Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supporting Information

Cobalt-Catalyzed Carbonylative Synthesis of Free (*NH*)-Tetrahydro-β-Carbolinones from Tryptamine Derivatives

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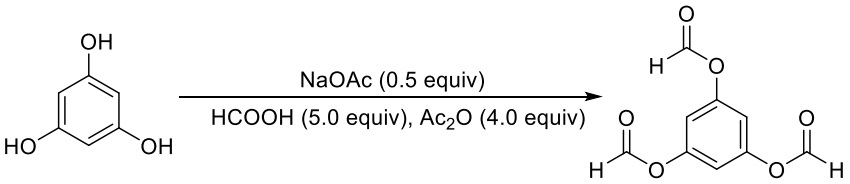
1. General experimental information

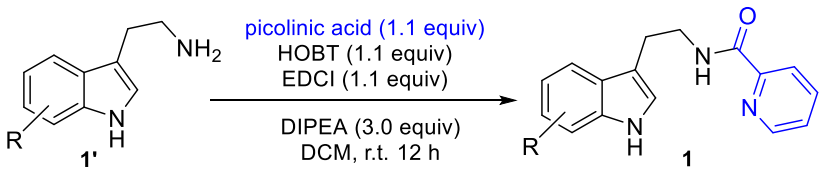
Unless otherwise noted, all reactions were carried out under nitrogen atmosphere. All commercially available reagents were used without further purification. All of the solvents were treated according to known methods. Column chromatography was performed on silica gel (200-400 mesh). ^{1}H NMR (400 MHz) chemical shifts were reported in ppm (δ) relative to tetramethylsilane (TMS) with the solvent resonance employed as the internal standard. ^{13}C NMR (100 MHz) chemical shifts were reported in ppm (δ) from tetramethylsilane (TMS) with the solvent resonance as the internal standard. Data were reported as follows: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, dd = doublet of doublets, td = triplet of doublets, qd = quartet of doublets, m = multiplet), coupling constants (Hz) and integration. HRMS measurements were obtained on a TOF analyzer.

2. Preparation of benzene-1,3,5-triyl triformate (TFBen)[1]



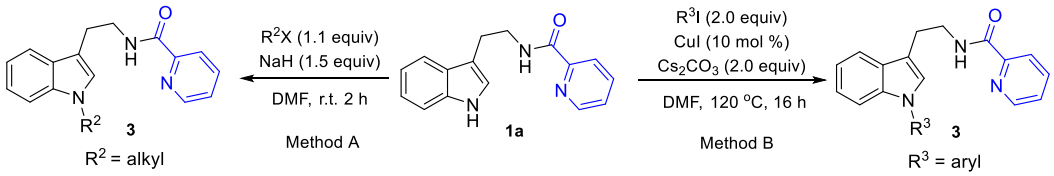
Formic acid (8.4 mL, 222.8 mmol, 5.0 equiv) was added to acetic anhydride (16.8 mL, 178.2 mmol, 4.0 equiv) at r.t. The mixture was stirred at 60 °C for 1 h and cooled to r.t. The resulting solution was poured into a flask containing 1,3,5-trihydroxybenzene (5.62 g, 44.6 mmol, 1.0 equiv) and AcONa (1.83 g, 22.3 mmol, 0.5 equiv). The mixture was stirred for 4 h in a water bath and then diluted with toluene (100 mL), washed with H_2O (50 mL) twice. Keep the organic phase in fridge (2-8 °C) for overnight. Then filtered and dried in vacuo to afford the desired product benzene-1,3,5-triyl triformate (TFBen) as a white solid (5.1 g, 55%).

3. General procedure for the synthesis of tryptamine derivatives (1a-1j)



Tryptamine **1'** (3.0 mmol, 1.0 equiv), picolinic acid (3.3 mmol, 1.1 equiv), HOBT (3.3 mmol, 1.1 equiv), DIPEA (9.0 mmol, 3.0 equiv), and EDCI (3.3 mmol, 1.1 equiv) were added to an oven-dried flask (50 mL). Then DCM (15 mL) was added into the flask via syringe. The flask was sealed and stirred at r.t. for 12 h. Upon the reaction was completed, the resulting mixture was purified by silica gel column using chromatography (PE / EA = 1:1) to obtain product **1**.

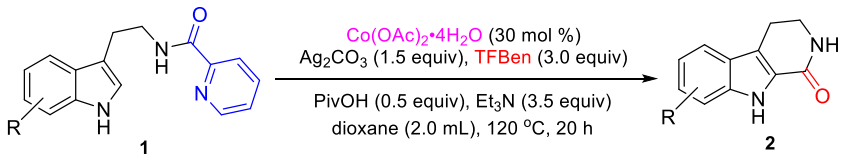
4. General procedure for the synthesis of *N*-substituted tryptamine derivatives (3a-3l)



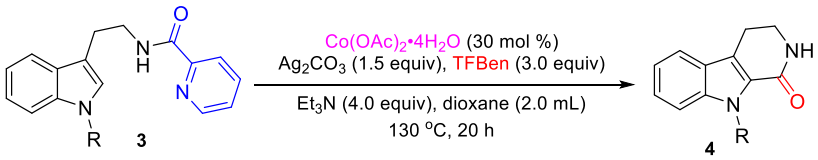
Method A: The tryptamine derivative **1a** (3.0 mmol, 1.0 equiv) and DMF (5.0 mL) were added to an oven-dried tube (15 mL). NaH (4.5 mmol, 1.5 equiv) was added dropwise via syringe at 0 °C and the reaction was stirred at r.t. for 1 h. Then an alkyl halide (3.0 mmol, 1.0 equiv) was added into the tube via syringe at 0 °C and the reaction was stirred at r.t. for 1 h. Upon the reaction was completed, the mixture was quenched with water, extracted with DCM, dried over Na_2SO_4 and purified by silica gel column using chromatography (PE / EA = 2:1) to obtain product **3**.

Method B: The tryptamine derivative **1a** (3.0 mmol, 1.0 equiv) , CuI (0.3 mmol, 10 mol %), Cs_2CO_3 (6.0 mmol, 2.0 equiv) were added to an oven-dried tube (15 mL) which was then placed under vacuum and refilled with nitrogen three times. Then an aryl iodide (6.0 mmol, 2.0 equiv) and DMF (5.0 mL) were added into the tube via syringe. The reaction was stirred at 120 °C for 16 h. Upon the reaction was completed, the mixture was quenched with water, extracted with DCM, dried over Na_2SO_4 and purified by silica gel column using chromatography (PE / EA = 2:1) to obtain product **3**.

5. General procedure for the synthesis of (*NH*)-tetrahydro-β-carbolinones (2a-2j, 4a-4l)

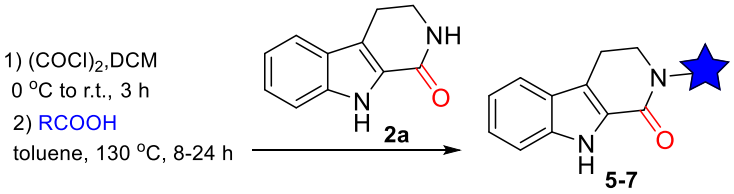


$Co(OAc)_2 \cdot 4H_2O$ (15.0 mg, 30 mol%), Ag_2CO_3 (82.5 mg, 1.5 equiv), tryptamine derivative **1** (0.2 mmol, 1.0 equiv), and TFBen (126.0 mg, 0.6 mmol, 3.0 equiv) were added to an oven-dried tube (15 mL) which was then placed under vacuum and refilled with nitrogen three times. Then Et_3N (70.5 mg, 0.7 mmol, 3.5 equiv), PivOH (10.1 mg, 0.1 mmol, 0.5 equiv) and dioxane (2.0 mL) were added into the tube via syringe. The tube was sealed and stirred at 120 °C for 20 h. Upon the reaction was completed, the resulting mixture was purified by silica gel column using chromatography (PE / EA = 1:1) to obtain product **2**.



$Co(OAc)_2 \cdot 4H_2O$ (15.0 mg, 30 mol%), Ag_2CO_3 (82.5 mg, 1.5 equiv), *N*-substituted tryptamine derivative **3** (0.2 mmol, 1.0 equiv), and TFBen (126.0 mg, 0.6 mmol, 3.0 equiv) were added to an oven-dried tube (15 mL) which was then placed under vacuum and refilled with nitrogen three times. Then Et_3N (80.5 mg, 0.8 mmol, 4.0 equiv) and dioxane (2.0 mL) were added into the tube via syringe. The tube was sealed and stirred at 130 °C for 20 h. Upon the reaction was completed, the resulting mixture was purified by silica gel column using chromatography (PE / EA = 1:1) to obtain product **4**.

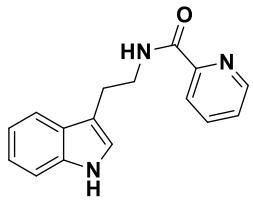
6. General procedure for the synthesis of bioactive molecules (5, 6, 7)



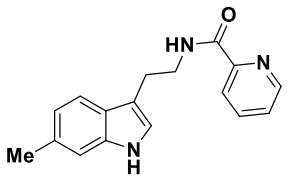
To a solution of carboxylic acid (1.5 mmol, 1.0 equiv) in DCM (10 mL) was added oxalyl chloride (3.0 mmol, 2.0 equiv) dropwise at 0 ºC. The reaction was stirred at r.t. for 3 h to give the acyl chloride without further purification.

The (*NH*)-tetrahydro-β-carbolinone **2a** (0.2 mmol, 1.0 equiv), the corresponding acyl chloride (0.8 mmol, 4.0 equiv), and toluene (2.0 mL) were added to an oven-dried tube (15 mL). The reaction was stirred at 130 ºC for 8-24 h. Upon the reaction was completed, the resulting mixture was purified by silica gel column using chromatography (PE / EA = 3:1) to obtain product **5, 6, 7**.

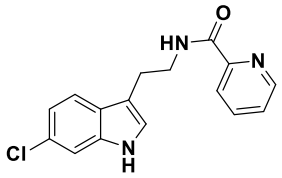
7. Characterization data of substrates (1a-1j, 3a-3l)



***N*-(2-(1*H*-indol-3-yl)ethyl)picolinamide (1a).** Yellow solid, mp: 115.6 – 116.3 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.49 (dd, *J* = 4.7, 0.6 Hz, 1H), 8.22 (d, *J* = 7.8 Hz, 2H), 7.83 (td, *J* = 7.7, 1.7 Hz, 1H), 7.67 (d, *J* = 7.9 Hz, 1H), 7.41 – 7.37 (m, 2H), 7.21 (t, *J* = 7.1 Hz, 1H), 7.13 (t, *J* = 7.0 Hz, 1H), 7.08 (d, *J* = 2.2 Hz, 1H), 3.83 (dd, *J* = 13.3, 7.0 Hz, 2H), 3.12 (t, *J* = 7.0 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) *δ* 164.4, 150.1, 148.1, 137.3, 136.5, 127.4, 126.1, 122.2, 122.12, 122.06, 119.4, 118.9, 113.1, 111.2, 39.8, 25.6.

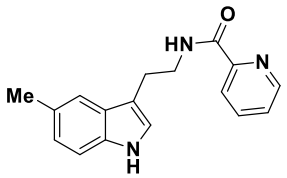


***N*-(2-(6-methyl-1*H*-indol-3-yl)ethyl)picolinamide (1b).** Yellow solid, mp: 146.3 – 147.2 °C; ^{1}H NMR (400 MHz, $CDCl_3$) *δ* 8.49 (d, *J* = 4.4 Hz, 1H), 8.21 (d, *J* = 7.8 Hz, 2H), 8.00 (s, 1H), 7.83 (td, *J* = 7.7, 1.5 Hz, 1H), 7.52 (d, *J* = 8.6 Hz, 1H), 7.39 (dd, *J* = 6.7, 5.0 Hz, 1H), 6.97 (s, 1H), 6.86 (d, *J* = 1.9 Hz, 1H), 6.79 (dd, *J* = 8.6, 2.1 Hz, 1H), 3.84 (s, 3H), 3.81 – 3.78 (m, 2H), 3.07 (t, *J* = 7.0 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) *δ* 164.4, 156.6, 150.1, 148.1, 137.3, 137.2, 126.1, 122.2, 121.9, 120.7, 119.5, 113.2, 109.4, 94.8, 55.7, 39.8, 25.7.

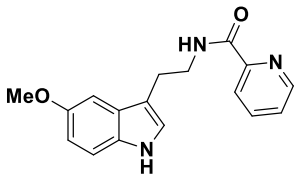


***N*-(2-(6-chloro-1*H*-indol-3-yl)ethyl)picolinamide (1c).** Yellow solid, mp: 154.6 – 155.5 °C; ^{1}H NMR (400 MHz, DMSO-d_6) *δ* 11.01 (s, 1H), 8.93 (t, *J* = 5.5 Hz, 1H), 8.66 (d, *J* = 3.9 Hz, 1H), 8.10 (d, *J* = 7.7 Hz, 1H), 8.03 (td, *J* = 7.6, 1.6 Hz, 1H), 7.66 (d, *J* = 8.4 Hz, 1H), 7.63 – 7.60 (m, 1H),

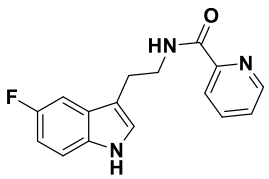
7.44 (d, J = 1.6 Hz, 1H), 7.29 (s, 1H), 7.04 (dd, J = 8.4, 1.8 Hz, 1H), 3.65 (dd, J = 13.7, 6.8 Hz, 2H), 3.01 (t, J = 7.3 Hz, 2H); ^{13}C NMR (100 MHz, DMSO- d_6) δ 164.3, 150.5, 148.8, 138.2, 137.1, 126.9, 126.6, 126.3, 124.3, 122.3, 120.3, 119.1, 112.7, 111.5, 25.5.



***N*-(2-(5-methyl-1*H*-indol-3-yl)ethyl)picolinamide (1d).** Yellow solid, mp: 153.1 – 154.0 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.53 (d, J = 4.7 Hz, 1H), 8.25 (d, J = 7.8 Hz, 1H), 8.09 (s, 1H), 7.87 (td, J = 7.7, 1.7 Hz, 1H), 7.47 (s, 1H), 7.43 (ddd, J = 7.5, 4.8, 1.1 Hz, 1H), 7.30 (t, 1H), 7.06 (d, J = 8.6 Hz, 2H), 3.85 (d, J = 6.8 Hz, 2H), 3.12 (t, J = 7.0 Hz, 2H), 2.47 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.4, 150.1, 148.1, 137.3, 134.8, 128.7, 127.7, 126.0, 123.7, 122.2, 118.6, 112.7, 110.9, 39.9, 25.6, 21.5.

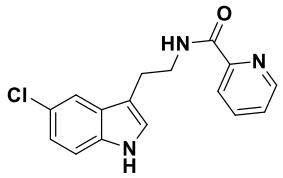


***N*-(2-(5-methoxy-1*H*-indol-3-yl)ethyl)picolinamide (1e).** Yellow solid, mp: 116.3 – 117.1 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.49 (d, J = 4.7 Hz, 1H), 8.21 (d, J = 7.8 Hz, 2H), 8.01 (s, 1H), 7.84 (td, J = 7.7, 1.6 Hz, 1H), 7.40 (ddd, J = 7.5, 4.8, 0.9 Hz, 1H), 7.27 – 7.25(m, 1H), 7.07 (t, J = 2.5 Hz, 2H), 6.86 (dd, J = 8.8, 2.4 Hz, 1H), 3.84 – 3.79 (m, 5H), 3.08 (t, J = 7.0 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.4, 154.1, 150.1, 148.1, 137.3, 131.5, 127.8, 126.1, 122.8, 122.2, 113.0, 112.5, 111.9, 100.6, 55.9, 39.8, 25.6.

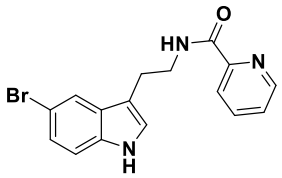


***N*-(2-(5-fluoro-1*H*-indol-3-yl)ethyl)picolinamide (1f).** Yellow solid, mp: 118.6 – 119.5 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.50 (d, J = 4.7 Hz, 1H), 8.40 (s, 1H), 8.23 (s, 1H), 8.20 (d, J = 7.8 Hz, 1H), 7.83 (td, J = 7.7, 1.2 Hz, 1H), 7.40 (dd, J = 7.0, 5.2 Hz, 1H), 7.29 – 7.25 (m, 2H), 7.10 (s, 1H),

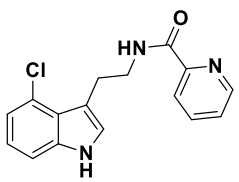
6.93 (td, *J* = 9.1, 2.3 Hz, 1H), 3.79 (q, *J* = 6.8 Hz, 2H), 3.05 (t, *J* = 7.0 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.5, 157.8 (d, *J* = 234.5 Hz), 149.9, 148.1, 137.4, 132.9, 127. 8 (d, *J* = 9.6 Hz), 126.2, 123.9, 122.2, 113.2 (d, *J* = 4.7 Hz), 111.9 (d, *J* = 9.6 Hz), 110.4 (d, *J* = 26.3 Hz), 103.7 (d, *J* = 23.4 Hz), 39.8, 25.5.



***N*-(2-(5-chloro-1*H*-indol-3-yl)ethyl)picolinamide (1g).** Yellow solid, mp: 119.8 – 120.8 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.50 (d, *J* = 4.6 Hz, 1H), 8.36 (s, 1H), 8.20 (d, *J* = 7.8 Hz, 1H), 7.83 (td, *J* = 7.7, 1.6 Hz, 1H), 7.59 (d, *J* = 1.7 Hz, 1H), 7.40 (ddd, *J* = 7.5, 4.8, 0.9 Hz, 1H), 7.27 (d, *J* = 6.8 Hz, 1H), 7.13 (dd, *J* = 8.6, 1.9 Hz, 1H), 7.09 (d, *J* = 2.1 Hz, 1H), 3.79 (q, *J* = 6.8 Hz, 2H), 3.05 (t, *J* = 7.0 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.5, 149.9, 148.1, 137.4, 134., 128.54, 126.2, 125.2, 123.5, 122.4, 122.2, 118.4, 113.0, 112.2, 39.9, 25.5.

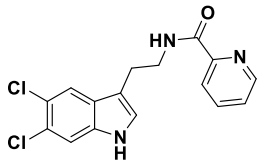


***N*-(2-(5-bromo-1*H*-indol-3-yl)ethyl)picolinamide (1h).** Yellow solid, mp: 139.6 – 139.9 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.58 (s, 1H), 8.50 (dd, *J* = 4.7, 0.6 Hz, 1H), 8.24 (s, 1H), 8.19 (d, *J* = 7.8 Hz, 1H), 7.82 (td, *J* = 7.7, 1.7 Hz, 1H), 7.74 (s, 1H), 7.39 (ddd, *J* = 7.6, 4.8, 1.1 Hz, 1H), 7.24 (dd, *J* = 8.6, 1.7 Hz, 1H), 7.20 (d, *J* = 8.5 Hz, 1H), 7.03 (d, *J* = 2.1 Hz, 1H), 3.78 (q, *J* = 6.9 Hz, 2H), 3.04 (t, *J* = 7.0 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.5, 149.9, 148.2, 137.4, 135.1, 129.2, 126.2, 124.9, 123.4, 122.2, 121.4, 112.8, 112.74, 112.65, 39.9, 25.4.

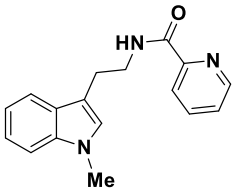


***N*-(2-(4-chloro-1*H*-indol-3-yl)ethyl)picolinamide (1i).** Yellow solid, mp: 140.8 – 141.5 ^{o}C; ^{11}H NMR (400 MHz, $CDCl_3$) δ 8.51 (d, *J* = 4.6 Hz, 1H), 8.42 (s, 1H), 8.21 (d, *J* = 7.8 Hz, 1H), 7.83 (td,

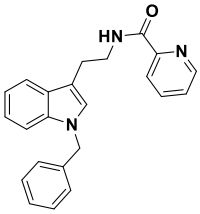
J = 7.7, 1.6 Hz, 1H), 7.40 (dd, *J* = 7.5, 4.8 Hz, 1H), 7.27 – 7.25 (m, 1H), 7.09 – 7.06 (m, 3H), 3.86 (q, *J* = 6.9 Hz, 2H), 3.34 (t, *J* = 7.1 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.4, 150.1, 148.1, 138.0, 137.3, 126.4, 126.1, 124.2, 123.8, 122.6, 122.2, 120.5, 113.4, 110.1, 40.9, 26.6.



***N*-(2-(5,6-dichloro-1*H*-indol-3-yl)ethyl)picolinamide (1j).** Yellow solid, mp: 185.6 – 186.3 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.16 (s, 1H), 8.96 (t, *J* = 6.0 Hz, 1H), 8.68 (d, *J* = 4.5 Hz, 1H), 8.09 (d, *J* = 7.7 Hz, 1H), 8.03 (td, *J* = 7.6, 1.6 Hz, 1H), 7.92 (s, 1H), 7.65 – 7.63 (m, 1H), 7.62 (s, 1H), 7.37 (d, *J* = 2.1 Hz, 1H), 3.61 (dd, *J* = 13.9, 6.9 Hz, 2H), 2.99 (t, *J* = 7.3 Hz, 2H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 164.2, 150.5, 148.8, 138.2, 135.6, 127.9, 126.9, 126.1, 123.7, 122.3, 121.4, 120.2, 113.3, 112.6, 25.4.

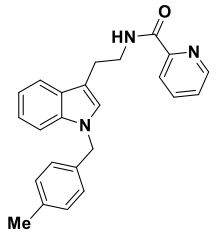


***N*-(2-(1-methyl-1*H*-indol-3-yl)ethyl)picolinamide (3a).** Yellow solid, mp: 62.3 – 63.1 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.50 (d, *J* = 4.6 Hz, 1H), 8.24 (d, *J* = 7.8 Hz, 1H), 7.82 (td, *J* = 7.7, 1.7 Hz, 1H), 7.68 (d, *J* = 7.9 Hz, 1H), 7.38 (ddd, *J* = 7.5, 4.8, 1.1 Hz, 1H), 7.32 (d, *J* = 8.1 Hz, 1H), 7.26 (d, *J* = 15.0 Hz, 1H), 7.14 (t, *J* = 7.4 Hz, 1H), 6.94 (s, 1H), 3.83 (q, *J* = 6.7 Hz, 2H), 3.74 (s, 3H), 3.12 (t, *J* = 7.1 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.4, 150.1, 148.1, 137.3, 137.2, 127.9, 126.8, 126.1, 122.2, 121.7, 119.0, 118.9, 111.7, 109.3, 40.0, 32.7, 25.6.

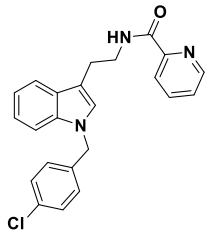


***N*-(2-(1-benzyl-1*H*-indol-3-yl)ethyl)picolinamide (3b).** Yellow solid, mp: 75.3 – 76.2 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.47 (d, *J* = 4.6 Hz, 1H), 8.21 (d, *J* = 7.8 Hz, 1H), 7.84 (td, *J* = 7.7, 1.6 Hz, 1H), 7.69 (d, *J* = 7.8 Hz, 1H), 7.40 (ddd, *J* = 7.4, 4.8, 0.9 Hz, 1H), 7.30 – 7.28 (m, 2H), 7.25 (d,

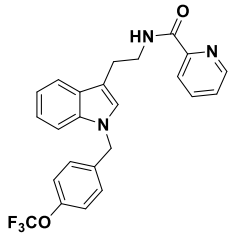
J = 5.4 Hz, 2H), 7.19 (t, *J* = 7.5 Hz, 1H), 7.13 (dd, *J* = 10.2, 4.3 Hz, 3H), 7.03 (s, 1H), 5.29 (s, 2H), 3.83 (q, *J* = 6.9 Hz, 2H), 3.12 (t, *J* = 7.0 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.3, 150.1, 148.0, 137.7, 137.3, 136.8, 128.8, 128.1, 127.6, 126.8, 126.3, 126.0, 122.2, 121.9, 119.2, 119.1, 112.3, 109.8, 50.0, 39.7, 25.6.



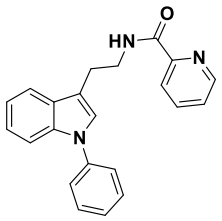
***N*-(2-(1-(4-methylbenzyl)-1*H*-indol-3-yl)ethyl)picolinamide (3c).** Yellow solid, mp: 96.5 – 97.3 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.50 (d, *J* = 4.6 Hz, 1H), 8.30 (d, *J* = 4.1 Hz, 1H), 8.26 (d, *J* = 8.4 Hz, 1H), 7.82 (t, *J* = 7.7 Hz, 1H), 7.73 (d, *J* = 7.7 Hz, 1H), 7.24 – 7.16 (m, 1H), 7.33 (d, *J* = 8.2 Hz, 1H), 7.25 – 7.15 (m, 2H), 7.11 (d, *J* = 8.0 Hz, 2H), 7.06 (d, *J* = 8.1 Hz, 2H), 7.04 (s, 1H), 5.24 (s, 2H), 3.90 – 3.84 (m, 2H), 3.16 (t, *J* = 7.0 Hz, 2H), 2.35 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.4, 150.2, 148.1, 137.35, 137.26, 136.9, 134.7, 129.5, 128.2, 127.0, 126.3, 126.1, 122.2, 121.9, 119.23, 119.17, 112.2, 109.9, 49.8, 39.9, 25.7, 21.2.



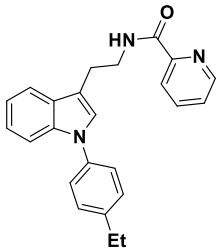
***N*-(2-(1-(4-chlorobenzyl)-1*H*-indol-3-yl)ethyl)picolinamide (3d).** Yellow solid, mp: 103.3 – 104.8 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.46 (d, *J* = 4.7 Hz, 1H), 8.21 (d, *J* = 7.8 Hz, 1H), 7.83 (td, *J* = 7.7, 1.6 Hz, 1H), 7.69 (d, *J* = 7.7 Hz, 1H), 7.40 (ddd, *J* = 7.5, 4.8, 0.9 Hz, 1H), 7.24 – 7.18 (m, 4H), 7.16 – 7.12 (m, 1H), 7.03 (s, 1H), 7.01 (s, 2H), 5.23 (s, 2H), 3.83 (q, *J* = 6.8 Hz, 2H), 3.12 (t, *J* = 7.0 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.3, 150.1, 148.0, 137.3, 136.7, 136.2, 133.4, 128.9, 128.1, 126.11, 126.09, 122.2, 122.1, 119.4, 119.2, 112.6, 109.7, 49.3, 39.7, 25.5.



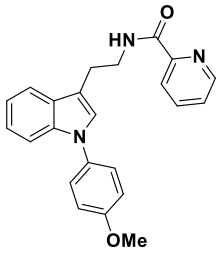
***N*-(2-(1-(4-(trifluoromethoxy)benzyl)-1*H*-indol-3-yl)ethyl)picolinamide (3e).** Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.46 (d, J = 4.7 Hz, 1H), 8.22 (d, J = 7.3 Hz, 1H), 7.83 (t, J = 7.7 Hz, 1H), 7.71 (d, J = 7.7 Hz, 1H), 7.41 – 7.37 (m, 1H), 7.23 (d, J = 3.5 Hz, 1H), 7.21 – 7.14 (m, 2H), 7.10 (s, 4H), 7.03 (s, 1H), 5.27 (s, 2H), 3.85 (q, J = 6.6 Hz, 2H), 3.14 (t, J = 7.0 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.3, 150.1, 148.5, 148.0, 137.3, 136.7, 136.5, 128.15, 128.09, 126.1 (d, J =4.7 Hz), 122.2 (d, J = 3.7 Hz), 121.2, 120.5 (q, J = 256.5 Hz), 119.4, 119.3, 112.7, 109.6, 49.2, 39.7, 25.5.



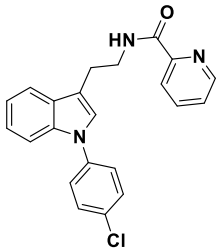
***N*-(2-(1-phenyl-1*H*-indol-3-yl)ethyl)picolinamide (3f).** Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.51 (d, J = 4.6 Hz, 1H), 8.29 (s, 1H), 8.24 (d, J = 7.8 Hz, 1H), 7.84 (td, J = 7.7, 1.6 Hz, 1H), 7.74 (d, J = 7.7 Hz, 1H), 7.59 (d, J = 8.1 Hz, 1H), 7.51 – 7.50 (m, 4H), 7.41 (ddd, J = 7.5, 4.8, 1.0 Hz, 1H), 7.34 (ddd, J = 8.6, 4.9, 3.5 Hz, 1H), 7.27 (d, J = 3.3 Hz, 1H), 7.26 – 7.24 (m, 1H), 7.22 – 7.18 (m, 1H), 3.88 (q, J = 6.9 Hz, 2H), 3.18 (t, J = 7.1 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.4, 150.1, 148.1, 139.8, 137.4, 136.3, 129.6, 128.8, 126.2, 126.1, 125.9, 124.2, 122.6, 122.2, 120.1, 119.3, 114.3, 110.6, 39.7, 25.6.



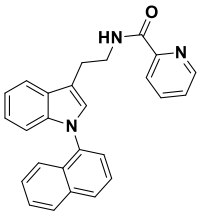
***N*-(2-(1-(4-ethylphenyl)-1*H*-indol-3-yl)ethyl)picolinamide (3g).** Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.51 (d, J = 4.6 Hz, 1H), 8.28 (s, 1H), 8.24 (d, J = 7.8 Hz, 1H), 7.84 (td, J = 7.7, 1.6 Hz, 1H), 7.73 (d, J = 7.7 Hz, 1H), 7.56 (d, J = 8.1 Hz, 1H), 7.42 – 7.39 (m, 3H), 7.33 (d, J = 8.3 Hz, 2H), 7.24 – 7.22 (m, 2H), 7.19 (t, J = 7.0 Hz, 1H), 3.87 (q, J = 6.9 Hz, 2H), 3.18 (t, J = 7.1 Hz, 2H), 2.74 (q, J = 7.6 Hz, 2H), 1.32 (t, J = 7.6 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.4, 150.1, 148.1, 142.4, 137.5, 137.3, 136.4, 129.0, 128.7, 126.1, 126.0, 124.2, 122.5, 122.2, 119.9, 119.2, 113.9, 110.7, 39.7, 28.5, 25.6, 15.6.



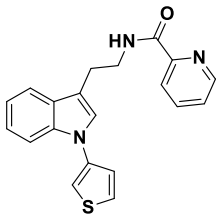
***N*-(2-(1-(4-methoxyphenyl)-1H-indol-3-yl)ethyl)picolinamide (3h).** Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.51 (dd, J = 4.7, 0.7 Hz, 1H), 8.27 (s, 1H), 8.23 (d, J = 7.8 Hz, 1H), 7.84 (td, J = 7.7, 1.6 Hz, 1H), 7.72 (d, J = 7.5 Hz, 1H), 7.47 (d, J = 8.1 Hz, 1H), 7.42 – 7.38 (m, 3H), 7.25 – 7.21 (m, 1H), 7.19 – 7.15 (m, 2H), 7.05 – 7.01 (m, 2H), 3.89 – 3.84 (m, 5H), 3.17 (t, J = 7.0 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.4, 158.1, 150.1, 148.1, 137.3, 136.7, 132.9, 128.4, 126.2, 126.1, 125.8, 122.4, 122.2, 119.8, 119.2, 114.8, 113.6, 110.5, 55.6, 39.7, 25.6.



***N*-(2-(1-(4-chlorophenyl)-1*H*-indol-3-yl)ethyl)picolinamide (3i).** Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.50 (dd, J = 4.7, 0.6 Hz, 1H), 8.28 (s, 1H), 8.24 (d, J = 7.8 Hz, 1H), 7.84 (td, J = 7.7, 1.7 Hz, 1H), 7.73 (d, J = 7.6 Hz, 1H), 7.53 (d, J = 8.1 Hz, 1H), 7.46 (d, J = 8.9 Hz, 2H), 7.40 (dd, J = 12.4, 5.0 Hz, 3H), 7.28 – 7.24 (m, 1H), 7.22 – 7.18 (m, 2H), 3.86 (q, J = 7.0 Hz, 2H), 3.16 (t, J = 7.1 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.4, 150.1, 148.1, 138.4, 137.4, 136.1, 131.7, 129.8, 129.0, 126.2, 125.6, 125.3, 122.9, 122.2, 120.4, 119.4, 114.8, 110.4, 39.6, 25.5.

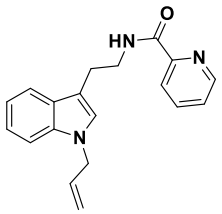


***N*-(2-(1-(naphthalen-1-yl)-1*H*-indol-3-yl)ethyl)picolinamide (3j).** Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.50 (d, J = 4.7 Hz, 1H), 8.35 (s, 1H), 8.25 (d, J = 7.8 Hz, 1H), 7.98 – 7.94 (m, 2H), 7.86 – 7.80 (m, 2H), 7.60 – 7.52 (m, 4H), 7.27 (d, J = 8.2 Hz, 2H), 7.41 – 7.35 (m, 2H), 7.24 – 7.20 (m, 2H), 7.19 – 7.15 (m, 1H), 7.07 (d, J = 8.0 Hz, 1H), 3.95 (td, J = 7.2, 1.3 Hz, 2H), 3.26 (t, J = 7.0 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.4, 150.2, 148.1, 138.5, 137.4, 136.1, 134.6, 130.6, 128.4, 128.3, 128.0, 127.8, 126.9, 126.7, 126.1, 125.6, 125.1, 123.5, 122.5, 122.2, 119.9, 119.2, 113.6, 111.0, 39.7, 25.7.



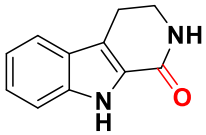
***N*-(2-(1-(thiophen-3-yl)-1*H*-indol-3-yl)ethyl)picolinamide (3k).** Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.51 (d, J = 4.7 Hz, 1H), 8.27 (s, 1H), 8.24 (d, J = 7.8 Hz, 1H), 7.85 (td, J = 7.7, 1.6 Hz,

1H), 7.72 (d, *J* = 7.8 Hz, 1H), 7.58 (d, *J* = 8.2 Hz, 1H), 7.45 (dd, *J* = 5.1, 3.2 Hz, 1H), 7.41 (ddd, *J* = 7.4, 4.8, 0.8 Hz, 1H), 7.30 – 7.27 (m, 2H), 7.26 (dd, *J* = 2.8, 1.3 Hz, 1H), 7.24 (s, 1H), 7.20 (t, *J* = 7.4 Hz, 1H), 3.87 (q, *J* = 6.9 Hz, 2H), 3.16 (t, *J* = 7.1 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.4, 150.1, 148.1, 138.6, 137.4, 136.5, 128.6, 126.2, 126.1, 125.9, 123.7, 122.8, 122.3, 120.2, 119.3, 114.4, 114.1, 110.8, 39.7, 25.6.

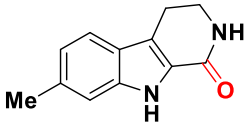


***N*-(2-(1-allyl-1*H*-indol-3-yl)ethyl)picolinamide (3l).** Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.49 (d, *J* = 4.2 Hz, 1H), 8.22 (d, *J* = 7.8 Hz, 1H), 7.83 (td, *J* = 7.7, 1.7 Hz, 1H), 7.67 (d, *J* = 7.9 Hz, 1H), 7.39 (ddd, *J* = 7.5, 4.8, 1.1 Hz, 1H), 7.31 (d, *J* = 8.2 Hz, 1H), 7.24 – 7.20 (m, 1H), 7.14 – 7.10 (m, 1H), 6.99 (s, 1H), 6.03 – 5.94 (m, 1H) 5.18 (dd, *J* = 10.3, 1.3 Hz, 1H), 5.09 (dd, *J* = 17.1, 1.3 Hz, 1H), 4.69 (dt, *J* = 5.3, 1.5 Hz, 2H), 3.81 (dd, *J* = 13.3, 7.0 Hz, 2H), 3.11 (t, *J* = 7.1 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.3, 150.1, 148.0, 137.3, 136.6, 133.6, 128.0, 126.0, 125.9, 122.2, 121.8, 119.1, 117.2, 112.0, 109.6, 48.7, 39.8, 25.6.

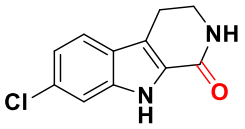
8. Characterization data of products (2a-2j , 4a-4l, 5, 6, 7)



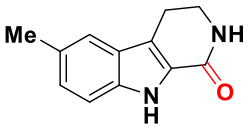
2,3,4,9-tetrahydro-1*H*-pyrido[3,4-*b*]indol-1-one (2a).[2] Yellow solid, 35.3 mg, 95% yield, mp: 185.5 – 186.3 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.65 (s, 1H), 7.64 (s, 1H), 7.62 (s, 1H), 7.45 (d, J = 8.3 Hz, 1H), 7.28 – 7.24 (m, 1H), 7.10 (t, J = 7.5 Hz, 1H), 3.56 (td, J = 7.0, 2.5 Hz, 2H), 2.96 (t, J = 7.0 Hz, 2H); ^{13}C NMR (101 MHz, DMSO-d_6) δ 162.4, 137.6, 127.7, 125.4, 124.5, 120.6, 119.9, 118.7, 113.0, 41.7, 20.8.



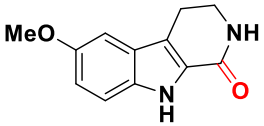
7-methyl-2,3,4,9-tetrahydro-1*H*-pyrido[3,4-*b*]indol-1-one (2b). Yellow solid, 36.0 mg, 90% yield, mp: 263.1 – 264.5 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.43 (s, 1H), 7.50 (d, J = 8.7 Hz, 1H), 7.44 (s, 1H), 6.89 (d, J = 2.2 Hz, 1H), 6.76 (dd, J = 8.7, 2.3 Hz, 1H), 3.82 (s, 3H), 3.52 (td, J = 7.0, 2.5 Hz, 2H), 2.91 (t, J = 7.0 Hz, 2H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 162.4, 158.0, 138.6, 126.6, 121.4, 119.8, 119.3, 111.1, 94.8, 55.6, 41.6, 20.9; HRMS (ESI-TOF) m/z: $[M+H]^+$ Calcd. for $C_{12}H_{13}N_2O^+$: 201.1022; found: 201.1022.



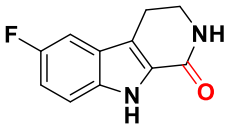
7-chloro-2,3,4,9-tetrahydro-1*H*-pyrido[3,4-*b*]indol-1-one (2c).[3] Yellow solid, 40.0 mg, 91% yield, mp: 211.2 – 212.5 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.80 (s, 1H), 7.67 (s, 1H), 7.65 (s, 1H), 7.44 (d, J = 1.6 Hz, 1H), 7.12 (dd, J = 8.5, 1.9 Hz, 1H), 3.55 (td, J = 7.0, 2.5 Hz, 2H), 2.96 (t, J = 7.0 Hz, 2H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 162.0, 137.8, 129.0, 128.7, 124.2, 122.2, 120.4, 118.8, 112.4, 41.5, 20.7.



