Supporting Information for

CdS/Mg-Fe layered double hydroxide: A versatile heterogeneous photocatalyst for the acylation of indoles with α-keto acids

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1. Experimental

1.1 General experimental information

All commercial reagents were used directly without further purification. X-ray diffraction analysis was carried out using a PANalytical X'Pert Pro X-ray diffractometer. The surface morphology and particle size were studied using a Hitachi S-4800 SEM instrument. Melting points were measured on an X-4 digital melting point apparatus (Gongyi, China) without correction. IR spectra were recorded in the range 4000-600 cm^{-1} using KBr pellets on a Thermo Fisher Nicolet IS50 spectrometer instrument. ^{1}H NMR and ^{13}C NMR spectra were recorded on Zhongke Niujin AS 400 spectrometer using DMSO-d6 as the solvent. Mass spectra were performed on a ThermoFinnigan LCQ Advantage instrument (ThermoFinnigan, USA) with an ESI source (4.5 KeV). A 10 W blue LED lamp (manufactured by Xi'an Walters Experimental Equipment Co., Ltd., WATTCAS: WP-TEC-1020LC) was used to carry out photocatalytic reaction by adjusting the condensed water to maintain a relatively constant temperature. The distance from the light source to the irradiation vessel was about 3 cm.

1.2 Synthesis of Mg-Fe LDH

To prepare Mg-Fe-LDHs, a solution containing $Fe(NO_3)_3 \cdot 9H_2O$ (0.06 mol/L) and $Mg(NO_3)_2 \cdot 6H_2O$ (0.24 mol/L) in 100 mL of deionized water was sonicated and stirred. Next, an alkaline mixed solution was prepared by dissolving Na_2CO_3 (0.16 g) and NaOH (0.16 g) in deionized water (15 mL). Then the above two solutions were gradually dropped into a three-neck round bottomed flask containing 100 mL of deionized water, while the pH of the reaction mixture was kept at 10 ± 0.2, then the suspension was aged for 18 h at room temperature. The product was collected by centrifugation and washed with ethanol and water alternately for some times until the pH of the supernatant reached 7.0. Finally, the target product Mg-Fe-LDH was dried in a vacuum oven for 6 h at 80 °C.

1.3 Preparation of CdS

$Cd(NO_3)_3 \cdot 4H_2O$ (1.0 g) was ultrasonically dispersed in deionized water (40 mL)

to form solution A. Then, thiourea (0.25 g) was dissolved in 50 mLof aqueous solution to obtained solution B. Solution B was added dropwise to the above solution A and stirred for another 30 min to obtain solution C. Subsequently, solution C was heated at 80 °C and NaOH aqueous solution (1 mol/L) was added dropwise to make the pH of the solution reach 10.0, and then keep at this temperature for 15 min. Subsequently, the precipitate produced was centrifuged and washed with water and dried under vacuum for 10 h at 80 °C.

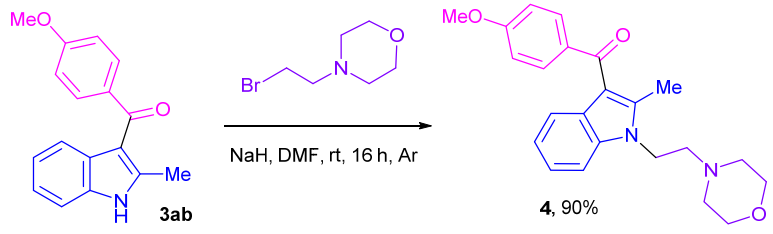
1.4 Preparation of Mg-Fe LDH/CdS

Typically, CdS (0.20 g) and Mg-Fe LDH (1.0 g) were added to a flask containing 80 ml of ethanol. The mixed solution was refluxed for 6 h, and then evaporated solvent. Finally, the resulting sample was obtained after drying.

1.5 General procedure for reduction of nitroarenes to aromatic amines

To a 25 mL tube equipped with a magnetic stir bar was added indoles (1 mmol), α-keto acid, Mg-Fe LDH /CdS (20 mg) and EtOH (1 mL). The reaction mixture was then irradiated using blue LEDs with stirring at room temperature for an appropriate time. After the reaction was completed (monitoring by TLC), the catalyst was separated by filtration, and the solvent was evaporated under reduced pressure. The crude product was purified by column chromatography using petroleum ether/EtOAc as eluent. The recovered catalyst was washed with ethanol and dried for further use.

1.6 Synthesis of pravadoline (4)



Methoxyphenyl)(2-methyl-1*H*-indol-3-yl)methanone (**3ab**) (265 mg, 1.0 mmol) was dissolved in anhydrous DMF before cooling to 0 ℃. NaH (60% dispersion in mineral oil, 44 mg, 1.1 mmol) was added in small portions over a period of 10-15 min. Once addition was complete, the reaction mixture was stirred at 0 ℃ for 0.5 h. Then

an anhydrous DMF (2 mL) solution of 4-(2-bromoethyl)morpholine (194 mg, 1.0 mmol) was slowly added, and the mixture was continued to stir at room temperature until completion. Subsequently, it was quenched by a dropwise addition of water. The solution was extracted with dichloromethane (2 × 10 mL), washed with water (2 × 10 mL) and brine (10 mL), then dried with $MgSO_4$ and concentrated. Purification by column chromatography (ethyl acetate/petroleum ether = 1/1, v/v) gave the product **4** as a pale yellow solid.

2. Photocatalytic parallel reactor

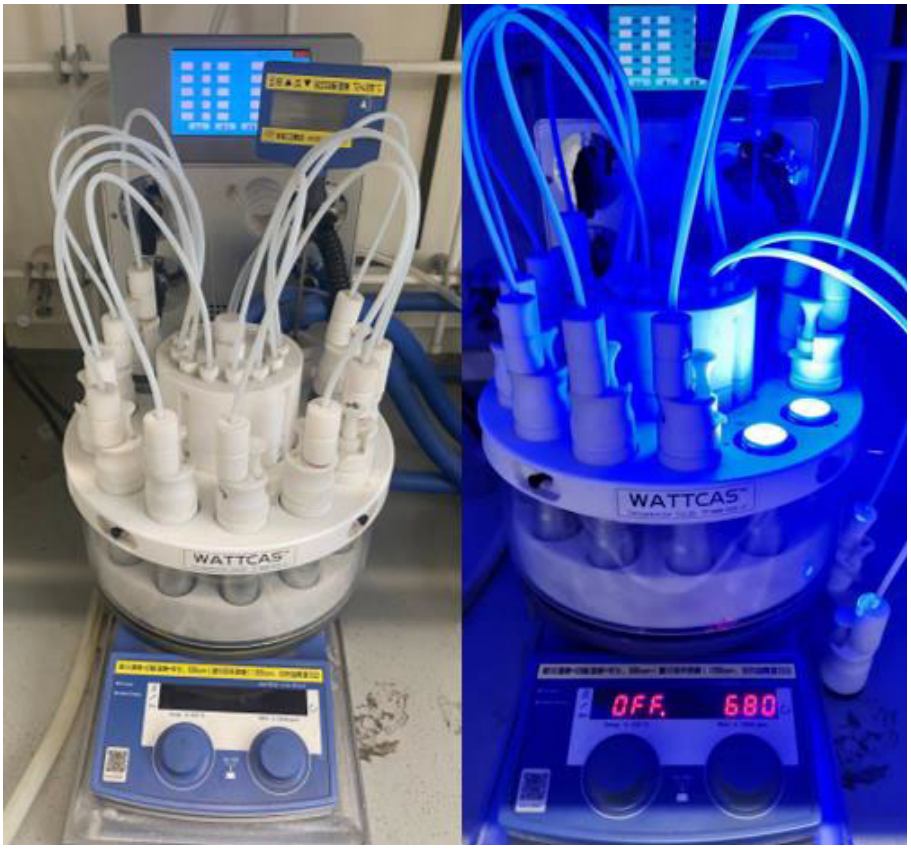


Fig. S1 Photocatalytic parallel reactor

3. Calculation of green chemistry metrics

Green chemistry metrics has been calculated for our optimized reaction on the basis of following parameters.

(1) Atom economy (AE) (%) $= \frac{\text{molecular mass of desired product}}{\text{Molecular mass of all reactants}} \times 100$

(2) Reaction mass efficiency (RME) (%) $= \frac{\text{mass of desired product}}{\text{mass of all reactants}} \times 100$

(3) Carbon efficiency (CE) (%) $= \frac{\text{amount of carbon in desired product total}}{\text{producttotal amount of carbon presented in all reactants}} \times 100$

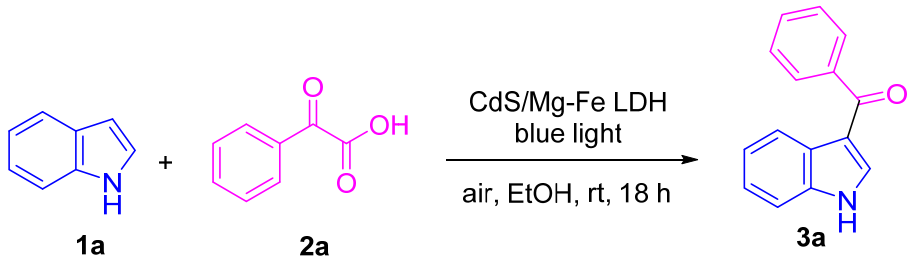
(4) Atom efficiency(AE_f) (%) = (% yield of product × % atom economy) × 100

(5) Environmental factor (E-factor) $= \frac{\text{Amount of waste}}{\text{Amount of product}}$

(6) Optimum efficiency (OE) $= \frac{\text{RME}}{\text{AE}} \times 100$

(7) Product mass intensity (PMI) $= \frac{\text{mass of all reactants + solvent}}{\text{mass of product}}$

Evaluation of green chemistry metrics for the synthesis of **3a**



1a
1.0 mmol
117.05 mg
C_8H_7N
117.05

2a
1.0 mmol
150.03 mg
$C_8H_6O_3$
150.03

3a
0.85 mmol
187.85 mg
$C_{15}H_{11}NO$
221.08

Reactant **1a**	1*H*-indole	117.05 mg	1.0 mmol	FW 117.05
Reactant **2a**	phenylglyoxylic acid	150.03 mg	1.0 mmol	FW 150.03
Solvent	EtOH (2.0 mL)	1578.0 mg	34.30 mmol	FW 46.04
Product **3a**	(1*H*-indol-3-yl)(phenyl)methanone	187.85 mg	0.85 mmol	FW 221.08

Yield of product **3a** = 85%

(1) AE $= \frac{221.08}{117.05 + 150.03} \times 100 = 82.8\%$

(2) RME $= \frac{187.85}{117.05 + 150.03} \times 100 = 70.3\%$

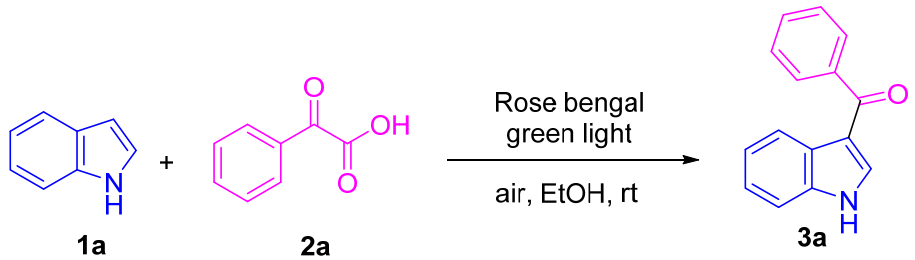
(3) CE $= \frac{0.85 \times 15}{8 + 8} \times 100 = 79.7\%$

(4) AE_f $= (0.85 \times 0.828) \times 100 = 70.4\%$

(5) E-Factor $= \frac{(117.05 + 150.03) - 187.85}{187.85} = 0.42$

(6) OE $= \frac{70.3}{82.8} \times 100 = 84.9\%$

(7) PMI $= \frac{117.05 + 150.03 + 1578.0}{187.85} = 9.82$



1a
0.3 mmol
35.12 mg
C_8H_7N
117.05

2a
0.6 mmol
90.02 mg
$C_8H_6O_3$
150.03

3a
0.237 mmol
52.4 mg
$C_{15}H_{11}NO$
221.08

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Reactant **1a**	1*H*-indole	35.12 mg	0.3 mmol	FW 117.05
Reactant **2a**	phenylglyoxylic acid	90.02 mg	0.6 mmol	FW 150.03
Solvent	EtOH (2.0 mL)	1578.0 mg	34.30 mmol	FW 46.04
Product **3a**	(1*H*-indol-3-yl)(phenyl)methanone	52.40 mg	0.85 mmol	FW 221.08

Yield of product **3a** = 79%

(1) AE $= \frac{221.08}{117.05 + 150.03} \times 100 = 82.8\%$

(2) RME $= \frac{54.40}{35.12 + 90.02} \times 100 = 43.5\%$

(3) CE $= \frac{0.79 \times 15}{8 + 8} \times 100 = 74.1\%$

(4) AE_f $= (0.79 \times 0.828) \times 100 = 65.4\%$

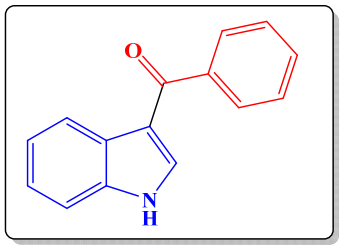
(5) E-Factor $= \frac{(35.12 + 90.02) - 54.40}{54.40} = 1.30$

(6) OE $= \frac{43.5}{82.8} \times 100 = 52.5\%$

(7) PMI $= \frac{35.12 + 90.02 + 1578.0}{52.40} = 35.50$

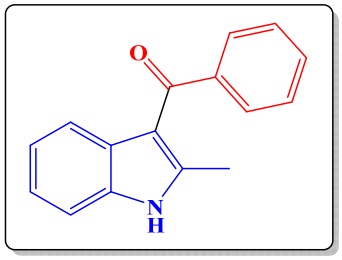
4. Spectra data of all products

(1*H*-Indol-3-yl)(phenyl)methanone (**3a**)



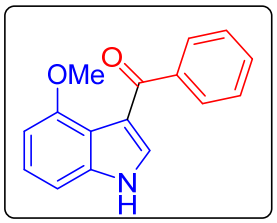
White solid; mp: 236-238 °C; IR (KBr): 3420, 3144, 1738, 1682, 1600, 1580, 1429, 1213, 749 cm^{-1}; ^1H NMR (400 MHz, DMSO-d_6) δ = 12.12 (s, 1H), 8.30 (d, J = 8.0 Hz, 1H), 7.97 (s, 1H), 7.82 (d, J = 7.2 Hz, 2H), 7.63 – 7.58 (m, 1H), 7.56 – 7.51 (m, 3H), 7.29 – 7.22 (m, 2H) ppm. ^{13}C NMR (100 MHz, -DMSO-d_6) δ = 190.44, 140.99, 137.17, 136.17, 131.47, 128.75, 126.71, 123.59, 122.29, 121.86, 115.45, 112.60 ppm.

(2-Methyl-1*H*-indol-3-yl)(phenyl)methanone (**3b**)



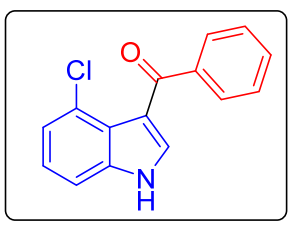
Light yellow solid; mp: 176-178 °C; IR (KBr): 3394, 3176, 2926, 1686, 1594, 1567, 1218, 883, 703 cm^{-1}; ^1H NMR (400 MHz, DMSO-d_6) δ = 11.97 (s, 1H), 7.62-7.58 (m, 3H), 7.53-7.50 (m, 2H), 7.41 (d, J = 7.9 Hz, 1H), 7.34 (d, J = 7.8 Hz, 1H), 7.15-7.11 (m, 1H), 7.04-7.00 (m, 1H), 2.39 (s, 3H) ppm. ^{13}C NMR (101 MHz, DMSO-d_6) δ = 192.32, 144.99, 142.11, 135.44, 131.55, 128.86, 128.48, 127.74, 122.36, 121.47, 120.48, 112.96, 111.75, 14.67 ppm.

(4-Methoxy-1*H*-indol-3-yl)(phenyl)methanone (**3c**)



White solid; mp: 174-177 °C; IR (KBr): 3387, 3216, 2936, 2843, 1739, 1617, 1574, 1203, 1124, 883 cm^{-1}; ^1H NMR (400 MHz, DMSO-d_6) δ = 11.90 (s, 1H), 7.74-7.71 (m, 3H), 7.61-7.57 (m, 1H), 7.50-7.46 (m, 2H), 7.24 – 7.07 (m, 2H), 6.62 (d, J = 7.2 Hz, 1H), 3.55 (s, 3H) ppm. ^{13}C NMR (101 MHz, DMSO-d_6) δ = 190.50, 153.92, 140.88, 138.65, 132.12, 132.02, 129.49, 128.38, 124.22, 116.78, 116.12, 105.73, 102.46, 55.34 ppm.

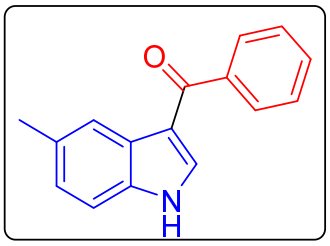
(4-Chloro-1*H*-indol-3-yl)(phenyl)methanone (**3d**)



Yellow solid; mp: 171-172 °C; IR (KBr): 3446, 3123, 1710, 1661, 1650, 1230, 824, 761, 626 cm^{-1}; ^1H NMR (400 MHz, DMSO-d_6) δ = 12.21 (s, 1H), 7.89 – 7.80 (m, 3H), 7.69 – 7.47 (m, 5H), 7.24-7.22 (m, 1H) ppm.^{13}C NMR (101 MHz,

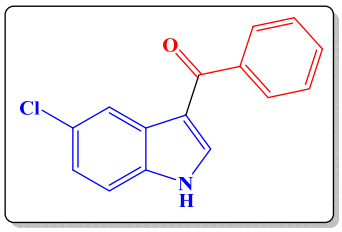
DMSO-d_6) δ = 189.41, 140.22, 138.80, 134.85, 132.69, 129.88, 128.88, 125.81, 124.15, 123.92, 122.78, 116.19, 111.85 ppm.

(5-Methyl-1*H*-indol-3-yl)(phenyl)methanone (**3e**)



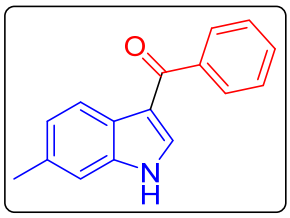
White solid; mp: 224-226 °C; IR (KBr): 3411, 3167, 293, 1726, 1584, 1568, 1218, 1140, 894, 719 cm^{-1}; ^1H NMR (400 MHz, DMSO-d_6) δ = 12.10 (s, 1H), 8.10 (d, J = 7.8 Hz, 1H), 7.88 (s, 1H), 7.79 (d, J = 6.9 Hz, 2H), 7.63-7.53 (m, 3H), 7.20 – 7.05 (m, 2H), 2.54 (s, 3H) ppm. ^{13}C NMR (101 MHz, DMSO-d_6) δ = 190.64, 141.02, 136.64, 135.80, 131.57, 128.91, 128.85, 126.50, 124.26, 122.66, 122.04, 119.51, 115.89, 17.16 ppm.

(5-Chloro-1*H*-indol-3-yl)(phenyl)methanone (**3f**)



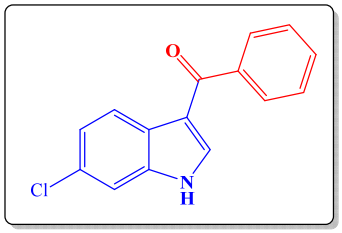
Light yellow solid; mp: 252-254 °C; IR (KBr): 3393, 3154, 1729, 1589, 1568, 1213, 894, 752, 722 cm^{-1}; ^1H NMR (400 MHz, DMSO-d_6) δ = 12.27 (s, 1H), 8.24 (d, J = 2.0 Hz, 1H), 8.05 (s, 2H), 7.80 (d, J = 7.2 Hz, 2H), 7.65 – 7.46 (m, 4H), 7.29 (dd, J = 8.4, 2.0 Hz, 2H) ppm. ^{13}C NMR (101 MHz, DMSO-d_6) δ = 190.31, 140.53, 137.61, 135.70, 131.81, 128.98, 128.91, 127.92, 127.13, 123.69, 121.05, 114.97, 114.43 ppm.

(6-Methyl-1*H*-indol-3-yl)(phenyl)methanone (**3g**)



Yellow solid; mp: 248-250 °C; IR (KBr): 3421, 3123, 2921, 1715,1600, 1567, 1216, 890, 718 cm^{-1};^1H NMR (400 MHz, DMSO-d_6) δ = 11.92 (s, 1H), 7.58-7.45 (m, 5H), 7.36 (d, J = 7.9 Hz, 1H), 7.30 (d, J = 7.8 Hz, 1H), 7.11-7.07 (m, 1H), 7.00-6.96 (m, 1H), 2.35 (s, 3H) ppm.^{13}C NMR (101 MHz, DMSO-d_6) δ = 192.33, 145.00, 142.12, 135.45, 131.55, 128.87, 128.49, 127.75, 122.36, 121.47, 120.48, 112.96, 111.76, 14.67 ppm.

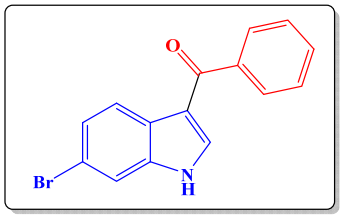
(6-Chloro-1*H*-indol-3-yl)(phenyl)methanone (**3h**)



White solid; mp: 272-273 °C; IR (KBr): 3420, 3129, 1698, 1595, 1564, 1213, 890, 755, 714 cm^{-1}; ^1H NMR (400 MHz, DMSO-d_6) δ = 12.21 (s, 1H), 8.27 (d, J = 8.4

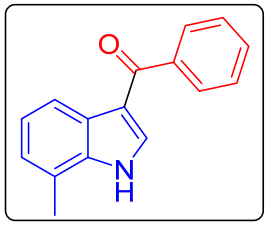
Hz, 1H), 8.03 (s, 1H), 7.85-7.80 (m, 2H), 7.67 – 7.55 (m, 4H), 7.30 (dd, J = 8.8, 2 Hz, 1H) ppm. ^{13}C NMR (101 MHz, DMSO-d_6) δ = 189.40, 140.21, 138.79, 134.83, 132.68, 129.87, 128.87, 125.81, 124.14, 123.92, 122.77, 111.83 ppm.

(6-Bromo-1*H*-indol-3-yl)(phenyl)methanone (**3i**)



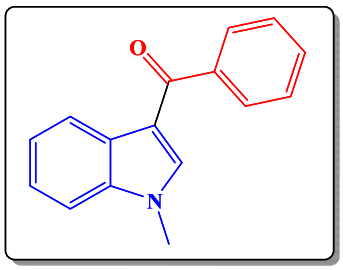
White solid; mp: 268-270 °C; IR(KBr): 3428, 3135, 1719, 1612, 1598, 1213, 822, 760, 657 cm^{-1}; ^{1}H NMR (400 MHz, DMSO-d_6) δ = 12.21 (s, 1H), 8.22 (d, J = 8.4 Hz, 1H), 8.02 (s, 1H), 7.82 (d, J = 7.2 Hz, 2H), 7.74 (s, 1H), 7.67-7.62 (m, 1H), 7.60-7.55 (m, 2H), 7.42 (d, J = 8.8 Hz, 1H) ppm. ^{13}C NMR (101 MHz, DMSO-d_6) δ = 190.33, 140.57, 138.08, 136.96, 131.83, 128.99, 128.81, 125.76, 125.18, 123.55, 116.12, 115.36 ppm.

(7-Methyl-1*H*-indol-3-yl)(phenyl)methanone (**3j**)



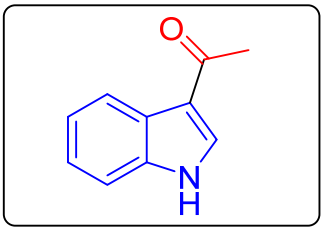
Light yellow solid; mp: 248-250 °C; IR (KBr): 3419, 3129, 2981, 1735,1610, 1557, 1214, 891, 708 cm^{-1}; ^{1}H NMR (400 MHz, DMSO-d_6) δ = 12.11 (s, 1H), 8.10 (d, J = 7.7 Hz, 1H), 7.88 (d, J = 2.8 Hz, 1H), 7.79 (d, J = 6.8 Hz, 2H), 7.62-7.53 (m, 3H), 7.18-7.14 (m, 1H), 7.09-7.07 (m, 1H) ppm. ^{13}C NMR (101 MHz, DMSO-d_6) δ = 190.65, 141.02, 136.64, 135.81, 131.57, 128.91, 128.85, 126.49, 124.26, 122.67, 122.04, 119.51, 115.89, 17.16 ppm.

