Supporting Information

Palladium-Catalyzed Carbonylative Cyclization of Benzyl Chlo-rides with Anthranils for the Synthesis of 3-Arylquinolin-2(1H)-ones

Jian-Li Liu,† Ren-Rui Xu, † Wei Wang,† Xinxin Qi,*,† Xiao-Feng Wu*,‡

†Department of Chemistry, Zhejiang Sci-Tech University, Hangzhou, Zhejiang 310018, People's Republic of China.

‡Dalian National Laboratory for Clean Energy, Dalian Institute of Chemical Physics, Chinese Academy of Sciences, 116023, Dalian, Liaoning, China; Leibniz-Institut für Katalyse e.V. an der, Institution Universität Rostock, Albert-Einstein-Straße 29a, Rostock 18059, Germany

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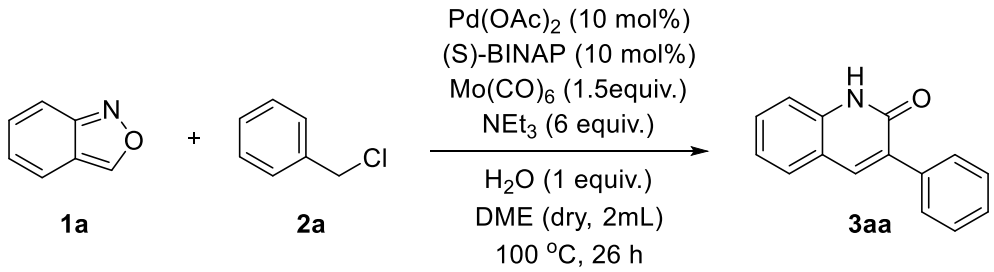
1. General Information

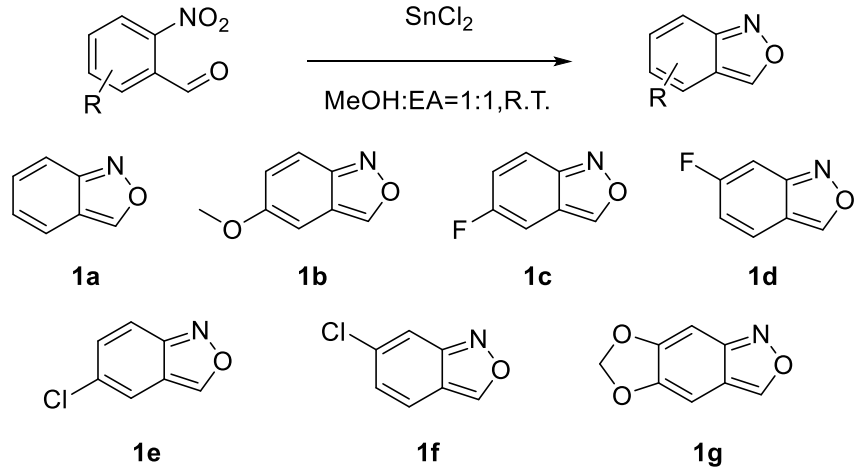
Unless otherwise noted, all reactions were carried out under a nitrogen atmosphere. All reagents were from commercial sources, all solvents are extra dry solvents and used as received without further purification. Column chromatography was performed on silica gel (200-300 meshes) using petroleum ether (b.p. 60 - 90 °C) and ethyl acetate as the eluents. ^{1}H and ^{13}C NMR spectra were taken on 400 MHz instruments and spectral data were reported in ppm relative to tetramethylsilane (TMS) as the internal standard and $CDCl_3$ or DMSO-D_6 as solvent. All coupling constants (*J*) are reported in Hz with the following abbreviations: s = singlet, d = doublet, dd = double doublet, ddd = double doublet of doublets, t = triplet, dt = double triplet, q = quartet, m = multiplet, br = broad. Gas (GC) analyses were performed on a Shimadzu GC-2014C chromatograph equipped with FID detector. Mass spectra (MS) were measured on spectrometer by direct inlet at 70 eV.

2. General Procedure



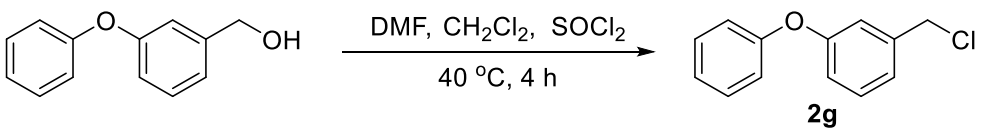
$Pd(OAc)_2$ (10 mol%, 11.3 mg), (*S*)-BINAP (10 mol%, 31.4 mg), $Mo(CO)_6$ (0.75 mmol, 198.0 mg), were added to an oven-dried tube (15.0 mL), which was then placed under vacuum and refilled with nitrogen for three times. **1a** (0.5 mmol, 59.5 mg), **2a** (1.25 mmol, 158.3 mg), NEt_3 (3.0 mmol, 303.6 mg), H_2O (0.5 mmol, 9.0 μL), and DME (2.0 mL) were added into the tube via a syringe. The tube was sealed and the mixture was stirred at 100 °C for 26 h. After the reaction was completed, the crude mixture was filtered and concentrated under vacuum. The crude product was purified by column chromatography (DCM/EA = 20/1 to 5/1) on silica gel to afford the products.

3.1 Synthesis of Substituted 2,1-Benzisoxazoles (1a - 1g[1])



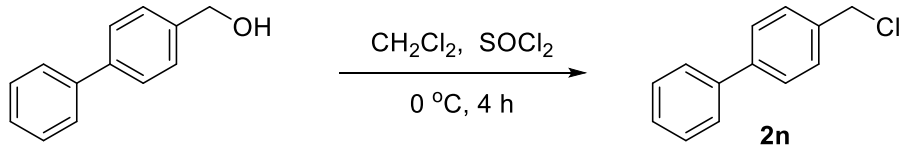
To a solution of substituted 2-nitroacylbenzene (3.0 mmol) in MeOH/EtOAc (1/1, 20.0 mL) was added $SnCl_2$ (9.0 mmol, 1.7 g) in three portions at room temperature. The mixture was stirred at room temperature for 24 h. The reaction was quenched by sat. $NaHCO_3$ (20.0 ml) and filtered. The aqueous phase was extracted with EtOAc (3 × 10.0 mL), the combined organic layers was washed with brine (30.0 mL), dried over with Na_2SO_4, filtered and concentrated. The residue was purified by silica gel column chromatography (petroleum ether/ethyl acetate = 20/1) to give **1a - 1g**.

3.2 Synthesis of Starting Materials (2g[2], 2n[3], 2q[4])



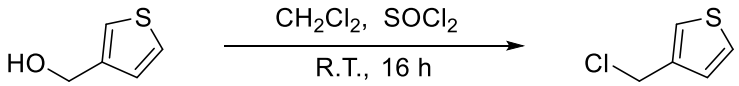
An oven-dried round-bottom flask was charged under air with 3-phenoxyphenol (4.0 mmol, 0.8 g), dichloromethane (20.0 mL), and thionyl chloride (24.0 mmol, 2.9 g), a catalytic amount of DMF was

added in slowly and stirred at room temperature, then stirred the reaction mixture at 40 °C for 4 h. The reaction mixture was then washed with H_2O (40.0 mL) and extracted with DCM (25.0 mL) for three times. The combined organic phases were dried over magnesium sulfate, filtered through short celite pad, and concentrated under reduced pressure. Purification by column chromatography (PE/EA = 100/1) afforded **2g** as a white solid (0.75 g, 86%).



2n

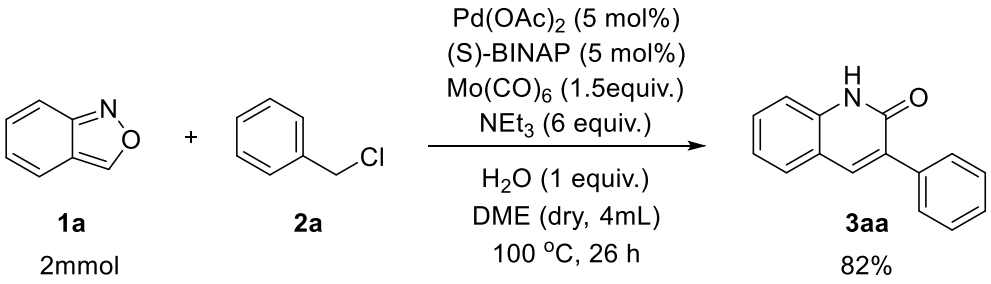
An oven-dried round-bottom flask was charged under air with 4-(hydroxymethyl)-1,1′-biphenyl (7.4 mmol, 1.4 g), dichloromethane (30.0 mL), and thionyl chloride (24.0 mmol, 1.4 g) was added in slowly and stirred in an ice bath, then stirred the reaction mixture for 4 h. The reaction mixture was then washed with H_2O (3×30.0 mL) and extracted with DCM (25.0 mL) for three times. The combined organic phases were dried over magnesium sulfate, filtered through short celite pad, and concentrated under reduced pressure. Purification by column chromatography (PE/EA = 100/1) afforded **2n** as a white solid (1.35 g, 90%).

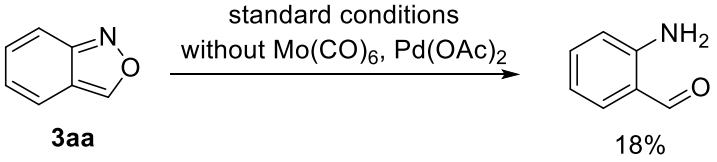


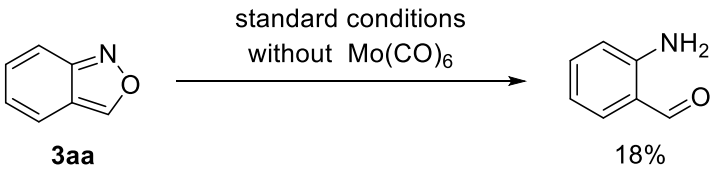
2q

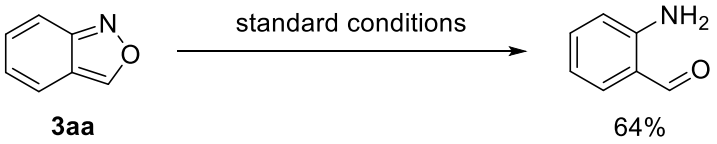
An oven-dried round-bottom flask was charged under air with 3-thienylmethanol (40.0 mmol, 4.6 g), dry dichloromethane (160.0 mL), and thionyl chloride (80.1 mmol, 9.5 g) was added in slowly and stirred in an ice bath for 10 min, then stirred the reaction mixture at room temperature for 16 h. Then the mixture was poured onto ice, the dichloromethane was separated, and the remaining aqueous layer was re-extracted with dichloromethane (3 × 70.0 mL) and dried over with $MgSO_4$. The solvent was removed under reduced pressure. Purification by column chromatography (PE/EA = 100/1) afforded **2q** as a brown oil (3.95 g, 67%).

4. 2 mmol scale reaction and mechanistic studies









i) $Pd(OAc)_2$ (5.0 mol%, 22.5 mg), (*S*)-BINAP (5.0 mol%, 62.8 mg), $Mo(CO)_6$ (3.0 mmol, 792.0 mg), were added to an oven-dried tube (15.0 mL), which was then placed under vacuum and refilled with nitrogen for three times. **1a** (2.0 mmol, 238.0 mg), **2a** (5.0 mmol, 633.2 mg), NEt_3 (12.0 mmol, 1214.4 mg), H_2O (2.0 mmol, 36.0 μL), and DME (4.0 mL) were added into the tube via a syringe. The tube was sealed and the mixture was stirred at 100 °C for 26 h. After the reaction was completed, the crude mixture was filtered and concentrated under vacuum. The crude product was purified by column chromatography (DCM/EA = 20/1) on silica gel to afford the products. the product **3aa** was observed in 82% yield (362.5 mg).

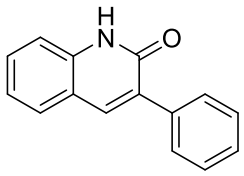
ii) An oven-dried tube (15.0 mL) was placed under vacuum and refilled with nitrogen for three times. **3aa** (0.5 mmol, 59.5 mg), NEt_3 (3.0 mmol, 303.6 mg), H_2O (0.5 mmol, 9.0 μL), and DME (2.0 mL) were added into the tube via a syringe. The tube was sealed and the mixture was stirred at 100 °C for 26 h. After the reaction was completed, the crude mixture was filtered and concentrated under vacuum. The crude product was purified by column chromatography (PE/EA = 40/1) on silica gel to afford the products. the product 2-aminobenzaldehyde was observed in 18% yield.

iii) $Pd(OAc)_2$ (10 mol%, 11.3 mg), (*S*)-BINAP (10 mol%, 31.4 mg), were added to an oven-dried tube (15.0 mL), which was then placed under vacuum and refilled with nitrogen for three times. **3aa** (0.5 mmol, 59.5 mg), NEt_3 (3.0 mmol, 303.6 mg), H_2O (0.5 mmol, 9 μL), and DME (2.0 mL) were added into the tube via a syringe. The tube was sealed and the mixture was stirred at 100 °C for 26 h. After the

reaction was completed, the crude mixture was filtered and concentrated under vacuum. The crude product was purified by column chromatography (PE/EA=40/1) on silica gel to afford the products. the product 2-aminobenzaldehyde was observed in 18% yield.

iv) $Pd(OAc)_2$ (10 mol%, 11.3 mg), (*S*)-BINAP (10 mol%, 31.4 mg), $Mo(CO)_6$ (0.75 mmol, 198.0 mg), were added to an oven-dried tube (15.0 mL), which was then placed under vacuum and refilled with nitrogen for three times. **3aa** (0.5 mmol, 59.5 mg), NEt_3 (3.0 mmol, 303.6 mg), H_2O (0.5 mmol, 9.0 μL), and DME (2.0 mL) were added into the tube via a syringe. The tube was sealed and the mixture was stirred at 100 °C for 26 h. After the reaction was completed, the crude mixture was filtered and concentrated under vacuum. The crude product was purified by column chromatography (PE/EA=40/1) on silica gel to afford the products. the product 2-aminobenzaldehyde was observed in 64% yield.

5 Characterization of Products



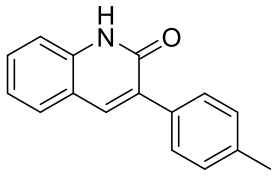
3-phenylquinolin-2(1*H*)-one (**3aa**)[5]

General Procedure was followed with $Pd(OAc)_2$ (10 mol%, 11.3 mg), (*S*)-BINAP (10 mol%, 31.4 mg), $Mo(CO)_6$ (0.75 mmol, 198.0 mg), were added to an oven-dried tube (15.0 mL), which was then placed under vacuum and refilled with nitrogen for three times. **1a** (0.5 mmol, 59.5 mg), **2a** (1.25 mmol, 158.3 mg), NEt_3 (3.0 mmol, 303.6 mg), H_2O (0.5 mmol, 9.0 μL), and DME (2.0 mL) were added into the tube via a syringe. The tube was sealed and the mixture was stirred at 100 °C for 26 h. After the reaction was completed, the crude mixture was filtered and concentrated under vacuum. The crude product was purified by column chromatography (DCM/EA = 20/1 to 5/1) on silica gel to afford the products titled product **3aa** as a **white solid** (100.6 mg, 91%).

^{1}H NMR (400 MHz, DMSO-d_6) δ 11.98 (s, 1H), 8.13 (s, 1H), 7.81 – 7.74 (m, 3H), 7.56 – 7.50 (m, 1H), 7.49 – 7.43 (m, 2H), 7.43 – 7.34 (m, 2H), 7.25 – 7.19 (m, 1H).

^{13}C NMR (101 MHz, DMSO-d_6) δ 161.0, 138.4, 137.6, 136.3, 131.5, 130.2, 128.7, 128.1, 127.9, 127.8, 121.9, 119.5, 114.7.

M.p. 191.2 – 193.0 °C



3-(*p*-tolyl)quinolin-2(1*H*)-one (**3ab**)[5]

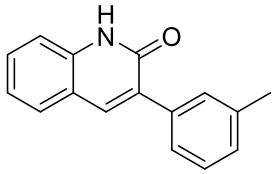
General Procedure was followed with $Pd(OAc)_2$ (10 mol%, 11.3 mg), (*S*)-BINAP (10 mol%, 31.4 mg), $Mo(CO)_6$ (0.75 mmol, 198.0 mg), were added to an oven-dried tube (15.0 mL), which was then placed under vacuum and refilled with nitrogen for three times. **1a** (0.5 mmol, 59.5 mg), **2b** (1.25 mmol, 175.8 mg), NEt_3 (3.0 mmol, 303.6 mg), H_2O (0.5 mmol, 9.0 μL), and DME (2.0 mL) were added into the tube

via a syringe. The tube was sealed and the mixture was stirred at 100 °C for 26 h. After the reaction was completed, the crude mixture was filtered and concentrated under vacuum. The crude product was purified by column chromatography (DCM/EA = 20/1 to 5/1) on silica gel to afford the products titled product **3ab** as a **white solid** (86.9 mg, 74%).

^{1}H NMR (400 MHz, DMSO-d_6) δ 11.98 (s, 1H), 8.10 (s, 1H), 7.77 – 7.73 (m, 1H), 7.72 – 7.67 (m, 2H), 7.54 – 7.48 (m, 1H), 7.35 (d, *J* = 8.2 Hz, 1H), 7.26 (d, *J* = 8.0 Hz, 2H), 7.24 – 7.19 (m, 1H), 2.38 (s, 3H).

^{13}C NMR (101 MHz, DMSO-d_6) δ 161.6, 138.7, 137.6, 137.5, 133.8, 131.9, 130.5, 129.0, 128.5, 122.3, 120.1, 115.1, 21.3.

M.p. 218.0 – 219.6 °C



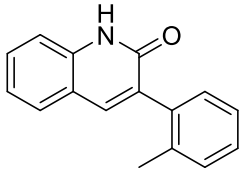
3-(*m*-tolyl)quinolin-2(1*H*)-one (**3ac**)[5]

General Procedure was followed with $Pd(OAc)_2$ (10 mol%, 11.3 mg), (*S*)-BINAP (10 mol%, 31.4 mg), $Mo(CO)_6$ (0.75 mmol, 198.0 mg), were added to an oven-dried tube (15.0 mL), which was then placed under vacuum and refilled with nitrogen for three times. **1a** (0.5 mmol, 59.5 mg), **2c** (1.25 mmol, 175.8 mg), NEt_3 (3.0 mmol, 303.6 mg), H_2O (0.5 mmol, 9.0 μL), and DME (2.0 mL) were added into the tube via a syringe. The tube was sealed and the mixture was stirred at 100 °C for 26 h. After the reaction was completed, the crude mixture was filtered and concentrated under vacuum. The crude product was purified by column chromatography (DCM/EA = 20/1 to 5/1) on silica gel to afford the products titled product **3ab** as a **white solid** (70.6 mg, 60%).

^{1}H NMR (400 MHz, DMSO-d_6) δ 11.99 (s, 1H), 7.87 (s, 1H), 7.78 – 7.74 (m, 3H), 7.56 – 7.50 (t, 1H), 7.38 (d, *J* = 8.2 Hz, 1H), 7.34 – 7.26 (m, 1H), 7.26 – 7.18 (m, 2H), 2.21 (s, 3H).

^{13}C NMR (101 MHz, DMSO-d_6) δ 161.5, 138.8, 137.4, 136.7, 132.1, 130.6, 129.7, 128.9, 128.3, 122.3, 120.1, 115.1, 21.6.

M.p. 220.8 – 222.3 °C



3-(*o*-tolyl)quinolin-2(1*H*)-one (**3ad**)[6]

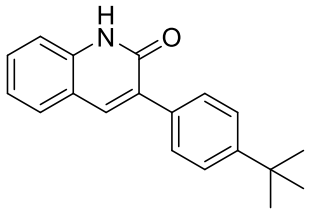
General Procedure was followed with $Pd(OAc)_2$ (10 mol%, 11.3 mg), (*S*)-BINAP (10 mol%, 31.4 mg), $Mo(CO)_6$ (0.75 mmol, 198.0 mg), were added to an oven-dried tube (15.0 mL), which was then placed under vacuum and refilled with nitrogen for three times. **1a** (0.5 mmol, 59.5 mg), **2d** (1.25 mmol, 175.8 mg), NEt_3 (3.0 mmol, 303.6 mg), H_2O (0.5 mmol, 9.0 μL), and DME (2.0 mL) were added into the tube via a syringe. The tube was sealed and the mixture was stirred at 100 °C for 26 h. After the reaction was completed, the crude mixture was filtered and concentrated under vacuum. The crude product was

purified by column chromatography (DCM/EA = 20/1 to 5/1) on silica gel to afford the products titled product **3ad** as a **white solid** (57.6 mg, 49%).

^{1}H NMR (400 MHz, DMSO-d_6) δ 11.99 (s, 1H), 7.87 (s, 1H), 7.77 – 7.67 (m, 1H), 7.61 – 7.50 (m, 1H), 7.38 (d, *J* = 8.2 Hz, 1H), 7.33 – 7.18 (m, 5H), 2.21 (s, 3H).

^{13}C NMR (101 MHz, DMSO-d_6) δ 161.2, 139.2, 139.1, 137.4, 137.1, 134.3, 130.6, 130.4, 130.1, 128.4, 128.3, 125.9, 122.3, 119.7, 115.3, 20.1.

M.p. 184.9 – 186.3°C



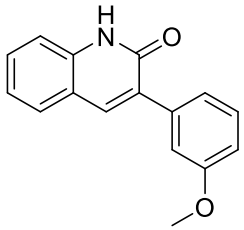
3-(4-(*tert*-butyl)phenyl)quinolin-2(1*H*)-one (**3ae**)[4]

General Procedure was followed with $Pd(OAc)_2$ (10 mol%, 11.3 mg), (*S*)-BINAP (10 mol%, 31.4 mg), $Mo(CO)_6$ (0.75 mmol, 198.0 mg), were added to an oven-dried tube (15.0 mL), which was then placed under vacuum and refilled with nitrogen for three times. **1a** (0.5 mmol, 59.5 mg), **2e** (1.25 mmol, 227.7 mg), NEt_3 (3.0 mmol, 303.6 mg), H_2O (0.5 mmol, 9.0 μL), and DME (2.0 mL) were added into the tube via a syringe. The tube was sealed and the mixture was stirred at 100 °C for 26 h. After the reaction was completed, the crude mixture was filtered and concentrated under vacuum. The crude product was purified by column chromatography (DCM/EA = 20/1 to 5/1) on silica gel to afford the products titled product **3ae** as a **white solid** (131.7 mg, 95%).

^{1}H NMR (400 MHz, DMSO-d_6) δ 11.97 (s, 1H), 8.10 (s, 1H), 7.78 – 7.69 (m, 3H), 7.54 – 7.49 (m, 1H), 7.47 (d, *J* = 8.5 Hz, 2H), 7.35 (d, *J* = 8.0 Hz, 1H), 7.25 – 7.19 (m, 1H), 1.34 (s, 9H).

^{13}C NMR (101 MHz, DMSO-d_6) δ 161.6, 150.8, 138.7, 137.6, 133.9, 131.9, 130.5, 128.9, 128.5, 125.2, 122.3, 120.1, 115.1, 34.8, 31.6.

M.p. 239.9 – 241.3 °C



3-(3-methoxyphenyl)quinolin-2(1*H*)-one (**3af**)[7]

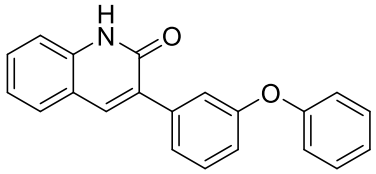
General Procedure was followed with $Pd(OAc)_2$ (10 mol%, 11.3 mg), (*S*)-BINAP (10 mol%, 31.4 mg), $Mo(CO)_6$ (0.75 mmol, 198.0 mg), were added to an oven-dried tube (15.0 mL), which was then placed under vacuum and refilled with nitrogen for three times. **1a** (0.5 mmol, 59.5 mg), **2f** (1.25 mmol, 195.1 mg), NEt_3 (3.0 mmol, 303.6 mg), H_2O (0.5 mmol, 9.0 μL), and DME (2.0 mL) were added into the tube via a syringe. The tube was sealed and the mixture was stirred at 100 °C for 26 h. After the reaction was completed, the crude mixture was filtered and concentrated under vacuum. The crude product was

purified by column chromatography (DCM/EA = 20/1 to 5/1) on silica gel to afford the products titled product **3af** as a **white solid** (131.7 mg, 83%).

^{1}H NMR (400 MHz, DMSO-d_6) δ 11.99 (s, 1H), 8.15 (s, 1H), 7.75 (d, *J* = 7.8 Hz, 1H), 7.52 (t, *J* = 7.8 Hz, 1H), 7.40 – 7.29 (m, 4H), 7.21 (t, *J* = 7.7 Hz, 1H), 7.05 – 6.93 (m, 1H), 3.82 (s, 3H).

^{13}C NMR (101 MHz, DMSO-d_6) δ 161.5, 159.3, 138.8, 138.3, 138.0, 131.7, 130.7, 129.4, 128.6, 122.4, 121.5, 120.0, 115.1, 114.9, 113.7, 55.6.

M.p. 147.2 – 148.6 °C



3-(3-phenoxyphenyl)quinolin-2(1*H*)-one (**3ag**)

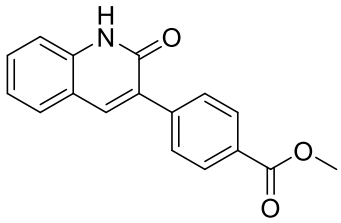
General Procedure was followed with $Pd(OAc)_2$ (10 mol%, 11.3 mg), (*S*)-BINAP (10 mol%, 31.4 mg), $Mo(CO)_6$ (0.75 mmol, 198.0 mg), were added to an oven-dried tube (15.0 mL), which was then placed under vacuum and refilled with nitrogen for three times. **1a** (0.5 mmol, 59.5 mg), **2g** (1.25 mmol, 272.6 mg), NEt_3 (3.0 mmol, 303.6 mg), H_2O (0.5 mmol, 9.0 μL), and DME (2 mL) were added into the tube via a syringe. The tube was sealed and the mixture was stirred at 100 °C for 26 h. After the reaction was completed, the crude mixture was filtered and concentrated under vacuum. The crude product was purified by column chromatography (DCM/EA = 20/1 to 5/1) on silica gel to afford the products titled product **3ag** as a **white solid** (134.7 mg, 86%).