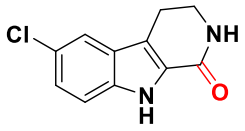
6-methyl-2,3,4,9-tetrahydro-1*H*-pyrido[3,4-*b*]indol-1-one (2d). Yellow solid, 35.6 mg, 89% yield, mp: 210.5 – 211.3 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.47 (s, 1H), 7.55 (s, 1H), 7.40 (s, 1H), 7.32 (d, J = 8.4 Hz, 1H), 7.09 (dd, J = 8.4, 1.2 Hz, 1H), 3.54 (td, J = 6.9, 2.4 Hz, 2H), 2.93 (t, J = 6.9 Hz, 2H), 2.42 (s, 3H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 162.4, 136.0, 128.5, 127.7, 126.3, 125.6, 119.9, 118.1, 112.7, 41.7, 21.6, 20.8; HRMS (ESI-TOF) m/z: $[M+H]^+$ Calcd. for $C_{12}H_{12}N_2NaO^+$: 223.0842; found: 223.0839.



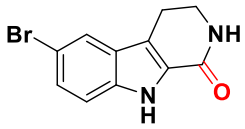
6-methoxy-2,3,4,9-tetrahydro-1*H*-pyrido[3,4-*b*]indol-1-one (2e).[4] Yellow solid, 29.8 mg, 69% yield, mp: 220.5 – 221.6 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.06 (s, 1H), 7.15 (s, 1H), 6.92 (d, J = 8.9 Hz, 1H), 6.69 (d, J = 2.3 Hz, 1H), 6.51 (dd, J = 8.9, 2.5 Hz, 1H), 3.14 (td, J = 6.9, 2.4 Hz, 2H), 2.98 (s, 3H), 2.53 (t, J = 6.9 Hz, 2H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 162.3, 154.0, 132.8, 128.2, 125.5, 118.2, 115.6, 113.8, 101.2, 55.8, 41.7, 20.9.



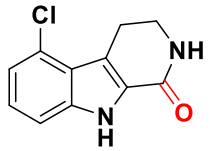
6-fluoro-2,3,4,9-tetrahydro-1*H*-pyrido[3,4-*b*]indol-1-one (2f).[5] Yellow solid, 29.4 mg, 72% yield, mp: 226.3 – 227.9 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.73 (s, 1H), 7.66 (s, 1H), 7.45 – 7.43 (m, 1H), 7.41 – 7.40 (m, 1H), 7.11 (td, J = 9.3, 2.5 Hz, 1H), 3.55 (td, J = 7.0, 2.6 Hz, 2H), 2.94 (t, J = 7.0 Hz, 2H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 162.0, 157.4 (d, J = 232.9 Hz), 134.2, 129.5, 125.4 (d, J = 10.1 Hz), 118.6 (d, J = 5.2 Hz), 114.2 (d, J = 9.7 Hz), 113.1 (d, J = 26.6 Hz), 105.0 (d, J = 23.0 Hz), 41.6, 20.7.



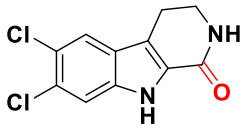
6-chloro-2,3,4,9-tetrahydro-1*H*-pyrido[3,4-*b*]indol-1-one (2g).[5] Yellow solid, 40.9 mg, 93% yield, mp: 232.1 – 233.0 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.84 (s, 1H), 7.72 (d, J = 1.9 Hz, 1H), 7.70 (s, 1H), 7.45 (d, J = 8.7 Hz, 1H), 7.25 (dd, J = 8.7, 2.1 Hz, 1H), 3.55 (td, J = 7.0, 2.5 Hz, 2H), 2.95 (t, J = 7.0 Hz, 2H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 162.0, 135.9, 129.2, 126.4, 124.5, 119.9, 118.2, 114.6, 41.5, 20.6.



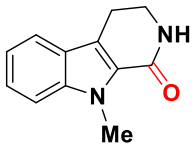
6-bromo-2,3,4,9-tetrahydro-1*H*-pyrido[3,4-*b*]indol-1-one (2h).[6] Yellow solid, 38.0 mg, 72% yield, mp: 259.3 – 259.9 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.86 (s, 1H), 7.87 (d, J = 1.7 Hz, 1H), 7.70 (s, 1H), 7.40 (d, J = 8.6 Hz, 1H), 7.36 (dd, J = 8.7, 1.8 Hz, 1H), 3.55 (td, J = 7.0, 2.5 Hz, 2H), 2.95 (t, J = 7.0 Hz, 2H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 161.4, 135.6, 128.5, 126.6, 126.4, 122.5, 117.6, 114.5, 111.8, 41.0, 20.1.



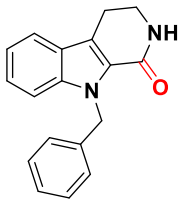
5-chloro-2,3,4,9-tetrahydro-1*H*-pyrido[3,4-*b*]indol-1-one (2i).[3] Yellow solid, 40.5 mg, 92% yield, mp: 208.3 – 209.5 °C; °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.00 (s, 1H), 7.74 (s, 1H), 7.40 (dd, J = 8.2, 0.5 Hz, 1H), 7.22 (t, J = 7.9 Hz, 1H), 7.12 (dd, J = 7.5, 0.5 Hz, 1H), 3.57 (td, J = 7.0, 2.5 Hz, 2H), 3.23 (t, J = 7.0 Hz, 2H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 161.8, 138.7, 128.8, 126.5, 125.1, 122.8, 120.3, 117.7, 112.2, 41.5, 22.3.



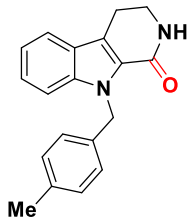
6,7-dichloro-2,3,4,9-tetrahydro-1*H*-pyrido[3,4-*b*]indol-1-one (2j).[7] Yellow solid, 48.3 mg, 95% yield, mp: 246.5 – 247.3 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.96 (s, 1H), 7.96 (s, 1H), 7.76 (s, 1H), 7.61 (s, 1H), 3.55 (td, J = 7.0, 2.5 Hz, 2H), 2.96 (t, J = 7.0 Hz, 2H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 161.6, 136.2, 130.0, 126.6, 125.3, 122.6, 122.0, 118.3, 114.3, 41.4, 20.5.



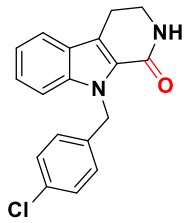
9-methyl-2,3,4,9-tetrahydro-1*H*-pyrido[3,4-*b*]indol-1-one (4a).[2] Yellow solid, 21.2 mg, 53% yield, mp: 157.6 – 158.3 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.71 (s, 1H), 7.67 (d, J = 8.0 Hz, 1H), 7.55 (d, J = 8.4 Hz, 1H), 7.37 – 7.33 (m, 1H), 7.18 – 7.14 (m, 1H), 4.07 (s, 3H), 3.52 (td, J = 6.9, 2.7 Hz, 2H), 2.96 (t, J = 6.9 Hz, 2H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 162.6, 138.9, 126.6, 124.8, 124.3, 120.8, 120.2, 119.4, 111.0, 41.3, 31.4, 21.0.



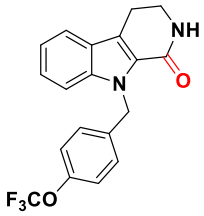
9-benzyl-2,3,4,9-tetrahydro-1*H*-pyrido[3,4-*b*]indol-1-one (4b).[2] Yellow solid, 35.9 mg, 65% yield, mp: 182.3 – 183.5 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.63 (d, J = 8.0 Hz, 1H), 7.36 (d, J = 8.4 Hz, 1H), 7.32 – 7.28 (m, 2H), 7.24 – 7.15 (m, 5H), 6.12 (s, 1H), 5.92 (s, 2H), 3.65 (td, J = 7.0, 2.7 Hz, 2H), 3.08 (t, J = 7.0 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.3, 138.7, 138.5, 128.5, 127.1, 126.9, 125.5, 125.2, 124.6, 120.54, 120.49, 120.3, 111.1, 47.8, 41.8, 21.2.



9-(4-methylbenzyl)-2,3,4,9-tetrahydro-1*H*-pyrido[3,4-*b*]indol-1-one (4c). Yellow solid, 30.7 mg, 53% yield, mp: 193.8 – 194.7 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.71 (s, 1H), 7.68 (d, J = 8.0 Hz, 1H), 7.52 (d, J = 8.4 Hz, 1H), 7.29 (t, J = 7.7 Hz, 1H), 7.14 (t, J = 7.4 Hz, 1H), 7.10 (s, 4H), 5.87 (s, 2H), 3.54 (td, J = 6.9, 2.6 Hz, 2H), 3.01 (t, J = 6.9 Hz, 2H), 2.26 (s, 3H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 162.5, 138.3, 136.6, 136.2, 129.4, 127.3, 126.1, 125.0, 124.7, 120.9, 120.4, 120.2, 111.7, 46.9, 41.3, 21.1, 21.0; HRMS (ESI-TOF) m/z: $[M+H]^+$ Calcd. for $C_{19}H_{19}N_2O^+$: 291.1492; found: 291.1494.

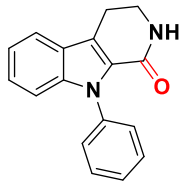


9-(4-chlorobenzyl)-2,3,4,9-tetrahydro-1*H*-pyrido[3,4-*b*]indol-1-one (4d). Yellow solid, 42.8 mg, 69% yield, mp: 186.5 – 187.8 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.75 (s, 1H), 7.70 (d, J = 7.9 Hz, 1H), 7.53 (d, J = 8.4 Hz, 1H), 7.37 (d, J = 8.5 Hz, 2H), 7.33 – 7.29 (m, 1H), 7.20 (d, J = 8.5 Hz, 2H), 7.16 (t, J = 7.5 Hz, 1H), 5.90 (s, 2H), 3.54 (td, J = 6.9, 2.6 Hz, 2H), 3.01 (t, J = 6.9 Hz, 2H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 162.5, 138.3, 132.1, 129.2, 128.9, 126.0, 125.2, 124.7, 121.0, 120.6, 120.4, 111.5, 46.5, 41.2, 21.0; HRMS (ESI-TOF) m/z: $[M+H]^+$ Calcd. for $C_{18}H_{15}ClN_2NaO^+$: 333.0765; found: 333.0761.

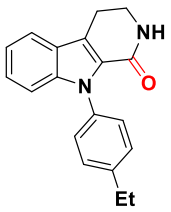


9-(4-(trifluoromethoxy)benzyl)-2,3,4,9-tetrahydro-1*H*-pyrido[3,4-*b*]indol-1-one (4e). Yellow solid, 46.8 mg, 65% yield, mp: 192.1 – 193.5 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.76 (s, 1H),

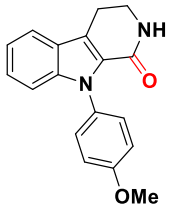
7.71 (d, *J* = 7.9 Hz, 1H), 7.56 (d, *J* = 8.4 Hz, 1H), 7.33 – 7.29 (m, 5H), 7.17 (t, *J* = 7.5 Hz, 1H), 5.95 (s, 2H), 3.55 (td, *J* = 7.0, 2.6 Hz, 2H), 3.02 (t, *J* = 6.9 Hz, 2H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 162.5, 147.8, 138.8, 138.3, 129.2, 129.1, 126.0, 125.2, 124.7, 121.5, 121.1, 120.6, 120.5 (q, *J* = 256.1 Hz), 120.4, 111.5, 46.5, 41.2, 21.0; HRMS (ESI-TOF) m/z: $[M+H]^+$ Calcd. for $C_{19}H_{16}F_3N_2O_2^+$: 361.1158; found: 361.1162.



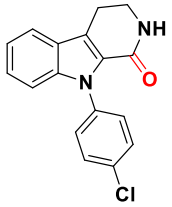
9-phenyl-2,3,4,9-tetrahydro-1*H*-pyrido[3,4-*b*]indol-1-one (4f).[2] Yellow solid, 28.8 mg, 55% yield, mp: 249.1 – 250.3 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.77 (d, *J* = 7.8 Hz, 1H), 7.64 (s, 1H), 7.55 (t, *J* = 7.5 Hz, 2H), 7.47 (dd, *J* = 8.5, 6.3 Hz, 1H), 7.42 – 7.40 (m, 2H), 7.34 – 7.30 (m, 1H), 7.23 (t, *J* = 7.1 Hz, 1H), 7.19 (d, *J* = 8.3 Hz, 1H), 3.59 (td, *J* = 6.8, 2.7 Hz, 2H), 3.06 (t, *J* = 6.8 Hz, 2H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 161.3, 139.9, 139.0, 129.7, 128.3, 128.2, 126.2, 125.5, 122.6, 121.7, 121.6, 111.9, 41.4, 21.8.



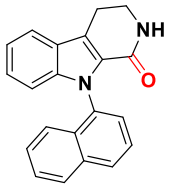
9-(4-ethylphenyl)-2,3,4,9-tetrahydro-1*H*-pyrido[3,4-*b*]indol-1-one (4g). Yellow solid, 34.8 mg, 60% yield, mp: 238.3 – 239.1 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.76 (d, *J* = 7.8 Hz, 1H), 7.62 (s, 1H), 7.37 (d, *J* = 8.3 Hz, 2H), 7.34 – 7.27 (m, 3H), 7.21 (dd, *J* = 10.9, 3.9 Hz, 1H), 7.17 (d, *J* = 8.3 Hz, 1H), 3.57 (td, *J* = 6.8, 2.7 Hz, 2H), 3.04 (t, *J* = 6.8 Hz, 2H), 2.75 (q, *J* = 7.6 Hz, 2H), 1.31 (t, *J* = 7.6 Hz, 3H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 160.9, 143.1, 139.5, 136.1, 128.5, 127.7, 127.6, 125.7, 125.0, 121.9, 121.1, 121.0, 111.4, 41.0, 28.3, 21.3, 15.9; HRMS (ESI-TOF) m/z: $[M+H]^+$ Calcd. for $C_{19}H_{18}N_2NaO^+$: 313.1311; found: 313.1313.



9-(4-methoxyphenyl)-2,3,4,9-tetrahydro-1*H*-pyrido[3,4-*b*]indol-1-one (4h). Yellow solid, 29.8 mg, 51% yield, mp: 253.8 – 254.5 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.75 (d, J = 7.9 Hz, 1H), 7.59 (s, 1H), 7.30 (dd, J = 11.8, 4.9 Hz, 3H), 7.21 (t, J = 7.1 Hz, 1H), 7.13 (d, J = 8.3 Hz, 1H), 7.09 – 7.07 (m, 1H), 3.88 (s, 3H), 3.57 (td, J = 6.8, 2.7 Hz, 2H), 3.04 (t, J = 6.8 Hz, 2H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 161.0, 158.7, 139.7, 131.3, 129.0, 127.8, 125.6, 124.8, 121.4, 121.0, 121.0, 114.4, 111.4, 55.8, 41.0, 21.2; HRMS (ESI-TOF) m/z: [M+H]$^+$ Calcd. for $C_{18}H_{17}N_2O_2^+$: 293.1285; found: 293.1286.

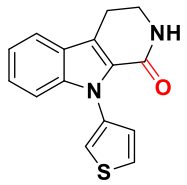


9-(4-chlorophenyl)-2,3,4,9-tetrahydro-1*H*-pyrido[3,4-*b*]indol-1-one (4i). Yellow solid, 38.5 mg, 65% yield, mp: 270.3 – 271.5 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.78 (d, J = 7.8 Hz, 1H), 7.68 (s, 1H), 7.62 – 7.58 (m, 2H), 7.48 – 7.44 (m, 2H), 7.34 (ddd, J = 8.2, 7.1, 1.1 Hz, 1H), 7.27 – 7.21 (m, 2H), 3.58 (td, J = 6.9, 2.7 Hz, 2H), 3.05 (t, J = 6.9 Hz, 2H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 160.9, 139.2, 137.4, 132.1, 129.6, 129.2, 127.6, 126.0, 125.2, 122.4, 121.4, 111.3, 40.9, 21.2; HRMS (ESI-TOF) m/z: [M+H]$^+$ Calcd. for $C_{17}H_{13}ClN_2NaO^+$: 319.0609; found: 319.0610.

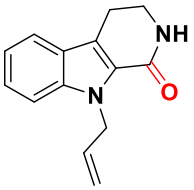


9-(naphthalen-1-yl)-2,3,4,9-tetrahydro-1*H*-pyrido[3,4-*b*]indol-1-one (4j). Yellow solid, 30.6 mg, 49% yield, mp: 232.5 – 233.7 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.11 (dd, J = 8.2, 2.9 Hz, 2H), 7.85 – 7.83 (m, 1H), 7.72 – 7.68 (m, 1H), 7.59 – 7.57 (m, 2H), 7.54 (s, 1H), 7.43 (ddd, J = 8.1, 6.9,

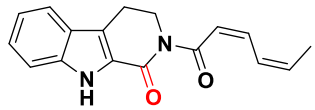
1.1 Hz, 1H), 7.26 – 7.21 (m, 2H), 7.03 (d, *J* = 8.4 Hz, 1H), 6.77 – 6.73 (m, 1H), 3.65 – 3.61 (m, 2H), 3.14 (dd, *J* = 12.6, 6.7 Hz, 2H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 160.9, 140.3, 135.4, 134.3, 131.4, 129.1, 128.8, 128.7, 127.4, 126.8, 126.5, 126.1, 125.7, 125.0, 122.8, 121.2, 121.1, 111.5, 41.2, 21.2; HRMS (ESI-TOF) m/z: $[M+H]^+$ Calcd. for $C_{21}H_{17}N_2O^+$: 313.1335; found: 313.1334.



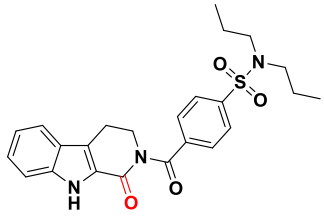
9-(thiophen-3-yl)-2,3,4,9-tetrahydro-1*H*-pyrido[3,4-*b*]indol-1-one (4k). Yellow solid, 32.7 mg, 61% yield, mp: 241.7 – 242.5 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.75 (d, *J* = 7.9 Hz, 1H), 7.67 – 7.65 (m, 2H), 7.63 (s, 1H), 7.37 – 7.33 (m, 1H), 7.27 (d, *J* = 8.3 Hz, 1H), 7.25 – 7.21 (m, 1H), 7.18 – 7.17 (m, 1H), 3.56 (td, *J* = 6.9, 2.7 Hz, 2H), 3.04 (t, *J* = 6.9 Hz, 2H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 160.9, 139.5, 136.3, 127.8, 127.5, 125.8, 125.4, 124.9, 121.8, 121.3, 121.0, 120.5, 111.7, 40.9, 21.2.; HRMS (ESI-TOF) m/z: $[M+H]^+$ Calcd. for $C_{15}H_{12}N_2NaOS^+$: 291.0563; found: 291.0558.



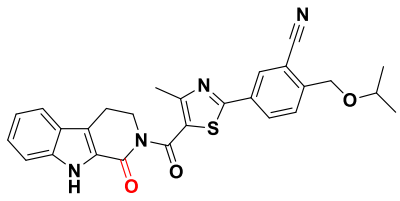
9-allyl-2,3,4,9-tetrahydro-1*H*-pyrido[3,4-*b*]indol-1-one (4l). Yellow solid, 26.2 mg, 58% yield, mp: 193.8 – 194.6 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.70 (s, 1H), 7.68 (s, 1H), 7.52 (d, *J* = 8.4 Hz, 1H), 7.33 (t, *J* = 7.6 Hz, 1H), 7.16 (t, *J* = 7.4 Hz, 1H), 5.99 (ddt, *J* = 15.5, 10.3, 5.2 Hz, 1H), 5.30 (d, *J* = 5.2 Hz, 2H), 5.09 (dd, *J* = 10.3, 1.4 Hz, 1H), 4.93 (dd, *J* = 17.1, 1.6 Hz, 1H), 3.52 (td, *J* = 6.9, 2.7 Hz, 2H), 2.99 (t, *J* = 6.9 Hz, 2H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 162.4, 138.2, 135.3, 126.1, 124.9, 124.5, 120.9, 120.4, 119.9, 116.3, 111.4, 46.3, 41.3, 21.0; HRMS (ESI-TOF) m/z: $[M+H]^+$ Calcd. for $C_{14}H_{15}N_2O^+$: 227.1179; found: 227.1179.



2-((2*Z*,4*Z*)-hexa-2,4-dienoyl)-2,3,4,9-tetrahydro-1*H*-pyrido[3,4-*b*]indol-1-one (5). Yellow solid, 43.7 mg, 78% yield, mp: >300 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.88 (s, 1H), 7.68 (d, J = 8.1 Hz, 1H), 7.47 (d, J = 8.3 Hz, 1H), 7.35 – 7.25 (m, 2H), 7.13 (t, J = 7.5 Hz, 1H), 6.87 (d, J = 15.1 Hz, 1H), 6.39 – 6.24 (m, 2H), 4.21 (t, J = 6.3 Hz, 2H), 3.06 (t, J = 6.3 Hz, 2H), 1.86 (d, J = 6.1 Hz, 3H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 168.8, 161.7, 143.2, 139.7, 139.1, 130.8, 126.8, 126.3, 124.7, 123.7, 123.5, 121.5, 120.5, 113.3, 45.0, 20.9, 18.9.



4-(1-oxo-2,3,4,9-tetrahydro-1*H*-pyrido[3,4-*b*]indole-2-carbonyl)-*N*,*N*-dipropylbenzenesulfon--amide (6). Yellow solid, 73.4 mg, 81% yield, mp: >300 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.86 (s, 1H), 7.88 (d, J = 8.4 Hz, 2H), 7.80 – 7.76 (m, 3H), 7.48 (d, J = 8.3 Hz, 1H), 7.38 (dd, J = 11.7, 4.4 Hz, 1H), 7.19 (t, J = 7.5 Hz, 1H), 4.32 (t, J = 6.3 Hz, 2H), 3.28 (t, J = 6.3 Hz, 2H), 3.12 – 3.08 (m, 4H), 1.58 – 1.49 (m, 4H), 0.87 (t, J = 7.4 Hz, 6H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 172.2, 161.3, 141.7, 141.0, 139.2, 129.0, 127.0, 126.6, 125.9, 124.9, 124.3, 121.6, 120.7, 113.3, 50.1, 46.7, 22.1, 21.0, 11.5.



2-(isopropoxymethyl)-5-(4-methyl-5-(1-oxo-2,3,4,9-tetrahydro-1*H*-pyrido[3,4-*b*]indole-2-car--bonyl)thiazol-2-yl)benzonitrile (7). Yellow solid, 30.6 mg, 32% yield, mp: >300 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.92 (s, 1H), 8.33 (d, J = 2.3 Hz, 1H), 8.26 (dd, J = 8.9, 2.3 Hz, 1H), 7.76 (d, J = 8.1 Hz, 1H), 7.50 (d, J = 8.4 Hz, 1H), 7.39 (t, J = 7.9 Hz, 2H), 7.19 (t, J = 7.5 Hz, 1H), 4.26

(t, *J* = 6.2 Hz, 2H), 4.05 (d, *J* = 6.5 Hz, 2H), 3.25 (t, *J* = 6.2 Hz, 2H), 2.51 (s, 3H), 2.14 (dt, *J* = 13.3, 6.6 Hz, 1H), 1.06 (d, *J* = 6.7 Hz, 6H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 165.8, 165.7, 162.5, 161.3, 156.3, 139.2, 133.4, 131.9, 128.6, 126.7, 126.0, 125.8, 124.9, 124.0, 121.6, 120.7, 115.8, 114.4, 113.4, 102.1, 75.6, 47.5, 28.1, 21.1, 19.2, 17.3.

9. References

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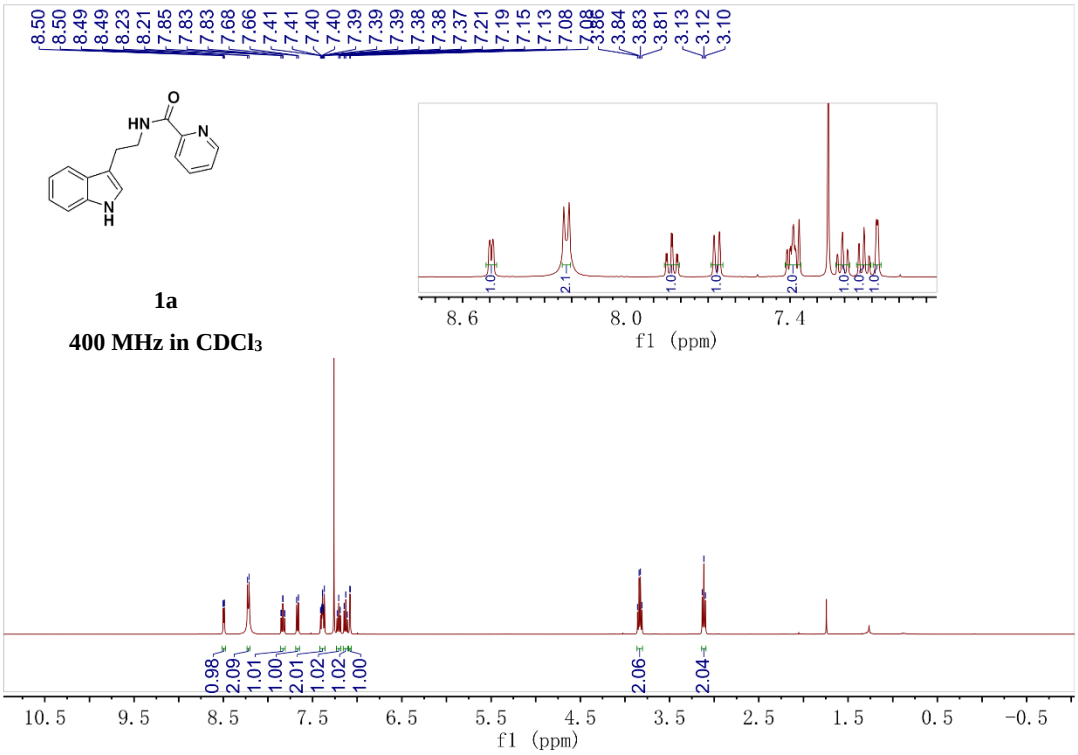
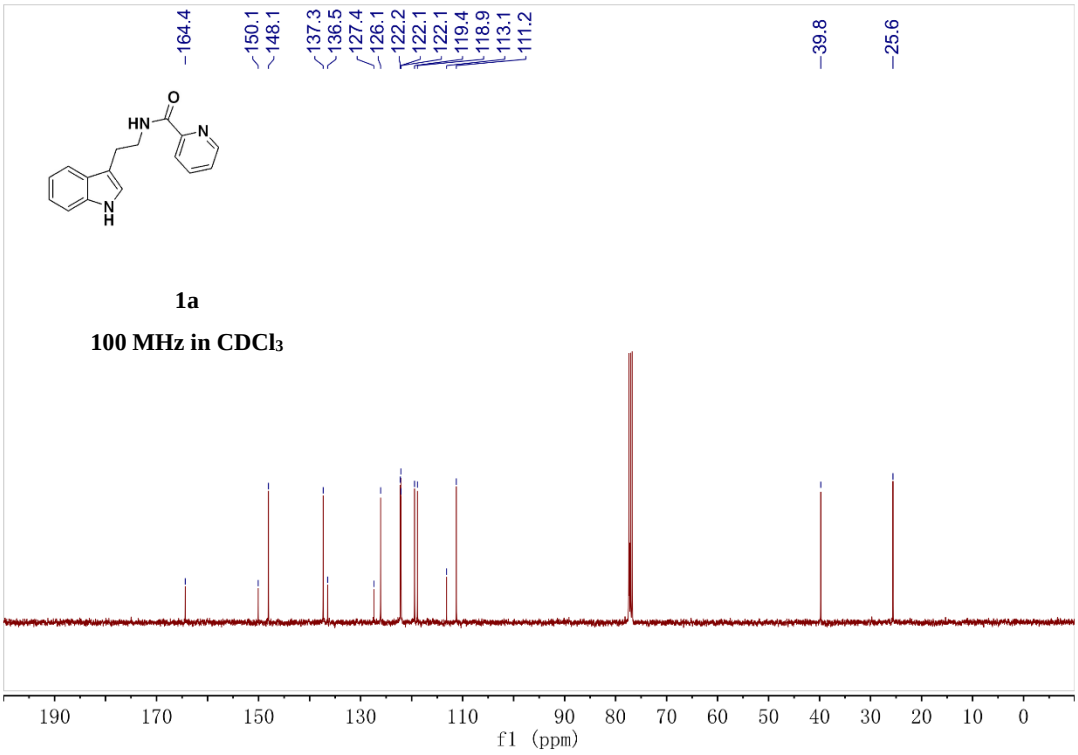
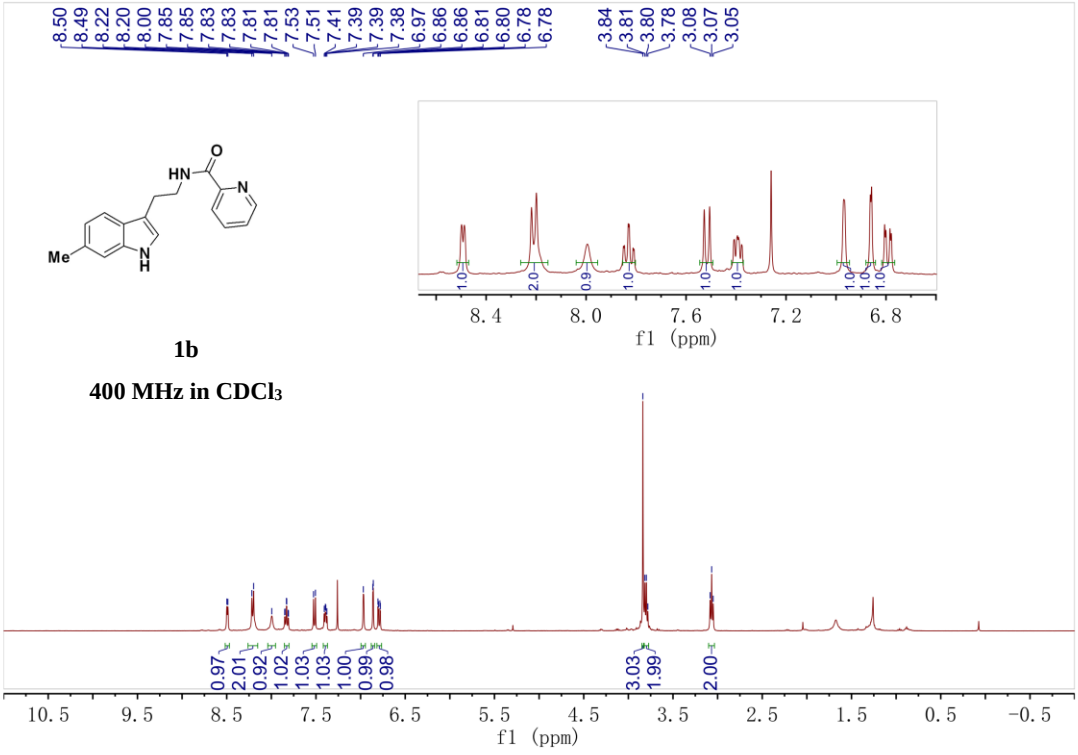
10. ^{1}H, ^{13}C spectra of substrates (1a-1j, 3a-3l) and products (2a-2j , 4a-4l, 5, 6, 7)

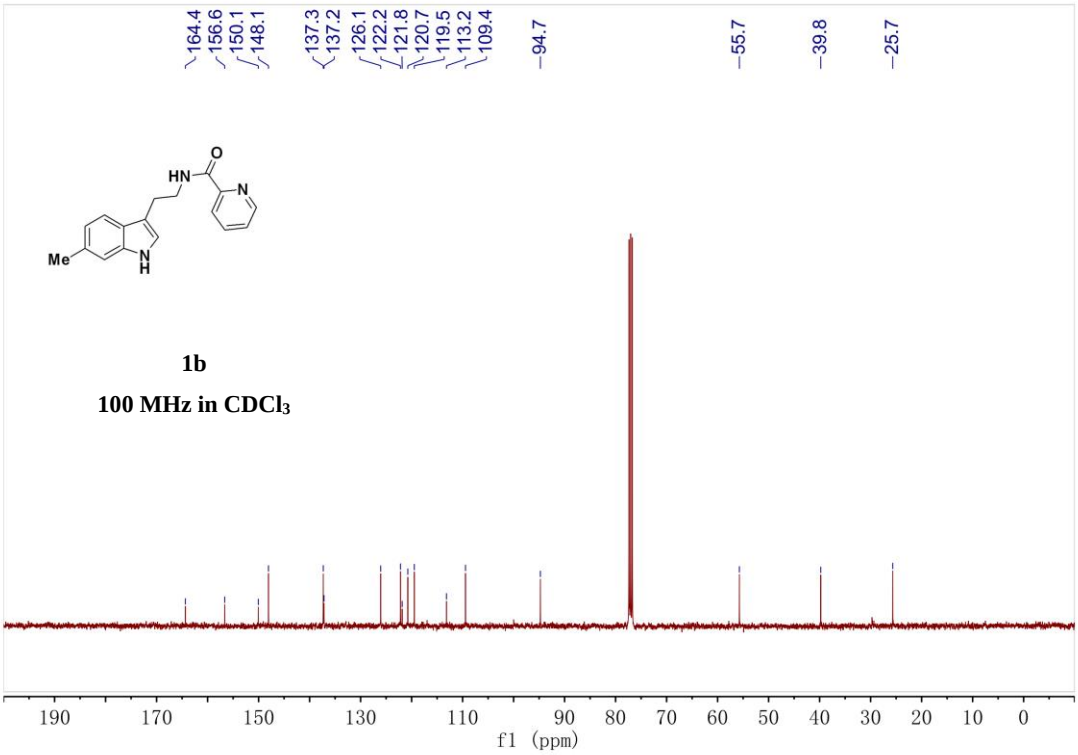






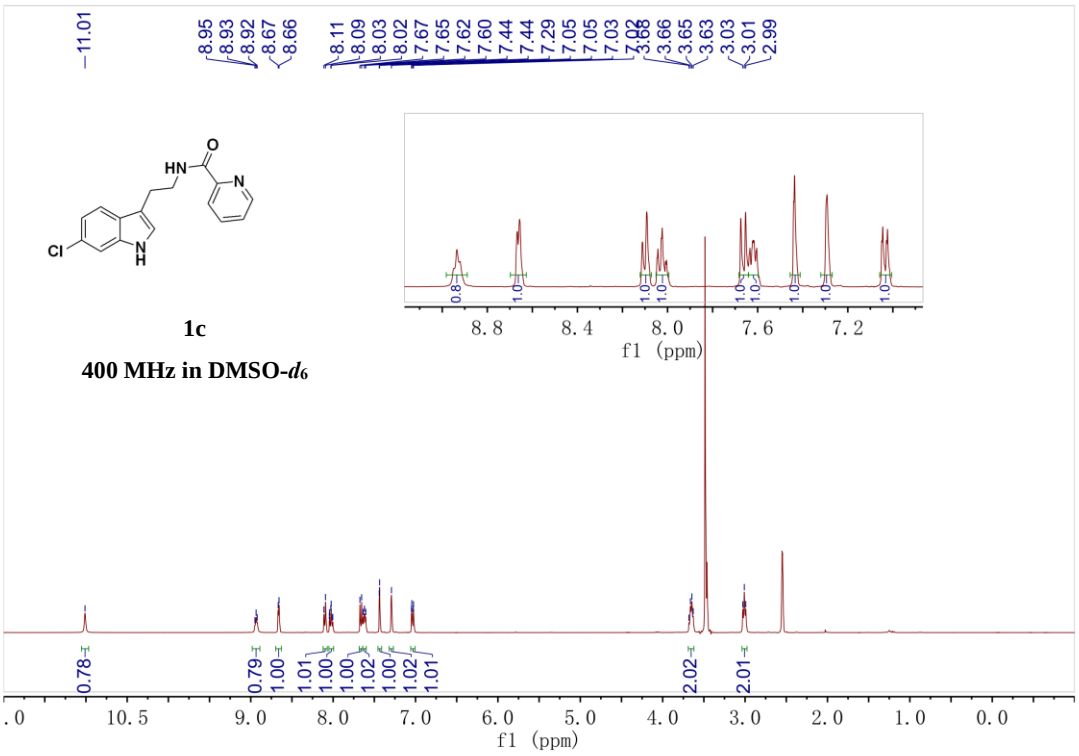
1b

400 MHz in $CDCl_3$



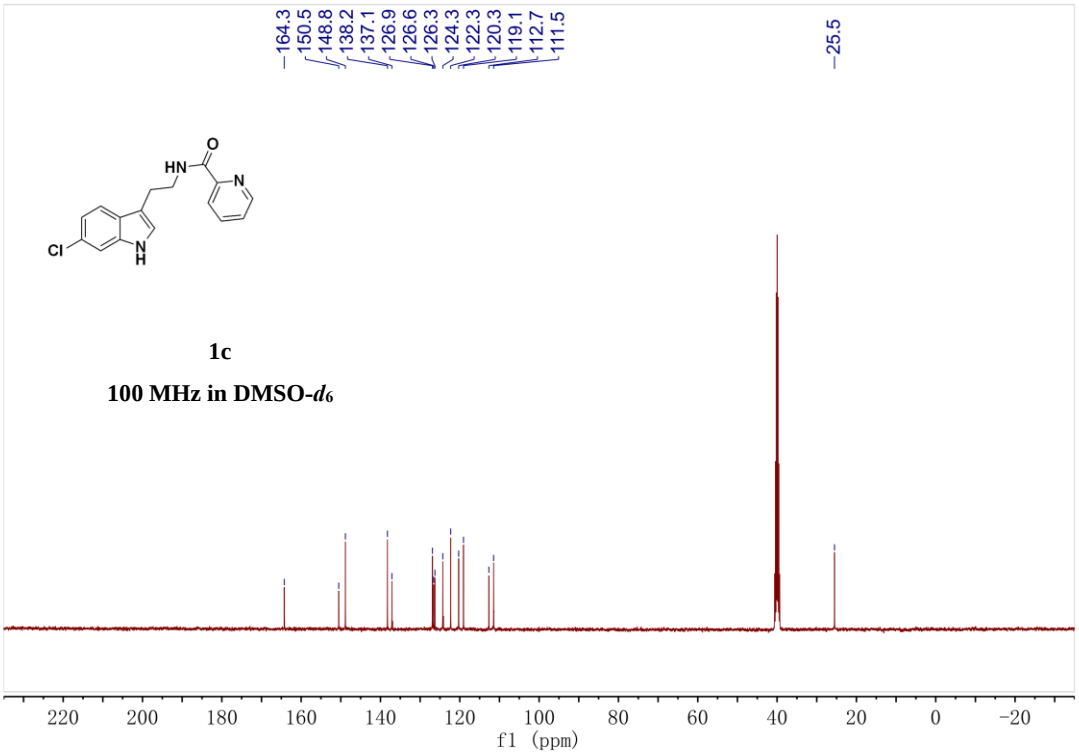
1b

100 MHz in $CDCl_3$



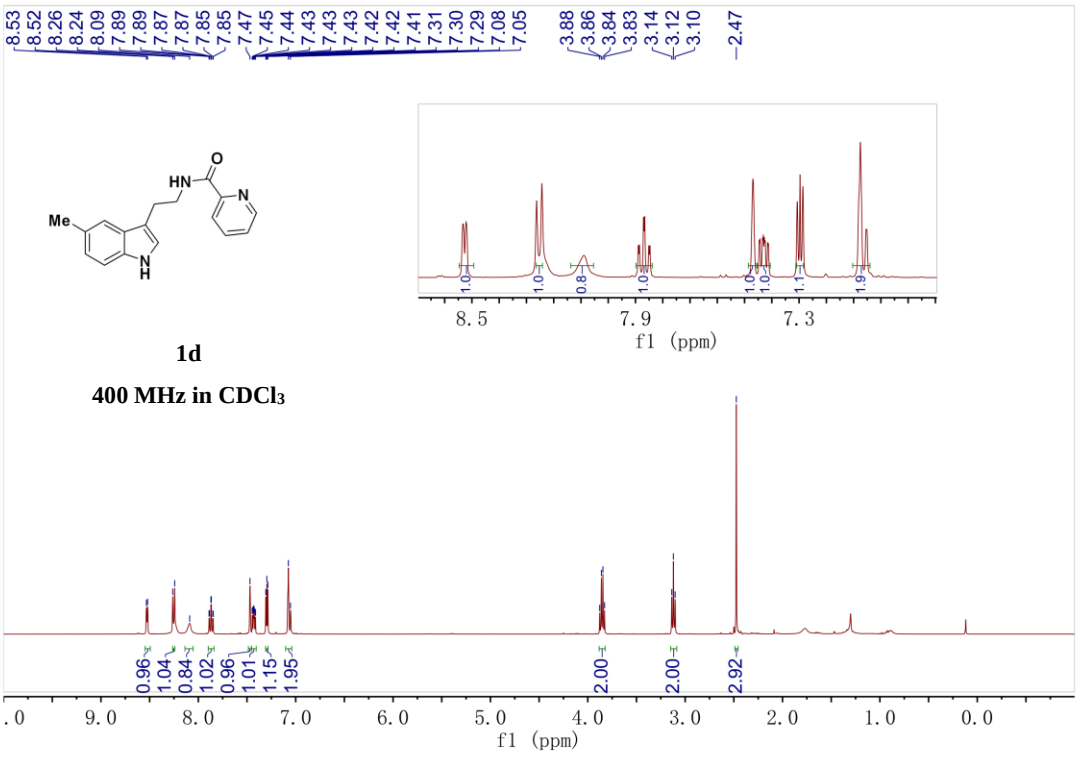
1c

400 MHz in DMSO-*d*$_6$



1c

100 MHz in DMSO-*d*$_6$



1d

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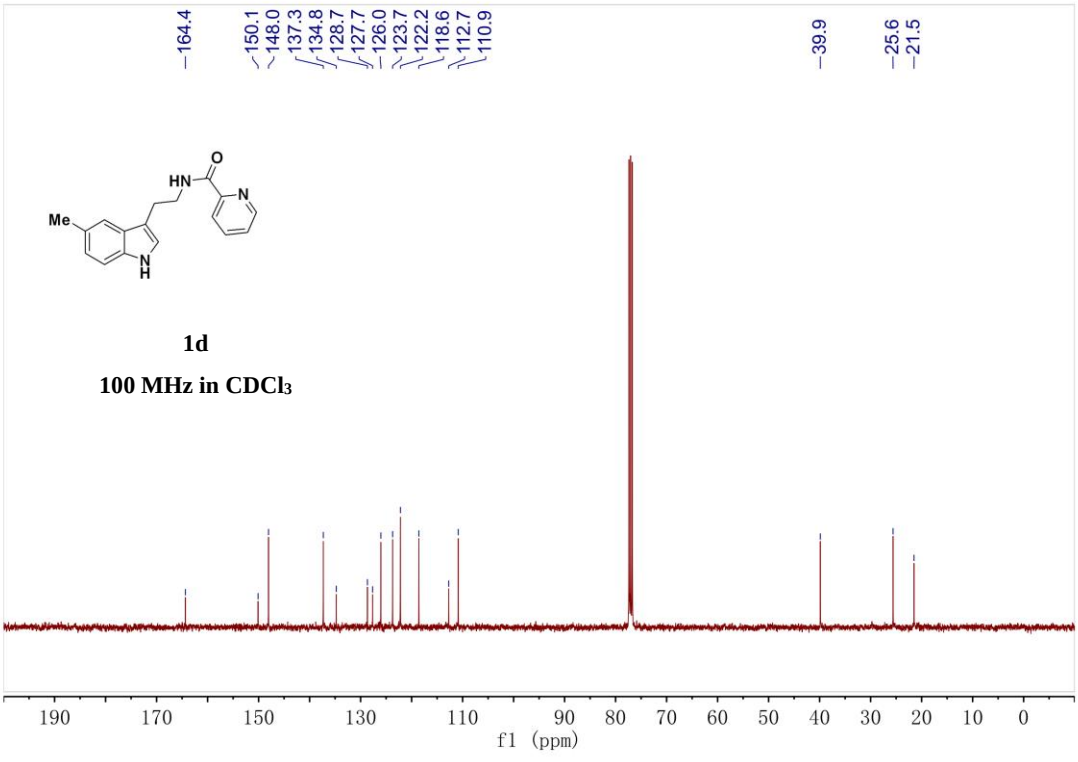