(1-Methyl-1*H*-indol-3-yl)(phenyl)methanone (**3k**)



Yellow oil; mp: 166-168 °C; IR (KBr):3346, 3123, 1697, 1647, 1581, 1212, 824, 761 cm^{-1}; ^{1}H NMR (400 MHz, DMSO-d_6) δ = 8.30 (d, J = 7.2 Hz, 1H), 8.02 (s, 1H), 7.79 (d, J = 6.8 Hz, 2H), 7.67 – 7.52 (m, 4H), 7.40 – 7.26 (m, 2H), 3.88 (s, 3H) ppm. ^{13}C NMR (101 MHz, DMSO-d_6) δ = 189.94, 140.98, 139.90, 137.82, 131.52, 128.88, 128.82, 127.14, 123.66, 122.76, 122.02, 114.25, 111.15, 33.70 ppm.

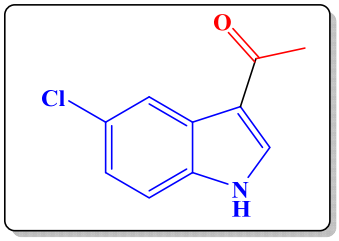
1-(1*H*-Indol-3-yl)ethan-1-one (**3l**)



White solid; mp: 164 - 168°C; IR (KBr): 3379, 3137, 1768, 1650, 1563, 1231, 821, 746, 553 cm^{-1};^{1}H NMR (400 MHz,

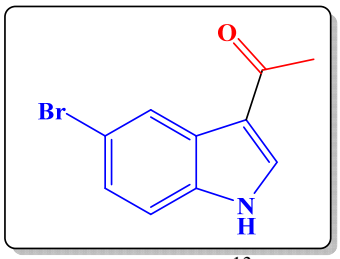
DMSO-d_6) δ = 11.93 (s, 1H), 8.32 (s, 1H), 8.25 – 8.19 (m, 1H), 7.50-7.48(m, 1H), 7.23-7.19 (m, 2H), 2.48 (s, 3H) ppm.^{13}C NMR (101 MHz, DMSO-d_6) δ = 193.12, 137.14, 134.81, 125.78, 123.19, 122.12, 121.81, 117.30, 112.55, 27.73 ppm.

1-(5-Chloro-1*H*-indol-3-yl)ethan-1-one (**3m**)



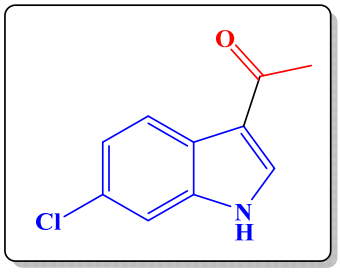
Light yellow solid; mp: 162-165 °C; IR (KBr): 3439, 3167, 1771, 1660, 1583, 1227, 823, 736, 557 cm^{-1}; ^{1}H NMR (400 MHz, DMSO-d_6) δ = 12.12 (s, 1H), 8.39 (d, J = 3.2 Hz, 1H), 8.17 (s, 1H), 7.51 (d, J = 8.4 Hz, 1H), 7.25 (d, J = 8.4 Hz, 1H), 2.47 (s, 3H) ppm. ^{13}C NMR (101 MHz, DMSO-d_6) δ = 193.37, 136.21, 135.60, 126.88, 126.86, 123.28, 120.83, 116.80, 114.25, 27.65 ppm.

1-(5-Bromo-1*H*-indol-3-yl)ethan-1-one (**3n**)



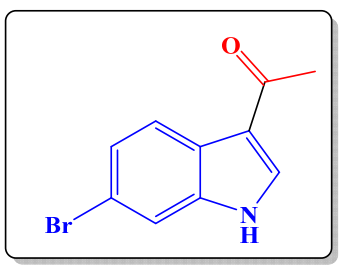
White solid; mp: 168-170 °C; IR (KBr): 3431, 3152, 1766, 1630, 1568, 1233, 873, 620, 589 cm^{-1}; ^{1}H NMR (400 MHz, DMSO-d_6) δ = 12.13 (s, 1H), 8.37 (s, 1H), 8.32 (s, 1H), 7.47 (d, J = 8.8 Hz, 1H), 7.36 (d, J = 8.8 Hz, 1H), 2.47 (s, 3H) ppm. ^{13}C NMR (101 MHz, DMSO-d_6) δ = 193.19, 136.06, 135.88, 127.52, 125.79, 123.89, 116.71, 114.92, 114.68, 27.66 ppm.

1-(6-Chloro-1*H*-indol-3-yl)ethan-1-one (**3o**)



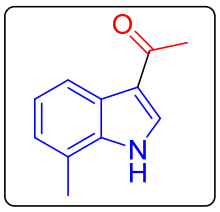
Light brown solid; mp: 170-174 °C; IR (KBr): 3421, 3157, 1732, 1622, 1590, 1214, 894, 721, 589 cm^{-1}; ^{1}H NMR (400 MHz, DMSO-d_6) δ = 12.05 (s, 1H), 8.37 (s, 1H), 8.15 (d, J = 8.8 Hz, 1H), 7.51 (s, 1H), 7.21-7.18 (m, 1H), 2.45 (s, 3H) ppm. ^{13}C NMR (101 MHz, DMSO-d_6) δ = 193.23, 137.58, 135.86, 127.76, 124.50, 123.08, 122.46, 117.16, 112.30, 27.69 ppm.

1-(6-Bromo-1*H*-indol-3-yl)ethan-1-one (**3p**)



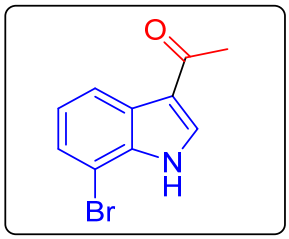
Yellow solid; mp: 172-176 °C; IR (KBr): 3423, 3160, 1735, 1624, 1571, 1222, 896, 620, 597 cm^{-1}; ^{1}H NMR (400 MHz, DMSO-d_6) δ = 12.04 (s, 1H), 8.35 (s, 1H), 8.10 (d, J = 8.4 Hz, 1H), 7.66 (s, 1H), 7.33-7.29 (m, 1H), 2.44 (s, 3H) ppm. ^{13}C NMR (101 MHz, DMSO-d_6) δ =

193.23, 138.02, 135.74, 125.05, 124.77, 123.47, 117.17, 115.81, 115.23, 27.71 ppm.



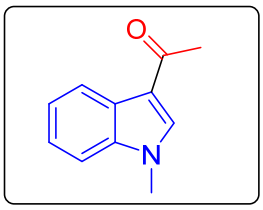
Light brown solid; mp: 172-176 °C; IR (KBr): 3443, 1695, 1604, 1574, 1321, 869, 650, 557 cm^{-1}; ^{1}H NMR (400 MHz, DMSO-d_6) δ =10.63 (s, 1H), 7.11 (d, J = 7.7 Hz, 1H), 6.82 – 6.74 (m, 2H), 6.68-6.64 (m, 1H), 2.52 (s, 3H), 2.44 (s, 3H) ppm.^{13}C NMR (101 MHz, DMSO-d_6) δ =136.93, 126.36, 123.51, 123.32, 121.20, 120.72, 119.41, 118.27, 28.69, 17.28 ppm.

1-(7-Bromo-1*H*-indol-3-yl)ethan-1-one (**3r**)



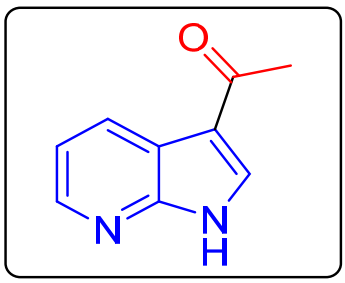
White solid; mp: 186-188 °C; IR (KBr): 3390, 3153, 1715, 1639, 1598, 1257, 883, 608 cm^{-1};^{1}H NMR (400 MHz, DMSO-d_6) δ = 12.17 (s, 1H), 8.37 (s, 1H), 8.21 (d, J = 7.9 Hz, 1H), 7.45 (d, J = 7.6 Hz, 1H), 7.16-7.12 (m, 1H), 2.50 (s, 3H) ppm.^{13}C NMR (101 MHz, DMSO-d_6) δ = 193.45, 135.65, 135.55, 127.46, 125.90, 123.65, 121.25, 118.14, 105.07, 27.88 ppm.

1-(1-Methyl-1*H*-indol-3-yl)ethan-1-one (**3s**)



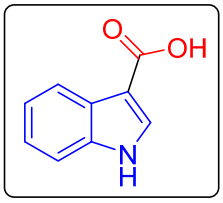
Light brown solid; mp: 206-208 °C; IR (KBr): 3433, 3166, 1702, 1632, 1222, 743, 614 cm^{-1};^{1}H NMR (400 MHz, DMSO-d_6) δ = 8.46 – 8.06 (m, 2H), 7.55 (d, J = 7.9 Hz, 1H), 7.31-7.22 (m, 2H), 3.88 (s, 3H), 2.45 (s, 3H) ppm.^{13}C NMR (101 MHz, DMSO-d_6) δ = 192.51, 138.49, 137.76, 126.17, 123.25, 122.47, 121.90, 116.08, 111.02, 27.71 ppm.

1-(1*H*-pyrrolo[2,3-*b*]pyridin-3-yl)ethan-1-one (**3t**)



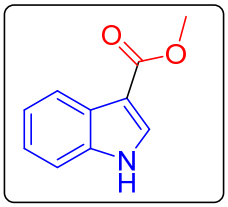
Light yellow solid; mp: 200-206 °C; IR (KBr): 3465, 3084, 1633, 1582, 1523, 1416, 1173, 769, 613 cm^{-1}; ^{1}H NMR (400 MHz, DMSO-d_6) δ = 12.46 (s, 1H), 8.51 – 8.44 (m, 2H), 8.34 -8.32 (m, 1H), 7.26-7.23 (m, 1H), 2.48 (s, 3H) ppm.^{13}C NMR (101 MHz, DMSO-d_6) δ = 193.36, 149.47, 144.62, 135.13, 130.04, 118.49, 118.07, 115.95, 27.40 ppm.

1*H*-Indole-3-carboxylic acid (**3u**)



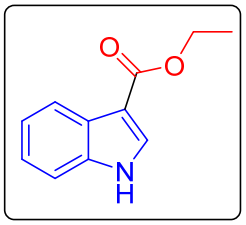
White solid; mp: 234-238 °C; IR (KBr): 3306, 3053, 1645, 1529, 1443, 1200, 763, 611 cm^{-1}; ^1H NMR (400 MHz, DMSO-d_6) δ = 11.81 (s, 2H), 8.02 (d, J = 9.4 Hz, 2H), 7.48 (d, J = 7.8 Hz, 1H), 7.26 – 7.10 (m, 2H) ppm.^{13}C NMR (101 MHz, DMSO-d_6) δ = 166.43, 136.90, 132.70, 126.49, 122.58, 121.41, 121.06, 112.65, 107.91 ppm.

Methyl 1*H*-indole-3-carboxylate (**3v**)



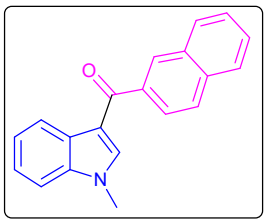
White solid; mp: 152-153 °C; IR (KBr): 3249, 1657, 1445, 1377, 1317, 1128, 777, 608 cm^{-1}; ^1H NMR (400 MHz, DMSO-d_6) δ = 11.95 (s, 1H), 8.11 (s, 1H), 8.10-8.02 (m, 1H), 7.51-7.49 (m, 1H), 7.24-7.18 (m, 2H) ppm. ^{13}C NMR (101 MHz, DMSO-d_6) δ = 165.26, 136.85, 132.90, 126.14, 122.84, 121.73, 120.90, 112.82, 106.82, 51.09 ppm.

Ethyl 1*H*-indole-3-carboxylate (**3w**)



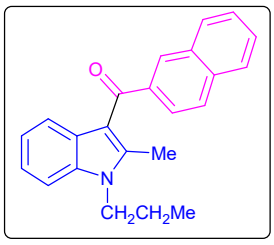
White solid; mp: 124-128 °C; IR (KBr): 3267, 3179, 1757, 1669, 1547, 1373, 1318, 1199, 1050, 688 cm^{-1}; ^1H NMR (400 MHz, DMSO-d_6) δ = 11.93 (s, 1H), 8.24 – 7.83 (m, 2H), 7.59 – 7.40 (m, 1H), 7.27 – 7.11 (m, 2H), 4.32-4.27 (m, 2H) ppm.^{13}C NMR (101 MHz, DMSO-d_6) δ = 164.88, 136.87, 132.86, 126.12, 122.80, 121.68, 120.95, 112.81, 107.12, 59.43, 40.64, 40.43, 40.23, 40.02, 39.81, 39.60, 39.39, 14.99 ppm.

1-Methyl-1H-indol-3-yl)(naphthalen-2-yl)methanone (**3x**)



White solid; mp: 166-172 °C; IR (KBr): 3421, 2254, 2127, 1844, 1643, 1384, 1277, 1004, 824, 762 cm^{-1}; ^1H NMR (400 MHz, DMSO) δ = 8.42 (s, 1H), 8.33 (d, J = 7.4 Hz, 1H), 8.14 – 7.90 (m, 4H), 7.90 -7.89 (m, 1H), 7.67-7.61 (m, 3H), 7.40 – 7.31 (m, 2H), 3.92 (s, 3H) ppm.;^{13}C NMR (101 MHz, DMSO) δ = 189.91, 140.20, 138.23, 137.90, 134.63, 132.66, 129.72, 129.31, 128.58, 128.14, 128.10, 127.24, 127.15, 125.72, 123.72, 122.80, 122.13, 114.55, 111.19, 33.68 ppm.

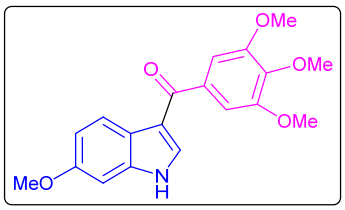
(2-Methyl-1-propyl-1*H*-indol-3-yl)(naphthalen-2-yl)methanone (**3y**)



Yellow solid; mp: 147-152 °C; IR (KBr):3431, 2254, 2127, 1651, 1314, 1026, 825, 764, 618 cm^{-1}; ^1H NMR (400 MHz, DMSO) δ = 8.23 (s, 1H), 8.09 – 8.03 (m, 3H), 7.79 – 7.75 (m,

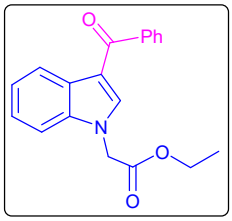
1H), 7.67-7.65 (m, 1H), 7.60 -7.58(m, 2H), 7.27 – 7.17 (m, 2H), 7.04 - 7.00 (m, 1H), 4.29 - 4.25 (m, 2H), 2.52 (s, 3H), 1.746 - 1.70 (m, 2H), 0.98 - 0.94 (m, 3H) ppm. ^{13}C NMR (101 MHz, DMSO) δ = 191.98, 144.93, 139.12, 136.26, 134.76, 132.69, 132.27, 129.57, 128.55, 128.28, 128.21, 127.25, 125.65, 122.37, 121.70, 120.45, 110.82, 43.11, 31.82, 20.09, 14.18, 12.83 ppm.

(6-Methoxy-1*H*-indol-3-yl)(3,4,5-trimethoxyphenyl)methanone (**3z**)



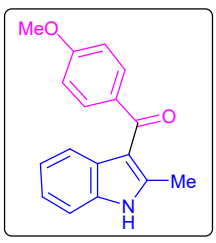
White solid; mp: 154-163 °C; IR (KBr): 3433, 2255, 2127, 1660, 1376, 1026, 999, 864, 612 cm^{-1}; ^{1}H NMR (400 MHz, DMSO) δ = 11.84 (s, 1H), 8.12 (s, 1H), 7.97 -7.96 (m, 1H), 7.10-7.09 (s, 2H), 7.01 (s, 1H), 6.90 (d, J = 8.7 Hz, 1H), 3.87 (s, 6H), 3.82 (s, 3H), 3.77 (s, 3H) ppm. ^{13}C NMR (101 MHz, DMSO) δ = 189.29, 157.01, 153.07, 140.46, 138.09, 136.26, 135.14, 122.59, 120.84, 115.40, 112.10, 106.47, 95.63, 60.59, 56.45, 55.73 ppm.

Ethyl 2-(3-benzoyl-1*H*-indol-1-yl)acetate (**3aa**)



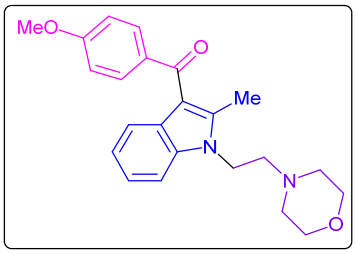
White solid; mp: 153-161 °C; IR (KBr): 3447, 2253, 2126, 1640, 1384, 1026, 1004, 824, 762 cm^{-1}; ^{1}H NMR (400 MHz, DMSO) δ = 8.31-8.30 (m, 1H), 8.09 (s, 1H), 7.80 (d, J = 7.0 Hz, 2H), 7.62-7.59 (m, 4H), 7.33-7.32 (m, 2H), 5.29 (s, 2H), 4.18 (q, J = 7.1 Hz, 2H), 1.24 (t, J = 7.1 Hz, 3H) ppm. ^{13}C NMR (101 MHz, DMSO) δ = 190.19, 168.81, 140.82, 140.21, 137.75, 131.68, 128.95, 126.96, 123.90, 122.89, 122.13, 115.10, 111.29, 61.68, 47.87, 14.53 ppm.

(4-Methoxyphenyl)(2-methyl-1H-indol-3-yl)methanone (**3ab**)



Light Yellow solid; mp: 179-185 °C; IR (KBr): 3470, 3229, 1606, 1558, 1456, 1302, 1008, 781, 605 cm^{-1}; ^{1}H NMR (400 MHz, DMSO) δ = 11.88 (s, 1H), 7.67-7.64 (m, 2H), 7.40 (d, J = 8.0 Hz, 1H), 7.36 (d, J = 7.9 Hz, 1H), 7.15 – 7.00 (m, 4H), 3.87 (s, 3H), 2.44 (s, 3H) ppm . ^{13}C NMR (101 MHz, DMSO) δ = 191.00, 162.35, 143.81, 135.40, 134.12, 131.21, 127.80, 122.08, 121.15, 120.40, 114.02, 113.15, 111.67, 55.87, 14.52 ppm.

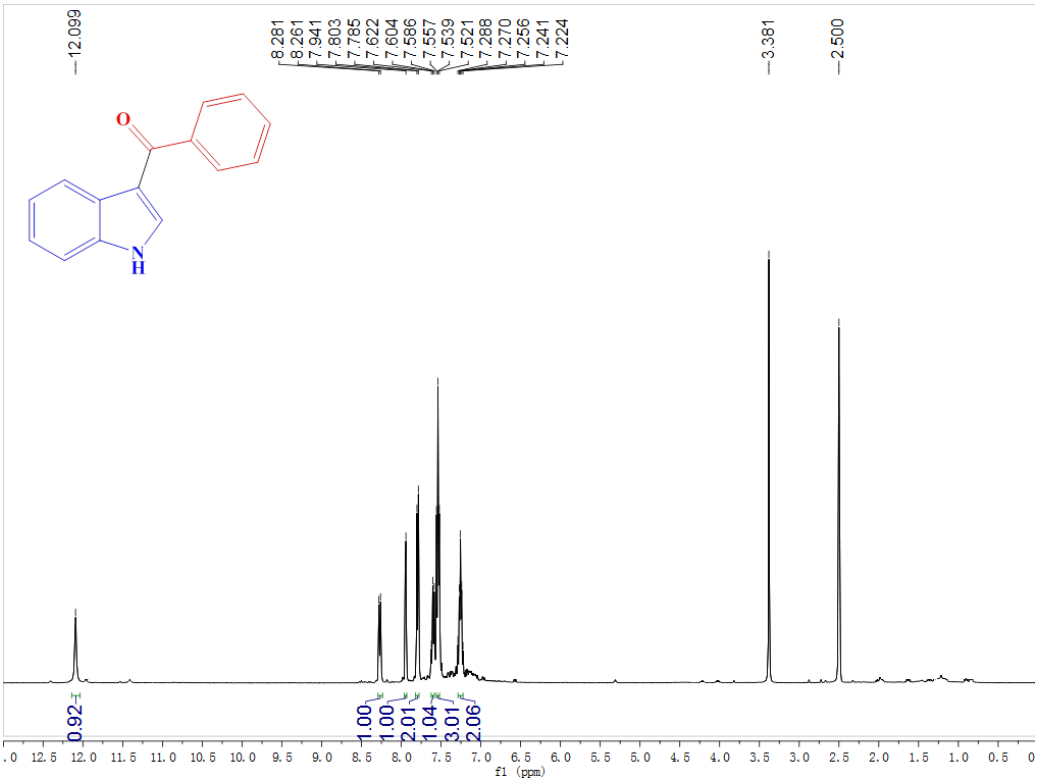
(4-Methoxyphenyl)(2-methyl-1-(2-morpholinoethyl)-1*H*-indol-3-yl)methanone (**4**)

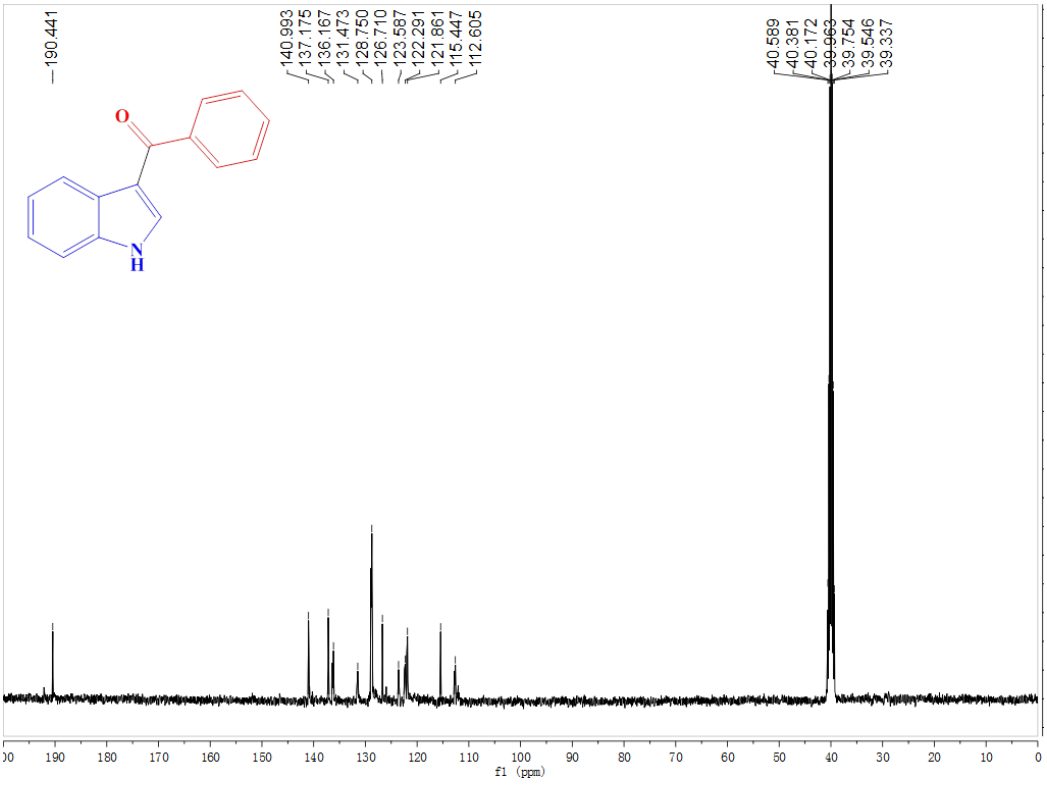


White solid; mp: 104-110 °C; IR (KBr): 3466, 1646, 1576, 1507, 1322, 1211, 1163, 1060, 1037, 896, 741, 616 cm^{-1}; ^{1}H NMR (400 MHz, DMSO) δ = 7.66 (d, J = 8.4 Hz, 2H), 7.55 (d, J = 8.2 Hz, 1H), 7.30 (d, J = 8.0 Hz, 1H), 7.20-7.17 (m, 1H), 7.06-7.04 (m, 3H), 4.36 (t, J = 6.5 Hz, 2H), 3.87 (s, 3H), 3.58-3.56 (m, 4H), 2.65 (t, J = 6.5 Hz, 2H), 2.52 (s, 3H), 2.48-2.46 (m, 4H) ppm . ^{13}C NMR (101 MHz, DMSO) δ = 190.90, 162.60, 144.23, 136.09, 133.88, 131.48, 127.19, 122.18, 121.47, 120.42, 114.08, 113.34, 110.63, 66.70, 57.59, 55.91, 54.11, 12.77 ppm.

