Supporting Information

Catalyst-free and Oxidant-free Cyclocondensation of 2-Aminobenzamides with Glycosides under Visible Light

Tiancheng Gong, ‡[a] Jian Wang, ‡[a] Zirui Zhuang,[b] Bing Sun,*[a] Fang-Lin Zhang*[a]

[a] School of Chemistry, Chemical Engineering and Life Sciences Wuhan University of Technology, Wuhan 430070, P. R. China.

[b] Wuhan Britain-China School, Wuhan 430070, P. R. China.

*E-mail: bing.sun@whut.edu.cn

*E-mail: fanglinzhang@whut.edu.cn

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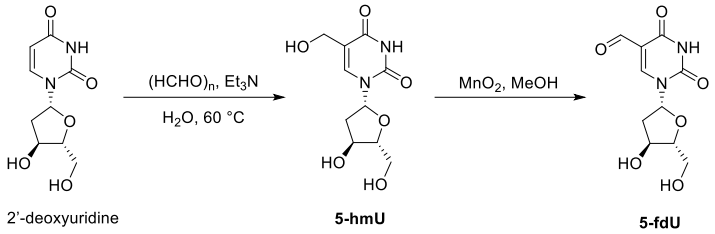
1. General Information

Aldehydes and amide were obtained from the commercial sources or synthesized following literature procedures. Solvents were obtained from Sigma-Aldrich, Alfa-Aesar, Oakwood, and Acros and used directly without further purification. Analytical thin layer chromatography was performed on 0.25 mm silica gel 60-F254. Visualization was carried out with UV light. ^{1}H NMR was recorded on Bruker instrument (500MHz). Chemical shifts were quoted in parts per million (ppm) referenced to 0.0 ppm for tetramethylsilane. The following abbreviations (or combinations thereof) were used to explain multiplicities: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, br = broad. Coupling constants, *J*, were reported in Hertz unit (Hz). ^{13}C NMR spectra were recorded on Bruker instrument (126 MHz), and were fully decoupled by broad band proton decoupling. Chemical shifts were reported in ppm referenced to either the center line of a triplet at 77.0 ppm of chloroform-*d* or referenced to the center line of a septet at 39.52 ppm of DMSO-d_6. High-resolution mass spectra (HRMS) were recorded on an Agilent Mass spectrometer using ESI-TOF (electrospray ionization-time of flight).

2. Experimental Section

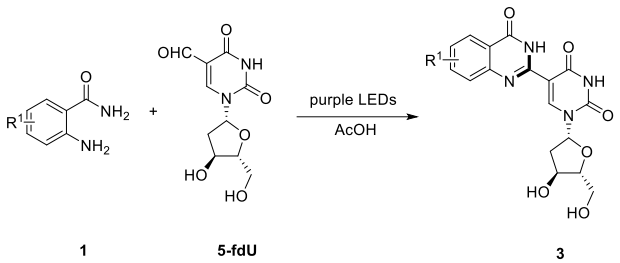
2.1 Synthesis of 3a-3g



The starting material **5-fdU** was prepared according to previous methond[1, 2]:

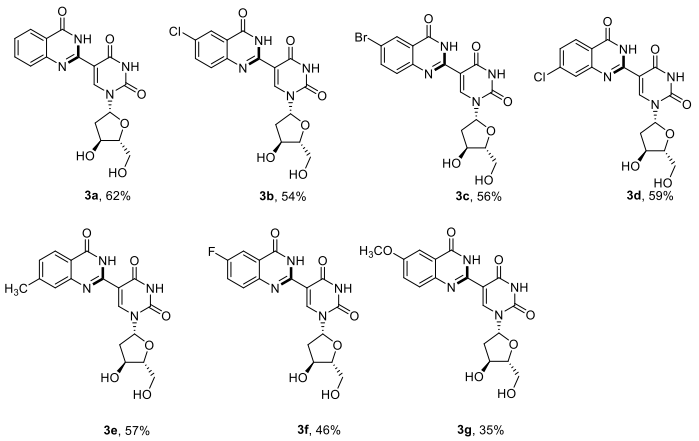
A suspension of 2'-deoxyuridine (5.25 g, 23.0 mmol) and paraformalclehyde (3.11 g, 103.5 mmol) in 80 mL H_2O was treated with 5.6 mL triethylamine and heated at 60 ℃ for 4 days. During the reaction, paraformaldehyde (4.49 g, 149.5 mmol) was added once daily, and triethylamine (1 mL) and water (10 mL) were supplied on the second day. After that, the solvent was evaporated under reduced pressure and the residue was recrystallized in MeOH to afford **5-hmU** as a white solid (4.11 g, 15.9 mmol). The obtained **5-hmU** (0.70 g, 2.7 mmol) was added into a 25 mL round-bottom flask and dissolved with 10 mL MeOH followed by activated manganese dioxide (0.94 g, 10.9 mmol). The suspension was heated with stirring at 50 °C for 24 h. After cooling to room temperature, the mixture was filtered with diatomite. The filtrate was collected and concentrated in *vacuo*. Further purification by silica gel column chromatography (CH_2Cl_2 : MeOH = 6:1) afforded **5-fdU** as a white solid (0.60 g, 2.35 mmol).Yield: 79%.

The product **3a** - **3g** were synthesized through ***general procedure A***:



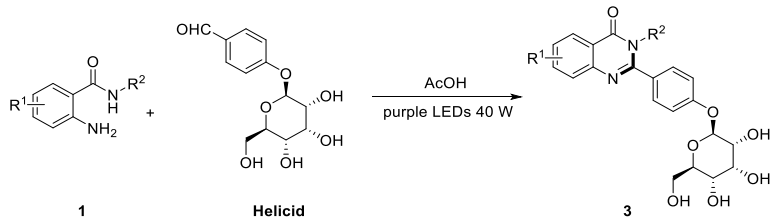
The starting material **1** (0.1 mmol) and **5-fdU** (0.11 mmol, 28.2 mg) were dissolved in AcOH (1 mL) and the mixture was stirred under 5 W purple LEDs at room temperature (25 ℃) for 12 - 24 h. After that, petroleum ether (10 mL) was added to the mixture and stirred for 1 h. Then the suspension was filtered and filter residue was washed with little

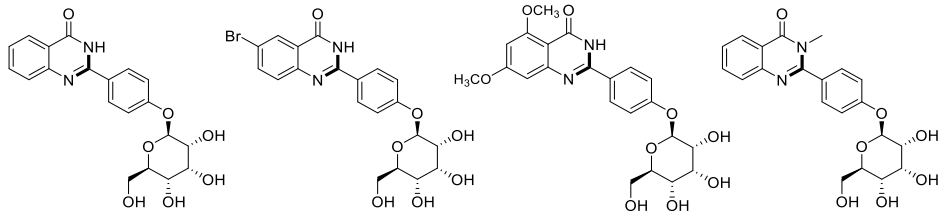
EtOAc and 95% EtOH. The collected solid was dried in vacuo to get the desired product.

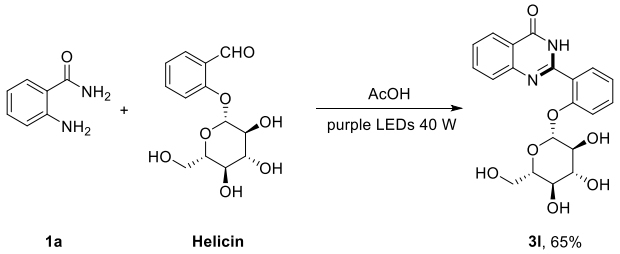


2.2 Synthesis of 3h - 3l

General produce B (3h-3l): Substitued anthranilamide (**1**, 0.20 mmol) and aldehyde (0.22 mmol) were dissolved in AcOH (2 mL) and the mixture was stirred under 5 W purple LEDs at room temperature (25 °C) for 12 - 24 h. After completion of the reaction (TLC monitored), the solvent was evaporated and the resulting residue was purified by silica gel column chromatography to afford the desired products.







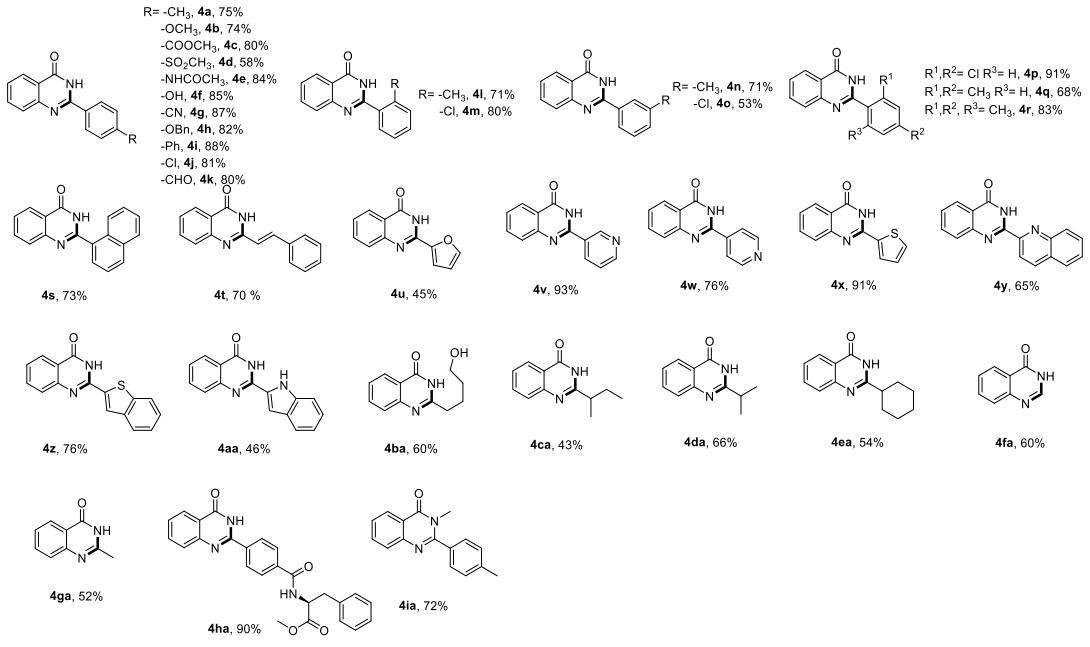
2.3 Sythesis of 4a – 4la

General producure C (**4a**, **4b**, **4c**, **4l - 4ga**)

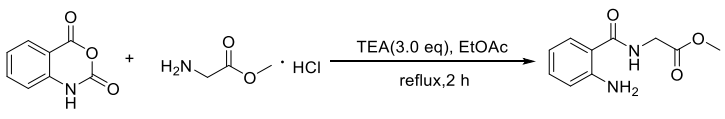
Anthranilamide (**1**, 0.30 mmol, 40.8 mg) and aldehyde (**2**, 0.33 mmol) were dissolved in AcOH (3 mL) and the mixture was stirred under 5 W purple LEDs at room temperature (25 ℃) for 4-24 h. After completion of the reaction, the solvent was evaporated and the resulting residue was purified by silica gel column chromatography to afford the desired products.

General producure D (**4d - 4k**, **4ha**, **4ia**)

Anthranilamide (**1**, 0.30 mmol, 40.8 mg) and aldehyde (**2**, 0.33 mmol) were dissolved in AcOH (3 mL) and the mixture was stirred under 5 W purple LEDs at room temperature (25 ℃) for 4-24 h. After completion of the reaction, H_2O (10 mL) was added to the reaction mixture and stirred for 1 h. Then the suspension was filtered and filter residue was washed with H_2O and petroleum ether : EtOAc (5:1). The collected solid was dried in vacuo to afford the desired product.



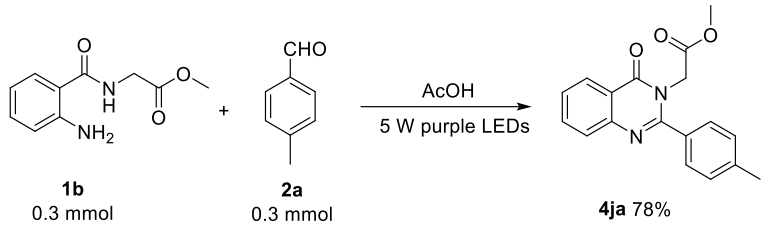
Synthesis of 4ja



The starting material **1b** was prepared according to previous methond[3]:

To a solution of isatoic anhydride (0.5 g, 3.1 mmol) in EtOAc (10 mL) was added methylglycinate hydrochloride (0.38 g, 3.1 mmol) and Et_3N (0.8 mL, 6.1 mmol) at room

temperature and reaction mixture was refluxed for 2 h. After completion of the reaction (as monitored by TLC), the solvent was removed under reduced pressure. The crude residue was purified by column chromatography over silica gel using PE/EtOAc (4:6, v/v) as eluent to afford the desired product **1b** (0.56 g from 0.5 g, 88%) as a white solid.

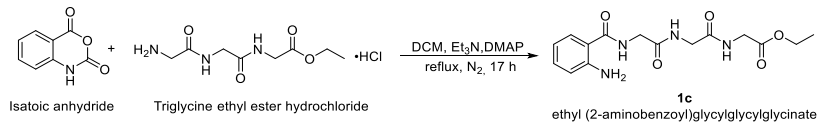


methyl 2-(4-oxo-2-(p-tolyl)quinazolin-3(4H)-yl)acetate (4ja)

4ja was isolated through a silica gel column chromatography (PE: EtOAc = 1:1) as a white solid (72 mg, 78% yield).

^{1}H NMR (500 MHz, Chloroform-*d*) δ 8.30 (d, *J* = 8.0 Hz, 1H), 7.80-7.72 (m, 2H), 7.53-7.47 (m, 1H), 7.43 (d, *J* = 8.0 Hz, 2H), 7.29 (d, *J* = 8.0 Hz, 2H), 4.66 (s, 1H), 3.74 (s, 1H), 2.41 (s, 1H). **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 168.6, 162.4, 155.8, 147.5, 140.7, 134.9, 132.0, 129.8, 127.9, 127.8, 127.3, 127.0, 120.5, 52.8, 47.8, 21.6.

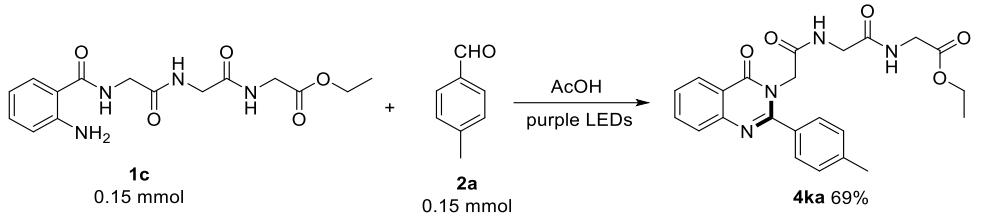
Synthesis of 4ka



The starting material **N-(2-Aminobenzoyl)triglycine ethyl ester (1c)** was prepared according to previous methond[4]:

Triglycine ethyl ester hydrochloride (0.40 g, 1.58 mmol) was dissolved in DCM (100 mL) and triethylamine (0.44 mL, 3.15 mmol). 4-Dimethylaminopyridine (20 mg, 0.16 mmol) was added and the suspension was heated to reflux temperature. Isatoic anhydride (1.79 g, 11.0 mmol) was added once the solution had cooled slightly and the resulting suspension was refluxed for 17 h, under nitrogen. The solid residue was collected by filtration. The remaining solution was washed with water (3 × 25 mL). The aqueous layer was washed with ethyl acetate (3 × 50 mL) and the organic layers were combined and dried over magnesium sulfate. The solvent was removed in *vacuo* and the resulting residue was combined with the solid collected by filtration. This was

dissolved in methanol and DCM, evaporated onto silica (2 g) and then purified twice by column chromatography (silica, ethyl acetate, followed by ethyl acetate–methanol 9 : 1 then 1 : 1) to give the product **1c** (0.3 g, 56%) as a cream powder.



1c
0.15 mmol

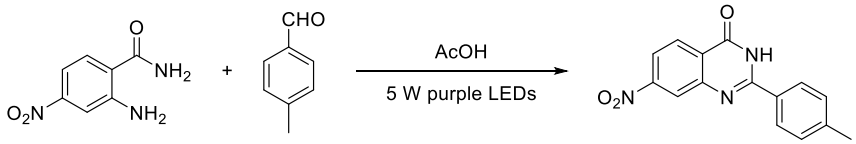
2a
0.15 mmol

4ka 69%

4ka was isolated through a silica gel column chromatography (PE: EtOAc from 1:1 to pure EtOAc) as a white solid (45 mg, 69% yield).

^{1}H NMR (500 MHz, DMSO-d_6) δ 8.50 (t, J = 6.0 Hz, 1H), 8.30 (t, J = 6.0 Hz, 1H), 8.15 (d, J = 8.0 Hz, 1H), 7.86 (t, J = 7.5 Hz, 1H), 7.69 (d, J = 8.0 Hz, 1H), 7.57 (t, J = 7.5 Hz, 1H), 7.50 (d, J = 8.0 Hz, 2H), 7.32 (d, J = 8.0 Hz, 2H), 4.53 (s, 2H), 4.09 (q, J = 7.0 Hz, 2H), 3.85 (d, J = 6.0 Hz, 2H), 3.76 (d, J = 5.5 Hz, 2H), 2.38 (s, 3H), 1.19 (t, J = 7.0 Hz, 3H). **^{13}C NMR** (126 MHz, DMSO-d_6) δ 169.7, 169.1, 167.1, 161.4, 156.2, 147.1, 139.6, 134.7, 132.2, 129.0, 128.2, 127.3, 127.0, 126.2, 120.2, 60.5, 48.7, 41.8, 40.7, 21.0, 14.1.

Synthesis of 4la



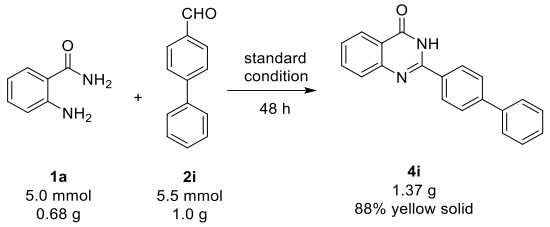
1d
0.3 mmol

2a
0.33 mmol

4la
less than 5%

4-Nitro-*o*-aminobenzamide (**1d**, 0.30 mmol, 54.3 mg) and *p*-Methyl benzaldehyde (**2a**, 0.33 mmol, 39.6 mg) were dissolved in AcOH (3 mL) and the mixture was stirred under 5 W purple LEDs at room temperature (25 °C) for 12 h. Reaction progress was monitored by thin-layer chromatography (TLC), which revealed negligible product formation upon completion of the reaction.

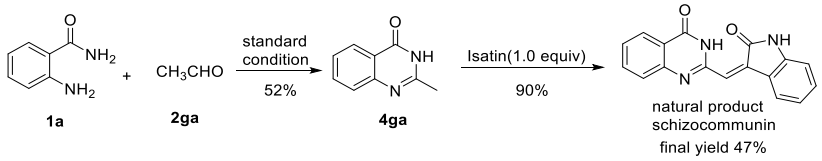
2.4 Gram-scale reaction: synthesis of 4i



Anthranilamide (**1a**, 5.0 mmol, 0.68 g) and 4-biphenylcarboxaldehyde (**2i**, 5.5 mmol, 1.0 g) were dissolved in AcOH (15 mL). Then the solution was stirred under purple LEDs at room temperature (25 ℃) for 48 h. After that, H_2O (10 mL) was added into the mixture and stirred for 30 minutes. The resulting suspension was filtured and the filter residue was washed with H_2O (5 mL), EtOAc (2 mL) for three times respectly. The collected yellow solid was dried in *vacuo* to get the desired product **4i** (1.37 g, 88%) without further purfication.

2.5 The synthesis of natural products: schizocommunin and mackinazolione

1) schizocommunin:

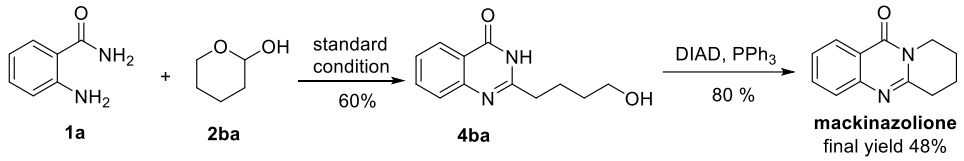


Anthranilamide (**1**, 0.4 mmol, 27.2 mg) and acetaldehyde (**2ga**, 0.6 mmol, 26.4 mg) were dissolved in AcOH(3 mL). Then the solution was stirred under 5 W purple LEDs at room temperature(25 ℃). After that, water was added the reaction mixture. The aqueous layer was extracted three times with 20 mL EtOAc. The combined organic layers were dried with anhydrous Na_2SO_4 , filtered. The solvent was evaporated and the crude mixture was purified by silica gel column chromatography (PE: EtOAc = 1:3) for pure product **4ga** as white solid(33 mg, 52%).

The next step carried out according to the literature[5]. A mixture of 2-methyl-4(3H)-quinazolinone (**4ga**, 80 mg, 0.5 mmol) and isatin (75 mg, 0.5 mmol) in glacial acetic acid (1 mL) was refluxed for 3.5 h. After the mixture was allowed to cool to rt, the precipitate was filtered, washed with methanol and dried to afford (Z)-2-((2'-oxoindolin-3'-ylidene)methyl)-quinazolin-4(3H)-one, **shizocommunin** (144.7 mg, 0.45 mmol, 90%) as an orange powder, which is a known compound. **^{1}H NMR** (500

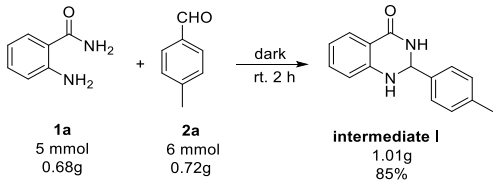
MHz, DMSO-d_6) δ 14.40 (s, 1H), 11.50 (s, 1H), 8.18 (d, J = 8.0 Hz, 1H), 7.95 (d, J = 7.5 Hz, 1H), 7.92-7.86 (m, 1H), 7.79 (d, J = 8.0 Hz, 1H), 7.61 (t, J = 7.5 Hz, 1H), 7.59 (s, 1H), 7.37 (t, J = 7.5 Hz, 1H), 7.09 (t, J = 7.5 Hz, 1H), 6.94 (d, J = 7.5 Hz, 1H). **^{13}C NMR** (126 MHz, DMSO-d_6) δ 168.8, 160.8, 150.4, 149.0, 141.6, 134.7, 134.3, 131.7, 130.0, 128.1, 128.0, 126.0, 123.3, 122.6, 122.0, 121.5, 110.6.

2) mackinazolione:



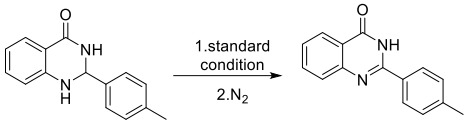
4ba was obtained through ***General producure B.*** and the next step was carried out according to litreature[6]. **4ba** (100 mg), diisopropyl azodicarboxylate (DIAD, 157 mg, 0.6 mmol, 1.2 equiv.), triphenylphosphine (144 mg, 0.55 mmol, 1.3 equiv.) and acetonitrile (8 mL) was added repectly to round-bottomed flask. The reaction mixture was stirred at room temperature and monitored by TLC. After completion, the reaction mixture was concentrated in *vacuo*. and the residue was purified through silica gel chromatography (PE: EtOAc =5:1) to give product **mackinazolione** (44.2 mg, 48%, m.p. 88–91 °C) which is a known compound. **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 8.26 (dd, J = 1.5, 8.0 Hz, 1H), 7.75 – 7.68 (m, 1H), 7.60 (d, J = 8.5 Hz, 1H), 7.45 – 7.39 (m, 1H), 4.09 (t, J = 6.0 Hz, 2H), 3.00 (t, J = 7.0 Hz, 2H), 2.06 – 1.91 (m, 4H). **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 162.4, 155.0, 147.5, 134.3, 126.8, 126.5, 126.2, 120.6, 42.5, 32.1, 22.3, 19.5.

2.6 Control experiments

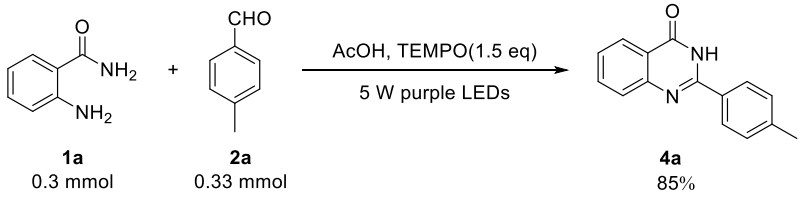


Anthranilamide (**1**, 5.0 mmol, 0.68 g) and *p*-Tolualdehyde (**2a**, 6.0 mmol, 0.72 g) were dissolved in AcOH (15 mL). Then the solution was stirred in the dark at room temperature (25 ℃) for 2 h. After that, H_2O (10 mL) was added into the mixture and stirred for 30 minutes. The resulting suspension was filtured and the filter residue was

washed with H_2O (5 mL), EtOAc (2 mL) for three times respectly. The collected white solid was dried in vacuo to get the desired product **intermediate I** (1.01 g, 85%) without further purification.**^{1}H NMR** (500 MHz, DMSO-d_6) δ 8.22 (s, 1H), 7.60 (dd, J = 2.0, 7.5 Hz, 1H), 7.37 (d, J = 8.0 Hz, 2H), 7.27-7.20 (m, 1H), 7.19 (d, J = 8.0 Hz, 2H), 7.04 (s, 1H), 6.73 (d, J = 7.5 Hz, 1H), 6.66 (t, J = 7.0 Hz, 1H), 5.70 (t, J = 2.0 Hz, 1H), 2.29 (s, 3H). **^{13}C NMR** (126 MHz, DMSO-d_6) δ 163.6, 147.9, 138.6, 137.7, 133.2, 128.8, 127.3, 126.8, 117.0, 115.0, 114.4, 66.4, 20.7.



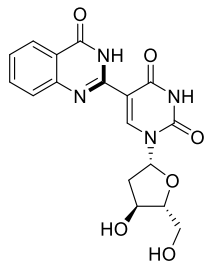
Intermediate I (0.2 mmol, 47.7 mg) was dissolved in AcOH (2 mL). Then the solution was stirred under 5 W purple LEDs at room temperature (25 ℃). After that, water was added the reaction mixture. The aqueous layer was extracted three times with 20 mL EtOAc. The combined organic layers were dried with anhydrous Na_2SO_4, filtered. Compound **4a** was isolated through a silica gel column chromatography (PE : EtOAc = 3:1) as a white solid (41.6 mg, 88% yield). Next, we put intermediate **I** in nitrogen to exclude oxygen in air and **4a** could also be gained in high yield (70%), demonstrating that oxygen is not necessary for the reaction.



Anthranilamide (**1a**, 0.30 mmol, 40.8 mg), aldehyde (**2a**, 0.33 mmol, 39.6mg) and TEMPO (0.45 mmol, 70.2 mg) were dissolved in AcOH (3 mL) and the mixture was stirred under 5 W purple LEDs at room temperature (25 ℃) for 4-24 h. After completion of the reaction, the solvent was evaporated and the resulting residue was purified by silica gel column chromatography (PE: EtOAc = 3:1) to afford a white solid (60.2 mg, 85% yield). This experiment indicates that the reaction was not involved with radical intermediates.

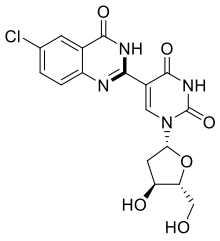
2.7 Characterization of Products

1-((2R,4S,5R)-4-hydroxy-5-(hydroxymethyl)tetrahydrofuran-2-yl)-5-(4-oxo-3,4-dihydroquinazolin-2-yl)pyrimidine-2,4(1H,3H)-dione (3a)


3a

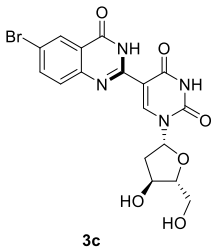
Compound **3a** was isolated through ***General Procedure A*** as a yellow solid (23.1 mg, 62% yield). **^{1}H NMR** (500 MHz, DMSO-d_6) δ 12.26-12.13 (m, N-H, 2H), 9.29 (s, 1H), 8.09 (d, *J* = 8.0 Hz, 1H), 7.81 (t, *J* = 7.5 Hz, 1H), 7.69 (d, *J* = 8.0 Hz, 1H), 7.47 (t, *J* = 7.5 Hz, 1H), 6.18 (t, *J* = 6.0 Hz, 1H), 5.33 (d, *J* = 4.5 Hz, 1H), 5.12 (t, *J* = 4.5 Hz, 1H), 4.33-4.27 (m, 1H), 3.93 (q, *J* = 3.5 Hz, 1H), 3.73-3.64 (m, 2H), 2.31-2.21 (m, 2H). **^{13}C NMR** (126 MHz, DMSO-d_6) δ 164.3, 160.8, 149.7, 149.2, 149.1, 145.4, 135.0, 127.7, 126.4, 126.3, 121.3, 103.6, 88.5, 86.5, 70.6, 61.4, 41.1. **HRMS (ESI)**: m/z calculated for $C_{17}H_{17}N_4O_6^+$ $[M+H]^+$ 373.1143, found 373.1143.

5-(6-chloro-4-oxo-3,4-dihydroquinazolin-2-yl)-1-((2R,4S,5R)-4-hydroxy-5-(hydroxymethyl)tetrahydrofuran-2-yl)pyrimidine-2,4(1H,3H)-dione (3b)


3b

Compound **3b** was isolated through ***General Procedure A*** as a yellow solid (22.0 mg, 54% yield). **^{1}H NMR** (500 MHz, DMSO-d_6) δ 12.29 (s, 1H), 12.23 (s, 1H), 9.32 (s, 1H), 8.02 (s, 1H), 7.84 (d, *J* = 9.0 Hz, 1H), 7.71 (d, *J* = 8.5 Hz, 1H), 6.17 (t, *J* = 6.5 Hz, 1H), 5.33 (d, *J* = 4.5 Hz, 1H), 5.14 (t, *J* = 4.5 Hz, 1H), 4.30 (t, *J* = 5.0 Hz, 1H), 3.93 (q, *J* = 3.5 Hz, 1H), 3.76-3.62 (m, 2H), 2.33-2.19 (m, 2H). **^{13}C NMR** (126 MHz, DMSO-d_6) δ 163.8, 159.3, 149.2, 149.1, 147.5, 145.3, 134.7, 130.1, 129.5, 124.8, 121.9, 102.8, 88.0, 86.1, 70.0, 60.9, 40.7. **HRMS (ESI)**: m/z calculated for $C_{17}H_{16}ClN_4O_6^+$ $[M+H]^+$ 407.0753, found 407.0750.

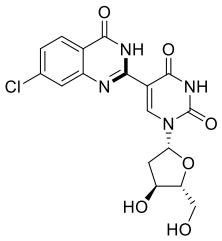
5-(6-bromo-4-oxo-3,4-dihydroquinazolin-2-yl)-1-((2R,4S,5R)-4-hydroxy-5-(hydroxymethyl)tetrahydrofuran-2-yl)pyrimidine-2,4(1H,3H)-dione (3c)


3c

Compound **3c** was isolated through ***General Procedure A*** as a yellow solid (25.3 mg, 56% yield). **^{1}H NMR** (500 MHz, DMSO-d_6) δ 12.29 (s, 1H), 12.24 (s, 1H), 9.31 (s, 1H), 8.15 (d, *J* = 2.5 Hz, 1H), 8.01 – 7.90 (m, 1H), 7.63 (d, *J* = 9.0 Hz, 1H), 6.17 (t, *J* = 6.0 Hz,

1H), 5.34 (d, *J* = 4.5 Hz, 1H), 5.14 (t, *J* = 4.5 Hz, 1H), 4.29 (q, *J* = 4.0, 4.5 Hz, 1H), 3.92 (q, *J* = 3.5 Hz, 1H), 3.76 – 3.59 (m, 2H), 2.33 – 2.19 (m, 2H). **^{13}C NMR** (126 MHz, DMSO-d_6) δ 163.8, 159.2, 149.3, 149.2, 147.8, 145.4, 137.4, 129.7, 128.0, 122.3, 118.2, 102.8, 88.1, 86.1, 70.1, 60.9, 40.7. **HRMS (ESI)**: m/z calculated for $C_{17}H_{15}BrN_4O_6^+$ $[M+H]^+$ 488.9807, found 488.9814.

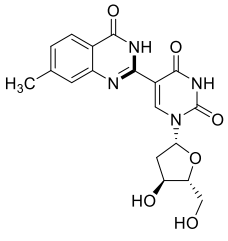
5-(7-chloro-4-oxo-3,4-dihydroquinazolin-2-yl)-1-((2R,4S,5R)-4-hydroxy-5-(hydroxymethyl)tetrahydrofuran-2-yl)pyrimidine-2,4(1H,3H)-dione (3d)



3d

Compound **3d** was isolated through ***General Procedure A*** as a yellow solid (24.0 mg, 59% yield). **^{1}H NMR** (500 MHz, DMSO-d_6) δ 12.31-12.19 (m, 2H), 9.40 (s, 1H), 8.07 (d, *J* = 8.5 Hz, 1H), 7.77 (s, 1H), 7.47 (d, *J* = 8.5 Hz, 1H), 6.18 (t, *J* = 6.0 Hz, 1H), 5.35 (d, *J* = 4.5 Hz, 1H), 5.23-5.18 (m, 1H), 4.31 (s, 1H), 3.93 (s, 1H), 3.77-3.63 (m, 2H), 2.33-2.19 (m, 2H). **^{13}C NMR** (126 MHz, DMSO-d_6) δ 163.8, 159.7, 150.2, 149.9, 149.2, 145.7, 139.2, 127.9, 126.3, 126.1, 119.6, 102.7, 88.0, 86.1, 70.0, 60.8, 40.8. **HRMS (ESI)**: m/z calculated for $C_{17}H_{16}ClN_4O_6^+$ $[M+H]^+$ 407.0753, found 407.0750.

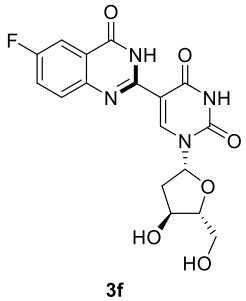
1-((2R,4S,5R)-4-hydroxy-5-(hydroxymethyl)tetrahydrofuran-2-yl)-5-(7-methyl-4-oxo-3,4-dihydroquinazolin-2-yl)pyrimidine-2,4(1H,3H)-dione (3e)



3e

Compound **3e** was isolated through ***General Procedure A*** as a yellow solid (22.0 mg, 57% yield). **^{1}H NMR** (500 MHz, DMSO-d_6) δ 12.19 (s, 1H), 12.08 (s, 1H), 9.26 (s, 1H), 7.97 (d, *J* = 8.0 Hz, 1H), 7.49 (s, 1H), 7.28 (d, *J* = 8.0 Hz, 1H), 6.18 (t, *J* = 6.5 Hz, 1H), 5.33 (d, *J* = 4.5 Hz, 1H), 5.11 (t, *J* = 4.7 Hz, 1H), 4.30 (t, *J* = 4.5 Hz, 1H), 3.93 (q, *J* = 4.0 Hz, 1H), 3.65-3.72(m, 2H), 2.46 (s, 3H), 2.32-2.22 (m, 2H). **^{13}C NMR** (126 MHz, DMSO-d_6) δ 164.2, 160.6, 149.7, 149.3, 149.1, 145.5, 145.3, 127.9, 127.3, 126.2, 118.9, 103.6, 88.5, 86.5, 70.6, 61.4, 41.1, 21.9. **HRMS (ESI)**: m/z calculated for $C_{18}H_{19}N_4O_6^+$ $[M+H]^+$ 387.1299, found 387.1298.

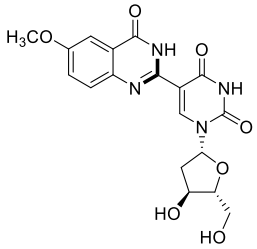
5-(6-fluoro-4-oxo-3,4-dihydroquinazolin-2-yl)-1-((2R,4S,5R)-4-hydroxy-5-(hydroxymethyl)tetrahydrofuran-2-yl)pyrimidine-2,4(1H,3H)-dione (3f)



3f

Compound **3f** was isolated through ***General Procedure A*** as a yellow solid (17.8 mg, 46% yield). **^{1}H NMR** (500 MHz, DMSO-d_6) δ 12.26 (s, 1H), 12.21 (s, 1H), 9.29 (s, 1H), 7.81-7.67 (m, 3H), 6.18 (t, *J* = 6.5 Hz, 1H), 5.32 (d, *J* = 4.5 Hz, 1H), 5.13 (t, *J* = 4.5 Hz, 1H), 4.33-4.25 (m, 1H), 3.92 (q, *J* = 3.5 Hz, 1H), 3.74-3.62 (m, 2H), 2.33-2.19 (m, 2H). **^{13}C NMR** (126 MHz, DMSO-d_6) δ 163.7, 159.7 (d, *J* = 3.2 Hz), 159.6 (d, *J* = 252.0 Hz), 149.2, 148.2, 145.7, 144.9, 130.0 (d, *J* = 7.9 Hz), 123.2, 123.0, 121.9, 121.8, 110.4 (d, *J* = 23.5 Hz), 103.0, 88.0, 86.0, 70.0, 60.9, 40.7. **^{19}F NMR** (471 MHz, DMSO-d6) δ -114.3 (q, *J* = 7.6 Hz). **HRMS (ESI)**: m/z calculated for $C_{17}H_{16}FN_4O_6^+$ $[M+H]^+$ 391.1048, found 391.1044.

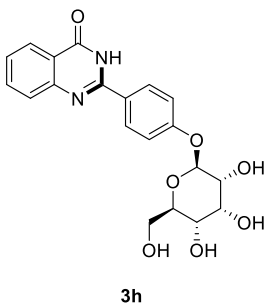
1-((2R,4S,5R)-4-hydroxy-5-(hydroxymethyl)tetrahydrofuran-2-yl)-5-(6-methoxy-4-oxo-3,4-dihydroquinazolin-2-yl)pyrimidine-2,4(1H,3H)-dione (3g)



3g

Compound **3g** was isolated through ***General Procedure A*** as a yellow solid (14.0 mg, 35% yield). **^{1}H NMR** (500 MHz, DMSO-d_6) δ 12.17 (s, 1H), 12.13 (s, 1H), 9.22 (s, 1H), 7.65 (d, *J* = 9.0 Hz, 1H), 7.49 (d, *J* = 3.0 Hz, 1H), 7.43 (dd, *J* = 3.0, 9.0 Hz, 1H), 6.18 (t, *J* = 6.5 Hz, 1H), 5.32 (d, *J* = 4.5 Hz, 1H), 5.11 (t, *J* = 4.5 Hz, 1H), 4.29 (q, *J* = 4.5 Hz, 1H), 3.92 (q, *J* = 4.0 Hz, 1H), 3.87 (s, 3H), 3.73-3.61 (m, 2H), 2.32-2.18 (m, 2H). **^{13}C NMR** (126 MHz, DMSO-d_6) δ 163.7, 160.0, 157.3, 149.2, 146.4, 144.2, 143.2, 129.0, 124.2, 121.5, 105.8, 103.4, 88.0, 85.9, 70.1, 61.0, 55.6, 40.6. **HRMS (ESI)**: m/z calculated for $C_{18}H_{19}N_4O_7^+$ $[M+H]^+$ 403.1248, found 403.1242.

2-(4-(((2S,3R,4R,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)tetrahydro-2H-pyran-2-yl)oxy)phenyl)quinazolin-4(3H)-one (3h)

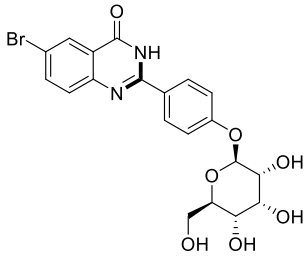


3h

Compound **3h** was isolated through a silica gel column chromatography (EtOAc : MeOH = 4:1) as a white solid (64.1 mg, 80% yield). **^{1}H NMR** (500 MHz, DMSO-d_6) δ 12.44 (s, 1H), 8.17 (d, *J* = 9.0 Hz, 2H), 8.14 (d, *J* = 8.0 Hz, 1H), 7.85-7.77 (m, 1H), 7.71 (d, *J* = 8.0 Hz, 1H), 7.49 (t, *J* = 7.5 Hz, 1H), 7.15 (d, *J* = 8.5 Hz, 2H), 5.25 (d, *J* = 8.0 Hz, 1H), 5.15 (d, *J* = 7.0 Hz,

1H), 5.02 (d, *J* = 4.0 Hz, 1H), 4.71 (d, *J* = 7.5 Hz, 1H), 4.55 (t, *J* = 5.5 Hz, 1H), 3.95 (q, *J* = 3.0 Hz, 1H), 3.78-3.66 (m, 2H), 3.52-3.40 (m, 3H). **^{13}C NMR** (126 MHz, DMSO-d_6) δ 162.3, 160.1, 151.9, 148.9, 134.6, 129.4, 127.3, 126.2, 125.9, 125.8, 120.7, 116.0, 98.2, 74.8, 71.5, 70.3, 67.0, 60.9. **HRMS (ESI)**: m/z calculated for $C_{20}H_{21}N_2O_7^+$ $[M+H]^+$ 401.1343, found 401.1355.

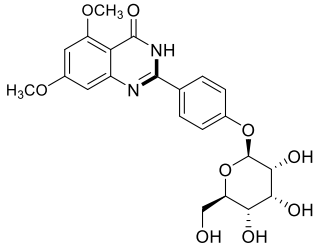
6-bromo-2-(4-(((2S,3R,4R,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)tetrahydro-2H-pyran-2-yl)oxy)phenyl)quinazolin-4(3H)-one (3i)



3i

Compound **3i** was isolated through a silica gel column chromatography (EtOAc : MeOH = 4:1) as a yellow solid (63.3 mg, 66% yield). **^{1}H NMR** (500 MHz, DMSO-d_6) δ 12.58 (s, 1H), 8.25 – 8.09 (m, 3H), 7.93 (d, *J* = 9.0 Hz, 1H), 7.64 (d, *J* = 9.0 Hz, 1H), 7.14 (d, *J* = 8.5 Hz, 2H), 5.24 (d, *J* = 8.0 Hz, 1H), 5.14 (s, 1H), 5.02 (s, 1H), 4.72 (s, 1H), 4.54 (s, 1H), 3.95 (s, 1H), 3.78-3.62 (m, 2H), 3.53-3.40 (m, 3H). **^{13}C NMR** (126 MHz, DMSO-d_6) δ 161.8, 160.2, 153.0, 148.0, 137.1, 129.6, 129.5, 128.0, 126.0, 122.3, 118.2, 116.0, 98.2, 74.8, 71.5, 70.2, 67.0, 60.9. **HRMS (ESI)**: m/z calculated for $C_{20}H_{20}BrN_2O_7^+$ $[M+H]^+$ 479.0448, found 479.0462.

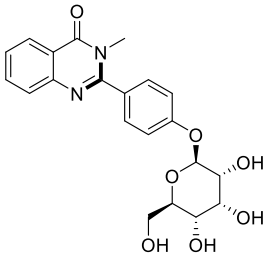
5,7-dimethoxy-2-(4-(((2S,3R,4R,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)tetrahydro-2H-pyran-2-yl)oxy)phenyl)quinazolin-4(3H)-one (3j)



3j

Compound **3j** was isolated through a silica gel column chromatography (EtOAc : MeOH = 5:1) as a yellow solid (35.0 mg, 38% yield). **^{1}H NMR** (500 MHz, DMSO-d_6) δ 11.95 (s, 1H), 8.14 (d, *J* = 8.5 Hz, 2H), 7.12 (d, *J* = 8.5 Hz, 2H), 6.51 (s, 1H), 5.23 (d, *J* = 8.0 Hz, 1H), 5.14 (s, 1H), 5.01 (s, 1H), 4.70 (s, 1H), 4.55 (s, 1H), 3.95 (s, 1H), 3.88 (s, 3H), 3.84 (s, 3H), 3.78-3.66 (m, 2H), 3.50-3.40 (m, 3H). **^{13}C NMR** (126 MHz, DMSO-d_6) δ 164.3, 161.0, 160.1, 159.9, 153.1, 152.5, 129.3, 125.6, 115.9, 104.6, 101.1, 98.2, 97.5, 74.8, 71.5, 70.3, 67.0, 60.9, 56.0, 55.6. **HRMS (ESI)**: m/z calculated for $C_{22}H_{25}N_2O_9^+$ $[M+H]^+$ 461.1555, found 461.1560.

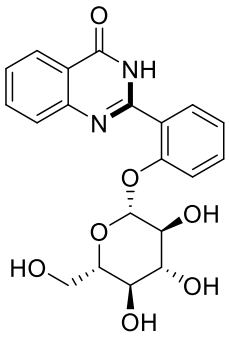
3-methyl-2-(4-(((2S,3R,4R,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)tetrahydro-2H-pyran-2-yl)oxy)phenyl)quinazolin-4(3H)-one (3k)



3k

Compound **3k** was isolated through a silica gel column chromatography (EtOAc : MeOH = 5:1) as a white solid (34.8 mg, 42% yield). **^{1}H NMR** (500 MHz, Chloroform-d) δ 8.16 (d, *J* = 8.0 Hz, 1H), 7.86 – 7.78 (m, 1H), 7.69 – 7.60 (m, 3H), 7.53 (t, *J* = 7.5 Hz, 1H), 7.15 (d, *J* = 8.5 Hz, 2H), 5.22 (d, *J* = 8.0 Hz, 2H), 5.14 (s, 1H), 4.90 (s, 1H), 4.61 (s, 1H), 3.98 (d, *J* = 3.0 Hz, 1H), 3.77 – 3.65 (m, 2H), 3.53-3.42 (m, 3H), 3.40 (s, 3H). **^{13}C NMR** (126 MHz, DMSO-d_6) δ 161.8, 158.7, 156.0, 147.1, 134.3, 130.0, 128.7, 127.1, 126.7, 126.1, 120.0, 115.8, 98.4, 74.8, 71.5, 70.3, 67.0, 60.9, 34.1. **HRMS (ESI)**: m/z calculated for $C_{21}H_{23}N_2O_7^+$ $[M+H]^+$ 415.1500, found 415.1508.

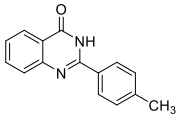
2-(2-(((2R,3S,4R,5R,6S)-3,4,5-trihydroxy-6-(hydroxymethyl)tetrahydro-2H-pyran-2-yl)oxy)phenyl)quinazolin-4(3H)-one (3l)



3l

Compound **3l** was isolated through a silica gel column chromatography (EtOAc : MeOH = 4:1) as a white solid (48.1 mg, 60% yield). **^{1}H NMR** (500 MHz, DMSO-d_6) δ 8.16 (d, *J* = 8.0 Hz, 1H), 7.91 (dd, *J* = 1.5, 8.0 Hz, 1H), 7.88 – 7.81 (m, 1H), 7.73 (d, *J* = 8.0 Hz, 1H), 7.61-7.51 (m, 2H), 7.41 (d, *J* = 8.5 Hz, 1H), 7.24 (t, *J* = 7.5 Hz, 1H), 5.26-5.13 (m, 2H), 5.11 (d, *J* = 7.5 Hz, 1H), 4.64 (t, *J* = 6.0 Hz, 1H), 3.77-3.69 (m, 1H), 3.57-3.48 (m, 1H), 3.45-3.37 (m, 2H), 3.35-3.31 (m, 3H), 3.31 (d, *J* = 9.0 Hz, 2H), 3.25-3.17 (m, 1H). **^{13}C NMR** (126 MHz, DMSO-d_6) δ 161.5, 155.4, 151.7, 148.7, 134.6, 132.7, 130.9, 127.3, 126.7, 125.8, 123.2, 122.9, 120.9, 117.2, 102.6, 77.5, 76.2, 73.4, 69.5, 60.6. **HRMS (ESI)**: m/z calculated for $C_{20}H_{21}N_2O_7^+$ $[M+H]^+$ 401.1343, found 401.1348.

