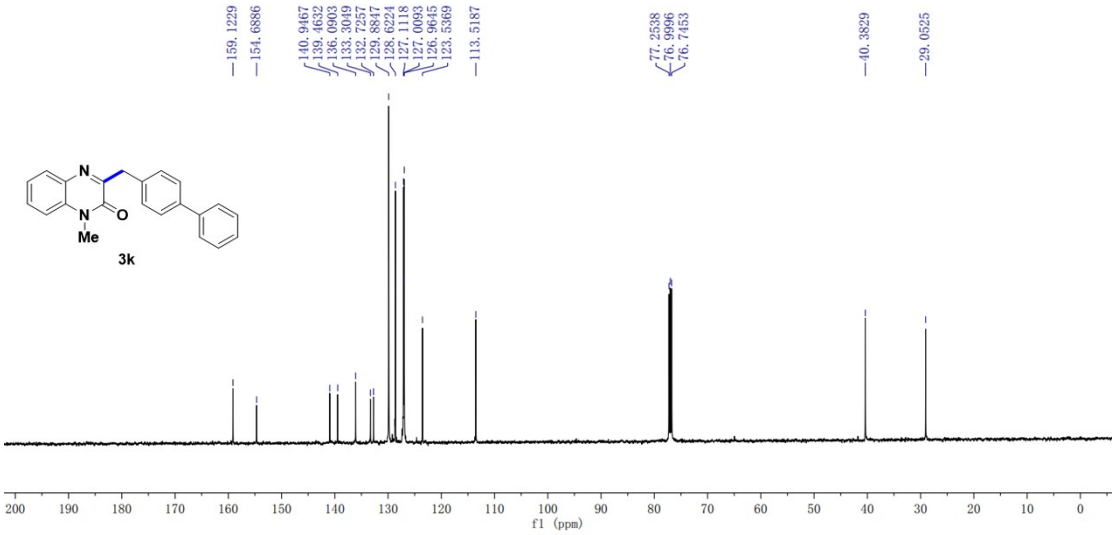
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123.5369
113.5187
77.2538
76.9996
76.7453
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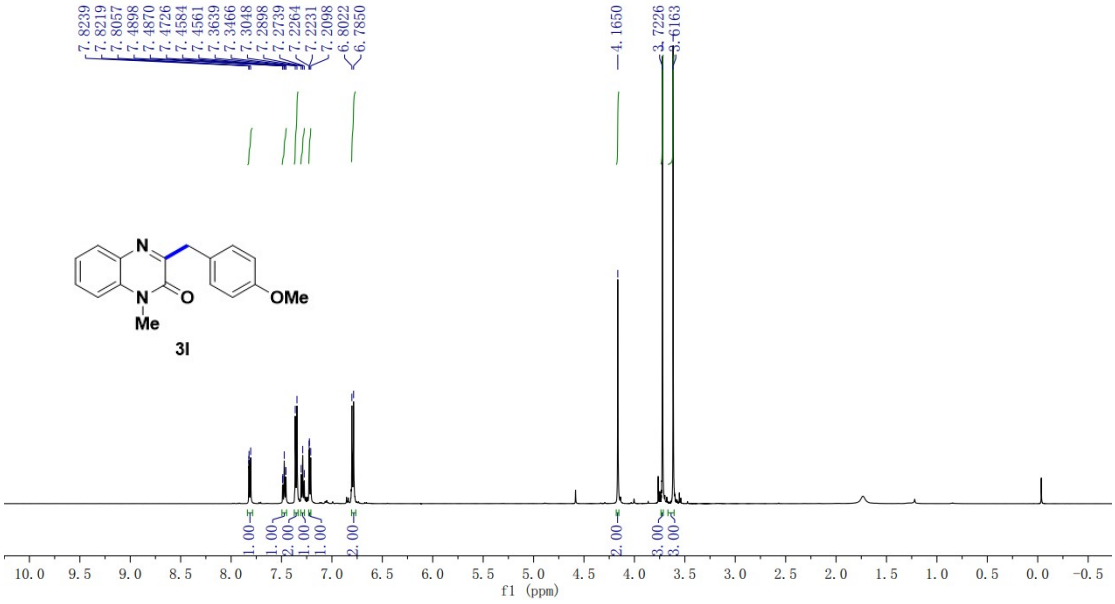
O
N
Me
3k
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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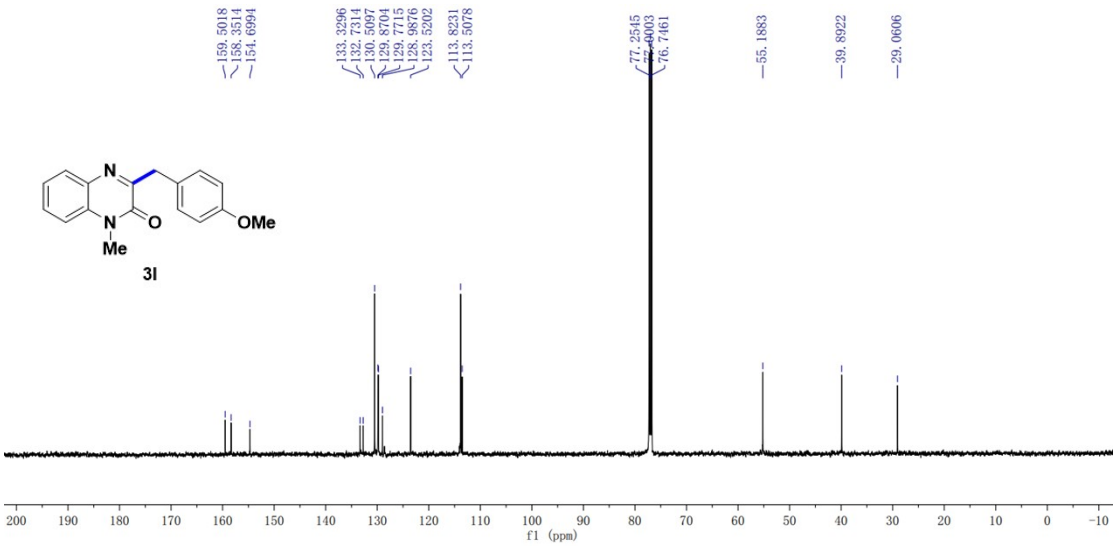
7.3048
7.2898
7.2739
7.2264
7.2231
7.2098
6.8022
6.7850
4.1650
3.7226
3.6163
N
O
N
Me
OMe
3l
1.00
1.00
2.00
1.00
1.00
2.00
2.00
3.00
3.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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113.5078
77.2545
77.0003
76.7461
55.1883
39.8922
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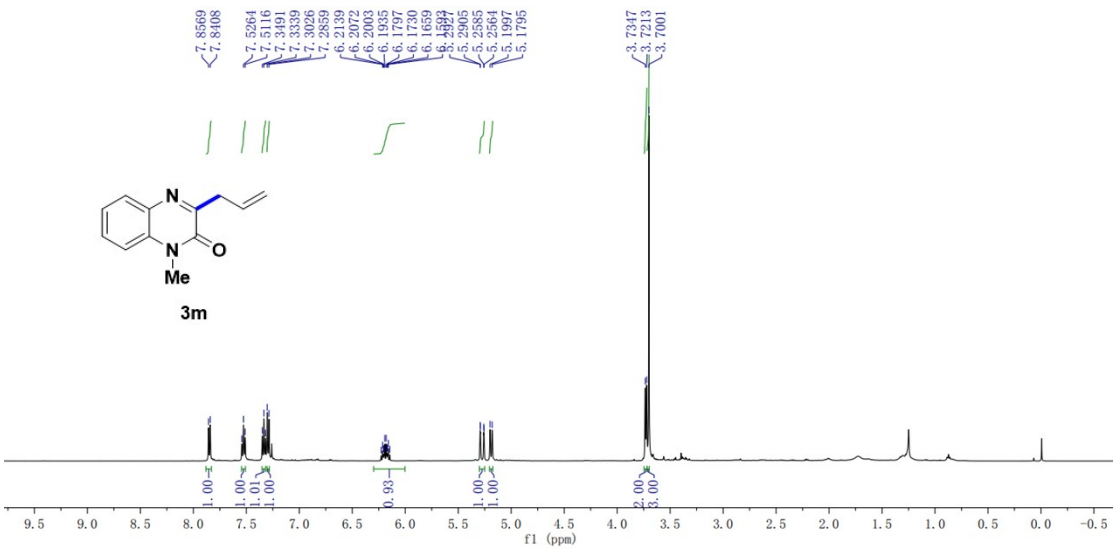
O
N
Me
OMe
3l
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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6.2003
6.1935
6.1797
6.1730
6.1659
5.2905
5.2585
5.2564
5.1997
5.1795
3.7347
3.7213
3.7001
N
N
O
Me
3m
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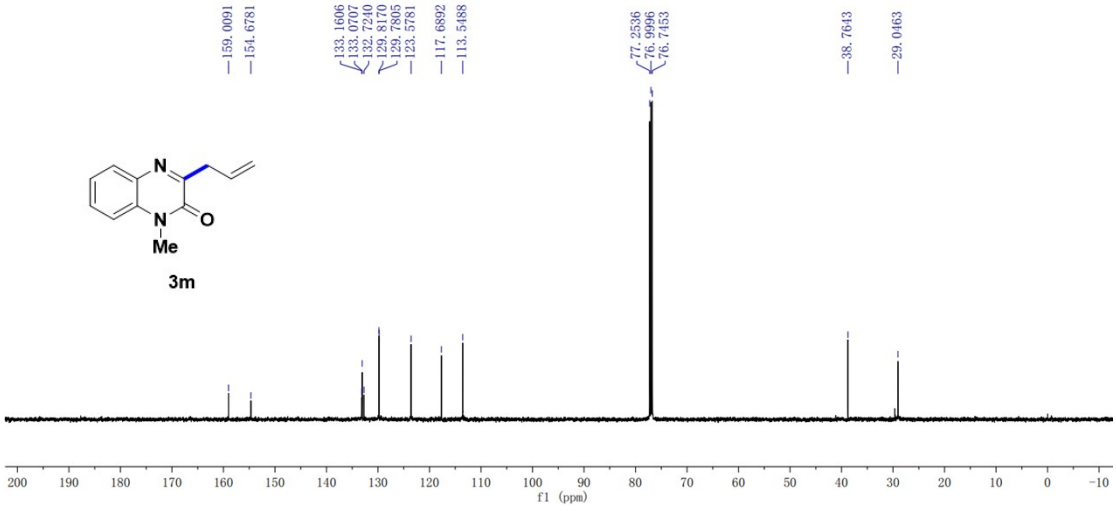
1.00
1.01
1.00
0.93
1.00
1.00
2.00
3.00
f1 (ppm)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76.9996
76.7453
38.7643
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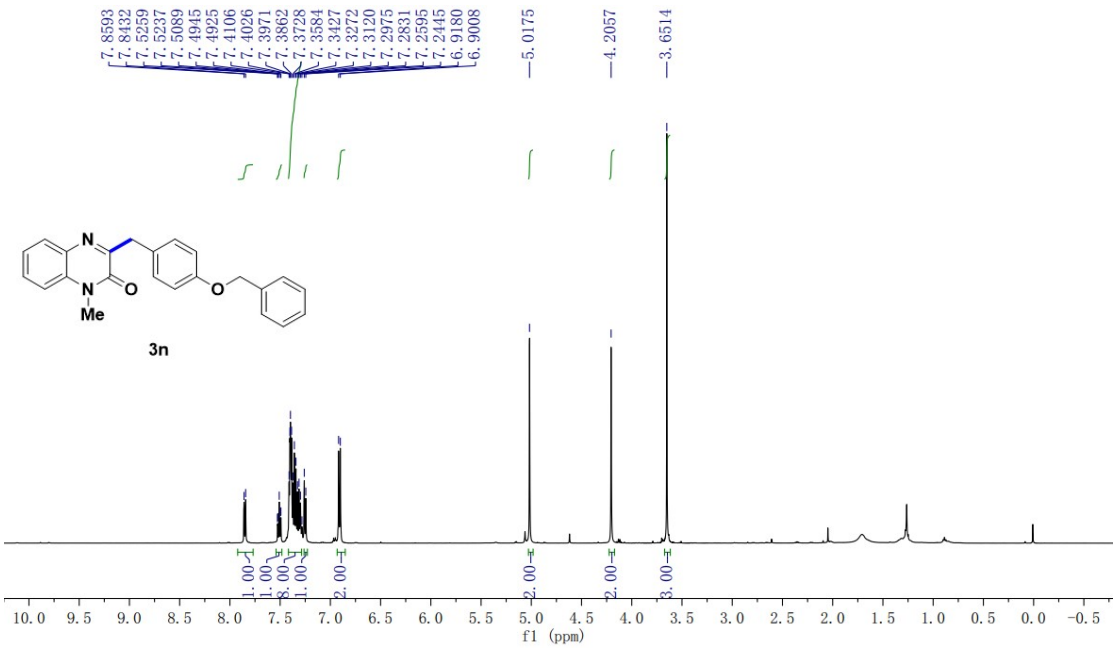
Me
3m
f1 (ppm)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7.3728
7.3584
7.3427
7.3272
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7.2595
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6.9180
6.9008
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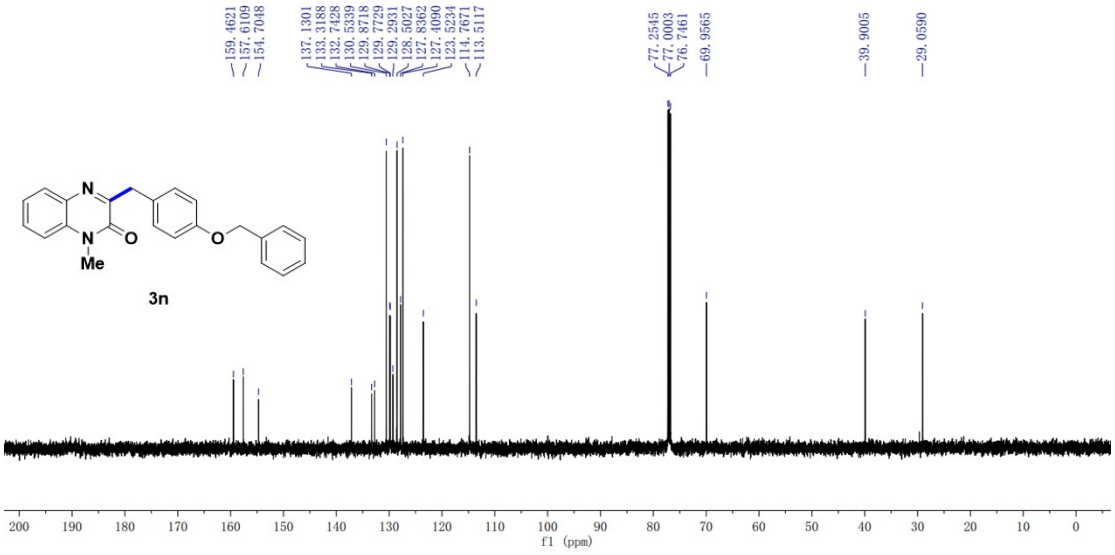
4.2057
3.6514
1.00
1.00
8.00
1.00
2.00
2.00
2.00
3.00
N
N
O
O
Me
3n
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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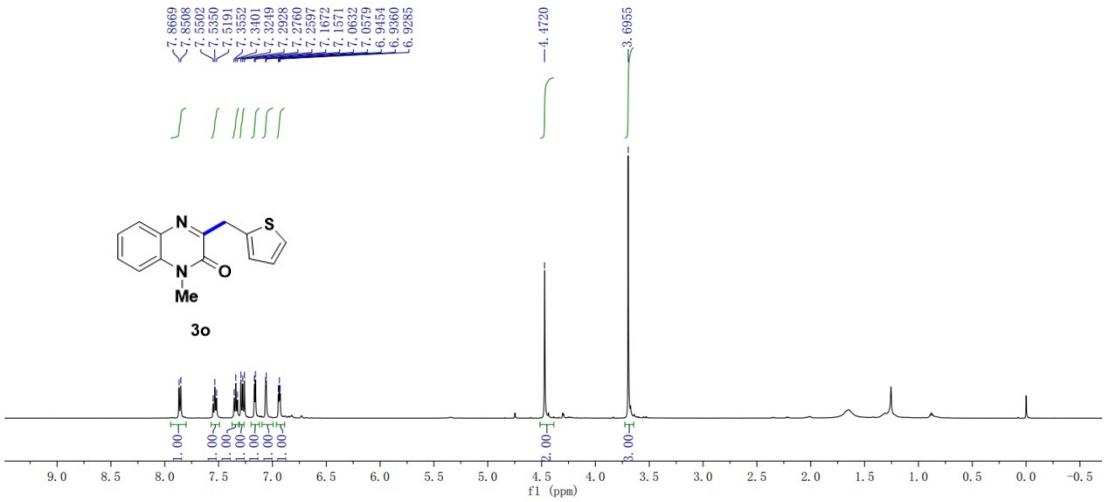
128.5027
127.8362
127.4090
123.5234
114.7671
113.5117
77.2545
77.0003
76.7461
69.9565
39.9005
29.0590
N
N
O
O
Me
3n
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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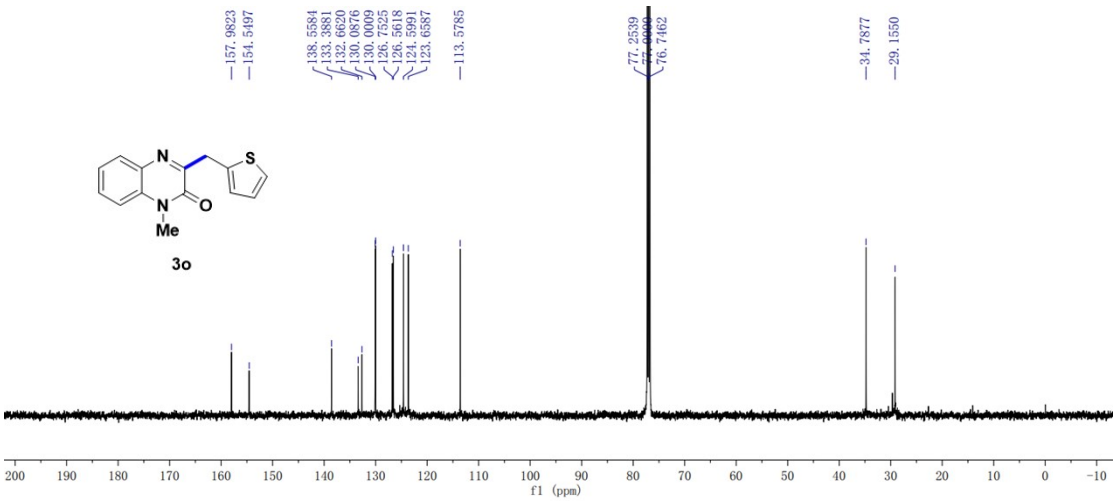
7.1672
7.1571
7.0632
7.0579
6.9454
6.9360
6.9285
4.4720
3.6955
N
S
N
O
Me
3o
1.00
1.00
1.00
1.00
1.00
1.00
1.00
2.00
3.00
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)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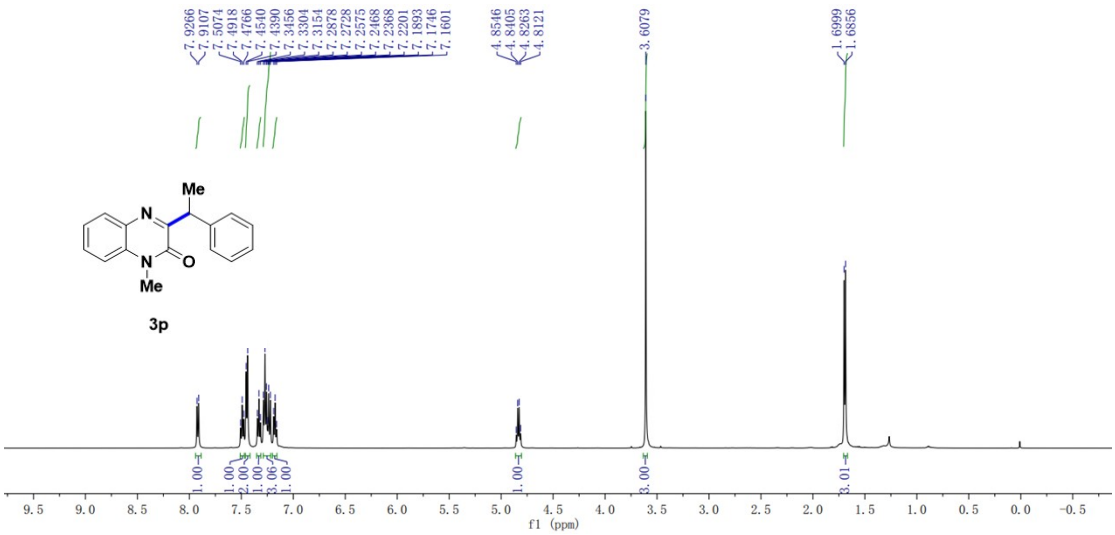
123.6587
113.5785
77.2539
76.7462
34.7877
29.1550
N
S
N
