

## Supplementary Information for:

### Copper-Catalyzed Intramolecular Dearomative Aza-Wacker Reaction of Indole

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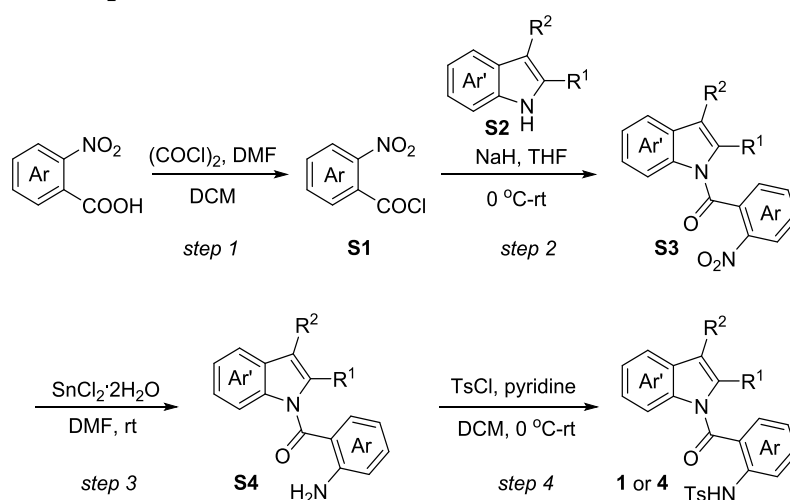
#### Table of Contents

1. General Information.....	S1
2. Procedure for Preparation of Substrates .....	S1
3. Procedure for Copper-Catalyzed Intramolecular Dearomatizing Oxidative Amination of Indoles <b>1</b> and <b>4</b> .....	S2
4. Characterization of Substrates and Products .....	S3
5. Crystal Report for the Mixture of <b>2b</b> and <b>6</b> .....	S24
6. Copies of NMR Spectra.....	S26

## 1. General Information

All reagents were purchased from commercial suppliers with the highest purity grade, and used directly without further purification.  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra were recorded on Bruker AVANCE III 400 MHz or 500 MHz using  $\text{CDCl}_3$  as solvent with TMS as the internal standard. Melting points were measured on a Büchi Melting Point B-545 apparatus and uncorrected. HRMS were recorded on Thermo Scientific LTQ Orbitrap XL or Agilent 6210 TOF LC/MS mass spectrometer. Solvents were purified prior to use according to conventional procedures. Reactions were monitored by thin layer chromatography (TLC) using silica gel plates. Column chromatography was carried out using silica gel (200-300 mesh).

## 2. Procedure for Preparation of Substrates



**Step 1:** To a solution of 2-nitrobenzoic acid (1.0 equiv) in anhydrous DCM was added oxalyl chloride (3.0 equiv) and DMF (two drops) at room temperature. The resulting mixture was allowed to stir for 2 h. When the reaction was completed, the solution was concentrated under reduced pressure. The obtained crude product was used for the next step without further purification.

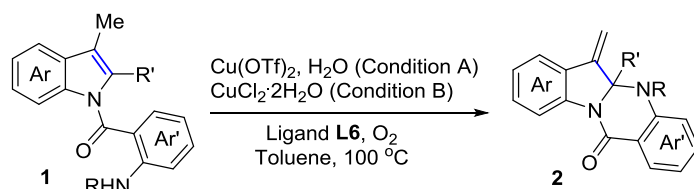
**Step 2: Synthesis of *N*-acylindoles **S3**.** To a dried Schlenk tube was charged with indole **S2** (1.0 equiv) and THF under  $\text{N}_2$  atmosphere. Sodium hydride (60 wt%, 1.5 equiv) was then added in portions at 0 °C. After stirring at 0 °C for 40 min, the above crude of 2-nitrobenzoic chloride derivatives **S1** (1.5 equiv) was added dropwise. The resulting mixture was allowed to stir at room temperature for 2 h. When the reaction was completed, the mixture was quenched with water and extracted with DCM. The combined organic layers were dried over  $\text{Na}_2\text{SO}_4$  and concentrated under reduced pressure. The residue was purified by flash column chromatography on silica gel eluting with petroleum ether/ethyl acetate (10:1) to afford **S3**.

**Step 3: Reduction of the nitro group.** To a solution of **S3** (1.0 equiv) in DMF in the Schlenk tube was added stannous chloride dihydrate ( $\text{SnCl}_2 \cdot 2\text{H}_2\text{O}$ , 9.0 equiv). The

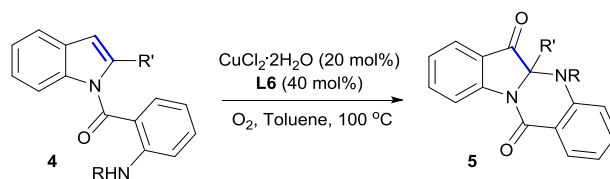
resulting mixture was stirred at room temperature for 3 h. When the reaction was completed, the reaction system was quenched with water and extracted with ethyl acetate. The combined organic layers were dried over Na<sub>2</sub>SO<sub>4</sub> and concentrated under reduced pressure. The residue was purified by flash chromatography on silica gel eluting with petroleum ether/ethyl acetate (20:1) to afford **S4**.

**Step 4: Acylation of amine.** To a solution of **S4** (1.0 equiv) in DCM in the Schlenk tube was added pyridine (1.5 equiv) and TsCl (1.2 equiv). The resulting mixture was allowed to stir at room temperature overnight. When the reaction was completed, the reaction mixture was extracted with ethyl acetate. The combined organic layers were dried over Na<sub>2</sub>SO<sub>4</sub> and concentrated under reduced pressure. The residue was purified by flash chromatography on silica gel eluting with petroleum ether/ethyl acetate (20:1) to afford products **1** or **4**.

### 3. Procedure for Copper-Catalyzed Intramolecular Dearomatizing Oxidative Amination of Indoles **1** and **4**



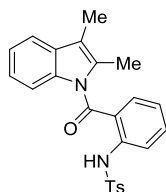
To a dried Schlenk tube were charged with **1** (0.2 mmol), Cu catalyst (0.04 mmol; For condition A: 14.5 mg Cu(OTf)<sub>2</sub> and 0.7 μL H<sub>2</sub>O; For condition B: 7.0 mg CuCl<sub>2</sub>·2H<sub>2</sub>O), and ligand **L6** (0.08 mmol, 12 μL) under O<sub>2</sub> atmosphere. Toluene (2.0 mL) was then introduced via a syringe. The tube was sealed with a Teflon cap. The resulting mixture was allowed to stir at 100 °C until the reaction was completed (monitored by TLC). The reaction mixture was then concentrated under reduced pressure and the residue was purified by flash chromatography on silica gel, eluting with petroleum ether/ethyl acetate (10:1) to afford product **2**.



To a dried Schlenk tube were charged with **4** (0.2 mmol), CuCl<sub>2</sub>·2H<sub>2</sub>O (0.04 mmol, 7.0 mg), and ligand **L6** (0.08 mmol, 12 μL) under O<sub>2</sub> atmosphere. Toluene (2.0 mL) was then introduced via a syringe. The tube was sealed with a Teflon cap. The resulting mixture was allowed to stir at 100 °C until the reaction was completed (monitored by TLC). The reaction mixture was then concentrated under reduced pressure and the residue was purified by flash chromatography on silica gel, eluting with petroleum ether/ethyl acetate (5:1) to afford product **5**.

#### 4. Characterization of Substrates and Products

##### *N*-(2-(2,3-Dimethyl-1H-indole-1-carbonyl)phenyl)-4-methylbenzenesulfonamide (1a)



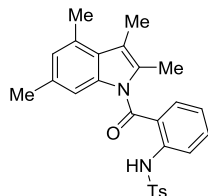
Purified by chromatography on silica gel, eluting with ethyl acetate/petroleum ether 1:10 (v/v); yellow solid, Mp = 130-131 °C; 34% yield (for the last step).

**<sup>1</sup>H NMR** (500 MHz, CDCl<sub>3</sub>) δ 9.36 (s, 1H), 7.92 (d, *J* = 8.38 Hz, 1H), 7.64 (d, *J* = 7.86 Hz, 2H), 7.56 (t, *J* = 7.89 Hz, 1H), 7.40 (d, *J* = 7.74 Hz, 1H), 7.27 (d, *J* = 7.64 Hz, 1H), 7.14 (t, *J* = 7.49 Hz, 1H), 7.06 (t, *J* = 7.59 Hz, 1H), 7.00 (d, *J* = 7.93 Hz, 2H), 6.84 (t, *J* = 7.76 Hz, 1H), 6.21 (d, *J* = 8.33 Hz, 1H), 2.21 (s, 3H), 2.20 (s, 3H), 2.15 (s, 3H).

**<sup>13</sup>C NMR** (125 MHz, CDCl<sub>3</sub>) δ 169.3, 144.1, 138.3, 136.2, 136.0, 134.0, 133.1, 132.1, 130.8, 129.7, 127.2, 124.7, 124.2, 123.6, 122.9, 122.6, 118.0, 115.8, 113.8, 21.4, 12.7, 8.7.

**HRMS** *m/z* (ESI+): Calculated for C<sub>24</sub>H<sub>23</sub>N<sub>2</sub>O<sub>3</sub>S<sup>+</sup> ([M+H]<sup>+</sup>): 419.1424, found 419.1430.

##### 4-Methyl-N-(2-(2,3,4,6-tetramethyl-1H-indole-1-carbonyl)phenyl)benzenesulfonamide (1b)



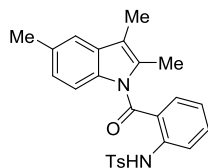
Purified by chromatography on silica gel, eluting with ethyl acetate/petroleum ether 1:10 (v/v); brown red solid, Mp = 130-131 °C; 65% yield (for the last step).

**<sup>1</sup>H NMR** (500 MHz, CDCl<sub>3</sub>) δ 9.53 (s, 1H), 7.90 (d, *J* = 8.30 Hz, 1H), 7.70-7.66 (m, 2H), 7.53 (td, *J* = 8.04, 1.68 Hz, 1H), 7.23 (dd, *J* = 7.85, 1.71 Hz, 1H), 7.10-7.01 (m, 3H), 6.71 (s, 1H), 6.21 (s, 1H), 2.64 (s, 3H), 2.36 (s, 3H), 2.20 (s, 3H), 2.15 (s, 3H), 1.98 (s, 3H).

**<sup>13</sup>C NMR** (125 MHz, CDCl<sub>3</sub>) δ 169.6, 143.9, 138.5, 136.9, 136.4, 134.0, 132.4, 132.3, 131.4, 129.9, 129.6, 127.2, 126.6, 126.2, 124.4, 124.0, 123.0, 116.4, 112.1, 21.4, 21.3, 20.1, 12.5, 11.9.

**HRMS** *m/z* (ESI+): Calculated for C<sub>26</sub>H<sub>27</sub>N<sub>2</sub>O<sub>3</sub>S<sup>+</sup> ([M+H]<sup>+</sup>): 447.1737, found 447.1737.

**4-methyl-N-(2-(2,3,5-trimethyl-1H-indole-1-carbonyl)phenyl)benzene-sulfonamide (1c)**



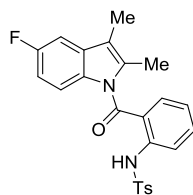
Purified by chromatography on silica gel, eluting with ethyl acetate/petroleum ether 1:10 (v/v); yellow solid, Mp = 120-121 °C; 45% yield (for the last step).

**<sup>1</sup>H NMR** (500 MHz, CDCl<sub>3</sub>) δ 9.31 (s, 1H), 7.91 (d, *J* = 8.29 Hz, 1H), 7.66-7.61 (m, 2H), 7.55 (td, *J* = 7.93, 1.64 Hz, 1H), 7.27 (dd, *J* = 7.79, 1.79 Hz, 1H), 7.18 (d, *J* = 1.6 Hz, 1H), 7.08 (s, 1H), 6.98 (d, *J* = 8.05 Hz, 2H), 6.64 (dd, *J* = 8.37, 1.77 Hz, 1H), 6.05 (d, *J* = 8.53 Hz, 1H), 2.40 (s, 3H), 2.19 (s, 6H), 2.14 (s, 3H).

**<sup>13</sup>C NMR** (125 MHz, CDCl<sub>3</sub>) δ 169.1, 144.0, 138.2, 136.2, 134.2, 133.8, 133.2, 132.1, 132.0, 131.1, 129.7, 127.2, 125.0, 124.22, 124.16, 123.6, 118.0, 115.8, 113.6, 21.3, 21.2, 12.8, 8.7.

**HRMS** *m/z* (ESI+): Calculated for C<sub>25</sub>H<sub>24</sub>N<sub>2</sub>O<sub>3</sub>NaS<sup>+</sup> ([M+Na]<sup>+</sup>): 455.1400, found 455.1404.

**N-(2-(5-Fluoro-2,3-dimethyl-1H-indole-1-carbonyl)phenyl)-4-methylbenzene-sulfonamide (1d)**



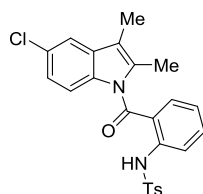
Purified by chromatography on silica gel, eluting with ethyl acetate/petroleum ether 1:10 (v/v); white solid, Mp = 117-128 °C; 69% yield (for the last step).

**<sup>1</sup>H NMR** (500 MHz, CDCl<sub>3</sub>) δ 9.26 (s, 1H), 7.91 (d, *J* = 8.26 Hz, 1H), 7.63 (d, *J* = 2.25 Hz, 2H), 7.61-7.50 (m, 1H), 7.24 (dd, *J* = 7.82, 1.67 Hz, 1H), 7.12-6.97 (m, 4H), 6.55 (td, *J* = 9.00, 2.59 Hz, 1H), 6.15 (dd, *J* = 8.97, 4.35 Hz, 1H), 2.18 (d, *J* = 2.17 Hz, 9H).

**<sup>13</sup>C NMR** (125 MHz, CDCl<sub>3</sub>) δ 169.0, 160.2 (d, *J* = 238.8 Hz), 144.1, 138.3, 136.3, 134.9, 134.1, 132.2, 132.0, 131.9 (d, *J* = 6.2 Hz), 129.7, 127.2, 124.6, 124.3, 123.7, 115.7 (d, *J* = 3.5 Hz), 114.7 (d, *J* = 9.2 Hz), 110.4 (d, *J* = 25.0 Hz), 103.8 (d, *J* = 25.8 Hz), 21.3, 12.9, 8.7.

**HRMS** *m/z* (ESI+): Calculated for C<sub>24</sub>H<sub>22</sub>N<sub>2</sub>O<sub>3</sub>SF<sup>+</sup> ([M+H]<sup>+</sup>): 437.1330, found 437.1335.

***N*-(2-(5-Chloro-2,3-dimethyl-1H-indole-1-carbonyl)phenyl)-4-methylbenzene-sulfonamide (1e)**



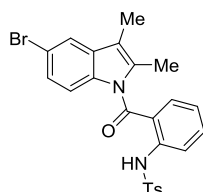
Purified by chromatography on silica gel, eluting with ethyl acetate/petroleum ether 1:10 (v/v); yellow solid, Mp = 123-124 °C; 57% yield (for the last step).

**<sup>1</sup>H NMR** (500 MHz, CDCl<sub>3</sub>) δ 9.26 (s, 1H), 7.92 (d, *J* = 8.36 Hz, 1H), 7.63 (d, *J* = 7.83 Hz, 2H), 7.58 (t, *J* = 7.88 Hz, 1H), 7.35 (d, *J* = 1.92 Hz, 1H), 7.23 (d, *J* = 7.75 Hz, 1H), 7.08 (t, *J* = 7.58 Hz, 1H), 7.00 (d, *J* = 7.94 Hz, 2H), 6.75 (dd, *J* = 8.71, 2.15 Hz, 1H), 6.00 (d, *J* = 8.80 Hz, 1H), 2.22 (s, 3H), 2.18 (s, 3H), 2.17 (s, 3H).

**<sup>13</sup>C NMR** (125 MHz, CDCl<sub>3</sub>) δ 169.1, 144.2, 138.3, 136.2, 134.8, 134.3, 132.1, 131.9, 129.7, 128.3, 127.2, 124.5, 124.4, 123.8, 122.9, 117.7, 115.2, 114.6, 21.3, 12.7, 8.6.

**HRMS** *m/z* (ESI<sup>+</sup>): Calculated for C<sub>24</sub>H<sub>21</sub>N<sub>2</sub>O<sub>3</sub>SClNa<sup>+</sup> ([M+Na]<sup>+</sup>): 475.0854, found 475.0861.

***N*-(2-(5-Bromo-2,3-dimethyl-1H-indole-1-carbonyl)phenyl)-4-methylbenzene-sulfonamide (1f)**



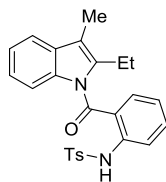
Purified by chromatography on silica gel, eluting with ethyl acetate/petroleum ether 1:10 (v/v); yellow solid, Mp = 168-169 °C; 80% yield (for the last step).

**<sup>1</sup>H NMR** (500 MHz, CDCl<sub>3</sub>) δ 9.26 (s, 1H), 7.93 (d, *J* = 8.23 Hz, 1H), 7.64-7.60 (m, 2H), 7.58 (td, *J* = 8.07, 1.72 Hz, 1H), 7.51 (d, *J* = 2.09 Hz, 1H), 7.22 (dd, *J* = 7.78, 1.68 Hz, 1H), 7.08 (t, *J* = 7.63 Hz, 1H), 6.99 (d, *J* = 8.07 Hz, 2H), 6.88 (dd, *J* = 8.71, 1.89 Hz, 1H), 5.92 (d, *J* = 8.72 Hz, 1H), 2.23 (s, 3H), 2.18 (s, 3H), 2.17 (s, 3H).

**<sup>13</sup>C NMR** (125 MHz, CDCl<sub>3</sub>) δ 169.0, 144.2, 138.3, 136.2, 134.7, 134.6, 134.3, 132.6, 131.9, 129.7, 127.2, 125.6, 124.5, 124.4, 123.9, 120.8, 115.9, 115.1, 115.0, 21.4, 12.7, 8.6.

**HRMS** *m/z* (ESI<sup>+</sup>): Calculated for C<sub>24</sub>H<sub>21</sub>N<sub>2</sub>O<sub>3</sub>SBrNa<sup>+</sup> ([M+Na]<sup>+</sup>): 519.0348, found 519.0356.

***N*-(2-(2-Ethyl-3-methyl-1H-indole-1-carbonyl)phenyl)-4-methylbenzene-sulfonamide (1g)**



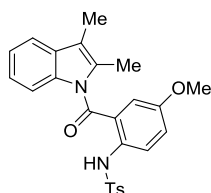
Purified by chromatography on silica gel, eluting with ethyl acetate/petroleum ether 1:10 (v/v); yellow solid, Mp = 131-132 °C; 53% yield (for the last step).

**<sup>1</sup>H NMR** (500 MHz, CDCl<sub>3</sub>) δ 9.50 (s, 1H), 7.94 (d, *J* = 8.58 Hz, 1H), 7.70-7.62 (m, 2H), 7.58 (td, *J* = 8.00, 1.67 Hz, 1H), 7.39 (d, *J* = 7.51 Hz, 1H), 7.33-7.24 (m, 1H), 7.11 (t, *J* = 7.54 Hz, 1H), 7.05 (t, *J* = 7.68 Hz, 1H), 6.98 (d, *J* = 8.04 Hz, 2H), 6.75-6.64 (m, 1H), 5.75 (d, *J* = 8.40 Hz, 1H), 2.93 (ddt, *J* = 162.08, 14.60, 7.45 Hz, 2H), 2.25 (s, 3H), 2.12 (s, 3H), 1.16 (t, *J* = 7.40 Hz, 3H).

**<sup>13</sup>C NMR** (125 MHz, CDCl<sub>3</sub>) δ 169.5, 144.1, 139.8, 138.7, 136.2, 136.0, 134.2, 132.2, 130.8, 129.7, 127.3, 124.24, 124.18, 123.4, 122.6, 122.2, 118.1, 115.2, 113.6, 21.4, 19.1, 14.3, 8.5.

**HRMS** *m/z* (ESI+): Calculated for C<sub>25</sub>H<sub>25</sub>N<sub>2</sub>O<sub>3</sub>S<sup>+</sup> ([M+H]<sup>+</sup>): 433.1580, found 433.1579.

***N*-(2-(2,3-Dimethyl-1H-indole-1-carbonyl)-4-methoxyphenyl)-4-methylbenzene-sulfonamide (1h)**



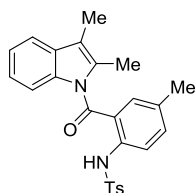
Purified by chromatography on silica gel, eluting with ethyl acetate/petroleum ether 1:10 (v/v); white solid, Mp = 111-112 °C; 42% yield (for the last step).

**<sup>1</sup>H NMR** (500 MHz, CDCl<sub>3</sub>) δ 8.84 (s, 1H), 7.83 (d, *J* = 9.09 Hz, 1H), 7.60-7.54 (m, 2H), 7.37 (d, *J* = 7.86 Hz, 1H), 7.19 -7.07 (m, 2H), 6.89 (d, *J* = 8.04 Hz, 2H), 6.84 (s, 1H), 6.74 (d, *J* = 2.90 Hz, 1H), 6.18 (d, *J* = 8.61 Hz, 1H), 3.61 (s, 3H), 2.21 (s, 3H), 2.19 (s, 3H), 2.06 (s, 3H).

**<sup>13</sup>C NMR** (125 MHz, CDCl<sub>3</sub>) δ 168.6, 156.5, 143.8, 136.1, 135.7, 133.1, 130.8, 130.6, 129.5, 127.23, 127.17, 122.9, 122.7, 119.8, 117.9, 116.1, 116.0, 114.1, 55.7, 21.3, 12.8, 8.7.

**HRMS** *m/z* (ESI+): Calculated for C<sub>25</sub>H<sub>24</sub>N<sub>2</sub>O<sub>4</sub>SNa<sup>+</sup> ([M+Na]<sup>+</sup>): 471.1349, found 471.1355.

***N*-(2-(2,3-Dimethyl-1H-indole-1-carbonyl)-4-methylphenyl)-4-methylbenzene-sulfonamide (1i)**



Purified by chromatography on silica gel, eluting with ethyl acetate/petroleum ether 1:10 (v/v); yellow solid, Mp = 110-111 °C; 32% yield (for the last step).

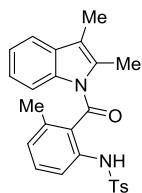
**<sup>1</sup>H NMR** (500 MHz, CDCl<sub>3</sub>) δ 9.16 (s, 1H), 7.81 (d, *J* = 8.42 Hz, 1H), 7.61 (d, *J* = 7.99 Hz, 2H), 7.38 (dd, *J* = 12.40, 7.96 Hz, 2H), 7.15 (t, *J* = 7.55 Hz, 1H), 7.07 (s,

1H), 6.96 (d,  $J = 7.79$  Hz, 2H), 6.84 (d,  $J = 7.82$  Hz, 1H), 6.21 (d,  $J = 8.30$  Hz, 1H), 2.22 (s, 3H), 2.19 (s, 3H), 2.18 (s, 3H), 2.12 (s, 3H).

$^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  169.3, 143.9, 136.2, 136.0, 135.6, 134.7, 134.4, 133.1, 132.1, 130.8, 129.6, 127.2, 125.1, 124.2, 122.9, 122.5, 117.9, 115.8, 113.8, 21.4, 20.5, 12.7, 8.7.

HRMS  $m/z$  (ESI+): Calculated for  $\text{C}_{25}\text{H}_{24}\text{N}_2\text{O}_3\text{SNa}^+$  ( $[\text{M}+\text{Na}]^+$ ): 455.1400, found 455.1408.

#### ***N*-(2-(2,3-Dimethyl-1H-indole-1-carbonyl)-3-methylphenyl)-4-methylbenzene-sulfonamide (1j)**



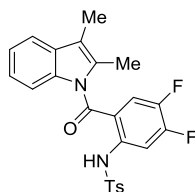
Purified by chromatography on silica gel, eluting with ethyl acetate/petroleum ether 1:10 (v/v); yellow solid, Mp = 105-106 °C; 46% yield (for the last step).

$^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.78 (s, 1H), 7.67 (d,  $J = 8.26$  Hz, 1H), 7.56 (d,  $J = 8.09$  Hz, 2H), 7.42-7.33 (m, 2H), 7.17 (t,  $J = 7.48$  Hz, 1H), 6.97 (d,  $J = 7.70$  Hz, 1H), 6.84 (d,  $J = 8.17$  Hz, 3H), 2.18 (s, 3H), 2.12 (s, 6H), 1.85 (s, 3H).

$^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  166.0, 157.8, 143.8, 136.7, 136.4, 135.5, 133.0, 132.6, 131.2, 129.4, 127.0, 123.3, 123.0, 117.9, 116.3, 115.8, 113.8, 108.1, 55.9, 21.4, 12.9, 8.7.

HRMS  $m/z$  (ESI+): Calculated for  $\text{C}_{25}\text{H}_{25}\text{N}_2\text{O}_3\text{S}^+$  ( $[\text{M}+\text{H}]^+$ ): 433.1586, found 433.1581.

#### ***N*-(2-(2,3-Dimethyl-1H-indole-1-carbonyl)-4,5-difluorophenyl)-4-methylbenzene-sulfonamide (1k)**



Purified by chromatography on silica gel, eluting with ethyl acetate/petroleum ether 1:10 (v/v); yellow solid, Mp = 125-126 °C; 54% yield (for the last step).

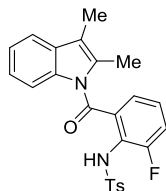
$^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  9.36 (s, 1H), 7.81 (dd,  $J = 11.52, 6.93$  Hz, 1H), 7.64 (d,  $J = 8.06$  Hz, 2H), 7.41 (d,  $J = 7.76$  Hz, 1H), 7.17 (t,  $J = 7.51$  Hz, 1H), 7.10 (dd,  $J = 9.98, 8.23$  Hz, 1H), 7.04 (d,  $J = 7.95$  Hz, 2H), 6.88 (t,  $J = 7.78$  Hz, 1H), 6.15 (d,  $J = 8.26$  Hz, 1H), 2.21 (s, 6H), 2.17 (s, 3H).

$^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  167.4, 154.4 (d,  $J = 12.8$  Hz), 152.4 (d,  $J = 14.6$  Hz), 147.8 (d,  $J = 12.4$  Hz), 145.7 (d,  $J = 12.4$  Hz), 144.6, 136.1 (d,  $J = 11.3$  Hz), 135.7 (d,  $J = 11$  Hz), 132.8, 130.9, 129.9, 127.2, 123.2, 121.0 (t,  $J = 4.2, 3.4$  Hz), 120.7 (d,  $J = 1.9$  Hz), 120.5, 118.3, 116.5, 113.4 (t,  $J = 10.8$  Hz), 12.6, 8.7.



**HRMS**  $m/z$  (ESI+): Calculated for  $C_{24}H_{21}N_2O_3SF_2^+$  ( $[M+H]^+$ ): 455.1235, found 455.1245.

***N*-(2-(2,3-Dimethyl-1H-indole-1-carbonyl)-6-fluorophenyl)-4-methylbenzenesulfonamide (1l)**



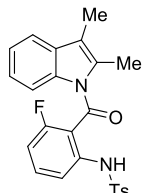
Purified by chromatography on silica gel, eluting with ethyl acetate/petroleum ether 1:10 (v/v); yellow solid, Mp = 182-183 °C; 58% yield (for the last step).

**$^1H$  NMR** (500 MHz,  $CDCl_3$ )  $\delta$  7.79 (s, 1H), 7.62 (d,  $J = 8.04$  Hz, 2H), 7.40 (d,  $J = 7.78$  Hz, 1H), 7.34 (t,  $J = 9.03$  Hz, 1H), 7.26 (dd,  $J = 11.70, 6.96$  Hz, 1H), 7.20 (d,  $J = 7.49$  Hz, 2H), 6.95 (dd,  $J = 39.40, 7.81$  Hz, 3H), 6.61 (d,  $J = 8.50$  Hz, 1H), 2.32 (s, 3H), 2.21 (s, 3H), 2.10 (s, 3H).

**$^{13}C$  NMR** (125 MHz,  $CDCl_3$ )  $\delta$  166.9, 159.8 (d,  $J = 252.5$  Hz), 143.8, 136.4, 135.8, 133.3 (d,  $J = 15.0$  Hz), 131.2, 129.2, 127.8 (d,  $J = 8.1$  Hz), 127.3, 126.3 (d,  $J = 3.8$  Hz), 124.4 (d,  $J = 13.4$  Hz), 123.1, 120.6, 120.4, 118.1, 116.3, 114.6, 21.3, 13.4, 8.7.

**HRMS**  $m/z$  (ESI+): Calculated for  $C_{24}H_{22}N_2O_3SF^+$  ( $[M+H]^+$ ): 437.1330, found 437.1333.

***N*-(2-(2,3-Dimethyl-1H-indole-1-carbonyl)-3-fluorophenyl)-4-methylbenzenesulfonamide (1m)**



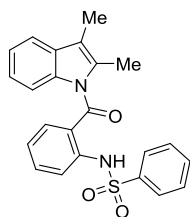
Purified by chromatography on silica gel, eluting with ethyl acetate/petroleum ether 1:10 (v/v); yellow solid, Mp = 110-111 °C; 47% yield (for the last step).

**$^1H$  NMR** (500 MHz,  $CDCl_3$ )  $\delta$  8.44 (s, 1H), 7.68 (d,  $J = 8.30$  Hz, 1H), 7.61 (d,  $J = 8.08$  Hz, 2H), 7.50 (td,  $J = 8.30, 5.98$  Hz, 1H), 7.38 (d,  $J = 7.69$  Hz, 1H), 7.19 (t,  $J = 7.52$  Hz, 1H), 6.91 (t,  $J = 8.40$  Hz, 3H), 6.84 (t,  $J = 8.73$  Hz, 1H), 6.57 (d,  $J = 8.38$  Hz, 1H), 2.18 (s, 3H), 2.12 (d,  $J = 2.55$  Hz, 6H).

**$^{13}C$  NMR** (125 MHz,  $CDCl_3$ )  $\delta$  163.6, 160.8 (d,  $J = 252.5$  Hz), 144.2, 137.7 (d,  $J = 2.8$  Hz), 136.2, 135.4, 133.7 (d,  $J = 9.8$  Hz), 132.3, 131.3, 129.6, 127.1, 123.7, 123.4, 119.7 (t,  $J = 3.4, 2.8$  Hz), 118.1, 116.8 (d,  $J = 4.1$  Hz), 113.3, 112.5 (d,  $J = 21.6$  Hz), 21.4, 12.7, 8.7.

**HRMS**  $m/z$  (ESI+): Calculated for  $C_{24}H_{22}N_2O_3SF^+$  ( $[M+H]^+$ ): 437.1330, found 437.1338.

***N*-(2-(2,3-Dimethyl-1H-indole-1-carbonyl)phenyl)benzenesulfonamide (1n)**



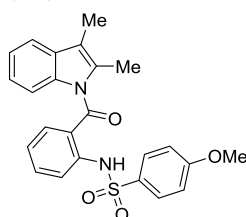
Purified by chromatography on silica gel, eluting with ethyl acetate/petroleum ether 1:10 (v/v); yellow solid, Mp = 63-64 °C; 38% yield (for the last step).

**<sup>1</sup>H NMR** (500 MHz, CDCl<sub>3</sub>) δ 9.44 (s, 1H), 7.93 (d, *J* = 8.27 Hz, 1H), 7.80 (d, *J* = 7.68 Hz, 2H), 7.56 (t, *J* = 7.78 Hz, 1H), 7.41 (d, *J* = 7.78 Hz, 1H), 7.34 (t, *J* = 7.43 Hz, 1H), 7.31-7.23 (m, 3H), 7.15 (t, *J* = 7.51 Hz, 1H), 7.07 (t, *J* = 7.57 Hz, 1H), 6.89 (t, *J* = 7.78 Hz, 1H), 6.39 (d, *J* = 8.40 Hz, 1H), 2.21 (s, 3H), 2.13 (s, 3H).

**<sup>13</sup>C NMR** (125 MHz, CDCl<sub>3</sub>) δ 169.4, 139.3, 138.3, 136.1, 134.1, 133.1, 132.9, 132.2, 130.8, 129.1, 127.2, 124.4, 124.2, 123.2, 123.0, 122.7, 118.1, 115.9, 113.8, 12.7, 8.7.

**HRMS** *m/z* (ESI+): Calculated for C<sub>23</sub>H<sub>21</sub>N<sub>2</sub>O<sub>3</sub>S<sup>+</sup> ([M+H]<sup>+</sup>): 405.1267, found 405.1266.

***N*-(2-(2,3-dimethyl-1H-indole-1-carbonyl)phenyl)-4-methoxybenzenesulfonamide (1o)**



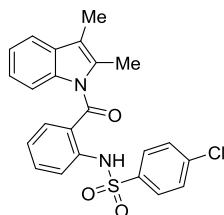
Purified by chromatography on silica gel, eluting with ethyl acetate/petroleum ether 1:10 (v/v); yellow solid, Mp = 134-135 °C; 23% yield (for the last step).

**<sup>1</sup>H NMR** (500 MHz, CDCl<sub>3</sub>) δ 9.32 (s, 1H), 7.92 (d, *J* = 8.4 Hz, 1H), 7.78-7.63 (m, 2H), 7.56 (td, *J* = 8.2, 1.7 Hz, 1H), 7.40 (d, *J* = 7.8 Hz, 1H), 7.34-7.25 (m, 1H), 7.14 (t, *J* = 7.4 Hz, 1H), 7.07 (t, *J* = 7.6 Hz, 1H), 6.83 (t, *J* = 7.8 Hz, 1H), 6.77-6.48 (m, 2H), 6.17 (d, *J* = 8.3 Hz, 1H), 3.59 (s, 3H), 2.22 (d, *J* = 5.9 Hz, 6H).

**<sup>13</sup>C NMR** (125 MHz, CDCl<sub>3</sub>) δ 169.3, 163.1, 138.4, 136.0, 134.0, 133.1, 132.1, 130.8, 130.6, 129.3, 124.8, 124.2, 123.7, 122.9, 122.6, 118.0, 115.9, 114.2, 113.8, 55.3, 12.7, 8.7.

**HRMS** *m/z* (ESI+): Calculated for C<sub>24</sub>H<sub>23</sub>N<sub>2</sub>O<sub>4</sub>S<sup>+</sup> ([M+H]<sup>+</sup>): 435.1373, found 435.1366.

**4-Chloro-N-(2-(2,3-dimethyl-1H-indole-1-carbonyl)phenyl)benzenesulfonamide  
(1p)**



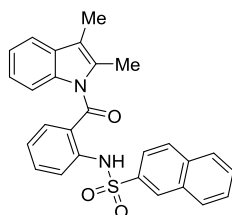
Purified by chromatography on silica gel, eluting with ethyl acetate/petroleum ether 1:10 (v/v); yellow solid, Mp = 146-147 °C; 19% yield (for the last step).

**<sup>1</sup>H NMR** (500 MHz, CDCl<sub>3</sub>) δ 9.36 (s, 1H), 7.91 (d, *J* = 8.30 Hz, 1H), 7.73-7.66 (m, 2H), 7.58 (td, *J* = 7.94, 1.64 Hz, 1H), 7.42 (d, *J* = 7.77 Hz, 1H), 7.32 (dd, *J* = 7.82, 1.67 Hz, 1H), 7.18 (dd, *J* = 8.18, 6.35 Hz, 3H), 7.11 (t, *J* = 7.70 Hz, 1H), 6.90 (t, *J* = 7.73 Hz, 1H), 6.26 (d, *J* = 8.27 Hz, 1H), 2.22 (s, 3H), 2.19 (s, 3H).

**<sup>13</sup>C NMR** (125 MHz, CDCl<sub>3</sub>) δ 169.3, 139.8, 137.73, 137.67, 135.9, 134.1, 132.9, 132.1, 130.9, 129.4, 128.6, 125.1, 124.7, 123.6, 123.2, 122.9, 118.3, 116.3, 113.6, 12.7, 8.7.

**HRMS** *m/z* (ESI+): Calculated for C<sub>23</sub>H<sub>20</sub>ClN<sub>2</sub>O<sub>3</sub>S<sup>+</sup> ([M+H]<sup>+</sup>): 439.0878, found 439.0872.

**N-(2-(2,3-Dimethyl-1H-indole-1-carbonyl)phenyl)naphthalene-2-sulfonamide  
(1q)**



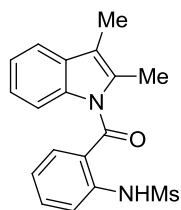
Purified by chromatography on silica gel, eluting with ethyl acetate/petroleum ether 1:10 (v/v); white solid, Mp = 158-159 °C; 23% yield (for the last step).

**<sup>1</sup>H NMR** (500 MHz, CDCl<sub>3</sub>) δ 9.47 (s, 1H), 8.35 (d, *J* = 2.3 Hz, 1H), 7.96 (d, *J* = 8.2 Hz, 1H), 7.78 (d, *J* = 8.0 Hz, 1H), 7.71 (d, *J* = 2.0 Hz, 1H), 7.63 (d, *J* = 8.1 Hz, 1H), 7.59-7.40 (m, 4H), 7.37-7.24 (m, 1H), 7.21 (dd, *J* = 7.8, 1.7 Hz, 1H), 7.01 (dt, *J* = 25.1, 7.5 Hz, 2H), 6.44 (t, *J* = 7.7 Hz, 1H), 6.12 (d, *J* = 8.3 Hz, 1H), 2.12 (s, 3H), 2.02 (s, 3H).

**<sup>13</sup>C NMR** (125 MHz, CDCl<sub>3</sub>) δ 169.3, 138.0, 136.0, 135.9, 134.9, 134.0, 132.7, 132.0, 131.9, 130.7, 129.7, 129.1, 128.8, 127.8, 127.5, 125.1, 124.4, 123.7, 122.8, 122.6, 122.0, 117.9, 116.0, 113.6, 12.6, 8.6.

**HRMS** *m/z* (ESI+): Calculated for C<sub>27</sub>H<sub>23</sub>N<sub>2</sub>O<sub>3</sub>S<sup>+</sup> ([M+H]<sup>+</sup>): 455.1424, found 455.1419.

### *N*-(2-(2,3-dimethyl-1H-indole-1-carbonyl)phenyl)methanesulfonamide (1r)



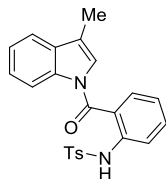
Purified by chromatography on silica gel, eluting with ethyl acetate/petroleum ether 1:10 (v/v); yellow solid, Mp = 50-51 °C; 50% yield (for the last step).

**<sup>1</sup>H NMR** (400 MHz, CDCl<sub>3</sub>) δ 8.98 (s, 1H), 7.88 (dd, *J*=8.4, 1.2 Hz, 1H), 7.64 (ddd, *J*=8.6, 7.4, 1.6 Hz, 1H), 7.51-7.43 (m, 2H), 7.22 (td, *J*=7.5, 1.0 Hz, 1H), 7.17 (td, *J*=7.6, 1.1 Hz, 1H), 7.08 (ddd, *J*=8.4, 7.1, 1.3 Hz, 1H), 6.96 (dt, *J*=8.3, 0.9 Hz, 1H), 3.11 (s, 3H), 2.36 (s, 3H), 2.26 (s, 3H).

**<sup>13</sup>C NMR** (100 MHz, CDCl<sub>3</sub>) δ 169.5, 138.7, 136.3, 134.4, 132.9, 132.4, 131.1, 123.8, 123.5, 123.4, 123.0, 120.8, 118.4, 116.3, 113.8, 40.4, 13.0, 8.7.

**HRMS** *m/z* (ESI+): Calculated for C<sub>18</sub>H<sub>19</sub>N<sub>2</sub>O<sub>3</sub>S<sup>+</sup> ([M+H]<sup>+</sup>): 343.1111, found 343.1105.

### 4-Methyl-*N*-(2-(3-methyl-1H-indole-1-carbonyl)phenyl)benzenesulfonamide (1v)



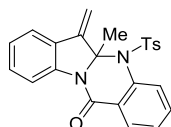
Purified by chromatography on silica gel, eluting with ethyl acetate/petroleum ether 1:10 (v/v); white solid, Mp = 142-143 °C; 75% yield (for the last step).

**<sup>1</sup>H NMR** (500 MHz, CDCl<sub>3</sub>) δ 8.57 (s, 1H), 8.32-8.11 (m, 1H), 7.82 (dd, *J* = 8.27, 1.20 Hz, 1H), 7.57 (td, *J* = 7.99, 1.67 Hz, 1H), 7.54-7.51 (m, 1H), 7.51-7.46 (m, 2H), 7.38 (ddd, *J* = 6.80, 4.95, 1.73 Hz, 2H), 7.35 (dd, *J* = 7.81, 1.67 Hz, 1H), 7.25 (td, *J* = 7.53, 1.27 Hz, 1H), 6.80 (d, *J* = 8.08 Hz, 2H), 6.45 (d, *J* = 1.57 Hz, 1H), 2.21 (d, *J* = 1.37 Hz, 3H), 2.05 (s, 3H).

**<sup>13</sup>C NMR** (125 MHz, CDCl<sub>3</sub>) δ 166.8, 143.8, 137.1, 135.9, 135.8, 132.6, 131.7, 130.0, 129.2, 127.0, 126.3, 126.2, 125.3, 124.8, 124.2, 124.0, 118.9, 118.2, 116.6, 21.3, 9.6.

**HRMS** *m/z* (ESI+): Calculated for C<sub>23</sub>H<sub>21</sub>N<sub>2</sub>O<sub>3</sub>S<sup>+</sup> ([M+H]<sup>+</sup>): 405.1267, found 405.1269.

### 5a-Methyl-6-methylene-5-tosyl-5a,6-dihydroindolo[2,1-b]quinazolin-12(5H)-one (2a)



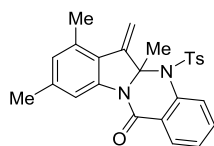
Purified by chromatography on silica gel, eluting with ethyl acetate/petroleum ether 1:10 (v/v); white solid, Mp = 125-126 °C; 78% yield.

**<sup>1</sup>H NMR** (500 MHz, CDCl<sub>3</sub>) δ 8.04 (d, *J* = 7.70 Hz, 1H), 7.85-7.64 (m, 3H), 7.52 (dd, *J* = 11.51, 7.26 Hz, 2H), 7.15 (dt, *J* = 28.38, 7.41 Hz, 2H), 6.96 (d, *J* = 8.01 Hz, 2H), 6.75 (d, *J* = 7.97 Hz, 2H), 6.11 (s, 1H), 5.74 (s, 1H), 2.17 (s, 3H), 1.59 (d, *J* = 4.87 Hz, 3H).

**<sup>13</sup>C NMR** (125 MHz, CDCl<sub>3</sub>) δ 158.3, 144.3, 141.9, 140.8, 139.5, 133.8, 132.8, 130.3, 129.4, 128.8, 128.1, 128.0, 127.7, 126.9, 124.5, 120.2, 116.0, 110.8, 82.4, 32.1, 21.3.

**HRMS** *m/z* (ESI+): Calculated for C<sub>24</sub>H<sub>21</sub>N<sub>2</sub>O<sub>3</sub>S<sup>+</sup> ([M+H]<sup>+</sup>): 417.1267, found 417.1275.

### 5a,7,9-Trimethyl-6-methylene-5-tosyl-5a,6-dihydroindolo[2,1-b]quinazolin-12(5H)-one (2b)



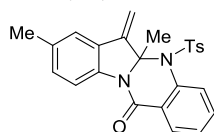
Purified by chromatography on silica gel, eluting with ethyl acetate/petroleum ether 1:10 (v/v); white solid, Mp = 175-176 °C; 77% yield.