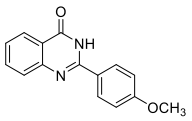
2-(4-tolyl) quinazolin-4(3H)-one (4a)



Compound **4a** was isolated through a silica gel column chromatography (PE : EtOAc = 3:1) as a white solid (35.4 mg, 75% yield) which is a known compound[6]. **^{1}H NMR** (500 MHz, DMSO-d_6) δ 12.47 (s, 1H),

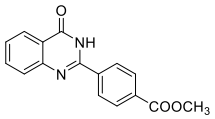
8.15 (d, *J* = 8.0 Hz, 1H), 8.10 (d, *J* = 8.5 Hz, 2H), 7.83 (t, *J* = 7.0 Hz, 1H), 7.73 (d, *J* = 8.0 Hz, 1H), 7.51 (t, *J* = 7.5 Hz, 1H), 7.35 (d, *J* = 8.0 Hz, 2H), 2.39 (s, 3H). **^{13}C NMR** (126 MHz, DMSO-d_6) δ 162.7, 152.7, 149.3, 141.9, 135.0, 130.4, 129.6, 128.1, 127.9, 126.8, 126.3, 121.4, 21.5.

2-(4-methoxyphenyl)quinazolin-4(3H)-one (4b)



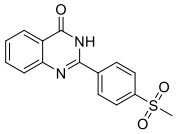
Compound **4b** was isolated through a silica gel column chromatography (PE: EtOAc = 3:1) as a white solid (37.3 mg, 74% yield) which is a known compound[6]. **^{1}H NMR** (500 MHz, DMSO-d_6) δ 12.40 (br, s, 1H), 8.19 (d, *J* = 9.0 Hz, 2H), 8.13 (d, *J* = 8.0 Hz, 1H), 7.81 (t, *J* = 7.0 Hz, 1H), 7.70 (d, *J* = 8.0 Hz, 1H), 7.48 (t, *J* = 7.0 Hz, 1H), 7.08 (d, *J* = 9.0 Hz, 2H), 3.84 (s, 3H). **^{13}C NMR** (126 MHz, DMSO-d_6) δ 162.8, 162.4, 152.4, 149.4, 135.0, 129.9, 127.8, 126.6, 126.3, 125.3, 121.2, 114.5, 55.9.

methyl 4-(4-oxo-3,4-dihydroquinazolin-2-yl)benzoate (4c)



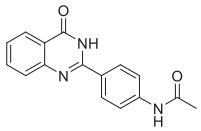
Compound **4c** was isolated through a silica gel column chromatography (PE: EtOAc = 2:1) as a white solid (44.8 mg, 80% yield) which is a known compound[7].**^{1}H NMR** (500 MHz, DMSO-d_6) δ 12.70 (s, 1H), 8.31 (d, *J* = 8.5 Hz, 2H), 8.17 (dd, *J* = 1.5, 8.0 Hz, 1H), 8.14 – 8.07 (m, 2H), 7.87 (ddd, *J* = 1.6, 7.0, 8.5 Hz, 1H), 7.78 (d, *J* = 8.0 Hz, 1H), 7.60 – 7.53 (m, 1H), 3.90 (s, 3H). **^{13}C NMR** (126 MHz, DMSO-d_6) δ 166.2, 162.6, 151.9, 149.0, 137.4, 135.2, 132.3, 129.8, 128.7, 128.2, 127.6, 126.4, 121.7, 52.9.

2-(4-(methylsulfonyl)phenyl)quinazolin-4(3H)-one (4d)



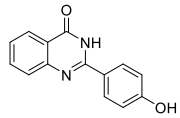
Compound **4d** was isolated through ***General Procedure D*** as a white solid (48.1 mg, 80% yield) which is a known compound[7]. **^{1}H NMR** (500 MHz, DMSO-d_6) δ 12.77 (s, 1H), 8.41 (d, *J* = 8.5 Hz, 2H), 8.18 (dd, *J* = 1.5, 8.0 Hz, 1H), 8.10 (d, *J* = 8.5 Hz, 2H), 7.87 (ddd, *J* = 1.5, 7.0, 8.5 Hz, 1H), 7.79 (d, *J* = 8.0 Hz, 1H), 7.60 – 7.55 (m, 1H), 3.31 (s, 3H). **^{13}C NMR** (126 MHz, DMSO-d_6) δ 162.6, 151.6, 148.9, 143.4, 137.8, 135.3, 129.3, 128.2, 127.7, 127.6, 126.4, 121.7, 43.8. **HRMS (ESI)**: m/z calculated for $C_{15}H_{13}N_2O_3S^+$ $[M+H]^+$ 301.0641, found 301.0645.

N-(4-(3,4-dihydro-4-oxo-2-quinazolinyl)phenyl)acetamide (4e)



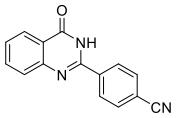
Compound **4e** was isolated through ***General Procedure D*** as a white solid (46.9 mg, 84% yield) which is a known compound[8]. **^{1}H NMR** (500 MHz, DMSO-d_6) δ 12.40 (s, 1H), 10.23 (s, 1H), 8.19-8.12 (m, 3H), 7.86-7.79 (m, 1H), 7.73 (dd, *J* = 15.5, 8.5 Hz, 3H), 7.53-7.47 (m, 1H), 2.10 (s, 3H). **^{13}C NMR** (126 MHz, DMSO-d_6) δ 162.2, 151.8, 148.9, 142.2, 134.5, 128.5, 127.3, 126.8, 126.2, 125.8, 120.8, 118.4, 24.1.

2-(4-hydroxyphenyl)quinazolin-4(3H)-one (4f)



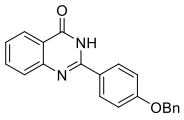
Compound **4f** was isolated through ***General Procedure D*** as a white solid (40.5 mg, 85% yield) which is a known compound[9]. **^{1}H NMR** (500 MHz, DMSO-d_6) δ 12.29 (s, 1H), 10.14 (s, 1H), 8.15-8.06 (m, 3H), 7.83-7.76 (m, 1H), 7.68 (d, *J* = 8.0 Hz, 1H), 7.46 (t, *J* = 8.0 Hz, 1H), 6.89 (d, *J* = 9.0 Hz, 2H). **^{13}C NMR** (126 MHz, DMSO-d_6) δ 162.3, 160.5, 152.1, 149.0, 134.5, 129.6, 127.2, 125.9, 125.8, 123.2, 120.6, 115.3.

4-(3,4-dihydro-4-oxo-2-quinazolinyl)benzonitrile (4g)



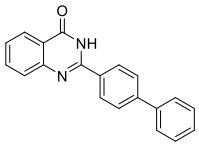
Compound **4g** was isolated through ***General Procedure D*** as a white solid (43.0 mg, 87% yield) which is a known compound[10].**^{1}H NMR** (500 MHz, DMSO-d_6) δ 12.70 (s, 1H), 8.35 (d, *J* = 8.5 Hz, 2H), 8.19 (d, *J* = 8.0 Hz, 1H), 8.04 (d, *J* = 8.5 Hz, 2H), 7.91-7.84 (m, 1H), 7.79 (d, *J* = 8.0 Hz, 1H), 7.58 (t, *J* = 7.0 Hz, 1H). **^{13}C NMR** (126 MHz, DMSO-d_6) δ 162.1, 151.0, 148.3, 136.9, 134.7, 132.5, 128.6, 127.7, 127.2, 125.9, 121.2, 118.3, 113.6.

2-(4-(benzyloxy)phenyl)quinazolin-4(3H)-one (4h)



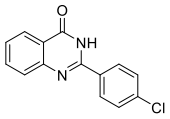
Compound **4h** was isolated through ***General Procedure D*** as a white solid (53.9 mg, 82% yield) which is a known compound[11].**^{1}H NMR** (500 MHz, DMSO-d_6) δ 12.4 (s, 1H), 8.2 (d, *J* = 9.0 Hz, 2H), 8.1 (d, *J* = 7.5 Hz, 1H), 7.82 (t, *J* = 7.0 Hz, 1H), 7.7 (d, *J* = 8.0 Hz, 1H), 7.5-7.5 (m, 3H), 7.5-7.4 (m, 2H), 7.4-7.3 (m, 1H), 7.2 (d, *J* = 9.0 Hz, 2H), 5.2 (s, 2H). **^{13}C NMR** (126 MHz, DMSO-d_6) δ 162.3, 161.0, 151.9, 148.9, 136.7, 134.6, 129.5, 128.5, 128.0, 127.8, 127.3, 126.1, 125.8, 125.0, 120.7, 114.8, 69.5

2-((1,1'-biphenyl)-4-yl)quinazolin-4(3H)-one (4i)



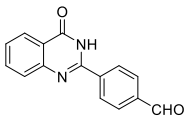
Compound **4i** was isolated through ***General Procedure D*** as a white solid (53.9 mg, 88% yield) which is a known compound[12].**^{1}H NMR** (500 MHz, DMSO-d_6) δ 12.58 (s, 1H), 8.32 (d, *J* = 8.5 Hz, 2H), 8.18 (d, *J* = 8.0 Hz, 1H), 7.92-7.84 (m, 1H), 7.82-7.75 (m, 3H), 7.53 (q, *J* = 7.5 Hz, 3H), 7.44 (t, *J* = 7.0 Hz, 1H). **^{13}C NMR** (126 MHz, DMSO-d_6) δ 162.2, 151.9, 148.8, 142.8, 139.0, 134.6, 131.6, 129.1, 128.4, 128.2, 127.5, 126.8, 126.7, 126.6, 125.9, 121.0.

2-(4-Chlorophenyl)quinazolin-4(3H)-one (4j)



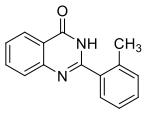
Compound **4j** was isolated through ***General Procedure D*** as a white solid (41.6 mg, 81% yield) which is a known compound[6].**^{1}H NMR** (500 MHz, DMSO-d_6) δ 12.61 (s, 1H), 8.20 (d, *J* = 8.5 Hz, 2H), 8.17 (d, *J* = 7.0 Hz, 1H), 7.88-7.81 (m, 1H), 7.76 (d, *J* = 8.0 Hz, 1H), 7.63 (d, *J* = 8.5 Hz, 2H), 7.54 (t, *J* = 7.0 Hz, 1H). **^{13}C NMR** (126 MHz, DMSO-d_6) δ 162.2, 151.4, 148.6, 136.3, 134.7, 131.6, 129.6, 128.7, 127.6, 126.8, 125.9, 121.0.

2-(4-Formyl-phenyl)-3H-quinazolin-4-one (4k)



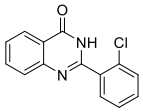
Compound **4k** was isolated through ***General Procedure D*** as a white solid (40.0 mg, 80% yield) which is a known compound[13].**^{1}H NMR** (500 MHz, DMSO-d_6) δ 12.71 (s, 1H), 10.11 (s, 1H), 8.39-8.34 (m, 2H), 8.17 (d, *J* = 8.0 Hz, 1H), 8.06 (d, *J* = 8.0 Hz, 2H), 7.86 (t, *J* = 7.5 Hz, 1H), 7.78 (d, *J* = 8.0 Hz, 1H), 7.56 (t, *J* = 7.5 Hz, 1H).**^{13}C NMR** (126 MHz, DMSO-d_6) δ 192.8, 162.1, 151.5, 148.4, 137.8, 137.7, 134.7, 129.5, 128.5, 127.9, 127.6, 125.9, 121.2.

2-(o-tolyl)quinazolin-4(3H)-one (4l)



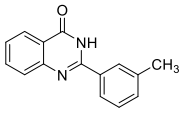
Compound **4l** was isolated through a silica gel column chromatography (PE: EtOAc = 5:1) as a white solid (33.6 mg, 71% yield) which is a known compound[7]. **^{1}H NMR** (500 MHz, DMSO-d_6) δ 12.44 (s, 1H), 8.17 (dd, *J* = 2.0, 8.0 Hz, 1H), 7.87-7.80 (m, 1H), 7.69 (d, *J* = 8.0 Hz, 1H), 7.57-7.48 (m, 2H), 7.43 (td, *J* = 1.5, 7.5 Hz, 1H), 7.37-7.29 (m, 2H), 2.39 (s, 3H). **^{13}C NMR** (126 MHz, DMSO-d_6) δ 161.7, 154.3, 148.7, 136.1, 134.4, 134.2, 130.5, 129.9, 129.1, 127.3, 126.6, 125.8, 125.7, 121.0, 19.5.

2-(2-Chlorophenyl)quinazolin-4(3H)-one (4m)



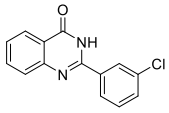
Compound **4m** was isolated through a silica gel column chromatography (PE: EtOAc = 3:1) as a white solid (41.1 mg, 80% yield) which is a known compound[9].**^{1}H NMR** (500 MHz, DMSO-d_6) δ 12.64 (s, 1H), 8.19 (dd, *J* = 1.5, 8.0 Hz, 1H), 7.85 (ddd, *J* = 2.0, 7.0, 8.5 Hz, 1H), 7.72 (d, *J* = 8.0 Hz, 1H), 7.67 (dd, *J* = 2.0, 7.5 Hz, 1H), 7.64 – 7.53 (m, 3H), 7.49 (td, *J* = 1.5, 7.5 Hz, 1H). **^{13}C NMR** (126 MHz, DMSO-d_6) δ 161.4, 152.2, 148.6, 134.6, 133.8, 131.6, 131.5, 130.9, 129.6, 127.5, 127.2, 127.1, 125.8, 121.2.

2-(m-tolyl)quinazolin-4(3H)-one (4n)



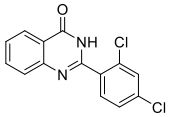
Compound **4n** was isolated through a silica gel column chromatography (PE: EtOAc = 2:1) as a white solid (33.6 mg, 71% yield) which is a known compound[12].**^{1}H NMR** (500 MHz, DMSO-d_6) δ 12.46 (s, 1H), 8.15 (dd, *J* = 1.5, 8.0 Hz, 1H), 8.02 (s, 1H), 7.97 (d, *J* = 7.5 Hz, 1H), 7.84 (ddd, *J* = 1.5, 7.0, 8.5 Hz, 1H), 7.74 (dd, *J* = 1.5, 8.5 Hz, 1H), 7.52 (ddd, *J* = 1.0, 7.0, 8.0 Hz, 1H), 7.47-7.38 (m, 2H), 2.41 (s, 3H). **^{13}C NMR** (126 MHz, DMSO-d_6) δ 162.2, 152.4, 148.8, 137.9, 134.6, 132.7, 132.0, 128.5, 128.3, 127.5, 126.6, 125.9, 124.9, 121.0, 21.0.

2-(3-Chlorophenyl)quinazolin-4(3H)-one (4o)



Compound **4o** was isolated through a silica gel column chromatography (PE: EtOAc = 2:1) as a white solid (27.2 mg, 53% yield) which is a known compound[14]. **^{1}H NMR** (500 MHz, DMSO-d_6) δ 12.63 (s, 1H), 8.26 (s, 1H), 8.20 – 8.13 (m, 2H), 7.87 (ddd, *J* = 1.5, 7.0, 8.5 Hz, 1H), 7.78 (d, *J* = 7.5 Hz, 1H), 7.67 (d, *J* = 8.0 Hz, 1H), 7.63-7.52 (m, 2H). **^{13}C NMR** (126 MHz, DMSO-d_6) δ 162.1, 151.0, 148.5, 134.8, 134.7, 133.5, 131.2, 130.6, 127.7, 127.6, 127.0, 126.5, 125.9, 121.2.

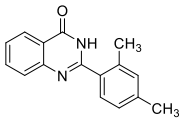
2-(2,4-Dichlorophenyl)quinazolin-4(3H)-one (4p)



Compound **4p** was isolated through a silica gel column chromatography (PE: EtOAc = 2:1) as a white solid (53.0 mg, 91% yield) which is a known compound[6]. **^{1}H NMR** (500 MHz, DMSO-d_6) δ 12.67 (s, 1H), 8.18 (dd, *J* = 1.5, 8.0 Hz, 1H), 7.88-7.81 (m, 1H), 7.80 (d, *J* = 2.0 Hz, 1H), 7.71 (dd, *J* = 2.5, 8.5 Hz, 2H), 7.62-7.54 (m, 3H). **^{13}C NMR** (126 MHz, DMSO-d_6) δ 161.4, 151.4, 148.5, 135.5, 134.7,

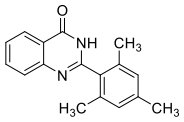
132.8, 132.7, 132.3, 129.2, 127.5, 127.3, 125.9, 121.3.

2-(2,4-Dimethylphenyl)quinazolin-4(3H)-one (4q)



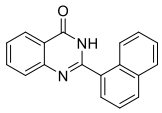
Compound **4q** was isolated through a silica gel column chromatography (PE: EtOAc = 3:1) as a white solid (34.0 mg, 68% yield) which is a known compound[12]. **^{1}H NMR** (500 MHz, DMSO-d_6) δ 12.37 (s, 1H), 8.16 (dd, *J* = 1.5, 8.0 Hz, 1H), 7.85-7.78 (m, 1H), 7.68 (d, *J* = 7.0 Hz, 1H), 7.56-7.49 (m, 1H), 7.40 (d, *J* = 8.0 Hz, 1H), 7.15 (s, 1H), 7.12 (d, *J* = 8.0 Hz, 1H), 2.36 (s, 3H), 2.34 (s, 3H). **^{13}C NMR** (126 MHz, DMSO-d_6) δ 162.2, 154.7, 149.0, 139.9, 136.3, 134.8, 131.5, 131.5, 129.3, 127.5, 126.9, 126.6, 126.0, 121.0, 21.1, 19.8.

2-Mesitylquinazolin-4(3H)-one (4r)



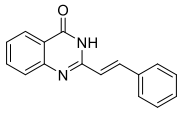
Compound **4r** was isolated through a silica gel column chromatography (PE: EtOAc = 4:1) as a white solid (43.3 mg, 83% yield) which is a known compound[10]. **^{1}H NMR** (500 MHz, DMSO-d_6) δ 12.40 (s, 1H), 8.17 (dd, *J* = 1.5, 8.0 Hz, 1H), 7.85-7.78 (m, 1H), 7.67 (d, *J* = 8.0 Hz, 1H), 7.57-7.48 (m, 1H), 6.95 (s, 2H), 2.28 (s, 3H), 2.12 (s, 6H). **^{13}C NMR** (126 MHz, DMSO-d_6) δ 161.9, 154.3, 149.0, 138.5, 135.5, 134.6, 132.0, 128.1, 127.4, 126.8, 125.9, 121.1, 20.8, 19.1.

2-(Naphthalen-1-yl) quinazolin-4(3H)-one (4s)



Compound **4s** was isolated through a silica gel column chromatography (PE: EtOAc = 4:1) as a white solid (39.2 mg, 72% yield) which is a known compound[6]. **^{1}H NMR** (500 MHz, DMSO-d_6) δ 12.66 (s, 1H), 8.22 (dd, *J* = 1.5, 8.0 Hz, 1H), 8.19-8.13 (m, 1H), 8.12 (d, *J* = 8.0 Hz, 1H), 8.08-8.02 (m, 1H), 7.90-7.83 (m, 1H), 7.79 (d, *J* = 7.0 Hz, 1H), 7.73 (d, *J* = 8.0 Hz, 1H), 7.68-7.62 (m, 1H), 7.64-7.55 (m, 2H). **^{13}C NMR** (126 MHz, DMSO-d_6) δ 161.9, 153.7, 148.7, 134.6, 133.2, 131.7, 130.4, 130.3, 128.4, 127.7, 127.5, 127.1, 126.8, 126.4, 125.9, 125.2, 125.1, 121.2.

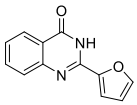
(E)-2-Styrylquinazolin-4(3H)-one (4t)



Compound **4t** was isolated through a silica gel column chromatography (PE: EtOAc = 4:1) as a white solid (34.8 mg, 70% yield) which is a known compound[6]. **^{1}H NMR** (500 MHz, DMSO-d_6) δ 12.33 (s, 1H), 8.11 (dd, *J* = 1.5,

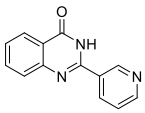
8.0 Hz, 1H), 7.95 (d, *J* = 16.5 Hz, 1H), 7.83-7.78 (m, 1H), 7.69-7.64 (m, 3H), 7.50-7.44 (m, 3H), 7.43-7.39 (m, 1H), 7.01 (d, *J* = 16.0 Hz, 1H). **^{13}C NMR** (126 MHz, DMSO-d_6) δ 161.8, 151.4, 149.0, 138.3, 135.0, 134.6, 129.8, 129.1, 128.6, 128.4, 128.4, 127.7, 127.2, 126.3, 125.9, 121.1, 121.1.

2-(Furan-2-yl)quinazolin-4(3H)-one (4u)



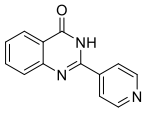
Compound **4u** was isolated through a silica gel column chromatography (PE: EtOAc = 2:1) as a white solid (19.1 mg, 45% yield) which is a known compound[12]. **^{1}H NMR** (500 MHz, DMSO-d_6) δ 12.49 (s, 1H), 8.12 (dd, *J* = 1.5, 8.0 Hz, 1H), 8.00 (s, 1H), 7.85-7.78 (m, 1H), 7.69 (d, *J* = 8.0 Hz, 1H), 7.63 (d, *J* = 3.5 Hz, 1H), 7.49 (t, *J* = 8.0 Hz, 1H), 6.77-6.73 (m, 1H). **^{13}C NMR** (126 MHz, DMSO-d_6) δ 161.6, 148.7, 146.6, 146.1, 144.1, 134.7, 127.2, 126.5, 126.0, 121.1, 114.5, 112.5.

2-(pyridin-3-yl)quinazolin-4(3H)-one (4v)



Compound **4v** was isolated through a silica gel column chromatography (PE: EtOAc = 2:1) as a white solid (41.5 mg, 93% yield) which is a known compound[8]. **^{1}H NMR** (500 MHz, DMSO-d_6) δ 12.72 (s, 1H), 9.29 (d, *J* = 2.5 Hz, 1H), 8.75 (dd, *J* = 1.5, 5.0 Hz, 1H), 8.49 (dt, *J* = 2.0, 8.0 Hz, 1H), 8.17 (dd, *J* = 1.5, 8.0 Hz, 1H), 7.89 – 7.82 (m, 1H), 7.77 (d, *J* = 8.0 Hz, 1H), 7.61-7.52 (m, 2H). **^{13}C NMR** (126 MHz, DMSO-d_6) δ 162.2, 151.8, 150.9, 148.8, 148.5, 135.4, 134.7, 128.8, 127.5, 127.0, 125.9, 123.6, 121.1.

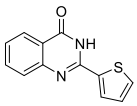
2-(Pyridin-4-yl)quinazolin-4(3H)-one (4w)



Compound **4w** was isolated through a silica gel column chromatography (PE: EtOAc = 2:1) as a white solid (33.9 mg, 76% yield) which is a known compound[12]. **^{1}H NMR** (500 MHz, DMSO-d_6) δ 12.77 (s, 1H), 8.81-8.76 (m, 2H), 8.18 (dd, *J* = 1.5, 8.0 Hz, 1H), 8.14-8.07 (m, 2H), 7.91-7.84 (m, 1H), 7.79 (d, *J* = 8.0 Hz, 1H), 7.62 – 7.55 (m, 1H). **^{13}C NMR** (126 MHz, DMSO-d_6) δ 162.1, 150.5, 150.3, 148.2, 139.9, 134.8, 127.7, 127.4, 125.9, 121.6, 121.5.

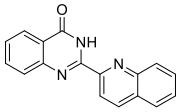
2-(Thiophen-2-yl)quinazolin-4(3H)-one (4x)

Compound **4x** was isolated through a silica gel column chromatography (PE: EtOAc =



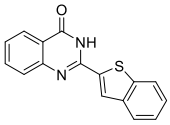
3:1) as a white solid (41.5 mg, 91% yield) which is a known compound[12]. **^{1}H NMR** (500 MHz, DMSO-d_6) δ 12.64 (s, 1H), 8.23 (dd, *J* = 1.0, 4.0 Hz, 1H), 8.12 (dd, *J* = 1.5, 8.0 Hz, 1H), 7.86 (dd, *J* = 1.0, 5.0 Hz, 1H), 7.83-7.76 (m, 1H), 7.65 (d, *J* = 8.0 Hz, 1H), 7.52-7.45 (m, 1H), 7.26-7.21 (m, 1H). **^{13}C NMR** (126 MHz, DMSO-d_6) δ 161.8, 148.6, 147.9, 137.4, 134.7, 132.2, 129.4, 128.5, 126.9, 126.3, 126.0, 120.9.

2-(Quinolin-2-yl)quinazolin-4(3H)-one (4y)



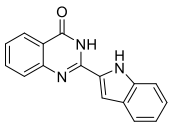
Compound **4y** was isolated through a silica gel column chromatography (PE: EtOAc = 1:1) as a white solid (35.5 mg, 65% yield) which is a known compound[12]. **^{1}H NMR** (500 MHz, Chloroform-d) δ 11.16 (s, 1H), 8.59 (dd, *J* = 2.0, 8.5 Hz, 1H), 8.34 (d, *J* = 8.0 Hz, 1H), 8.30 (d, *J* = 8.5 Hz, 1H), 8.10 (d, *J* = 8.5 Hz, 1H), 7.87-7.81 (m, 2H), 7.81-7.72 (m, 2H), 7.60 (t, *J* = 7.5 Hz, 1H), 7.51 (t, *J* = 7.5 Hz, 1H). **^{13}C NMR** (126 MHz, Chloroform-d) δ 161.5, 149.2, 149.0, 148.1, 146.8, 137.7, 134.7, 130.5, 129.7, 129.4, 128.3, 127.8, 127.6, 126.9, 122.7, 118.5.

2-(Benzo[b]thiophen-2-yl)quinazolin-4(3H)-one (4z)



Compound **4z** was isolated through a silica gel column chromatography (PE: EtOAc = 3:1) as a white solid (42.3 mg, 76% yield) which is a known compound[8]. **^{1}H NMR** (500 MHz, DMSO-d_6) δ 12.87 (s, 1H), 8.58 (s, 1H), 8.16 (d, *J* = 8.0 Hz, 1H), 8.05 (d, *J* = 8.0 Hz, 1H), 7.94 (d, *J* = 7.5 Hz, 1H), 7.88-7.81 (m, 1H), 7.71 (d, *J* = 8.0 Hz, 1H), 7.57-7.42 (m, 2H). **^{13}C NMR** (126 MHz, DMSO-d_6) δ 161.6, 148.3, 147.9, 140.7, 139.4, 137.5, 134.8, 127.2, 126.9, 126.7, 126.3, 126.0, 125.2, 125.1, 122.6, 121.2.

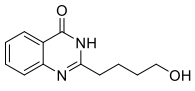
2-(1H-Indol-2-yl)quinazolin-4(3H)-one (4aa)



Compound **4aa** was isolated through a silica gel column chromatography (PE: EtOAc = 1:1) as a white solid (19.9 mg, 46% yield) which is a known compound[12]. **^{1}H NMR** (500 MHz, DMSO-d_6) δ 12.59 (s, 1H), 11.78 (s, 1H), 8.16 (dd, *J* = 1.5, 8.0 Hz, 1H), 7.88-7.81 (m, 1H), 7.74 (d, *J* = 8.0 Hz, 1H), 7.69-7.62 (m, 2H), 7.57-7.48 (m, 2H), 7.27-7.20 (m, 1H), 7.06 (t, *J* = 7.0 Hz, 1H). **^{13}C NMR** (126 MHz, DMSO-d_6) δ 161.8, 148.7, 146.6, 137.7, 134.7,

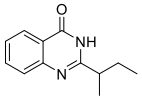
130.0, 127.5, 126.9, 126.3, 126.1, 124.1, 121.5, 121.2, 120.0, 112.4, 105.0.

2-(4-Hydroxybutyl)quinazolin-4(3H)-one (4ba)



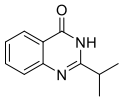
Compound **4ba** was isolated through a silica gel column chromatography (PE: EtOAc = 1:1) as a white solid (26.2 mg, 60% yield) which is a known compound[6].**^{1}H NMR** (500 MHz, DMSO-d_6) δ 12.15 (s, 1H), 8.07 (d, *J* = 8.0 Hz, 1H), 7.76 (t, *J* = 7.0 Hz, 1H), 7.59 (d, *J* = 8.0 Hz, 1H), 7.45 (t, *J* = 7.5 Hz, 1H), 4.42 (t, *J* = 5.0 Hz, 1H), 3.42 (q, *J* = 6.5 Hz, 2H), 2.60 (t, *J* = 7.6 Hz, 2H), 1.75 (p, *J* = 7.5 Hz, 2H), 1.52-1.41 (m, 2H). **^{13}C NMR** (126 MHz, DMSO-d_6) δ 161.8, 157.5, 148.9, 134.3, 126.8, 125.9, 125.7, 120.8, 60.4, 34.3, 31.9, 23.5.

2-(1-Methylpropyl)quinazolinone-4(3H)-one (4ca)



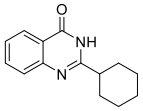
Compound **4ca** was isolated through a silica gel column chromatography (PE: EtOAc = 1:1) as a white solid (17.4 mg, 43% yield) which is a known compound[15]. **^{1}H NMR** (500 MHz, DMSO-d_6) δ 12.11 (s, 1H), 8.08 (dd, *J* = 1.5, 8.0 Hz, 1H), 7.79-7.72 (m, 1H), 7.60 (d, *J* = 8.0 Hz, 1H), 7.48-7.41 (m, 1H), 2.72-2.61 (m, 1H), 1.85-1.72 (m, 1H), 1.62-1.49 (m, 1H), 1.23 (d, *J* = 7.0 Hz, 3H), 0.83 (t, *J* = 7.5 Hz, 3H). **^{13}C NMR** (126 MHz, DMSO-d_6) δ 162.0, 161.0, 148.9, 134.3, 127.0, 126.0, 125.7, 120.9, 40.4, 27.5, 18.3, 11.7.

2-Isopropylquinazolin-4(3H)-one (4da)



Compound **4da** was isolated through a silica gel column chromatography (PE: EtOAc = 1:1) as a white solid (15.6 mg, 66% yield) which is a known compound[6]. **^{1}H NMR** (500 MHz, DMSO-d_6) δ 12.12 (s, 1H), 8.08 (dd, *J* = 1.5, 8.0 Hz, 1H), 7.79-7.72 (m, 1H), 7.60 (d, *J* = 8.0 Hz, 1H), 7.48-7.41 (m, 1H), 2.94-2.82 (m, 1H), 1.25 (d, *J* = 7.0 Hz, 6H). **^{13}C NMR** (126 MHz, DMSO-d_6) δ 161.9, 161.6, 148.9, 134.2, 126.9, 125.9, 125.7, 120.9, 33.3, 20.4.

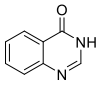
2-Cyclohexylquinazolin-4(3H)-one (4ea)



Compound **4ea** was isolated through a silica gel column chromatography (PE: EtOAc = 1:1) as a white solid (24.7 mg, 54% yield) which is a known compound[12]. **^{1}H NMR** (500 MHz, DMSO-d_6) δ 12.05 (s, 1H), 8.07 (dd, *J* = 1.5, 8.0 Hz, 1H), 7.78 – 7.71 (m, 1H), 7.59 (d, *J* = 8.0 Hz, 1H), 7.44 (t, *J* = 7.5 Hz, 1H), 2.61 –

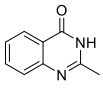
2.53 (m, 1H), 1.90 (d, *J* = 12.5 Hz, 2H), 1.82-1.75 (m, 2H), 1.67 (d, *J* = 13.0 Hz, 1H), 1.62-1.54 (m, 2H), 1.35-1.20 (m, 3H). **^{13}C NMR** (126 MHz, DMSO-d_6) δ 161.9, 160.7, 148.9, 134.2, 126.9, 125.8, 125.6, 120.9, 42.8, 30.2, 25.5, 25.3.

Quinazolin-4(3H)-one (4fa)



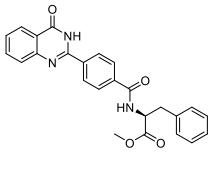
Compound **4fa** was isolated through a silica gel column chromatography (PE: EtOAc = 1:1) as a white solid (17.5 mg, 60% yield) which is a known compound[6]. **^{1}H NMR** (500 MHz, DMSO-d_6) δ 12.23 (s, 1H), 8.12 (dd, *J* = 1.5, 8.0 Hz, 1H), 8.09 (s, 1H), 7.83-7.77 (m, 1H), 7.66 (d, *J* = 8.0 Hz, 1H), 7.54-7.48 (m, 1H). **^{13}C NMR** (126 MHz, DMSO-d_6) δ 160.7, 148.8, 145.4, 134.3, 127.2, 126.8, 125.8, 122.6.

2-Methylquinazolin-4(3H)-one (4ga)



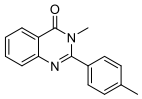
Compound **4ga** was isolated through a silica gel column chromatography (PE: EtOAc from 1:3) as a white solid (16.7 mg, 52% yield) which is a known compound[16]. **^{1}H NMR** (500 MHz, DMSO-d_6) δ 12.18 (s, 1H), 8.07 (dd, *J* = 1.5, 8.0 Hz, 1H), 7.80-7.71 (m, 1H), 7.56 (d, *J* = 8.0 Hz, 1H), 7.49-7.39 (m, 1H), 2.34 (s, 3H). **^{13}C NMR** (126 MHz, DMSO-d_6) δ 161.7, 154.3, 149.0, 134.3, 126.6, 125.8, 125.7, 120.6, 21.4.

Methyl (4-(4-oxo-3,4-dihydroquinazolin-2-yl)benzoyl)-L-phenylalaninate (4ha)



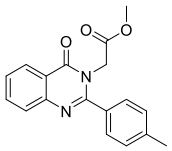
Compound **4ha** was isolated through ***General Produce D*** as a white solid (76.9 mg, 90% yield). **^{1}H NMR** (500 MHz, DMSO-d_6) δ 12.62 (s, 1H), 9.04 (d, *J* = 8.0 Hz, 1H), 8.26 (d, *J* = 8.5 Hz, 2H), 8.17 (dd, *J* = 1.5, 8.0 Hz, 1H), 7.96 (d, *J* = 8.5 Hz, 2H), 7.88-7.84 (m, 1H), 7.77 (d, *J* = 8.0 Hz, 1H), 7.57-7.53 (m, 1H), 7.32-7.26 (m, 4H), 7.22-7.18 (m, 1H), 4.74-4.69 (m, 1H), 3.66 (s, 3H), 3.24-3.08 (m, 2H). **^{13}C NMR** (126 MHz, DMSO-d_6) δ 172.0, 165.6, 162.1, 151.6, 148.6, 137.6, 135.8, 135.3, 134.7, 129.0, 128.2, 127.7, 127.6, 127.6, 126.9, 126.5, 125.9, 121.1, 54.3, 52.0, 36.2. **HRMS (ESI)**: m/z calculated for $C_{25}H_{22}N_3O_4^+$ $[M+H]^+$ 428.1605, found 428.1609.

3-methyl-2-(p-tolyl)quinazolin-4(3H)-one (4ia)



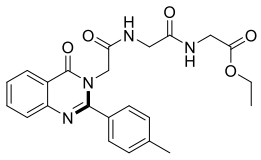
Compound 4Ia was isolated through ***General Produce D*** as a white solid (54.0 mg, 72% yield) which is a known compound[17]. **^{1}H NMR** (500 MHz, Chloroform-d) δ 8.3 (d, *J* = 7.0 Hz, 1H), 7.7 (dd, *J* = 2.0, 6.0 Hz, 2H), 7.5 – 7.4 (m, 3H), 7.3 (d, *J* = 8.0 Hz, 2H), 3.5 (s, 3H), 2.4 (s, 3H). **^{13}C NMR** (126 MHz, Chloroform-d) δ 162.7, 156.2, 147.2, 140.2, 134.1, 132.4, 129.4, 127.9, 127.3, 126.8, 126.5, 120.3, 34.2, 21.3.

methyl 2-(4-oxo-2-(p-tolyl)quinazolin-3(4H)-yl)acetate (4ja)



4ja was isolated through a silica gel column chromatography (PE: EtOAc = 1:1) as a white solid (72 mg, 78% yield). **^{1}H NMR** (500 MHz, Chloroform-d) δ 8.30 (d, *J* = 8.0 Hz, 1H), 7.80-7.72 (m, 2H), 7.53-7.47 (m, 1H), 7.43 (d, *J* = 8.0 Hz, 2H), 7.29 (d, *J* = 8.0 Hz, 2H), 4.66 (s, 1H), 3.74 (s, 1H), 2.41 (s, 1H). **^{13}C NMR** (126 MHz, Chloroform-d) δ 168.6, 162.4, 155.8, 147.5, 140.7, 134.9, 132.0, 129.8, 127.9, 127.8, 127.3, 127.0, 120.5, 52.8, 47.8, 21.6. **HRMS (ESI)**: m/z calculated for $C_{18}H_{17}N_2O_3^+$ $[M+H]^+$ 309.1234, found 309.1225.

ethyl (2-(4-oxo-2-(p-tolyl)quinazolin-3(4H)-yl)acetyl)glycylglycinate (4ka)



4ka was isolated through a silica gel column chromatography (PE: EtOAc from 1:1 to pure EtOAc) as a white solid (45 mg, 69% yield). **^{1}H NMR** (500 MHz, DMSO-d_6) δ 8.50 (t, *J* = 6.0 Hz, 1H), 8.30 (t, *J* = 6.0 Hz, 1H), 8.15 (d, *J* = 8.0 Hz, 1H), 7.86 (t, *J* = 7.5 Hz, 1H), 7.69 (d, *J* = 8.0 Hz, 1H), 7.57 (t, *J* = 7.5 Hz, 1H), 7.50 (d, *J* = 8.0 Hz, 2H), 7.32 (d, *J* = 8.0 Hz, 2H), 4.53 (s, 2H), 4.09 (q, *J* = 7.0 Hz, 2H), 3.85 (d, *J* = 6.0 Hz, 2H), 3.76 (d, *J* = 5.5 Hz, 2H), 2.38 (s, 3H), 1.19 (t, *J* = 7.0 Hz, 3H). **^{13}C NMR** (126 MHz, DMSO-d_6) δ 169.7, 169.1, 167.1, 161.4, 156.2, 147.1, 139.6, 134.7, 132.2, 129.0, 128.2, 127.3, 127.0, 126.2, 120.2, 60.5, 48.7, 41.8, 40.7, 21.0, 14.1. **HRMS (ESI)**: m/z calculated for $C_{24}H_{25}N_4O_5^+$ $[M+H]^+$ 437.1819, found 437.1813.

3. References

[1] Zhou, Q.;Li, K.;Liu, Y.-H.;Li, L.-L.;Yu, K.-K.;Zhang, H.;Yu, X.-Q. *Chem. Commun.* 2018, **54**, 13722-13725.

[2] Wang, C.-J.;Xie, F.;Zhang, W.-B. *Chin. J. Org. Chem.* 2008, **28**, 503-505.

[3] Barak, D. S.;Mukhopadhyay, S.;Dahatonde, D. J.;Batra, S. *Tetrahedron Lett.* 2019, **60**, 248-251.

[4] Warfield, R.;Bardelang, P.;Saunders, H.;Chan, W. C.;Penfold, C.;James, R.;Thomas, N. R. *Org. Biomol. Chem.* 2006, **4**, 3626-3638.

[5] Uehata, K.;Kimura, N.;Hasegawa, K.;Arai, S.;Nishida, M.;Hosoe, T.;Kawai, K.-i.;Nishida, A. *J. Nat. Prod.* 2013, **76**, 2034-2039.

[6] Cao, L.;Huo, H.;Zeng, H.;Yu, Y.;Lu, D.;Gong, Y. *Adv. Synth. Catal.* 2018, **360**, 4764-4773.

[7] Ma, Z.;Song, T.;Yuan, Y.;Yang, Y. *Chem. Sci.* 2019, **10**, 10283-10289.

[8] Sharif, M.;Opalach, J.;Langer, P.;Beller, M.;Wu, X.-F. *RSC Adv.* 2014, **4**, 8-17.

[9] Tian, X.;Song, L.;Li, E.;Wang, Q.;Yu, W.;Chang, J. *RSC Adv.* 2015, **5**, 62194-62201.

[10] Alam, M. T.;Maiti, S.;Mal, P. *Beilstein J. Org. Chem.* 2018, **14**, 2396-2403.

[11] Brown, C. E.;Kong, T.;McNulty, J.;D'Aiuto, L.;Williamson, K.;McClain, L.;Piazza, P.;Nimgaonkar, V. L. *Bioorg. Med. Chem. Lett.* 2017, **27**, 4601-4605.

[12] Rao, K. R.;Mekala, R.;Raghunadh, A.;Meruva, S. B.;Kumar, S. P.;Kalita, D.;Laxminarayana, E.;Prasad, B.;Pal, M. *RSC Adv.* 2015, **5**, 61575-61579.

[13] Vemula, S. R.;Kumar, D.;Cook, G. R. *Tetrahedron Lett.* 2018, **59**, 3801-3805.

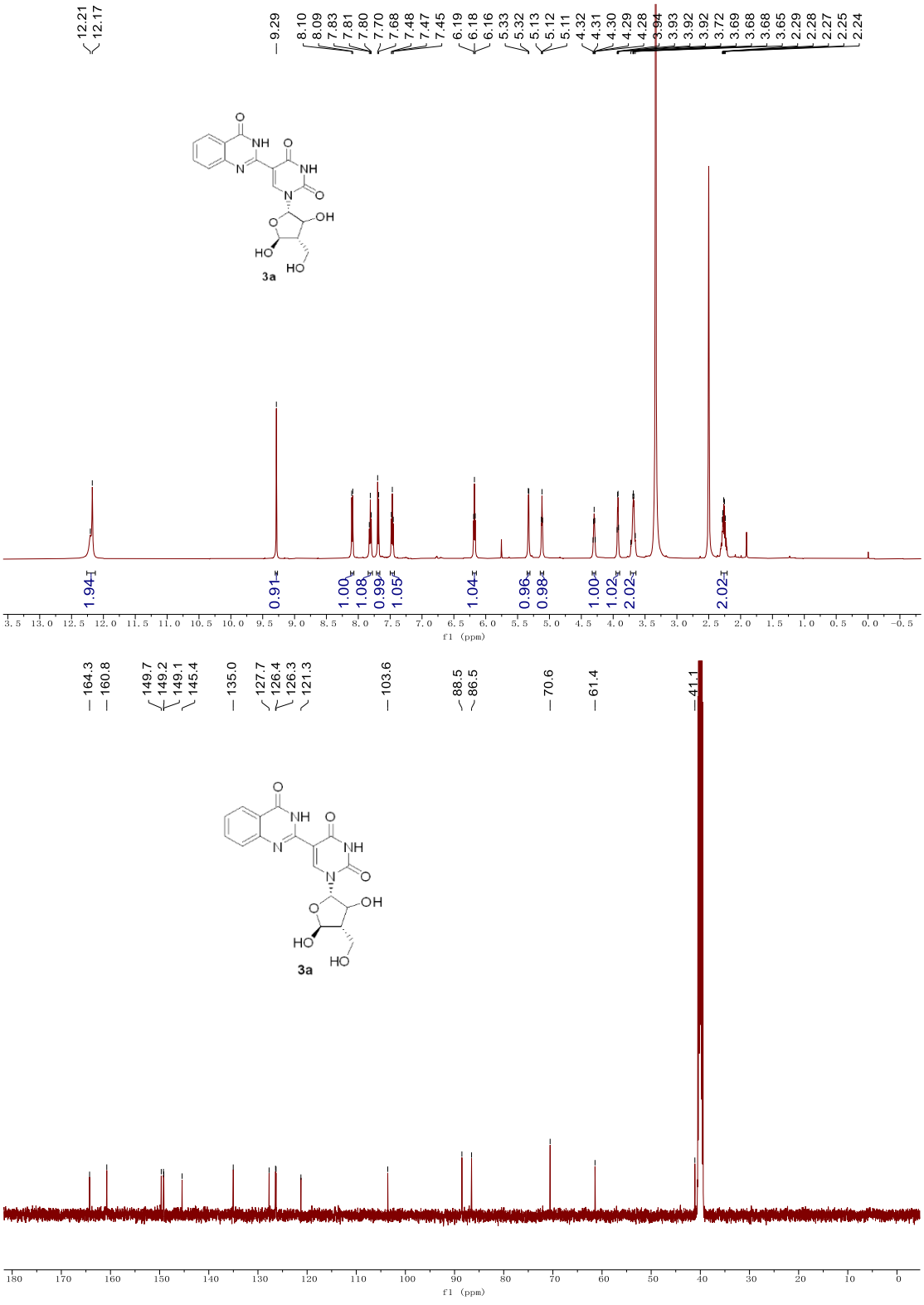
[14] Das, S.;Sinha, S.;Samanta, D.;Mondal, R.;Chakraborty, G.;Brandao, P.;Paul, N. D. *J. Org. Chem.* 2019, **84**, 10160-10171.

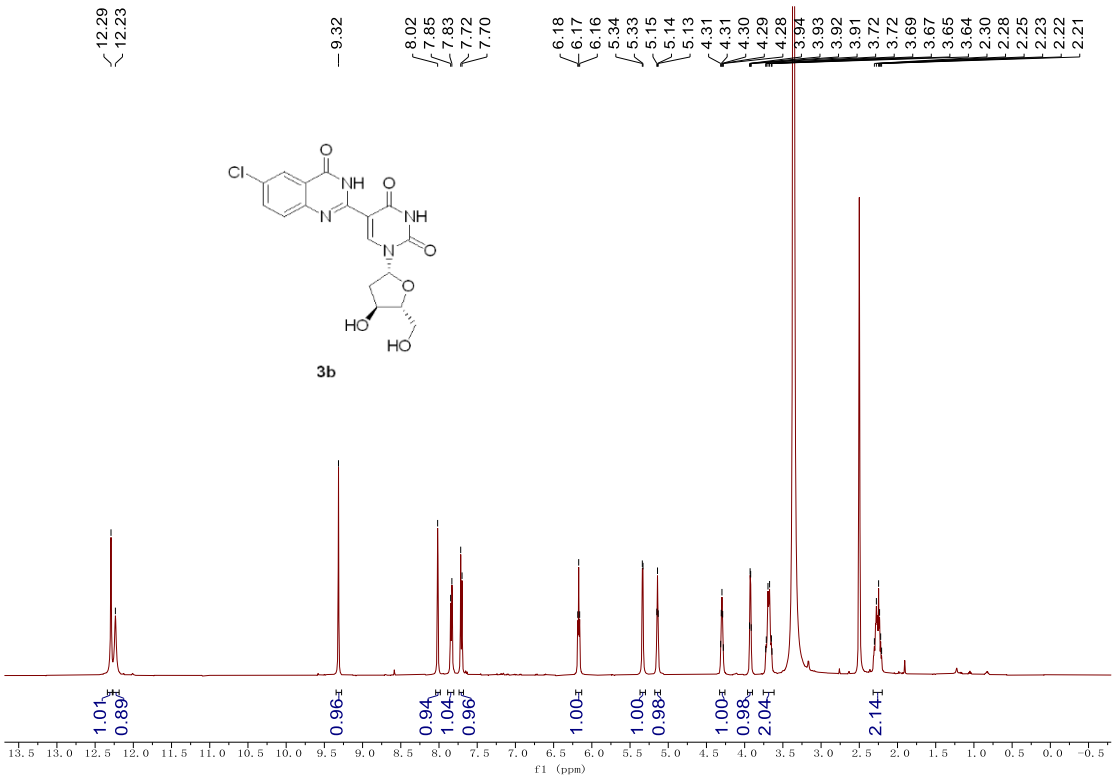
[15] Xu, W.;Fu, H. *J. Org. Chem.* 2011, **76**, 3846-3852.

[16] Bhargava Reddy, M.;Prasanth, K.;Anandhan, R. *Org. Biomol. Chem.* 2020, **18**, 9601-9605.

[17] Jang, Y.;Lee, S. B.;Hong, J.;Chun, S.;Lee, J.;Hong, S. *Org. Biomol. Chem.* 2020, **18**, 5435-5441.

