# Total Synthesis of Tetracyclic Spirooxindole Alkaloids via a Double Oxidative Rearrangement/Cyclization Cascade

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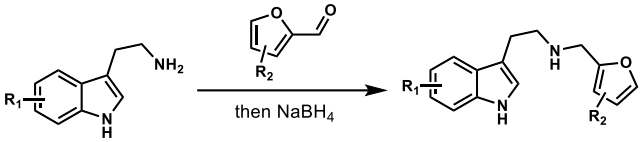
## General Information

All reactions were carried out under an atmosphere of argon in flame-dried glassware with magnetic stirring unless otherwise indicated. Reactions were monitored by UPLC/MS, and thin layer chromatography (TLC) and visualization was accomplished with a 254 nm UV light and by staining with $KMnO_4$ solution with heating. All Flash silica gel column chromatography was performed using silica gel with particle size of 300-400 mesh. $^1H$ and $^{13}C$ NMR spectra were recorded on Varian Inova-400 spectrometers. Data for $^1H$ NMR spectra are reported relative to $CDCl_3$ (7.26 ppm), $CD_3OD$ (3.31 ppm), or DMSO-$d_6$ (2.50 ppm) as an internal standard and are reported as follows: chemical shift ($\delta$ ppm), multiplicity (*s* = singlet, *d* = doublet, *t* = triplet, *q* = quartet, *sept* = septet, *m* = multiplet, *br* = broad), coupling constant *J* (Hz), and integration. Data for $^{13}C$ NMR spectra are reported relative to $CDCl_3$ (77.16 ppm), $CD_3OD$ (49.00 ppm), DMSO-$d_6$ (39.52 ppm) as an internal standard and are reported in terms of chemical shift ($\delta$ ppm). All $^{13}C$ NMR spectra were recorded with complete proton decoupling. UPLC-MS analyses were performed on a Waters system (Column: BEH C18, 1.7 µm, 2.1*50 mm) with a Photodiode Array (PDA) detector and a Single Quadrupole (SQ) detector. High Resolution Mass spectra were obtained from on an Agilent 1290 LC-6540 QTOF Mass Spectrometer or an Agilent Technologies 7250 GCQTOF.

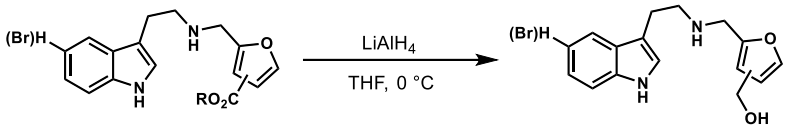
## General Procedure for the Synthesis of Substrates

**General Procedure A**: Synthesis of rearrangement substrates



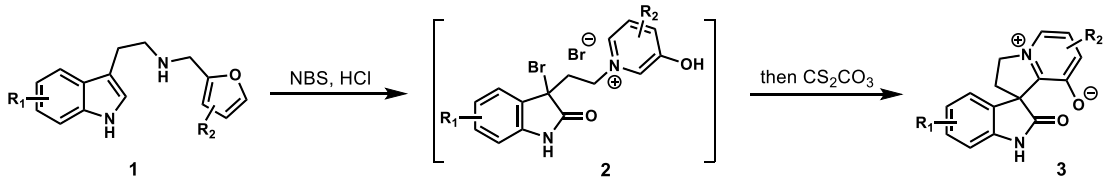

To a stirred solution of tryptamine derivatives (2.0 mmol, 1.0 equiv.) in MeOH (20 mL) was added furfural derivatives (2.0 mmol, 1.0 equiv.) in one portion. The reaction was stirred at rt for 1 hour. Then $NaBH_4$ (2.0 mmol, 1.0 equiv.) was added in portions at rt and monitored by TLC analysis. After completion, the reaction was quenched by addition of $H_2O$ (30 mL) and then transferred to a separatory funnel. The mixture was extracted with DCM (3×15 mL) and the organic phase was collected. The combined organic layers were washed with brine (20 mL), dried over $Na_2SO_4$ and concentrated in vacuo. The crude product was purified by column chromatography on silica gel (DCM/MeOH=60/1 to 10/1) to give the product.

**General Procedure B**: Synthesis of rearrangement substrates




To a stirred solution of starting material (0.2 mmol, 1.0 equiv.) in THF (5 mL) was added $LiAlH_4$ (7.6 mg, 0.2 mmol, 1.0 equiv.) in portions at 0 °C. The resulting mixture was stirred at 0 °C for 1 hour. After completion, the reaction was quenched by addition of $Na_2SO_4 \cdot 10H_2O$ in portions. The resulting suspension was filtrated through a pad of celite and the filtrate was concentrated in vacuo. The crude product was purified by column chromatography on silica gel (DCM/MeOH=50/1 to 10/1) to give the product

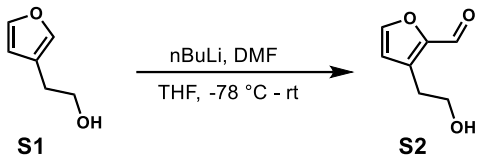
**General Procedure C**: Synthesis of the pyridinium products




To a stirred solution of starting material (0.2 mmol, 1.0 equiv.) in THF (2 mL) was added HCl (0.8 mL of 2.5 M solution in $H_2O$, 2.0 mmol, 10.0 equiv.) in one portion at rt. Then the reaction mixture was cooled to 0 °C and NBS (110 mg, 0.62 mmol, 3.1 equiv.) in THF (2.0 mL) was added dropwise to the reaction. The resulting mixture was stirred at 0 °C for 0.5-3 hours (depends on the complete transformation from **1** to **2**) before the reaction mixture was added dropwise to the solution of $Cs_2CO_3$ (969 mg, 3.0 mmol, 15.0 equiv.) in $H_2O$ (60 mL) at rt. After addition, the resulting mixture was concentrated in vacuo. The crude product was purified by column chromatography on silica gel (DCM/MeOH=30/1 to 7/1, with 0.1% $NH_3 \cdot H_2O$) to give the product.

## Spectral Data of Substrates

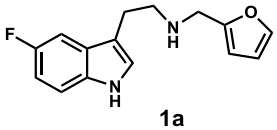
Procedure for the synthesis of **S2** (starting material of **1n**)




To a stirred solution of **S1**[1] (3.8 g, 33.9 mmol, 1.0 equiv.) in THF (70 mL) was added nBuLi (28.5 mL of 2.5 M solution in hexane, 71.2 mmol, 2.1 equiv.) dropwise to the reaction in 30 min at -78 °C. The resulting mixture was stirred at -78 °C for 30 min and stirred at 0 °C for another 30 min. DMF (8.0 mL, 101.7 mmol, 3.0 equiv.) was added dropwise to the reaction in 5 min. The resulting mixture was moved to rt and stirred for 2 hours. After completion, the reaction was quenched by addition of $H_2O$ (10 mL) and then transferred to a separatory funnel. The organic phase was separated. The aqueous phase was concentrated in vacuo and the residue was washed with EA (10 mL×2). The organic phase was combined, dried over $Na_2SO_4$, and concentrated in vacuo. The crude product was purified by column chromatography on silica gel (PE/EA=2/1 to 1/1) to give **S2** as a yellow oil (2.45g, 52% yield). **S2** was subsequently used for the synthesis of **1n**.

**$^1$H NMR (400 MHz, DMSO-*d*$_6$)** δ 9.69 (d, J = 0.7 Hz, 1H), 7.96 (d, J = 1.7 Hz, 1H), 6.71 (d, J = 1.7 Hz, 1H), 4.78 (t, J = 5.3 Hz, 1H), 3.61 (td, J = 6.5, 5.3 Hz, 2H), 2.90 (t, J = 6.5 Hz, 2H).

**$^{13}$C NMR (100 MHz, DMSO-*d*$_6$)** δ 177.95, 148.63, 148.19, 136.74, 114.77, 60.42, 27.88.



**1a**

**2-(5-fluoro-1*H*-indol-3-yl)-*N*-(furan-2-ylmethyl)ethan-1-amine**

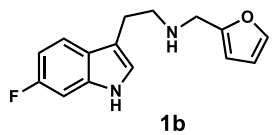
Prepared according to General Procedure A, isolated as a yellow solid (95% yield).

**$^1$H NMR (400 MHz, $CDCl_3$)** *δ* 8.10 (s, *J* = 92.6 Hz, 1H), 7.33 (dd, *J* = 1.9, 0.9 Hz, 1H), 7.25 – 7.20 (m, 1H), 7.15 – 7.03 (m, 1H), 6.99 – 6.88 (m, 1H), 6.29 (dd, *J* = 3.1, 1.8 Hz, 1H), 6.14 (dq, *J* = 3.1, 0.7 Hz, 1H), 3.81 (d, *J* = 1.6 Hz, 2H), 3.03 – 2.81 (m, 4H).

**$^{13}$C NMR (100 MHz, $CDCl_3$)** *δ* 158.82, 156.49, 153.70, 141.87 (d, *J* = 3.4 Hz), 132.97, 127.74 (d, *J* = 9.5 Hz), 124.02, 113.68 (d, *J* = 4.7 Hz), 111.84 (d, *J* = 9.8 Hz), 111.40 – 109.46 (m), 107.09, 103.73 (d, *J* = 23.2 Hz), 48.92, 46.17, 25.69.

**$^{19}$F NMR (376 MHz, $CDCl_3$)** *δ* -124.84 – -124.94 (m).

**HRMS (ESI, m/z):** calc'd for $C_{15}H_{15}FN_2O$ $[M+H]^+$ 259.1246, found: 259.1236.



**1b**

**2-(6-fluoro-1*H*-indol-3-yl)-*N*-(furan-2-ylmethyl)ethan-1-amine**

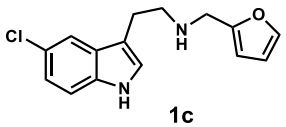
Prepared according to General Procedure A, isolated as a brown solid (85% yield).

**$^1$H NMR (400 MHz, $CDCl_3$)** *δ* 8.20 (d, *J* = 21.1 Hz, 1H), 7.49 (dd, *J* = 8.7, 5.3 Hz, 1H), 7.33 (dt, *J* = 1.7, 0.8 Hz, 1H), 7.14 – 6.92 (m, 3H), 6.87 (tdd, *J* = 9.4, 2.3, 0.8 Hz, 1H), 6.29 (dd, *J* = 3.2, 1.8 Hz, 1H), 6.14 (ddt, *J* = 3.1, 1.5, 0.8 Hz, 1H), 3.80 (d, *J* = 2.1 Hz, 3H), 2.96 (d, *J* = 1.9 Hz, 5H).

**$^{13}$C NMR (100 MHz, $CDCl_3$)** *δ* 161.06, 158.71, 153.47, 141.84, 136.34 (d, *J* = 12.5 Hz), 123.97 (d, *J* = 2.9 Hz), 122.49 (d, *J* = 3.6 Hz), 120.78 – 116.50 (m), 113.30, 110.15, 109.01 – 103.34 (m), 98.54 – 94.90 (m), 48.94, 45.99, 25.53.

**$^{19}$F NMR (376 MHz, $CDCl_3$)** δ -121.39 (dtd, *J* = 18.8, 9.7, 5.4 Hz).

**HRMS (ESI, m/z):** calc'd for $C_{15}H_{15}FN_2O$ $[M+H]^+$ 259.1246, found: 259.1236.



**1c**

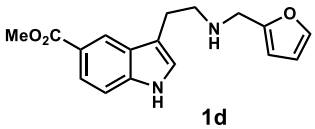
**2-(5-chloro-1H-indol-3-yl)-N-(furan-2-ylmethyl)ethan-1-amine**

Prepared according to General Procedure A, isolated as a yellow solid (78% yield).

**$^1$H NMR (400 MHz, $CDCl_3$)** δ 8.61 (s, 1H), 7.55 (d, J = 2.0 Hz, 1H), 7.34 (d, J = 1.8 Hz, 1H), 7.20 (d, J = 8.6 Hz, 1H), 7.12 (dd, J = 8.6, 2.0 Hz, 1H), 6.97 (d, J = 2.4 Hz, 1H), 6.30 (dd, J = 3.2, 1.8 Hz, 1H), 6.16 (d, J = 3.1 Hz, 1H), 3.82 (s, 2H), 2.98 – 2.91 (m, 4H).

**$^{13}$C NMR (100 MHz, $CDCl_3$)** δ 153.64, 141.87, 134.75, 128.48, 124.90, 123.57, 122.19, 118.35, 113.36, 112.21, 110.16, 107.07, 77.42, 77.10, 76.78, 48.91, 46.10, 25.55.

**HRMS (ESI, m/z):** calc'd for $C_{15}H_{15}ClN_2O$ $[M+H]^+$ 275.0951, found: 275.0938.



**1d**

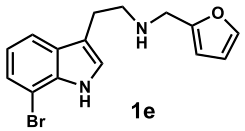
**methyl 3-(2-((furan-2-ylmethyl)amino)ethyl)-1H-indole-5-carboxylate**

Prepared according to General Procedure A, isolated as a yellow solid (92% yield).

**$^1$H NMR (400 MHz, $CDCl_3$)** δ 8.74 (s, 1H), 8.37 (dt, J = 1.5, 0.7 Hz, 1H), 7.88 (dd, J = 8.6, 1.6 Hz, 1H), 7.36 – 7.29 (m, 2H), 7.07 – 7.02 (m, 1H), 6.28 (dd, J = 3.2, 1.8 Hz, 1H), 6.15 (dq, J = 3.2, 0.8 Hz, 1H), 3.93 (s, 3H), 3.81 (d, J = 0.7 Hz, 2H), 3.02 – 2.96 (m, 4H).

**$^{13}$C NMR (100 MHz, $CDCl_3$)** δ 168.43, 153.45, 141.88, 139.11, 127.01, 123.60, 123.23, 121.85, 121.04, 114.88, 110.98, 110.14, 107.14, 51.90, 49.04, 46.01, 25.46.

**HRMS (ESI, m/z):** calc'd for $C_{17}H_{18}N_2O_3$ $[M+H]^+$ 299.1395, found: 299.1385.



**1e**

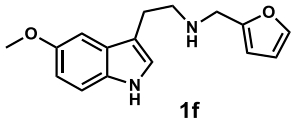
**2-(7-bromo-1*H*-indol-3-yl)-*N*-(furan-2-ylmethyl)ethan-1-amine**

Prepared according to General Procedure A, isolated as a yellow oil (91% yield).

**$^1$H NMR (400 MHz, $CDCl_3$)** *δ* 8.35 (s, 1H), 7.53 (dd, *J* = 7.9, 0.9 Hz, 1H), 7.43 – 7.31 (m, 2H), 7.07 (d, *J* = 2.3 Hz, 1H), 6.99 (t, *J* = 7.8 Hz, 1H), 6.29 (dd, *J* = 3.2, 1.9 Hz, 1H), 6.22 – 5.88 (m, 1H), 3.80 (d, *J* = 0.6 Hz, 2H), 2.96 (s, 4H).

**$^{13}$C NMR (100 MHz, $CDCl_3$)** *δ* 153.74, 141.92, 135.14, 128.73, 124.43, 122.71, 120.54, 118.23, 115.17, 110.20, 107.10, 104.90, 49.06, 46.21, 25.90.

**HRMS (ESI, m/z):** calc'd for $C_{15}H_{15}BrN_2O$ $[M+H]^+$ 319.0446, found: 319.0433.



**1f**

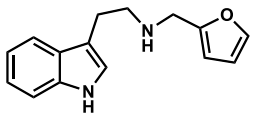
***N*-(furan-2-ylmethyl)-2-(5-methoxy-1*H*-indol-3-yl)ethan-1-amine**

Prepared according to General Procedure A, isolated as a brown solid (89% yield).

**$^1$H NMR (400 MHz, $CDCl_3$)** δ 7.96 (d, J = 52.6 Hz, 1H), 7.33 (dd, J = 1.8, 0.9 Hz, 1H), 7.26 – 7.17 (m, 1H), 7.04 (d, J = 2.4 Hz, 1H), 6.99 (t, J = 2.4 Hz, 1H), 6.86 (dd, J = 8.8, 2.4 Hz, 1H), 6.29 (dd, J = 3.1, 1.8 Hz, 1H), 6.14 (dd, J = 3.1, 0.8 Hz, 1H), 3.85 (s, 3H), 3.81 (d, J = 0.8 Hz, 2H), 2.96 (d, J = 1.5 Hz, 4H).

**$^{13}$C NMR (100 MHz, $CDCl_3$)** δ 153.83, 153.80, 141.81, 131.58, 127.77, 122.97, 113.29, 112.19, 111.97, 110.13, 106.97, 100.59, 55.93, 49.11, 46.18, 25.72.

**HRMS (ESI, m/z):** calc'd for $C_{16}H_{18}N_2O_2$ $[M+H]^+$ 271.1446, found: 271.1434.



**1g**

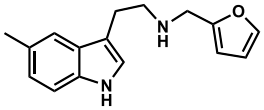
**N-(furan-2-ylmethyl)-2-(1H-indol-3-yl)ethan-1-amine**

Prepared according to General Procedure A, isolated as a brown solid (95% yield).

**$^1$H NMR (400 MHz, $CDCl_3$)** δ 8.33 (s, 1H), 7.63 (dd, J = 7.8, 1.2 Hz, 1H), 7.37 – 7.32 (m, 2H), 7.21 (ddd, J = 8.2, 6.9, 1.2 Hz, 1H), 7.14 (ddd, J = 8.0, 7.0, 1.1 Hz, 1H), 6.99 (d, J = 2.2 Hz, 1H), 6.31 (dd, J = 3.2, 1.8 Hz, 1H), 6.18 – 6.13 (m, 1H), 3.82 (s, 2H), 3.01 (d, J = 2.3 Hz, 4H).

**$^{13}$C NMR (100 MHz, $CDCl_3$)** δ 153.38, 141.62, 136.25, 127.15, 122.13, 121.60, 118.89, 117.68, 113.45, 111.12, 109.96, 106.38, 48.87, 45.82, 25.37.

**HRMS (ESI, m/z):** calc'd for $C_{15}H_{16}N_2O$ $[M+H]^+$ 241.1341, found: 241.1329.



**1h**

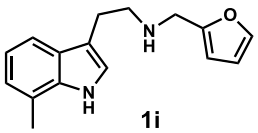
**N-(furan-2-ylmethyl)-2-(5-methyl-1H-indol-3-yl)ethan-1-amine**

Prepared according to General Procedure A, isolated as a yellow oil (85% yield).

**$^1$H NMR (400 MHz, $CDCl_3$)** δ 8.21 (s, 1H), 7.41 (s, 1H), 7.37 – 7.34 (m, 1H), 7.24 (d, J = 8.3 Hz, 1H), 7.04 (dd, J = 8.2, 1.6 Hz, 1H), 6.96 (d, J = 2.3 Hz, 1H), 6.31 (dd, J = 3.2, 1.8 Hz, 1H), 6.17 (d, J = 3.1 Hz, 1H), 3.83 (s, 2H), 2.99 (s, 4H), 2.48 (s, 3H).

**$^{13}$C NMR (100 MHz, $CDCl_3$)** δ 153.73, 141.82, 134.74, 128.97, 127.62, 124.17, 122.30, 118.54, 113.06, 110.88, 110.12, 107.01, 51.49, 46.14, 26.95, 21.56.

**HRMS (ESI, m/z):** calc'd for $C_{16}H_{18}N_2O$ $[M+H]^+$ 255.1497, found: 255.1485



**1i**

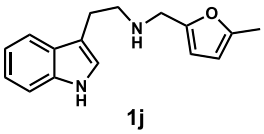
**N-(furan-2-ylmethyl)-2-(7-methyl-1H-indol-3-yl)ethan-1-amine**

Prepared according to General Procedure A, isolated as a brown oil (59% yield).

**$^1$H NMR (400 MHz, $CDCl_3$)** δ 8.05 – 7.98 (m, 1H), 7.46 (d, J = 7.7 Hz, 1H), 7.34 (dd, J = 1.9, 0.8 Hz, 1H), 7.09 – 6.99 (m, 3H), 6.29 (dd, J = 3.2, 1.9 Hz, 1H), 6.18 (d, J = 3.2 Hz, 1H), 3.82 (s, 2H), 3.05 – 2.96 (m, 4H), 2.48 (s, 3H).

**$^{13}$C NMR (100 MHz, $CDCl_3$)** δ 153.28, 142.36, 136.34, 127.22, 122.92, 122.28, 120.78, 119.90, 116.93, 114.23, 110.56, 107.90, 49.26, 46.22, 25.83, 17.01.

**HRMS (ESI, m/z):** calc'd for $C_{16}H_{18}N_2O$ $[M+H]^+$ 255.1497, found: 255.1484



**1j**

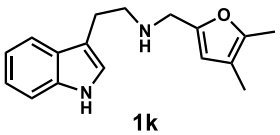
**2-(1*H*-indol-3-yl)-*N*-((5-methylfuran-2-yl)methyl)ethan-1-amine**

Prepared according to General Procedure A, isolated as a brown solid (93% yield).

**$^1$H NMR (400 MHz, $CDCl_3$)** *δ* 8.28 (s, 0H), 8.20 (s, 1H), 7.66 – 7.59 (m, 1H), 7.35 (dq, *J* = 8.1, 1.0 Hz, 1H), 7.20 (ddt, *J* = 8.2, 7.0, 1.3 Hz, 1H), 7.12 (ddt, *J* = 7.9, 7.0, 1.4 Hz, 1H), 7.01 (q, *J* = 2.3 Hz, 1H), 6.02 (t, *J* = 2.7 Hz, 1H), 5.87 (td, *J* = 2.7, 1.2 Hz, 1H), 3.76 (d, *J* = 2.3 Hz, 2H), 3.06 – 2.94 (m, 4H), 2.25 (d, *J* = 1.1 Hz, 3H).

**$^{13}$C NMR (100 MHz, $CDCl_3$)** *δ* 152.22, 151.80, 136.78, 127.73, 122.54, 122.21, 119.46, 119.19, 113.85, 111.58, 108.14, 106.26, 49.44, 46.61, 26.02, 13.94.

**HRMS (ESI, m/z):** calc'd for $C_{16}H_{18}N_2O$ $[M+H]^+$ 255.1497, found: 255.1485



**1k**

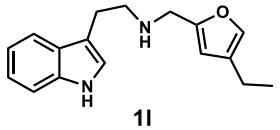
***N*-((4,5-dimethylfuran-2-yl)methyl)-2-(1*H*-indol-3-yl)ethan-1-amine**

Prepared according to General Procedure A, isolated as a brown solid (86% yield).

**$^1$H NMR (400 MHz, $CDCl_3$)** *δ* 8.33 (d, *J* = 94.3 Hz, 1H), 7.63 (dd, *J* = 7.9, 3.8 Hz, 1H), 7.39 – 7.28 (m, 1H), 7.21 (tdd, *J* = 8.2, 4.2, 1.8 Hz, 1H), 7.16 – 7.08 (m, 1H), 6.99 (dd, *J* = 6.5, 2.6 Hz, 1H), 5.92 (d, *J* = 5.0 Hz, 1H), 3.72 (d, *J* = 6.1 Hz, 2H), 3.00 (dt, *J* = 6.2, 2.7 Hz, 4H), 2.16 (d, *J* = 3.7 Hz, 3H), 1.90 (d, *J* = 4.8 Hz, 3H).

**$^{13}$C NMR (100 MHz, $CDCl_3$)** *δ* 150.58, 146.58, 136.46, 127.40, 122.24, 121.83, 119.08, 118.86, 114.26, 113.49, 111.27, 110.35, 49.11, 46.24, 25.72, 11.36, 9.89.

**HRMS (ESI, m/z):** calc'd for $C_{17}H_{20}N_2O$ $[M+H]^+$ 269.1654, found:269.1641



**1l**

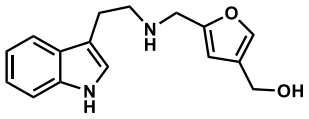
***N*-((4-ethylfuran-2-yl)methyl)-2-(1*H*-indol-3-yl)ethan-1-amine**

Prepared according to General Procedure A, isolated as a light yellow solid (86% yield).

**$^1$H NMR (400 MHz, $CDCl_3$)** *δ* 8.03 (s, 1H), 7.61 (dd, J = 7.8, 0.8 Hz, 1H), 7.36 (dt, J = 8.2, 0.8 Hz, 1H), 7.19 (ddd, J = 8.2, 7.1, 1.2 Hz, 1H), 7.11 (ddd, J = 8.7, 4.6, 1.1 Hz, 2H), 7.03 (d, J = 2.3 Hz, 1H), 6.03 (s, 1H), 3.76 – 3.73 (m, 2H), 3.49 (s, 1H), 2.99 (dd, J = 4.3, 1.7 Hz, 4H), 2.38 (q, J = 7.5, 1.1 Hz, 2H), 1.14 (t, J = 7.5 Hz, 3H).

**$^{13}$C NMR (100 MHz, $CDCl_3$)** *δ* 153.68, 137.39, 136.43, 127.58, 127.39, 122.13, 121.92, 119.17, 118.85, 113.56, 111.20, 108.31, 49.08, 46.27, 25.63, 18.23, 14.28.

**HRMS (ESI, m/z):** calc'd for $C_{17}H_{20}N_2O$ $[M+H]^+$ 269.1654, found:269.1642



**1m**

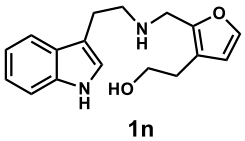
**(5-(((2-(1H-indol-3-yl)ethyl)amino)methyl)furan-3-yl)methanol**

Prepared according to General Procedure B, isolated as a yellow oil (87% yield).

**$^1$H NMR (400 MHz, $CD_3OD$)** δ 7.51 (dt, J = 7.8, 1.0 Hz, 1H), 7.36 (t, J = 1.1 Hz, 1H), 7.32 (dt, J = 8.2, 1.0 Hz, 1H), 7.08 (ddd, J = 8.2, 7.0, 1.2 Hz, 1H), 7.03 (s, 1H), 6.98 (ddd, J = 8.0, 6.9, 1.1 Hz, 1H), 6.27 (d, J = 1.0 Hz, 1H), 4.40 (d, J = 0.9 Hz, 2H), 3.76 (s, 2H), 3.01 – 2.85 (m, 4H).

**$^{13}$C NMR (100 MHz, $CD_3OD$)** δ 154.03, 140.65, 138.21, 128.54, 127.67, 123.49, 122.41, 119.64, 119.22, 112.90, 112.29, 109.54, 56.57, 56.32, 49.87, 46.11, 25.68.

**HRMS (ESI, m/z):** calc'd for $C_{16}H_{18}N_2O_2$ $[M+H]^+$ 271.1446, found: 271.1437



**1n**

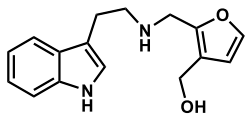
**2-(2-(((2-(1H-indol-3-yl)ethyl)amino)methyl)furan-3-yl)ethan-1-ol**

Prepared according to General Procedure A, isolated as a yellow oil (81% yield).

**$^1$H NMR (400 MHz, $CD_3OD$)** δ 7.57 – 7.52 (m, 2H), 7.37 (dd, J = 8.1, 1.0 Hz, 1H), 7.16 (d, J = 1.1 Hz, 1H), 7.12 (ddd, J = 8.2, 7.0, 1.2 Hz, 1H), 7.04 (ddd, J = 8.0, 7.0, 1.1 Hz, 1H), 6.43 (d, J = 1.8 Hz, 1H), 4.22 (s, 2H), 3.69 (t, J = 6.0 Hz, 2H), 3.30 – 3.24 (m, 2H), 3.17 – 3.10 (m, 2H), 2.67 (t, J = 5.9 Hz, 2H).

**$^{13}$C NMR (100 MHz, $CD_3OD$)** δ 144.67, 144.41, 138.17, 128.12, 124.42, 124.09, 122.63, 119.94, 118.45, 113.39, 112.49, 110.62, 62.42, 48.65, 43.38, 28.74, 23.79.

**HRMS (ESI, m/z):** calc'd for $C_{17}H_{20}N_2O_2$ $[M+H]^+$ 285.1603, found:285.1591



**1o**

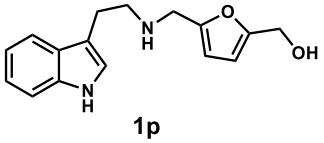
**(2-(((2-(1H-indol-3-yl)ethyl)amino)methyl)furan-3-yl)methanol**

Prepared according to General Procedure B, isolated as a yellow oil (91% yield).

**$^1$H NMR (400 MHz, $CDCl_3$)** δ 8.29 (s, 1H), 7.60 (d, J = 7.9 Hz, 1H), 7.34 (t, J = 6.6 Hz, 1H), 7.25 – 7.17 (m, 2H), 7.15 – 7.08 (m, 1H), 6.99 (d, J = 2.0 Hz, 1H), 6.27 (d, J = 1.6 Hz, 1H), 4.53 (s, 2H), 3.83 (s, 2H), 3.01 – 2.92 (m, 4H).

**$^{13}$C NMR (100 MHz, $CDCl_3$)** δ 149.92, 140.35, 136.43, 127.18, 122.32, 122.07, 119.33, 118.70, 112.96, 111.27, 111.13, 77.36, 77.04, 76.73, 57.01, 48.79, 45.38, 25.30.

**HRMS (ESI, m/z):** calc'd for $C_{16}H_{18}N_2O_2$ $[M+H]^+$ 271.1446, found:271.1434



**1p**

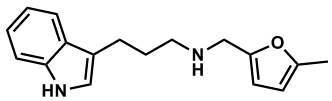
**(5-(((2-(1H-indol-3-yl)ethyl)amino)methyl)furan-2-yl)methanol**

Prepared according to General Procedure A, isolated as a yellow oil (92% yield).

**$^1$H NMR (400 MHz, $CDCl_3$)** δ 8.08 (s, 1H), 7.59 (dd, J = 7.9, 1.0 Hz, 1H), 7.36 (dd, J = 8.1, 0.9 Hz, 1H), 7.19 (ddd, J = 8.2, 7.1, 1.2 Hz, 1H), 7.10 (ddd, J = 8.0, 7.0, 1.1 Hz, 1H), 7.00 (d, J = 2.2 Hz, 1H), 6.17 (d, J = 3.1 Hz, 1H), 6.08 (d, J = 3.1 Hz, 1H), 4.50 (s, 2H), 3.76 (s, 2H), 3.01 – 2.95 (m, 4H).

**$^{13}$C NMR (100 MHz, $CDCl_3$)** δ 154.12, 152.77, 136.52, 127.26, 122.61, 121.81, 121.79, 119.05, 118.70, 112.62, 111.44, 108.21, 108.12, 108.10, 56.72, 48.48, 45.74, 25.17.

**HRMS (ESI, m/z):** calc'd for $C_{16}H_{18}N_2O_2$ $[M+H]^+$ 271.1446, found:271.1434



**1q**

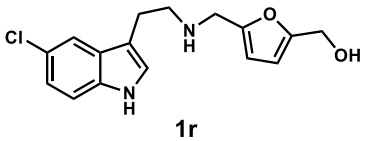
**3-(1*H*-indol-3-yl)-*N*-((5-methylfuran-2-yl)methyl)propan-1-amine**

Prepared according to General Procedure A, isolated as a yellow solid (75% yield).

**$^1$H NMR (400 MHz, $CDCl_3$)** *δ* 8.21 (s, *J* = 30.9 Hz, 1H), 7.61 (dd, *J* = 7.9, 1.2 Hz, 1H), 7.34 (dq, *J* = 8.1, 1.0 Hz, 1H), 7.19 (ddt, *J* = 8.1, 6.9, 1.1 Hz, 1H), 7.16 – 7.07 (m, 1H), 6.94 (td, *J* = 2.4, 1.2 Hz, 1H), 6.04 (t, *J* = 2.7 Hz, 1H), 5.89 (dp, *J* = 3.5, 1.1 Hz, 1H), 3.74 (d, *J* = 2.1 Hz, 2H), 2.85 – 2.78 (m, 2H), 2.74 (td, *J* = 7.2, 2.1 Hz, 2H), 2.28 (t, *J* = 1.3 Hz, 3H), 1.95 (pd, *J* = 7.4, 1.8 Hz, 4H).

**$^{13}$C NMR (100 MHz, $CDCl_3$)** *δ* 151.89, 151.54, 136.41, 127.52, 121.83, 121.36, 119.07, 118.92, 116.08, 111.20, 107.90, 106.01, 49.00, 46.34, 30.26, 22.94, 13.70.

**HRMS (ESI, m/z):** calc'd for $C_{17}H_{20}N_2O$ $[M+H]^+$ 269.1654, found: 269.1643



**1r**

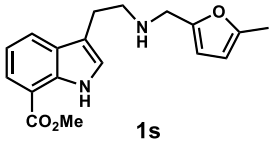
**(5-(((2-(5-chloro-1H-indol-3-yl)ethyl)amino)methyl)furan-2-yl)methanol**

Prepared according to General Procedure A, isolated as a yellow oil (94% yield).

**$^1$H NMR (400 MHz, $CDCl_3$)** δ 8.10 (s, 1H), 7.53 (dt, J = 2.0, 0.6 Hz, 1H), 7.13 (dd, J = 8.6, 2.0 Hz, 1H), 7.03 (d, J = 2.3 Hz, 1H), 6.19 (d, J = 3.1 Hz, 1H), 6.10 (d, J = 3.1 Hz, 1H), 4.52 (s, 2H), 3.78 (s, 2H), 2.94 (q, J = 1.3, 0.9 Hz, 4H).

**$^{13}$C NMR (100 MHz, $CDCl_3$)** δ 154.06, 152.55, 134.84, 128.28, 124.59, 124.05, 121.93, 118.05, 112.45, 112.26, 108.38, 108.22, 56.60, 48.20, 45.57, 24.94.

**HRMS (ESI, m/z):** calc'd for $C_{16}H_{17}ClN_2O_2$ $[M+H]^+$ 305.1057, found: 305.1042.




**1s**

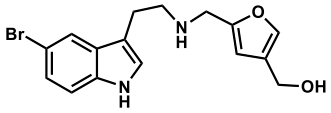
**methyl 3-(2-(((5-methylfuran-2-yl)methyl)amino)ethyl)-1H-indole-7-carboxylate**

Prepared according to General Procedure A, isolated as a yellow solid (72% yield).

**$^1$H NMR (400 MHz, $CDCl_3$)** $\delta$ 9.63 (s, 1H), 7.88 (dd, *J* = 7.5, 1.1 Hz, 1H), 7.82 (d, *J* = 7.8 Hz, 1H), 7.20 – 6.99 (m, 2H), 6.00 (d, *J* = 3.0 Hz, 1H), 5.91 – 5.79 (m, 1H), 3.98 (s, 3H), 3.74 (s, 2H), 2.98 (dq, *J* = 10.8, 5.8 Hz, 4H), 2.35 – 2.07 (m, 3H).

**$^{13}$C NMR (100 MHz, $CDCl_3$)** $\delta$ 167.56, 151.62, 151.10, 135.87, 128.41, 124.26, 124.01, 122.70, 118.17, 113.62, 112.09, 107.41, 105.56, 51.54, 48.85, 45.97, 25.24, 13.28.

**HRMS (ESI, m/z):** calc'd for $C_{18}H_{20}N_2O_3$ $[M+H]^+$ 313.1552, found: 313.1543.




**1t**

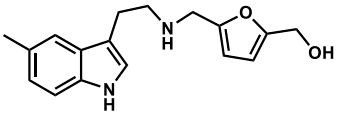
**(5-(((2-(5-bromo-1H-indol-3-yl)ethyl)amino)methyl)furan-3-yl)methanol**

Prepared according to General Procedure B, isolated as a light yellow oil (95% yield).

**$^1$H NMR (400 MHz, $CDCl_3$)** δ 8.75 – 8.69 (m, 1H), 7.66 (d, J = 1.8 Hz, 1H), 7.24 – 7.20 (m, 2H), 7.15 (d, J = 8.6 Hz, 1H), 6.89 (d, J = 2.2 Hz, 1H), 6.13 (s, 1H), 4.44 (s, 2H), 3.70 (s, 2H), 2.88 (s, 3H).

**$^{13}$C NMR (100 MHz, $CDCl_3$)** δ 154.21, 139.02, 135.04, 129.04, 126.03, 124.68, 123.58, 121.36, 112.88, 112.73, 112.38, 107.51, 56.33, 48.61, 45.94, 25.29.

**HRMS (ESI, m/z):** calc'd for $C_{16}H_{17}BrN_2O_2$ $[M+H]^+$ 349.0551, found: 349.0538.




**1u**

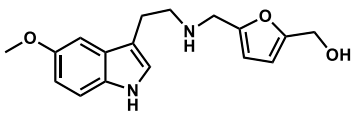
**(6-(((2-(5-methyl-1H-indol-3-yl)ethyl)amino)methyl)furan-2-yl)methanol.**

Prepared according to General Procedure A, isolated as a light yellow oil (95% yield).

**$^1$H NMR (400 MHz, $CDCl_3$)** δ 8.03 (s, 1H), 7.36 (s, 1H), 7.22 (t, *J* = 11.3 Hz, 1H), 7.01 (d, *J* = 8.3 Hz, 1H), 6.94 (t, *J* = 7.0 Hz, 1H), 6.16 (d, *J* = 3.0 Hz, 1H), 6.08 (d, *J* = 3.0 Hz, 1H), 4.50 (s, 2H), 3.73 (d, *J* = 20.3 Hz, 2H), 2.97 (d, *J* = 19.9 Hz, 4H), 2.47 (d, *J* = 19.7 Hz, 3H).

**$^{13}$C NMR (100 MHz, $CDCl_3$)** δ 153.48, 134.72, 128.41, 127.54, 123.56, 122.33, 118.46, 112.89, 110.84, 108.20, 107.90, 57.31, 48.74, 46.07, 25.43, 21.48.

**HRMS (ESI, m/z):** calc'd for $C_{17}H_{20}N_2O_2$ $[M+H]^+$ 285.1603, found: 285.1588.




**1v**

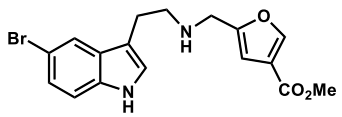
(**5-(((2-(5-methoxy-1H-indol-3-yl)ethyl)amino)methyl)furan-2-yl)methanol**

Prepared according to General Procedure A, isolated as a light yellow solid (95% yield).

**$^1$H NMR (400 MHz, $CDCl_3$)** δ 8.19 (s, 1H), 7.22 (dd, J = 8.8, 0.6 Hz, 1H), 7.00 (d, J = 2.4 Hz, 1H), 6.92 (d, J = 2.4 Hz, 1H), 6.84 (dd, J = 8.7, 2.4 Hz, 1H), 6.14 (d, J = 3.1 Hz, 1H), 6.07 (d, J = 3.1 Hz, 1H), 4.47 (d, J = 1.4 Hz, 2H), 3.83 (s, 3H), 3.73 (d, J = 1.7 Hz, 2H), 2.93 (d, J = 1.3 Hz, 4H).

**$^{13}$C NMR (100 MHz, $CDCl_3$)** δ 154.25, 153.62, 152.65, 131.79, 127.61, 123.51, 112.21, 111.89, 108.29, 108.08, 100.60, 56.63, 55.96, 48.35, 45.66, 25.15.

**HRMS (ESI, m/z):** calc'd for $C_{17}H_{20}N_2O_3$ $[M+H]^+$ 301.1552, found: 301.1538.




**1w**

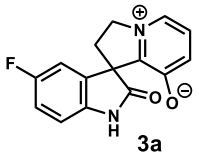
**methyl 5-(((2-(5-bromo-1H-indol-3-yl)ethyl)amino)methyl)furan-3-carboxylate**

Prepared according to General Procedure A, isolated as a brown oil (95% yield).

**$^{1}$H NMR (400 MHz, $CDCl_3$)** δ 8.08 (s, 1H), 7.89 (d, J = 0.8 Hz, 1H), 7.70 (dd, J = 1.8, 0.8 Hz, 1H), 7.23 (dd, J = 8.6, 0.5 Hz, 1H), 7.03 (d, J = 2.4 Hz, 1H), 6.49 (t, J = 0.7 Hz, 1H), 3.82 (s, 3H), 3.79 (s, 2H), 2.93 (s, 5H).

**$^{13}$C NMR (100 MHz, $CDCl_3$)** δ 163.85, 155.79, 147.21, 135.16, 129.10, 124.97, 123.78, 121.24, 119.54, 112.90, 112.68, 112.28, 107.06, 51.68, 48.81, 45.69, 26.08.

**HRMS (ESI, m/z):** calc'd for $C_{17}H_{17}BrN_2O_3$ $[M+H]^+$ 377.0501, found: 377.0484.




**3a**

**5-fluoro-2-oxo-2',3'-dihydrospiro[indoline-3,1'-indolizin]-4'-ium-8'-olate**

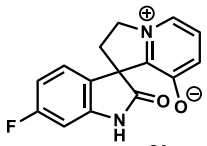
Prepared according to General Procedure C, isolated as a white solid (83% yield).

**$^{1}$H NMR (400 MHz, $CD_3OD$)** *δ* 7.99 – 7.84 (m, 1H), 7.54 (dd, *J* = 8.7, 5.7 Hz, 1H), 7.27 (dd, *J* = 8.7, 0.9 Hz, 1H), 7.13 – 6.99 (m, 2H), 6.94 (dd, *J* = 8.5, 4.3 Hz, 1H), 5.11 (dt, *J* = 12.9, 8.0 Hz, 1H), 4.99 (ddd, *J* = 13.3, 8.9, 5.3 Hz, 1H), 2.90 (ddd, *J* = 13.1, 8.9, 7.6 Hz, 1H), 2.66 (ddd, *J* = 13.5, 8.4, 5.3 Hz, 1H).

**$^{13}$C NMR (100 MHz, $CD_3OD$)** *δ* 178.93, 163.13 (d, J = 248.5 Hz), 159.52, 145.83, 139.58 (d, J = 2.3 Hz), 134.41, 133.22 (d, J = 8.3 Hz), 128.84, 125.38, 116.40 (d, J = 23.9 Hz), 112.18 (d, J = 25.4 Hz), 111.98, 60.11, 58.58, 35.21.

**$^{19}$F NMR (376 MHz, $CD_3OD$)** δ -122.42 – -122.54 (m).

**HRMS (ESI, m/z):** calc'd for $C_{15}H_{11}FN_2O_2$ $[M+H]^+$ 271.0883, found: 271.0875.




**3b**

**6-fluoro-2-oxo-2',3'-dihydrospiro[indoline-3,1'-indolizin]-4'-ium-8'-olate**

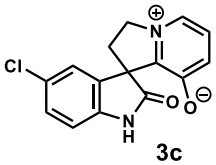
Prepared according to General Procedure C, isolated as a white solid (62% yield).

**$^{1}$H NMR (400 MHz, $CD_3OD$)** *δ* 7.76 (d, *J* = 5.6 Hz, 1H), 7.69 (s, 0H), 7.46 (dd, *J* = 8.7, 5.6 Hz, 1H), 7.24 – 7.03 (m, 2H), 6.83 – 6.59 (m, 2H), 5.07 (dt, *J* = 12.8, 8.2 Hz, 1H), 2.86 (ddd, *J* = 13.1, 9.0, 8.2 Hz, 1H), 2.58 (ddd, *J* = 13.1, 8.2, 4.8 Hz, 1H).

**$^{13}$C NMR (100 MHz, $CD_3OD$)** *δ* 179.51, 166.20, 164.84 (d, J = 243.7 Hz), 145.14 (d, J = 12.5 Hz), 134.79, 128.56, 127.61 (d, J = 3.1 Hz), 125.33 (d, J = 10.1 Hz), 123.32, 109.68 (d, J = 23.0 Hz), 99.60 (d, J = 27.7 Hz), 59.28, 58.38, 34.81.

**$^{19}$F NMR (376 MHz, $CD_3OD$)** *δ* -110.01 – -118.80 (m).

**HRMS (ESI, m/z):** calc'd for $C_{15}H_{11}FN_2O_2$ $[M+H]^+$ 271.0883, found: 271.0874.




**3c**

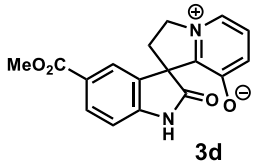
**5-chloro-2-oxo-2',3'-dihydrospiro[indoline-3,1'-indolizin]-4'-ium-8'-olate**

Prepared according to General Procedure C, isolated as a yellow solid (79% yield).

**$^1$H NMR (400 MHz, $CD_3OD$)** δ 7.92 (dt, J = 5.6, 0.8 Hz, 1H), 7.55 (dd, J = 8.7, 5.7 Hz, 1H), 7.28 (dd, J = 2.2, 0.5 Hz, 1H), 7.27 – 7.26 (m, 1H), 7.25 (d, J = 2.1 Hz, 1H), 6.94 (dd, J = 8.2, 0.6 Hz, 1H), 5.11 (dt, J = 13.0, 8.0 Hz, 1H), 4.99 (ddd, 1H), 2.89 (ddd, J = 13.2, 8.9, 7.6 Hz, 1H), 2.66 (ddd, J = 13.4, 8.4, 5.4 Hz, 2H).

**$^{13}$C NMR (100 MHz, $CD_3OD$)** δ 178.56, 163.87, 145.54, 142.30, 134.21, 133.45, 130.18, 128.95, 128.89, 125.84, 124.70, 112.48, 59.80, 58.65, 34.70.

**HRMS (ESI, m/z):** calc'd for $C_{15}H_{11}ClN_2O_2$ $[M+H]^+$ 287.0587, found: 287.0576.




**3d**

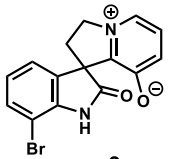
**5-(methoxycarbonyl)-2-oxo-2',3'-dihydrospiro[indoline-3,1'-indolizin]-4'-ium-8'-olate**

Prepared according to General Procedure C, isolated as a white solid (67% yield).

**$^1$H NMR (400 MHz, $CD_3OD$)** δ 8.00 (dd, J = 8.2, 1.7 Hz, 1H), 7.97 – 7.94 (m, 1H), 7.81 (dd, J = 1.7, 0.5 Hz, 1H), 7.56 (dd, J = 8.7, 5.7 Hz, 1H), 7.28 (dd, J = 8.7, 0.9 Hz, 1H), 7.05 (dd, J = 8.3, 0.5 Hz, 1H), 5.15 (dt, J = 13.0, 8.0 Hz, 1H), 5.03 (ddd, J = 13.0, 9.0, 5.4 Hz, 1H), 3.83 (s, 3H), 2.93 (ddd, J = 13.3, 9.0, 7.5 Hz, 1H), 2.70 (ddd, J = 13.5, 8.5, 5.4 Hz, 1H).

**$^{13}$C NMR (100 MHz, $CD_3OD$)** δ 179.29, 168.24, 166.10, 148.23, 146.22, 134.88, 132.66, 132.26, 128.71, 125.71, 125.29, 123.63, 111.00, 59.47, 58.52, 52.45, 34.65.

**HRMS (ESI, m/z):** calc'd for $C_{17}H_{14}N_2O_4$ $[M+H]^+$ 311.1032, found: 311.1019.




**3e**

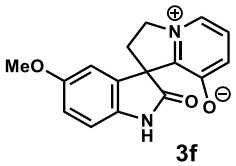
**7-bromo-8'-hydroxy-2-oxo-2',3'-dihydrospiro[indoline-3,1'-indolizin]-4'-ium**

Prepared according to General Procedure C, isolated as a white solid (58% yield).

**$^1$H NMR (400 MHz, $CD_3OD$)** *δ* 7.80 (d, *J* = 5.6 Hz, 1H), 7.48 (dd, *J* = 8.7, 5.6 Hz, 1H), 7.41 (dd, *J* = 8.1, 1.0 Hz, 1H), 7.18 (d, *J* = 8.7 Hz, 1H), 7.15 (s, 0H), 6.91 (dd, *J* = 8.2, 7.4 Hz, 1H), 5.08 (dt, *J* = 12.9, 8.1 Hz, 1H), 4.97 (ddd, *J* = 13.4, 9.1, 5.0 Hz, 1H), 2.89 (ddd, *J* = 13.2, 9.0, 8.0 Hz, 1H), 2.62 (ddd, *J* = 13.2, 8.2, 4.9 Hz, 1H).

**$^{13}$C NMR (100 MHz, $CD_3OD$)** *δ* 178.52, 165.72, 145.91, 143.07, 134.75, 133.45, 133.08, 128.69, 125.10, 123.87, 123.05, 104.01, 60.60, 58.48, 35.01.

**HRMS (ESI, m/z):** calc'd for $C_{15}H_{11}BrN_2O_2$ $[M+H]^+$ 331.0082, found: 331.0071.




**3f**

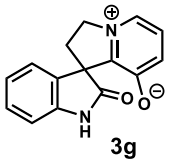
**5-methoxy-2-oxo-2',3'-dihydrospiro[indoline-3,1'-indolizin]-4'-ium-8'-olate**

Prepared according to General Procedure C, isolated as a yellow solid (73% yield).

**$^1$H NMR (400 MHz, $CD_3OD$)** δ 7.89 (dd, J = 5.7, 0.9 Hz, 1H), 7.52 (dd, J = 8.7, 5.6 Hz, 1H), 7.24 (dd, J = 8.7, 1.0 Hz, 1H), 6.91 – 6.80 (m, 3H), 5.18 – 5.06 (m, 1H), 4.97 (ddd, J = 17.1, 9.0, 4.5 Hz, 1H), 3.71 (s, 3H), 2.88 (ddd, J = 13.1, 9.0, 7.7 Hz, 1H), 2.63 (ddd, J = 13.3, 8.4, 5.2 Hz, 1H).

**$^{13}$C NMR (100 MHz, $CD_3OD$)** δ 178.95, 164.37, 157.76, 146.28, 136.62, 134.22, 132.93, 128.67, 125.21, 114.99, 111.80, 111.21, 60.27, 58.61, 56.24, 34.96.

**HRMS (ESI, m/z):** calc'd for $C_{16}H_{14}N_2O_3$ $[M+H]^+$ 283.1082, found: 283.1074.



**3g**

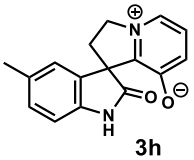
**2-oxo-2',3'-dihydrospiro[indoline-3,1'-indolizin]-4'-ium-8'-olate**

Prepared according to General Procedure C, isolated as a white solid (70% yield).

**$^1$H NMR (400 MHz, $CD_3OD$)** δ 7.78 (d, J = 5.6 Hz, 1H), 7.47 (dd, J = 8.7, 5.6 Hz, 1H), 7.25 (td, J = 7.7, 1.3 Hz, 1H), 7.21 – 7.10 (m, 2H), 7.06 – 6.91 (m, 2H), 5.09 (dt, J = 12.9, 8.2 Hz, 1H), 5.02 – 4.91 (m, 1H), 2.87 (dt, J = 13.1, 8.7 Hz, 1H), 2.59 (ddd, J = 12.9, 8.1, 4.6 Hz, 1H).

**$^{13}$C NMR (100 MHz, $CD_3OD$)** δ 179.21, 165.95, 143.45, 134.64, 132.00, 130.13, 128.52, 123.99, 123.82, 123.53, 111.35, 59.80, 58.49, 34.97.

**HRMS (ESI, m/z):** calc'd for $C_{15}H_{12}N_2O_2$ $[M+H]^+$ 253.0977, found: 253.0970.



**3h**

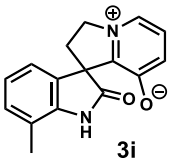
**5-methyl-2-oxo-2',3'-dihydrospiro[indoline-3,1'-indolizin]-4'-ium-8'-olate**

Prepared according to General Procedure C, isolated as a yellow solid (74% yield).

**$^1$H NMR (400 MHz, DMSO-*$d_6$*)** δ 10.73 (s, 1H), 7.96 (d, J = 5.6 Hz, 1H), 7.48 (dd, J = 8.7, 5.6 Hz, 1H), 7.08 – 6.96 (m, 3H), 6.77 (d, J = 7.8 Hz, 1H), 5.10 (dt, J = 13.1, 8.5 Hz, 1H), 4.93 (ddd, J = 13.1, 9.1, 3.8 Hz, 1H), 2.72 (dt, J = 12.9, 9.1 Hz, 1H), 2.49 – 2.42 (m, 1H), 2.19 (s, 3H).

**$^{13}$C NMR (100 MHz, DMSO-*$d_6$*)** δ 176.05, 160.58, 144.32, 139.89, 139.73, 130.82, 130.75, 130.47, 128.99, 127.25, 123.88, 109.37, 57.66, 57.23, 33.35, 20.62.

**HRMS (ESI, m/z):** calc'd for $C_{16}H_{14}N_2O_2$ $[M+H]^+$ 267.1133, found: 267.1123.



**3i**

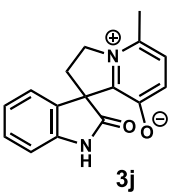
**7-methyl-2-oxo-2',3'-dihydrospiro[indoline-3,1'-indolizin]-4'-ium-8'-olate**

Prepared according to General Procedure C, isolated as a light yellow solid (42% yield).

**$^1$H NMR (400 MHz, $CD_3OD$)** δ 7.91 (d, J = 5.6 Hz, 1H), 7.51 (dd, / = 8.7, 5.6 Hz, 1H), 7.23 (dd, J = 8.7, 0.9 Hz, 1H), 7.08 (dt, J = 7.7, 1.1 Hz, 1H), 6.99 – 6.95 (m, 1H), 6.89 (t, J = 7.5 Hz, 1H), 5.11 (dt, J = 12.9, 8.2 Hz, 1H), 4.98 (ddd, J = 13.2, 9.1, 4.5 Hz, 1H), 2.89 (dt, J = 13.1, 8.7 Hz, 1H), 2.59 (ddd, J = 12.9, 8.2, 4.6 Hz, 1H), 2.30 (s, 3H).

**$^{13}$C NMR (100 MHz, $CD_3OD$)** δ 179.12, 163.65, 146.34, 141.86, 133.85, 131.58, 131.35, 128.63, 125.70, 123.86, 121.46, 121.20, 59.89, 58.66, 35.17, 16.85.

**HRMS (ESI, m/z):** calc'd for $C_{16}H_{14}N_2O_2$ $[M+H]^+$ 267.1133, found: 267.1124.



**3j**

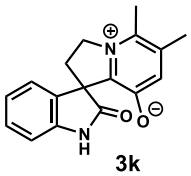
**5'-methyl-2-oxo-2',3'-dihydrospiro[indoline-3,1'-indolizin]-4'-ium-8'-olate**

Prepared according to General Procedure C, isolated as a white solid (88% yield).

**$^1$H NMR (400 MHz, $CD_3OD$)** *δ* 7.35 (d, *J* = 8.7 Hz, 1H), 7.25 (td, *J* = 7.7, 1.2 Hz, 1H), 7.21 – 7.13 (m, 2H), 7.04 – 6.92 (m, 2H), 4.96 (dt, *J* = 13.1, 8.4 Hz, 2H), 2.87 (ddd, *J* = 13.1, 9.2, 8.3 Hz, 1H), 2.67 – 2.53 (m, 4H).

**$^{13}$C NMR (100 MHz, $CD_3OD$)** *δ* 179.35, 162.70, 145.27, 143.33, 135.65, 135.54, 132.27, 130.08, 129.37, 123.99, 123.80, 111.29, 59.89, 56.27, 34.61, 18.20.

**HRMS (ESI, m/z):** calc'd for $C_{16}H_{14}N_2O_2$ $[M+H]^+$ 267.1133, found: 267.1125.



**3k**

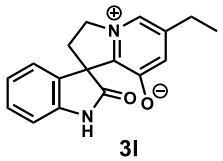
**5',6'-dimethyl-2-oxo-2',3'-dihydrospiro[indoline-3,1'-indolizin]-4'-ium-8'-olate**

Prepared according to General Procedure C, isolated as a white solid (80% yield).

**$^1$H NMR (400 MHz, $CD_3OD$)** *δ* 7.87 (d, *J* = 8.1 Hz, 1H), 7.48 (dd, *J* = 8.1, 3.6 Hz, 2H), 7.34 (d, *J* = 8.7 Hz, 1H), 7.09 (t, *J* = 7.7 Hz, 1H), 5.10 – 5.00 (m, 1H), 3.96 (s, 4H), 2.95 (dt, *J* = 13.3, 8.5 Hz, 1H), 2.78 – 2.59 (m, 4H).

**$^{13}$C NMR (100 MHz, $CD_3OD$)** *δ* 179.64, 162.60, 143.38, 143.28, 138.15, 136.77, 134.06, 132.58, 129.95, 123.93, 123.75, 111.27, 59.80, 56.76, 34.72, 19.05, 15.37.

**HRMS (ESI, m/z):** calc'd for $C_{17}H_{16}N_2O_2$ $[M+H]^+$ 281.1290, found: 281.1281.



**3l**

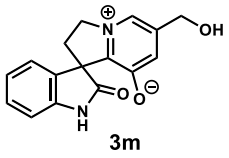
**6'-ethyl-2-oxo-2',3'-dihydrospiro[indoline-3,1'-indolizin]-4'-ium-8'-olate**

Prepared according to General Procedure C, isolated as a white solid (73% yield).

**$^1$H NMR (400 MHz, $CD_3OD$)** δ 7.99 (s, 1H), 7.27 (td, *J* = 7.7, 1.2 Hz, 1H), 7.22 – 7.15 (m, 2H), 6.99 (ddd, J = 7.7, 6.2, 2.4 Hz, 2H), 5.17 – 5.09 (m, 1H), 5.05 – 4.97 (m, 2H), 2.94 – 2.86 (m, 1H), 2.73 – 2.63 (m, 4H), 1.27 (t, *J* = 7.6 Hz, 3H).

**$^{13}$C NMR (100 MHz, $CD_3OD$)** δ 179.42, 165.71, 146.02, 144.44, 143.40, 134.08, 132.18, 130.05, 123.98, 123.80, 122.92, 111.34, 59.50, 58.33, 35.07, 26.81, 15.31.

**HRMS (ESI, m/z):** calc'd for $C_{17}H_{16}N_2O_2$ $[M+H]^+$ 281.1290, found: 281.1282.



**3m**

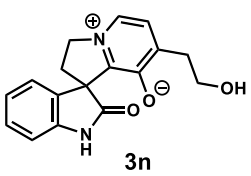
**6'-(hydroxymethyl)-2-oxo-2',3'-dihydrospiro[indoline-3,1'-indolizin]-4'-ium-8'-olate**

Prepared according to General Procedure C, isolated as a white solid (74% yield).

**$^1$H NMR (400 MHz, DMSO-$d_6$)** δ 7.43 (s, 1H), 7.18 (td, J = 7.7, 1.3 Hz, 1H), 7.16 – 7.10 (m, 1H), 6.89 – 6.79 (m, 2H), 6.63 (s, 1H), 5.39 (s, 1H), 4.98 (dt, J = 12.8, 8.5 Hz, 1H), 4.80 (ddd, J = 12.8, 9.1, 3.8 Hz, 1H), 4.38 (s, 2H), 2.65 (dd, J = 11.0, 7.2 Hz, 1H), 2.40 – 2.31 (m, 1H).

**$^{13}$C NMR (100 MHz, DMSO-$d_6$)** δ 176.93, 164.40, 142.92, 142.42, 142.15, 131.33, 129.08, 128.27, 122.91, 121.46, 115.47, 109.39, 60.21, 57.34, 56.67, 33.31.

**HRMS (ESI, m/z):** calc'd for $C_{16}H_{14}N_2O_3$ $[M+H]^+$ 283.1082, found: 283.1074.



**3n**

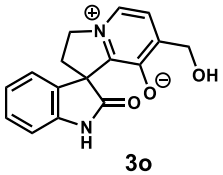
**7'-(2-hydroxyethyl)-2-oxo-2',3'-dihydrospiro[indoline-3,1'-indolizin]-4'-ium-8'-olate**

Prepared according to General Procedure C, isolated as a light yellow solid (60% yield).

**$^1$H NMR (400 MHz, $CD_3OD$)** δ 7.77 (d, J = 5.8 Hz, 1H), 7.46 (d, J = 5.8 Hz, 1H), 7.25 (td, J = 7.7, 1.2 Hz, 1H), 7.15 – 7.10 (m, 1H), 7.02 – 6.94 (m, 2H), 5.06 (dt, J = 12.7, 8.3 Hz, 1H), 4.97 – 4.91 (m, 1H), 3.73 (t, J = 6.2 Hz, 2H), 2.93 – 2.85 (m, 1H), 2.82 (td, J = 5.9, 1.7 Hz, 2H), 2.58 (ddd, J = 12.7, 8.0, 4.3 Hz, 1H).

**$^{13}$C NMR (100 MHz, $CD_3OD$)** δ 179.36, 163.51, 148.00, 144.58, 143.33, 132.17, 130.09, 128.51, 124.06, 123.93, 123.84, 111.34, 61.53, 59.64, 58.01, 35.43, 34.58.

**HRMS (ESI, m/z):** calc'd for $C_{17}H_{16}N_2O_3$ $[M+H]^+$ 297.1239, found: 297.1230.



**3o**

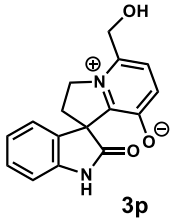
**7'-(hydroxymethyl)-2-oxo-2',3'-dihydrospiro[indoline-3,1'-indolizin]-4'-ium-8'-olate**

Prepared according to General Procedure C, isolated as a light yellow solid (71% yield).

**$^1$H NMR (400 MHz, DMSO-$d_6$)** δ 7.54 (d, *J* = 5.6 Hz, 1H), 7.30 (t, *J* = 6.8 Hz, 1H), 7.18 (td, *J* = 7.7, 1.2 Hz, 1H), 7.15 – 7.09 (m, 1H), 6.85 (ddd, *J* = 8.6, 4.5, 1.0 Hz, 2H), 5.25 (s, 1H), 4.97 (dt, *J* = 12.5, 8.3 Hz, 1H), 4.79 (ddd, *J* = 12.7, 9.1, 3.7 Hz, 1H), 4.30 (t, *J* = 10.3 Hz, 2H), 2.65 (dt, *J* = 12.8, 9.1 Hz, 1H), 2.42 – 2.33 (m, 1H).

**$^{13}$C NMR (100 MHz, DMSO-$d_6$)** δ 177.09, 162.40, 146.98, 142.38, 140.69, 131.53, 128.26, 122.98, 121.88, 121.50, 117.43, 109.39, 59.42, 57.16, 56.10, 33.69.

**HRMS (ESI, m/z):** calc'd for $C_{16}H_{14}N_2O_3$ $[M+H]^+$ 283.1082, found: 283.1073.



**3p**

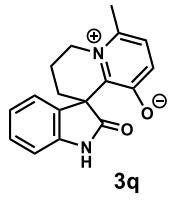
**5'-(hydroxymethyl)-2-oxo-2',3'-dihydrospiro[indoline-3,1'-indolizin]-4'-ium-8'-olate**

Prepared according to General Procedure C, isolated as a light yellow solid (74% yield).

**$^1$H NMR (400 MHz, DMSO-$d_6$)** δ 10.65 (s, 1H), 7.25 (d, *J* = 8.8 Hz, 1H), 7.17 (tt, *J* = 15.8, 7.9 Hz, 1H), 7.10 (d, *J* = 7.4 Hz, 1H), 6.86 (ddd, *J* = 21.3, 10.7, 4.2 Hz, 2H), 6.71 (d, *J* = 8.8 Hz, 1H), 5.65 (s, 1H), 5.03 – 4.83 (m, 2H), 4.63 – 4.45 (m, 2H), 2.64 (dt, *J* = 12.8, 9.3 Hz, 1H), 2.38 (ddd, *J* = 12.7, 7.5, 3.7 Hz, 1H).

**$^{13}$C NMR (100 MHz, DMSO-$d_6$)** δ 177.28, 164.02, 144.67, 142.89, 132.19, 131.75, 130.34, 128.74, 127.35, 123.20, 121.88, 109.89, 59.27, 57.92, 54.31, 33.57.

**HRMS (ESI, m/z):** calc'd for $C_{16}H_{14}N_2O_3$ $[M+H]^+$ 283.1082, found: 283.1073.



**3q**

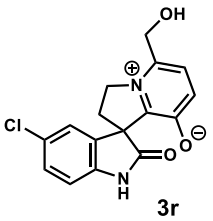
**6'-methyl-2-oxo-3',4'-dihydro-2'H-spiro[indoline-3,1'-quinolizin]-5'-ium-9'-olate**

Prepared according to General Procedure C, isolated as a white solid (89% yield).

**$^1$H NMR (400 MHz, $CD_3OD$)** *δ* 7.31 (d, *J* = 8.8 Hz, 1H), 7.21 (td, *J* = 7.7, 1.3 Hz, 1H), 7.05 (dd, *J* = 8.2, 4.6 Hz, 2H), 7.01 – 6.83 (m, 2H), 4.66 (dt, *J* = 14.3, 4.1 Hz, 1H), 4.32 (ddd, *J* = 14.8, 11.1, 5.0 Hz, 1H), 2.53 – 2.38 (m, 1H), 2.32 (ddp, *J* = 13.9, 5.2, 3.0 Hz, 1H), 2.20 (td, *J* = 12.9, 3.0 Hz, 1H), 1.93 – 1.76 (m, 1H).

**$^{13}$C NMR (100 MHz, $CD_3OD$)** *δ* 182.40, 165.81, 143.69, 143.48, 136.46, 135.42, 133.29, 129.11, 128.71, 123.51, 122.89, 110.86, 53.25, 52.78, 32.45, 19.80, 19.53.

**HRMS (ESI, m/z):** calc'd for $C_{17}H_{16}N_2O_2$ $[M+H]^+$ 281.1290, found: 281.1282.



**3r**

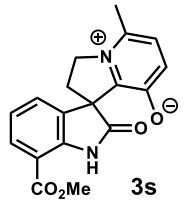
**5-chloro-5'-(hydroxymethyl)-2-oxo-2',3'-dihydrospiro[indoline-3,1'-indolizin]-4'-ium-8'-olate**

Prepared according to General Procedure C, isolated as a white solid (81% yield).

**$^1$H NMR (400 MHz, DMSO-*d*$_6$)** δ 10.76 (s, 1H), 7.26 (ddd, *J* = 10.4, 6.7, 2.6 Hz, 3H), 6.84 (d, *J* = 8.3 Hz, 1H), 6.74 (d, *J* = 8.8 Hz, 1H), 5.58 (s, 1H), 5.07 – 4.82 (m, 2H), 4.66 – 4.43 (m, 2H), 2.63 (dt, *J* = 12.9, 9.2 Hz, 1H), 2.48 – 2.38 (m, 1H).

**$^{13}$C NMR (100 MHz, DMSO-*d*$_6$)** δ 176.73, 163.62, 143.50, 141.52, 133.30, 132.03, 130.13, 128.10, 126.96, 125.50, 123.11, 110.74, 58.82, 57.63, 53.85, 32.75.

**HRMS (ESI, m/z):** calc'd for $C_{16}H_{13}ClN_2O_3$ $[M+H]^+$ 317.0693, found: 317.0684.



**3s**

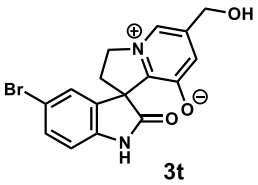
**7-(methoxycarbonyl)-5'-methyl-2-oxo-2',3'-dihydrospiro[indoline-3,1'-indolizin]-4'-ium-8'-olate**

Prepared according to General Procedure C, isolated as a white solid (83% yield).

**$^1$H NMR (400 MHz, CD$_3$OD)** *δ* 7.35 (d, *J* = 8.7 Hz, 1H), 7.25 (td, *J* = 7.7, 1.2 Hz, 1H), 7.21 – 7.13 (m, 2H), 7.04 – 6.92 (m, 2H), 4.96 (dt, *J* = 13.1, 8.4 Hz, 2H), 2.87 (ddd, *J* = 13.1, 9.2, 8.3 Hz, 1H), 2.67 – 2.53 (m, 4H).

**$^{13}$C NMR (100 MHz, CD$_3$OD)** *δ* 179.35, 162.70, 145.27, 143.33, 135.65, 135.54, 132.27, 130.08, 129.37, 123.99, 123.80, 111.29, 59.89, 56.27, 34.61, 18.20.

**HRMS (ESI, m/z):** calc'd for $C_{18}H_{16}N_2O_4$ $[M+H]^+$ 325.1188, found: 325.1178.



**3t**

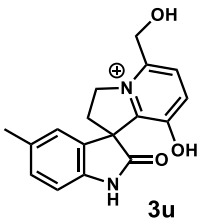
**5-bromo-6'-(hydroxymethyl)-2-oxo-2',3'-dihydrospiro[indoline-3,1'-indolizin]-4'-ium-8'-olate**

Prepared according to General Procedure C, isolated as a light yellow solid (58% yield).

**$^1$H NMR (400 MHz, DMSO-*d*$_6$)** δ 10.75 (s, 1H), 7.48 – 7.39 (m, 2H), 7.35 (dt, *J* = 11.8, 5.9 Hz, 1H), 6.79 (d, *J* = 8.2 Hz, 1H), 6.66 (s, 1H), 5.39 (s, 1H), 5.03 (dt, *J* = 12.7, 8.4 Hz, 1H), 4.78 (td, *J* = 9.0, 4.5 Hz, 1H), 4.39 (s, 2H), 2.62 (dt, *J* = 13.0, 9.0 Hz, 1H), 2.46 – 2.33 (m, 1H).

**$^{13}$C NMR (100 MHz, DMSO-*d*$_6$)** δ 176.65, 164.26, 142.32, 142.20, 141.85, 133.64, 130.93, 129.23, 125.87, 116.03, 113.26, 111.23, 60.17, 57.46, 56.67, 32.85.

**HRMS (ESI, m/z):** calc'd for $C_{16}H_{13}BrN_2O_3$ $[M+H]^+$ 361.0188, found: 361.0179.



**3u**

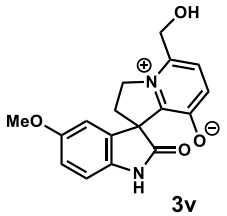
**8'-hydroxy-5'-(hydroxymethyl)-5-methyl-2-oxo-2',3'-dihydrospiro[indoline-3,1'-indolizin]-4'-ium**

Prepared according to General Procedure C, isolated as an off-white solid (82% yield).

**$^1$H NMR (400 MHz, DMSO-$d_6$)** δ 10.51 (s, 1H), 7.27 (d, *J* = 8.8 Hz, 1H), 6.99 (d, *J* = 7.8 Hz, 1H), 6.94 (s, 1H), 6.79 – 6.66 (m, 2H), 5.59 (s, 1H), 5.02 – 4.83 (m, 2H), 4.63 – 4.50 (m, 2H), 2.68 – 2.55 (m, 1H), 2.37 (ddd, *J* = 20.2, 9.3, 5.5 Hz, 1H), 2.19 (s, 3H).

**$^{13}$C NMR (100 MHz, DMSO-$d_6$)** δ 176.84, 163.47, 144.38, 140.09, 131.85, 131.44, 130.61, 130.36, 128.55, 126.91, 123.42, 109.29, 58.80, 57.59, 53.95, 33.28, 20.66.

**HRMS (ESI, m/z):** calc'd for $C_{17}H_{16}N_2O_3$ $[M+H]^+$ 297.1239, found: 297.1230.




**3v**

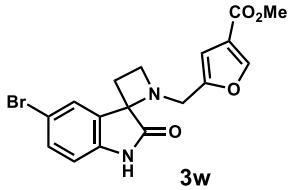
**5'-(hydroxymethyl)-5-methoxy-2-oxo-2',3'-dihydrospiro[indoline-3,1'-indolizin]-4'-ium-8'-olate**

Prepared according to General Procedure C, isolated as a brown solid (83% yield).

**$^1$H NMR (400 MHz, DMSO-$d_6$)** δ 10.47 (s, 1H), 7.23 (d, J = 8.8 Hz, 1H), 6.76 (d, J = 2.6 Hz, 1H), 6.74 – 6.67 (m, 3H), 5.64 (s, 1H), 4.96 (dt, J = 12.9, 8.4 Hz, 1H), 4.86 (ddd, J = 12.9, 9.2, 3.7 Hz, 1H), 4.60 – 4.47 (m, 2H), 3.63 (s, 3H), 2.61 (dt, J = 12.8, 9.1 Hz, 1H), 2.37 (ddd, J = 12.9, 7.9, 3.7 Hz, 1H).

**$^{13}$C NMR (100 MHz, DMSO-$d_6$)** δ 176.82, 164.02, 154.94, 144.20, 135.83, 132.68, 131.84, 129.13, 126.94, 112.61, 110.26, 109.58, 58.86, 57.98, 55.54, 53.76, 33.09.

**HRMS (ESI, m/z):** calc'd for $C_{17}H_{16}N_2O_4$ $[M+H]^+$ 313.1188, found: 313.1178.




**3w**

**methyl 5-((5'-bromo-2'-oxospiro[azetidine-2,3'-indolin]-1-yl)methyl)furan-3-carboxylate**

Prepared according to General Procedure C, isolated as a yellow oil (81% yield).

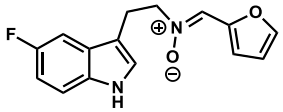
**$^1$H NMR (400 MHz, $CDCl_3$)** δ 8.59 (s, 1H), 7.92 – 7.90 (m, 1H), 7.48 (d, J = 2.0 Hz, 1H), 7.36 (dd, J = 8.3, 2.0 Hz, 1H), 6.79 (d, J = 8.2 Hz, 1H), 6.56 (d, J = 1.7 Hz, 1H), 4.07 – 3.86 (m, 2H), 3.83 (s, 3H), 3.00 – 2.87 (m, 3H), 2.62 (dq, J = 13.9, 5.4, 4.9 Hz, 1H).

**$^{13}$C NMR (100 MHz, $CDCl_3$)** δ 175.68, 163.35, 151.99, 147.70, 138.91, 133.12, 131.56, 127.87, 119.79, 115.64, 112.47, 110.03, 61.19, 60.55, 54.11, 51.72, 37.65.

**HRMS (ESI, m/z):** calc'd for $C_{17}H_{15}BrN_2O_4$ $[M-H]^-$ 389.0136, found: 389.0141.

Note: **3w** is unstable at rt and needed to be stored at -20 °C.

## Spectral Data of Products from Different Oxidative Conditions



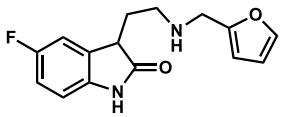
**5**

**(Z)-N-(2-(5-fluoro-1H-indol-3-yl)ethyl)-1-(furan-2-yl)methanimine oxide**

**$^1$H NMR (400 MHz, $CDCl_3$)** δ 8.15 (s, 1H), 7.80 (dd, J = 3.5, 0.7 Hz, 1H), 7.42 (dd, J = 1.7, 0.7 Hz, 1H), 7.29 – 7.26 (m, 2H), 7.26 – 7.23 (m, 1H), 7.06 (d, J = 2.4 Hz, 1H), 6.94 (td, J = 9.0, 2.5 Hz, 1H), 6.55 (dd, J = 3.6, 1.7 Hz, 1H), 4.12 (t, J = 6.8 Hz, 3H), 3.39 (t, J = 6.8 Hz, 3H).

**$^{13}$C NMR (100 MHz, $CDCl_3$)** δ 157.83 (d, J = 235.1 Hz), 146.50, 143.71, 132.70, 127.26 (d, J = 9.8 Hz), 126.08, 124.65, 115.54, 112.30, 112.01 (d, J = 9.6 Hz), 111.43, 110.55 (d, J = 26.3 Hz), 103.27 (d, J = 23.5 Hz), 65.89, 23.64.

**HRMS (ESI, m/z):** calc'd for $C_{15}H_{13}FN_2O_2$ $[M+H]^+$ 273.1039, found: 273.1033.



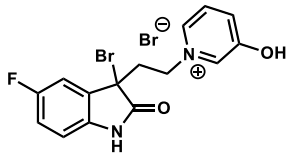
**6**

**5-fluoro-3-(2-((furan-2-ylmethyl)amino)ethyl)indolin-2-one**

**$^1$H NMR (400 MHz, $CDCl_3$)** δ 8.58 (s, 1H), 7.34 (dd, J = 1.9, 0.9 Hz, 1H), 6.94 – 6.91 (m, 1H), 6.91 – 6.87 (m, 1H), 6.80 (dd, J = 8.3, 4.3 Hz, 1H), 6.30 (dd, J = 3.2, 1.9 Hz, 1H), 6.19 (dd, J = 3.1, 0.8 Hz, 1H), 3.87 – 3.73 (m, 2H), 3.56 (t, J = 6.4 Hz, 1H), 2.93 – 2.70 (m, 2H), 2.30 – 2.06 (m, 2H).

**$^{13}$C NMR (100 MHz, $CDCl_3$)** δ 180.57, 158.96 (d, J = 239.8 Hz), 152.89, 141.99, 137.53, 130.93 (d, J = 8.3 Hz), 114.23 (d, J = 23.6 Hz), 112.09 (d, J = 24.8 Hz), 110.32 (d, J = 8.1 Hz), 110.20, 107.47, 45.61, 45.22, 44.66, 29.99.

**HRMS (ESI, m/z):** calc'd for $C_{15}H_{15}FN_2O_2$ $[M-H]^-$ 273.1039, found: 273.1047.



**2a**

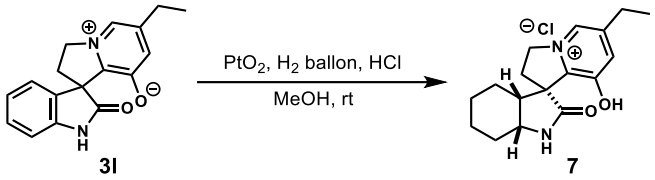
**1-(2-(3-bromo-5-fluoro-2-oxoindolin-3-yl)ethyl)-3-hydroxypyridin-1-ium**

**$^1$H NMR (400 MHz, DMSO-*$d_6$*)** δ 11.80 (s, 1H), 11.05 (s, 1H), 8.49 – 8.41 (m, 2H), 7.95 (ddd, J = 8.8, 2.3, 1.2 Hz, 1H), 7.85 (dd, J = 8.7, 6.3 Hz, 1H), 7.43 (dd, J = 8.3, 2.7 Hz, 1H), 7.14 (ddd, J = 9.5, 8.6, 2.7 Hz, 1H), 6.93 (dd, J = 8.6, 4.4 Hz, 1H), 4.60 (t, J = 7.1 Hz, 2H), 3.19 (dd, J = 14.6, 7.2 Hz, 1H), 3.01 (dt, J = 14.2, 6.9 Hz, 1H).

**$^{13}$C NMR (100 MHz, DMSO-*$d_6$*)** δ 173.84, 158.25 (d, J = 238.4 Hz), 156.73, 136.79, 135.87, 133.30, 131.53, 130.28 (d, J = 8.8 Hz), 128.36, 117.41 (d, J = 23.5 Hz), 112.57 (d, J = 25.6 Hz), 111.84 (d, J = 8.2 Hz), 57.23, 54.38, 37.44.

**HRMS (ESI, m/z):** calc'd for $C_{15}H_{13}BrFN_2O_2^+$ $[M]^+$ 351.0139, found: 351.013.

## General Procedure for the Selective Dearomatization and the Spectral Data



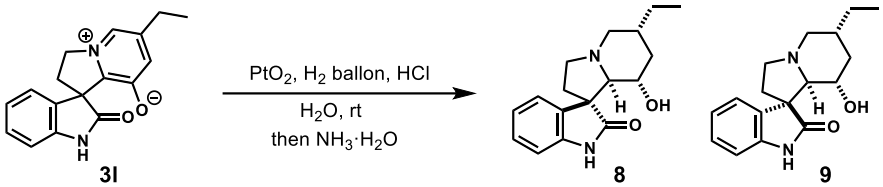

To a stirred solution of **3l** (29 mg, 0.1 mmol, 1.0 equiv.) in MeOH (4 mL) was added HCl (80 μL of 2.5 M solution in $H_2O$, 0.2 mmol, 2.0 equiv.) and $PtO_2$ (9.1 mg, 0.04 mmol, 0.4 equiv.) at rt. After addition, the resulting mixture was stirred under a hydrogen atmosphere for 16 hours. After completion, the reaction mixture was filtrated through a pad of celite and the filtrate was concentrated in vacuo. The crude product was purified by column chromatography on silica gel (DCM/MeOH 30:1 to 7:1) to afford **7** as a white solid (24 mg, 75% yield).

**Rf** = 0.52, DCM/MeOH = 5/1.

**$^1$H NMR (400 MHz, DMSO-*d*$_6$)** δ 8.44 (s, 1H), 7.94 (s, 1H), 7.64 (s, 1H), 4.85 (td, J = 12.4, 5.7 Hz, 1H), 4.77 (dd, J = 12.7, 8.6 Hz, 1H), 3.86 (q, J = 4.2 Hz, 1H), 2.69 (q, J = 7.5 Hz, 2H), 2.62 (dd, J = 12.4, 5.7 Hz, 1H), 2.54 (d, J = 5.1 Hz, 1H), 2.26 (td, J = 12.1, 8.6 Hz, 1H), 1.96 – 1.90 (m, 1H), 1.90 (s, 1H), 1.55 (d, J = 12.6 Hz, 1H), 1.50 (s, 1H), 1.44 (d, J = 3.8 Hz, 1H), 1.29 (q, J = 12.1 Hz, 1H), 1.20 (t, J = 7.5 Hz, 3H), 1.12 (dd, J = 13.6, 5.6 Hz, 1H), 1.00 (q, J = 12.7 Hz, 1H).

**$^{13}$C NMR (100 MHz, DMSO-*d*$_6$)** δ 173.77, 155.90, 143.66, 141.57, 131.04, 130.38, 61.57, 57.13, 50.39, 43.74, 32.35, 26.69, 24.91, 22.90, 22.80, 19.65, 14.49.

**HRMS (ESI, m/z):** calc'd for $C_{17}H_{23}N_2O_2^+$ $[M]^+$ 287.1759, found: 287.1748.




To a stirred solution of **3l** (29 mg, 0.1 mmol, 1.0 equiv.) in $H_2O$ (4 mL) at rt was added HCl (32 μL of 2.5 M solution in $H_2O$, 0.08 mmol, 0.8 equiv.) and $PtO_2$ (9.1 mg, 0.04 mmol, 0.4 equiv.). After addition, the resulting mixture was stirred under a hydrogen atmosphere for 30 hours. Then $NH_3{\cdot}H_2O$ (0.1 mL) was added and stirred for another 1 hour. The resulting mixture was filtrated through a pad of celite, and the filtrate was concentrated in vacuo. The crude product was purified by column chromatography on silica gel (DCM/MeOH 70:1 to 10:1) to afford **8** (less polar) as a white solid (19 mg, 64% yield) and **9** (more polar) as a white solid (4 mg, 14%).

Data for **8**

**Rf** = 0.58, DCM/MeOH = 10/1.

**$^1$H NMR (400 MHz, DMSO-*d*$_6$)** δ 10.14 (s, 1H), 7.21 (dd, J = 7.3, 1.3 Hz, 1H), 7.11 (td, J = 7.7, 1.3 Hz, 1H), 6.90 (td, J = 7.5, 1.1 Hz, 1H), 6.77 (dd, J = 7.7, 1.3 Hz, 1H), 4.16 (d, J = 5.8 Hz, 1H), 3.20 (td, J = 8.4, 2.4 Hz, 1H), 3.07 – 3.02 (m, 1H), 2.97 (dddd, J = 10.6, 9.2, 5.9, 4.6 Hz, 1H), 2.33 (q, J = 8.7 Hz, 1H), 2.18 – 2.06 (m, 2H), 1.83 – 1.76 (m, 1H), 1.76 – 1.70 (m, 1H), 1.56 (t, J = 10.6 Hz, 1H), 1.42 (dddt, J = 14.2, 10.6, 6.8, 3.4 Hz, 1H), 1.19 (ddt, J = 16.5, 13.6, 6.8 Hz, 2H), 0.85 (t, J = 7.4 Hz, 3H), 0.79 – 0.70 (m, 1H).

**$^{13}$C NMR (100 MHz, DMSO-*d*$_6$)** δ 180.61, 142.19, 134.18, 127.09, 124.16, 120.82, 108.94, 76.70, 67.08, 57.89, 54.46, 53.27, 40.36, 36.72, 35.65, 26.31, 11.64, 11.62.

**HRMS (ESI, m/z):** calc'd for $C_{17}H_{22}N_2O_2$ $[M+H]^+$ 287.1759, found: 287.1750.

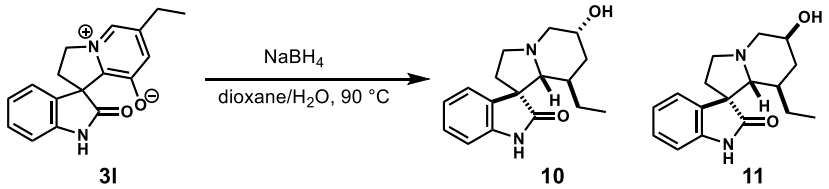
Data for **9**

**Rf** = 0.35, DCM/MeOH = 10/1.

**$^1$H NMR (400 MHz, DMSO-*d*$_6$)** δ 10.08 (s, 1H), 7.17 (dd, J = 7.4, 1.2 Hz, 1H), 7.06 (td, J = 7.6, 1.2 Hz, 1H), 6.88 (td, J = 7.5, 1.1 Hz, 1H), 6.70 (d, J = 7.6 Hz, 1H), 4.10 (d, J = 6.1 Hz, 1H), 3.60 (dddd, J = 10.7, 9.1, 6.2, 4.5 Hz, 1H), 3.08 (t, J = 7.8 Hz, 1H), 3.01 (dd, J = 10.4, 3.7 Hz, 1H), 2.47 – 2.41 (m, 1H), 2.18 – 2.06 (m, 2H), 1.81 (dt, J = 12.9, 3.9 Hz, 1H), 1.69 (dd, J = 12.2, 6.3 Hz, 1H), 1.58 (t, J = 10.5 Hz, 1H), 1.46 (tt, J = 10.9, 3.5 Hz, 1H), 1.18 (dhept, J = 13.5, 6.9 Hz, 2H), 0.83 (t, J = 7.4 Hz, 3H), 0.67 (q, J = 11.7 Hz, 1H).

**$^{13}$C NMR (100 MHz, DMSO-*d*$_6$)** δ 180.09, 140.52, 136.64, 126.80, 122.61, 121.17, 108.61, 79.80, 66.99, 57.34, 54.06, 53.51, 41.99, 38.05, 36.70, 26.39, 12.27.

**HRMS (ESI, m/z):** calc'd for $C_{17}H_{22}N_2O_2$ [M+H]$^+$ 287.1759, found: 287.1750.




**3l** **10** **11**

To a stirred solution of **3l** (56 mg, 0.2 mmol, 1.0 equiv.) in dioxane/$H_2O$ = 10/1 (2 mL) was added $NaBH_4$ (76 mg, 2 mmol, 10.0 equiv.) in potions at rt. After addition, the resulting mixture was stirred at 90 °C for 12 hours. After completion, the reaction mixture was concentrated in vacuo and the crude product was purified by column chromatography on silica gel (DCM/MeOH 60:1 to 10:1) to afford **10** (more polar) as a light yellow solid (11 mg, 19% yield) and **11** (less polar) as a light yellow solid (7 mg, 12% yield).

Data for **10**

**Rf** = 0.27, DCM/MeOH = 10/1.

**$^1$H NMR (400 MHz, $CD_3OD$)** δ 7.28 (d, J = 7.4 Hz, 1H), 7.20 (t, J = 7.6 Hz, 1H), 7.04 (t, J = 7.6 Hz, 1H), 6.88 (d, J = 6.8 Hz, 0H), 3.85 (p, J = 2.7 Hz, 1H), 3.20 (t, 1H), 3.16 (td, 1H), 2.58 – 2.46 (m, 1H), 2.35 – 2.28 (m, 1H), 2.27 – 2.19 (m, 2H), 2.02 – 1.96 (m, 1H), 1.95 – 1.87 (m, 2H), 1.02 (tdd, J = 12.1, 5.0, 2.5 Hz, 1H), 0.88 (ddd, J = 11.7, 7.1, 3.0 Hz, 1H), 0.61 – 0.57 (m, 3H), 0.57 – 0.49 (m, 1H).

**$^{13}$C NMR (100 MHz, $CD_3OD$)** δ 184.09, 141.97, 137.81, 128.54, 124.04, 122.94, 109.52, 78.84, 66.60, 59.47, 57.10, 55.52, 38.17, 37.55, 35.19, 25.86, 10.72.

**HRMS (ESI, m/z):** calc'd for $C_{17}H_{22}N_2O_2$ [M+H]$^+$ 287.1759, found: 287.1750.

Data for **11**

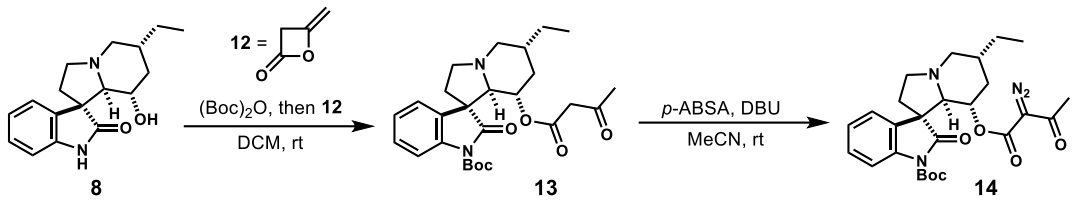
**Rf** = 0.33, DCM/MeOH = 10/1.

**$^1$H NMR (400 MHz, $CD_3OD$)** δ 7.26 (d, J = 7.4 Hz, 1H), 7.16 (t, J = 7.7 Hz, 1H), 7.01 (t, J = 7.5 Hz, 1H), 6.83 (d, J = 7.7 Hz, 1H), 3.74 (tt, J = 9.9, 4.5 Hz, 1H), 3.26 (d, J = 5.0 Hz, 1H), 3.18 (t, J = 8.5 Hz, 1H), 2.59 (q, J = 9.6, 8.7 Hz, 1H), 2.36 – 2.32 (m, 1H), 2.29 (d, J = 10.0 Hz, 1H), 2.05 (dd, J = 12.6, 5.2 Hz, 1H), 1.92 (dd, J = 12.4, 7.9 Hz, 2H), 1.82 – 1.70 (m, 1H), 0.89 (ddt, J = 8.9, 5.8, 3.1 Hz, 1H), 0.84 – 0.76 (m, 1H), 0.58 (d, J = 6.7 Hz, 3H), 0.55 – 0.47 (m, 1H).

**$^{13}$C NMR (100 MHz, $CD_3OD$)** δ 182.90, 142.66, 135.40, 129.16, 124.05, 123.81, 110.86, 77.43, 67.44, 60.83, 55.74, 54.76, 39.52, 38.32, 38.04, 24.87, 10.70.