^{1}H NMR (400 MHz, DMSO-d_6) δ 12.01 (s, 1H), 8.19 (s, 1H), 7.75 (dd, *J* = 8.0, 1.4 Hz, 1H), 7.61 – 7.52 (m, 3H), 7.47 (t, *J* = 7.9 Hz, 1H), 7.45 – 7.39 (m, 2H), 7.38 – 7.32 (m, 1H), 7.24 – 7.19 (m, 1H), 7.18 – 7.13 (m, 1H), 7.10 – 7.06 (m, 2H), 7.05 – 7.00 (m, 1H).

^{13}C NMR (101 MHz, DMSO-d_6) δ 161.3, 157.3, 156.5, 138.9, 138.6, 138.5, 130.9, 130.9, 130.5, 130.0, 128.7, 124.4, 123.8, 122.4, 119.9, 119.7, 118.8, 118.6, 115.2.

HRMS (ESI): $[M+H]^+$ calcd. for $C_{21}H_{16}NO_2^+$ 314.1176, found 314.1182.

M.p. 169.8 – 171.5 °C



methyl 4-(2-*oxo*-1,2-dihydroquinolin-3-yl)benzoate (**3ah**)

General Procedure was followed with $Pd(OAc)_2$ (10 mol%, 11.3 mg), (*S*)-BINAP (10 mol%, 31.4 mg), $Mo(CO)_6$ (0.75 mmol, 198.0 mg), were added to an oven-dried tube (15.0 mL), which was then placed under vacuum and refilled with nitrogen for three times. **1a** (0.5 mmol, 59.5 mg), **2h** (1.25 mmol, 230.1 mg), NEt_3 (3.0 mmol, 303.6 mg), H_2O (0.5 mmol, 9.0 μL), and DME (2.0 mL) were added into the tube via a syringe. The tube was sealed and the mixture was stirred at 100 °C for 26 h. After the reaction was completed, the crude mixture was filtered and concentrated under vacuum. The crude product was

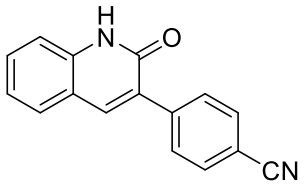
purified by column chromatography (DCM/EA = 20/1 to 5/1) on silica gel to afford the products titled product **3ah** as a **white solid** (96.3 mg, 69%).

^{1}H NMR (400 MHz, DMSO-d_6) δ 12.11 (s, 1H), 8.27 (s, 1H), 8.09 – 7.92 (m, 4H), 7.79 (dd, *J* = 8.0, 1.4 Hz, 1H), 7.59 – 7.53 (m, 1H), 7.37 (d, *J* = 8.2 Hz, 1H), 7.28 – 7.21 (m, 1H), 3.91 (s, 3H).

^{13}C NMR (101 MHz, DMSO-d_6) δ 166.6, 161.2, 141.5, 139.3, 139.1, 131.2, 130.6, 129.4, 129.3, 129.1, 128.9, 122.5, 119.9, 115.3, 52.7.

HRMS (ESI): $[M+H]^+$ calcd. for $C_{17}H_{13}NO_3^+$ 280.0968, found 280.0969.

M.p. 265.8 – 266.9 °C



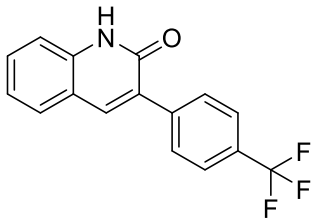
4-(2-*oxo*-1,2-dihydroquinolin-3-yl)benzonitrile (**3ai**)[6]

General Procedure was followed with $Pd(OAc)_2$ (10 mol%, 11.3 mg), (*S*)-BINAP (10 mol%, 31.4 mg), $Mo(CO)_6$ (0.75 mmol, 198.0 mg), were added to an oven-dried tube (15.0 mL), which was then placed under vacuum and refilled with nitrogen for three times. **1a** (0.5 mmol, 59.5 mg), **2i** (1.25 mmol, 188.8 mg), NEt_3 (3.0 mmol, 303.6 mg), H_2O (0.5 mmol, 9.0 μL), and DME (2 mL) were added into the tube via a syringe. The tube was sealed and the mixture was stirred at 100 °C for 26 h. After the reaction was completed, the crude mixture was filtered and concentrated under vacuum. The crude product was purified by column chromatography (DCM/EA = 20/1 to 5/1) on silica gel to afford the products titled product **3ah** as a **white solid** (119.4 mg, 97%).

^{1}H NMR (400 MHz, DMSO-d_6) δ 12.12 (s, 1H), 8.28 (s, 1H), 8.04 – 7.88 (m, 4H), 7.77 (d, *J* = 8.1 Hz, 1H), 7.60 – 7.52 (m, 1H), 7.37 (d, *J* = 8.2 Hz, 1H), 7.28 – 7.21 (m, 1H).

^{13}C NMR (101 MHz, DMSO-d_6) δ 161.1, 141.5, 139.7, 139.2, 132.3, 131.4, 130.0, 129.9, 129.0, 122.6, 119.8, 119.4, 115.3, 110.6.

M.p. 271.6 – 273.4 °C



3-(4-(trifluoromethyl)phenyl)quinolin-2(1*H*)-one (**3aj**)[6]

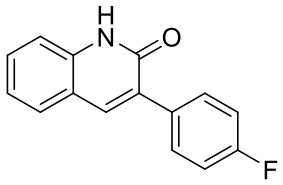
General Procedure was followed with $Pd(OAc)_2$ (10 mol%, 11.3 mg), (*S*)-BINAP (10 mol%, 31.4 mg), $Mo(CO)_6$ (0.75 mmol, 198.0 mg), were added to an oven-dried tube (15.0 mL), which was then placed under vacuum and refilled with nitrogen for three times. **1a** (0.5 mmol, 59.5 mg), **2j** (1.25 mmol, 242.6 mg), NEt_3 (3.0 mmol, 303.6 mg), H_2O (0.5 mmol, 9.0 μL), and DME (2 mL) were added into the tube via a syringe. The tube was sealed and the mixture was stirred at 100 °C for 26 h. After the reaction was completed, the crude mixture was filtered and concentrated under vacuum. The crude product was

purified by column chromatography (DCM/EA = 20/1 to 5/1) on silica gel to afford the products titled product **3aj** as a **white solid** (128.7mg, 89%).

^{1}H NMR (400 MHz, DMSO-d_6) δ 12.13 (s, 1H), 8.27 (s, 1H), 8.03 (d, *J* = 8.1 Hz, 2H), 7.82 (d, *J* = 8.2 Hz, 2H), 7.78 (d, *J* = 7.9, 1H), 7.60 – 7.52 (m, 1H), 7.38 (d, *J* = 8.1 Hz, 1H), 7.29 – 7.19 (m, 1H).

^{13}C NMR (101 MHz, DMSO-d_6) δ 161.2, 140.8, 139.4, 139.1, 131.3, 130.4, 129.9, 128.50 (d, *J* = 31.7 Hz), 125.3 (d, J = 3.8 Hz), 124.8 (q, *J* = 275.1 Hz), 122.5, 119.8, 115.3.

M.p. 265.8 – 267.6 °C



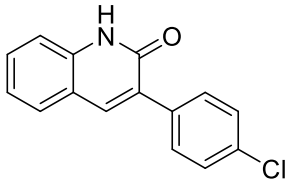
3-(4-fluorophenyl)quinolin-2(1*H*)-one (**3ak**)[6]

General Procedure was followed with $Pd(OAc)_2$ (10 mol%, 11.3 mg), (*S*)-BINAP (10 mol%, 31.4 mg), $Mo(CO)_6$ (0.75 mmol, 198.0 mg), were added to an oven-dried tube (15.0 mL), which was then placed under vacuum and refilled with nitrogen for three times. **1a** (0.5 mmol, 59.5 mg), **2k** (1.25 mmol, 180.1 mg), NEt_3 (3.0 mmol, 303.6 mg), H_2O (0.5 mmol, 9.0 μL), and DME (2 mL) were added into the tube via a syringe. The tube was sealed and the mixture was stirred at 100 °C for 26 h. After the reaction was completed, the crude mixture was filtered and concentrated under vacuum. The crude product was purified by column chromatography (DCM/EA = 20/1 to 5/1) on silica gel to afford the products titled product **3ak** as a **white solid** (90.9 mg, 76%).

^{1}H NMR (400 MHz, DMSO-d_6) δ 12.05 (s, 1H), 8.14 (s, 1H), 7.88 – 7.81 (m, 2H), 7.74 (d, *J* = 7.9 Hz, 1H), 7.58 – 7.48 (m, 1H), 7.36 (d, *J* = 8.2 Hz, 1H), 7.34 – 7.25 (m, 2H), 7.25 – 7.18 (m, 1H).

^{13}C NMR (101 MHz, DMSO-d_6) δ 162.3 (d, *J* = 244.9 Hz),161.5, 138.8, 138.1, 133.05 (d, *J* = 3.1 Hz), 131.3, 131.2, 130.77 (d, *J* = 10.3 Hz), 128.6, 122.4, 120.0, 115.3 (d, *J* = 21.2 Hz), 115.2.

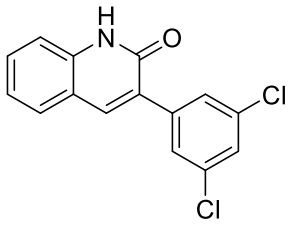
M.p. 249.9 – 251.8 °C



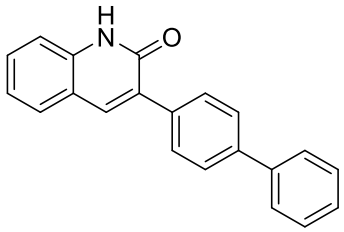
3-(4-chlorophenyl)quinolin-2(1*H*)-one (**3al**)[5]

General Procedure was followed with $Pd(OAc)_2$ (10 mol%, 11.3 mg), (*S*)-BINAP (10 mol%, 31.4 mg), $Mo(CO)_6$ (0.75 mmol, 198.0 mg), were added to an oven-dried tube (15.0 mL), which was then placed under vacuum and refilled with nitrogen for three times. **1a** (0.5 mmol, 59.5 mg), **2l** (1.25 mmol, 200.0 mg), NEt_3 (3.0 mmol, 303.6 mg), H_2O (0.5 mmol, 9.0 μL), and DME (=2.0 mL) were added into the tube via a syringe. The tube was sealed and the mixture was stirred at 100 °C for 26 h. After the reaction was completed, the crude mixture was filtered and concentrated under vacuum. The crude product was purified by column chromatography (DCM/EA = 20/1 to 5/1) on silica gel to afford the products titled product **3al** as a **white solid** (103.3 mg, 81%).

^{1}H NMR (400 MHz, DMSO-d_6) δ 12.06 (s, 1H), 8.18 (s, 1H), 7.84 (d, *J* = 8.5 Hz, 2H), 7.76 (d, *J* = 7.8 Hz, 1H), 7.60 – 7.48 (m, 3H), 7.36 (d, *J* = 8.2 Hz, 1H), 7.23 (t, *J* = 7.5 Hz, 1H).
^{13}C NMR (101 MHz, DMSO-d_6) δ 161.4, 139.0, 138.5, 135.6, 133.1, 131.0, 130.6, 128.8, 128.5, 122.6, 120.0, 115.3.
M.p. 255.4 – 257.2 °C

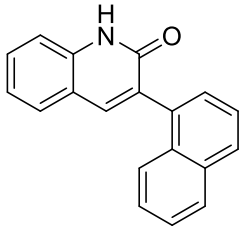


3-(3,5-dichlorophenyl)quinolin-2(1*H*)-one (**3am**)
General Procedure was followed with $Pd(OAc)_2$ (10 mol%, 11.3 mg), (*S*)-BINAP (10 mol%, 31.4 mg), $Mo(CO)_6$ (0.75 mmol, 198.0 mg), were added to an oven-dried tube (15.0 mL), which was then placed under vacuum and refilled with nitrogen for three times. **1a** (0.5 mmol, 59.5 mg), **2m** (1.25 mmol, 242.5 mg), NEt_3 (3.0 mmol, 303.6 mg), H_2O (0.5 mmol, 9.0 μL), and DME (2.0 mL) were added into the tube via a syringe. The tube was sealed and the mixture was stirred at 100 °C for 26 h. After the reaction was completed, the crude mixture was filtered and concentrated under vacuum. The crude product was purified by column chromatography (DCM/EA = 20/1 to 5/1) on silica gel to afford the products titled product **3am** as a **white solid** (101.2 mg, 70%).
^{1}H NMR (400 MHz, DMSO-d_6) δ 12.13 (s, 1H), 8.35 (s, 1H), 7.91 (d, *J* = 2.0 Hz, 2H), 7.78 (dd, *J* = 8.0, 1.4 Hz, 1H), 7.64 (t, *J* = 2.0 Hz, 1H), 7.60 – 7.53 (m, 1H), 7.37 (d, *J* = 8.1 Hz, 1H), 7.31 – 7.20 (m, 1H).
^{13}C NMR (101 MHz, DMSO-d_6) δ 161.0, 140.0, 139.7, 139.1, 134.1, 131.5, 129.0, 128.6, 127.6, 122.6, 119.7, 115.3.
HRMS (ESI): $[M+H]^+$ calcd. for $C_{15}H_{10}NOCl_2^+$ 290.0134, found 290.0139.
M.p. 282.8 – 284.6 °C

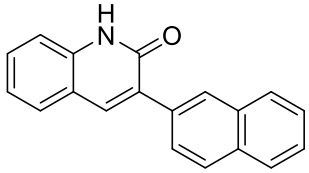


3-([1,1'-biphenyl]-4-yl)quinolin-2(1*H*)-one (**3an**)[10]
General Procedure was followed with $Pd(OAc)_2$ (10 mol%, 11.3 mg), (*S*)-BINAP (10 mol%, 31.4 mg), $Mo(CO)_6$ (0.75 mmol, 198.0 mg), were added to an oven-dried tube (15.0 mL), which was then placed under vacuum and refilled with nitrogen for three times. **1a** (0.5 mmol, 59.5 mg), **2n** (1.25 mmol, 252.6 mg), NEt_3 (3.0 mmol, 303.6 mg), H_2O (0.5 mmol, 9.0 μL), and DME (2.0 mL) were added into the tube via a syringe. The tube was sealed and the mixture was stirred at 100 °C for 26 h. After the reaction was completed, the crude mixture was filtered and concentrated under vacuum. The crude product was purified by column chromatography (DCM/EA = 20/1 to 5/1) on silica gel to afford the products titled product **3an** as a **white solid** (142.6 mg, 96%).

^{1}H NMR (400 MHz, DMSO-d_6) δ 12.04 (s, 1H), 8.22 (s, 1H), 7.92 (d, *J* = 8.1 Hz, 2H), 7.84 – 7.67 (m, 5H), 7.59 – 7.47 (m, 3H), 7.46 – 7.34 (m, 2H), 7.24 (t, *J* = 7.5 Hz, 1H).
^{13}C NMR (101 MHz, DMSO-d_6) δ 161.6, 140.2, 140.0, 138.8, 138.0, 135.8, 131.4, 130.7, 129.7, 129.5, 128.6, 128.1, 127.1, 126.7, 122.4, 120.1, 115.2.
M.p. 315.5 – 317.1 °C

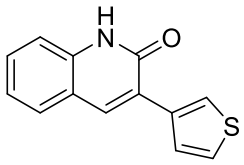


3-(naphthalen-1-yl)quinolin-2(1*H*)-one (**3ao**)[8]
General Procedure was followed with $Pd(OAc)_2$ (10 mol%, 11.3 mg), (*S*)-BINAP (10 mol%, 31.4 mg), $Mo(CO)_6$ (0.75 mmol, 198.0 mg), were added to an oven-dried tube (15.0 mL), which was then placed under vacuum and refilled with nitrogen for three times. **1a** (0.5 mmol, 59.5 mg), **2o** (1.25 mmol, 220.1 mg), NEt_3 (3.0 mmol, 303.6 mg), H_2O (0.5 mmol, 9.0 μL), and DME (2.0 mL) were added into the tube via a syringe. The tube was sealed and the mixture was stirred at 100 °C for 26 h. After the reaction was completed, the crude mixture was filtered and concentrated under vacuum. The crude product was purified by column chromatography (DCM/EA = 20/1 to 5/1) on silica gel to afford the products titled product **3ao** as a **white solid** (86.8 mg, 64%).
^{1}H NMR (400 MHz, DMSO-d_6) δ 12.06 (s, 1H), 8.04 (s, 1H), 8.03 – 7.97 (m, 2H), 7.76 (dd, *J* = 7.9, 1.4 Hz, 1H), 7.69 (dd, *J* = 8.4, 1.2 Hz, 1H), 7.64 – 7.60 (m, 1H), 7.59 – 7.55 (m, 2H), 7.52 – 7.47 (m, 2H), 7.45 – 7.41 (m, 1H), 7.29 – 7.22 (m, 1H).
^{13}C NMR (101 MHz, DMSO-d_6) δ 161.8, 140.2, 139.3, 135.5, 133.5, 133.1, 132.0, 130.8, 128.6, 128.6, 128.5, 127.9, 126.5, 126.4, 126.3, 125.9, 122.4, 119.8, 115.4.
M.p. 258.2 – 259.9 °C

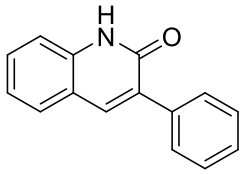


3-(naphthalen-2-yl)quinolin-2(1*H*)-one (**3ap**)[5]
General Procedure was followed with $Pd(OAc)_2$ (10 mol%, 11.3 mg), (*S*)-BINAP (10 mol%, 31.4 mg), $Mo(CO)_6$ (0.75 mmol, 198.0 mg), were added to an oven-dried tube (15.0 mL), which was then placed under vacuum and refilled with nitrogen for three times. **1a** (0.5 mmol, 59.5 mg), **2p** (1.25 mmol, 220.1 mg), NEt_3 (3.0 mmol, 303.6 mg), H_2O (0.5 mmol, 9.0 μL), and DME (2.0 mL) were added into the tube via a syringe. The tube was sealed and the mixture was stirred at 100 °C for 26 h. After the reaction was completed, the crude mixture was filtered and concentrated under vacuum. The crude product was purified by column chromatography (DCM/EA = 20/1 to 5/1) on silica gel to afford the products titled product **3ap** as a **white solid** (134.2 mg, 99%).

^{1}H NMR (400 MHz, DMSO-d_6) δ 12.08 (s, 1H), 8.41 (d, *J* = 1.7 Hz, 1H), 8.32 (s, 1H), 8.11 – 7.95 (m, 4H), 7.82 (dd, *J* = 8.0, 1.4 Hz, 1H), 7.67 – 7.52 (m, 3H), 7.41 (d, *J* = 8.2 Hz, 1H), 7.35 – 7.24 (m, 1H).
^{13}C NMR (101 MHz, DMSO-d_6) δ 161.7, 138.9, 138.6, 134.4, 133.2, 132.9, 131.8, 130.8, 128.7, 128.1, 127.9, 127.6, 127.3, 126.8, 126.7, 122.4, 120.1, 115.2.
M.p. 305.3 – 306.8 °C



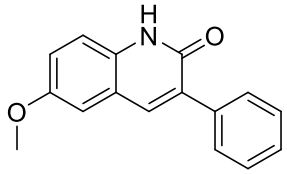
3-(thiophen-3-yl)quinolin-2(1*H*)-one (**3aq**)
General Procedure was followed with $Pd(OAc)_2$ (10 mol%, 11.3 mg), (*S*)-BINAP (10 mol%, 31.4 mg), $Mo(CO)_6$ (0.75 mmol, 198.0 mg), were added to an oven-dried tube (15.0 mL), which was then placed under vacuum and refilled with nitrogen for three times. **1a** (0.5 mmol, 59.5 mg), **2r** (1.25 mmol, 165.0 mg), NEt_3 (3.0 mmol, 303.6 mg), H_2O (0.5 mmol, 9.0 μL), and DME (2.0 mL) were added into the tube via a syringe. The tube was sealed and the mixture was stirred at 100 °C for 26 h. After the reaction was completed, the crude mixture was filtered and concentrated under vacuum. The crude product was purified by column chromatography (DCM/EA = 20/1 to 5/1) on silica gel to afford the products titled product **3ar** as a **white solid** (104.5 mg, 92%).
^{1}H NMR (400 MHz, DMSO-d_6) δ 12.04 (s, 1H), 8.45 (dd, *J* = 3.0, 1.3 Hz, 1H), 8.41 (s, 1H), 7.79 (dd, *J* = 5.1, 1.3 Hz, 1H), 7.75 (dd, *J* = 7.9, 1.4 Hz, 1H), 7.63 (dd, *J* = 5.1, 3.0 Hz, 1H), 7.56 – 7.49 (m, 1H), 7.37 (d, *J* = 8.2 Hz, 1H), 7.27 – 7.19 (m, 1H).
^{13}C NMR (101 MHz, DMSO-d_6) δ 161.3, 138.2, 136.6, 136.0, 130.5, 128.4, 127.6, 126.3, 125.9, 125.4, 122.4, 119.9, 115.2.
HRMS (ESI): $[M+H]^+$ calcd. for $C_{21}H_{16}NO_2^+$ 228.0478, found 228.0485.
M.p. 246.7 – 248.1 °C



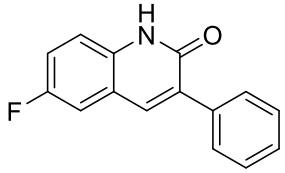
from Benzyl bromide.

3-phenylquinolin-2(1*H*)-one[4]
General Procedure was followed with $Pd(OAc)_2$ (10 mol%, 11.3 mg), (*S*)-BINAP (10 mol%, 31.4 mg), $Mo(CO)_6$ (0.75 mmol, 198.0 mg), were added to an oven-dried tube (15.0 mL), which was then placed under vacuum and refilled with nitrogen for three times. **1a** (0.5 mmol, 59.5 mg), **2r** (1.25 mmol, 213.8 mg), NEt_3 (3.0 mmol, 303.6 mg), H_2O (0.5 mmol, 9.0 μL), and DME (2.0 mL) were added into the tube via a syringe. The tube was sealed and the mixture was stirred at 100 °C for 26 h. After the reaction was completed, the crude mixture was filtered and concentrated under vacuum. The crude product was purified by column chromatography (DCM/EA = 20/1 to 5/1) on silica gel to afford the products titled product as a **white solid** (53.1 mg, 48%)..

^{1}H NMR (400 MHz, DMSO-d_6) δ 12.00 (s, 1H), 8.13 (s, 1H), 7.85 – 7.71 (m, 3H), 7.57 – 7.50 (m, 1H), 7.46 (dd, *J* = 8.2, 6.4 Hz, 2H), 7.42 – 7.39 (m, 1H), 7.36 (d, *J* = 8.2 Hz, 1H), 7.28 – 7.14 (m, 1H)..
^{13}C NMR (101 MHz, DMSO-d_6) δ 161.5, 138.8, 138.1, 136.7, 132.0, 130.7, 129.2, 128.6, 128.4, 128.3, 122.4, 120.0, 115.1.
M.p. 191.2 – 193 °C

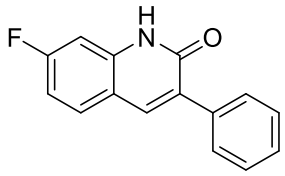


6-methoxy-3-phenylquinolin-2(1*H*)-one (**3ba**)[4]
General Procedure was followed with $Pd(OAc)_2$ (10 mol%, 11.3 mg), (*S*)-BINAP (10 mol%, 31.4 mg), $Mo(CO)_6$ (0.75 mmol, 198.0 mg), were added to an oven-dried tube (15.0 mL), which was then placed under vacuum and refilled with nitrogen for three times. **1b** (0.5 mmol, 74.5 mg), **2a** (1.25 mmol, 158.3 mg), NEt_3 (3.0 mmol, 303.6 mg), H_2O (0.5 mmol, 9.0 μL), and DME (2.0 mL) were added into the tube via a syringe. The tube was sealed and the mixture was stirred at 100 °C for 26 h. After the reaction was completed, the crude mixture was filtered and concentrated under vacuum. The crude product was purified by column chromatography (DCM/EA = 20/1 to 5/1) on silica gel to afford the products titled product **3ba** as a **white solid** (114.3 mg, 91%).
^{1}H NMR (400 MHz, DMSO-d_6) δ 11.90 (s, 1H), 8.08 (s, 1H), 7.90 – 7.64 (m, 2H), 7.53 – 7.42 (m, 2H), 7.42 – 7.37 (m, 1H), 7.34 – 7.24 (m, 2H), 7.19 (dd, *J* = 8.9, 2.8 Hz, 1H), 3.82 (s, 3H).
^{13}C NMR (101 MHz, DMSO-d_6) δ 161.1, 154.7, 137.7, 136.9, 133.4, 132.3, 129.2, 128.4, 128.3, 120.6, 120.0, 116.5, 109.8, 55.9.
M.p. 242.7 – 244.1 °C

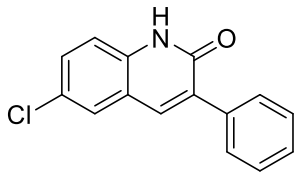


6-fluoro-3-phenylquinolin-2(1*H*)-one (**3ca**)[5]
General Procedure was followed with $Pd(OAc)_2$ (10 mol%, 11.3 mg), (*S*)-BINAP (10 mol%, 31.4 mg), $Mo(CO)_6$ (0.75 mmol, 198.0 mg), were added to an oven-dried tube (15.0 mL), which was then placed under vacuum and refilled with nitrogen for three times. **1c** (0.5 mmol, 68.5 mg), **2a** (1.25 mmol, 158.3 mg), NEt_3 (3.0 mmol, 303.6 mg), H_2O (0.5 mmol, 9.0 μL), and DME (2.0 mL) were added into the tube via a syringe. The tube was sealed and the mixture was stirred at 100 °C for 26 h. After the reaction was completed, the crude mixture was filtered and concentrated under vacuum. The crude product was purified by column chromatography (DCM/EA = 20/1 to 5/1) on silica gel to afford the products titled product **3ca** as a **white solid** (81.3 mg, 67%).
^{1}H NMR (400 MHz, DMSO-d_6) δ 12.08 (s, 1H), 8.11 (s, 1H), 7.83 – 7.71 (m, 2H), 7.61 (dd, *J* = 9.2, 2.8 Hz, 1H), 7.48 – 7.44 (m, 2H), 7.44 – 7.42 (m, 1H), 7.42 – 7.35 (m, 2H).

