

Supporting Information

Alkali Ion Tuned Chemoselective Indolation of Allylic Alcohols by Base Catalysis

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Contents

1. General information	1
2. General analytical information.....	2
3. General experiment	2
3.1 Reaction optimization	2
3.2 General method for the substrate screenings	3
4. The synthesis of allylic alcohols.....	3
4.1 Route 1 of primary allylic alcohols	3
4.2 Route 2 of primary allylic alcohols	4
4.3 The synthesis of 1o.....	5
4.4 The synthesis of 1b-D	5
4.5 The synthesis of N-N-B	5
5. Mechanism investigation	6
5.1 Deuterium hydrogen labeling experiment for 3t-D.....	6
5.2 Deuterium hydrogen labeling experiment for 5q-D.....	6
5.3 The kinetic isotope effect of parallel reactions for 1,2-addition.....	8
5.4 The kinetic isotope effect of parallel reactions for 1,4-addition.....	9
6. Density functional theory studies	9
6.1 Density functional theory studies for 1,2-addition	9
6.2 Density functional theory studies for 1,4-addition	10
7. Characterization data of all products	11
8. References.....	25
9. ¹ H and ¹³ C NMR spectra of all products	27
10. Crystallographic details of 5n	112
11. Cartesian coordinates	112

1. General information

General Information: Commercial reagents were purchased and used without further purification.

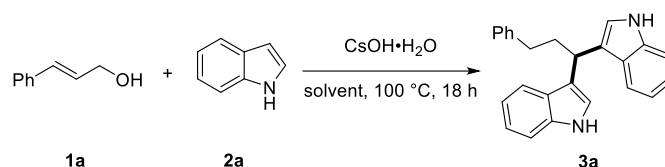
All glassware was dried and reactions were performed under a nitrogen atmosphere, unless otherwise stated. Flash column chromatography was performed using silica gel from Qindao Haiyang. Anhydrous solvents tetrahydrofuran (THF), Ethanol, *N,N*-dimethylformamide (DMF), ethyl acetate (EtOAc), acetonitrile (CH₃CN), Toluene and water were purchased and used as received. ¹H and ¹³C NMR data was acquired on a Bruker 400 MHz spectrometer and referenced to residual protic solvent. High-resolution mass spectrometry was performed at the University of Sun Yat-sen at the test center.

2. General analytical information

All new compounds were characterized by NMR spectroscopy, and high-resolution mass spectroscopy. NMR spectra were recorded on a Bruker Ascend TM 400 spectrometer and were calibrated using TMS or residual deuterated solvent as an internal reference (CDCl₃: 7.26 ppm for ¹H NMR and 77.16 ppm for ¹³C NMR; DMSO: 2.5 ppm for ¹H NMR and 39.6 ppm for ¹³C NMR).

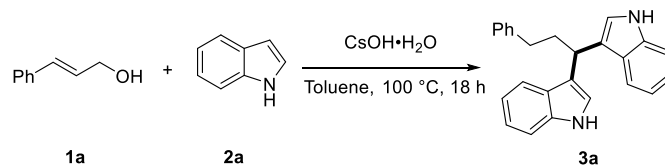
3. General experiment

3.1 Reaction optimization



Entry	Solvent	T/°C	t/h	^a Y%/ ^c 3a
1	THF	100	18	85
2	DMF	100	18	n.r.
3	EtOH	100	18	trace
4	H ₂ O	100	18	n.r.
5	MeCN	100	18	n.d.
6	Toluene	100	18	88

Table S1 The investigation of solvent for **3a**: ^aReaction conditions: **1a** (0.3 mmol), **2a** (0.75 mmol), CsOH•H₂O (0.3 mmol), toluene (1 mL), 100 °C, 24 h, N₂; ^bIsolated yield; ^cYield determined by ¹H NMR spectroscopy, using 1,3,5-trimethoxybenzene as the internal standard.



Entry	1a/2a	T/°C	Base(x eq.)	t/h	Y%/ 3a
1	1/2	100	1	18	74
2	1/2.5	100	1	18	88
3	1/2.5	80	1	18	23
4	1/2.5	100	0.5	18	66

5	1/2.5	100	0.5	24	71
6	1/2.5	120	0.5	18	96
7	1/2.5	120	0.5	24	87^b/100

Table S2 The parameters optimization for **3a**: ^aReaction conditions: **1a** (0.3 mmol), **2a** (0.75 mmol), CsOH•H₂O (0.3 mmol), toluene (1 mL), 100 °C, 24 h, N₂; ^bIsolated yield; ^cYield determined by ¹H NMR spectroscopy, using 1,3,5-trimethoxybenzene as the internal standard.

Reaction scheme: 1a + 2a $\xrightarrow{\text{NaO}^t\text{Bu, toluene}}$ 5a + 6a

Entry	1a/2a	1 eq. base	T/°C	t/h	Y%/ 5a	Y%/6a
1	1/2.5	NaO ^t Bu	120	18	99	-
2	1/1.5	NaO ^t Bu	120	18	99	7
3	1/1	NaO ^t Bu	120	18	89	-
4	1/1.5	NaO^tBu (0.5)	120	24	67^b/99	9
5	1/1.5	NaO ^t Bu (0.5)	100	24	78	-

Table S3 The optimization of reaction conditions of **5a**: ^aReaction conditions: **1a** (0.3 mmol), **2a** (0.75 mmol), NaO^tBu (0.3 mmol), toluene (1 mL), 100 °C, 24 h, N₂; ^bIsolated yield; ^cYield determined by ¹H NMR spectroscopy, using 1,3,5-trimethoxybenzene as the internal standard.

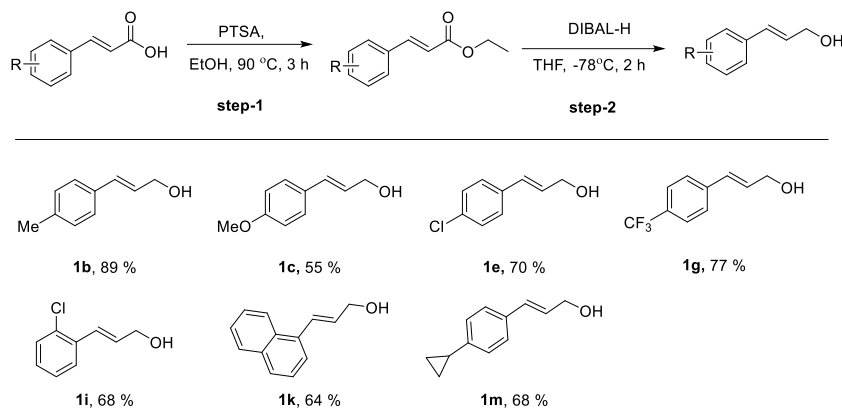
3.2 General method for the substrate screenings

Procedure for bis(indolyl)methane derivatives: To a 15 mL reaction tube in a glovebox, was added allylic alcohol (0.3 mmol), indole (0.75 mmol) CsOH•H₂O, and toluene (1 mL). Then the tube was closed and removed from the glovebox. The reaction mixture was stirred for 24 h at 120 °C. The reaction was completed, cooled to room temperature, and quenched with methanol. The solvent was evaporated to dryness and the corresponding bis(indolyl)methane derivative was purified by column chromatography with silica gel (ethyl acetate/ petroleum ether). The yields were calculated based on isolated products.

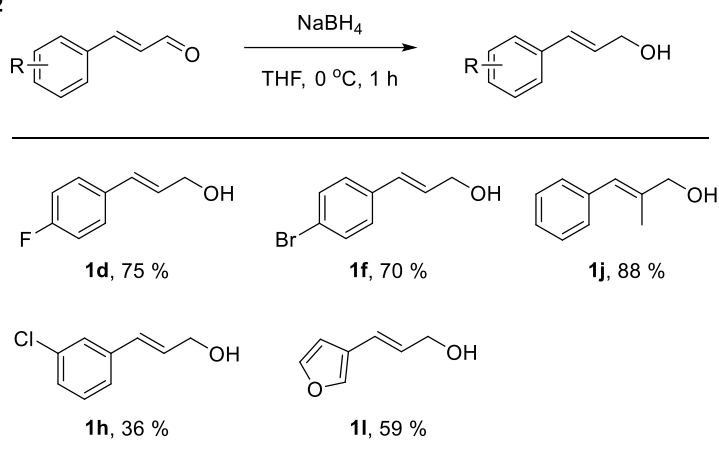
Procedure for 1,4-addition reaction: To a 15 mL reaction tube in a glovebox, was added allylic alcohol (0.3 mmol), indole (0.45 mmol) NaO^tBu, and toluene (1 mL). Then the tube was closed and removed from the glovebox. The reaction mixture was stirred for 24 h at 120 °C. The reaction was completed, cooled to room temperature, and quenched with methanol. The solvent was evaporated to dryness and the corresponding product was purified by column chromatography with silica gel (ethyl acetate/ petroleum ether). The yields were calculated based on isolated products.

4. The synthesis of allylic alcohols

4.1 Route 1 of primary allylic alcohols

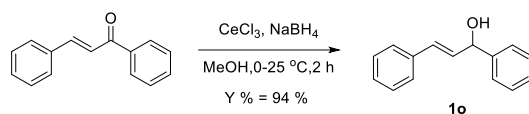
Route 1

The mixture of cinnamic acid derivatives (1 equiv.) and 4-methylbenzenesulfonic acid (0.3 equiv.) in EtOH was stirred under 90 °C for 3 h. After completion of the reaction, ethanol was removed under reduced pressure. The residue was diluted with ethyl acetate and saturated sodium bicarbonate solution. The organic layer was washed with brine, dried with anhydrous MgSO_4 , and concentrated under vacuum. Diisobutylaluminum hydride was slowly added to a stirred solution of ester in THF at -78 °C and was stirred for 1 h, then slowly warmed to room temperature, and stirred for another 1 h. After completion, the reaction was quenched by 0.5M hydrochloric acid solution and extracted with ethyl acetate. The organic layer was dried over anhydrous Na_2SO_4 , concentrated, and purified by silica gel column chromatography using (ethyl acetate/ether 10:1) to afford corresponding cinnamyl alcohol. ^[1]

4.2 Route 2 of primary allylic alcohols**Route 2**

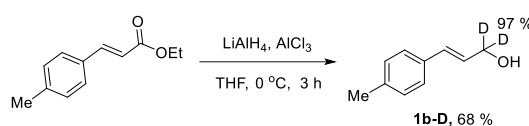
NaBH_4 was slowly poured into a solution of aldehyde in THF at 0 °C and was stirred for 1 h. After completion, the reaction was quenched with cold water and extracted with ethyl acetate. The organic layer was dried over anhydrous Na_2SO_4 , concentrated, and purified by silica gel column chromatography using (ethyl acetate/ether 10:1) to afford corresponding cinnamyl alcohol. ^[2]

4.3 The synthesis of **1o**



To a mixture of (*E*)-chalcone(500 mg, 2.4 mmol) and CeCl_3 (2.4 mmol) was added prepared NaBH_4 (2.4mmol) at 0 °C and stirred for 2 h. The reaction was quenched by the addition of 1 M HCl and extracted with CH_2Cl_2 . The combined organic extracts were washed with brine, dried over anhydrous MgSO_4 , filtered, concentrated, and purified on silica gel chromatography to give **1o**.^[3]

4.4 The synthesis of **1b-D**



To a solution of cinnamic acid derivative(10 mmol) in dry THF (30 mL) was added dropwise to a well-stirred suspension of LiAlH_4 (24 mmol) and AlCl_3 (10 mmol) in THF (15 mL) at 0 °C. The reaction mixture was stirred at this temperature for 4 h, checked by TLC, the reaction was quenched by cold water. The solid residue was removed by filtration and washed with DCM-EtOH. The filtrate was dried over anhydrous Na_2SO_4 , concentrated, and purified by silica gel column chromatography using (ethyl acetate/ether 10:1) to afford white solid(**1b-D**, 1.1 g, 68 %).^[4] ^1H NMR (400 MHz, Chloroform- d) δ 7.28 (t, J = 7.7 Hz, 2H), 7.13 (d, J = 7.9 Hz, 2H), 6.59 (d, J = 15.8 Hz, 1H), 6.32 (d, J = 15.9 Hz, 1H), 2.34 (s, 3H), 1.51 (s, 1H). ^{13}C NMR (100 MHz, Chloroform- d) δ 137.6, 133.9, 131.4, 129.3, 127.3, 126.4, 63.2, 21.2.

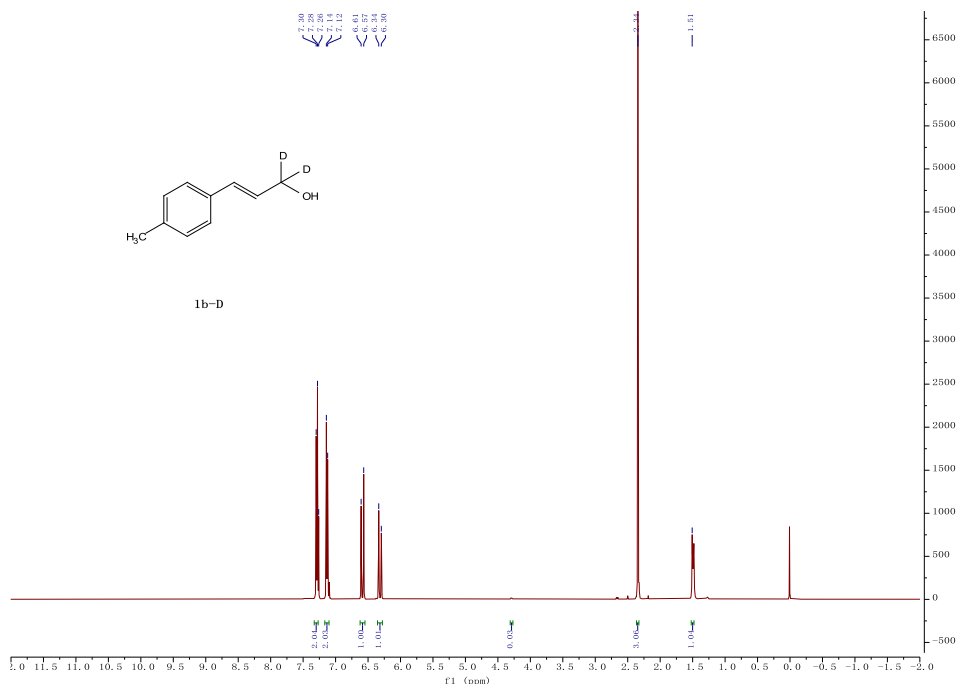
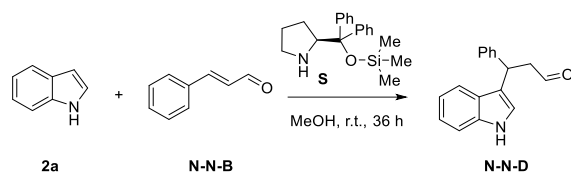


Figure S1 ^1H NMR of **1b-D**

4.5 The synthesis of N-N-B



To a solution of **N-N-B** (1 eq.) and **S** (0.2 eq.) in MeOH was added indole (**2a**, 1.2eq.). The mixture was stirred at room temperature for 36 h. The reaction was quenched by water and extracted with CH_2Cl_2 . The combined organic extracts were washed with brine, dried over anhydrous MgSO_4 , filtered, concentrated, and purified on silica gel chromatography to afford **N-N-D**.^[5]

5. Mechanism investigation

5.1 Deuterium hydrogen labeling experiment for 3t-D

The mixture of (*E*)-3-(*p*-tolyl)prop-2-en-1,1-d₂-1-ol (**1b-D**, 0.3 mmol), indole (**2a**, 0.75 mmol) and $\text{CsOH}\cdot\text{H}_2\text{O}$ (0.15 mmol) was stirred at 120°C for 48 h under N_2 . The reaction was quenched by MeOH and concentrated and purified on silica gel chromatography (PE/EA=5/1) to afford **3,3'-(3-(*p*-tolyl)propane-1,1-diyl-1,3-d₂)bis(1*H*-indole)** (**3t-D**) as a white solid (93.2 mg, 85 %). ¹H NMR (400 MHz, Chloroform-*d*) δ 7.79 (s, 2H), 7.62 (d, *J* = 7.9 Hz, 2H), 7.38 – 7.32 (m, 2H), 7.25 – 7.19 (m, 2H), 7.18 – 7.07 (m, 6H), 6.99 (d, *J* = 2.4 Hz, 2H), 4.56 (s, 0.06H), 2.74 (d, *J* = 8.4 Hz, 1.64H), 2.59 (dd, *J* = 8.7, 6.4 Hz, 2H), 2.40 (s, 3H). ¹³C NMR (100 MHz, Chloroform-*d*) δ 139.6, 139.6, 136.7, 135.1, 129.0, 128.5, 127.1, 121.8, 121.6, 120.1, 119.7, 119.1, 111.2, 37.5, 37.4, 34.0, 21.1.