**<sup>1</sup>H NMR** (500 MHz, CDCl<sub>3</sub>) δ 8.04 (dd, *J* = 7.86, 1.69 Hz, 1H), 7.78 (d, *J* = 8.14 Hz, 1H), 7.68-7.63 (m, 1H), 7.56 (s, 1H), 7.51 (t, *J* = 7.56 Hz, 1H), 7.01-6.94 (m, 2H), 6.79-6.72 (m, 3H), 6.03 (d, *J* = 1.46 Hz, 1H), 5.76 (d, *J* = 1.56 Hz, 1H), 2.53 (s, 3H), 2.30 (s, 3H), 2.16 (s, 3H), 1.58 (s, 3H).

**<sup>13</sup>C NMR** (125 MHz, CDCl<sub>3</sub>) δ 158.3, 144.2, 142.5, 141.8, 139.6, 139.3, 134.20, 134.18, 132.6, 130.3, 128.6, 128.0, 127.9, 127.7, 127.0, 122.6, 114.1, 113.7, 82.7, 32.5, 21.5, 21.3, 21.3.

**HRMS** *m/z* (ESI+): Calculated for C<sub>26</sub>H<sub>25</sub>N<sub>2</sub>O<sub>3</sub>S<sup>+</sup> ([M+H]<sup>+</sup>): 445.1580, found 445.1585.

### 5a,8-Dimethyl-6-methylene-5-tosyl-5a,6-dihydroindolo[2,1-b]quinazolin-12(5H)-one (2c)



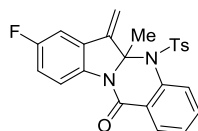
Purified by chromatography on silica gel, eluting with ethyl acetate/petroleum ether 1:10 (v/v); white solid, Mp = 140-141 °C; 70% yield.

**<sup>1</sup>H NMR** (500 MHz, CDCl<sub>3</sub>) δ 8.02 (dd, *J* = 7.8, 1.7 Hz, 1H), 7.79 (d, *J* = 8.1 Hz, 1H), 7.67 (td, *J* = 7.8, 1.7 Hz, 1H), 7.62 (d, *J* = 8.2 Hz, 1H), 7.51 (t, *J* = 7.6 Hz, 1H), 7.32 (d, *J* = 1.6 Hz, 1H), 7.00 (dd, *J* = 8.3, 1.6 Hz, 1H), 6.95 (d, *J* = 8.1 Hz, 2H), 6.76 (d, *J* = 8.1 Hz, 2H), 6.06 (d, *J* = 1.4 Hz, 1H), 5.69 (d, *J* = 1.4 Hz, 1H), 2.41 (s, 3H), 2.18 (s, 3H), 1.58 (s, 3H).

$^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  158.0, 144.2, 142.0, 139.4, 138.7, 134.4, 133.8, 132.6, 130.3, 130.2, 128.8, 128.08, 128.05, 127.7, 127.6, 127.0, 120.5, 115.8, 110.4, 82.6, 32.0, 21.4, 21.2.

**HRMS**  $m/z$  (ESI+): Calculated for  $\text{C}_{25}\text{H}_{23}\text{N}_2\text{O}_3\text{S}^+$  ( $[\text{M}+\text{H}]^+$ ): 431.1429, found 431.1432.

**8-Fluoro-5a-methyl-6-methylene-5-tosyl-5a,6-dihydroindolo[2,1-b]quinazolin-12 (5H)-one (2d)**



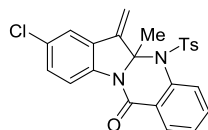
Purified by chromatography on silica gel, eluting with ethyl acetate/petroleum ether 1:10 (v/v); white solid, Mp = 175-176 °C; 99% yield.

$^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  8.03 (dd,  $J = 7.73, 1.66$  Hz, 1H), 7.80 (d,  $J = 8.01$  Hz, 1H), 7.75-7.65 (m, 2H), 7.53 (t,  $J = 7.51$  Hz, 1H), 7.18 (dd,  $J = 8.09, 2.62$  Hz, 1H), 6.98 (d,  $J = 8.07$  Hz, 2H), 6.89 (td,  $J = 8.93, 2.65$  Hz, 1H), 6.82 (d,  $J = 7.94$  Hz, 2H), 6.09 (d,  $J = 1.78$  Hz, 1H), 5.79 (d,  $J = 1.76$  Hz, 1H), 2.20 (s, 3H), 1.60 (s, 3H).

$^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  161.1 (d,  $J = 242.5$  Hz), 158.0, 144.5, 141.3 (d,  $J = 3.4$  Hz), 139.4, 137.0, 133.4 (d,  $J = 138.9$  Hz), 130.3, 129.2, 129.9 (d,  $J = 6.3$  Hz), 128.8, 128.2, 128.1, 127.6, 126.6, 117.1 (d,  $J = 8.1$  Hz), 116.1 (d,  $J = 23.2$  Hz), 112.3, 106.9 (d,  $J = 24.9$  Hz), 82.7, 32.0, 21.3.

**HRMS**  $m/z$  (ESI+): Calculated for  $\text{C}_{24}\text{H}_{20}\text{N}_2\text{O}_3\text{SF}^+$  ( $[\text{M}+\text{H}]^+$ ): 435.1173, found 435.1179.

**8-Chloro-5a-methyl-6-methylene-5-tosyl-5a,6-dihydroindolo[2,1-b]quinazolin-12 (5H)-one (2e)**



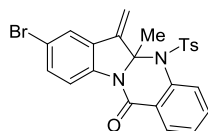
Purified by chromatography on silica gel, eluting with ethyl acetate/petroleum ether 1:10 (v/v); white solid, Mp = 171-172 °C; 89% yield.

$^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  8.03 (dd,  $J = 7.74, 1.73$  Hz, 1H), 7.79 (d,  $J = 7.98$  Hz, 1H), 7.75-7.65 (m, 2H), 7.53 (t,  $J = 7.50$  Hz, 1H), 7.45 (d,  $J = 2.23$  Hz, 1H), 7.14 (dd,  $J = 8.71, 2.19$  Hz, 1H), 6.99 (d,  $J = 8.08$  Hz, 2H), 6.82 (d,  $J = 8.04$  Hz, 2H), 6.10 (d,  $J = 1.77$  Hz, 1H), 5.78 (d,  $J = 1.78$  Hz, 1H), 2.21 (s, 3H), 1.60 (s, 3H).

$^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  158.3, 144.5, 140.9, 139.4, 139.3, 134.0, 133.0, 130.3, 129.9, 129.2, 128.9, 128.2, 128.1, 127.8, 126.5, 120.3, 117.0, 112.4, 82.6, 32.0, 21.3.

**HRMS**  $m/z$  (ESI+): Calculated for  $\text{C}_{24}\text{H}_{20}\text{N}_2\text{O}_3\text{SCl}^+$  ( $[\text{M}+\text{H}]^+$ ): 451.0878, found 451.0885.

**8-Bromo-5a-methyl-6-methylene-5-tosyl-5a,6-dihydroindolo[2,1-b]quinazolin-12(5H)-one (2f)**



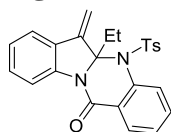
Purified by chromatography on silica gel, eluting with ethyl acetate/petroleum ether 1:10 (v/v); white solid, Mp = 178-179 °C; 92% yield.

**<sup>1</sup>H NMR** (500 MHz, CDCl<sub>3</sub>) δ 8.03 (dd, *J* = 7.6, 1.7 Hz, 1H), 7.78 (d, *J* = 8.1 Hz, 1H), 7.68 (td, *J* = 7.7, 1.7 Hz, 1H), 7.64 (d, *J* = 8.6 Hz, 1H), 7.59 (d, *J* = 2.1 Hz, 1H), 7.52 (t, *J* = 7.5 Hz, 1H), 7.27 (dd, *J* = 8.3, 2.2 Hz, 1H), 6.99 (d, *J* = 8.3 Hz, 2H), 6.81 (d, *J* = 7.9 Hz, 2H), 6.09 (d, *J* = 1.8 Hz, 1H), 5.77 (d, *J* = 1.8 Hz, 1H), 2.20 (s, 3H), 1.58 (s, 3H).

**<sup>13</sup>C NMR** (125 MHz, CDCl<sub>3</sub>) δ 158.3, 144.6, 140.7, 139.7, 139.4, 134.0, 133.0, 132.0, 130.3, 129.6, 128.9, 128.21, 128.17, 127.8, 126.4, 123.3, 117.3, 117.2, 112.5, 82.5, 32.0, 21.4.

**HRMS** *m/z* (ESI<sup>+</sup>): Calculated for C<sub>24</sub>H<sub>20</sub>N<sub>2</sub>O<sub>3</sub>SBr<sup>+</sup> ([M+H]<sup>+</sup>): 495.0373, found 495.0381.

**5a-Ethyl-6-methylene-5-tosyl-5a,6-dihydroindolo[2,1-b]quinazolin-12(5H)-one (2g)**



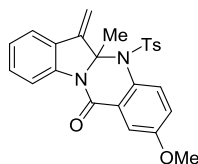
Purified by chromatography on silica gel, eluting with ethyl acetate/petroleum ether 1:10 (v/v); white solid, Mp = 134-135 °C; 88% yield.

**<sup>1</sup>H NMR** (500 MHz, CDCl<sub>3</sub>) δ 8.04 (d, *J* = 7.61 Hz, 1H), 7.75 (dd, *J* = 18.54, 8.01 Hz, 2H), 7.66 (t, *J* = 7.64 Hz, 1H), 7.55-7.41 (m, 2H), 7.11 (dt, *J* = 28.34, 7.70 Hz, 2H), 6.98 (d, *J* = 8.12 Hz, 2H), 6.74 (d, *J* = 7.80 Hz, 2H), 6.18 (s, 1H), 5.75 (s, 1H), 2.15 (s, 3H), 1.99 (dt, *J* = 14.52, 7.21 Hz, 1H), 1.85 (dd, *J* = 14.19, 7.32 Hz, 1H), 0.64 (t, *J* = 7.26 Hz, 3H).

**<sup>13</sup>C NMR** (125 MHz, CDCl<sub>3</sub>) δ 158.3, 144.2, 141.8, 139.5, 139.3, 134.1, 132.7, 130.4, 129.2, 128.7, 128.5, 128.1, 128.0, 127.7, 126.7, 124.4, 119.7, 115.7, 111.3, 85.4, 36.2, 21.3, 6.9.

**HRMS** *m/z* (ESI<sup>+</sup>): Calculated for C<sub>25</sub>H<sub>23</sub>N<sub>2</sub>O<sub>3</sub>S<sup>+</sup> ([M+H]<sup>+</sup>): 431.1424, found 431.1415.

**2-Methoxy-5a-methyl-6-methylene-5-tosyl-5a,6-dihydroindolo[2,1-b]quinazolin-12(5H)-one (2h)**



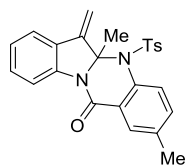
Purified by chromatography on silica gel, eluting with ethyl acetate/petroleum ether 1:10 (v/v); white solid, Mp = 177-178 °C; 83% yield.

**<sup>1</sup>H NMR** (400 MHz, CDCl<sub>3</sub>) δ 7.74-7.66 (m, 2H), 7.50 (dd, *J* = 7.43, 1.99 Hz, 2H), 7.22-7.16 (m, 2H), 7.15-7.08 (m, 1H), 6.94 (d, *J* = 8.37 Hz, 2H), 6.75 (t, *J* = 7.07 Hz, 2H), 6.09 (d, *J* = 1.38 Hz, 1H), 5.71 (d, *J* = 1.46 Hz, 1H), 3.92 (s, 3H), 2.16 (s, 3H), 1.58 (s, 3H).

**<sup>13</sup>C NMR** (125 MHz, CDCl<sub>3</sub>) δ 159.3, 158.2, 144.2, 141.8, 140.7, 133.7, 132.3, 131.5, 129.4, 128.7, 128.0, 127.8, 127.6, 124.6, 120.2, 119.8, 116.0, 110.8, 110.7, 82.6, 55.8, 32.0, 21.3.

**HRMS** *m/z* (ESI+): Calculated for C<sub>25</sub>H<sub>23</sub>N<sub>2</sub>O<sub>4</sub>S<sup>+</sup> ([M+H]<sup>+</sup>): 447.1373, found 447.1378.

### 2,5a-Dimethyl-6-methylene-5-tosyl-5a,6-dihydroindolo[2,1-b]quinazolin-12(5H)-one (2i)



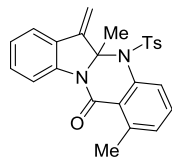
Purified by chromatography on silica gel, eluting with ethyl acetate/petroleum ether 1:10 (v/v); white solid, Mp = 155-156 °C; 77% yield.

**<sup>1</sup>H NMR** (400 MHz, CDCl<sub>3</sub>) δ 7.83 (d, *J* = 2.19 Hz, 1H), 7.73-7.69 (m, 1H), 7.66 (d, *J* = 8.14 Hz, 1H), 7.52-7.44 (m, 2H), 7.15 (td, *J* = 7.65, 1.43 Hz, 1H), 7.09 (td, *J* = 7.46, 1.24 Hz, 1H), 6.99-6.92 (m, 2H), 6.73 (d, *J* = 7.93 Hz, 2H), 6.09 (d, *J* = 1.45 Hz, 1H), 5.71 (d, *J* = 1.42 Hz, 1H), 2.48 (s, 3H), 2.15 (s, 3H), 1.58 (s, 3H).

**<sup>13</sup>C NMR** (125 MHz, CDCl<sub>3</sub>) δ 158.5, 144.2, 141.9, 140.8, 138.4, 136.9, 133.9, 133.6, 130.1, 129.3, 128.7, 128.0, 127.6, 126.5, 124.4, 120.1, 116.0, 110.8, 82.4, 32.0, 21.3, 21.1.

**HRMS** *m/z* (ESI+): Calculated for C<sub>25</sub>H<sub>23</sub>N<sub>2</sub>O<sub>3</sub>S<sup>+</sup> ([M+H]<sup>+</sup>): 431.1424, found 431.1425.

### 1,5a-Dimethyl-6-methylene-5-tosyl-5a,6-dihydroindolo[2,1-b]quinazolin-12(5H)-one (2j)



Purified by chromatography on silica gel, eluting with ethyl acetate/petroleum ether 1:10 (v/v); white solid, Mp = 138-139 °C; 37% yield.

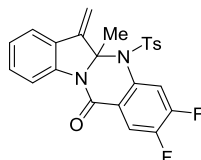
**<sup>1</sup>H NMR** (500 MHz, CDCl<sub>3</sub>) δ 7.76 (d, *J* = 8.11 Hz, 1H), 7.64 (d, *J* = 7.84 Hz, 1H), 7.54-7.47 (m, 2H), 7.30 (d, *J* = 7.60 Hz, 1H), 7.12 (dt, *J* = 28.40, 7.46 Hz, 2H), 7.02 (d, *J* = 8.20 Hz, 2H), 6.77 (d, *J* = 7.98 Hz, 2H), 6.07 (d, *J* = 1.40 Hz, 1H), 5.68 (d, *J* = 1.41 Hz, 1H), 2.74 (s, 3H), 2.17 (s, 3H), 1.57 (s, 3H).



$^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  159.0, 144.1, 142.2, 141.2, 141.0, 140.2, 134.1, 131.6, 131.5, 129.3, 128.6, 128.2, 127.5, 125.2, 124.3, 120.1, 116.2, 110.4, 81.8, 31.7, 21.5, 21.3.

**HRMS**  $m/z$  (ESI+): Calculated for  $\text{C}_{25}\text{H}_{23}\text{N}_2\text{O}_3\text{S}^+$  ( $[\text{M}+\text{H}]^+$ ): 431.1424, found 431.1432.

**2,3-Difluoro-5a-methyl-6-methylene-5-tosyl-5a,6-dihydroindolo[2,1-b]quinazolin-12(5H)-one (2k)**



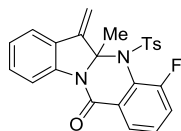
Purified by chromatography on silica gel, eluting with ethyl acetate/petroleum ether 1:10 (v/v); white solid,  $\text{Mp} = 177\text{-}178\text{ }^\circ\text{C}$ ; 60% yield.

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.83 (dd,  $J = 9.80, 8.34$  Hz, 1H), 7.69-7.65 (m, 1H), 7.65-7.62 (m, 1H), 7.53-7.44 (m, 1H), 7.20-7.09 (m, 2H), 7.00-6.93 (m, 2H), 6.76 (d,  $J = 8.14$  Hz, 2H), 6.11 (d,  $J = 1.53$  Hz, 1H), 5.71 (d,  $J = 1.57$  Hz, 1H), 2.16 (s, 3H), 1.60 (s, 3H).

$^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  156.5, 153.5 (d,  $J = 13.4$  Hz), 151.4 (dd,  $J = 35.1, 13.4$  Hz), 149.2 (d,  $J = 13.5$  Hz), 144.8, 141.3, 140.4, 136.5 (dd,  $J = 9.6, 3.2$  Hz), 133.4, 129.5, 128.9, 128.0, 127.5, 124.9, 124.0, 120.3, 119.8 (d,  $J = 20.0$  Hz), 116.1 (d,  $J = 18.4$  Hz), 111.4, 82.8, 32.0, 21.4.

**HRMS**  $m/z$  (ESI+): Calculated for  $\text{C}_{24}\text{H}_{19}\text{N}_2\text{O}_3\text{SF}_2^+$  ( $[\text{M}+\text{H}]^+$ ): 453.1079, found 453.1084.

**4-Fluoro-5a-methyl-6-methylene-5-tosyl-5a,6-dihydroindolo[2,1-b]quinazolin-12(5H)-one (2l)**



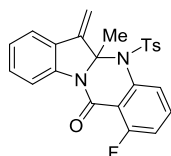
Purified by chromatography on silica gel, eluting with ethyl acetate/petroleum ether 1:10 (v/v); white solid,  $\text{Mp} = 145\text{-}146\text{ }^\circ\text{C}$ ; 67% yield.

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.95-7.87 (m, 1H), 7.87-7.76 (m, 1H), 7.56-7.41 (m, 3H), 7.29 (s, 1H), 7.26 (s, 1H), 7.17 (td,  $J = 7.71, 1.40$  Hz, 1H), 7.10 (td,  $J = 7.49, 1.17$  Hz, 1H), 6.85 (d,  $J = 8.11$  Hz, 2H), 5.97 (d,  $J = 1.51$  Hz, 1H), 5.55 (d,  $J = 1.55$  Hz, 1H), 2.18 (s, 3H), 1.58 (s, 3H).

$^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  160.0 (d,  $J = 255.0$  Hz), 157.7, 144.5, 141.3, 140.7, 135.1, 129.5, 129.1 (d,  $J = 7.9$  Hz), 128.9, 128.7, 128.5, 128.1 (d,  $J = 13.0$  Hz), 127.4, 124.7, 123.6 (d,  $J = 3.5$  Hz), 120.9 (d,  $J = 20.9$  Hz), 120.2, 116.3, 110.6, 82.6, 31.7, 21.3.

**HRMS**  $m/z$  (ESI+): Calculated for  $\text{C}_{24}\text{H}_{20}\text{N}_2\text{O}_3\text{SF}^+$  ( $[\text{M}+\text{H}]^+$ ): 435.1173, found 435.1179.

**1-Fluoro-5a-methyl-6-methylene-5-tosyl-5a,6-dihydroindolo[2,1-b]quinazolin-12(5H)-one (2m)**



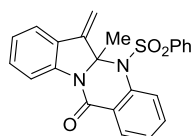
Purified by chromatography on silica gel, eluting with ethyl acetate/petroleum ether 1:10 (v/v); white solid, Mp = 185-186 °C; 76% yield.

**<sup>1</sup>H NMR** (400 MHz, CDCl<sub>3</sub>) δ 7.76-7.71 (m, 1H), 7.64-7.57 (m, 2H), 7.48 (dd, *J* = 7.32, 1.54 Hz, 1H), 7.25-7.18 (m, 1H), 7.18-7.08 (m, 2H), 7.01 (d, *J* = 8.40 Hz, 2H), 6.77 (d, *J* = 8.04 Hz, 2H), 6.09 (d, *J* = 1.52 Hz, 1H), 5.69 (d, *J* = 1.53 Hz, 1H), 2.16 (s, 3H), 1.60 (s, 3H).

**<sup>13</sup>C NMR** (125 MHz, CDCl<sub>3</sub>) δ 162.5 (d, *J* = 261.3 Hz), 155.2, 144.6, 141.7, 140.9 (d, *J* = 26.8 Hz), 133.7, 133.1 (d, *J* = 9.9 Hz), 129.5, 129.0, 128.0, 127.5, 126.5 (d, *J* = 3.6 Hz), 124.7, 120.1, 116.6 (d, *J* = 21.5 Hz), 116.4, 115.7 (d, *J* = 7.5 Hz), 111.0, 82.4, 31.7, 21.3.

**HRMS** *m/z* (ESI+): Calculated for C<sub>24</sub>H<sub>20</sub>N<sub>2</sub>O<sub>3</sub>SF<sup>+</sup> ([M+H]<sup>+</sup>): 435.1173, found 435.1181.

**5a-Methyl-6-methylene-5-(phenylsulfonyl)-5a,6-dihydroindolo[2,1-b]quinazolin-12(5H)-one (2n)**



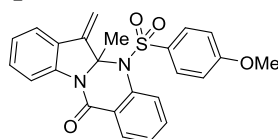
Purified by chromatography on silica gel, eluting with ethyl acetate/petroleum ether 1:10 (v/v); white solid, Mp = 183-184 °C; 80% yield.

**<sup>1</sup>H NMR** (500 MHz, CDCl<sub>3</sub>) δ 8.02 (dd, *J* = 7.6, 1.7 Hz, 1H), 7.82 (d, *J* = 8.1 Hz, 1H), 7.74 (d, *J* = 8.0 Hz, 1H), 7.69 (td, *J* = 7.7, 1.7 Hz, 1H), 7.54 (q, *J* = 8.0, 7.4 Hz, 2H), 7.26 (dd, *J* = 13.7, 6.5 Hz, 1H), 7.16 (dt, *J* = 28.4, 7.5 Hz, 2H), 7.04 (d, *J* = 7.6 Hz, 2H), 6.99 (t, *J* = 7.6 Hz, 2H), 6.12 (d, *J* = 1.5 Hz, 1H), 5.72 (d, *J* = 1.4 Hz, 1H), 1.60 (s, 3H).

**<sup>13</sup>C NMR** (125 MHz, CDCl<sub>3</sub>) δ 158.1, 142.0, 140.7, 139.3, 136.5, 133.3, 132.8, 130.2, 129.9, 128.3, 128.2, 127.9, 127.8, 127.5, 127.1, 124.7, 120.3, 116.2, 110.7, 82.5, 32.1.

**HRMS** *m/z* (ESI+): Calculated for C<sub>23</sub>H<sub>19</sub>N<sub>2</sub>O<sub>3</sub>S<sup>+</sup> ([M+H]<sup>+</sup>): 403.1111, found 403.1107.

**5-((4-Methoxyphenyl)sulfonyl)-5a-methyl-6-methylene-5a,6-dihydroindolo[2,1-b]quinazolin-12(5H)-one (2o)**



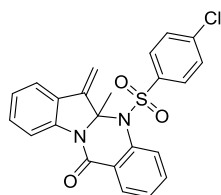
Purified by chromatography on silica gel, eluting with ethyl acetate/petroleum ether 1:10 (v/v); white solid, Mp = 141-142 °C; 60% yield.

**<sup>1</sup>H NMR** (500 MHz, CDCl<sub>3</sub>) δ 8.05 (dd, *J* = 7.8, 1.6 Hz, 1H), 7.80 (dd, *J* = 7.9, 4.2 Hz, 2H), 7.68 (td, *J* = 7.8, 1.6 Hz, 1H), 7.52 (dt, *J* = 7.5, 3.6 Hz, 2H), 7.15 (dt, *J* = 26.1, 7.3 Hz, 2H), 7.01 (d, *J* = 9.0 Hz, 2H), 6.42 (d, *J* = 8.7 Hz, 2H), 6.11 (d, *J* = 1.5 Hz, 1H), 5.74 (d, *J* = 1.5 Hz, 1H), 3.68 (s, 3H), 1.60 (d, *J* = 4.7 Hz, 5H).

**<sup>13</sup>C NMR** (125 MHz, CDCl<sub>3</sub>) δ 163.3, 158.3, 141.9, 140.8, 139.6, 132.8, 130.4, 130.2, 129.5, 128.3, 128.1, 127.7, 127.6, 126.9, 124.5, 120.2, 116.2, 113.4, 110.8, 82.4, 55.4, 32.1.

**HRMS** *m/z* (ESI+): Calculated for C<sub>24</sub>H<sub>21</sub>N<sub>2</sub>O<sub>4</sub>S<sup>+</sup> ([M+H]<sup>+</sup>): 433.1217, found 433.1211.

**5-((4-Chlorophenyl)sulfonyl)-5a-methyl-6-methylene-5a,6-dihydroindolo[2,1-b]-quinazolin-12(5H)-one (2p)**



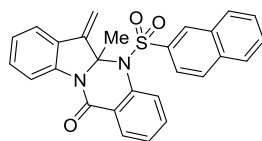
Purified by chromatography on silica gel, eluting with ethyl acetate/petroleum ether 1:10 (v/v); white solid, Mp = 144-145 °C; 46% yield.

**<sup>1</sup>H NMR** (500 MHz, CDCl<sub>3</sub>) δ 8.06 (dd, *J* = 7.8, 1.7 Hz, 1H), 7.78 (t, *J* = 7.4 Hz, 2H), 7.69 (td, *J* = 7.8, 1.7 Hz, 1H), 7.53 (dd, *J* = 16.4, 7.8 Hz, 2H), 7.24 (t, *J* = 7.7 Hz, 1H), 7.15 (t, *J* = 7.6 Hz, 1H), 7.00 (d, *J* = 8.8 Hz, 2H), 6.95-6.89 (m, 2H), 6.12 (d, *J* = 1.6 Hz, 1H), 5.73 (d, *J* = 1.6 Hz, 1H), 1.61 (s, 3H).

**<sup>13</sup>C NMR** (125 MHz, CDCl<sub>3</sub>) δ 158.2, 141.6, 140.7, 140.1, 139.1, 135.1, 132.9, 130.3, 130.0, 129.3, 128.4, 127.9, 127.3, 126.8, 124.8, 120.2, 116.0, 111.1, 82.5, 32.0.

**HRMS** *m/z* (ESI+): Calculated for C<sub>23</sub>H<sub>18</sub>ClN<sub>2</sub>O<sub>3</sub>S<sup>+</sup> ([M+H]<sup>+</sup>): 437.0721, found 437.0713.

**5a-Methyl-6-methylene-5-(naphthalen-2-ylsulfonyl)-5a,6-dihydroindolo[2,1-b]-quinazolin-12(5H)-one (2q)**



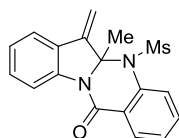
Purified by chromatography on silica gel, eluting with ethyl acetate/petroleum ether 1:10 (v/v); white solid, Mp = 158-159 °C; 15% yield.

**<sup>1</sup>H NMR** (500 MHz, CDCl<sub>3</sub>) δ 8.05 (d, *J* = 7.8 Hz, 1H), 7.86 (d, *J* = 8.0 Hz, 1H), 7.80 (s, 1H), 7.77-7.62 (m, 2H), 7.59-7.50 (m, 3H), 7.45 (t, *J* = 7.1 Hz, 2H), 7.39 (dd, *J* = 20.0, 7.7 Hz, 2H), 6.92 (d, *J* = 8.7 Hz, 1H), 6.82 (t, *J* = 7.6 Hz, 1H), 6.70 (t, *J* = 7.8 Hz, 1H), 6.15 (s, 1H), 5.77 (s, 1H), 1.60 (s, 3H).

$^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  158.2, 142.0, 140.5, 139.5, 134.7, 133.5, 132.8, 131.4, 131.0, 130.3, 129.32, 129.28, 129.0, 128.6, 128.2, 127.8, 127.5, 127.1, 127.0, 126.8, 124.6, 122.2, 119.8, 115.6, 110.8, 82.4, 32.0.

**HRMS**  $m/z$  (ESI+): Calculated for  $\text{C}_{27}\text{H}_{21}\text{N}_2\text{O}_3\text{S}^+$  ( $[\text{M}+\text{H}]^+$ ): 453.1267, found 453.1262.

**5a-methyl-6-methylene-5-(methylsulfonyl)-5a,6-dihydroindolo[2,1-b]quinazolin-12(5H)-one (2r)**



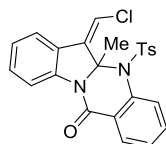
Purified by chromatography on silica gel, eluting with ethyl acetate/petroleum ether 1:10 (v/v); white solid,  $\text{Mp} = 212\text{-}213\text{ }^\circ\text{C}$ ; 41% yield.

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.33 (d,  $J=8.4$  Hz, 1H), 8.16 (dd,  $J=7.6, 1.5$  Hz, 1H), 7.67-7.60 (m, 3H), 7.56-7.51 (m, 1H), 7.42 (td,  $J=7.9, 1.3$  Hz, 1H), 7.26-7.20 (m, 1H), 6.11 (d,  $J=1.4$  Hz, 1H), 5.66 (d,  $J=1.7$  Hz, 1H), 2.65 (s, 3H), 1.69 (s, 3H).

$^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  158.9, 142.2, 140.6, 138.9, 133.2, 130.9, 129.7, 128.4, 128.2, 127.1, 126.7, 125.2, 121.0, 116.5, 110.4, 82.7, 39.7, 31.8.

**HRMS**  $m/z$  (ESI+): Calculated for  $\text{C}_{18}\text{H}_{17}\text{N}_2\text{O}_3\text{S}^+$  ( $[\text{M}+\text{H}]^+$ ): 341.0954, found 341.0942.

**(Z)-6-(Chloromethylene)-5a-methyl-5-tosyl-5a,6-dihydroindolo[2,1-b]quinazolin-12(5H)-one (3)**



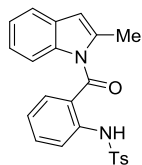
Purified by chromatography on silica gel, eluting with ethyl acetate/petroleum ether 1:10 (v/v); white solid,  $\text{Mp} = 223\text{-}224\text{ }^\circ\text{C}$ ; 63% yield.

$^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.82 (dd,  $J = 38.9, 7.8$  Hz, 2H), 7.68 (d,  $J = 8.0$  Hz, 1H), 7.61 (t,  $J = 7.7$  Hz, 1H), 7.47-7.37 (m, 2H), 7.23-7.13 (m, 1H), 7.07 (t,  $J = 7.4$  Hz, 1H), 6.90 (s, 1H), 6.68 (s, 4H), 2.15 (s, 3H), 1.72 (s, 3H).

$^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  157.7, 144.5, 140.3, 138.8, 137.4, 133.1, 132.9, 130.2, 129.9, 128.9, 128.4, 127.9, 127.7, 127.6, 126.4, 124.8, 119.7, 116.2, 115.4, 82.7, 26.4, 21.5.

**HRMS**  $m/z$  (ESI+): Calculated for  $\text{C}_{24}\text{H}_{20}\text{ClN}_2\text{O}_3\text{S}^+$  ( $[\text{M}+\text{H}]^+$ ): 451.0878, found 451.0884.

**4-Methyl-N-(2-(2-methyl-1H-indole-1-carbonyl)phenyl)benzenesulfonamide (4a)**



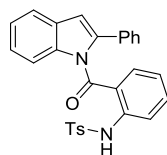
Purified by chromatography on silica gel, eluting with ethyl acetate/petroleum ether 1:10 (v/v); yellow solid, Mp = 135-136 °C; 46% yield (for the last step).

**<sup>1</sup>H NMR** (500 MHz, CDCl<sub>3</sub>) δ 9.32 (s, 1H), 7.93 (d, *J* = 8.70 Hz, 1H), 7.70-7.62 (m, 2H), 7.61-7.56 (m, 1H), 7.42 (d, *J* = 7.70 Hz, 1H), 7.28 (s, 1H), 7.09 (dt, *J* = 17.87, 7.55 Hz, 2H), 7.01 (d, *J* = 7.97 Hz, 2H), 6.82 (t, *J* = 7.85 Hz, 1H), 6.40 (s, 1H), 6.19 (d, *J* = 8.23 Hz, 1H), 2.29 (s, 3H), 2.15 (s, 3H).

**<sup>13</sup>C NMR** (125 MHz, CDCl<sub>3</sub>) δ 169.6, 144.1, 138.4, 137.9, 136.7, 136.2, 134.3, 132.1, 129.7, 129.4, 127.2, 124.4, 124.3, 123.7, 122.8, 122.6, 119.8, 114.0, 109.2, 21.4, 15.3.

**HRMS** *m/z* (ESI+): Calculated for C<sub>23</sub>H<sub>21</sub>N<sub>2</sub>O<sub>3</sub>S<sup>+</sup> ([M+H]<sup>+</sup>): 405.1267, found 405.1276.

#### 4-Methyl-N-(2-(2-phenyl-1H-indole-1-carbonyl)phenyl)benzenesulfonamide (4b)



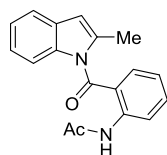
Purified by chromatography on silica gel, eluting with ethyl acetate/petroleum ether 1:10 (v/v); yellow solid, Mp = 135-136 °C; 40% yield (for the last step).

**<sup>1</sup>H NMR** (500 MHz, CDCl<sub>3</sub>) δ 9.69 (s, 1H), 7.75 (t, *J* = 8.71 Hz, 3H), 7.61 (d, *J* = 7.67 Hz, 1H), 7.46-7.37 (m, 2H), 7.27 (dd, *J* = 6.90, 3.14 Hz, 2H), 7.22 (q, *J* = 4.32, 3.82 Hz, 3H), 7.14 (d, *J* = 8.04 Hz, 2H), 7.06 (t, *J* = 7.75 Hz, 1H), 6.91 (t, *J* = 7.58 Hz, 1H), 6.85-6.79 (m, 2H), 2.28 (s, 3H).

**<sup>13</sup>C NMR** (125 MHz, CDCl<sub>3</sub>) δ 170.4, 144.1, 141.4, 139.5, 137.9, 136.7, 134.6, 132.7, 132.5, 129.8, 129.4, 128.4, 127.9, 127.8, 127.3, 124.1, 123.4, 123.3, 122.4, 121.0, 120.9, 113.7, 110.3, 21.5.

**HRMS** *m/z* (ESI+): Calculated for C<sub>28</sub>H<sub>23</sub>N<sub>2</sub>O<sub>3</sub>S<sup>+</sup> ([M+H]<sup>+</sup>): 467.1424, found 467.1424.

#### N-(2-(2-Methyl-1H-indole-1-carbonyl)phenyl)acetamide (4c)



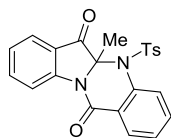
Purified by chromatography on silica gel, eluting with ethyl acetate/petroleum ether 1:10 (v/v); yellow solid, Mp = 141-142 °C; 81% yield (for the last step).

**<sup>1</sup>H NMR** (500 MHz, CDCl<sub>3</sub>) δ 9.77 (s, 1H), 8.58 (d, *J* = 8.3 Hz, 1H), 7.62 (ddd, *J* = 8.7, 7.3, 1.7 Hz, 1H), 7.49 (d, *J* = 7.7 Hz, 1H), 7.42 (dd, *J* = 7.8, 1.7 Hz, 1H), 7.18 (ddd, *J* = 8.1, 6.2, 1.9 Hz, 1H), 7.13-6.99 (m, 3H), 6.47 (d, *J* = 1.3 Hz, 1H), 2.41 (d, *J* = 1.2 Hz, 3H), 2.22 (s, 3H).

**<sup>13</sup>C NMR** (125 MHz, CDCl<sub>3</sub>) δ 170.5, 169.0, 139.4, 137.7, 137.2, 134.4, 131.8, 129.6, 123.2, 123.1, 123.0, 122.31, 122.27, 120.0, 114.2, 109.3, 25.1, 15.6.

**HRMS** *m/z* (ESI+): Calculated for C<sub>18</sub>H<sub>17</sub>N<sub>2</sub>O<sub>2</sub><sup>+</sup> ([M+H]<sup>+</sup>): 293.1285, found 293.1291.

### 5a-Methyl-5-tosyl-5,5a-dihydroindolo[2,1-b]quinazoline-6,12-dione (5a)



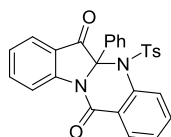
Purified by chromatography on silica gel, eluting with ethyl acetate/petroleum ether 1:10 (v/v); white solid, Mp = 155-156 °C; 37% yield.

**<sup>1</sup>H NMR** (400 MHz, CDCl<sub>3</sub>) δ 8.24 (d, *J* = 8.26 Hz, 1H), 8.06-7.97 (m, 2H), 7.75 (ddd, *J* = 8.44, 7.25, 1.41 Hz, 1H), 7.69-7.66 (m, 2H), 7.55-7.48 (m, 1H), 7.38 (td, *J* = 7.55, 0.91 Hz, 1H), 7.03-6.87 (m, 4H), 2.32 (s, 3H), 1.54 (s, 3H).

**<sup>13</sup>C NMR** (125 MHz, CDCl<sub>3</sub>) δ 191.2, 157.8, 148.7, 144.9, 139.0, 137.5, 133.9, 133.6, 129.3, 128.6, 128.5, 128.3, 127.7, 127.4, 125.4, 125.2, 122.7, 117.1, 78.7, 25.7, 21.6.

**HRMS** *m/z* (ESI<sup>+</sup>): Calculated for C<sub>23</sub>H<sub>19</sub>N<sub>2</sub>O<sub>4</sub>S<sup>+</sup> ([M+H]<sup>+</sup>): 419.1060, found 419.1070.

### 5a-Phenyl-5-tosyl-5,5a-dihydroindolo[2,1-b]quinazoline-6,12-dione (5b)



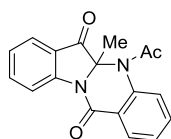
Purified by chromatography on silica gel, eluting with ethyl acetate/petroleum ether 1:10 (v/v); yellow solid, Mp = 182-183 °C; 54% yield.

**<sup>1</sup>H NMR** (400 MHz, CDCl<sub>3</sub>) δ 8.50-8.38 (m, 1H), 7.93 (dt, *J* = 7.6, 1.2 Hz, 1H), 7.89-7.78 (m, 2H), 7.58-7.46 (m, 2H), 7.44-7.35 (m, 2H), 7.31 (td, *J* = 7.5, 1.4 Hz, 1H), 7.20-7.12 (m, 5H), 7.06 (d, *J* = 8.2 Hz, 2H), 2.39 (s, 3H).

**<sup>13</sup>C NMR** (100 MHz, CDCl<sub>3</sub>) δ 188.4, 158.7, 149.8, 145.0, 139.5, 137.5, 135.6, 134.4, 133.5, 129.4, 129.1, 129.0, 128.3, 128.2, 127.9, 127.82, 127.77, 126.0, 125.9, 125.5, 122.1, 116.5, 82.9, 21.6.

**HRMS** *m/z* (ESI<sup>+</sup>): Calculated for C<sub>28</sub>H<sub>21</sub>N<sub>2</sub>O<sub>4</sub>S<sup>+</sup> ([M+H]<sup>+</sup>): 481.1217, found 481.1205.

### 5-Acetyl-5a-methyl-5,5a-dihydroindolo[2,1-b]quinazoline-6,12-dione (5c)



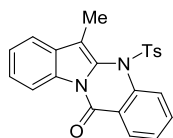
Purified by chromatography on silica gel, eluting with ethyl acetate/petroleum ether 1:10 (v/v); yellow solid, Mp = 214-215 °C; 33% yield.

**<sup>1</sup>H NMR** (500 MHz, CDCl<sub>3</sub>) δ 8.46 (d, *J* = 8.2 Hz, 1H), 8.22 (d, *J* = 7.7 Hz, 1H), 7.99 (d, *J* = 7.7 Hz, 1H), 7.72 (q, *J* = 6.8 Hz, 2H), 7.55 (d, *J* = 8.3 Hz, 2H), 7.35 (t, *J* = 7.7 Hz, 1H), 2.05 (s, 3H), 1.45 (s, 3H).

**<sup>13</sup>C NMR** (125 MHz, CDCl<sub>3</sub>) δ 192.1, 172.2, 158.5, 148.0, 139.9, 136.6, 133.6, 129.2, 128.3, 127.2, 126.5, 125.2, 125.0, 123.9, 117.0, 76.0, 29.7, 22.4.

**HRMS** *m/z* (ESI<sup>+</sup>): Calculated for C<sub>18</sub>H<sub>15</sub>N<sub>2</sub>O<sub>3</sub><sup>+</sup> ([M+H]<sup>+</sup>): 307.1077, found 307.1073.

### 6-Methyl-5-tosylindolo[2,1-b]quinazolin-12(5H)-one (7)



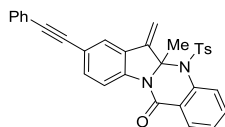
Purified by chromatography on silica gel, eluting with ethyl acetate/petroleum ether 1:10 (v/v); yellow solid, Mp = 206-207 °C; 59% yield.

**<sup>1</sup>H NMR** (500 MHz, CDCl<sub>3</sub>) δ 8.35 (d, *J* = 7.8 Hz, 2H), 7.95-7.81 (m, 3H), 7.59 (t, *J* = 7.4 Hz, 1H), 7.53 (t, *J* = 7.8 Hz, 1H), 7.45 (t, *J* = 7.6 Hz, 1H), 7.18 (d, *J* = 8.1 Hz, 2H), 6.98 (d, *J* = 8.0 Hz, 2H), 2.33 (s, 3H), 2.21 (s, 3H).

**<sup>13</sup>C NMR** (125 MHz, CDCl<sub>3</sub>) δ 159.1, 154.3, 146.7, 145.7, 140.1, 134.7, 131.2, 131.0, 130.1, 129.0, 128.2, 128.0, 126.9, 126.7, 126.4, 126.3, 121.5, 116.7, 72.3, 21.7, 17.4.

**HRMS** *m/z* (ESI+): Calculated for C<sub>23</sub>H<sub>19</sub>N<sub>2</sub>O<sub>3</sub>S<sup>+</sup> ([M+H]<sup>+</sup>): 403.1111, found 403.1106

### 5a-Methyl-6-methylene-8-(phenylethynyl)-5-tosyl-5a,6-dihydroindolo[2,1-b]quinazolin-12(5H)-one (8)



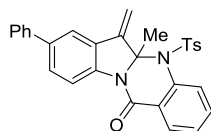
Purified by chromatography on silica gel, eluting with ethyl acetate/petroleum ether 1:10 (v/v); white solid, Mp = 180-181 °C; 76% yield.

**<sup>1</sup>H NMR** (400 MHz, CDCl<sub>3</sub>) δ 8.03 (dd, *J* = 7.71, 1.67 Hz, 1H), 7.79 (dd, *J* = 8.01, 1.14 Hz, 1H), 7.74-7.63 (m, 3H), 7.59-7.55 (m, 2H), 7.51 (td, *J* = 7.53, 1.19 Hz, 1H), 7.42-7.31 (m, 4H), 6.98 (d, *J* = 8.37 Hz, 2H), 6.81 (d, *J* = 8.11 Hz, 2H), 6.14 (d, *J* = 1.61 Hz, 1H), 5.76 (d, *J* = 1.60 Hz, 1H), 2.20 (s, 3H), 1.59 (s, 3H).

**<sup>13</sup>C NMR** (125 MHz, CDCl<sub>3</sub>) δ 158.3, 144.5, 141.1, 140.4, 139.5, 133.9, 133.0, 132.9, 131.6, 131.5, 130.4, 129.0, 128.9, 128.7, 128.5, 128.4, 128.2, 128.1, 127.9, 127.81, 127.76, 126.6, 123.3, 123.1, 119.4, 115.9, 111.9, 89.4, 89.0, 82.7, 32.1, 21.4.

**HRMS** *m/z* (ESI+): Calculated for C<sub>32</sub>H<sub>25</sub>N<sub>2</sub>O<sub>3</sub>S<sup>+</sup> ([M+H]<sup>+</sup>): 517.1580, found 517.1588.