**HRMS (ESI, m/z):** calc'd for $C_{17}H_{22}N_2O_2$ [M+H]$^+$ 287.1759, found: 287.1750.

## General Procedure for the Formal Synthesis of Rhynchophylline and Isorhynchophylline



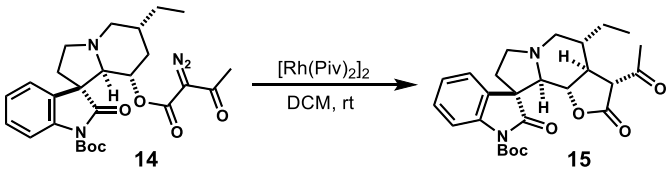

To a stirred solution of **8** (1.0 g, 3.5 mmol, 1.0 equiv.) in DCM (400 mL) was added TEA (0.58 mL, 4.2 mmol, 1.2 equiv.), DMAP (15 mg, 0.7 mmol, 0.2 equiv.) and $Boc_2O$ (0.96 mL, 4.2 mmol, 1.2 equiv.) at rt. The resulting mixture was stirred at rt for 3 hours until the starting material was consumed completely monitored by TLC analysis. The resulting mixture was added **12** in one portion (0.67 mL, 8.7 mmol, 2.5 equiv.). After addition, the resulting mixture was stirred at rt for 30 min. After completion, the reaction was quenched by addition of $H_2O$ (100 mL). The solution was transferred to a separatory funnel, and the organic phase was collected. The aqueous phase was extracted with DCM (2×30 mL). The combined organic layers were washed with brine (100 mL), dried over $Na_2SO_4$, and concentrated in vacuo. The crude residue was purified by column chromatography on silica gel (PE/EA 8:1 to 5:1) to afford **13** as a light yellow oil (1.18g). Then to a stirred solution of **13** (1.18 g, 2.5 mmol, 1.0 equiv.) in MeCN (30 mL) was sequentially added *p*-ABSA (900 mg, 3.75 mmol, 1.5 equiv.) and DBU (0.56 mL, 3.75 mmol, 1.5 equiv.) at rt. After addition, the reaction mixture was concentrated in vacuo. The resulting oil was purified by column chromatography on silica gel (PE/EA 8:1 to 5:1) to afford **14** as a light yellow solid (1.19 g, 69% yield, 2 steps).

**Rf** = 0.47, PE/EA = 5/1.

**$^1$H NMR (400 MHz, $CDCl_3$)** δ 7.72 – 7.68 (m, 1H), 7.45 – 7.43 (m, 1H), 7.30 – 7.25 (m, 1H), 7.22 – 7.17 (m, 1H), 4.48 (ddd, J = 10.6, 9.5, 4.6 Hz, 1H), 3.31 (td, J = 8.5, 2.2 Hz, 1H), 3.16 (dd, J = 10.7, 3.1 Hz, 1H), 2.66 – 2.56 (m, 2H), 2.44 (ddd, J = 13.1, 9.1, 2.1 Hz, 1H), 2.24 (d, J = 0.6 Hz, 3H), 2.11 – 1.99 (m, 2H), 1.77 (t, J = 10.8 Hz, 1H), 1.70 – 1.63 (m, 1H), 1.60 (d, J = 0.6 Hz, 9H), 1.35 – 1.20 (m, 2H), 1.00 – 0.92 (m, 1H), 0.91 – 0.86 (m, 3H).

**$^{13}$C NMR (100 MHz, $CDCl_3$)** δ 189.51, 178.06, 159.04, 148.91, 138.84, 130.82, 128.35, 124.80, 124.57, 114.11, 84.72, 75.38, 71.42, 57.76, 54.87, 53.86, 37.08, 36.88, 36.35, 28.06, 27.98, 27.96, 26.38, 11.50.

**HRMS (ESI, m/z):** calc'd for $C_{26}H_{32}N_4O_6$ $[M+H]^+$ 497.2400, found: 497.2385.




To a stirred solution of **14** (20 mg, 0.04 mmol, 1.0 equiv.) in DCM (1.0 mL) was added $[Rh(Piv)_2]_2$ (0.49 mg, 0.0008 mmol, 0.02 equiv.) at rt. The resulting mixture was stirred for 30 min under argon atmosphere. After completion, the reaction mixture was concentrated in vacuo and the resulting oil was purified by column chromatography on silica gel (PE/EA 10/1 to 5/1) to afford **15** as a white solid (15.5 mg, 82% yield).

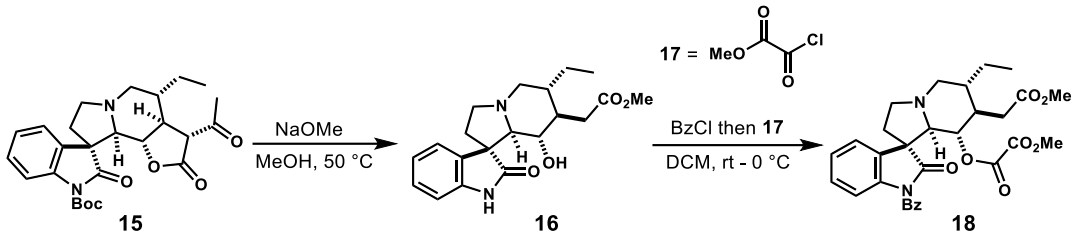
Note: When the reaction scale of **14** was increased to 1.19g (2.4 mmol) while other conditions were not changed, the yield of **15** slightly decreased to 70%.

**Rf** = 0.5, PE/EA = 2/1.

**$^1$H NMR (400 MHz, $CDCl_3$)** δ 7.87 (dd, J = 8.2, 0.9 Hz, 1H), 7.36 (dd, J = 7.4, 1.6 Hz, 1H), 7.30 (tt, J = 8.0, 1.1 Hz, 1H), 7.13 (tt, J = 7.5, 1.0 Hz, 1H), 3.44 – 3.38 (m, 1H), 3.37 – 3.33 (m, 1H), 3.32 – 3.28 (m, 2H), 2.87 (d, J = 9.2 Hz, 1H), 2.76 (dt, J = 9.3, 8.0 Hz, 1H), 2.52 (tt, J = 10.1, 9.3, 3.0 Hz, 1H), 2.32 (d, J = 0.8 Hz, 3H), 2.30 – 2.22 (m, 1H), 2.12 – 2.05 (m, 1H), 2.02 (t, J = 10.7 Hz, 1H), 1.64 (s, 9H), 1.60 – 1.52 (m, 1H), 1.17 (ddd, J = 17.9, 8.5, 6.1 Hz, 2H), 0.88 – 0.81 (m, 3H).

**$^{13}$C NMR (100 MHz, $CDCl_3$)** δ 202.43, 177.74, 172.14, 149.08, 139.46, 131.15, 128.46, 124.28, 123.96, 116.69, 84.42, 78.96, 73.42, 57.35, 56.58, 55.14, 52.82, 49.00, 40.44, 36.57, 30.55, 28.09, 23.77, 11.50.

**HRMS (ESI, m/z):** calc'd for $C_{26}H_{32}N_2O_6$ $[M+H]^+$ 469.2338, found: 469.2324.



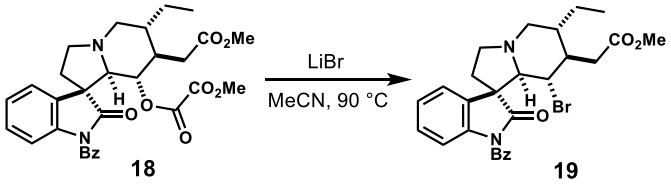

To a stirred solution of **15** (500 mg, 1.07 mmol, 1.0 equiv.) in MeOH (20 mL) at rt was added NaOMe (2.0 mL of 5.4 M solution in MeOH, 10.7 mmol, 10.0 equiv.) in one portion. The resulting mixture was stirred at 50 °C for 12 hours. After completion, the reaction was quenched by addition of sat. aq. $NH_4Cl$ (5 mL) and $H_2O$ (20mL). The solution was transferred to a separatory funnel and extracted with DCM (3×20 mL). The combined organic layers were washed with brine (20 mL), dried over $Na_2SO_4$, and concentrated in vacuo. The resulting yellow foam was redissolved in DCM (10 ml), then TEA (0.19 mL, 1.39 mmol, 1.3 equiv.), DMAP (26 mg, 0.21 mmol, 0.2 equiv.) and BzCl (0.15 ml, 1.28 mmol, 1.2 equiv.) were added in sequence. The resulting mixture was stirred at rt for 1 hour until the starting material was consumed completely by TLC analysis. Then DCM (10 mL) and TEA (2.0 mL, 15.0 mmol, 14.0 equiv.) was added and the resulting mixture was cooled to 0 °C. **17** (1.38 mL, 15.0 mmol, 14.0 equiv.) was added dropwise to the reaction at 0 °C. The resulting mixture was stirred at 0 °C for 1 hour. After completion, the reaction was quenched by addition of $H_2O$ (30 mL). The solution was transferred to a separatory funnel, and the organic phase was collected. The aqueous phase was extracted with DCM (2×15 mL). The combined organic extracts were washed with brine (20 mL), dried over $Na_2SO_4$, and concentrated in vacuo. The resulting oil was purified by column chromatography on silica gel (PE/EA 10/1 to 2/1) to afford **18** as a yellow solid (420 mg, 72% yield, 2 steps).

**Rf** = 0.5, PE/EA = 5/1.

**$^1$H NMR (400 MHz, $CDCl_3$)** δ 7.86 – 7.82 (m, 1H), 7.75 – 7.72 (m, 2H), 7.61 – 7.56 (m, 1H), 7.51 – 7.45 (m, 3H), 7.34 (td, J = 7.8, 1.6 Hz, 1H), 7.29 (dd, J = 7.4, 1.2 Hz, 1H), 4.79 (t, J = 10.0 Hz, 1H), 3.67 (s, 3H), 3.56 (s, 3H), 3.31 (t, J = 8.2 Hz, 1H), 3.26 (dd, J = 11.1, 4.1 Hz, 1H), 2.77 (d, J = 9.8 Hz, 1H), 2.55 (dt, J = 10.0, 8.1 Hz, 1H), 2.44 – 2.35 (m, 1H), 2.25 (d, J = 4.8 Hz, 2H), 2.16 (ddd, J = 13.0, 10.3, 8.0 Hz, 1H), 1.97 – 1.83 (m, 2H), 1.83 – 1.73 (m, 1H), 1.55 – 1.50 (m, 1H), 1.28 – 1.14 (m, 1H), 0.91 (t, J = 7.5 Hz, 3H).

**$^{13}$C NMR (100 MHz, $CDCl_3$)** δ 179.76, 172.48, 169.16, 156.97, 155.33, 139.40, 134.39, 132.40, 130.73, 129.23, 128.82, 128.20, 128.02, 128.00, 125.73, 124.49, 115.16, 76.78, 75.29, 56.77, 55.19, 54.66, 53.51, 51.62, 43.06, 40.69, 38.19, 33.06, 23.23, 11.00.

**HRMS (ESI, m/z):** calc'd for $C_{30}H_{32}N_2O_8$ $[M+H]^+$ 549.2237, found: 549.2227.



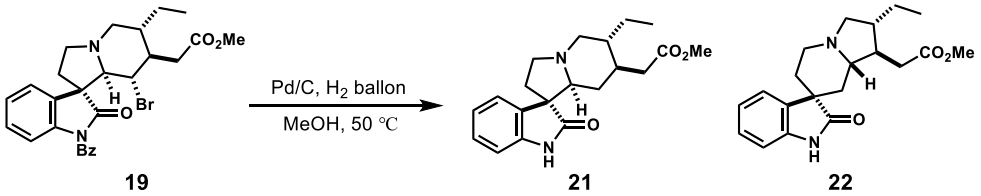

To a stirred solution of **18** (100 mg, 0.18 mmol, 1.0 equiv.) in MeCN (8 mL) was added LiBr in one portion (476 mg, 14.6 mmol, 30.0 equiv.) at rt. The resulting mixture was stirred at 90 °C for 8 hours. After completion, the reaction was quenched by addition of $H_2O$ (20mL). The solution was transferred to a separatory funnel and extracted with EA (3×5 mL). The combined organic extracts were washed with brine (10 mL), dried over $Na_2SO_4$, and concentrated in vacuo. The resulting oil was purified by column chromatography on silica gel (PE/EA 10:1 to 5:1) to afford **19** as a white solid (38 mg, 40% yield).

**Rf** = 0.63, PE/EA = 5/1.

**$^1$H NMR (400 MHz, $CDCl_3$)** δ 7.90 – 7.87 (m, 1H), 7.81 – 7.78 (m, 2H), 7.57 (tt, J = 6.9, 1.3 Hz, 1H), 7.49 – 7.43 (m, 3H), 7.39 (ddd, J = 8.1, 7.6, 1.4 Hz, 1H), 7.29 – 7.24 (m, 1H), 3.83 (t, J = 10.5 Hz, 1H), 3.63 (s, 3H), 3.28 (ddd, J = 12.5, 7.1, 3.0 Hz, 2H), 2.94 (d, J = 10.3 Hz, 1H), 2.61 (d, J = 4.3 Hz, 2H), 2.55 (dd, J = 9.5, 8.5 Hz, 1H), 2.38 (ddd, J = 13.0, 8.4, 1.8 Hz, 1H), 2.10 (ddd, J = 13.0, 9.6, 8.3 Hz, 1H), 1.97 – 1.85 (m, 2H), 1.70 – 1.58 (m, 2H), 1.19 (ddd, J = 13.9, 9.1, 7.0 Hz, 1H), 0.90 (t, J = 7.4 Hz, 3H).

**$^{13}$C NMR (100 MHz, $CDCl_3$)** δ 179.52, 172.41, 169.31, 140.20, 134.44, 132.56, 131.55, 131.53, 129.49, 128.49, 128.04, 124.95, 124.06, 115.27, 77.81, 56.80, 56.71, 56.56, 54.05, 51.66, 46.20, 42.06, 38.70, 35.43, 23.87, 11.02.

**HRMS (ESI, m/z):** calc'd for $C_{27}H_{29}BrN_2O_4$ $[M+H]^+$ 525.1389, found: 525.1378.




**19** **21** **22**

To a stirred solution of **19** (30 mg, 0.057 mmol, 1.0 equiv.) in MeOH (3 mL) was added Pd/C (50 wt.%, 15 mg) at rt. The resulting mixture was stirred at 50 °C for 12 hours under a hydrogen atmosphere. After completion, the reaction was filtrated through a pad of celite and the filtrate was concentrated in vacuo. The crude residue was purified by column chromatography on silica gel (DCM/MeOH 100:1 to 20:1) to afford **21** as a white solid (6.7 mg, 34% yield) and **22** as a white solid (7.9 mg, 40% yield).

Data for **21**

**Rf** = 0.4, DCM/MeOH = 10/1.

**$^1$H NMR (400 MHz, $CD_3OD$)** δ 7.61 (d, J = 7.6 Hz, 1H), 7.24 (tt, J = 7.7, 1.3 Hz, 1H), 7.02 (tt, J = 7.6, 1.3 Hz, 1H), 6.96 (d, J = 7.7 Hz, 1H), 3.54 (d, J = 1.2 Hz, 3H), 3.11 (ddd, J = 12.1, 4.7, 2.1 Hz, 1H), 2.93 (dd, J = 9.6, 2.6 Hz, 1H), 2.74 (dd, J = 12.4, 2.8 Hz, 1H), 2.70 – 2.63 (m, 1H), 2.54 (t, J = 10.3 Hz, 1H), 2.37 (dt, J = 6.4, 1.7 Hz, 2H), 2.28 – 2.16 (m, 1H), 1.86 – 1.79 (m, 1H), 1.79 – 1.76 (m, 1H), 1.76 – 1.71 (m, 1H), 1.62 (dd, J = 13.1, 2.0 Hz, 1H), 1.59 – 1.53 (m, 1H), 1.49 (d, J = 3.9 Hz, 1H), 1.47 – 1.41 (m, 1H), 0.95 (td, J = 7.4, 1.3 Hz, 3H).

**$^{13}$C NMR (100 MHz, $CD_3OD$)** δ 183.73, 174.61, 142.16, 136.12, 129.07, 126.34, 122.95, 111.30, 65.43, 58.97, 51.99, 49.37, 48.76, 44.92, 37.65, 37.30, 35.83, 33.03, 29.38, 13.27.

**HRMS (ESI, m/z):** calc'd for $C_{20}H_{26}N_2O_3$ $[M+H]^+$ 343.2021, found: 343.2013.

Data for **22**

**Rf** = 0.6, DCM/MeOH = 10/1.

**$^1$H NMR (400 MHz, DMSO-*$d_6$*)** δ 10.36 (s, 1H), 7.22 (dd, J = 7.4, 1.3 Hz, 1H), 7.15 (td, J = 7.7, 1.3 Hz, 1H), 6.95 (td, J = 7.5, 1.1 Hz, 1H), 6.81 (dd, J = 7.8, 1.0 Hz, 1H), 3.47 (s, 3H), 3.27 – 3.17 (m, 2H), 2.47 (dd, J = 15.0, 3.3 Hz, 1H), 2.30 (q, J = 8.7 Hz, 1H), 2.22 (dd, J = 11.4, 2.7 Hz, 1H), 2.17 (ddd, J = 12.2, 9.4, 2.5 Hz, 1H), 1.92 – 1.78 (m, 2H), 1.70 (t, J = 10.8 Hz, 1H), 1.54 – 1.43 (m, 1H), 1.41 – 1.32 (m, 1H), 1.21 – 1.12 (m, 1H), 1.10 – 0.97 (m, 2H), 0.83 (t, J = 7.4 Hz, 3H), 0.60 (q, J = 11.8 Hz, 1H).

**$^{13}$C NMR (100 MHz, DMSO-*$d_6$*)** δ 180.00, 172.72, 141.40, 133.53, 127.48, 124.41, 121.45, 109.19, 70.95, 56.99, 55.98, 53.32, 51.17, 40.58, 37.31, 36.63, 34.67, 31.54, 22.82, 10.83.

**HRMS (ESI, m/z):** calc'd for $C_{20}H_{26}N_2O_3$ $[M+H]^+$ 343.2021, found: 343.2011.

## NMR Spectral Data Comparison of 21

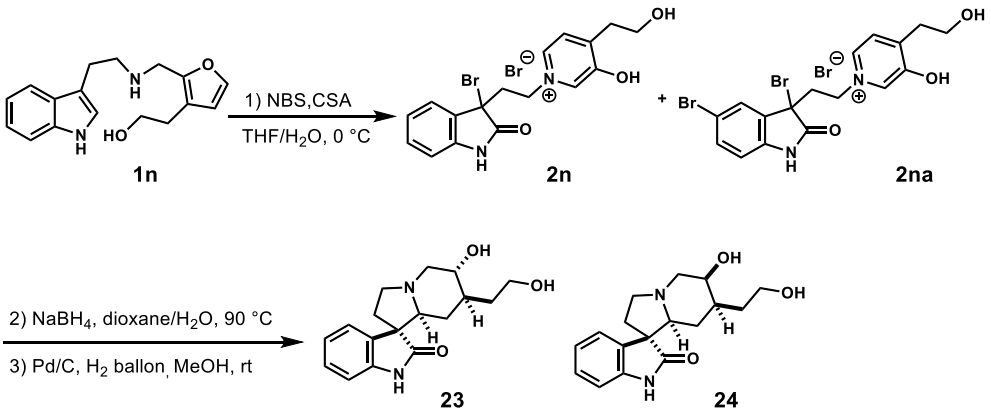
**Table S1**. Comparison of $^1$H NMR data of Oishi's intermediate **21**

| **21** (reported by Martin)[2] $^1$H NMR (500 MHz, DMSO-$d_6$, ppm) | **21** (reported by Tong)[3] $^1$H NMR (400 MHz, DMSO-$d_6$, ppm) | **21** (our synthetic sample) $^1$H NMR (400 MHz, DMSO-$d_6$, ppm) |
|---|---|---|
| 10.32 (s, 1 H) | 10.36 (s, 1 H) | 10.36 (s, 1 H) |
| 7.21 (d, J = 7.4 Hz, 1 H) | 7.22 (d, J = 7.4 Hz, 1 H) | 7.22 (dd, J = 7.4, 1.3 Hz, 1 H) |
| 7.14 (td, J = 7.6, 1.2 Hz, 1 H) | 7.15 (t, J = 7.7, 1 H) | 7.15 (td, J = 7.7, 1.3 Hz, 1H) |
| 6.94 (td, J = 7.4, 0.8 Hz, 1 H) | 6.95 (t, J = 7.5, 1 H) | 6.95 (td, J = 7.5, 1.1 Hz, 1H) |
| 6.80 (d, J = 7.6 Hz, 1 H) | 6.82 (d, J = 7.7 Hz, 1 H) | 6.81 (dd, J = 7.8, 1.0 Hz, 1H) |
| 3.46 (s, 3H) | 3.47 (s, 3H) | 3.47 (s, 3H) |
| 3.24 – 3.17 (comp, 2 H) | 3.26 – 3.20 (m, 2 H) | 3.27 – 3.17 (m, 2 H) |
| 2.45 (dd, J = 15.5, 3.8 Hz, 1 H) | 2.45 (dd, J = 15.5, 3.8 Hz, 1 H) | 2.47 (dd, J = 15.0, 3.3 Hz, 1 H) |
| 2.30 (app q, J = 8.7 Hz, 1 H) | 2.31 (m, 1 H) | 2.30 (q, J = 8.7 Hz, 1H), |
| 2.22 (dd, J = 11.3, 2.3 Hz, 1 H) | 2.22 (m, 1 H) | 2.22 (dd, J = 11.4, 2.7 Hz, 1H) |
| 2.16 (ddd, J = 12.8, 9.5, 2.4 Hz, 1 H) | 2.16 (m, 1 H) | 2.17 (ddd, J = 12.2, 9.4, 2.5 Hz, 1H), |
| 1.90 – 1.79 (comp, 2 H) | 1.93 – 1.80 (m, 2 H) | 1.92 – 1.78 (m, 2H) |
| 1.69 (app t, J = 10.9 Hz, 1 H) | 1.70 (t, J = 10.4 Hz, 1 H) | 1.70 (t, J = 10.8 Hz, 1 H) |
| 1.52 – 1.44 (m, 1 H) | 1.55 – 1.44 (m, 1 H) | 1.54 – 1.43 (m, 1 H) |
| 1.42 – 1.34 (m, 1 H) | 1.42 – 1.34 (m, 1 H) | 1.41 – 1.32 (m, 1 H) |
| 1.20 – 1.12 (m, 1 H) | 1.20 – 1.12 (m, 1 H) | 1.21 – 1.12 (m, 1 H) |
| 1.08 – 0.98 (comp, 2 H) | 1.11 – 0.96 (m, 2 H) | 1.10 – 0.97 (m, 2 H) |
| 0.82 (t, J = 7.4 Hz, 3 H) | 0.83 (t, J = 7.5 Hz, 3 H) | 0.83 (t, J = 7.4 Hz, 3 H) |
| 0.60 (app q, J = 11.9, 1 H) | 0.61 (q, J = 11.9 Hz, 1 H) | 0.60 (q, J = 11.8 Hz, 1 H) |

**Table S2**. Comparison of $^{13}C$ NMR data of Oishi's intermediate **21**

| **21** (reported by Martin)[2] $^{13}C$ NMR (125 MHz, DMSO-$d_6$, ppm) | **21** (reported by Tong)[3] $^{13}C$ NMR (100 MHz, DMSO-$d_6$, ppm) | **21** (our synthetic sample) $^{13}C$ NMR (100 MHz, DMSO-$d_6$, ppm) |
|---|---|---|
| 179.9 | 179.92 | 180.00 |
| 172.6 | 172.62 | 172.72 |
| 141.4 | 141.37 | 141.40 |
| 133.5 | 133.45 | 133.53 |
| 127.4 | 127.44 | 127.48 |
| 124.3 | 124.38 | 124.41 |
| 121.4 | 121.39 | 121.45 |
| 109.1 | 109.16 | 109.19 |
| 70.9 | 70.91 | 70.95 |
| 56.9 | 56.95 | 56.99 |
| 55.9 | 55.92 | 55.98 |
| 53.2 | 53.26 | 53.32 |
| 51.1 | 51.1 | 51.17 |
| 40.5 | 40.53 | 40.58 |
| 37.3 | 37.27 | 37.31 |
| 36.6 | 36.58 | 36.63 |
| 34.6 | 34.64 | 34.67 |
| 31.5 | 31.48 | 31.54 |
| 22.7 | 22.76 | 22.82 |
| 10.7 | 10.75 | 10.83 |

## General Procedure for the Total Synthesis of 7(*R*)-Geissoschizol Oxindole and 7(*S*)-Geissoschizol Oxindole




To a stirred solution of **1n** (1.0 g, 3.5 mmol, 1.0 equiv.) in THF/$H_2O$ = 10/1 (35 mL) was added CSA (1.22 g, 5.25 mmol, 1.5 equiv.) in one portion at rt. After addition, the resulting mixture was cooled to 0 °C. NBS (1.92 g, 10.85mmol, 3.1 equiv.) in THF (10 mL) was added dropwise to the reaction and the resulting mixture was stirred at 0 °C for 2 hours. After completion, the mixture was directly concentrated in vacuo and the crude product was purified by column chromatography on silica gel (DCM/MeOH 50/1 to 10/1) to afford **2n** and **2na** (**2n**/**2na** = 5/1 according to the $^1$H NMR spectrum) as a yellow solid. Then the mixture of **2n**/**2na** was dissolved in dioxane/$H_2O$ = 10/1 (40 mL) and $NaBH_4$ (669 mg, 17.5 mmol, 5.0 equiv.) was added in portions at rt. After addition, the resulting mixture was heated to 90 °C and stirred for 12 hours. After completion, the resulting mixture was concentrated in vacuo and the crude product was redissolved in MeOH. Pd/C (10 wt. %, 100 mg) was added in one portion and the resulting mixture was stirred under a hydrogen atmosphere for 1 hour. The resulting mixture was filtrated through a pad of celite, and the filtrate was concentrated in vacuo. The crude product was purified by column chromatography on silica gel (DCM/MeOH=70/1 to 10/1, with 0.1% $NH_3 \cdot H_2O$) to afford **23** (less polar) as a white solid (120 mg, 11.3% yield, 3 steps) and **24** (more polar) as a white solid (100 mg, 9.4% yield, 3 steps).

Data for **23**

**Rf** = 0.45, DCM/MeOH = 10/1 (with 1 drop of $NH_3 \cdot H_2O$).

**$^1$H NMR (400 MHz, DMSO-*d*$_6$)** δ 10.36 (s, 1H), 7.20 (d, J = 7.3 Hz, 1H), 7.14 (td, J = 7.6, 1.3 Hz, 1H), 6.94 (t, J = 7.5 Hz, 1H), 6.81 (d, J = 7.7 Hz, 1H), 4.77 (d, J = 5.7 Hz, 1H), 4.34 (t, J = 5.1 Hz, 1H), 3.35 – 3.21 (m, 2H), 3.21 – 3.15 (m, 2H), 3.06 (tt, J = 9.9, 5.1 Hz, 1H), 2.31 (q, J = 8.7 Hz, 1H), 2.27 – 2.13 (m, 2H), 1.92 – 1.78 (m, 3H), 1.24 – 1.08 (m, 2H), 0.92 (ddt, J = 13.9, 8.3, 5.7 Hz, 1H), 0.46 (q, J = 12.3 Hz, 1H).

**$^{13}$C NMR (100 MHz, DMSO-*d*$_6$)** δ 180.19, 141.45, 133.66, 133.64, 127.51, 124.44, 121.49, 109.25, 71.00, 70.54, 60.24, 58.85, 55.69, 52.95, 39.81, 35.23, 35.10, 29.59.

**HRMS (ESI, m/z):** calc'd for $C_{17}H_{22}N_2O_3$ $[M+H]^+$ 303.1708, found: 303.1701.

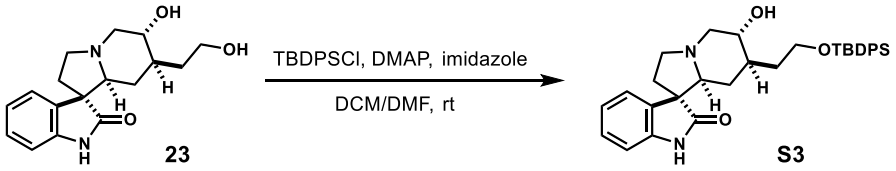
Data for **24**

**Rf** = 0.26, DCM/MeOH = 10/1 (with 1 drop of $NH_3 \cdot H_2O$).

**$^1$H NMR (400 MHz, $CD_3OD$)** δ 7.49 (dd, J = 7.5, 1.3 Hz, 1H), 7.18 (td, J = 7.7, 1.3 Hz, 1H), 7.02 (td, J = 7.5, 1.1 Hz, 1H), 6.90 – 6.85 (m, 1H), 3.72 (p, J = 1.9 Hz, 1H), 3.49 (dq, J = 10.5, 5.1, 4.7 Hz, 2H), 3.28 – 3.20 (m, 2H), 2.46 (t, J = 7.9 Hz, 1H), 2.44 – 2.39 (m, 1H), 2.32 – 2.23 (m, 2H), 2.02 (dt, J = 12.8, 8.6 Hz, 1H), 1.63 – 1.51 (m, 2H), 1.35 – 1.28 (m, 1H), 1.04 (q, J = 11.8 Hz, 1H), 0.92 (dt, J = 12.8, 3.4 Hz, 1H).

**$^{13}$C NMR (100 MHz, $CD_3OD$)** δ 183.71, 142.31, 135.09, 128.78, 126.12, 123.47, 110.59, 73.13, 67.99, 60.39, 60.18, 58.26, 54.82, 37.73, 36.19, 35.79, 28.11.

**HRMS (ESI, m/z):** calc'd for $C_{17}H_{22}N_2O_3$ $[M+H]^+$ 303.1708, found: 303.1700.



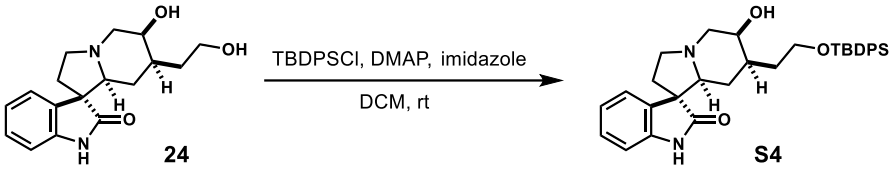
To a stirred solution of **23** (150 mg, 0.5 mmol, 1.0 equiv.) in DCM/DMF = 3/1 (8 mL) at rt was added DMAP (12 mg, 0.1 mmol, 0.2 equiv.) and imidazole (68 mg, 1.0 mmol, 2.0 equiv.). Then TBDPSCl (206 mg, 0.75 mmol, 1.5 equiv.) was added dropwise to the reaction and the resulting mixture was stirred for 2 hours at rt. After completion, the reaction was directly concentrated in vacuo. The resulting oil was purified by column chromatography on silica gel (PE/EA 1/1 to pure EA) to afford **S3** as a white solid (210 mg, 78% yield).

**Rf** = 0.17, PE/EA = 1/1.

**$^1$H NMR (400 MHz, DMSO-*d*$_6$)** δ10.37 (s, 1H), 7.50 (ddd, J = 11.3, 7.8, 1.6 Hz, 4H), 7.45 – 7.34 (m, 6H), 7.19 (d, J = 7.3 Hz, 1H), 7.17 – 7.11 (m, 1H), 6.93 (t, J = 7.5 Hz, 1H), 6.81 (d, J = 7.7 Hz, 1H), 4.70 (d, J = 5.8 Hz, 1H), 3.50 (t, J = 6.3 Hz, 2H), 3.19 (dt, J = 13.4, 6.5 Hz, 2H), 3.07 (p, J = 6.3, 5.5 Hz, 1H), 2.32 (d, J = 8.6 Hz, 1H), 2.26 (dd, J = 11.0, 2.1 Hz, 1H), 2.23 – 2.14 (m, 1H), 2.05 – 1.96 (m, 1H), 1.91 – 1.79 (m, 2H), 1.07 – 0.95 (m, 1H), 0.88 (s, 10H), 0.51 (t, J = 12.2 Hz, 1H).

**$^{13}$C NMR (100 MHz, DMSO-*d*$_6$)** δ180.12, 162.34, 141.48, 134.96, 133.58, 133.14, 129.78, 127.86, 127.42, 124.34, 121.40, 109.23, 71.00, 70.22, 61.98, 60.27, 55.61, 52.92, 35.23, 34.20, 29.58, 26.59, 18.61.

**HRMS (ESI, m/z):** calc'd for $C_{33}H_{40}N_2O_3Si$ $[M+H]^+$ 541.2886, found: 541.2875.



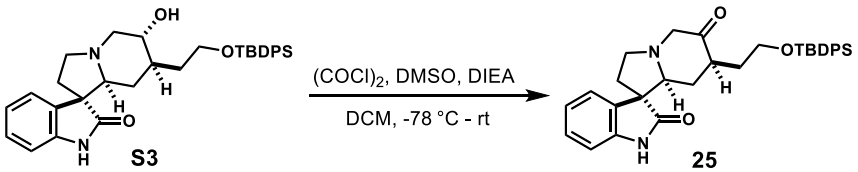

To a stirred solution of **24** (440 mg, 1.45 mmol, 1.0 equiv.) in DCM (15 mL) at rt was added DMAP (35 mg, 0.29 mmol, 0.2 equiv.) and imidazole (198mg, 2.9 mmol, 2.0 equiv.). Then TBDPSCl (598 mg, 2.18 mmol, 1.5 equiv.) was added dropwise to the reaction. The resulting mixture was stirred for 2 hours at rt. After completion, the reaction was quenched by addition of $H_2O$ (15mL). The solution was transferred to a separatory funnel and the organic layer was collected. The aqueous layer was extracted with DCM (2 × 10 mL). The combined organic layers were washed with brine (15 mL), dried over $Na_2SO_4$, and concentrated in vacuo. The resulting oil was purified by column chromatography on silica gel (DCM/MeOH 100/1 to 50/1) to afford **S4** as a white solid (630 mg, 80% yield).

**Rf** = 0.4, DCM/MeOH = 20/1.

**$^1$H NMR (400 MHz, CDCl$_3$)** δ 7.64 (s, 1H), 7.61 – 7.56 (m, 4H), 7.44 – 7.27 (m, 7H), 7.21 (td, J = 7.7, 1.2 Hz, 1H), 7.05 (t, J = 7.5 Hz, 1H), 6.87 (dt, J = 7.8, 0.8 Hz, 1H), 3.76 – 3.50 (m, 3H), 3.27 (d, J = 10.5 Hz, 2H), 2.57 (dd, J = 25.4, 10.2 Hz, 2H), 2.42 (t, J = 9.4 Hz, 1H), 2.27 (d, J = 11.3 Hz, 1H), 2.04 (q, J = 10.0, 8.4 Hz, 1H), 1.60 (d, J = 12.5 Hz, 2H), 1.43 – 1.31 (m, 1H), 1.16 – 1.07 (m, 1H), 0.98 (s, 9H), 0.92 – 0.80 (m, 1H).

**$^{13}$C NMR (100 MHz, CDCl$_3$)** δ 181.86, 140.30, 135.50, 133.76, 129.57, 127.80, 127.63, 124.48, 122.74, 109.87, 71.23, 67.16, 61.47, 59.06, 57.07, 53.16, 36.40, 34.79, 26.84, 26.71, 19.12.

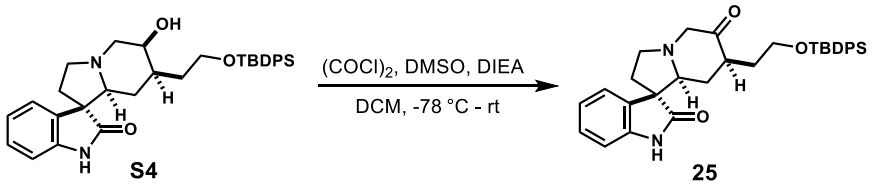
**HRMS (ESI, m/z):** calc'd for $C_{33}H_{40}N_2O_3Si$ $[M+H]^+$ 541.2886, found: 541.2876.




To a round bottom flask was added $(COCl)_2$ (84 µL, 1.0 mmol, 5.0 equiv.), then DCM (4 mL) was added through a syringe at rt. The resulting solution was cooled to -78 °C. DMSO (84 µL, 1.2 mmol, 6.0 equiv.) in DCM (0.3 mL) was added dropwise to the reaction and the resulting mixture was stirred for 20 min. **S3** (109 mg, 0.2 mmol, 1.0 equiv.) in DCM (6.0 mL) was added dropwise to the reaction and the resulting mixture was stirred for 2 hours at -78 °C. DIEA (350 µL, 2.0 mmol, 10.0 equiv.) was added dropwise to the reaction and the resulting mixture was stirred for 10 min. Then the reaction was moved to rt and stirred for 30 min. After completion, the reaction was quenched by addition of $H_2O$ (10mL). The solution was transferred to a separatory funnel and the organic layer was collected. The aqueous layer was extracted with DCM (2 × 10 mL). The combined organic layers were washed with brine (15 mL), dried over $Na_2SO_4$, and concentrated in vacuo. The resulting oil was purified by column chromatography on silica gel (PE/EA 5/1 to 1/1) to afford **25** as a white solid (102 mg, 95% yield).

Data for **25**

See below the synthesis of **25** from **S4**.




S4 25

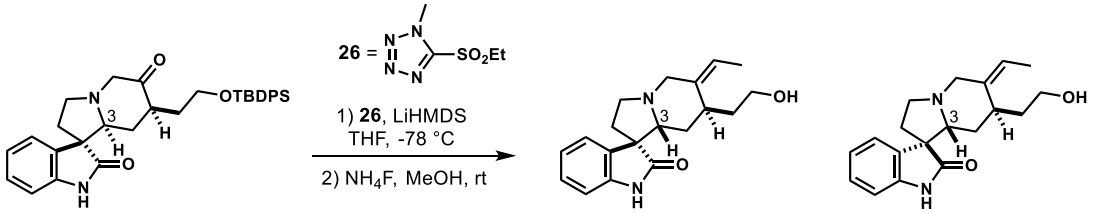
To a round bottom flask was added $(COCl)_2$ (167 µL, 1.94 mmol, 5.0 equiv.), then DCM (10 mL) was added through a syringe at rt. The resulting solution was cooled to -78 °C. DMSO (170 µL, 2.33 mmol, 6.0 equiv.) in DCM (0.5 mL) was added dropwise to the reaction and the resulting mixture was stirred for 30 min. **S4** (210 mg, 0.39 mmol, 1.0 equiv.) in DCM (4.0 mL) was added dropwise to the reaction and the resulting mixture was stirred for 2 hours at -78 °C. DIEA (674 µL, 3.88 mmol, 10.0 equiv.) was added dropwise to the reaction and the resulting mixture was stirred for 10 min. Then the reaction was moved to rt and stirred for 30 min. After completion, the reaction was quenched by addition of $H_2O$ (10mL). The solution was transferred to a separatory funnel and the organic layer was collected. The aqueous layer was extracted with DCM (2 × 10 mL). The combined organic layers were washed with brine (15 mL), dried over $Na_2SO_4$, and concentrated in vacuo. The resulting oil was purified by column chromatography on silica gel (PE/EA 5/1 to 1/1) to afford **25** as a white solid (196 mg, 94% yield).

**Rf** = 0.48, PE/EA = 1/1.

**$^1$H NMR (400 MHz, $CDCl_3$)** δ 8.54 (s, 1H), 7.59 – 7.52 (m, 4H), 7.41 – 7.32 (m, 6H), 7.31 (d, J = 1.8 Hz, 1H), 7.20 (td, J = 7.7, 1.3 Hz, 1H), 7.02 (td, J = 7.6, 1.0 Hz, 1H), 6.94 – 6.88 (m, 1H), 3.65 – 3.50 (m, 3H), 3.33 (td, J = 8.6, 2.8 Hz, 1H), 3.05 (dd, J = 11.2, 2.4 Hz, 1H), 2.93 (d, J = 13.1 Hz, 1H), 2.63 (q, J = 8.7 Hz, 1H), 2.53 (ddd, J = 12.6, 9.6, 2.8 Hz, 1H), 2.41 (dq, J = 12.6, 6.1 Hz, 1H), 2.20 – 2.04 (m, 2H), 1.64 (ddd, J = 12.8, 6.1, 2.5 Hz, 1H), 1.34 – 1.17 (m, 1H), 1.10 – 1.01 (m, 1H), 0.95 (s, 9H).

**$^{13}$C NMR (100 MHz, $CDCl_3$)** δ 206.51, 181.40, 140.03, 135.47, 133.63, 132.92, 129.58, 127.97, 127.63, 125.12, 122.76, 109.77, 69.93, 63.77, 61.40, 56.25, 53.75, 43.72, 35.73, 31.16, 30.90, 29.70, 26.81, 19.07.

**HRMS (ESI, m/z):** calc'd for $C_{33}H_{38}N_2O_3Si$ $[M+H]^+$ 539.2730, found: 539.2720.




25 27 28

To a round bottom flask was added **26** (166 mg, 0.94 mmol, 4.0 equiv.), then THF (6 mL) was added through a syringe. The resulting solution was cooled to -78 °C. LiHMDS (1.15 mL, 1.15 mmol, 5.0 equiv.) was added dropwise to the reaction and the resulting mixture was stirred at -78 °C for 30 min. Then **25** (120 mg, 0.22 mmol, 1.0 equiv.) in THF (1.5 mL) was added dropwise to the reaction and the resulting mixture was stirred for 30 min. After completion, the reaction was quenched by addition of sat. aq. $NH_4Cl$ (2 mL) and $H_2O$ (10 mL). The solution was transferred to a separatory funnel and extracted with EA (3 × 5 mL). The organic layers were combined and washed with brine (10 mL), dried over $Na_2SO_4$, and concentrated in vacuo. The crude product was dissolved in MeOH (12 mL) and $NH_4F$ (1.77 g, 48 mmol, 218 equiv.) was added in one portion. The resulting mixture was stirred at rt for 12 hours. DCM (40 mL) was added to the reaction and the solid was filtrated and the filtrate was concentrated in vacuo. The crude product was purified by column chromatography on silica gel (DCM/MeOH 70/1 to 10/1) to afford **27** as a light yellow solid (31 mg, 45% yield, 2 steps) and **28** as a light yellow solid (11 mg, 16% yield, 2 steps).

Data for **27**

**Rf** = 0.25, DCM/MeOH = 10/1.

**$^1$H NMR (400 MHz, $CDCl_3$)** δ 8.45 (s, 1H), 7.22 (d, J = 7.8 Hz, 1H), 7.20 (td, J = 7.7, 1.4 Hz, 1H), 7.05 (td, J = 7.5, 1.0 Hz, 1H), 6.88 (d, J = 7.7 Hz, 1H), 5.47 (q, J = 6.1 Hz, 1H), 3.53 dt (10.4, 6.4, 1H), 3.48 dt (10.4, 6.4, 1H), 3.44 (d, J = 11.8 Hz, 1H), 3.40 – 3.33 (m, 1H), 2.91 dt (9.2, 4.8, 1H), 2.85 (d, J = 11.6 Hz, 1H), 2.59 (d, J = 11.9 Hz, 1H), 2.53 – 2.48 (m, 1H), 2.48 – 2.43 (m, 1H), 2.09 – 1.99 (m, 1H), 1.80 – 1.77 (m, 1H), 1.75 – 1.71 (m, 1H), 1.59 (dd, J = 6.8, 1.7 Hz, 3H), 1.50 – 1.38 (m, 1H), 1.23 (d, J = 8.8 Hz, 1H)

**$^{13}$C NMR (100 MHz, $CDCl_3$)** δ 181.3, 140.9, 135.8, 133.7, 128.1, 123.1, 122.8, 121.8, 109.6, 70.4, 61.4, 58.1, 55.8, 54.8, 35.0, 34.9, 30.4, 30.1, 13.1.

**$^1$H NMR (400 MHz, $CD_3OD$)** δ 7.29 (d, J = 7.5 Hz, 1H), 7.20 (td, J = 7.7, 1.2 Hz, 1H), 7.04 (td, J = 7.6, 1.0 Hz, 1H), 6.86 (d, J = 7.7 Hz, 1H), 5.46 (q, J = 7.4, 6.9 Hz, 1H), 3.39 (ddd, J = 9.0, 6.7, 3.6 Hz, 2H), 3.30 (s, 1H), 3.22 (td, J = 8.5, 1.4 Hz, 1H), 3.00 – 2.91 (m, 1H), 2.87 (dt, J = 11.8, 2.0 Hz, 1H), 2.66 (dd, J = 12.2, 2.5 Hz, 1H), 2.52 (dt, J = 10.1, 8.5 Hz, 1H), 2.35 (ddd, J = 13.1, 10.1, 8.1 Hz, 1H), 2.04 (ddd, J = 13.0, 8.1, 1.5 Hz, 1H), 1.74 – 1.63 (m, 2H), 1.62 (dd, J = 6.8, 1.8 Hz, 3H), 1.43 (tt, J = 13.4, 6.4 Hz, 1H), 1.22 (dt, J = 12.7, 2.2 Hz, 1H).

**$^{13}$C NMR (100 MHz, $CD_3OD$)** δ 182.77, 143.04, 137.36, 134.67, 129.16, 124.01, 123.62, 122.33, 110.44, 71.11, 60.63, 58.98, 56.95, 55.40, 35.60, 35.32, 30.79, 13.15.

**HRMS (ESI, m/z):** calc'd for $C_{19}H_{24}N_2O_2$ $[M+H]^+$ 313.1916, found: 313.1906.

Data for **28**

**Rf** = 0.32, DCM/MeOH = 10/1.

**$^1$H NMR (400 MHz, $CDCl_3$)** δ 8.47 (s, 1H), 7.37 (d, J = 7.4 Hz, 1H), 7.17 (td, J = 7.7, 1.3 Hz, 1H), 7.00 (td, J = 7.5, 1.1 Hz, 1H), 6.87 (d, J = 7.6 Hz, 1H), 5.45 (q, J = 7.2, 6.7 Hz, 1H), 3.57 (dt, J = 12.5, 6.4 Hz, 1H), 3.53 – 3.46 (m, 1H), 3.35 (d, J = 11.9 Hz, 1H), 3.29 (td, J = 8.6, 2.1 Hz, 1H), 2.93 (d, J = 12.0 Hz, 1H), 2.88 – 2.80 (m, 1H), 2.76 (dd, J = 11.6, 3.1 Hz, 1H), 2.51 (q, J = 8.9 Hz, 1H), 2.40 (ddd, J = 12.8, 9.0, 2.0 Hz, 1H), 2.06 (dt, J = 12.8, 8.4 Hz, 1H), 1.81 (ddt, J = 13.8, 9.5, 6.2 Hz, 1H), 1.58 (dd, J = 6.8, 1.6 Hz, 3H), 1.56 – 1.52 (m, 1H), 1.23 – 1.15 (m, 1H), 1.12 (dt, J = 13.0, 2.7 Hz, 1H).

**$^{13}$C NMR (100 MHz, $CDCl_3$)** δ 182.3, 140.3, 136.9, 133.6, 127.6, 125.3, 122.4, 120.7, 109.6, 67.7, 61.0, 58.3, 56.6, 54.1, 35.3, 35.0, 31.0, 29.9, 13.0.

**$^1$H NMR (400 MHz, $CD_3OD$)** δ 7.39 (dd, J = 7.5, 0.7 Hz, 1H), 7.19 (td, J = 7.7, 1.3 Hz, 1H), 7.00 (td, J = 7.6, 1.1 Hz, 1H), 6.88 (d, J = 7.5 Hz, 1H), 5.49 (q, J = 7.3, 6.4 Hz, 1H), 3.51 – 3.41 (m, 2H), 3.38 (d, J = 12.0 Hz, 1H), 3.26 (ddd, J = 8.7, 7.9, 1.8 Hz, 1H), 2.94 (dt, J = 11.9, 1.9 Hz, 1H), 2.89 (dt, J = 10.0, 3.2 Hz, 1H), 2.74 (dd, J = 12.1, 2.7 Hz, 1H), 2.48 (q, J = 9.0 Hz, 1H), 2.32 (ddd, J = 13.1, 8.7, 1.8 Hz, 1H), 2.03 (ddd, J = 13.1, 9.6, 8.3 Hz, 1H), 1.74 (dddd, J = 15.4, 8.0, 6.6, 4.1 Hz, 1H), 1.61 (dd, J = 6.8, 1.8 Hz, 3H), 1.59 – 1.50 (m, 1H), 1.20 (ddd, J = 13.1, 12.1, 5.4 Hz, 1H), 1.08 (dt, J = 13.1, 2.4 Hz, 1H).

**$^{13}$C NMR (100 MHz, $CD_3OD$)** δ 184.48, 142.50, 137.72, 134.50, 128.98, 126.08, 123.34, 122.21, 110.73, 69.03, 60.67, 59.42, 57.79, 55.21, 36.22, 35.86, 32.46, 30.79, 13.12.

**HRMS (ESI, m/z):** calc'd for $C_{19}H_{24}N_2O_2$ $[M+H]^+$ 313.1916, found: 313.1908.

## NMR Spectral Data Comparison of Geissoschizol Oxindoles (Natural) and 27/28 (Synthetic)

Table **S3**. Comparison of $^1$H NMR data of 7(*R*)-geissoschizol oxindole (natural) and **27** (synthetic).

| Position of hydrogens | 7(*R*)-geissoschizol oxindole (natural)[4] $^1$H-NMR (400 MHz, $CDCl_3$, ppm) | **27** (our synthetic) $^1$H-NMR (400 MHz, $CDCl_3$, ppm) | Chemical shift, Δδ (ppm) |
|---|---|---|---|
| 2 | - | - | - |
| 3 | 2.58 dd (12, 2.2) | 2.59 (d, J = 11.9 Hz, 1H) | -0.01 |
| 5 | 2.47 m (α) | 2.53 – 2.48 (m, 1H) | -0.03 |
| | 3.37 m (β) | 3.40 – 3.33 (m, 1H) | 0 |
| 6 | 2.03 m (α) | 2.09 – 1.99 (m, 1H) | -0.01 |
| | 2.47 m (β) | 2.48 – 2.43 (m, 1H) | -0.01 |
| 7 | - | - | - |
| 8 | - | - | - |
| 9 | 7.21 d (7.5) | 7.22 (d, J = 7.8 Hz, 1H) | -0.01 |
| 10 | 7.03 td (7.5, 1) | 7.05 (td, *J* = 7.5, 1.0 Hz, 1H) | -0.02 |
| 11 | 7.19 td (7.5, 1) | 7.20 (td, *J* = 7.7, 1.4 Hz, 1H) | -0.01 |
| 12 | 6.90 d (7.5) | 6.88 (d, *J* = 7.7 Hz, 1H) | -0.02 |
| 13 | - | - | - |
| 14 | 1.24 br d (12) (α) | 1.23 (d, J = 8.8 Hz, 1H) | 0.01 |
| | 1.75 td (12, 5.5) (β) | 1.75 – 1.71 (m, 1H) | 0.02 |
| 15 | 2.91 dt (10.0, 5.5) | 2.91 dt (9.2, 4.8, 1H) | 0 |
| 16 | 1.44 m | 1.50 – 1.38 (m, 1H) | 0 |
| | 1.77 m | 1.80 – 1.77 (m, 1H) | -0.01 |
| 17 | 3.48 dt (10.5, 6.5) | 3.48 dt (10.4, 6.4, 1H) | 0 |
| | 3.52 dt (10.5, 6.5) | 3.53 dt (10.4, 6.4, 1H) | -0.01 |
| 18 | 1.59 dd (6.8, 1.3) | 1.59 (dd, J = 6.8, 1.7 Hz, 3H) | 0 |
| 19 | 5.46 q (6.8) | 5.47 (q, J = 6.1 Hz, 1H) | -0.01 |
| 20 | - | - | - |
| 21 | 2.84 d (11.5) (α) | 2.85 (d, J = 11.6 Hz, 1H) | -0.01 |
| | 3.43 d (11.5) (β) | 3.44 (d, J = 11.8 Hz, 1H) | -0.01 |
| NH | 9.03 br s | 8.45 (s, 1H) | 0.58 |

Table **S4**. Comparison of $^{13}C$ NMR data of 7(*R*)-geissoschizol oxindole (natural) and **27** (synthetic).

| Position of carbons | 7(*R*)-geissoschizol oxindole (natural)[4] $^{13}C$ NMR (100 MHz, $CDCl_3$, ppm) | **27** (our synthetic) $^{13}C$ NMR (100 MHz, $CDCl_3$, ppm) | Chemical shift, Δδ (ppm) |
|---|---|---|---|
| 2 | 181.9 | 181.3 | 0.6 |
| 3 | 70.3 | 70.4 | -0.1 |
| 5 | 54.8 | 54.8 | 0 |
| 6 | 34.8 | 34.9 | -0.1 |
| 7 | 55.8 | 55.8 | 0 |
| 8 | 133.7 | 133.7 | 0 |
| 9 | 122.9 | 123.1 | -0.2 |
| 10 | 122.6 | 122.8 | -0.2 |
| 11 | 128.0 | 128.1 | -0.1 |
| 12 | 109.8 | 109.6 | 0.2 |
| 13 | 141.2 | 140.9 | 0.3 |
| 14 | 30.3 | 30.4 | -0.1 |
| 15 | 30.0 | 30.1 | -0.1 |
| 16 | 34.9 | 35.0 | -0.1 |
| 17 | 61.1 | 61.4 | -0.3 |
| 18 | 13.0 | 13.1 | -0.1 |
| 19 | 121.6 | 121.8 | -0.2 |
| 20 | 135.8 | 135.8 | 0 |
| 21 | 58.0 | 58.1 | -0.1 |

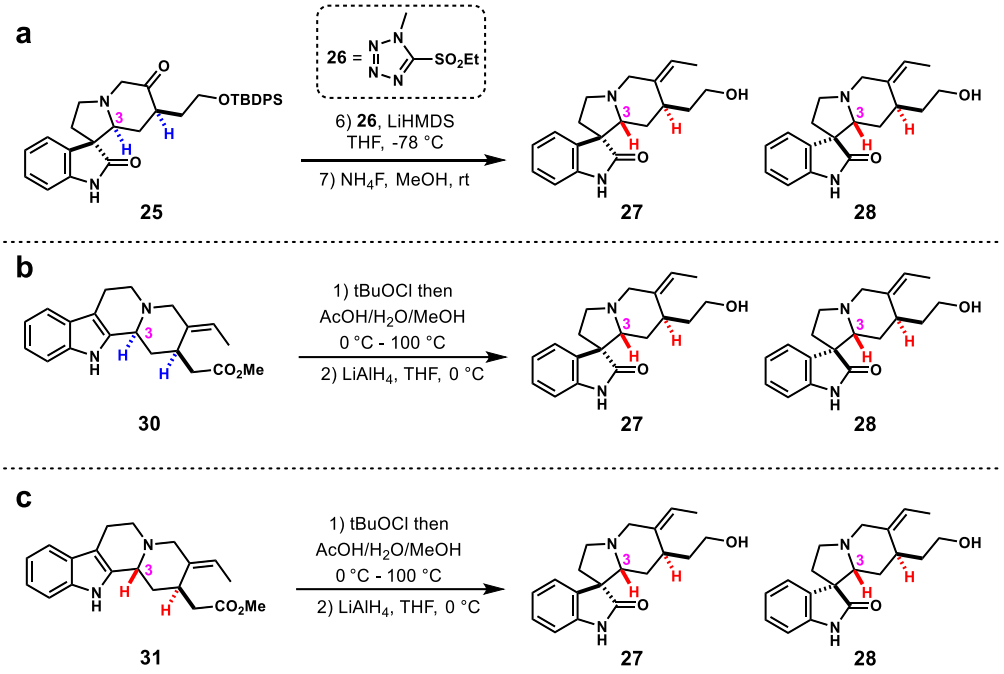
Table **S5**. Comparison of $^{1}$H NMR data of 7(*S*)-geissoschizol oxindole (natural) and **28** (synthetic).

| Position of hydrogens | 7(*S*)-geissoschizol oxindole (natural)[4] $^{1}$H-NMR (400 MHz, $CDCl_3$, ppm) | **28** (our synthetic) $^{1}$H NMR (400 MHz, $CDCl_3$, ppm) | Chemical shift, Δδ (ppm) |
|---|---|---|---|
| 2 | - | - | - |
| 3 | 2.76 dd (12, 3) | 2.76 (dd, *J* = 11.6, 3.1 Hz, 1H) | 0 |
| 5 | 2.51 q (9) (α) | 2.51 (q, *J* = 8.9 Hz, 1H) | 0 |
| | 3.30 td (9, 2) (β) | 3.29 (td, *J* = 8.6, 2.1 Hz, 1H) | 0.01 |
| 6 | 2.06 dt (12.9, 9) (α) | 2.06 (dt, J = 12.8, 8.4 Hz, 1H) | 0 |
| | 2.39 ddd (12.9, 9, 2) (β) | 2.40 (ddd, J = 12.8, 9.0, 2.0 Hz, 1H) | -0.01 |
| 7 | - | - | - |
| 8 | - | - | - |
| 9 | 7.38 d (7.5) | 7.37 (d, *J* = 7.4 Hz, 1H) | 0.01 |
| 10 | 7.01 td (7.5, 1.1) | 7.00 (t, *J* = 7.5 Hz, 1.1 Hz, 1H) | 0.01 |
| 11 | 7.17 td (7.5, 1.1) | 7.18 (td, *J* = 7.7, 1.3 Hz, 1H) | -0.01 |
| 12 | 6.87 d (7.5) | 6.87 (d, *J* = 7.6 Hz, 1H) | 0 |
| 13 | - | - | - |
| 14 | 1.13 dt (12, 3) (α) | 1.12 (dt, J = 13.0, 2.7 Hz, 1H) | 0.01 |
| | 1.19 td (12, 5.4) (β) | 1.23 – 1.15 (m, 1H) | 0 |
| 15 | 2.85 m | 2.88 – 2.80 (m, 1H) | 0.01 |
| 16 | 1.57 m | 1.56 – 1.52 (m, 1H) | 0.03 |
| | 1.80 ddt (13.9, 9.5, 6.5) | 1.81 (ddt, J = 13.8, 9.5, 6.2 Hz, 1H) | -0.01 |
| 17 | 3.51 dt (10.7, 6.5) | 3.53 – 3.46 (m, 1H), | 0.01 |
| | 3.57 dt (10.7, 6.5) | 3.57 (dt, *J* = 12.5, 6.4 Hz, 1H) | 0 |
| 18 | 1.59 dd (6.8, 1.7) | 1.58 (dd, J = 6.8, 1.6 Hz, 3H) | 0.01 |
| 19 | 5.45 q (6.8) | 5.45 (q, *J* = 6.7 Hz, 1H) | 0 |
| 20 | - | - | - |
| 21 | 2.94 d (11.9) (α) | 2.93 (d, J = 12.0 Hz, 1H) | 0.01 |
| | 3.36 d (11.9) (β) | 3.35 (d, *J* = 11.9 Hz, 1H) | 0.01 |
| NH | 8.56 br s | 8.47 (br s, 1H) | 0.09 |

Table **S6**. Comparison of $^{13}C$ NMR data of 7(*S*)-geissoschizol oxindole (natural) and **28** (synthetic).

| Position of carbons | 7(*S*)-geissoschizol oxindole (natural)[4] $^{13}C$-NMR (100 MHz, $CDCl_3$, ppm) | **28** (our synthetic) $^{13}C$ NMR (100 MHz, $CDCl_3$, ppm) | Chemical shift, Δδ (ppm) |
|---|---|---|---|
| 2 | 182.2 | 182.3 | -0.1 |
| 3 | 67.6 | 67.7 | -0.1 |
| 5 | 53.9 | 54.1 | -0.2 |
| 6 | 35 | 35.3 | -0.3 |
| 7 | 56.4 | 56.6 | -0.2 |
| 8 | 133.1 | 133.6 | -0.5 |
| 9 | 125.3 | 125.3 | 0 |
| 10 | 122.4 | 122.4 | 0 |
| 11 | 127.6 | 127.6 | 0 |
| 12 | 109.6 | 109.6 | 0 |
| 13 | 140.3 | 140.3 | 0 |
| 14 | 30.7 | 31.0 | -0.3 |
| 15 | 29.7 | 29.9 | -0.2 |
| 16 | 34.8 | 35.0 | -0.2 |
| 17 | 60.7 | 61.0 | -0.3 |
| 18 | 12.9 | 13.0 | -0.1 |
| 19 | 121 | 120.7 | 0.3 |
| 20 | 136.2 | 136.9 | -0.7 |
| 21 | 58.1 | 58.3 | -0.2 |

## Different Methods for the Synthesis of 27/28 and their NMR Spectrum Comparison.




Note: **29** and **30** were synthesized from tryptamine in 5 steps according to the reported procedures[5].

Procedures for **b** and **c** (depicted in Scheme S-1): To a stirred solution of **30** (or **31**) (80 mg, 0.25 mmol, 1.0 equiv.) in DCM (5 mL) was added TEA (69 μL, 0.50 mmol, 2.0 equiv.) at rt. Then the tube was cooled to 0 °C. *t*-BuOCl (56 mg, 0.50 mmol, 2.0 eq) was added dropwise to the stirred solution at 0 °C. The resulting mixture was stirred at 0 °C for 20 min. After the complete consumption of the starting material detected by TLC analysis, the reaction mixture was concentrated in vacuo. In the same tube, the residue was redissolved in the mixture of MeOH (2.0 mL) and $H_2O$ (2.0 mL). To the suspension was added AcOH (0.2 mL) in one portion. The tube was then sealed and the reaction mixture was stirred at 100 °C for 2 hours. Then the reaction was quenched by addition of sat. aq. $NaHCO_3$ and extracted by EA, dried over $Na_2SO_4$ and concentrated in vacuo. The crude product was redissolved in THF (4.0 mL) and cooled to 0 °C. $LiAlH_4$ was added in portions at 0 °C before the reaction mixture was moved to rt and stirred for 1 hour. $Na_2SO_4 \cdot 10H_2O$ was added in portions to quench the reaction and the result suspension was stirred for 30 min before filtrated through a pad of celite. The filtrate was concentrated in vacuo and the crude product was purified by column chromatography on silica gel (DCM/MeOH 70/1 to 10/1).

For process b from **30**: **27** (36 mg, 46%) and **28** (24 mg, 31%).

For process c from **31**: **27** (21 mg, 27%) and **28** (10 mg, 13%).

**Figure S1.** $^{1}$H NMR spectrum comparison of **27** (400 MHz, $CD_3OD$).

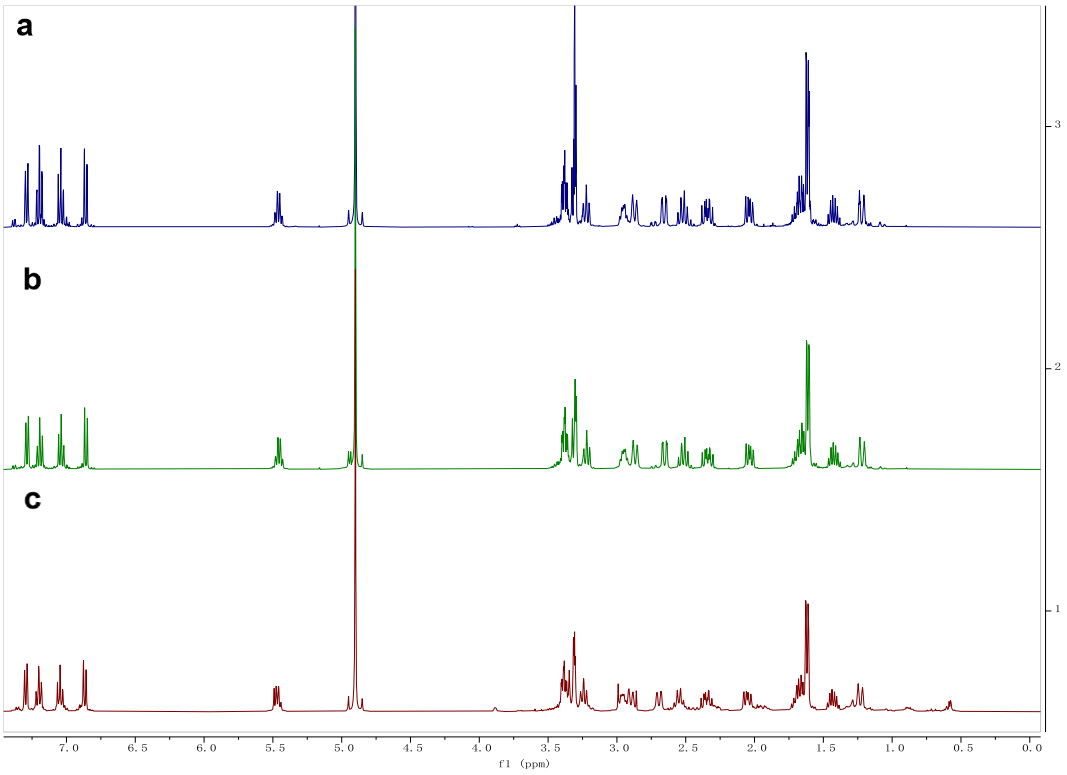
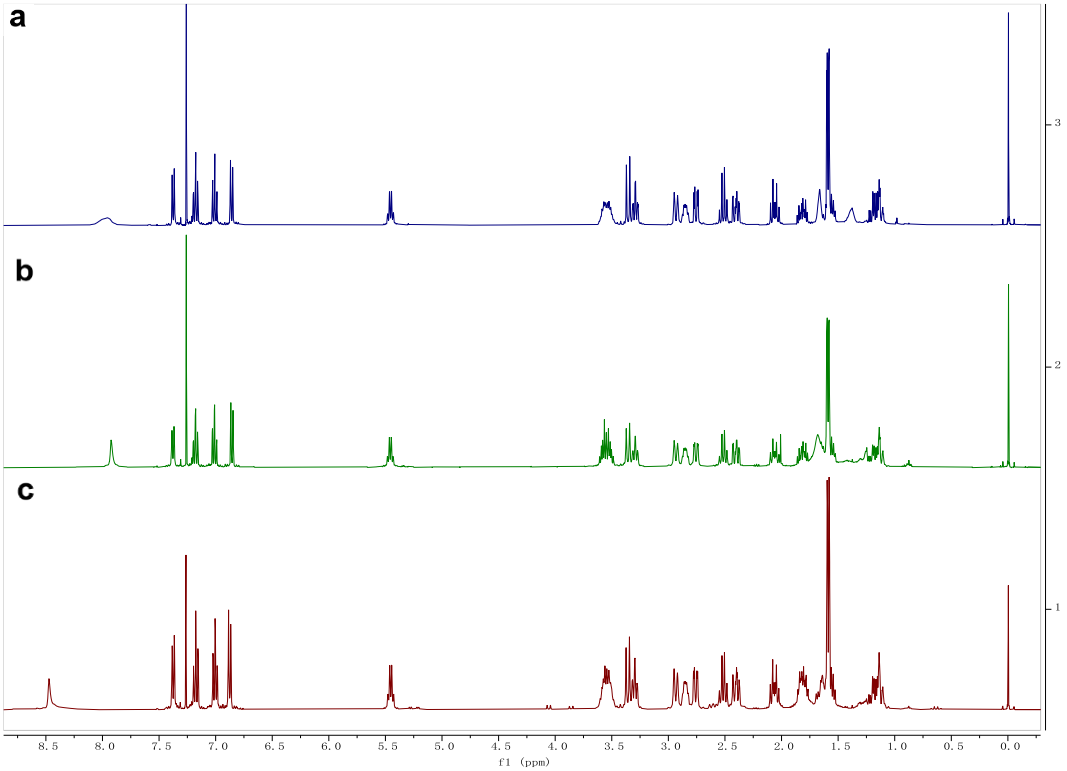



**Figure S2.** $^{1}$H NMR spectrum comparison of **28** (400 MHz, $CDCl_3$).



## NMR Spectra Comparison of Geissoschizol Oxindoles (Natural) and 27/28 (Synthetic)

**Figure S3.** $^{1}$H NMR spectrum comparison of 7(*R*)-geissoschizol oxindole (natural) and **27** (synthetic).

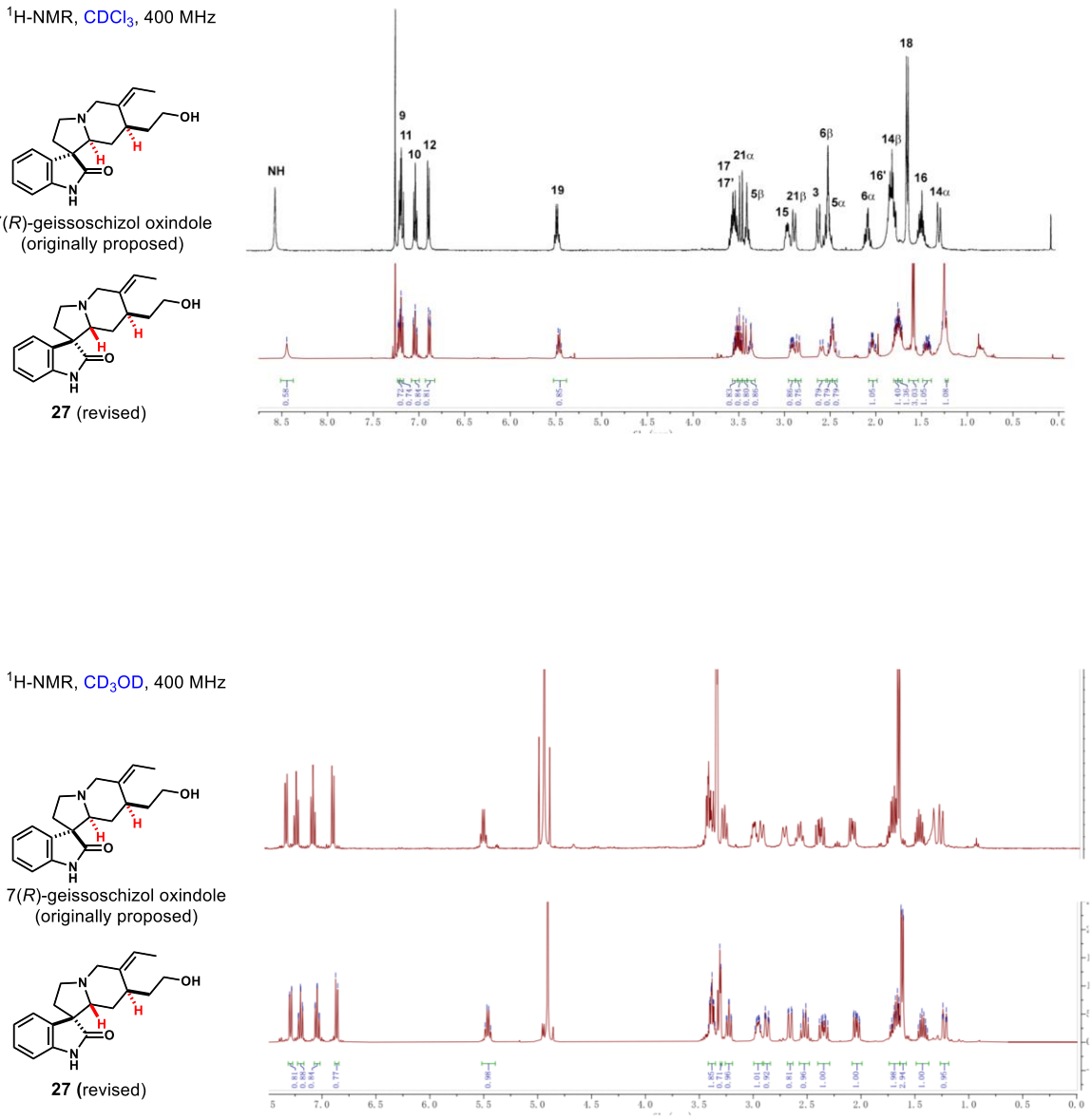
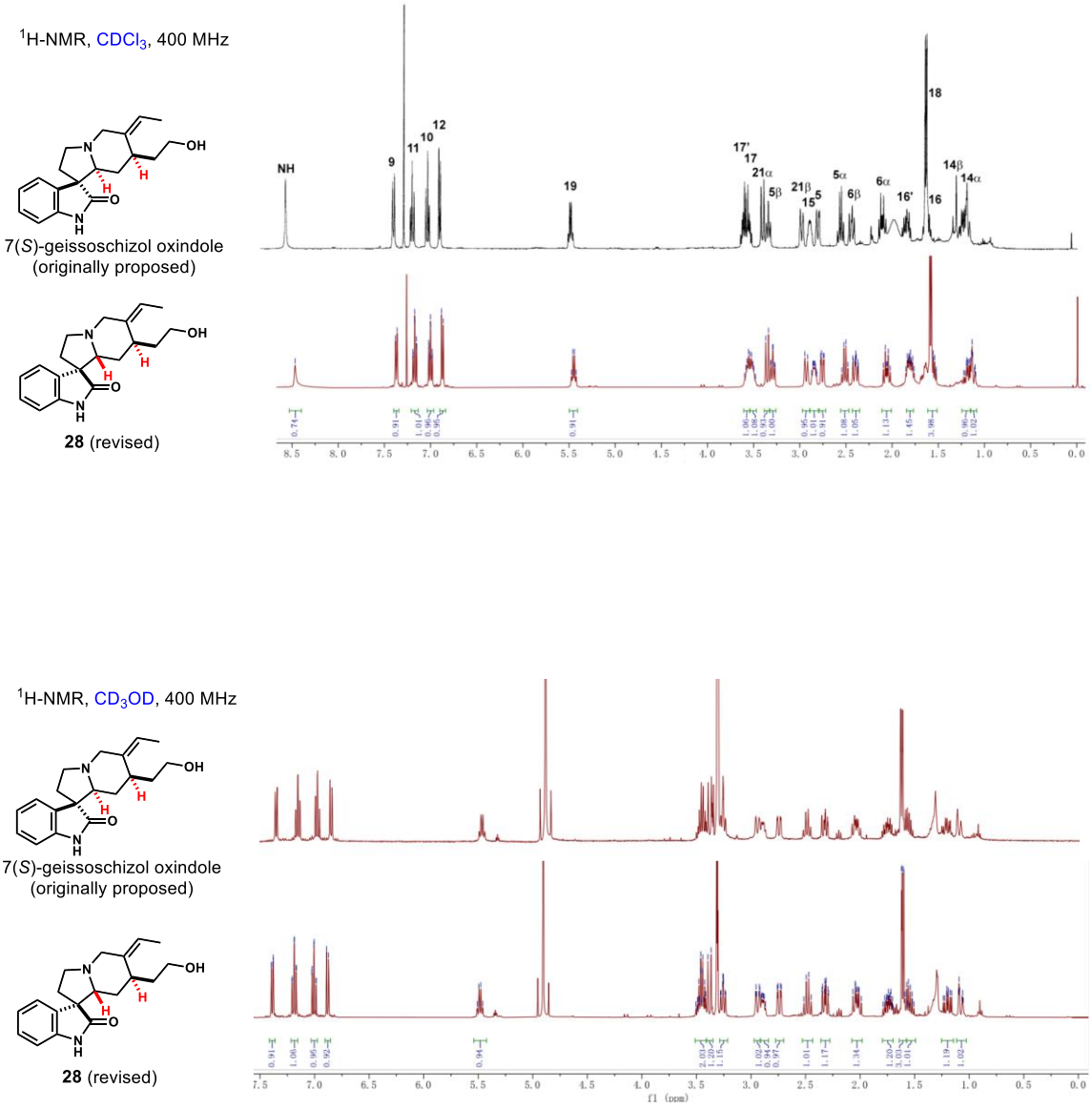


**Figure S4.** $^{1}$H NMR spectrum comparison of 7(*S*)-geissoschizol oxindole (natural) and **28** (synthetic).



## Mixed NMR Spectrum of Geissoschizol Oxindoles (Natural) and 27/28 (Synthetic)

**Figure S5.** $^{1}$H NMR spectrum of a mixture of 7(*R*)-geissoschizol oxindole (natural, 1.5 mg) and **27** (synthetic, 1.5 mg) (400 MHz, $CD_3OD$).

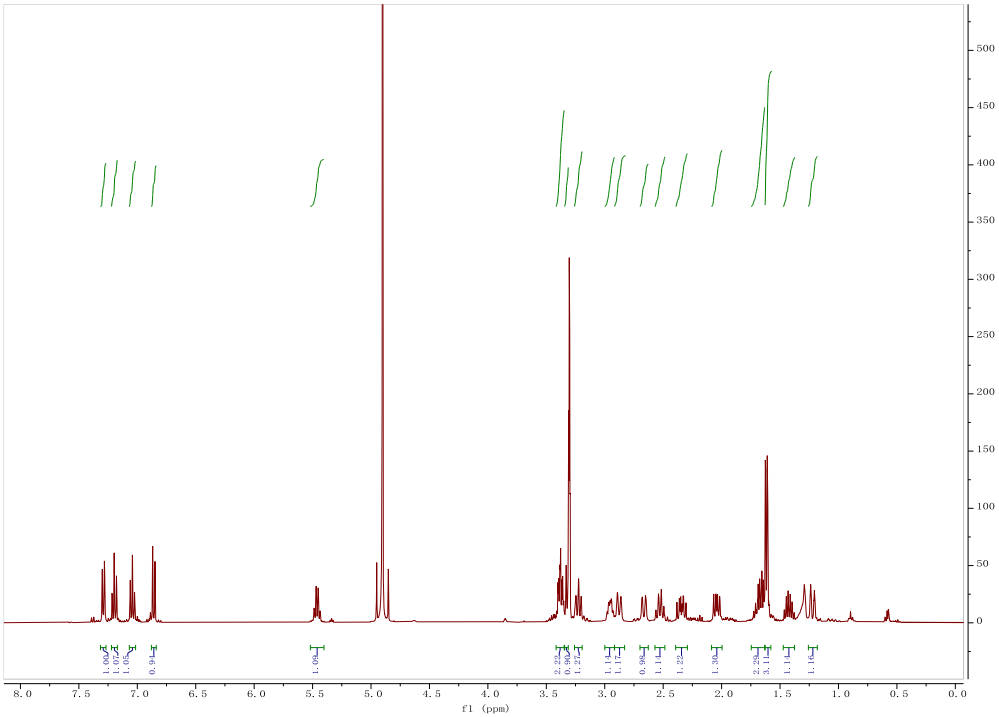
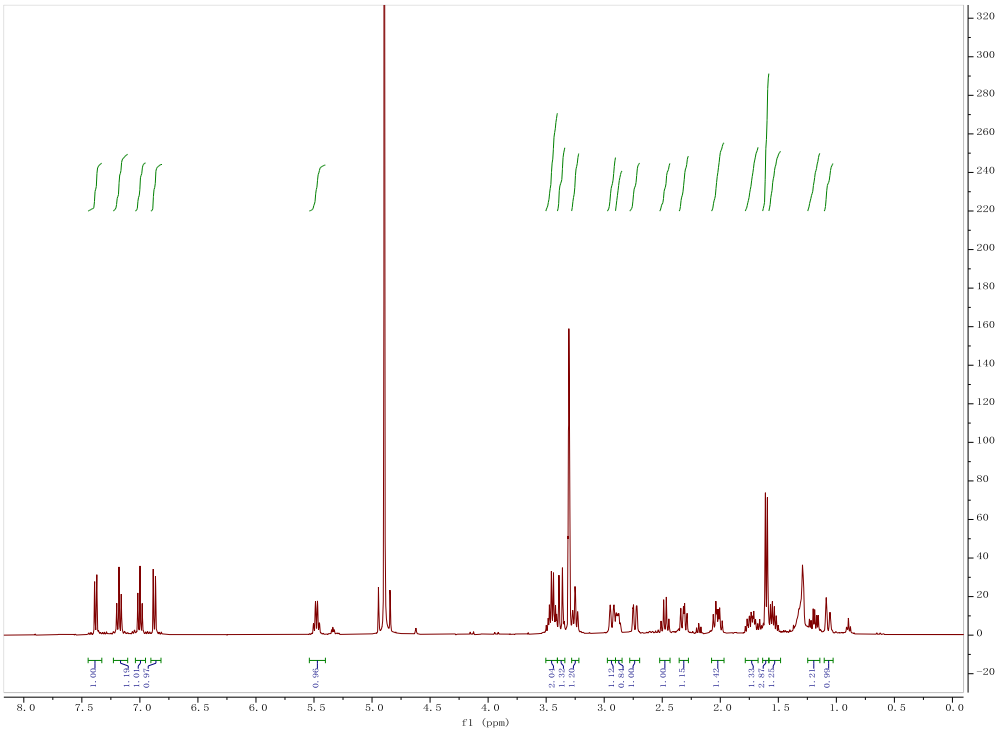



**Figure S6.** $^{1}$H NMR spectrum of a mixture of 7(*S*)-geissoschizol oxindole (natural, 1.5 mg) and **28** (synthetic, 1.5 mg) (400 MHz, $CD_3OD$).



## Computational Information

In our calculations, geometry optimizations were performed by Gaussian 16[6] program in gas phase, B3LYP[7] hybrid functional with dispersion correction of D3[8] (BJ)[9] were used. Def2-SVP[10] basis set and IEFPCM (water)[11] solvent model was applied for all elements. The vibrational frequencies calculations were conducted at the same level of theory to be sure whether every optimized stationary point is an energy minimum (No imaginary frequency) and evaluate their thermal corrections at 298 K. The single point energies were calculated based on the optimized structures with M06-2X functional[12] and D3[8] dispersion correction. Def2-TZVP[10] basis set and SMD (water)[13] solvent model was applied in calculations. In order to adjust the Gibbs free energies from 1 atm to 1 mol/L, a correction of RTln (Csol/Cgas) (1.89 kcal/mol) is added to energies of all species. Csol represents the standard molar concentration in solution (1 mol/L), Cgas represents the standard molar concentration in gas phase (0.0446 mol/L), and R represents the gas constant.

To ensure the conformation of the intermediates we optimized were global minimum, we conducted the conformation search calculation of flexible intermediates. We preform 2 ns molecular dynamic simulation with the temperature of 350K with GAFF[14] forcefield by gromacs-2023.1 program[15-22]. 1000 conformers were then extracted from the trajectory, optimized under GFN0-xTB[23] level by xtb-6.5.1[24] package. After clustered by molclus-1.9.9.9 program[25], the clustered conformers were optimized under GFN2-xTB[26] level, and the results were then clustered by molclus. The first 10 clusters were optimized by DFT level above, and finally got the best conformation.

