Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Electronic Supplementary Information

Divergent Electrosynthesis of 3-Iodoindoles and Indoles from 2-Ethynylanilines under Ambient and Aqueous Conditions

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1. General and experimental details

1.1 General information:

All commercially available reagents (AR grade) were directly used as received without further purification. The electrochemical reactions were performed on DJS-292B potentiostats (made in China) in constant current mode with high purity metal or graphite electrodes (> 99.99%). All yields of products refer to the isolated yields after chromatography that performed on 200 ~ 300 mesh silica gel with PE (petroleum ether) / EtOAc or PE / DCM (dichloromethane) as eluents. After each electrochemical reaction, the electrodes were washed with DCM, acetone, deionized water, 1.0 M HCl and wiped with lens tissue, and if necessary, gentle polish was further conducted using 2000 and 8000 mesh sandpapers.

^{1}H NMR (400 MHz), ^{13}C NMR (101 MHz) and ^{19}F NMR (376 MHz) spectra were recorded on a Bruker AV-400 spectrometer with $CDCl_3$ as the solvent. For ^{1}H NMR, the signal of $CDCl_3$ (δ = 7.26 ppm), DMSO-d_6 (δ = 2.50 ppm), or tetramethylsilane (TMS, δ = 0.00 ppm) serves as the internal standard; for ^{13}C NMR, the signal of $CDCl_3$ (δ = 77.16 ppm) or DMSO-d_6 (δ = 39.52 ppm), serve as the internal standard. Data are reported as follows: chemical shift (in ppm), multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, p = quintet, hept = heptet, m = multiplet, br = broad), coupling constant (in Hz), and integration.

Infrared spectra were measured on an FT/IR instrument. GC analysis was performed on a 7890B/Agilent, while GC-MS analysis was performed on a 7890A-5975C/Agilent. HR-MS spectra were recorded on a Bruker Esquire LC mass spectrometer using electrospray ionization. CV measurements were conducted on a CHI-760E electrochemical workstation.

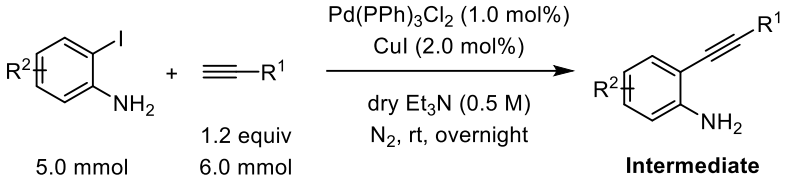
1.2 Preparation of substrates

Substrates **1a** – **26a**, **28a** – **35a**, **42a** – **46a** were prepared via **General Procedure 1** (**GP1**). For **42a** – **44a**, the condensation between carboxylic acid and alcohol building blocks before **GP1** was carried out via **General Procedure 2** (**GP2**). While **27a**, [1] **36a** – **38a**, [2] **39a**, [3] and **40a** – **41a** [16] were prepared according to the protocols in corresponding literature. For the reported substrates, all characterization data are in good accordance with those in previous literature: (**1a** – **4a**, **7a**, **8a**, **17a**,

20a, **24a**), [4] (**5a**, **23a**), [5] **10a**, [6] (**11a**, **26a**), [7] (**12a**, **15a**, **16a**, **27a**), [1] (**19a**, **21a**, **28a** – **30a**, **36a** – **38a**), [2] **22a**, [8] (**25a**, **39a**). [3]

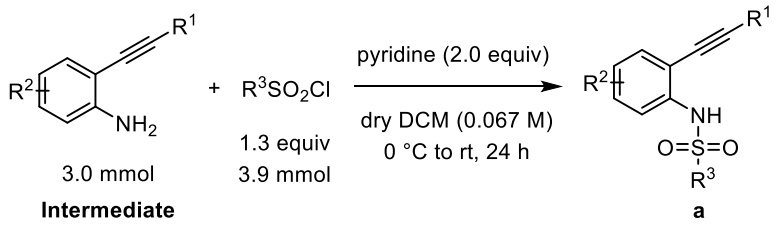
1.2.1 General Procedure 1 (GP1)

Step 1:



To an oven-dried 25 mL flask with a magnetic stir bar were added 2-iodoaniline derivative (5.0 mmol, 1.0 equiv), $Pd(PPh_3)_2Cl_2$ (35.1 mg, 0.05 mmol, 1.0 mol%) and CuI (19.0 mg, 0.1 mmol, 2.0 mol%). Then the flask was closed with a septum, and the atmosphere inside was replaced with N_2. Dry Et_3N (10 mL, 0.5 M) and specific terminal alkyne (6.0 mmol, 1.2 equiv) were successively added via syringe (soild alkynes were added after dissolution in minimized amount of dry THF). The mixture was stirred overnight at room temperature. Upon completion, the reaction mixture was filtered through a short pad of silica gel, concentrated under reduced pressure, and subjected to column chromatography to yield 2-alkynyl aniline **intermediate** (yield generally > 90%).

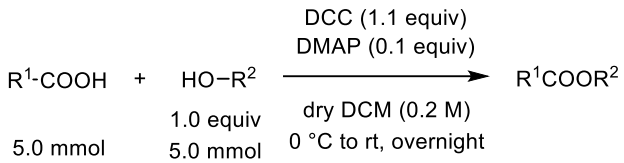
Step 2:



The second step was carried out with 3.0 mmol of the 2-alkynyl aniline intermediate: To an oven-dried 100 mL flask with a magnetic stir bar was added **intermediate** (3.0 mmol), dry DCM (30 mL) and pyridine (0.48 mL, 6.0 mmol, 2.0 equiv). The flask was then equipped with a constant pressure drip funnel containing sulfonyl chloride (3.9 mmol, 1.3 equiv) in DCM (15 mL) and cooled with ice-water bath. The solution of sulfonyl chloride was added dropwise over 15 min. The reaction mixture was stirred at room temperature for 24 h. Upon completion, 1 M HCl (10 mL) was added, and the resulting mixture was stirred for an additional 5 min. The organic phase was washed with water for three times and then dried over anhydrous Na_2SO_4. The mixture was concentrated under

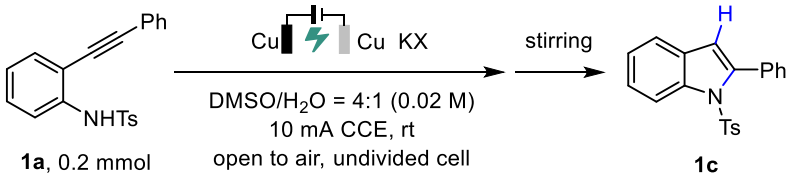
reduced pressure, and subjected to column chromatography to yield substrate **a** in good to excellent yields.

1.2.2 General Procedure 2 (GP2)



To an oven-dried 100 mL flask were added carboxylic acid (5.0 mmol, 1.0 equiv), the corresponding alcohol (5.0 mmol, 1.0 equiv), 4-dimethylaminopyridine (DMAP, 61 mg, 0.5 mmol, 0.1 equiv) and dry DCM (20 mL). The system was cooled with ice-water bath, then a solution of dicyclohexylcarbodiimide (DCC, 1.13 g, 5.5 mmol, 1.1 equiv) in 5 mL dry DCM was added dropwise. After 30 min stirring at 0 °C, the mixture was heated to room temperature and stirred overnight. Upon completion, the reaction mixture was filtered through a short pad of silica gel, concentrated under reduced pressure, and subjected to column chromatography to yield the desired ester product.

1.3 Brief optimization of Condition B

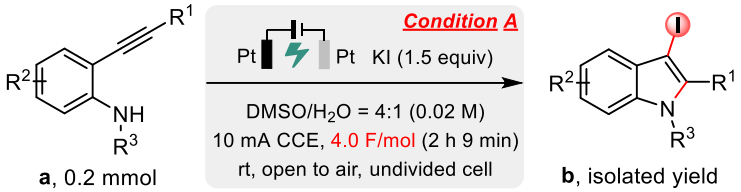


Entry	Conditions	Yield (%)
1	KI (1.5 equiv), 0.1 F/mol, stirred for 3 h	98 [a]
2	KI (0.5 equiv), 0.1 F/mol, stirred for 3 h	98 [a,b]
3	KI (0.5 equiv), 0.05 F/mol, stirred for 7 h	95
4	KBr (0.5 equiv), 0.1 F/mol, stirred for 3 h	21
5	KCl (0.5 equiv), 0.1 F/mol, stirred for 3 h	40
6	KPF_6 (0.5 equiv), 0.1 F/mol, stirred for 3 h	33

Table S1. Brief optimization of **Condition B**. [a] Reaction completion at ~ 2.5 h of additional stirring as revealed by TLC analysis; [b] when applied amount of electrolyte KI was lower than 0.5 equiv, the cell voltage would reach > 20 V.

1.4 General procedure for electrochemical reactions

1.4.1 Iodocyclization under Condition A



To a 25 mL three-necked flask with a magnetic stir bar was added substrate **a** (0.2 mmol) and KI (49.8 mg, 0.3 mmol, 1.5 equiv), followed by solvent DMSO (8.0 mL). *For substrate **42a** which showed poor solubility, additional 5.0 mL DCM was added.* Then water (2.0 mL) was added into the mixture (slightly exothermic), after which the flask was equipped with two platinum plate electrodes (10×10×0.2 mm, approximately 2 cm apart). The 10 mA constant current electrolysis was performed at room temperature under air atmosphere with vigorous stirring. After 4 F/mol charges passed (129 min), EtOAc (~ 5 mL) was added into the system, and the resulting mixture was stirred for additional 1 min. The mixture was then poured into brine and extracted with EtOAc for three times. The combined organic layer was dried over anhydrous Na_2SO_4, and the solvent was then removed under reduced pressure. The resulting mixture was purified by column chromatography on silica gel (eluted with EtOAc/PE) to afford the desired product **b**.

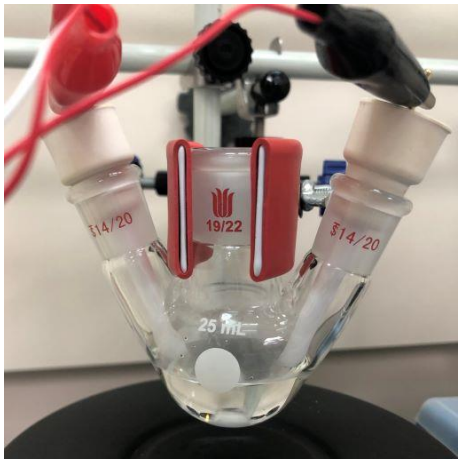
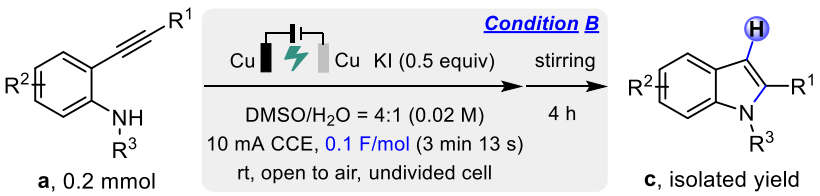


Fig. S1 Setup for the electrochemical iodocyclization with Pt electrodes (**Condition A**).

1.4.2 Hydrocyclization under Condition B



To a 25 mL three-necked flask with a magnetic stir bar was added substrate **a** (0.2 mmol) and KI (17.5 mg, 0.1 mmol, 0.5 equiv), followed by solvent DMSO (8.0 mL). *For substrate **42a** which showed poor solubility, additional 5.0 mL DCM was added.* Then water (2.0 mL) was added into the mixture (slightly exothermic), after which the flask was equipped with two copper rod electrodes (*Φ* 6 mm, 10 cm in length, approximately 1 cm immersed and 2 cm apart, gently sanded before use). The 10 mA constant current electrolysis was performed at room temperature under air atmosphere with vigorous stirring. After 0.1 F/mol charges passed (3 min 13 s), the electrodes were detached from the power source and the system was stirred for additional 4 h. Upon completion, EtOAc (~ 5 mL) was added into the system, and the resulting mixture was stirred for ~ 1 min. The mixture was then poured into brine and extracted with EtOAc for three times. The combined organic layer was dried over anhydrous Na_2SO_4, and the solvent was then removed under reduced pressure. The resulting mixture was purified by column chromatography on silica gel (eluted with EtOAc/PE) to afford the desired product **c**.

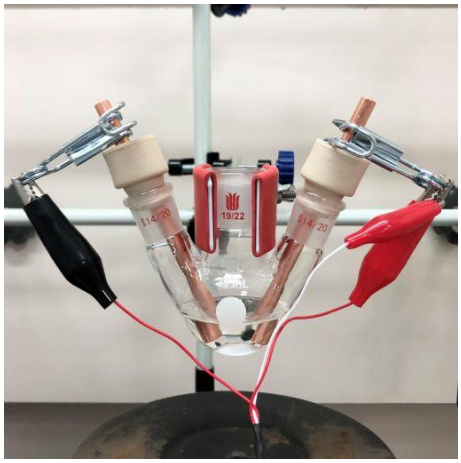
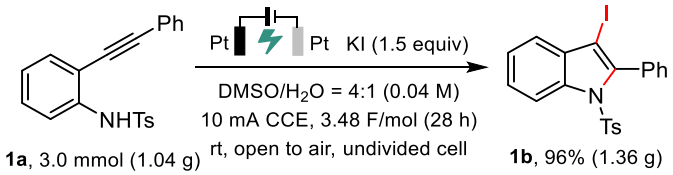


Fig. S2 Setup for the electrochemical hydrocyclization with Cu electrodes (**Condition B**).

1.5 Procedure for gram-scale electrochemical reactions

1.5.1 Procedure for gram-scale electrosynthesis of 1b from 1a with Pt electrodes (3.0 mmol)



1a, 3.0 mmol (1.04 g) **1b**, 96% (1.36 g)

A piece of paperboard was drilled with three holes: two for electrode fixation (approximately 3 cm apart), and one for TLC sample taken. Substrate **1a** (3.0 mmol, 1.04 g) and KI (4.5 mmol, 747 mg) were placed in a 100 mL beaker with a magnetic stir bar. Solvent DMSO (60 mL) was then added, after which the mixture was stirred for several minutes until the dissolution of **1a**. Then water (15 mL) was added into the mixture (slightly exothermic). The beaker was equipped with two Pt electrodes (10 x 10 x 0.2 mm, fixed on the paperboard), and the system was electrolyzed with 10 mA constant current. The reaction was monitored by TLC until the disappearance of **1a** (28 h, 3.48 F/mol). The reaction mixture was poured into brine and extracted with EtOAc for 3 times. After dried over anhydrous Na_2SO_4, the solvent was evaporated, and the resulting mixture was subjected to column chromatography to yield product **1b** (1.36 g, 96%).

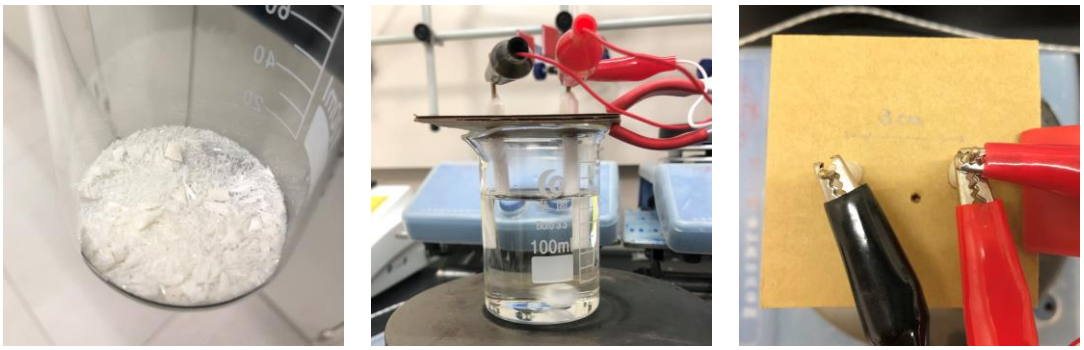
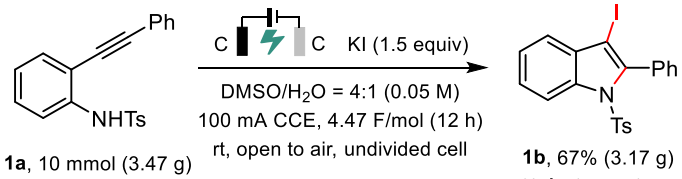


Fig. S3 Setup for 3.0 mmol scale electrochemical iodocyclization.

1.5.2 Procedure for gram-scale electrosynthesis of 1b from 1a with graphite electrodes (10 mmol)



1a, 10 mmol (3.47 g) **1b**, 67% (3.17 g) with 25% **1a** (0.87 g) recovered

Substrate **1a** (10.0 mmol, 3.47 g) and KI (15.0 mmol, 2.49 g) were placed in a 250 mL beaker with a magnetic stir bar. Solvent DMSO (160 mL) was then added, after which the mixture was stirred for several minutes until the dissolution of **1a**. Then water (40 mL) was added into the mixture (slightly exothermic). The beaker was equipped with two graphite rod electrodes (Φ 10 mm, about 4 cm apart and 5 cm immersed in the solution), and the system was electrolyzed with 100 mA constant current. The reaction was monitored by TLC until the conversion of **1a** was no more obvious (12 h, 4.48 F/mol). The reaction mixture was poured into brine and extracted with EtOAc for 3 times. After dried over anhydrous Na_2SO_4, the solvent was evaporated, and the resulting mixture was subjected to column chromatography to yield product **1b** (3.17 g, 67%) with the recovery of part of starting material **1a** (0.87 g, 25%).

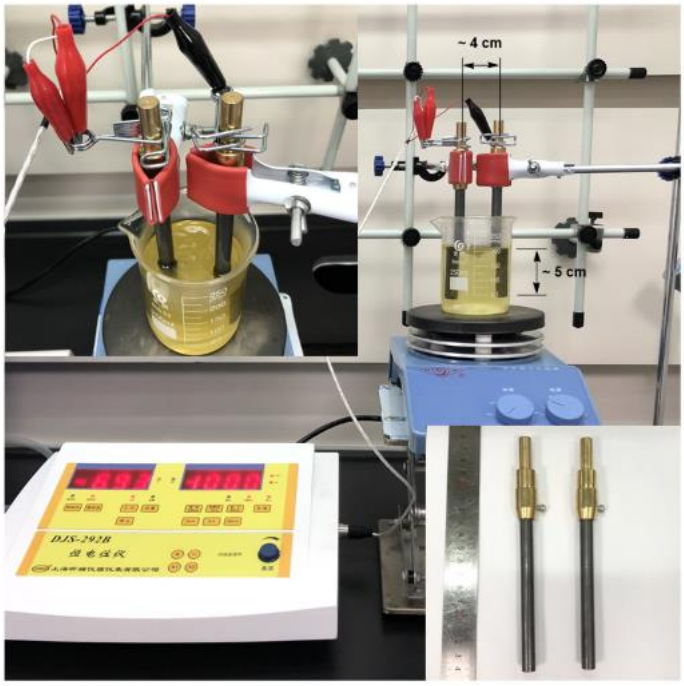
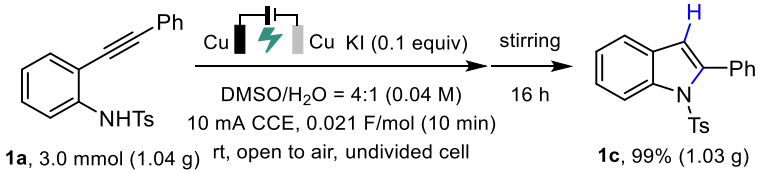


Fig. S4 Setup for 10 mmol scale electrochemical iodocyclization.

1.5.3 Procedure for gram-scale electrosynthesis of 1c from 1a with Cu electrodes (3.0 mmol)



A piece of paperboard was drilled with two holes for the fixation of electrodes (approximately 3 cm apart). Substrate **1a** (3.0 mmol, 1.04 g) and KI (0.3 mmol, 49.8 mg) were placed in a 100 mL beaker with a magnetic stir bar. Solvent DMSO (60 mL) was then added, after which the mixture was stirred for several minutes until the dissolution of **1a**. Then water (15 mL) was added into the mixture (slightly exothermic). The beaker was equipped with two Cu rod electrodes (*Φ* 6 mm, 10 cm in length, approximately 3 cm immersed, gently sanded before use), and the system was electrolyzed with 10 mA constant current. After 10 min (0.021 F/mol), the electrodes were detached from the power source and the system was stirred under ambient conditions. Upon completion as revealed by TLC analysis (16 h), the reaction mixture was poured into brine and extracted with EtOAc for 3 times. After dried over anhydrous Na_2SO_4, the solvent was evaporated, and the resulting mixture was subjected to column chromatography to yield product **1c** (1.03 g, 99%).

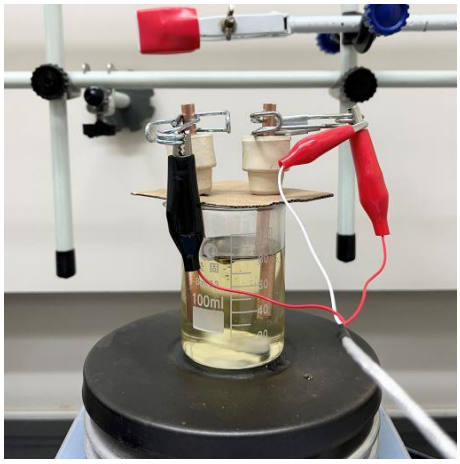
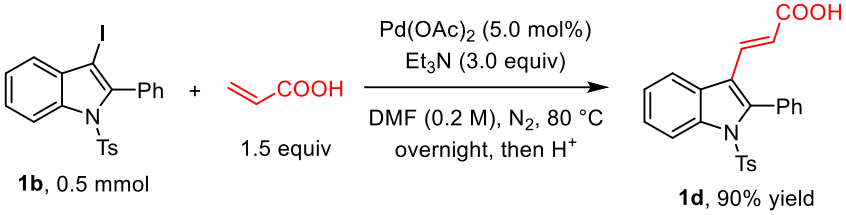


Fig. S5 Setup for 3.0 mmol scale electrochemical hydrocyclization.

1.6 Procedure for synthetic applications

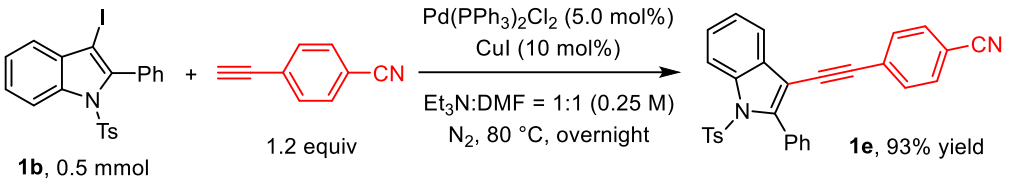
1.6.1 Heck Cross-Coupling



To an oven-dried 10 mL flask with a magnetic stir bar were added **1b** (236.7 mg, 0.5 mmol, 1.0 equiv), $Pd(OAc)_2$ (5.6 mg, 0.025 mmol, 5.0 mol%). Then the flask was capped with a rubber

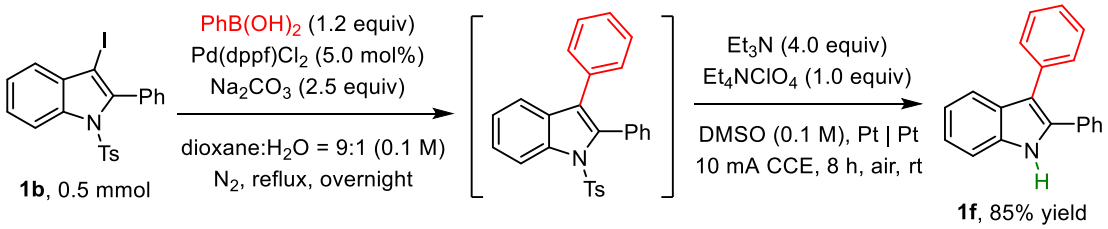
septum, and the atmosphere inside was replaced with N_2. Dry Et_3N (0.2 mL, 1.5 mmol, 3.0 equiv) and dry DMF (2.5 mL) were successively added via syringe. The mixture was then stirred overnight at 80 °C. Upon completion, acidification of the reaction mixture was carried out by adding 2M HCl aq., then the system was extracted with DCM for 3 times. The combined organic layer was then washed with water and dried over anhydrous Na_2SO_4. After removal of solvent under reduced pressure, the mixture was purified by column chromatography to afford **1d** as a white solid (187.9 mg, 90%).

1.6.2 Sonogashira Cross-Coupling



To an oven-dried 10 mL flask with a magnetic stir bar were added **1b** (236.7 mg, 0.5 mmol, 1.0 equiv), $Pd(PPh_3)_2Cl_2$ (17.6 mg, 0.025 mmol, 5.0 mol%) and CuI (9.5 mg, 0.05 mmol, 10 mol%). Then the flask was capped with a rubber septum, and the atmosphere inside was replaced with N_2. Dry Et_3N (1 mL), and 4-ethynylbenzonitrile (76.3 mg, 0.6 mmol, 1.2 equiv) in dry DMF (1 mL) were successively added via syringe. The mixture was then stirred overnight at 80 °C. Upon completion, the reaction mixture was poured into brine and extracted with EtOAc for 3 times. The combined organic layer was dried over anhydrous Na_2SO_4, and the solvent was then removed under reduced pressure. The resulting mixture was purified by column chromatography to afford **1e** as a light yellow solid (219.8 mg, 93%).

1.6.3 Suzuki Cross-Coupling followed by electrochemical deprotection

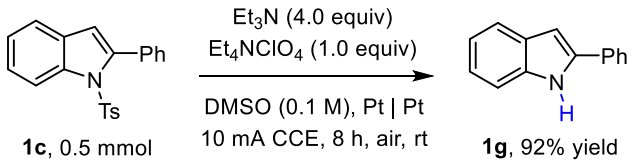


To an oven-dried two-necked 25 mL flask with a magnetic stir bar were added **1b** (236.7 mg, 0.5 mmol, 1.0 equiv), phenylboronic acid (73.2 mg, 0.6 mmol, 1.2 equiv) and Na_2CO_3 (132.5

mg, 1.25 mmol, 2.5 equiv). The flask was then equipped with a rubber septum and a reflux condenser with a nitrogen balloon. After replacing the atmosphere with N_2, 4.5 mL of dioxane and 0.5 mL of deionized water were added successively via syringe. The system was heated to reflux overnight. Upon completion, the reaction mixture was diluted with water and extracted 3 times with DCM, and dried over anhydrous Na_2SO_4. Column chromatography afforded the intermediate compound as a white solid (200.5 mg, 95% yield), which was transferred with 5.0 mL DMSO to a three-necked flask and directly subjected to the following electrochemical procedure.

To the three-necked flask were added electrolyte Et_4NClO_4 (114.9 mg, 0.5 mmol, 1.0 equiv) and Et_3N (202.4 mg, 2.0 mmol, 4.0 equiv), after which the flask was equipped with two platinum plate electrodes (10×10×0.2 mm, approximately 2 cm apart) and a magnetic stir bar. The 10 mA constant current electrolysis was performed at room temperature under air atmosphere with vigorous stirring. After completion as revealed by TLC analysis (8 h), the mixture was poured into brine and extracted with EtOAc for three times. The combined organic layer was dried over anhydrous Na_2SO_4, and the solvent was then removed under reduced pressure. The resulting mixture was purified by column chromatography to afford **1f** as a white solid (114.5 mg, 85% over two steps).

1.6.4 Electrochemical deprotection of 1c



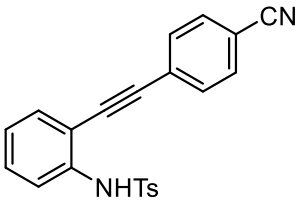
1c, 0.5 mmol **1g**, 92% yield

To a three-necked flask were added **1c** (173.7 mg, 0.5 mmol, 1.0 equiv), electrolyte Et_4NClO_4 (114.9 mg, 0.5 mmol, 1.0 equiv) and Et_3N (202.4 mg, 2.0 mmol, 4.0 equiv), after which the flask was equipped with two platinum plate electrodes (10×10×0.2 mm, approximately 2 cm apart) and a magnetic stir bar. The 10 mA constant current electrolysis was performed at room temperature under air atmosphere with vigorous stirring. After completion as revealed by TLC analysis (8 h), the mixture was poured into brine and extracted with EtOAc for three times. The combined organic layer was dried over anhydrous Na_2SO_4, and the solvent was then removed

under reduced pressure. The resulting mixture was purified by column chromatography to afford **1g** as a white solid (88.9 mg, 92%).

2. Characterization data

2.1 Characterization data for unreported substrates (a)



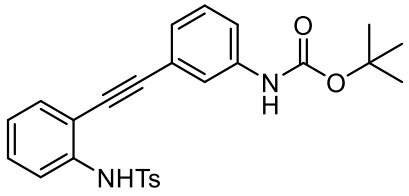
N-(2-((4-cyanophenyl)ethynyl)phenyl)-4-methylbenzenesulfonamide (**6a**)

Light yellow solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.72 – 7.63 (m, 4H), 7.60 (dd, J = 8.3, 1.1 Hz, 1H), 7.58 – 7.51 (m, 2H), 7.40 (dd, J = 7.7, 1.5 Hz, 1H), 7.34 (td, J = 7.9, 1.6 Hz, 1H), 7.23 – 7.13 (m, 3H), 7.10 (td, J = 7.6, 1.2 Hz, 1H), 2.35 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 144.35, 137.91, 136.19, 132.52, 132.34, 132.18, 130.67, 129.83, 127.35, 127.03, 124.88, 120.67, 118.39, 113.77, 112.43, 94.18, 88.15, 21.68.

HRMS (ESI) calculated for $C_{22}H_{17}N_2O_2S^+$ m/z $[M+H]^+$: 373.1005, found: 373.1008.



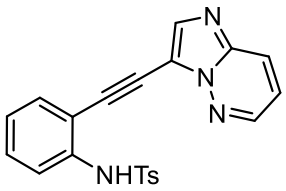
Tert-butyl (3-((2-((4-methylphenyl)sulfonamido)phenyl)ethynyl)phenyl)carbamate (**9a**)

Light yellow solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.72 – 7.56 (m, 4H), 7.38 – 7.21 (m, 5H), 7.20 – 7.15 (m, 2H), 7.12 (dq, J = 7.4, 1.6 Hz, 1H), 7.06 (tt, J = 7.6, 1.6 Hz, 1H), 6.66 (s, 1H), 2.33 (s, 3H), 1.54 (s, 9H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 152.71, 144.18, 138.80, 137.60, 136.05, 132.16, 129.77, 129.73, 129.26, 127.38, 126.22, 124.83, 122.79, 121.33, 120.79, 119.23, 114.93, 95.98, 83.77, 81.03, 28.43, 21.64.

HRMS (ESI) calculated for $C_{26}H_{27}N_2O_4S^+$ m/z $[M+H]^+$: 463.1686, found: 463.1684.



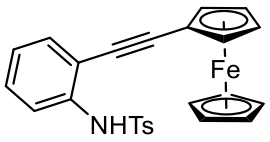
N-(2-(imidazo[1,2-*b*]pyridazin-3-ylethynyl)phenyl)-4-methylbenzenesulfonamide (**13a**)

Yellow solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.85 (dd, J = 4.5, 1.5 Hz, 1H), 8.77 (s, 1H), 8.09 (dd, J = 9.2, 1.6 Hz, 1H), 7.99 (s, 1H), 7.75 (dd, J = 8.5, 1.1 Hz, 1H), 7.73 – 7.67 (m, 2H), 7.37 (dd, J = 7.7, 1.6 Hz, 1H), 7.34 – 7.22 (m, 2H), 7.12 (d, J = 8.1 Hz, 2H), 7.05 (td, J = 7.6, 1.1 Hz, 1H), 2.31 (s, 3H).

^{13}C NMR (400 MHz, $CDCl_3$) δ 144.94, 143.93, 140.20, 138.43, 136.42, 135.96, 130.06, 130.03, 129.68, 127.40, 126.27, 123.85, 118.85, 118.75, 112.64, 112.54, 96.02, 83.92, 21.62.

HRMS (ESI) calculated for $C_{21}H_{17}N_4O_2S^+$ m/z $[M+H]^+$: 389.1067, found: 389.1063.



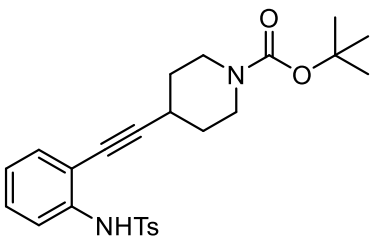
N-(2-(ferrocenylethynyl)phenyl)-4-methylbenzenesulfonamide (**14a**)

Orange solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.73 – 7.68 (m, 2H), 7.60 (dd, J = 8.2, 1.2 Hz, 1H), 7.32 (dd, J = 7.8, 1.5 Hz, 1H), 7.29 – 7.18 (m, 5H), 7.02 (td, J = 7.6, 1.1 Hz, 1H), 4.50 (s, 2H), 4.31 (s, 2H), 4.26 (s, 5H), 2.36 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 144.14, 137.61, 136.32, 131.75, 129.79, 129.13, 127.41, 124.39, 119.45, 114.93, 96.21, 80.19, 71.67, 70.26, 69.48, 63.70, 21.71.

HRMS (ESI) calculated for $C_{25}H_{22}FeNO_2S^+$ m/z $[M+H]^+$: 456.0715, found: 456.0715.



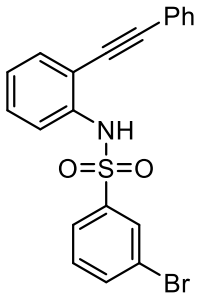
Tert-butyl-4-((2-((4-methylphenyl)sulfonamido)phenyl)ethynyl)piperidine-1-carboxylate (**18a**)

Light yellow solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.66 (d, J = 8.0 Hz, 2H), 7.59 (d, J = 8.2 Hz, 1H), 7.32 – 7.15 (m, 5H), 7.02 (tt, J = 7.6, 1.1 Hz, 1H), 3.79 – 3.68 (m, 2H), 3.27 – 3.16 (m, 2H), 2.86 – 2.75 (m, 1H), 2.38 (s, 3H), 1.94 – 1.81 (m, 3H), 1.68 – 1.57 (m, 2H), 1.50 (s, 9H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 154.79, 144.12, 137.58, 136.22, 132.11, 129.69, 129.22, 127.24, 124.42, 119.76, 114.59, 99.32, 79.80, 76.73, 31.40, 28.52, 27.88, 21.62.

HRMS (ESI) calculated for $C_{25}H_{31}N_2O_4S^+$ m/z $[M+H]^+$: 455.1999, found: 455.1994.



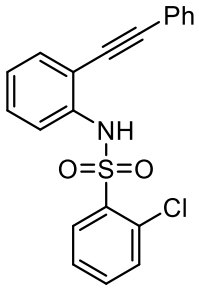
3-Bromo-*N*-(2-(phenylethynyl)phenyl)benzenesulfonamide (**31a**)

White solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.95 (t, J = 1.9 Hz, 1H), 7.68 – 7.57 (m, 3H), 7.50 – 7.43 (m, 2H), 7.43 – 7.37 (m, 4H), 7.34 (td, J = 7.9, 1.6 Hz, 1H), 7.26 – 7.17 (m, 2H), 7.13 (td, J = 7.6, 1.2 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 140.81, 136.88, 136.32, 132.25, 131.78, 130.52, 130.19, 129.88, 129.32, 128.74, 125.86, 125.54, 123.10, 121.84, 121.53, 115.62, 96.38, 83.52.

HRMS (ESI) calculated for $C_{20}H_{15}BrNO_2S^+$ m/z $[M+H]^+$: 412.0001, found: 412.0001.



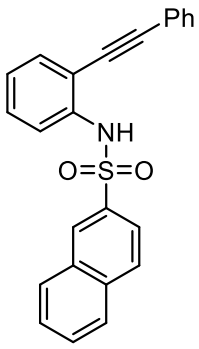
2-Chloro-*N*-(2-(phenylethynyl)phenyl)benzenesulfonamide (**32a**)

White solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.15 (dd, J = 7.9, 1.5 Hz, 1H), 7.91 (s, 1H), 7.60 – 7.52 (m, 3H), 7.49 – 7.34 (m, 7H), 7.21 (ddd, J = 8.5, 7.5, 1.6 Hz, 1H), 7.00 (td, J = 7.6, 1.2 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 137.26, 136.23, 134.41, 132.47, 132.16, 132.03, 131.75, 129.74, 129.21, 128.71, 127.13, 123.97, 122.20, 117.26, 113.12, 96.87, 83.65.

HRMS (ESI) calculated for $C_{20}H_{15}ClNO_2S^+$ m/z $[M+H]^+$: 368.0507, found: 368.0509.



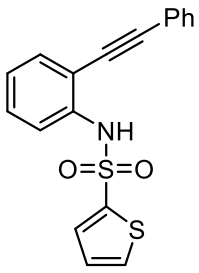
N-(2-(phenylethynyl)phenyl)naphthalene-2-sulfonamide (**33a**)

White solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.39 (d, J = 1.9 Hz, 1H), 7.87 – 7.79 (m, 3H), 7.73 (dd, J = 8.7, 1.9 Hz, 1H), 7.69 (d, J = 8.2 Hz, 1H), 7.60 (ddd, J = 8.2, 6.8, 1.3 Hz, 1H), 7.54 (ddd, J = 8.2, 6.9, 1.3 Hz, 1H), 7.43 – 7.27 (m, 8H), 7.05 (td, J = 7.6, 1.2 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 137.51, 136.12, 135.14, 132.16, 131.70, 129.81, 129.46, 129.42, 129.20, 129.07, 129.04, 128.68, 128.02, 127.60, 124.94, 122.38, 122.04, 120.77, 115.01, 96.31, 83.79.

HRMS (ESI) calculated for $C_{24}H_{18}NO_2S^+$ m/z $[M+H]^+$: 384.1053, found: 384.1051.



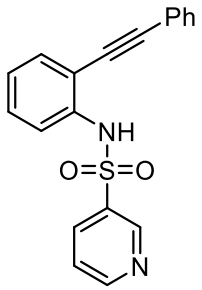
N-(2-(phenylethynyl)phenyl)thiophene-2-sulfonamide (**34a**)

White solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.70 (dd, J = 8.4, 3.4 Hz, 1H), 7.55 – 7.45 (m, 4H), 7.45 – 7.32 (m, 5H), 7.29 (s, 1H), 7.17 – 7.09 (m, 1H), 7.01 – 6.92 (m, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 139.43, 137.23, 132.98, 132.86, 132.17, 131.77, 129.80, 129.25, 128.70, 127.45, 125.29, 122.05, 121.08, 115.35, 96.37, 83.62.

HRMS (ESI) calculated for $C_{18}H_{13}NNaO_2S_2^+$ m/z $[M+Na]^+$: 362.0280, found: 362.0281.



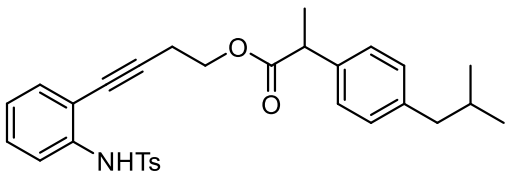
N-(2-(phenylethynyl)phenyl)pyridine-3-sulfonamide (**35a**)

White solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.97 (s, 1H), 8.72 (dd, J = 4.9, 1.6 Hz, 1H), 8.00 (dt, J = 8.2, 2.0 Hz, 1H), 7.66 (d, J = 8.2 Hz, 1H), 7.50 – 7.27 (m, 9H), 7.14 (td, J = 7.6, 1.2 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 153.73, 148.18, 136.55, 135.72, 135.01, 132.41, 131.71, 129.99, 129.43, 128.79, 125.85, 123.65, 121.84, 121.78, 115.86, 96.49, 83.49.

HRMS (ESI) calculated for $C_{19}H_{15}N_2O_2S^+$ m/z $[M+H]^+$: 335.0849, found: 335.0836.



4-(2-((4-Methylphenyl)sulfonamido)phenyl)but-3-yn-1-yl 2-(4-isobutylphenyl)propanoate

(**42a**, *Ibuprofen derivative*)

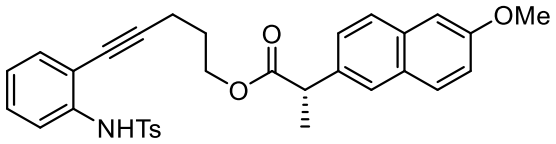
Light brown oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.70 – 7.63 (m, 2H), 7.56 (dd, J = 8.3, 1.1 Hz, 1H), 7.25 – 7.15 (m, 7H), 7.04 (d, J = 7.9 Hz, 2H), 6.98 (td, J = 7.6, 1.2 Hz, 1H), 4.22 (td, J = 6.6, 3.3 Hz, 2H), 3.80 (q,

J = 7.1 Hz, 1H), 2.68 (t, J = 6.5 Hz, 2H), 2.40 (d, *J* = 7.2 Hz, 2H), 2.35 (s, 3H), 1.87 – 1.72 (m, 1H), 1.51 (d, *J* = 7.2 Hz, 3H), 0.87 (d, *J* = 6.6, 6H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 174.88, 144.05, 140.69, 137.89, 137.58, 136.33, 132.14, 129.67, 129.46, 129.32, 127.35, 127.26, 124.35, 119.94, 114.46, 92.95, 76.93, 62.21, 45.10, 45.05, 30.24, 22.48, 21.64, 20.19, 18.72.

HRMS (ESI) calculated for $C_{30}H_{34}NO_4S^+$ m/z $[M+H]^+$: 504.2203, found: 504.2202.



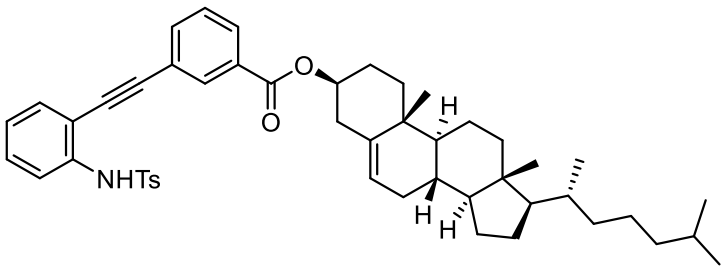
5-(2-((4-Methylphenyl)sulfonamido)phenyl)pent-4-yn-1-yl (*S*)-2-(6-methoxynaphthalen-2-yl)propanoate (**43a**, *Naproxen derivative*)

Light brown oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.74 – 7.67 (m, 3H), 7.65 – 7.60 (m, 2H), 7.54 (dd, *J* = 8.3, 1.1 Hz, 1H), 7.43 (dd, *J* = 8.4, 1.9 Hz, 1H), 7.26 – 7.17 (m, 3H), 7.16 – 7.10 (m, 4H), 6.96 (td, *J* = 7.6, 1.2 Hz, 1H), 4.26 – 4.15 (m, 2H), 3.92 – 3.88 (m, 4H), 2.39 – 2.26 (m, 5H), 1.83 (p, *J* = 6.7 Hz, 2H), 1.60 (d, *J* = 7.1 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 174.80, 157.76, 144.03, 137.75, 136.27, 135.75, 133.82, 132.18, 129.66, 129.39, 129.13, 129.03, 127.35, 127.33, 126.29, 126.06, 124.30, 119.61, 119.17, 114.64, 105.69, 95.95, 76.17, 63.12, 55.42, 45.57, 27.77, 21.62, 18.59, 16.22.

HRMS (ESI) calculated for $C_{32}H_{32}NO_5S^+$ m/z $[M+H]^+$: 542.1996, found: 542.1995.



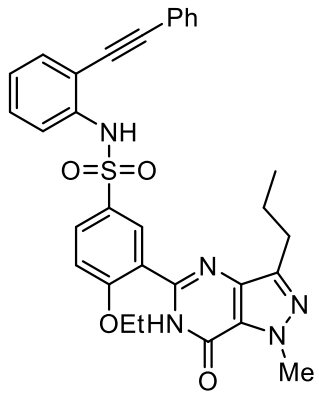
(3*S*,8*S*,9*S*,10*R*,13*R*,14*S*,17*R*)-10,13-dimethyl-17-((*R*)-6-methylheptan-2-yl)-2,3,4,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-1*H*-cyclopenta[*a*]phenanthren-3-yl 3-((2-((4-methylphenyl)sulfonamido)phenyl)ethynyl)benzoate (**44a**, *Cholesterol derivative*)

Light yellow solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.14 – 8.02 (m, 2H), 7.71 – 7.58 (m, 4H), 7.47 (t, J = 7.8 Hz, 1H), 7.39 (dd, J = 7.7, 1.6 Hz, 1H), 7.32 (td, J = 7.9, 1.6 Hz, 1H), 7.22 – 7.13 (m, 3H), 7.09 (td, J = 7.6, 1.2 Hz, 1H), 5.44 (d, J = 5.0 Hz, 1H), 4.98 – 4.83 (m, 1H), 2.54 – 2.44 (m, 2H), 2.34 (s, 3H), 2.08 – 1.90 (m, 4H), 1.89 – 1.72 (m, 2H), 1.65 – 1.42 (m, 6H), 1.40 – 0.96 (m, 17H), 0.92 (d, J = 6.5 Hz, 3H), 0.88 (d, J = 1.9 Hz, 3H), 0.86 (d, J = 1.9 Hz, 3H), 0.69 (s, 3H).

^{13}C NMR (400 MHz, $CDCl_3$) δ 165.16, 144.23, 139.60, 137.69, 136.15, 135.59, 132.71, 132.31, 131.44, 130.15, 130.05, 129.79, 128.77, 127.35, 124.91, 123.11, 122.45, 120.98, 114.62, 94.96, 84.61, 75.22, 56.80, 56.24, 50.15, 42.43, 39.84, 39.63, 38.33, 37.14, 36.77, 36.30, 35.92, 32.06, 31.98, 28.37, 28.14, 28.01, 24.42, 23.95, 22.97, 22.70, 21.69, 21.17, 19.52, 18.84, 11.99.

HRMS (ESI) calculated for $C_{49}H_{62}NO_4S^+$ m/z $[M+H]^+$: 760.4394, found: 760.4396.



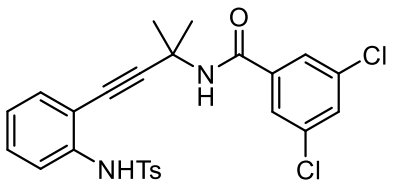
4-Ethoxy-3-(1-methyl-7-oxo-3-propyl-6,7-dihydro-1*H*-pyrazolo[4,3-*d*]pyrimidin-5-yl)-*N*-(2-(phenylethynyl)phenyl)benzenesulfonamide (**45a**, *Sildenafil derivative*)

Light yellow solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 10.64 (s, 1H), 8.88 (d, J = 2.4 Hz, 1H), 7.74 – 7.66 (m, 2H), 7.35 (ddt, J = 11.5, 6.9, 1.5 Hz, 4H), 7.25 – 7.14 (m, 4H), 7.11 (td, J = 7.6, 1.2 Hz, 1H), 6.93 (d, J = 8.8 Hz, 1H), 4.32 – 4.17 (m, 5H), 2.87 (t, J = 7.6 Hz, 2H), 1.82 (h, J = 7.4 Hz, 2H), 1.56 (t, J = 6.9 Hz, 3H), 1.02 (t, J = 7.3 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 159.56, 153.64, 147.14, 146.39, 138.43, 137.21, 132.39, 132.27, 131.53, 131.13, 131.04, 129.81, 128.98, 128.46, 125.44, 124.55, 122.20, 121.87, 121.26, 115.84, 112.99, 96.02, 83.81, 66.10, 38.32, 27.70, 22.45, 14.57, 14.16.

HRMS (ESI) calculated for $C_{31}H_{30}N_5O_4S^+$ m/z $[M+H]^+$: 568.2013, found: 568.2013.



3,5-Dichloro-*N*-(2-methyl-4-(2-((4-methylphenyl)sulfonamido)phenyl)but-3-yn-2-yl)benzamide

(**46a**, *Propyzamide derivative*)

Light yellow solid.

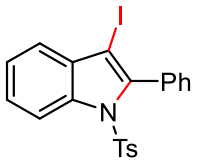
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.40 (s, 1H), 7.83 – 7.78 (m, 2H), 7.74 (d, J = 1.9 Hz, 2H), 7.68 – 7.63 (m, 1H), 7.49 (t, J = 1.9 Hz, 1H), 7.25 – 7.19 (m, 2H), 7.19 – 7.13 (m, 2H), 6.98 – 6.90 (m, 1H), 6.29 (s, 1H), 2.34 (s, 3H), 1.75 (s, 6H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 164.47, 143.59, 139.60, 137.43, 137.20, 135.61, 131.71, 131.38, 129.65, 129.53, 127.44, 126.05, 123.47, 118.96, 113.07, 98.11, 48.38, 29.35, 21.66.

HRMS (ESI) calculated for $C_{25}H_{23}Cl_2N_2O_3S^+$ m/z $[M+H]^+$: 501.0801, found: 501.0805.

2.2 Characterization data for products

2.2.1 Characterization data for iodocyclization products (b)

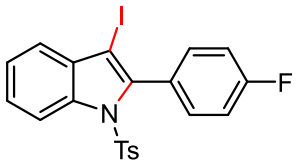


3-Iodo-2-phenyl-1-tosyl-1*H*-indole (**1b**) [4]

Light yellow solid, 89.0 mg, 94% yield under **Condition A**.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.36 – 8.28 (m, 1H), 7.54 – 7.41 (m, 5H), 7.40 – 7.30 (m, 5H), 7.10 (dd, J = 8.4, 1.9 Hz, 2H), 2.33 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 145.14, 141.19, 137.10, 135.16, 132.36, 131.86, 131.66, 129.60, 129.43, 127.63, 127.03, 126.20, 124.77, 122.31, 116.13, 75.93, 21.71.

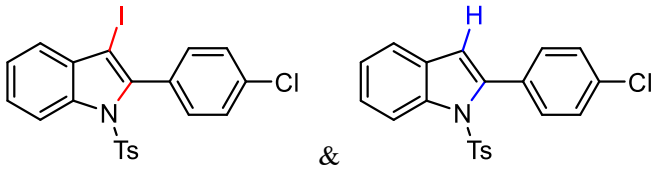


2-(4-Fluorophenyl)-3-iodo-1-tosyl-1*H*-indole (**2b**) [4]

Light yellow solid, 80.6 mg, 82% yield under **Condition A**.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.34 – 8.29 (m, 1H), 7.49 – 7.28 (m, 7H), 7.19 – 7.13 (m, 2H), 7.10 (d, J = 8.2 Hz, 2H), 2.33 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 163.39 (d, J = 249.5 Hz), 145.30, 140.07, 137.09, 135.11, 133.80 (d, J = 8.2 Hz), 132.21, 129.68, 127.55 (d, J = 3.6 Hz), 126.94, 126.37, 124.86, 122.34, 116.14, 114.89 (d, J = 21.9 Hz), 76.26, 21.74.



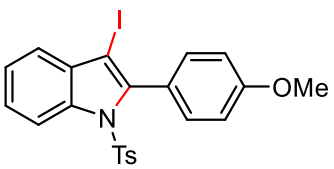
2-(4-Chlorophenyl)-3-iodo-1-tosyl-1*H*-indole (**3b**) [4]

& 2-(4-Chlorophenyl)-1-tosyl-1*H*-indole (**3c**) [9]

Light yellow solid mixture, 87.7 mg, **3:1** by ^{1}H NMR (1:0.33), consisting of 70.1 mg of **3b** (69% yield) and 17.6 mg of **3c** (23% yield) under **Condition A**.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.36 – 8.26 (m, 1.33H), 7.50 – 7.23 (m, 12H), 7.10 (d, J = 8.1 Hz, 2H), 7.05 (d, J = 8.1 Hz, 0.66H), 6.55 (s, 0.33H), 2.33 (s, 3H), 2.29 (s, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 145.35, 144.86, 140.92, 139.89, 138.43, 137.13, 135.58, 134.94, 134.88, 134.50, 133.13, 132.32, 131.59, 130.98, 130.55, 130.07, 129.69, 129.41, 128.03, 127.94, 126.92, 126.83, 126.47, 125.19, 124.94, 124.61, 122.41, 120.92, 116.82, 116.18, 114.19, 76.46, 21.74, 21.67.

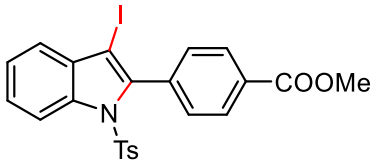


3-Iodo-2-(4-methoxyphenyl)-1-tosyl-1*H*-indole (**4b**) [4]

Light yellow solid, 88.6 mg, 88% yield under **Condition A**.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.31 (dt, J = 8.3, 0.9 Hz, 1H), 7.46 – 7.34 (m, 3H), 7.33 – 7.27 (m, 4H), 7.09 (d, J = 8.1 Hz, 2H), 7.01 – 6.96 (m, 2H), 3.91 (s, 3H), 2.32 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 160.39, 145.07, 141.16, 137.10, 135.16, 133.25, 132.38, 129.56, 127.00, 126.03, 124.73, 123.64, 122.16, 116.20, 113.05, 75.85, 55.40, 21.72.



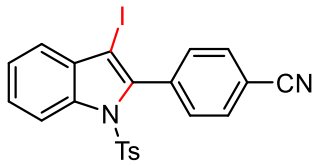
Methyl 4-(3-iodo-1-tosyl-1*H*-indol-2-yl)benzoate (**5b**)

Light yellow solid, 79.7 mg, 75% yield under **Condition A**.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.33 – 8.27 (m, 1H), 8.17 – 8.10 (m, 2H), 7.50 – 7.35 (m, 5H), 7.33 – 7.28 (m, 2H), 7.13 – 7.07 (m, 2H), 3.98 (s, 3H), 2.33 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 166.88, 145.41, 140.06, 137.25, 136.34, 134.91, 132.45, 131.90, 130.81, 129.72, 128.89, 126.95, 126.62, 125.01, 122.53, 116.22, 76.68, 52.44, 21.74.

HRMS (ESI) calculated for $C_{23}H_{19}INO_4S^+$ m/z $[M+H]^+$: 532.0074, found: 532.0073.



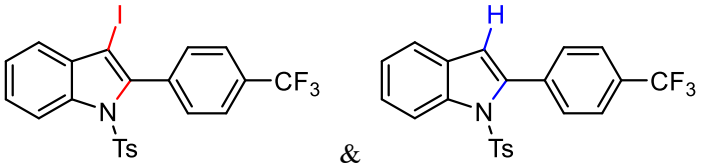
4-(3-Iodo-1-tosyl-1*H*-indol-2-yl)benzonitrile (**6b**)

White solid, 68.8 mg, 69% yield under **Condition A**.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.29 (d, J = 8.5 Hz, 1H), 7.80 – 7.73 (m, 2H), 7.57 – 7.52 (m, 2H), 7.51 – 7.45 (m, 1H), 7.45 – 7.36 (m, 2H), 7.32 – 7.27 (m, 2H), 7.11 (d, J = 8.2 Hz, 2H), 2.33 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 145.64, 139.00, 137.28, 136.49, 134.60, 132.48, 132.41, 131.46, 129.82, 127.00, 126.84, 125.24, 122.70, 118.71, 116.27, 113.03, 21.76 (C-I signal overlapped by the signals of $CDCl_3$).

HRMS (ESI) calculated for $C_{22}H_{16}IN_2O_2S^+$ m/z $[M+H]^+$: 498.9972, found: 498.9969.



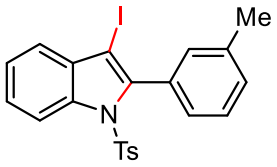
3-Iodo-1-tosyl-2-(4-(trifluoromethyl)phenyl)-1*H*-indole (**7b**) [4]

& 1-Tosyl-2-(4-(trifluoromethyl)phenyl)-1*H*-indole (**7c**) [10]

White solid mixture, 91.7 mg, **8.3:1** by ^{1}H NMR (1:0.12), consisting of 83.9 mg of **7b** (78% yield) and 7.8 mg of **7c** (9% yield) under **Condition A**.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.30 (d, J = 8.4 Hz, 1.12H), 7.72 (d, J = 8.1 Hz, 2H), 7.70 – 7.62 (m, 0.48H), 7.56 – 7.35 (m, 5.24H), 7.34 – 7.24 (m, 2.24H), 7.11 (d, J = 8.1 Hz, 2H), 7.05 (d, J = 8.1 Hz, 0.24H), 6.61 (s, 0.12H), 2.33 (s, 3H), 2.29 (s, 0.36H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 145.50, 145.00, 139.52, 138.63, 137.20, 136.15, 135.40, 134.79, 132.36, 132.19, 131.17 (q, J = 32.4 Hz), 130.52, 129.76, 128.16 (q, J = 264.0 Hz), 126.93, 126.73, 125.54, 125.51, 125.07, 124.76, 124.67 (q, J = 3.7 Hz), 122.80, 122.57, 121.14, 116.88, 116.22, 115.15, 76.94, 21.75. (Some signals of **7c** were missing due to low content and overlapping)

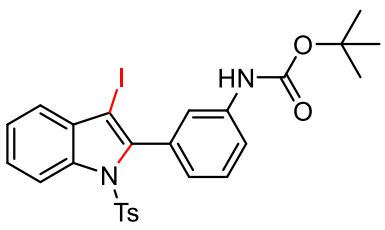


3-Iodo-2-(*m*-tolyl)-1-tosyl-1*H*-indole (**8b**) [4]

Light yellow oil, 87.7 mg, 90% yield under **Condition A**.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.32 (dt, J = 8.3, 0.9 Hz, 1H), 7.48 – 7.40 (m, 2H), 7.40 – 7.28 (m, 5H), 7.18 (dt, J = 7.6, 1.7 Hz, 1H), 7.13 – 7.05 (m, 3H), 2.42 (s, 3H), 2.33 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 145.07, 141.35, 137.13, 137.08, 135.24, 132.46, 132.30, 131.47, 130.19, 129.53, 128.86, 127.51, 127.08, 126.10, 124.69, 122.25, 116.08, 75.66, 21.71, 21.55.



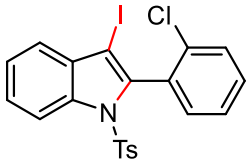
Tert-butyl (3-(3-iodo-1-tosyl-1*H*-indol-2-yl)phenyl)carbamate (**9b**)

Light yellow oil. 104.8 mg, 89% yield under **Condition A**.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.28 (dd, J = 8.4, 3.0 Hz, 1H), 7.57 (d, J = 8.3 Hz, 1H), 7.47 – 7.30 (m, 6H), 7.30 – 7.22 (m, 1H), 7.09 (dd, J = 8.4, 2.9 Hz, 2H), 7.04 – 6.95 (m, 1H), 6.58 (s, 1H), 2.30 (s, 3H), 1.53 (s, 9H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 152.69, 145.11, 140.74, 137.91, 137.02, 135.15, 132.41, 132.26, 129.66, 128.35, 127.18, 126.42, 126.18, 124.71, 122.32, 121.79, 119.30, 116.04, 80.77, 75.86, 28.50, 21.72.

HRMS (ESI) calculated for $C_{26}H_{26}IN_2O_4S^+$ m/z $[M+H]^+$: 589.0652, found: 589.0650.



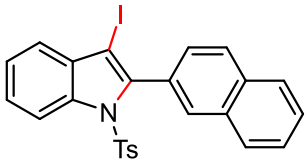
2-(2-Chlorophenyl)-3-iodo-1-tosyl-1*H*-indole (**10b**)

White solid, 92.4 mg, 91% yield under **Condition A**.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.27 (d, J = 8.8 Hz, 1H), 7.54 – 7.43 (m, 6H), 7.41 – 7.35 (m, 2H), 7.28 (dd, J = 7.6, 1.7 Hz, 1H), 7.15 (d, J = 8.1 Hz, 2H), 2.34 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 145.33, 137.99, 136.34, 135.90, 135.52, 133.58, 131.67, 131.31, 131.06, 129.76, 129.57, 127.29, 126.31, 126.14, 124.42, 122.30, 115.27, 76.11, 21.75.

HRMS (ESI) calculated for $C_{21}H_{16}ClINO_2S^+$ m/z $[M+H]^+$: 507.9629, found: 507.9627.



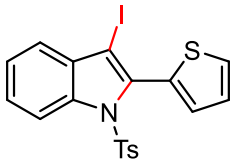
3-Iodo-2-(naphthalen-2-yl)-1-tosyl-1*H*-indole (**11b**)

Light yellow solid, 91.1 mg, 87% yield under **Condition A**.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.36 (dd, J = 8.3, 1.1 Hz, 1H), 7.97 – 7.91 (m, 2H), 7.88 (dd, J = 7.3, 2.2 Hz, 1H), 7.77 (s, 1H), 7.62 – 7.51 (m, 3H), 7.51 – 7.43 (m, 2H), 7.42 – 7.37 (m, 1H), 7.34 – 7.27 (m, 2H), 7.06 (d, J = 8.1 Hz, 2H), 2.32 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 145.19, 141.13, 137.22, 135.11, 133.56, 132.50, 132.47, 131.37, 129.58, 129.19, 129.15, 128.44, 128.07, 127.13, 127.06, 126.51, 126.30, 124.83, 122.38, 116.17, 76.44, 21.72.

HRMS (ESI) calculated for $C_{25}H_{19}INO_2S^+$ m/z $[M+H]^+$: 524.0176, found: 524.0176.



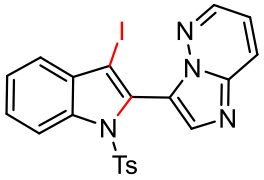
3-Iodo-2-(thiophen-2-yl)-1-tosyl-1*H*-indole (**12b**)

Light yellow oil, 84.3 mg, 88% yield under **Condition A**.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.30 (dt, J = 8.4, 0.9 Hz, 1H), 7.57 (dd, J = 5.0, 1.3 Hz, 1H), 7.49 – 7.34 (m, 5H), 7.19 – 7.09 (m, 4H), 2.34 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 145.21, 137.28, 135.20, 134.07, 132.36, 131.92, 131.44, 129.69, 129.00, 127.09, 126.63, 126.60, 124.73, 122.49, 115.97, 78.89, 21.75.

HRMS (ESI) calculated for $C_{19}H_{14}INNaO_2S_2^+$ m/z $[M+Na]^+$: 501.9403, found: 501.9402.



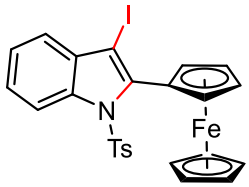
3-(3-Iodo-1-tosyl-1*H*-indol-2-yl)imidazo[1,2-b]pyridazine (**13b**)

Light yellow solid, 96.7 mg, 94% yield under **Condition A**.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.37 – 8.27 (m, 2H), 8.09 (dd, J = 9.2, 1.7 Hz, 1H), 7.89 (s, 1H), 7.52 – 7.44 (m, 2H), 7.43 – 7.33 (m, 3H), 7.16 (dd, J = 9.2, 4.3 Hz, 1H), 7.07 (d, J = 8.1 Hz, 2H), 2.29 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 145.31, 143.38, 140.10, 137.32, 136.94, 135.01, 131.90, 129.75, 128.22, 127.04, 126.92, 125.81, 124.66, 122.76, 119.73, 118.20, 115.67, 79.97, 21.68.

HRMS (ESI) calculated for $C_{21}H_{16}IN_4O_2S^+$ m/z $[M+H]^+$: 515.0033, found: 515.0037.



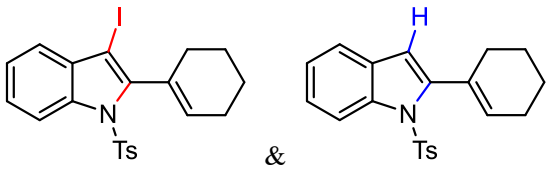
3-Iodo-2-(2-(ferrocenylethynyl)phenyl)-1-tosyl-1*H*-indole (**14b**)

Red solid, 81.4 mg, 70% yield under **Condition A**.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.13 (d, J = 8.1 Hz, 1H), 7.44 – 7.17 (m, 3H), 7.06 – 6.85 (m, 4H), 5.09 (s, 2H), 4.49 (s, 2H), 4.26 (s, 5H), 2.22 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 144.58, 141.58, 138.53, 135.41, 132.57, 128.87, 126.98, 125.62, 121.40, 118.36, 72.05, 70.15, 68.20, 21.65 (the C-I signal was overlapped by the signals of $CDCl_3$).

HRMS (ESI) calculated for $C_{25}H_{21}FeINO_2S^+$ m/z $[M+H]^+$: 581.9682, found: 581.9680.



2-(Cyclohex-1-en-1-yl)-3-iodo-1-tosyl-1*H*-indole (**15b**)

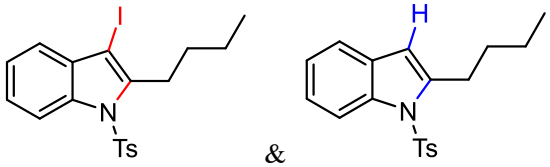
& 2-(Cyclohex-1-en-1-yl)-1-tosyl-1*H*-indole (**15c**) [11]

Colorless oil mixture, 84.4 mg, **6.25:1** by ^{1}H NMR (1:0.16), consisting of 75.4 mg of **15b** (79% yield) and 9.0 mg of **15c** (13% yield) under **Condition A**.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.24 – 8.14 (m, 1.16H), 7.62 – 7.55 (m, 2H), 7.52 (d, J = 8.4 Hz, 0.32H), 7.40 – 7.27 (m, 3.32H), 7.20 (td, J = 7.4, 1.1 Hz, 0.16H), 7.14 (d, J = 8.1 Hz, 2H), 7.09 (d, J = 8.0 Hz, 0.32H), 6.35 (s, 0.16H), 5.76 (dq, J = 3.7, 1.8 Hz, 0.16H), 5.57 (tt, J = 3.7, 1.7 Hz, 1H), 2.73 – 2.53 (m, 1H), 2.48 – 2.41 (m, 0.32H), 2.36 – 2.21 (m, 5.80H), 2.15 – 1.98 (m, 1H), 1.93 – 1.78 (m, 3.32H), 1.78 – 1.64 (m, 1.32H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 145.01, 144.97, 144.50, 143.57, 137.83, 136.67, 135.52, 135.06, 133.21, 132.59, 132.32, 131.63, 130.79, 129.59, 129.51, 129.32, 126.96, 126.87, 125.68, 124.37, 124.04, 122.19, 120.57, 116.13, 115.50, 111.05, 73.63, 30.63, 29.95, 25.79, 25.70, 22.80, 22.72, 22.07, 21.94, 21.70, 21.64.

HRMS (ESI) calculated for (**15b**) $C_{21}H_{21}INO_2S^+$ m/z $[M+H]^+$: 478.0332, found: 478.0334.



2-Butyl-3-iodo-1-tosyl-1*H*-indole (**16b**)

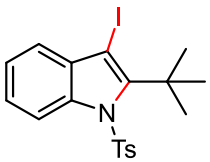
& 2-Butyl-1-tosyl-1*H*-indole (**16c**) [9]

Light yellow oil mixture, 79.3 mg, **9:1** by ^{1}H NMR (1:0.11), consisting of 73.4 mg of **16b** (81% yield) and 5.9 mg of **16c** (9% yield) under **Condition A**.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.21 – 8.08 (m, 1.11H), 7.66 – 7.52 (m, 2.22H), 7.41 – 7.37 (m, 0.11H), 7.35 – 7.10 (m, 5.44H), 6.37 (s, 0.11H), 3.16 – 3.07 (m, 2H), 3.01 – 2.95 (m, 0.22H), 2.30 (s, 3.33H), 1.75 – 1.64 (m, 2.22H), 1.51 – 1.40 (m, 2.22H), 0.96 (t, J = 7.4 Hz, 3.33H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 145.10, 144.69, 142.62, 142.26, 137.31, 136.75, 136.34, 135.86, 131.97, 130.00, 129.87, 126.43, 126.35, 125.30, 124.28, 123.86, 123.56, 121.56, 120.15, 115.21, 114.93, 108.73, 73.62, 32.30, 31.08, 29.64, 28.85, 22.78, 22.59, 21.66, 14.06, 13.98.

HRMS (ESI) calculated for (**16b**) $C_{19}H_{21}INO_2S^+$ m/z $[M+H]^+$: 454.0332, found: 454.0337.

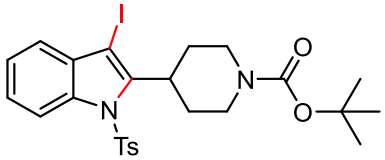


2-(*Tert*-butyl)-3-iodo-1-tosyl-1*H*-indole (**17b**) [4]

Light yellow solid, 84.3 mg, 93% yield under **Condition A**.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.92 (d, J = 8.2 Hz, 1H), 7.26 – 7.18 (m, 3H), 7.17 – 7.08 (m, 2H), 6.94 (d, J = 8.2 Hz, 2H), 2.23 (s, 3H), 1.79 (s, 9H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 151.61, 144.37, 139.70, 136.53, 131.80, 128.63, 126.93, 125.87, 125.49, 122.05, 118.43, 80.41, 36.53, 31.98, 21.64.



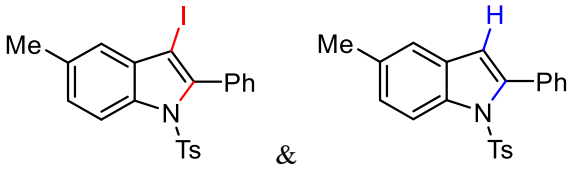
Tert-butyl 4-(3-iodo-1-tosyl-1*H*-indol-2-yl)piperidine-1-carboxylate (**18b**)

Light yellow oil, 95.1 mg, 82% yield under **Condition A**.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.25 (d, J = 7.8 Hz, 1H), 7.60 (d, J = 8.4 Hz, 2H), 7.43 – 7.29 (m, 3H), 7.23 (d, J = 8.1 Hz, 2H), 4.31 – 4.05 (m, 2H), 3.79 (tt, J = 12.2, 3.6 Hz, 1H), 2.82 – 2.56 (m, 2H), 2.52 – 2.39 (m, 2H), 2.37 (s, 3H), 1.49 (s, 9H), 1.42 – 1.28 (m, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 155.00, 145.44, 141.04, 136.79, 136.46, 132.20, 130.13, 126.40, 125.79, 124.19, 121.67, 115.28, 79.69, 69.10, 45.06, 44.28, 35.33, 29.28, 28.59, 21.74.

HRMS (ESI) calculated for $C_{25}H_{30}IN_2O_4S^+$ m/z $[M+H]^+$: 581.0965, found: 581.0961.



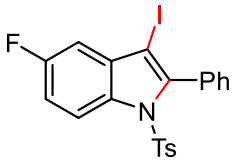
3-Iodo-5-methyl-2-phenyl-1-tosyl-1*H*-indole (**20b**) [4]

& 5-Methyl-2-phenyl-1-tosyl-1*H*-indole (**20c**) [9]

Light yellow oil mixture, 83.2 mg, **4:1** by ^{1}H NMR (1:0.25), consisting of 70.2 mg of **20b** (72% yield) and 13.0 mg of **20c** (18% yield) under **Condition A**.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.16 (dd, J = 8.5, 2.4 Hz, 1.25H), 7.52 – 7.41 (m, 3.75H), 7.39 – 7.33 (m, 2H), 7.33 – 7.27 (m, 2H), 7.27 – 7.14 (m, 3.25H), 7.08 (d, J = 8.1 Hz, 2H), 7.03 (d, J = 8.0 Hz, 0.5H), 6.47 (s, 0.25H), 2.47 (s, 3H), 2.40 (s, 0.75H), 2.31 (s, 3H), 2.27 (s, 0.75H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 145.02, 144.53, 142.37, 141.24, 136.61, 135.30, 135.10, 134.67, 134.11, 132.56, 131.84, 131.73, 130.96, 130.39, 129.56, 129.37, 129.29, 128.70, 127.60, 127.01, 126.92, 126.29, 122.15, 120.77, 116.50, 115.94, 113.75, 75.95, 21.72, 21.66, 21.41.

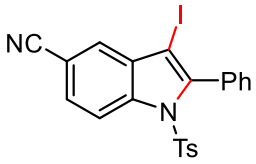


5-Fluoro-3-iodo-2-phenyl-1-tosyl-1*H*-indole (**21b**) [12]

Light yellow solid, 83.5 mg, 85% yield under **Condition A**.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.27 (dd, J = 9.1, 4.4 Hz, 1H), 7.54 – 7.43 (m, 3H), 7.39 – 7.33 (m, 2H), 7.31 – 7.24 (m, 3H), 7.16 (td, J = 9.0, 2.6 Hz, 1H), 7.13 – 7.06 (m, 3H), 2.34 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 160.55 (d, J = 242.2 Hz), 145.38, 143.00, 134.85, 133.89 (d, J = 10.2 Hz), 133.36, 131.78, 131.31, 129.67 (d, J = 2.4 Hz), 127.70, 127.03, 117.62 (d, J = 9.3 Hz), 114.07 (d, J = 25.0 Hz), 108.06 (d, J = 25.0 Hz), 74.98 (d, J = 3.7 Hz), 21.76.