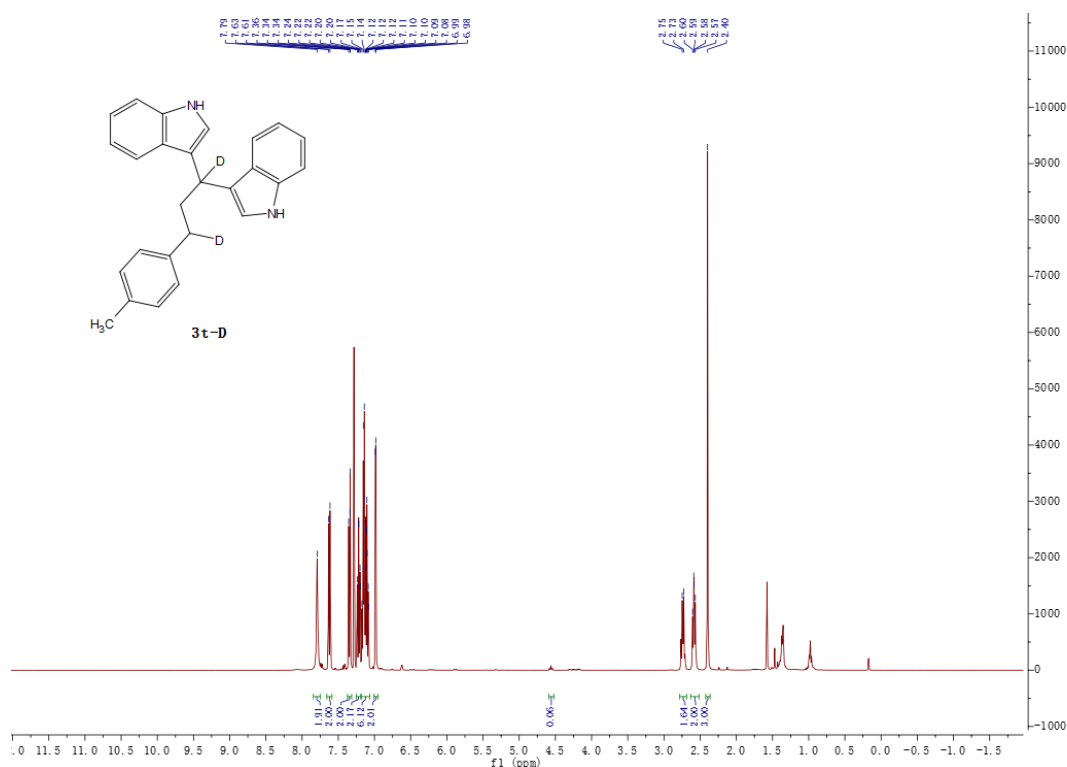


Figure S2 ¹H NMR of 3t-D

5.2 Deuterium hydrogen labeling experiment for 5q-D

The mixture of (*E*)-3-(*p*-tolyl)prop-2-en-1,1-d₂-1-ol (**1b-D**, 0.3 mmol), indole (**2a**, 0.45 mmol) and

NaO^tBu(0.15 mmol) was stirred at 120 °C for 24 h under N₂. The reaction was quenched by MeOH and concentrated and purified on silica gel chromatography (PE/EA=3/1) to afford 3-(1*H*-indol-3-yl)-3-(*p*-tolyl)propan-1,1-d₂-1-ol(**5q-D**) as a white solid(54.0 mg, 68 %). ¹H NMR (400 MHz, Chloroform-*d*) δ 8.05 (s, 1H), 7.51 (d, *J* = 8, 1H), 7.37 – 7.32 (m, 1H), 7.25 (d, *J* = 8.0 Hz, 2H), 7.21-7.17 (m, 1H), 7.12 (d, *J* = 8 Hz, 2H), 7.09 – 7.02 (m, 2H), 4.39 (t, *J* = 7.7 Hz, 1H), 3.69 (q, *J* = 6.8 Hz, 0.03H), 2.47 (dd, *J* = 13.5, 7.0 Hz, 1H), 2.34 (s, 3H), 2.28 (dd, *J* = 13.6, 8.5 Hz, 1H), 1.50 (s, 1H). ¹³C NMR (100 MHz, Chloroform-*d*) δ 141.8, 136.7, 135.7, 129.3, 127.8, 127.0, 122.1, 121.6, 112.0, 119.63, 119.4, 111.2, 60.8, 38.9, 38.7, 21.1. ESI-HRMS: *m/z* calculated for C₁₈H₁₈D₂NO[M+H]⁺: 268.1665; found: 268.1665.

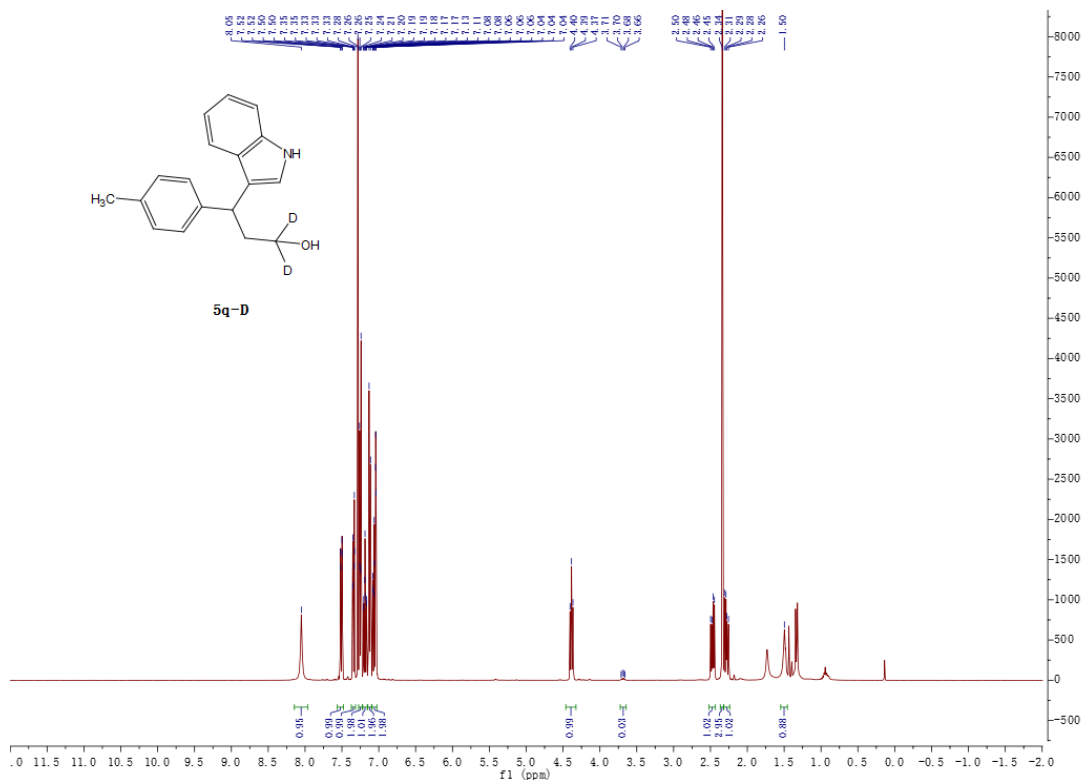


Figure S3 ¹H NMR of **5q-D**

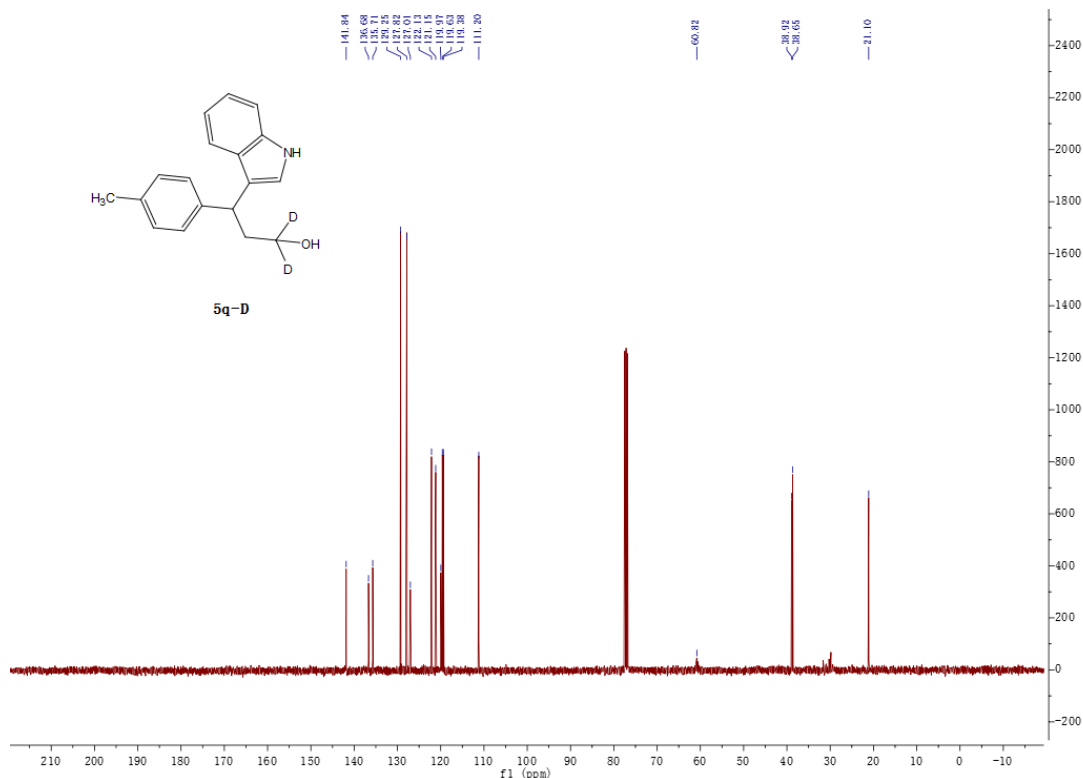


Figure S4 ^{13}C NMR of 5q-D

5.3 The kinetic isotope effect of parallel reactions for 1,2-addition.

Twelve parallel reactions, six with (*E*)-3-(*p*-tolyl)prop-2-en-1-ol (**1b**, 0.15 mmol) and other six with (*E*)-3-(*p*-tolyl)prop-2-en-1,1-d₂-1-ol (**1b-D**, 0.15 mmol), were carried out under standard condition for 1,2-addition reaction. To a 15 mL reaction tube in a glovebox, was added indole (0.375 mmol), CsOH•H₂O (0.075 mmol) and toluene (0.5 mL). Then the tube was sealed and removed from the glovebox. The reaction mixture was stirred at 120 °C, the reaction vessels were taken after 80, 90, 100, 110, 120, and 130 min. Yields of products were determined by ^1H NMR spectroscopy, using 1,3,5-trimethoxybenzene as the internal standard. The calculated KIE ($k_{\text{H}}/k_{\text{D}}$) was 2.5 (Figure S5), which suggested that the isomerization of the allylic alcohol is involved in the rate-determining step (RDS) of the reaction.

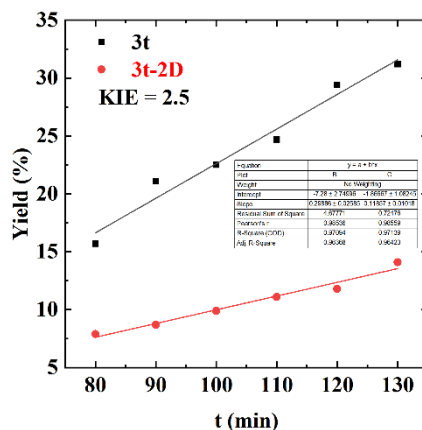


Figure S5 parallel reactions for 1,2-addition

5.4 The kinetic isotope effect of parallel reactions for 1,4-addition.

Twelve parallel reactions, six with (*E*)-3-(*p*-tolyl)prop-2-en-1-ol (**1b**, 0.15 mmol) and other six with (*E*)-3-(*p*-tolyl)prop-2-en-1,1-d₂-1-ol (**1b-D**, 0.15 mmol), were carried out under standard condition for 1,4-addition reaction. To a 15 mL reaction tube in a glovebox, was added indole (0.225 mmol), NaO^tBu (0.075 mmol) and toluene (0.5 mL). Then the tube was sealed and removed from the glovebox. The reaction mixture was stirred at 120 °C, the reaction vessel was taken after 4, 5, 6, 8, and 9 min. Yields of products were determined by ¹H NMR spectroscopy, using 1,3,5-trimethoxybenzene as the internal standard. The calculated KIE (k_H/k_D) was 2.5 (Figure S6), which suggested that hydrogen transfer of the allylic alcohol is involved in the rate-determining step (RDS) of the reaction.

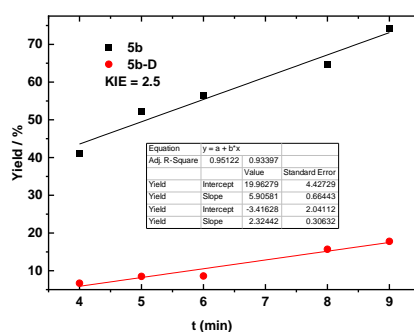


Figure S6 Parallel reactions for 1,4-addition

6. Density functional theory studies

All the calculations were performed by the Gaussian 09 program.⁶ The 3D structures were displayed by the VMD program.⁷

All the structures were optimized by the density functional theory(B3LYP with D3 empirical dispersion correction) with basis set I (BSI, SDD for metal element and 6-31G* for nonmetal element) in the gas phase. Frequency analysis calculation was applied to the optimized structures to make sure it's the minimum point (no imaginary frequency) or transition state (one imaginary frequency). IRC calculation was taken to confirm the transition state was connected to two minima. Based on the optimized structures, the energy results were refined by calculating the single point energy with B3LYP (D3 empirical dispersion correction) and basis set II (BSII, SDD for metal element and 6-311g** nonmetal for nonmetal element) with the correction of solvent effect (SMD,solvent=toluene).

6.1 Density functional theory studies for 1,2-addition

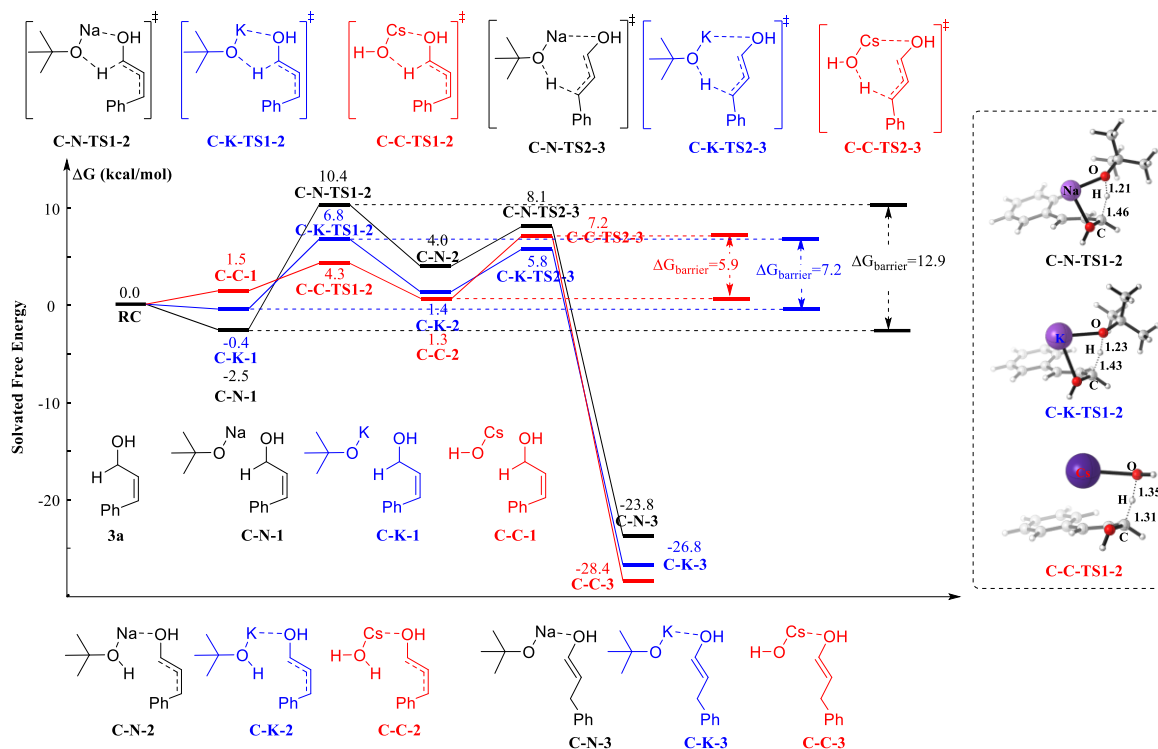


Figure S7 Calculated Gibbs free energy profiles for 1,2-addition pathways at the B3LYP-D3/BSII/SMD(toluene)/B3LYP-D3/BSI. Value are given in kcal/mol.