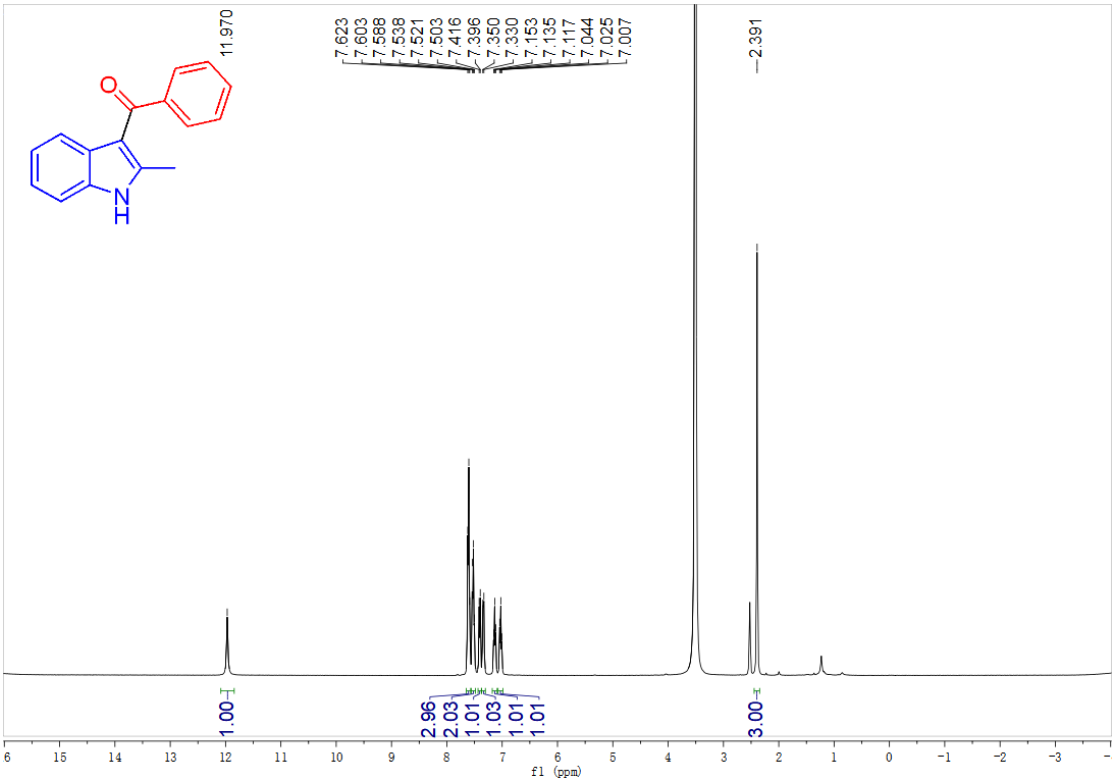
Copies of NMR spectra for all products

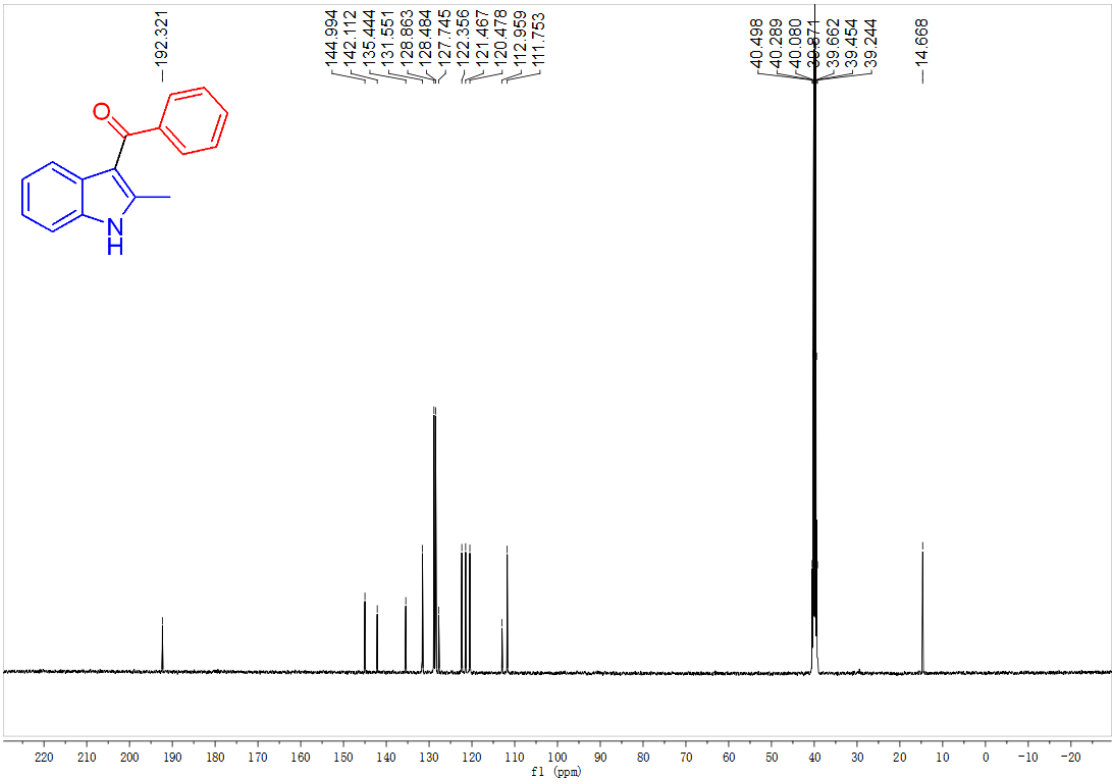
^{1}H NMR and ^{13}C NMR of compound **3a**



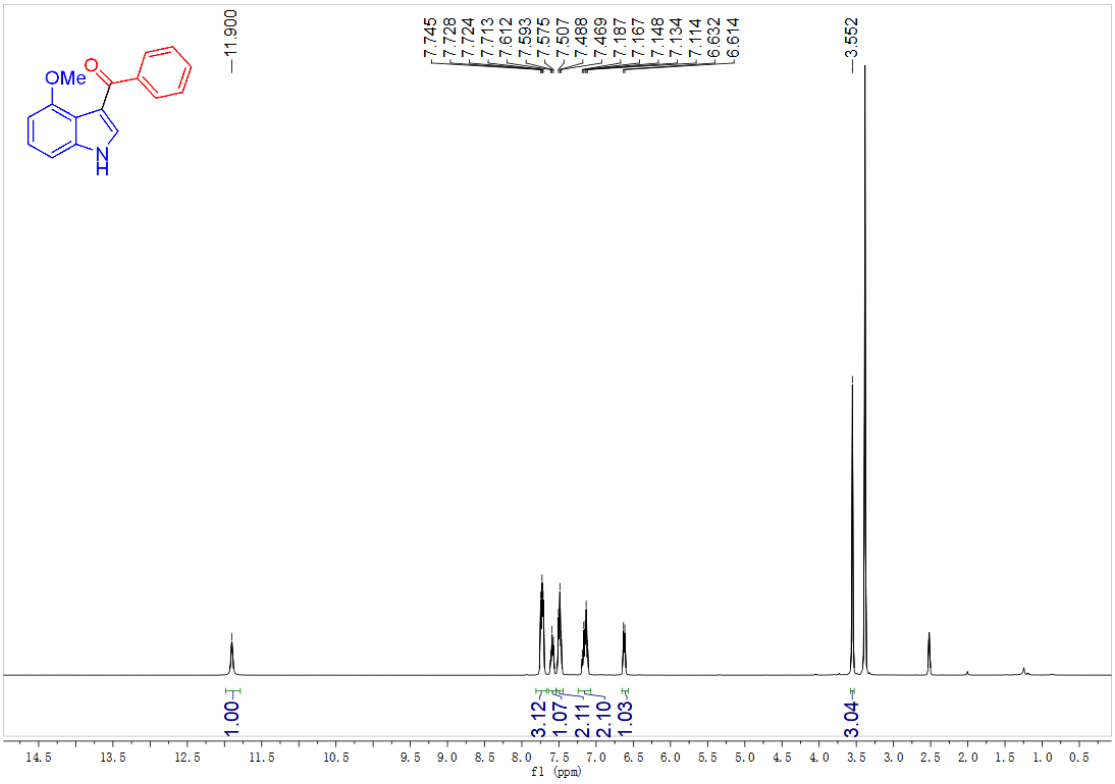


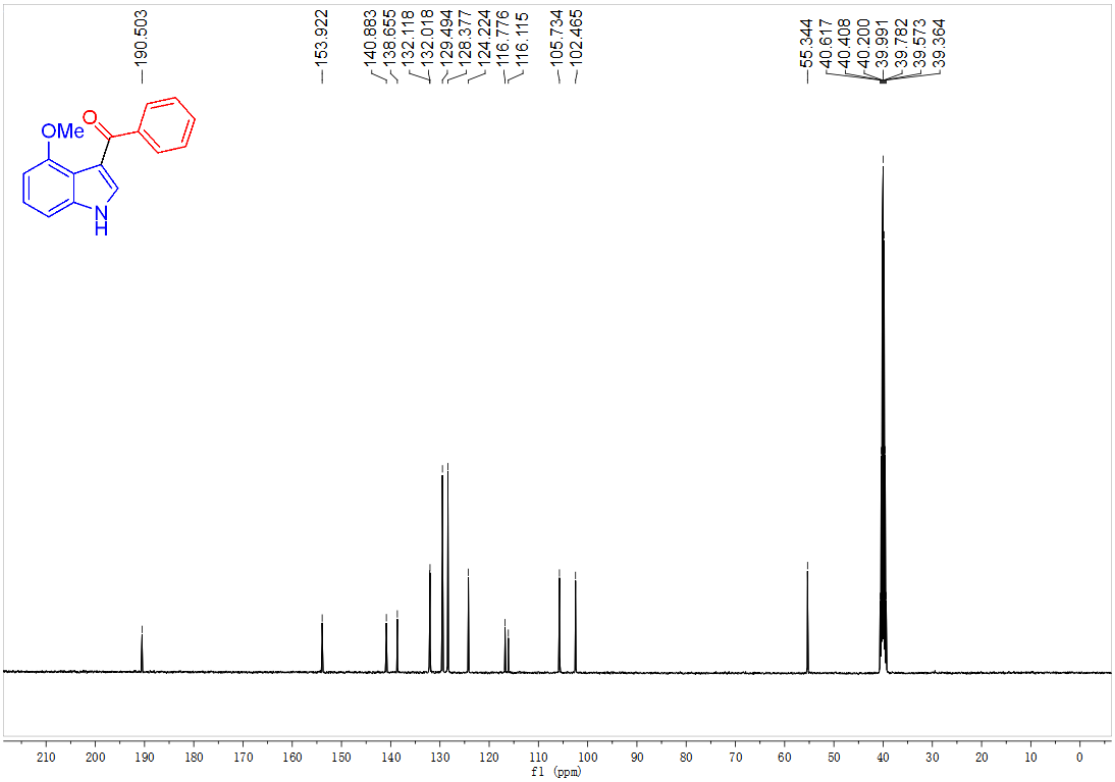
^{1}H NMR and ^{13}C NMR of compound **3b**



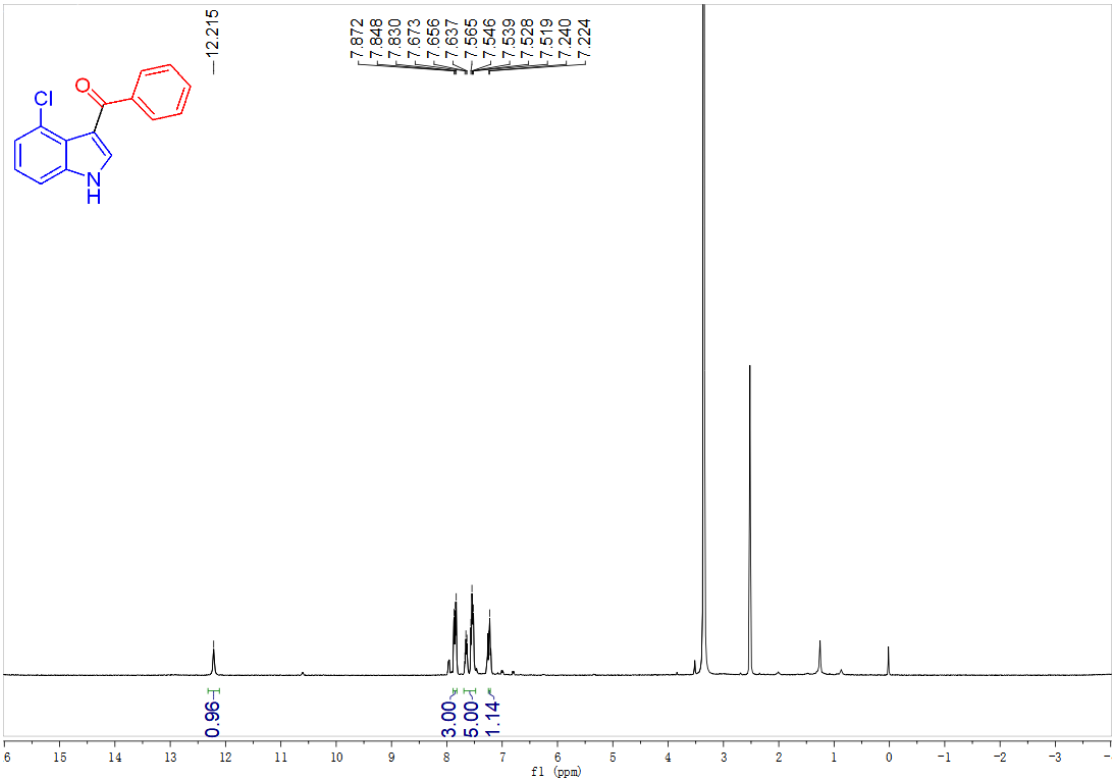


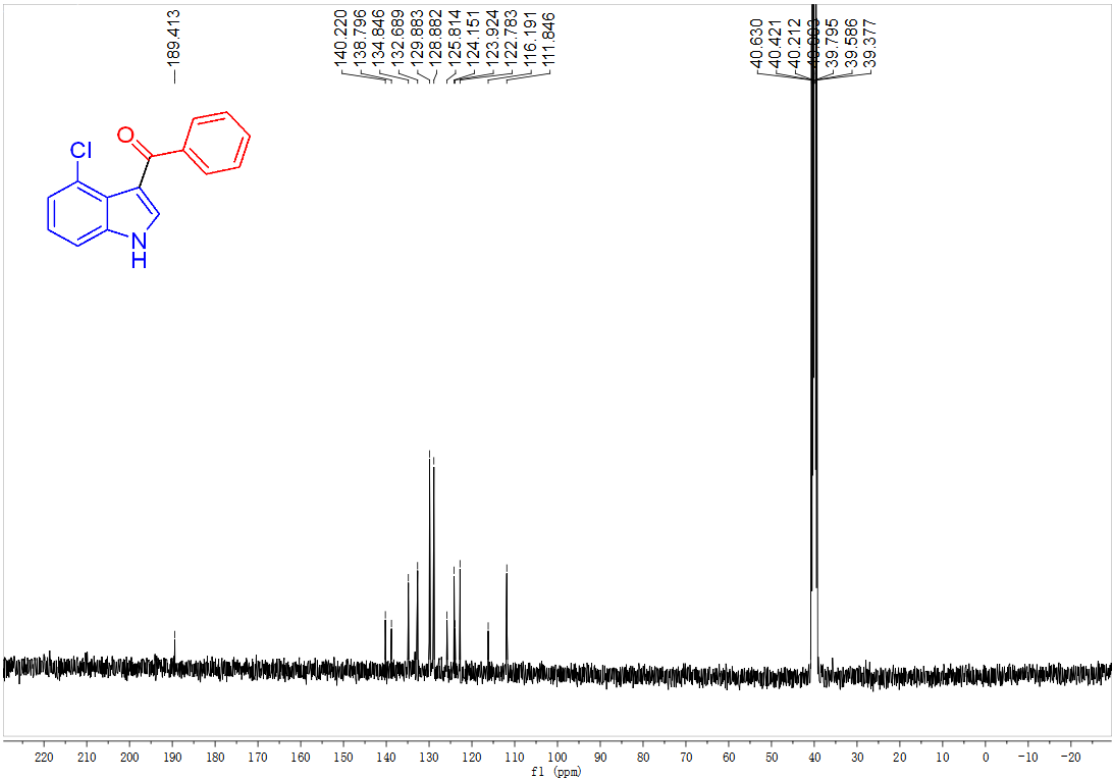
^{1}H NMR and ^{13}C NMR of compound **3c**



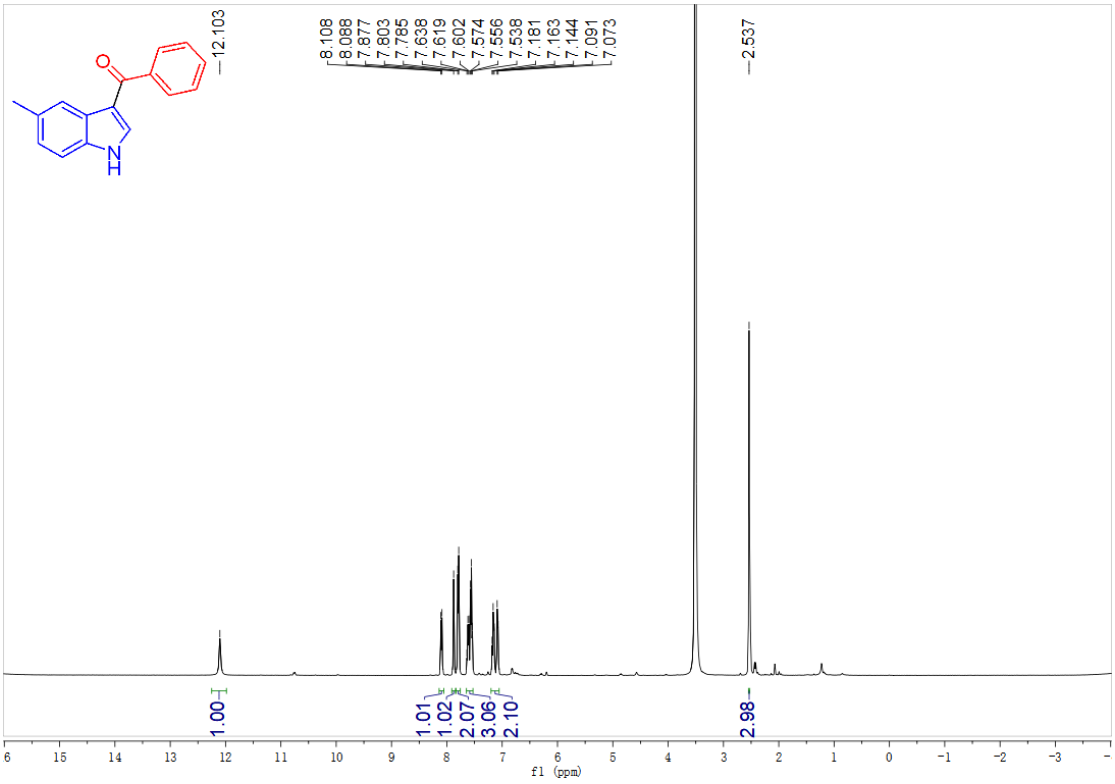


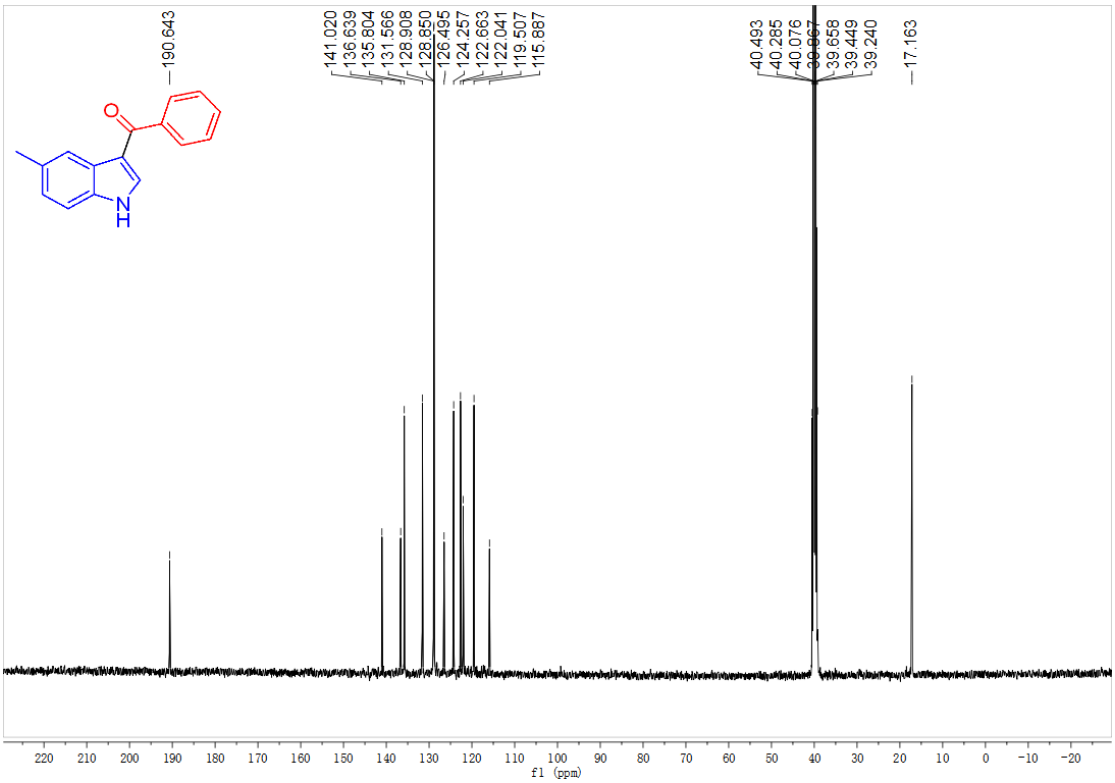
^{1}H NMR and ^{13}C NMR of compound **3d**