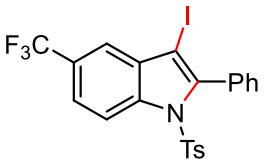


3-Iodo-2-phenyl-1-tosyl-1*H*-indole-5-carbonitrile (**22b**) [13]

White solid, 91.7 mg, 92% yield under **Condition A**.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.43 (dd, J = 8.7, 0.6 Hz, 1H), 7.78 (d, J = 1.6 Hz, 1H), 7.69 (dd, J = 8.7, 1.7 Hz, 1H), 7.57 – 7.50 (m, 1H), 7.49 – 7.42 (m, 2H), 7.32 – 7.26 (m, 4H), 7.13 (d, J = 8.2 Hz, 2H), 2.36 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 145.94, 143.39, 139.00, 134.86, 132.39, 131.78, 130.54, 129.97, 129.89, 128.91, 127.83, 127.76, 127.14, 119.10, 116.85, 108.20, 73.89, 21.80.



3-Iodo-2-phenyl-1-tosyl-5-(trifluoromethyl)-1*H*-indole (**23b**)

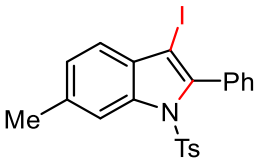
White solid, 89.9 mg, 83% yield under **Condition A**.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.44 (d, J = 8.7 Hz, 1H), 7.74 – 7.65 (m, 2H), 7.55 – 7.42 (m, 3H), 7.35 – 7.28 (m, 4H), 7.12 (d, J = 8.2 Hz, 2H), 2.35 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 145.70, 142.92, 138.69, 134.99, 132.11, 131.84, 130.94, 129.83, 127.78, 127.11, 127.06 (q, J = 32.8 Hz), 124.45 (q, J = 272.1 Hz), 122.75 (q, J = 3.5 Hz), 119.91 (q, J = 4.1 Hz), 116.47, 74.80, 21.78.

^{19}F NMR (376 MHz, $CDCl_3$) δ -61.26.

HRMS (ESI) calculated for $C_{22}H_{16}F_3INO_2S^+$ m/z $[M+H]^+$: 541.9893, found: 541.9890.

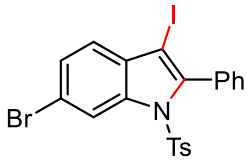


3-Iodo-6-methyl-2-phenyl-1-tosyl-1*H*-indole (**24b**) [4]

White solid, 88.7 mg, 91% under **Condition A**.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.12 (s, 1H), 7.51 – 7.40 (m, 3H), 7.37 – 7.24 (m, 5H), 7.18 (dd, J = 8.1, 1.4 Hz, 1H), 7.09 (d, J = 8.1 Hz, 2H), 2.56 (s, 3H), 2.32 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 145.03, 140.46, 137.42, 136.48, 135.22, 131.87, 131.77, 130.23, 129.58, 129.30, 127.58, 126.99, 126.22, 121.81, 116.18, 75.95, 22.23, 21.73.



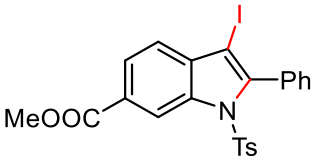
6-Bromo-3-iodo-2-phenyl-1-tosyl-1*H*-indole (**25b**)

White solid, 99.3 mg, 90% under **Condition A**.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.52 (d, J = 1.6 Hz, 1H), 7.53 – 7.41 (m, 4H), 7.34 – 7.24 (m, 5H), 7.12 (d, J = 8.2 Hz, 2H), 2.34 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 145.51, 141.67, 137.54, 134.97, 131.84, 131.22, 131.13, 129.76, 129.66, 128.02, 127.70, 127.12, 123.41, 119.83, 118.95, 74.95, 21.78.

HRMS (ESI) calculated for $C_{21}H_{16}BrINO_2S^+$ m/z $[M+H]^+$: 551.9124, found: 551.9125.



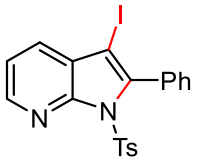
Methyl 3-iodo-2-phenyl-1-tosyl-1*H*-indole-6-carboxylate (**26b**)

Light yellow solid, 82.8 mg, 78% yield under **Condition A**.

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.01 (d, J = 1.4 Hz, 1H), 8.06 (dd, J = 8.3, 1.4 Hz, 1H), 7.56 – 7.43 (m, 4H), 7.38 – 7.29 (m, 4H), 7.11 (d, J = 8.1 Hz, 2H), 4.01 (s, 3H), 2.33 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 167.28, 145.50, 144.12, 136.55, 135.82, 134.97, 131.74, 131.14, 129.80, 129.76, 127.89, 127.74, 127.16, 125.85, 122.09, 117.78, 75.09, 52.54, 21.76.

HRMS (ESI) calculated for $C_{23}H_{19}INO_4S^+$ m/z $[M+H]^+$: 532.0074, found: 532.0071.



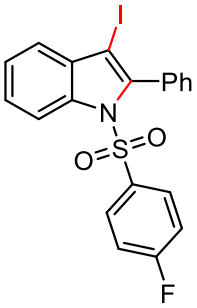
3-Iodo-2-phenyl-1-tosyl-1*H*-pyrrolo[2,3-*b*]pyridine (**27b**)

Light yellow solid, 60.7 mg, 64% yield under **Condition A**.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.61 – 8.46 (m, 1H), 7.82 (d, J = 7.8 Hz, 2H), 7.75 – 7.65 (m, 1H), 7.58 – 7.48 (m, 3H), 7.47 – 7.39 (m, 2H), 7.33 – 7.24 (m, 1H), 7.20 (d, J = 7.9 Hz, 2H), 2.34 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 148.73, 146.07, 145.27, 141.47, 135.71, 132.07, 131.01, 130.27, 129.56, 128.05, 127.91, 124.94, 120.22, 70.57, 21.74.

HRMS (ESI) calculated for $C_{20}H_{16}IN_2O_2S^+$ m/z $[M+H]^+$: 474.9972, found: 474.9970.



1-((4-Fluorophenyl)sulfonyl)-3-iodo-2-phenyl-1*H*-indole (**28b**)

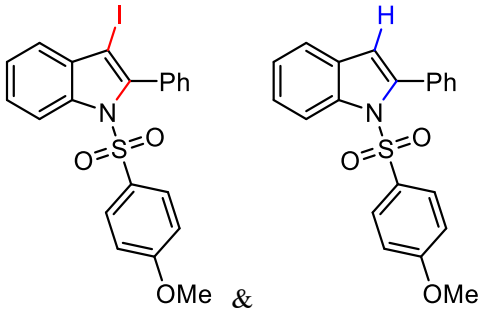
Light yellow solid, 82.1 mg, 86% yield under **Condition A**.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.29 (d, J = 8.3 Hz, 1H), 7.54 – 7.38 (m, 8H), 7.38 – 7.33 (m, 2H), 6.98 (t, J = 8.5 Hz, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 165.84 (d, J = 257.3 Hz), 141.02, 137.08, 134.01, 133.97, 132.47, 131.86, 131.40, 129.90 (d, J = 9.7 Hz), 129.60, 127.75, 126.45, 125.07, 122.52, 116.49, 116.19 (d, J = 15.1 Hz), 76.44.

^{19}F NMR (376 MHz, $CDCl_3$) δ -102.33.

HRMS (ESI) calculated for $C_{20}H_{14}FINO_2S^+$ m/z $[M+H]^+$: 477.9768, found: 477.9770.



3-Iodo-1-((4-methoxyphenyl)sulfonyl)-2-phenyl-1*H*-indole (**29b**)

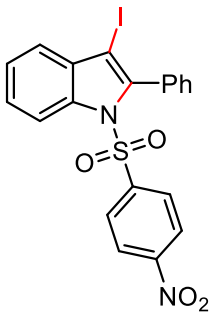
& 1-((4-Methoxyphenyl)sulfonyl)-2-phenyl-1*H*-indole (**29c**) [2]

Light yellow solid mixture, 87.3 mg, 12.5:1 by ^{1}H NMR (1:0.08), consisting of 82.2 mg of **29b** (84% yield) and 5.1 mg of **29c** (7% yield) under **Condition A**.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.31 (d, J = 8.3 Hz, 1.08H), 7.54 – 7.40 (m, 5.40H), 7.40 – 7.25 (m, 5.40H), 6.78 – 6.72 (m, 2H), 6.70 (d, J = 9.0 Hz, 0.16H), 6.55 (s, 0.08H), 3.78 (s, 3H), 3.75 (s, 0.24H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 163.92, 141.21, 137.14, 132.37, 131.87, 131.73, 130.46, 129.72, 129.41, 129.31, 129.15, 128.76, 127.64, 126.16, 124.88, 124.71, 124.40, 122.30, 120.81, 116.80, 116.14, 114.14, 113.85, 75.78, 55.74.

HRMS (ESI) calculated for (**29b**) $C_{21}H_{17}INO_3S^+$ m/z $[M+H]^+$: 489.9968, found: 489.9964.



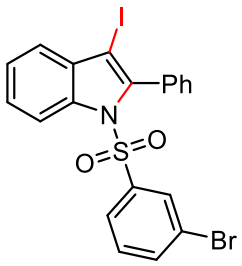
3-Iodo-1-((4-nitrophenyl)sulfonyl)-2-phenyl-1*H*-indole (**30b**)

Light yellow solid, 32.3 mg, 32% yield under **Condition A**.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.29 (dt, J = 8.4, 0.9 Hz, 1H), 8.18 – 8.12 (m, 2H), 7.63 – 7.57 (m, 2H), 7.56 – 7.46 (m, 4H), 7.45 – 7.41 (m, 2H), 7.40 – 7.35 (m, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 150.72, 142.91, 140.76, 136.88, 132.67, 131.81, 130.99, 129.88, 128.34, 127.92, 126.86, 125.61, 124.22, 122.85, 116.09, 77.54.

HRMS (ESI) calculated for $C_{20}H_{14}IN_2O_4S^+$ m/z $[M+H]^+$: 504.9713, found: 504.9715.



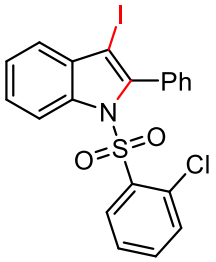
1-((3-Bromophenyl)sulfonyl)-3-iodo-2-phenyl-1*H*-indole (**31b**)

Light yellow solid, 88.3 mg, 82% yield under **Condition A**.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.29 (d, J = 8.3 Hz, 1H), 7.61 (ddd, J = 8.0, 2.0, 1.0 Hz, 1H), 7.56 – 7.46 (m, 5H), 7.46 – 7.39 (m, 2H), 7.40 – 7.32 (m, 3H), 7.18 (t, J = 8.0 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 140.87, 139.47, 137.05, 136.95, 132.35, 131.94, 131.15, 130.55, 130.21, 129.74, 127.79, 126.54, 125.33, 125.14, 122.81, 122.53, 116.01, 76.58.

HRMS (ESI) calculated for $C_{20}H_{14}BrINO_2S^+$ m/z $[M+H]^+$: 537.8968, found: 537.8963.



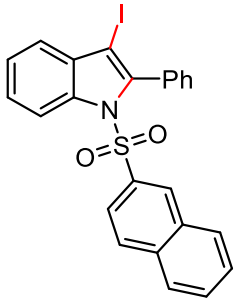
1-((2-chlorophenyl)sulfonyl)-3-iodo-2-phenyl-1H-indole (**32b**)

Light yellow solid, 88.9 mg, 90% yield under **Condition A**.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.24 (dt, J = 8.4, 0.9 Hz, 1H), 7.51 – 7.47 (m, 1H), 7.47 – 7.41 (m, 1H), 7.41 – 7.35 (m, 3H), 7.35 – 7.29 (m, 1H), 7.26 – 7.22 (m, 1H), 7.20 (t, J = 7.8 Hz, 2H), 7.08 – 7.03 (m, 2H), 6.99 (ddd, J = 8.2, 6.4, 2.3 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 139.95, 138.10, 137.07, 134.50, 133.14, 131.98, 131.69, 131.61, 130.88, 130.56, 129.26, 127.66, 126.70, 126.06, 124.16, 122.31, 116.09, 74.44.

HRMS (ESI) calculated for $C_{20}H_{14}ClINO_2S^+$ m/z $[M+H]^+$: 493.9473, found: 493.9475.



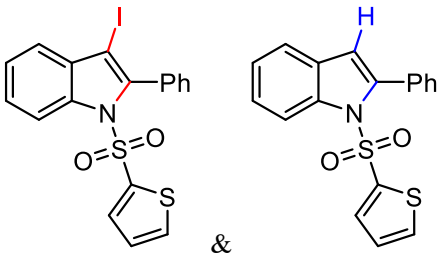
3-Iodo-1-(naphthalen-2-ylsulfonyl)-2-phenyl-1*H*-indole (**33b**)

White solid, 78.4 mg, 77% yield under **Condition A**.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.41 (dt, J = 8.3, 0.8 Hz, 1H), 7.93 (d, J = 1.9 Hz, 1H), 7.84 – 7.71 (m, 3H), 7.62 (ddd, J = 8.2, 6.8, 1.5 Hz, 1H), 7.57 (ddd, J = 8.1, 6.9, 1.4 Hz, 1H), 7.54 – 7.44 (m, 3H), 7.44 – 7.35 (m, 4H), 7.34 – 7.29 (m, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 141.06, 137.17, 135.32, 134.94, 132.24, 132.03, 131.66, 131.51, 129.60, 129.56, 129.54, 129.44, 129.26, 128.01, 127.83, 127.62, 126.31, 124.82, 122.37, 121.47, 116.10, 75.94.

HRMS (ESI) calculated for $C_{24}H_{17}INO_2S^+$ m/z $[M+H]^+$: 510.0019, found: 510.0019.



3-Iodo-2-phenyl-1-(thiophen-2-ylsulfonyl)-1*H*-indole (**34b**)

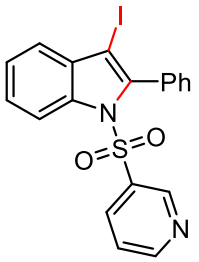
& 2-Phenyl-1-(thiophen-2-ylsulfonyl)-1*H*-indole (**34c**)

Light yellow solid mixture, 77.1 mg, 10:1 by ^{1}H NMR (1:0.1), consisting of 71.7 mg of **34b** (77% yield) and 5.4 mg of **34c** (8% yield) under **Condition A**.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.32 – 8.21 (m, 1.1H), 7.58 – 7.37 (m, 9.8H), 7.34 – 7.28 (m, 1.1H), 7.23 (dd, J = 3.8, 1.4 Hz, 0.1H), 6.90 (dd, J = 5.0, 3.8 Hz, 1H), 6.85 (dd, J = 5.0, 3.8 Hz, 0.1H), 6.62 (s, 0.1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 142.35, 141.24, 138.22, 137.57, 137.29, 136.79, 133.72, 133.46, 133.14, 132.95, 132.75, 132.40, 131.64, 131.58, 131.02, 130.26, 129.50, 128.86, 127.75, 127.69, 127.22, 126.97, 126.40, 125.19, 125.13, 124.89, 122.47, 120.98, 116.98, 116.31, 114.51, 76.96.

HRMS (ESI) calculated for (**34b**) $C_{18}H_{13}INO_2S_2^+$ m/z $[M+H]^+$: 465.9427, found: 465.9424.



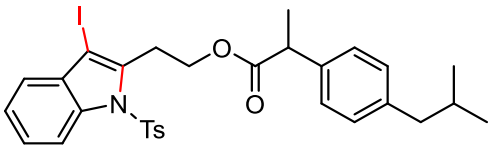
3-Iodo-2-phenyl-1-(pyridin-3-ylsulfonyl)-1*H*-indole (**35b**)

Light yellow solid, 71.8 mg, 78% yield under **Condition A**.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.70 (dd, J = 4.9, 1.6 Hz, 1H), 8.62 (d, J = 2.4 Hz, 1H), 8.29 (d, J = 8.3 Hz, 1H), 7.69 (dt, J = 8.2, 2.0 Hz, 1H), 7.55 – 7.35 (m, 8H), 7.29 – 7.22 (m, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 154.36, 147.68, 140.85, 136.85, 134.61, 134.48, 132.60, 131.74, 131.14, 129.79, 127.92, 126.74, 125.44, 123.58, 122.70, 116.09, 77.20.

HRMS (ESI) calculated for $C_{19}H_{14}IN_2O_2S^+$ m/z $[M+H]^+$: 460.9815, found: 460.9810.



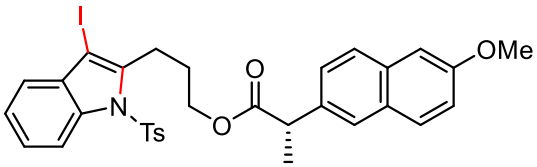
2-(3-Iodo-1-tosyl-1*H*-indol-2-yl)ethyl 2-(4-isobutylphenyl)propanoate (**42b**, *Ibuprofen derivative*)

Light yellow oil, 103.2 mg, 82% yield under **Condition A**.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.11 (dt, J = 7.8, 1.2 Hz, 1H), 7.59 – 7.51 (m, 2H), 7.40 – 7.28 (m, 3H), 7.14 (d, J = 7.9 Hz, 4H), 7.00 – 6.92 (m, 2H), 4.49 (dt, J = 10.9, 6.4 Hz, 1H), 4.33 (dt, J = 10.9, 6.6 Hz, 1H), 3.69 (q, J = 7.2 Hz, 1H), 3.49 (td, J = 6.6, 4.1 Hz, 2H), 2.39 (d, J = 7.2 Hz, 2H), 2.32 (s, 3H), 1.80 (hept, J = 6.6 Hz, 1H), 1.46 (d, J = 7.2 Hz, 3H), 0.87 (d, J = 6.6 Hz, 6H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 174.68, 145.35, 140.54, 137.74, 137.41, 136.84, 135.51, 131.87, 130.12, 129.35, 127.38, 126.42, 125.87, 124.47, 122.00, 115.26, 76.27, 63.63, 45.21, 45.14, 30.28, 29.46, 22.55, 21.71, 18.67.

HRMS (ESI) calculated for $C_{30}H_{33}INO_4S^+$ m/z $[M+H]^+$: 630.1169, found: 630.1171.



3-(3-Iodo-1-tosyl-1*H*-indol-2-yl)propyl (*S*)-2-(6-methoxynaphthalen-2-yl)propanoate

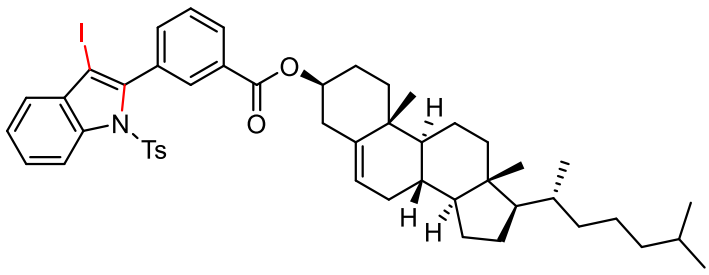
(**43b**, *Naproxen derivative*)

Colorless oil, 120.2 mg, 90% yield under **Condition A**.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.11 (dt, J = 8.3, 1.0 Hz, 1H), 7.73 – 7.67 (m, 3H), 7.56 – 7.50 (m, 2H), 7.46 (dd, J = 8.5, 1.8 Hz, 1H), 7.32 (dt, J = 8.4, 4.4 Hz, 1H), 7.29 – 7.23 (m, 4H), 7.16 – 7.07 (m, 4H), 4.18 (hept, J = 6.1, 5.7 Hz, 2H), 3.96 – 3.84 (m, 4H), 3.20 – 3.04 (m, 2H), 2.30 (s, 3H), 2.09 – 1.97 (m, 2H), 1.61 (d, J = 7.1 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 174.84, 157.71, 145.21, 140.69, 136.71, 135.93, 135.58, 133.83, 131.83, 130.06, 129.46, 129.08, 127.30, 126.60, 126.41, 126.26, 125.58, 124.39, 121.71, 119.08, 115.18, 105.66, 74.27, 64.23, 55.43, 45.70, 29.19, 26.86, 21.68, 18.70.

HRMS (ESI) calculated for $C_{32}H_{31}INO_5S^+$ m/z $[M+H]^+$: 668.0962, found: 668.0961.



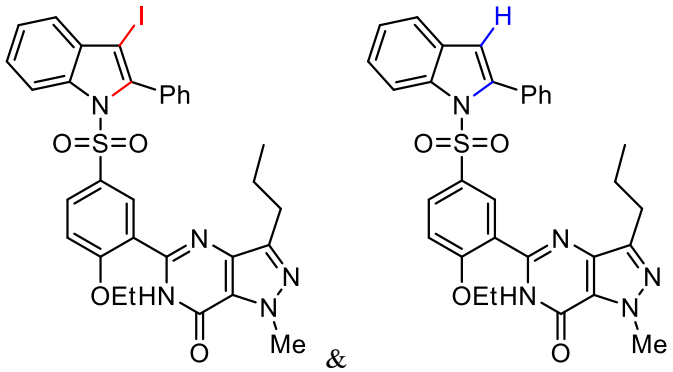
(3*S*,8*S*,9*S*,10*R*,13*R*,14*S*,17*R*)-10,13-Dimethyl-17-((*R*)-6-methylheptan-2-yl)-2,3,4,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-1*H*-cyclopenta[*a*]phenanthren-3-yl 3-(3-iodo-1-tosyl-1*H*-indol-2-yl)benzoate (**44b**, *Cholesterol derivative*)

Light yellow oil, 170.1 mg, 96% yield under **Condition A** (with additional 5.0 mL DCM as co-solvent).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.31 (d, J = 8.3 Hz, 1H), 8.18 (dt, J = 7.5, 1.6 Hz, 1H), 7.97 (t, J = 1.8 Hz, 1H), 7.63 – 7.52 (m, 2H), 7.50 – 7.35 (m, 3H), 7.34 – 7.28 (m, 2H), 7.10 (d, J = 8.1 Hz, 2H), 5.49 – 5.38 (m, 1H), 4.97 – 4.84 (m, 1H), 2.49 (d, J = 7.9 Hz, 2H), 2.32 (s, 3H), 2.09 – 1.69 (m, 6H), 1.65 – 1.44 (m, 6H), 1.40 – 0.96 (m, 17H), 0.93 (d, J = 6.5 Hz, 3H), 0.88 (d, J = 1.9 Hz, 3H), 0.86 (d, J = 1.9 Hz, 3H), 0.69 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 165.56, 145.34, 140.07, 139.73, 137.06, 136.14, 135.01, 132.76, 132.27, 132.03, 130.51, 130.43, 129.74, 127.81, 126.98, 126.46, 124.89, 123.00, 122.42, 116.08, 76.43, 74.93, 56.81, 56.24, 50.15, 42.44, 39.85, 39.64, 38.39, 37.16, 36.78, 36.30, 35.93, 32.07, 31.99, 28.38, 28.15, 28.06, 27.03, 24.43, 23.95, 22.98, 22.71, 21.76, 21.18, 19.54, 18.85, 12.00.

HRMS (ESI) calculated for $C_{49}H_{61}INO_4S^+$ m/z $[M+H]^+$: 886.3360, found: 886.3363.



5-(2-Ethoxy-5-((3-iodo-2-phenyl-1*H*-indol-1-yl)sulfonyl)phenyl)-1-methyl-3-propyl-1,6-dihydro-7*H*-pyrazolo[4,3-*d*]pyrimidin-7-one (**45b**) &

5-(2-Ethoxy-5-((2-phenyl-1*H*-indol-1-yl)sulfonyl)phenyl)-1-methyl-3-propyl-1,6-dihydro-7*H*-pyrazolo[4,3-*d*]pyrimidin-7-one (**45c**)

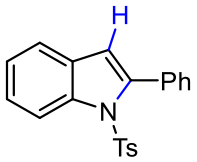
Light yellow solid mixture, 129.2 mg, 8.3:1 by ^{1}H NMR (1:0.12), consisting of 117.9 mg of **43b** (85% yield) and 11.3 mg of **43c** (10% yield) under **Condition A**.

^{1}H NMR (400 MHz, $CDCl_3$) δ 10.71 (s, 1.12H), 8.54 (d, J = 2.6 Hz, 1H), 8.47 (d, J = 2.5 Hz, 0.12H), 8.31 (d, J = 8.4 Hz, 1.12H), 7.57 – 7.33 (m, 10.08H), 6.91 (d, J = 8.9 Hz, 1H), 6.86 (d, J = 8.9 Hz, 0.12H), 6.58 (s, 0.12H), 4.30 – 4.21 (m, 5.60H), 2.96 (t, J = 7.6 Hz, 2.24H), 1.88 (h, J = 7.4 Hz, 2.24H), 1.57 (t, J = 7.0 Hz, 3.36H), 1.07 (t, J = 7.4 Hz, 3.36H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 160.04, 159.78, 153.60, 147.05, 146.05, 142.21, 141.16, 138.37, 138.33, 138.22, 136.92, 132.48, 131.68, 130.98, 130.95, 130.88, 130.72, 130.59, 130.40, 130.32, 129.46, 128.82, 127.74, 127.70, 126.31, 125.04, 124.97, 124.64, 124.51, 122.42, 121.08, 120.96, 116.67, 116.03, 114.01, 112.85, 112.60, 76.39, 66.25, 38.35, 27.70, 22.54, 14.55, 14.24.

HRMS (ESI) calculated for (**43b**) $C_{31}H_{29}IN_5O_4S^+$ m/z $[M+H]^+$: 694.0979, found: 694.0978.

2.2.2 Characterization data for hydrocyclization products (c)

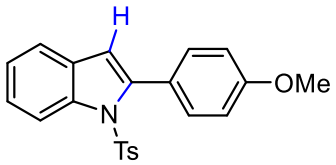


2-Phenyl-1-tosyl-1*H*-indole (**1c**) [9]

Light yellow solid, 68.1 mg, 98% yield under **Condition B**.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.31 (dd, J = 8.4, 1.0 Hz, 1H), 7.52 – 7.48 (m, 2H), 7.46 – 7.38 (m, 4H), 7.35 (ddd, J = 8.5, 7.2, 1.4 Hz, 1H), 7.29 – 7.23 (m, 3H), 7.03 (d, J = 8.1 Hz, 2H), 6.54 (s, 1H), 2.27 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 144.66, 142.26, 138.40, 134.74, 132.55, 130.69, 130.46, 129.33, 128.78, 127.63, 126.92, 124.91, 124.45, 120.82, 116.79, 113.77, 21.65.

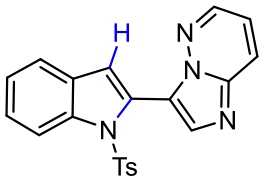


2-(4-Methoxyphenyl)-1-tosyl-1*H*-indole (**4c**) [9]

White solid, 70.2 mg, 93% yield under **Condition B**.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.30 (dd, J = 8.4, 1.0 Hz, 1H), 7.45 – 7.37 (m, 3H), 7.33 (ddd, J = 8.5, 7.3, 1.4 Hz, 1H), 7.29 – 7.20 (m, 3H), 7.02 (d, J = 8.1 Hz, 2H), 6.98 – 6.91 (m, 2H), 6.47 (s, 1H), 3.87 (s, 3H), 2.26 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 160.10, 144.59, 142.14, 138.25, 134.75, 131.76, 130.76, 129.29, 126.87, 124.81, 124.64, 124.39, 120.61, 116.78, 113.07, 113.03, 55.41, 21.62.



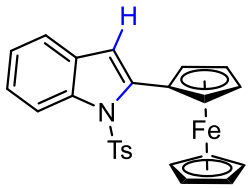
3-(1-Tosyl-1*H*-indol-2-yl)imidazo[1,2-*b*]pyridazine (**13c**)

Light yellow solid, 72.2 mg, 93% yield under **Condition B**.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.36 (dd, J = 4.4, 1.6 Hz, 1H), 8.31 (dd, J = 8.4, 0.9 Hz, 1H), 8.04 (dd, J = 9.2, 1.7 Hz, 1H), 7.86 (s, 1H), 7.54 (dt, J = 7.7, 1.0 Hz, 1H), 7.44 – 7.35 (m, 3H), 7.32 – 7.26 (m, 1H), 7.12 (dd, J = 9.2, 4.4 Hz, 1H), 7.06 (d, J = 8.1 Hz, 2H), 6.89 (s, 1H), 2.27 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 144.92, 143.23, 140.17, 138.01, 135.76, 135.02, 129.81, 129.55, 126.86, 126.75, 125.79, 125.72, 124.16, 121.42, 120.64, 117.75, 115.93, 21.59.

HRMS (ESI) calculated for $C_{21}H_{17}N_4O_2S^+$ m/z $[M+H]^+$: 389.1067, found: 389.1071.



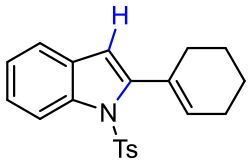
2-(2-(Ferrocenylethynyl)phenyl)-1-tosyl-1*H*-indole (**14c**)

Orange solid, 83.8 mg, 92% yield under **Condition B**.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.25 (d, J = 8.2 Hz, 1H), 7.46 (d, J = 8.2 Hz, 1H), 7.34 – 7.18 (m, 5H), 7.01 (d, J = 8.0 Hz, 2H), 6.84 (s, 1H), 4.53 (s, 2H), 4.31 (s, 2H), 4.17 (s, 5H), 2.27 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 144.43, 139.57, 138.13, 135.29, 130.15, 129.24, 126.97, 124.36, 124.12, 120.31, 116.23, 113.65, 77.85, 72.95, 69.98, 68.08, 21.65.

HRMS (ESI) calculated for $C_{25}H_{22}FeNO_2S^+$ m/z $[M+H]^+$: 456.0715, found: 456.0717.

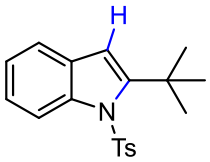


2-(Cyclohex-1-en-1-yl)-1-tosyl-1*H*-indole (**15c**) [11]

White solid, 67.5 mg, 96% yield under **Condition B**.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.17 (dd, J = 8.3, 0.9 Hz, 1H), 7.55 – 7.47 (m, 2H), 7.36 (dt, J = 7.6, 1.0 Hz, 1H), 7.30 – 7.24 (m, 1H), 7.19 (td, J = 7.5, 1.1 Hz, 1H), 7.12 – 7.05 (m, 2H), 6.34 (d, J = 0.8 Hz, 1H), 5.75 (s, 1H), 2.49 – 2.39 (m, 2H), 2.28 (s, 3H), 2.26 – 2.18 (m, 2H), 1.86 – 1.77 (m, 2H), 1.76 – 1.67 (m, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 144.99, 144.52, 137.84, 135.08, 132.61, 130.81, 129.52, 129.33, 126.88, 124.38, 124.04, 120.58, 116.14, 111.06, 30.64, 25.79, 22.81, 22.08, 21.66.

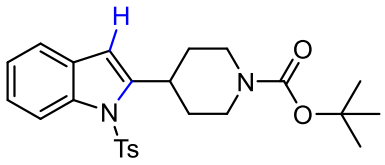


2-(*Tert*-butyl)-1-tosyl-1*H*-indole (**17c**) [9]

Light yellow oil, 63.5 mg, 97% yield under **Condition B**.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.09 – 8.00 (m, 1H), 7.48 – 7.37 (m, 3H), 7.23 – 7.14 (m, 2H), 7.10 (d, J = 8.3 Hz, 2H), 6.63 (s, 1H), 2.29 (s, 3H), 1.61 (s, 9H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 152.83, 144.15, 139.04, 136.91, 129.58, 129.34, 126.09, 124.24, 123.73, 120.42, 116.19, 110.87, 35.10, 31.46, 21.56.



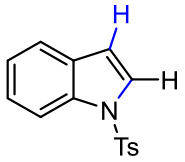
Tert-butyl 4-(1-tosyl-1*H*-indol-2-yl)piperidine-1-carboxylate (**18c**)

Colorless oil, 82.7 mg, 91% yield under **Condition B**.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.21 – 8.09 (m, 1H), 7.54 (d, J = 8.4 Hz, 2H), 7.45 – 7.37 (m, 1H), 7.30 – 7.13 (m, 4H), 6.42 (s, 1H), 4.23 (d, J = 13.3 Hz, 2H), 3.47 (tt, J = 11.7, 3.3 Hz, 1H), 2.87 (td, J = 13.1, 2.4 Hz, 2H), 2.32 (s, 3H), 2.08 (dt, J = 13.0, 2.7 Hz, 2H), 1.60 – 1.50 (m, 2H), 1.48 (s, 9H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 154.95, 146.33, 144.85, 137.45, 135.99, 129.97, 129.90, 126.18, 124.35, 123.87, 120.49, 115.42, 108.13, 79.67, 44.28, 35.98, 33.29, 28.58, 21.67.

HRMS (ESI) calculated for $C_{25}H_{31}N_2O_4S^+$ m/z $[M+H]^+$: 455.1999, found: 455.1996.

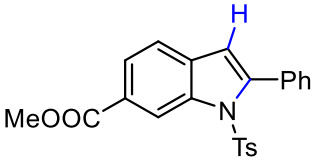


1-Tosyl-1*H*-indole (**19c**) [2]

White solid, 48.8 mg, 90% yield under **Condition B** (stirred for 24 h after electrolysis).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.01 (dd, J = 8.3, 1.0 Hz, 1H), 7.80 – 7.74 (m, 2H), 7.58 (d, J = 3.7 Hz, 1H), 7.53 (dt, J = 7.8, 1.0 Hz, 1H), 7.32 (ddd, J = 8.4, 7.2, 1.3 Hz, 1H), 7.25 – 7.18 (m, 3H), 6.66 (dd, J = 3.8, 0.8 Hz, 1H), 2.32 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 145.04, 135.34, 134.89, 130.84, 129.97, 126.90, 126.43, 124.65, 123.37, 121.48, 113.62, 109.14, 21.64.

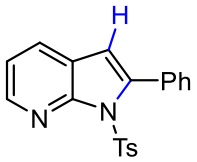


Methyl 2-phenyl-1-tosyl-1*H*-indole-6-carboxylate (**26c**) [10]

Light yellow solid, 77.8 mg, 96% yield under **Condition B**.

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.01 (s, 1H), 7.98 (dd, J = 8.2, 1.5 Hz, 1H), 7.53 – 7.40 (m, 6H), 7.31 – 7.23 (m, 2H), 7.05 (d, J = 8.1 Hz, 2H), 6.58 (s, 1H), 3.99 (s, 3H), 2.29 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 167.53, 145.24, 145.03, 137.79, 134.60, 134.28, 131.94, 130.51, 129.49, 129.25, 127.72, 126.99, 126.59, 125.69, 120.51, 118.37, 113.23, 52.41, 21.68.

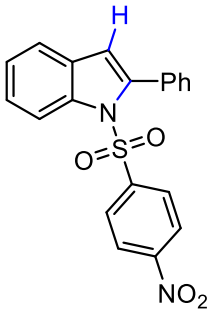


2-Phenyl-1-tosyl-1*H*-pyrrolo[2,3-*b*]pyridine (**27c**) [1]

White solid, 60.6 mg, 87% yield under **Condition B** (stirred for 12 h after electrolysis).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.48 (dd, J = 4.8, 1.6 Hz, 1H), 7.82 – 7.71 (m, 3H), 7.59 – 7.52 (m, 2H), 7.49 – 7.42 (m, 3H), 7.22 – 7.13 (m, 3H), 6.50 (s, 1H), 2.33 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 150.24, 144.86, 144.83, 142.37, 135.77, 132.78, 130.02, 129.40, 129.02, 128.88, 127.88, 127.80, 122.52, 119.71, 109.22, 21.73.

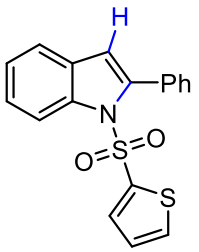


1-((4-Nitrophenyl)sulfonyl)-2-phenyl-1*H*-indole (**30c**) [2]

Light yellow solid, 68.1 mg, 90% yield under **Condition B**.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.29 (dd, J = 8.4, 0.9 Hz, 1H), 8.12 – 8.05 (m, 2H), 7.57 – 7.38 (m, 9H), 7.31 (td, J = 7.5, 1.0 Hz, 1H), 6.61 (s, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 150.54, 142.35, 142.05, 138.18, 131.84, 130.89, 130.30, 129.23, 128.20, 127.93, 125.55, 125.31, 123.91, 121.30, 116.83, 114.91.



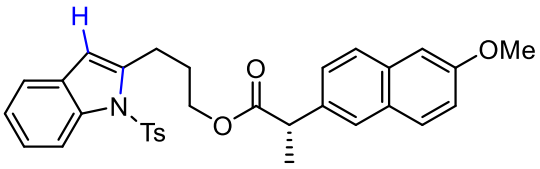
2-Phenyl-1-(thiophen-2-ylsulfonyl)-1*H*-indole (**34c**)

White solid, 62.4 mg, 92% yield under **Condition B**.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.29 (d, J = 8.3 Hz, 1H), 7.60 – 7.53 (m, 2H), 7.52 – 7.36 (m, 6H), 7.32 (t, J = 7.5 Hz, 1H), 7.23 (dd, J = 3.8, 1.4 Hz, 1H), 6.85 (t, J = 4.4 Hz, 1H), 6.62 (s, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 142.36, 138.23, 137.31, 133.13, 132.95, 132.41, 131.03, 130.27, 128.85, 127.69, 126.96, 125.12, 124.89, 120.98, 116.98, 114.50.

HRMS (ESI) calculated for $C_{18}H_{14}NO_2S_2^+$ m/z $[M+H]^+$: 340.0460, found: 340.0460.



3-(1-Tosyl-1*H*-indol-2-yl)propyl (*S*)-2-(6-methoxynaphthalen-2-yl)propanoate

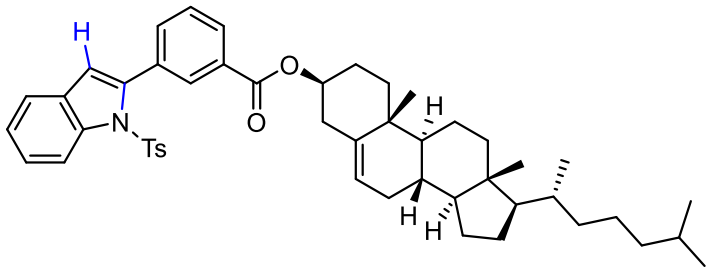
(**43c**, *Naproxen derivative*)

White solid, 101.8 mg, 94% yield under **Condition B**.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.12 (dd, J = 8.3, 1.0 Hz, 1H), 7.76 – 7.65 (m, 3H), 7.56 – 7.50 (m, 2H), 7.43 (dd, J = 8.5, 1.9 Hz, 1H), 7.31 – 7.26 (m, 1H), 7.26 – 7.05 (m, 6H), 6.11 (d, J = 1.0 Hz, 1H), 4.20 – 4.10 (m, 2H), 3.96 – 3.81 (m, 4H), 3.05 – 2.86 (m, 2H), 2.28 (s, 3H), 2.04 (p, J = 7.1 Hz, 2H), 1.59 (d, J = 7.2 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 174.79, 157.73, 144.78, 140.73, 137.30, 135.98, 135.88, 133.81, 129.89, 129.75, 129.43, 129.04, 127.34, 126.42, 126.29, 126.05, 124.12, 123.65, 120.28, 119.12, 114.93, 109.62, 105.66, 63.98, 55.41, 45.61, 28.22, 25.75, 21.62, 18.56.

HRMS (ESI) calculated for $C_{32}H_{32}NO_5S^+$ m/z $[M+H]^+$: 542.1996, found: 542.1993.



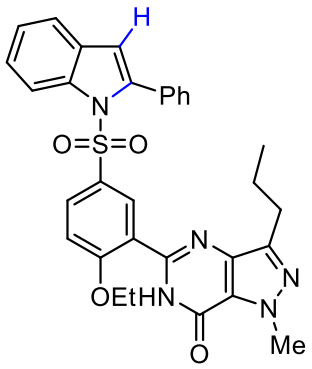
(3*S*,8*S*,9*S*,10*R*,13*R*,14*S*,17*R*)-10,13-Dimethyl-17-((*R*)-6-methylheptan-2-yl)-2,3,4,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-1*H*-cyclopenta[*a*]phenanthren-3-yl 3-(1-tosyl-1*H*-indol-2-yl)benzoate (**44c**)

White solid, 138.3 mg, 91% yield under **Condition B** (with additional 5.0 mL DCM as co-solvent, stirred for 12 h after electrolysis).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.31 (d, J = 8.4 Hz, 1H), 8.15 – 8.06 (m, 2H), 7.75 (dt, J = 7.8, 1.5 Hz, 1H), 7.51 (t, J = 7.7 Hz, 1H), 7.46 (dd, J = 7.7, 1.2 Hz, 1H), 7.38 (ddd, J = 8.5, 7.3, 1.3 Hz, 1H), 7.32 – 7.22 (m, 3H), 7.05 (d, J = 8.1 Hz, 2H), 6.60 (s, 1H), 5.49 – 5.38 (m, 1H), 4.91 (dtd, J = 12.3, 8.4, 4.4 Hz, 1H), 2.49 (d, J = 8.1 Hz, 2H), 2.28 (s, 3H), 2.08 – 1.70 (m, 6H), 1.64 – 1.45 (m, 6H), 1.43 – 0.96 (m, 17H), 0.93 (d, J = 6.5 Hz, 3H), 0.88 (d, J = 1.9 Hz, 3H), 0.86 (d, J = 1.9 Hz, 3H), 0.69 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 165.79, 144.85, 141.04, 139.76, 138.37, 135.19, 134.59, 132.83, 130.81, 130.54, 130.47, 129.88, 129.45, 127.61, 126.87, 125.21, 124.57, 122.99, 120.99, 116.73, 114.33, 74.89, 56.82, 56.24, 50.16, 42.45, 39.86, 39.65, 38.38, 37.17, 36.79, 36.31, 35.93, 32.08, 32.00, 28.38, 28.15, 28.05, 24.43, 23.95, 22.98, 22.71, 21.69, 21.19, 19.54, 18.86, 12.00.

HRMS (ESI) calculated for $C_{49}H_{62}NO_4S^+$ m/z $[M+H]^+$: 760.4394, found: 760.4384.



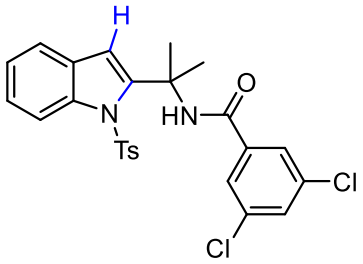
5-(2-Ethoxy-5-((2-phenyl-1*H*-indol-1-yl)sulfonyl)phenyl)-1-methyl-3-propyl-1,6-dihydro-7*H*-pyrazolo[4,3-*d*]pyrimidin-7-one (**45c**)

White solid, 111.3 mg, 98% yield under **Condition B**.

^{1}H NMR (400 MHz, $CDCl_3$) δ 10.70 (s, 1H), 8.47 (d, J = 2.5 Hz, 1H), 8.32 (d, J = 8.4 Hz, 1H), 7.59 – 7.51 (m, 2H), 7.50 – 7.39 (m, 5H), 7.39 – 7.33 (m, 1H), 7.29 – 7.22 (m, 1H), 6.85 (d, J = 8.9 Hz, 1H), 6.57 (s, 1H), 4.28 – 4.18 (m, 5H), 2.96 (t, J = 7.6 Hz, 2H), 1.88 (h, J = 7.4 Hz, 2H), 1.54 (t, J = 7.0 Hz, 3H), 1.08 (t, J = 7.4 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 159.78, 153.61, 147.01, 146.17, 142.20, 138.34, 138.21, 132.46, 130.88, 130.74, 130.69, 130.38, 130.32, 128.82, 127.70, 125.04, 124.64, 124.50, 120.96, 120.74, 116.66, 114.01, 112.60, 66.12, 38.33, 27.68, 22.49, 14.53, 14.20.

HRMS (ESI) calculated for $C_{31}H_{30}N_5O_4S^+$ m/z $[M+H]^+$: 568.2013, found: 568.2013.



3,5-Dichloro-*N*-(2-(1-tosyl-1*H*-indol-2-yl)propan-2-yl)benzamide (**46c**)

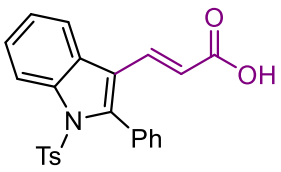
White solid, 97.3 mg, 97% yield under **Condition B** (stirred for 12 h after electrolysis).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.97 – 7.88 (m, 1H), 7.57 – 7.50 (m, 1H), 7.41 – 7.31 (m, 3H), 7.25 – 7.16 (m, 2H), 7.06 (s, 1H), 7.01 – 6.95 (m, 3H), 6.93 – 6.85 (m, 2H), 2.19 (s, 3H), 2.07 (s, 6H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 163.38, 145.55, 144.41, 139.15, 137.52, 136.94, 135.08, 131.02, 129.71, 128.40, 125.56, 125.29, 125.14, 124.10, 121.44, 115.71, 112.68, 53.33, 30.21, 21.51.

HRMS (ESI) calculated for $C_{25}H_{23}Cl_2N_2O_3S^+$ m/z $[M+H]^+$: 501.0801, found: 501.0801.

2.2.3 Characterization data for products of synthetic diversification



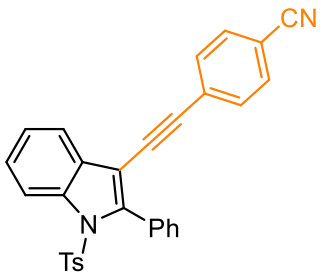
(*E*)-3-(2-Phenyl-1-tosyl-1*H*-indol-3-yl)acrylic acid (**1d**)

White solid, 187.9 mg, 90% yield.

^{1}H NMR (400 MHz, DMSO-d_6) δ 12.38 (br, 1H), 8.24 (dd, J = 8.5, 1.9 Hz, 1H), 7.95 (d, J = 7.9 Hz, 1H), 7.62 – 7.46 (m, 4H), 7.45 – 7.38 (m, 5H), 7.34 – 7.26 (m, 2H), 7.18 (dt, J = 16.2, 2.8 Hz, 1H), 6.47 (dt, J = 16.2, 1.7 Hz, 1H), 2.29 (s, 3H).

^{13}C NMR (101 MHz, DMSO-d_6) δ 167.46, 145.73, 142.84, 136.34, 135.05, 133.95, 131.41, 130.16, 129.70, 129.64, 127.83, 126.94, 126.55, 125.96, 125.20, 120.89, 119.88, 117.72, 115.45, 21.07.

HRMS (ESI) calculated for $C_{24}H_{20}NO_4S^+$ m/z $[M+H]^+$: 418.1108, found: 418.1108.



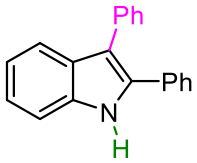
4-((2-Phenyl-1-tosyl-1*H*-indol-3-yl)ethynyl)benzonitrile (**1e**)

Light yellow solid, 219.8 mg, 93% yield.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.42 – 8.30 (m, 1H), 7.68 – 7.59 (m, 3H), 7.59 – 7.54 (m, 2H), 7.54 – 7.48 (m, 3H), 7.48 – 7.43 (m, 1H), 7.42 – 7.35 (m, 3H), 7.32 – 7.27 (m, 2H), 7.07 (d, J = 8.1 Hz, 2H), 2.30 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 145.25, 144.80, 137.10, 134.64, 132.12, 131.89, 131.37, 130.47, 130.24, 129.58, 128.13, 127.51, 126.98, 126.14, 124.96, 120.07, 118.63, 116.71, 111.39, 107.17, 93.10, 86.45, 21.70.

HRMS (ESI) calculated for $C_{30}H_{21}N_2O_2S^+$ m/z $[M+H]^+$: 473.1318, found: 473.1321.

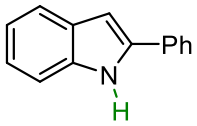


2,3-Diphenyl-1*H*-indole (**1f**) [14]

White solid, 114.5 mg, 85% yield over two steps.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.15 (s, 1H), 7.68 (dd, J = 7.9, 1.1 Hz, 1H), 7.48 – 7.33 (m, 7H), 7.33 – 7.18 (m, 5H), 7.14 (ddd, J = 8.0, 7.0, 1.1 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 135.98, 135.16, 134.20, 132.78, 130.27, 128.84, 128.81, 128.66, 128.30, 127.82, 126.36, 122.82, 120.55, 119.82, 115.12, 111.03.



2-Phenyl-1*H*-indole (**1g**) [15]

White solid, 88.9 mg, 92% yield.

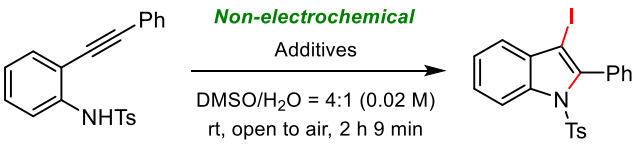
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.27 (s, 1H), 7.73 – 7.54 (m, 3H), 7.50 – 7.25 (m, 4H), 7.25 – 7.07 (m, 2H), 6.82 (s, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 138.00, 136.91, 132.46, 129.37, 129.15, 127.85, 125.28, 122.48, 120.80, 120.40, 111.05, 100.10.

3. Mechanistic studies

3.1 Control reactions under non-electrochemical conditions

3.1.1 Control reactions for iodocyclization



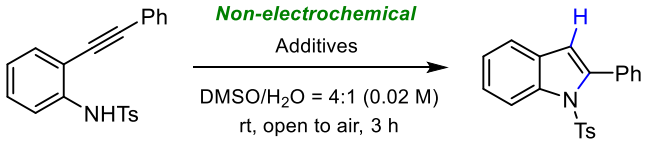
1a, 0.2 mmol

Additives	1b
1) KI (1.5 equiv)	0% yield
2) I_2 (1.5 equiv)	33% yield
3) NIS (1.5 equiv)	56% yield
4) I_2 (1.5 equiv) + KOH (1.5 equiv)	79% yield
5) KI (1.5 equiv) + KOH (1.5 equiv)	0% yield

Table S2. Non-electrochemical control reactions for iodocyclization.

To a 25 mL flask with a magnetic stir bar was added **1a** (0.2 mmol, 1.0 equiv) and the corresponding additives (0.3 mmol, 1.5 equiv), followed by solvent DMSO (8.0 mL). Then water (2.0 mL) was added into the mixture (slightly exothermic), after which the system was stirred for 129 min under ambient conditions. The mixture was then poured into brine and extracted with EtOAc for three times. The combined organic layer was dried over anhydrous Na_2SO_4, and the solvent was then removed under reduced pressure. The resulting mixture was purified by column chromatography on silica gel (eluted with EtOAc/PE) to afford the desired product **1b**.

3.1.2 Control reactions for hydrocyclization



1a, 0.2 mmol

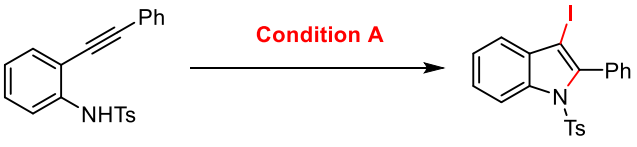
Additives	1c
1) KI (0.5 equiv)	0% yield
2) KOH (0.1 equiv)	0% yield
3) KI (0.5 equiv) + KOH (0.1 equiv)	0% yield
4) Cu powder (0.1 equiv)	0% yield
5) Cu powder (0.1 equiv) + KOH (0.1 equiv)	0% yield
6) Cu powder (0.1 equiv) + KI (0.5 equiv)	0% yield
7) CuI (0.1 equiv)	10% yield
8) CuI (0.1 equiv) + KOH (0.1 equiv)	96% yield
9) Cu powder (0.1 equiv) + KOH (0.1 equiv) + KI (0.5 equiv)	28% yield

Table S3. Non-electrochemical control reactions for hydrocyclization.

To a 25 mL flask with a magnetic stir bar was added **1a** (0.2 mmol, 1.0 equiv) and the corresponding additives (0.02 mmol for 0.1 equiv, 0.1 mmol for 0.5 equiv), followed by solvent DMSO (8.0 mL). Then water (2.0 mL) was added into the mixture (slightly exothermic), after which the system was stirred for 3 h under ambient conditions. The mixture was then poured into brine and extracted with EtOAc for three times. The combined organic layer was dried over anhydrous Na_2SO_4, and the solvent was then removed under reduced pressure. The resulting mixture was purified by column chromatography on silica gel (eluted with EtOAc/PE) to afford the desired product **1c**.

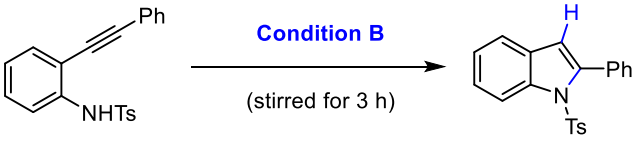
3.2 Control reactions under electrochemical conditions

3.2.1 Addition of radical scavengers



1a, 0.2 mmol

Variations	1b
1) Standard **Condition A**	94% yield
2) With additional TEMPO (2.0 equiv)	22% yield
3) With additional BHT (2.0 equiv)	5% yield



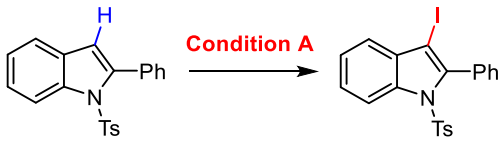
1a, 0.2 mmol

Variations	1c
1) Standard **Condition B**	98% yield
2) With additional TEMPO (2.0 equiv)	90% yield
3) With additional BHT (2.0 equiv)	82% yield

Table S4. Radical trapping experiments under electrochemical conditions.

Under standard electrochemical conditions (**A** or **B**), **1a** was treated with 2.0 equiv of additional radical trapping reagents (TEMPO or BHT). The iodocyclization was obviously inhibited, while the efficiency of hydrocyclization was only affected slightly. **No radical adduct was detected in all reaction systems.**

3.2.2 Other control reactions



1c, 0.2 mmol **1b**, 0% (99% recovery of **1c**)

To a 25 mL three-necked flask with a magnetic stir bar was added **1c** (69.5 mg, 0.2 mmol) and KI (49.8 mg, 0.3 mmol, 1.5 equiv), followed by solvent DMSO (8.0 mL). Then water (2.0 mL) was added into the mixture (slightly exothermic), after which the flask was equipped with two platinum plate electrodes (10 × 10 × 0.2 mm, approximately 2 cm apart). The 10 mA constant current electrolysis was performed at room temperature under air atmosphere with vigorous stirring. After 4 F/mol charges passed (129 min), EtOAc (~ 5 mL) was added into the system, and the resulting mixture was stirred for additional 1 min. The mixture was then poured into brine and extracted with EtOAc for three times. The combined organic layer was dried over anhydrous Na_2SO_4, and the solvent was then removed under reduced pressure. The resulting mixture was purified by column chromatography on silica gel (eluted with EtOAc/PE) to afford a compound which was then proven by ^{1}H-NMR to be unreacted **1c** (68.6 mg, 99%).

3.3 Cyclic voltammetry studies

The electrolyte solution for CV studies was prepared with ^{n}Bu$_4$NPF$_6$ (0.1 M) in DMSO/H_2O (4:1, v:v). The samples were prepared with 0.1 mmol of compound in 10 mL electrolyte solution (0.01 M). Measurements employed a glassy carbon or a Cu rod working electrode (WE), platinum plate counter electrode (CE) and a saturated calomel electrode (SCE) reference electrode (RE). The scan rate applied was 0.1 V/s, and the scans start from 0 V (initial E) to +2 V (high E), then back to 0 V (low E).

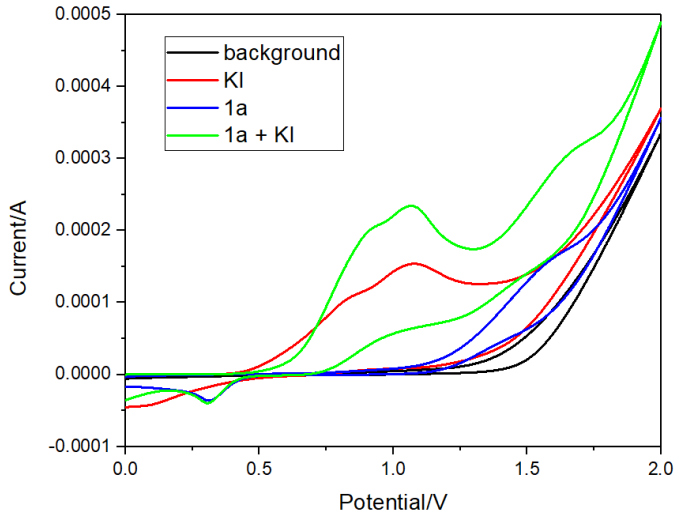


Fig. S6 CV plot of reaction components with glassy carbon as working electrode.

From the above results, it can be concluded that KI (unseparated oxidation peaks at +~0.83 V and +1.08 V vs. SCE) would be oxidized at lower potential than **1a** (possible oxidation peak +~1.57 V vs. SCE) with a GC working electrode in the reaction solvent.

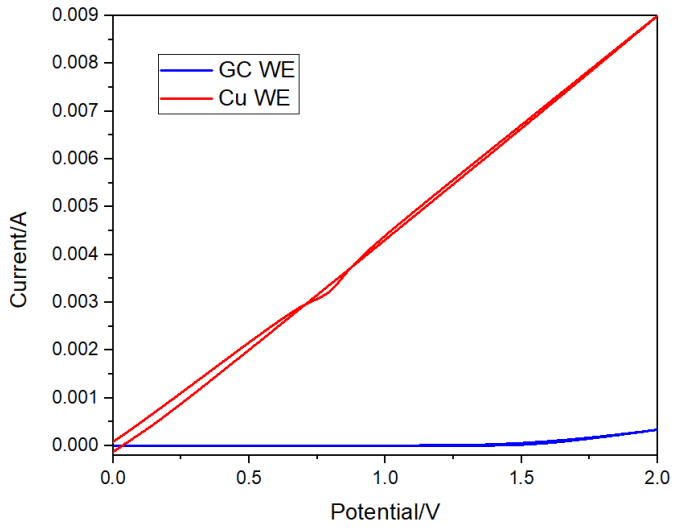


Fig. S7 CV plot in electrolyte solution with glassy carbon and Cu rod as working electrodes.

From such a plot, it can be speculated that under an oxidative potential, the Cu working electrode releases cupric ions, [17] which results in a dramatic enhancement of the system conductivity (higher currents than that with a GC WE under the same potentials).

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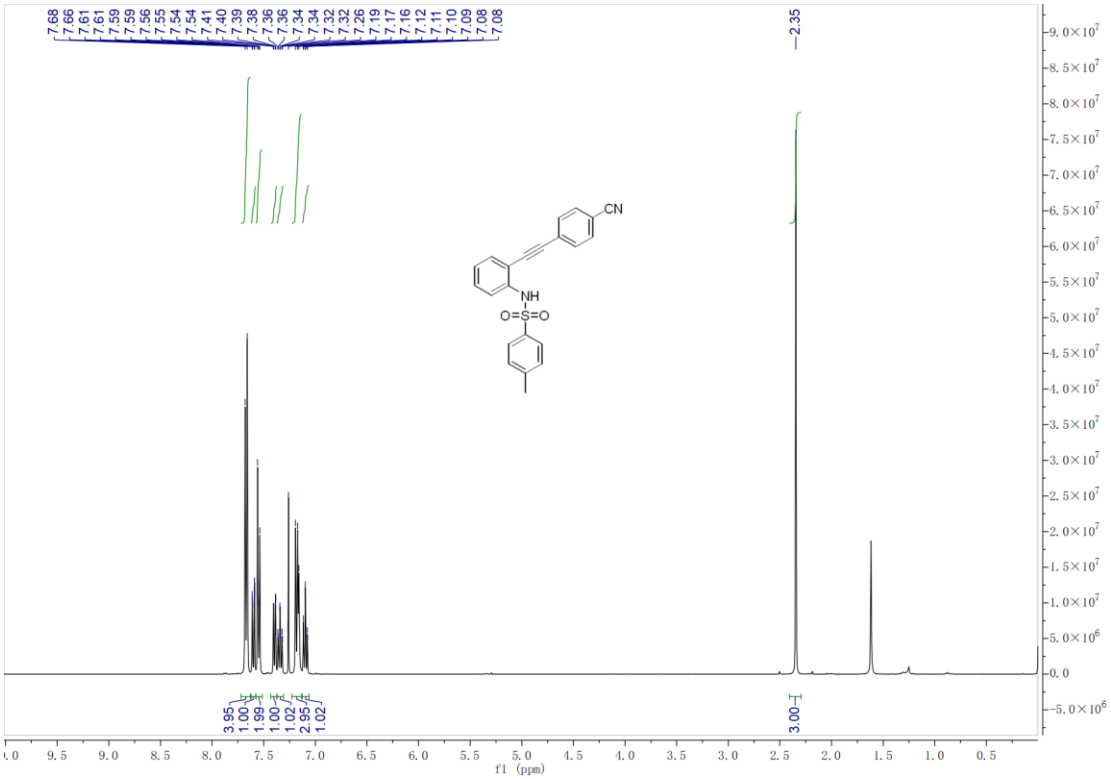
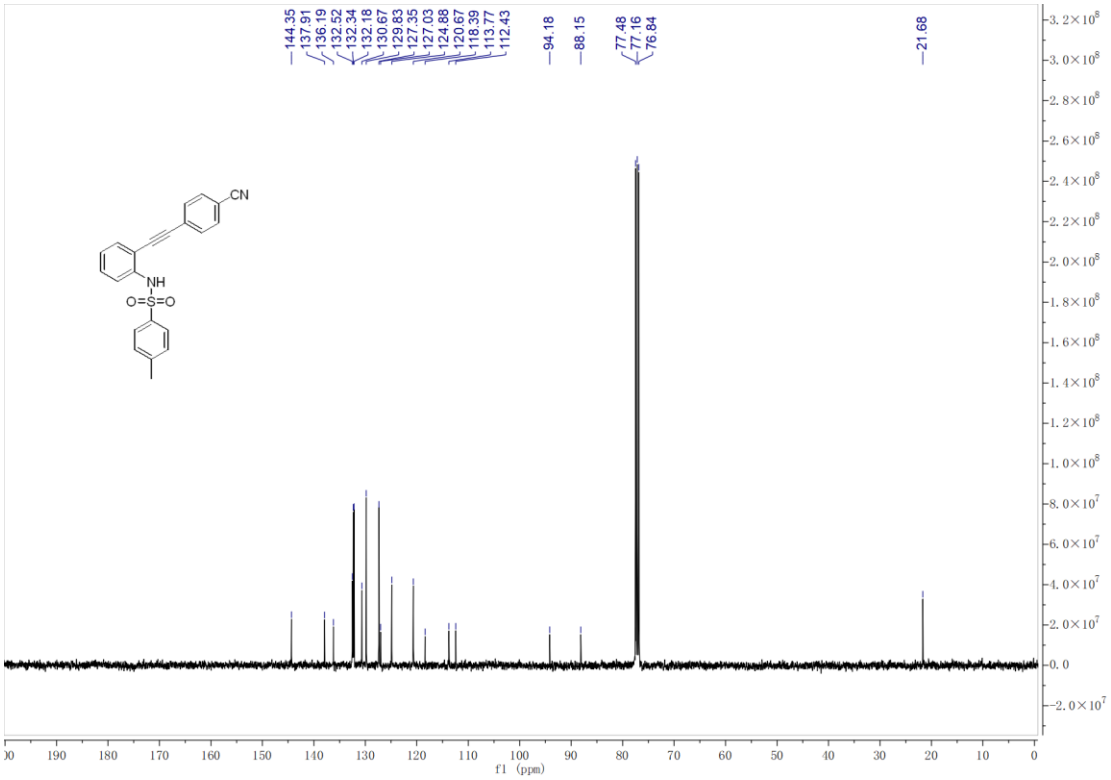
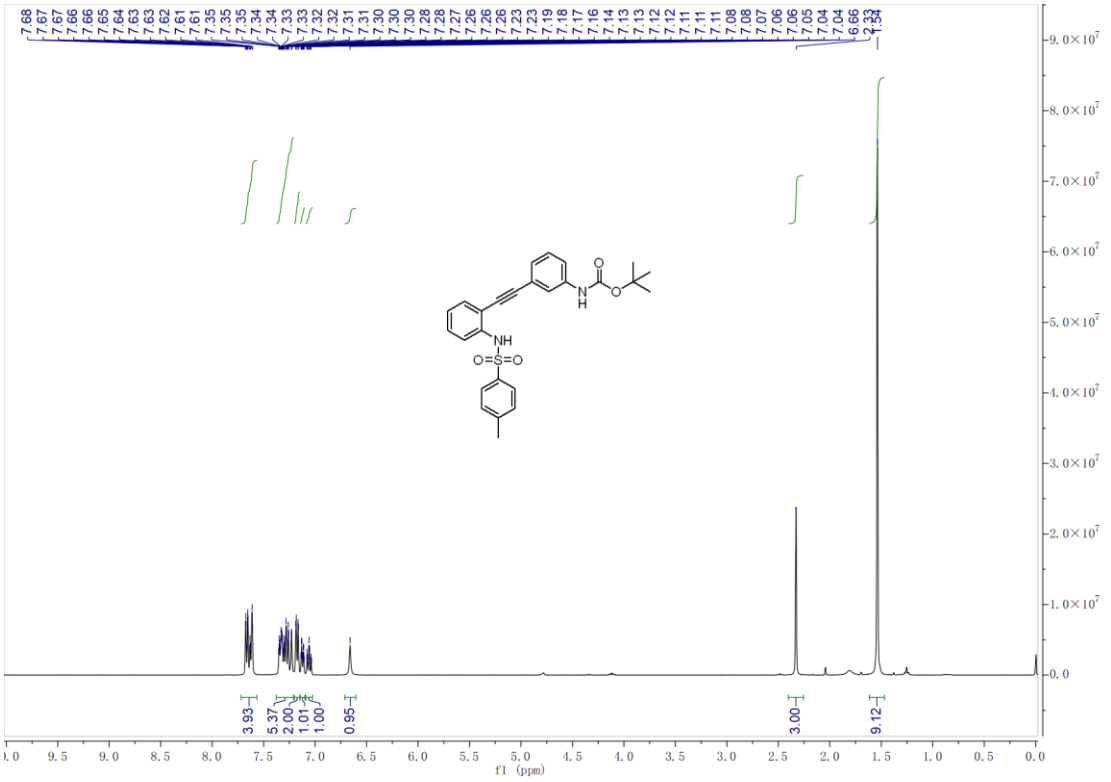
5. Copies of NMR spectra

6a, ^{1}H + ^{13}C





9a, $^{1}H + {}^{13}C$


7.68 7.67 7.67 7.66 7.66 7.65 7.64 7.63 7.63 7.62 7.61 7.61 7.35 7.35 7.35 7.34 7.34 7.33 7.33 7.32 7.32 7.31 7.31 7.30 7.30 7.30 7.28 7.28 7.27 7.26 7.26 7.26 7.23 7.23 7.19 7.18 7.17 7.16 7.14 7.13 7.13 7.12 7.12 7.11 7.11 7.11 7.08 7.08 7.07 7.06 7.06 7.05 7.04 7.04 6.66 2.33 1.54
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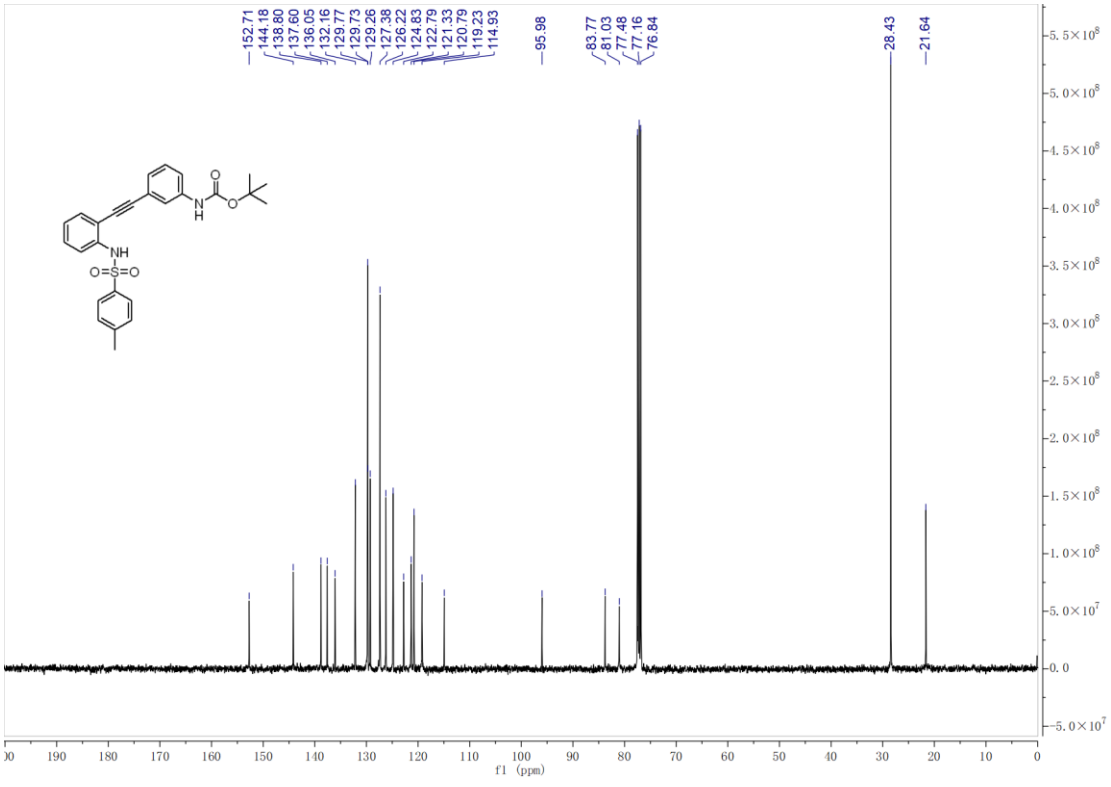
f1 (ppm)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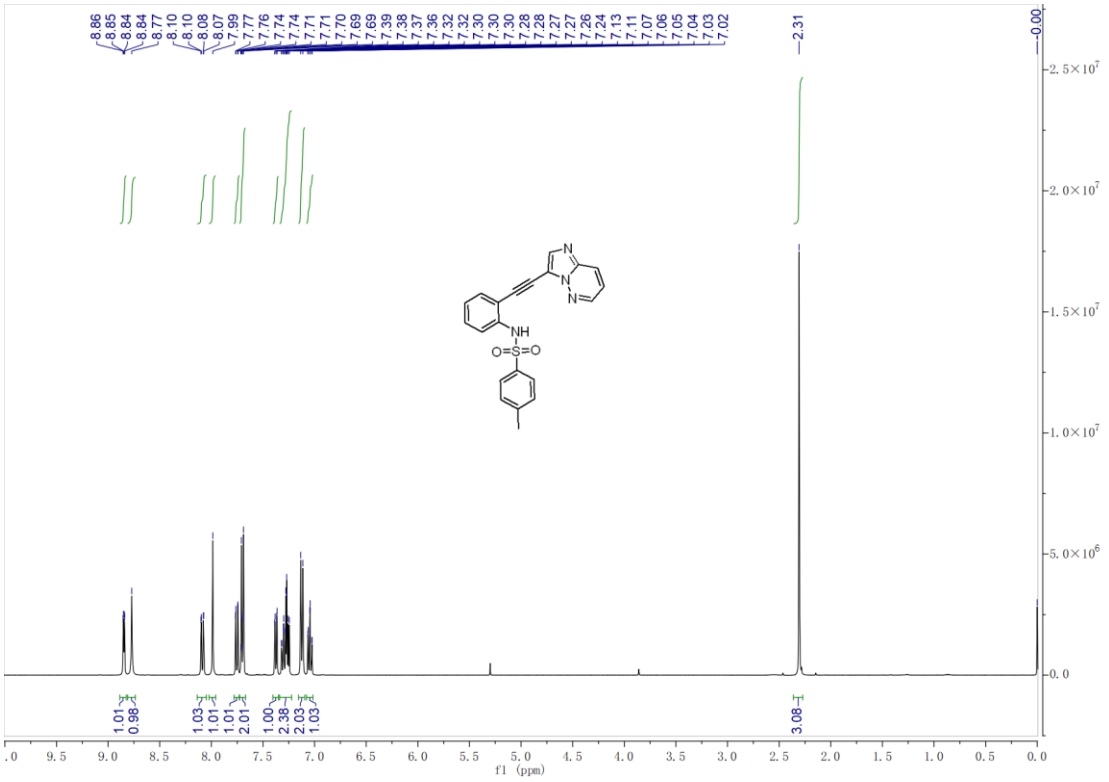
f1 (ppm)