^{13}C NMR (101 MHz, DMSO-d_6) δ 161.2, 157.45 (d, *J* = 237.8 Hz), 137.26 (d, J = 3.2 Hz), 136.5, 135.6, 133.2, 129.2, 128.5, 128.4, 120.7 (d, *J* = 9.4 Hz), 118.7 (d, *J* = 24.5 Hz), 117.0 (d, *J* = 8.5 Hz), 113.1 (d, *J* = 22.8 Hz).
M.p. 299.9 – 301.4 °C

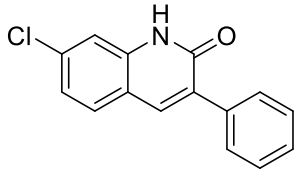


7-fluoro-3-phenylquinolin-2(1*H*)-one (**3da**)[5]
General Procedure was followed with $Pd(OAc)_2$ (10 mol%, 11.3 mg), (*S*)-BINAP (10 mol%, 31.4 mg), $Mo(CO)_6$ (0.75 mmol, 198.0 mg), were added to an oven-dried tube (15.0 mL), which was then placed under vacuum and refilled with nitrogen for three times. **1d** (0.5 mmol, 68.5 mg), **2a** (1.25 mmol, 158.3 mg), NEt_3 (3.0 mmol, 303.6 mg), H_2O (0.5 mmol, 9.0 μL), and DME (2.0 mL) were added into the tube via a syringe. The tube was sealed and the mixture was stirred at 100 °C for 26 h. After the reaction was completed, the crude mixture was filtered and concentrated under vacuum. The crude product was purified by column chromatography (DCM/EA = 20/1 to 5/1) on silica gel to afford the products titled product **3da** as a **white solid** (80.1 mg, 68%).
^{1}H NMR (400 MHz, DMSO-d_6) δ 12.07 (s, 1H), 8.13 (s, 1H), 7.81 (dd, *J* = 9.3, 6.3 Hz, 1H), 7.78 – 7.73 (m, 2H), 7.45 (dd, *J* = 8.3, 6.4 Hz, 2H), 7.42 – 7.36 (m, 1H), 7.09 (dd, *J* = 9.3, 7.1 Hz, 2H).
^{13}C NMR (101 MHz, DMSO-d_6) δ 163.44 (d, *J* = 246.9 Hz), 161.6, 140.3 (d, *J* = 12.4 Hz), 137.7, 136.5, 131.2, 131.1, 131.06 (d, *J* = 2.5 Hz), 129.1, 128.36 (d, *J* = 10.9 Hz), 117.1, 110.60 (d, *J* = 23.3 Hz), 101.1 (d, *J* = 25.5 Hz).
M.p. 201.3 – 202.8 °C

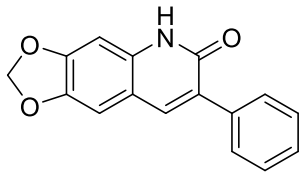


6-chloro-3-phenylquinolin-2(1*H*)-one (**3ea**)[5]
General Procedure was followed with $Pd(OAc)_2$ (10 mol%, 11.3 mg), (*S*)-BINAP (10 mol%, 31.4 mg), $Mo(CO)_6$ (0.75 mmol, 198.0 mg), were added to an oven-dried tube (15.0 mL), which was then placed under vacuum and refilled with nitrogen for three times. **1e** (0.5 mmol, 76.5 mg), **2a** (1.25 mmol, 158.3 mg), NEt_3 (3.0 mmol, 303.6 mg), H_2O (0.5 mmol, 9.0 μL), and DME (2.0 mL) were added into the tube via a syringe. The tube was sealed and the mixture was stirred at 100 °C for 26 h. After the reaction was completed, the crude mixture was filtered and concentrated under vacuum. The crude product was purified by column chromatography (DCM/EA = 20/1 to 5/1) on silica gel to afford the products titled product **3ea** as a **white solid** (121.2 mg, 97%).
^{1}H NMR (400 MHz, DMSO-d_6) δ 12.13 (s, 1H), 8.11 (s, 1H), 7.86 (d, *J* = 2.3 Hz, 1H), 7.81 – 7.74 (m, 2H), 7.56 (dd, *J* = 8.8, 2.1 Hz, 1H), 7.51 – 7.45 (m, 2H), 7.45 – 7.41 (m, 1H), 7.37 (d, *J* = 8.7 Hz, 1H).

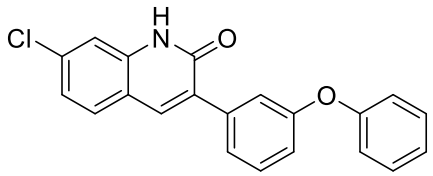
^{13}C NMR (101 MHz, DMSO-d_6) δ 161.3, 137.5, 137.0, 136.4, 133.2, 130.5, 129.2, 128.6, 128.5, 127.5, 126.1, 121.2, 117.1.
M.p. 249.1 – 250.9 °C



7-chloro-3-phenylquinolin-2(1*H*)-one (**3fa**)[5]
General Procedure was followed with $Pd(OAc)_2$ (10 mol%, 11.3 mg), (*S*)-BINAP (10 mol%, 31.4 mg), $Mo(CO)_6$ (0.75 mmol, 198.0 mg), were added to an oven-dried tube (15.0 mL), which was then placed under vacuum and refilled with nitrogen for three times. **1f** (0.5 mmol, 76.5 mg), **2a** (1.25 mmol, 158.3 mg), NEt_3 (3.0 mmol, 303.6 mg), H_2O (0.5 mmol, 9.0 μL), and DME (2.0 mL) were added into the tube via a syringe. The tube was sealed and the mixture was stirred at 100 °C for 26 h. After the reaction was completed, the crude mixture was filtered and concentrated under vacuum. The crude product was purified by column chromatography (DCM/EA = 20/1 to 5/1) on silica gel to afford the products titled product **3fa** as a **white solid** (123.7 mg, 95%).
^{1}H NMR (400 MHz, DMSO-d_6) δ 12.07 (s, 1H), 8.14 (s, 1H), 7.81 – 7.71 (m, 3H), 7.49 – 7.43 (m, 2H), 7.43 – 7.39 (m, 1H), 7.37 (d, *J* = 2.0 Hz, 1H), 7.25 (dd, *J* = 8.4, 2.0 Hz, 1H).
^{13}C NMR (101 MHz, DMSO-d_6) δ 161.4, 139.6, 137.5, 136.4, 135.0, 132.3, 130.4, 129.1, 128.5, 128.4, 122.5, 118.9, 114.4.
M.p. 248.8 – 250.6 °C



7-phenyl-[1,3]dioxolo[4,5-*g*]quinolin-6(5*H*)-one (**3ga**)[9]
General Procedure was followed with $Pd(OAc)_2$ (10 mol%, 11.3 mg), (*S*)-BINAP (10 mol%, 31.4 mg), $Mo(CO)_6$ (0.75 mmol, 198.0 mg), were added to an oven-dried tube (15.0 mL), which was then placed under vacuum and refilled with nitrogen for three times. **1g** (0.5 mmol, 76.5 mg), **2a** (1.25 mmol, 158.3 mg), NEt_3 (3.0 mmol, 303.6 mg), H_2O (0.5 mmol, 9.0 μL), and DME (2.0 mL) were added into the tube via a syringe. The tube was sealed and the mixture was stirred at 100 °C for 26 h. After the reaction was completed, the crude mixture was filtered and concentrated under vacuum. The crude product was purified by column chromatography (DCM/EA = 20/1 to 5/1) on silica gel to afford the products titled product **3ga** as a **white solid** (81.5 mg, 88%).
^{1}H NMR (400 MHz, DMSO-d_6) δ 11.89 (s, 1H), 8.01 (s, 1H), 7.78 – 7.74 (m, 2H), 7.51 – 7.40 (m, 2H), 7.39 – 7.35 (m, 1H), 7.25 (s, 1H), 6.86 (s, 1H), 6.12 (s, 2H).
^{13}C NMR (101 MHz, DMSO-d_6) δ 161.2, 150.5, 143.7, 137.9, 137.0, 135.8, 128.9, 128.8, 128.4, 127.9, 114.3, 105.8, 102.2, 95.2.
M.p. 317.8 – 319.2 °C



7-chloro-3-(3-phenoxyphenyl)quinolin-2(1*H*)-one (**3ha**)[6]

General Procedure was followed with $Pd(OAc)_2$ (10 mol%, 11.3 mg), (*S*)-BINAP (10 mol%, 31.4 mg), $Mo(CO)_6$ (0.75 mmol, 198.0 mg), were added to an oven-dried tube (15.0 mL), which was then placed under vacuum and refilled with nitrogen for three times. **1f** (0.5 mmol, 76.5 mg), **2g** (1.25 mmol, 272.7 mg), NEt_3 (3.0 mmol, 303.6 mg), H_2O (0.5 mmol, 9.0 μL), and DME (2.0 mL) were added into the tube via a syringe. The tube was sealed and the mixture was stirred at 100 °C for 26 h. After the reaction was completed, the crude mixture was filtered and concentrated under vacuum. The crude product was purified by column chromatography (DCM/EA = 20/1 to 5/1) on silica gel to afford the products titled product **3ha** as a **Brown liquid** (149.3 mg, 86%).

^{1}H NMR (400 MHz, DMSO-d_6) δ 12.08 (s, 1H), 8.22 (s, 1H), 7.79 (d, *J* = 8.5 Hz, 2H), 7.62 – 7.55 (m, 2H), 7.55 – 7.52 (m, 1H), 7.48 (t, *J* = 7.9 Hz, 1H), 7.45 – 7.40 (m, 2H), 7.37 (d, *J* = 2.0 Hz, 1H), 7.27 (dd, *J* = 8.4, 2.1 Hz, 1H), 7.22 – 7.13 (m, 1H), 7.10 – 7.05 (m, 3H).

^{13}C NMR (101 MHz, DMSO-d_6) δ 161.2, 157.2, 156.5, 139.7, 138.3, 137.8, 135.2, 131.2, 130.5, 130.0, 124.3, 123.8, 122.6, 119.7, 118.8, 118.7, 114.4.

6. References

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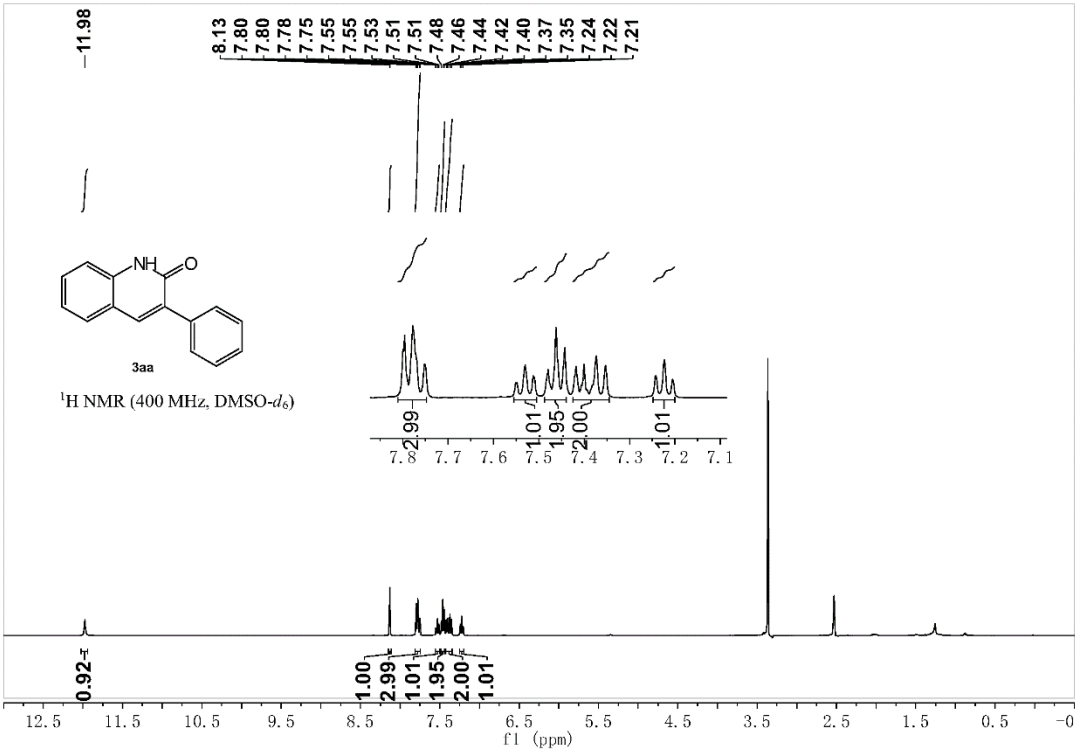
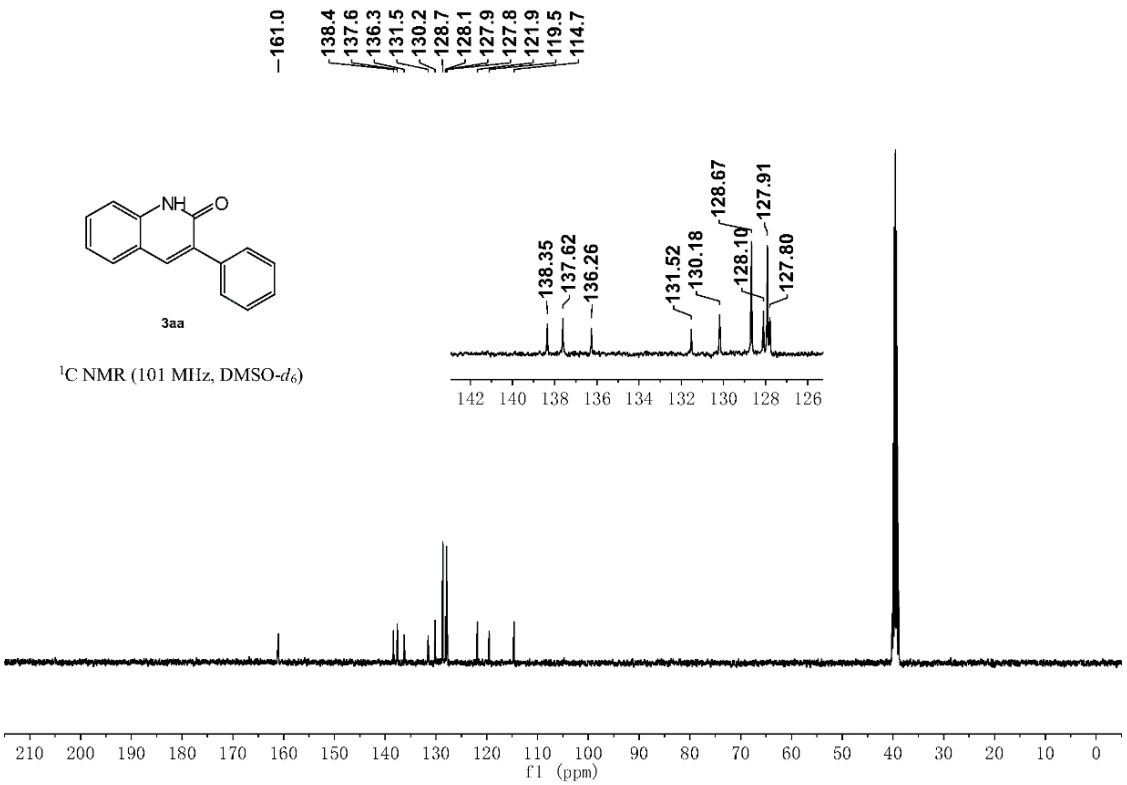
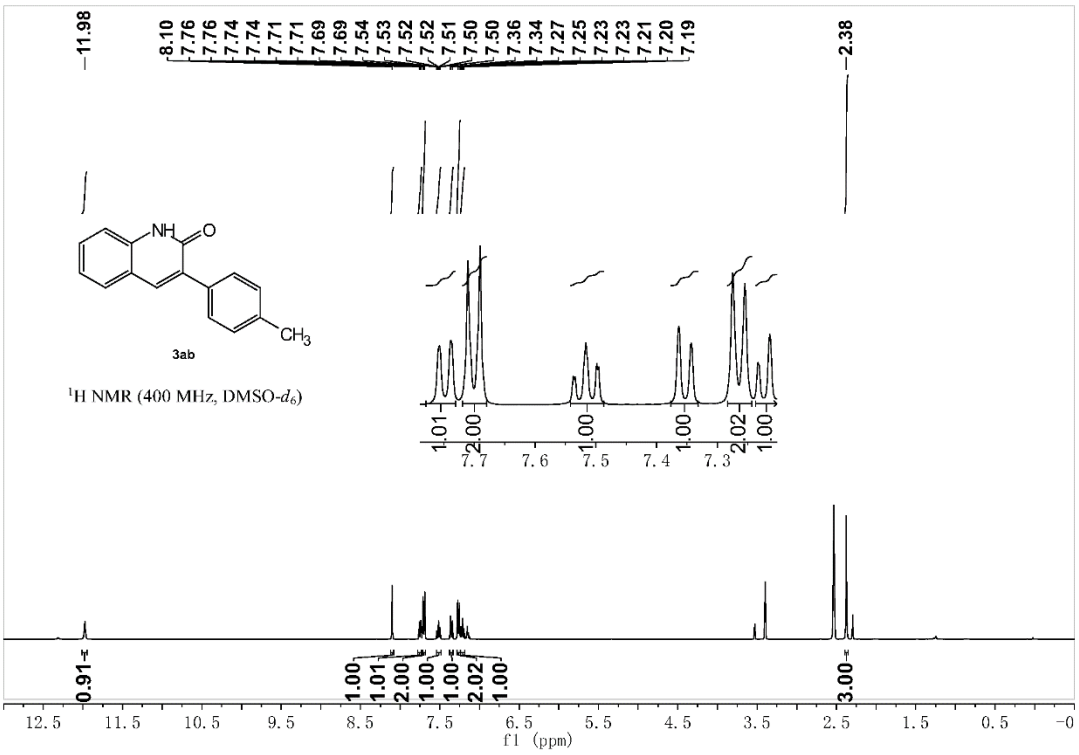
7. Copy of ^{1}H and ^{13}C NMR Spectra of Products



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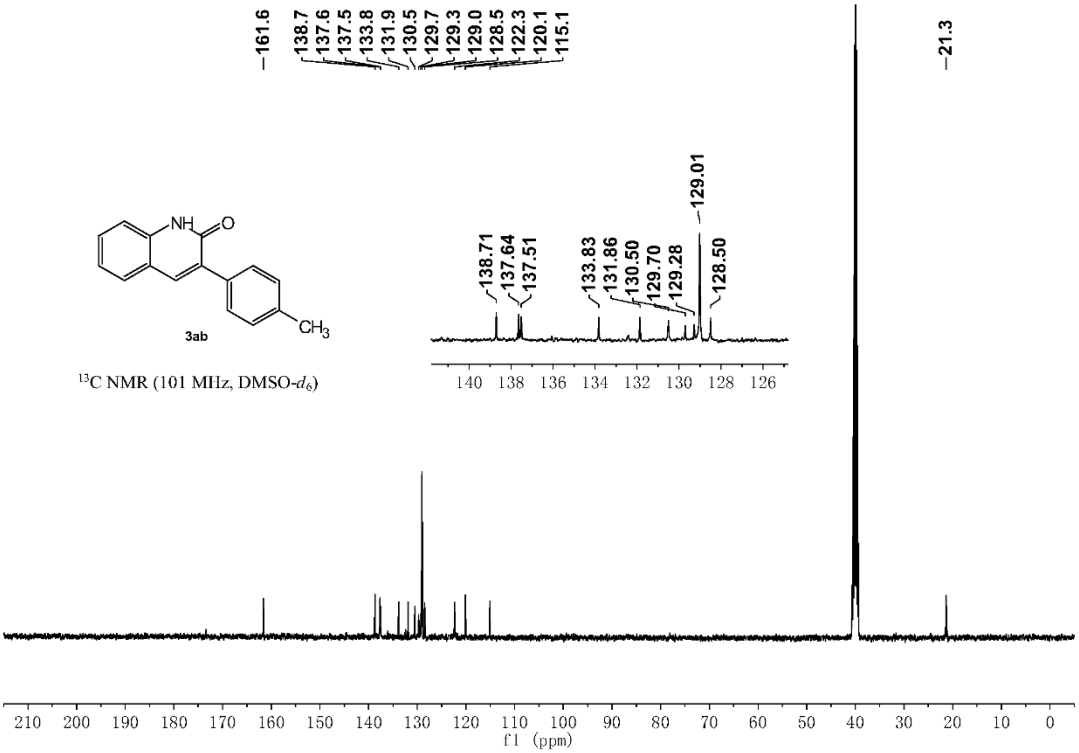
8.10
7.76
7.76
7.74
7.74
7.71
7.71
7.69
7.69
7.54
7.53
7.52
7.52
7.51
7.50
7.50
7.36
7.34
7.27
7.25
7.23
7.23
7.21
7.20
7.19
2.38
NH
O
CH3
3ab
1H NMR (400 MHz, DMSO-d6)
1.01
2.00
1.00
1.00
2.02
1.00
7.7
7.6
7.5
7.4
7.3
0.91
1.00
1.01
2.00
1.00
1.00
2.02
1.00
3.00
f1 (ppm)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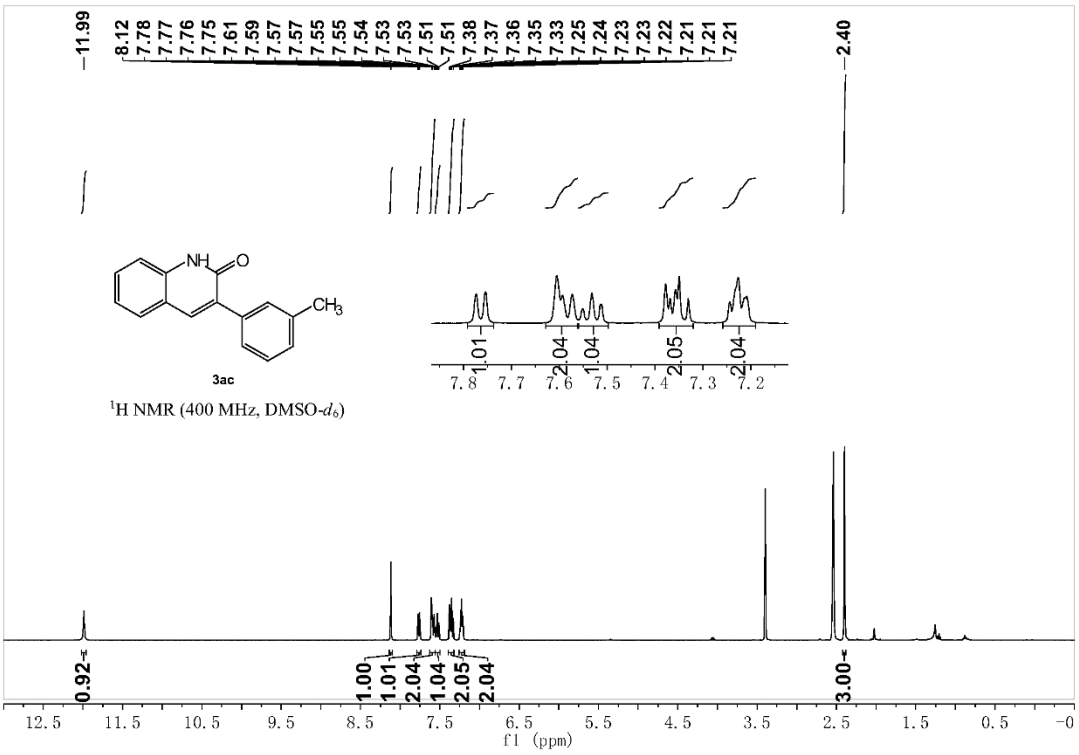
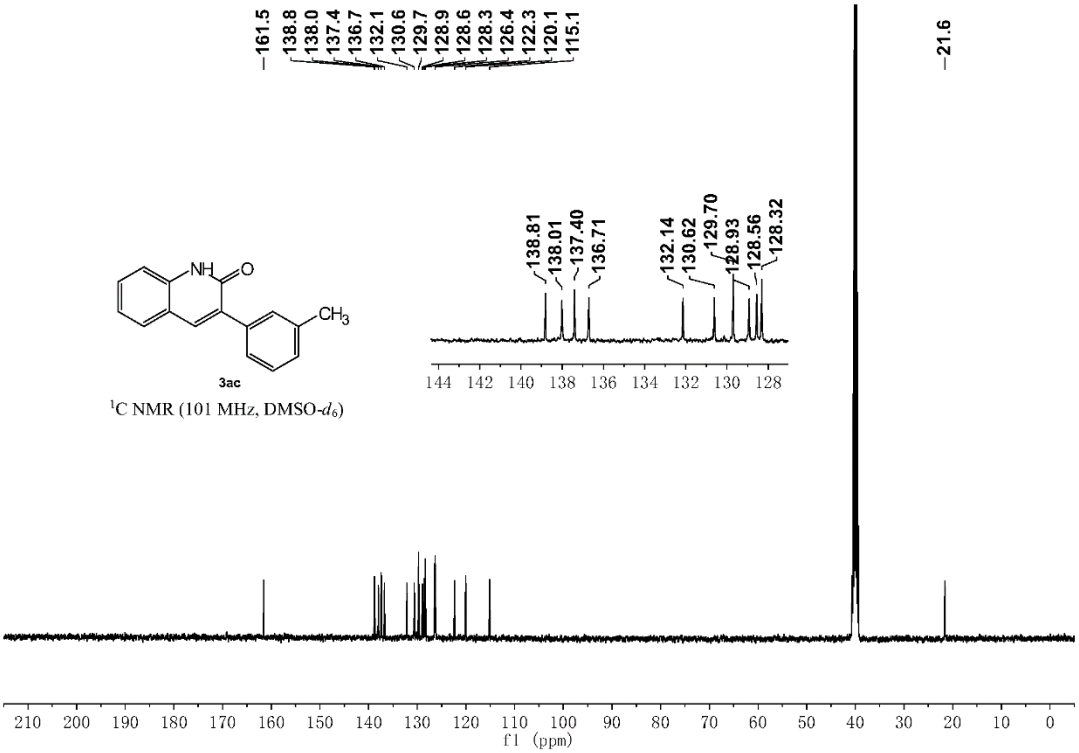
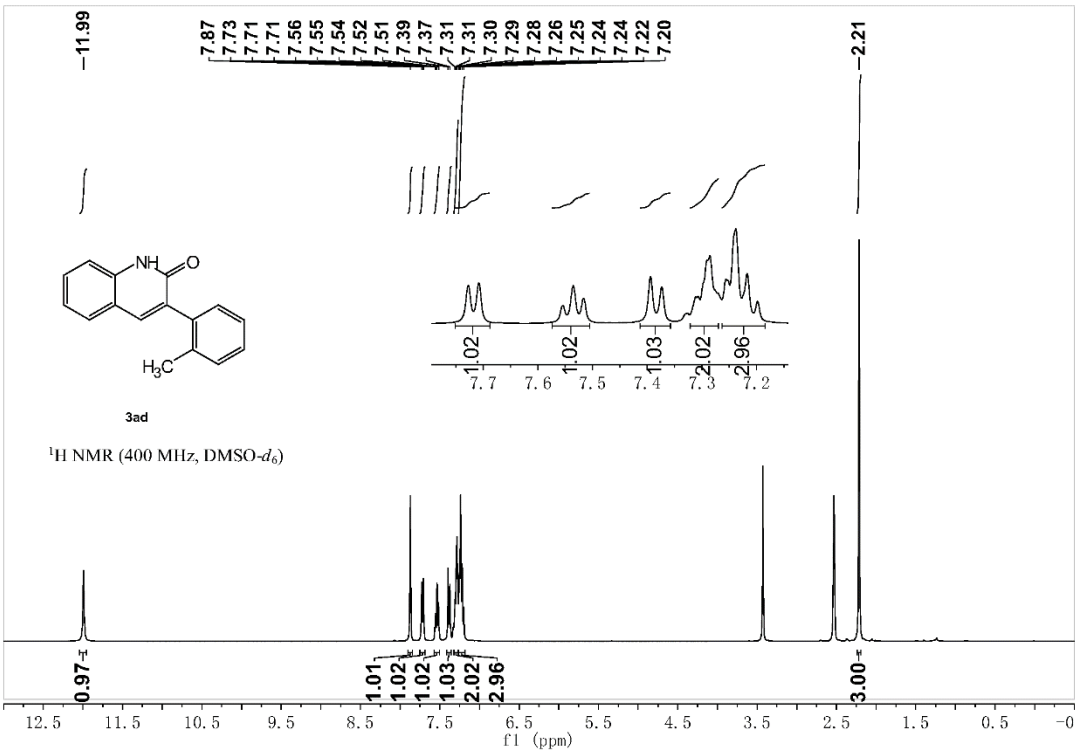
138.7
137.6
137.5
133.8
131.9
130.5
129.7
129.3
129.0
128.5
122.3
120.1
115.1
21.3
129.01
138.71
137.64
137.51
133.83
131.86
130.50
129.70
129.28
128.50
NH
O
CH3
3ab
13C NMR (101 MHz, DMSO-d6)
f1 (ppm)