### 5a-Methyl-6-methylene-8-phenyl-5-tosyl-5a,6-dihydroindolo[2,1-b]quinazolin-12(5H)-one (9)



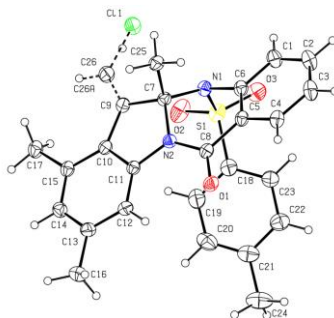
Purified by chromatography on silica gel, eluting with ethyl acetate/petroleum ether 1:10 (v/v); white solid, Mp = 90-91 °C; 64% yield.

**<sup>1</sup>H NMR** (400 MHz, CDCl<sub>3</sub>) δ 8.05 (dd, *J* = 7.76, 1.66 Hz, 1H), 7.79 (d, *J* = 8.11 Hz, 2H), 7.72-7.58 (m, 4H), 7.50 (dt, *J* = 10.64, 7.50 Hz, 3H), 7.44-7.34 (m, 2H), 7.01 (d, *J* = 8.12 Hz, 2H), 6.75 (d, *J* = 8.04 Hz, 2H), 6.26-6.04 (m, 1H), 5.88-5.50 (m, 1H), 2.15 (s, 3H), 1.62 (s, 3H).

$^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  158.3, 144.3, 141.8, 140.6, 140.1, 139.5, 138.0, 134.0, 132.8, 130.4, 129.0, 128.9, 128.8, 128.4, 128.21, 128.16, 128.12, 127.8, 127.5, 126.9, 126.7, 126.5, 118.6, 116.2, 111.3, 82.7, 32.1, 21.4.

HRMS  $m/z$  (ESI+): Calculated for  $\text{C}_{30}\text{H}_{25}\text{N}_2\text{O}_3\text{S}^+$  ( $[\text{M}+\text{H}]^+$ ): 493.1580, found 493.1589.

## 5. Crystal Report for the Mixture of 2b and 6



### Datablock: mo\_211221\_wb\_2f\_0m

Bond precision:	C-C = 0.0028 Å	Wavelength=0.71073	
Cell:	a=10.908 (4)	b=15.648 (6)	c=14.141 (5)
	alpha=90	beta=112.321 (10)	gamma=90
Temperature:	170 K		
	Calculated	Reported	
Volume	2232.9 (14)	2232.8 (14)	
Space group	P 21/n	P 1 21/n 1	
Hall group	-P 2yn	-P 2yn	
Moiety formula	C26 H23.63 Cl0.37 N2 O3 S	C26 H23.63 Cl0.37 N2 O3 S	
Sum formula	C26 H23.63 Cl0.37 N2 O3 S	C26 H23.62 Cl0.38 N2 O3 S	
Mr	457.34	457.53	
Dx, g cm <sup>-3</sup>	1.360	1.361	
Z	4	4	
Mu (mm <sup>-1</sup> )	0.221	0.222	
F000	959.8	960.0	
F000'	960.91		
h, k, lmax	14, 20, 18	13, 20, 18	
Nref	4945	4935	
Tmin, Tmax	0.904, 0.927	0.684, 0.746	
Tmin'	0.901		
Correction method=	# Reported T Limits: Tmin=0.684 Tmax=0.746		
AbsCorr =	MULTI-SCAN		
Data completeness=	0.998	Theta(max) = 27.137	
R(reflections)=	0.0423 ( 4186)	wR2(reflections)=	
S =	1.040	0.1145 ( 4935)	
	Npar= 303		



The following ALERTS were generated. Each ALERT has the format  
**test-name\_ALERT\_alert-type\_alert-level.**  
Click on the hyperlinks for more details of the test.

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**Alert level C**

PLAT041_ALERT_1_C	Calc. and Reported SumFormula	Strings Differ	Please Check
PLAT077_ALERT_4_C	Unitcell Contains Non-integer Number of Atoms ..		Please Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance .....		2.970 Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L=	0.600	2 Report

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**Alert level G**

FORMU01\_ALERT\_1\_G There is a discrepancy between the atom counts in the  
\_chemical\_formula\_sum and \_chemical\_formula\_moiety. This is  
usually due to the moiety formula being in the wrong format.  
Atom count from \_chemical\_formula\_sum: C26 H23.62 Cl0.38 N2 O3 S1  
Atom count from \_chemical\_formula\_moiety:C26 H23.63 Cl0.37 N2 O3 S1  
CELLZ01\_ALERT\_1\_G Difference between formula and atom\_site contents detected.  
CELLZ01\_ALERT\_1\_G ALERT: check formula stoichiometry or atom site occupancies.  
From the CIF: \_cell\_formula\_units\_Z 4  
From the CIF: \_chemical\_formula\_sum C26 H23.62 Cl0.38 N2 O3 S  
TEST: Compare cell contents of formula and atom\_site data

atom	Z*formula	cif sites	diff
C	104.00	104.00	0.00
H	94.48	94.51	-0.03
Cl	1.52	1.49	0.03
N	8.00	8.00	0.00
O	12.00	12.00	0.00
S	4.00	4.00	0.00

PLAT068_ALERT_1_G	Reported F000 Differs from Calcd (or Missing)...		Please Check
PLAT168_ALERT_4_G	The CIF-Embedded .res File Contains EXYZ Records		1 Report
PLAT171_ALERT_4_G	The CIF-Embedded .res File Contains EADP Records		1 Report
PLAT301_ALERT_3_G	Main Residue Disorder .....	(Resd 1 )	4% Note
PLAT380_ALERT_4_G	Incorrectly? Oriented X(sp2)-Methyl Moiety .....		C17 Check
PLAT793_ALERT_4_G	Model has Chirality at C7	(Centro SPGR)	S Verify
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L=	0.600	8 Note
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.		8 Info

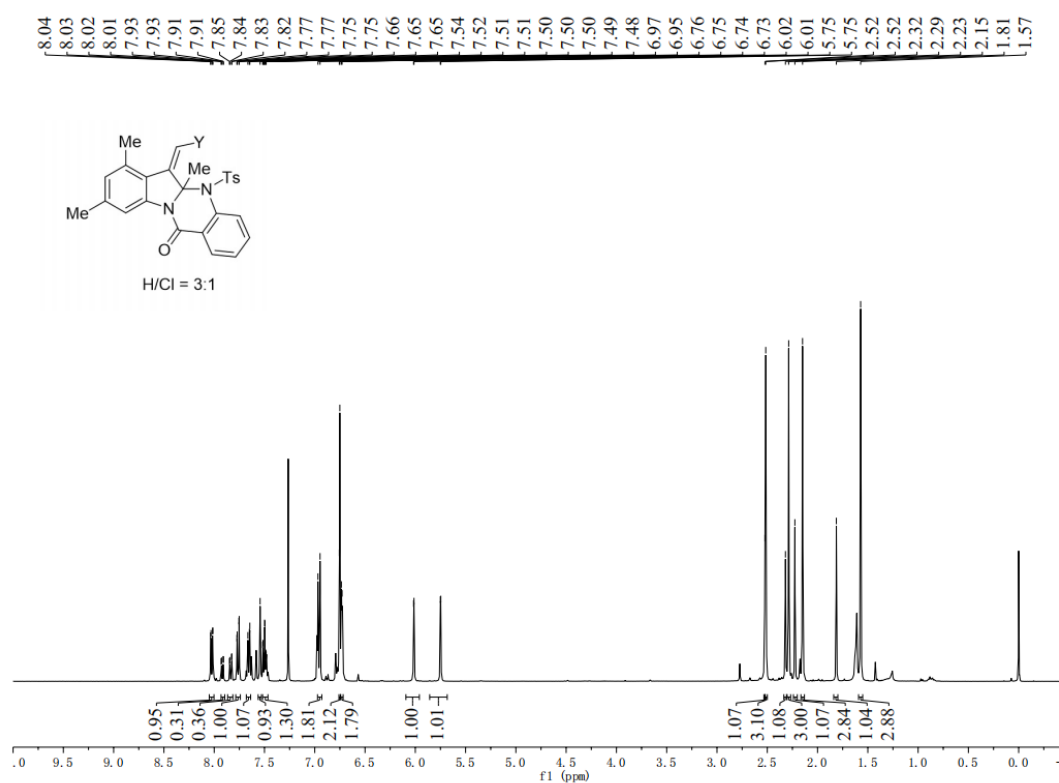
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0 **ALERT level A** = Most likely a serious problem - resolve or explain  
0 **ALERT level B** = A potentially serious problem, consider carefully  
4 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
11 **ALERT level G** = General information/check it is not something unexpected

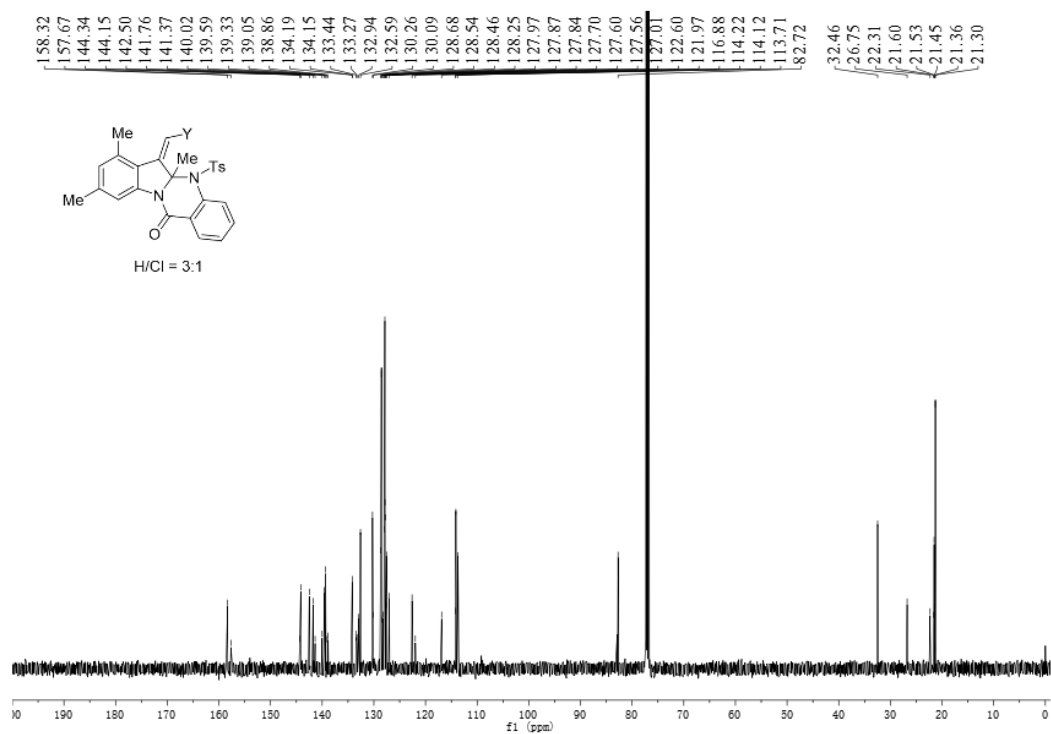
5 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
1 ALERT type 2 Indicator that the structure model may be wrong or deficient  
3 ALERT type 3 Indicator that the structure quality may be low  
6 ALERT type 4 Improvement, methodology, query or suggestion  
0 ALERT type 5 Informative message, check

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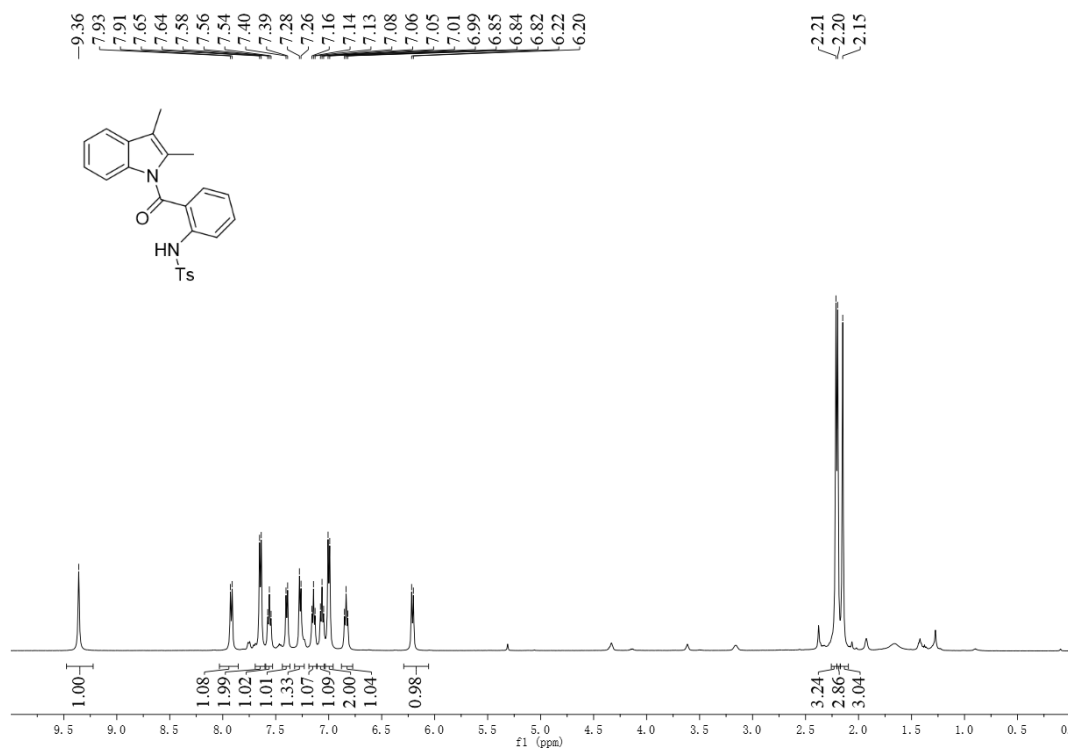
## 6. Copies of NMR spectra



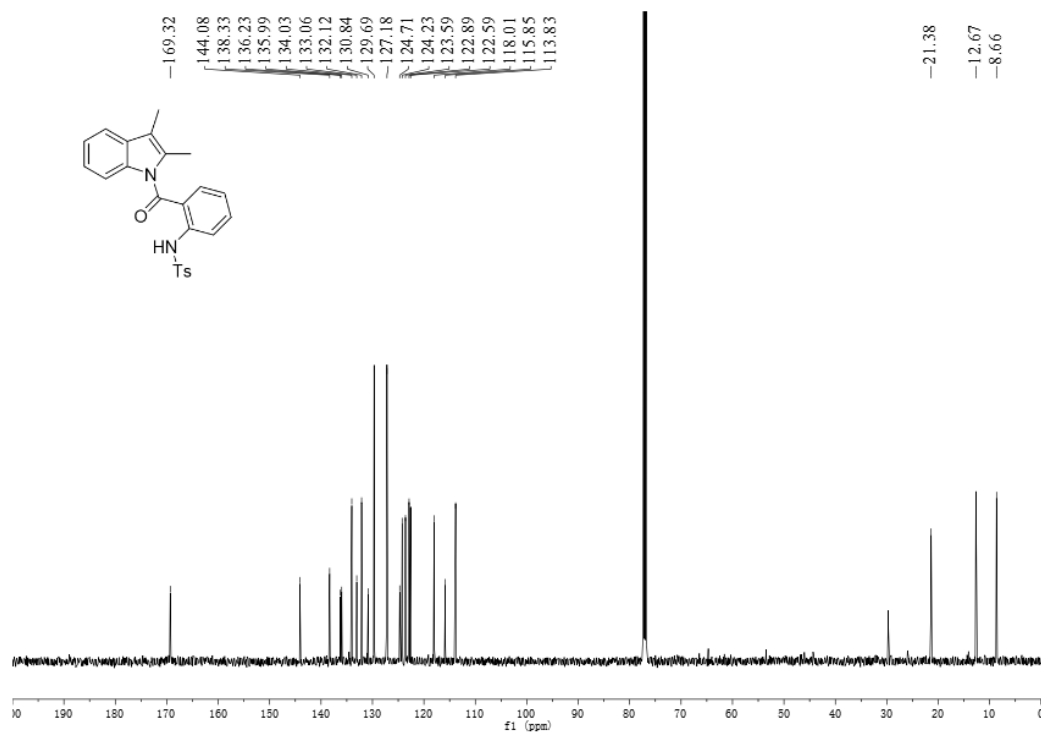
<sup>1</sup>H NMR spectrum of mixture (2b and 6)



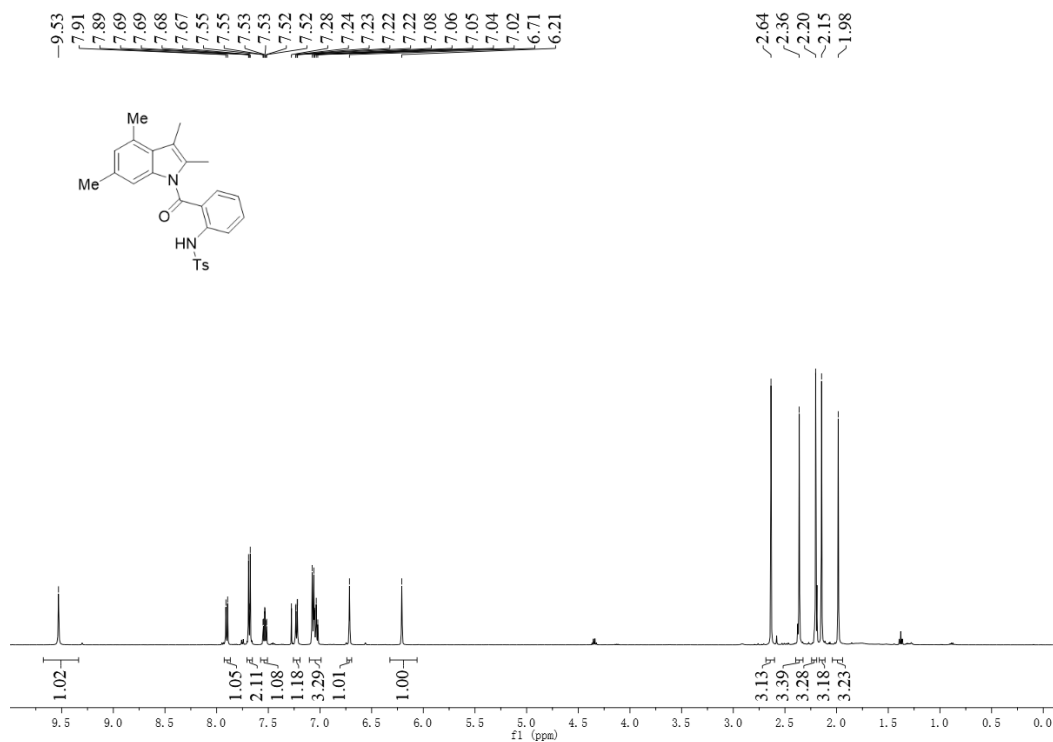
<sup>13</sup>C NMR spectrum of mixture (2b and 6)



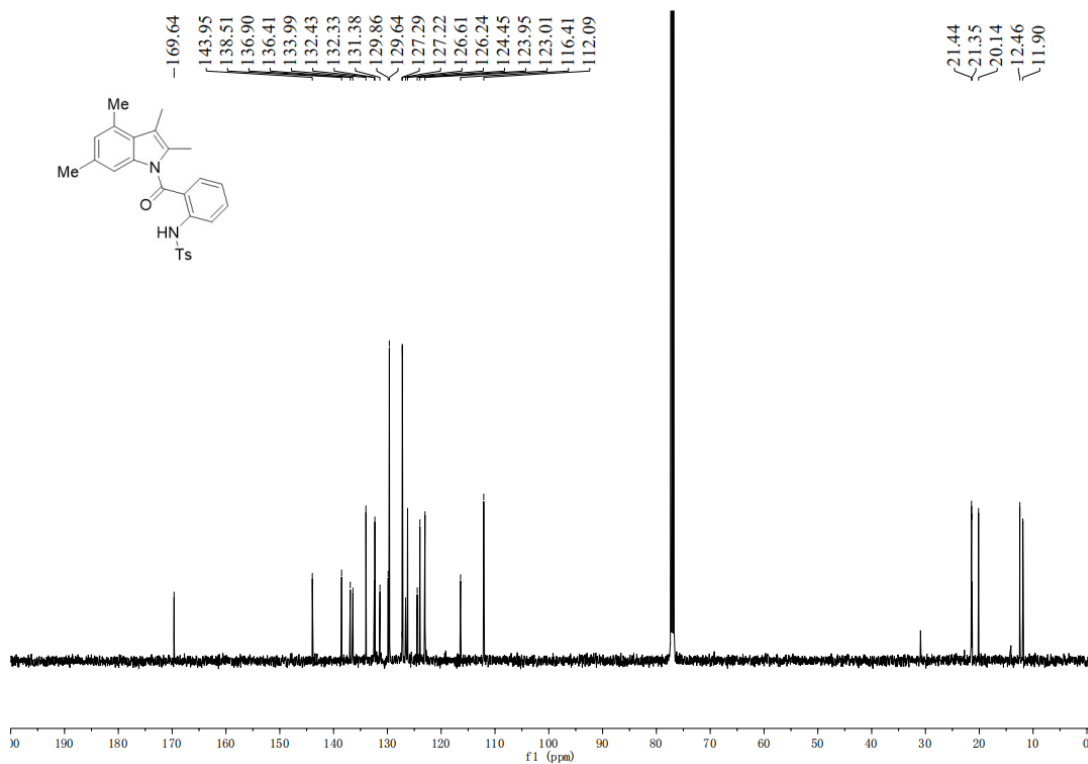
<sup>1</sup>H NMR spectrum of compound 1a



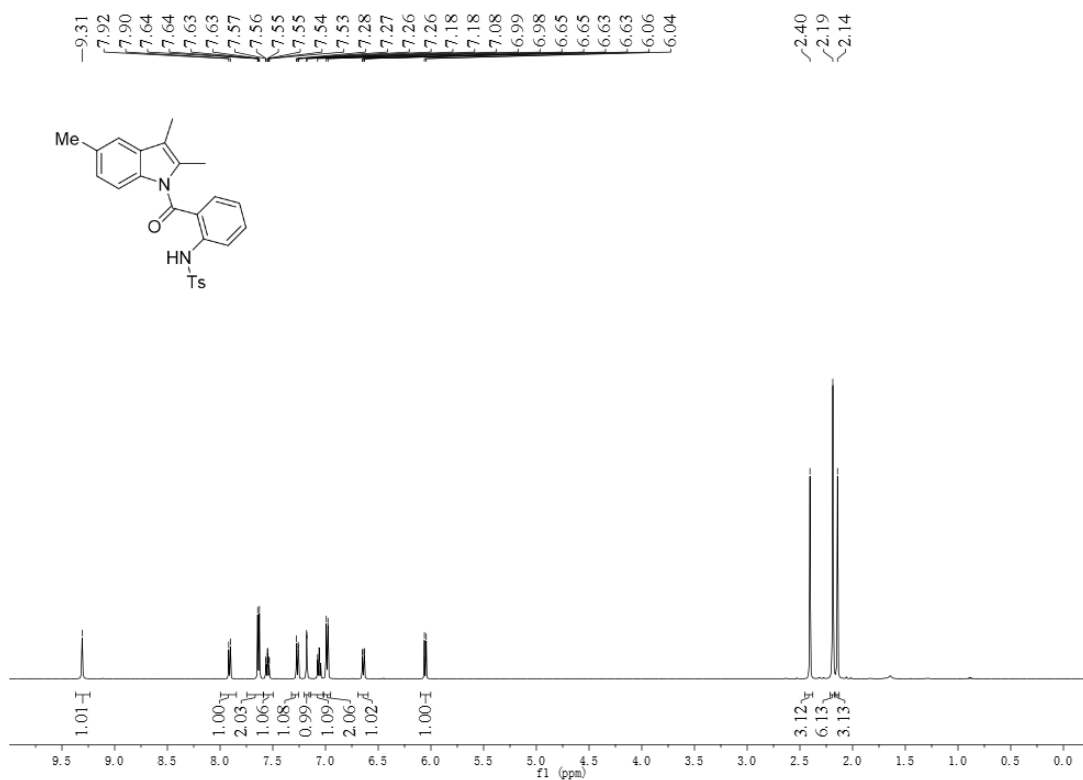
<sup>13</sup>C NMR spectrum of compound 1a



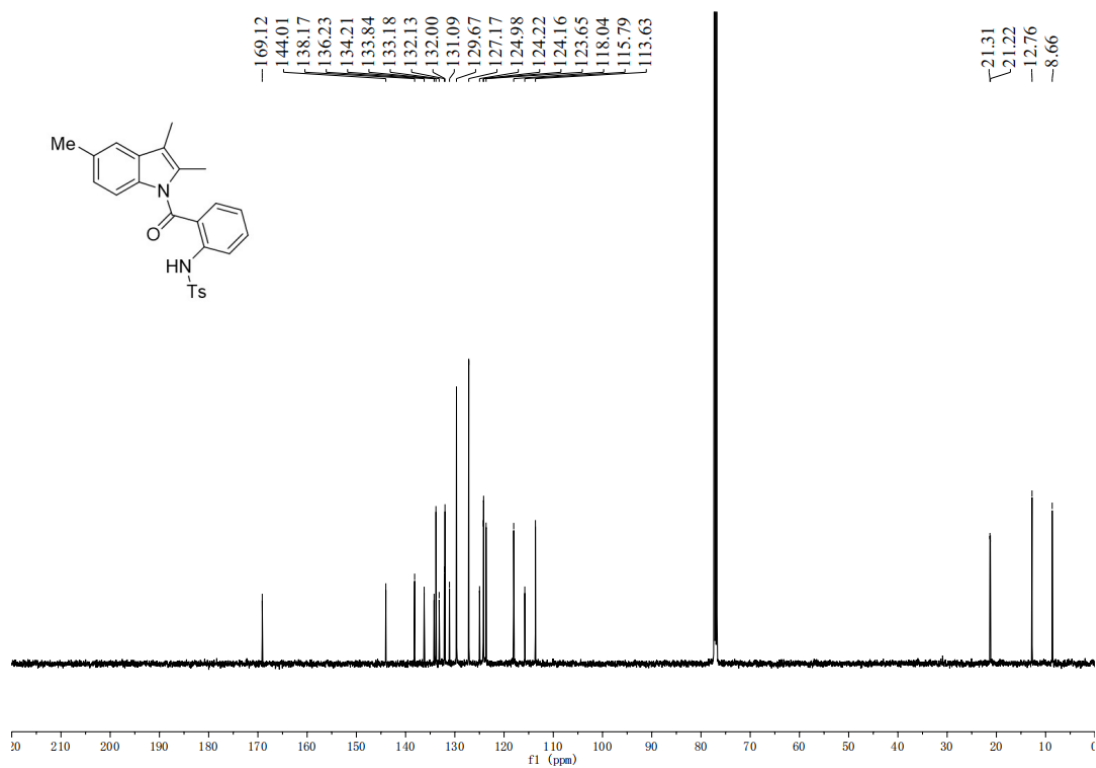
<sup>1</sup>H NMR spectrum of compound **1b**



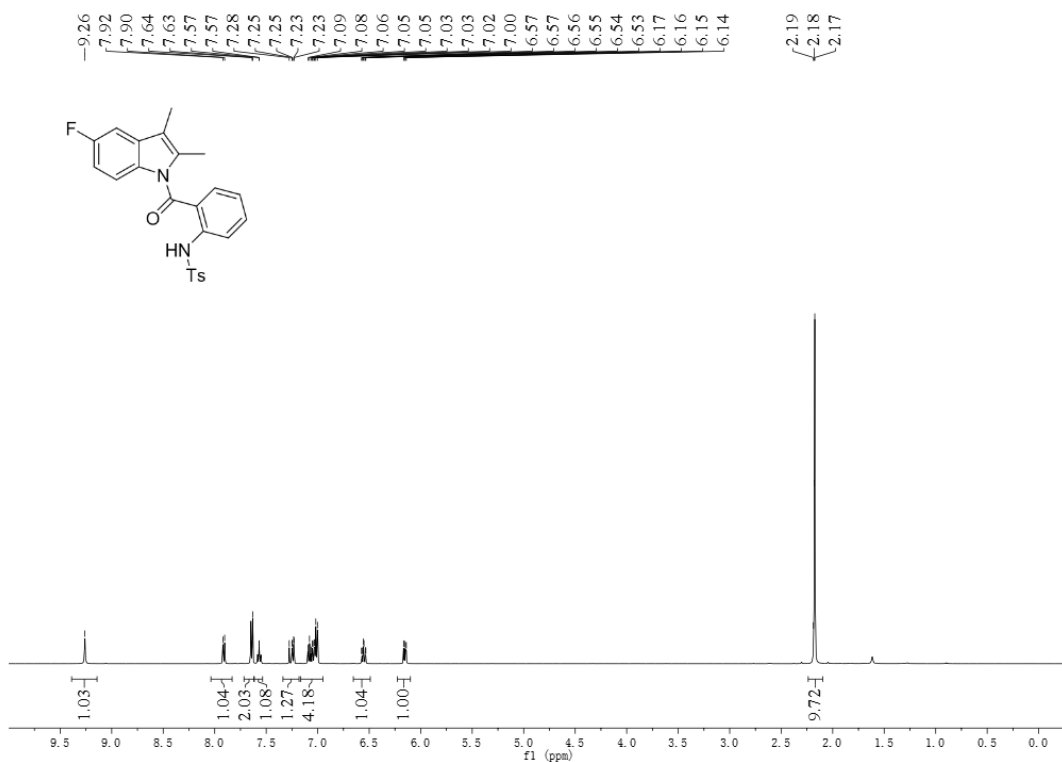
<sup>13</sup>C NMR spectrum of compound **1b**



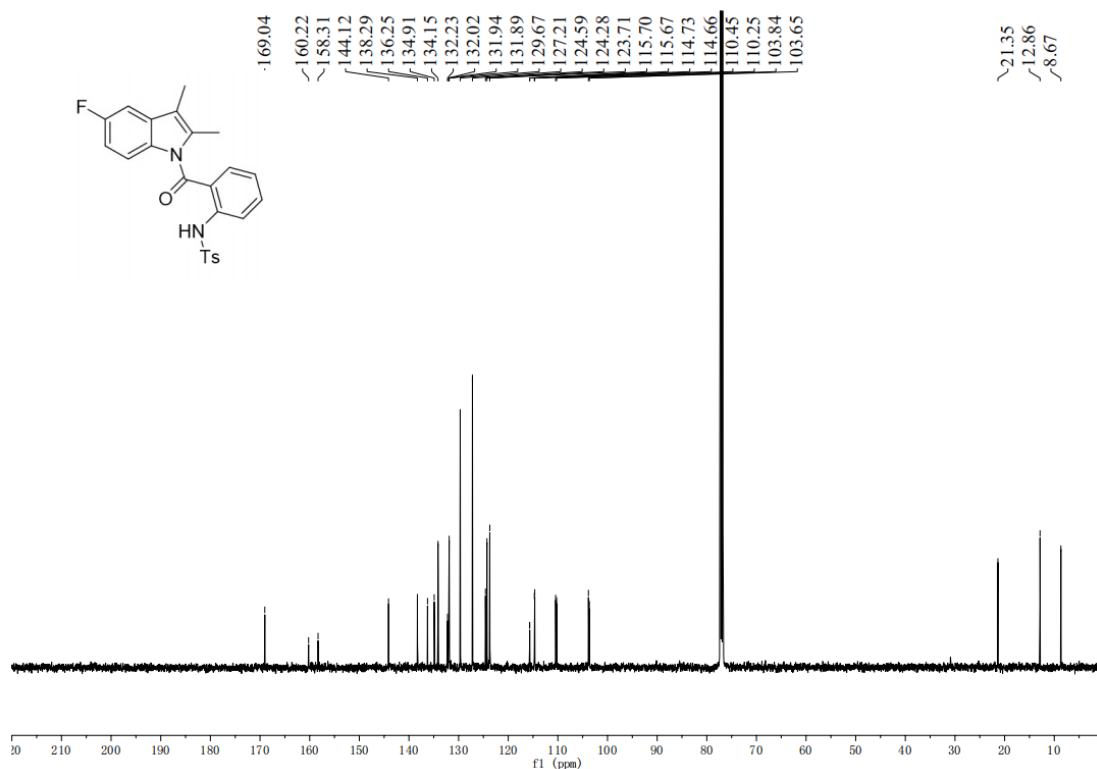
<sup>1</sup>H NMR spectrum of compound **1c**



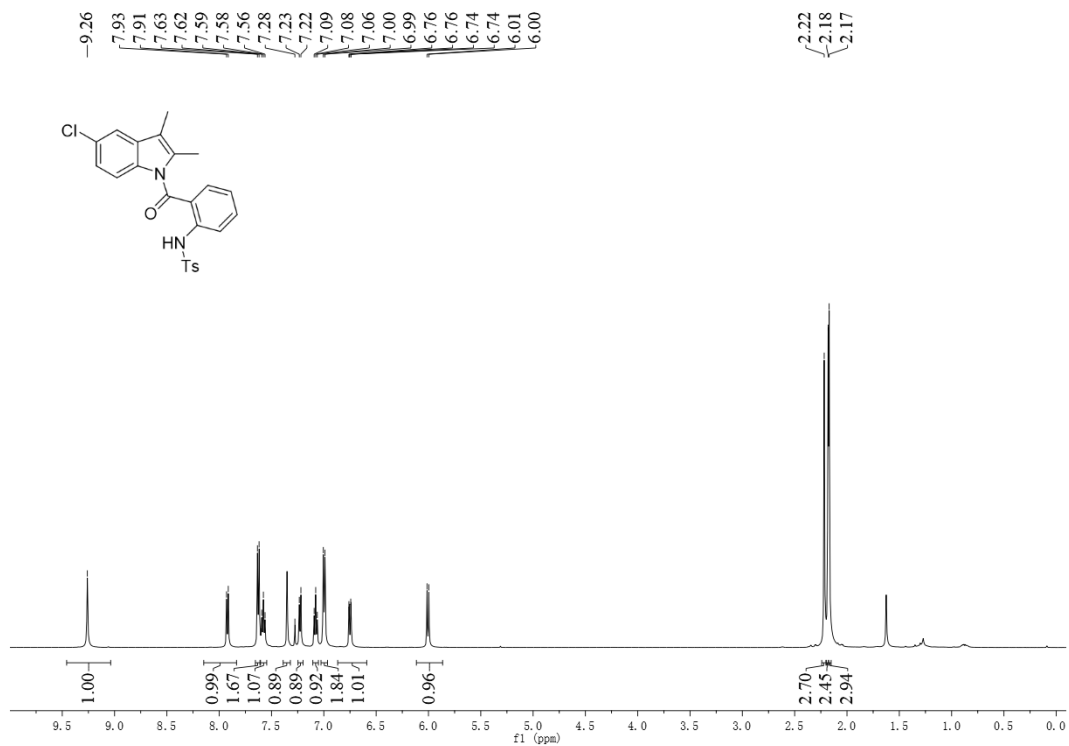
<sup>13</sup>C NMR spectrum of compound **1c**



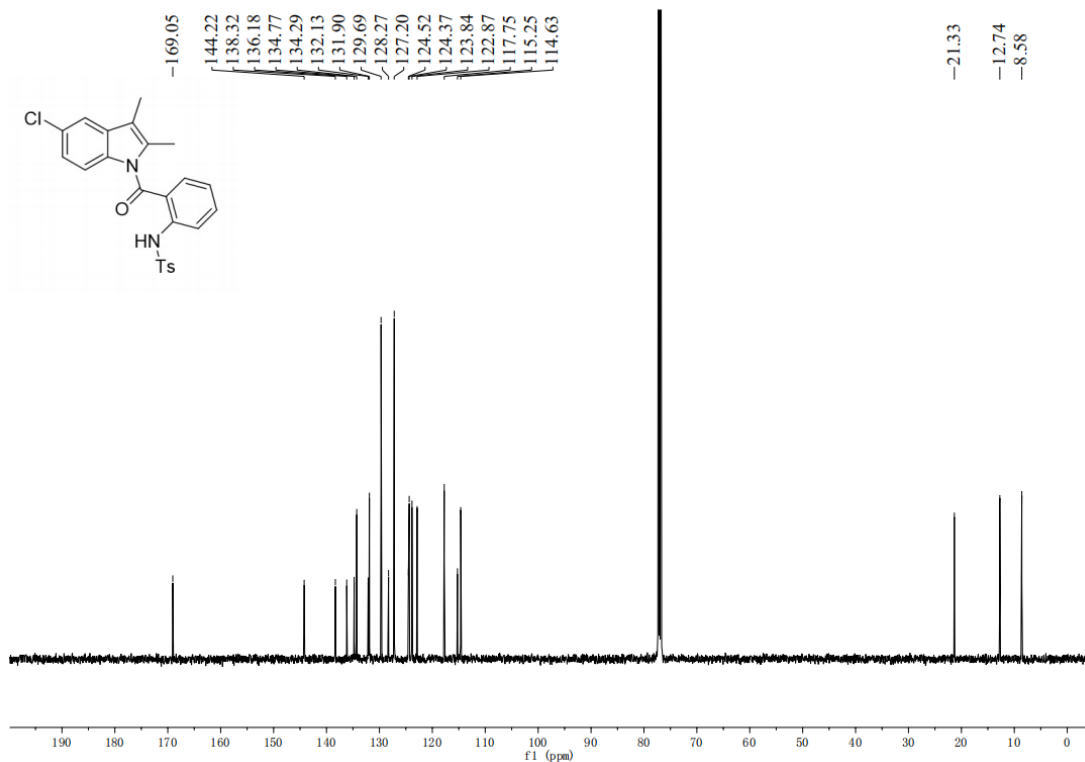
$^1\text{H}$  NMR spectrum of compound **1d**



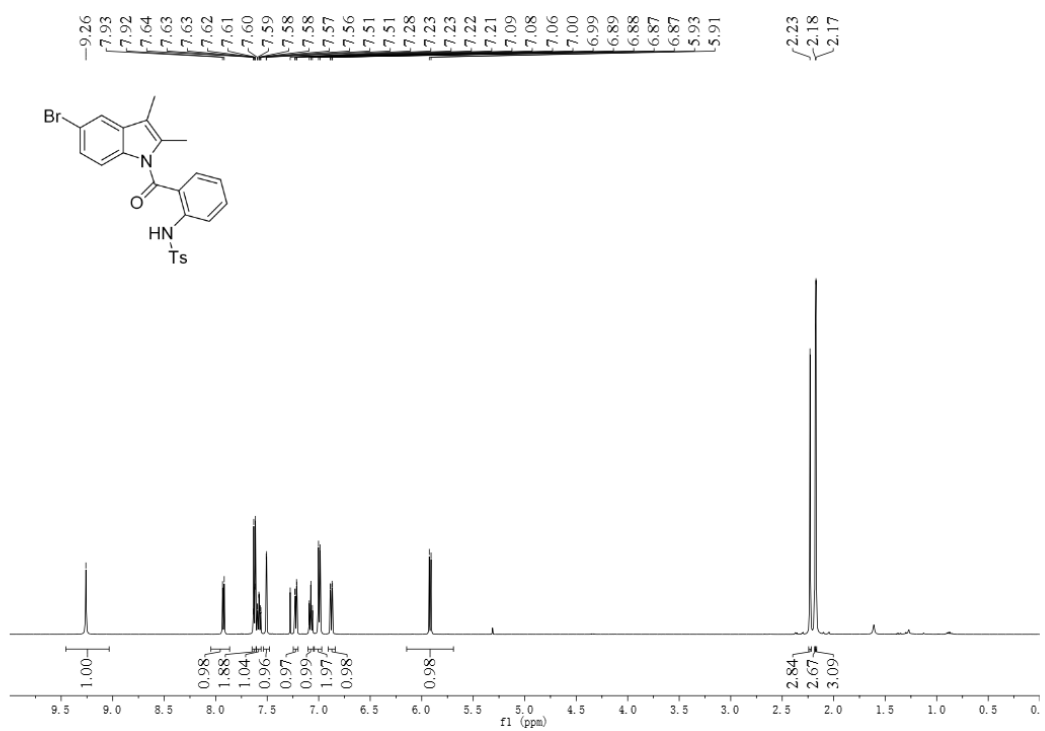
$^{13}\text{C}$  NMR spectrum of compound **1d**



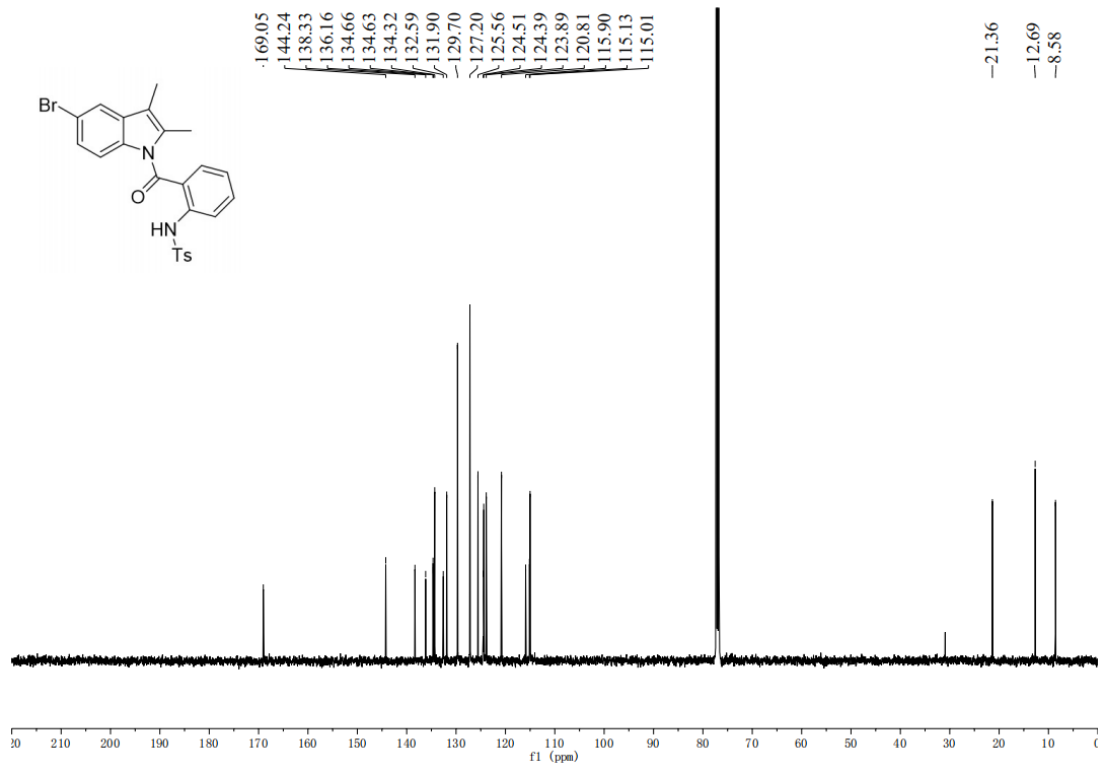
<sup>1</sup>H NMR spectrum of compound 1e