13a, $^{1}H + ^{13}C$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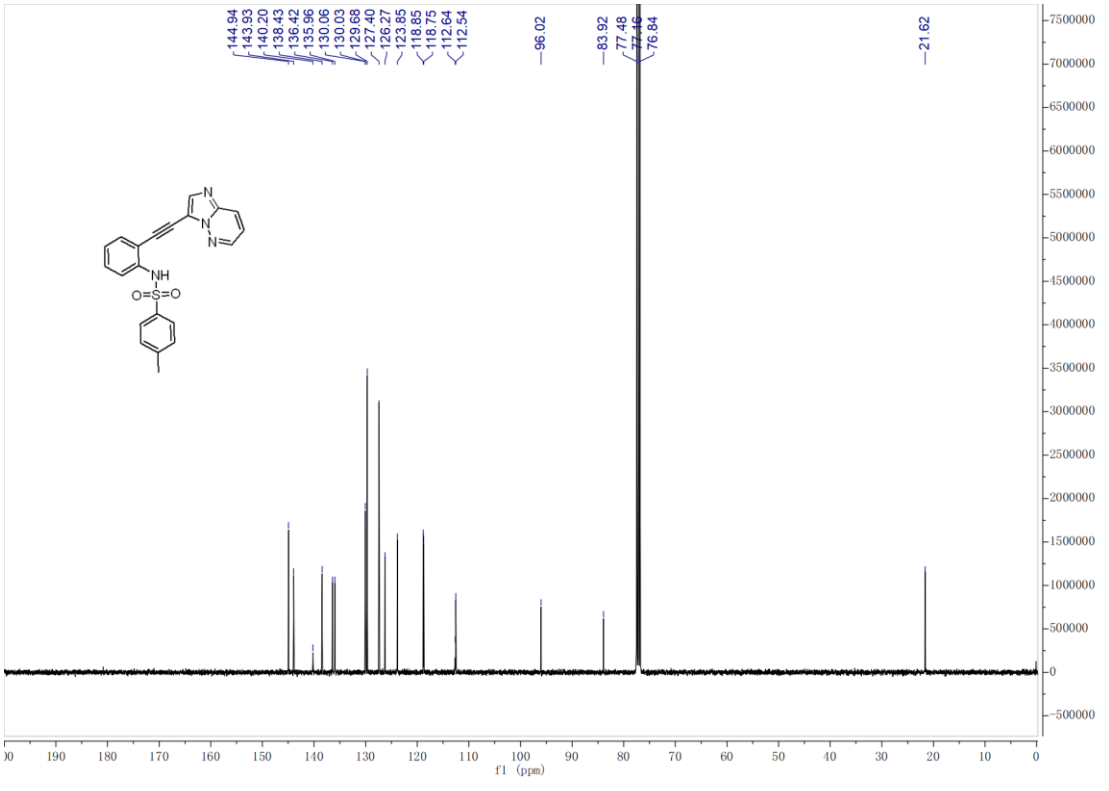
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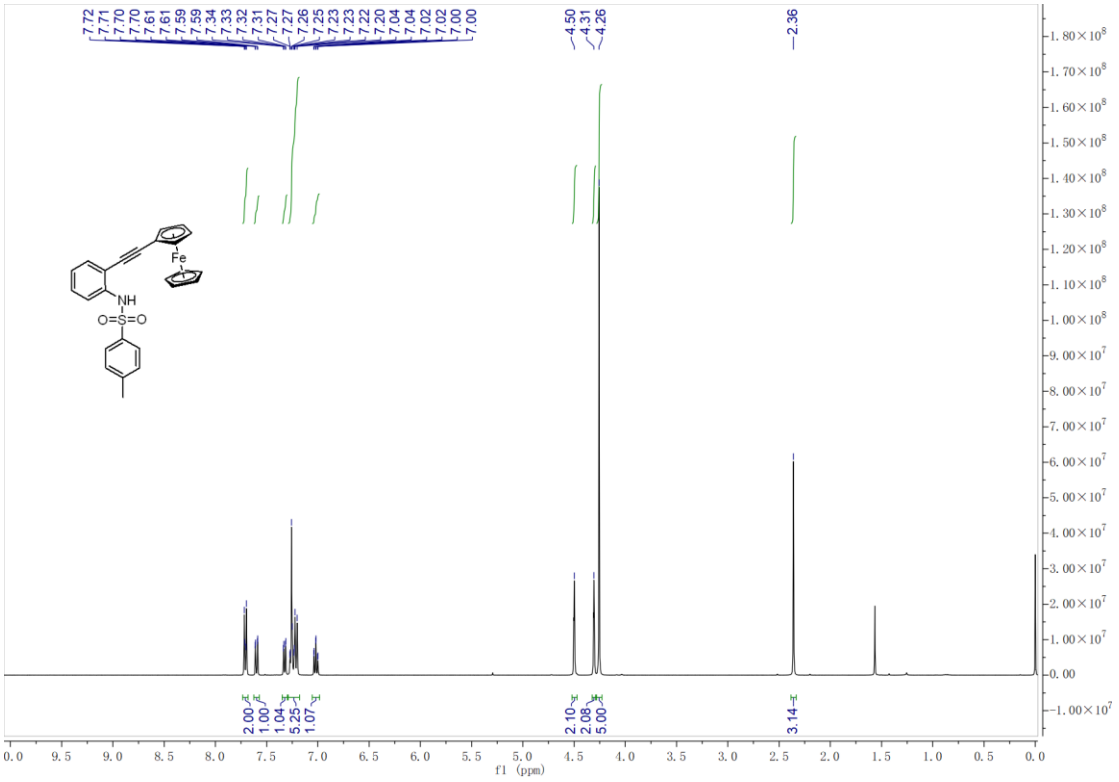
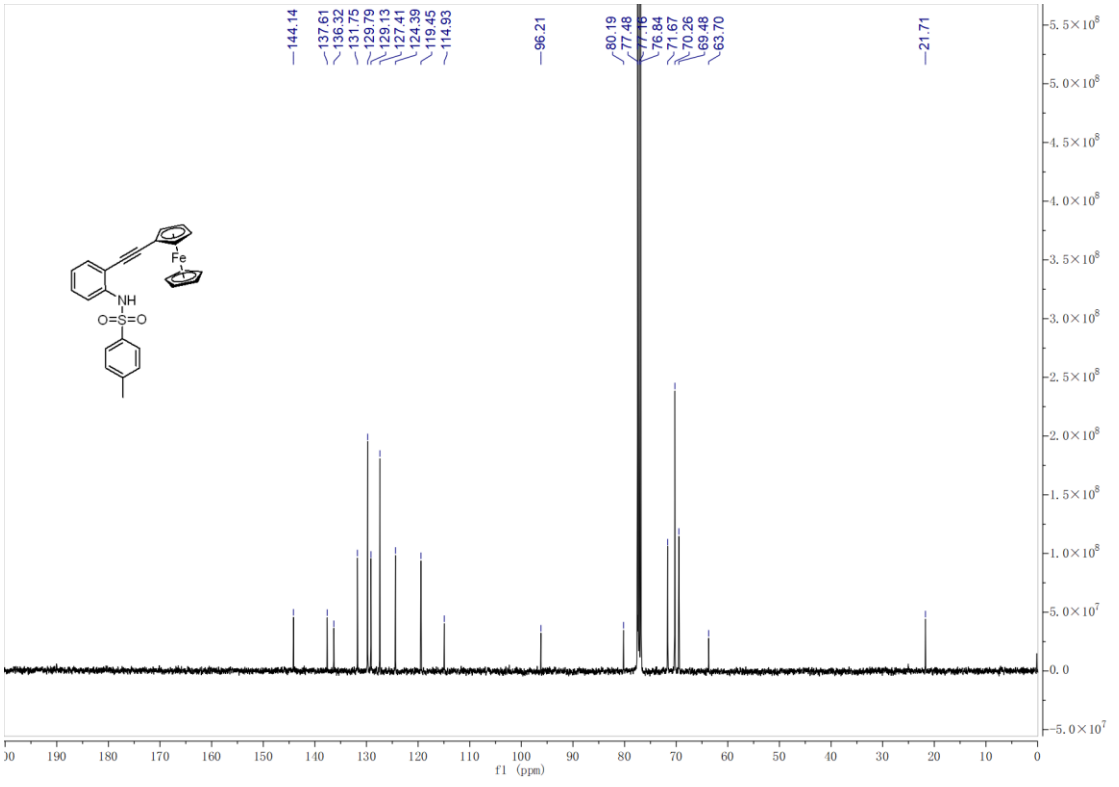
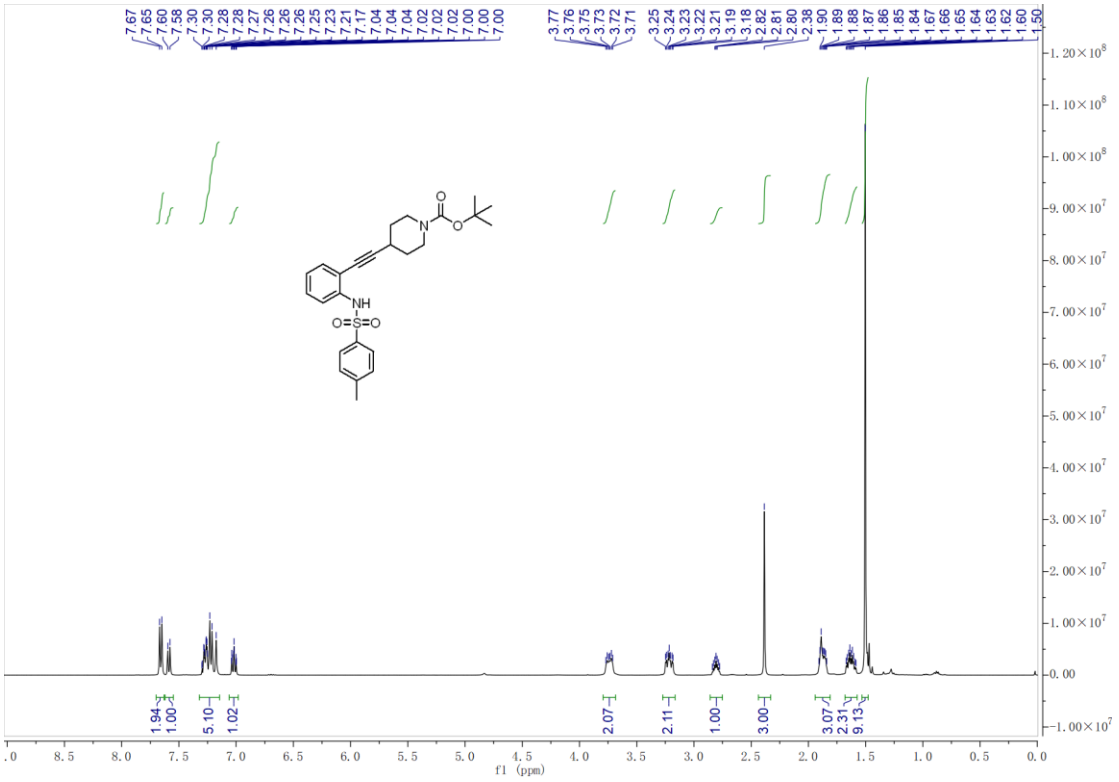
118.75
112.64
112.54
96.02
83.92
77.48
77.16
76.84
21.62
f1 (ppm)

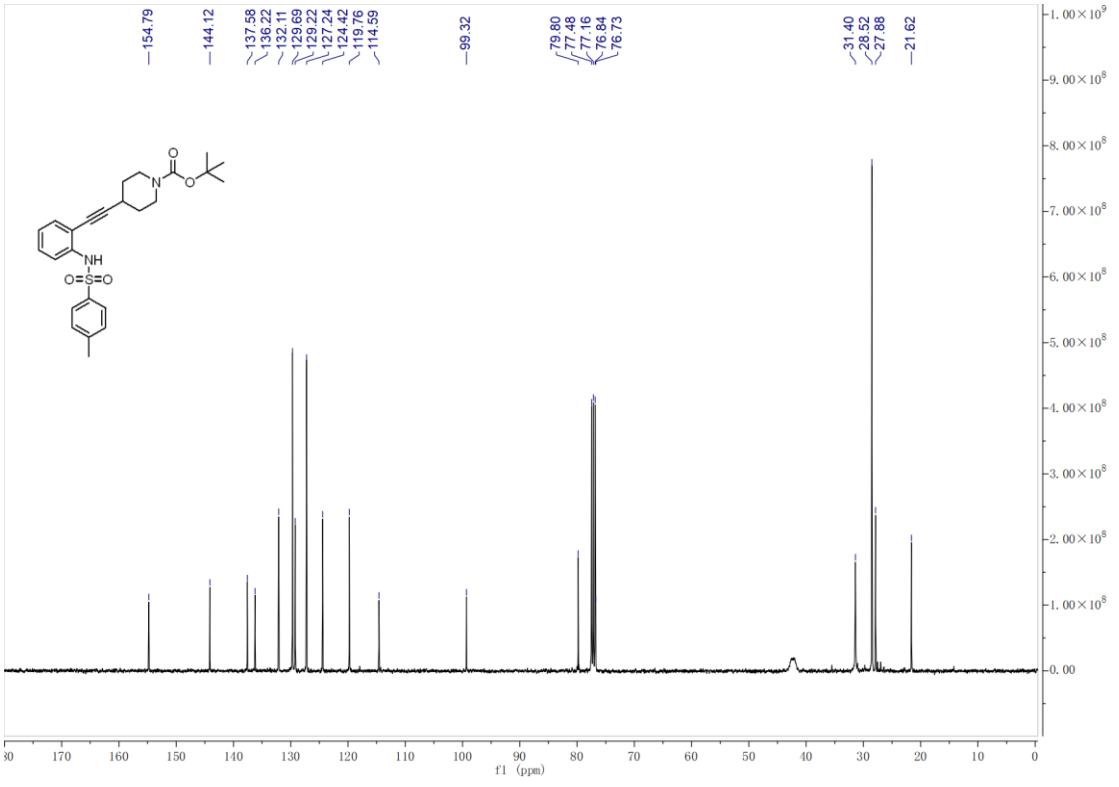
14a, $^{1}H + ^{13}C$


7.72
7.71
7.70
7.70
7.61
7.59
7.59
7.34
7.33
7.32
7.31
7.27
7.27
7.26
7.25
7.23
7.23
7.22
7.20
7.04
7.04
7.02
7.02
7.00
7.00
4.50
4.31
4.26
2.36
Fe
NH
O=S=O
2.00
1.00
1.04
5.25
1.07
2.10
2.08
5.00
3.14
f1 (ppm)

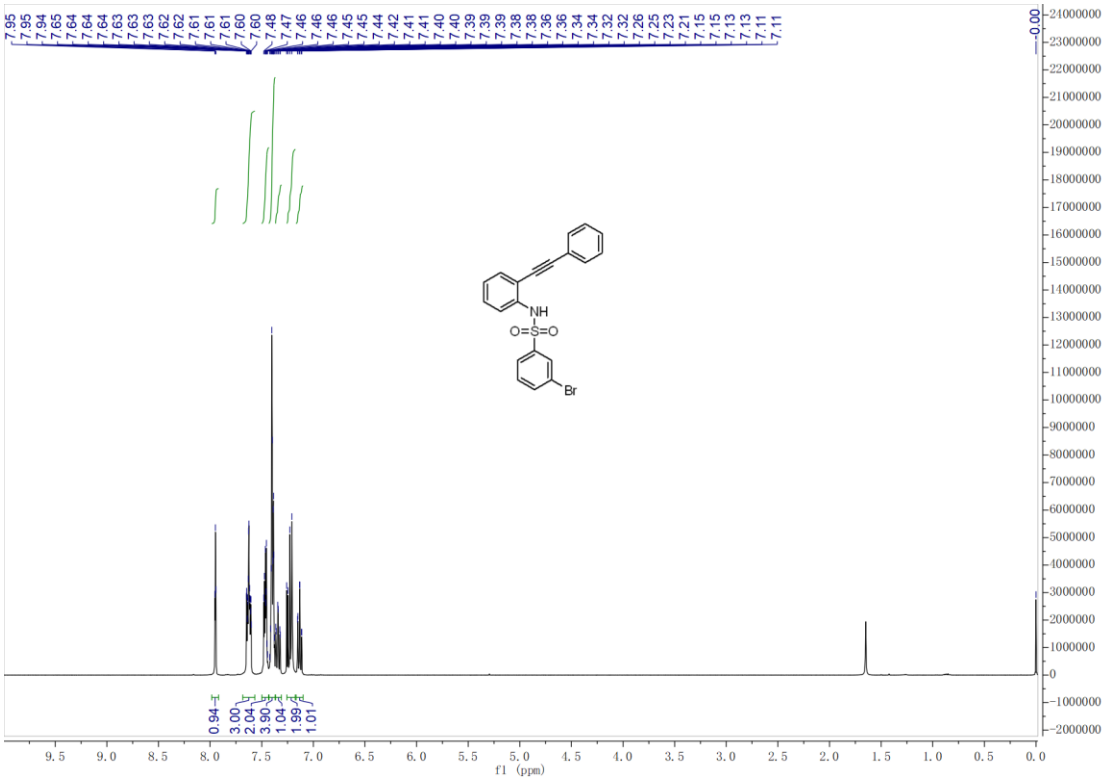

144.14
137.61
136.32
131.75
129.79
129.13
127.41
124.39
119.45
114.93
96.21
80.19
77.48
77.16
76.84
71.67
70.26
69.48
63.70
21.71
Fe
NH
O=S=O
f1 (ppm)

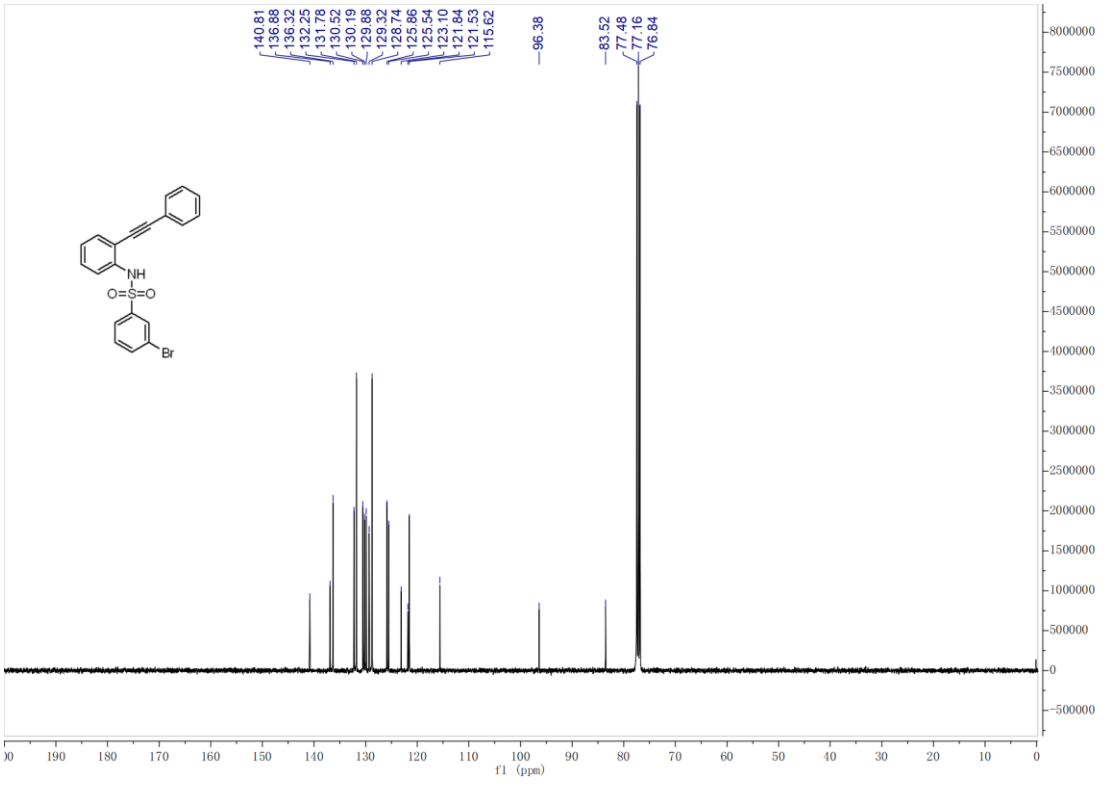
18a, $^{1}H + ^{13}C$


7.67
7.65
7.60
7.58
7.30
7.30
7.28
7.28
7.27
7.26
7.26
7.26
7.25
7.23
7.21
7.17
7.04
7.04
7.04
7.02
7.02
7.02
7.00
7.00
7.00
3.77
3.76
3.75
3.73
3.72
3.71
3.25
3.24
3.23
3.22
3.21
3.19
3.18
2.82
2.81
2.80
2.38
1.90
1.89
1.88
1.87
1.86
1.85
1.84
1.67
1.66
1.65
1.64
1.63
1.62
1.60
1.50
1.94
1.00
5.10
1.02
2.07
2.11
1.00
3.00
3.07
2.31
9.13
f1 (ppm)

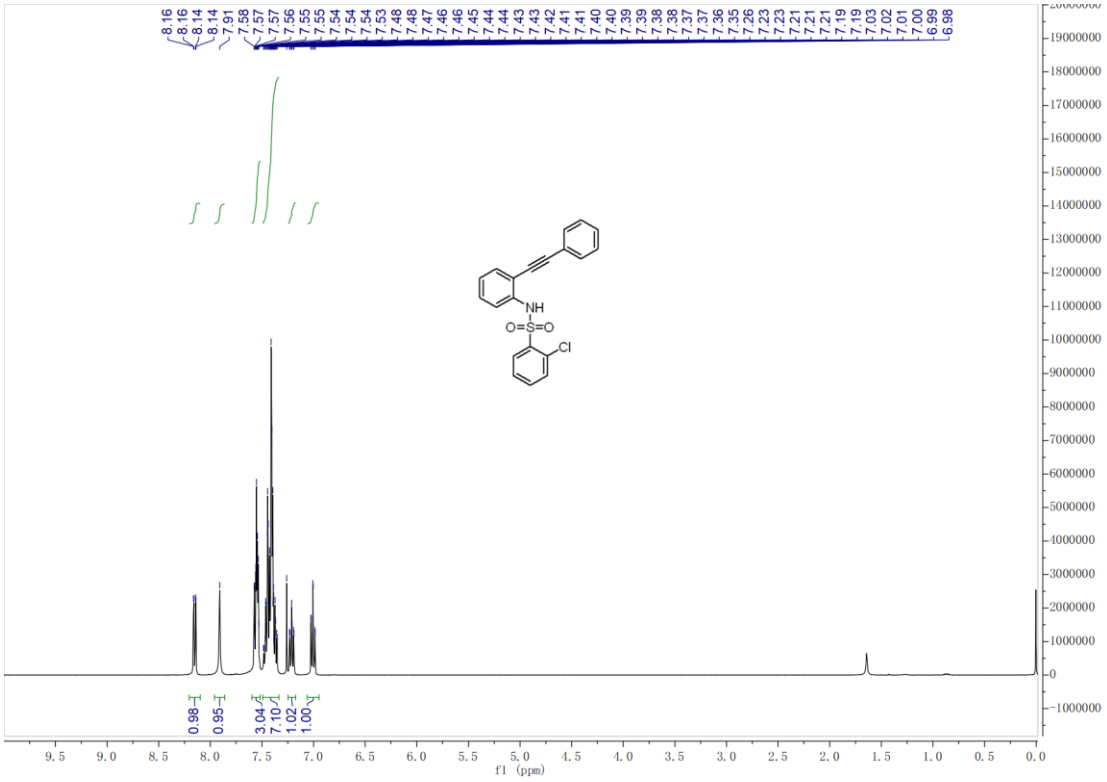

154.79
144.12
137.58
136.22
132.11
129.69
129.22
127.24
124.42
119.76
114.59
99.32
79.80
77.48
77.16
76.84
76.73
31.40
28.52
27.88
21.62
f1 (ppm)

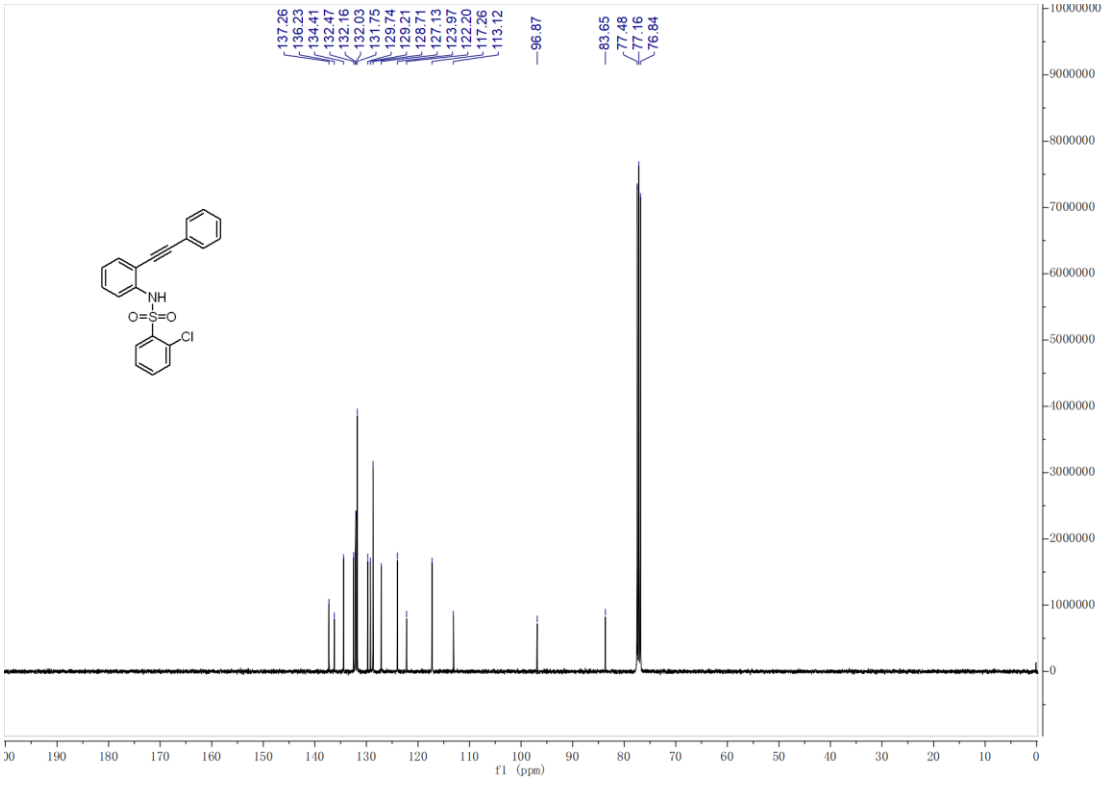
31a, $^{1}H + ^{13}C$


7.95 7.95 7.94 7.65 7.64 7.64 7.63 7.63 7.63 7.62 7.62 7.61 7.61 7.60 7.60 7.48 7.47 7.46 7.46 7.46 7.45 7.45 7.44 7.42 7.41 7.41 7.40 7.40 7.39 7.39 7.38 7.38 7.36 7.36 7.34 7.34 7.32 7.32 7.26 7.25 7.23 7.21 7.15 7.15 7.13 7.13 7.11 7.11
0.00
0.94 3.00 2.04 3.90 1.04 1.99 1.01
NH
O=S=O
Br
f1 (ppm)

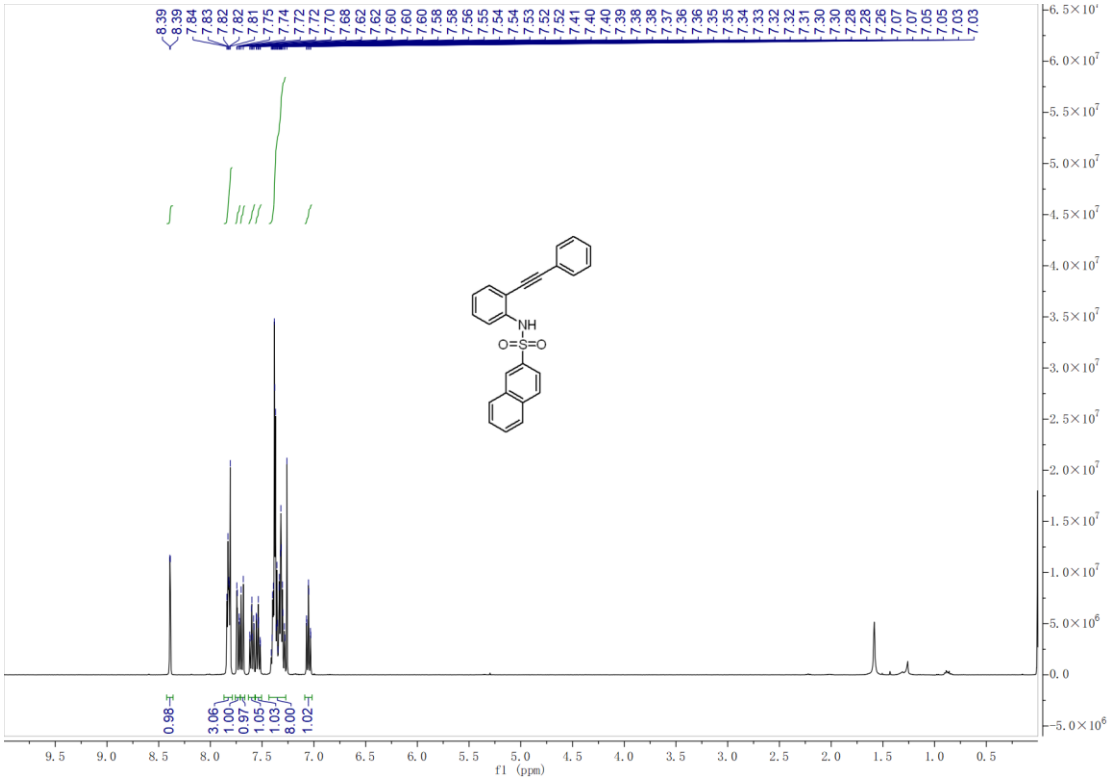

140.81 136.88 136.32 132.25 131.78 130.52 130.19 129.88 129.32 128.74 125.86 125.54 123.10 121.84 121.53 115.62
96.38
83.52 77.48 77.16 76.84
NH
O=S=O
Br
f1 (ppm)

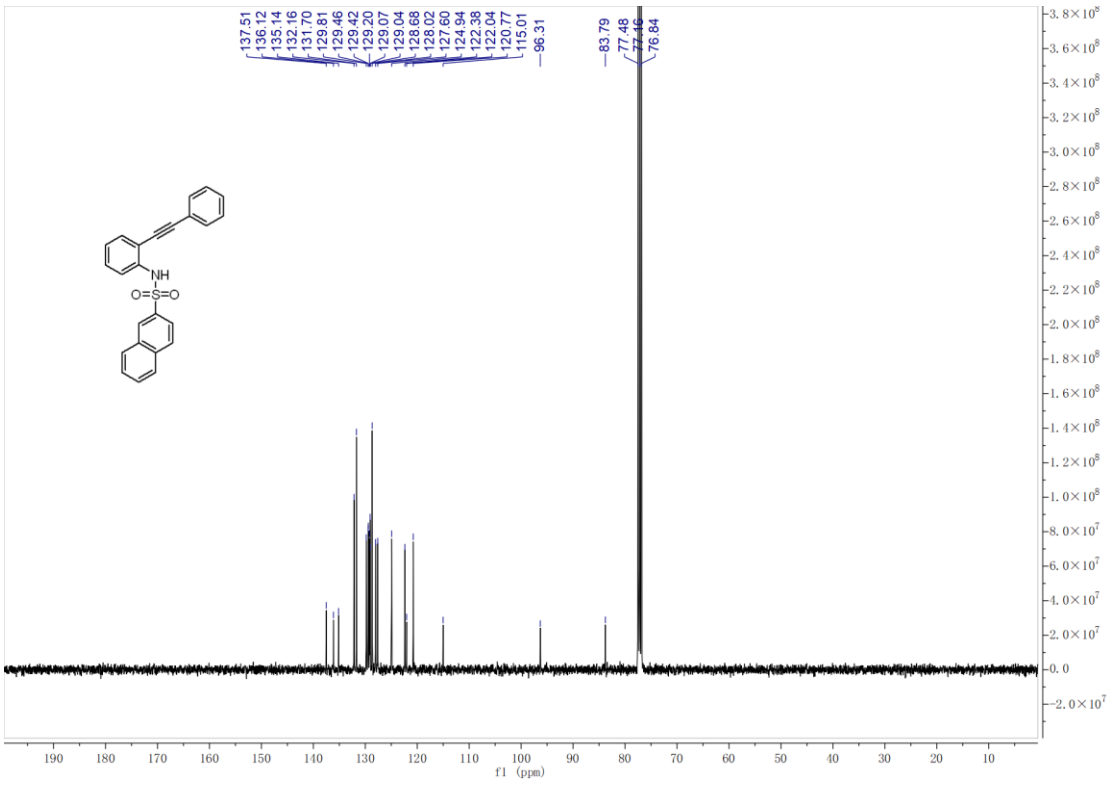
32a, $^{1}H + ^{13}C$


8.16
8.16
8.14
8.14
7.91
7.58
7.57
7.57
7.56
7.55
7.55
7.54
7.54
7.54
7.53
7.48
7.48
7.47
7.46
7.46
7.45
7.44
7.44
7.43
7.43
7.42
7.41
7.41
7.40
7.40
7.39
7.39
7.38
7.38
7.37
7.37
7.36
7.35
7.26
7.23
7.23
7.21
7.21
7.21
7.19
7.19
7.03
7.02
7.01
7.00
6.99
6.98
NH
O=S=O
Cl
0.98
0.95
3.04
7.10
1.02
1.00
f1 (ppm)

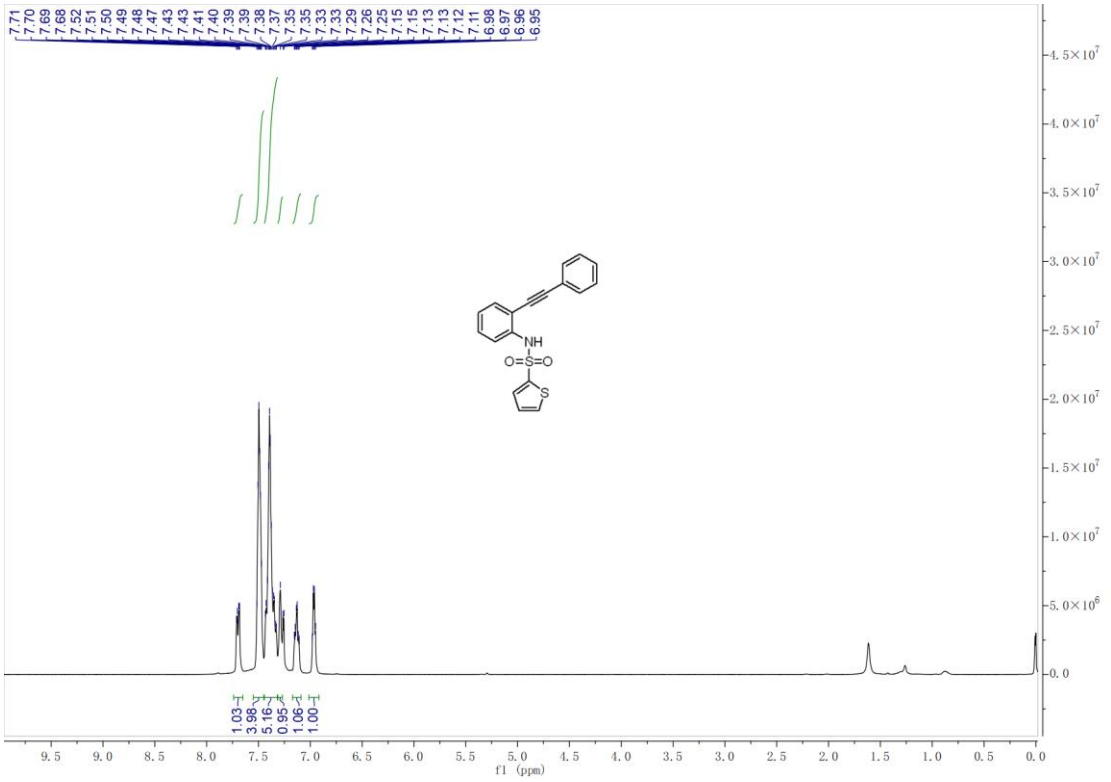

137.26
136.23
134.41
132.47
132.16
132.03
131.75
129.74
129.21
128.71
127.13
123.97
122.20
117.26
113.12
96.87
83.65
77.48
77.16
76.84
NH
O=S=O
Cl
f1 (ppm)

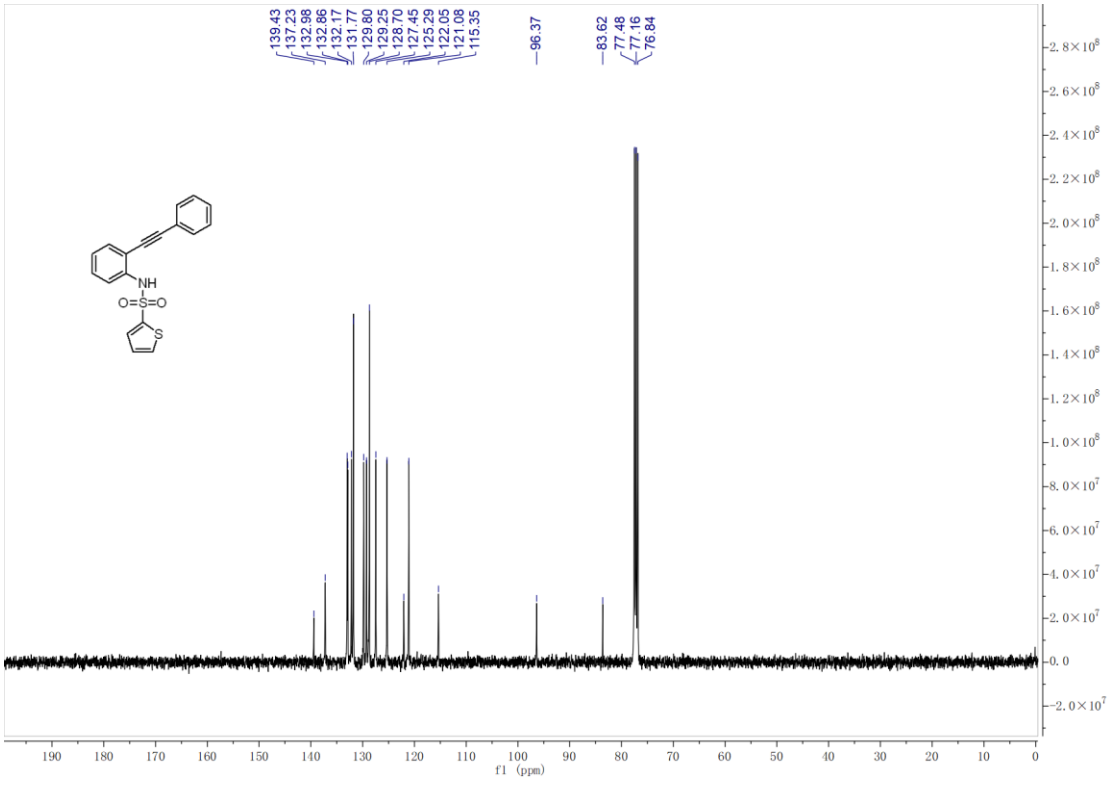
33a, $^{1}H + ^{13}C$


8.39
8.39
7.84
7.83
7.82
7.82
7.81
7.75
7.74
7.72
7.72
7.70
7.68
7.62
7.62
7.60
7.60
7.60
7.58
7.58
7.56
7.55
7.54
7.54
7.53
7.52
7.52
7.41
7.40
7.40
7.39
7.38
7.38
7.37
7.36
7.36
7.35
7.35
7.34
7.33
7.32
7.32
7.31
7.30
7.30
7.28
7.28
7.26
7.07
7.07
7.05
7.05
7.03
7.03
NH
O=S=O
0.98
3.06
1.00
0.97
1.05
1.03
8.00
1.02
f1 (ppm)

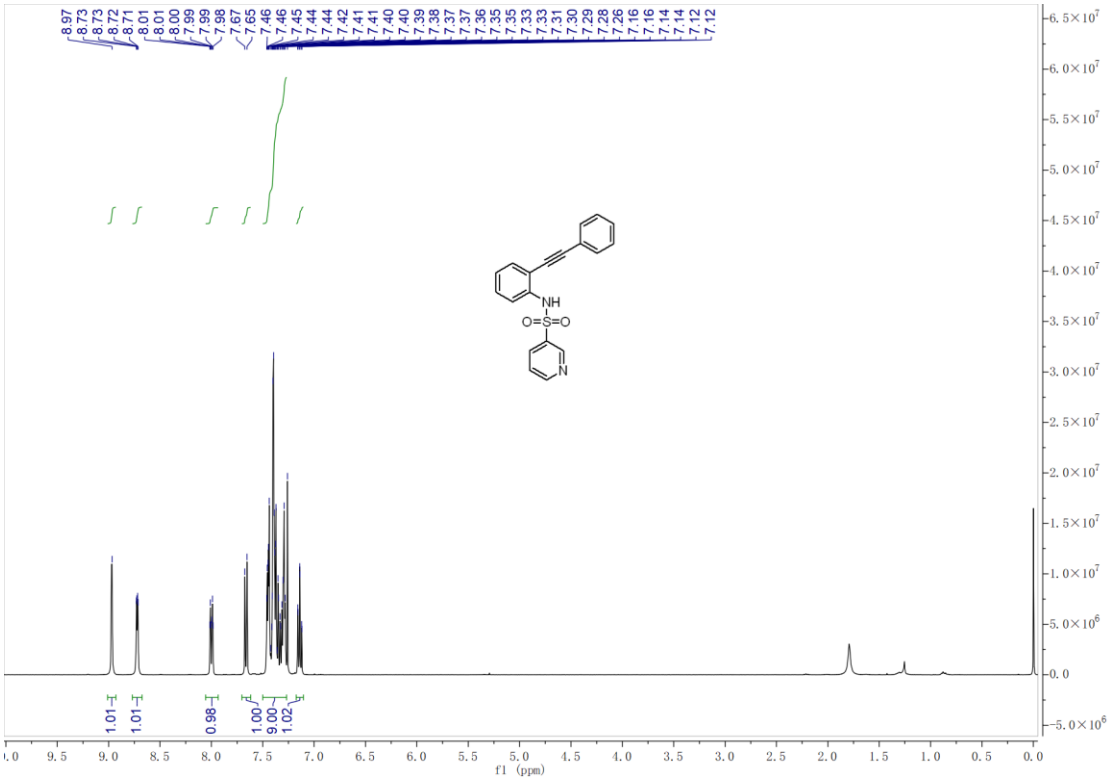

137.51
136.12
135.14
132.16
131.70
129.81
129.46
129.42
129.20
129.07
129.04
128.68
128.02
127.60
124.94
122.38
122.04
120.77
115.01
96.31
83.79
77.48
77.16
76.84
NH
O=S=O
f1 (ppm)

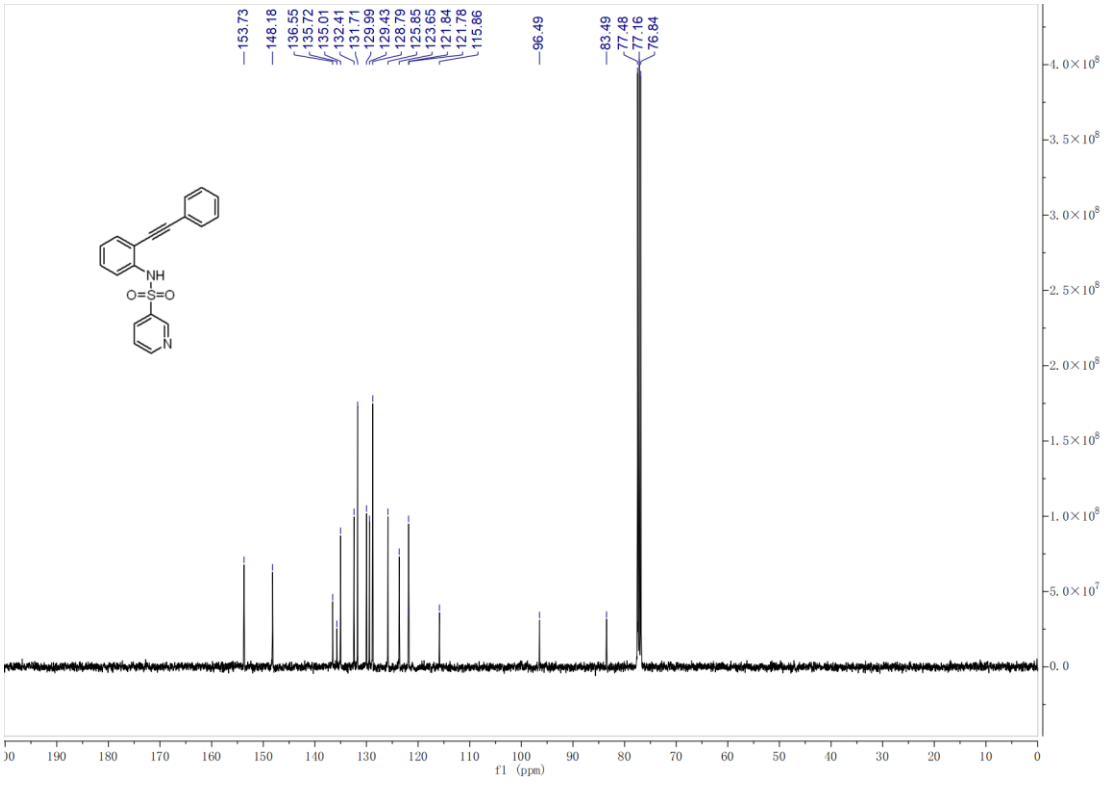
34a, $^{1}H + ^{13}C$


7.71
7.70
7.69
7.68
7.52
7.51
7.50
7.49
7.48
7.47
7.43
7.43
7.41
7.40
7.39
7.39
7.38
7.37
7.35
7.35
7.33
7.33
7.29
7.26
7.25
7.15
7.15
7.13
7.13
7.12
7.11
6.98
6.97
6.96
6.95
1.03
3.98
5.16
0.95
1.06
1.00
NH
O=S=O
S
f1 (ppm)

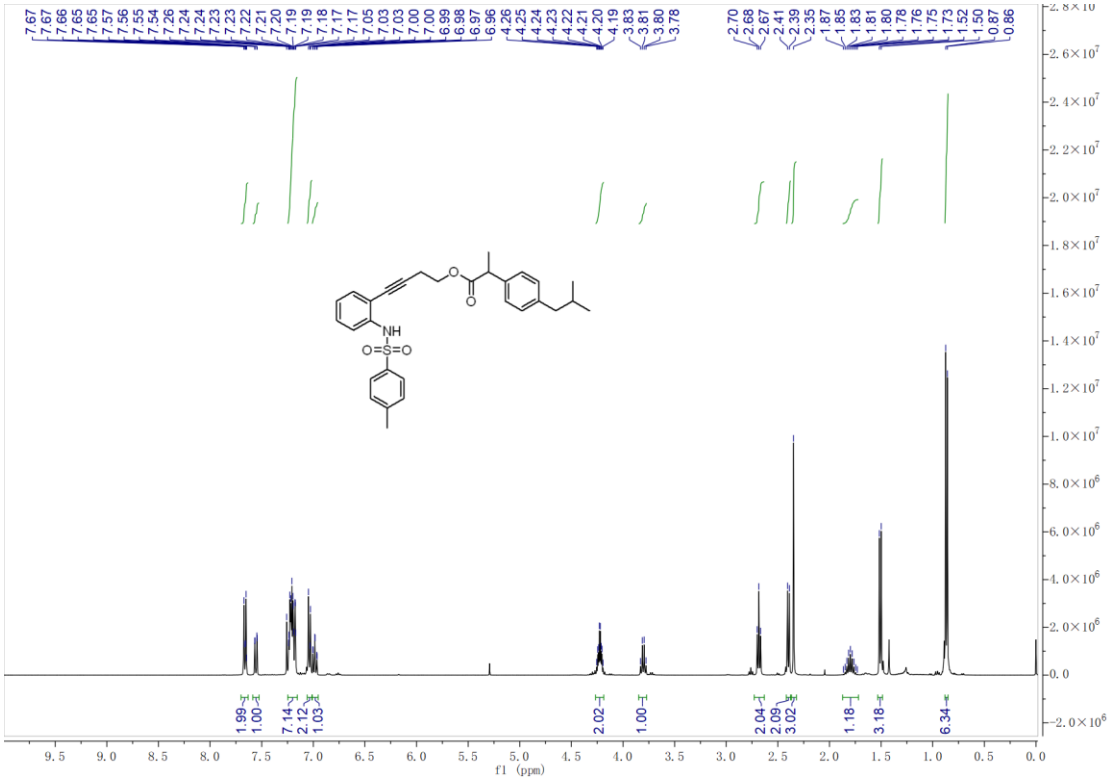

139.43
137.23
132.98
132.86
132.17
131.77
129.80
129.25
128.70
127.45
125.29
122.05
121.08
115.35
96.37
83.62
77.48
77.16
76.84
NH
O=S=O
S
f1 (ppm)

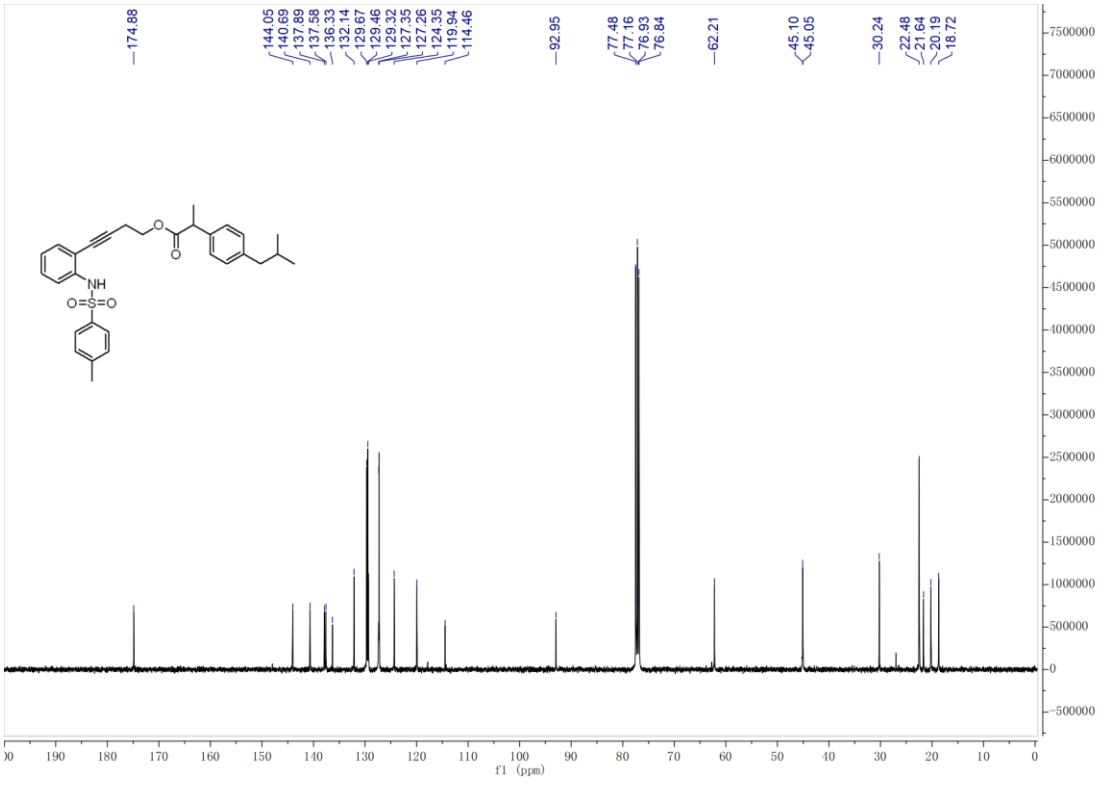
35a, $^{1}H + ^{13}C$


8.97
8.73
8.73
8.72
8.71
8.01
8.01
8.00
7.99
7.99
7.98
7.67
7.65
7.46
7.46
7.45
7.44
7.44
7.42
7.41
7.41
7.40
7.40
7.39
7.38
7.37
7.37
7.36
7.35
7.35
7.33
7.33
7.31
7.30
7.29
7.28
7.26
7.16
7.16
7.14
7.14
7.12
7.12
NH
O=S=O
N
1.01
1.01
0.98
1.00
9.00
1.02
f1 (ppm)

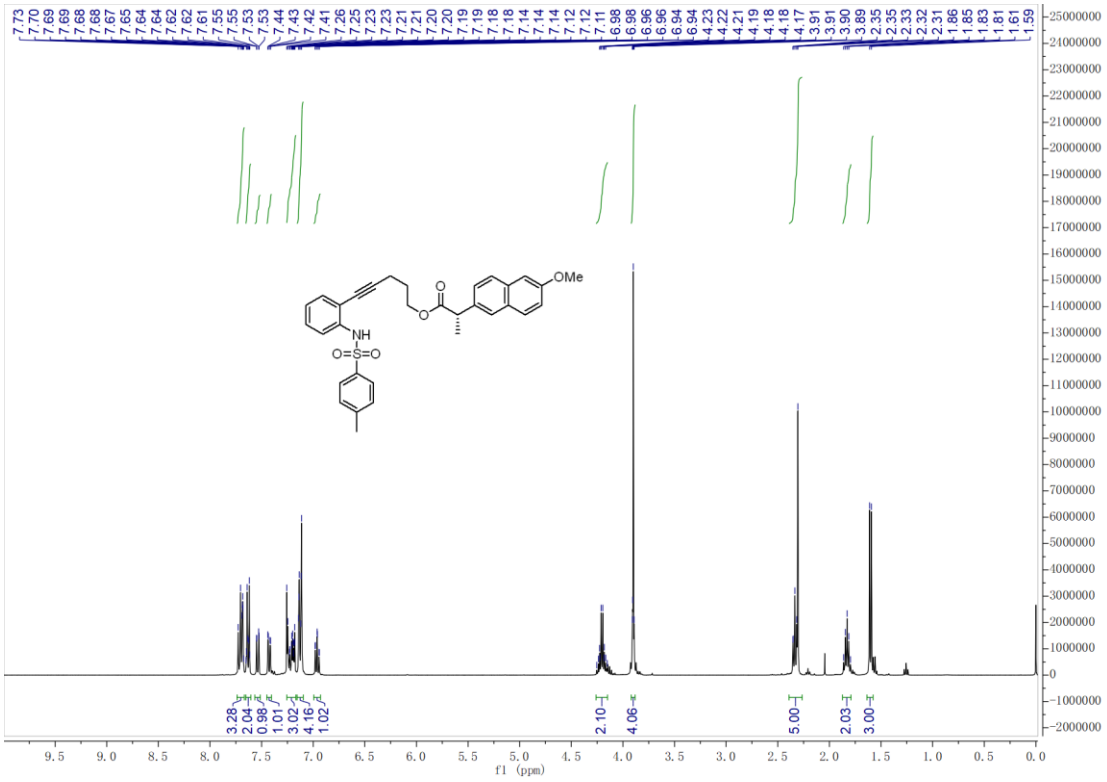

153.73
148.18
136.55
135.72
135.01
132.41
131.71
129.99
129.43
128.79
125.85
123.65
121.84
121.78
115.86
96.49
83.49
77.48
77.16
76.84
NH
O=S=O
N
f1 (ppm)

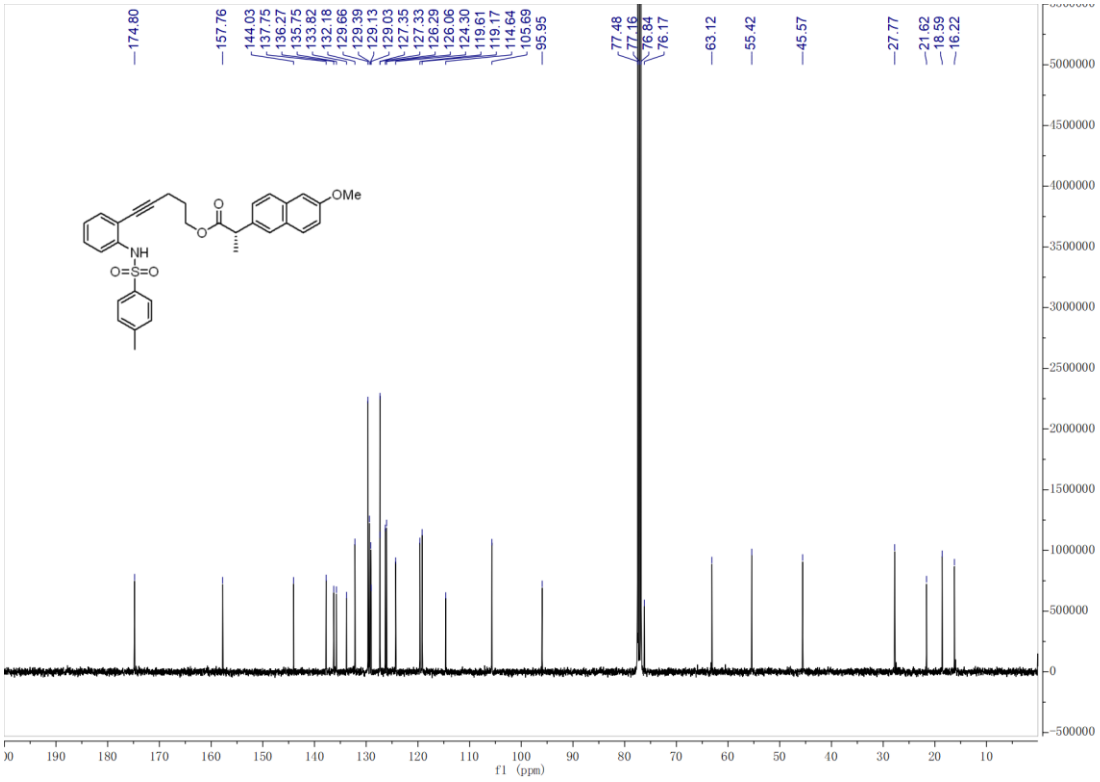
40a, $^{1}H + {}^{13}C$


7.67
7.67
7.66
7.65
7.65
7.57
7.56
7.55
7.54
7.26
7.24
7.24
7.23
7.23
7.22
7.21
7.20
7.19
7.19
7.18
7.17
7.17
7.05
7.03
7.03
7.00
7.00
6.99
6.98
6.97
6.96
4.26
4.25
4.24
4.23
4.22
4.21
4.20
4.19
3.83
3.81
3.80
3.78
2.70
2.68
2.67
2.41
2.39
2.35
1.87
1.85
1.83
1.81
1.80
1.78
1.76
1.75
1.73
1.52
1.50
0.87
0.86
NH
O=S=O
1.99
1.00
7.14
2.12
1.03
2.02
1.00
2.04
2.09
3.02
1.18
3.18
6.34
f1 (ppm)

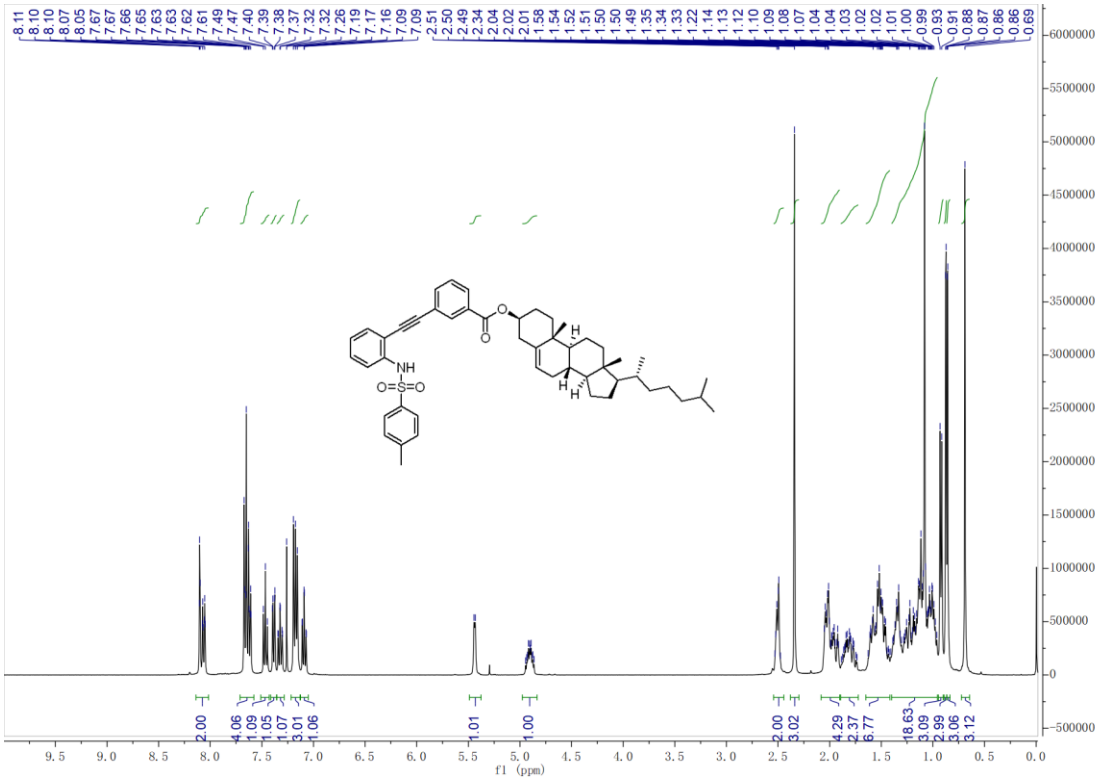

174.88
144.05
140.69
137.89
137.58
136.33
132.14
129.67
129.46
129.32
127.35
127.26
124.35
119.94
114.46
92.95
77.48
77.16
76.93
76.84
62.21
45.10
45.05
30.24
22.48
21.64
20.19
18.72
NH
O=S=O
f1 (ppm)

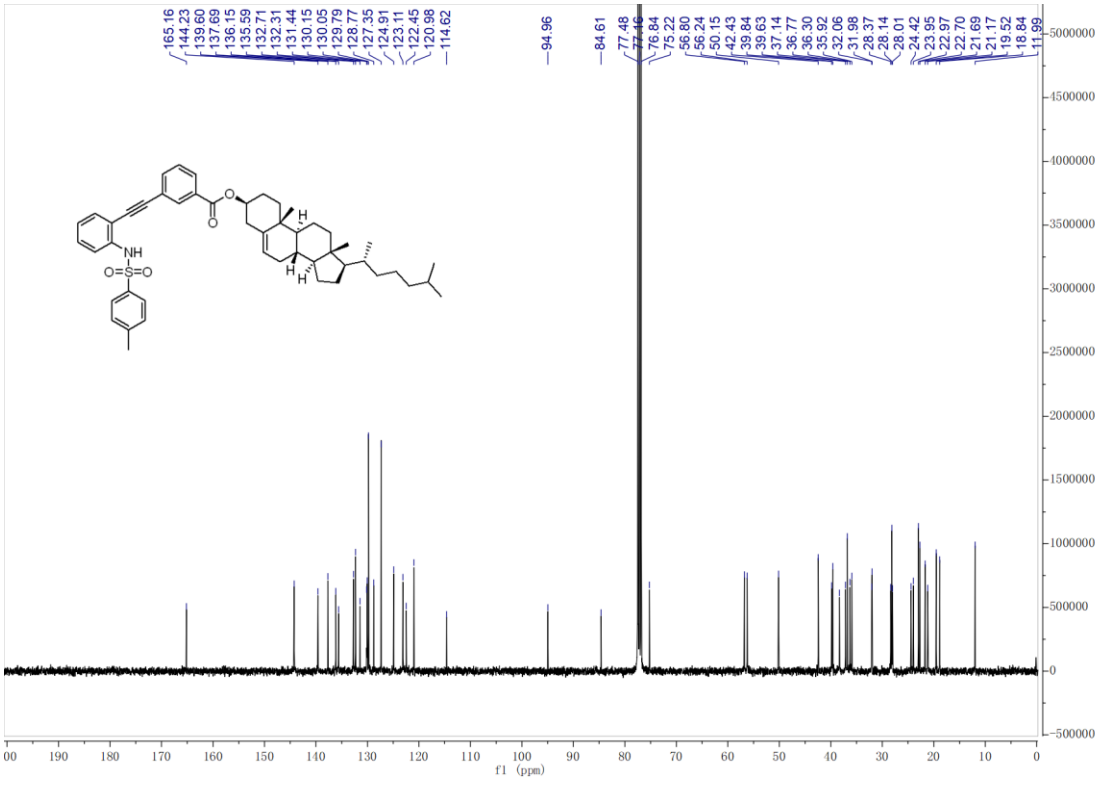
41a, $^{1}H + {}^{13}C$



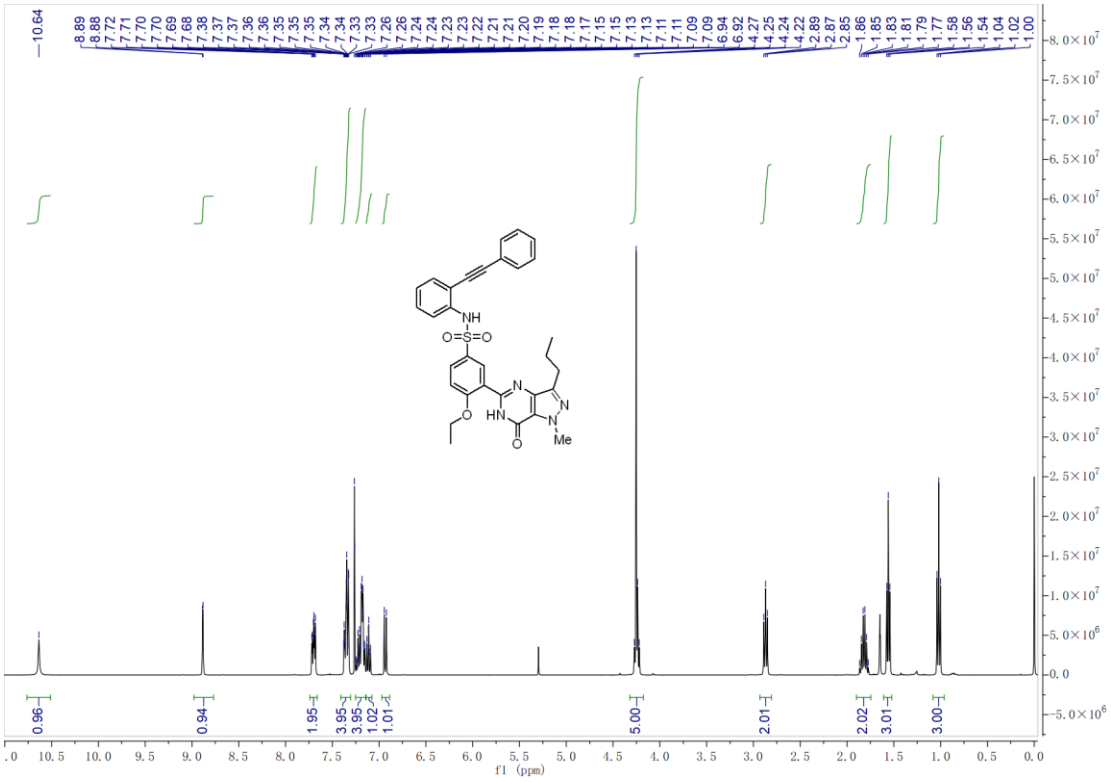


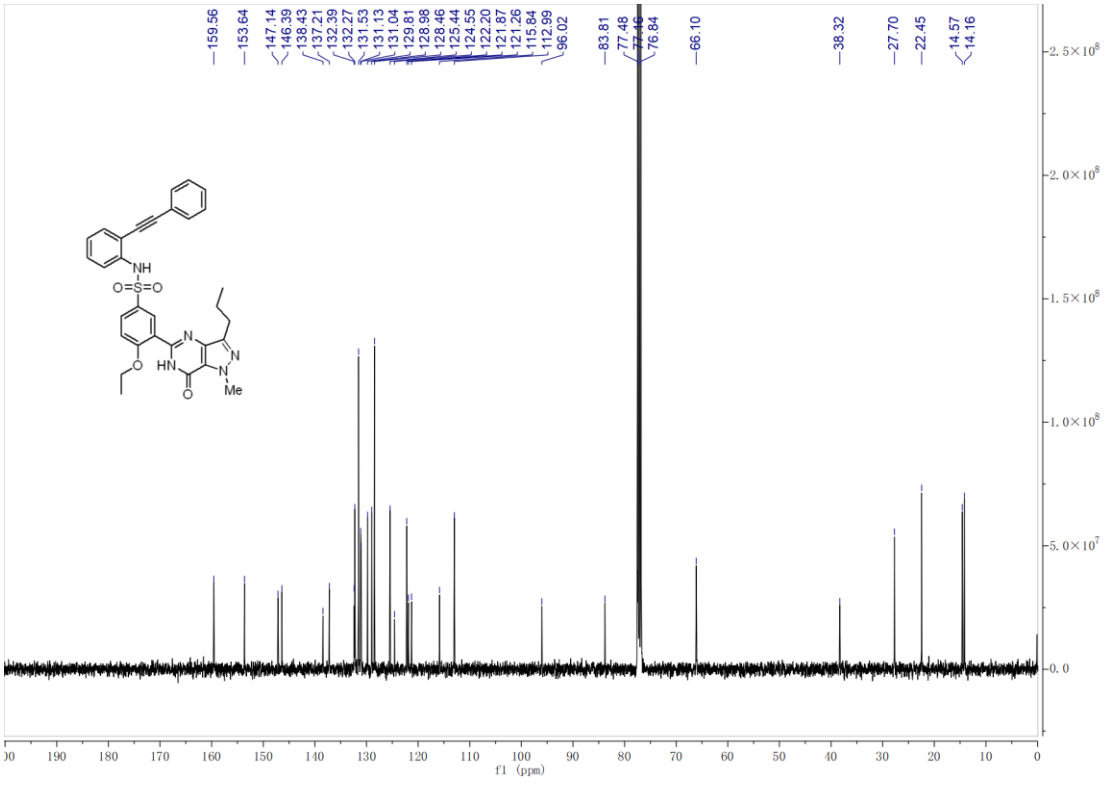
42a, $^{1}H + ^{13}C$



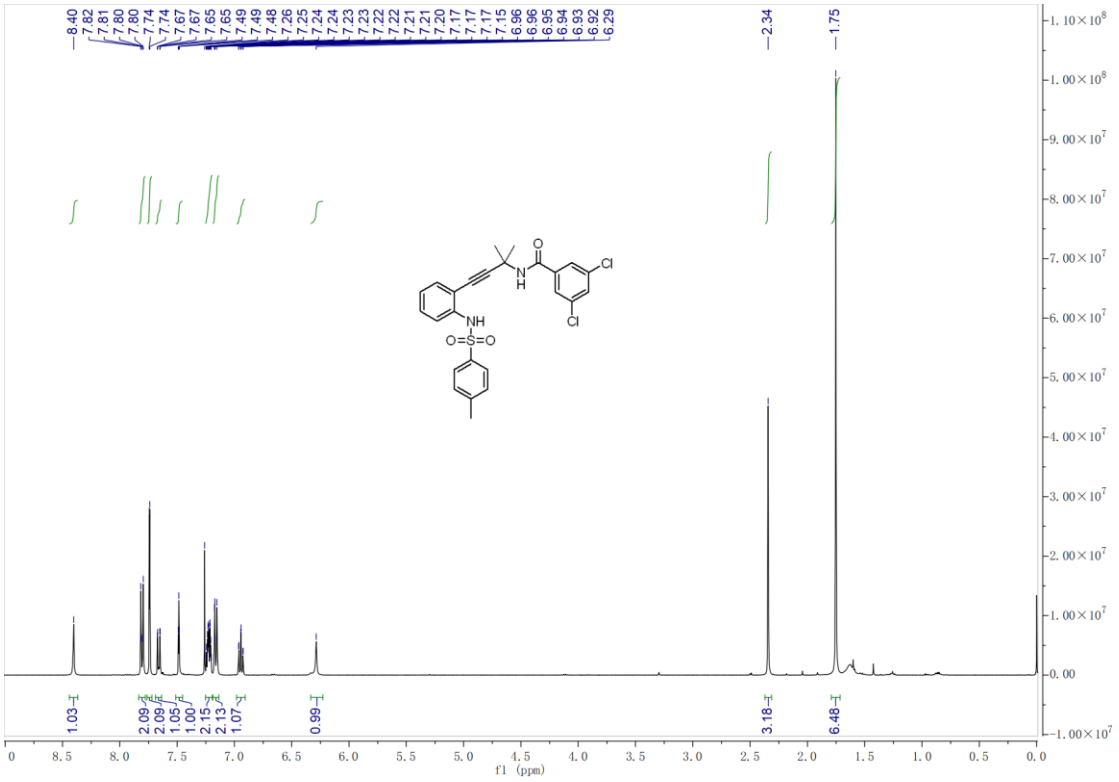


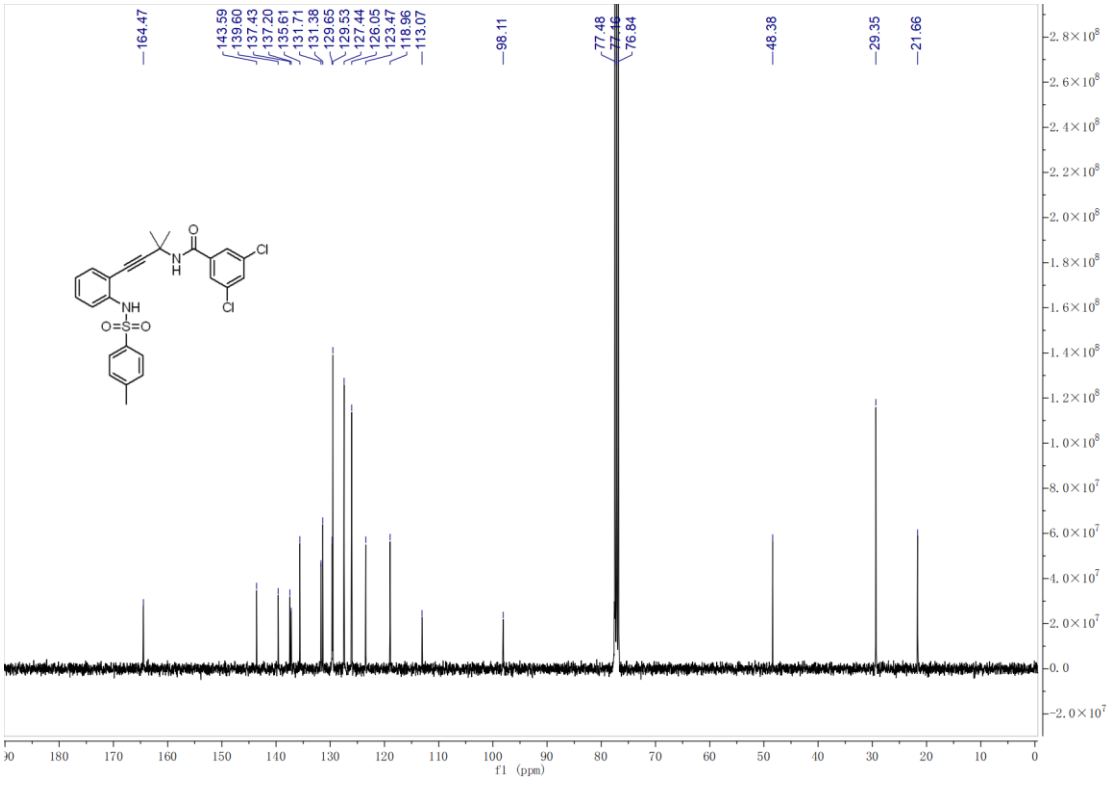
43a, $^{1}H + ^{13}C$



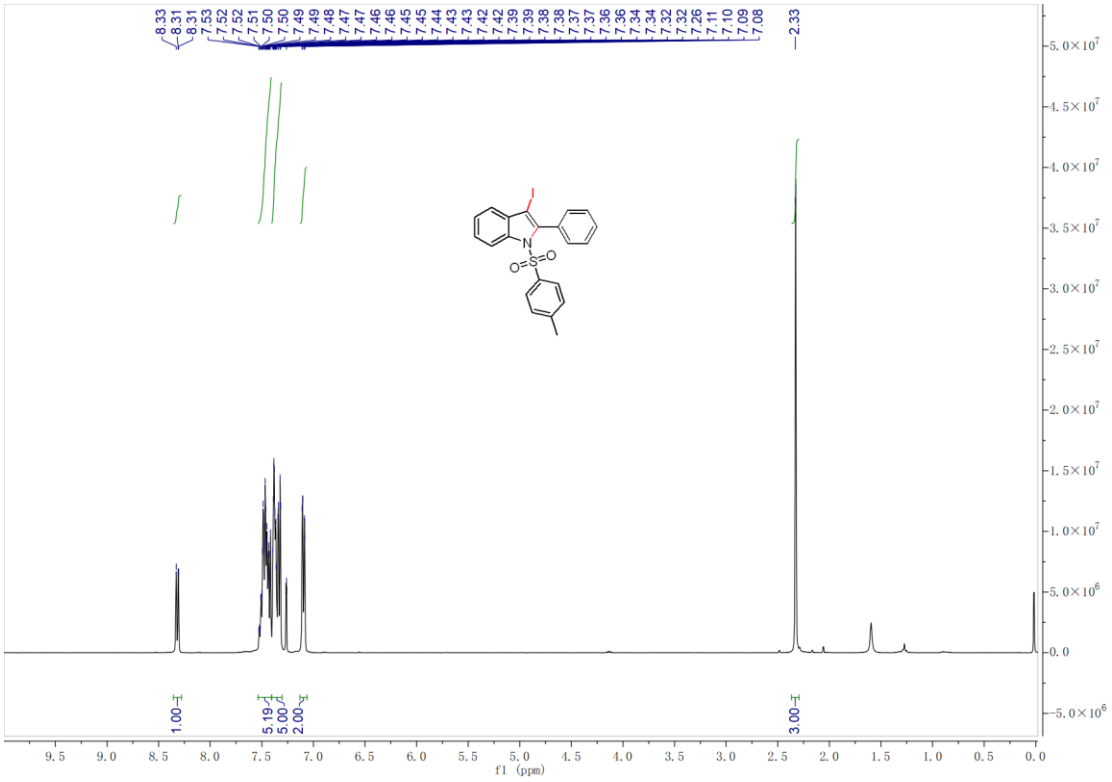


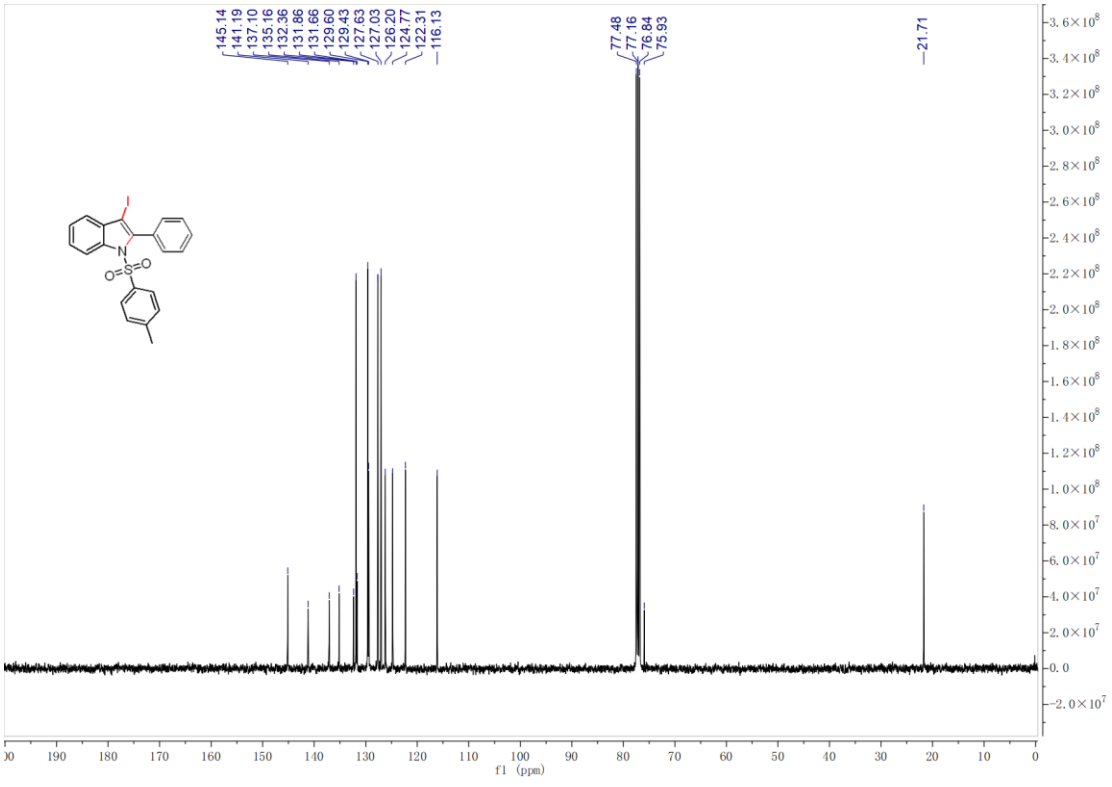
44a, $^{1}H + ^{13}C$


8.40
7.82
7.81
7.80
7.80
7.74
7.74
7.67
7.67
7.65
7.65
7.49
7.49
7.48
7.26
7.25
7.24
7.24
7.23
7.23
7.22
7.22
7.21
7.21
7.20
7.17
7.17
7.15
6.96
6.96
6.95
6.94
6.93
6.92
6.29
2.34
1.75
1.03
2.09
2.09
1.05
1.00
2.15
2.13
1.07
0.99
3.18
6.48
f1 (ppm)