6.2 Density functional theory studies for 1,4-addition

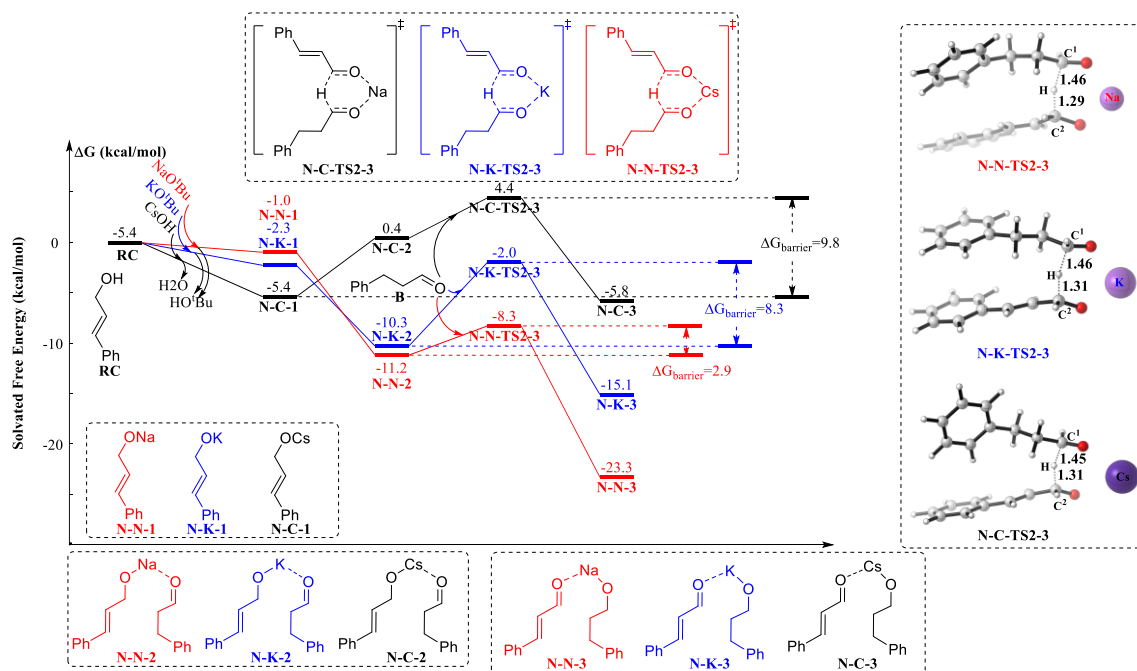
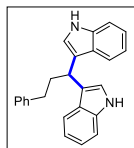


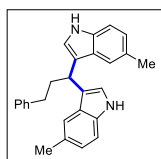
Figure S8 Calculated Gibbs free energy profiles for 1,4-addition pathways at the B3LYP-D3/BSII/SMD(toluene)/B3LYP-D3/BSI for metal,. Value are given in kcal/mol.

7. Characterization data of all products

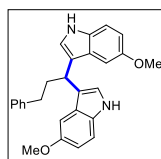
3,3'-(3-phenylpropane-1,1-diyl)bis(1H-indole)(3a)^[8]: Purified by silica-gel column chromatography (EA/PE=1/5). White solid. Yield: 91.4 mg, 87 %. ¹H NMR (400 MHz, Chloroform-*d*) δ 7.80 (s, 2H), 7.57 – 7.48 (m, 2H), 7.33 – 7.21 (m, 4H), 7.20 – 7.10 (m, 5H), 7.02 (td, *J* = 7.5, 6.9, 1.1 Hz, 2H), 6.95 (d, *J* = 2.4 Hz, 2H), 4.49 (t, *J* = 7.4 Hz, 1H), 2.73-1.69 (m, 2H), 2.60 – 2.45 (m, 2H). ¹³C NMR (100 MHz, Chloroform-*d*) δ 142.8, 136.7, 128.7, 128.4, 127.2, 125.8, 121.9, 121.7, 120.1, 119.8, 119.2, 111.2, 37.5, 34.6, 33.6.



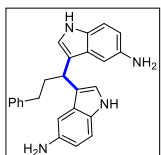
3,3'-(3-phenylpropane-1,1-diyl)bis(5-methyl-1H-indole)(3b): Purified by silica-gel column chromatography (EA/PE=1/5). White solid. Yield: 112 mg, 99 %. ¹H NMR (400 MHz, Chloroform-*d*) δ 7.61 (s, 2H), 7.48 (s, 2H), 7.44 (t, *J* = 7.4 Hz, 2H), 7.38 – 7.30 (m, 3H), 7.27 (d, *J* = 6.6 Hz, 2H), 7.12 (dd, *J* = 8.3, 1.6 Hz, 2H), 6.91 (d, *J* = 2.4 Hz, 2H), 4.58 (t, *J* = 7.3 Hz, 1H), 2.89-2.85 (m, 2H), 2.67-2.60 (m, 2H), 2.56 (s, 6H). ¹³C NMR (100 MHz, Chloroform-*d*) δ 142.9, 135.1, 128.8, 128.4, 128.3, 127.4, 125.9, 123.5, 122.0, 119.6, 119.4, 111.0, 37.6, 34.6, 33.4, 21.7; **ESI-HRMS**: *m/z* calculated for C₂₇H₂₅N₂[M-H]⁻: 377.2023; found: 377.2023



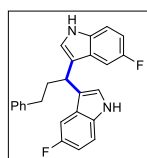
3,3'-(3-phenylpropane-1,1-diyl)bis(5-methoxy-1H-indole)(3c): Purified by silica-gel column chromatography (EA/PE=1/3). White solid. Yield: 111.9 mg, 89 %. ¹H NMR (400 MHz, Chloroform-*d*) δ 7.80 (s, 2H), 7.35 (t, *J* = 7.5 Hz, 2H), 7.30 – 7.22 (m, 4H), 7.21 (s, 1H), 7.00 (dd, *J* = 22.7, 2.4 Hz, 4H), 6.89 (dd, *J* = 8.7, 2.4 Hz, 2H), 4.43 (t, *J* = 7.3 Hz, 1H), 3.82 (s, 6H), 2.78 (t, *J* = 7.5 Hz, 2H), 2.65 – 2.52 (m, 2H). ¹³C NMR (100 MHz, Chloroform-*d*) δ 153.7, 142.8, 131.9, 128.8, 128.4, 127.6, 125.8, 122.5, 119.7, 111.9, 111.8, 101.8, 56.0, 37.3, 34.3, 33.0. **ESI-HRMS**: *m/z* calculated for C₂₇H₂₅N₂O₂[M-H]⁻: 409.1921; found: 409.1922.



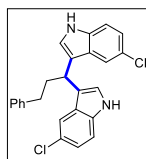
3,3'-(3-phenylpropane-1,1-diyl)bis(1H-indol-5-amine)(3d): Purified by silica-gel column chromatography (DCM/MeOH=10/1). Red solid. Yield: 50.2 mg, 44 %. ¹H NMR (400 MHz, DMSO-*d*₆) δ 10.26 (s, 2H), 7.35 – 7.24 (m, 2H), 7.18 (d, *J* = 7.4 Hz, 3H), 7.04 (d, *J* = 8.5 Hz, 2H), 6.97 (d, *J* = 2.1 Hz, 2H), 6.71 (d, *J* = 2.0 Hz, 2H), 6.46 (dd, *J* = 8.5, 2.1 Hz, 2H), 4.39-4.15 (m, 5H), 2.65-2.61 (m, 2H), 2.43-2.37 (m, 2H). ¹³C NMR (100 MHz, DMSO-*d*₆) δ 143.0, 140.6, 131.0, 128.8, 128.7, 128.0, 126.0, 122.3, 117.6, 112.0, 111.9, 103.1, 37.4, 34.7, 34.0; **ESI-HRMS**: *m/z* calculated for C₂₅H₂₅N₄[M+H]⁺: 381.2074; found: 381.2074.



3,3'-(3-phenylpropane-1,1-diyl)bis(5-fluoro-1H-indole)(3e): Purified by silica-gel column chromatography (PE/EA=5/1). Yellow solid. Yield: 114.6 mg, 99 %. ¹H NMR (400 MHz, Chloroform-*d*) δ 7.76 (s, 2H), 7.19 (dd, *J* = 8.1, 6.8 Hz, 2H), 7.12 – 7.04 (m, 5H), 7.01 (dd, *J* = 9.9, 2.6 Hz, 2H), 6.94 (d, *J* = 2.4 Hz, 2H), 6.78 (td, *J* = 9.1, 2.5 Hz, 2H), 4.22 (t, *J* = 7.4 Hz, 1H), 2.60-2.56 (m, 2H), 2.46 – 2.34 (m, 2H). ¹³C NMR (100 MHz, Chloroform-*d*) δ 158.7, 156.4, 142.4, 133.3, 128.6 (d, *J*-F = 15.8 Hz), 127.3 (d, *J*-F = 9.7 Hz), 126.0, 123.4, 119.8 (d, *J*-F = 4.7 Hz), 111.8 (d, *J*-F = 9.7 Hz), 110.4 (d, *J*-F = 26.4 Hz), 104.6 (d, *J*-F = 23.5 Hz), 36.9, 34.4, 33.7. **ESI-HRMS**: *z/s* calculated for C₂₅H₁₉F₂N₂[M-H]⁻: 385.1521; found: 385.1522.

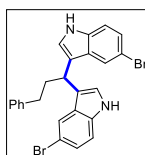


3,3'-(3-phenylpropane-1,1-diyl)bis(5-chloro-1H-indole)(3f): Purified by silica-gel column



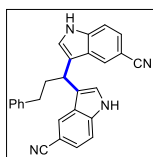
chromatography (PE/EA=3/1). Yellow solid. Yield: 112.8 mg, 90 %. ^1H NMR (400 MHz, Chloroform-*d*) δ 7.99 (s, 2H), 7.43 (d, J = 2.0 Hz, 2H), 7.34 – 7.26 (m, 3H), 7.22 (d, J = 10.7 Hz, 2H), 7.20 – 7.14 (m, 2H), 7.14 – 7.02 (m, 4H), 4.35 (t, J = 7.4 Hz, 1H), 2.71-2.67 (m, 2H), 2.60 – 2.44 (m, 2H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 142.2, 135.0, 128.6, 128.4, 127.9, 125.9, 124.9, 122.9, 122.3, 119.3, 119.0, 112.2, 36.8, 34.3, 33.4. **ESI-HRMS:** z/s calculated for $\text{C}_{25}\text{H}_{19}\text{Cl}_2\text{N}_2[\text{M}-\text{H}]^-$: 417.0930; found: 417.0930.

3,3'-(3-phenylpropane-1,1-diyl)bis(5-bromo-1H-indole)(3g): Purified by silica-gel column



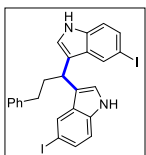
chromatography (PE/EA=5/1). White solid. Yield: 124.7 mg, 82 %. ^1H NMR (400 MHz, Chloroform-*d*) δ 8.01 – 7.90 (m, 2H), 7.59 (d, J = 1.7 Hz, 2H), 7.34 – 7.28 (m, 2H), 7.25 – 7.14 (m, 7H), 7.04 (d, J = 2.4 Hz, 2H), 4.34 (t, J = 7.4 Hz, 1H), 2.71-2.67 (m, 2H), 2.58 – 2.44 (m, 2H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 142.1, 135.3, 128.6, 128.6, 128.4, 125.9, 124.8, 122.7, 122.1, 119.2, 112.6, 112.5, 36.9, 34.3, 33.3. **ESI-HRMS:** z/s calculated for $\text{C}_{25}\text{H}_{19}\text{Br}_2\text{N}_2[\text{M}-\text{H}]^-$: 506.9900; found: 506.9902.

3,3'-(3-phenylpropane-1,1-diyl)bis(1H-indole-5-carbonitrile)(3j): Purified by silica-gel column



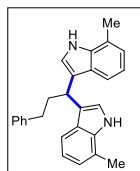
chromatography (DCM/MeOH=10/1). White solid. Yield: 30.1 mg, 25 %. ^1H NMR (400 MHz, DMSO-*d*₆) δ 11.46 (d, J = 2.4 Hz, 2H), 8.02 (s, 2H), 7.70 (d, J = 2.3 Hz, 2H), 7.48 (d, J = 8.4 Hz, 2H), 7.35 (dd, J = 8.4, 1.6 Hz, 2H), 7.27 (dd, J = 8.2, 6.9 Hz, 2H), 7.18 (d, J = 7.3 Hz, 3H), 4.52 (t, J = 7.2 Hz, 1H), 2.62-2.57 (m, 2H), 2.56 – 2.52 (m, 2H). ^{13}C NMR (100 MHz, DMSO-*d*₆) δ 142.5, 138.7, 128.8, 128.7, 126.6, 126.2, 125.6, 125.0, 124.0, 121.4, 119.6, 113.2, 100.6, 36.8, 34.4, 33.2. **ESI-HRMS:** z/s calculated for $\text{C}_{27}\text{H}_{21}\text{N}_4\text{O}[\text{M}+\text{OH}]^+$: 417.1721; found: 417.1721.

3,3'-(3-phenylpropane-1,1-diyl)bis(5-iodo-1H-indole)(3h): Purified by silica-gel column

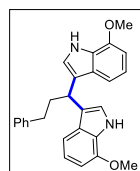


chromatography (PE/EA=3/1). White solid. Yield: 114.4 mg, 63 %. ^1H NMR (400 MHz, Chloroform-*d*) δ 7.92 (s, 2H), 7.81 (d, J = 1.7 Hz, 2H), 7.40 (dd, J = 8.5, 1.7 Hz, 2H), 7.33 (t, J = 7.5 Hz, 2H), 7.25 – 7.14 (m, 3H), 7.10 (d, J = 8.5 Hz, 2H), 6.95 (d, J = 2.4 Hz, 2H), 4.32 (t, J = 7.4 Hz, 1H), 2.68 (dd, J = 8.8, 6.4 Hz, 2H), 2.58 – 2.42 (m, 2H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 142.2, 135.8, 130.7, 129.5, 128.7, 128.6, 128.5, 126.1, 122.4, 119.0, 113.3, 82.9, 37.0, 34.3, 33.1. **ESI-HRMS:** z/s calculated for $\text{C}_{25}\text{H}_{19}\text{I}_2\text{N}_2[\text{M}-\text{H}]^-$: 600.9643; found: 600.9643.