Table **S7**. Zero-point correction (ZPE), thermal correction to enthalpy (TCH), thermal correction to Gibbs free energy (TCG), electronic energies (EE), Gibbs free energies(G), free energies of solute in the solution (ΔGsolu), enthalpies (H) and free energies of solvation (ΔGsoln) (in Hartree), and imaginary frequencies (Im) of the structures calculated in corresponding level.

| Entry | ZPE | TCH | TCG | EE | G |
|---|---|---|---|---|---|
| **25'_conf_01** | 0.351135 | 0.371050 | 0.302360 | -995.046941 | -994.741569 |
| **25'_conf_02** | 0.351047 | 0.371031 | 0.302799 | -995.046954 | -994.741143 |
| **25'_conf_03** | 0.350986 | 0.371044 | 0.302466 | -995.046201 | -994.740723 |
| **25'_conf_04** | 0.350986 | 0.370961 | 0.302758 | -995.045586 | -994.739816 |
| **25'_conf_05** | 0.350990 | 0.371060 | 0.302596 | -995.045309 | -994.739701 |
| **25'_conf_06** | 0.351760 | 0.371253 | 0.304177 | -995.046175 | -994.738986 |
| **25'_conf_07** | 0.351009 | 0.370982 | 0.302746 | -995.044235 | -994.738477 |
| **25'_conf_08** | 0.352091 | 0.371527 | 0.304633 | -995.044966 | -994.737321 |
| **25'_conf_09** | 0.353139 | 0.372061 | 0.307577 | -995.043664 | -994.733075 |
| **25'_conf_10** | 0.353302 | 0.372140 | 0.307838 | -995.043221 | -994.732371 |
| **3-epi-25'_conf_01** | 0.351327 | 0.371194 | 0.303563 | -995.042958 | -994.736383 |
| **3-epi-25'_conf_02** | 0.351244 | 0.371122 | 0.303584 | -995.042662 | -994.736066 |
| **3-epi-25'_conf_03** | 0.352496 | 0.371702 | 0.306148 | -995.044649 | -994.735489 |
| **3-epi-25'_conf_04** | 0.352246 | 0.371521 | 0.305282 | -995.043719 | -994.735425 |
| **3-epi-25'_conf_05** | 0.351816 | 0.371474 | 0.303590 | -995.040311 | -994.733709 |
| **3-epi-25'_conf_06** | 0.351526 | 0.371421 | 0.303608 | -995.040104 | -994.733484 |
| **3-epi-25'_conf_07** | 0.351492 | 0.371417 | 0.303575 | -995.039812 | -994.733225 |
| **3-epi-25'_conf_08** | 0.351864 | 0.371513 | 0.304660 | -995.040795 | -994.733123 |
| **3-epi-25'_conf_09** | 0.352743 | 0.371911 | 0.306154 | -995.041598 | -994.732432 |
| **3-epi-25'_conf_10** | 0.352524 | 0.371761 | 0.306135 | -995.041116 | -994.731969 |
| **3-epi-27_conf_01** | 0.402526 | 0.424169 | 0.352172 | -998.403344 | -998.048160 |
| **3-epi-27_conf_02** | 0.402566 | 0.424240 | 0.352622 | -998.403153 | -998.047520 |
| **3-epi-27_conf_03** | 0.402959 | 0.424643 | 0.352563 | -998.401789 | -998.046214 |
| **3-epi-27_conf_04** | 0.403211 | 0.424814 | 0.353192 | -998.401606 | -998.045402 |

| | | | | | |
|---|---|---|---|---|---|
| **3-epi-27_conf_05** | 0.402243 | 0.424261 | 0.350669 | -998.397063 | -998.043382 |
| **3-epi-27_conf_06** | 0.402080 | 0.424096 | 0.351004 | -998.397373 | -998.043357 |
| **3-epi-27_conf_07** | 0.402221 | 0.424128 | 0.351912 | -998.398259 | -998.043335 |
| **3-epi-27_conf_08** | 0.402512 | 0.424281 | 0.352461 | -998.398446 | -998.042973 |
| **3-epi-27_conf_09** | 0.402762 | 0.424422 | 0.353531 | -998.399443 | -998.042900 |
| **3-epi-27_conf_10** | 0.402441 | 0.424210 | 0.352440 | -998.397377 | -998.041925 |
| **27_conf_01** | 0.402980 | 0.424435 | 0.353686 | -998.410241 | -998.053543 |
| **27_conf_02** | 0.402983 | 0.424514 | 0.353647 | -998.405506 | -998.048847 |
| **27_conf_03** | 0.402847 | 0.424603 | 0.352987 | -998.402946 | -998.046947 |
| **27_conf_04** | 0.402993 | 0.424698 | 0.353229 | -998.403165 | -998.046925 |
| **27_conf_05** | 0.403098 | 0.424748 | 0.353107 | -998.402662 | -998.046543 |
| **27_conf_06** | 0.402886 | 0.424446 | 0.353808 | -998.402904 | -998.046085 |
| **27_conf_07** | 0.403317 | 0.424763 | 0.354264 | -998.403300 | -998.046024 |
| **27_conf_08** | 0.403196 | 0.424690 | 0.354128 | -998.403096 | -998.045956 |
| **27_conf_09** | 0.403056 | 0.424685 | 0.353149 | -998.402111 | -998.045950 |
| **27_conf_10** | 0.402929 | 0.424485 | 0.353690 | -998.398392 | -998.041690 |

Optimized molecule coordination

25'_conf_01

Charge = 0 Multi = 1

| | | | |
|---|---|---|---|
| H | 4.609233 | -2.027558 | 1.405551 |
| O | 3.699102 | -2.351390 | 1.465977 |
| H | 3.841765 | -3.393889 | -0.343518 |
| H | 2.220220 | -3.011989 | 0.258001 |
| C | 3.238864 | -2.606994 | 0.149019 |
| H | 4.265255 | -1.042782 | -0.929815 |
| H | 2.793914 | -1.614895 | -1.712086 |
| C | 3.228457 | -1.359262 | -0.730250 |
| O | 3.503745 | 1.225077 | -1.774704 |
| N | 0.460464 | 1.920930 | -0.230213 |
| H | 0.510286 | -0.745469 | -0.859650 |
| H | 0.839416 | -1.293883 | 0.797971 |
| C | 0.968251 | -0.455016 | 0.098024 |
| H | 2.904267 | 0.018762 | 0.882198 |
| C | 2.468952 | -0.184211 | -0.115716 |
| C | 2.681690 | 1.109361 | -0.888497 |
| H | 1.921127 | 3.087802 | -1.193110 |
| H | 2.312764 | 2.687130 | 0.503608 |
| C | 1.842529 | 2.296990 | -0.433169 |
| H | -0.716311 | 3.642368 | -0.585789 |
| H | 0.085129 | 3.612370 | 1.004455 |
| H | 0.656044 | 0.979905 | 1.671136 |
| H | -2.574175 | 2.469693 | 0.402258 |
| H | -1.701996 | 2.496681 | 1.952062 |
| C | -0.421851 | 2.981495 | 0.245029 |
| C | 0.266654 | 0.775927 | 0.645928 |
| C | -1.616811 | 2.239277 | 0.887234 |
| C | -1.276710 | 0.729437 | 0.759342 |

| | | | |
|---|---|---|---|
| O | -1.424590 | 0.123156 | 3.146581 |
| N | -2.507704 | -1.118067 | 1.526539 |
| H | -2.927697 | -1.805927 | 2.142548 |
| H | -1.406860 | 1.110052 | -2.151789 |
| H | -2.723170 | -0.400628 | -3.667988 |
| H | -3.978021 | -2.325451 | -2.725969 |
| H | -3.957797 | -2.780584 | -0.266648 |
| C | -1.721391 | -0.090619 | 1.985602 |
| C | -1.973714 | 0.269016 | -1.749017 |
| C | -2.706003 | -0.584652 | -2.591570 |
| C | -3.411897 | -1.669590 | -2.060282 |
| C | -3.407554 | -1.934126 | -0.681747 |
| C | -2.675856 | -1.077684 | 0.136021 |
| C | -1.961738 | 0.017900 | -0.382710 |

25'_conf_02

Charge = 0 Multi = 1

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|---|---|---|---|
| H | 3.118327 | -2.023366 | 1.984351 |
| O | 3.794004 | -2.415784 | 1.416254 |
| H | 3.862402 | -3.374291 | -0.372403 |
| H | 2.219794 | -3.036803 | 0.190067 |
| C | 3.239335 | -2.613292 | 0.124297 |
| H | 4.284745 | -1.029100 | -0.893437 |
| H | 2.821983 | -1.578300 | -1.718258 |
| C | 3.243652 | -1.343972 | -0.725525 |
| O | 3.502772 | 1.238566 | -1.768719 |
| N | 0.463231 | 1.927949 | -0.220396 |
| H | 0.522067 | -0.729391 | -0.868884 |
| H | 0.831868 | -1.294512 | 0.783997 |
| C | 0.972807 | -0.448095 | 0.094691 |
| H | 2.910246 | 0.039352 | 0.888294 |
| C | 2.475437 | -0.175761 | -0.108474 |
| C | 2.685119 | 1.121997 | -0.879478 |
| H | 1.924411 | 3.101438 | -1.174262 |
| H | 2.313615 | 2.692411 | 0.521136 |
| C | 1.845405 | 2.306827 | -0.418434 |
| H | -0.716087 | 3.648239 | -0.572385 |
| H | 0.080904 | 3.613644 | 1.020012 |
| H | 0.655928 | 0.976427 | 1.676373 |
| H | -2.574284 | 2.467957 | 0.405765 |
| H | -1.706472 | 2.490231 | 1.958068 |
| C | -0.422642 | 2.984840 | 0.256717 |
| C | 0.268595 | 0.778535 | 0.649211 |
| C | -1.617845 | 2.237426 | 0.892439 |
| C | -1.274721 | 0.728679 | 0.759188 |
| O | -1.424454 | 0.112852 | 3.143846 |
| N | -2.502934 | -1.124341 | 1.517585 |
| H | -2.922968 | -1.815062 | 2.130372 |
| H | -1.400284 | 1.119369 | -2.150999 |
| H | -2.709735 | -0.389372 | -3.674908 |

| | | | |
|---|---|---|---|
| H | -3.962010 | -2.320260 | -2.742027 |
| H | -3.945845 | -2.783753 | -0.284251 |
| C | -1.719659 | -0.097032 | 1.981761 |
| C | -1.965780 | 0.275531 | -1.752175 |
| C | -2.694340 | -0.576987 | -2.599098 |
| C | -3.398816 | -1.665358 | -2.072936 |
| C | -3.396723 | -1.934615 | -0.695320 |
| C | -2.668656 | -1.079296 | 0.126838 |
| C | -1.956045 | 0.019707 | -0.386697 |

25'_conf_03

Charge = 0 Multi = 1

| | | | |
|---|---|---|---|
| H | -5.236827 | 2.697706 | 0.465873 |
| O | -4.359919 | 3.086888 | 0.591205 |
| H | -2.491693 | 2.520210 | 1.100280 |
| H | -3.755798 | 1.563856 | 1.895987 |
| C | -3.469974 | 2.041459 | 0.936363 |
| H | -4.380149 | 0.574051 | -0.347948 |
| H | -3.041418 | 1.451608 | -1.091741 |
| C | -3.373036 | 0.977234 | -0.152537 |
| O | -3.465906 | -1.398492 | -1.618233 |
| N | -0.235939 | -1.974514 | -0.454540 |
| H | -0.636544 | 0.728762 | -0.580914 |
| H | -0.854004 | 0.944336 | 1.167865 |
| C | -0.964133 | 0.226298 | 0.341756 |
| H | -2.758688 | -0.619651 | 1.164943 |
| C | -2.442716 | -0.183486 | 0.195227 |
| C | -2.583249 | -1.341780 | -0.787408 |
| H | -1.645583 | -3.125557 | -1.507920 |
| H | -1.916322 | -3.082606 | 0.257265 |
| C | -1.581750 | -2.477629 | -0.621822 |
| H | 1.084872 | -3.442806 | -1.211980 |
| H | 0.437773 | -3.798782 | 0.408726 |
| H | -0.348723 | -1.410814 | 1.597378 |
| H | 2.888924 | -2.248227 | -0.152534 |
| H | 2.166389 | -2.648969 | 1.422467 |
| C | 0.798625 | -2.983688 | -0.252275 |
| C | -0.084697 | -0.985073 | 0.600722 |
| C | 1.959362 | -2.223620 | 0.430680 |
| C | 1.448128 | -0.767758 | 0.604124 |
| O | 1.758017 | -0.563575 | 3.043517 |
| N | 2.538133 | 1.060636 | 1.597168 |
| H | 2.937476 | 1.680467 | 2.293962 |
| H | 1.339788 | -0.628644 | -2.329605 |
| H | 2.331240 | 1.269988 | -3.643049 |
| H | 3.453337 | 3.147098 | -2.466491 |
| H | 3.620238 | 3.170848 | 0.028350 |
| C | 1.916964 | -0.119937 | 1.921228 |
| C | 1.847060 | 0.195567 | -1.825416 |
| C | 2.397475 | 1.264502 | -2.552917 |

| | | | |
|---|---|---|---|
| C | 3.028588 | 2.322293 | -1.889377 |
| C | 3.127897 | 2.345668 | -0.489414 |
| C | 2.575507 | 1.278672 | 0.213407 |
| C | 1.938748 | 0.207229 | -0.439210 |

25'_conf_04

Charge = 0 Multi = 1

| | | | |
|---|---|---|---|
| H | 5.673650 | -0.633892 | 1.872815 |
| O | 4.740300 | -0.870548 | 1.796434 |
| H | 5.012546 | -0.966585 | -0.274992 |
| H | 5.008964 | -2.539272 | 0.564005 |
| C | 4.549843 | -1.531028 | 0.553299 |
| H | 2.894730 | -2.253030 | -0.613220 |
| H | 2.617251 | -2.241936 | 1.138147 |
| C | 3.054650 | -1.666271 | 0.305451 |
| O | 3.351639 | -0.000962 | -1.959613 |
| N | 0.389221 | 1.492517 | -0.992802 |
| H | 0.371193 | -1.150595 | -0.279507 |
| H | 0.633712 | -0.859148 | 1.453375 |
| C | 0.806232 | -0.447439 | 0.446878 |
| H | 2.728810 | 0.348397 | 0.976760 |
| C | 2.323080 | -0.327665 | 0.200607 |
| C | 2.571387 | 0.393242 | -1.116282 |
| H | 1.908206 | 2.015301 | -2.348658 |
| H | 2.262331 | 2.461575 | -0.653193 |
| C | 1.788943 | 1.687318 | -1.305963 |
| H | -0.705503 | 2.869542 | -2.166785 |
| H | 0.052505 | 3.574720 | -0.717267 |
| H | 0.499979 | 1.567411 | 1.133931 |
| H | -2.634062 | 2.340728 | -0.823375 |
| H | -1.806139 | 3.083042 | 0.564729 |
| C | -0.460128 | 2.672481 | -1.111013 |
| C | 0.130856 | 0.907211 | 0.314084 |
| C | -1.700504 | 2.349019 | -0.246077 |
| C | -1.415456 | 0.952306 | 0.371359 |
| O | -1.652099 | 1.555310 | 2.752247 |
| N | -2.742614 | -0.279537 | 1.867603 |
| H | -3.207838 | -0.581501 | 2.717059 |
| H | -1.447305 | -0.093298 | -2.374024 |
| H | -2.783483 | -2.111523 | -3.050673 |
| H | -4.145475 | -3.325868 | -1.366154 |
| H | -4.213289 | -2.558083 | 1.012753 |
| C | -1.926298 | 0.823266 | 1.819193 |
| C | -2.059974 | -0.628730 | -1.646855 |
| C | -2.804044 | -1.762285 | -2.016049 |
| C | -3.570268 | -2.446666 | -1.066267 |
| C | -3.615508 | -2.024414 | 0.271639 |
| C | -2.870527 | -0.900709 | 0.618024 |
| C | -2.096573 | -0.200845 | -0.325676 |

25'_conf_05

Charge = 0 Multi = 1

| | | | |
|---|---|---|---|
| H | 6.227597 | -2.065324 | 0.976405 |
| O | 5.286328 | -2.229044 | 0.833127 |
| H | 4.726577 | -0.397228 | 1.676126 |
| H | 5.061270 | -0.358463 | -0.075252 |
| C | 4.631795 | -0.975157 | 0.733940 |
| H | 3.069450 | -1.791486 | -0.494422 |
| H | 2.771169 | -1.890670 | 1.248721 |
| C | 3.159762 | -1.234388 | 0.452650 |
| O | 3.382445 | 0.591156 | -1.698444 |
| N | 0.232193 | 1.689554 | -0.818193 |
| H | 0.484115 | -0.977027 | -0.247210 |
| H | 0.620629 | -0.760044 | 1.510768 |
| C | 0.795493 | -0.273054 | 0.539110 |
| H | 2.578213 | 0.705725 | 1.217761 |
| C | 2.300958 | 0.027316 | 0.386664 |
| C | 2.527867 | 0.850061 | -0.876027 |
| H | 1.750225 | 2.463983 | -2.048920 |
| H | 1.961493 | 2.837976 | -0.312364 |
| C | 1.614753 | 2.059386 | -1.035660 |
| H | -0.945957 | 3.010030 | -1.976358 |
| H | -0.360680 | 3.696921 | -0.440331 |
| H | 0.218337 | 1.650774 | 1.311848 |
| H | -2.870364 | 2.165462 | -0.799004 |
| H | -2.228212 | 2.920113 | 0.677800 |
| C | -0.740874 | 2.771377 | -0.920700 |
| C | -0.025033 | 1.001768 | 0.437851 |
| C | -1.982661 | 2.252064 | -0.159280 |
| C | -1.566924 | 0.864993 | 0.404153 |
| O | -1.999776 | 1.300786 | 2.793922 |
| N | -2.813276 | -0.596575 | 1.756260 |
| H | -3.282429 | -0.999085 | 2.560639 |
| H | -1.331114 | -0.019326 | -2.388125 |
| H | -2.375394 | -2.139710 | -3.241053 |
| H | -3.665524 | -3.600173 | -1.701681 |
| H | -3.949889 | -2.981211 | 0.704857 |
| C | -2.134687 | 0.595496 | 1.811053 |
| C | -1.910882 | -0.663630 | -1.725146 |
| C | -2.491885 | -1.854497 | -2.193244 |
| C | -3.217744 | -2.677399 | -1.325157 |
| C | -3.383557 | -2.339677 | 0.027164 |
| C | -2.799476 | -1.157002 | 0.471976 |
| C | -2.067557 | -0.318535 | -0.388597 |

25'_conf_06

Charge = 0 Multi = 1

| | | | |
|---|---|---|---|
| H | 4.861627 | -0.809499 | -0.548937 |
| O | 5.285881 | -1.402196 | 0.101300 |
| H | 4.771749 | -2.193325 | 1.893034 |

| | | | |
|---|---|---|---|
| H | 4.708231 | -0.423467 | 1.861314 |
| C | 4.489272 | -1.334220 | 1.261661 |
| H | 2.794497 | -2.155474 | 0.214184 |
| H | 2.496003 | -1.785439 | 1.913837 |
| C | 2.980033 | -1.403170 | 1.000252 |
| O | 3.653576 | 0.241873 | -1.304413 |
| N | 0.394507 | 1.456251 | -0.984696 |
| H | 0.425461 | -1.071846 | 0.027352 |
| H | 0.447682 | -0.579533 | 1.732909 |
| C | 0.726585 | -0.267595 | 0.714974 |
| H | 2.531155 | 0.672537 | 1.401414 |
| C | 2.258557 | -0.093888 | 0.647384 |
| C | 2.661736 | 0.555127 | -0.666998 |
| H | 2.054043 | 1.924847 | -2.188195 |
| H | 2.137403 | 2.608672 | -0.542246 |
| C | 1.805997 | 1.720602 | -1.136677 |
| H | -0.622345 | 2.584297 | -2.456873 |
| H | -0.096708 | 3.526010 | -1.039393 |
| H | 0.225448 | 1.788361 | 1.113829 |
| H | -2.672707 | 2.100472 | -1.288862 |
| H | -2.063884 | 3.060388 | 0.078961 |
| C | -0.501190 | 2.544663 | -1.362681 |
| C | 0.002135 | 1.013614 | 0.343409 |
| C | -1.819541 | 2.242721 | -0.613158 |
| C | -1.538721 | 0.954362 | 0.208024 |
| O | -2.108210 | 1.822801 | 2.446193 |
| N | -2.976409 | -0.177109 | 1.681084 |
| H | -3.529091 | -0.405975 | 2.500421 |
| H | -1.165025 | -0.416187 | -2.365348 |
| H | -2.290869 | -2.590247 | -2.928968 |
| H | -3.785904 | -3.684922 | -1.275757 |
| H | -4.197610 | -2.641038 | 0.959196 |
| C | -2.222011 | 0.965889 | 1.589318 |
| C | -1.833923 | -0.900986 | -1.652261 |
| C | -2.461626 | -2.120586 | -1.957872 |
| C | -3.303010 | -2.737316 | -1.025548 |
| C | -3.541123 | -2.160240 | 0.231628 |
| C | -2.909493 | -0.952852 | 0.516018 |
| C | -2.061313 | -0.319868 | -0.411013 |

25'_conf_07

Charge = 0 Multi = 1

| | | | |
|---|---|---|---|
| H | -1.626375 | 3.629341 | -0.019294 |
| O | -1.781693 | 2.956087 | 0.656155 |
| H | -3.862831 | 3.090236 | 0.641872 |
| H | -3.166918 | 2.083112 | -0.646965 |
| C | -3.053263 | 2.369217 | 0.414041 |
| H | -2.953145 | 1.423014 | 2.332748 |
| H | -4.300309 | 0.888816 | 1.316218 |
| C | -3.229896 | 1.143685 | 1.302546 |

| | | | |
|---|---|---|---|
| O | -3.993233 | -0.383049 | -0.933493 |
| N | -0.728366 | -1.622422 | -0.903868 |
| H | -0.657394 | 0.897200 | 0.187655 |
| H | -0.559374 | 0.350454 | 1.862879 |
| C | -0.913749 | 0.069538 | 0.858736 |
| H | -2.654792 | -0.895304 | 1.646381 |
| C | -2.443756 | -0.107413 | 0.894885 |
| C | -2.960003 | -0.730083 | -0.397098 |
| H | -2.476095 | -2.093781 | -1.973771 |
| H | -2.418863 | -2.794281 | -0.332397 |
| C | -2.147350 | -1.897217 | -0.942907 |
| H | 0.147936 | -2.742265 | -2.469735 |
| H | -0.221535 | -3.685312 | -1.004395 |
| H | -0.373888 | -1.999907 | 1.162537 |
| H | 2.291594 | -2.197709 | -1.515846 |
| H | 1.859887 | -3.209826 | -0.118816 |
| C | 0.137368 | -2.699992 | -1.368945 |
| C | -0.226098 | -1.202675 | 0.396114 |
| C | 1.520800 | -2.381563 | -0.756223 |
| C | 1.297551 | -1.121781 | 0.123728 |
| O | 2.088115 | -2.040027 | 2.273304 |
| N | 2.825052 | 0.009862 | 1.503316 |
| H | 3.438601 | 0.232445 | 2.279857 |
| H | 0.670023 | 0.306000 | -2.365398 |
| H | 1.668366 | 2.537475 | -2.948297 |
| H | 3.259654 | 3.635667 | -1.389902 |
| H | 3.896709 | 2.538067 | 0.765478 |
| C | 2.100109 | -1.154408 | 1.438230 |
| C | 1.383046 | 0.791974 | -1.697424 |
| C | 1.938338 | 2.043873 | -2.012163 |
| C | 2.834252 | 2.662549 | -1.133252 |
| C | 3.199131 | 2.055297 | 0.078540 |
| C | 2.636924 | 0.816342 | 0.372924 |
| C | 1.736002 | 0.181053 | -0.500842 |

25'_conf_08

Charge = 0 Multi = 1

| | | | |
|---|---|---|---|
| H | -4.281096 | 1.234589 | -0.544995 |
| O | -4.333984 | 2.079951 | -0.060501 |
| H | -2.309106 | 2.323820 | 0.408824 |
| H | -3.490855 | 2.849881 | 1.613837 |
| C | -3.279830 | 2.056517 | 0.877778 |
| H | -2.702300 | 0.910909 | 2.612850 |
| H | -4.166831 | 0.343292 | 1.809060 |
| C | -3.148015 | 0.721273 | 1.622652 |
| O | -3.710662 | -0.403849 | -1.003208 |
| N | -0.489598 | -1.553639 | -0.976342 |
| H | -0.613926 | 0.854993 | 0.342439 |
| H | -0.447729 | 0.154145 | 1.965819 |
| C | -0.787478 | -0.051546 | 0.939150 |

| | | | |
|---|---|---|---|
| H | -2.401045 | -1.290077 | 1.587188 |
| C | -2.296857 | -0.377914 | 0.967480 |
| C | -2.739339 | -0.839760 | -0.408765 |
| H | -2.206510 | -2.088661 | -2.062581 |
| H | -2.084072 | -2.884730 | -0.463454 |
| C | -1.884663 | -1.938504 | -1.022519 |
| H | 0.450617 | -2.434543 | -2.653260 |
| H | 0.185079 | -3.546978 | -1.287049 |
| H | -0.055552 | -2.074563 | 1.043600 |
| H | 2.563379 | -1.827969 | -1.668016 |
| H | 2.223189 | -2.980135 | -0.356489 |
| C | 0.454762 | -2.504310 | -1.554004 |
| C | 0.005330 | -1.205658 | 0.347050 |
| C | 1.816427 | -2.131208 | -0.923157 |
| C | 1.508050 | -0.968587 | 0.059862 |
| O | 2.414080 | -1.986074 | 2.116732 |
| N | 2.983160 | 0.165112 | 1.493782 |
| H | 3.598710 | 0.372607 | 2.273014 |
| H | 0.705895 | 0.600913 | -2.292589 |
| H | 1.530121 | 2.934853 | -2.721120 |
| H | 3.085526 | 4.021215 | -1.118729 |
| H | 3.856458 | 2.811518 | 0.929784 |
| C | 2.342567 | -1.040781 | 1.353362 |
| C | 1.399741 | 1.084274 | -1.602855 |
| C | 1.859215 | 2.392325 | -1.832230 |
| C | 2.734704 | 3.004120 | -0.928483 |
| C | 3.173804 | 2.334346 | 0.224240 |
| C | 2.706143 | 1.040286 | 0.434942 |
| C | 1.827047 | 0.410861 | -0.465237 |

25'_conf_09

Charge = 0 Multi = 1

| | | | |
|---|---|---|---|
| H | 1.289460 | 1.250492 | 0.944756 |
| O | 1.441630 | 2.207972 | 0.748641 |
| H | 2.900807 | 3.391233 | -0.029320 |
| H | 3.499307 | 1.884984 | 0.668811 |
| C | 2.671315 | 2.316931 | 0.068767 |
| H | 2.003569 | 2.253255 | -1.993827 |
| H | 3.706957 | 1.830289 | -1.738705 |
| C | 2.690340 | 1.698700 | -1.333334 |
| O | 4.339876 | -0.855904 | -0.678830 |
| N | 1.201870 | -0.570350 | 1.050979 |
| H | 0.266279 | 0.879761 | -1.162394 |
| H | 0.418913 | -0.515515 | -2.241101 |
| C | 0.791497 | -0.072647 | -1.305651 |
| H | 2.671237 | -0.150356 | -2.409503 |
| C | 2.320360 | 0.191818 | -1.425521 |
| C | 3.186628 | -0.572947 | -0.426136 |
| H | 3.207064 | -0.443614 | 1.707024 |
| H | 2.757098 | -2.035319 | 1.061737 |

| | | | |
|---|---|---|---|
| C | 2.600526 | -0.942770 | 0.933595 |
| H | 0.319112 | -0.216794 | 2.949667 |
| H | 1.103505 | -1.802095 | 2.796007 |
| H | 0.736472 | -2.038288 | -0.408321 |
| H | -1.669200 | -1.481527 | 2.403749 |
| H | -0.702535 | -2.762346 | 1.628705 |
| C | 0.498482 | -1.054819 | 2.256920 |
| C | 0.457904 | -0.996375 | -0.143628 |
| C | -0.813189 | -1.674182 | 1.743834 |
| C | -1.009418 | -1.068222 | 0.334608 |
| O | -1.564486 | -3.155430 | -0.858046 |
| N | -2.866366 | -1.261617 | -1.092351 |
| H | -3.550839 | -1.646455 | -1.734721 |
| H | -0.808342 | 1.600896 | 1.632964 |
| H | -2.448826 | 3.422184 | 1.230357 |
| H | -4.352259 | 3.082506 | -0.329606 |
| H | -4.661644 | 0.892581 | -1.499538 |
| C | -1.819175 | -1.994269 | -0.598338 |
| C | -1.643042 | 1.433095 | 0.953494 |
| C | -2.569499 | 2.463752 | 0.721124 |
| C | -3.640355 | 2.271928 | -0.157015 |
| C | -3.821325 | 1.049041 | -0.820704 |
| C | -2.894240 | 0.040424 | -0.576721 |
| C | -1.801946 | 0.219675 | 0.294497 |

25'_conf_10

Charge = 0 Multi = 1

| | | | |
|---|---|---|---|
| H | 1.431164 | 0.822040 | 1.341927 |
| O | 1.545891 | 1.802185 | 1.433669 |
| H | 3.003549 | 3.165161 | 1.027295 |
| H | 3.583296 | 1.501814 | 1.142756 |
| C | 2.746167 | 2.125054 | 0.765992 |
| H | 1.982814 | 2.775510 | -1.154038 |
| H | 3.689162 | 2.296746 | -1.143369 |
| C | 2.690475 | 2.026348 | -0.762165 |
| O | 4.343968 | -0.586038 | -1.232389 |
| N | 1.389680 | -0.880452 | 0.793113 |
| H | 0.270090 | 1.239037 | -0.893191 |
| H | 0.366814 | 0.132183 | -2.256062 |
| C | 0.778765 | 0.341584 | -1.258318 |
| H | 2.570424 | 0.710732 | -2.437218 |
| C | 2.298101 | 0.650934 | -1.373935 |
| C | 3.220971 | -0.418988 | -0.802169 |
| H | 3.440050 | -1.170419 | 1.189804 |
| H | 2.754890 | -2.325127 | 0.025963 |
| C | 2.720367 | -1.264951 | 0.361042 |
| H | 1.275039 | -1.661498 | 2.760884 |
| H | 0.839108 | -2.817759 | 1.464171 |
| H | 0.571777 | -1.784350 | -0.914260 |
| H | -0.770614 | -0.383017 | 2.418706 |

| | | | |
|---|---|---|---|
| H | -1.370435 | -2.037713 | 2.174484 |
| C | 0.775703 | -1.758879 | 1.785519 |
| C | 0.457512 | -0.839957 | -0.345100 |
| C | -0.671658 | -1.281243 | 1.793490 |
| C | -0.967367 | -0.893025 | 0.306546 |
| O | -1.472449 | -3.163216 | -0.527771 |
| N | -2.987337 | -1.438683 | -0.774968 |
| H | -3.719344 | -1.968161 | -1.236302 |
| H | -0.780782 | 1.948247 | 1.082754 |
| H | -2.631183 | 3.586728 | 0.687624 |
| H | -4.723055 | 2.868889 | -0.442855 |
| H | -5.018683 | 0.499432 | -1.188872 |
| C | -1.802998 | -2.001534 | -0.376153 |
| C | -1.707549 | 1.630811 | 0.598676 |
| C | -2.745942 | 2.548969 | 0.367199 |
| C | -3.923261 | 2.144617 | -0.271058 |
| C | -4.098743 | 0.818833 | -0.695813 |
| C | -3.057856 | -0.075473 | -0.462571 |
| C | -1.865981 | 0.315570 | 0.174603 |

27_conf_01

Charge = 0 Multi = 1

| | | | |
|---|---|---|---|
| H | -3.629627 | 3.376987 | 0.949216 |
| O | -4.196463 | 2.704544 | 0.545306 |
| H | -4.257758 | 1.528644 | -1.098524 |
| H | -3.601080 | 3.151781 | -1.406890 |
| C | -3.604247 | 2.312750 | -0.684556 |
| H | -1.787017 | 1.547427 | -1.526356 |
| H | -1.543944 | 2.581589 | -0.120094 |
| C | -2.185573 | 1.777164 | -0.524566 |
| N | -0.597977 | -1.643849 | -0.814966 |
| H | -0.094213 | 1.128825 | 1.089324 |
| H | -0.629035 | -0.481985 | 1.629807 |
| C | -0.626888 | 0.215422 | 0.779207 |
| H | -2.605798 | 0.827129 | 1.337170 |
| C | -2.087721 | 0.552018 | 0.408853 |
| C | -2.754428 | -0.679174 | -0.183428 |
| H | -1.937259 | -0.741398 | -2.185068 |
| H | -2.439100 | -2.323332 | -1.545359 |
| C | -1.955178 | -1.375401 | -1.264461 |
| H | 0.280283 | -1.709078 | -2.749358 |
| H | -0.013262 | -3.301581 | -1.995120 |
| H | 0.159636 | 0.284338 | -1.223541 |
| H | 2.476580 | -2.023379 | -1.849534 |
| H | 1.882215 | -3.061228 | -0.531675 |
| C | 0.287400 | -2.263534 | -1.782852 |
| C | 0.098339 | -0.445091 | -0.382698 |
| C | 1.669209 | -2.156780 | -1.117594 |
| C | 1.564380 | -0.933700 | -0.154719 |
| O | 1.279431 | -2.287343 | 1.905106 |

| | | | |
|---|---|---|---|
| N | 2.698495 | -0.472803 | 1.855629 |
| H | 3.018396 | -0.538499 | 2.816003 |
| H | 2.414065 | 0.771695 | -2.399996 |
| H | 4.124455 | 2.581109 | -2.164385 |
| H | 5.211830 | 2.998137 | 0.029596 |
| H | 4.621412 | 1.615563 | 2.028435 |
| C | 1.791556 | -1.354275 | 1.315623 |
| C | 2.894032 | 0.953686 | -1.435257 |
| C | 3.854768 | 1.970654 | -1.299961 |
| C | 4.466940 | 2.204307 | -0.063980 |
| C | 4.142696 | 1.434647 | 1.064251 |
| C | 3.191077 | 0.430630 | 0.907952 |
| C | 2.565534 | 0.182510 | -0.327758 |
| C | -3.955390 | -1.151934 | 0.190181 |
| H | -4.301096 | -2.073561 | -0.296294 |
| C | -4.895431 | -0.569394 | 1.206454 |
| H | -5.932398 | -0.607217 | 0.832492 |
| H | -4.884364 | -1.157614 | 2.142186 |
| H | -4.666741 | 0.477571 | 1.445889 |

27_conf_02

Charge = 0 Multi = 1

| | | | |
|---|---|---|---|
| H | 1.743894 | 3.243660 | -1.282969 |
| O | 2.142559 | 3.669598 | -0.512706 |
| H | 2.039200 | 3.572049 | 1.508680 |
| H | 0.662100 | 2.818503 | 0.693391 |
| C | 1.760703 | 2.944526 | 0.646760 |
| H | 3.548312 | 1.772201 | 0.850300 |
| H | 2.156322 | 1.106354 | 1.704165 |
| C | 2.464525 | 1.595384 | 0.765462 |
| N | 0.971696 | -1.417083 | 1.074763 |
| H | 0.171260 | 1.254834 | -0.897709 |
| H | 0.652468 | -0.311417 | -1.553381 |
| C | 0.736250 | 0.338407 | -0.669701 |
| H | 2.634173 | 1.118117 | -1.323394 |
| C | 2.225041 | 0.635130 | -0.420993 |
| C | 2.959412 | -0.677567 | -0.190209 |
| H | 2.682281 | -2.576663 | 0.781336 |
| H | 1.704922 | -2.363756 | -0.680003 |
| C | 2.081057 | -1.839684 | 0.226230 |
| H | 0.421771 | -2.866186 | 2.549553 |
| H | 0.187348 | -3.374560 | 0.856265 |
| H | -0.000609 | 0.430842 | 1.334025 |
| H | -1.515852 | -1.407166 | 2.475512 |
| H | -2.069860 | -2.739527 | 1.436303 |
| C | 0.123336 | -2.513885 | 1.546621 |
| C | 0.124463 | -0.338896 | 0.549837 |
| C | -1.304953 | -1.957683 | 1.545862 |
| C | -1.300724 | -0.948199 | 0.376648 |
| O | -0.819865 | -2.586923 | -1.422660 |

| | | | |
|---|---|---|---|
| N | -2.514610 | -1.040027 | -1.633642 |
| H | -2.822808 | -1.320528 | -2.558647 |
| H | -2.261865 | 1.120658 | 2.241985 |
| H | -4.152871 | 2.661864 | 1.702244 |
| H | -5.337811 | 2.479152 | -0.472771 |
| H | -4.658494 | 0.757111 | -2.154265 |
| C | -1.473444 | -1.656415 | -0.981748 |
| C | -2.780768 | 1.038341 | 1.283775 |
| C | -3.845080 | 1.904392 | 0.978311 |
| C | -4.511927 | 1.800477 | -0.246826 |
| C | -4.139230 | 0.836957 | -1.197451 |
| C | -3.083344 | -0.010756 | -0.875689 |
| C | -2.402999 | 0.078236 | 0.353322 |
| C | 4.283882 | -0.832236 | -0.346941 |
| H | 4.710235 | -1.816687 | -0.113769 |
| C | 5.265549 | 0.199342 | -0.821029 |
| H | 4.782496 | 1.125048 | -1.164594 |
| H | 5.974487 | 0.472522 | -0.019027 |
| H | 5.877267 | -0.193298 | -1.651598 |

27_conf_03

Charge = 0 Multi = 1

| | | | |
|---|---|---|---|
| H | -4.965743 | 3.690764 | -0.018381 |
| O | -4.084436 | 3.426014 | 0.275985 |
| H | -4.743648 | 1.538849 | 0.898909 |
| H | -4.231535 | 1.638456 | -0.800469 |
| C | -4.007431 | 2.011426 | 0.217063 |
| H | -1.890034 | 2.060613 | -0.077157 |
| H | -2.385481 | 2.015126 | 1.615365 |
| C | -2.604239 | 1.592592 | 0.620048 |
| N | -0.251304 | -0.678031 | -1.185215 |
| H | -0.757111 | 0.254095 | 2.086528 |
| H | -0.990864 | -1.374279 | 1.459563 |
| C | -0.996068 | -0.312338 | 1.173949 |
| H | -3.126148 | -0.320933 | 1.418635 |
| C | -2.410136 | 0.064750 | 0.677545 |
| C | -2.671153 | -0.603333 | -0.661500 |
| H | -1.576659 | 0.727460 | -1.955751 |
| H | -1.771071 | -0.907552 | -2.608038 |
| C | -1.581711 | -0.343288 | -1.682084 |
| H | 0.341218 | -2.492122 | -2.085187 |
| H | -0.794880 | -2.706359 | -0.736246 |
| H | 0.198942 | 1.024196 | -0.041620 |
| H | 2.141519 | -2.606205 | -0.508542 |
| H | 0.949353 | -2.791763 | 0.793733 |
| C | 0.064069 | -2.103913 | -1.091127 |
| C | 0.076922 | -0.061773 | 0.102282 |
| C | 1.225338 | -2.181292 | -0.077267 |
| C | 1.460078 | -0.716736 | 0.383575 |
| O | 1.406649 | -1.157549 | 2.821334 |

| | | | |
|---|---|---|---|
| N | 3.087177 | 0.101022 | 1.872096 |
| H | 3.607781 | 0.274922 | 2.725174 |
| H | 2.020328 | -0.080995 | -2.427576 |
| H | 4.044575 | 1.219480 | -3.162181 |
| H | 5.676780 | 2.039210 | -1.479169 |
| H | 5.335038 | 1.578184 | 0.956429 |
| C | 1.931225 | -0.641048 | 1.851170 |
| C | 2.753572 | 0.273926 | -1.701998 |
| C | 3.883333 | 1.008240 | -2.102667 |
| C | 4.802142 | 1.470410 | -1.154433 |
| C | 4.620807 | 1.216539 | 0.214281 |
| C | 3.497045 | 0.486230 | 0.590532 |
| C | 2.564908 | 0.011870 | -0.350667 |
| C | -3.727583 | -1.380740 | -0.951859 |
| H | -3.763064 | -1.812150 | -1.961426 |
| C | -4.895601 | -1.725006 | -0.075816 |
| H | -5.013994 | -2.818933 | 0.010705 |
| H | -4.811467 | -1.311132 | 0.938414 |
| H | -5.835749 | -1.346675 | -0.514597 |

27_conf_04

Charge = 0 Multi = 1

| | | | |
|---|---|---|---|
| H | -3.617728 | 3.825938 | -0.347423 |
| O | -4.212133 | 3.419246 | 0.298417 |
| H | -4.745852 | 1.572232 | 0.936974 |
| H | -4.274581 | 1.621141 | -0.770483 |
| C | -4.022484 | 2.015768 | 0.232260 |
| H | -1.898810 | 2.053343 | -0.094515 |
| H | -2.373425 | 2.022754 | 1.605502 |
| C | -2.608121 | 1.594820 | 0.616421 |
| N | -0.251172 | -0.682450 | -1.185156 |
| H | -0.758721 | 0.255440 | 2.084700 |
| H | -0.993949 | -1.373172 | 1.458926 |
| C | -0.997629 | -0.311418 | 1.172416 |
| H | -3.127509 | -0.318078 | 1.416354 |
| C | -2.411140 | 0.066363 | 0.674810 |
| C | -2.671922 | -0.603379 | -0.663722 |
| H | -1.574208 | 0.721826 | -1.961549 |
| H | -1.770226 | -0.914903 | -2.608194 |
| C | -1.580836 | -0.347935 | -1.683920 |
| H | 0.339685 | -2.499435 | -2.080285 |
| H | -0.796288 | -2.709073 | -0.730516 |
| H | 0.199162 | 1.022164 | -0.044975 |
| H | 2.140713 | -2.608985 | -0.504179 |
| H | 0.948823 | -2.792940 | 0.798598 |
| C | 0.063078 | -2.108313 | -1.087239 |
| C | 0.076317 | -0.063485 | 0.101209 |
| C | 1.224480 | -2.183720 | -0.073372 |
| C | 1.459037 | -0.718336 | 0.385035 |
| O | 1.403126 | -1.154694 | 2.823507 |

| | | | |
|---|---|---|---|
| N | 3.084626 | 0.102182 | 1.873687 |
| H | 3.604397 | 0.277650 | 2.726955 |
| H | 2.022045 | -0.087782 | -2.426712 |
| H | 4.046709 | 1.211913 | -3.161652 |
| H | 5.677110 | 2.034925 | -1.478500 |
| H | 5.333162 | 1.578056 | 0.957558 |
| C | 1.928717 | -0.639957 | 1.852971 |
| C | 2.754504 | 0.268617 | -1.701057 |
| C | 3.884480 | 1.002491 | -2.101927 |
| C | 4.802279 | 1.466509 | -1.153611 |
| C | 4.619703 | 1.214978 | 0.215369 |
| C | 3.495723 | 0.485113 | 0.591830 |
| C | 2.564614 | 0.008909 | -0.349448 |
| C | -3.730006 | -1.378554 | -0.954110 |
| H | -3.765349 | -1.811739 | -1.962895 |
| C | -4.900597 | -1.716700 | -0.079261 |
| H | -5.837936 | -1.330842 | -0.517587 |
| H | -5.026476 | -2.809922 | 0.004918 |
| H | -4.814057 | -1.305684 | 0.935937 |

27_conf_05

Charge = 0 Multi = 1

| | | | |
|---|---|---|---|
| H | -3.130090 | 3.023084 | 0.310410 |
| O | -3.420069 | 3.187942 | -0.596544 |
| H | -2.688137 | 2.995157 | -2.477703 |
| H | -1.455791 | 2.843897 | -1.217722 |
| C | -2.495541 | 2.570734 | -1.479230 |
| H | -3.630261 | 0.810324 | -1.984548 |
| H | -1.890398 | 0.665754 | -2.250142 |
| C | -2.647092 | 1.051720 | -1.547244 |
| N | -0.285879 | -1.539512 | -0.230274 |
| H | -1.034266 | 1.700170 | 0.636779 |
| H | -1.354650 | 0.286233 | 1.620699 |
| C | -1.235740 | 0.620784 | 0.579943 |
| H | -3.374548 | 0.741442 | 0.432016 |
| C | -2.552597 | 0.340809 | -0.178680 |
| C | -2.735815 | -1.158171 | -0.329102 |
| H | -1.407432 | -1.549875 | -1.980363 |
| H | -1.670651 | -2.947642 | -0.926498 |
| C | -1.528996 | -1.856089 | -0.925482 |
| H | 0.255742 | -3.215805 | 0.931030 |
| H | -1.023642 | -2.226286 | 1.666007 |
| H | 0.168643 | 0.343133 | -1.046320 |
| H | 1.873505 | -1.839850 | 2.040240 |
| H | 0.545609 | -0.876271 | 2.718430 |
| C | -0.090189 | -2.178500 | 1.071740 |
| C | -0.043934 | -0.104767 | -0.061548 |
| C | 0.953875 | -1.295229 | 1.788217 |
| C | 1.252297 | -0.136656 | 0.797637 |
| O | 0.921285 | 1.728854 | 2.394697 |

| | | | |
|---|---|---|---|
| N | 2.783113 | 1.632070 | 1.040674 |
| H | 3.226796 | 2.478622 | 1.380494 |
| H | 2.132832 | -2.193775 | -1.104172 |
| H | 4.314188 | -2.065372 | -2.349960 |
| H | 5.832731 | -0.130112 | -2.007023 |
| H | 5.219468 | 1.704475 | -0.420149 |
| C | 1.580180 | 1.182619 | 1.528026 |
| C | 2.816419 | -1.356917 | -0.954532 |
| C | 4.033899 | -1.273083 | -1.652183 |
| C | 4.888609 | -0.182576 | -1.459441 |
| C | 4.554756 | 0.851748 | -0.570999 |
| C | 3.345575 | 0.749747 | 0.111097 |
| C | 2.476013 | -0.341702 | -0.069072 |
| C | -3.832557 | -1.844998 | 0.031437 |
| H | -3.812603 | -2.931844 | -0.126328 |
| C | -5.107326 | -1.312507 | 0.615991 |
| H | -5.963116 | -1.532089 | -0.046365 |
| H | -5.331701 | -1.800670 | 1.580326 |
| H | -5.083608 | -0.226781 | 0.783394 |

27_conf_06

Charge = 0 Multi = 1

| | | | |
|---|---|---|---|
| H | -0.110459 | 3.828798 | 0.222973 |
| O | 0.363108 | 3.032609 | 0.497181 |
| H | 1.824261 | 3.441451 | -0.943588 |
| H | 2.204912 | 3.983062 | 0.708781 |
| C | 1.727552 | 3.170507 | 0.126838 |
| H | 3.552354 | 2.102299 | 0.404216 |
| H | 2.230380 | 1.512743 | 1.403966 |
| C | 2.475871 | 1.871354 | 0.390669 |
| N | 1.150978 | -1.134275 | 1.178312 |
| H | 0.168879 | 1.177475 | -1.129854 |
| H | 0.724897 | -0.446825 | -1.590105 |
| C | 0.779938 | 0.324918 | -0.806763 |
| H | 2.612131 | 1.110923 | -1.610697 |
| C | 2.252033 | 0.737886 | -0.637050 |
| C | 3.065284 | -0.487574 | -0.241085 |
| H | 2.922074 | -2.227603 | 1.015699 |
| H | 1.904559 | -2.296614 | -0.432084 |
| C | 2.266175 | -1.619357 | 0.372920 |
| H | 0.707459 | -2.366080 | 2.871686 |
| H | 0.493764 | -3.147844 | 1.283509 |
| H | 0.059060 | 0.669417 | 1.159665 |
| H | -1.320787 | -1.060355 | 2.602986 |
| H | -1.794860 | -2.574680 | 1.799721 |
| C | 0.379802 | -2.194403 | 1.831105 |
| C | 0.226888 | -0.204662 | 0.509351 |
| C | -1.082161 | -1.738082 | 1.768943 |
| C | -1.153841 | -0.927419 | 0.455537 |
| O | -0.579609 | -2.792933 | -1.076680 |

| | | | |
|---|---|---|---|
| N | -2.386128 | -1.422715 | -1.483497 |
| H | -2.684831 | -1.866626 | -2.345435 |
| H | -2.225690 | 1.351562 | 1.982537 |
| H | -4.237696 | 2.645840 | 1.259790 |
| H | -5.443948 | 2.028946 | -0.821844 |
| H | -4.666325 | 0.108572 | -2.224002 |
| C | -1.292187 | -1.851598 | -0.769568 |
| C | -2.758077 | 1.074940 | 1.069621 |
| C | -3.888014 | 1.803236 | 0.659370 |
| C | -4.566582 | 1.455390 | -0.513478 |
| C | -4.139136 | 0.379331 | -1.307359 |
| C | -3.018172 | -0.328560 | -0.883347 |
| C | -2.326741 | 0.004624 | 0.296417 |
| C | 4.391449 | -0.600617 | -0.419793 |
| H | 4.874526 | -1.517995 | -0.058217 |
| C | 5.306535 | 0.391756 | -1.075919 |
| H | 6.005532 | 0.835802 | -0.344503 |
| H | 5.932655 | -0.098087 | -1.841454 |
| H | 4.765507 | 1.217326 | -1.559921 |

27_conf_07

Charge = 0 Multi = 1

| | | | |
|---|---|---|---|
| H | 4.642133 | -2.657639 | -1.043678 |
| O | 4.916611 | -1.734175 | -1.136509 |
| H | 4.291142 | -0.023859 | -2.014223 |
| H | 3.992287 | -1.478183 | -2.993028 |
| C | 3.967111 | -1.075351 | -1.961942 |
| H | 1.870626 | -0.662622 | -2.142317 |
| H | 2.231265 | -2.214439 | -1.389756 |
| C | 2.543787 | -1.154471 | -1.420574 |
| N | 0.169479 | 1.393833 | 0.007875 |
| H | 0.792143 | -1.952106 | 0.495009 |
| H | 1.053907 | -0.693421 | 1.695536 |
| C | 1.009679 | -0.879849 | 0.612512 |
| H | 3.146888 | -1.037413 | 0.620027 |
| C | 2.386140 | -0.554008 | -0.007978 |
| C | 2.611580 | 0.948157 | 0.007009 |
| H | 1.393891 | 1.552514 | -1.663176 |
| H | 1.629625 | 2.822901 | -0.453133 |
| C | 1.459961 | 1.742133 | -0.576069 |
| H | -0.383771 | 2.944347 | 1.327478 |
| H | 0.815071 | 1.824632 | 2.009804 |
| H | -0.285241 | -0.364404 | -1.046784 |
| H | -2.114119 | 1.513341 | 2.163532 |
| H | -0.862697 | 0.433011 | 2.810543 |
| C | -0.082142 | 1.884477 | 1.362978 |
| C | -0.119926 | -0.041848 | -0.005435 |
| C | -1.196392 | 0.966340 | 1.909577 |
| C | -1.464168 | -0.064148 | 0.778067 |
| O | -1.282237 | -2.102823 | 2.174821 |

| | | | |
|---|---|---|---|
| N | -3.052943 | -1.797812 | 0.732497 |
| H | -3.539127 | -2.661177 | 0.949917 |
| H | -2.173284 | 2.218626 | -0.925602 |
| H | -4.279203 | 2.302274 | -2.300154 |
| H | -5.866504 | 0.392345 | -2.264345 |
| H | -5.398180 | -1.626900 | -0.862610 |
| C | -1.870574 | -1.444177 | 1.336228 |
| C | -2.887298 | 1.393971 | -0.910681 |
| C | -4.062417 | 1.428577 | -1.681402 |
| C | -4.955854 | 0.352313 | -1.661770 |
| C | -4.703406 | -0.784995 | -0.878502 |
| C | -3.535138 | -0.799589 | -0.121714 |
| C | -2.627969 | 0.275984 | -0.127566 |
| C | 3.702219 | 1.557658 | 0.500974 |
| H | 3.707309 | 2.656008 | 0.486333 |
| C | 4.931652 | 0.910621 | 1.073752 |
| H | 5.037901 | -0.137369 | 0.762203 |
| H | 5.835805 | 1.450339 | 0.746261 |
| H | 4.930328 | 0.952262 | 2.178267 |

27_conf_08

Charge = 0 Multi = 1

| | | | |
|---|---|---|---|
| H | 5.732775 | -1.653156 | -1.382235 |
| O | 4.819158 | -1.823907 | -1.118729 |
| H | 4.283596 | 0.002867 | -1.981295 |
| H | 3.987235 | -1.434106 | -2.995194 |
| C | 3.963136 | -1.055603 | -1.954856 |
| H | 1.870034 | -0.655128 | -2.135989 |
| H | 2.249348 | -2.211474 | -1.391225 |
| C | 2.544956 | -1.148356 | -1.417836 |
| N | 0.166271 | 1.393697 | 0.030179 |
| H | 0.785660 | -1.957520 | 0.480890 |
| H | 1.043898 | -0.712737 | 1.696127 |
| C | 1.003426 | -0.886774 | 0.610891 |
| H | 3.140033 | -1.044206 | 0.626284 |
| C | 2.382480 | -0.556132 | -0.001276 |
| C | 2.609745 | 0.945600 | 0.023506 |
| H | 1.392204 | 1.570510 | -1.637260 |
| H | 1.628349 | 2.826490 | -0.412515 |
| C | 1.457563 | 1.747351 | -0.547845 |
| H | -0.383326 | 2.928872 | 1.369084 |
| H | 0.808824 | 1.794840 | 2.039281 |
| H | -0.286486 | -0.351805 | -1.046189 |
| H | -2.123702 | 1.493482 | 2.176399 |
| H | -0.878754 | 0.403463 | 2.819634 |
| C | -0.086465 | 1.867308 | 1.390972 |
| C | -0.123972 | -0.041543 | -0.000683 |
| C | -1.206018 | 0.946548 | 1.922162 |
| C | -1.470564 | -0.071754 | 0.778810 |
| O | -1.294172 | -2.124592 | 2.155331 |

| | | | |
|---|---|---|---|
| N | -3.058226 | -1.805565 | 0.707834 |
| H | -3.545054 | -2.671266 | 0.914173 |
| H | -2.174502 | 2.229742 | -0.901324 |
| H | -4.274666 | 2.327395 | -2.283915 |
| H | -5.860588 | 0.416004 | -2.276441 |
| H | -5.396741 | -1.618565 | -0.895510 |
| C | -1.878876 | -1.457623 | 1.320798 |
| C | -2.888002 | 1.404509 | -0.898793 |
| C | -4.059843 | 1.446950 | -1.674107 |
| C | -4.952521 | 0.369873 | -1.670416 |
| C | -4.702561 | -0.776003 | -0.898888 |
| C | -3.537551 | -0.798242 | -0.137257 |
| C | -2.631178 | 0.277981 | -0.127191 |
| C | 3.708970 | 1.548669 | 0.506298 |
| H | 3.718383 | 2.647058 | 0.498785 |
| C | 4.946120 | 0.893249 | 1.052303 |
| H | 5.846738 | 1.425196 | 0.702958 |
| H | 4.971541 | 0.935321 | 2.156446 |
| H | 5.035935 | -0.156253 | 0.740573 |

27_conf_09

Charge = 0 Multi = 1

| | | | |
|---|---|---|---|
| H | -2.993100 | 4.098411 | -0.441635 |
| O | -3.219107 | 3.161866 | -0.513008 |
| H | -2.532638 | 3.009378 | -2.483270 |
| H | -1.301066 | 2.752388 | -1.229357 |
| C | -2.364491 | 2.572593 | -1.479202 |
| H | -3.647797 | 0.911064 | -1.949352 |
| H | -1.934212 | 0.637469 | -2.262898 |
| C | -2.637885 | 1.077896 | -1.538308 |
| N | -0.311930 | -1.541842 | -0.234286 |
| H | -1.048376 | 1.694576 | 0.669952 |
| H | -1.371746 | 0.264308 | 1.629394 |
| C | -1.245794 | 0.616901 | 0.595050 |
| H | -3.372843 | 0.776815 | 0.438608 |
| C | -2.561104 | 0.359711 | -0.171287 |
| C | -2.760888 | -1.135515 | -0.336682 |
| H | -1.431430 | -1.535259 | -1.985237 |
| H | -1.710051 | -2.933419 | -0.936798 |
| C | -1.558008 | -1.843190 | -0.931378 |
| H | 0.211170 | -3.232204 | 0.915186 |
| H | -1.055845 | -2.232779 | 1.658081 |
| H | 0.156463 | 0.345549 | -1.033288 |
| H | 1.848081 | -1.881302 | 2.026722 |
| H | 0.531708 | -0.912951 | 2.720745 |
| C | -0.122498 | -2.191826 | 1.062990 |
| C | -0.059465 | -0.109495 | -0.052316 |
| C | 0.932421 | -1.325580 | 1.784460 |
| C | 1.237518 | -0.159165 | 0.805397 |
| O | 0.922809 | 1.690327 | 2.424587 |

| | | | |
|---|---|---|---|
| N | 2.774616 | 1.603035 | 1.056456 |
| H | 3.223105 | 2.444356 | 1.402837 |
| H | 2.106552 | -2.205973 | -1.112387 |
| H | 4.283492 | -2.074320 | -2.365796 |
| H | 5.807818 | -0.144858 | -2.015826 |
| H | 5.205133 | 1.680203 | -0.413895 |
| C | 1.573630 | 1.151346 | 1.547462 |
| C | 2.792838 | -1.371882 | -0.959629 |
| C | 4.007776 | -1.286145 | -1.661548 |
| C | 4.865756 | -0.198911 | -1.464840 |
| C | 4.537818 | 0.830064 | -0.567980 |
| C | 3.331169 | 0.726129 | 0.118347 |
| C | 2.458290 | -0.362080 | -0.065804 |
| C | -3.868343 | -1.813331 | 0.008248 |
| H | -3.859549 | -2.899395 | -0.156608 |
| C | -5.142279 | -1.269100 | 0.584153 |
| H | -5.995467 | -1.478714 | -0.084822 |
| H | -5.379381 | -1.755866 | 1.546272 |
| H | -5.107200 | -0.183888 | 0.752740 |

27_conf_10

Charge = 0 Multi = 1

| | | | |
|---|---|---|---|
| H | 0.258975 | 3.984137 | -0.280890 |
| O | 0.634707 | 3.179042 | 0.098811 |
| H | 2.225392 | 3.310766 | -1.254024 |
| H | 2.533161 | 3.998623 | 0.358819 |
| C | 2.029916 | 3.167114 | -0.172339 |
| H | 3.728907 | 1.984774 | 0.350012 |
| H | 2.290469 | 1.629015 | 1.308243 |
| C | 2.637148 | 1.849634 | 0.286378 |
| N | 1.057154 | -0.692759 | 1.383352 |
| H | 0.370228 | 1.192037 | -1.323859 |
| H | 0.824480 | -0.505387 | -1.575421 |
| C | 0.875114 | 0.332251 | -0.866287 |
| H | 2.817424 | 0.856160 | -1.604752 |
| C | 2.364963 | 0.631736 | -0.624630 |
| C | 3.020753 | -0.618244 | -0.050976 |
| H | 2.636814 | -2.061108 | 1.510558 |
| H | 1.632892 | -2.273697 | 0.059635 |
| C | 2.079987 | -1.513804 | 0.735837 |
| H | -0.201057 | -0.621392 | 3.051540 |
| H | 0.728101 | -2.130771 | 2.900311 |
| H | -0.181186 | 0.904791 | 0.908005 |
| H | -1.913570 | -2.041248 | 2.082914 |
| H | -0.718036 | -2.926168 | 1.103548 |
| C | 0.184092 | -1.363811 | 2.330323 |
| C | 0.165706 | -0.028397 | 0.440111 |
| C | -0.986201 | -1.937055 | 1.502752 |
| C | -1.145897 | -0.944821 | 0.320002 |
| O | -0.479663 | -2.570445 | -1.424908 |

| | | | |
|---|---|---|---|
| N | -2.335652 | -1.231584 | -1.689173 |
| H | -2.609742 | -1.579058 | -2.601874 |
| H | -2.432116 | 0.940497 | 2.185396 |
| H | -4.543445 | 2.162052 | 1.644928 |
| H | -5.675596 | 1.805633 | -0.537132 |
| H | -4.726259 | 0.216355 | -2.220198 |
| C | -1.234388 | -1.702543 | -1.016946 |
| C | -2.929558 | 0.778969 | 1.225887 |
| C | -4.116926 | 1.466077 | 0.919329 |
| C | -4.754150 | 1.264422 | -0.309507 |
| C | -4.229923 | 0.375042 | -1.260897 |
| C | -3.056180 | -0.298588 | -0.935420 |
| C | -2.401484 | -0.108571 | 0.296206 |
| C | 4.317686 | -0.930870 | -0.198374 |
| H | 4.677256 | -1.844495 | 0.293721 |
| C | 5.353732 | -0.166979 | -0.970221 |
| H | 4.930503 | 0.676219 | -1.534316 |
| H | 6.130737 | 0.239085 | -0.298078 |
| H | 5.878465 | -0.824565 | -1.684934 |

3-epi-25'_conf_01

Charge = 0 Multi = 1

| | | | |
|---|---|---|---|
| H | 4.632421 | 2.594501 | 1.407058 |
| O | 4.647409 | 2.912627 | 0.493625 |
| H | 4.321508 | 2.210134 | -1.378278 |
| H | 4.871954 | 0.965707 | -0.243999 |
| C | 4.217702 | 1.851614 | -0.340623 |
| H | 2.658567 | 1.143227 | 0.971611 |
| H | 2.134929 | 2.360374 | -0.204234 |
| C | 2.764705 | 1.463714 | -0.079605 |
| O | 3.954787 | -1.339867 | -1.004053 |
| N | 1.042786 | -1.141133 | 1.065509 |
| H | 0.242785 | 1.153965 | -1.335249 |
| H | 0.420514 | -0.568202 | -1.709843 |
| C | 0.713092 | 0.218460 | -0.997702 |
| H | 2.584765 | 0.570965 | -2.040409 |
| C | 2.242488 | 0.352558 | -1.015767 |
| C | 2.856924 | -0.982530 | -0.623737 |
| H | 2.672782 | -2.453330 | 0.904247 |
| H | 1.507179 | -2.606617 | -0.425442 |
| C | 1.997187 | -1.873950 | 0.256094 |
| H | 0.597272 | -2.086184 | 2.933061 |
| H | 0.111348 | -2.998544 | 1.479972 |
| H | 0.259140 | 0.807378 | 1.005769 |
| H | -1.241423 | -0.531306 | 2.690752 |
| H | -2.007388 | -2.014515 | 2.079281 |
| C | 0.192942 | -1.985076 | 1.911024 |
| C | 0.219801 | -0.119975 | 0.404817 |
| C | -1.182483 | -1.307485 | 1.912736 |
| C | -1.251098 | -0.614709 | 0.532875 |

| | | | |
|---|---|---|---|
| O | -1.054493 | -2.664810 | -0.846683 |
| N | -2.713951 | -1.112636 | -1.236743 |
| H | -3.145831 | -1.586470 | -2.023052 |
| H | -1.865486 | 1.926791 | 1.894814 |
| H | -3.747464 | 3.416058 | 1.200826 |
| H | -5.216099 | 2.779633 | -0.697909 |
| H | -4.834494 | 0.645767 | -1.946148 |
| C | -1.619980 | -1.617761 | -0.578280 |
| C | -2.508514 | 1.644969 | 1.057394 |
| C | -3.568286 | 2.481112 | 0.665746 |
| C | -4.394965 | 2.121639 | -0.403857 |
| C | -4.190015 | 0.926284 | -1.110937 |
| C | -3.134790 | 0.113215 | -0.708424 |
| C | -2.294784 | 0.458498 | 0.367030 |

3-epi-25'_conf_02

Charge = 0 Multi = 1

| | | | |
|---|---|---|---|
| H | 5.500973 | 3.066552 | 0.460582 |
| O | 4.568196 | 2.852557 | 0.593216 |
| H | 4.334814 | 2.173752 | -1.373898 |
| H | 4.857738 | 0.940216 | -0.206166 |
| C | 4.216369 | 1.832863 | -0.325327 |
| H | 2.647846 | 1.157816 | 0.973629 |
| H | 2.141747 | 2.365063 | -0.218541 |
| C | 2.762333 | 1.463852 | -0.079290 |
| O | 3.951243 | -1.340801 | -1.006140 |
| N | 1.040975 | -1.139400 | 1.066938 |
| H | 0.241868 | 1.156228 | -1.333667 |
| H | 0.418900 | -0.565874 | -1.708813 |
| C | 0.711926 | 0.220451 | -0.996502 |
| H | 2.583672 | 0.571384 | -2.039905 |
| C | 2.241294 | 0.353731 | -1.015190 |
| C | 2.854863 | -0.981742 | -0.623180 |
| H | 2.672536 | -2.449779 | 0.907462 |
| H | 1.506930 | -2.606446 | -0.421781 |
| C | 1.996132 | -1.872098 | 0.258566 |
| H | 0.594975 | -2.084385 | 2.934387 |
| H | 0.109214 | -2.996652 | 1.481135 |
| H | 0.257686 | 0.809178 | 1.007031 |
| H | -1.243229 | -0.528855 | 2.691132 |
| H | -2.009490 | -2.012150 | 2.080183 |
| C | 0.190914 | -1.983191 | 1.912243 |
| C | 0.218490 | -0.118109 | 0.406000 |
| C | -1.184367 | -1.305413 | 1.913471 |
| C | -1.252469 | -0.612995 | 0.533397 |
| O | -1.054470 | -2.663240 | -0.845930 |
| N | -2.714406 | -1.111877 | -1.236740 |
| H | -3.145958 | -1.586267 | -2.022891 |
| H | -1.868156 | 1.928825 | 1.894075 |
| H | -3.750520 | 3.417172 | 1.198922 |

| | | | |
|---|---|---|---|
| H | -5.218307 | 2.779486 | -0.700060 |
| H | -4.835401 | 0.645331 | -1.947448 |
| C | -1.620450 | -1.616383 | -0.577774 |
| C | -2.510825 | 1.646495 | 1.056557 |
| C | -3.570797 | 2.482110 | 0.664231 |
| C | -4.396990 | 2.121944 | -0.405497 |
| C | -4.191336 | 0.926426 | -1.112108 |
| C | -3.135937 | 0.113897 | -0.708948 |
| C | -2.296409 | 0.459866 | 0.366699 |

3-epi-25'_conf_03

Charge = 0 Multi = 1

| | | | |
|---|---|---|---|
| H | 4.865714 | 0.969370 | -0.977453 |
| O | 4.881642 | 1.898504 | -0.682436 |
| H | 4.523582 | 1.112550 | 1.210845 |
| H | 4.383953 | 2.869538 | 1.040176 |
| C | 4.164990 | 1.913797 | 0.536900 |
| H | 2.194242 | 1.564639 | 1.332716 |
| H | 2.223225 | 2.740511 | 0.005556 |
| C | 2.646726 | 1.783581 | 0.352275 |
| O | 4.092937 | -0.812599 | -0.697374 |
| N | 1.012202 | -1.177434 | 1.038877 |
| H | 0.214785 | 1.452262 | -0.993091 |
| H | 0.520357 | -0.168180 | -1.636735 |
| C | 0.722709 | 0.498876 | -0.785179 |
| H | 2.627229 | 1.053277 | -1.658460 |
| C | 2.238460 | 0.712142 | -0.686487 |
| C | 2.921083 | -0.617121 | -0.415005 |
| H | 2.720489 | -2.368858 | 0.773317 |
| H | 1.670794 | -2.311645 | -0.658586 |
| C | 2.062989 | -1.705708 | 0.190688 |
| H | 0.513017 | -2.455218 | 2.681190 |
| H | 0.179706 | -3.126362 | 1.062820 |
| H | 0.106208 | 0.706562 | 1.253302 |
| H | -1.403337 | -0.981087 | 2.570896 |
| H | -2.032085 | -2.375174 | 1.664212 |
| C | 0.167890 | -2.200418 | 1.664282 |
| C | 0.167550 | -0.102323 | 0.501968 |
| C | -1.245792 | -1.607373 | 1.679753 |
| C | -1.272405 | -0.691455 | 0.435145 |
| O | -0.849601 | -2.457513 | -1.252391 |
| N | -2.586589 | -0.960827 | -1.493618 |
| H | -2.936825 | -1.316334 | -2.376999 |
| H | -2.140474 | 1.541001 | 2.154399 |
| H | -4.072802 | 3.018425 | 1.584574 |
| H | -5.375490 | 2.633934 | -0.494453 |
| H | -4.773938 | 0.769514 | -2.050049 |
| C | -1.502266 | -1.507318 | -0.852977 |
| C | -2.709950 | 1.370854 | 1.237403 |
| C | -3.798010 | 2.200379 | 0.915393 |

| | | | |
|---|---|---|---|
| C | -4.531151 | 1.982906 | -0.255861 |
| C | -4.202471 | 0.939524 | -1.135684 |
| C | -3.121082 | 0.130793 | -0.799617 |
| C | -2.373844 | 0.334192 | 0.375772 |

3-epi-25'_conf_04

Charge = 0 Multi = 1

| | | | |
|---|---|---|---|
| H | 4.975694 | 0.737193 | -0.318458 |
| O | 5.085940 | 1.556065 | 0.198335 |
| H | 4.099284 | 3.290402 | 0.543495 |
| H | 4.026062 | 2.756773 | -1.146515 |
| C | 3.993518 | 2.398350 | -0.095757 |
| H | 2.575170 | 1.409569 | 1.203029 |
| H | 1.865657 | 2.572905 | 0.071615 |
| C | 2.620805 | 1.774210 | 0.163170 |
| O | 4.101677 | -0.861281 | -0.714655 |
| N | 1.032786 | -1.171823 | 1.011113 |
| H | 0.187331 | 1.334147 | -1.153270 |
| H | 0.503504 | -0.324513 | -1.685121 |
| C | 0.709617 | 0.403604 | -0.886462 |
| H | 2.587561 | 0.932256 | -1.822037 |
| C | 2.224565 | 0.646150 | -0.820281 |
| C | 2.921094 | -0.664592 | -0.479217 |
| H | 2.718210 | -2.393218 | 0.739800 |
| H | 1.641602 | -2.354307 | -0.673948 |
| C | 2.058274 | -1.735966 | 0.154215 |
| H | 0.571615 | -2.393248 | 2.705792 |
| H | 0.175121 | -3.107750 | 1.119930 |
| H | 0.161757 | 0.737636 | 1.154199 |
| H | -1.322626 | -0.885758 | 2.606080 |
| H | -2.003970 | -2.304339 | 1.778611 |
| C | 0.196463 | -2.164365 | 1.693502 |
| C | 0.184620 | -0.112694 | 0.447753 |
| C | -1.206582 | -1.549155 | 1.735601 |
| C | -1.264163 | -0.683374 | 0.456372 |
| O | -0.924795 | -2.523483 | -1.169891 |
| N | -2.648887 | -1.012193 | -1.413161 |
| H | -3.034221 | -1.398095 | -2.268754 |
| H | -2.040660 | 1.631298 | 2.109477 |
| H | -3.971732 | 3.112525 | 1.545777 |
| H | -5.352129 | 2.661912 | -0.468870 |
| H | -4.831100 | 0.725954 | -1.964959 |
| C | -1.550292 | -1.548047 | -0.788222 |
| C | -2.644536 | 1.431662 | 1.220893 |
| C | -3.731947 | 2.263372 | 0.902391 |
| C | -4.508848 | 2.008673 | -0.232590 |
| C | -4.225609 | 0.924974 | -1.078802 |
| C | -3.144061 | 0.114725 | -0.746937 |
| C | -2.353252 | 0.355200 | 0.392395 |

3-epi-25'_conf_05

Charge = 0 Multi = 1

| | | | |
|---|---|---|---|
| H | -4.905385 | -1.124307 | -0.376552 |
| O | -4.668792 | -1.389251 | -1.276385 |
| H | -4.369562 | -0.462385 | -3.059095 |
| H | -4.984196 | 0.613480 | -1.789631 |
| C | -4.285824 | -0.222316 | -1.986789 |
| H | -2.178592 | -0.629881 | -1.888146 |
| H | -2.577012 | 1.006135 | -2.423755 |
| C | -2.852605 | 0.221677 | -1.698884 |
| O | -4.026832 | -0.258999 | 1.347296 |
| N | -0.516323 | -0.707619 | 1.138722 |
| H | -0.921359 | 1.967346 | -0.982413 |
| H | -1.136099 | 1.999452 | 0.760673 |
| C | -1.179315 | 1.339202 | -0.117693 |
| H | -3.333354 | 1.629350 | -0.143815 |
| C | -2.617341 | 0.803597 | -0.285021 |
| C | -2.943203 | -0.223807 | 0.789636 |
| H | -1.921693 | -1.988956 | 0.247679 |
| H | -2.104473 | -1.788090 | 2.001743 |
| C | -1.857291 | -1.254326 | 1.073111 |
| H | 0.078404 | -0.809292 | 3.161067 |
| H | -0.960622 | 0.584567 | 2.801236 |
| H | -0.097833 | -0.374641 | -0.894387 |
| H | 1.983524 | 0.517648 | 2.567558 |
| H | 0.885926 | 1.877251 | 2.252803 |
| C | -0.147750 | -0.050537 | 2.395112 |
| C | -0.162050 | 0.199163 | 0.043924 |
| C | 1.074405 | 0.817969 | 2.030516 |
| C | 1.258315 | 0.640097 | 0.497422 |
| O | 1.314219 | 3.047056 | -0.083153 |
| N | 2.908614 | 1.587784 | -0.884244 |
| H | 3.452584 | 2.269939 | -1.401877 |
| H | 1.673607 | -2.218613 | 1.028160 |
| H | 3.607194 | -3.520250 | 0.084479 |
| H | 5.272812 | -2.395355 | -1.374455 |
| H | 5.054469 | 0.036361 | -1.917738 |
| C | 1.783541 | 1.927207 | -0.174660 |
| C | 2.419203 | -1.735751 | 0.394786 |
| C | 3.499350 | -2.457237 | -0.142222 |
| C | 4.436949 | -1.823426 | -0.964463 |
| C | 4.324385 | -0.459145 | -1.275160 |
| C | 3.248344 | 0.238067 | -0.733336 |
| C | 2.298697 | -0.383994 | 0.097563 |

3-epi-25'_conf_06

Charge = 0 Multi = 1

| | | | |
|---|---|---|---|
| H | -4.571144 | 3.345025 | 0.800905 |
| O | -4.710513 | 2.918422 | -0.056214 |
| H | -5.122021 | 1.068103 | 0.836215 |

| | | | |
|---|---|---|---|
| H | -4.667226 | 1.072352 | -0.875590 |
| C | -4.442414 | 1.537688 | 0.097181 |
| H | -2.333697 | 1.742866 | -0.252983 |
| H | -2.785450 | 1.772942 | 1.453575 |
| C | -2.992595 | 1.269763 | 0.492940 |
| O | -3.881195 | -1.597834 | -0.878330 |
| N | -0.420366 | -0.969400 | -1.102441 |
| H | -1.046318 | 0.220268 | 2.062340 |
| H | -1.119609 | -1.465888 | 1.575606 |
| C | -1.219182 | -0.437885 | 1.198459 |
| H | -3.371454 | -0.654187 | 1.387251 |
| C | -2.653033 | -0.226029 | 0.669953 |
| C | -2.869616 | -0.966250 | -0.643791 |
| H | -1.842050 | 0.200302 | -2.102850 |
| H | -1.907296 | -1.533568 | -2.482319 |
| C | -1.747732 | -0.812522 | -1.668017 |
| H | 0.316118 | -2.825113 | -1.785754 |
| H | -0.786260 | -2.971446 | -0.402035 |
| H | -0.149827 | 0.885330 | -0.150259 |
| H | 2.134290 | -2.565578 | -0.246353 |
| H | 0.976620 | -2.736478 | 1.088709 |
| C | 0.014675 | -2.343565 | -0.841833 |
| C | -0.165624 | -0.185503 | 0.108803 |
| C | 1.182696 | -2.194141 | 0.155694 |
| C | 1.269931 | -0.671684 | 0.456321 |
| O | 1.223788 | -0.846173 | 2.926722 |
| N | 2.798365 | 0.447436 | 1.849855 |
| H | 3.288350 | 0.763578 | 2.679945 |
| H | 1.798515 | -0.289138 | -2.408147 |
| H | 3.700675 | 1.108010 | -3.275062 |
| H | 5.234531 | 2.247173 | -1.688367 |
| H | 4.913403 | 2.016503 | 0.781944 |
| C | 1.714914 | -0.393473 | 1.908571 |
| C | 2.486464 | 0.208525 | -1.723098 |
| C | 3.548480 | 0.996706 | -2.199199 |
| C | 4.411843 | 1.638720 | -1.305161 |
| C | 4.241150 | 1.515694 | 0.082712 |
| C | 3.184120 | 0.730652 | 0.534337 |
| C | 2.308790 | 0.076200 | -0.351555 |

3-epi-25'_conf_07

Charge = 0 Multi = 1

| | | | |
|---|---|---|---|
| H | -5.497045 | 3.129554 | 0.159044 |
| O | -4.602683 | 2.909689 | 0.451115 |
| H | -5.121727 | 0.925595 | 0.877259 |
| H | -4.571472 | 1.227781 | -0.785391 |
| C | -4.408782 | 1.519284 | 0.270460 |
| H | -2.290152 | 1.763906 | 0.061300 |
| H | -2.836613 | 1.547397 | 1.724801 |
| C | -2.986335 | 1.188864 | 0.693130 |

| | | | |
|---|---|---|---|
| O | -3.866665 | -1.500686 | -1.049635 |
| N | -0.434622 | -0.789522 | -1.219027 |
| H | -1.037139 | -0.068662 | 2.089552 |
| H | -1.112858 | -1.669890 | 1.370662 |
| C | -1.215017 | -0.599183 | 1.142772 |
| H | -3.367356 | -0.840371 | 1.312228 |
| C | -2.652734 | -0.316554 | 0.657662 |
| C | -2.872738 | -0.871797 | -0.743489 |
| H | -1.865087 | 0.520562 | -2.010759 |
| H | -1.930703 | -1.132641 | -2.661047 |
| C | -1.766623 | -0.548341 | -1.744496 |
| H | 0.293201 | -2.523325 | -2.176665 |
| H | -0.799678 | -2.873569 | -0.822383 |
| H | -0.149548 | 0.903368 | -0.006271 |
| H | 2.121957 | -2.499860 | -0.628176 |
| H | 0.972349 | -2.864610 | 0.674723 |
| C | -0.000836 | -2.187724 | -1.169320 |
| C | -0.168252 | -0.193717 | 0.092810 |
| C | 1.174178 | -2.190220 | -0.168872 |
| C | 1.268066 | -0.729180 | 0.353276 |
| O | 1.239177 | -1.267602 | 2.770681 |
| N | 2.812835 | 0.164649 | 1.884714 |
| H | 3.310746 | 0.352919 | 2.748293 |
| H | 1.774656 | 0.075637 | -2.426623 |
| H | 3.676504 | 1.579506 | -3.091917 |
| H | 5.228776 | 2.463528 | -1.366457 |
| H | 4.925991 | 1.868041 | 1.044746 |
| C | 1.725099 | -0.670857 | 1.827055 |
| C | 2.470727 | 0.462667 | -1.680996 |
| C | 3.532647 | 1.309244 | -2.043435 |
| C | 4.406370 | 1.807520 | -1.071174 |
| C | 4.246217 | 1.479386 | 0.284216 |
| C | 3.189205 | 0.639415 | 0.622804 |
| C | 2.303654 | 0.127533 | -0.343072 |

3-epi-25'_conf_08

Charge = 0 Multi = 1

| | | | |
|---|---|---|---|
| H | -3.888382 | -2.429222 | -1.259725 |
| O | -4.431063 | -1.686434 | -0.960640 |
| H | -4.426857 | -0.953063 | -2.917413 |
| H | -5.033522 | 0.124761 | -1.642595 |
| C | -4.252943 | -0.617152 | -1.878595 |
| H | -2.108467 | -0.755190 | -1.911761 |
| H | -2.741509 | 0.736292 | -2.601539 |
| C | -2.875452 | 0.025219 | -1.769111 |
| O | -3.861611 | 0.246517 | 1.547472 |
| N | -0.579152 | -0.570457 | 1.139254 |
| H | -0.925575 | 1.839030 | -1.295668 |
| H | -1.149876 | 2.105749 | 0.427416 |
| C | -1.196255 | 1.335421 | -0.355737 |

| | | | |
|---|---|---|---|
| H | -3.344474 | 1.645313 | -0.431116 |
| C | -2.643240 | 0.795980 | -0.454182 |
| C | -2.948158 | -0.026555 | 0.793634 |
| H | -1.981986 | -1.887262 | 0.305519 |
| H | -2.176225 | -1.594555 | 2.053351 |
| C | -1.927070 | -1.119243 | 1.093955 |
| H | -0.004589 | -0.477834 | 3.167361 |
| H | -1.050805 | 0.867374 | 2.670757 |
| H | -0.105104 | -0.459560 | -0.904158 |
| H | 1.888532 | 0.827815 | 2.493193 |
| H | 0.780019 | 2.121250 | 1.993099 |
| C | -0.229559 | 0.205070 | 2.332371 |
| C | -0.192694 | 0.214087 | -0.036835 |
| C | 0.990155 | 1.046681 | 1.901383 |
| C | 1.217622 | 0.697316 | 0.404535 |
| O | 1.307552 | 3.023553 | -0.441132 |
| N | 2.916720 | 1.478785 | -1.021301 |
| H | 3.481306 | 2.096392 | -1.594816 |
| H | 1.596920 | -2.086355 | 1.263307 |
| H | 3.552141 | -3.489875 | 0.535335 |
| H | 5.270847 | -2.539796 | -0.985084 |
| H | 5.084048 | -0.182888 | -1.804405 |
| C | 1.771696 | 1.898981 | -0.391106 |
| C | 2.365567 | -1.679036 | 0.604877 |
| C | 3.458122 | -2.458733 | 0.187548 |
| C | 4.425687 | -1.923423 | -0.669357 |
| C | 4.331293 | -0.602307 | -1.134332 |
| C | 3.242703 | 0.153753 | -0.709094 |
| C | 2.262786 | -0.368684 | 0.154659 |

3-epi-25'_conf_09

Charge = 0 Multi = 1

| | | | |
|---|---|---|---|
| H | 4.962066 | 0.543166 | -0.995811 |
| O | 5.077827 | 1.498241 | -0.839966 |
| H | 4.553607 | 1.073651 | 1.130278 |
| H | 4.630602 | 2.783959 | 0.677900 |
| C | 4.319417 | 1.789497 | 0.318801 |
| H | 2.287546 | 1.811188 | 1.037979 |
| H | 2.518881 | 2.711521 | -0.477206 |
| C | 2.806568 | 1.796709 | 0.067011 |
| O | 3.994601 | -1.103158 | -0.504098 |
| N | 1.016140 | -0.614483 | 1.298422 |
| H | 0.385065 | 1.461047 | -1.279135 |
| H | 0.568291 | -0.251448 | -1.666695 |
| C | 0.791673 | 0.509571 | -0.907044 |
| H | 2.758024 | 0.720405 | -1.782454 |
| C | 2.318940 | 0.598307 | -0.780324 |
| C | 2.862556 | -0.721977 | -0.254466 |
| H | 2.500671 | -2.107920 | 1.327401 |
| H | 1.389417 | -2.255877 | -0.061857 |

| | | | |
|---|---|---|---|
| C | 1.910615 | -1.531228 | 0.601508 |
| H | -0.110472 | -0.426658 | 3.047655 |
| H | 0.647878 | -2.021717 | 2.836663 |
| H | -0.132850 | 1.068614 | 0.964726 |
| H | -2.026183 | -1.625897 | 2.190867 |
| H | -1.006536 | -2.676205 | 1.179277 |
| C | 0.145017 | -1.201834 | 2.305130 |
| C | 0.126857 | 0.143209 | 0.426509 |
| C | -1.129674 | -1.650937 | 1.556876 |
| C | -1.243921 | -0.674219 | 0.351138 |
| O | -0.681635 | -2.362520 | -1.368997 |
| N | -2.498921 | -0.967599 | -1.616815 |
| H | -2.809801 | -1.325416 | -2.513789 |
| H | -2.374144 | 1.351913 | 2.172998 |
| H | -4.432417 | 2.661743 | 1.639154 |
| H | -5.644746 | 2.280232 | -0.494786 |
| H | -4.828385 | 0.579227 | -2.137715 |
| C | -1.398480 | -1.460887 | -0.964852 |
| C | -2.904370 | 1.181316 | 1.232810 |
| C | -4.063119 | 1.917272 | 0.930640 |
| C | -4.745582 | 1.701323 | -0.271126 |
| C | -4.296079 | 0.749576 | -1.199964 |
| C | -3.148674 | 0.030035 | -0.880223 |
| C | -2.448976 | 0.234023 | 0.323873 |

3-epi-25'_conf_10

Charge = 0 Multi = 1

| | | | |
|---|---|---|---|
| H | -5.202239 | 0.021398 | -0.250712 |
| O | -5.324254 | 0.464862 | -1.109395 |
| H | -4.191473 | -1.091654 | -1.905305 |
| H | -4.508829 | 0.286282 | -2.969072 |
| C | -4.264115 | 0.012939 | -1.929936 |
| H | -2.114949 | 0.104653 | -2.112176 |
| H | -2.878515 | 1.684087 | -1.876310 |
| C | -2.910488 | 0.629510 | -1.557422 |
| O | -3.999874 | -1.117583 | 0.855252 |
| N | -0.415598 | -1.146518 | 0.817256 |
| H | -1.002857 | 2.040885 | -0.322328 |
| H | -1.184251 | 1.499192 | 1.336889 |
| C | -1.209950 | 1.153961 | 0.293570 |
| H | -3.369623 | 1.280098 | 0.428090 |
| C | -2.617489 | 0.623330 | -0.034214 |
| C | -2.876978 | -0.763144 | 0.530613 |
| H | -1.698735 | -2.189571 | -0.468077 |
| H | -1.924430 | -2.550352 | 1.250395 |
| C | -1.707150 | -1.736583 | 0.543625 |
| H | 0.181875 | -1.859324 | 2.711235 |
| H | -0.934806 | -0.481240 | 2.796087 |
| H | -0.039024 | -0.146204 | -0.992880 |
| H | 2.012602 | -0.318246 | 2.594057 |

| | | | |
|---|---|---|---|
| H | 0.843505 | 1.010800 | 2.731885 |
| C | -0.086847 | -0.908835 | 2.223594 |
| C | -0.127129 | 0.085999 | 0.080862 |
| C | 1.085224 | 0.094465 | 2.176069 |
| C | 1.268297 | 0.437913 | 0.670544 |
| O | 1.176786 | 2.901696 | 0.906951 |
| N | 2.846472 | 1.879660 | -0.309988 |
| H | 3.344720 | 2.723628 | -0.572012 |
| H | 1.860528 | -2.408696 | 0.248729 |
| H | 3.858098 | -3.214245 | -1.048072 |
| H | 5.438610 | -1.578699 | -2.045696 |
| H | 5.069724 | 0.880328 | -1.770109 |
| C | 1.710368 | 1.902466 | 0.460349 |
| C | 2.568825 | -1.702027 | -0.186141 |
| C | 3.684635 | -2.143722 | -0.917987 |
| C | 4.574296 | -1.222199 | -1.480239 |
| C | 4.377334 | 0.159599 | -1.331213 |
| C | 3.267139 | 0.577012 | -0.602775 |
| C | 2.364477 | -0.336836 | -0.028961 |

3-epi-27_conf_01

Charge = 0 Multi = 1

| | | | |
|---|---|---|---|
| H | -2.420467 | 3.804439 | 1.873477 |
| O | -2.746908 | 3.004049 | 1.442029 |
| H | -2.783148 | 3.878640 | -0.458461 |
| H | -1.231432 | 3.150297 | 0.011253 |
| C | -2.328779 | 3.027750 | 0.086339 |
| H | -3.859039 | 1.694373 | -0.608337 |
| H | -2.413961 | 1.738073 | -1.625565 |
| C | -2.758823 | 1.728532 | -0.577112 |
| N | -0.619461 | -1.953030 | -0.432251 |
| H | -0.292264 | 0.810340 | -0.772953 |
| H | -0.349443 | 1.175321 | 0.951549 |
| C | -0.695025 | 0.461190 | 0.189091 |
| H | -2.618806 | 0.472540 | 1.154886 |
| C | -2.233203 | 0.459099 | 0.122957 |
| C | -2.741226 | -0.799701 | -0.567141 |
| H | -1.308151 | -0.938259 | -2.181971 |
| H | -2.124152 | -2.464803 | -1.790229 |
| C | -1.687737 | -1.560906 | -1.335785 |
| H | 0.790371 | -2.318217 | -1.996247 |
| H | 0.230344 | -3.767938 | -1.135886 |
| H | -0.439825 | -1.190079 | 1.532994 |
| H | 2.609951 | -2.703158 | -0.389436 |
| H | 1.450363 | -3.163703 | 0.891399 |
| C | 0.486398 | -2.702732 | -0.997715 |
| C | -0.135246 | -0.921972 | 0.503328 |
| C | 1.608491 | -2.510802 | 0.019042 |
| C | 1.422863 | -1.042175 | 0.470392 |
| O | 1.729755 | -1.379577 | 2.894960 |

| | | | |
|---|---|---|---|
| N | 2.943159 | 0.216075 | 1.750117 |
| H | 3.481266 | 0.564902 | 2.536115 |
| H | 1.409170 | -0.275194 | -2.401174 |
| H | 2.880782 | 1.500823 | -3.334763 |
| H | 4.443185 | 2.746384 | -1.856682 |
| H | 4.565524 | 2.225768 | 0.587482 |
| C | 2.021269 | -0.793498 | 1.868426 |
| C | 2.097830 | 0.258657 | -1.744252 |
| C | 2.926962 | 1.264175 | -2.269706 |
| C | 3.805116 | 1.964935 | -1.437347 |
| C | 3.880684 | 1.681431 | -0.065373 |
| C | 3.051914 | 0.681201 | 0.434911 |
| C | 2.159968 | -0.036149 | -0.386296 |
| C | -4.005529 | -1.244490 | -0.484726 |
| H | -4.254851 | -2.164819 | -1.028028 |
| C | -5.133596 | -0.619425 | 0.282892 |
| H | -5.656100 | -1.376448 | 0.892073 |
| H | -4.799236 | 0.185281 | 0.952864 |
| H | -5.892733 | -0.192377 | -0.396861 |

3-epi-27_conf_02

Charge = 0 Multi = 1

| | | | |
|---|---|---|---|
| H | -4.077558 | 3.800525 | 0.443232 |
| O | -3.121454 | 3.942169 | 0.399617 |
| H | -1.407238 | 2.945462 | 0.777545 |
| H | -2.729659 | 2.509278 | 1.876915 |
| C | -2.489217 | 2.746039 | 0.819925 |
| H | -3.950137 | 1.452337 | -0.069973 |
| H | -2.550184 | 1.771821 | -1.101043 |
| C | -2.852137 | 1.554418 | -0.061669 |
| N | -0.507039 | -1.951462 | -0.651547 |
| H | -0.358186 | 0.843030 | -0.513057 |
| H | -0.334870 | 0.898898 | 1.247880 |
| C | -0.686949 | 0.307310 | 0.389350 |
| H | -2.561634 | 0.018149 | 1.419072 |
| C | -2.225983 | 0.220381 | 0.386307 |
| C | -2.693724 | -0.929437 | -0.498769 |
| H | -1.334092 | -0.688193 | -2.163856 |
| H | -2.044053 | -2.308340 | -2.022360 |
| C | -1.636929 | -1.473632 | -1.429762 |
| H | 0.839715 | -1.953941 | -2.310728 |
| H | 0.406015 | -3.561974 | -1.692892 |
| H | -0.268246 | -1.532679 | 1.408699 |
| H | 2.757462 | -2.490093 | -0.870176 |
| H | 1.692272 | -3.236204 | 0.357070 |
| C | 0.609042 | -2.521869 | -1.382773 |
| C | -0.034072 | -1.070365 | 0.430747 |
| C | 1.768870 | -2.435129 | -0.394382 |
| C | 1.524085 | -1.080247 | 0.312588 |
| O | 1.975864 | -1.805762 | 2.626670 |

| | | | |
|---|---|---|---|
| N | 3.041185 | 0.032692 | 1.723922 |
| H | 3.601005 | 0.274965 | 2.534523 |
| H | 1.311623 | 0.167387 | -2.377697 |
| H | 2.634871 | 2.163189 | -3.051835 |
| H | 4.209264 | 3.229043 | -1.450892 |
| H | 4.491816 | 2.305403 | 0.856955 |
| C | 2.181380 | -1.036608 | 1.705691 |
| C | 2.006005 | 0.621359 | -1.668810 |
| C | 2.751554 | 1.750659 | -2.047521 |
| C | 3.636344 | 2.350164 | -1.146019 |
| C | 3.801242 | 1.840863 | 0.150783 |
| C | 3.053987 | 0.721555 | 0.505978 |
| C | 2.157578 | 0.102414 | -0.387137 |
| C | -3.925338 | -1.462067 | -0.453391 |
| H | -4.144414 | -2.285321 | -1.144992 |
| C | -5.053927 | -1.057510 | 0.448822 |
| H | -5.524988 | -1.944796 | 0.904194 |
| H | -4.733304 | -0.389091 | 1.260659 |
| H | -5.850654 | -0.538508 | -0.113909 |

3-epi-27_conf_03

Charge = 0 Multi = 1

| | | | |
|---|---|---|---|
| H | -4.418899 | 2.695455 | -0.553456 |
| O | -3.510231 | 2.939534 | -0.780654 |
| H | -3.674082 | 2.177751 | -2.721499 |
| H | -2.045834 | 2.387996 | -2.057577 |
| C | -3.066765 | 2.062347 | -1.803070 |
| H | -4.124281 | 0.294183 | -1.212134 |
| H | -2.710062 | -0.010371 | -2.231037 |
| C | -3.076668 | 0.591553 | -1.383015 |
| N | -0.306428 | -0.800373 | 1.701491 |
| H | -0.385804 | -0.307433 | -1.026284 |
| H | -0.526517 | 1.454623 | -0.831396 |
| C | -0.738445 | 0.487099 | -0.351242 |
| H | -2.548503 | 1.108687 | 0.598171 |
| C | -2.256733 | 0.317935 | -0.118507 |
| C | -2.479725 | -0.991513 | 0.622184 |
| H | -1.870401 | -1.950803 | 2.469202 |
| H | -2.125385 | -0.188782 | 2.602138 |
| C | -1.727265 | -0.996655 | 1.940441 |
| H | 0.695335 | -1.813392 | 3.264894 |
| H | 0.111800 | -0.183526 | 3.691949 |
| H | -0.276772 | 1.318181 | 1.569989 |
| H | 2.708511 | -0.844320 | 2.363359 |
| H | 2.145836 | 0.706845 | 3.025687 |
| C | 0.553993 | -0.793118 | 2.874297 |
| C | 0.004230 | 0.417527 | 0.972703 |
| C | 1.867223 | -0.139303 | 2.382580 |
| C | 1.553202 | 0.377420 | 0.948158 |
| O | 1.971216 | 2.780703 | 1.322901 |

| | | | |
|---|---|---|---|
| N | 2.891960 | 1.672784 | -0.482968 |
| H | 3.386152 | 2.461774 | -0.885905 |
| H | 1.361805 | -2.441233 | 0.159385 |
| H | 2.531770 | -3.378767 | -1.860782 |
| H | 3.914263 | -1.897812 | -3.297000 |
| H | 4.168486 | 0.530157 | -2.754235 |
| C | 2.142844 | 1.771041 | 0.664367 |
| C | 1.984828 | -1.807062 | -0.473417 |
| C | 2.634988 | -2.321107 | -1.608372 |
| C | 3.412707 | -1.485935 | -2.417967 |
| C | 3.562449 | -0.121748 | -2.122318 |
| C | 2.909642 | 0.368482 | -0.994693 |
| C | 2.126253 | -0.459080 | -0.169698 |
| C | -3.173107 | -2.089635 | 0.272036 |
| H | -3.171693 | -2.895934 | 1.017571 |
| C | -3.963034 | -2.430166 | -0.960861 |
| H | -3.770751 | -3.478095 | -1.244140 |
| H | -5.048979 | -2.359560 | -0.767999 |
| H | -3.736305 | -1.802878 | -1.828170 |

3-epi-27_conf_04

Charge = 0 Multi = 1

| | | | |
|---|---|---|---|
| H | -4.899132 | 2.025307 | 2.409952 |
| O | -5.248104 | 1.509425 | 1.669357 |
| H | -4.400002 | -0.297135 | 2.303898 |
| H | -4.774586 | -0.127919 | 0.582649 |
| C | -4.376274 | 0.413388 | 1.453683 |
| H | -2.917870 | 1.728988 | 0.544033 |
| H | -2.490651 | 1.170007 | 2.156094 |
| C | -2.933040 | 0.844581 | 1.198343 |
| N | -0.044618 | -1.572792 | -1.003732 |
| H | -0.330083 | 0.947340 | 0.112671 |
| H | -0.327806 | 0.348662 | 1.788723 |
| C | -0.557822 | 0.076616 | 0.746036 |
| H | -2.220879 | -1.166353 | 1.244620 |
| C | -2.059287 | -0.266501 | 0.617705 |
| C | -2.317475 | -0.713660 | -0.816423 |
| H | -1.619892 | -2.221738 | -2.209243 |
| H | -1.721929 | -2.774842 | -0.516402 |
| C | -1.449355 | -1.909191 | -1.168406 |
| H | 1.009408 | -2.750220 | -2.409428 |
| H | 0.599503 | -3.595470 | -0.893894 |
| H | 0.142334 | -1.921910 | 1.081920 |
| H | 3.004240 | -1.883141 | -1.372792 |
| H | 2.628970 | -2.935475 | 0.010551 |
| C | 0.915718 | -2.618641 | -1.319771 |
| C | 0.295068 | -1.110030 | 0.330493 |
| C | 2.227046 | -2.150843 | -0.645172 |
| C | 1.827216 | -0.912323 | 0.209386 |
| O | 2.470285 | -1.778397 | 2.429079 |

| | | | |
|---|---|---|---|
| N | 3.136458 | 0.317783 | 1.723013 |
| H | 3.658257 | 0.578770 | 2.552811 |
| H | 1.333791 | 0.476021 | -2.327422 |
| H | 2.238614 | 2.768864 | -2.829960 |
| H | 3.606702 | 3.965348 | -1.137765 |
| H | 4.108213 | 2.910930 | 1.074310 |
| C | 2.500770 | -0.893004 | 1.593824 |
| C | 1.949174 | 1.008568 | -1.600464 |
| C | 2.451328 | 2.293216 | -1.870011 |
| C | 3.220990 | 2.967474 | -0.915618 |
| C | 3.508843 | 2.384953 | 0.328807 |
| C | 3.001497 | 1.112585 | 0.577072 |
| C | 2.228579 | 0.420794 | -0.373334 |
| C | -3.096212 | -0.188659 | -1.781027 |
| H | -3.036405 | -0.708771 | -2.746543 |
| C | -4.029743 | 0.988708 | -1.830310 |
| H | -3.605414 | 1.774333 | -2.481035 |
| H | -4.981000 | 0.688260 | -2.301565 |
| H | -4.266830 | 1.448803 | -0.867515 |

3-epi-27_conf_05

Charge = 0 Multi = 1

| | | | |
|---|---|---|---|
| H | 4.240945 | 3.707131 | -0.773167 |
| O | 4.636583 | 3.085517 | -0.146270 |
| H | 4.472975 | 1.474611 | -1.472831 |
| H | 4.628939 | 1.101549 | 0.254070 |
| C | 4.152289 | 1.790941 | -0.459935 |
| H | 2.337815 | 2.026288 | 0.664103 |
| H | 2.179973 | 2.407352 | -1.055864 |
| C | 2.635497 | 1.693288 | -0.345549 |
| N | 0.249684 | -0.928011 | 1.362051 |
| H | 0.139341 | 1.243393 | -0.136243 |
| H | 0.165448 | 0.463317 | -1.728325 |
| C | 0.500052 | 0.360504 | -0.684677 |
| H | 2.417114 | -0.026931 | -1.612174 |
| C | 2.053834 | 0.294710 | -0.624473 |
| C | 2.508121 | -0.734650 | 0.400778 |
| H | 1.838448 | 0.149330 | 2.249379 |
| H | 2.020214 | -1.611003 | 2.303507 |
| C | 1.677363 | -0.779100 | 1.666466 |
| H | -0.650737 | -1.885505 | 3.019285 |
| H | 0.074166 | -3.000842 | 1.834523 |
| H | 0.253317 | -1.773056 | -0.602425 |
| H | -2.685041 | -1.913833 | 1.741993 |
| H | -1.910737 | -3.078733 | 0.643487 |
| C | -0.478702 | -2.042760 | 1.941869 |
| C | -0.104203 | -0.875551 | -0.045567 |
| C | -1.794911 | -2.098252 | 1.126155 |
| C | -1.645375 | -1.007023 | 0.027886 |
| O | -1.971173 | -2.445323 | -1.951079 |

| | | | |
|---|---|---|---|
| N | -3.104247 | -0.445083 | -1.724894 |
| H | -3.622563 | -0.486372 | -2.595889 |
| H | -1.620360 | 0.948614 | 2.217882 |
| H | -3.025331 | 3.033857 | 2.203451 |
| H | -4.517050 | 3.517289 | 0.277798 |
| H | -4.648608 | 1.941520 | -1.660177 |
| C | -2.234034 | -1.431775 | -1.329189 |
| C | -2.288456 | 1.168580 | 1.383702 |
| C | -3.072167 | 2.335201 | 1.365158 |
| C | -3.911709 | 2.607636 | 0.279598 |
| C | -3.993137 | 1.730203 | -0.813227 |
| C | -3.208373 | 0.581000 | -0.776602 |
| C | -2.359463 | 0.292225 | 0.308054 |
| C | 3.537600 | -1.581982 | 0.230439 |
| H | 3.745962 | -2.283427 | 1.048401 |
| C | 4.465564 | -1.685459 | -0.943245 |
| H | 4.145394 | -1.079869 | -1.802079 |
| H | 5.484209 | -1.357926 | -0.669273 |
| H | 4.556088 | -2.733060 | -1.276593 |