O
Me
3o
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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7.2368
7.2201
7.1893
7.1746
7.1601
4.8546
4.8405
4.8263
4.8121
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1.6856
Me
N
N
O
Me
3p
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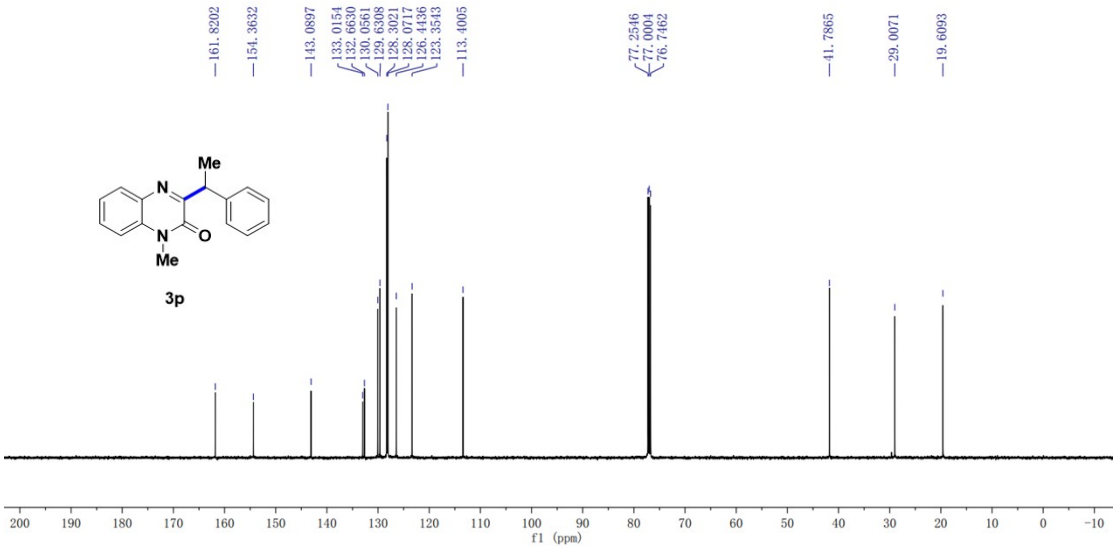
1.00
2.00
1.00
3.06
1.00
1.00
3.00
3.01
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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113.4005
77.2546
77.0004
76.7462
41.7865
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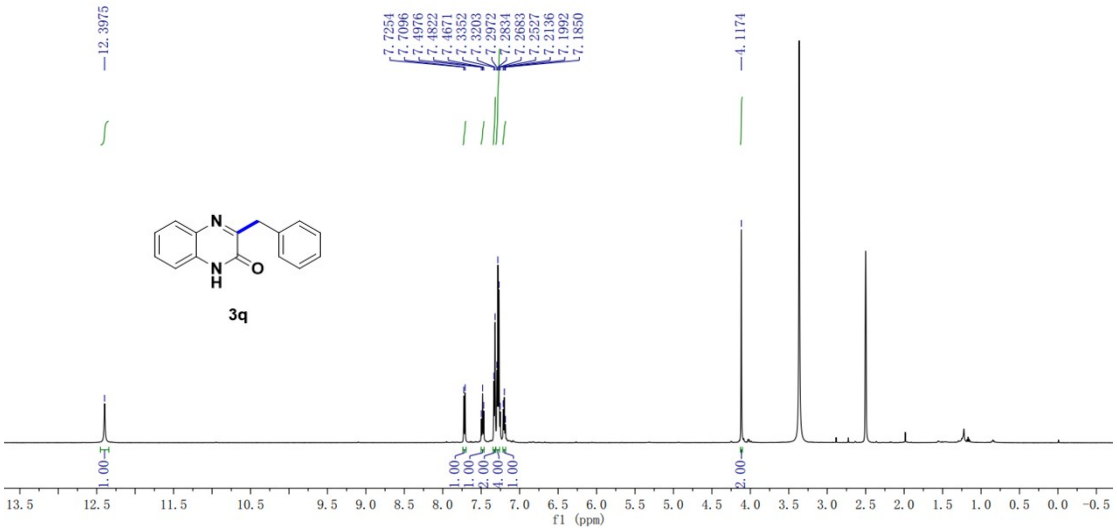
19.6093
Me
N
N
O
Me
3p
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.3203
7.2972
7.2834
7.2683
7.2527
7.2136
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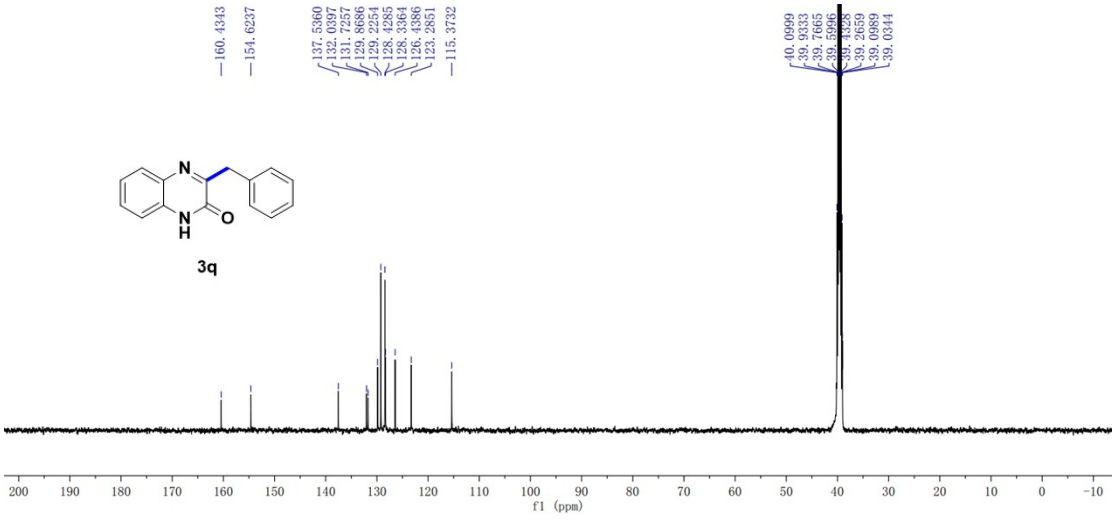
3q
1.00
1.00
1.00
2.00
4.00
1.00
2.00
f1 (ppm)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123.2851
115.3732
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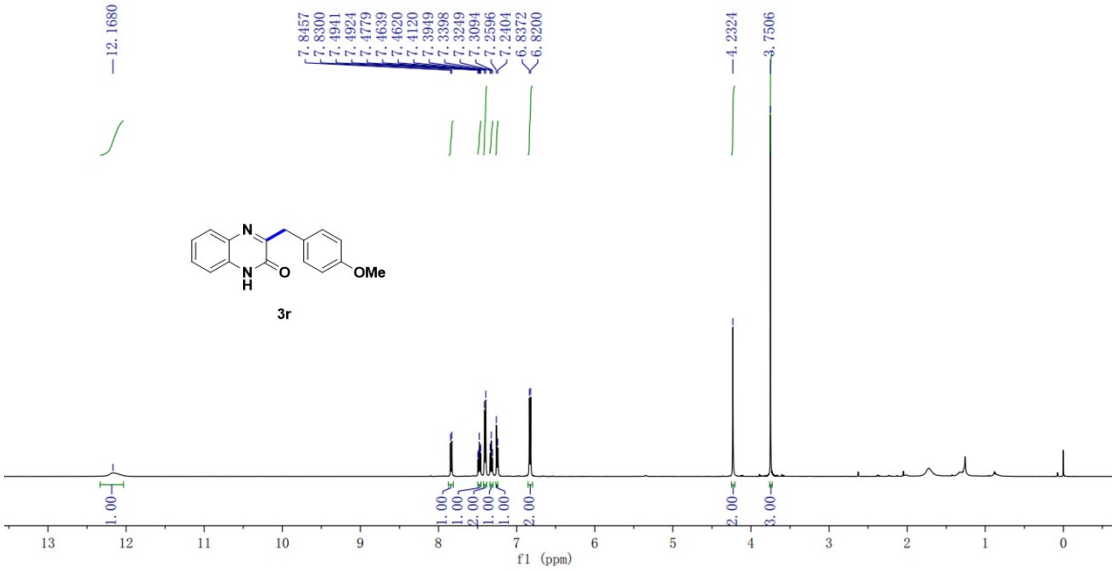
39.7665
39.5996
39.4328
39.2659
39.0989
39.0344
3q
f1 (ppm)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7.2404
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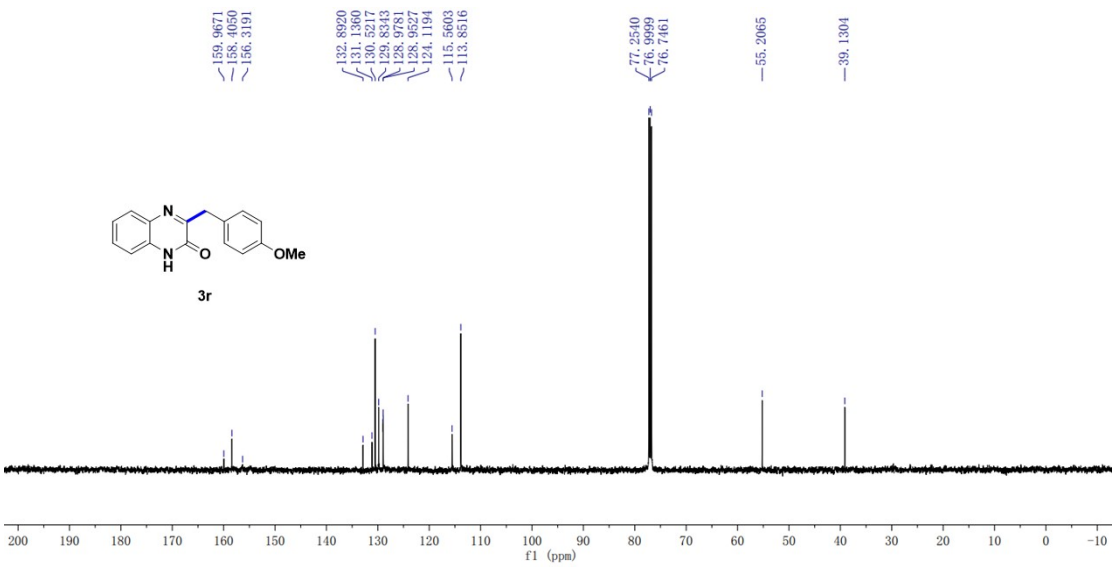
6.8200
4.2324
3.7506
OMe
3r
f1 (ppm)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76.9999
76.7461
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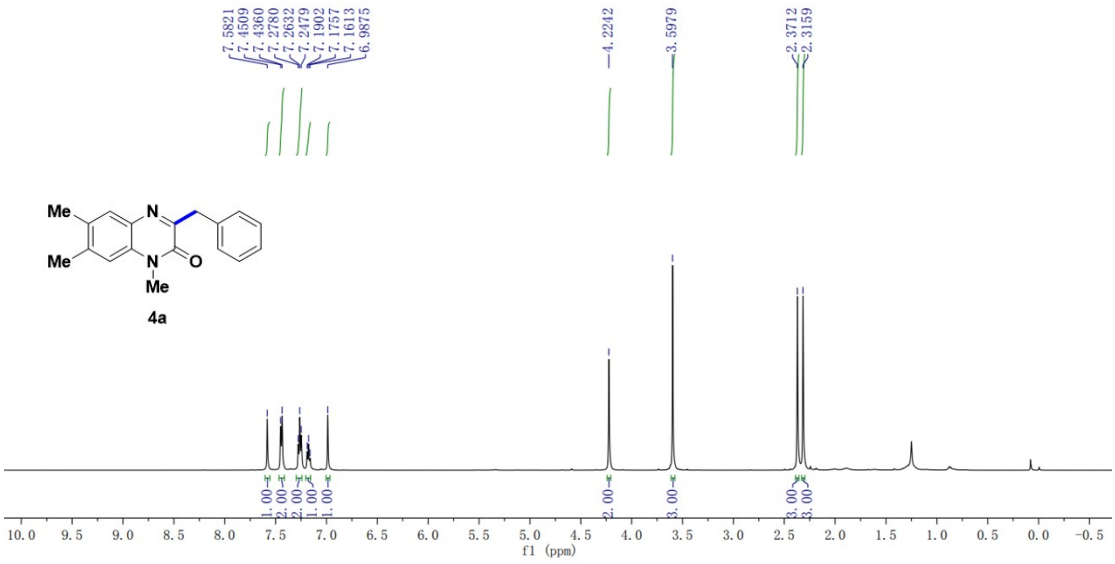
39.1304
OMe
3r
f1 (ppm)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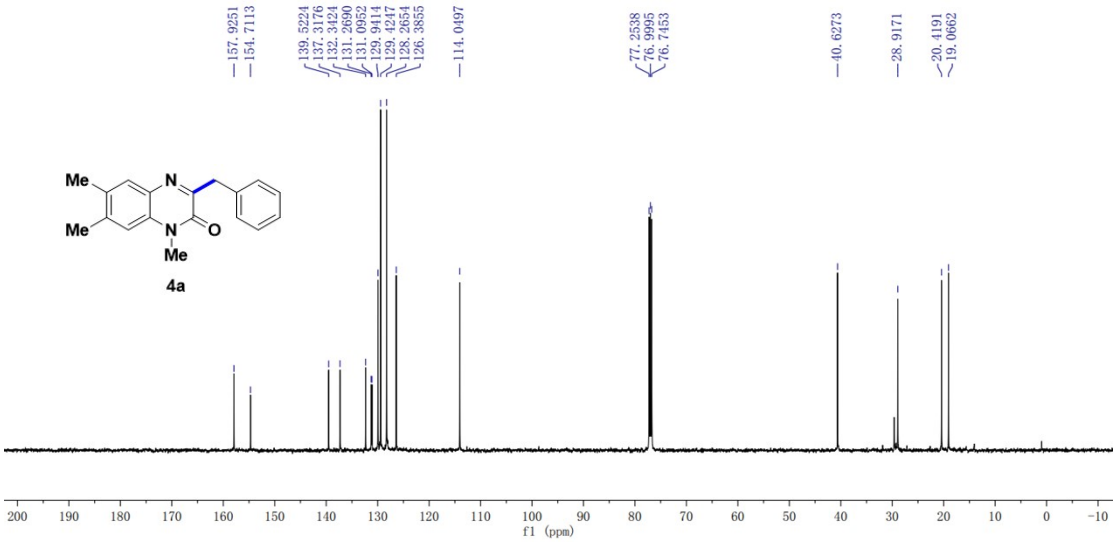
7.1613
6.9875
4.2242
3.5979
2.3712
2.3159
Me
Me
N
O
N
Me
4a
1.00
2.00
2.00
2.00
1.00
1.00
2.00
3.00
3.00
3.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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77.2538
76.9995
76.7453
40.6273
28.9171
20.4191
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Me
N
O
N
Me
4a
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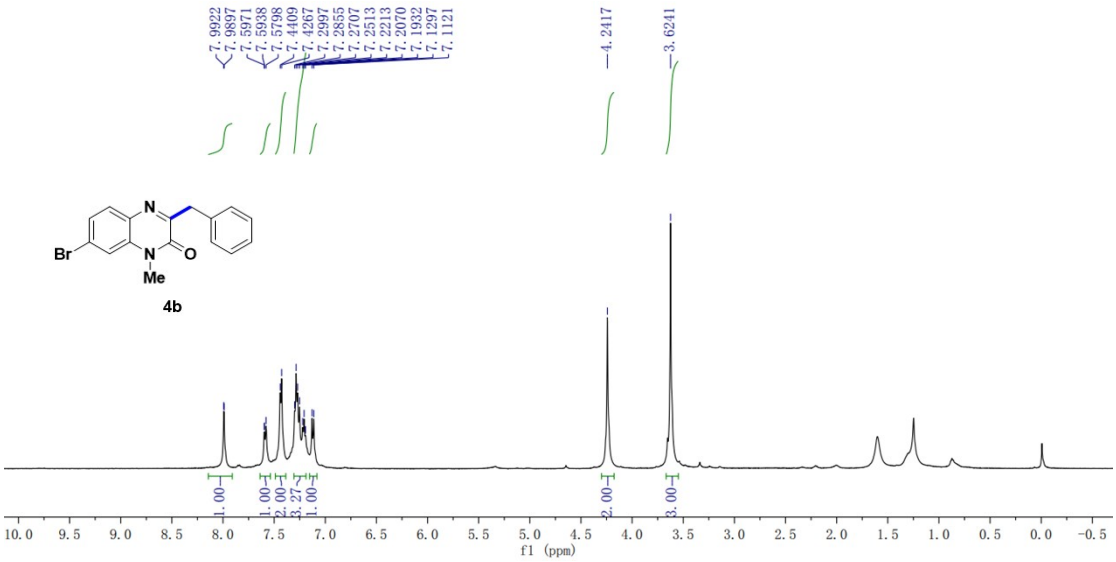
f1 (ppm)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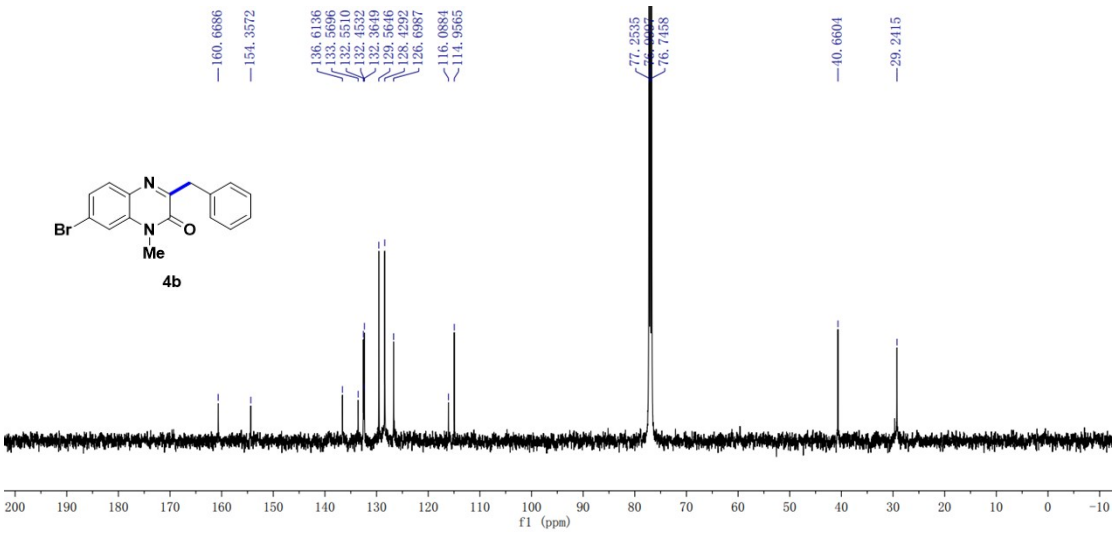
7.2213
7.2070
7.1932
7.1297
7.1121
4.2417
3.6241
Br
N
O
Me
4b
1.00
1.00
2.00
3.27
1.00
2.00
3.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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114.9565
77.2535
76.7458
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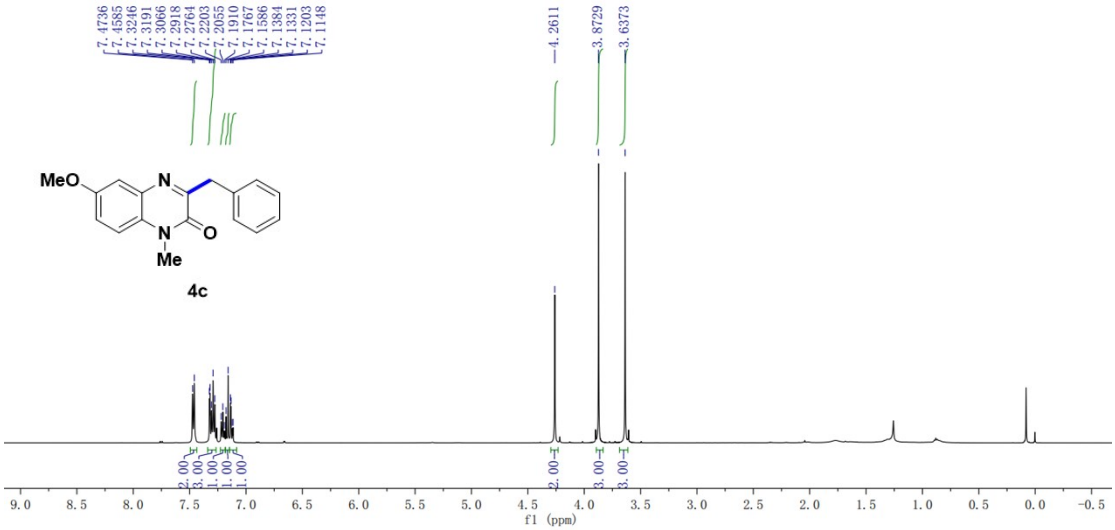
Br
N