4. $^{1}H\&^{13}C$ NMR Spectra




12.29
12.23
9.32
8.02
7.85
7.83
7.72
7.70
6.18
6.17
6.16
5.34
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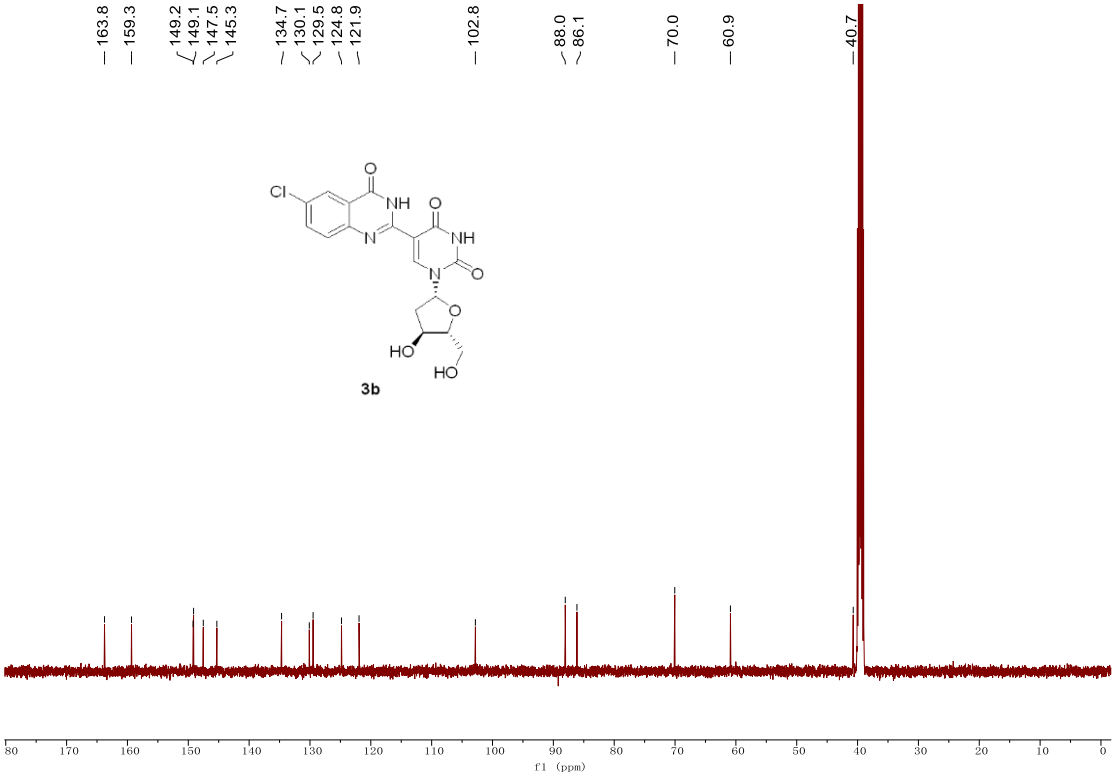
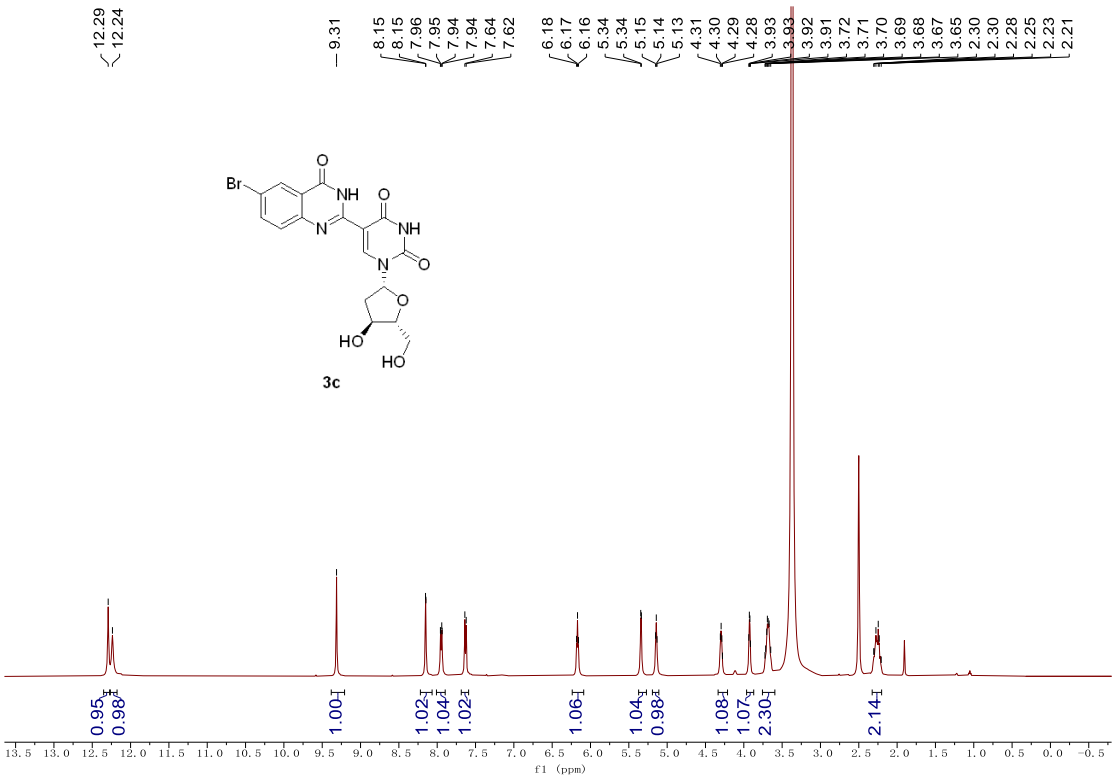
5.15
5.14
5.13
4.31
4.31
4.30
4.29
4.28
3.94
3.93
3.92
3.91
3.72
3.72
3.69
3.67
3.65
3.64
2.30
2.28
2.25
2.23
2.22
2.21
Cl
NH
O
NH
N
N
O
O
HO
HO
3b
1.01
0.89
0.96
0.94
1.04
0.96
1.00
1.00
0.98
1.00
0.98
2.04
2.14
f1 (ppm)


163.8
159.3
149.2
149.1
147.5
145.3
134.7
130.1
129.5
124.8
121.9
102.8
88.0
86.1
70.0
60.9
40.7
Cl
NH
O
NH
N
N
O
O
HO
HO
3b
f1 (ppm)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7.94
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7.62
6.18
6.17
6.16
5.34
5.34
5.15
5.14
5.13
4.31
4.30
4.29
4.28
3.93
3.93
3.92
3.91
3.72
3.71
3.70
3.69
3.68
3.67
3.65
2.30
2.30
2.28
2.25
2.23
2.21
Br
NH
O
N
NH
O
N
O
HO
HO
3c
0.95
0.98
1.00
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1.04
1.02
1.06
1.04
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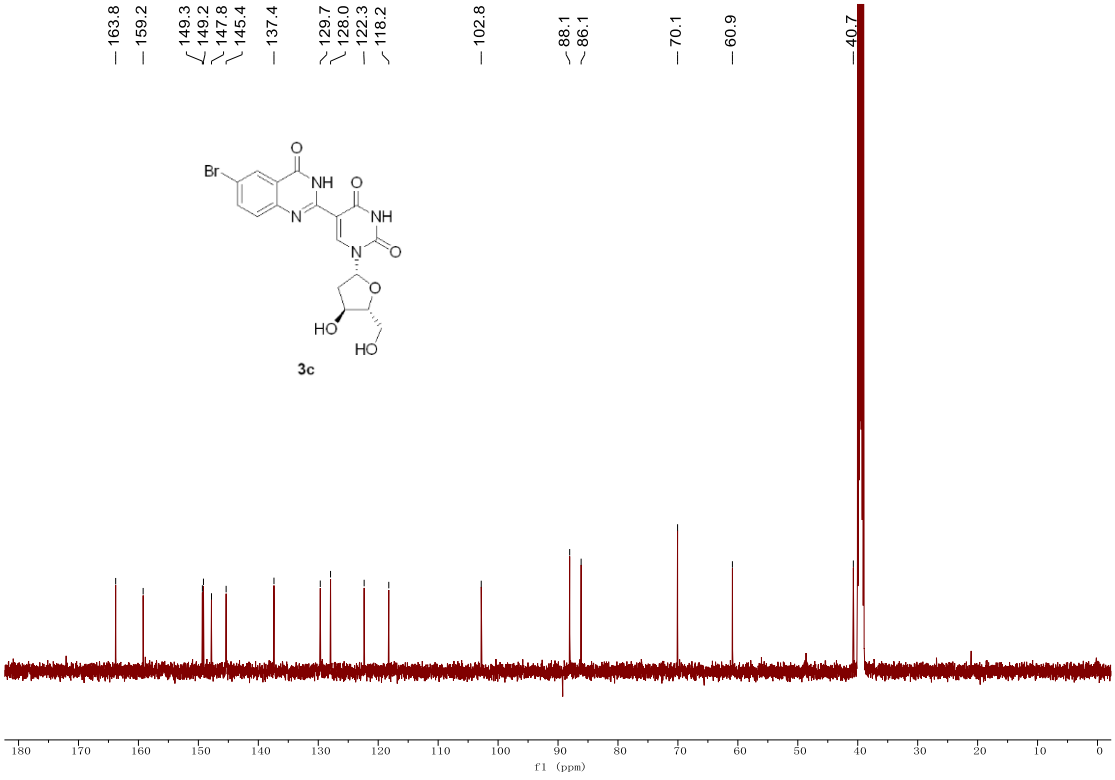
1.08
1.07
2.30
2.14
f1 (ppm)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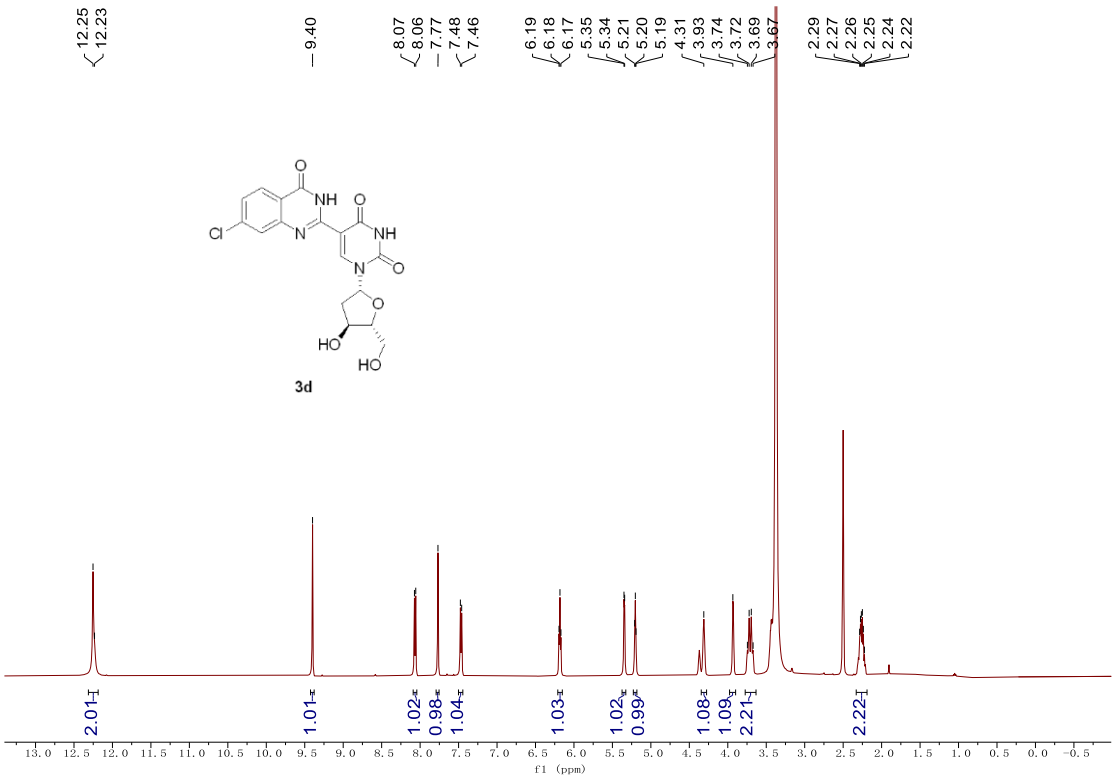
149.2
147.8
145.4
137.4
129.7
128.0
122.3
118.2
102.8
88.1
86.1
70.1
60.9
40.7
Br
NH
O
N
NH
O
N
O
HO
HO
3c
f1 (ppm)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6.18
6.17
5.35
5.34
5.21
5.20
5.19
4.31
3.93
3.74
3.72
3.69
3.67
2.29
2.27
2.26
2.25
2.24
2.22
2.01
1.01
1.02
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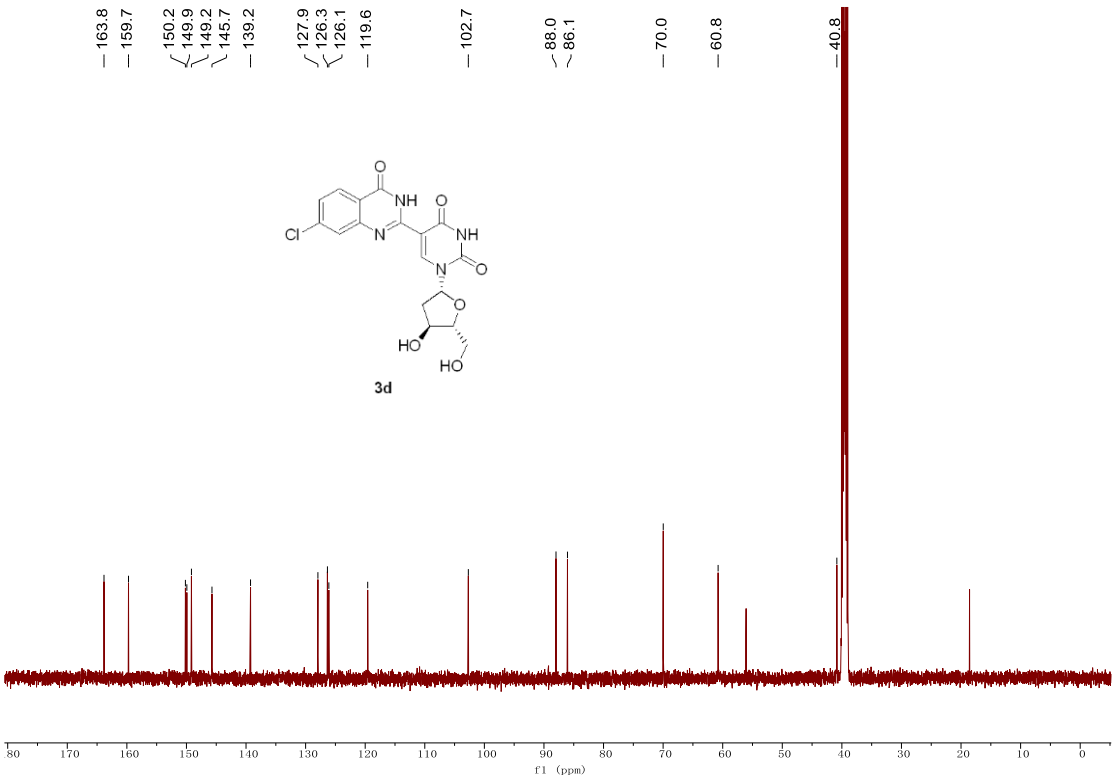
1.03
1.02
0.99
1.08
1.09
2.21
2.22
f1 (ppm)

3d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139.2
127.9
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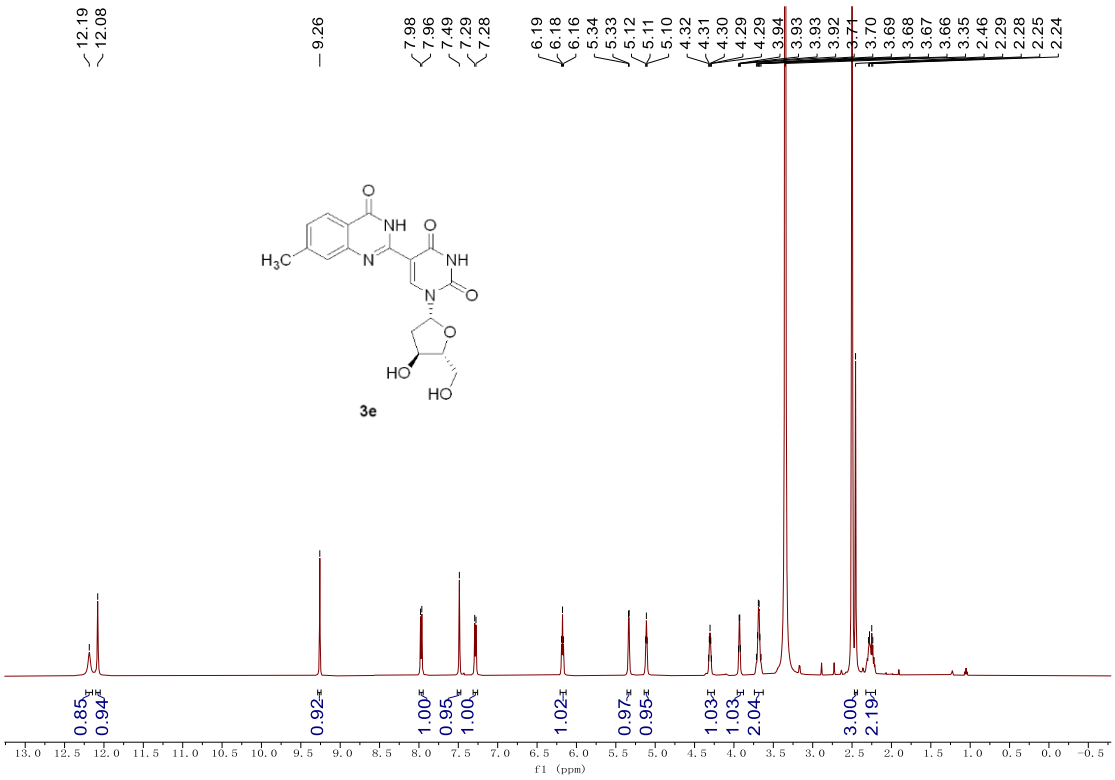
126.1
119.6
102.7
88.0
86.1
70.0
60.8
40.8
f1 (ppm)

3d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7.28
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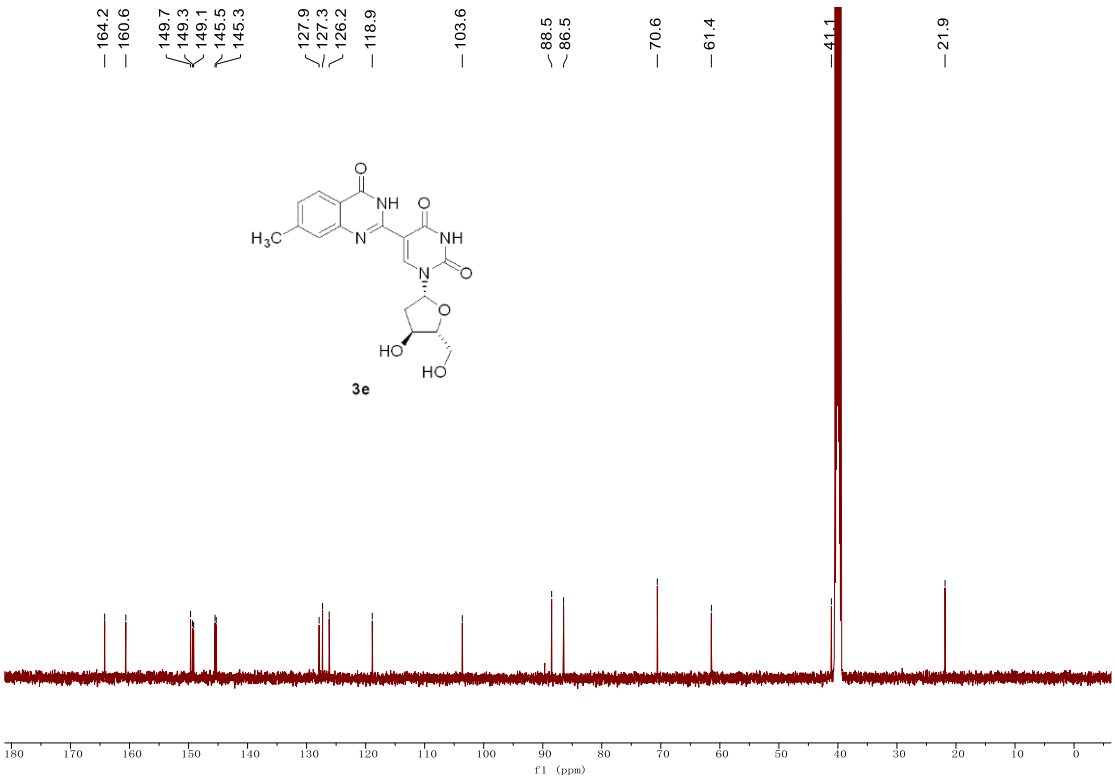
6.18
6.16
5.34
5.33
5.12
5.11
5.10
4.32
4.31
4.30
4.29
4.29
3.94
3.93
3.93
3.92
3.71
3.70
3.69
3.68
3.67
3.66
3.35
2.46
2.29
2.28
2.25
2.24
0.85
0.94
0.92
1.00
0.95
1.00
1.02
0.97
0.95
1.03
1.03
2.04
3.00
2.19
f1 (ppm)
3e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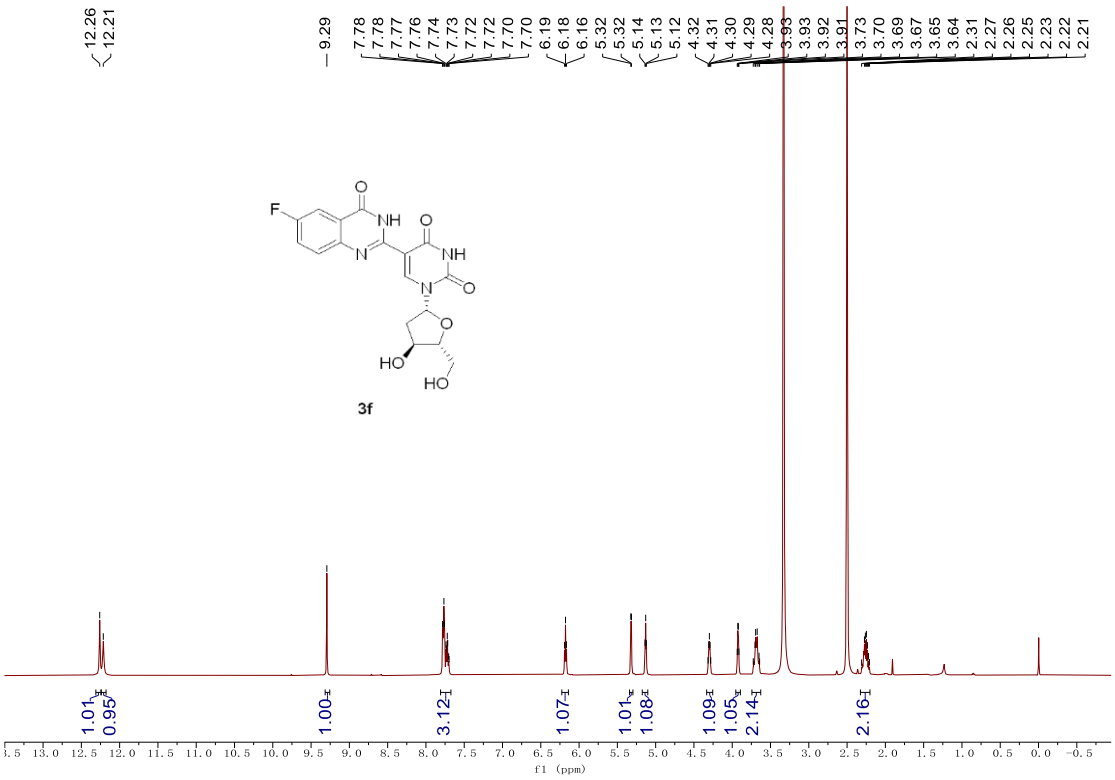
149.7
149.3
149.1
145.5
145.3
127.9
127.3
126.2
118.9
103.6
88.5
86.5
70.6
61.4
41.1
21.9
f1 (ppm)
3e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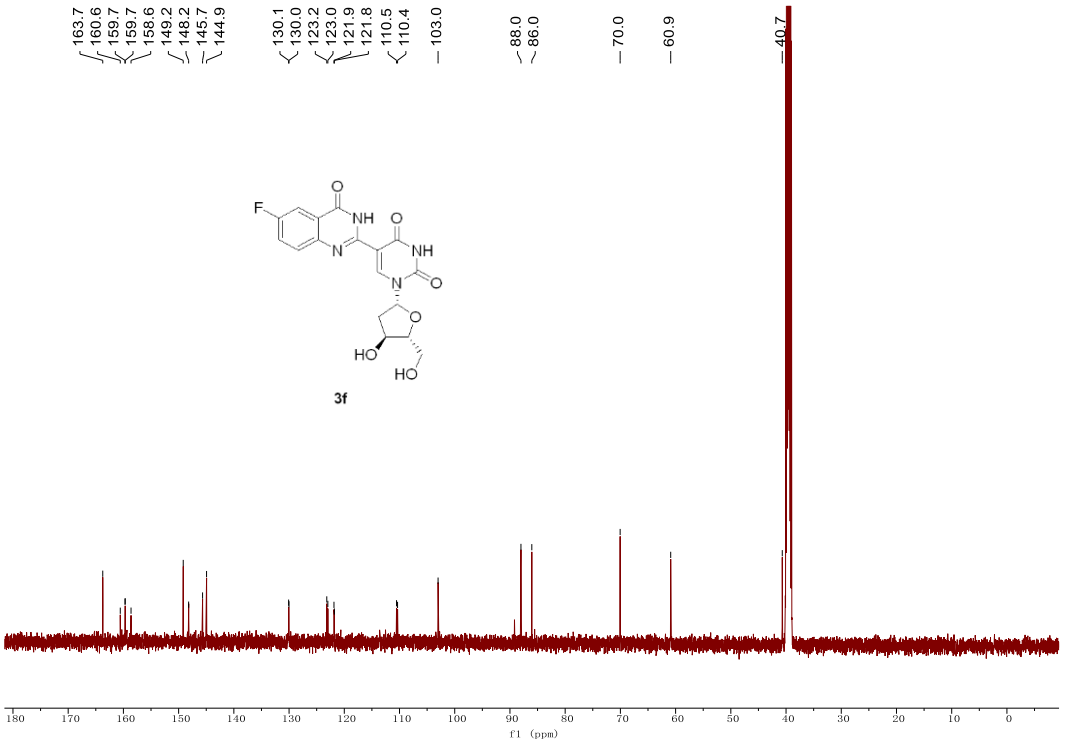
7.72
7.72
7.70
6.19
6.18
6.16
5.32
5.32
5.14
5.13
5.12
4.32
4.31
4.30
4.29
4.28
3.93
3.93
3.92
3.91
3.73
3.70
3.69
3.67
3.65
3.64
2.31
2.27
2.26
2.25
2.23
2.22
2.21
F
NH
O
NH
N
O
HO
HO
3f
1.01
0.95
1.00
3.12
1.07
1.01
1.08
1.09
1.05
2.14
2.16
f1 (ppm)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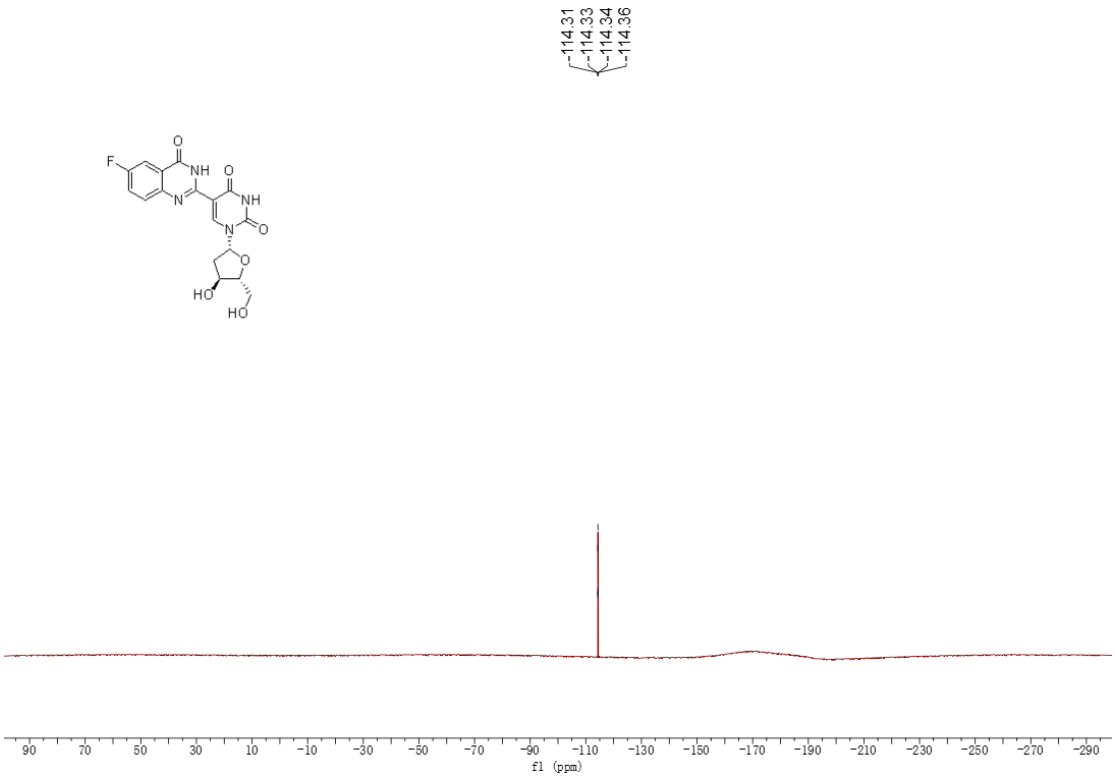
160.6
159.7
159.7
158.6
149.2
148.2
145.7
144.9
130.1
130.0
123.2
123.0
121.9
121.8
110.5
110.4
103.0
88.0
86.0
70.0
60.9
40.7
F
NH
O
NH
N
O
HO
HO
3f
f1 (ppm)


-114.31
-114.33
-114.34
-114.36
F
O
NH
N
O
NH
N
O
O
HO
HO
90
70
50
30
10
-10
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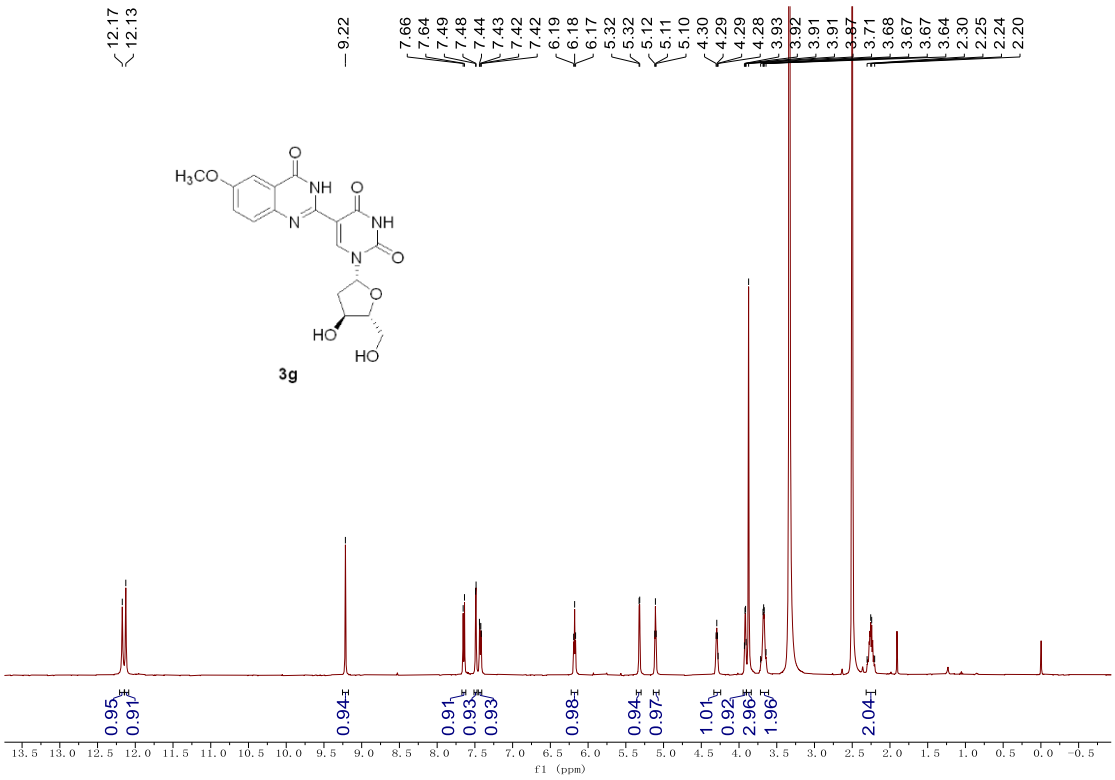
-210
-230
-250
-270
-290
f1 (ppm)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12.13
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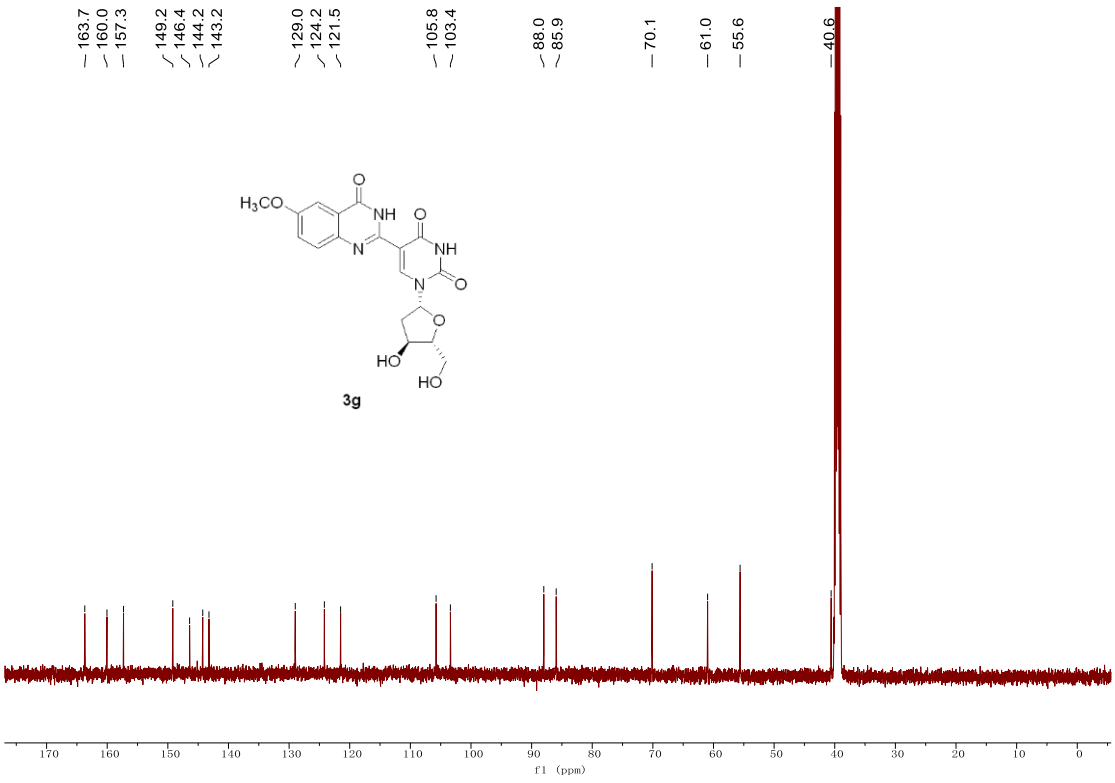
7.64
7.49
7.48
7.44
7.43
7.42
7.42
6.19
6.18
6.17
5.32
5.32
5.12
5.11
5.10
4.30
4.29
4.29
4.28
3.93
3.92
3.91
3.91
3.87
3.71
3.68
3.67
3.67
3.64
2.30
2.25
2.24
2.20
0.95
0.91
0.94
0.91
0.93
0.93
0.98
0.94
0.97
1.01
0.92
2.96
1.96
2.04
f1 (ppm)

H3CO
NH
O
N
NH
O
N
O
HO
HO

3g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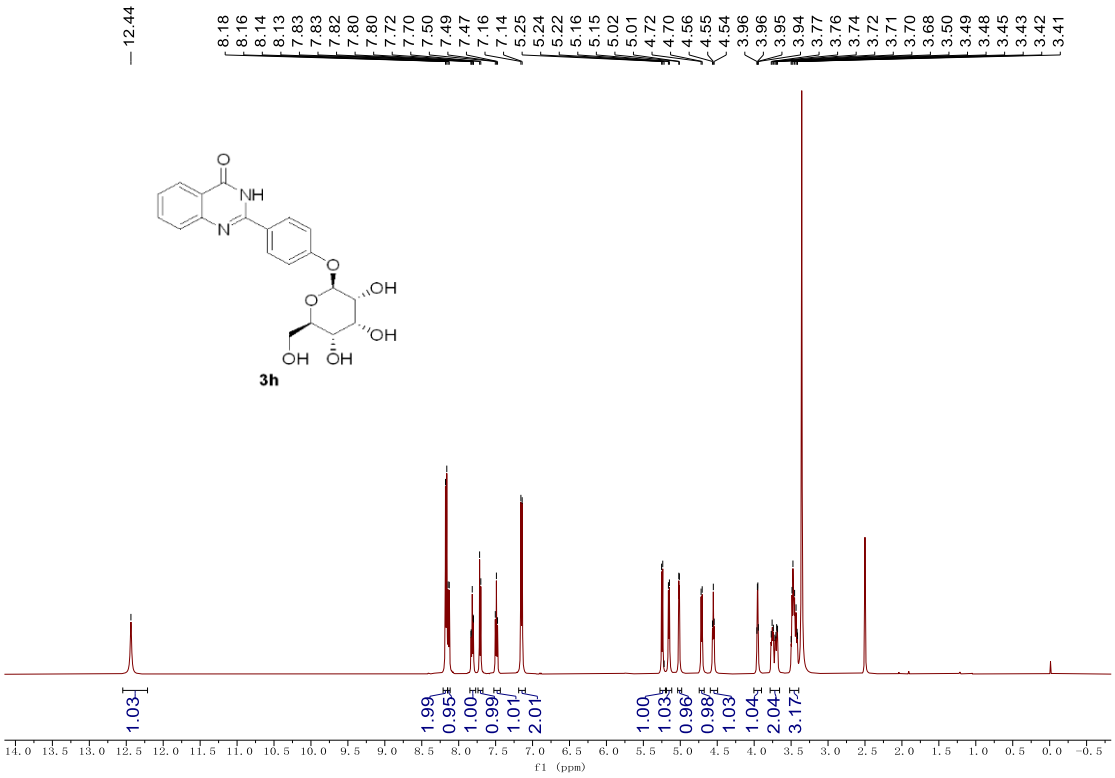
160.0
157.3
149.2
146.4
144.2
143.2
129.0
124.2
121.5
105.8
103.4
88.0
85.9
70.1
61.0
55.6
40.6
f1 (ppm)

H3CO
NH
O
N
NH
O
N
O
HO
HO

3g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8.18
8.16
8.14
8.13
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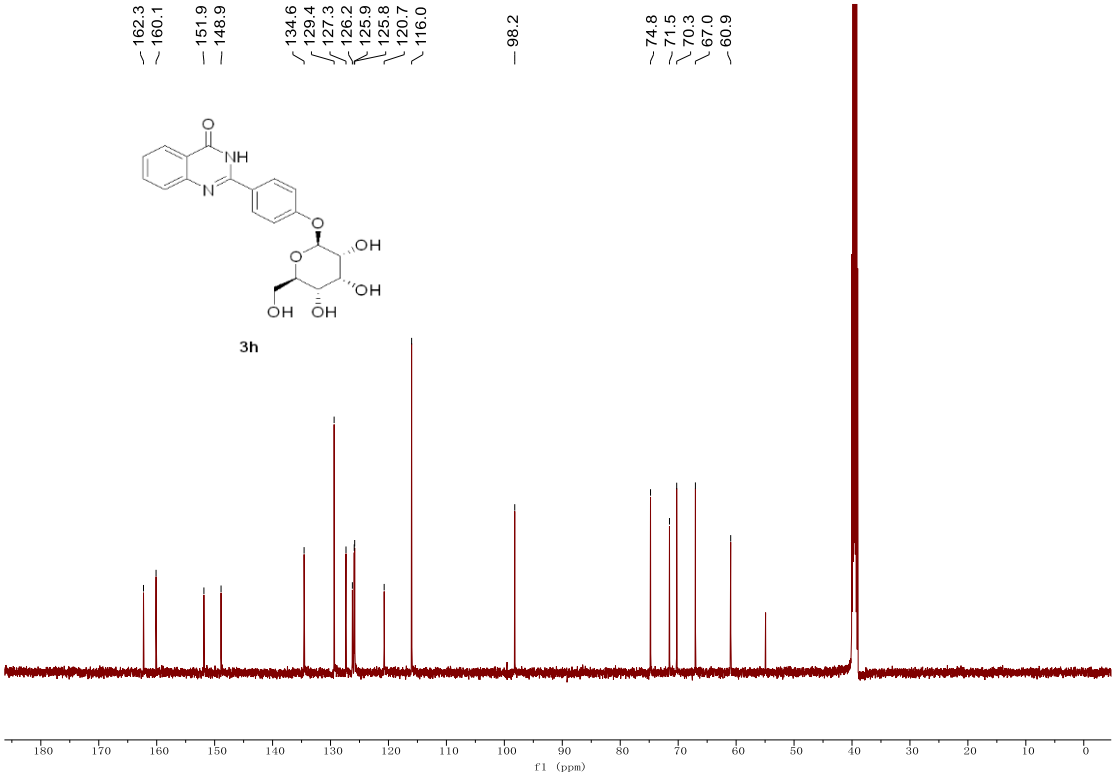
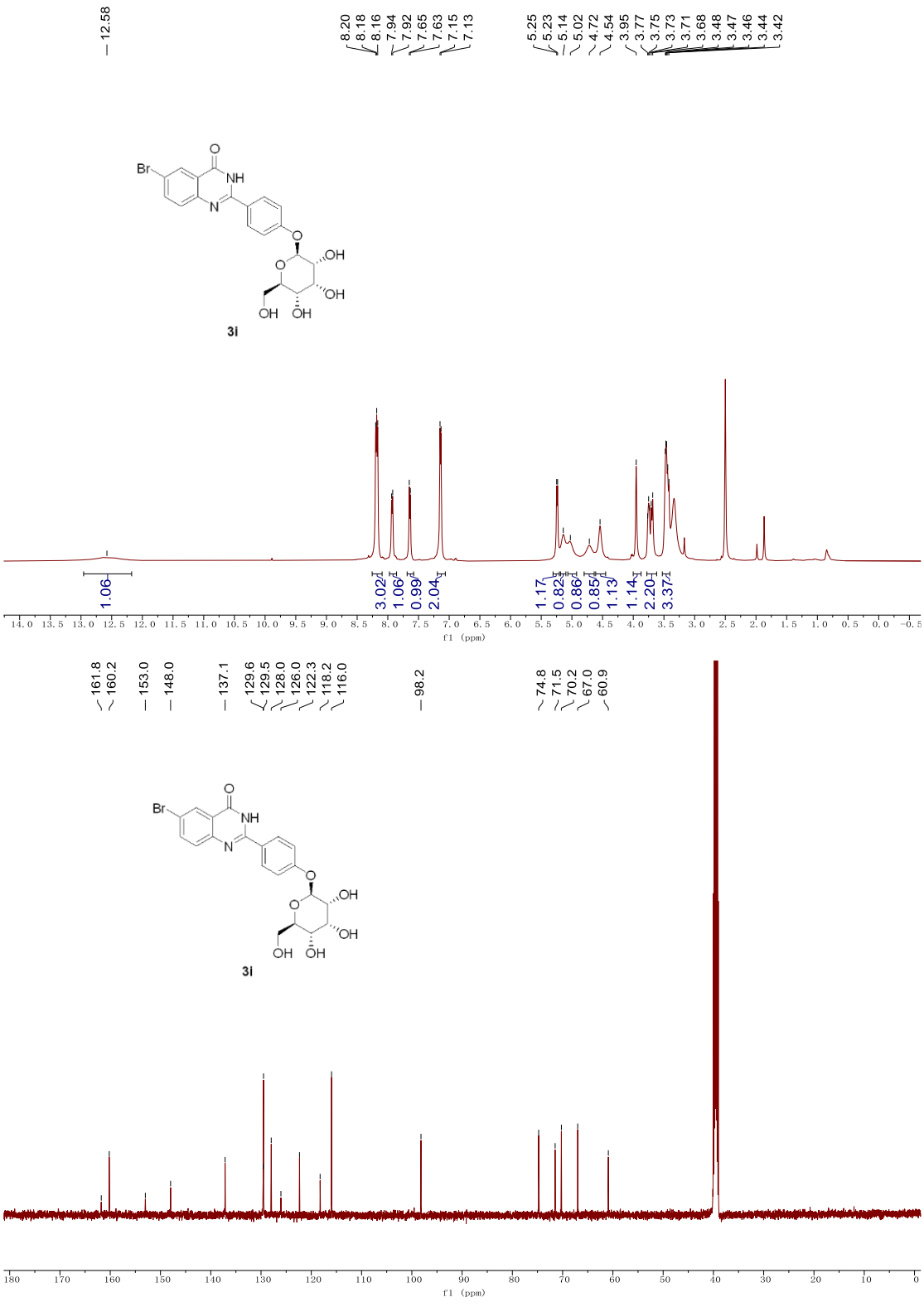
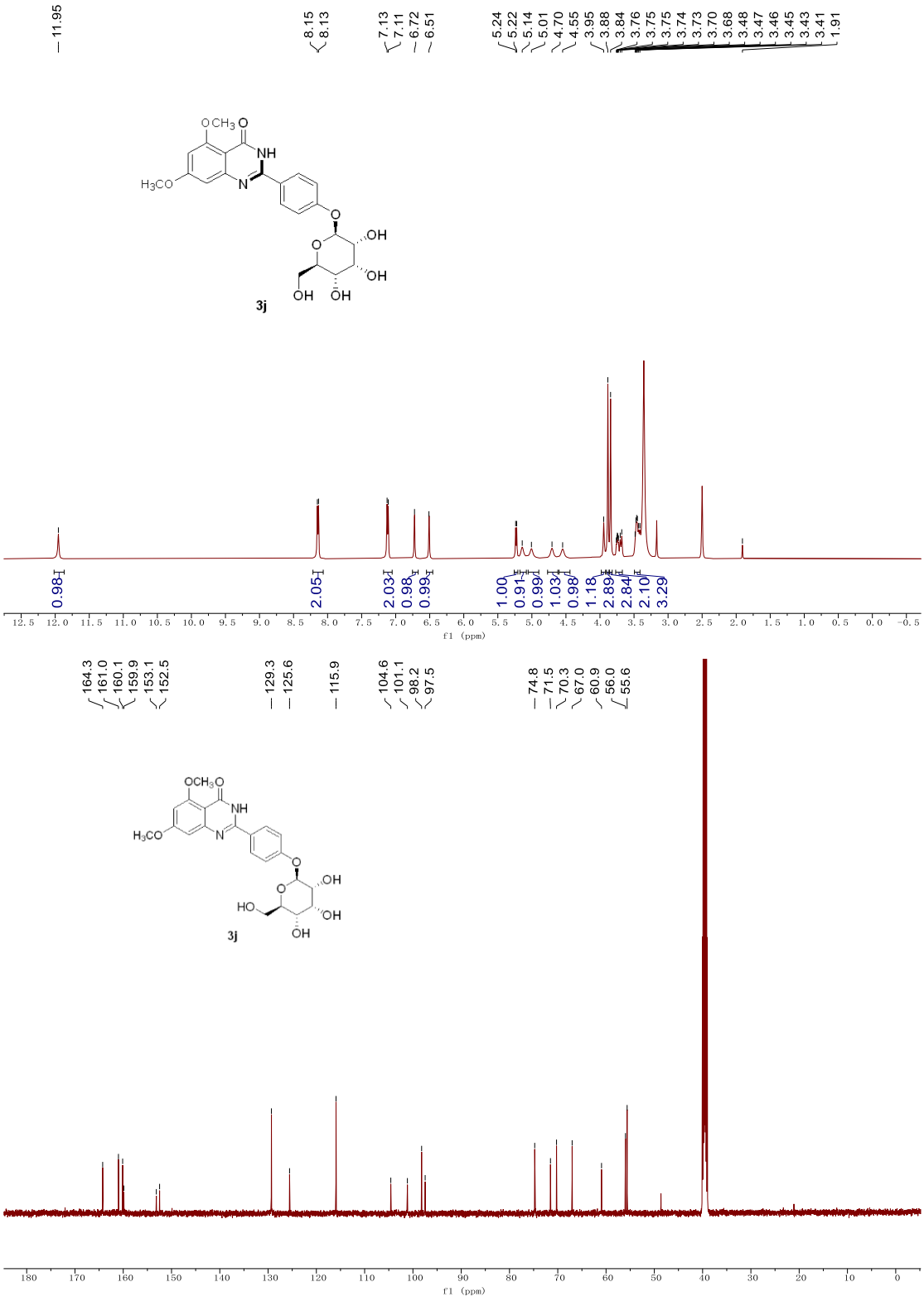
7.83
7.82
7.80
7.80
7.72
7.70
7.50
7.49
7.47
7.16
7.14
5.25
5.24
5.22
5.16
5.15
5.02
5.01
4.72
4.70
4.56
4.55
4.54
3.96
3.96
3.95
3.94
3.77
3.76
3.74
3.72
3.71
3.70
3.68
3.50
3.49
3.48
3.45
3.43
3.42
3.41
NH
N
O
OH
OH
OH
OH
3h
1.03
1.99
0.95
1.00
0.99
1.01
2.01
1.00
1.03
0.96
0.98
1.03
1.04
2.04
3.17
f1 (ppm)