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



^{1}C NMR (101 MHz, DMSO-d_6)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7.87
7.73
7.71
7.71
7.56
7.55
7.54
7.52
7.51
7.39
7.37
7.31
7.31
7.30
7.29
7.28
7.26
7.25
7.24
7.24
7.22
7.20
2.21
NH
O
H3C
3ad
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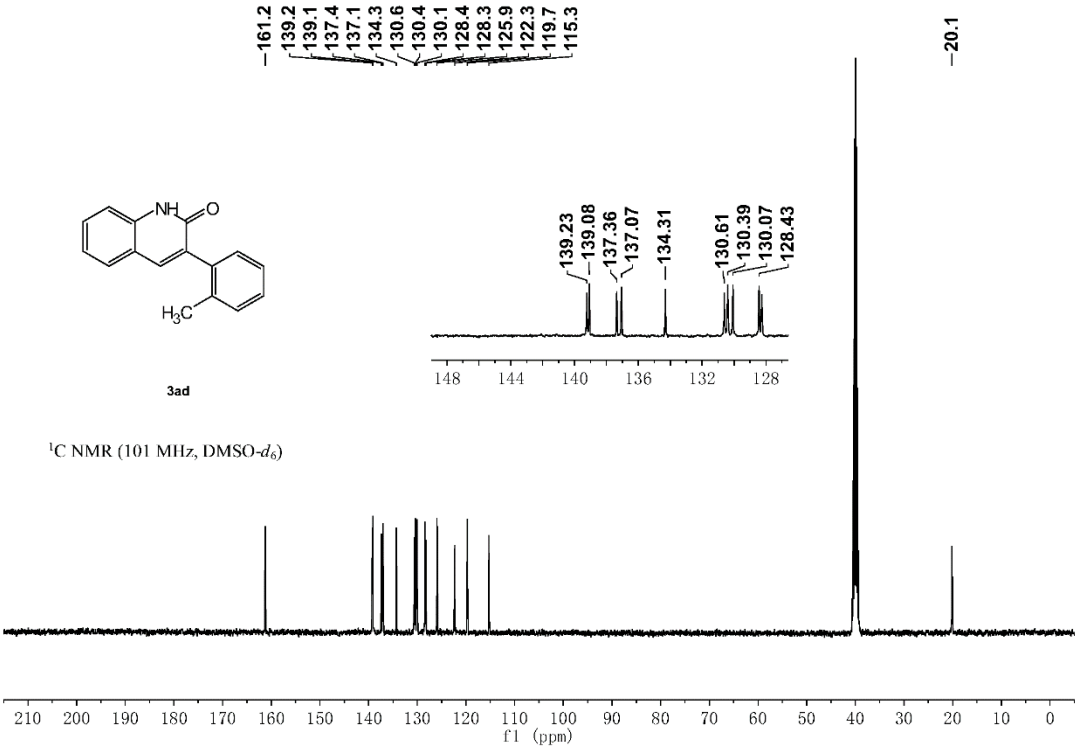
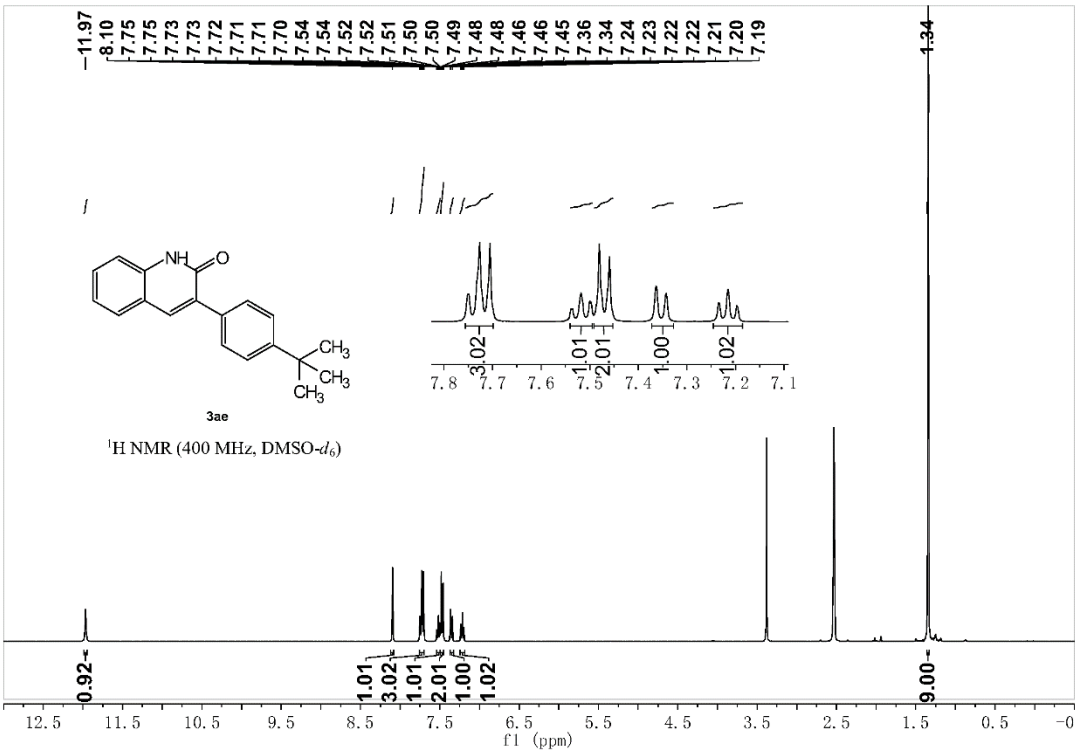
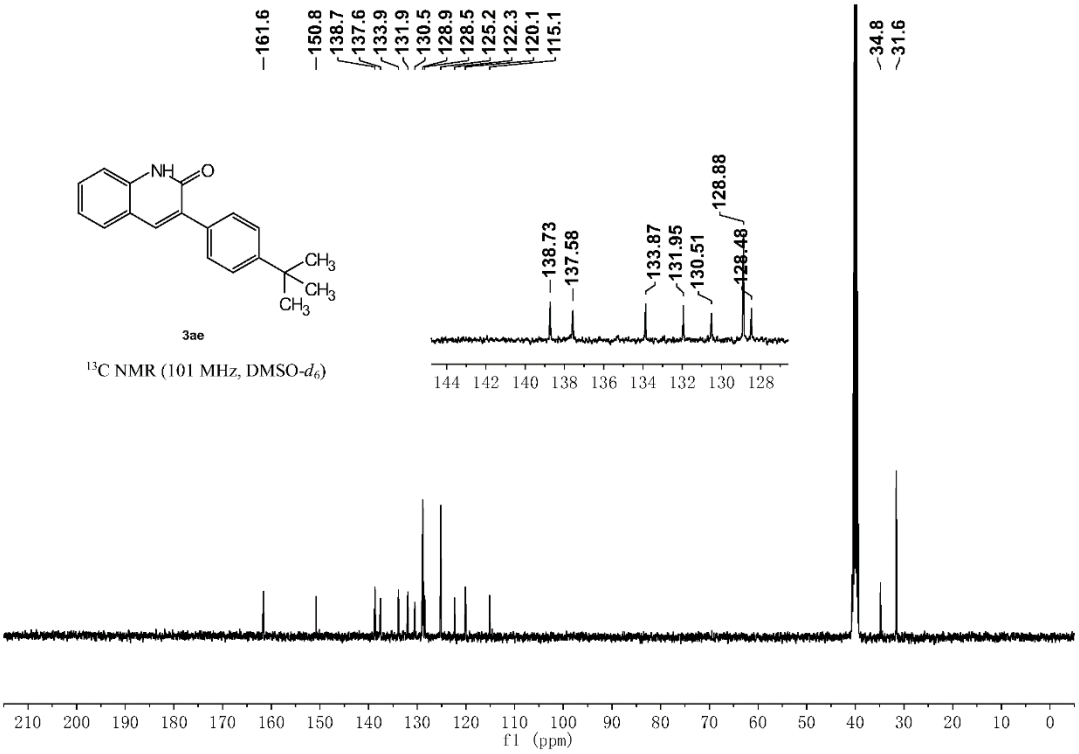
1.02
1.02
1.03
2.02
2.96
3.00
f1 (ppm)


161.2
139.2
139.1
137.4
137.1
134.3
130.6
130.4
130.1
128.4
128.3
125.9
122.3
119.7
115.3
20.1
139.23
139.08
137.36
137.07
134.31
130.61
130.39
130.07
128.43
NH
O
H3C
3ad
13C NMR (101 MHz, DMSO-d6)
f1 (ppm)



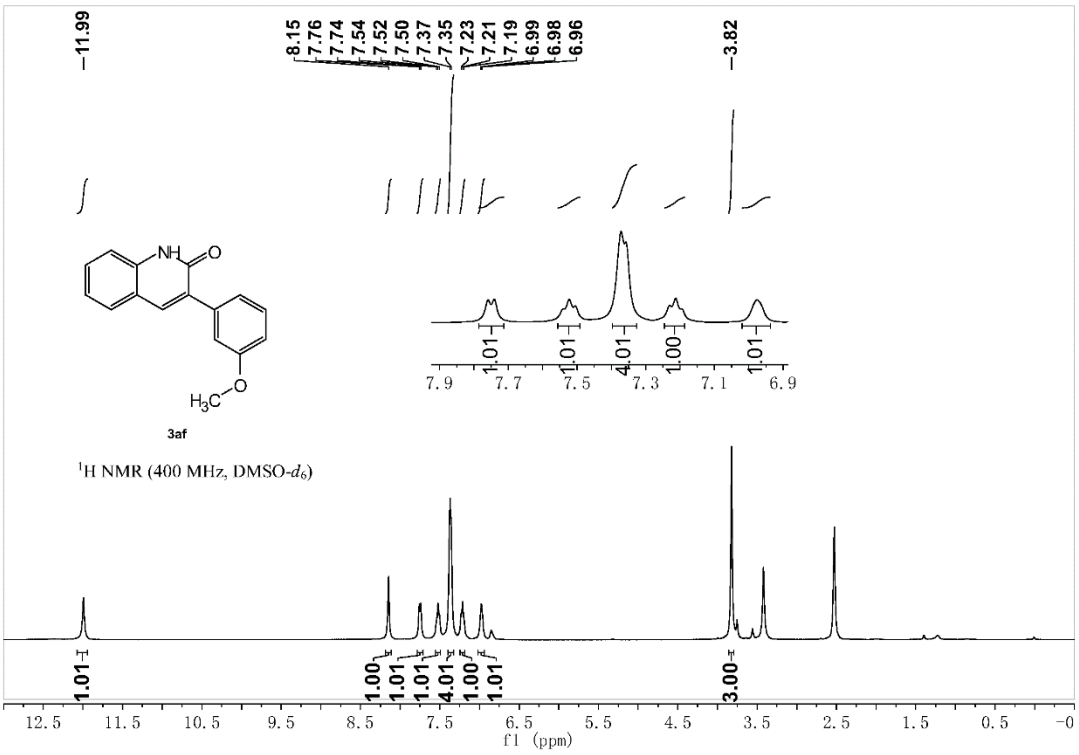
3ae

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



3ae

^{13}C NMR (101 MHz, DMSO-d_6)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7.52
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7.37
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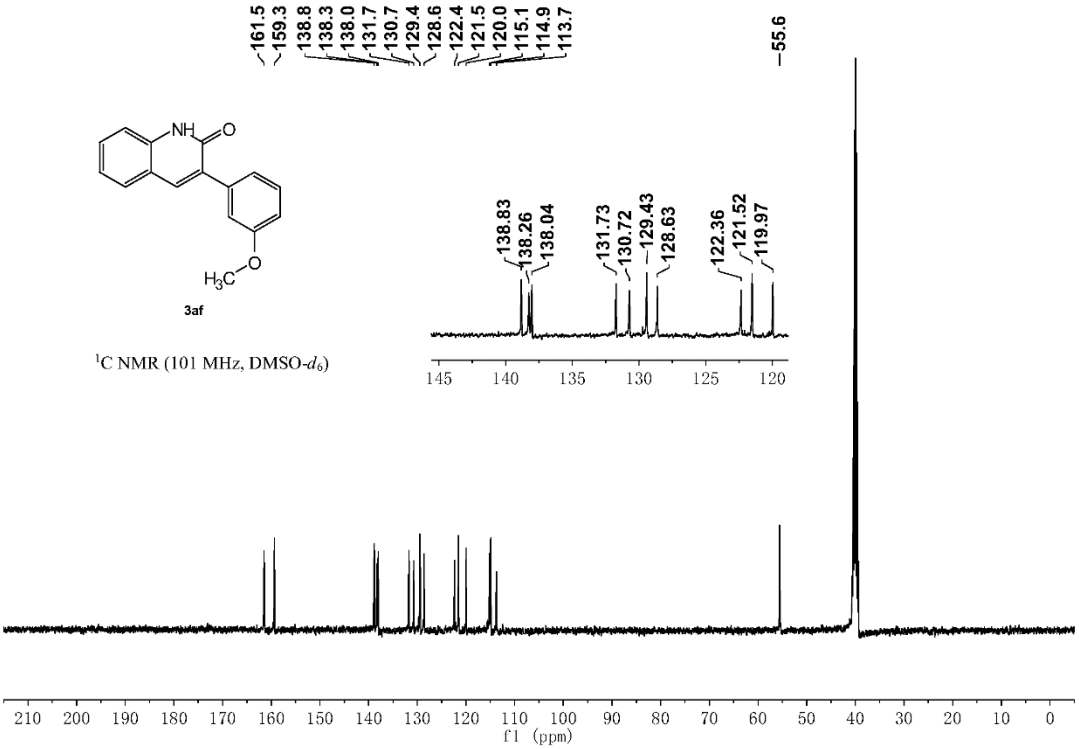
7.23
7.21
7.19
6.99
6.98
6.96
3.82
NH
O
H3C
O
3af
1H NMR (400 MHz, DMSO-d6)
1.01
1.00
1.01
1.01
4.01
1.00
1.01
3.00
12.5 11.5 10.5 9.5 8.5 7.5 6.5 5.5 4.5 3.5 2.5 1.5 0.5 −0
f1 (ppm)


161.5
159.3
138.8
138.3
138.0
131.7
130.7
129.4
128.6
122.4
121.5
120.0
115.1
114.9
113.7
55.6
NH
O
H3C
O
3af
13C NMR (101 MHz, DMSO-d6)
138.83
138.26
138.04
131.73
130.72
129.43
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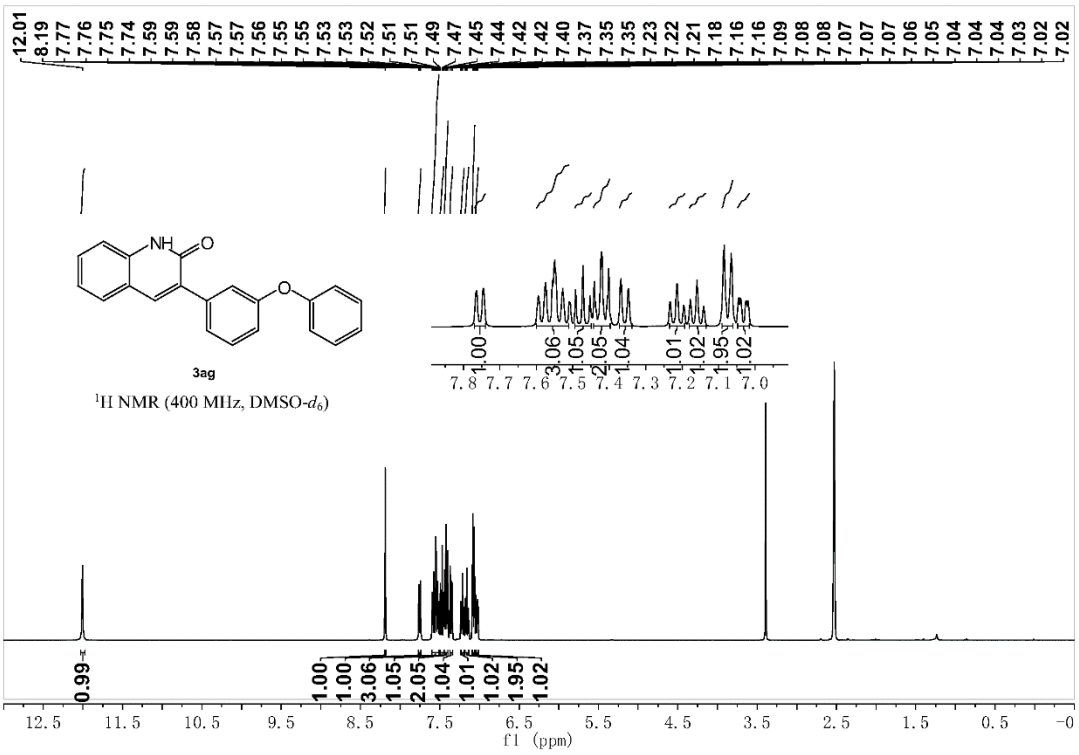
f1 (ppm)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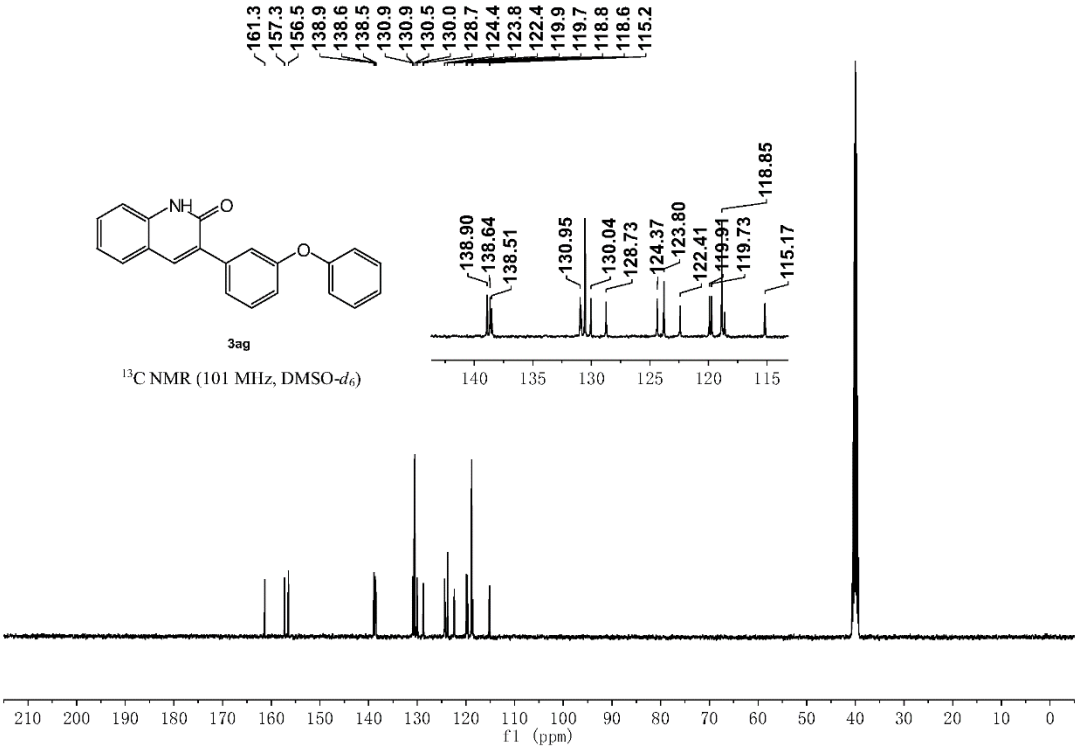
7.42
7.40
7.37
7.35
7.35
7.23
7.22
7.21
7.18
7.16
7.16
7.09
7.08
7.08
7.07
7.07
7.07
7.06
7.05
7.04
7.04
7.04
7.03
7.02
7.02
NH
O
O
3ag
1H NMR (400 MHz, DMSO-d6)
1.00
3.06
1.05
2.05
1.04
1.01
1.02
1.95
1.02
7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0
0.99
1.00
1.00
3.06
1.05
2.05
1.04
1.01
1.02
1.95
1.02
12.5 11.5 10.5 9.5 8.5 7.5 6.5 5.5 4.5 3.5 2.5 1.5 0.5 −0
f1 (ppm)