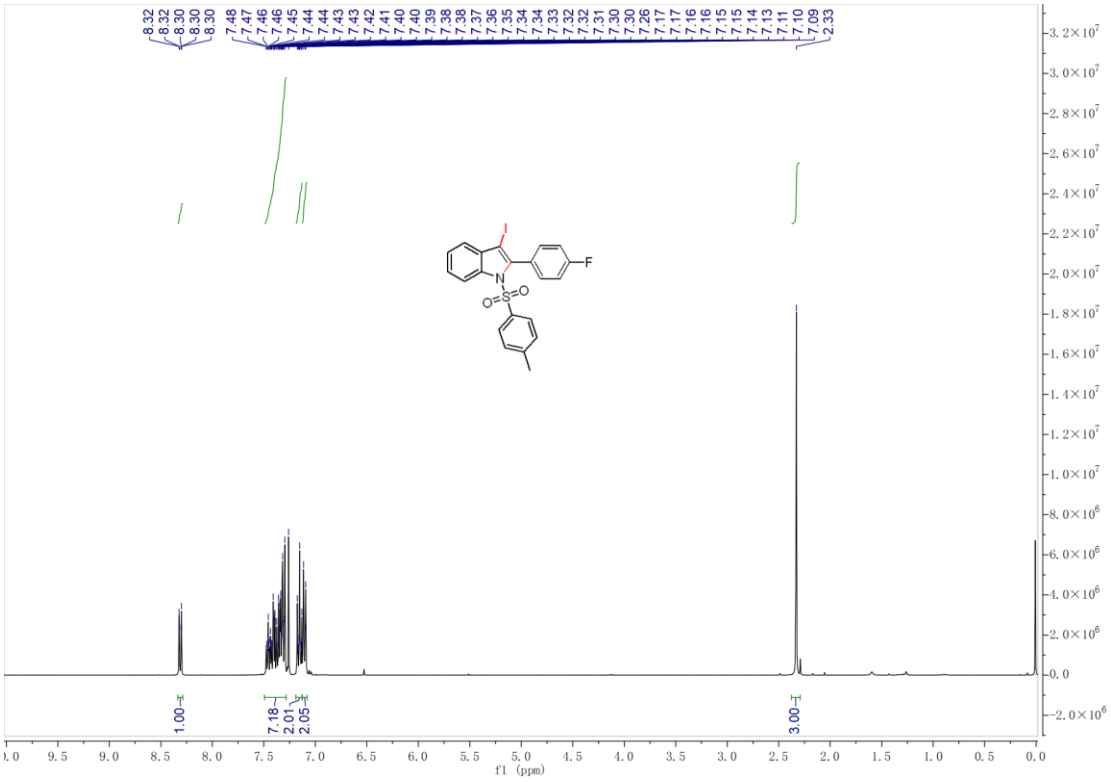

164.47
143.59
139.60
137.43
137.20
135.61
131.71
131.38
129.65
129.53
127.44
126.05
123.47
118.96
113.07
98.11
77.48
77.16
76.84
48.38
29.35
21.66
f1 (ppm)

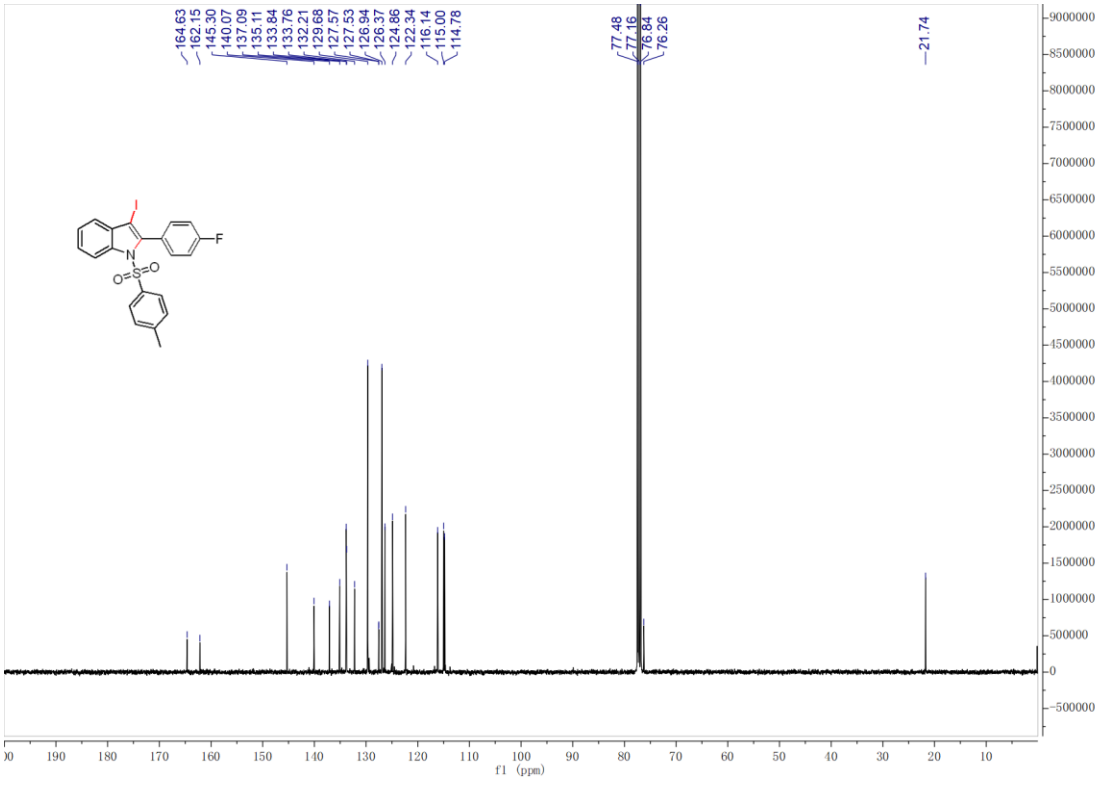
1b, $^{1}H + ^{13}C$


8.33
8.31
8.31
7.53
7.52
7.52
7.51
7.50
7.50
7.49
7.49
7.48
7.47
7.47
7.46
7.46
7.45
7.45
7.44
7.43
7.43
7.42
7.42
7.39
7.39
7.38
7.38
7.37
7.37
7.36
7.36
7.34
7.34
7.32
7.26
7.11
7.10
7.09
7.08
2.33
1.00
5.19
5.00
2.00
3.00
f1 (ppm)

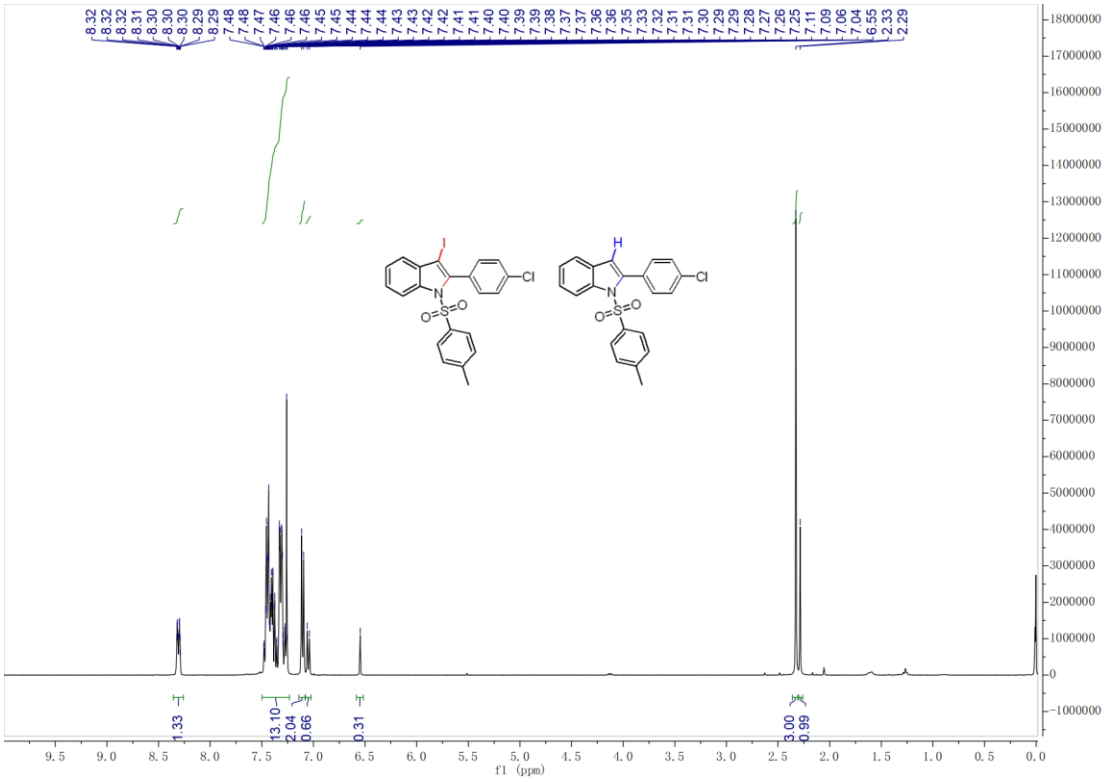

145.14
141.19
137.10
135.16
132.36
131.86
131.66
129.60
129.43
127.63
127.03
126.20
124.77
122.31
116.13
77.48
77.16
76.84
75.93
21.71
f1 (ppm)

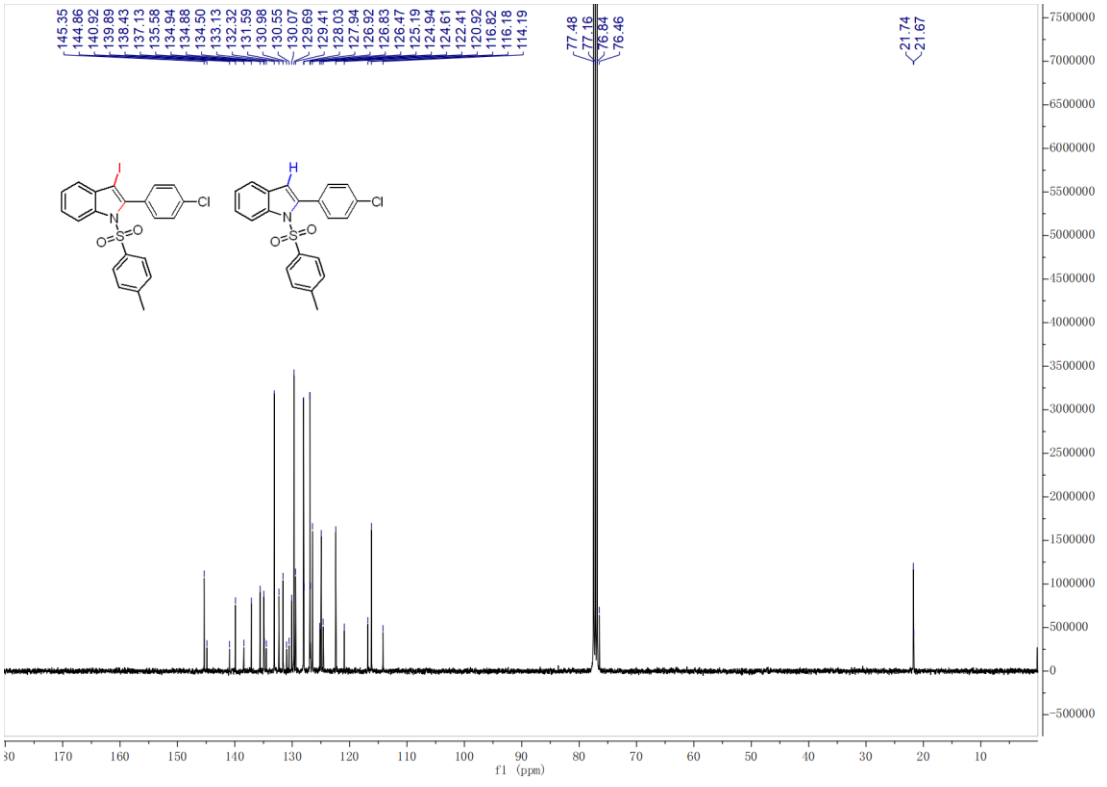
2b, $^{1}H + ^{13}C$


8.32
8.32
8.30
8.30
8.30
7.48
7.47
7.46
7.46
7.45
7.44
7.44
7.43
7.43
7.42
7.41
7.40
7.40
7.39
7.38
7.38
7.37
7.36
7.35
7.34
7.34
7.33
7.32
7.31
7.30
7.30
7.26
7.17
7.17
7.16
7.16
7.15
7.15
7.14
7.13
7.11
7.10
7.09
2.33
I
F
N
O=S=O
1.00
7.18
2.01
2.05
3.00
f1 (ppm)

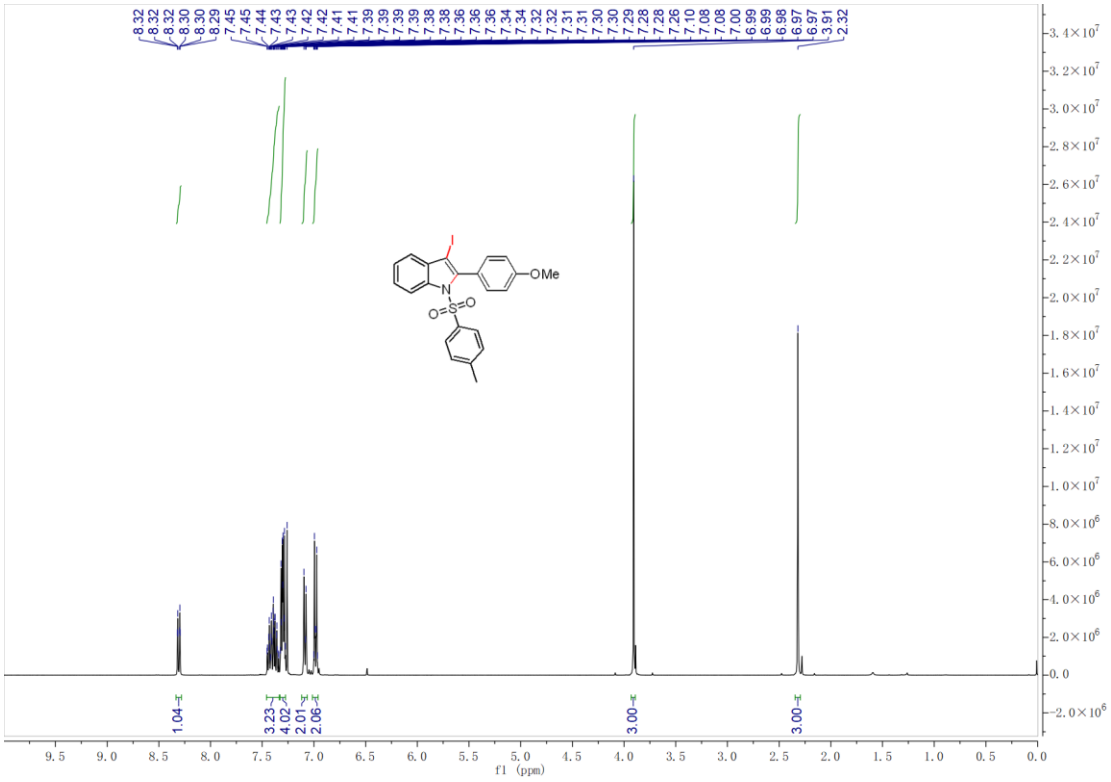

164.63
162.15
145.30
140.07
137.09
135.11
133.84
133.76
132.21
129.68
127.57
127.53
126.94
126.37
124.86
122.34
116.14
115.00
114.78
77.48
77.16
76.84
76.26
21.74
I
F
N
O=S=O
f1 (ppm)

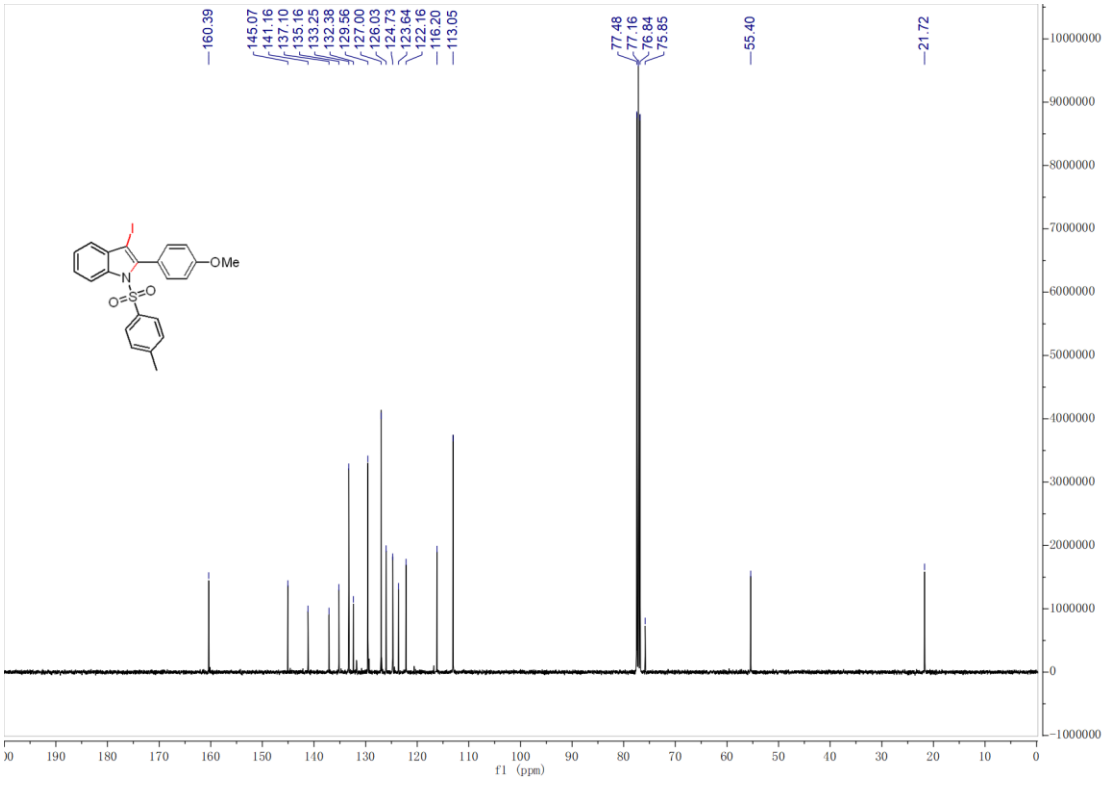
3b & 3c (3:1), $^{1}H + {}^{13}C$



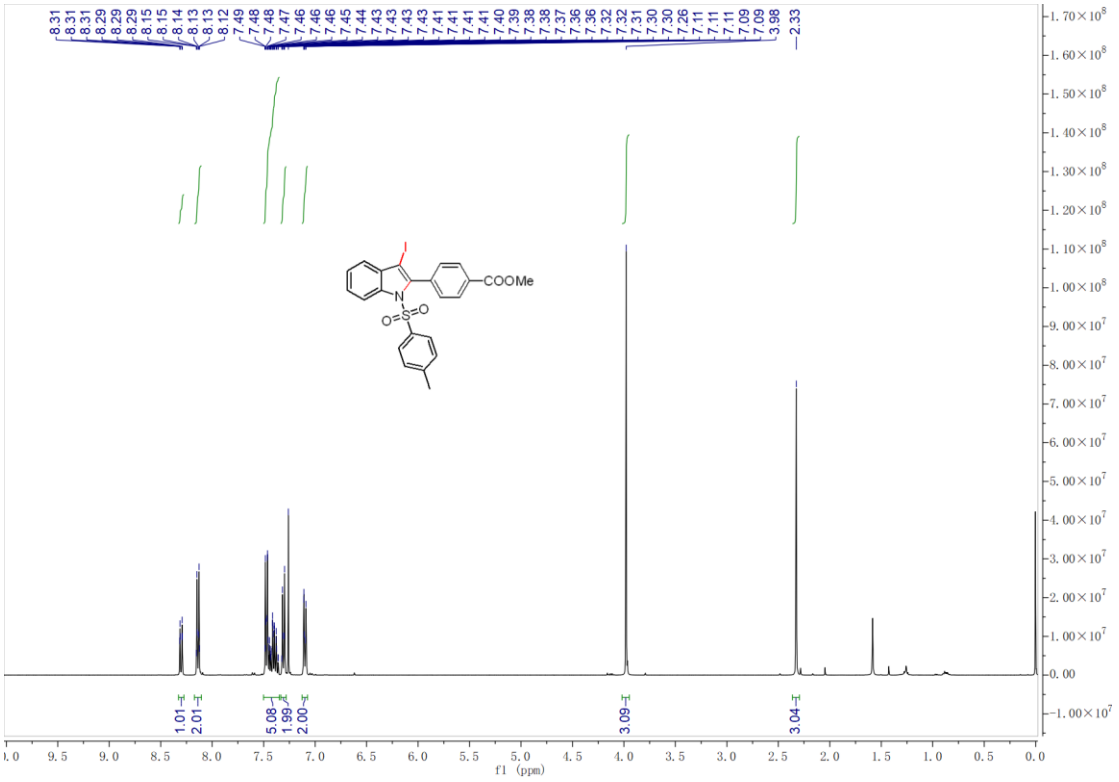


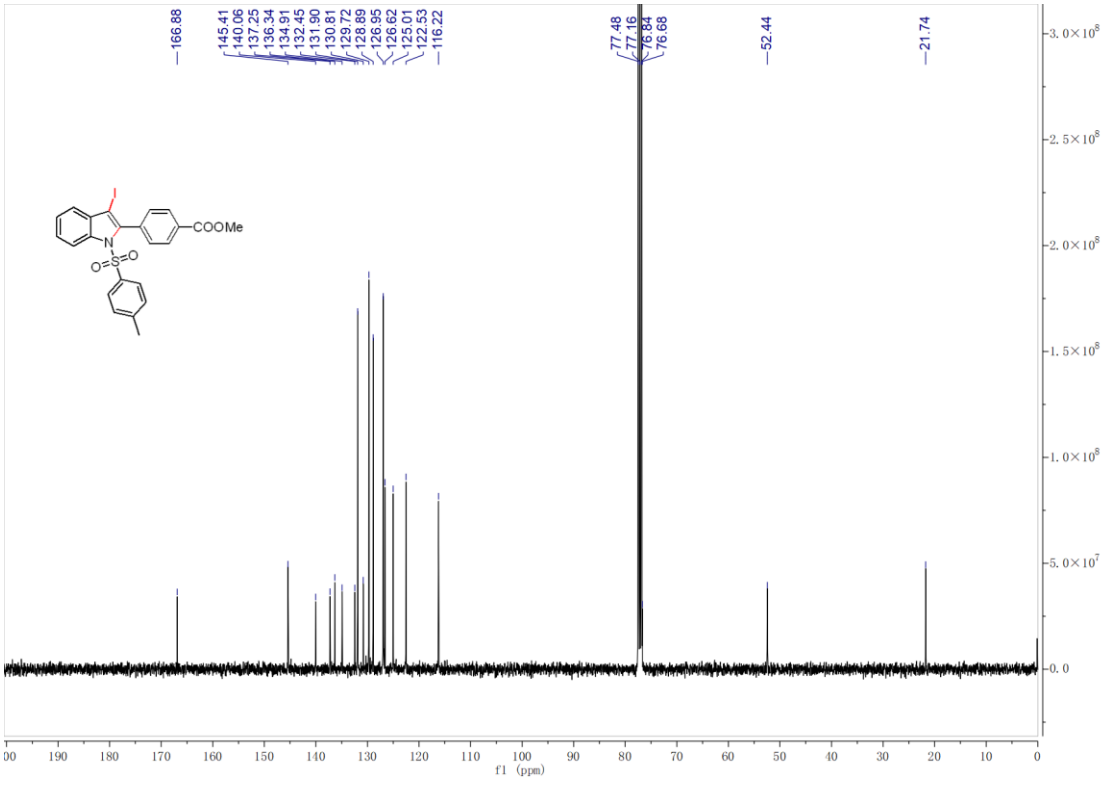
4b, $^{1}H + ^{13}C$


8.32
8.32
8.32
8.30
8.30
8.29
7.45
7.44
7.43
7.43
7.42
7.42
7.41
7.41
7.39
7.39
7.39
7.38
7.38
7.36
7.36
7.36
7.34
7.34
7.32
7.32
7.31
7.31
7.30
7.30
7.29
7.28
7.28
7.26
7.10
7.08
7.08
7.00
6.99
6.99
6.98
6.97
6.97
3.91
2.32
OMe
1.04
3.23
4.02
2.01
2.06
3.00
3.00
f1 (ppm)

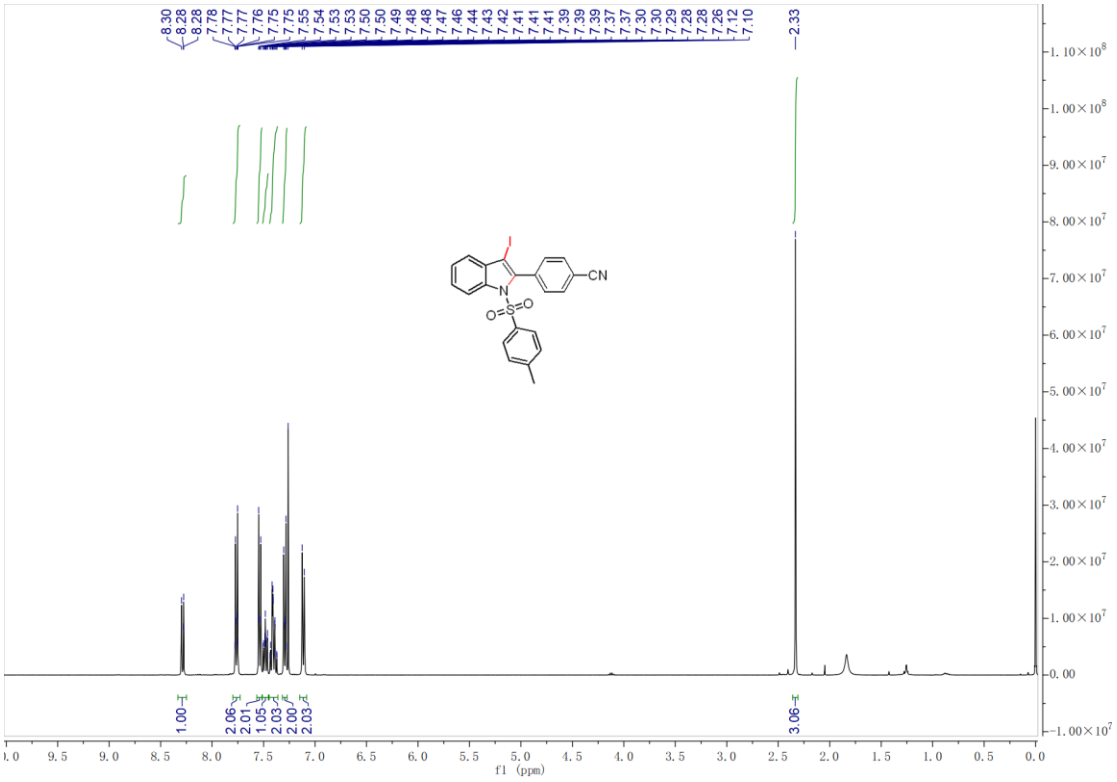

160.39
145.07
141.16
137.10
135.16
133.25
132.38
129.56
127.00
126.03
124.73
123.64
122.16
116.20
113.05
77.48
77.16
76.84
75.85
55.40
21.72
OMe
f1 (ppm)

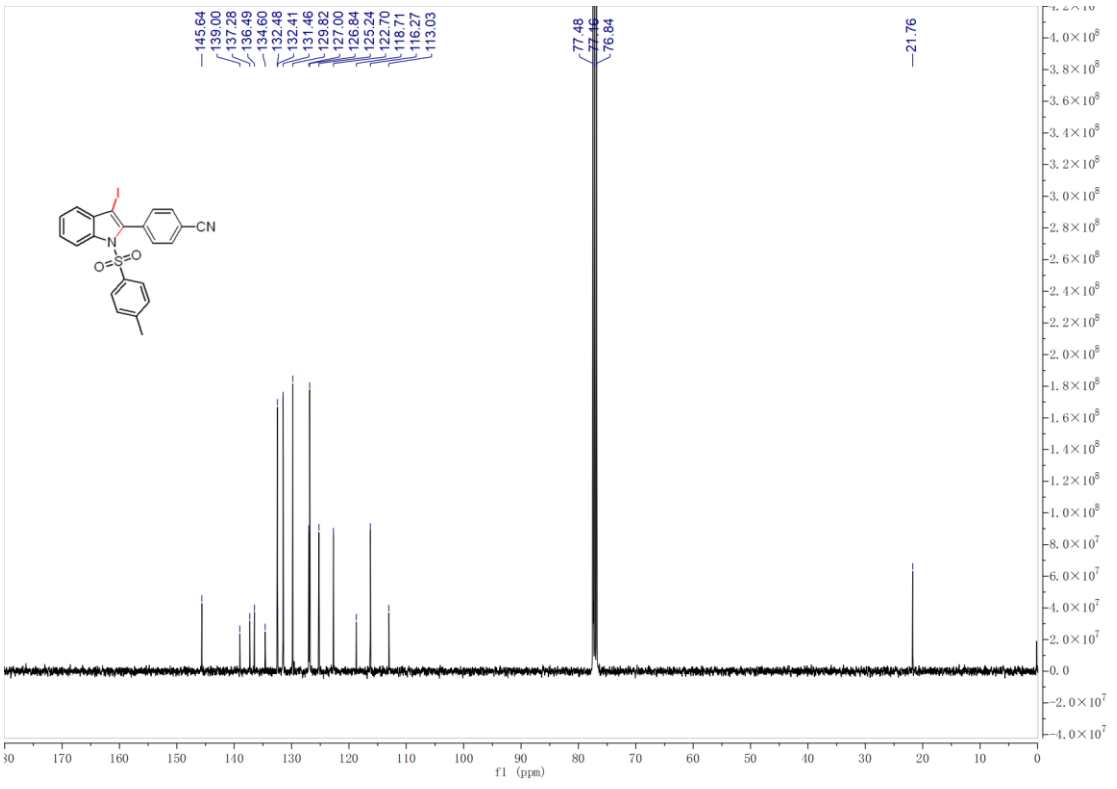
5b, $^{1}H + ^{13}C$


8.31
8.31
8.31
8.29
8.29
8.29
8.15
8.14
8.13
8.13
8.12
7.49
7.48
7.48
7.47
7.46
7.46
7.46
7.45
7.44
7.43
7.43
7.43
7.41
7.41
7.41
7.41
7.40
7.39
7.38
7.38
7.37
7.36
7.36
7.32
7.31
7.30
7.30
7.26
7.11
7.11
7.11
7.09
7.09
3.98
2.33
COOMe
1.01
2.01
5.08
1.99
2.00
3.09
3.04
f1 (ppm)

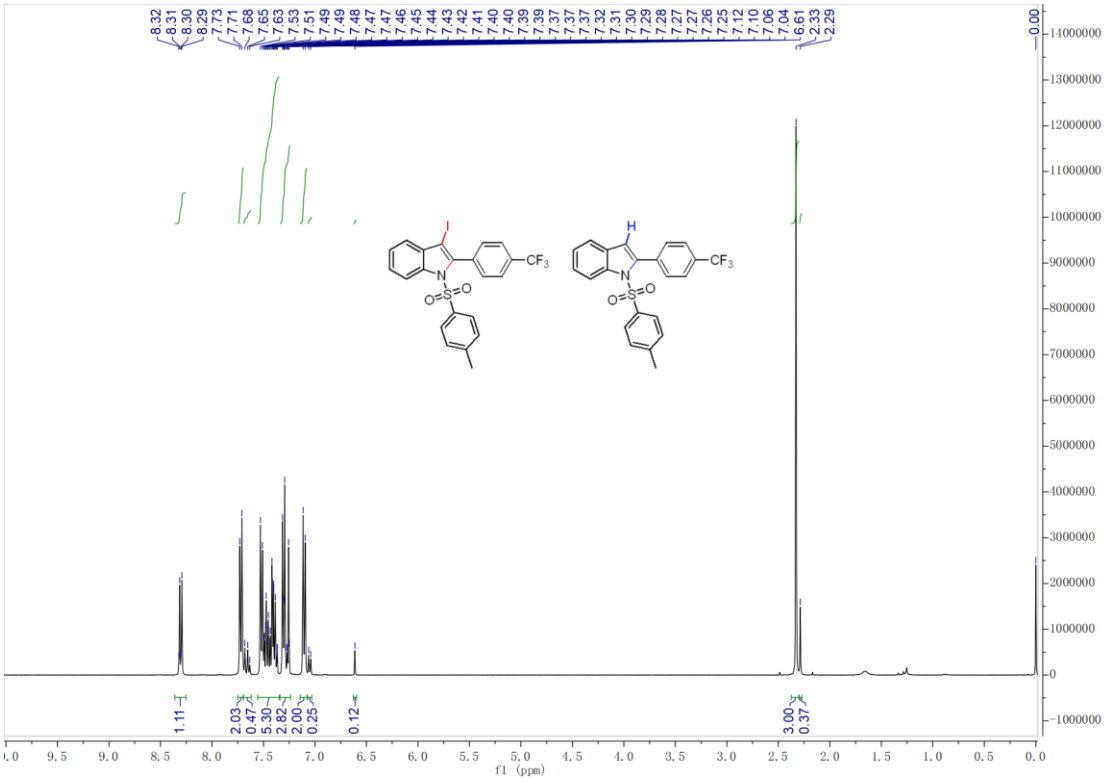

166.88
145.41
140.06
137.25
136.34
134.91
132.45
131.90
130.81
129.72
128.89
126.95
126.62
125.01
122.53
116.22
77.48
77.16
76.84
76.68
52.44
21.74
COOMe
f1 (ppm)

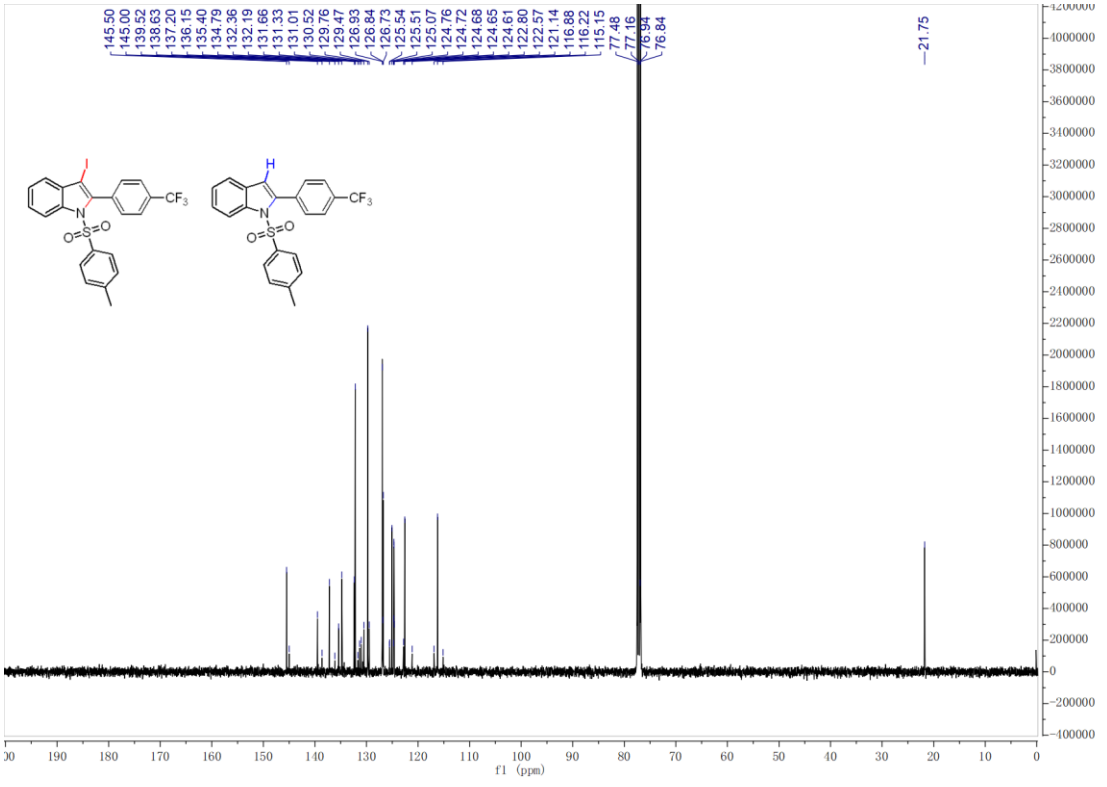
6b, $^{1}H + ^{13}C$


8.30
8.28
8.28
7.78
7.77
7.77
7.76
7.75
7.75
7.55
7.54
7.53
7.53
7.50
7.50
7.49
7.48
7.48
7.47
7.46
7.44
7.43
7.42
7.41
7.41
7.41
7.39
7.39
7.39
7.37
7.37
7.30
7.30
7.29
7.28
7.28
7.26
7.12
7.10
2.33
CN
1.00
2.06
2.01
1.05
2.03
2.00
2.03
3.06
f1 (ppm)

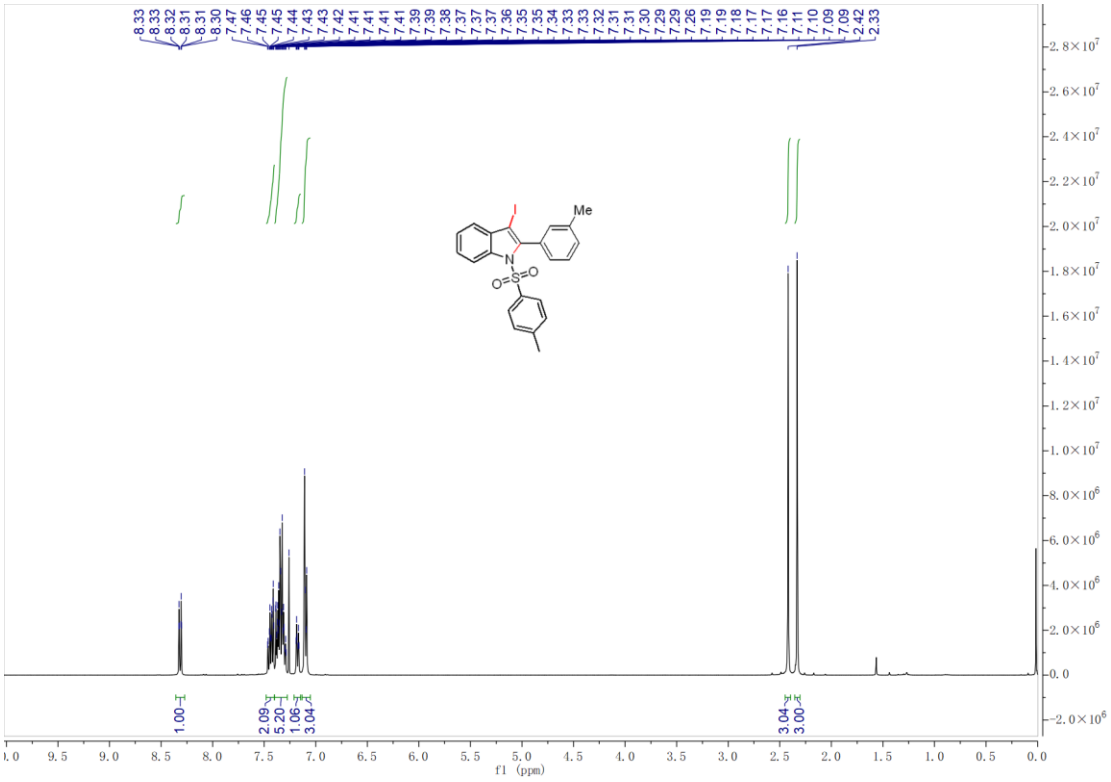

145.64
139.00
137.28
136.49
134.60
132.48
132.41
131.46
129.82
127.00
126.84
125.24
122.70
118.71
116.27
113.03
77.48
77.16
76.84
21.76
CN
f1 (ppm)

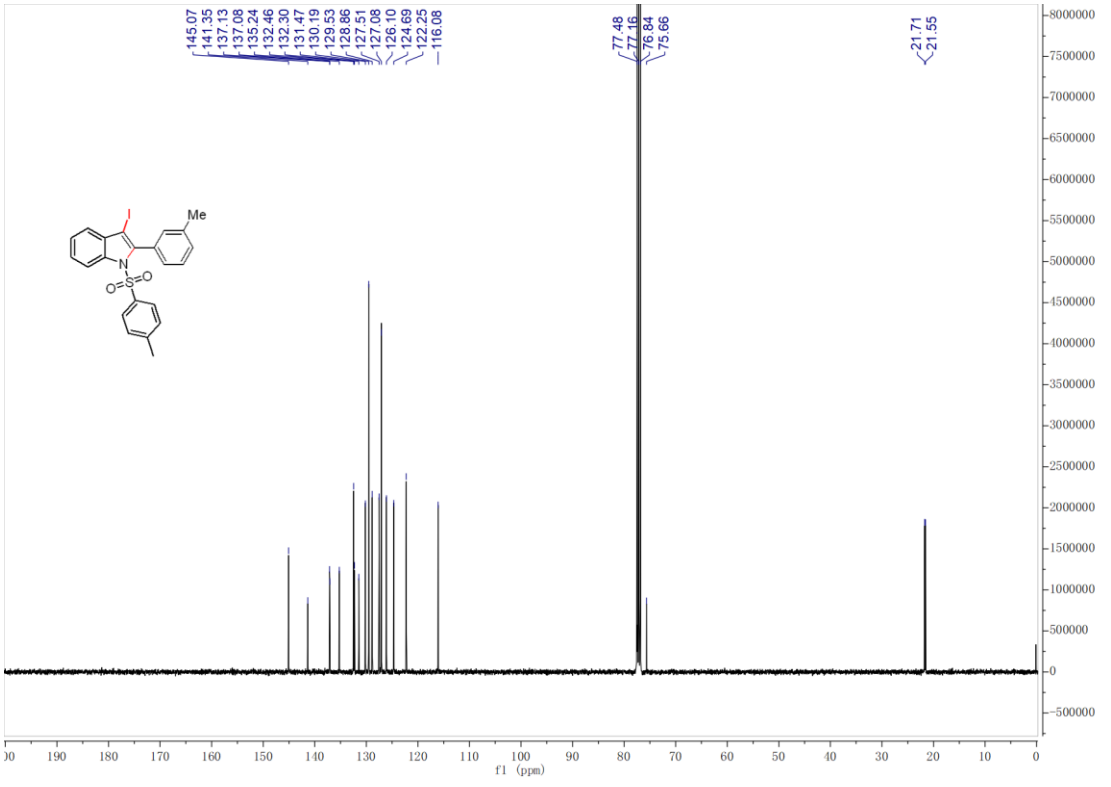
7b & 7c (8.3:1), $^{1}H + ^{13}C$



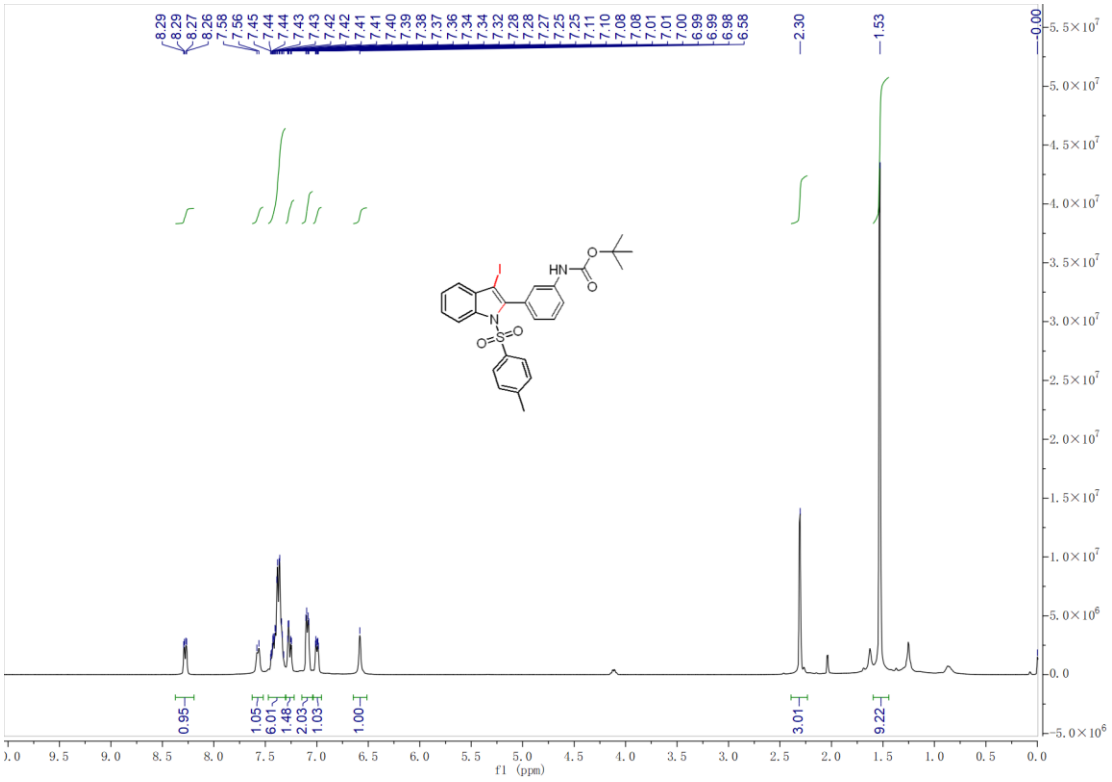


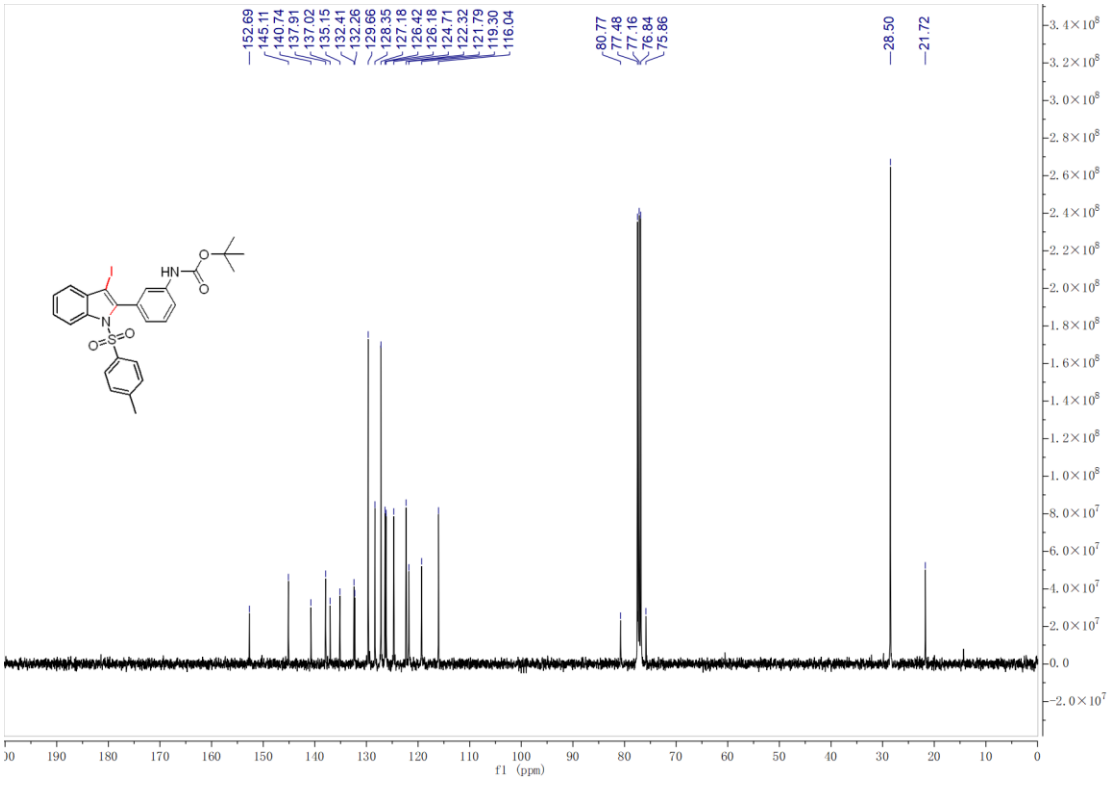
8b, $^{1}H + ^{13}C$


8.33
8.33
8.32
8.31
8.31
8.30
7.47
7.46
7.45
7.45
7.44
7.43
7.43
7.42
7.41
7.41
7.41
7.41
7.39
7.39
7.38
7.37
7.37
7.36
7.35
7.35
7.34
7.33
7.33
7.32
7.31
7.31
7.30
7.29
7.29
7.26
7.19
7.19
7.18
7.17
7.17
7.16
7.11
7.10
7.09
7.09
2.42
2.33
Me
1.00
2.09
5.20
1.06
3.04
3.04
3.00
f1 (ppm)

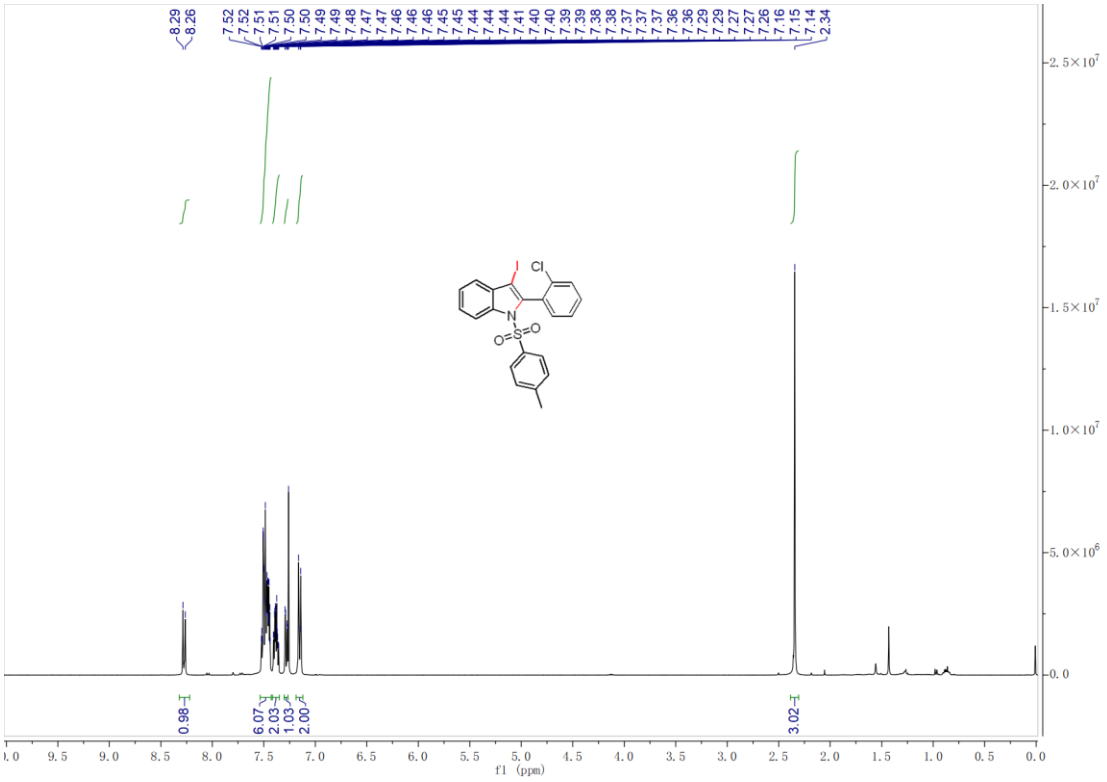

145.07
141.35
137.13
137.08
135.24
132.46
132.30
131.47
130.19
129.53
128.86
127.51
127.08
126.10
124.69
122.25
116.08
77.48
77.16
76.84
75.66
21.71
21.55
Me
f1 (ppm)

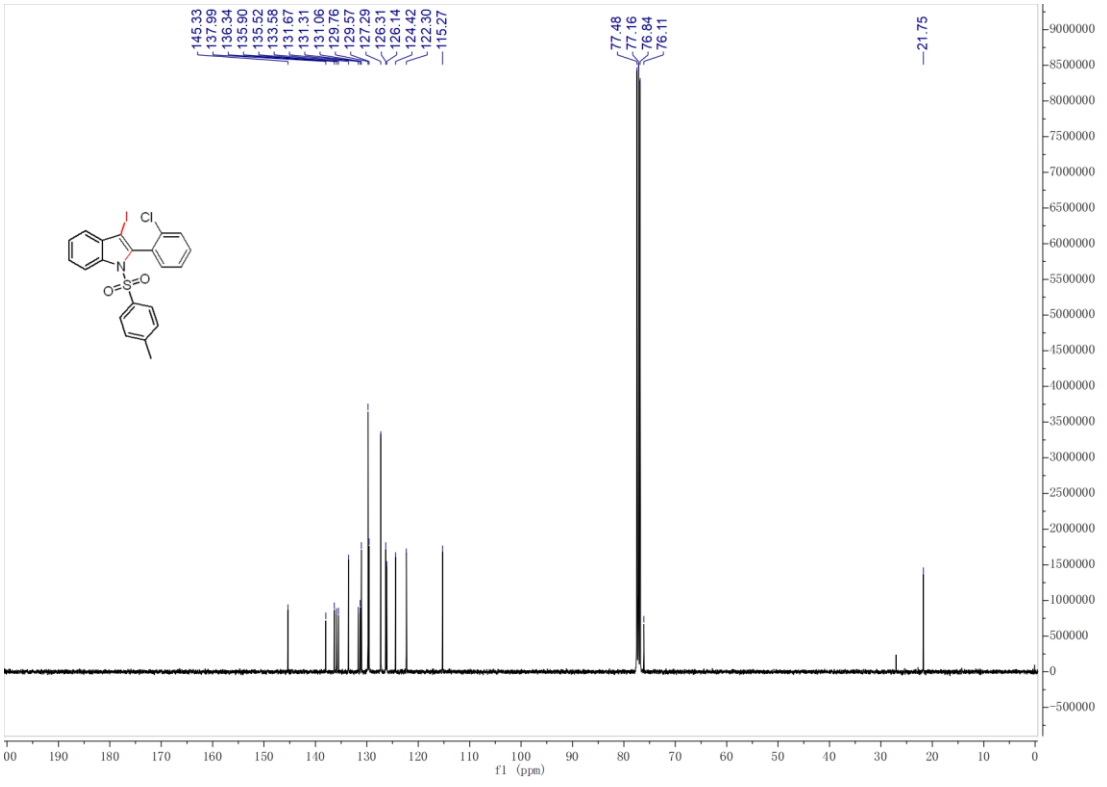
9b, $^{1}H + ^{13}C$


8.29
8.29
8.27
8.26
7.58
7.56
7.45
7.44
7.44
7.43
7.43
7.42
7.42
7.41
7.41
7.40
7.39
7.38
7.37
7.36
7.34
7.34
7.32
7.28
7.28
7.27
7.25
7.25
7.11
7.10
7.08
7.08
7.01
7.01
7.00
6.99
6.99
6.98
6.58
2.30
1.53
0.00
HN
O
O
I
N
O=S=O
0.95
1.05
6.01
1.48
2.03
1.03
1.00
3.01
9.22
f1 (ppm)

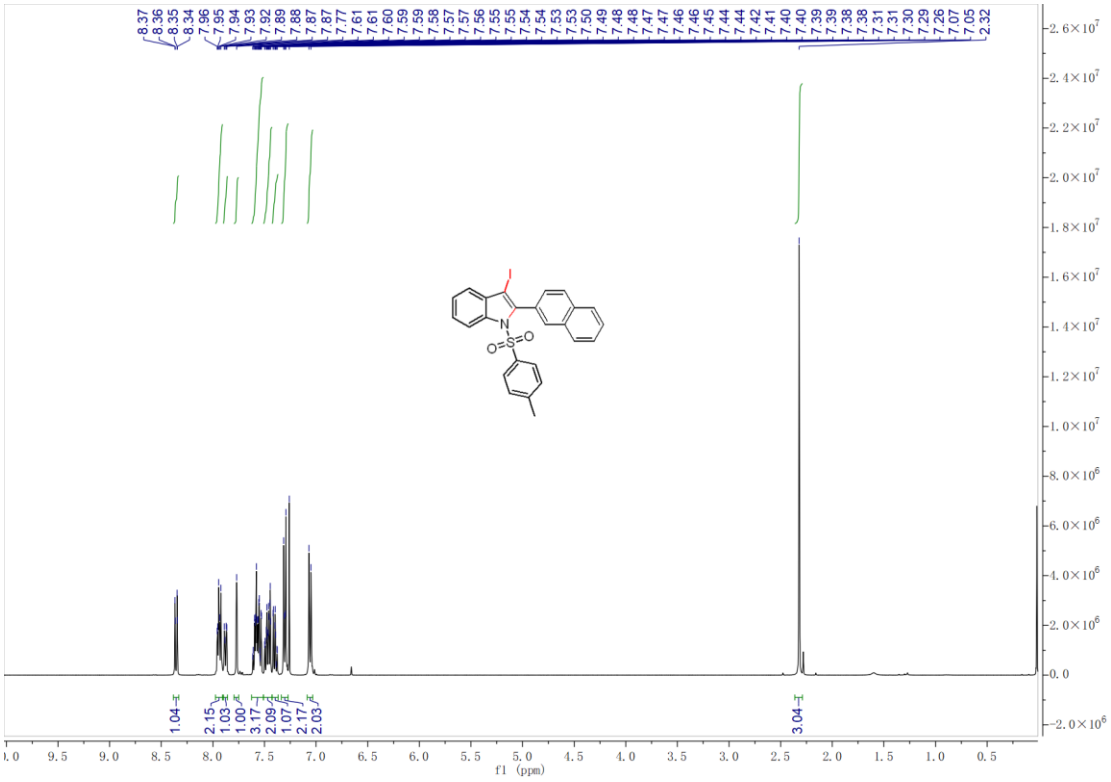

152.69
145.11
140.74
137.91
137.02
135.15
132.41
132.26
129.66
128.35
127.18
126.42
126.18
124.71
122.32
121.79
119.30
116.04
80.77
77.48
77.16
76.84
75.86
28.50
21.72
HN
O
O
I
N
O=S=O
f1 (ppm)

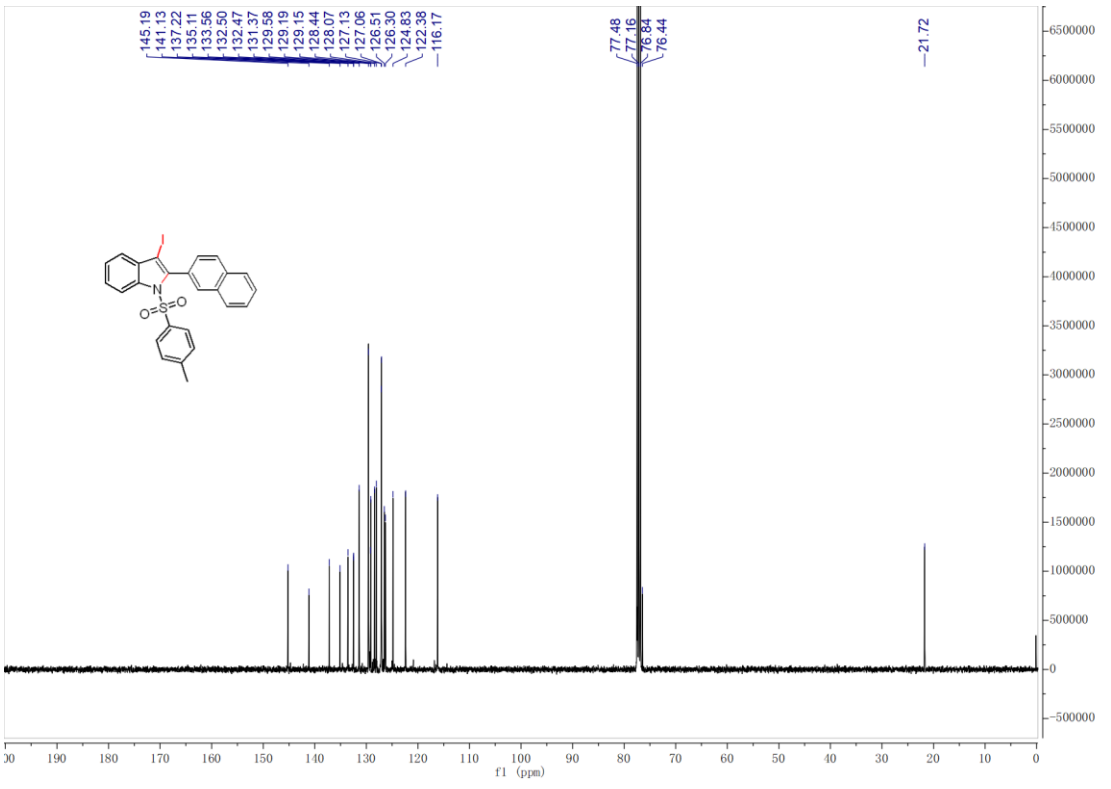
10b, $^{1}H + ^{13}C$


8.29
8.26
7.52
7.52
7.51
7.51
7.50
7.50
7.49
7.49
7.48
7.47
7.47
7.46
7.46
7.46
7.45
7.45
7.44
7.44
7.44
7.41
7.40
7.40
7.39
7.39
7.38
7.38
7.37
7.37
7.37
7.36
7.36
7.29
7.29
7.27
7.27
7.26
7.16
7.15
7.14
2.34
Cl
0.98
6.07
2.03
1.03
2.00
3.02
f1 (ppm)

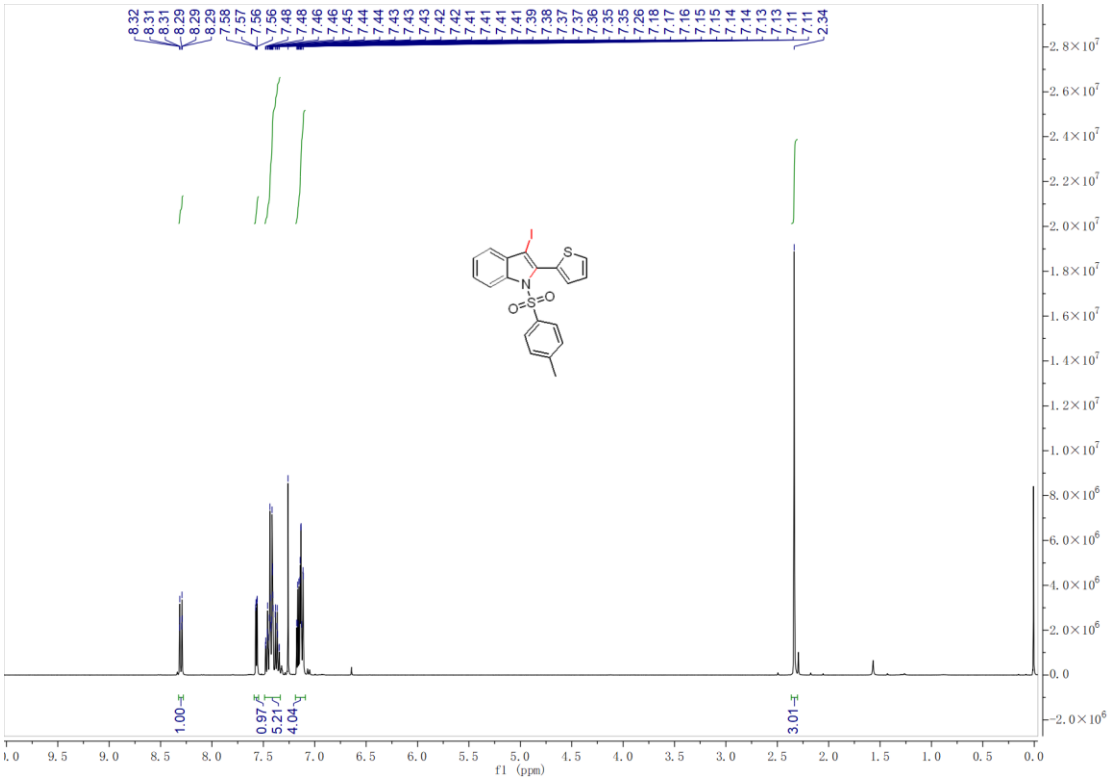

145.33
137.99
136.34
135.90
135.52
133.58
131.67
131.31
131.06
129.76
129.57
127.29
126.31
126.14
124.42
122.30
115.27
77.48
77.16
76.84
76.11
21.75
Cl
f1 (ppm)