O
Me
4b
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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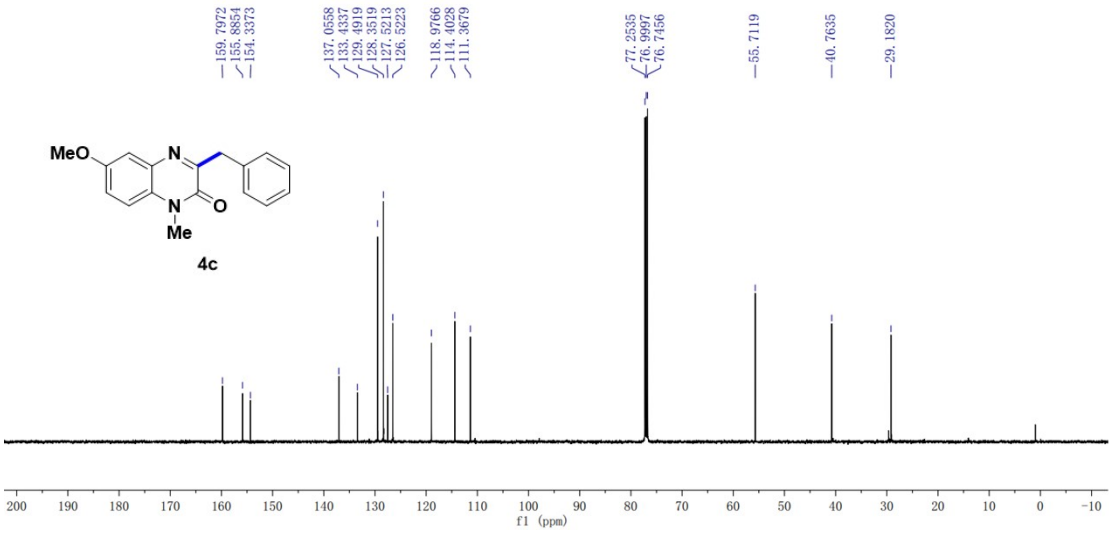
7.1586
7.1384
7.1331
7.1203
7.1148
4.2611
3.8729
3.6373
MeO
N
N
O
Me
4c
2.00
3.00
1.00
1.00
2.00
3.00
3.00
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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128.3519
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114.4028
111.3679
77.2535
76.9997
76.7456
55.7119
40.7635
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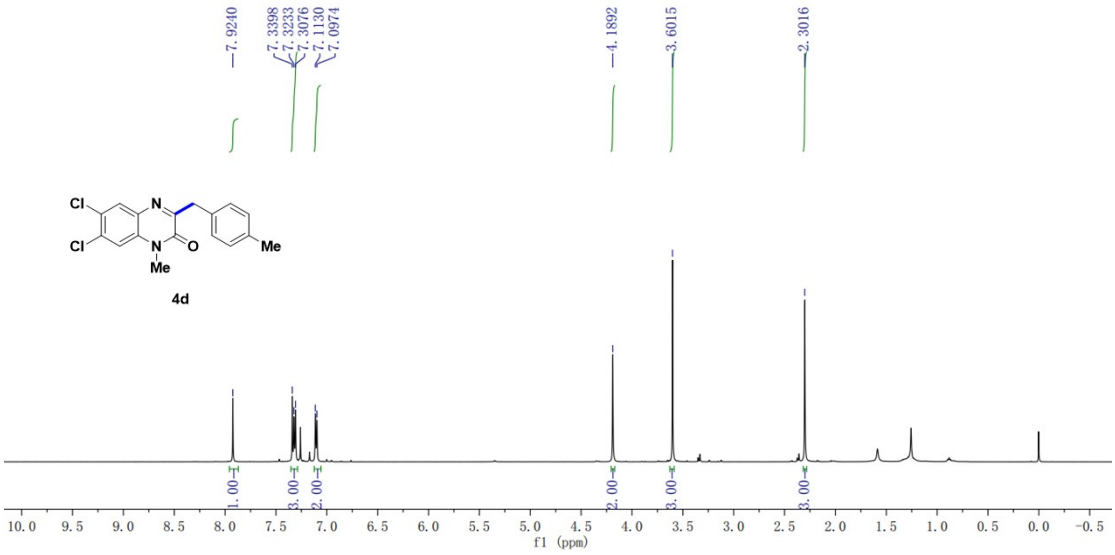
N
N
O
Me
4c
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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2.3016
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Cl
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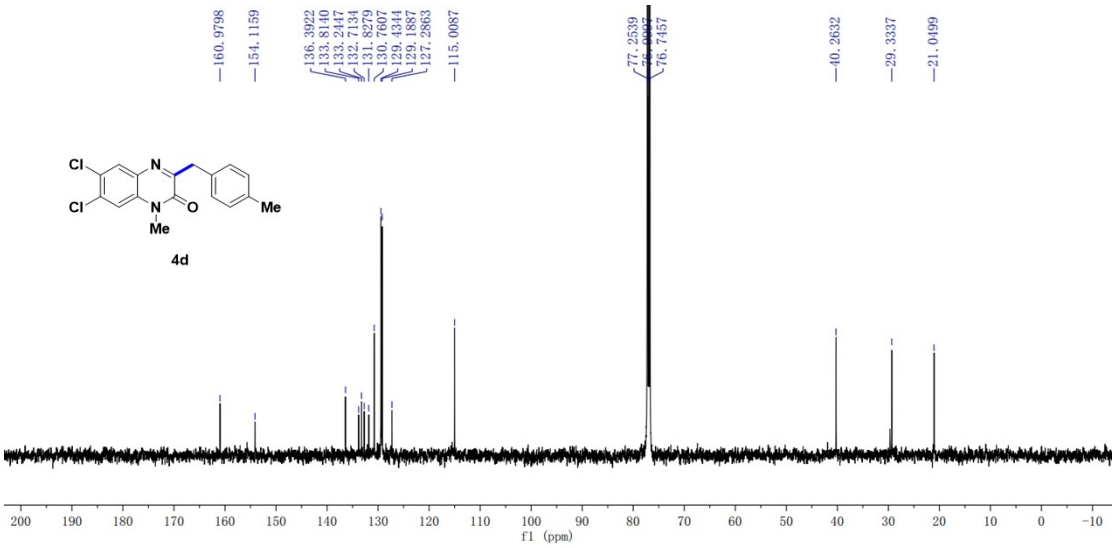
N
O
Me
Me
4d
1.00
3.00
2.00
2.00
3.00
3.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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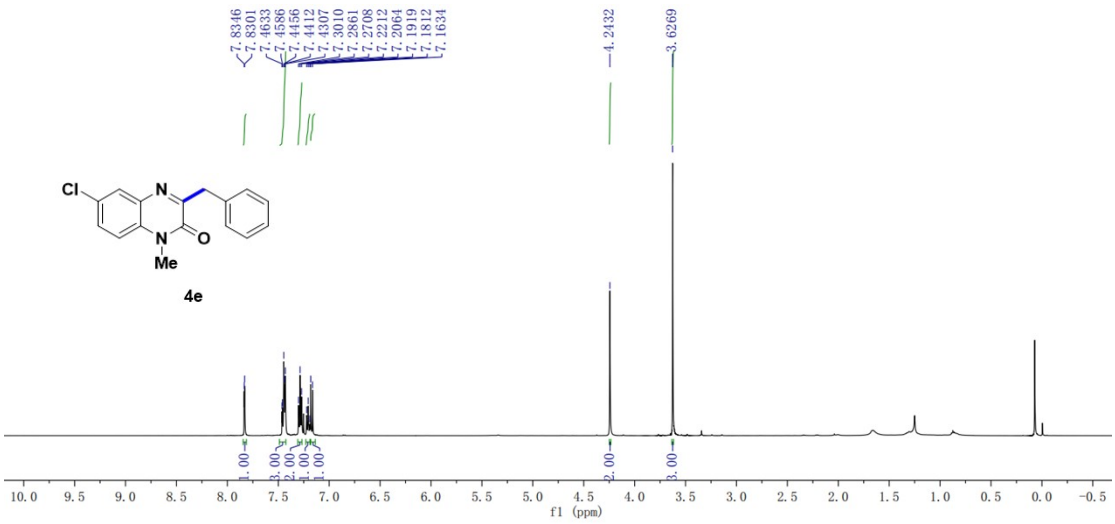
115.0087
77.2539
76.7457
40.2632
29.3337
21.0499
Cl
Cl
N
N
O
Me
Me
4d
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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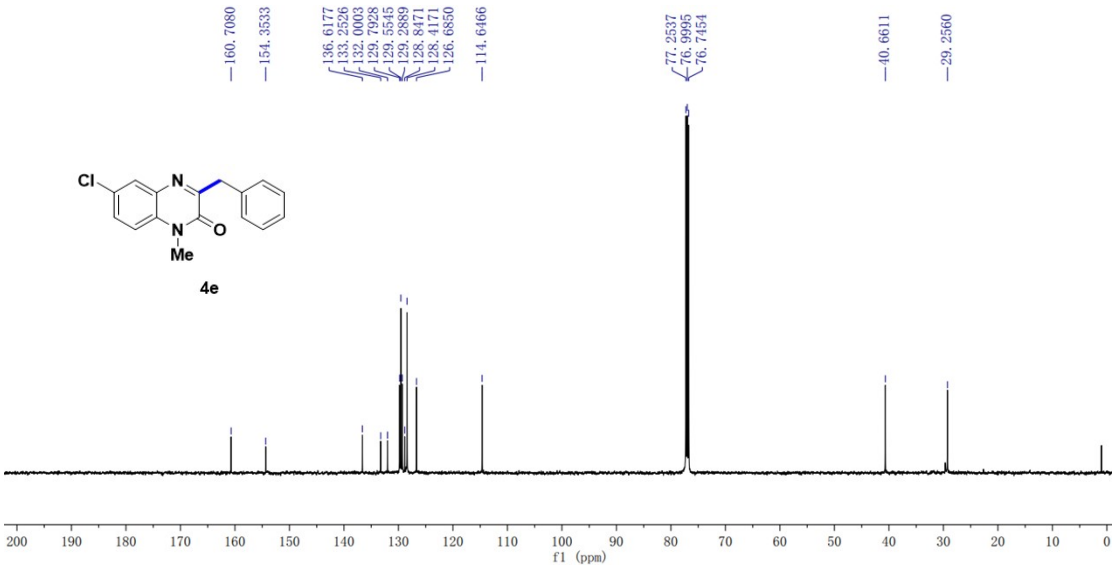
7.2064
7.1919
7.1812
7.1634
4.2432
3.6269
Cl
N
N
O
Me
4e
1.00
3.00
2.00
1.00
1.00
2.00
3.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 −0.5
f1 (ppm)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N
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Me
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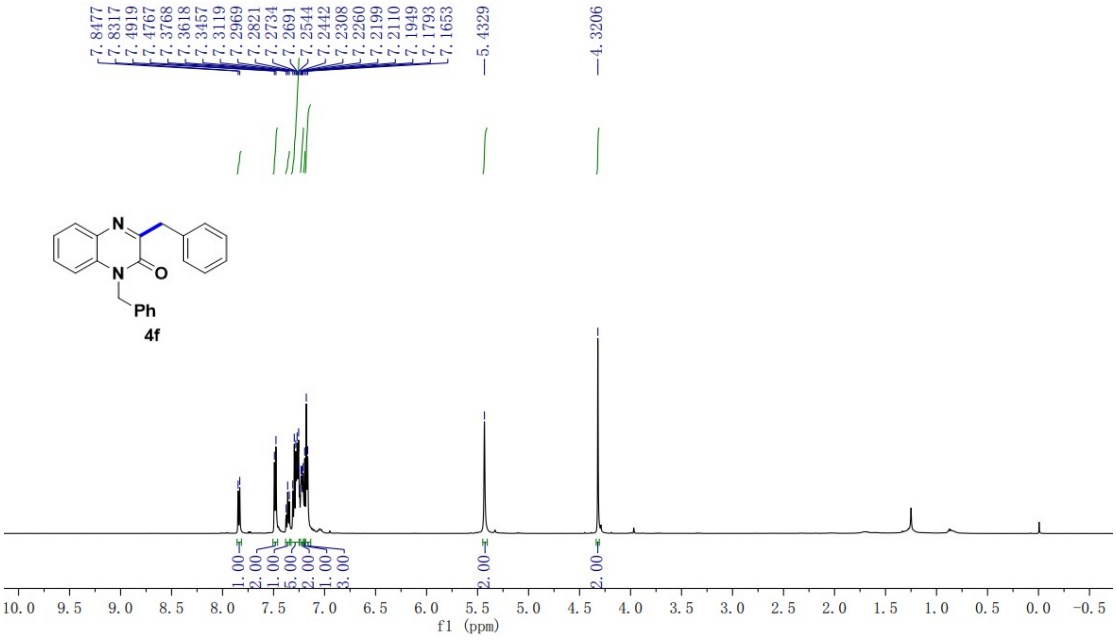
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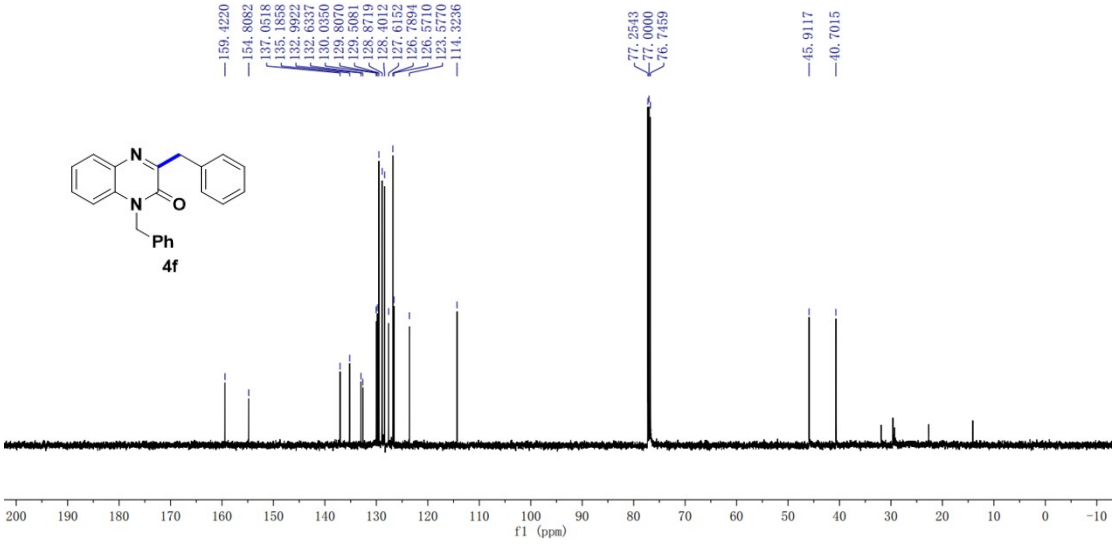
7.2544
7.2442
7.2308
7.2260
7.2199
7.2110
7.1949
7.1793
7.1653
5.4329
4.3206
N
N
O
Ph
4f
1.00
2.00
1.00
5.00
2.00
1.00
3.00
2.00
2.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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128.4012
127.6152
126.7894
126.5710
123.5770
114.3236
77.2543
77.0000
76.7459
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N
N
O
Ph
4f
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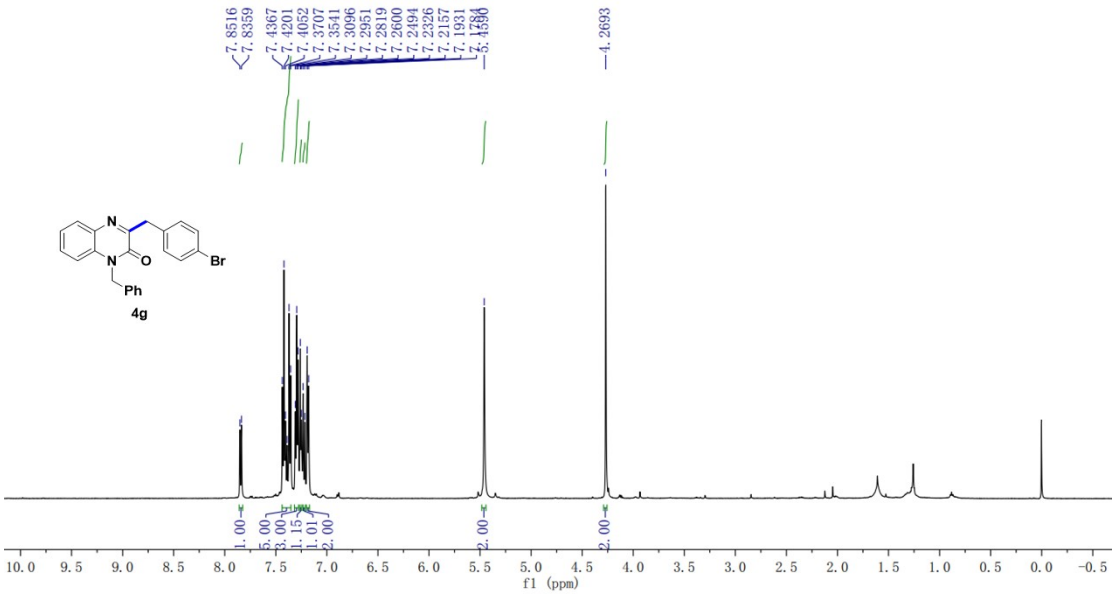
f1 (ppm)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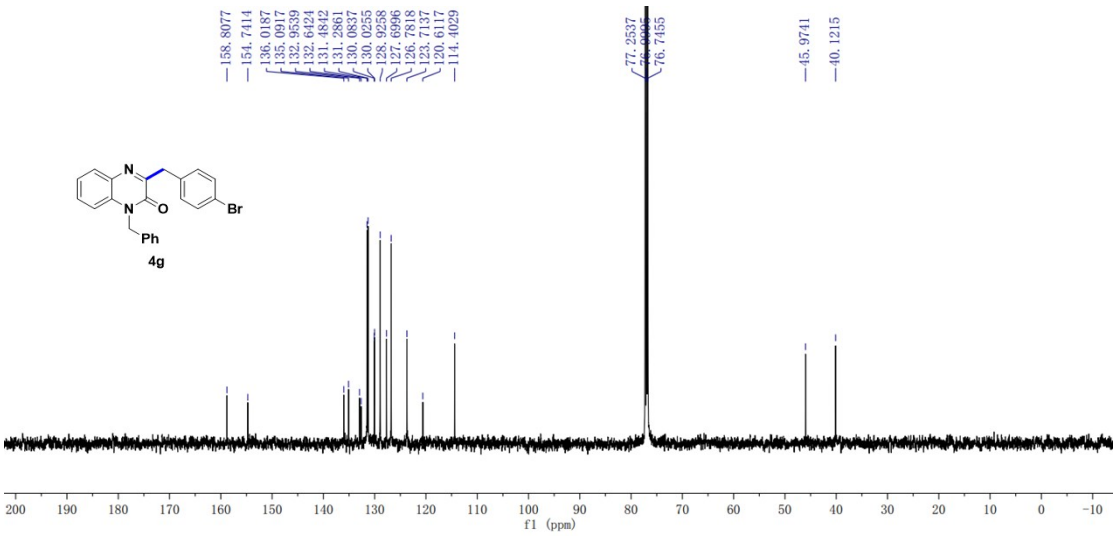
7.2494
7.2326
7.2157
7.1931
7.1784
5.4590
4.2693
N
O
N
Br
Ph
4g
1.00
5.00
3.00
1.15
1.01
2.00
2.00