161.3
157.3
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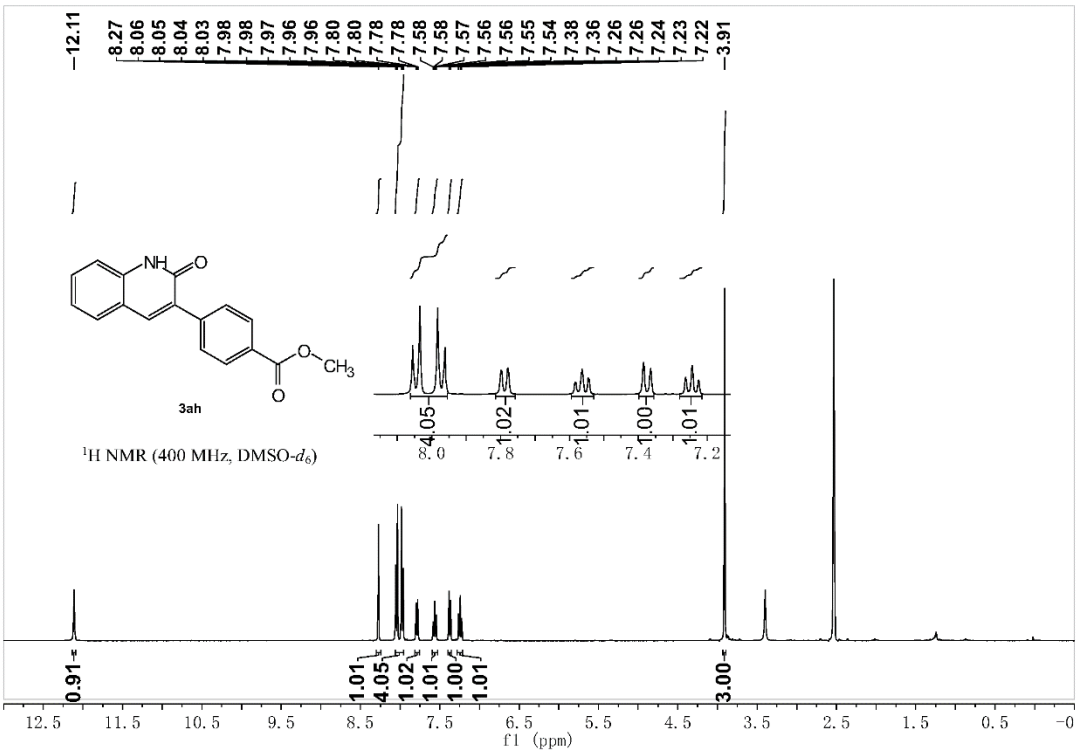
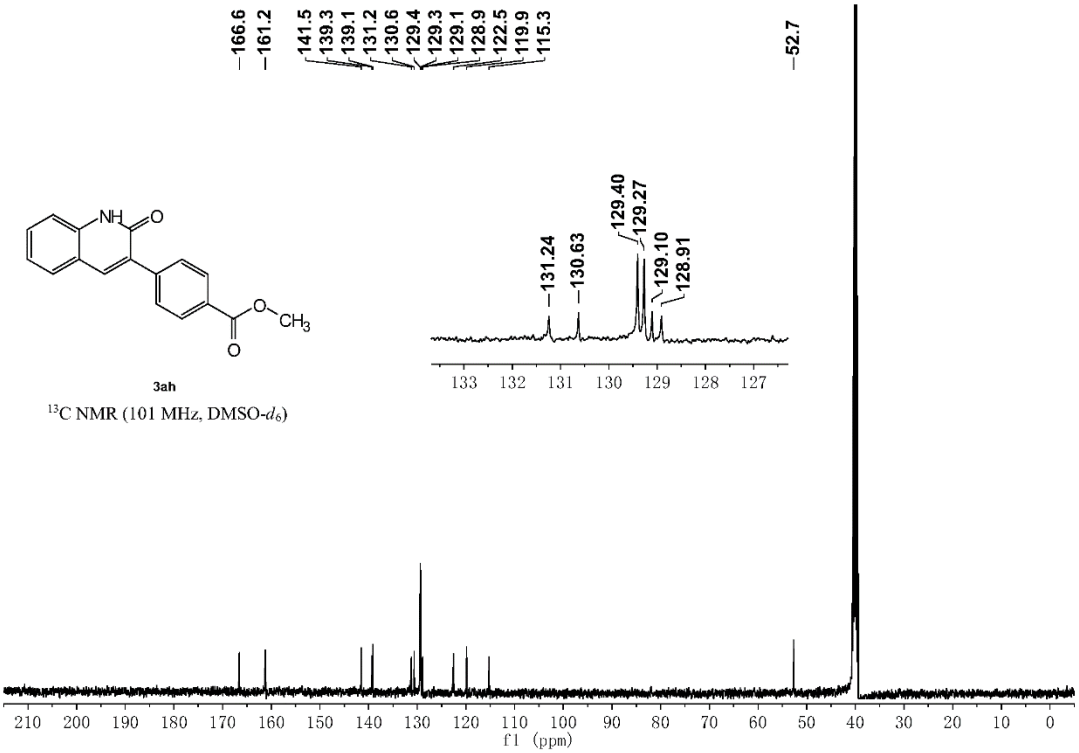
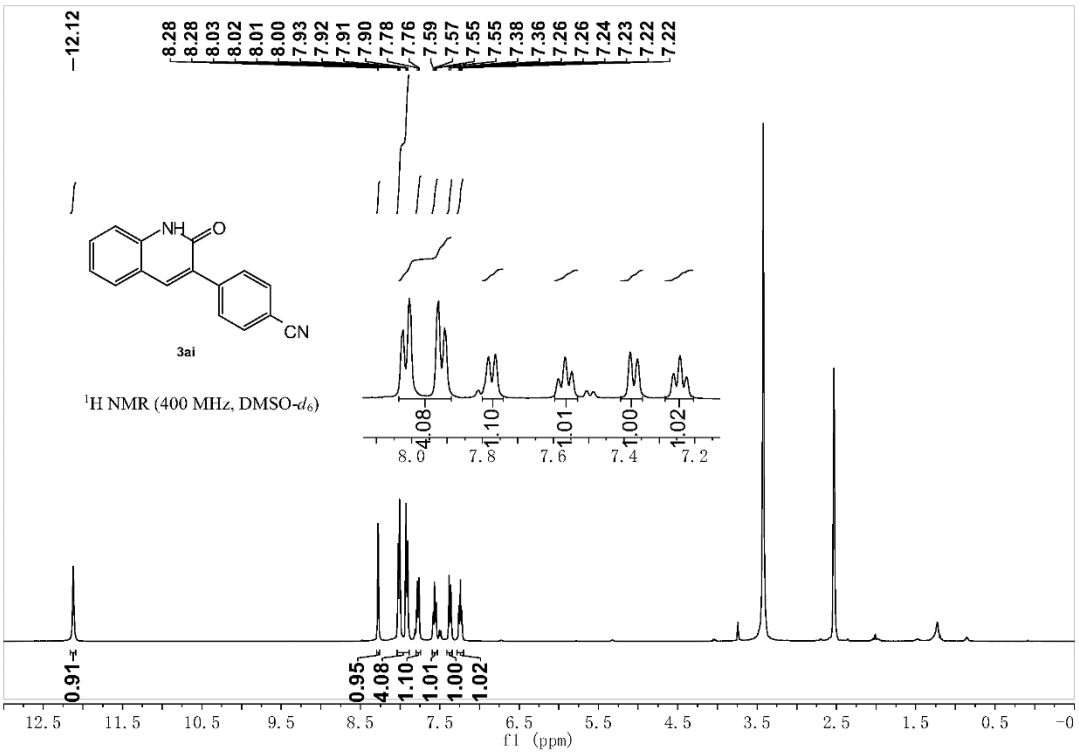
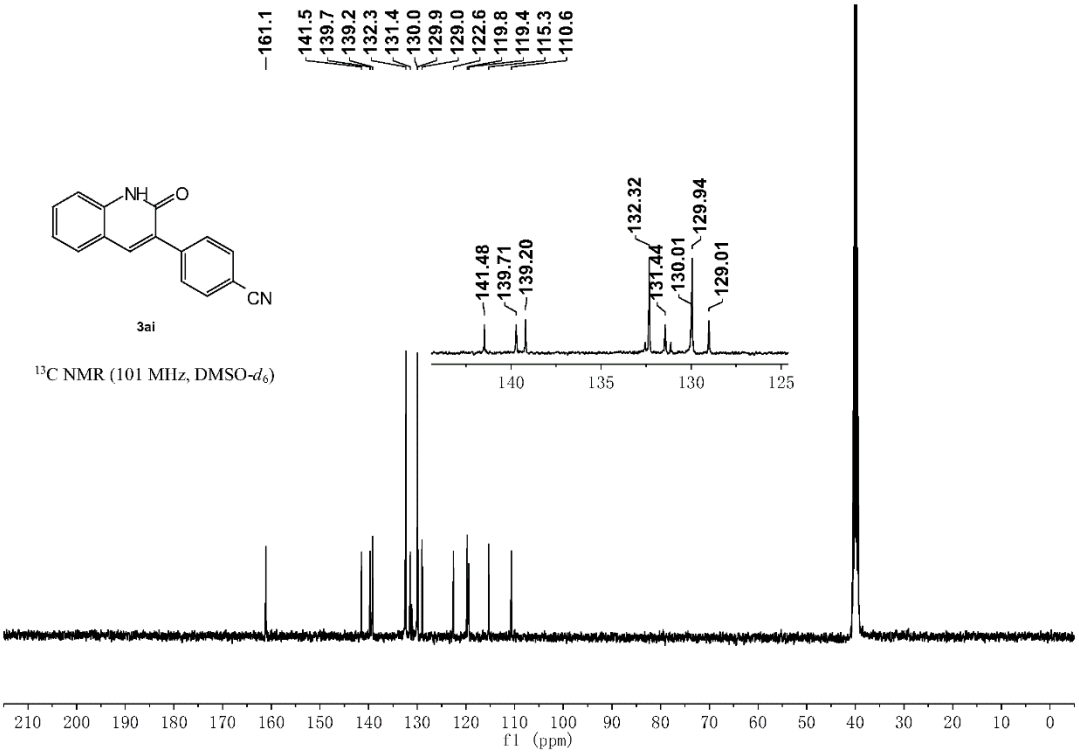
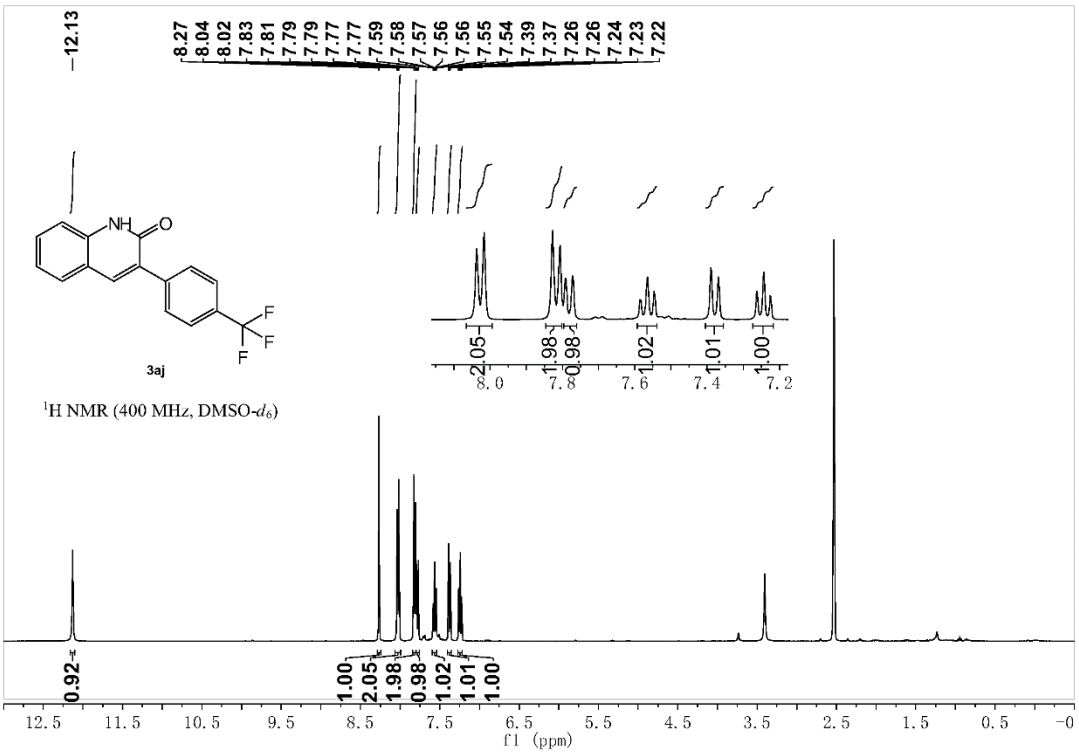
138.5
130.9
130.9
130.5
130.0
128.7
124.4
123.8
122.4
119.9
119.7
118.8
118.6
115.2
NH
O
O
3ag
13C NMR (101 MHz, DMSO-d6)
138.90
138.64
138.51
130.95
130.04
128.73
124.37
123.80
122.41
119.94
119.73
118.85
115.17
140 135 130 125 120 115
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


12.11
8.27
8.06
8.05
8.04
8.03
7.98
7.98
7.97
7.96
7.96
7.80
7.80
7.78
7.78
7.58
7.58
7.57
7.56
7.56
7.55
7.54
7.38
7.36
7.26
7.26
7.24
7.23
7.22
3.91
NH
O
O
O
CH3
3ah
1H NMR (400 MHz, DMSO-d6)
4.05
1.02
1.01
1.00
1.01
8.0
7.8
7.6
7.4
7.2
0.91
1.01
4.05
1.02
1.01
1.00
1.01
3.00
12.5
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
−0
f1 (ppm)

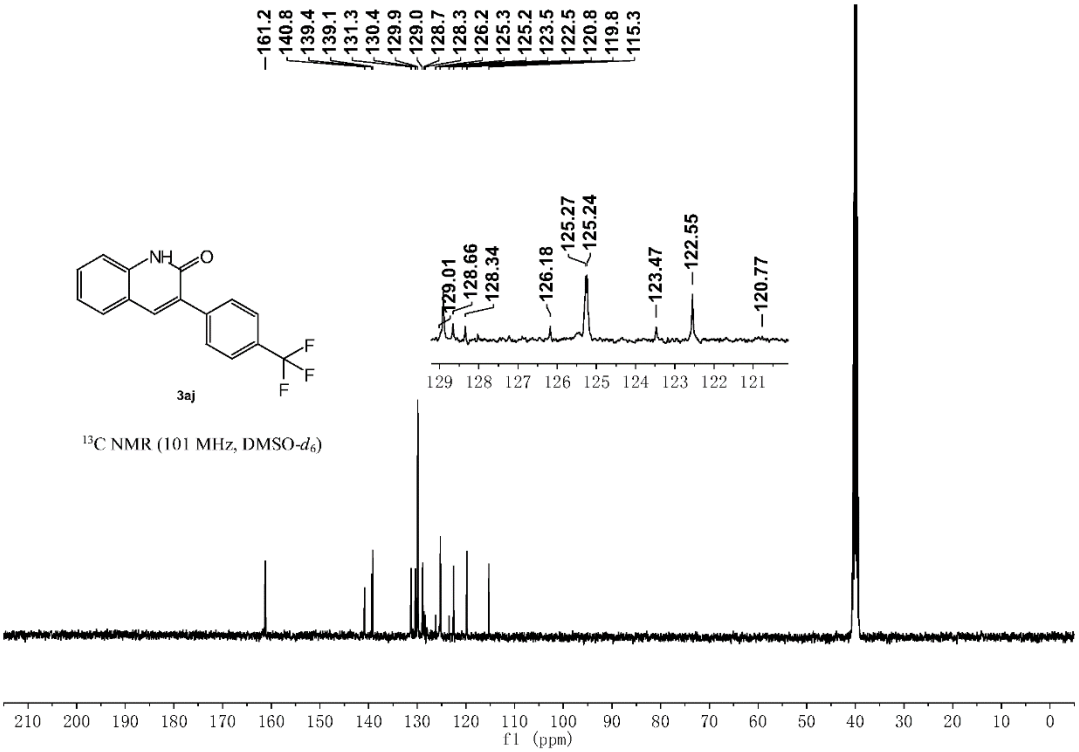

166.6
161.2
141.5
139.3
139.1
131.2
130.6
129.4
129.3
129.1
128.9
122.5
119.9
115.3
52.7
NH
O
O
O
CH3
3ah
13C NMR (101 MHz, DMSO-d6)
131.24
130.63
129.40
129.27
129.10
128.91
133
132
131
130
129
128
127
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


12.12
8.28
8.28
8.03
8.02
8.01
8.00
7.93
7.92
7.91
7.90
7.78
7.76
7.59
7.57
7.55
7.55
7.38
7.36
7.26
7.26
7.24
7.23
7.22
7.22
NH
O
CN
3ai
1H NMR (400 MHz, DMSO-d6)
4.08
1.10
1.01
1.00
1.02
8.0
7.8
7.6
7.4
7.2
0.91
0.95
4.08
1.10
1.01
1.00
1.02
12.5
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
−0
f1 (ppm)

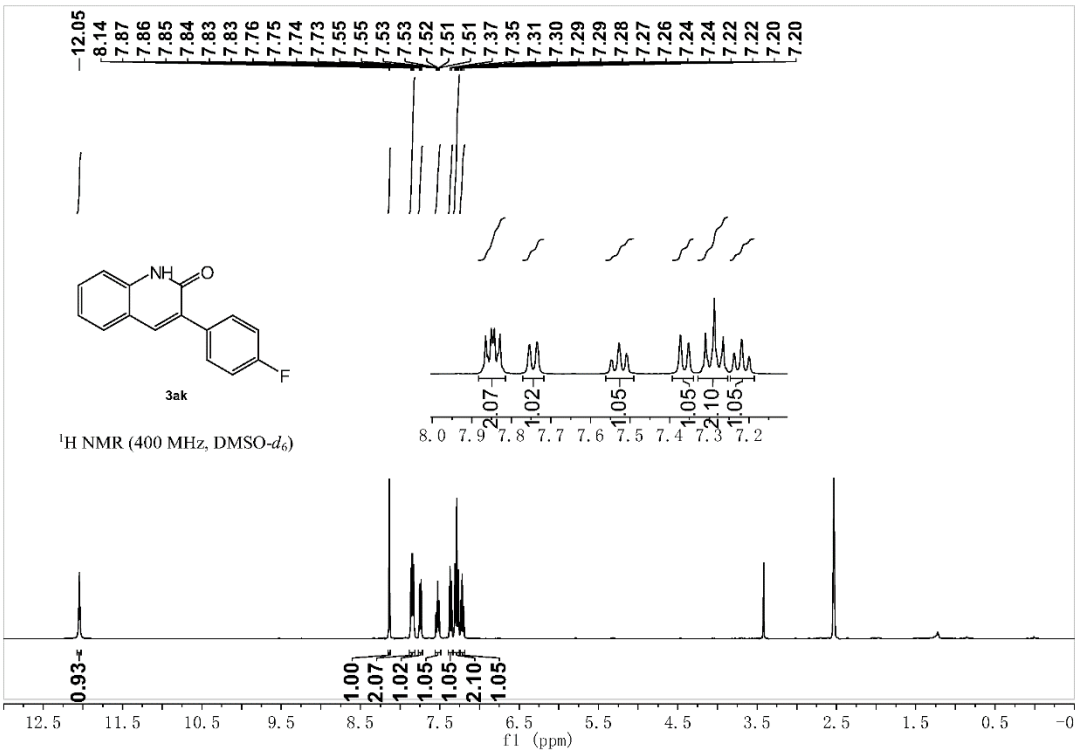

161.1
141.5
139.7
139.2
132.3
131.4
130.0
129.9
129.0
122.6
119.8
119.4
115.3
110.6
NH
O
CN
3ai
13C NMR (101 MHz, DMSO-d6)
141.48
139.71
139.20
132.32
131.44
130.01
129.94
129.01
140
135
130
125
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)



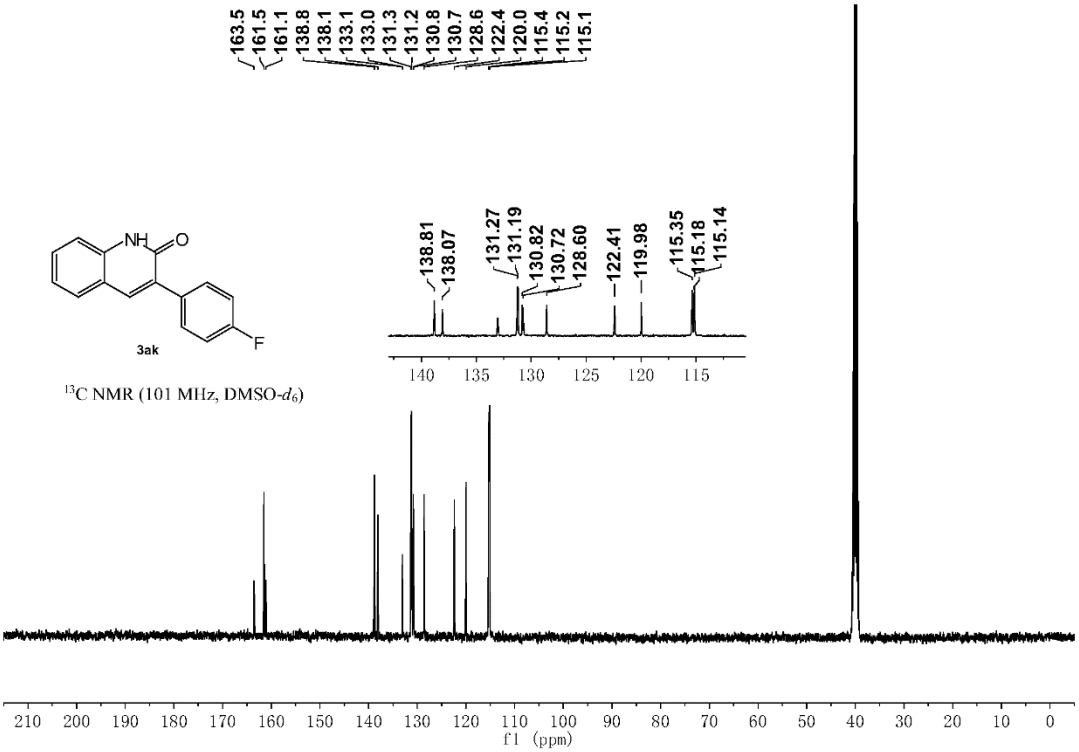
^{1}H NMR (400 MHz, DMSO-d_6)



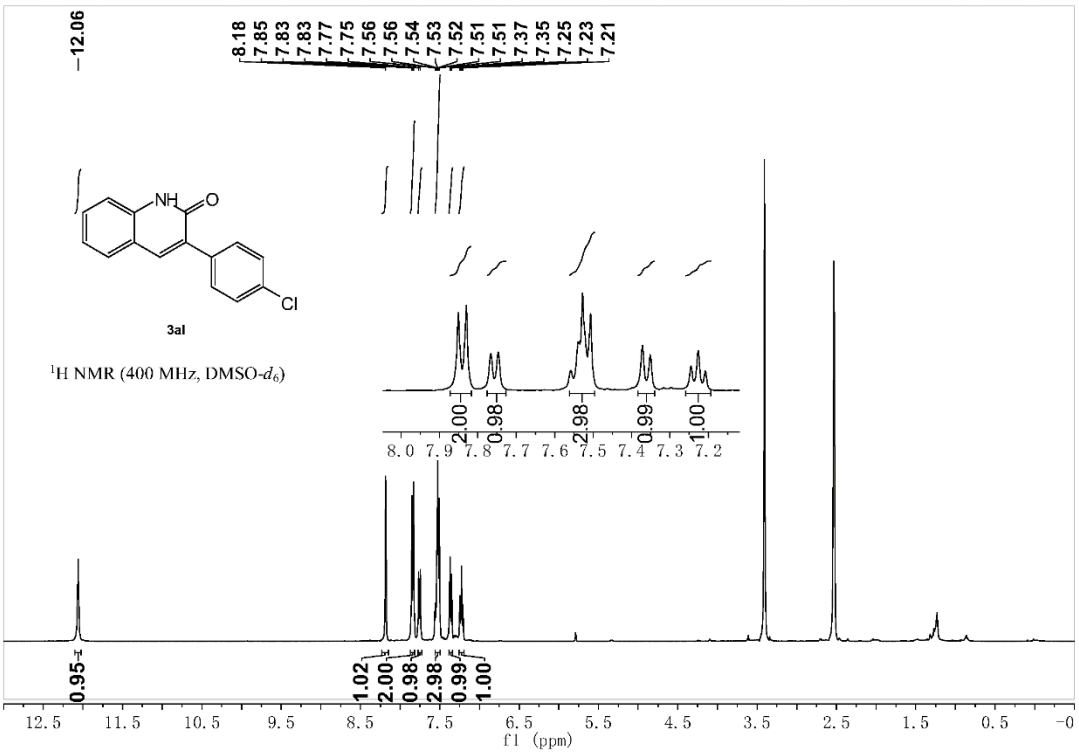
^{13}C NMR (101 MHz, DMSO-d_6)