1d

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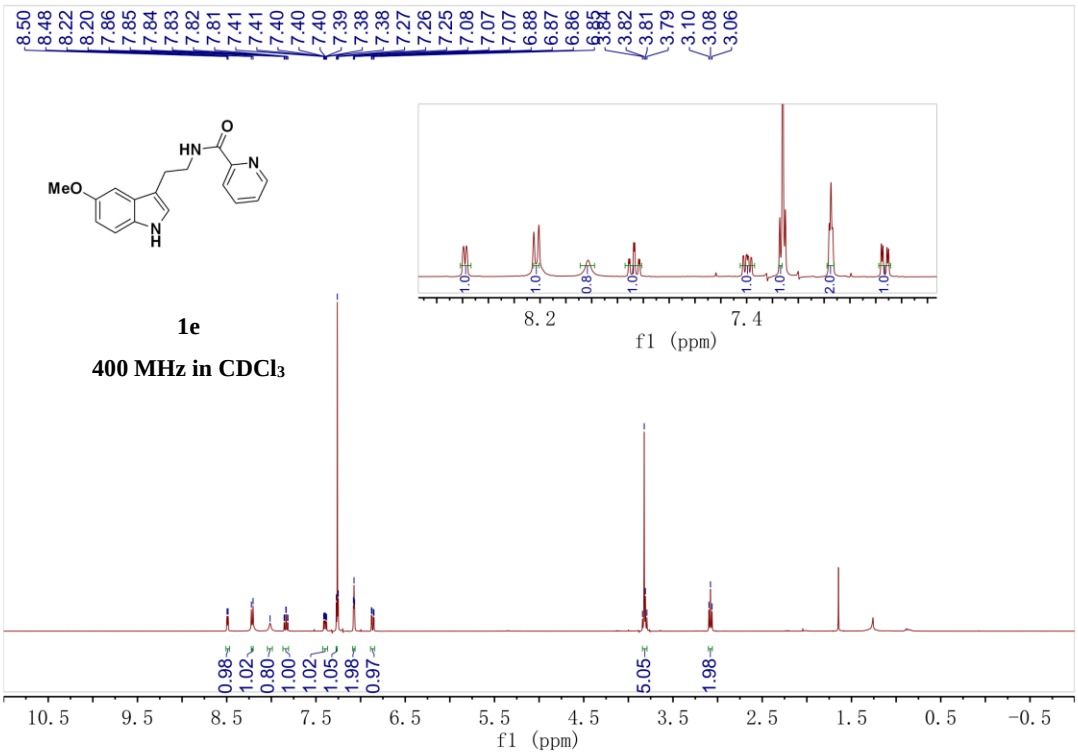
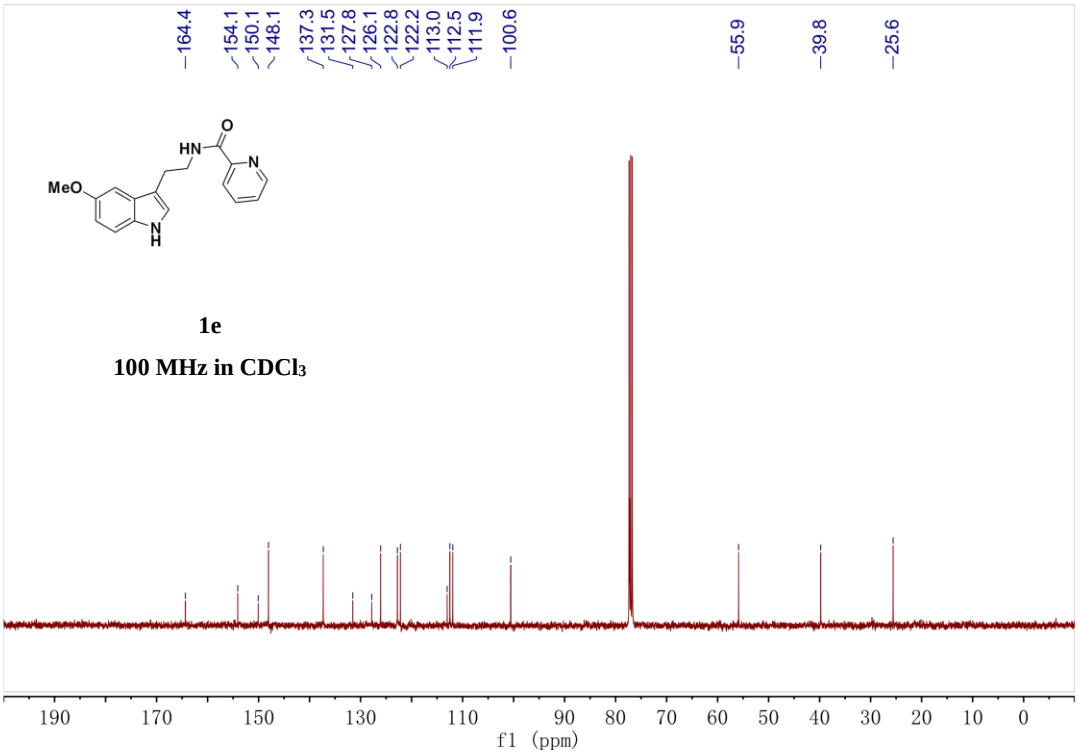


1e

400 MHz in $CDCl_3$



1e

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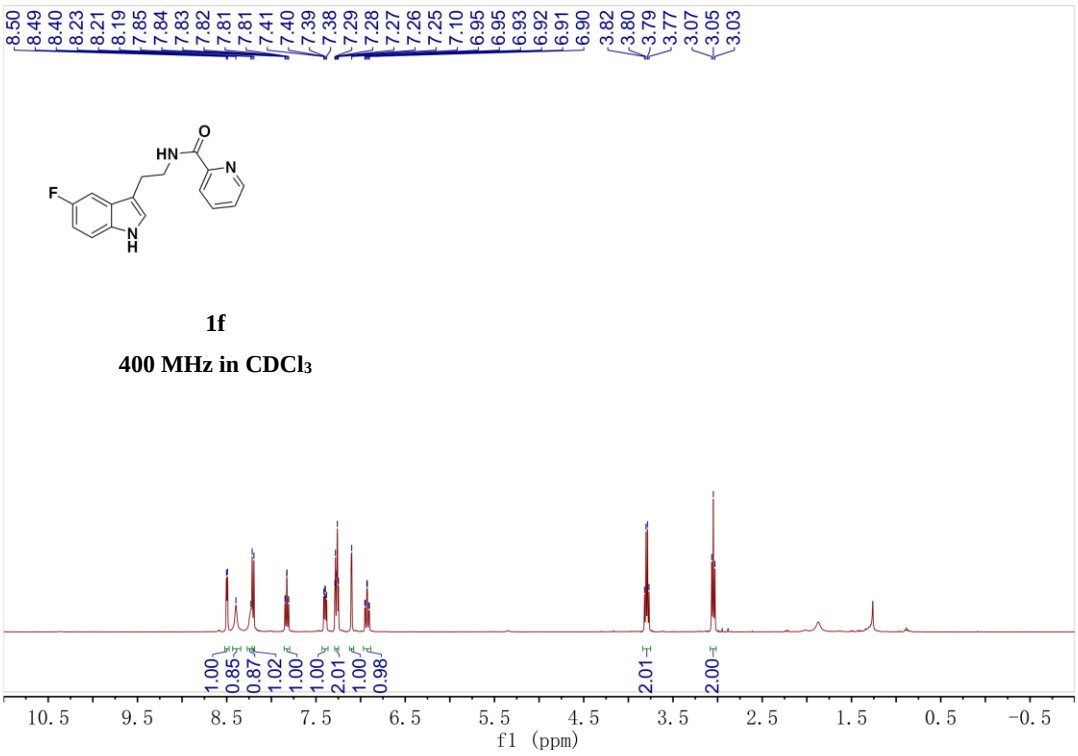
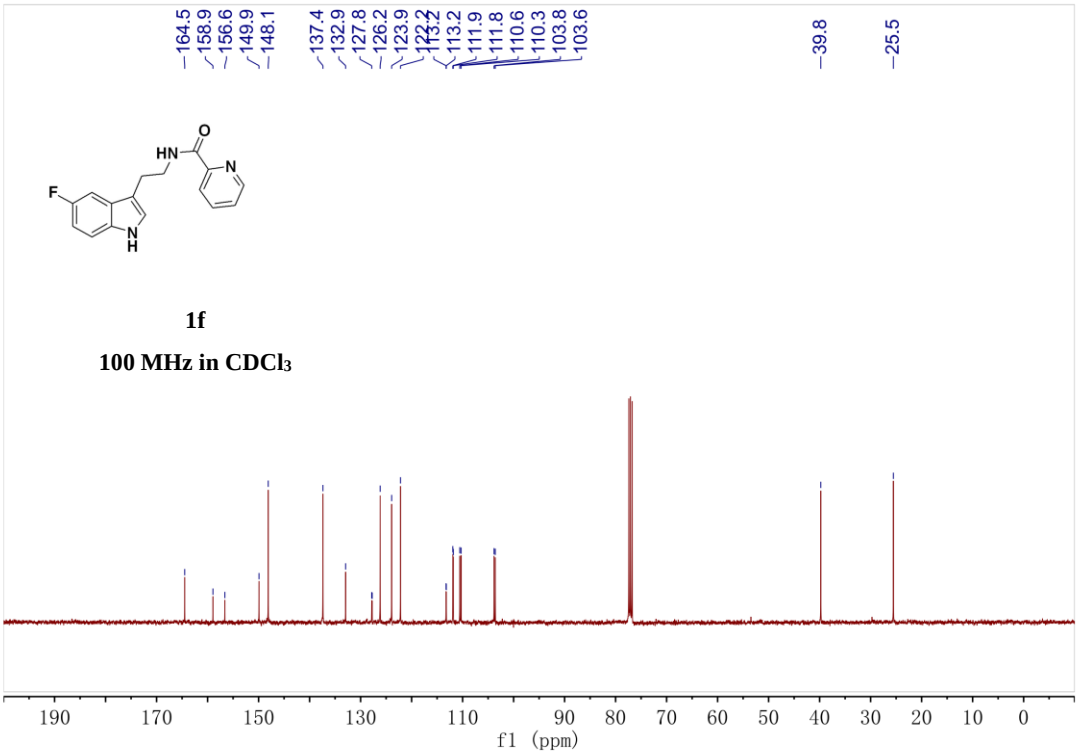


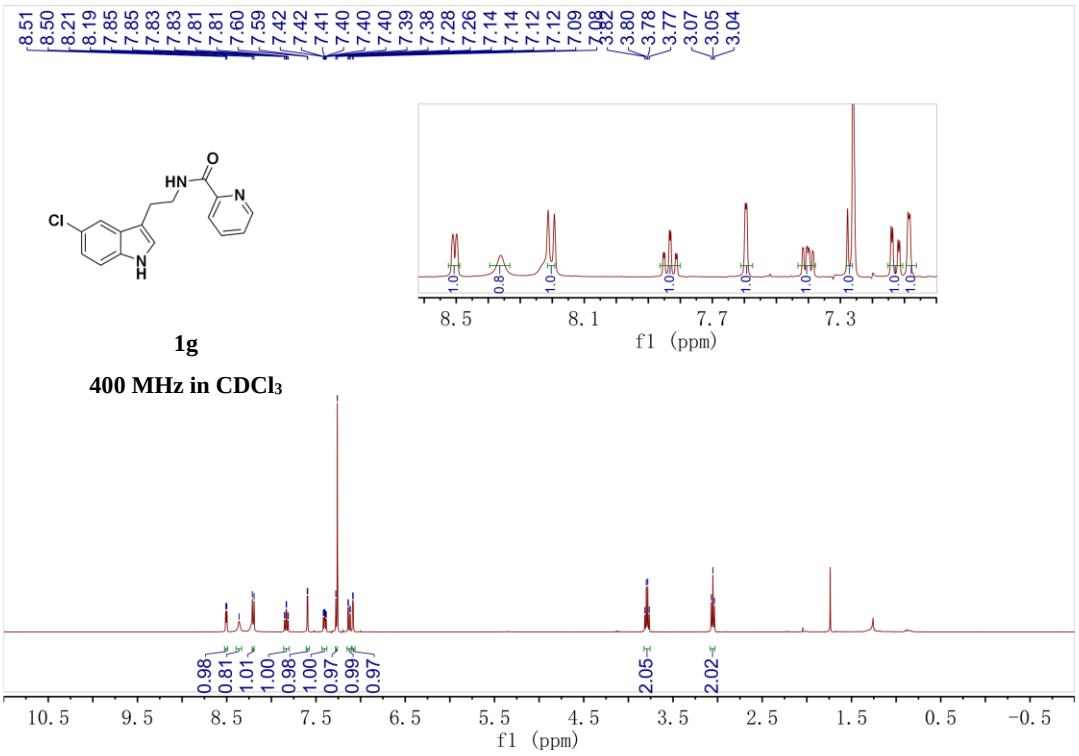
1f

400 MHz in $CDCl_3$



1f

100 MHz in $CDCl_3$



1g

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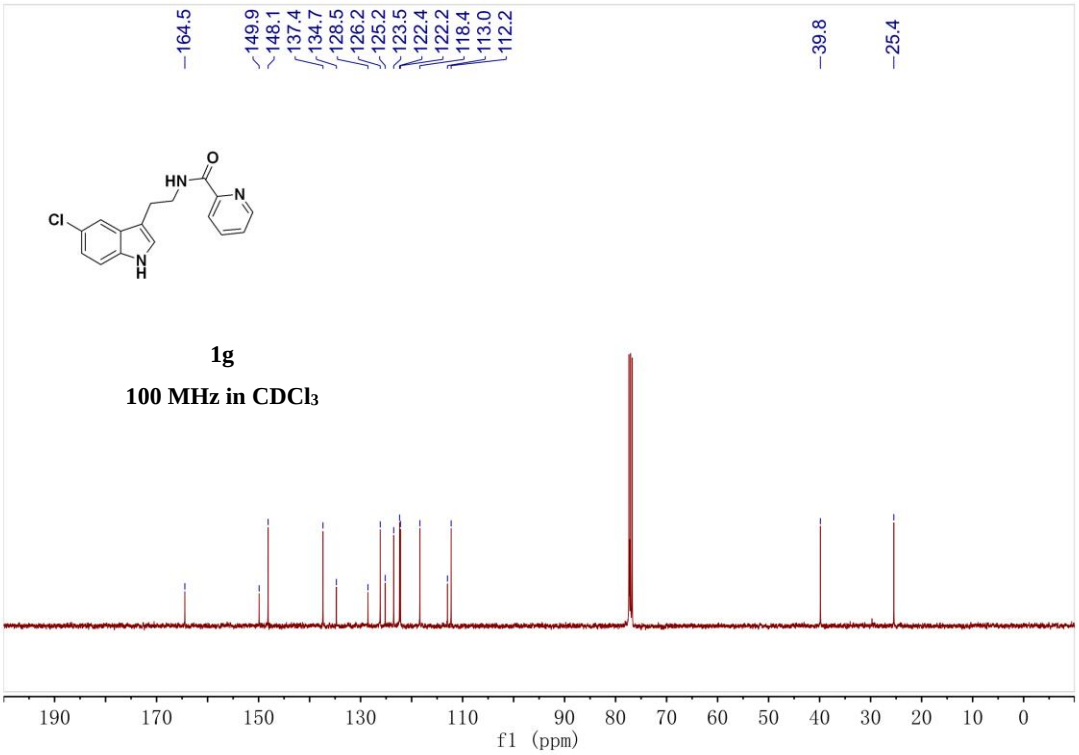

1g

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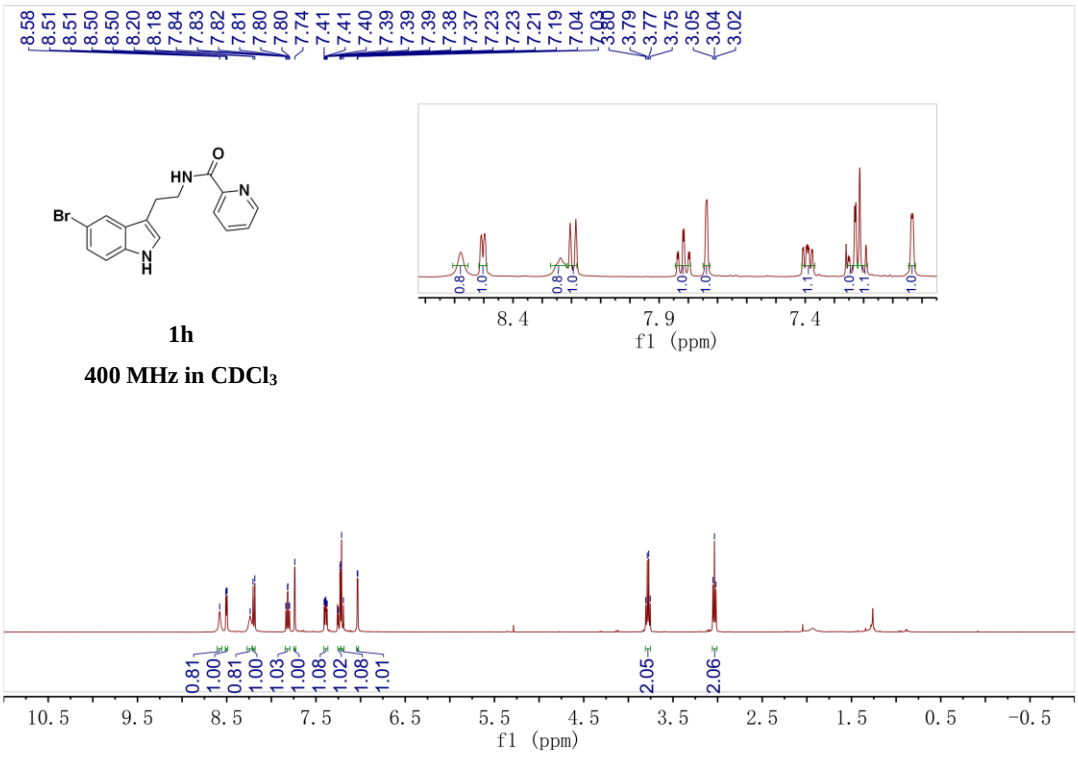
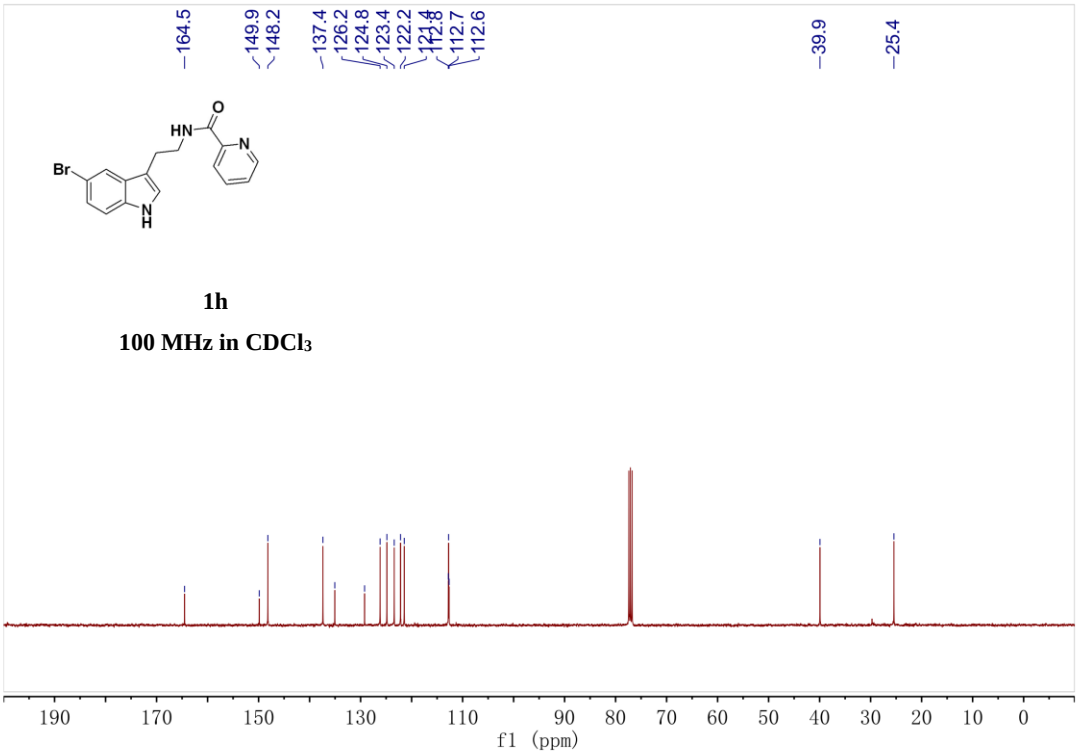


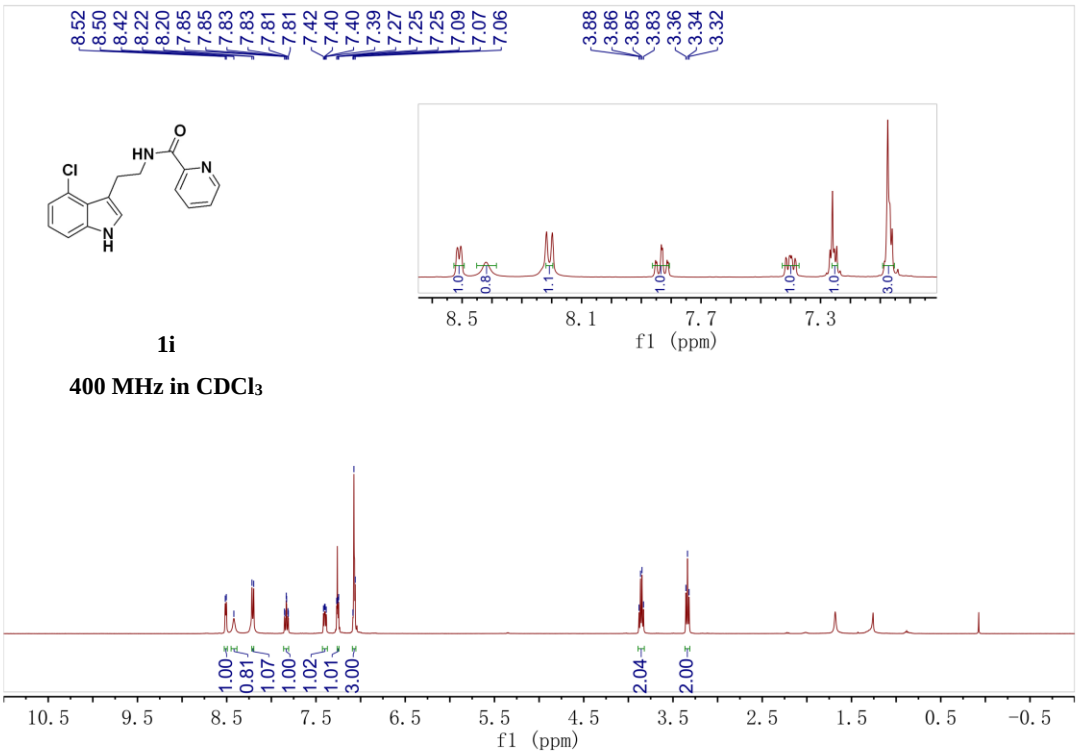
1h

400 MHz in $CDCl_3$



1h

100 MHz in $CDCl_3$



1i

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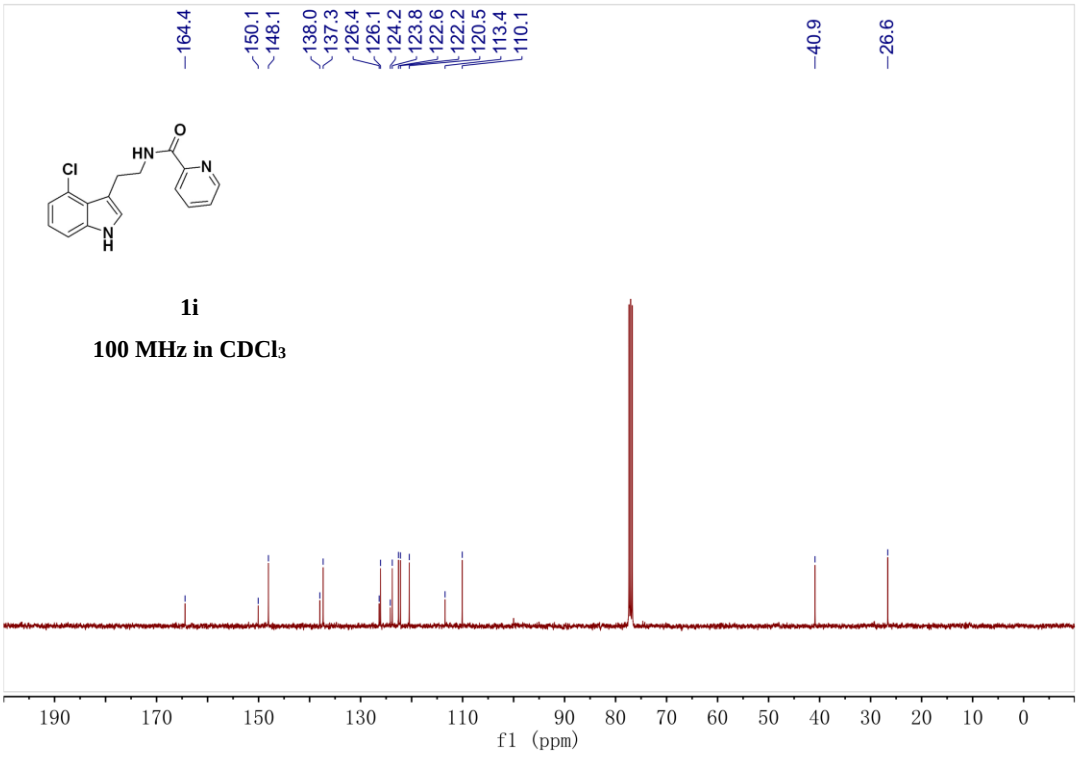
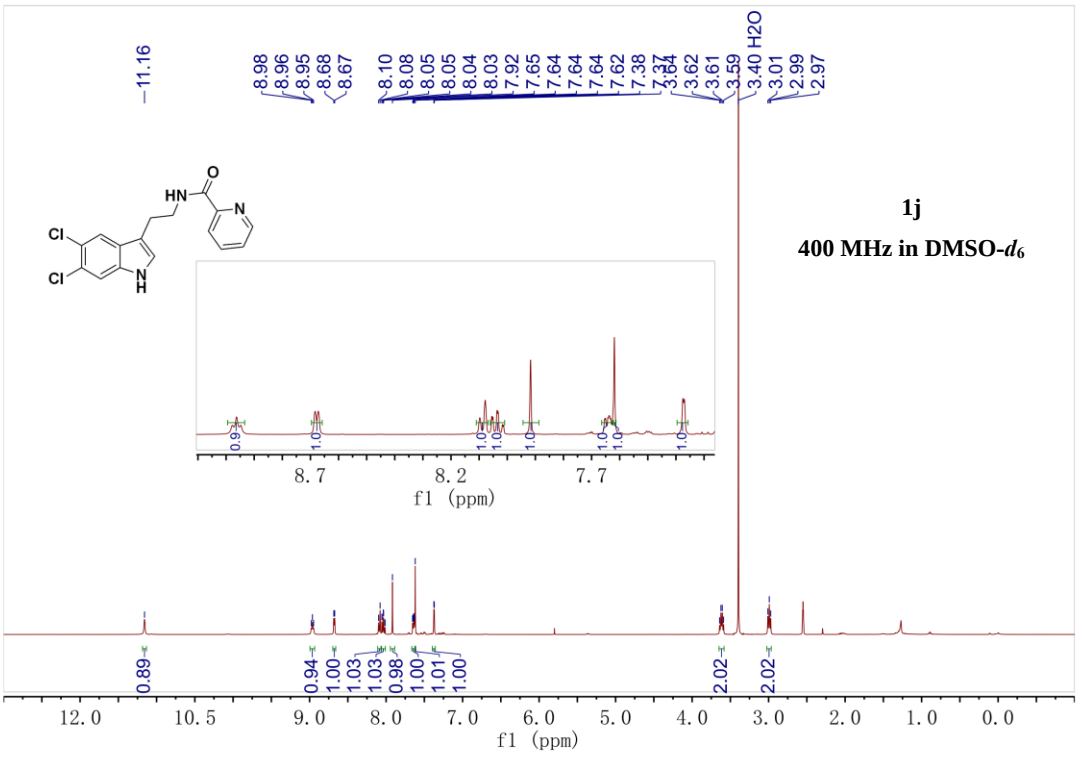
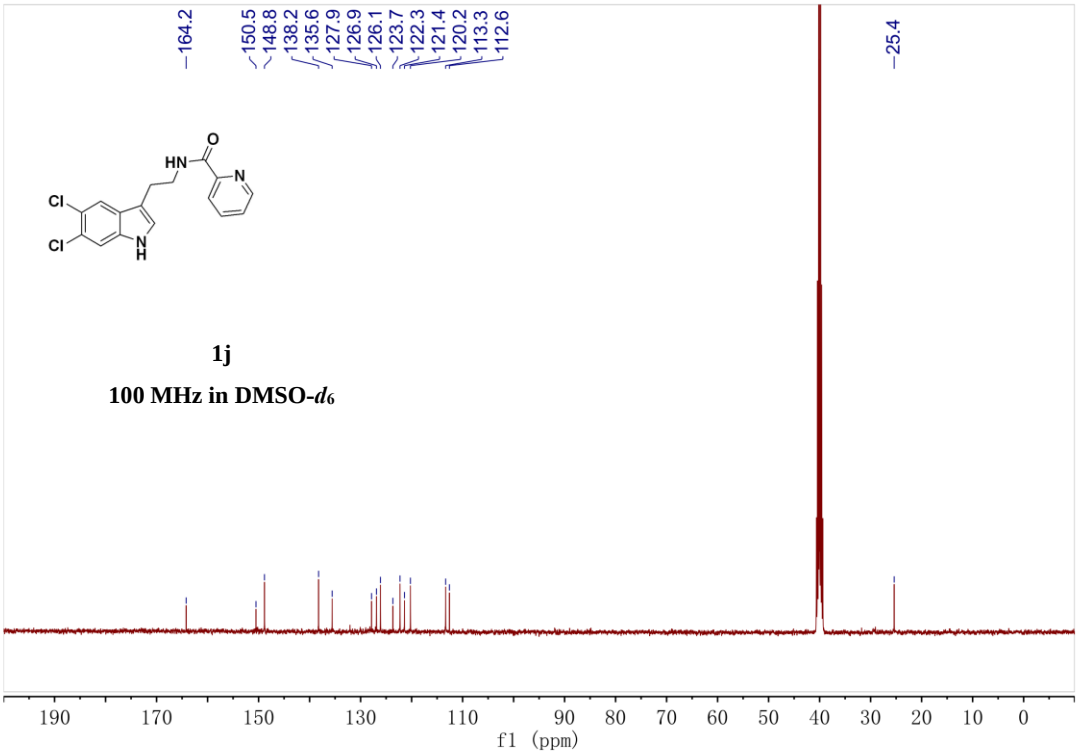
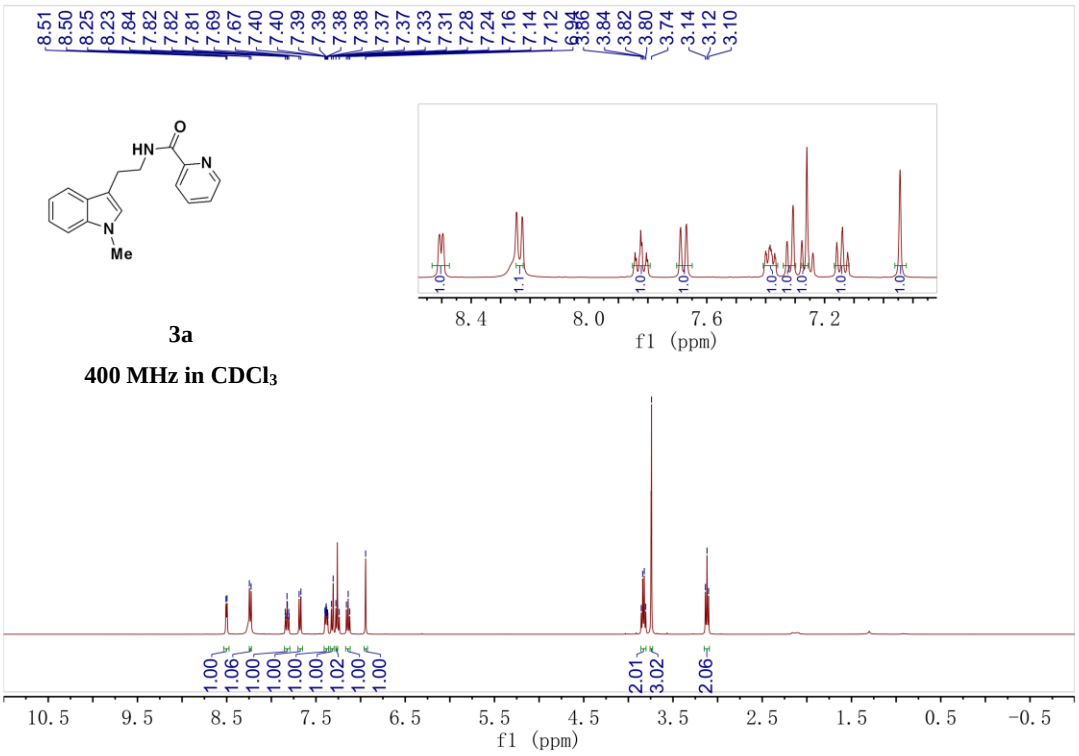


