Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supporting Information

Rh^{III}-Catalyzed One-Pot Cascade Synthesis of Quinazolines with *N*-Alkoxyamide as an Amidating Reagent

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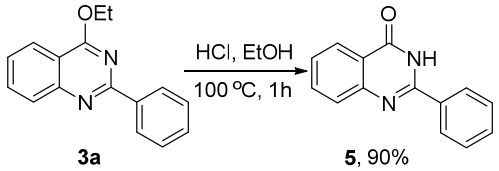
1. General methods

NMR data were obtained for ^{1}H at 400 MHz or 600 MHz, and for ^{13}C at 100 MHz or 151MHz. Chemical shifts were reported in ppm from tetramethylsilane with the solvent resonance as the internal standard in $CDCl_3$ solution. ESI HRMS was recorded on a Waters SYNAPT G2 and Water XEVO G2 Q-ToF. UV detection was monitored at 220 nm. TLC was performed on glass-backed silica plates. Column chromatography was performed on silica gel (200-300 mesh), eluting with ethyl acetate and petroleum ether. *N*-methoxybenzamide **1a**[1] and aryl imidate **2**[2] were prepared according to the literature procedures.

2. General procedure for the C−H activation/amidation/annulation cascade

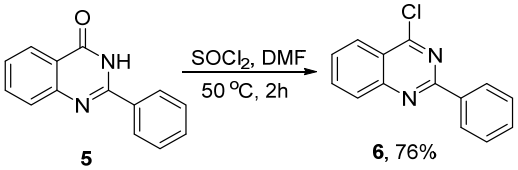
Ethyl benzimidate **1** (0.15 mmol), *N*-methoxybenzamide **2** (0.1 mmol), $[Cp^*RhCl_2]_2$ (1.5 mg, 2.5 mol%), $AgBF_4$ (1.9 mg, 10 mol%) were stirred in DCE (1 mL) under an Ar atmosphere at 120 °C for 3 h. After completion, the reaction mixture was purified by flash chromatography eluting with ethyl acetate and petroleum ether (1:15) to give the product **3** as an off-white solid.

3. Synthetic application of 3



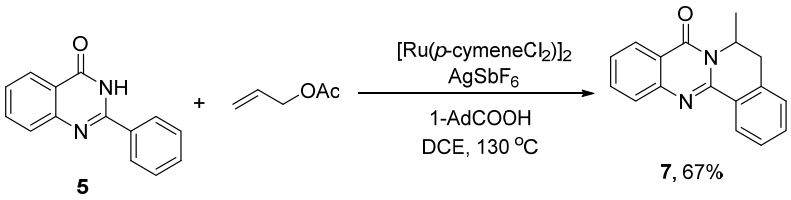
3a **5**, 90%

4-Ethoxy-2-phenylquinazoline **3a** (0.2 mmol, 50 mg) was dissolved in EtOH (6 mL). Hydrochloric acid (3 mL, 35%) was slowly added to the solution. The reaction was heated at 100 °C for one hour. After cooling down to room temperature and concentrating in vacuum, the mixture was washed with saturated aqueous sodium bicarbonate and extracted by DCM (3×15 mL). The organic phase was combined and dried over magnesium sulphate. The solvent was removed under reduced pressure to give 2-phenylquinazolin-4(3*H*)-one **5** without further purification as white solid (40 mg, 90%).



5 **6**, 76%

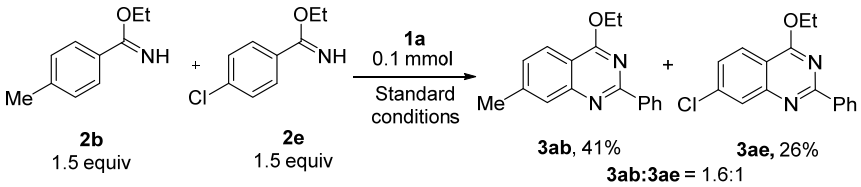
To a mixture of 2-phenylquinazolin-4(3H)-one **5** (0.1 mmol, 22.2 mg) and thionyl chloride (0.2 mmol, 24 mg) 8μL of dimethylformamide (0.5 mL) was slowly added. The mixture was heated at 50 °C for 2 hours. After cooling down to room temperature the mixture was washed with saturated aqueous sodium bicarbonate and extracted by DCM (3×15 mL). The organic phase was combined, dried and purified through column chromatography to afford the pure product **6** as yellow solid (18.3 mg, 76%).



A mixture of 2-phenylquinazolin-4(3*H*)-one (0.1 mmol), [Ru(*p*-cymene)Cl_2]$_2$ (5 mol %), $AgSbF_6$ (20 mol %) and $AdCO_2H$ (0.2 mmol, 2.0 equiv) was taken in a 15-mL pressure tube. To this reaction mixture, DCE (0.5 mL) and the corresponding allyl acetate (0.5 mmol) were added via micro syringe and the closed reaction mixture was allowed to stir at 130 °C for 10 min. After completion as indicated by TLC, the reaction mixture was cooled to ambient temperature. Further the reaction mixture was diluted with dichloromethane and washed with 1N NaOH solution to neutralize the excess acid and dried over anhydrous Na_2SO_4, and concentrated under reduced pressure. The crude product was purified by column chromatography using ethyl acetate/hexane as eluent to afford the desired isoquinolino[1,2-b]quinazolinone product **7** (17.5 mg, 67%).

4. Mechanism study

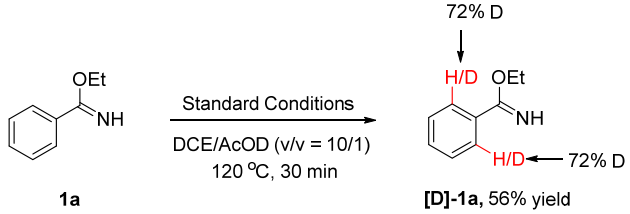
4.1 Intermolecular competition experiment

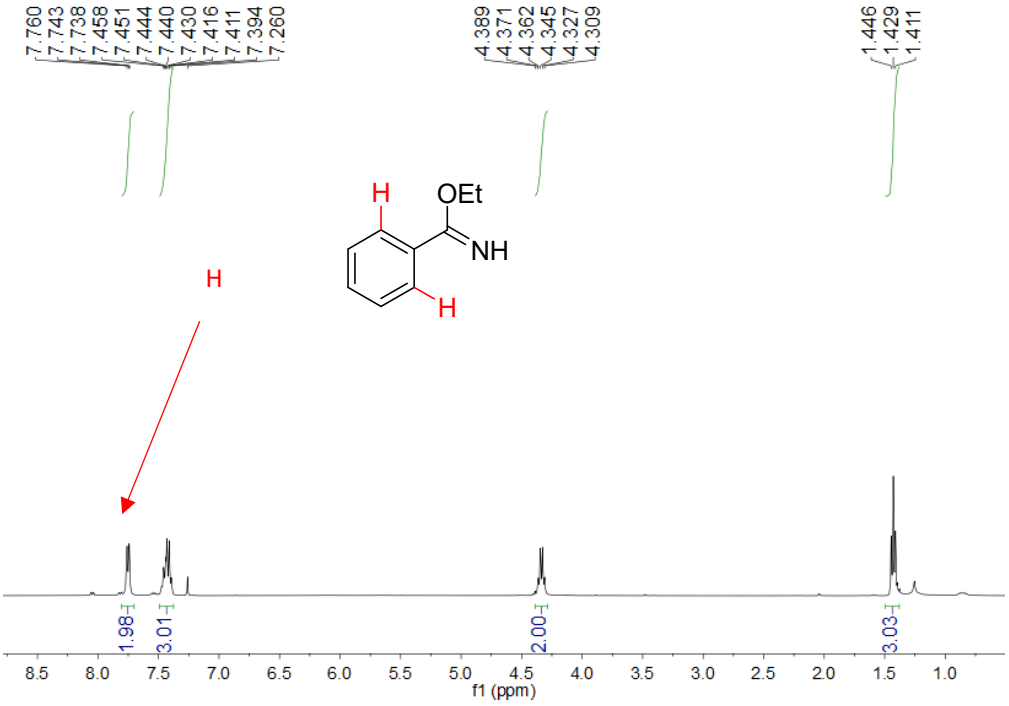


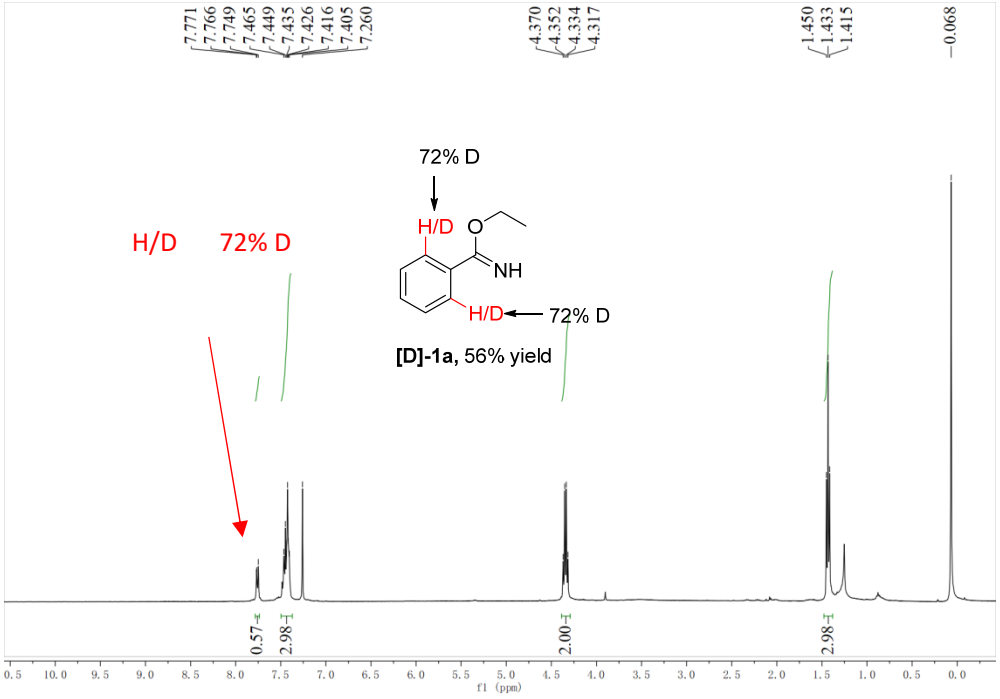
To a tube with a stir bar was added benzimidates (**2b**, 0.15 mmol) and (**2e**, 0.15 mmol), *N*-methoxybenzamide **1a** (0.10 mmol), [Cp*$RhCl_2$]$_2$ (3 mg), $AgBF_4$ (6 mg) were stirred in DCE (1 mL) at 120 °C for 3 h. After completion, the reaction mixture was purified by flash chromatography eluting with ethyl acetate and petroleum ether (1:15) to give the product **3ab** and **3ae** in 41% and 26% yield, respectively. The ratio of the products is 1.6:1, which revealed that electronic effect of benzimidates have slightly affected the reaction.

4.2 Deuterium-labeling experiment

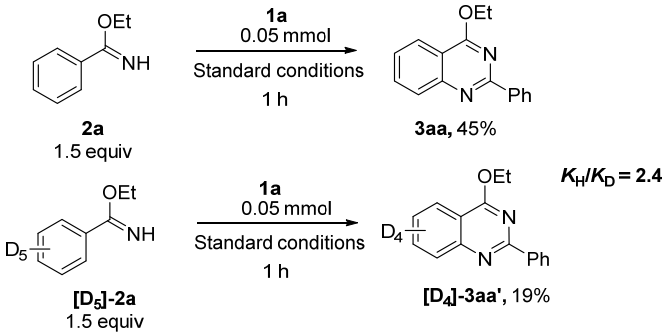
Deuterium-labeling experiment was proceeded to investigate the mechanism of this reaction. Ethyl benzimidate **1a** was stirred in the absence of *N*-methoxybenzamide at 120 °C for 30 min under standard condition with AcOD/DCE, and the deuterium rate was obtained from ^{1}H NMR. This suggested that C−H bond activation could occur at the first step.







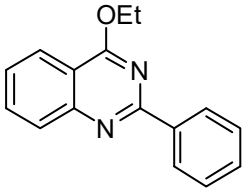
4.3 KIE experiments (parallel experiments)



Two Schlenk tubes each was charged with Ethyl benzimidate **2a** (0.075 mmol) or [**D_5**]-**2a** (0.075 mmol) and *N*-methoxybenzamide **1a** (0.05 mmol), $[Cp^*RhCl_2]_2$ (5 mol%,), $AgBF_4$ (0.03 equiv), and DCE (0.5 mL). The reaction mixture was stirred at 120 ºC for 1h under argon atmosphere. After rapidly evaporating the two mixtures solely, the product **3aa** and [**D_4**]-**3aa** were purified by flash column chromatography on silicagel (eluent:PE/EA = 15:1). The KIE value was determined to be k_H/k_D = 2.4 on the yield ratio of **3aa** and [**D_4**]-**3aa**, which indicated that the cleavage of the C−H bond is likely involved in the rate-limiting step.

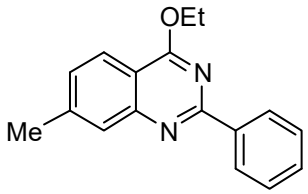
5 Characterization data for compounds

4-ethoxy-2-phenylquinazoline (3aa)[2]



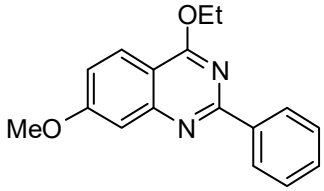
23.8mg (95%); off-white solid; mp = 109.3-113.1ºC; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.59 (dd, *J* = 7.5, 2.2 Hz, 2H), 8.18 (dd, *J* = 8.1, 1.6 Hz, 1H), 8.01 (d, *J* = 8.4 Hz, 1H), 7.81 (ddd, *J* = 8.4, 6.9, 1.5 Hz, 1H), 7.51 (dt, *J* = 7.0, 4.4 Hz, 4H), 4.79 (q, *J* = 7.1 Hz, 2H), 1.58 (t, *J* = 7.1 Hz, 3H).^{13}C NMR (101 MHz, Chloroform-*d*) δ 166.7, 160.1, 151.6, 138.1, 133.5, 130.5, 128.5, 128.4, 127.8, 126.3, 123.5, 115.4, 62.9, 14.4.

4-ethoxy-7-methyl-2-phenylquinazoline (3ab)[2]

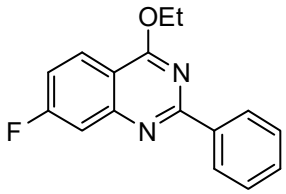


22.7 mg (86%); off-white solid; mp = 92.3-93.5ºC; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.74 – 8.41 (m, 2H), 8.05 (d, *J* = 8.3 Hz, 1H), 7.80 (s, 1H), 7.62 – 7.42 (m, 3H), 7.33 (dd, *J* = 8.3, 1.6 Hz, 1H), 4.77 (q, *J* = 7.1 Hz, 2H), 2.56 (s, 3H), 1.57 (t, *J* = 7.1 Hz, 3H).^{13}C NMR (101 MHz, Chloroform-*d*) δ 166.6, 160.1, 152.0, 144.2, 138.3, 130.4, 128.4, 128.4, 128.3, 127.1, 123.2, 113.2, 62.7, 22.1, 14.4.

4-ethoxy-7-methoxy-2-phenylquinazoline (3ac)[2]



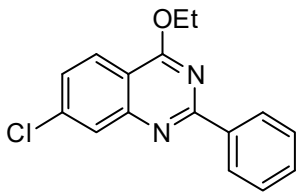
25.5 mg (91%); off-white solid; mp = 126.4-129.3ºC; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.63 – 8.51 (m, 2H), 8.05 (d, *J* = 9.0 Hz, 1H), 7.55 – 7.45 (m, 3H), 7.35 (d, *J* = 2.5 Hz, 1H), 7.11 (dd, *J* = 9.0, 2.5 Hz, 1H), 4.75 (q, *J* = 7.1 Hz, 2H), 3.97 (s, 3H), 1.55 (t, *J* = 7.1 Hz, 3H).^{13}C NMR (101 MHz, Chloroform-*d*) δ 166.4, 163.8, 160.8, 154.0, 138.2, 130.4, 128.5, 128.4, 124.8, 118.6, 109.7, 106.4, 62.7, 55.7, 14.5.



4-ethoxy-7-fluoro-2-phenylquinazoline (3ad)[2]

23.6 mg (88%); off-white solid; mp = 88.5-93.3ºC; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.58 (dd, *J* = 6.8, 3.0 Hz, 2H), 8.19 (dd, *J* = 9.0, 6.1 Hz, 1H), 7.86 – 7.39 (m, 4H), 7.39 – 7.04 (m, 2H), 4.78 (q, *J* = 7.0 Hz, 2H), 1.57 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 167.1, 166.6, 164.6, 161.3, 130.8, 128.6, 128.5, 126.3, 126.2, 116.2 (d, *J* = 25 Hz), 112.3, 112.0 (q, *J* = 20 Hz), 111.9, 63.1, 14.4.

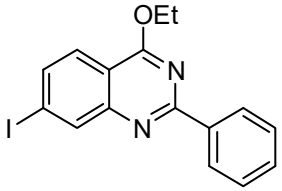
7-chloro-4-ethoxy-2-phenylquinazoline (3ae)[2]



22.7 mg (80%); off-white solid; mp = 104.0-108.7ºC; ^{1}H NMR (400

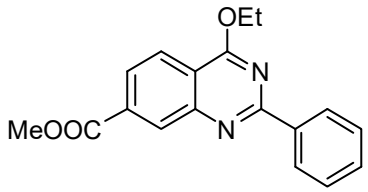
MHz, Chloroform-*d*) δ 8.56 (dd, *J* = 6.8, 3.0 Hz, 2H), 8.18 – 7.92 (m, 2H), 7.62 – 7.34 (m, 4H), 4.77 (q, *J* = 7.1 Hz, 2H), 1.57 (t, *J* = 7.1 Hz, 3H).^{13}C NMR (101 MHz, Chloroform-*d*) δ 166.6, 161.2, 152.5, 139.6, 137.7, 130.8, 128.6, 128.4, 127.2, 127.0, 125.0, 113.7, 63.2, 14.4.

4-ethoxy-7-iodo-2-phenylquinazoline (3af)[2]



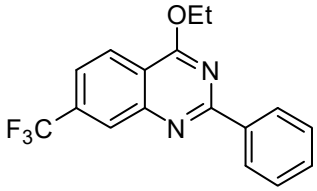
35.7 mg (95%); off-white solid; mp = 89.6-93.4ºC; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.69 – 8.12 (m, 3H), 7.96 – 7.65 (m, 2H), 7.50 (dd, *J* = 5.0, 2.0 Hz, 3H), 4.76 (q, *J* = 7.1 Hz, 2H), 1.56 (t, *J* = 7.1 Hz, 3H).^{13}C NMR (101 MHz, Chloroform-*d*) δ 166.8, 160.8, 152.4, 137.7, 136.8, 135.2, 130.8, 128.6, 128.5, 124.7, 114.4, 100.7, 63.2, 14.4.

methyl 4-ethoxy-2-phenylquinazoline-7-carboxylate (3ag)[2]



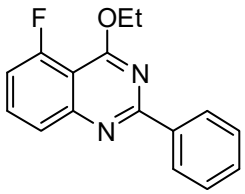
26.8 mg (87%); off-white solid; mp = 138.2-146.8ºC; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.68 (d, *J* = 1.7 Hz, 1H), 8.63 – 8.52 (m, 2H), 8.21 (d, *J* = 8.4 Hz, 1H), 8.09 (dd, *J* = 8.5, 1.5 Hz, 1H), 7.51 (dd, *J* = 5.1, 2.0 Hz, 3H), 4.79 (qd, *J* = 7.1, 1.2 Hz, 2H), 4.01 (s, 3H), 1.58 (t, *J* = 7.1 Hz, 3H).^{13}C NMR (101 MHz, Chloroform-*d*) δ 166.6, 166.4, 160.8, 151.4, 137.7, 134.6, 130.8, 130.1, 128.6, 128.5, 125.9, 123.9, 117.8, 63.3, 52.6, 14.4.

4-ethoxy-2-phenyl-7-(trifluoromethyl)quinazoline (3ah)[2]



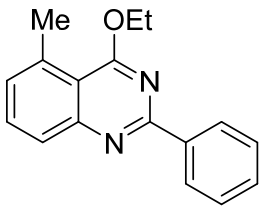
26.1 mg (82%); off-white solid; mp = 100.5-106.0ºC; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.62 – 8.54 (m, 2H), 8.28 (dd, *J* = 5.0, 3.4 Hz, 2H), 7.68 (dd, *J* = 8.7, 1.6 Hz, 1H), 7.57 – 7.48 (m, 3H), 4.81 (q, *J* = 7.1 Hz, 2H), 1.59 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 166.9, 158.6, 151.5, 141.4, 133.7, 132.0 (d, *J* = 32 Hz), 128.7, 127.9, 126.9, 125.3 (q, *J* = 4 Hz), 124.2 (s, *J* = 270 Hz),123.6, 115.5, 63.1, 14.4.

4-ethoxy-5-fluoro-2-phenylquinazoline (3ai)[2]



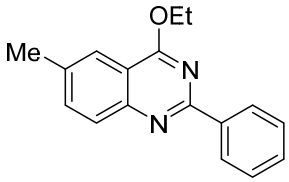
25.5 mg (95%); off-white solid; mp = 92.0-94.3ºC; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.57 (dd, *J* = 6.7, 3.0 Hz, 2H), 7.85 – 7.76 (m, 1H), 7.72 (td, *J* = 8.1, 5.3 Hz, 1H), 7.51 (dd, *J* = 5.1, 2.0 Hz, 3H), 7.14 (ddd, *J* = 10.5, 7.8, 1.2 Hz, 1H), 4.80 (q, *J* = 7.1 Hz, 2H), 1.59 (t, *J* = 7.1 Hz, 3H).^{13}C NMR (101 MHz, Chloroform-*d*) δ 165.8 (d, *J* = 5 Hz), 160.6 (d, *J* = 2 Hz), 158.6 (d, *J* = 260 Hz), 153.8, 137.6, 133.3 (d, *J* = 10 Hz), 130.8, 128.5, 128.4, 123.8 (d, *J* = 5 Hz), 112.0 (d, *J* = 22 Hz), 106.0 (d, *J* = 12 Hz), 63.3, 14.3.

4-ethoxy-5-methyl-2-phenylquinazoline (3aj)[2]



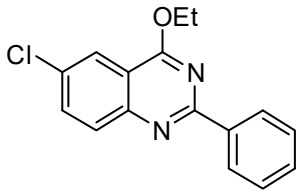
18.2 mg (69%); off-white solid; mp = 76.3-80.9ºC; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.59 (dd, *J* = 7.4, 2.4 Hz, 2H), 7.93 (d, *J* = 8.3 Hz, 1H), 7.65 (dd, *J* = 8.4, 7.2 Hz, 1H), 7.58 – 7.40 (m, 3H), 7.32 – 7.27 (m, 1H), 4.77 (q, *J* = 7.1 Hz, 2H), 2.86 (s, 3H), 1.58 (t, *J* = 7.1 Hz, 3H).^{13}C NMR (101 MHz, Chloroform-*d*) δ 167.9, 159.3, 136.9, 133.0, 130.7, 129.0, 128.5, 128.4, 125.7, 114.9, 63.2, 23.9, 14.4.

4-ethoxy-6-methyl-2-phenylquinazoline (3ak)[2]



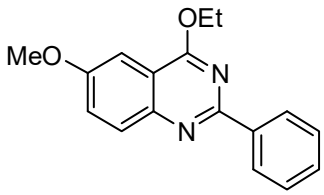
25.6 mg (97%); off-white solid; mp = 109.3-113.1°C; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.64 – 8.49 (m, 2H), 8.05 – 7.85 (m, 2H), 7.64 (dd, *J* = 8.5, 2.0 Hz, 1H), 7.57 – 7.46 (m, 3H), 4.78 (q, *J* = 7.1 Hz, 2H), 2.54 (s, 3H), 1.58 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 166.3, 159.3, 136.5, 135.5, 130.3, 128.4, 127.5, 122.5, 115.2, 62.8, 21.6, 14.5.

6-chloro-4-ethoxy-2-phenylquinazoline (3al)[2]



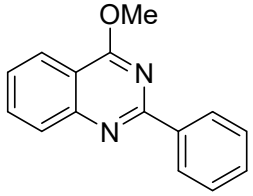
22.4 mg (79%); off-white solid; mp = 138.4-144.3°C; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.56 (dd, *J* = 6.7, 3.0 Hz, 2H), 8.13 (d, *J* = 2.4 Hz, 1H), 7.93 (d, *J* = 8.9 Hz, 1H), 7.73 (dd, *J* = 8.9, 2.4 Hz, 1H), 7.50 (dd, *J* = 5.1, 2.0 Hz, 3H), 4.77 (q, *J* = 7.1 Hz, 2H), 1.57 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 165.9, 160.3, 150.2, 137.7, 134.2, 131.8, 130.7, 129.5, 128.5, 128.4, 122.8, 116.0, 63.2, 14.4.

4-ethoxy-6-methoxy-2-phenylquinazoline (3am)



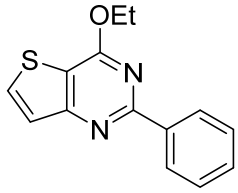
11.7 mg (42%); off-white solid; mp = 109.3-113.1°C; IR (cm^{-1}) *v*: 2982, 1622, 1584, 1438, 1348, 1210, 1158,1019, 768, 703. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.59 – 8.49 (m, 2H), 7.91 (d, *J* = 9.0 Hz, 1H), 7.47 (dtd, *J* = 24.1, 8.2, 2.5 Hz, 5H), 4.78 (q, *J* = 7.1 Hz, 2H), 3.95 (s, 3H), 1.58 (t, *J* = 7.1 Hz, 3H).^{13}C NMR (101 MHz, Chloroform-*d*) δ 165.8, 158.1, 157.8, 147.4, 138.3, 130.1, 129.4, 128.4, 128.1, 125.4, 115.8, 101.5, 62.8, 55.7, 14.5. HRMS: m/z (ESI) calcd for $C_{17}H_{17}N_2O_2[M+H]^+$: 281.1285, found: 282.1281.

4-methoxy-2-phenylquinazoline (3an)

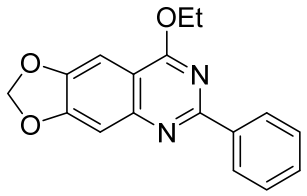


20.7 mg (88%); off-white solid; mp = 109.3-113.1°C; IR (cm^{-1}) *v*: 3058, 1620, 1557, 1501, 1444, 1375, 1103, 911, 759, 672. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.74 – 8.44 (m, 2H), 8.17 (d, *J* = 8.2 Hz, 1H), 8.05 (d, *J* = 8.4 Hz, 1H), 7.83 (t, *J* = 7.8 Hz, 1H), 7.52 (d, *J* = 6.9 Hz, 4H), 4.31 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 167.3, 160.0, 133.8, 130.9, 128.7, 128.5, 127.5, 126.7, 123.5, 115.2, 54.4. HRMS: m/z (ESI) calcd for $C_{15}H_{13}N_2O$ $[M+H]^+$: 237.1022, found: 237.1026.

4-ethoxy-2-phenylthieno[2,3-d]pyrimidine (3ap)[2]



20.2 mg (79%); off-white solid; mp = 74.6-83.1°C; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.53 (dd, *J* = 7.6, 2.1 Hz, 2H), 7.84 (d, *J* = 5.4 Hz, 1H), 7.66 – 7.37 (m, 4H), 4.78 (q, *J* = 7.1 Hz, 2H), 1.55 (t, *J* = 7.1 Hz, 3H).^{13}C NMR (101 MHz, Chloroform-*d*) δ 164.1, 162.7, 161.1, 137.8, 133.9, 130.3, 128.4, 128.3, 124.7, 115.9, 62.9, 14.5.

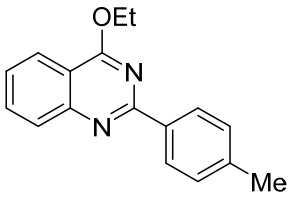


8-ethoxy-6-phenyl-[1,3]dioxolo[4,5-g]quinazoline (3aq)

23.8 mg (81%); off-white solid; mp = 56.2-62.1 °C; IR (cm^{-1}) *v*: 3066, 2976, 2921, 1620, 1573, 1497, 1324, 1105, 760, 680. ^{1}H NMR (400

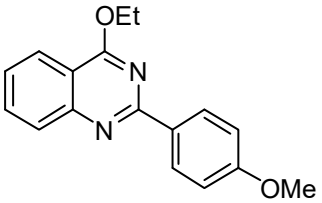
MHz, Chloroform-*d*) δ 8.50 (dd, *J* = 6.8, 3.0 Hz, 2H), 7.69 (d, *J* = 8.5 Hz, 1H), 7.40 (p, *J* = 3.5 Hz, 3H), 7.03 (d, *J* = 8.5 Hz, 1H), 6.18 (s, 2H), 4.67 (q, *J* = 7.1 Hz, 2H), 1.47 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 166.4, 160.4, 150.6, 140.4, 137.8, 130.7, 128.6, 128.3, 118.4, 111.4, 109.5, 102.8, 62.9, 14.4. HRMS: m/z (ESI) calcd for: $C_{17}H_{15}N_2O_3[M+H]^+$:295.1083, found: 295.1084.

4-ethoxy-2-(p-tolyl)quinazoline (3ba)[2]



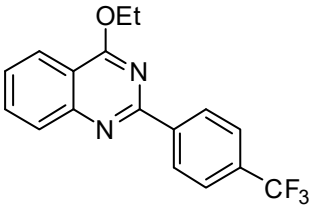
22.9 mg (87%); off-white solid; mp = 74.6-78.5 ºC; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.57 – 8.41 (m, 2H), 8.16 (ddd, *J* = 8.2, 1.6, 0.7 Hz, 1H), 8.00 (d, *J* = 8.4 Hz, 1H), 7.80 (ddd, *J* = 8.5, 7.0, 1.5 Hz, 1H), 7.49 (ddd, *J* = 8.1, 6.9, 1.1 Hz, 1H), 7.37 – 7.28 (m, 2H), 4.78 (q, *J* = 7.1 Hz, 2H), 2.44 (s, 3H), 1.57 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 166.6, 160.2, 151.7, 140.7, 135.4, 133.4, 129.2, 128.5, 127.7, 126.1, 123.5, 115.3, 62.8, 21.5, 14.4.

4-ethoxy-2-(4-methoxyphenyl)quinazoline (3ca)[2]



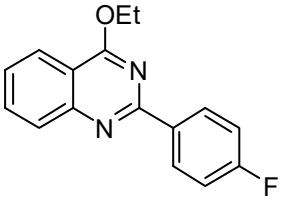
22.4 mg (80%); off-white solid; mp = 68.9-75.4 ºC; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.64 – 8.45 (m, 2H), 8.14 (dd, *J* = 8.1, 1.4 Hz, 1H), 7.96 (d, *J* = 8.5 Hz, 1H), 7.78 (ddd, *J* = 8.5, 6.9, 1.5 Hz, 1H), 7.47 (ddd, *J* = 8.0, 6.9, 1.1 Hz, 1H), 7.12 – 6.93 (m, 2H), 4.76 (q, *J* = 7.1 Hz, 2H), 3.89 (s, 3H), 1.57 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 166.6, 161.7, 159.9, 151.8, 133.4, 130.8, 130.1, 127.5, 125.9, 123.5, 115.1, 113.7, 62.8, 55.4, 14.4.

4-ethoxy-2-(4-(trifluoromethyl)phenyl)quinazoline (3da)[2]

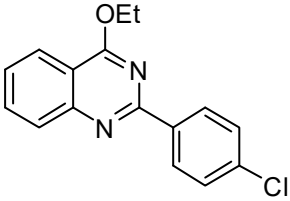


25.7 mg (81%); off-white solid; mp = 124.8-128.7 ºC; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.75 – 8.61 (m, 2H), 8.19 (dd, *J* = 8.2, 1.4 Hz, 1H), 8.00 (d, *J* = 8.4 Hz, 1H), 7.84 (ddd, *J* = 8.5, 6.9, 1.5 Hz, 1H), 7.75 (d, *J* = 8.2 Hz, 2H), 7.55 (ddd, *J* = 8.1, 6.9, 1.2 Hz, 1H), 4.78 (q, *J* = 7.1 Hz, 2H), 1.59 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 166.9, 158.6, 151.5, 141.4, 133.7, 132.0 (d, *J* = 30 Hz), 128.7, 127.9, 126.9, 125.3 (q, *J* = 3 Hz), 124.2 (q, *J* = 270 Hz), 123.6, 115.5, 63.1, 14.4.

4-ethoxy-2-(4-fluorophenyl)quinazoline (3ea)[2]



24.9 mg (93%); off-white solid; mp = 107.3-111.9 ºC; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.68 – 8.45 (m, 2H), 8.17 (dd, *J* = 8.2, 1.5 Hz, 1H), 7.99 (d, *J* = 8.4 Hz, 1H), 7.81 (ddd, *J* = 8.5, 6.9, 1.6 Hz, 1H), 7.51 (ddd, *J* = 8.1, 6.9, 1.2 Hz, 1H), 7.23 – 7.07 (m, 2H), 4.77 (q, *J* = 7.1 Hz, 2H), 1.58 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 166.8, 164.6 (d, *J* = 250 Hz), 159.1, 151.5, 134.2 (d, *J* = 10 Hz), 133.6, 130.5 (d, *J* = 10 Hz), 127.6, 126.4, 123.6, 115.3 (d, *J* = 20 Hz), 63.0, 14.4.

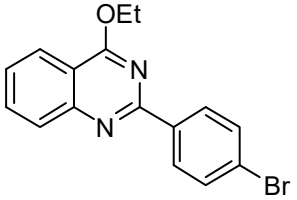


2-(4-chlorophenyl)-4-ethoxyquinazoline (3fa)[2]

24.2 mg (86%); off-white solid; mp = 109.3-113.1ºC; ^{1}H NMR (400

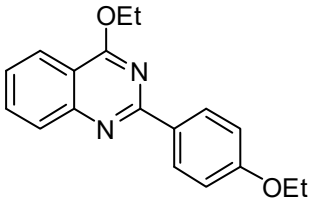
MHz, Chloroform-*d*) δ 8.63 – 8.43 (m, 2H), 8.16 (dd, *J* = 8.2, 1.4 Hz, 1H), 7.97 (d, *J* = 8.4 Hz, 1H), 7.81 (ddd, *J* = 8.5, 7.0, 1.5 Hz, 1H), 7.60 – 7.40 (m, 3H), 4.76 (q, *J* = 7.1 Hz, 2H), 1.57 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 166.77, 159.02, 151.61, 136.63, 133.57, 129.80, 128.59, 127.78, 126.52, 123.58, 115.35, 62.97, 14.4.