162.3
160.1
151.9
148.9
134.6
129.4
127.3
126.2
125.9
125.8
120.7
116.0
98.2
74.8
71.5
70.3
67.0
60.9
NH
N
O
OH
OH
OH
OH
3h
f1 (ppm)


12.58
8.20
8.18
8.16
7.94
7.92
7.65
7.63
7.15
7.13
5.25
5.23
5.14
5.02
4.72
4.54
3.95
3.77
3.75
3.73
3.71
3.68
3.48
3.47
3.46
3.44
3.42
Br
O
NH
N
O
OH
O
OH
OH
OH
3i
1.06
3.02
1.06
0.99
2.04
1.17
0.82
0.86
0.85
1.13
1.14
2.20
3.37
f1 (ppm)
161.8
160.2
153.0
148.0
137.1
129.6
129.5
128.0
126.0
122.3
118.2
116.0
98.2
74.8
71.5
70.2
67.0
60.9
Br
O
NH
N
O
OH
O
OH
OH
OH
3i
f1 (ppm)


11.95
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7.11
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6.51
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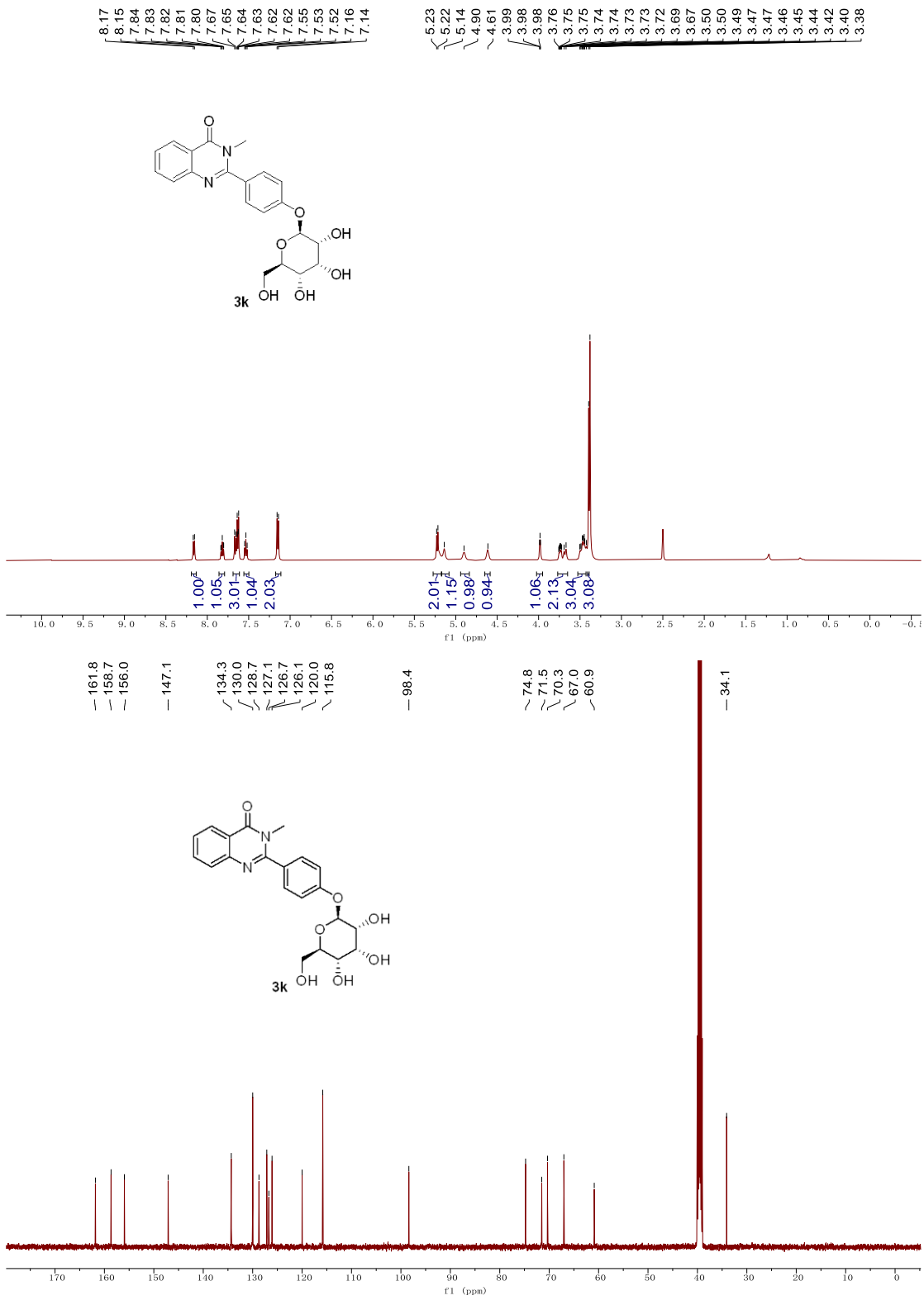
5.22
5.14
5.01
4.70
4.55
3.95
3.88
3.84
3.76
3.75
3.75
3.74
3.73
3.70
3.68
3.48
3.47
3.46
3.45
3.43
3.41
1.91
OCH3
O
NH
N
H3CO
O
OH
O
OH
OH
OH
3j
0.98
2.05
2.03
0.98
0.99
1.00
0.91
0.99
1.03
0.98
1.18
2.89
2.84
2.10
3.29
f1 (ppm)
164.3
161.0
160.1
159.9
153.1
152.5
129.3
125.6
115.9
104.6
101.1
98.2
97.5
74.8
71.5
70.3
67.0
60.9
56.0
55.6
OCH3
O
NH
N
H3CO
O
OH
HO
OH
OH
3j
f1 (ppm)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7.82
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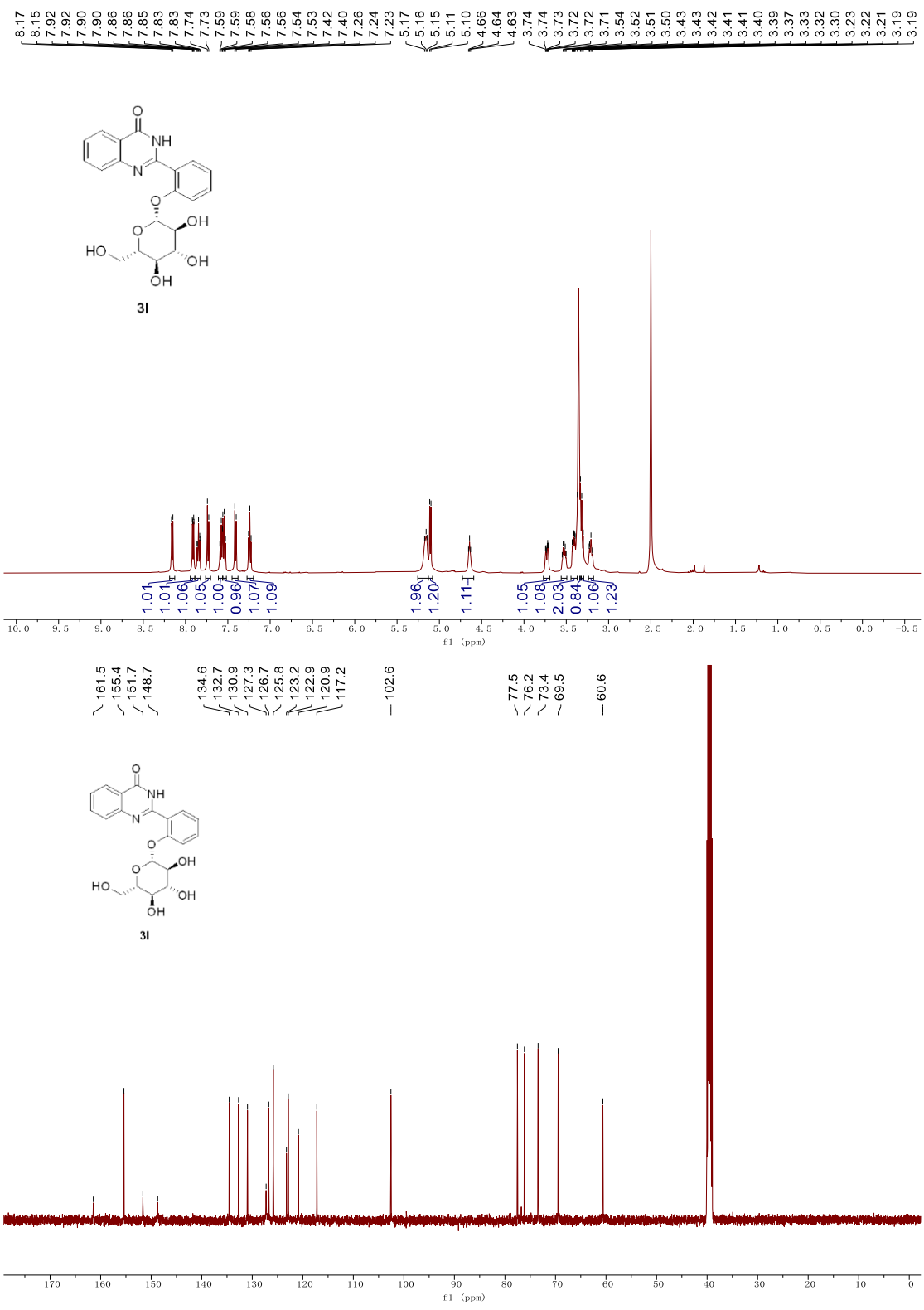
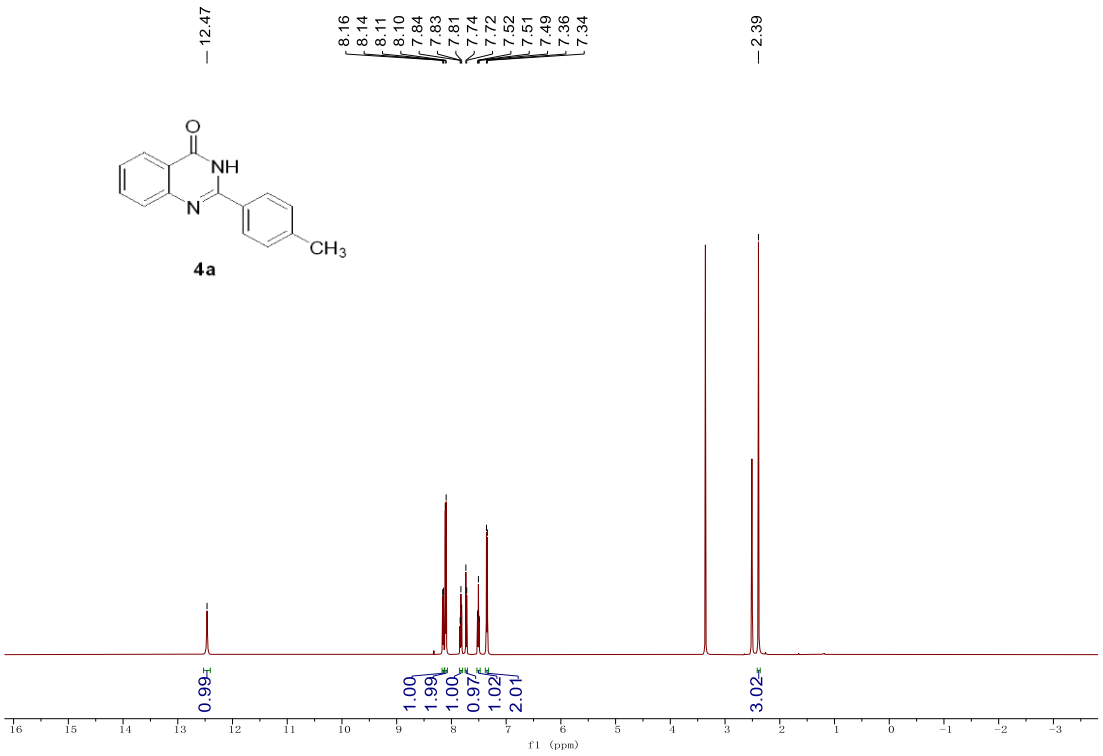
7.80
7.67
7.65
7.64
7.63
7.62
7.62
7.55
7.53
7.52
7.16
7.14
5.23
5.22
5.14
4.90
4.61
3.99
3.98
3.98
3.76
3.75
3.75
3.74
3.74
3.73
3.73
3.72
3.69
3.67
3.50
3.50
3.49
3.47
3.47
3.46
3.45
3.44
3.42
3.40
3.38
3k
1.00
1.05
3.01
1.04
2.03
2.01
1.15
0.98
0.94
1.06
2.13
3.04
3.08
f1 (ppm)
161.8
158.7
156.0
147.1
134.3
130.0
128.7
127.1
126.7
126.1
120.0
115.8
98.4
74.8
71.5
70.3
67.0
60.9
34.1
3k
f1 (ppm)


8.17 8.15 7.92 7.92 7.90 7.90 7.86 7.86 7.85 7.83 7.83 7.74 7.73 7.59 7.59 7.58 7.56 7.56 7.54 7.53 7.42 7.40 7.26 7.24 7.23 5.17 5.16 5.15 5.11 5.10 4.66 4.64 4.63 3.74 3.74 3.73 3.72 3.72 3.71 3.54 3.52 3.51 3.50 3.43 3.43 3.42 3.41 3.41 3.40 3.39 3.37 3.33 3.32 3.30 3.23 3.22 3.21 3.19 3.19
NH
N
O
OH
HO
OH
OH
3l
1.01 1.01 1.06 1.05 1.00 0.96 1.07 1.09 1.96 1.20 1.11 1.05 1.08 2.03 0.84 1.06 1.23
f1 (ppm)
161.5 155.4 151.7 148.7 134.6 132.7 130.9 127.3 126.7 125.8 123.2 122.9 120.9 117.2 102.6 77.5 76.2 73.4 69.5 60.6
3l
f1 (ppm)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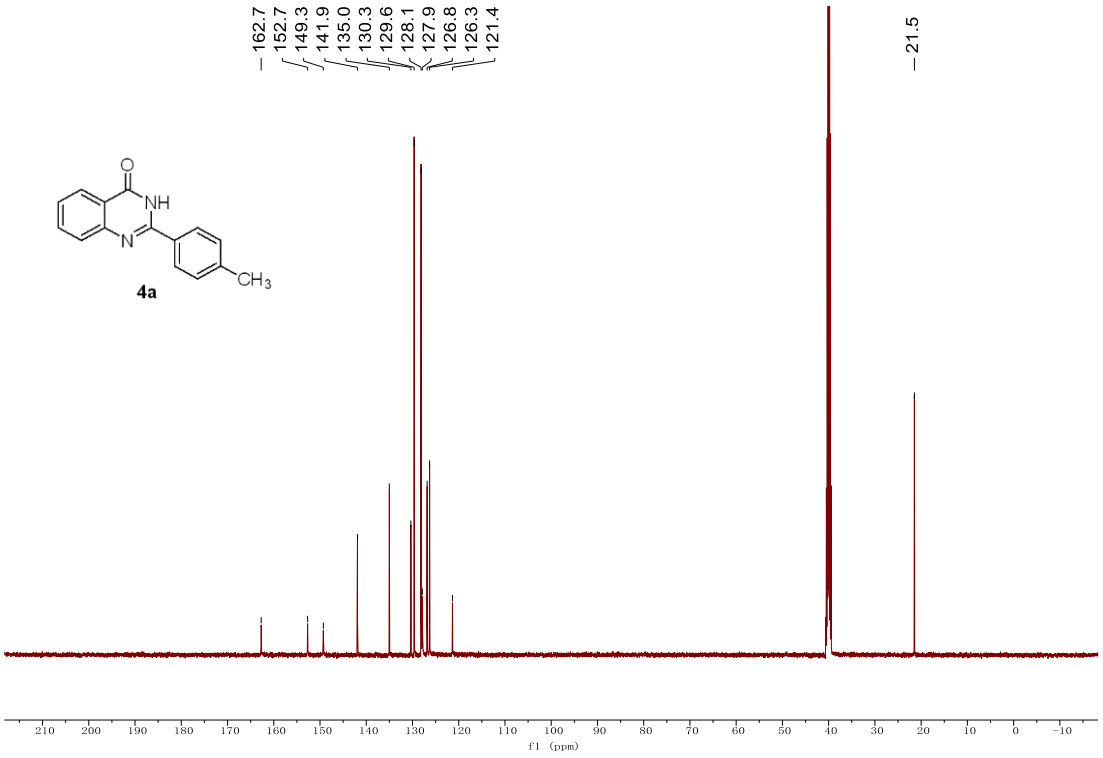
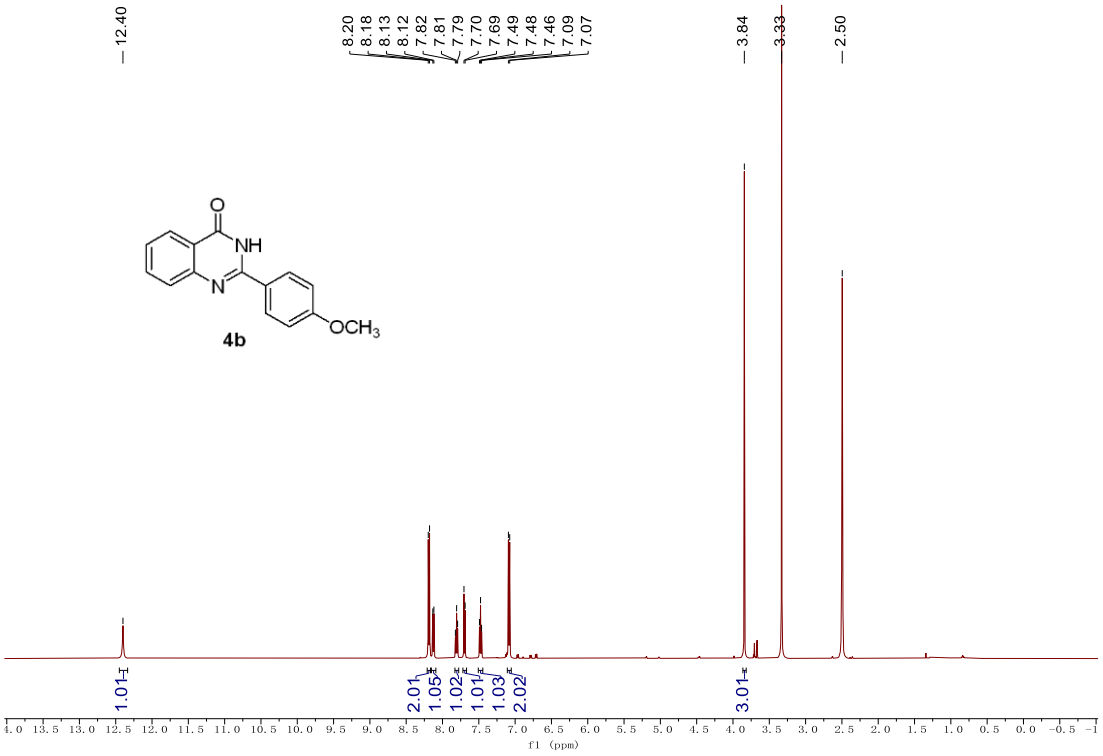
8.11
8.10
7.84
7.83
7.81
7.74
7.72
7.52
7.51
7.49
7.36
7.34
2.39
NH
N
O
CH3
4a
0.99
1.00
1.99
1.00
0.97
1.02
2.01
3.02
f1 (ppm)


162.7
152.7
149.3
141.9
135.0
130.3
129.6
128.1
127.9
126.8
126.3
121.4
21.5
NH
N
O
CH3
4a
f1 (ppm)


12.40
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8.12
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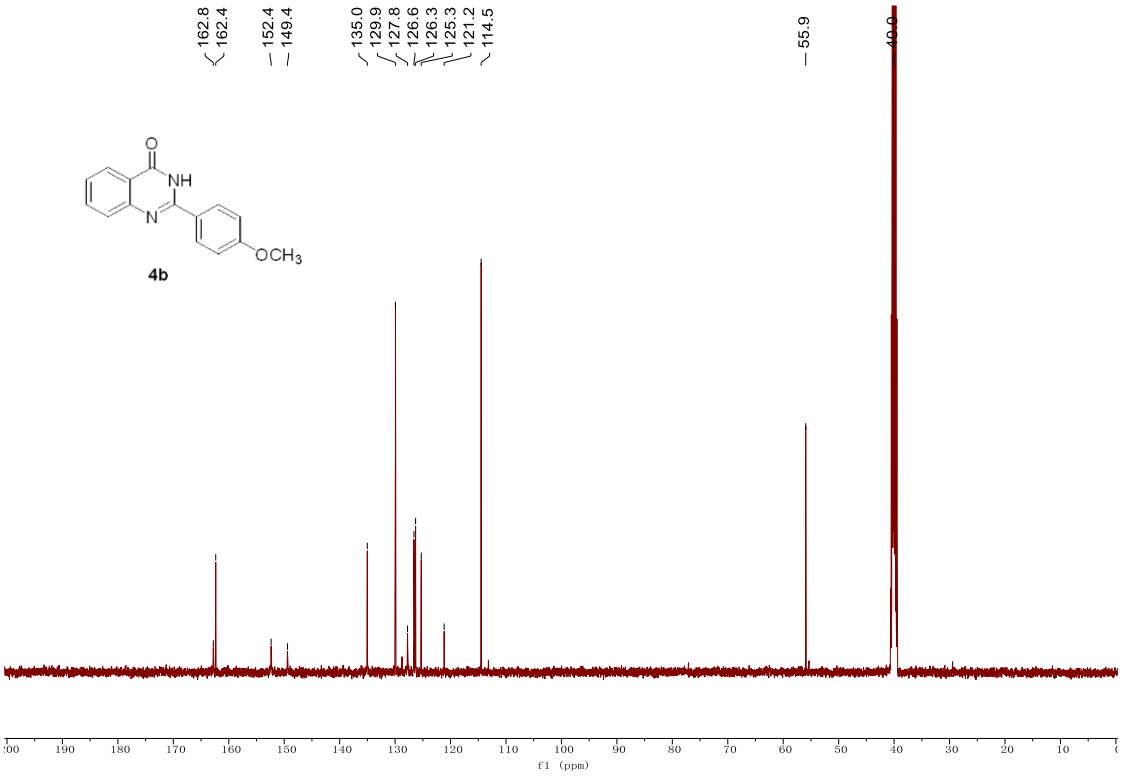
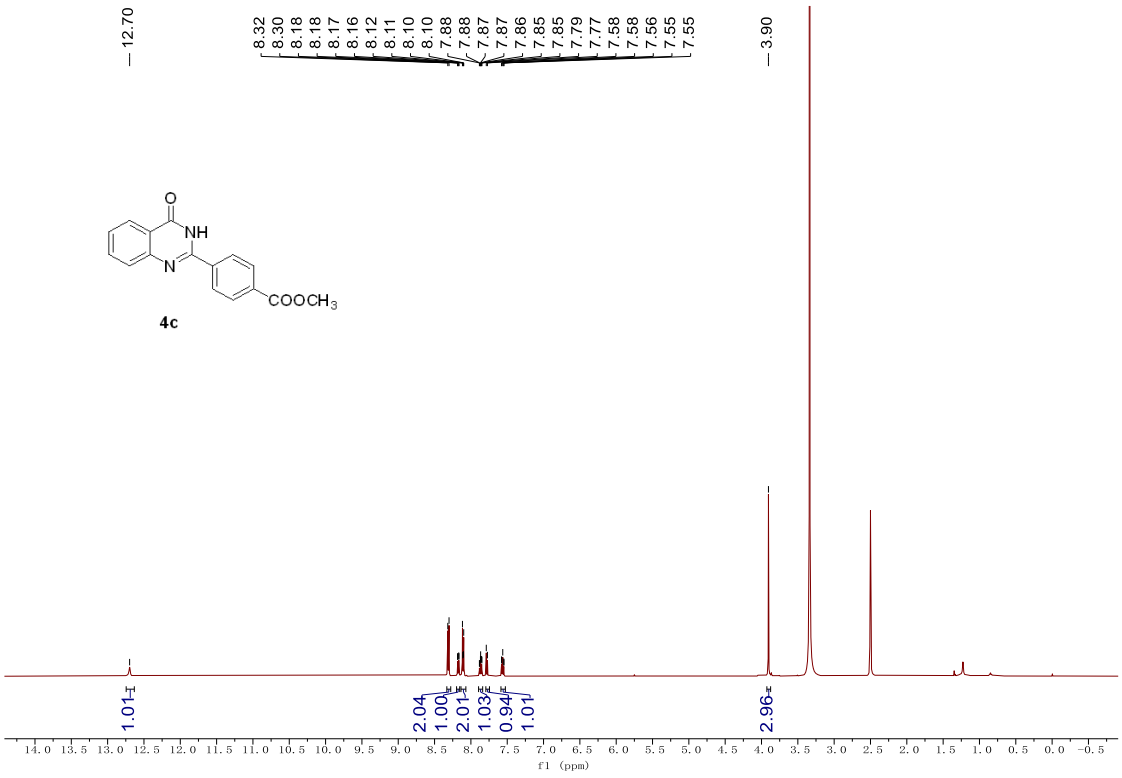
7.81
7.79
7.70
7.69
7.49
7.48
7.46
7.09
7.07
3.84
3.33
2.50
O
NH
N
OCH3
4b
1.01
2.01
1.05
1.02
1.01
1.03
2.02
3.01
f1 (ppm)


162.8
162.4
152.4
149.4
135.0
129.9
127.8
126.6
126.3
125.3
121.2
114.5
55.9
40.0
O
NH
N
OCH3
4b
f1 (ppm)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8.18
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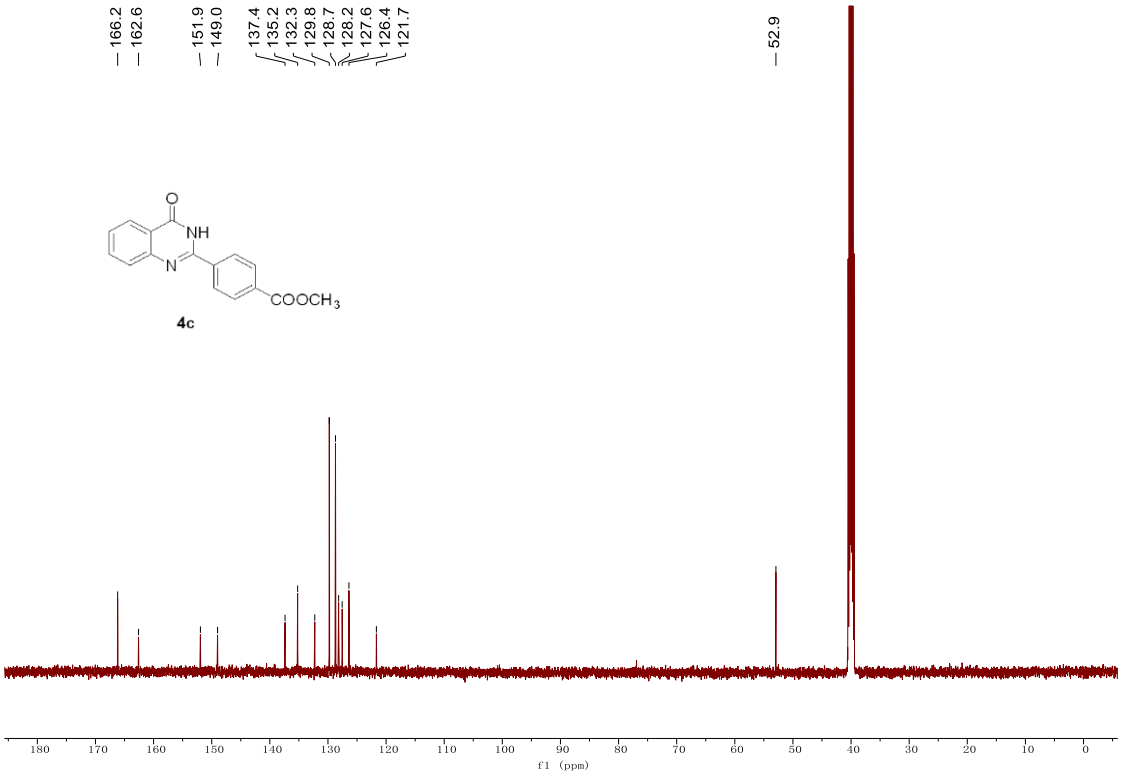
8.16
8.12
8.11
8.10
8.10
7.88
7.88
7.87
7.87
7.86
7.85
7.85
7.79
7.77
7.58
7.58
7.56
7.55
7.55
3.90
O
NH
N
COOCH3
4c
1.01
2.04
1.00
2.01
1.03
0.94
1.01
2.96
f1 (ppm)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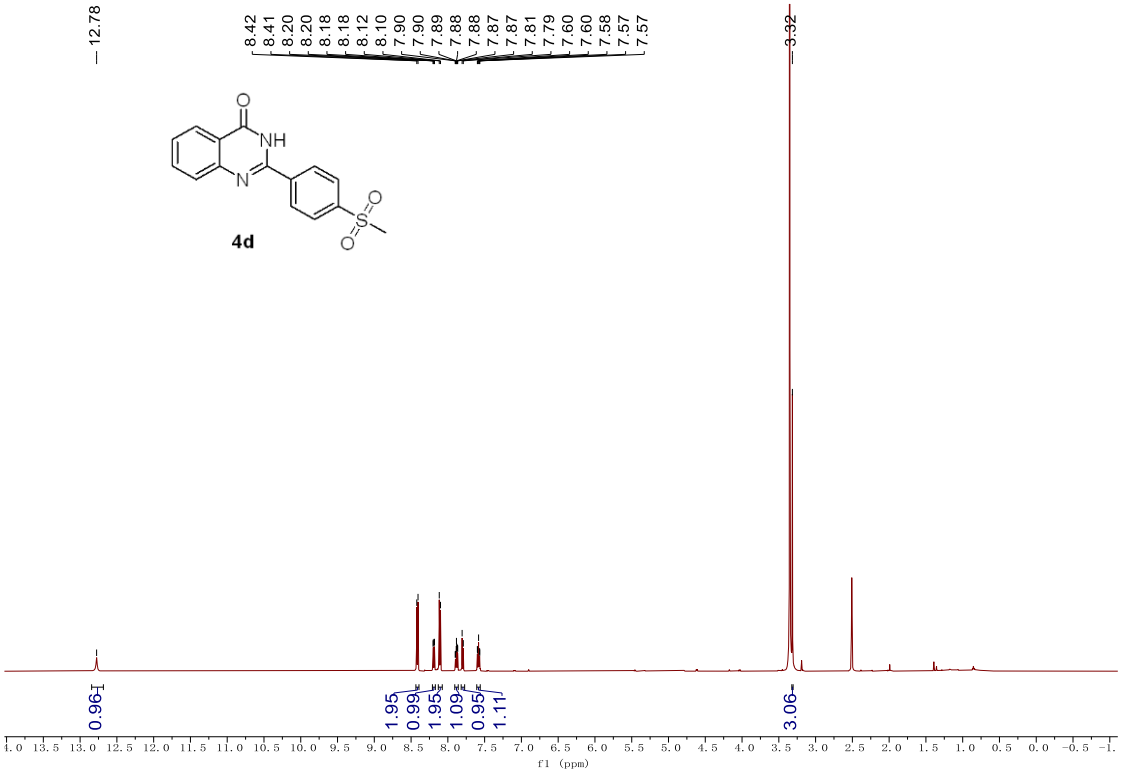
162.6
151.9
149.0
137.4
135.2
132.3
129.8
128.7
128.2
127.6
126.4
121.7
52.9
O
NH
N
COOCH3
4c
f1 (ppm)