3-epi-27_conf_06

Charge = 0 Multi = 1

| | | | |
|---|---|---|---|
| H | -2.615430 | 3.932632 | 1.639235 |
| O | -2.900222 | 3.108514 | 1.223249 |
| H | -2.857713 | 3.903828 | -0.711375 |
| H | -1.313214 | 3.242342 | -0.129029 |
| C | -2.409379 | 3.090006 | -0.108126 |
| H | -3.860396 | 1.665482 | -0.795607 |
| H | -2.386685 | 1.737611 | -1.774217 |
| C | -2.762887 | 1.751062 | -0.736649 |
| N | -0.368613 | -1.523839 | -1.023179 |
| H | -0.220328 | 1.071243 | -0.731410 |
| H | -0.364419 | 1.166971 | 1.033875 |
| C | -0.662636 | 0.582191 | 0.150670 |
| H | -2.612174 | 0.601904 | 1.055021 |
| C | -2.207224 | 0.540247 | 0.035178 |
| C | -2.681155 | -0.772746 | -0.573419 |
| H | -1.711521 | -0.817466 | -2.490309 |
| H | -2.104905 | -2.415913 | -1.840654 |
| C | -1.729408 | -1.418785 | -1.559300 |
| H | 0.491706 | -3.250485 | -1.889960 |
| H | -0.404790 | -3.557405 | -0.379617 |
| H | -0.623250 | -1.346747 | 1.090249 |
| H | 2.447656 | -2.704080 | -0.608926 |
| H | 1.542670 | -3.210413 | 0.835728 |
| C | 0.253856 | -2.828519 | -0.900261 |
| C | -0.128768 | -0.834441 | 0.230889 |
| C | 1.517529 | -2.553893 | -0.045072 |
| C | 1.390521 | -1.072135 | 0.417203 |
| O | 1.390056 | -1.455541 | 2.855305 |

| | | | |
|---|---|---|---|
| N | 2.726486 | 0.167558 | 1.898459 |
| H | 3.153834 | 0.508943 | 2.752696 |
| H | 1.766947 | -0.349802 | -2.402013 |
| H | 3.357825 | 1.448280 | -3.151507 |
| H | 4.699152 | 2.700474 | -1.478291 |
| H | 4.493946 | 2.189115 | 0.961686 |
| C | 1.807018 | -0.853373 | 1.882282 |
| C | 2.370110 | 0.202289 | -1.679512 |
| C | 3.257055 | 1.212584 | -2.089736 |
| C | 4.011845 | 1.918506 | -1.146546 |
| C | 3.904278 | 1.639839 | 0.225216 |
| C | 3.019384 | 0.636917 | 0.611367 |
| C | 2.254055 | -0.082864 | -0.324959 |
| C | -3.864702 | -1.339415 | -0.284492 |
| H | -4.104254 | -2.290676 | -0.776798 |
| C | -4.926323 | -0.806054 | 0.631960 |
| H | -4.625412 | 0.116309 | 1.147826 |
| H | -5.852477 | -0.586129 | 0.071774 |
| H | -5.199570 | -1.554321 | 1.396080 |

3-epi-27_conf_07

Charge = 0 Multi = 1

| | | | |
|---|---|---|---|
| H | 1.241352 | 4.190875 | -1.270564 |
| O | 1.762494 | 3.484594 | -0.867270 |
| H | 0.779438 | 3.574346 | 0.978496 |
| H | -0.018325 | 2.579151 | -0.252082 |
| C | 0.971957 | 2.873478 | 0.141869 |
| H | 2.658315 | 1.995481 | 1.125119 |
| H | 1.107533 | 1.213898 | 1.486684 |
| C | 1.706911 | 1.657265 | 0.679489 |
| N | 0.759660 | -1.298360 | 1.114374 |
| H | -0.010523 | 0.705907 | -1.136568 |
| H | 1.033192 | -0.379497 | -2.051643 |
| C | 0.777424 | -0.052876 | -1.033151 |
| H | 2.581276 | 1.105974 | -1.180964 |
| C | 2.031187 | 0.587632 | -0.386264 |
| C | 2.892633 | -0.513478 | 0.190217 |
| H | 2.480616 | -1.033042 | 2.252895 |
| H | 2.566108 | -2.421941 | 1.152128 |
| C | 2.201590 | -1.373081 | 1.237429 |
| H | -0.147482 | -1.945253 | 2.913958 |
| H | 0.513747 | -3.257393 | 1.912966 |
| H | 0.517466 | -2.197575 | -0.798367 |
| H | -2.225908 | -2.301615 | 1.742377 |
| H | -1.403246 | -3.408140 | 0.617887 |
| C | -0.007720 | -2.278473 | 1.871140 |
| C | 0.252447 | -1.266770 | -0.246693 |
| C | -1.342042 | -2.423122 | 1.102267 |
| C | -1.280012 | -1.341581 | 0.001463 |
| O | -1.880249 | -2.742371 | -1.939385 |

| | | | |
|---|---|---|---|
| N | -2.830032 | -0.659555 | -1.623154 |
| H | -3.419500 | -0.655060 | -2.448683 |
| H | -1.030405 | 0.536037 | 2.255805 |
| H | -2.294014 | 2.696868 | 2.374491 |
| H | -3.852067 | 3.333840 | 0.547965 |
| H | -4.202243 | 1.822360 | -1.413681 |
| C | -2.013827 | -1.716617 | -1.297590 |
| C | -1.722947 | 0.817634 | 1.461921 |
| C | -2.432050 | 2.029206 | 1.521393 |
| C | -3.309092 | 2.387352 | 0.492226 |
| C | -3.511447 | 1.547505 | -0.614395 |
| C | -2.802490 | 0.349978 | -0.652226 |
| C | -1.903745 | -0.017273 | 0.366756 |
| C | 4.159540 | -0.776746 | -0.169800 |
| H | 4.645390 | -1.638375 | 0.308385 |
| C | 5.018125 | -0.029197 | -1.146640 |
| H | 5.380839 | -0.698904 | -1.946095 |
| H | 4.494968 | 0.812096 | -1.621608 |
| H | 5.919447 | 0.372573 | -0.650667 |

3-epi-27_conf_08

Charge = 0 Multi = 1

| | | | |
|---|---|---|---|
| H | 3.428251 | 3.105543 | -1.193349 |
| O | 3.958340 | 2.511750 | -0.642787 |
| H | 3.811561 | 1.485847 | 1.092256 |
| H | 3.063048 | 3.097391 | 1.153241 |
| C | 3.199994 | 2.200225 | 0.518304 |
| H | 1.303515 | 1.392162 | 1.144591 |
| H | 1.230795 | 2.328194 | -0.347093 |
| C | 1.840364 | 1.588770 | 0.204180 |
| N | 0.456579 | -1.075020 | 1.210867 |
| H | -0.124242 | 0.672497 | -1.230065 |
| H | 0.631098 | -0.677898 | -2.087078 |
| C | 0.535015 | -0.198490 | -1.101591 |
| H | 2.507556 | 0.548088 | -1.532451 |
| C | 1.928187 | 0.298676 | -0.634843 |
| C | 2.633392 | -0.813183 | 0.111410 |
| H | 2.255906 | -0.884697 | 2.240309 |
| H | 2.073793 | -2.443801 | 1.413907 |
| C | 1.875337 | -1.352486 | 1.312348 |
| H | -0.500363 | -1.201649 | 3.096515 |
| H | -0.000800 | -2.768132 | 2.421745 |
| H | 0.050682 | -2.235352 | -0.526925 |
| H | -2.622138 | -1.628906 | 2.028114 |
| H | -1.905947 | -2.976357 | 1.112243 |
| C | -0.408686 | -1.771699 | 2.155509 |
| C | -0.096359 | -1.206079 | -0.127555 |
| C | -1.758112 | -1.931696 | 1.421772 |
| C | -1.615992 | -1.067094 | 0.147790 |
| O | -2.418894 | -2.712773 | -1.506264 |

| | | | |
|---|---|---|---|
| N | -3.225216 | -0.547867 | -1.481029 |
| H | -3.867306 | -0.635687 | -2.261494 |
| H | -1.013175 | 1.168686 | 1.965741 |
| H | -2.112291 | 3.414538 | 1.774435 |
| H | -3.787362 | 3.836345 | -0.010226 |
| H | -4.409792 | 2.032562 | -1.626267 |
| C | -2.448187 | -1.589895 | -1.036584 |
| C | -1.757485 | 1.358776 | 1.191642 |
| C | -2.373163 | 2.616690 | 1.075714 |
| C | -3.316172 | 2.853797 | 0.069926 |
| C | -3.672433 | 1.848523 | -0.842685 |
| C | -3.051633 | 0.609495 | -0.710926 |
| C | -2.098353 | 0.355603 | 0.293021 |
| C | 3.827658 | -1.324959 | -0.227895 |
| H | 4.192776 | -2.177379 | 0.360780 |
| C | 4.737257 | -0.853251 | -1.328335 |
| H | 5.791633 | -0.949037 | -1.021421 |
| H | 4.623656 | -1.464472 | -2.242470 |
| H | 4.560262 | 0.199563 | -1.588700 |

3-epi-27_conf_09

Charge = 0 Multi = 1

| | | | |
|---|---|---|---|
| H | -0.566608 | 3.441661 | 0.815916 |
| O | 0.138325 | 3.810500 | 0.264133 |
| H | -0.255640 | 2.239714 | -1.035946 |
| H | 1.183425 | 3.216730 | -1.376315 |
| C | 0.599383 | 2.754195 | -0.562065 |
| H | 2.346491 | 2.296958 | 0.596299 |
| H | 0.914098 | 1.363479 | 1.055272 |
| C | 1.473425 | 1.755750 | 0.194861 |
| N | 0.948032 | -1.220287 | 1.100829 |
| H | -0.008451 | 0.293844 | -1.537301 |
| H | 1.212245 | -0.825587 | -2.124703 |
| C | 0.842392 | -0.323699 | -1.219236 |
| H | 2.473593 | 1.023247 | -1.545447 |
| C | 1.972943 | 0.581691 | -0.671359 |
| C | 2.975267 | -0.275174 | 0.075036 |
| H | 2.686674 | -0.812109 | 2.156672 |
| H | 2.832744 | -2.198702 | 1.060745 |
| C | 2.392203 | -1.178815 | 1.156617 |
| H | 0.223841 | -1.767180 | 3.011935 |
| H | 0.850913 | -3.124680 | 2.047269 |
| H | 0.634570 | -2.402262 | -0.634680 |
| H | -1.934165 | -2.221411 | 2.031129 |
| H | -1.185319 | -3.451071 | 0.986521 |
| C | 0.287983 | -2.169499 | 1.987039 |
| C | 0.380833 | -1.398990 | -0.221281 |
| C | -1.100745 | -2.414772 | 1.343057 |
| C | -1.137330 | -1.467978 | 0.125362 |
| O | -1.822595 | -3.069748 | -1.622243 |

| | | | |
|---|---|---|---|
| N | -2.699815 | -0.931856 | -1.538598 |
| H | -3.303432 | -1.004114 | -2.350898 |
| H | -0.936090 | 0.560487 | 2.249563 |
| H | -2.227157 | 2.707821 | 2.208662 |
| H | -3.709706 | 3.235116 | 0.284420 |
| H | -4.034611 | 1.582317 | -1.562892 |
| C | -1.914342 | -1.975098 | -1.099740 |
| C | -1.604821 | 0.787655 | 1.418697 |
| C | -2.319816 | 1.997852 | 1.382882 |
| C | -3.168136 | 2.286759 | 0.307007 |
| C | -3.354140 | 1.367739 | -0.737009 |
| C | -2.654650 | 0.164911 | -0.670298 |
| C | -1.759604 | -0.118728 | 0.378619 |
| C | 4.297640 | -0.289923 | -0.159033 |
| H | 4.901852 | -0.981097 | 0.445011 |
| C | 5.077963 | 0.534706 | -1.139362 |
| H | 5.824698 | 1.159375 | -0.617950 |
| H | 5.647234 | -0.109027 | -1.832751 |
| H | 4.446744 | 1.203999 | -1.740031 |

3-epi-27_conf_10

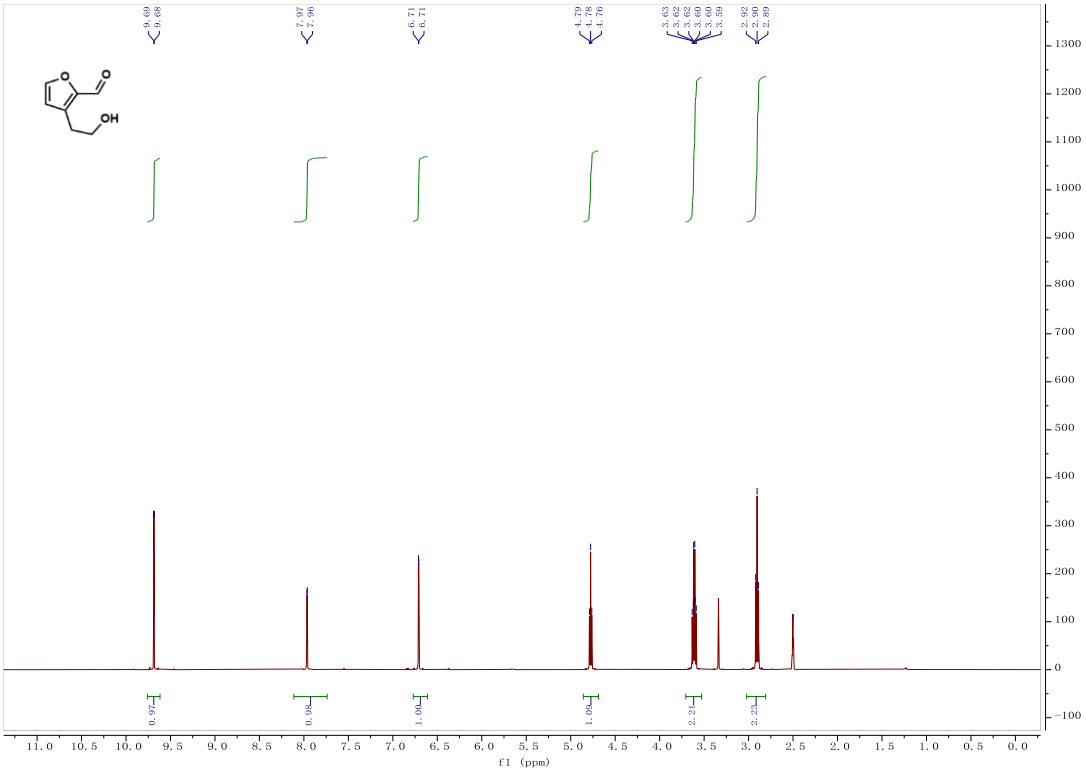
Charge = 0 Multi = 1

| | | | |
|---|---|---|---|
| H | 3.167582 | 2.305879 | 1.676216 |
| O | 3.746183 | 2.074834 | 0.936502 |
| H | 2.908023 | 3.550978 | -0.272234 |
| H | 3.783979 | 2.237270 | -1.081748 |
| C | 3.082571 | 2.457305 | -0.259302 |
| H | 1.161988 | 1.761613 | 0.432886 |
| H | 1.179797 | 2.308236 | -1.241193 |
| C | 1.757414 | 1.737287 | -0.493824 |
| N | 0.639931 | -0.645772 | 1.243183 |
| H | -0.246171 | 0.438845 | -1.459238 |
| H | 0.508373 | -1.043170 | -2.065241 |
| C | 0.474223 | -0.353643 | -1.208709 |
| H | 2.364013 | 0.338773 | -1.987261 |
| C | 1.875326 | 0.286331 | -1.004324 |
| C | 2.682626 | -0.617800 | -0.099746 |
| H | 2.508557 | -0.054536 | 1.967098 |
| H | 2.373243 | -1.804696 | 1.677460 |
| C | 2.082205 | -0.807275 | 1.279181 |
| H | -0.188599 | -0.332364 | 3.168699 |
| H | 0.409402 | -1.981692 | 2.888051 |
| H | 0.205180 | -2.216361 | -0.128672 |
| H | -2.321412 | -1.200058 | 2.441721 |
| H | -1.533408 | -2.665326 | 1.808660 |
| C | -0.101165 | -1.124457 | 2.404147 |
| C | 0.001799 | -1.133226 | 0.029647 |
| C | -1.472313 | -1.568171 | 1.850504 |
| C | -1.499665 | -1.030822 | 0.401254 |
| O | -2.275142 | -3.078513 | -0.736338 |

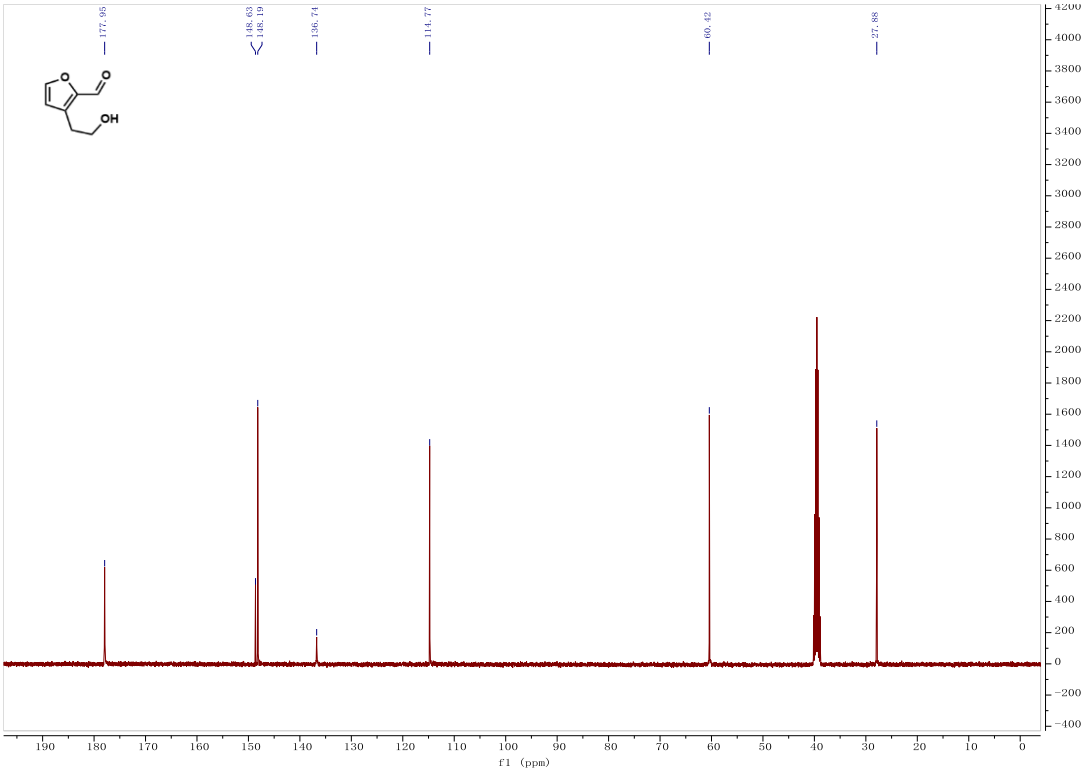
| | | | |
|---|---|---|---|
| N | -3.263347 | -1.031260 | -1.148432 |
| H | -3.950639 | -1.348809 | -1.823680 |
| H | -0.967586 | 1.614276 | 1.582250 |
| H | -2.272633 | 3.665747 | 0.971555 |
| H | -4.104570 | 3.528531 | -0.700148 |
| H | -4.679486 | 1.349535 | -1.784704 |
| C | -2.367781 | -1.879852 | -0.544234 |
| C | -1.779199 | 1.559870 | 0.855675 |
| C | -2.511467 | 2.707191 | 0.505792 |
| C | -3.542863 | 2.629311 | -0.436099 |
| C | -3.873418 | 1.411681 | -1.051244 |
| C | -3.136528 | 0.286811 | -0.691140 |
| C | -2.093303 | 0.348644 | 0.251821 |
| C | 3.802156 | -1.270686 | -0.450738 |
| H | 4.237709 | -1.947207 | 0.297105 |
| C | 4.567040 | -1.179043 | -1.738019 |
| H | 4.673836 | -2.172941 | -2.206947 |
| H | 4.099238 | -0.508075 | -2.471647 |
| H | 5.593231 | -0.812528 | -1.557412 |

## NMR Spectra

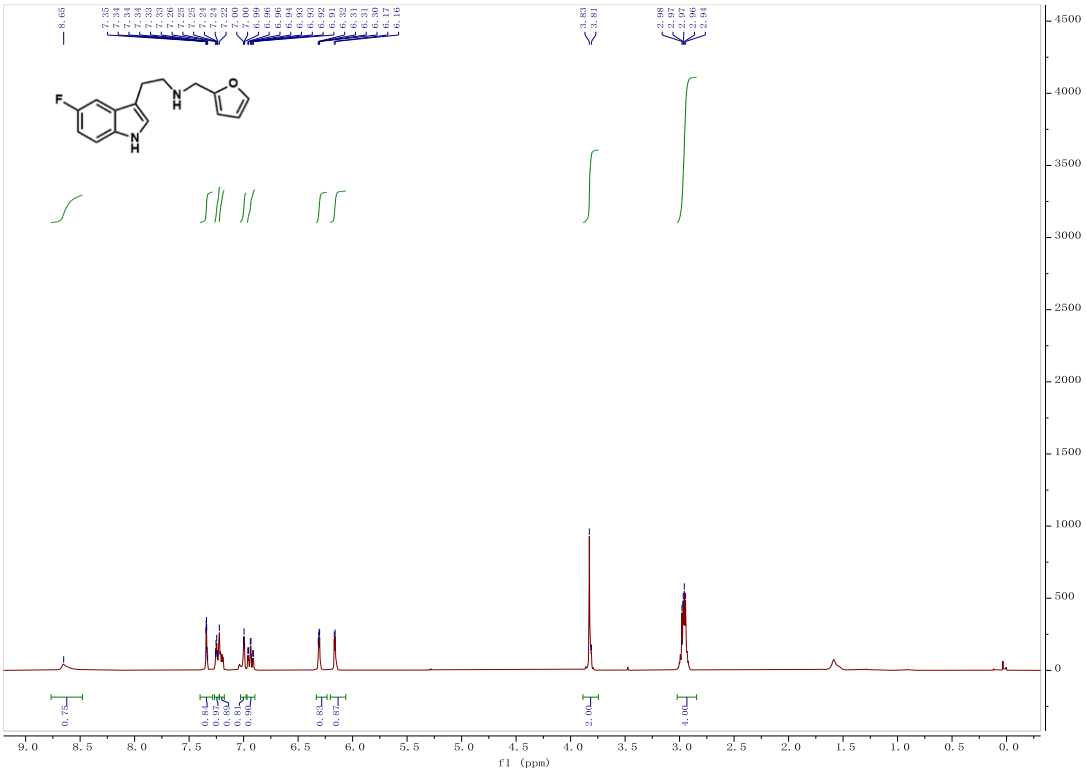
$^{1}$H NMR Spectrum of **S2** (400 MHz, DMSO-$d_6$):



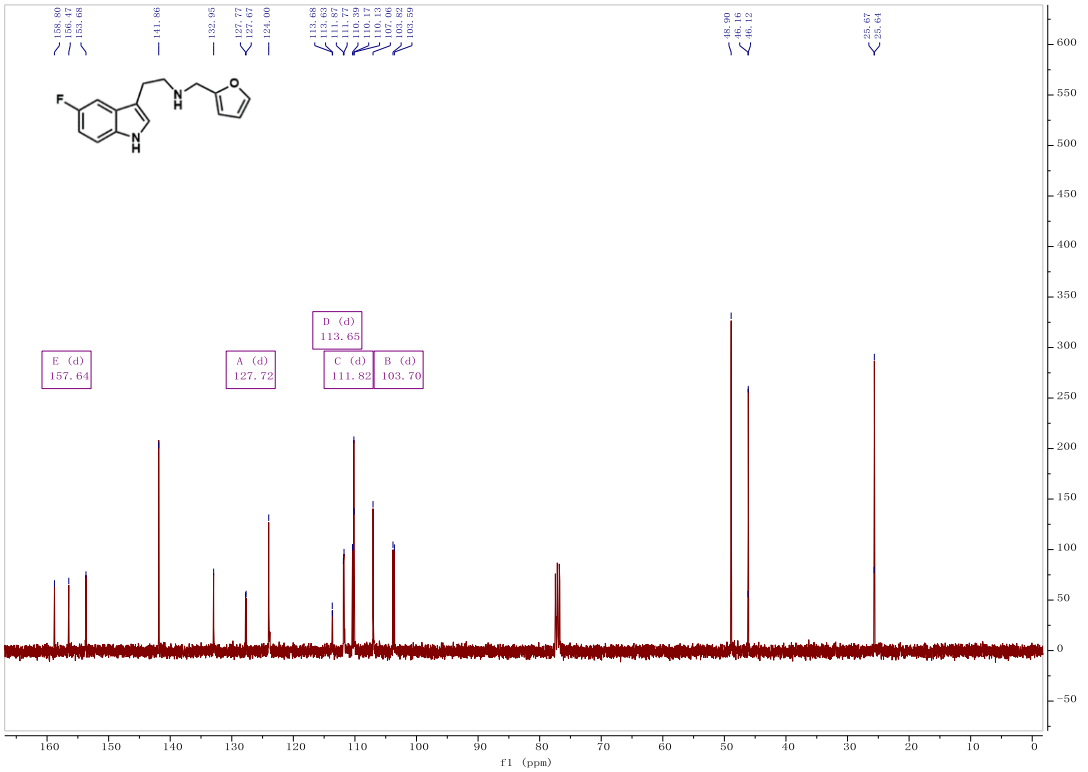

$^{13}$C NMR Spectrum of **S2** (100 MHz, DMSO-$d_6$):



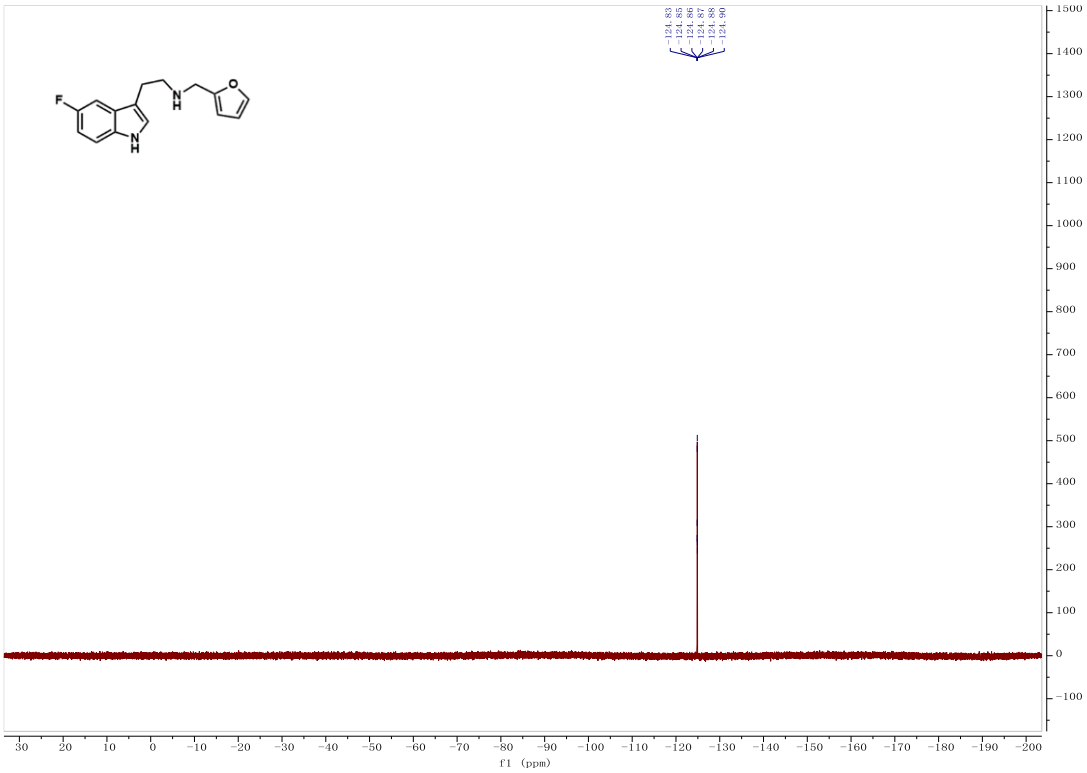
$^{1}$H NMR Spectrum of **1a** (400 MHz, $CDCl_3$):



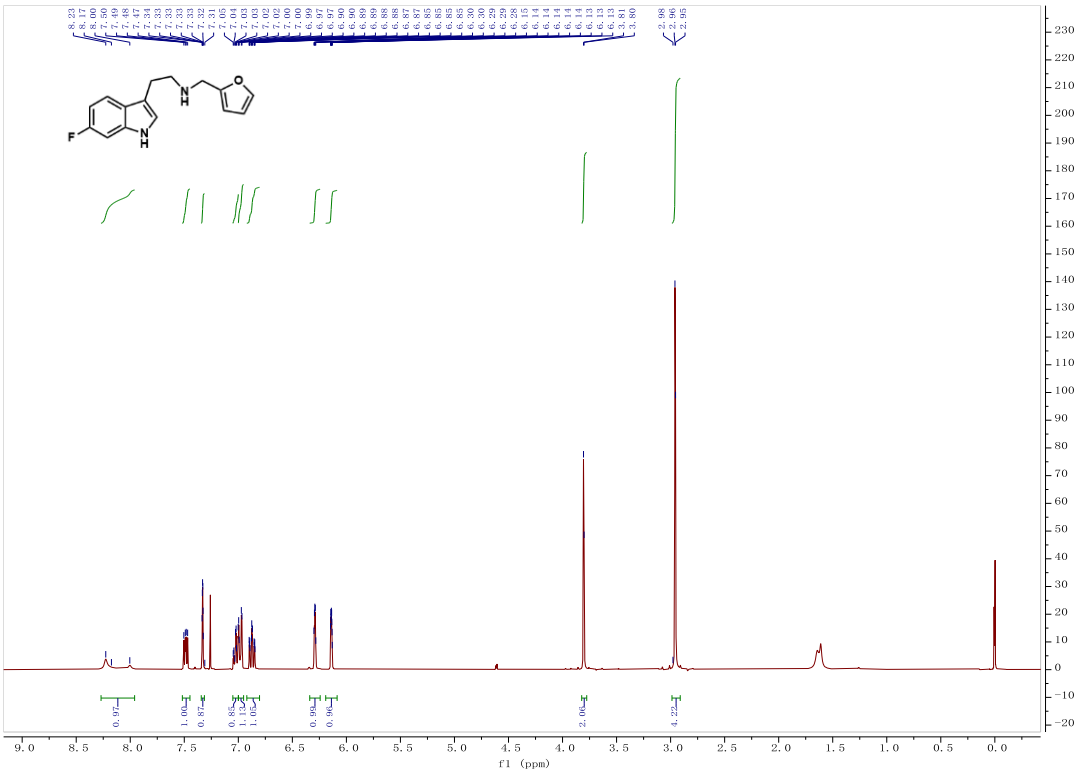
$^{13}$C NMR Spectrum of **1a** (100 MHz, $CDCl_3$):



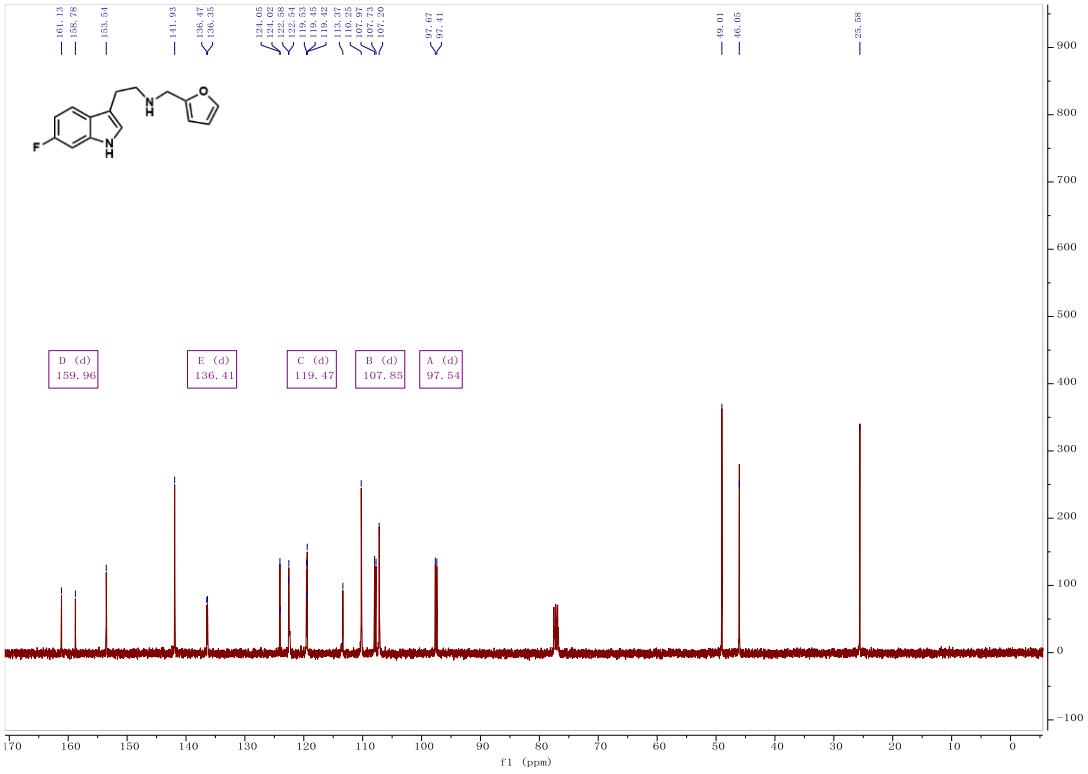
$^{19}$F NMR Spectrum of **1a** (376 MHz, $CDCl_3$):



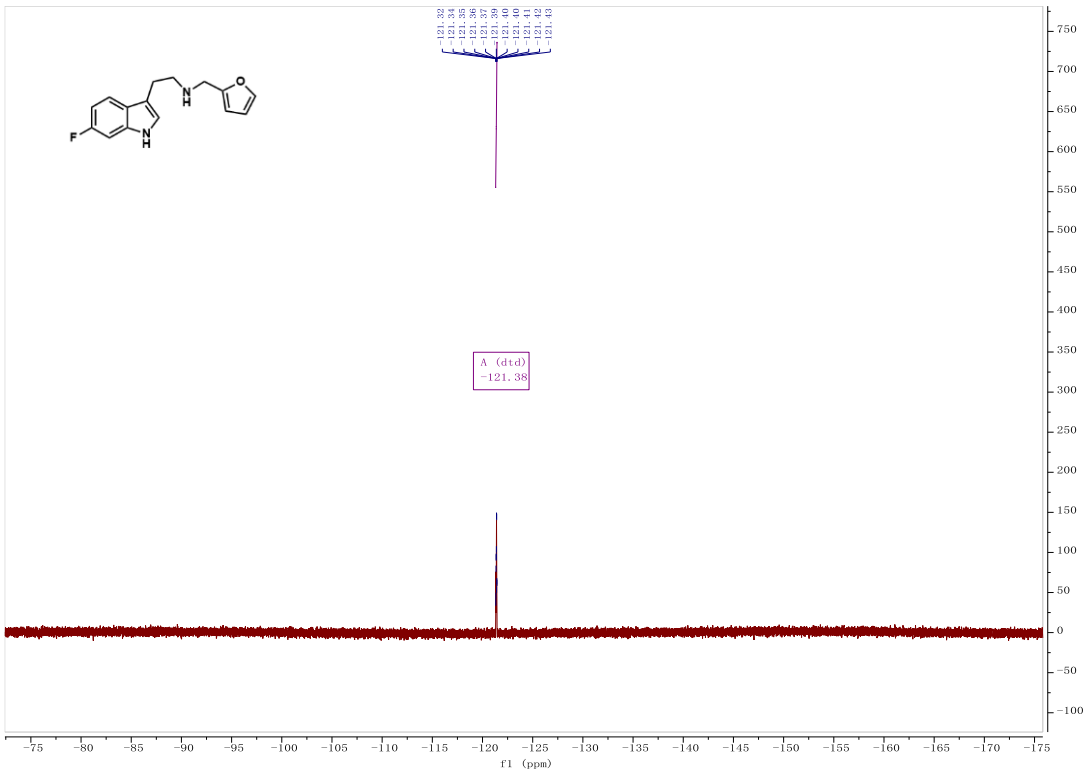

$^{1}$H NMR Spectrum of **1b** (400 MHz, $CDCl_3$):



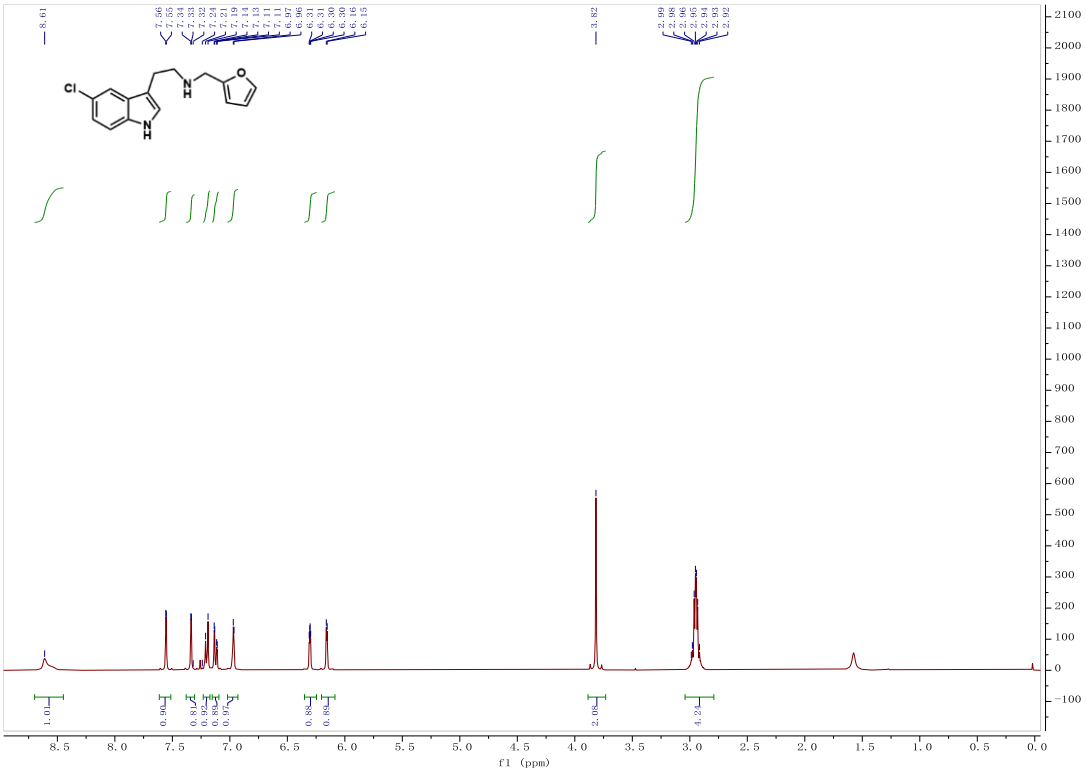
$^{13}$C NMR Spectrum of **1b** (100 MHz, $CDCl_3$):



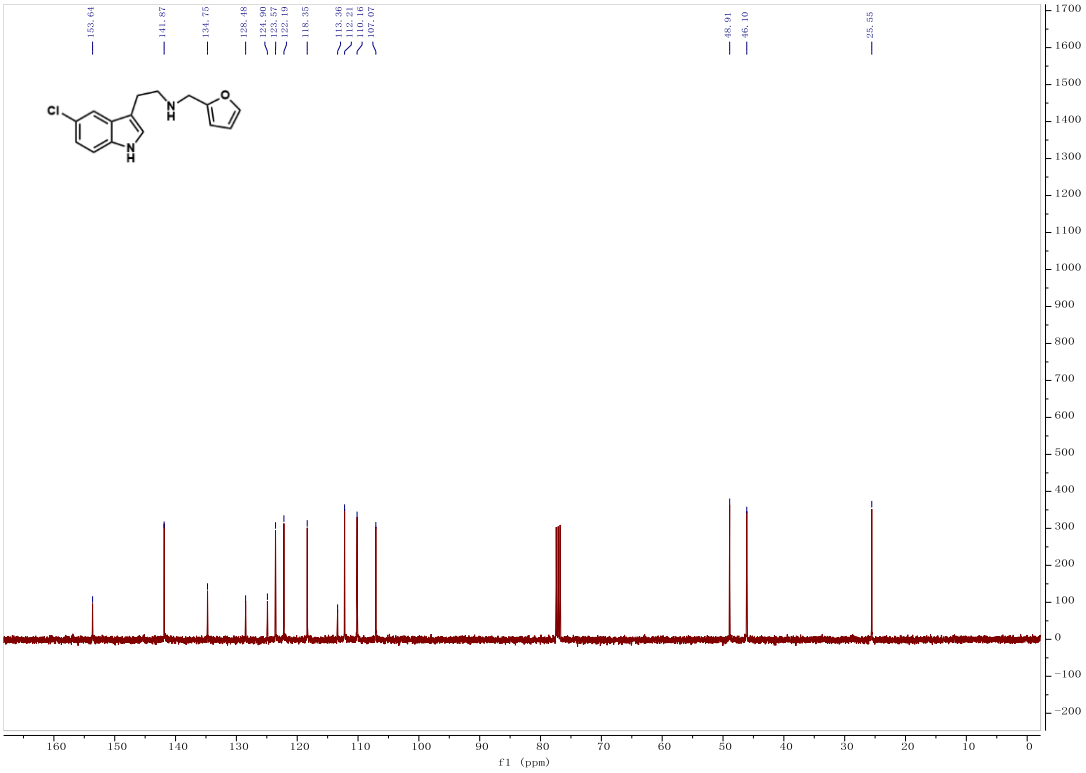

$^{19}$F NMR Spectrum of **1b** (376 MHz, $CDCl_3$):



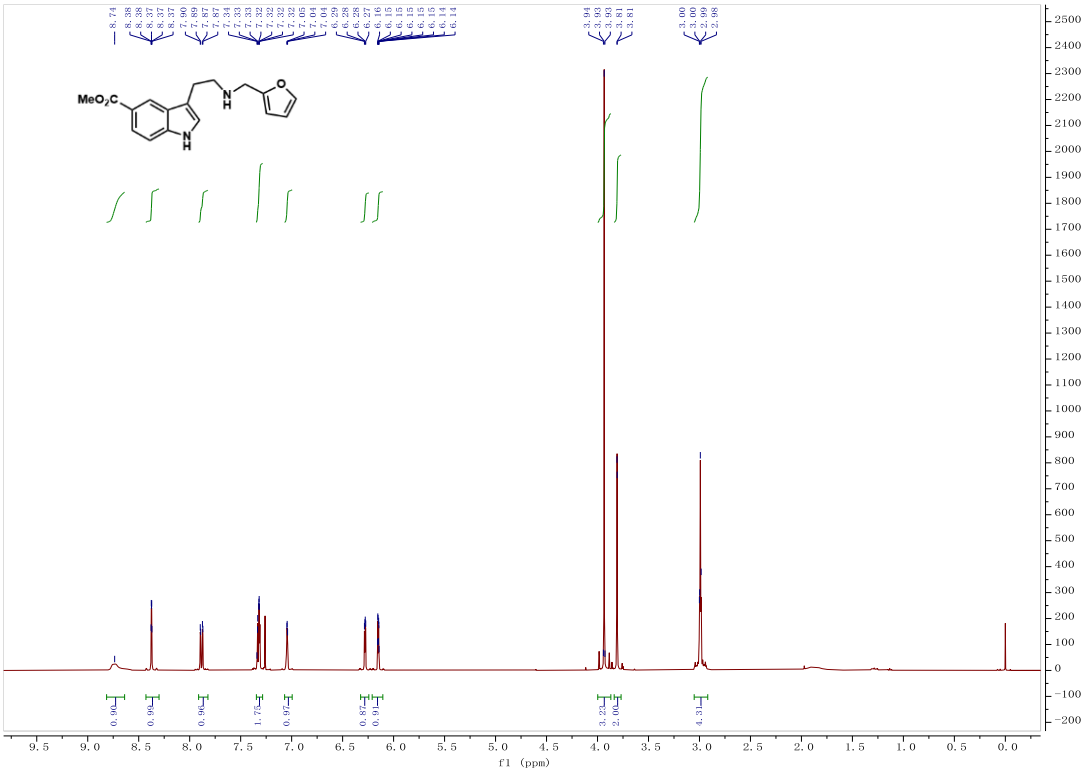
$^{1}$H NMR Spectrum of **1c** (400 MHz, $CDCl_3$):



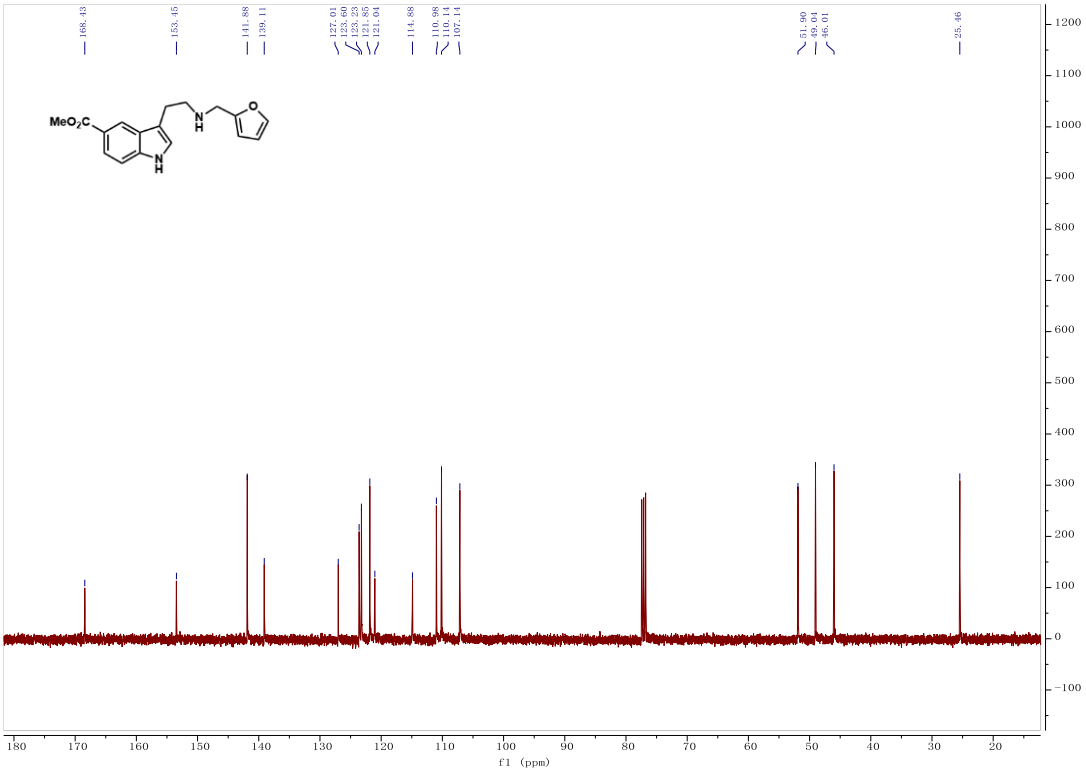

$^{13}$C NMR Spectrum of **1c** (100 MHz, $CDCl_3$):



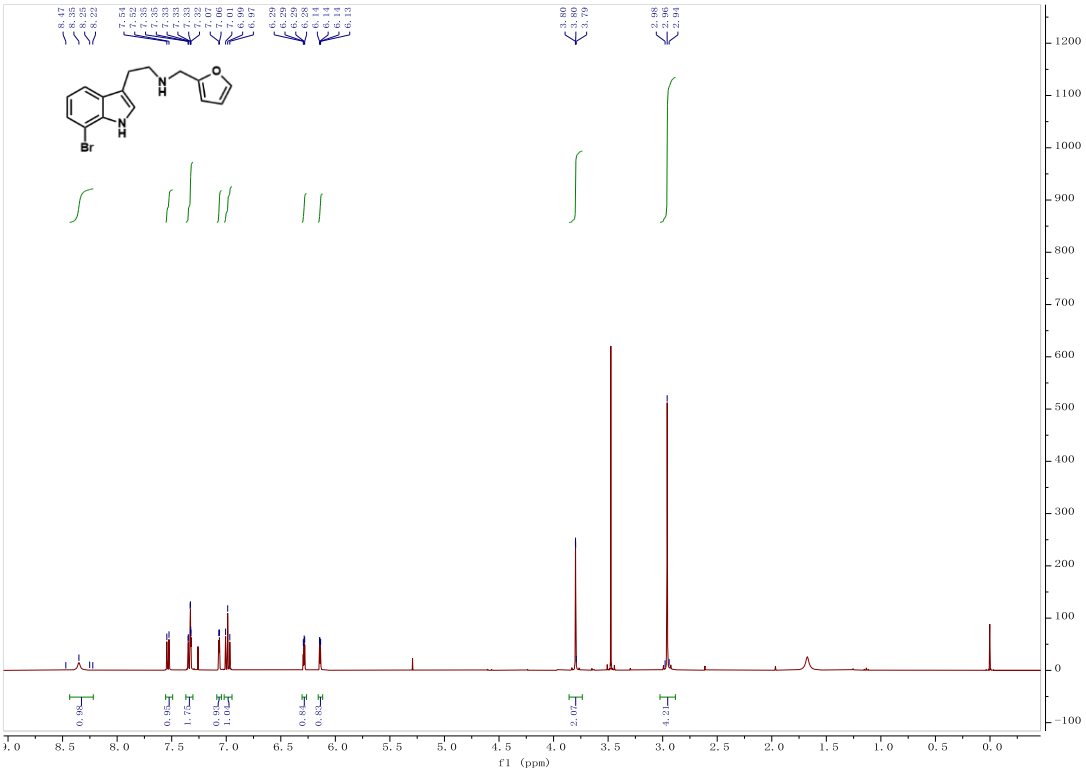
$^{1}$H NMR Spectrum of **1d** (400 MHz, $CDCl_3$):



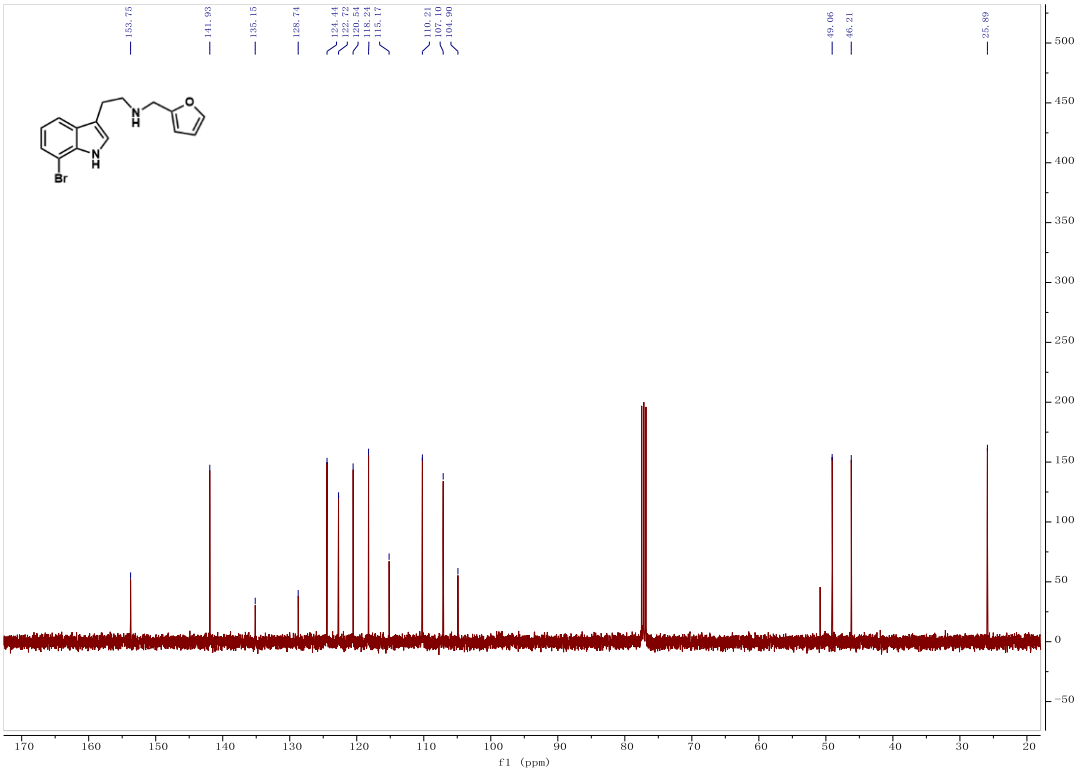
$^{13}$C NMR Spectrum of **1d** (100 MHz, $CDCl_3$):



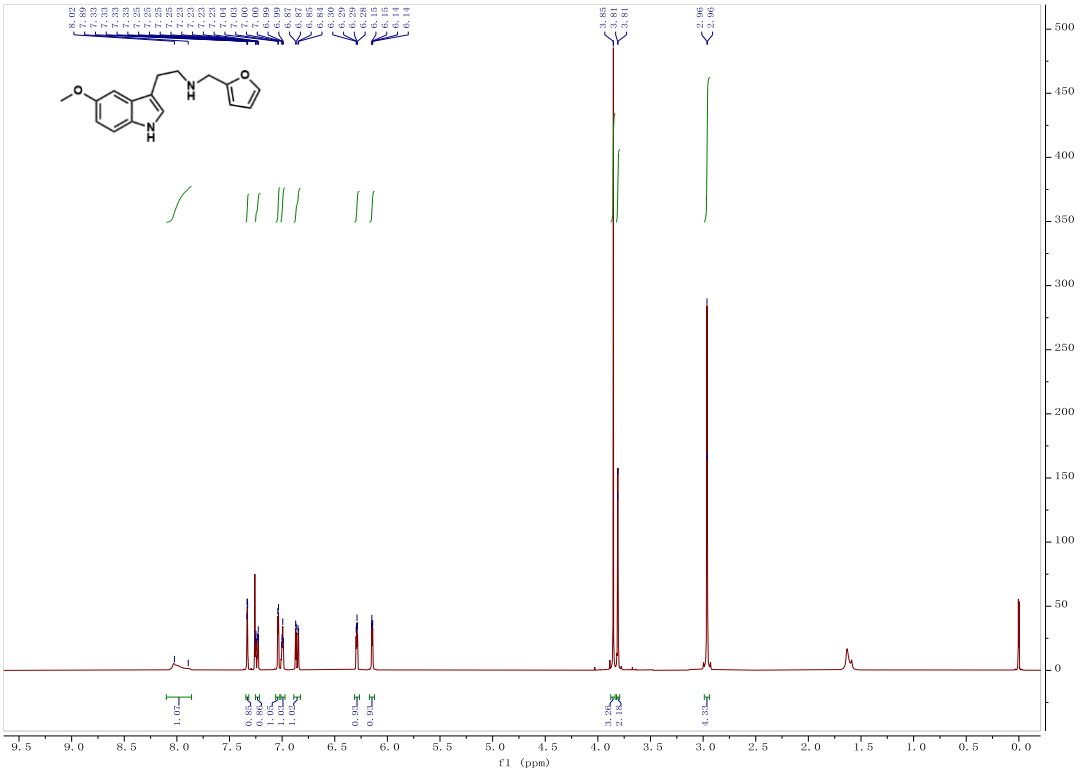
$^{1}$H NMR Spectrum of **1e** (400 MHz, $CDCl_3$):



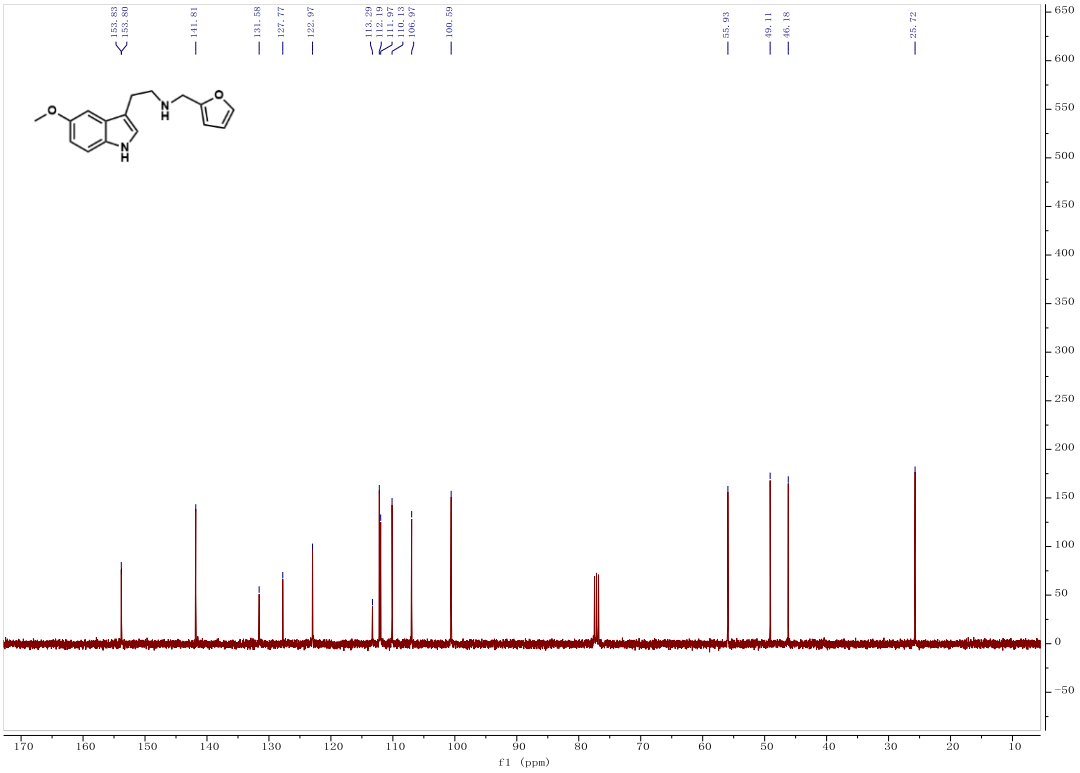

$^{13}$C NMR Spectrum of **1e** (100 MHz, $CDCl_3$):



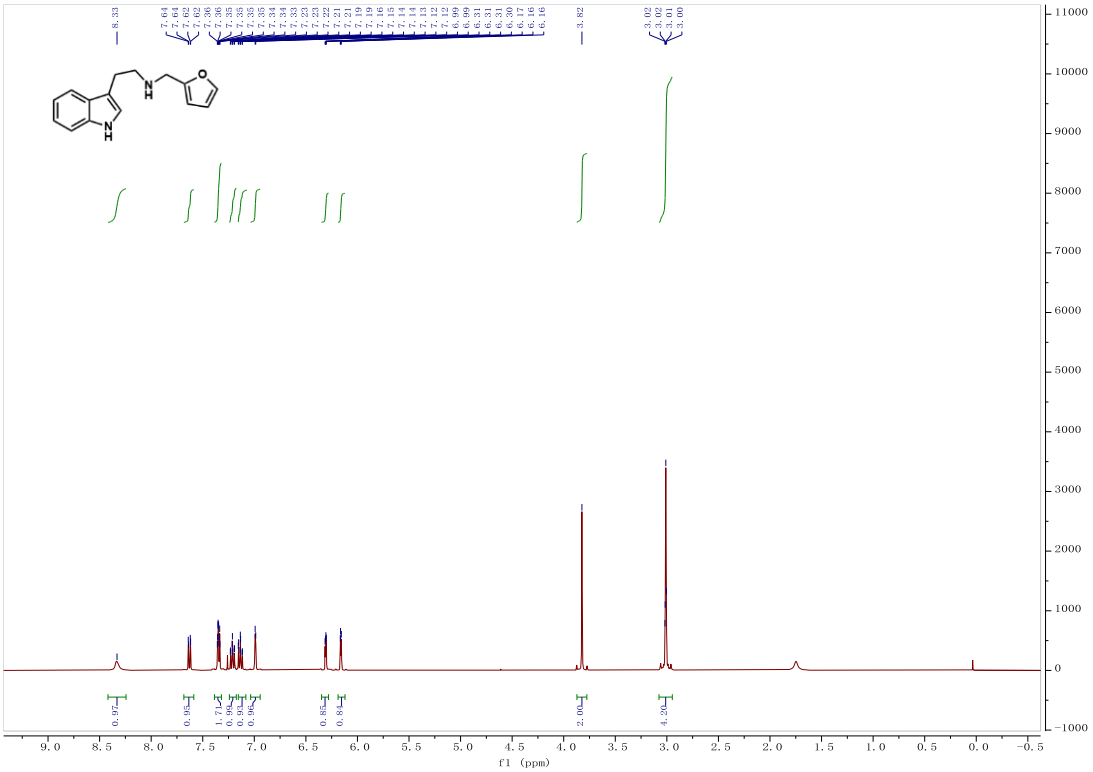
$^{1}$H NMR Spectrum of **1f** (400 MHz, $CDCl_3$):



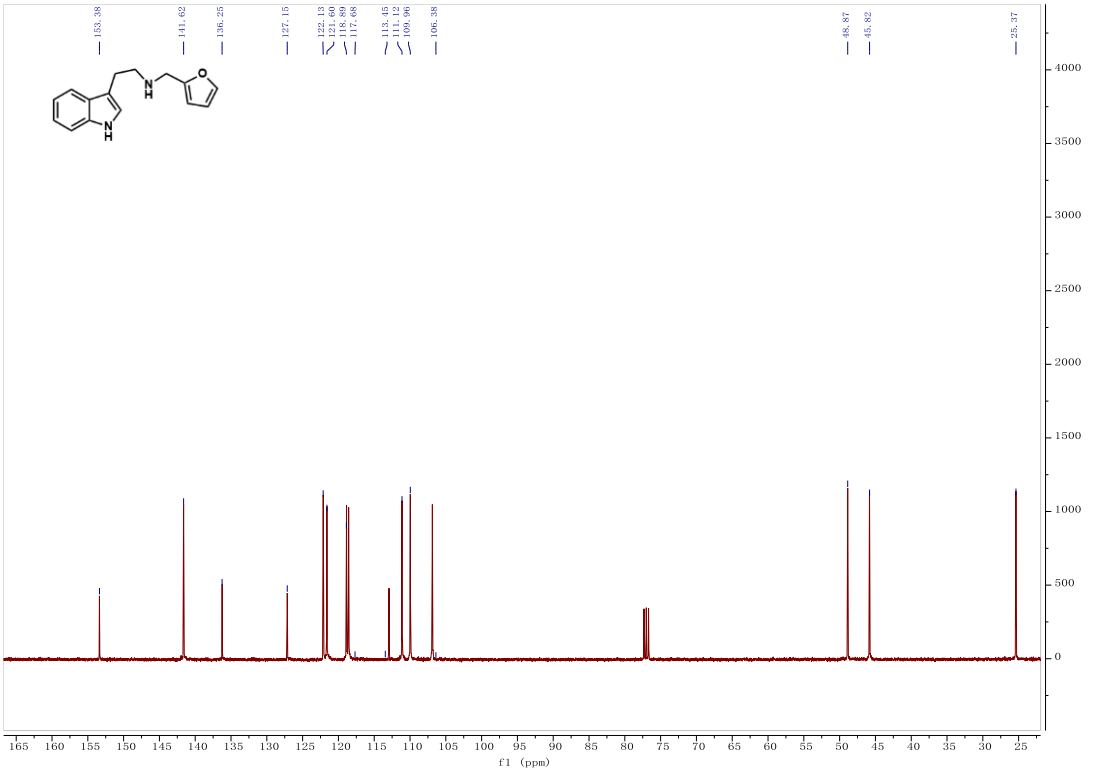
$^{13}$C NMR Spectrum of **1f** (100 MHz, $CDCl_3$):



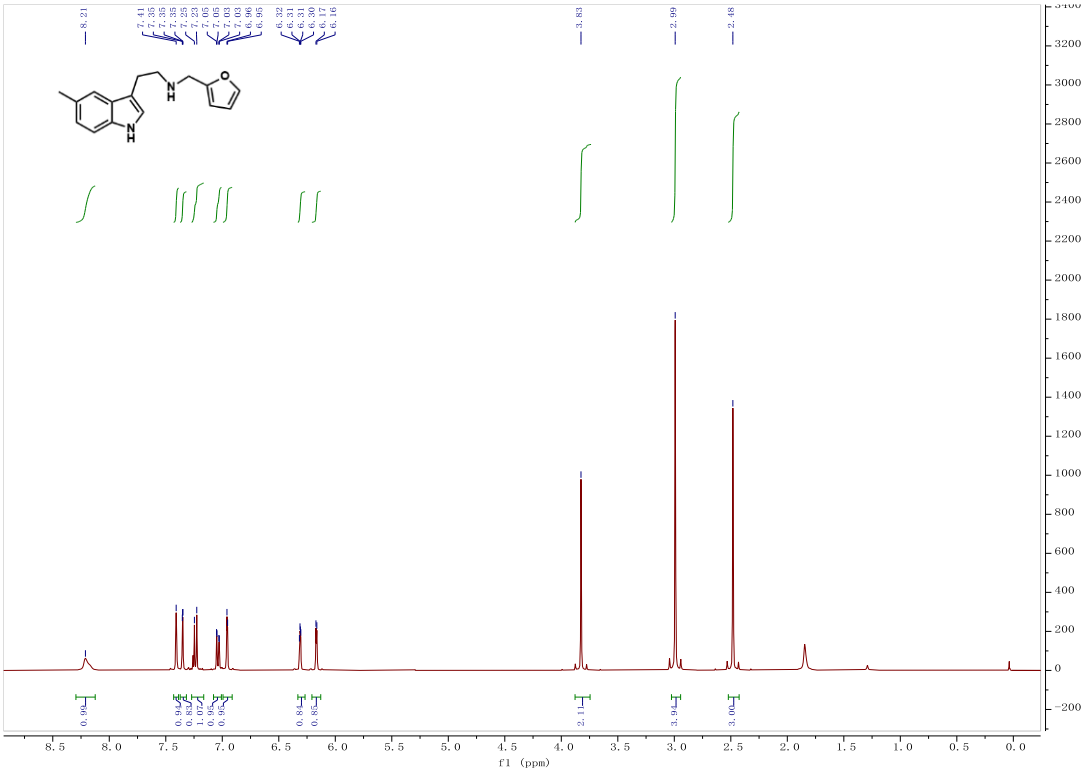
$^{1}$H NMR Spectrum of **1g** (400 MHz, $CDCl_3$):



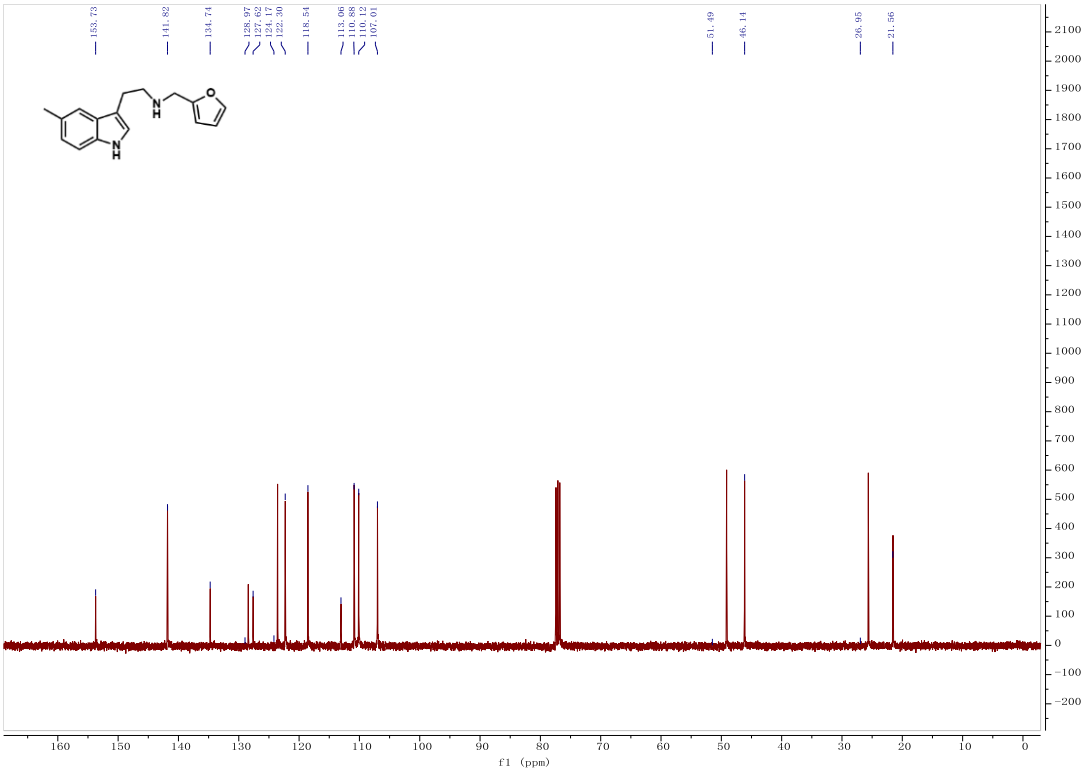
$^{13}$C NMR Spectrum of **1g** (100 MHz, $CDCl_3$):



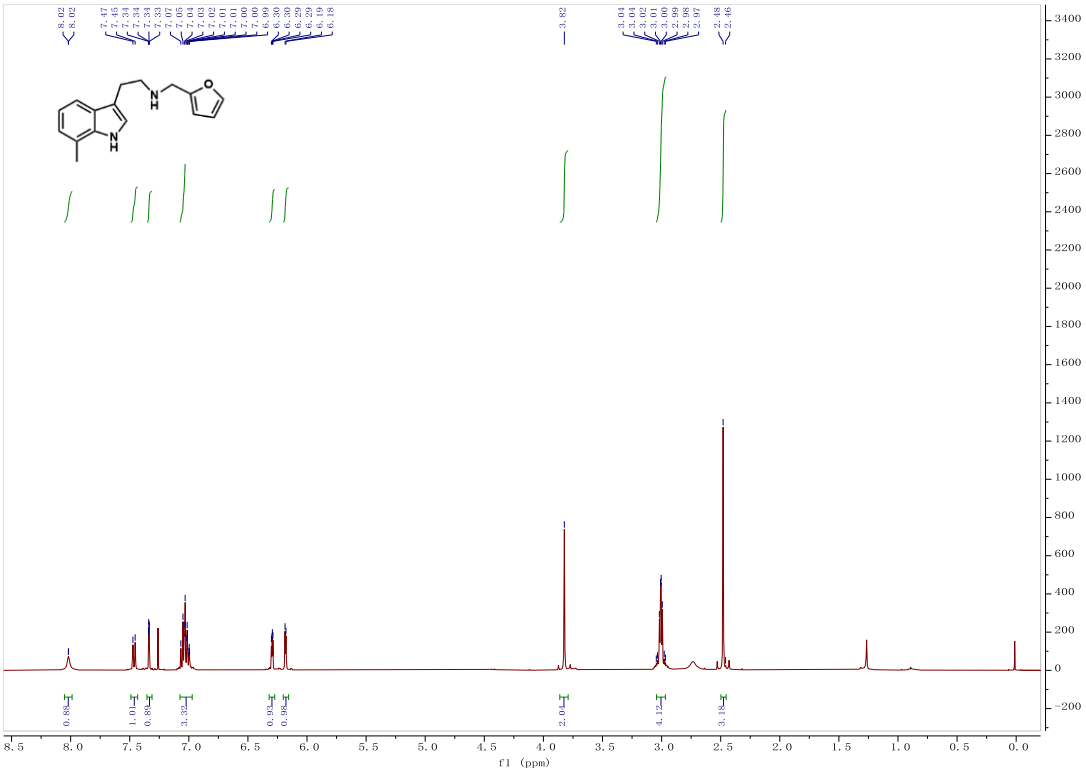
$^{1}$H NMR Spectrum of **1h** (400 MHz, $CDCl_3$):



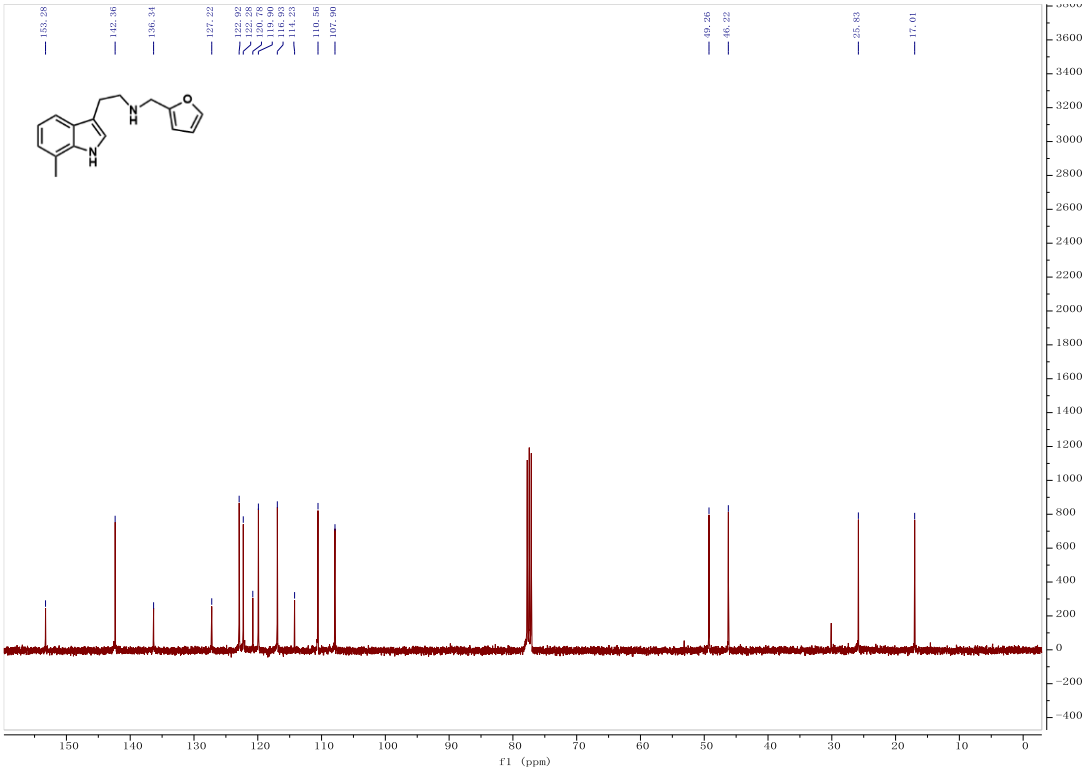

$^{13}$C NMR Spectrum of **1h** (100 MHz, $CDCl_3$):



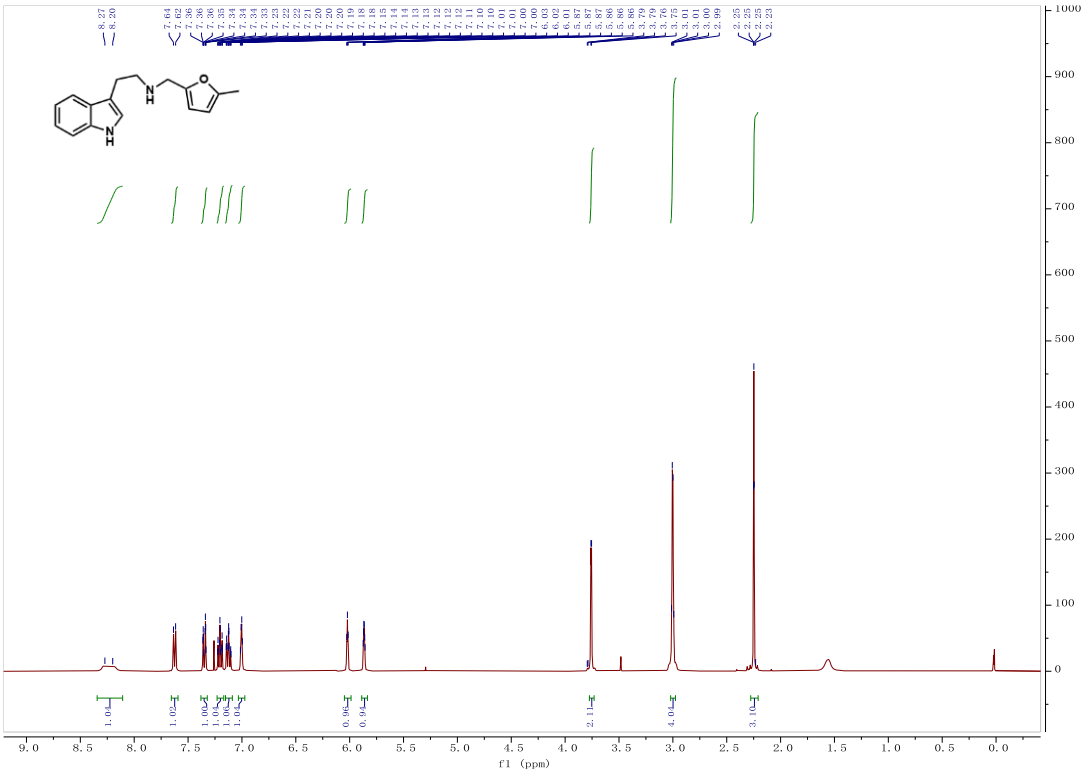
$^{1}$H NMR Spectrum of **1i** (400 MHz, $CDCl_3$):



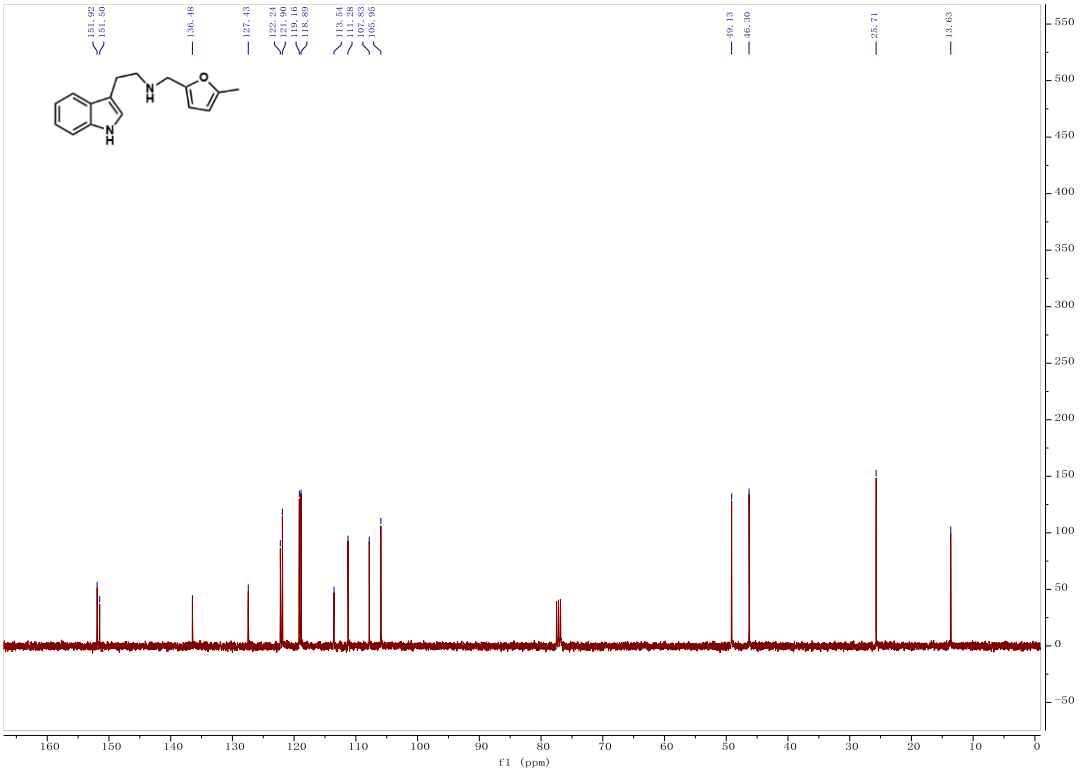
$^{13}$C NMR Spectrum of **1i** (100 MHz, $CDCl_3$):



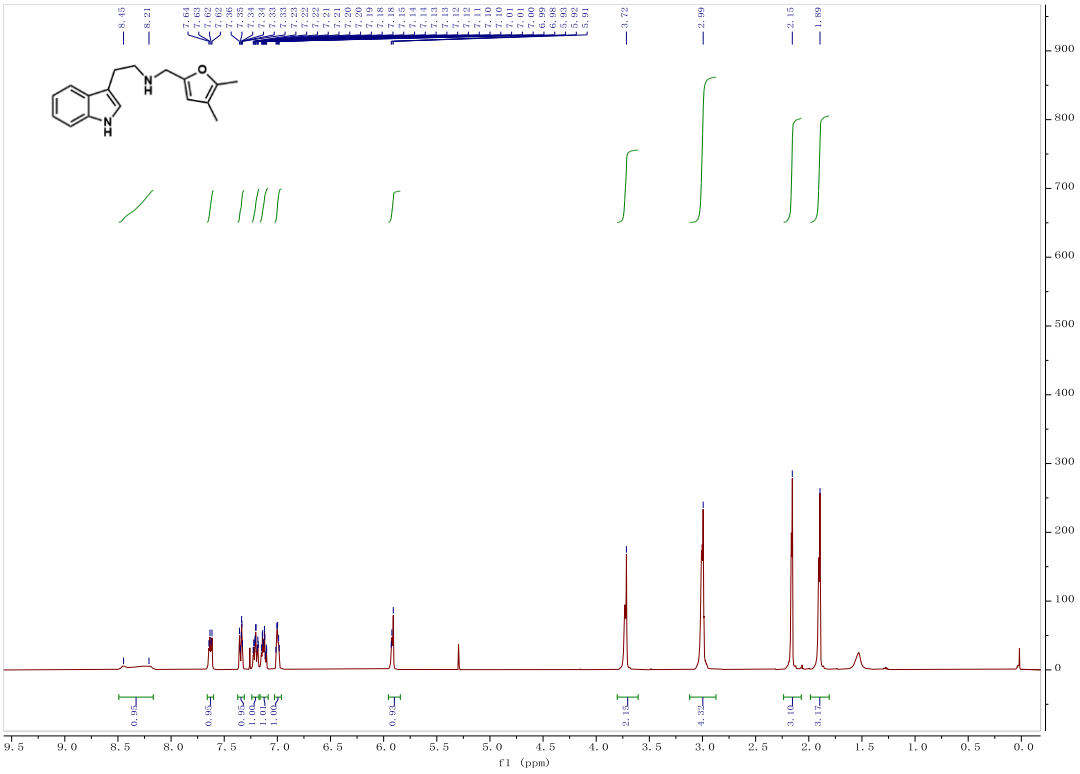
$^{1}$H NMR Spectrum of **1j** (400 MHz, $CDCl_3$):



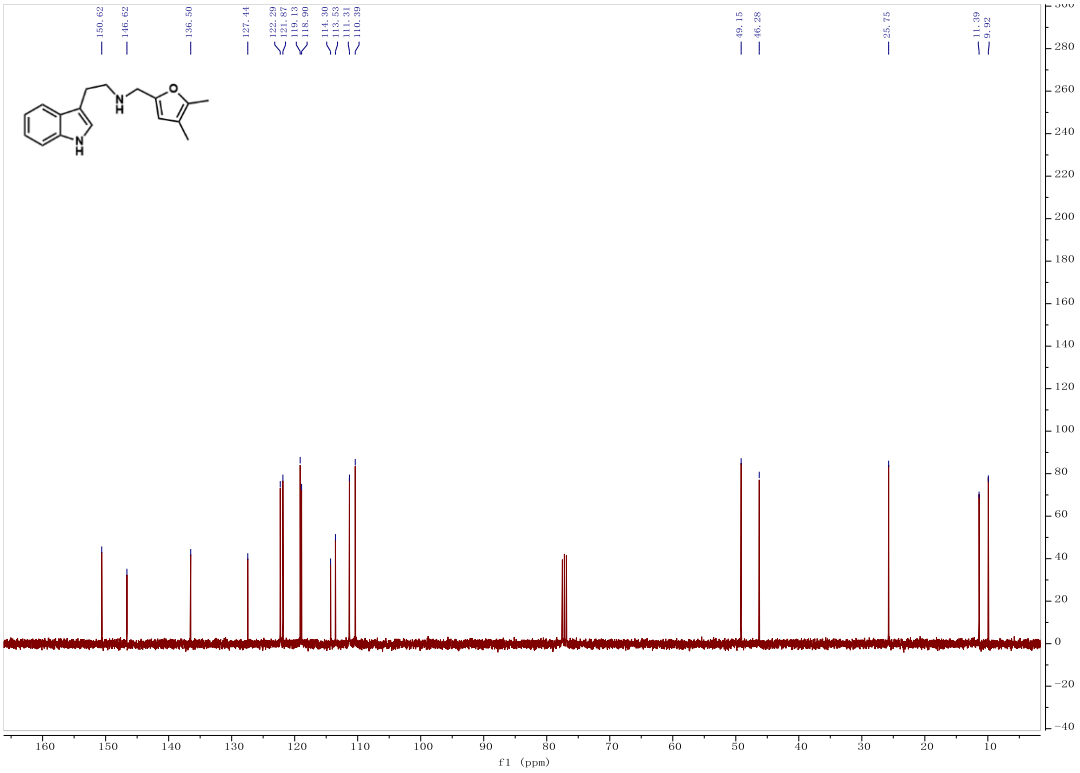
$^{13}$C NMR Spectrum of **1j** (100 MHz, $CDCl_3$):



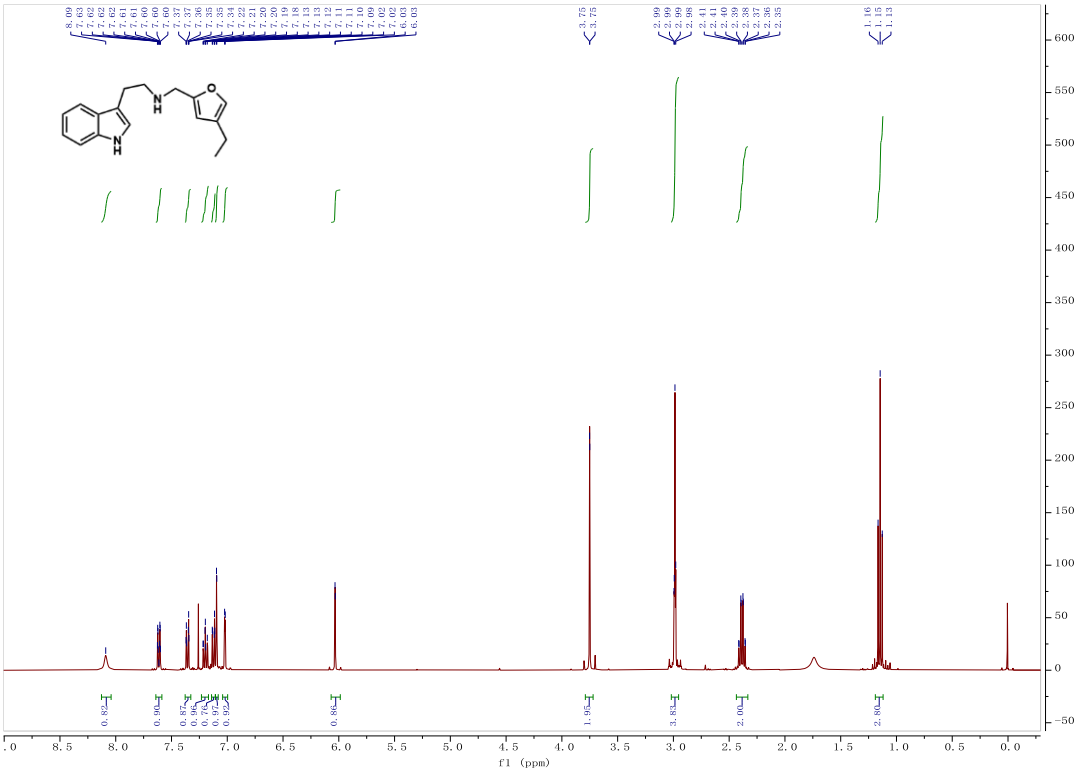
$^{1}$H NMR Spectrum of **1k** (400 MHz, $CDCl_3$):



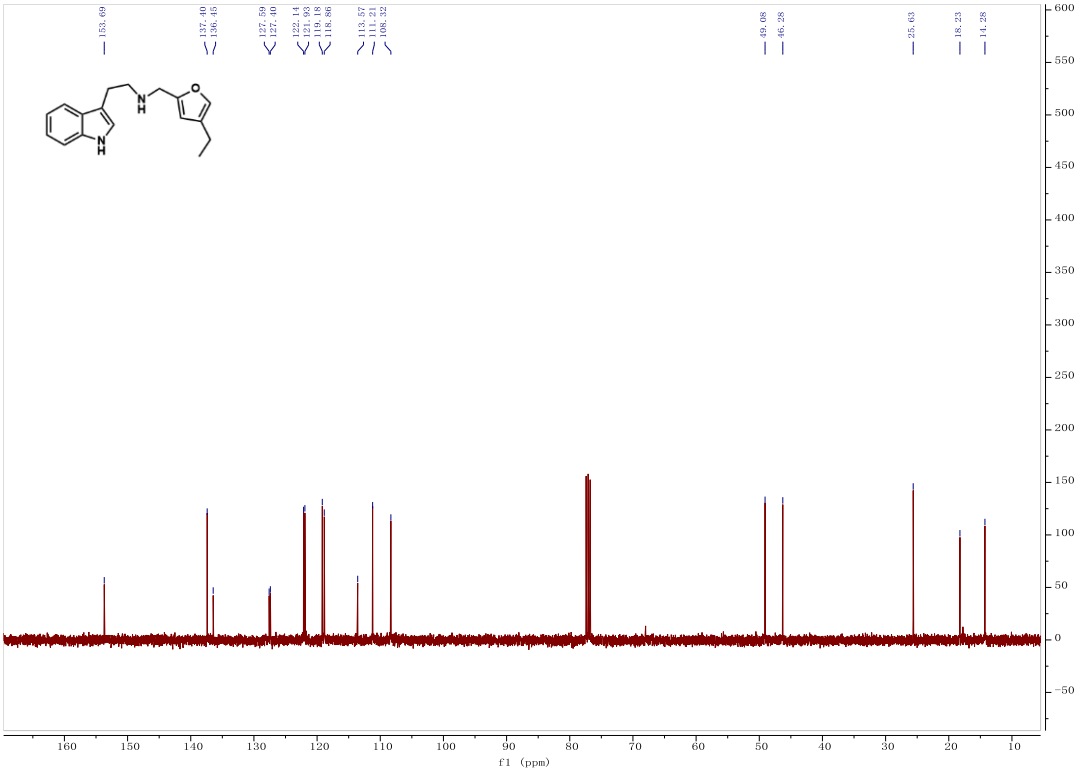
$^{13}$C NMR Spectrum of **1k** (100 MHz, $CDCl_3$):