2-(4-bromophenyl)-4-ethoxyquinazoline (3ga)[2]



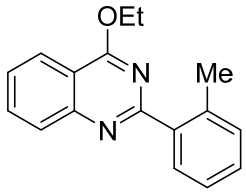
23.6 mg (72%); off-white solid; mp = 109.3-113.1°C; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.46 (d, *J* = 8.3 Hz, 2H), 8.17 (dd, *J* = 8.2, 1.4 Hz, 1H), 7.97 (d, *J* = 8.4 Hz, 1H), 7.81 (ddd, *J* = 8.4, 7.0, 1.4 Hz, 1H), 7.62 (d, *J* = 8.3 Hz, 2H), 7.56 – 7.46 (m, 1H), 4.76 (q, *J* = 7.1 Hz, 2H), 1.57 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 166.8, 159.1, 151.6, 137.1, 133.6, 131.6, 130.1, 127.8, 126.5, 125.2, 123.6, 115.4, 63.0, 14.4.

4-ethoxy-2-(4-ethoxyphenyl)quinazoline (3ha)



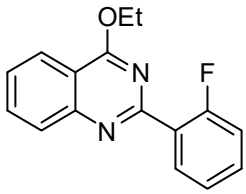
21.2 mg (72%); off-white solid; mp = 102.5-109.7°C; IR (cm^{-1}) *v*:3070, 2980, 2936, 1601, 1573, 1421, 1326, 1249, 1153, 760, 659, 541. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.60 – 8.48 (m, 2H), 8.20 – 8.09 (m, 1H), 7.97 (d, *J* = 8.4 Hz, 1H), 7.78 (ddd, *J* = 8.4, 6.9, 1.5 Hz, 1H), 7.46 (ddt, *J* = 7.9, 6.8, 0.9 Hz, 1H), 7.08 – 6.94 (m, 2H), 4.84 – 4.68 (m, 2H), 4.12 (q, *J* = 7.0 Hz, 2H), 1.57 (t, *J* = 7.1 Hz, 3H), 1.46 (t, *J* = 7.0 Hz, 3H).^{13}C NMR (101 MHz, Chloroform-*d*) δ 166.6, 161.2, 159.9, 151.6, 133.4, 130.5, 130.1, 127.4, 125.8, 123.5, 115.0, 114.2, 63.6, 62.8, 14.8, 14.4. HRMS: m/z (ESI) calcd. for $[C_{18}H_{19}N_2O_2+H]^+$: 295.1447 , found: 295.1447.

4-ethoxy-2-(o-tolyl)quinazoline (3ia)[2]



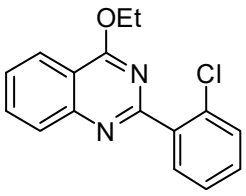
11.9 mg (45%); off-white solid; mp = 109.3-113.1°C; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.21 (ddd, *J* = 8.1, 1.5, 0.7 Hz, 1H), 8.00 (dt, *J* = 8.4, 0.9 Hz, 1H), 7.94 (dd, *J* = 7.4, 1.8 Hz, 1H), 7.83 (ddd, *J* = 8.5, 7.0, 1.5 Hz, 1H), 7.55 (ddd, *J* = 8.2, 6.9, 1.2 Hz, 1H), 7.33 (tdd, *J* = 8.7, 4.7, 2.2 Hz, 3H), 4.71 (q, *J* = 7.1 Hz, 2H), 2.65 (s, 3H), 1.54 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 166.3, 163.1, 151.4, 138.7, 137.3, 133.4, 131.2, 130.5, 129.2, 127.8, 126.5, 125.8, 123.4, 114.7, 63.0, 21.4, 14.5.

4-ethoxy-2-(2-fluorophenyl)quinazoline (3ja)[2]



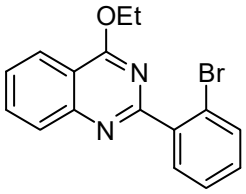
22.8 mg (85%); off-white solid; mp = 109.3-113.1°C; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.17 (td, *J* = 8.0, 4.4 Hz, 2H), 8.01 (d, *J* = 8.4 Hz, 1H), 7.86 – 7.76 (m, 1H), 7.57 – 7.49 (m, 1H), 7.43 (tdd, *J* = 7.5, 4.8, 1.8 Hz, 1H), 7.27 (t, *J* = 7.5 Hz, 1H), 7.20 (dd, *J* = 11.1, 8.2 Hz, 1H), 4.72 (q, *J* = 7.1 Hz, 2H), 1.54 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 166.6, 161.4 (d, *J* = 254 Hz), 158.8 (d, *J* = 5 Hz), 151.6, 133.5, 132.0, 131.9, 131.3 (d, *J* = 9 Hz), 128.0, 127.3 (d, *J* = 10 Hz), 126.81, 124.0 (d, *J* = 4 Hz), 123.47, 116.8 (d, *J* = 23 Hz), 115.1, 63.1, 14.4.

2-(2-chlorophenyl)-4-ethoxyquinazoline (3ka)[2]



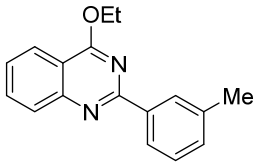
20.4 mg (72%); off-white solid; mp = 80.9-87.5°C; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.23 (dd, *J* = 8.1, 1.4 Hz, 1H), 8.04 (d, *J* = 8.4 Hz, 1H), 7.98 – 7.80 (m, 2H), 7.59 (ddd, *J* = 8.1, 7.0, 1.0 Hz, 1H), 7.55 – 7.48 (m, 1H), 7.43 – 7.35 (m, 2H), 4.72 (q, *J* = 7.1 Hz, 2H), 1.54 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 166.6, 161.0, 151.1, 138.2, 133.7, 133.0, 131.7, 130.6, 130.2, 127.7, 127.1, 126.8, 123.6, 115.1, 63.4, 14.5.

2-(2-bromophenyl)-4-ethoxyquinazoline (3la)[2]



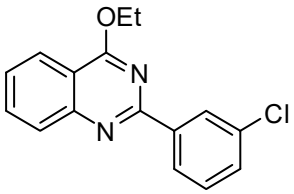
14.4 mg (44%); off-white solid; mp = 90.8-95.8°C; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.23 (dd, *J* = 8.2, 1.4 Hz, 1H), 8.04 (d, *J* = 8.4 Hz, 1H), 7.91 – 7.75 (m, 2H), 7.71 (dd, *J* = 7.9, 1.2 Hz, 1H), 7.59 (ddd, *J* = 8.1, 7.0, 1.2 Hz, 1H), 7.44 (td, *J* = 7.5, 1.2 Hz, 1H), 7.30 (td, *J* = 7.7, 1.8 Hz, 1H), 4.74 (q, *J* = 7.1 Hz, 2H), 1.54 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 166.6, 161.8, 133.8, 133.8, 131.7, 130.4, 127.6, 127.4, 127.2, 123.6, 121.9, 115.1, 63.6, 14.5.

4-ethoxy-2-(m-tolyl)quinazoline (3ma)[2]



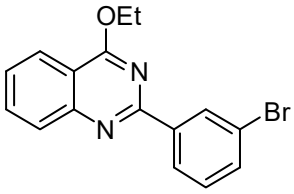
19.1 mg (72%); off-white solid; mp = 69.6-71.2°C; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.39 (dd, *J* = 9.2, 1.9 Hz, 2H), 8.17 (dd, *J* = 8.2, 1.4 Hz, 1H), 8.02 (d, *J* = 8.4 Hz, 1H), 7.81 (ddd, *J* = 8.5, 6.9, 1.5 Hz, 1H), 7.50 (ddd, *J* = 8.1, 7.0, 1.1 Hz, 1H), 7.41 (t, *J* = 7.6 Hz, 1H), 7.35 – 7.27 (m, 1H), 4.79 (q, *J* = 7.1 Hz, 2H), 2.49 (s, 3H), 1.58 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 166.7, 160.3, 151.7, 138.0, 133.4, 131.4, 129.0, 128.3, 127.8, 126.3, 125.7, 123.5, 115.3, 62.9, 21.6, 14.4.

2-(3-chlorophenyl)-4-ethoxyquinazoline (3na)[2]



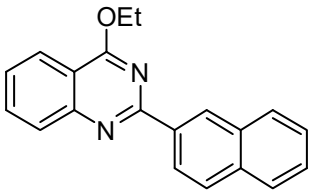
25.6 mg (90%); off-white solid; mp = 78.9-84.1°C; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.56 (d, *J* = 2.1 Hz, 1H), 8.47 (dt, *J* = 6.8, 1.8 Hz, 1H), 8.16 (dd, *J* = 8.1, 1.4 Hz, 1H), 7.97 (d, *J* = 8.4 Hz, 1H), 7.81 (ddd, *J* = 8.5, 6.9, 1.6 Hz, 1H), 7.52 (ddd, *J* = 8.1, 6.9, 1.1 Hz, 1H), 7.49 – 7.31 (m, 2H), 4.76 (q, *J* = 7.1 Hz, 2H), 1.57 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (101 MHz, Chloroform-d) δ 166.8, 158.6, 151.5, 140.0, 134.5, 133.6, 130.3, 129.6, 128.5, 127.8, 126.6, 126.6, 123.5, 115.4, 63.0, 14.4.

2-(3-bromophenyl)-4-ethoxyquinazoline (3oa)[2]



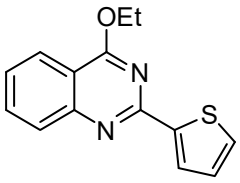
23.3 mg (71%); off-white solid; mp = 109.3-113.1°C; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.23 (ddd, *J* = 8.2, 1.5, 0.7 Hz, 1H), 8.03 (d, *J* = 8.4 Hz, 1H), 7.95 – 7.77 (m, 2H), 7.71 (dd, *J* = 8.0, 1.1 Hz, 1H), 7.59 (ddd, *J* = 8.1, 7.0, 1.1 Hz, 1H), 7.44 (td, *J* = 7.5, 1.2 Hz, 1H), 7.29 (ddd, *J* = 8.0, 7.4, 1.8 Hz, 1H), 4.73 (q, *J* = 7.1 Hz, 2H), 1.54 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 166.6, 161.9, 151.2, 140.2, 133.7, 133.7, 131.6, 130.2, 127.8, 127.4, 127.0, 123.6, 121.9, 115.1, 63.4, 14.5.

4-ethoxy-2-(naphthalen-2-yl)quinazoline (3pa)[2]



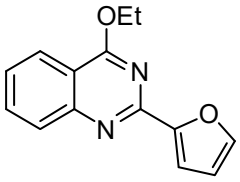
26.4 mg (88%); off-white solid; mp = 109.3-113.1°C; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.11 (d, *J* = 1.6 Hz, 1H), 8.71 (dd, *J* = 8.6, 1.7 Hz, 1H), 8.20 (dd, *J* = 8.2, 1.4 Hz, 1H), 8.07 – 8.01 (m, 2H), 7.96 (d, *J* = 8.7 Hz, 1H), 7.92 – 7.87 (m, 1H), 7.83 (ddd, *J* = 8.4, 7.0, 1.5 Hz, 1H), 7.56 – 7.49 (m, 3H), 4.85 (q, *J* = 7.1 Hz, 2H), 1.62 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 166.7, 160.1, 151.8, 135.6, 134.7, 133.5, 133.3, 129.2, 128.7, 128.0, 127.8, 127.7, 126.9, 126.4, 126.1, 125.5, 123.6, 115.4, 63.0, 14.5.

4-ethoxy-2-(thiophen-2-yl)quinazoline (3qa)[2]



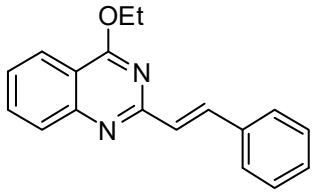
21.5 mg (84%); off-white solid; mp = 109.3-113.1°C; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.24 (dd, *J* = 3.7, 1.3 Hz, 1H), 8.13 (dd, *J* = 8.2, 1.4 Hz, 1H), 8.02 (d, *J* = 8.4 Hz, 1H), 7.82 (ddd, *J* = 8.5, 7.0, 1.5 Hz, 1H), 7.58 – 7.46 (m, 2H), 7.19 (dd, *J* = 5.0, 3.7 Hz, 1H), 4.75 (q, *J* = 7.1 Hz, 2H), 1.57 (t, *J* = 7.1 Hz, 3H).^{13}C NMR (101 MHz, Chloroform-*d*) δ 166.9, 156.4, 149.8, 142.4, 134.3, 130.8, 130.2, 128.6, 126.6, 126.2, 123.7, 114.9, 63.7, 14.3.

4-ethoxy-2-(furan-2-yl)quinazoline (3ra)[2]



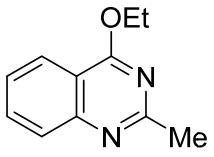
20.9 mg (87%); off-white solid; mp = 78.1-86.5°C; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.13 (dd, *J* = 8.1, 1.5 Hz, 1H), 8.03 (d, *J* = 8.4 Hz, 1H), 7.79 (ddd, *J* = 8.5, 7.0, 1.5 Hz, 1H), 7.66 (dd, *J* = 1.7, 0.9 Hz, 1H), 7.48 (ddd, *J* = 8.1, 7.0, 1.1 Hz, 1H), 7.38 (d, *J* = 3.4 Hz, 1H), 6.57 (dd, *J* = 3.4, 1.8 Hz, 1H), 4.71 (q, *J* = 7.1 Hz, 2H), 1.54 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 166.7, 153.1, 152.6, 151.3, 145.1, 133.7, 127.7, 126.3, 123.6, 115.4, 113.9, 112.0, 63.1, 14.3.

(E)-4-ethoxy-2-styrylquinazoline (3sa)



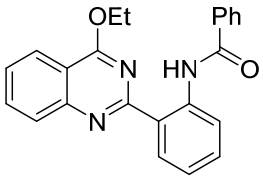
24.3 mg (88%); off-white solid; mp = 72.1-74.5°C; IR (cm^{-1}) *v*: 3058, 2979, 1614, 1573, 1325, 1102, 970, 765, 678. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.15 (dd, *J* = 8.2, 1.4 Hz, 1H), 8.05 (d, *J* = 15.8 Hz, 1H), 7.91 (d, *J* = 8.4 Hz, 1H), 7.79 (ddd, *J* = 8.5, 7.0, 1.5 Hz, 1H), 7.66 (dd, *J* = 7.3, 1.7 Hz, 2H), 7.49 (ddd, *J* = 8.2, 6.9, 1.2 Hz, 1H), 7.40 (dd, *J* = 8.2, 6.5 Hz, 2H), 7.37 – 7.27 (m, 2H), 4.75 (q, *J* = 7.1 Hz, 2H), 1.57 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 166.2, 160.4, 151.3, 138.2, 136.3, 133.6, 128.9, 128.8, 128.1, 127.7, 127.2, 126.3, 123.7, 115.4, 62.9, 14.4. HRMS: m/z (ESI) calcd. for $[C_{24}H_{21}N_2O+H]^+$: 353.1654 found: 353.1652.

4-ethoxy-2-methylquinazoline (3ta)



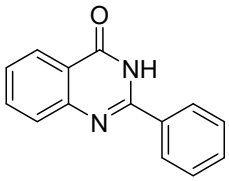
12.7 mg (68%); off-white solid; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.12 (d, *J* = 8.1 Hz, 1H), 7.82 (d, *J* = 8.3 Hz, 1H), 7.76 (t, *J* = 7.6 Hz, 1H), 7.46 (t, *J* = 7.5 Hz, 1H), 4.61 (q, *J* = 7.1 Hz, 2H), 2.71 (s, 3H), 1.50 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 166.5, 163.9, 151.3, 133.3, 126.8, 125.9, 123.4, 114.7, 62.7, 26.5, 14.4. HRMS: m/z (ESI) calcd. for $[C_{11}H_{12}N_2O+Na]^+$: 211.0842 , found: 211.0846.

***N*-(2-(4-ethoxyquinazolin-2-yl)phenyl)benzamide (4a)**[2d]



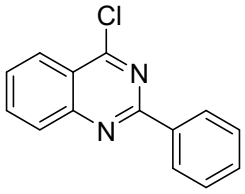
26.7 mg (73%); yellow solid; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 14.24 (s, 1H), 9.00 (dd, *J* = 8.5, 1.2 Hz, 1H), 8.75 (dd, *J* = 8.1, 1.6 Hz, 1H), 8.22 – 8.11 (m, 3H), 7.84 – 7.75 (m, 2H), 7.65 – 7.49 (m, 5H), 7.25 – 7.17 (m, 1H), 4.91 – 4.63 (m, 2H), 1.57 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 166.6, 166.2, 160.8, 149.6, 140.6, 136.6, 134.0, 132.0, 131.7, 131.0, 128.6, 127.9, 127.0, 126.2, 123.8, 123.1, 122.8, 120.8, 114.9, 63.4, 14.4.

2-phenylquinazolin-4(3H)-one (5)[3]



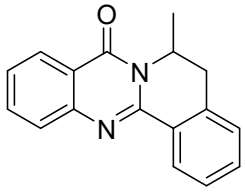
40.0 mg (90%); white solid; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 11.53 (s, 1H), 8.33 (dd, *J* = 8.0, 1.5 Hz, 1H), 8.29 – 8.21 (m, 2H), 7.89 – 7.76 (m, 2H), 7.59 (p, *J* = 3.4, 2.8 Hz, 3H), 7.51 (ddd, *J* = 8.2, 6.8, 1.4 Hz, 1H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 163.7, 151.7, 149.4, 134.9, 132.7, 131.7, 129.1, 128.0, 127.4, 126.8, 126.4, 120.9.

4-chloro-2-phenylquinazoline (6)[3]



18.3 mg (76%); yellow solid; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.60 (dd, *J* = 6.7, 3.0 Hz, 2H), 8.26 (dd, *J* = 8.4, 1.4 Hz, 1H), 8.10 (d, *J* = 8.4 Hz, 1H), 7.94 (ddd, *J* = 8.5, 6.9, 1.4 Hz, 1H), 7.67 (ddd, *J* = 8.1, 6.8, 1.1 Hz, 1H), 7.53 (dd, *J* = 5.0, 2.0 Hz, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 162.5, 160.1, 151.9, 136.7, 134.8, 131.1, 128.9, 128.7, 128.6, 128.2, 125.8, 122.5.

6-methyl-5,6-dihydro-8H-isoquinolino[1,2-b]quinazolin-8-one (7)[4]

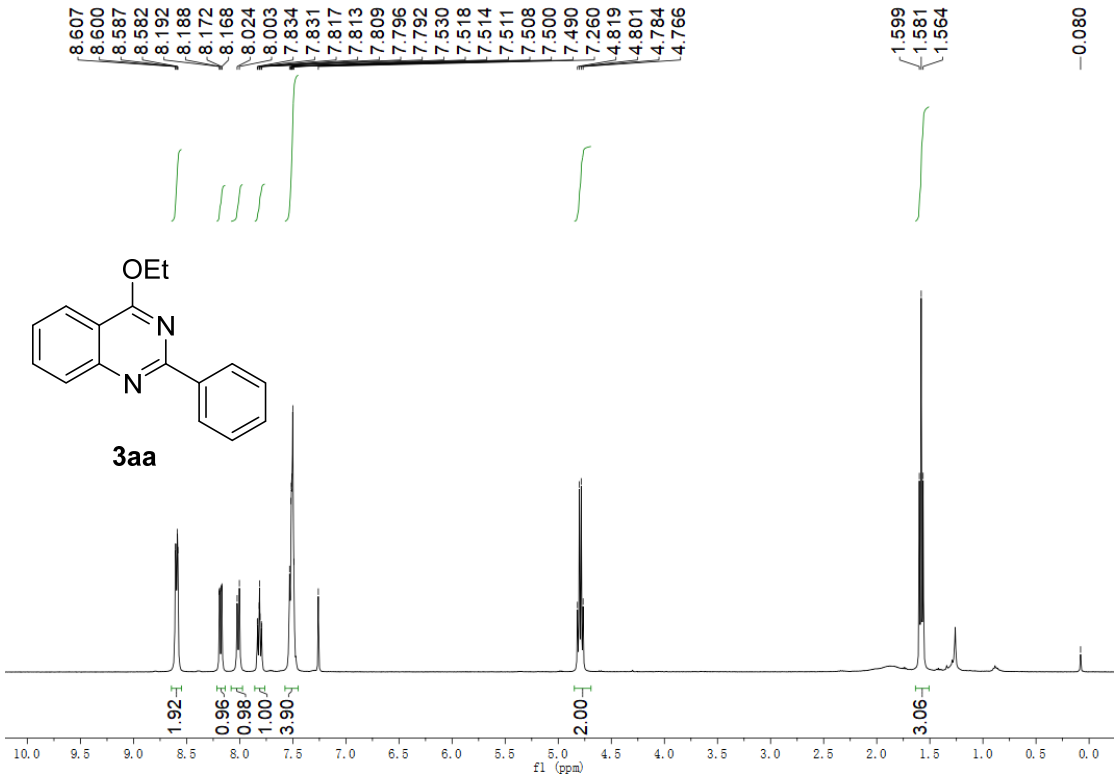


17.5 mg (67%); white solid; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.42 (dd, *J* = 7.7, 1.5 Hz, 1H), 8.27 – 8.19 (m, 1H), 7.68 (dd, *J* = 6.3, 1.6 Hz, 2H), 7.47 – 7.32 (m, 3H), 7.24 – 7.15 (m, 1H), 5.49 (qd, *J* = 6.7, 1.8 Hz, 1H), 3.30 (dd, *J* = 16.0, 5.9 Hz, 1H), 2.83 (dd, *J* = 16.0, 1.7 Hz, 1H), 1.17 (d, *J* = 6.7 Hz, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 161.3, 148.6, 147.8, 134.8, 134.2, 131.9, 129.0, 128.6, 127.9, 127.6, 126.8, 126.5, 120.9, 45.4, 33.6, 18.0.

Reference

(1) G. D. Ju, G. B. Li, G. W. Qian, J. Y. Zhang and Y. S. Zhao., *Org.Lett.* 2019, **21**, 7333−7336.
(2) (a) H. Wang, M. M. Lorion, and L. Ackermann. *Angew. Chem., Int. Ed.*, 2016, **55**, 10386−10390; (b) J. Wang, S. K. Zha, K. H. Chen, F. F. Zhang, C. Song and J. Zhu. *Org. Lett.*, 2016, **18**, 2062−2065; (c) X. M. Wang, A. Lerchen, and F. Glorius. *Org. Lett.*, 2016, **18**, 2090−2093; (d) F. Wang, H. Wang, Q. Wang, S. J. Yu and X. W. Li. *Org. Lett.*, 2016, **18**, 1306−1309.
(3) X. Y. Wang and N. Jiao. *Org. Lett.*, 2016, **18**, 2150−2153.
(4) G. Bairy, S. Das, H. M. Begam and R. Jana. *Org. Lett.* 2018, **20**, 7107−7112.