<sup>13</sup>C NMR spectrum of compound 1e

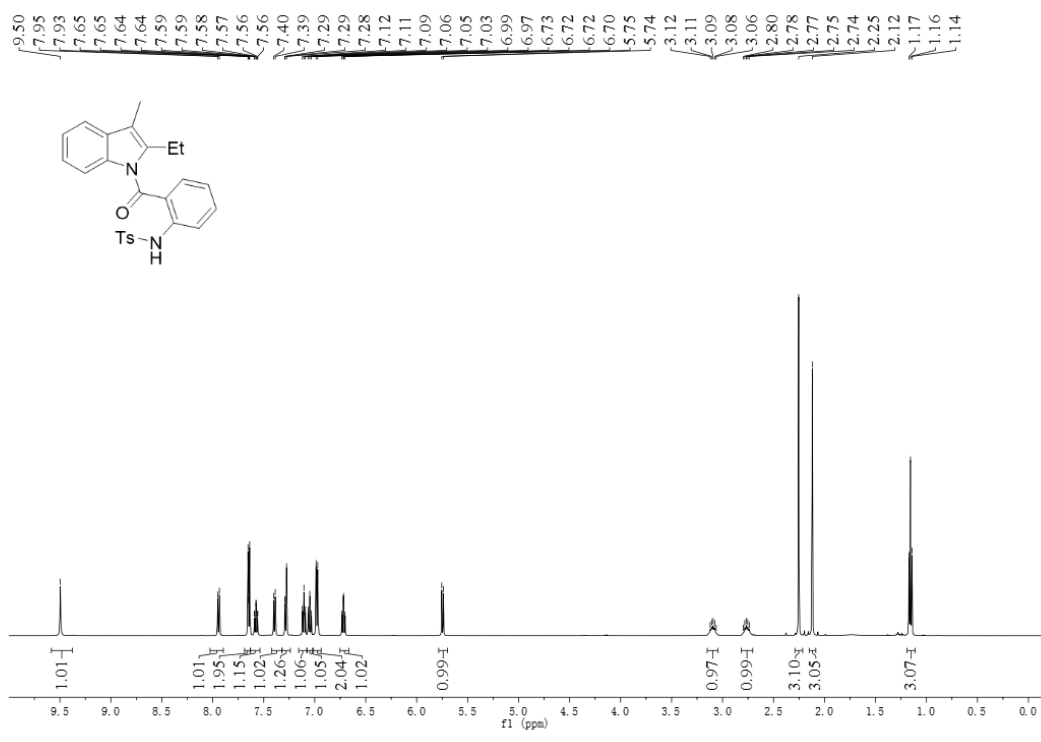


<sup>1</sup>H NMR spectrum of compound **1f**

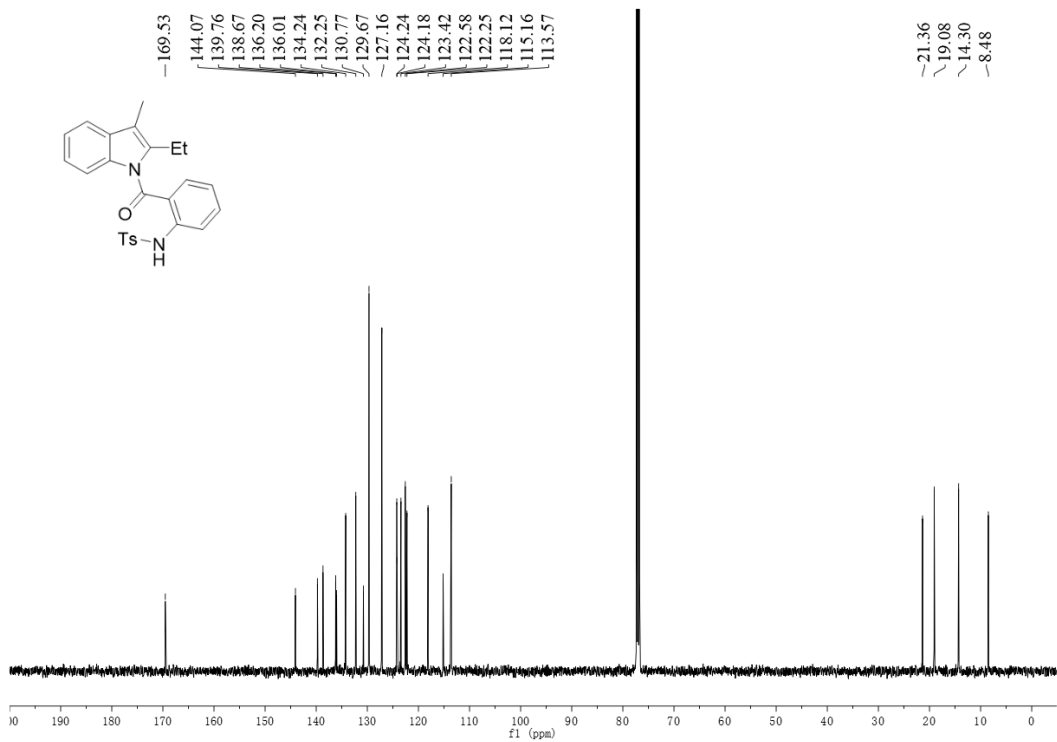


<sup>13</sup>C NMR spectrum of compound **1f**

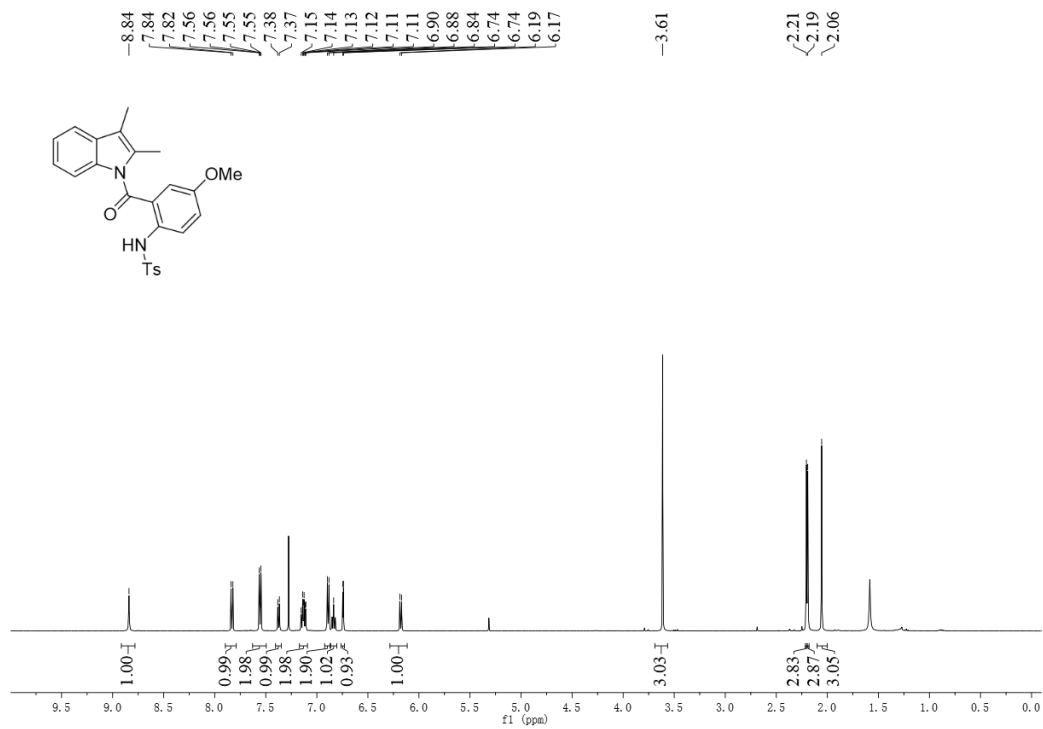




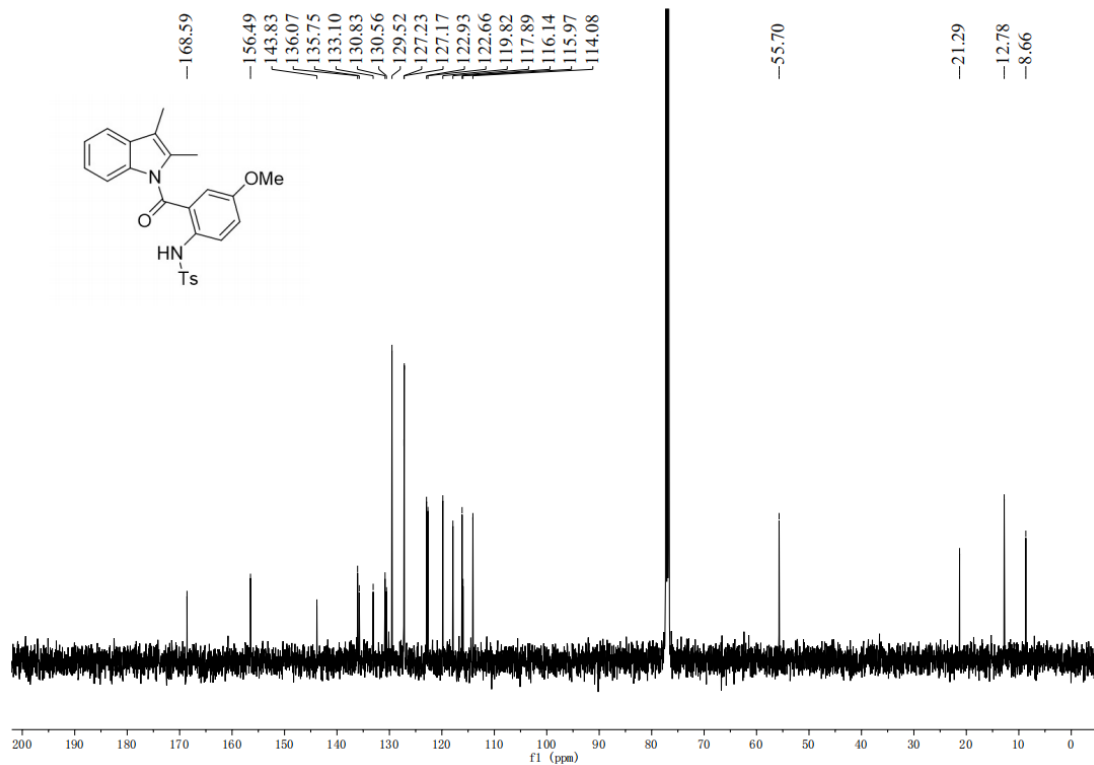
**<sup>1</sup>H NMR spectrum of compound **1g****



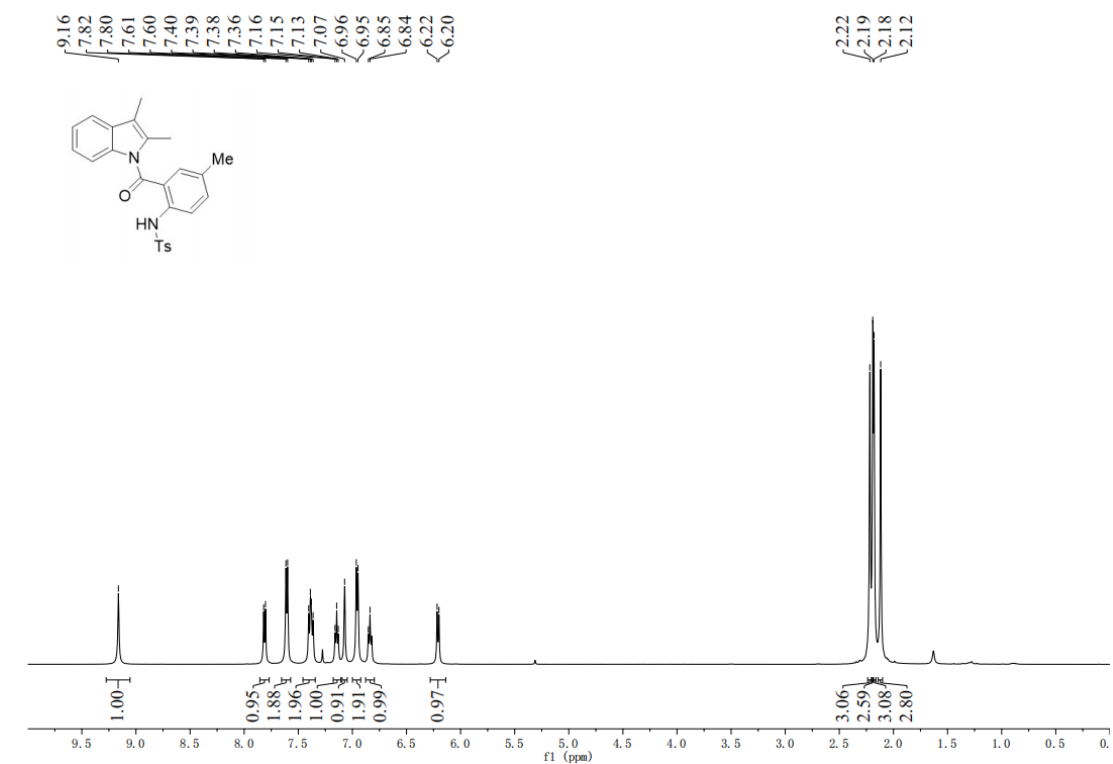
**<sup>13</sup>C NMR spectrum of compound **1g****



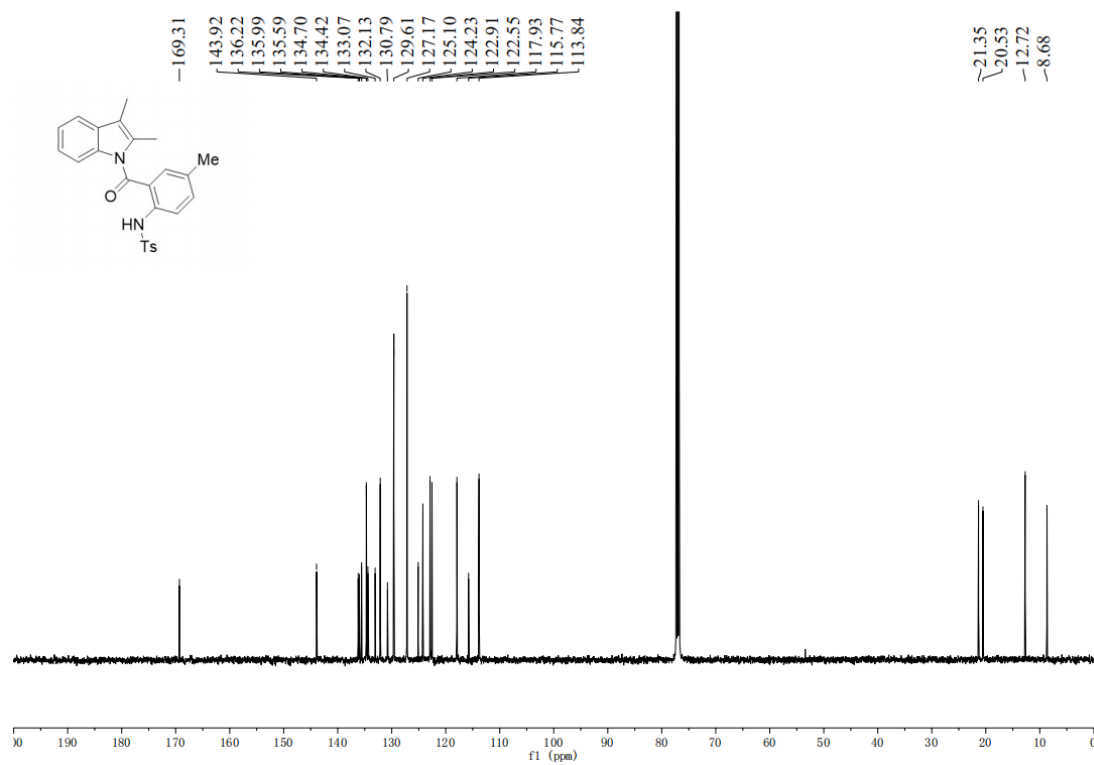
**<sup>1</sup>H NMR spectrum of compound **1h****



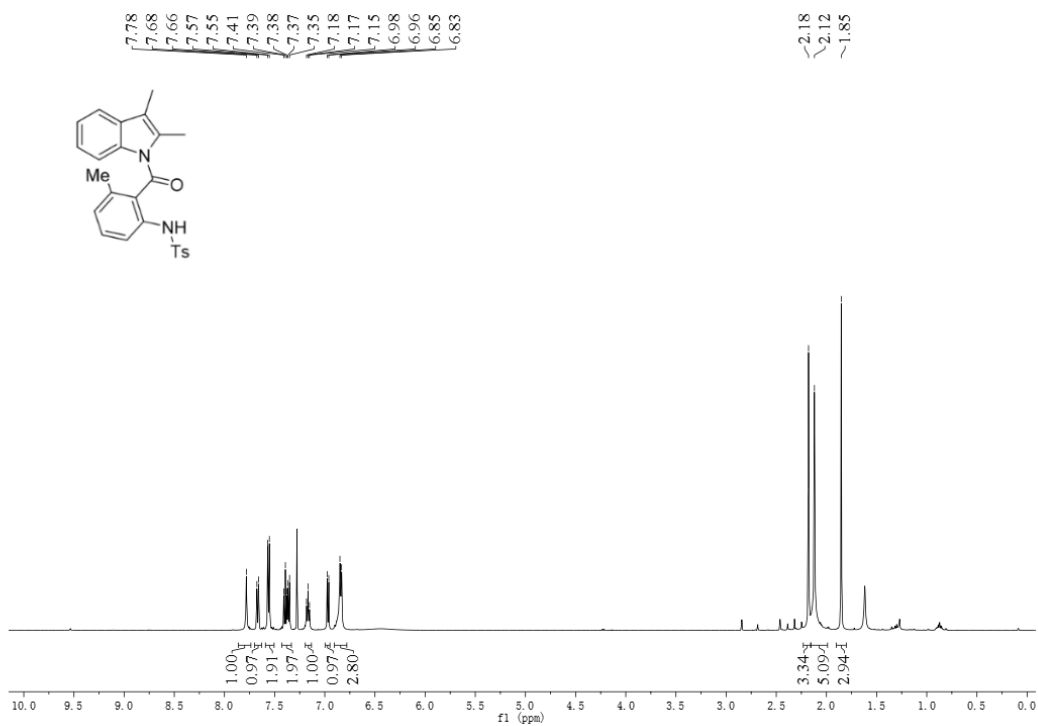
**<sup>13</sup>C NMR spectrum of compound **1h****



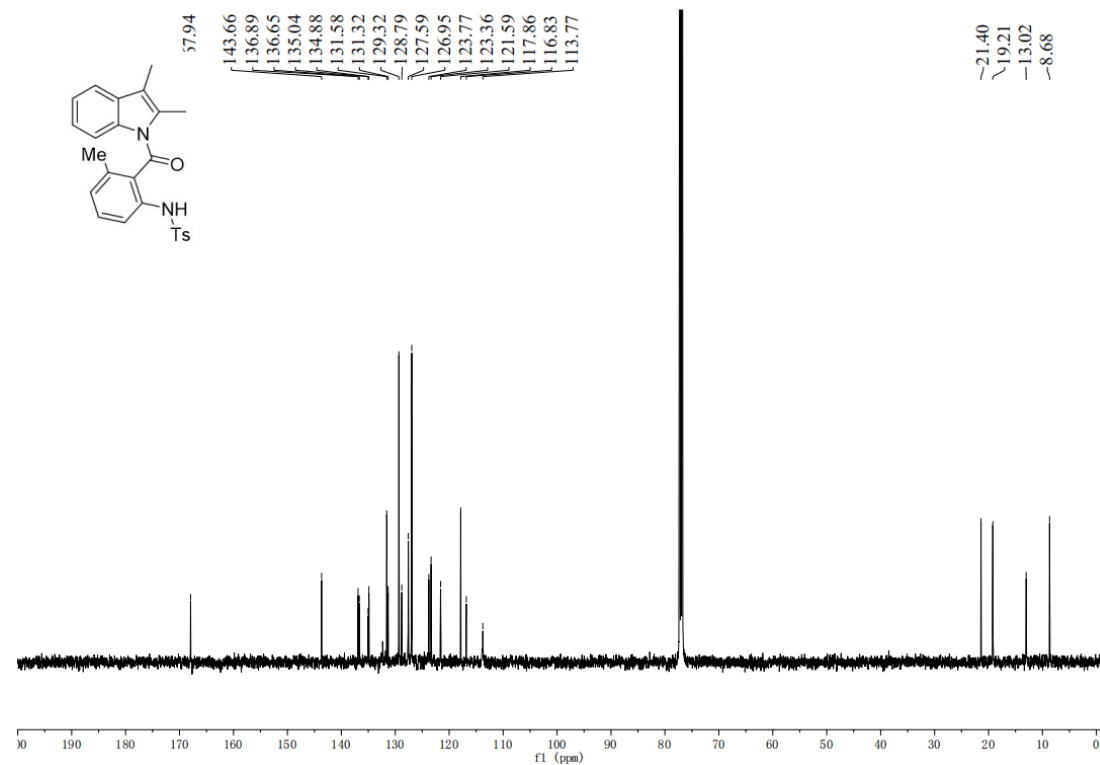
<sup>1</sup>H NMR spectrum of compound **1i**



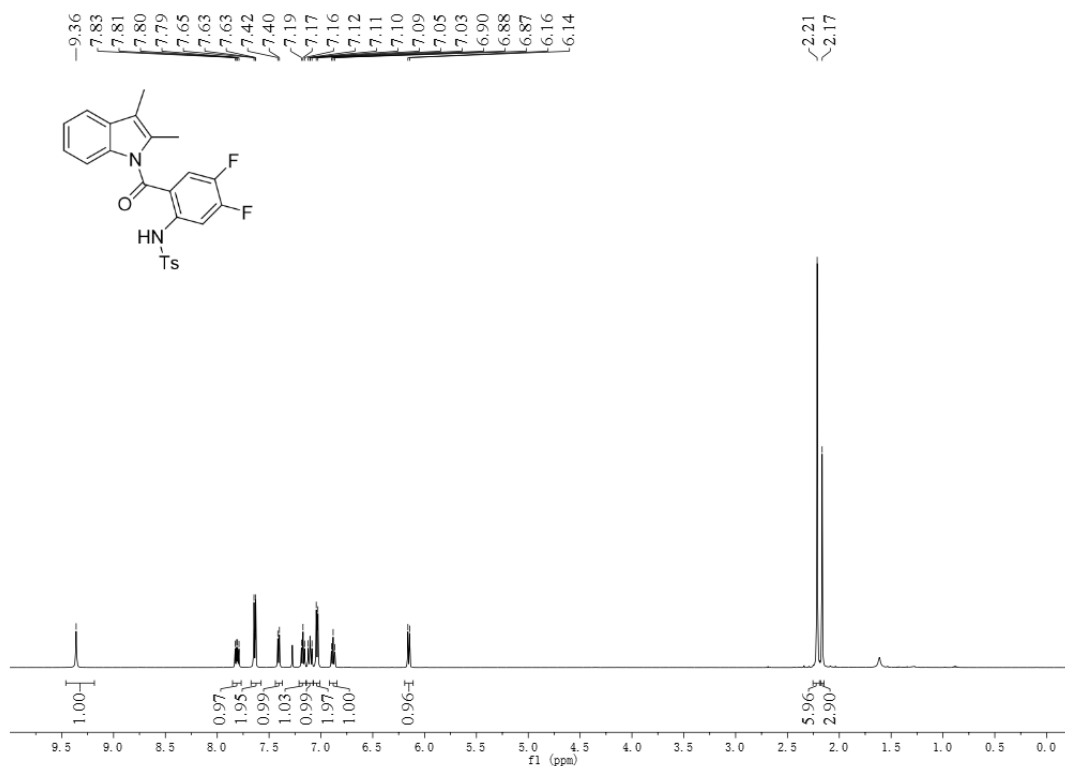
<sup>13</sup>C NMR spectrum of compound **1i**



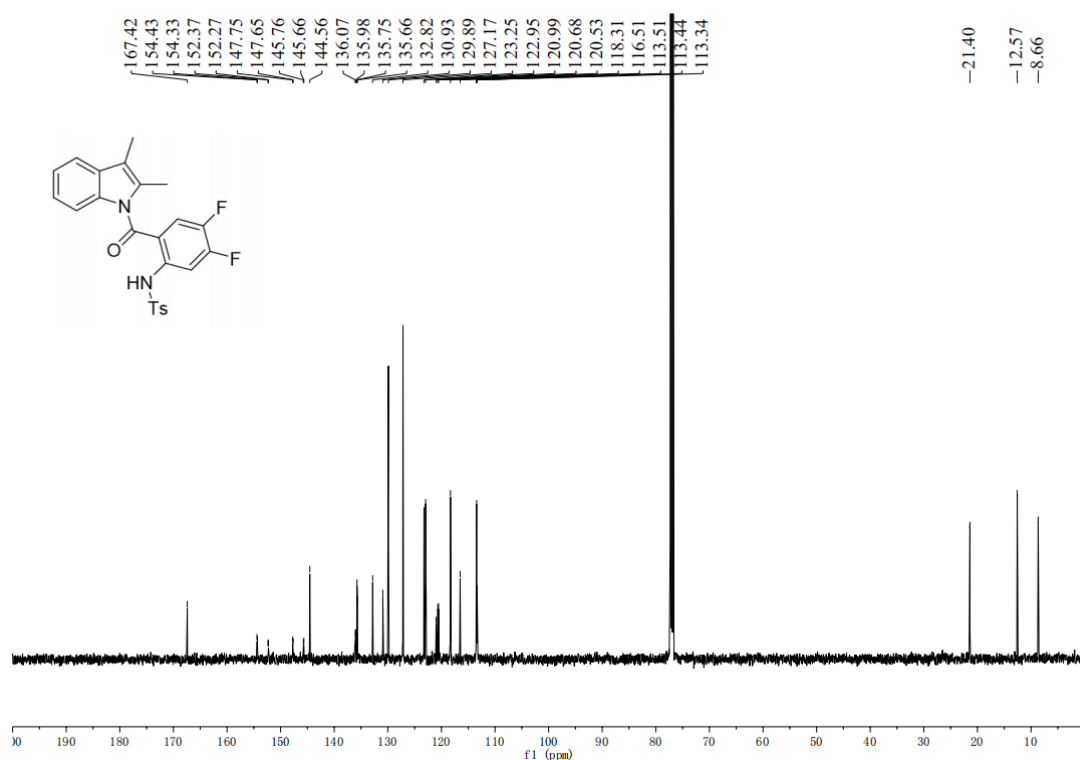
<sup>1</sup>H NMR spectrum of compound **1j**



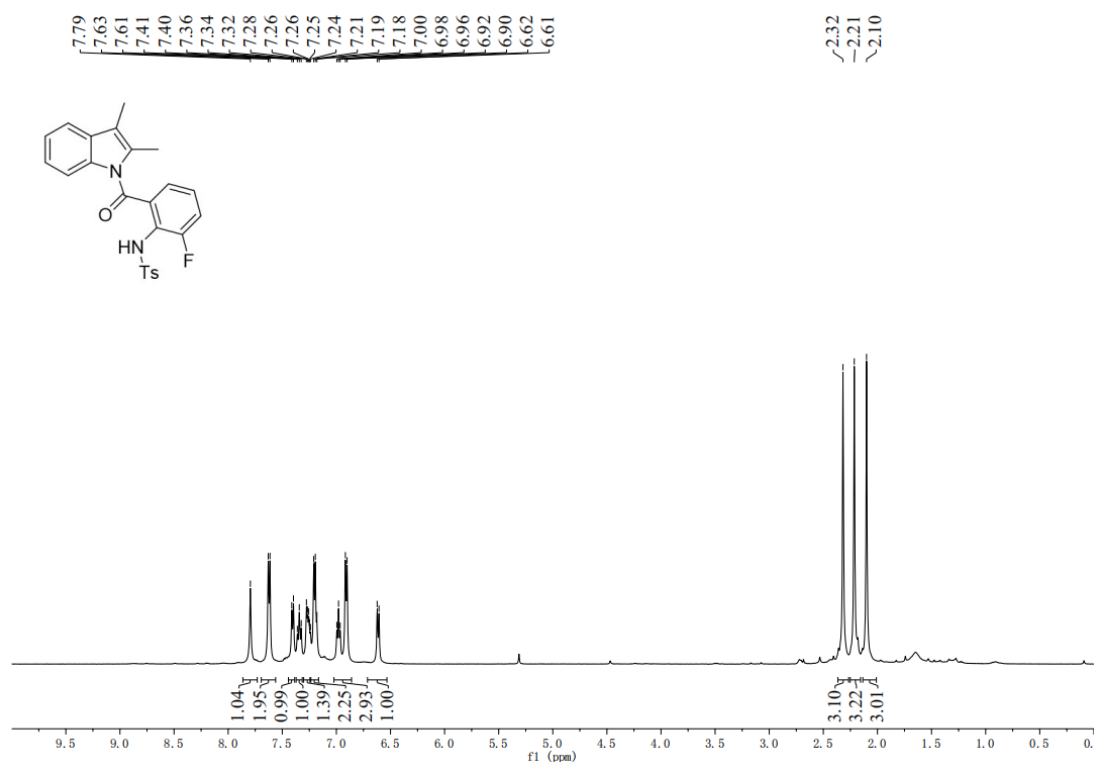
<sup>13</sup>C NMR spectrum of compound **1j**



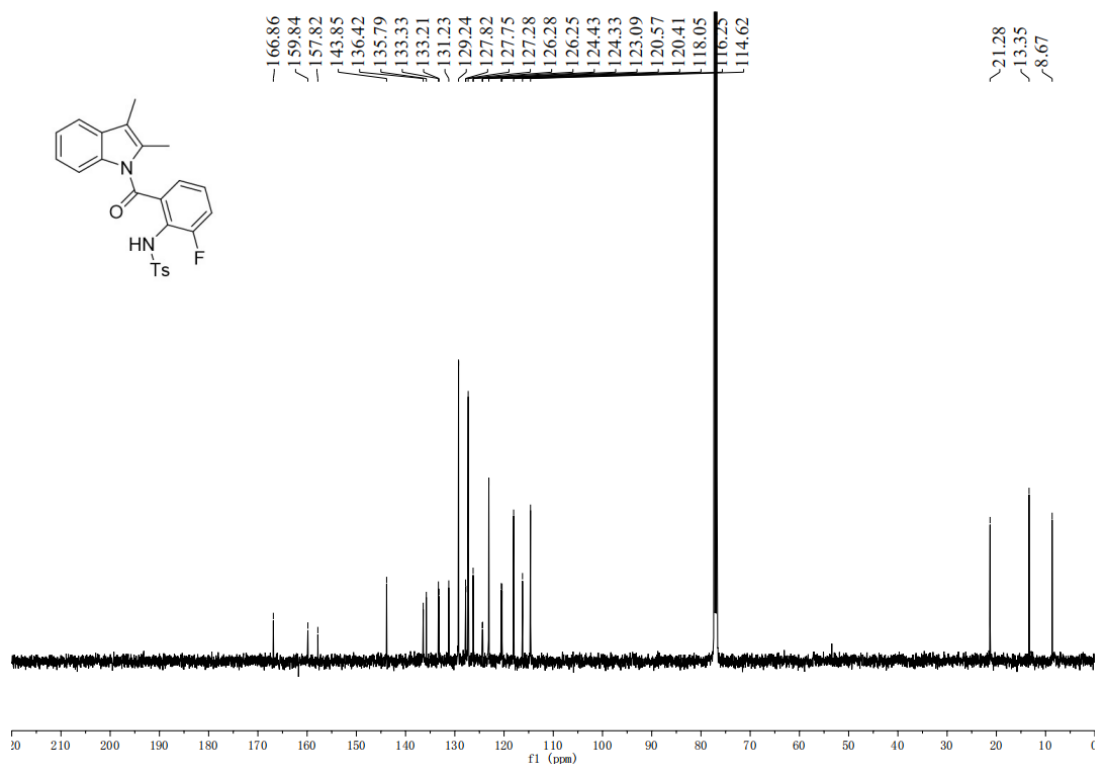
<sup>1</sup>H NMR spectrum of compound **1k**



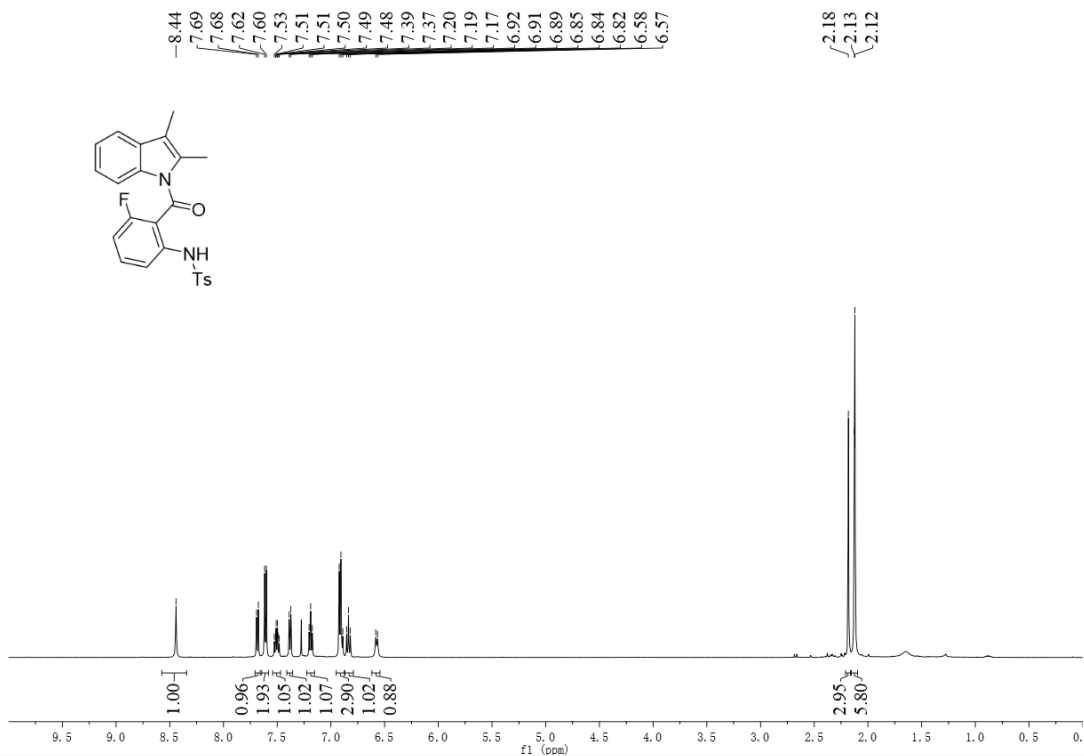
<sup>13</sup>C NMR spectrum of compound **1k**



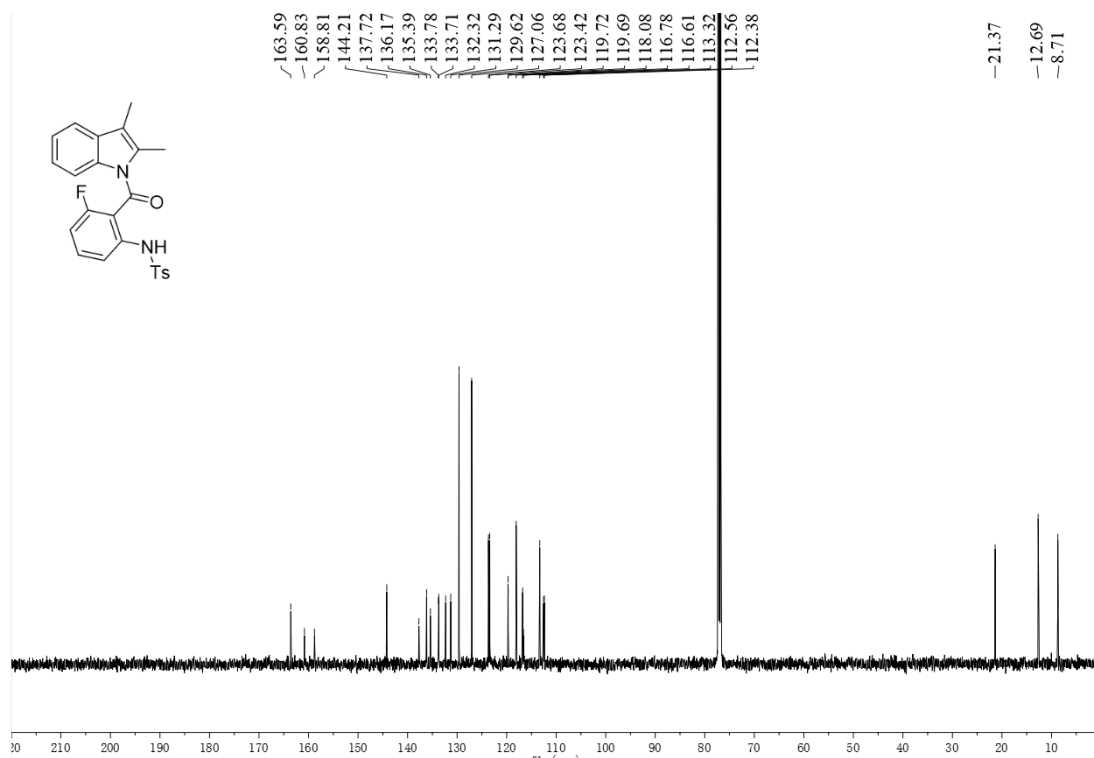
<sup>1</sup>H NMR spectrum of compound **11**



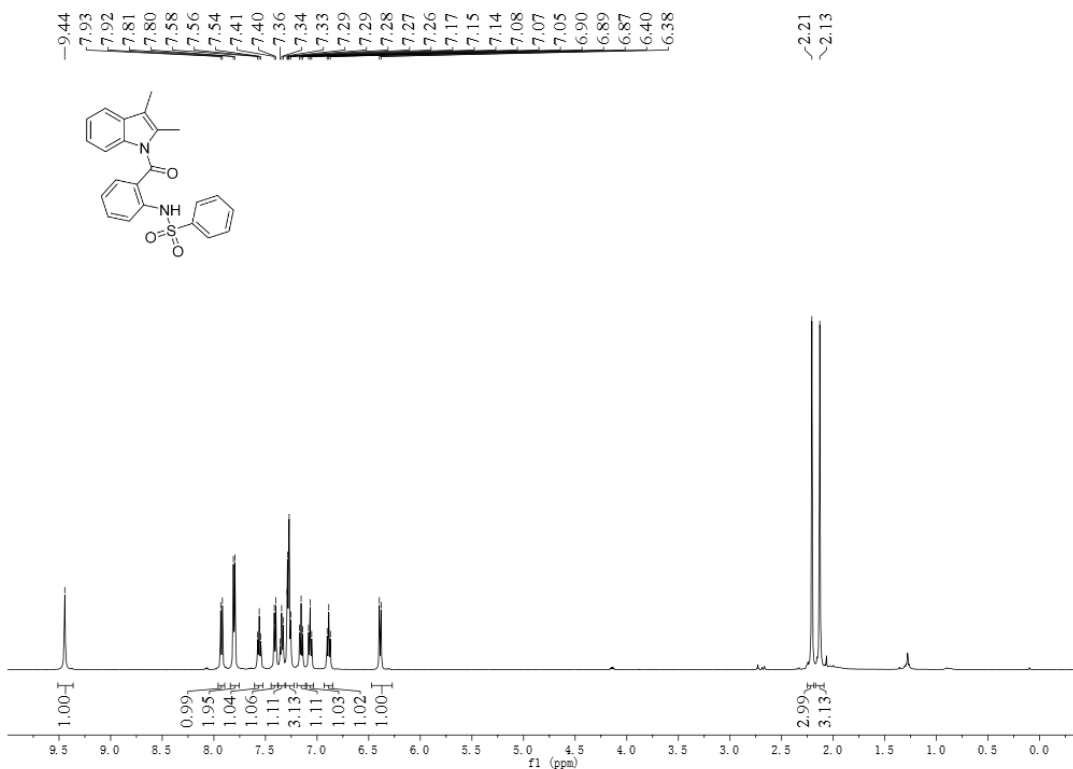
<sup>13</sup>C NMR spectrum of compound **11**



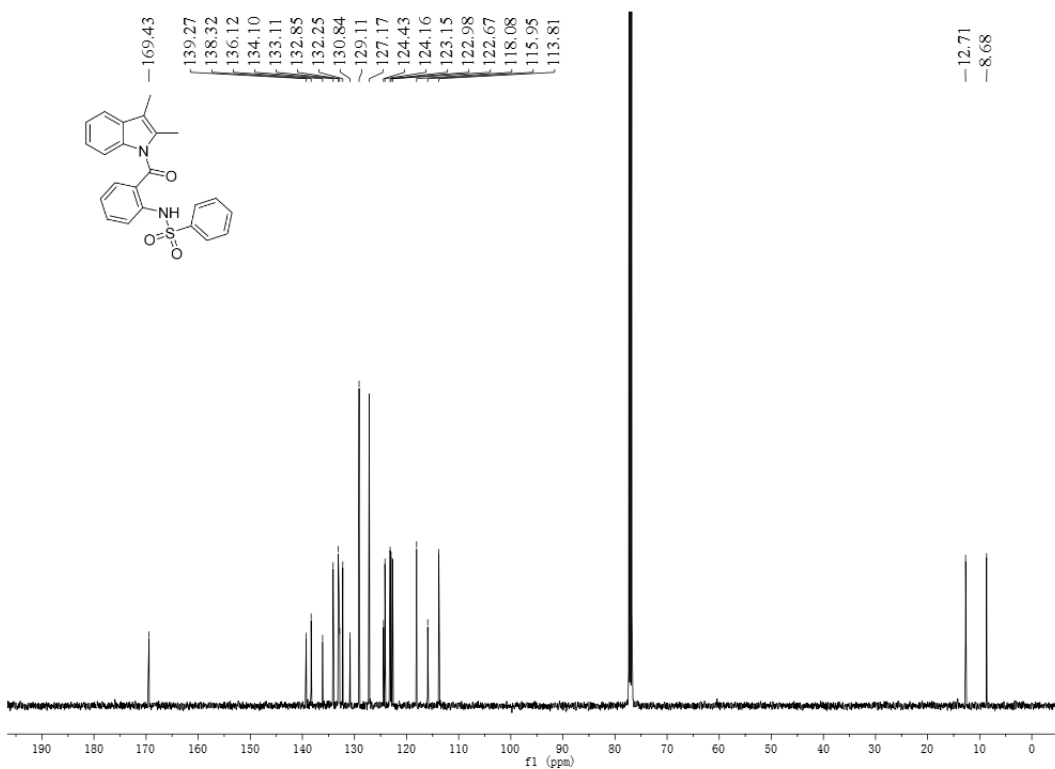
<sup>1</sup>H NMR spectrum of compound **1m**