2.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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126.7818
123.7137
120.6117
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76.7455
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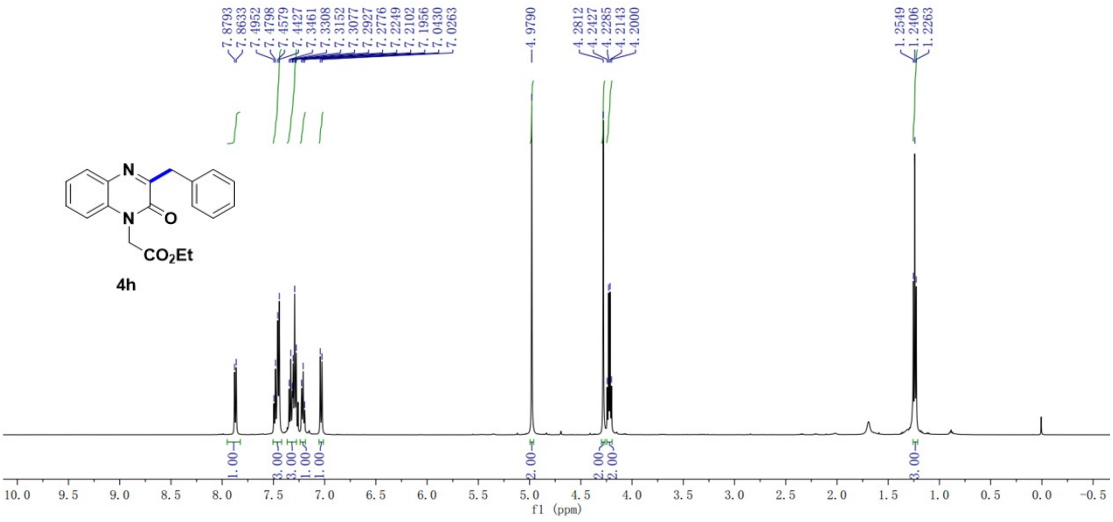
O
N
Br
Ph
4g
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.2102
7.1956
7.0430
7.0263
4.9790
4.2812
4.2427
4.2285
4.2143
4.2000
1.2549
1.2406
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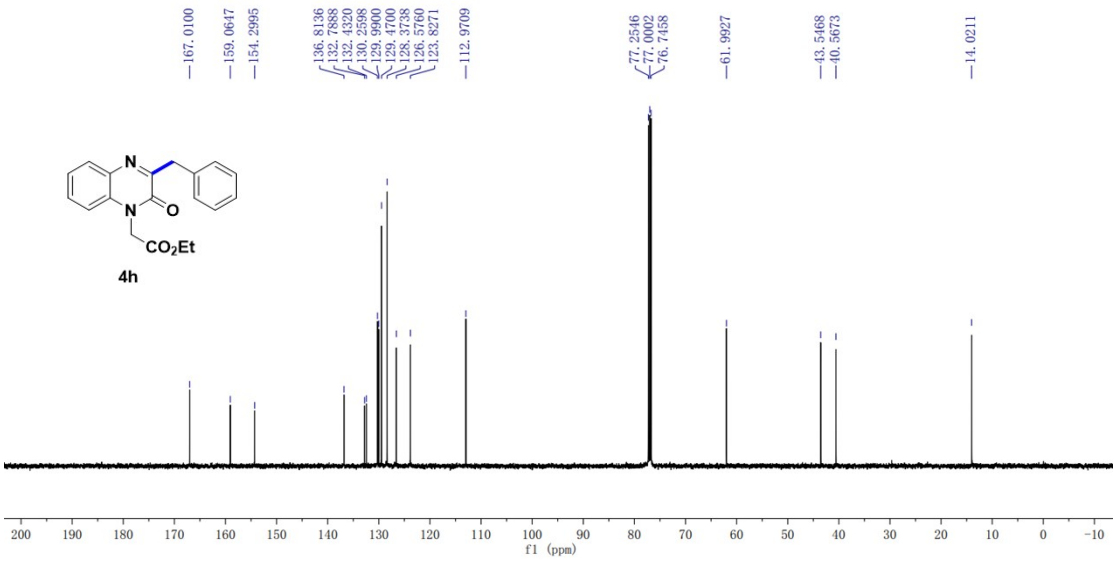
3.00
3.00
1.00
1.00
2.00
2.00
2.00
3.00
4h
f1 (ppm)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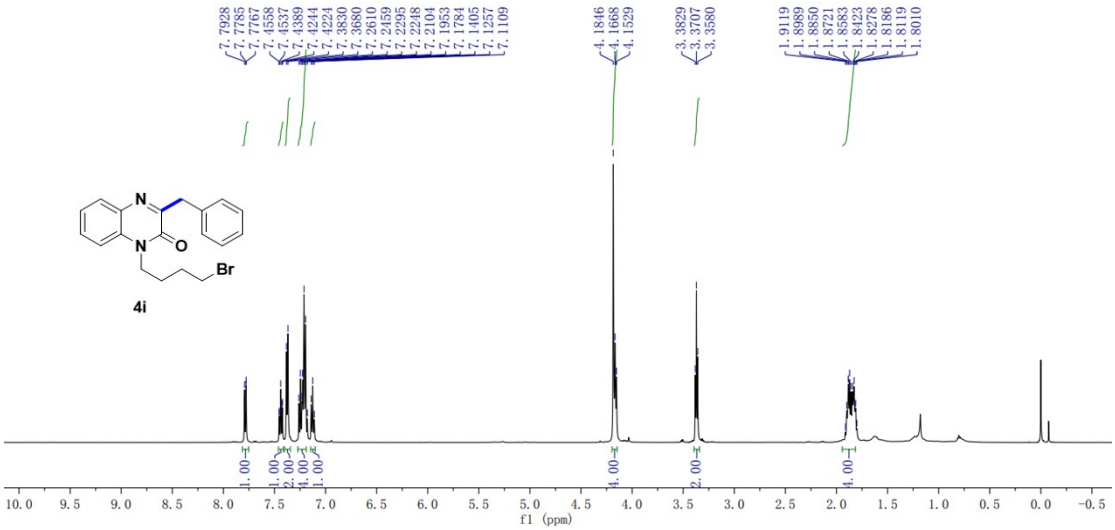
40.5673
14.0211
4h
f1 (ppm)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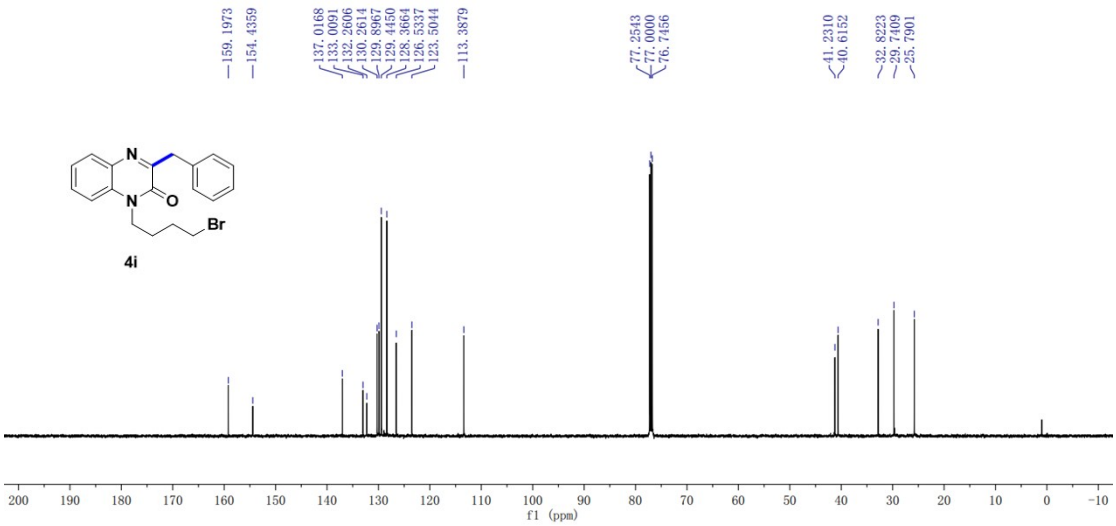
7.3680
7.2610
7.2459
7.2295
7.2248
7.2104
7.1953
7.1784
7.1405
7.1257
7.1109
4.1846
4.1668
4.1529
3.3829
3.3707
3.3580
1.9119
1.8989
1.8850
1.8721
1.8583
1.8423
1.8278
1.8186
1.8119
1.8010
N
N
O
Br
4i
1.00
1.00
2.00
4.00
1.00
4.00
2.00
4.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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77.2543
77.0000
76.7456
41.2310
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32.8223
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N
N
O
Br
4i
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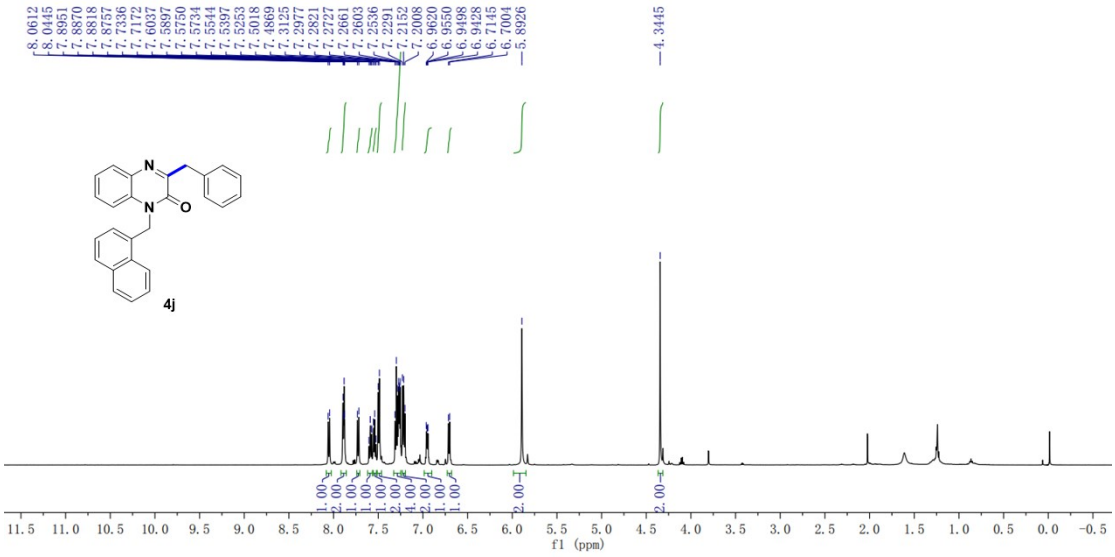
f1 (ppm)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7.5734
7.5544
7.5397
7.5253
7.5018
7.4869
7.3125
7.2977
7.2821
7.2727
7.2661
7.2603
7.2536
7.2291
7.2152
7.2008
6.9620
6.9550
6.9498
6.9428
6.7145
6.7004
5.8926
4.3445
4j
1.00
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1.00
1.00
1.00
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4.00
2.00
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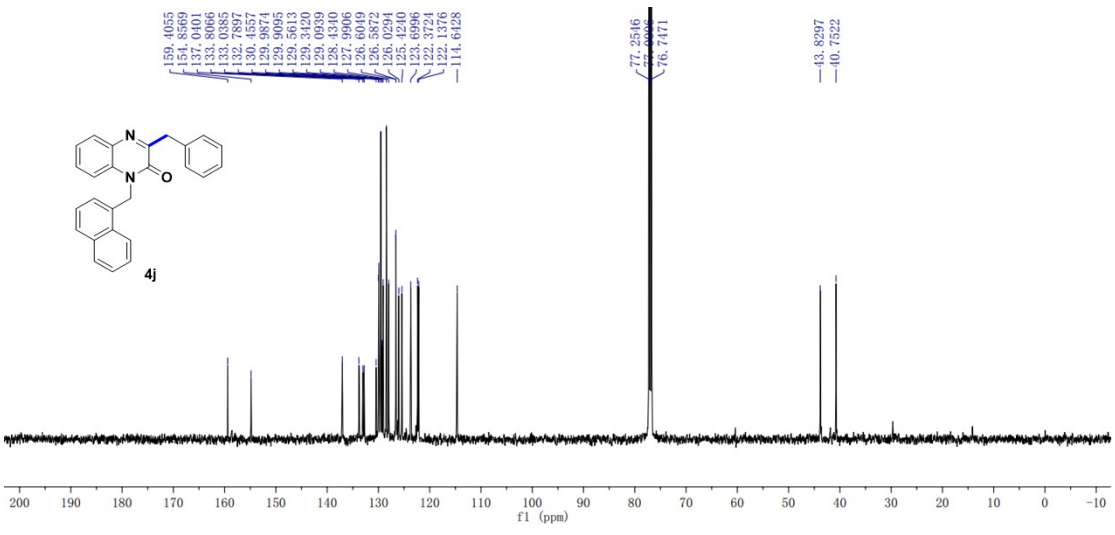
1.00
2.00
2.00
f1 (ppm)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127.9906
126.6049
126.5872
126.0294
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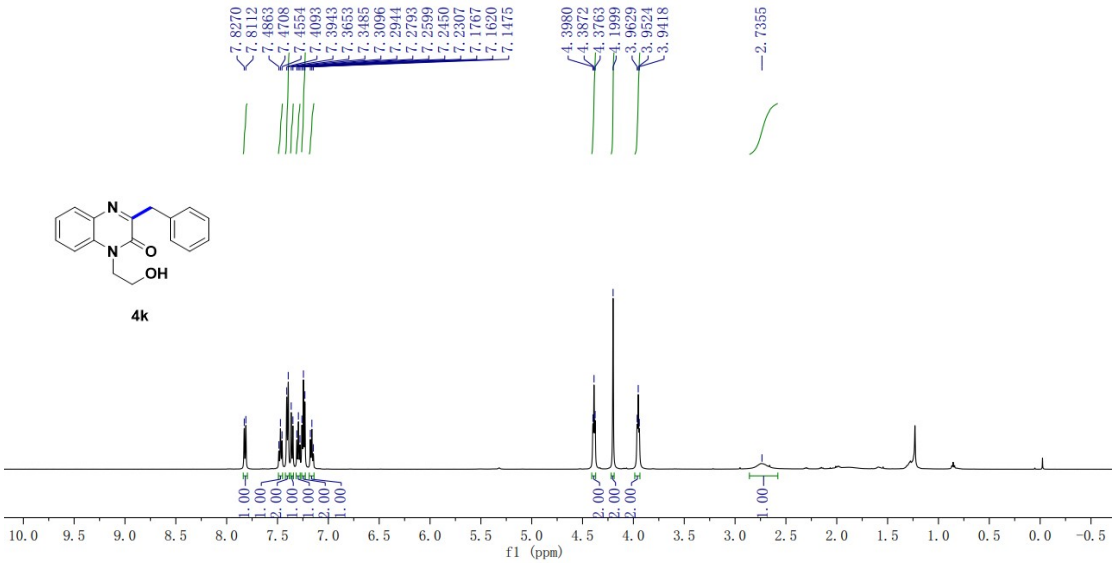
43.8297
40.7522
4j
f1 (ppm)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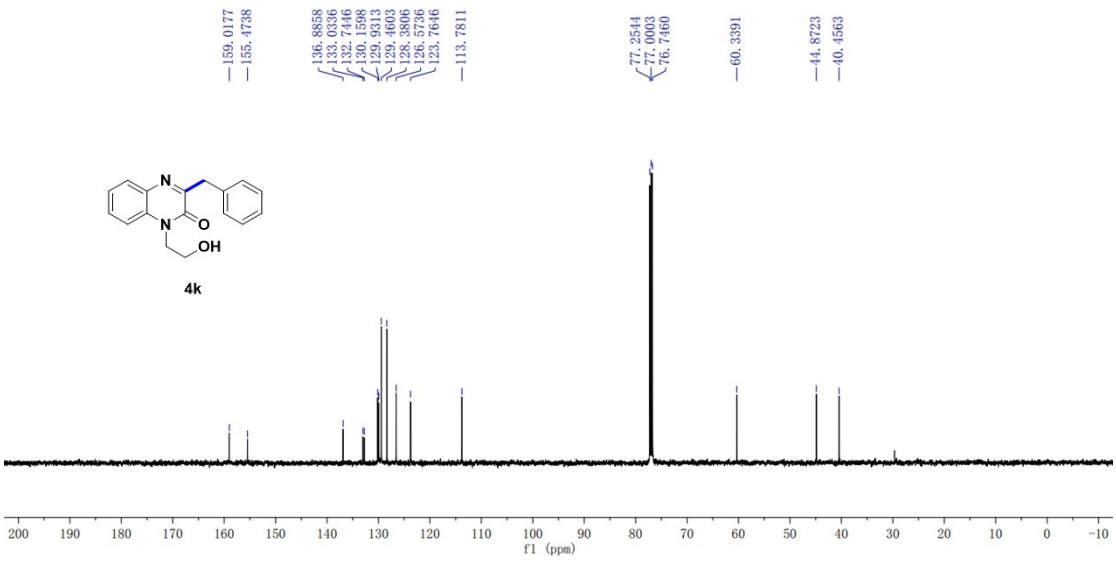
7.2944
7.2793
7.2599
7.2450
7.2307
7.1767
7.1620
7.1475
4.3980
4.3872
4.3763
4.1999
3.9629
3.9524
3.9418
2.7355
N
N
O
OH
4k
1.00
1.00
2.00
1.00
1.00
2.00
1.00
2.00
2.00
2.00
1.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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113.7811