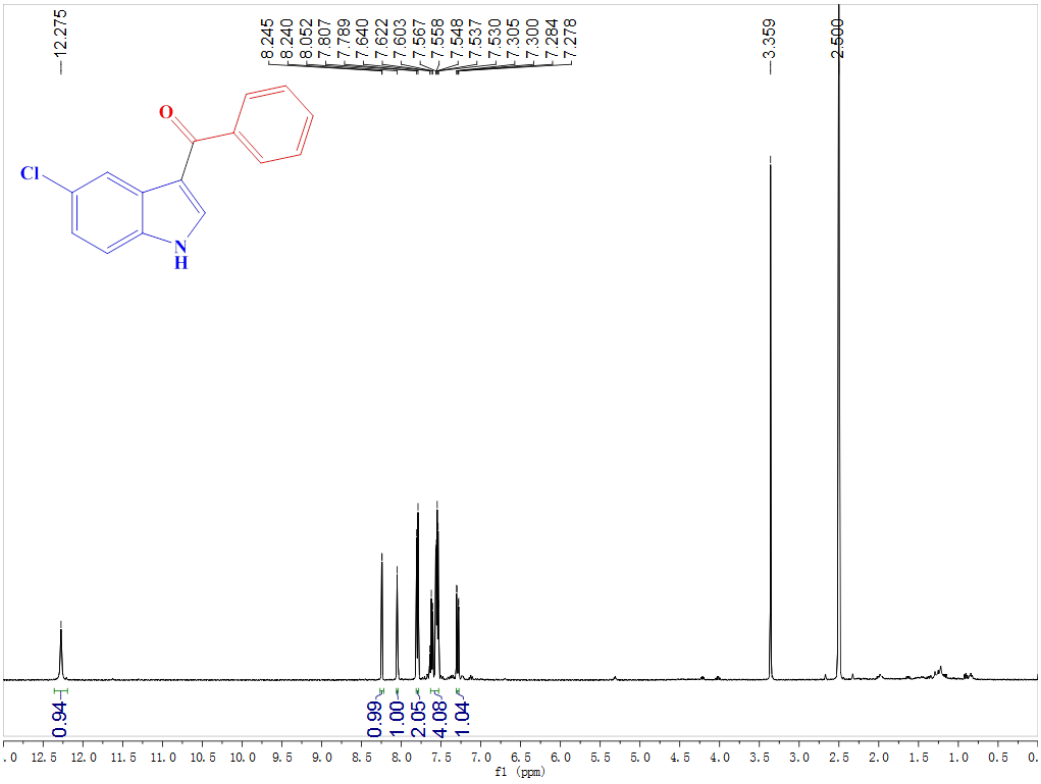


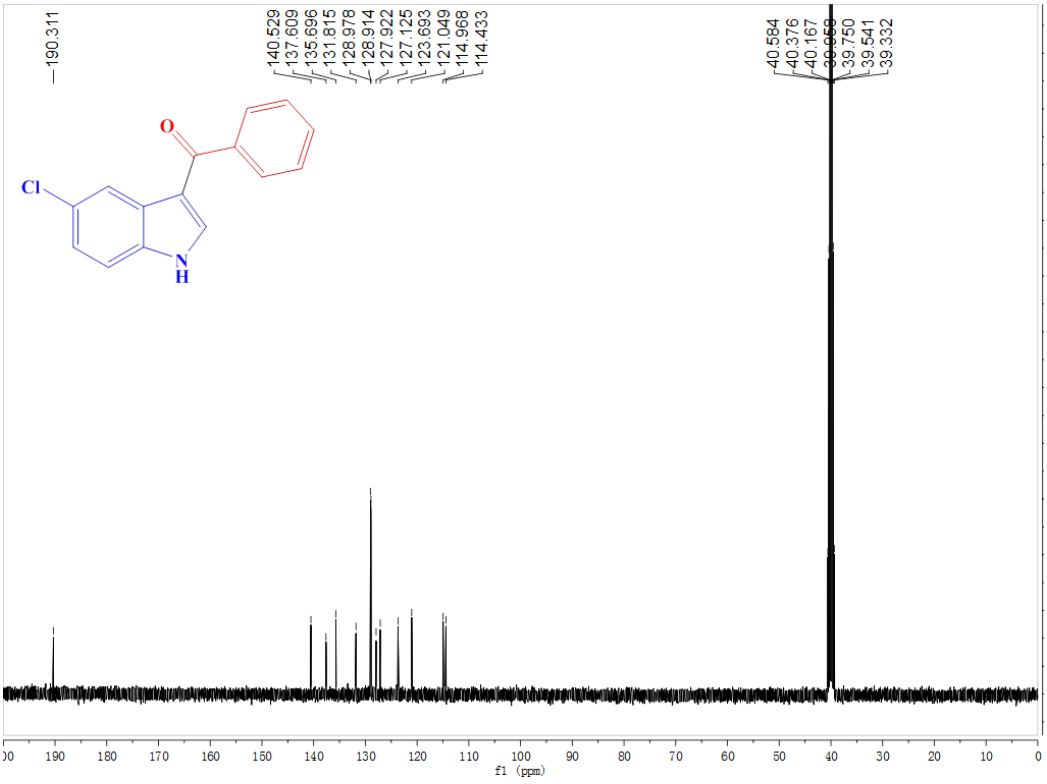
^{1}H NMR and ^{13}C NMR of compound **3e**



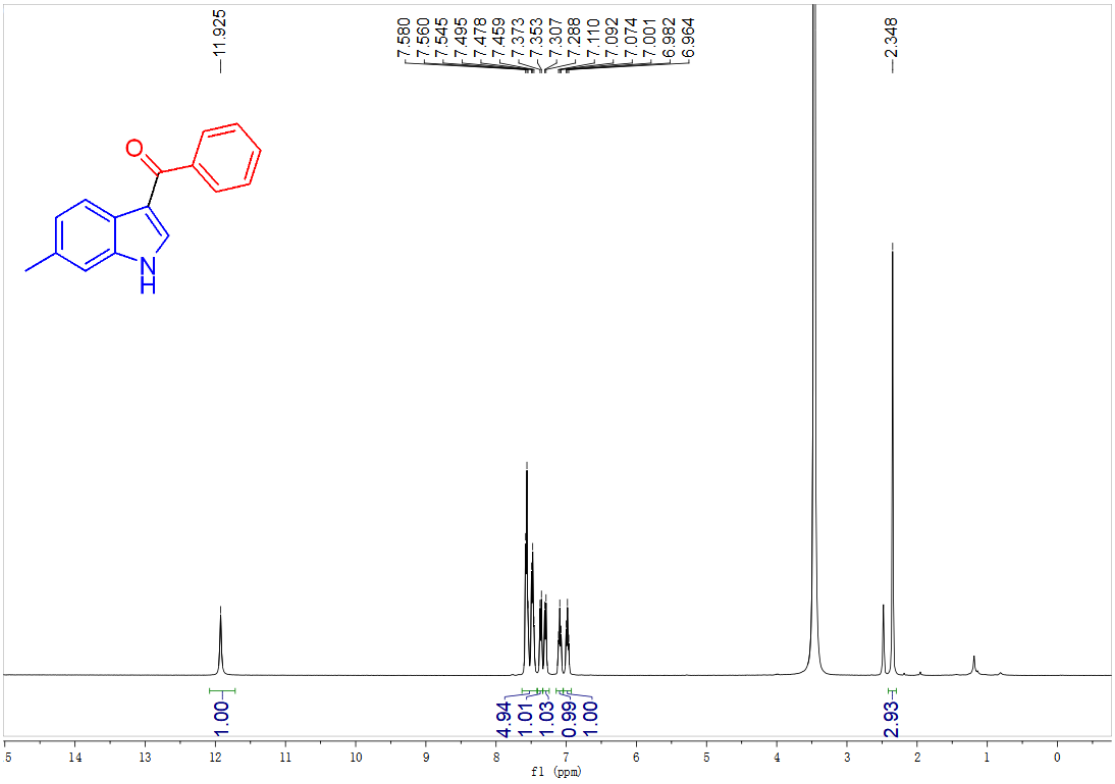


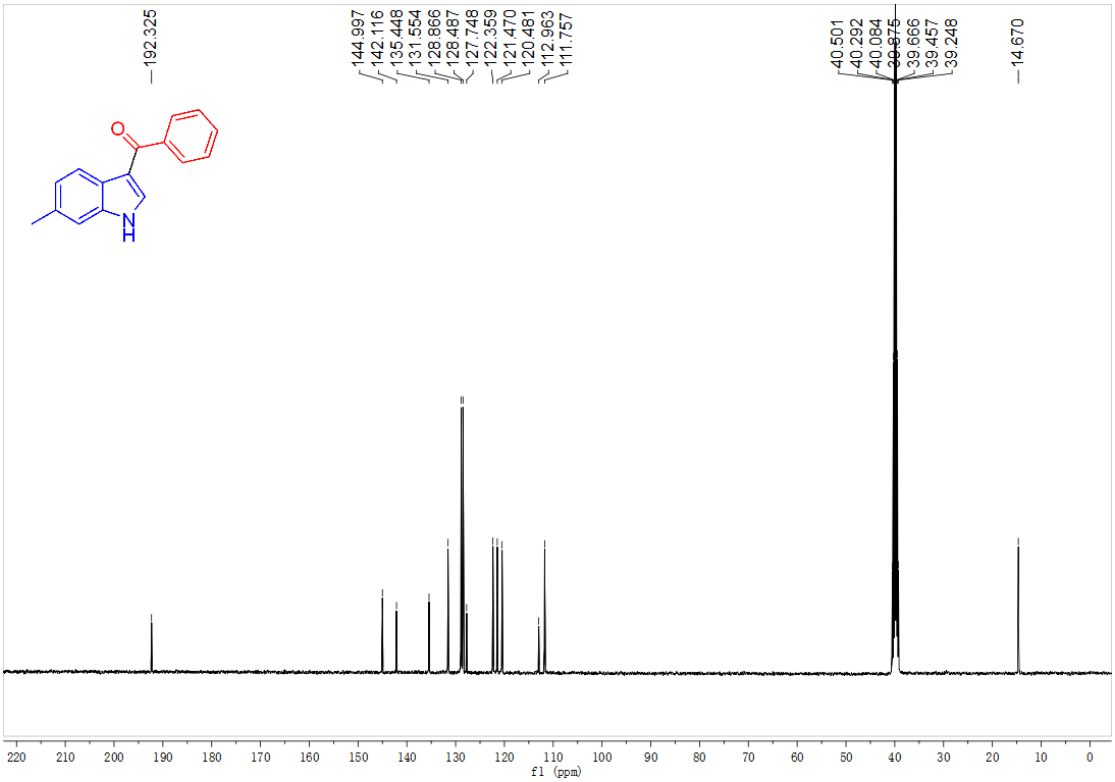
^{1}H NMR and ^{13}C NMR of compound **3f**



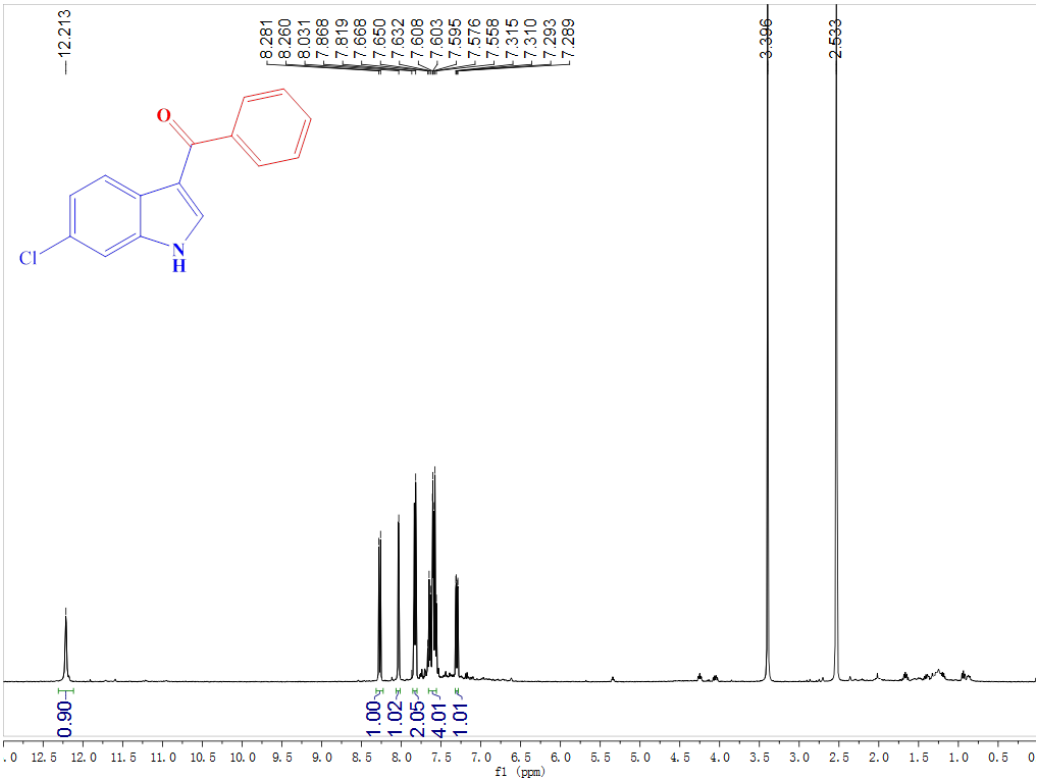


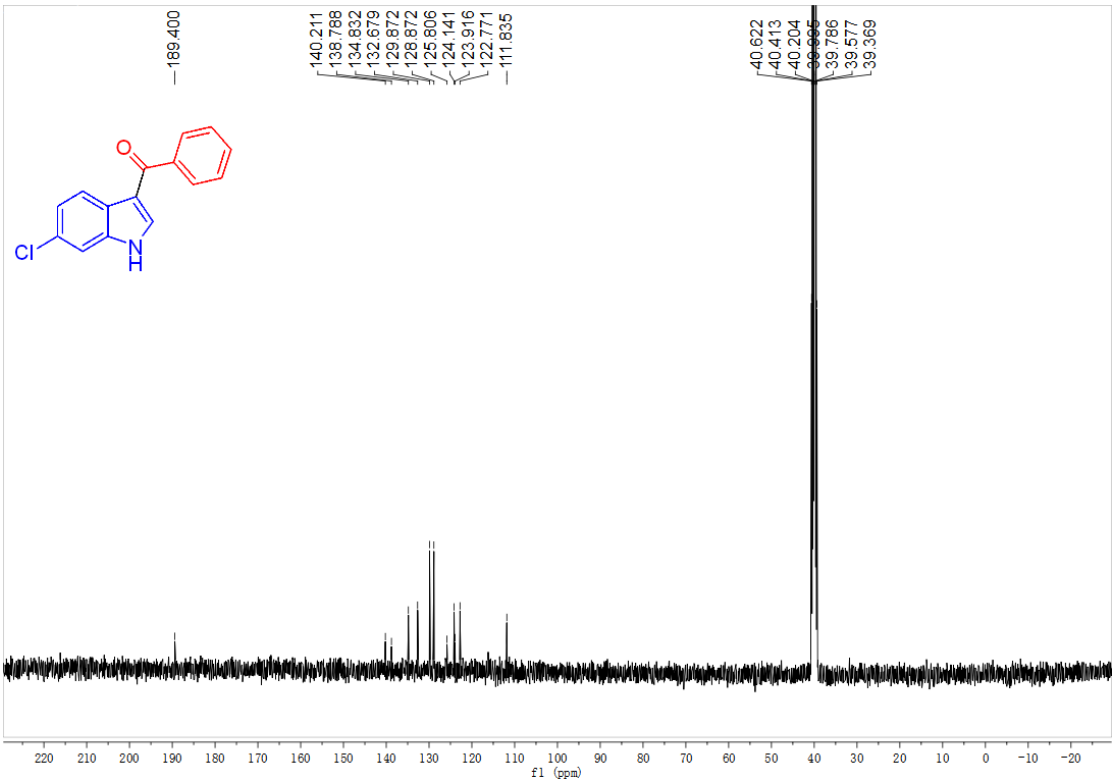
^{1}H NMR and ^{13}C NMR of compound **3g**



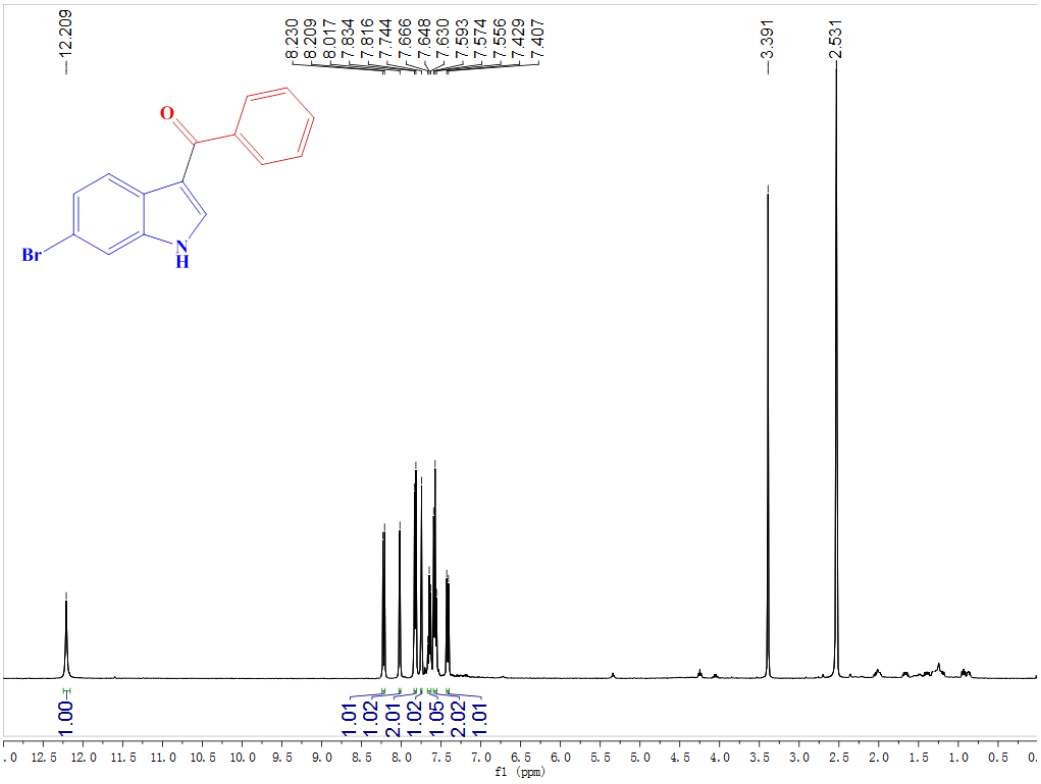


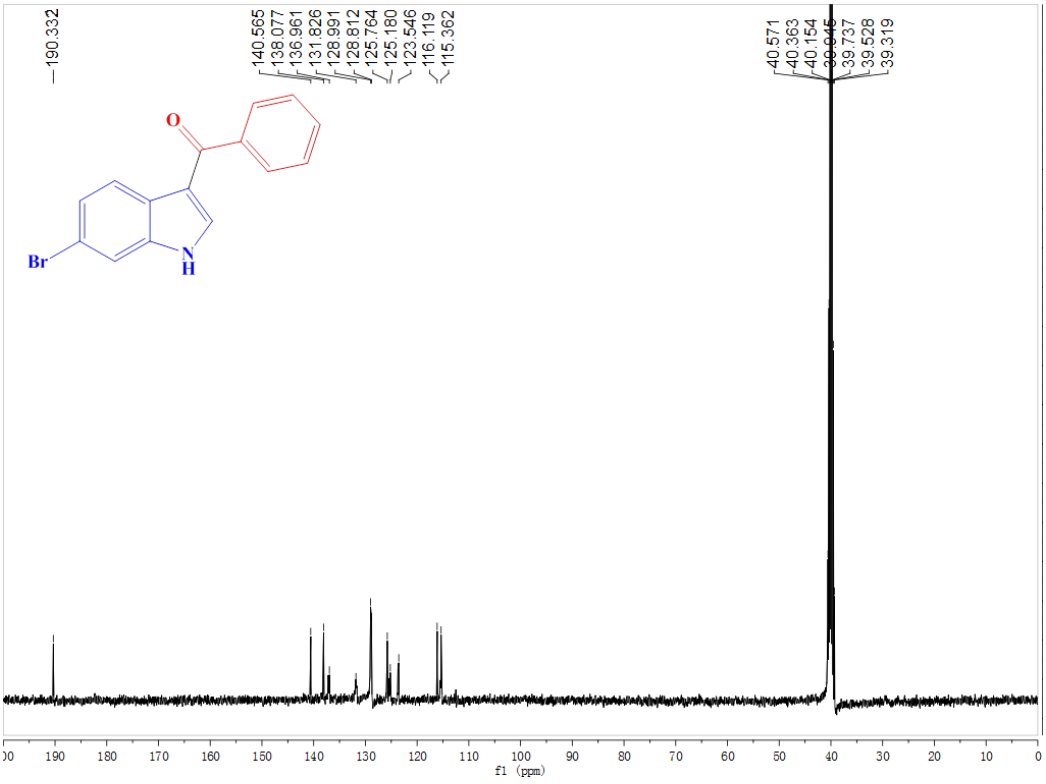
^{1}H NMR and ^{13}C NMR of compound **3h**



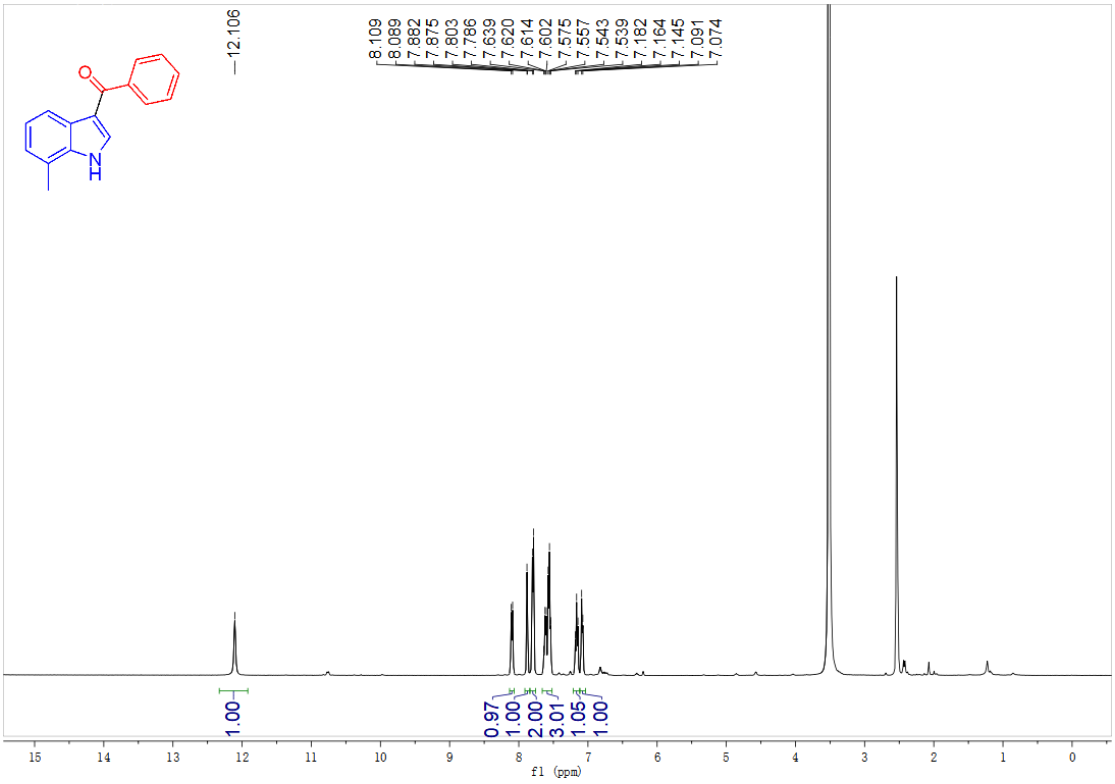


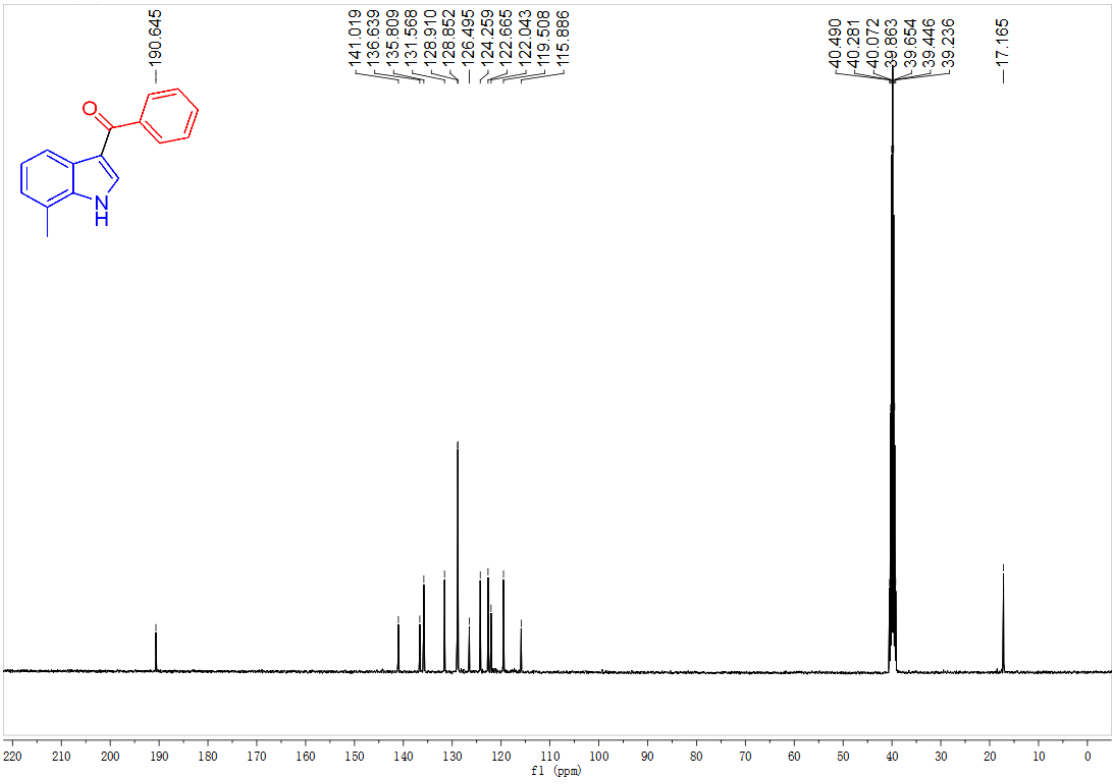
^{1}H NMR and ^{13}C NMR of compound **3i**