1i

100 MHz in $CDCl_3$

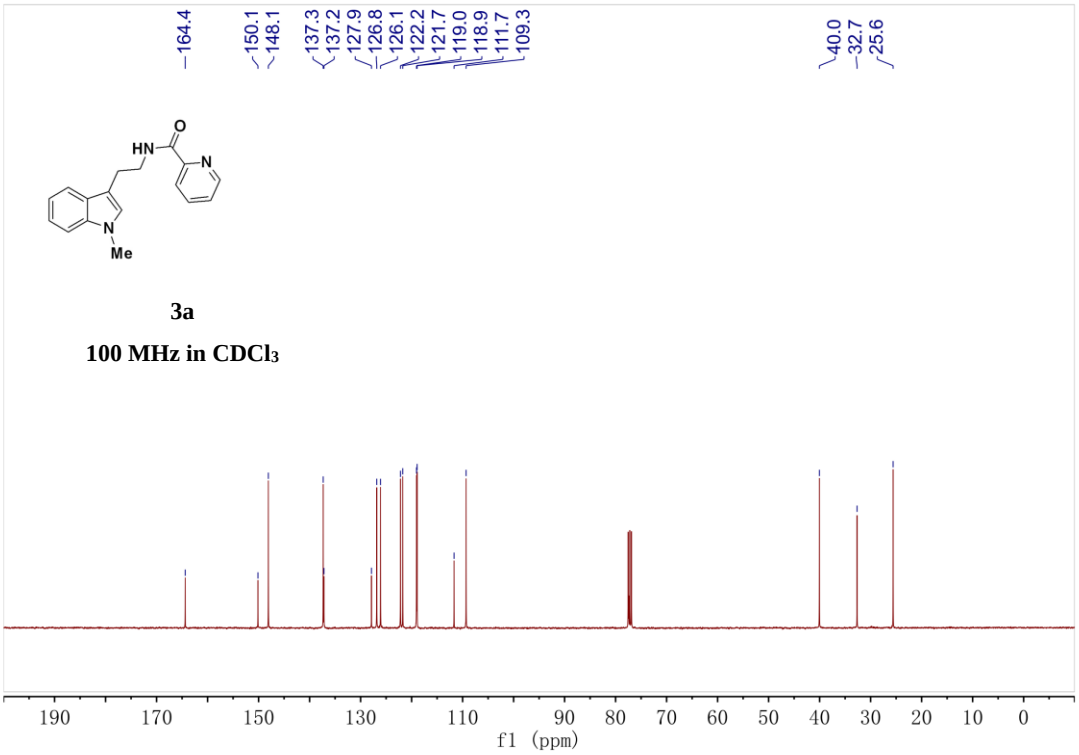

11.16
8.98
8.96
8.95
8.68
8.67
8.10
8.08
8.05
8.05
8.04
8.03
7.92
7.65
7.64
7.64
7.64
7.62
7.38
3.64
3.62
3.61
3.59
3.40 H2O
3.01
2.99
2.97
HN
O
N
Cl
Cl
N
H
1j
400 MHz in DMSO-d6
0.89
0.94
1.00
1.03
1.03
0.98
1.00
1.01
1.00
2.02
2.02
f1 (ppm)


164.2
150.5
148.8
138.2
135.6
127.9
126.9
126.1
123.7
122.3
121.4
120.2
113.3
112.6
25.4
HN
O
N
Cl
Cl
N
H
1j
100 MHz in DMSO-d6
f1 (ppm)



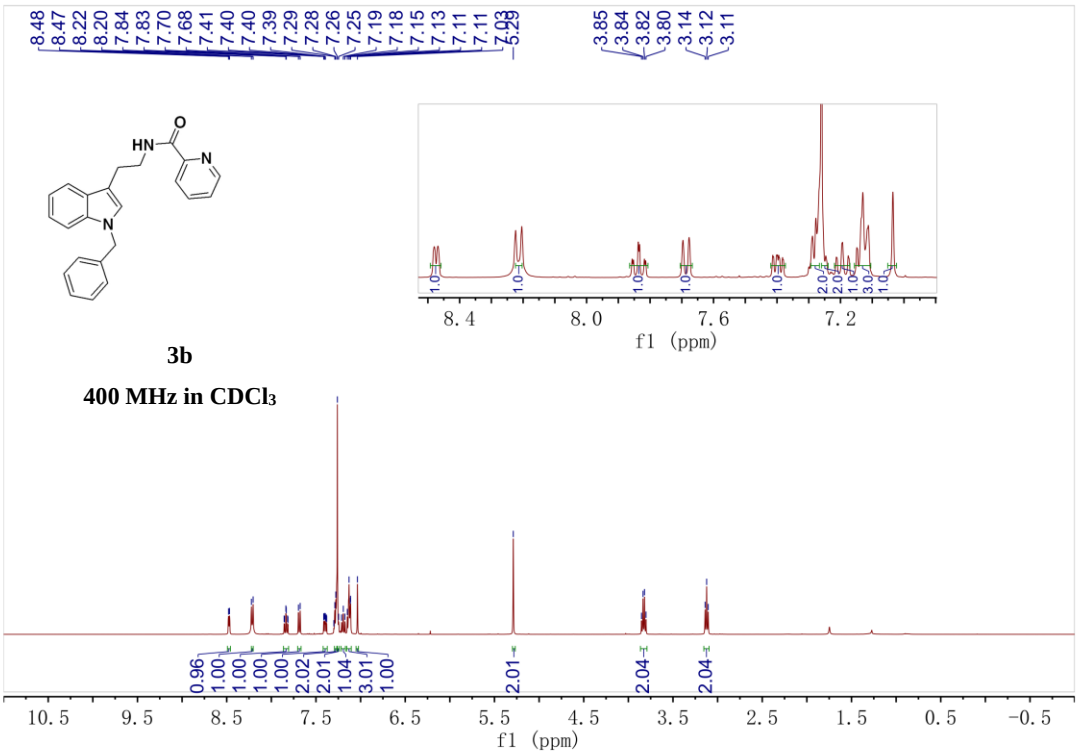
3a

400 MHz in $CDCl_3$



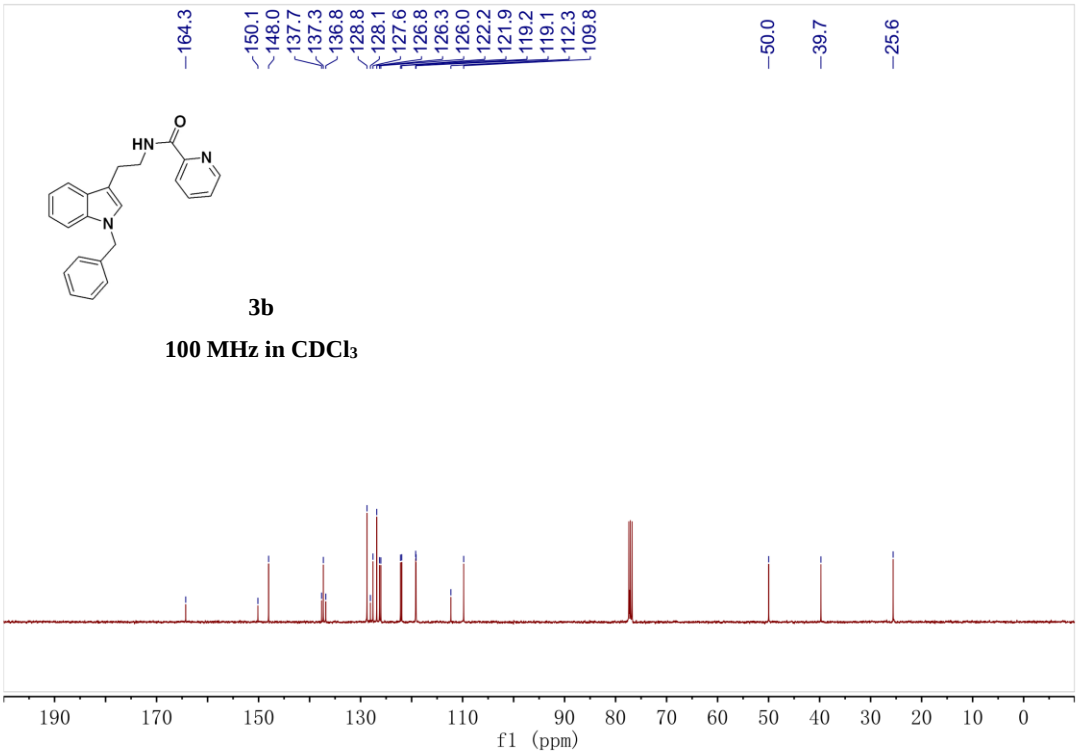
3a

100 MHz in $CDCl_3$



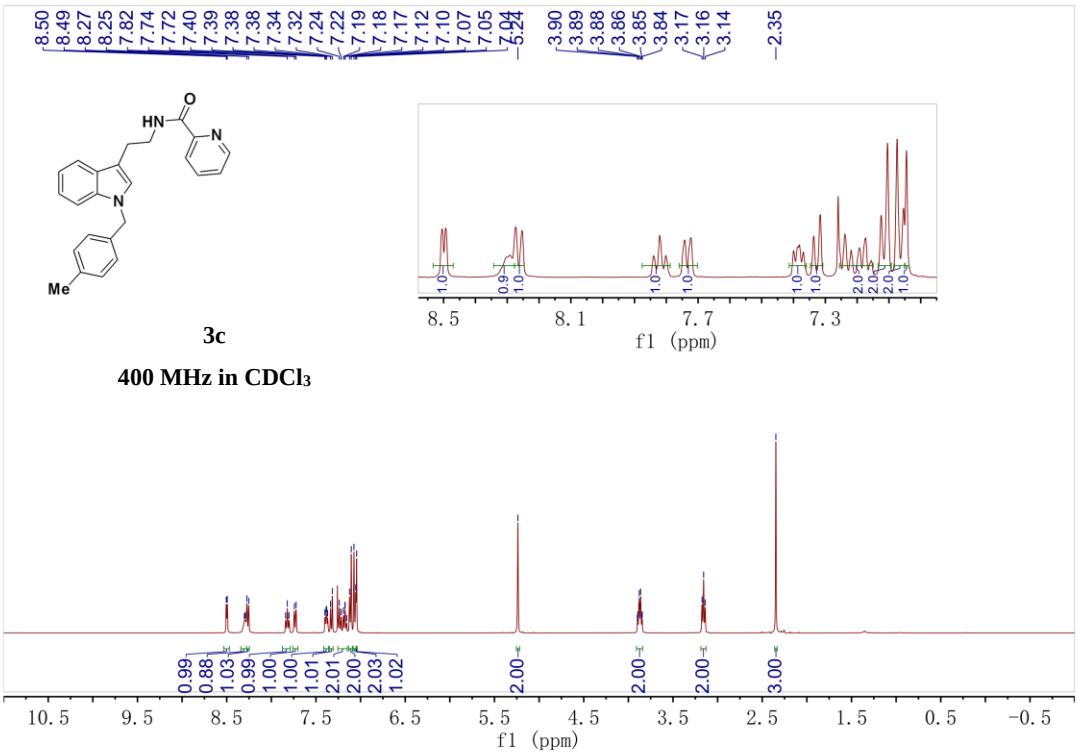
3b

400 MHz in $CDCl_3$



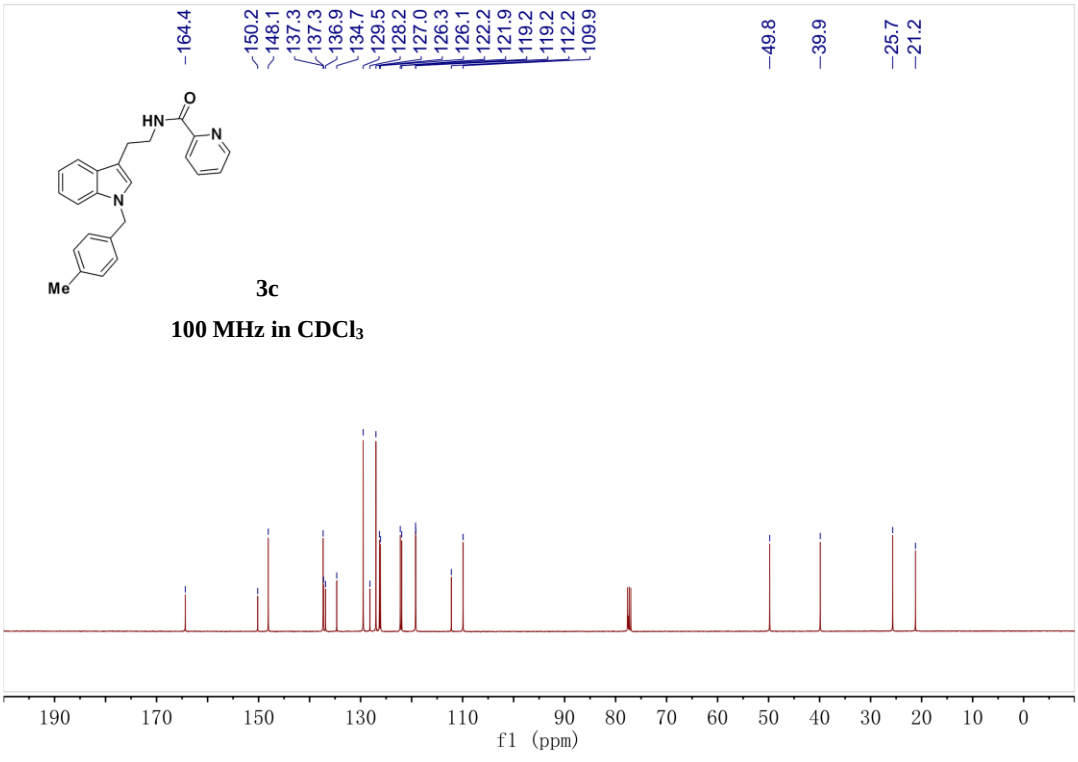
3b

100 MHz in $CDCl_3$



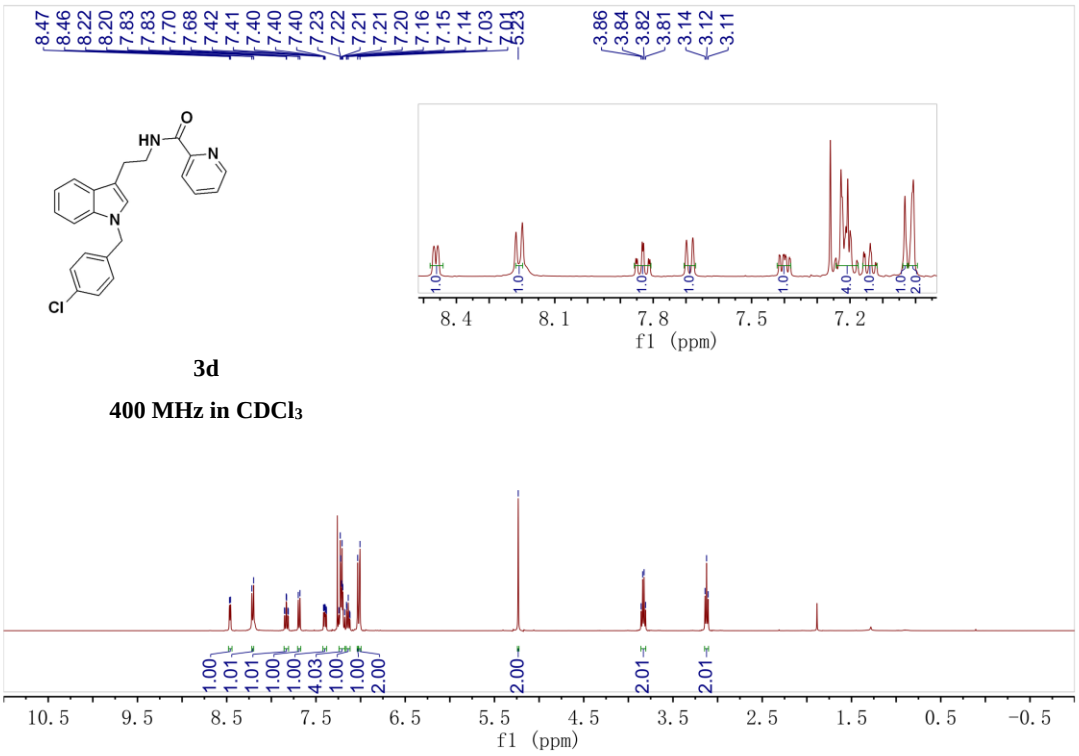
3c

400 MHz in $CDCl_3$



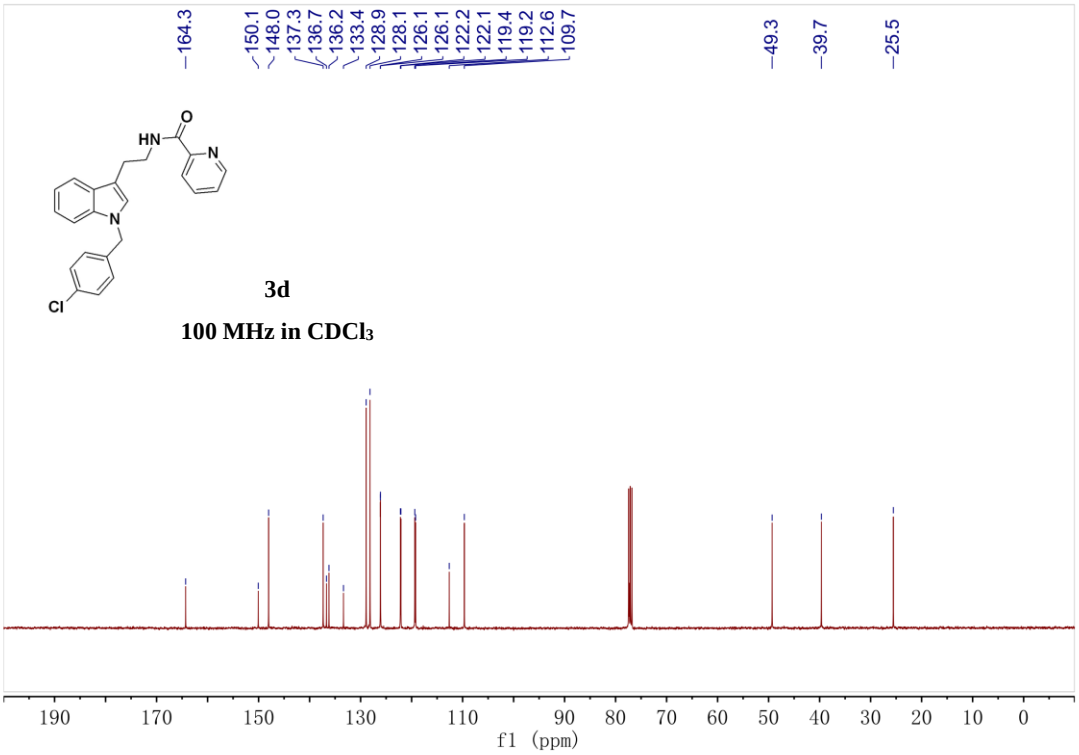
3c

100 MHz in $CDCl_3$



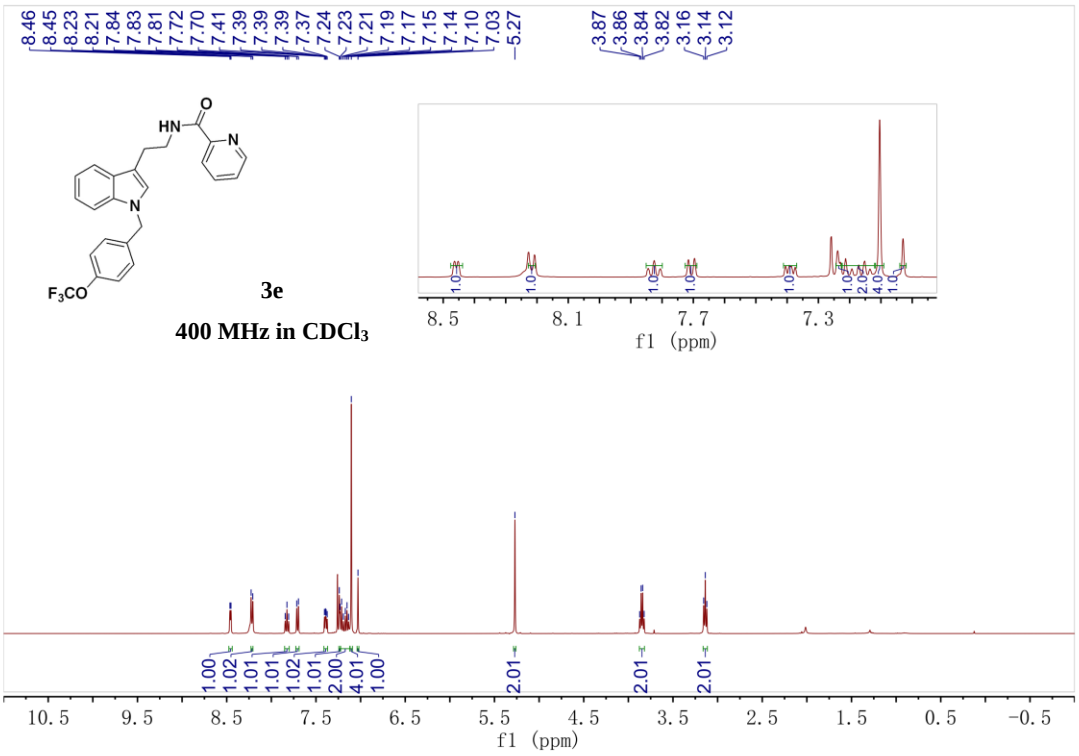
3d

400 MHz in $CDCl_3$



3d

100 MHz in $CDCl_3$


8.46
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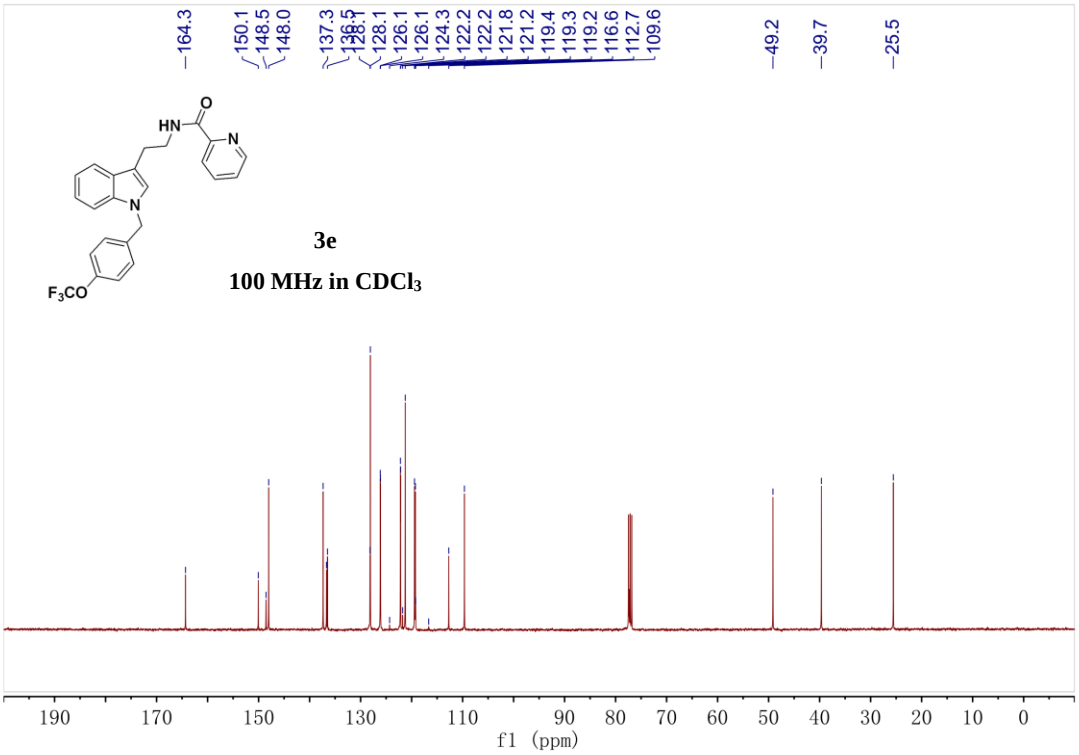
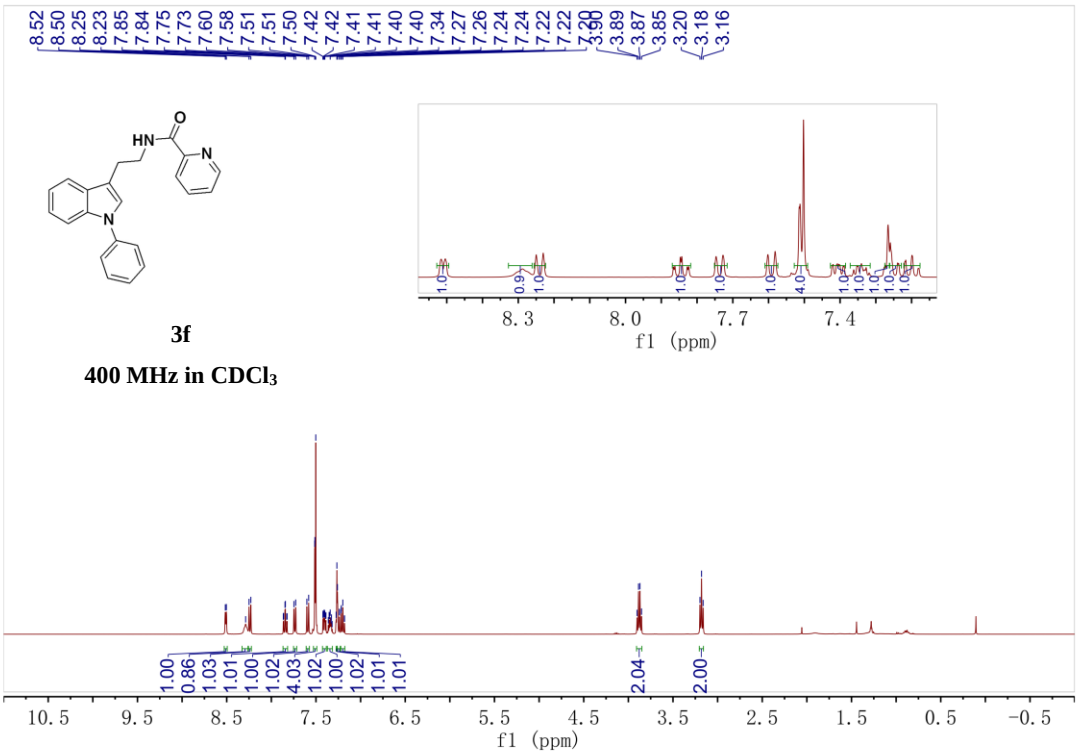
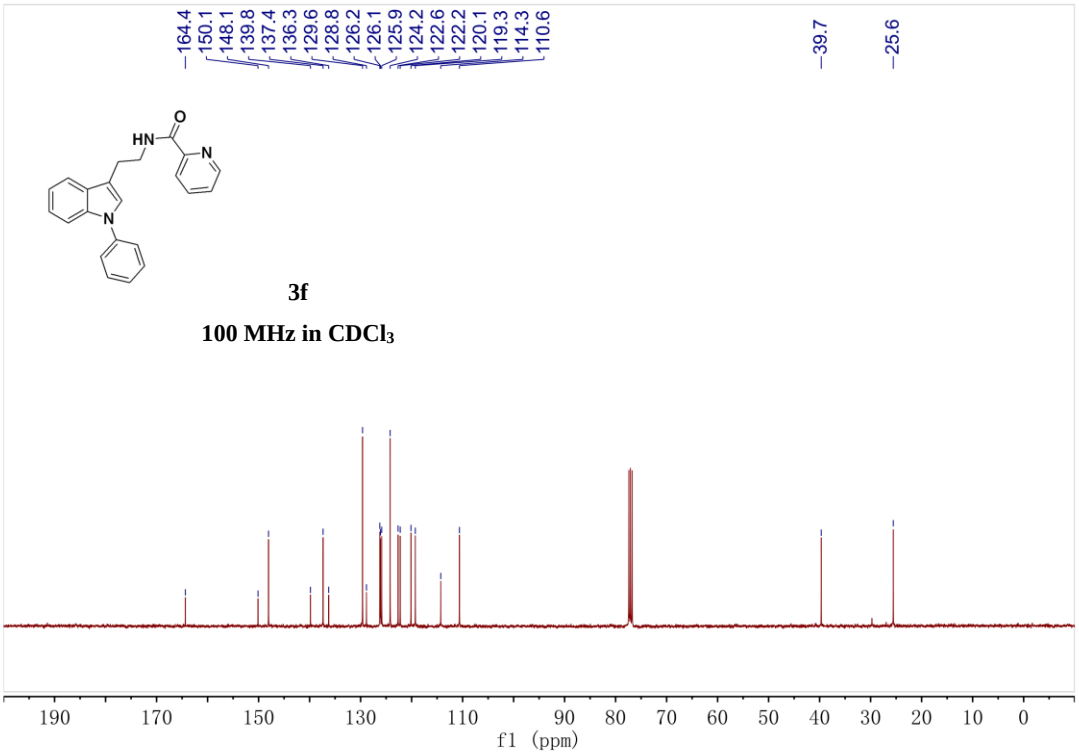
7.83
7.81
7.72
7.70
7.41
7.39
7.39
7.39
7.37
7.24
7.23
7.21
7.19
7.17
7.15
7.14
7.10
7.03
5.27
3.87
3.86
3.84
3.82
3.16
3.14
3.12
HN
O
N
N
F3CO
3e
400 MHz in CDCl3
8.5
8.1
7.7
7.3
f1 (ppm)
1.00
1.02
1.01
1.01
1.02
1.01
2.00
4.01
1.00
2.01
2.01
2.01
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
−0.5
f1 (ppm)


164.3
150.1
148.5
148.0
137.3
136.5
128.1
128.1
126.1
126.1
124.3
122.2
122.2
121.8
121.2
119.4
119.3
119.2
116.6
112.7
109.6
49.2
39.7
25.5
HN
O
N
N
F3CO
3e
100 MHz in CDCl3
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)