77.2544
77.0003
76.7460
60.3391
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40.4563
N
N
O
OH
4k
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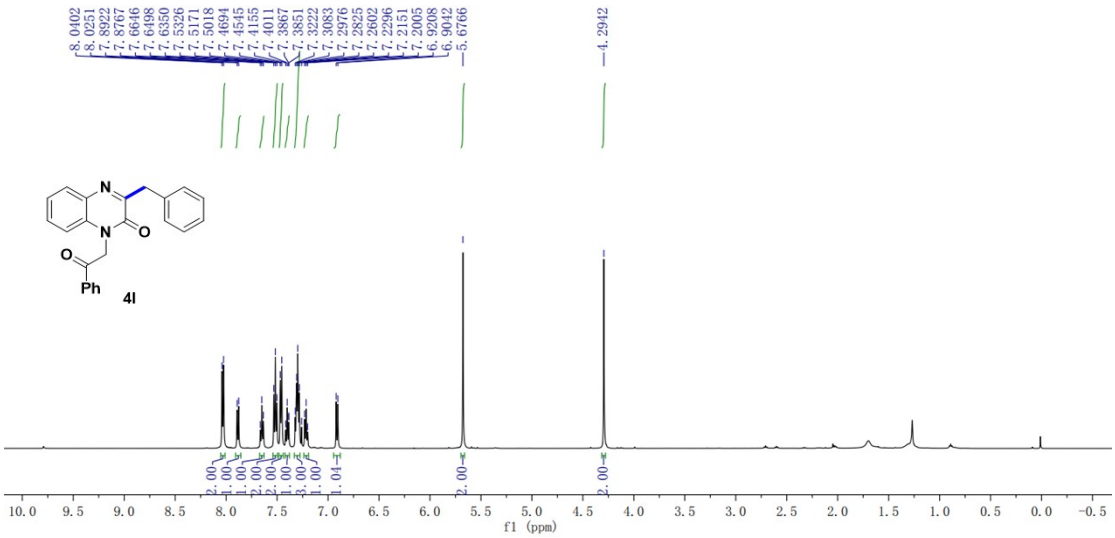
f1 (ppm)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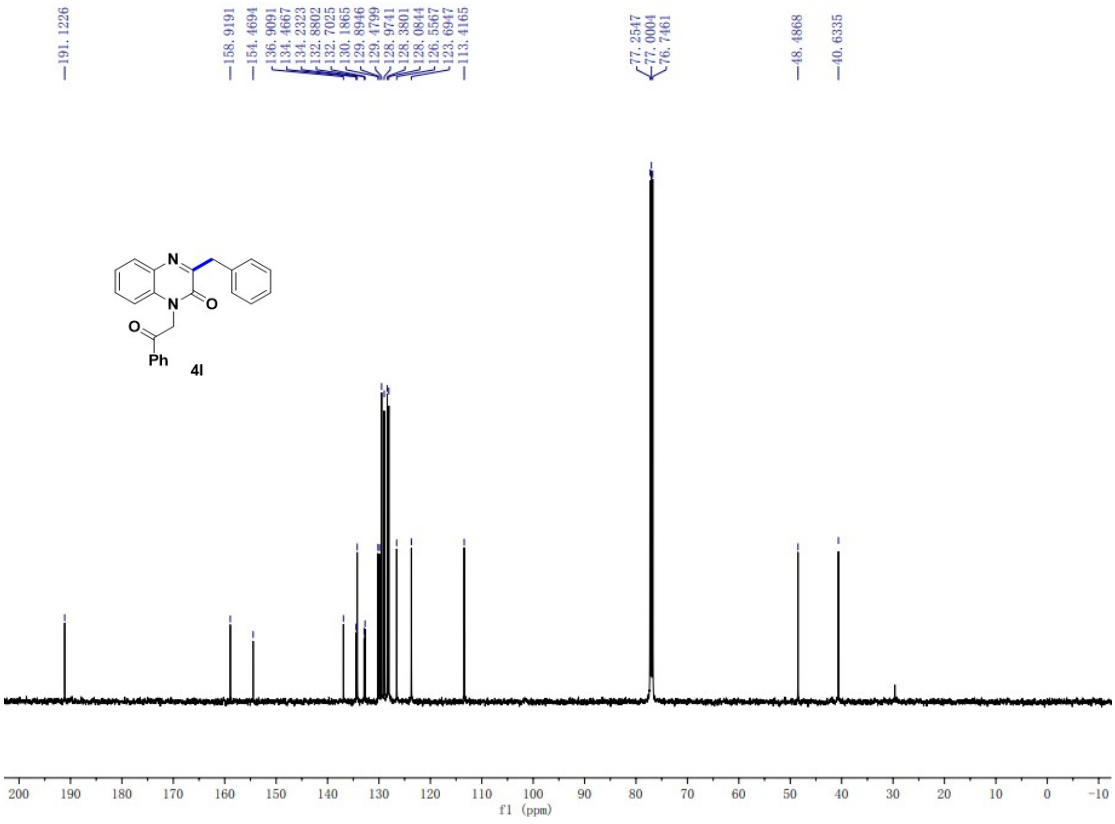
7.4545
7.4155
7.4011
7.3867
7.3851
7.3222
7.3083
7.2976
7.2825
7.2602
7.2296
7.2151
7.2005
6.9208
6.9042
5.6766
4.2942
N
O
N
O
Ph
4l
2.00
1.00
1.00
2.00
2.00
1.00
3.00
1.00
1.04
2.00
2.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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128.0844
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O
N
O
Ph
4l
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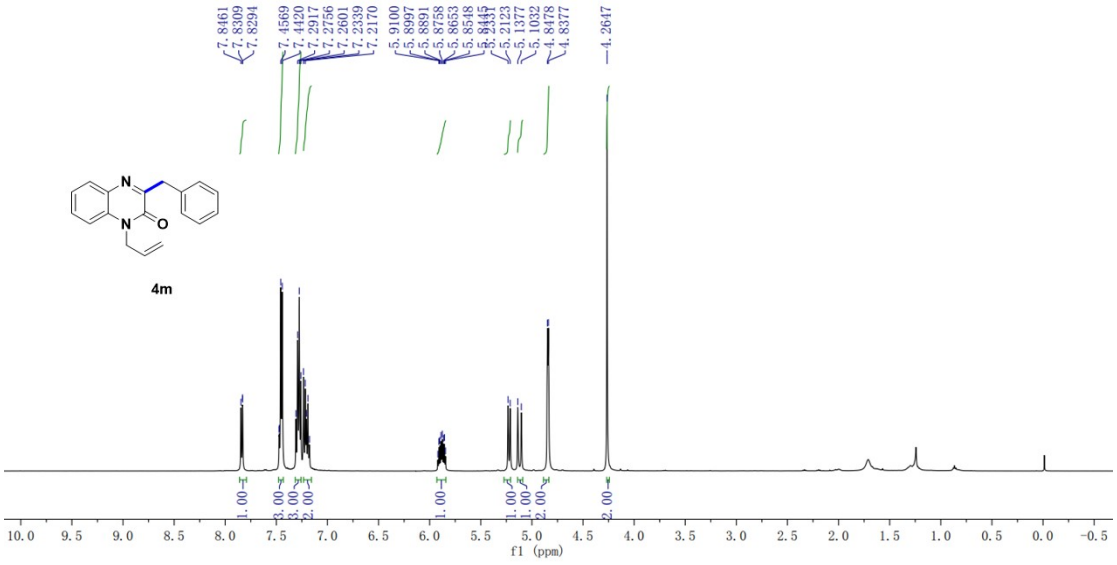
f1 (ppm)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5.8653
5.8548
5.2123
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4.8377
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1.00
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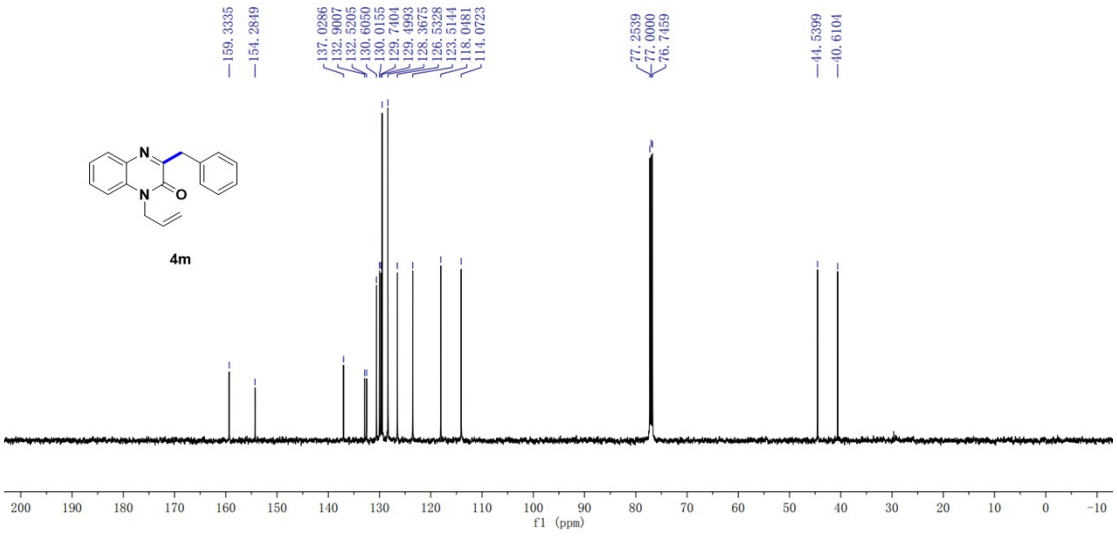
2.00
f1 (ppm)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126.5328
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77.0000
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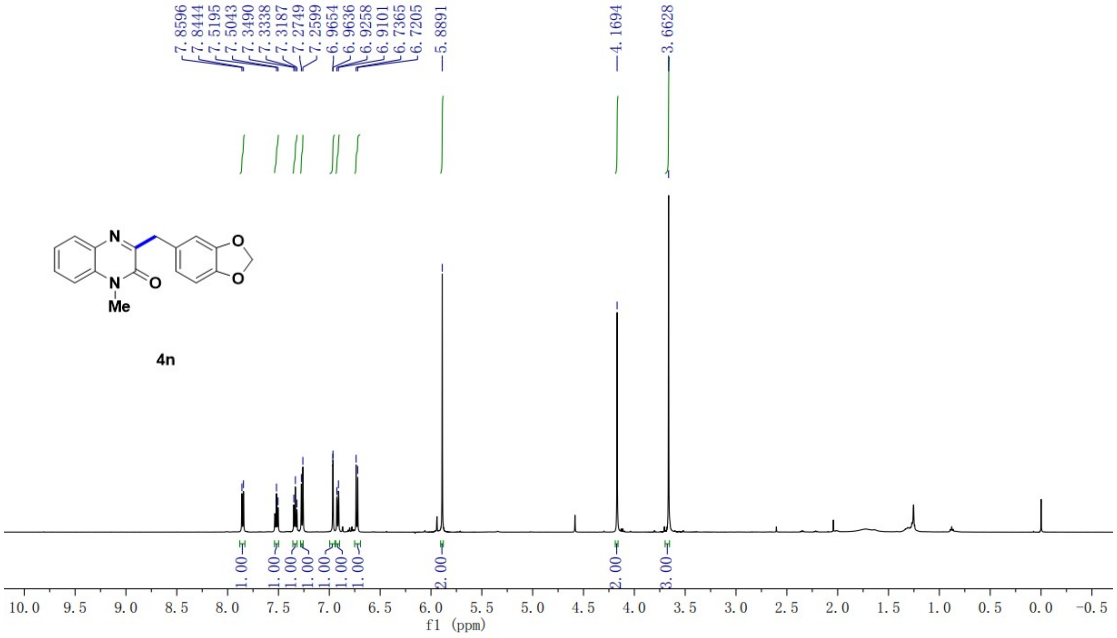
44.5399
40.6104
4m
f1 (ppm)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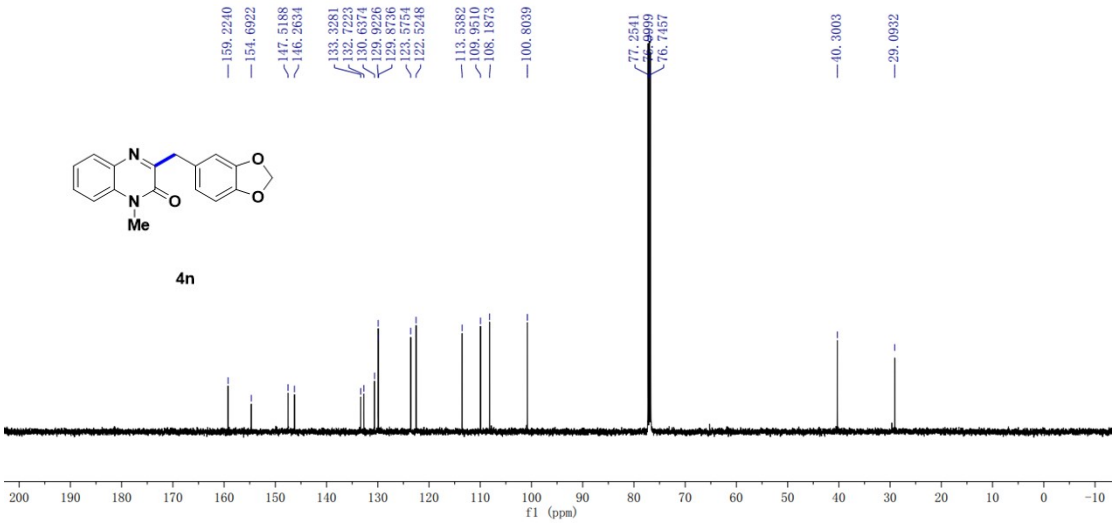
6.9258
6.9101
6.7365
6.7205
5.8891
4.1694
3.6628
N
O
N
O
Me
O
O
4n
1.00
1.00
1.00
1.00
1.00
1.00
2.00
2.00
3.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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108.1873
100.8039
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77.0999
76.7457
40.3003
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O
Me
O
O
4n
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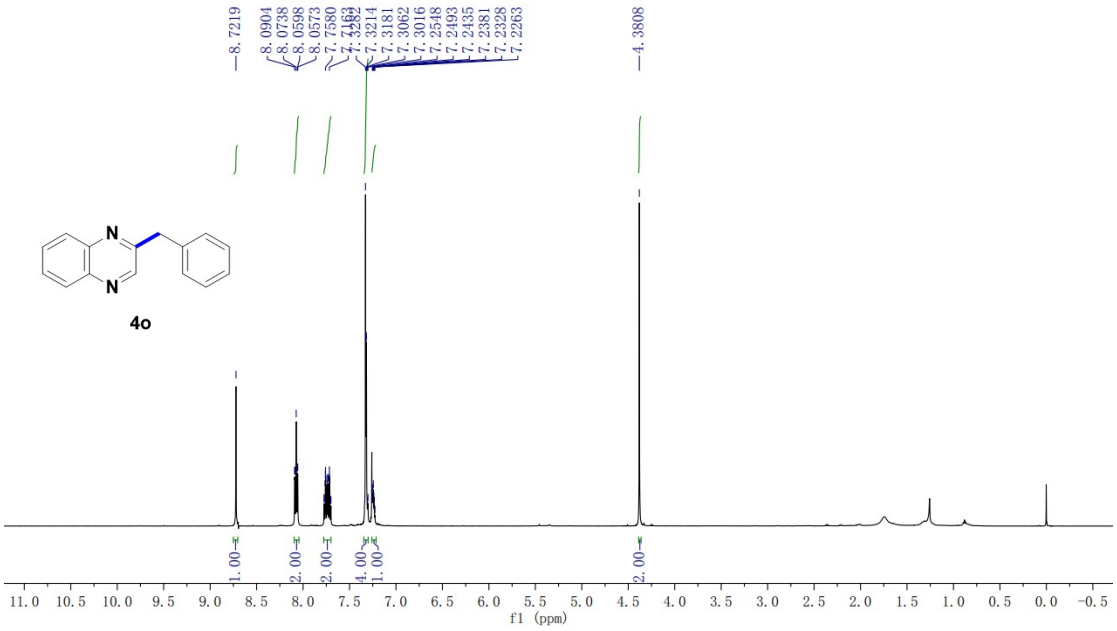
f1 (ppm)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7.3016
7.2548
7.2493
7.2435
7.2381
7.2328
7.2263
4.3808
1.00
2.00
2.00
4.00
1.00
2.00
f1 (ppm)

4o

155.8002
145.9230
142.0498
141.1914
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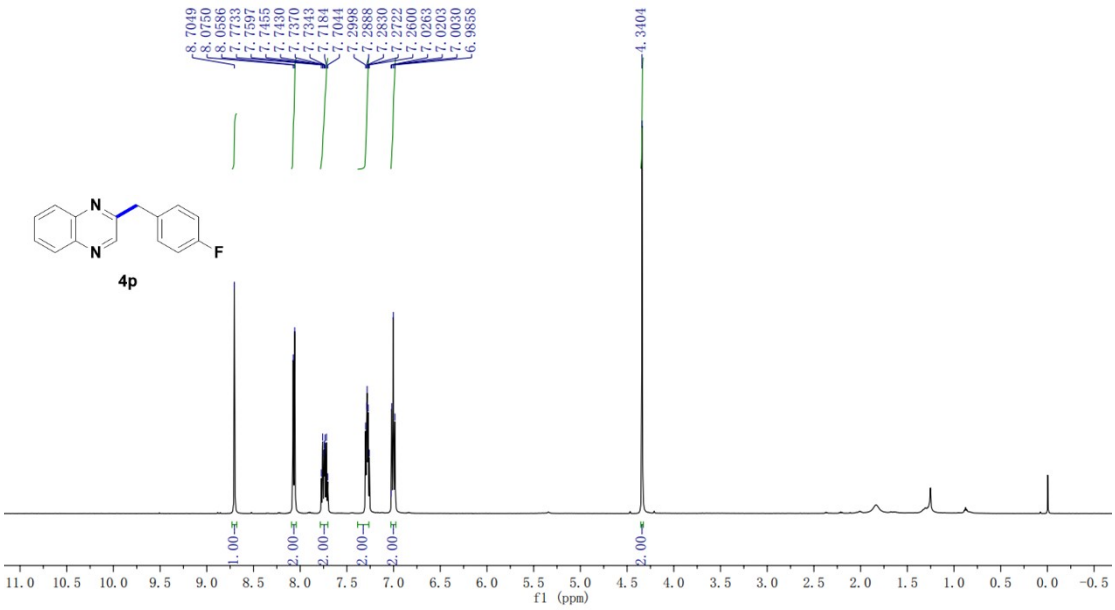
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7.0030
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4.3404
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N
F
4p
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2.00
2.00
2.00