6 ^{1}H and ^{13}C NMR spectra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8.168
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7.813
7.809
7.796
7.792
7.530
7.518
7.514
7.511
7.508
7.500
7.490
7.260
4.819
4.801
4.784
4.766
1.599
1.581
1.564
0.080
OEt
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N
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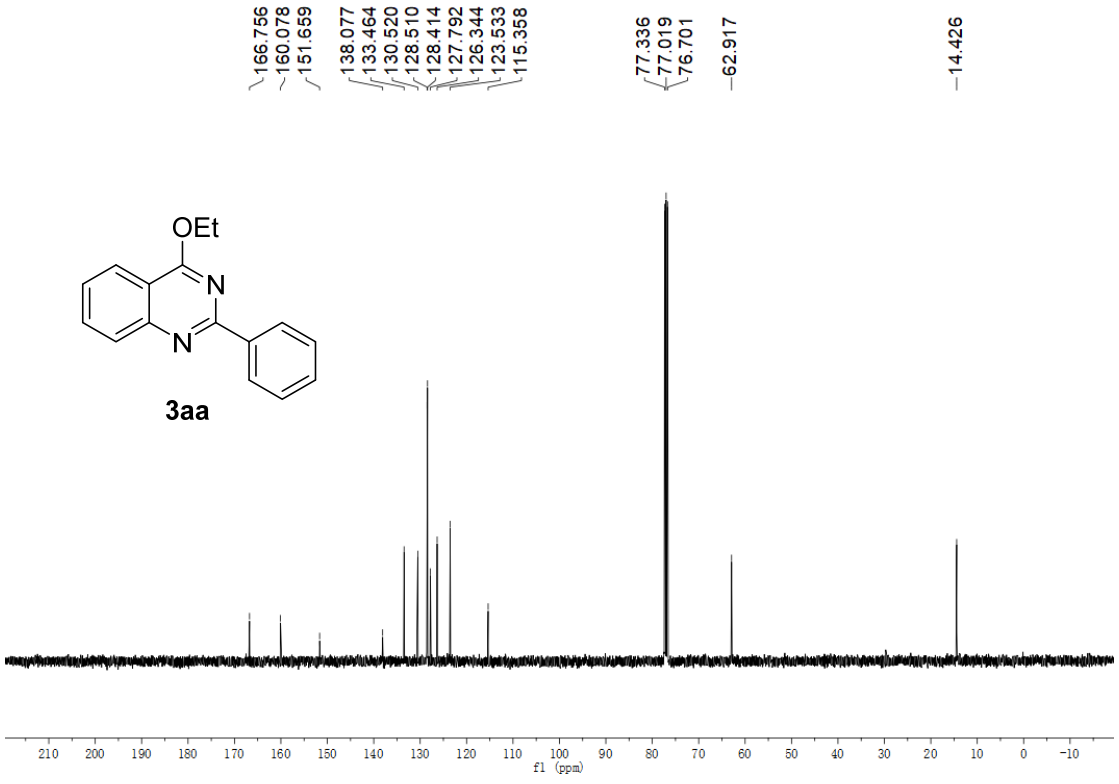
0.96
0.98
1.00
3.90
2.00
3.06
f1 (ppm)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76.701
62.917
14.426
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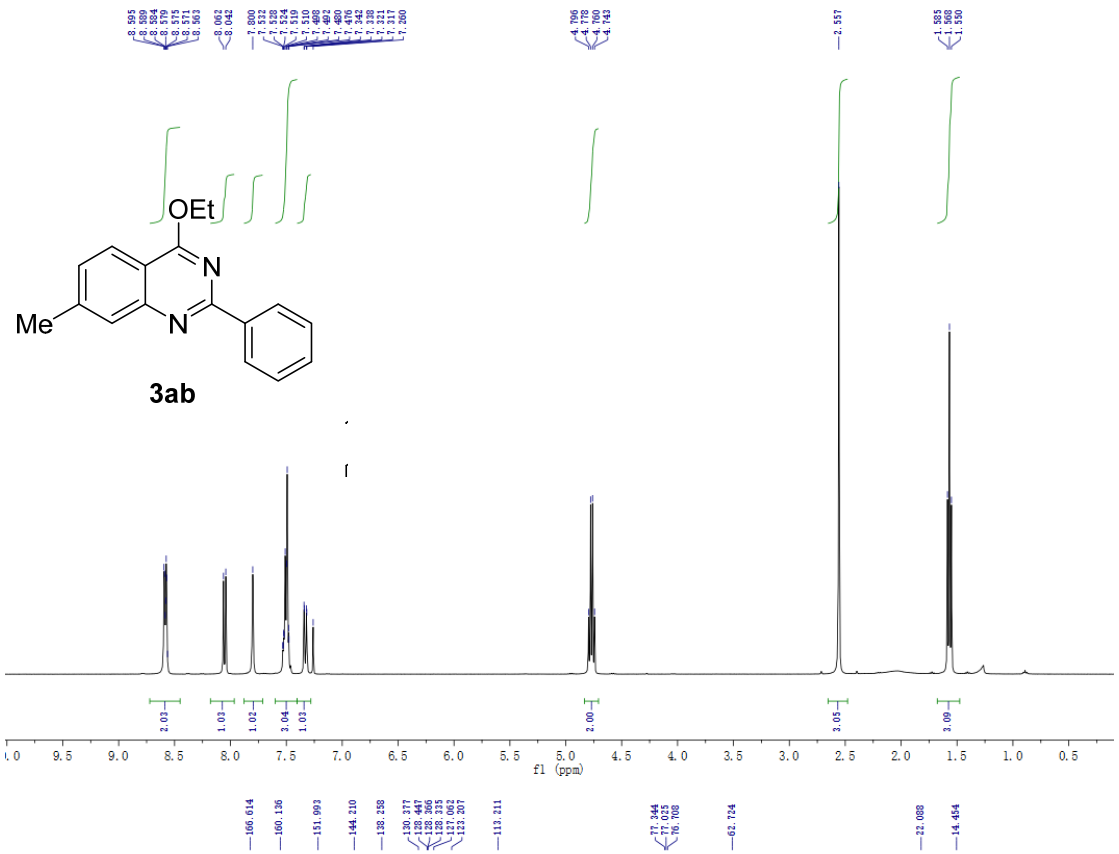
N
N
3aa
f1 (ppm)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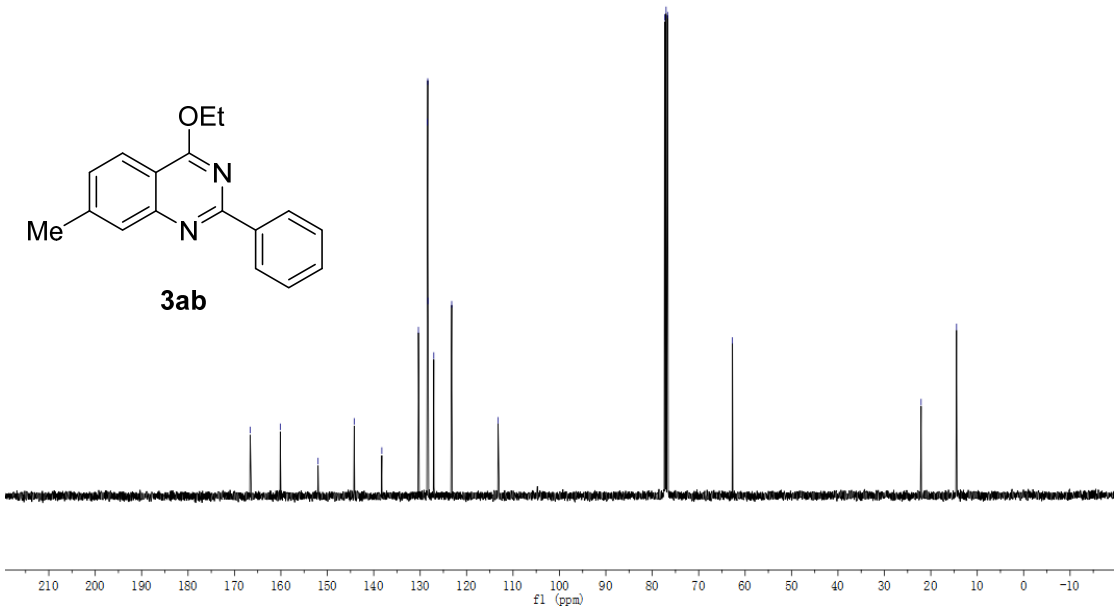
f1 (ppm)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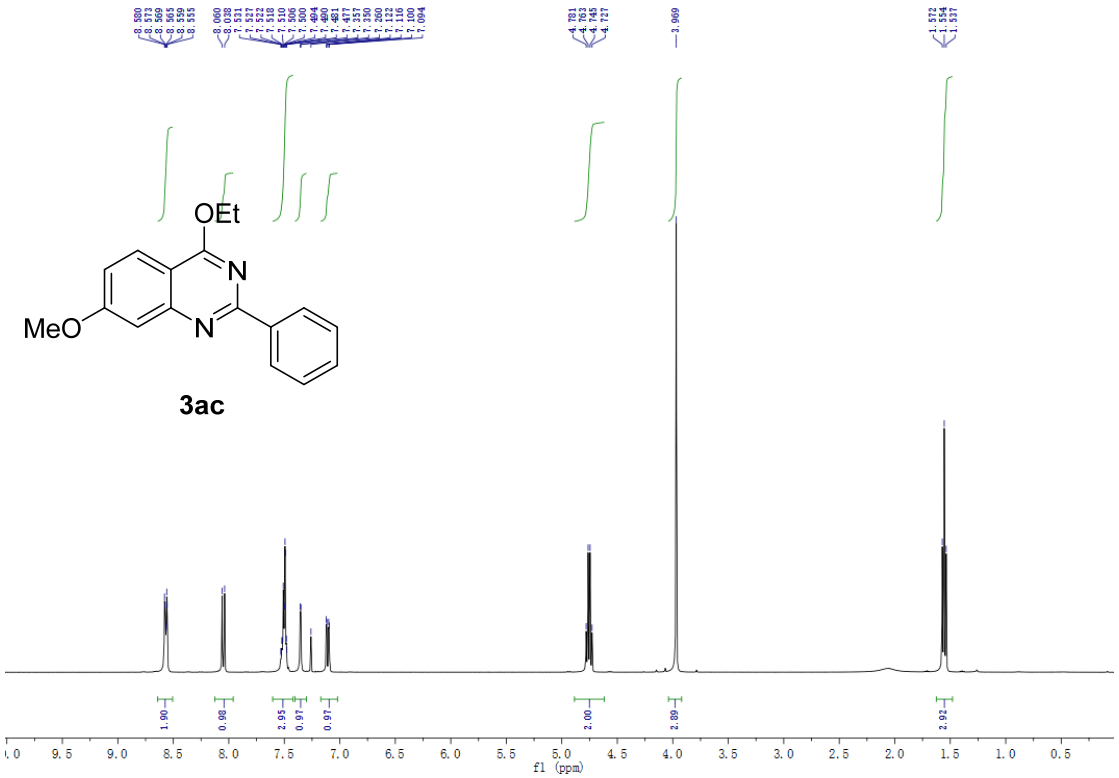
Me
N
3ab
f1 (ppm)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MeO
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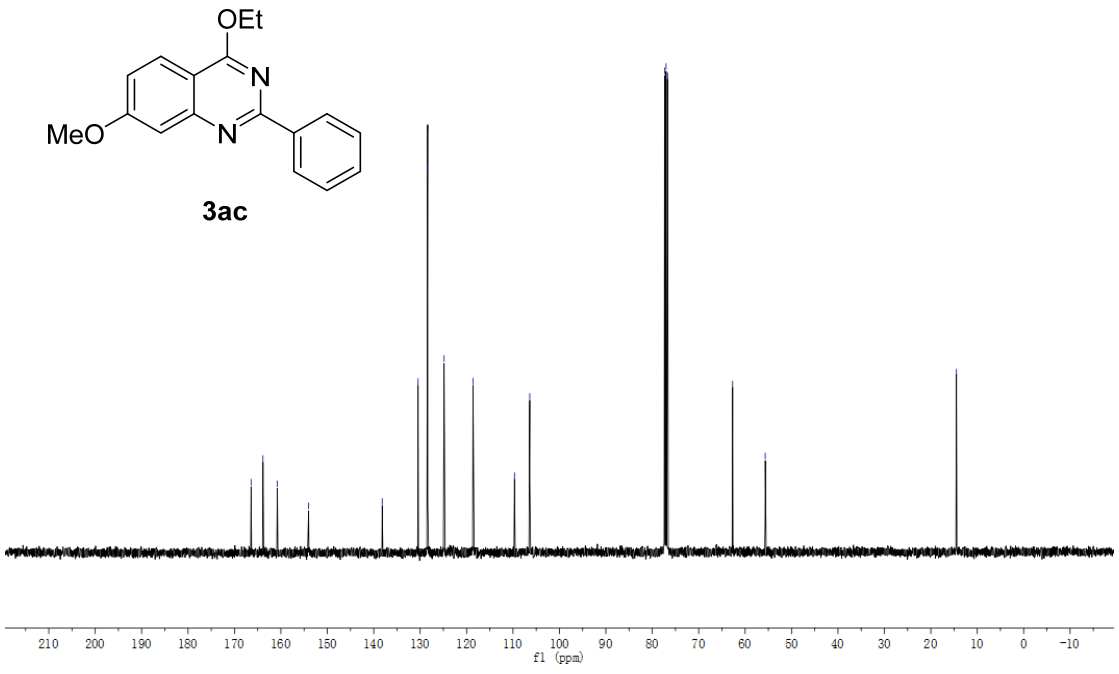
f1 (ppm)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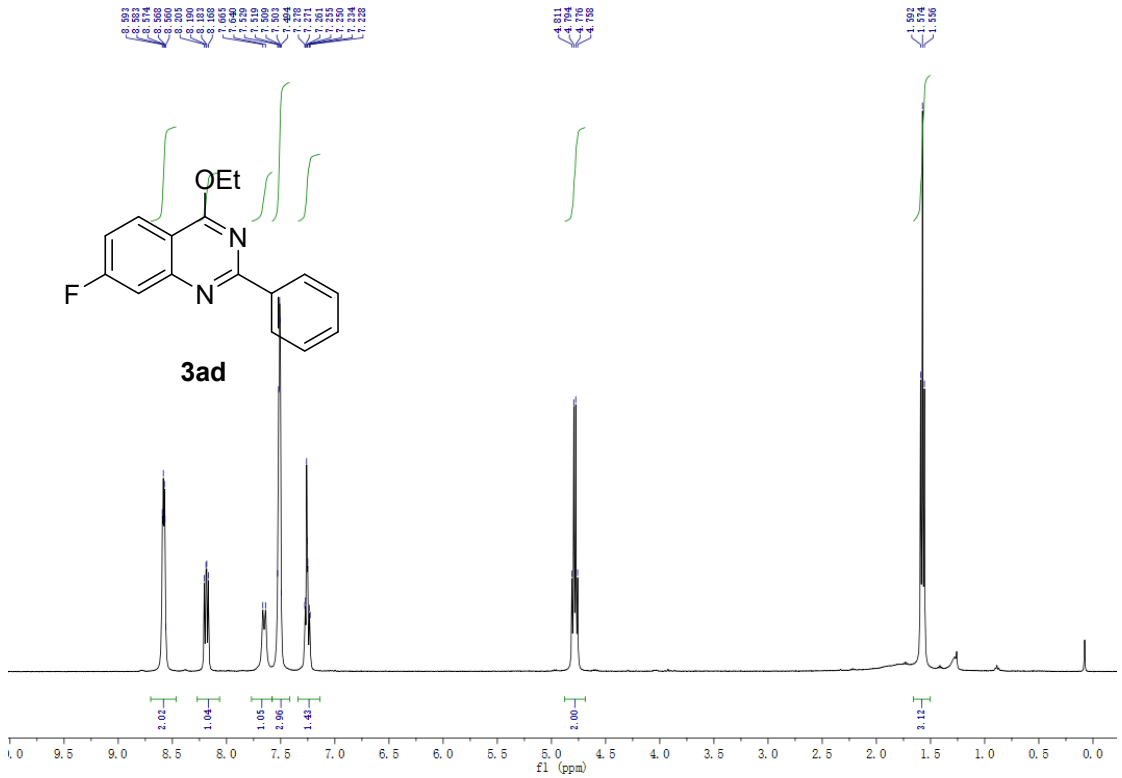
MeO
N
3ac
f1 (ppm)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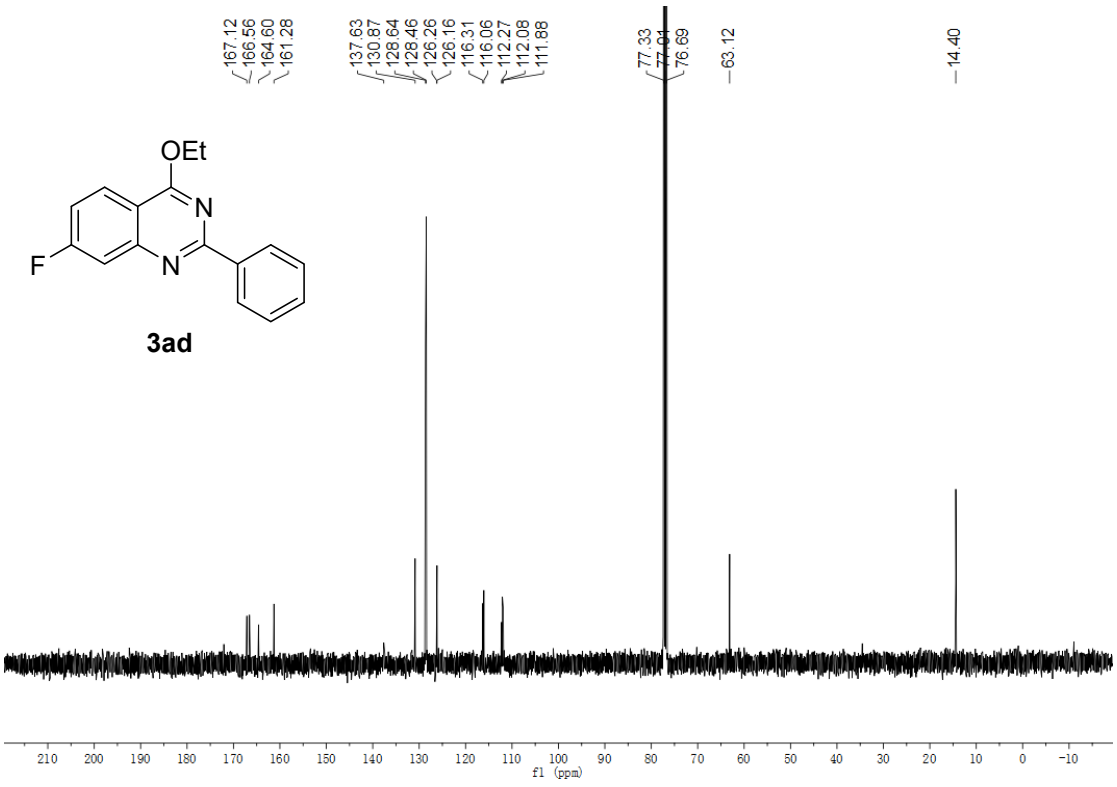
F
N
3ad
f1 (ppm)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F
N
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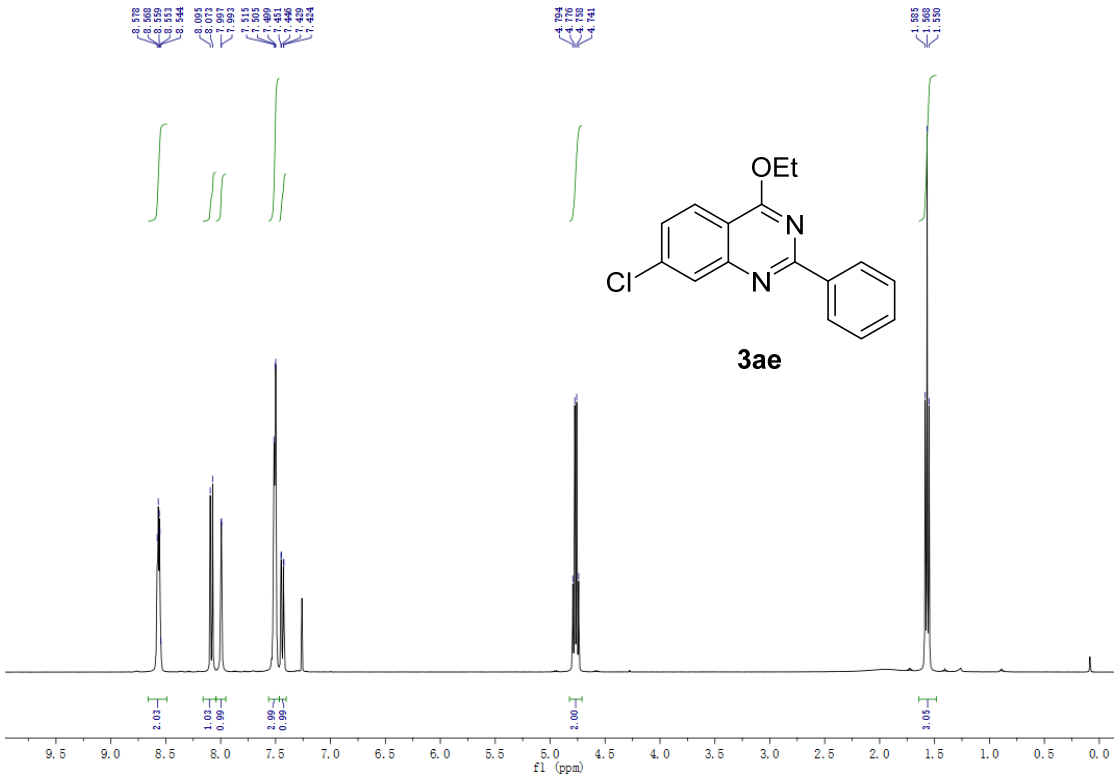
f1 (ppm)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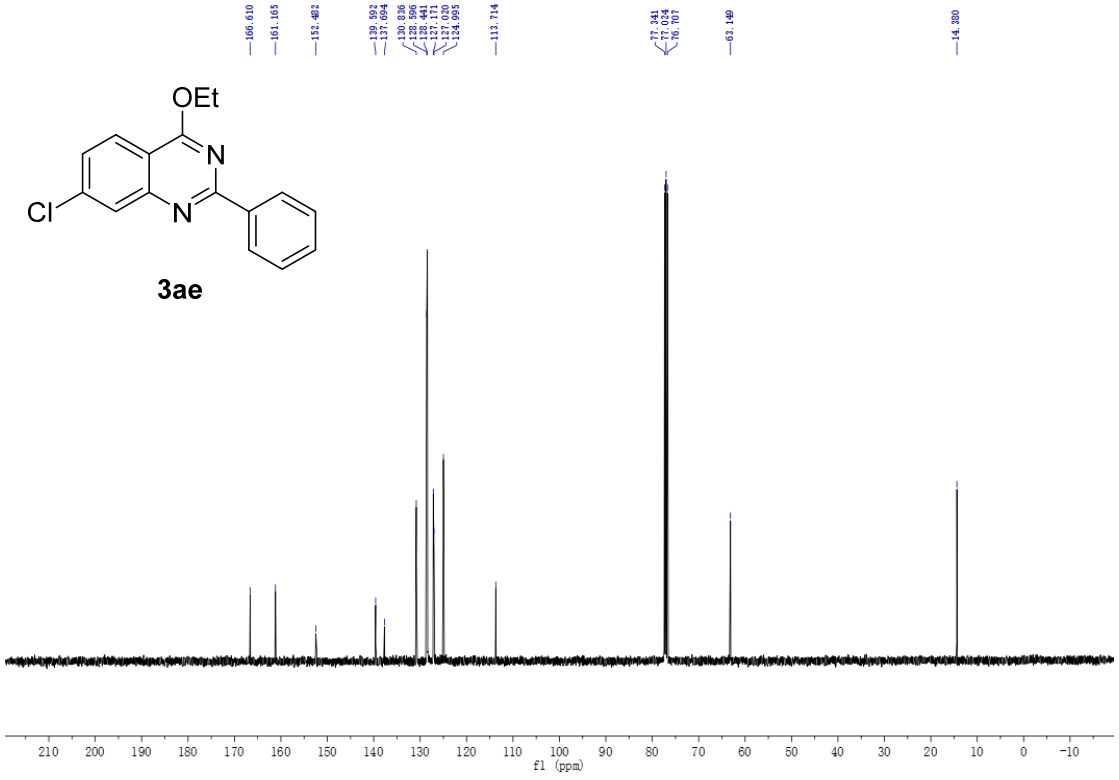
N
Cl
N
3ae
fl (ppm)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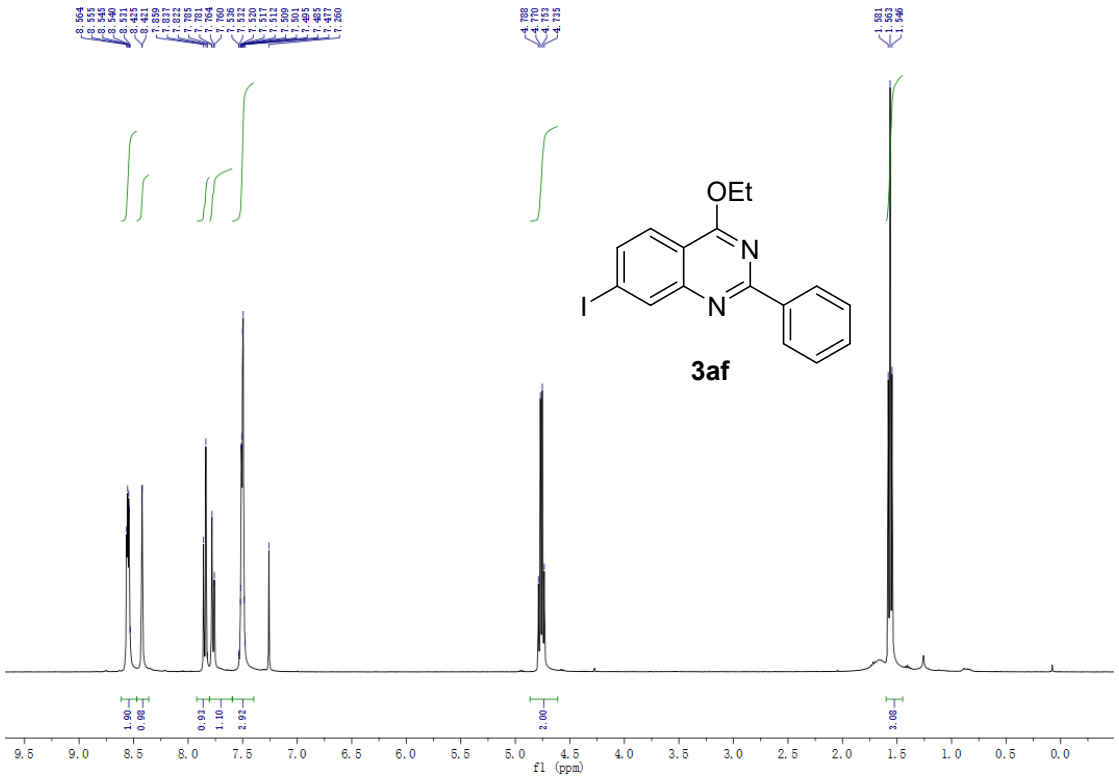
Cl
N
3ae
fl (ppm)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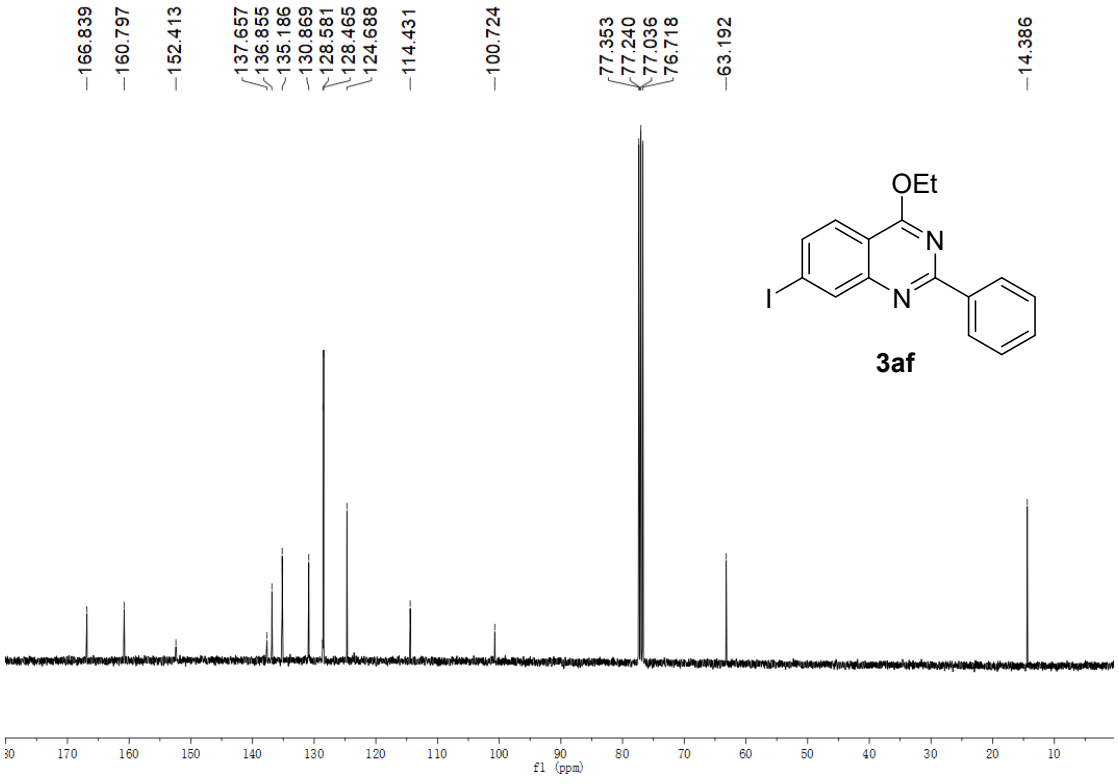
N
N
I
3af
f1 (ppm)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77.036
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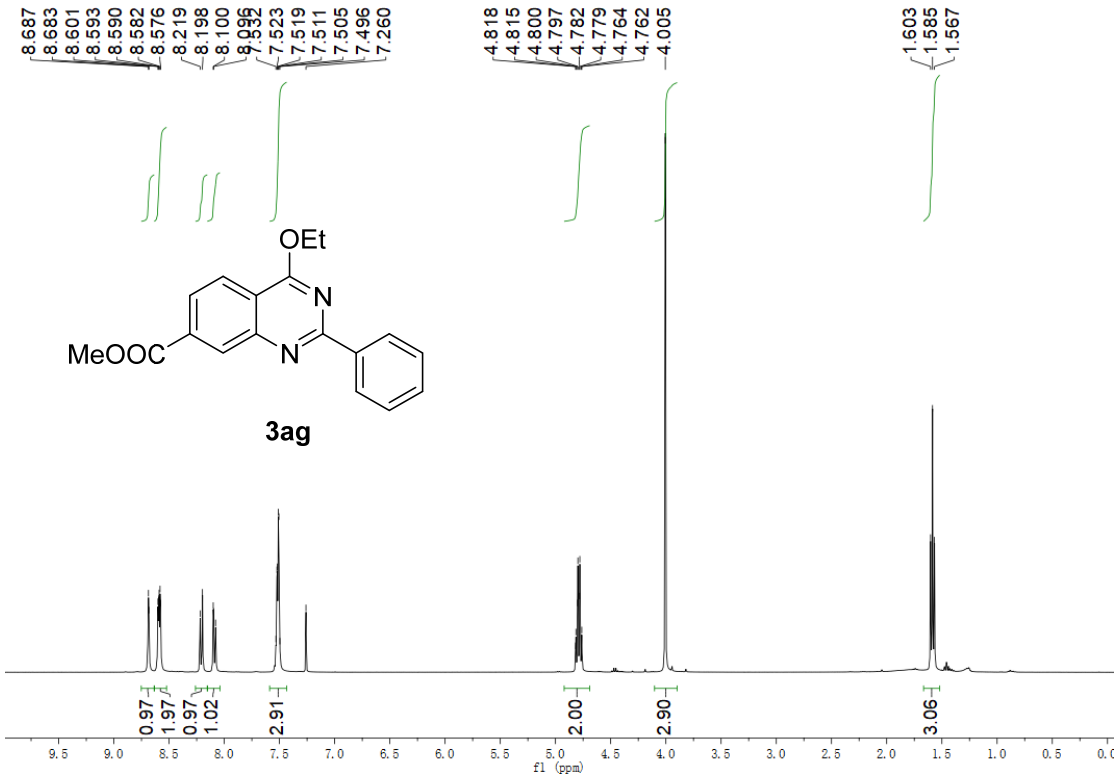
OEt
N
N
I
3af
f1 (ppm)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8.582
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7.511
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7.496
7.260
4.818
4.815
4.800
4.797
4.782
4.779
4.764
4.762
4.005
1.603
1.585
1.567
OEt
N
MeOOC
N
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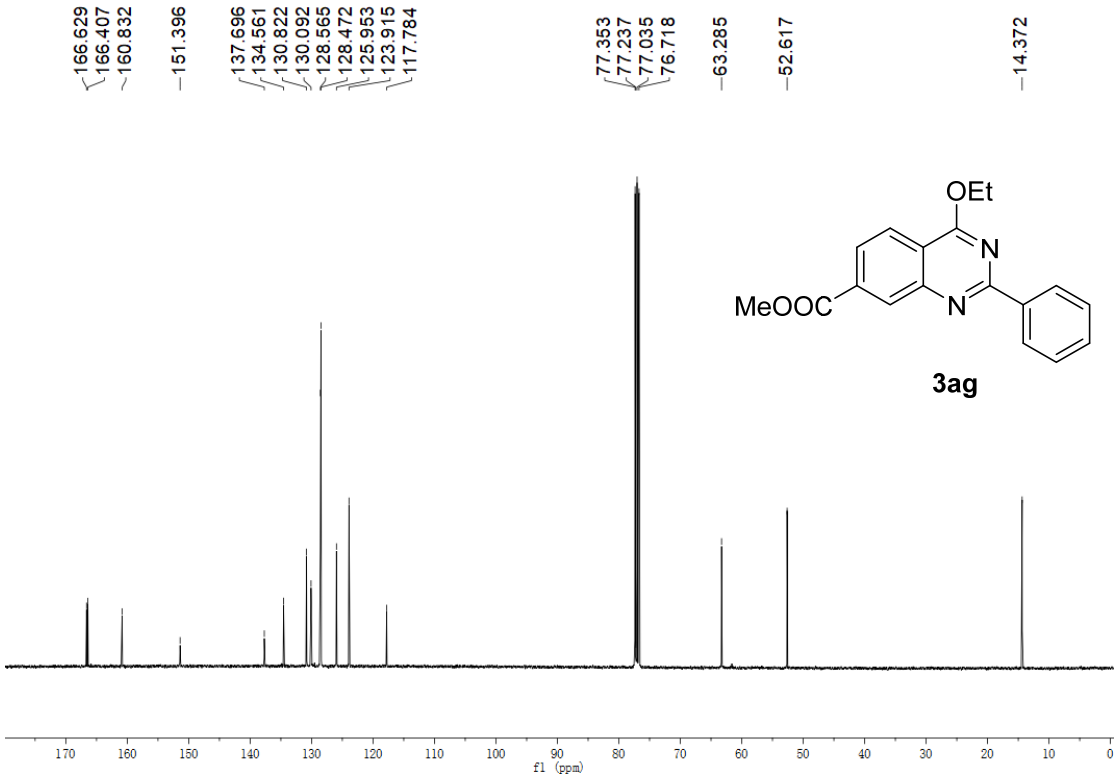
1.97
0.97
1.02
2.91
2.00
2.90
3.06
f1 (ppm)

3ag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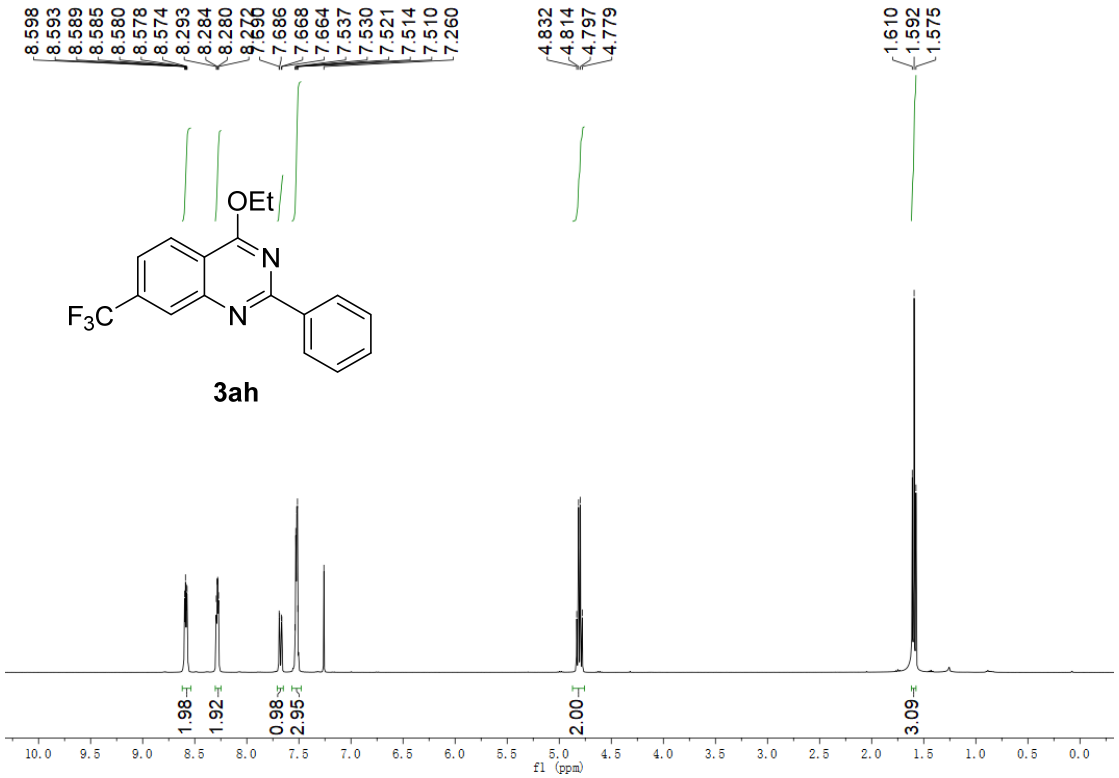
52.617
14.372
OEt
N
MeOOC
N
f1 (ppm)