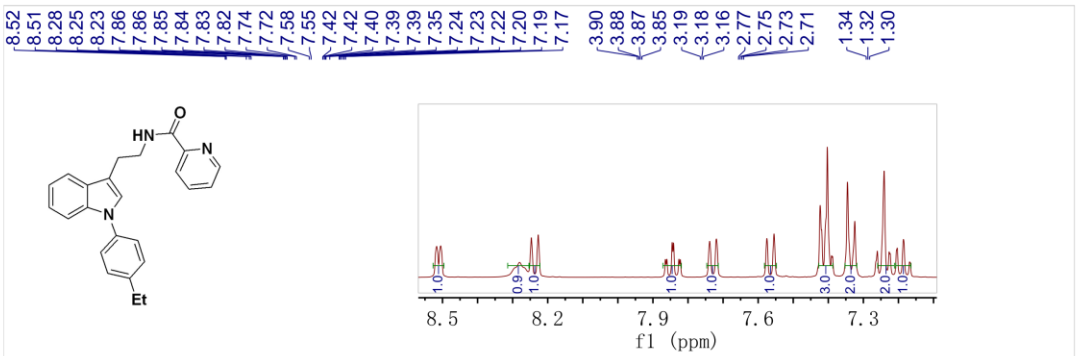
3f

400 MHz in $CDCl_3$



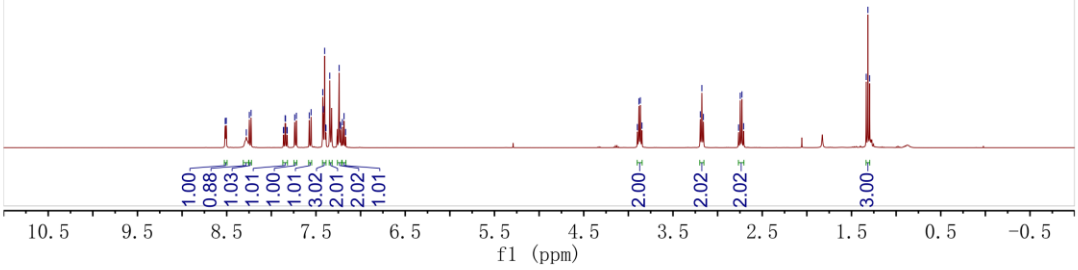
3f

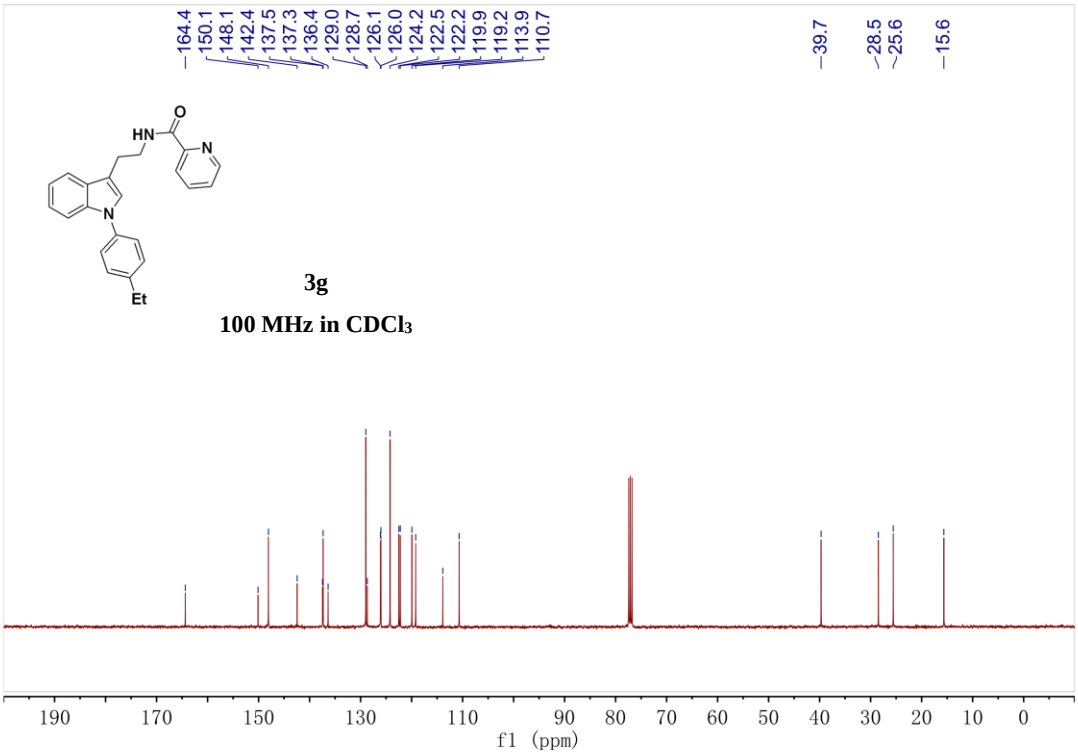
100 MHz in $CDCl_3$



3g

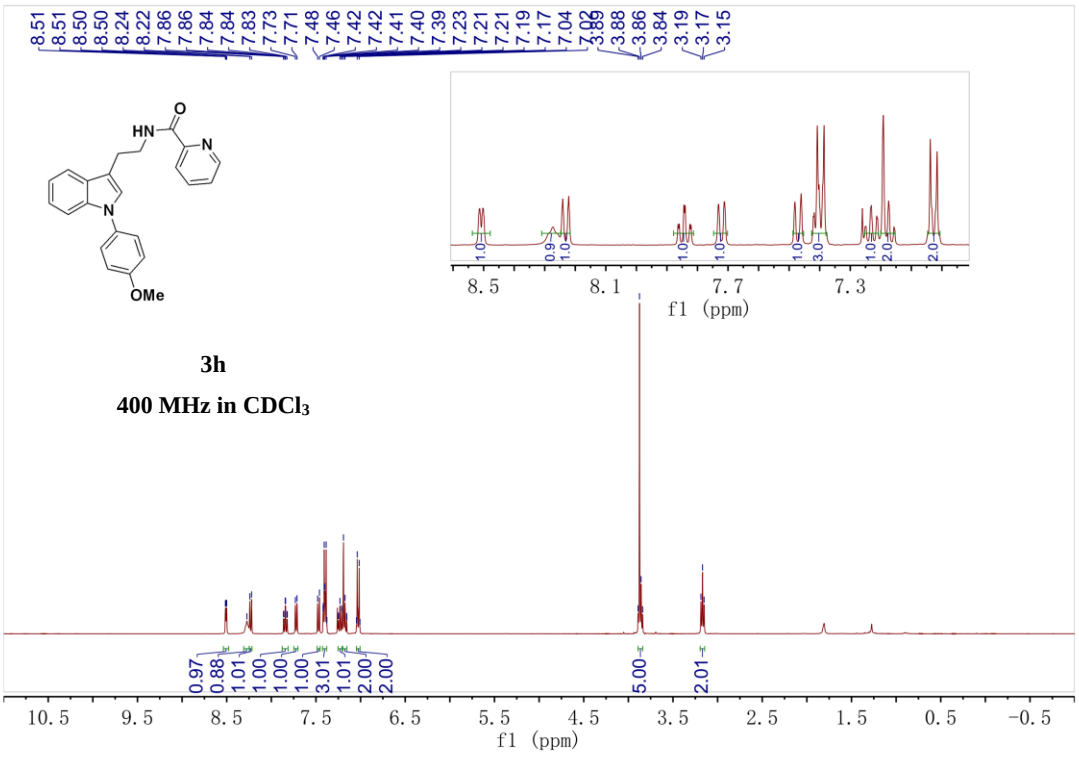
400 MHz in $CDCl_3$





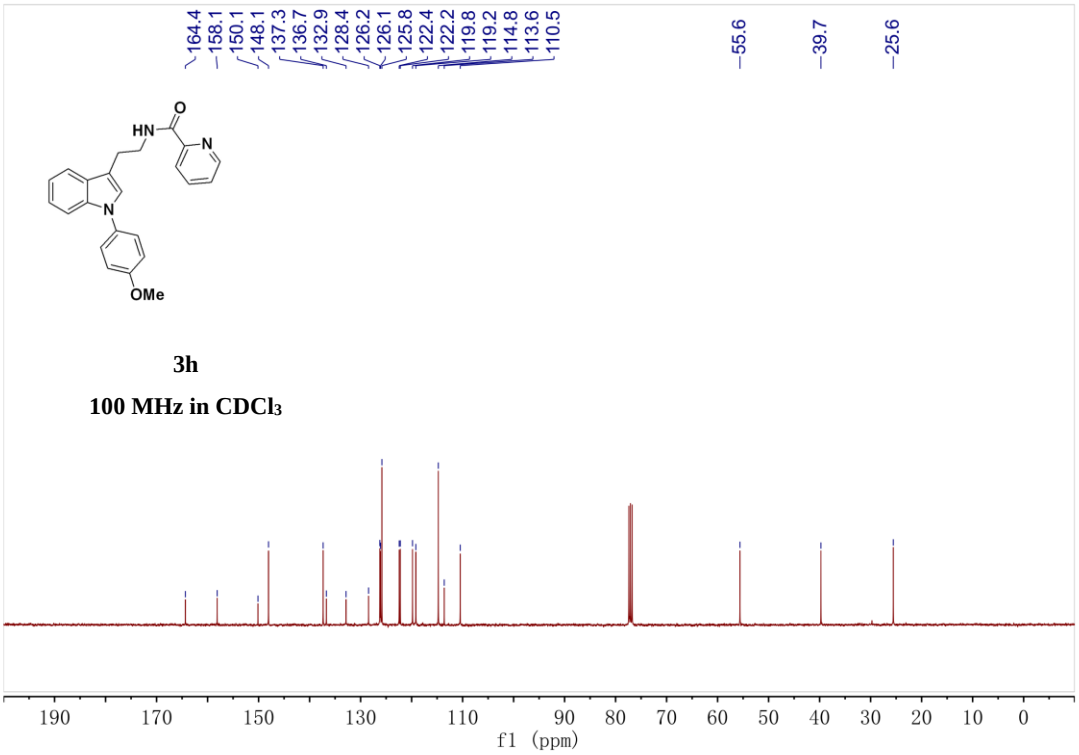
3g

100 MHz in $CDCl_3$



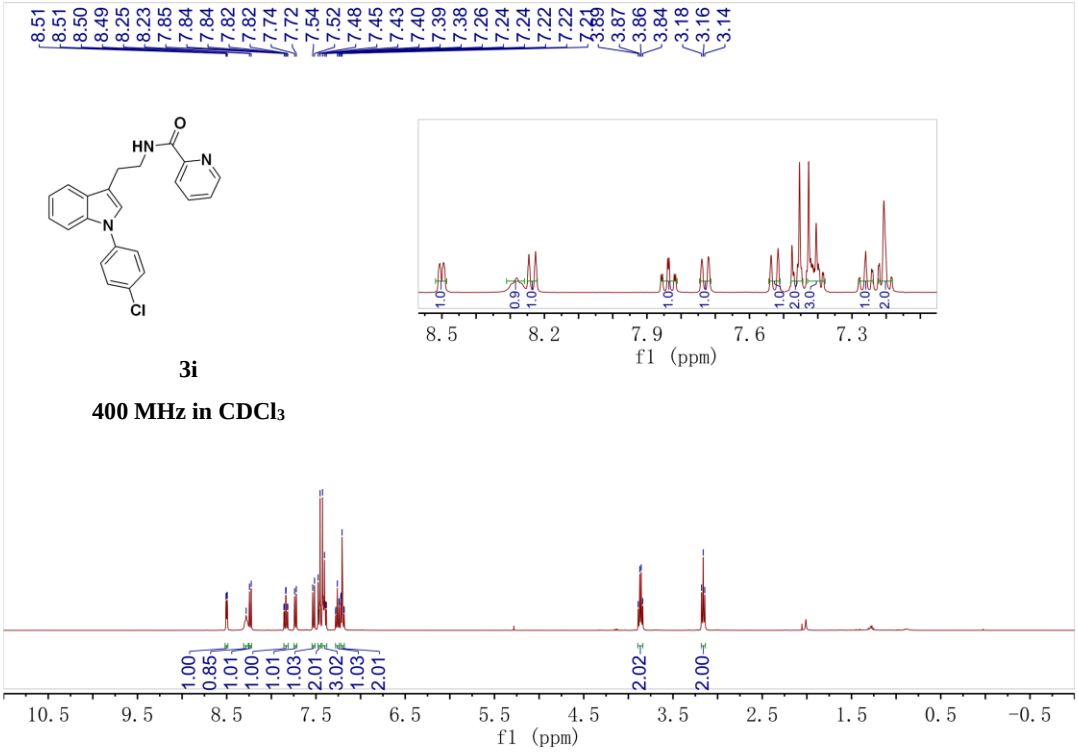
3h

400 MHz in $CDCl_3$



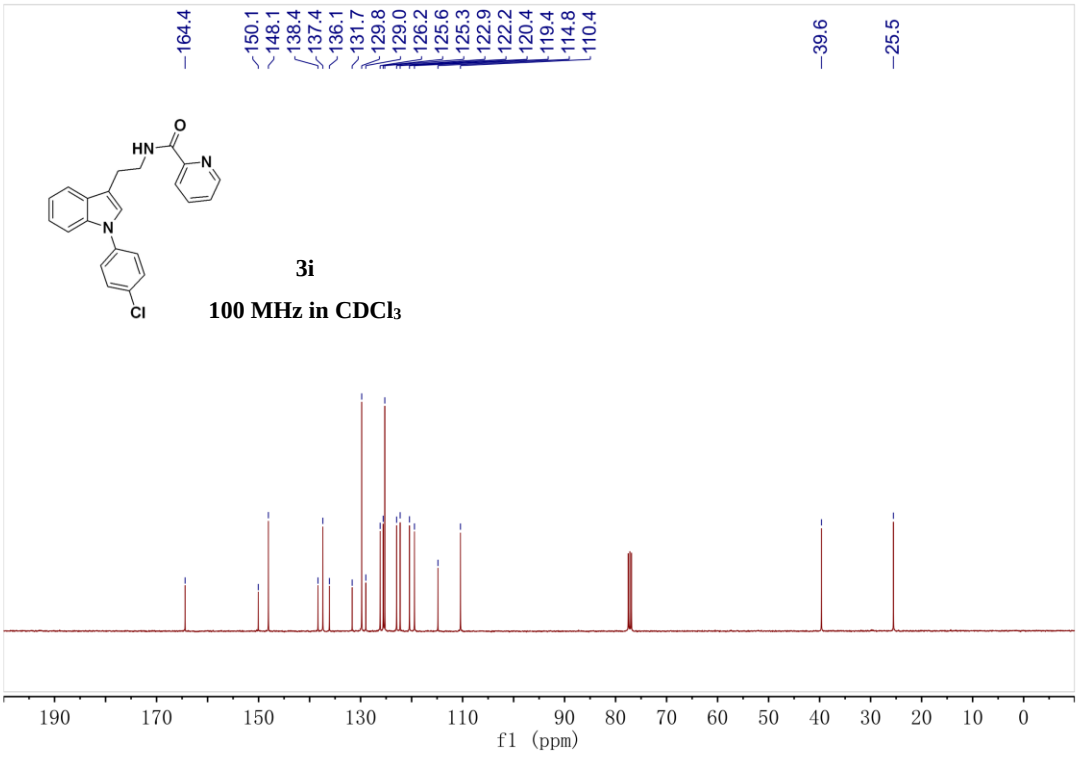
3h

100 MHz in $CDCl_3$



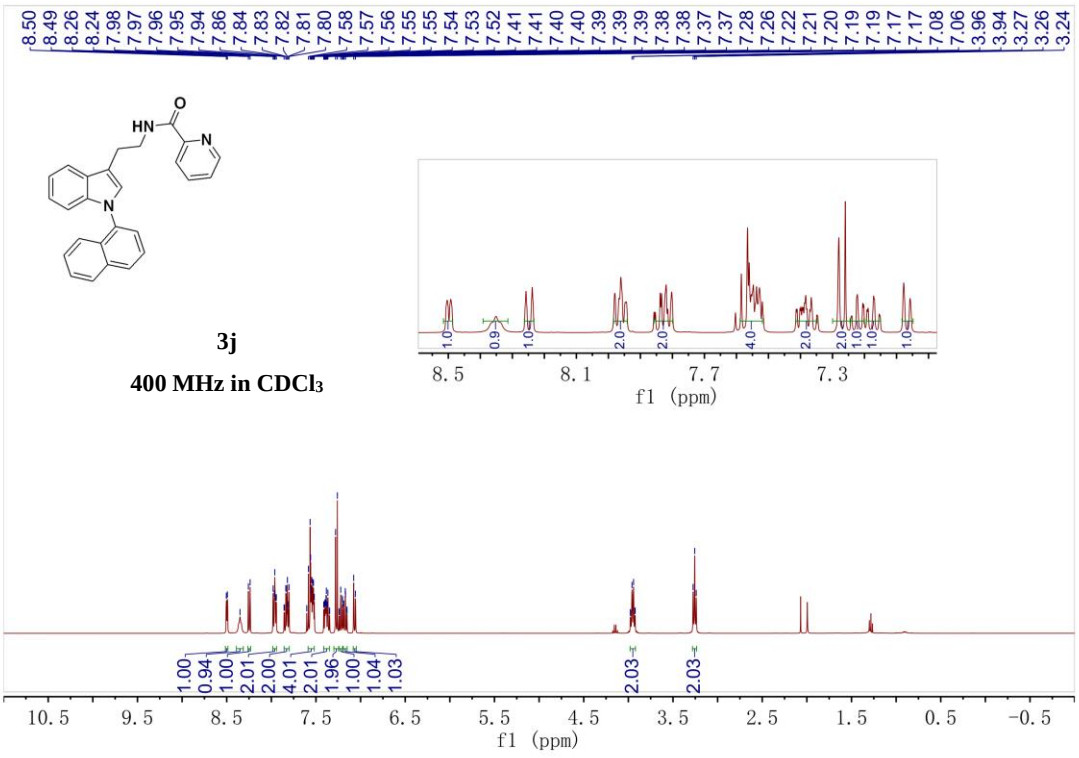
3i

400 MHz in $CDCl_3$



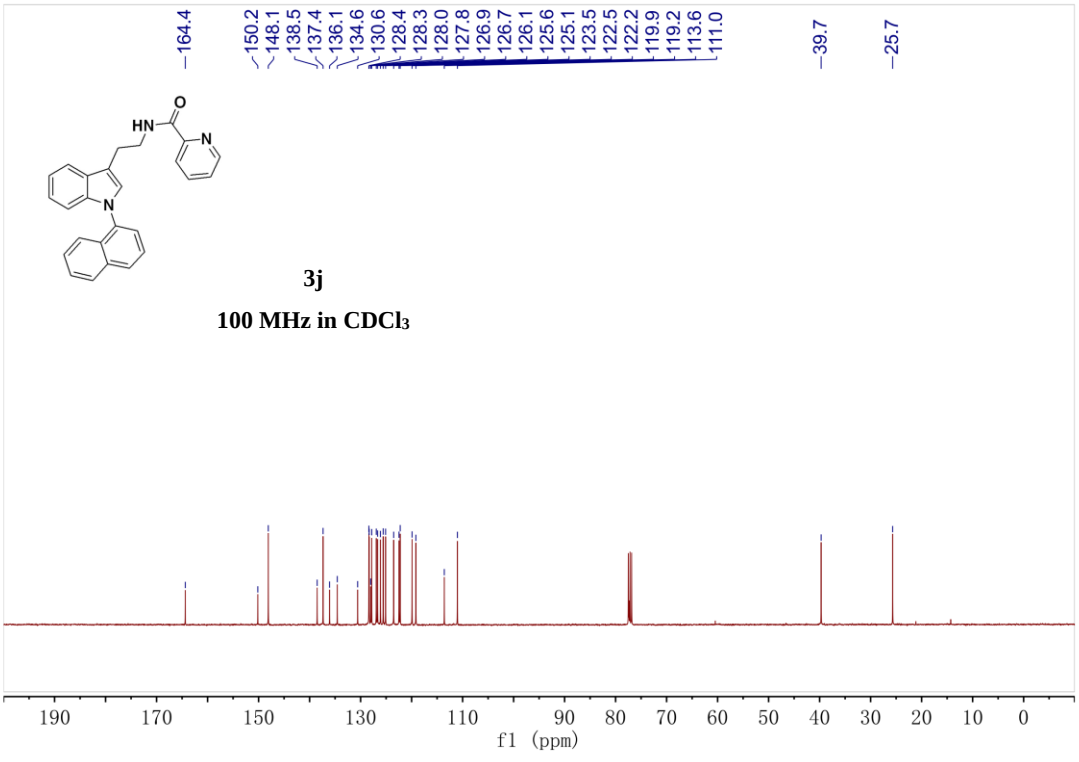
3i

100 MHz in $CDCl_3$



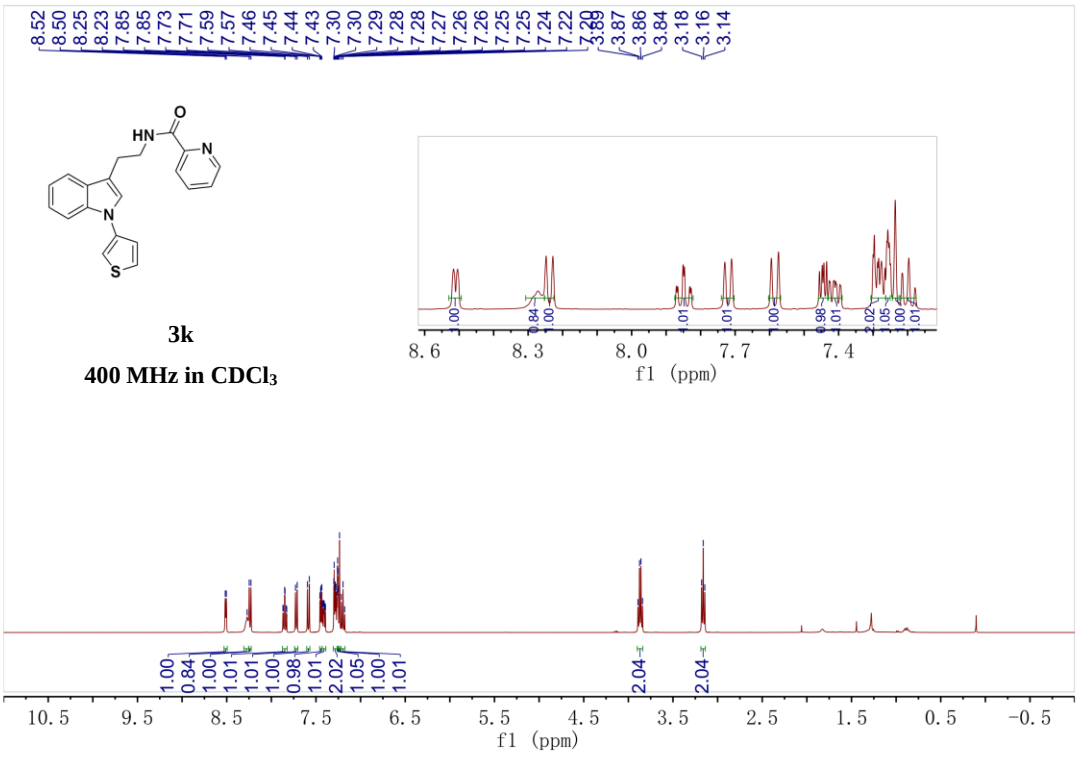
3j

400 MHz in $CDCl_3$



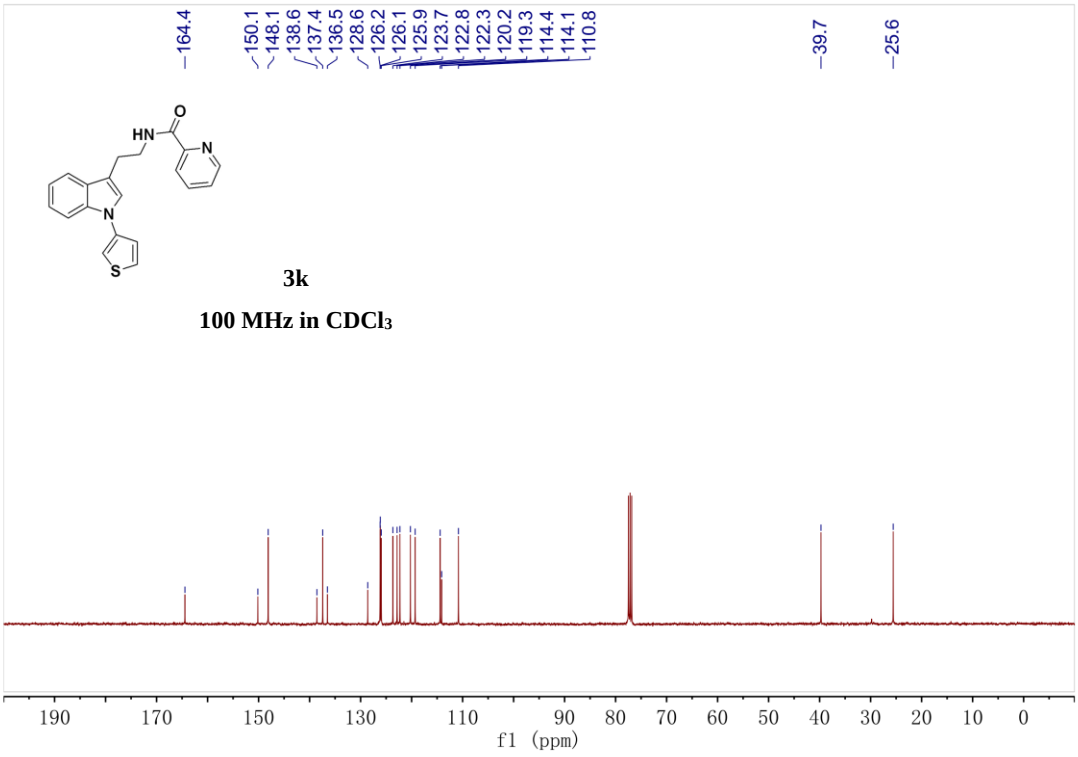
3j

100 MHz in $CDCl_3$



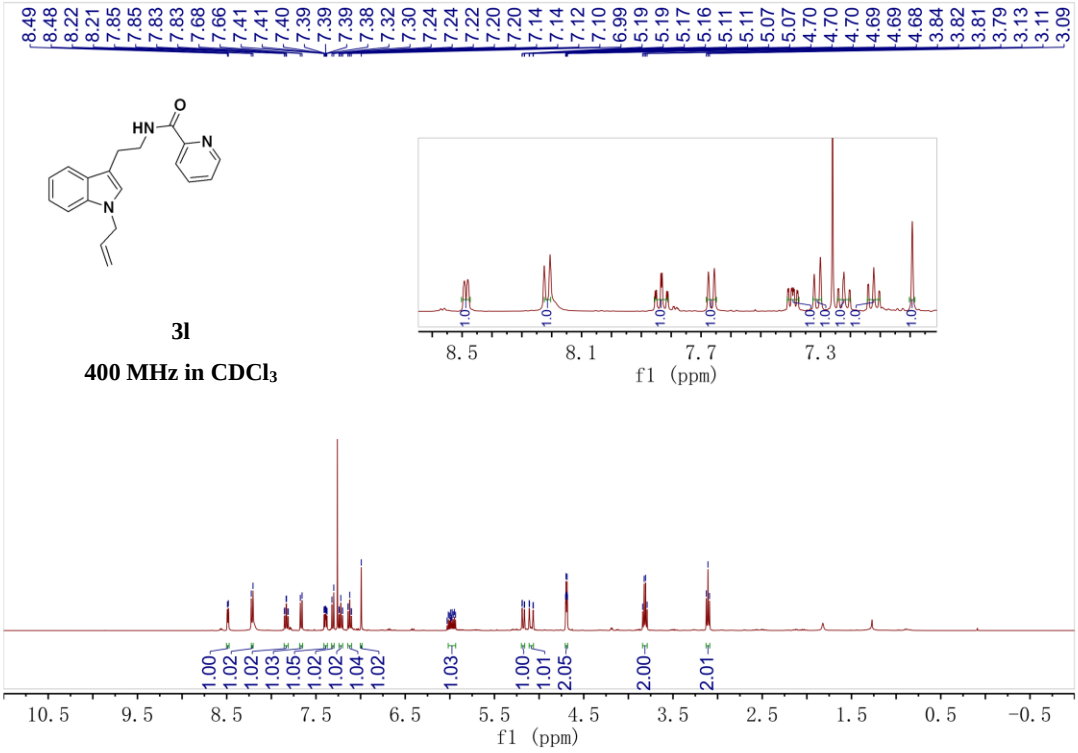
3k

400 MHz in $CDCl_3$



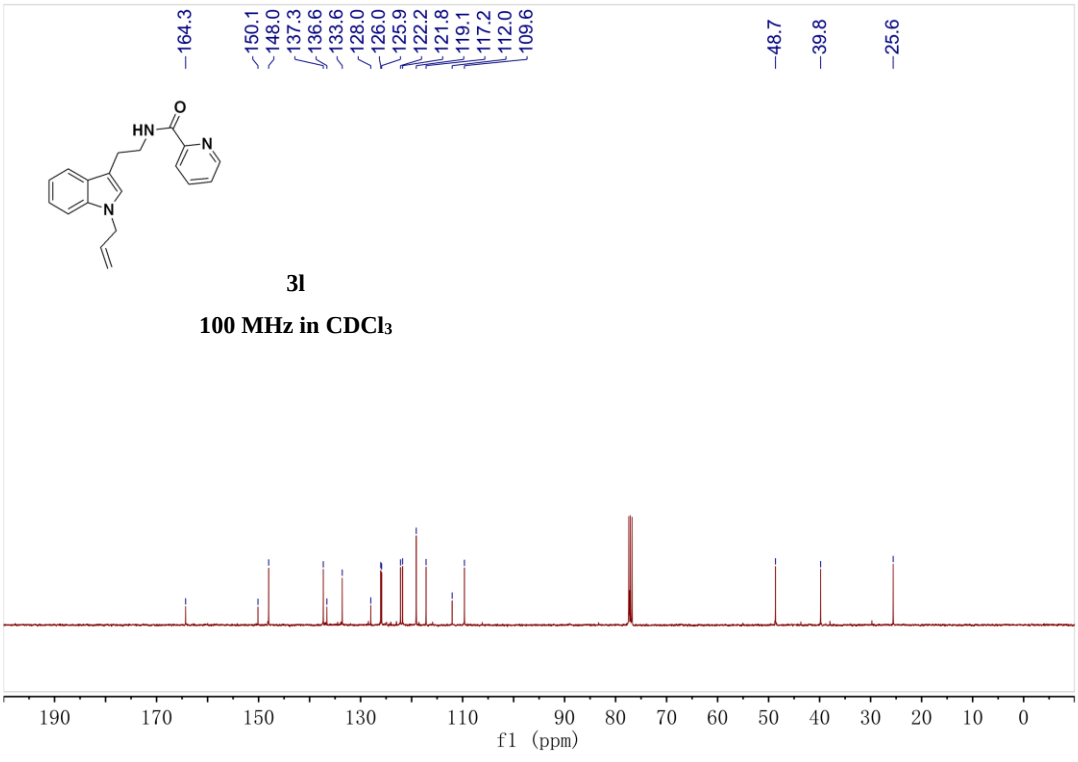
3k

100 MHz in $CDCl_3$



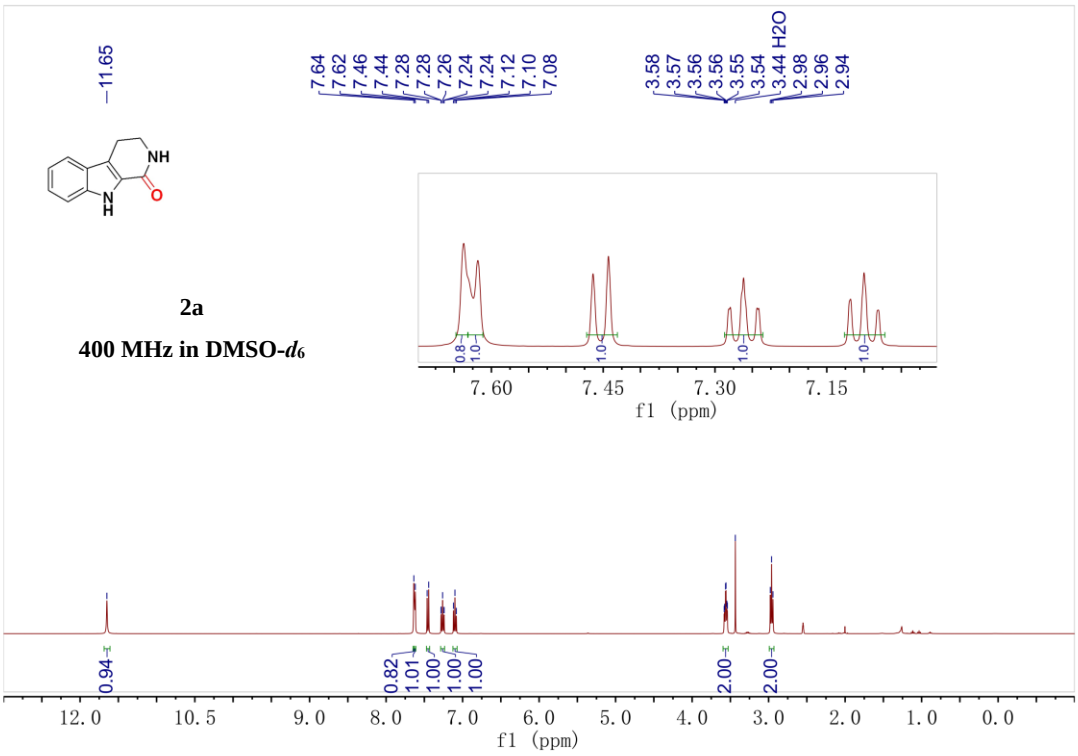
3l

400 MHz in $CDCl_3$



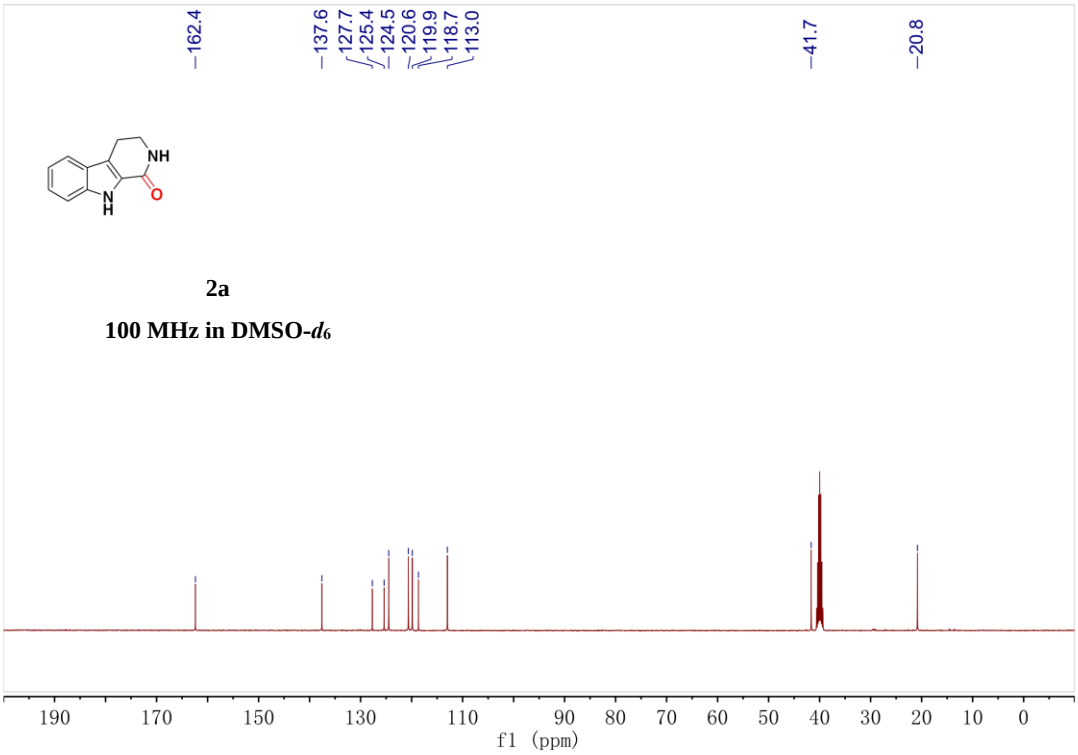
3l

100 MHz in $CDCl_3$



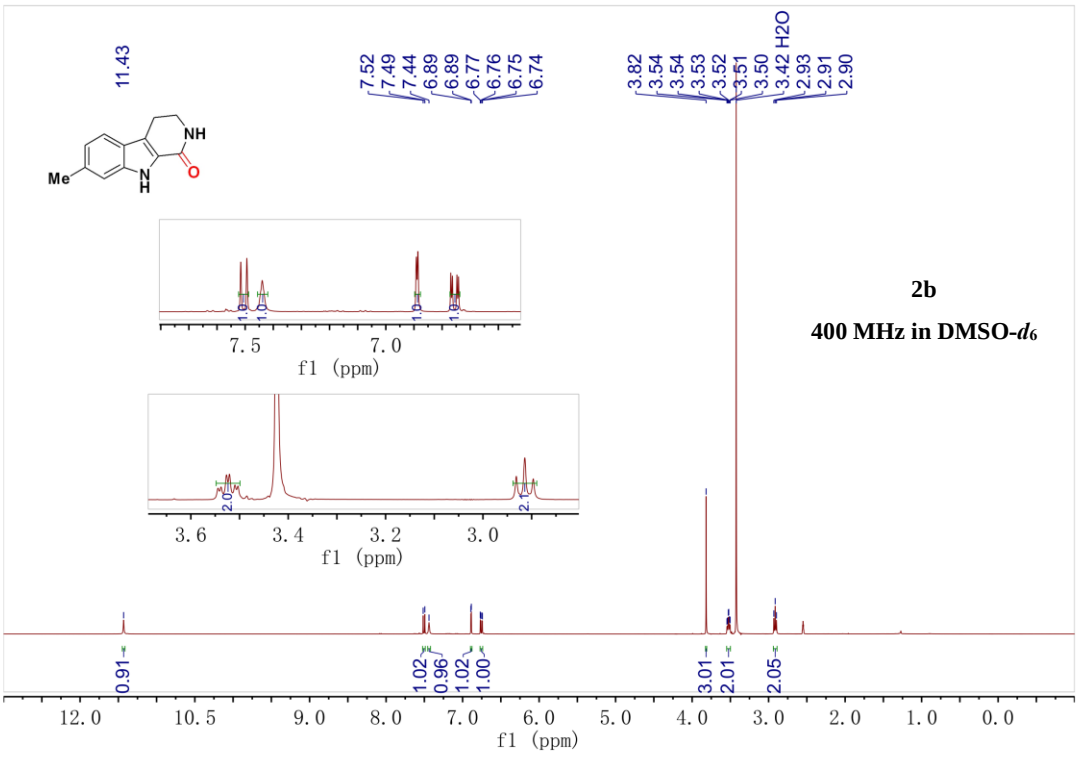
2a

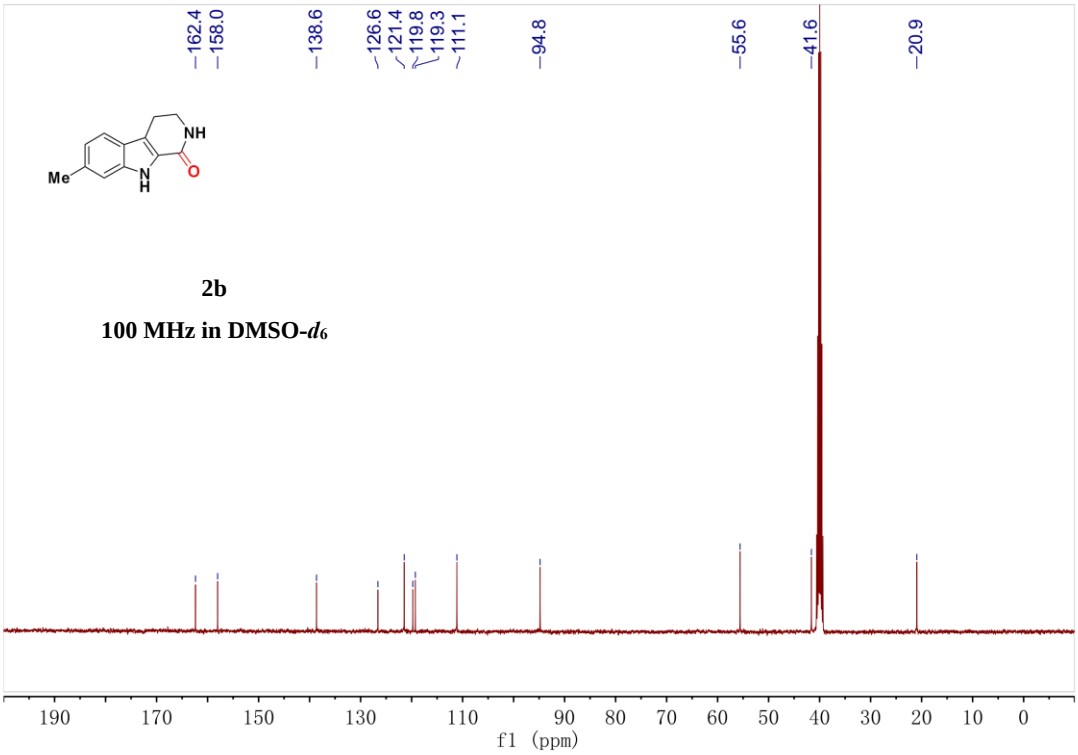
400 MHz in DMSO-*d*$_6$

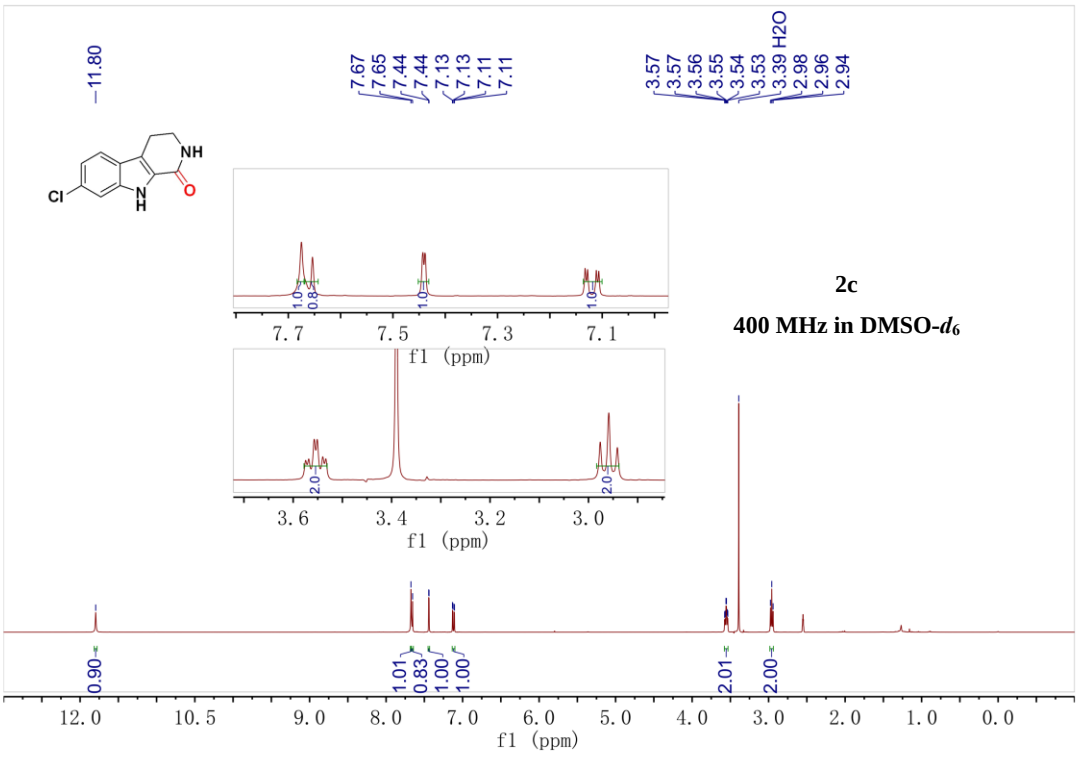


2a

100 MHz in DMSO-*d*$_6$

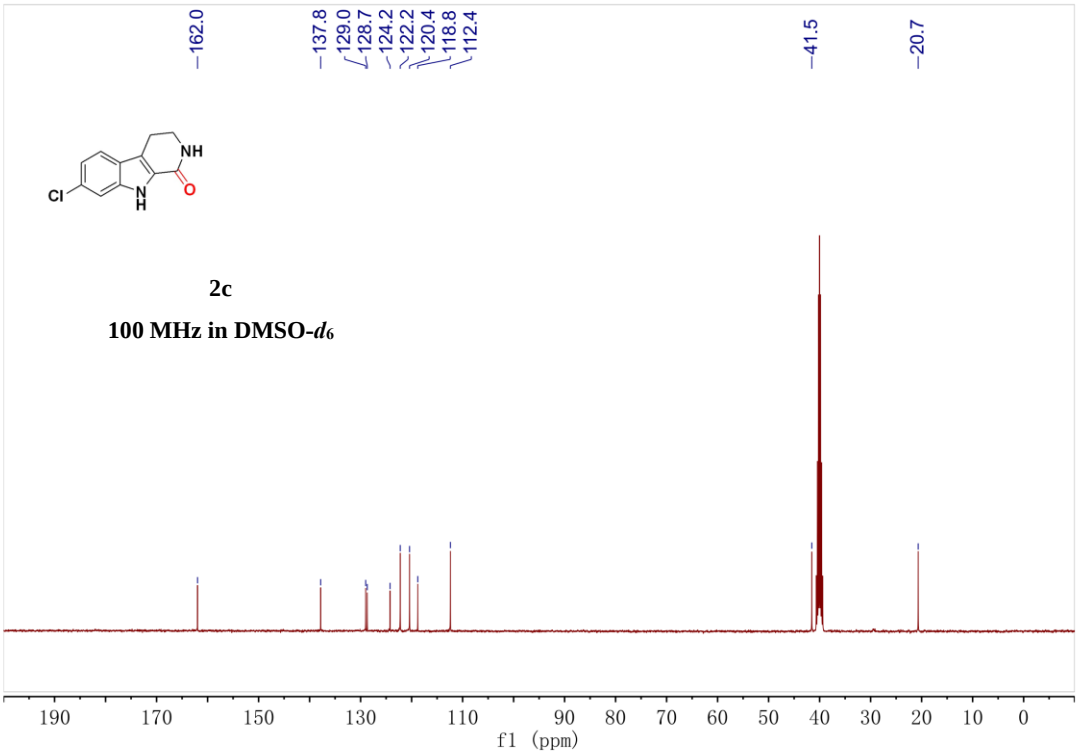

11.43
7.52
7.49
7.44
6.89
6.89
6.77
6.76
6.75
6.74
3.82
3.54
3.54
3.53
3.52
3.51
3.50
3.42 H2O
2.93
2.91
2.90
NH
Me
N
H
O
7.5
7.0
f1 (ppm)
3.6
3.4
3.2
3.0
f1 (ppm)
2b
400 MHz in DMSO-d6
0.91
1.02
0.96
1.02
1.00
3.01
2.01
2.05
12.0
10.5
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)


162.4
158.0
138.6
126.6
121.4
119.8
119.3
111.1
94.8
55.6
41.6
20.9
NH
Me
N
H
O
2b
100 MHz in DMSO-d6
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)