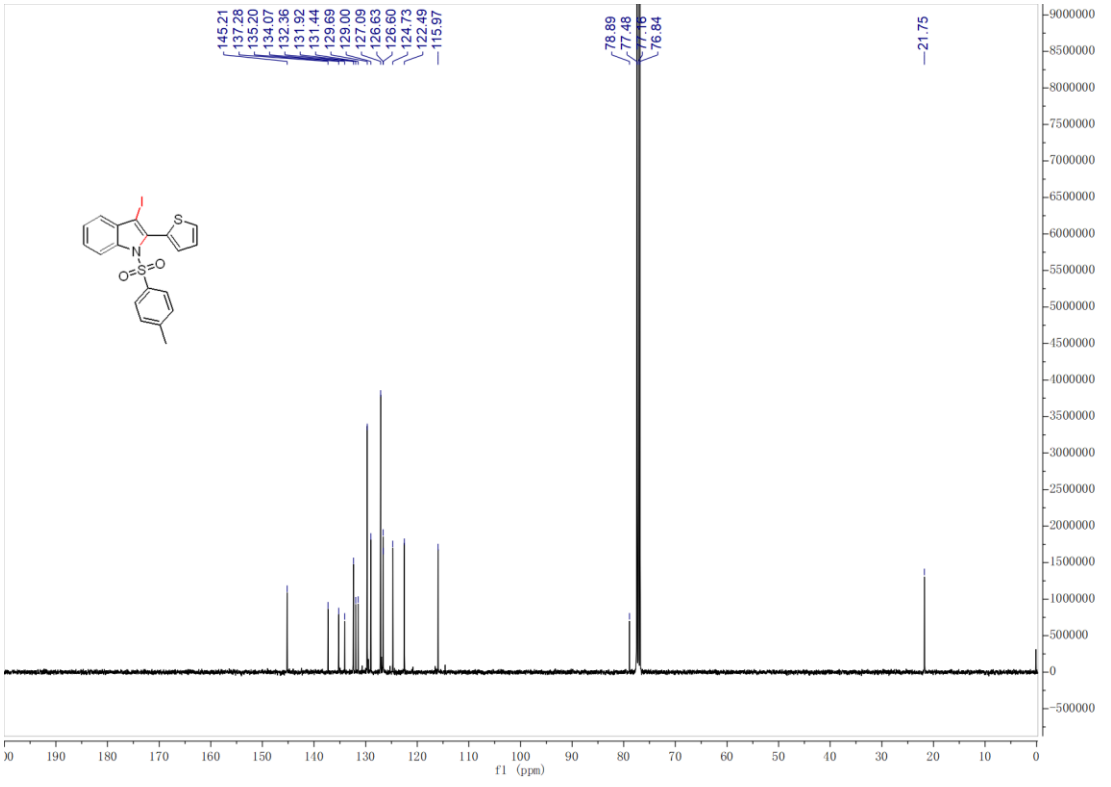
11b, $^{1}H + ^{13}C$


8.37
8.36
8.35
8.34
7.96
7.95
7.94
7.93
7.92
7.89
7.88
7.87
7.87
7.77
7.61
7.61
7.60
7.59
7.59
7.58
7.57
7.57
7.56
7.55
7.55
7.54
7.54
7.53
7.53
7.50
7.49
7.48
7.48
7.47
7.47
7.46
7.46
7.45
7.44
7.44
7.42
7.41
7.40
7.40
7.39
7.39
7.38
7.38
7.31
7.31
7.30
7.29
7.26
7.07
7.05
2.32
1.04
2.15
1.03
1.00
3.17
2.09
1.07
2.17
2.03
3.04
f1 (ppm)

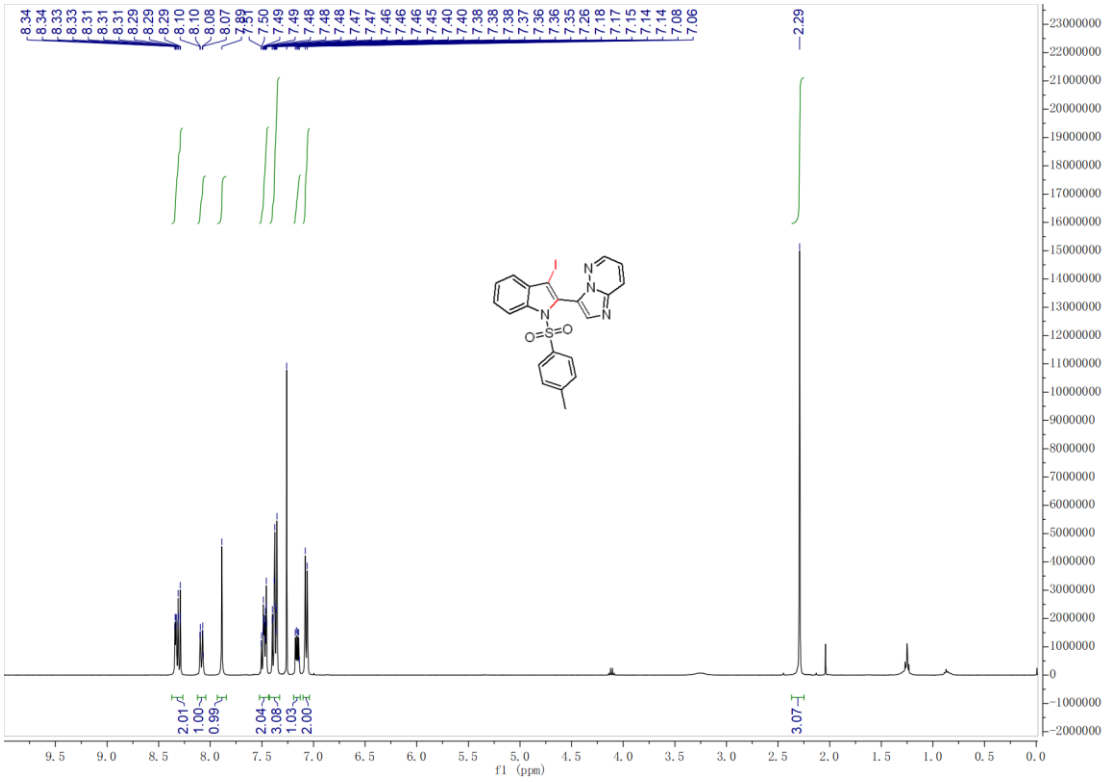

145.19
141.13
137.22
135.11
133.56
132.50
132.47
131.37
129.58
129.19
129.15
128.44
128.07
127.13
127.06
126.51
126.30
124.83
122.38
116.17
77.48
77.16
76.84
76.44
21.72
f1 (ppm)

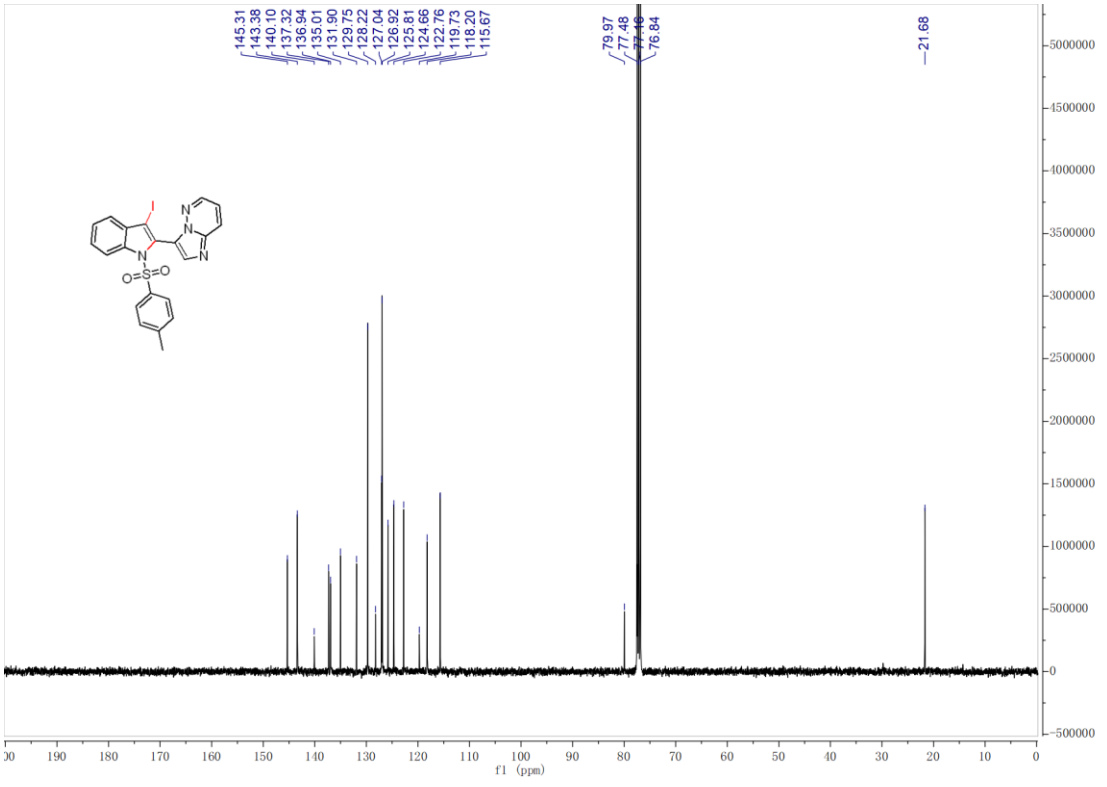
12b, $^{1}H + {}^{13}C$


8.32
8.31
8.31
8.29
8.29
8.29
7.58
7.57
7.56
7.56
7.48
7.48
7.46
7.46
7.45
7.44
7.44
7.43
7.43
7.43
7.42
7.42
7.41
7.41
7.41
7.41
7.39
7.38
7.37
7.37
7.36
7.35
7.35
7.26
7.18
7.17
7.16
7.15
7.15
7.14
7.14
7.13
7.13
7.11
7.11
2.34
1.00
0.97
5.21
4.04
3.01
f1 (ppm)

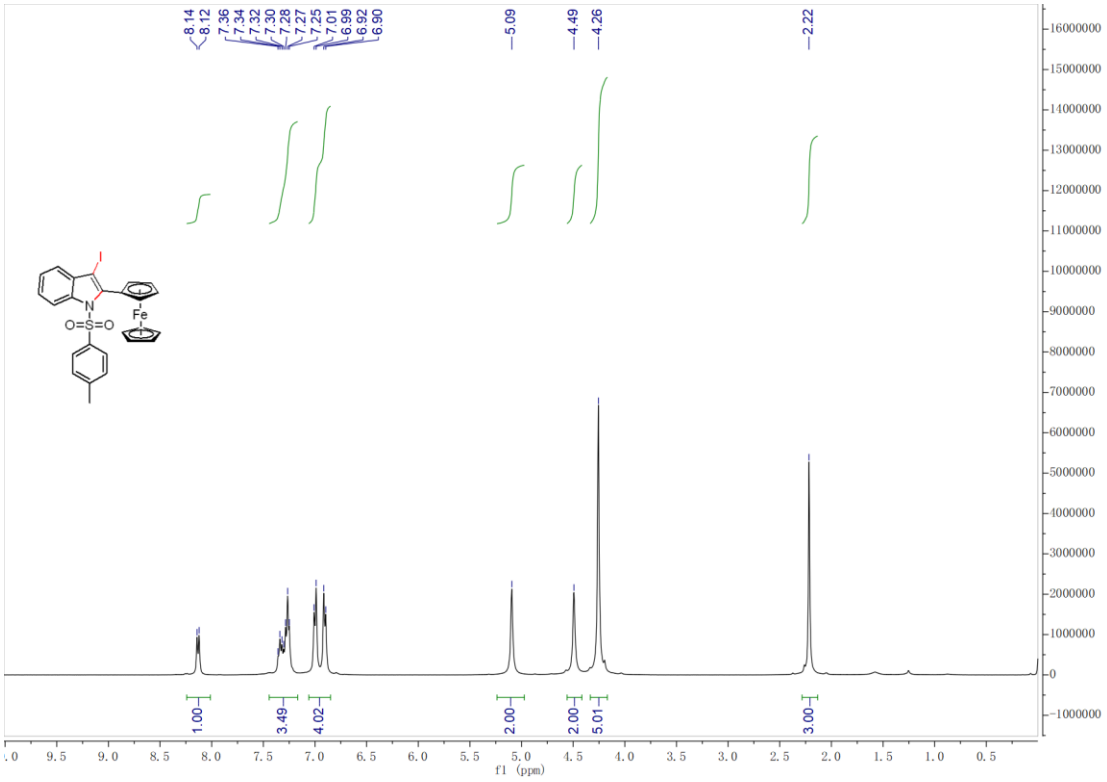

145.21
137.28
135.20
134.07
132.36
131.92
131.44
129.69
129.00
127.09
126.63
126.60
124.73
122.49
115.97
78.89
77.48
77.16
76.84
21.75
f1 (ppm)

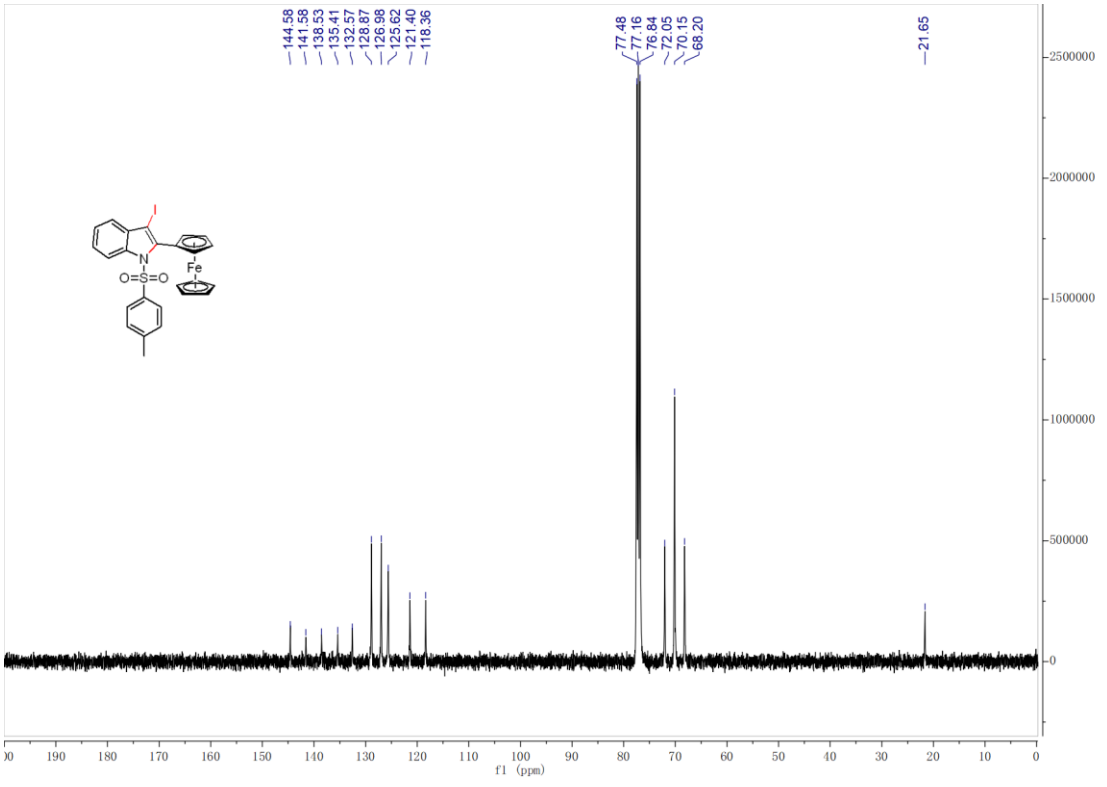
13b, $^{1}H + ^{13}C$


8.34
8.34
8.33
8.31
8.31
8.29
8.29
8.10
8.08
8.07
7.50
7.49
7.48
7.47
7.46
7.45
7.40
7.38
7.37
7.36
7.35
7.26
7.18
7.17
7.15
7.14
7.08
7.06
2.29
2.01
1.00
0.99
2.04
3.08
1.03
2.00
3.07
f1 (ppm)

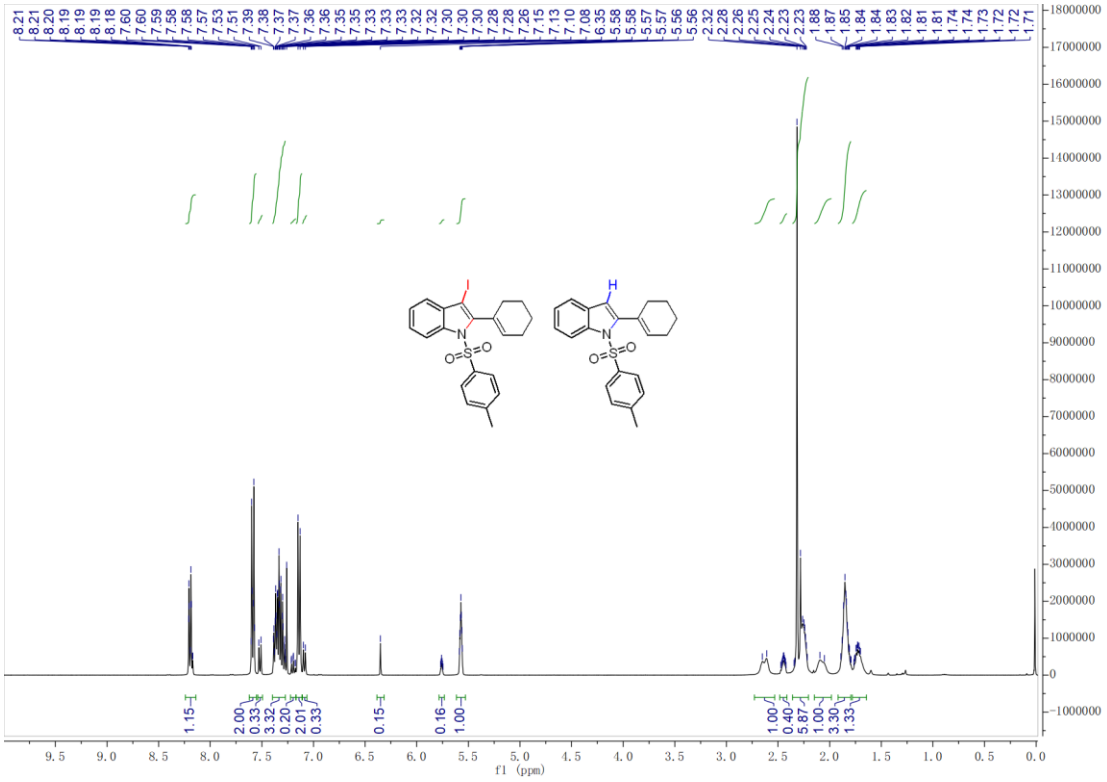

145.31
143.38
140.10
137.32
136.94
135.01
131.90
129.75
128.22
127.04
126.92
125.81
124.66
122.76
119.73
118.20
115.67
79.97
77.48
77.16
76.84
21.68
f1 (ppm)

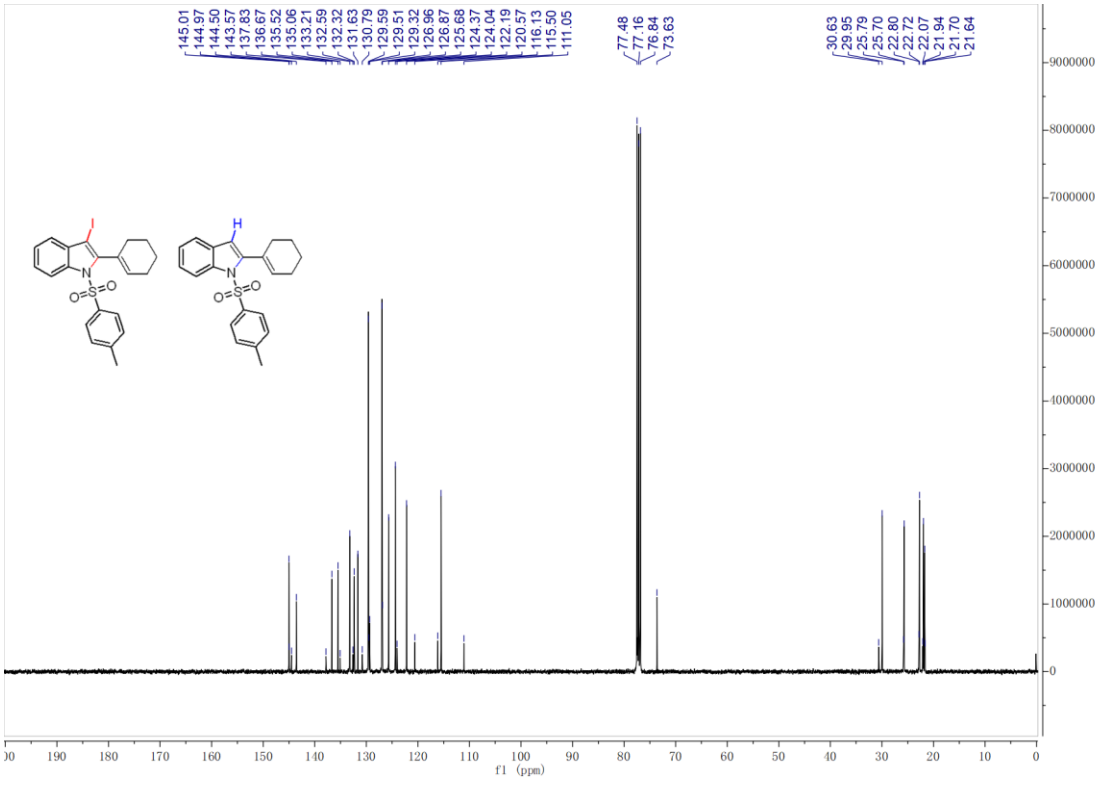
14b, $^{1}H + {}^{13}C$


8.14
8.12
7.36
7.34
7.32
7.30
7.28
7.27
7.25
7.01
6.99
6.92
6.90
5.09
4.49
4.26
2.22
1.00
3.49
4.02
2.00
2.00
5.01
3.00
f1 (ppm)

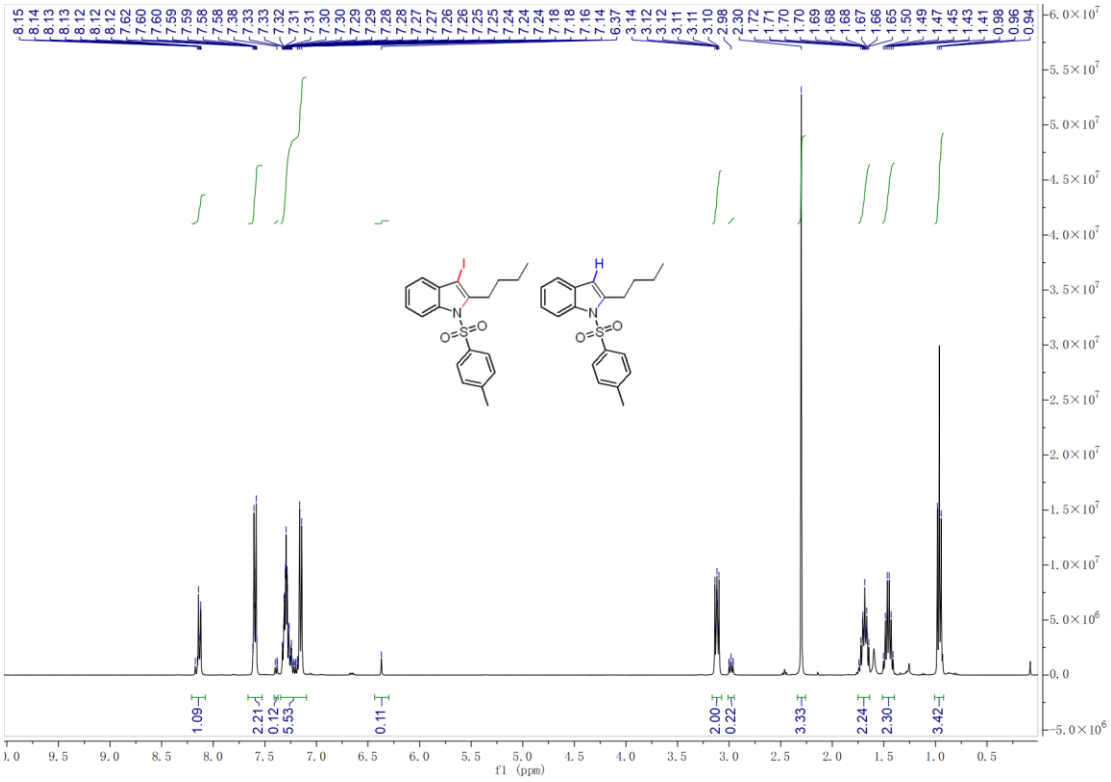

144.58
141.58
138.53
135.41
132.57
128.87
126.98
125.62
121.40
118.36
77.48
77.16
76.84
72.05
70.15
68.20
21.65
f1 (ppm)

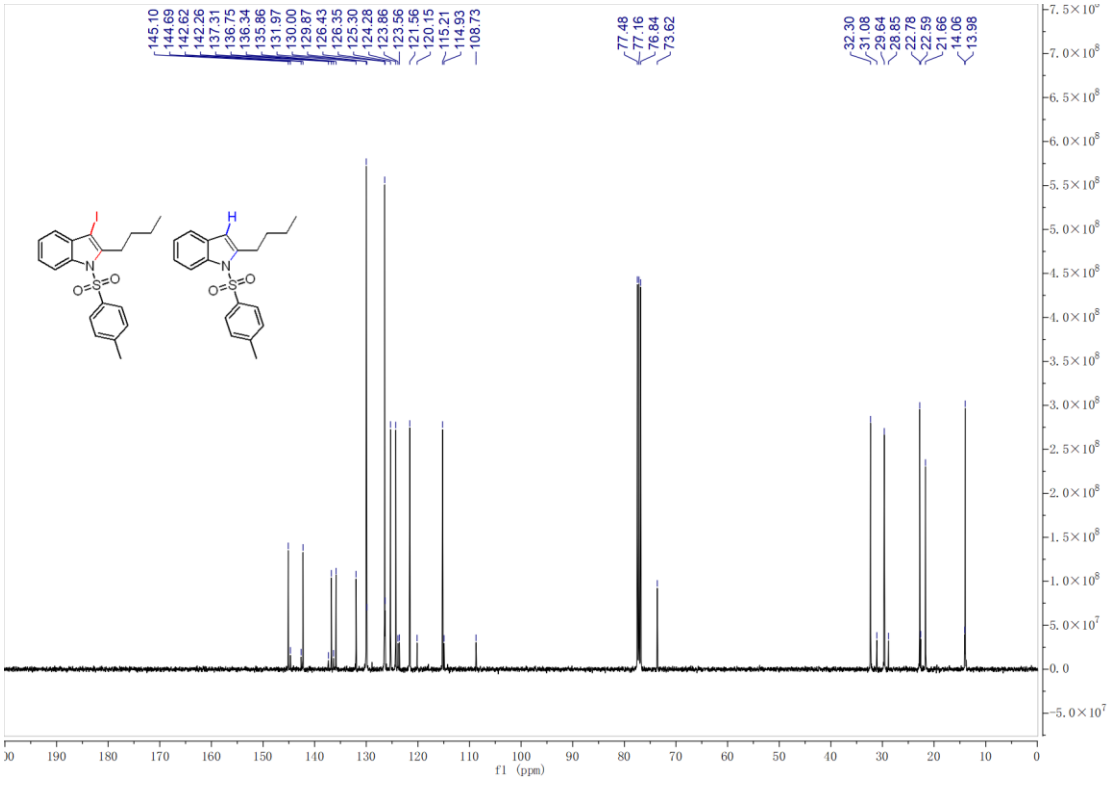
15b & 15c (6.25:1), $^{1}H + {}^{13}C$



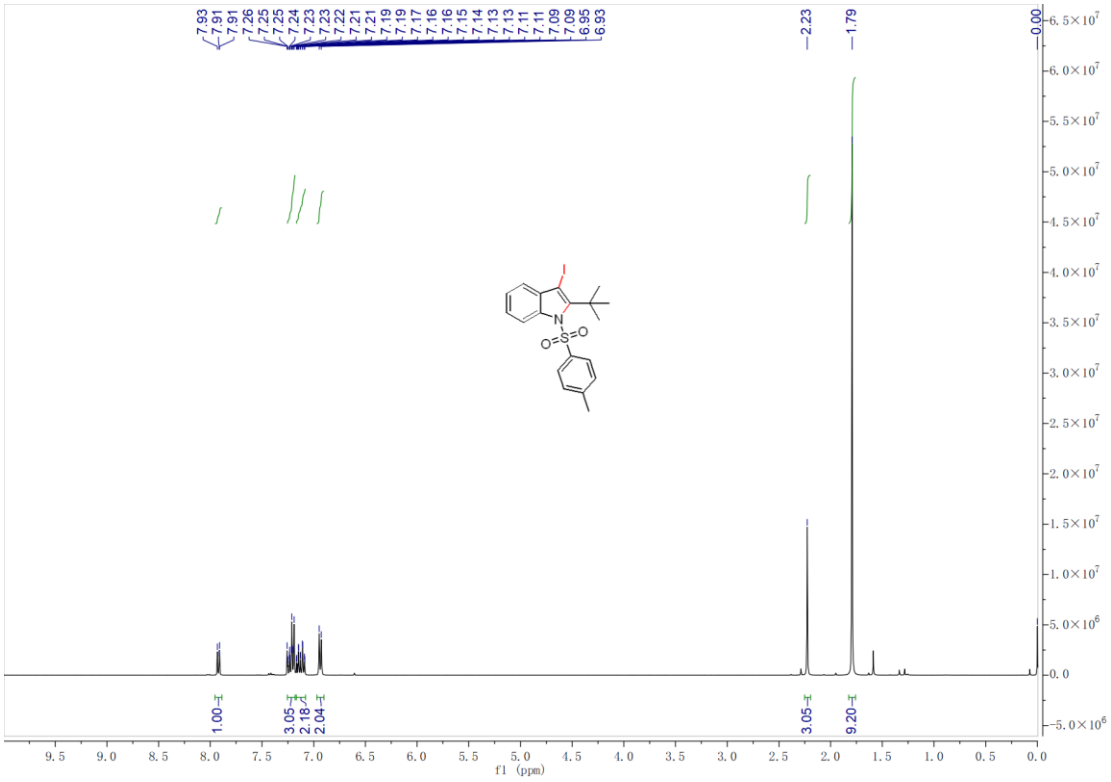


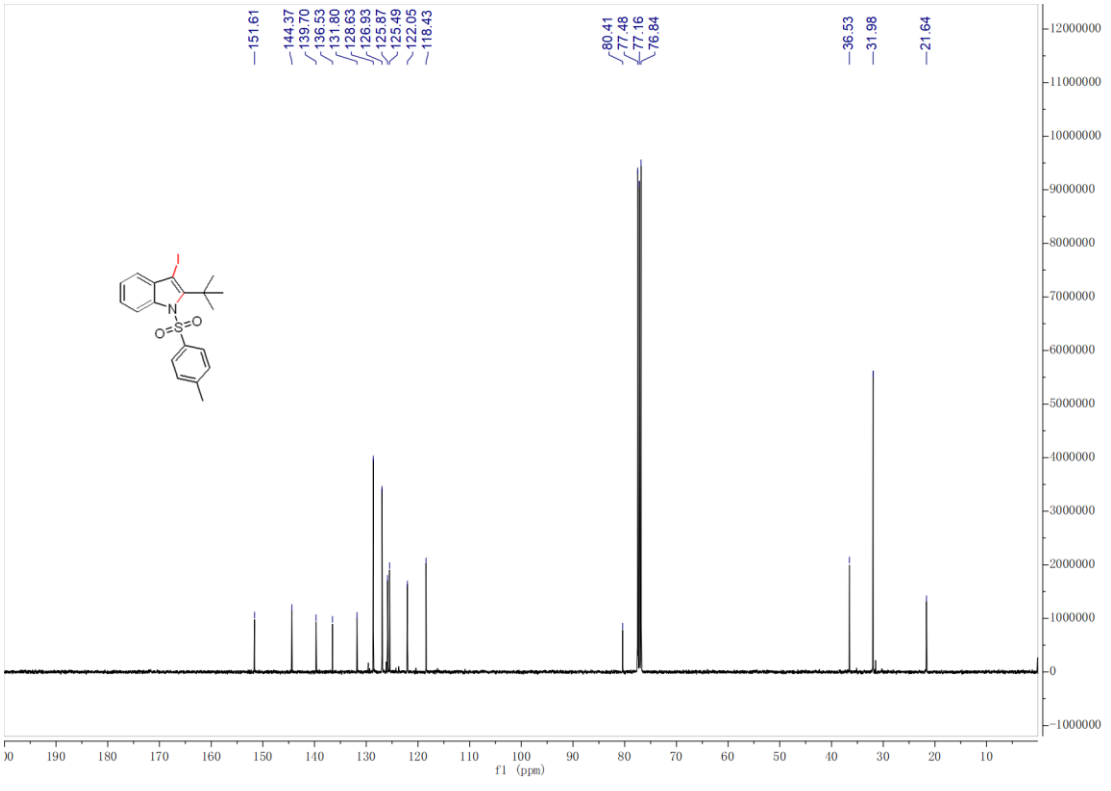
16b & 16c (9:1), $^{1}H + {}^{13}C$



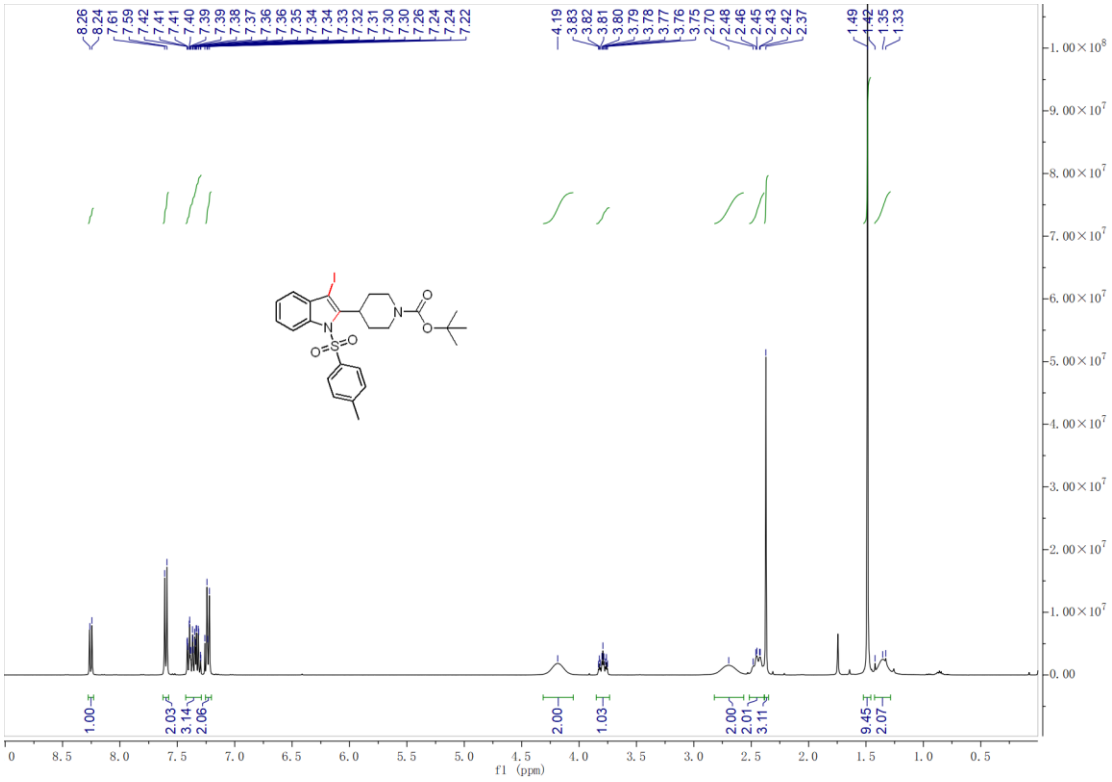


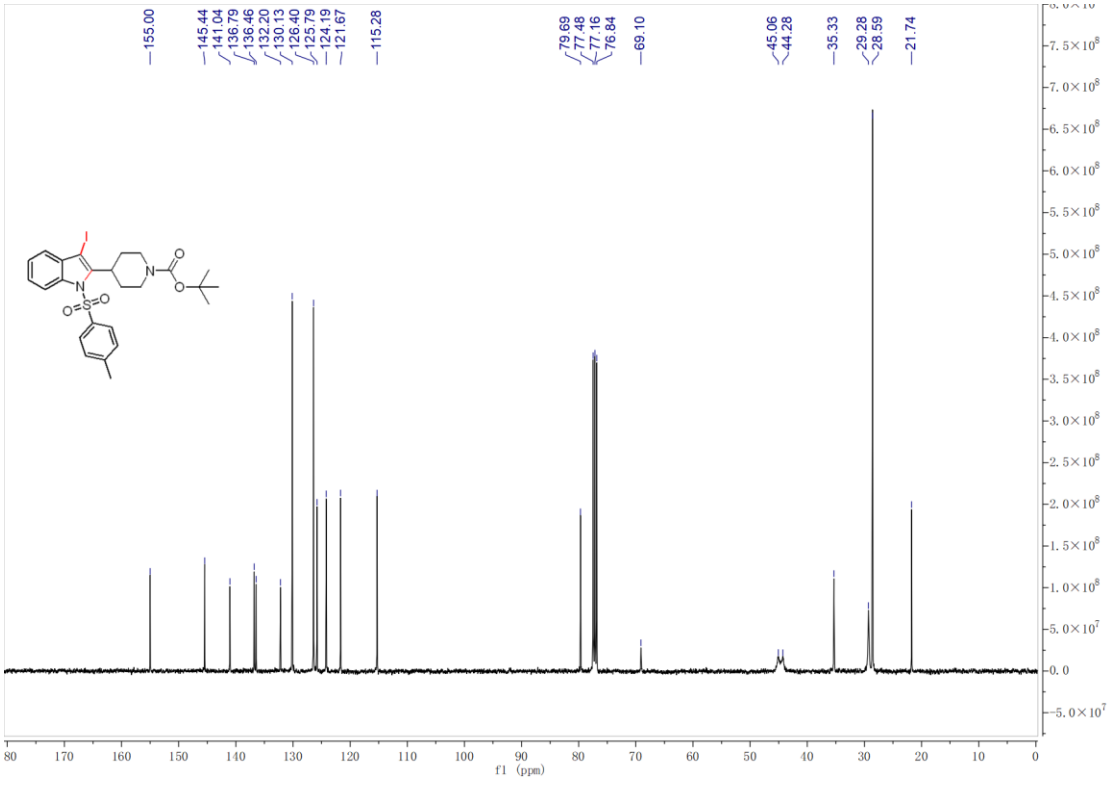
17b, $^{1}H + ^{13}C$


7.93
7.91
7.91
7.26
7.25
7.25
7.24
7.23
7.23
7.22
7.21
7.21
7.19
7.19
7.17
7.16
7.16
7.15
7.14
7.13
7.13
7.11
7.11
7.09
7.09
6.95
6.93
2.23
1.79
0.00
1.00
3.05
2.18
2.04
3.05
9.20
f1 (ppm)

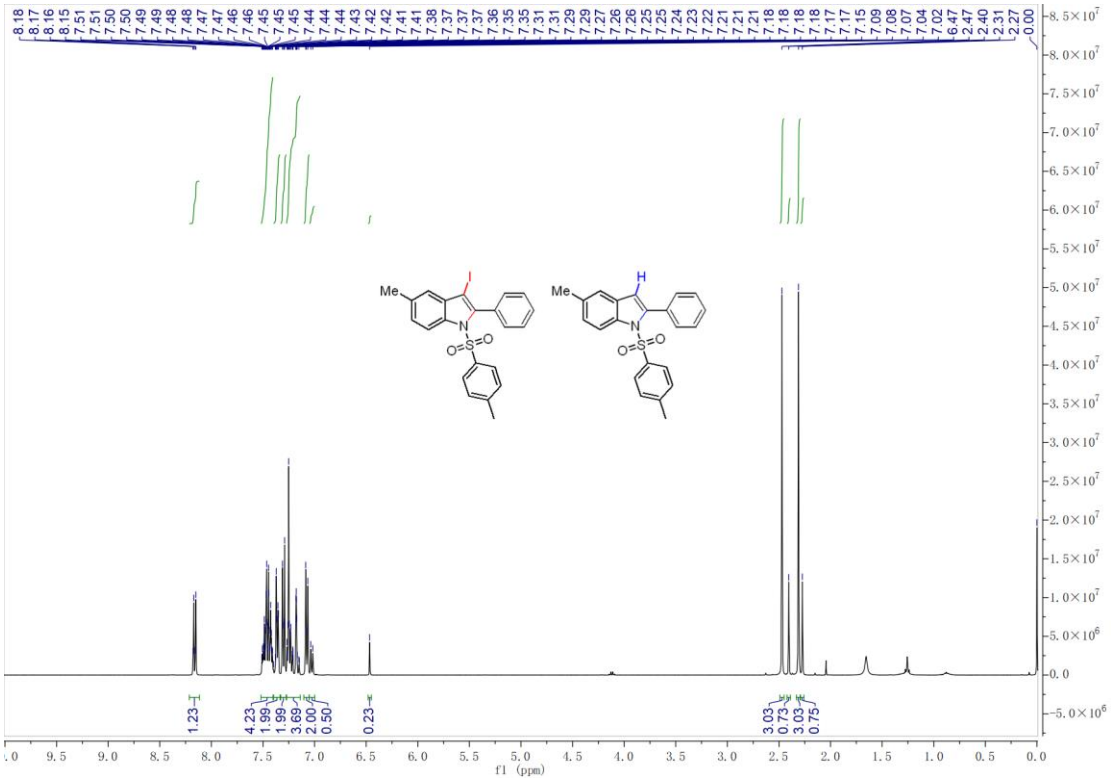

151.61
144.37
139.70
136.53
131.80
128.63
126.93
125.87
125.49
122.05
118.43
80.41
77.48
77.16
76.84
36.53
31.98
21.64
f1 (ppm)

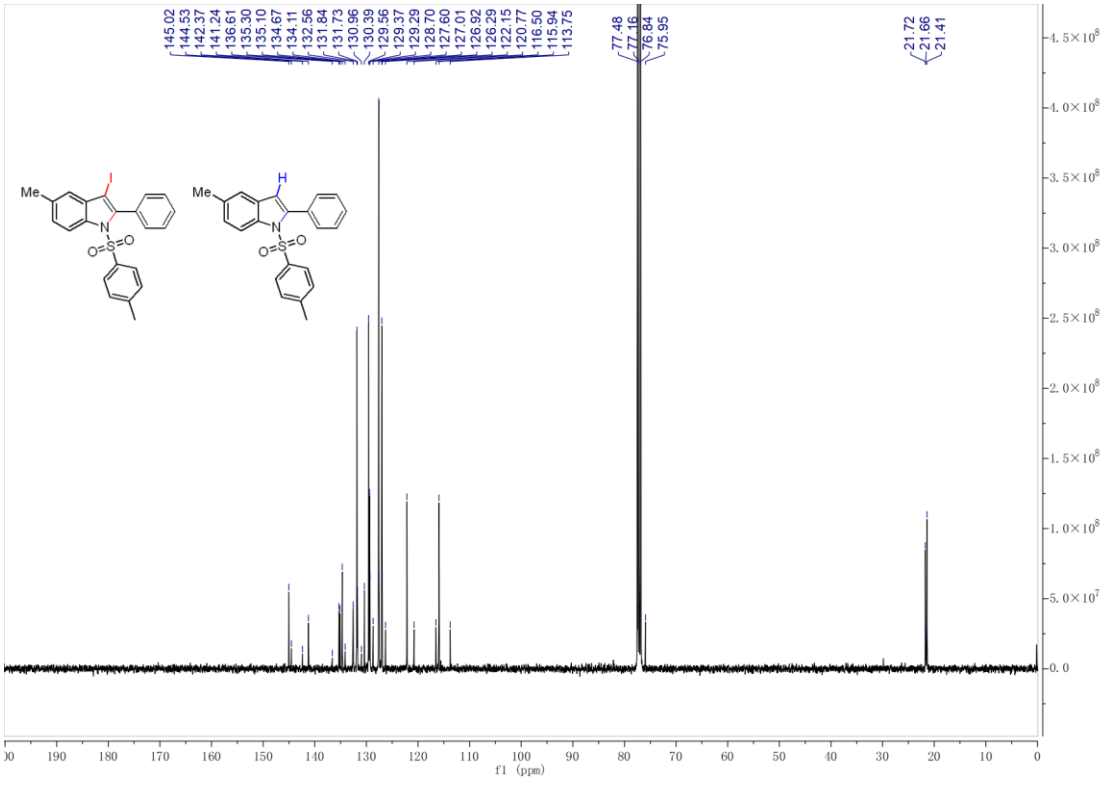
18b, $^{1}H + {}^{13}C$


8.26
8.24
7.61
7.59
7.42
7.41
7.41
7.40
7.39
7.39
7.38
7.37
7.36
7.36
7.35
7.34
7.34
7.33
7.32
7.31
7.30
7.30
7.26
7.24
7.24
7.22
4.19
3.83
3.82
3.81
3.80
3.79
3.78
3.77
3.76
3.75
2.70
2.48
2.46
2.45
2.43
2.42
2.37
1.49
1.42
1.35
1.33
1.00
2.03
3.14
2.06
2.00
1.03
2.00
2.01
3.11
9.45
2.07
f1 (ppm)

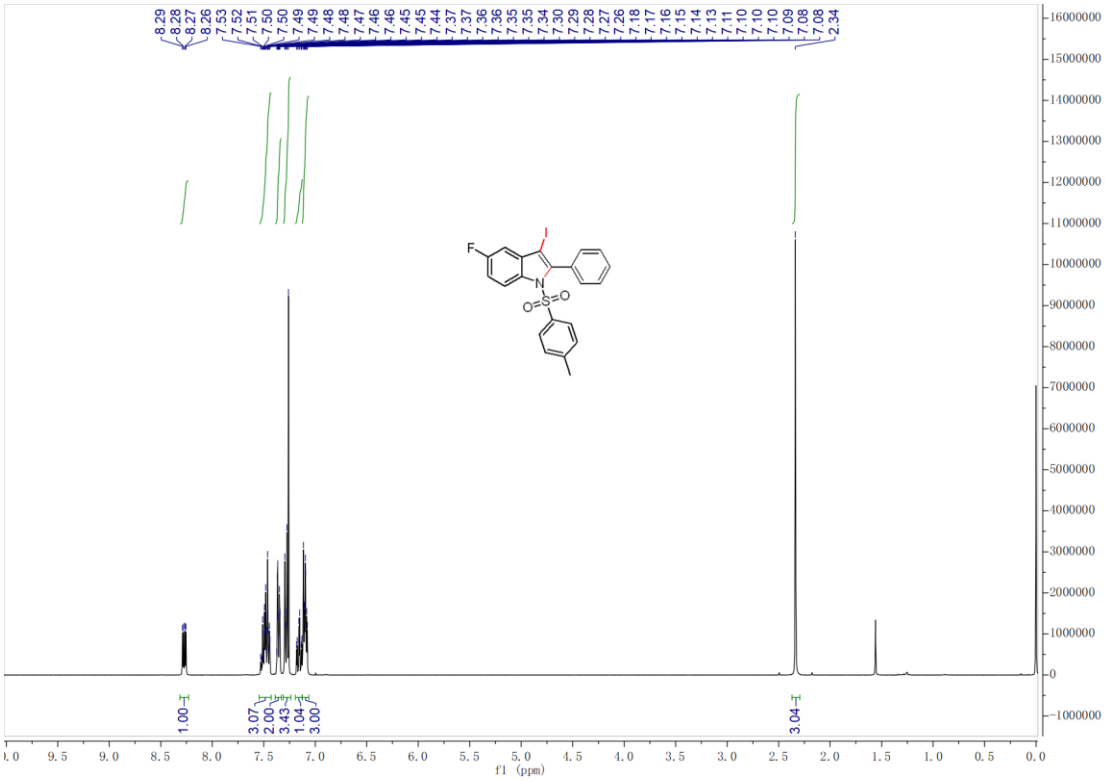

155.00
145.44
141.04
136.79
136.46
132.20
130.13
126.40
125.79
124.19
121.67
115.28
79.69
77.48
77.16
76.84
69.10
45.06
44.28
35.33
29.28
28.59
21.74
f1 (ppm)

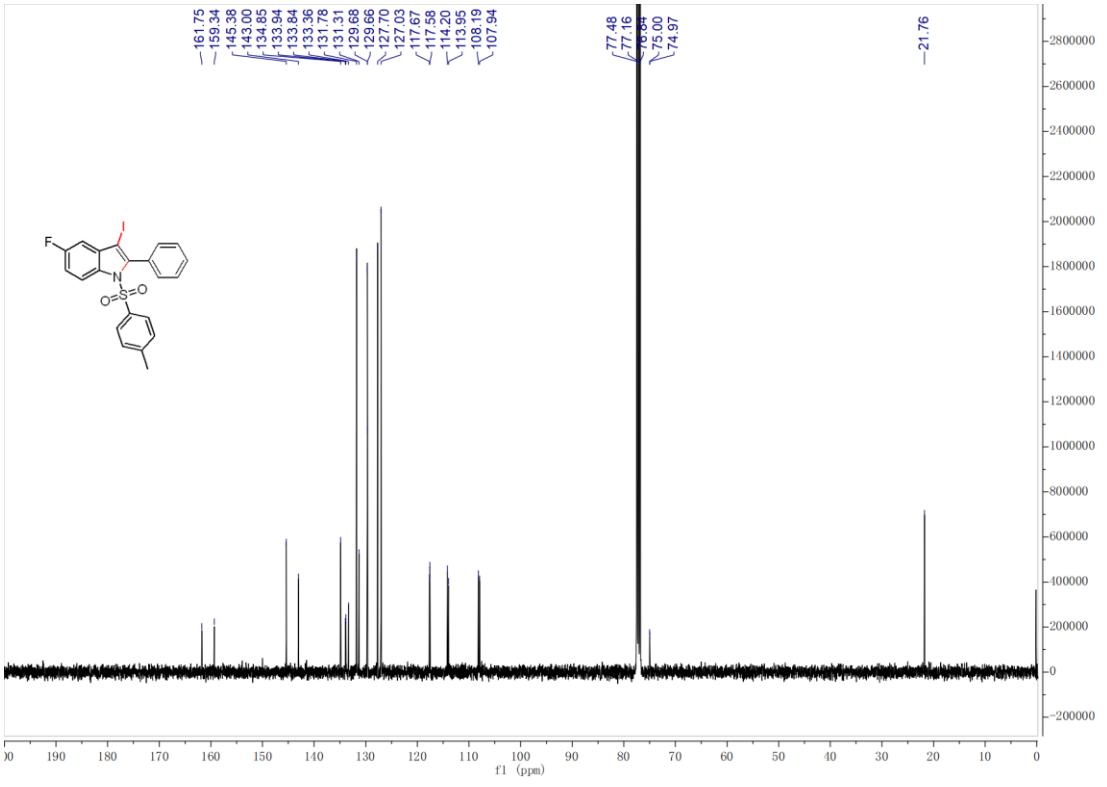
20b & 20c (4:1), $^{1}H + {}^{13}C$



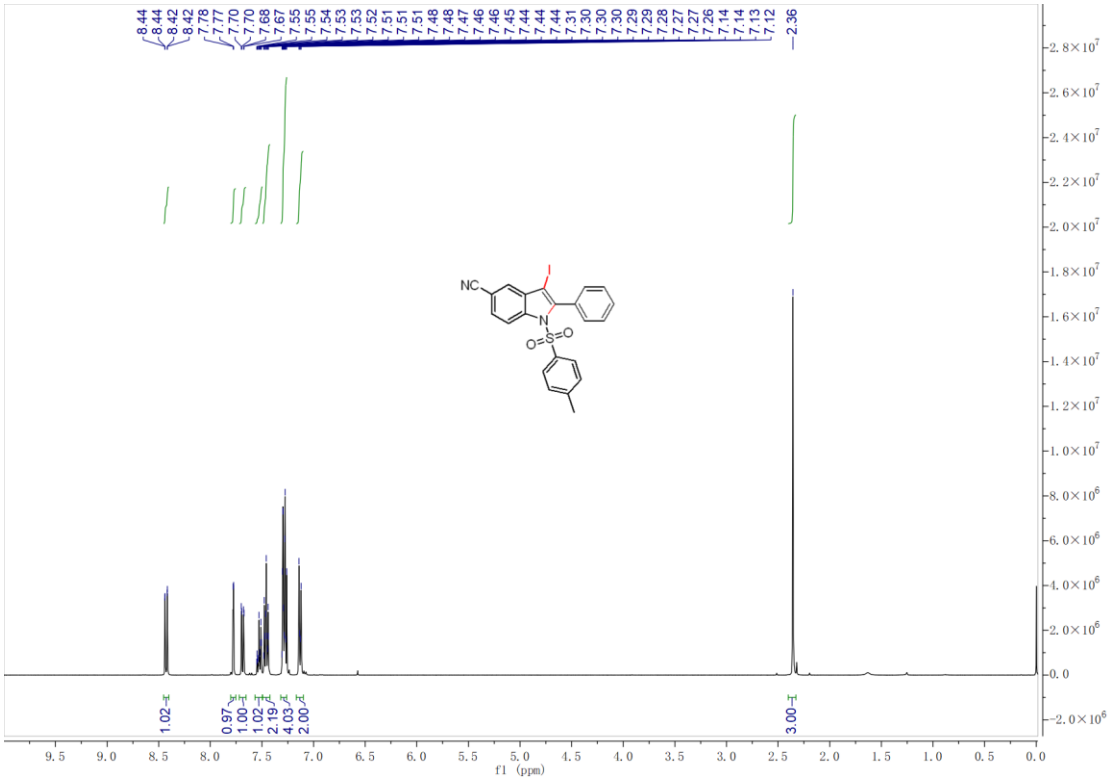


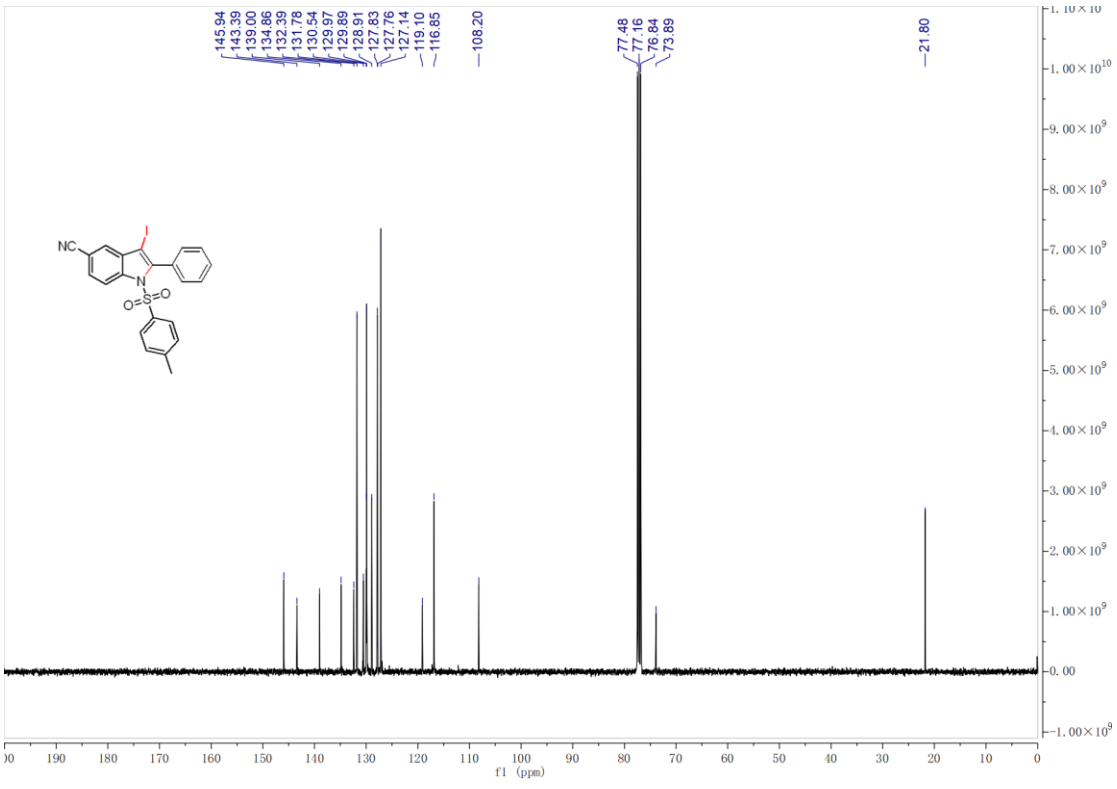
21b, $^{1}H + ^{13}C$


8.29
8.28
8.27
8.26
7.53
7.52
7.51
7.50
7.50
7.49
7.49
7.48
7.48
7.47
7.46
7.46
7.45
7.45
7.44
7.37
7.36
7.36
7.35
7.34
7.30
7.29
7.28
7.27
7.26
7.18
7.17
7.16
7.15
7.14
7.13
7.11
7.10
7.10
7.10
7.09
7.08
7.08
2.34
1.00
3.07
2.00
3.43
1.04
3.00
3.04
f1 (ppm)

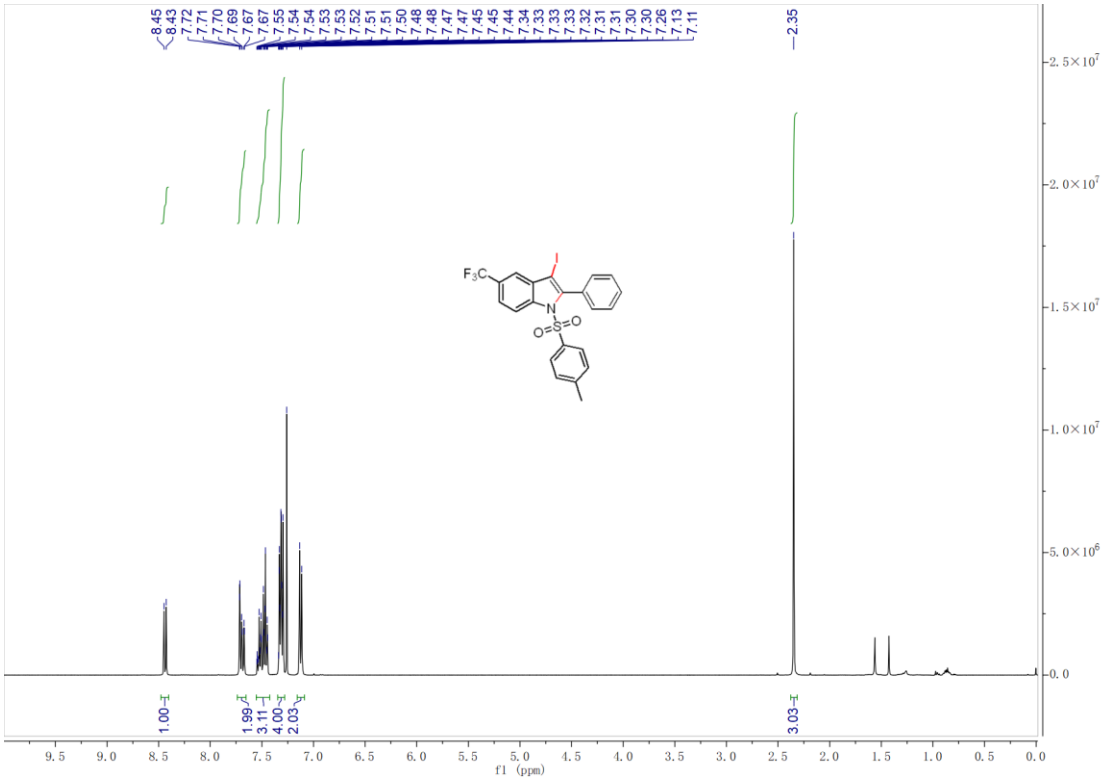

161.75
159.34
145.38
143.00
134.85
133.94
133.84
133.36
131.78
131.31
129.68
129.66
127.70
127.03
117.67
117.58
114.20
113.95
108.19
107.94
77.48
77.16
76.84
75.00
74.97
21.76
f1 (ppm)

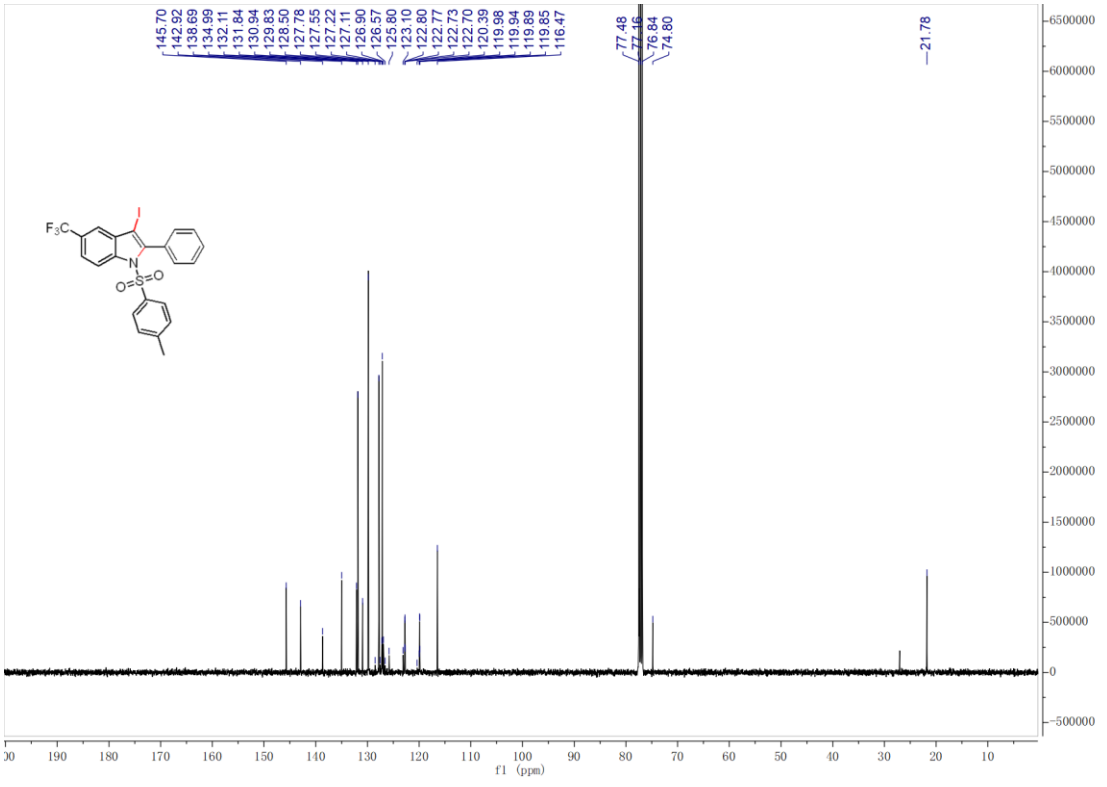
22b, $^{1}H + ^{13}C$

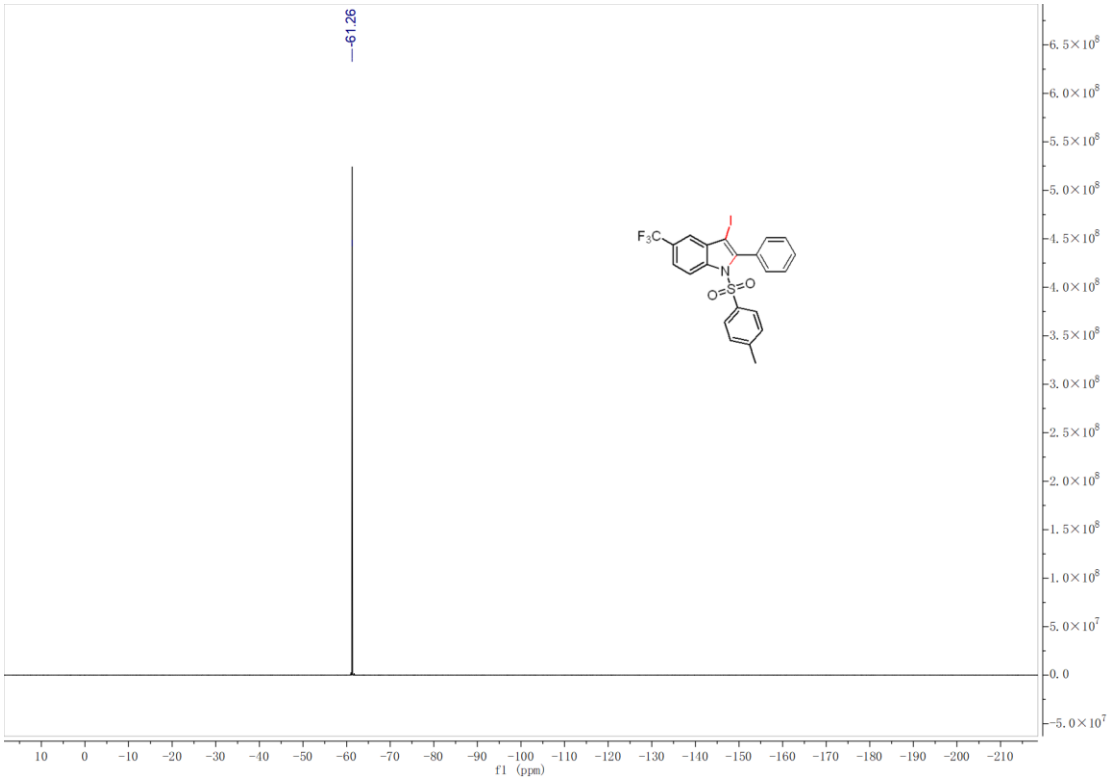

8.44
8.44
8.42
8.42
7.78
7.77
7.70
7.70
7.68
7.67
7.55
7.55
7.54
7.53
7.53
7.52
7.51
7.51
7.51
7.48
7.47
7.46
7.46
7.45
7.44
7.44
7.44
7.31
7.30
7.30
7.30
7.29
7.29
7.28
7.27
7.27
7.26
7.14
7.14
7.13
7.12
2.36
NC
O=S=O
1.02
0.97
1.00
1.02
2.19
4.03
2.00
3.00
f1 (ppm)


145.94
143.39
139.00
134.86
132.39
131.78
130.54
129.97
129.89
128.91
127.83
127.76
127.14
119.10
116.85
108.20
77.48
77.16
76.84
73.89
21.80
NC
O=S=O
f1 (ppm)

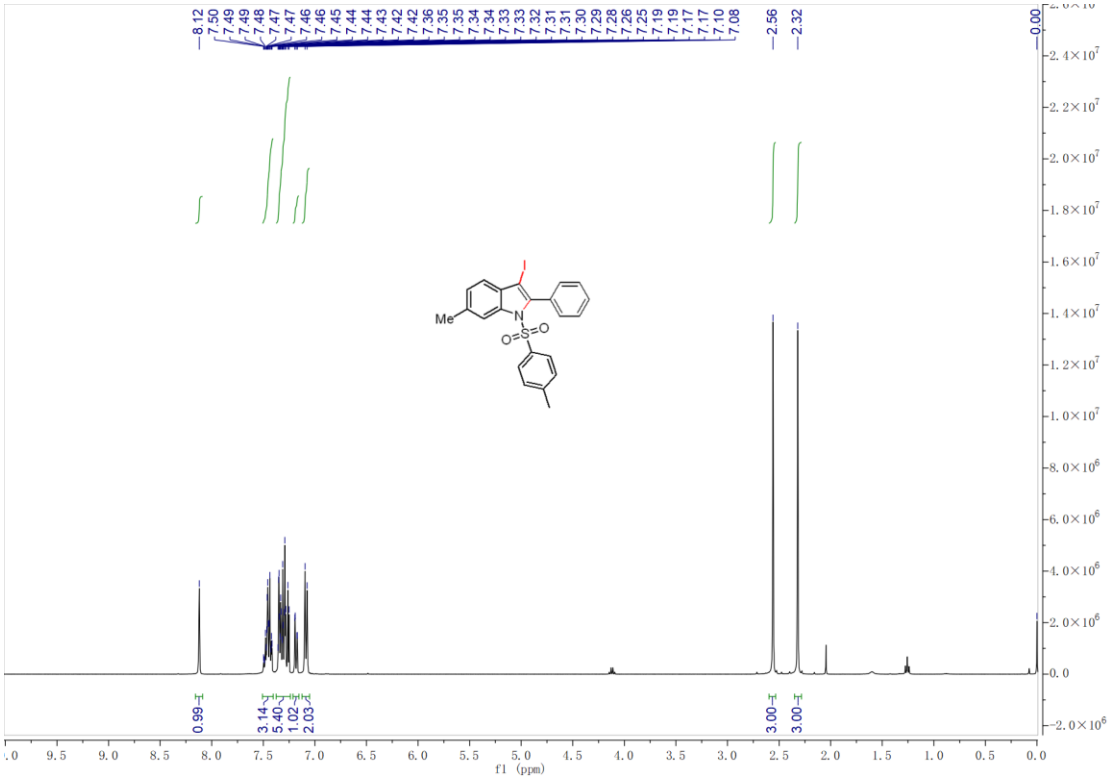
23b, $^{1}H + ^{13}C + ^{19}F$

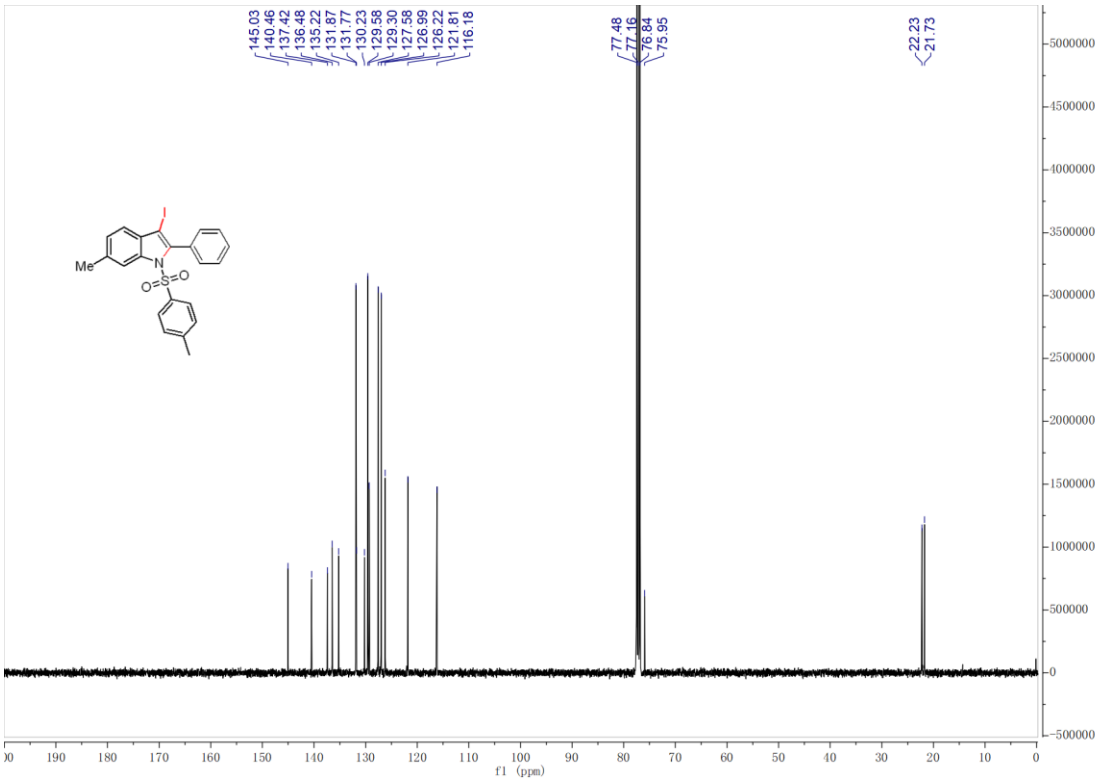




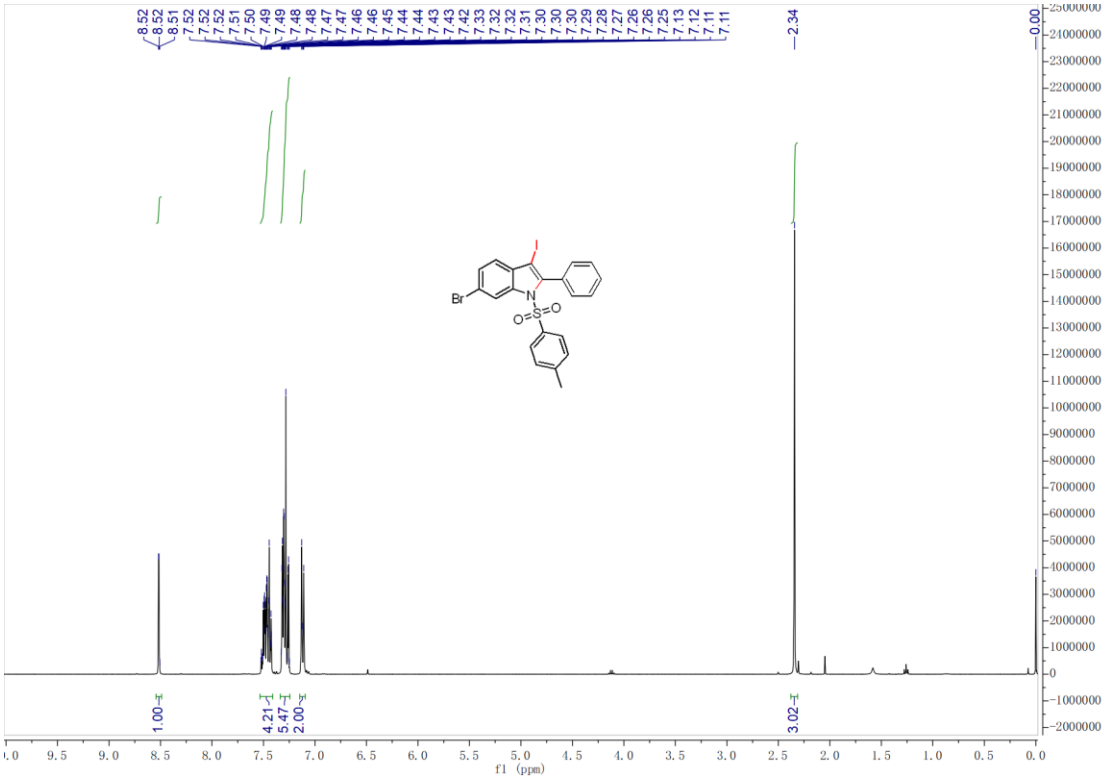

-61.26
F3C
I
N
O=S=O
f1 (ppm)