3ag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4.797
4.779
1.610
1.592
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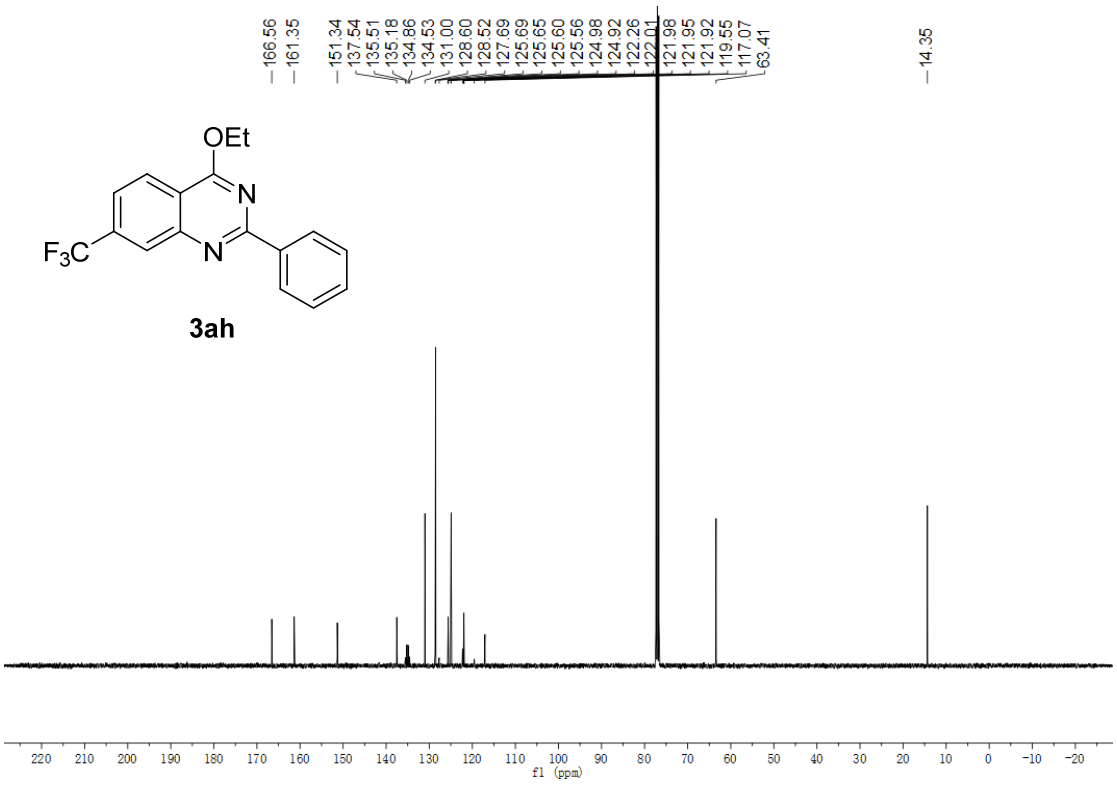
3.09
f1 (ppm)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128.60
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127.69
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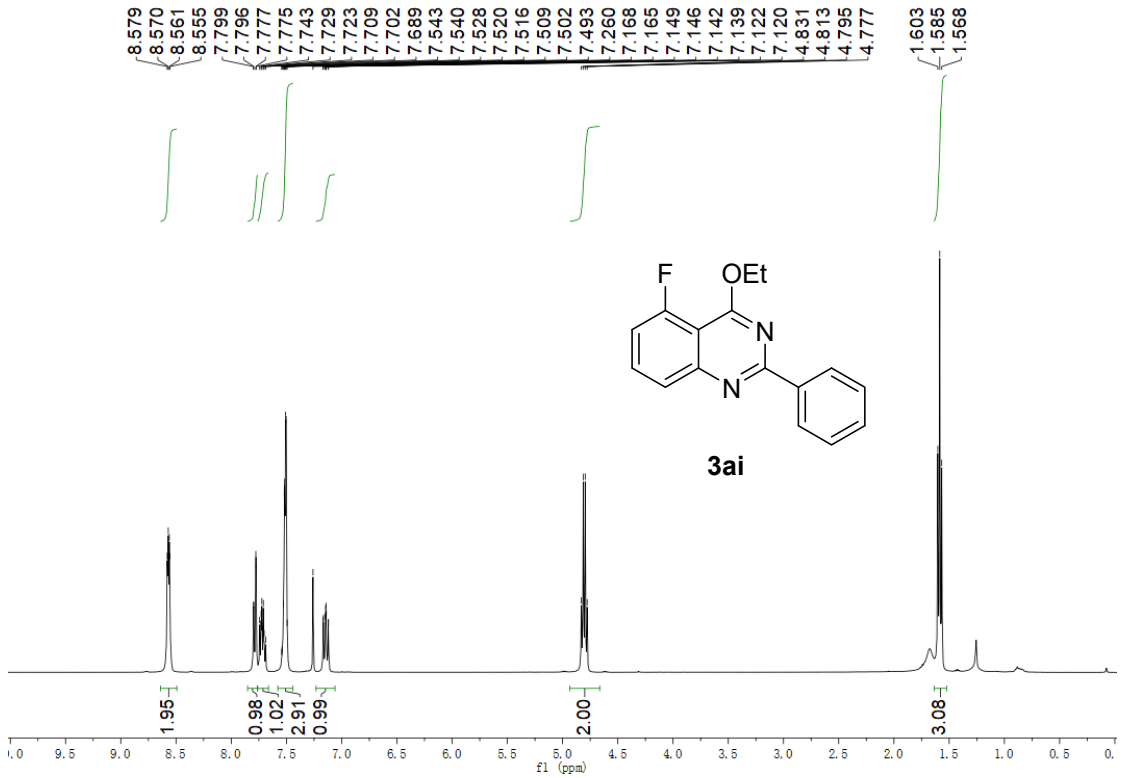
125.65
125.60
125.56
124.98
124.92
122.26
122.01
121.98
121.95
121.92
119.55
117.07
63.41
14.35
OEt
N
N
F3C
3ah
f1 (ppm)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4.777
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1.585
1.568
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OEt
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N
3ai
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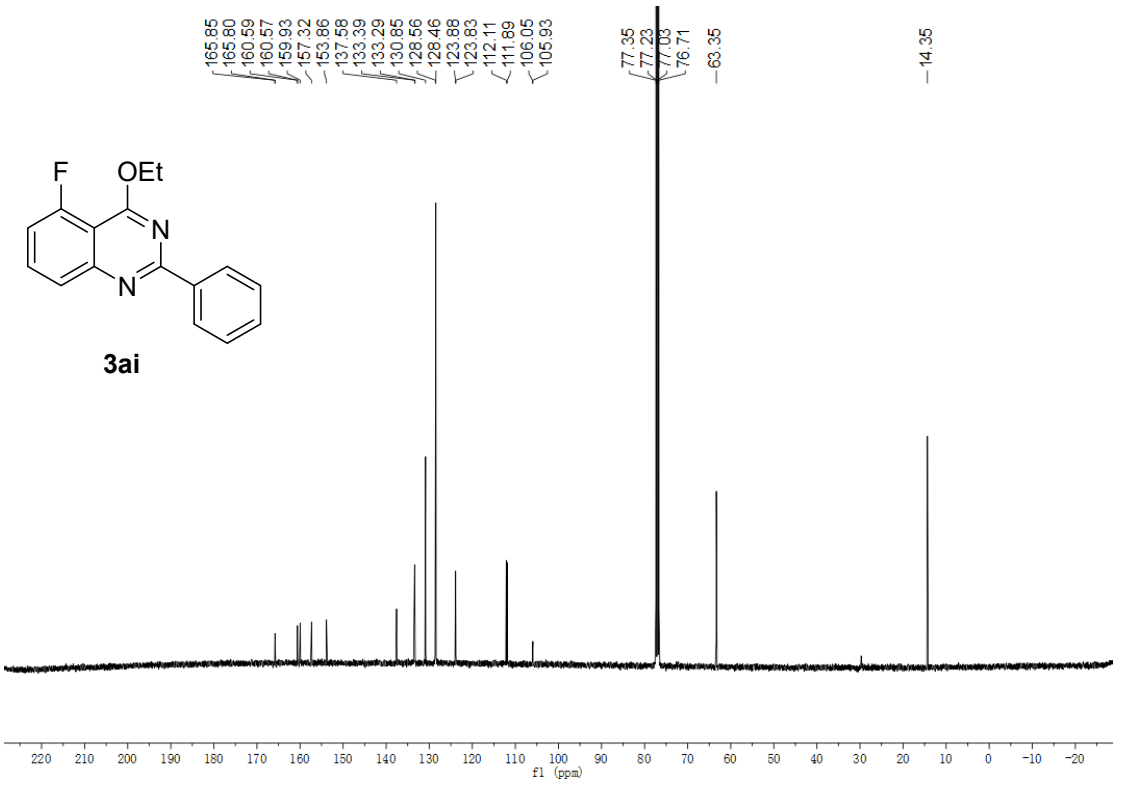
3.08
f1 (ppm)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133.29
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128.46
123.88
123.83
112.11
111.89
106.05
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F
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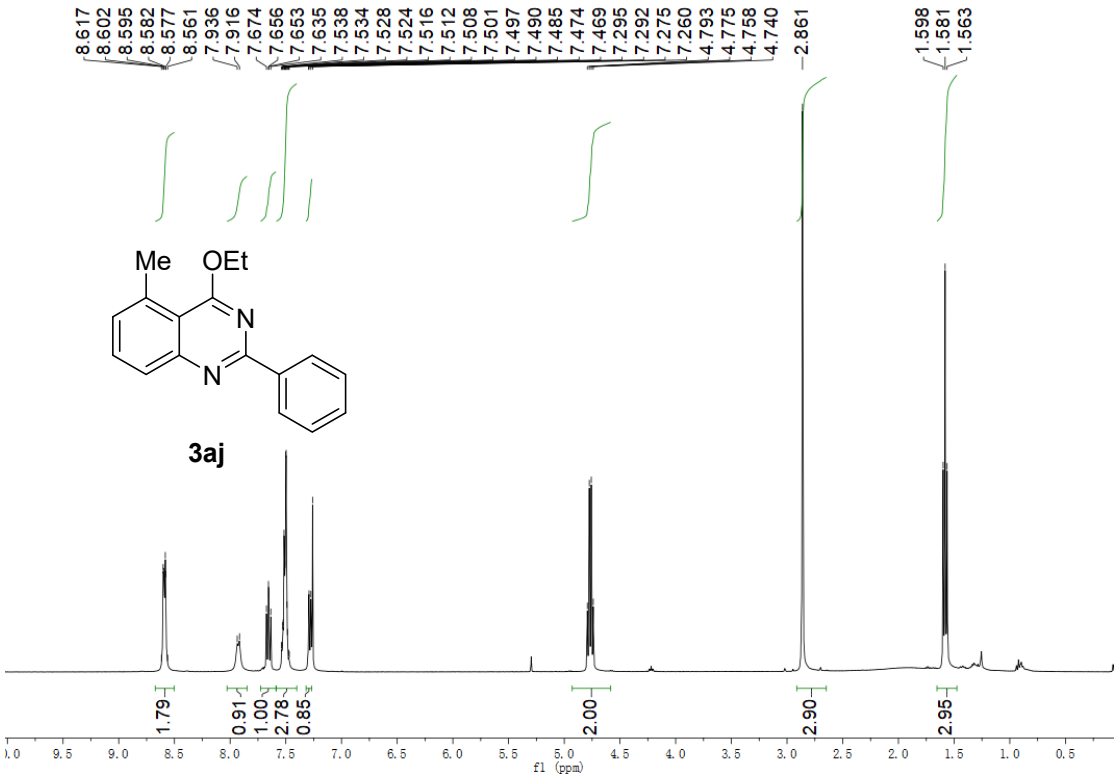
N
N
3ai
f1 (ppm)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7.534
7.528
7.524
7.516
7.512
7.508
7.501
7.497
7.490
7.485
7.474
7.469
7.295
7.292
7.275
7.260
4.793
4.775
4.758
4.740
2.861
1.598
1.581
1.563
Me
OEt
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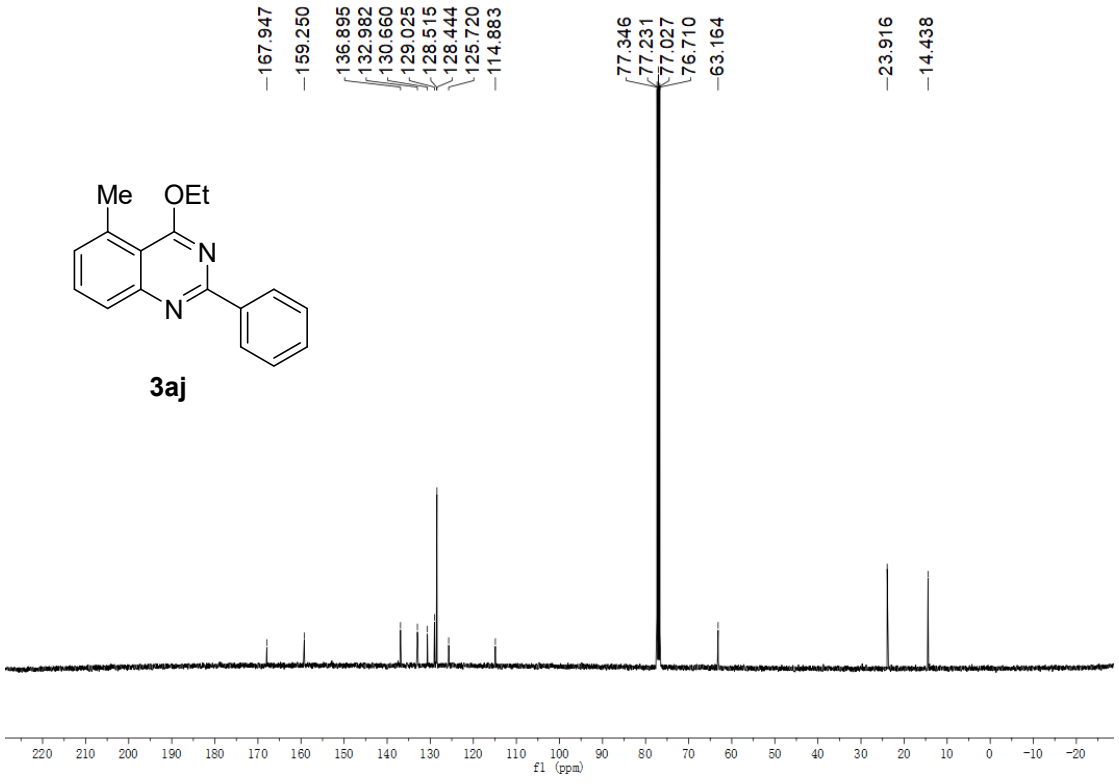
2.95
f1 (ppm)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76.710
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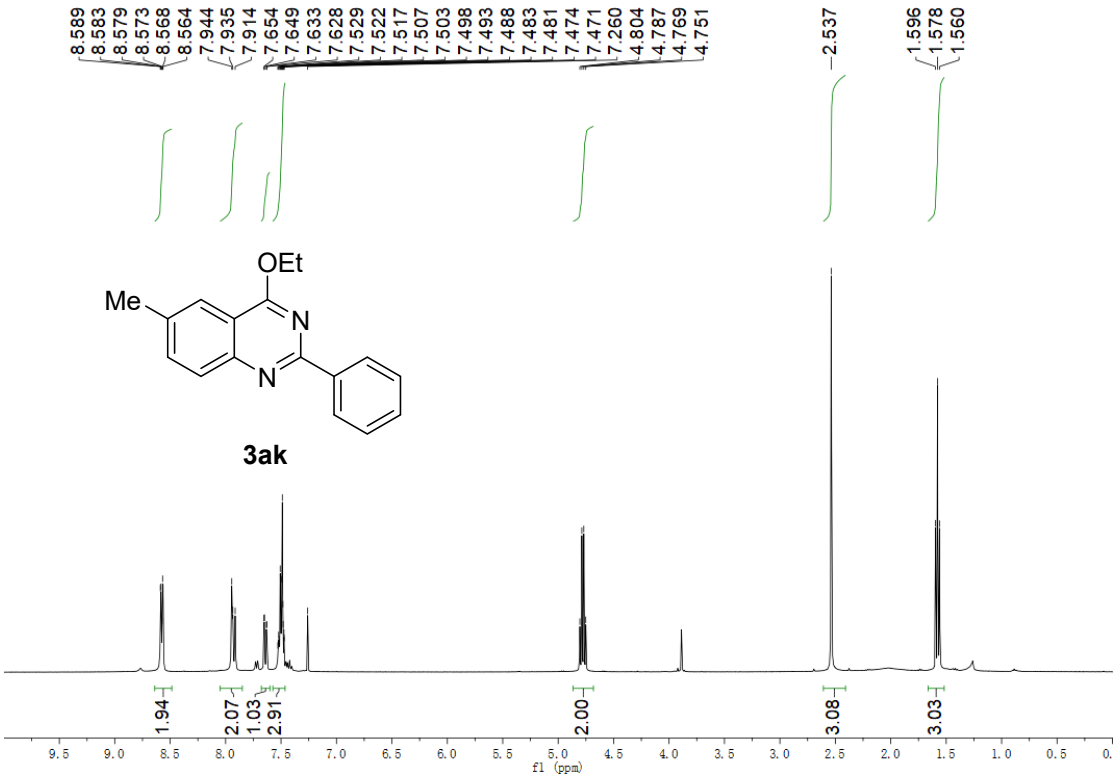
23.916
14.438
Me
OEt
N
N
3aj
f1 (ppm)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7.633
7.628
7.529
7.522
7.517
7.507
7.503
7.498
7.493
7.488
7.483
7.481
7.474
7.471
7.260
4.804
4.787
4.769
4.751
2.537
1.596
1.578
1.560
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1.03
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2.00
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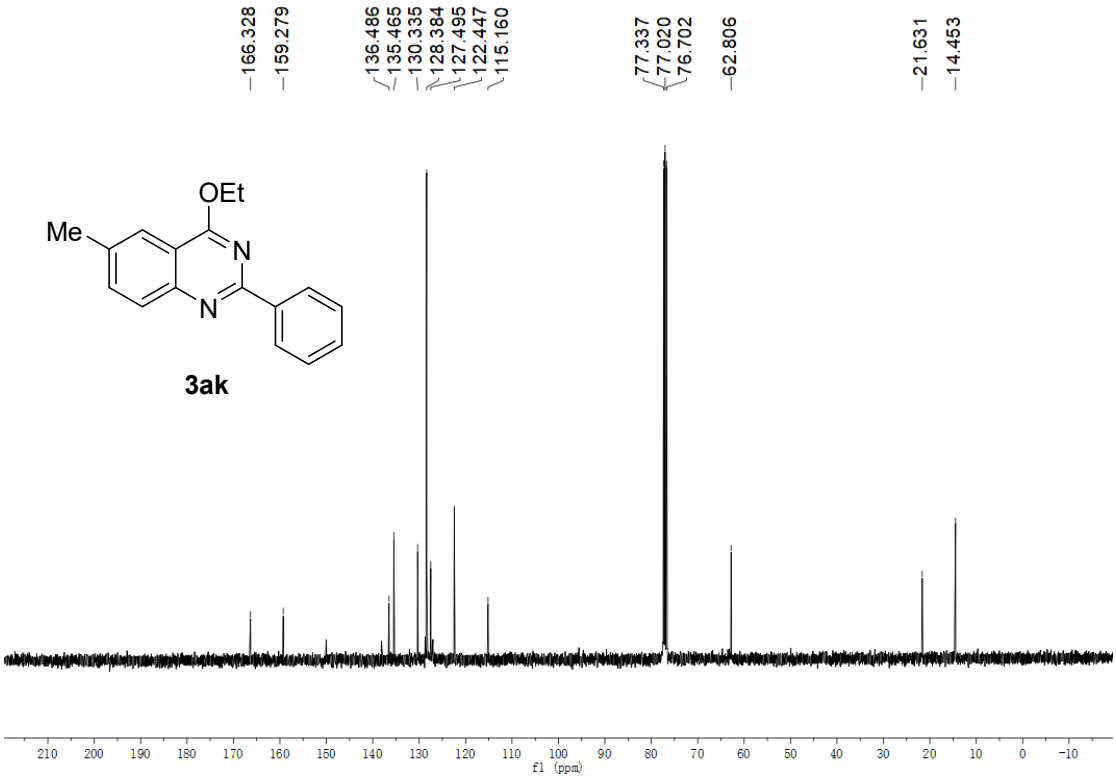
3.03
f1 (ppm)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Me
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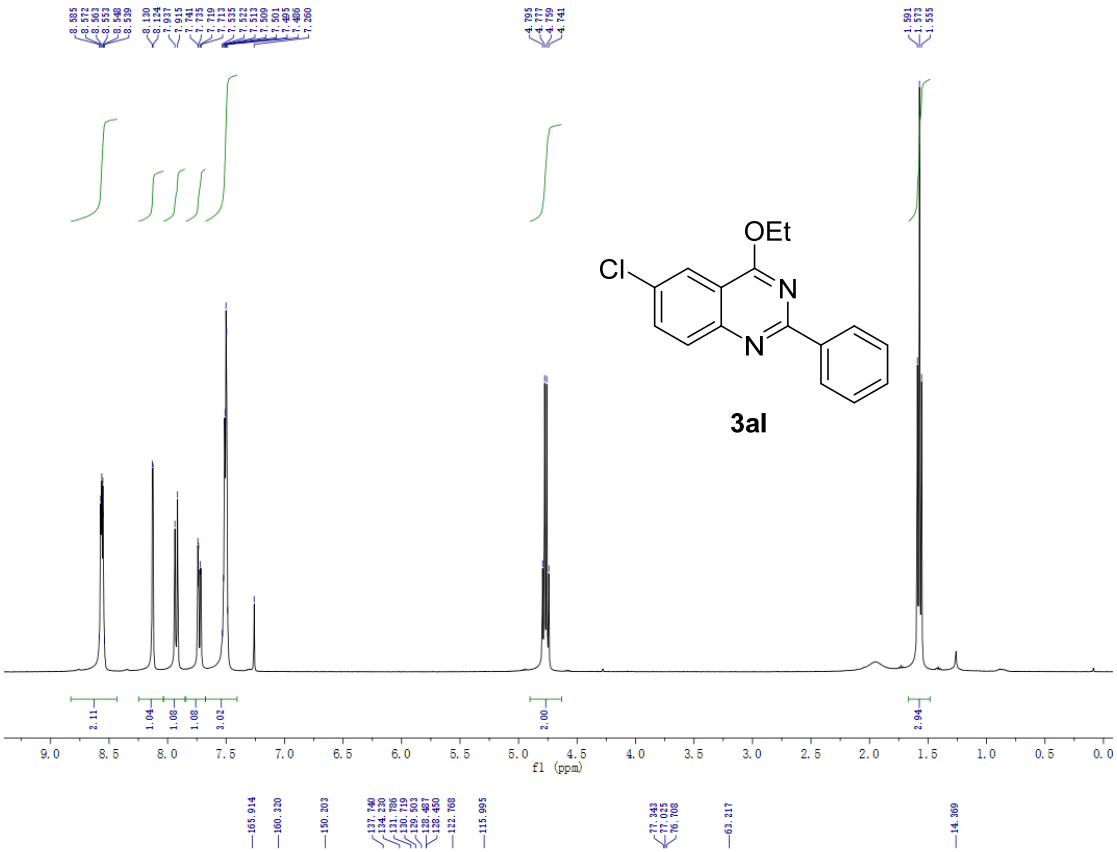
N
3ak
f1 (ppm)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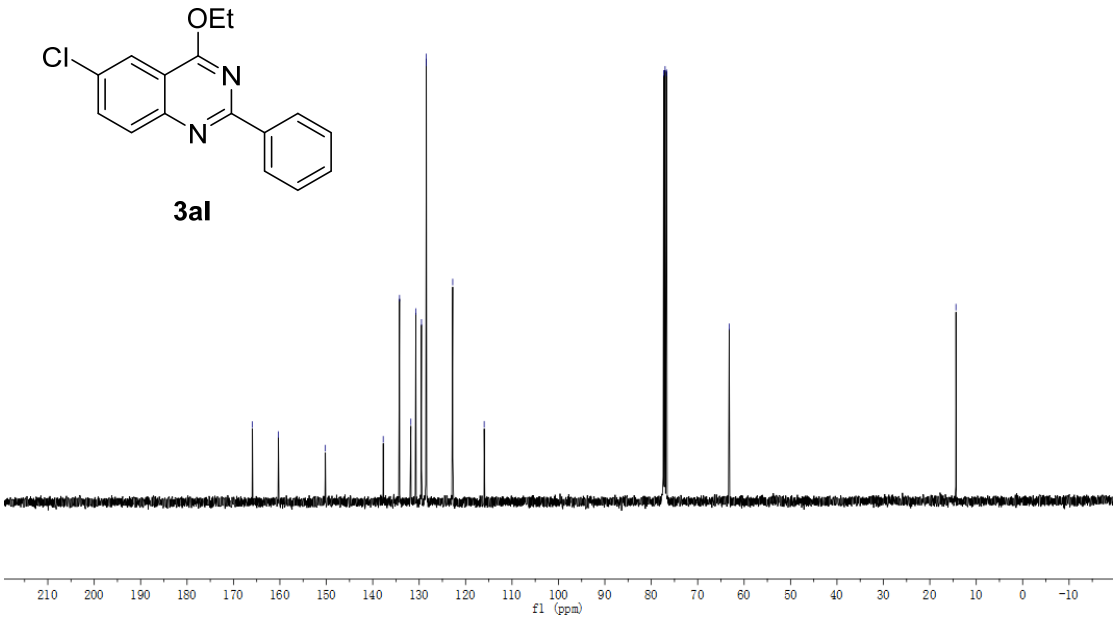
Cl
N
N
3al
f1 (ppm)


OEt
Cl
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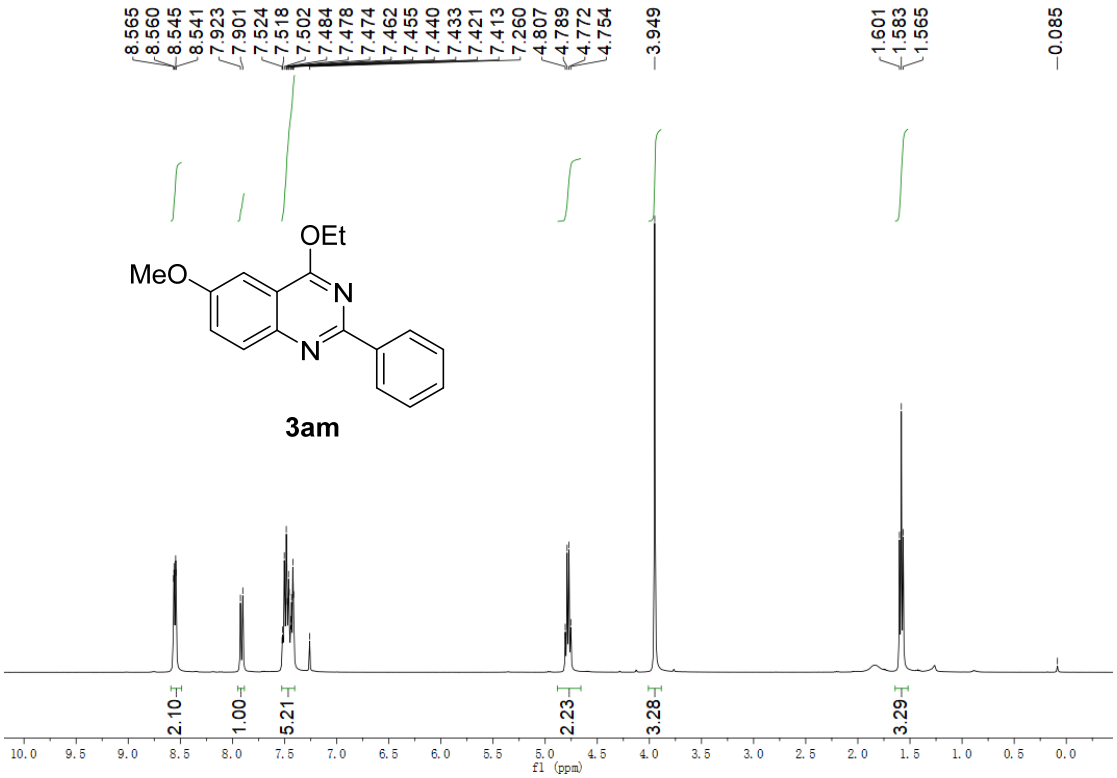
N
3al
f1 (ppm)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7.462
7.455
7.440
7.433
7.421
7.413
7.260
4.807
4.789
4.772
4.754
3.949
1.601
1.583
1.565
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OEt
MeO
N
N
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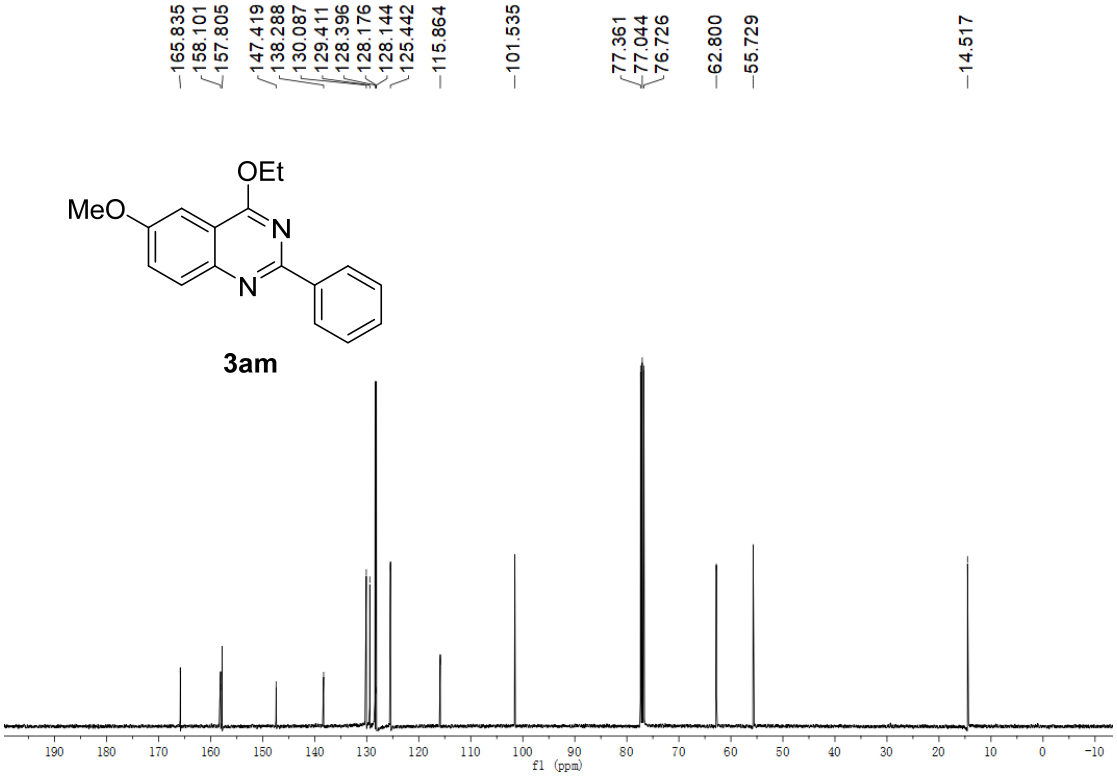
1.00
5.21
2.23
3.28
3.29
f1 (ppm)

3am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129.411
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115.864
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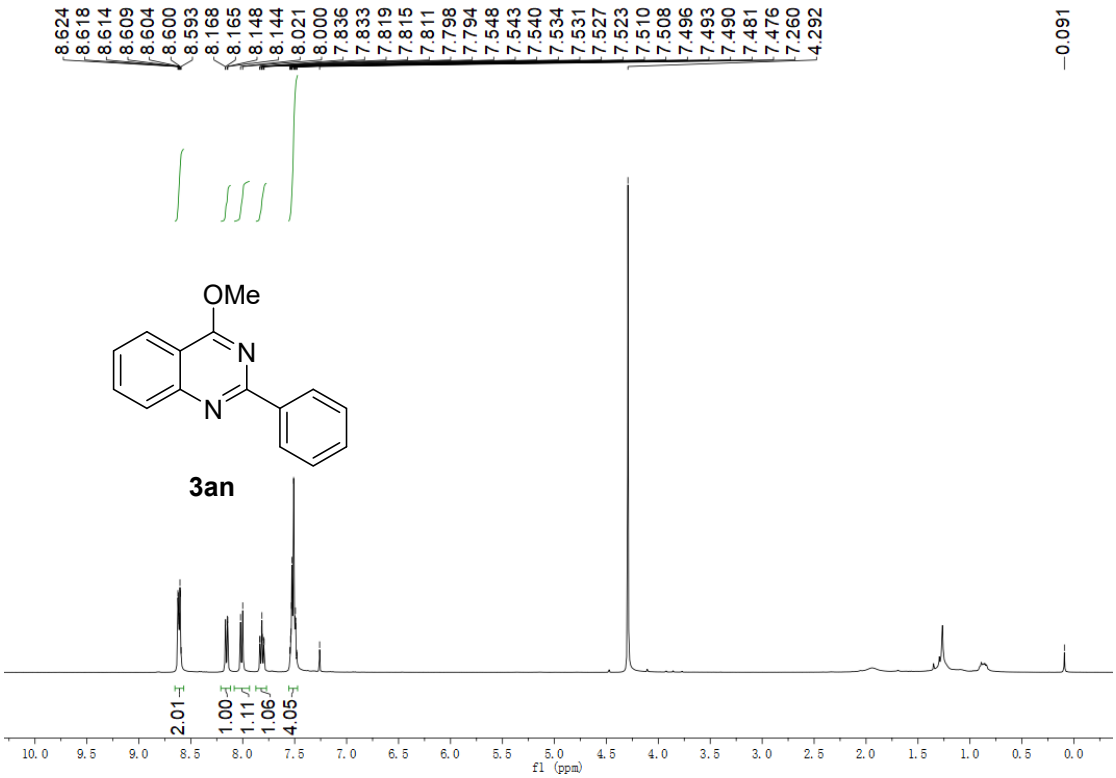
77.044
76.726
62.800
55.729
14.517
OEt
MeO
N
N
f1 (ppm)

3am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8.144
8.021
8.000
7.836
7.833
7.819
7.815
7.811
7.798
7.794
7.548
7.543
7.540
7.534
7.531
7.527
7.523
7.510
7.508
7.496
7.493
7.490
7.481
7.476
7.260
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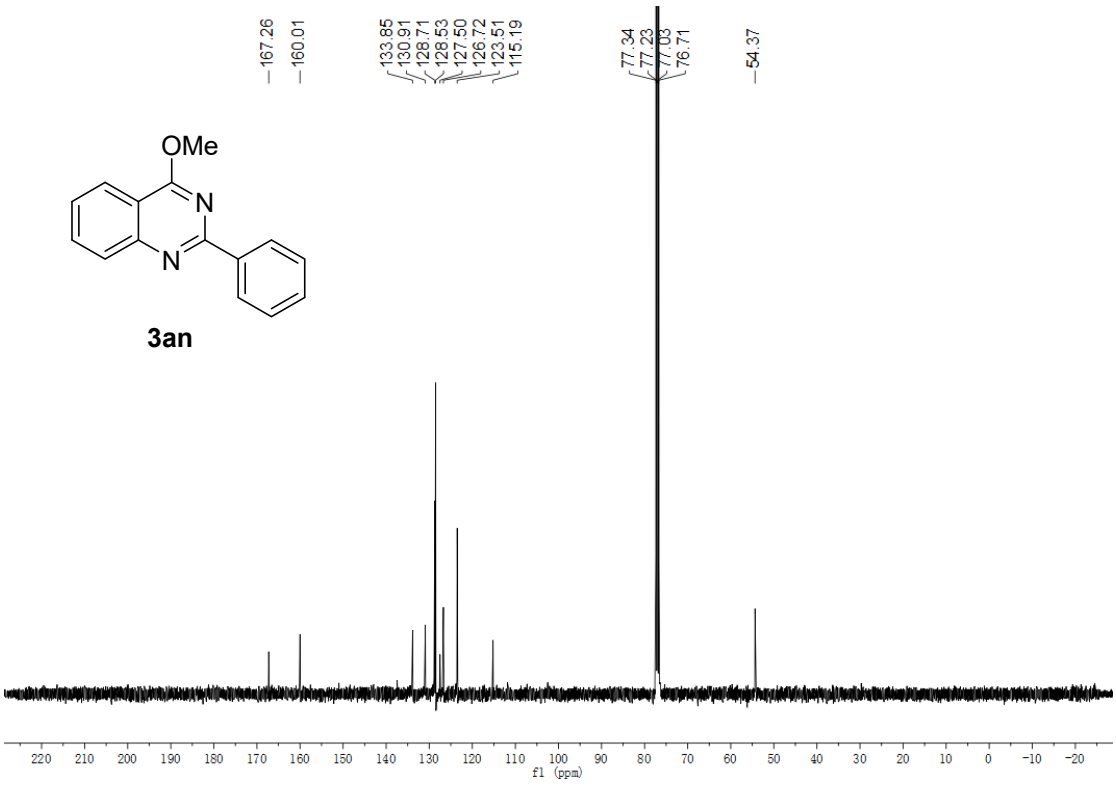
0.091
OMe
N
N
3an
2.01
1.00
1.11
1.06
4.05
f1 (ppm)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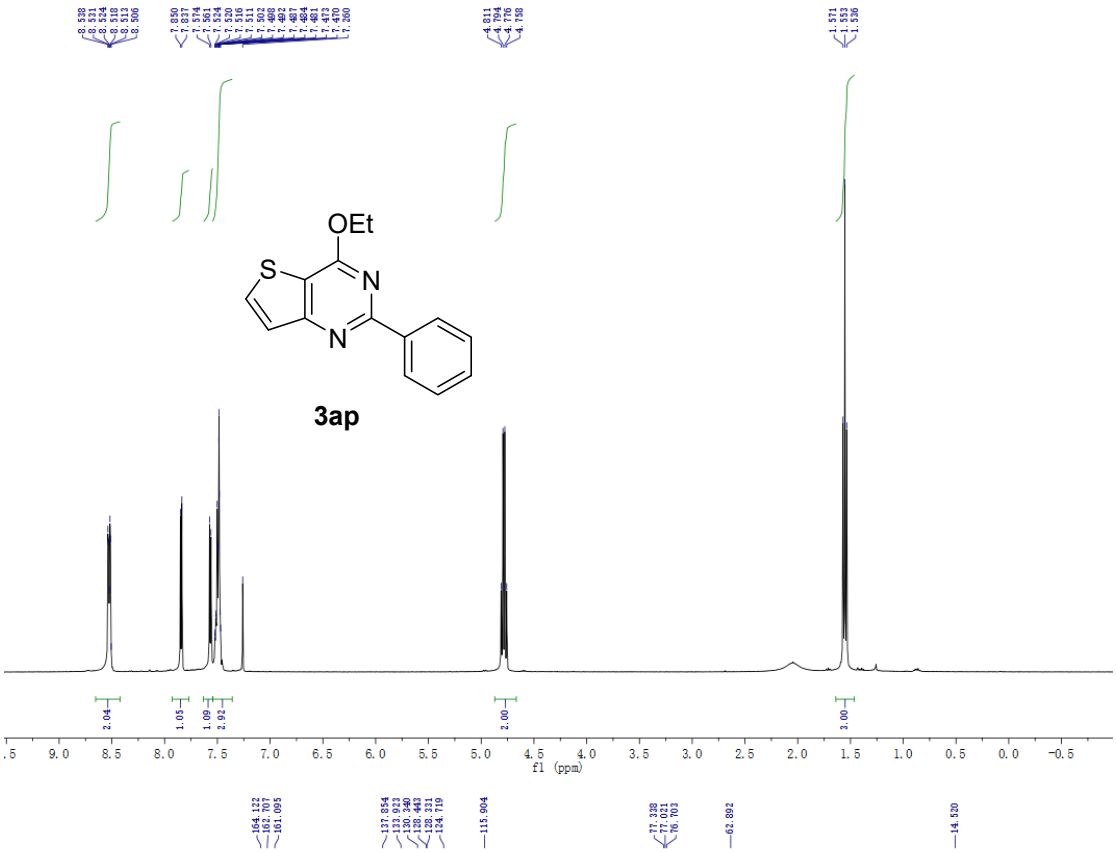
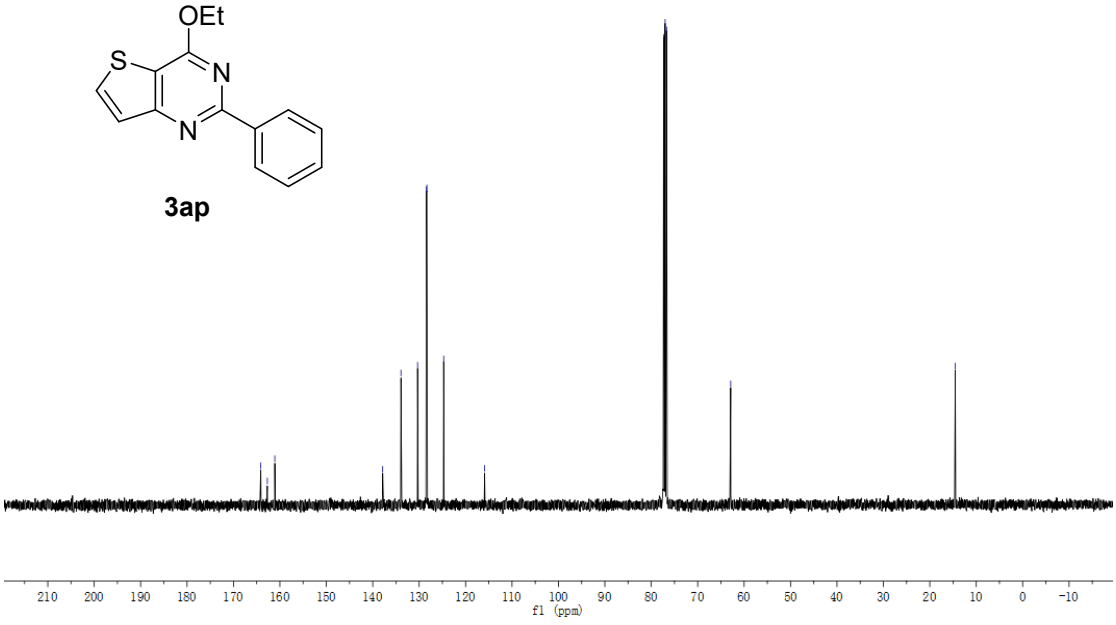
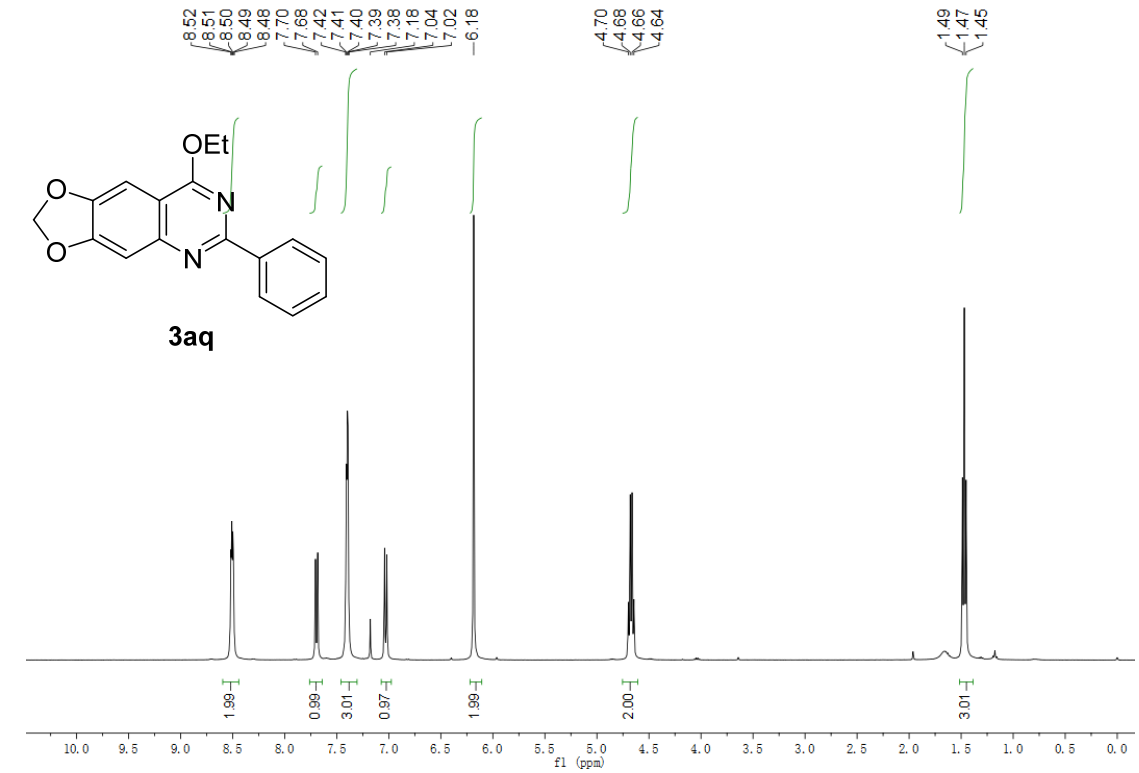
128.53
127.50
126.72
123.51
115.19
77.34
77.23
77.03
76.71
54.37
OMe
N
N
3an
f1 (ppm)