12.78
8.42
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8.20
8.20
8.18
8.18
8.12
8.10
7.90
7.90
7.89
7.88
7.88
7.87
7.87
7.81
7.79
7.60
7.60
7.58
7.57
7.57
3.32
NH
N
O
S
O
O
4d
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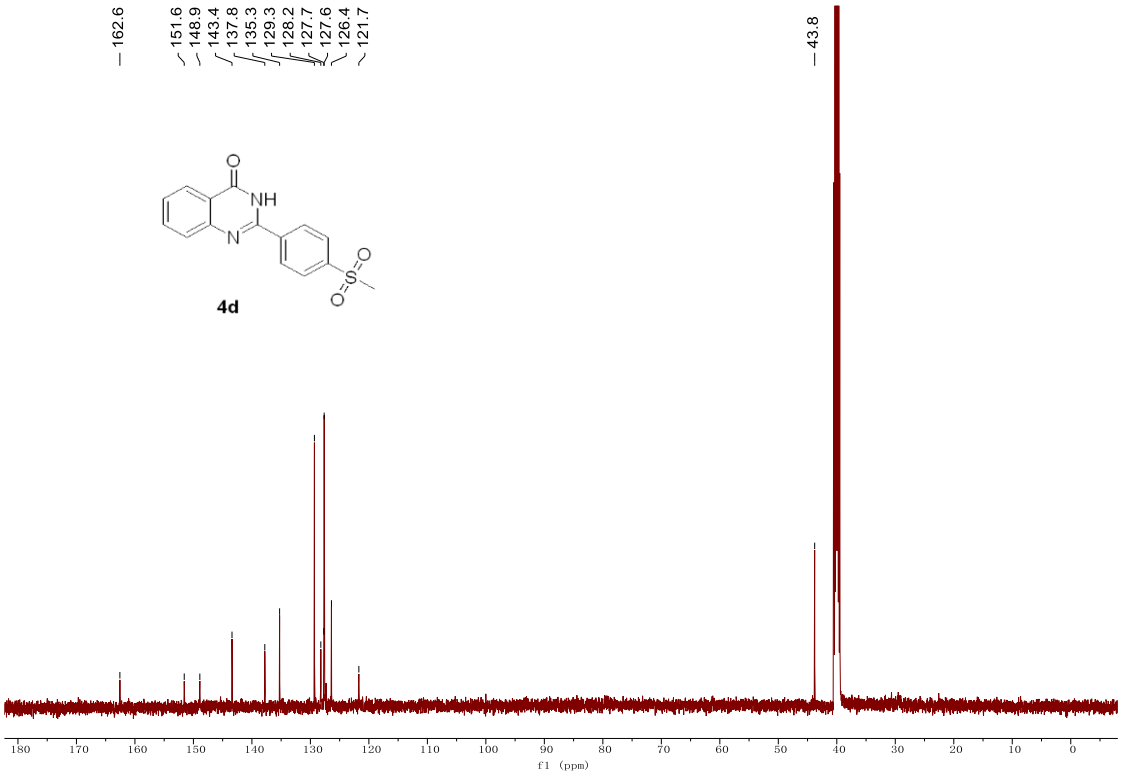
1.95
0.99
1.95
1.09
0.95
1.11
3.06
f1 (ppm)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135.3
129.3
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127.6
126.4
121.7
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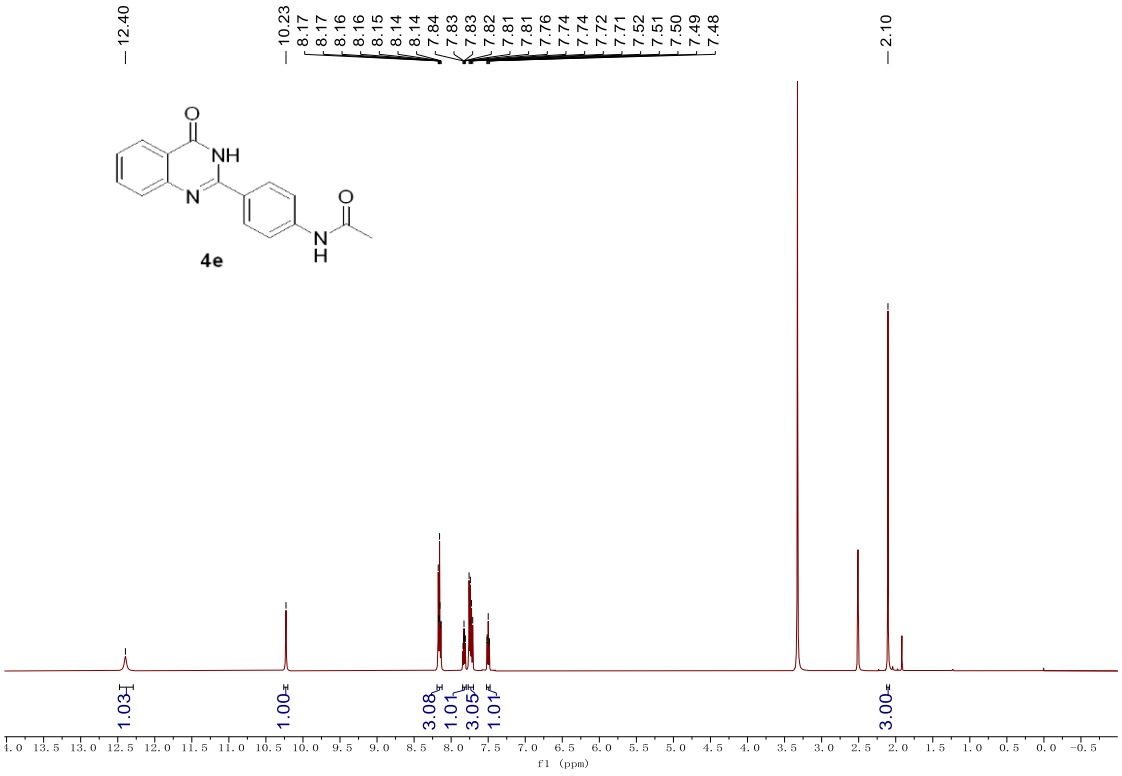
O
S
O
O
4d
f1 (ppm)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8.14
8.14
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7.83
7.83
7.82
7.81
7.81
7.76
7.74
7.74
7.72
7.71
7.52
7.51
7.50
7.49
7.48
2.10
NH
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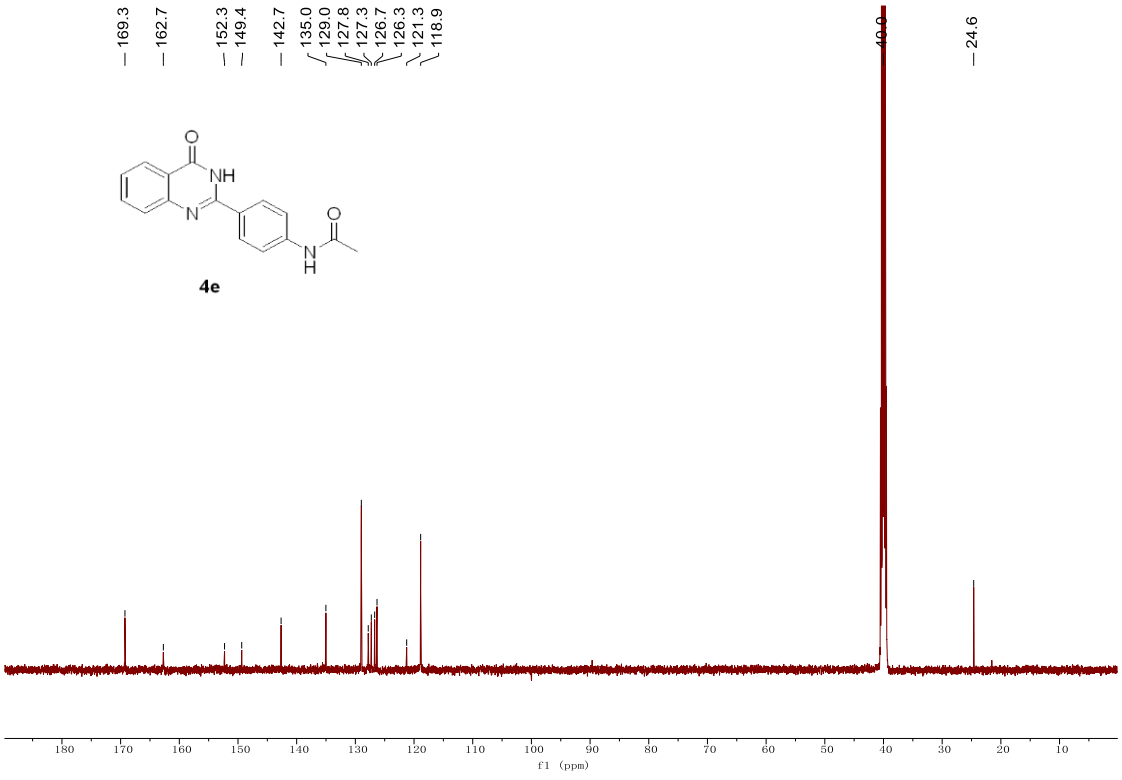
H
O
4e
1.03
1.00
3.08
1.01
3.05
1.01
3.00
f1 (ppm)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129.0
127.8
127.3
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121.3
118.9
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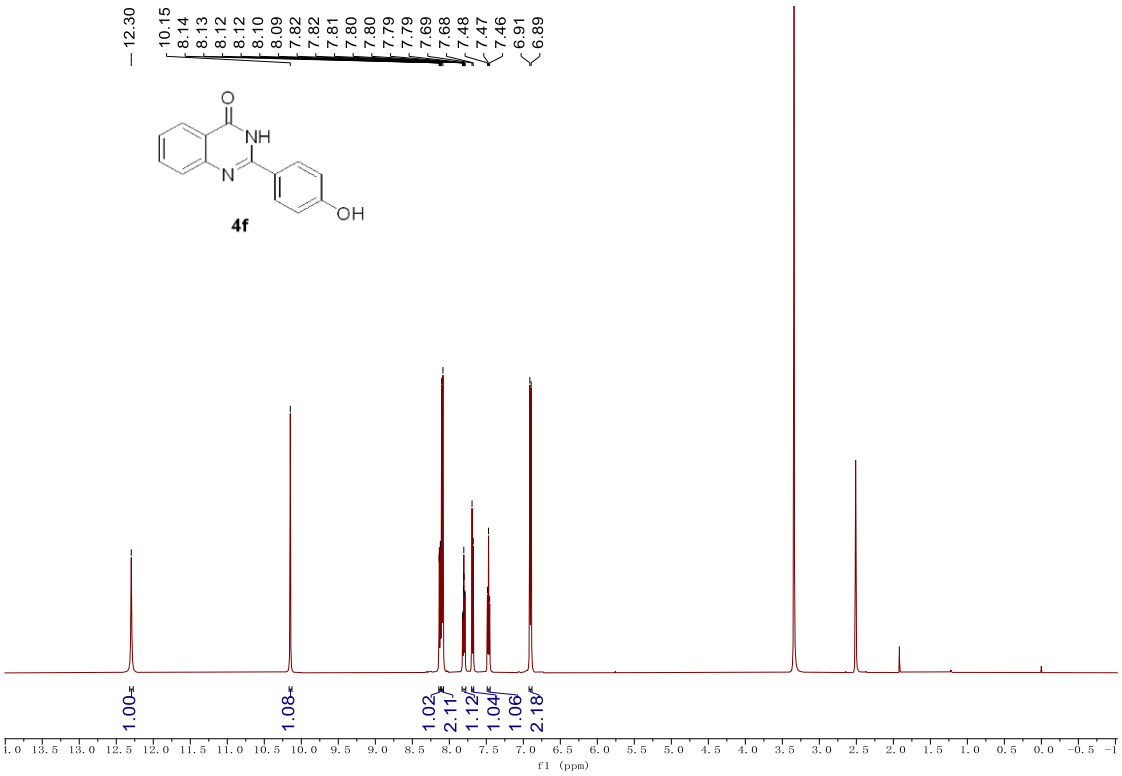
NH
N
O
N
H
O
4e
f1 (ppm)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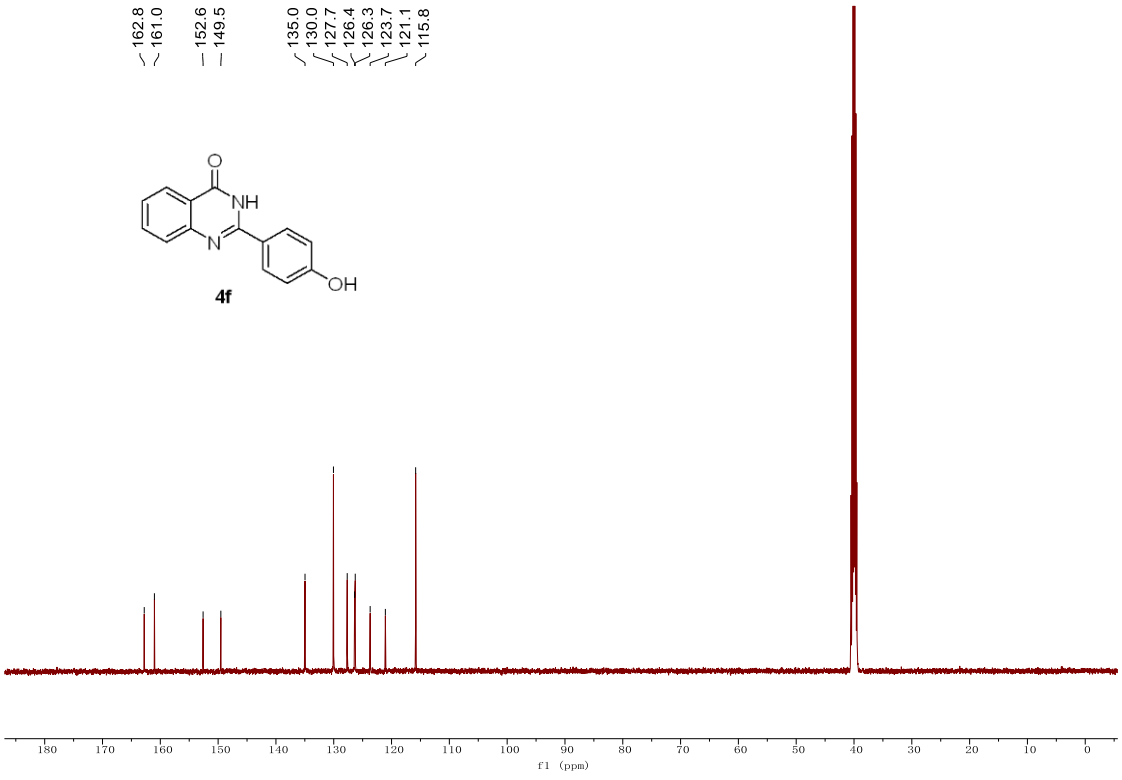
8.10
8.09
7.82
7.82
7.81
7.80
7.80
7.79
7.79
7.69
7.68
7.48
7.47
7.46
6.91
6.89
O
NH
N
OH
4f
1.00
1.08
1.02
2.11
1.12
1.04
1.06
2.18
f1 (ppm)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130.0
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121.1
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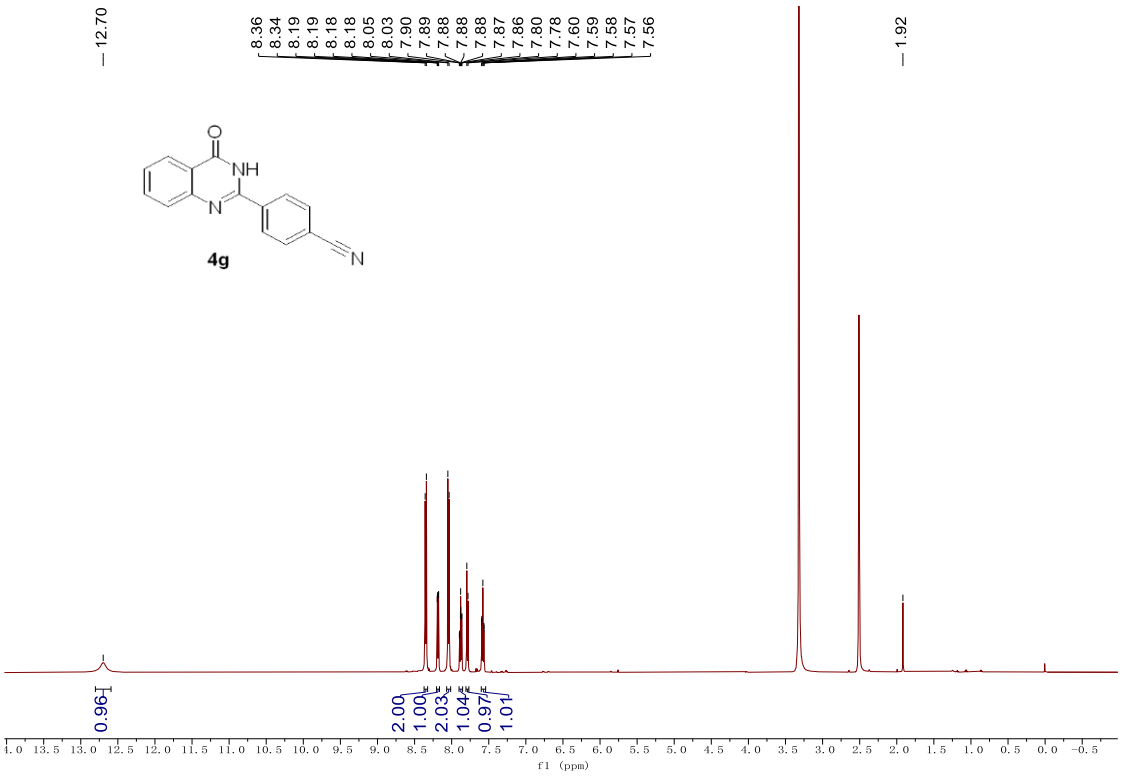
N
OH
4f
f1 (ppm)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7.89
7.88
7.88
7.88
7.87
7.86
7.80
7.78
7.60
7.59
7.58
7.57
7.56
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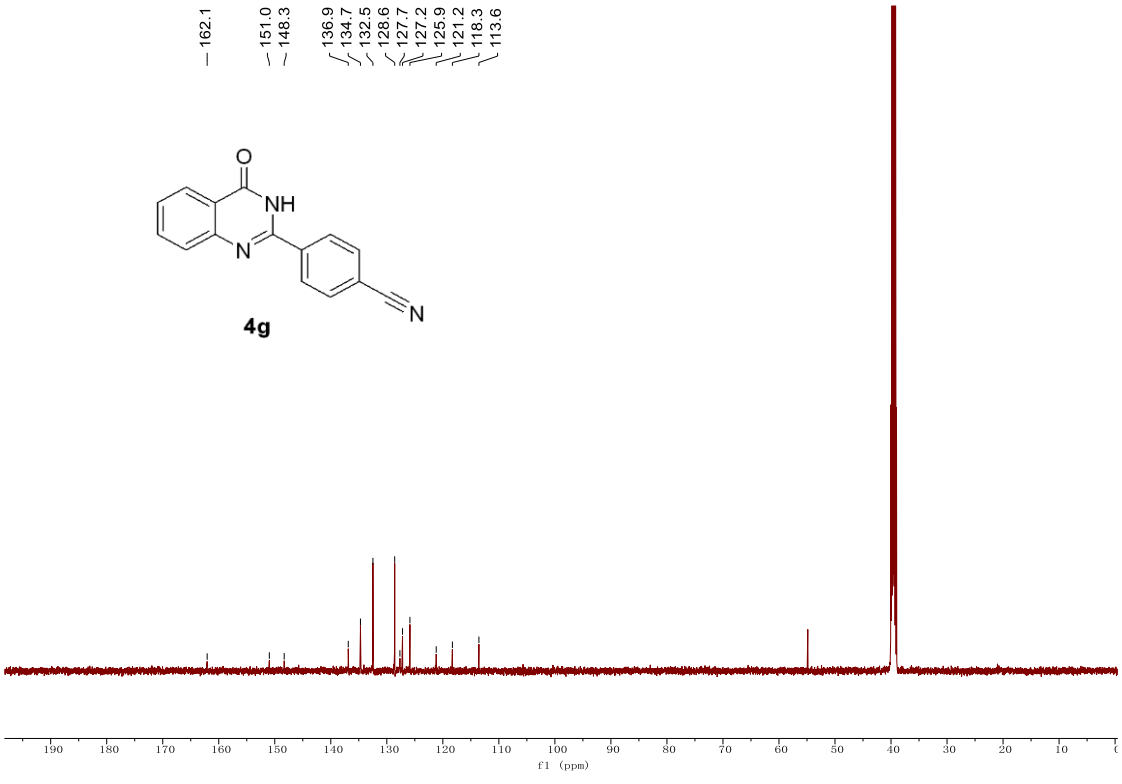
N
4g
0.96
2.00
1.00
2.03
1.04
0.97
1.01
f1 (ppm)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121.2
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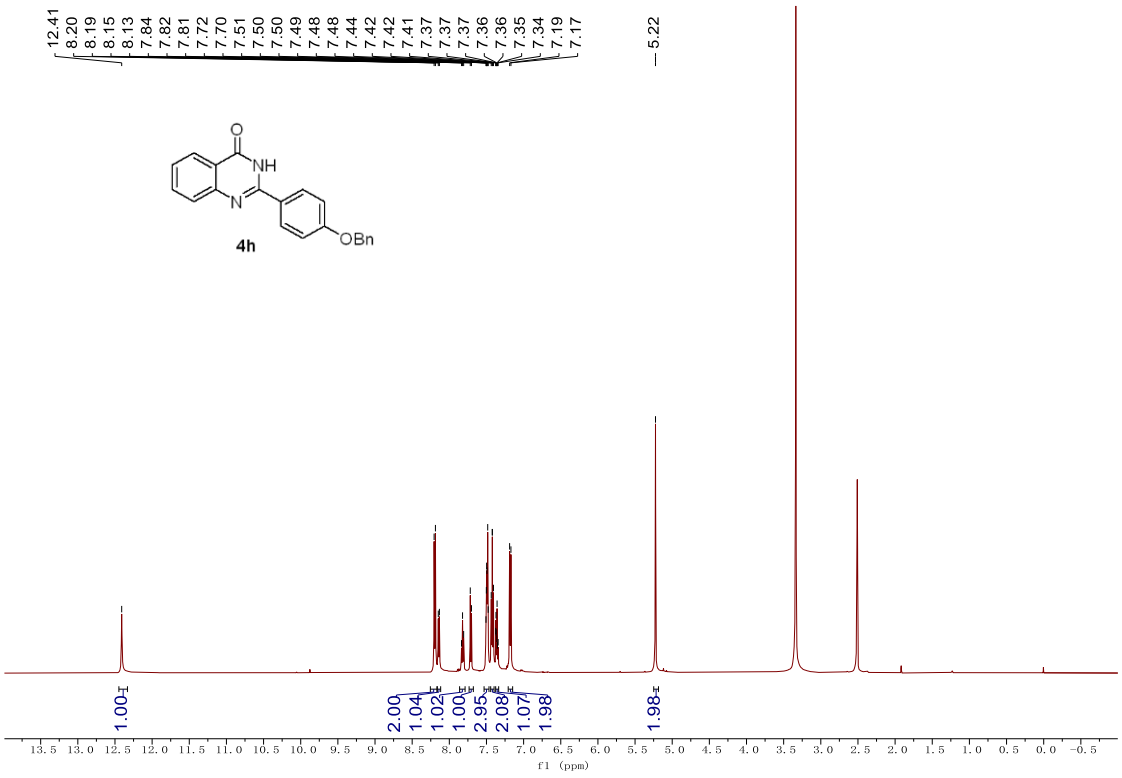
N
N
4g
f1 (ppm)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7.72
7.70
7.51
7.50
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7.49
7.48
7.48
7.44
7.42
7.42
7.41
7.37
7.37
7.37
7.36
7.36
7.35
7.34
7.19
7.17
5.22
O
NH
N
OBn
4h
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1.04
1.02
1.00
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2.08
1.07
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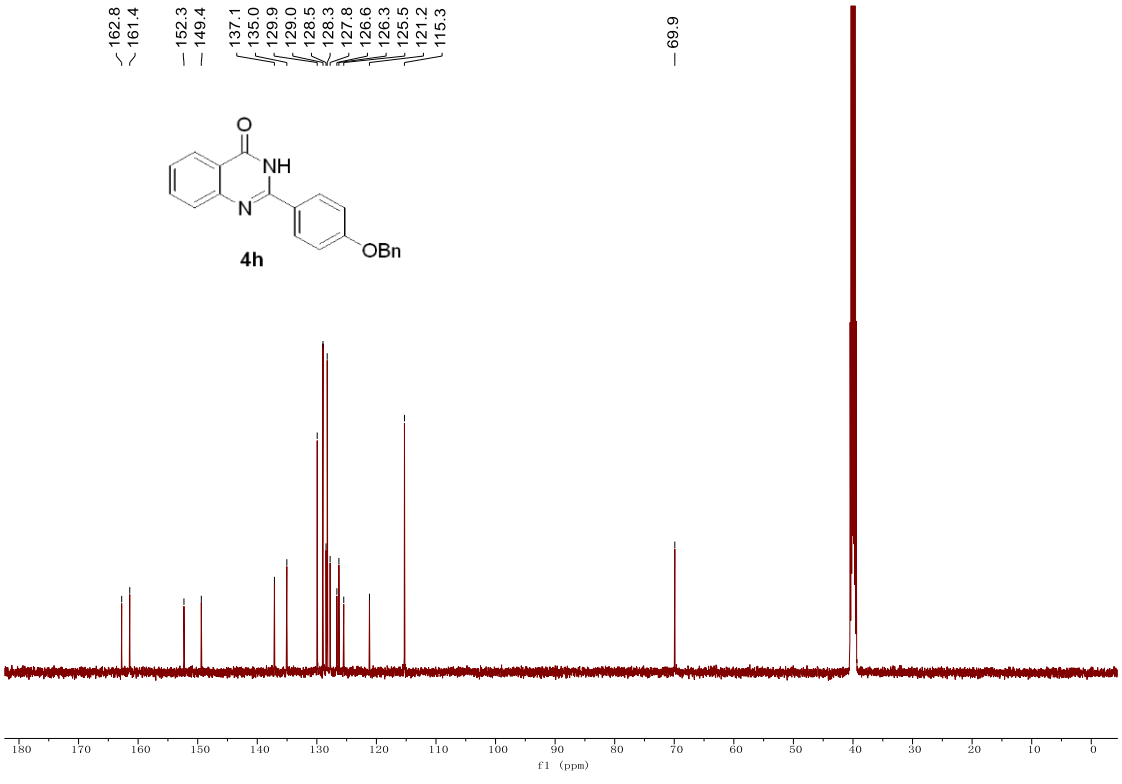
1.98
f1 (ppm)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129.9
129.0
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128.3
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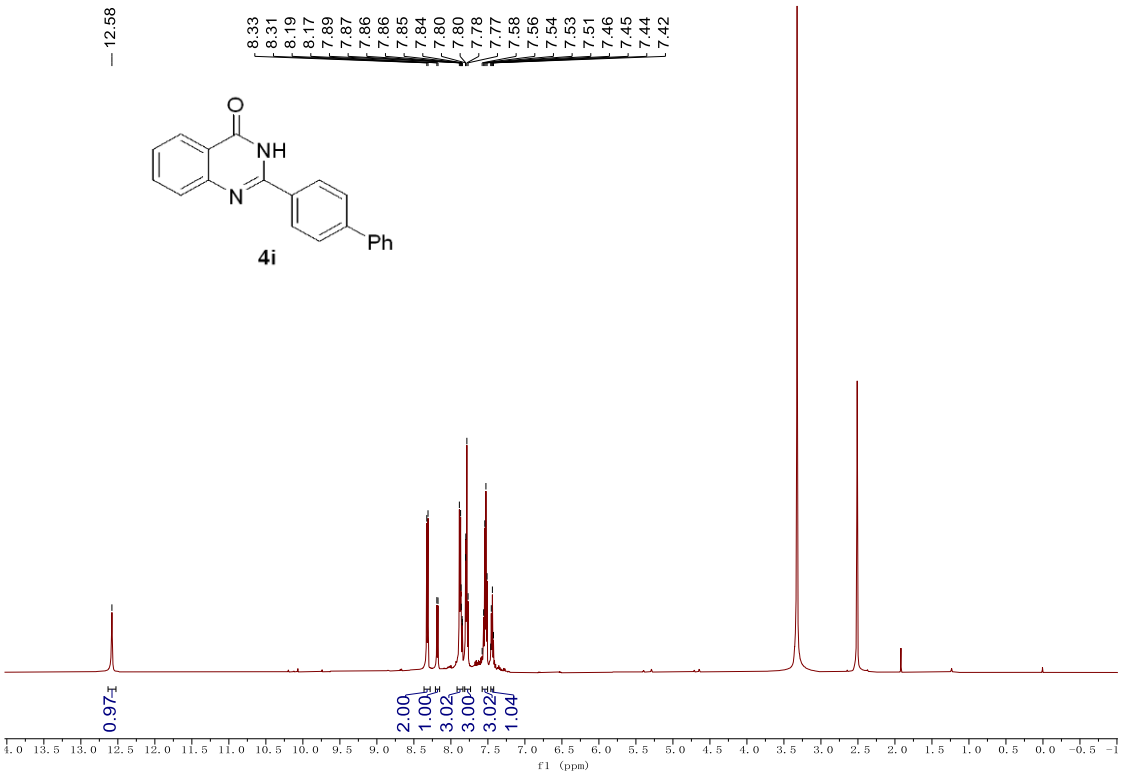
125.5
121.2
115.3
69.9
O
NH
N
OBn
4h
f1 (ppm)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7.80
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7.78
7.77
7.58
7.56
7.54
7.53
7.51
7.46
7.45
7.44
7.42
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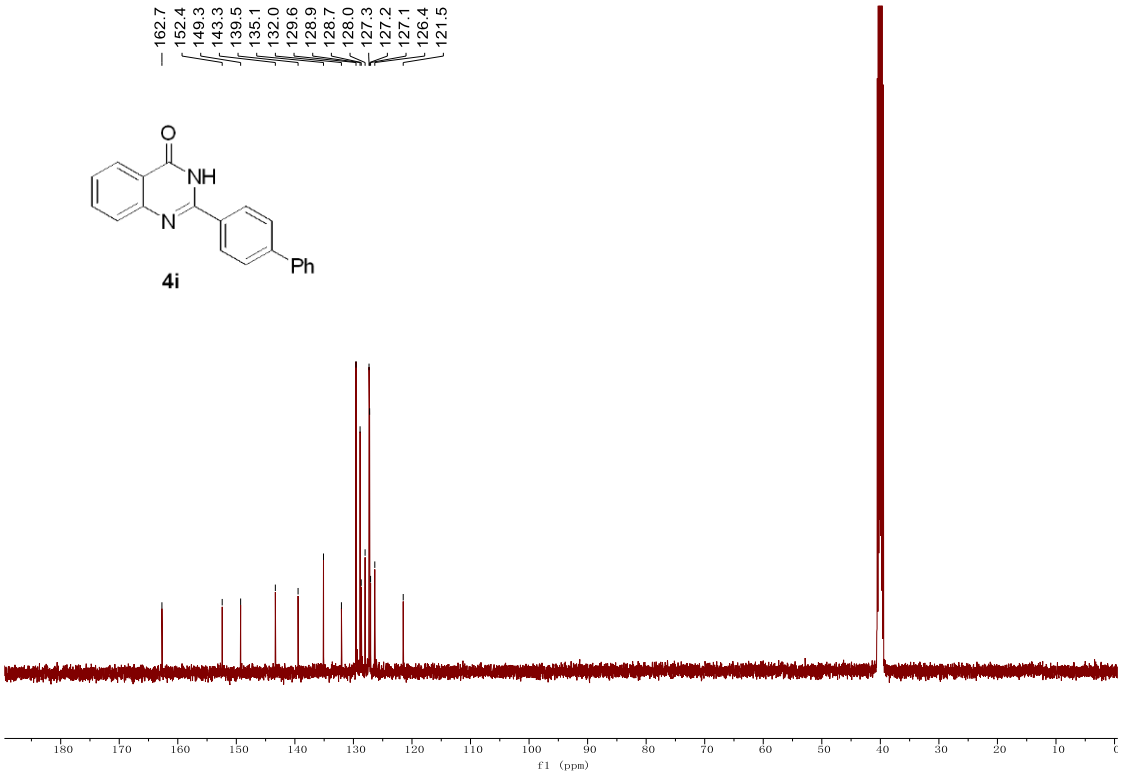
NH
N
Ph
4i
0.97
2.00
1.00
3.02
3.00
3.02
1.04
f1 (ppm)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143.3
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135.1
132.0
129.6
128.9
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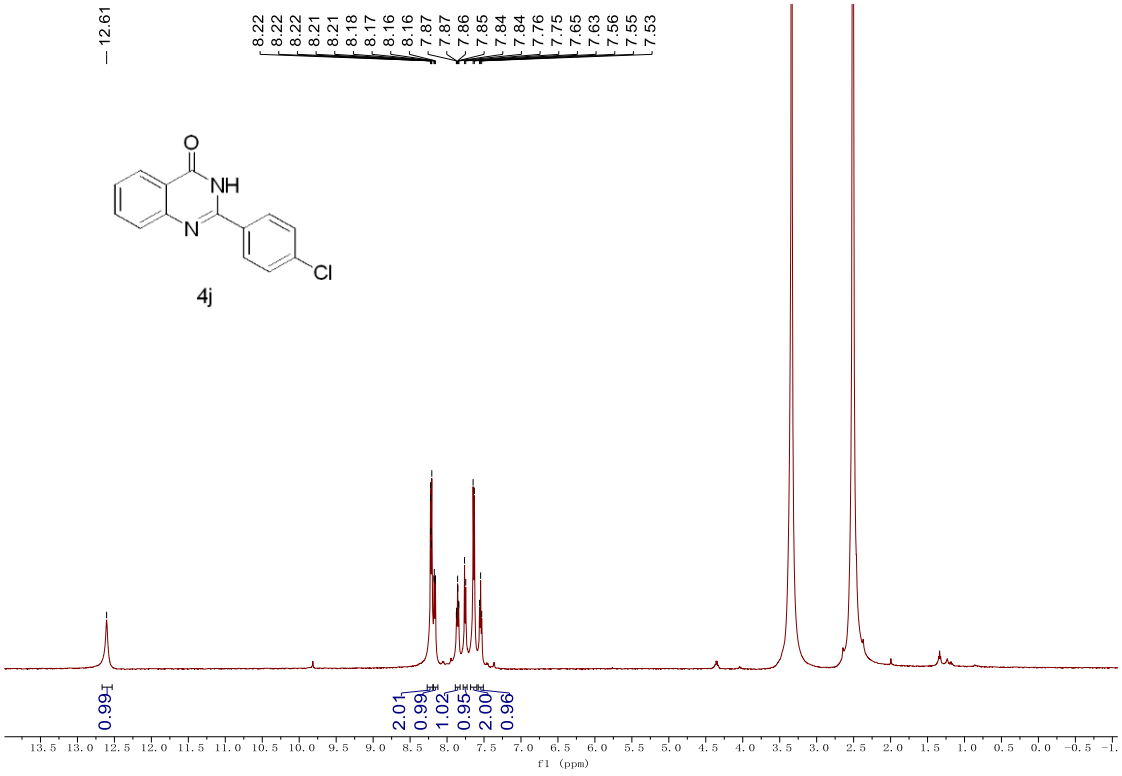
127.3
127.2
127.1
126.4
121.5
O
NH
N
Ph
4i
f1 (ppm)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8.21
8.18
8.17
8.16
8.16
7.87
7.87
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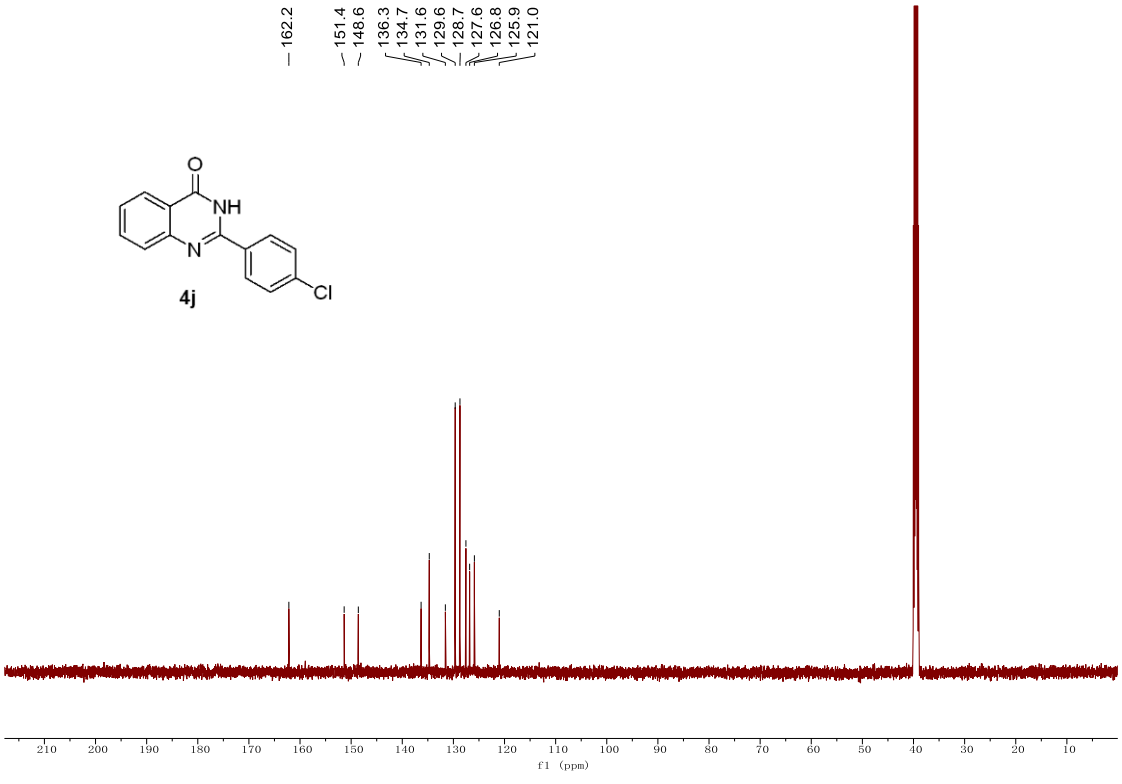
7.85
7.84
7.84
7.76
7.75
7.65
7.63
7.56
7.55
7.53
O
NH
N
Cl
4j
0.99
2.01
0.99
1.02
0.95
2.00
0.96
f1 (ppm)