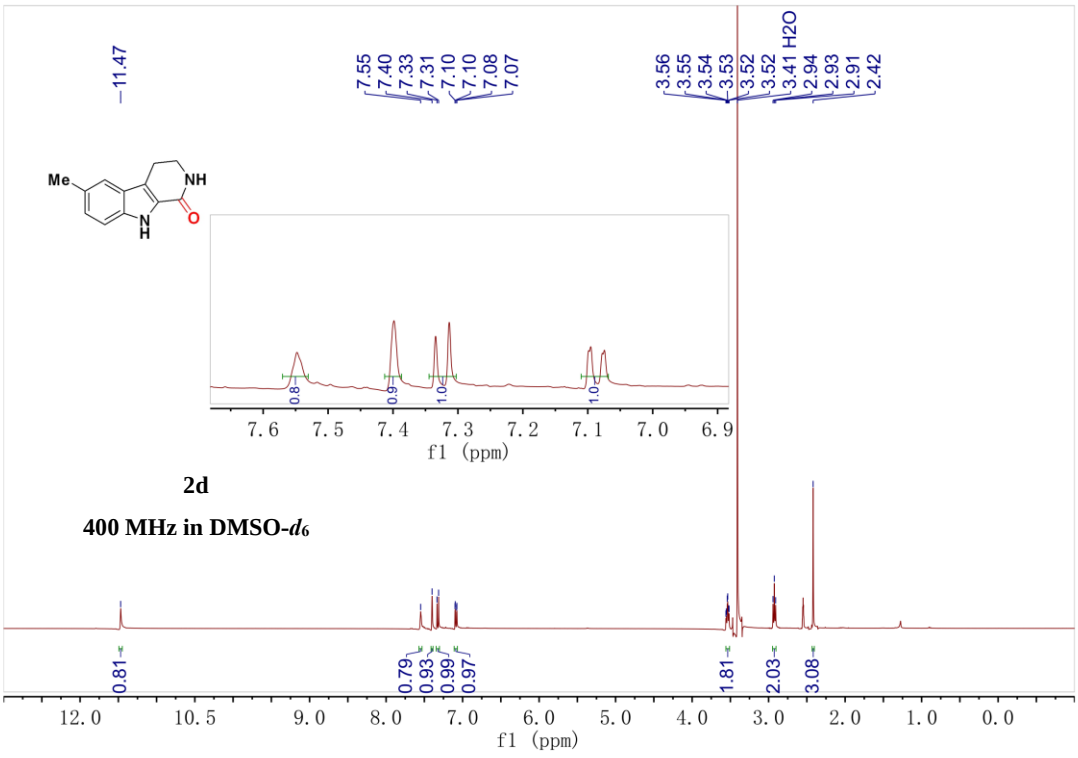
2c

400 MHz in DMSO-d_6



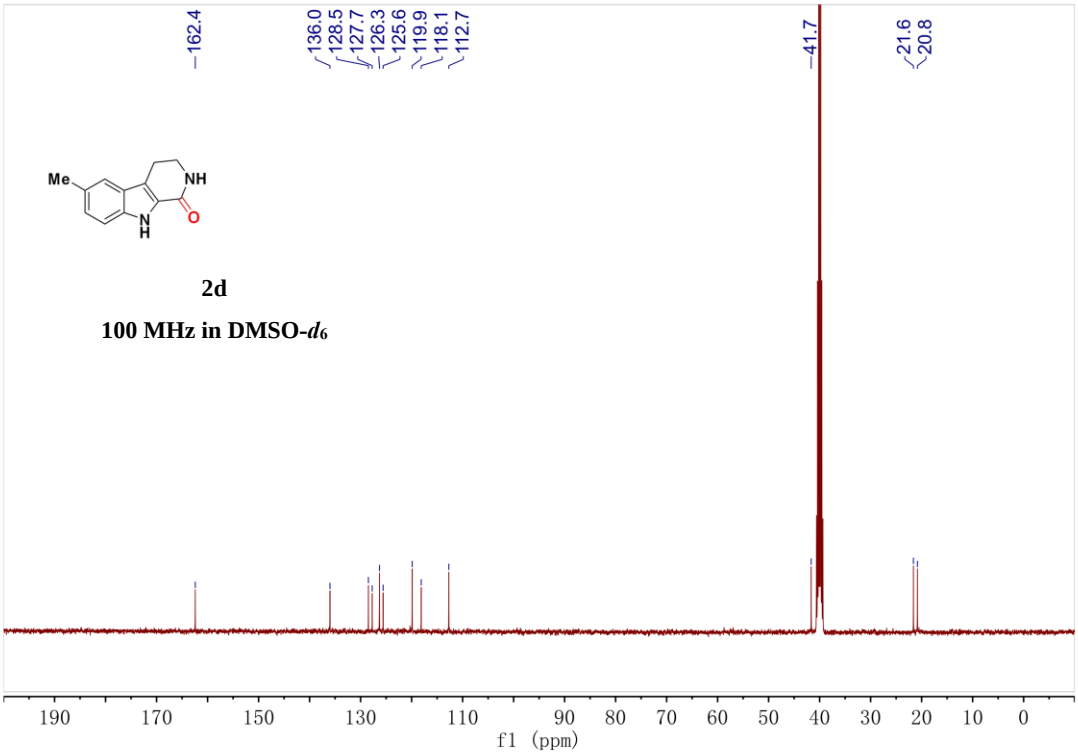
2c

100 MHz in DMSO-d_6



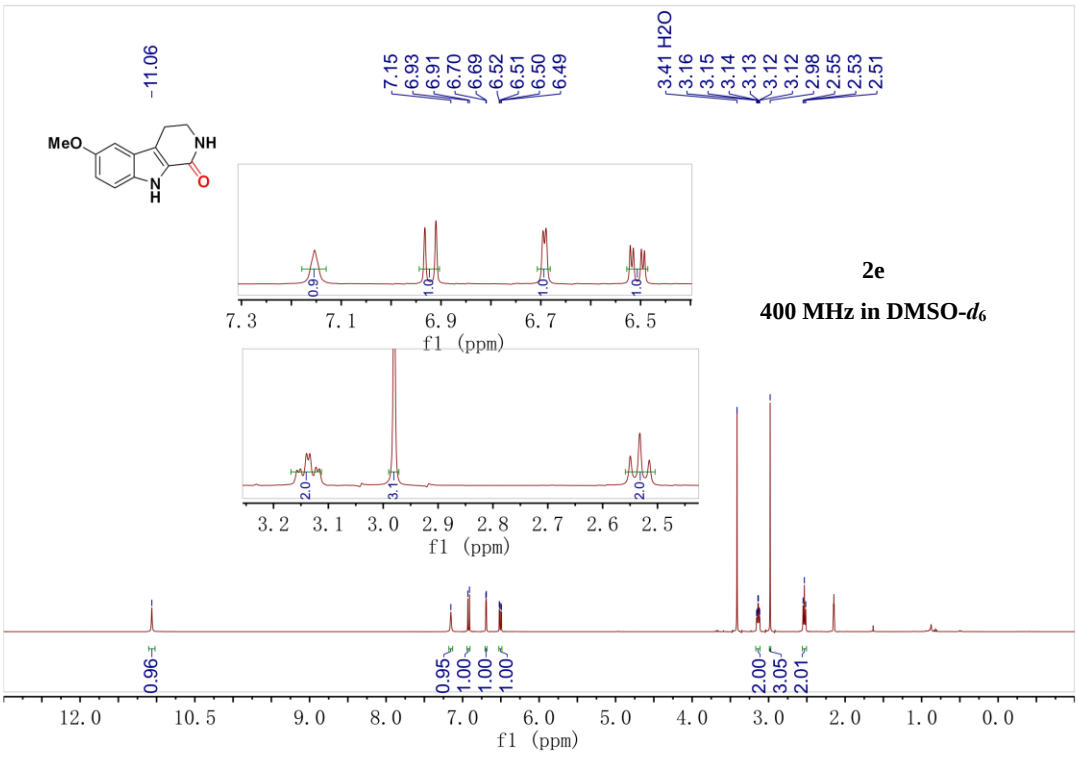
2d

400 MHz in DMSO-*d*$_6$



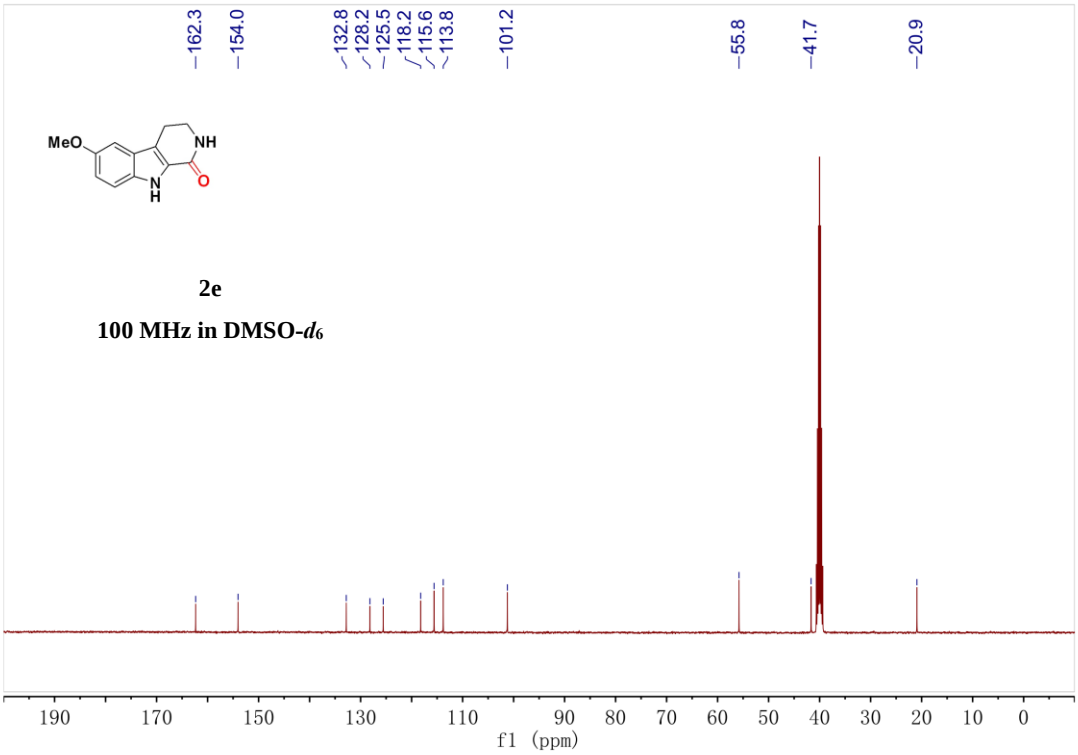
2d

100 MHz in DMSO-*d*$_6$



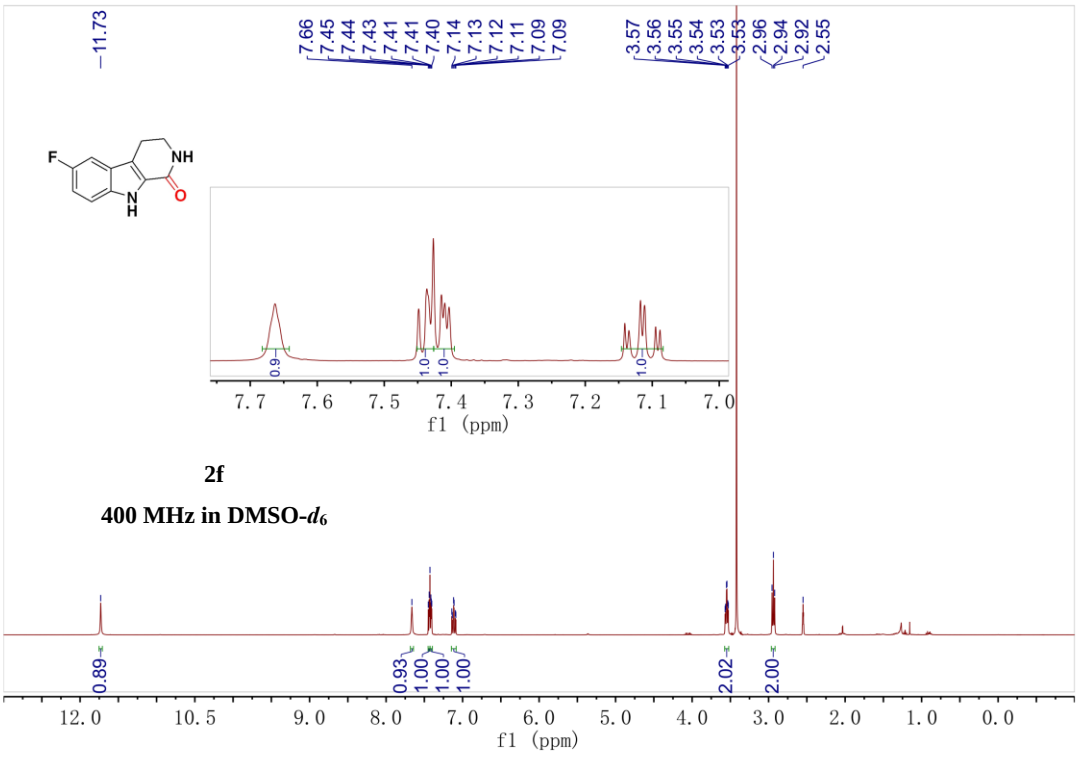
2e

400 MHz in DMSO-*d*$_6$



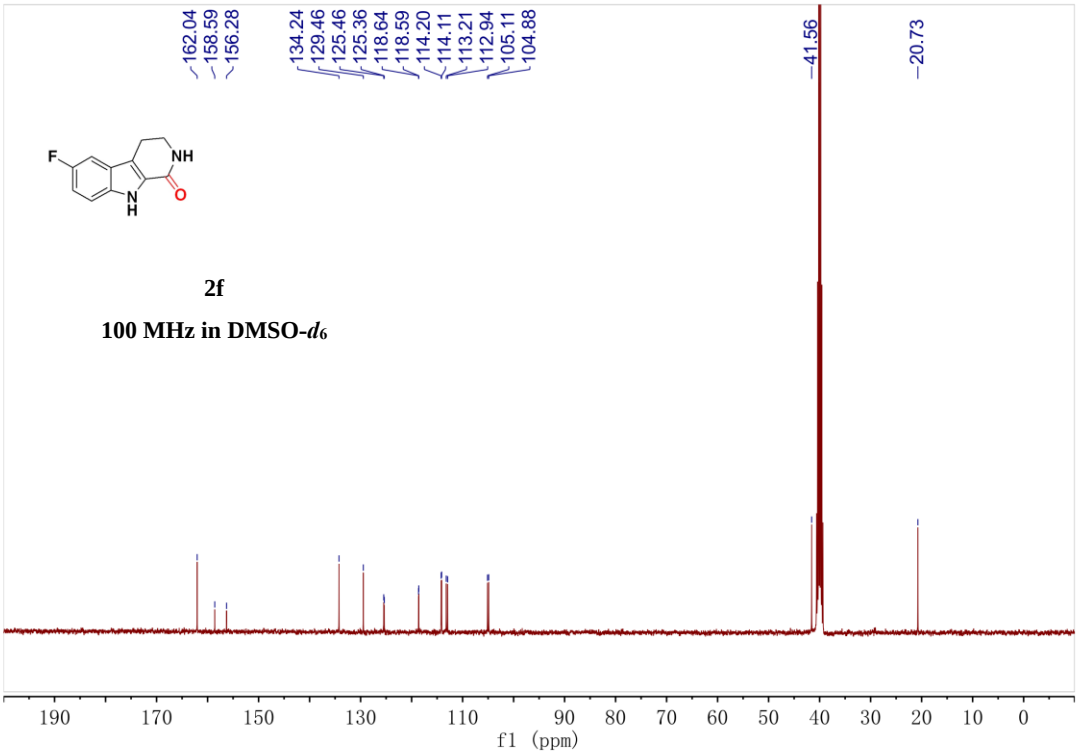
2e

100 MHz in DMSO-*d*$_6$



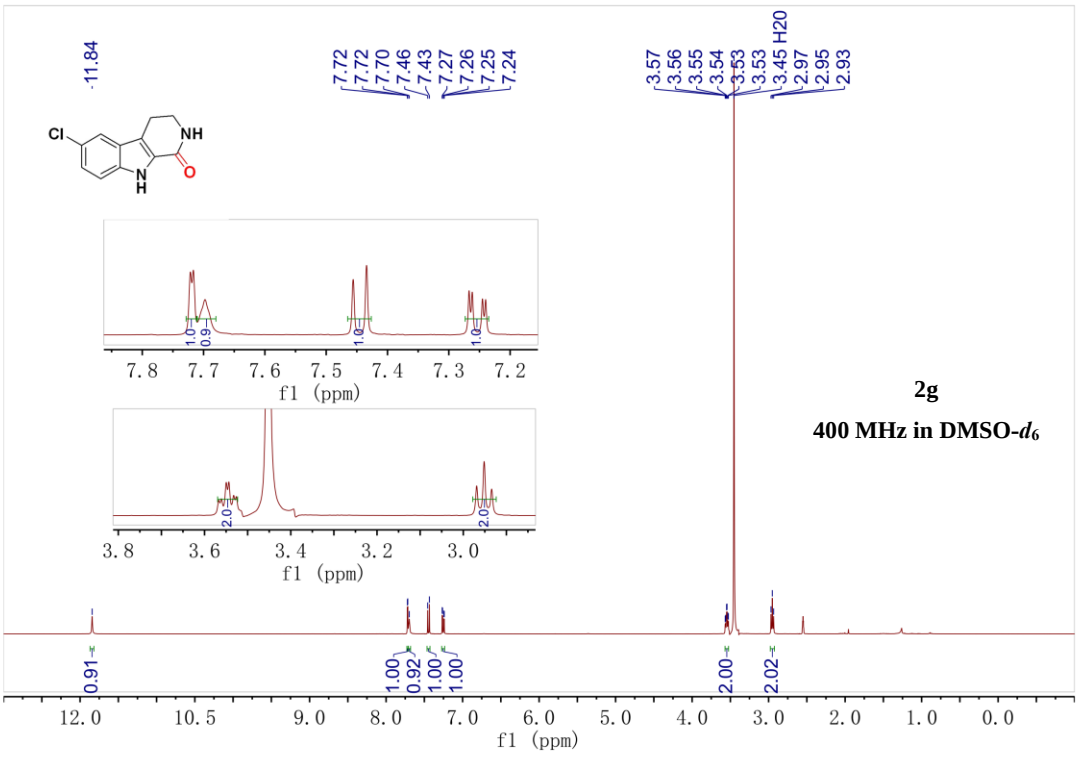
2f

400 MHz in DMSO-d_6



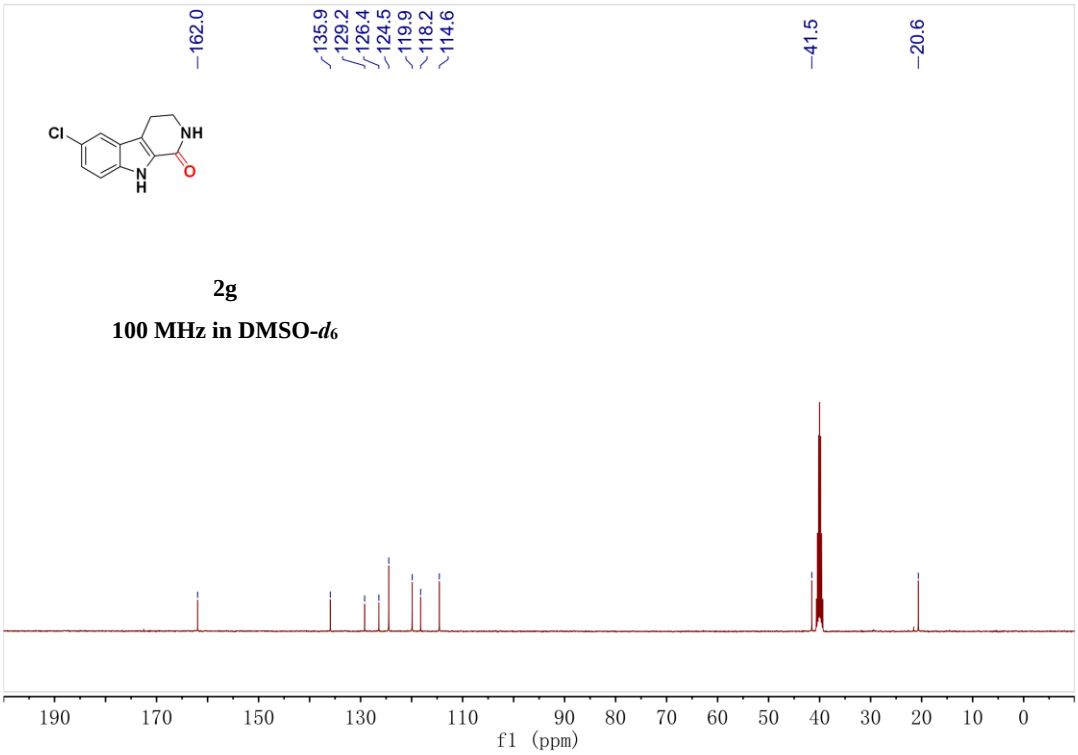
2f

100 MHz in DMSO-d_6



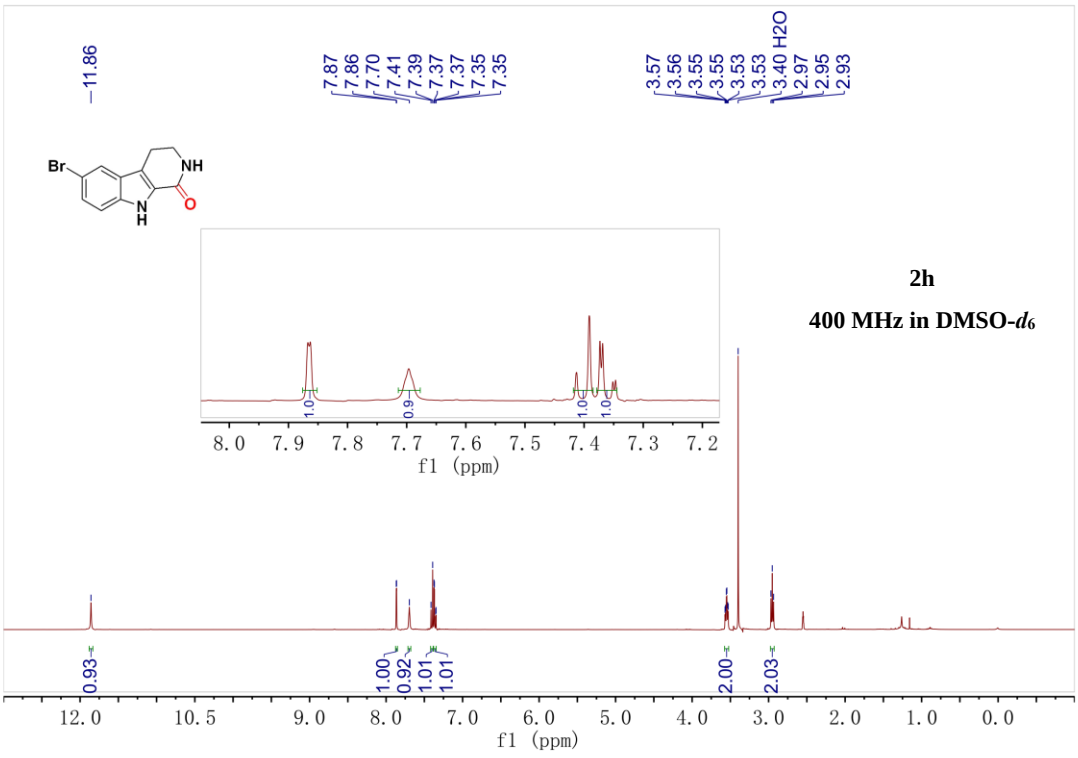
2g

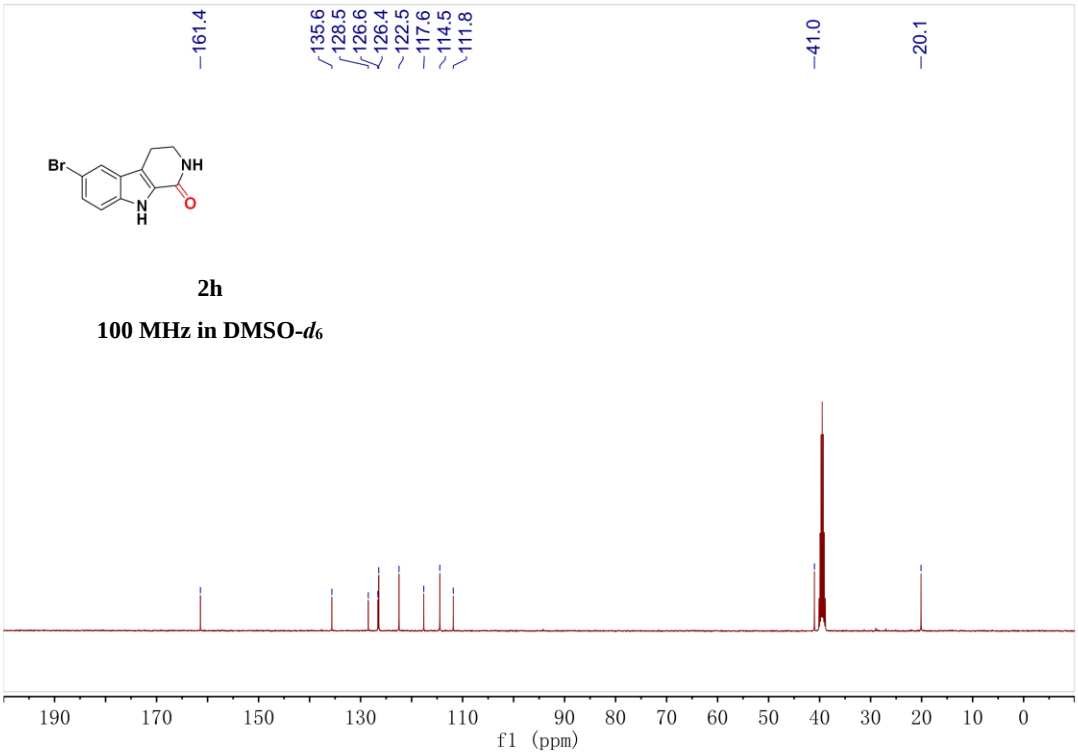
400 MHz in DMSO-d_6

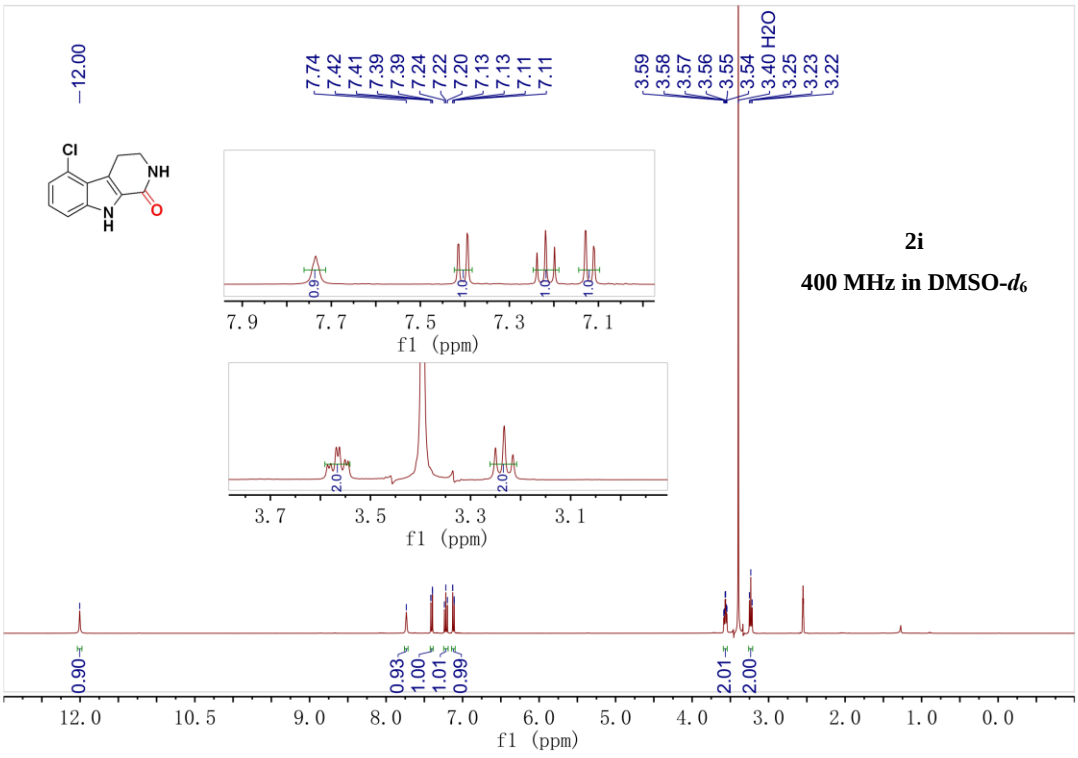


2g

100 MHz in DMSO-d_6

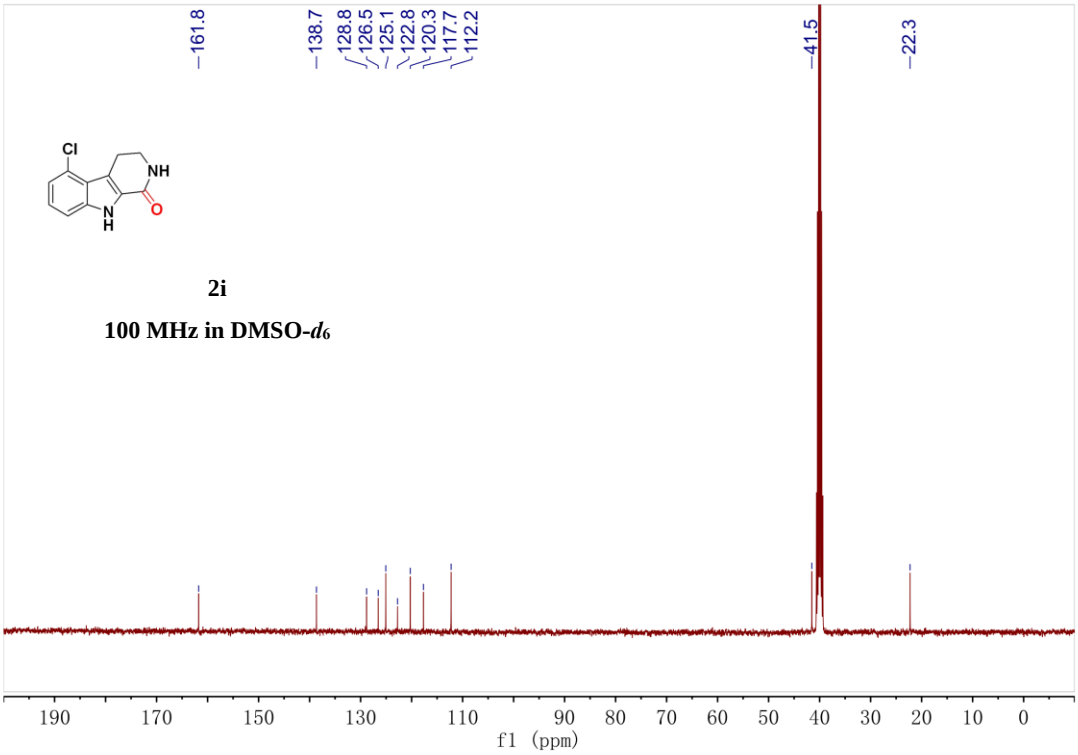

11.86
7.87
7.86
7.70
7.41
7.39
7.37
7.37
7.35
7.35
3.57
3.56
3.55
3.55
3.53
3.53
3.40 H2O
2.97
2.95
2.93
Br
NH
N
H
O
2h
400 MHz in DMSO-d6
f1 (ppm)
0.93
1.00
0.92
1.01
1.01
2.00
2.03


161.4
135.6
128.5
126.6
126.4
122.5
117.6
114.5
111.8
41.0
20.1
Br
NH
N
H
O
2h
100 MHz in DMSO-d6
f1 (ppm)