OEt
S
N
N
3ap
f1 (ppm)


OEt
S
N
N
3ap
f1 (ppm)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7.42
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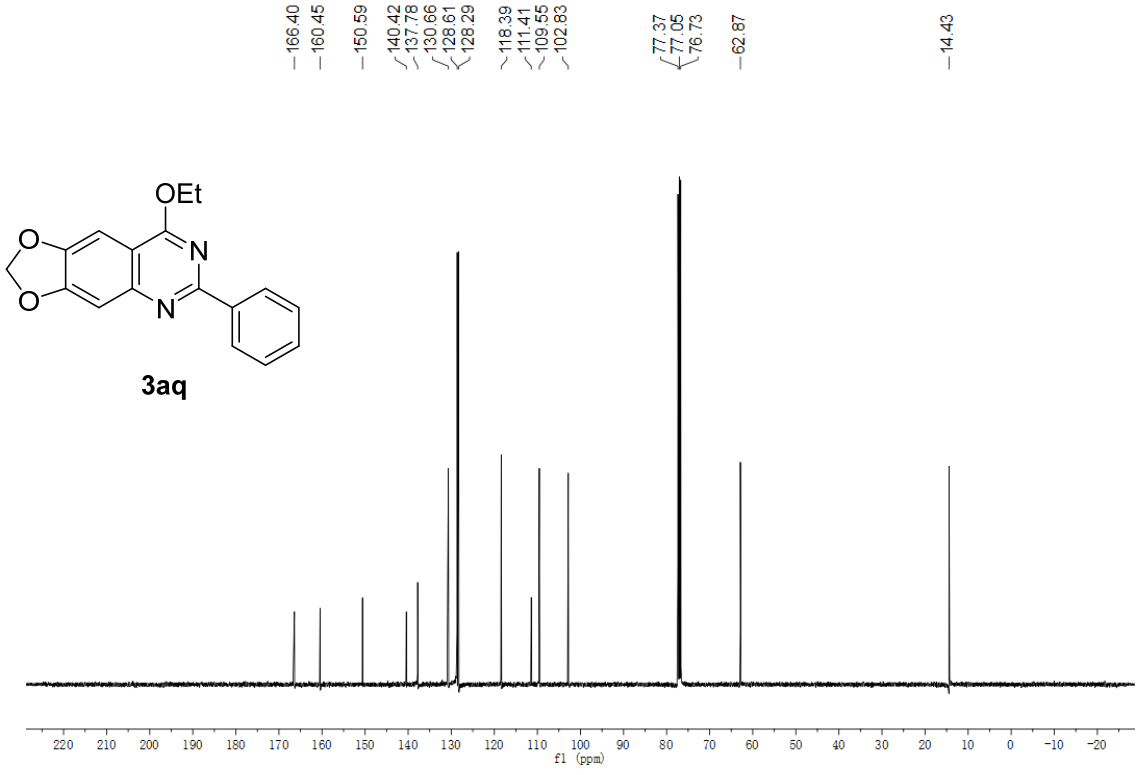
7.39
7.38
7.18
7.04
7.02
6.18
4.70
4.68
4.66
4.64
1.49
1.47
1.45
OEt
O
O
N
N
3aq
1.99
0.99
3.01
0.97
1.99
2.00
3.01
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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111.41
109.55
102.83
77.37
77.05
76.73
62.87
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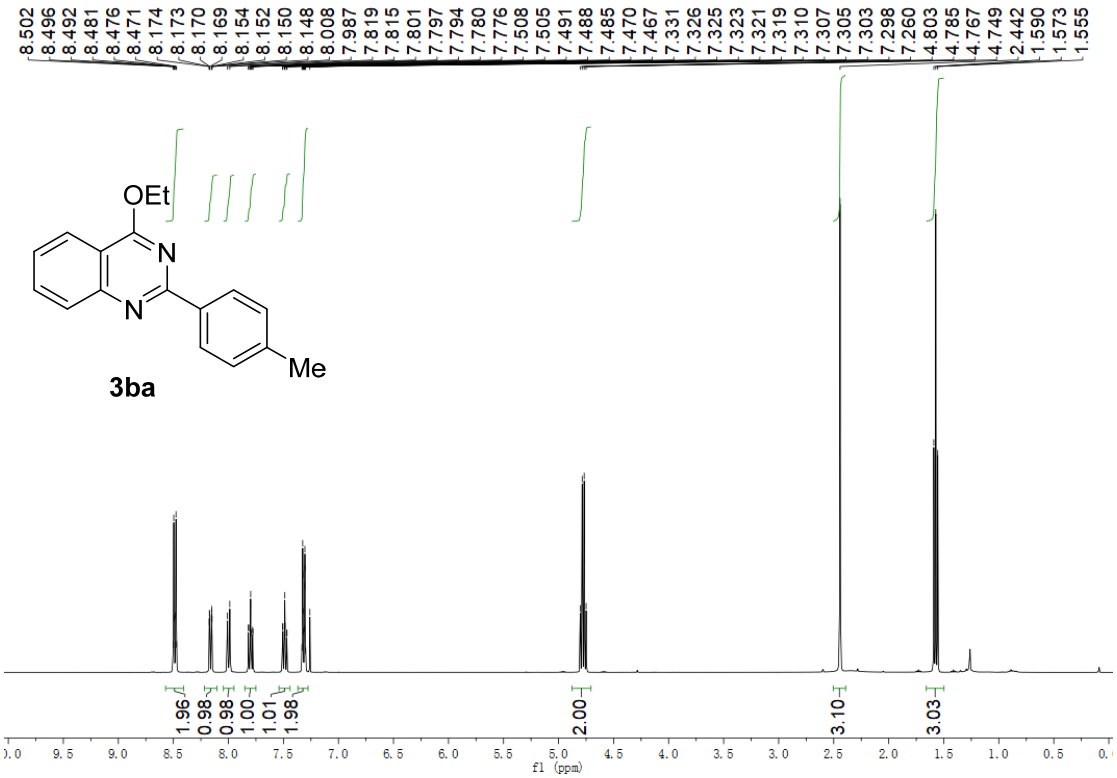
O
O
N
N
3aq
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)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8.173
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8.169
8.154
8.152
8.150
8.148
8.008
7.987
7.819
7.815
7.801
7.797
7.794
7.780
7.776
7.508
7.505
7.491
7.488
7.485
7.470
7.467
7.331
7.326
7.325
7.323
7.321
7.319
7.310
7.307
7.305
7.303
7.298
7.260
4.803
4.785
4.767
4.749
2.442
1.590
1.573
1.555
OEt
N
N
Me
3ba
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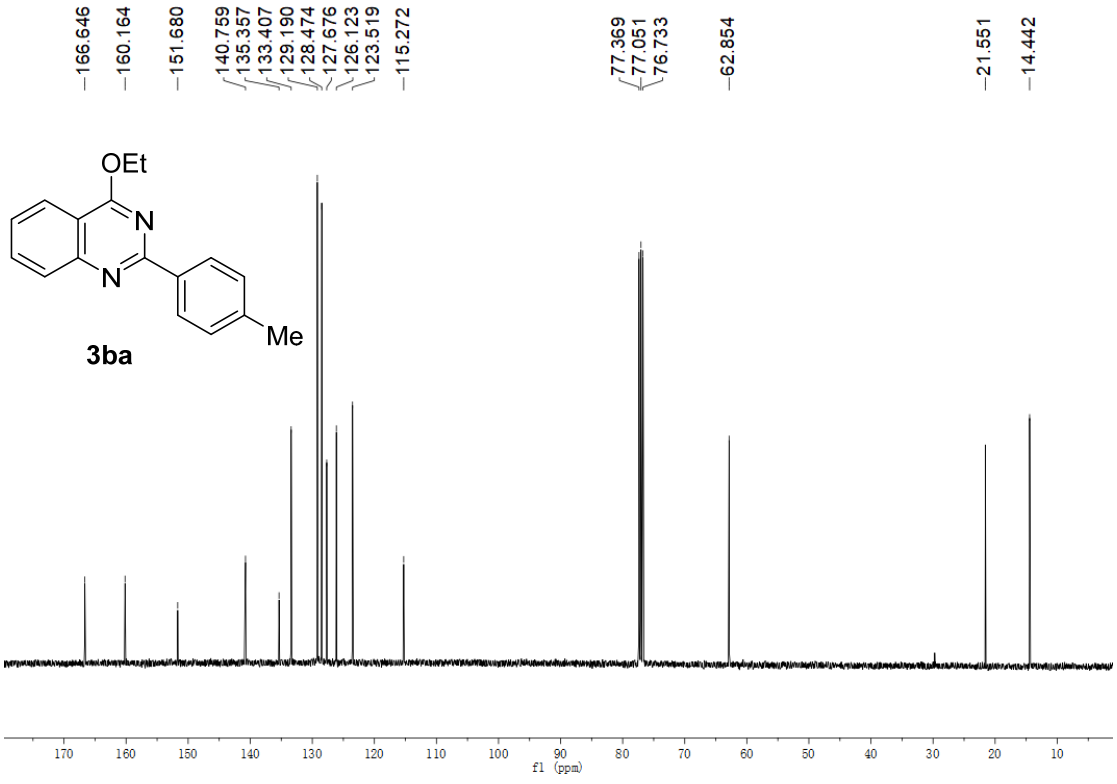
0.98
0.98
1.00
1.01
1.98
2.00
3.10
3.03
f1 (ppm)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123.519
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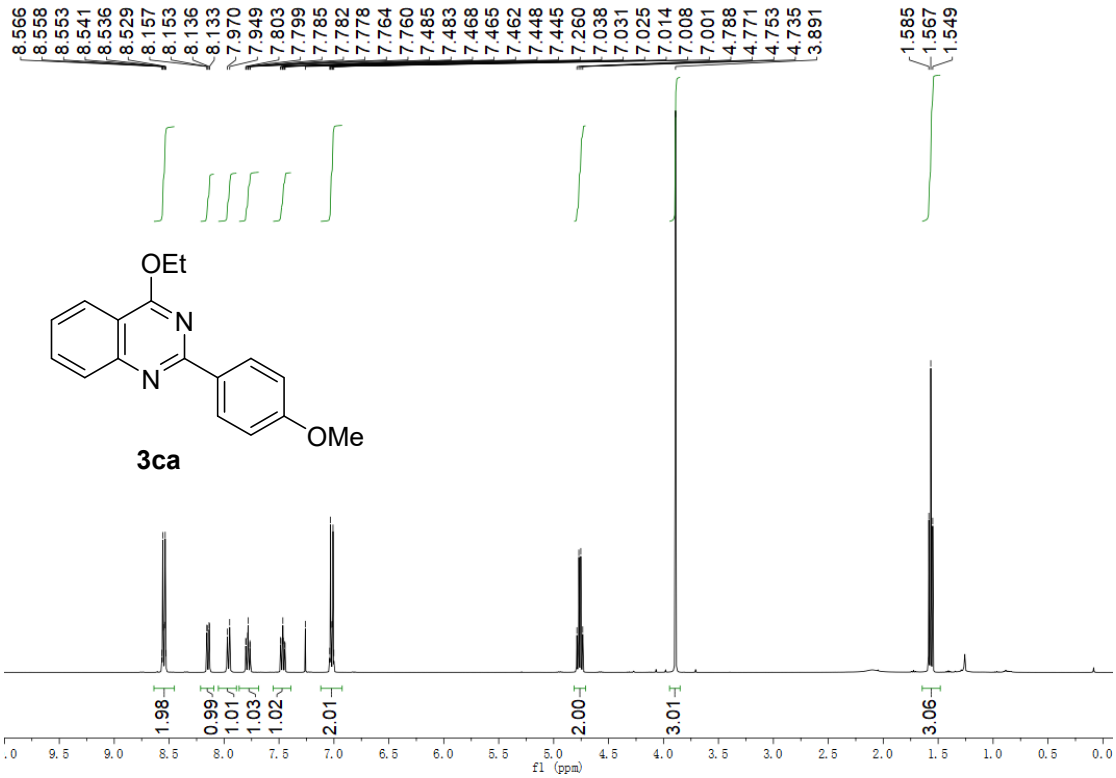
77.051
76.733
62.854
21.551
14.442
OEt
N
N
Me
3ba
f1 (ppm)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8.153
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8.133
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7.803
7.799
7.785
7.782
7.778
7.764
7.760
7.485
7.483
7.468
7.465
7.462
7.448
7.445
7.260
7.038
7.031
7.025
7.014
7.008
7.001
4.788
4.771
4.753
4.735
3.891
1.585
1.567
1.549
OEt
N
N
OMe
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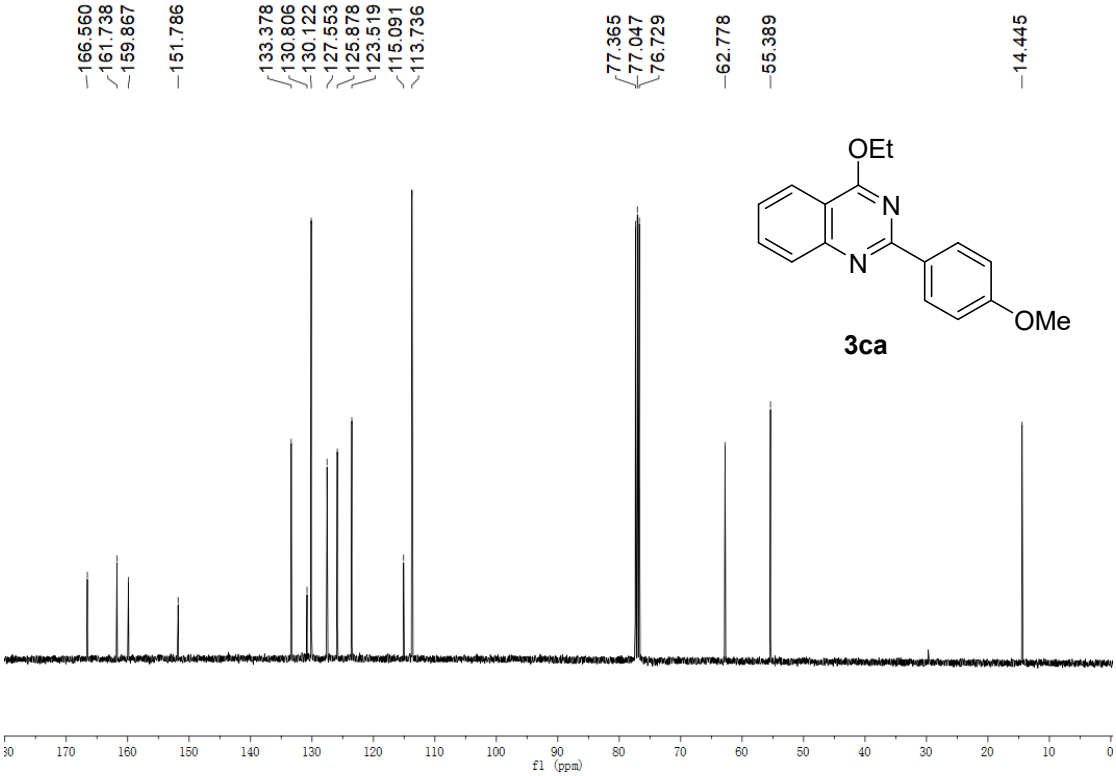
1.01
1.03
1.02
2.01
2.00
3.01
3.06
f1 (ppm)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76.729
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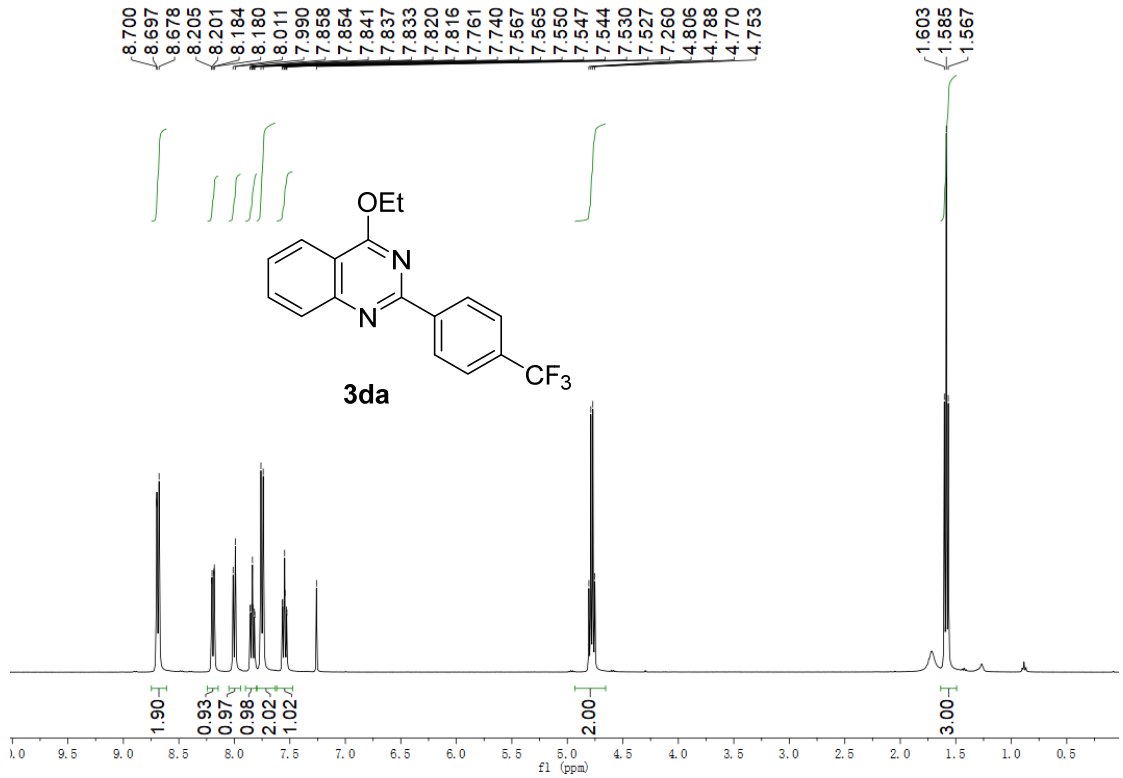
OEt
N
N
OMe
3ca
f1 (ppm)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7.837
7.833
7.820
7.816
7.761
7.740
7.567
7.565
7.550
7.547
7.544
7.530
7.527
7.260
4.806
4.788
4.770
4.753
1.603
1.585
1.567
OEt
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N
CF3
3da
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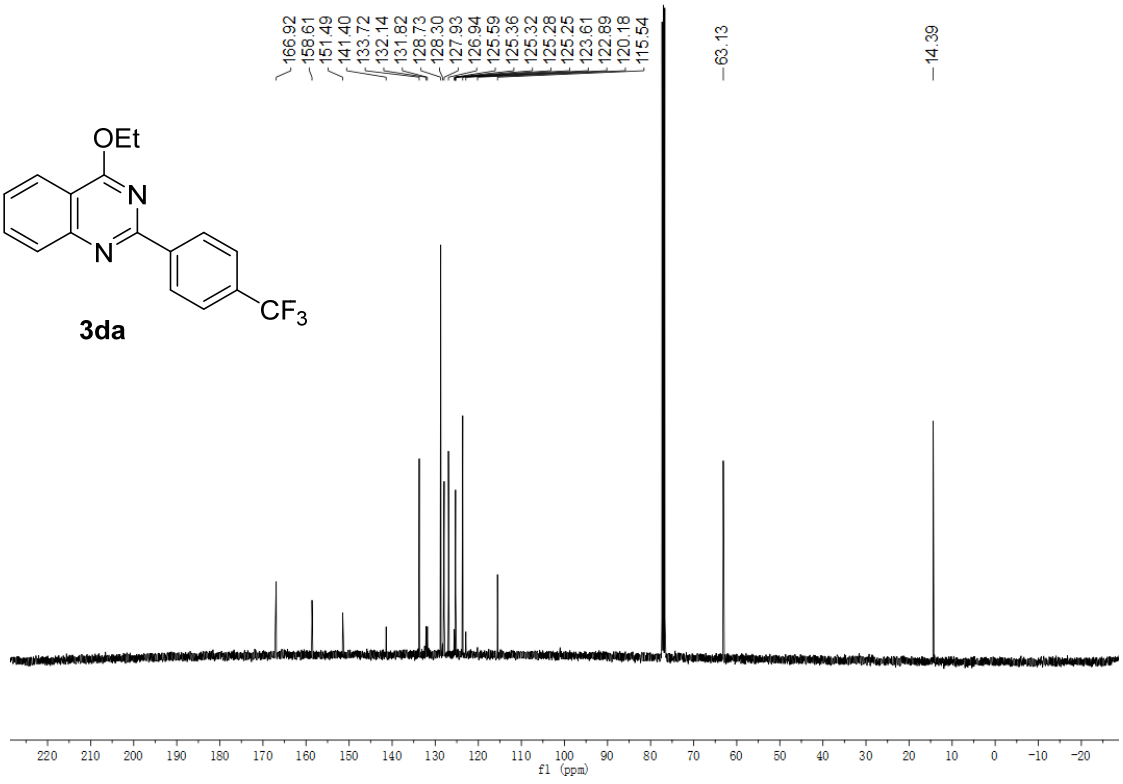
1.02
2.00
3.00
f1 (ppm)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125.36
125.32
125.28
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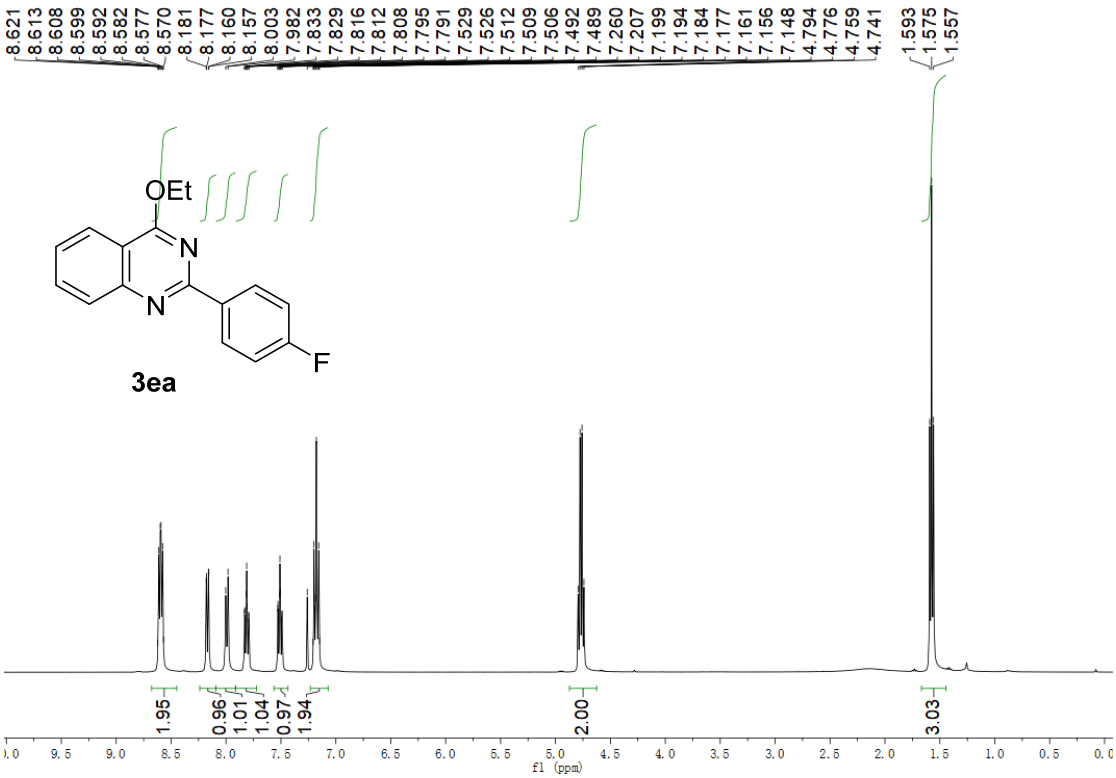
14.39
OEt
N
N
CF3
3da
f1 (ppm)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7.833
7.829
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7.812
7.808
7.795
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7.526
7.512
7.509
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7.199
7.194
7.184
7.177
7.161
7.156
7.148
4.794
4.776
4.759
4.741
1.593
1.575
1.557
OEt
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N
F
3ea
1.95
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1.04
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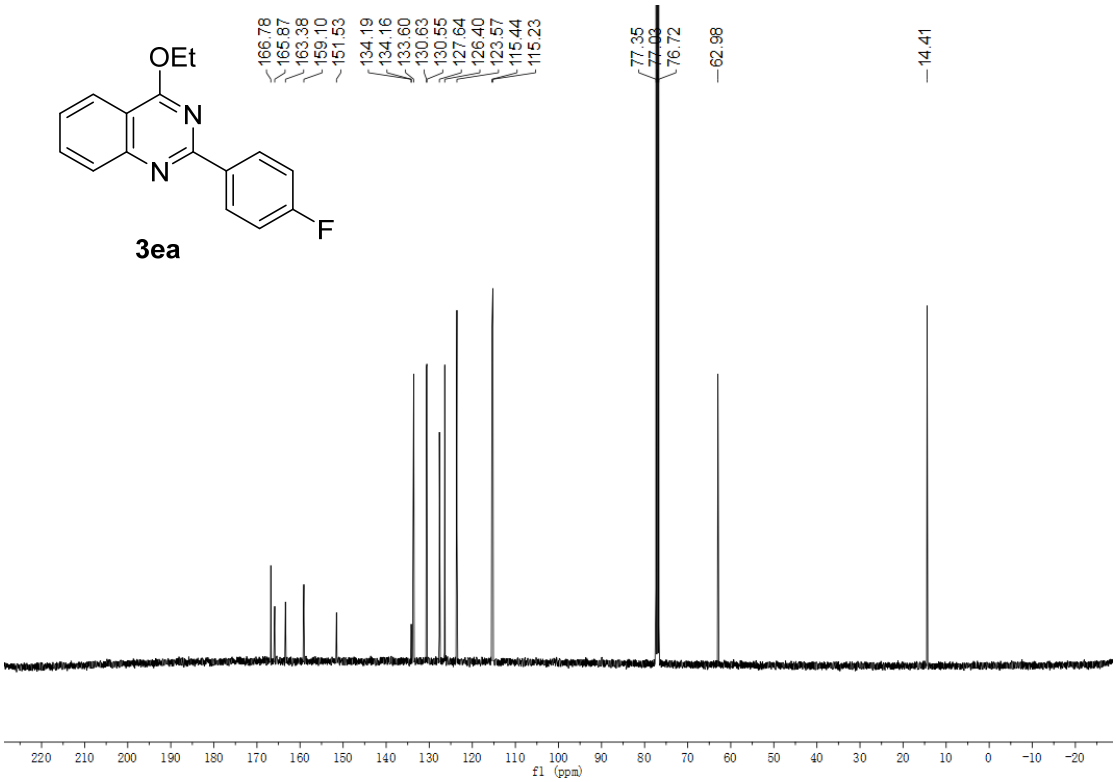
2.00
3.03
f1 (ppm)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123.57
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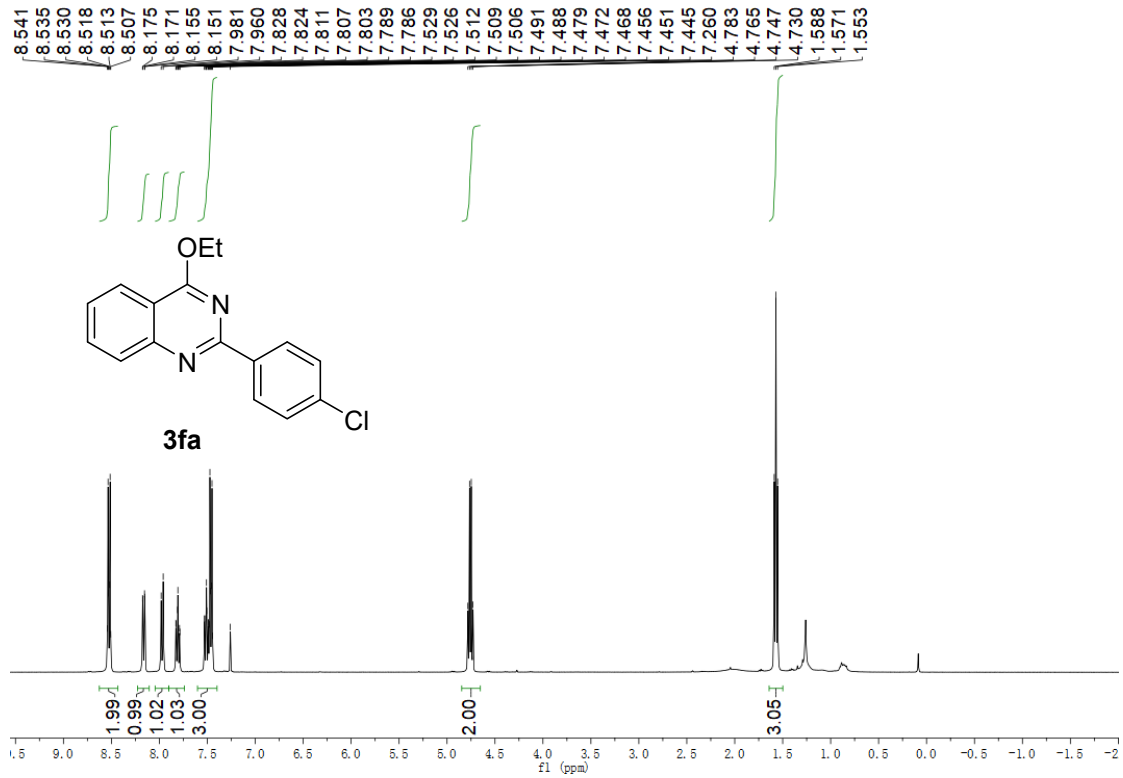
OEt
N
N
F
3ea
f1 (ppm)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7.824
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7.803
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7.509
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7.491
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7.472
7.468
7.456
7.451
7.445
7.260
4.783
4.765
4.747
4.730
1.588
1.571
1.553
OEt
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Cl
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1.03
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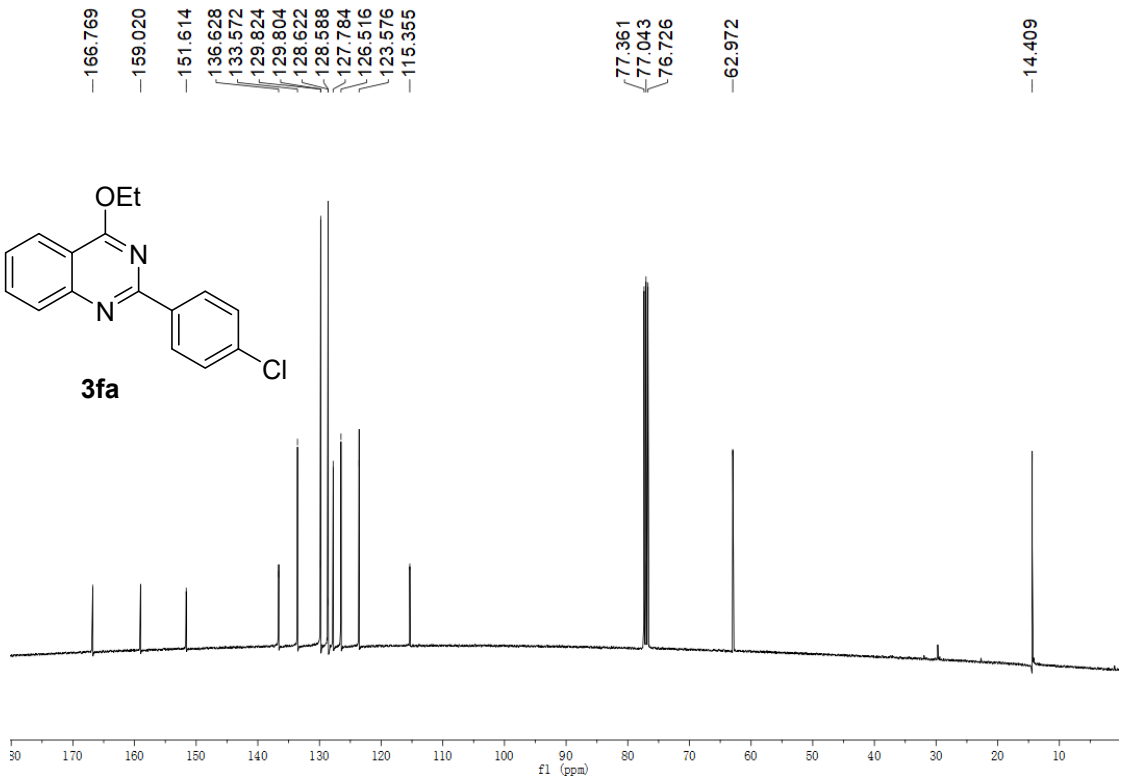
f1 (ppm)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77.043
76.726
62.972
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OEt
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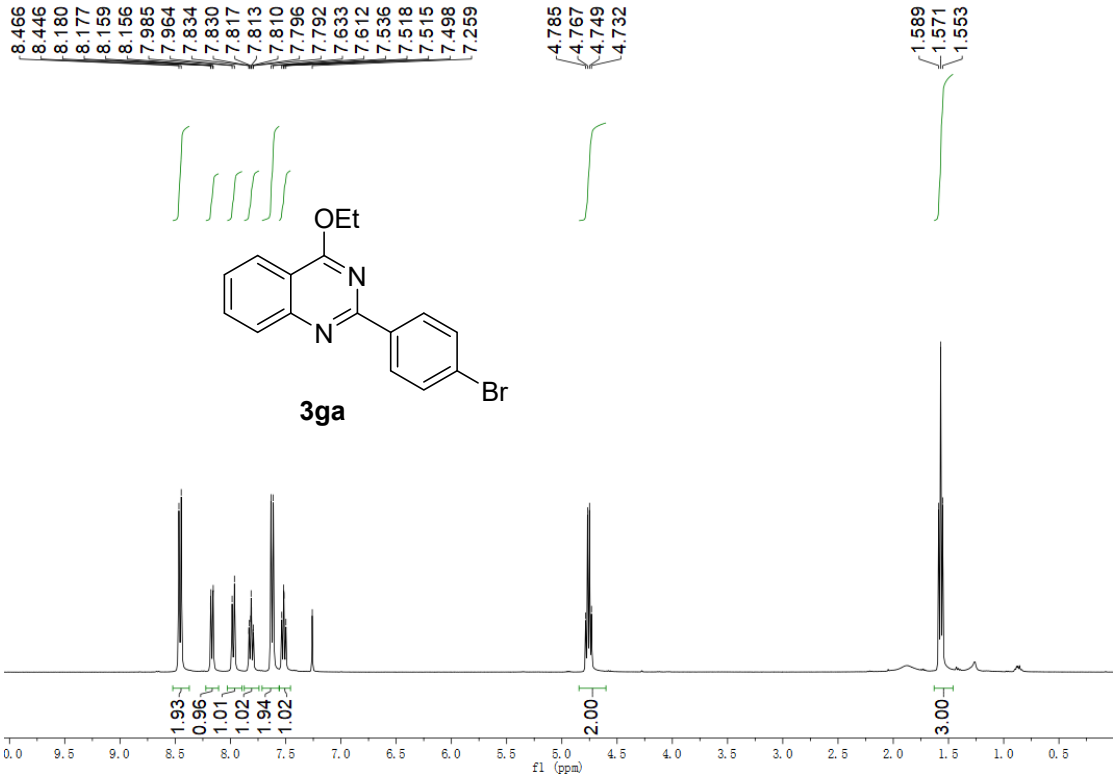
N
Cl
3fa
f1 (ppm)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7.259
4.785
4.767
4.749
4.732
1.589
1.571
1.553
OEt
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Br
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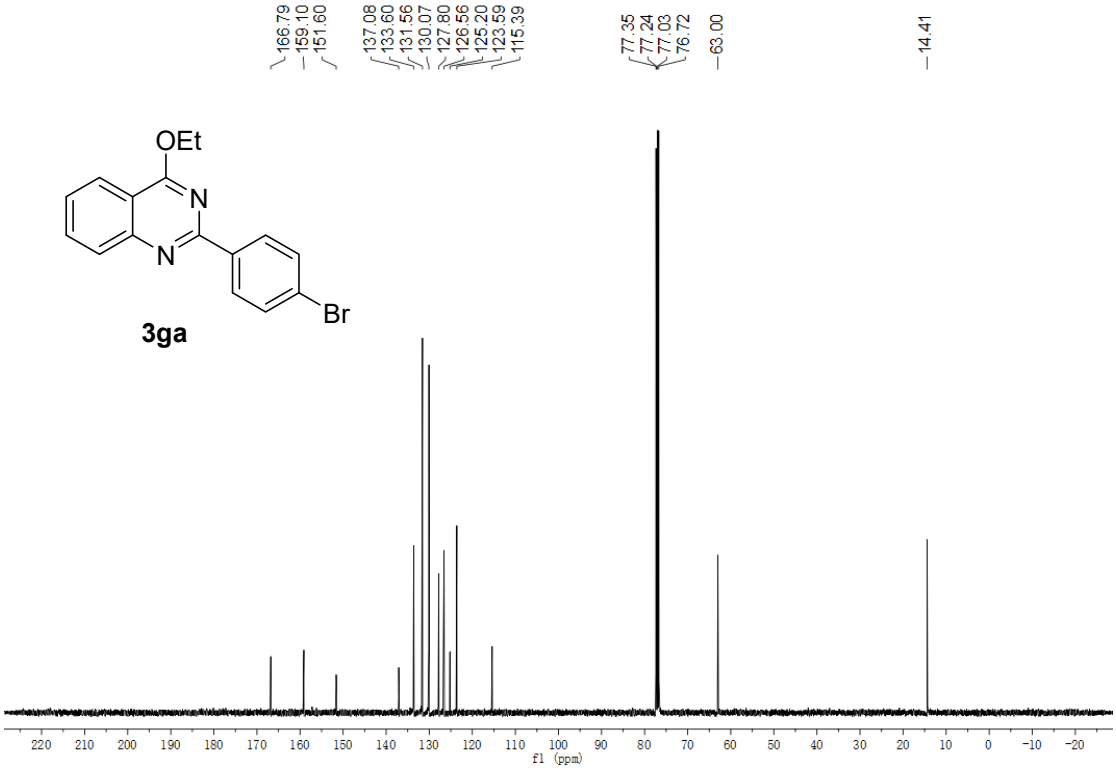
1.02
1.94
1.02
2.00
3.00
f1 (ppm)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123.59
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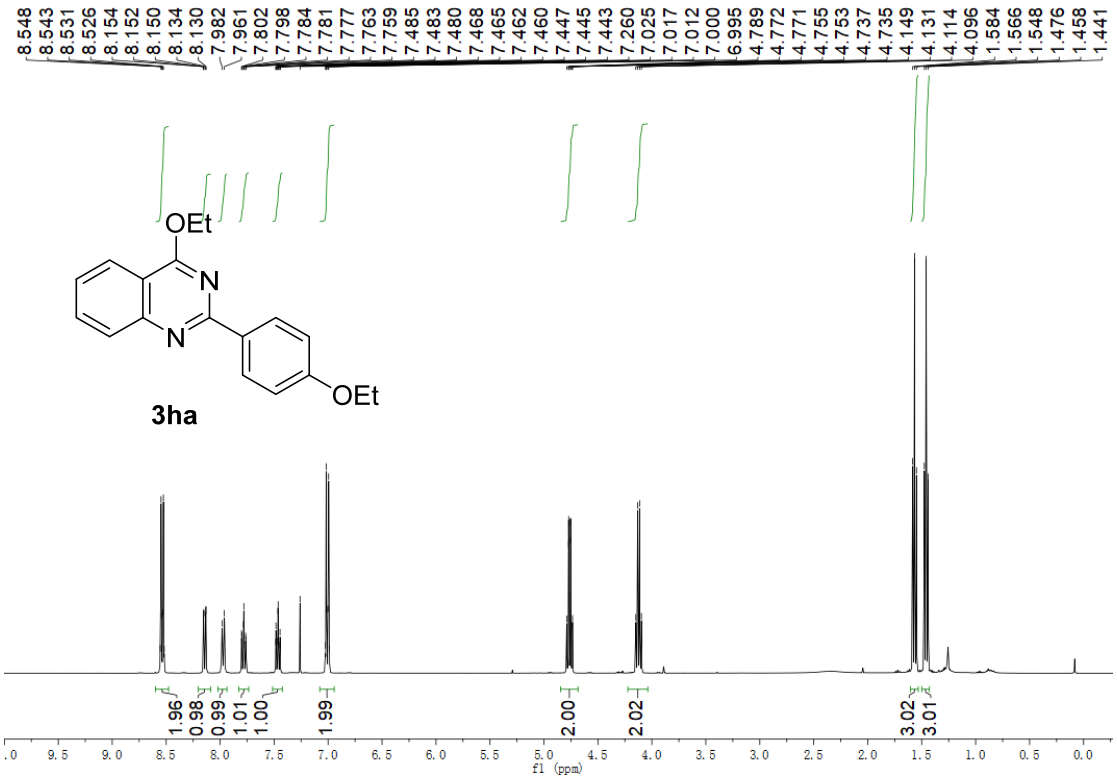
77.03
76.72
63.00
14.41
OEt
N
N
Br
3ga
f1 (ppm)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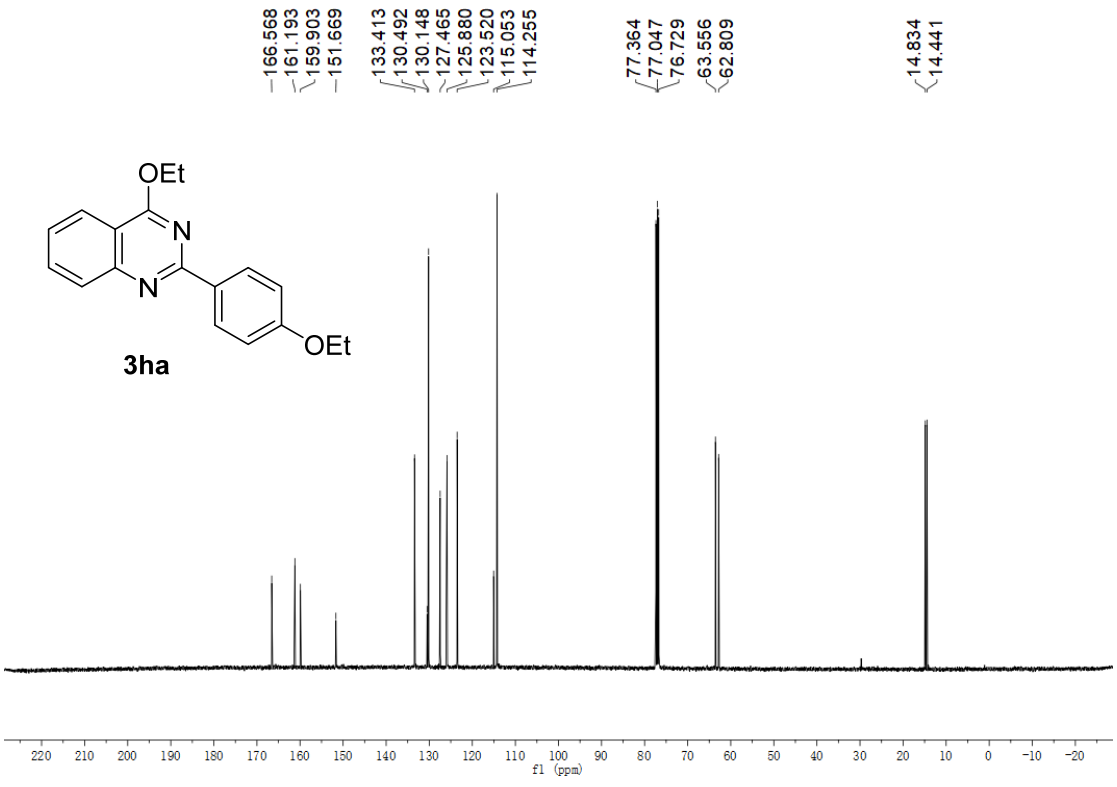
1.566
1.548
1.476
1.458
1.441
OEt
N
N
OEt
3ha
1.96
0.98
0.99
1.01
1.00
1.99
2.00
2.02
3.02
3.01
f1 (ppm)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127.465
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123.520
115.053
114.255
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77.047
76.729
63.556
62.809
14.834
14.441
OEt
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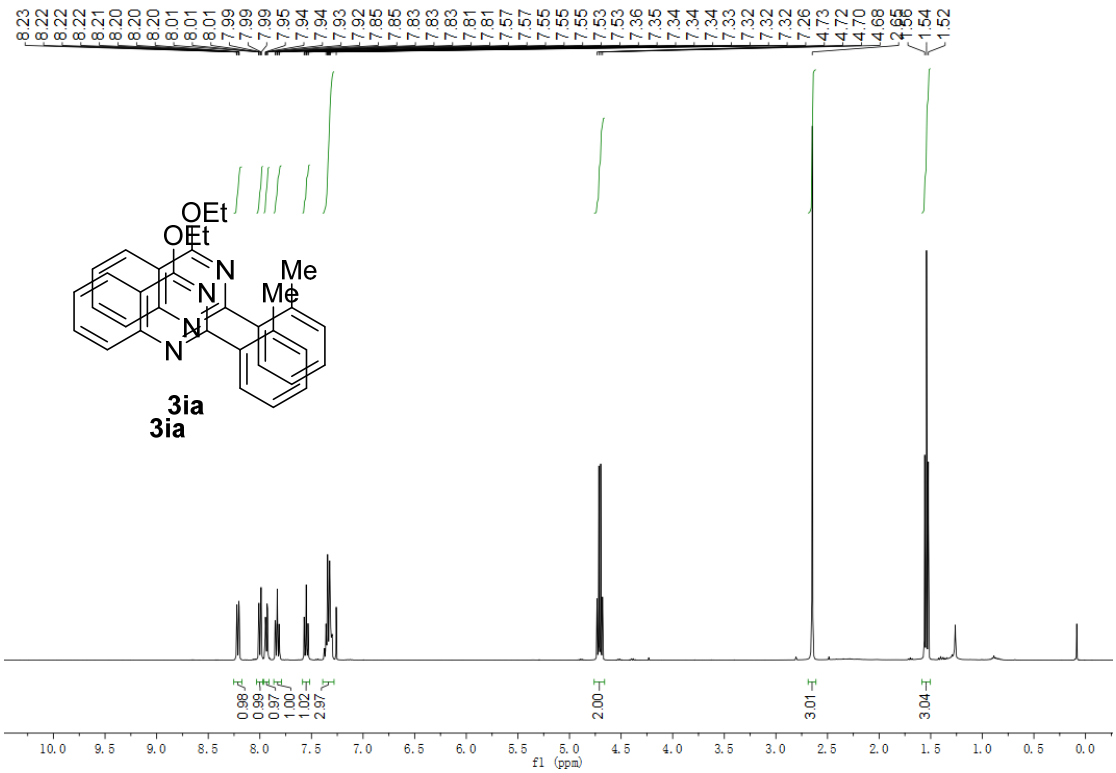
N
OEt
3ha
f1 (ppm)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OEt
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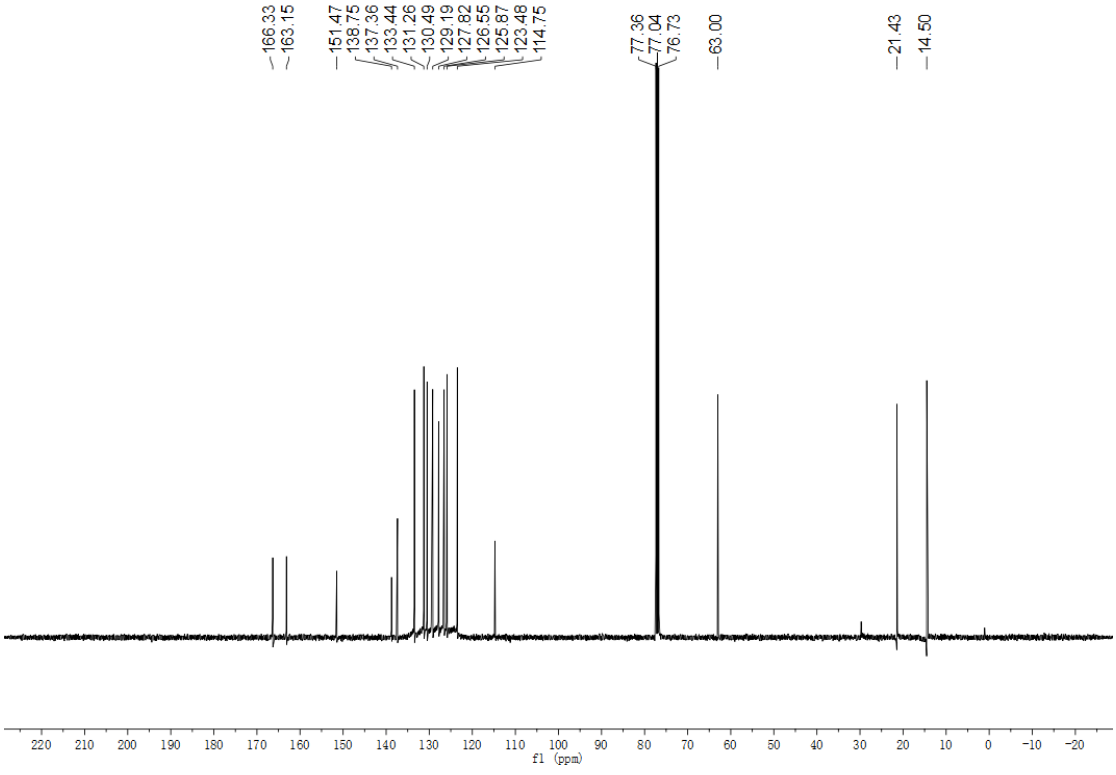
N
N
Me
Me
3ia
3ia
f1 (ppm)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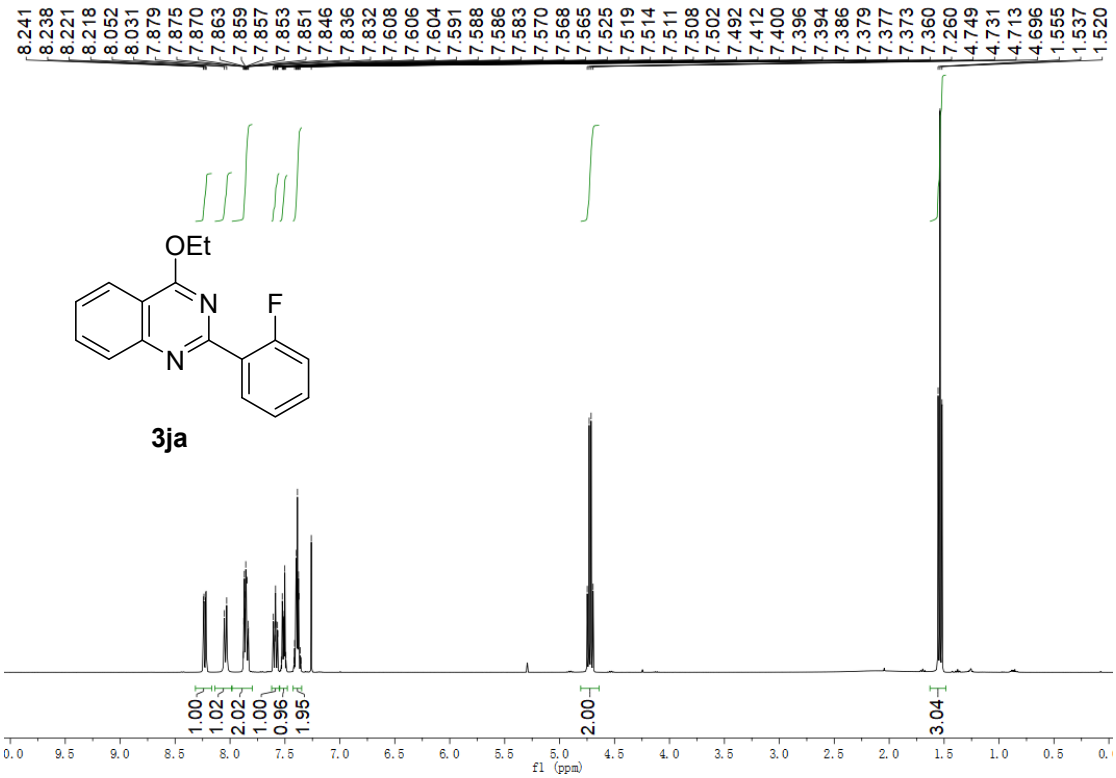
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7.875
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7.863
7.859
7.857
7.853
7.851
7.846
7.836
7.832
7.608
7.606
7.604
7.591
7.588
7.586
7.583
7.570
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7.565
7.525
7.519
7.514
7.511
7.508
7.502
7.492
7.412
7.400
7.396
7.394
7.386
7.379
7.377
7.373
7.360
7.260
4.749
4.731
4.713
4.696
1.555
1.537
1.520
OEt
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F
N
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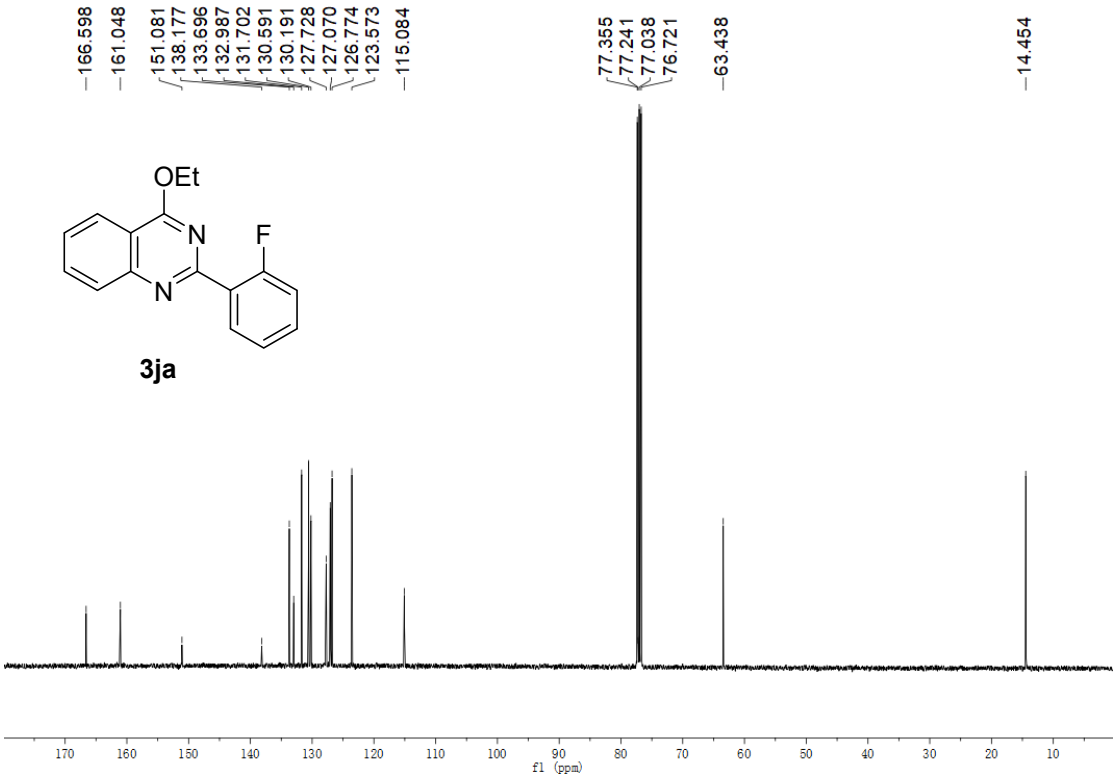
1.02
2.02
1.00
0.96
1.95
2.00
3.04
f1 (ppm)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126.774
123.573
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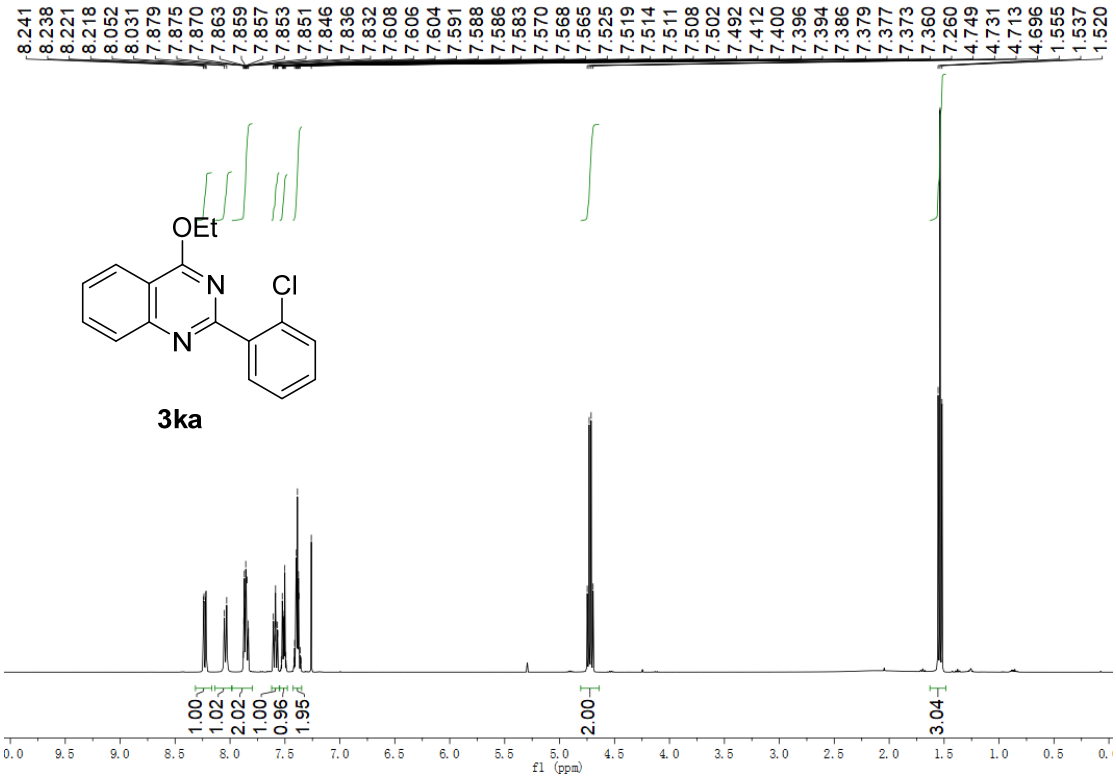
77.241
77.038
76.721
63.438
14.454
OEt
N
F
N
3ja
f1 (ppm)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7.846
7.836
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7.608
7.606
7.604
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7.519
7.514
7.511
7.508
7.502
7.492
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7.400
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7.394
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7.379
7.377
7.373
7.360
7.260
4.749
4.731
4.713
4.696
1.555
1.537
1.520
OEt
N
Cl
N
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1.00
1.02
2.02
1.00
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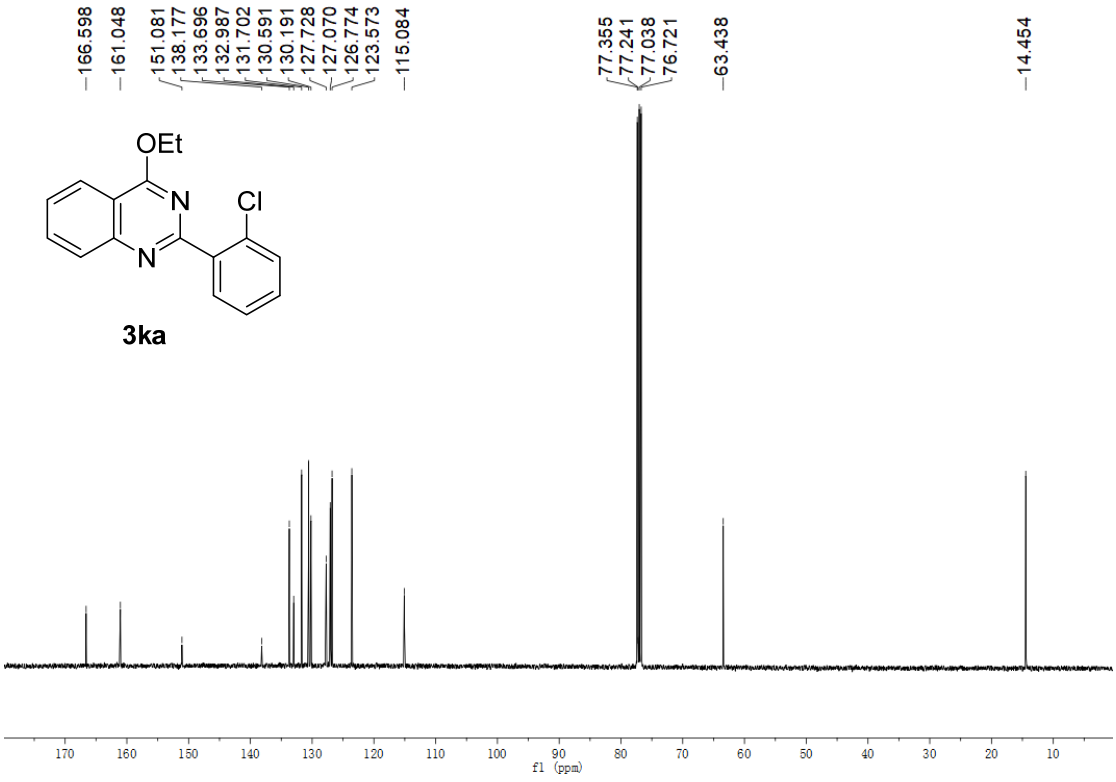
1.95
2.00
3.04
f1 (ppm)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123.573
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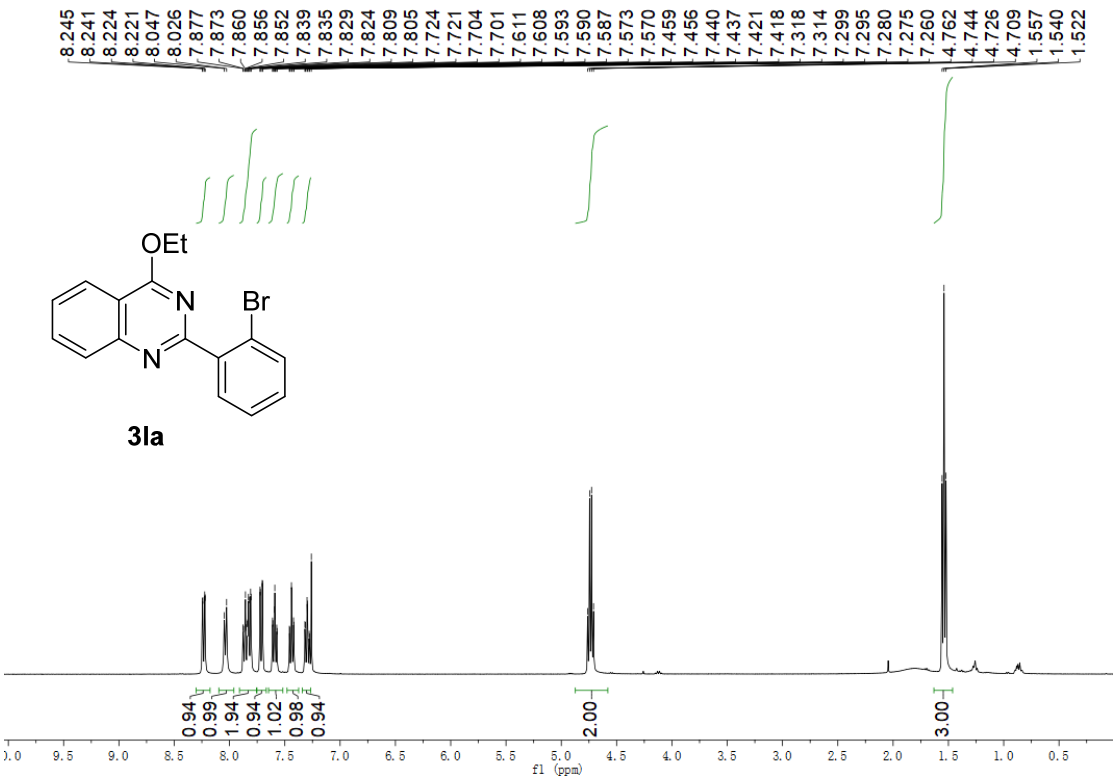
77.241
77.038
76.721
63.438
14.454
OEt
N
Cl
N
3ka
f1 (ppm)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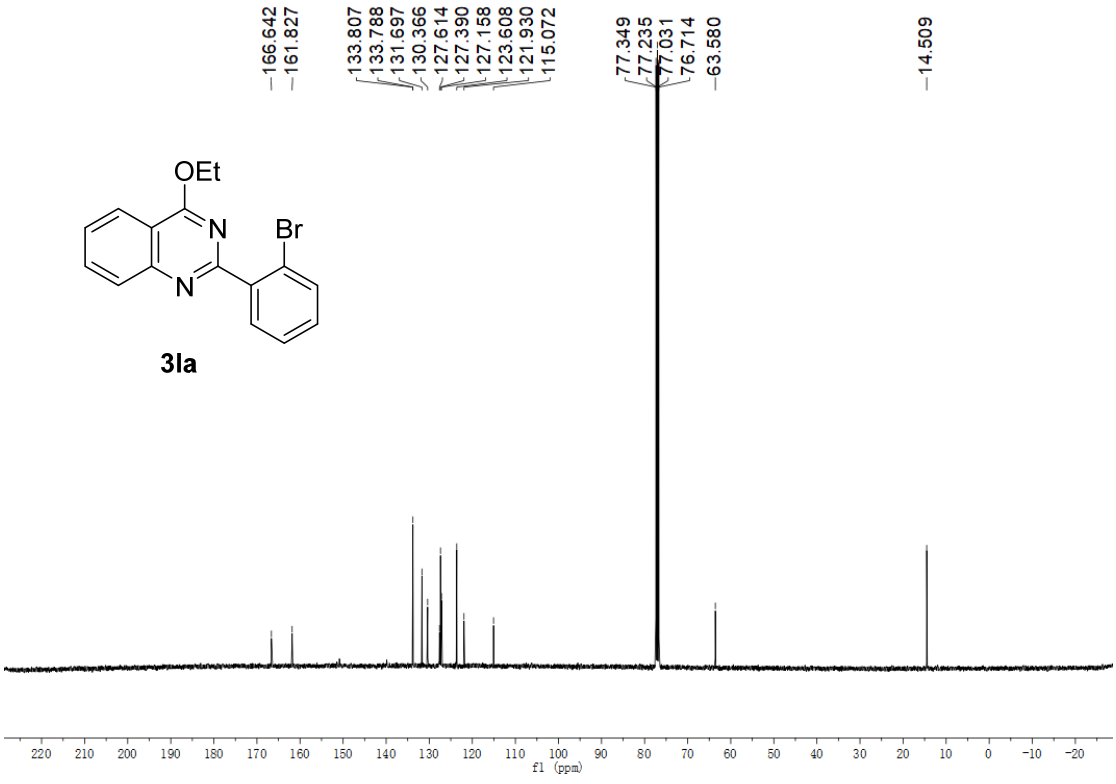
7.835
7.829
7.824
7.809
7.805
7.724
7.721
7.704
7.701
7.611
7.608
7.593
7.590
7.587
7.573
7.570
7.459
7.456
7.440
7.437
7.421
7.418
7.318
7.314
7.299
7.295
7.280
7.275
7.260
4.762
4.744
4.726
4.709
1.557
1.540
1.522
OEt
N
Br
N
0.94
0.99
1.94
0.94
1.02
0.98
0.94
2.00
3.00
f1 (ppm)