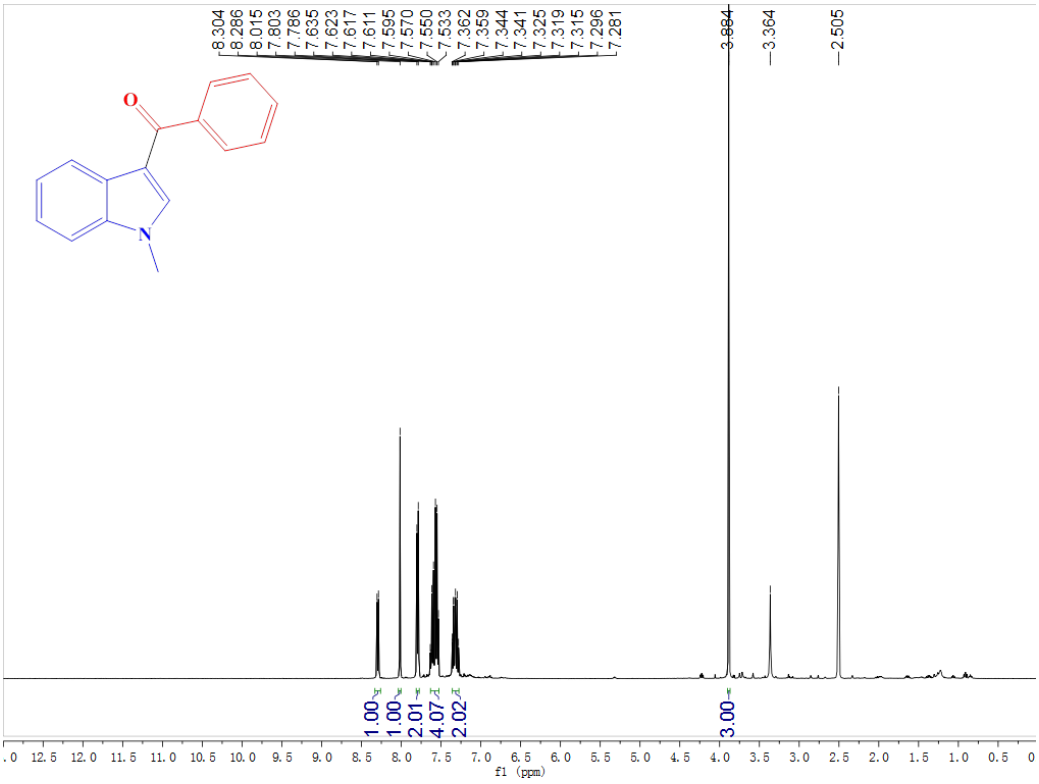


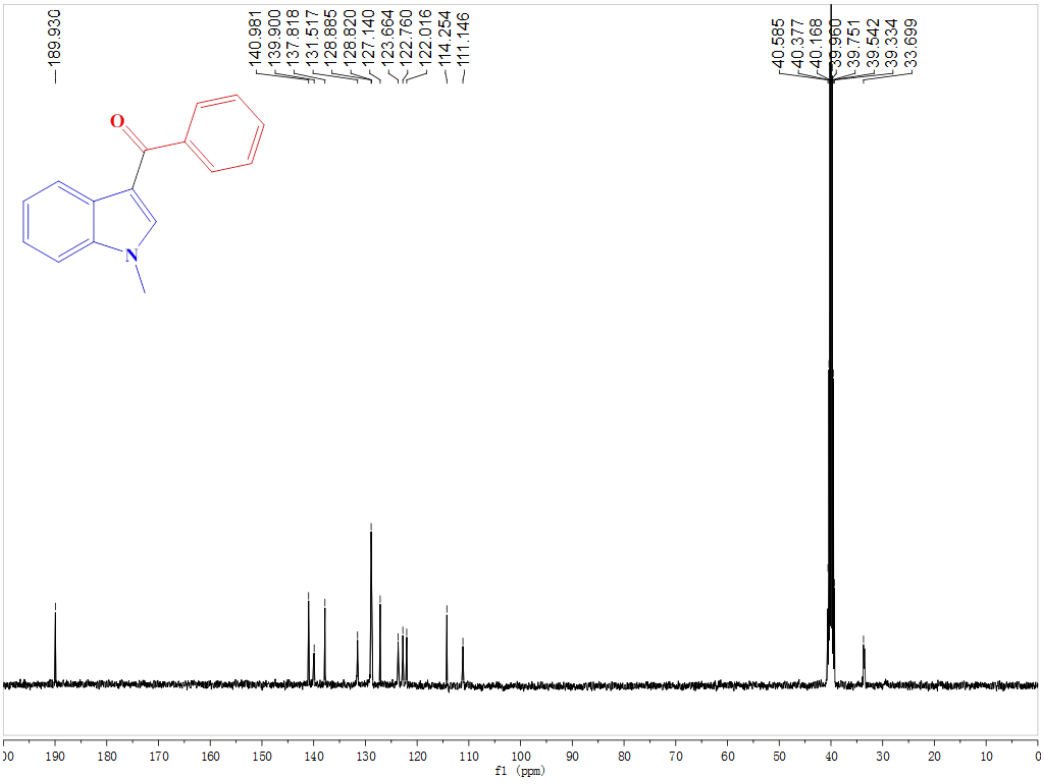
^{1}H NMR and ^{13}C NMR of compound **3j**



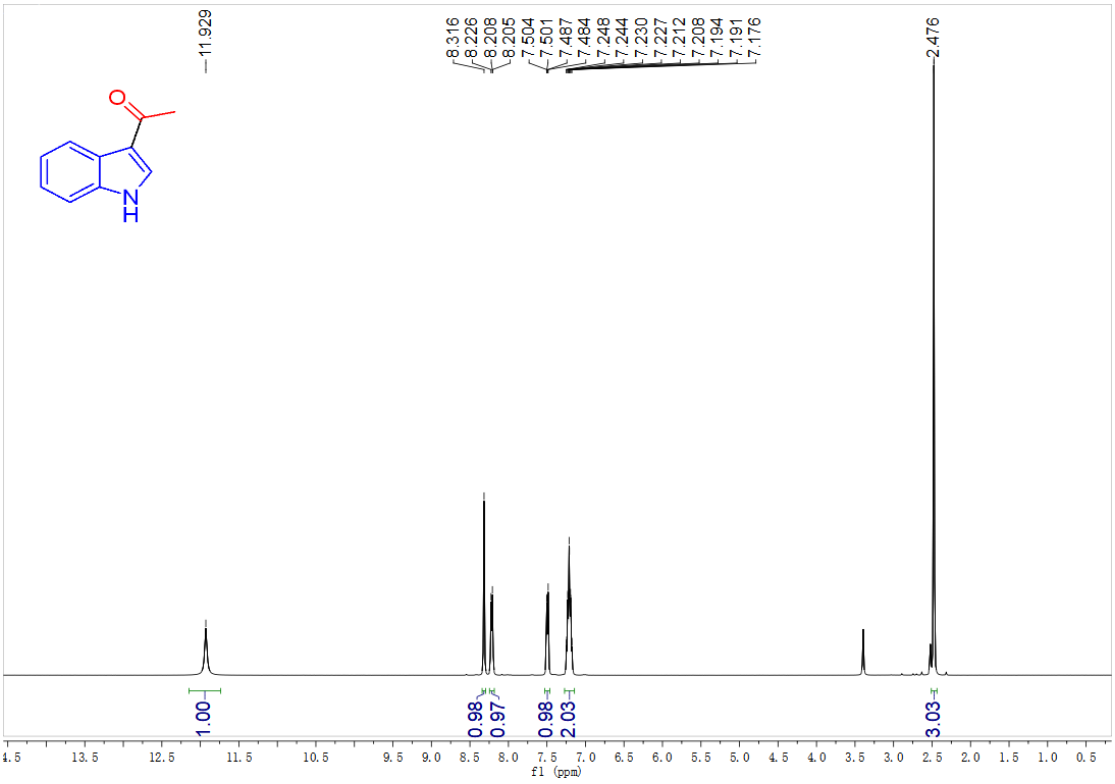


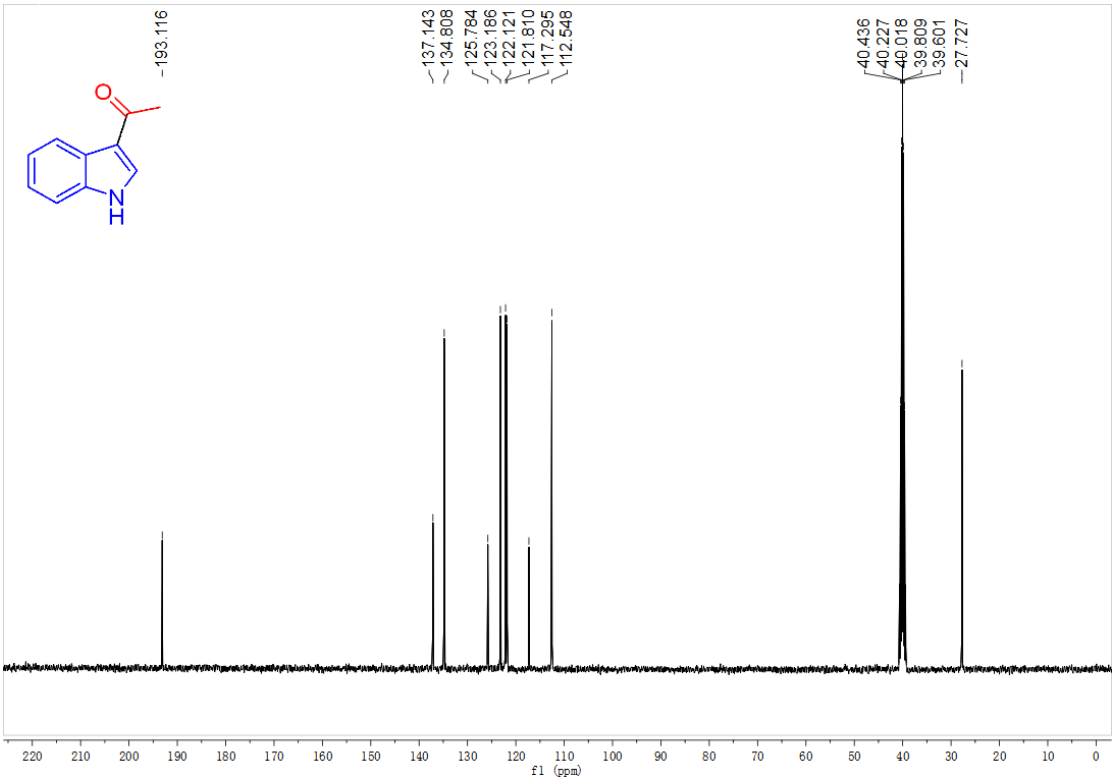
^{1}H NMR and ^{13}C NMR of compound **3k**



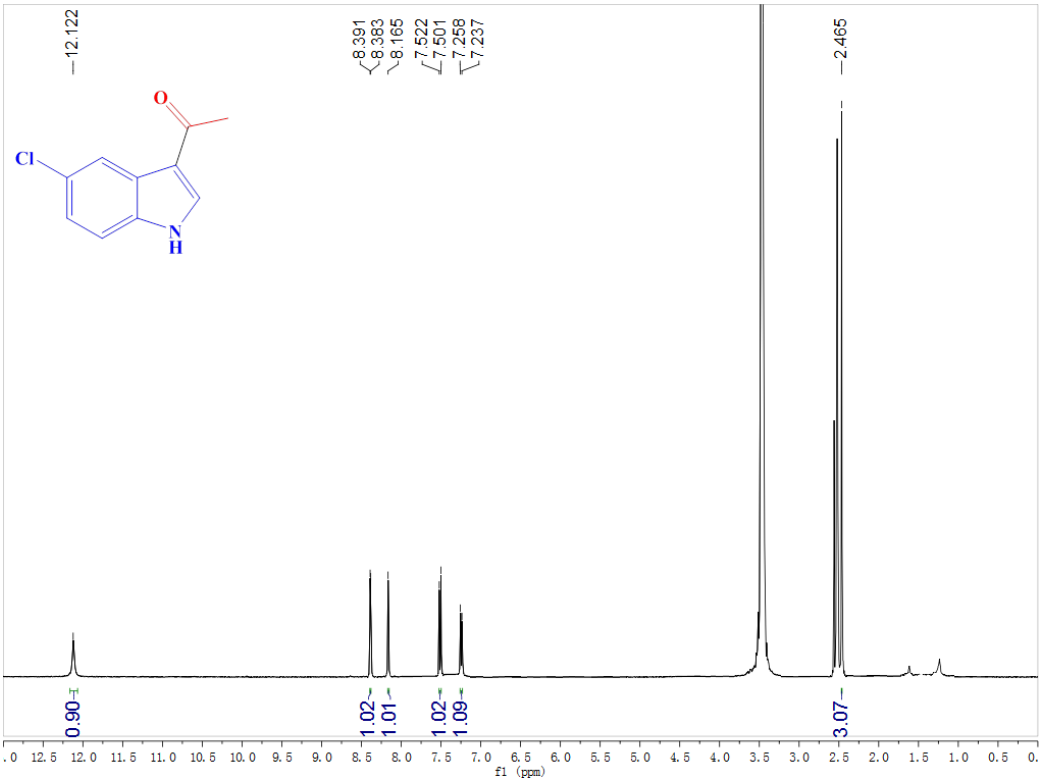


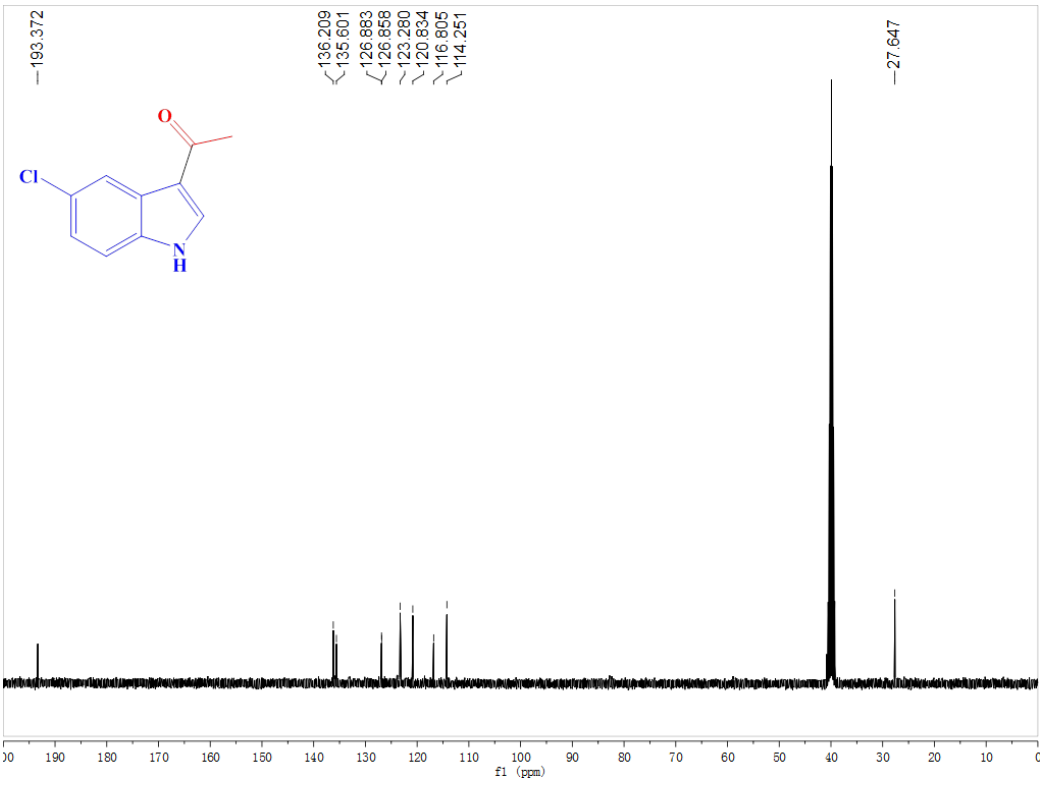
^{1}H NMR and ^{13}C NMR of compound **3l**



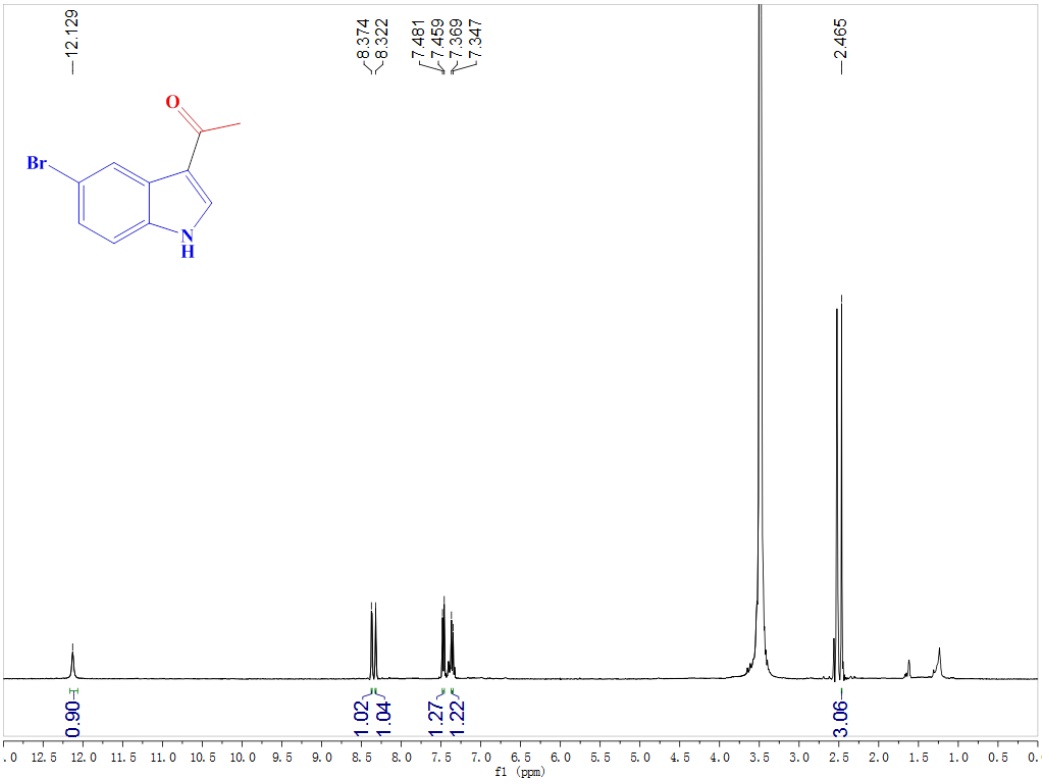


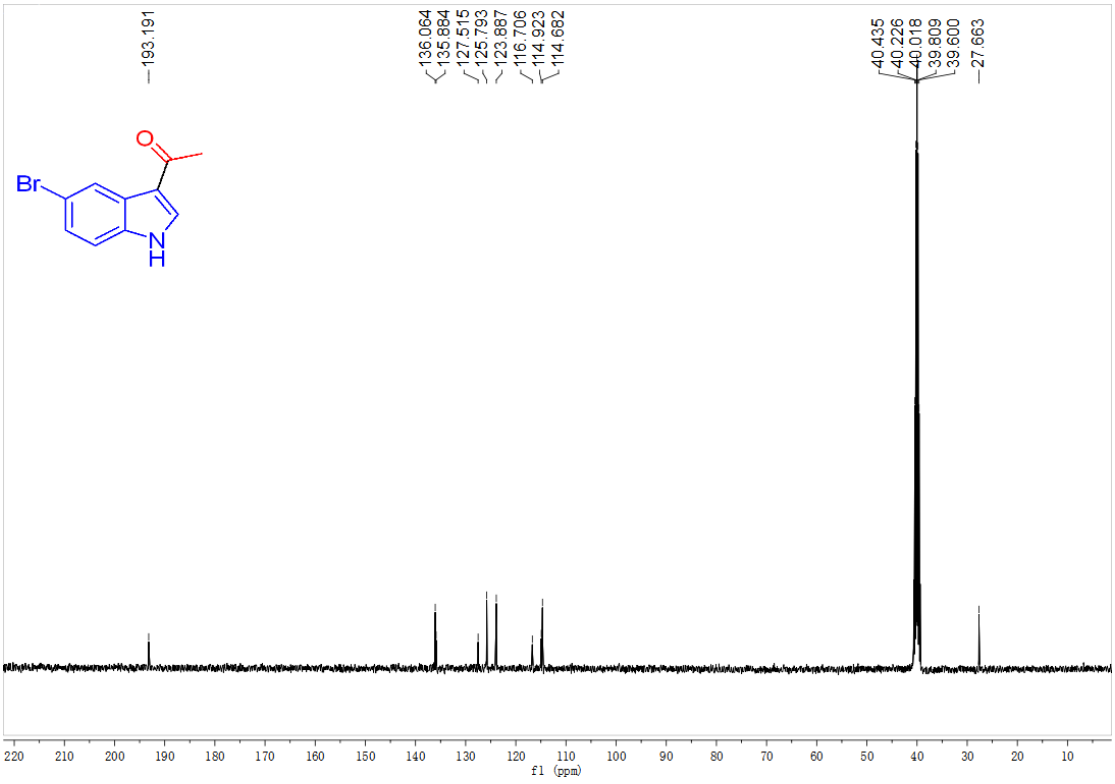
^{1}H NMR and ^{13}C NMR of compound **3m**



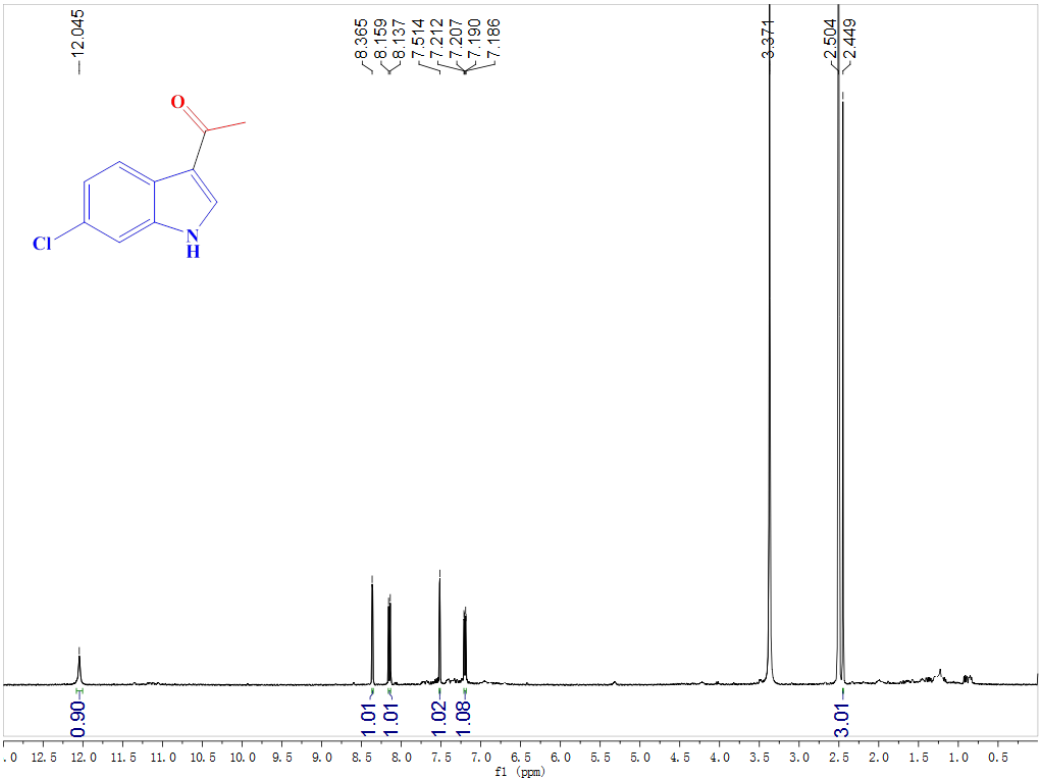


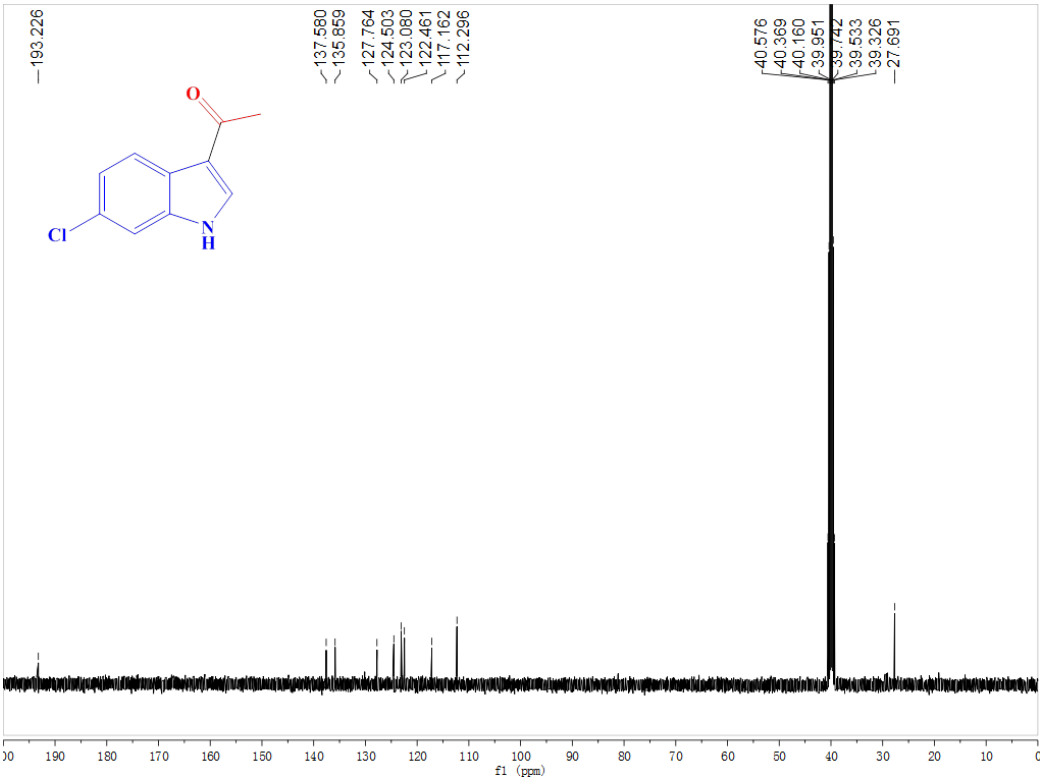
^{1}H NMR and ^{13}C NMR of compound **3n**