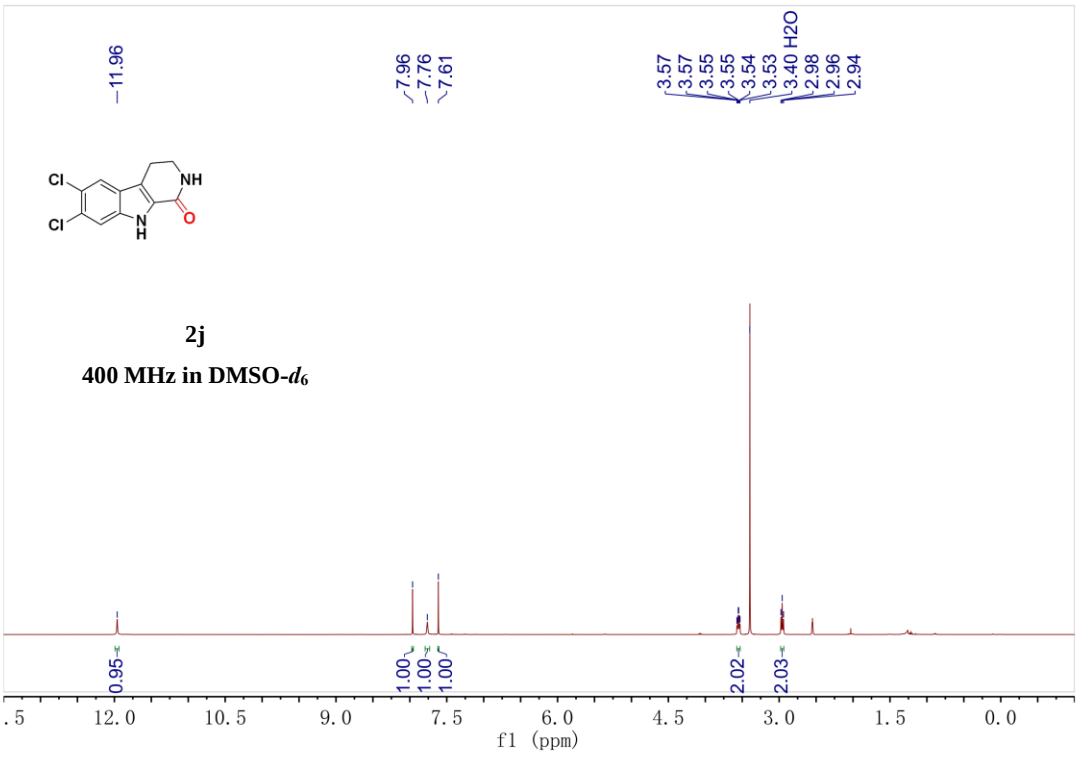
2i

400 MHz in DMSO-d_6



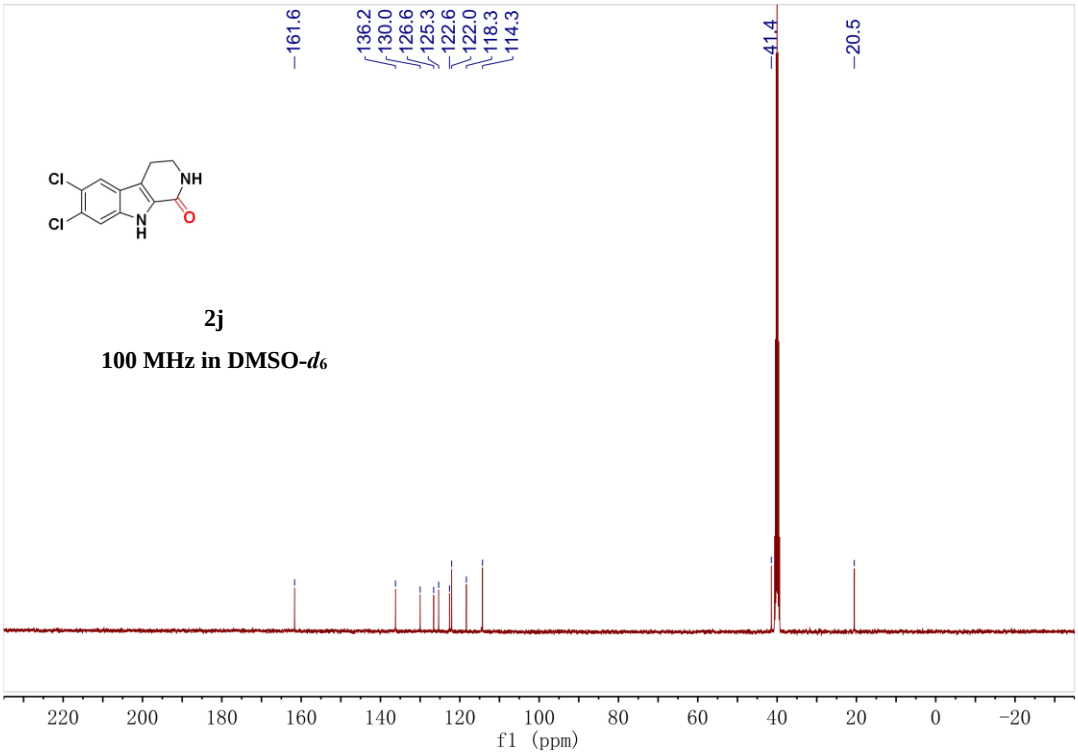
2i

100 MHz in DMSO-d_6



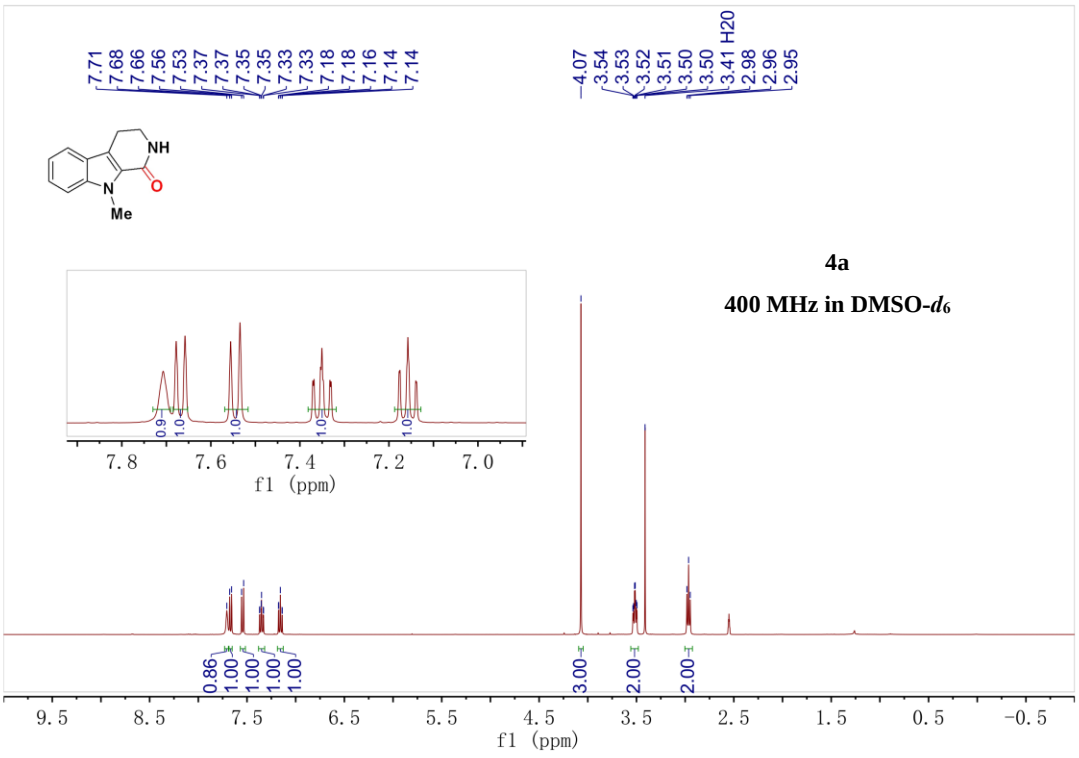
2j

400 MHz in DMSO-d_6



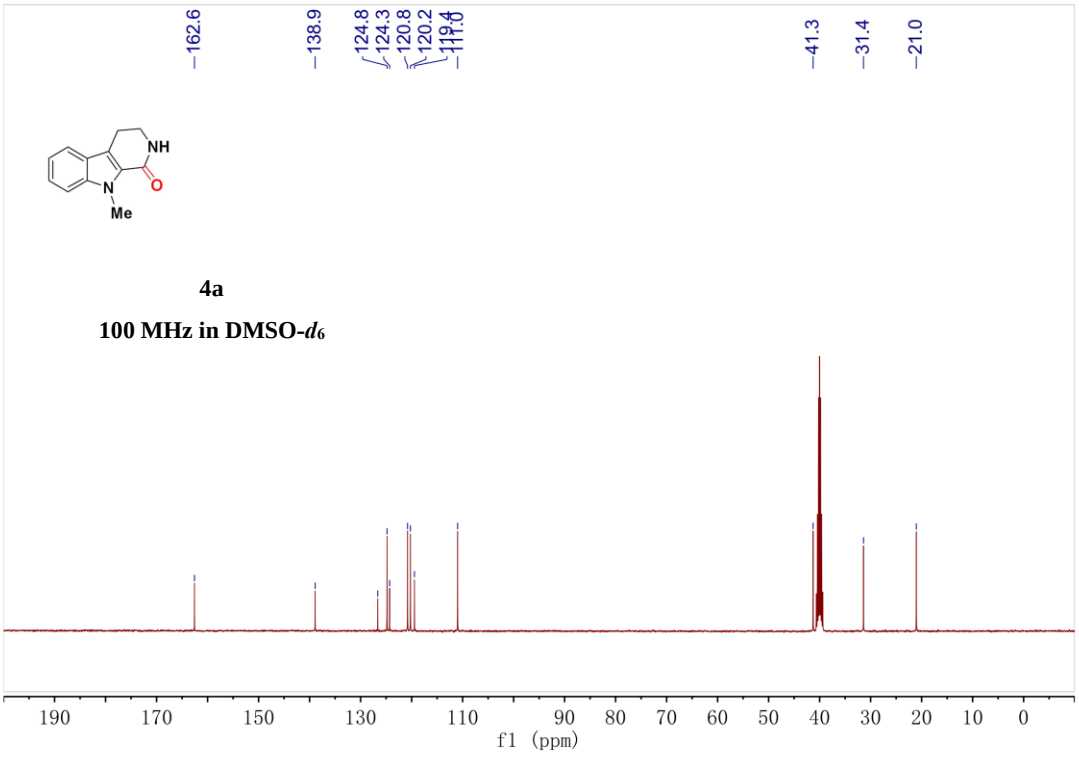
2j

100 MHz in DMSO-d_6



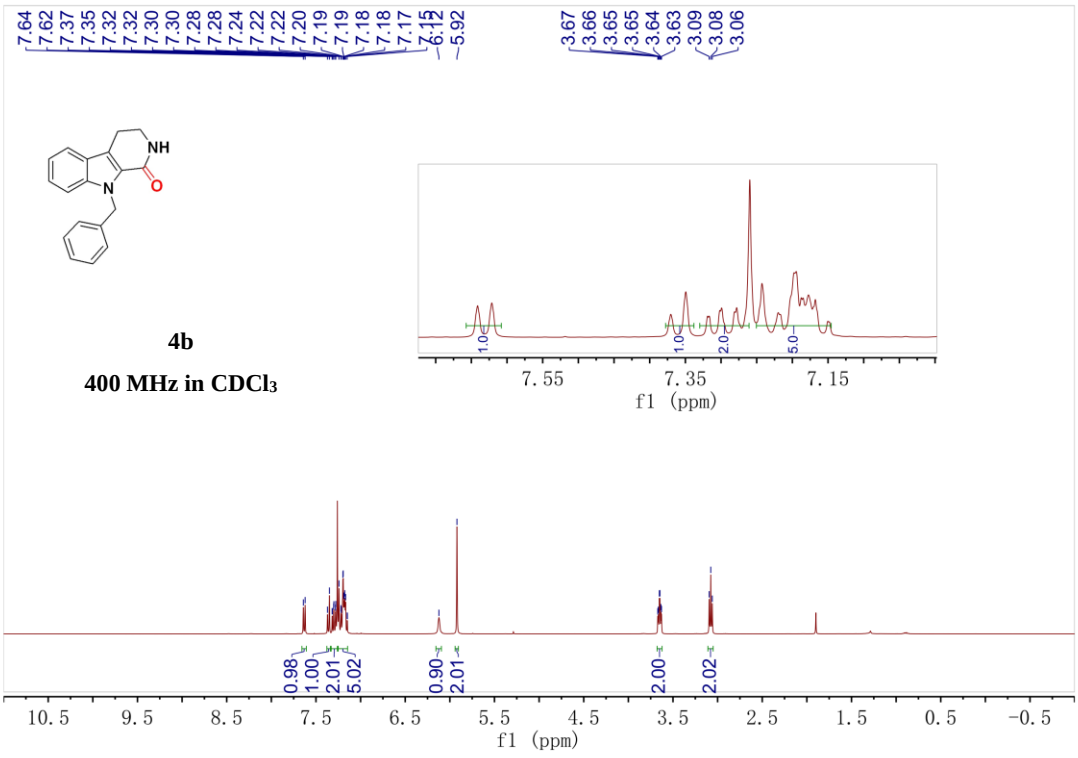
4a

400 MHz in DMSO-*d*$_6$



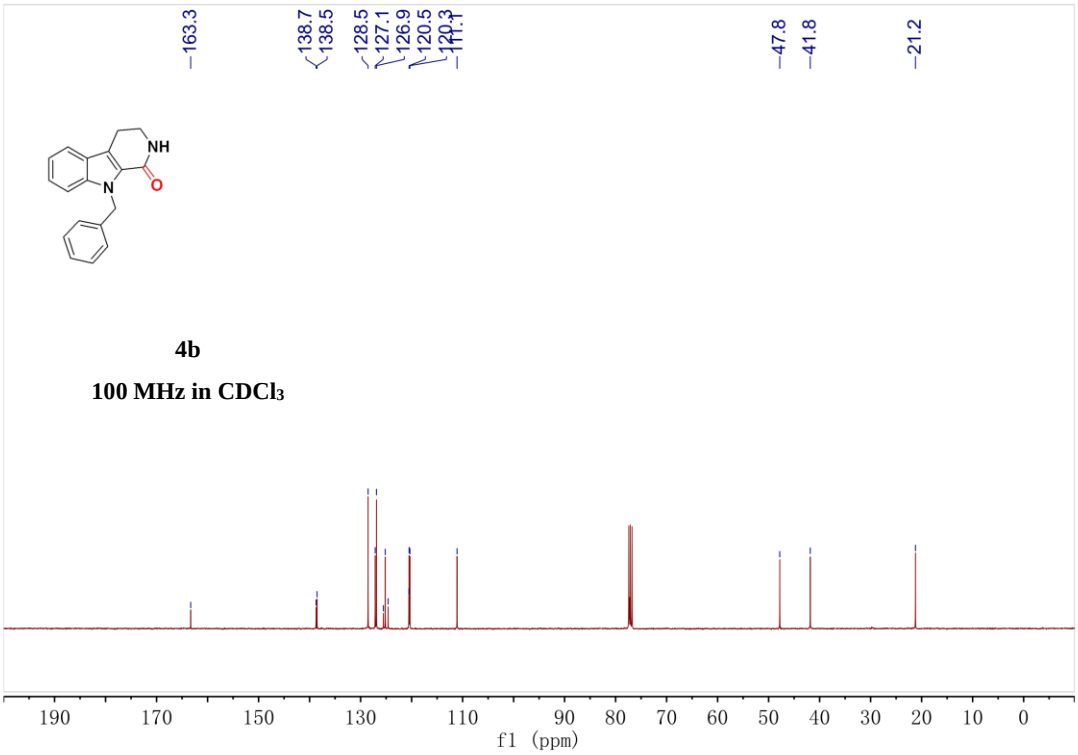
4a

100 MHz in DMSO-*d*$_6$



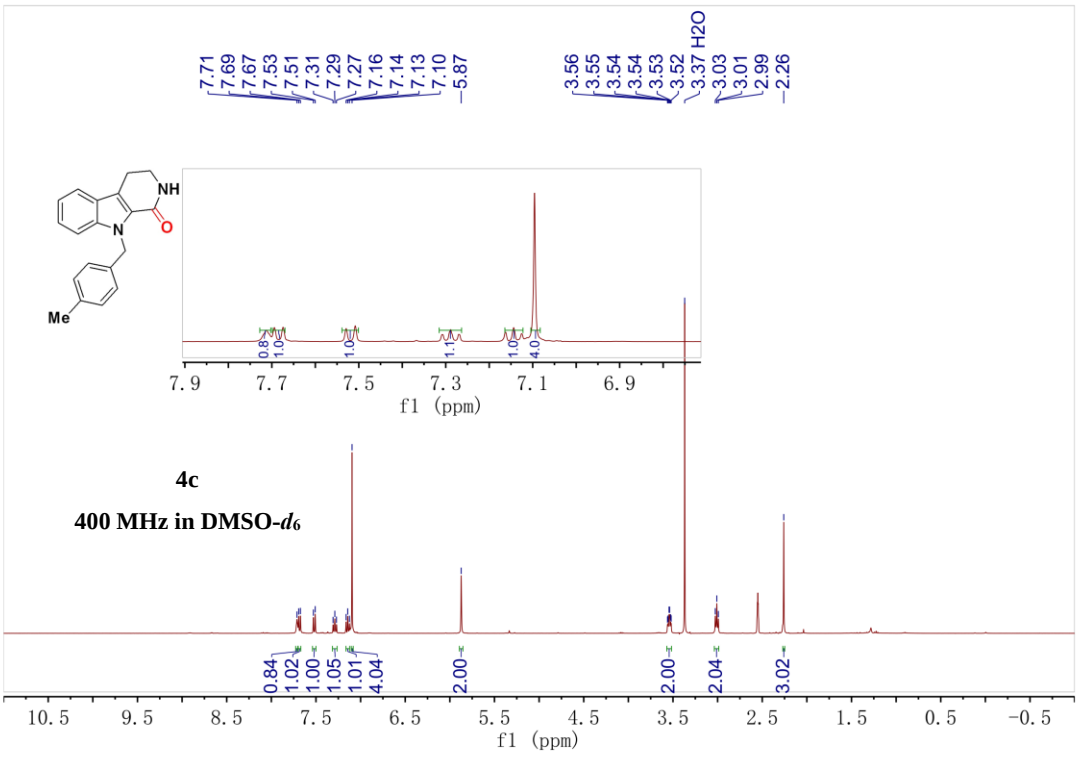
4b

400 MHz in $CDCl_3$



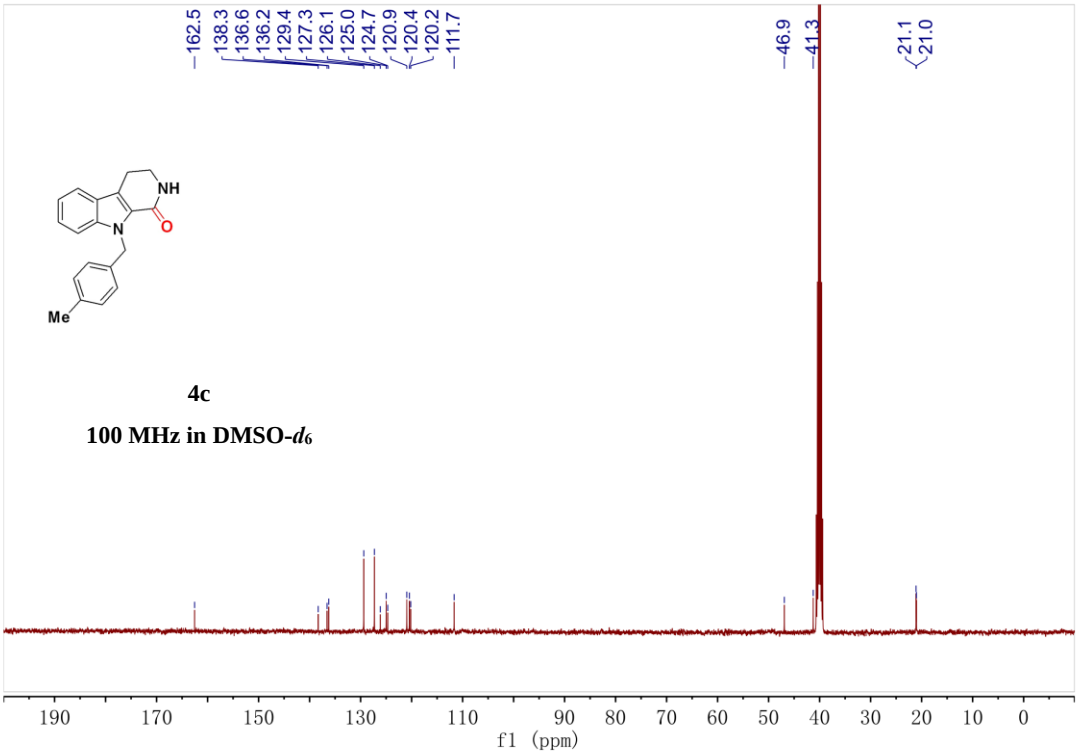
4b

100 MHz in $CDCl_3$



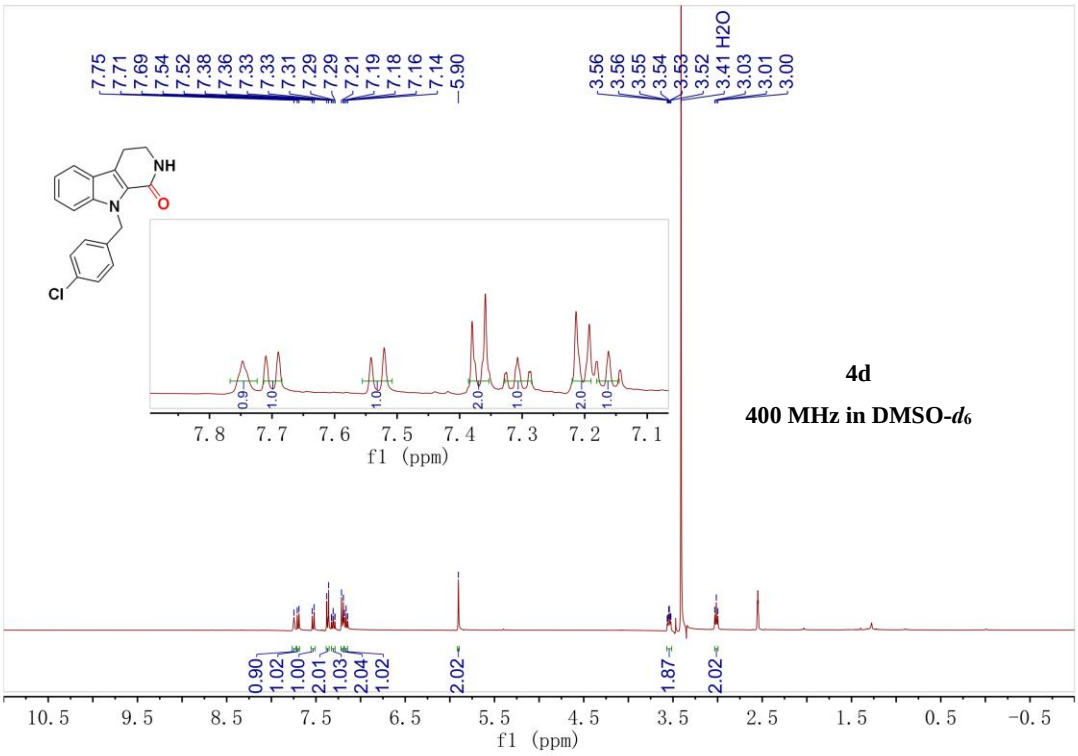
4c

400 MHz in DMSO-*d*$_6$



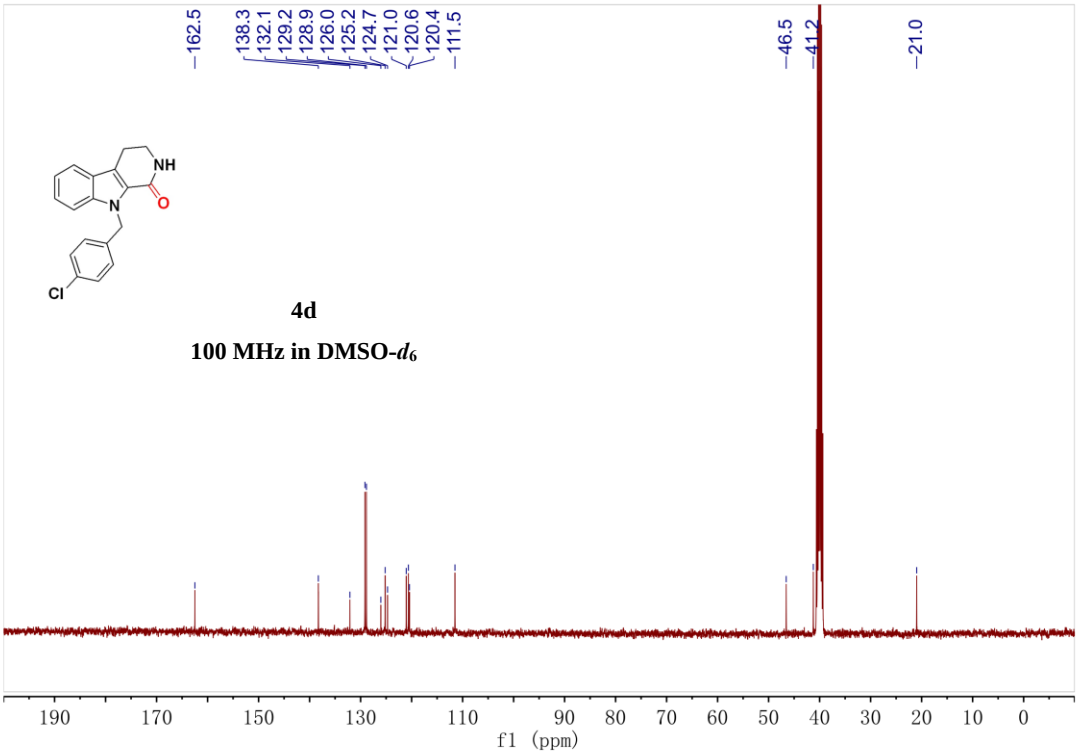
4c

100 MHz in DMSO-*d*$_6$



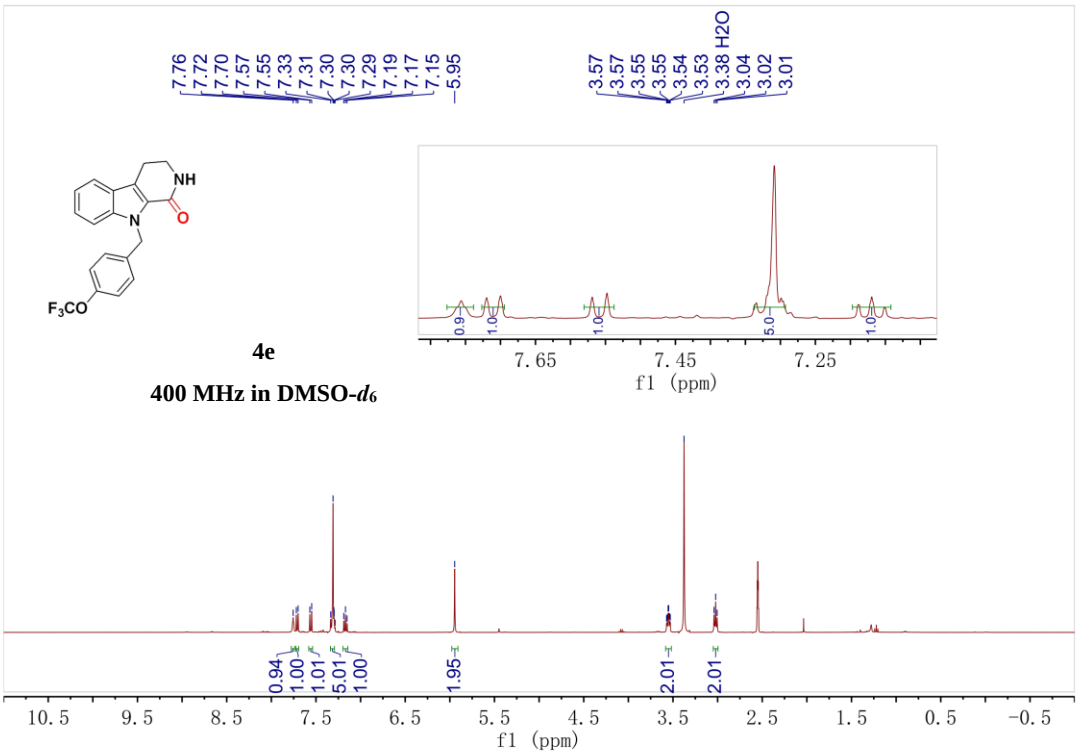
4d

400 MHz in DMSO-d_6



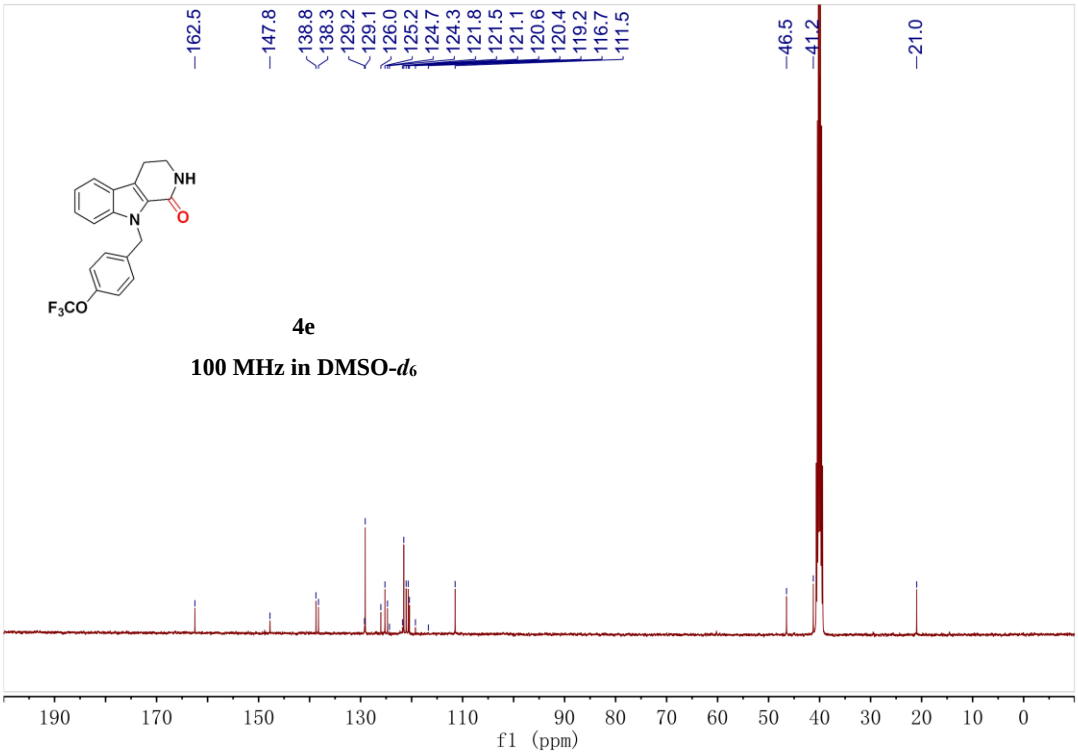
4d

100 MHz in DMSO-d_6



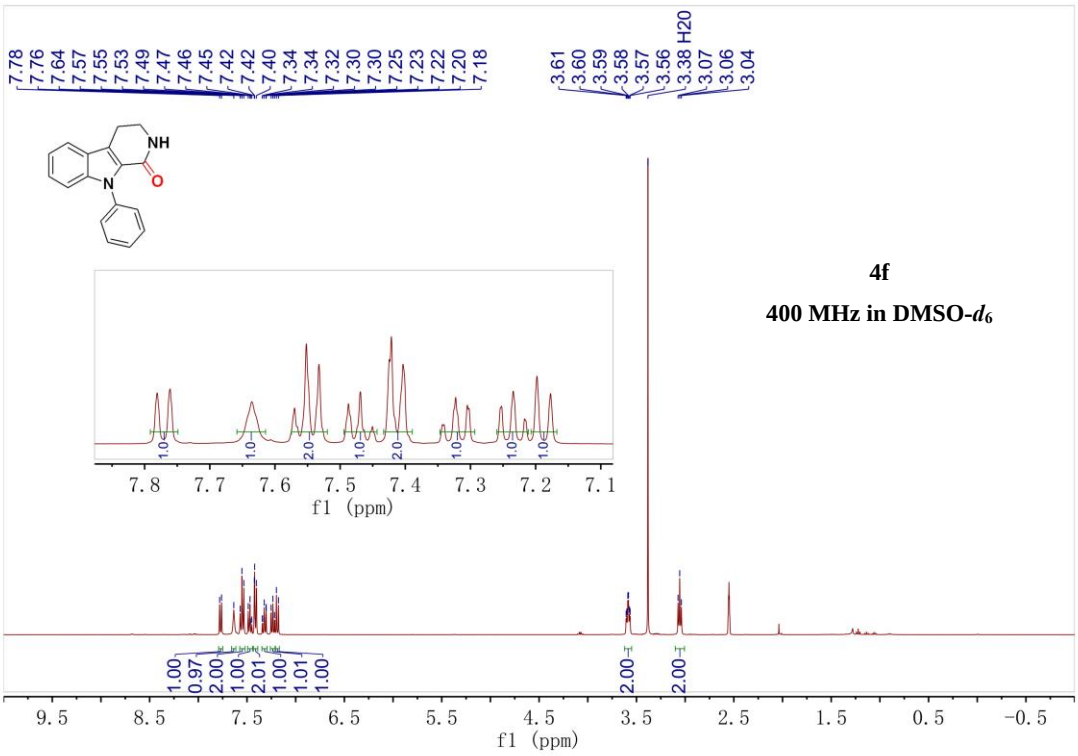
4e

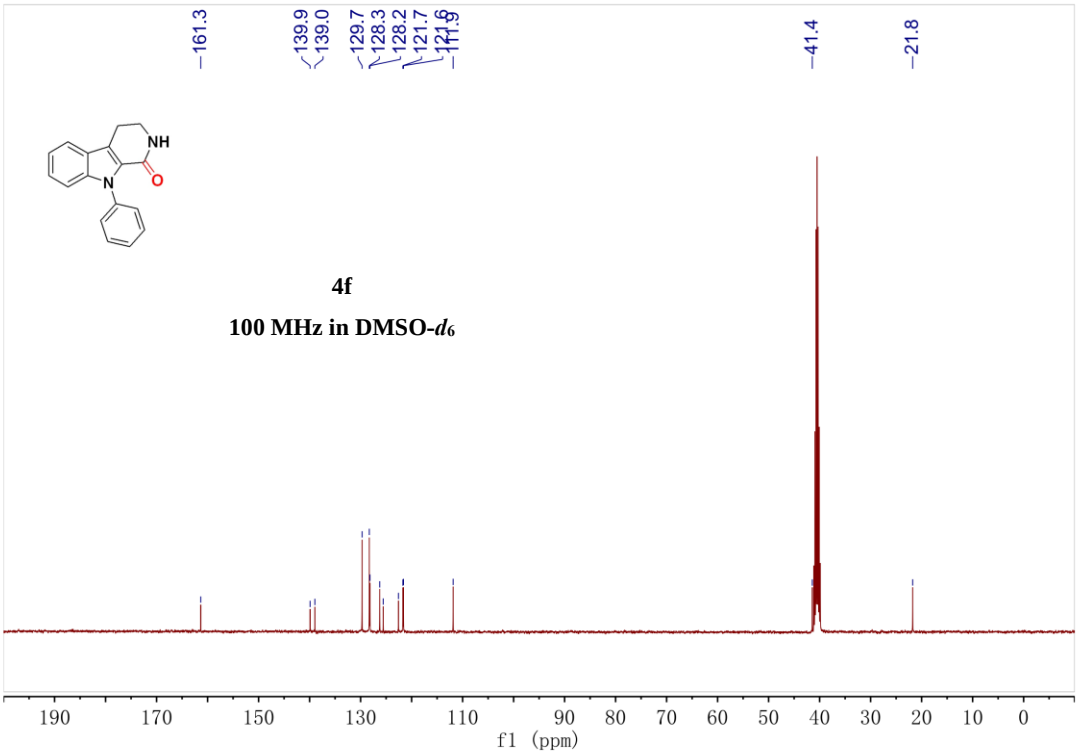
400 MHz in DMSO-*d*$_6$

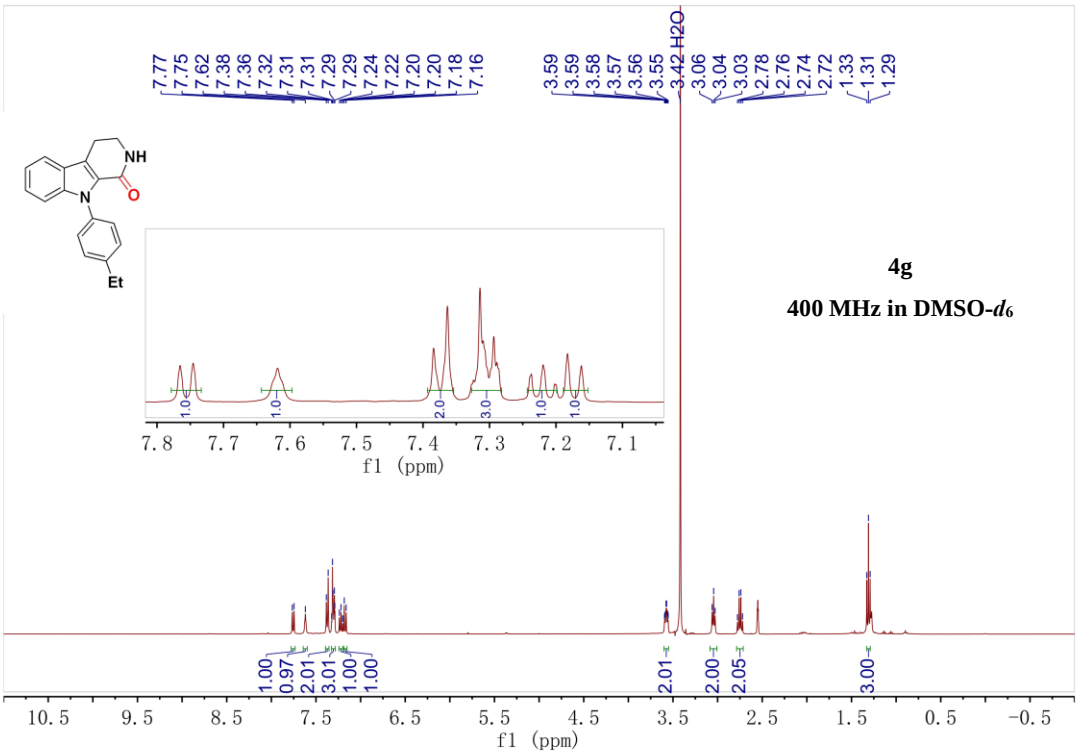


4e

100 MHz in DMSO-*d*$_6$

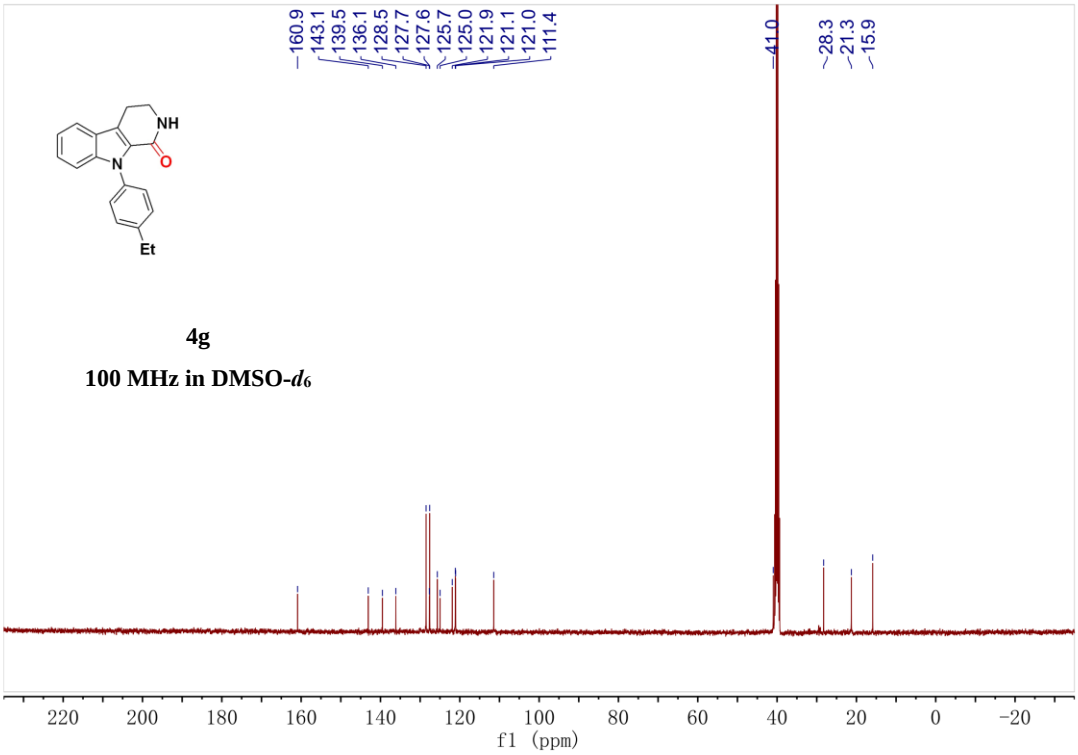

7.78
7.76
7.64
7.57
7.55
7.53
7.49
7.47
7.46
7.45
7.42
7.42
7.40
7.34
7.34
7.32
7.30
7.30
7.25
7.23
7.22
7.20
7.18
3.61
3.60
3.59
3.58
3.57
3.56
3.38 H20
3.07
3.06
3.04
NH
O
N
4f
400 MHz in DMSO-d6
f1 (ppm)
1.00
0.97
2.00
1.00
2.01
1.00
1.01
1.00
2.00
2.00


161.3
139.9
139.0
129.7
128.3
128.2
121.7
121.6
111.9
41.4
21.8
NH
O
N
4f
100 MHz in DMSO-d6
f1 (ppm)