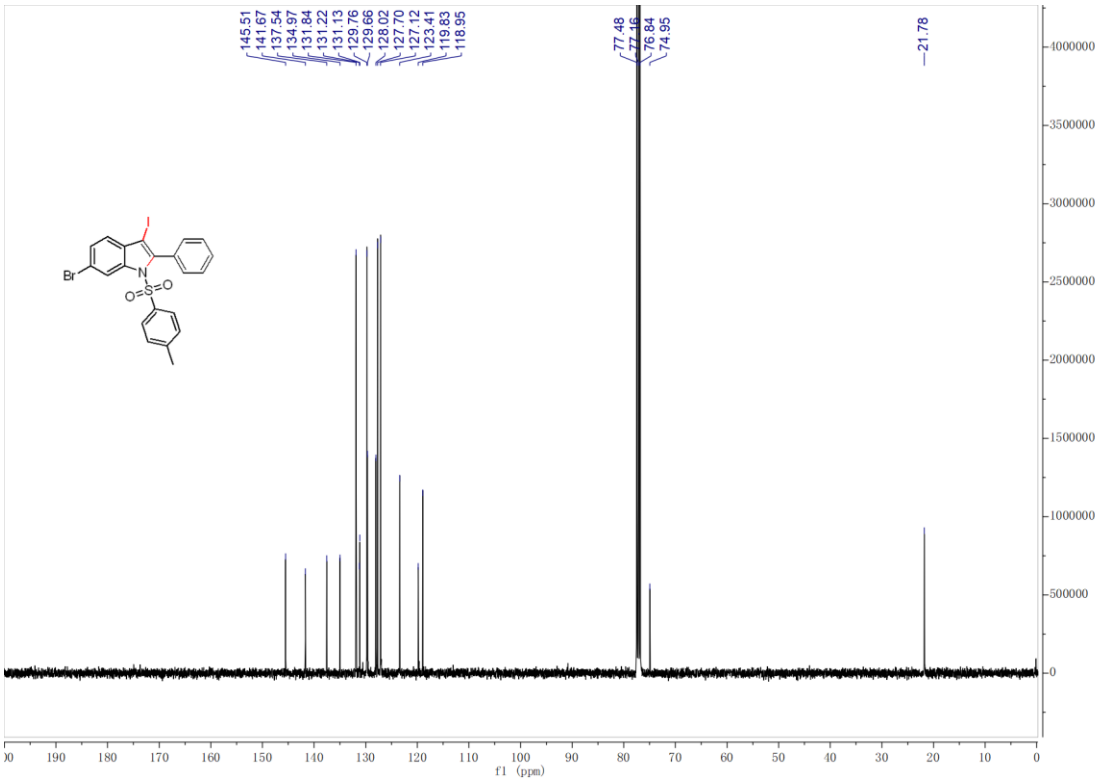
24b, $^{1}H + ^{13}C$


8.12
7.50
7.49
7.49
7.48
7.47
7.47
7.46
7.46
7.45
7.44
7.44
7.43
7.42
7.42
7.36
7.35
7.35
7.34
7.34
7.33
7.33
7.32
7.31
7.31
7.30
7.29
7.28
7.26
7.25
7.19
7.19
7.17
7.17
7.10
7.08
2.56
2.32
0.00
Me
I
N
O=S=O
0.99
3.14
5.40
1.02
2.03
3.00
3.00
f1 (ppm)

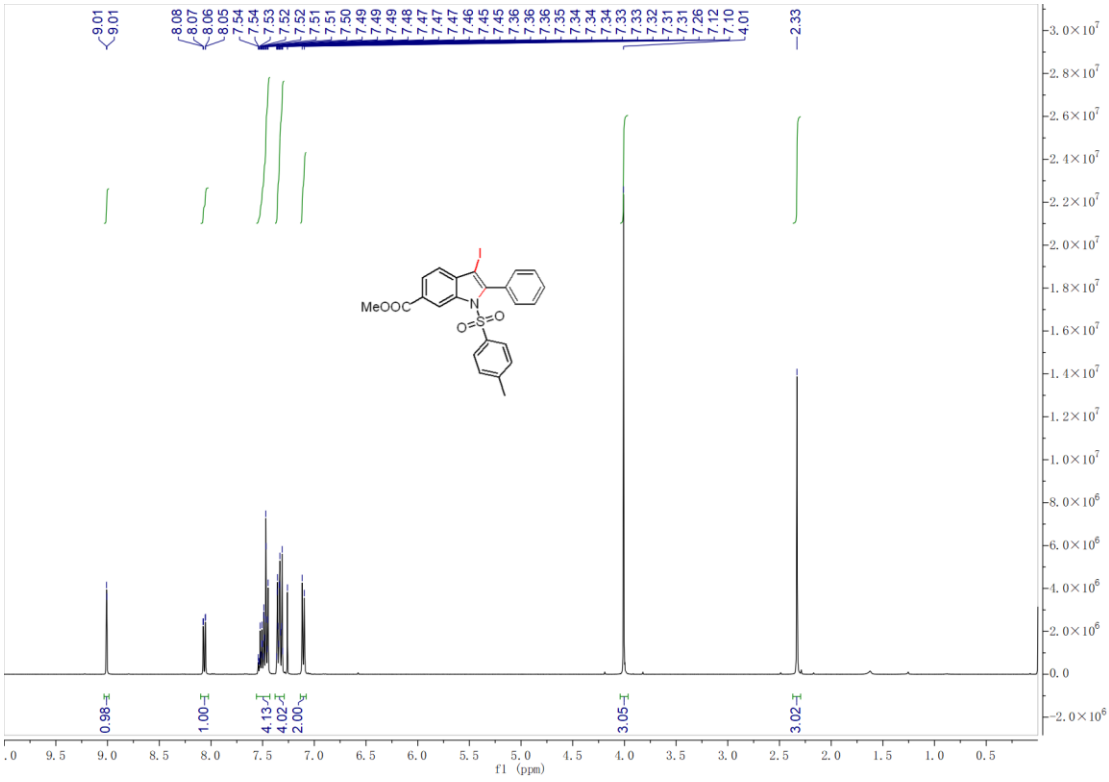

145.03
140.46
137.42
136.48
135.22
131.87
131.77
130.23
129.58
129.30
127.58
126.99
126.22
121.81
116.18
77.48
77.16
76.84
75.95
22.23
21.73
Me
I
N
O=S=O
f1 (ppm)

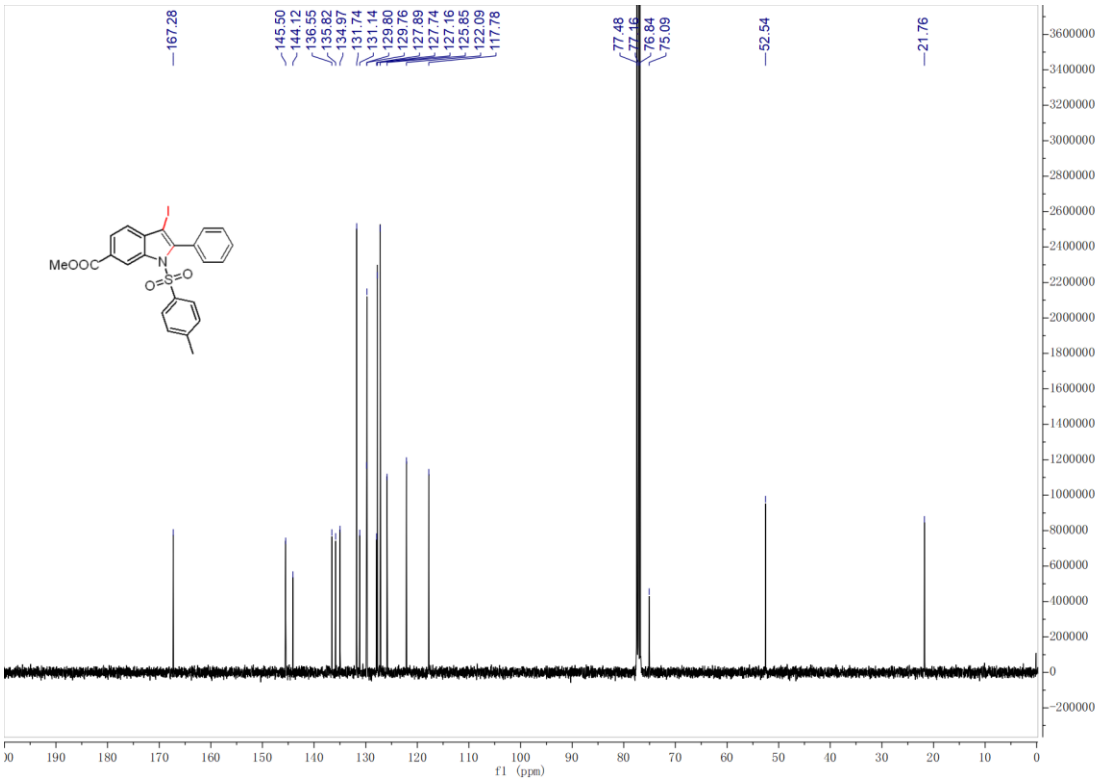
25b, $^{1}H + ^{13}C$


8.52
8.52
8.51
7.52
7.52
7.52
7.51
7.50
7.49
7.49
7.48
7.48
7.47
7.47
7.46
7.46
7.45
7.44
7.44
7.43
7.43
7.42
7.33
7.32
7.32
7.31
7.30
7.30
7.30
7.29
7.28
7.27
7.26
7.26
7.25
7.13
7.12
7.11
7.11
2.34
0.00
1.00
4.21
5.47
2.00
3.02
Br
I
N
O=S=O
f1 (ppm)

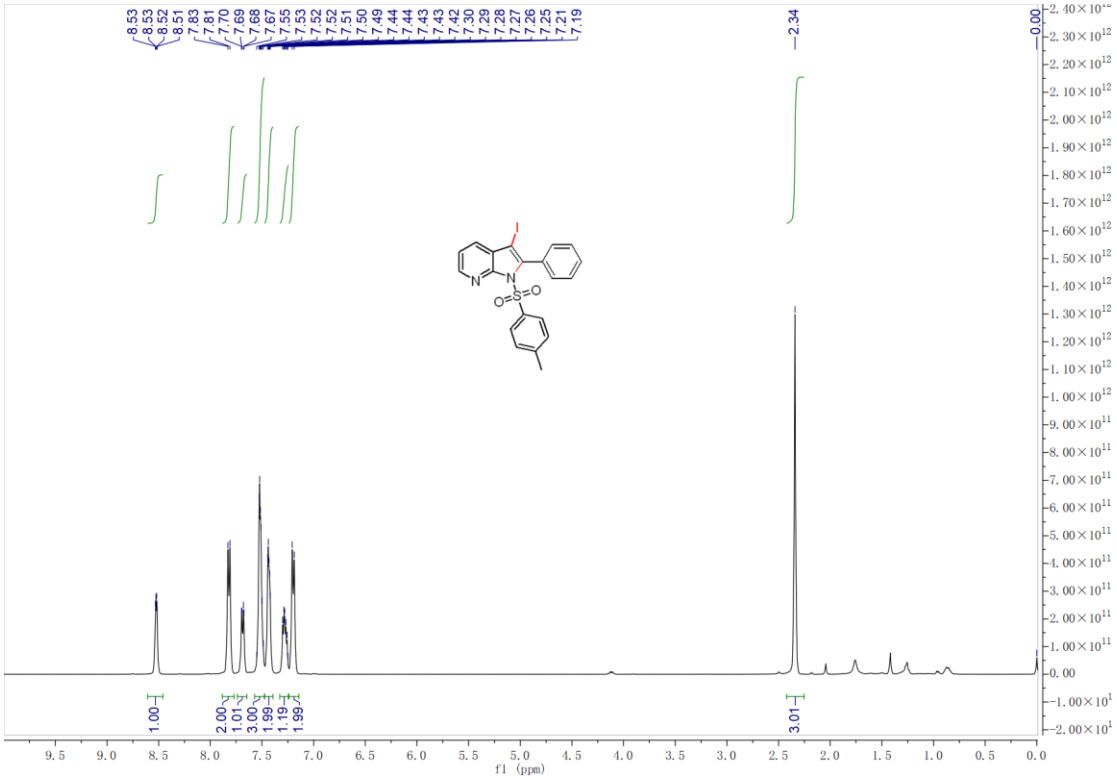

145.51
141.67
137.54
134.97
131.84
131.22
131.13
129.78
129.66
128.02
127.70
127.12
123.41
119.83
118.95
77.48
77.16
76.84
74.95
21.78
Br
N
O=S=O
f1 (ppm)

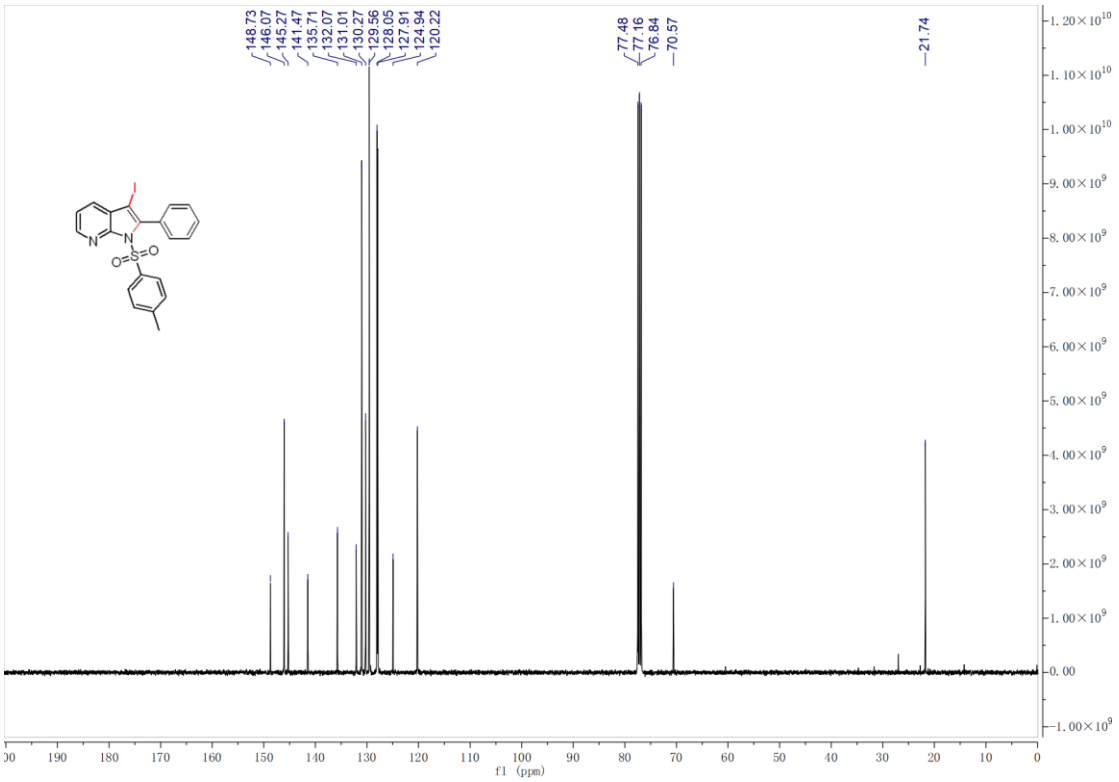
26b, $^{1}H + ^{13}C$


9.01
8.08
8.07
8.06
8.05
7.54
7.53
7.52
7.51
7.50
7.49
7.48
7.47
7.46
7.45
7.36
7.35
7.34
7.33
7.32
7.31
7.26
7.12
7.10
4.01
2.33
MeOOC
N
O=S=O
0.98
1.00
4.13
4.02
2.00
3.05
3.02
f1 (ppm)

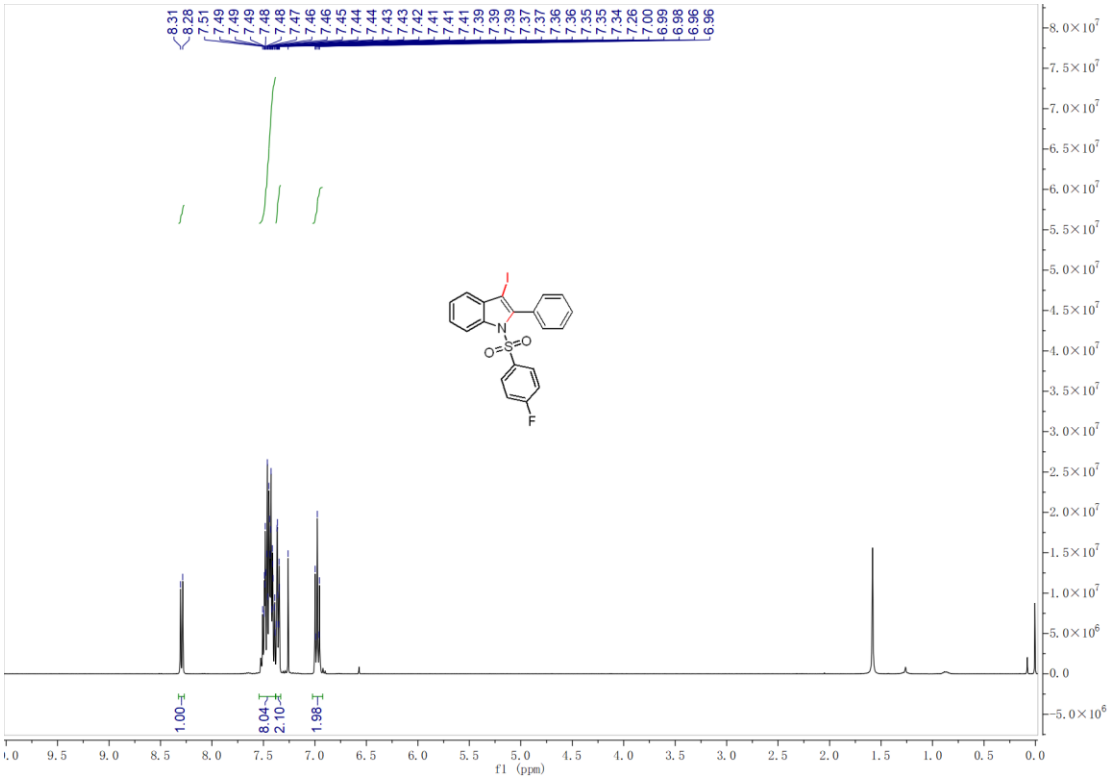

167.28
145.50
144.12
136.55
135.82
134.97
131.74
131.14
129.80
129.76
127.89
127.74
127.16
125.85
122.09
117.78
77.48
77.16
76.84
75.09
52.54
21.76
MeOOC
f1 (ppm)

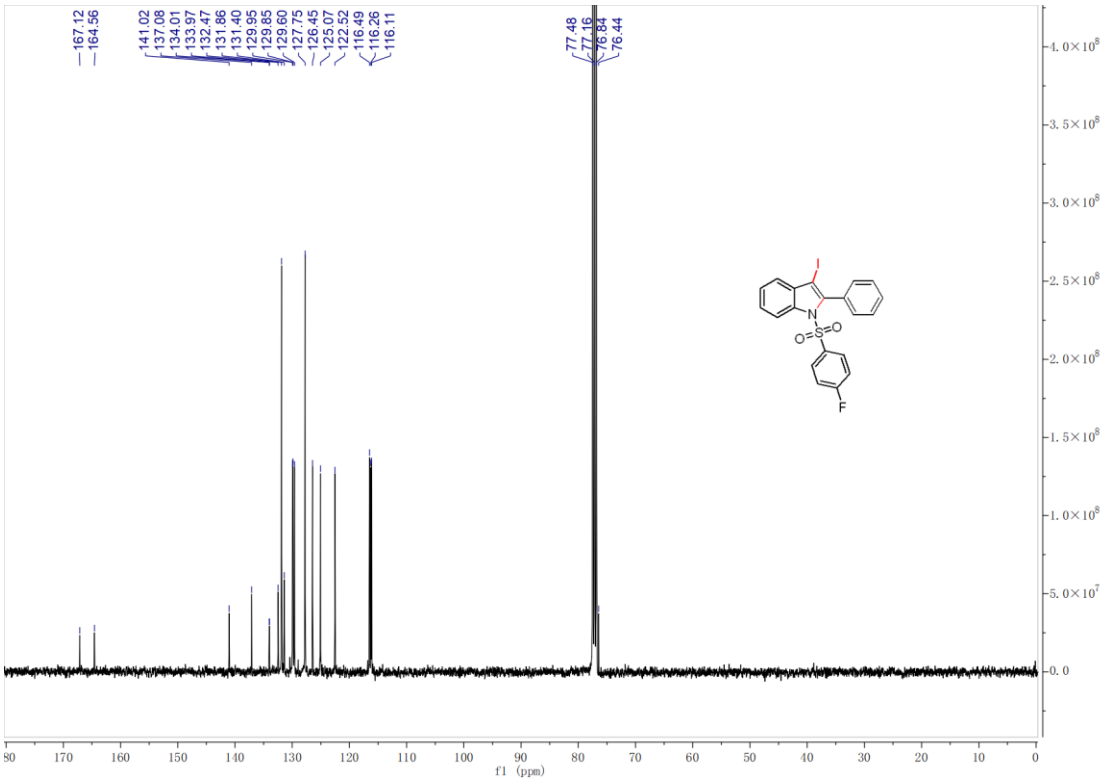
27b, $^{1}H + ^{13}C$

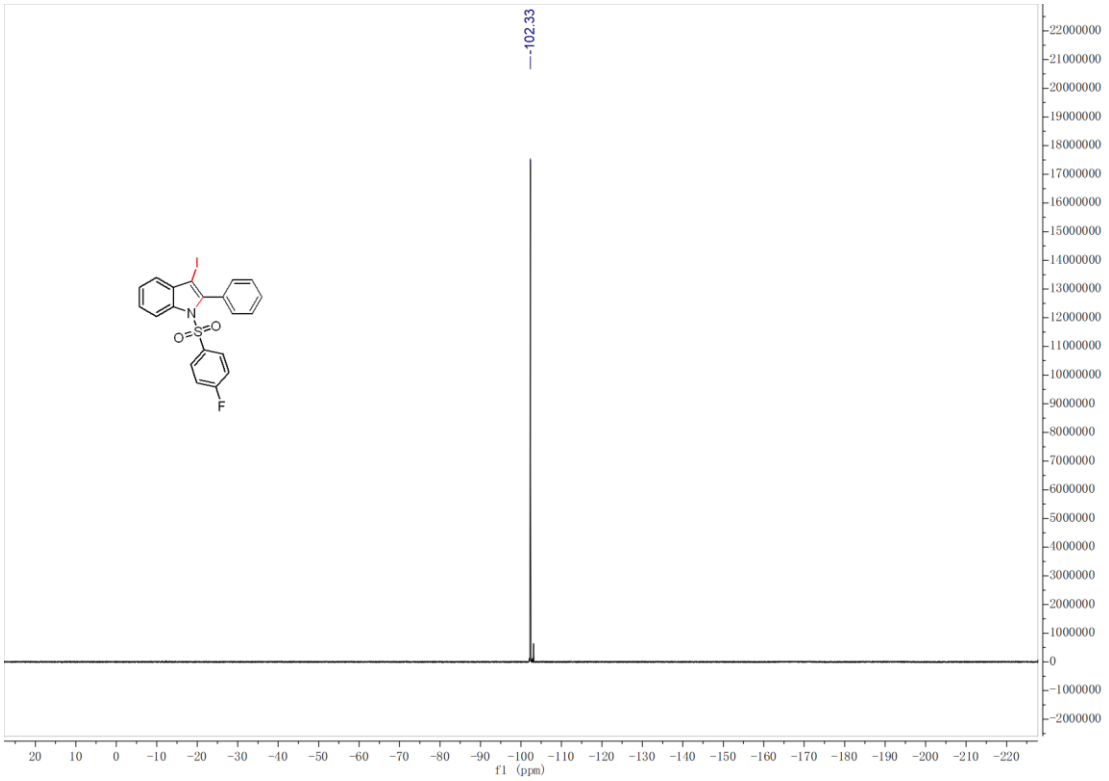

8.53
8.53
8.52
8.51
7.83
7.81
7.70
7.69
7.68
7.67
7.55
7.53
7.52
7.52
7.51
7.50
7.49
7.44
7.44
7.43
7.43
7.42
7.30
7.29
7.28
7.27
7.26
7.25
7.21
7.19
2.34
0.00
1.00
2.00
1.01
3.00
1.99
1.19
1.99
3.01
f1 (ppm)



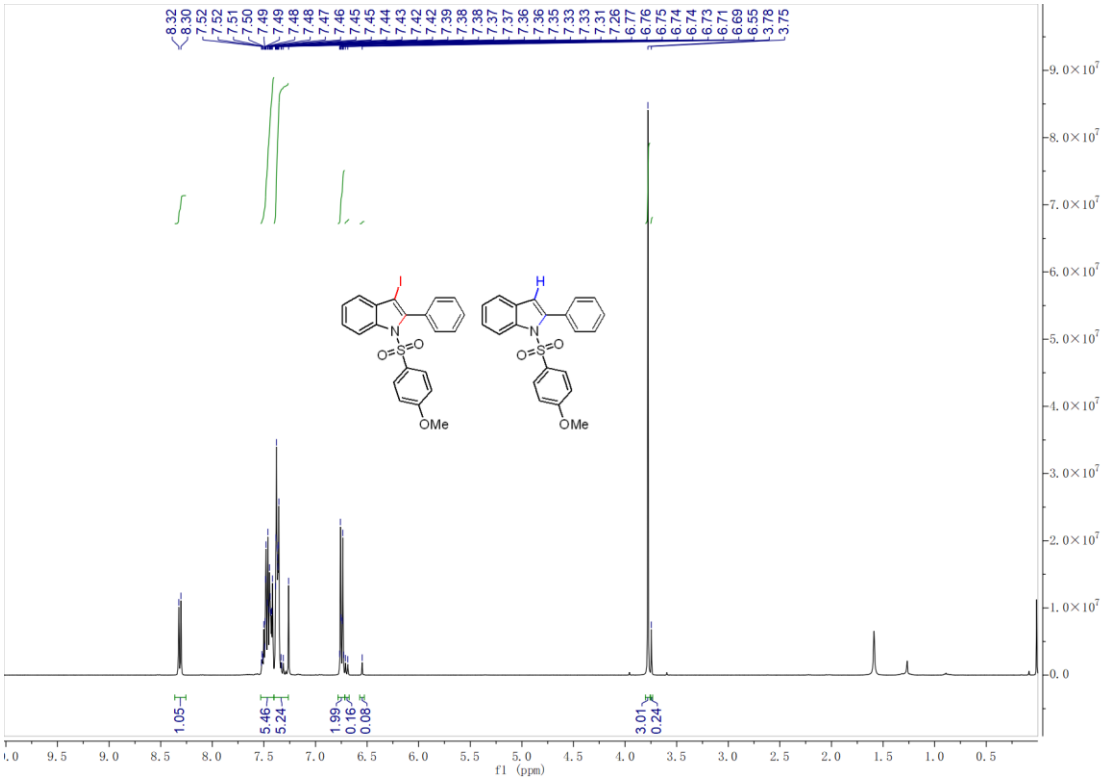
28b, $^{1}H + ^{13}C + ^{19}F$

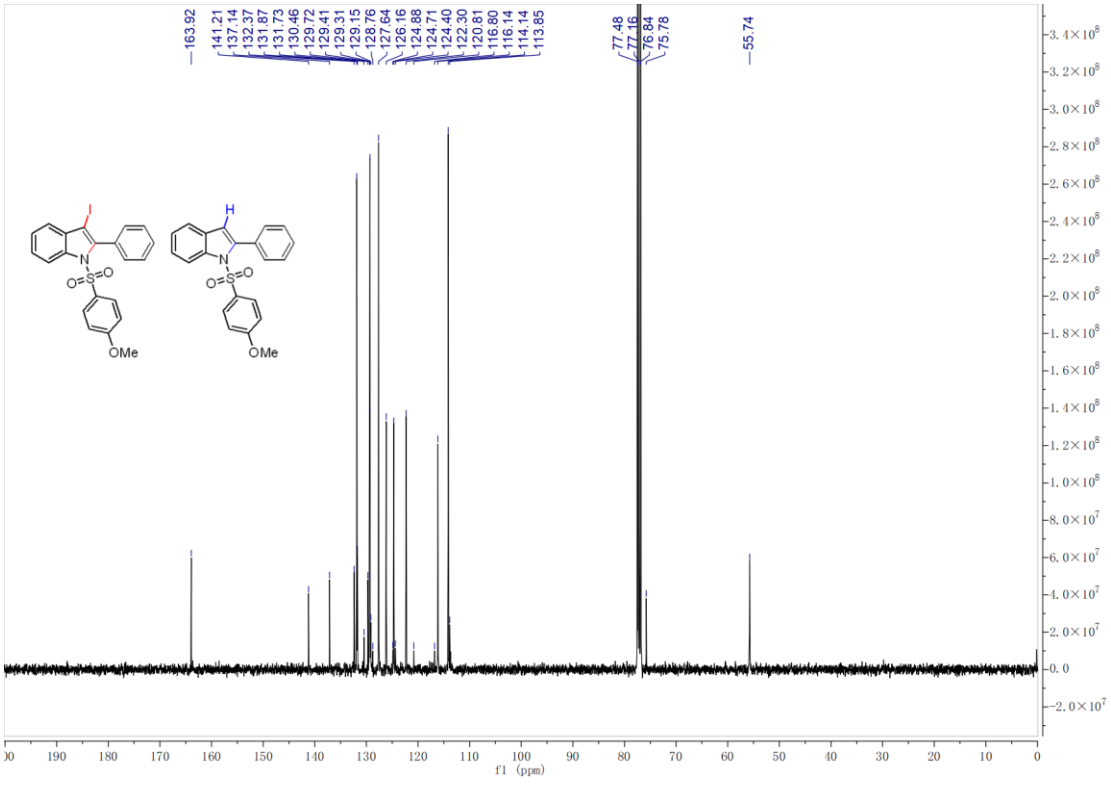



167.12
164.56
141.02
137.08
134.01
133.97
132.47
131.86
131.40
129.95
129.85
129.60
127.75
126.45
125.07
122.52
116.49
116.26
116.11
77.48
77.16
76.84
76.44
f1 (ppm)

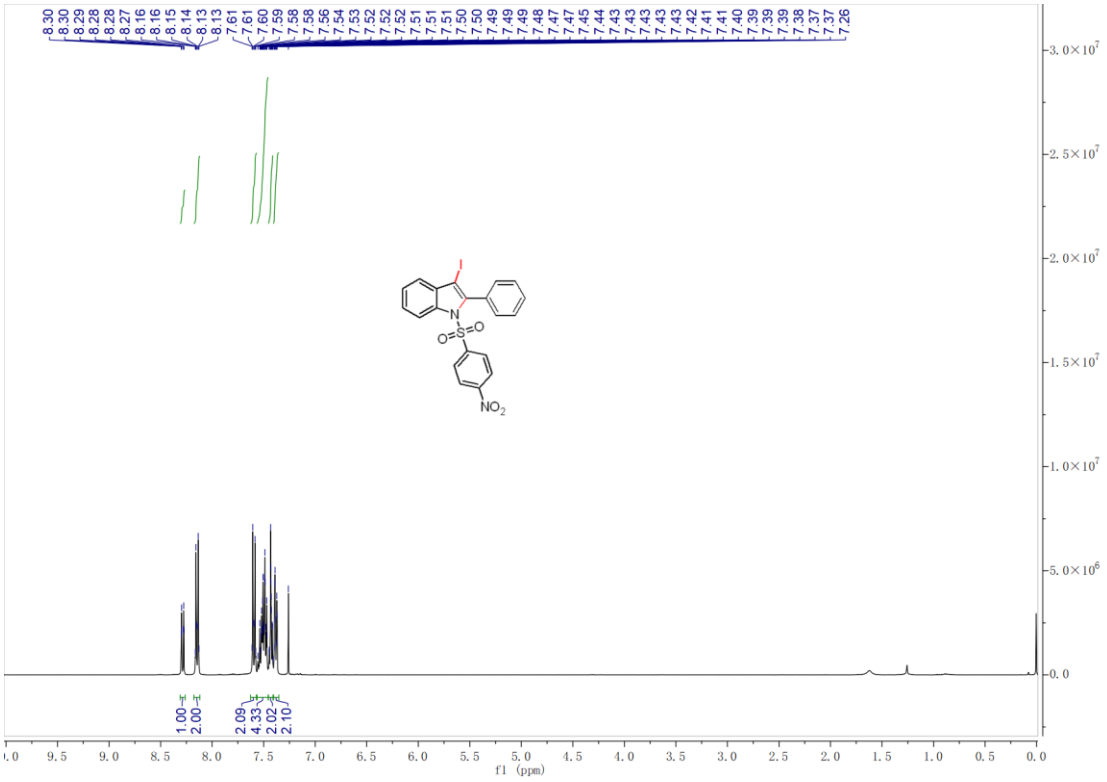

-102.33
f1 (ppm)

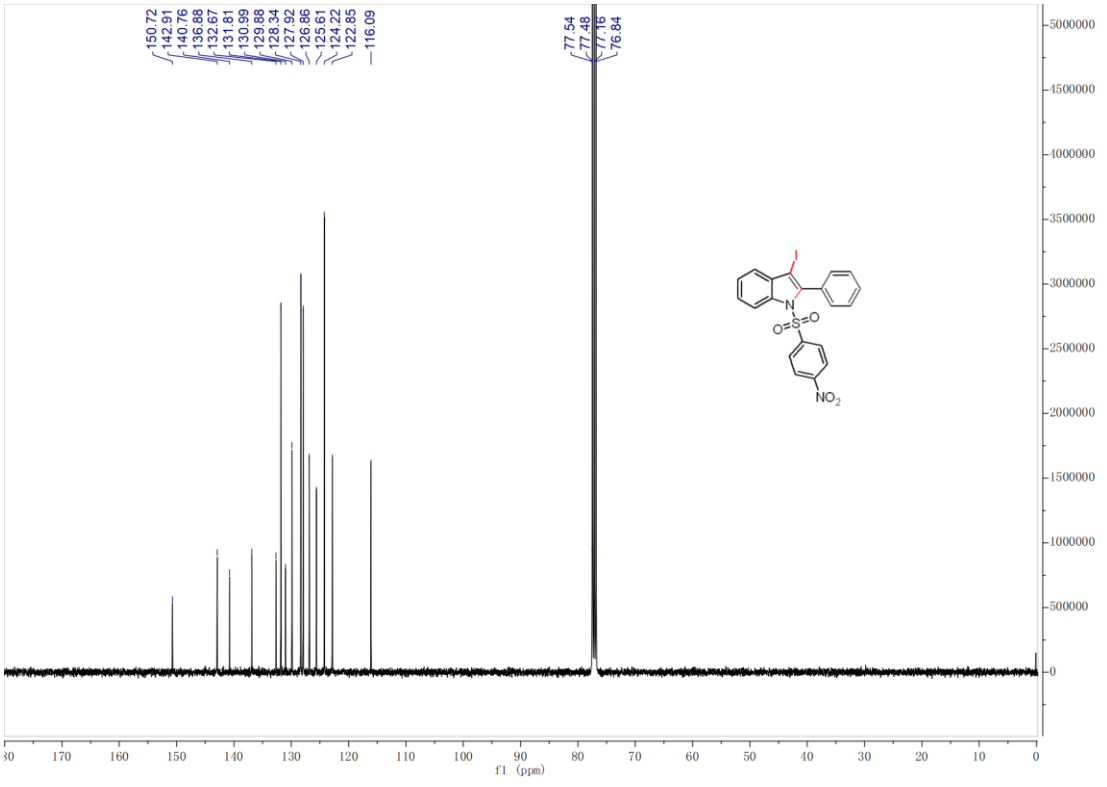
29b & 29c (12.5:1), $^{1}H + {}^{13}C$



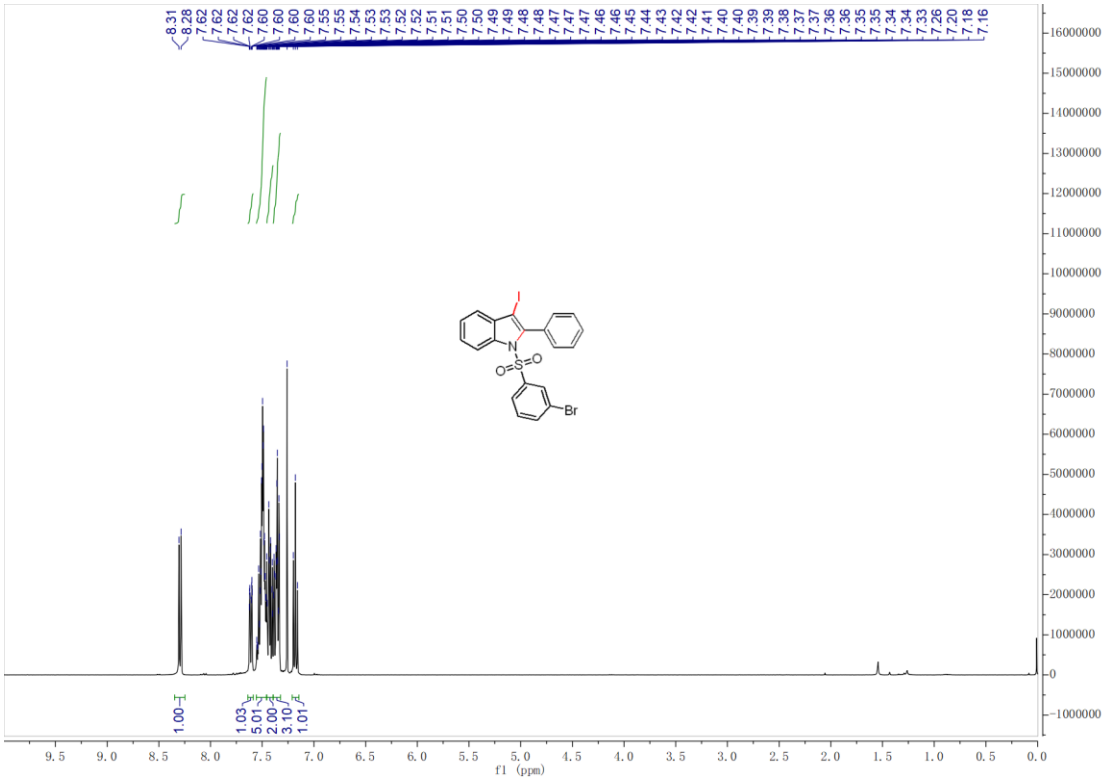


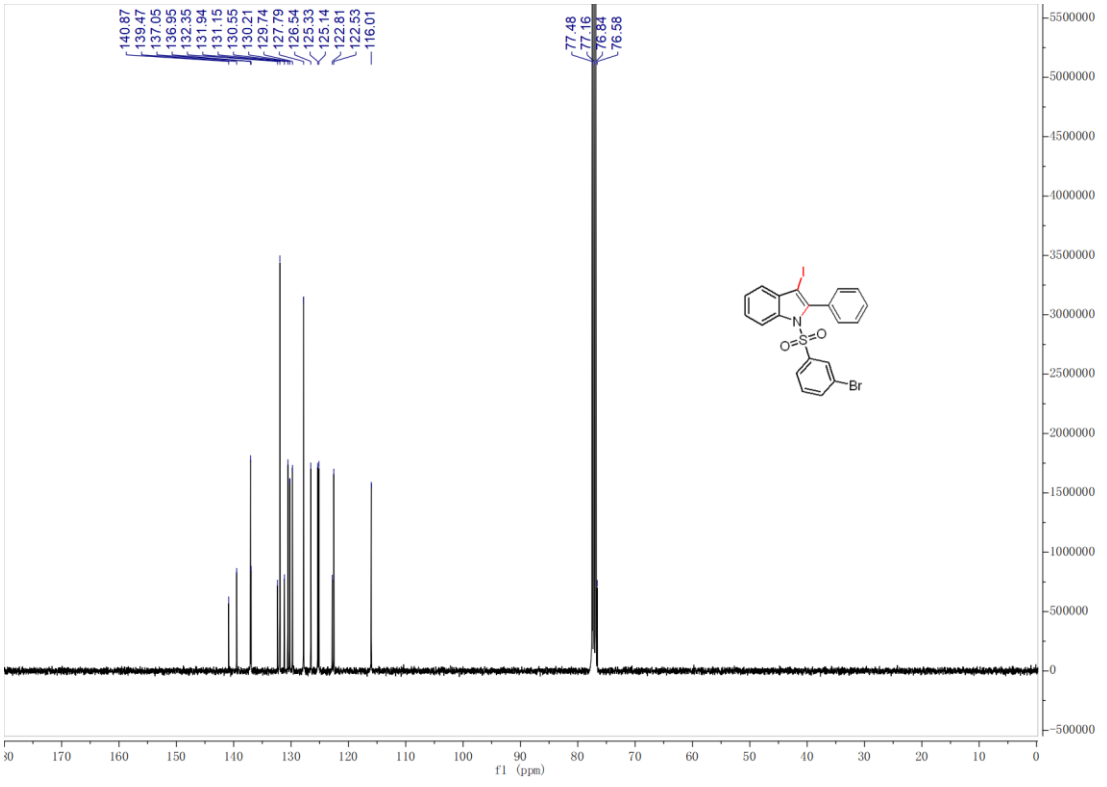
30b, $^{1}H + ^{13}C$


8.30
8.29
8.28
8.27
8.16
8.15
8.14
8.13
7.61
7.60
7.59
7.58
7.56
7.54
7.53
7.52
7.51
7.50
7.49
7.48
7.47
7.45
7.44
7.43
7.42
7.41
7.40
7.39
7.38
7.37
7.26
1.00
2.00
2.09
4.33
2.02
2.10
f1 (ppm)

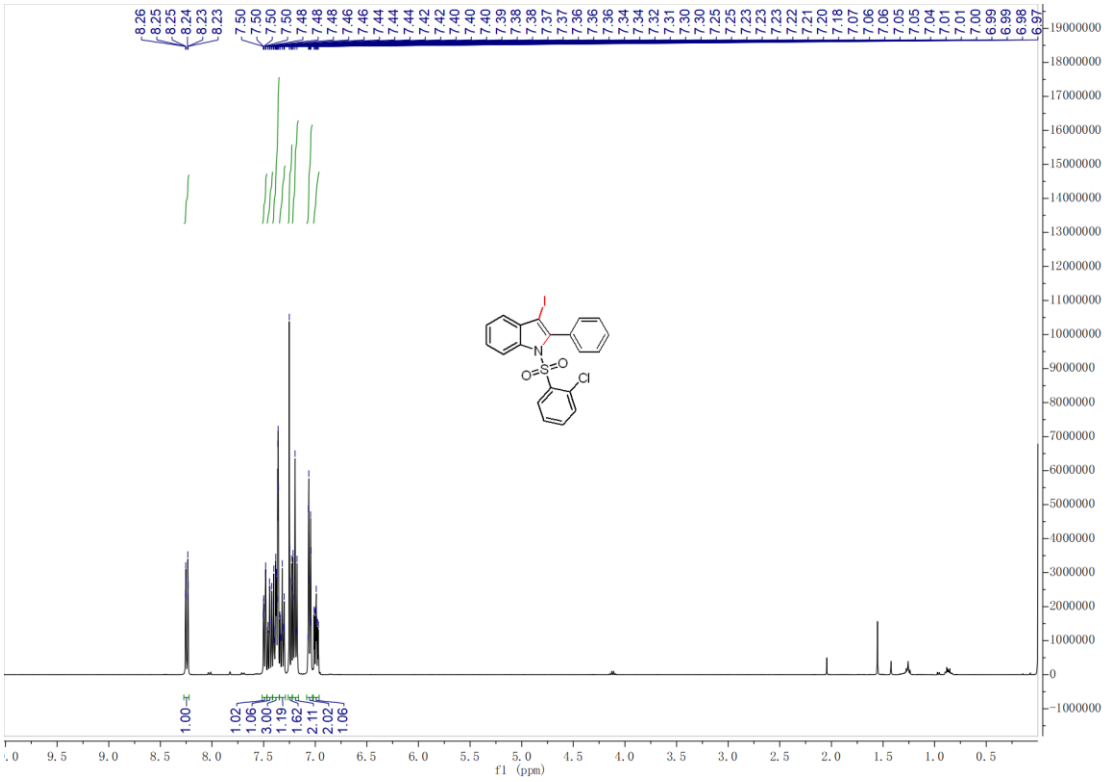

150.72
142.91
140.76
136.88
132.67
131.81
130.99
129.88
128.34
127.92
126.86
125.61
124.22
122.85
116.09
77.54
77.48
77.16
76.84
f1 (ppm)

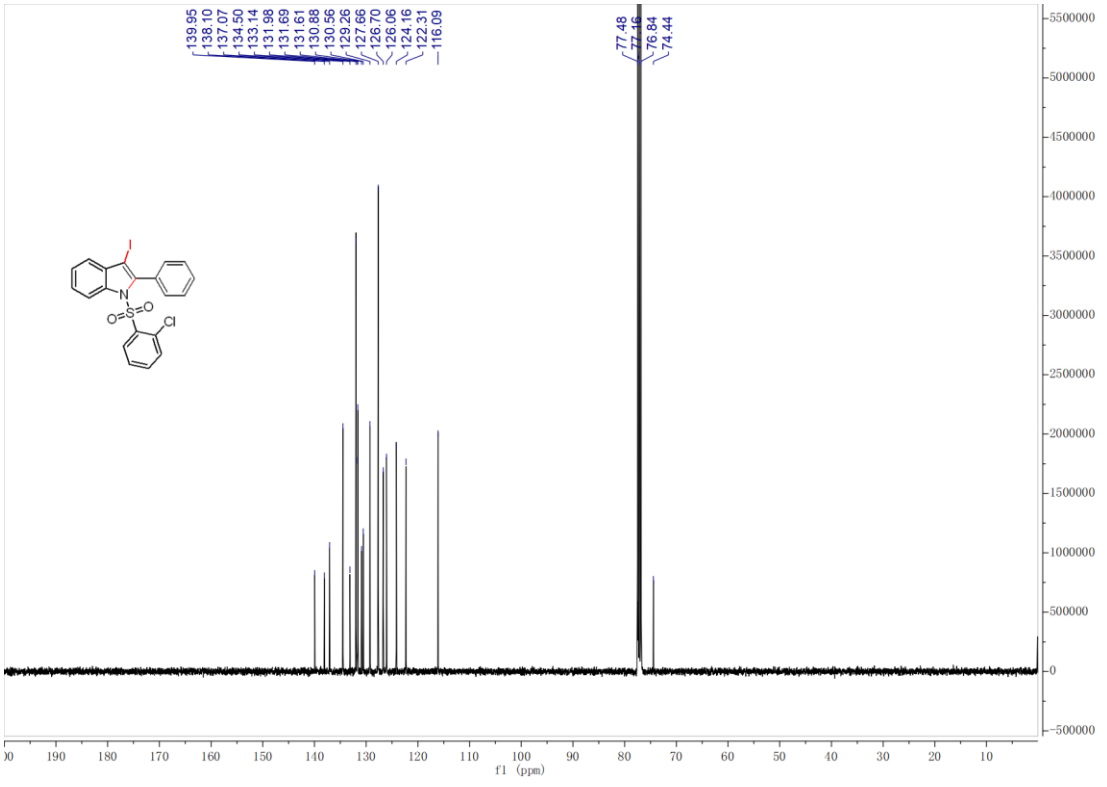
31b, $^{1}H + ^{13}C$


8.31
8.28
7.62
7.62
7.62
7.60
7.60
7.60
7.60
7.55
7.55
7.54
7.53
7.53
7.52
7.52
7.51
7.51
7.50
7.50
7.49
7.49
7.48
7.48
7.47
7.47
7.46
7.46
7.45
7.44
7.43
7.42
7.42
7.41
7.40
7.40
7.39
7.39
7.38
7.37
7.37
7.36
7.36
7.35
7.35
7.34
7.34
7.33
7.26
7.20
7.18
7.16
1.00
1.03
5.01
2.00
3.10
1.01
Br
f1 (ppm)

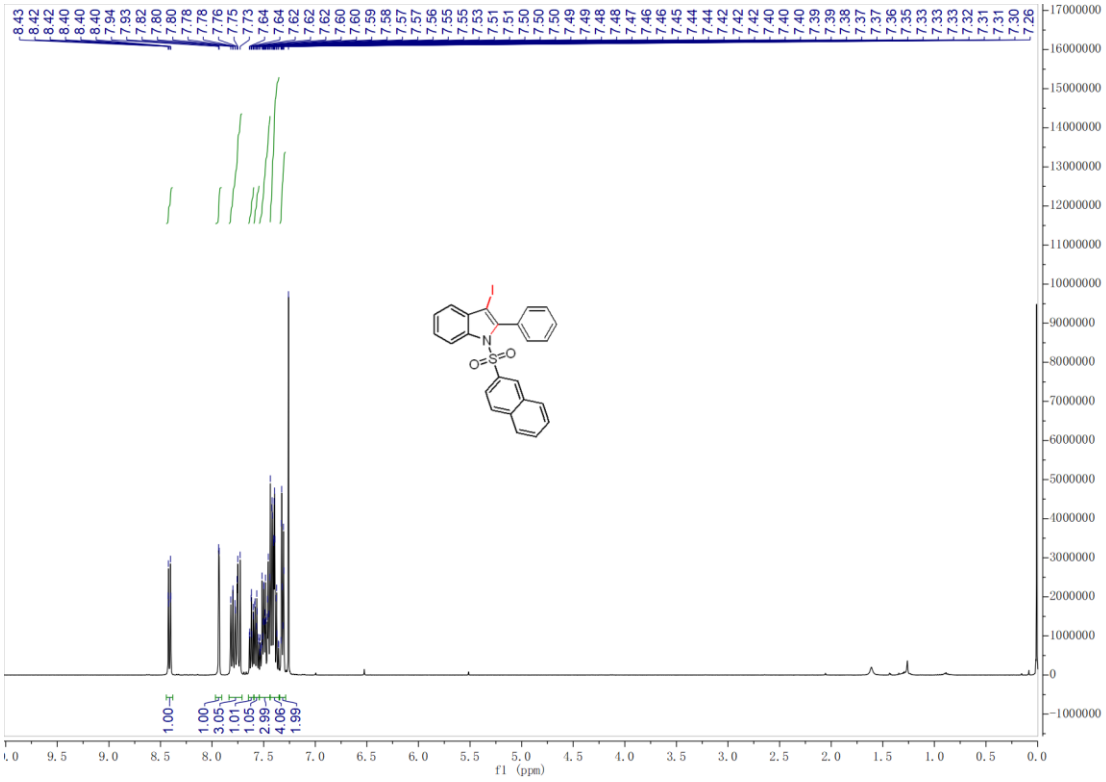

140.87
139.47
137.05
136.95
132.35
131.94
131.15
130.55
130.21
129.74
127.79
126.54
125.33
125.14
122.81
122.53
116.01
77.48
77.16
76.84
76.58
Br
f1 (ppm)

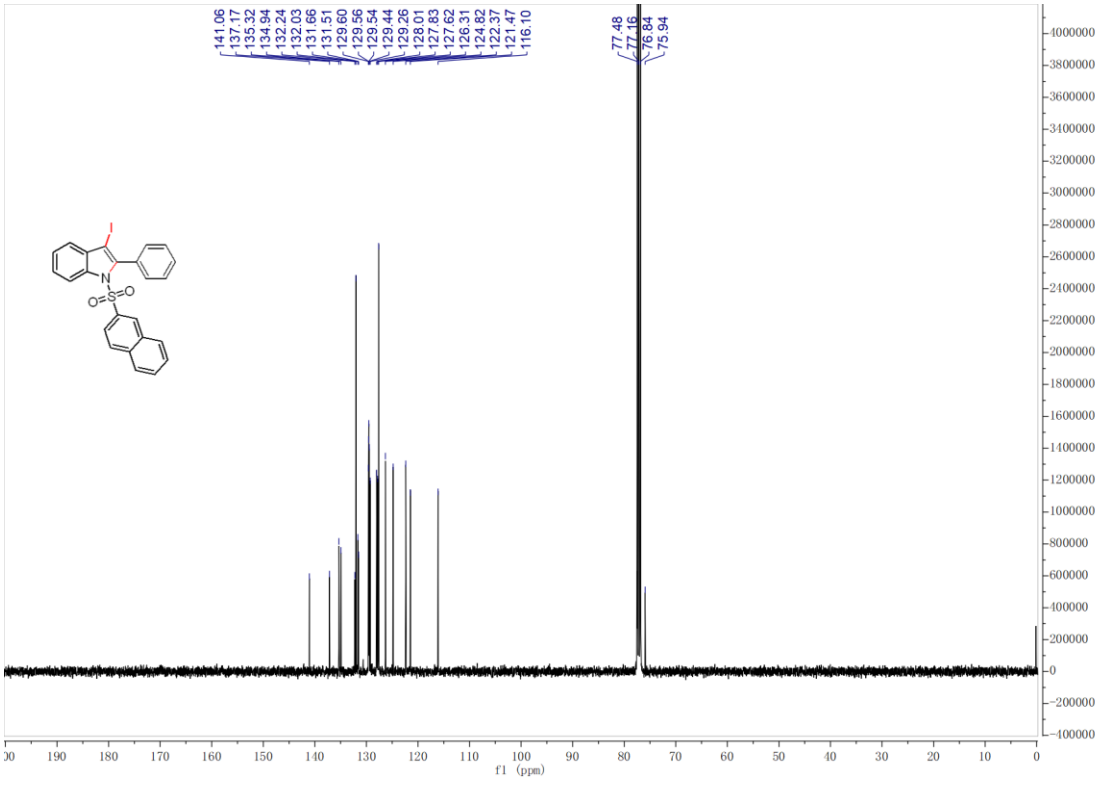
32b, $^{1}H + ^{13}C$


8.26
8.25
8.25
8.24
8.23
8.23
7.50
7.50
7.50
7.50
7.48
7.48
7.48
7.46
7.46
7.44
7.44
7.44
7.42
7.42
7.40
7.40
7.40
7.39
7.38
7.38
7.37
7.37
7.36
7.36
7.36
7.34
7.34
7.32
7.31
7.30
7.30
7.25
7.25
7.23
7.23
7.23
7.22
7.21
7.20
7.18
7.07
7.06
7.06
7.05
7.05
7.04
7.01
7.01
7.00
6.99
6.99
6.98
6.97
1.00
1.02
1.06
3.00
1.19
1.62
2.11
2.02
1.06
f1 (ppm)

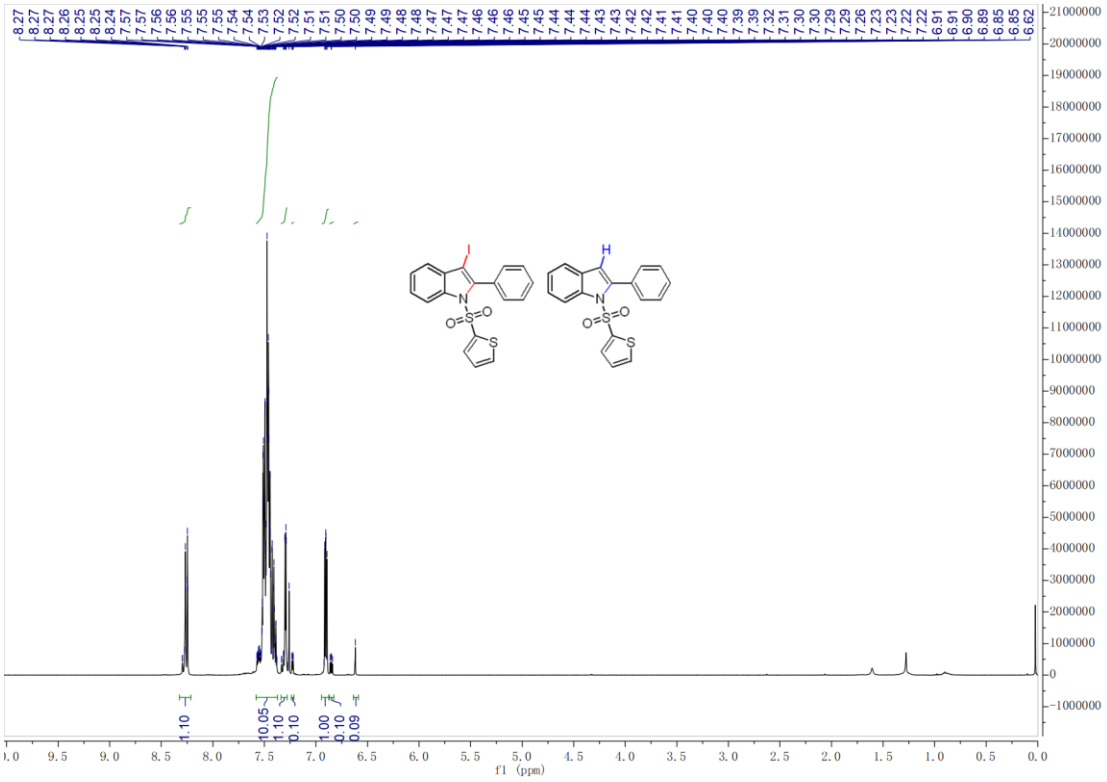

139.95
138.10
137.07
134.50
133.14
131.98
131.69
131.61
130.88
130.56
129.26
127.66
126.70
126.06
124.16
122.31
116.09
77.48
77.16
76.84
74.44
f1 (ppm)

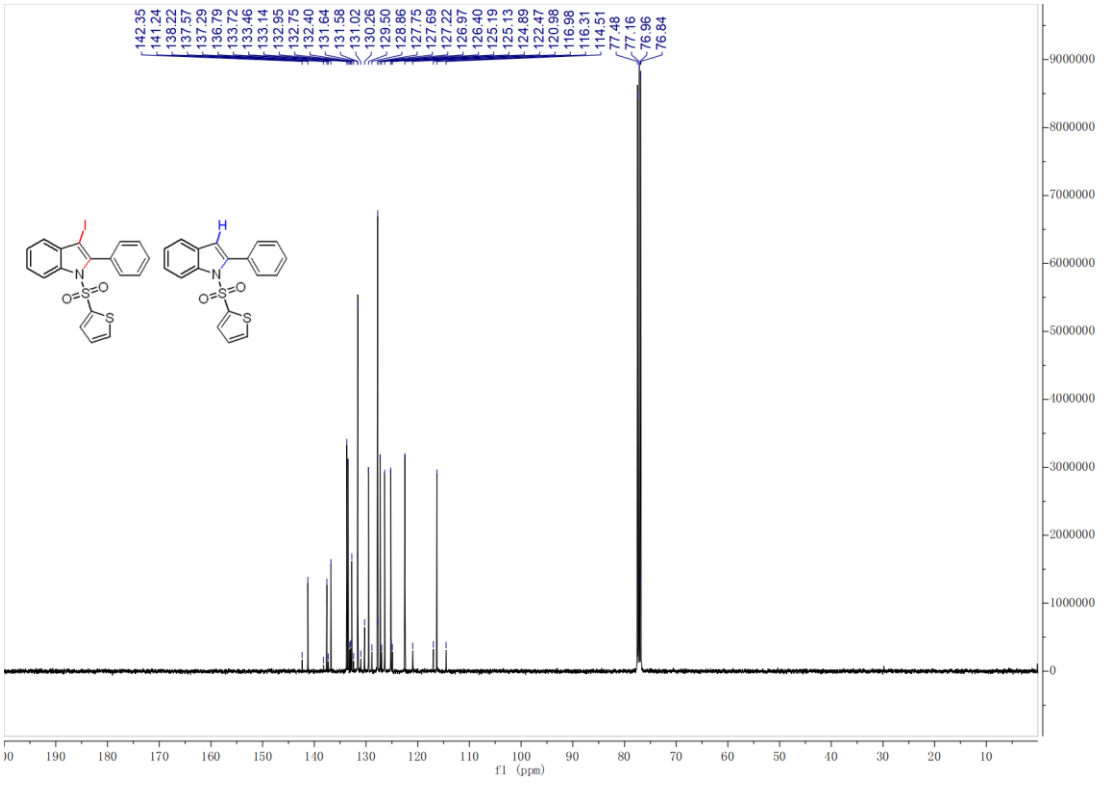
33b, $^{1}H + ^{13}C$


8.43 8.42 8.42 8.40 8.40 8.40 7.94 7.93 7.82 7.80 7.80 7.78 7.78 7.76 7.75 7.73 7.64 7.64 7.62 7.62 7.60 7.60 7.59 7.58 7.57 7.57 7.56 7.55 7.55 7.53 7.51 7.51 7.50 7.50 7.50 7.49 7.49 7.48 7.48 7.47 7.46 7.46 7.45 7.44 7.44 7.42 7.42 7.40 7.40 7.40 7.39 7.39 7.38 7.37 7.37 7.36 7.35 7.33 7.33 7.32 7.31 7.31 7.30 7.26
1.00 1.00 3.05 1.01 1.05 2.99 4.06 1.99
f1 (ppm)

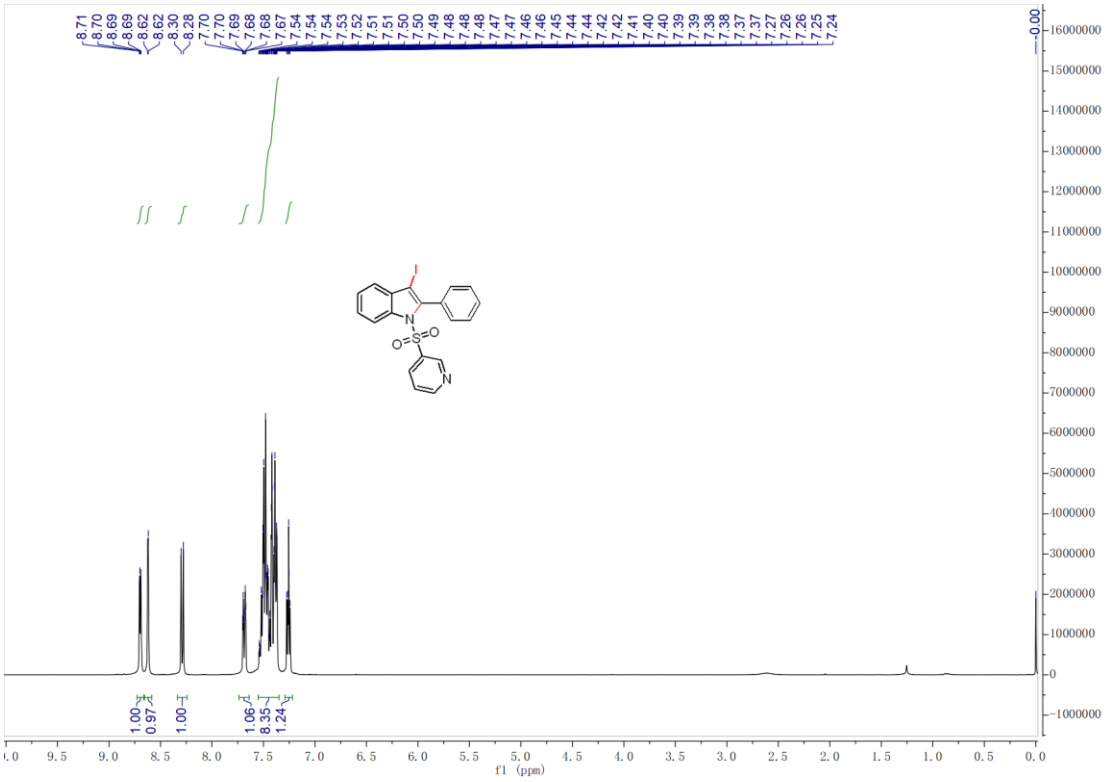

141.06 137.17 135.32 134.94 132.24 132.03 131.66 131.51 129.60 129.56 129.54 129.44 129.26 128.01 127.83 127.62 126.31 124.82 122.37 121.47 116.10
77.48 77.16 76.84 75.94
f1 (ppm)

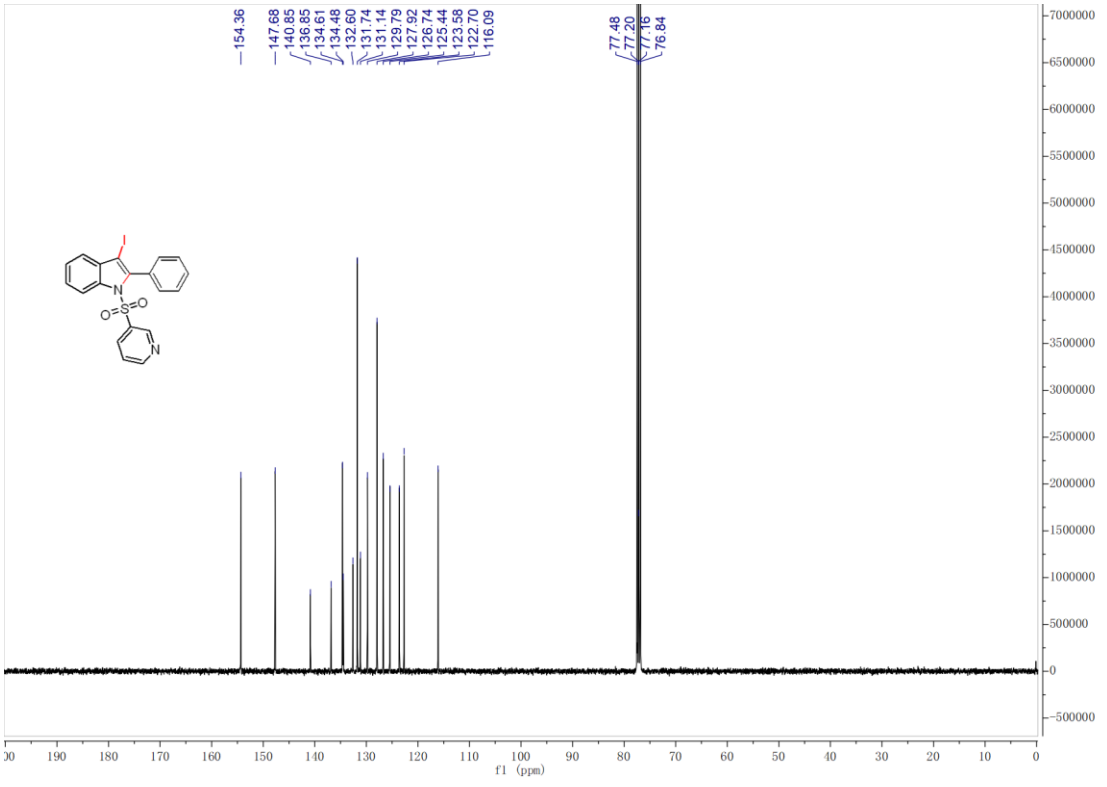
34b & 34c (10:1), $^{1}H + {}^{13}C$



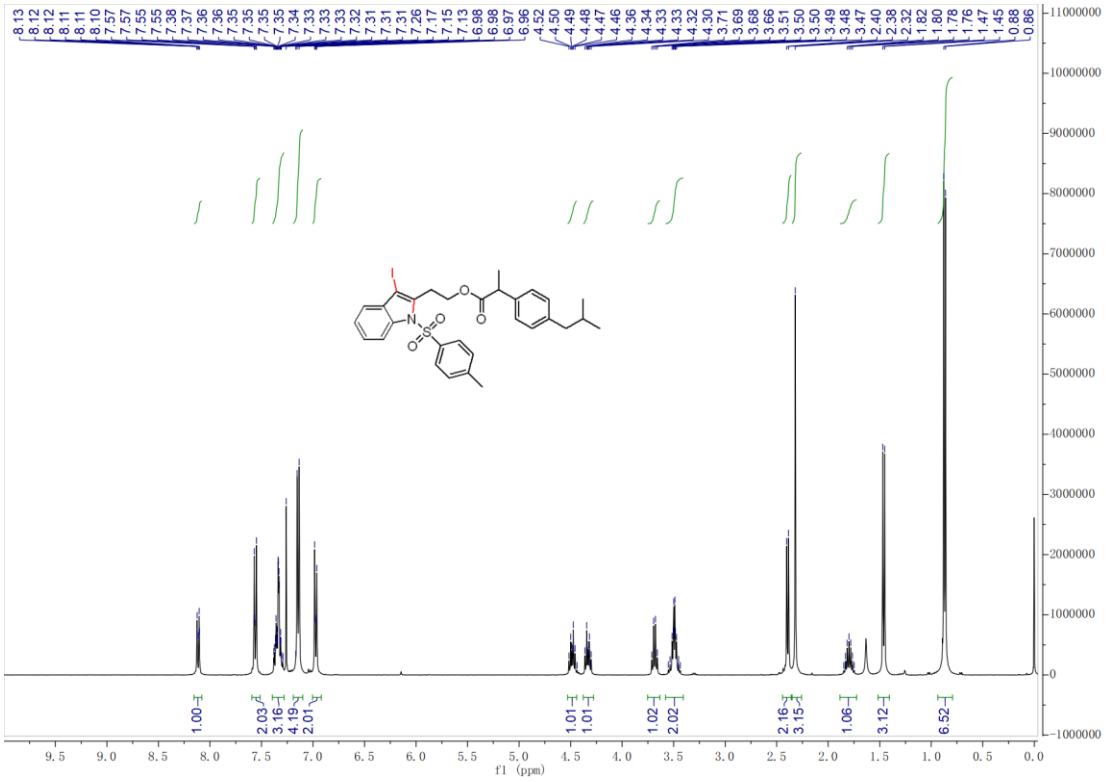


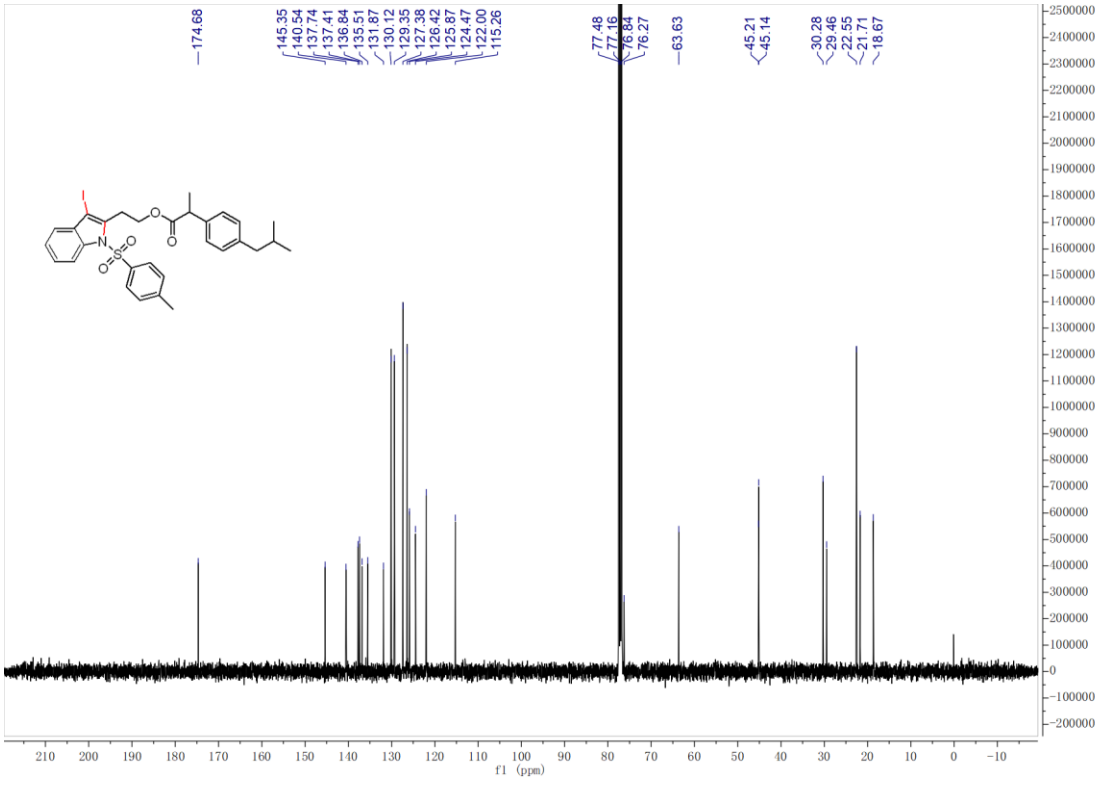
35b, $^{1}H + ^{13}C$


8.71
8.70
8.69
8.69
8.62
8.62
8.30
8.28
7.70
7.70
7.69
7.68
7.68
7.67
7.54
7.54
7.54
7.53
7.52
7.51
7.51
7.50
7.50
7.49
7.48
7.48
7.48
7.47
7.47
7.46
7.46
7.45
7.44
7.44
7.42
7.42
7.41
7.40
7.40
7.39
7.39
7.38
7.38
7.37
7.37
7.27
7.26
7.26
7.25
7.24
0.00
1.00
0.97
1.00
1.06
8.35
1.24
f1 (ppm)