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2.00
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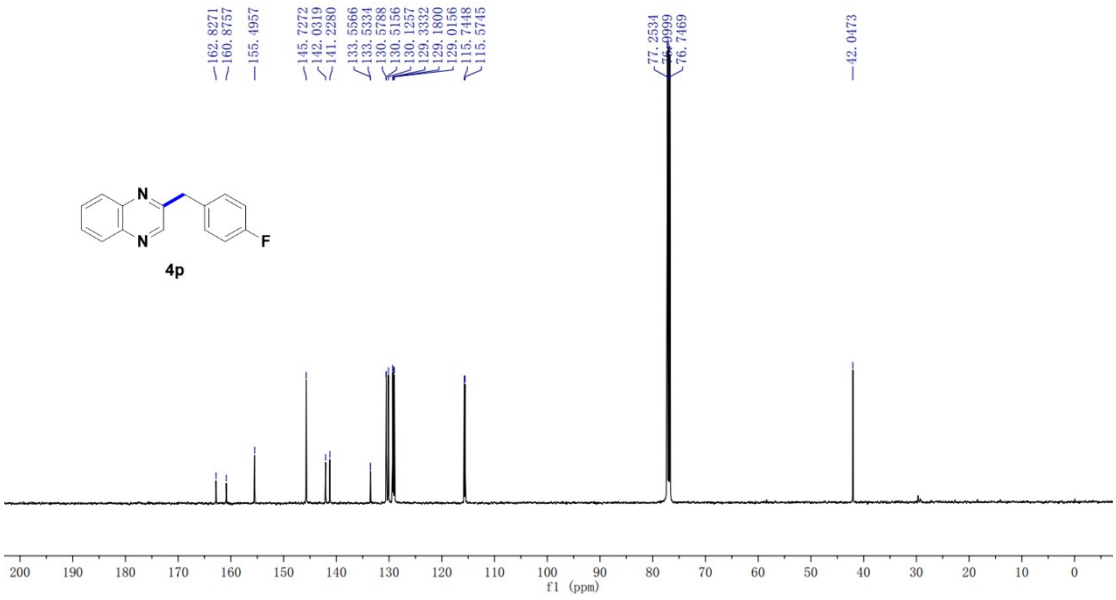
f1 (ppm)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115.7448
115.5745
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F
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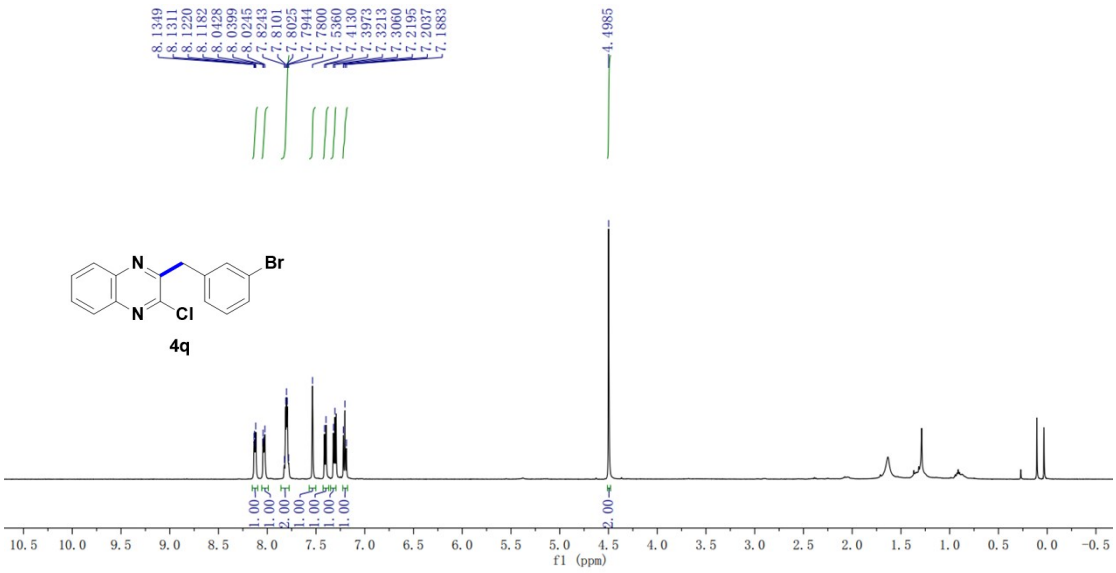
f1 (ppm)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7.3060
7.2195
7.2037
7.1883
4.4985
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Cl
Br
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1.00
2.00
1.00
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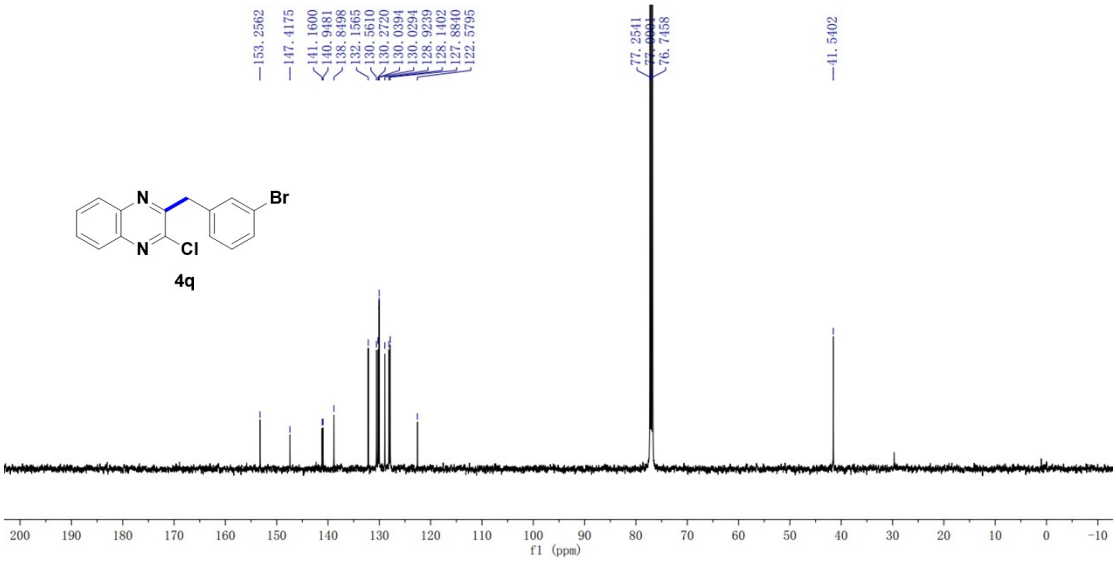
1.00
1.00
2.00
f1 (ppm)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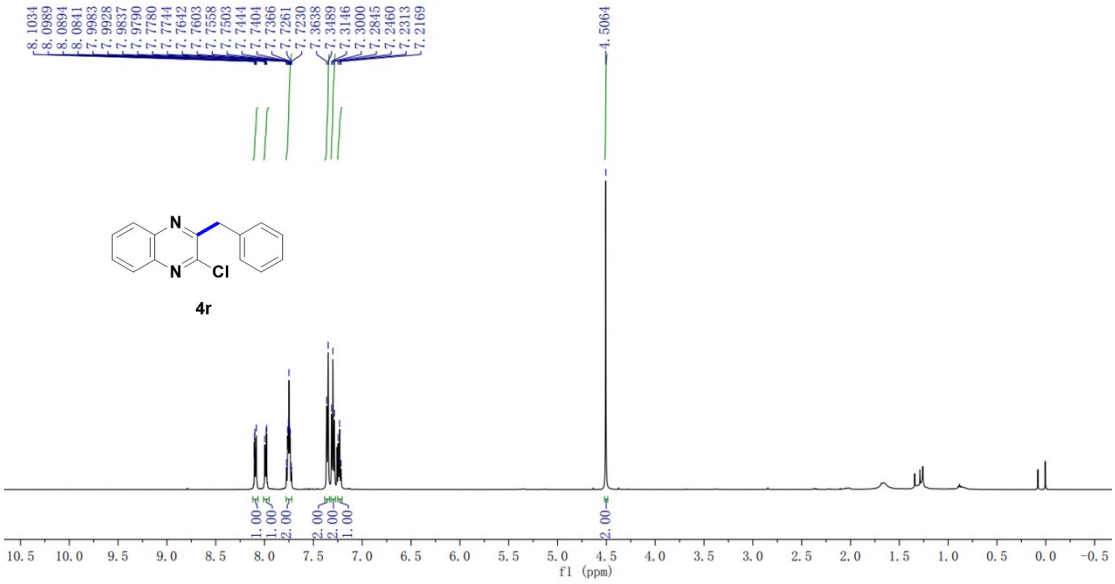
76.7458
41.5402
N
N
Cl
Br
4q
f1 (ppm)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7.7558
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7.3146
7.3000
7.2845
7.2460
7.2313
7.2169
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Cl
4r
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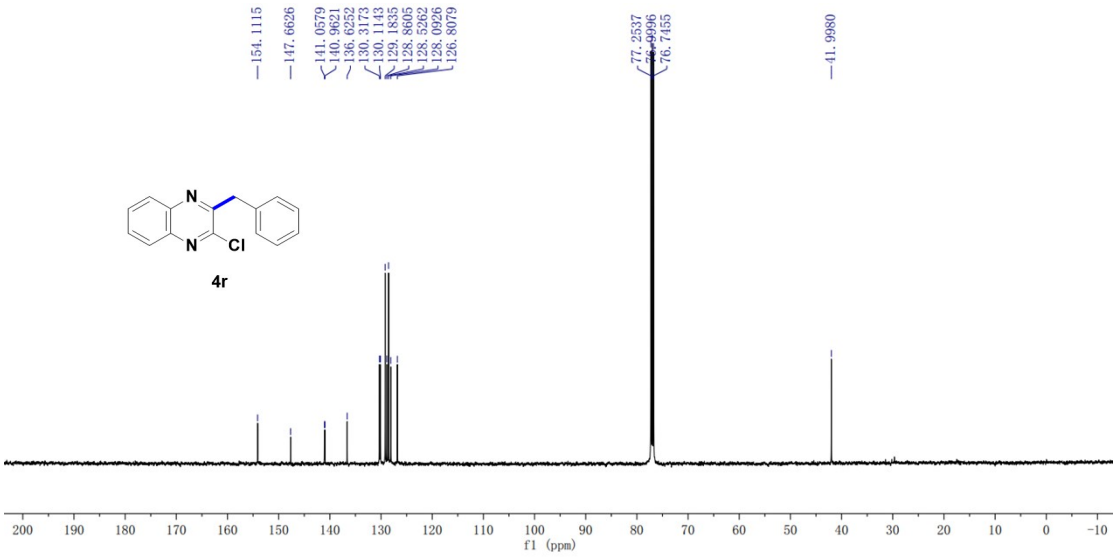
1.00
2.00
2.00
2.00
1.00
2.00
f1 (ppm)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76.7455
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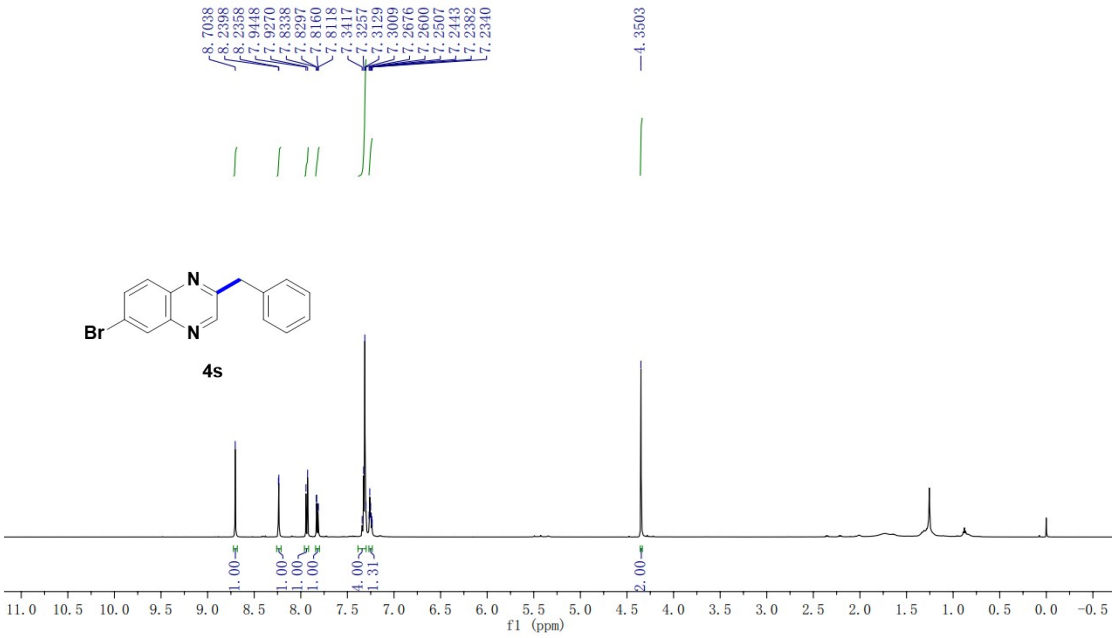
Cl
4r
f1 (ppm)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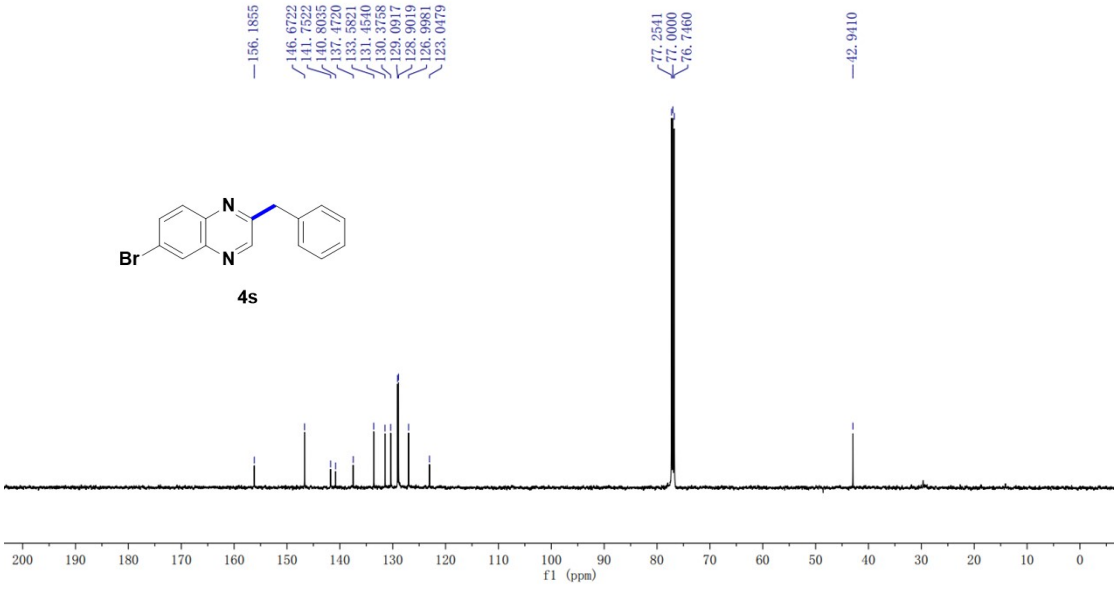
7.8297
7.8160
7.8118
7.3417
7.3257
7.3129
7.3009
7.2676
7.2600
7.2507
7.2443
7.2382
7.2340
4.3503
Br
N
N
4s
1.00
1.00
1.00
4.00
1.31
2.00
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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146.6722
141.7522
140.8035
137.4720
133.5821
131.4540
130.3758
129.0917
128.9019
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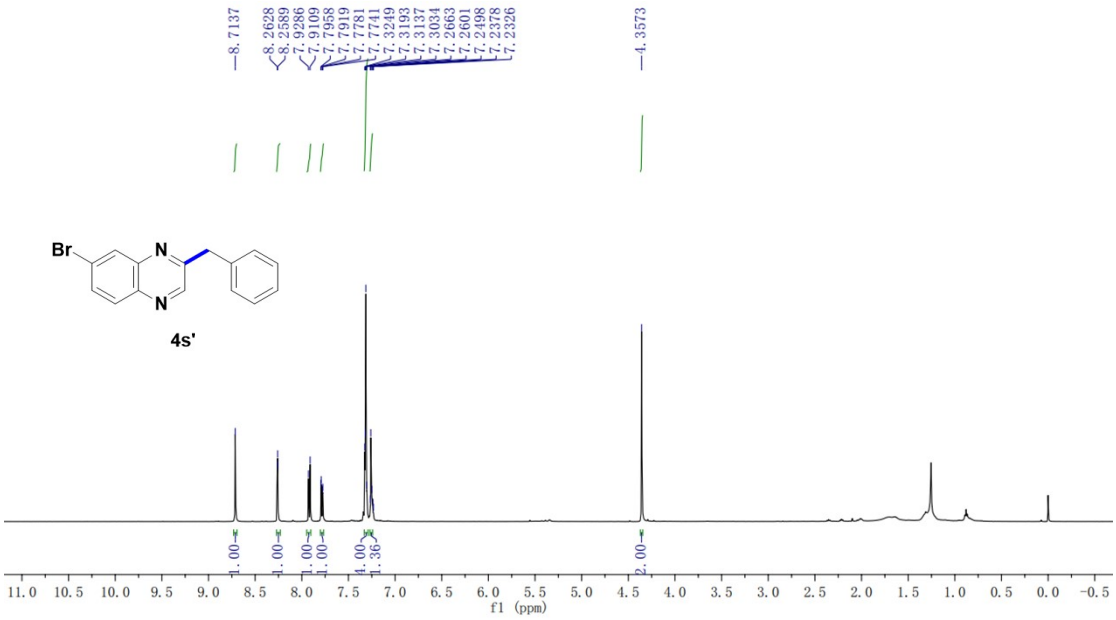
123.0479
77.2541
77.0000
76.7460
42.9410
Br
N
N
4s
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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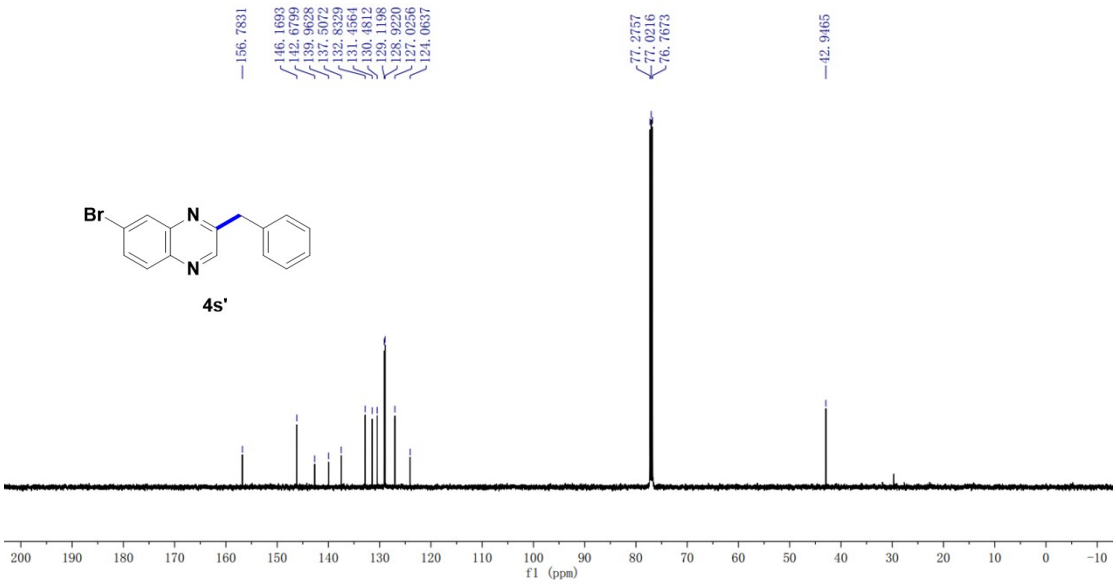
7.3193
7.3137
7.3034
7.2663
7.2601
7.2498
7.2378
7.2326
4.3573
Br
N
N
4s'
1.00
1.00
1.00
1.00
4.00
1.36
2.00
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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142.6799
139.9628
137.5072
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131.4564
130.4812
129.1198
128.9220
127.0256
124.0637
77.2757