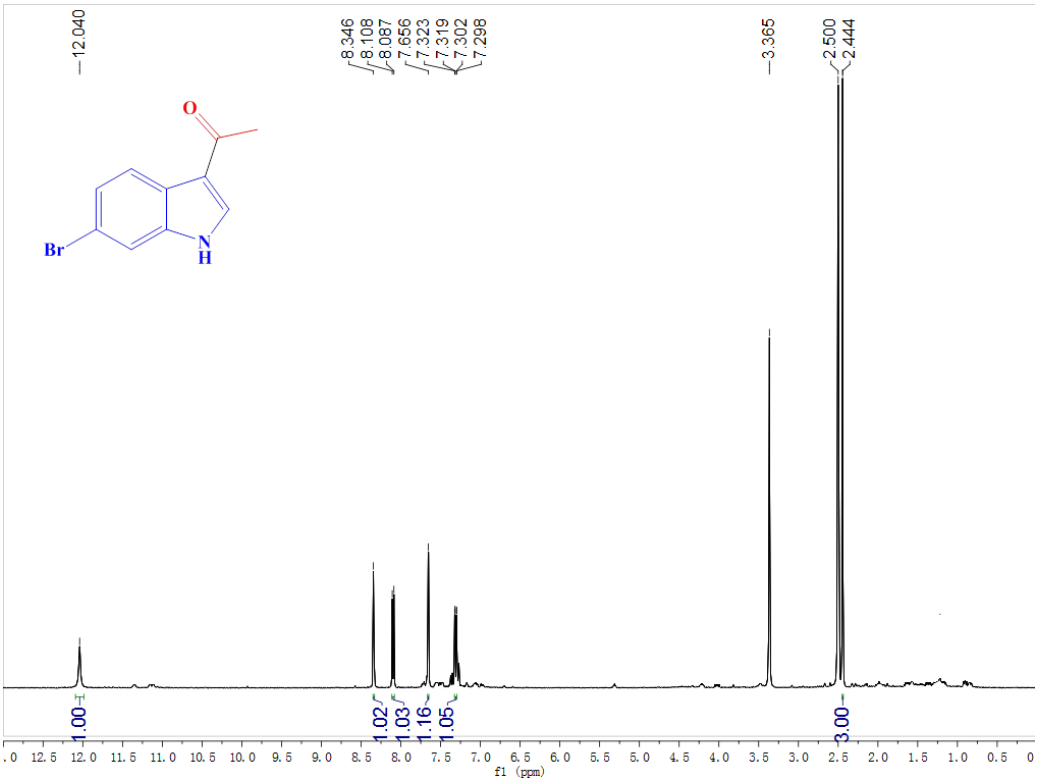


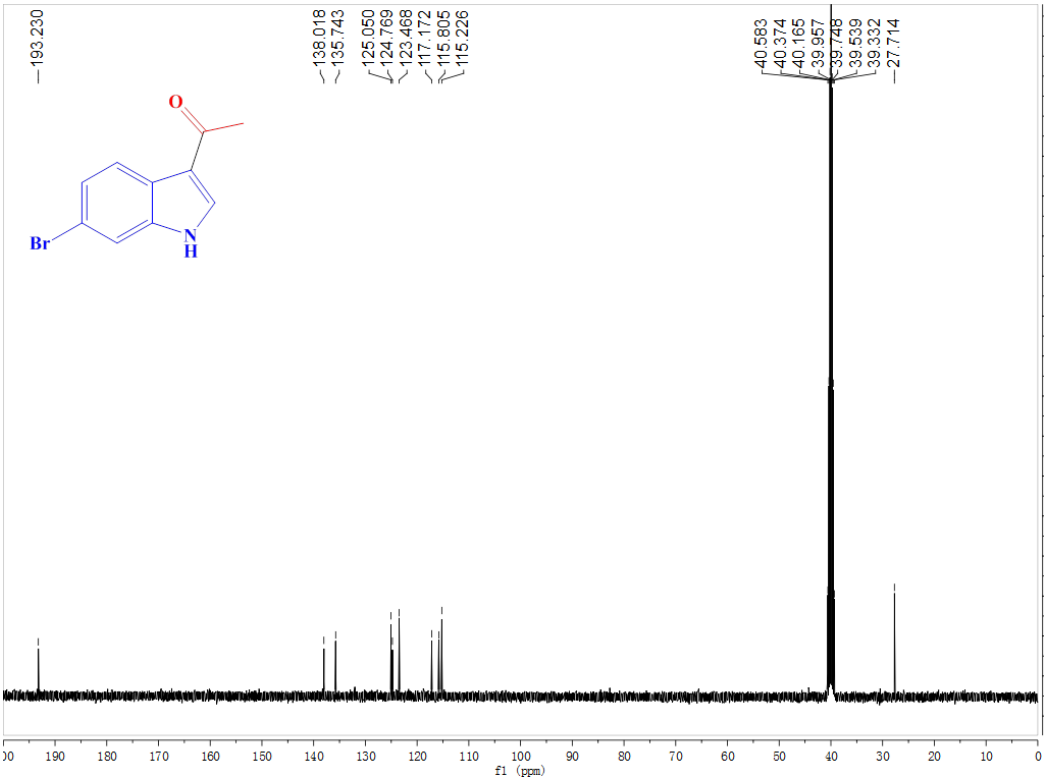
^{1}H NMR and ^{13}C NMR of compound **3o**



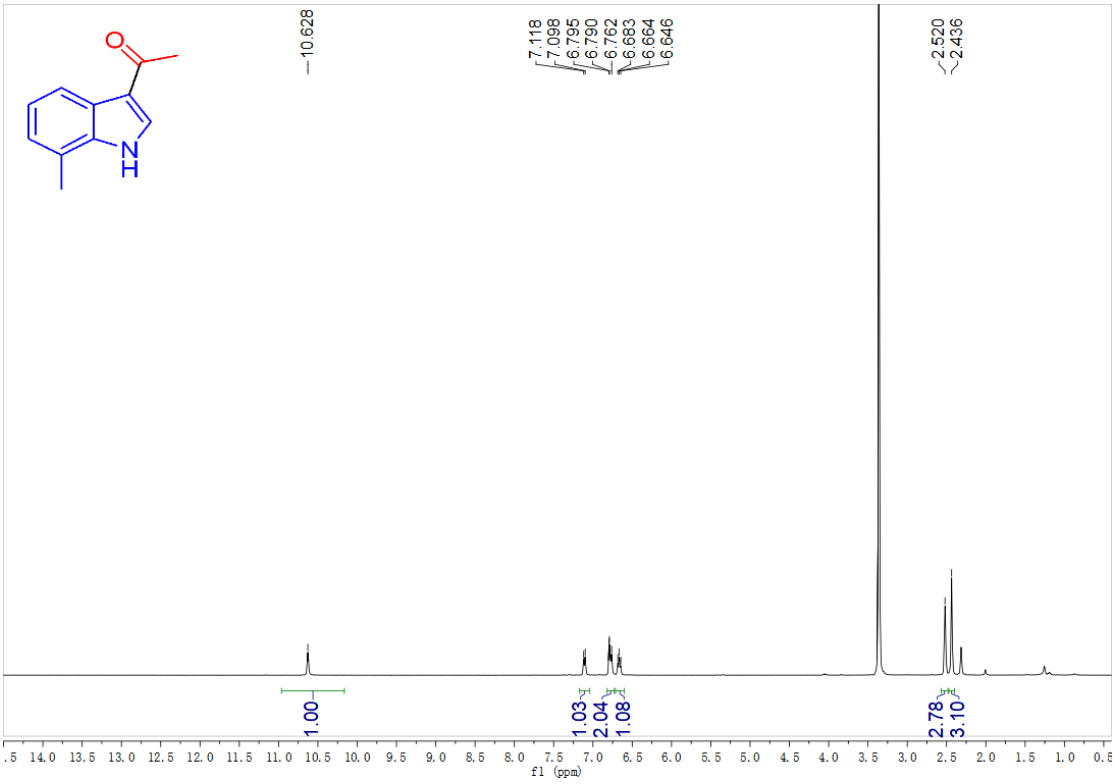


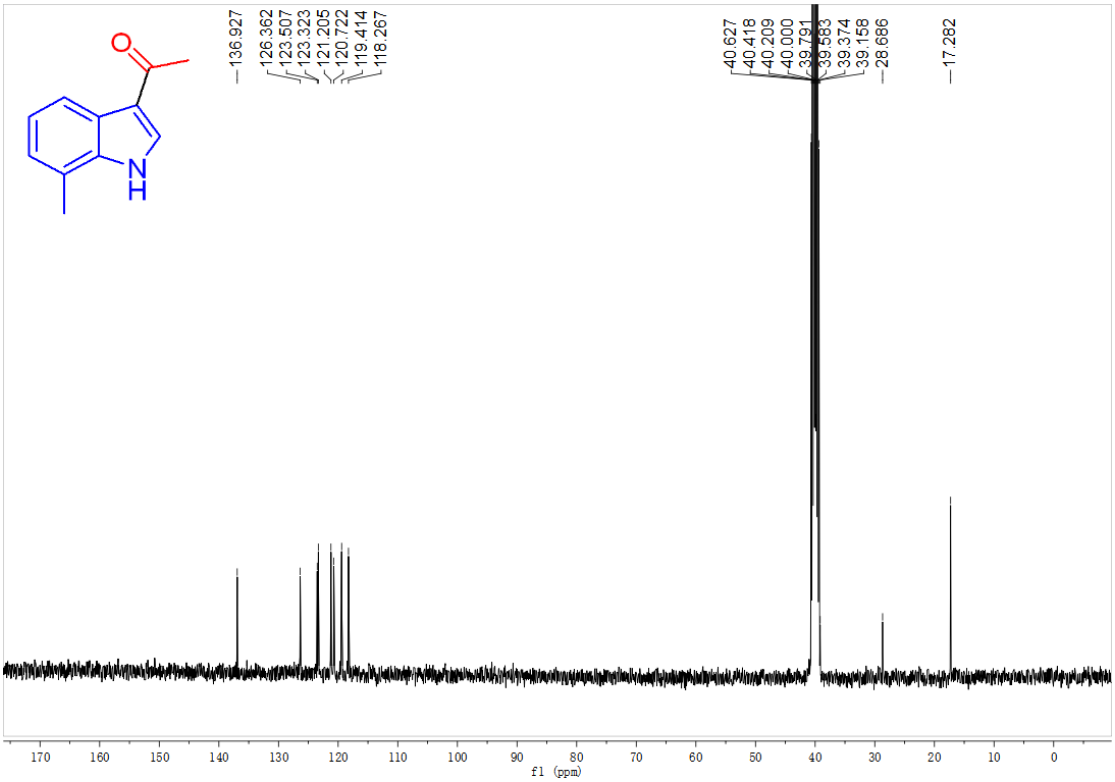
^{1}H NMR and ^{13}C NMR of compound **3p**



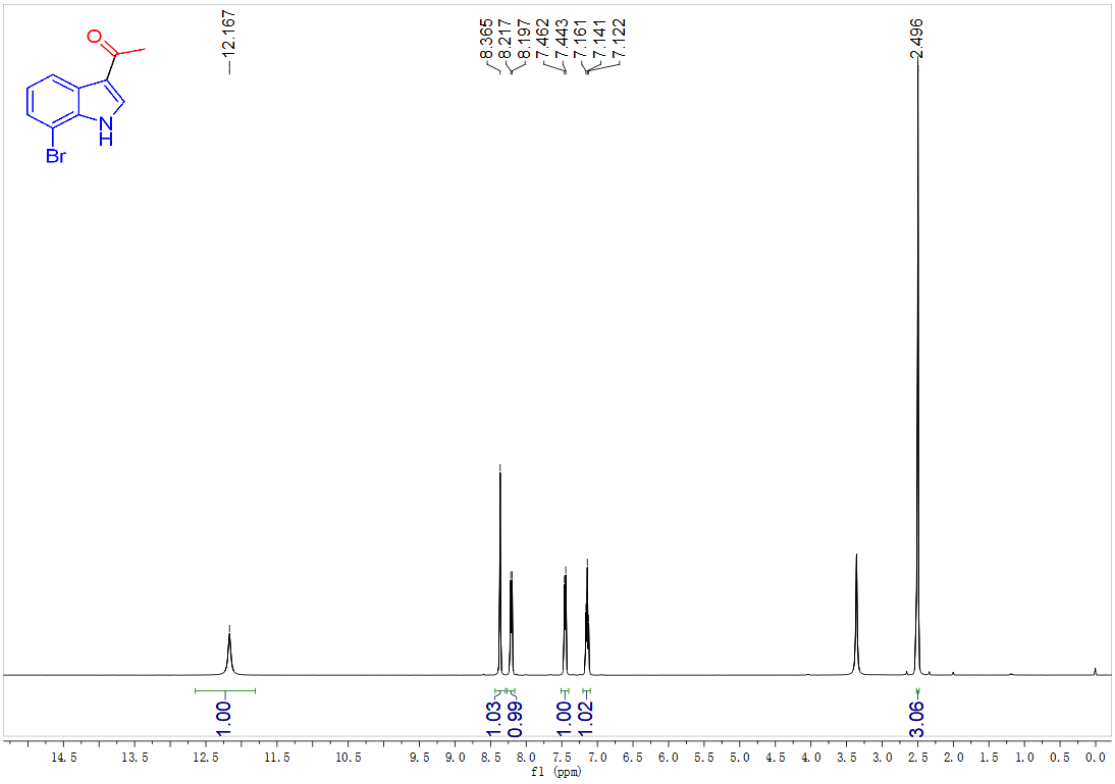


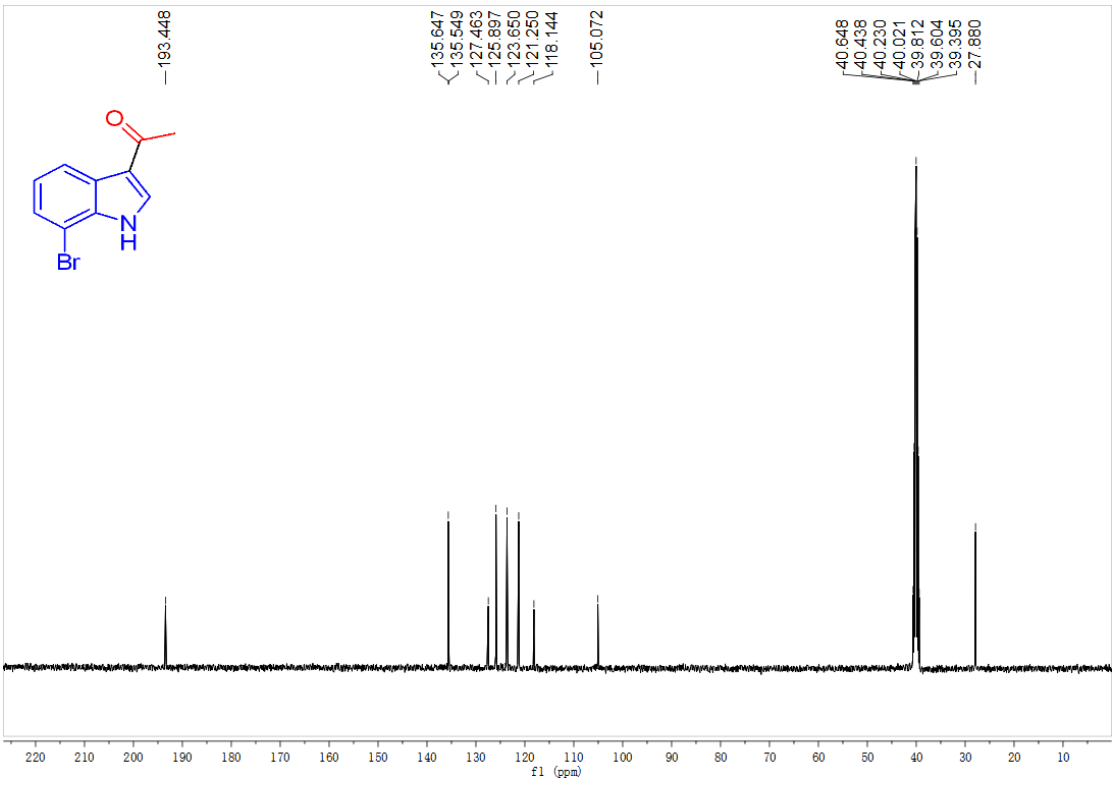
^{1}H NMR and ^{13}C NMR of compound **3q**



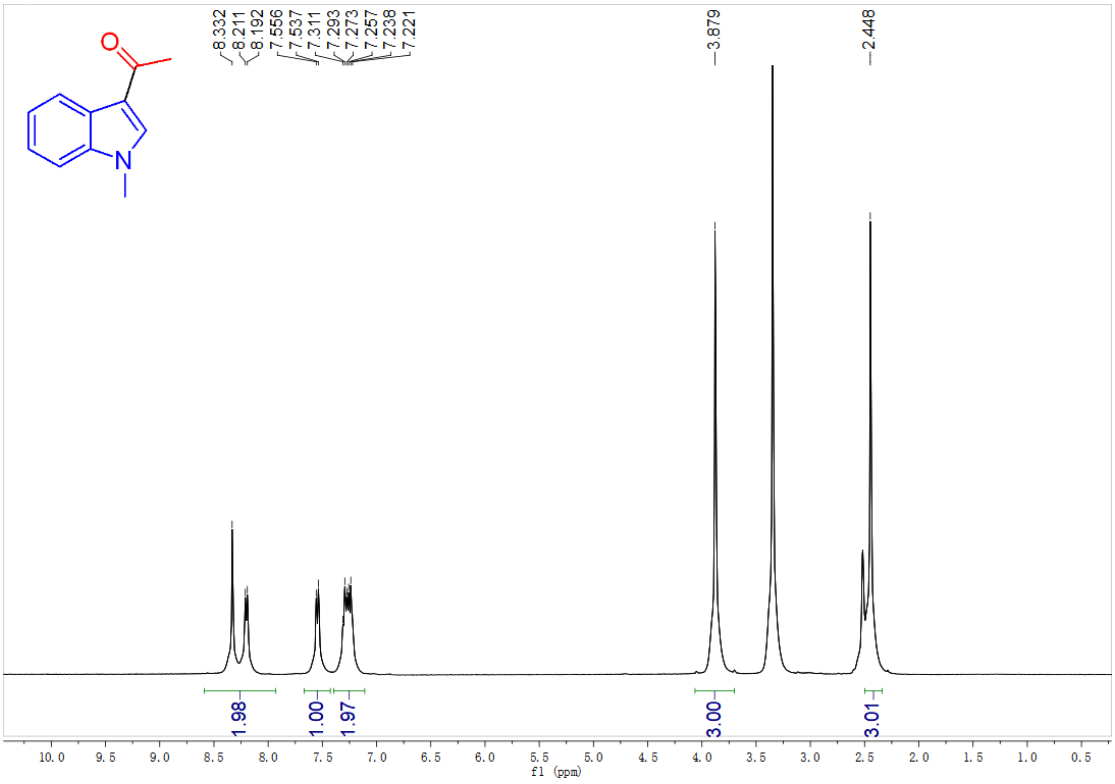


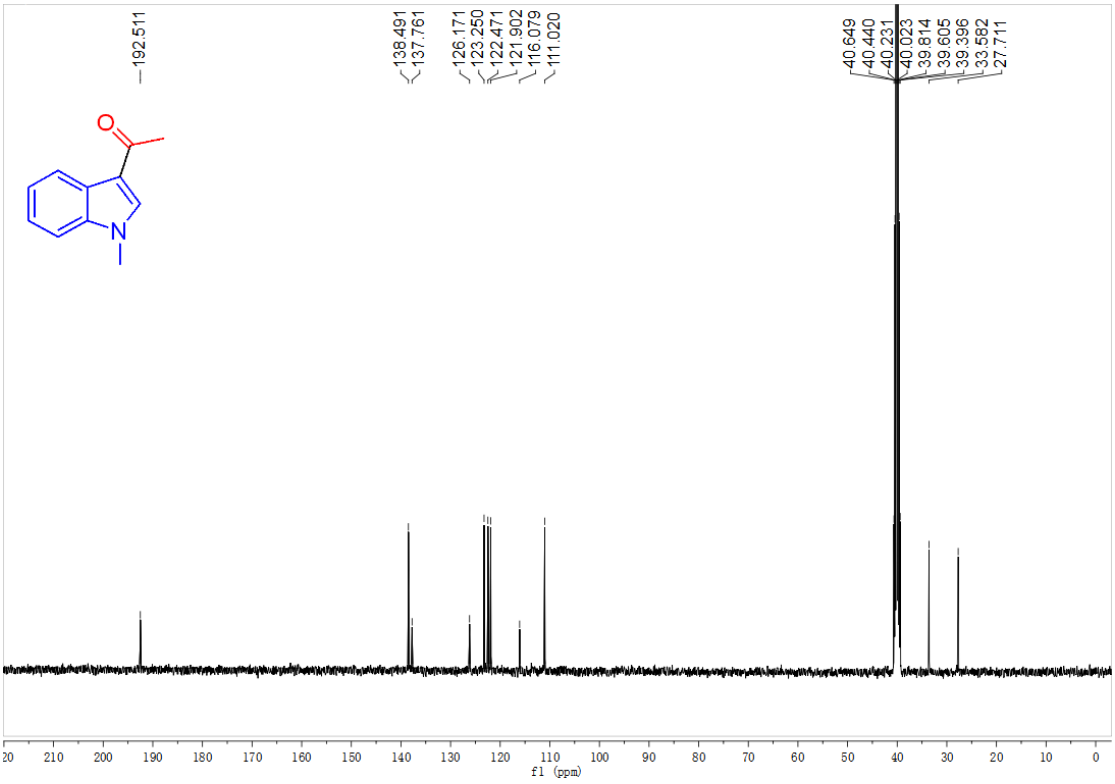
^{1}H NMR and ^{13}C NMR of compound **3r**