3,3'-(3-phenylpropane-1,1-diyl)bis(7-methyl-1H-indole)(3m): Purified by silica-gel column



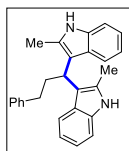
chromatography (PE/EA=3/1). White solid. Yield: 101 mg, 89 %. ^1H NMR (400 MHz, Chloroform-*d*) δ 7.56 (s, 2H), 7.38 (dd, J = 6.7, 2.3 Hz, 2H), 7.24 (dd, J = 8.0, 6.6 Hz, 2H), 7.19 – 7.12 (m, 3H), 7.01 – 6.86 (m, 4H), 6.81 (d, J = 2.4 Hz, 2H), 4.44 (t, J = 7.3 Hz, 1H), 2.71-2.67 (m, 2H), 2.59 – 2.43 (m, 2H), 2.37 (s, 6H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 142.8, 136.3, 128.7, 128.4, 126.8, 125.8, 122.4, 121.4, 120.7, 120.3, 119.4, 117.5, 37.5, 34.6, 33.8, 16.6. **ESI-HRMS:** m/z calculated for $\text{C}_{27}\text{H}_{25}\text{N}_2[\text{M}-\text{H}]^-$: 377.2023; found: 377.2023.



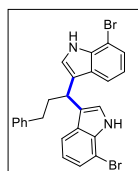
3,3'-(3-phenylpropane-1,1-diyl)bis(7-methoxy-1H-indole)(3n): Purified by silica-gel column chromatography (PE/EA=5/1). White solid. Yield: 96.8 mg, 79 %. ^1H NMR (400 MHz, Chloroform-*d*) δ 8.20 (s, 2H), 7.33 (d, J = 7.2 Hz, 2H), 7.26 – 7.21 (m, 5H),

7.10 – 6.94 (m, 4H), 6.68 (d, $J = 7.7$ Hz, 2H), 4.53 (t, $J = 7.4$ Hz, 1H), 3.98 (s, 6H), 2.84 – 2.74 (m, 2H), 2.61 (d, $J = 8.0$ Hz, 2H). ^{13}C NMR (100 MHz, Chloroform- d) δ 146.2, 142.8, 128.7, 128.6, 128.4, 127.2, 125.7, 121.5, 120.7, 119.5, 112.7, 101.8, 55.4, 37.6, 34.6, 33.9. **ESI-HRMS**: m/z calculated for $\text{C}_{27}\text{H}_{25}\text{N}_2\text{O}_2[\text{M}-\text{H}]^-$: 409.1921; found: 409.1922.

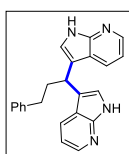
3,3'-(3-phenylpropane-1,1-diyl)bis(2-methyl-1H-indole)(3k)^[9]: Purified by silica-gel column chromatography (PE/EA=3/1). Pale yellow solid. Yield: 86 mg, 76 %. ^1H NMR (400 MHz, Chloroform- d) δ 7.65 (s, 2H), 7.62 (d, $J = 8$ Hz, 2H), 7.27-7.21 (m, 4H), 7.19 – 7.11 (m, 3H), 7.05 (ddd, $J = 8.0, 7.0, 1.3$ Hz, 2H), 6.98 (ddd, $J = 8.0, 7.0, 1.2$ Hz, 2H), 4.45 (t, $J = 7.3$ Hz, 1H), 2.83 – 2.66 (m, 4H), 2.28 (s, 6H). ^{13}C NMR (100 MHz, Chloroform- d) δ 142.7, 135.3, 131.0, 128.7, 128.6, 128.4, 125.8, 120.6, 119.5, 119.2, 114.7, 110.3, 36.4, 35.0, 34.5, 12.9.



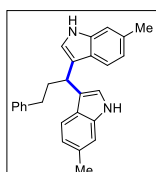
3,3'-(3-phenylpropane-1,1-diyl)bis(7-bromo-1H-indole)(3o): Purified by silica-gel column chromatography (PE/EA=10/1). Pink solid. Yield: 106.6 mg, 70 %. ^1H NMR (400 MHz, Chloroform- d) δ 8.08 (s, 2H), 7.50 (d, $J = 8.0$ Hz, 2H), 7.40-7.35 (m, 4H), 7.29 (d, $J = 7.3$ Hz, 1H), 7.25 – 7.19 (m, 2H), 7.02 (d, $J = 2.4$ Hz, 2H), 6.97 (t, $J = 7.8$ Hz, 2H), 4.49 (t, $J = 7.4$ Hz, 1H), 2.79-2.75 (m, 2H), 2.68 – 2.49 (m, 2H). ^{13}C NMR (100 MHz, Chloroform- d) δ 142.3, 135.3, 128.6, 128.5, 128.2, 126.0, 124.4, 122.2, 121.0, 120.5, 118.9, 104.9, 37.2, 34.4, 33.8. **ESI-HRMS**: z/s calculated for $\text{C}_{25}\text{H}_{19}\text{Br}_2\text{N}_2[\text{M}-\text{H}]^-$: 506.9900; found: 506.9902.



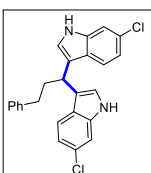
3,3'-(3-phenylpropane-1,1-diyl)bis(1H-pyrrolo[2,3-b]pyridine)(3p): Purified by silica-gel column chromatography (PE/EA=1/1). White solid. Yield: 90.7 mg, 86 %. ^1H NMR (400 MHz, DMSO- d_6) δ 11.40 (s, 2H), 8.14 (dt, $J = 4.6, 1.9$ Hz, 2H), 7.85 (dd, $J = 7.9, 1.6$ Hz, 2H), 7.49 (t, $J = 2.9$ Hz, 2H), 7.32 – 7.19 (m, 2H), 7.17 (dd, $J = 7.5, 4.7$ Hz, 3H), 6.93 (dd, $J = 7.9, 4.6$ Hz, 2H), 4.75 – 4.05 (m, 1H), 2.71 – 2.56 (m, 2H), 2.57 – 2.50 (m, 2H). ^{13}C NMR (100 MHz, DMSO- d_6) δ 149.4, 149.3, 142.7, 142.6, 128.9, 128.8, 127.5, 126.2, 123.1, 119.7, 117.4, 115.6, 36.6, 34.4, 34.0. **ESI-HRMS**: m/z calculated for $\text{C}_{23}\text{H}_{21}\text{N}_4[\text{M}+\text{H}]^+$: 353.1761; found: 353.1761.



3,3'-(3-phenylpropane-1,1-diyl)bis(6-methyl-1H-indole)(3q): Purified by silica-gel column chromatography (PE/EA=5/1). Blue solid. Yield: 99.5 mg, 83 %. ^1H NMR (400 MHz, Chloroform- d) δ 7.62 (s, 2H), 7.48 (d, $J = 8.1$ Hz, 2H), 7.33 (t, $J = 7.3$ Hz, 2H), 7.26 – 7.20 (m, 3H), 7.11 (s, 2H), 6.93 (dd, $J = 8.1, 1.4$ Hz, 2H), 6.87 (d, $J = 2.3$ Hz, 2H), 4.50 (t, $J = 7.3$ Hz, 1H), 2.79-2.75 (m, 2H), 2.61 – 2.54 (m, 2H), 2.50 (s, 6H). ^{13}C NMR (100 MHz, Chloroform- d) δ 142.9, 137.2, 131.6, 128.7, 128.4, 125.8, 125.1, 121.0, 120.9, 120.0, 119.4, 111.2, 37.5, 34.6, 33.7, 21.8. **ESI-HRMS**: m/z calculated for $\text{C}_{27}\text{H}_{25}\text{N}_2[\text{M}-\text{H}]^-$: 377.2023; found: 377.2023.

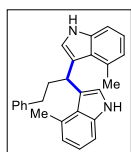


3,3'-(3-phenylpropane-1,1-diyl)bis(6-chloro-1H-indole)(3r): Purified by silica-gel column chromatography (PE/EA=3/1). White solid. Yield: 90.1 mg, 72 %. ^1H NMR (400 MHz, Chloroform- d) δ 7.91 (s, 2H), 7.37 (d, $J = 8.5$ Hz, 2H), 7.33 – 7.26 (m, 4H), 7.24 – 7.19 (m, 1H), 7.19 – 7.13 (m, 2H), 7.00 (t, $J = 2.4$ Hz, 3H), 6.98 (d, $J = 1.8$ Hz, 1H), 4.41 (t, $J = 7.4$ Hz, 1H), 2.71-2.67 (m, 2H), 2.60 – 2.43 (m, 2H). ^{13}C NMR (100 MHz, Chloroform- d) δ 142.4, 137.1, 128.7, 128.5, 128.0, 126.0, 125.7, 122.2, 120.5,



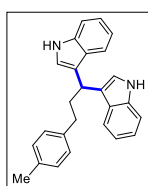
120.1, 120.0, 111.2, 37.3, 34.4, 33.4. **ESI-HRMS:** m/z calculated for $C_{25}H_{19}Cl_2N_2[M-H]^+$: 417.0930; found: 417.0931.

3,3'-(3-phenylpropane-1,1-diyl)bis(4-methyl-1H-indole)(3s): Purified by silica-gel column chromatography (PE/EA=3/1). Yellow solid. Yield: 49 mg, 43 %.



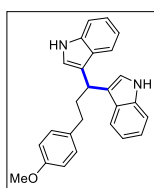
1H NMR (400 MHz, Chloroform-*d*) δ 7.79 (s, 2H), 7.30 (dd, $J = 8.5, 6.4$ Hz, 2H), 7.24 – 7.16 (m, 5H), 7.08 (t, $J = 7.6$ Hz, 2H), 6.83 (d, $J = 7.1$ Hz, 2H), 6.76 (d, $J = 2.5$ Hz, 2H), 5.12 (t, $J = 7.2$ Hz, 1H), 2.96-2.92 (m, 2H), 2.55 (s, 6H), 2.43 – 2.33 (m, 2H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 142.7, 137.3, 131.1, 128.7, 128.4, 125.9, 125.5, 122.2, 122.0, 121.9, 121.2, 109.1, 40.4, 34.9, 34.6, 20.2; **ESI-HRMS:** m/z calculated for $C_{27}H_{25}N_2[M-H]^+$: 377.2023; found: 377.2023.

3,3'-(3-(*p*-tolyl)propane-1,1-diyl)bis(1H-indole)(3t): Purified by silica-gel column chromatography



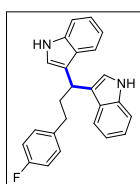
(PE/EA=3/1). White solid. Yield: 94.4 mg, 86 %. 1H NMR (400 MHz, Chloroform-*d*) δ 7.68 (s, 2H), 7.64 (d, $J = 7.9$ Hz, 2H), 7.31 (d, $J = 8.1$ Hz, 2H), 7.25 – 7.21 (m, 2H), 7.20 – 7.09 (m, 6H), 6.92 (d, $J = 2.4$ Hz, 2H), 4.57 (t, $J = 7.3$ Hz, 1H), 2.77-2.74 (m, 2H), 2.68 – 2.52 (m, 2H), 2.42 (s, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 139.6, 136.6, 135.2, 129.1, 128.5, 127.1, 121.8, 121.7, 120.1, 119.7, 119.1, 111.2, 37.6, 34.1, 33.6, 21.1. **ESI-HRMS:** m/z calculated for $C_{26}H_{23}N_2[M-H]^+$: 363.1866; found: 363.1867.

3,3'-(3-(4-methoxyphenyl)propane-1,1-diyl)bis(1H-indole)(3u): Purified by silica-gel column



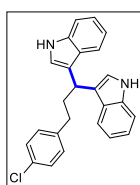
chromatography (PE/EA=3/1). White solid. Yield: 85.8 mg, 75 %. 1H NMR (400 MHz, Chloroform-*d*) δ 7.78 (s, 2H), 7.64 – 7.57 (m, 2H), 7.32 (d, $J = 8.1$ Hz, 2H), 7.23 – 7.16 (m, 2H), 7.15 – 7.06 (m, 4H), 6.94 (d, $J = 2.4$ Hz, 2H), 6.88 (d, $J = 8.6$ Hz, 2H), 4.53 (t, $J = 7.3$ Hz, 1H), 3.83 (s, 3H), 2.72-2.68 (m, 2H), 2.62 – 2.48 (m, 2H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 157.7, 136.7, 134.8, 129.6, 127.1, 121.9, 121.7, 120.1, 119.7, 119.1, 113.8, 111.2, 55.4, 37.7, 33.6, 33.4. **ESI-HRMS:** m/z calculated for $C_{26}H_{23}N_2O[M-H]^+$: 379.1815; found: 379.1516.

3,3'-(3-(4-fluorophenyl)propane-1,1-diyl)bis(1H-indole)(3v): Purified by silica-gel column



chromatography (PE/EA=5/1). Off-white solid. Yield: 75.1 mg, 68 %. 1H NMR (400 MHz, Chloroform-*d*) δ 7.86 (s, 2H), 7.56 (d, $J = 7.9$ Hz, 2H), 7.33 (d, $J = 8.1$ Hz, 2H), 7.18 (dd, $J = 8.2, 6.9$ Hz, 2H), 7.12 (dd, $J = 8.3, 5.5$ Hz, 2H), 7.06 (t, $J = 7.5$ Hz, 2H), 7.02 – 6.93 (m, 4H), 4.50 (t, $J = 7.4$ Hz, 1H), 2.72-2.69 (m, 2H), 2.57-2.51 (m, 2H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 162.5, 160.1, 138.28 (d, $J_{C-F} = 3.1$ Hz), 136.7, 123.0 (d, $J_{C-F} = 7.7$ Hz), 127.1, 121.8 (d, $J_{C-F} = 33.3$ Hz), 120.0, 119.7, 119.2, 115.1 (d, $J_{C-F} = 21.0$ Hz), 111.3, 37.6, 33.75, 33.5. ^{19}F NMR (400 MHz, Chloroform-*d*) δ -117.98. **ESI-HRMS:** m/z calculated for $C_{25}H_{20}FN_2[M-H]^+$: 367.1616; found: 367.1616.

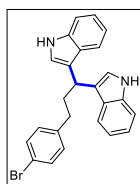
3,3'-(3-(4-chlorophenyl)propane-1,1-diyl)bis(1H-indole)(3w): Purified by silica-gel column



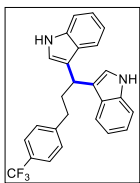
chromatography (PE/EA=5/1). Pale yellow solid. Yield: 107.3 mg, 93 %. 1H NMR (400 MHz, Chloroform-*d*) δ 7.91 (s, 2H), 7.55 (d, $J = 8.0$, 2H), 7.34 (d, $J = 8.1$, 2H), 7.25 – 7.21 (m, 2H), 7.19-7.15 (m, 2H), 7.11 – 6.98 (m, 6H), 4.49 (t, $J = 7.4$ Hz, 1H), 2.71-2.67 (m, 2H), 2.62 – 2.48 (m, 2H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 141.1, 136.7, 131.4, 130.0, 128.4, 127.1, 122.0, 121.6, 119.9, 119.7, 119.2, 111.3, 37.4, 33.9, 33.5.

ESI-HRMS: m/z calculated for $C_{25}H_{20}ClN_2[M-H]^+$: 383.1320; found: 383.1320.

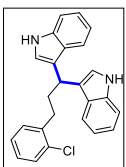
3,3'-(3-(4-bromophenyl)propane-1,1-diyl)bis(1H-indole)(3x): Purified by silica-gel column chromatography (PE/EA=5/1). Off-white solid. Yield: 107.8 mg, 84 %. ¹H NMR (400 MHz, Chloroform-*d*) δ 7.84 (s, 2H), 7.57 (d, *J* = 8.0, 2H), 7.42 – 7.37 (m, 2H), 7.33 (d, *J* = 8.0, 2H), 7.20-7.16 (m, 2H), 7.10 – 7.00 (m, 4H), 6.97 (d, *J* = 2.4 Hz, 2H), 4.48 (d, *J* = 7.4 Hz, 1H), 2.70-2.66 (m, 2H), 2.64 – 2.48 (m, 2H). ¹³C NMR (100 MHz, Chloroform-*d*) δ 141.7, 136.7, 131.4, 130.5, 127.1, 122.0, 121.6, 119.9, 119.7, 119.5, 119.3, 111.3, 37.3, 33.9, 33.5; **ESI-HRMS:** *m/z* calculated for C₂₅H₂₀BrN₂[M-H]⁻: 427.0815, 429.0794; found: 427.0815, 429.0798.