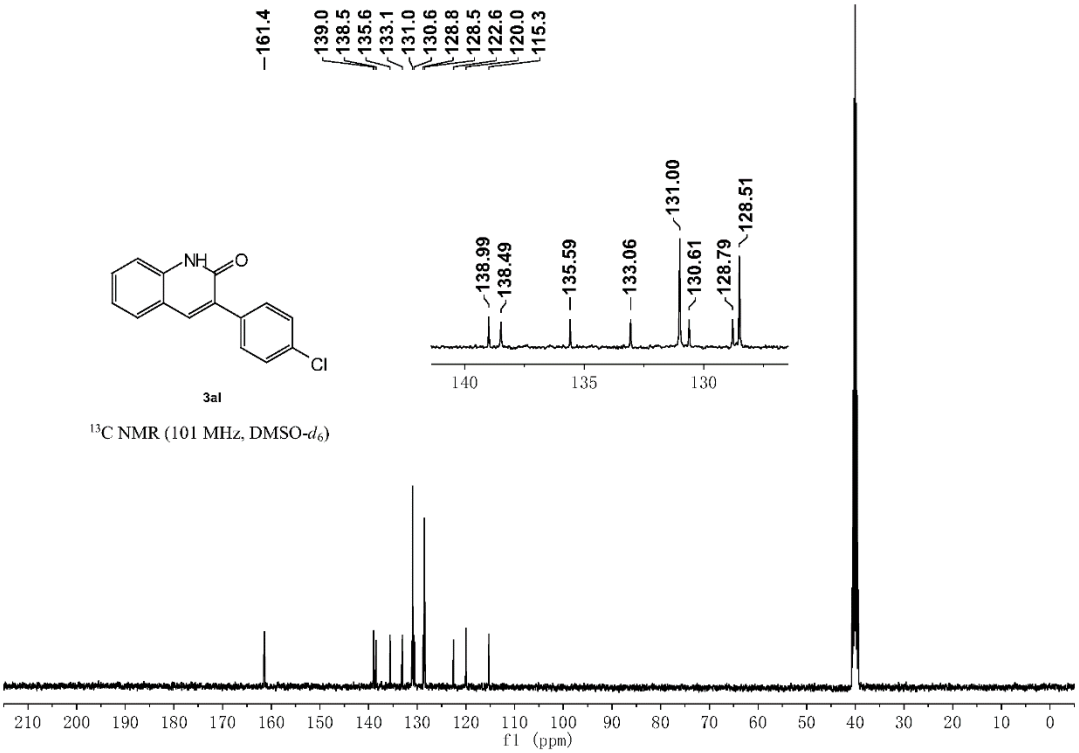


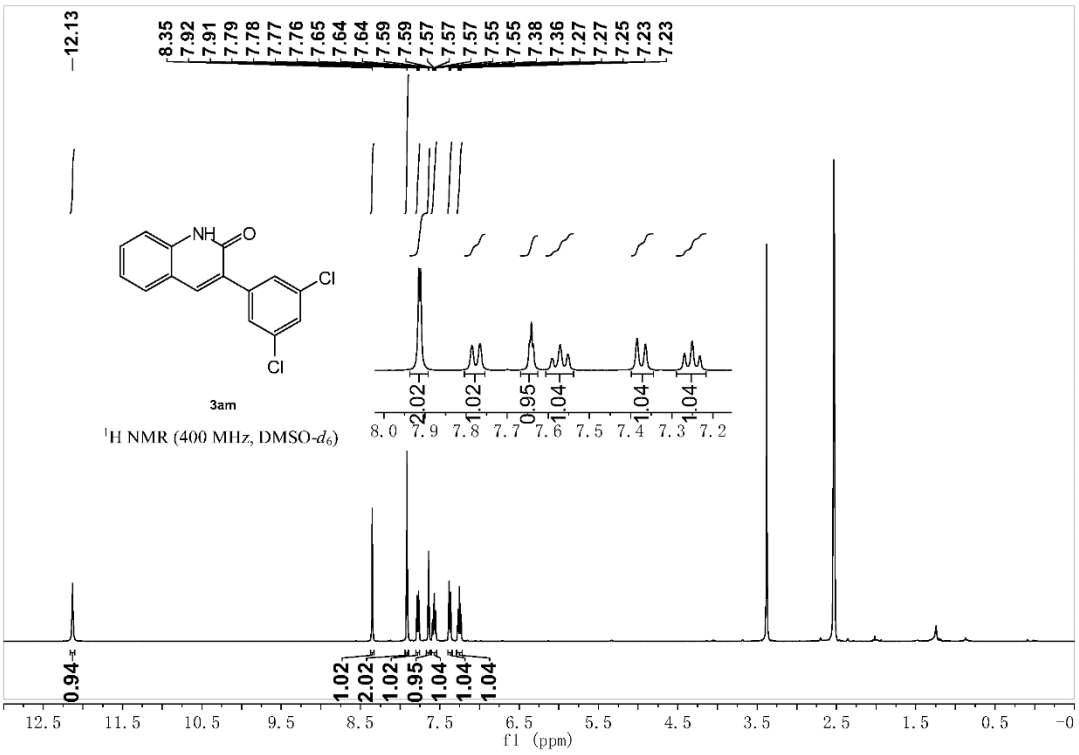
^{1}H NMR (400 MHz, DMSO-d_6)

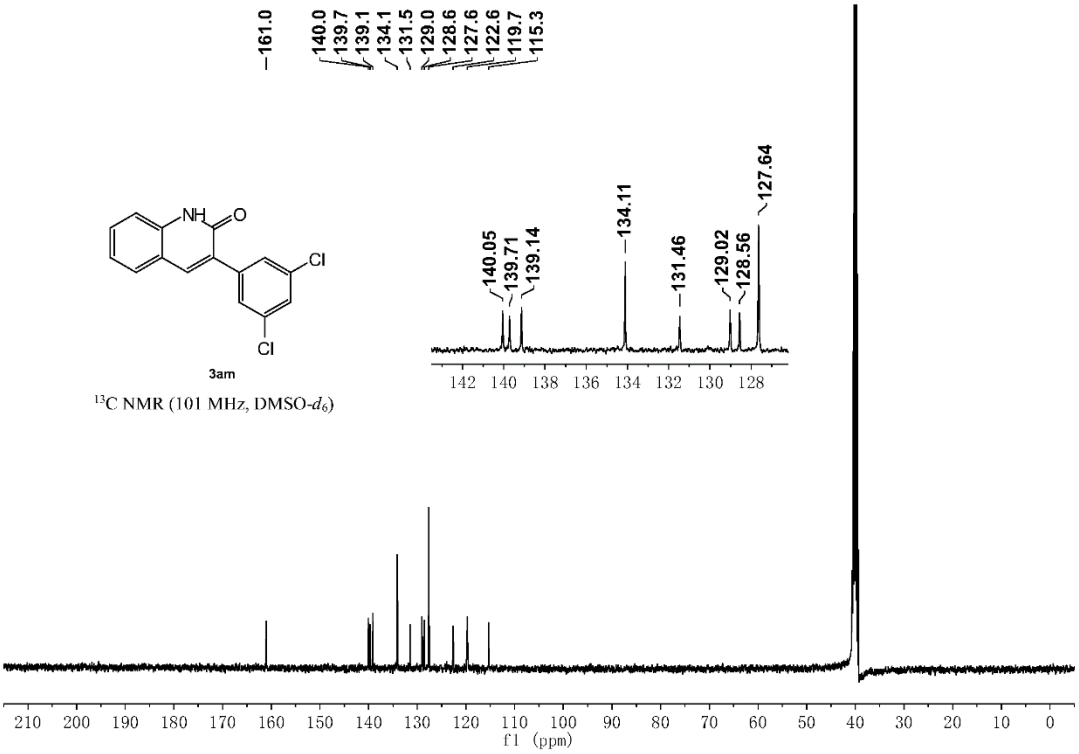


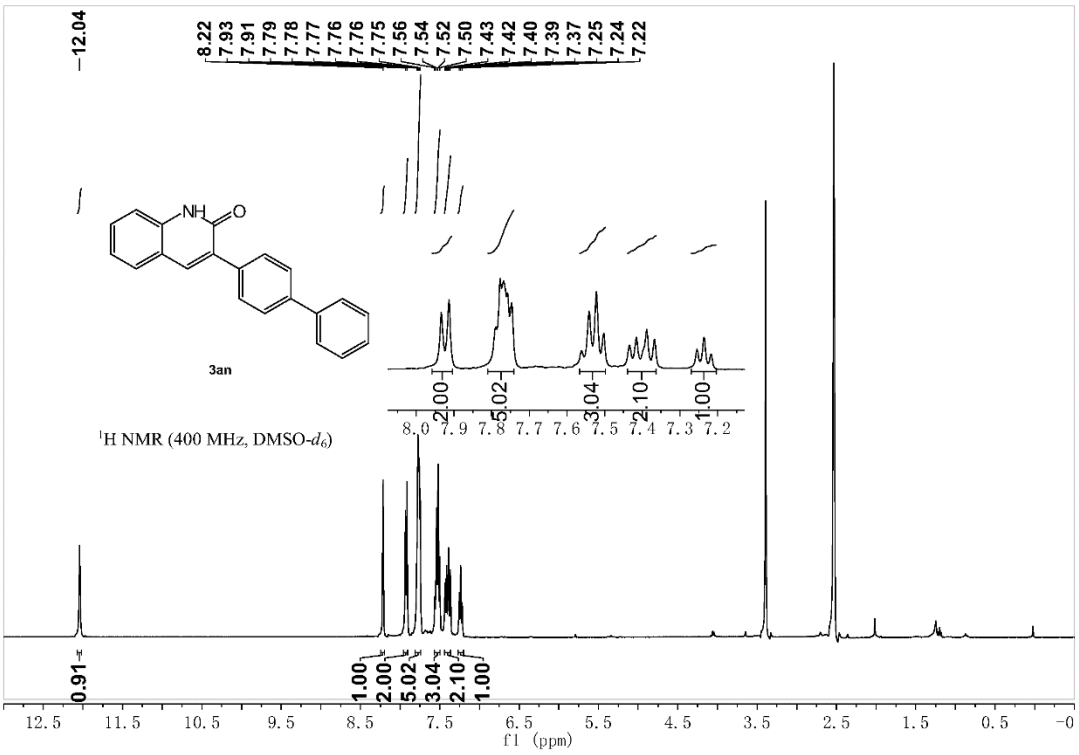
^{13}C NMR (101 MHz, DMSO-d_6)

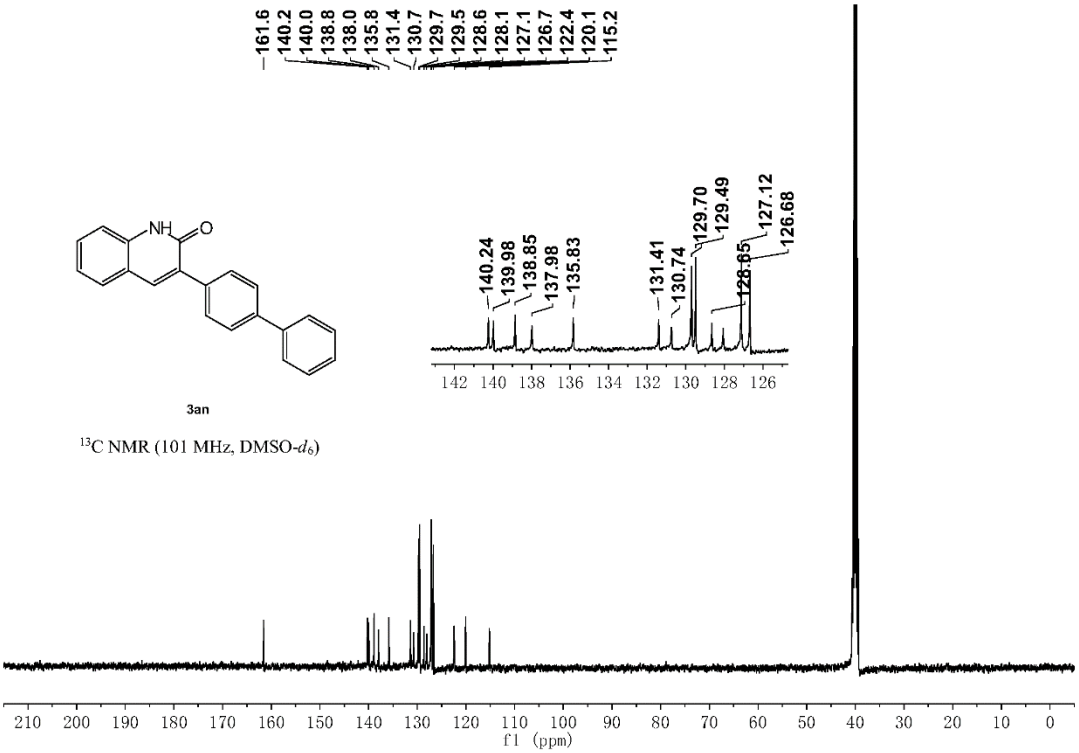

12.06
8.18
7.85
7.83
7.83
7.77
7.75
7.56
7.56
7.54
7.53
7.52
7.51
7.51
7.37
7.35
7.25
7.23
7.21
NH
O
Cl
3al
1H NMR (400 MHz, DMSO-d6)
2.00
0.98
2.98
0.99
1.00
8.0 7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2
0.95
1.02
2.00
0.98
2.98
0.99
1.00
12.5 11.5 10.5 9.5 8.5 7.5 6.5 5.5 4.5 3.5 2.5 1.5 0.5 -0
f1 (ppm)

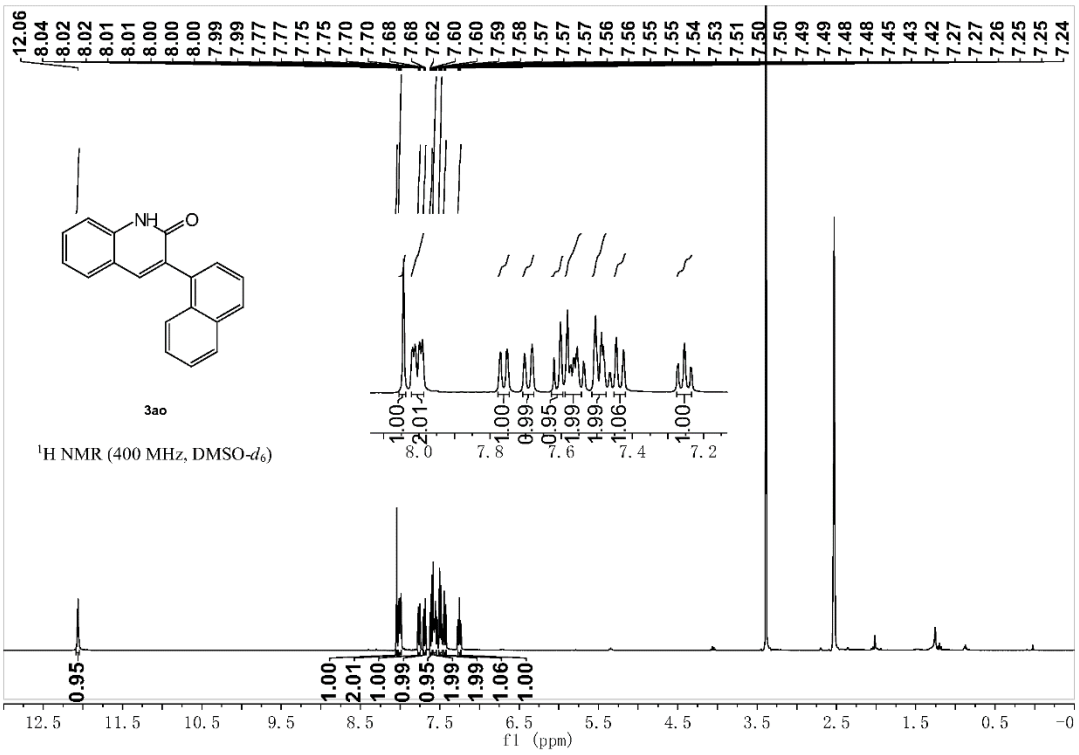

161.4
139.0
138.5
135.6
133.1
131.0
130.6
128.8
128.5
122.6
120.0
115.3
NH
O
Cl
3al
13C NMR (101 MHz, DMSO-d6)
138.99
138.49
135.59
133.06
131.00
130.61
128.79
128.51
140
135
130
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

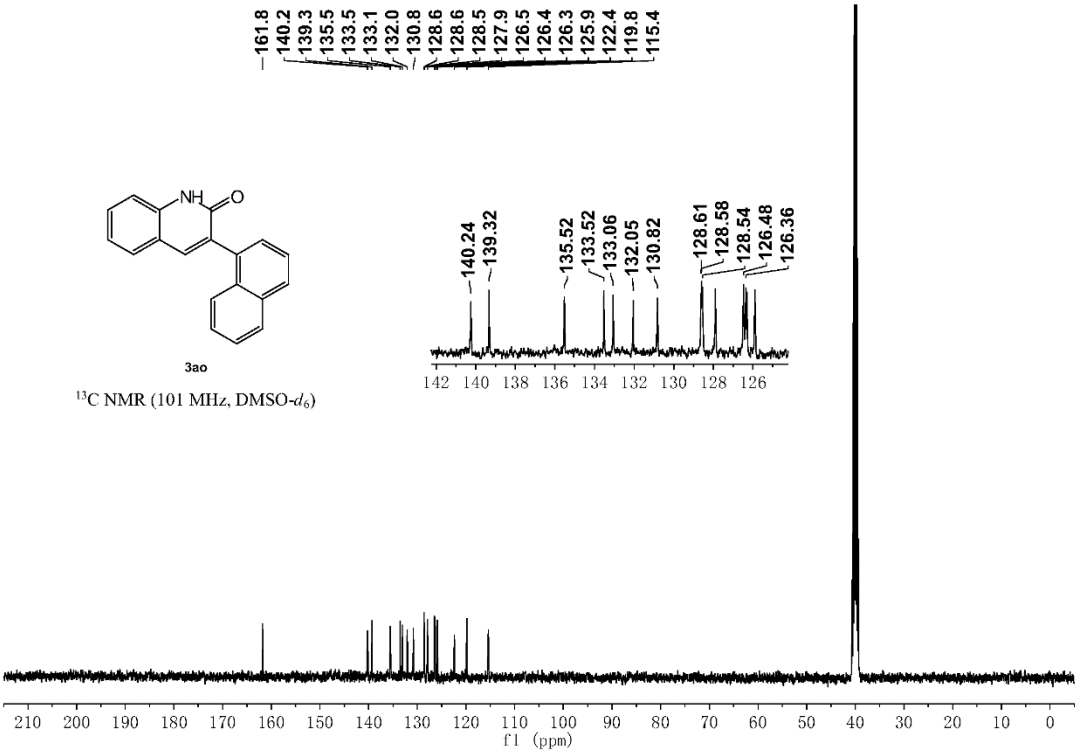

12.13
8.35
7.92
7.91
7.79
7.78
7.77
7.76
7.65
7.64
7.64
7.59
7.59
7.57
7.57
7.57
7.55
7.55
7.38
7.36
7.27
7.27
7.25
7.23
7.23
NH
O
Cl
Cl
3am
1H NMR (400 MHz, DMSO-d6)
2.02
1.02
1.02
0.95
1.04
1.04
1.04
0.94
1.02
2.02
1.02
0.95
1.04
1.04
1.04
f1 (ppm)

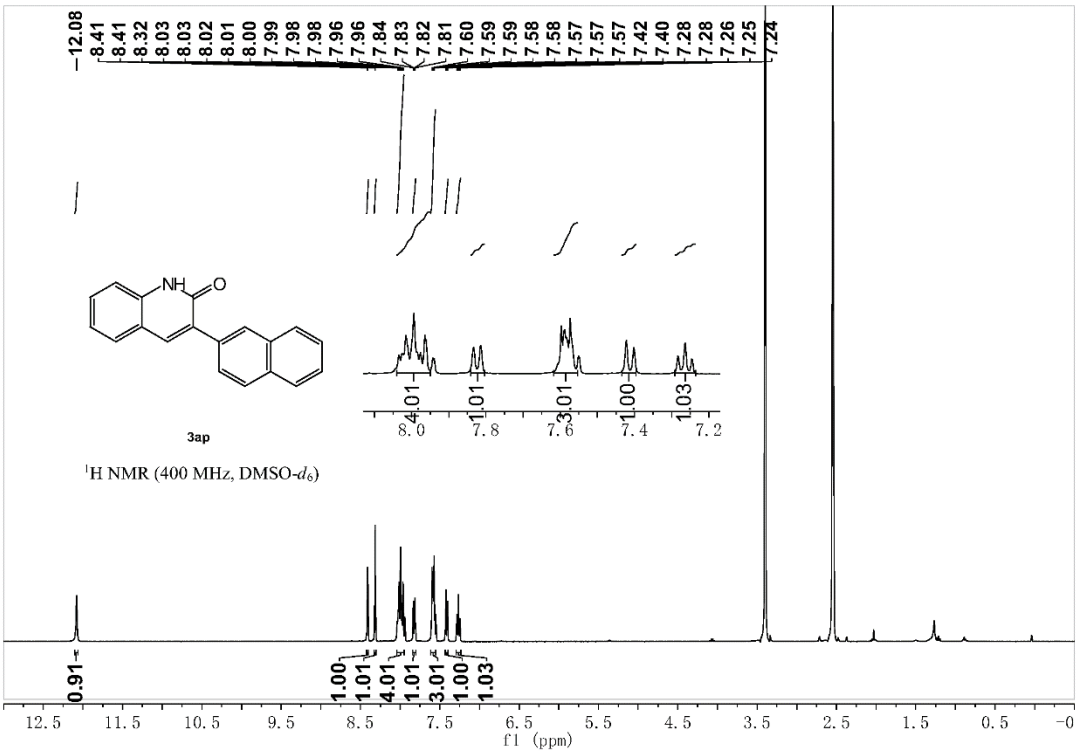

161.0
140.0
139.7
139.1
134.1
131.5
129.0
128.6
127.6
122.6
119.7
115.3
NH
O
Cl
Cl
3am
13C NMR (101 MHz, DMSO-d6)
140.05
139.71
139.14
134.11
131.46
129.02
128.56
127.64
f1 (ppm)


12.04
8.22
7.93
7.91
7.79
7.78
7.77
7.76
7.76
7.75
7.56
7.54
7.52
7.50
7.43
7.42
7.40
7.39
7.37
7.25
7.24
7.22
NH
O
3an
2.00
5.02
3.04
2.10
1.00
8.0 7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2
^{1}H NMR (400 MHz, DMSO-d_6)
0.91
1.00
2.00
5.02
3.04
2.10
1.00
12.5 11.5 10.5 9.5 8.5 7.5 6.5 5.5 4.5 3.5 2.5 1.5 0.5 −0
f1 (ppm)


161.6
140.2
140.0
138.8
138.0
135.8
131.4
130.7
129.7
129.5
128.6
128.1
127.1
126.7
122.4
120.1
115.2
NH
O
3an
140.24
139.98
138.85
137.98
135.83
131.41
130.74
129.70
129.49
127.12
126.68
142 140 138 136 134 132 130 128 126
^{13}C NMR (101 MHz, DMSO-d_6)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

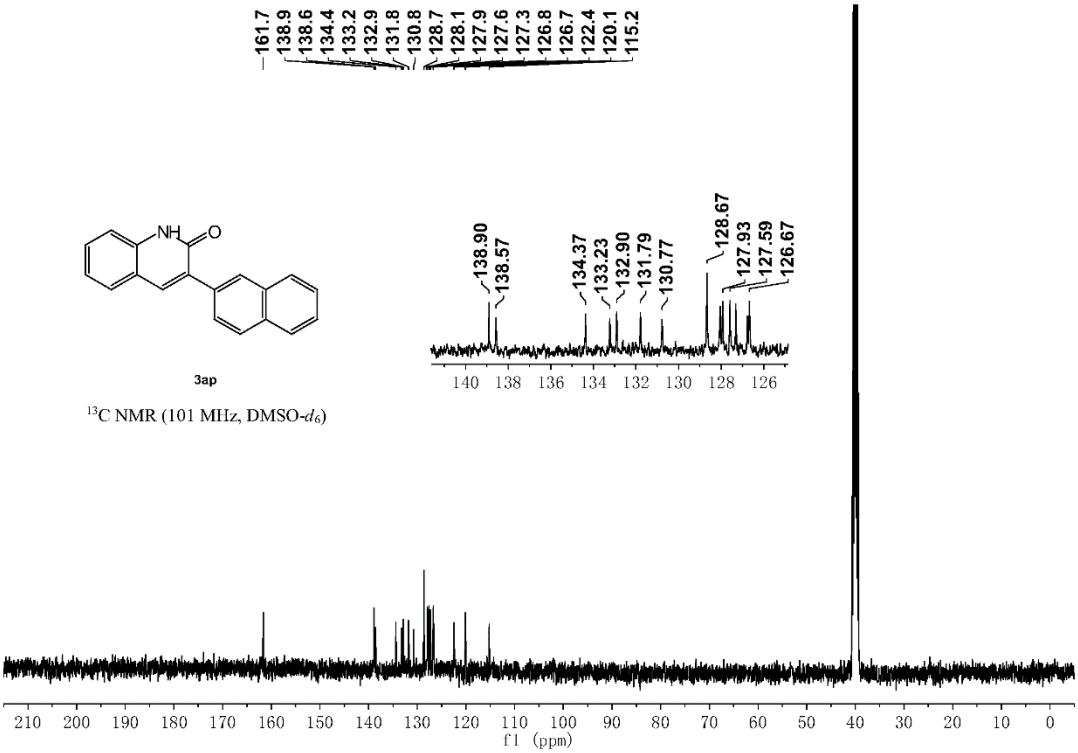

12.06
8.04
8.02
8.02
8.01
8.01
8.00
8.00
8.00
7.99
7.99
7.77
7.77
7.75
7.75
7.70
7.70
7.68
7.68
7.62
7.60
7.60
7.59
7.58
7.57
7.57
7.57
7.56
7.56
7.55
7.55
7.54
7.53
7.51
7.50
7.50
7.49
7.49
7.48
7.48
7.45
7.43
7.42
7.27
7.27
7.26
7.25
7.25
7.24
NH
O
3ao
^{1}H NMR (400 MHz, DMSO-d_6)
0.95
1.00
2.01
1.00
0.99
0.95
1.99
1.99
1.06
1.00
12.5
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
−0
f1 (ppm)


161.8
140.2
139.3
135.5
133.5
133.1
132.0
130.8
128.6
128.6
128.5
127.9
126.5
126.4
126.3
125.9
122.4
119.8
115.4
NH
O
3ao
^{13}C NMR (101 MHz, DMSO-d_6)
140.24
139.32
135.52
133.52
133.06
132.05
130.82
128.61
128.58
128.54
126.48
126.36
142 140 138 136 134 132 130 128 126
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)