3la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127.390
127.158
123.608
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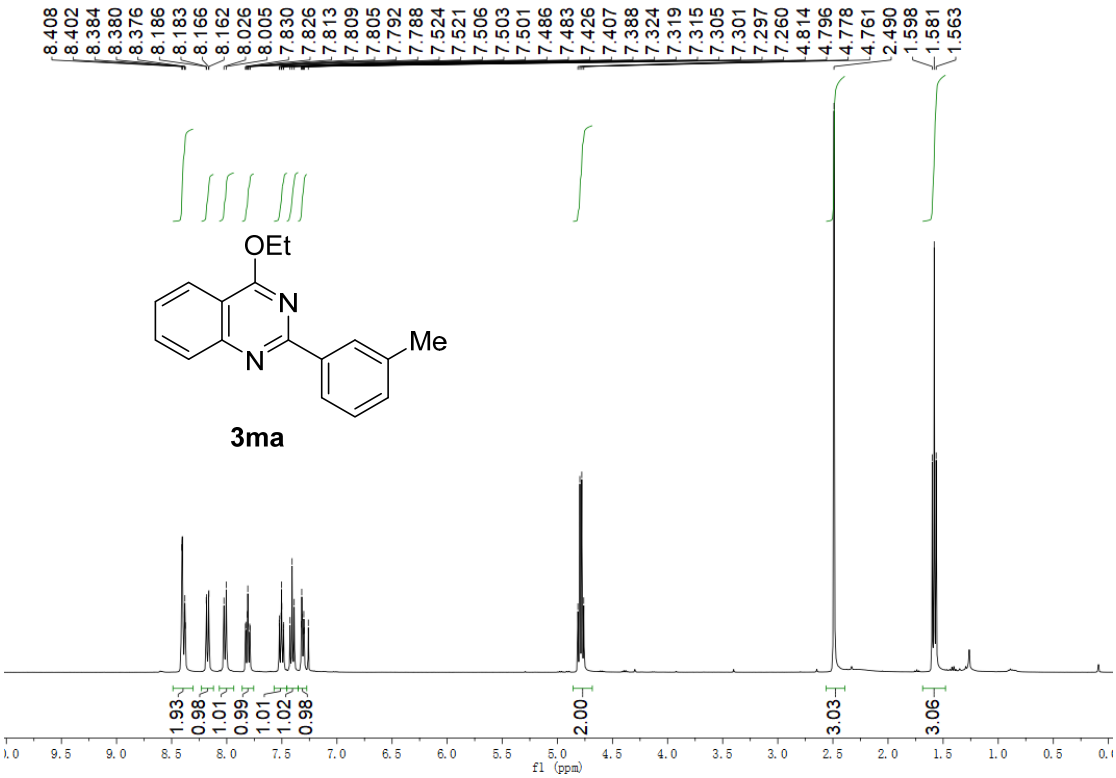
77.235
77.031
76.714
63.580
14.509
OEt
N
Br
N
f1 (ppm)