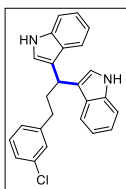
3,3'-(3-(4-(trifluoromethyl)phenyl)propane-1,1-diyl)bis(1H-indole)(3y): Purified by silica-gel column chromatography (PE/EA=3/1). Yellow solid. Yield: 45 mg, 36 %. ¹H NMR (400 MHz, Chloroform-*d*) δ 7.91 (s, 2H), 7.57 – 7.54 (m, 2H), 7.52 (d, *J* = 8.0 Hz, 2H), 7.35 (d, *J* = 8.2, 2H), 7.25 (s, 2H), 7.20-7.15 (m, 2H), 7.07-7.03 (m, 2H), 7.02 (d, *J* = 2.4 Hz, 2H), 4.51 (t, *J* = 7.4 Hz, 1H), 2.80-2.76 (m, 2H), 2.61 – 2.53 (m, 2H). ¹³C NMR (100 MHz, Chloroform-*d*) δ 146.9, 136.8, 129.0, 128.8, 127.1, 125.3, 125.3, 122.1, 121.6, 119.9, 119.7, 119.3, 111.3, 37.2, 34.5, 33.7. ¹⁹F NMR (400 MHz, Chloroform-*d*) δ -62.19. **ESI-HRMS:** *m/z* calculated for C₂₆H₂₀F₃N₂[M-H]⁻: 417.1584; found: 417.1584.



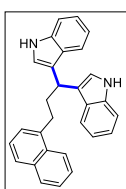
3,3'-(3-(2-chlorophenyl)propane-1,1-diyl)bis(1H-indole)(3z): Purified by silica-gel column chromatography (PE/EA=10/1). White solid. Yield: 103.1 mg, 92 %. ¹H NMR (400 MHz, Chloroform-*d*) δ 7.85 (s, 2H), 7.61 (d, *J* = 8.0, 2H), 7.37-7.32 (m, 3H), 7.22 – 7.10 (m, 5H), 7.09-7.05 (m, 2H), 7.01 (d, *J* = 2.4, 2H), 4.58 (t, *J* = 7.4 Hz, 1H), 2.95 – 2.82 (m, 2H), 2.63 – 2.49 (m, 2H). ¹³C NMR (100 MHz, Chloroform-*d*) δ 140.4, 136.7, 134.1, 130.7, 129.6, 127.3, 127.2, 126.8, 121.9, 121.7, 120.0, 119.7, 119.2, 111.2, 35.8, 34.0, 32.8. **ESI-HRMS:** *m/z* calculated for C₂₅H₂₀ClN₂[M-H]⁻: 383.1320; found: 383.1320.



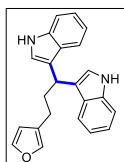
3,3'-(3-(3-chlorophenyl)propane-1,1-diyl)bis(1H-indole)(3aa): Purified by silica-gel column chromatography (PE/EA=10/1). Pale yellow solid. Yield: 107 mg, 93 %. ¹H NMR (400 MHz, Chloroform-*d*) δ 7.81 (s, 2H), 7.58 (d, *J* = 7.9, 2H), 7.33 (d, *J* = 8.1 Hz, 2H), 7.25 – 7.15 (m, 5H), 7.12 – 7.02 (m, 3H), 6.96 (d, *J* = 2.4 Hz, 2H), 4.51 (t, *J* = 7.4 Hz, 1H), 2.73-2.69 (m, 2H), 2.63 – 2.46 (m, 2H). ¹³C NMR (100 MHz, Chloroform-*d*) δ 144.8, 136.7, 134.1, 129.6, 128.8, 127.1, 126.9, 126.0, 122.0, 121.7, 119.9, 119.7, 119.3, 111.3, 37.3, 34.2, 33.6; **ESI-HRMS:** *m/z* calculated for C₂₅H₂₀ClN₂[M-H]⁻: 383.1320; found: 383.1320.



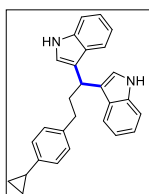
3,3'-(3-(naphthalen-1-yl)propane-1,1-diyl)bis(1H-indole)(3ab): Purified by silica-gel column chromatography (PE/EA=3/1). White solid. Yield: 102.9 mg, 86 %. ¹H NMR (400 MHz, Chloroform-*d*) δ 7.74 (q, *J* = 4.4 Hz, 4H), 7.60 (d, *J* = 8.2 Hz, 1H), 7.46 (d, *J* = 7.9 Hz, 2H), 7.34 (t, *J* = 7.5 Hz, 1H), 7.29-7.24 (m, 2H), 7.20 (t, *J* = 8.6 Hz, 3H), 7.06 (t, *J* = 7.6 Hz, 2H), 6.94 (d, *J* = 7.6 Hz, 2H), 6.90 (d, *J* = 2.5 Hz, 2H), 4.52 (t, *J* = 7.4 Hz, 1H), 3.15 – 3.01 (m, 2H), 2.66 – 2.52 (m, 2H). ¹³C NMR (100 MHz, Chloroform-*d*) δ 139.0, 136.8, 134.0, 128.8, 127.2, 126.6, 126.1, 125.8, 125.7, 125.5, 124.2, 122.0, 121.7, 120.1, 119.8, 119.2, 111.2, 36.9, 34.3, 31.9; **ESI-HRMS:** *m/z* calculated for C₂₉H₂₃N₂[M-H]⁻: 399.1866; found: 399.1867.



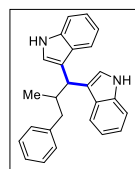
3,3'-(3-(furan-3-yl)propane-1,1-diyl)bis(1H-indole)(3ac): Purified by silica-gel column



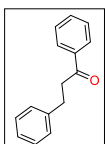
chromatography (PE/EA=5/1). Off-white solid. Yield: 88.9 mg, 87 %. ^1H NMR (400 MHz, Chloroform-*d*) δ 7.77 (s, 2H), 7.61 (d, J = 7.9 Hz, 2H), 7.38 (d, J = 1.8 Hz, 1H), 7.32 (d, J = 8.1 Hz, 2H), 7.24 – 7.15 (m, 2H), 7.09 (t, J = 7.4 Hz, 2H), 6.94 (d, J = 2.4 Hz, 2H), 6.34 (d, J = 3.1, 1H), 6.02 (d, J = 3.1 Hz, 1H), 4.55 (t, J = 7.4 Hz, 1H), 2.77 (t, J = 7.6 Hz, 2H), 2.60 (q, J = 7.5 Hz, 2H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 156.4, 140.9, 136.7, 127.1, 121.9, 121.7, 119.8, 119.7, 119.2, 111.2, 110.3, 105.1, 33.9, 33.5, 26.8; **ESI-HRMS**: m/z calculated for $\text{C}_{23}\text{H}_{19}\text{N}_2\text{O}$ [M-H] $^-$: 339.1502; found: 339.1503.



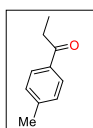
3,3'-(3-(4-cyclopropylphenyl)propane-1,1-diyl)bis(1H-indole)(3ad): Purified by silica-gel column chromatography (PE/EA=5/1). White solid. Yield: 107.7 mg, 92 %. ^1H NMR (400 MHz, Chloroform-*d*) δ 7.73 (s, 2H), 7.52 (d, J = 8 Hz, 2H), 7.26 (d, J = 8 Hz, 2H), 7.12 (t, J = 7.5 Hz, 2H), 7.06 – 6.95 (m, 6H), 6.90 (d, J = 2.4 Hz, 2H), 4.46 (t, J = 7.3 Hz, 1H), 2.67–2.63 (m, 2H), 2.56 – 2.45 (m, 2H), 1.88–1.81 (m, 1H), 0.97 – 0.86 (m, 2H), 0.67–0.63 (m, 2H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 141.3, 139.8, 136.7, 128.6, 127.2, 125.7, 121.9, 121.7, 120.2, 119.8, 119.2, 111.2, 37.6, 34.1, 33.6, 15.2, 9.1. **ESI-HRMS**: m/z calculated for $\text{C}_{28}\text{H}_{25}\text{N}_2$ [M-H] $^-$: 389.2023; found: 389.2032.



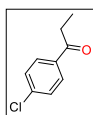
3,3'-(2-methyl-3-phenylpropane-1,1-diyl)bis(1H-indole)(3ae): Purified by silica-gel column chromatography (PE/EA=5/1). Off-white solid. Yield: 67.8 mg, 62 %. ^1H NMR (400 MHz, Chloroform-*d*) δ 7.91 (s, 2H), 7.74 – 7.61 (m, 2H), 7.35 – 7.30 (m, 2H), 7.28–7.24 (m, 2H), 7.20–7.12 (m, 7H), 7.10–7.05 (m, 2H), 4.49 (d, J = 7.8 Hz, 1H), 3.03 (dd, J = 13.3, 3.8 Hz, 1H), 2.92 – 2.73 (m, 1H), 2.35 (dd, J = 13.3, 10.0 Hz, 1H), 0.95 (d, J = 6.6 Hz, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 142.2, 136.7, 136.5, 129.5, 128.3, 128.0, 127.8, 125.8, 122.1, 122.0, 122.0, 121.9, 112.0, 119.9, 119.8, 119.4, 119.3, 119.1, 111.3, 111.2, 42.2, 40.3, 39.9, 18.2. **ESI-HRMS**: m/z calculated for $\text{C}_{26}\text{H}_{24}\text{N}_2\text{Na}$ [M+Na] $^+$: 387.1832; found: 387.1820.



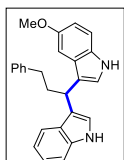
1,3-diphenylpropan-1-one(3ag)^[10]: Purified by silica-gel column chromatography (PE/EA=10/1). Off-white oil. Yield: 30.9 mg, 49 %. ^1H NMR (400 MHz, Chloroform-*d*) δ 8.00 (dd, J = 8.4, 1.3 Hz, 2H), 7.58 (d, J = 7.4 Hz, 1H), 7.49 (dd, J = 8.2, 6.9 Hz, 2H), 7.37 – 7.28 (m, 4H), 7.25 (s, 1H), 3.39 – 3.28 (m, 2H), 3.18 – 3.02 (m, 2H).



1-(p-tolyl)propan-1-one(3ah)^[11]: Purified by silica-gel column chromatography (PE/EA=30/1). Pale yellow oil. Yield: 23.3 mg, 52 %. ^1H NMR (400 MHz, Chloroform-*d*) δ 7.87 (d, J = 8.3 Hz, 2H), 7.25 (d, J = 8.3 Hz, 2H), 2.97 (q, J = 7.2 Hz, 2H), 2.41 (s, 3H), 1.22 (t, J = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 200.5, 143.6, 134.5, 129.2, 128.1, 31.7, 21.6, 8.3.



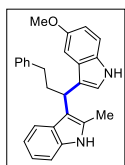
1-(4-chlorophenyl)propan-1-one(3ai)^[11]: Purified by silica-gel column chromatography (PE/EA=30/1). Pale yellow oil. Yield: 35.9 mg, 71 %. ^1H NMR (400 MHz, Chloroform-*d*) δ 7.89 (d, J = 8.6 Hz, 2H), 7.41 (d, J = 8.6 Hz, 2H), 2.96 (q, J = 7.2 Hz, 2H), 1.21 (t, J = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 199.6, 139.4, 135.3, 129.5, 129.0, 31.9, 8.3.



3-(1-(1H-indol-3-yl)-3-phenylpropyl)-5-methoxy-1H-indole(4a): Purified by silica-gel column chromatography (PE/EA=5/1). Pale yellow solid. Yield: 54.7 mg, 48 %. ^1H NMR (400 MHz, Chloroform-*d*) δ 7.89 (s, 1H), 7.76 (s, 1H), 7.57 (d, J = 7.9, 1H), 7.37 – 7.27 (m, 3H), 7.24 – 7.14 (m, 5H), 7.06–7.04 (m, 1H), 7.00 (d, J = 2.4 Hz, 1H), 6.96 (t, J = 2.9

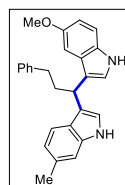
Hz, 2H), 6.84 (dd, $J = 8.8, 2.4$ Hz, 1H), 4.46 (t, $J = 7.3$ Hz, 1H), 3.77 (s, 3H), 2.81 – 2.69 (m, 2H), 2.65 – 2.43 (m, 2H). ^{13}C NMR (100 MHz, Chloroform- d) δ 153.7, 142.8, 136.8, 131.9, 128.8, 128.4, 127.6, 127.3, 125.8, 122.5, 121.9, 121.7, 120.0, 112.0, 119.8, 119.2, 111.9, 111.9, 111.2, 101.8, 56.0, 37.4, 34.5, 33.4; **ESI-HRMS**: m/z calculated for $\text{C}_{26}\text{H}_{23}\text{N}_2\text{O}[\text{M}+\text{H}]^+$: 381.1962; found: 381.1961.

5-methoxy-3-(1-(2-methyl-1H-indol-3-yl)-3-phenylpropyl)-1H-indole(4b)^[12]: Purified by silica-gel



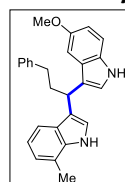
column chromatography (PE/EA=5/1). Yellow solid. Yield: 75.4 mg, 64 %. ^1H NMR (400 MHz, Chloroform- d) δ 7.74 (s, 1H), 7.72 (s, 1H), 7.66 (d, $J = 7.8$, 1H), 7.27 (d, $J = 10.7$ Hz, 4H), 7.23 – 7.14 (m, 4H), 7.05 – 6.99 (m, 2H), 6.82 (d, $J = 2.5$ Hz, 1H), 6.78 (dd, $J = 8.7, 2.4$ Hz, 1H), 4.43 – 4.32 (m, 1H), 3.71 (s, 3H), 2.80 – 2.54 (m, 4H), 2.33 (s, 3H). ^{13}C NMR (100 MHz, Chloroform- d) δ 153.6, 142.8, 135.6, 131.8, 131.2, 128.7, 128.4, 128.3, 127.8, 125.8, 122.0, 120.7, 120.3, 119.6, 119.0, 113.6, 111.8, 111.7, 110.4, 101.6, 55.8, 36.0, 34.5, 33.0, 12.4.

5-methoxy-3-(1-(6-methyl-1H-indol-3-yl)-3-phenylpropyl)-1H-indole(4c): Purified by silica-gel



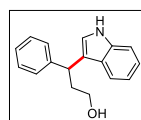
column chromatography (PE/EA=5/1). White solid. Yield: 58.8 mg, 50 %. ^1H NMR (400 MHz, Chloroform- d) δ 7.78 (s, 1H), 7.76 (s, 1H), 7.44 (d, $J = 8.1$ Hz, 1H), 7.33 – 7.27 (m, 2H), 7.23 – 7.16 (m, 4H), 7.13 (s, 1H), 6.96 (d, $J = 2.7$ Hz, 3H), 6.88 (d, $J = 8.2$, 1H), 6.83 (dd, $J = 8.7, 2.5$ Hz, 1H), 4.43 (t, $J = 7.3$ Hz, 1H), 3.77 (s, 3H), 2.76–2.74 (m, 2H), 2.62 – 2.47 (m, 2H), 2.45 (s, 3H). ^{13}C NMR (100 MHz, Chloroform- d) δ 153.7, 142.8, 137.3, 131.9, 131.7, 128.8, 128.4, 127.6, 125.8, 125.1, 122.5, 121.0, 120.9, 120.1, 119.8, 119.5, 111.9, 111.8, 111.2, 101.8, 56.0, 37.4, 34.5, 33.4, 21.8; **ESI-HRMS**: m/s calculated for $\text{C}_{27}\text{H}_{26}\text{N}_2\text{O}[\text{M}-\text{H}]^-$: 393.1972; found: 393.1972.