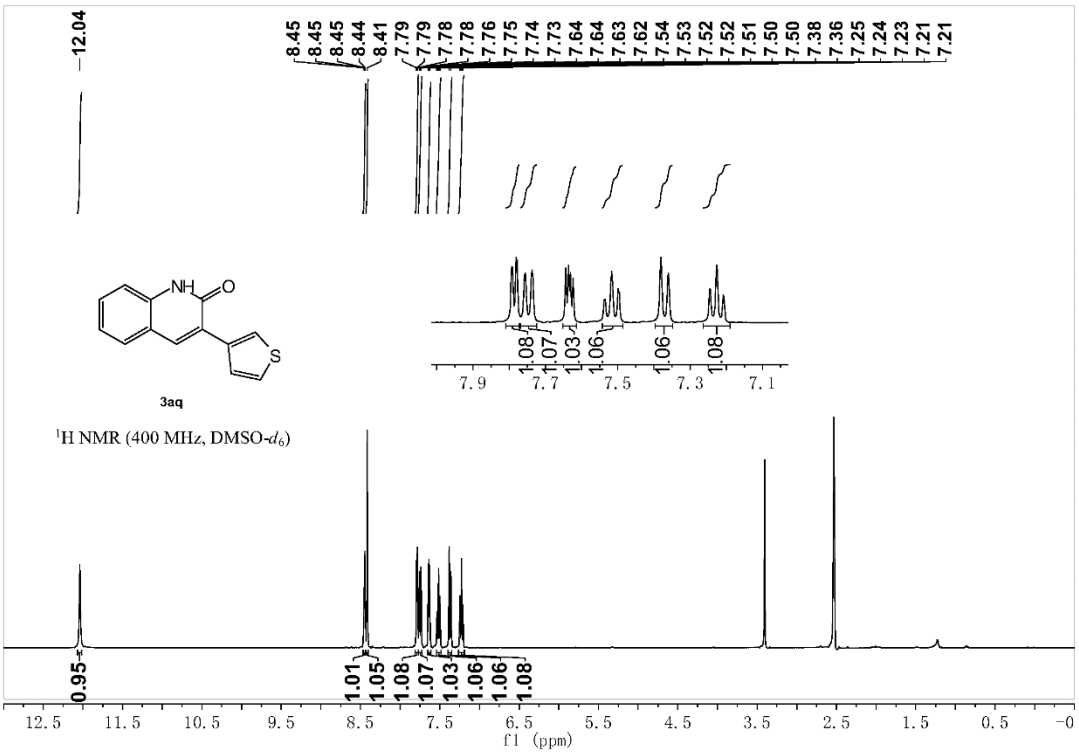
3ap

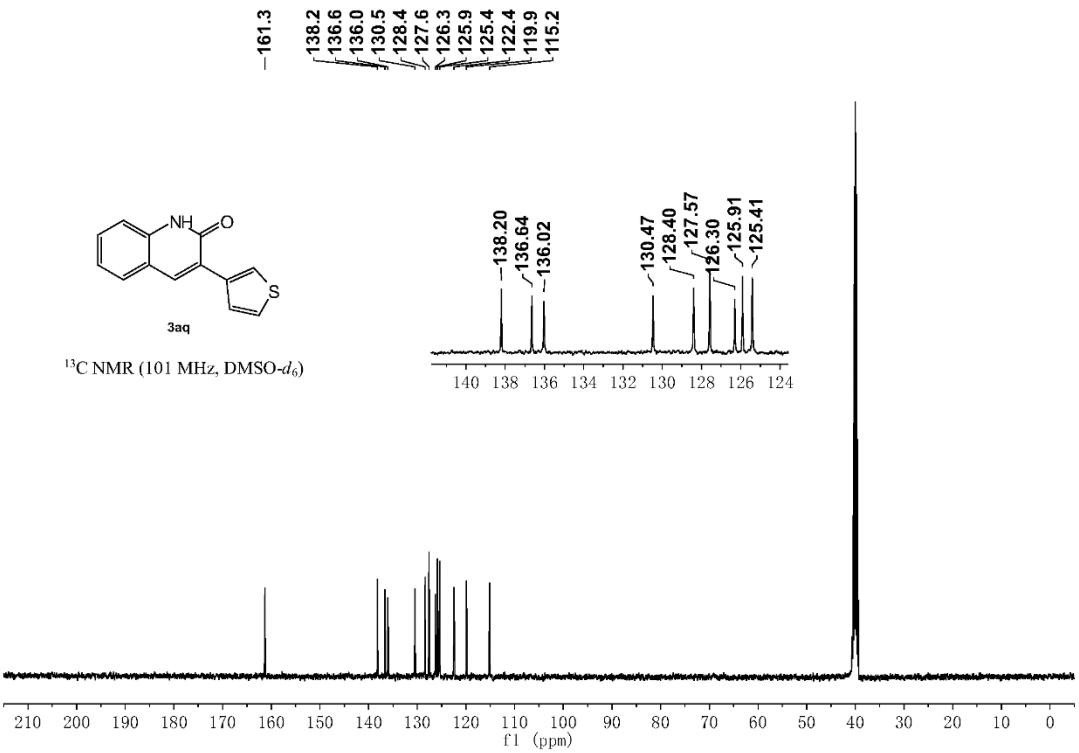
^{1}H NMR (400 MHz, DMSO-d_6)

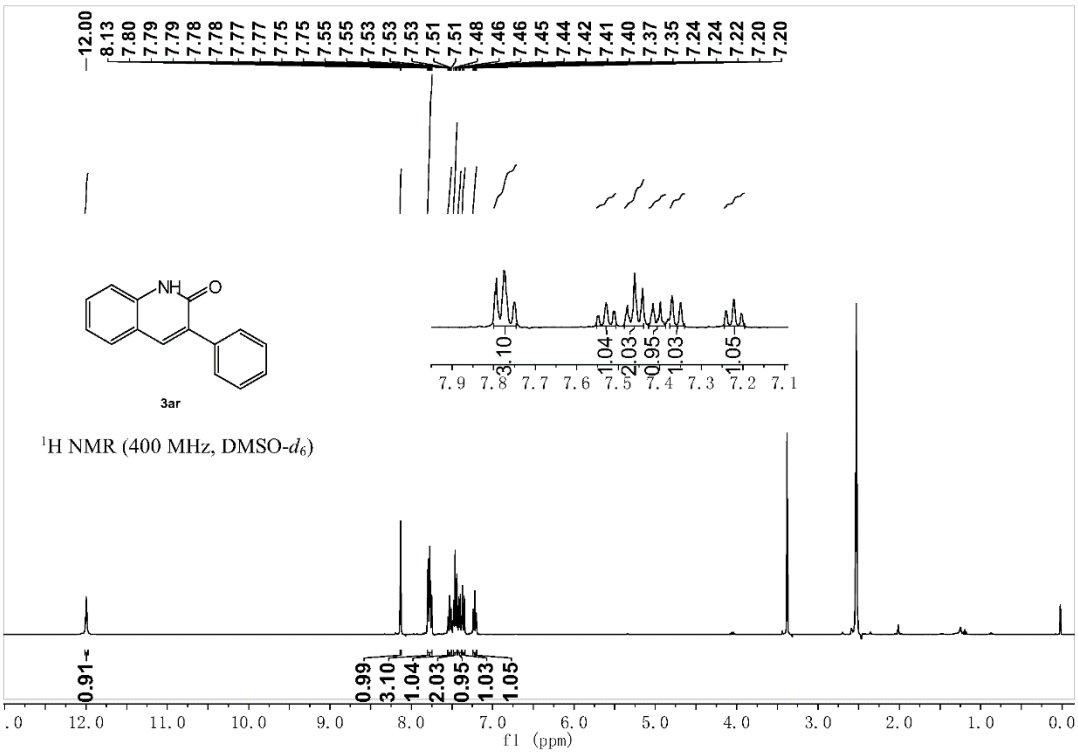


3ap

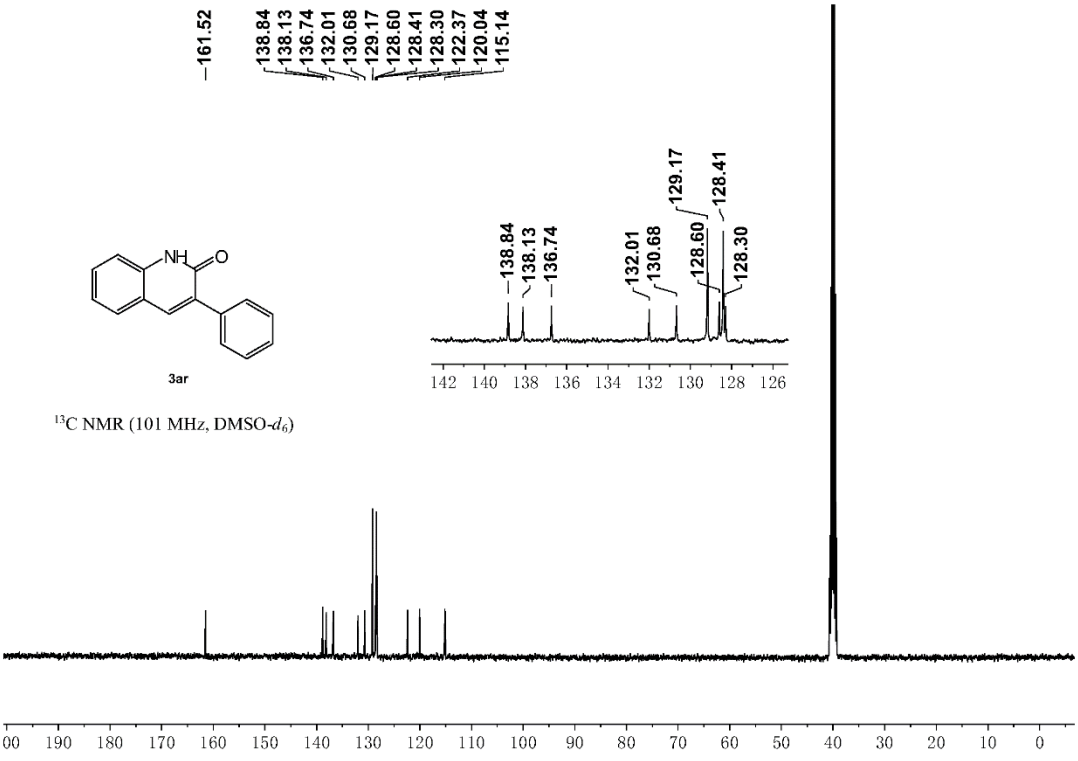
^{13}C NMR (101 MHz, DMSO-d_6)


12.04
8.45 8.45 8.45 8.44 8.41 7.79 7.79 7.78 7.78 7.76 7.75 7.74 7.73 7.64 7.64 7.63 7.62 7.54 7.53 7.52 7.52 7.51 7.50 7.50 7.38 7.36 7.25 7.24 7.23 7.21 7.21
NH
O
S
3aq
1.08 1.07 1.03 1.06 1.06 1.08
7.9 7.7 7.5 7.3 7.1
¹H NMR (400 MHz, DMSO-d6)
0.95 1.01 1.05 1.08 1.07 1.03 1.06 1.06 1.08
12.5 11.5 10.5 9.5 8.5 7.5 6.5 5.5 4.5 3.5 2.5 1.5 0.5 −0
f1 (ppm)

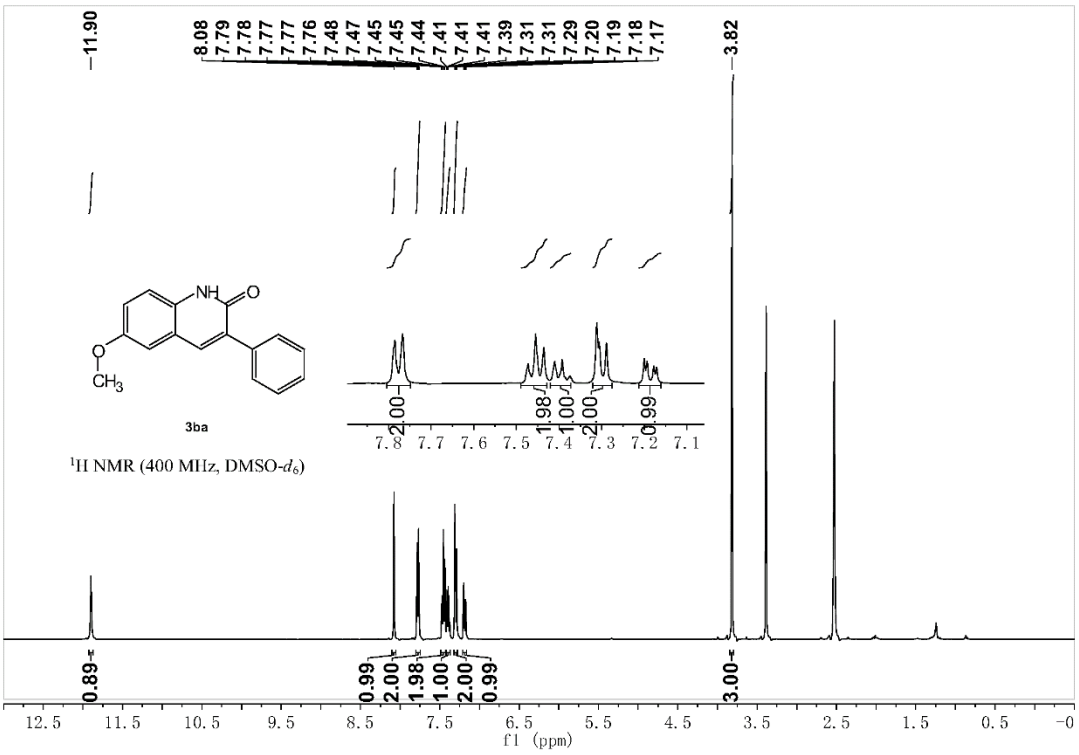

161.3
138.2 136.6 136.0 130.5 128.4 127.6 126.3 125.9 125.4 122.4 119.9 115.2
NH
O
S
3aq
138.20 136.64 136.02 130.47 128.40 127.57 126.30 125.91 125.41
140 138 136 134 132 130 128 126 124
¹³C NMR (101 MHz, DMSO-d6)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

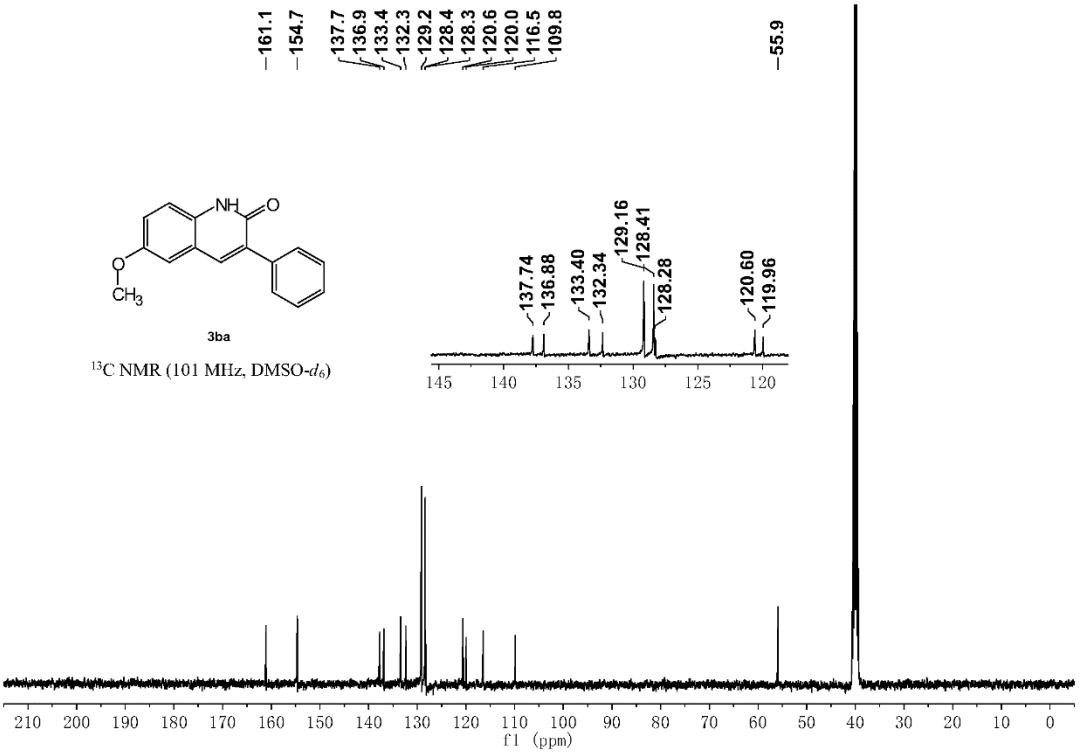


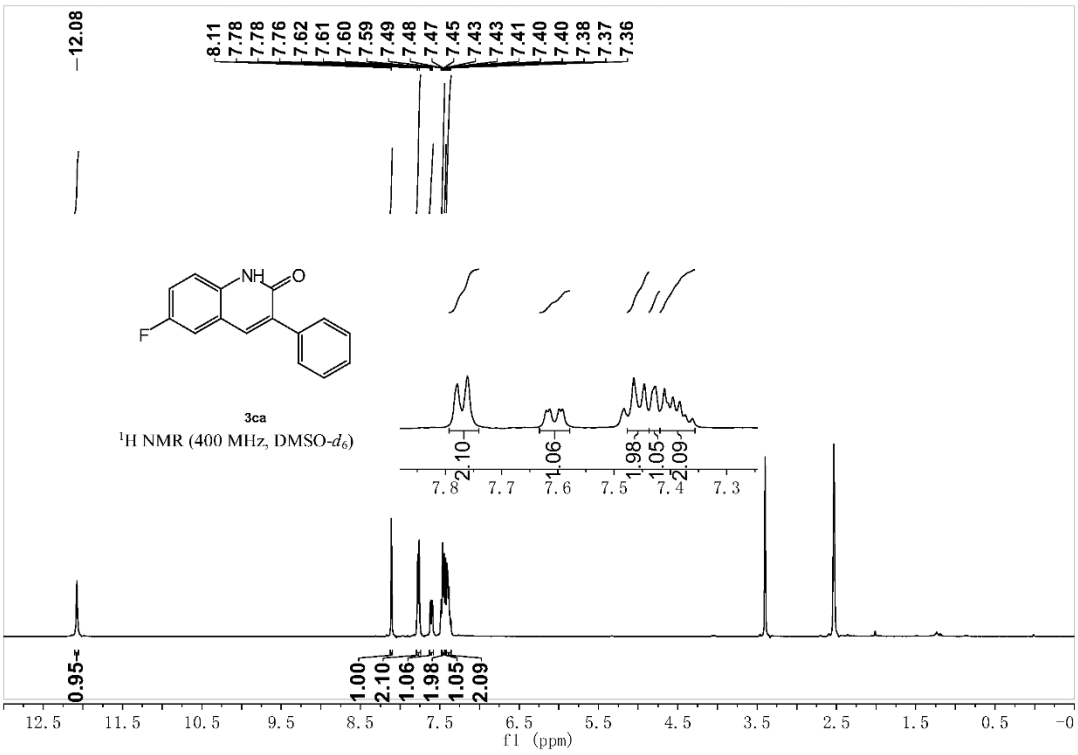
^{1}H NMR (400 MHz, DMSO-d_6)

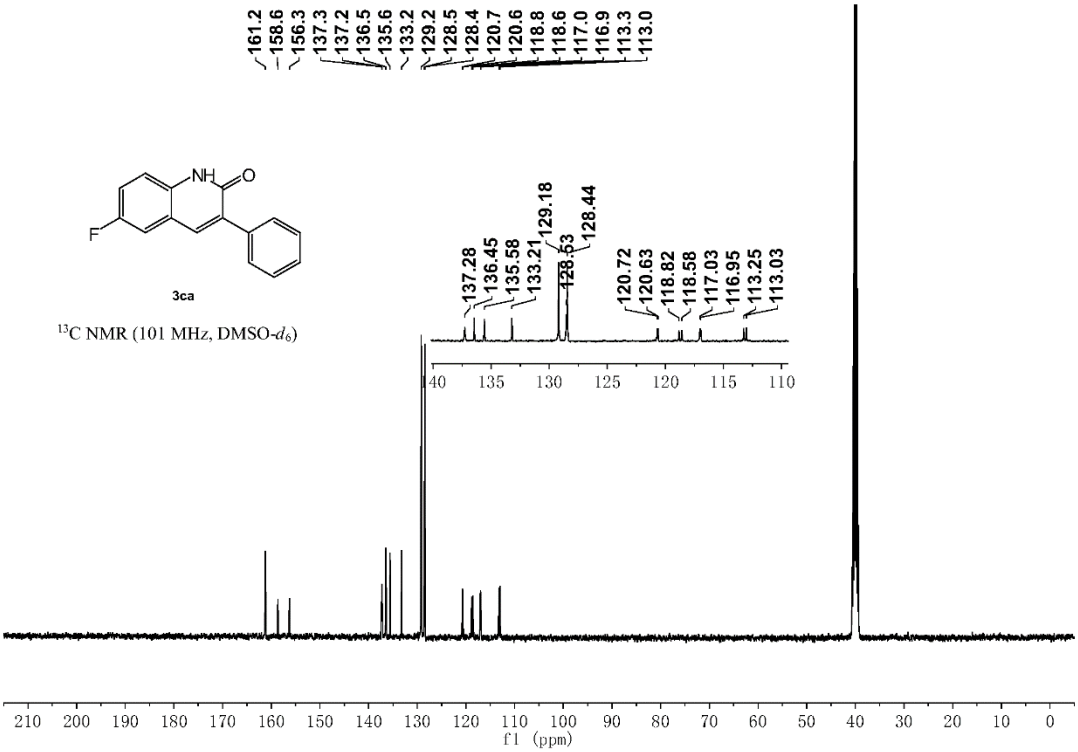


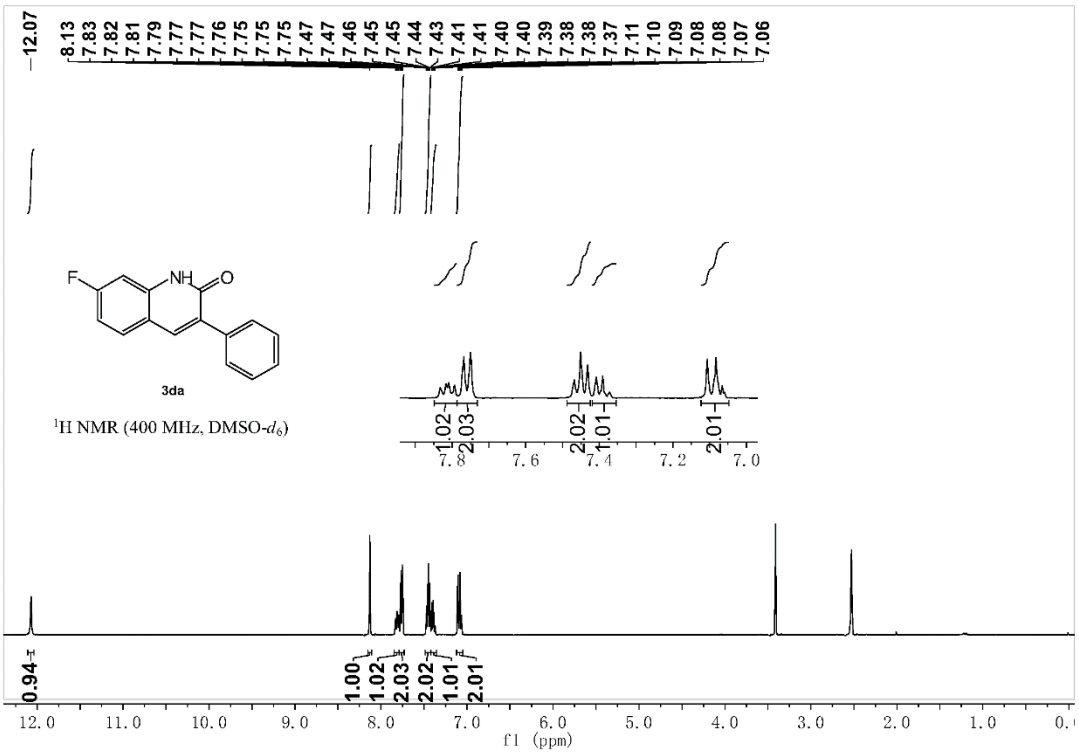
^{13}C NMR (101 MHz, DMSO-d_6)

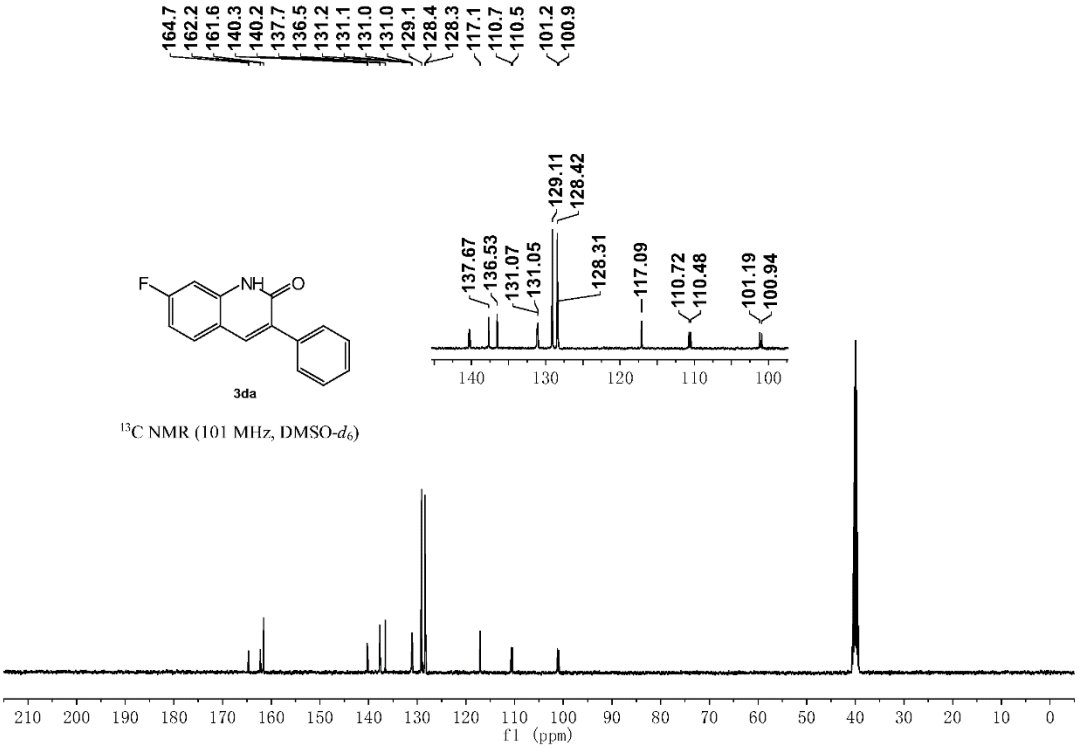

11.90
8.08
7.79
7.78
7.77
7.77
7.76
7.48
7.47
7.45
7.45
7.44
7.41
7.41
7.41
7.39
7.31
7.31
7.29
7.20
7.19
7.18
7.17
3.82
NH
O
O
CH3
3ba
1H NMR (400 MHz, DMSO-d6)
2.00
1.98
1.00
2.00
0.99
7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1
0.89
0.99
2.00
1.98
1.00
2.00
0.99
3.00
12.5 11.5 10.5 9.5 8.5 7.5 6.5 5.5 4.5 3.5 2.5 1.5 0.5 -0
f1 (ppm)