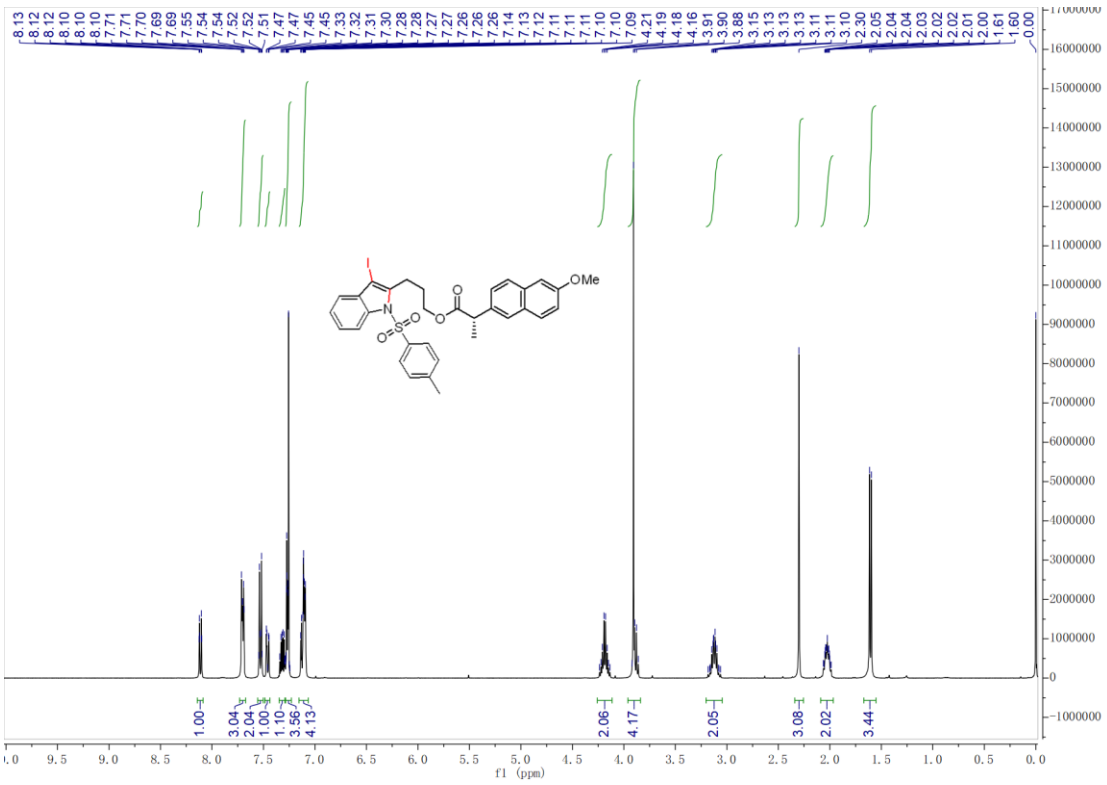

154.36
147.68
140.85
136.85
134.61
134.48
132.60
131.74
131.14
129.79
127.92
126.74
125.44
123.58
122.70
116.09
77.48
77.20
76.84
f1 (ppm)

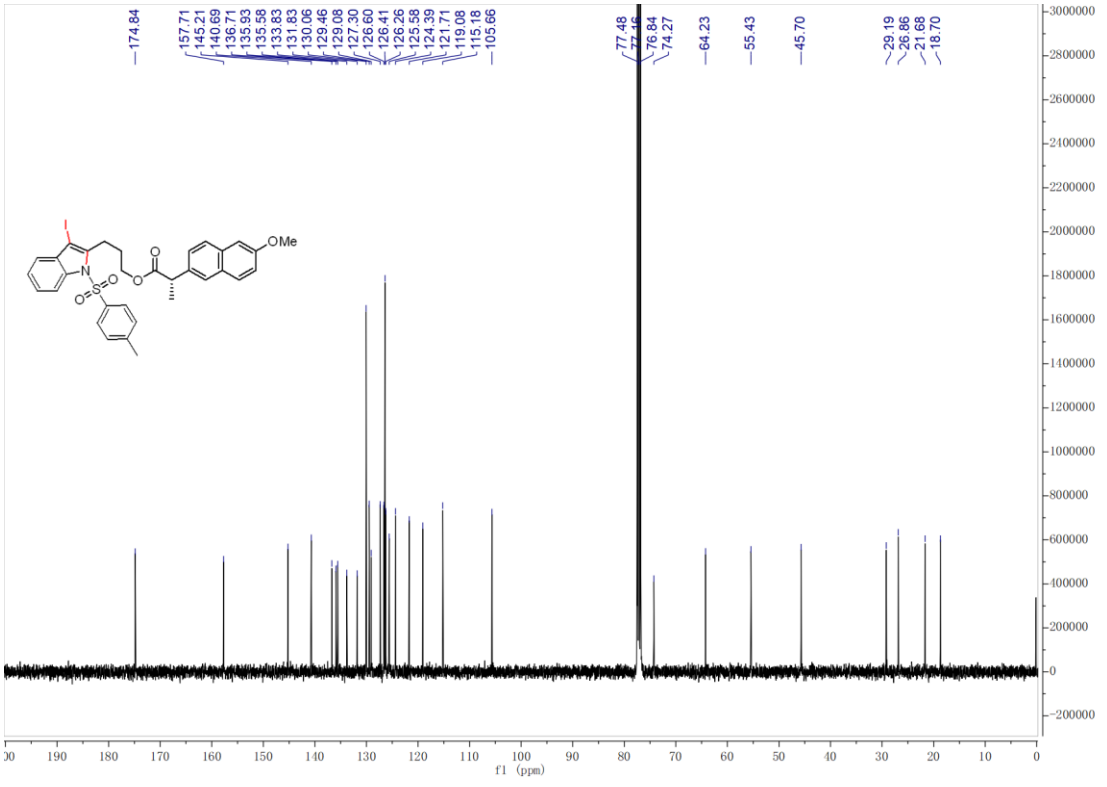
42b, $^{1}H + ^{13}C$


8.13 8.12 8.12 8.11 8.11 8.10 7.57 7.57 7.55 7.55 7.38 7.37 7.36 7.36 7.35 7.35 7.35 7.35 7.34 7.33 7.33 7.32 7.31 7.31 7.31 7.26 7.17 7.15 7.13 6.98 6.98 6.97 6.96 4.52 4.50 4.49 4.48 4.47 4.46 4.36 4.34 4.33 4.33 4.32 4.30 3.71 3.69 3.68 3.66 3.51 3.50 3.50 3.49 3.48 3.47 2.40 2.38 2.32 1.82 1.80 1.78 1.76 1.47 1.45 0.88 0.86
1.00 2.03 3.16 4.19 2.01 1.01 1.01 1.02 2.02 2.16 3.15 1.06 3.12 6.52
f1 (ppm)

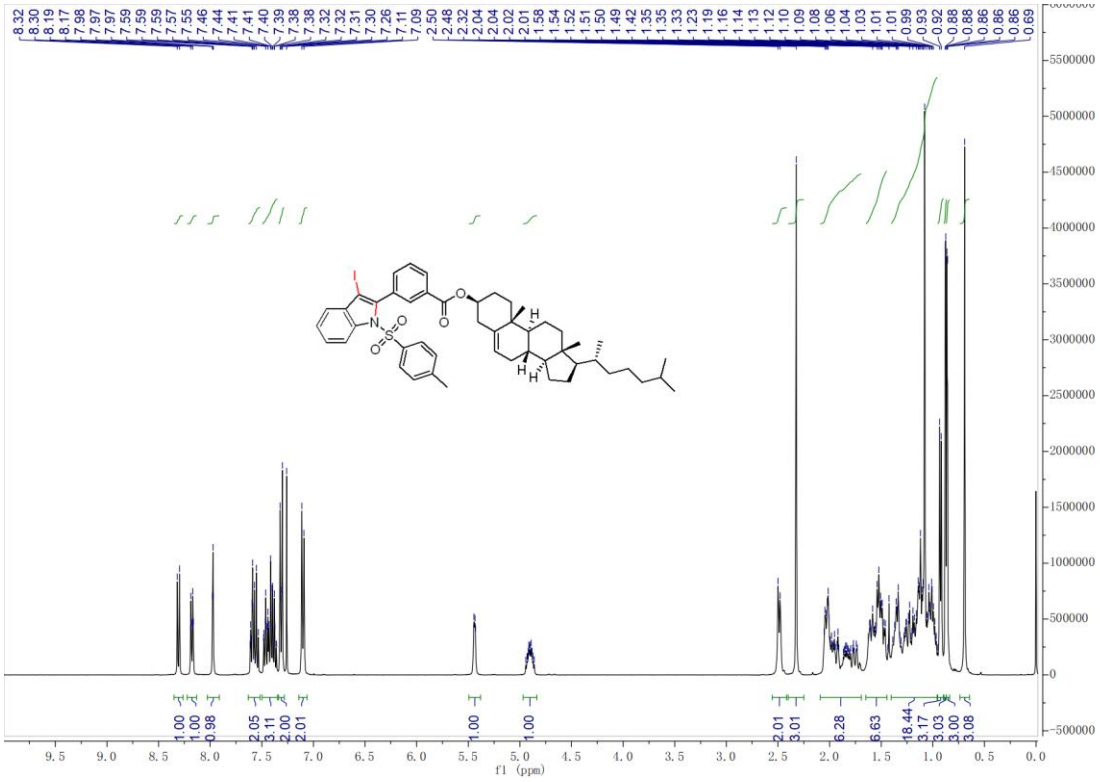

174.68
145.35 140.54 137.74 137.41 136.84 135.51 131.87 130.12 129.35 127.38 126.42 125.87 124.47 122.00 115.26
77.48 77.16 76.84 76.27
63.63
45.21 45.14
30.28 29.46 22.55 21.71 18.67
f1 (ppm)

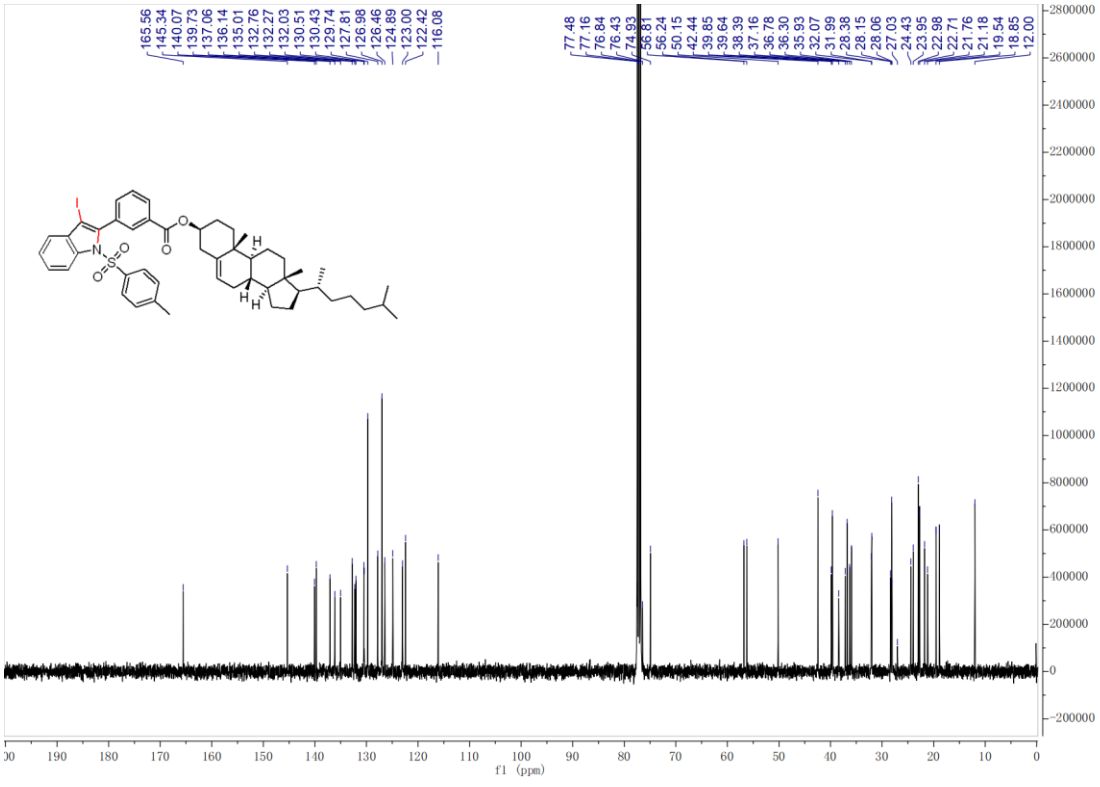
43b, $^{1}H + {}^{13}C$


8.13
8.12
8.12
8.10
8.10
8.10
7.71
7.71
7.70
7.69
7.69
7.55
7.54
7.54
7.52
7.52
7.51
7.47
7.47
7.45
7.45
7.33
7.32
7.31
7.30
7.28
7.28
7.27
7.27
7.26
7.26
7.26
7.14
7.13
7.12
7.11
7.11
7.11
7.10
7.10
7.09
4.21
4.19
4.18
4.16
3.91
3.90
3.88
3.15
3.13
3.13
3.13
3.11
3.11
3.10
2.30
2.05
2.04
2.04
2.03
2.02
2.02
2.01
2.00
1.61
1.60
0.00
OMe
1.00
3.04
2.04
1.00
1.10
3.56
4.13
2.06
4.17
2.05
3.08
2.02
3.44
f1 (ppm)

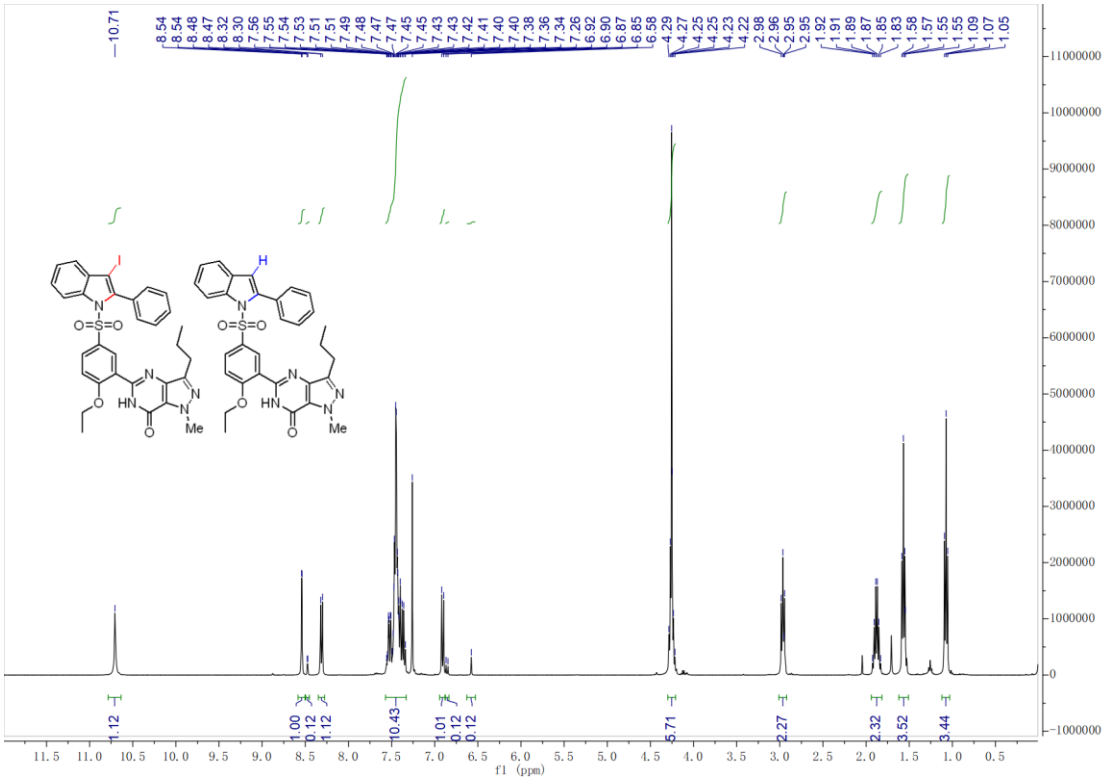

174.84
157.71
145.21
140.69
136.71
135.93
135.58
133.83
131.83
130.06
129.46
129.08
127.30
126.60
126.41
126.26
125.58
124.39
121.71
119.08
115.18
105.66
77.48
77.16
76.84
74.27
64.23
55.43
45.70
29.19
26.86
21.68
18.70
OMe
f1 (ppm)

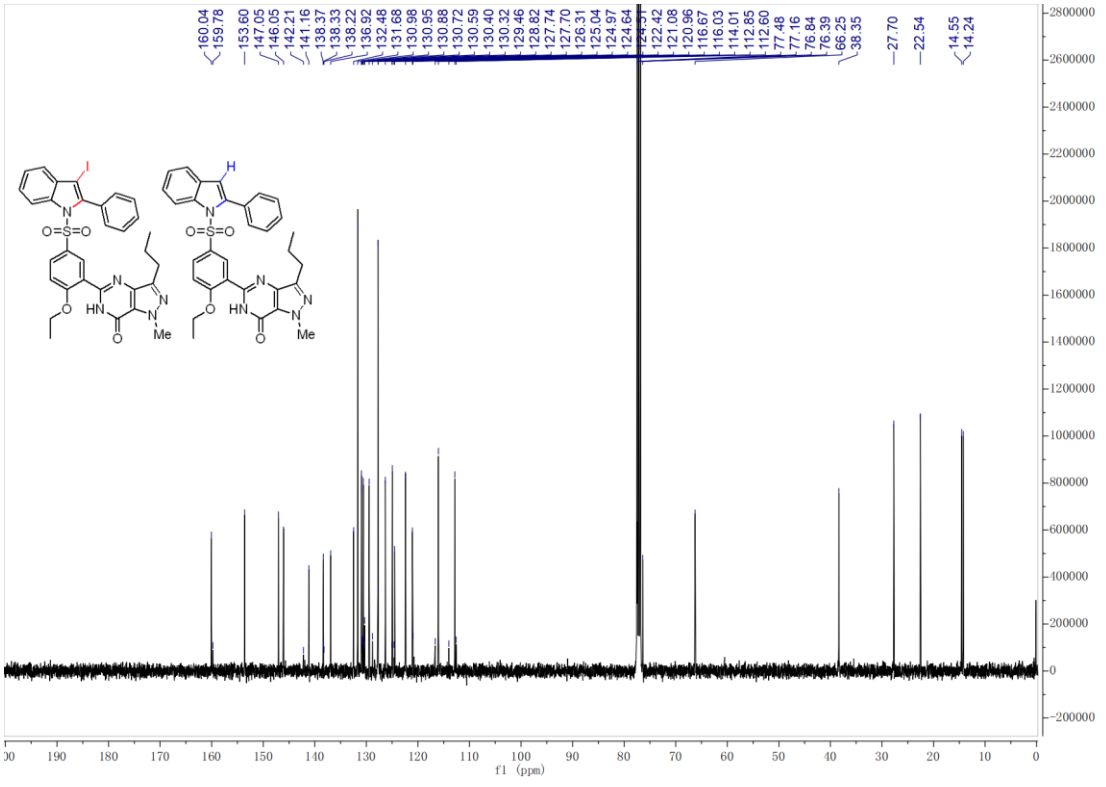
44b, $^{1}H + ^{13}C$



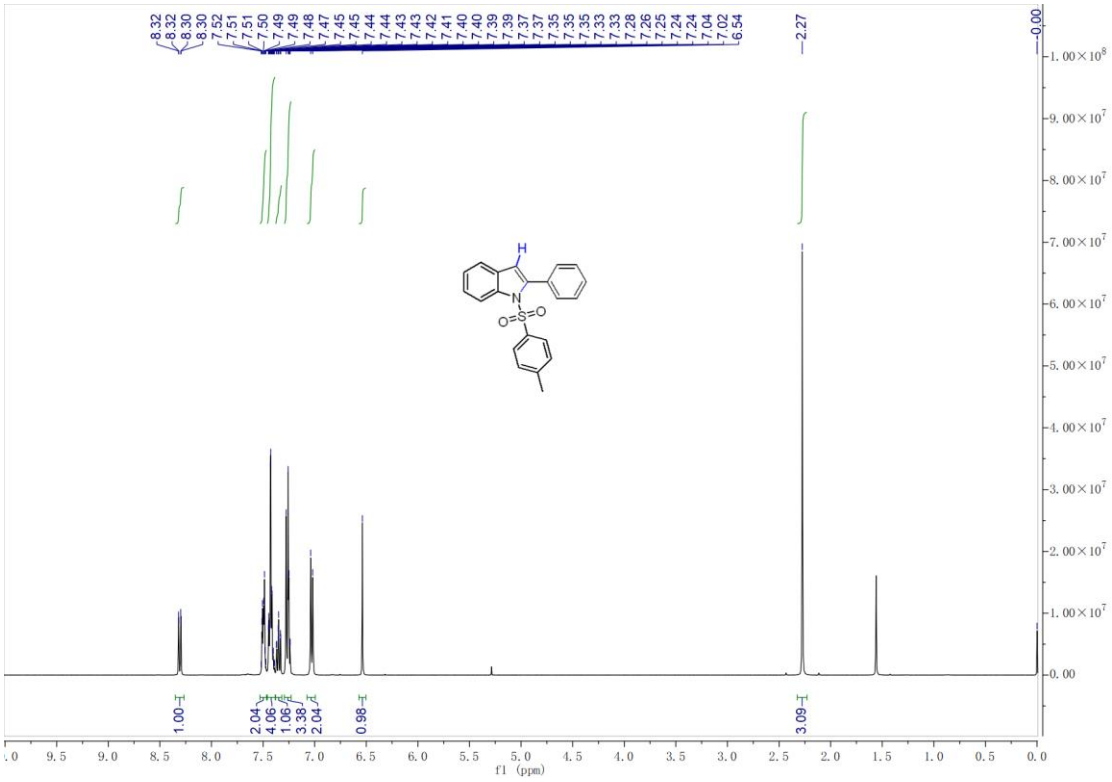


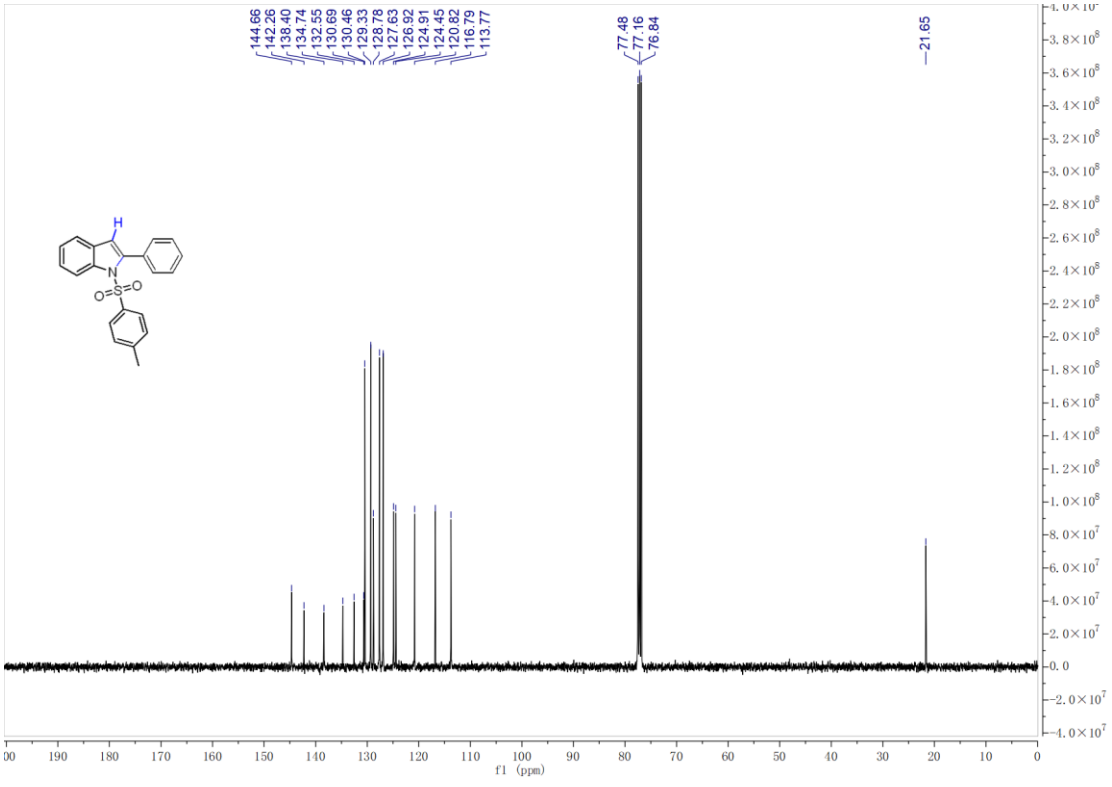
45b & 45c (8.3:1), $^{1}H + ^{13}C$



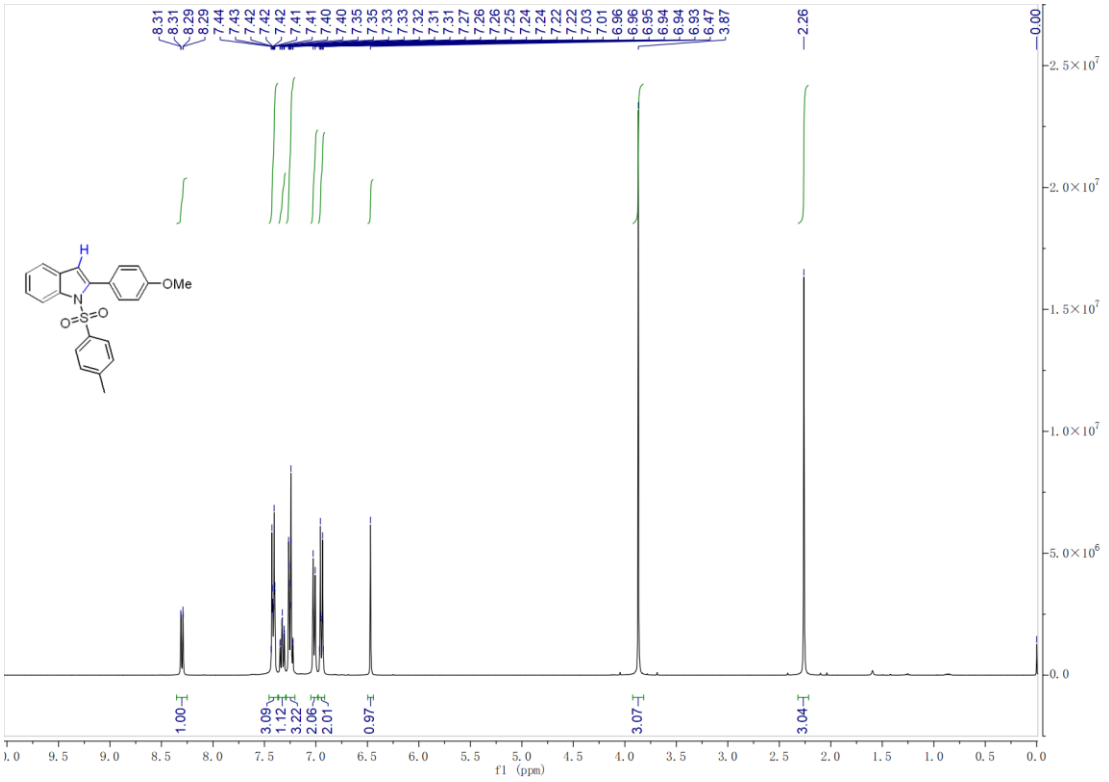


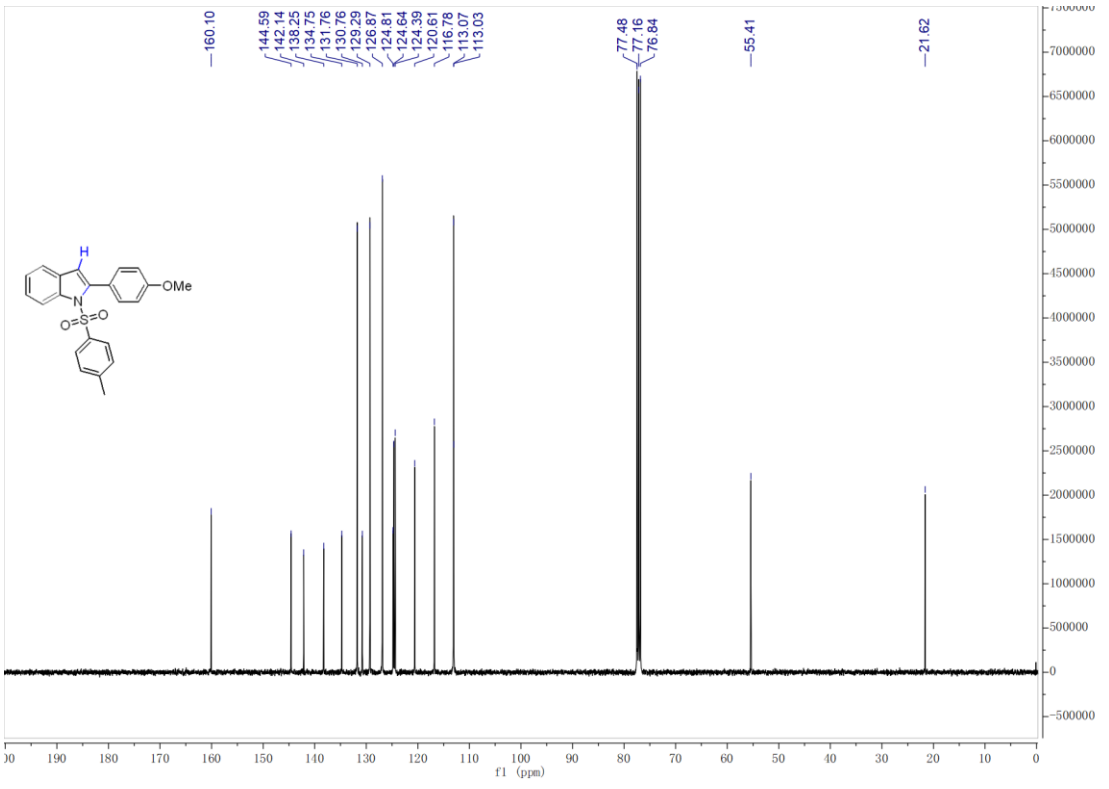
1c, $^{1}H + ^{13}C$


8.32
8.32
8.30
8.30
7.52
7.51
7.51
7.50
7.49
7.49
7.48
7.47
7.45
7.45
7.44
7.44
7.43
7.43
7.42
7.41
7.40
7.39
7.39
7.37
7.37
7.35
7.35
7.33
7.33
7.28
7.26
7.25
7.24
7.24
7.04
7.02
6.54
2.27
0.00
1.00
2.04
4.06
1.06
3.38
2.04
0.98
3.09
f1 (ppm)

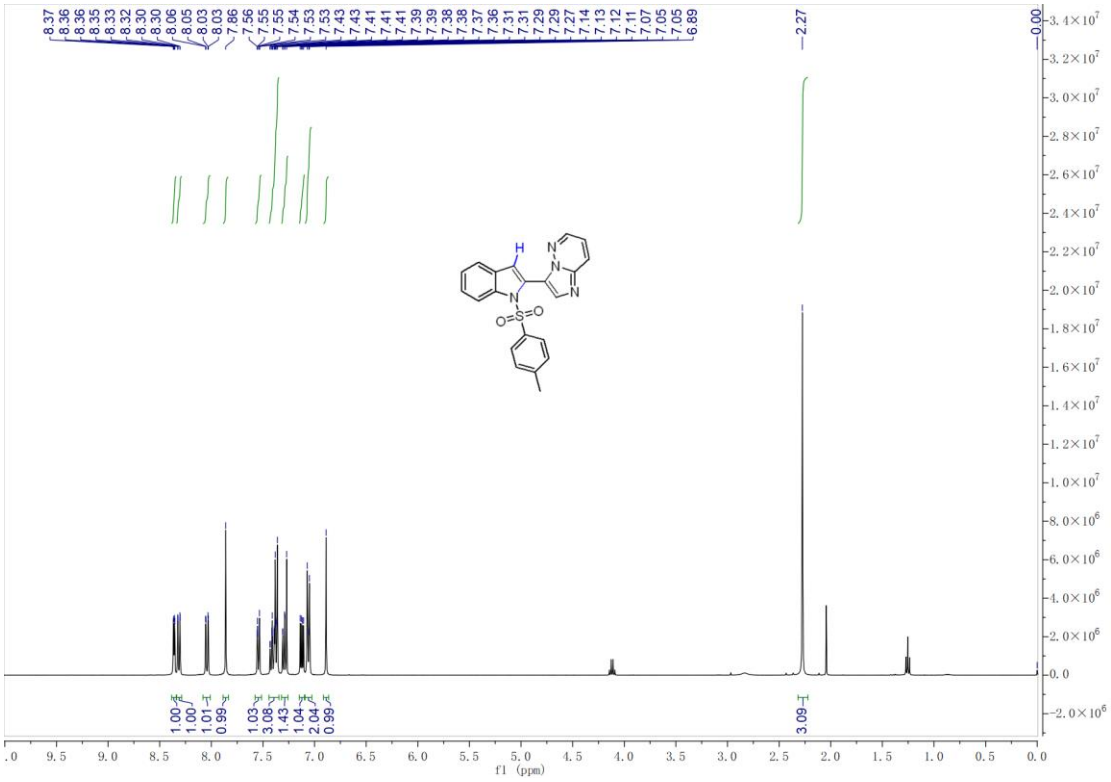

144.66
142.26
138.40
134.74
132.55
130.69
130.46
129.33
128.78
127.63
126.92
124.91
124.45
120.82
116.79
113.77
77.48
77.16
76.84
21.65
f1 (ppm)

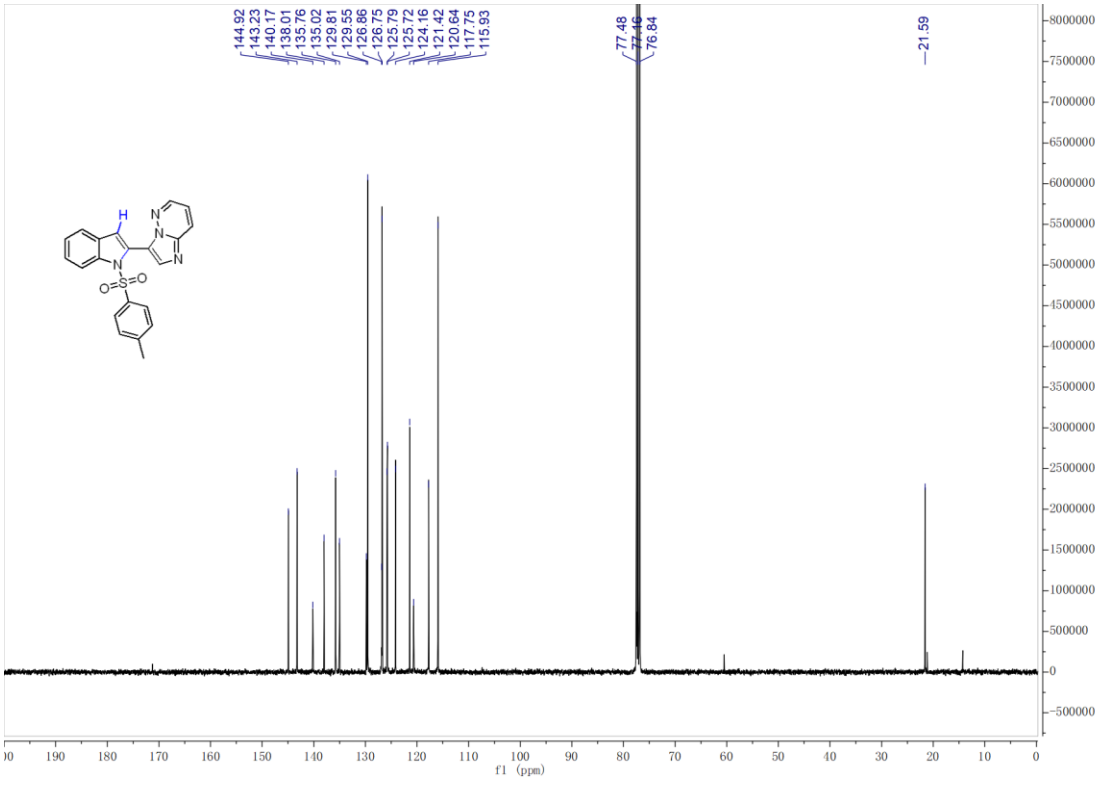
4c, $^{1}H + ^{13}C$


8.31
8.31
8.29
8.29
7.44
7.43
7.42
7.42
7.42
7.41
7.41
7.40
7.40
7.35
7.33
7.33
7.32
7.31
7.31
7.27
7.26
7.26
7.25
7.24
7.24
7.22
7.22
7.03
7.01
6.96
6.96
6.95
6.94
6.94
6.93
6.47
3.87
2.26
0.00
OMe
1.00
3.09
1.12
3.22
2.06
2.01
0.97
3.07
3.04
f1 (ppm)

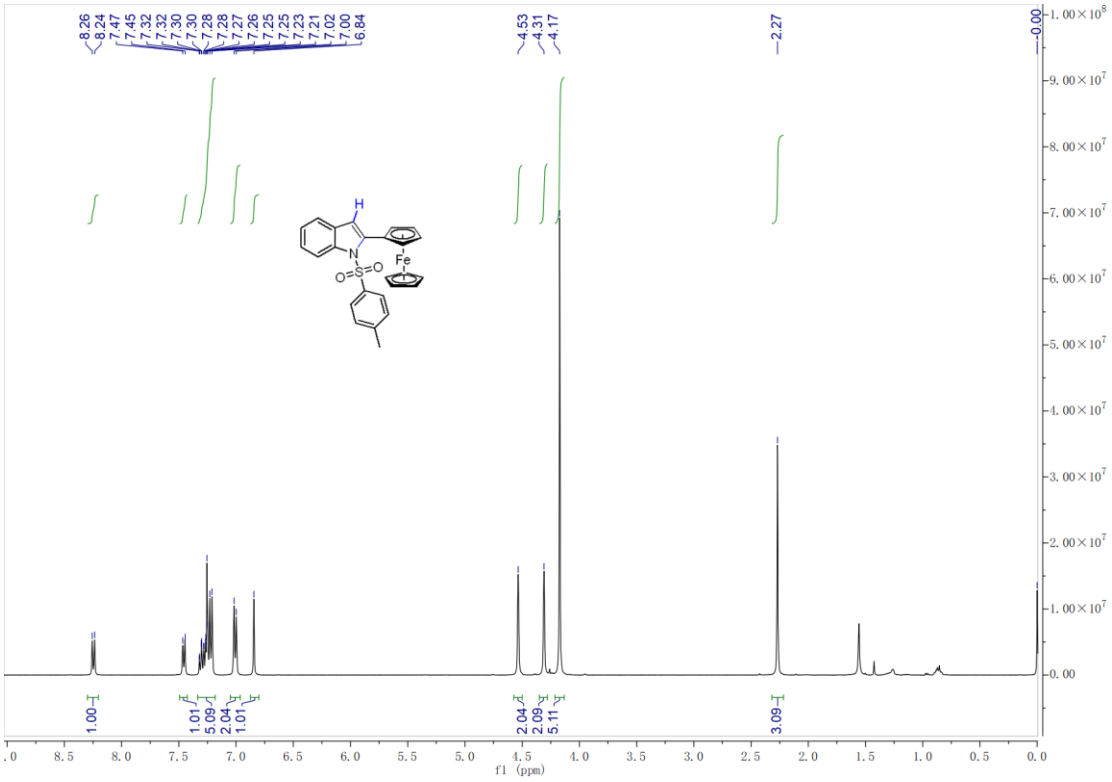

160.10
144.59
142.14
138.25
134.75
131.76
130.76
129.29
126.87
124.81
124.64
124.39
120.61
116.78
113.07
113.03
77.48
77.16
76.84
55.41
21.62
OMe
f1 (ppm)

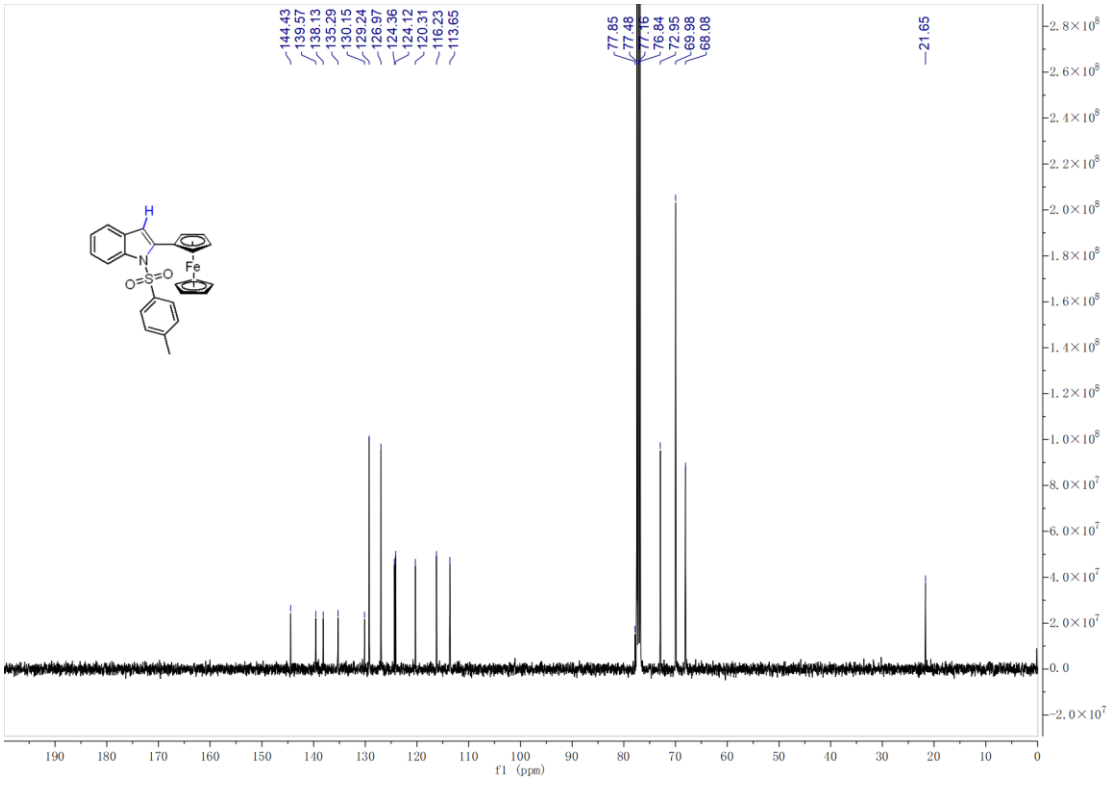
13c, $^{1}H + ^{13}C$


8.37
8.36
8.36
8.35
8.33
8.32
8.30
8.30
8.06
8.05
8.03
8.03
7.86
7.56
7.55
7.55
7.54
7.53
7.43
7.41
7.41
7.41
7.39
7.39
7.38
7.38
7.37
7.36
7.31
7.31
7.29
7.29
7.27
7.14
7.13
7.12
7.11
7.07
7.05
7.05
6.89
2.27
0.00
1.00
1.00
1.01
0.99
1.03
3.08
1.43
1.04
2.04
0.99
3.09
f1 (ppm)

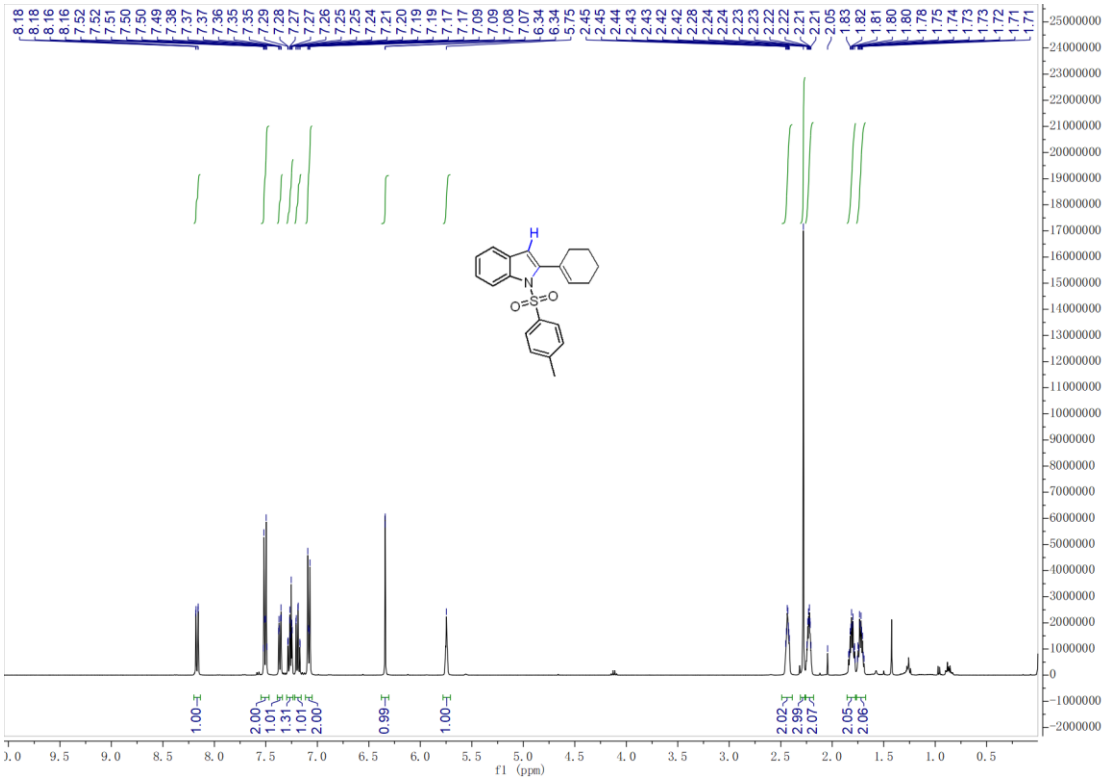

144.92
143.23
140.17
138.01
135.76
135.02
129.81
129.55
126.86
126.75
125.79
125.72
124.16
121.42
120.64
117.75
115.93
77.48
77.16
76.84
21.59
f1 (ppm)

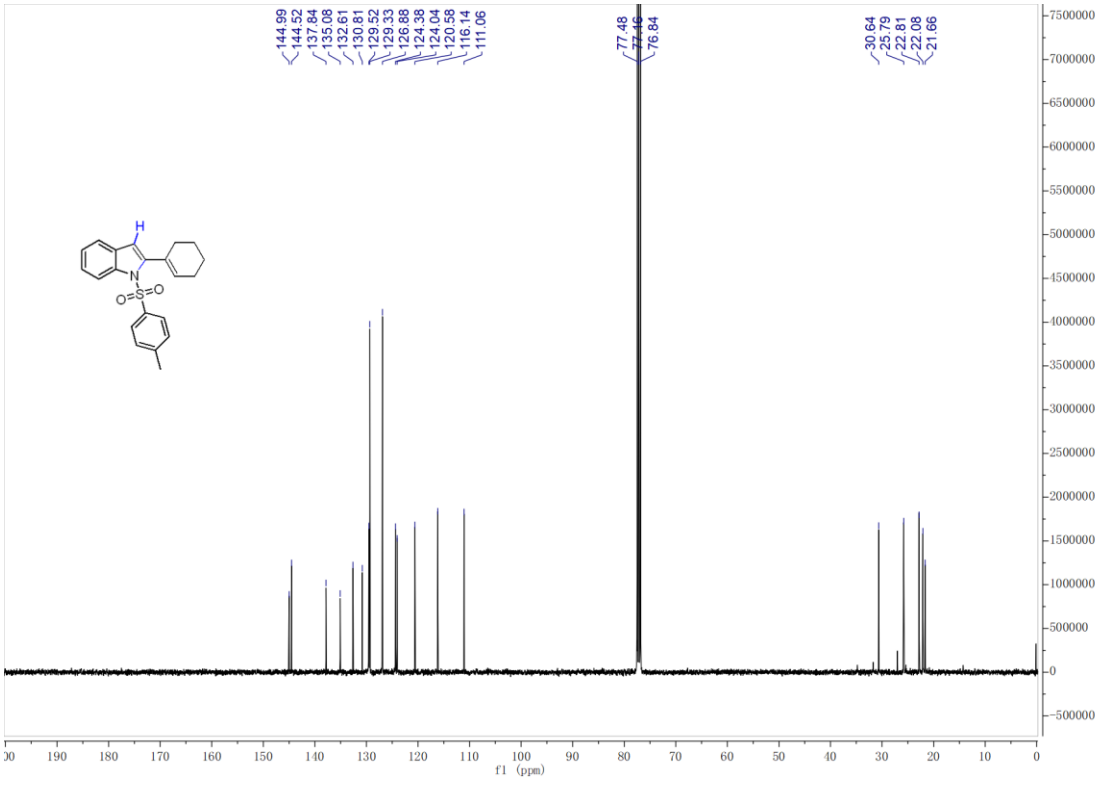
14c, $^{1}H + {}^{13}C$


8.26
8.24
7.47
7.45
7.32
7.32
7.30
7.30
7.28
7.28
7.27
7.26
7.25
7.25
7.23
7.21
7.02
7.00
6.84
4.53
4.31
4.17
2.27
0.00
1.00
1.01
5.09
2.04
1.01
2.04
2.09
5.11
3.09
f1 (ppm)

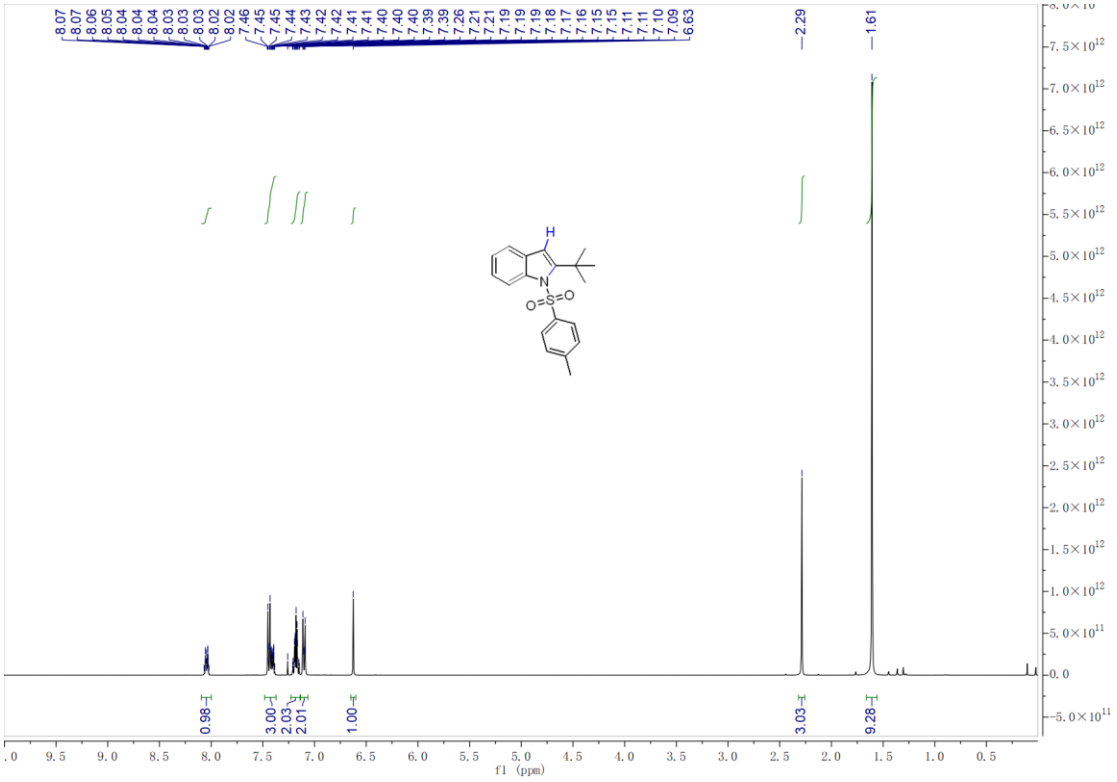

144.43
139.57
138.13
135.29
130.15
129.24
126.97
124.36
124.12
120.31
116.23
113.65
77.85
77.48
77.16
76.84
72.95
69.98
68.08
21.65
f1 (ppm)

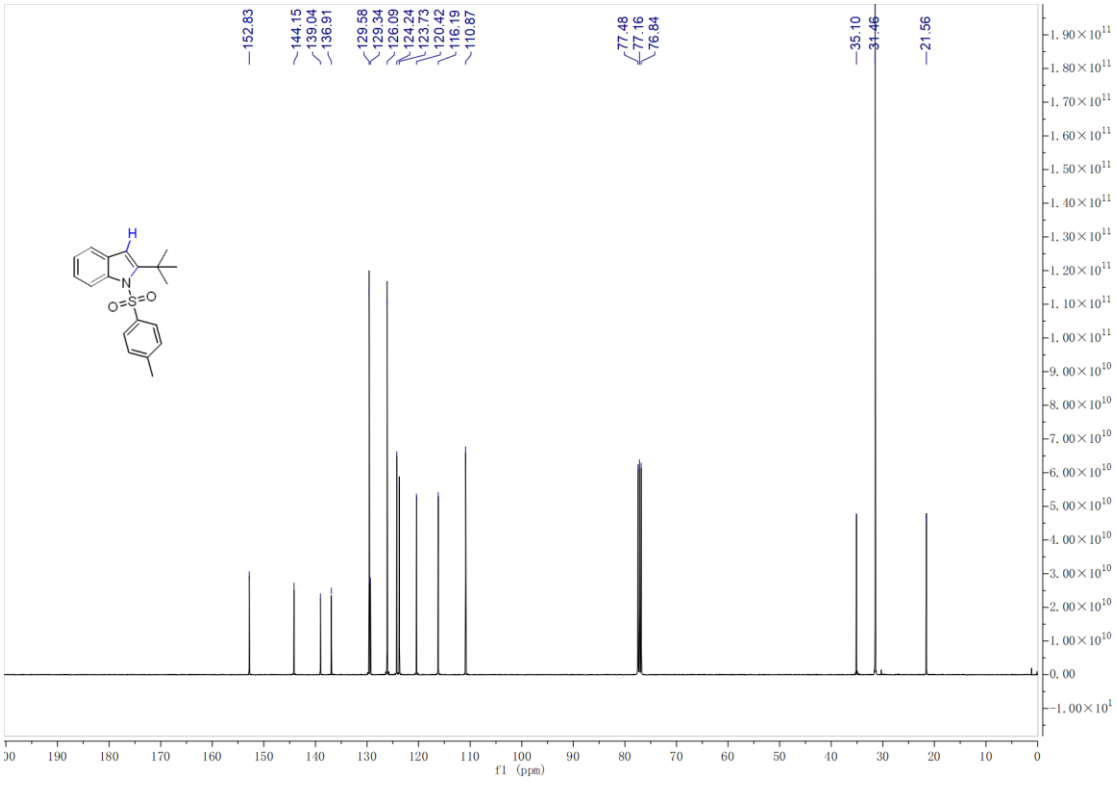
15c, $^{1}H + {}^{13}C$


8.18
8.16
7.52
7.51
7.50
7.49
7.38
7.37
7.36
7.35
7.29
7.28
7.27
7.26
7.25
7.24
7.21
7.20
7.19
7.17
7.09
7.08
7.07
6.34
5.75
2.45
2.44
2.43
2.42
2.28
2.24
2.23
2.22
2.21
2.05
1.83
1.82
1.81
1.80
1.78
1.75
1.74
1.73
1.72
1.71
1.00
2.00
1.01
1.31
1.01
2.00
0.99
1.00
2.02
2.99
2.07
2.05
2.06
f1 (ppm)

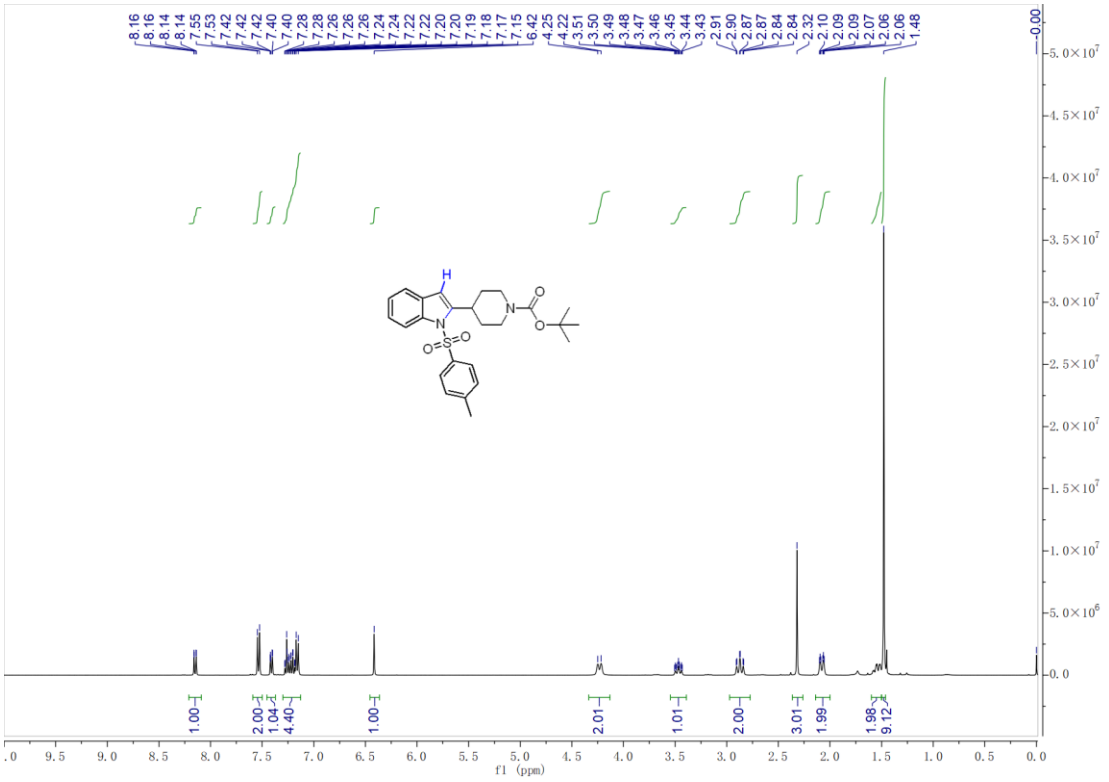

144.99
144.52
137.84
135.08
132.61
130.81
129.52
129.33
126.88
124.38
124.04
120.58
116.14
111.06
77.48
77.16
76.84
30.64
25.79
22.81
22.08
21.66
f1 (ppm)

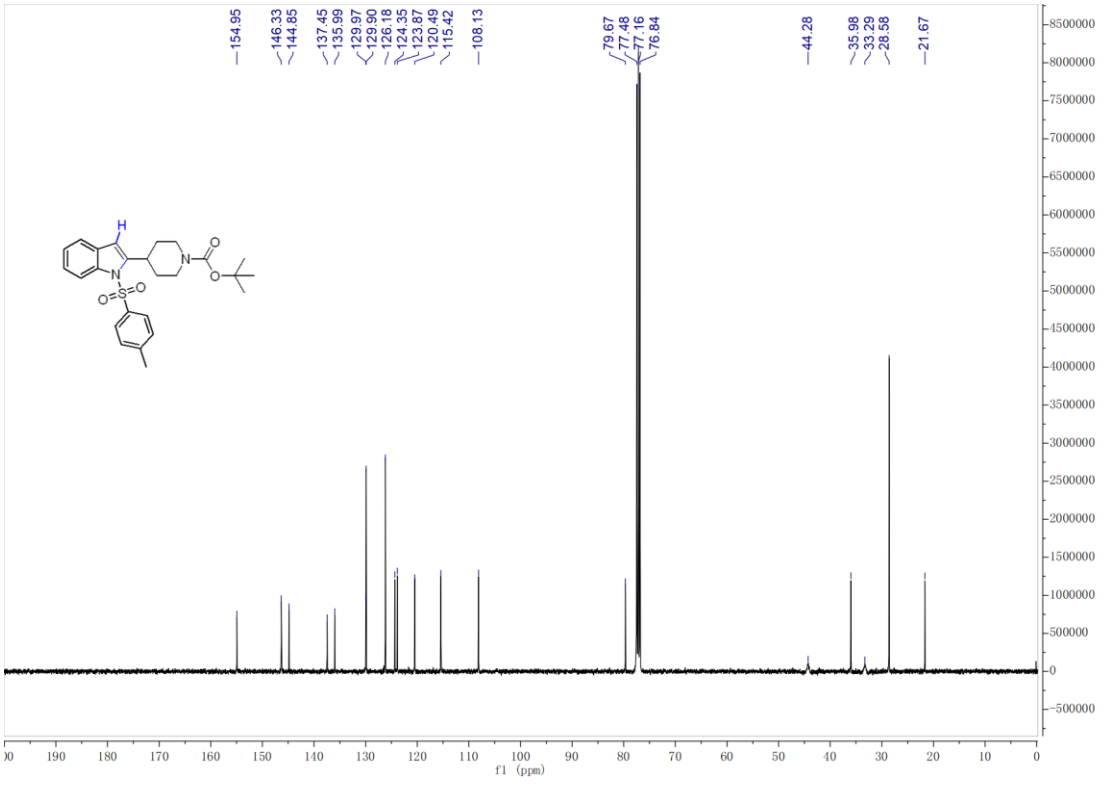
17c, $^{1}H + {}^{13}C$


8.07
8.07
8.06
8.05
8.04
8.04
8.04
8.03
8.03
8.03
8.02
8.02
7.46
7.45
7.45
7.44
7.43
7.42
7.42
7.41
7.41
7.40
7.40
7.40
7.39
7.39
7.26
7.21
7.21
7.19
7.19
7.19
7.18
7.17
7.16
7.15
7.15
7.11
7.11
7.10
7.09
6.63
2.29
1.61
0.98
3.00
2.03
2.01
1.00
3.03
9.28
f1 (ppm)

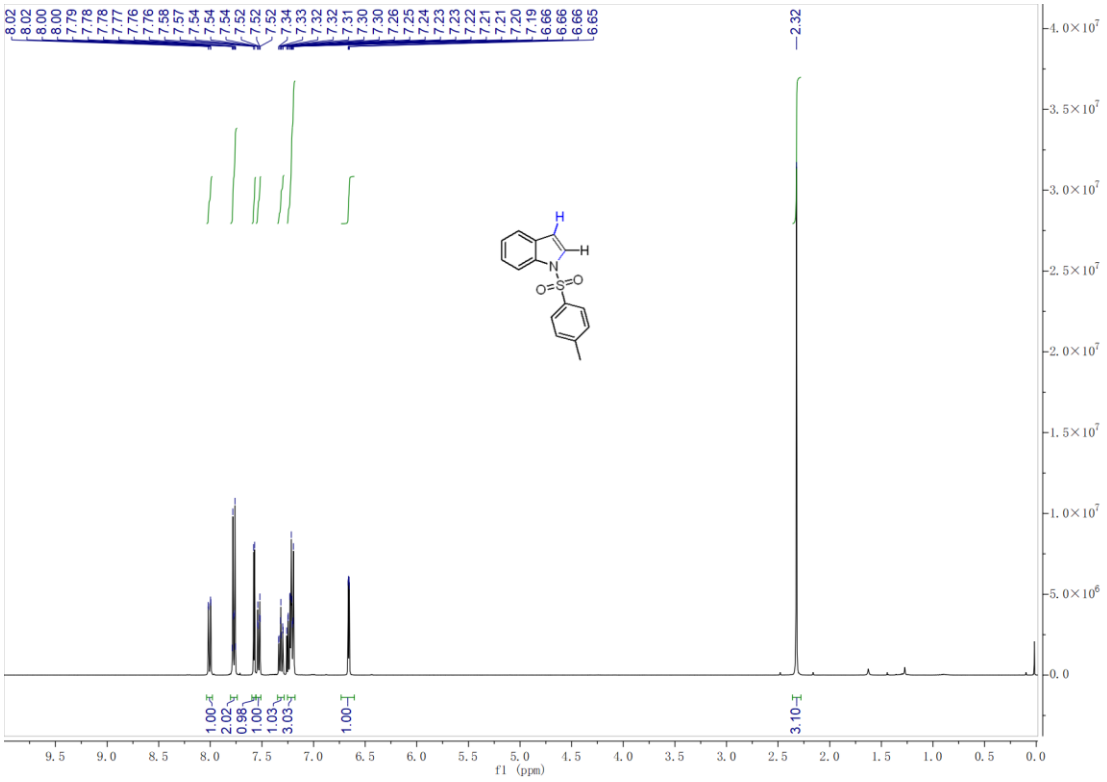

152.83
144.15
139.04
136.91
129.58
129.34
126.09
124.24
123.73
120.42
116.19
110.87
77.48
77.16
76.84
35.10
31.46
21.56
f1 (ppm)

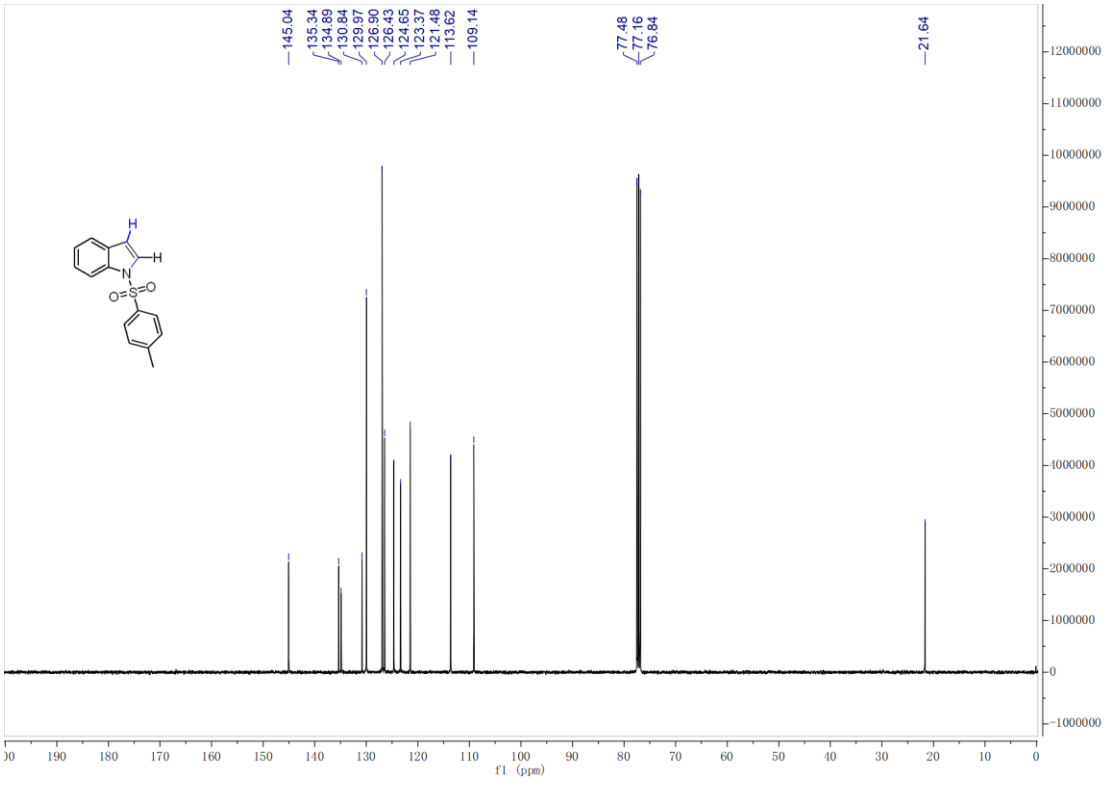
18c, $^{1}H + {}^{13}C$


8.16
8.16
8.14
8.14
7.55
7.53
7.42
7.42
7.42
7.40
7.40
7.28
7.28
7.26
7.26
7.26
7.24
7.24
7.22
7.22
7.20
7.20
7.19
7.18
7.17
7.15
6.42
4.25
4.22
3.51
3.50
3.49
3.48
3.47
3.46
3.45
3.44
3.43
2.91
2.90
2.87
2.87
2.84
2.84
2.32
2.10
2.09
2.09
2.07
2.06
2.06
1.48
0.00
1.00
2.00
1.04
4.40
1.00
2.01
1.01
2.00
3.01
1.99
1.98
9.12
f1 (ppm)

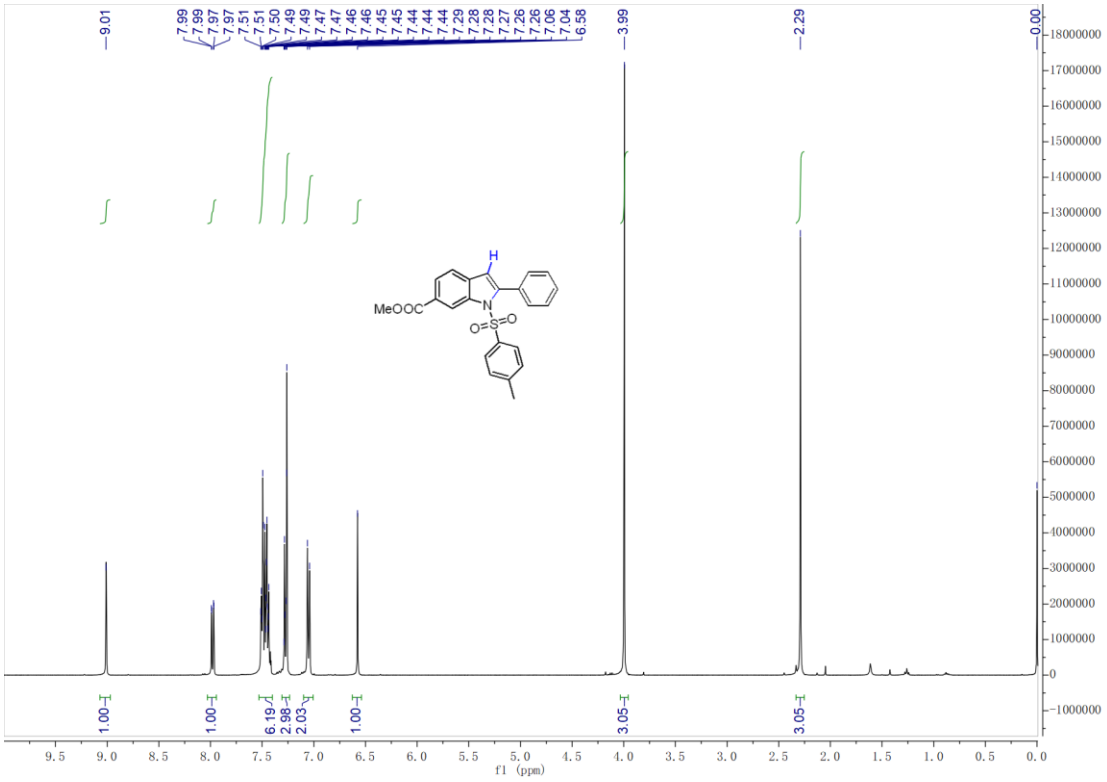

154.95
146.33
144.85
137.45
135.99
129.97
129.90
126.18
124.35
123.87
120.49
115.42
108.13
79.67
77.48
77.16
76.84
44.28
35.98
33.29
28.58
21.67
f1 (ppm)