5-methoxy-3-(1-(7-methyl-1H-indol-3-yl)-3-phenylpropyl)-1H-indole(4d): Purified by silica-gel



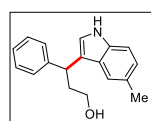
column chromatography (PE/EA=5/1). Pale yellow solid. Yield: 47.2 mg, 50 %. ^1H NMR (400 MHz, Chloroform- d) δ 7.84 (s, 1H), 7.76 (s, 1H), 7.47 – 7.39 (m, 1H), 7.33 – 7.26 (m, 3H), 7.23 – 7.16 (m, 4H), 7.02 (d, $J = 2.4$ Hz, 1H), 7.00 – 6.94 (m, 4H), 6.83 (dd, $J = 8.8, 2.5$ Hz, 1H), 4.45 (t, $J = 7.4$ Hz, 1H), 3.77 (s, 3H), 2.80 – 2.70 (m, 2H), 2.63–2.50 (m, 2H), 2.47 (s, 3H). ^{13}C NMR (100 MHz, Chloroform- d) δ 153.7, 142.8, 136.4, 131.9, 128.8, 128.4, 127.6, 126.8, 125.8, 122.5, 121.4, 120.6, 120.4, 120.1, 119.4, 117.6, 111.9, 111.8, 101.8, 56.0, 37.4, 34.5, 33.5, 16.7. **ESI-HRMS**: m/s calculated for $\text{C}_{27}\text{H}_{26}\text{N}_2\text{O}[\text{M}-\text{H}]^-$: 393.1972; found: 393.1972.

3-(1H-indol-3-yl)-3-phenylpropan-1-ol(5a)^[13]: Purified by silica-gel column chromatography



(PE/EA=3/1). White solid. Yield: 50.6 mg, 67 %. ^1H NMR (400 MHz, Chloroform- d) δ 8.00 (s, 1H), 7.44 (d, $J = 8.0$ Hz, 1H), 7.33 – 7.28 (m, 3H), 7.28 – 7.23 (m, 2H), 7.19 – 7.09 (m, 2H), 7.04 – 6.96 (m, 2H), 4.37 (t, $J = 7.7$ Hz, 1H), 3.70–3.61 (m, 2H), 2.50–2.41 (m, 1H), 2.33 – 2.21 (m, 1H), 1.40 (s, 1H). ^{13}C NMR (100 MHz, Chloroform- d) δ 144.9, 136.7, 128.6, 128.0, 127.0, 126.3, 122.2, 121.2, 119.8, 119.6, 119.4, 111.2, 61.5, 39.3, 38.8.

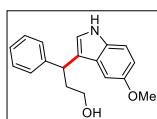
3-(5-methyl-1H-indol-3-yl)-3-phenylpropan-1-ol(5b)^[14]: Purified by silica-gel column



chromatography (PE/EA=3/1). Pale yellow solid. Yield: 53.5 mg, 67 %. ^1H NMR (400 MHz, Chloroform- d) δ 7.92 (s, 1H), 7.34 (d, $J = 7.1$ Hz, 2H), 7.31 – 7.26 (m, 3H), 7.23–7.17 (m, 2H), 7.03 – 6.93 (m, 2H), 4.37 (t, $J = 7.8$ Hz, 1H), 3.78 – 3.59 (m, 2H), 2.52 – 2.42 (m, 1H), 2.39 (s, 3H), 2.32–2.25 (m, 1H), 1.39 (s, 1H). ^{13}C NMR (100 MHz, Chloroform- d) δ

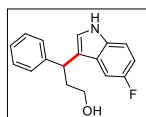
145.0, 135.0, 128.7, 128.6, 128.0, 127.3, 126.3, 123.9, 121.4, 119.3, 119.2, 110.9, 61.6, 39.3, 39.0, 21.7.

3-(5-methoxy-1H-indol-3-yl)-3-phenylpropan-1-ol(5c)^[14]: Purified by silica-gel column



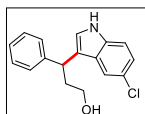
chromatography (PE/EA=3/1). Pale yellow solid. Yield: 58.2 mg, 69 %. ¹H NMR (400 MHz, Chloroform-*d*) δ 8.01 (s, 1H), 7.36 – 7.31 (m, 2H), 7.29 (d, *J* = 7.4 Hz, 2H), 7.23 – 7.13 (m, 2H), 7.01 (d, *J* = 2.4 Hz, 1H), 6.87 (d, *J* = 2.5 Hz, 1H), 6.82 (dd, *J* = 8.7, 2.5 Hz, 1H), 4.34 (t, *J* = 7.7 Hz, 1H), 3.75 (s, 3H), 3.69-3.65 (m, 2H), 2.49-2.41 (m, 1H), 2.35 – 2.19 (m, 1H). ¹³C NMR (100 MHz, Chloroform-*d*) δ 153.7, 144.8, 131.8, 128.5, 128.0, 127.4, 126.3, 122.0, 119.3, 112.1, 111.9, 101.6, 61.4, 55.9, 39.3, 38.7.

3-(5-fluoro-1H-indol-3-yl)-3-phenylpropan-1-ol(5d): Purified by silica-gel column chromatography



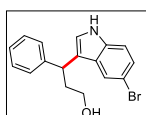
(PE/EA=3/1). Pale yellow solid. Yield: 58.3 mg, 72 %. ¹H NMR (400 MHz, Chloroform-*d*) δ 8.08 (s, 1H), 7.32-7.26 (m, 4H), 7.24-7.17 (m, 2H), 7.10-7.06 (m, 2H), 6.89 (t, *J* = 9.0 Hz, 1H), 4.32 (t, *J* = 7.8 Hz, 1H), 3.69-3.64 (m, 2H), 2.48-2.40 (m, 1H), 2.33 – 2.21 (m, 1H), 1.48 (s, 1H). ¹³C NMR (100 MHz, Chloroform-*d*) δ 157.7 (d, *J*_{C-F} = 234.3 Hz), 144.5, 133.2, 128.7, 127.9, 127.4 (d, *J*_{C-F} = 9.8 Hz), 126.5, 123.0, 120.0 (d, *J*_{C-F} = 4.7 Hz), 111.8 (d, *J*_{C-F} = 9.8 Hz), 110.6 (d, *J*_{C-F} = 26.5 Hz), 104.5 (d, *J*_{C-F} = 23.5 Hz), 61.3, 39.3, 38.6. ¹⁹F NMR (400 MHz, Chloroform-*d*) δ -124.52(m). **ESI-HRMS**: *m/z* calculated for C₁₇H₁₇FNO[M+H]⁺: 270.1289; found: 270.1289.

3-(5-chloro-1H-indol-3-yl)-3-phenylpropan-1-ol(5e): Purified by silica-gel column chromatography



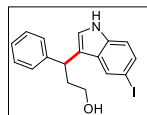
(PE/EA=3/1). Pale yellow solid. Yield: 52.7 mg, 61 %. ¹H NMR (400 MHz, Chloroform-*d*) δ 8.14 (s, 1H), 7.42 (d, *J* = 2.0 Hz, 1H), 7.35 – 7.27 (m, 4H), 7.22-7.18 (m, 2H), 7.09 (dd, *J* = 8.7, 2.0 Hz, 1H), 7.05 (d, *J* = 2.5 Hz, 1H), 4.32 (t, *J* = 8.0, 1H), 3.70-3.60 (m, 2H), 2.46-2.38 (m, 1H), 2.30-2.21(m, 1H), 1.57 (s, 1H). ¹³C NMR (100 MHz, Chloroform-*d*) δ 144.4, 135.0, 128.7, 128.1, 127.9, 126.5, 125.1, 122.6, 122.5, 119.6, 119.0, 112.2, 61.3, 39.1, 38.7. **ESI-HRMS**: *m/z* calculated for C₁₈H₂₀NO[M+H]⁺: 286.0999; found: 286.0999.

3-(5-bromo-1H-indol-3-yl)-3-phenylpropan-1-ol(5f)^[15]: Purified by silica-gel column



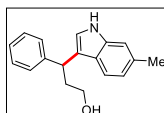
chromatography (PE/EA=3/1). White solid. Yield: 67.1 mg, 68 %. ¹H NMR (400 MHz, Chloroform-*d*) δ 8.11 (s, 1H), 7.58 (d, *J* = 1.8 Hz, 1H), 7.30 (s, 2H), 7.29 (d, *J* = 1.7 Hz, 2H), 7.24-7.17 (m, 3H), 7.04 (dd, *J* = 2.5, 0.9 Hz, 1H), 4.41 – 4.25 (m, 1H), 3.68-3.63 (m, 2H), 2.46-2.38 (m, 1H), 2.30-2.21 (m, 1H), 1.45 (s, 1H); ¹³C NMR (100 MHz, Chloroform-*d*) δ 144.3, 135.2, 128.74, 128.7, 127.9, 126.5, 125.0, 122.5, 122.1, 119.5, 112.7, 61.3, 39.1, 38.7.

3-(5-iodo-1H-indol-3-yl)-3-phenylpropan-1-ol(5g): Purified by silica-gel column chromatography



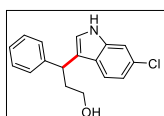
(PE/EA=3/1). Off-white solid. Yield: 83.8 mg, 74 %. ¹H NMR (400 MHz, Chloroform-*d*) δ 8.09 (s, 1H), 7.88 – 7.74 (m, 1H), 7.39 (dd, *J* = 8.5, 1.7 Hz, 1H), 7.33 – 7.27 (m, 4 H), 7.24 – 7.16 (m, 1H), 7.10 (d, *J* = 8.5 Hz, 1H), 7.00 (d, *J* = 2.5, 1H), 4.32 (t, *J* = 8.0 Hz 1H), 3.68-3.60 (m, 2H), 2.46-2.37 (m, 1H), 2.30-2.20 (m, 1H), 1.40 (s, 1H). ¹³C NMR (100 MHz, Chloroform-*d*) δ 144.3, 135.7, 130.6, 129.6, 128.7, 128.4, 127.9, 126.5, 122.0, 119.3, 113.2, 83.0, 61.3, 39.0, 38.8; **ESI-HRMS**: *m/z* calculated for C₁₇H₁₇INO[M+H]⁺: 378.0355; found: 378.0349.

3-(6-methyl-1H-indol-3-yl)-3-phenylpropan-1-ol(5i): Purified by silica-gel column chromatography



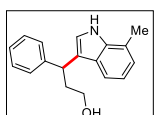
(PE/EA=3/1). White solid. Yield: 48.6 mg, 61 %. ^1H NMR (400 MHz, Chloroform-*d*) δ 7.89 (s, 1H), 7.34-7.31 (m, 3H), 7.28 (d, J = 7.3 Hz, 1H), 7.25 (s, 1H), 7.20 – 7.13 (m, 1H), 7.12 (s, 1H), 7.02 – 6.93 (m, 1H), 6.85 (d, J = 8.1, 1H), 4.36 (t, J = 7.7 Hz, 1H), 3.72-3.63 (m, 2H), 2.54 – 2.36 (m, 4H), 2.34 – 2.20 (m, 1H), 1.39 (s, 1H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 145.0, 137.2, 132.0, 128.5, 128.0, 126.2, 124.9, 121.2, 120.6, 119.6, 119.3, 111.2, 61.5, 39.5, 38.8, 21.8; **ESI-HRMS:** m/z calculated for $\text{C}_{18}\text{H}_{20}\text{NO}[\text{M}+\text{H}]^+$: 266.1545; found: 266.1539.

3-(6-chloro-1H-indol-3-yl)-3-phenylpropan-1-ol(5j): Purified by silica-gel column chromatography



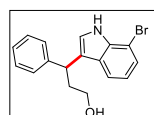
(PE/EA=3/1). Pale yellow solid. Yield: 63.7 mg, 74 %. ^1H NMR (400 MHz, Chloroform-*d*) δ 8.14 (s, 1H), 7.36 – 7.29 (m, 5H), 7.28 (s, 1H), 7.25 – 7.17 (m, 1H), 7.04 (d, J = 4, 1H), 6.99 (dd, J = 8.5, 1.9 Hz, 1H), 4.49 – 4.25 (m, 1H), 3.69 (t, J = 5.9 Hz, 2H), 2.48-2.41 (m, 1H), 2.34 – 2.21 (m, 1H), 1.57 (s, 1H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 144.5, 137.0, 128.6, 128.1, 127.9, 126.5, 125.6, 121.8, 120.5, 120.1, 112.0, 111.1, 61.3, 39.2, 38.6; **ESI-HRMS:** m/z calculated for $\text{C}_{18}\text{H}_{20}\text{NO}[\text{M}+\text{H}]^+$: 286.0999; found: 286.0993.

3-(7-methyl-1H-indol-3-yl)-3-phenylpropan-1-ol(5k): Purified by silica-gel column



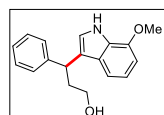
chromatography (PE/EA=3/1). White solid. Yield: 51 mg, 64 %. ^1H NMR (400 MHz, Chloroform-*d*) δ 7.98 (s, 1H), 7.37 – 7.26 (m, 5H), 7.21 – 7.14 (m, 1H), 7.11 – 7.04 (m, 1H), 7.01 – 6.91 (m, 2H), 4.39 (t, J = 7.7 Hz, 1H), 3.74-3.66 (m, 2H), 2.54 – 2.38 (m, 4H), 2.37 – 2.22 (m, 1H), 1.56 (s, 1H); ^{13}C NMR (100 MHz, Chloroform-*d*) δ 144.9, 136.2, 128.6, 128.0, 126.6, 126.3, 122.7, 120.9, 120.4, 120.3, 119.7, 117.4, 61.5, 39.5, 38.8, 16.7.

3-(7-bromo-1H-indol-3-yl)-3-phenylpropan-1-ol(5l): Purified by silica-gel column chromatography

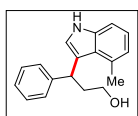


(PE/EA=3/1). White solid. Yield: 68.9 mg, 70 %. ^1H NMR (400 MHz, Chloroform-*d*) δ 8.33 (s, 1H), 7.39 (d, J = 7.9 Hz, 1H), 7.34 – 7.26 (m, 5H), 7.23 – 7.15 (m, 1H), 7.09 (d, J = 2.5 Hz, 1H), 6.90 (t, J = 7.8 Hz, 1H), 4.39-4.36 (m, 1H), 3.69-3.61(m, 2H), 2.49-2.40 (m, 1H), 2.35 – 2.20 (m, 1H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 144.4, 135.3, 128.6, 128.2, 127.9, 126.4, 124.5, 121.8, 121.0, 120.6, 118.9, 104.8, 61.2, 39.3, 38.6. **ESI-HRMS:** m/z calculated for $\text{C}_{17}\text{H}_{17}\text{BrNO}[\text{M}+\text{H}]^+$: 330.0494, 332.0473; found: 330.0488, 332.0473.

3-(7-methoxy-1H-indol-3-yl)-3-phenylpropan-1-ol(5m): Purified by silica-gel column



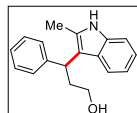
chromatography (PE/EA=3/1). White solid. Yield: 65.9 mg, 78 %. ^1H NMR (400 MHz, Chloroform-*d*) δ 8.35 (s, 1H), 7.36 – 7.26 (m, 4H), 7.19 (d, J = 7.3 Hz, 1H), 7.09 (d, J = 8.0 Hz, 1H), 7.01 (d, J = 2.4 Hz, 1H), 6.96 (t, J = 7.9 Hz, 1H), 6.62 (d, J = 7.6 Hz, 1H), 4.38 (t, J = 7.7 Hz, 1H), 3.94 (s, 3H), 3.68 (d, J = 6.5 Hz, 2H), 2.51-2.43 (m, 1H), 2.35 – 2.22 (m, 1H), 1.57 (s, 1H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 146.2, 145.0, 128.5, 128.4, 128.0, 127.2, 126.2, 120.9, 120.1, 119.8, 112.4, 102.0, 61.4, 55.4, 39.5, 38.8; **ESI-HRMS:** m/z calculated for $\text{C}_{18}\text{H}_{20}\text{NO}_2[\text{M}+\text{H}]^+$: 282.1494; found: 282.1489.



3-(4-methyl-1H-indol-3-yl)-3-phenylpropan-1-ol(5n): Purified by silica-gel column chromatography (PE/EA=3/1). Yellow solid. Yield: 26.1 mg, 33 %. ^1H NMR (400 MHz, Chloroform-*d*) δ 8.10 (s, 1H), 7.30 – 7.26 (m, 1H), 7.25 (d, J = 1.8 Hz, 3H), 7.20-7.14 (m, 2H), 7.11 (d, J = 2.6 Hz, 1H), 7.04 (t, J = 7.6 Hz, 1H), 6.77 (d, J = 7.1 Hz, 1H), 4.73 (t, J = 7.6 Hz, 1H), 3.78-3.69 (m, 2H), 2.55 (s, 3H), 2.45 – 2.31 (m, 1H), 2.31 – 2.14 (m, 1H), 1.42 (s, 1H). ^{13}C NMR

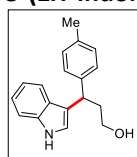
(100 MHz, Chloroform-*d*) δ 146.1, 137.0, 131.2, 128.5, 128.2, 126.1, 125.8, 122.3, 121.8, 121.4, 120.1, 109.1, 61.5, 40.9, 39.8, 21.0; **ESI-HRMS**: m/z calculated for C₁₈H₂₀NO[M+H]⁺: 266.1545; found: 266.1539.