<sup>13</sup>C NMR spectrum of compound **1m**

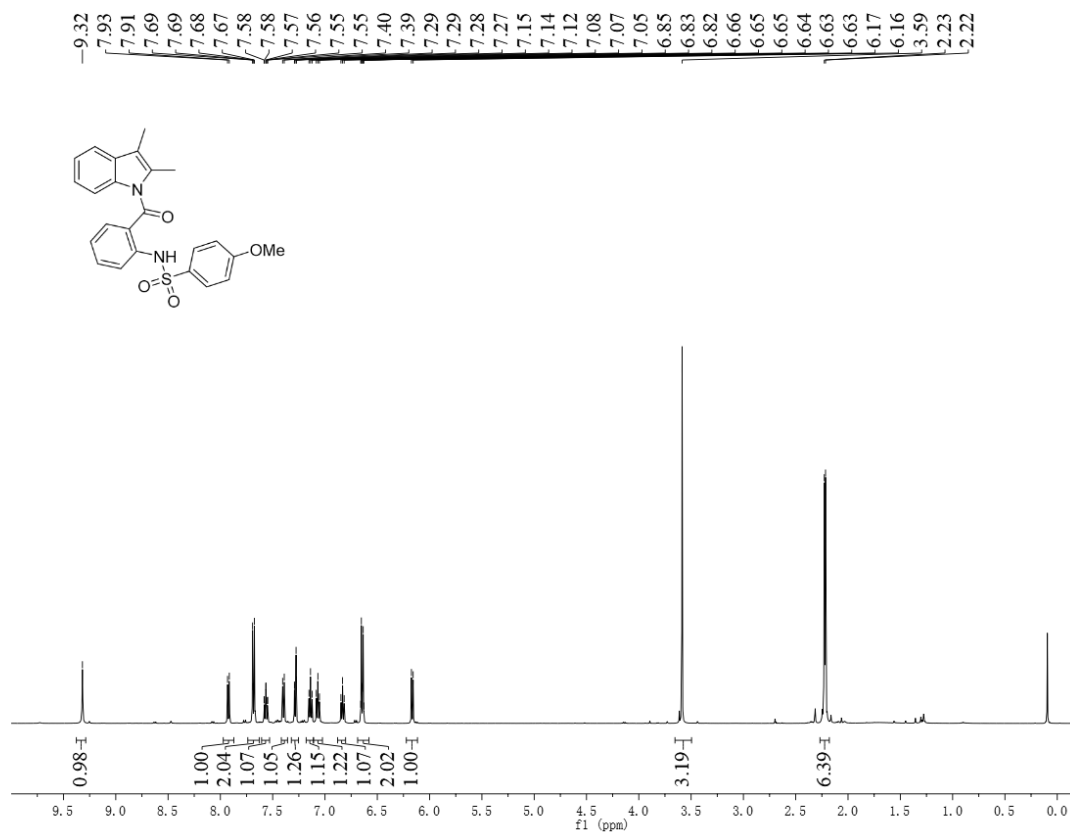


<sup>1</sup>H NMR spectrum of compound **1n**

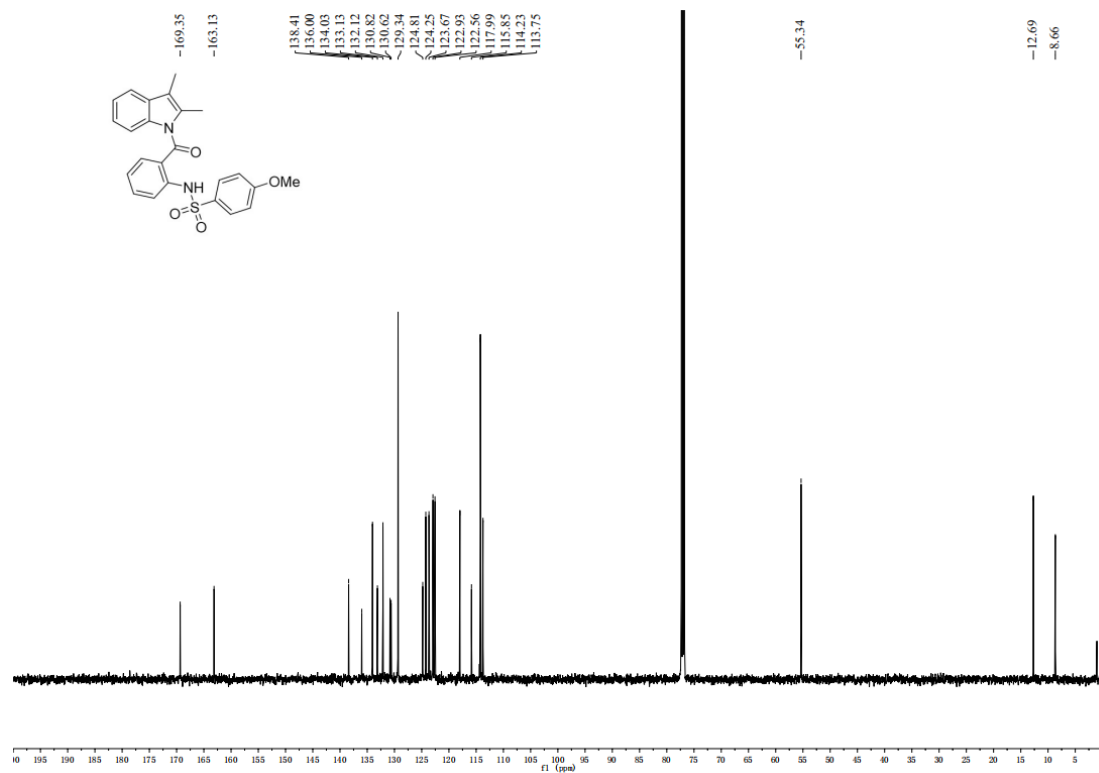


<sup>13</sup>C NMR spectrum of compound **1n**

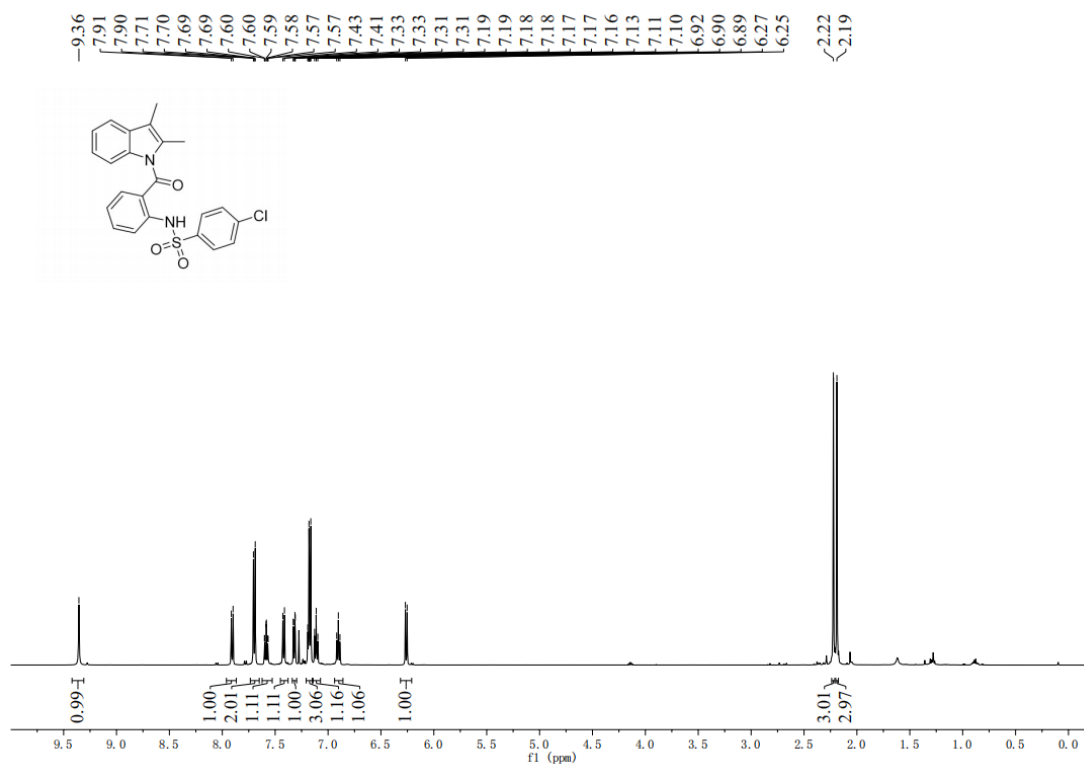




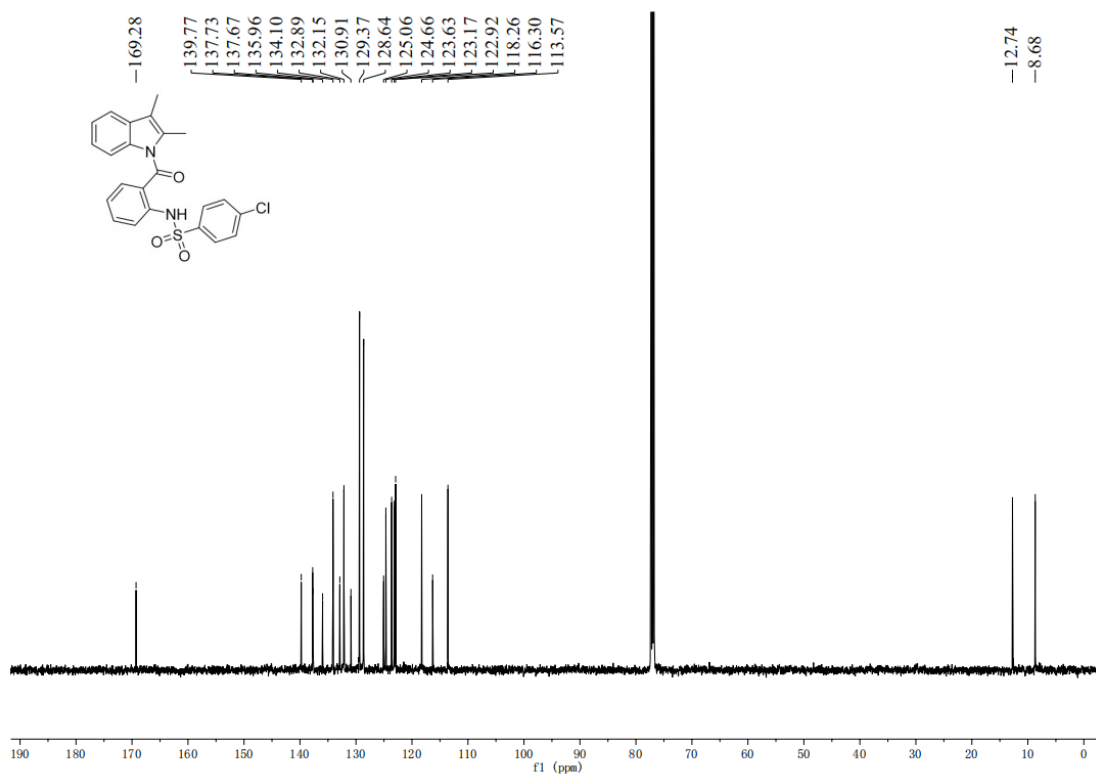
<sup>1</sup>H NMR spectrum of compound **1o**



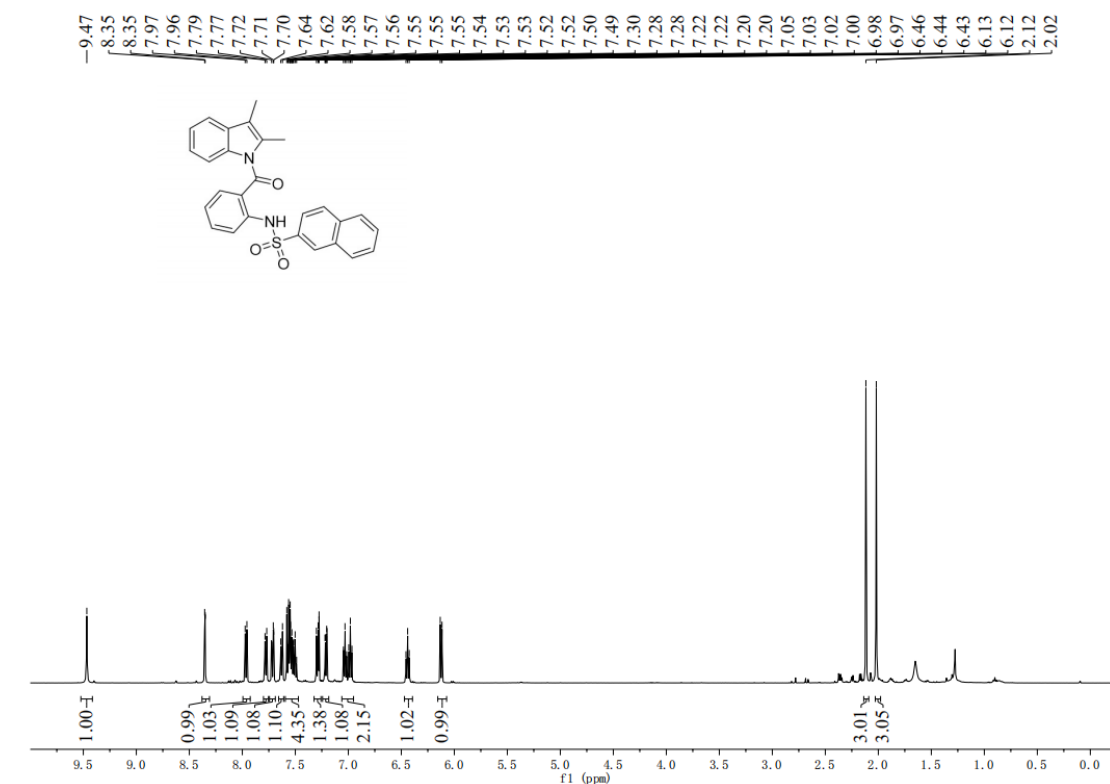
<sup>13</sup>C NMR spectrum of compound **1o**



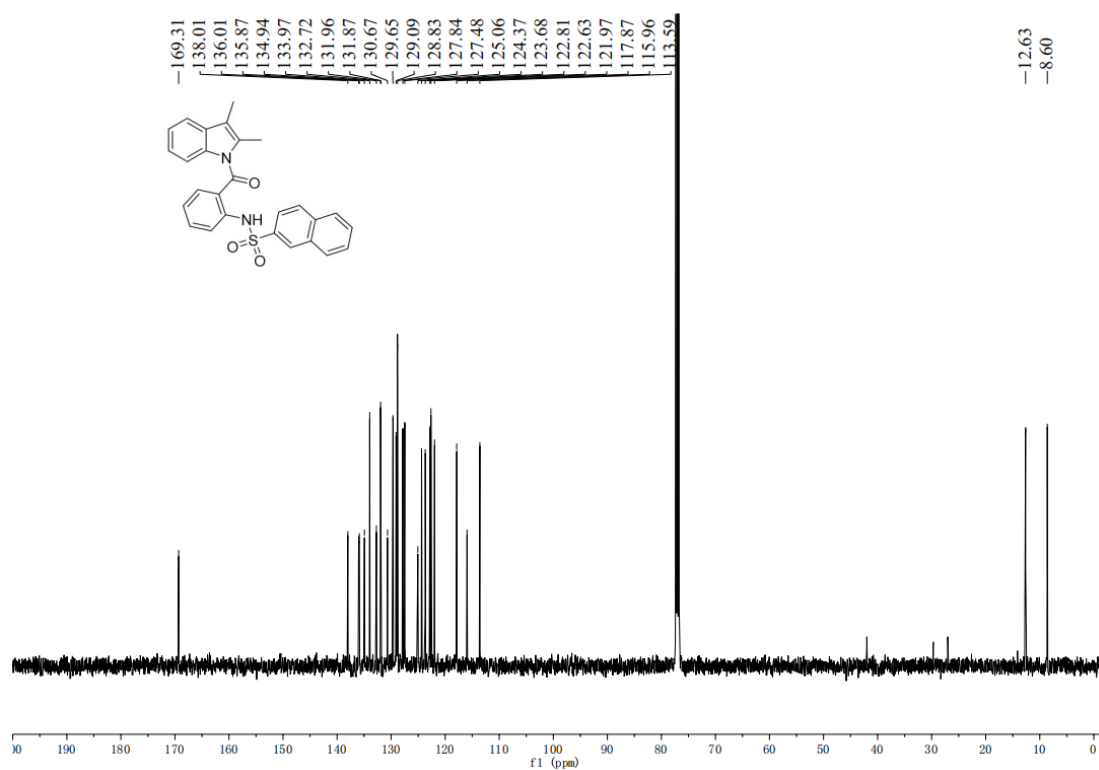
<sup>1</sup>H NMR spectrum of compound **1p**



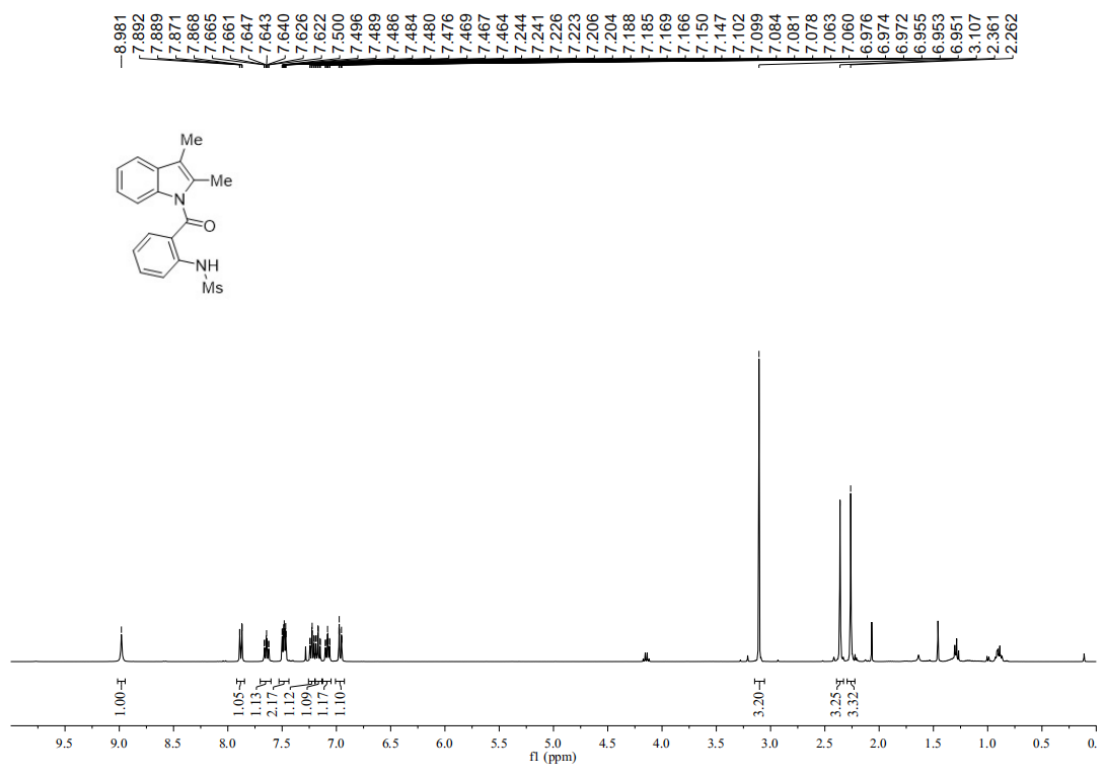
<sup>13</sup>C NMR spectrum of compound **1p**



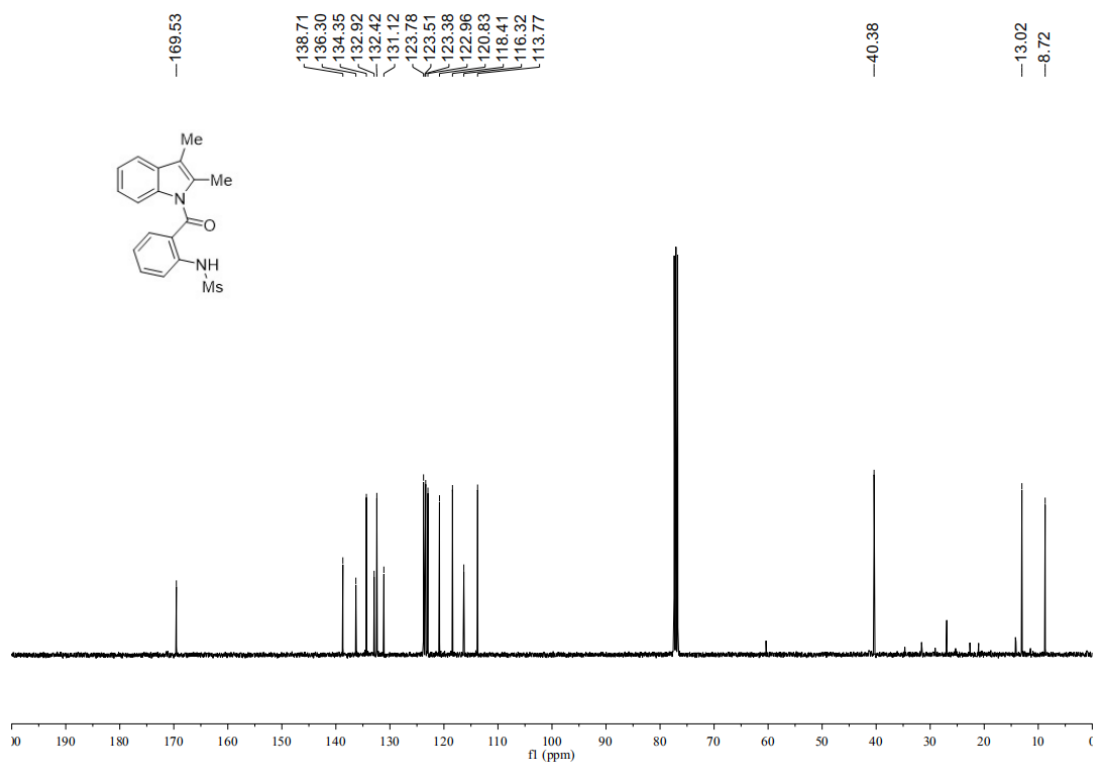
<sup>1</sup>H NMR spectrum of compound **1q**



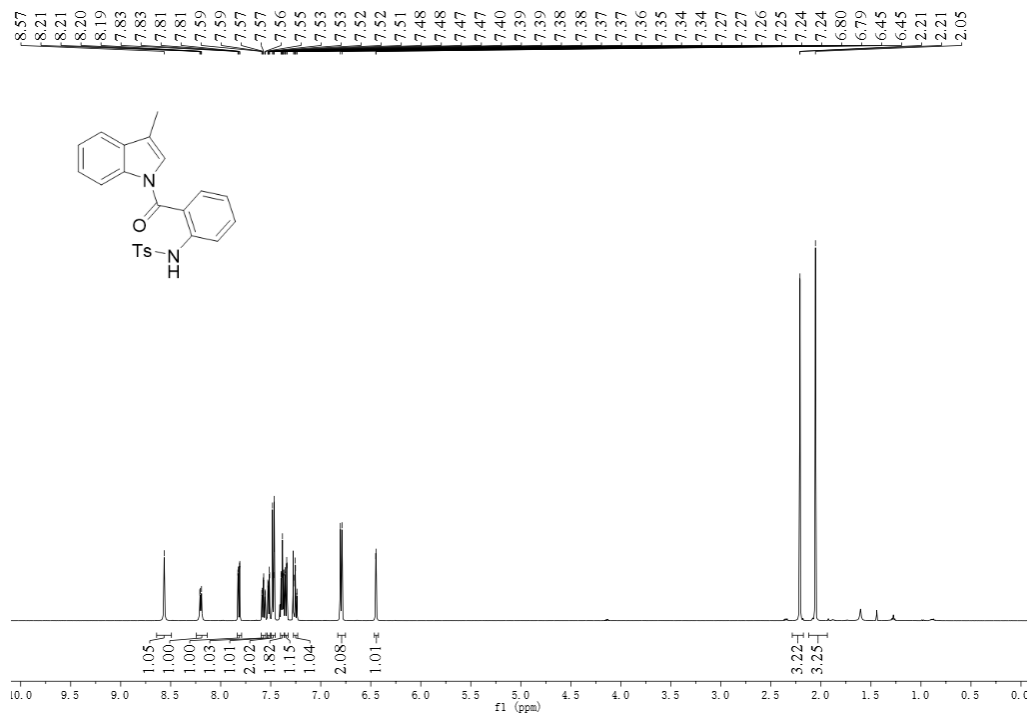
<sup>13</sup>C NMR spectrum of compound **1q**



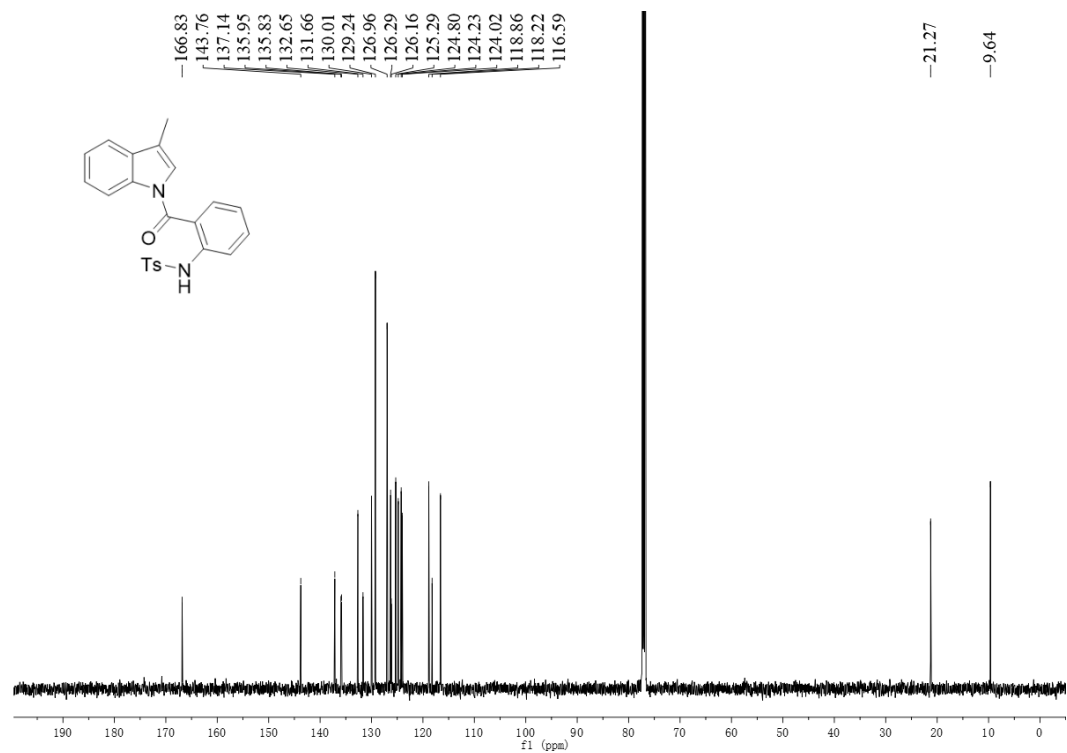
<sup>1</sup>H NMR spectrum of compound **1r**



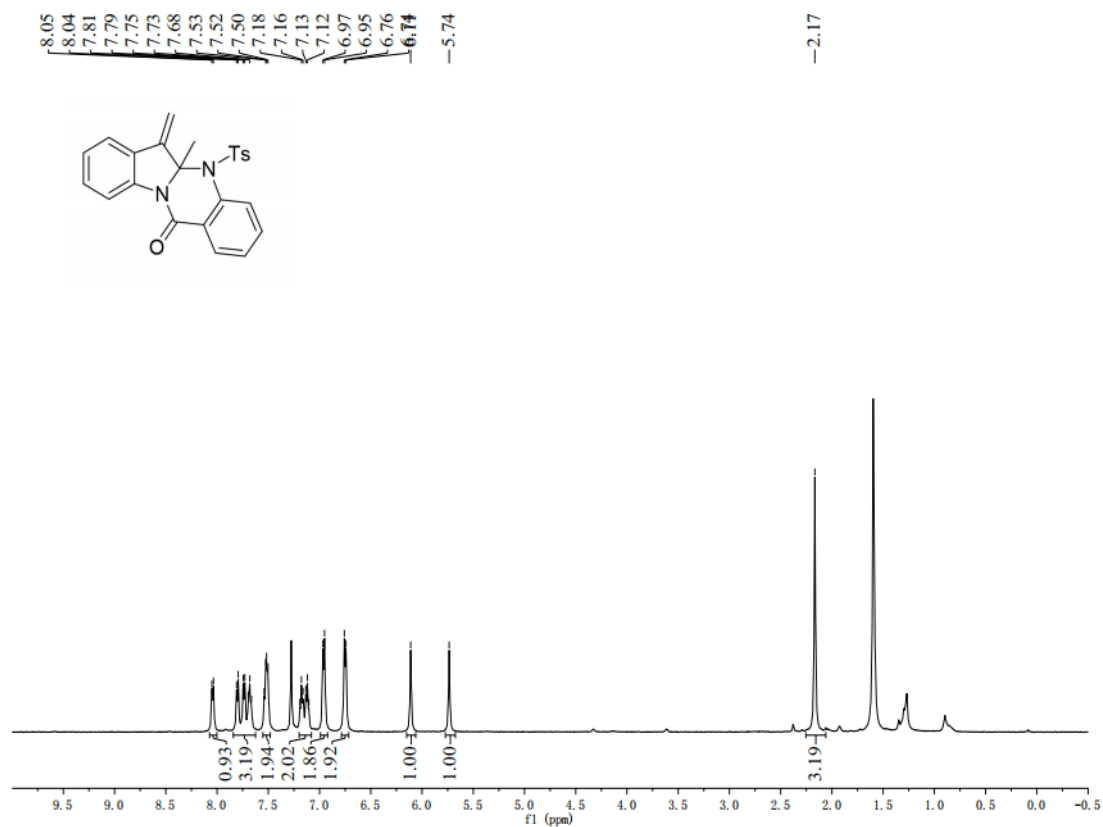
<sup>13</sup>C NMR spectrum of compound **1r**



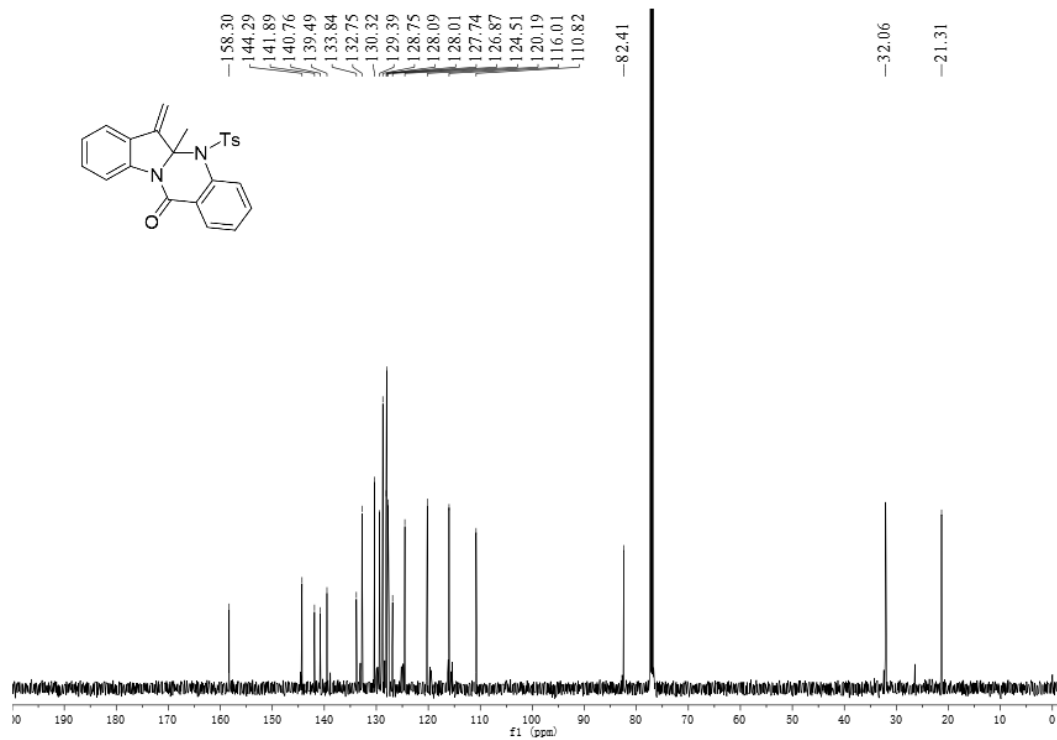
$^1\text{H}$  NMR spectrum of compound **1v**



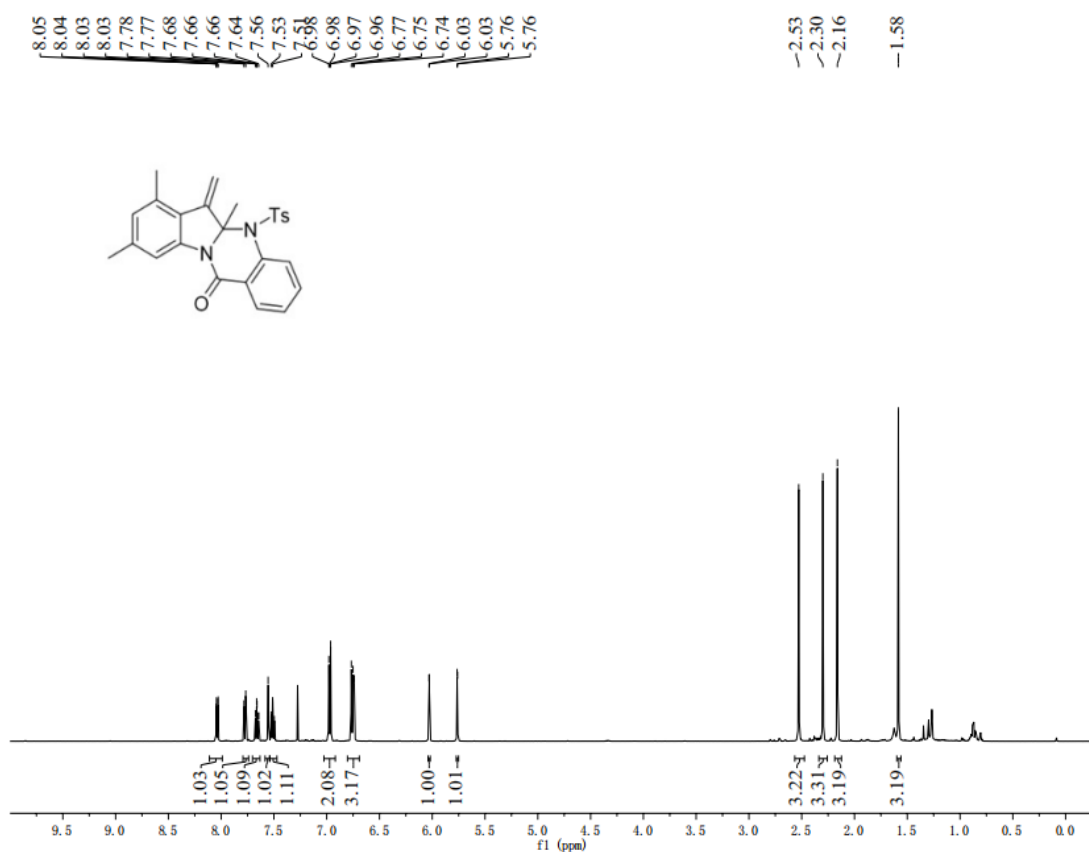
$^{13}\text{C}$  NMR spectrum of compound **1v**



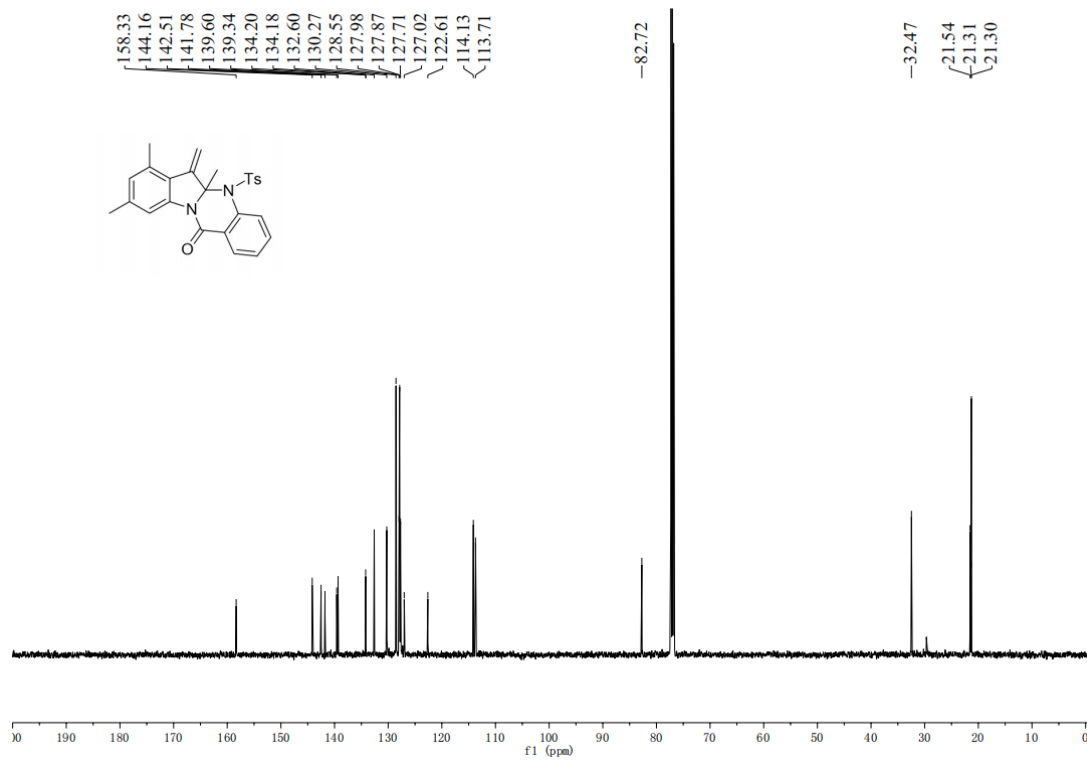
<sup>1</sup>H NMR spectrum of compound **2a**



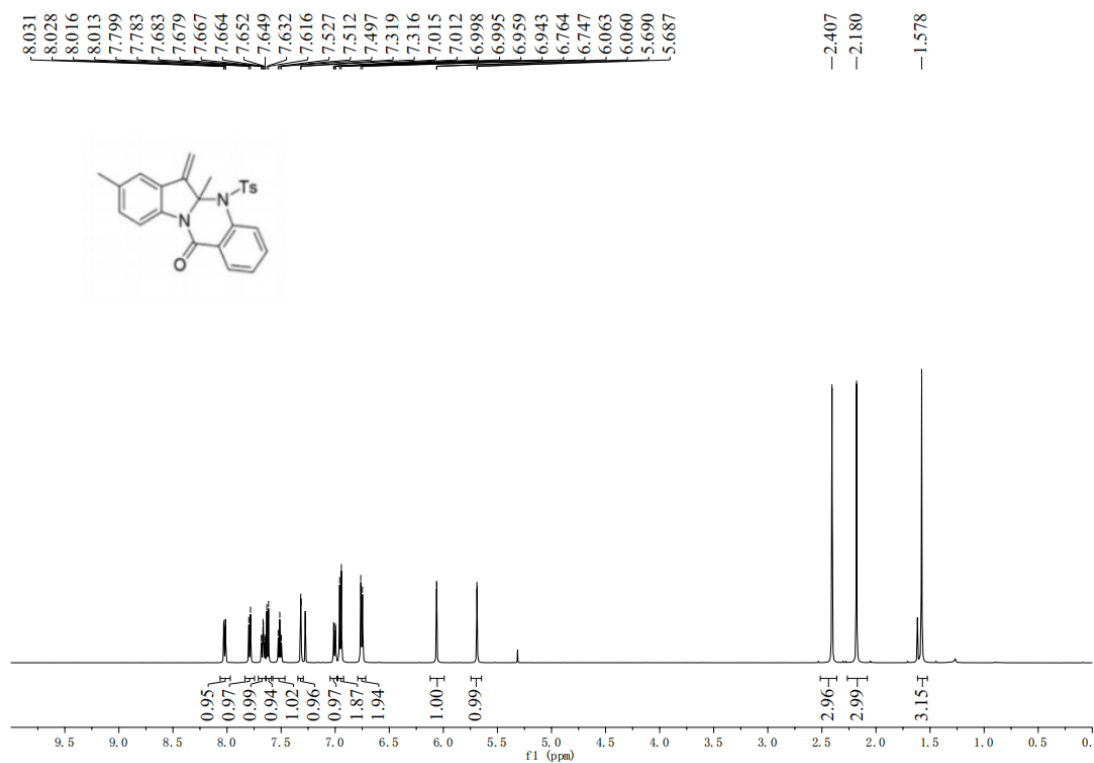
<sup>13</sup>C NMR spectrum of compound **2a**



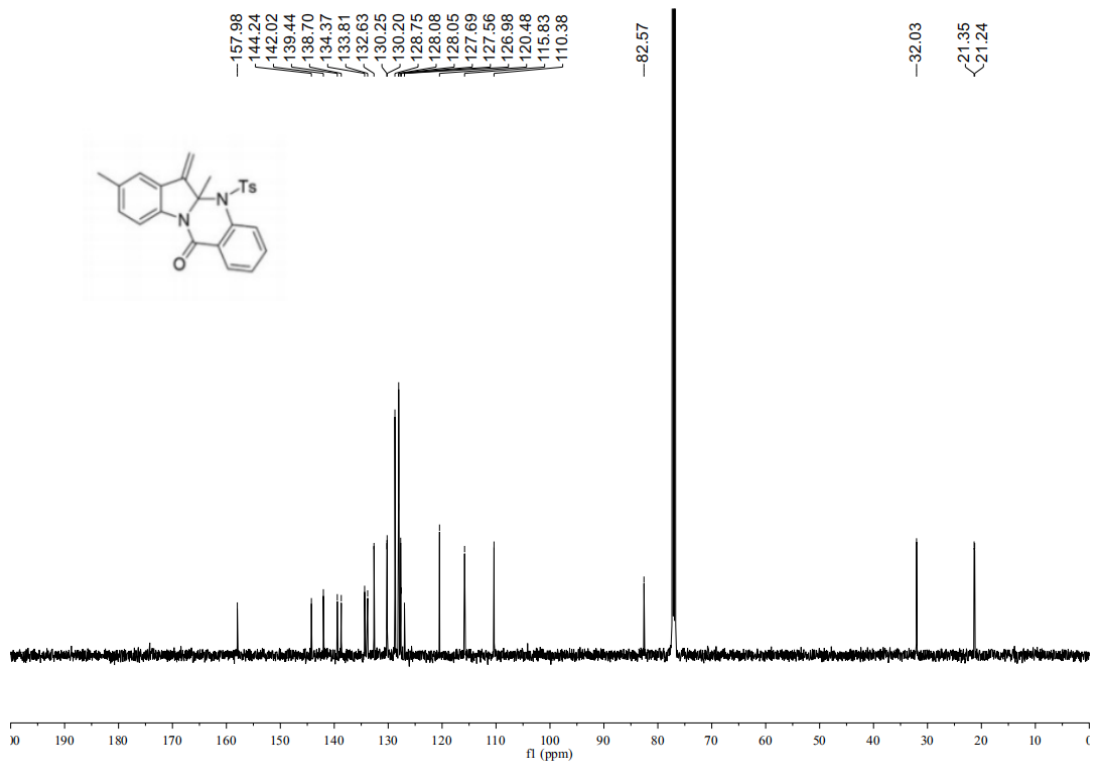
<sup>1</sup>H NMR spectrum of compound **2b**