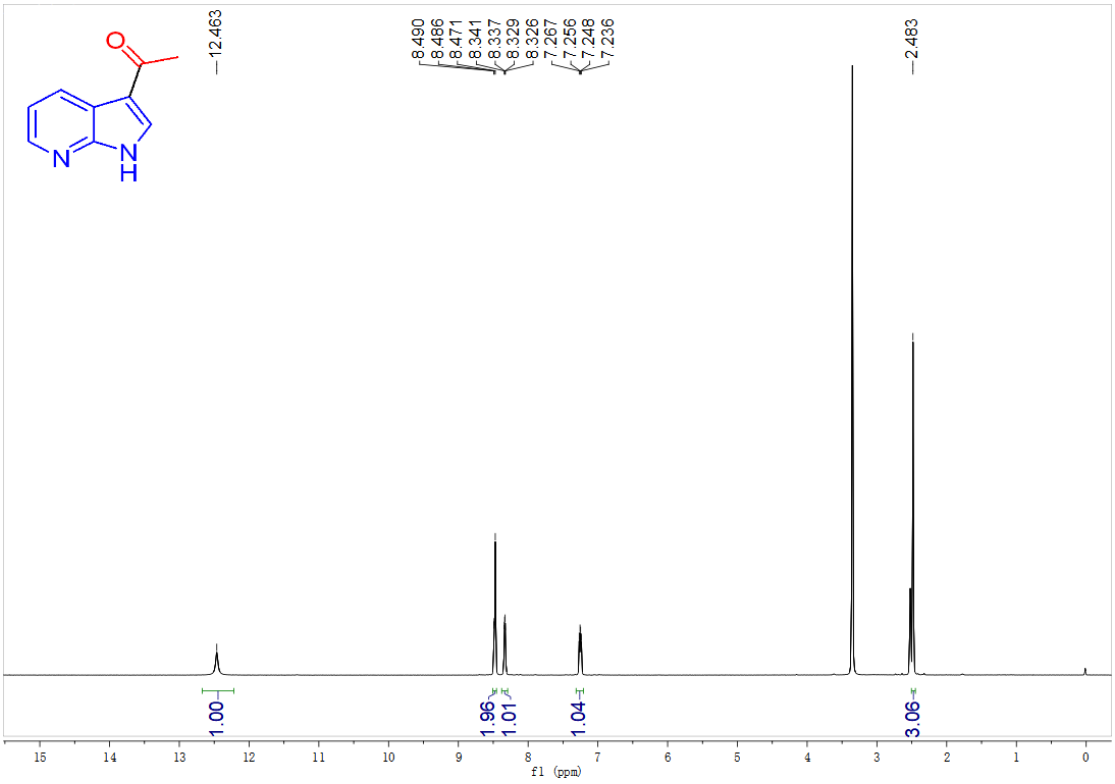


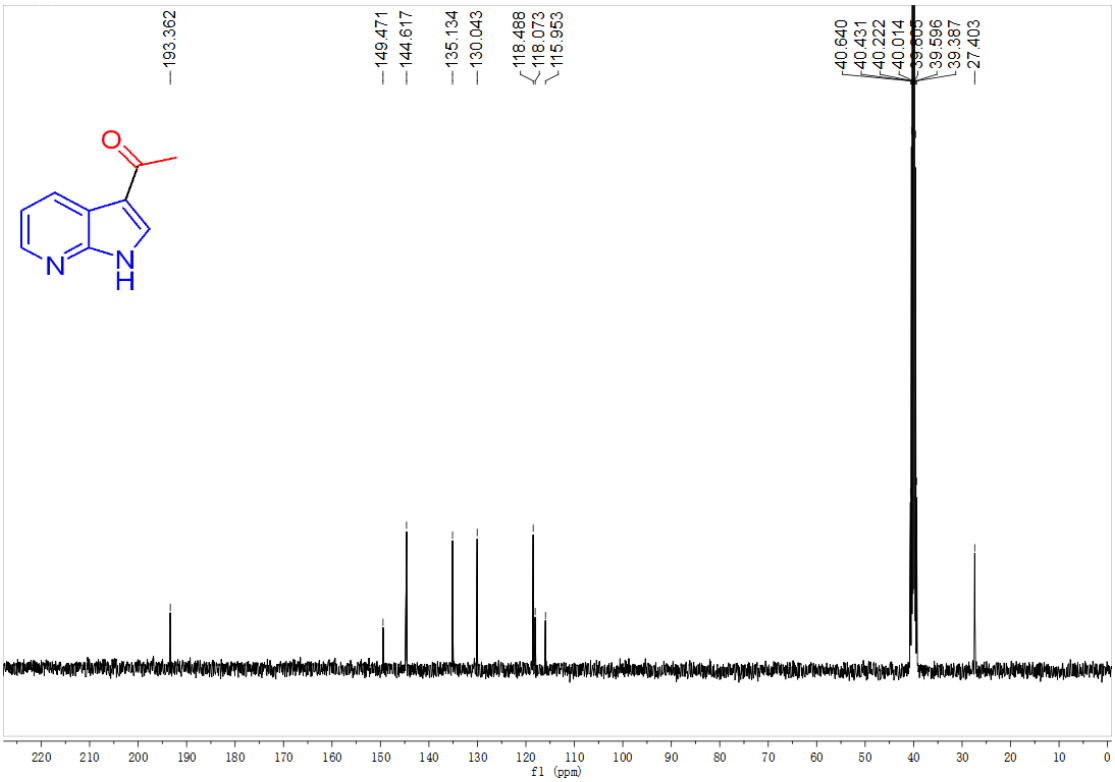
^{1}H NMR and ^{13}C NMR of compound **3s**



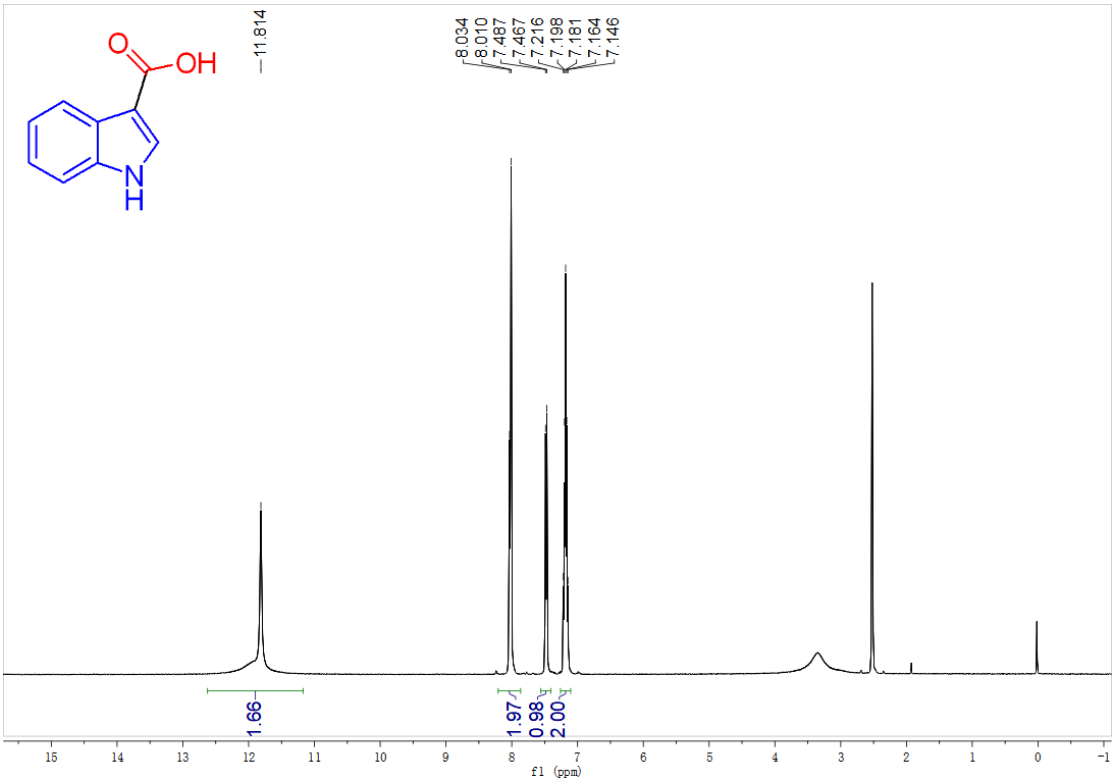


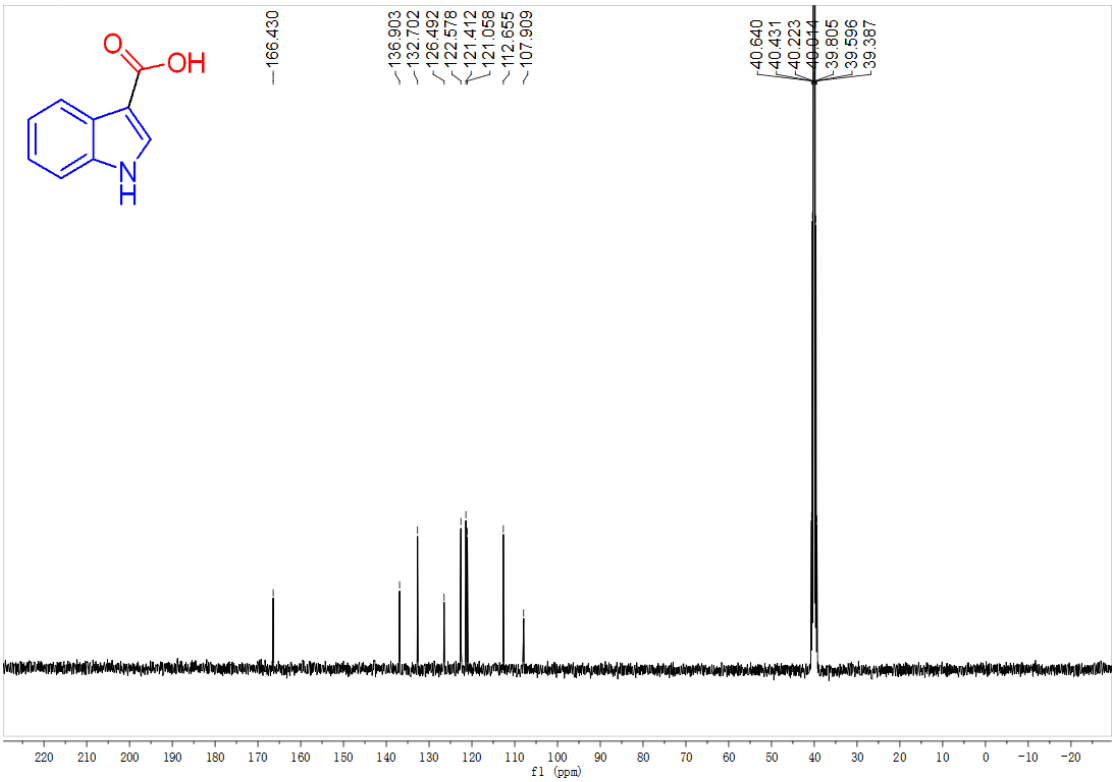
^{1}H NMR and ^{13}C NMR of compound **3t**



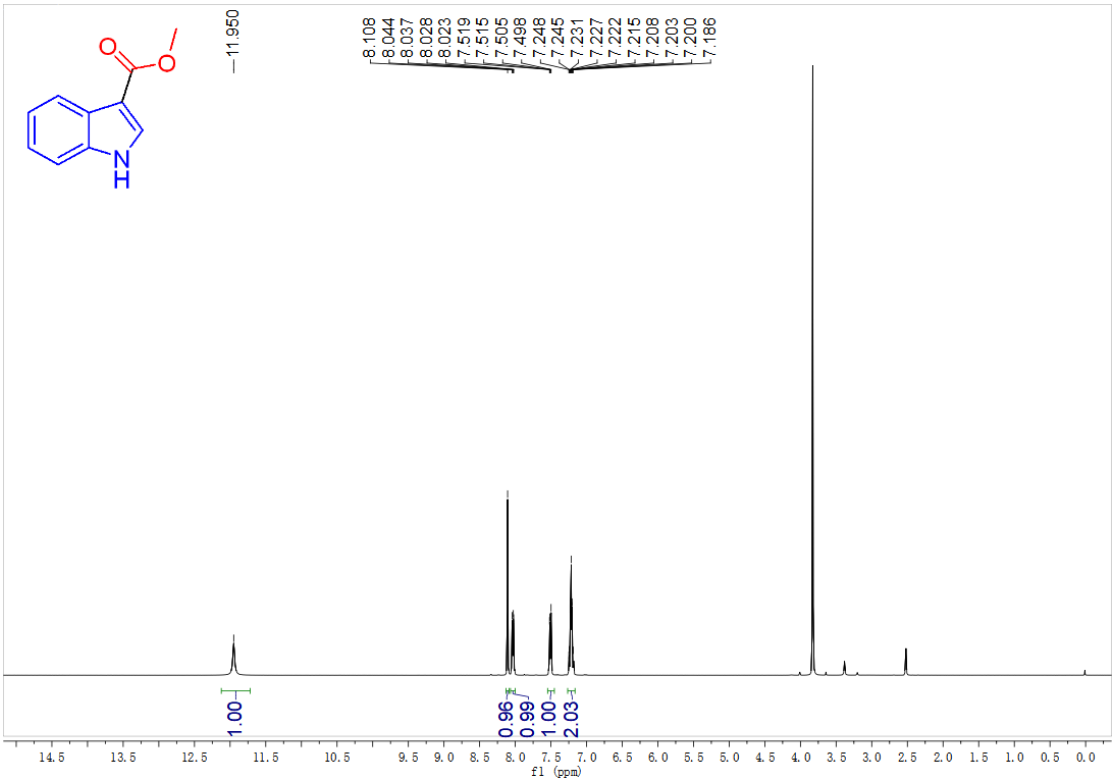


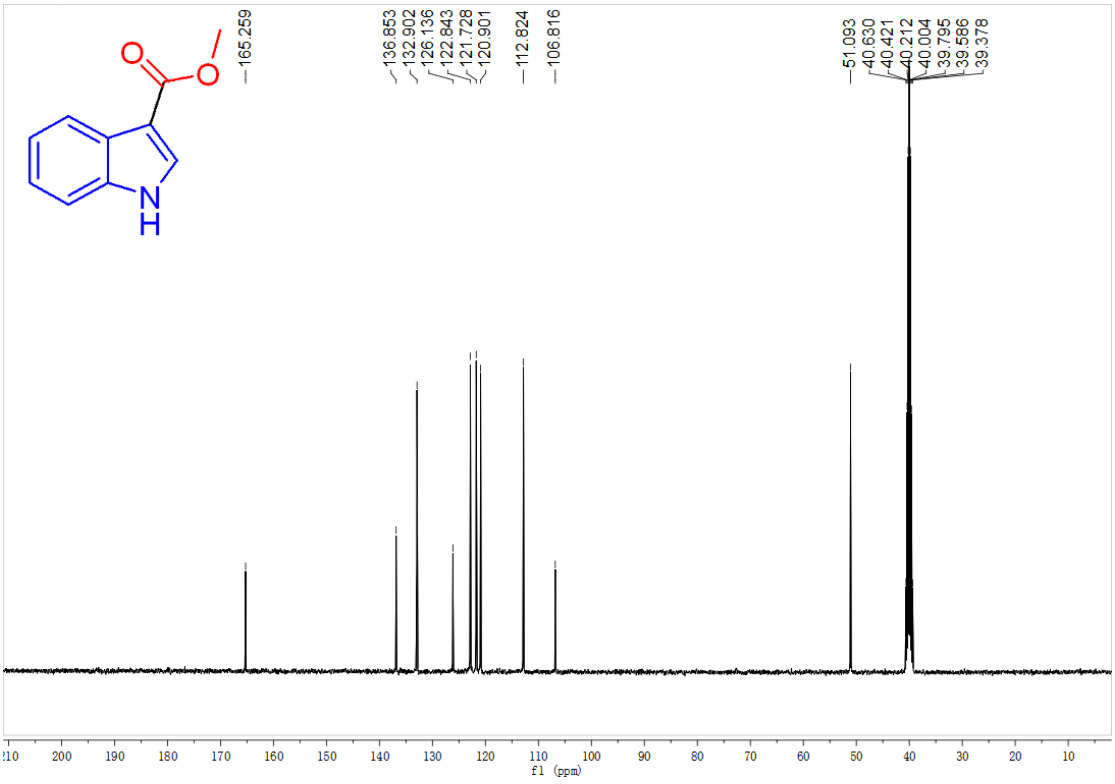
^{1}H NMR and ^{13}C NMR of compound **3u**



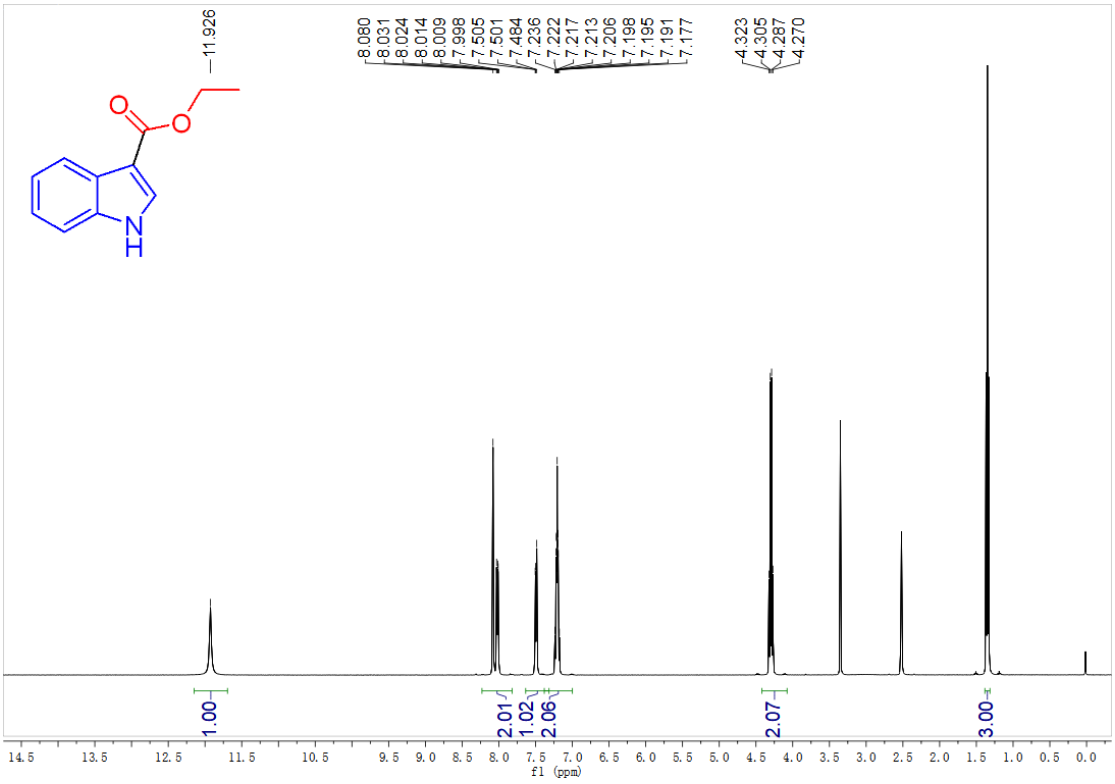


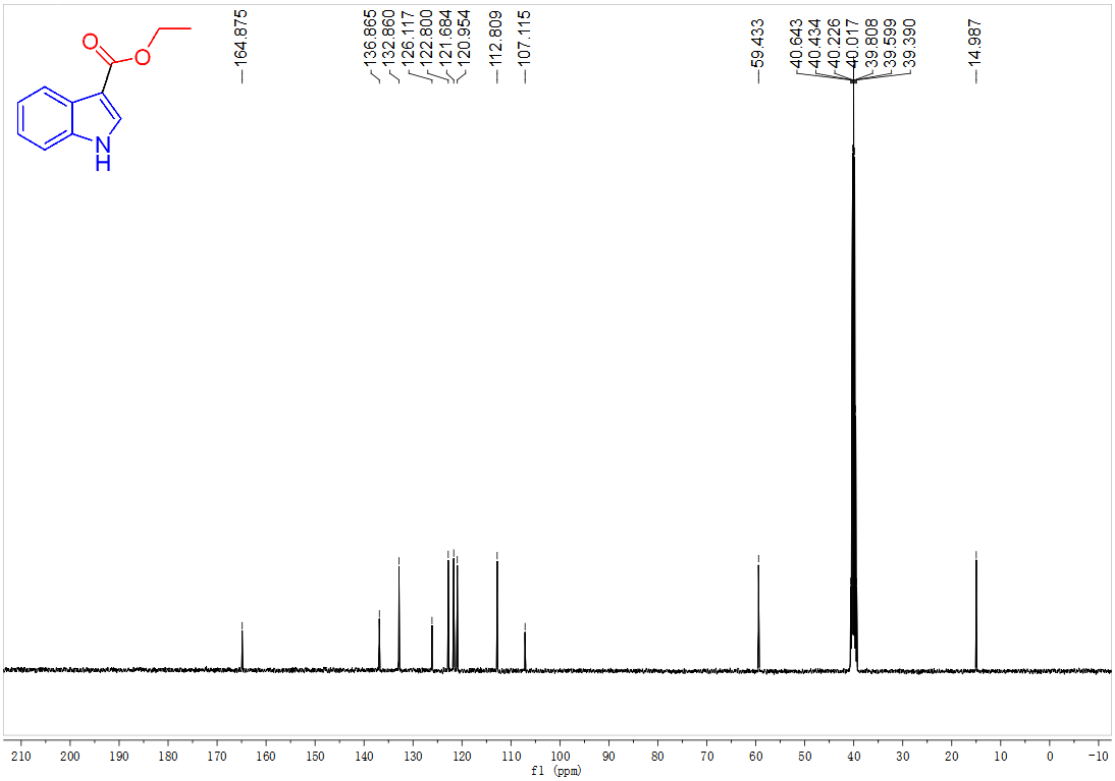
^{1}H NMR and ^{13}C NMR of compound **3v**



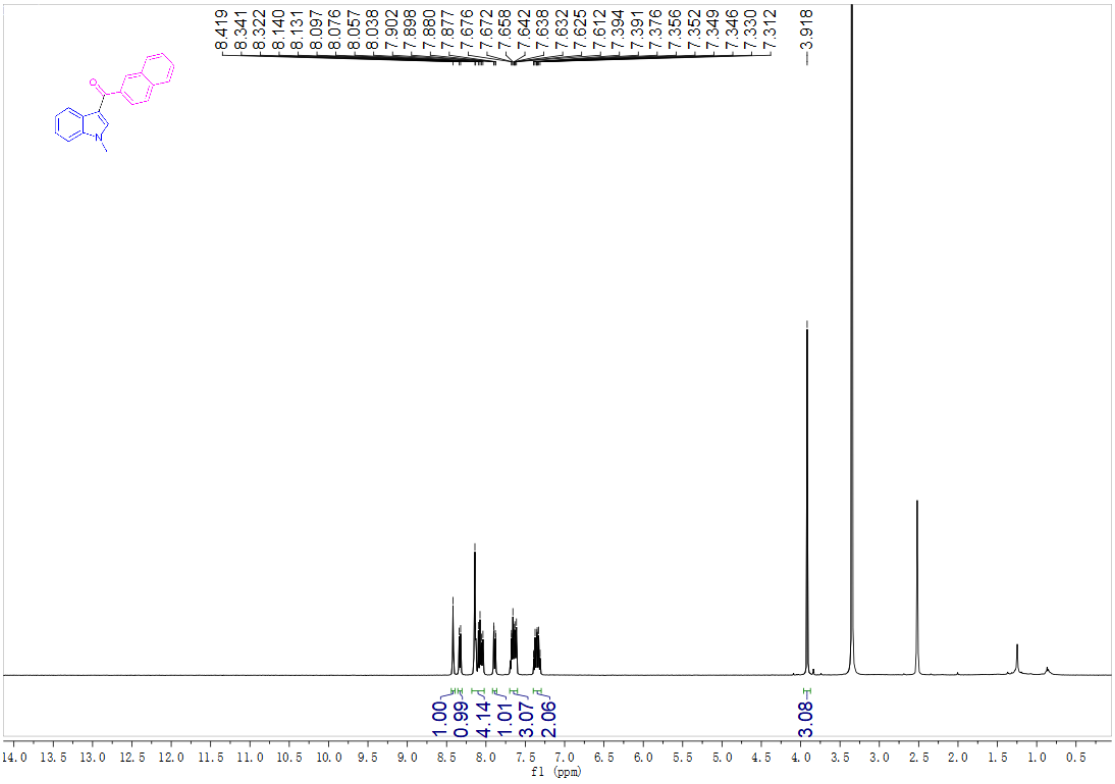


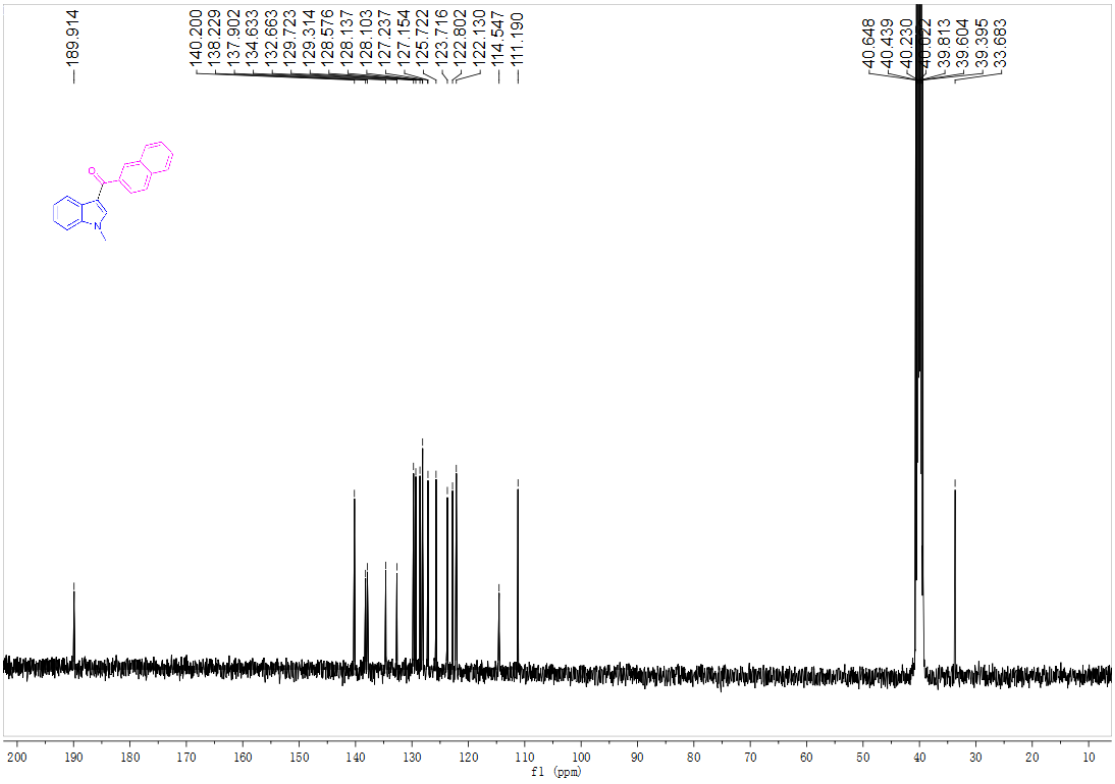
^{1}H NMR and ^{13}C NMR of compound **3w**