3la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7.813
7.809
7.805
7.792
7.788
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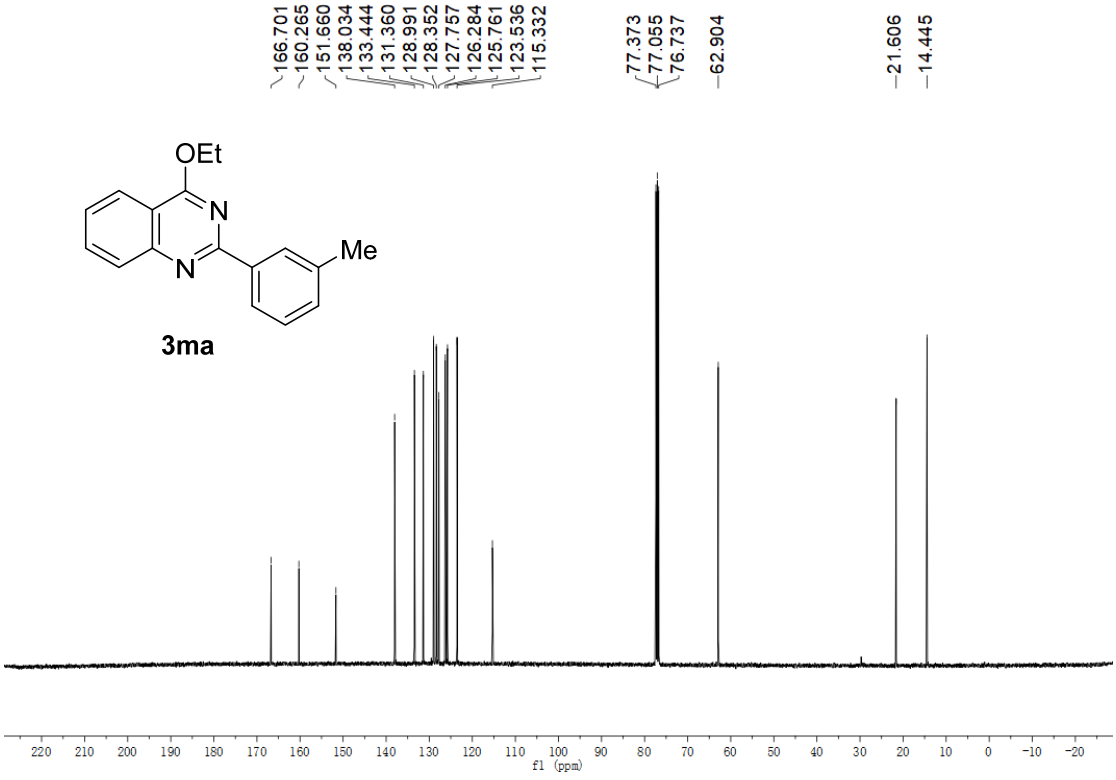
7.521
7.506
7.503
7.501
7.486
7.483
7.426
7.407
7.388
7.324
7.319
7.315
7.305
7.301
7.297
7.260
4.814
4.796
4.778
4.761
2.490
1.598
1.581
1.563
OEt
N
N
Me
3ma
1.93
0.98
1.01
0.99
1.01
1.02
0.98
2.00
3.03
3.06
f1 (ppm)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77.055
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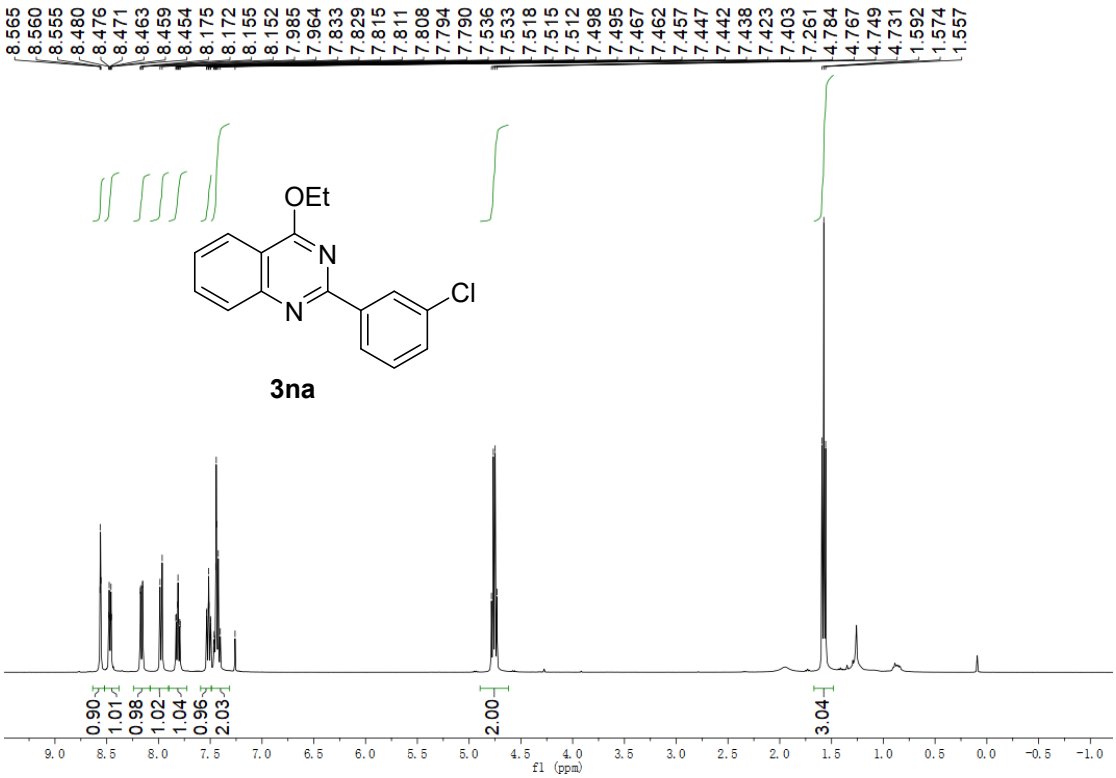
14.445
OEt
N
N
Me
3ma
f1 (ppm)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8.459
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8.175
8.172
8.155
8.152
7.985
7.964
7.833
7.829
7.815
7.811
7.808
7.794
7.790
7.536
7.533
7.518
7.515
7.512
7.498
7.495
7.467
7.462
7.457
7.447
7.442
7.438
7.423
7.403
7.261
4.784
4.767
4.749
4.731
1.592
1.574
1.557
OEt
N
N
Cl
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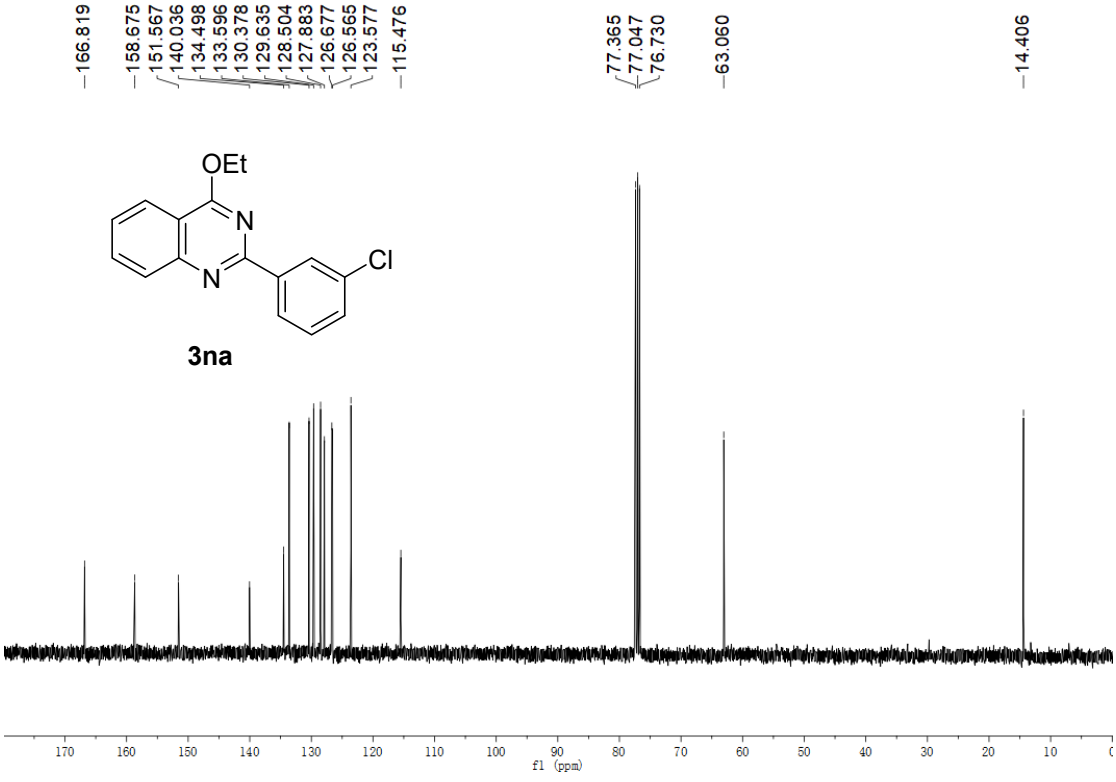
1.01
0.98
1.02
1.04
0.96
2.03
2.00
3.04
f1 (ppm)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77.047
76.730
63.060
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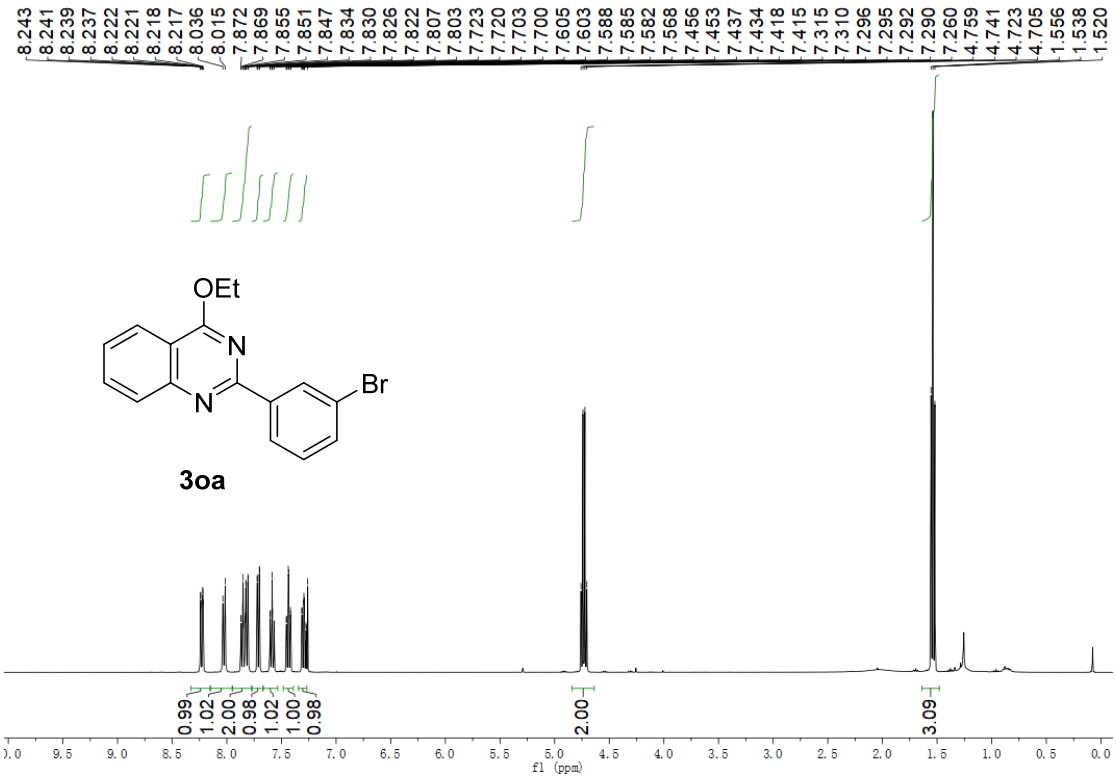
OEt
N
N
Cl
3na
f1 (ppm)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7.869
7.855
7.851
7.847
7.834
7.830
7.826
7.822
7.807
7.803
7.723
7.720
7.703
7.700
7.605
7.603
7.588
7.585
7.582
7.568
7.456
7.453
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7.434
7.418
7.415
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7.295
7.292
7.290
7.260
4.759
4.741
4.723
4.705
1.556
1.538
1.520
OEt
N
N
Br
3oa
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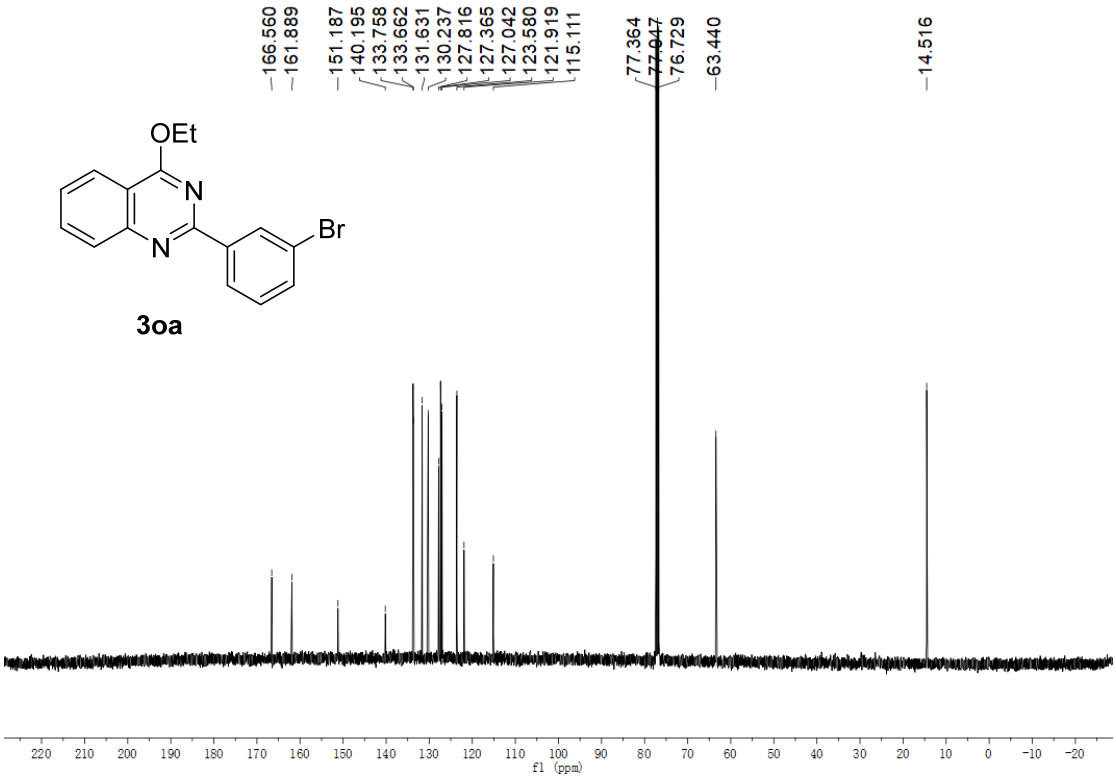
1.02
2.00
0.98
1.02
1.00
0.98
2.00
3.09
f1 (ppm)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123.580
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77.047
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OEt
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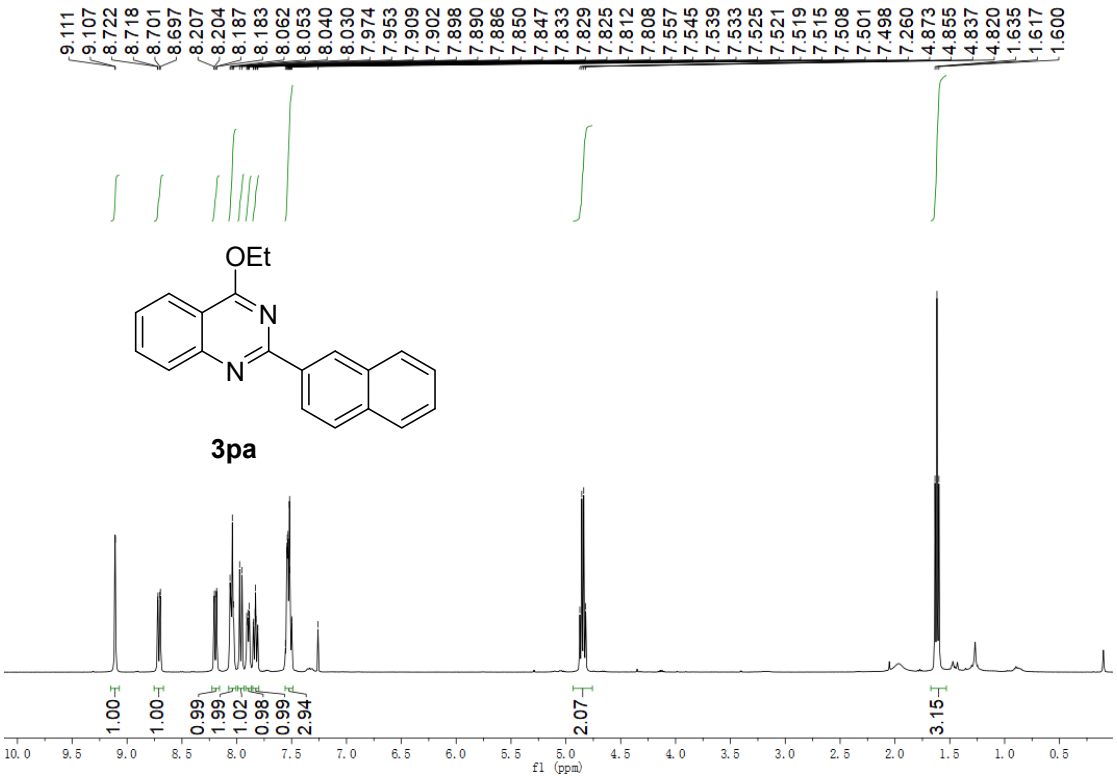
N
Br
3oa
f1 (ppm)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8.183
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8.053
8.040
8.030
7.974
7.953
7.909
7.902
7.898
7.890
7.886
7.850
7.847
7.833
7.829
7.825
7.812
7.808
7.557
7.545
7.539
7.533
7.525
7.521
7.519
7.515
7.508
7.501
7.498
7.260
4.873
4.855
4.837
4.820
1.635
1.617
1.600
OEt
N
N
3pa
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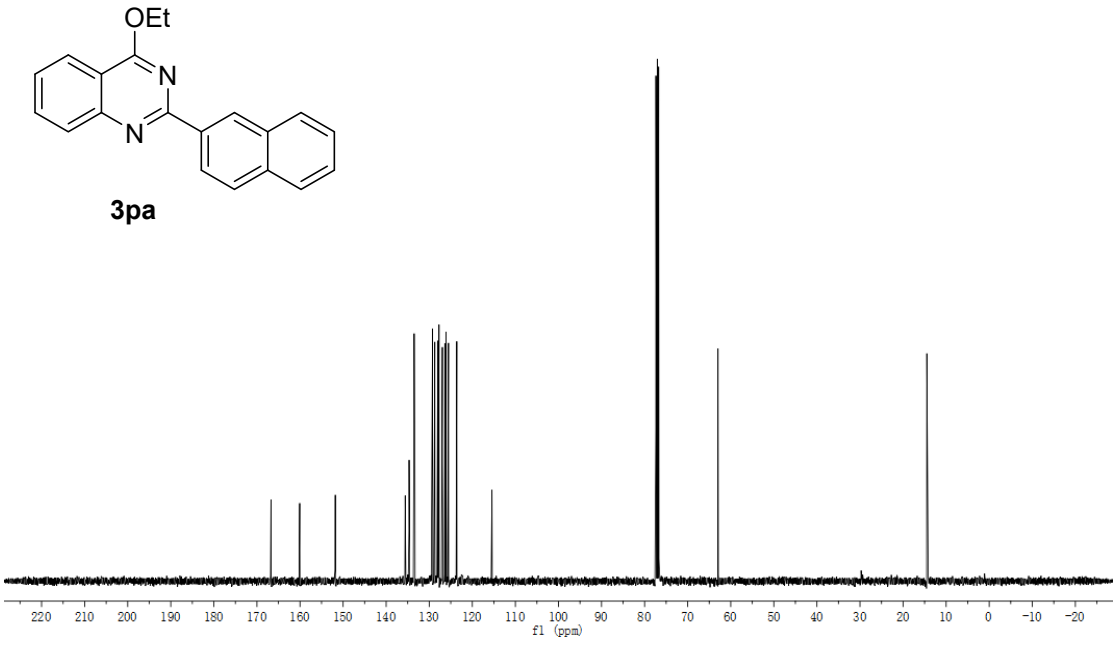
1.00
0.99
1.99
1.02
0.98
0.99
2.94
2.07
3.15
f1 (ppm)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126.95
126.37
126.12
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77.37
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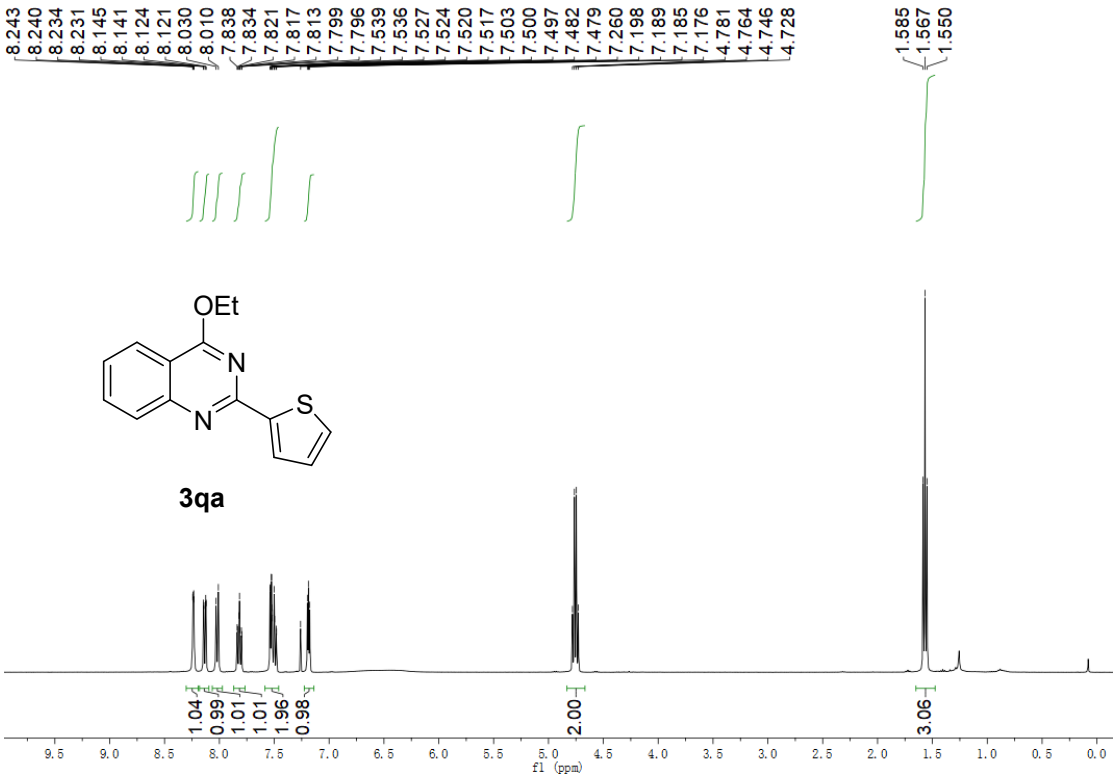
76.74
62.96
14.48
OEt
N
N
3pa
f1 (ppm)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7.821
7.817
7.813
7.799
7.796
7.539
7.536
7.527
7.524
7.520
7.517
7.503
7.500
7.497
7.482
7.479
7.260
7.198
7.189
7.185
7.176
4.781
4.764
4.746
4.728
1.585
1.567
1.550
OEt
N
N
S
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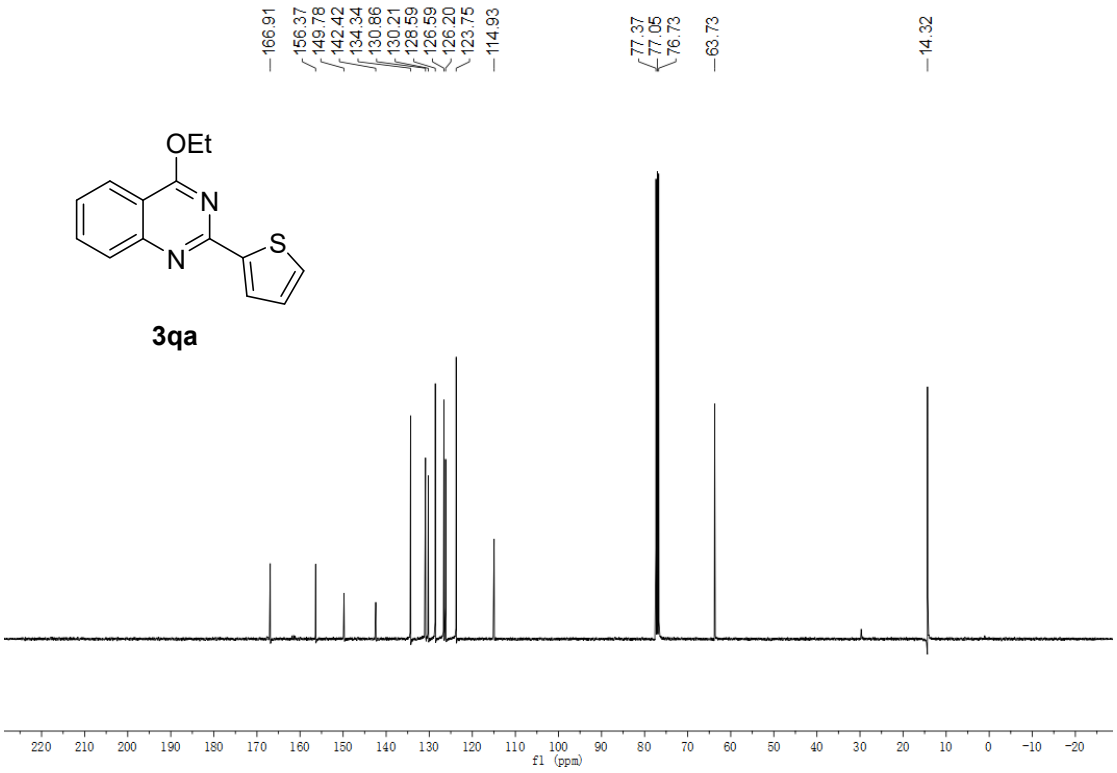
0.99
1.01
1.01
1.96
0.98
2.00
3.06
f1 (ppm)

3qa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128.59
126.59
126.20
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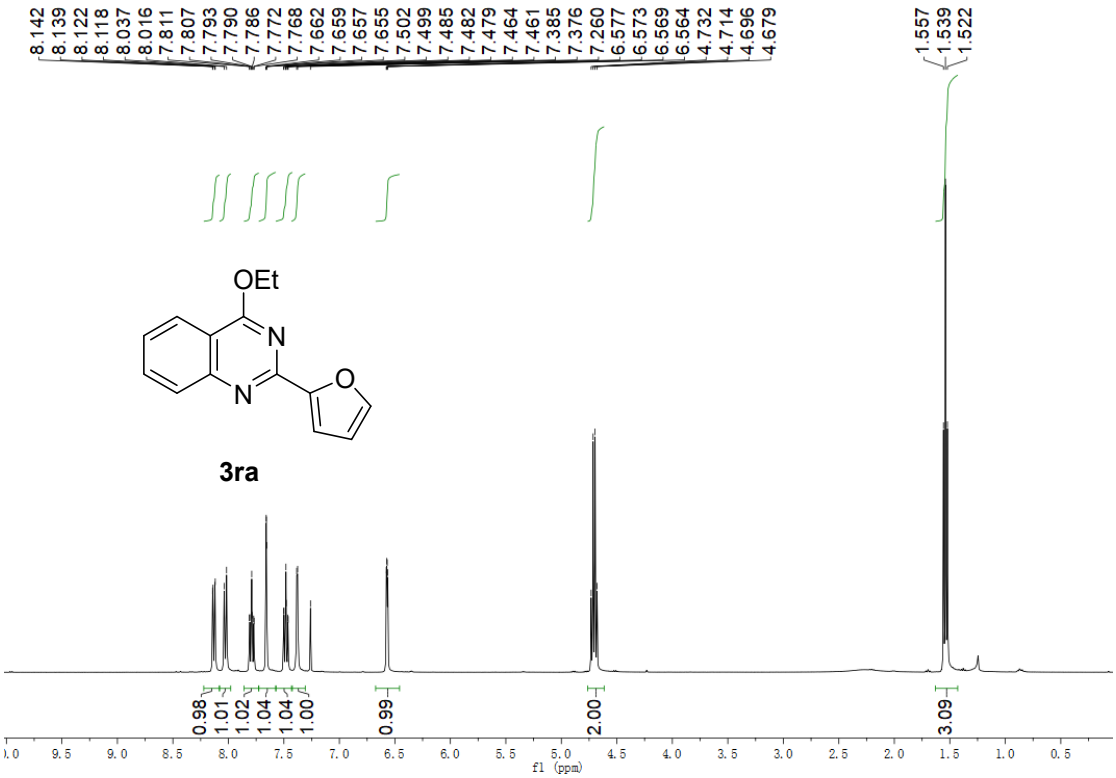
77.37
77.05
76.73
63.73
14.32
OEt
N
N
S
f1 (ppm)