<sup>13</sup>C NMR spectrum of compound **2b**

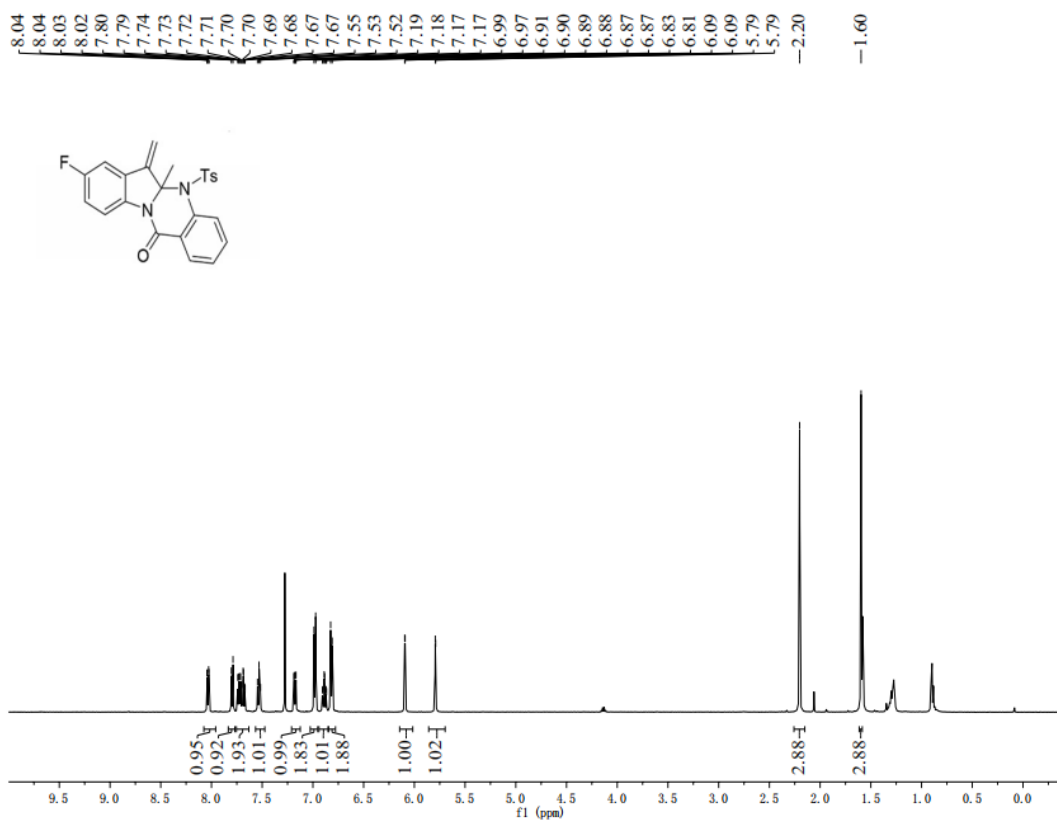


<sup>1</sup>H NMR spectrum of compound **2c**

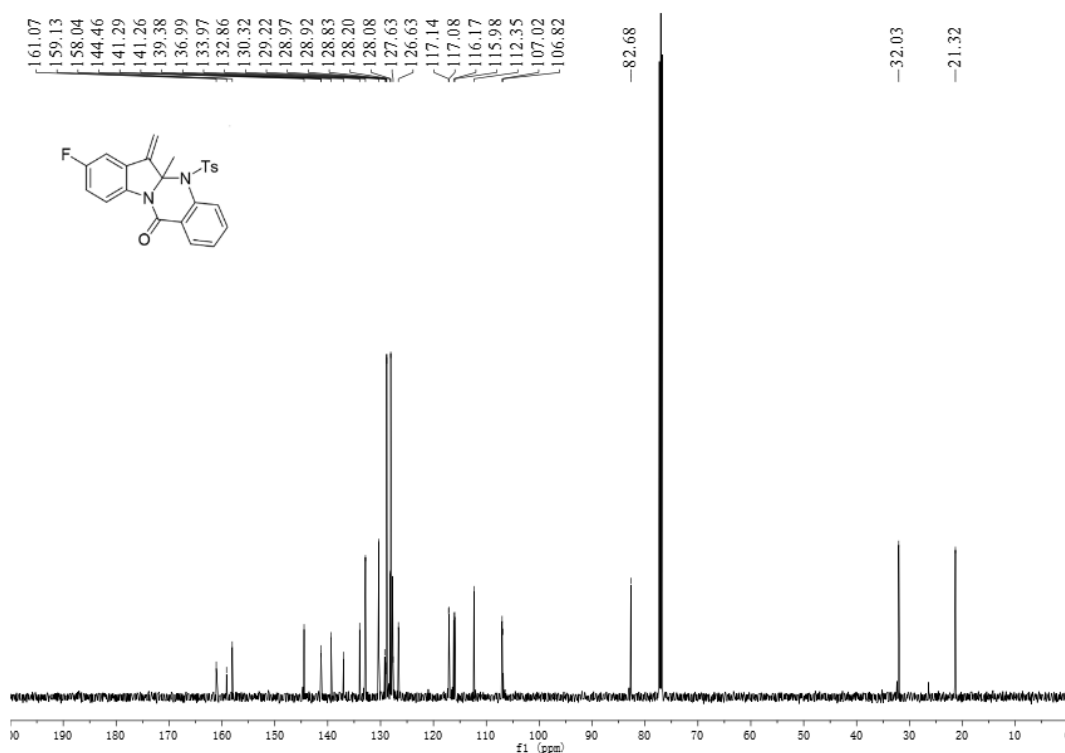


<sup>13</sup>C NMR spectrum of compound **2c**

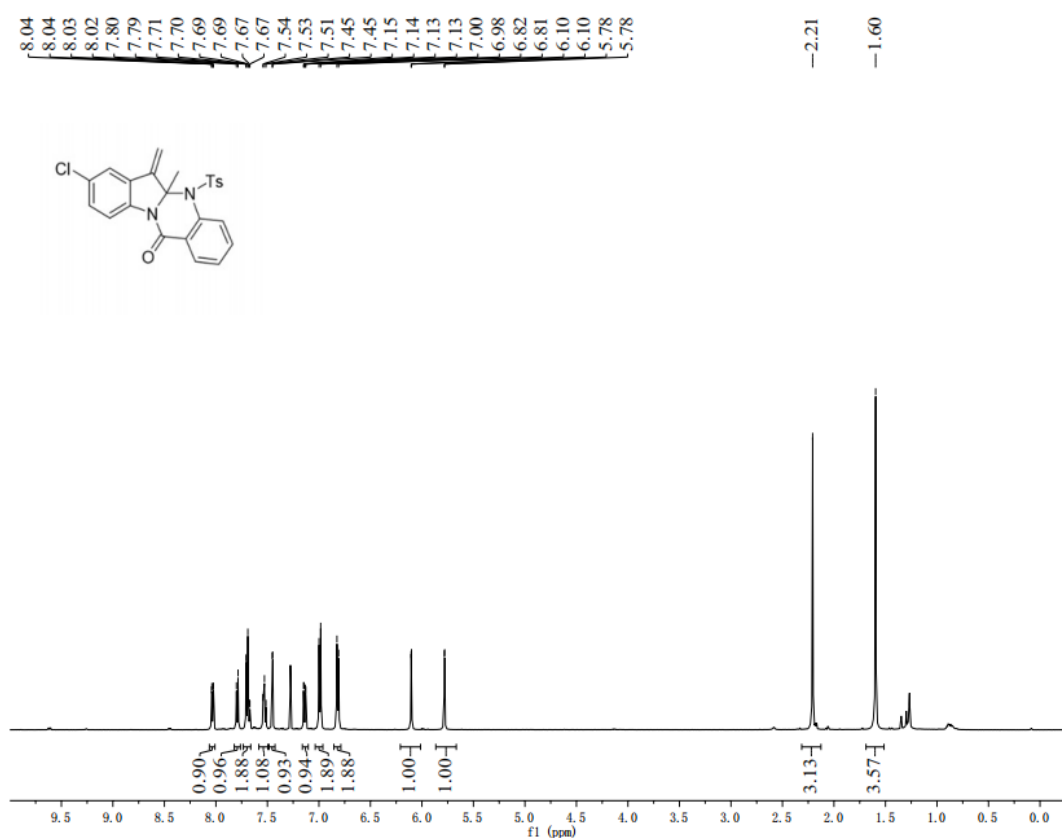




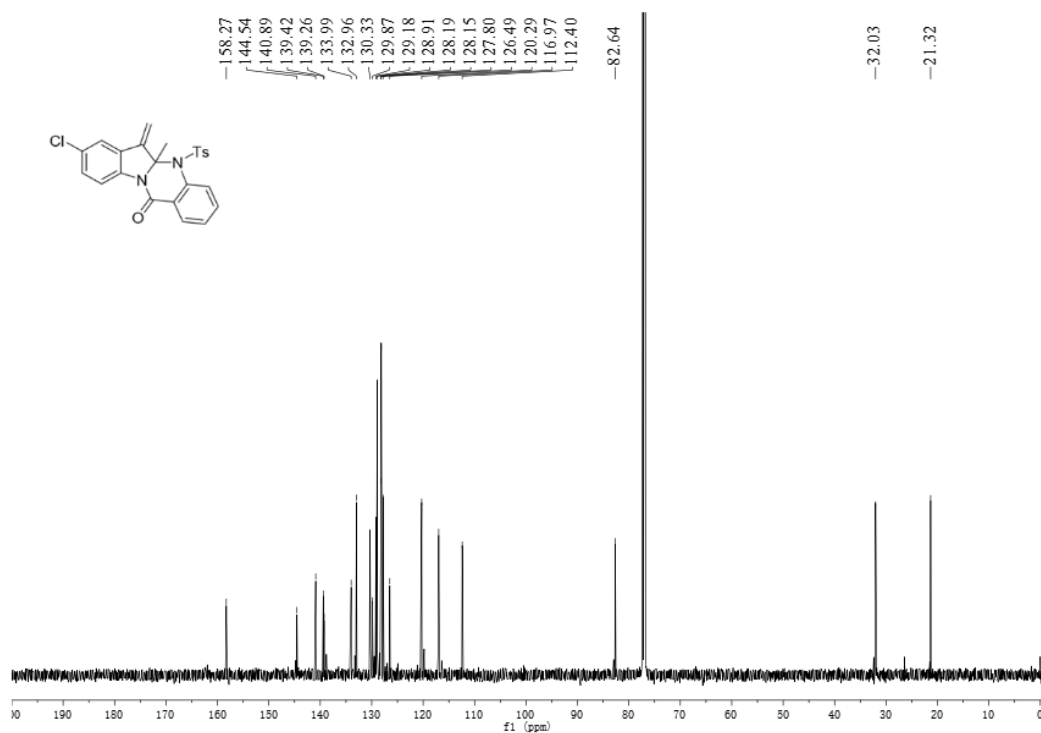
<sup>1</sup>H NMR spectrum of compound 2d



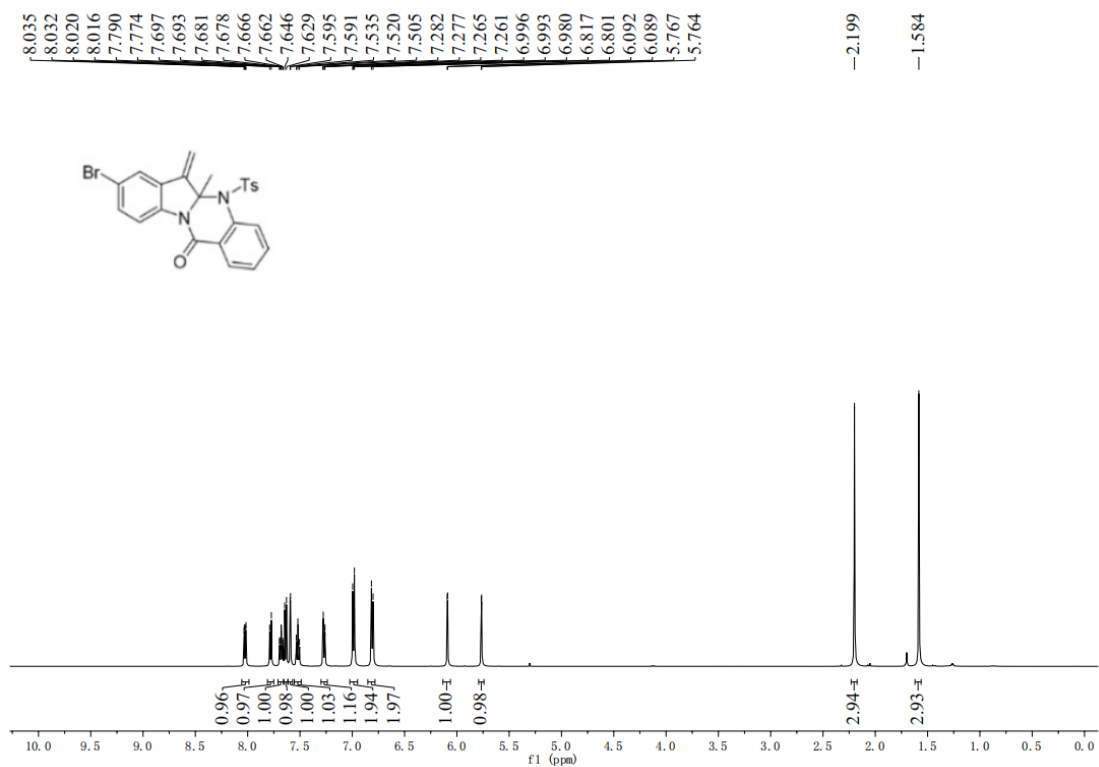
<sup>13</sup>C NMR spectrum of compound 2d



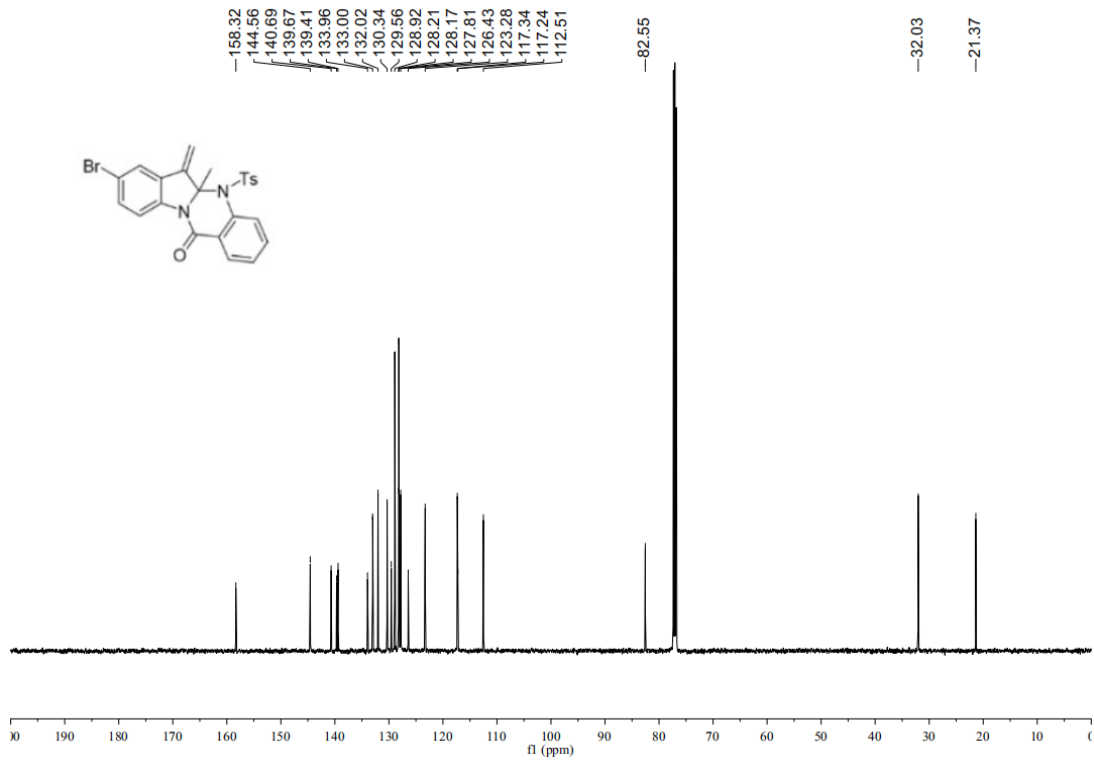
<sup>1</sup>H NMR spectrum of compound 2e



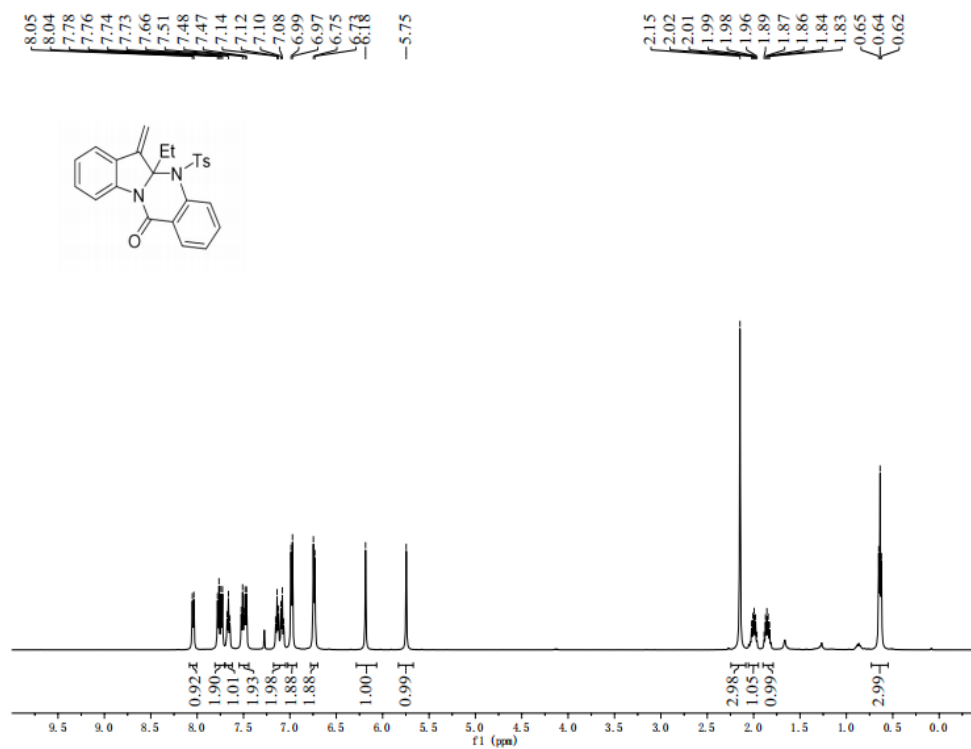
<sup>13</sup>C NMR spectrum of compound 2e



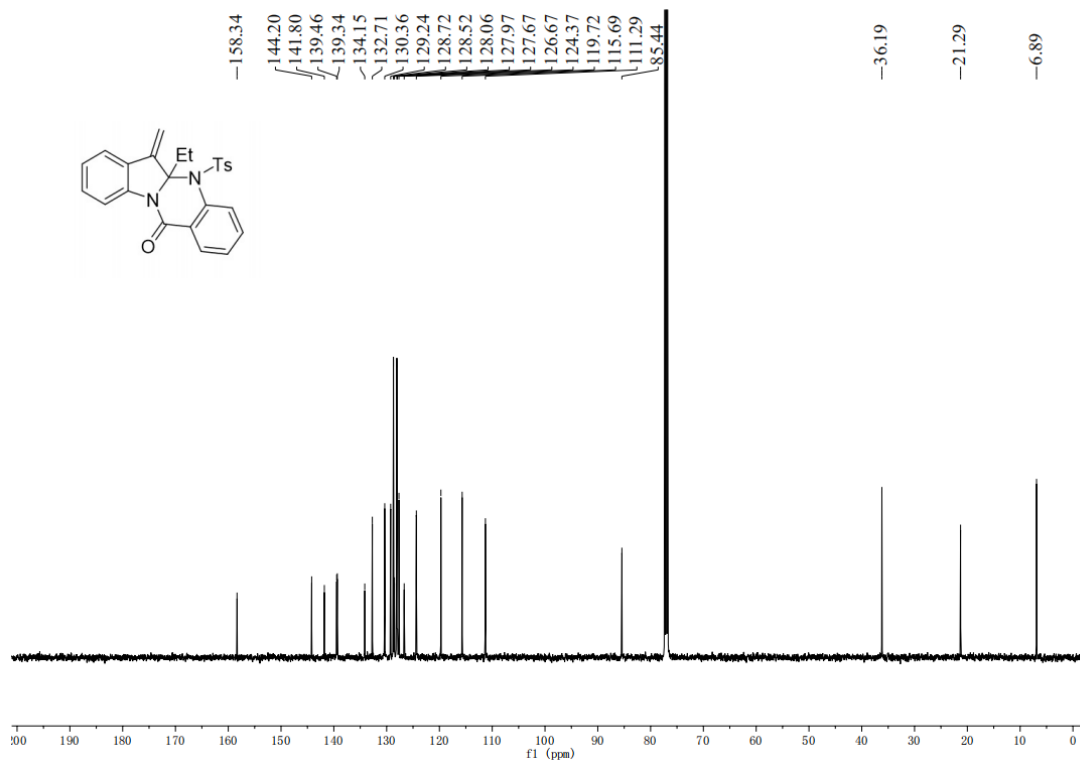
<sup>1</sup>H NMR spectrum of compound **2f**



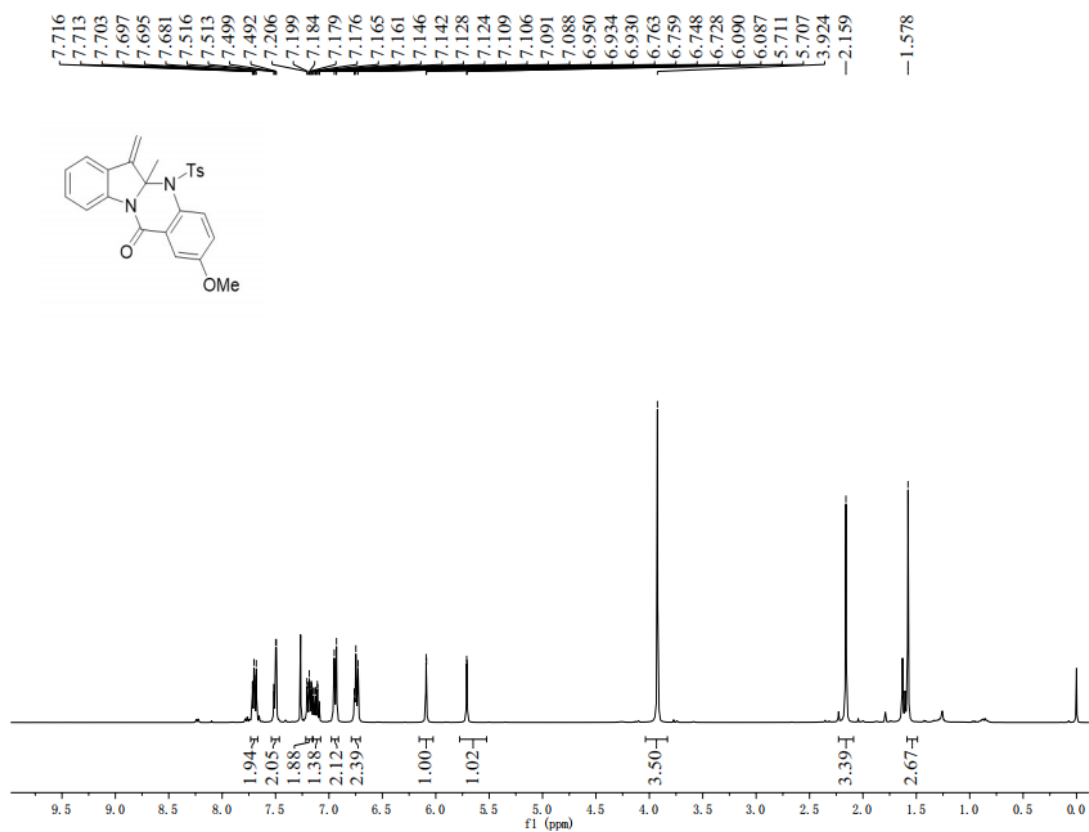
<sup>13</sup>C NMR spectrum of compound **2f**



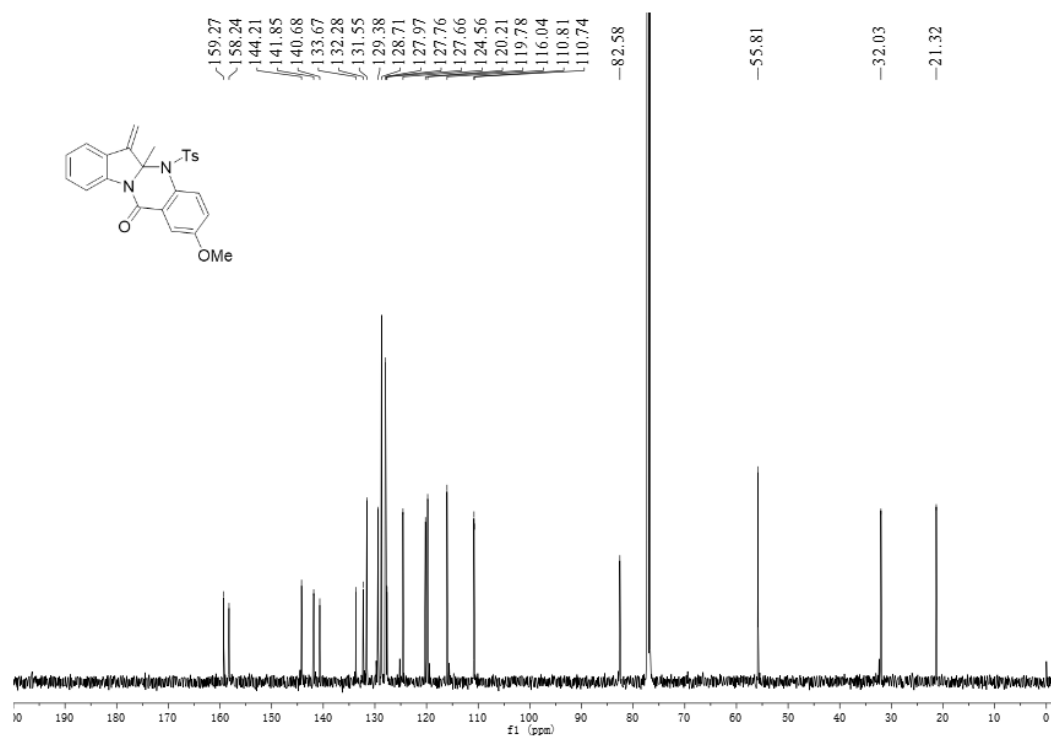
**<sup>1</sup>H NMR spectrum of compound 2g**



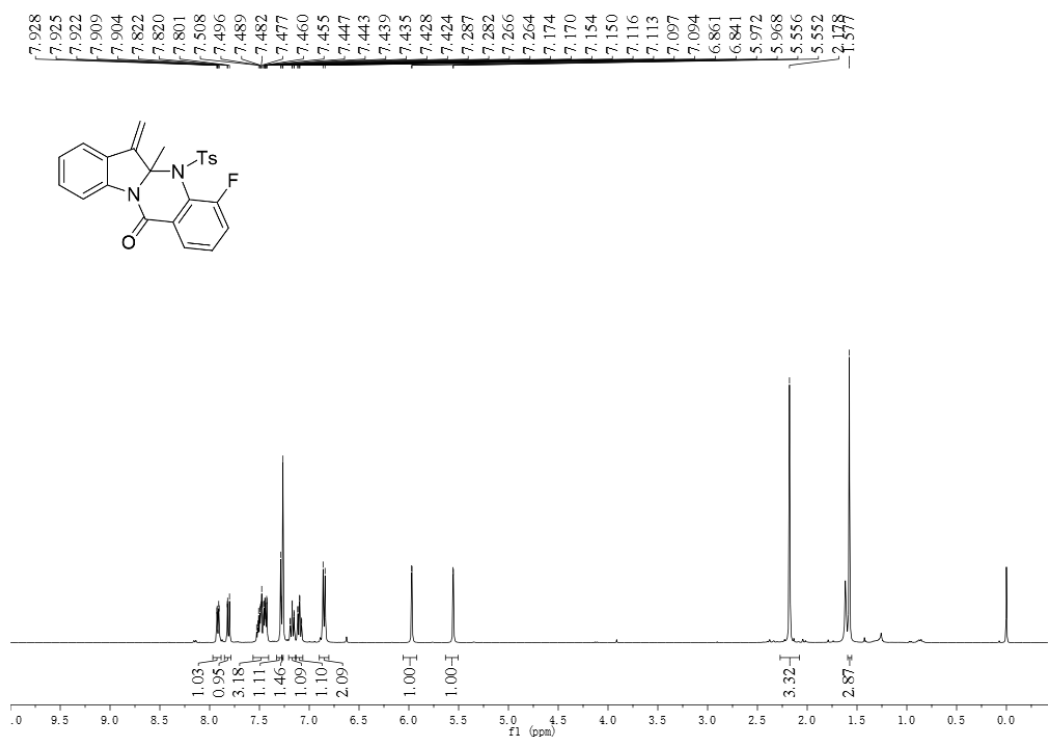
**<sup>13</sup>C NMR spectrum of compound 2g**



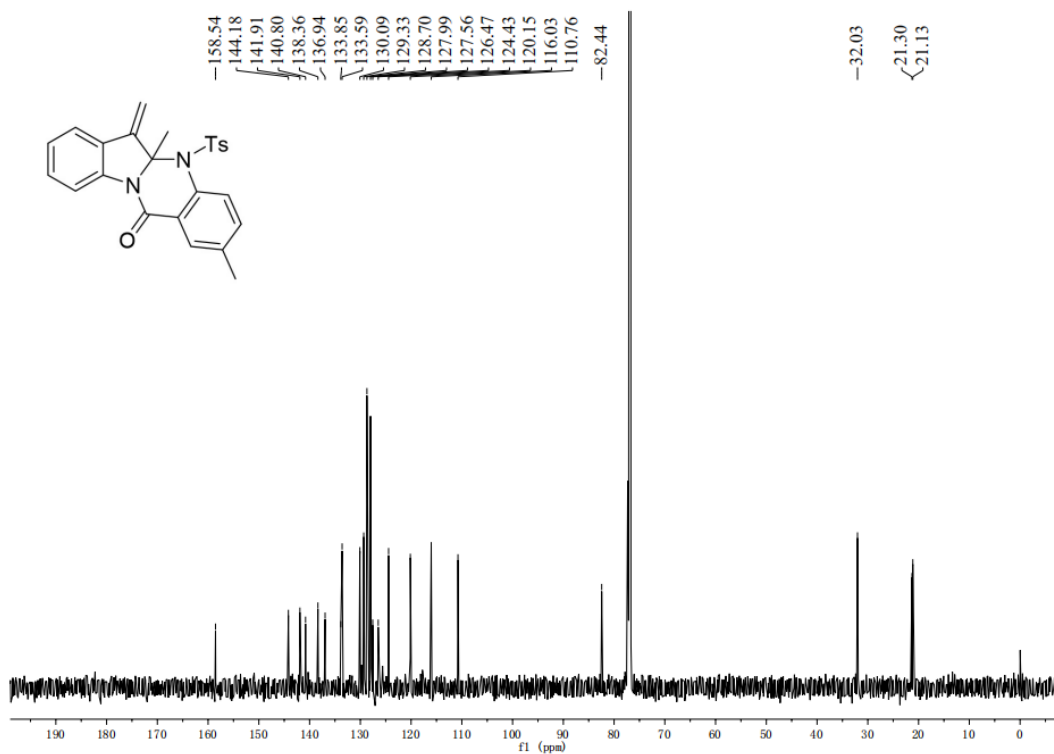
<sup>1</sup>H NMR spectrum of compound 2h



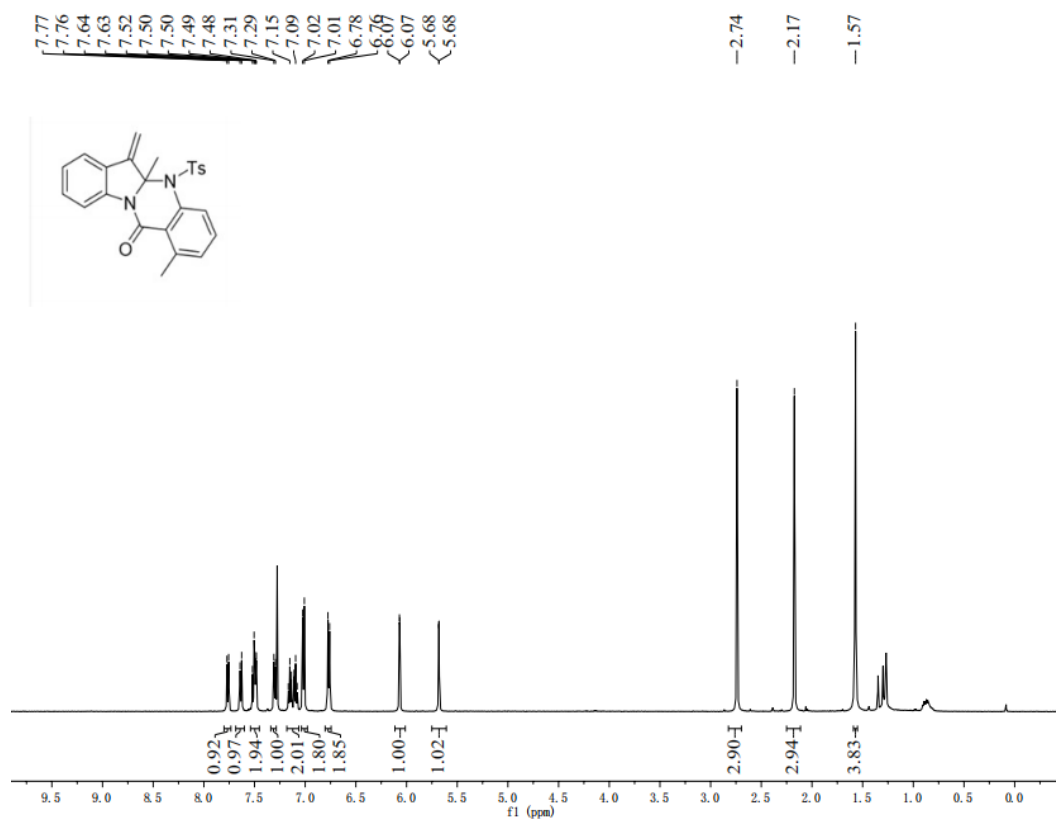
<sup>13</sup>C NMR spectrum of compound 2h



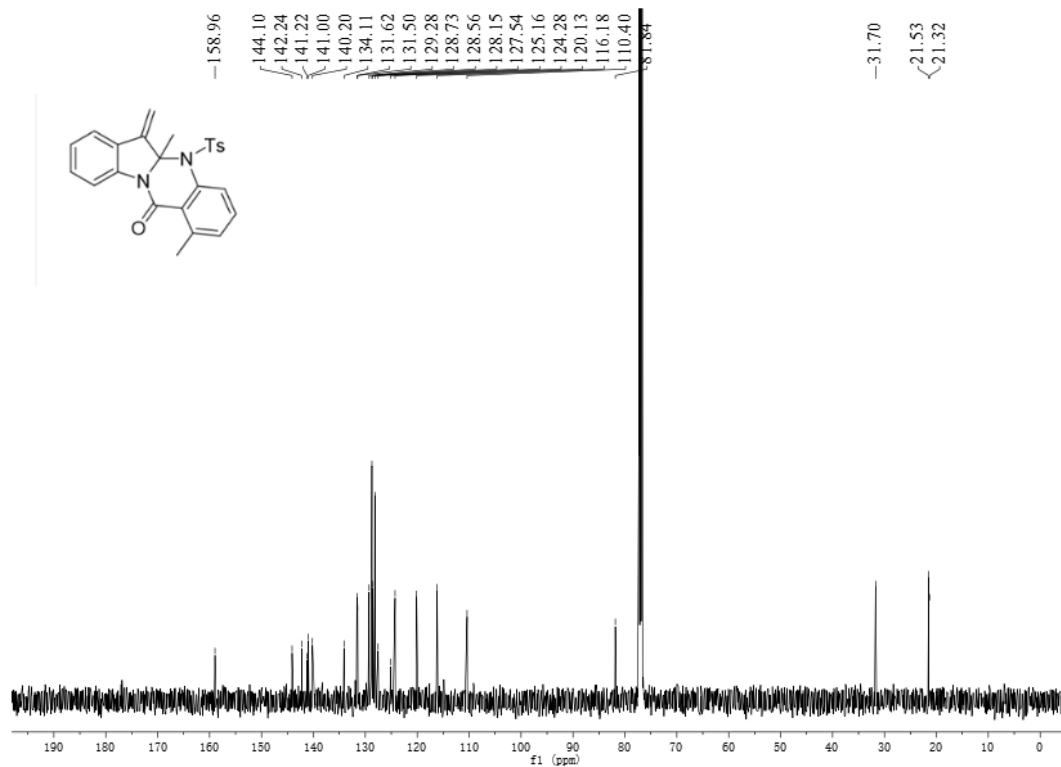
<sup>1</sup>H NMR spectrum of compound **2i**



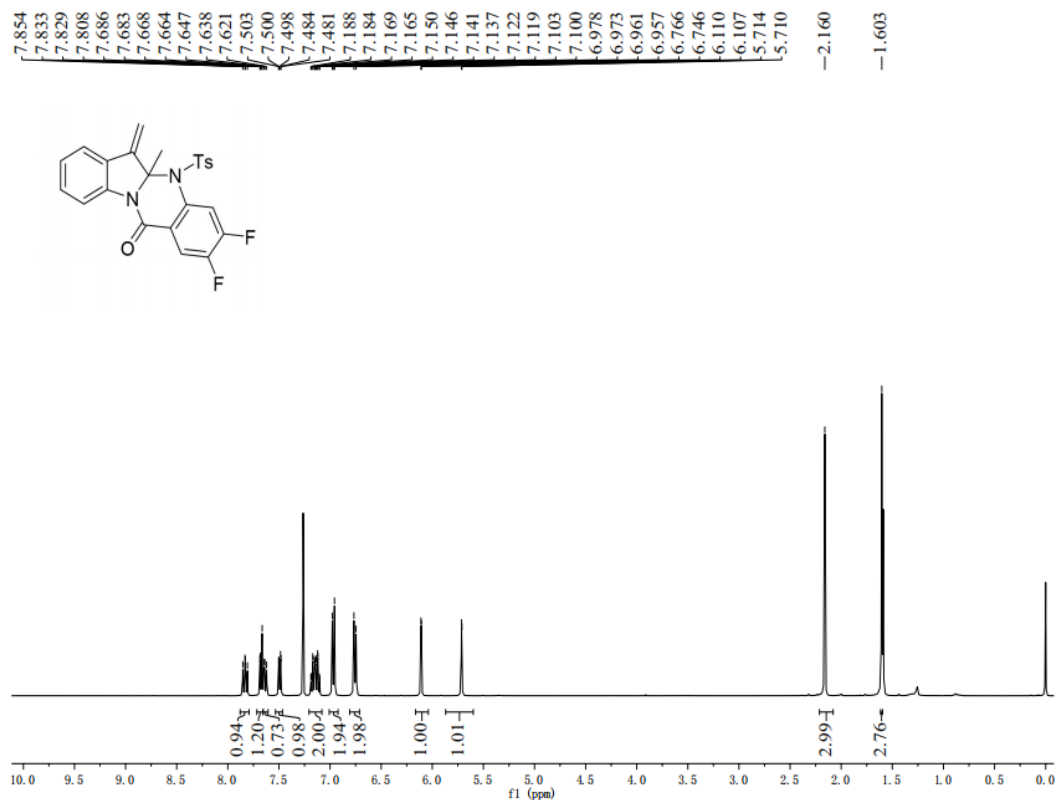
<sup>13</sup>C NMR spectrum of compound **2i**



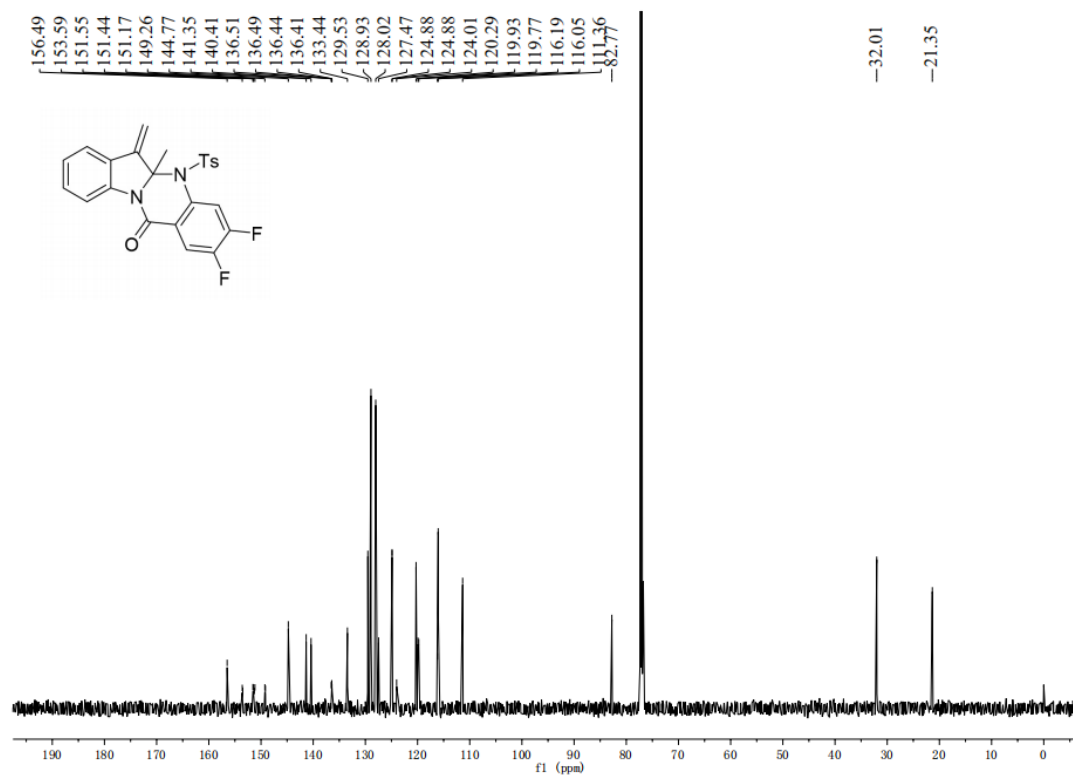
<sup>1</sup>H NMR spectrum of compound **2j**