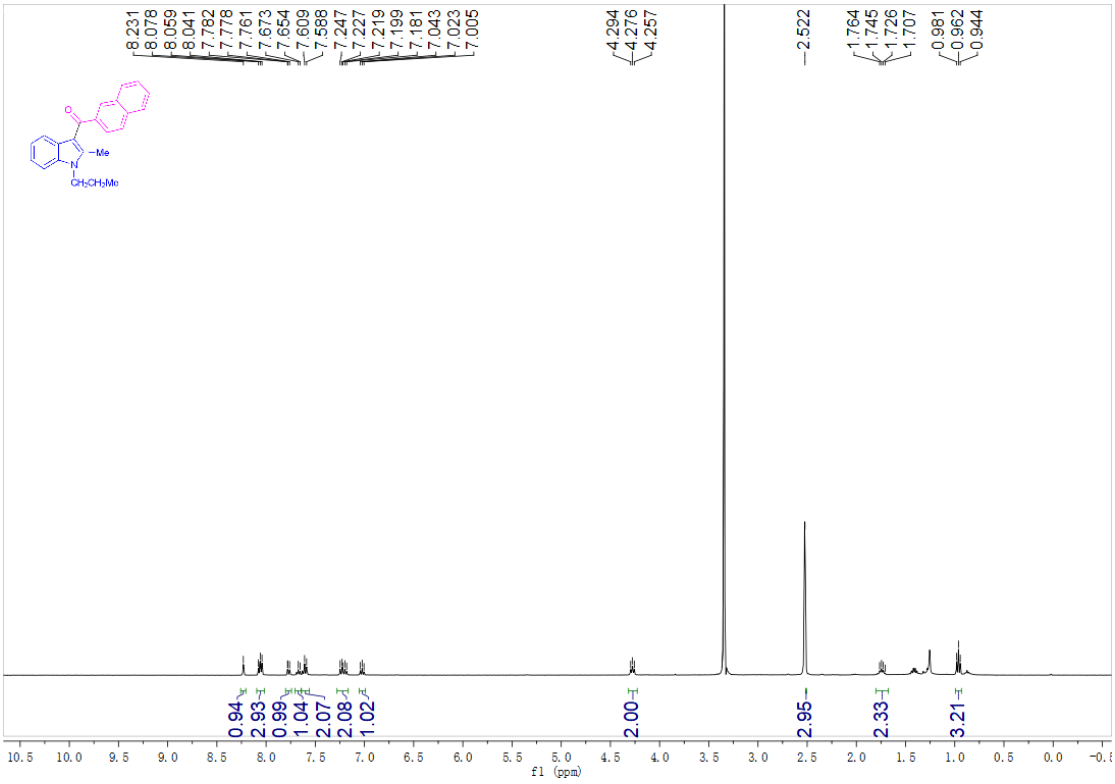


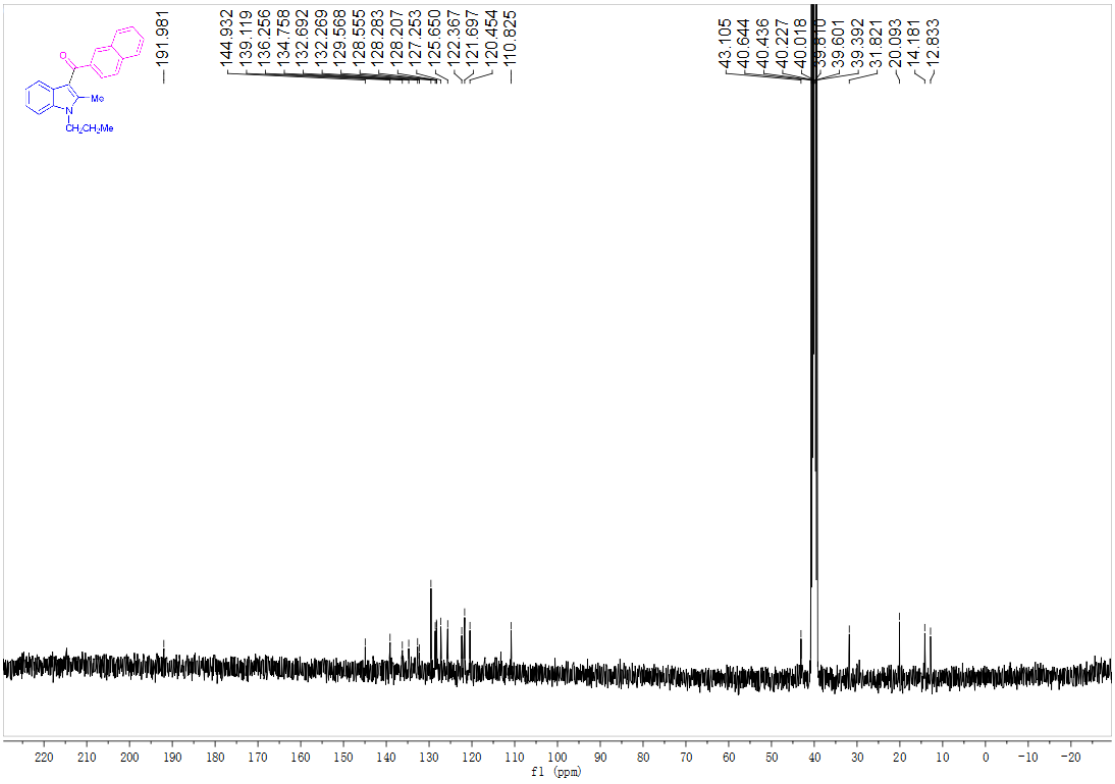
^{1}H NMR and ^{13}C NMR of compound **3x**



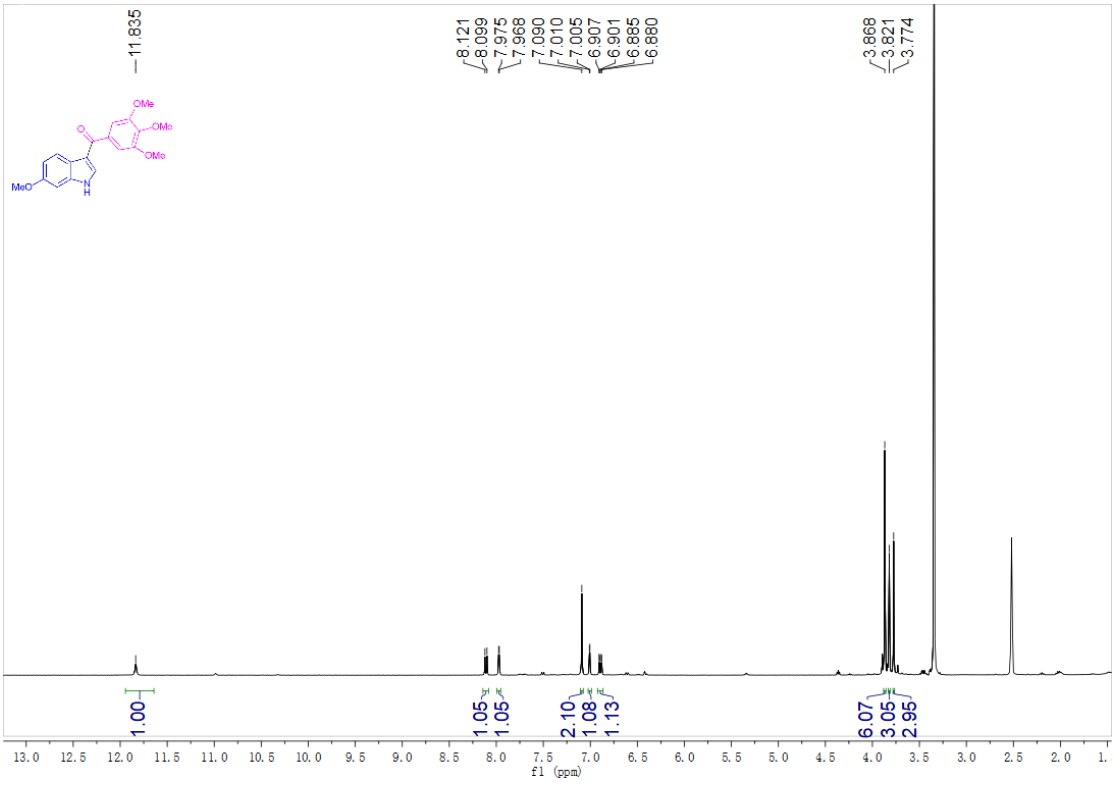


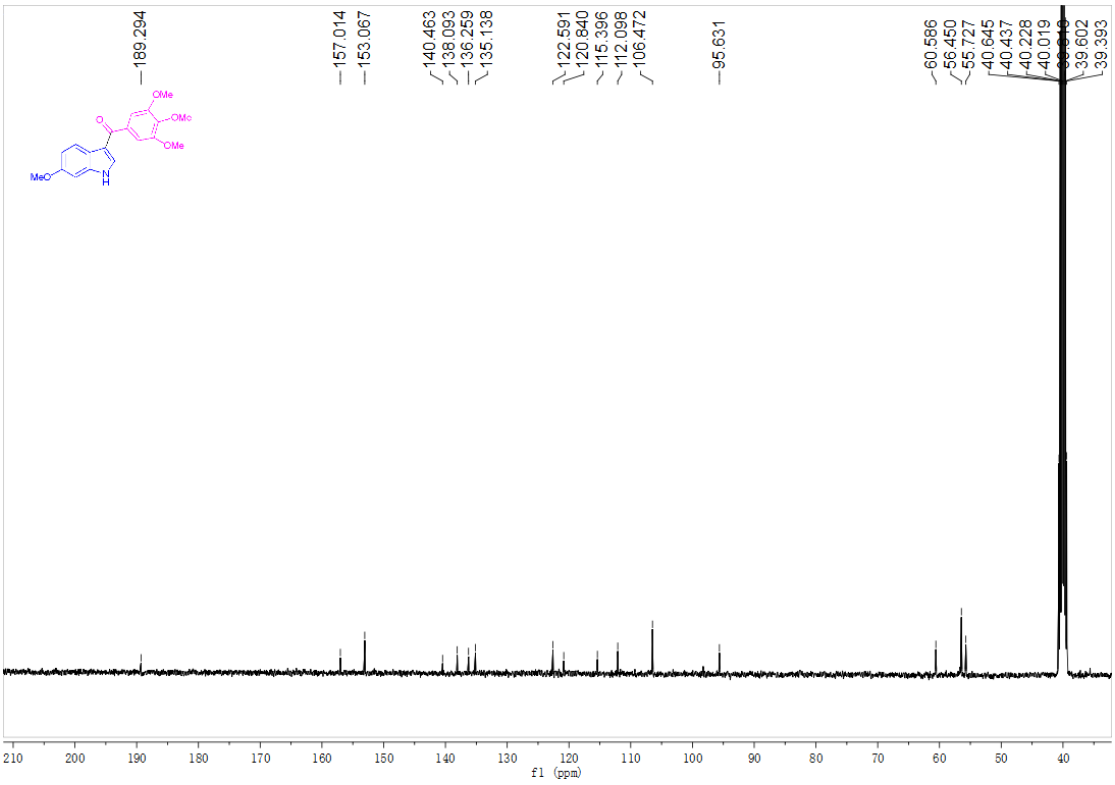
^{1}H NMR and ^{13}C NMR of compound **3y**



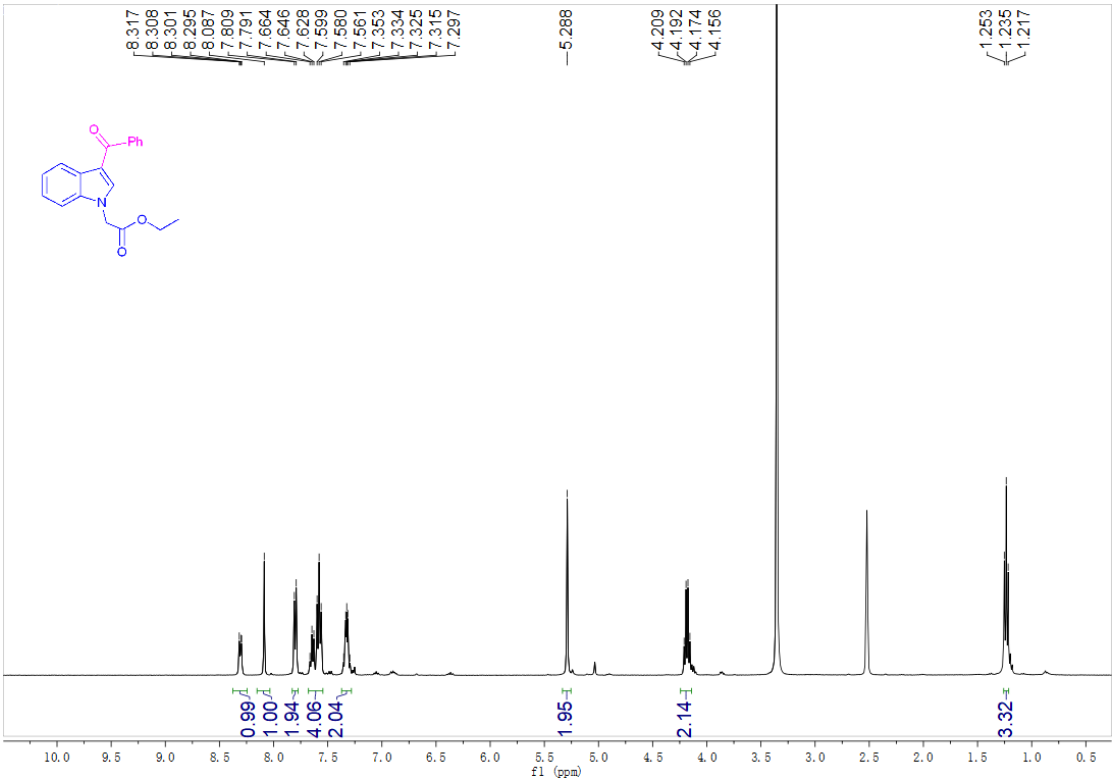


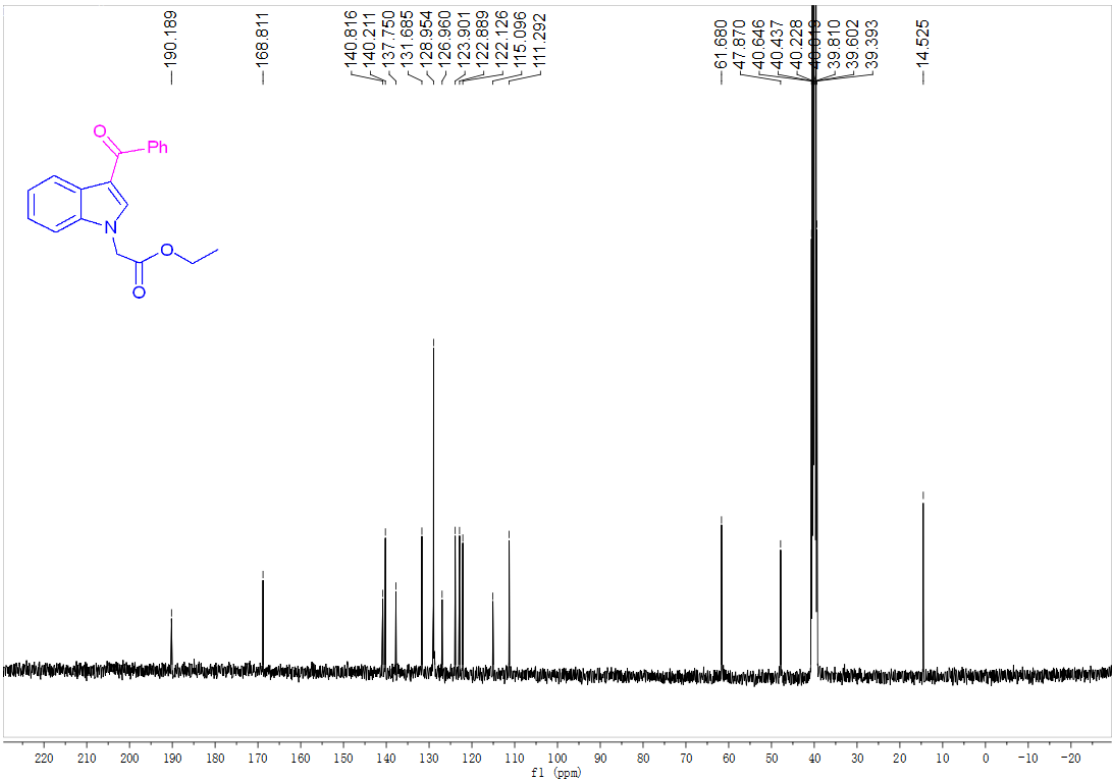
^{1}H NMR and ^{13}C NMR of compound **3z**



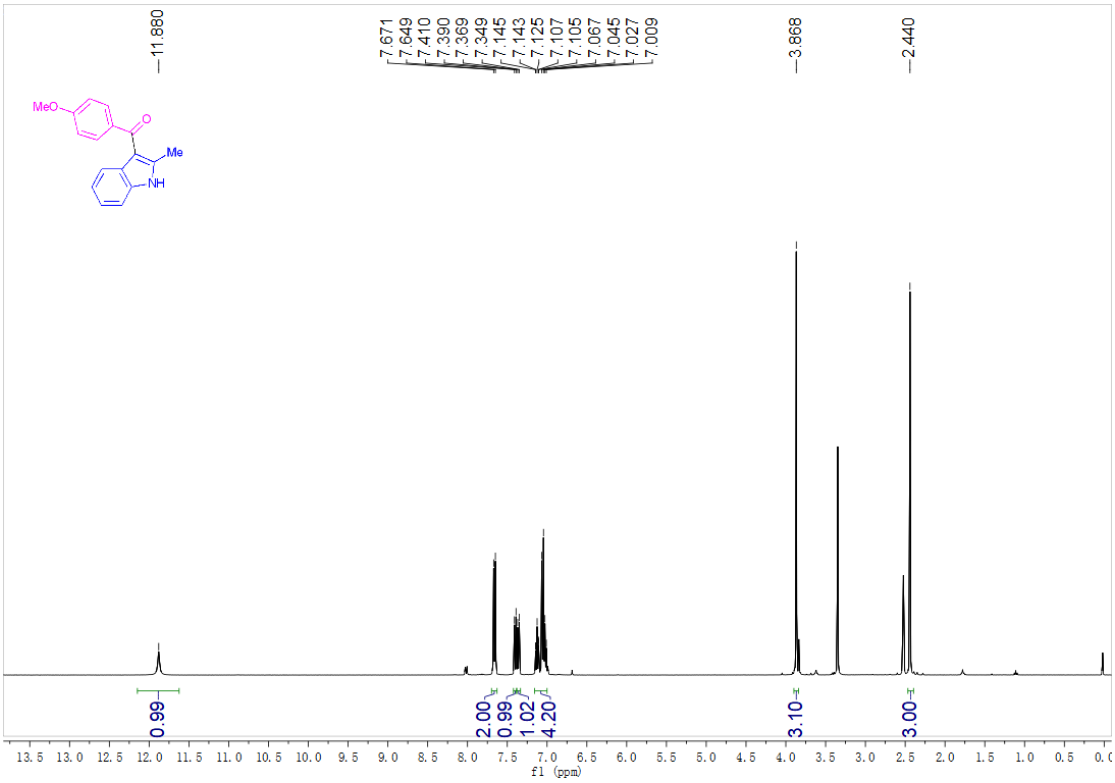


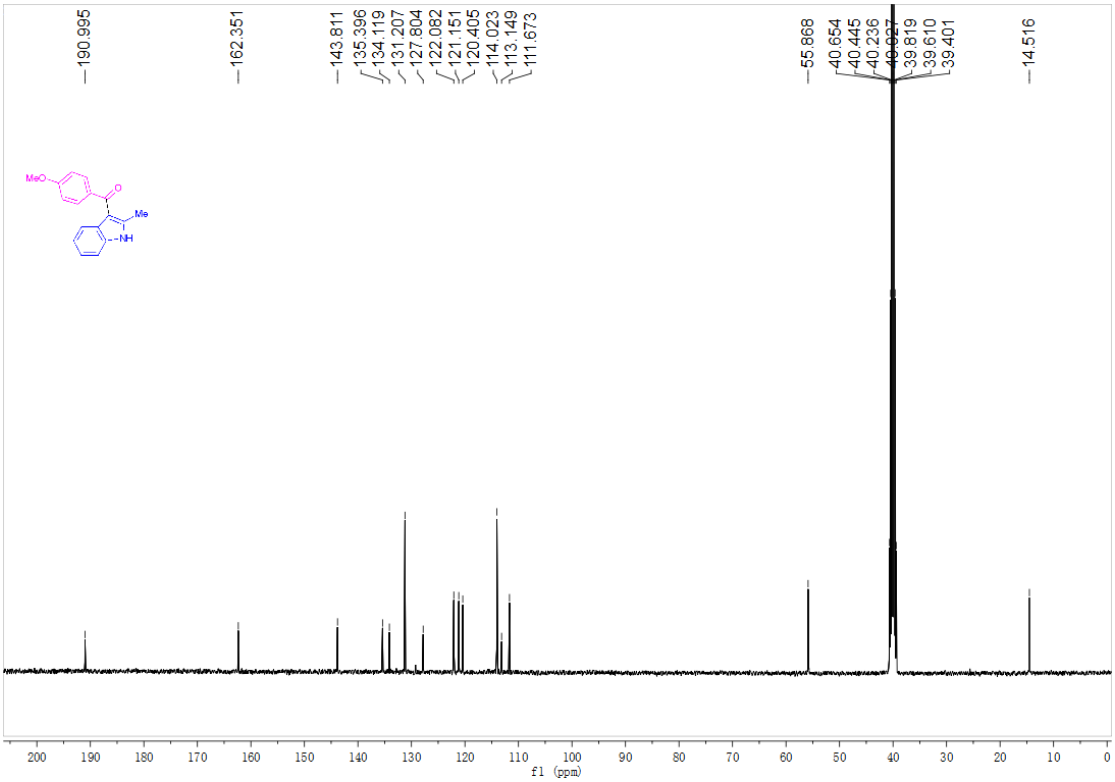
^{1}H NMR and ^{13}C NMR of compound **3aa**





^{1}H NMR and ^{13}C NMR of compound **3ab**





^{1}H NMR and ^{13}C NMR of compound **4**