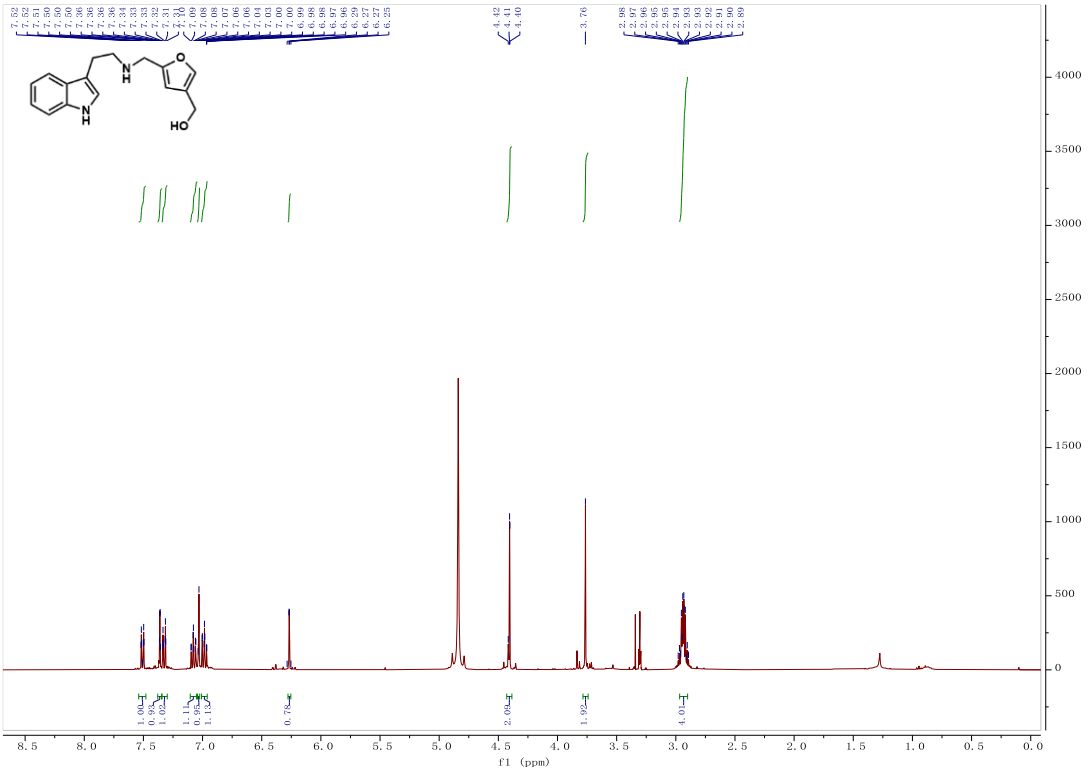
$^{1}$H NMR Spectrum of **1l** (400 MHz, $CDCl_3$):



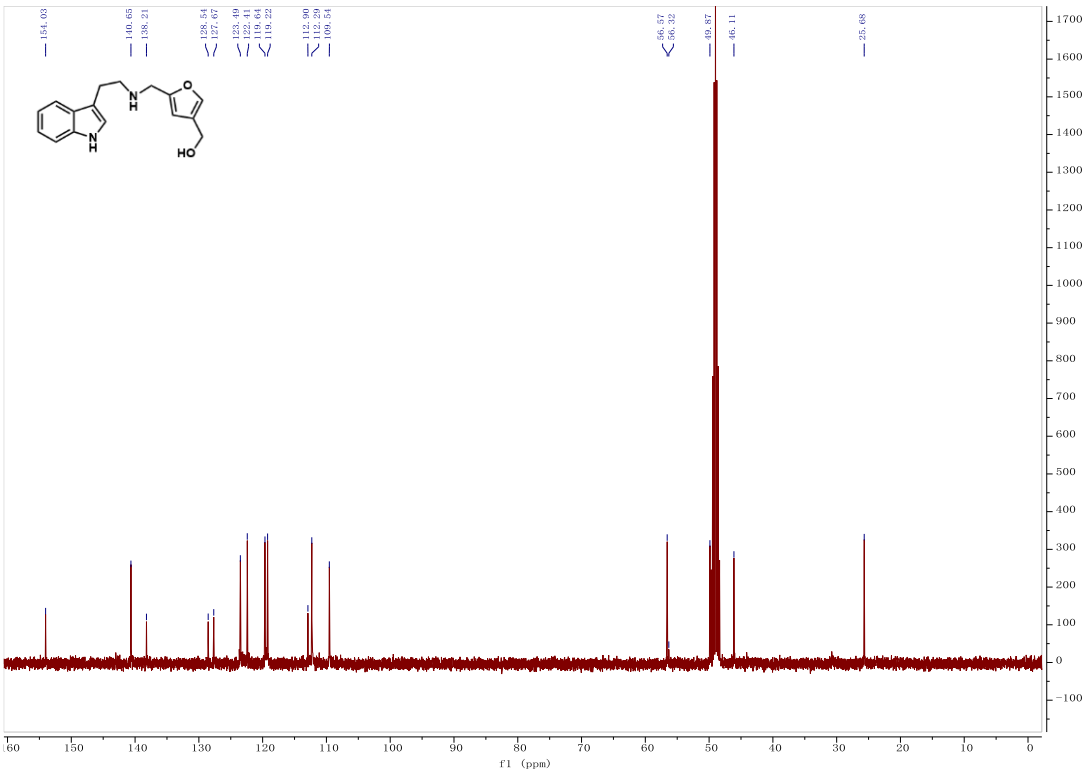
$^{13}$C NMR Spectrum of **1l** (100 MHz, $CDCl_3$):



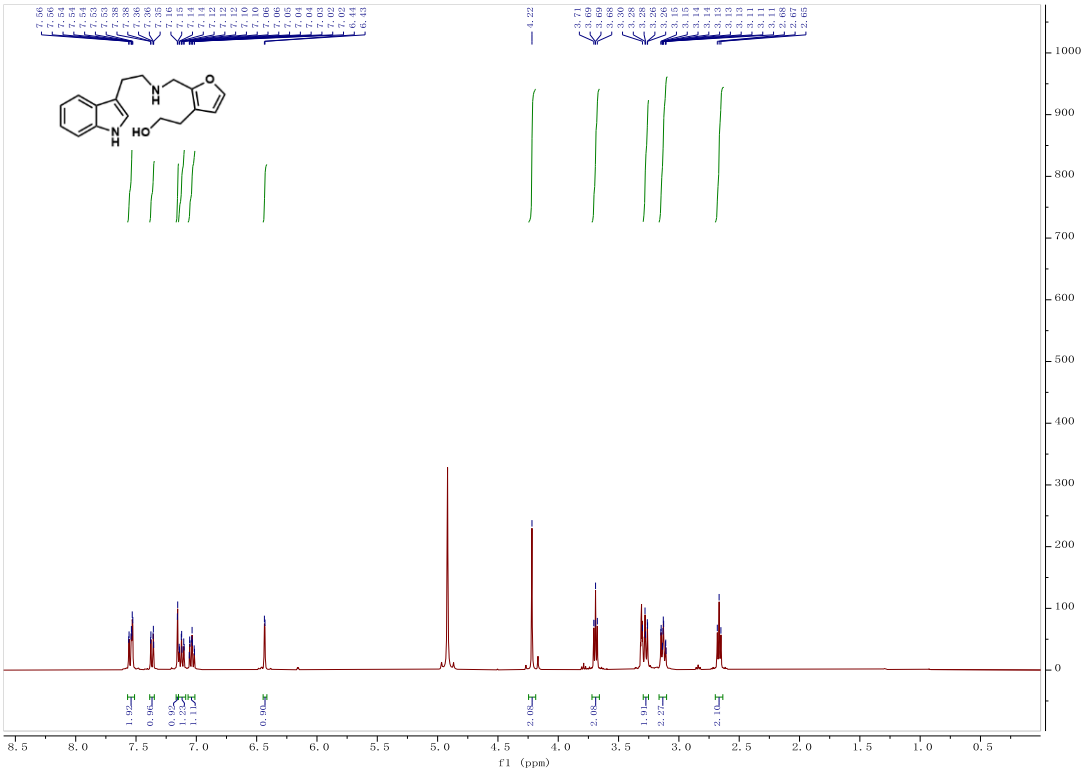
$^{1}$H NMR Spectrum of **1m** (400 MHz, $CDCl_3$):



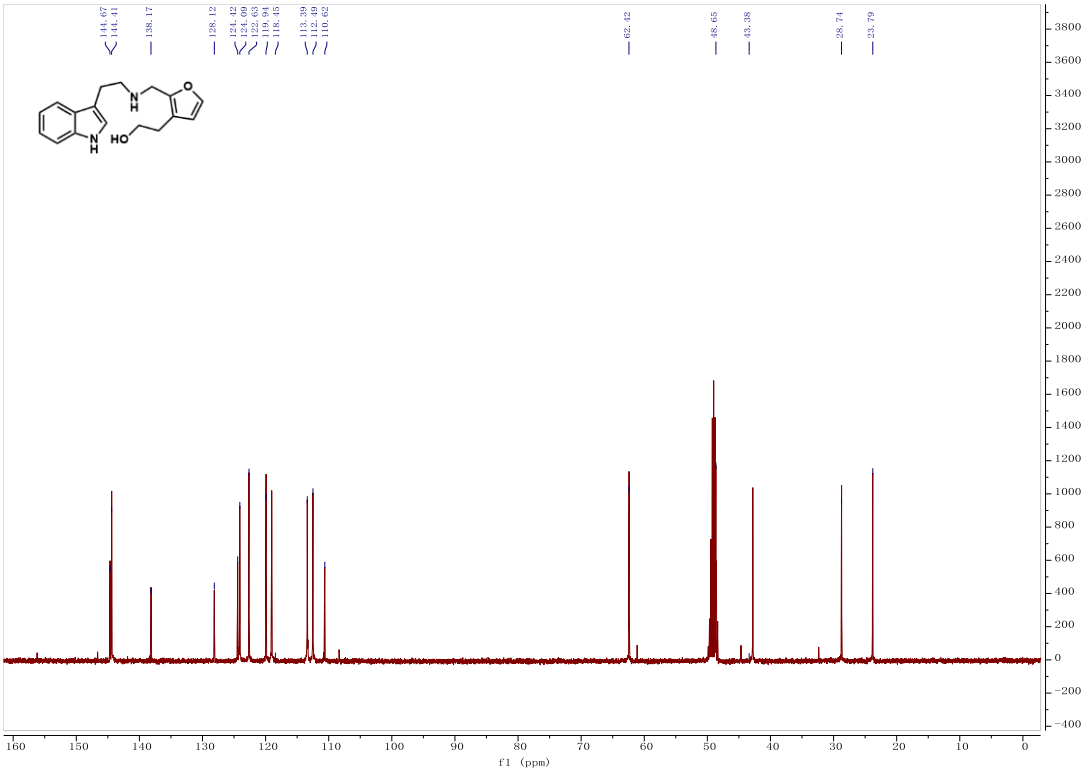
$^{13}$C NMR Spectrum of **1m** (100 MHz, $CDCl_3$):



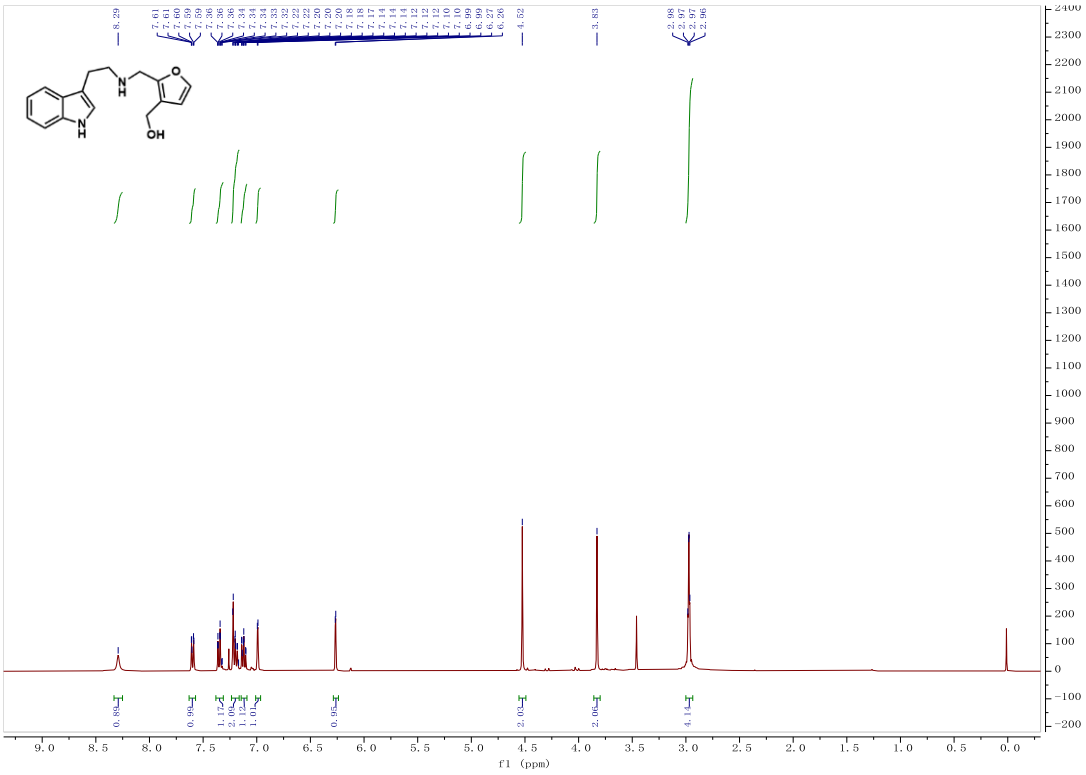
$^{1}$H NMR Spectrum of **1n** (400 MHz, $CD_3OD$):



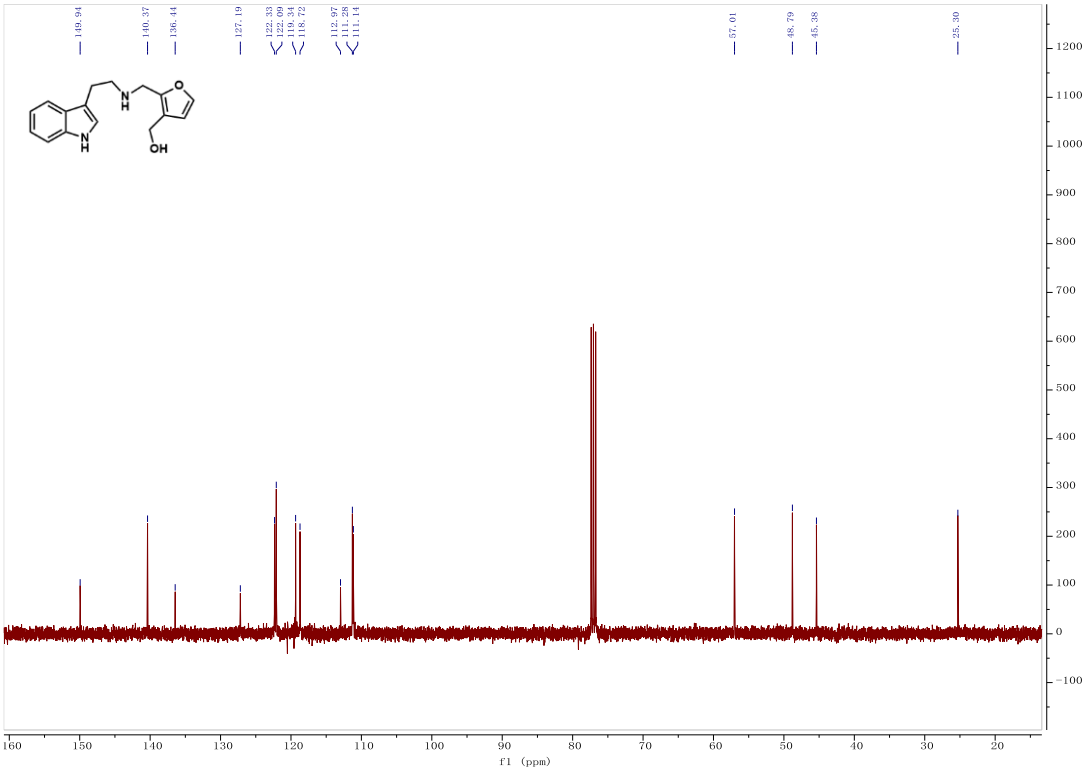
$^{13}$C NMR Spectrum of **1n** (100 MHz, $CD_3OD$):



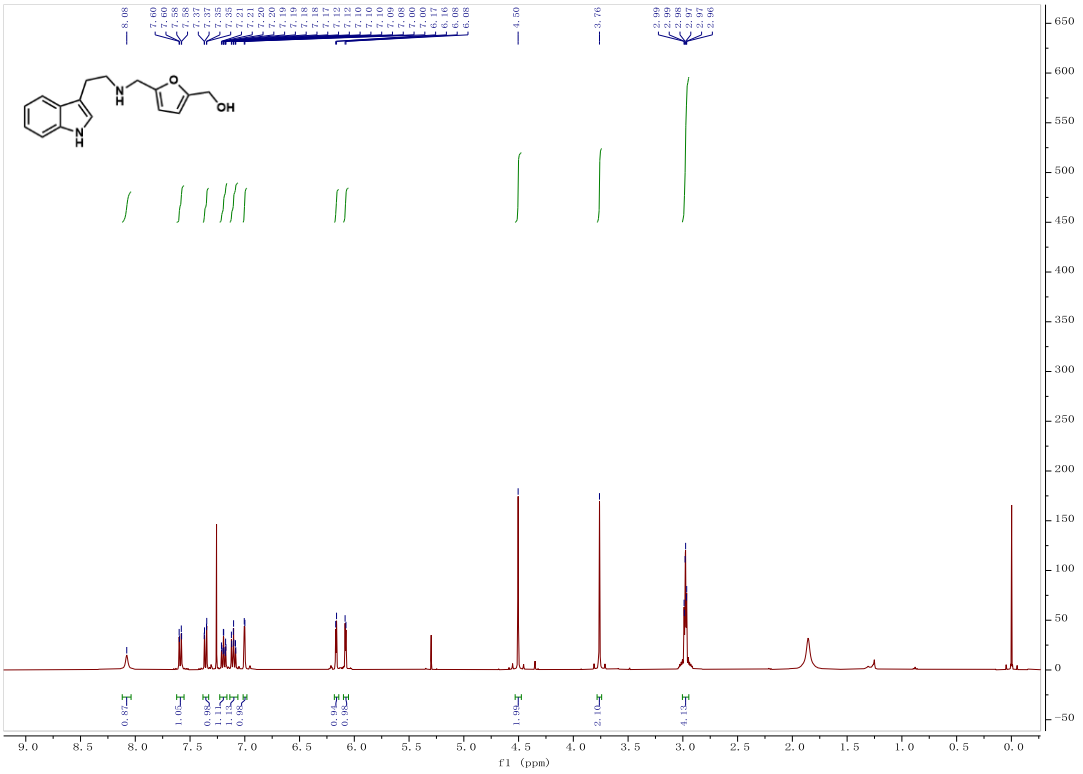
$^{1}$H NMR Spectrum of **1o** (400 MHz, $CDCl_3$):



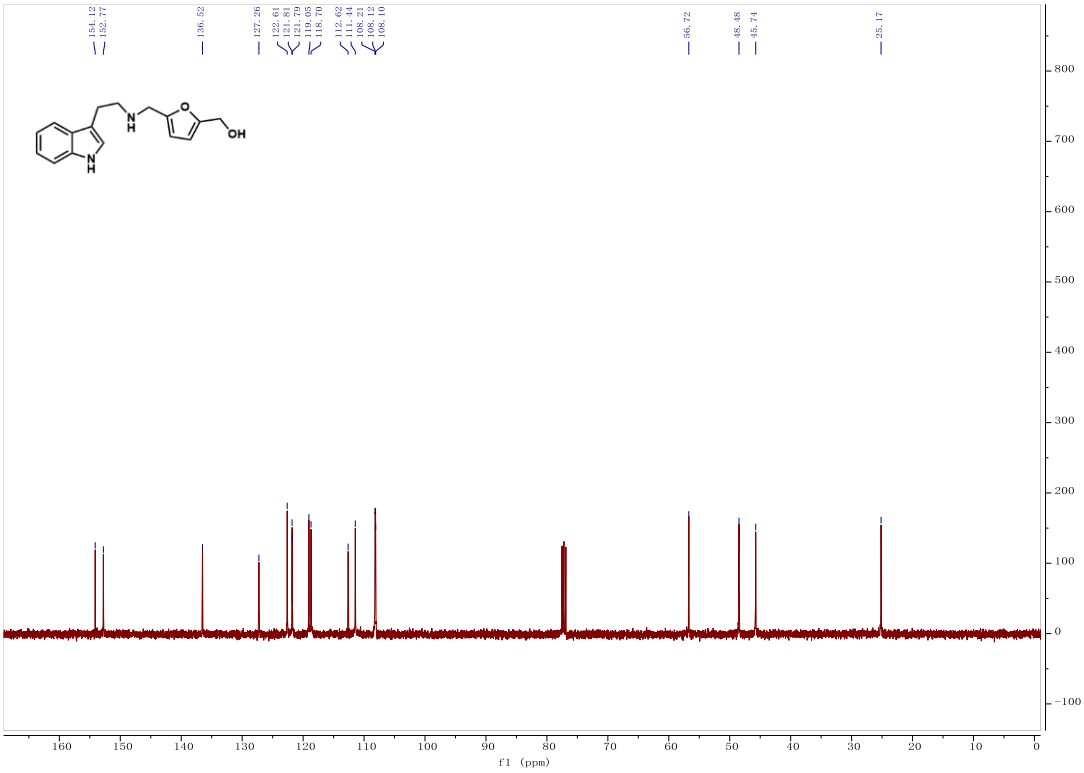
$^{13}$C NMR Spectrum of **1o** (100 MHz, $CDCl_3$):



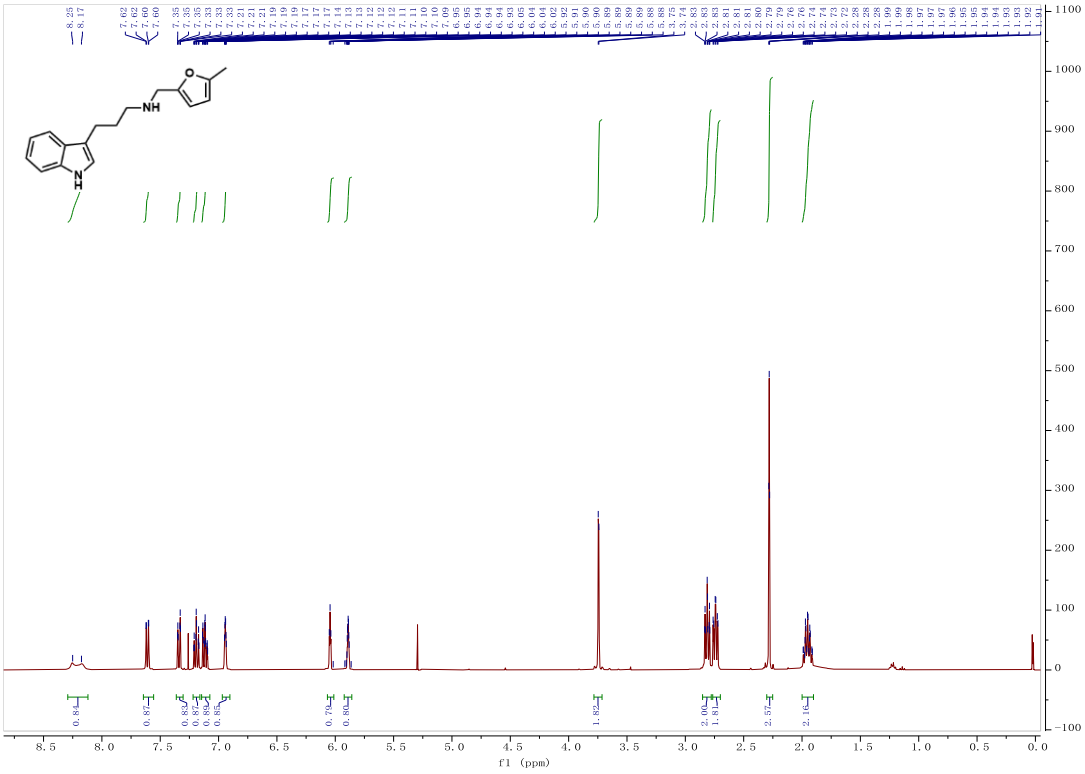
$^{1}$H NMR Spectrum of **1p** (400 MHz, $CDCl_3$):



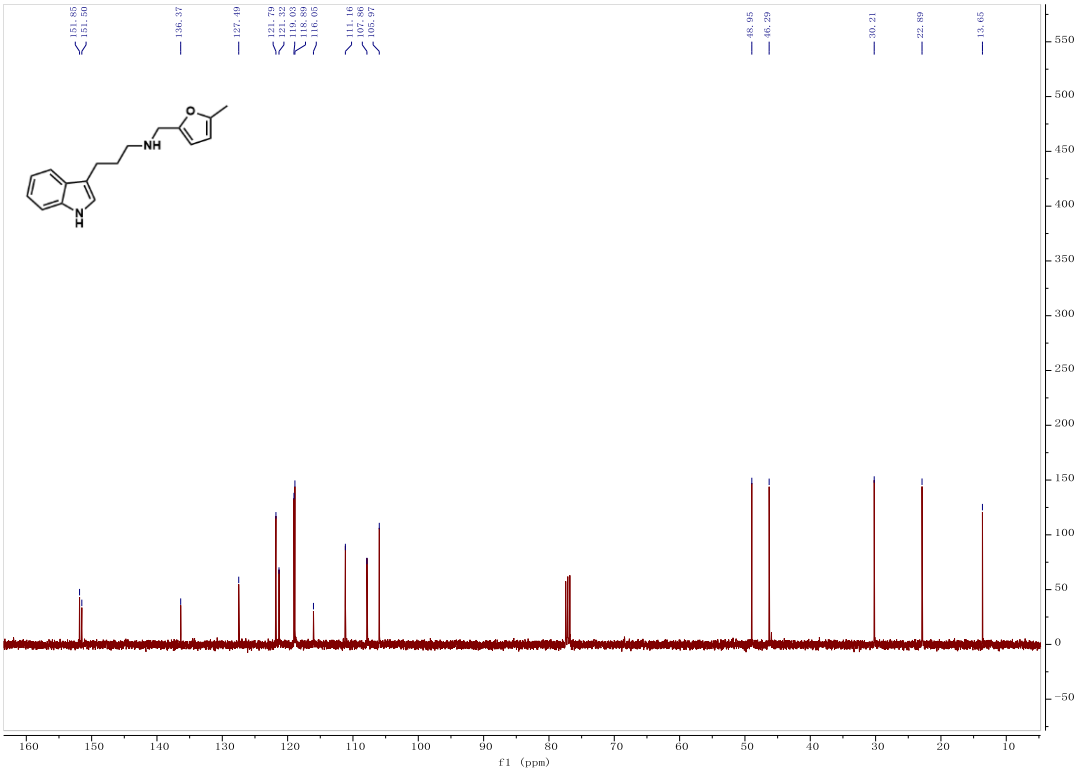
$^{13}$C NMR Spectrum of **1p** (100 MHz, $CDCl_3$):



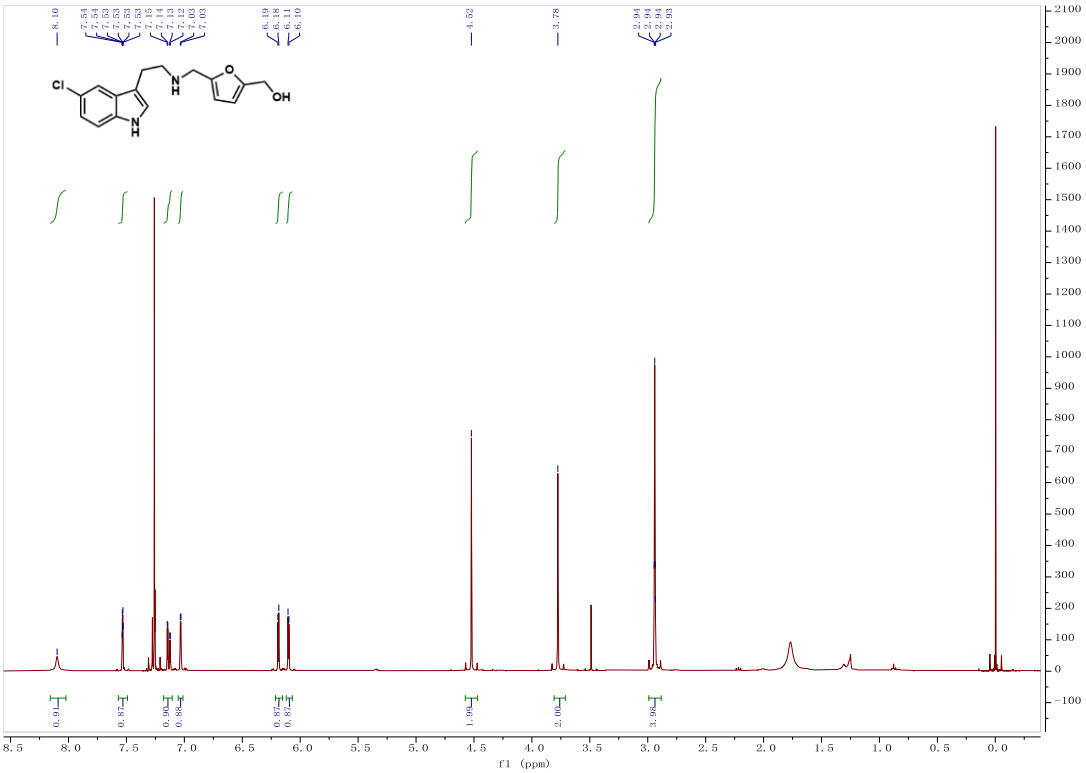
$^{1}$H NMR Spectrum of **1q** (400 MHz, $CDCl_3$):



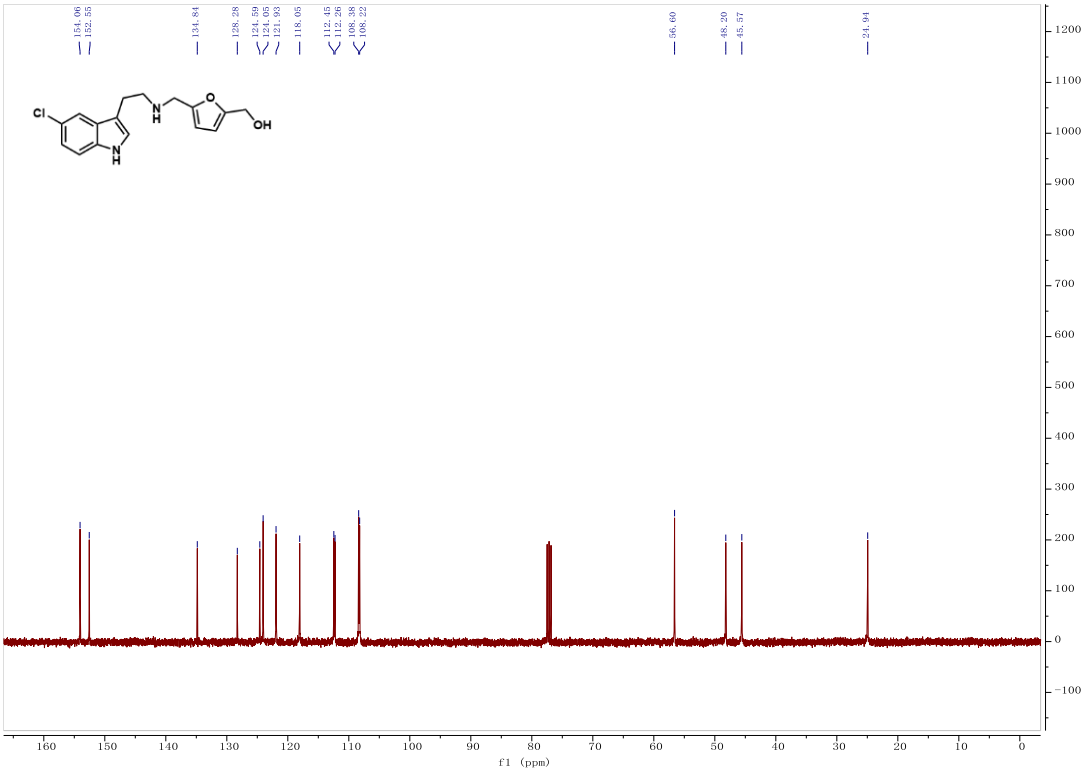
$^{13}$C NMR Spectrum of **1q** (100 MHz, $CDCl_3$):



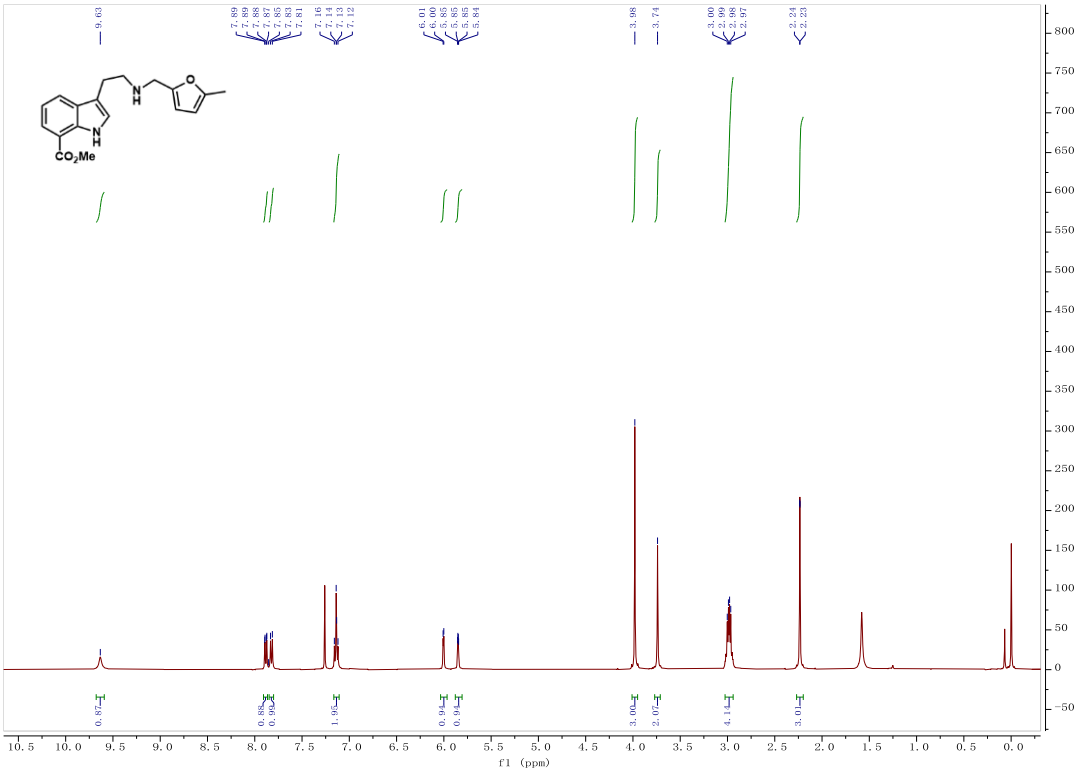
$^{1}$H NMR Spectrum of **1r** (400 MHz, $CDCl_3$):



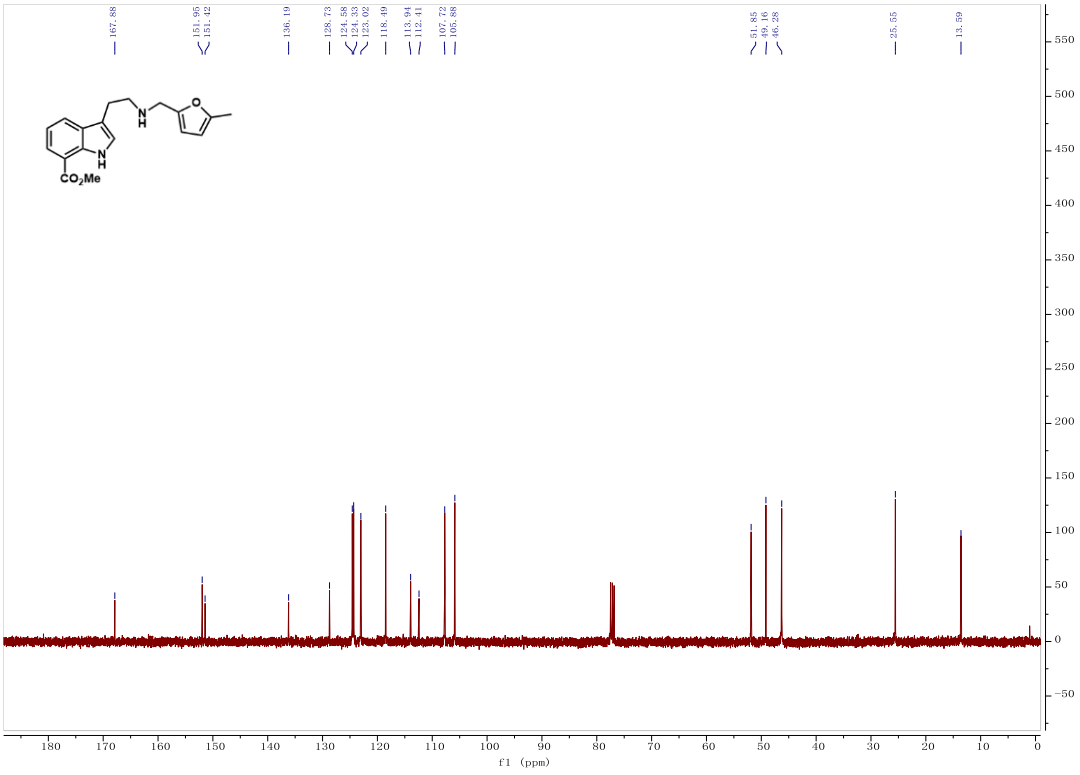

$^{13}$C NMR Spectrum of **1r** (100 MHz, $CDCl_3$):



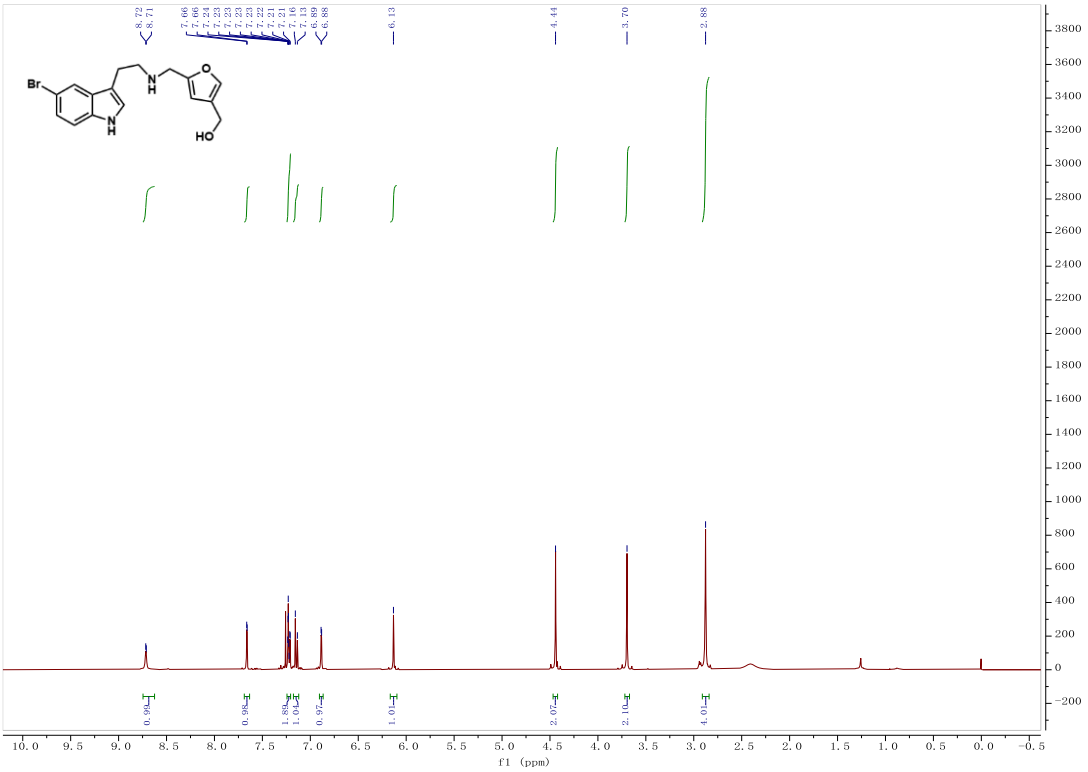
$^{1}$H NMR Spectrum of **1s** (400 MHz, $CDCl_3$):



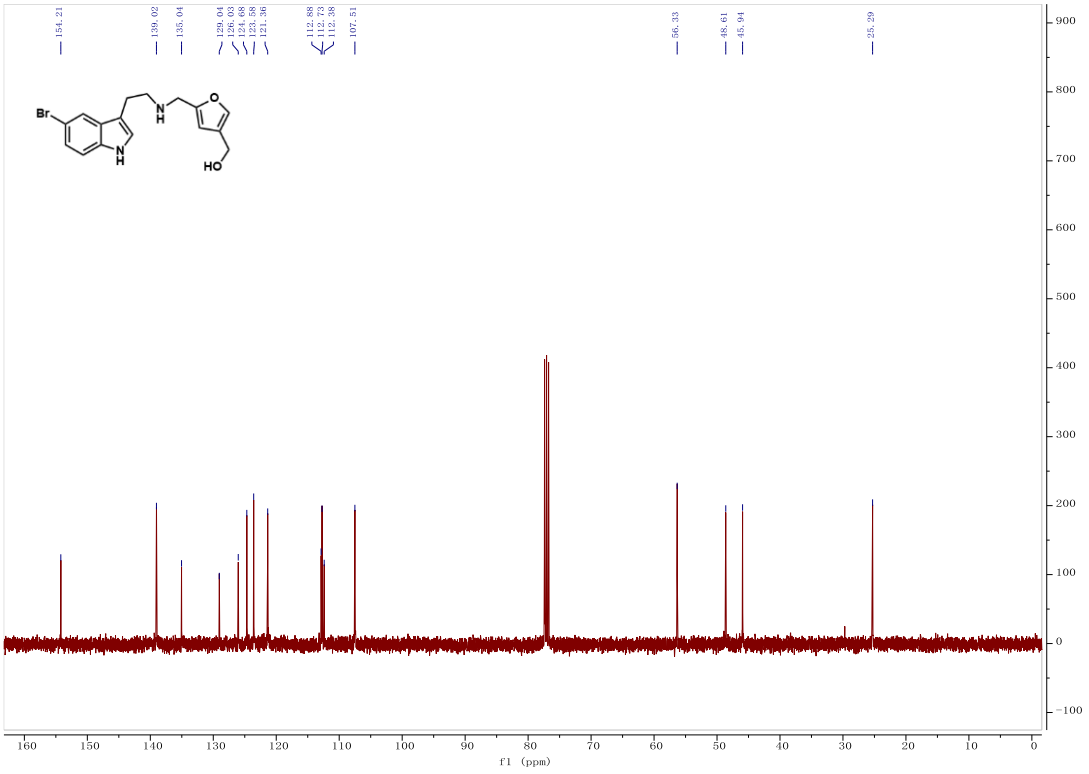

$^{13}$C NMR Spectrum of **1s** (100 MHz, $CDCl_3$):



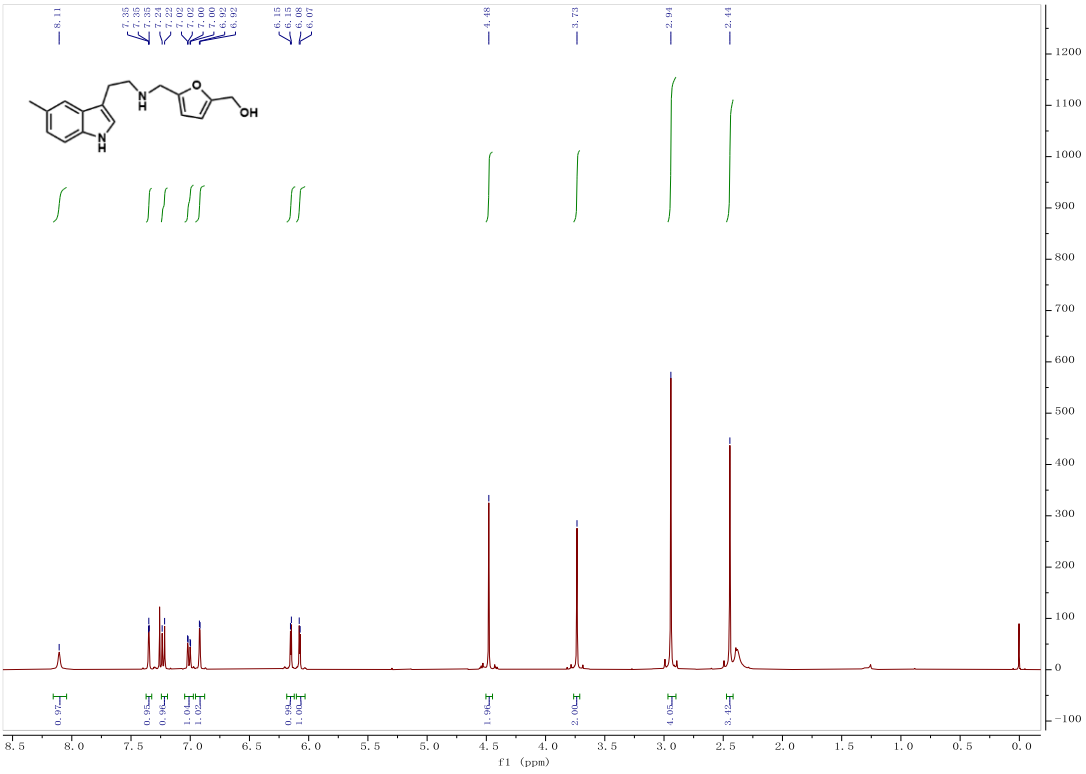
$^{1}$H NMR Spectrum of **1t** (400 MHz, $CDCl_3$):



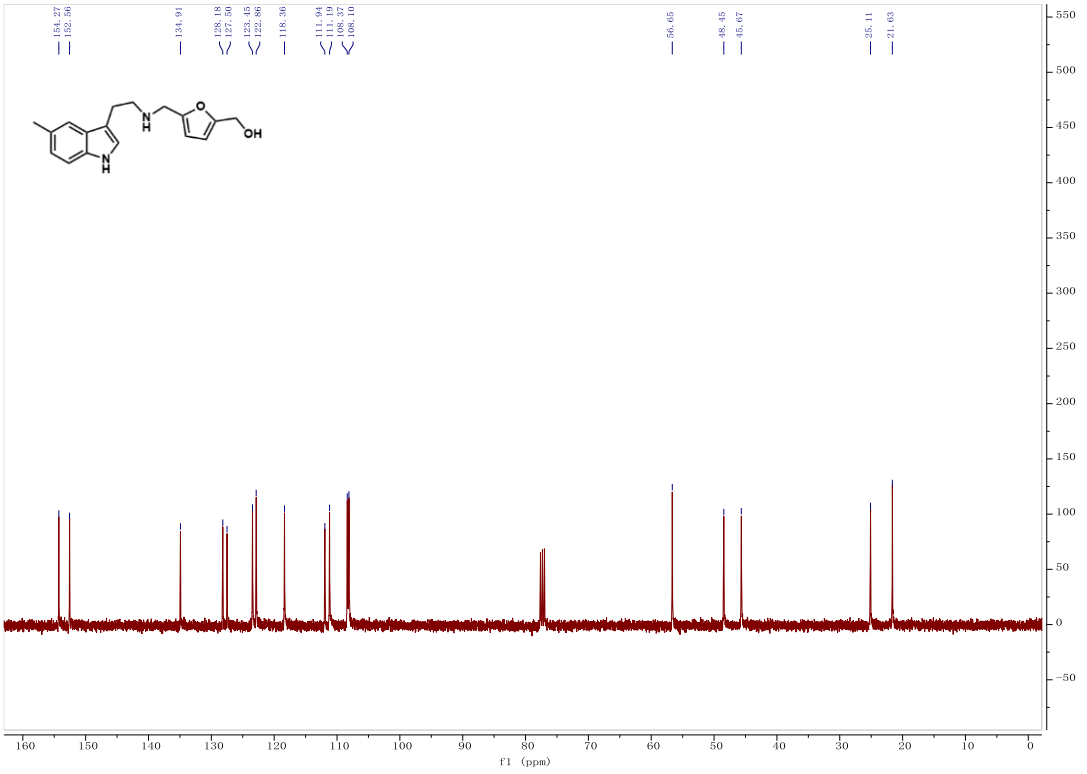

$^{13}$C NMR Spectrum of **1t** (100 MHz, $CDCl_3$):



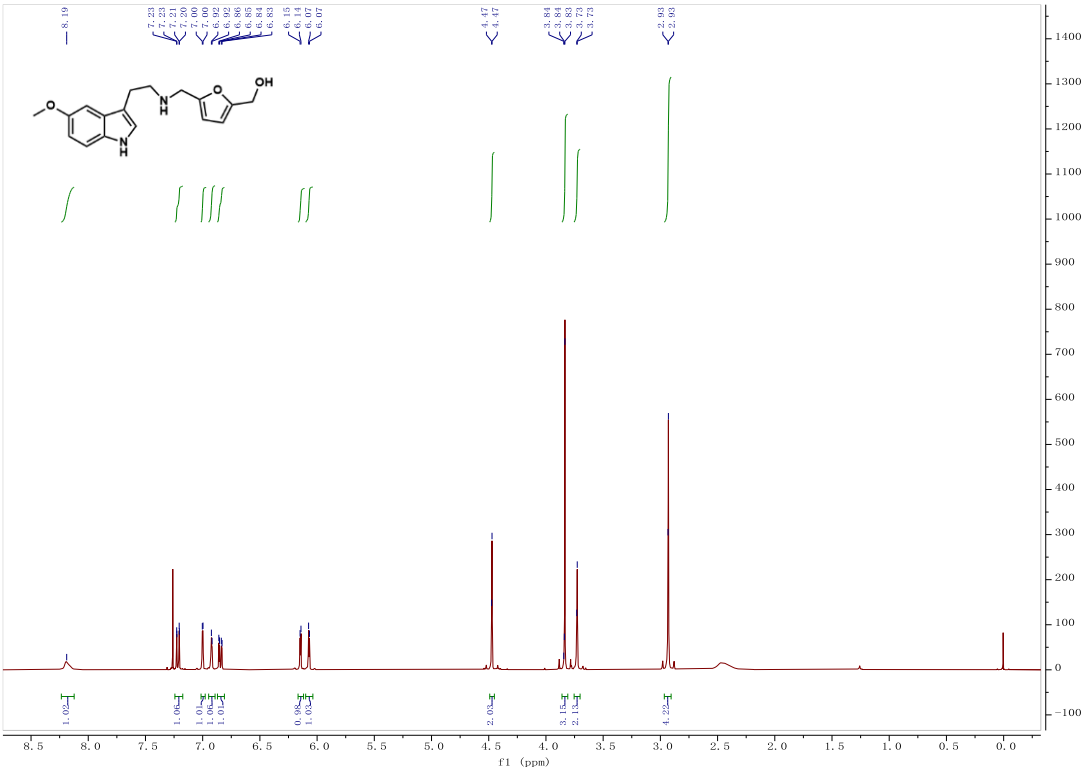
$^{1}$H NMR Spectrum of **1u** (400 MHz, $CDCl_3$):



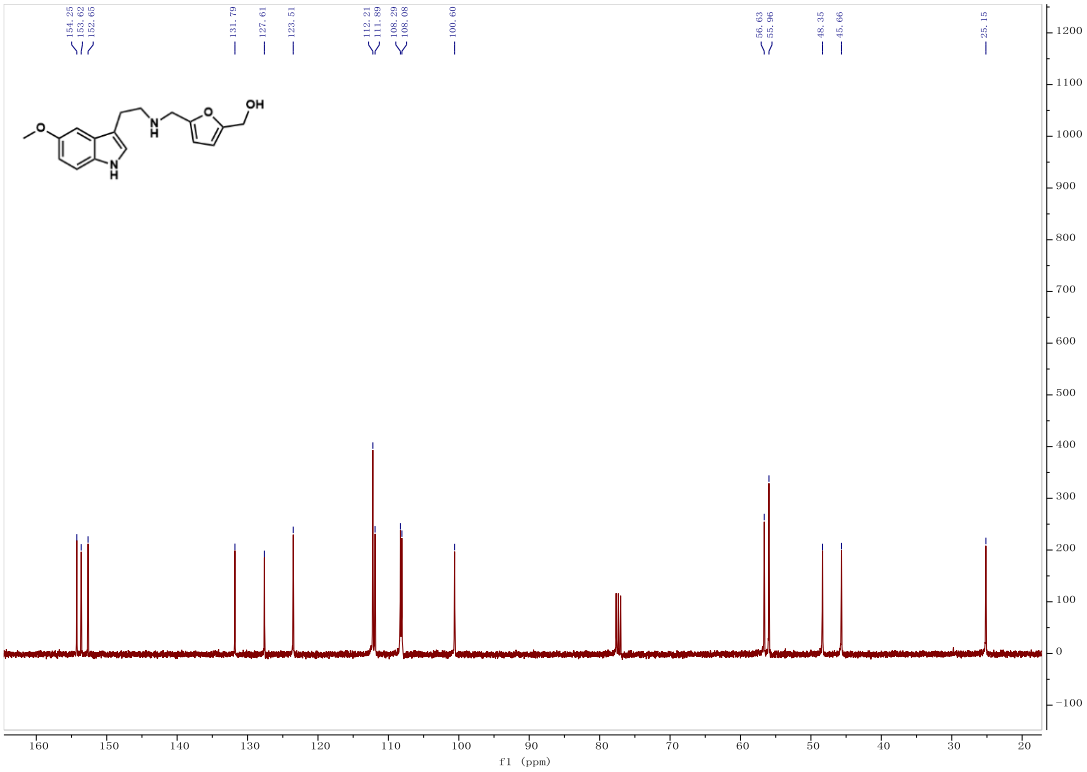

$^{13}$C NMR Spectrum of **1u** (100 MHz, $CDCl_3$):



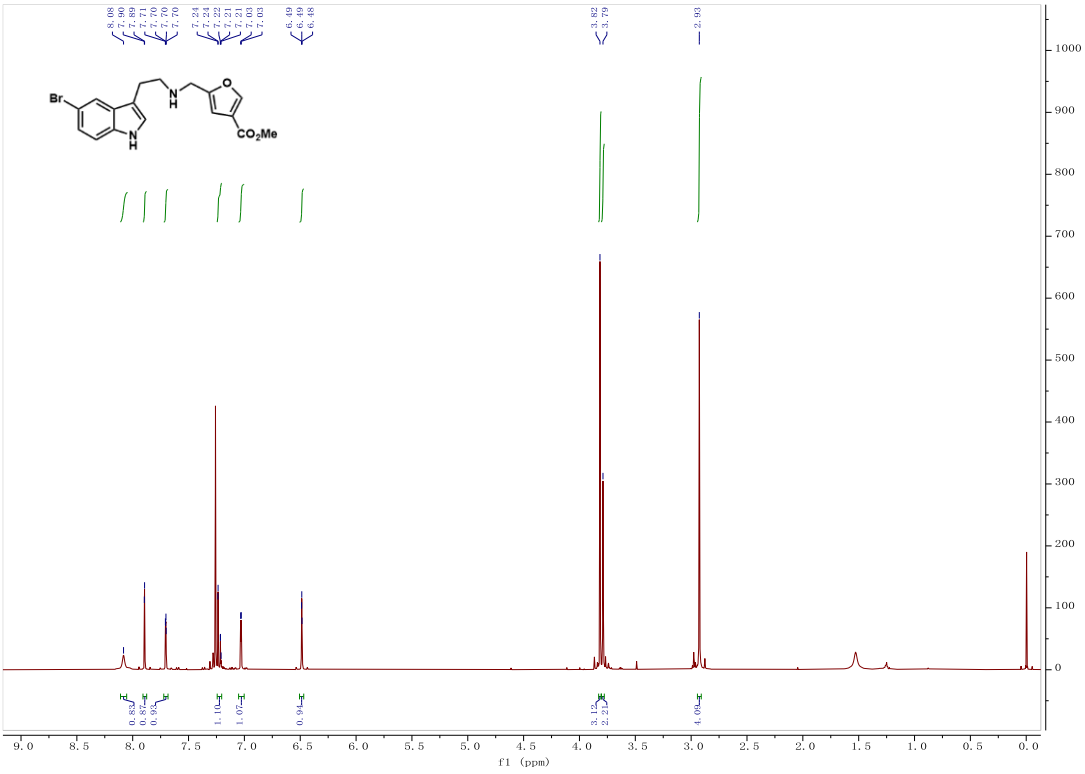
$^{1}$H NMR Spectrum of **1v** (400 MHz, $CDCl_3$):



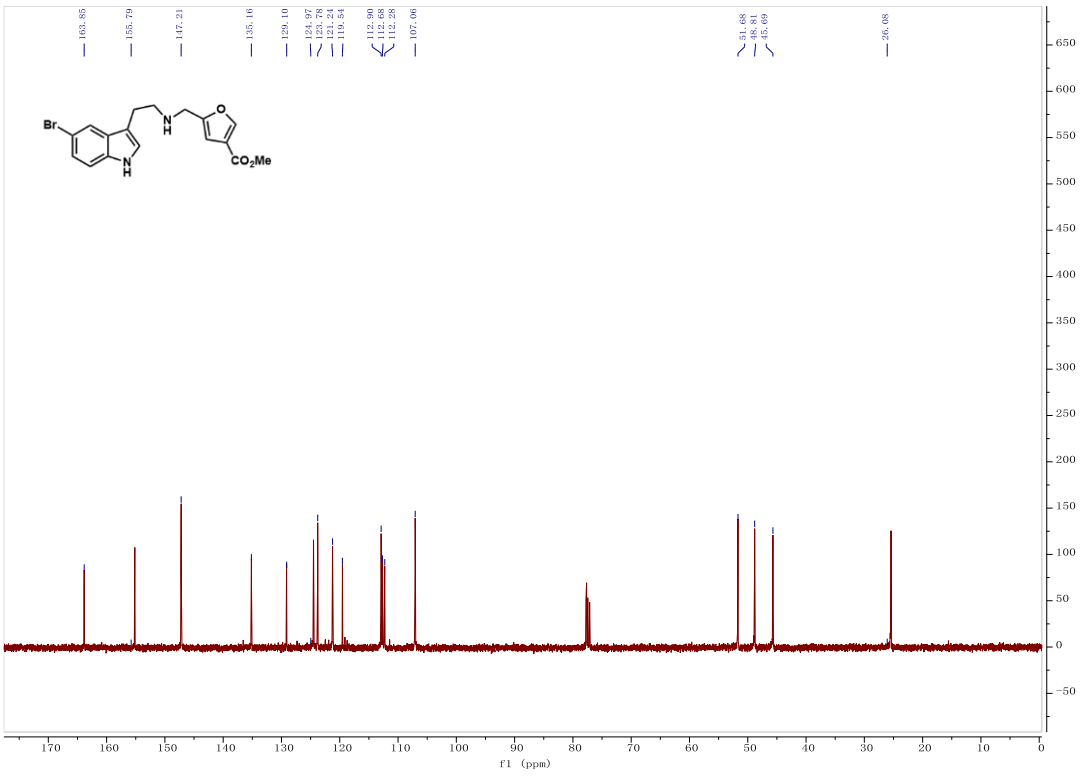
$^{13}$C NMR Spectrum of **1v** (100 MHz, $CDCl_3$):



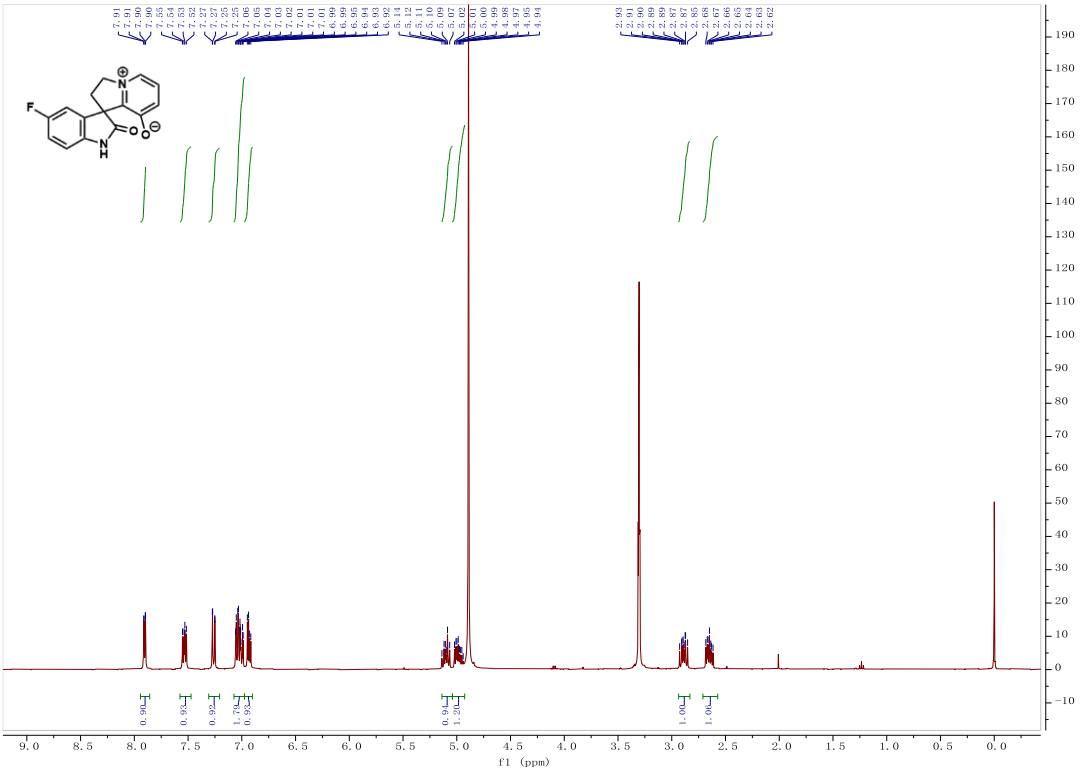
$^{1}$H NMR Spectrum of **1w** (400 MHz, $CDCl_3$):



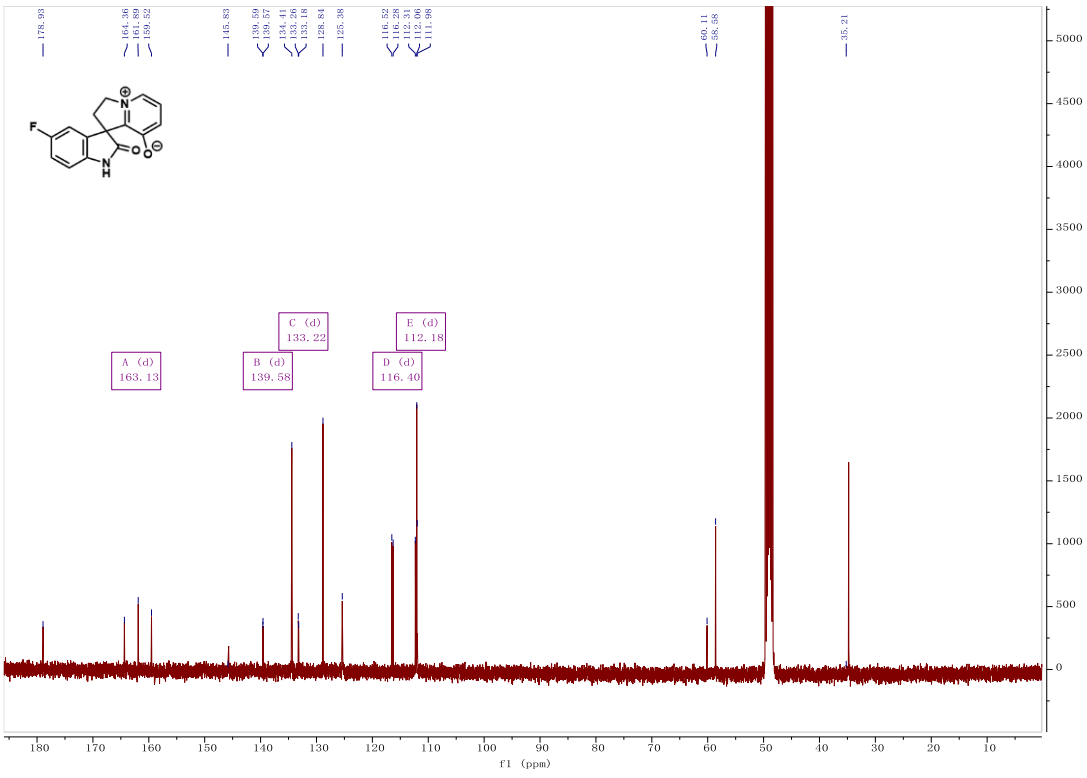

$^{13}$C NMR Spectrum of **1w** (100 MHz, $CDCl_3$):



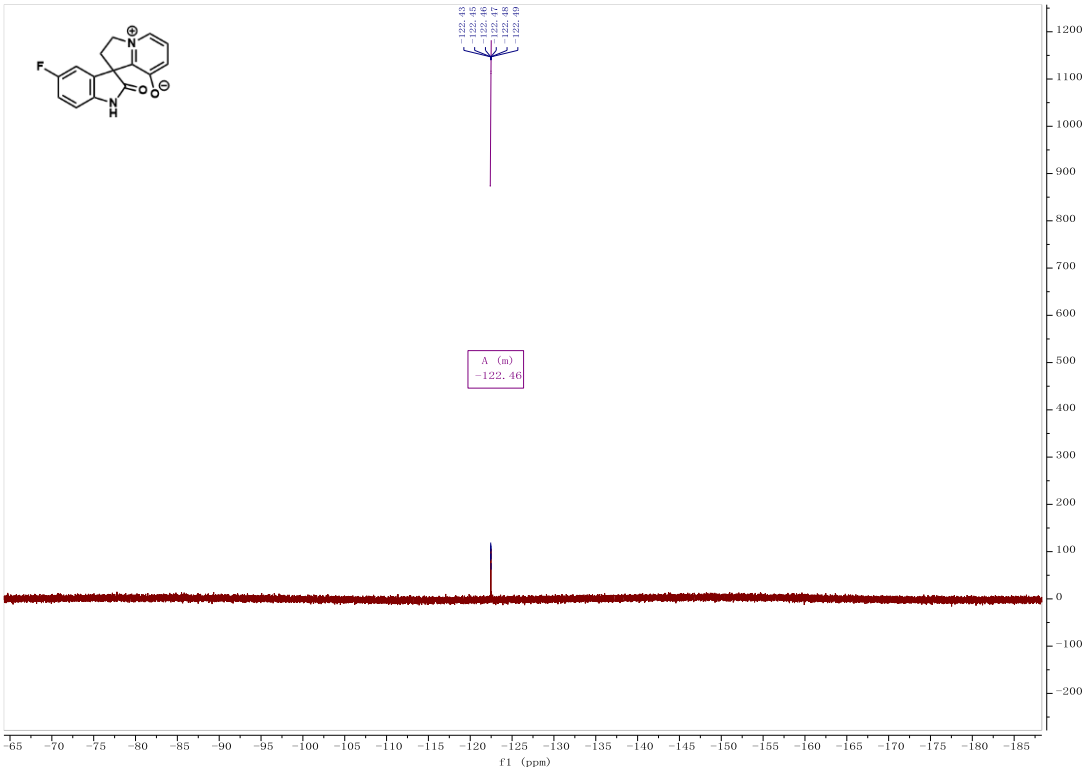
$^{1}$H NMR Spectrum of **3a** (400 MHz, $CD_3OD$):



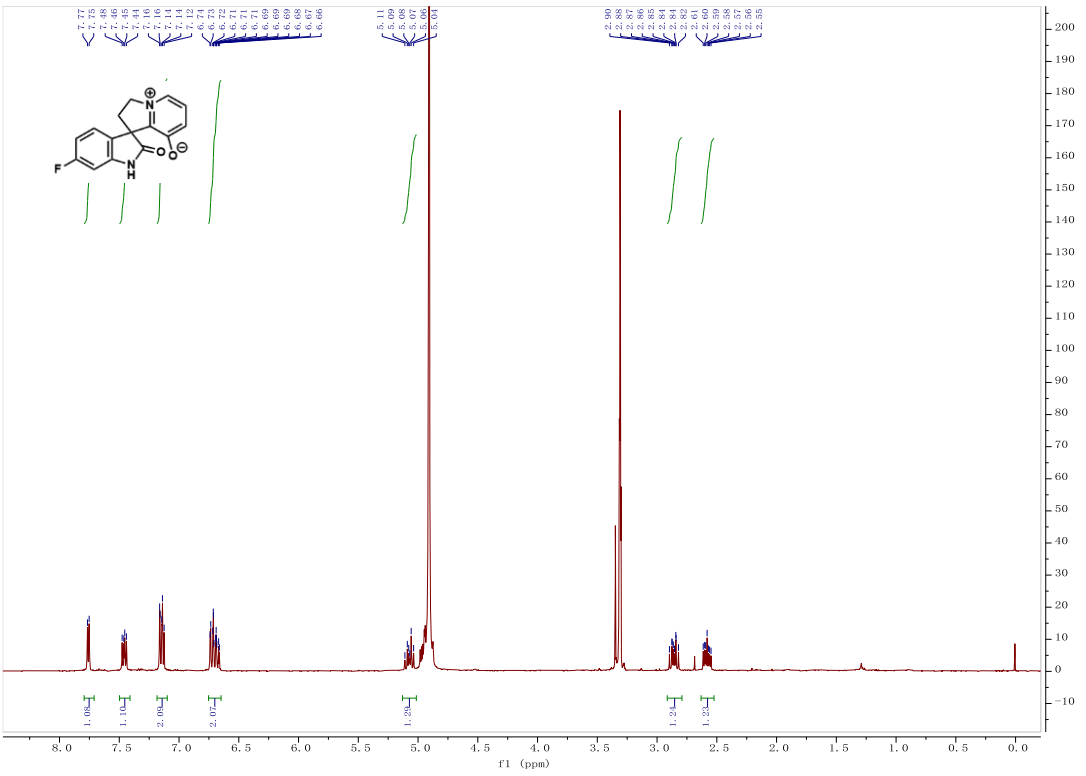
$^{13}$C NMR Spectrum of **3a** (100 MHz, $CD_3OD$):



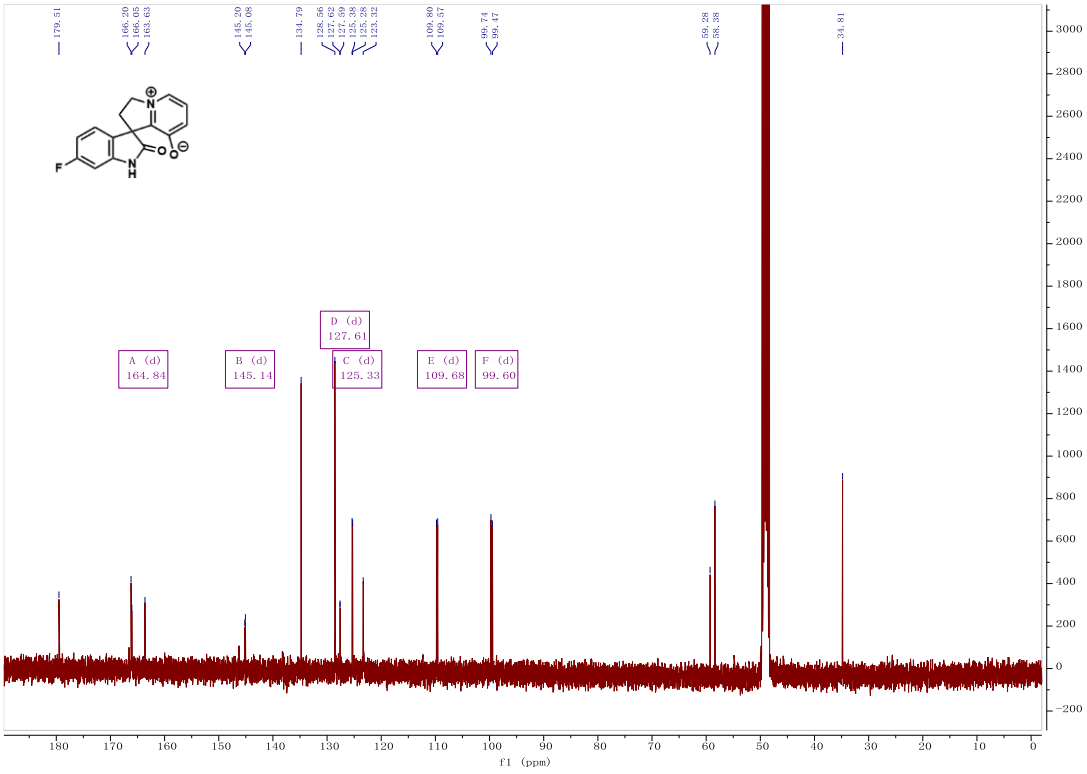
$^{19}$F NMR Spectrum of **3a** (376 MHz, $CD_3OD$):



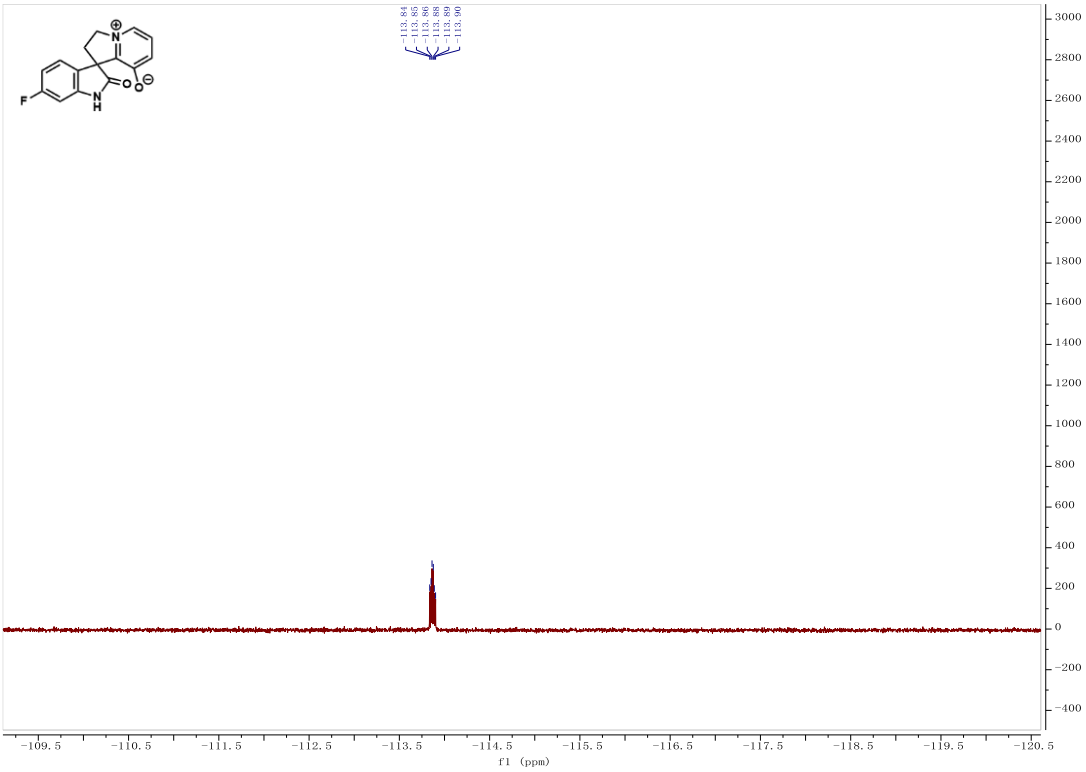

$^{1}$H NMR Spectrum of **3b** (400 MHz, $CD_3OD$):



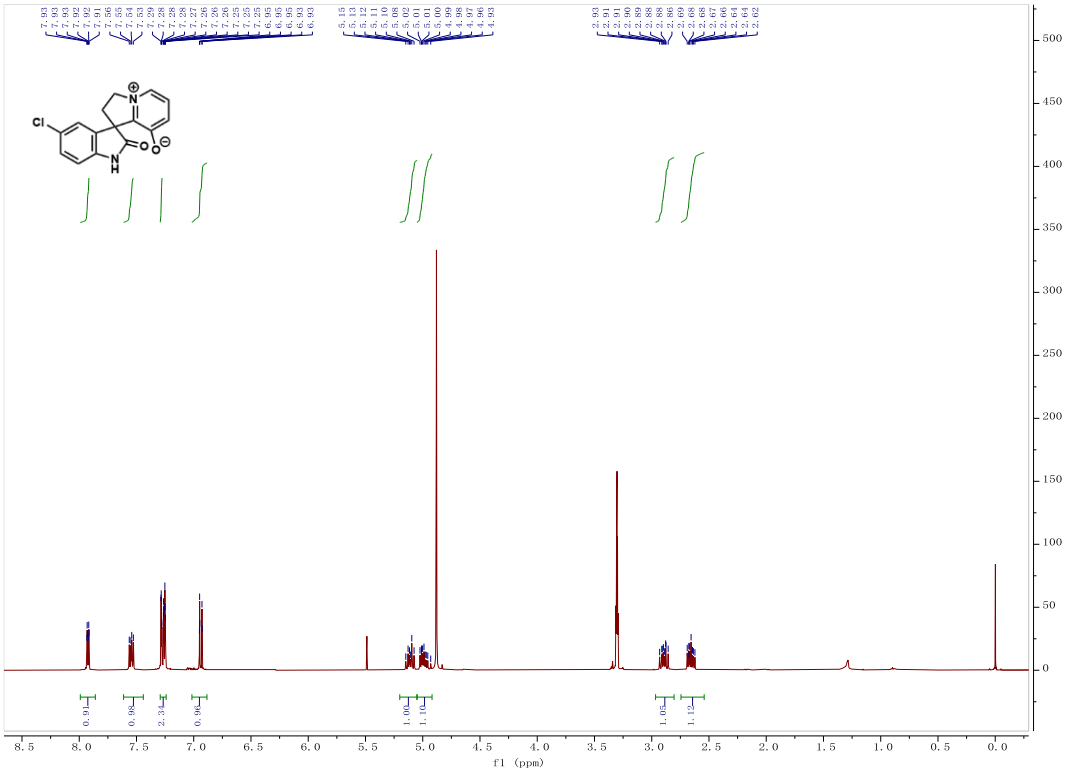
$^{13}$C NMR Spectrum of **3b** (100 MHz, $CD_3OD$):



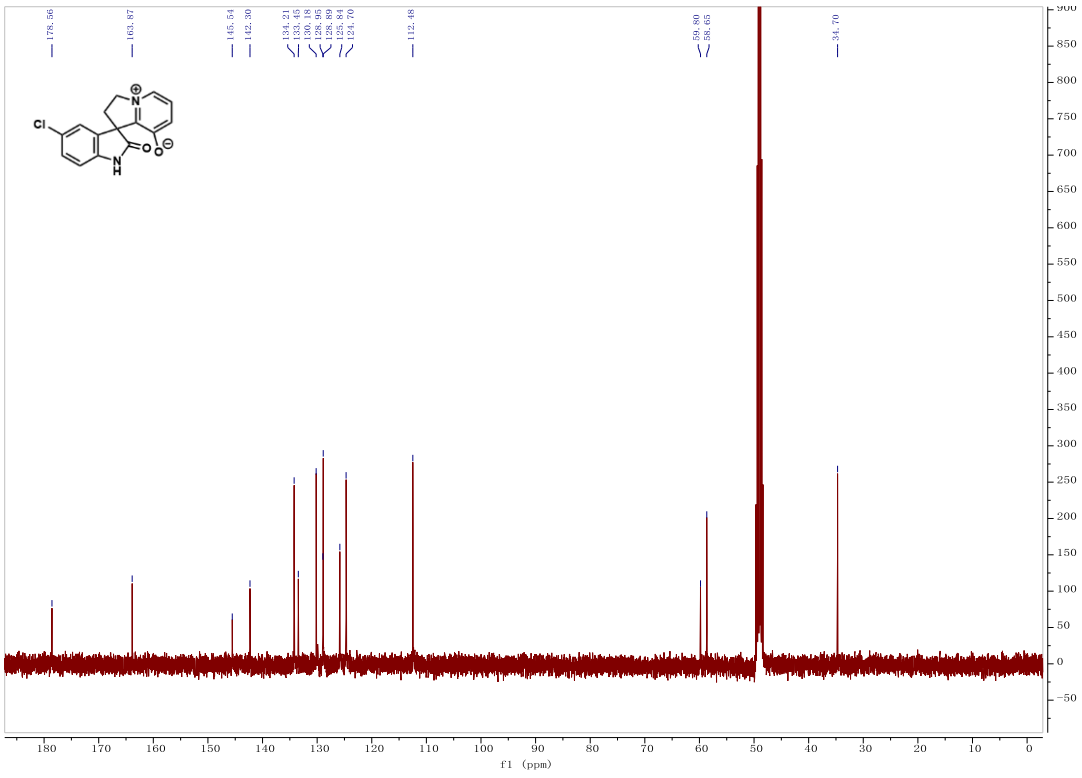

$^{19}$F NMR Spectrum of **3b** (376 MHz, $CD_3OD$):



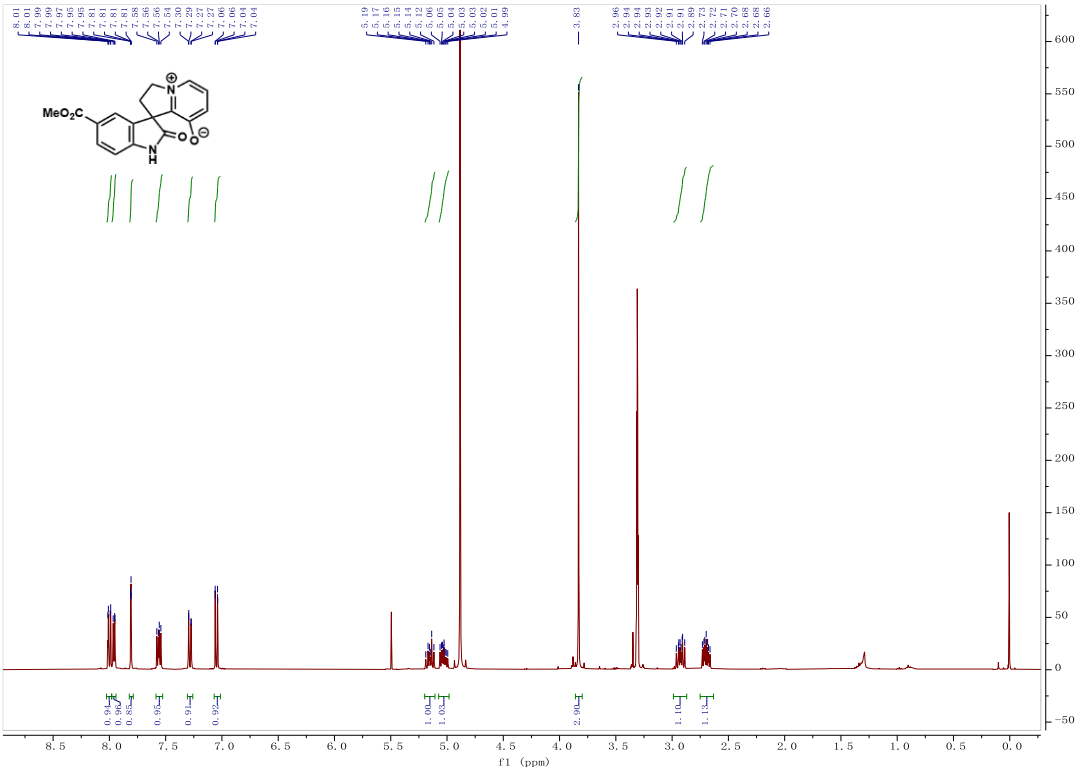
$^{1}$H NMR Spectrum of **3c** (400 MHz, $CD_3OD$):



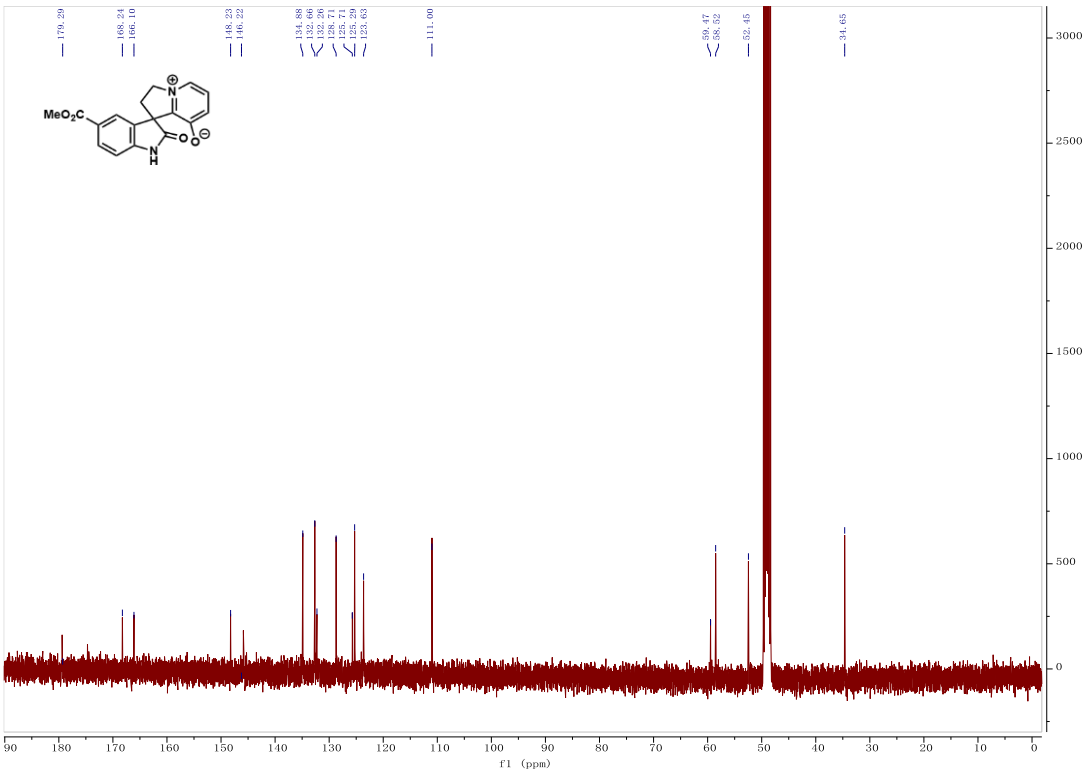
$^{13}$C NMR Spectrum of **3c** (100 MHz, $CD_3OD$):



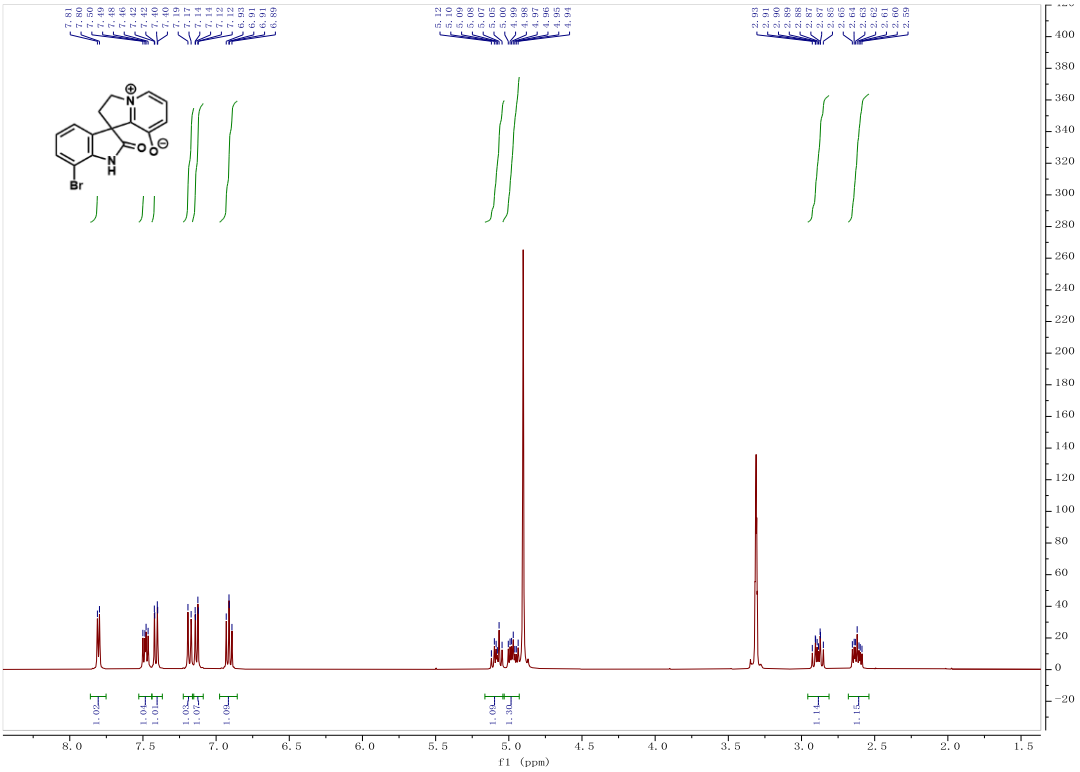
$^{1}$H NMR Spectrum of **3d** (400 MHz, $CD_3OD$):