<sup>13</sup>C NMR spectrum of compound **2j**

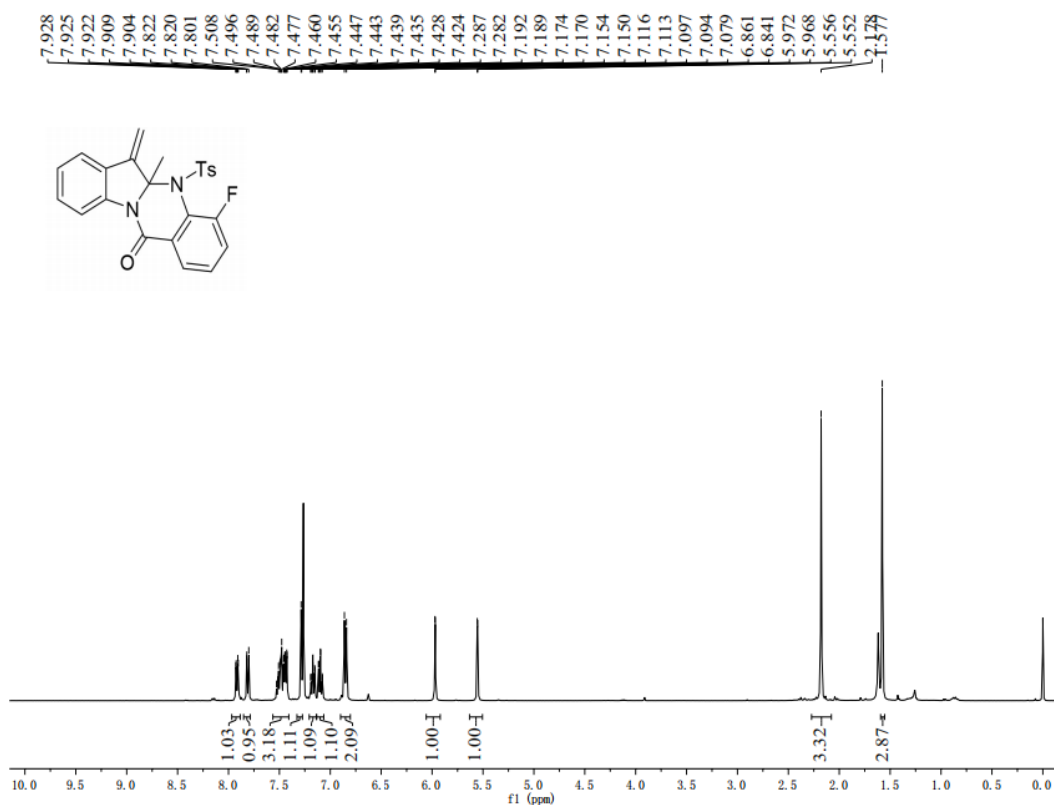


<sup>1</sup>H NMR spectrum of compound **2k**

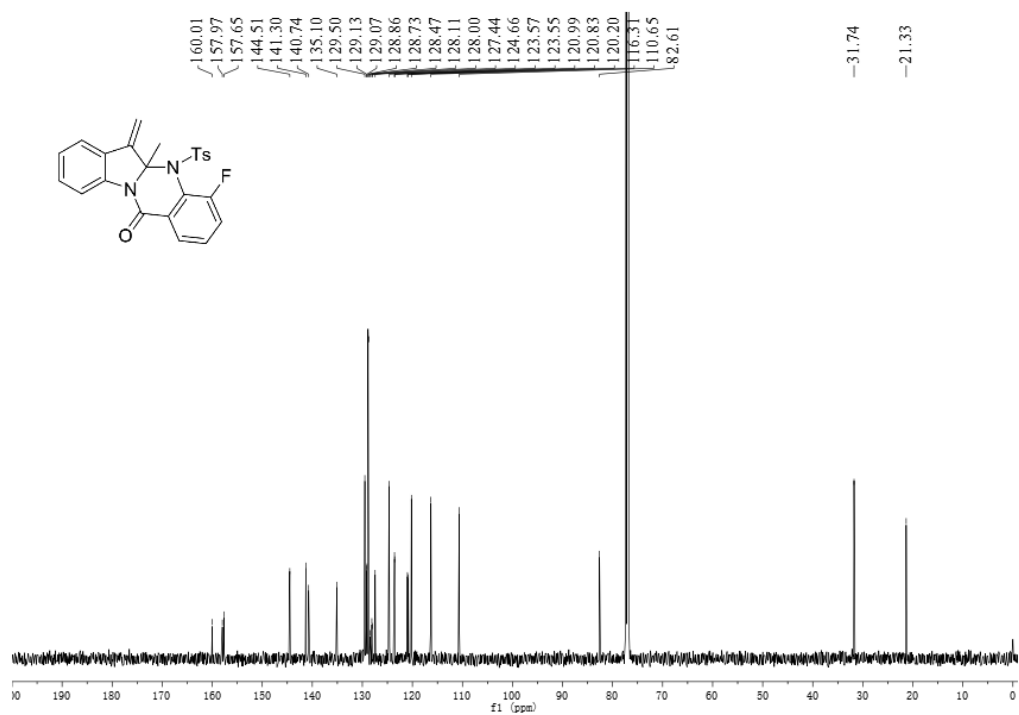


<sup>13</sup>C NMR spectrum of compound **2k**

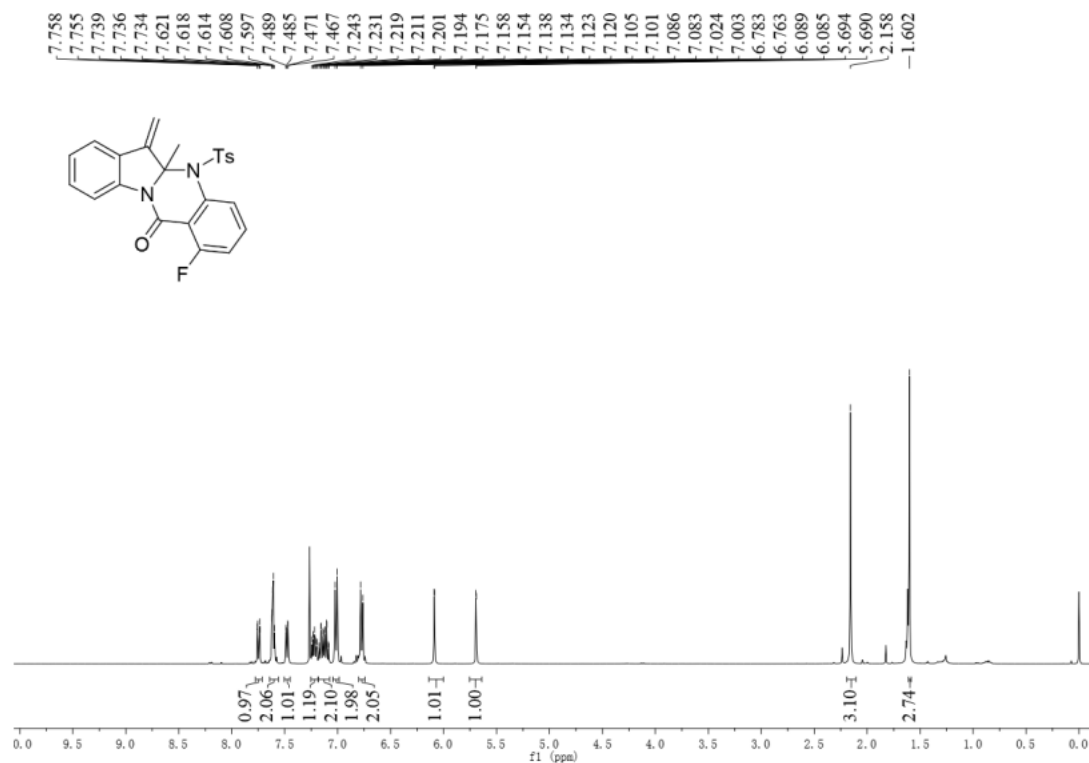




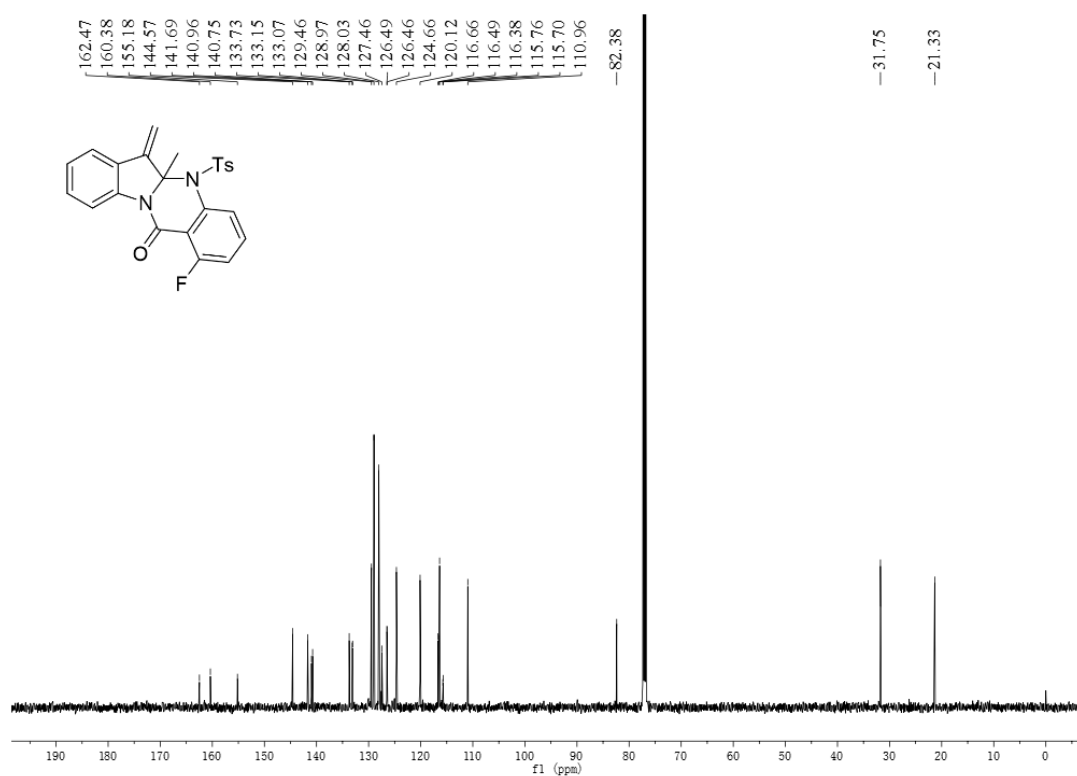
<sup>1</sup>H NMR spectrum of compound 21



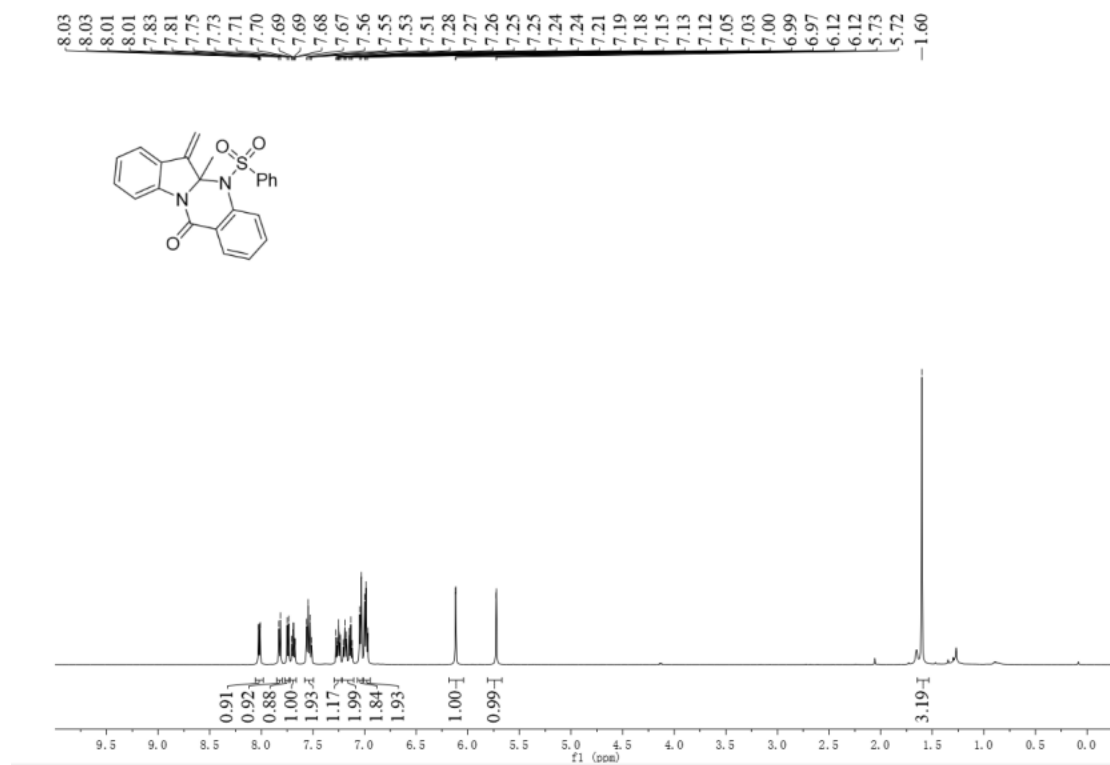
<sup>13</sup>C NMR spectrum of compound 21



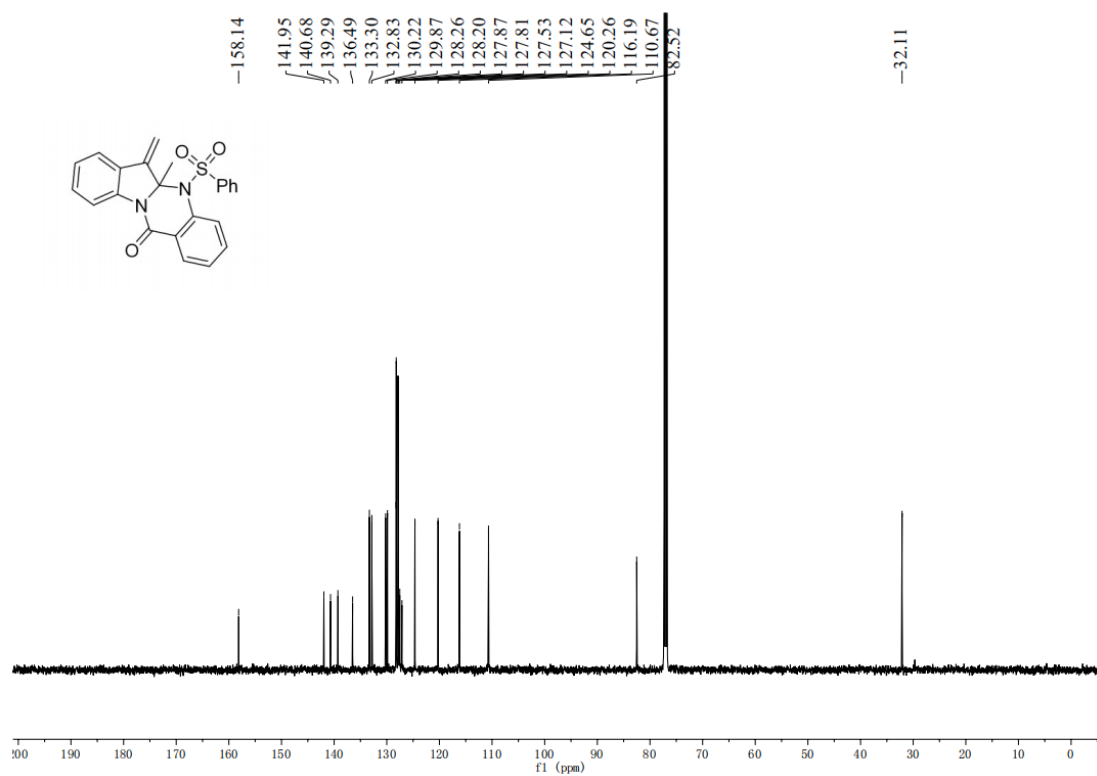
<sup>1</sup>H NMR spectrum of compound **2m**



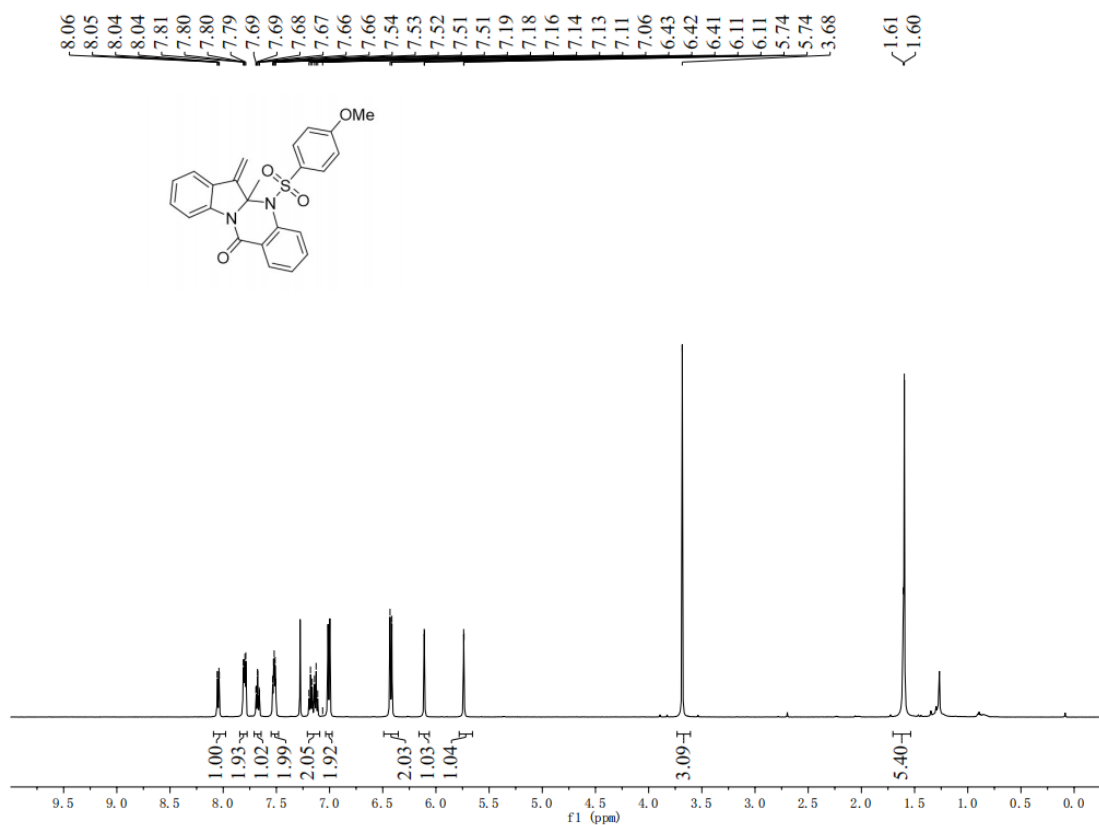
<sup>13</sup>C NMR spectrum of compound **2m**



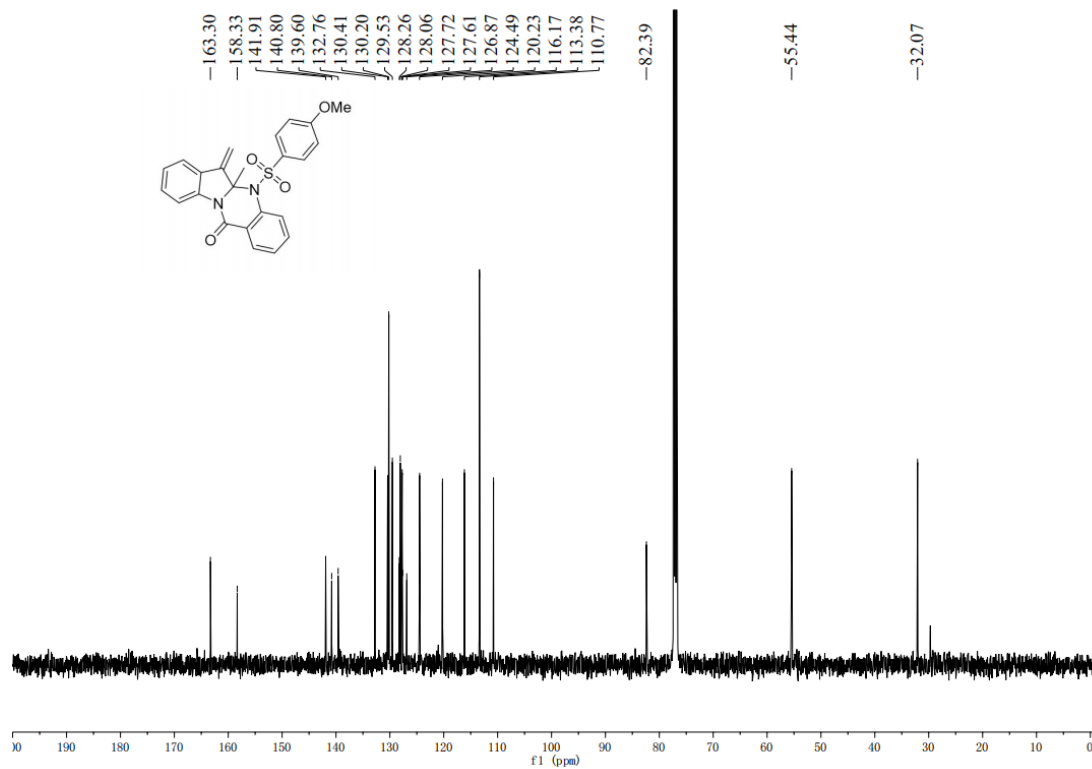
<sup>1</sup>H NMR spectrum of compound **2n**



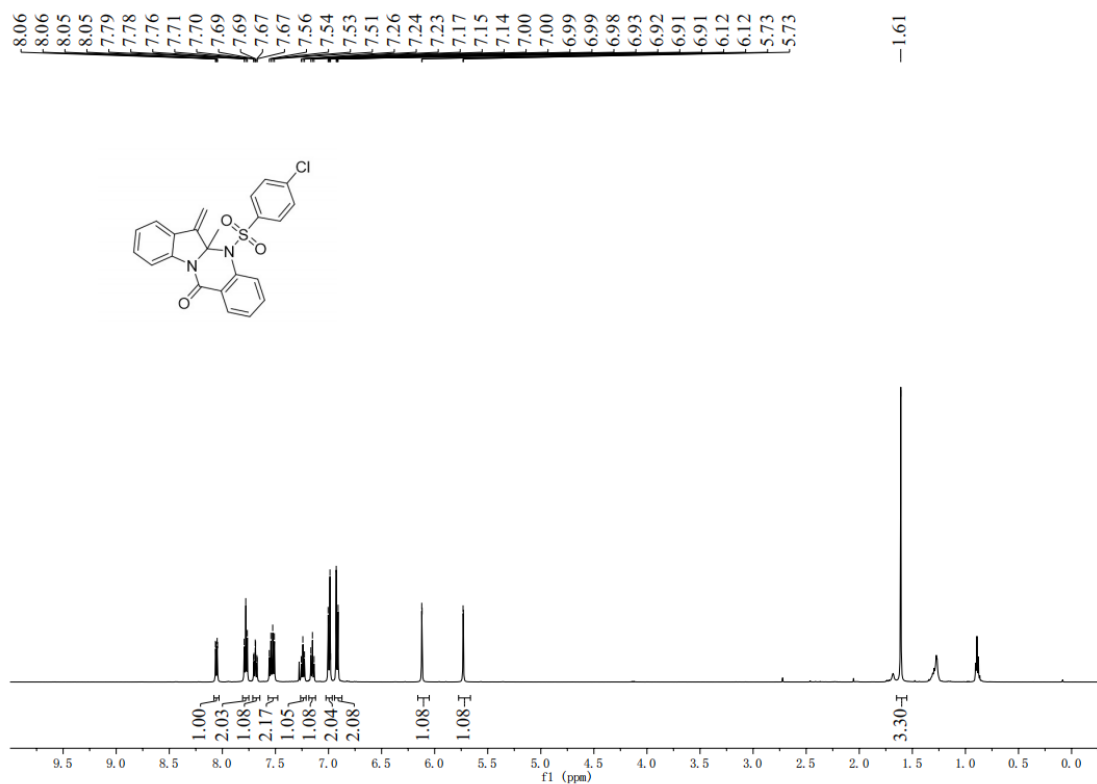
<sup>13</sup>C NMR spectrum of compound **2n**



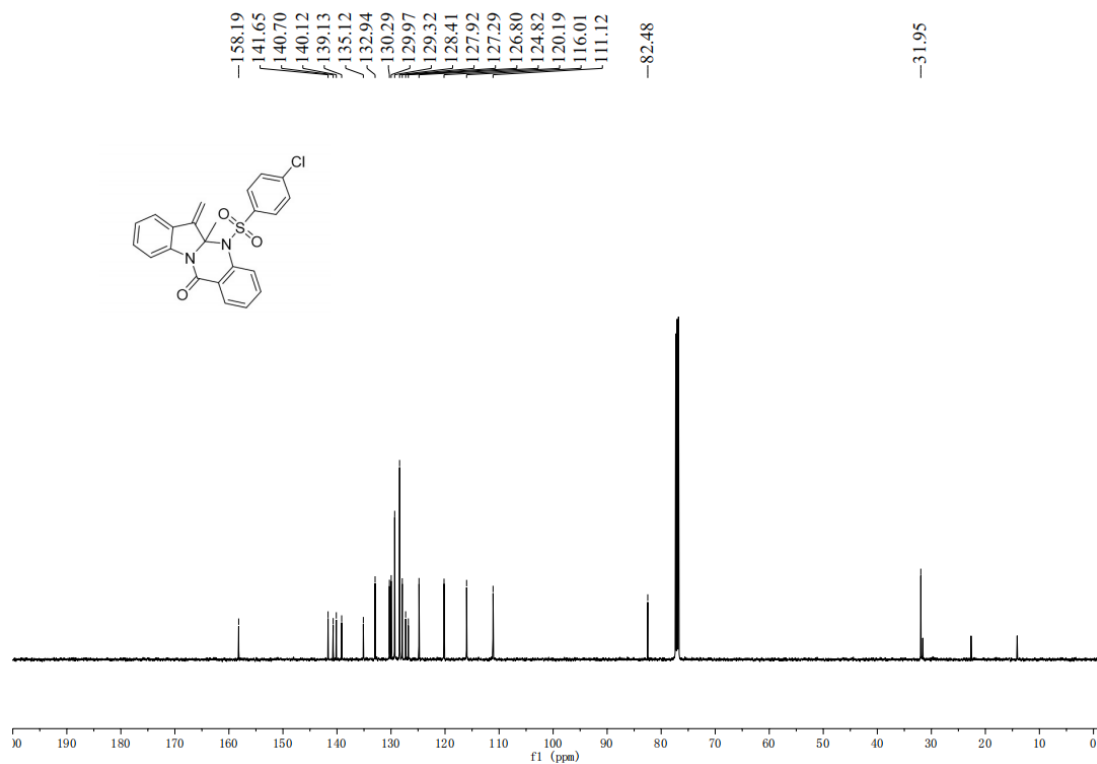
<sup>1</sup>H NMR spectrum of compound **2o**



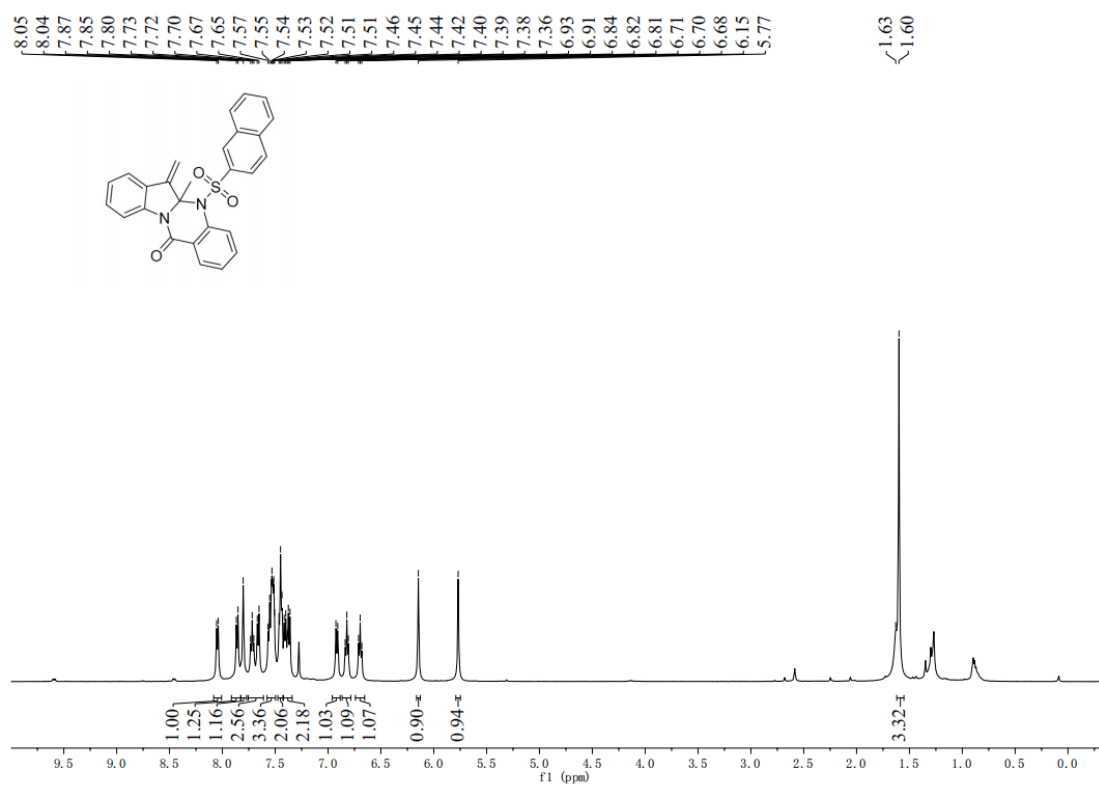
<sup>13</sup>C NMR spectrum of compound **2o**



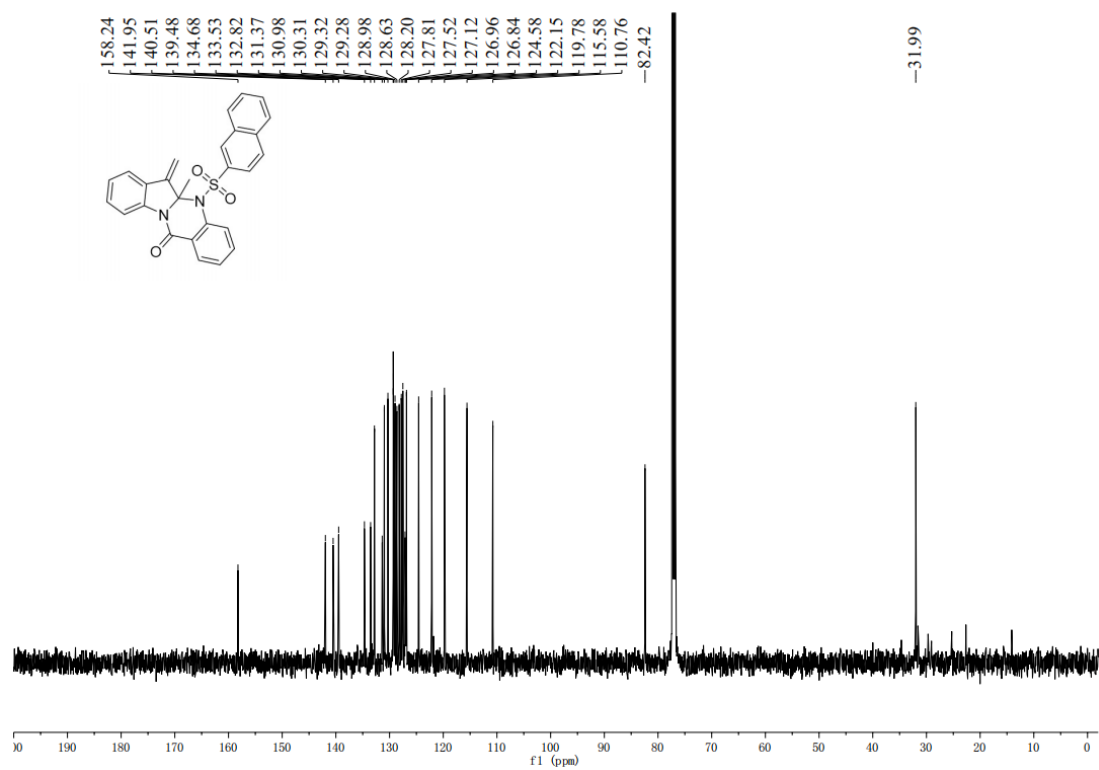
<sup>1</sup>H NMR spectrum of compound **2p**



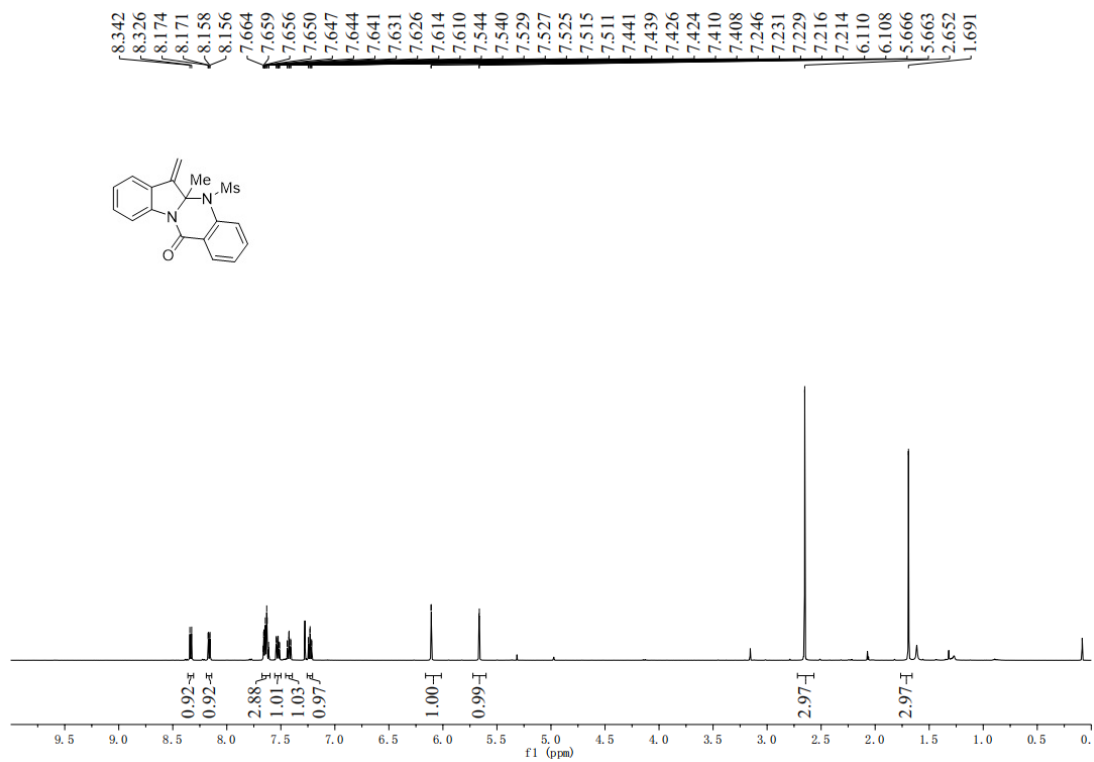
<sup>13</sup>C NMR spectrum of compound **2p**



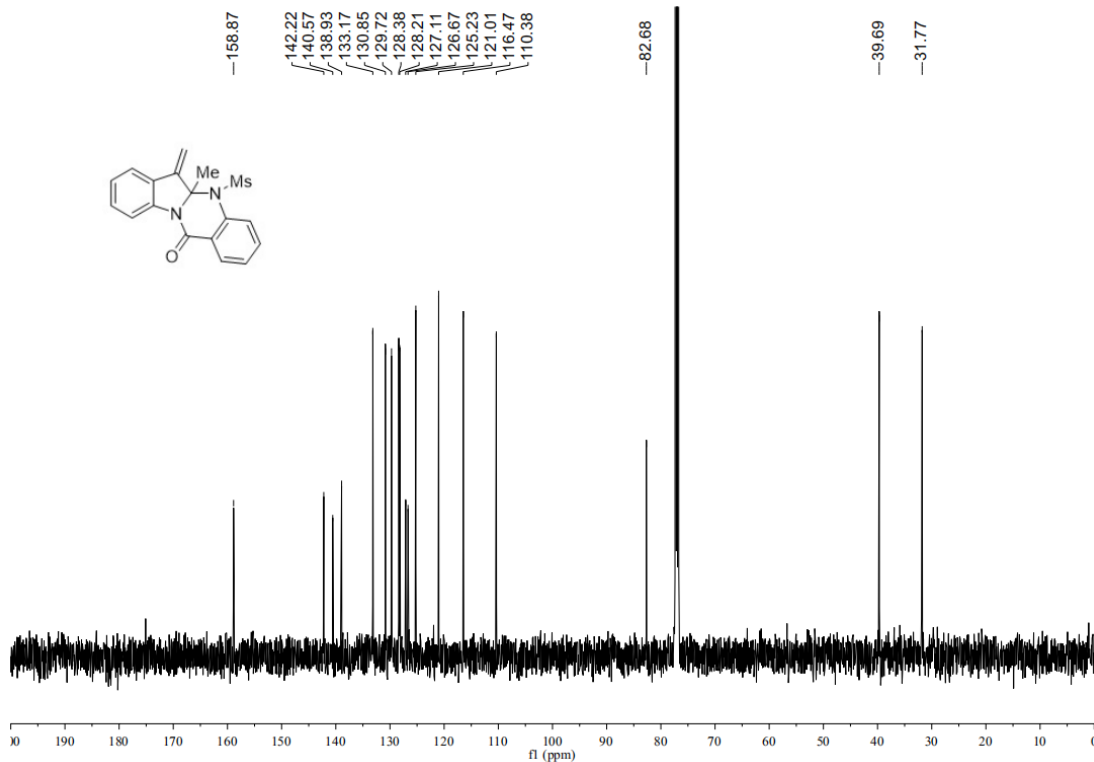
<sup>1</sup>H NMR spectrum of compound 2q



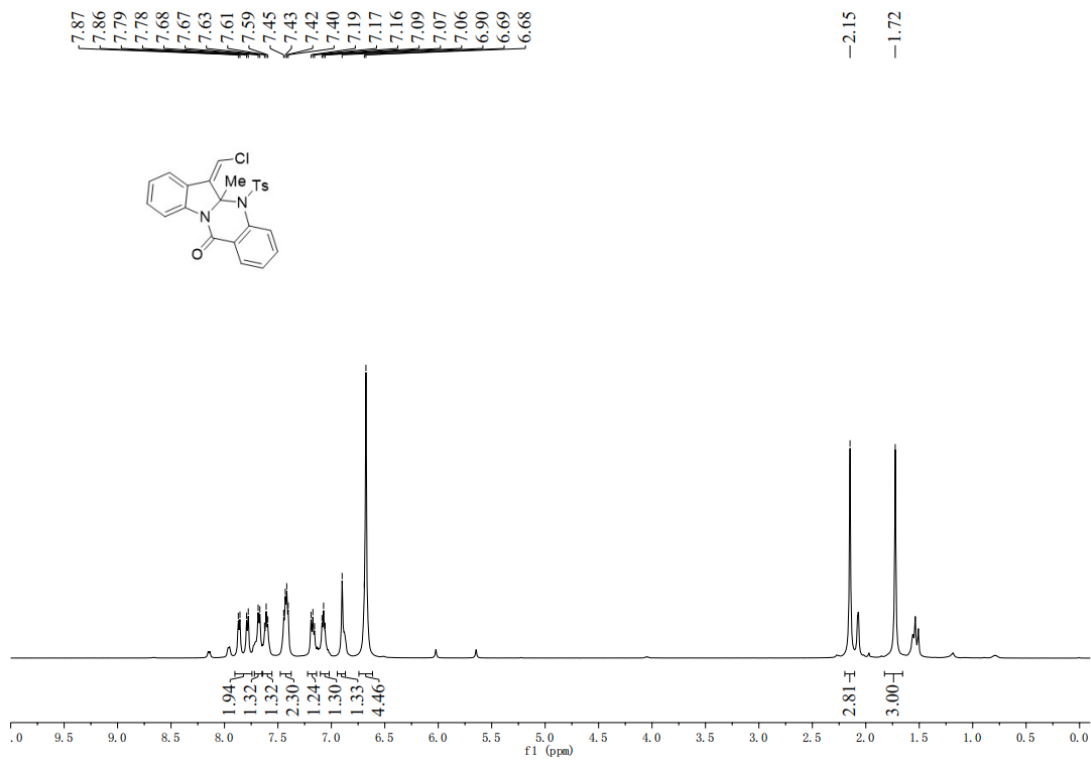
<sup>13</sup>C NMR spectrum of compound 2q



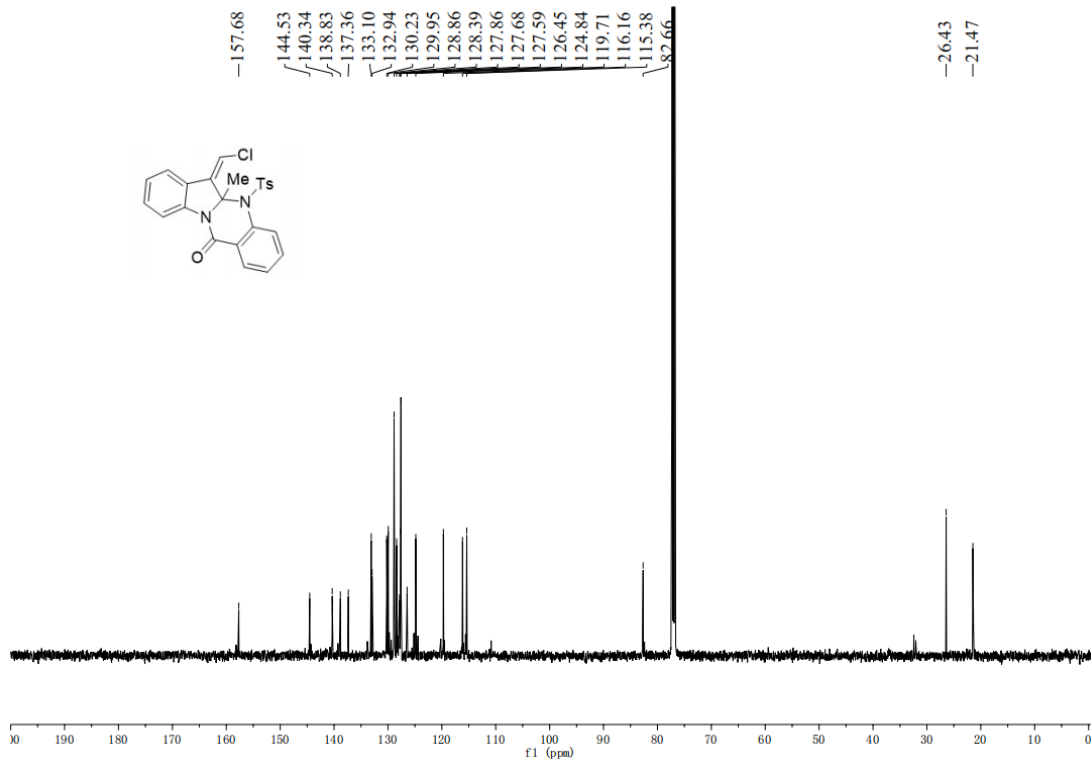
<sup>1</sup>H NMR spectrum of compound **2r**



<sup>13</sup>C NMR spectrum of compound **2r**

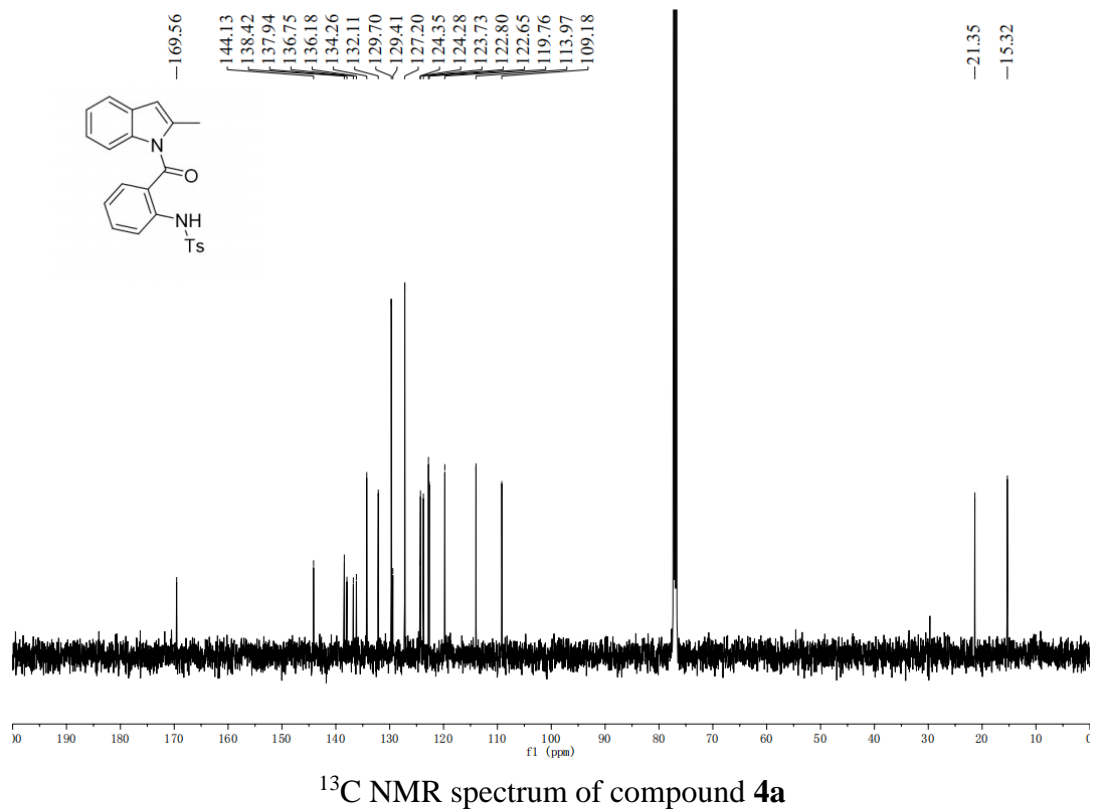
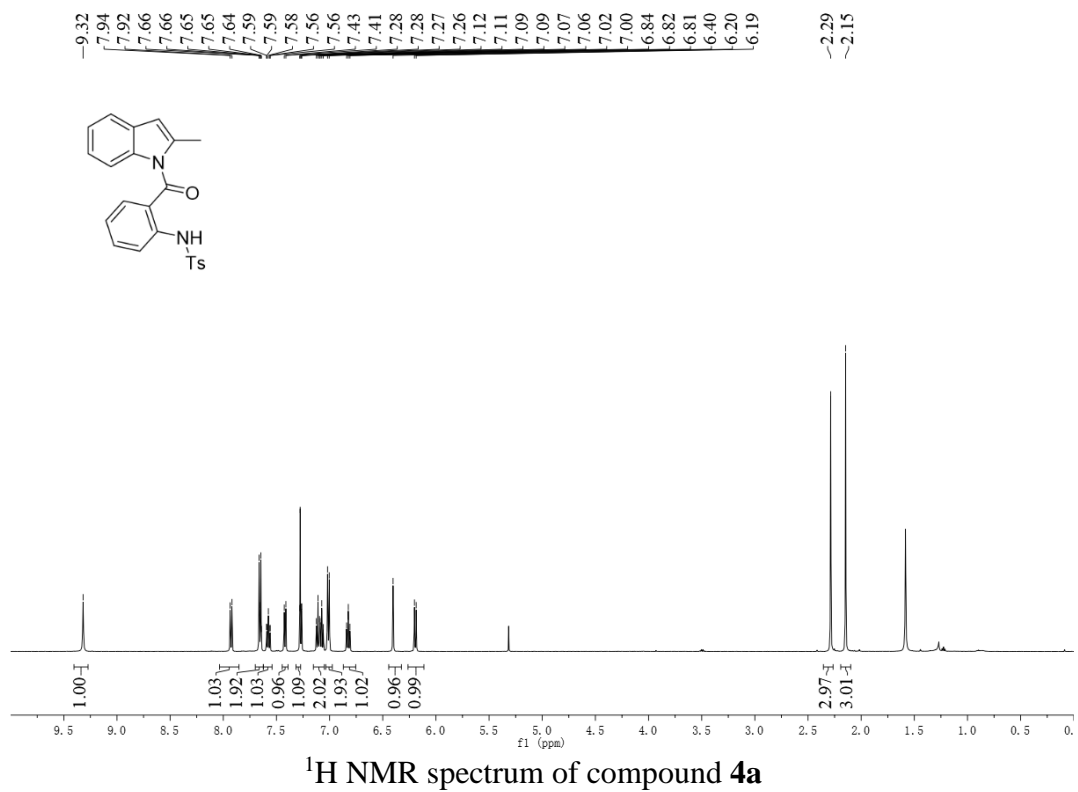