162.2
151.4
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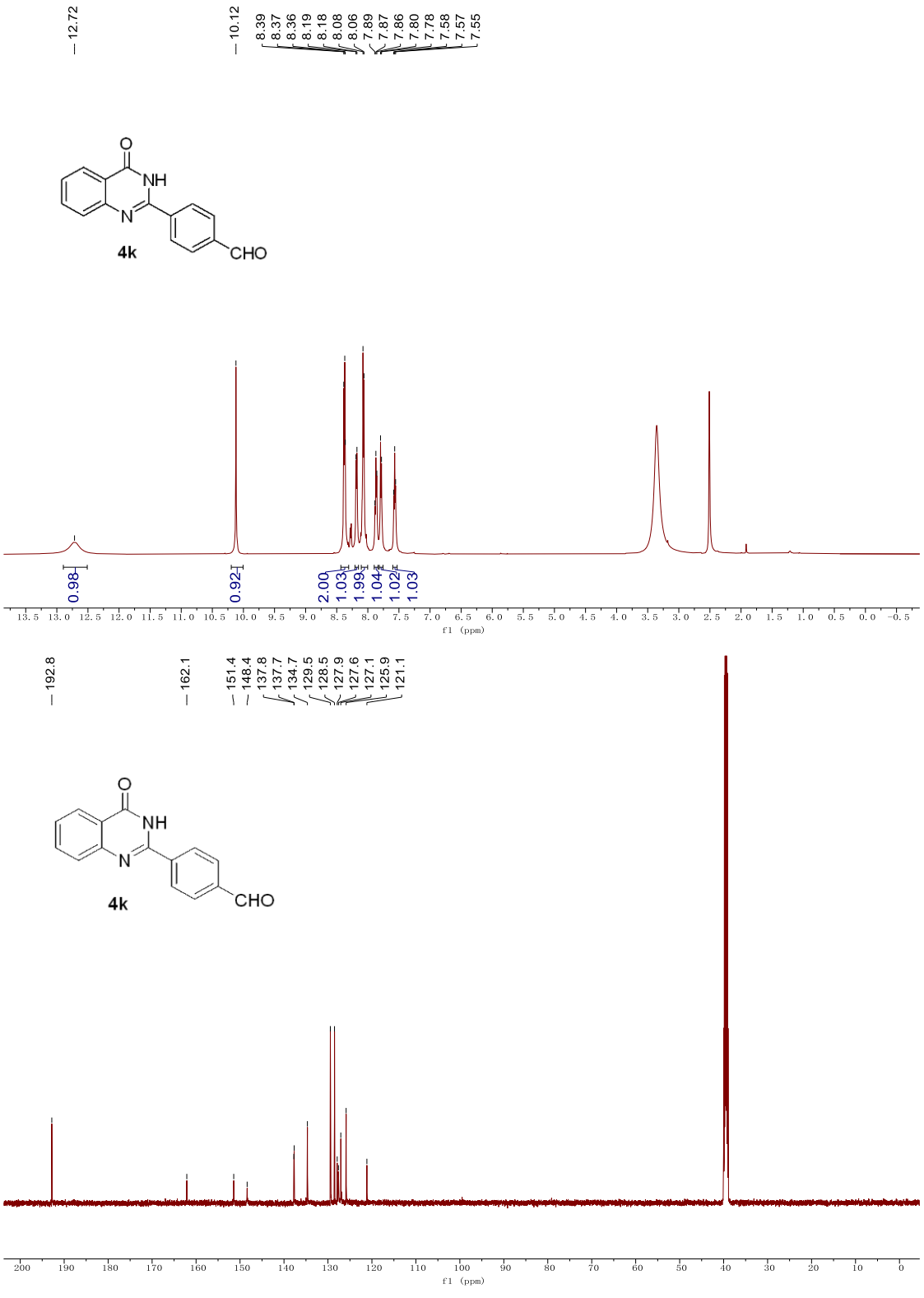
136.3
134.7
131.6
129.6
128.7
127.6
126.8
125.9
121.0
O
NH
N
Cl
4j
f1 (ppm)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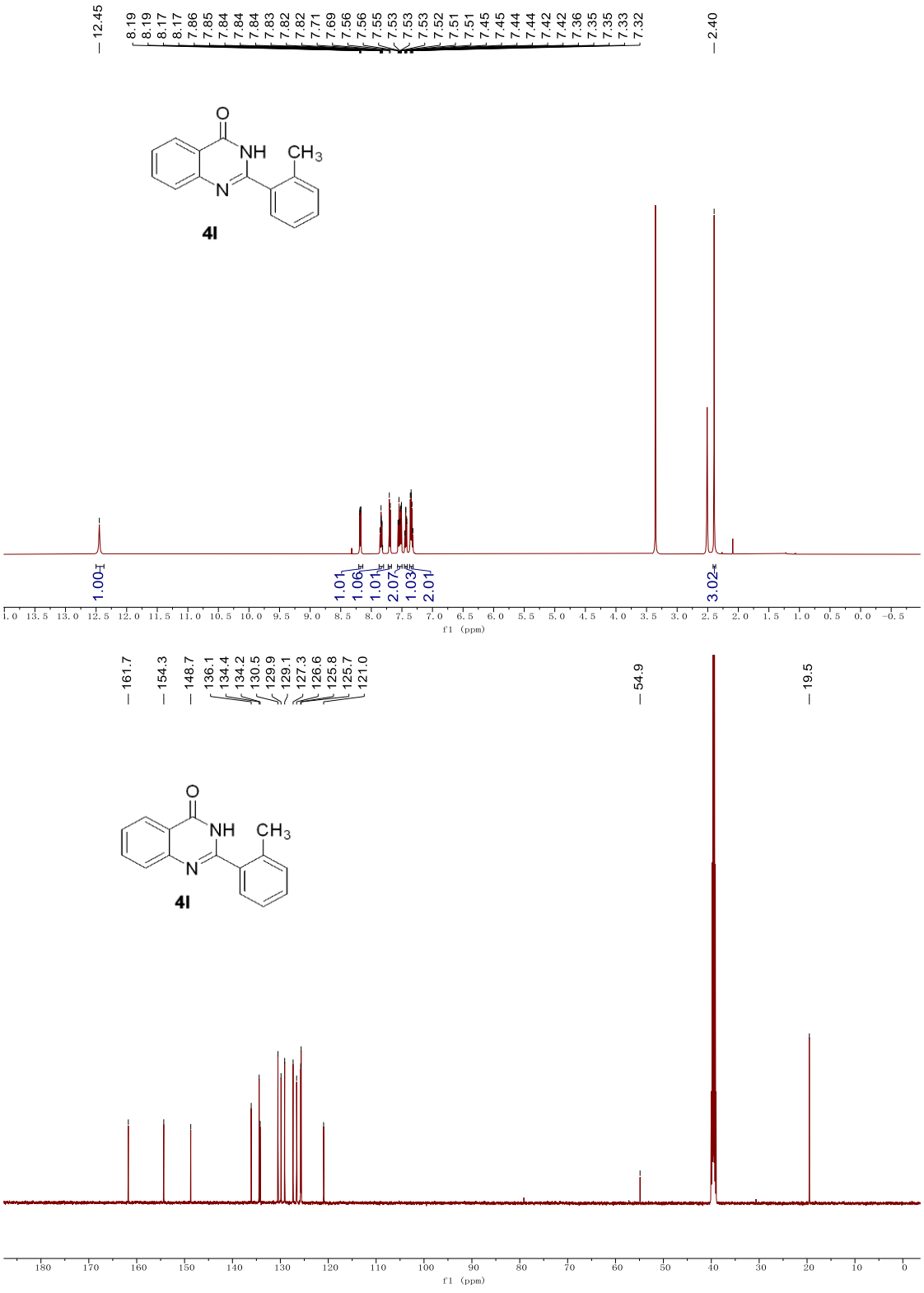
8.18
8.08
8.06
7.89
7.87
7.86
7.80
7.78
7.58
7.57
7.55
O
NH
N
CHO
4k
0.98
0.92
2.00
1.03
1.99
1.04
1.02
1.03
f1 (ppm)
192.8
162.1
151.4
148.4
137.8
137.7
134.7
129.5
128.5
127.9
127.6
127.1
125.9
121.1
O
NH
N
CHO
4k
f1 (ppm)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7.84
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7.82
7.71
7.69
7.56
7.55
7.53
7.53
7.52
7.51
7.51
7.45
7.44
7.44
7.42
7.42
7.36
7.35
7.35
7.33
7.32
2.40
O
NH
CH3
N
4l
1.00
1.01
1.06
1.01
2.07
1.03
2.01
3.02
f1 (ppm)
161.7
154.3
148.7
136.1
134.4
134.2
130.5
129.9
129.1
127.3
126.6
125.8
125.7
121.0
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O
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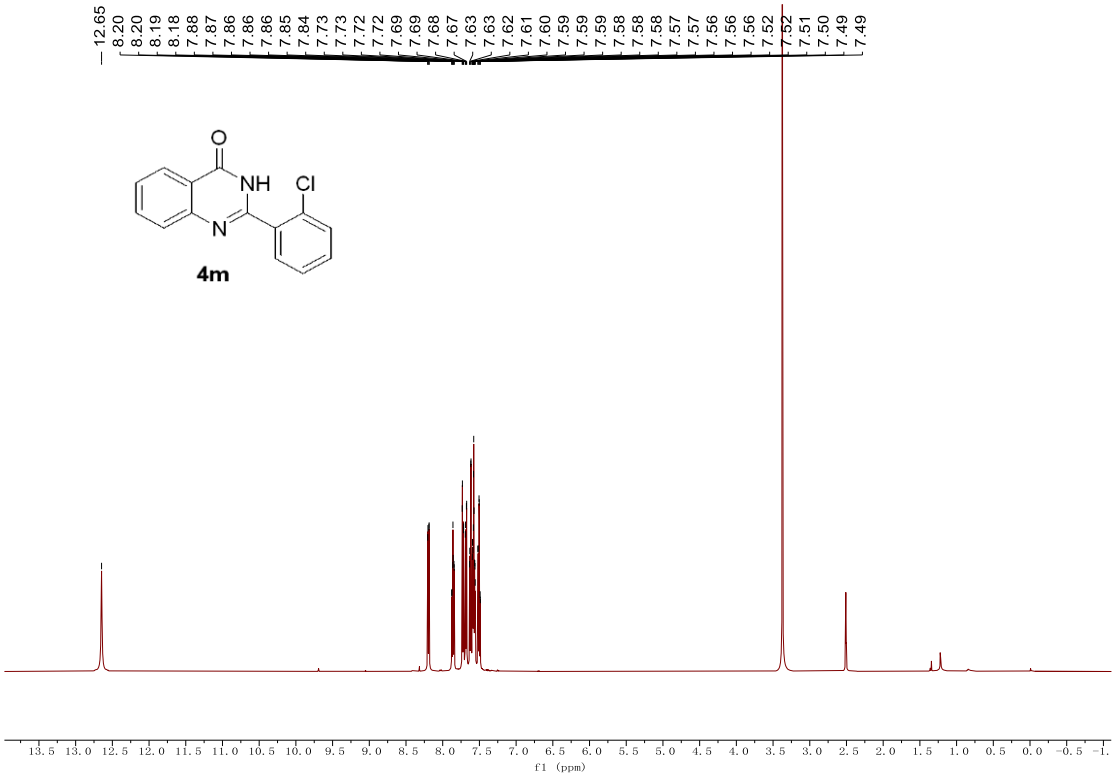
CH3
N
4l
f1 (ppm)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7.73
7.72
7.72
7.69
7.69
7.68
7.67
7.63
7.62
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7.60
7.59
7.59
7.59
7.58
7.58
7.58
7.57
7.57
7.56
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7.51
7.50
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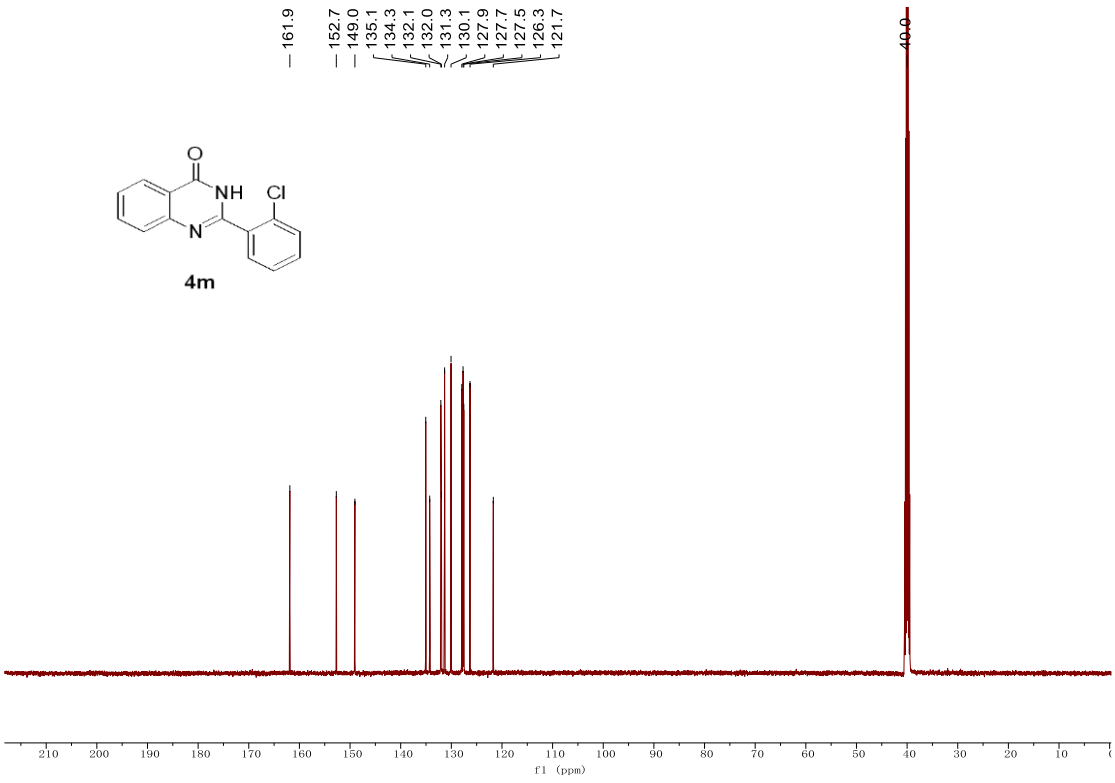
O
NH
Cl
N
4m
f1 (ppm)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132.0
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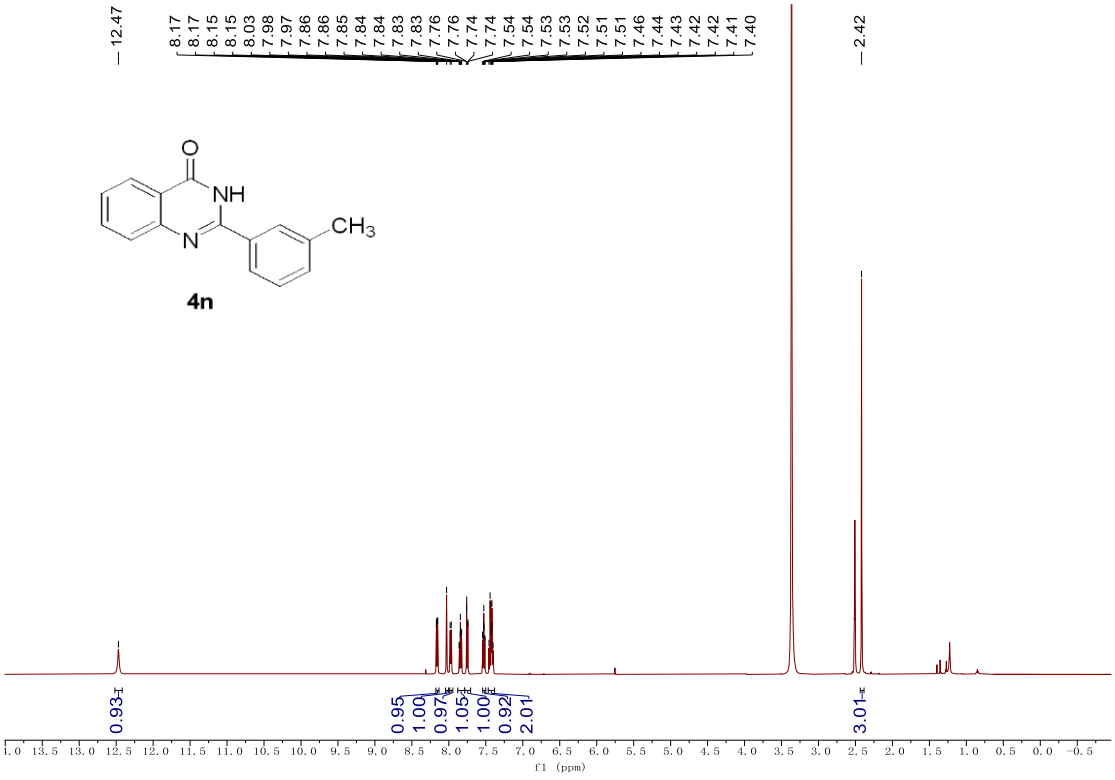
127.7
127.5
126.3
121.7
40.0
O
NH
Cl
N
4m
f1 (ppm)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7.84
7.83
7.83
7.76
7.76
7.74
7.74
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7.53
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7.52
7.51
7.51
7.46
7.44
7.43
7.42
7.42
7.41
7.40
2.42
O
NH
N
CH3
4n
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0.95
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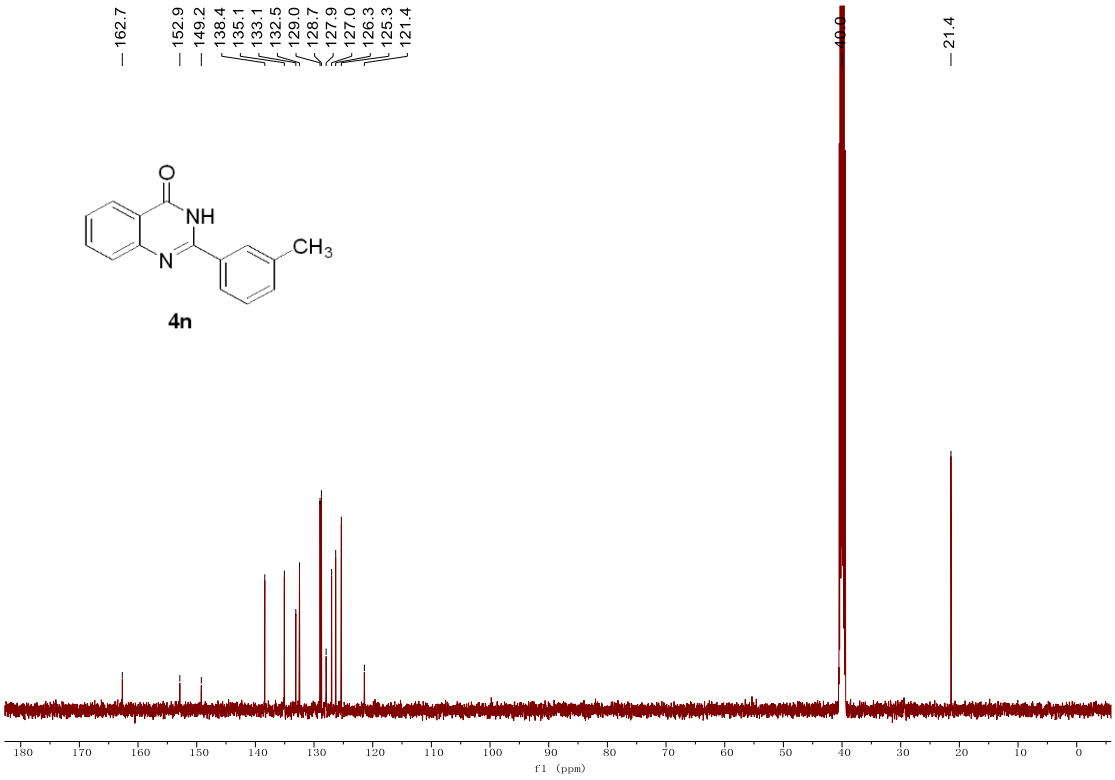
0.97
1.05
1.00
0.92
2.01
3.01
f1 (ppm)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133.1
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129.0
128.7
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126.3
125.3
121.4
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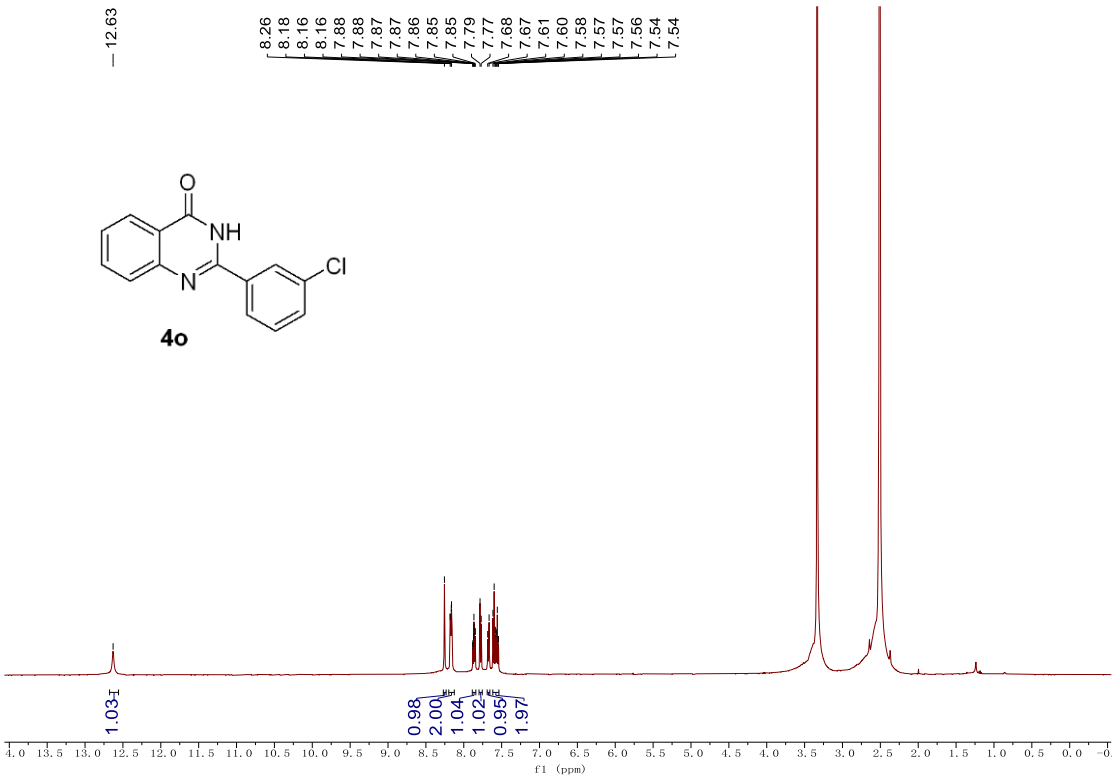
O
NH
N
CH3
4n
f1 (ppm)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7.61
7.60
7.58
7.57
7.57
7.56
7.54
7.54
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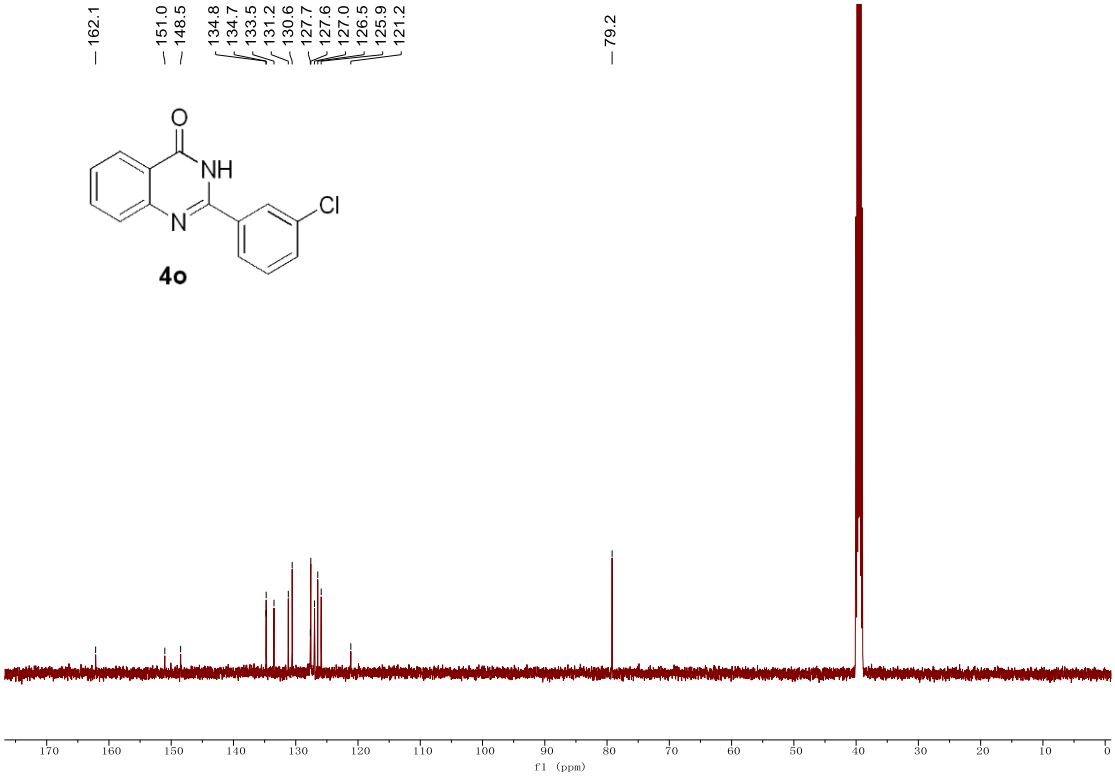
Cl
4o
1.03
0.98
2.00
1.04
1.02
0.95
1.97
f1 (ppm)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133.5
131.2
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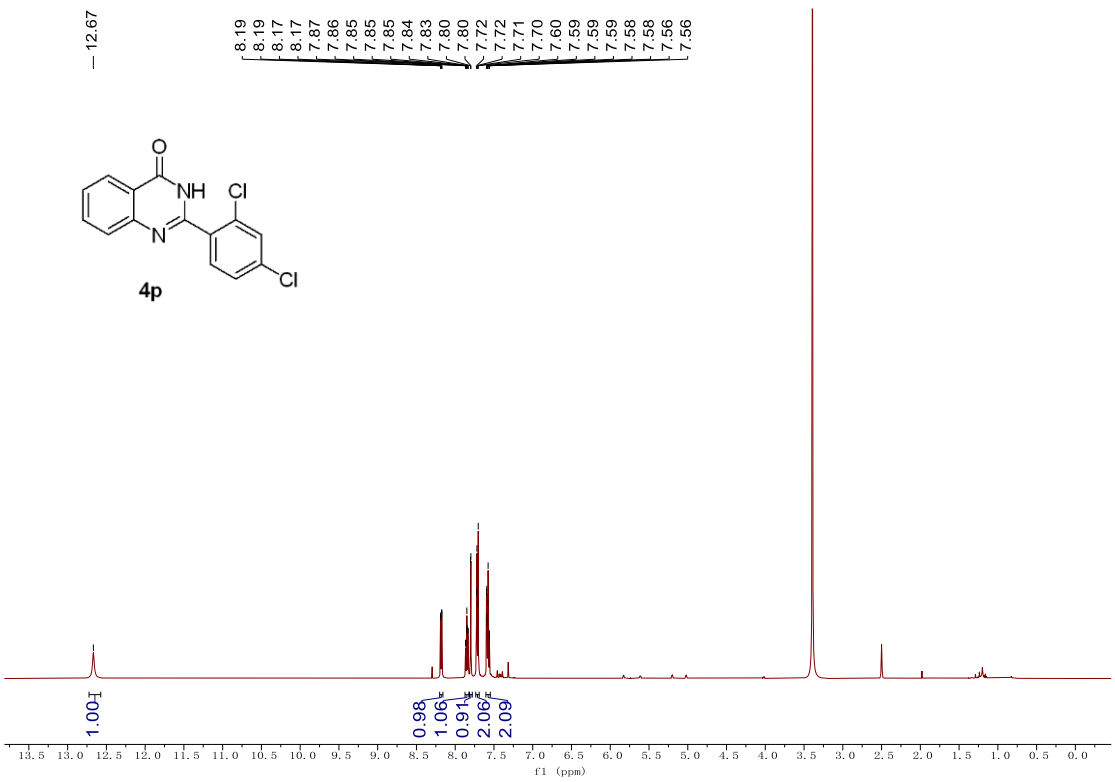
127.0
126.5
125.9
121.2
79.2
O
NH
N
Cl
4o
f1 (ppm)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7.59
7.59
7.59
7.58
7.58
7.56
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Cl
N
Cl
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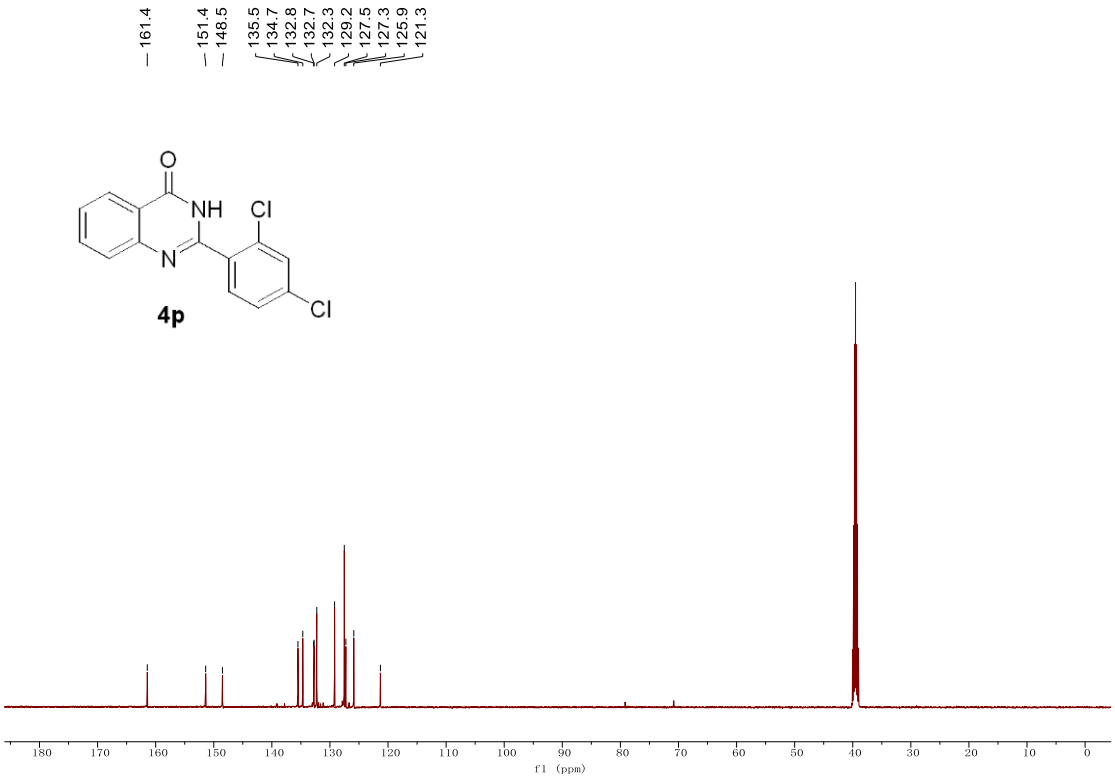
1.06
0.91
2.06
2.09
f1 (ppm)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134.7
132.8
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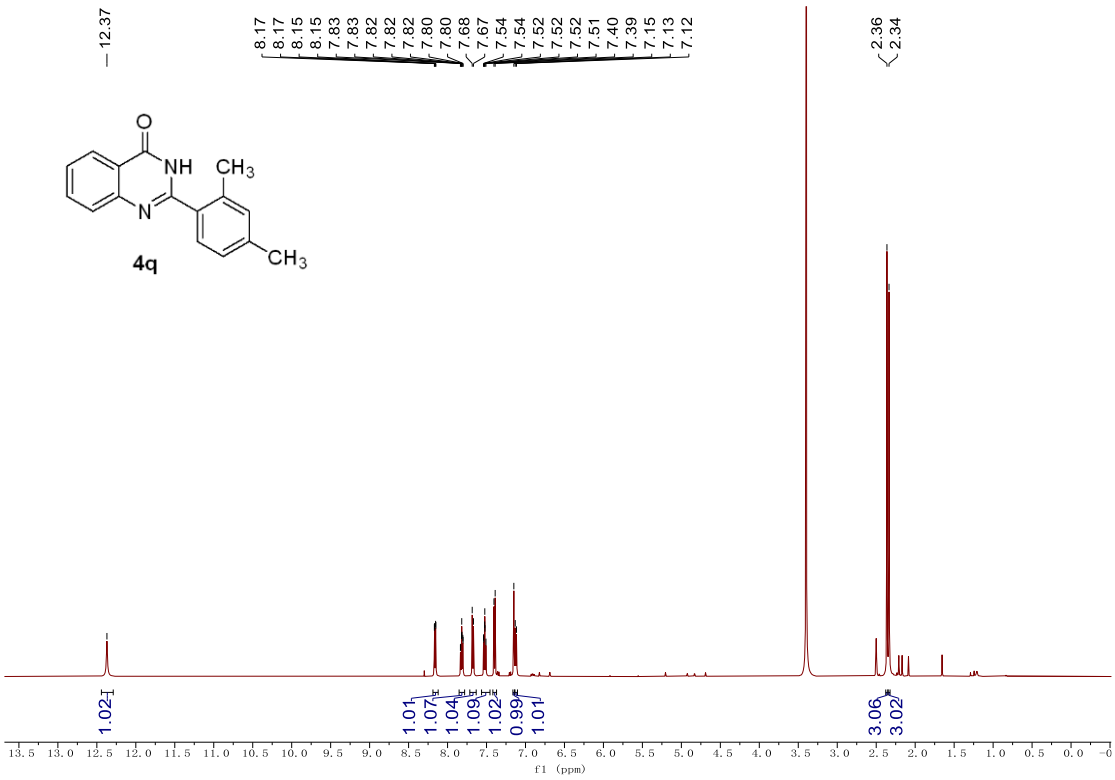
127.3
125.9
121.3
O
NH
Cl
N
Cl
4p
f1 (ppm)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7.82
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7.39
7.15
7.13
7.12
2.36
2.34
O
NH
CH3
N
CH3
4q
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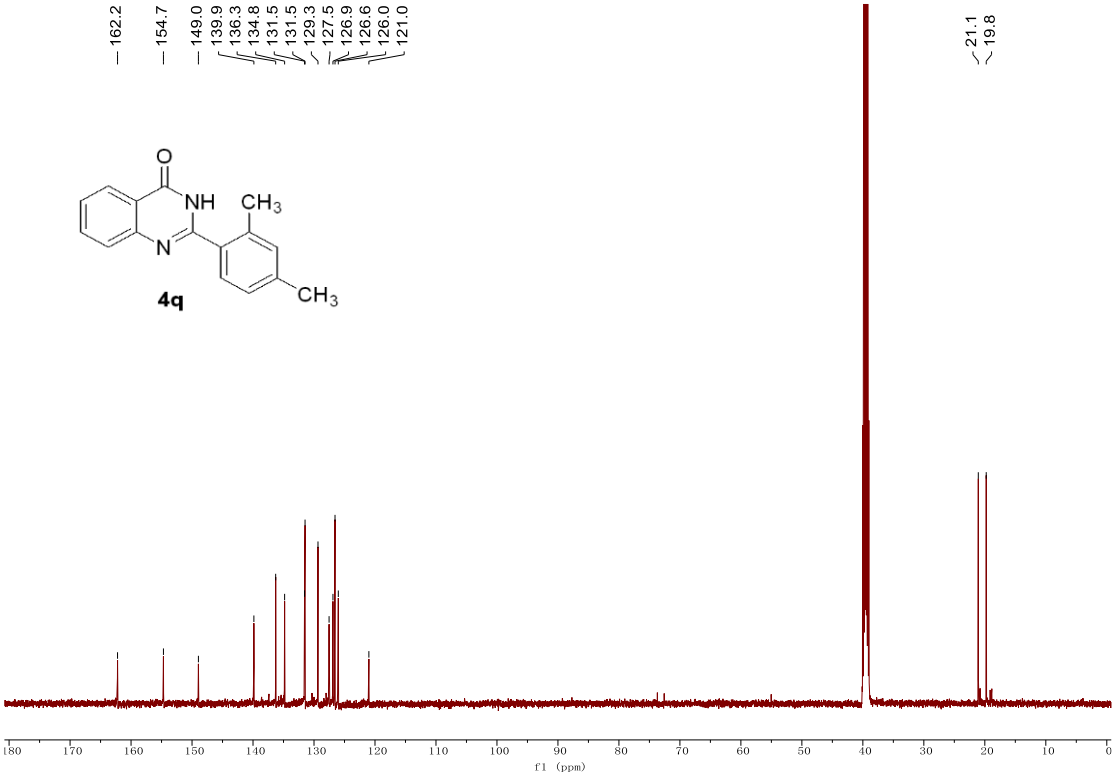
1.07
1.04
1.09
1.02
0.99
1.01
3.06
3.02
f1 (ppm)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129.3
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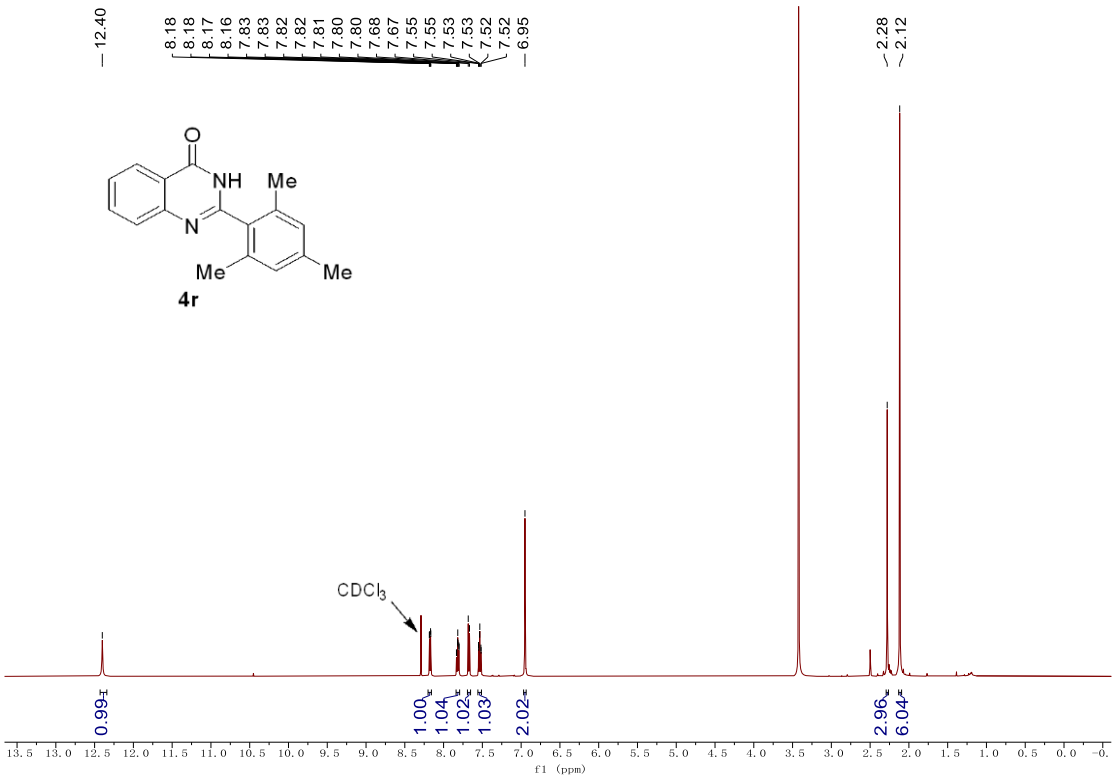
NH
CH3
N
CH3
4q
f1 (ppm)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7.53
7.53
7.52
7.52
6.95
2.28
2.12
O
NH
Me
N
Me
Me
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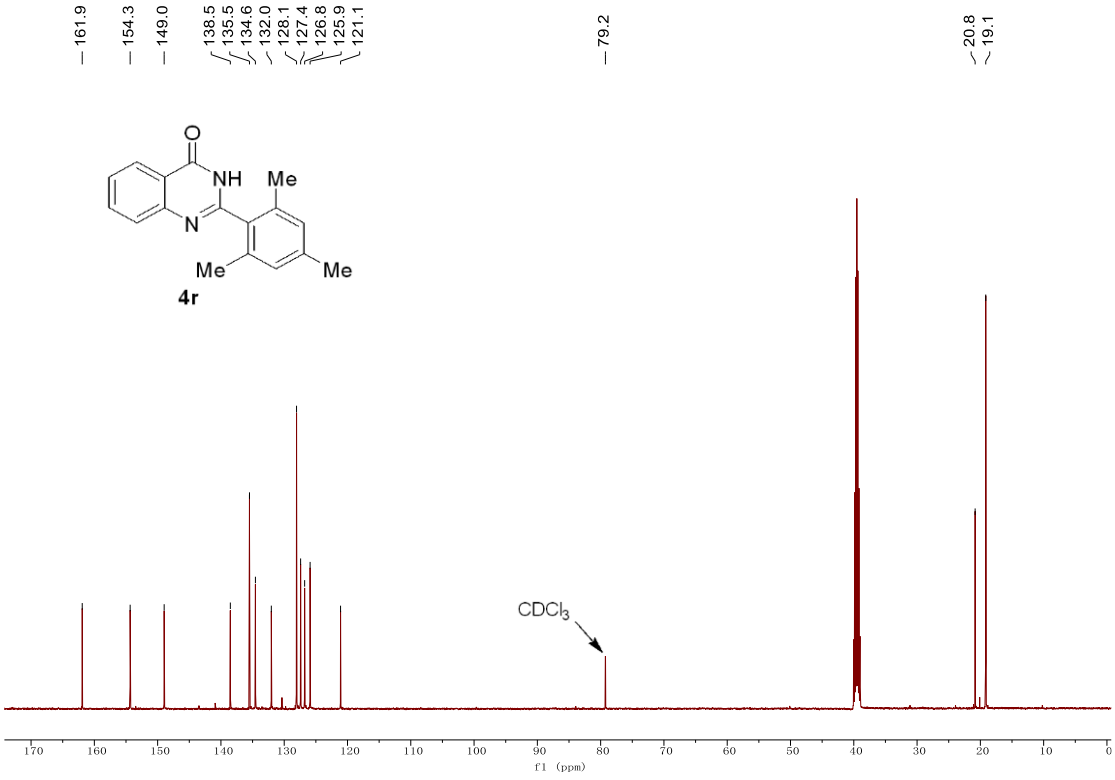
1.02
1.03
2.02
2.96
6.04
f1 (ppm)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134.6
132.0
128.1
127.4
126.8
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20.8
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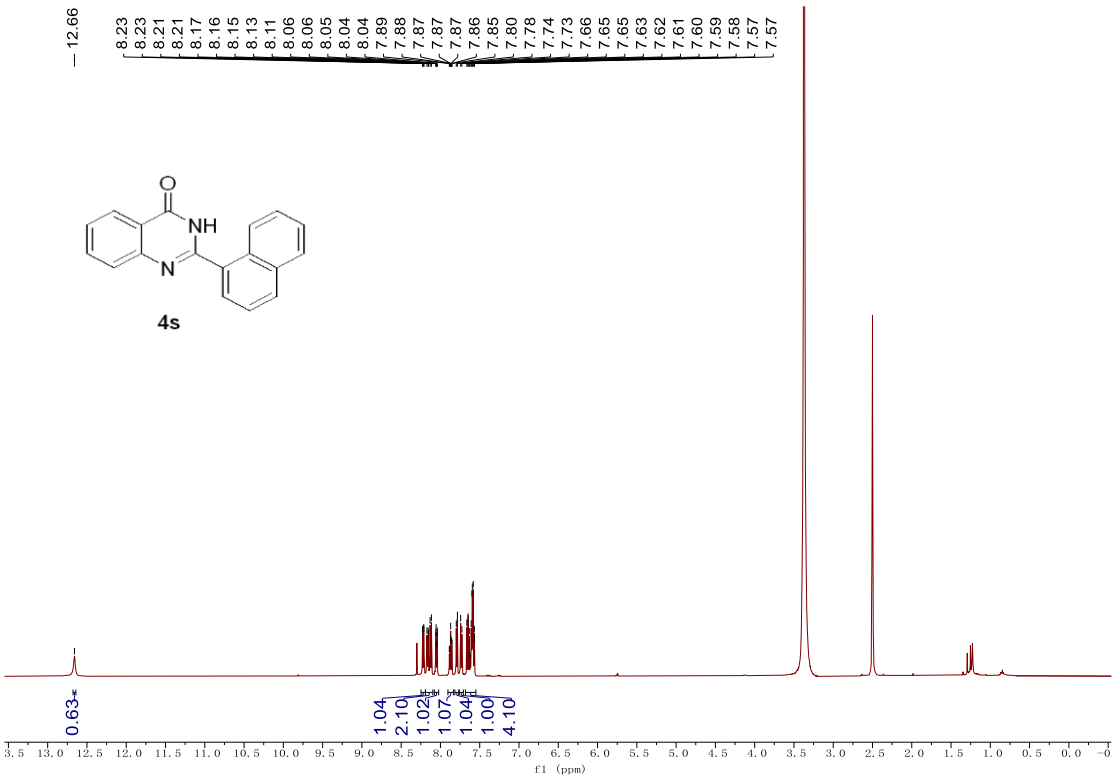
O
NH
Me
N
Me
Me
4r
CDCl3
f1 (ppm)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7.73
7.66
7.65
7.65
7.63
7.62
7.61
7.60
7.59
7.58
7.57
7.57
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NH
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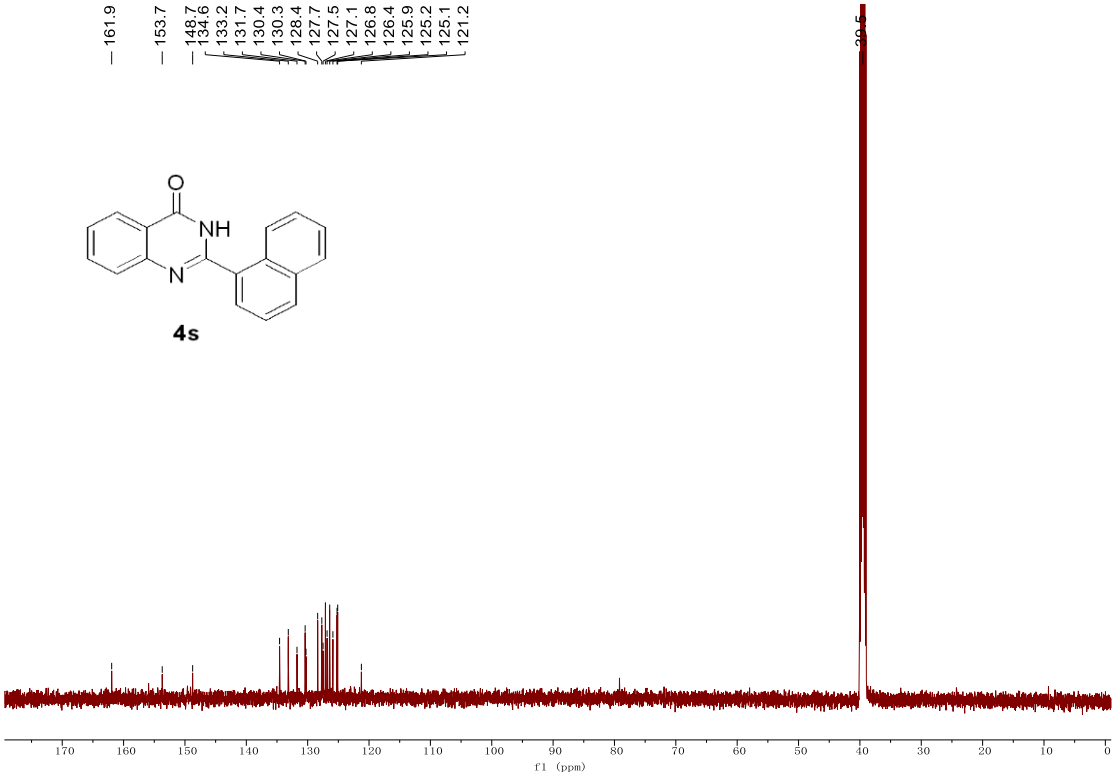
2.10
1.02
1.07
1.04
1.00
4.10
f1 (ppm)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133.2
131.7
130.4
130.3
128.4
127.7
127.5
127.1
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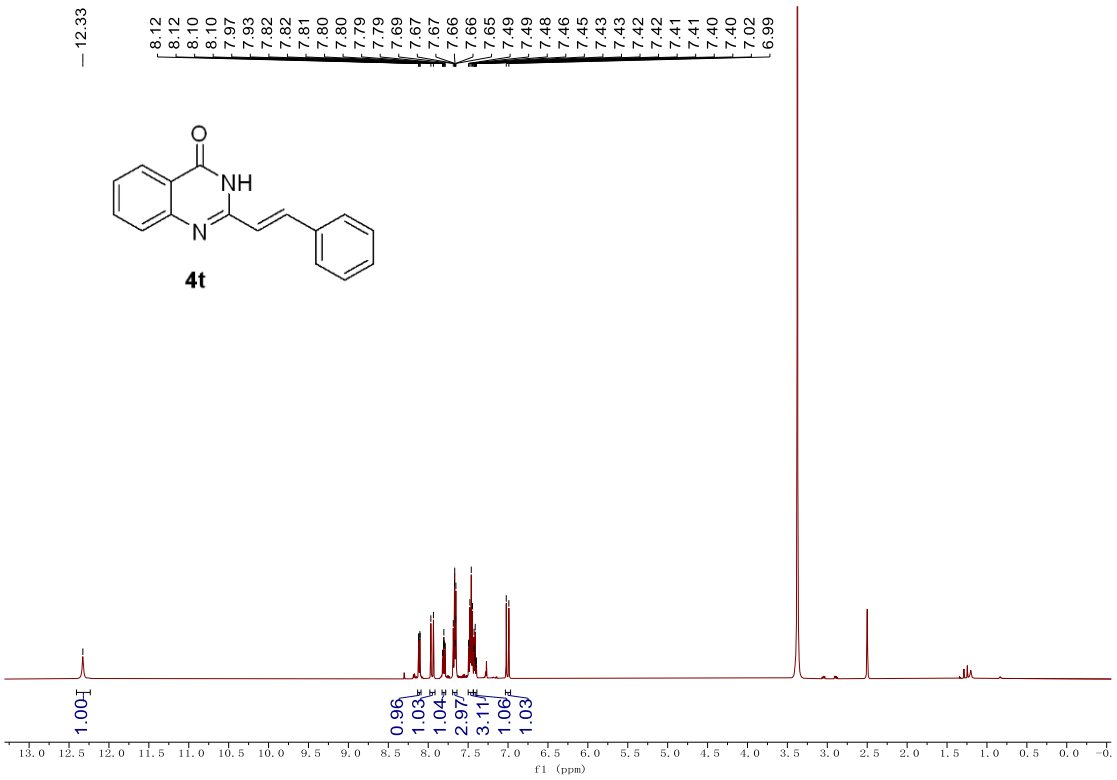
126.4
125.9
125.2
125.1
121.2
39.5
O
NH
N
4s
f1 (ppm)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7.82
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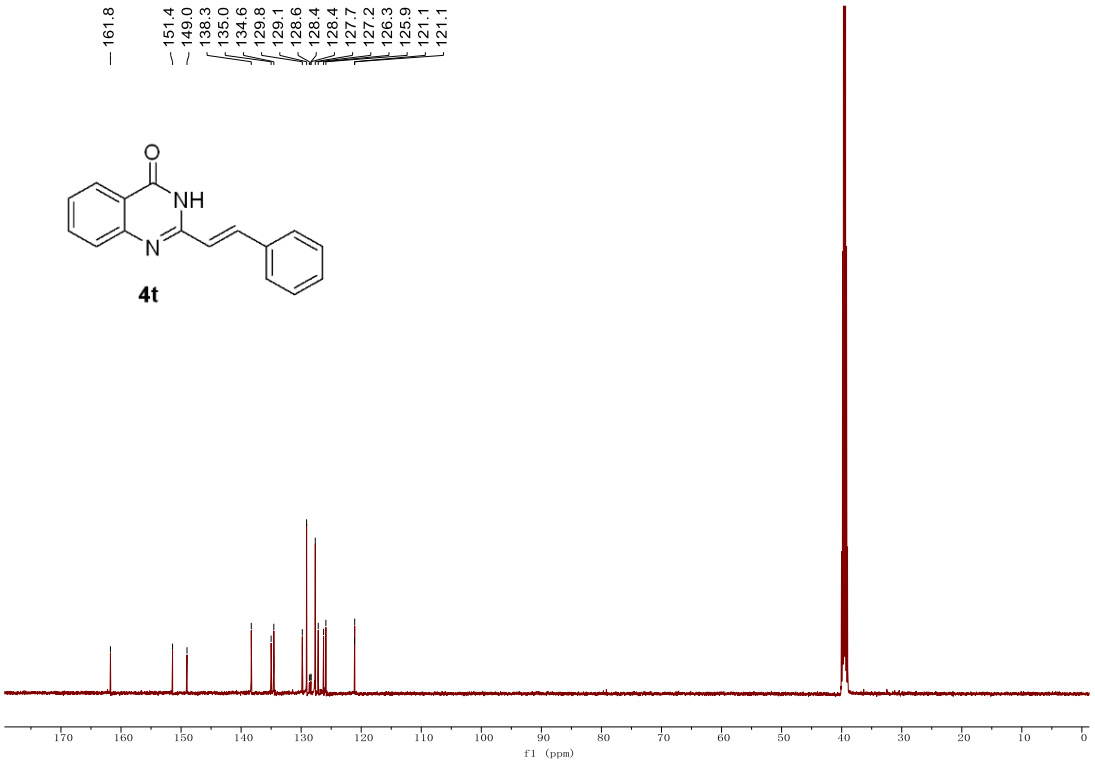
7.80
7.80
7.79
7.79
7.69
7.67
7.67
7.66
7.66
7.65
7.49
7.49
7.48
7.46
7.45
7.43
7.43
7.42
7.42
7.41
7.41
7.40
7.40
7.02
6.99
O
NH
N
4t
1.00
0.96
1.03
1.04
2.97
3.11
1.06
1.03
f1 (ppm)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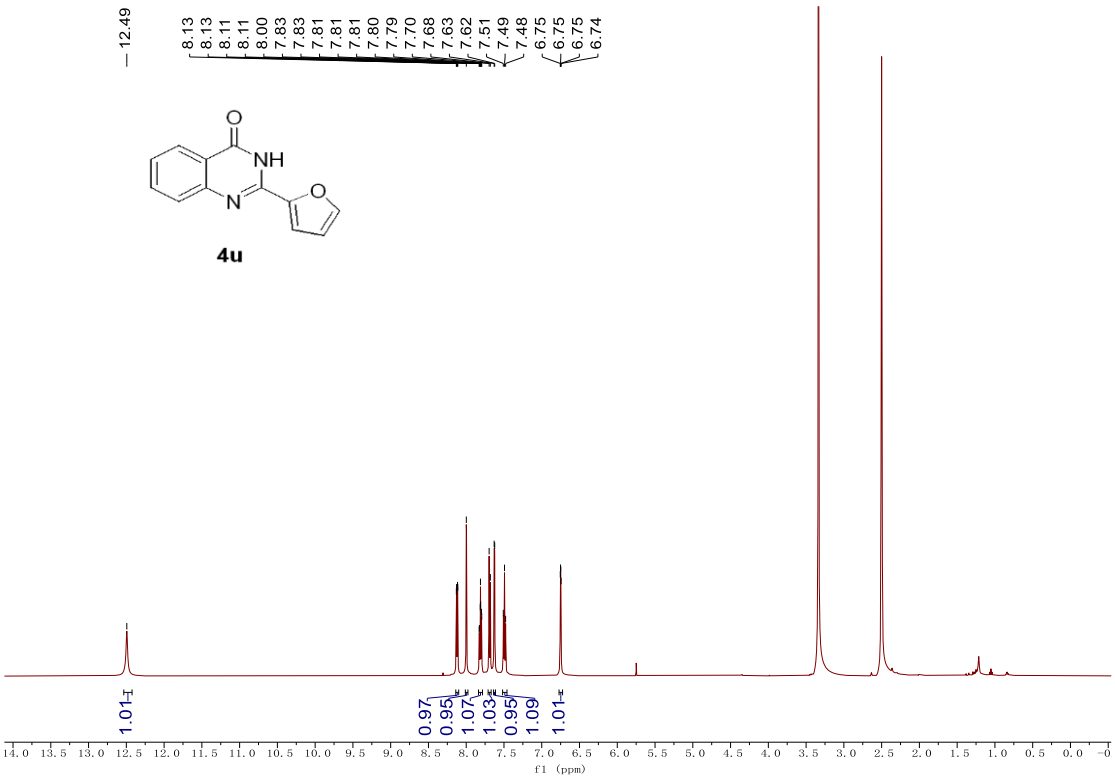
134.6
129.8
129.1
128.6
128.4
128.4
127.7
127.2
126.3
125.9
121.1
121.1
O
NH
N
4t
f1 (ppm)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8.11
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7.83
7.81
7.81
7.81
7.80
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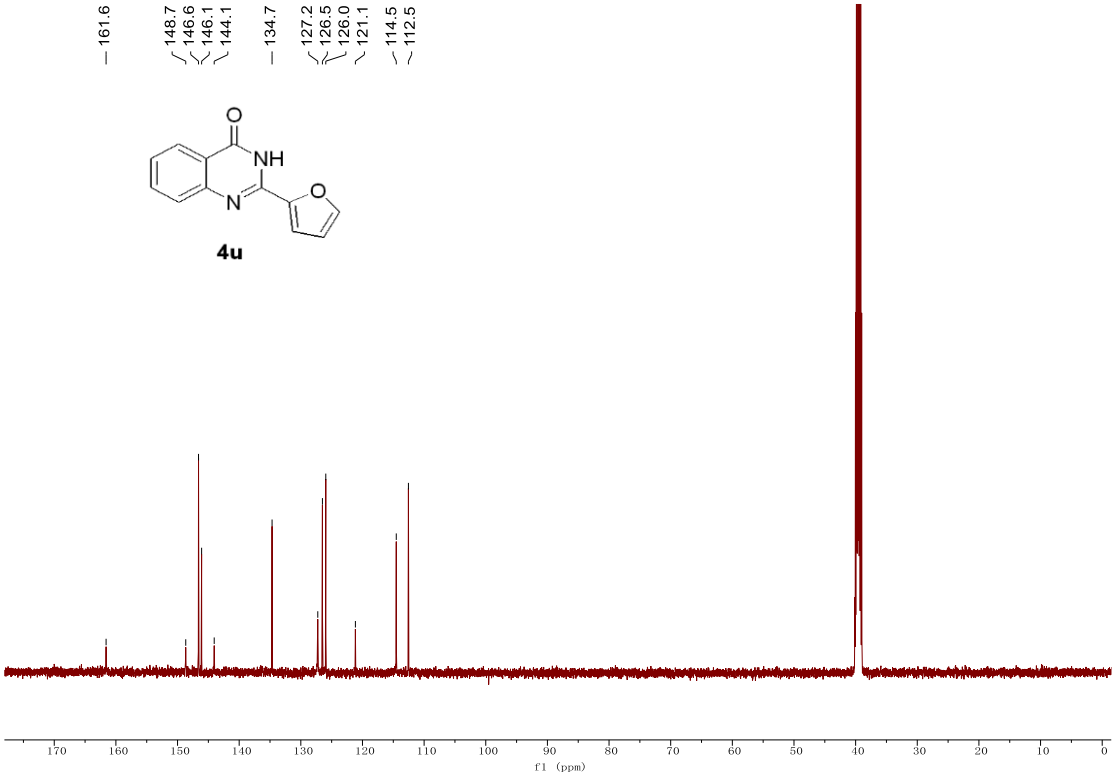
7.70
7.68
7.63
7.62
7.51
7.49
7.48
6.75
6.75
6.74
O
NH
N
O
4u
1.01
0.97
0.95
1.07
1.03
0.95
1.09
1.01
f1 (ppm)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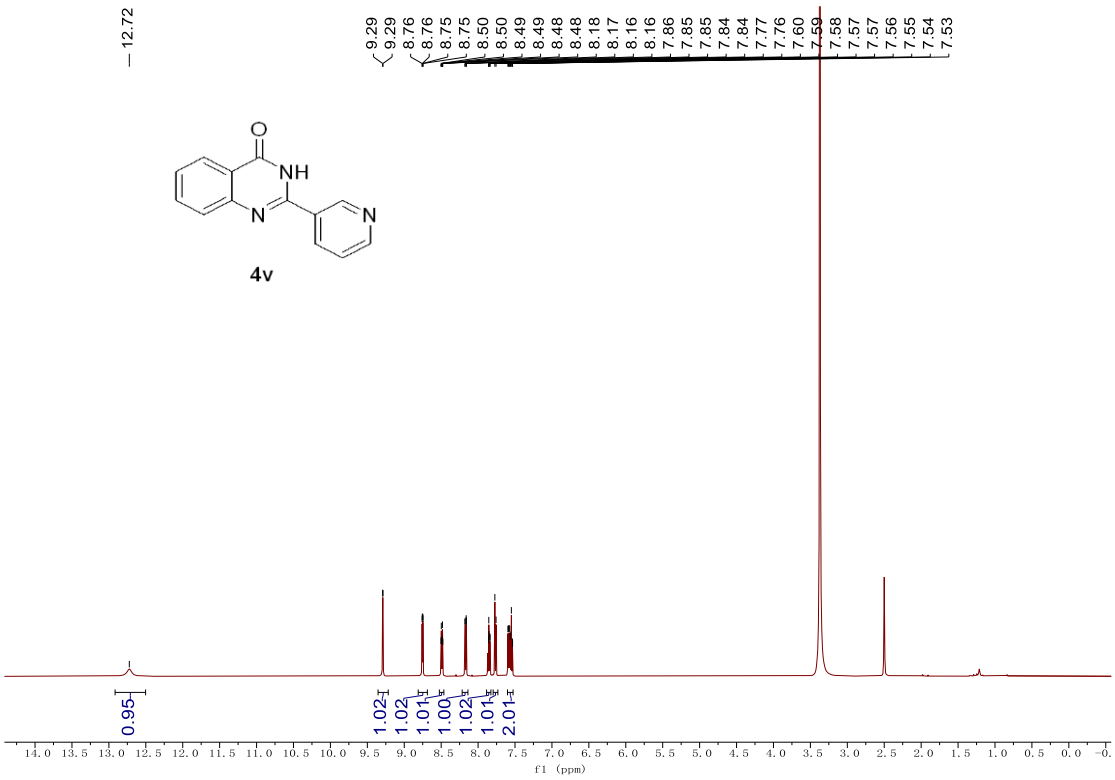
148.7
146.6
146.1
144.1
134.7
127.2
126.5
126.0
121.1
114.5
112.5
O
NH
N
O
4u
f1 (ppm)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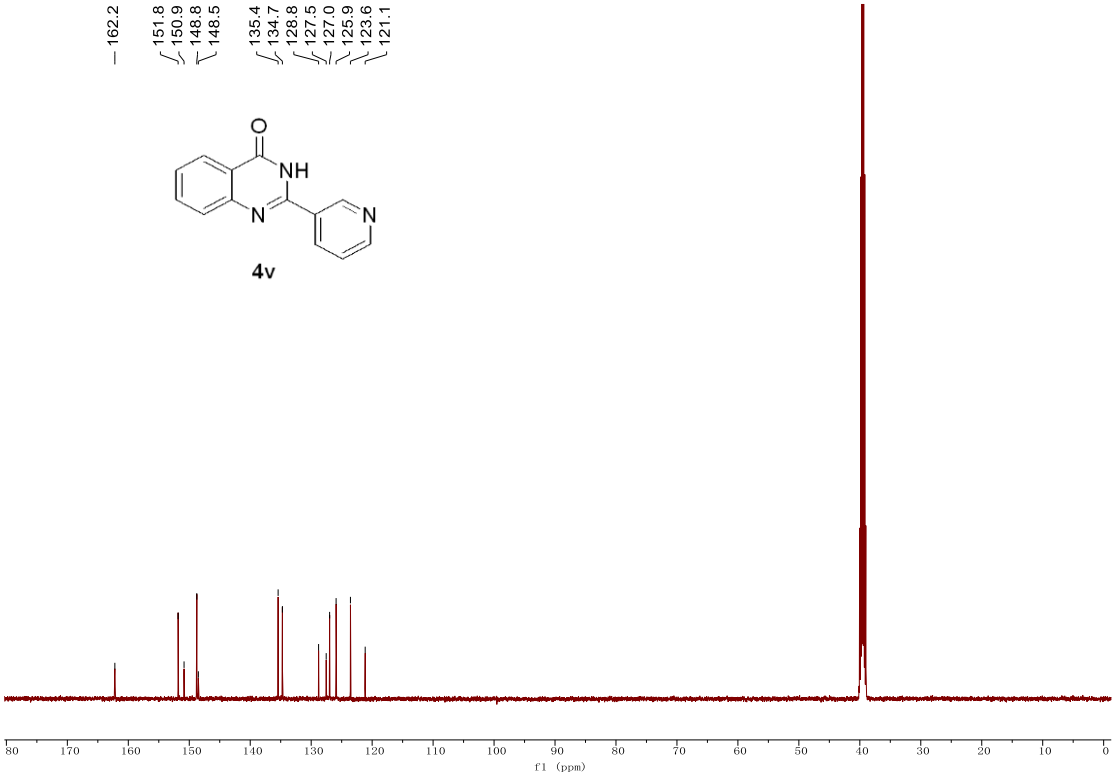
9.29
9.29
8.76
8.76
8.75
8.75
8.50
8.50
8.49
8.49
8.48
8.48
8.18
8.17
8.16
8.16
7.86
7.85
7.85
7.84
7.84
7.77
7.76
7.60
7.59
7.58
7.57
7.57
7.56
7.55
7.54
7.53
NH
N
N
4v
0.95
1.02
1.02
1.01
1.00
1.02
1.01
2.01
f1 (ppm)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151.8
150.9
148.8
148.5
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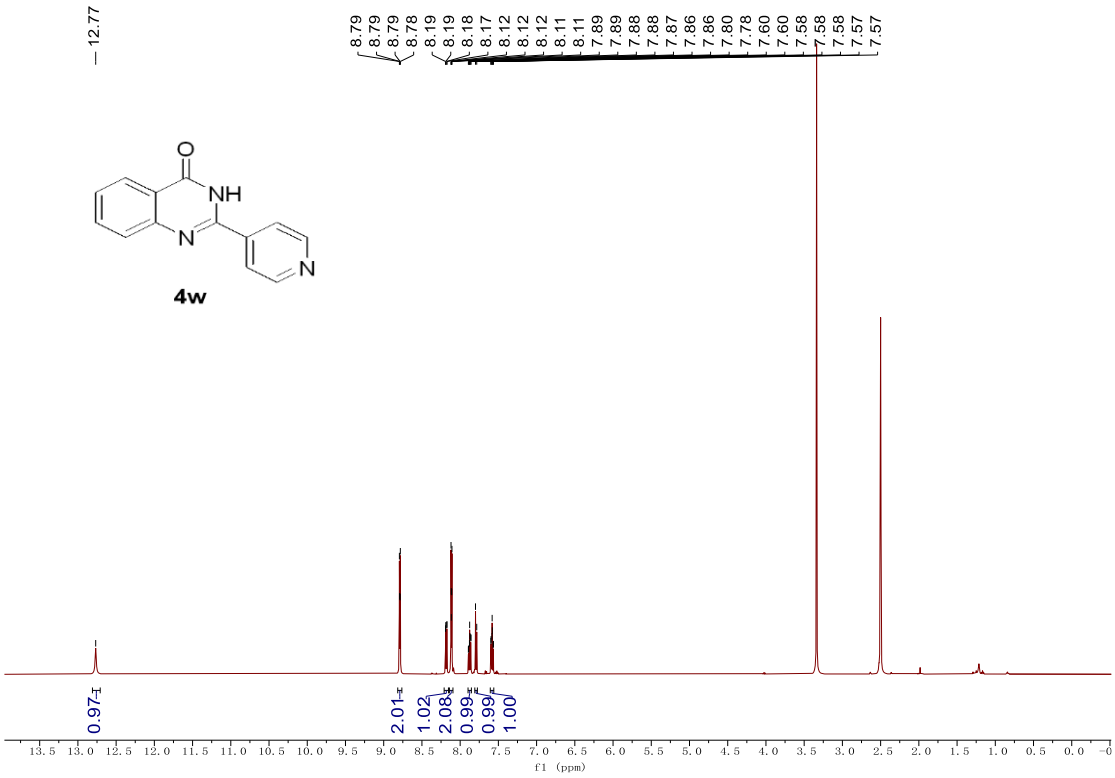
134.7
128.8
127.5
127.0
125.9
123.6
121.1
NH
N
N
4v
f1 (ppm)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8.79
8.79
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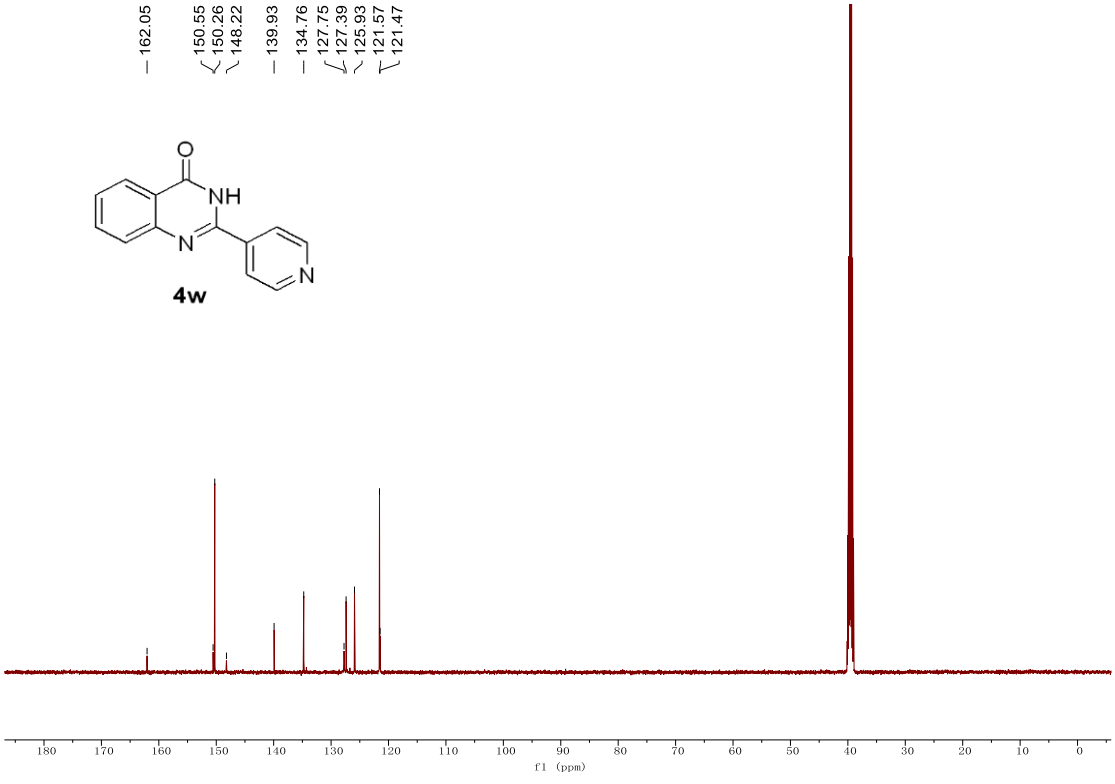
8.19
8.19
8.18
8.17
8.12
8.12
8.12
8.11
8.11
7.89
7.89
7.88
7.88
7.87
7.86
7.86
7.80
7.78
7.60
7.58
7.58
7.58
7.57
7.57
O
NH
N
N
4w
0.97
2.01
1.02
2.08
0.99
0.99
1.00
f1 (ppm)