77.0216
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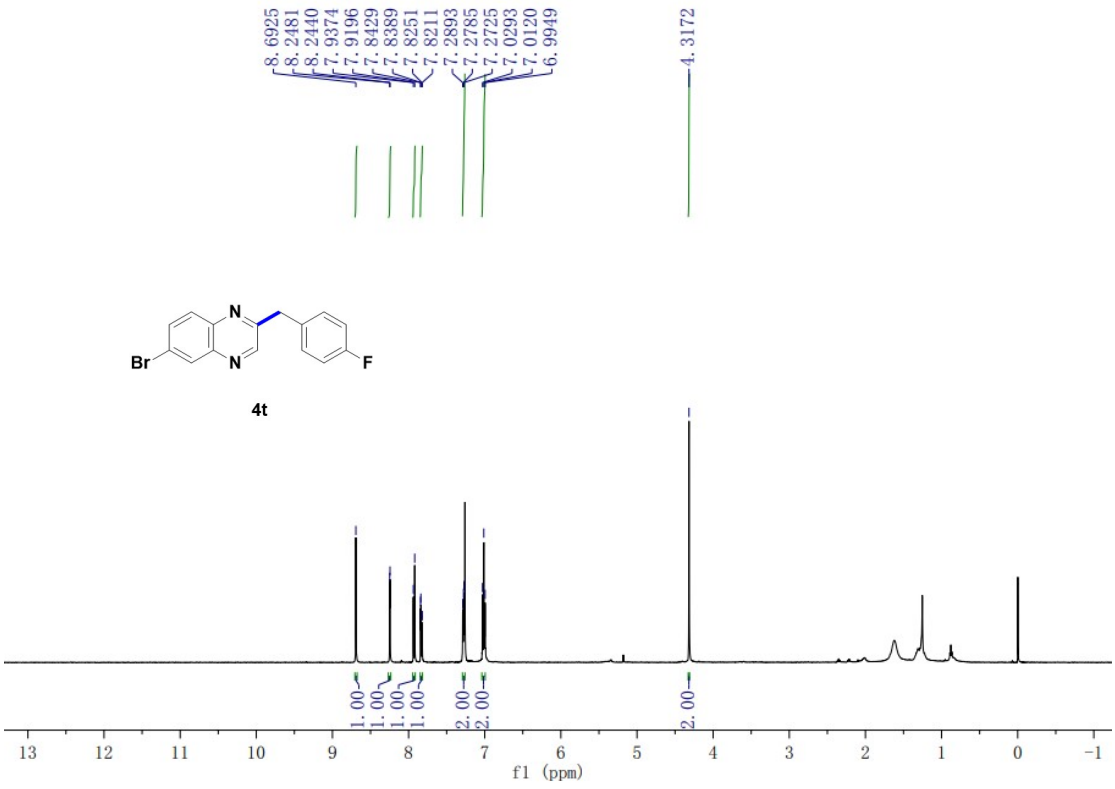
Br
N
N
4s'
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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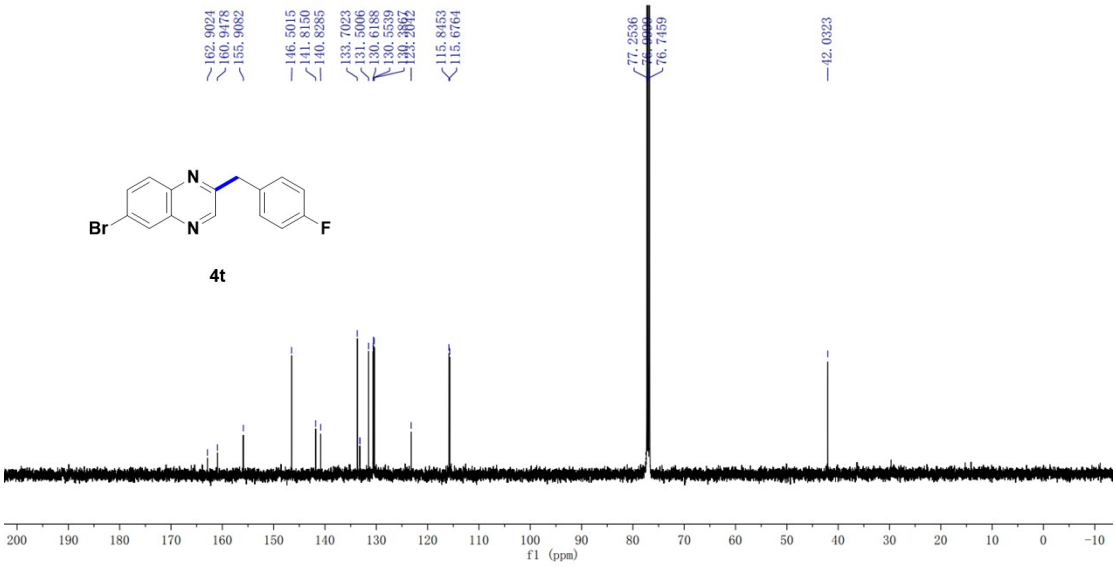
8.2440
7.9374
7.9196
7.8429
7.8389
7.8251
7.8211
7.2893
7.2785
7.2725
7.0293
7.0120
6.9949
4.3172
Br
N
N
F
4t
1.00
1.00
1.00
1.00
2.00
2.00
2.00
13
12
11
10
9
8
7
6
5
4
3
2
1
0
−1
f1 (ppm)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141.8150
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133.7023
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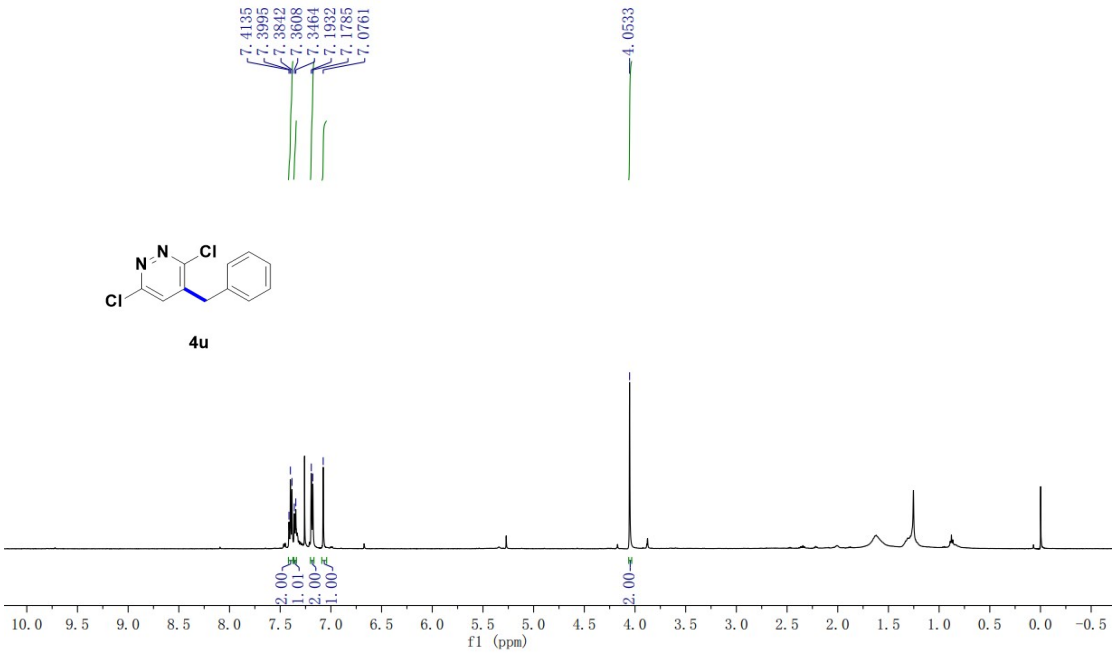
115.8453
115.6764
77.2536
76.7459
42.0323
Br
N
N
F
4t
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)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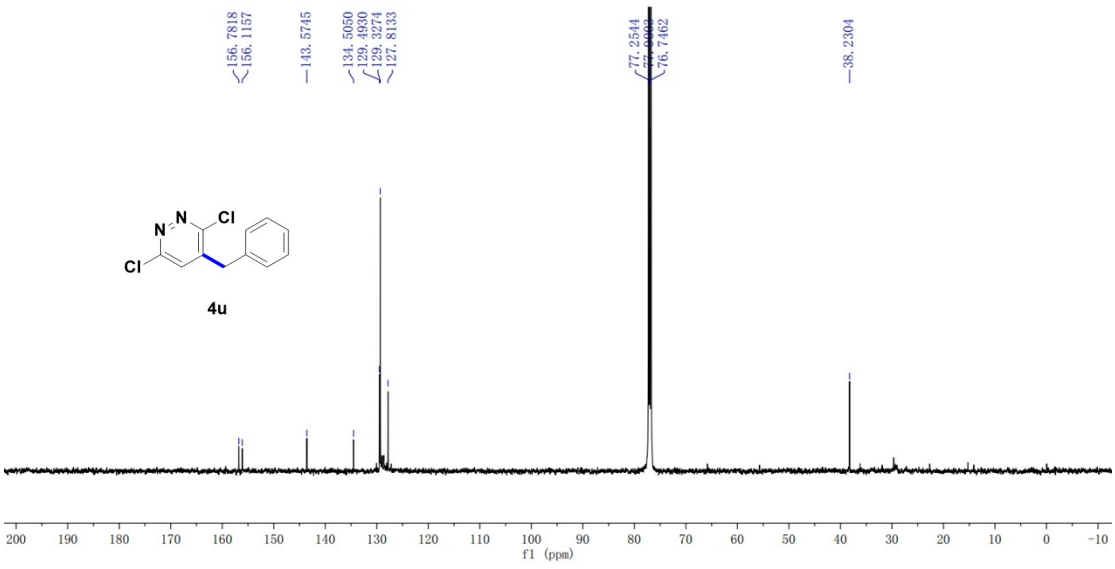
7.3995
7.3842
7.3608
7.3464
7.1932
7.1785
7.0761
4.0533
Cl
N
N
Cl
4u
2.00
1.01
2.00
1.00
2.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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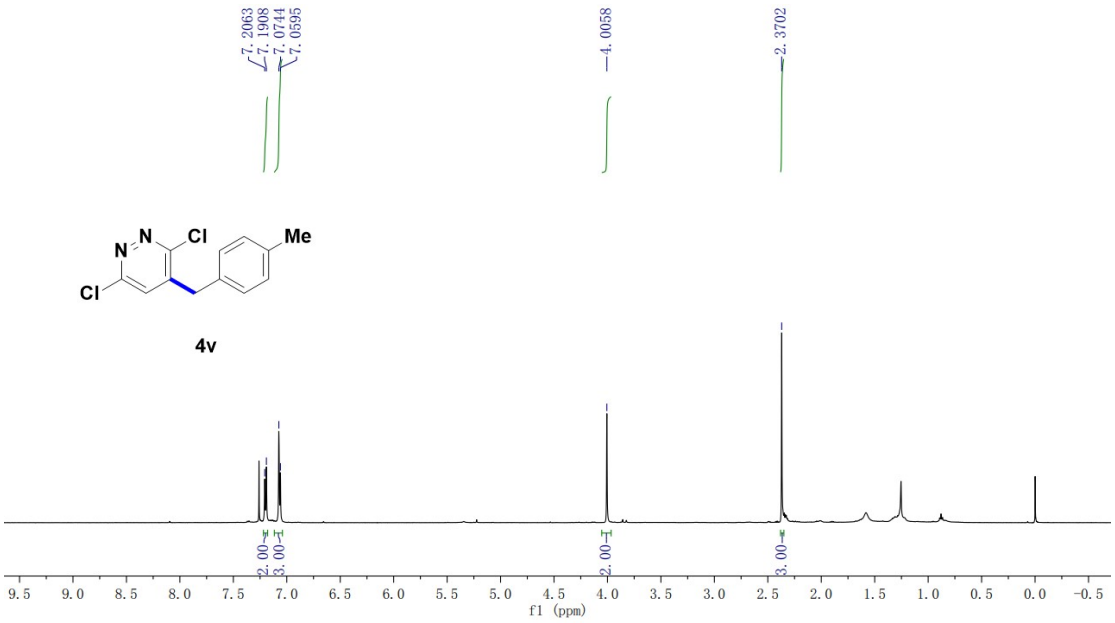
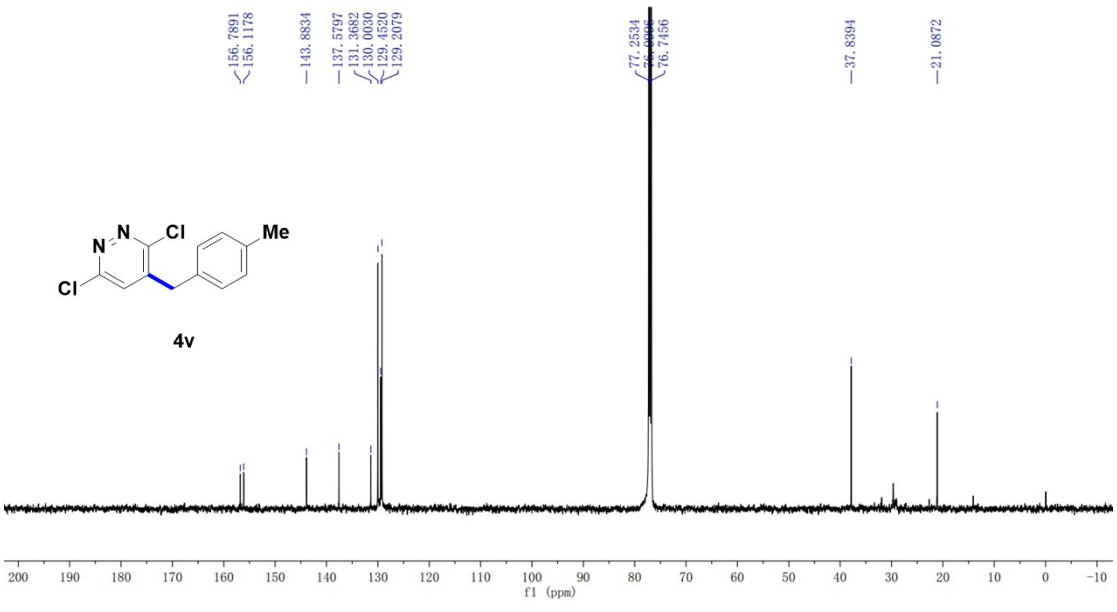
156.1157
143.5745
134.5050
129.4930
129.3274
127.8133
77.2544
76.7462
38.2304
Cl
N
N
Cl
4u
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


7.2063
7.1908
7.0744
7.0595
4.0058
2.3702
N
N
Cl
Cl
Me
4v
2.00
3.00
2.00
3.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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156.1178
143.8834
137.5797
131.3682
130.0030
129.4520
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77.2534
76.7456
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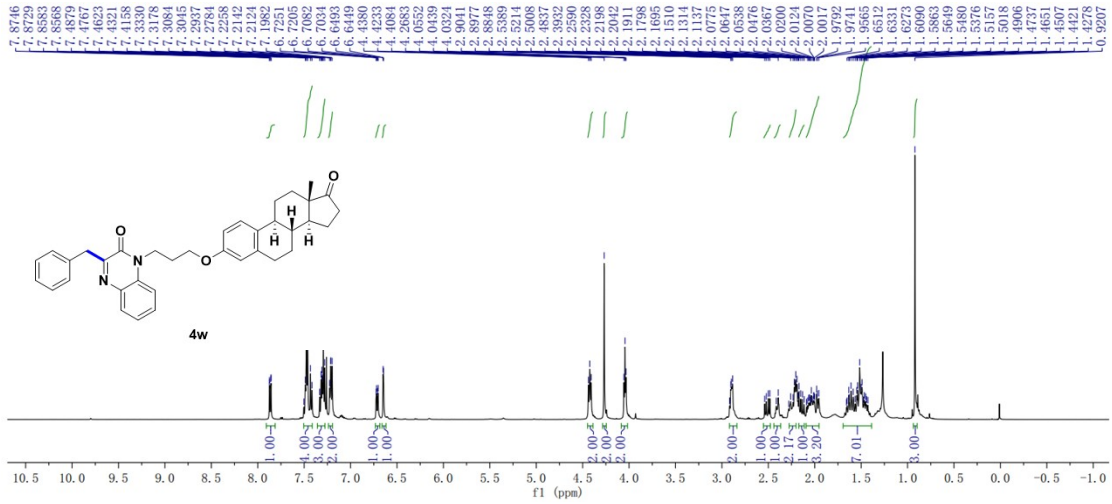
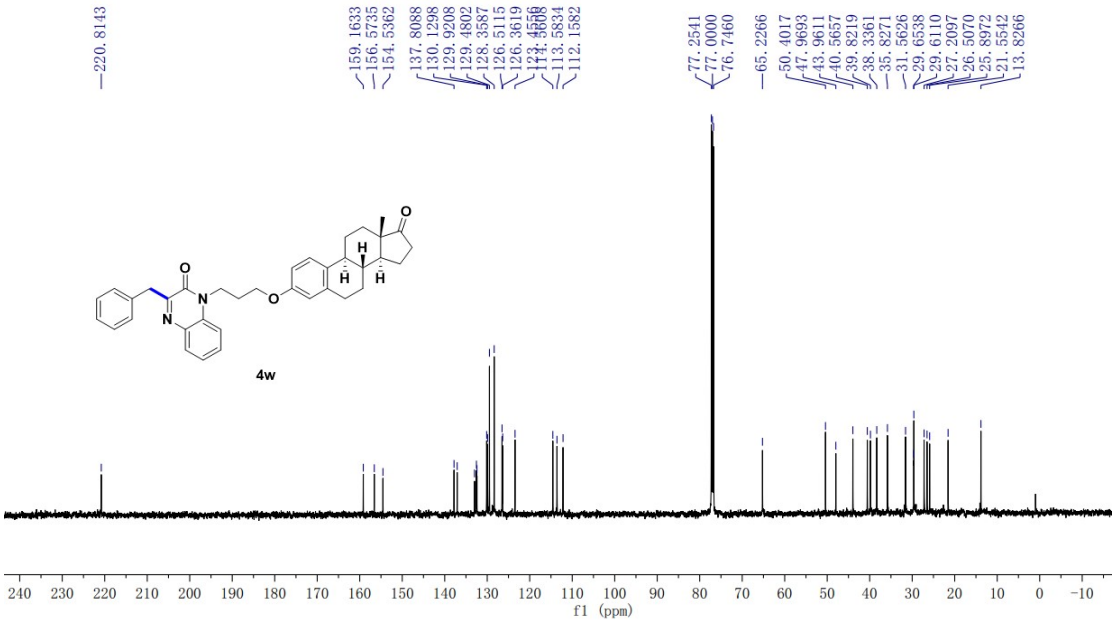
N
N
Cl
Cl
Me
4v
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


4w
f1 (ppm)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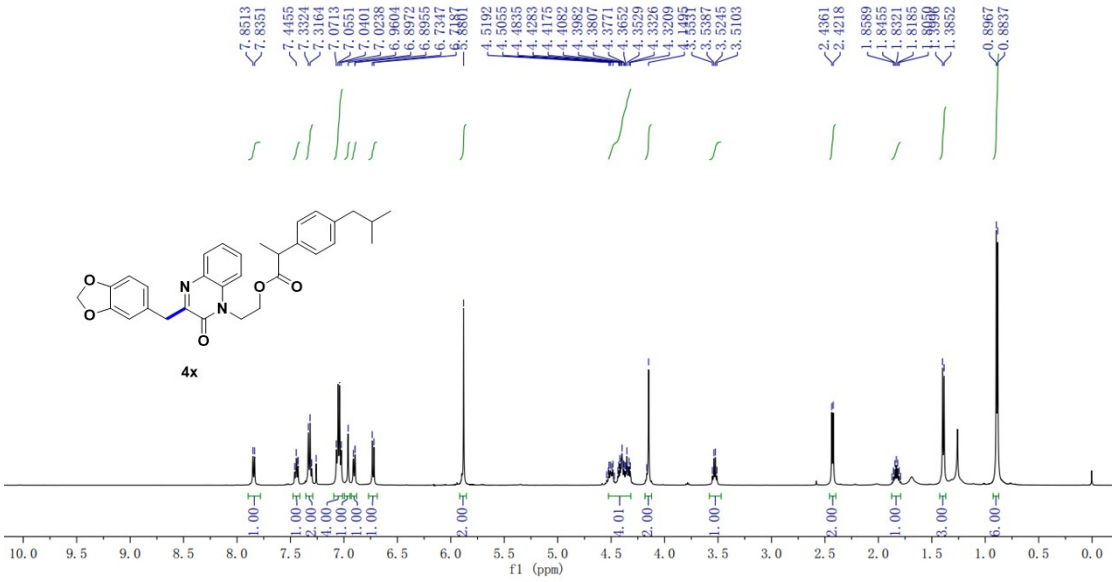
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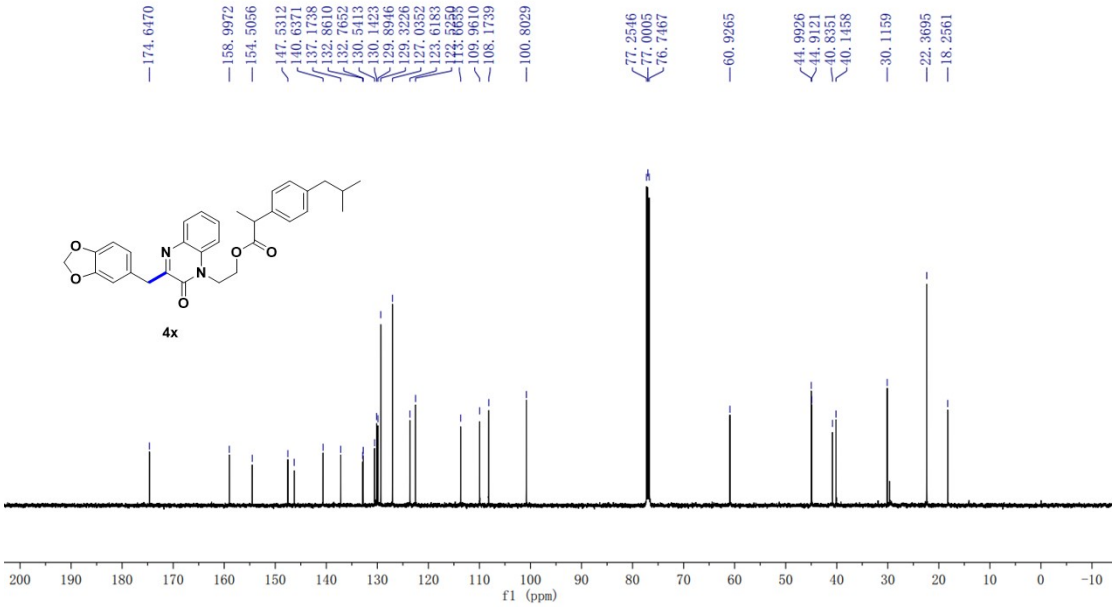
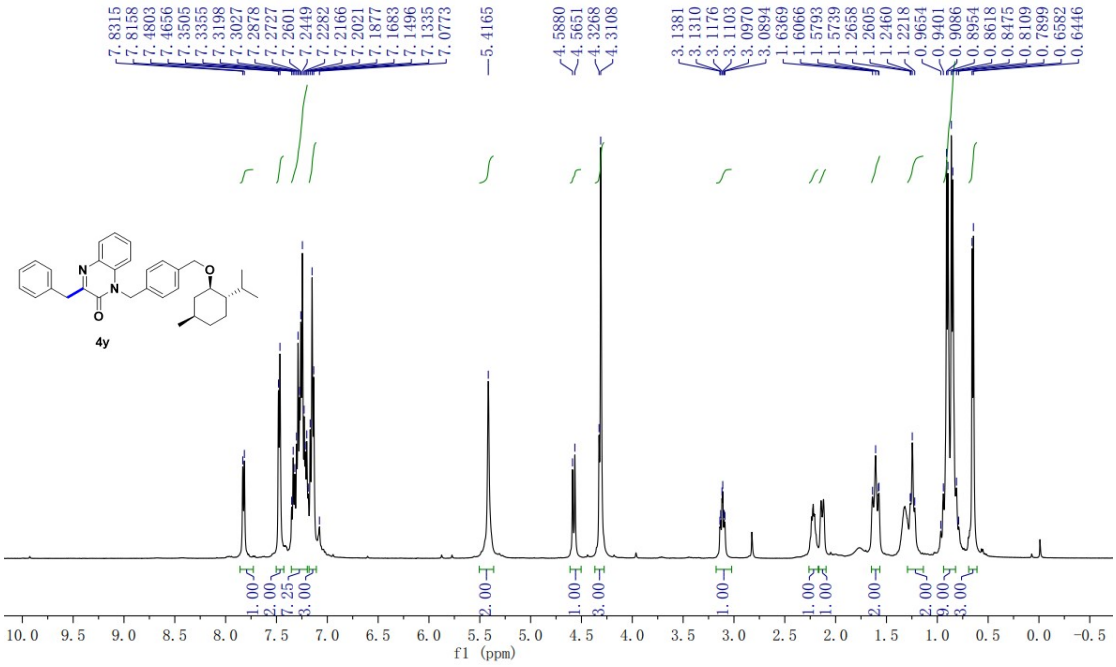
f1 (ppm)


4x
f1 (ppm)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7.2601
7.2449
7.2282
7.2166
7.2021
7.1877
7.1683
7.1496
7.1335
7.0773
5.4165
4.5880
4.5651
4.3268
4.3108
3.1381
3.1310
3.1176
3.1103
3.0970
3.0894
1.6369
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1.5793
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1.2658
1.2605
1.2460
1.2218
0.9654