3qa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7.768
7.662
7.659
7.657
7.655
7.502
7.499
7.485
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7.479
7.464
7.461
7.385
7.376
7.260
6.577
6.573
6.569
6.564
4.732
4.714
4.696
4.679
1.557
1.539
1.522
OEt
N
N
O
3ra
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1.04
1.04
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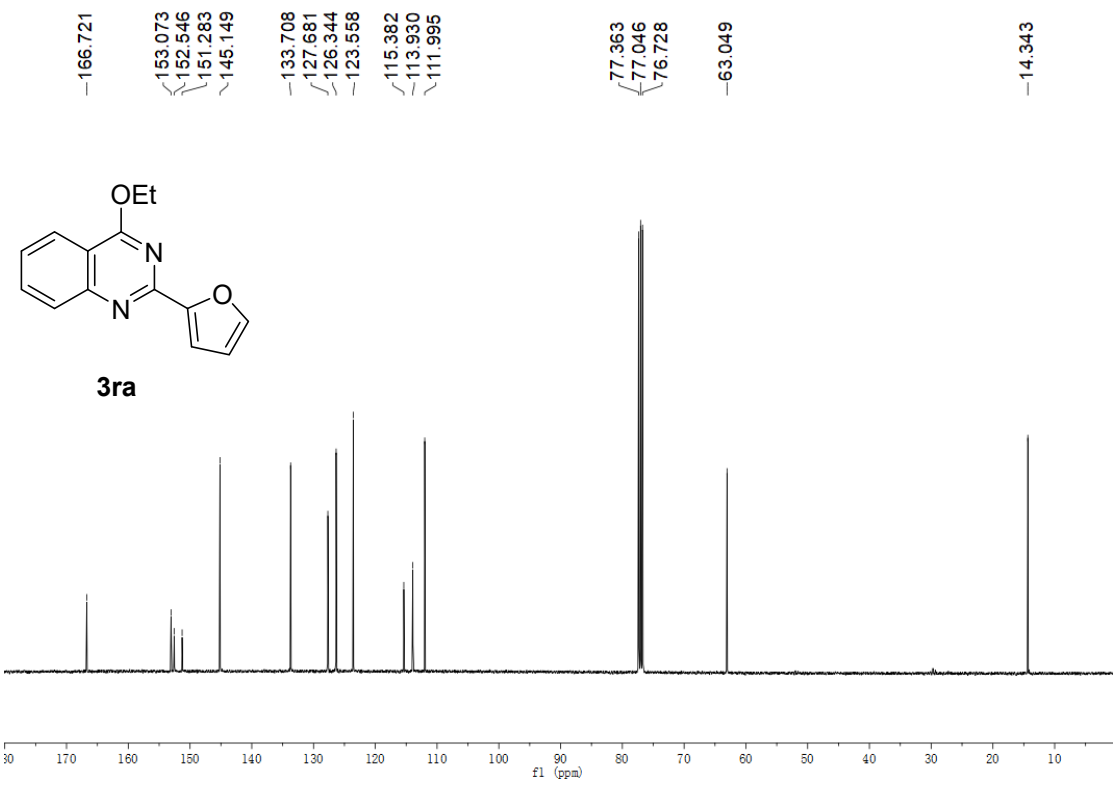
0.99
2.00
3.09
f1 (ppm)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115.382
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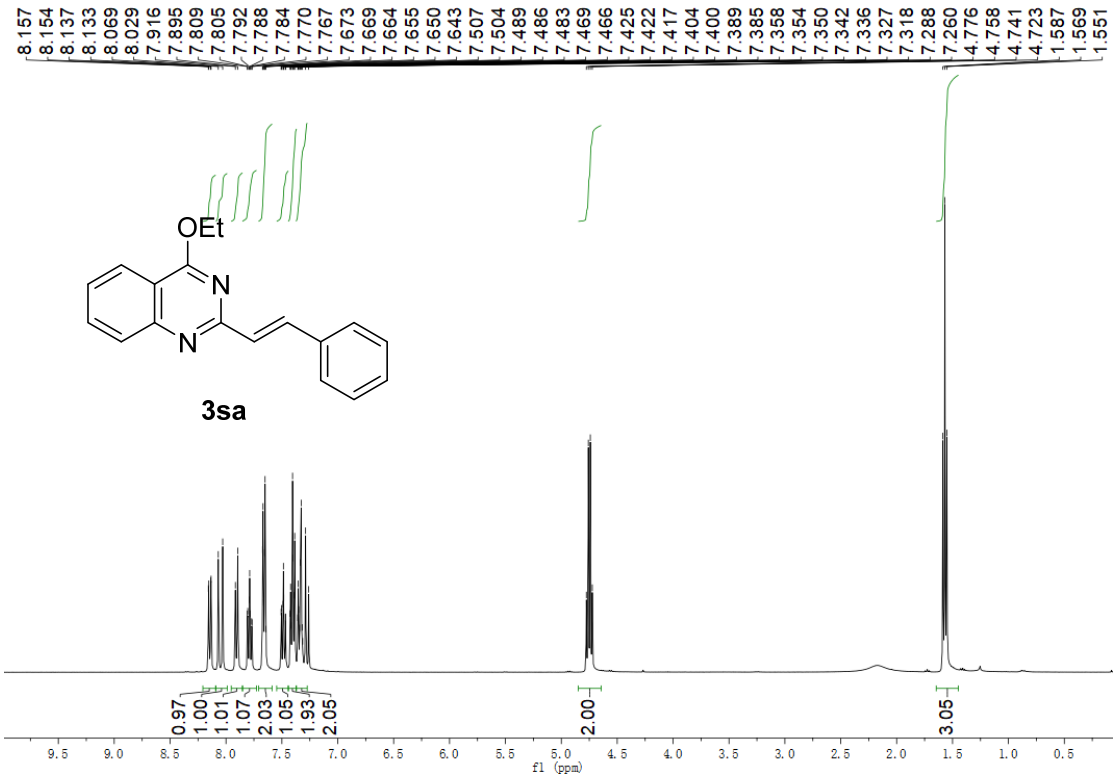
77.046
76.728
63.049
14.343
OEt
N
N
O
3ra
f1 (ppm)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7.788
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7.770
7.767
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7.669
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7.354
7.350
7.342
7.336
7.327
7.318
7.288
7.260
4.776
4.758
4.741
4.723
1.587
1.569
1.551
OEt
N
N
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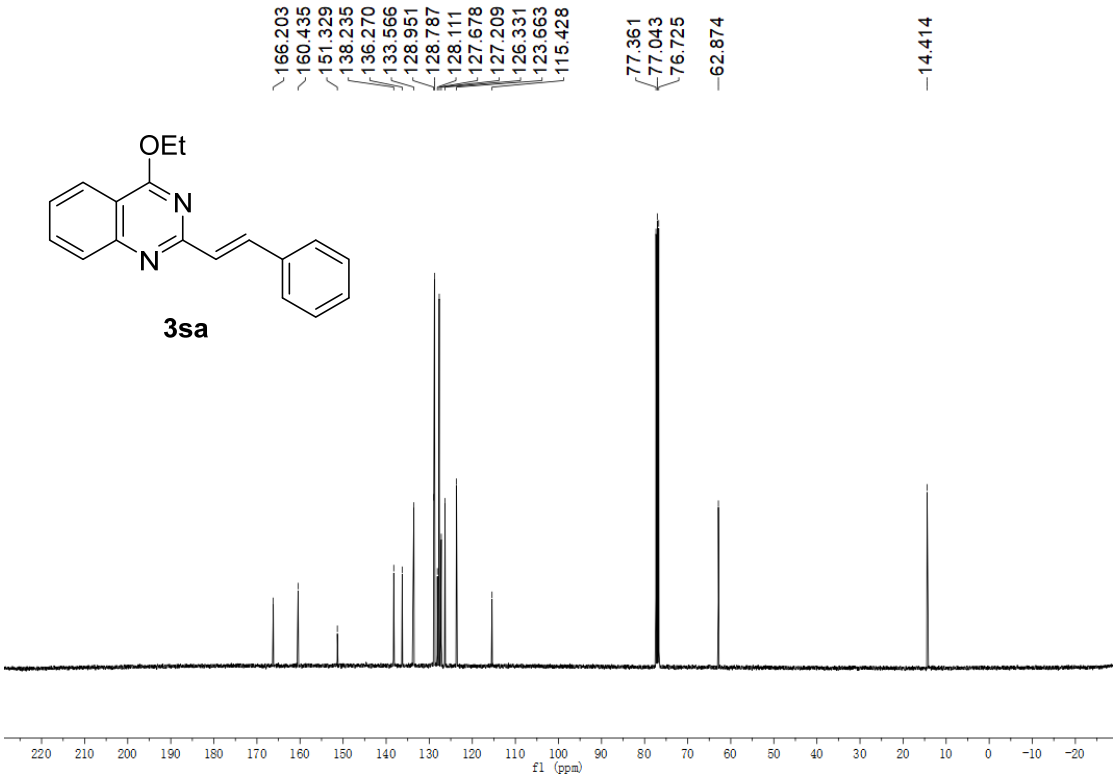
1.07
2.03
1.05
1.93
2.05
2.00
3.05
f1 (ppm)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128.787
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127.678
127.209
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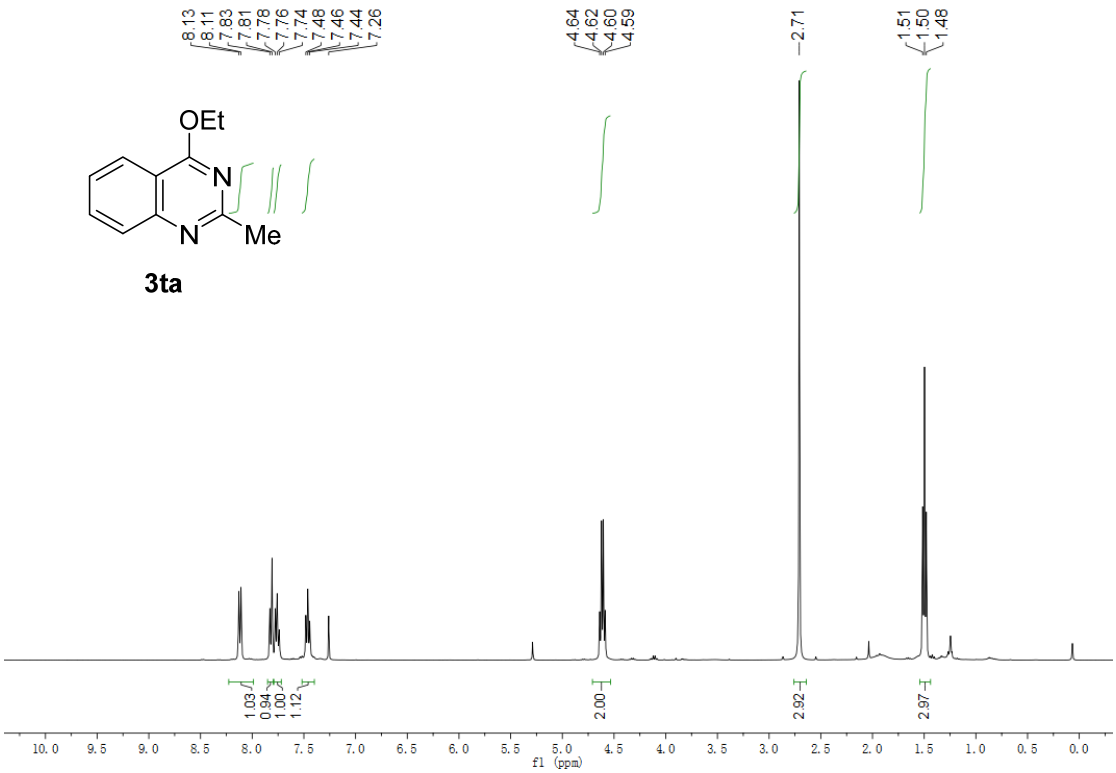
77.043
76.725
62.874
14.414
OEt
N
N
3sa
f1 (ppm)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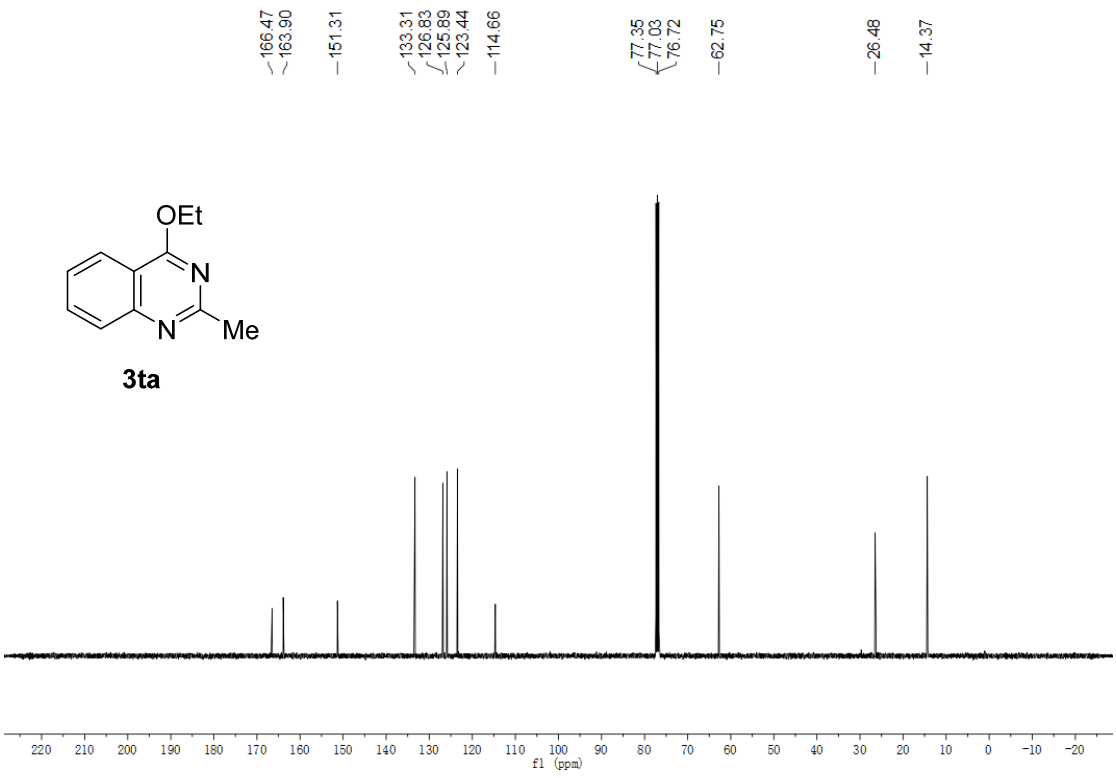
7.46
7.44
7.26
4.64
4.62
4.60
4.59
2.71
1.51
1.50
1.48
OEt
N
N
Me
3ta
1.03
0.94
1.00
1.12
2.00
2.92
2.97
f1 (ppm)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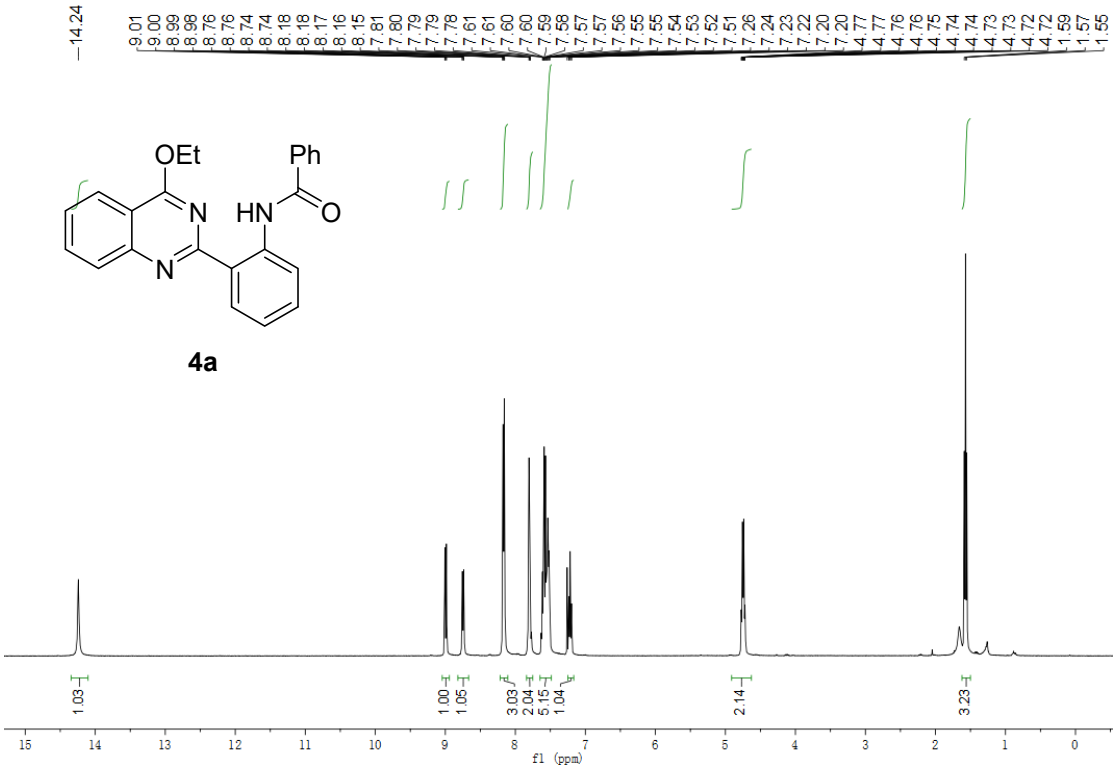
OEt
N
N
Me
3ta
f1 (ppm)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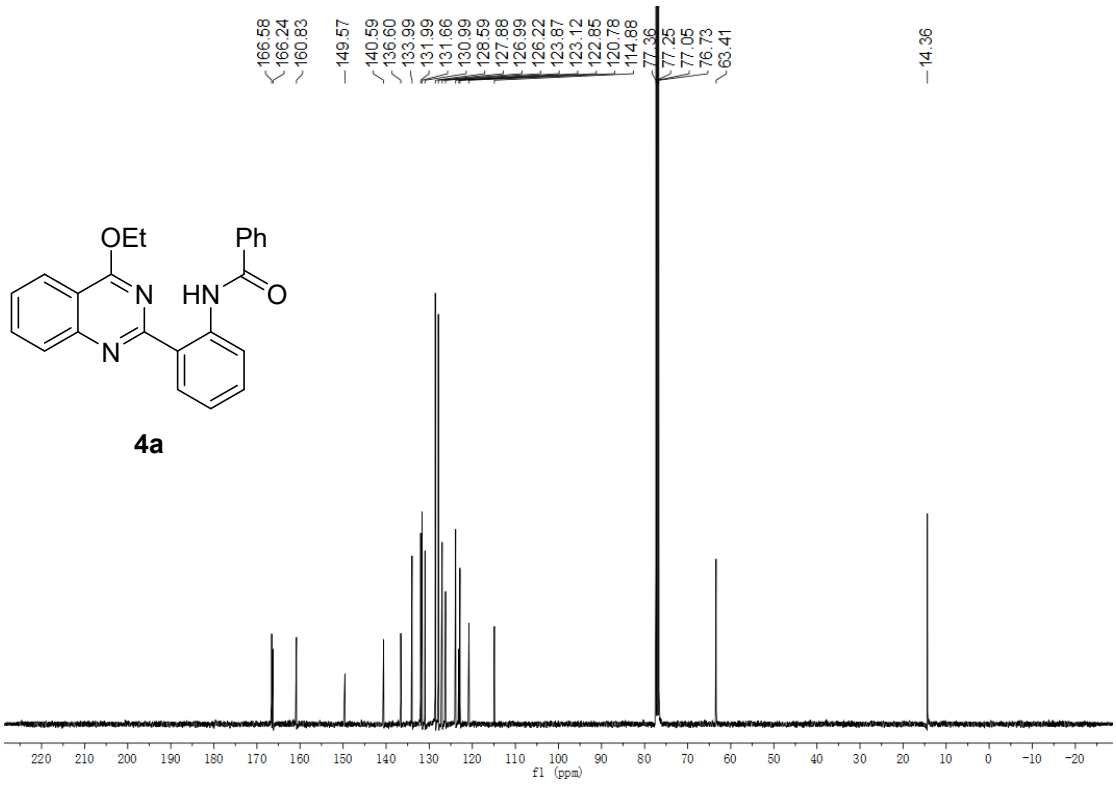
8.18
8.18
8.17
8.16
8.15
7.81
7.80
7.79
7.79
7.78
7.61
7.61
7.60
7.60
7.59
7.58
7.57
7.57
7.56
7.55
7.55
7.54
7.53
7.52
7.51
7.26
7.24
7.23
7.22
7.20
7.20
4.77
4.77
4.76
4.76
4.75
4.74
4.74
4.73
4.73
4.72
4.72
1.59
1.57
1.55
OEt
Ph
N
HN
O
N
1.03
1.00
1.05
3.03
2.04
5.15
1.04
2.14
3.23
f1 (ppm)

4a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166.24
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140.59
136.60
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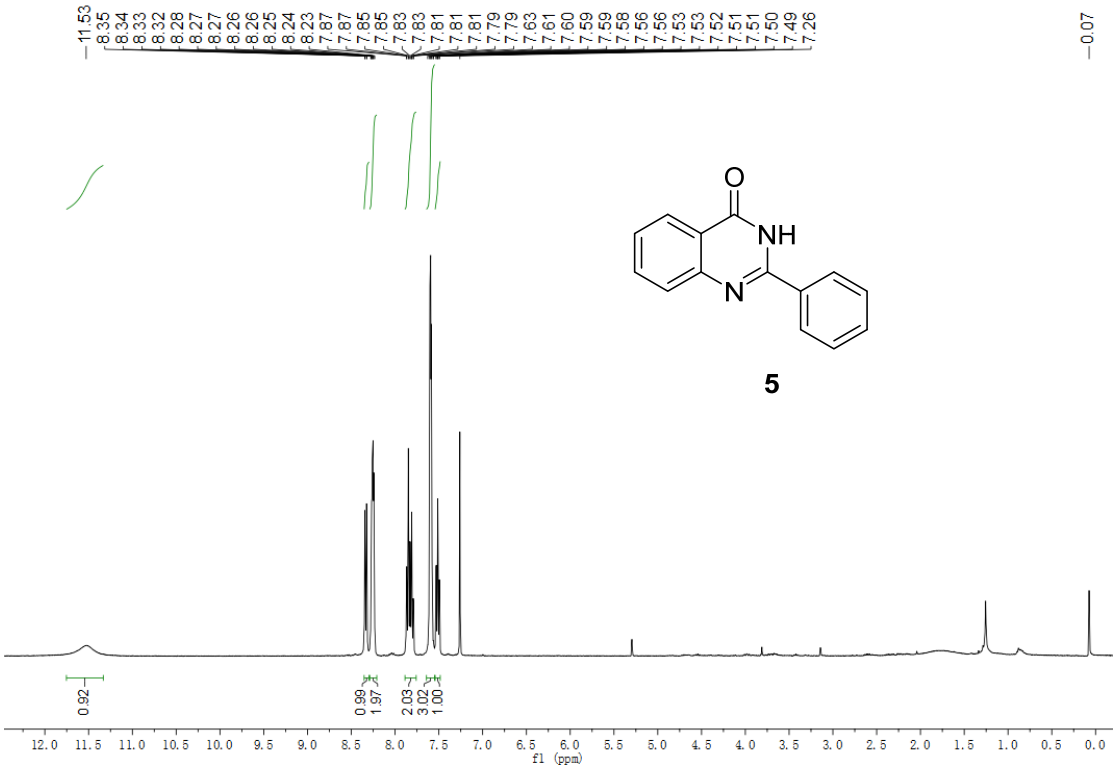
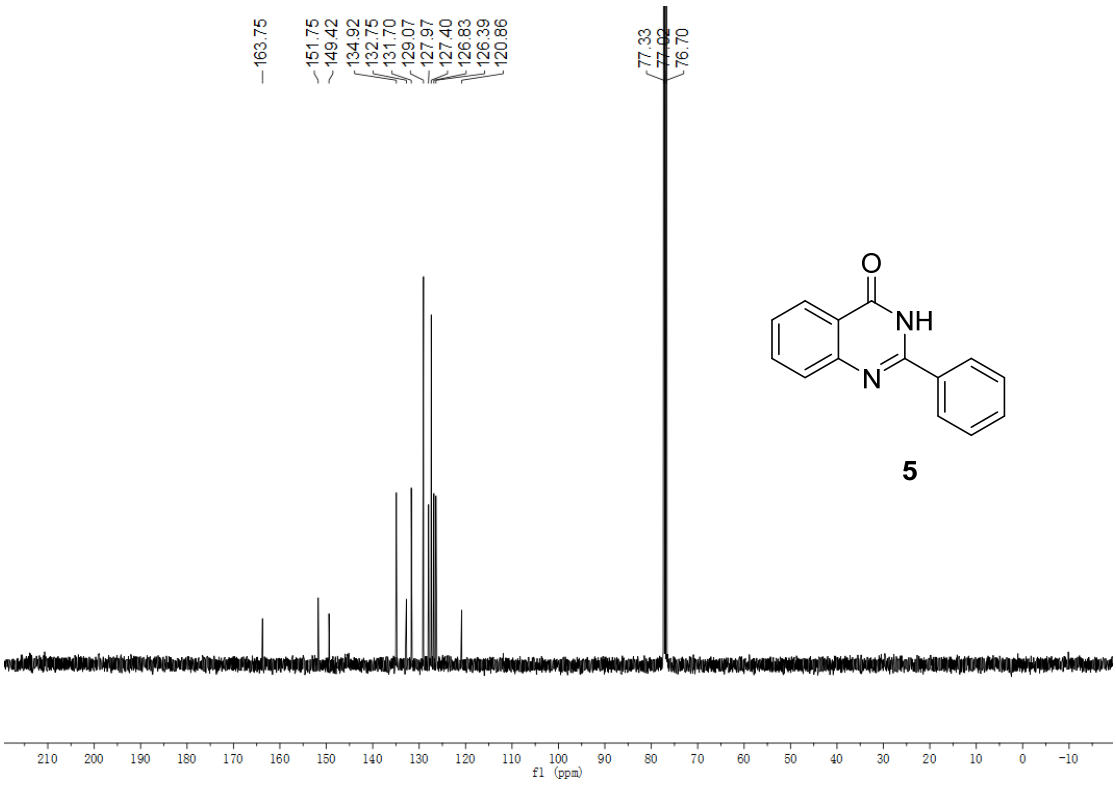
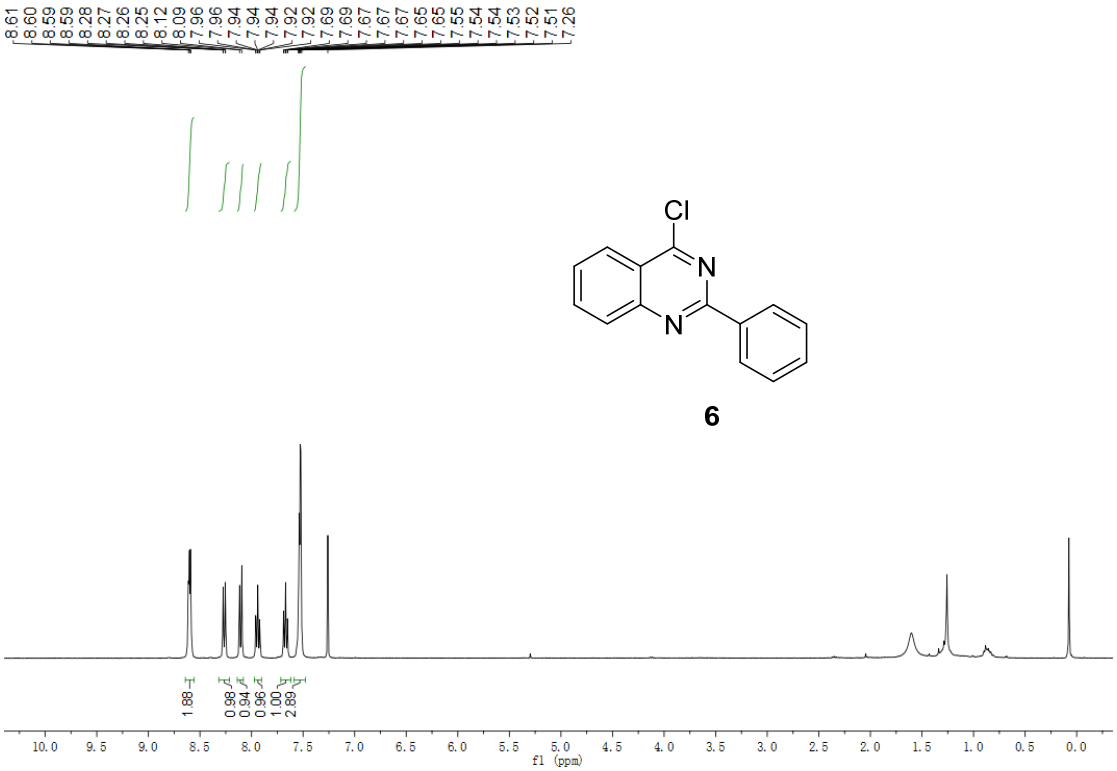
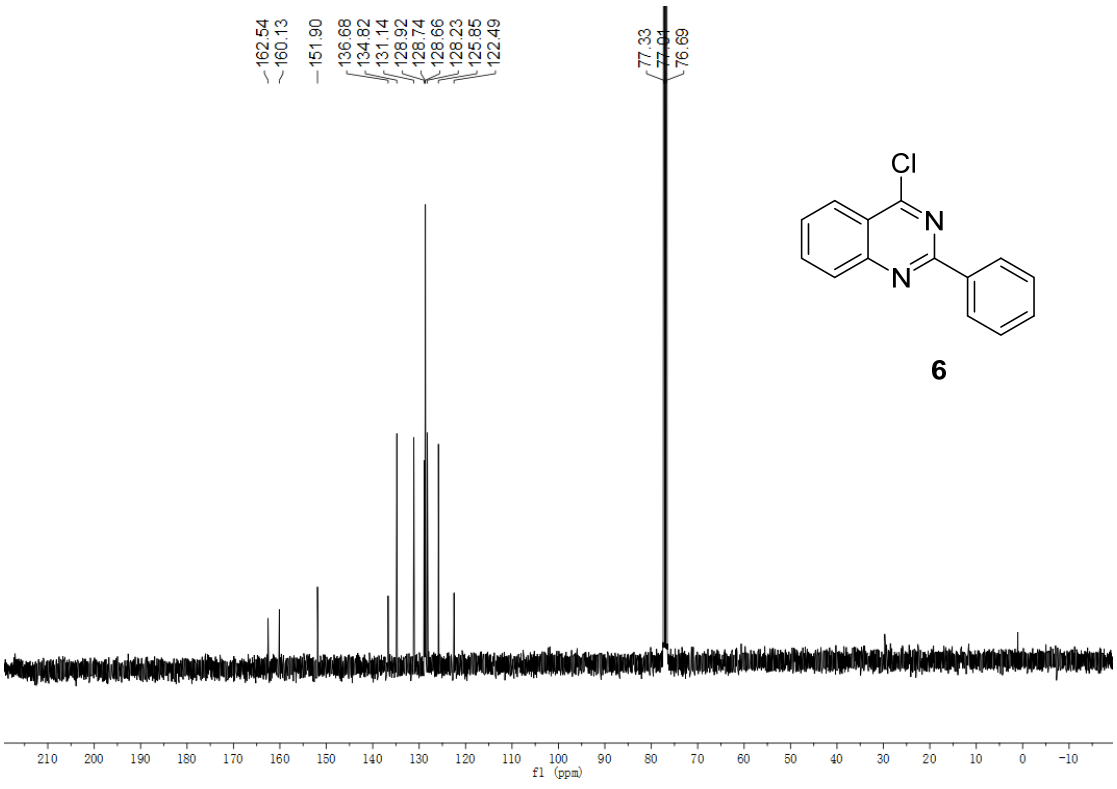
131.99
131.66
130.99
128.59
127.88
126.99
126.22
123.87
123.12
122.85
120.78
114.88
77.36
77.25
77.05
76.73
63.41
14.36
OEt
Ph
N
HN
O
N
f1 (ppm)

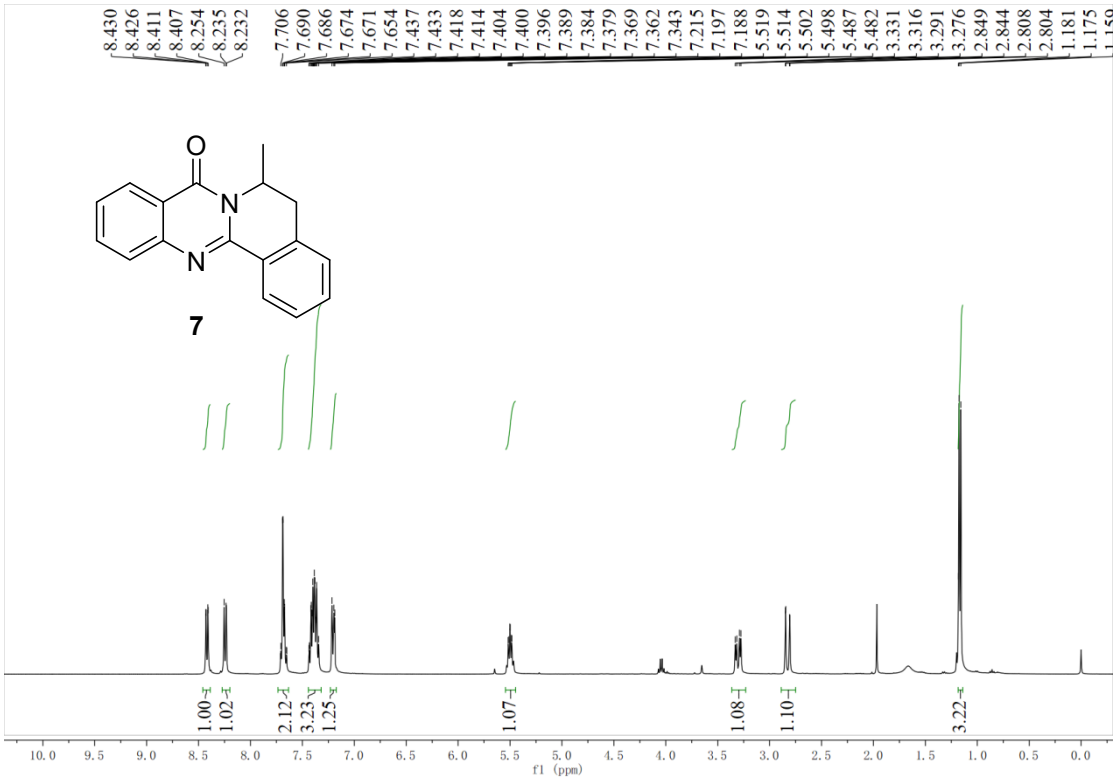
4a

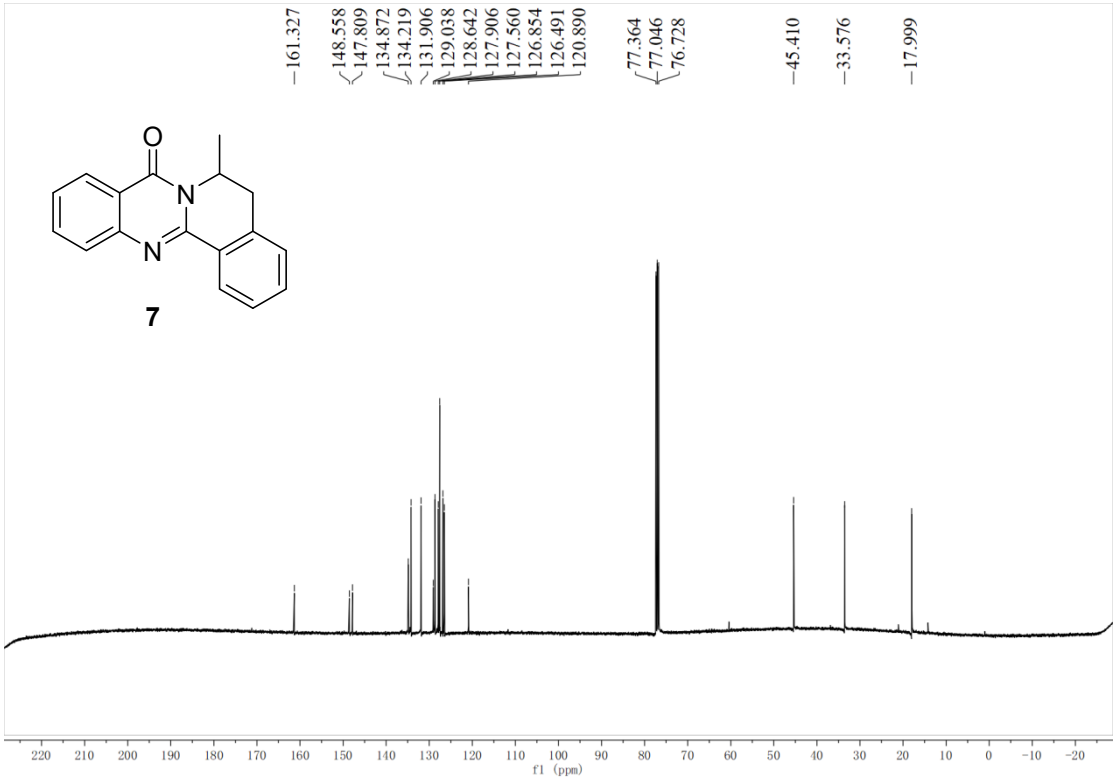

11.53
8.35
8.34
8.33
8.32
8.28
8.27
8.27
8.26
8.26
8.25
8.24
8.23
7.87
7.87
7.85
7.85
7.83
7.83
7.81
7.81
7.81
7.79
7.79
7.63
7.61
7.60
7.59
7.59
7.58
7.56
7.56
7.53
7.53
7.52
7.51
7.51
7.50
7.49
7.26
0.07
O
NH
N
5
0.92
0.99
1.97
2.03
3.02
1.00
f1 (ppm)


163.75
151.75
149.42
134.92
132.75
131.70
129.07
127.97
127.40
126.83
126.39
120.86
77.33
77.02
76.70
O
NH
N
5
f1 (ppm)


8.61
8.60
8.59
8.59
8.28
8.27
8.26
8.25
8.12
8.09
7.96
7.96
7.94
7.94
7.94
7.92
7.92
7.69
7.69
7.67
7.67
7.67
7.65
7.65
7.55
7.54
7.54
7.53
7.52
7.51
7.26
Cl
N
N
6
1.88
0.98
0.94
0.96
1.00
2.89
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
f1 (ppm)


162.54
160.13
151.90
136.68
134.82
131.14
128.92
128.74
128.66
128.23
125.85
122.49
77.33
77.01
76.69
Cl
N
N
6
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


8.430
8.426
8.411
8.407
8.254
8.235
8.232
7.706
7.690
7.686
7.674
7.671
7.654
7.437
7.433
7.418
7.414
7.404
7.400
7.396
7.389
7.384
7.379
7.369
7.362
7.343
7.215
7.197
7.188
5.519
5.514
5.502
5.498
5.487
5.482
3.331
3.316
3.291
3.276
2.849
2.844
2.808
2.804
1.181
1.175
O
N
N
7
1.00
1.02
2.12
3.23
1.25
1.07
1.08
1.10
3.22
f1 (ppm)


161.327
148.558
147.809
134.872
134.219
131.906
129.038
128.642
127.906
127.560
126.854
126.491
120.890
77.364
77.046
76.728
45.410
33.576
17.999
O
N
N
7
f1 (ppm)