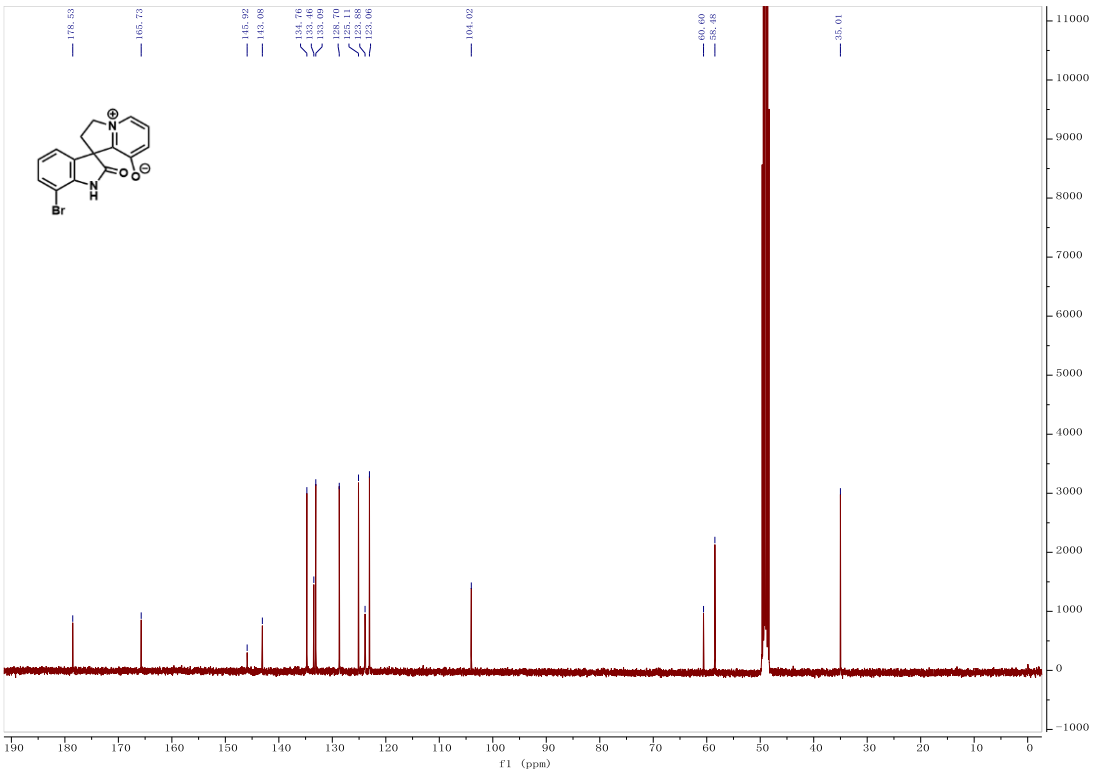
$^{13}$C NMR Spectrum of **3d** (100 MHz, $CD_3OD$):



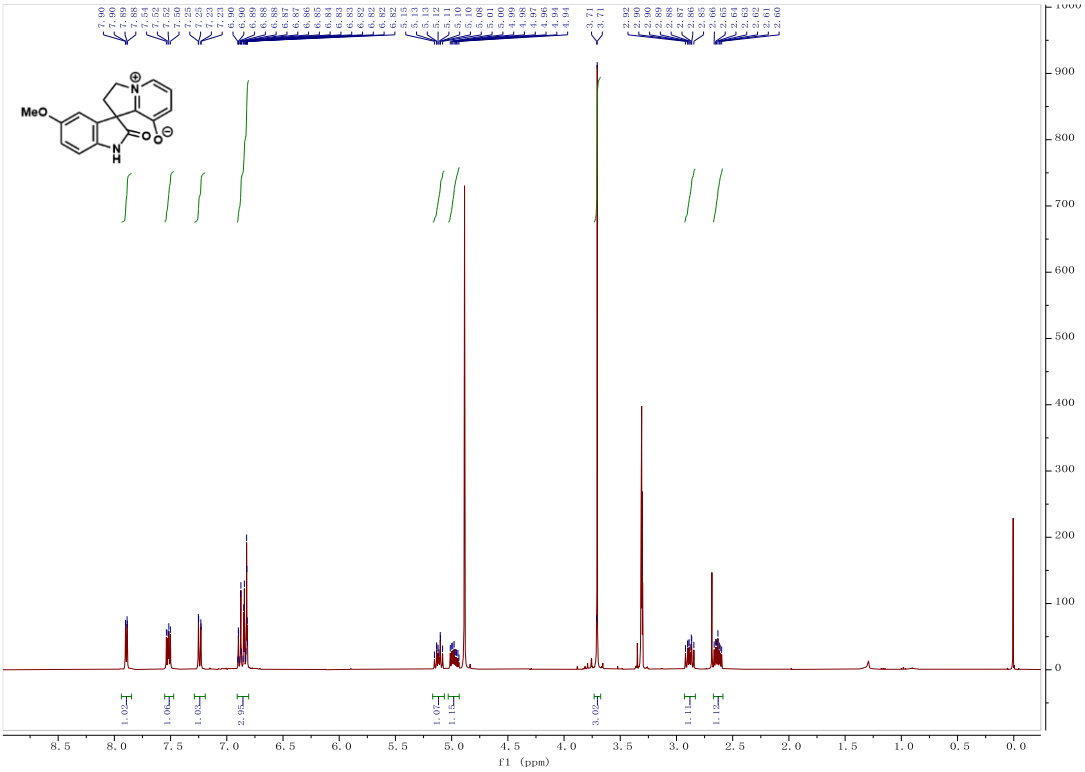
$^{1}$H NMR Spectrum of **3e** (400 MHz, $CD_3OD$):



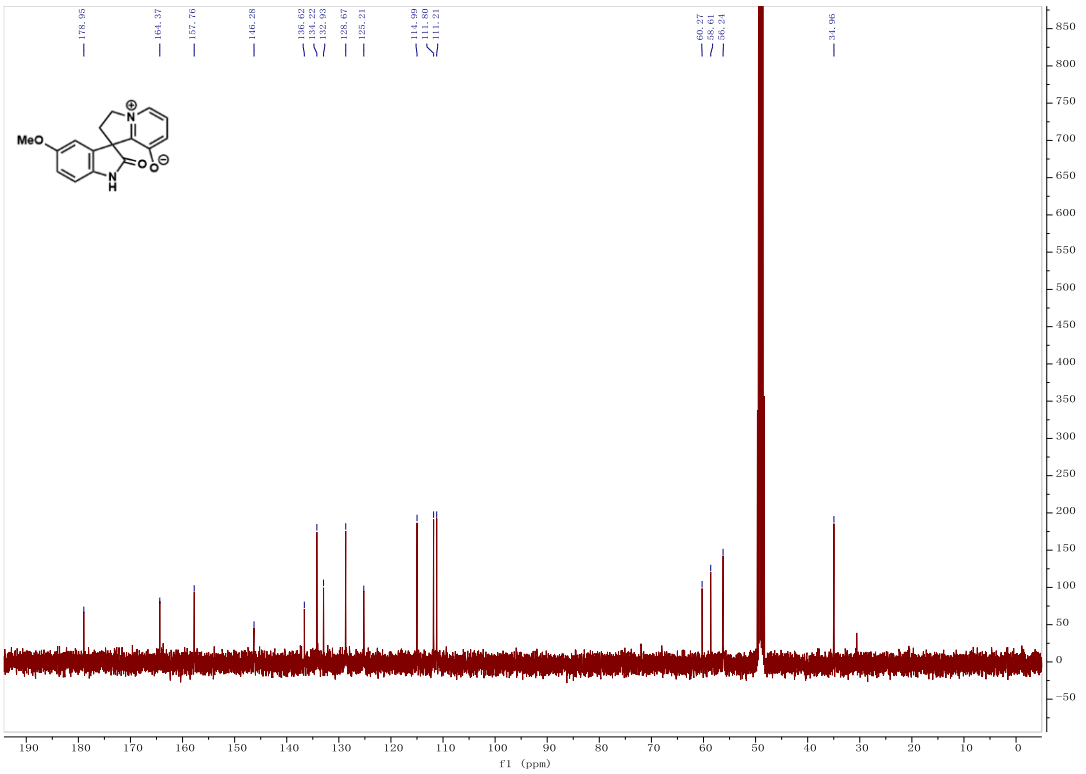
$^{13}$C NMR Spectrum of **3e** (100 MHz, $CD_3OD$):



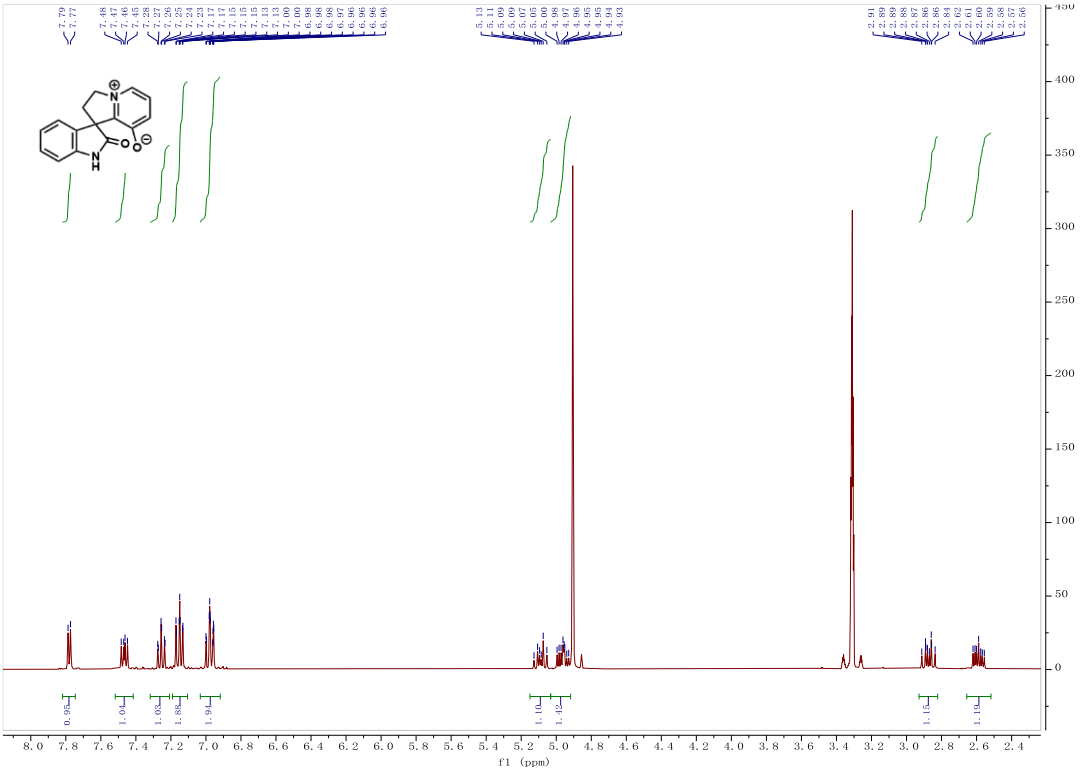
$^{1}$H NMR Spectrum of **3f** (400 MHz, $CD_3OD$):



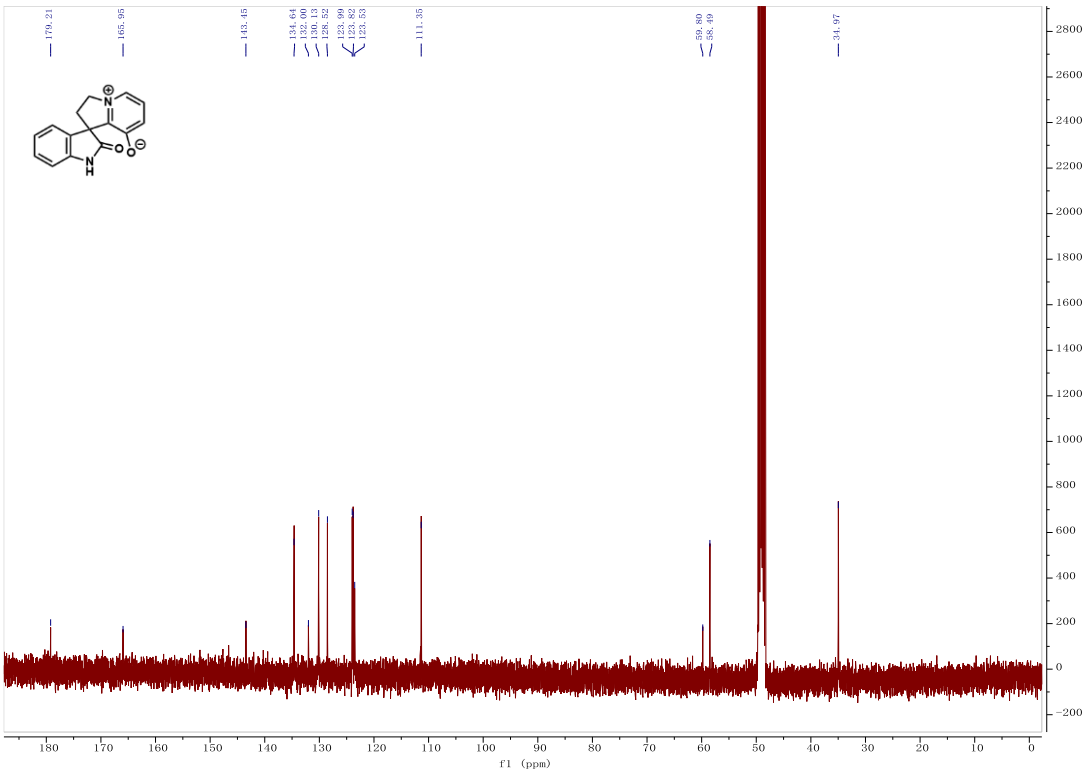
$^{13}$C NMR Spectrum of **3f** (100 MHz, $CD_3OD$):



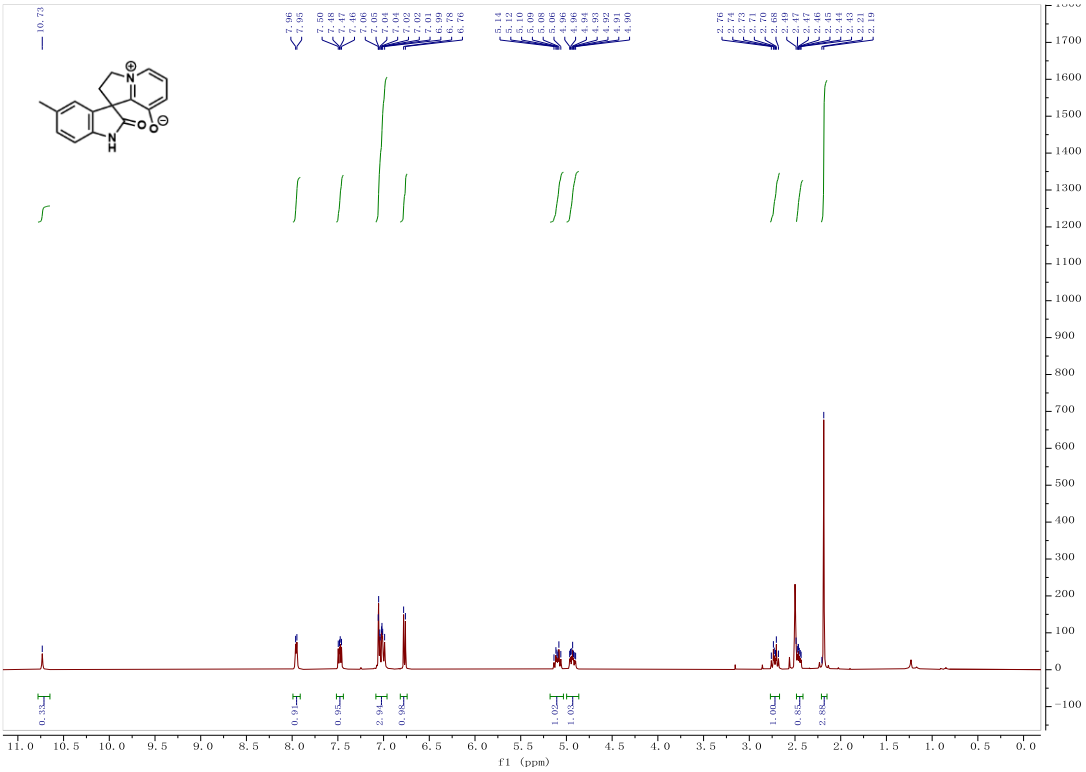
$^{1}$H NMR Spectrum of **3g** (400 MHz, $CD_3OD$):



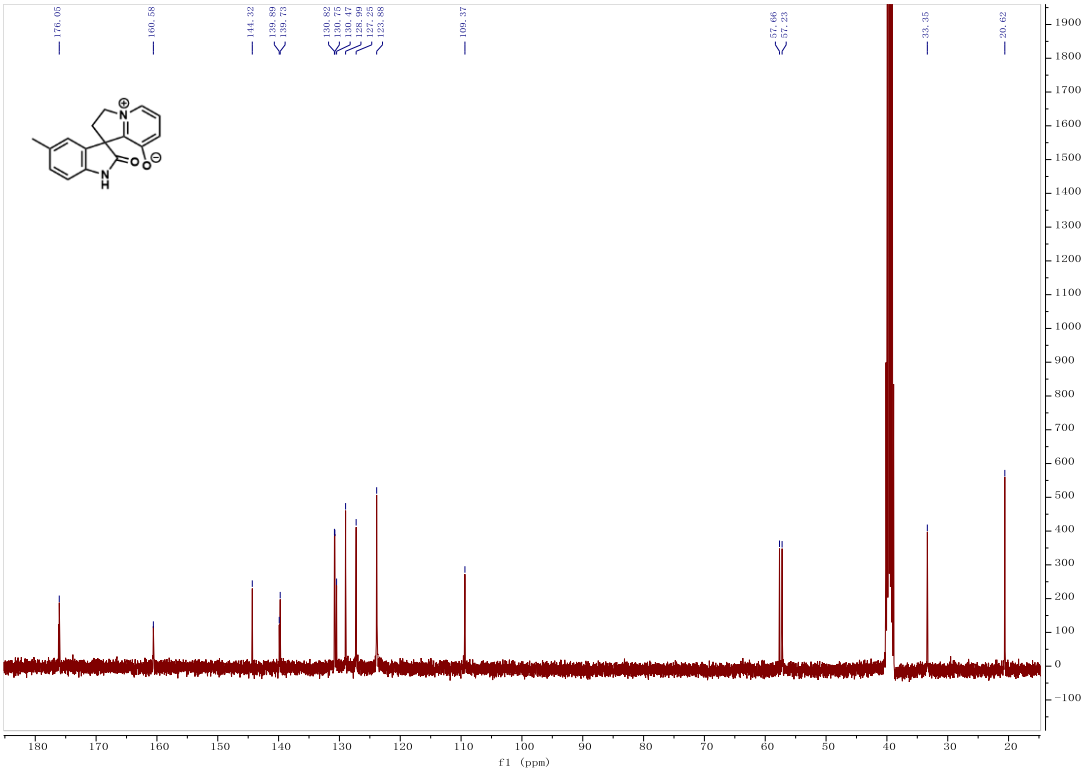
$^{13}$C NMR Spectrum of **3g** (100 MHz, $CD_3OD$):



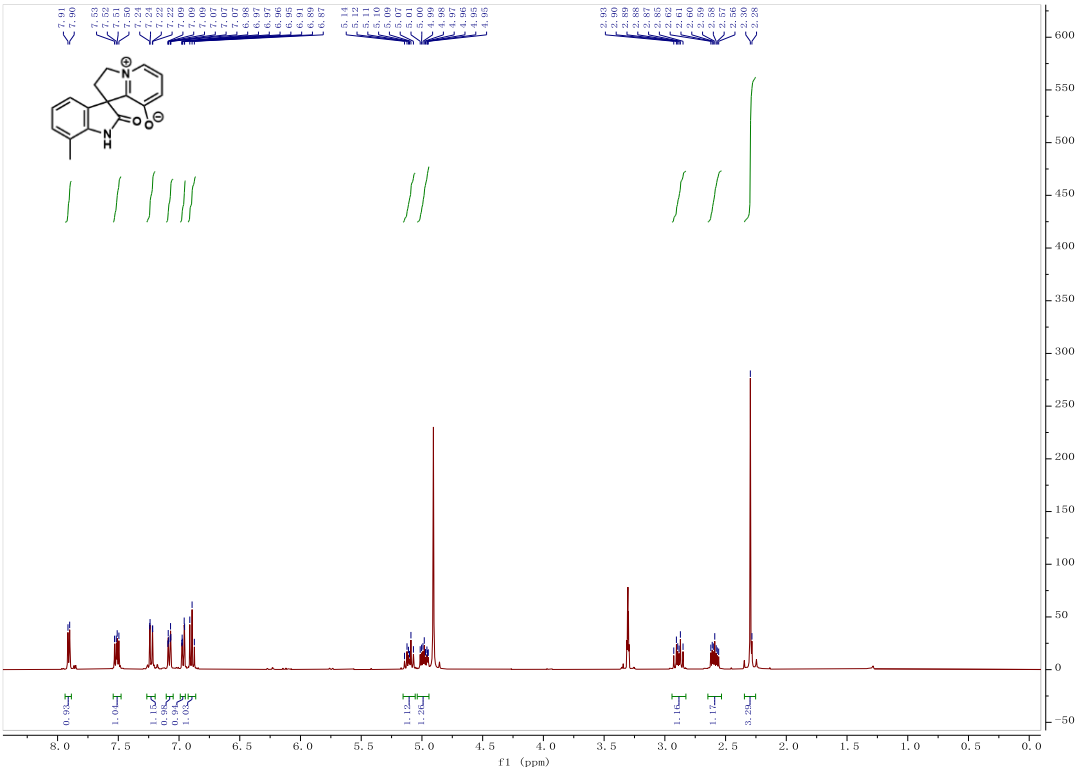
$^{1}$H NMR Spectrum of **3h** (400 MHz, DMSO-$d_6$):



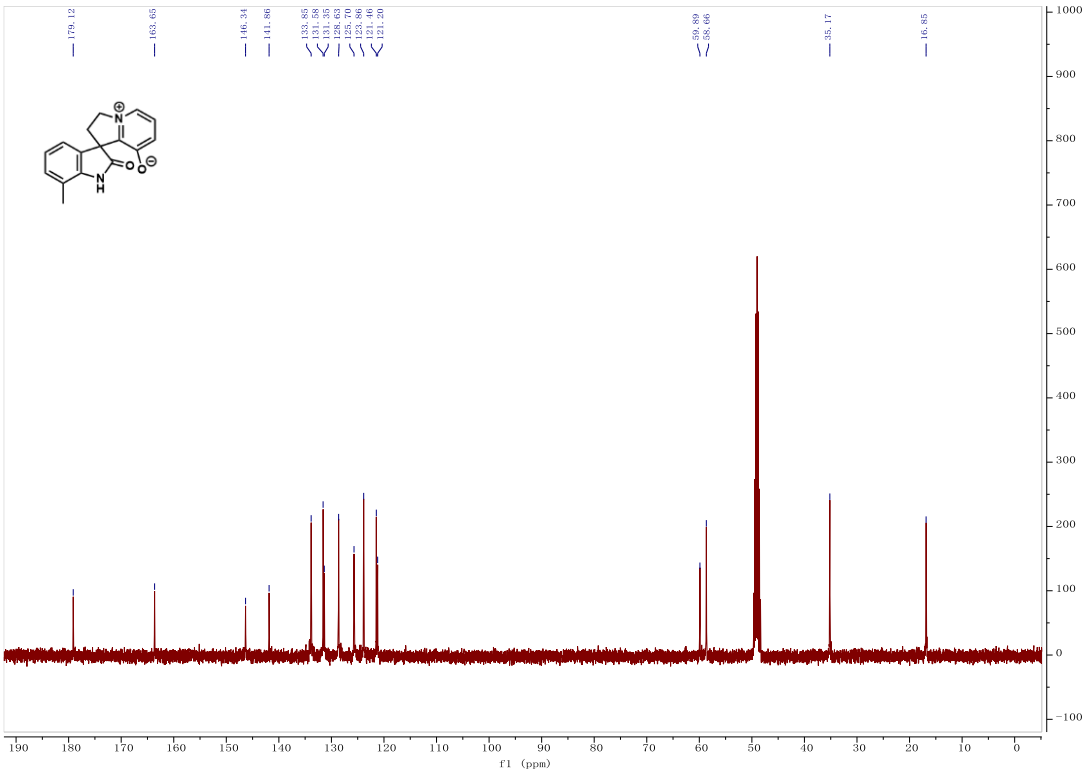
$^{13}$C NMR Spectrum of **3h** (100 MHz, DMSO-$d_6$):



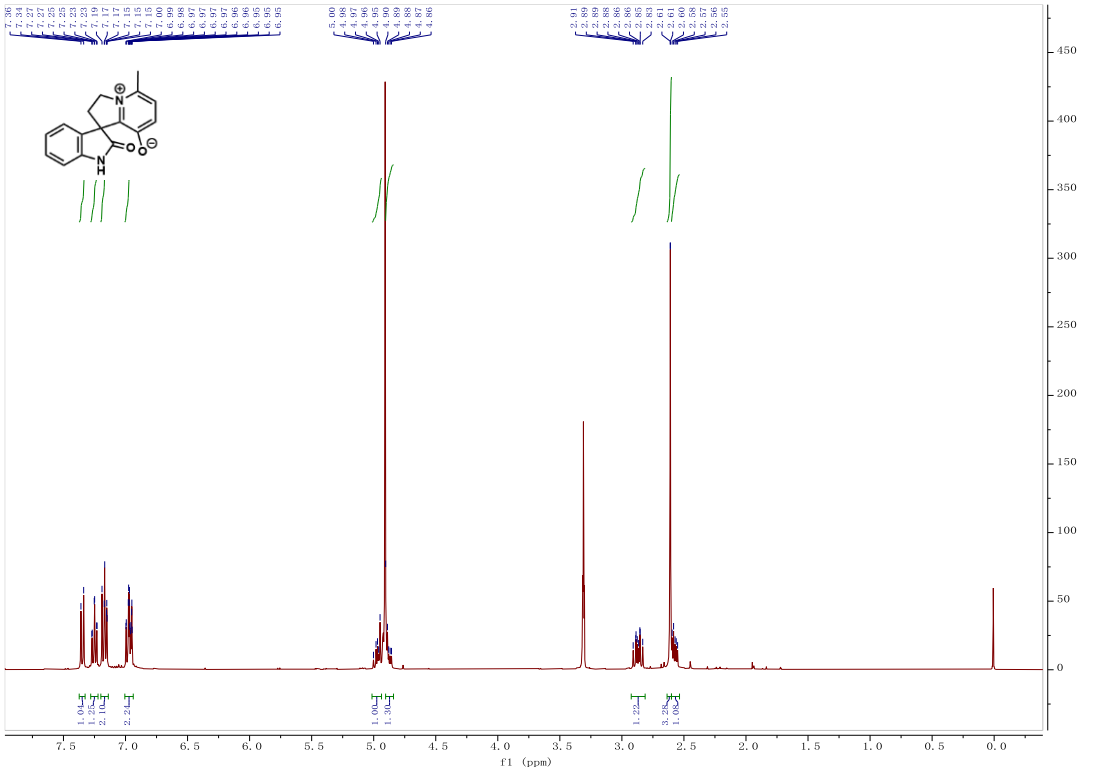
$^{1}$H NMR Spectrum of **3i** (400 MHz, $CD_3OD$):



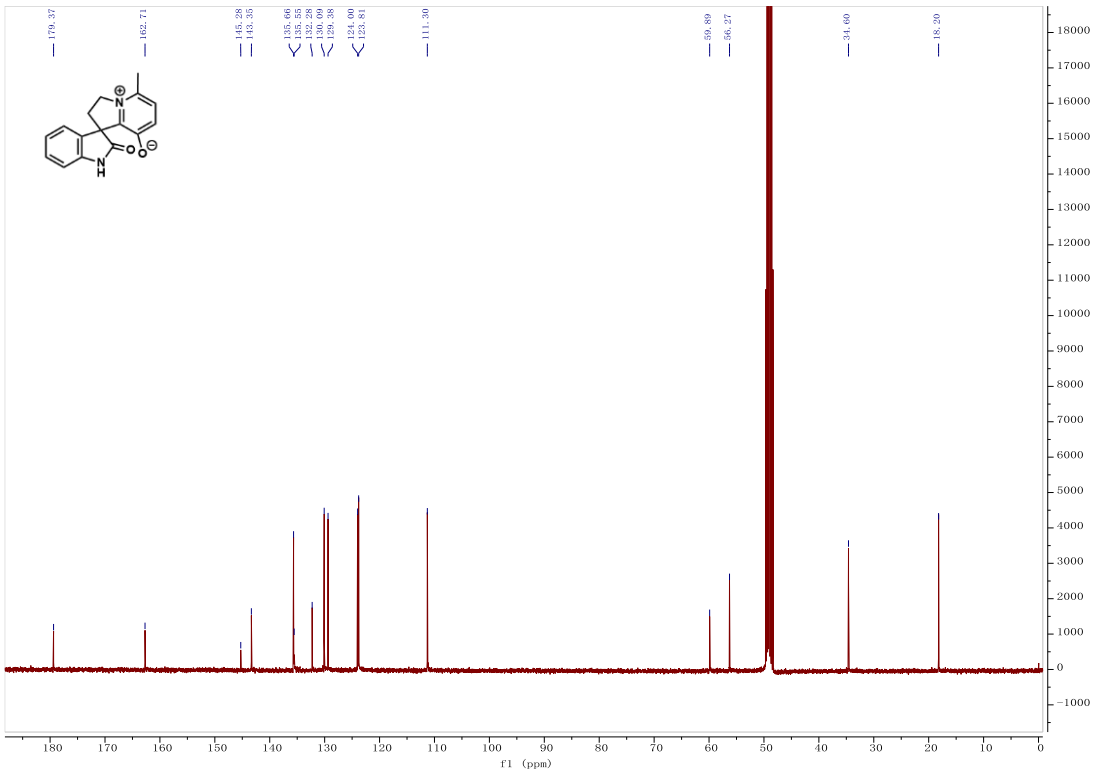
$^{13}$C NMR Spectrum of **3i** (100 MHz, $CD_3OD$):



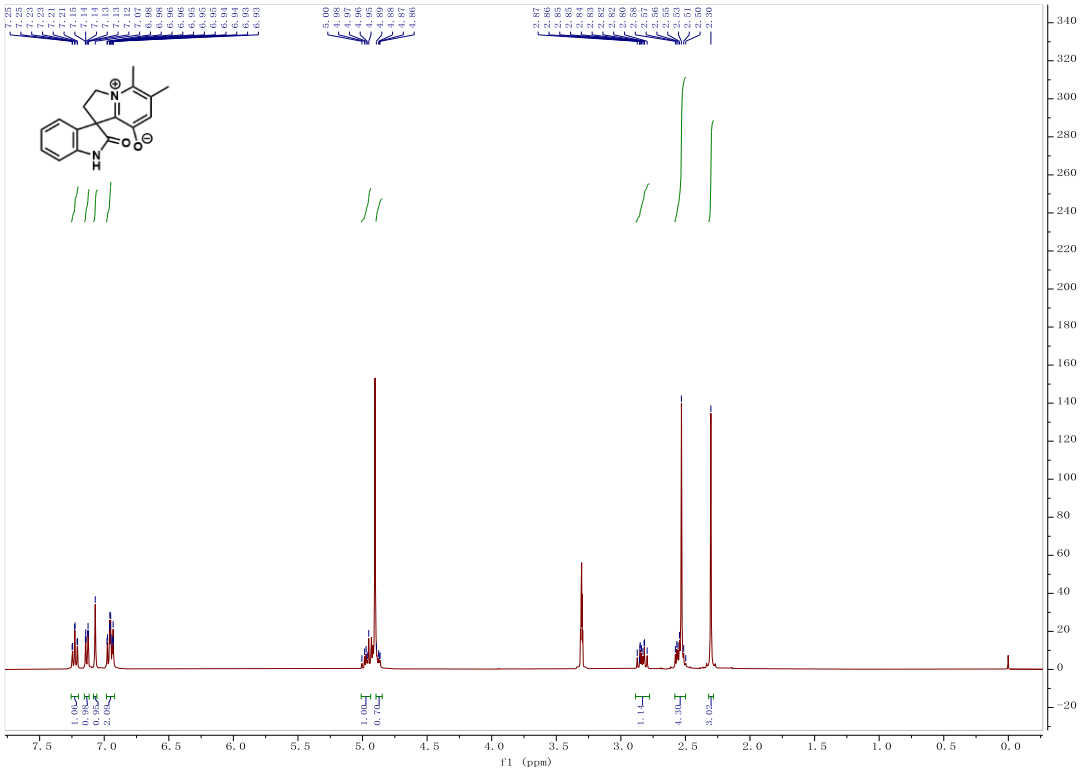
$^{1}$H NMR Spectrum of **3j** (400 MHz, $CD_3OD$):



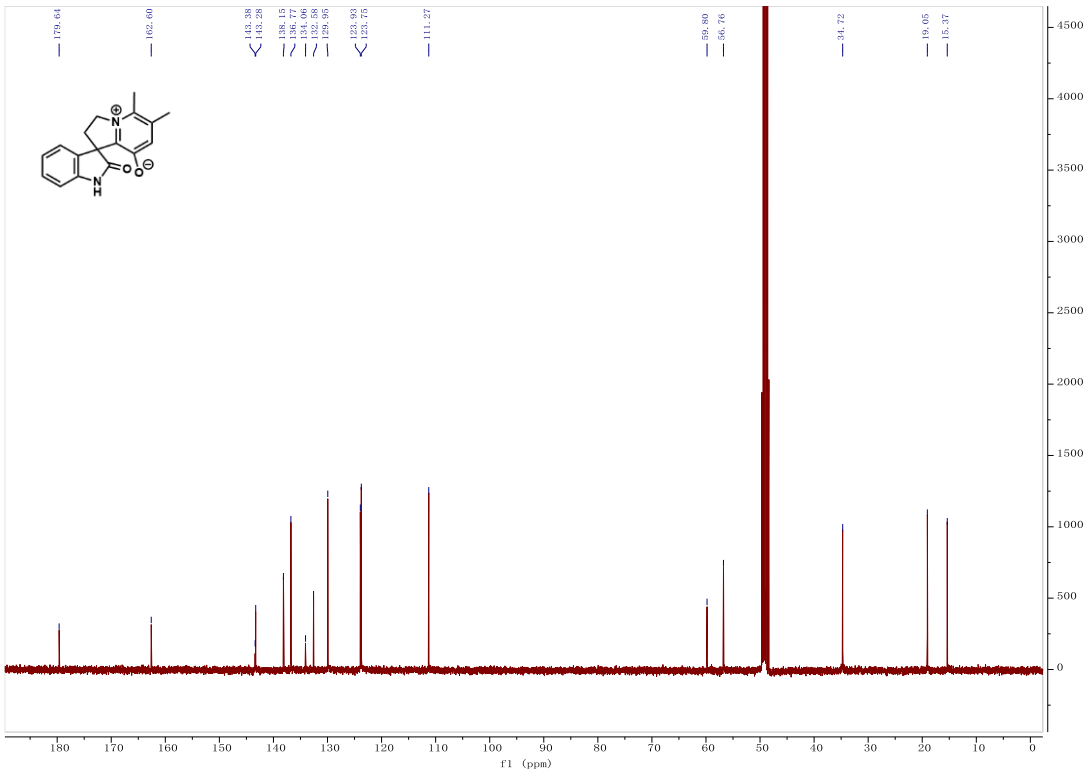
$^{13}$C NMR Spectrum of **3j** (100 MHz, $CD_3OD$):



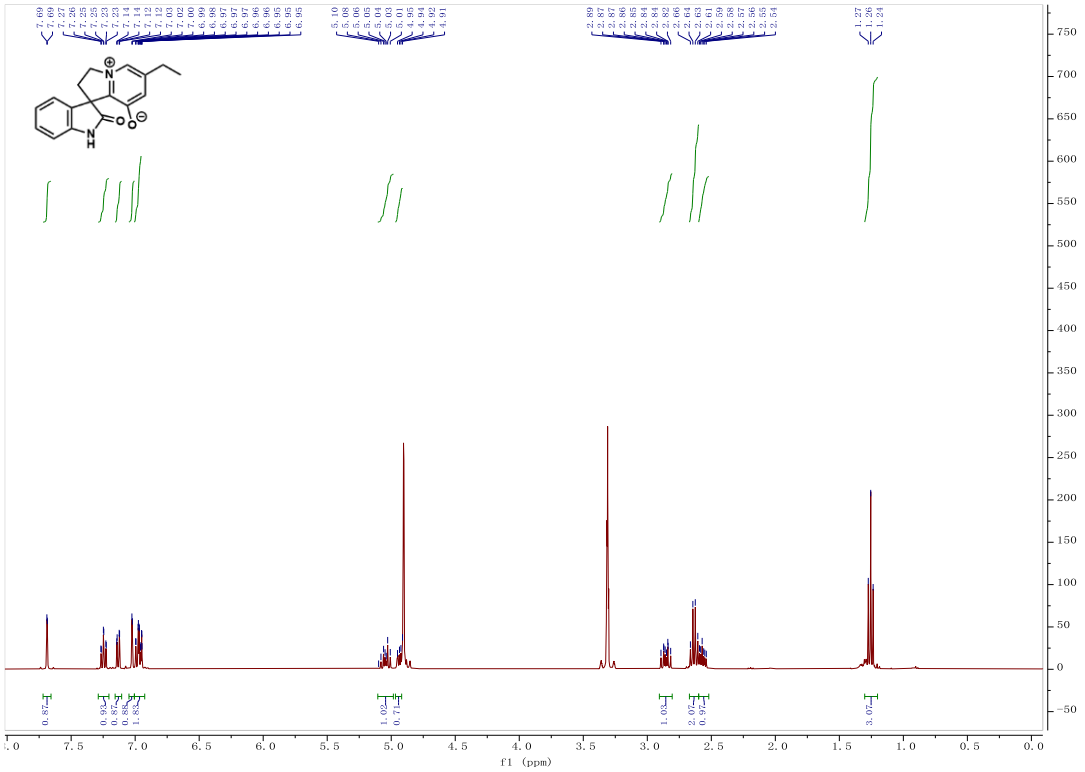
$^{1}$H NMR Spectrum of **3k** (400 MHz, $CD_3OD$):



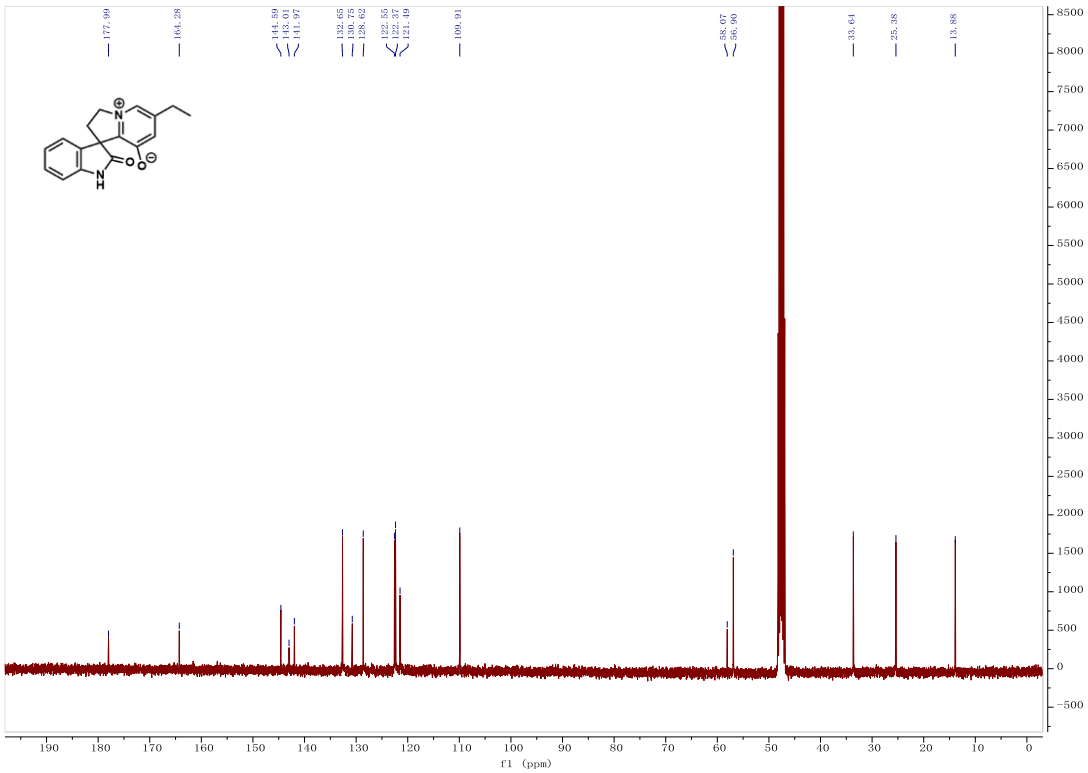
$^{13}$C NMR Spectrum of **3k** (100 MHz, $CD_3OD$):



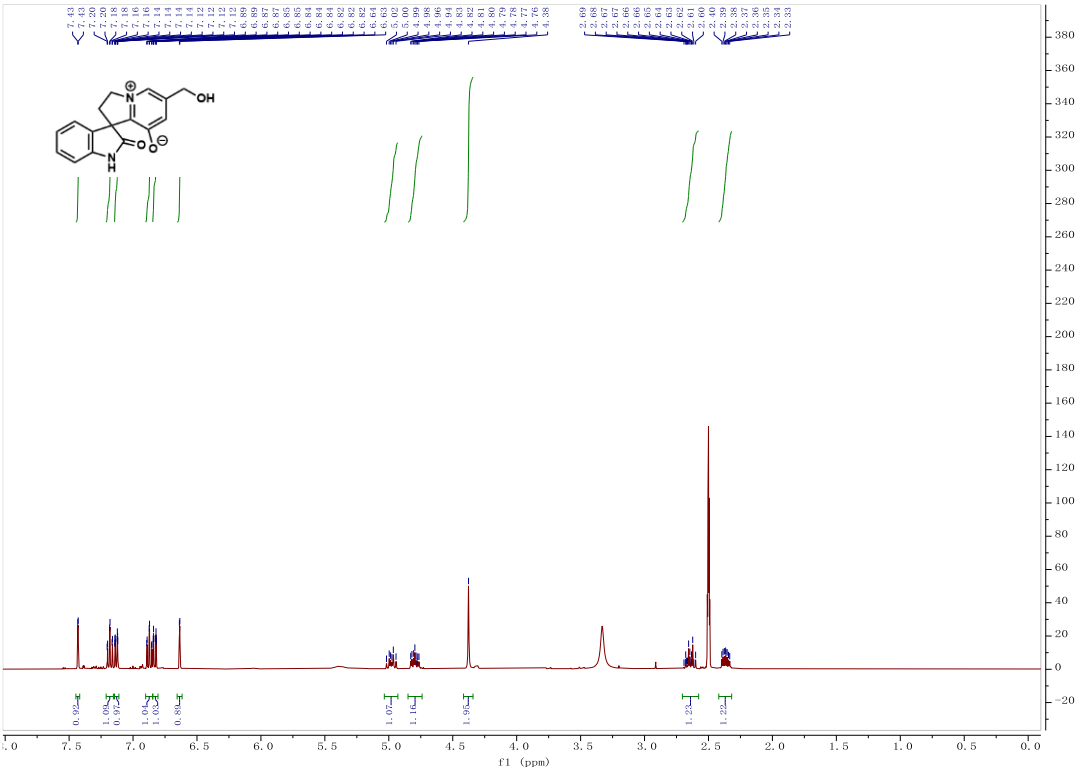
$^{1}$H NMR Spectrum of **3l** (400 MHz, $CD_3OD$):



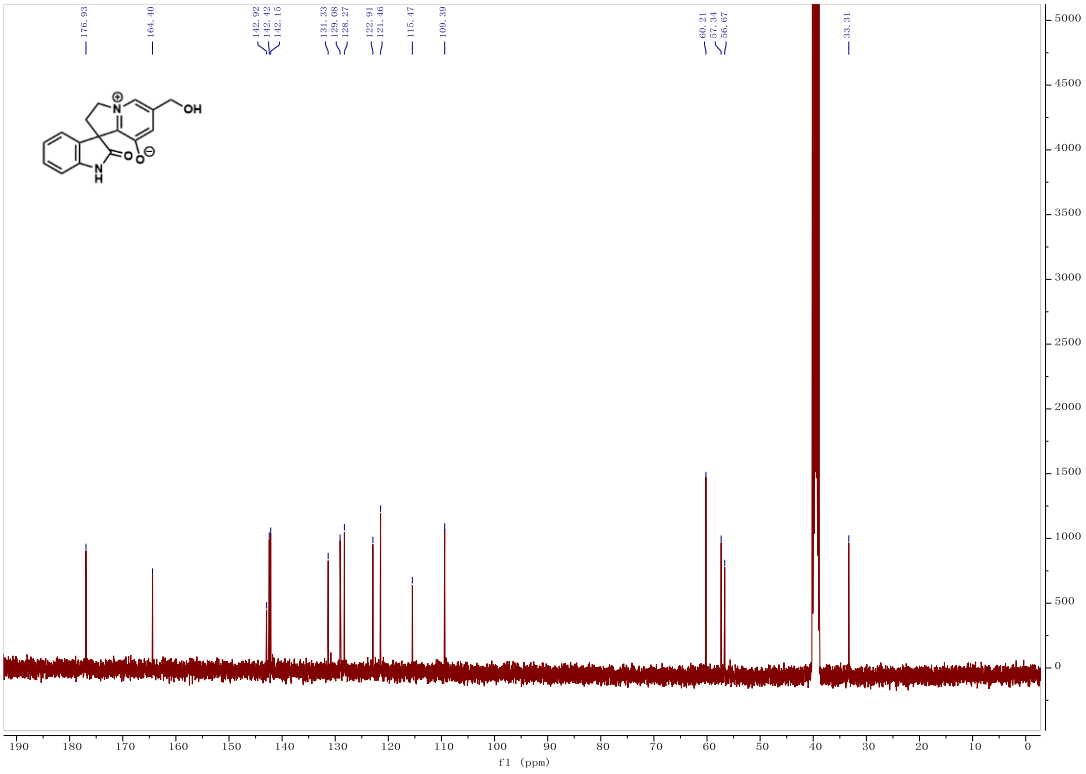
$^{13}$C NMR Spectrum of **3l** (100 MHz, $CD_3OD$):



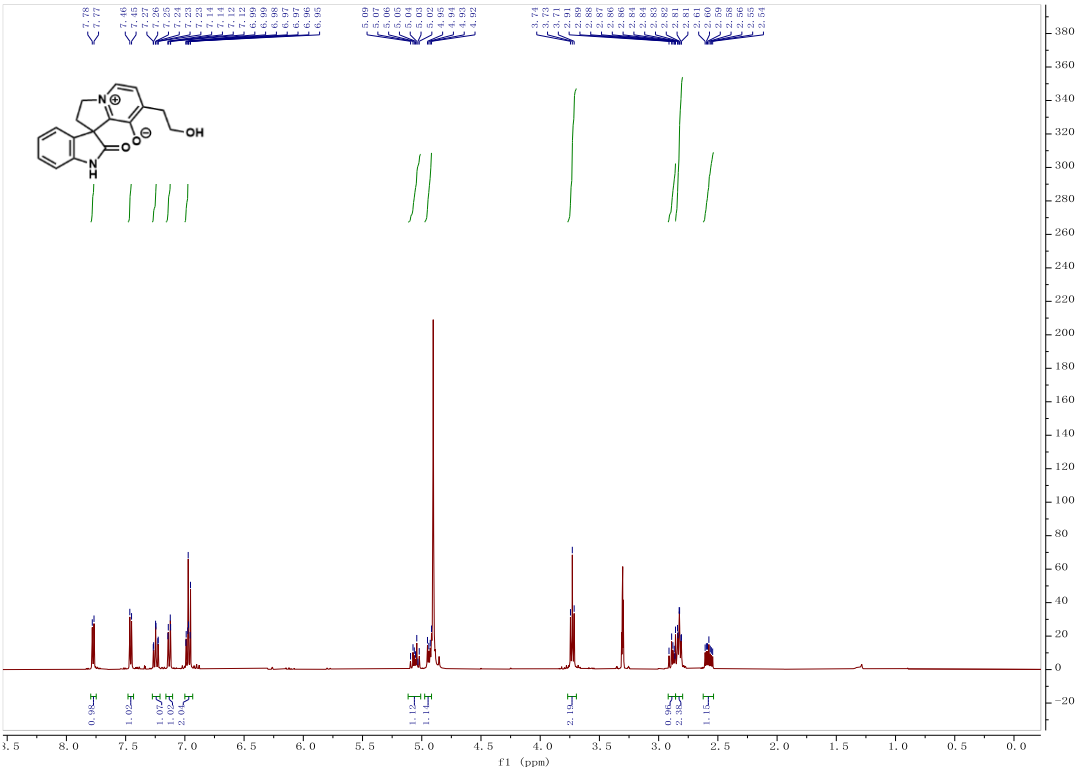
$^{1}$H NMR Spectrum of **3m** (400 MHz, DMSO-$d_6$):



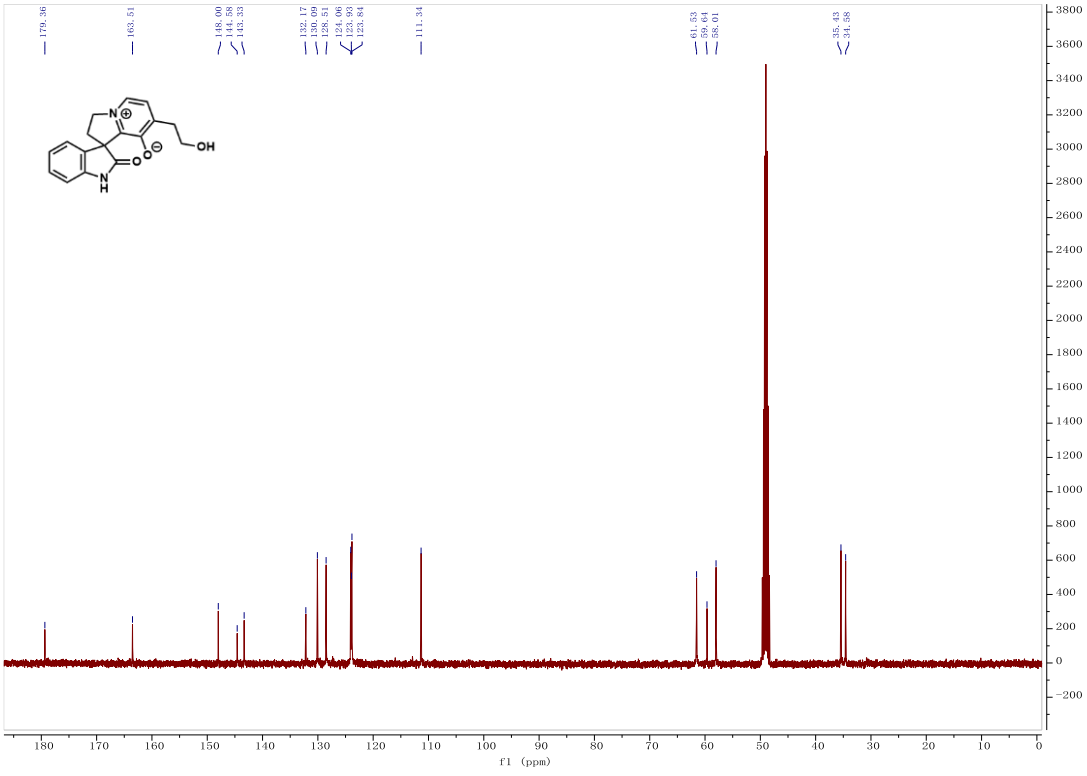
$^{13}$C NMR Spectrum of **3m** (100 MHz, DMSO-$d_6$):



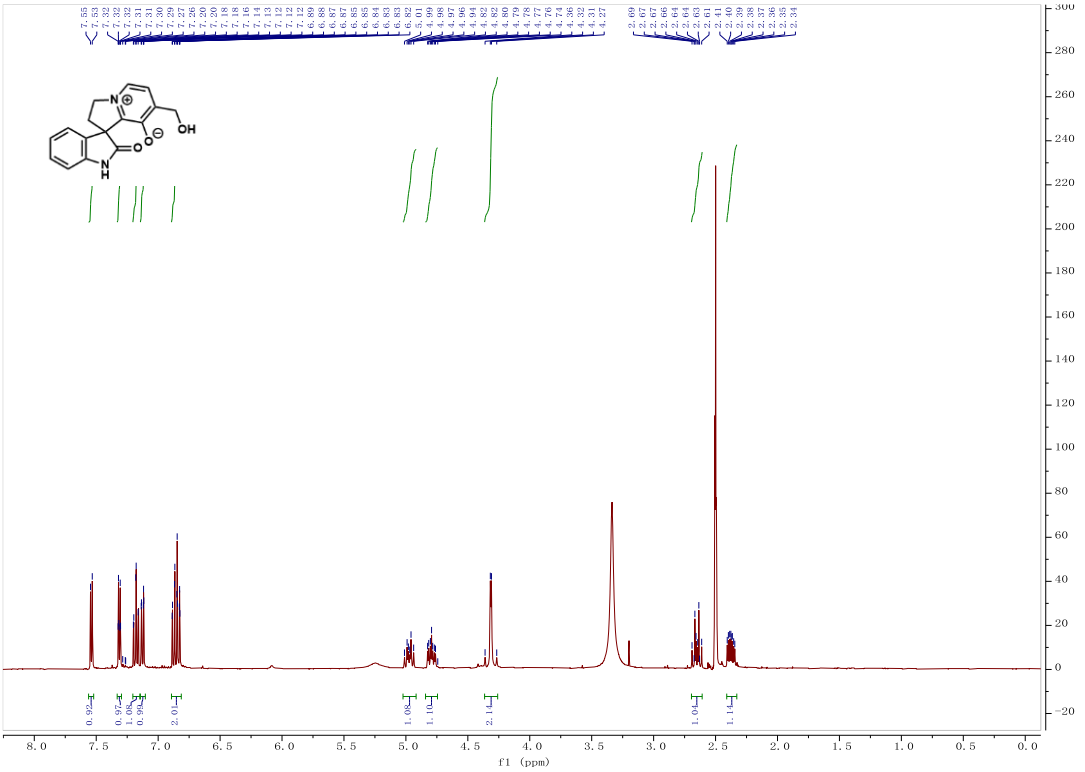
$^{1}$H NMR Spectrum of **3n** (400 MHz, $CD_3OD$):



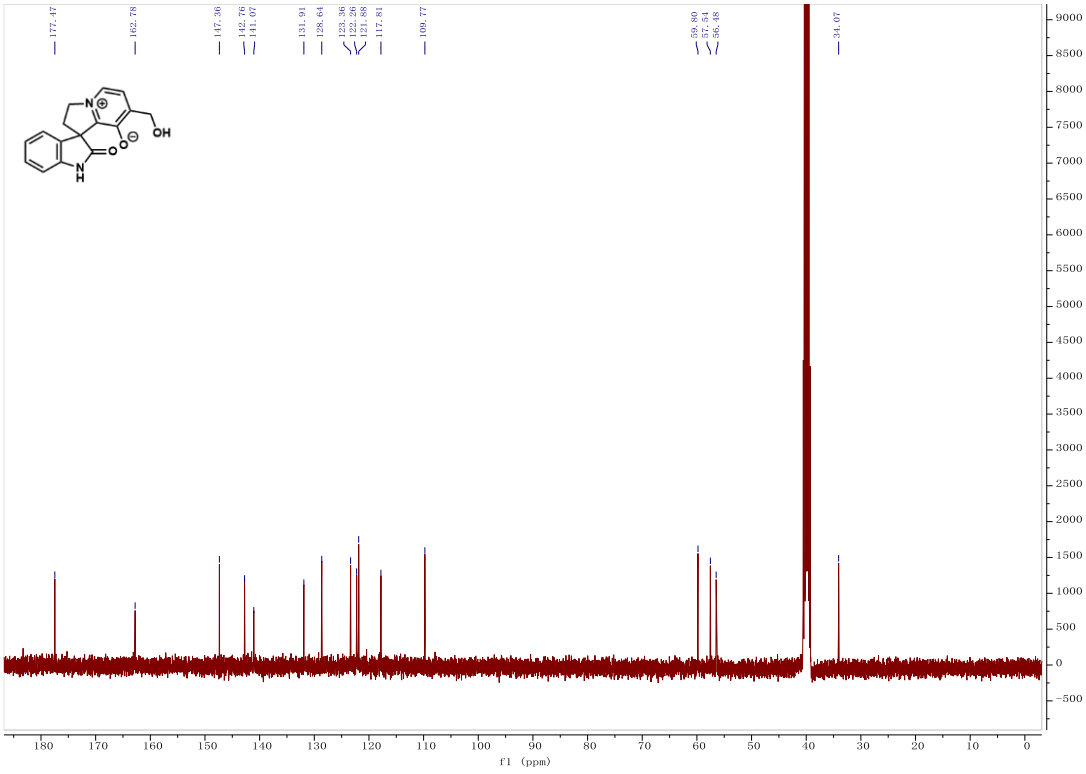
$^{13}$C NMR Spectrum of **3n** (100 MHz, $CD_3OD$):



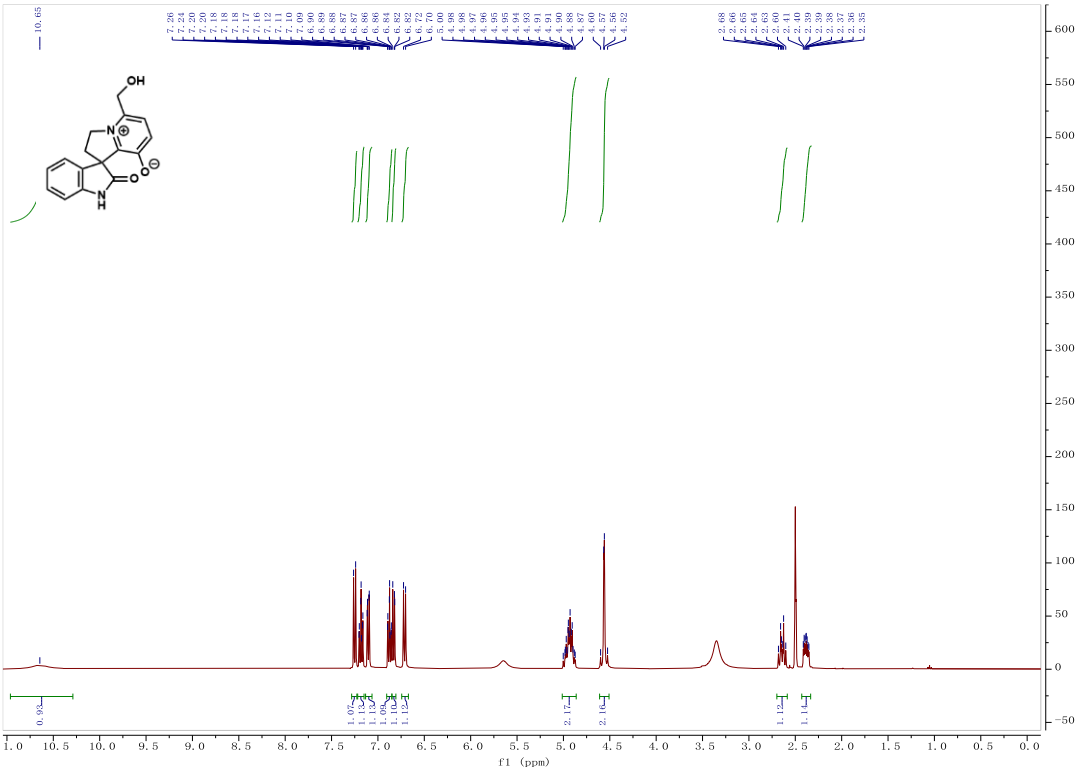
$^{1}$H NMR Spectrum of **3o** (400 MHz, DMSO-$d_6$):



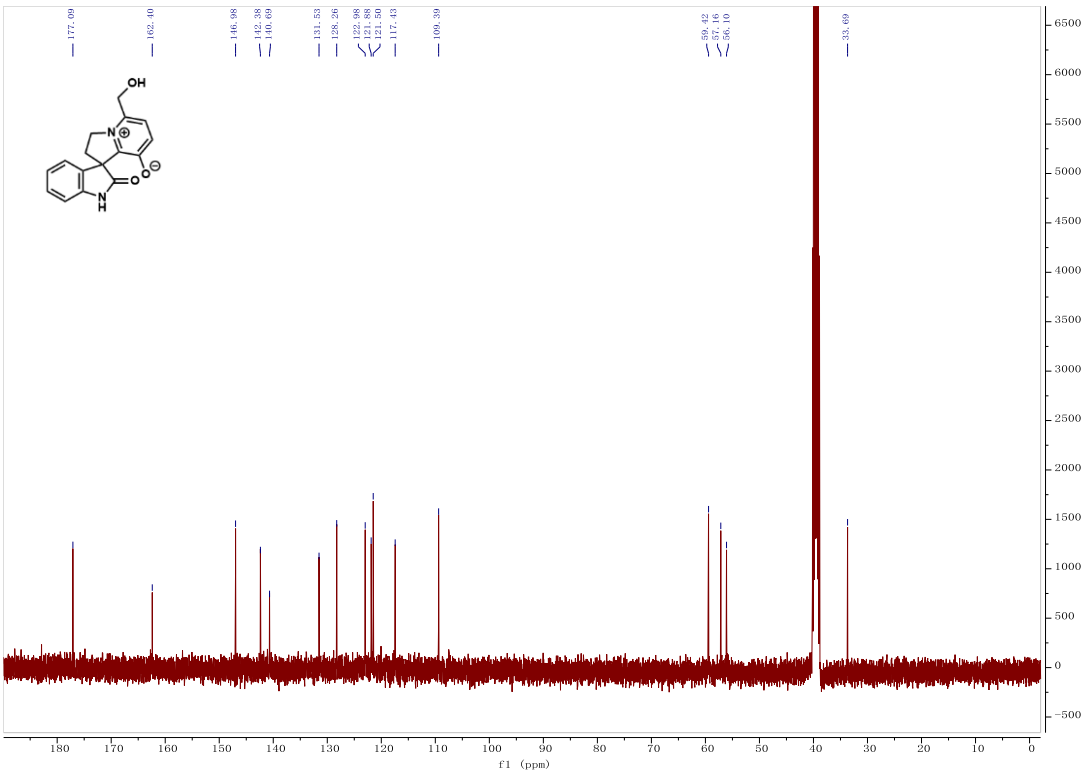
$^{13}$C NMR Spectrum of **3o** (100 MHz, DMSO-$d_6$):



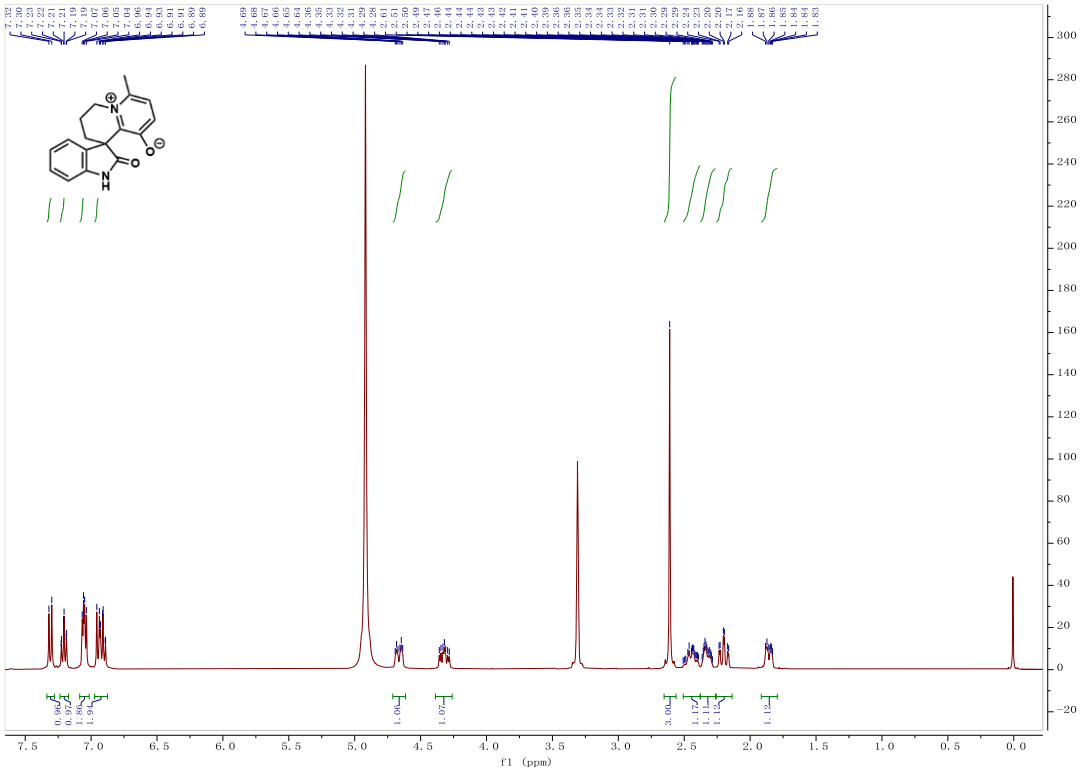
$^{1}$H NMR Spectrum of **3p** (400 MHz, DMSO-$d_6$):



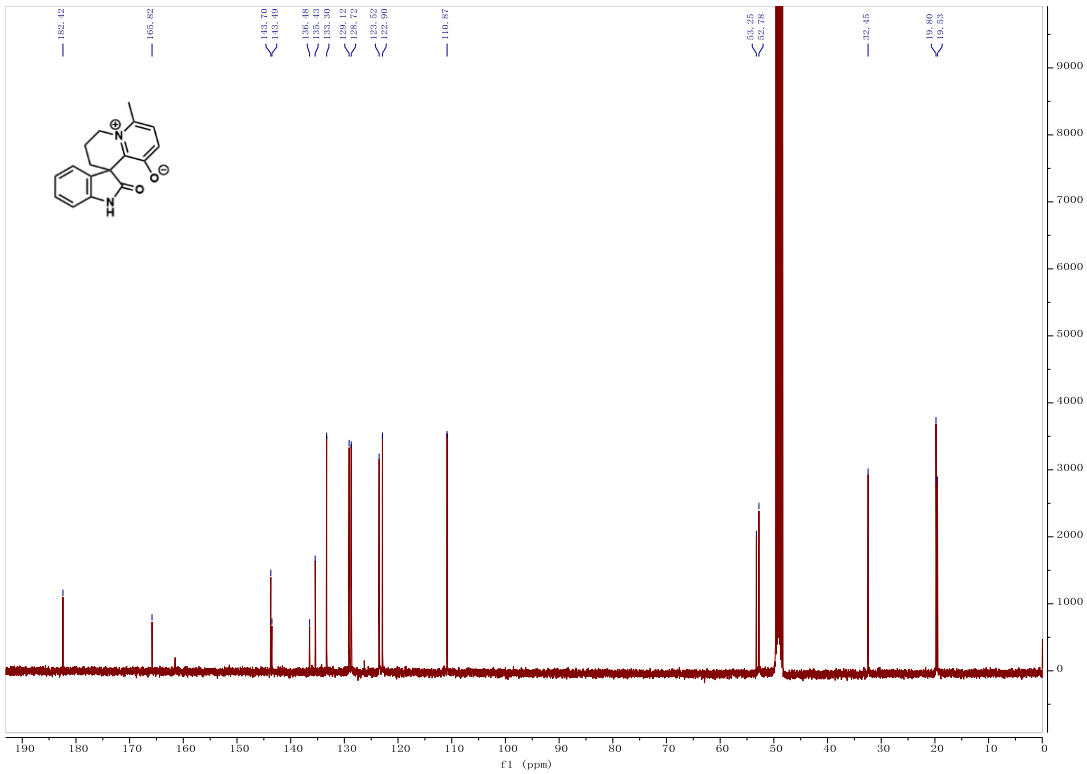
$^{13}$C NMR Spectrum of **3p** (100 MHz, DMSO-$d_6$):



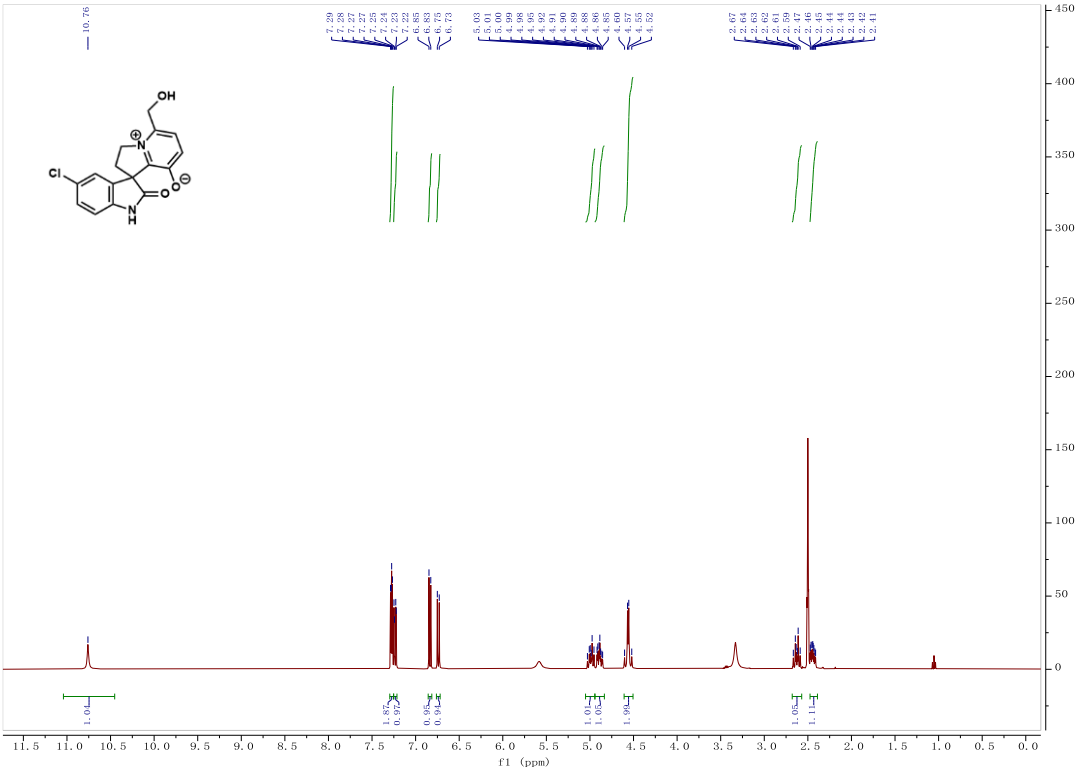
$^{1}$H NMR Spectrum of **3q** (400 MHz, $CD_3OD$):



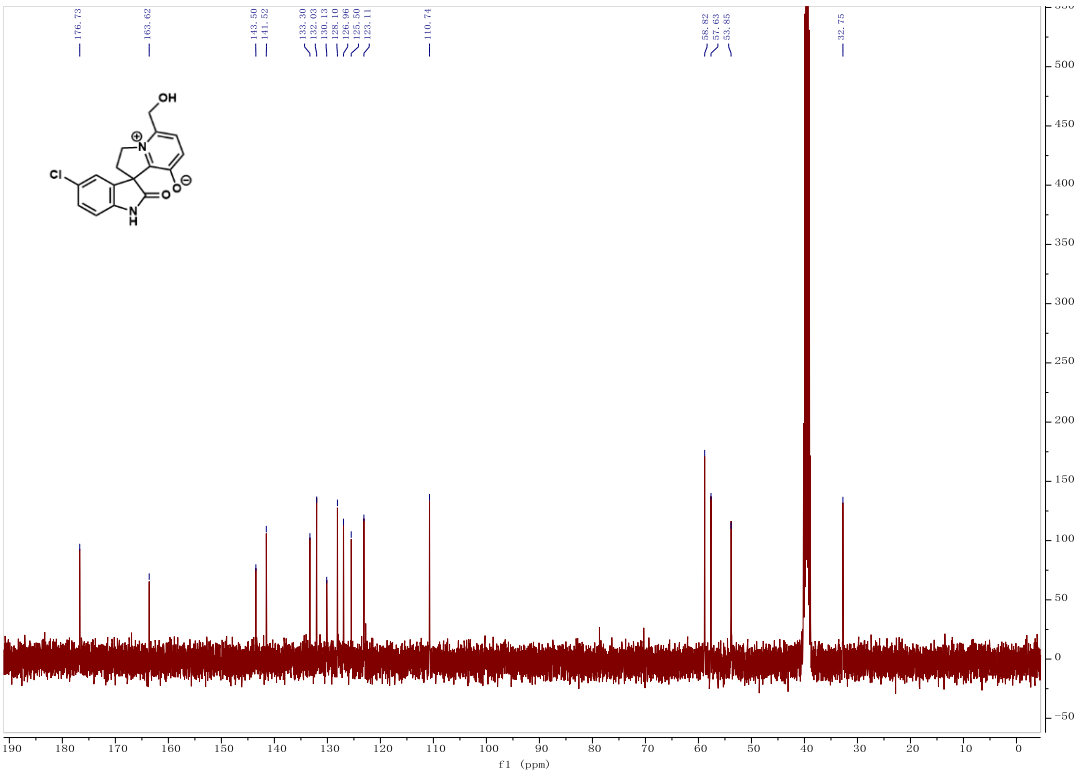
$^{13}$C NMR Spectrum of **3q** (100 MHz, $CD_3OD$):



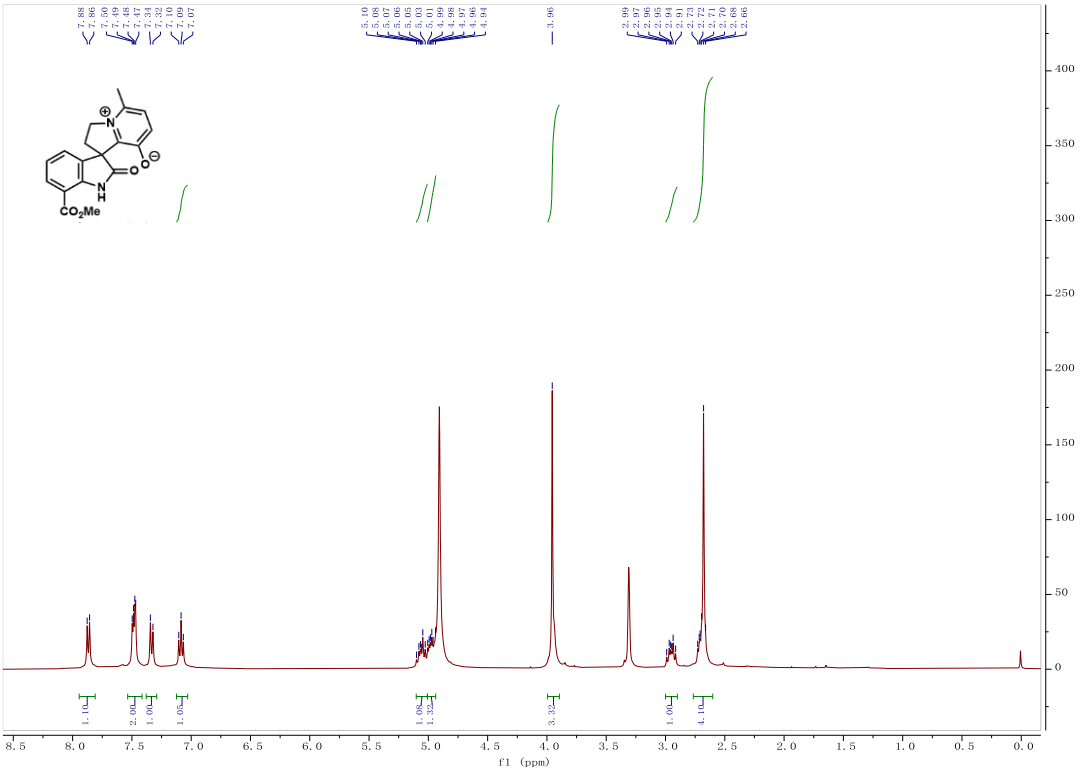
$^{1}$H NMR Spectrum of **3r** (400 MHz, DMSO-$d_6$):



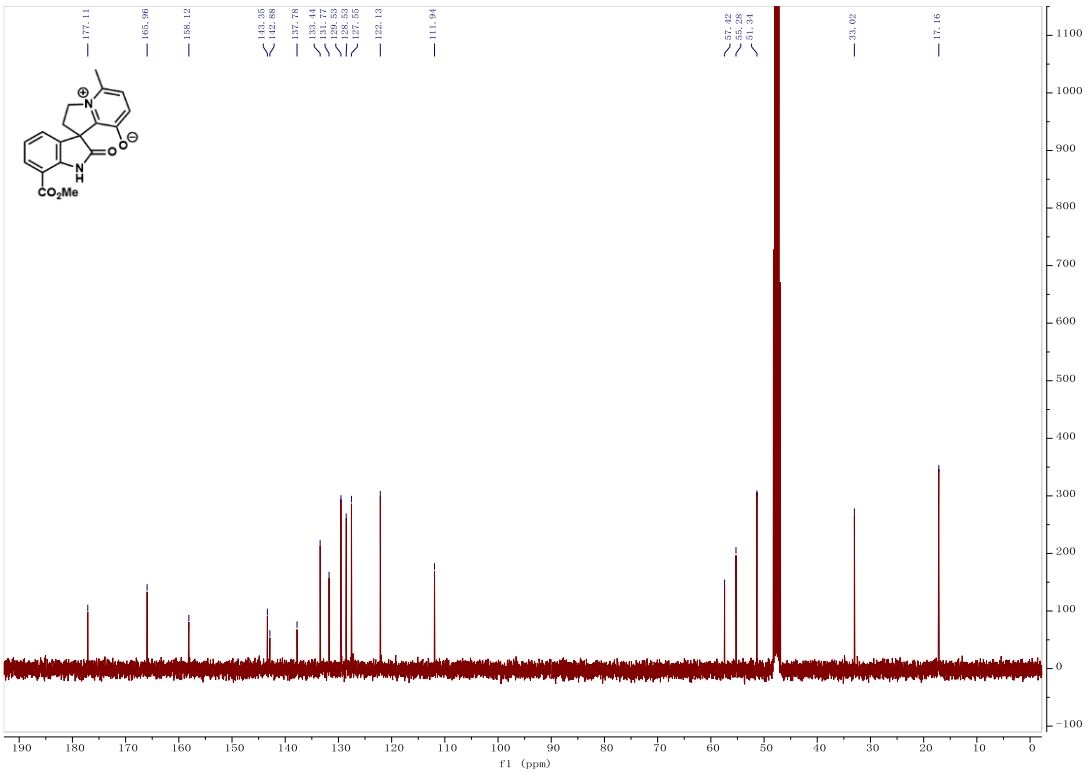
$^{13}$C NMR Spectrum of **3r** (100 MHz, DMSO-$d_6$):



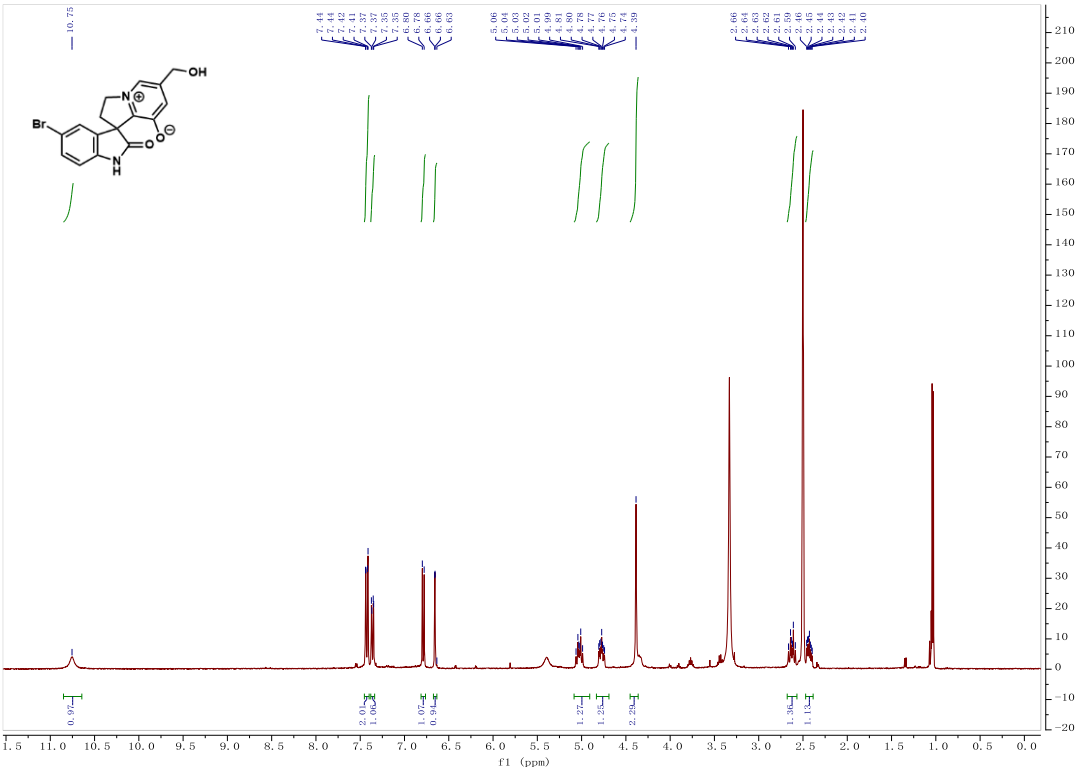
$^{1}$H NMR Spectrum of **3s** (400 MHz, $CD_3OD$):



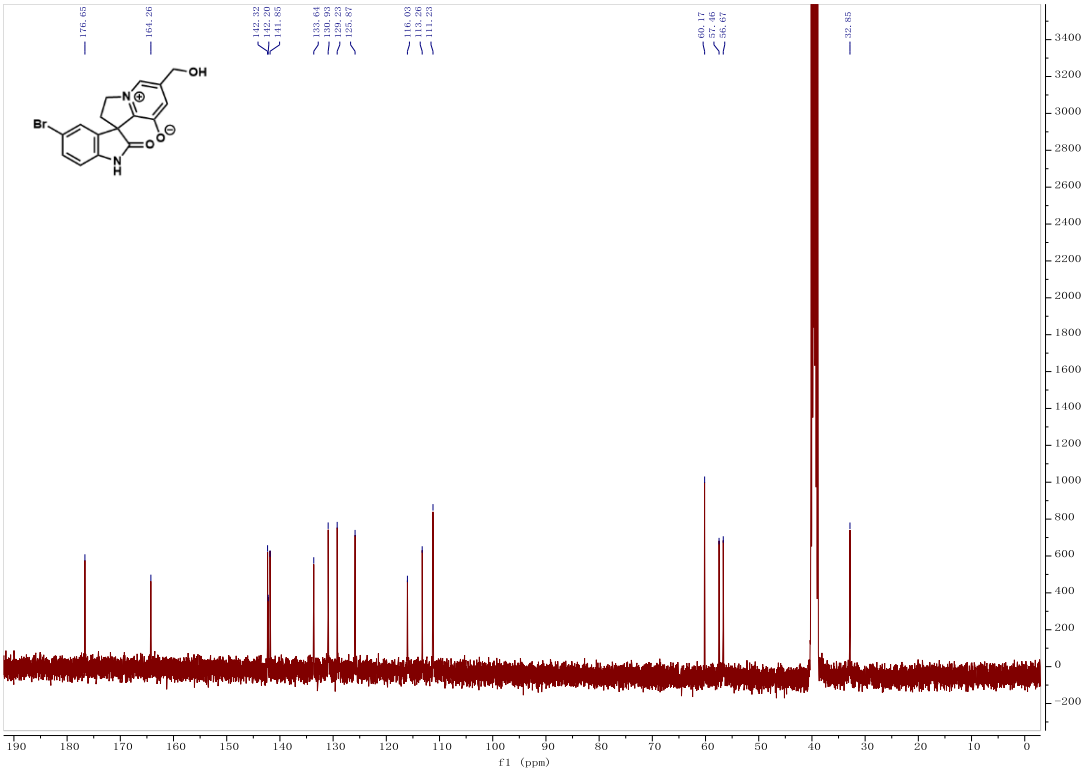
$^{13}$C NMR Spectrum of **3s** (100 MHz, $CD_3OD$):



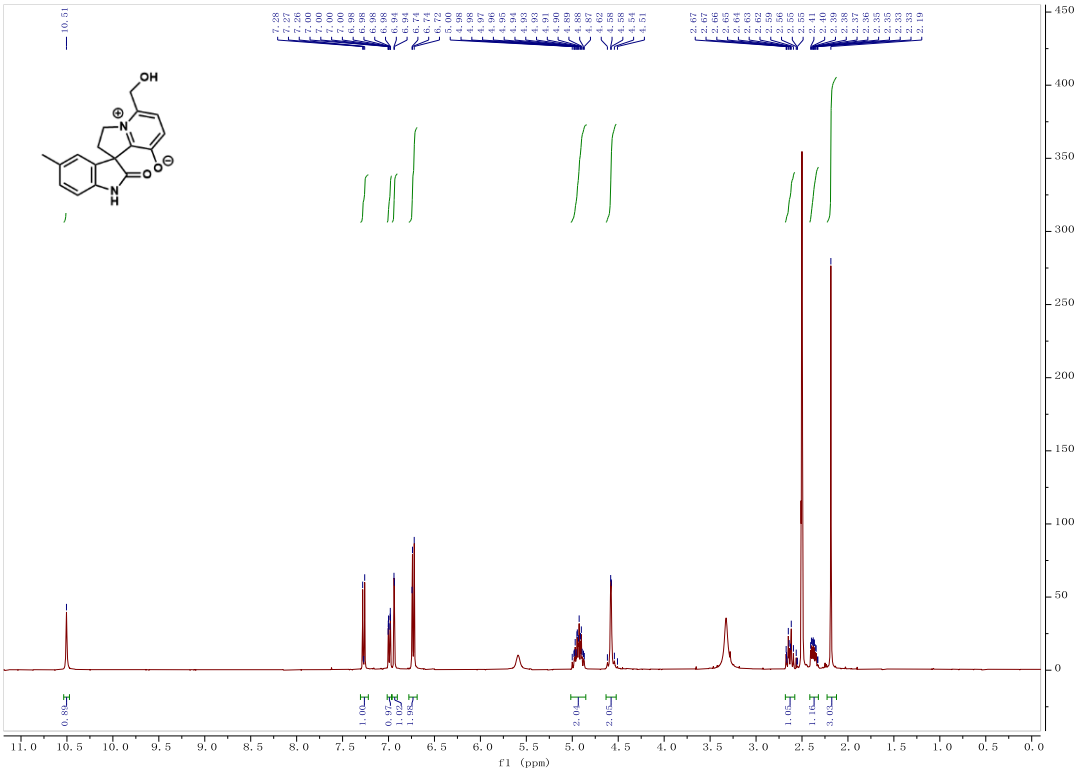
$^{1}$H NMR Spectrum of **3t** (400 MHz, DMSO-$d_6$):



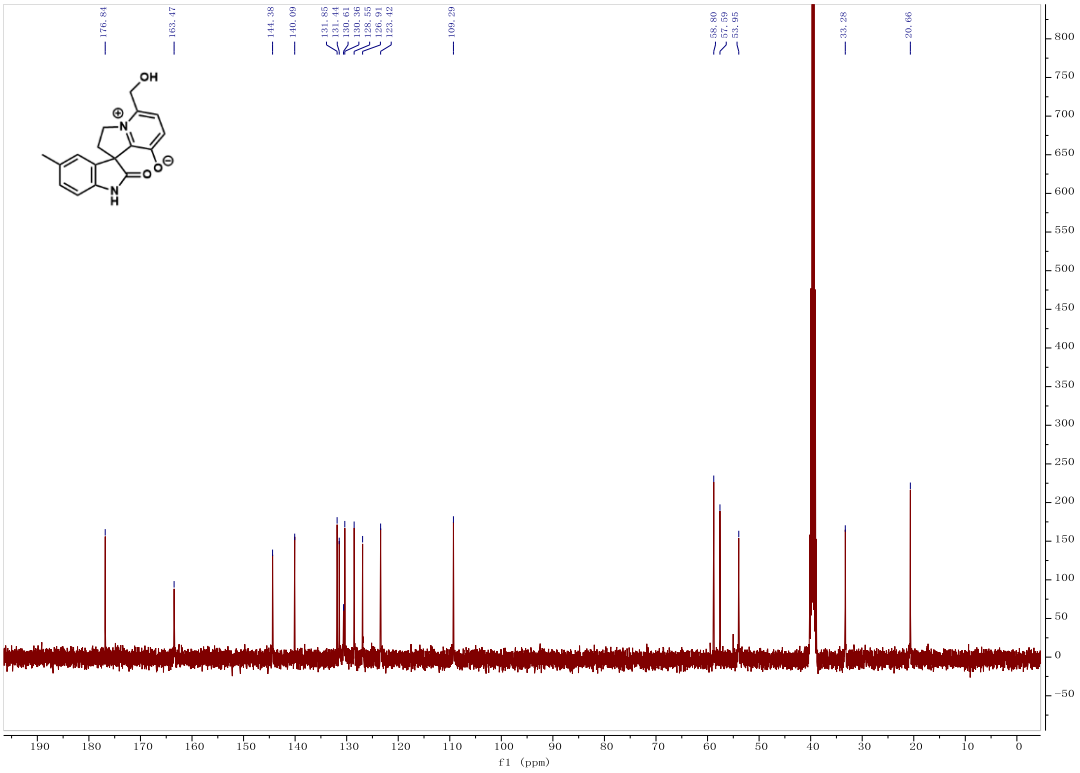
$^{13}$C NMR Spectrum of **3t** (100 MHz, DMSO-$d_6$):



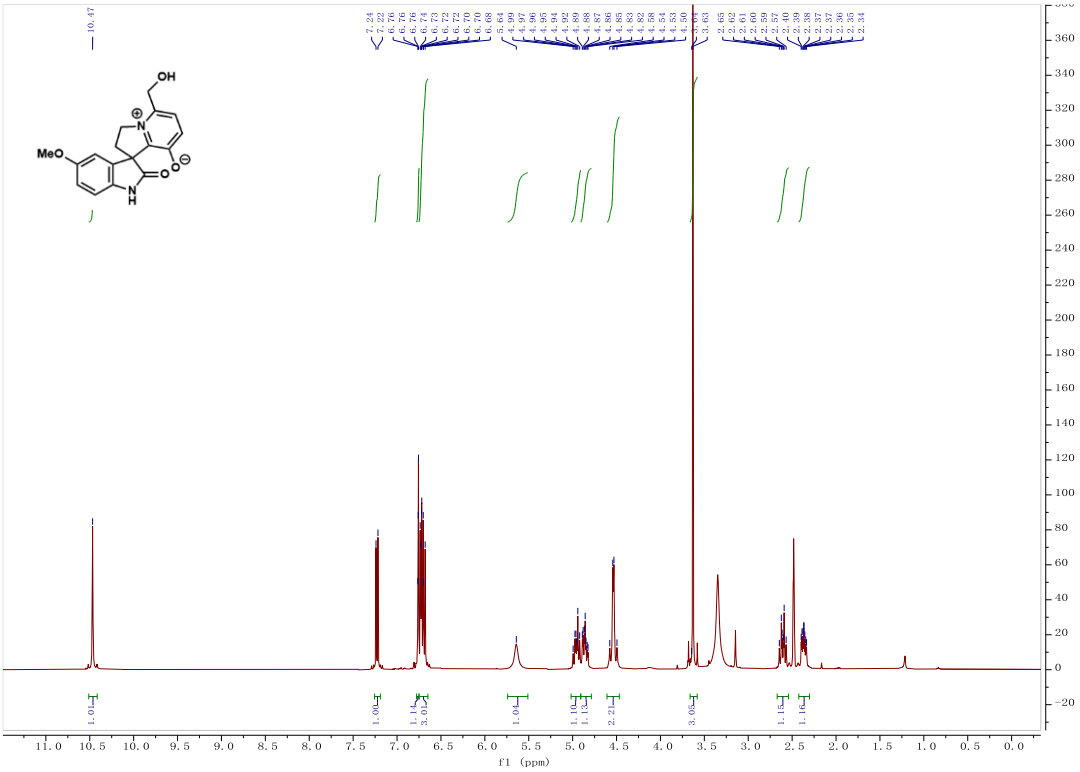
$^{1}$H NMR Spectrum of **3u** (400 MHz, DMSO-$d_6$):