0.9401
0.9086
0.8954
0.8618
0.8475
0.8109
0.7899
0.6582
0.6446
1.00
2.00
7.25
3.00
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1.00
1.00
1.00
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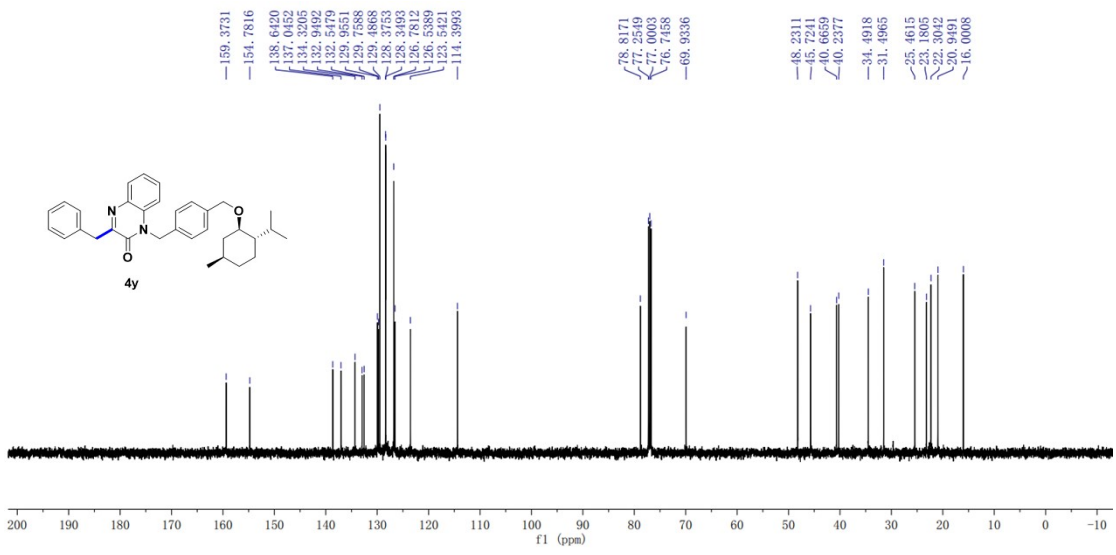
3.00
f1 (ppm)
4y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123.5421
114.3993
78.8171
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40.6659
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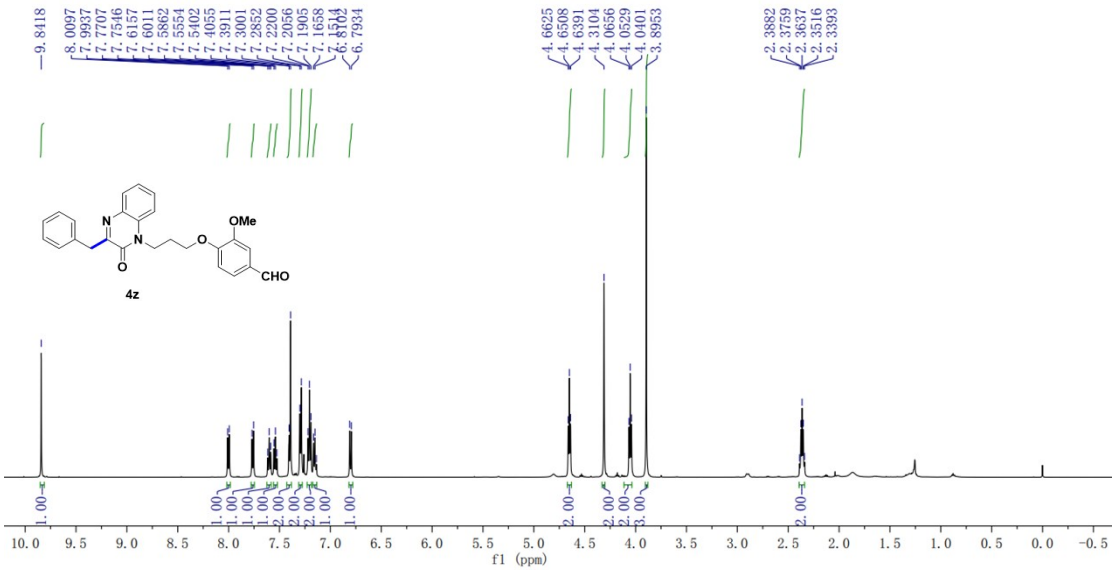
4y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7.7546
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7.5554
7.5402
7.4055
7.3911
7.3001
7.2852
7.2200
7.2056
7.1905
7.1658
7.1514
6.8102
6.7934
4.6625
4.6508
4.6391
4.3104
4.0656
4.0529
4.0401
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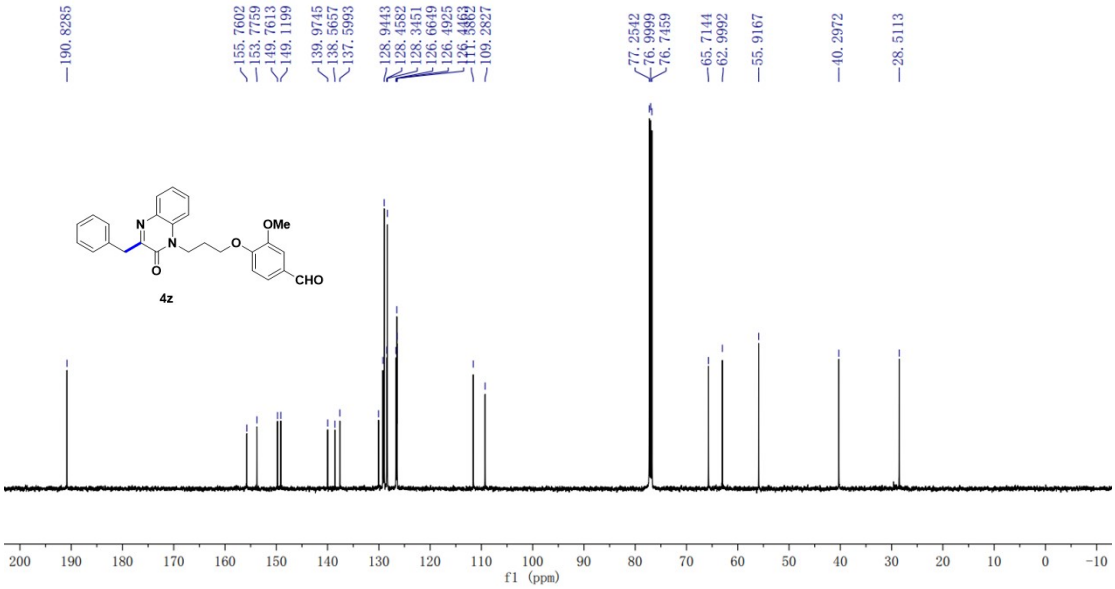
2.3882
2.3759
2.3637
2.3516
2.3393
OMe
CHO
4z
f1 (ppm)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126.4925
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111.3862
109.2827
77.2542
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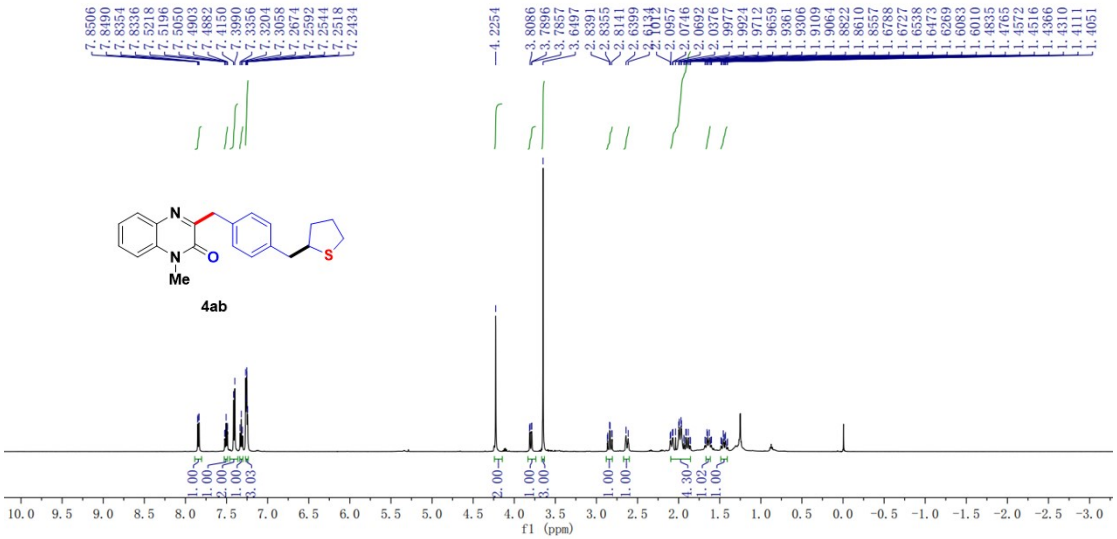
65.7144
62.9992
55.9167
40.2972
28.5113
OMe
CHO
4z
f1 (ppm)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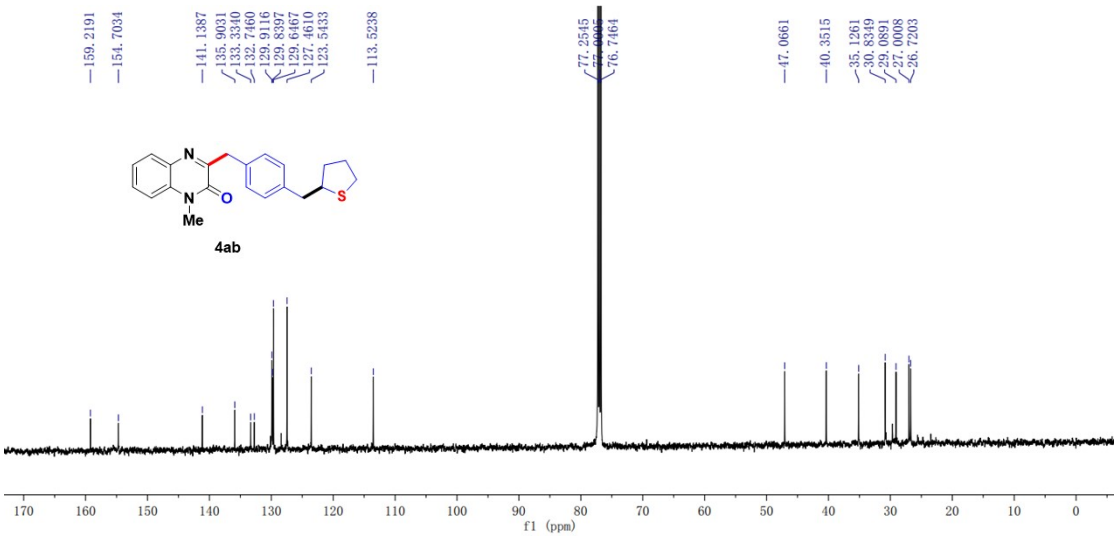
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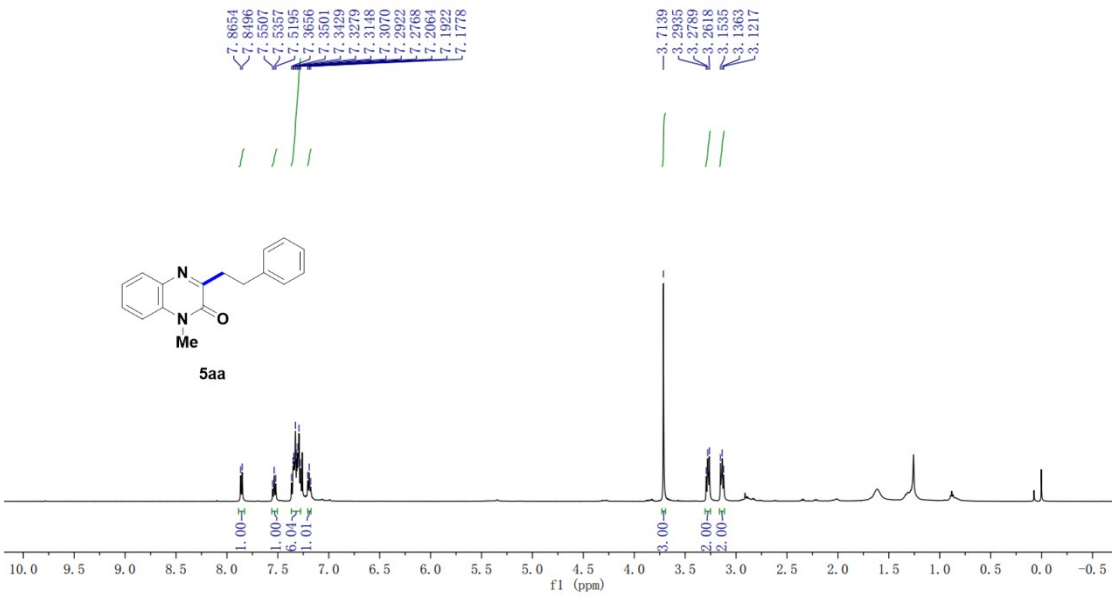
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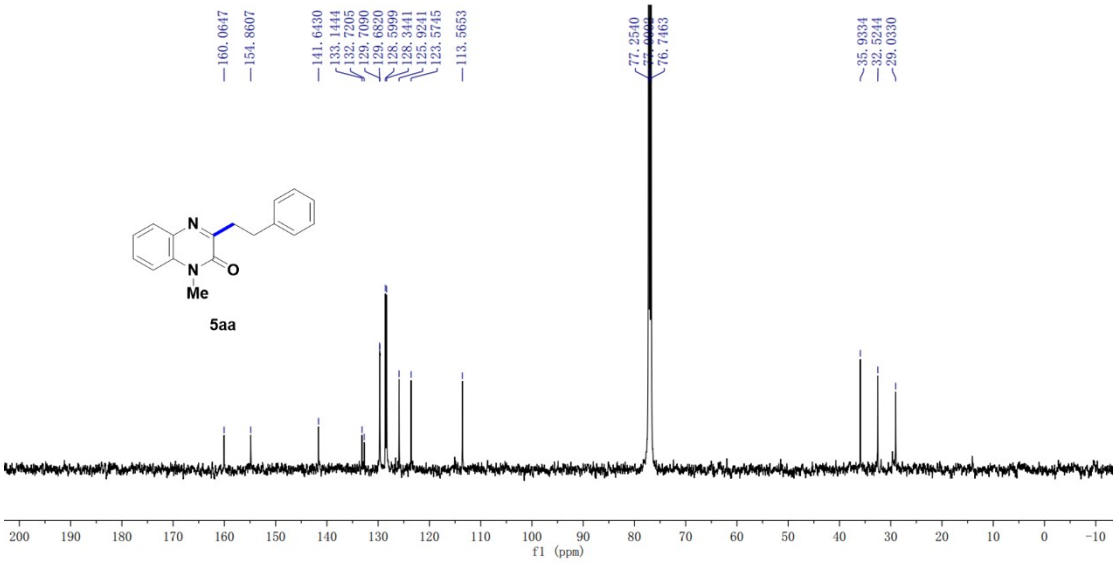
7.3070
7.2922
7.2768
7.2064
7.1922
7.1778
3.7139
3.2935
3.2789
3.2618
3.1535
3.1363
3.1217
N
N
O
Me
5aa
1.00
1.00
6.04
1.01
3.00
2.00
2.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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123.5745
113.5653
77.2540
77.0008
76.7463
35.9334
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N
N
O
Me
5aa
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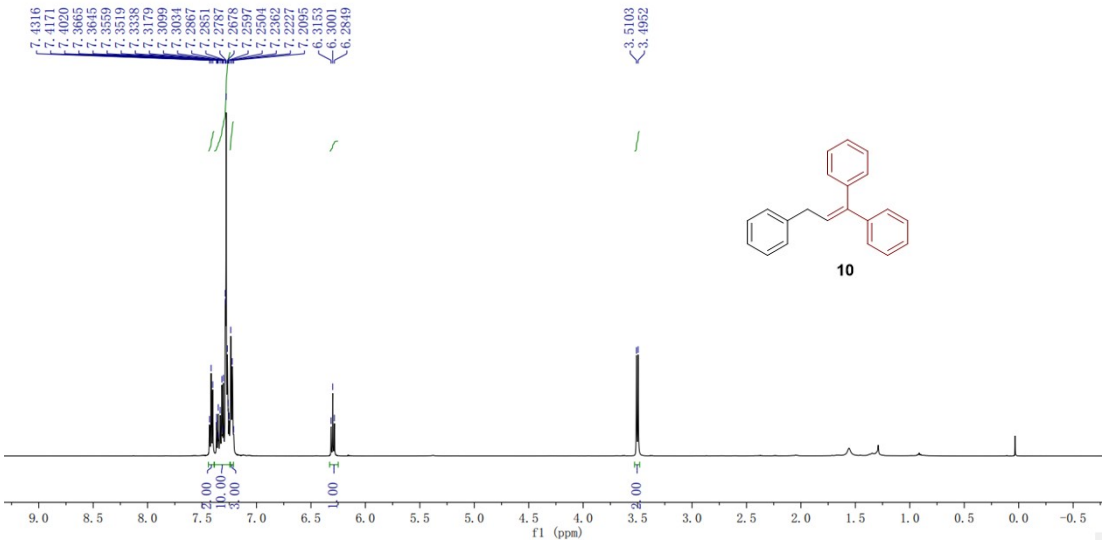
f1 (ppm)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7.3099
7.3034
7.2867
7.2851
7.2787
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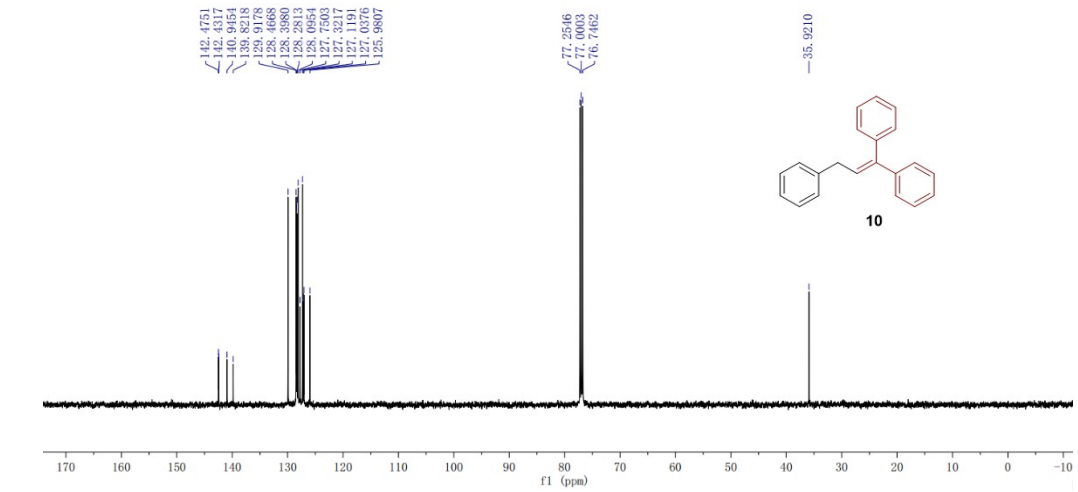
7.2597
7.2504
7.2362
7.2227
7.2095
7.2153
6.3001
6.2849
3.5103
3.4962
2.00
10.00
3.00
1.00
2.00
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)
10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127.0376
125.9807
77.2546
77.0003
76.7462
35.9210
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)
10