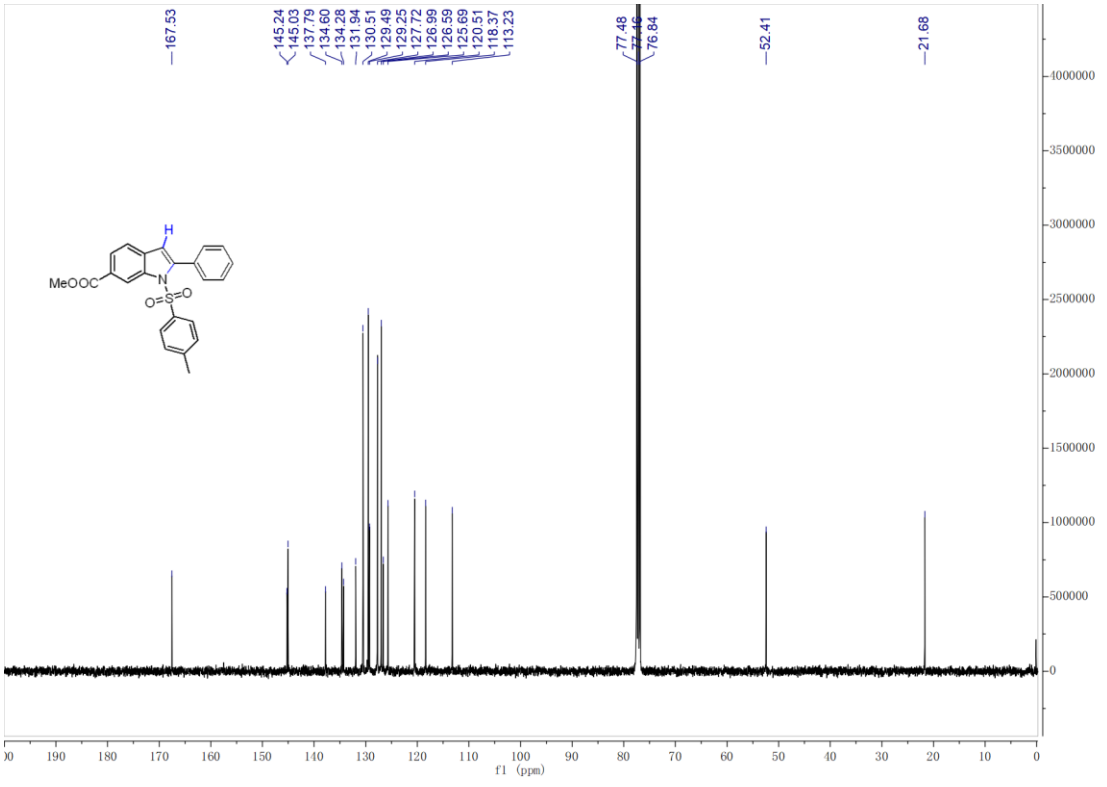
19c, $^{1}H + {}^{13}C$


8.02
8.02
8.00
8.00
7.79
7.78
7.78
7.77
7.76
7.76
7.58
7.57
7.54
7.54
7.54
7.52
7.52
7.52
7.34
7.33
7.32
7.32
7.31
7.30
7.30
7.26
7.25
7.24
7.23
7.23
7.22
7.21
7.21
7.20
7.19
6.66
6.66
6.66
6.65
2.32
1.00
2.02
0.98
1.00
1.03
3.03
1.00
3.10
f1 (ppm)

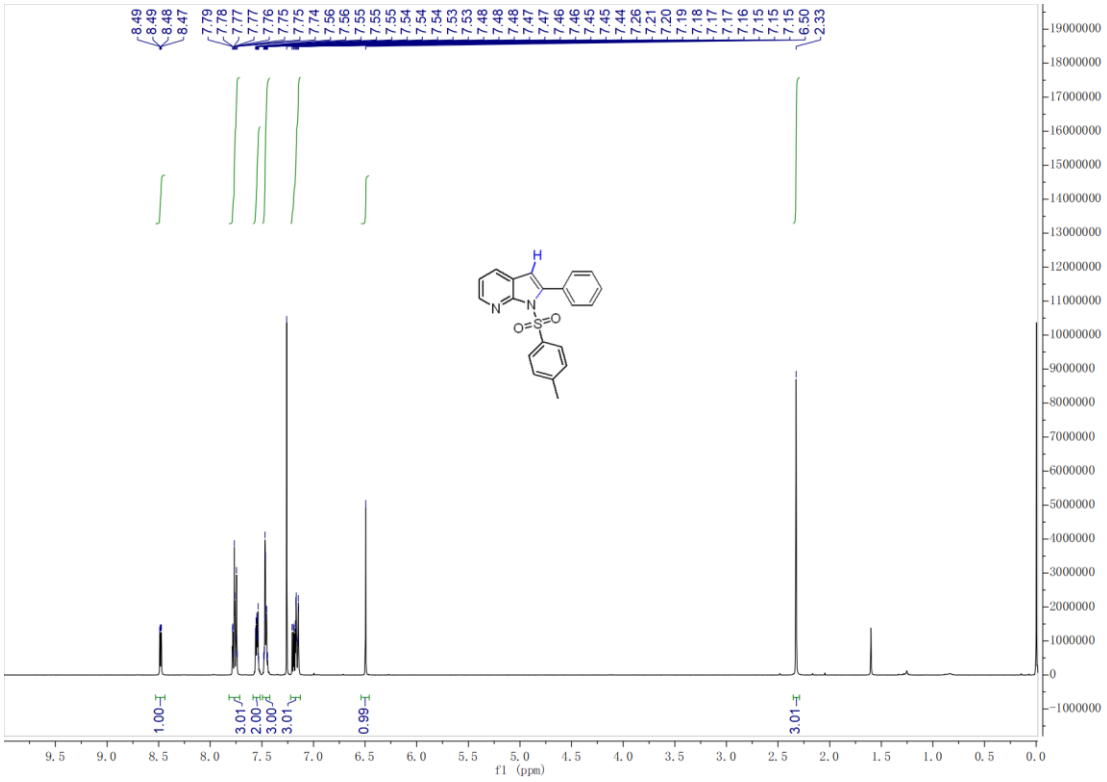

145.04
135.34
134.89
130.84
129.97
126.90
126.43
124.65
123.37
121.48
113.62
109.14
77.48
77.16
76.84
21.64
f1 (ppm)

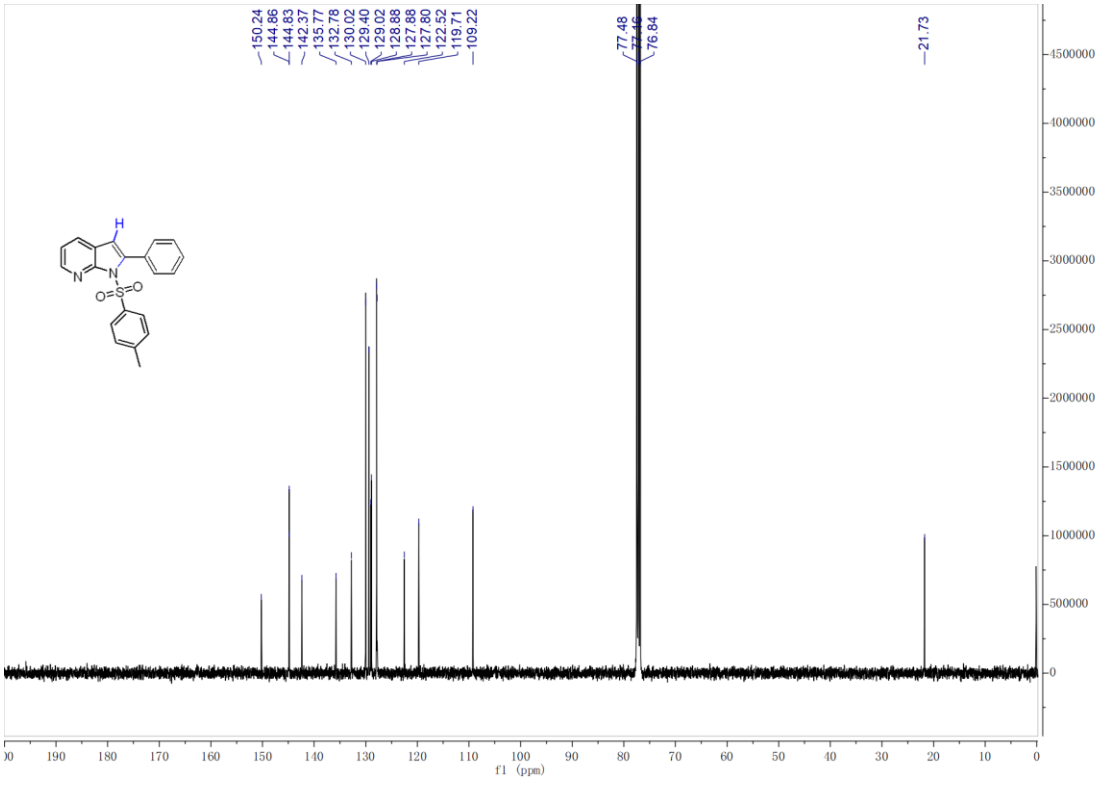
26c, $^{1}H + {}^{13}C$


9.01
7.99
7.97
7.51
7.50
7.49
7.47
7.46
7.45
7.44
7.29
7.28
7.27
7.26
7.06
7.04
6.58
3.99
2.29
0.00
MeOOC
1.00
1.00
6.19
2.98
2.03
1.00
3.05
3.05
f1 (ppm)

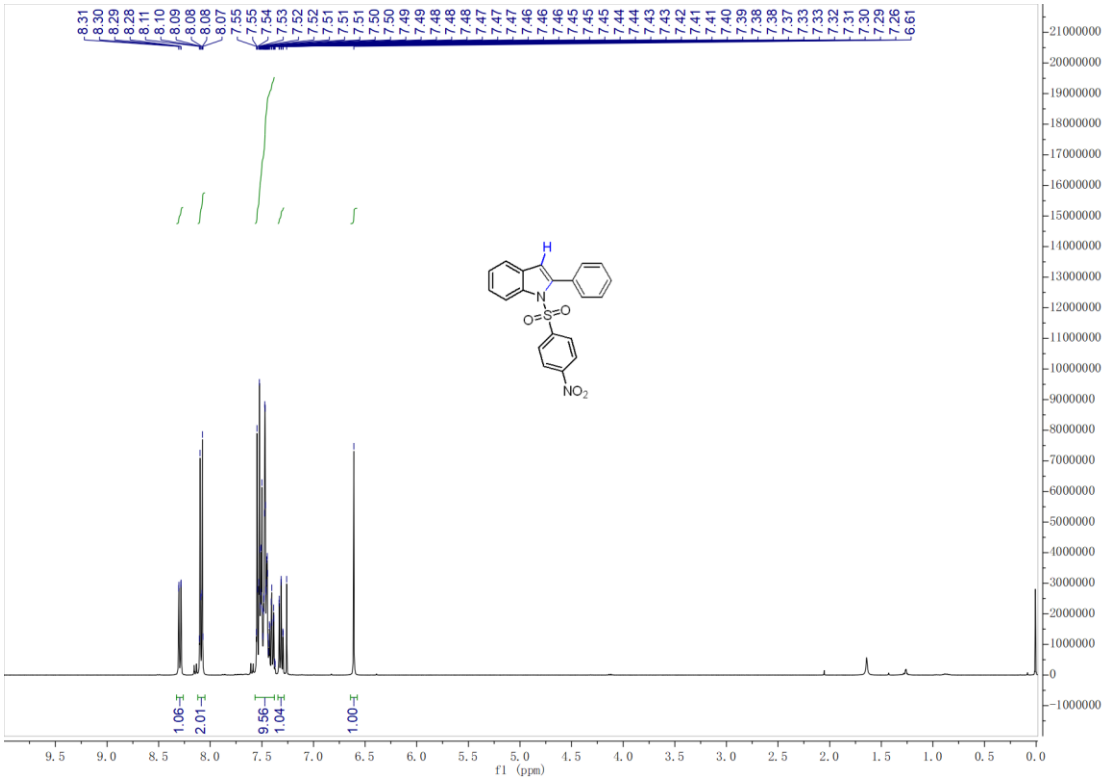

167.53
145.24
145.03
137.79
134.60
134.28
131.94
130.51
129.49
129.25
127.72
126.99
126.59
125.69
120.51
118.37
113.23
77.48
77.16
76.84
52.41
21.68
MeOOC
f1 (ppm)

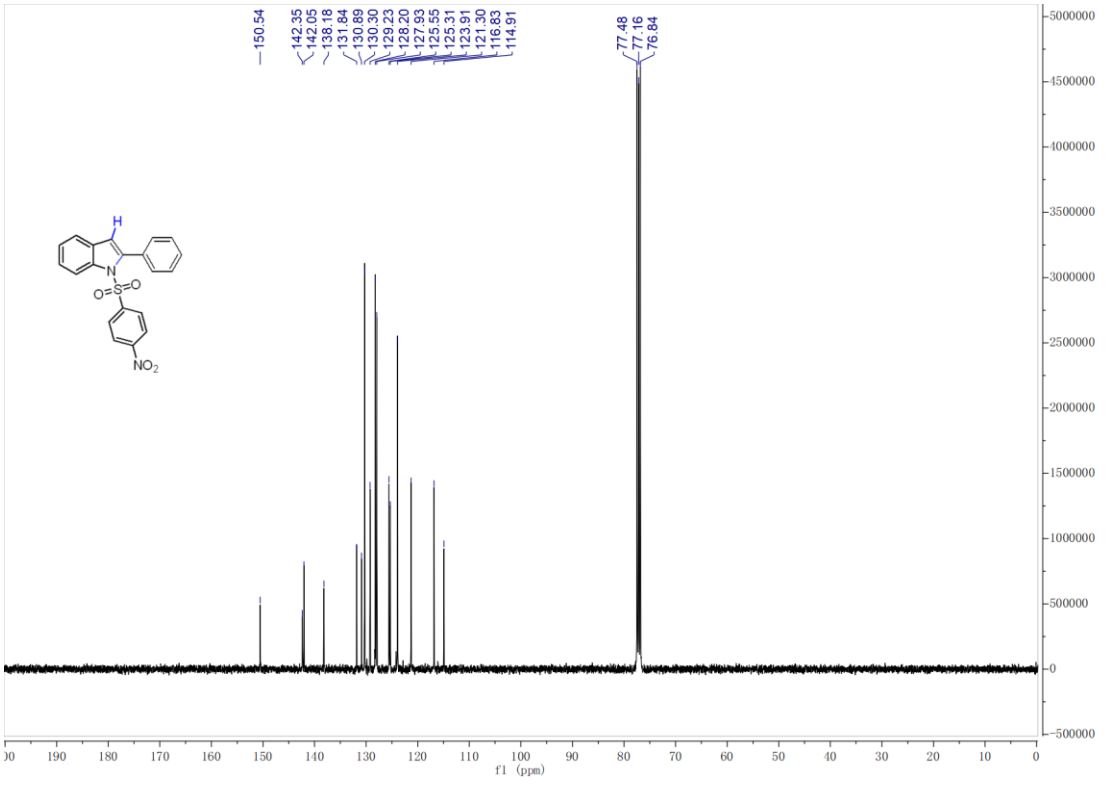
27c, $^{1}H + {}^{13}C$


8.49
8.48
8.47
7.79
7.78
7.77
7.76
7.75
7.74
7.56
7.55
7.54
7.53
7.48
7.47
7.46
7.45
7.44
7.26
7.21
7.20
7.19
7.18
7.17
7.16
7.15
6.50
2.33
1.00
3.01
2.00
3.00
3.01
0.99
3.01
f1 (ppm)

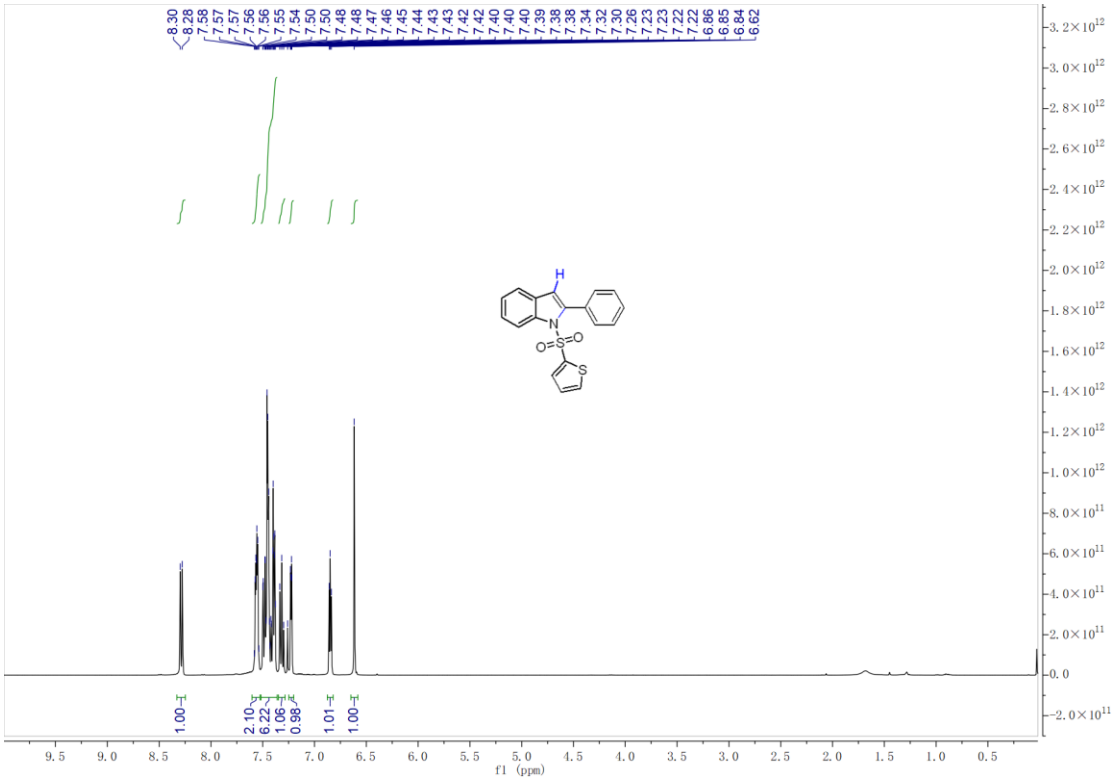

150.24
144.86
144.83
142.37
135.77
132.78
130.02
129.40
129.02
128.88
127.88
127.80
122.52
119.71
109.22
77.48
77.16
76.84
21.73
f1 (ppm)

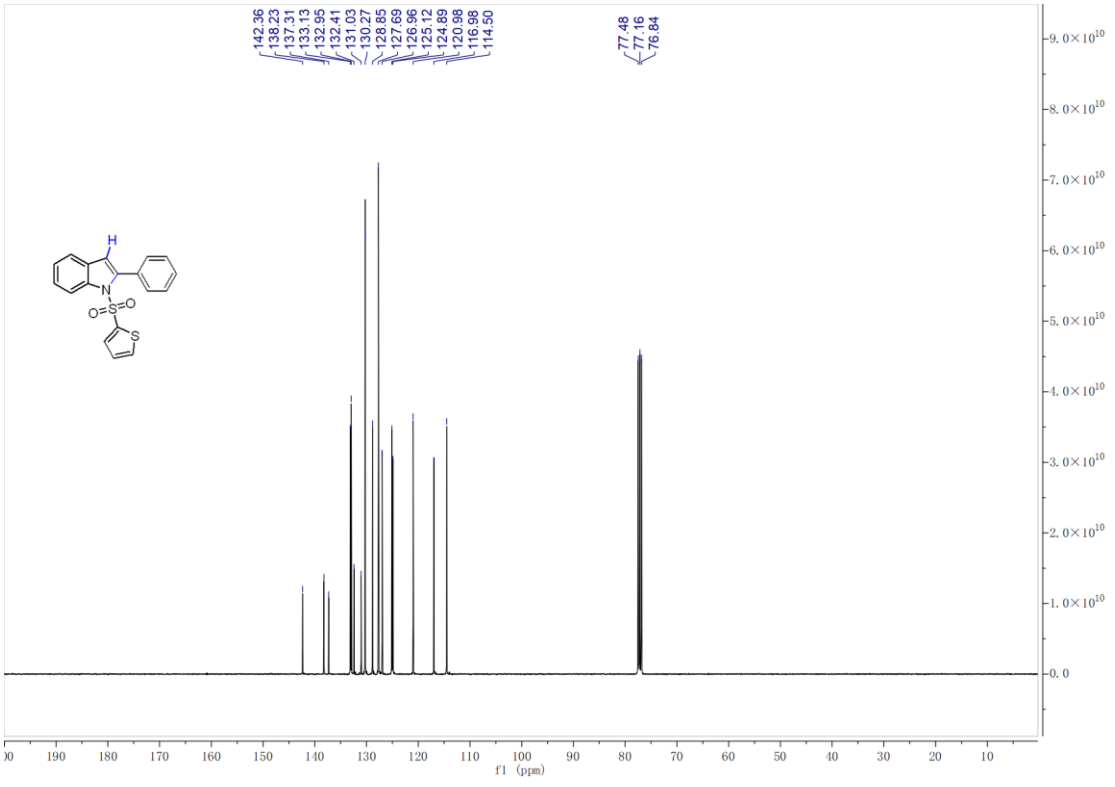
30c, $^{1}H + {}^{13}C$


8.31
8.30
8.29
8.28
8.11
8.10
8.09
8.08
8.08
8.07
7.55
7.54
7.53
7.52
7.52
7.51
7.51
7.51
7.50
7.50
7.49
7.49
7.48
7.48
7.47
7.47
7.47
7.46
7.46
7.45
7.45
7.45
7.44
7.44
7.43
7.43
7.42
7.41
7.41
7.40
7.39
7.38
7.38
7.37
7.33
7.33
7.32
7.31
7.30
7.29
7.26
6.61
H
N
O=S=O
NO2
1.06
2.01
9.56
1.04
1.00
f1 (ppm)

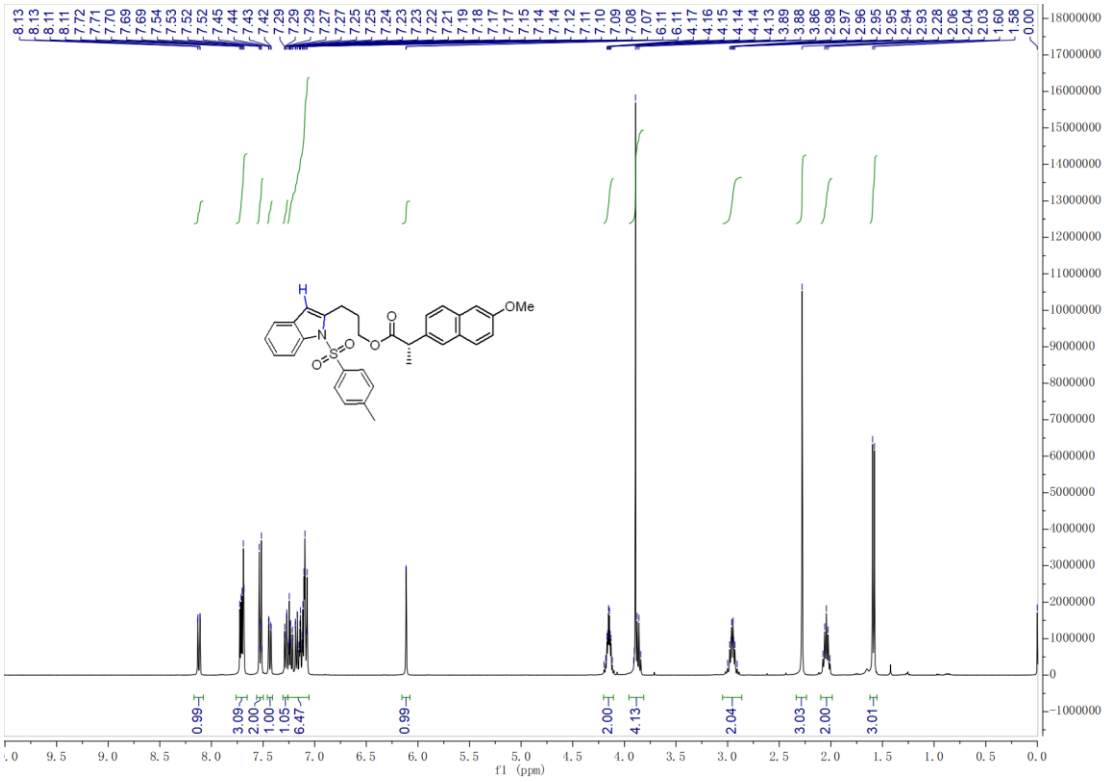

150.54
142.35
142.05
138.18
131.84
130.89
130.30
129.23
128.20
127.93
125.55
125.31
123.91
121.30
116.83
114.91
77.48
77.16
76.84
H
N
O=S=O
NO2
f1 (ppm)

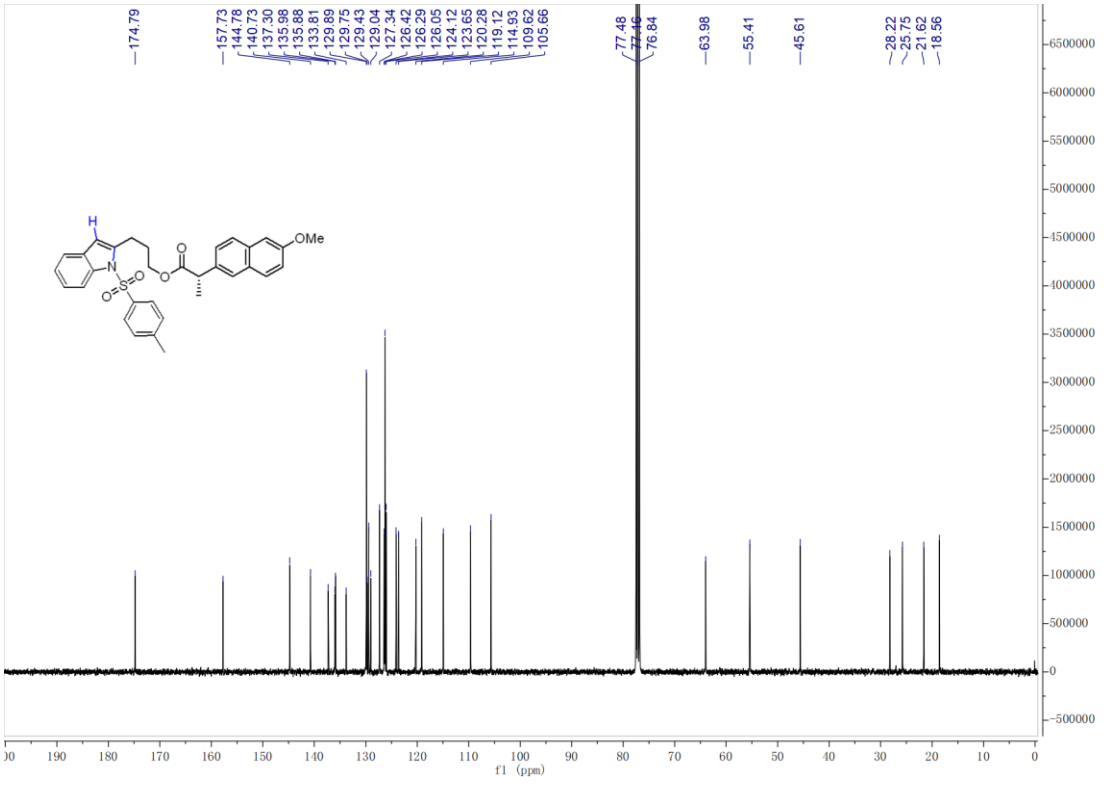
34c, $^{1}H + {}^{13}C$


8.30
8.28
7.58
7.57
7.57
7.56
7.56
7.55
7.54
7.50
7.50
7.48
7.48
7.47
7.46
7.45
7.44
7.43
7.43
7.42
7.42
7.40
7.40
7.40
7.39
7.38
7.38
7.34
7.32
7.30
7.26
7.23
7.22
7.22
6.86
6.85
6.84
6.62
1.00
2.10
6.22
1.06
0.98
1.01
1.00
f1 (ppm)

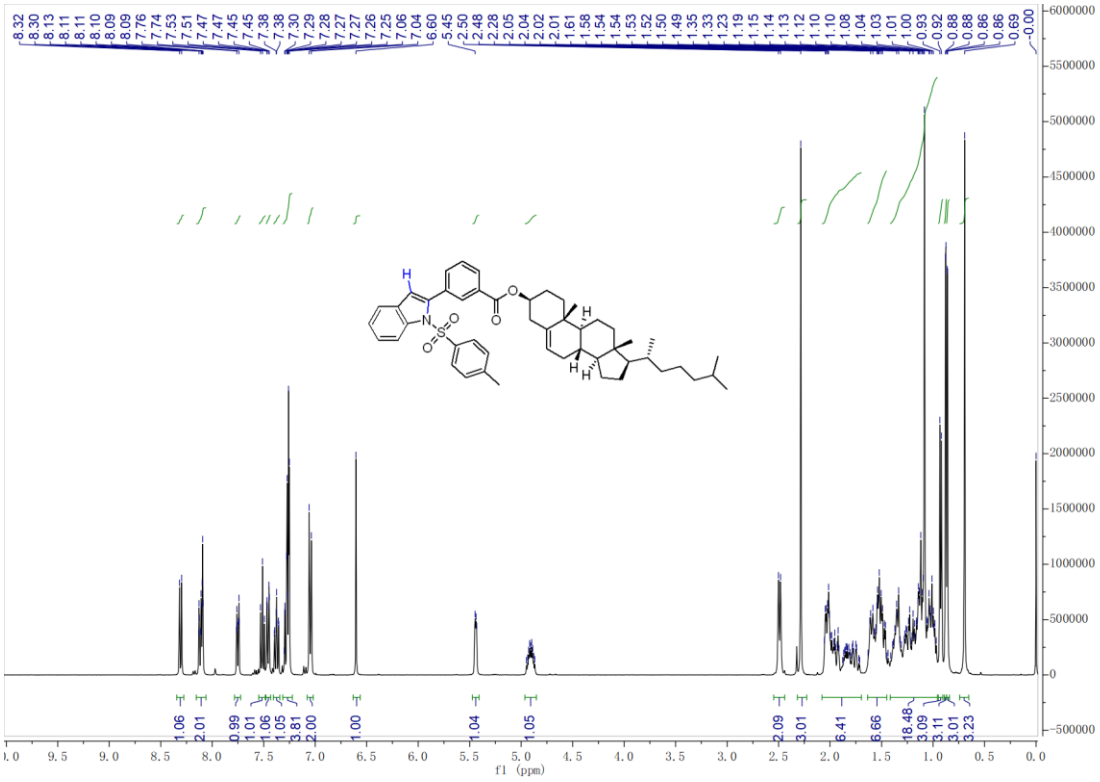

142.36
138.23
137.31
133.13
132.95
132.41
131.03
130.27
128.85
127.69
126.96
125.12
124.89
120.98
116.98
114.50
77.48
77.16
76.84
f1 (ppm)

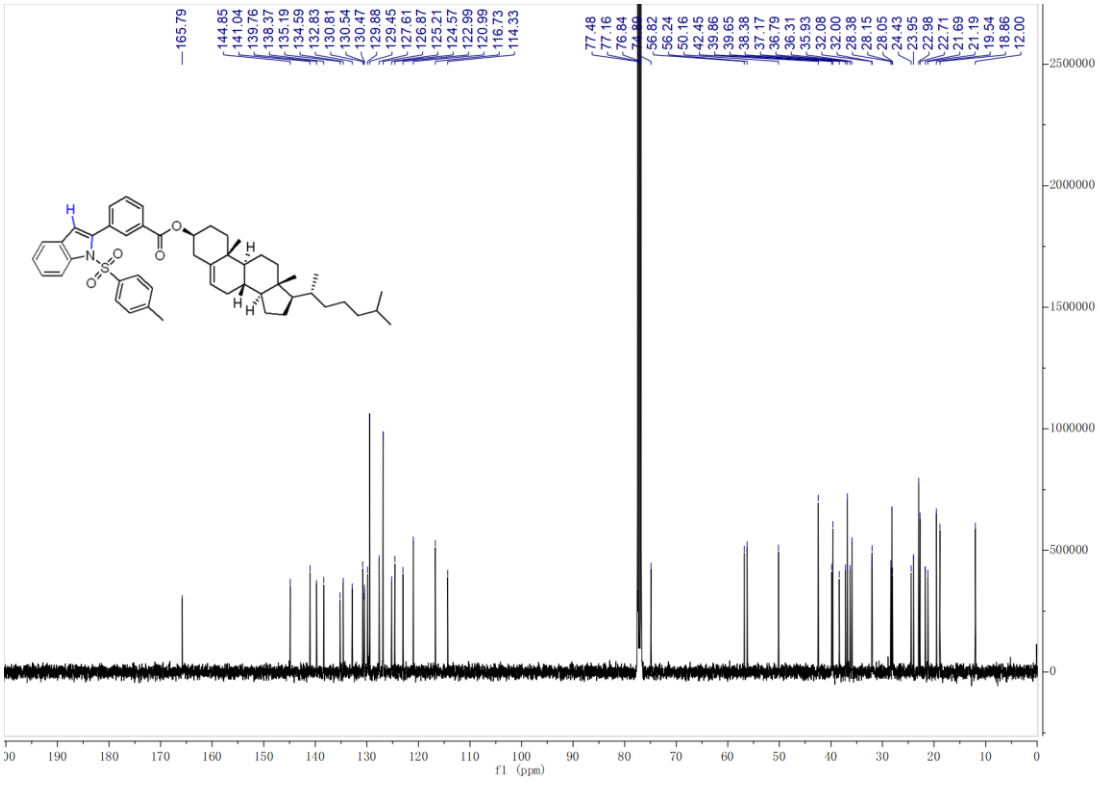
43c, $^{1}H + {}^{13}C$


8.13
8.13
8.11
8.11
7.72
7.71
7.70
7.69
7.69
7.54
7.53
7.52
7.52
7.45
7.44
7.43
7.42
7.29
7.29
7.29
7.27
7.27
7.25
7.25
7.24
7.23
7.23
7.22
7.21
7.19
7.18
7.17
7.17
7.15
7.14
7.14
7.12
7.11
7.10
7.09
7.08
7.07
6.11
6.11
4.17
4.16
4.15
4.14
4.14
4.13
3.89
3.88
3.86
2.98
2.97
2.96
2.95
2.95
2.94
2.93
2.28
2.06
2.04
2.03
1.60
1.58
0.00
OMe
0.99
3.09
2.00
1.00
1.05
6.47
0.99
2.00
4.13
2.04
3.03
2.00
3.01
f1 (ppm)

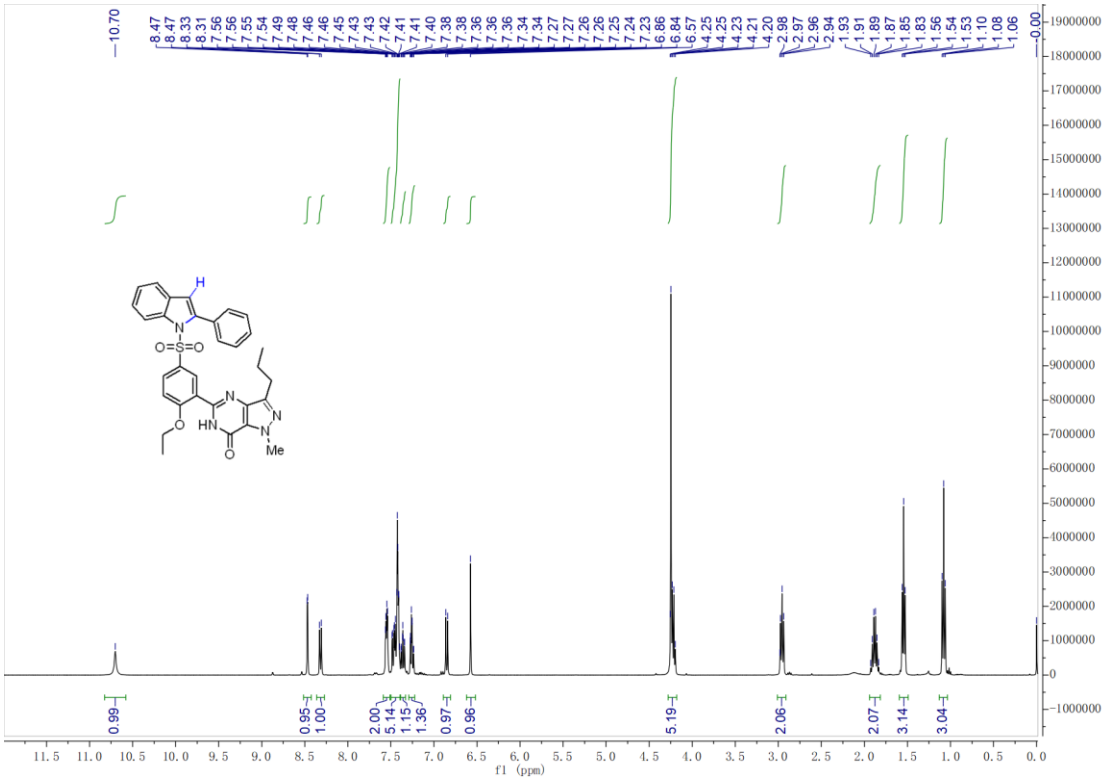

174.79
157.73
144.78
140.73
137.30
135.98
135.88
133.81
129.89
129.75
129.43
129.04
127.34
126.42
126.29
126.05
124.12
123.65
120.28
119.12
114.93
109.62
105.66
77.48
77.16
76.84
63.98
55.41
45.61
28.22
25.75
21.62
18.56
OMe
f1 (ppm)

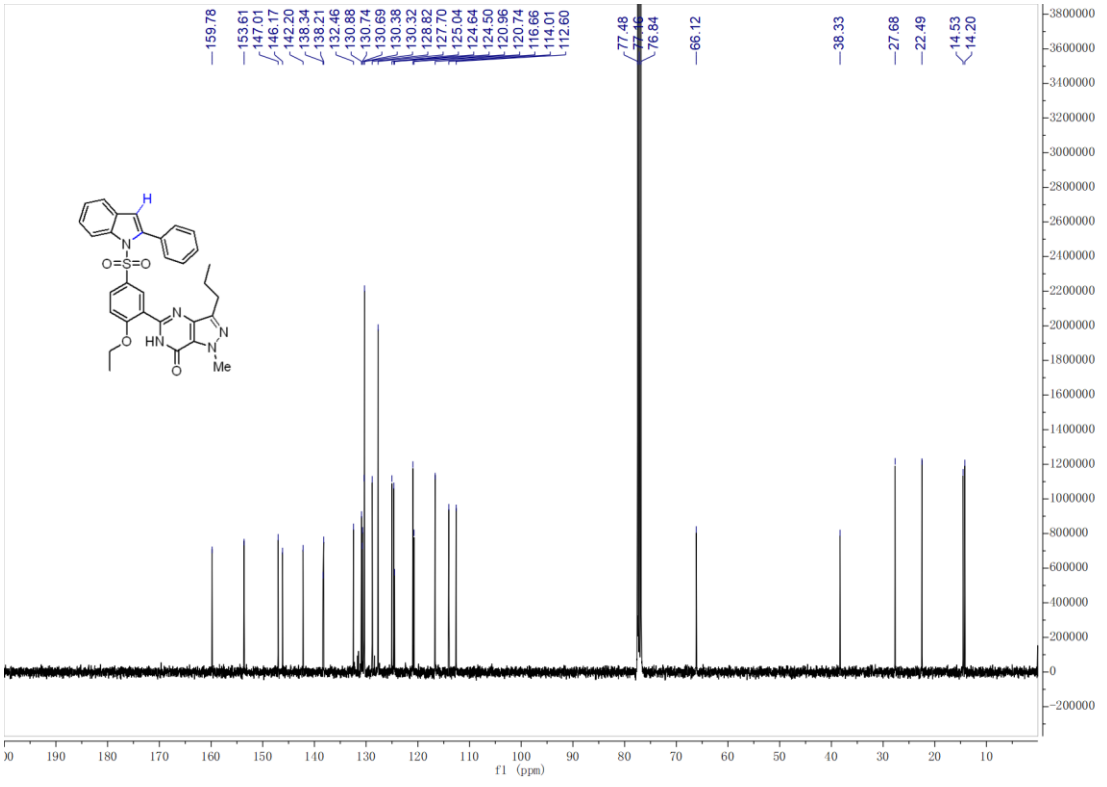
44c, $^{1}H + {}^{13}C$



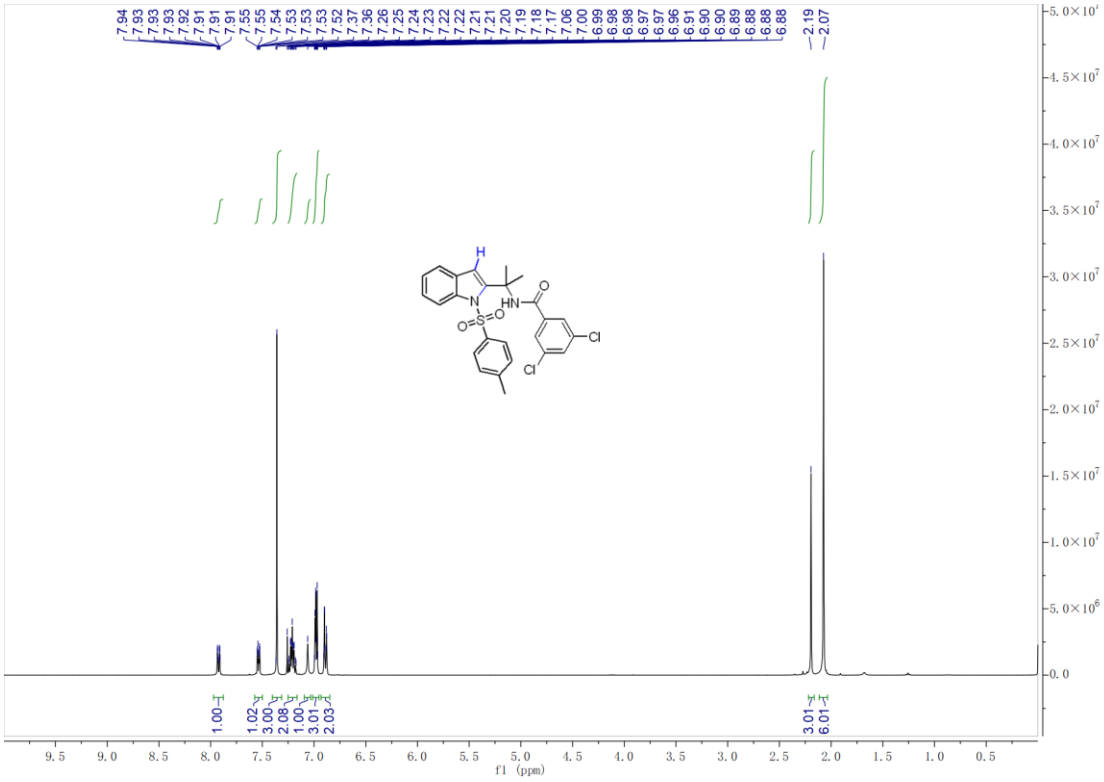


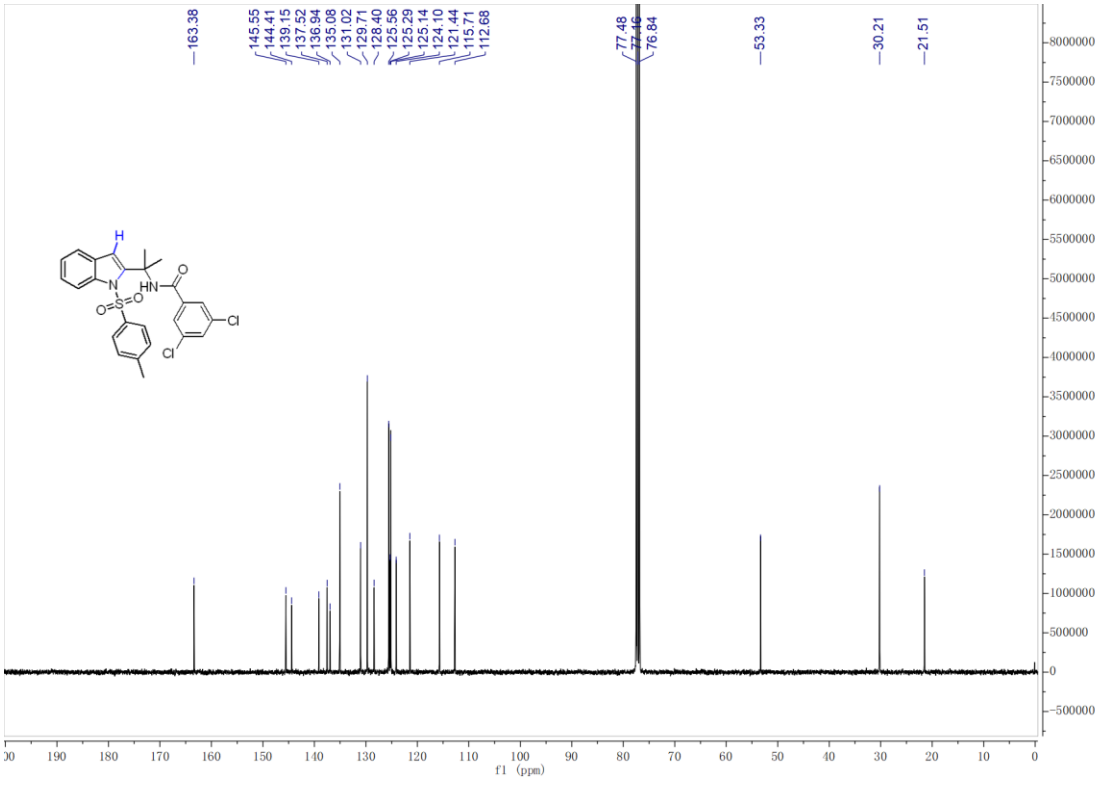
45c, $^{1}H + {}^{13}C$


10.70
8.47
8.47
8.33
8.31
7.56
7.56
7.55
7.54
7.49
7.48
7.46
7.46
7.45
7.43
7.43
7.42
7.41
7.41
7.40
7.38
7.38
7.36
7.36
7.36
7.34
7.34
7.27
7.27
7.26
7.26
7.25
7.24
7.23
6.86
6.84
6.57
4.25
4.25
4.23
4.21
4.20
2.98
2.97
2.96
2.94
1.93
1.91
1.89
1.87
1.85
1.83
1.56
1.54
1.53
1.10
1.08
1.06
0.00
0.99
0.95
1.00
2.00
5.14
1.15
1.36
0.97
0.96
5.19
2.06
2.07
3.14
3.04
f1 (ppm)

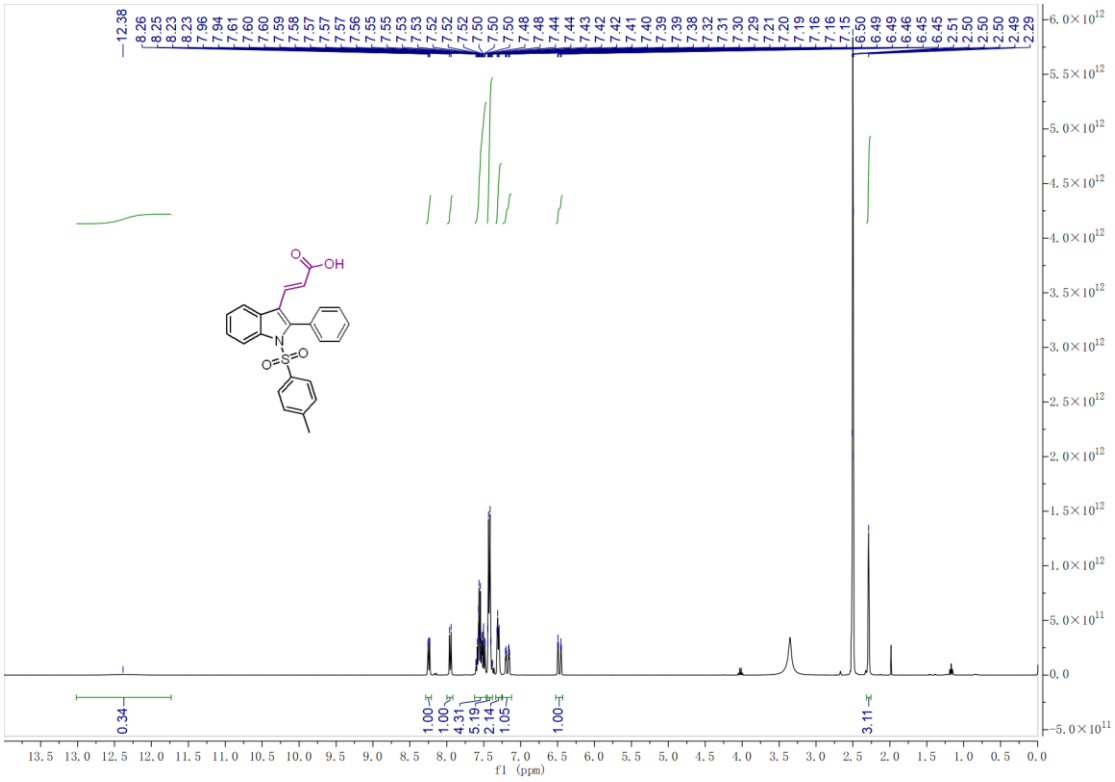

159.78
153.61
147.01
146.17
142.20
138.34
138.21
132.46
130.88
130.74
130.69
130.38
130.32
128.82
127.70
125.04
124.64
124.50
120.96
120.74
116.66
114.01
112.60
77.48
77.16
76.84
66.12
38.33
27.68
22.49
14.53
14.20
f1 (ppm)

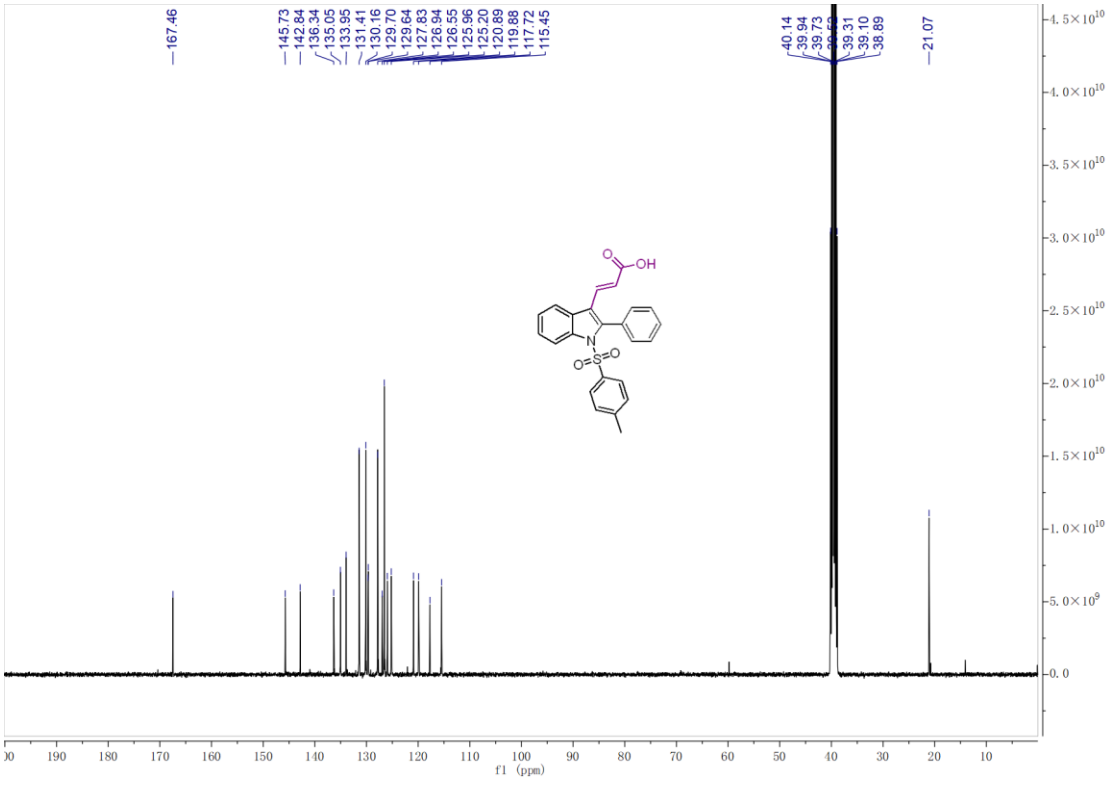
46c, $^{1}H + {}^{13}C$


7.94
7.93
7.93
7.93
7.92
7.91
7.91
7.91
7.55
7.55
7.54
7.53
7.53
7.53
7.52
7.37
7.36
7.26
7.25
7.24
7.23
7.22
7.22
7.21
7.21
7.20
7.19
7.18
7.17
7.06
7.00
6.99
6.98
6.98
6.97
6.97
6.96
6.91
6.90
6.90
6.89
6.88
6.88
6.88
2.19
2.07
1.00
1.02
3.00
2.08
1.00
3.01
2.03
3.01
6.01
f1 (ppm)

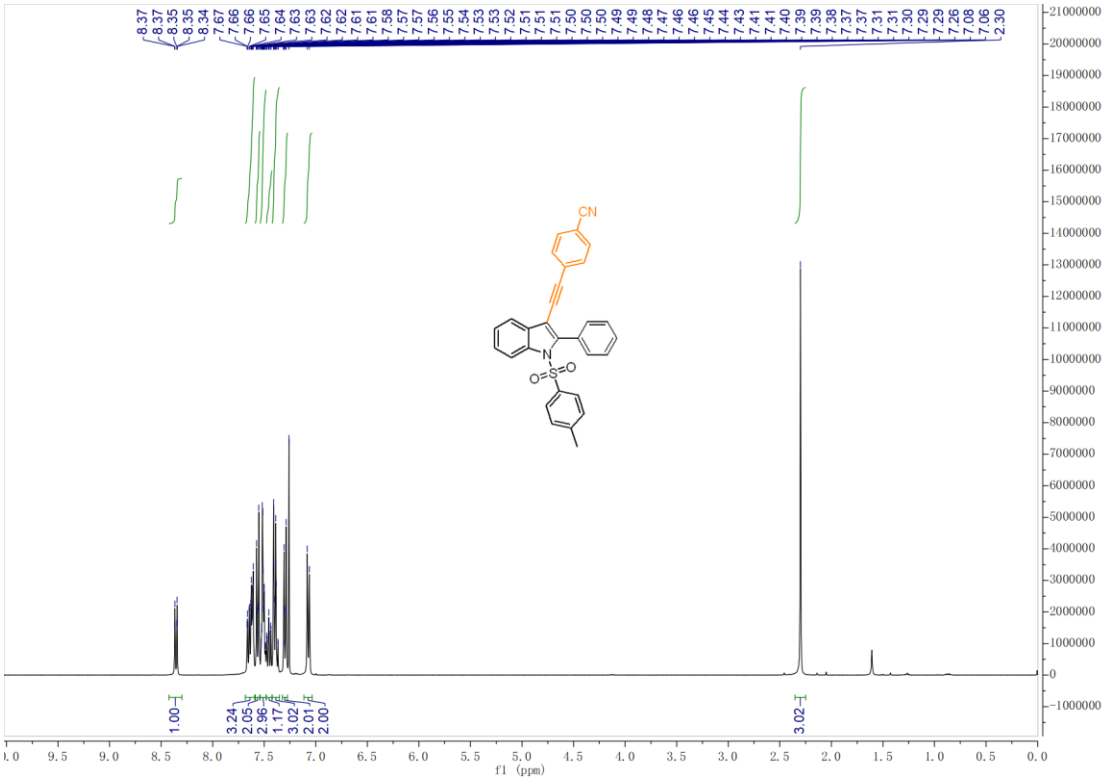

163.38
145.55
144.41
139.15
137.52
136.94
135.08
131.02
129.71
128.40
125.56
125.29
125.14
124.10
121.44
115.71
112.68
77.48
77.16
76.84
53.33
30.21
21.51
f1 (ppm)

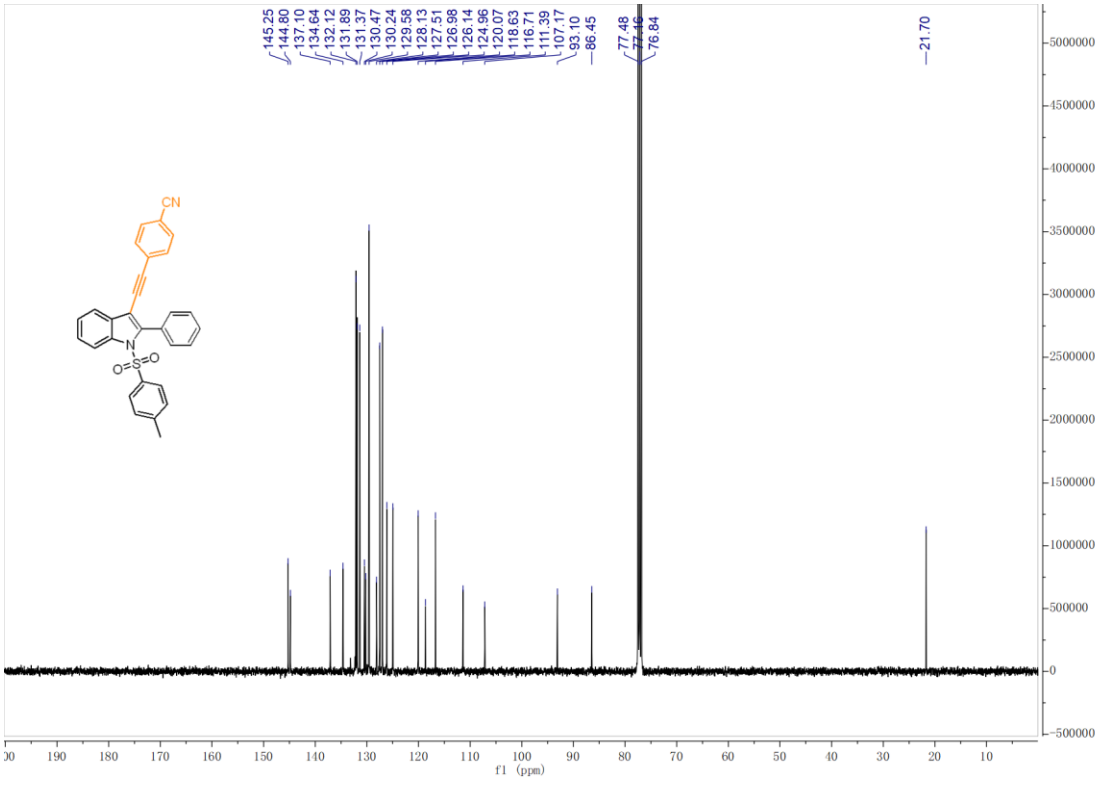
1d, $^{1}H + ^{13}C$


12.38
8.26
8.25
8.23
8.23
7.96
7.94
7.61
7.60
7.60
7.59
7.58
7.57
7.57
7.57
7.56
7.55
7.55
7.53
7.53
7.52
7.52
7.52
7.50
7.50
7.50
7.48
7.48
7.44
7.44
7.43
7.42
7.42
7.41
7.40
7.39
7.39
7.38
7.32
7.31
7.30
7.29
7.21
7.20
7.19
7.16
7.16
7.15
6.50
6.49
6.49
6.46
6.45
6.45
2.51
2.50
2.50
2.50
2.49
2.29
OH
O
N
O=S=O
0.34
1.00
1.00
4.31
5.19
2.14
1.05
1.00
3.11
f1 (ppm)

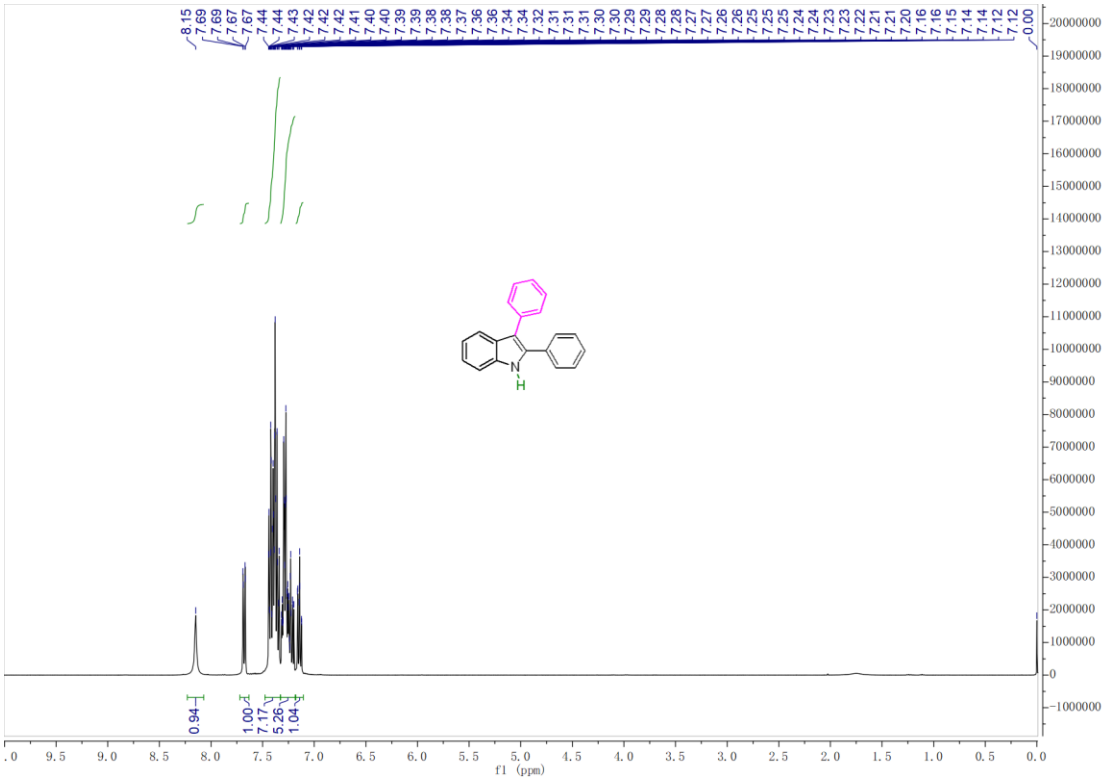

167.46
145.73
142.84
136.34
135.05
133.95
131.41
130.16
129.70
129.64
127.83
126.94
126.55
125.96
125.20
120.89
119.88
117.72
115.45
40.14
39.94
39.73
39.52
39.31
39.10
38.89
21.07
OH
O
N
O=S=O
f1 (ppm)

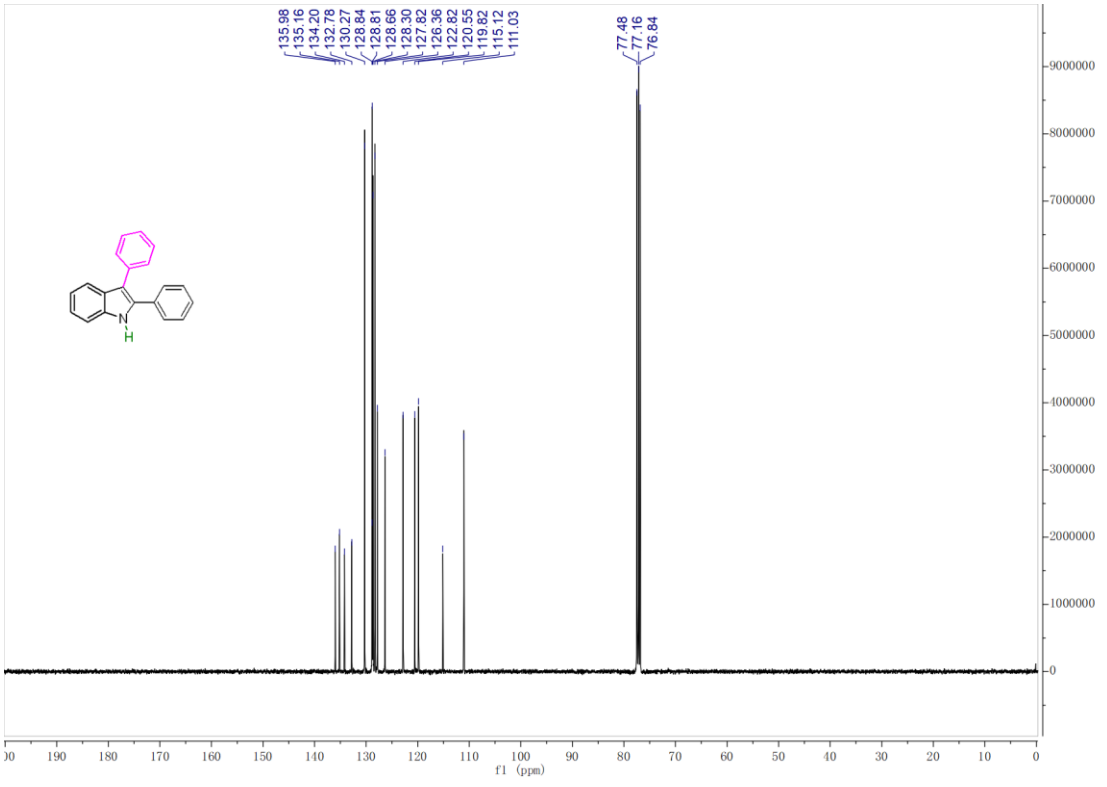
1e, $^{1}H + ^{13}C$


8.37
8.37
8.35
8.35
8.34
7.67
7.66
7.66
7.65
7.64
7.64
7.63
7.63
7.62
7.62
7.61
7.61
7.58
7.57
7.57
7.56
7.55
7.54
7.53
7.53
7.52
7.51
7.51
7.51
7.50
7.50
7.50
7.49
7.49
7.48
7.47
7.46
7.46
7.45
7.44
7.43
7.41
7.41
7.40
7.39
7.39
7.38
7.37
7.37
7.31
7.31
7.30
7.29
7.29
7.26
7.08
7.06
2.30
CN
1.00
3.24
2.05
2.96
1.17
3.02
2.01
2.00
3.02
f1 (ppm)

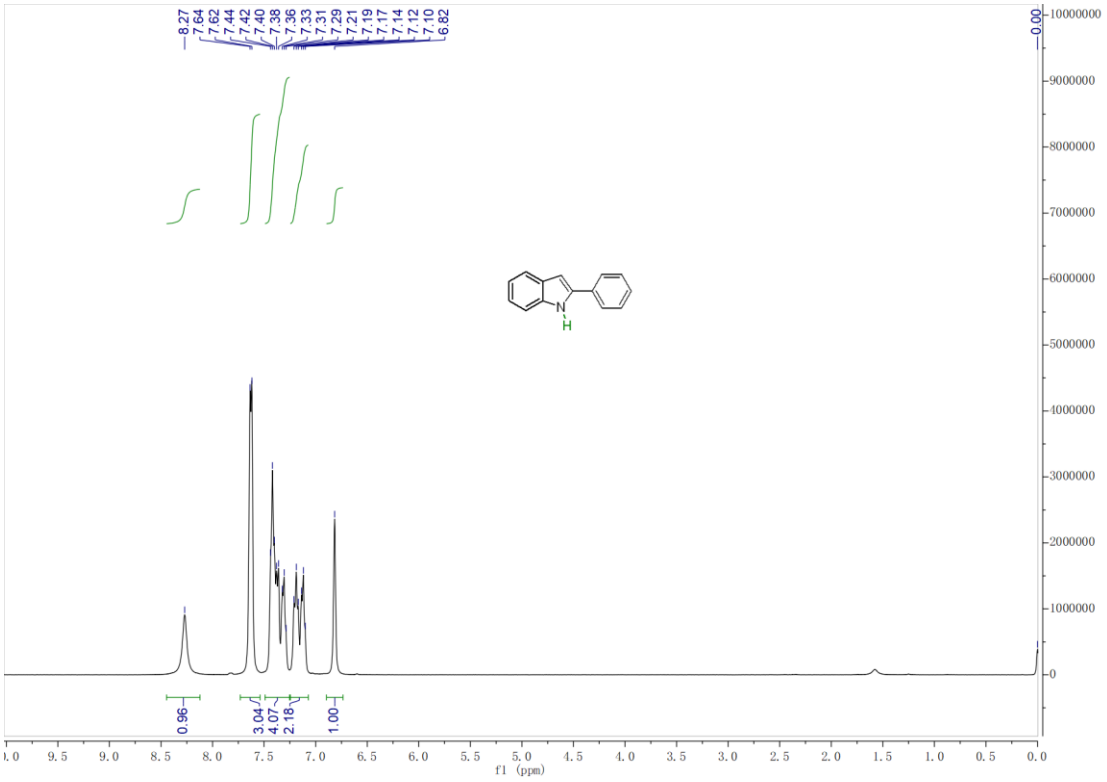

145.25
144.80
137.10
134.64
132.12
131.89
131.37
130.47
130.24
129.58
128.13
127.51
126.98
126.14
124.96
120.07
118.63
116.71
111.39
107.17
93.10
86.45
77.48
77.16
76.84
21.70
CN
f1 (ppm)

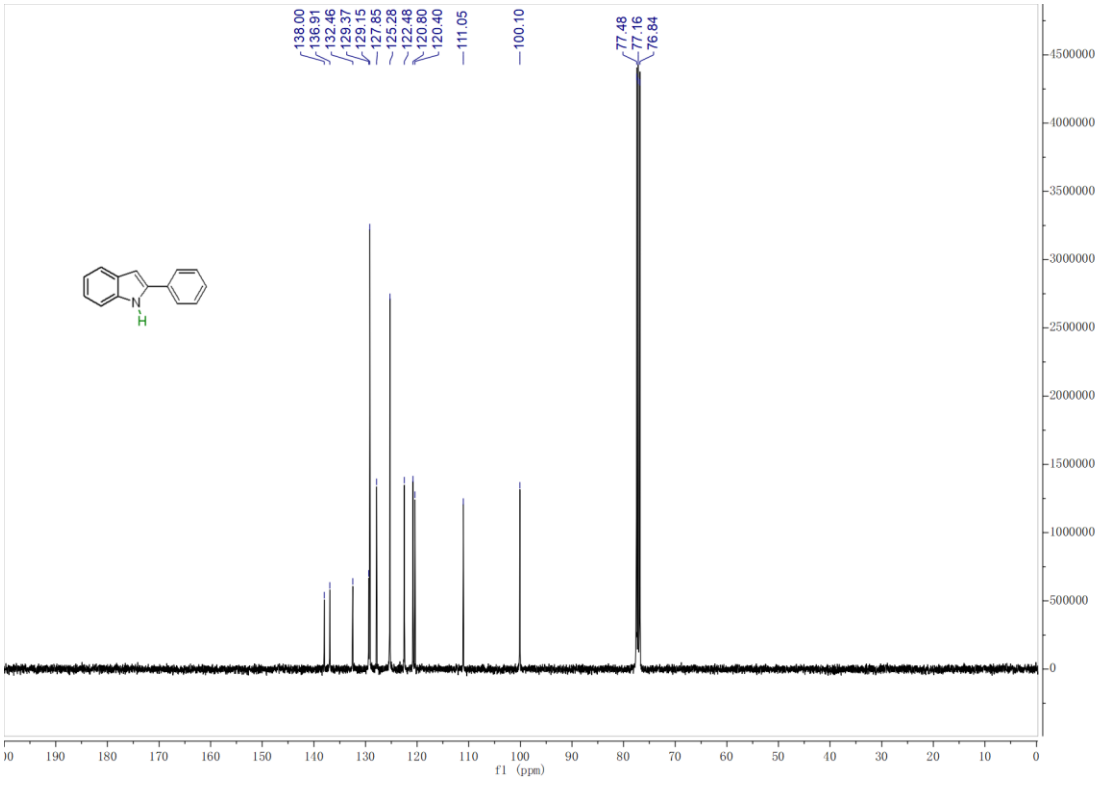
1f, $^{1}H + {}^{13}C$


8.15
7.69
7.69
7.67
7.67
7.44
7.44
7.43
7.42
7.42
7.42
7.41
7.40
7.40
7.39
7.39
7.38
7.38
7.37
7.36
7.36
7.34
7.34
7.32
7.31
7.31
7.30
7.30
7.29
7.29
7.28
7.28
7.27
7.27
7.26
7.26
7.25
7.25
7.24
7.24
7.23
7.23
7.22
7.21
7.21
7.20
7.16
7.16
7.15
7.14
7.14
7.12
7.12
0.00
0.94
1.00
7.17
5.26
1.04
f1 (ppm)


135.98
135.16
134.20
132.78
130.27
128.84
128.81
128.66
128.30
127.82
126.36
122.82
120.55
119.82
115.12
111.03
77.48
77.16
76.84
f1 (ppm)

1g, $^{1}H + ^{13}C$


8.27
7.64
7.62
7.44
7.42
7.40
7.38
7.36
7.33
7.31
7.29
7.21
7.19
7.17
7.14
7.12
7.10
6.82
0.00
0.96
3.04
4.07
2.18
1.00
f1 (ppm)


138.00
136.91
132.46
129.37
129.15
127.85
125.28
122.48
120.80
120.40
111.05
100.10
77.48
77.16
76.84
f1 (ppm)