162.05
150.55
150.26
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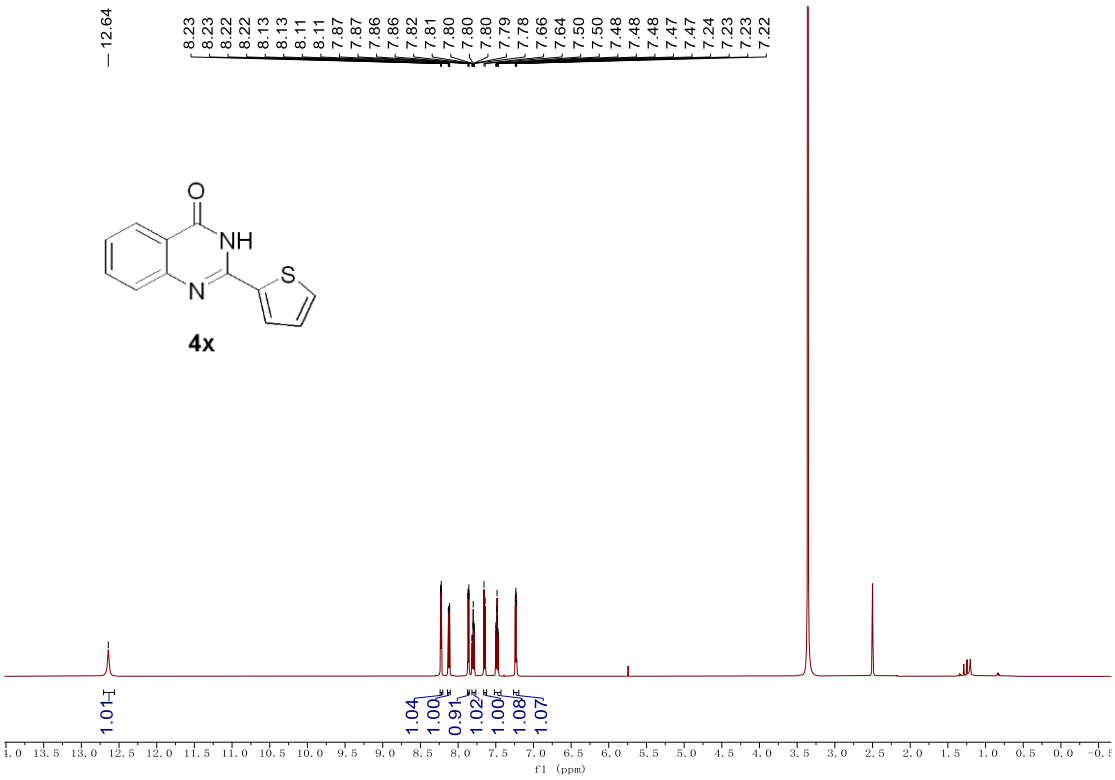
139.93
134.76
127.75
127.39
125.93
121.57
121.47
O
NH
N
N
4w
f1 (ppm)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8.22
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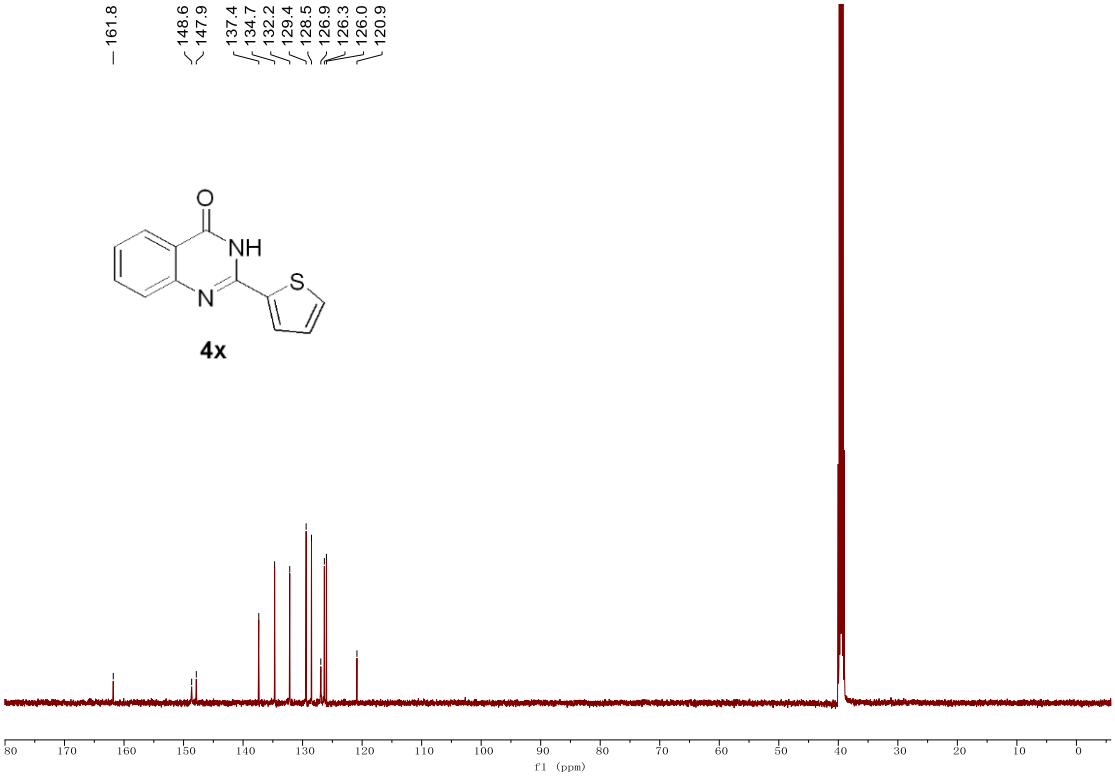
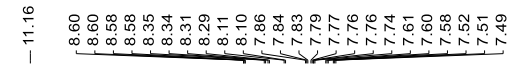
8.13
8.11
8.11
7.87
7.87
7.86
7.86
7.82
7.81
7.80
7.80
7.80
7.79
7.78
7.66
7.64
7.50
7.50
7.48
7.48
7.48
7.47
7.47
7.24
7.23
7.23
7.22
O
NH
N
S
4x
1.01
1.04
1.00
0.91
1.02
1.00
1.08
1.07
f1 (ppm)


161.8
148.6
147.9
137.4
134.7
132.2
129.4
128.5
126.9
126.3
126.0
120.9
O
NH
N
S
4x
f1 (ppm)


11.16
8.60
8.60
8.58
8.58
8.35
8.34
8.31
8.29
8.11
8.10
7.86
7.84
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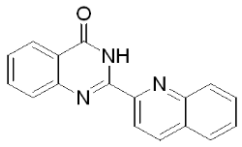
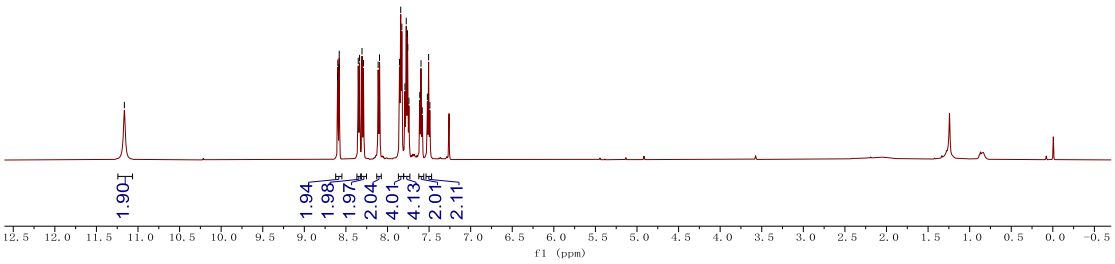
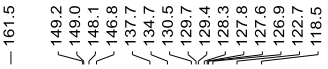
7.61
7.60
7.58
7.52
7.51
7.49


O
NH
N
N

4y


1.90
1.94
1.98
1.97
2.04
4.01
4.13
2.01
2.11
12.5 12.0 11.5 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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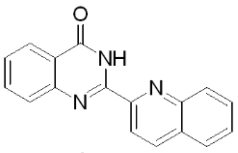
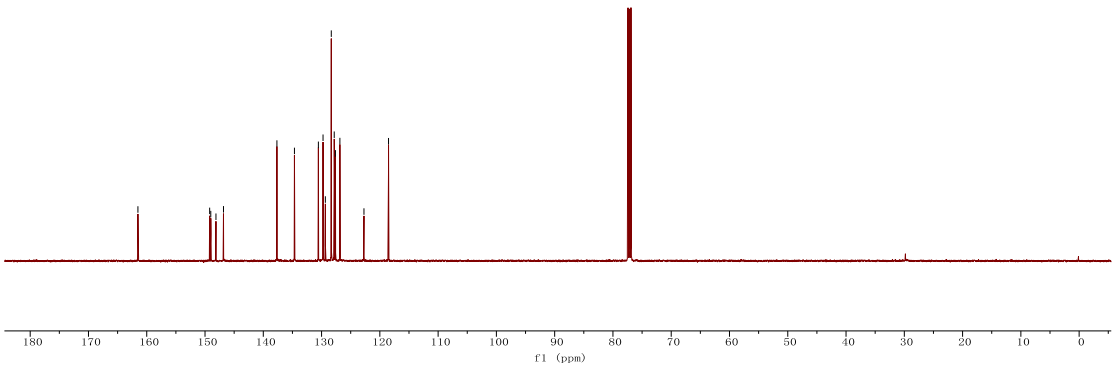
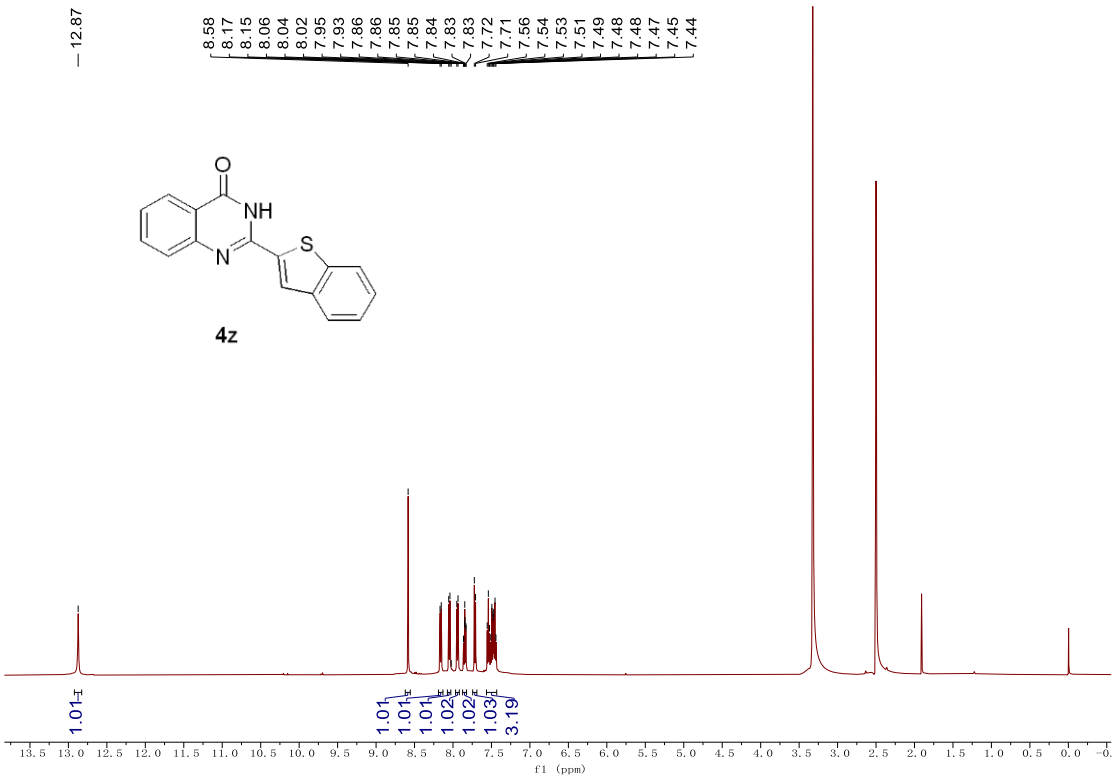
149.2
149.0
148.1
146.8
137.7
134.7
130.5
129.7
129.4
128.3
127.8
127.6
126.9
122.7
118.5


O
NH
N
N

4y


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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8.04
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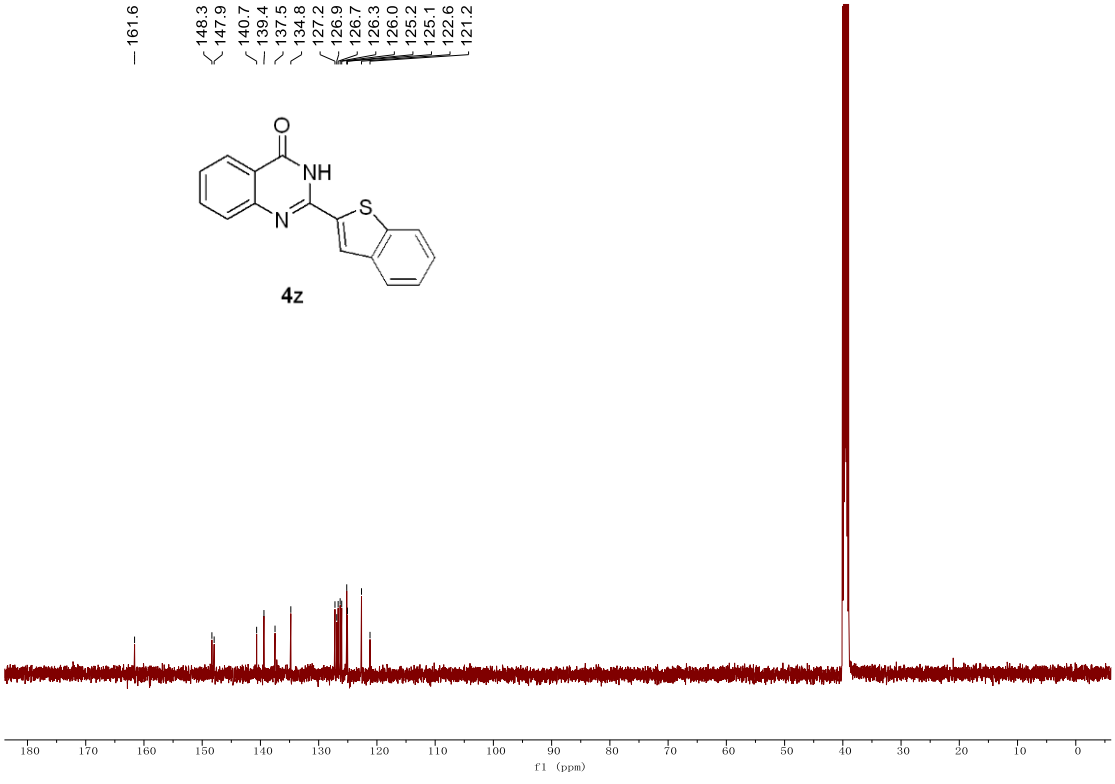
7.95
7.93
7.86
7.86
7.85
7.85
7.84
7.83
7.83
7.72
7.71
7.56
7.54
7.53
7.51
7.49
7.48
7.48
7.47
7.45
7.44
O
NH
N
S
4z
1.01
1.01
1.01
1.01
1.02
1.02
1.03
3.19
f1 (ppm)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139.4
137.5
134.8
127.2
126.9
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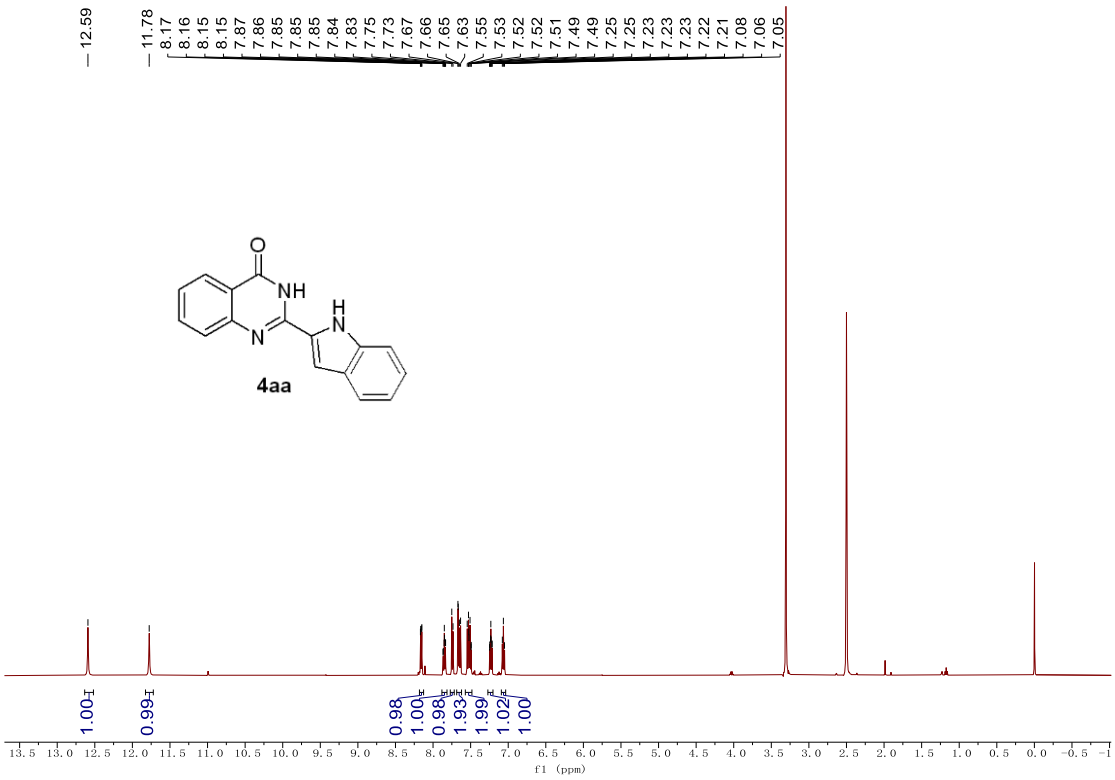
126.3
126.0
125.2
125.1
122.6
121.2
O
NH
N
S
4z
f1 (ppm)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7.85
7.85
7.85
7.84
7.83
7.75
7.73
7.67
7.66
7.65
7.63
7.55
7.53
7.52
7.52
7.51
7.49
7.49
7.25
7.25
7.23
7.23
7.22
7.21
7.08
7.06
7.05
O
NH
H
N
N
4aa
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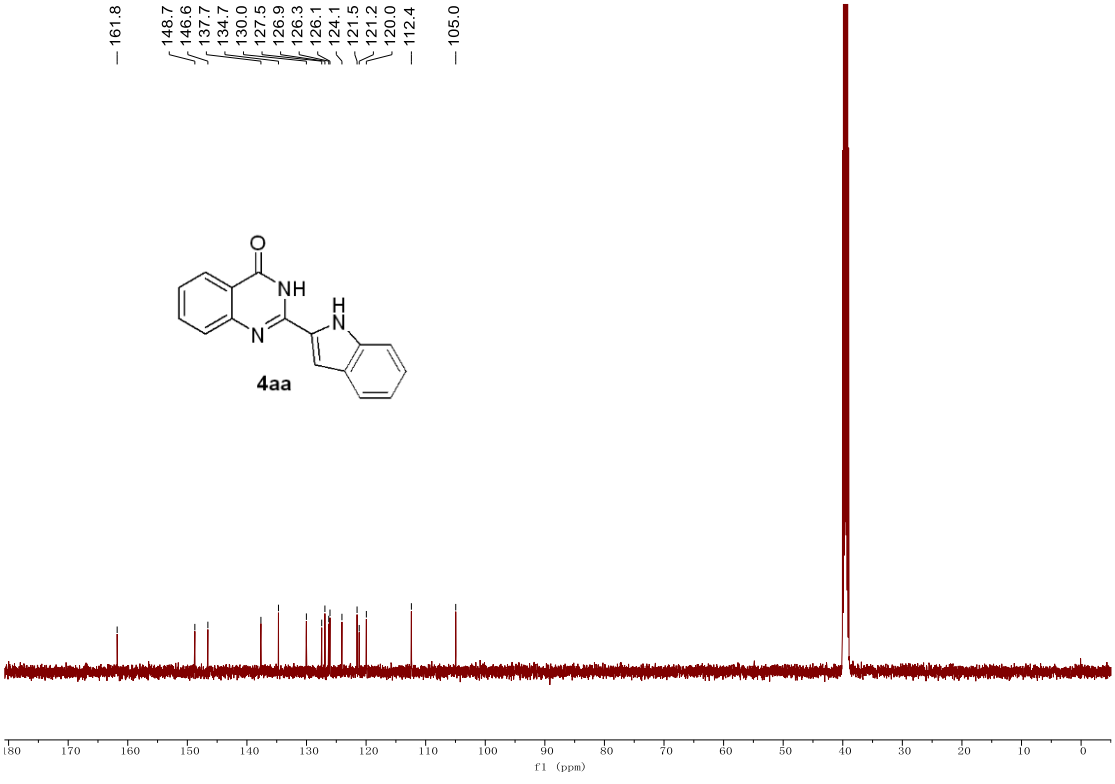
0.99
0.98
1.00
0.98
1.93
1.99
1.02
1.00
f1 (ppm)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130.0
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126.9
126.3
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124.1
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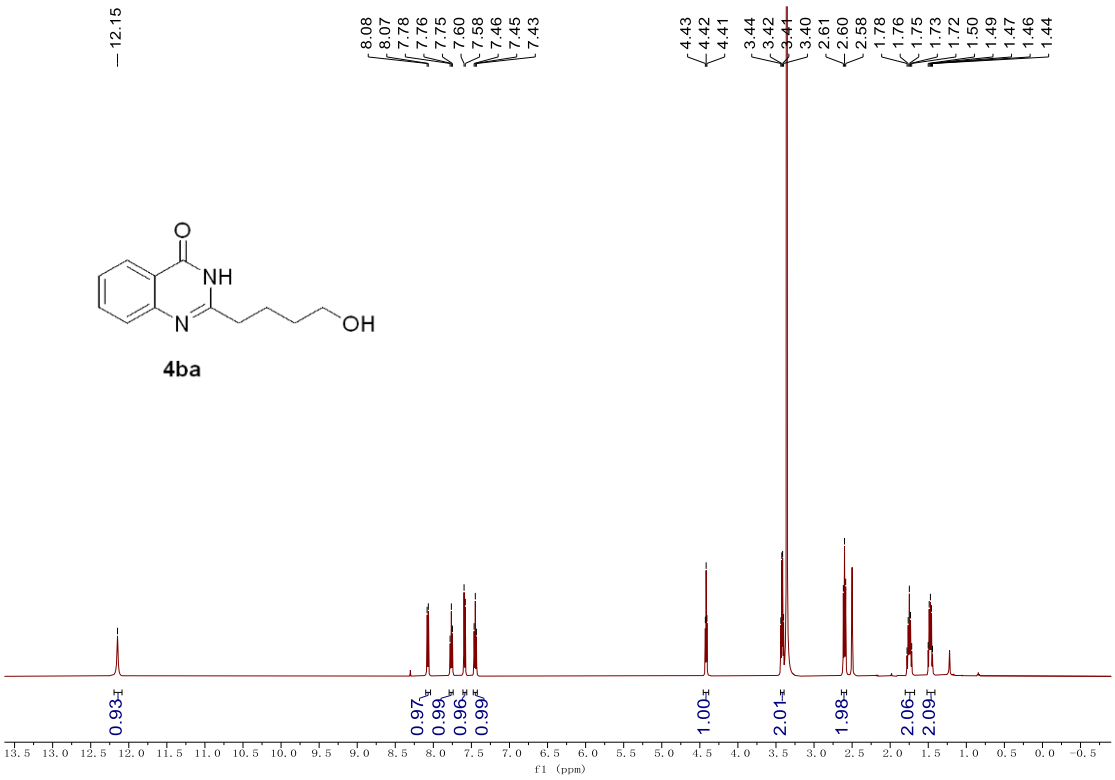
121.2
120.0
112.4
105.0
O
NH
H
N
N
4aa
f1 (ppm)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7.58
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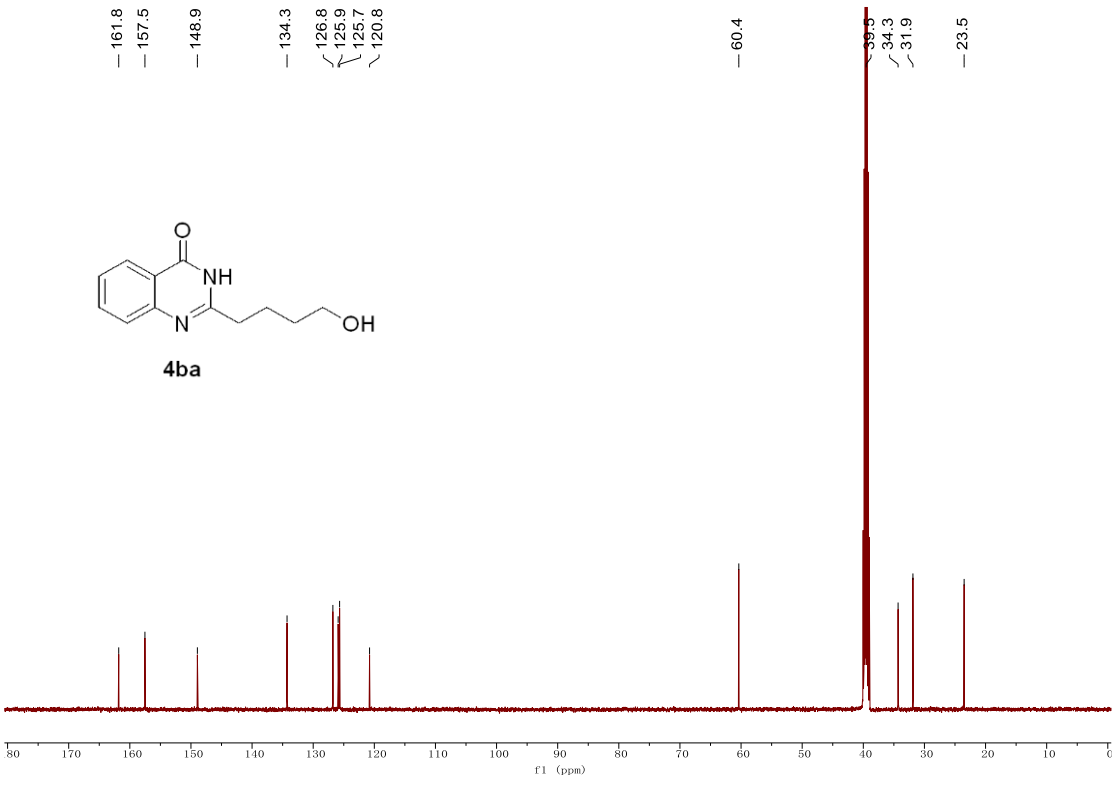
7.45
7.43
4.43
4.42
4.41
3.44
3.42
3.41
3.40
2.61
2.60
2.58
1.78
1.76
1.75
1.73
1.72
1.50
1.49
1.47
1.46
1.44
O
NH
N
OH
4ba
0.93
0.97
0.99
0.96
0.99
1.00
2.01
1.98
2.06
2.09
f1 (ppm)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134.3
126.8
125.9
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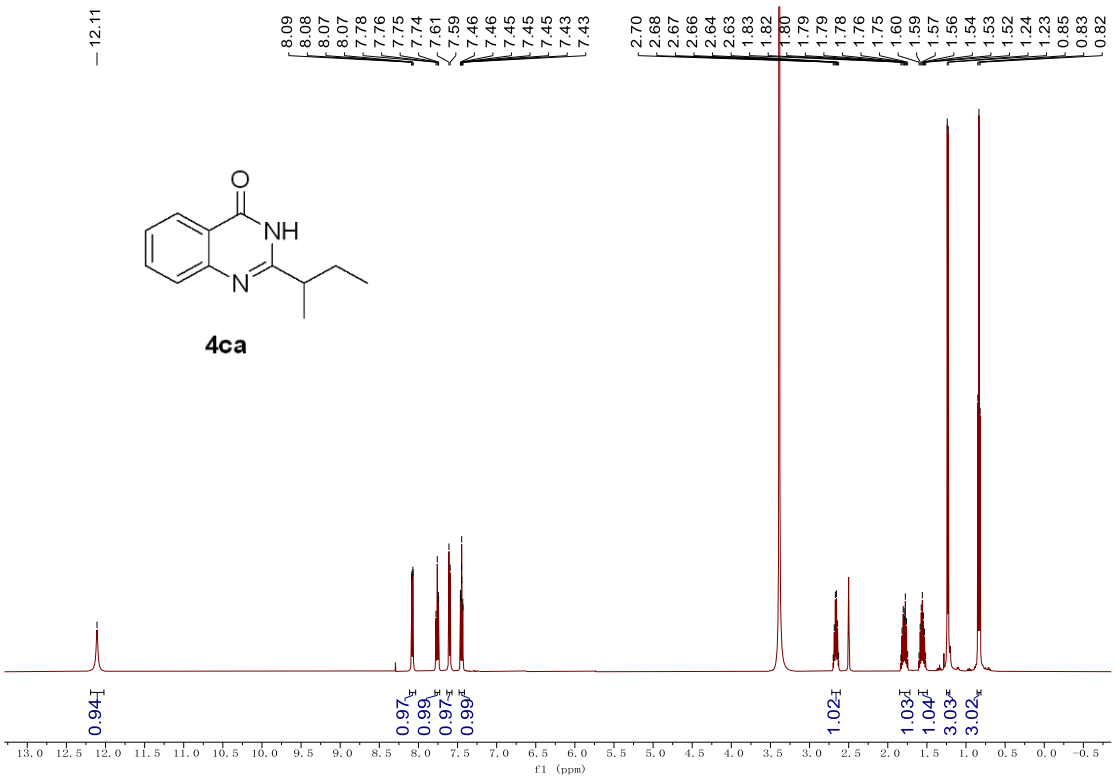
120.8
60.4
39.5
34.3
31.9
23.5
O
NH
N
OH
4ba
f1 (ppm)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7.75
7.74
7.61
7.59
7.46
7.46
7.45
7.45
7.45
7.43
7.43
2.70
2.68
2.67
2.66
2.64
2.63
1.83
1.82
1.80
1.79
1.79
1.78
1.76
1.75
1.60
1.59
1.57
1.56
1.54
1.53
1.52
1.24
1.23
0.85
0.83
0.82
O
NH
N
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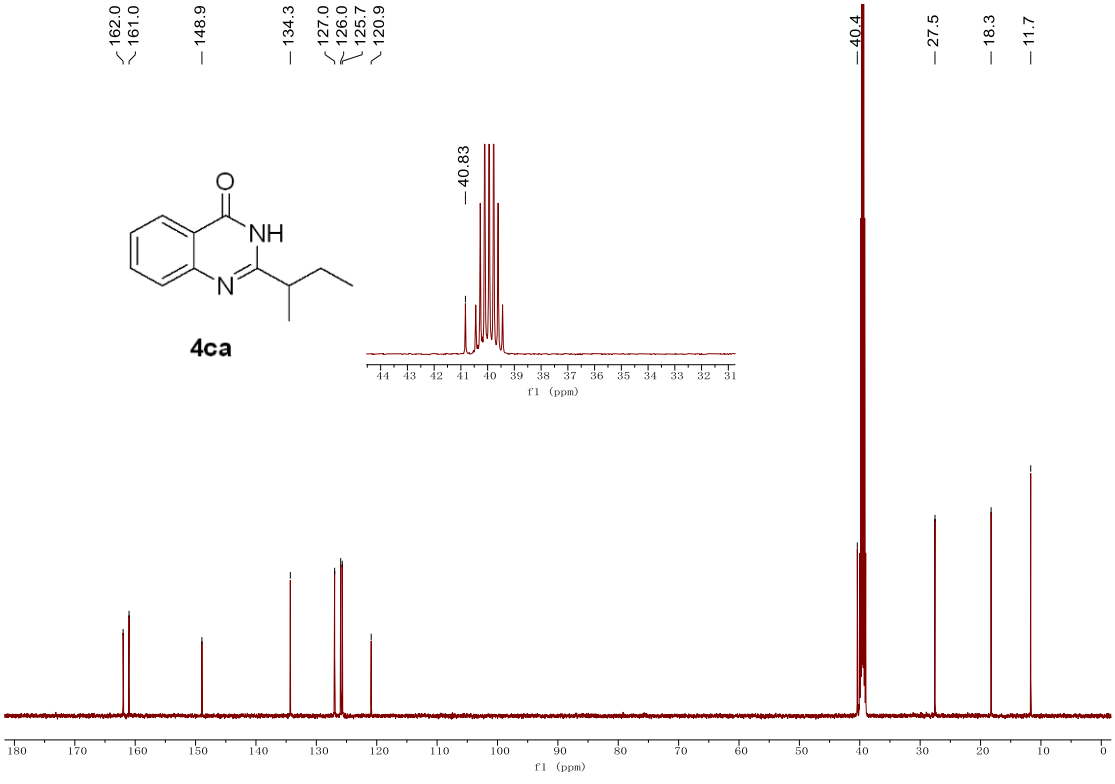
0.99
0.97
0.99
1.02
1.03
1.04
3.03
3.02
f1 (ppm)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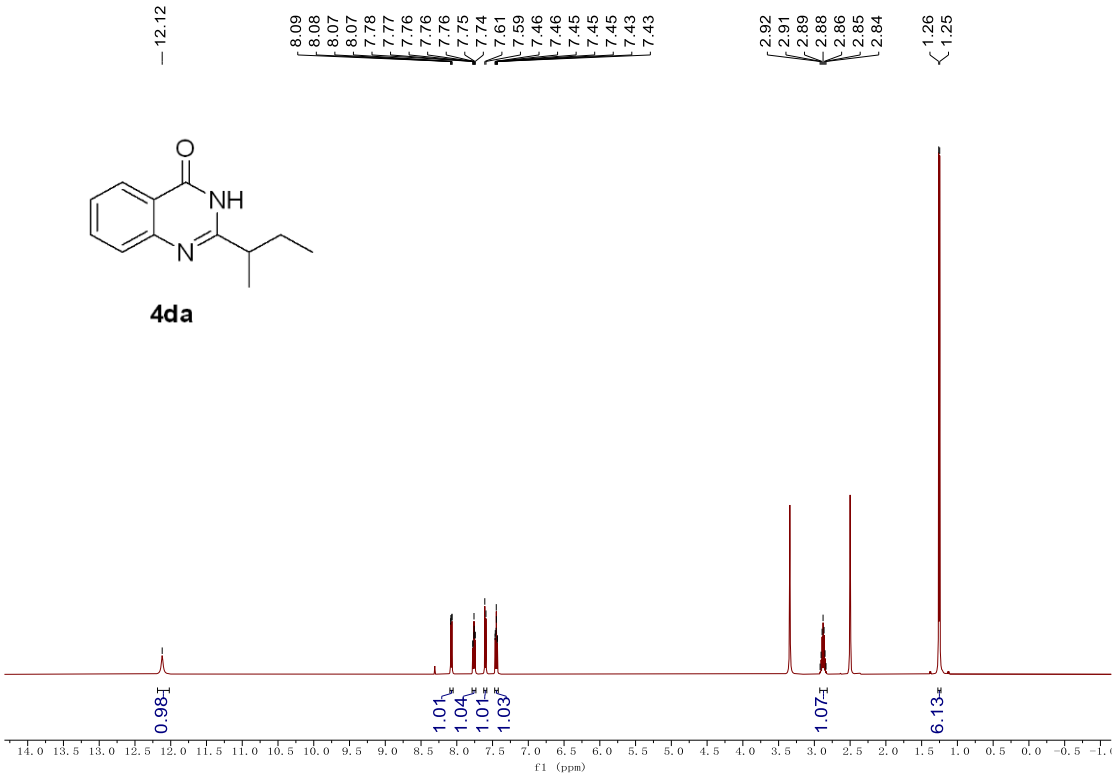
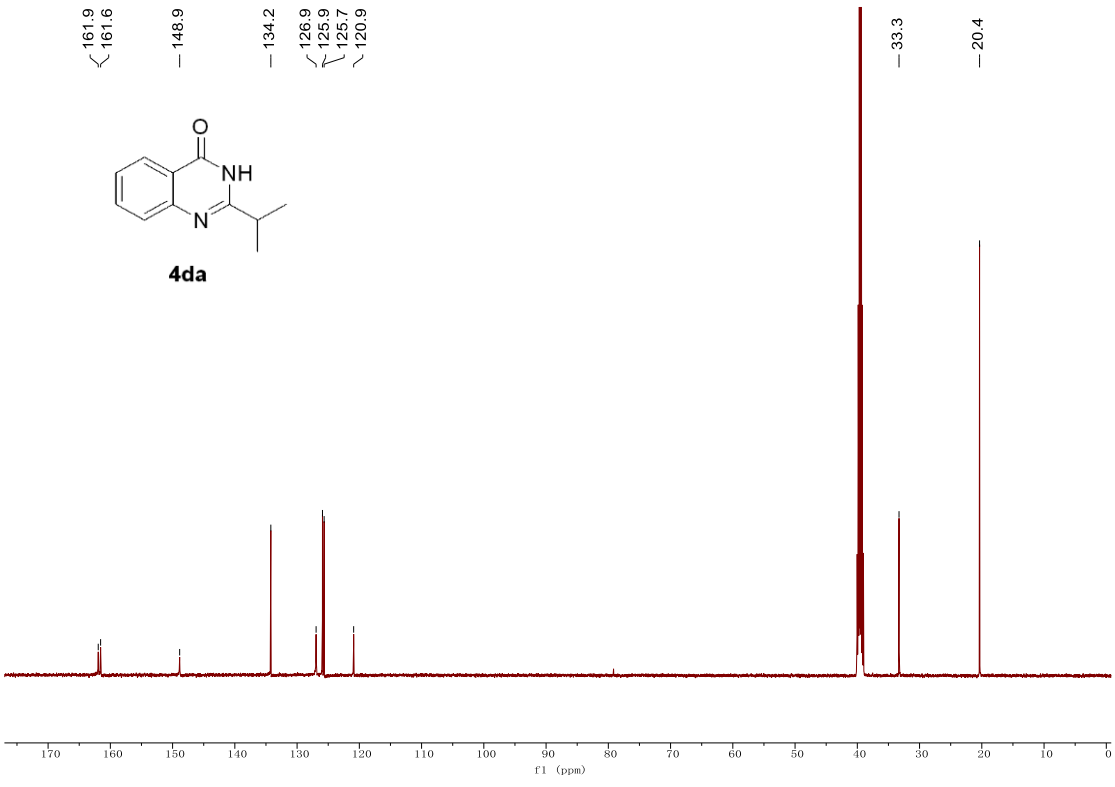
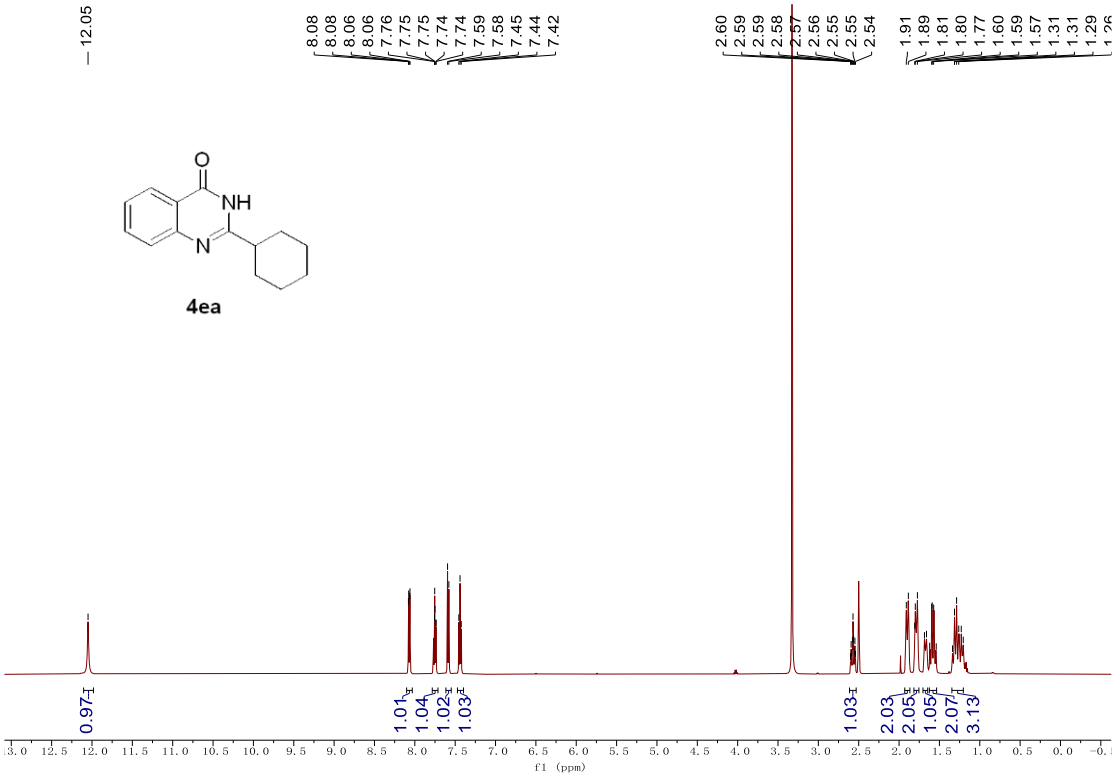
161.0
148.9
134.3
127.0
126.0
125.7
120.9
40.4
27.5
18.3
11.7
40.83
O
NH
N
4ca
f1 (ppm)


12.12
8.09
8.08
8.07
8.07
7.78
7.77
7.76
7.76
7.76
7.75
7.74
7.61
7.59
7.46
7.46
7.45
7.45
7.45
7.43
7.43
2.92
2.91
2.89
2.88
2.86
2.85
2.84
1.26
1.25
O
NH
N
4da
0.98
1.01
1.04
1.01
1.03
1.07
6.13
f1 (ppm)


161.9
161.6
148.9
134.2
126.9
125.9
125.7
120.9
33.3
20.4
O
NH
N
4da
f1 (ppm)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8.08
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8.06
7.76
7.75
7.75
7.74
7.74
7.59
7.58
7.45
7.44
7.42
2.60
2.59
2.59
2.58
2.57
2.56
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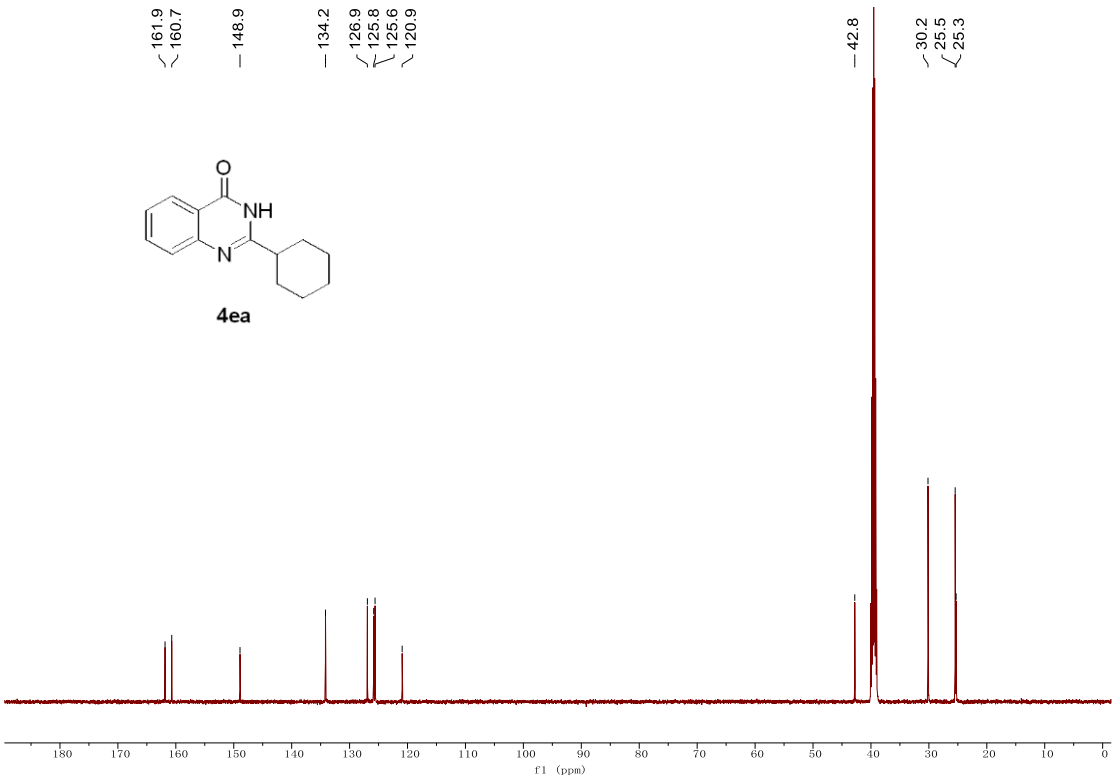
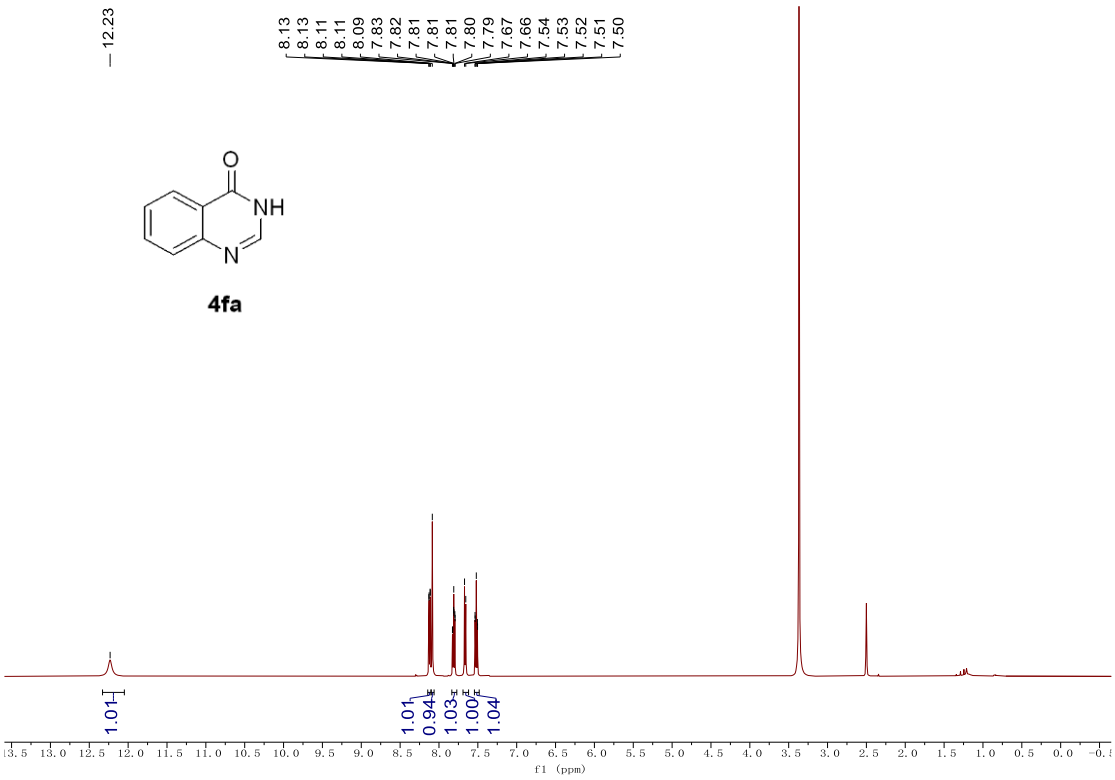
2.55
2.54
1.91
1.89
1.81
1.80
1.77
1.60
1.59
1.57
1.31
1.31
1.29
0.97
1.01
1.04
1.02
1.03
1.03
2.03
2.05
1.05
2.07
3.13
f1 (ppm)
O
NH
N
4ea


161.9
160.7
148.9
134.2
126.9
125.8
125.6
120.9
42.8
30.2
25.5
25.3
f1 (ppm)
O
NH
N
4ea