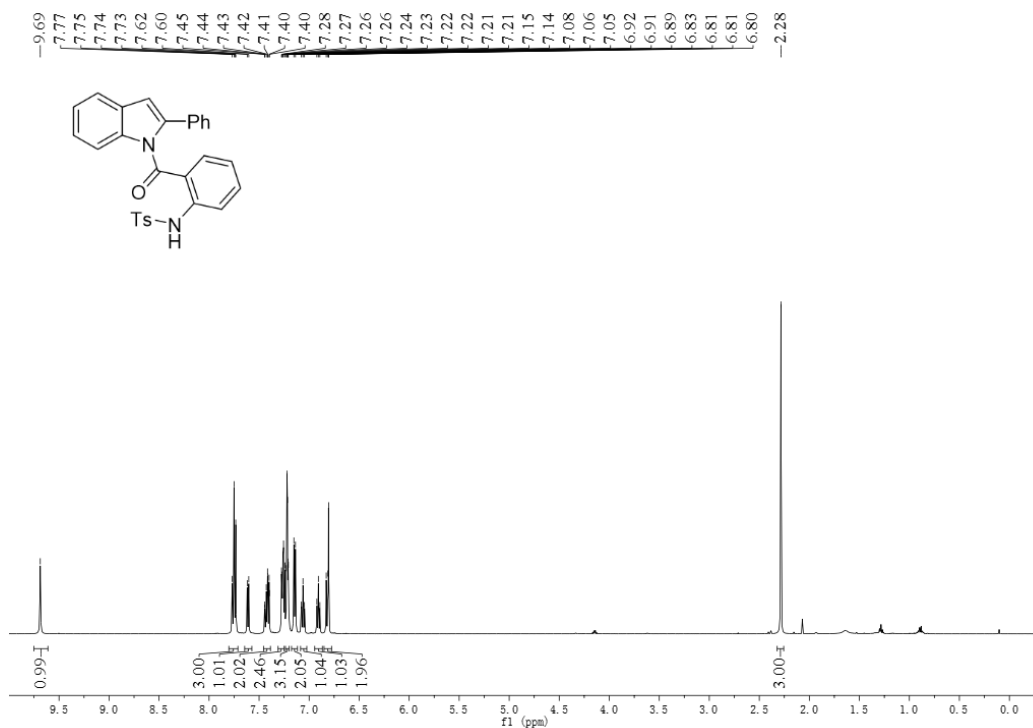
<sup>1</sup>H NMR spectrum of compound **3**



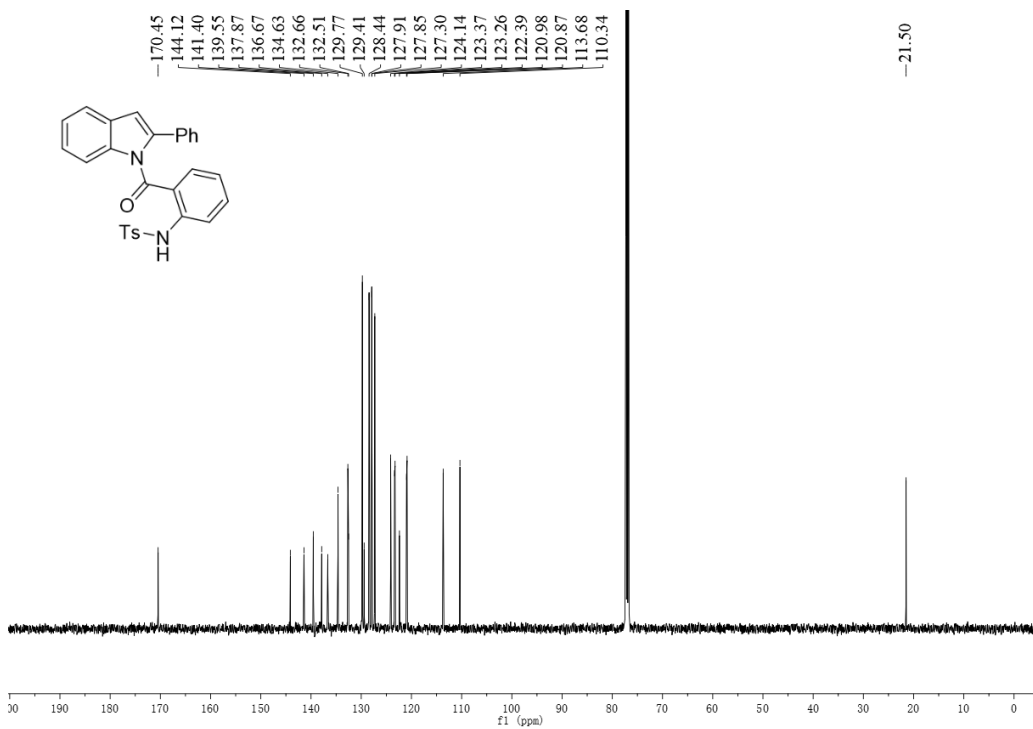
<sup>13</sup>C NMR spectrum of compound **3**



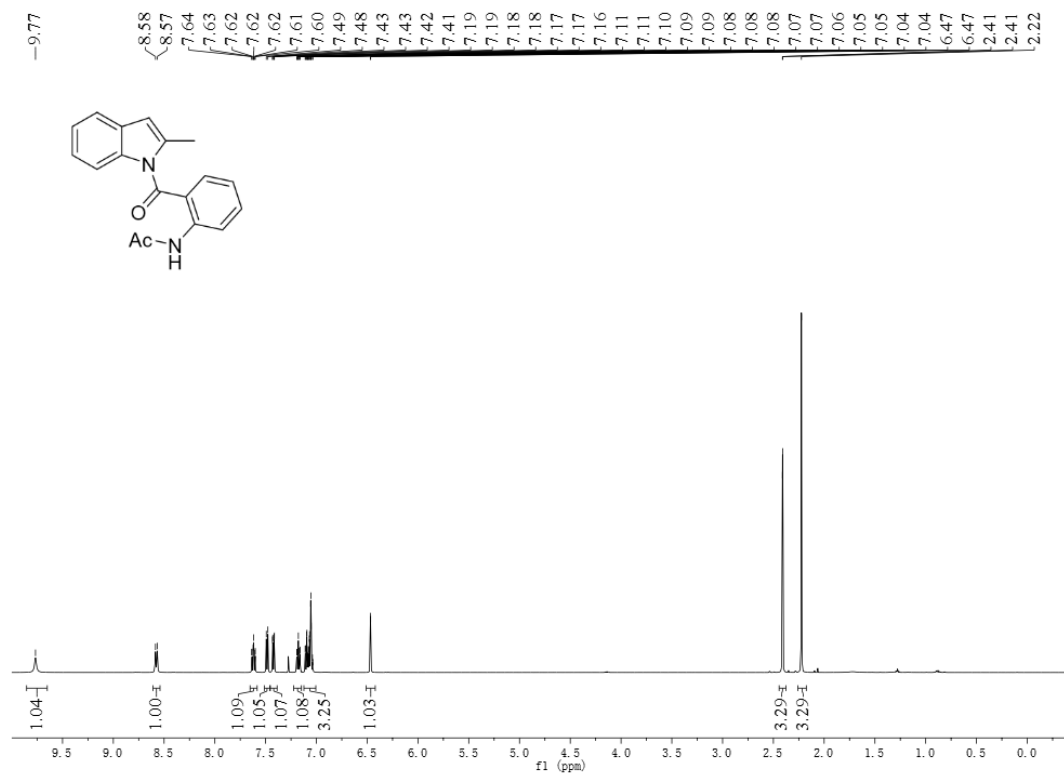




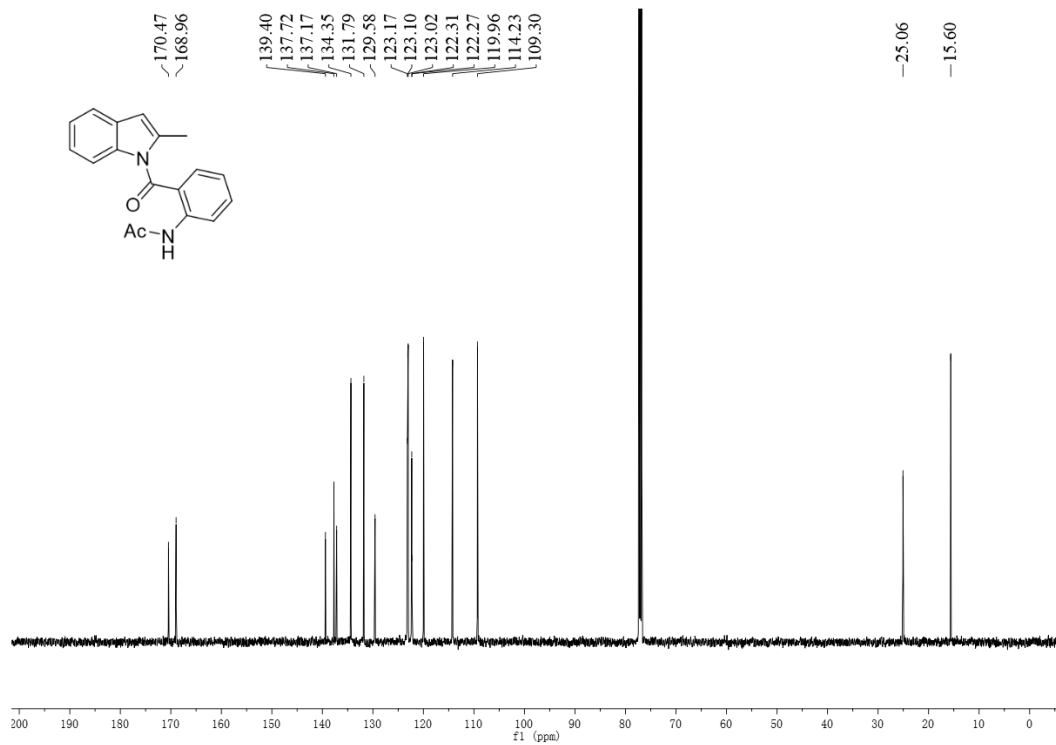
<sup>1</sup>H NMR spectrum of compound 4b



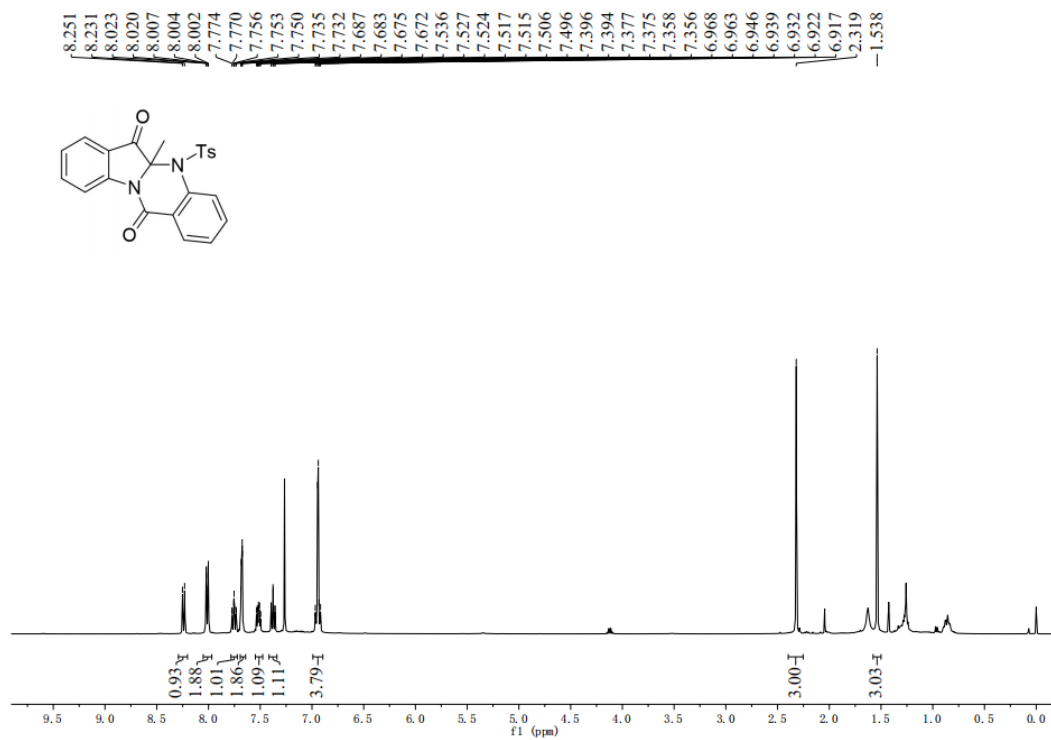
<sup>13</sup>C NMR spectrum of compound 4b



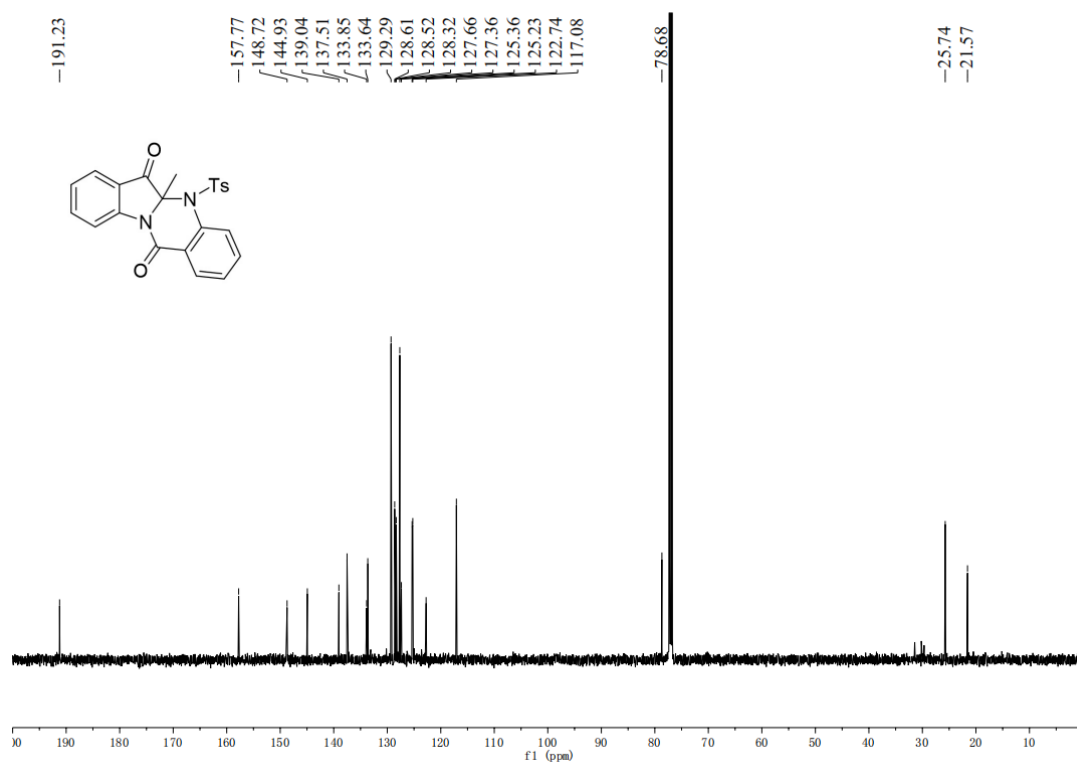
$^1\text{H NMR}$  spectrum of compound 4c



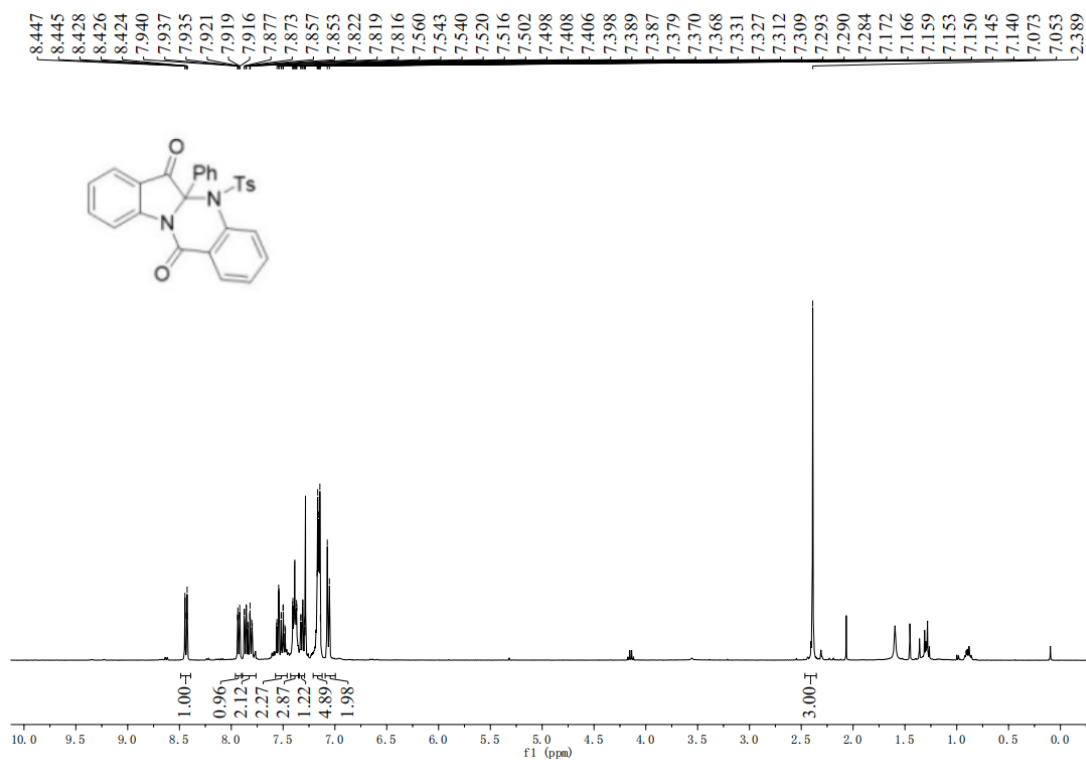
$^{13}\text{C NMR}$  spectrum of compound 4c



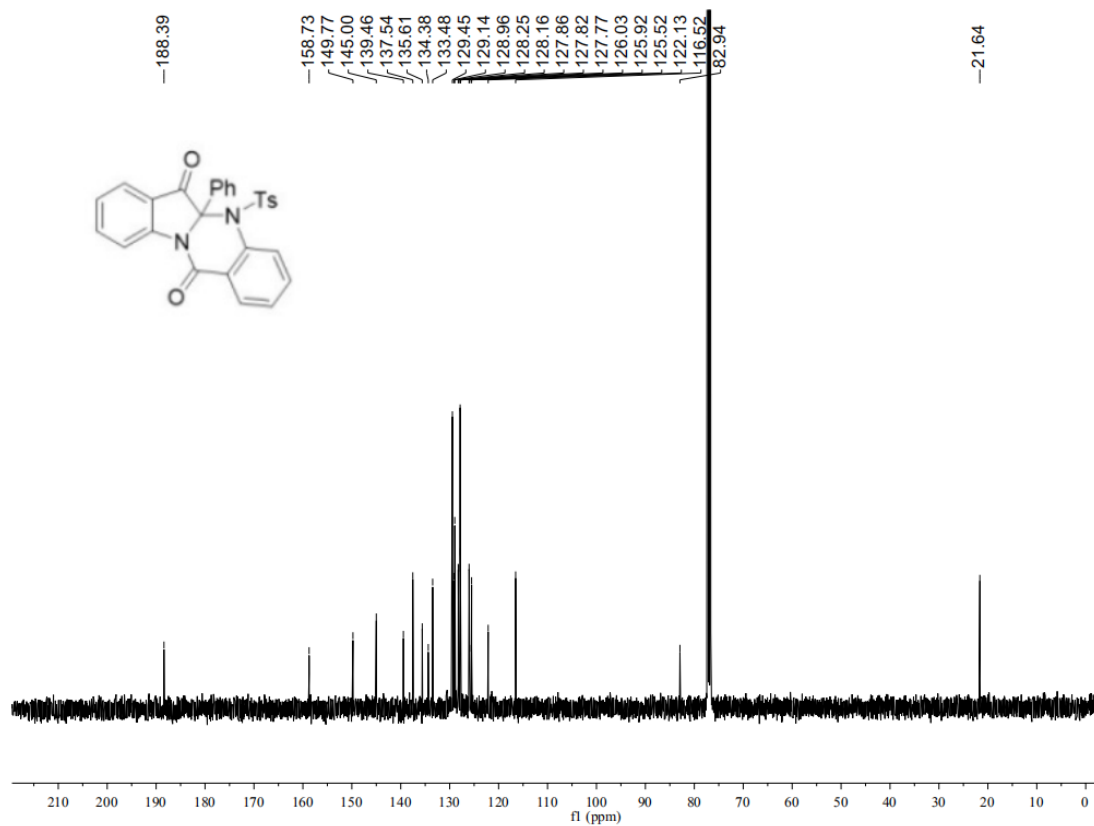
<sup>1</sup>H NMR spectrum of compound 5a



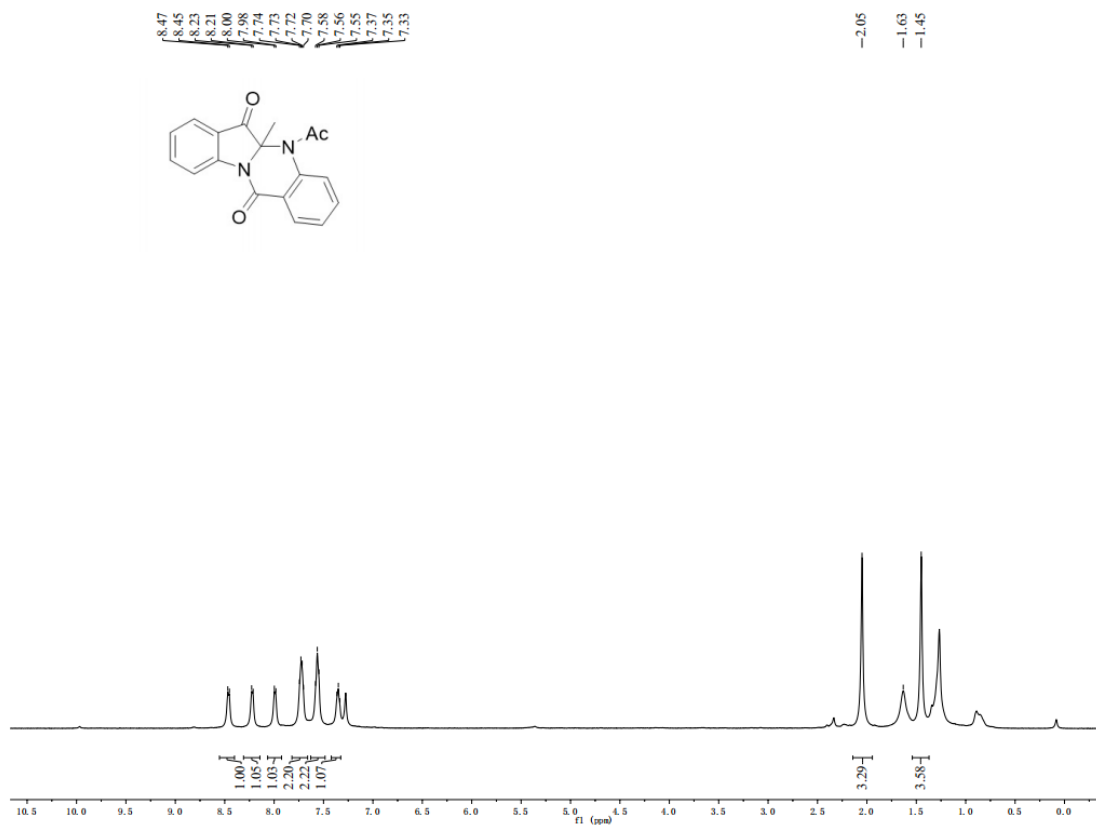
<sup>13</sup>C NMR spectrum of compound 5a



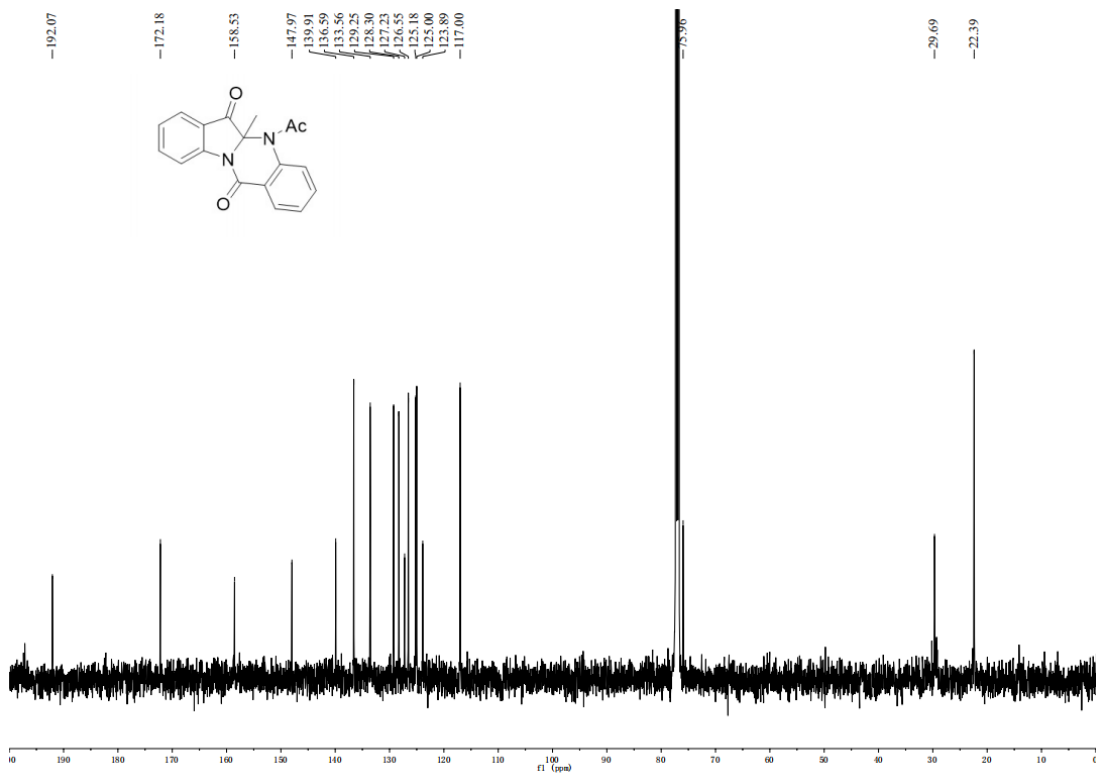
$^1\text{H}$  NMR spectrum of compound **5b**



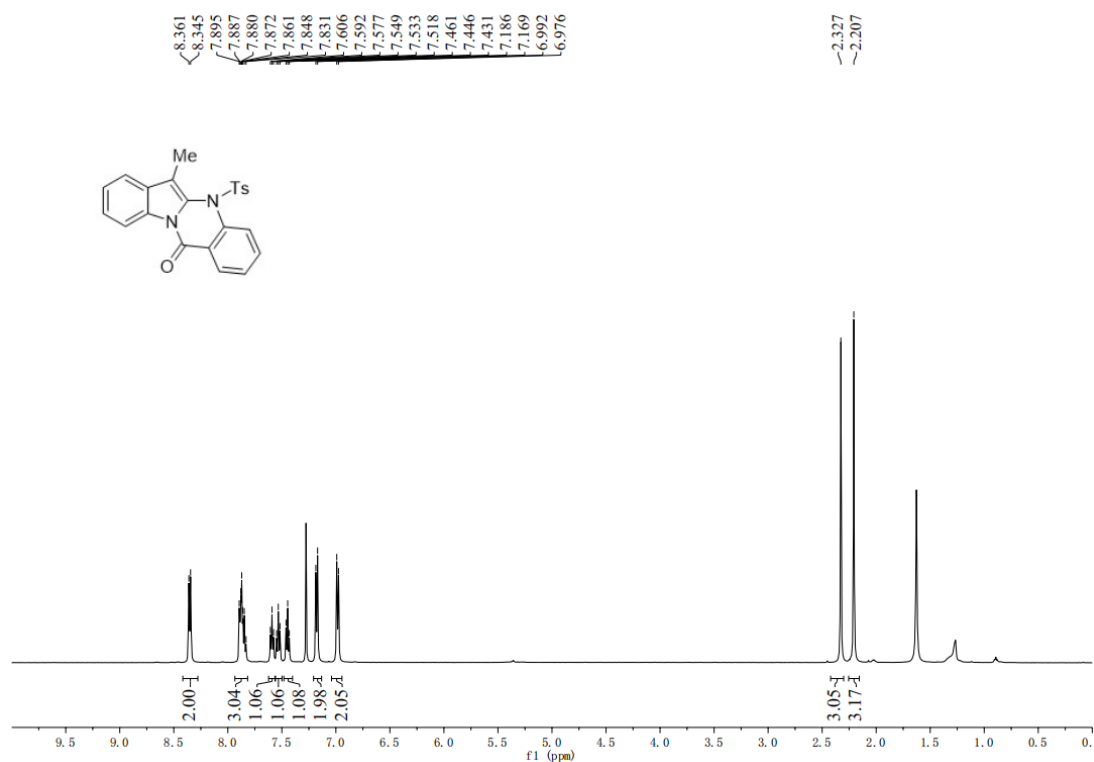
$^{13}\text{C}$  NMR spectrum of compound **5b**



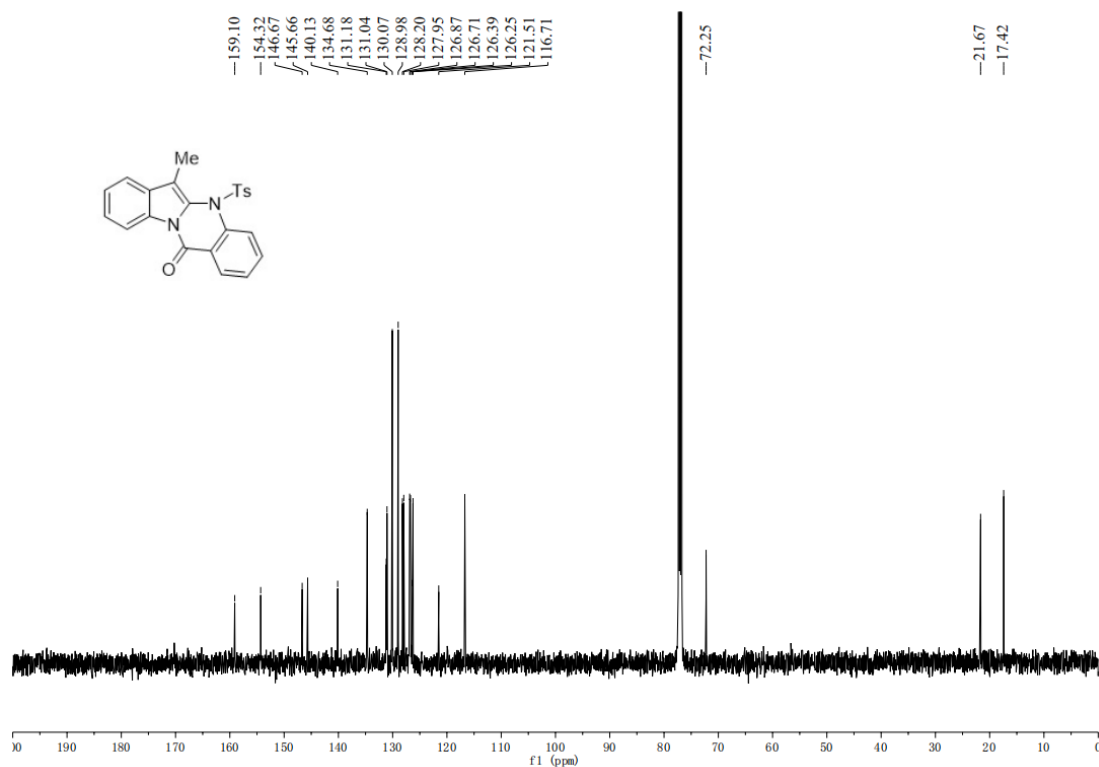
$^1\text{H NMR}$  spectrum of compound **5c**



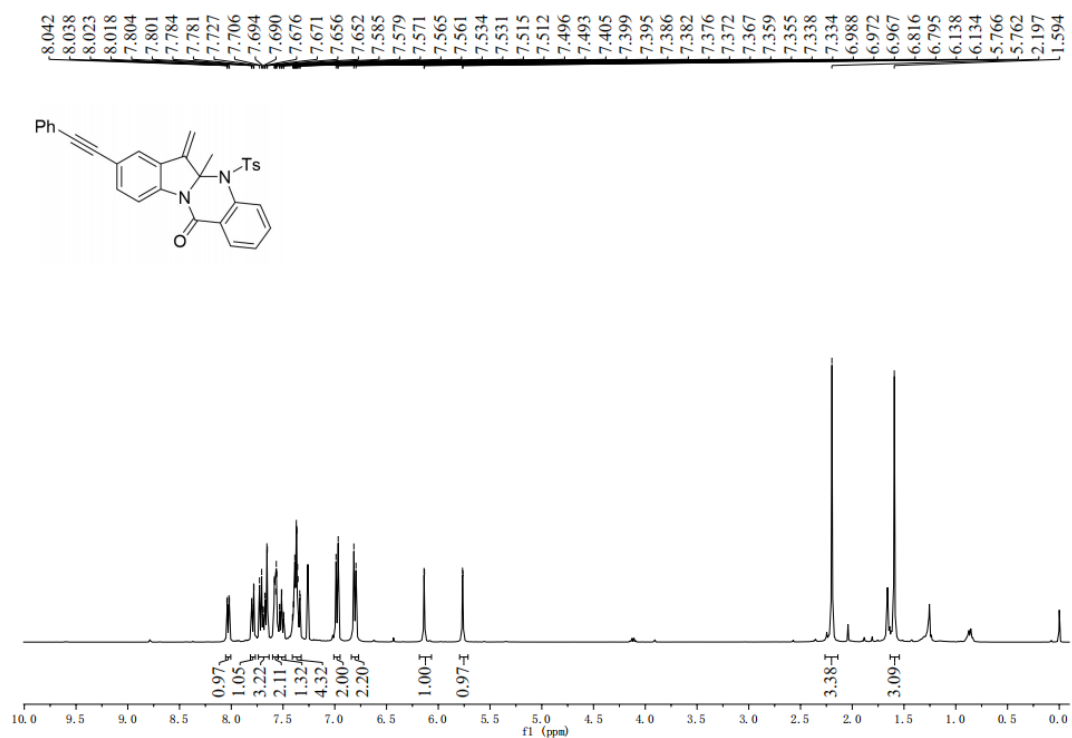
$^{13}\text{C NMR}$  spectrum of compound **5c**



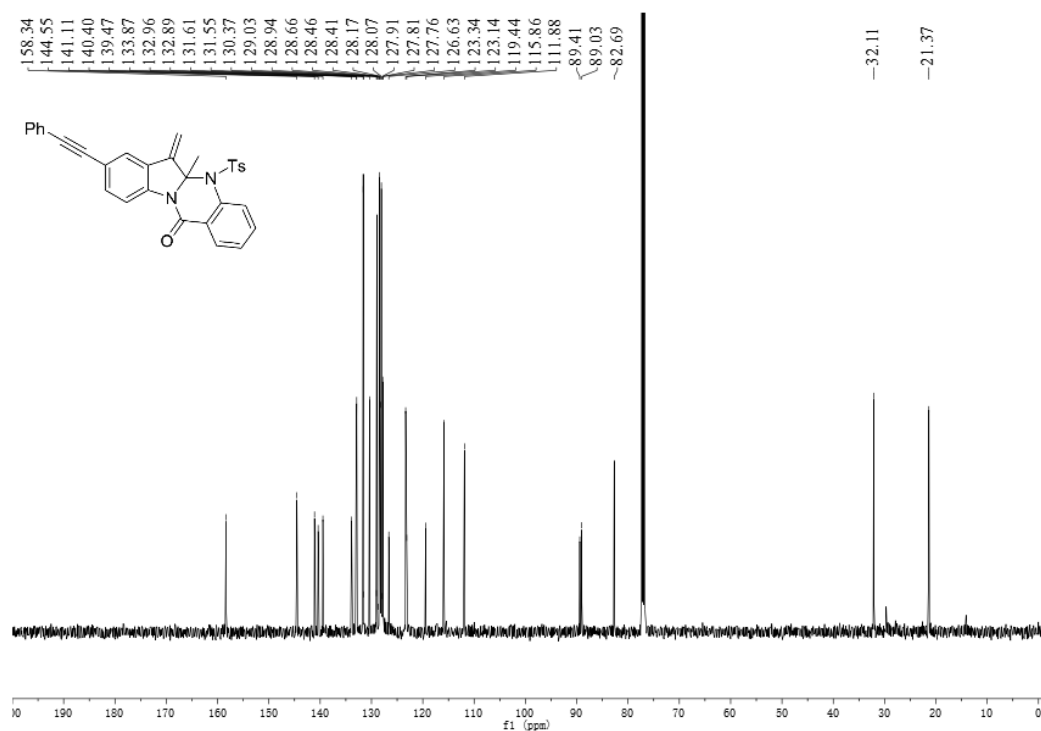
<sup>1</sup>H NMR spectrum of compound 7



<sup>13</sup>C NMR spectrum of compound 7

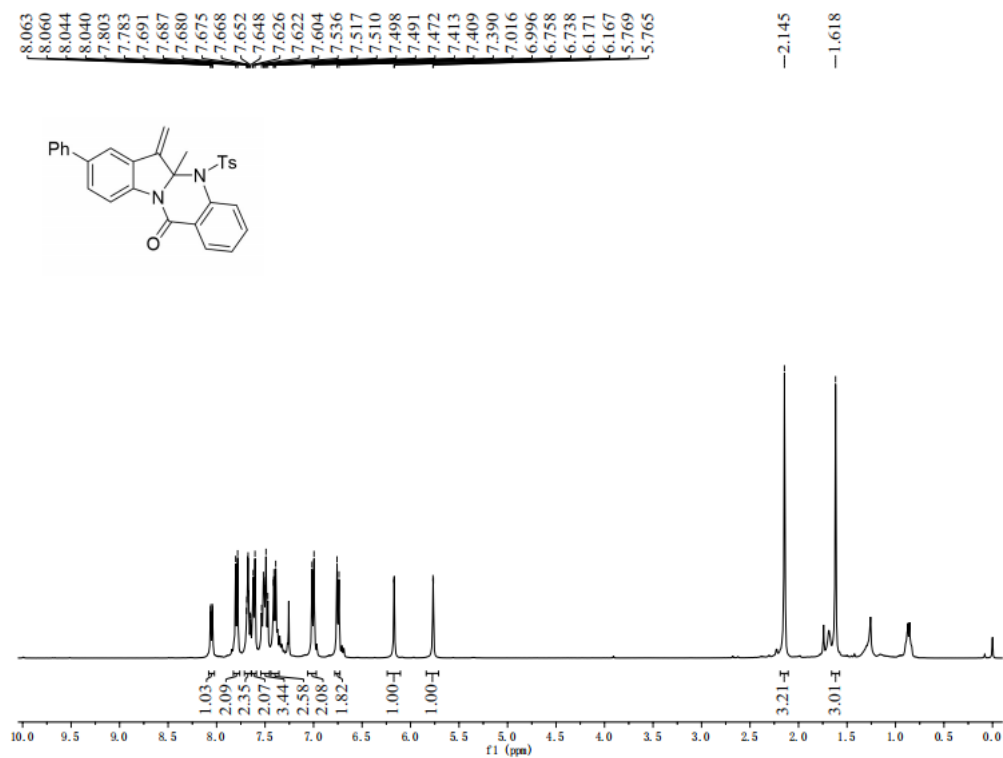


$^1\text{H}$  NMR spectrum of compound **8**

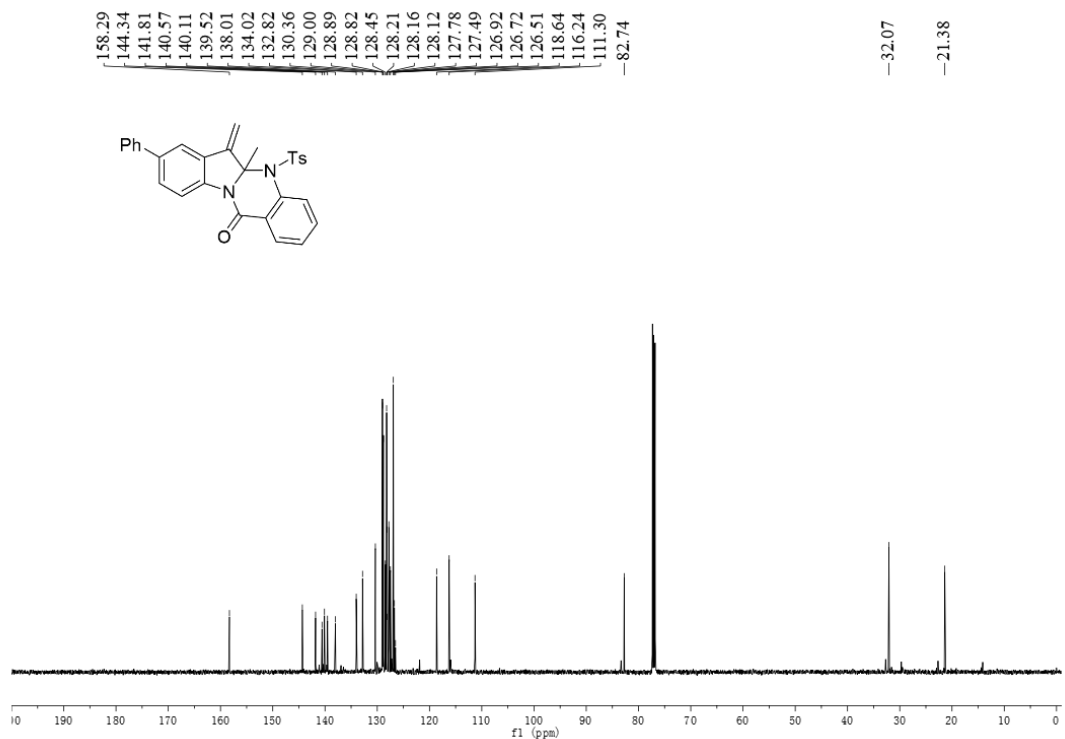


$^{13}\text{C}$  NMR spectrum of compound **8**





$^1\text{H}$  NMR spectrum of compound 9



$^{13}\text{C}$  NMR spectrum of compound 9