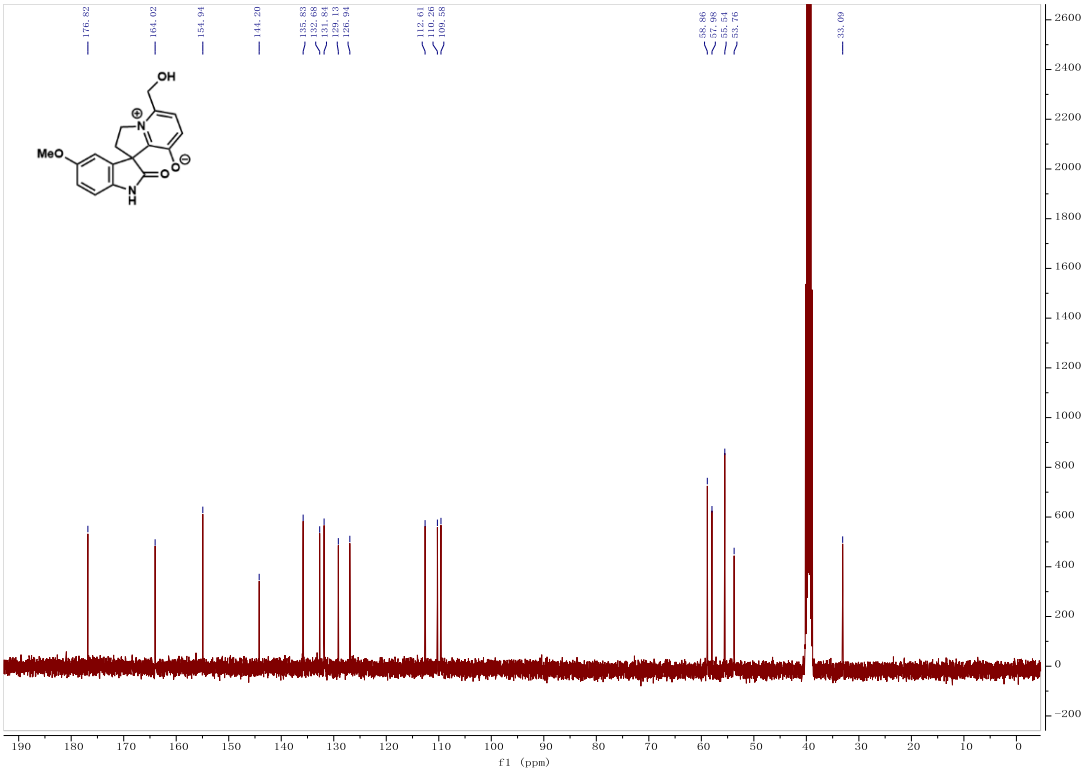
$^{13}$C NMR Spectrum of **3u** (100 MHz, DMSO-$d_6$):



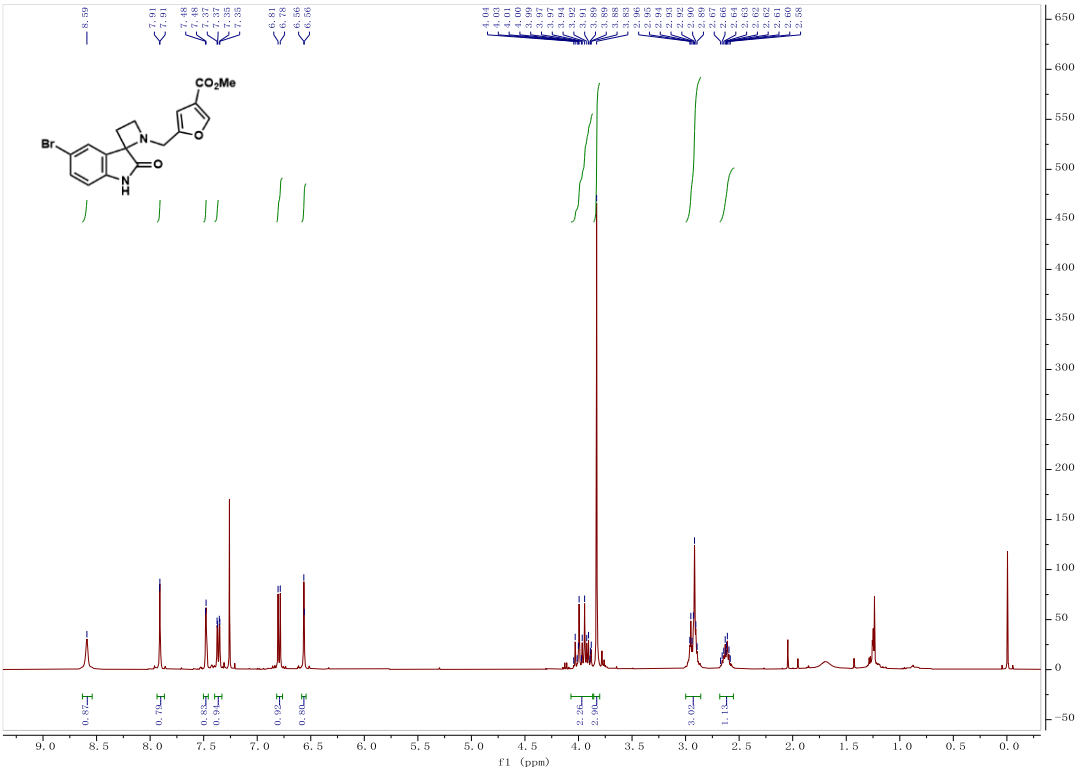
$^{1}$H NMR Spectrum of **3v** (400 MHz, DMSO-$d_6$):



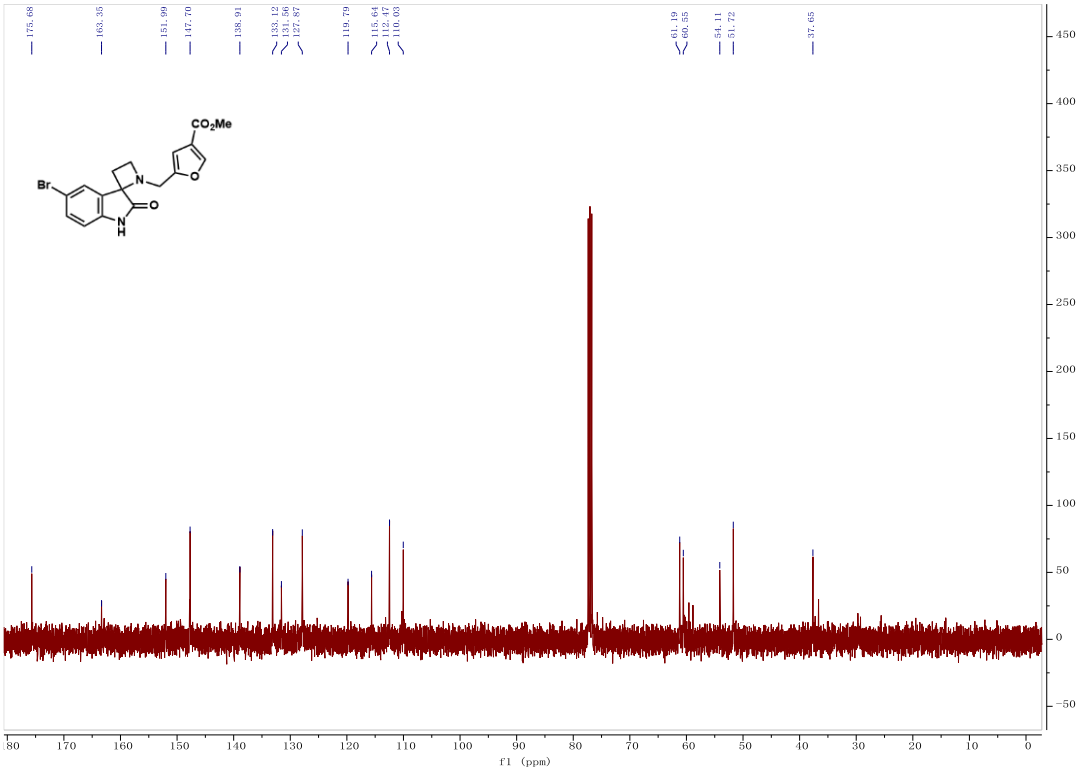

$^{13}$C NMR Spectrum of **3v** (100 MHz, DMSO-$d_6$):



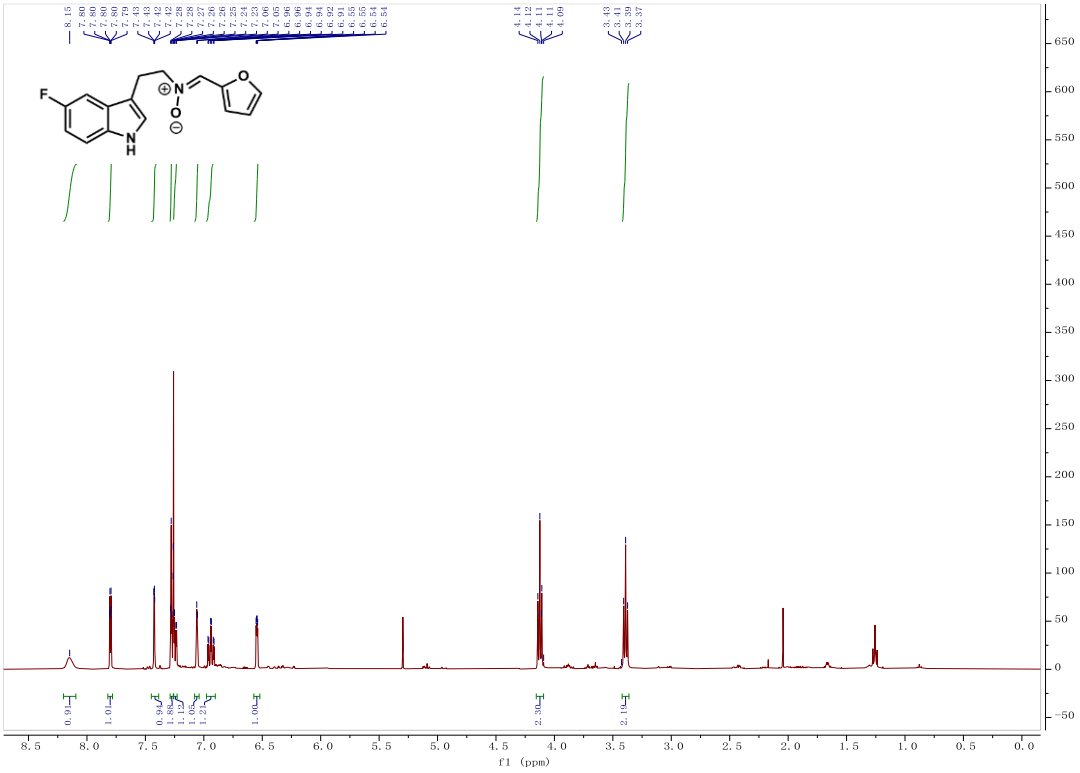
$^{1}$H NMR Spectrum of **3w** (400 MHz, $CDCl_3$):



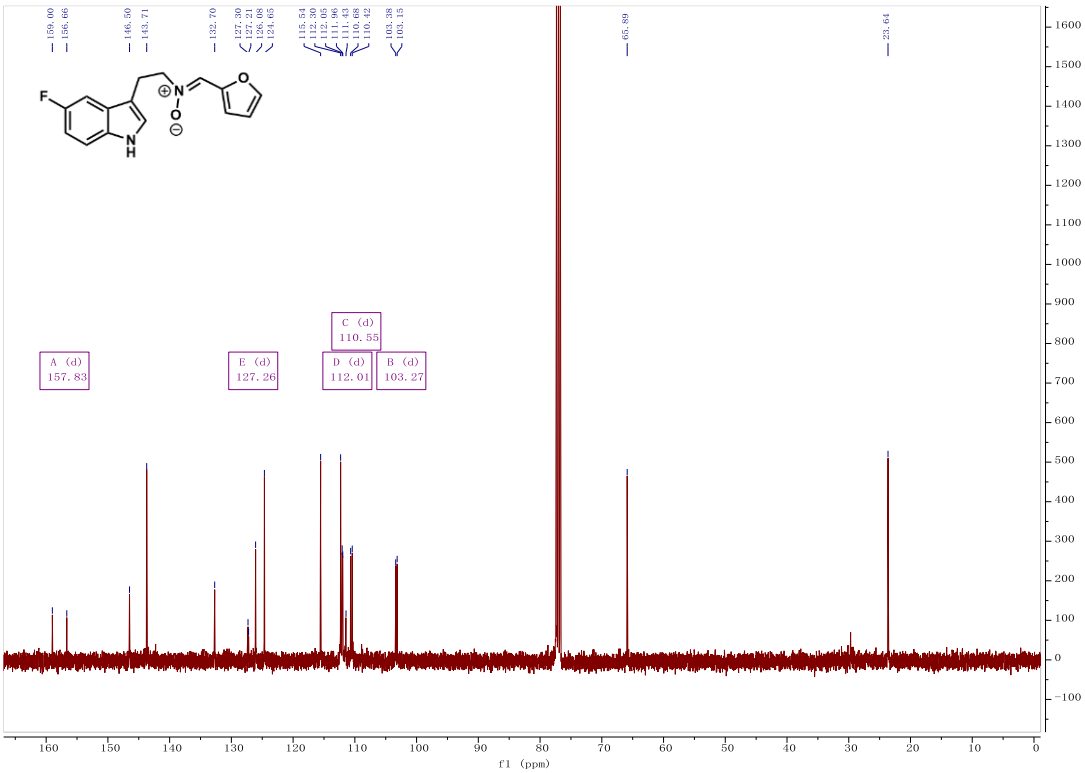
$^{13}$C NMR Spectrum of **3w** (100 MHz, $CDCl_3$):



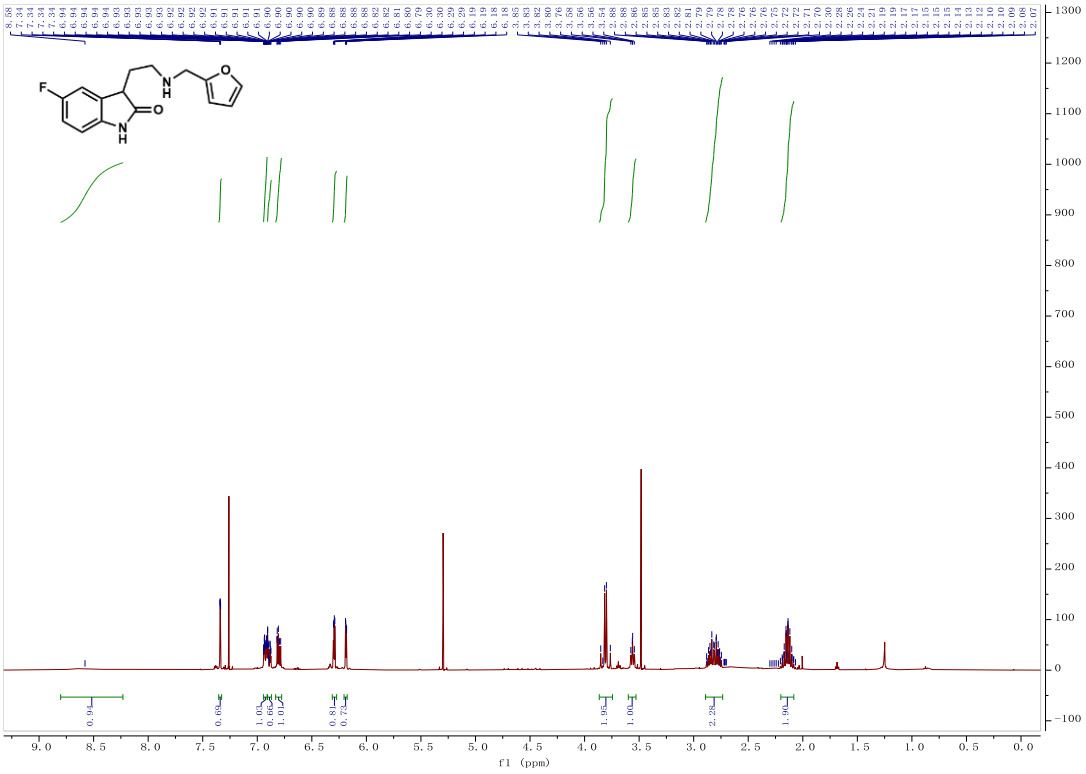
$^{1}$H NMR Spectrum of **5** (400 MHz, $CDCl_3$):



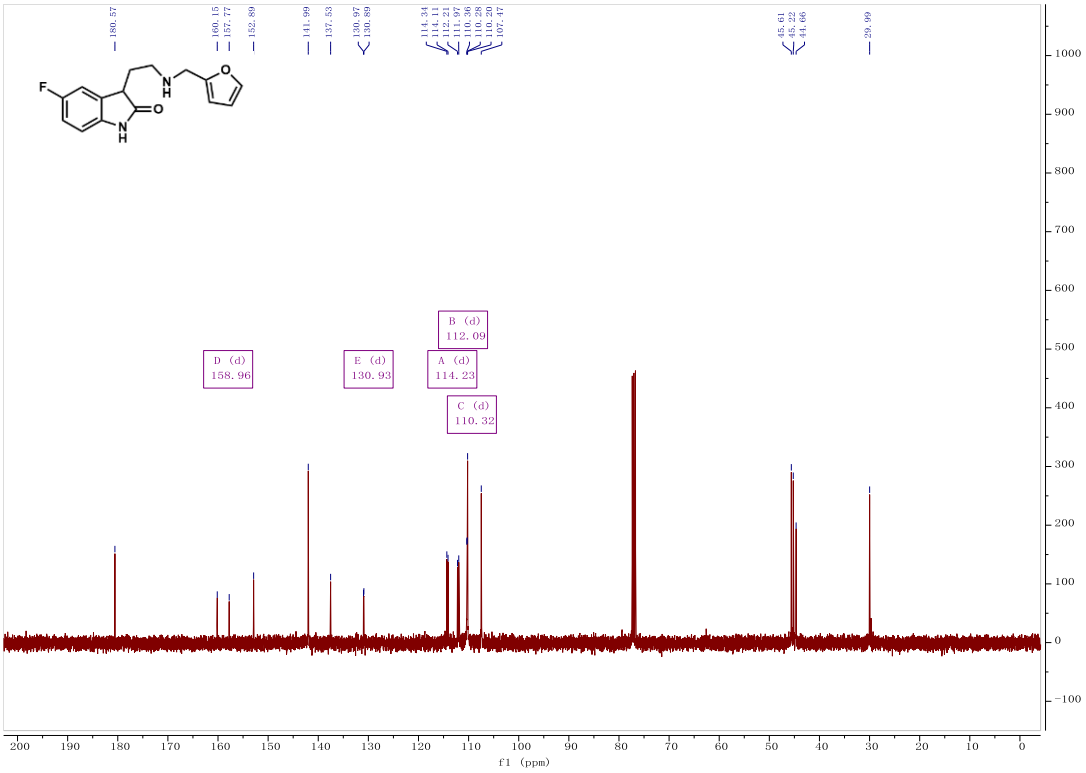
$^{13}$C NMR Spectrum of **5** (100 MHz, $CDCl_3$):



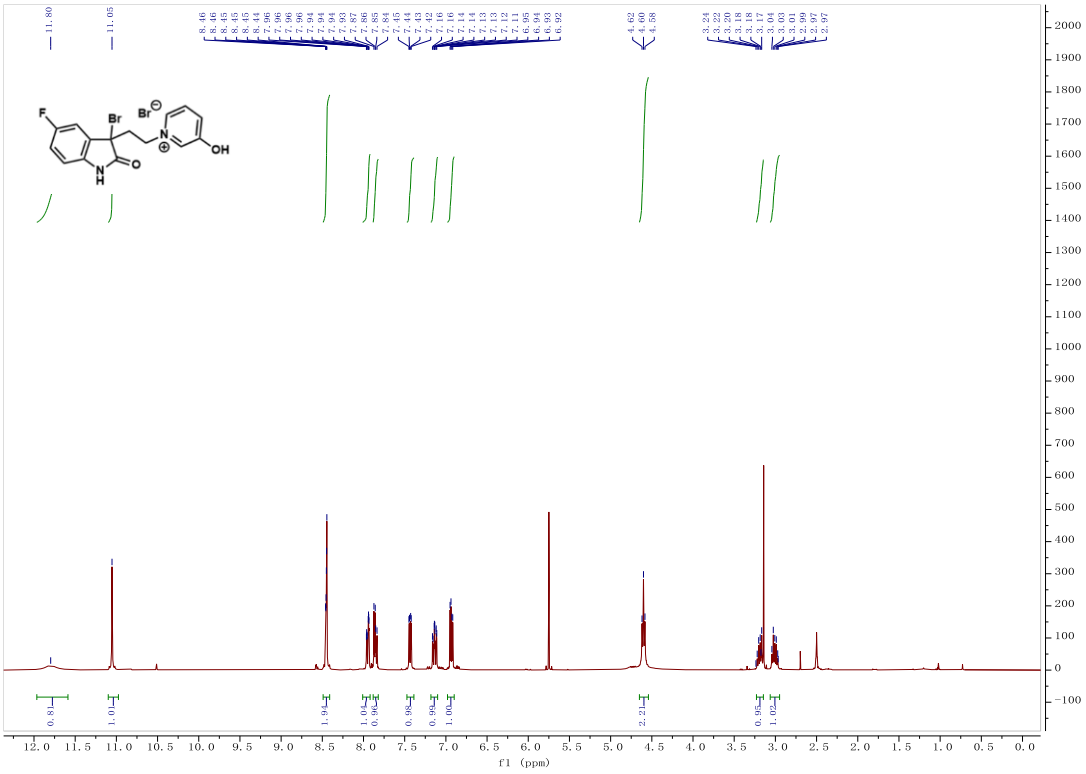
$^{1}$H NMR Spectrum of **6** (400 MHz, $CDCl_3$):



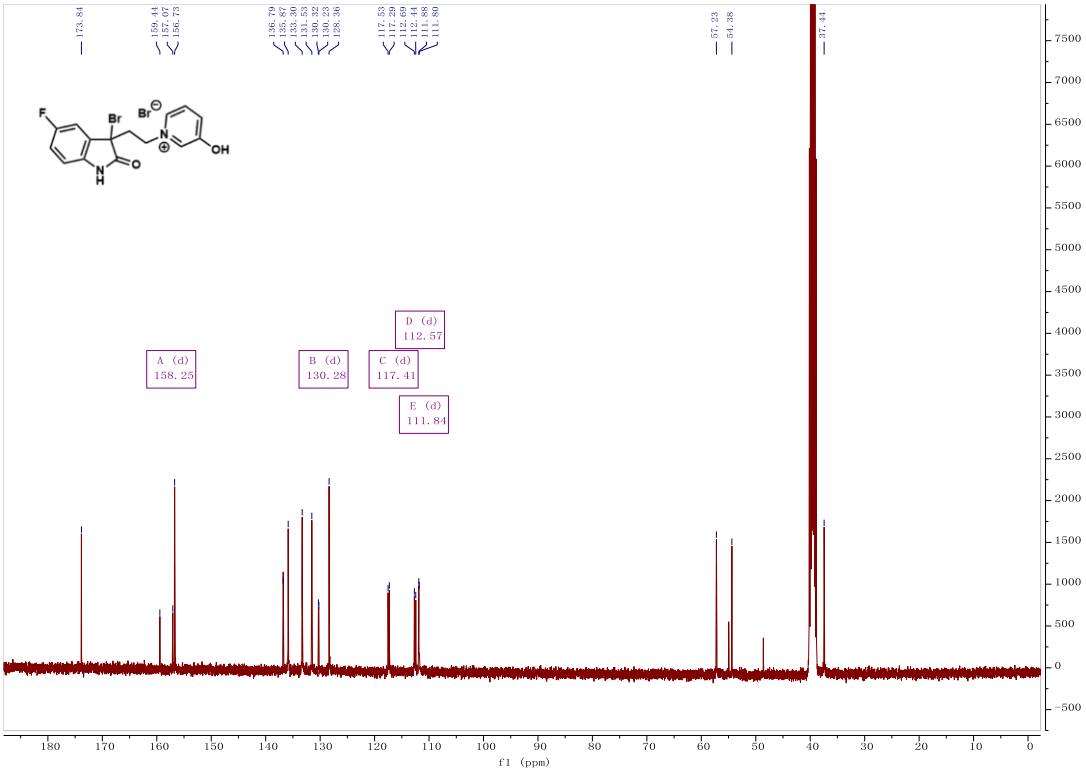

$^{13}$C NMR Spectrum of **6** (100 MHz, $CDCl_3$):



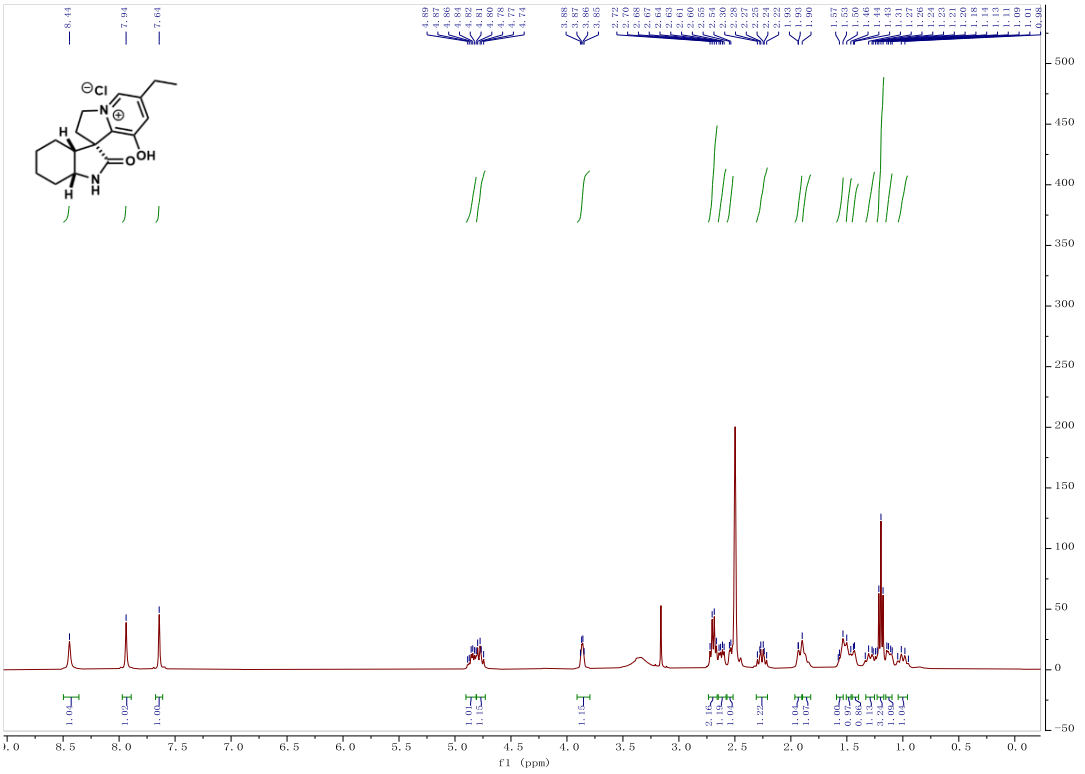
$^{1}$H NMR Spectrum of **2a** (400 MHz, DMSO-$d_6$):



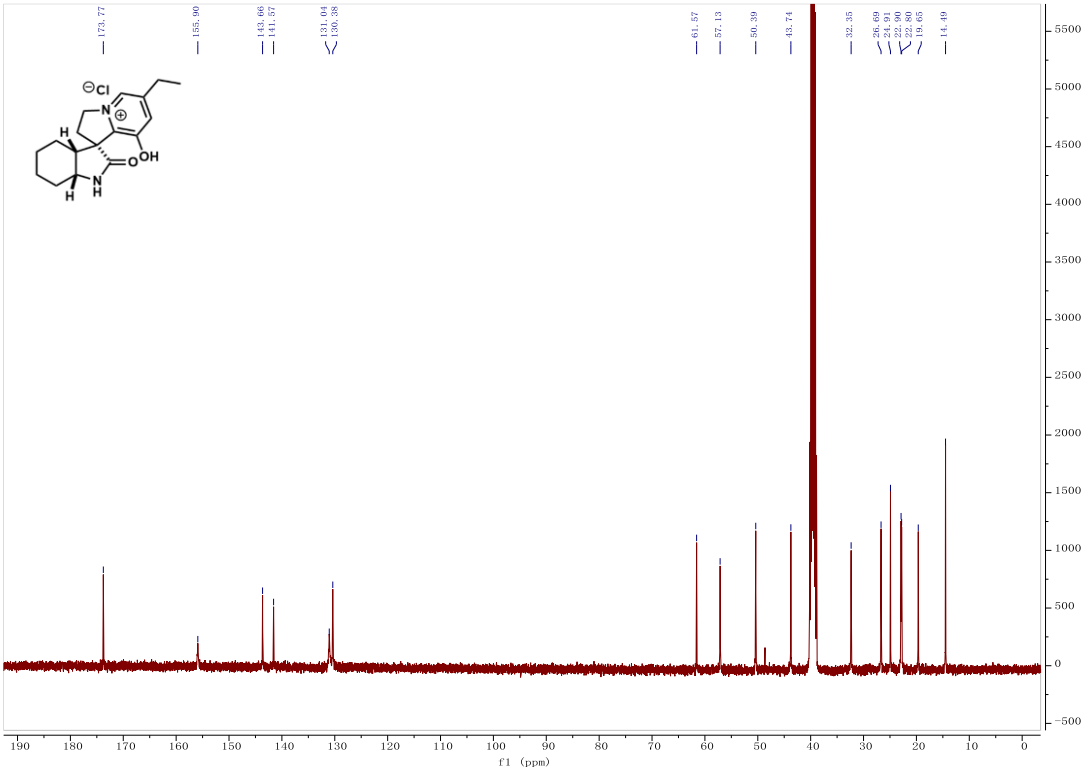
$^{13}$C NMR Spectrum of **2a** (100 MHz, DMSO-$d_6$):



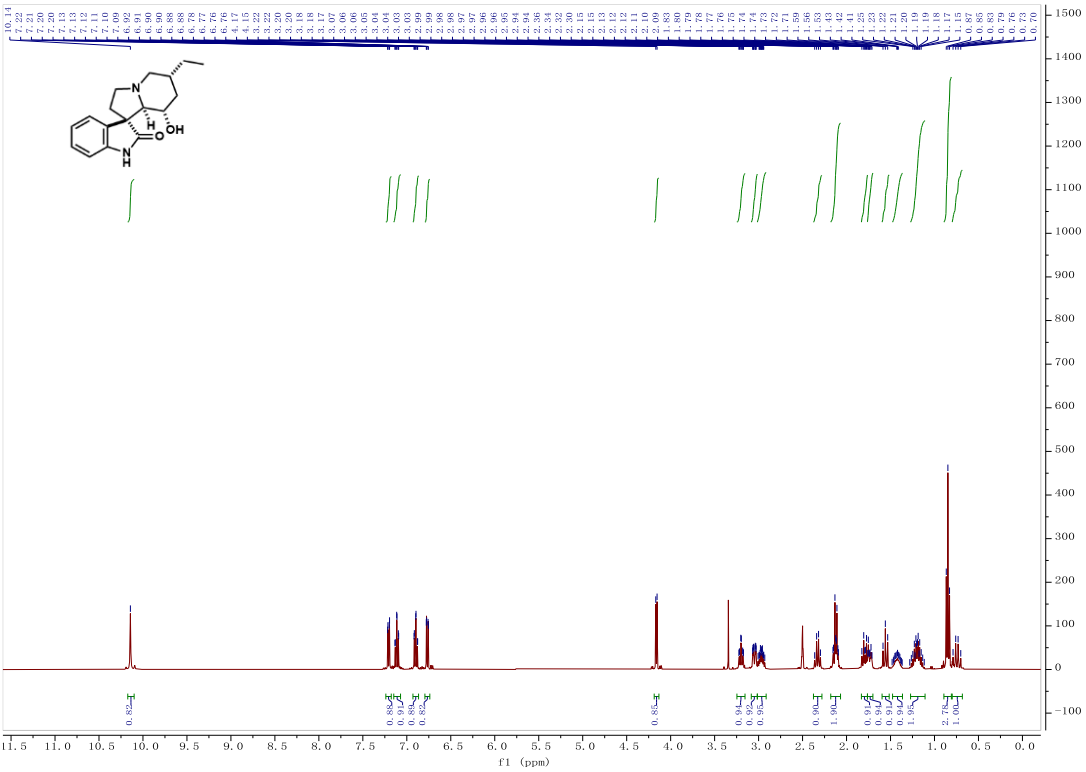
$^{1}$H NMR Spectrum of **7** (400 MHz, DMSO-$d_6$):



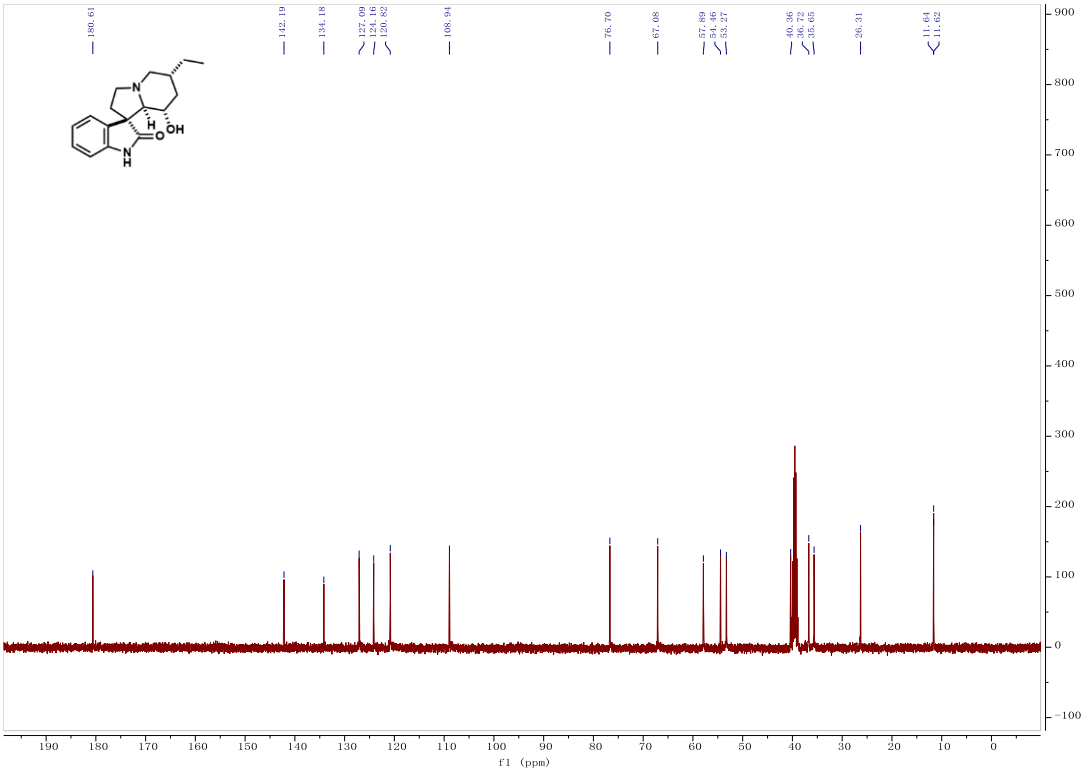
$^{13}$C NMR Spectrum of **7** (100 MHz, DMSO-$d_6$):



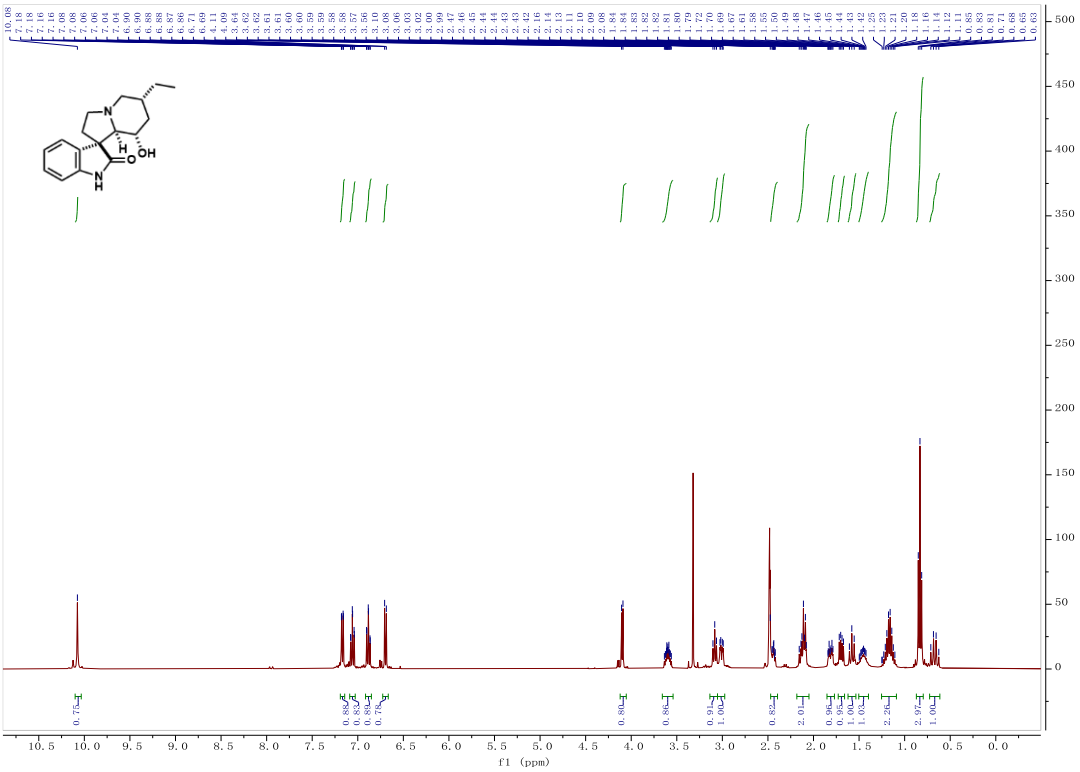
$^{1}$H NMR Spectrum of **8** (400 MHz, DMSO-$d_6$):



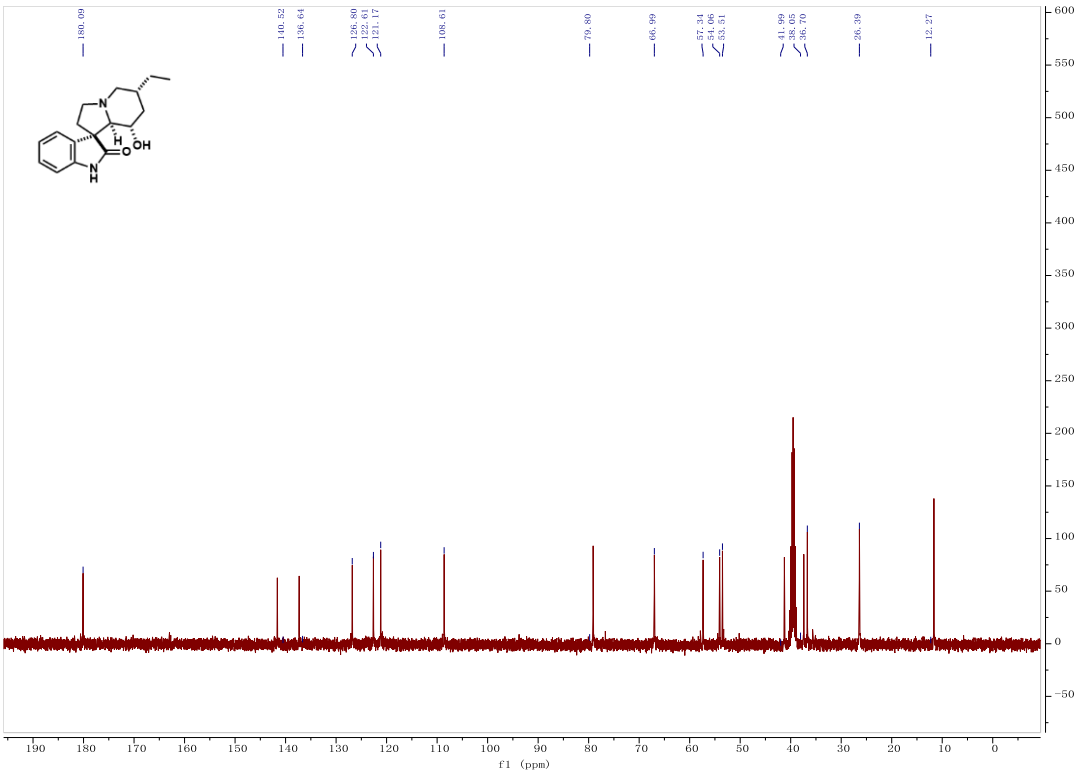
$^{13}$C NMR Spectrum of **8** (100 MHz, DMSO-$d_6$):



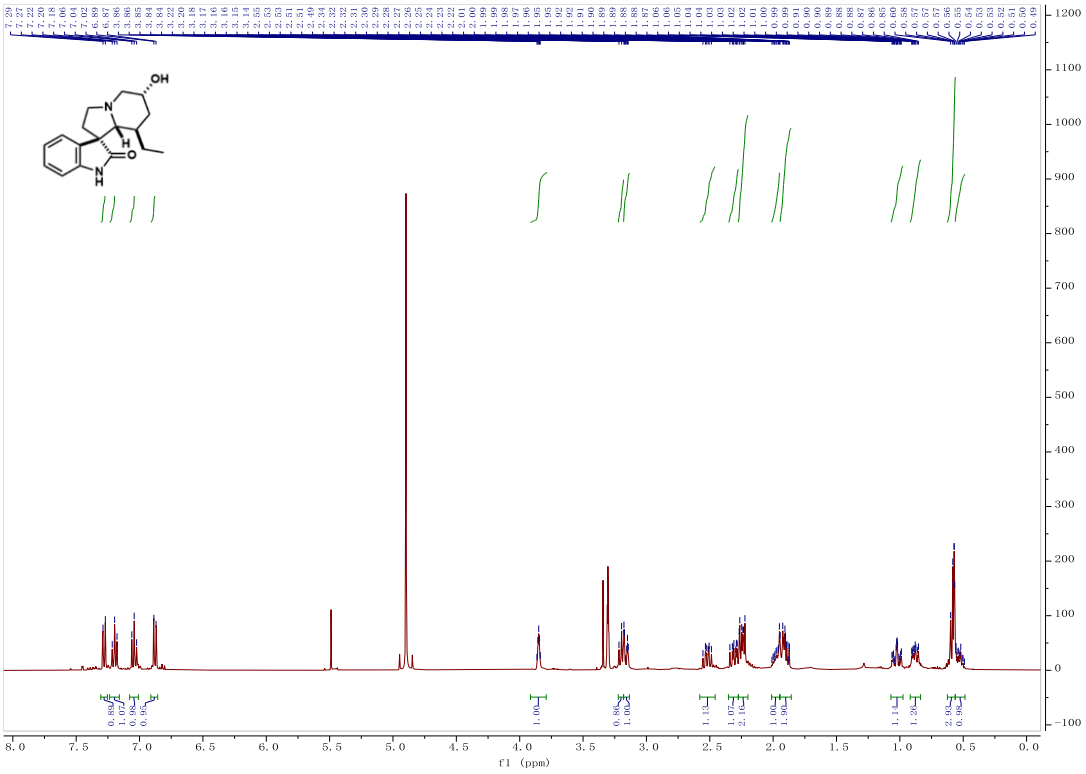
$^{1}$H NMR Spectrum of **9** (400 MHz, DMSO-$d_6$):



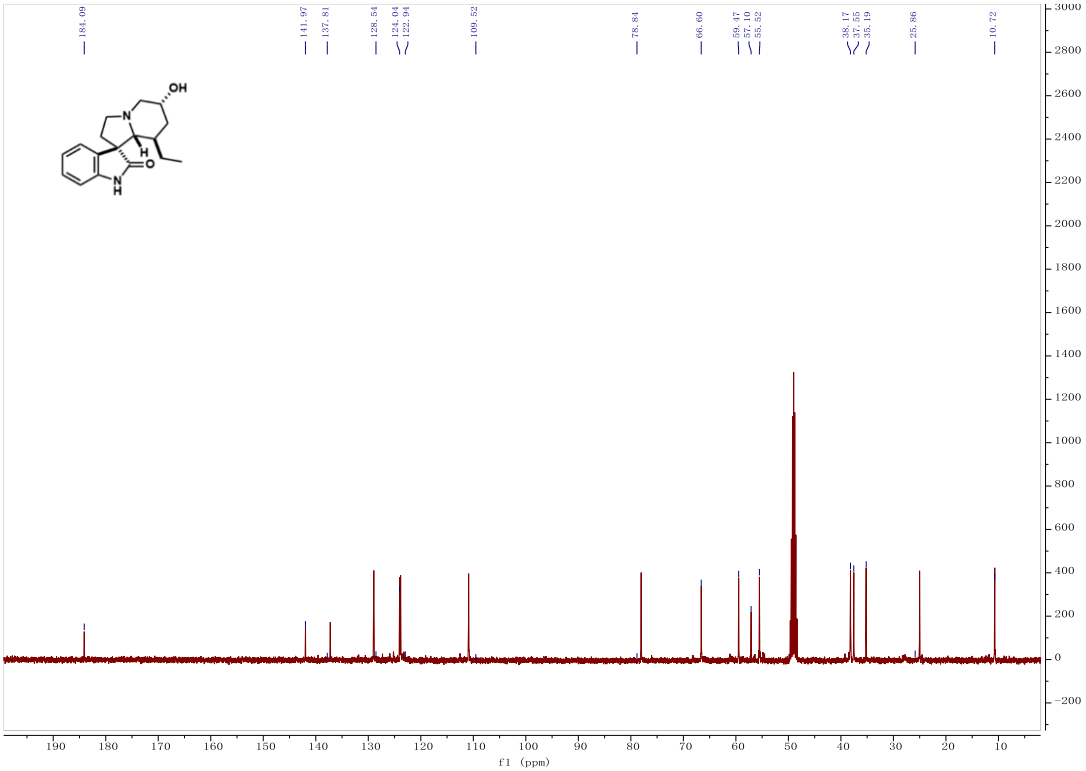
$^{13}$C NMR Spectrum of **9** (100 MHz, DMSO-$d_6$):



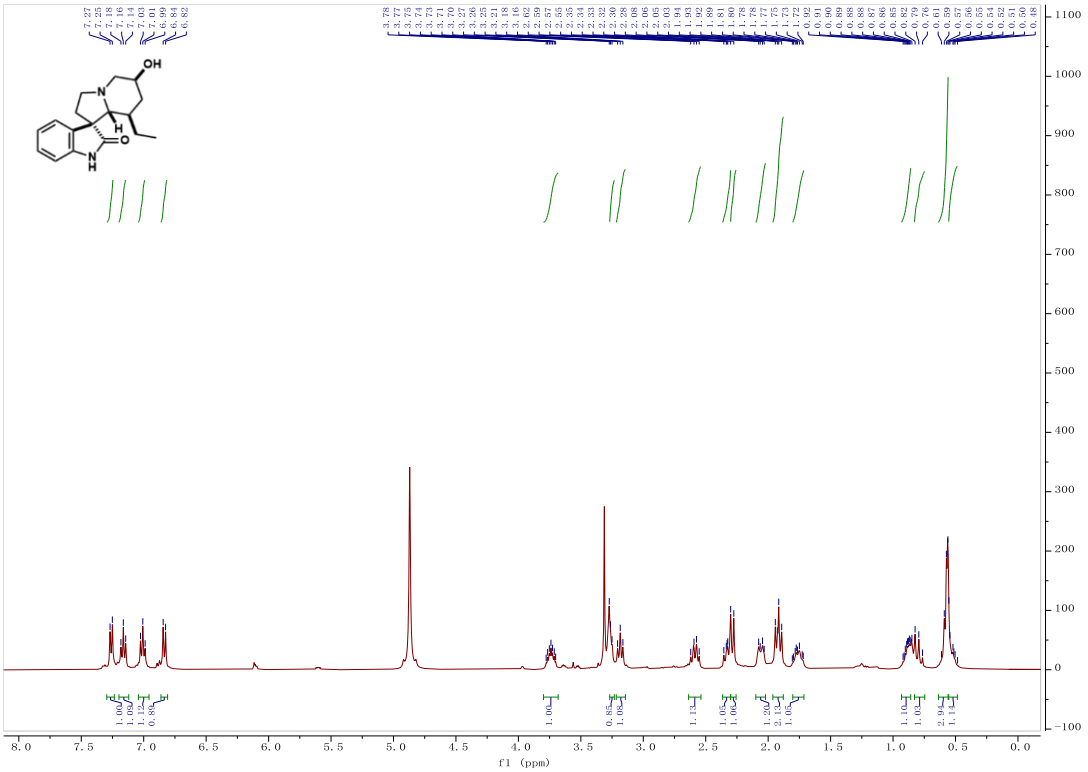
$^{1}$H NMR Spectrum of **10** (400 MHz, $CD_3OD$):



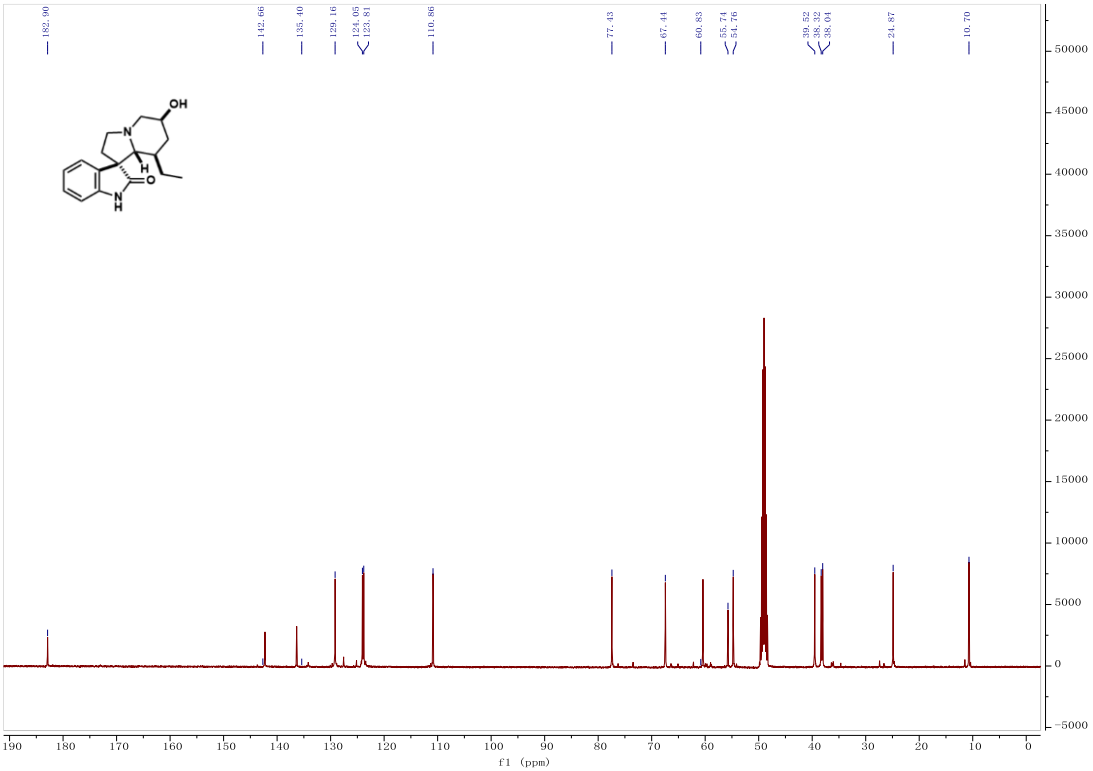
$^{13}$C NMR Spectrum of **10** (100 MHz, $CD_3OD$):



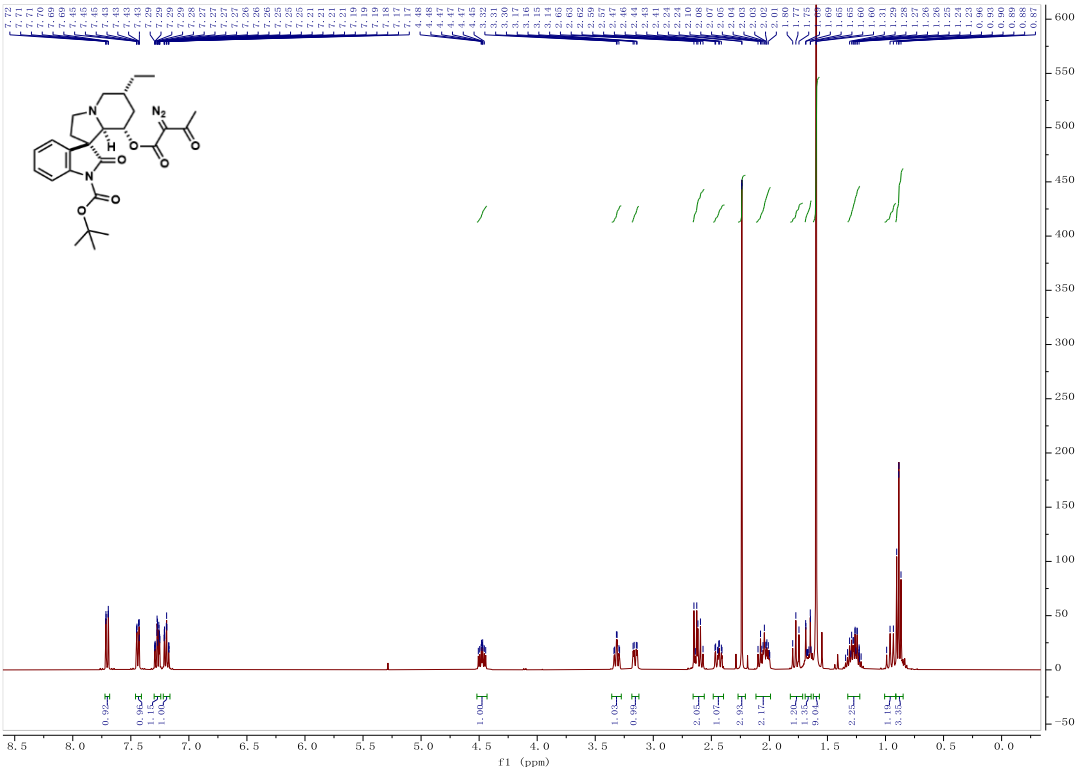
$^{1}$H NMR Spectrum of **11** (400 MHz, $CD_3OD$):



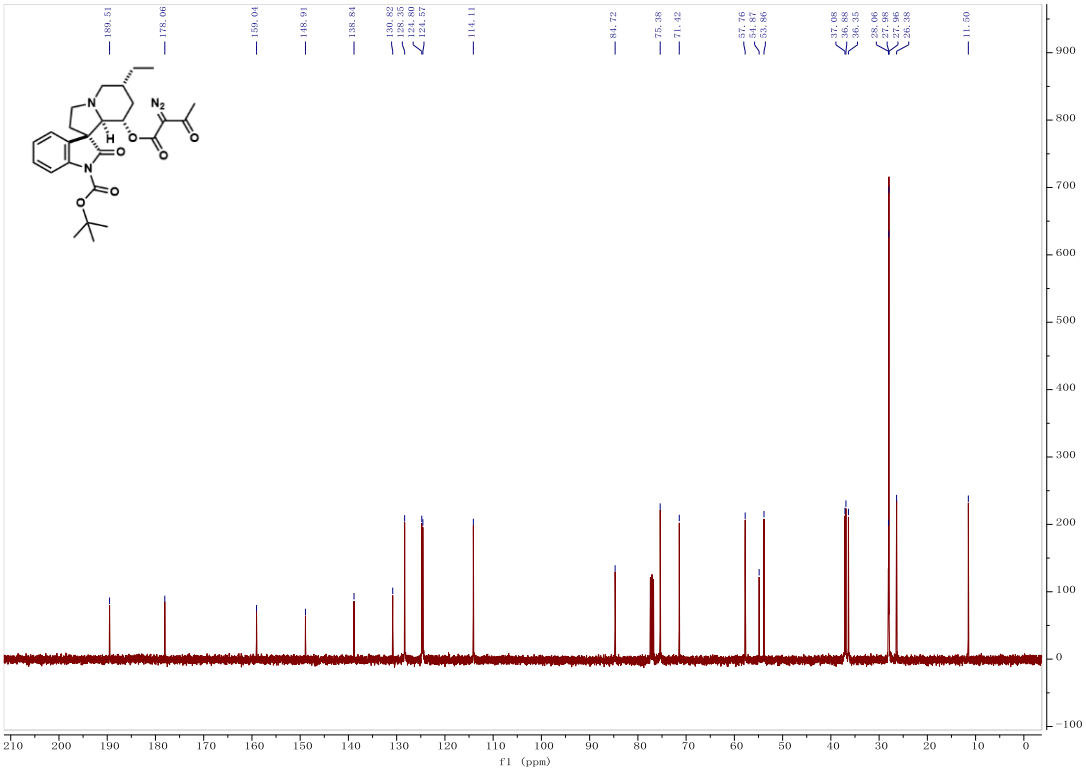
$^{13}$C NMR Spectrum of **11** (100 MHz, $CD_3OD$):



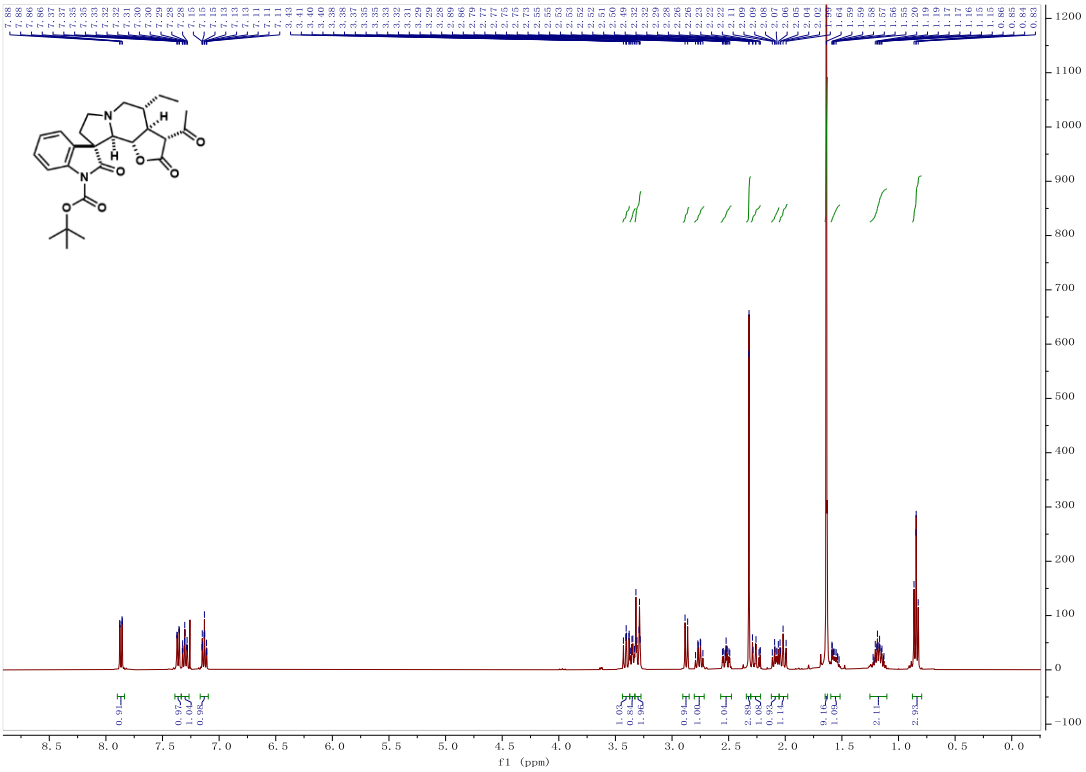
$^{1}$H NMR Spectrum of **14** (400 MHz, $CDCl_3$):



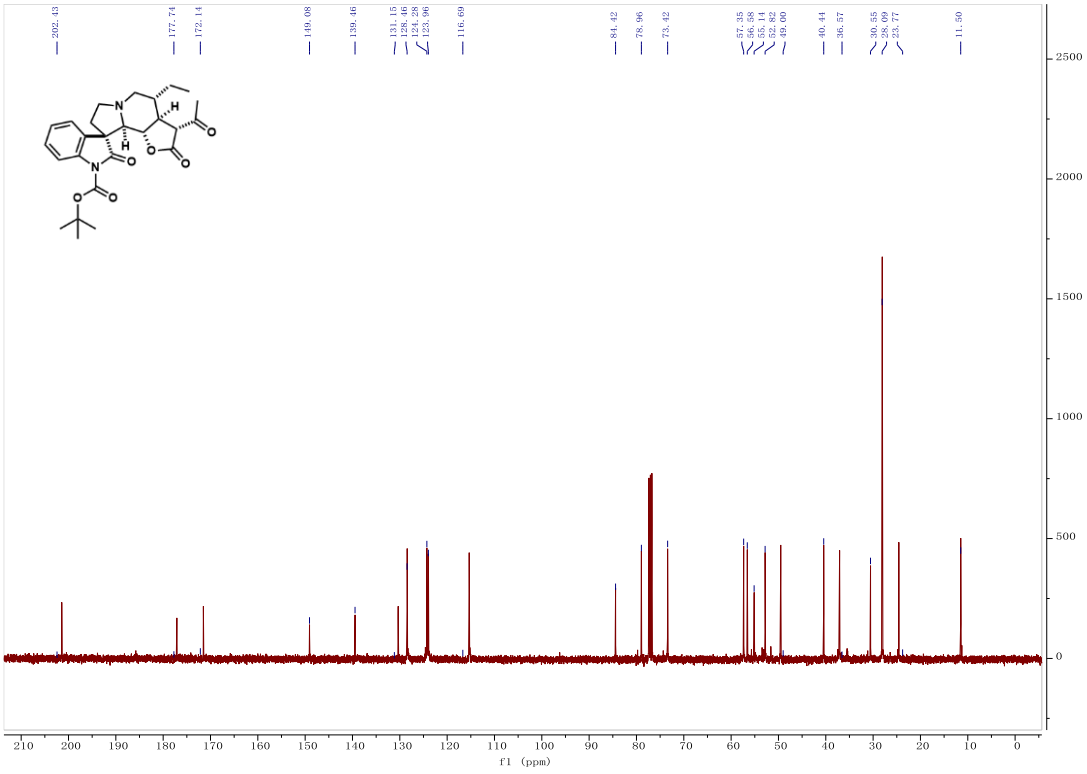
$^{13}$C NMR Spectrum of **14** (100 MHz, $CDCl_3$):



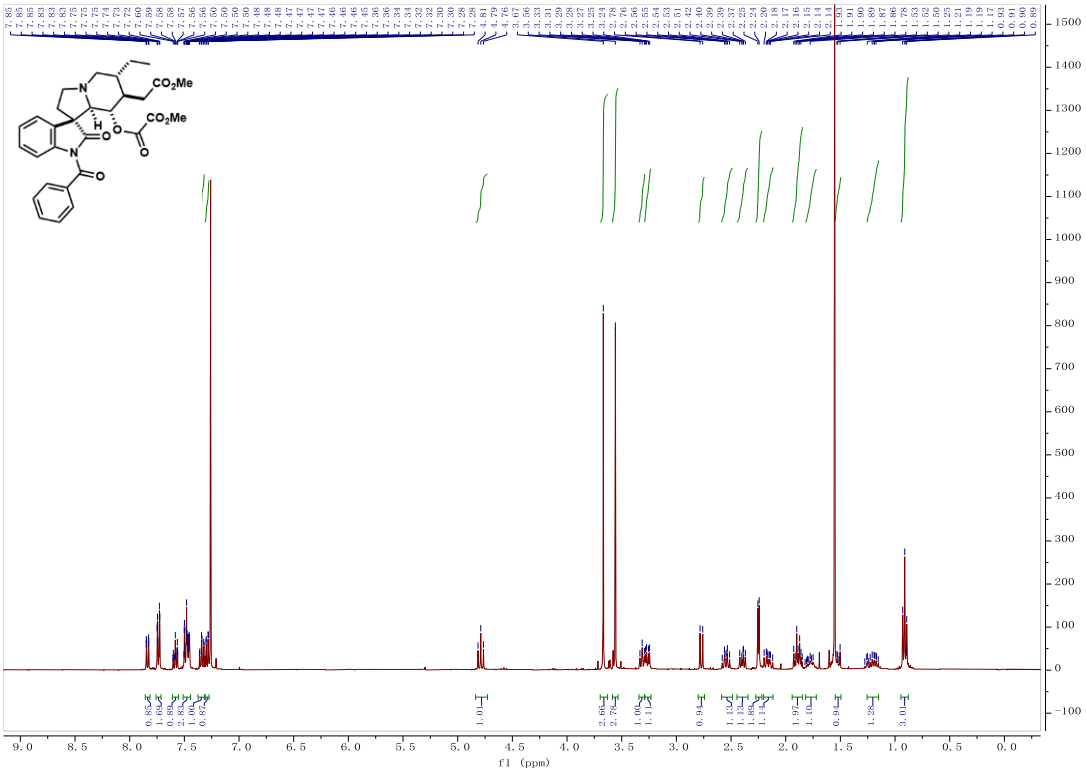
$^{1}$H NMR Spectrum of **15** (400 MHz, $CDCl_3$):



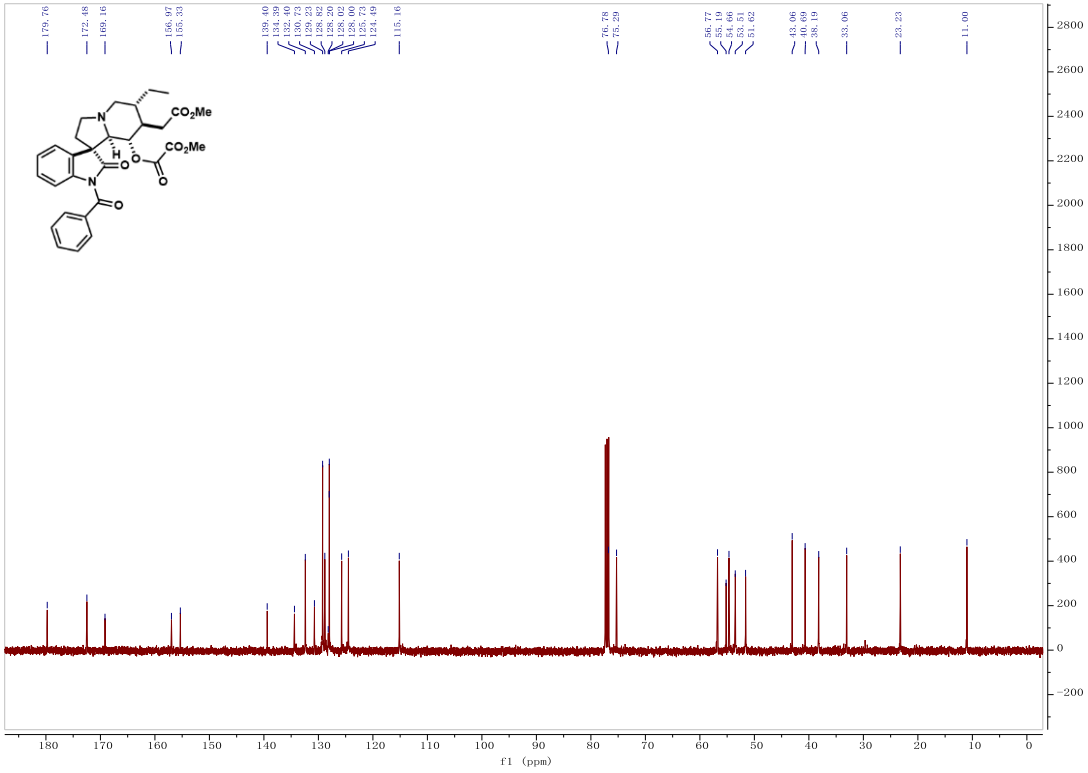
$^{13}$C NMR Spectrum of **15** (100 MHz, $CDCl_3$):



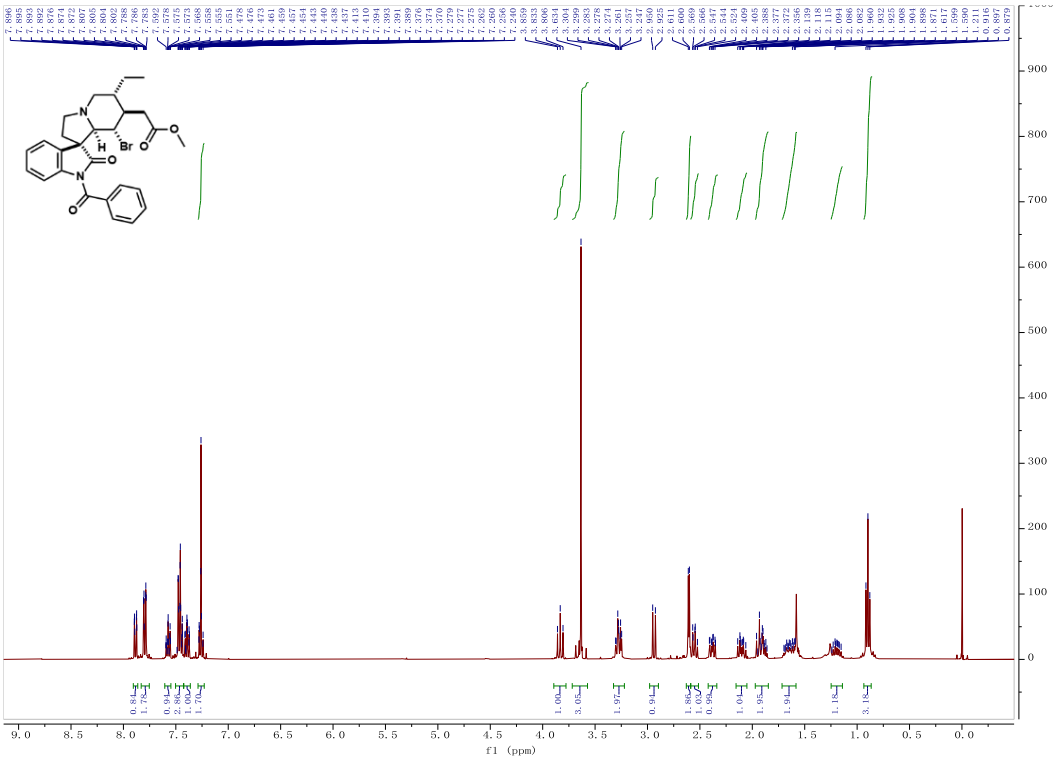
$^{1}$H NMR Spectrum of **18** (400 MHz, $CDCl_3$):



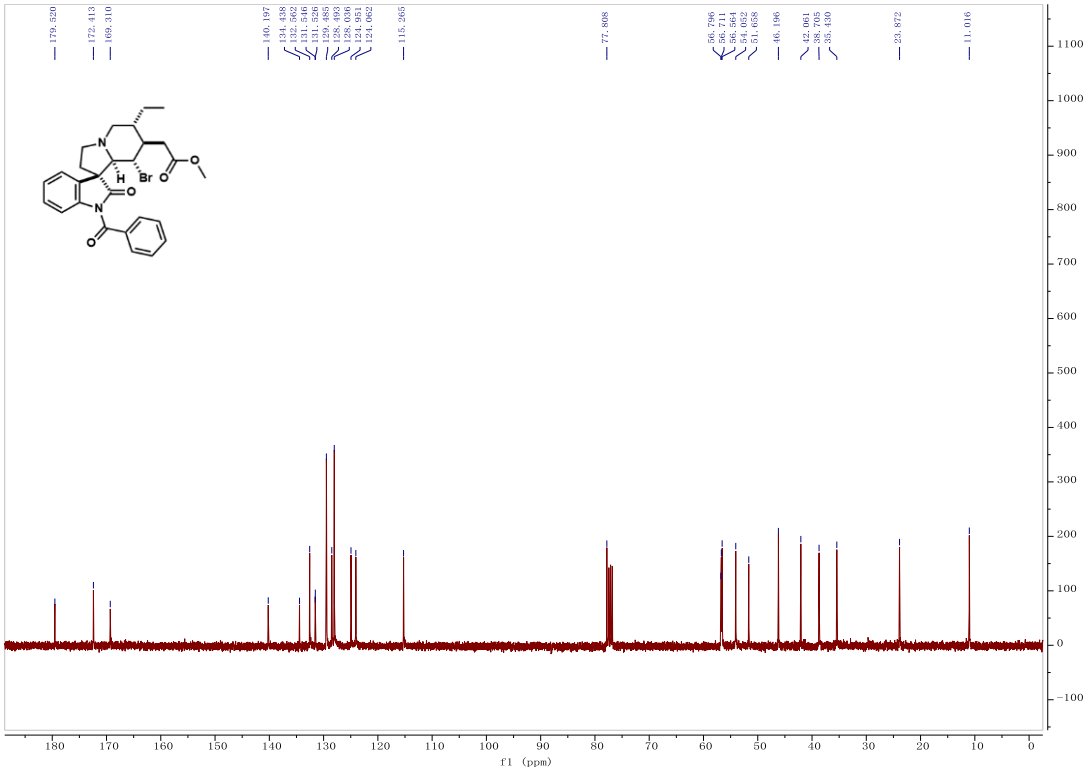
$^{13}$C NMR Spectrum of **18** (100 MHz, $CDCl_3$):



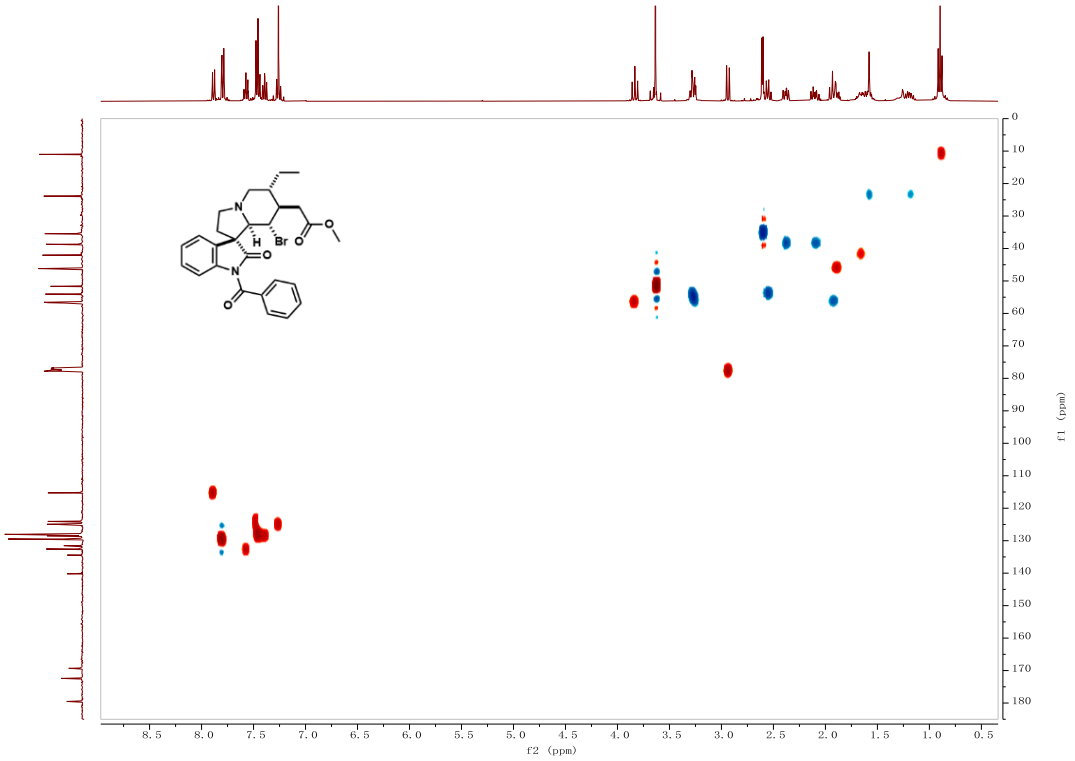
$^{1}$H NMR Spectrum of **19** (400 MHz, $CDCl_3$):



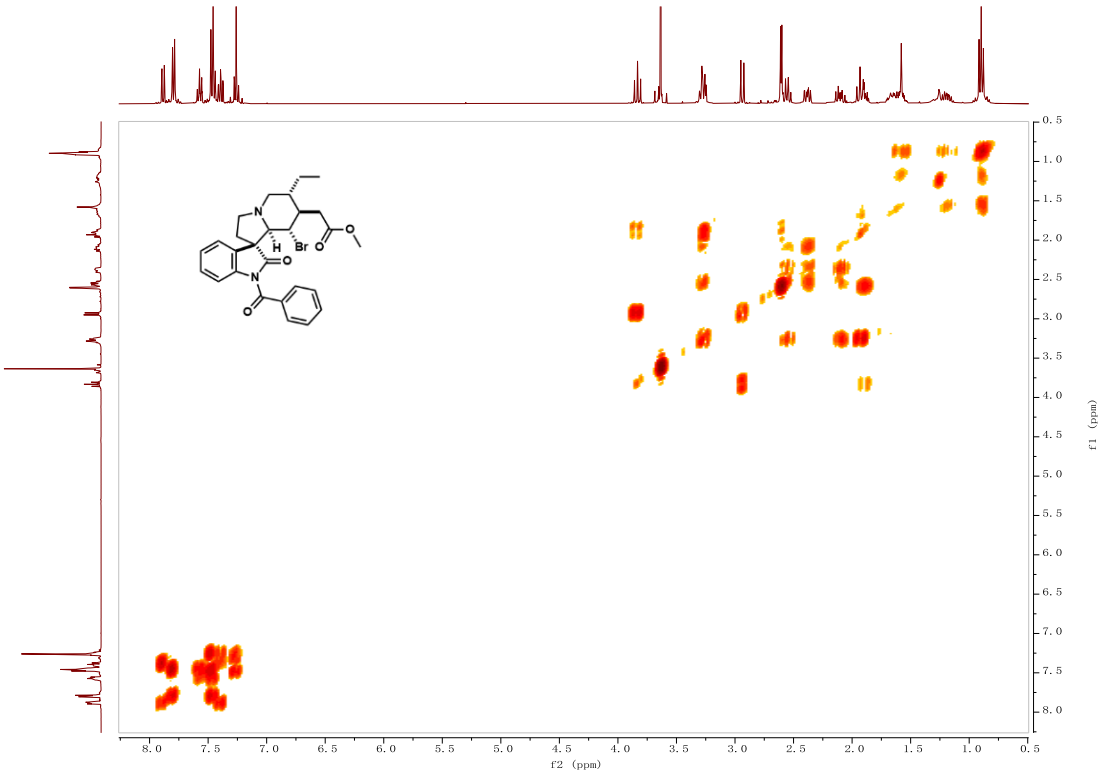
$^{13}$C NMR Spectrum of **19** (100 MHz, $CDCl_3$):



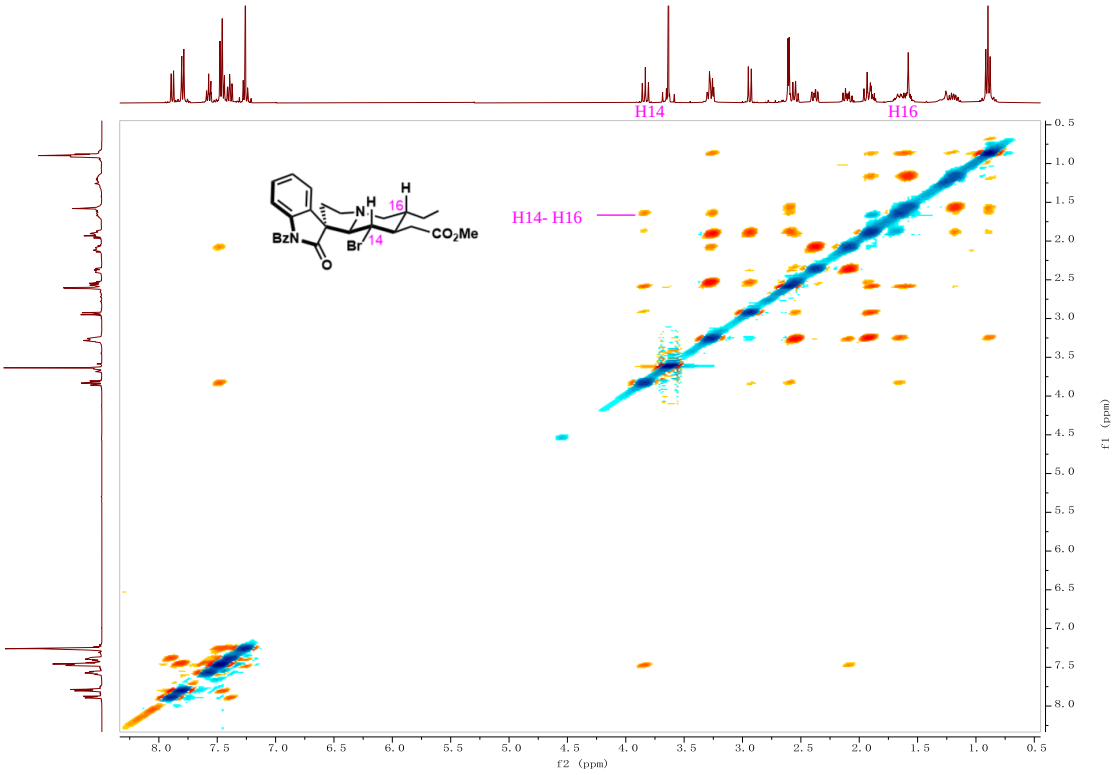
HSQC of **19** (400 MHz, $CDCl_3$):



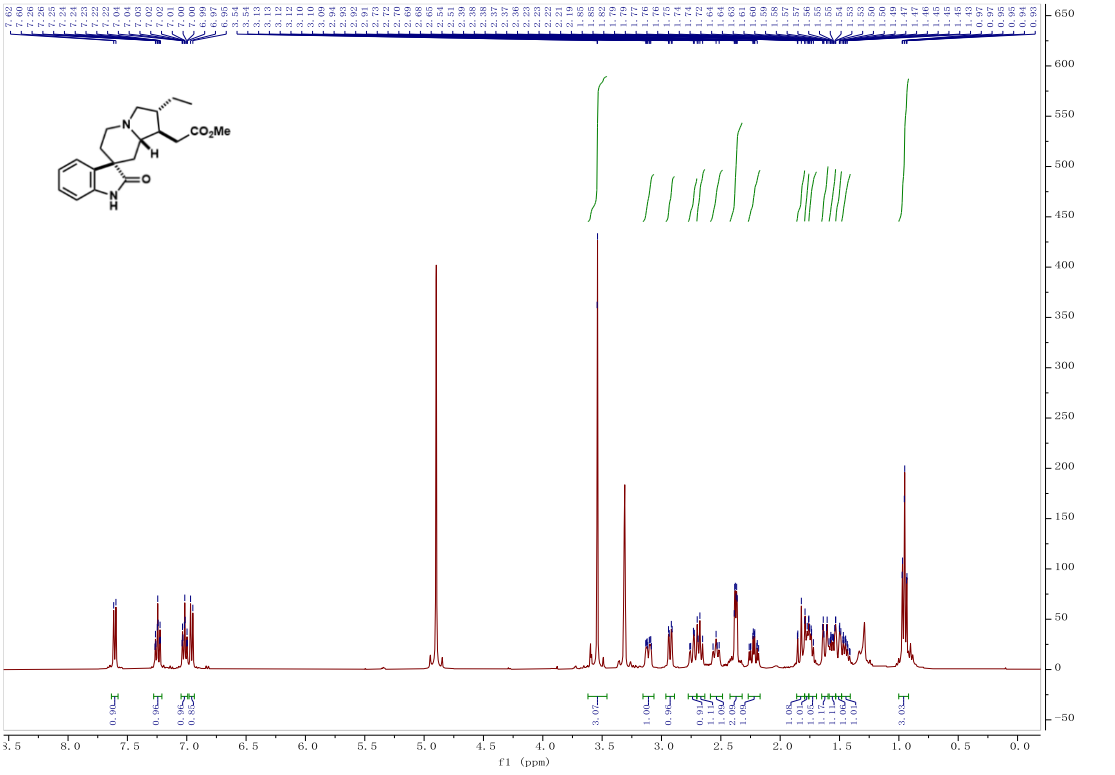

COSY of **19** (400 MHz, $CDCl_3$):



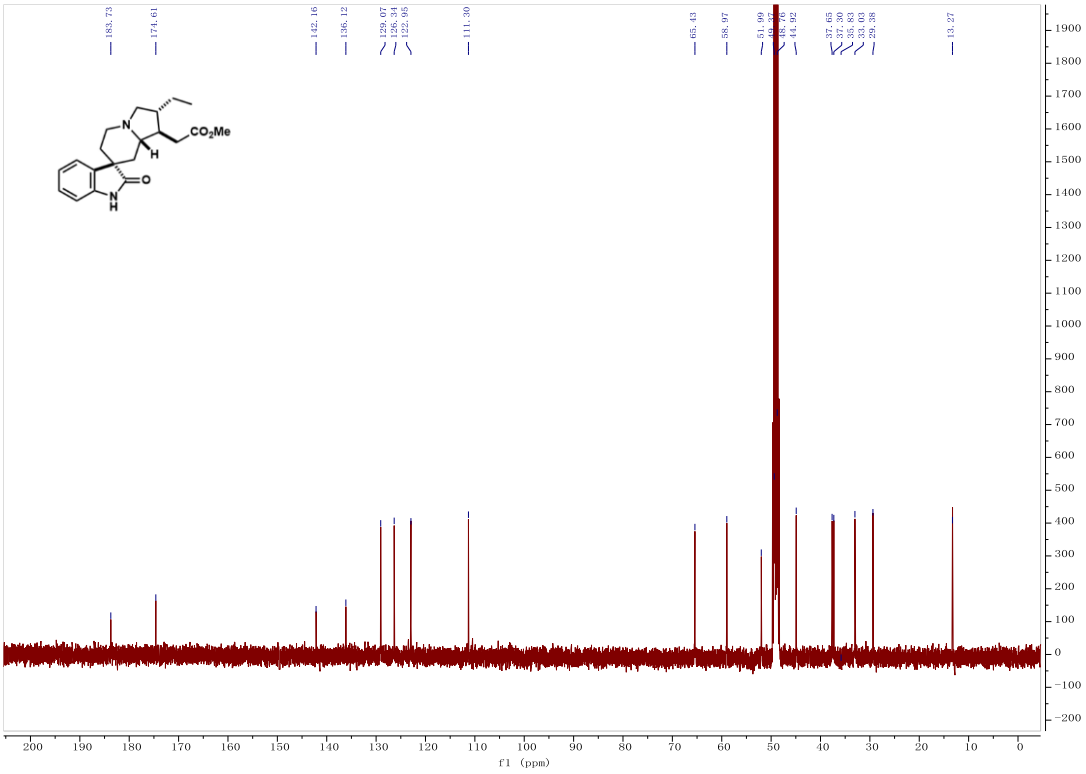
NOESY of **19** (400 MHz, $CDCl_3$):



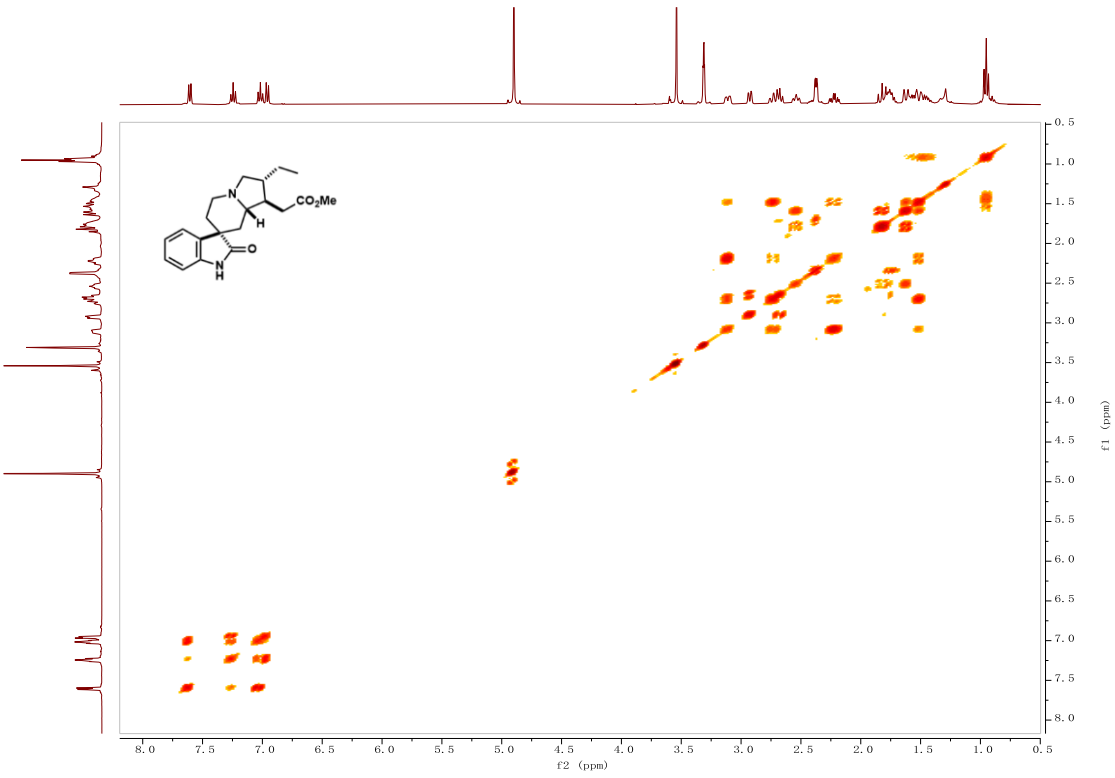

$^1$H NMR Spectrum of **21** (400 MHz, $CD_3OD$):



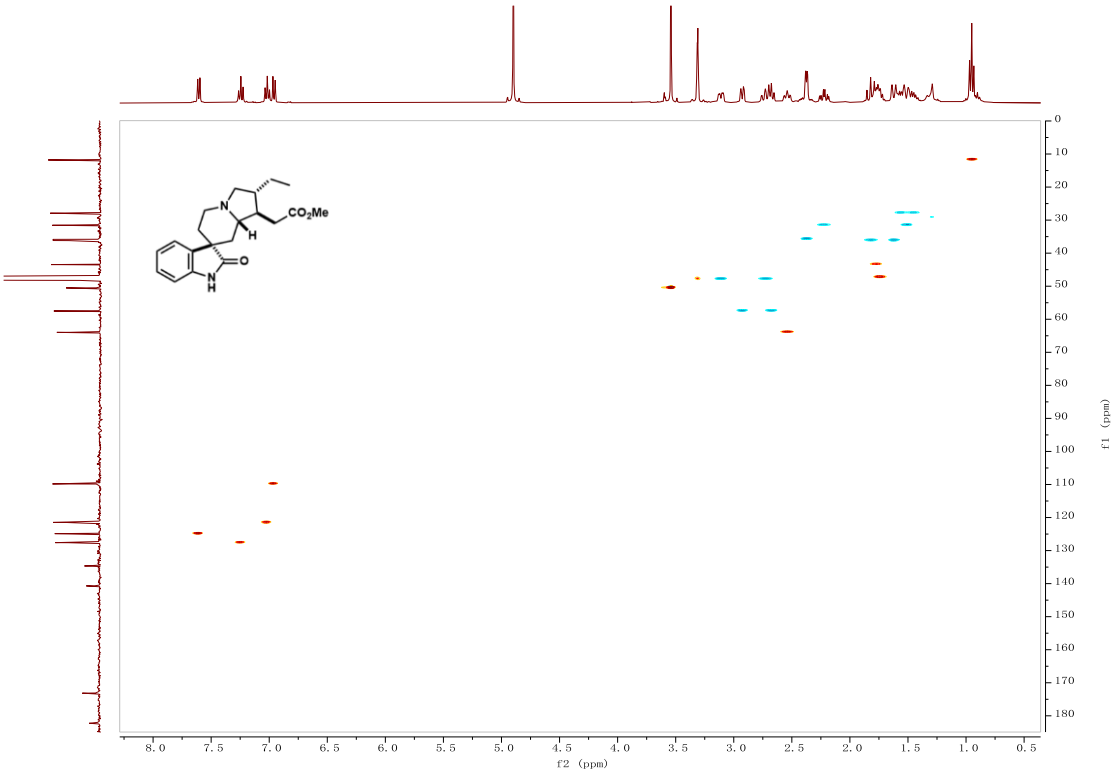
$^{13}$C NMR Spectrum of **21** (100 MHz, $CD_3OD$):