3-(2-methyl-1H-indol-3-yl)-3-phenylpropan-1-ol(5o): Purified by silica-gel column



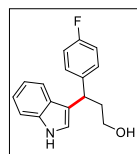
chromatography (PE/EA=3/1). Yellow oil. Yield: 58.2 mg, 73 %. ¹H NMR (400 MHz, Chloroform-*d*) δ 7.79 (s, 1H), 7.52 (dd, J = 8.0, 1.3 Hz, 1H), 7.37 (dd, J = 8.0, 1.4 Hz, 2H), 7.27 (d, J = 8.9 Hz, 2H), 7.25-7.24 (m, 1H), 7.16 (t, J = 7.3 Hz, 1H), 7.13 – 7.06 (m, 1H), 7.03-6.99 (m, 1H), 4.43 (t, J = 8.0 Hz, 1H), 3.69-3.63 (m, 1H), 3.61-3.55 (m, 1H), 2.57 – 2.48 (m, 2H), 2.37 (s, 3H), 1.42 – 1.34 (m, 1H). ¹³C NMR (100 MHz, Chloroform-*d*) δ 145.1, 135.6, 131.8, 128.4, 127.9, 127.8, 125.9, 121.0, 119.4, 119.3, 113.5, 110.5, 61.78, 38.2, 37.0, 12.4; **ESI-HRMS**: m/z calculated for C₁₈H₂₀NO[M+H]⁺: 266.1545; found: 266.1539.

3-(1H-indol-3-yl)-3-(p-tolyl)propan-1-ol(5q)^[14]: Purified by silica-gel column chromatography



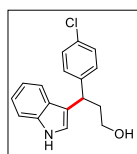
(PE/EA=3/1). White solid. Yield: 50.2 mg, 66 %. ¹H NMR (400 MHz, Chloroform-*d*) δ 8.01 (s, 1H), 7.48 (d, J = 7.9 Hz, 1H), 7.32 (d, J = 8.1 Hz, 1H), 7.25 – 7.20 (m, 2H), 7.16 (t, J = 7.6 Hz, 1H), 7.09 (d, J = 7.6 Hz, 2H), 7.06 – 6.99 (m, 2H), 4.36 (t, J = 7.8 Hz, 1H), 3.67 (d, J = 7.2 Hz, 2H), 2.51-2.42 (m, 1H), 2.31 (s, 4H), 1.41 (s, 1H). ¹³C NMR (100 MHz, Chloroform-*d*) δ 141.8, 136.7, 135.7, 129.3, 127.8, 127.0, 122.2, 121.1, 120.0, 119.6, 119.4, 111.2, 61.6, 39.0, 38.9, 21.1.

3-(4-fluorophenyl)-3-(1H-indol-3-yl)propan-1-ol(5r)^[14]: Purified by silica-gel column



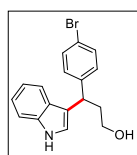
chromatography (PE/EA=3/1). White solid. Yield: 53.8 mg, 67 %. ¹H NMR (400 MHz, Chloroform-*d*) δ 8.04 (s, 1H), 7.42 (d, J = 8.0 Hz, 1H), 7.34 (d, J = 8.1 Hz, 1H), 7.31 – 7.26 (m, 2H), 7.17 (t, J = 7.6 Hz, 1H), 7.08 – 7.00 (m, 2H), 6.96 (t, J = 8.5 Hz, 2H), 4.40 (t, J = 7.7 Hz, 1H), 3.72-3.62 (m, 2H), 2.50-2.42 (m, 1H), 2.33 – 2.16 (m, 1H), 1.41 (s, 1H). ¹⁹F NMR (400 MHz, Chloroform-*d*) δ -117.25. ¹³C NMR (100 MHz, Chloroform-*d*) δ 162.7, 160.3, 140.6 (d, J -F = 3.1 Hz), 136.8, 129.4 (d, J -F = 7.9 Hz), 126.9, 122.3, 121.2, 119.7, 119.6 (d, J -F = 1.9 Hz), 115.3 (d, J -F = 21.0 Hz), 111.3, 61.3, 38.9, 38.5.

3-(4-chlorophenyl)-3-(1H-indol-3-yl)propan-1-ol(5s)^[14]: Purified by silica-gel column



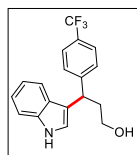
chromatography (PE/EA=3/1). White solid. Yield: 47 mg, 55 %. ¹H NMR (400 MHz, Chloroform-*d*) δ 7.97 (s, 1H), 7.32 (d, J = 8.0 Hz, 1H), 7.24 (d, J = 8.2 Hz, 1H), 7.17 (d, J = 1.1 Hz, 2H), 7.13 (s, 2H), 7.08 (t, J = 7.6 Hz, 1H), 6.98 – 6.87 (m, 2H), 4.30 (t, J = 7.7 Hz, 1H), 3.62-3.52 (m, 2H), 2.40-2.32 (m, 1H), 2.21 – 2.08 (m, 1H), 1.35 (s, 1H). ¹³C NMR (100 MHz, Chloroform-*d*) δ 143.5, 136.7, 131.9, 129.4, 128.7, 126.8, 122.4, 121.2, 119.6, 119.5, 119.3, 111.3, 61.2, 38.6.

3-(4-bromophenyl)-3-(1H-indol-3-yl)propan-1-ol(5t)^[14]: Purified by silica-gel column



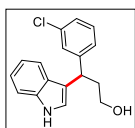
chromatography (PE/EA=3/1). White solid. Yield: 61.5 mg, 62 %. ¹H NMR (400 MHz, Chloroform-*d*) δ 8.03 (s, 1H), 7.42-7.37 (m, 3H), 7.34 (d, J = 8.2 Hz, 1H), 7.23 – 7.12 (m, 3H), 7.09 – 6.97 (m, 2H), 4.38 (t, J = 7.7 Hz, 1H), 3.70-3.63 (m, 2H), 2.54 – 2.38 (m, 1H), 2.28-2.19 (m, 1H), 1.32 (s, 1H). ¹³C NMR (100 MHz, Chloroform-*d*) δ 144.0, 136.8, 131.7, 129.8, 126.9, 122.4, 121.2, 120.0, 119.7, 119.6, 119.3, 111.3, 61.2, 38.8, 38.6.

3-(1*H*-indol-3-yl)-3-(4-(trifluoromethyl)phenyl)propan-1-ol(5u)^[14]: Purified by silica-gel column



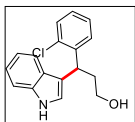
chromatography (PE/EA=3/1). White solid. Yield: 50 mg, 52 %. ¹H NMR (400 MHz, Chloroform-*d*) δ 8.10 (s, 1H), 7.52 (d, *J* = 8.1 Hz, 2H), 7.47 – 7.39 (m, 3H), 7.35 (d, *J* = 8.2, 1H), 7.26 (s, 1H), 7.20-7.16 (m, 1H), 7.09 (dd, *J* = 2.5, 0.8 Hz, 1H), 7.04 (d, *J* = 8.0, 1H), 4.49 (t, *J* = 7.7 Hz, 1H), 3.73-3.61 (m, 2H), 2.53-2.45 (m, 1H), 2.31-2.23 (m, 1H), 1.46 (s, 1H). ¹⁹F NMR (400 MHz, Chloroform-*d*) δ -62.26. ¹³C NMR (100 MHz, Chloroform-*d*) δ 149.2, 136.7, 128.7, 128.3, 126.8, 125.5 (q, *J*-*F* = 4.0 Hz), 122.5, 121.3, 119.7, 119.4, 118.8, 111.4, 61.0, 39.0, 38.5.

3-(3-chlorophenyl)-3-(1*H*-indol-3-yl)propan-1-ol(5v)^[14]: Purified by silica-gel column



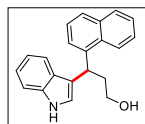
chromatography (PE/EA=3/1). White solid. Yield: 57.0 mg, 67 %. ¹H NMR (400 MHz, Chloroform-*d*) δ 8.09 (s, 1H), 7.45 (d, *J* = 8.0, 1H), 7.34 (d, *J* = 8.2, 1H), 7.30 (d, *J* = 1.9 Hz, 1H), 7.24 – 7.13 (m, 4H), 7.08 – 7.02 (m, 2H), 4.39 (t, *J* = 7.7 Hz, 1H), 3.70- 3.60 (m, 2H), 2.48-2.40 (m, 1H), 2.31 – 2.17 (m, 1H), 1.54 (s, 1H). ¹³C NMR (100 MHz, Chloroform-*d*) δ 147.2, 136.7, 134.3, 129.8, 128.1, 126.9, 126.5, 126.3, 122.4, 121.3, 119.6, 119.4, 119.0, 111.3, 61.1, 38.9, 38.6.

3-(2-chlorophenyl)-3-(1*H*-indol-3-yl)propan-1-ol(5w)^[14]: Purified by silica-gel column



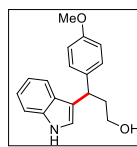
chromatography (PE/EA=3/1). White solid. Yield: 52.6 mg, 61 %. ¹H NMR (400 MHz, Chloroform-*d*) δ 8.07 (s, 1H), 7.47 (d, *J* = 8.0, 1H), 7.41 – 7.36 (m, 1H), 7.34 (d, *J* = 8.2, 1H), 7.25 – 7.21 (m, 1H), 7.19 – 7.07 (m, 4H), 7.05-7.01 (mz, 1H), 4.96 (t, *J* = 8.0, 1H), 3.74-3.69 (m, 2H), 2.52-2.44 (m, 1H), 2.30-2.21 (m, 1H), 1.52 (s, 1H). ¹³C NMR (100 MHz, Chloroform-*d*) δ 142.4, 136.6, 133.7, 129.6, 129.2, 127.5, 127.2, 127.1, 122.4, 121.5, 119.7, 119.6, 118.9, 111.2, 61.4, 38.6, 35.1.

3-(1*H*-indol-3-yl)-3-(naphthalen-2-yl)propan-1-ol(5x): Purified by silica-gel column

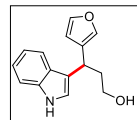


chromatography (PE/EA=3/1). White solid. Yield: 38.6 mg, 47 %. ¹H NMR (400 MHz, Chloroform-*d*) δ 8.43 – 8.22 (m, 1H), 7.99 (s, 1H), 7.91 – 7.80 (m, 1H), 7.73 (d, *J* = 8.0, 1H), 7.53 – 7.43 (m, 4H), 7.42 – 7.36 (m, 1H), 7.32 (d, *J* = 8.3, 1H), 7.18-7.14 (m, 1H), 7.03-6.99 (m, 1H), 6.98 (d, *J* = 2.5, 1H), 5.30 (t, *J* = 7.4 Hz, 1H), 3.80-3.69 (m, 2H), 2.30-2.52 (m, 1H), 2.49-2.41 (m, 1H), 1.47 (t, *J* = 4.1, 1H); ¹³C NMR (100 MHz, Chloroform-*d*) δ 140.7, 136.6, 134.1, 131.9, 128.9, 127.1, 126.9, 126.0, 125.5, 125.4, 124.7, 123.5, 122.1, 122.0, 119.7, 119.5, 119.4, 111.1, 61.5, 38.9, 33.9. **ESI-HRMS**: *m/z* calculated for C₂₁H₂₀NO[M+H]⁺: 302.1545; found: 302.1539.

3-(1*H*-indol-3-yl)-3-(4-methoxyphenyl)propan-1-ol(5y)^[14]: Purified by silica-gel column



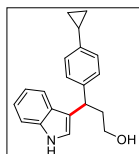
chromatography (PE/EA=3/1). White solid. Yield: 51.2 mg, 61 %. ¹H NMR (400 MHz, Chloroform-*d*) δ 8.05 (s, 1H), 7.46 (d, *J* = 8.0 Hz, 1H), 7.32 (d, *J* = 8.1 Hz, 1H), 7.25 – 7.21 (m, 2H), 7.20 – 7.11 (m, 1H), 7.07 – 6.98 (m, 2H), 6.86 – 6.76 (m, 2H), 4.35 (t, *J* = 7.7 Hz, 1H), 3.77 (s, 3H), 3.72-3.62 (m, 2H), 2.49-2.41 (m, 1H), 2.29-2.21 (m, 1H), 1.49 (s, 1H). ¹³C NMR (100 MHz, Chloroform-*d*) δ 158.0, 137.0, 136.7, 128.9, 127.0, 122.1, 121.1, 120.1, 119.7, 119.4, 114.0, 111.2, 61.5, 55.3, 38.9, 38.5.



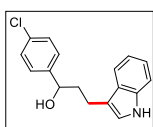
3-(furan-3-yl)-3-(1*H*-indol-3-yl)propan-1-ol(5z): Purified by silica-gel column chromatography (PE/EA=3/1). Off-white solid. Yield: 41.4 mg, 61 %. ¹H NMR (400 MHz, Chloroform-*d*) δ 8.07 (s, 1H), 7.59 (d, *J* = 8.0, 1H), 7.38 – 7.29 (m, 2H), 7.21-7.17(m, 1H), 7.13 – 7.03 (m, 2H), 6.29 (dd, *J* = 3.2, 1.9 Hz, 1H), 6.10 (d, *J* = 3.2, 1H), 4.50 (t, *J* = 7.7

Hz, 1H), 3.69-3.66 (m, 2H), 2.52 – 2.22 (m, 2H), 1.51 (s, 1H). ¹³C NMR (100 MHz, Chloroform-*d*) δ 157.9, 141.3, 136.6, 126.6, 122.2, 121.9, 119.5, 119.5, 116.9, 111.4, 110.2, 105.4, 61.2, 37.1, 33.2. **ESI-HRMS**:m/s calculated for C₁₅H₁₆NO₂[M+H]⁺: 242.1176; found: 242.1176.

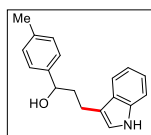
3-(4-cyclopropylphenyl)-3-(1H-indol-3-yl)propan-1-ol(5aa): Purified by silica-gel column chromatography (PE/EA=3/1). White solid. Yield: 28.3 mg, 65 %. ¹H NMR (400 MHz, Chloroform-*d*) δ 7.92 (s, 1H), 7.39 (d, *J* = 8.0 Hz, 1H), 7.24 (d, *J* = 8.0 Hz, 1H), 7.12 (d, *J* = 8.0 Hz, 2H), 7.10 – 7.05 (m, 1H), 6.97 – 6.92 (m, 2H), 6.92 – 6.86 (m, 2H), 4.26 (t, *J* = 8 Hz, 1H), 3.63-3.54 (m, 2H), 2.41-2.32 (m, 1H), 2.27 – 2.09 (m, 1H), 1.79-1.72 (m, 1H), 1.26 (s, 1H), 0.90 – 0.79 (m, 2H), 0.63 – 0.49 (m, 2H). ¹³C NMR (100 MHz, Chloroform-*d*) δ 141.9, 141.8, 136.7, 127.9, 127.0, 125.8, 122.2, 121.1, 120.1, 119.7, 119.4, 111.2, 61.6, 38.9, 38.8, 15.14. **ESI-HRMS**:m/s calculated for C₂₀H₂₂NO [M+H]⁺: 292.1696; found: 292.1696.