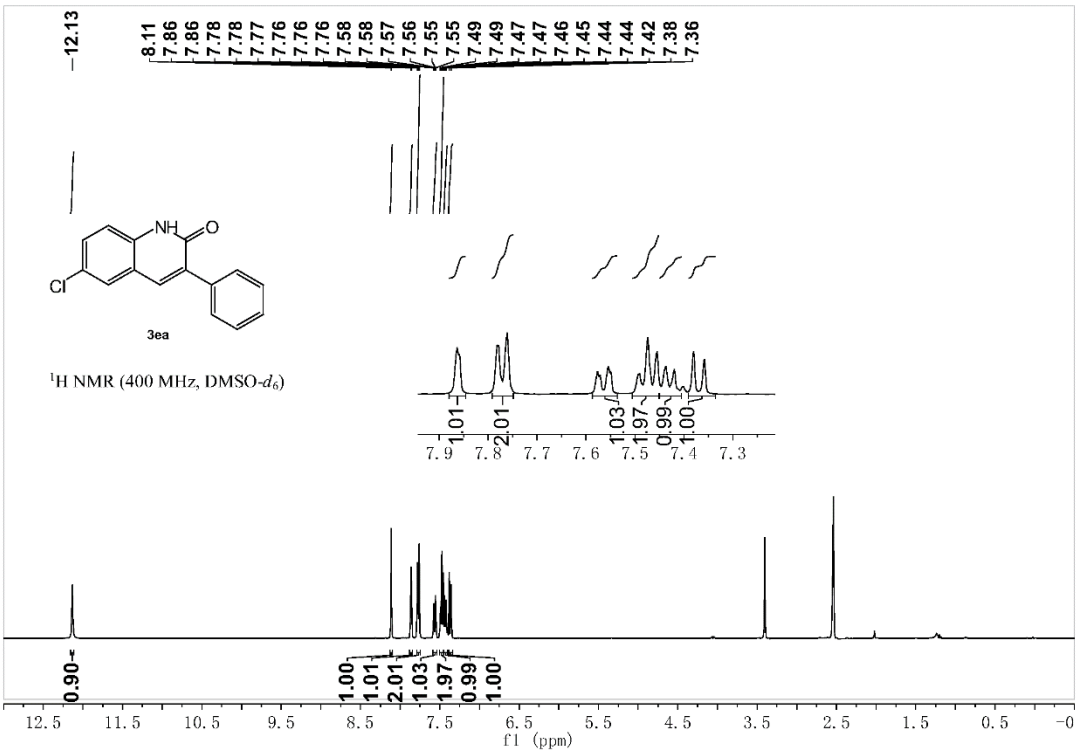

161.1
154.7
137.7
136.9
133.4
132.3
129.2
128.4
128.3
120.6
120.0
116.5
109.8
55.9
NH
O
O
CH3
3ba
13C NMR (101 MHz, DMSO-d6)
137.74
136.88
133.40
132.34
129.16
128.41
128.28
120.60
119.96
145 140 135 130 125 120
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

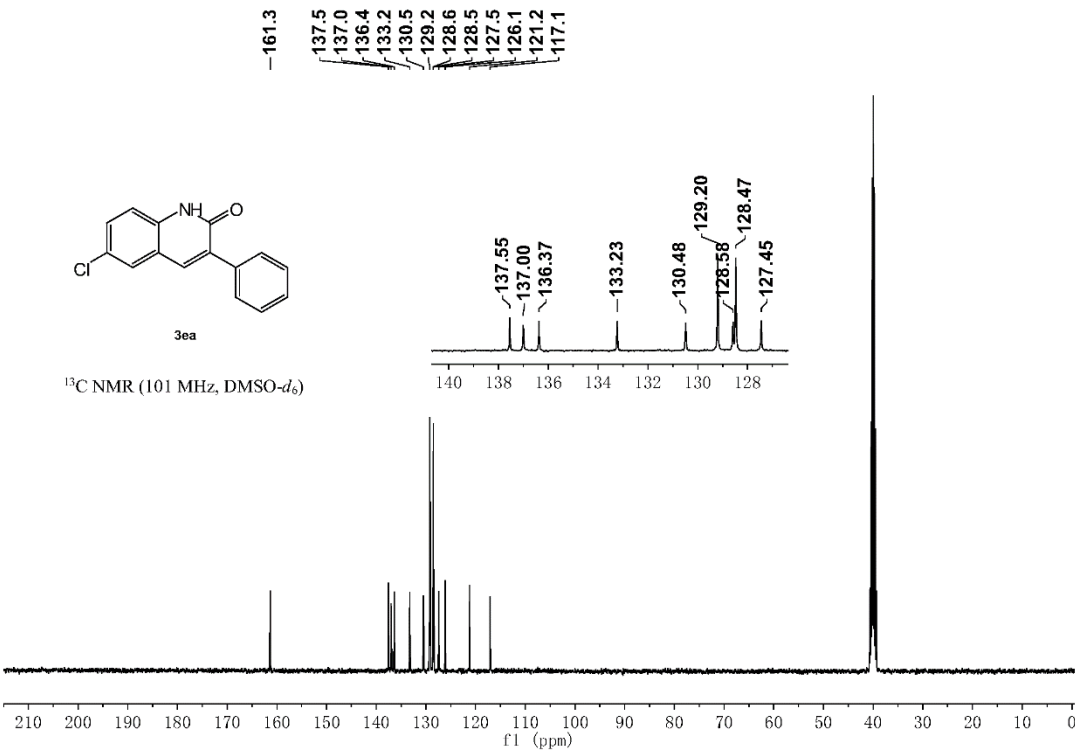

12.08
8.11
7.78
7.78
7.76
7.62
7.61
7.60
7.59
7.49
7.48
7.47
7.45
7.43
7.43
7.41
7.40
7.40
7.38
7.37
7.36
NH
O
F
3ca
1H NMR (400 MHz, DMSO-d6)
2.10
1.06
1.98
1.05
2.09
7.8
7.7
7.6
7.5
7.4
7.3
0.95
1.00
2.10
1.06
1.98
1.05
2.09
12.5
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
−0
f1 (ppm)

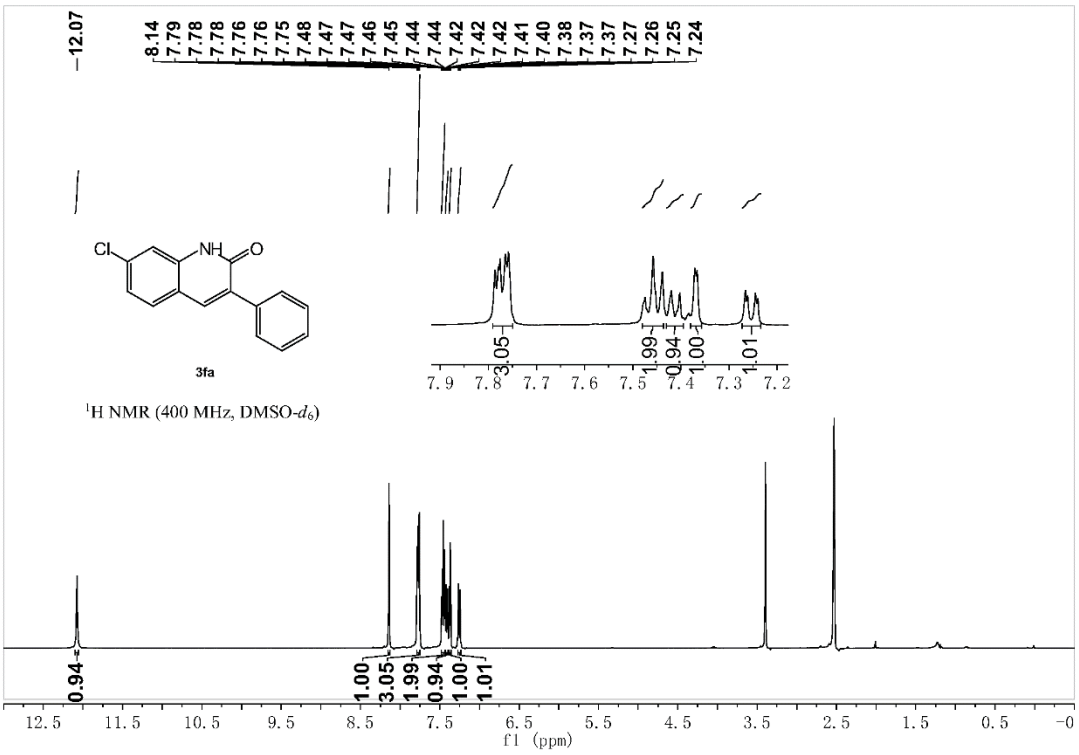

161.2
158.6
156.3
137.3
137.2
136.5
135.6
133.2
129.2
128.5
128.4
120.7
120.6
118.8
118.6
117.0
116.9
113.3
113.0
NH
O
F
3ca
13C NMR (101 MHz, DMSO-d6)
137.28
136.45
135.58
133.21
129.18
128.53
128.44
120.72
120.63
118.82
118.58
117.03
116.95
113.25
113.03
140
135
130
125
120
115
110
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


12.07
8.13
7.83
7.82
7.81
7.79
7.77
7.77
7.76
7.75
7.75
7.75
7.47
7.47
7.46
7.45
7.45
7.44
7.43
7.41
7.41
7.40
7.40
7.39
7.38
7.38
7.37
7.11
7.10
7.09
7.08
7.08
7.07
7.06
F
NH
O
3da
1H NMR (400 MHz, DMSO-d6)
1.02
2.03
2.02
1.01
2.01
0.94
1.00
1.02
2.03
2.02
1.01
2.01
f1 (ppm)

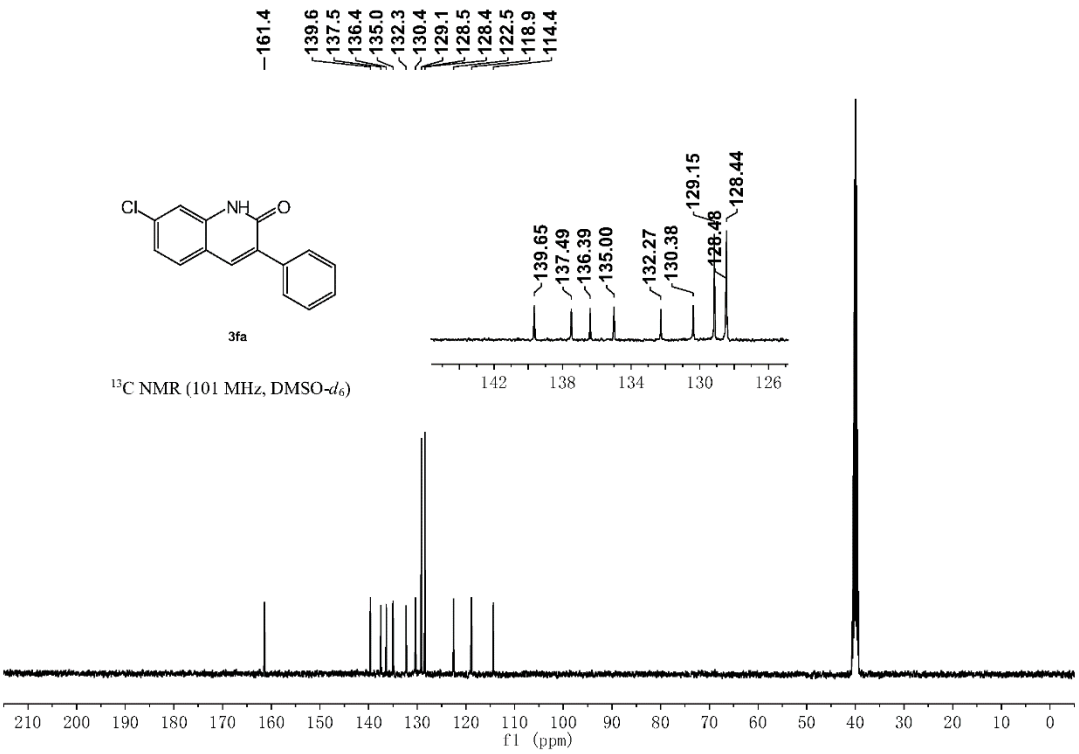

164.7
162.2
161.6
140.3
140.2
137.7
136.5
131.2
131.1
131.0
131.0
129.1
128.4
128.3
117.1
110.7
110.5
101.2
100.9
F
NH
O
3da
13C NMR (101 MHz, DMSO-d6)
129.11
128.42
137.67
136.53
131.07
131.05
128.31
117.09
110.72
110.48
101.19
100.94
f1 (ppm)


12.13
8.11
7.86
7.86
7.78
7.78
7.77
7.76
7.76
7.76
7.58
7.58
7.57
7.56
7.55
7.55
7.49
7.49
7.47
7.47
7.46
7.45
7.44
7.44
7.42
7.38
7.36
NH
O
Cl
3ea
1H NMR (400 MHz, DMSO-d6)
1.01
2.01
1.03
1.97
0.99
1.00
7.9 7.8 7.7 7.6 7.5 7.4 7.3
0.90
1.00
1.01
2.01
1.03
1.97
0.99
1.00
12.5 11.5 10.5 9.5 8.5 7.5 6.5 5.5 4.5 3.5 2.5 1.5 0.5 −0
f1 (ppm)

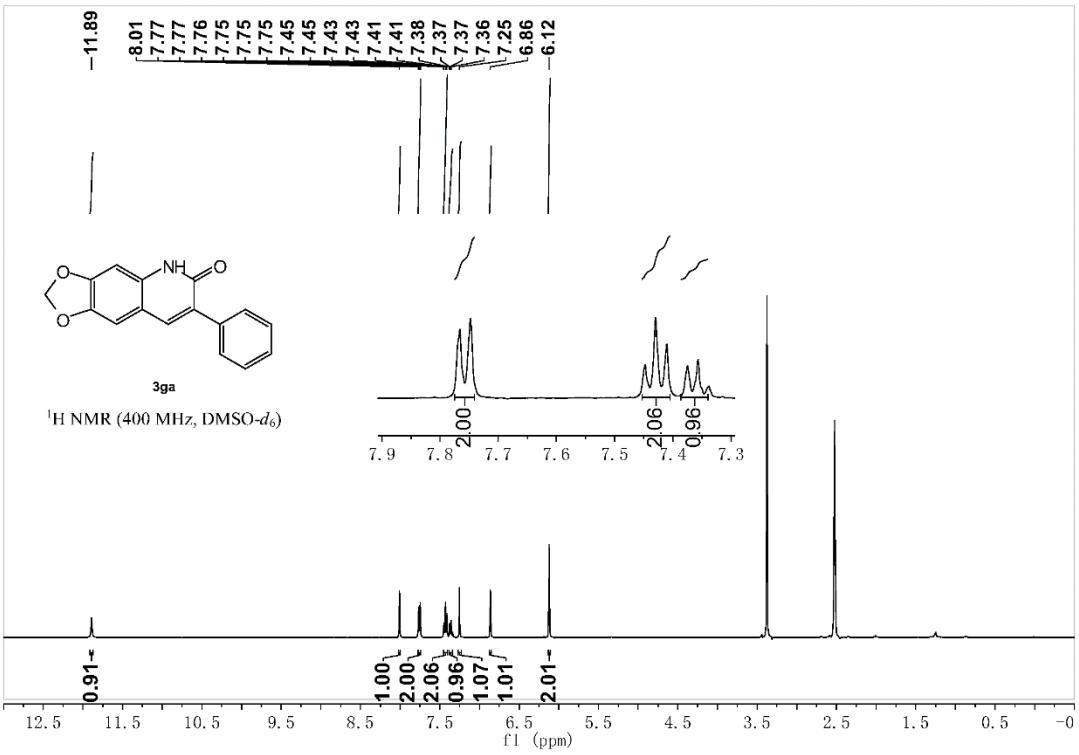

161.3
137.5
137.0
136.4
133.2
130.5
129.2
128.6
128.5
127.5
126.1
121.2
117.1
NH
O
Cl
3ea
13C NMR (101 MHz, DMSO-d6)
137.55
137.00
136.37
133.23
130.48
129.20
128.58
128.47
127.45
140 138 136 134 132 130 128
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

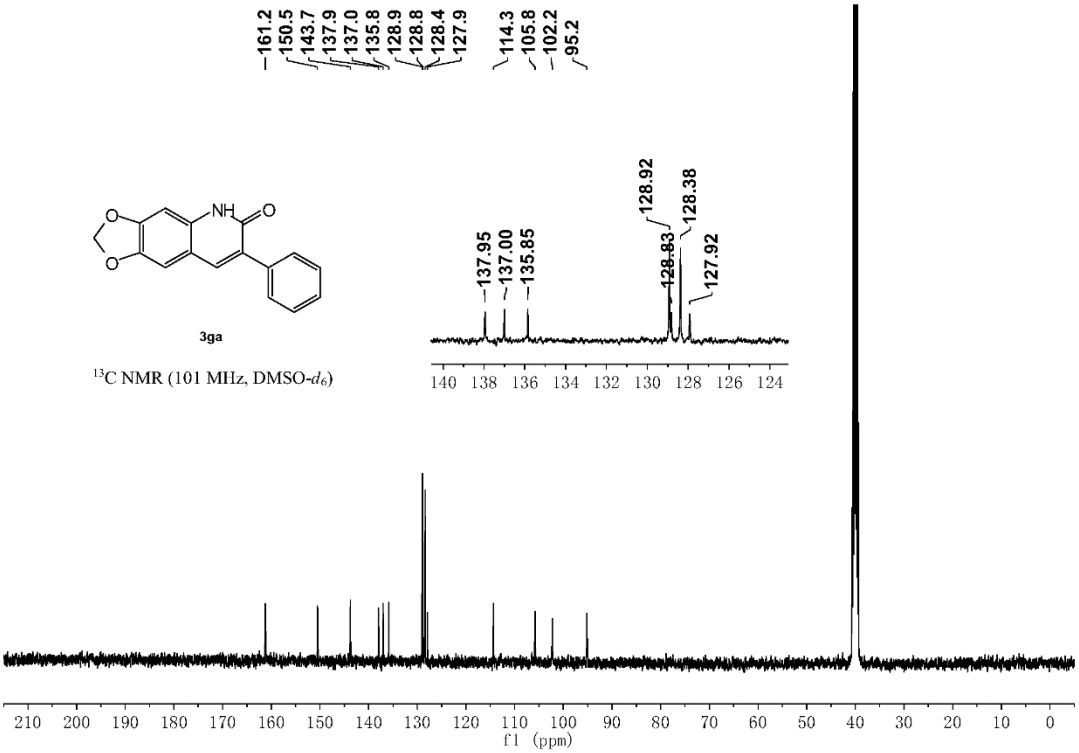


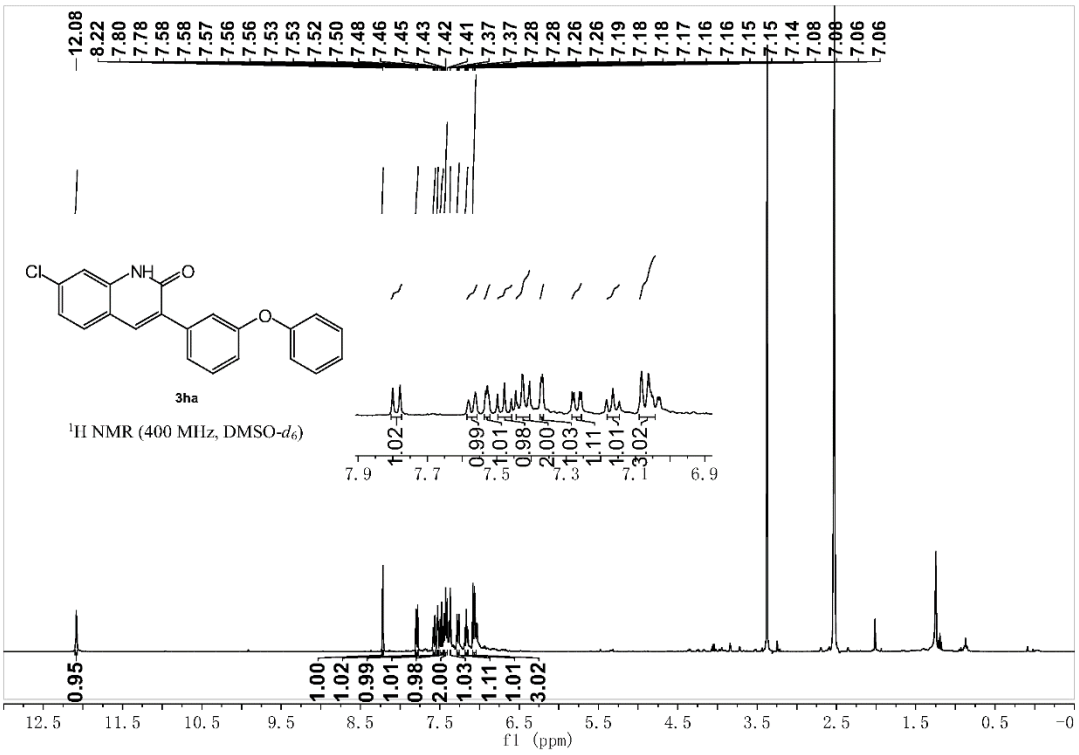
^{1}H NMR (400 MHz, DMSO-d_6)

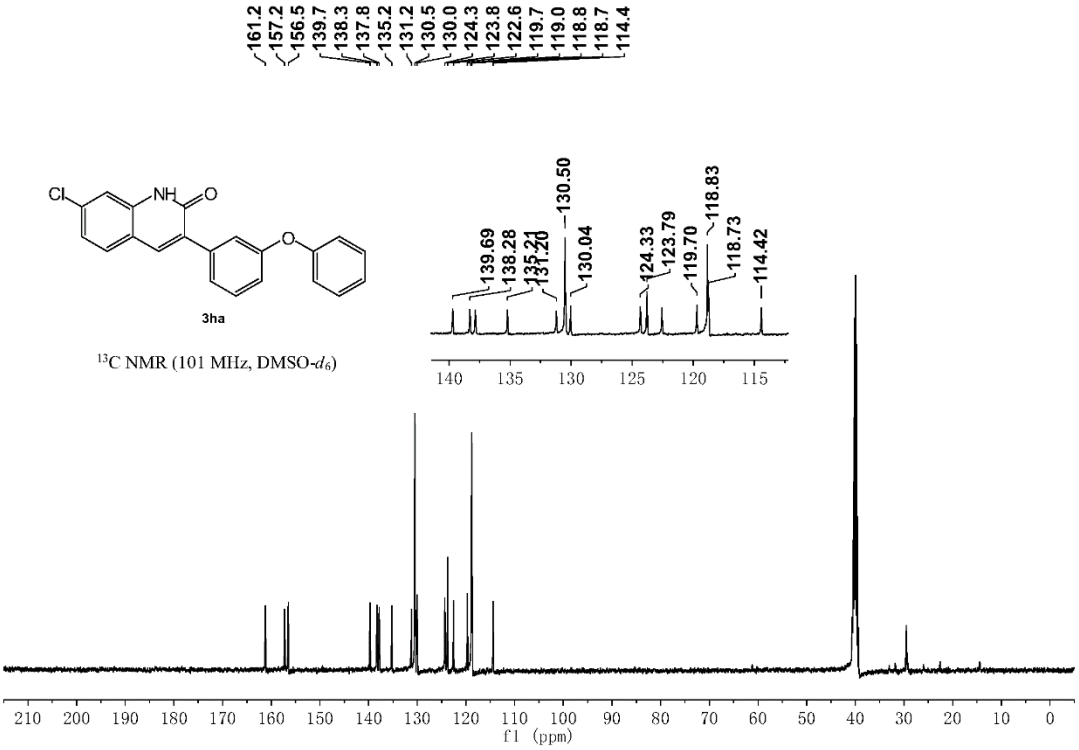


^{13}C NMR (101 MHz, DMSO-d_6)


11.89
8.01
7.77
7.77
7.76
7.75
7.75
7.75
7.45
7.45
7.43
7.43
7.41
7.41
7.38
7.37
7.37
7.36
7.25
6.86
6.12
NH
O
O
O
3ga
1H NMR (400 MHz, DMSO-d6)
2.00
2.06
0.96
7.9
7.8
7.7
7.6
7.5
7.4
7.3
0.91
1.00
2.00
2.06
0.96
1.07
1.01
2.01
12.5
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
f1 (ppm)


161.2
150.5
143.7
137.9
137.0
135.8
128.9
128.8
128.4
127.9
114.3
105.8
102.2
95.2
NH
O
O
O
3ga
13C NMR (101 MHz, DMSO-d6)
137.95
137.00
135.85
128.92
128.38
128.83
127.92
140
138
136
134
132
130
128
126
124
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


12.08
8.22
7.80
7.78
7.58
7.58
7.57
7.56
7.56
7.53
7.53
7.52
7.50
7.48
7.46
7.45
7.43
7.42
7.41
7.37
7.37
7.28
7.28
7.26
7.26
7.19
7.18
7.18
7.17
7.16
7.16
7.15
7.15
7.14
7.08
7.08
7.06
7.06
Cl
NH
O
O
3ha
1H NMR (400 MHz, DMSO-d6)
1.02
0.99
1.01
0.98
2.00
1.03
1.11
1.01
3.02
7.9
7.7
7.5
7.3
7.1
6.9
0.95
1.00
1.02
0.99
1.01
0.98
2.00
1.03
1.11
1.01
3.02
12.5
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
−0
f1 (ppm)


161.2
157.2
156.5
139.7
138.3
137.8
135.2
131.2
130.5
130.0
124.3
123.8
122.6
119.7
119.0
118.8
118.7
114.4
Cl
NH
O
O
3ha
13C NMR (101 MHz, DMSO-d6)
139.69
138.28
135.21
131.20
130.50
130.04
124.33
123.79
119.70
118.83
118.73
114.42
140
135
130
125
120
115
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)