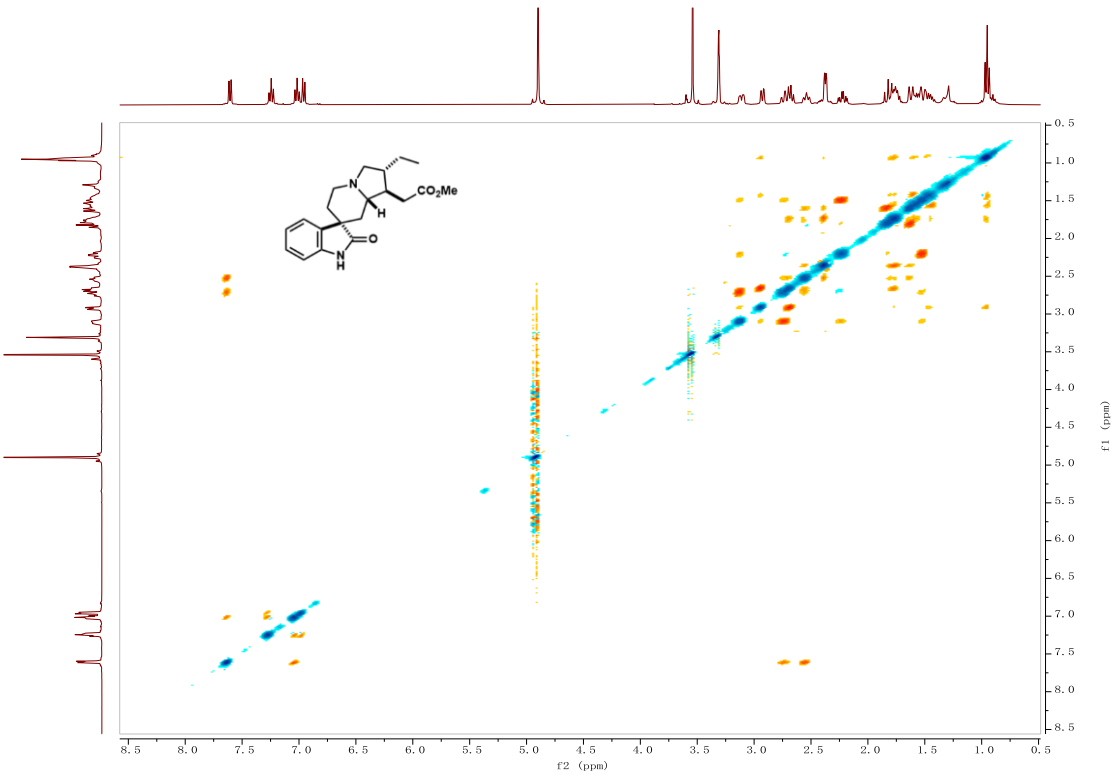

COSY of **21** (400 MHz, $CD_3OD$):



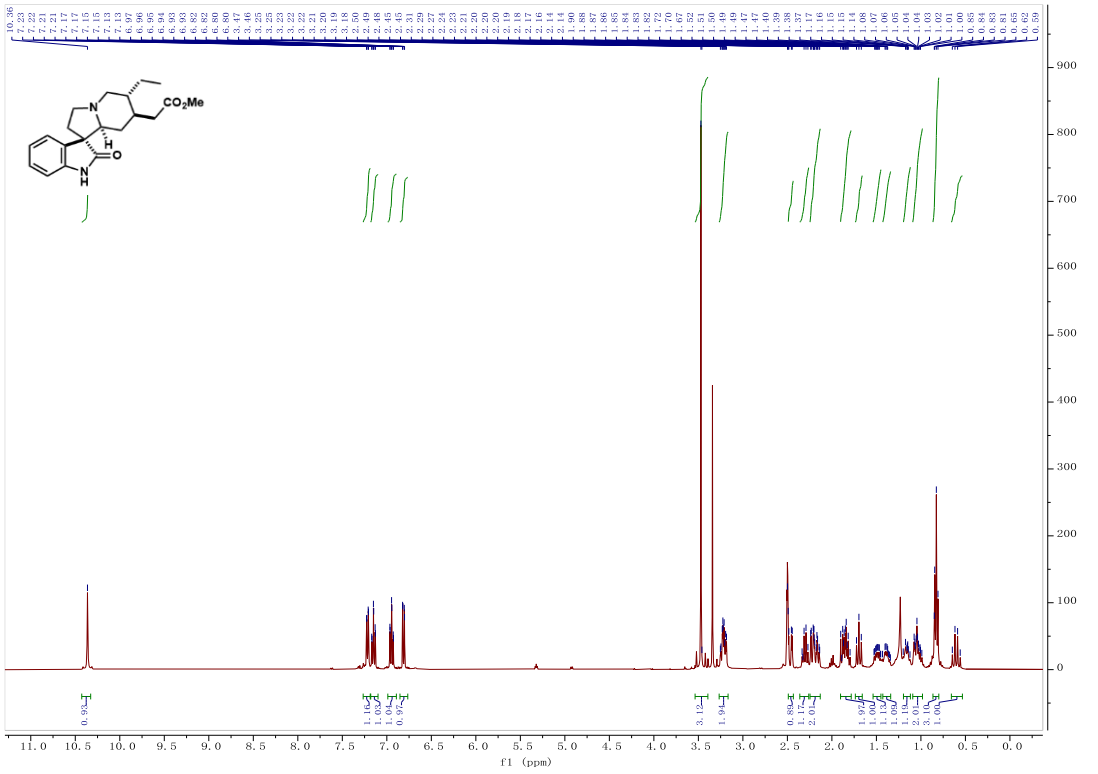
HSQC of **21** (400 MHz, $CD_3OD$):



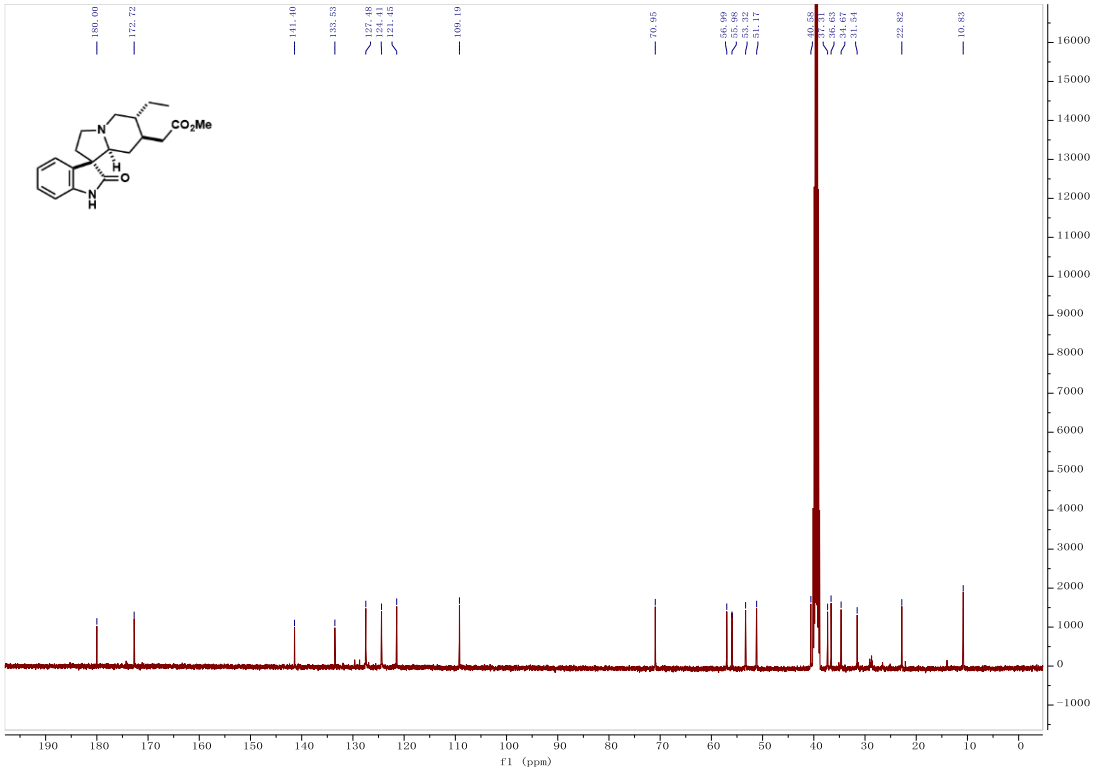

NOESY of **21** (400 MHz, $CD_3OD$):



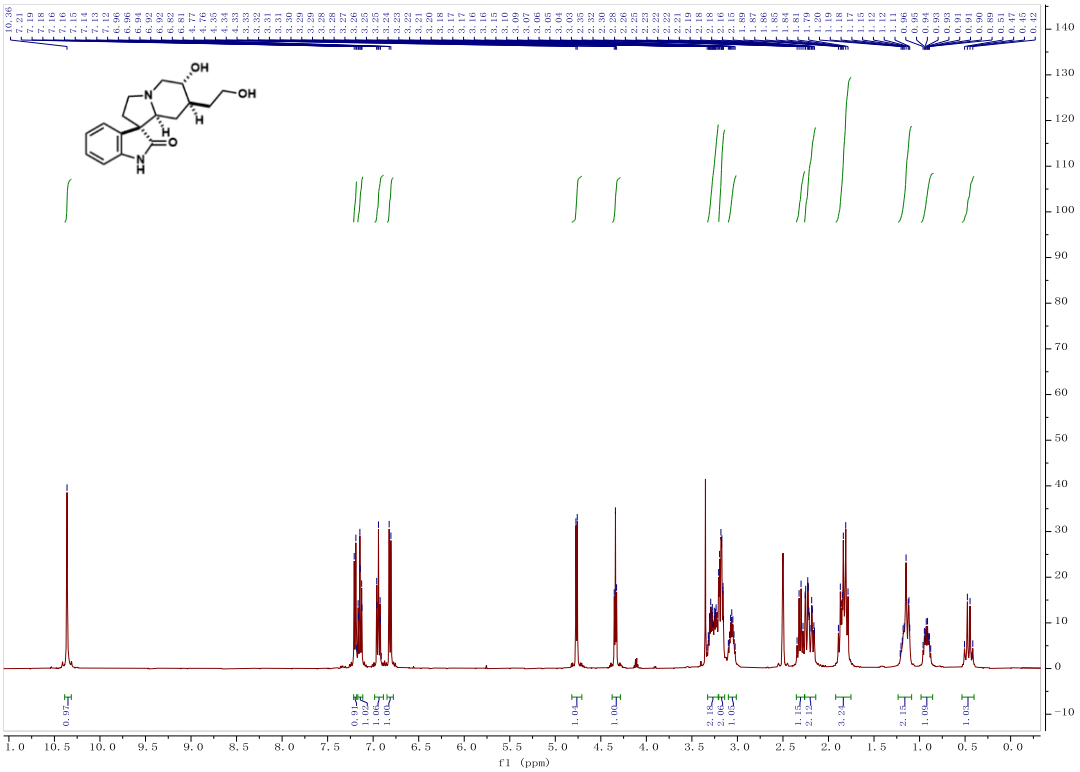
$^{1}$H NMR Spectrum of **22** (400 MHz, DMSO-$d_6$):



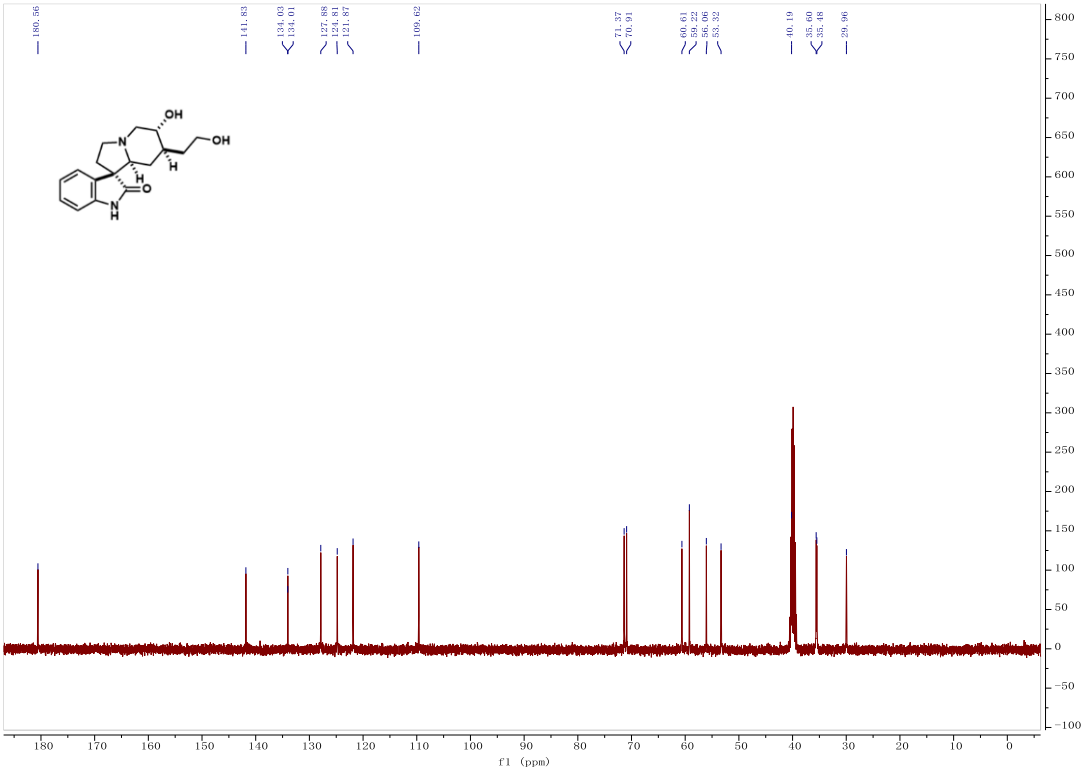

$^{13}$C NMR Spectrum of **22** (100 MHz, DMSO-$d_6$):



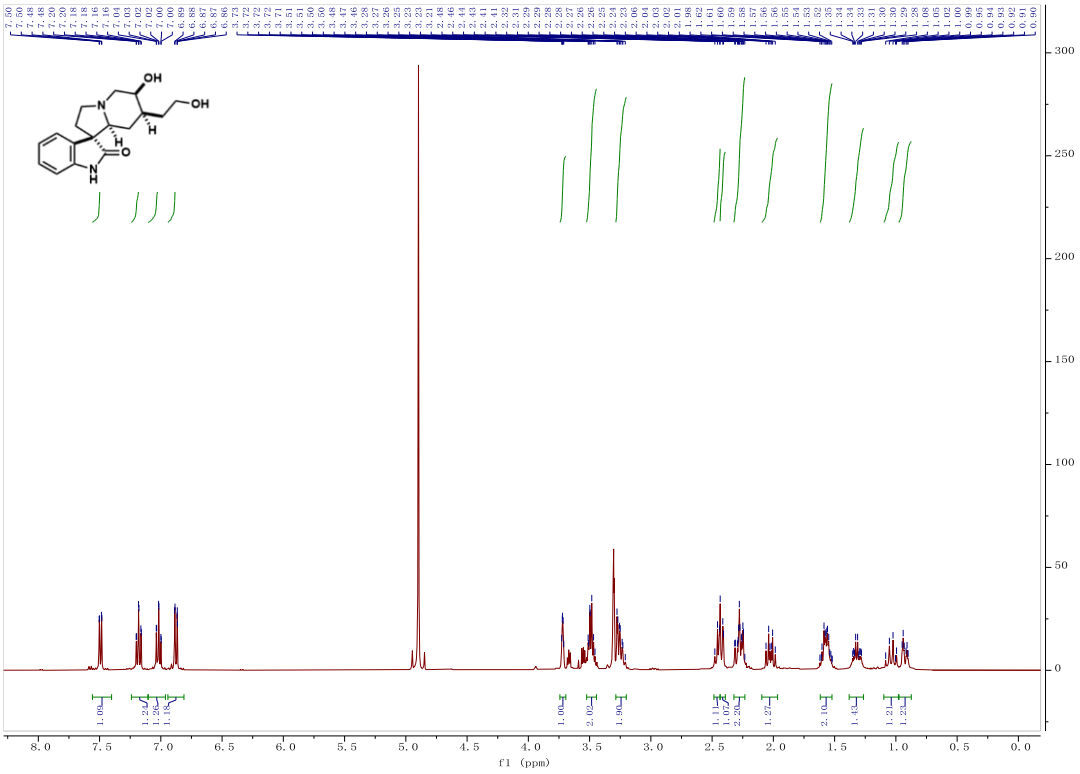
$^{1}$H NMR Spectrum of **23** (400 MHz, DMSO-$d_6$):



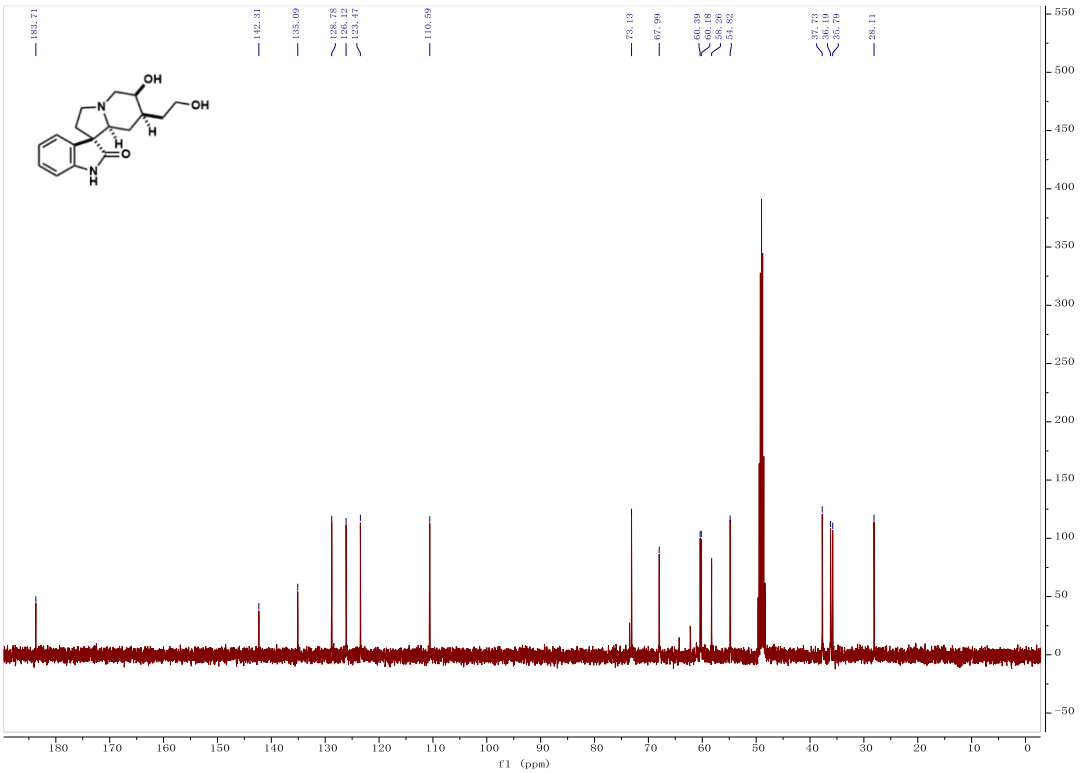
$^{13}$C NMR Spectrum of **23** (100 MHz, DMSO-$d_6$):



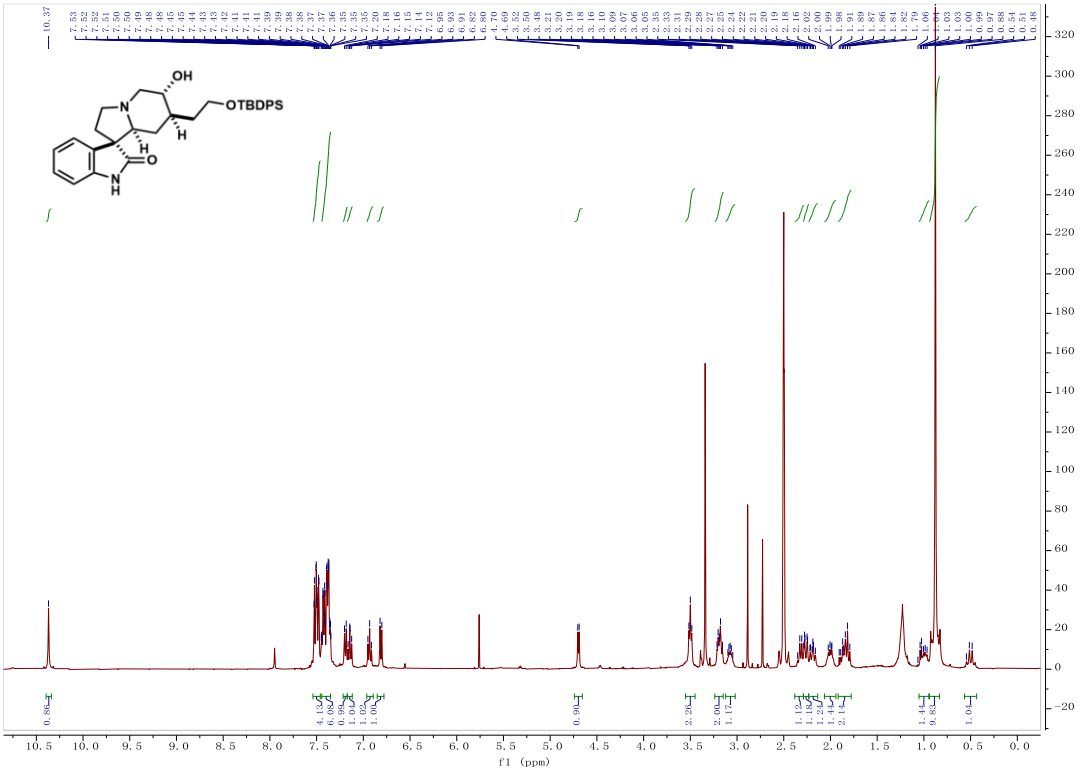
$^{1}$H NMR Spectrum of **24** (400 MHz, $CD_3OD$):



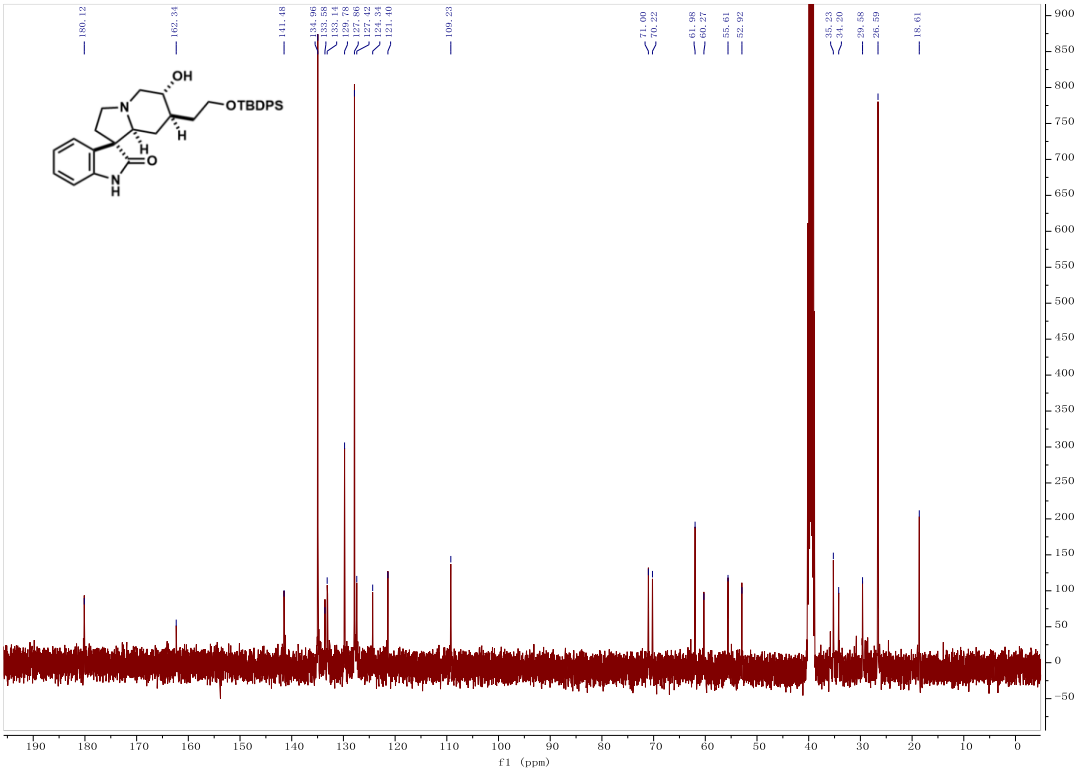
$^{13}$C NMR Spectrum of **24** (100 MHz, $CD_3OD$):



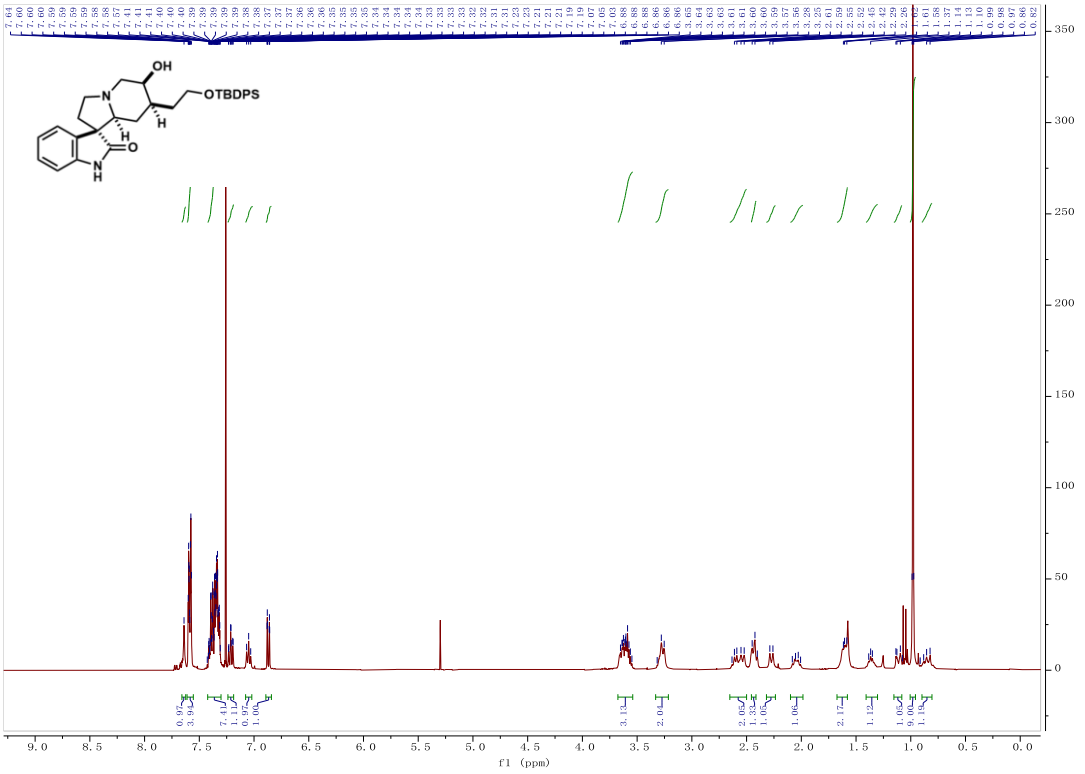
$^{1}$H NMR Spectrum of **S3** (400 MHz, DMSO-$d_6$):



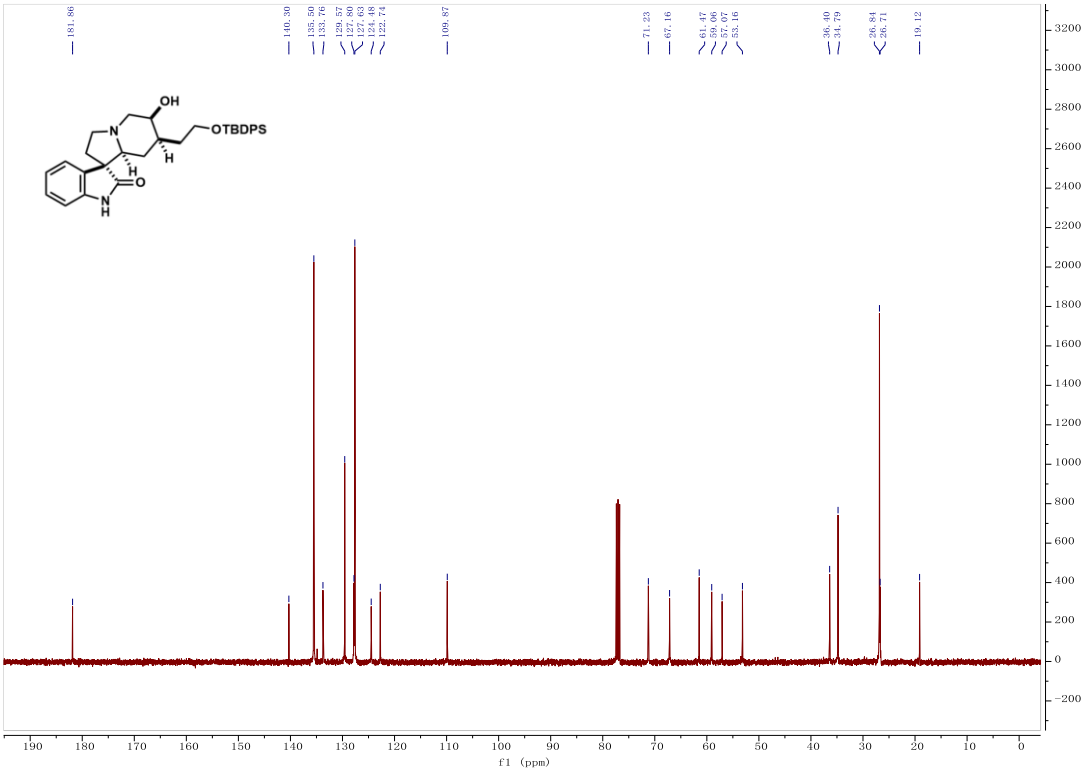

$^{13}$C NMR Spectrum of **S3** (100 MHz, DMSO-$d_6$):



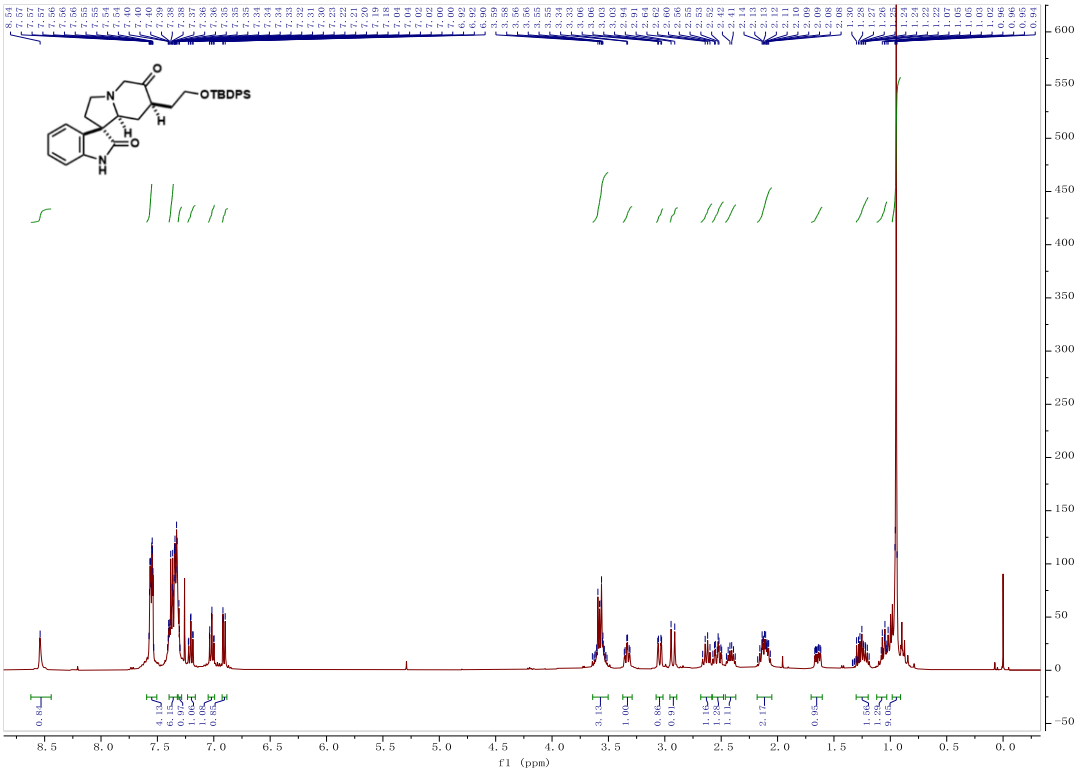
$^1$H NMR Spectrum of **S4** (400 MHz, $CDCl_3$):



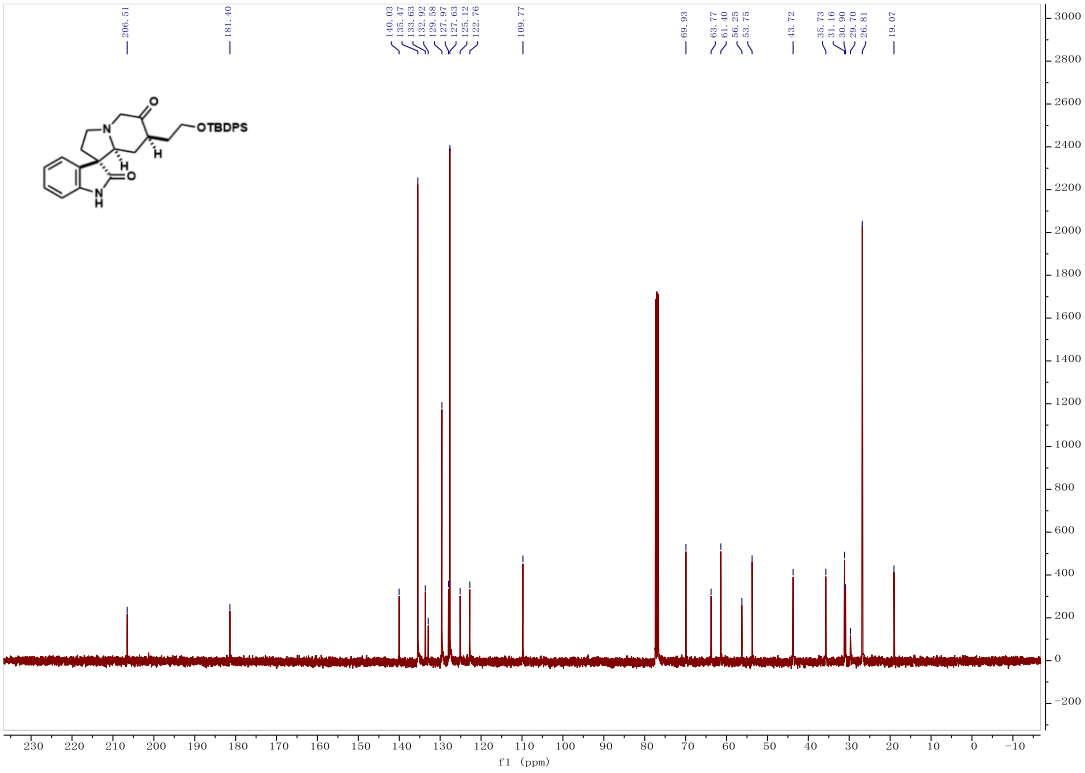

$^1$H NMR Spectrum of **S4** (100 MHz, $CDCl_3$):



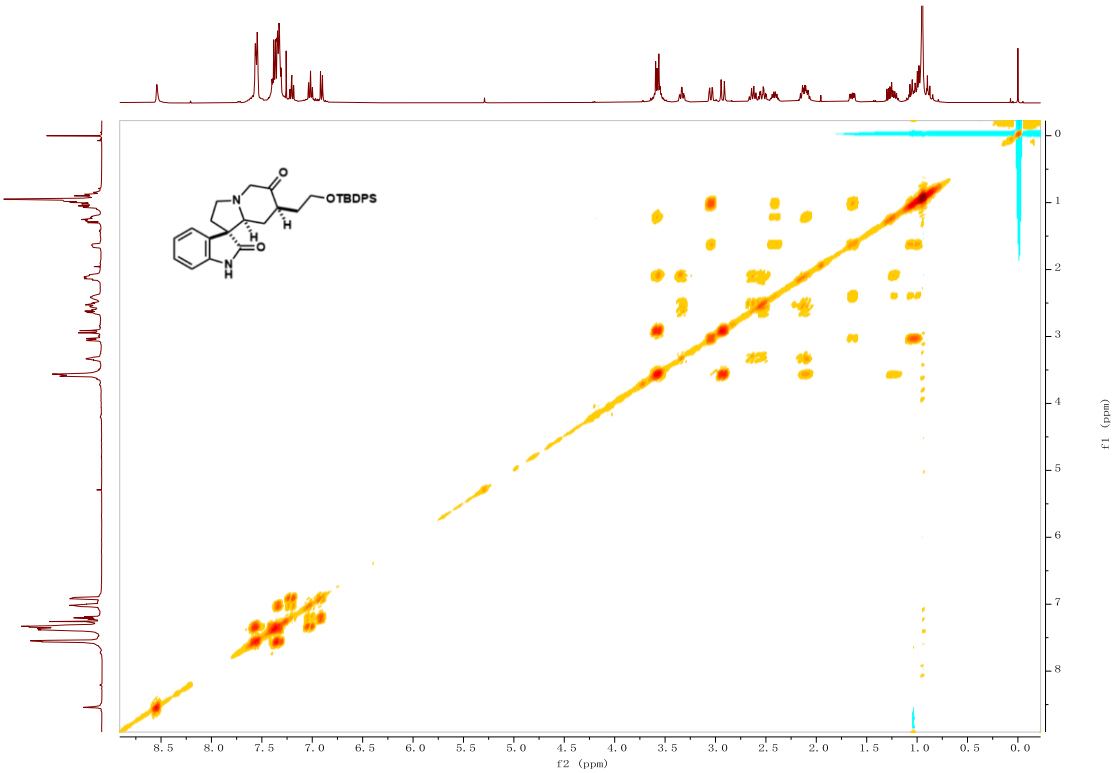
$^{1}$H NMR Spectrum of **25** (400 MHz, $CDCl_3$):



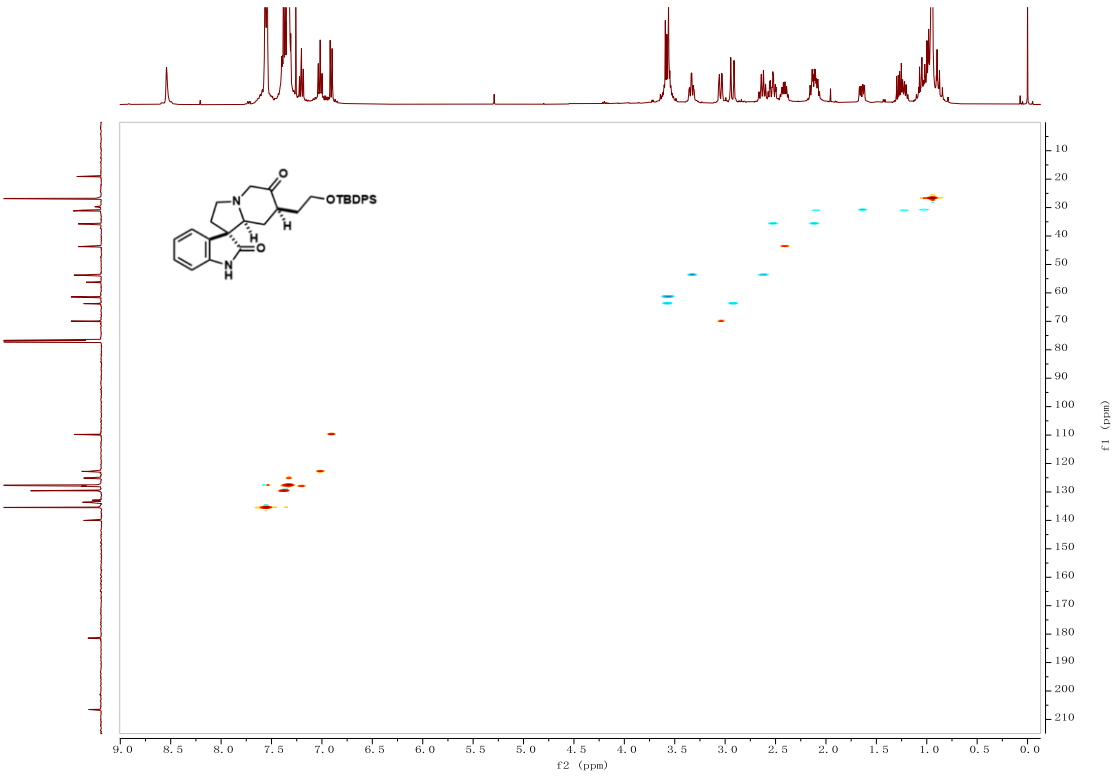

$^{13}$C NMR Spectrum of **25** (100 MHz, $CDCl_3$):



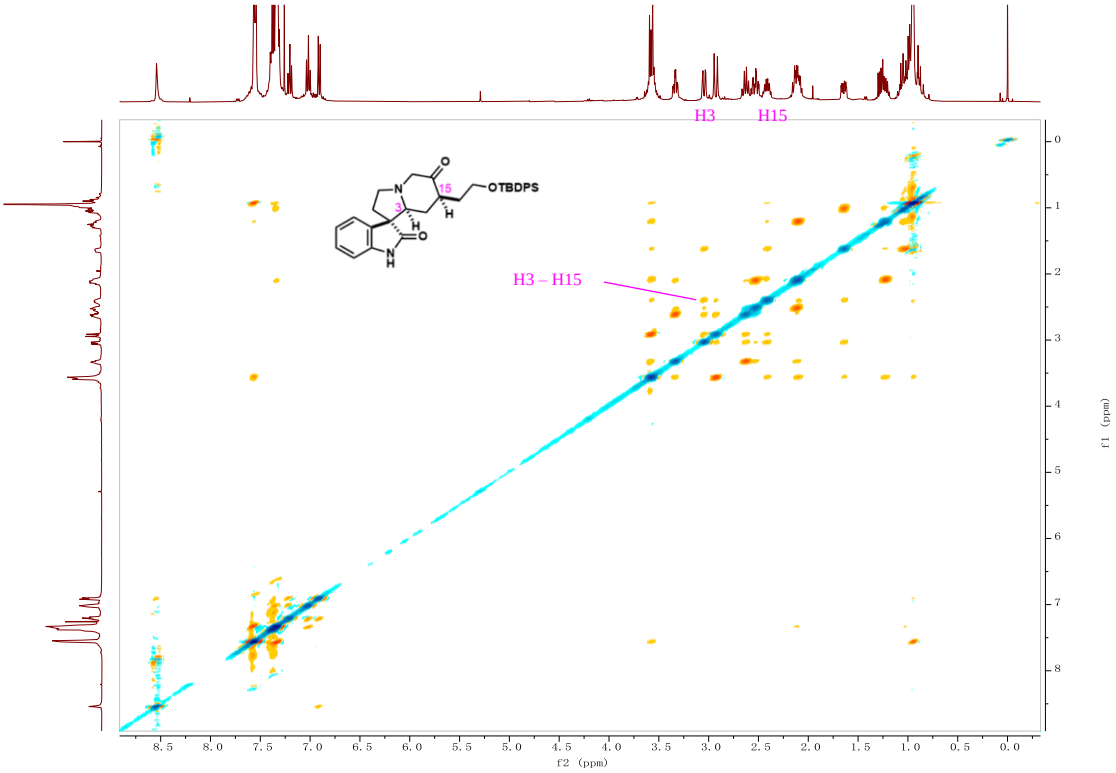
COSY of **25** (400 MHz, $CDCl_3$):



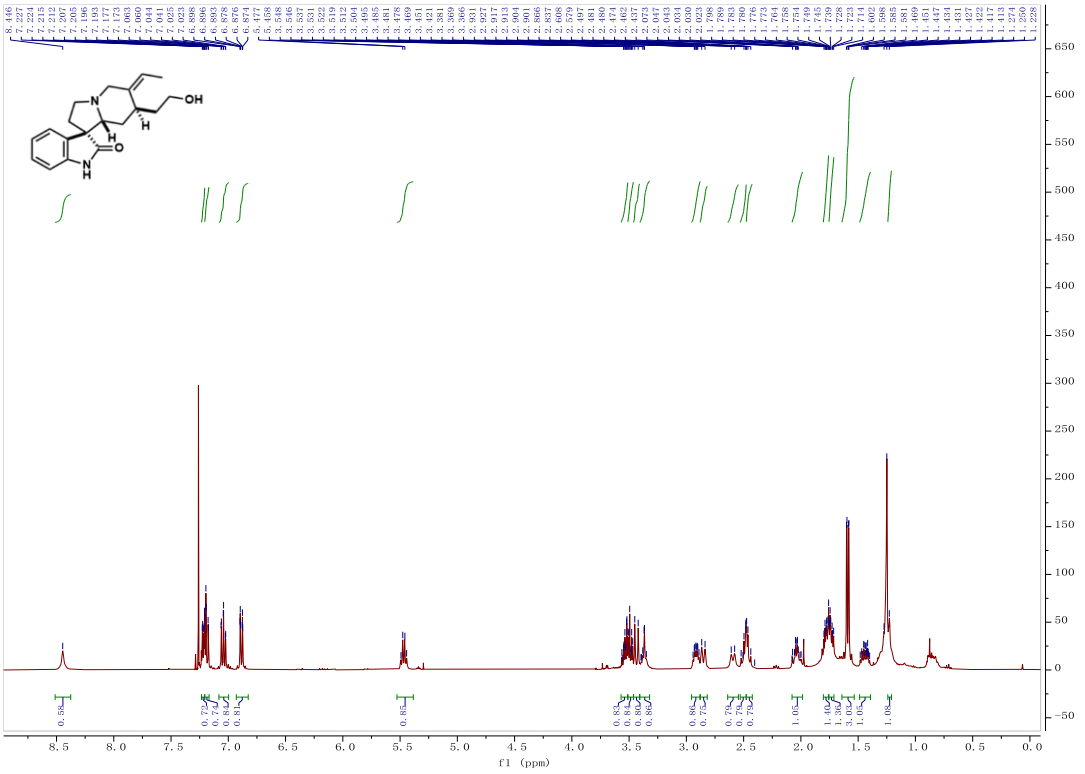

HSQC of **25** (400 MHz, $CDCl_3$):



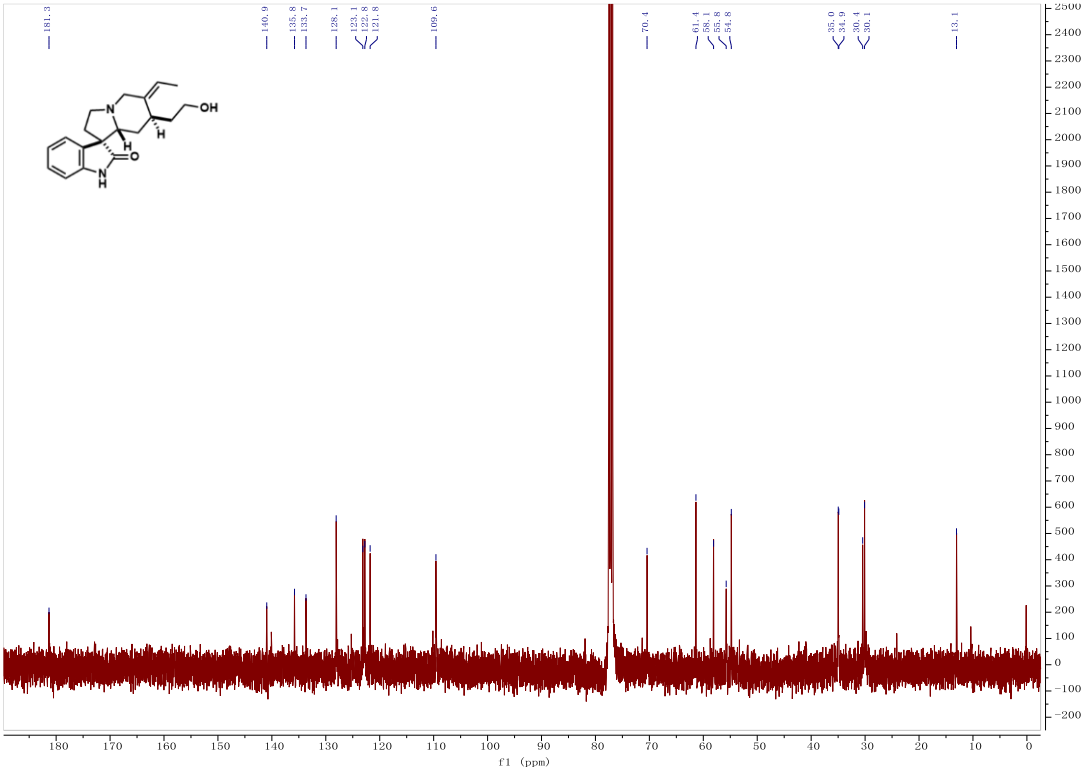
NOESY of **25** (400 MHz, $CDCl_3$):



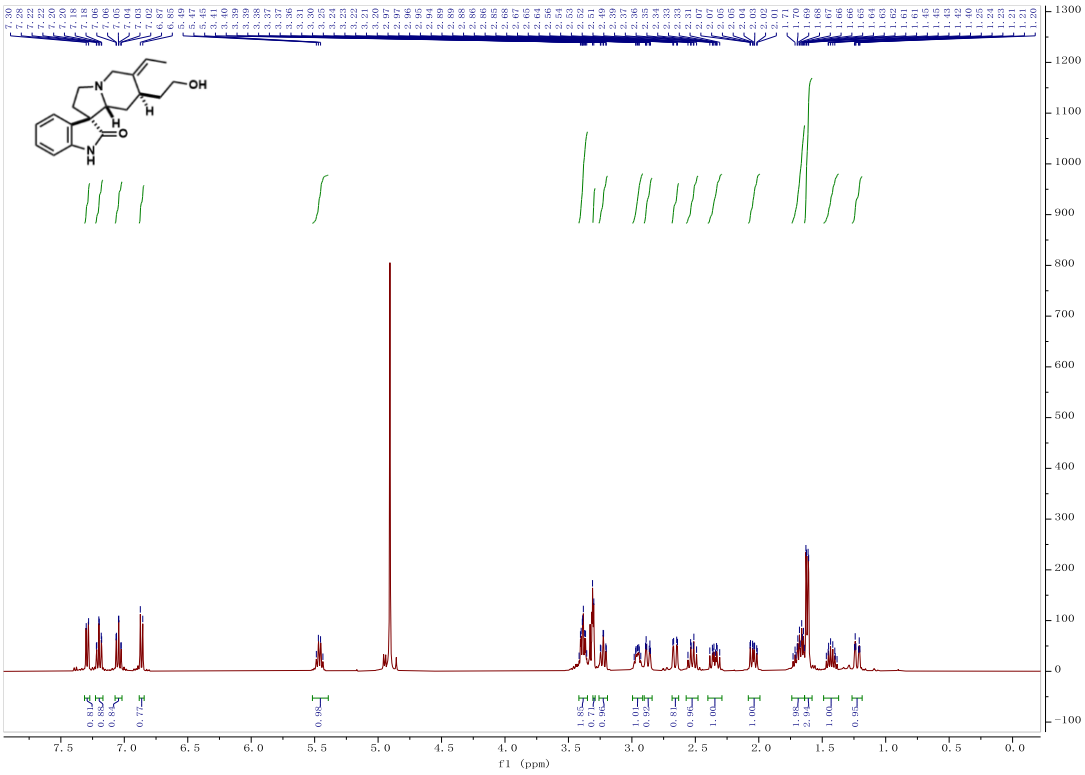
$^{1}$H NMR Spectrum of **27** (400 MHz, $CDCl_3$):



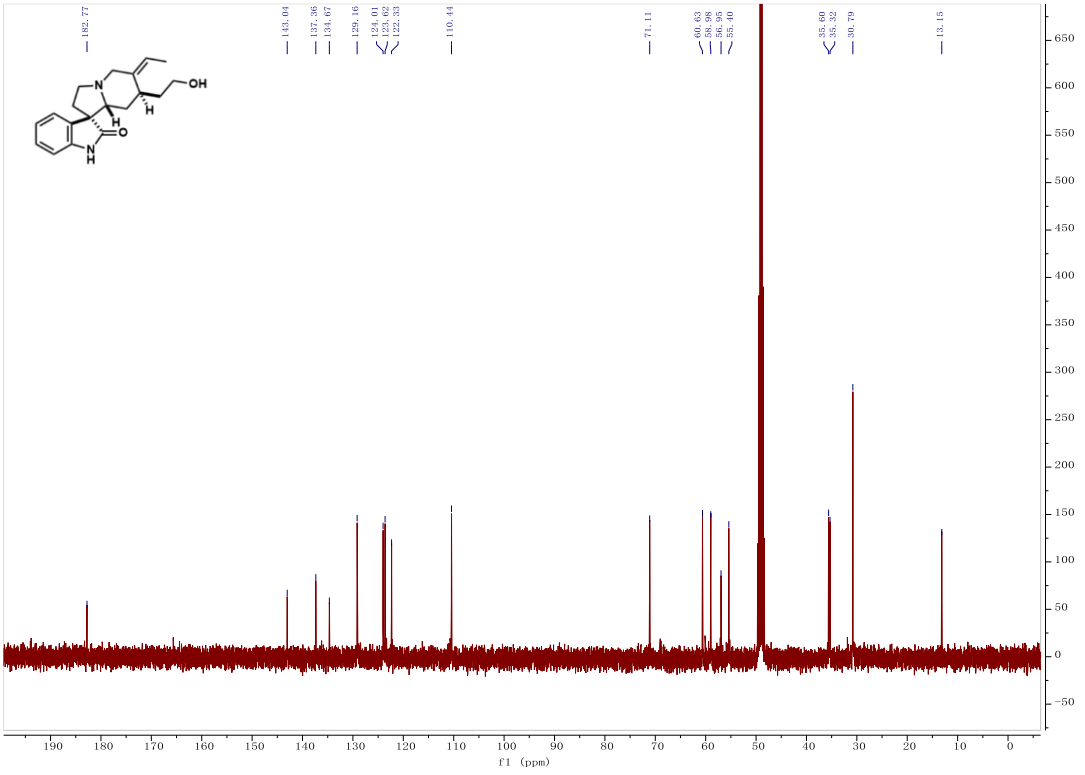
$^{13}$C NMR Spectrum of **27** (100 MHz, $CDCl_3$):



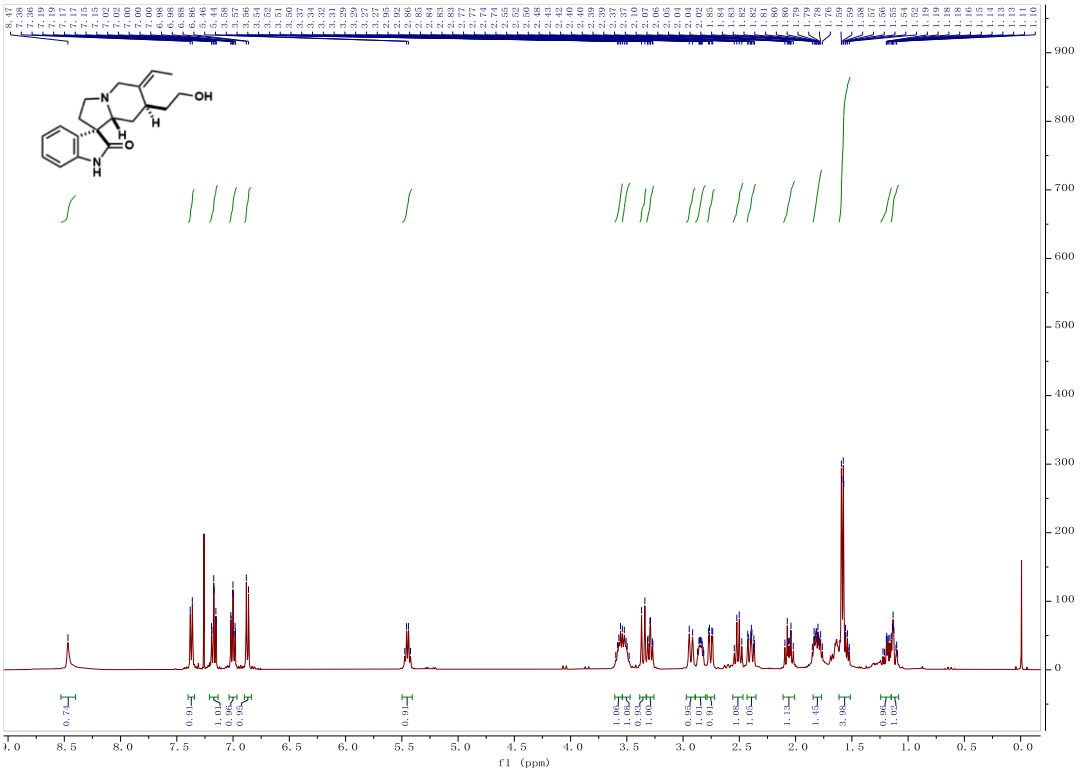
$^{1}$H NMR Spectrum of **27** (400 MHz, $CD_3OD$):



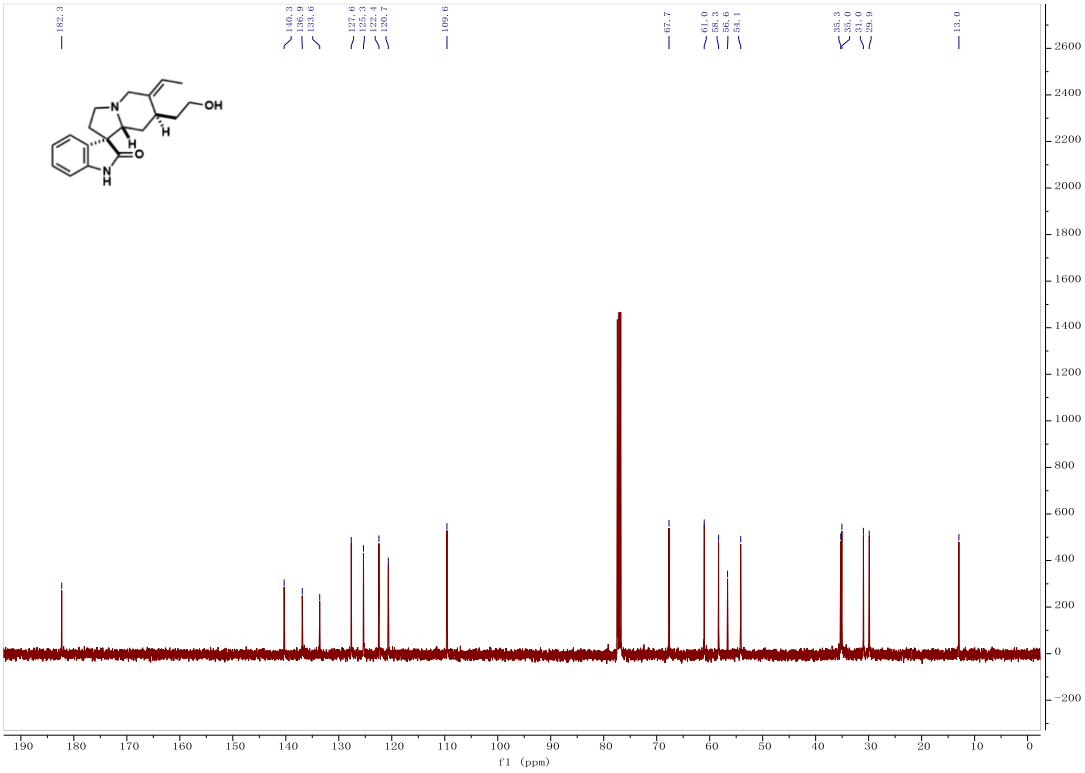
$^{13}$C NMR Spectrum of **27** (100 MHz, $CD_3OD$):



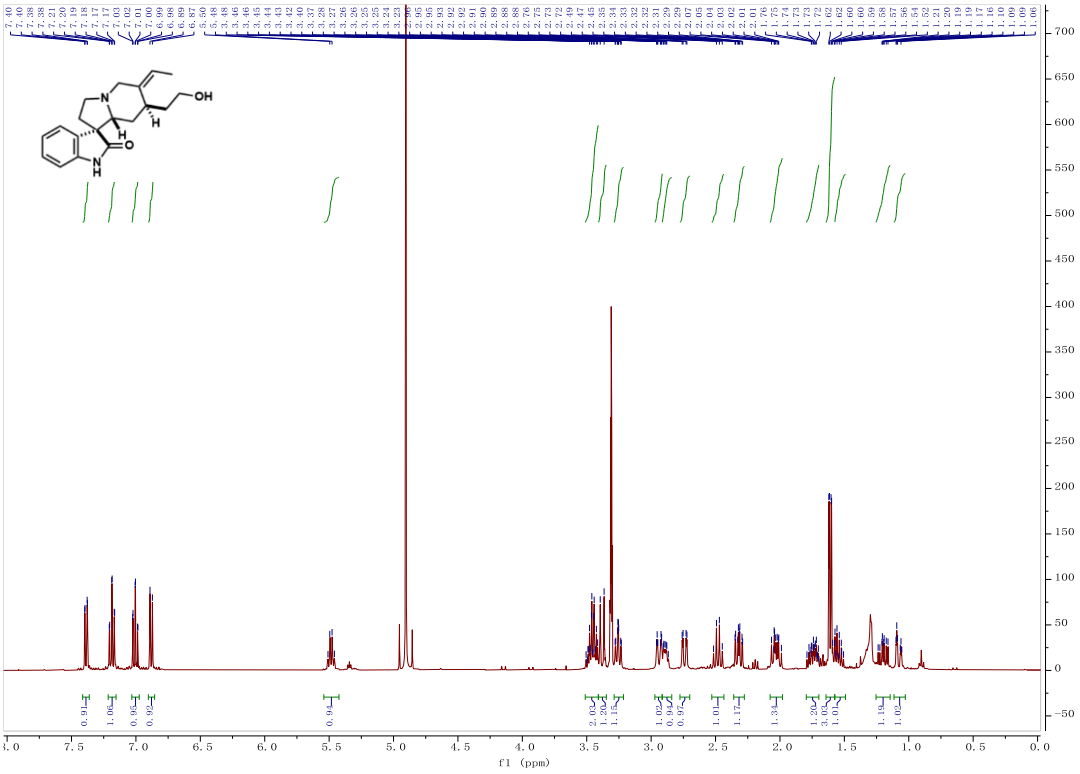
$^{1}$H NMR Spectrum of **28** (400 MHz, $CDCl_3$):



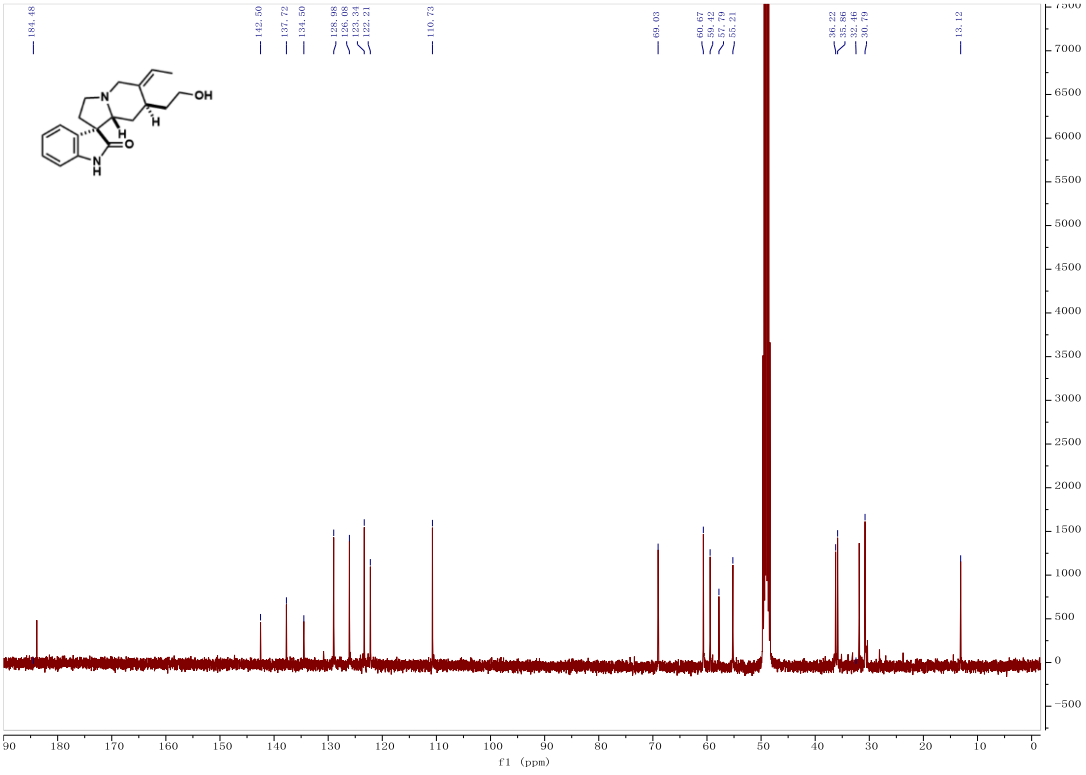

$^{13}$C NMR Spectrum of **28** (100 MHz, $CDCl_3$):



$^{1}$H NMR Spectrum of **28** (400 MHz, $CD_3OD$):



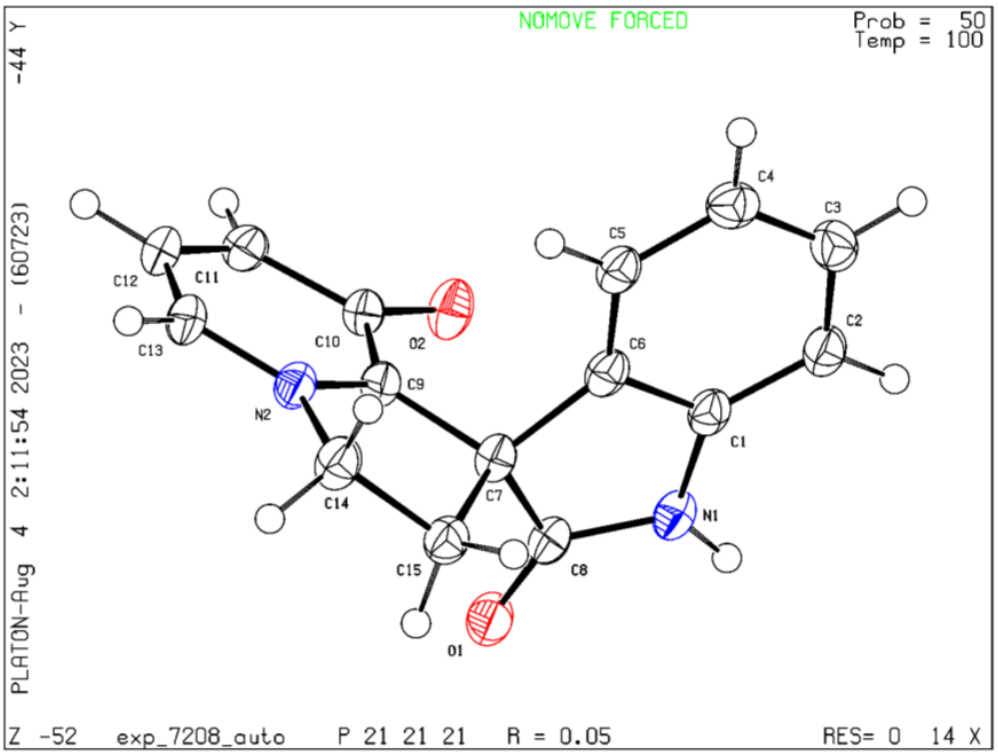

$^{13}$C NMR Spectrum of **28** (100 MHz, $CD_3OD$):



## Crystallographic Information

The crystal data of compound **3g** has been deposited in CCDC with number 2282680.

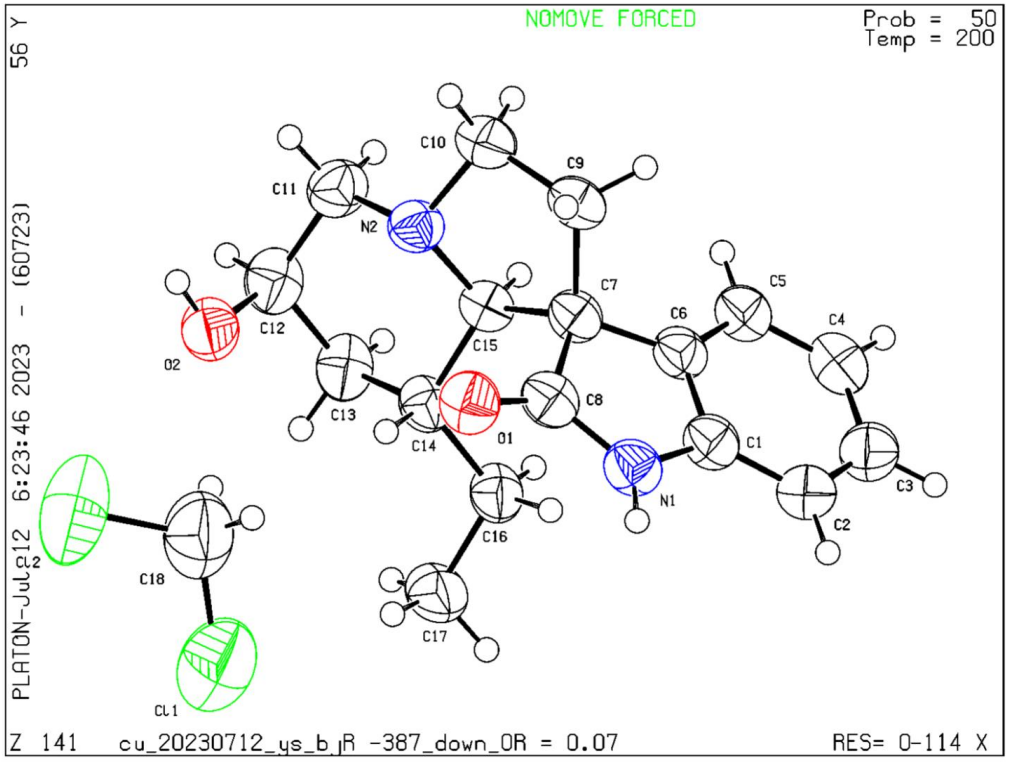
**Datablock exp_7208_auto** - ellipsoid plot




| The crystal data of compound **3g** | |
|---|---|
| Empirical formula | $C_{15}H_{12}N_2O_2$ |
| Formula weight | 252.27 |
| Temperature/K | 99.99(10) |
| Crystal system | orthorhombic |
| Space group | $P2_12_12_1$ |
| a/Å | 14.3604(3) |
| b/Å | 9.4124(2) |
| c/Å | 8.6308(2) |
| α/° | 90 |
| β/° | 90 |
| γ/° | 90 |
| Volume/Å$^3$ | 1166.59(4) |
| Z | 4 |
| $\rho_{calc}$g/cm$^3$ | 1.436 |
| μ/mm$^{-1}$ | 0.792 |
| F(000) | 528.0 |
| Crystal size/mm$^3$ | 0.3 × 0.2 × 0.2 |
| Radiation | CuKα (λ = 1.54184) |
| 2Θ range for data collection/° | 11.24 to 152.214 |

| | |
|---|---|
| Index ranges | -13 ≤ h ≤ 18, -9 ≤ k ≤ 11, -10 ≤ l ≤ 10 |
| Reflections collected | 7195 |
| Independent reflections | 2302 [$R_{int}$ = 0.0452, $R_{sigma}$ = 0.0356] |
| Data/restraints/parameters | 2302/0/172 |
| Goodness-of-fit on $F^2$ | 1.080 |
| Final R indexes [I>=2σ (I)] | $R_1$ = 0.0466, $wR_2$ = 0.1222 |
| Final R indexes [all data] | $R_1$ = 0.0475, $wR_2$ = 0.1228 |
| Largest diff. peak/hole / e $Å^{-3}$ | 0.42/-0.25 |
| Flack parameter | 0.45(17) |

The crystal data of compound **10** has been deposited in CCDC with number 2282806.

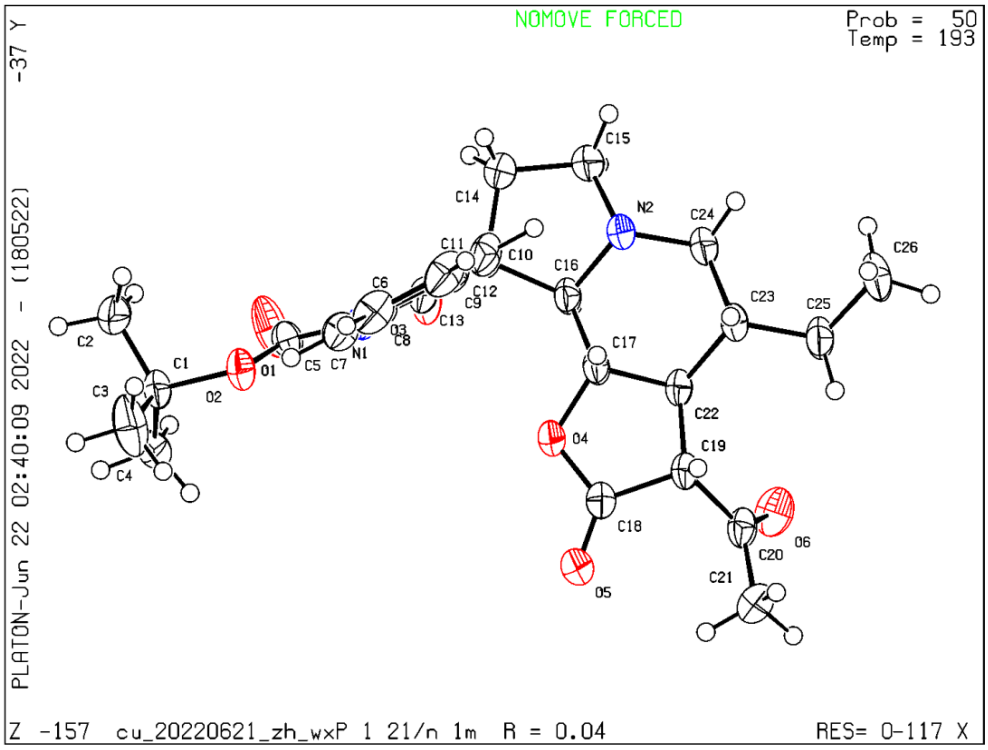



The crystal data of compound **10**

| | |
|---|---|
| Empirical formula | $C_{18}H_{24}Cl_2N_2O_2$ |
| Formula weight | 371.29 |
| Temperature/K | 200.00 |
| Crystal system | trigonal |
| Space group | R-3 |
| a/Å | 25.6161(14) |
| b/Å | 25.6161(14) |
| c/Å | 16.3068(13) |
| $\alpha$/° | 90 |
| $\beta$/° | 90 |
| $\gamma$/° | 120 |

| | |
|---|---|
| Volume/Å$^3$ | 9266.7(13) |
| Z | 18 |
| $\rho_{calc}$g/cm$^3$ | 1.198 |
| $\mu$ /mm$^{-1}$ | 2.927 |
| F(000) | 3528.0 |
| Crystal size/mm$^3$ | 0.14 × 0.12 × 0.11 |
| Radiation | CuK$\alpha$ ($\lambda$ = 1.54178) |
| 2$\Theta$ range for data collection/° | 11.562 to 136.792 |
| Index ranges | -30 ≤ h ≤ 27, -30 ≤ k ≤ 30, -19 ≤ l ≤ 18 |
| Reflections collected | 11974 |
| Independent reflections | 3752 [$R_{int}$ = 0.0841, $R_{sigma}$ = 0.0645] |
| Data/restraints/parameters | 3752/0/220 |
| Goodness-of-fit on F$^2$ | 1.034 |
| Final R indexes [I>=2$\sigma$ (I)] | $R_1$ = 0.0741, w$R_2$ = 0.2047 |
| Final R indexes [all data] | $R_1$ = 0.1152, w$R_2$ = 0.2383 |
| Largest diff. peak/hole / e Å$^{-3}$ | 1.13/-0.46 |

The crystal data of compound **15** has been deposited in CCDC with number 2282684.

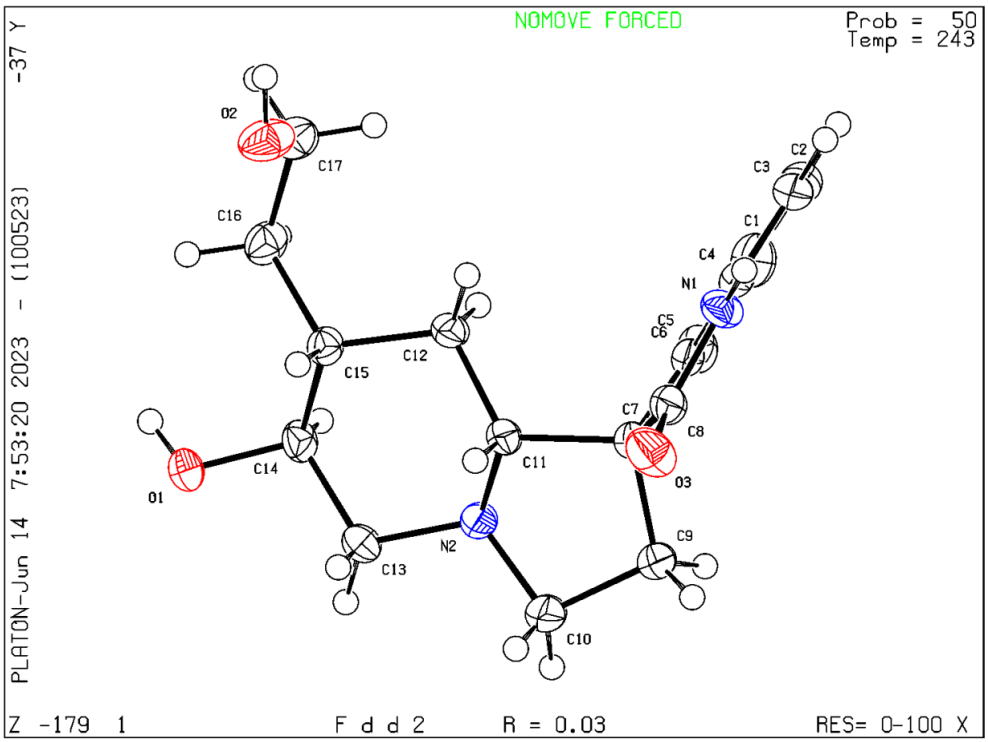



The crystal data of compound **15**

| | |
|---|---|
| Empirical formula | $C_{26}H_{32}N_2O_6$ |
| Formula weight | 468.53 |
| Temperature/K | 193.00 |

| | |
|---|---|
| Crystal system | monoclinic |
| Space group | $P2_1/n$ |
| a/Å | 8.6768(2) |
| b/Å | 14.2601(3) |
| c/Å | 20.0588(4) |
| α/° | 90 |
| β/° | 92.1130(10) |
| γ/° | 90 |
| Volume/Å$^3$ | 2480.23(9) |
| Z | 4 |
| $\rho_{calc}$g/cm$^3$ | 1.255 |
| μ/mm$^{-1}$ | 0.730 |
| F(000) | 1000.0 |
| Crystal size/mm$^3$ | 0.16 × 0.13 × 0.12 |
| Radiation | CuKα (λ = 1.54178) |
| 2Θ range for data collection/° | 7.608 to 136.598 |
| Index ranges | -10 ≤ h ≤ 10, -17 ≤ k ≤ 15, -23 ≤ l ≤ 24 |
| Reflections collected | 37603 |
| Independent reflections | 4540 [$R_{int}$ = 0.0384, $R_{sigma}$ = 0.0207] |
| Data/restraints/parameters | 4540/0/312 |
| Goodness-of-fit on $F^2$ | 1.029 |
| Final R indexes [I>=2σ (I)] | $R_1$ = 0.0414, $wR_2$ = 0.1038 |
| Final R indexes [all data] | $R_1$ = 0.0492, $wR_2$ = 0.1100 |
| Largest diff. peak/hole / e Å$^{-3}$ | 0.66/-0.42 |

The crystal data of compound **23** has been deposited in CCDC with number 2283109.

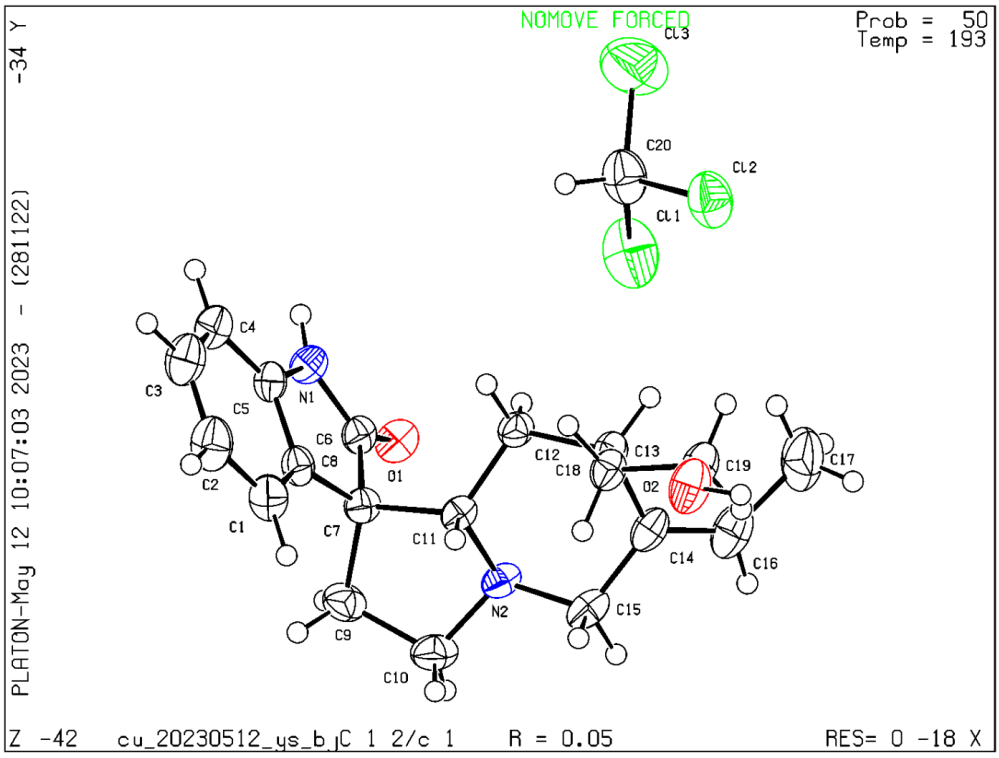



The crystal data of compound **23**

| | |
|---|---|
| Empirical formula | $C_{17}H_{22}N_2O_3$ |
| Empirical formula | |
| Formula weight | 302.36 |
| Temperature/K | 243.00 |
| Crystal system | orthorhombic |
| Space group | Fdd2 |
| a/Å | 17.4203(4) |
| b/Å | 42.9305(13) |
| c/Å | 8.1319(2) |
| α/° | 90 |
| β/° | 90 |
| γ/° | 90 |
| Volume/Å$^3$ | 6081.5(3) |
| Z | 16 |
| $\rho_{calc}$g/cm$^3$ | 1.321 |
| μ/mm$^{-1}$ | 0.737 |
| F(000) | 2592.0 |
| Crystal size/mm$^3$ | 0.13 × 0.12 × 0.11 |
| Radiation | CuKα (λ = 1.54178) |
| 2Θ range for data collection/° | 8.238 to 136.534 |
| Index ranges | -20 ≤ h ≤ 20, -51 ≤ k ≤ 51, -9 ≤ l ≤ 8 |
| Reflections collected | 45205 |
| Independent reflections | 2740 [$R_{int}$ = 0.0402, $R_{sigma}$ = 0.0164] |

| | |
|---|---|
| Data/restraints/parameters | 2740/1/202 |
| Goodness-of-fit on $F^2$ | 1.074 |
| Final R indexes [I>=2σ (I)] | $R_1$ = 0.0299, $wR_2$ = 0.0842 |
| Final R indexes [all data] | $R_1$ = 0.0305, $wR_2$ = 0.0848 |
| Largest diff. peak/hole / e $Å^{-3}$ | 0.39/-0.18 |

The crystal data of compound **27** has been deposited in CCDC with number 2283107.

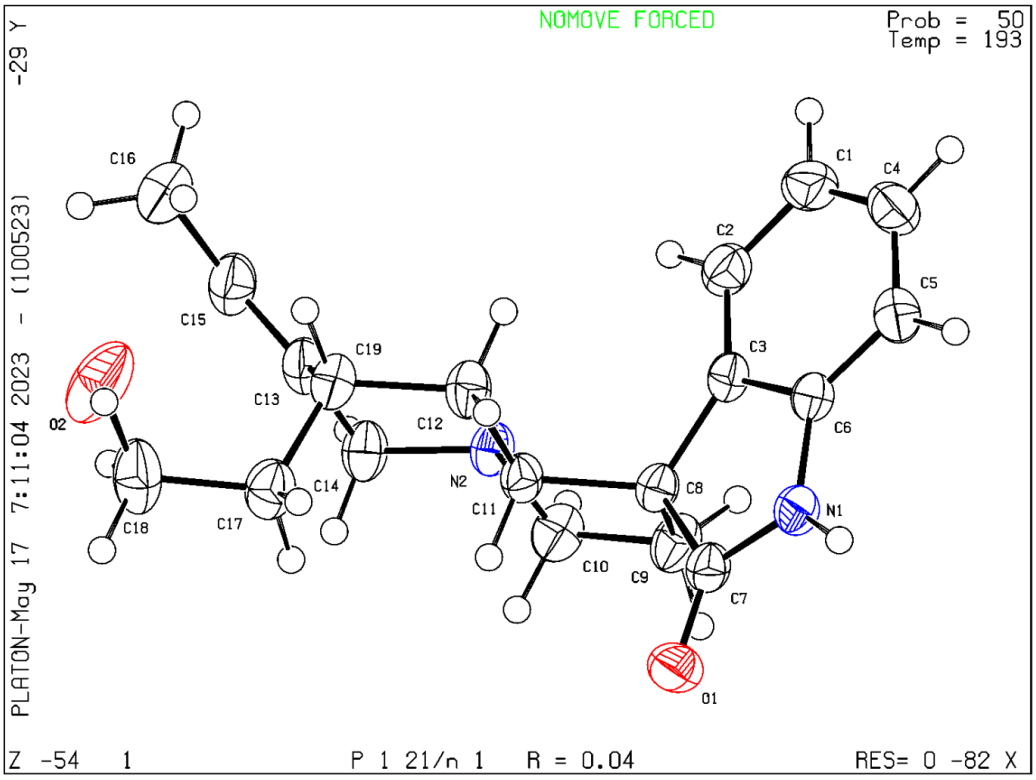



The crystal data of compound **27**

| | |
|---|---|
| Empirical formula | $C_{20}H_{25}Cl_3N_2O_2$ |
| Formula weight | 431.77 |
| Temperature/K | 193.15 |
| Crystal system | monoclinic |
| Space group | C2/c |
| a/Å | 20.2581(7) |
| b/Å | 10.2318(3) |
| c/Å | 20.6978(5) |
| α/° | 90 |
| β/° | 97.037(2) |
| γ/° | 90 |
| Volume/$Å^3$ | 4257.9(2) |
| Z | 8 |
| $\rho_{calc}g/cm^3$ | 1.347 |
| $\mu/mm^{-1}$ | 4.037 |
| F(000) | 1808.0 |
| Crystal size/$mm^3$ | 0.13 × 0.11 × 0.1 |

| | |
|---|---|
| Radiation | CuKα (λ = 1.54178) |
| 2Θ range for data collection/° | 8.608 to 136.648 |
| Index ranges | -24 ≤ h ≤ 24, -12 ≤ k ≤ 12, -24 ≤ l ≤ 24 |
| Reflections collected | 51503 |
| Independent reflections | 3910 [$R_{int}$ = 0.0553, $R_{sigma}$ = 0.0235] |
| Data/restraints/parameters | 3910/0/246 |
| Goodness-of-fit on $F^2$ | 1.096 |
| Final R indexes [I>=2σ (I)] | $R_1$ = 0.0497, $wR_2$ = 0.1403 |
| Final R indexes [all data] | $R_1$ = 0.0556, $wR_2$ = 0.1457 |
| Largest diff. peak/hole / e $Å^{-3}$ | 0.81/-0.71 |

The crystal data of compound **28** has been deposited in CCDC with number 2283108.




The crystal data of compound **28**

| | |
|---|---|
| Empirical formula | $C_{19}H_{24}N_2O_2$ |
| Formula weight | 312.40 |
| Temperature/K | 193.00 |
| Crystal system | monoclinic |
| Space group | $P2_1/n$ |
| a/Å | 13.7001(5) |
| b/Å | 6.7852(2) |
| c/Å | 19.5638(6) |
| α/° | 90 |
| β/° | 107.516(2) |

| | |
|---|---|
| γ/° | 90 |
| Volume/Å$^3$ | 1734.29(10) |
| Z | 4 |
| $\rho_{calc}$g/cm$^3$ | 1.196 |
| μ/mm$^{-1}$ | 0.618 |
| F(000) | 672.0 |
| Crystal size/mm$^3$ | 0.13 × 0.12 × 0.11 |
| Radiation | CuKα (λ = 1.54178) |
| 2Θ range for data collection/° | 6.994 to 136.634 |
| Index ranges | -16 ≤ h ≤ 16, -8 ≤ k ≤ 6, -19 ≤ l ≤ 23 |
| Reflections collected | 13998 |
| Independent reflections | 3140 [$R_{int}$ = 0.0548, $R_{sigma}$ = 0.0381] |
| Data/restraints/parameters | 3140/0/210 |
| Goodness-of-fit on F$^2$ | 1.067 |
| Final R indexes [I>=2σ (I)] | $R_1$ = 0.0448, w$R_2$ = 0.1214 |
| Final R indexes [all data] | $R_1$ = 0.0531, w$R_2$ = 0.1264 |
| Largest diff. peak/hole / e Å$^{-3}$ | 0.22/-0.23 |

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