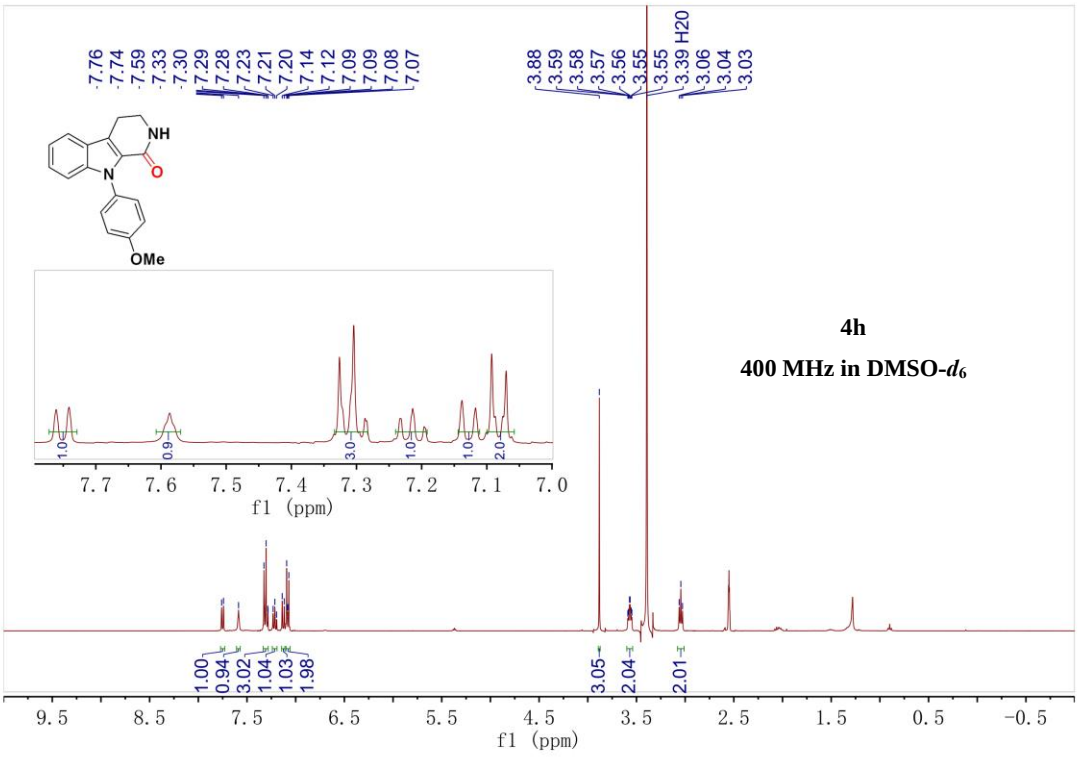
4g

400 MHz in DMSO-*d*$_6$



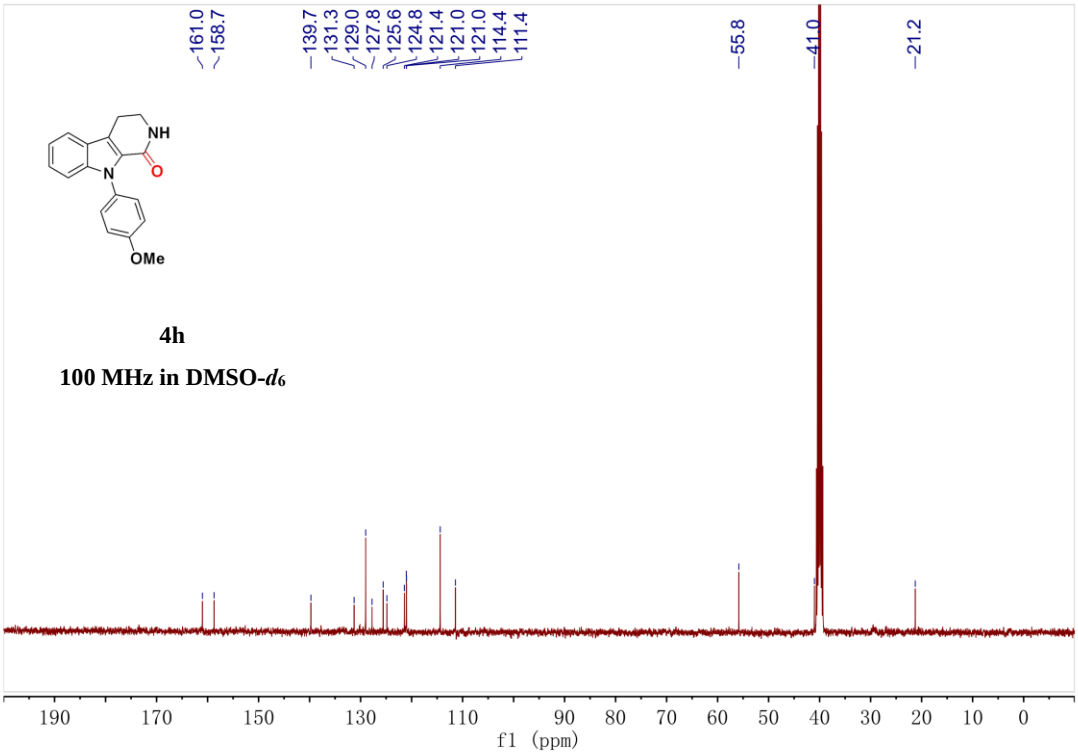
4g

100 MHz in DMSO-*d*$_6$



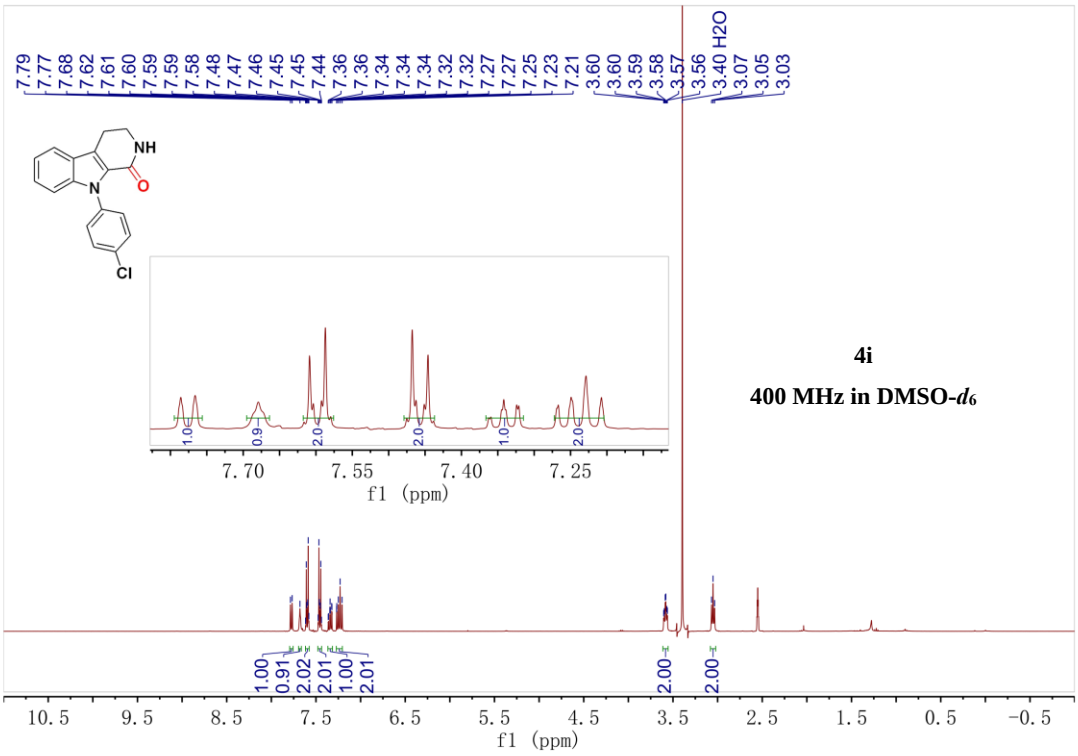
4h

400 MHz in DMSO-*d*$_6$



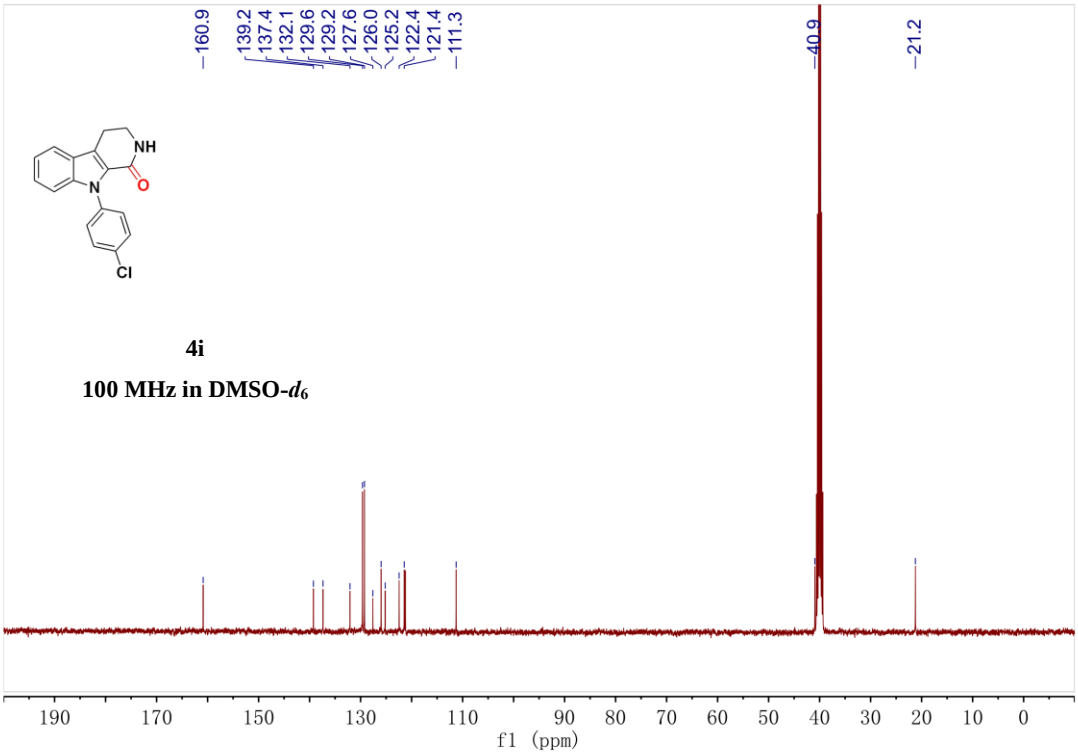
4h

100 MHz in DMSO-*d*$_6$



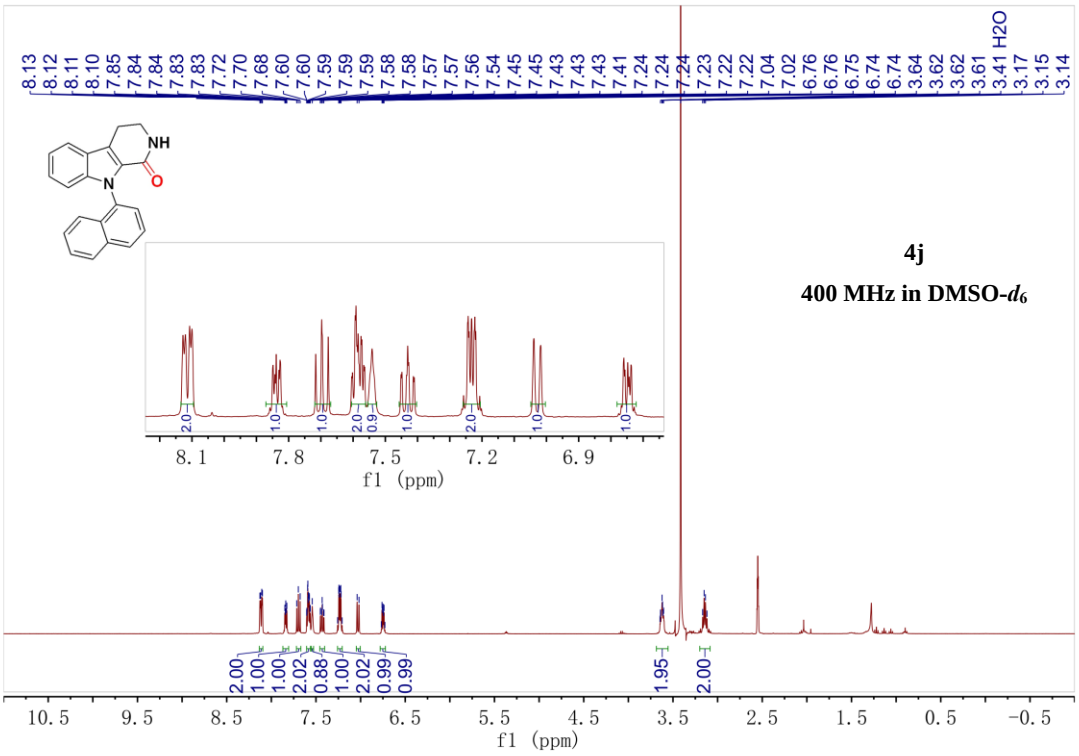
4i

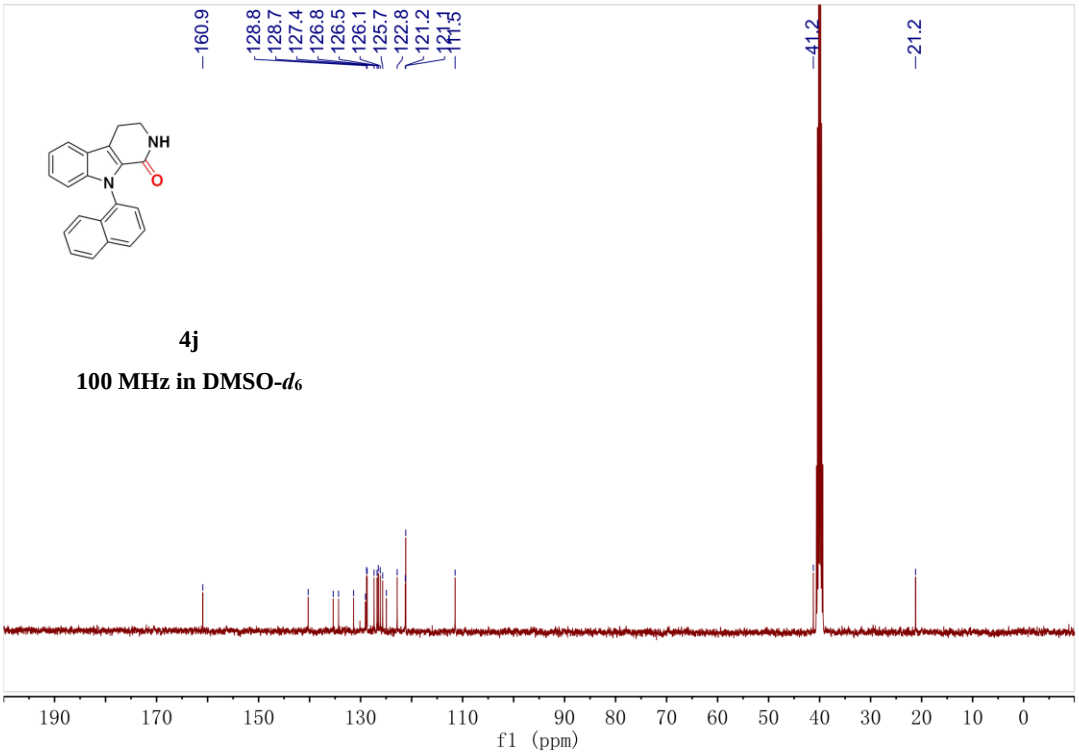
400 MHz in DMSO-*d*$_6$

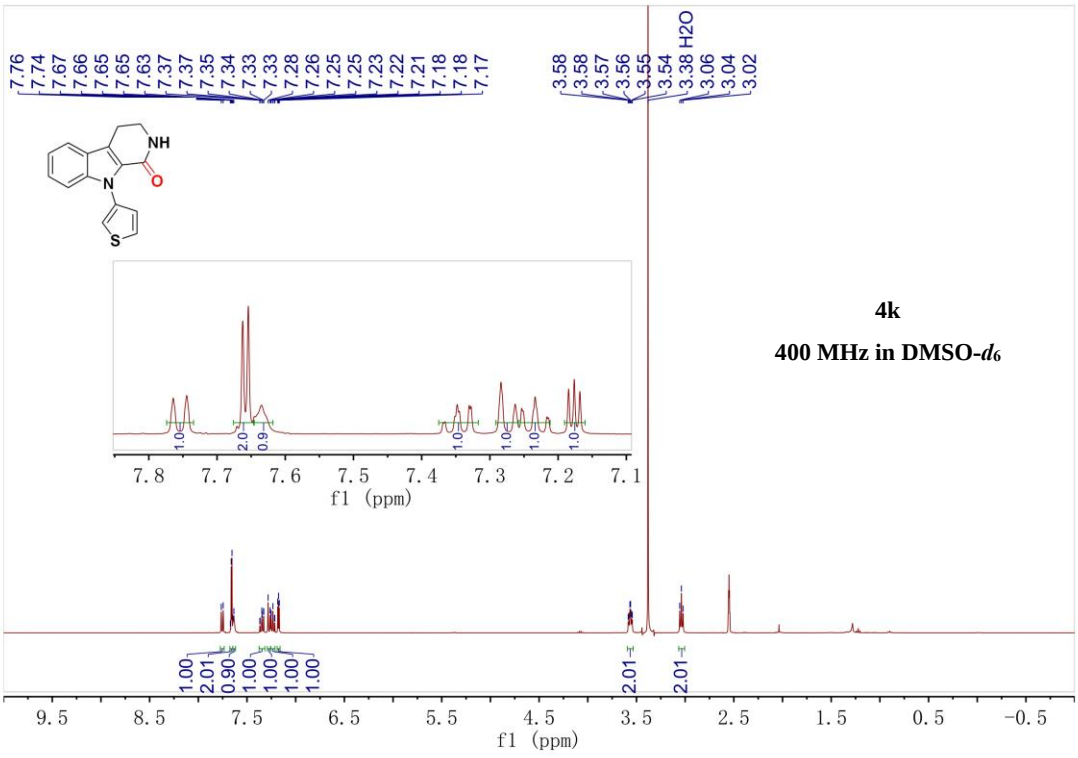


4i

100 MHz in DMSO-*d*$_6$

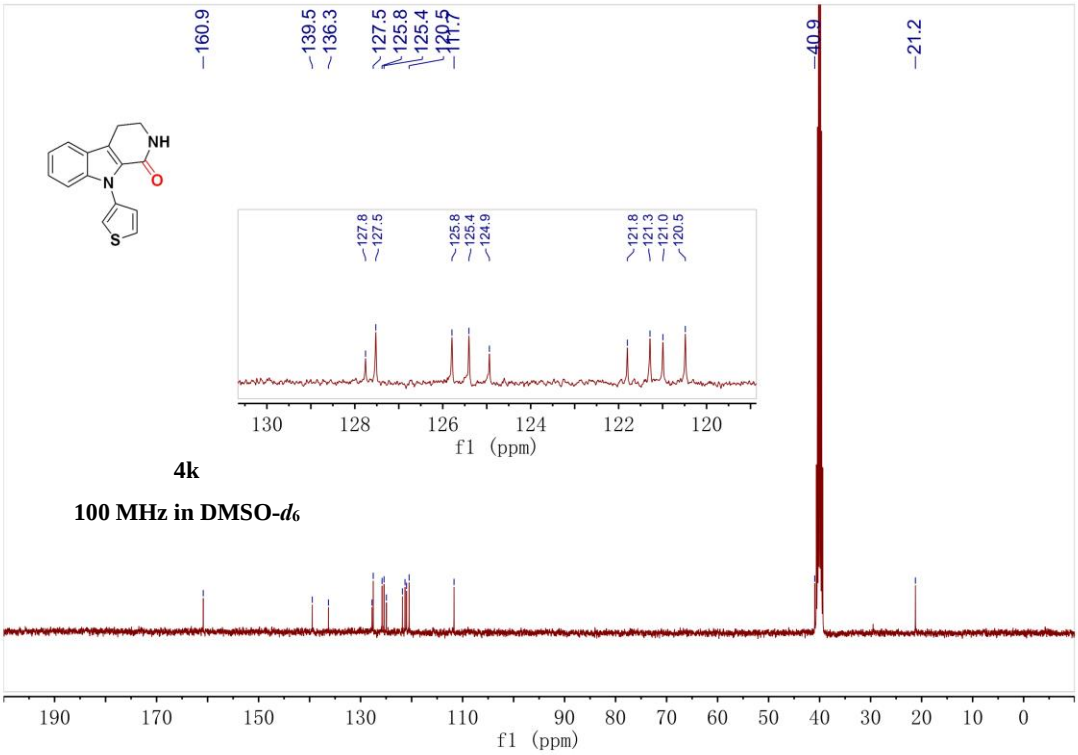

8.13 8.12 8.11 8.10 7.85 7.84 7.84 7.83 7.83 7.72 7.70 7.68 7.60 7.60 7.59 7.59 7.59 7.58 7.58 7.57 7.57 7.56 7.54 7.45 7.45 7.43 7.43 7.43 7.41 7.24 7.24 7.24 7.23 7.22 7.22 7.04 7.02 6.76 6.76 6.75 6.74 6.74 3.64 3.62 3.61 3.41 H2O 3.17 3.15 3.14
NH
O
N
4j
400 MHz in DMSO-d_6
f1 (ppm)
2.00 1.00 1.00 2.02 0.88 1.00 2.02 0.99 0.99 1.95 2.00
f1 (ppm)


160.9 128.8 128.7 127.4 126.8 126.5 126.1 125.7 122.8 121.2 121.1 111.5 41.2 21.2
NH
O
N
4j
100 MHz in DMSO-d_6
f1 (ppm)



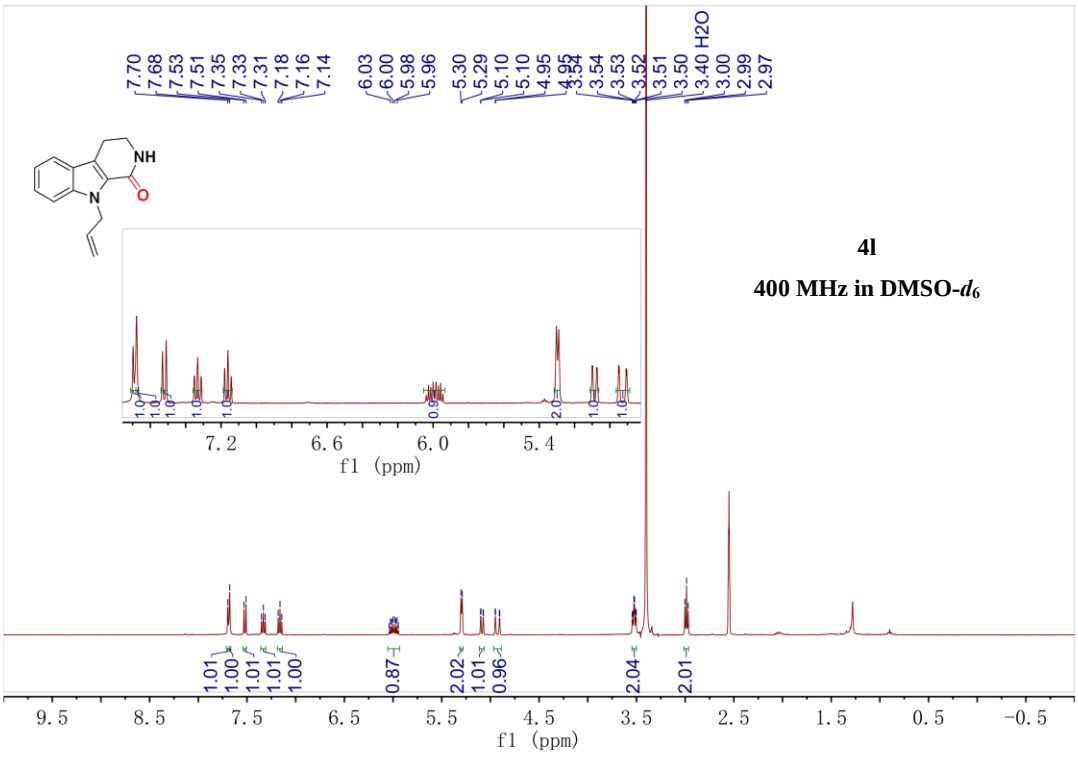
4k

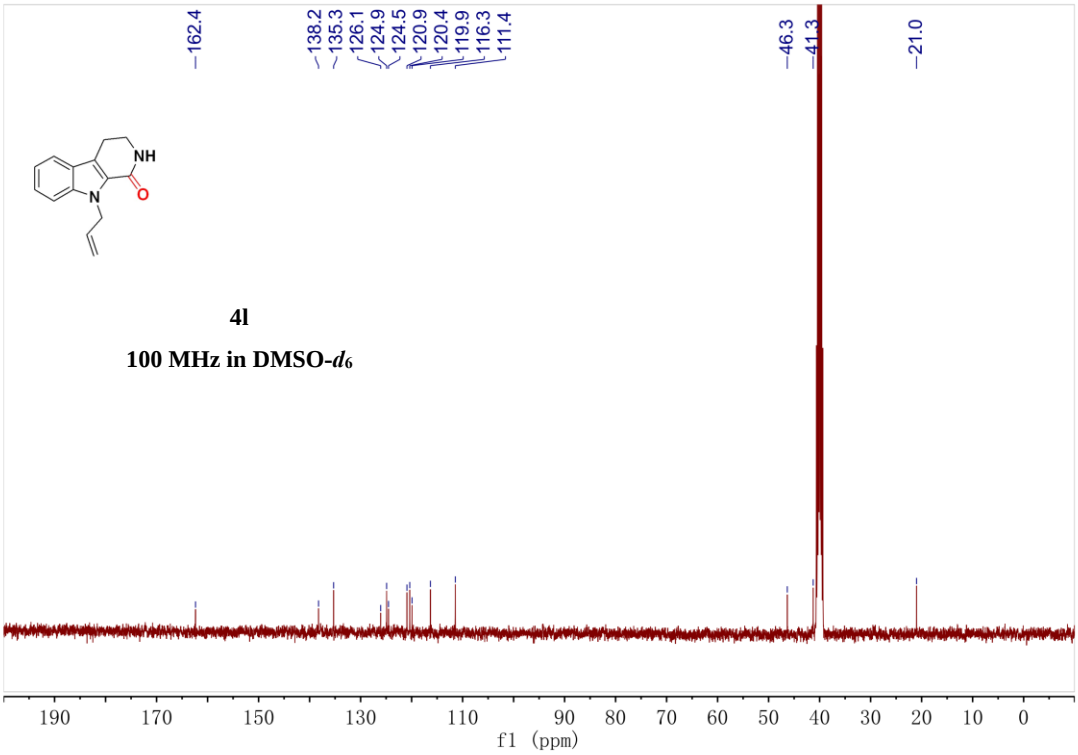
400 MHz in DMSO-*d*$_6$

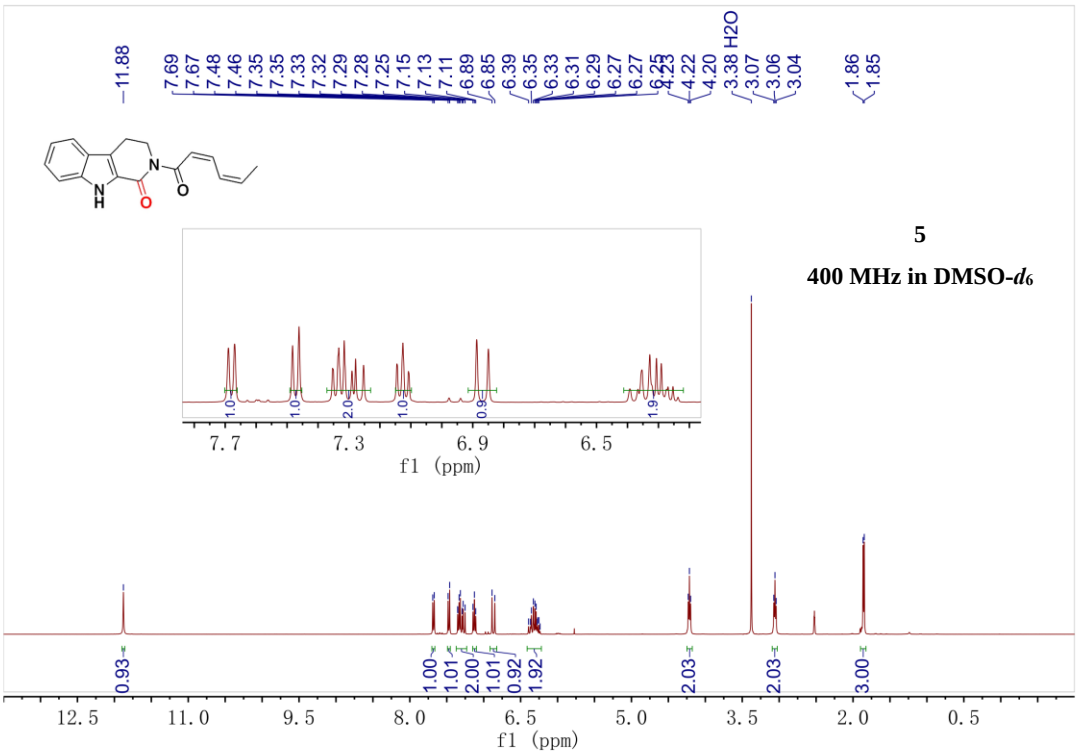


4k

100 MHz in DMSO-*d*$_6$

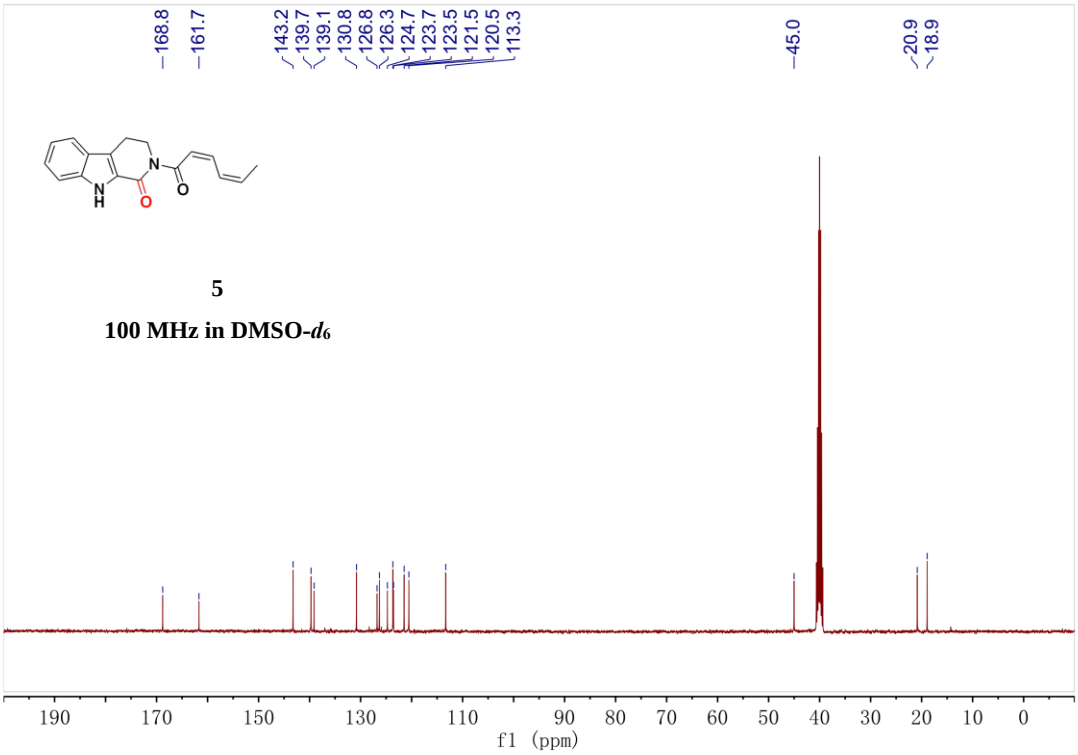

7.70
7.68
7.53
7.51
7.35
7.33
7.31
7.18
7.16
7.14
6.03
6.00
5.98
5.96
5.30
5.29
5.10
5.10
4.95
3.54
3.53
3.52
3.51
3.50
3.40 H2O
3.00
2.99
2.97
NH
N
O
4l
400 MHz in DMSO-d6
f1 (ppm)
1.01
1.00
1.01
1.01
1.00
0.87
2.02
1.01
0.96
2.04
2.01


162.4
138.2
135.3
126.1
124.9
124.5
120.9
120.4
119.9
116.3
111.4
46.3
41.3
21.0
NH
N
O
4l
100 MHz in DMSO-d6
f1 (ppm)



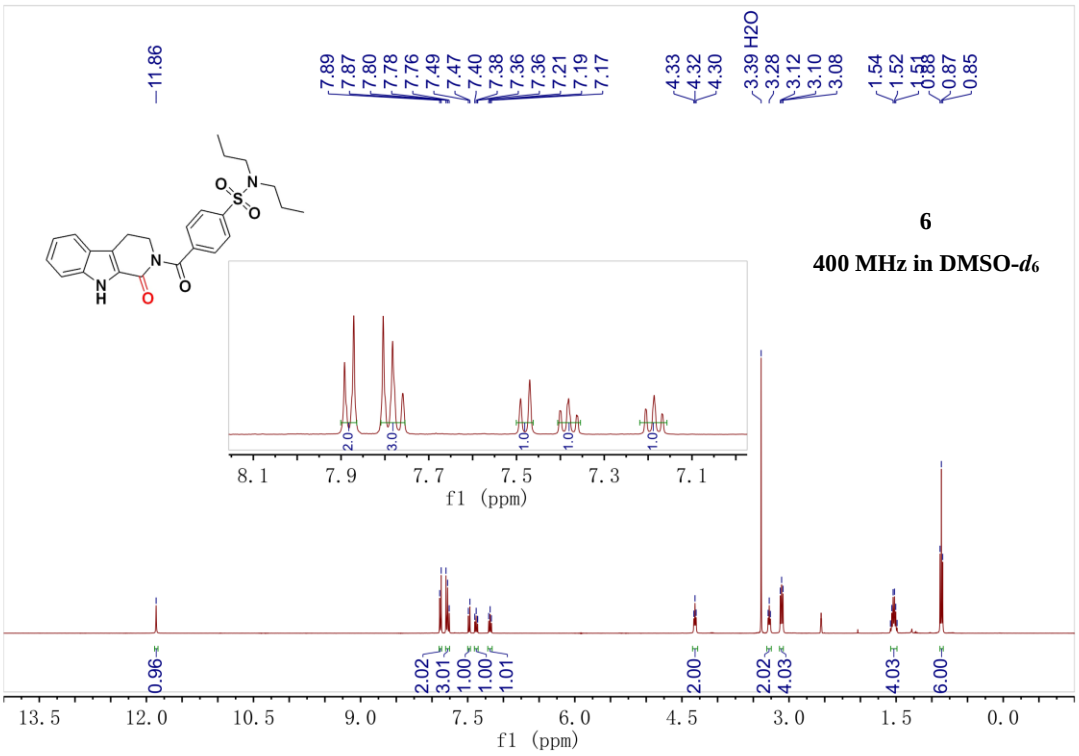
5

400 MHz in DMSO-*d*$_6$



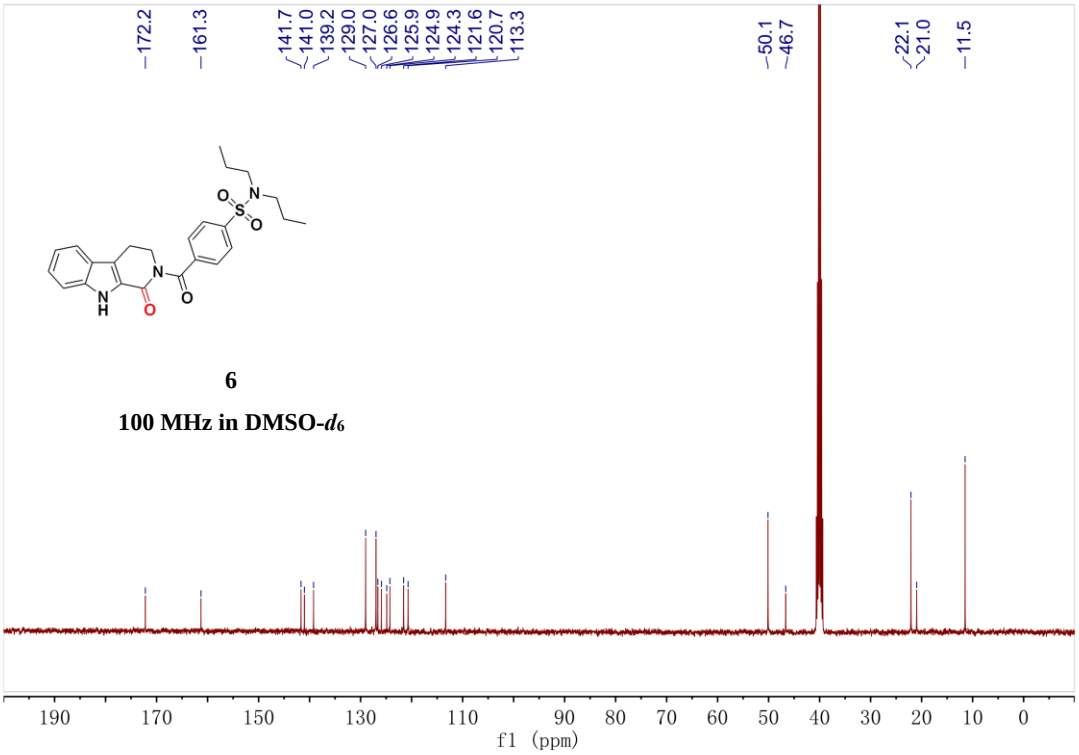
5

100 MHz in DMSO-*d*$_6$



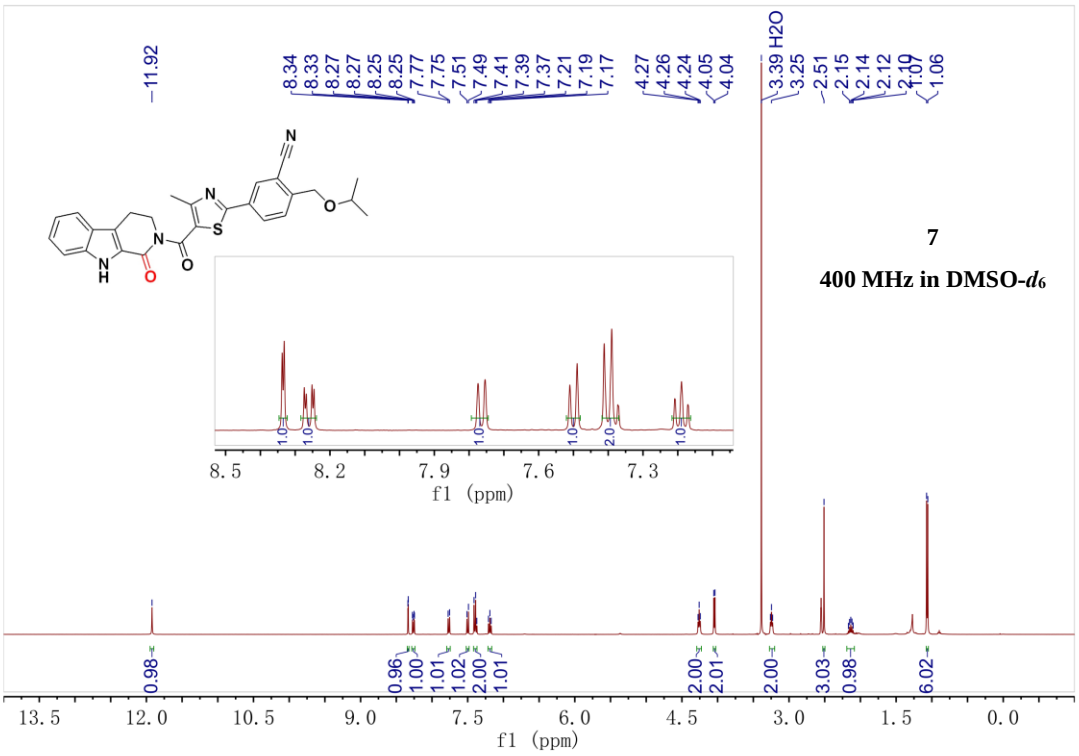
6

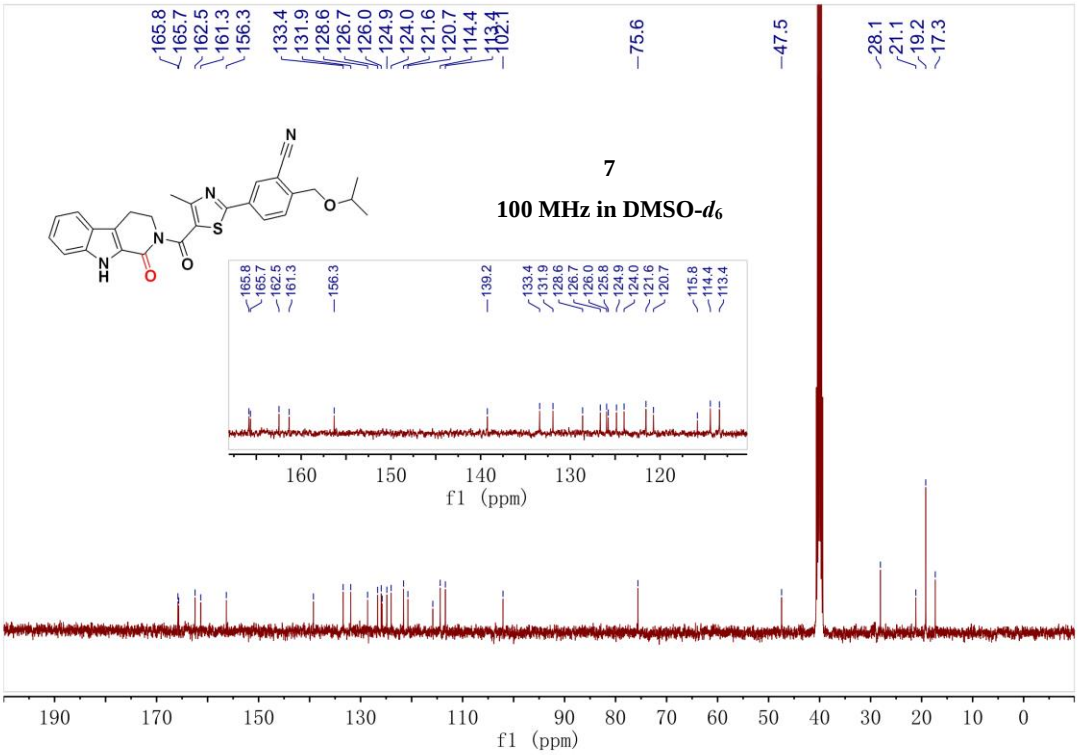
400 MHz in DMSO-*d*$_6$



6

100 MHz in DMSO-*d*$_6$


11.92
8.34
8.33
8.27
8.27
8.25
8.25
7.77
7.75
7.51
7.49
7.41
7.39
7.37
7.21
7.19
7.17
4.27
4.26
4.24
4.05
4.04
3.39 H2O
3.25
2.51
2.15
2.14
2.12
2.10
2.07
1.06
7
400 MHz in DMSO-d6
0.98
0.96
1.00
1.01
1.02
2.00
1.01
2.00
2.01
2.00
3.03
0.98
6.02
f1 (ppm)


165.8
165.7
162.5
161.3
156.3
133.4
131.9
128.6
126.7
126.0
124.9
124.0
121.6
120.7
114.4
113.4
102.1
75.6
47.5
28.1
21.1
19.2
17.3
7
100 MHz in DMSO-d6
f1 (ppm)