12.23
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7.82
7.81
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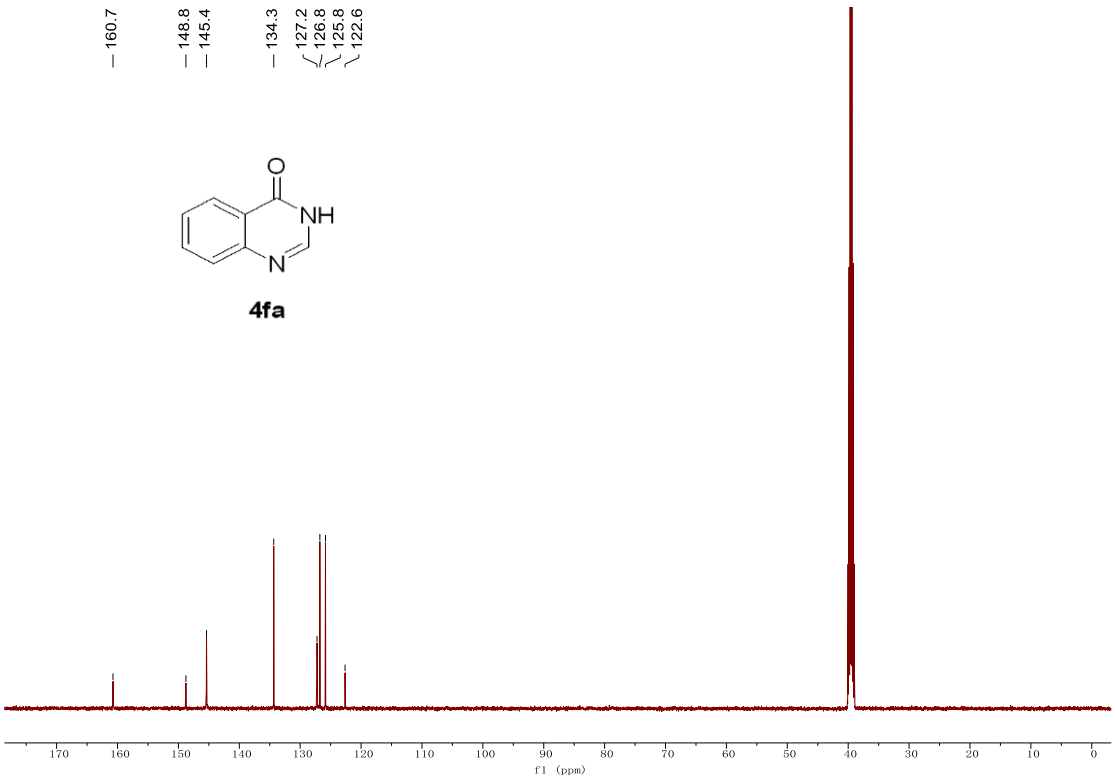
7.81
7.80
7.79
7.67
7.66
7.54
7.53
7.52
7.51
7.50
NH
N
4fa
1.01
1.01
0.94
1.03
1.00
1.04
f1 (ppm)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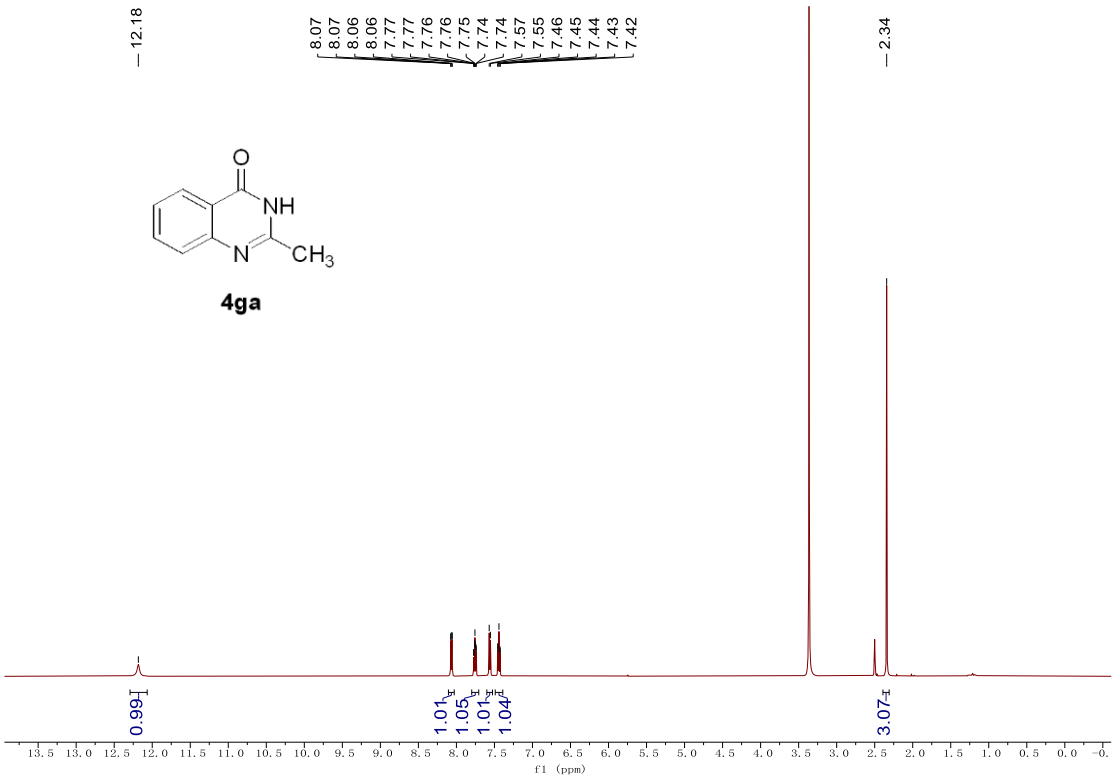
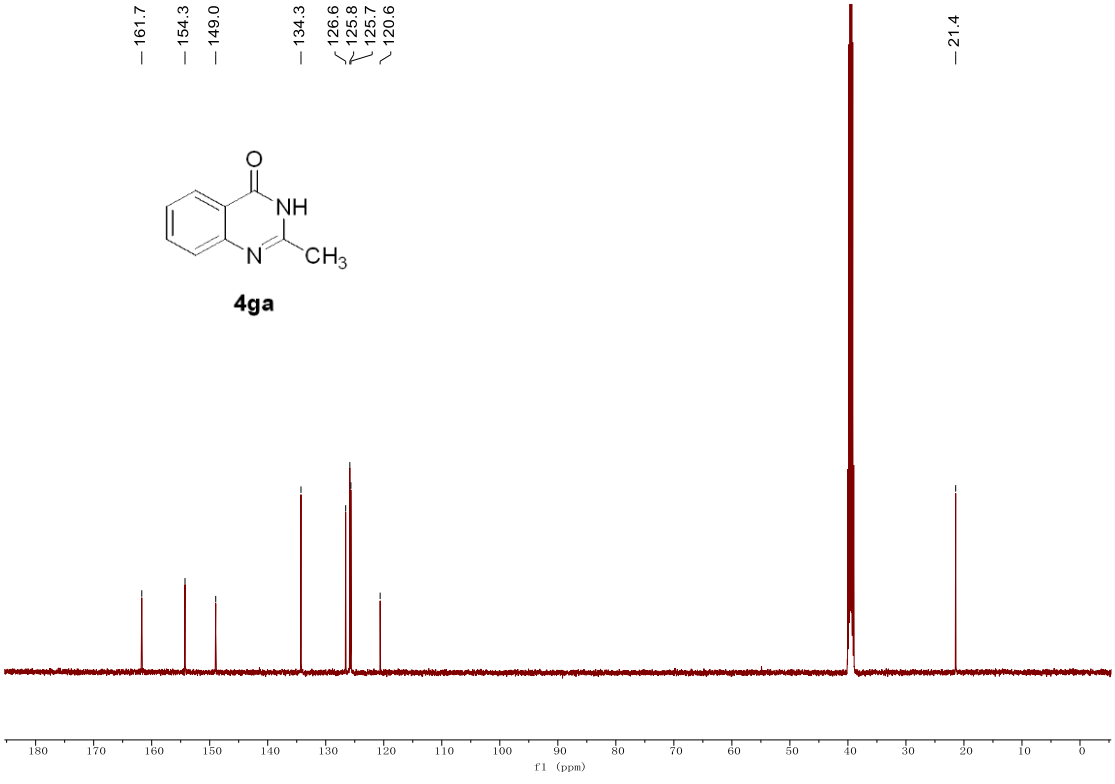
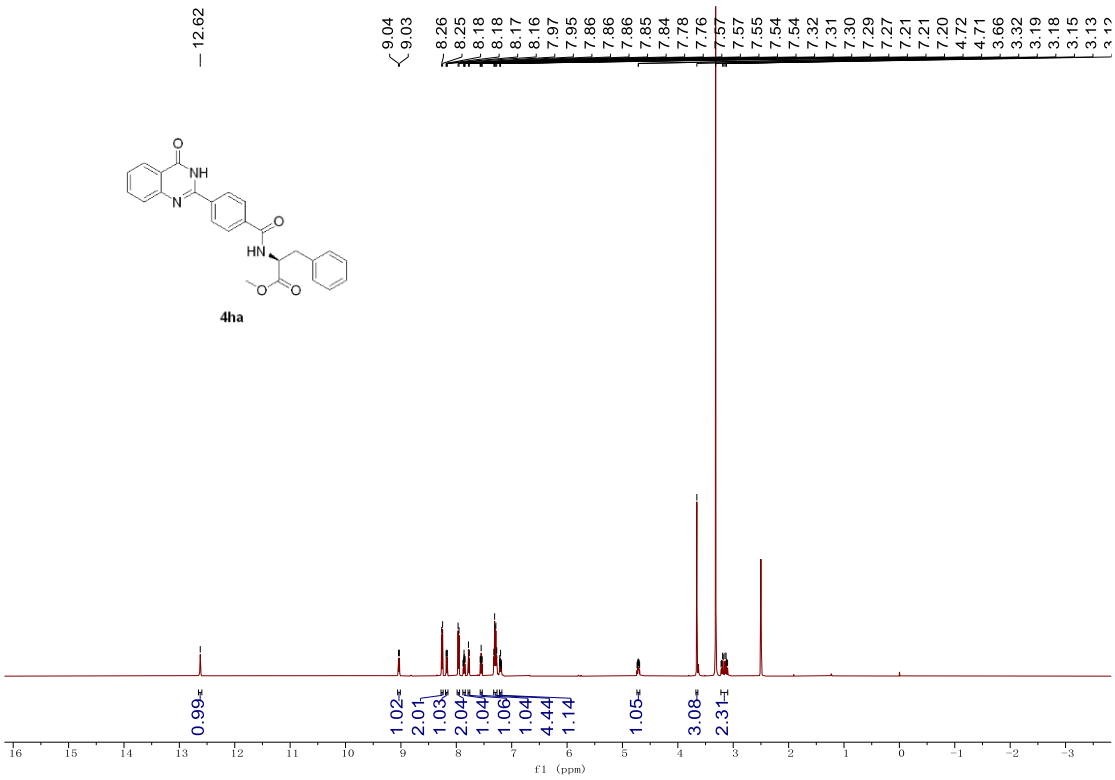
148.8
145.4
134.3
127.2
126.8
125.8
122.6
NH
N
4fa
f1 (ppm)


12.18
8.07
8.07
8.06
8.06
7.77
7.77
7.76
7.76
7.75
7.74
7.74
7.57
7.55
7.46
7.45
7.44
7.43
7.42
2.34
O
NH
N
CH3
4ga
0.99
1.01
1.05
1.01
1.04
3.07
f1 (ppm)


161.7
154.3
149.0
134.3
126.6
125.8
125.7
120.6
21.4
O
NH
N
CH3
4ga
f1 (ppm)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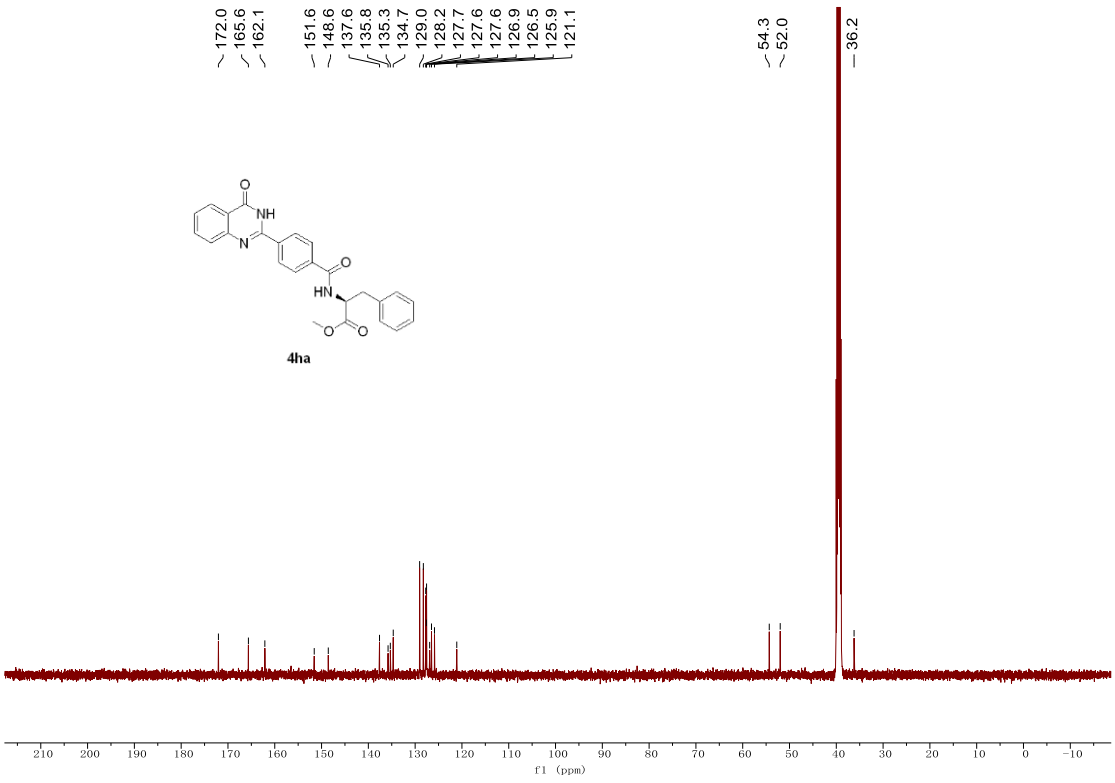
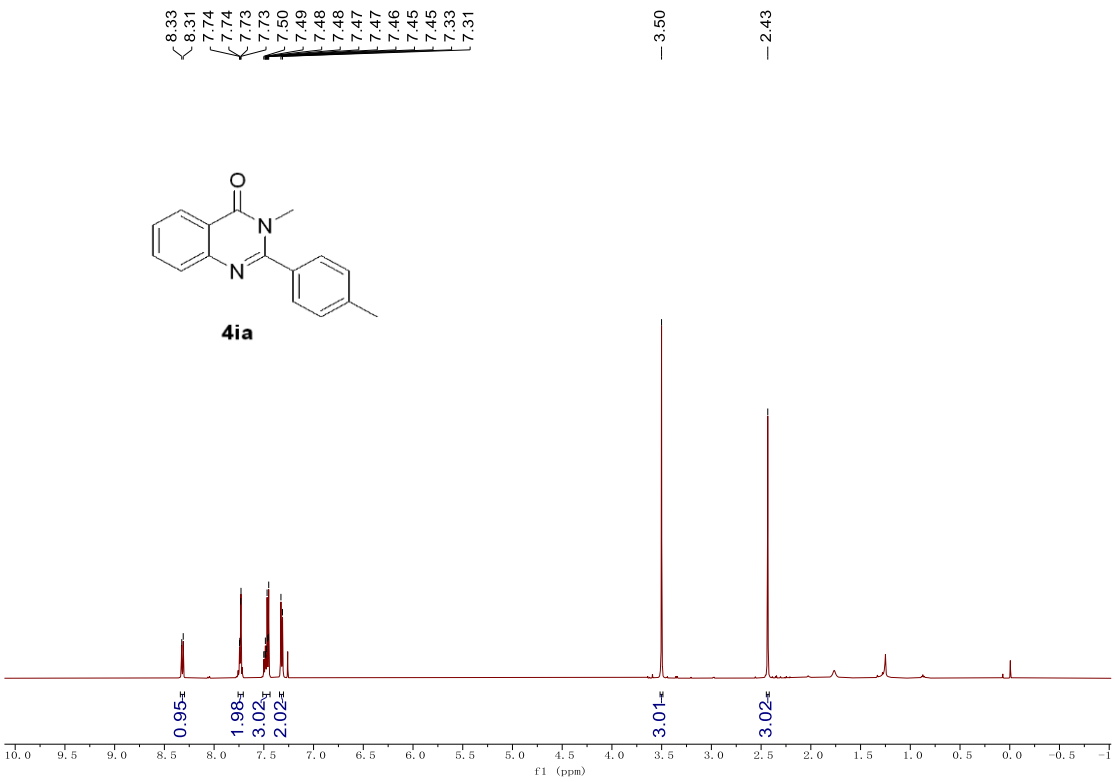
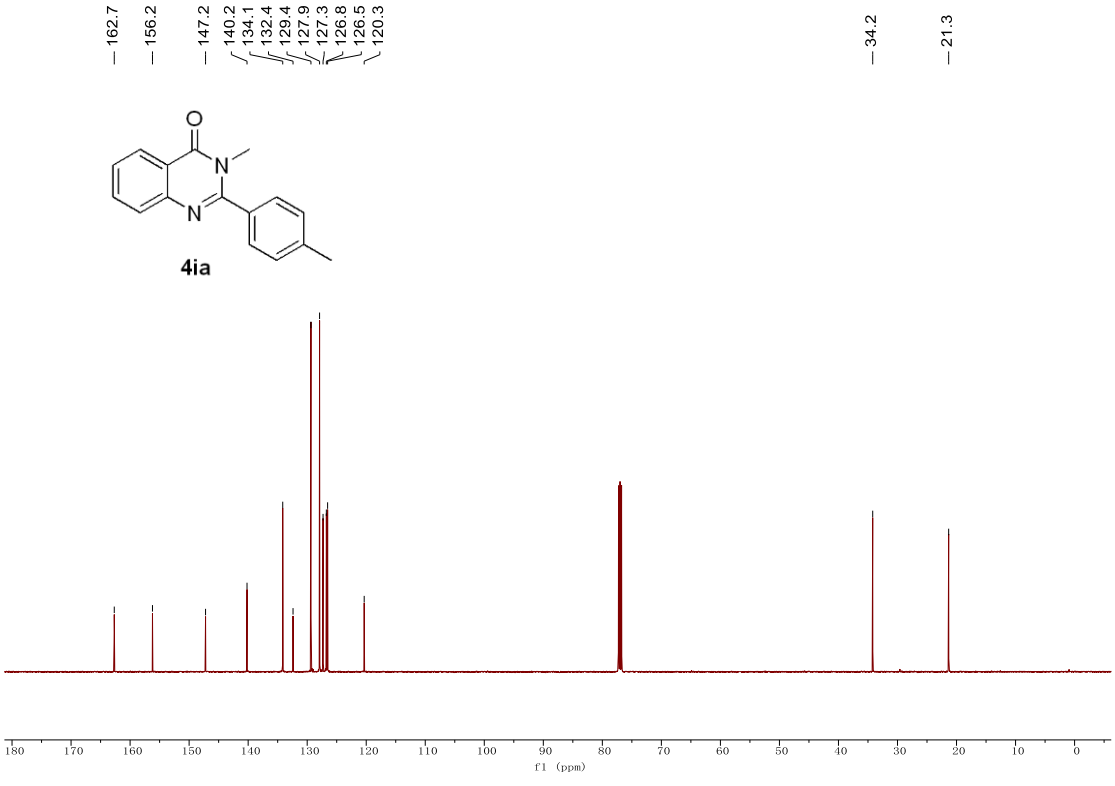
9.04
9.03
8.26
8.25
8.18
8.17
8.16
7.97
7.95
7.86
7.86
7.86
7.85
7.84
7.78
7.76
7.57
7.57
7.55
7.54
7.54
7.32
7.31
7.30
7.29
7.27
7.21
7.21
7.20
4.72
4.71
3.66
3.32
3.19
3.18
3.15
3.13
0.99
1.02
2.01
1.03
2.04
1.04
1.06
1.04
4.44
1.14
1.05
3.08
2.31
f1 (ppm)

4ha


172.0
165.6
162.1
151.6
148.6
137.6
135.8
135.3
134.7
129.0
128.2
127.7
127.6
127.6
126.9
126.5
125.9
121.1
54.3
52.0
36.2
f1 (ppm)

4ha


8.33
8.31
7.74
7.74
7.73
7.73
7.50
7.49
7.48
7.48
7.47
7.47
7.46
7.45
7.45
7.33
7.31
3.50
2.43
4ia
0.95
1.98
3.02
2.02
3.01
3.02
f1 (ppm)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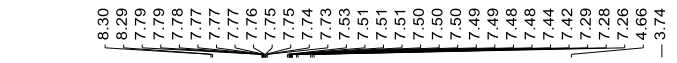
156.2
147.2
140.2
134.1
132.4
129.4
127.9
127.3
126.8
126.5
120.3
34.2
21.3
4ia
f1 (ppm)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7.79
7.78
7.77
7.77
7.77
7.76
7.75
7.75
7.74
7.73
7.53
7.51
7.51
7.50
7.50
7.50
7.49
7.49
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7.48
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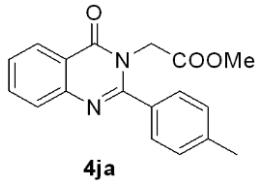
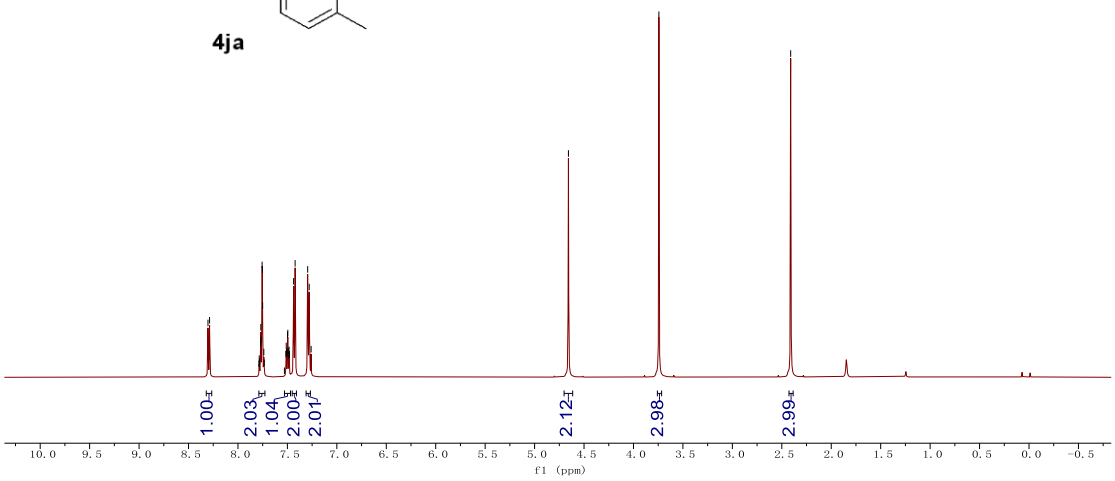
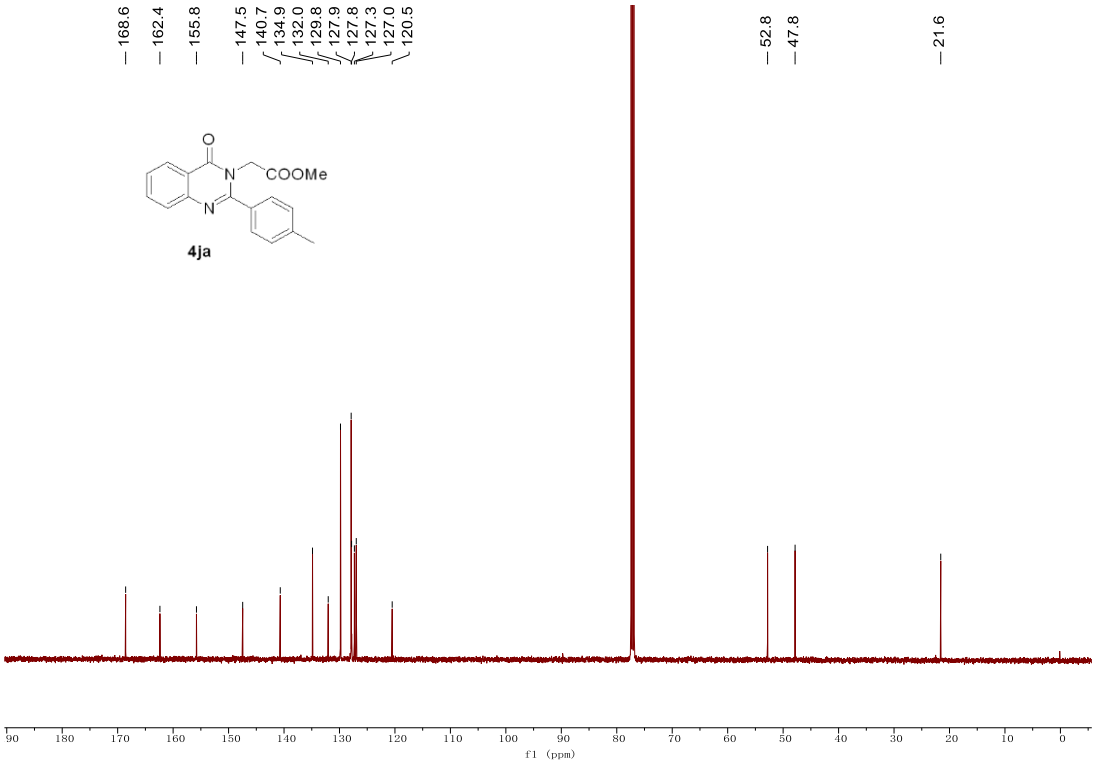
7.42
7.29
7.28
7.26
4.66
3.74
2.41


O
N
COOMe
N

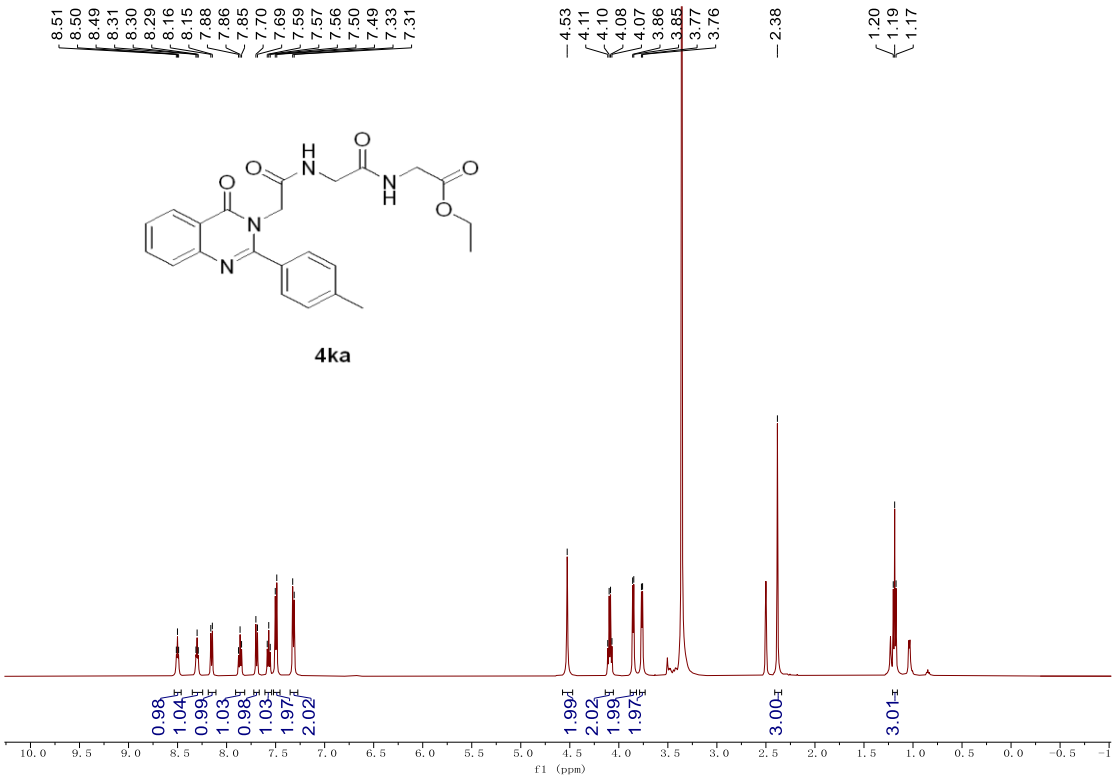
4ja


1.00
2.03
1.04
2.00
2.01
2.12
2.98
2.99
f1 (ppm)


168.6
162.4
155.8
147.5
140.7
134.9
132.0
129.8
127.9
127.8
127.3
127.0
120.5
52.8
47.8
21.6
f1 (ppm)

O
N
COOMe
N

4ja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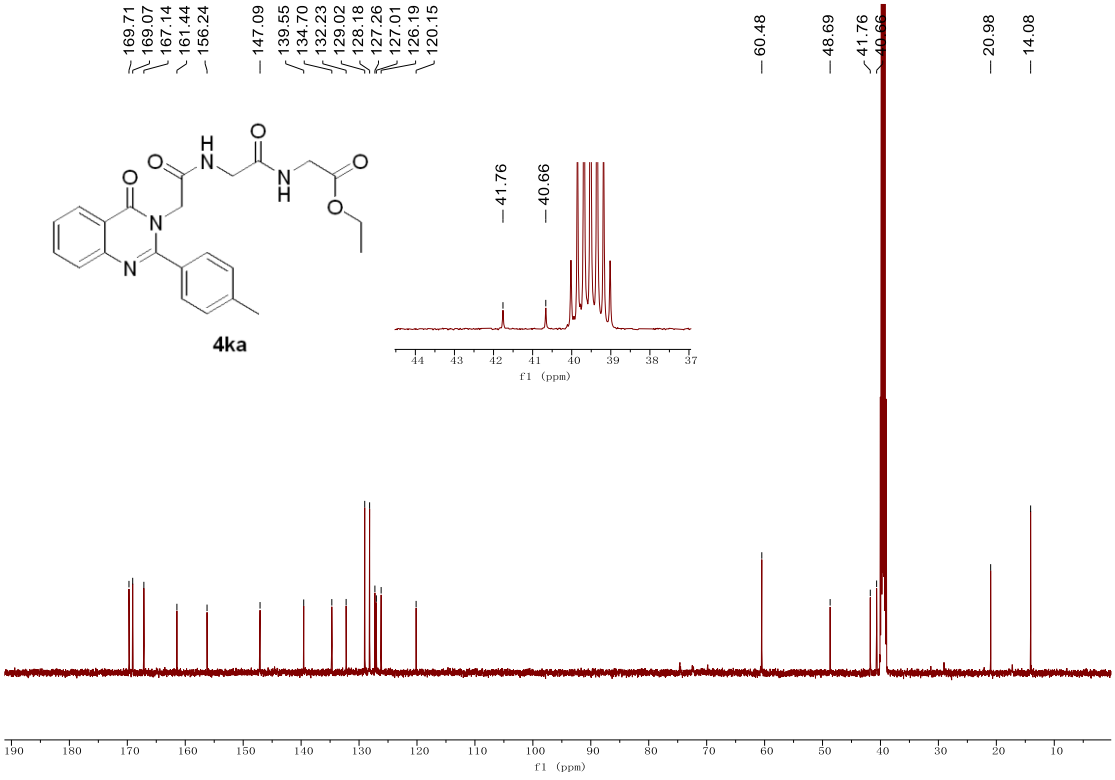
7.86
7.85
7.70
7.69
7.59
7.57
7.56
7.50
7.49
7.33
7.31
4.53
4.11
4.10
4.08
4.07
3.86
3.85
3.77
3.76
2.38
1.20
1.19
1.17
4ka
0.98
1.04
0.99
1.03
0.98
1.03
1.97
2.02
1.99
2.02
1.99
1.97
3.00
3.01
f1 (ppm)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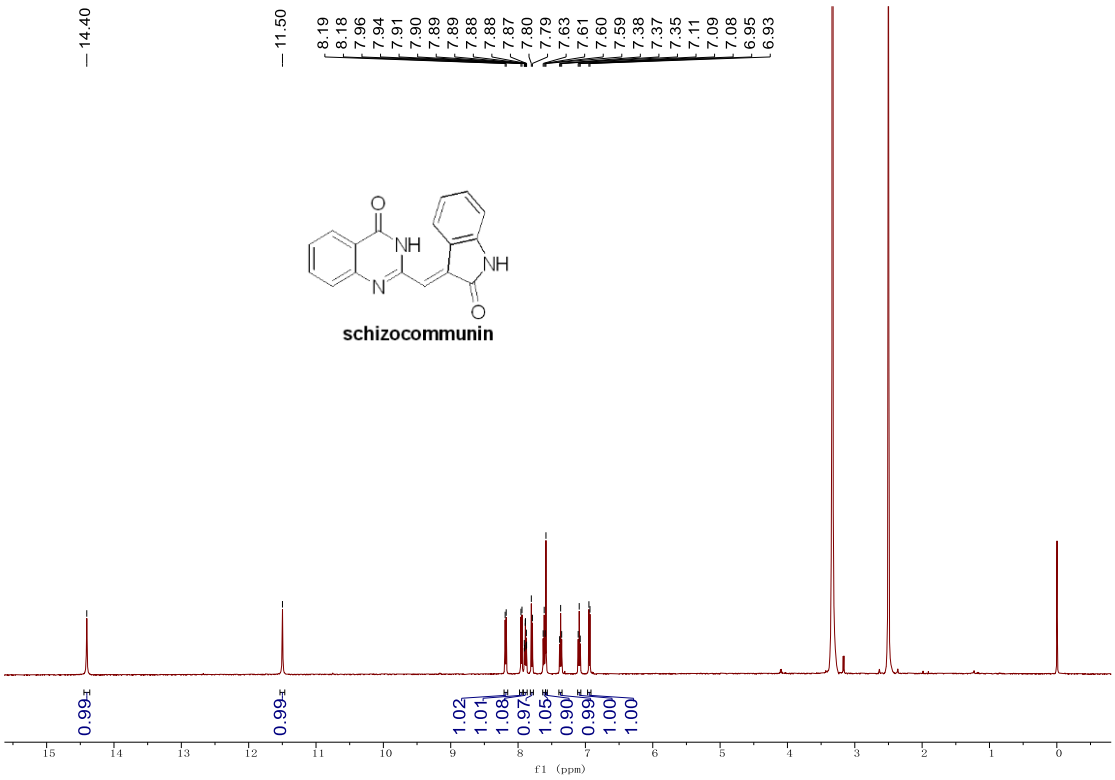
169.07
167.14
161.44
156.24
147.09
139.55
134.70
132.23
129.02
128.18
127.26
127.01
126.19
120.15
60.48
48.69
41.76
40.66
20.98
14.08
4ka
41.76
40.66
f1 (ppm)
f1 (ppm)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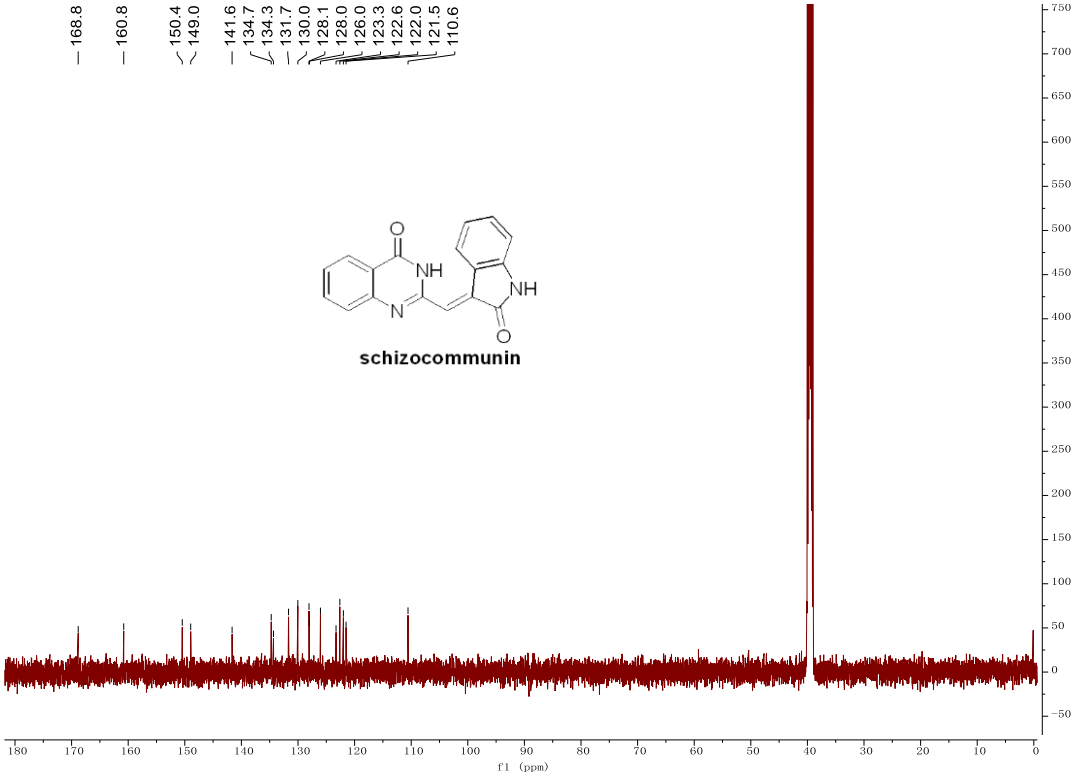
7.94
7.91
7.90
7.89
7.89
7.88
7.88
7.87
7.80
7.79
7.63
7.61
7.60
7.59
7.38
7.37
7.35
7.11
7.09
7.08
6.95
6.93
NH
NH
O
O
N
schizocommunin
0.99
0.99
1.02
1.01
1.08
0.97
1.05
0.90
0.99
1.00
1.00
f1 (ppm)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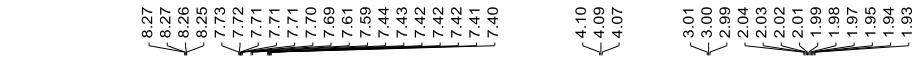
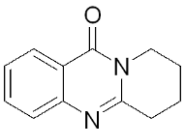
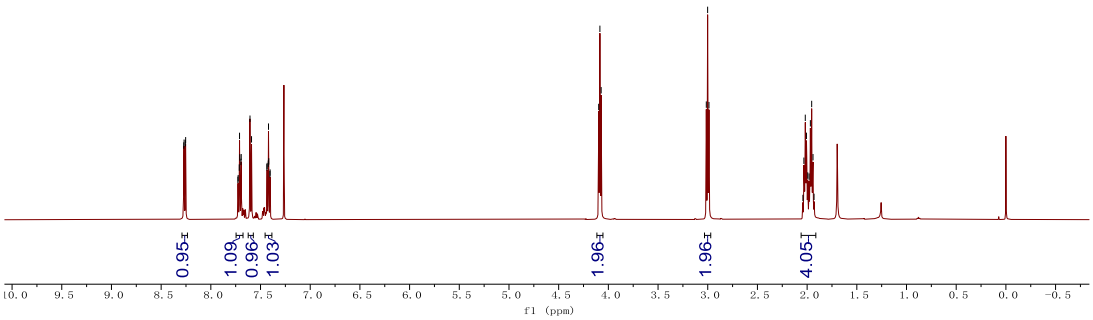
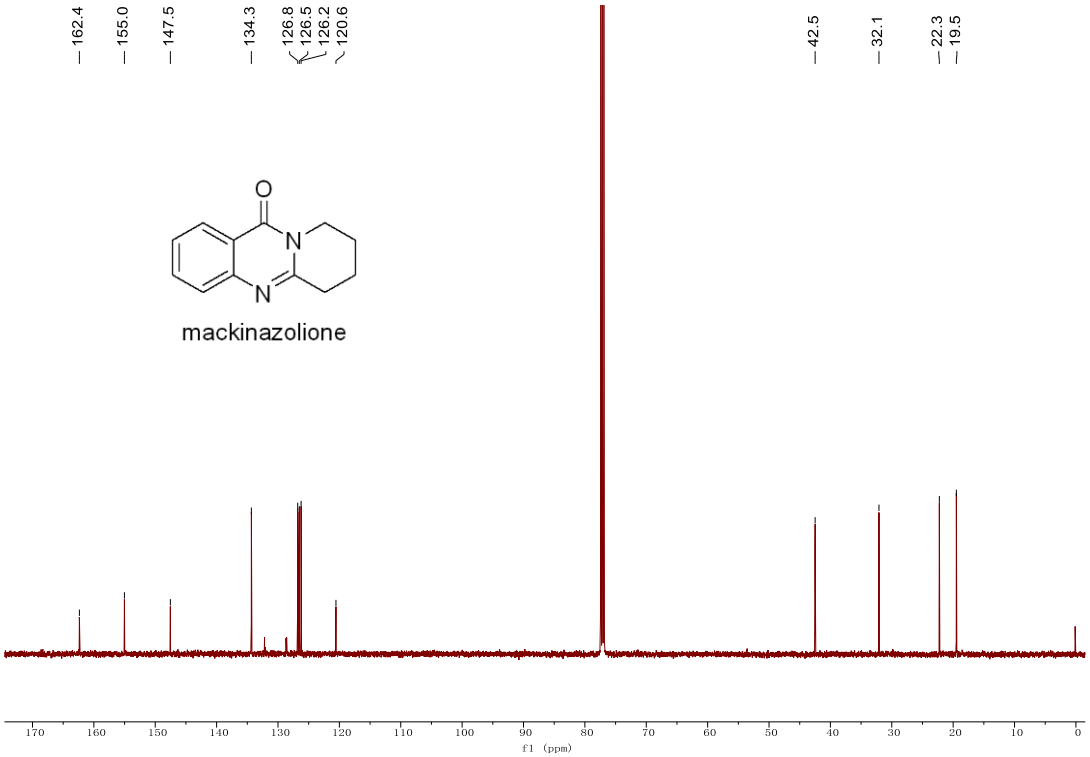
160.8
150.4
149.0
141.6
134.7
134.3
131.7
130.0
128.1
128.0
126.0
123.3
122.6
122.0
121.5
110.6
NH
NH
O
O
N
schizocommunin
f1 (ppm)





mackinazolione





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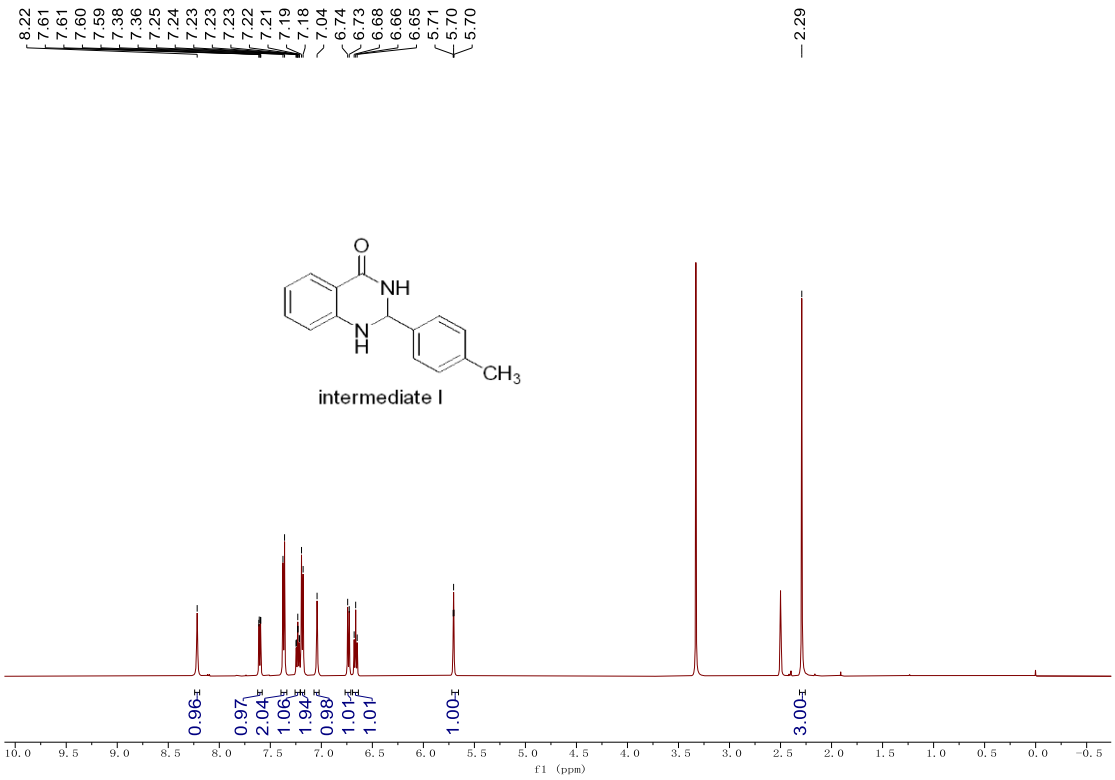
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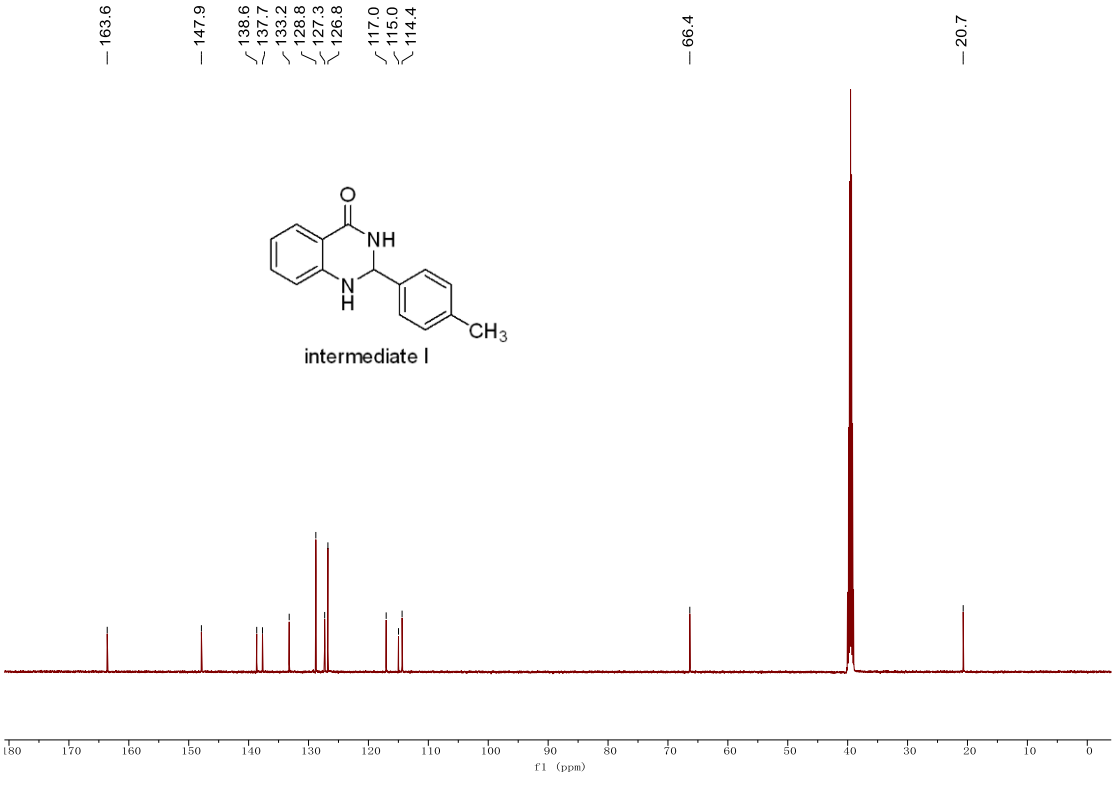
7.24
7.23
7.23
7.23
7.22
7.21
7.19
7.18
7.04
6.74
6.73
6.68
6.66
6.65
5.71
5.70
5.70
2.29
O
NH
N
H
CH3
intermediate I
0.96
0.97
2.04
1.06
1.94
0.98
1.01
1.01
1.00
3.00
f1 (ppm)


163.6
147.9
138.6
137.7
133.2
128.8
127.3
126.8
117.0
115.0
114.4
66.4
20.7
O
NH
N
H
CH3
intermediate I
f1 (ppm)