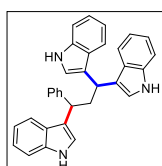
1-(4-chlorophenyl)-3-(1H-indol-3-yl)propan-1-one(5ab): Purified by silica-gel column chromatography (PE/EA=3/1). Light pink solid. Yield: 26.4 mg, 31 %. ¹H NMR (400 MHz, Chloroform-*d*) δ 7.95 (s, 1H), 7.58 (d, *J* = 7.9 Hz, 1H), 7.40 – 7.28 (m, 5H), 7.23 – 7.17 (m, 1H), 7.12 (t, *J* = 7.4 Hz, 1H), 6.98 (d, *J* = 2.3 Hz, 1H), 4.74 (dd, *J* = 7.9, 5.2 Hz, 1H), 2.91-2.71 (m, 2H), 2.26 – 2.04 (m, 2H), 1.87 (s, 1H). ¹³C NMR (100 MHz, Chloroform-*d*) δ 143.3, 136.5, 133.3, 128.7, 127.5, 122.2, 121.4, 119.4, 119.0, 115.9, 111.3, 73.6, 39.4, 21.5. **ESI-HRMS**: m/z calculated for C₁₇H₁₅ClNO[M-H]⁻: 284.0847, 286.0818; found: 284.0848, 286.0823.



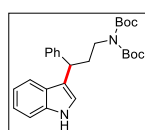
3-(1H-indol-3-yl)-1-(p-tolyl)propan-1-one(5ac): Purified by silica-gel column chromatography (PE/EA=3/1). Pale yellow solid. Yield: 31.4 mg, 40 %. ¹H NMR (400 MHz, Chloroform-*d*) δ 7.96 (s, 1H), 7.62 (d, *J* = 7.8 Hz, 1H), 7.38 (d, *J* = 8.1 Hz, 1H), 7.30 (d, *J* = 8.4 Hz, 2H), 7.25 – 7.19 (m, 3H), 7.16-7.11 (m, 1H), 7.04 – 6.99 (m, 1H), 4.76 (dd, *J* = 7.8, 5.4 Hz, 1H), 3.27 – 2.75 (m, 2H), 2.39 (s, 3H), 2.35 – 2.01 (m, 2H), 1.79 (s, 1H). ¹³C NMR (100 MHz, Chloroform-*d*) δ 141.8, 137.3, 136.4, 129.2, 127.5, 126.0, 122.0, 121.2, 119.2, 119.0, 116.1, 111.1, 74.1, 39.1, 21.5, 21.2.



3,3',3''-(3-phenylpropane-1,1,3-triyl)tris(1H-indole)(6a)^[15]: ¹H NMR (400 MHz, Chloroform-*d*) δ 7.86 (d, *J* = 7.7 Hz, 2H), 7.74 (s, 1H), 7.44 (d, *J* = 7.9 Hz, 1H), 7.34 (dd, *J* = 8.0, 3.5 Hz, 2H), 7.32 – 7.25 (m, 8H), 7.25 – 7.19 (m, 2H), 7.18-7.10 (m, 4H), 7.07 – 6.90 (m, 6H), 6.82 (d, *J* = 2.3 Hz, 1H), 4.45 (dd, *J* = 8.9, 6.0 Hz, 1H), 4.27 (dd, *J* = 8.9, 6.1 Hz, 1H), 3.11-3.04 (m, 1H), 2.95-2.88 (m, 1H). ¹³C NMR (100 MHz, Chloroform-*d*) δ 145.2, 136.7, 136.6, 136.5, 128.3, 128.3, 127.2, 127.1, 126.9, 126.1, 121.9, 121.9, 121.8, 121.7, 121.6, 121.1, 120.7, 120.5, 112.0, 119.7, 119.6, 119.4, 119.1, 119.0, 111.0, 42.1, 40.7, 31.7.

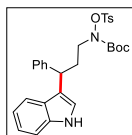


Di-tert-butyl (3-(1H-indol-3-yl)-3-phenylpropyl)iminodicarbonate(6): Purified by silica-gel column chromatography (PE/EA=5/1). Off-white oil. Yield: 84.5 mg, 47 %. ¹H NMR (400 MHz, Chloroform-*d*) δ 7.98 (s, 1H), 7.33 (d, *J* = 8 Hz, 1H), 7.25-7.16 (m, 5H), 7.10 – 7.02 (m, 3H), 6.92 (t, *J* = 8 Hz, 1H), 4.13 (t, *J* = 8 Hz, 1H), 3.66-3.59 (m, 1H), 3.52-3.45 (m, 1H), 2.42-2.35 (m, 1H), 2.26-2.17 (m, 1H), 1.39 (s, 18H). ¹³C NMR (100 MHz, Chloroform-*d*) δ 152.7, 144.8, 128.52, 127.9, 127.1, 126.3, 122.1, 119.6, 119.5, 119.4, 111.2, 82.3, 46.0, 41.1, 35.3,



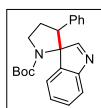
28.2.

Tert-butyl(3-(1H-indol-3-yl)-3-phenylpropyl)(tosyloxy)carbamate(8)^[13]: Purified by silica-gel



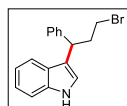
column chromatography (PE/EA=5/1). Off-white oil. Yield: 92.8 mg, 90 %. ¹H NMR (400 MHz, Chloroform-*d*) δ 8.16 (s, 1H), 7.90 – 7.76 (m, 2H), 7.42 (d, *J* = 8.0 Hz, 1H), 7.35 (d, *J* = 8.1 Hz, 1H), 7.30 (d, *J* = 1.9 Hz, 3H), 7.28-7.26 (m, 2H), 7.23 – 7.14 (m, 2H), 7.10 (d, *J* = 2.3 Hz, 1H), 7.10-7.05 (m, 1H), 4.18 (t, *J* = 7.6 Hz, 1H), 3.63 (d, *J* = 44.2 Hz, 2H), 2.44 (s, 5H), 1.25 (s, 9H).

Tert-butyl 3'-phenylspiro[indole-3,2'-pyrrolidine]-1'-carboxylate(10)^[13]: Purified by silica-gel



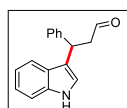
column chromatography (PE/EA=5/1). White solid. Yield: 49.2 mg, 75 %. ¹H NMR (400 MHz, Chloroform-*d*) δ 7.64 (s, 1H), 7.37 – 7.12 (m, 4H), 7.09-7.01 (m, 3H), 6.69 (d, *J* = 7.4 Hz, 2H), 4.03 (t, *J* = 9.5 Hz, 1H), 3.85 – 3.54 (m, 2H), 2.61-2.50 (m, 1H), 2.3-2.31 (m, 1H), 0.88 (s, 9H). ¹³C NMR (100 MHz, Chloroform-*d*) δ 172.3, 154.8, 153.4, 140.5, 135.2, 128.8, 128.3, 127.9, 127.2, 126.7, 121.4, 120.9, 80.4, 79.0, 55.4, 47.0, 29.0, 27.7.

3-(3-bromo-1-phenylpropyl)-1H-indole(11): Purified by silica-gel column chromatography (PE/EA=10/1). Pale yellow oil. Yield: 50 mg, 93 %. ¹H NMR (400 MHz, Chloroform-*d*)



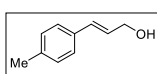
δ 7.98 (s, 1H), 7.52 (d, *J* = 8.0 Hz, 1H), 7.42 – 7.31 (m, 5H), 7.27 – 7.18 (m, 2H), 7.14 – 7.02 (m, 2H), 4.52 (t, *J* = 7.6 Hz, 1H), 3.54 – 3.29 (m, 2H), 2.82-2.73 (m, 1H), 2.66 – 2.54 (m, 1H). ¹³C NMR (100 MHz, Chloroform-*d*) δ 143.7, 136.7, 128.7, 128.0, 126.9, 126.6, 122.3, 121.3, 119.6, 119.6, 118.9, 111.3, 41.2, 38.8, 32.5. **ESI-HRMS**: *m/z* calculated for C₁₇H₁₇BrN[M+H]⁺: 314.0539, 316.0519; found: 314.0539, 316.0520.

3-(1H-indol-3-yl)-3-phenylpropanal(N-N-D)^[5]: Purified by silica-gel column chromatography (PE/EA=5/1). Pale yellow oil. Yield: 263.5 mg, 18 %. ¹H NMR (400 MHz, Chloroform-*d*)



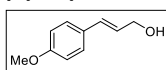
δ 9.79 (t, *J* = 2.4 Hz, 1H), 8.09 (s, 1H), 7.43 (d, *J* = 8.0 Hz, 1H), 7.39 – 7.30 (m, 5H), 7.27 – 7.16 (m, 2H), 7.11 – 7.01 (m, 2H), 4.90 (t, *J* = 7.7 Hz, 1H), 3.22 (dd, *J* = 8.3, 2.7 Hz, 1H), 3.13 (dd, *J* = 16.5, 7.2 Hz, 1H). ¹³C NMR (100 MHz, Chloroform-*d*) δ 201.9, 143.4, 136.7, 128.7, 127.7, 126.6, 126.5, 122.4, 121.7, 119.6, 119.4, 118.3, 49.8, 37.3.

(E)-3-(p-tolyl)prop-2-en-1-ol(1b)^[1]: Purified by silica-gel column chromatography (PE/EA=3/1).



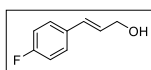
white solid. yield: 700 mg, 89 %; ¹H NMR (400 MHz, Chloroform-*d*) δ 7.29 (d, *J* = 8.0 Hz, 2H), 7.13 (d, *J* = 7.9 Hz, 2H), 6.58 (d, *J* = 16.0, 1H), 6.32 (dt, *J* = 16.0, 5.8 Hz, 1H), 4.30 (d, *J* = 5.6, 2H), 2.35 (s, 3H), 1.76 (s, 1H). ¹³C NMR (100 MHz, Chloroform-*d*) δ 137.7, 134.0, 131.3, 129.4, 127.5, 126.5, 63.9, 21.3

(E)-3-(4-methoxyphenyl)prop-2-en-1-ol (1c)^[1]: Purified by silica-gel column chromatography



(PE/EA=1/1). white solid. yield: 400 mg, 55 %; ¹H NMR (400 MHz, Chloroform-*d*) δ 7.35 (d, *J* = 8.7 Hz, 2H), 6.88 (d, *J* = 8.7 Hz, 2H), 6.58 (d, *J* = 16.0 Hz, 1H), 6.26 (d, *J* = 16.0 Hz, 1H), 4.72 – 4.04 (m, 3H), 3.83 (s, 4H), 1.69 (s, 1H).

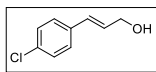
(E)-3-(4-fluorophenyl)prop-2-en-1-ol(1d)^[2]: Purified by silica-gel column chromatography



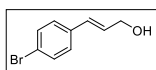
(PE/EA=3/1). white solid. yield: 700 mg, 75 %; ¹H NMR (400 MHz, Chloroform-*d*) δ 7.42 – 7.29 (m, 2H), 7.00 (t, *J* = 8.7 Hz, 2H), 6.58 (d, *J* = 15.9 Hz, 1H), 6.28 (dt, *J* = 15.9, 5.7 Hz, 1H), 4.31 (s, 2H), 1.63 (s, 1H). ¹⁹F NMR (400 MHz, Chloroform-*d*) δ -114.33. ¹³C NMR (100 MHz, Chloroform-*d*) δ 162.4 (d, *J*_{C-F} = 247.0 Hz), 132.8 (d, *J*_{C-F} = 3.3 Hz), 130.0, 128.2 (d, *J*_{C-F} =

2.3 Hz), 128.0 (d, J_{C-F} = 8.0 Hz), 115.5 (d, J_{C-F} = 21.6 Hz), 63.6.

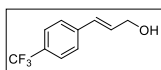
(E)-3-(4-chlorophenyl)prop-2-en-1-ol(1e)^[1]: Purified by silica-gel column chromatography (PE/EA=3/1). white solid. yiled: 1.28 g, 70 %; ¹H NMR (400 MHz, Chloroform-*d*) δ 7.33 – 7.26 (m, 4H), 6.56 (d, J = 15.9 Hz, 1H), 6.33 (dt, J = 15.9, 5.6 Hz, 1H), 4.31 (d, J = 5.6 Hz, 2H), 1.78 (s, 1H). ¹³C NMR (100 MHz, Chloroform-*d*) δ 135.3, 133.4, 129.9, 129.3, 128.9, 127.8, 63.6.



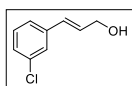
(E)-3-(4-bromophenyl)prop-2-en-1-ol(1f)^[2]: Purified by silica-gel column chromatography (PE/EA=3/1). Pale yellow solid. yiled: 700 mg, 70 %; ¹H NMR (400 MHz, Chloroform-*d*) δ 7.43 (d, J = 8.5 Hz, 2H), 7.24 (d, J = 8.4 Hz, 2H), 6.55 (d, J = 15.9 Hz, 1H), 6.34 (dt, J = 15.9, 5.6 Hz, 1H), 4.31 (dd, J = 5.5, 1.6 Hz, 2H), 1.73 (s, 1H). ¹³C NMR (100 MHz, Chloroform-*d*) δ 135.6, 131.7, 129.8, 129.3, 128.0, 121.5, 63.5.



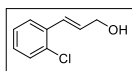
(E)-3-(4-(trifluoromethyl)phenyl)prop-2-en-1-ol(1g)^[1]: Purified by silica-gel column chromatography (PE/EA=3/1). White solid. yiled: 1.57 g, 77 %; ¹H NMR (400 MHz, Chloroform-*d*) δ 7.53 (d, J = 8.1 Hz, 2H), 7.42 (d, J = 8.1 Hz, 2H), 6.70 – 6.59 (d, J = 15.9, 1H), 6.43 (dt, J = 15.9, 5.3 Hz, 1H), 4.34 (dd, J = 5.4, 1.7 Hz, 2H), 2.49 (s, 1H). ¹⁹F NMR (400 MHz, Chloroform-*d*) δ -62.51. ¹³C NMR (100 MHz, Chloroform-*d*) δ 140.3, 131.4, 129.7, 129.4, 126.7, 125.7 (q, J_{C-F} = 3.9 Hz), 123.0, 63.4.



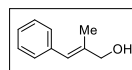
(E)-3-(3-chlorophenyl)prop-2-en-1-ol(1h)^[2]: Purified by silica-gel column chromatography (PE/EA=3/1). Pale yellow liquid. yiled: 365 mg, 36 %; ¹H NMR (400 MHz, Chloroform-*d*) δ 7.35 (s, 1H), 7.22 (h, J = 4.1 Hz, 3H), 6.54 (d, J = 15.9 Hz, 1H), 6.35 (dt, J = 15.9, 5.5 Hz, 1H), 4.31 (dd, J = 5.5, 1.6 Hz, 2H), 2.06 (s, 1H). ¹³C NMR (100 MHz, Chloroform-*d*) δ 138.7, 134.6, 130.2, 129.9, 129.5, 127.7, 126.5, 124.7, 63.4.



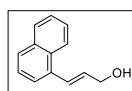
(E)-3-(2-chlorophenyl)prop-2-en-1-ol(1i)^[1]: Purified by silica-gel column chromatography (PE/EA=3/1). Off-white liquid. yiled: 1.15 g, 68 %; ¹H NMR (400 MHz, Chloroform-*d*) δ 7.50 (dd, J = 7.5, 2.0 Hz, 1H), 7.33 (dd, J = 7.5, 1.8 Hz, 1H), 7.18 (pd, J = 7.3, 1.7 Hz, 2H), 6.99 (d, J = 15.9 Hz, 1H), 6.33 (dt, J = 15.9, 5.6 Hz, 1H), 4.34 (dd, J = 5.6, 1.7 Hz, 2H), 2.52 (s, 1H).



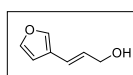
(E)-2-methyl-3-phenylprop-2-en-1-ol(1j)^[2]: Purified by silica-gel column chromatography (PE/EA=3/1). Pale yellow oil. yiled: 1.4 g, 88 %; ¹H NMR (400 MHz, Chloroform-*d*) δ 7.23 (t, J = 7.5 Hz, 2H), 7.18 (d, J = 6.8 Hz, 2H), 7.13 (d, J = 7.9 Hz, 1H), 6.42 (d, J = 2.4 Hz, 1H), 4.07 (s, 2H), 2.37 – 2.09 (m, 1H), 1.79 (s, 3H). ¹³C NMR (100 MHz, Chloroform-*d*) δ 137.7, 137.7, 128.9, 128.2, 126.5, 125.0, 68.9, 15.3.



(E)-3-(naphthalen-1-yl)prop-2-en-1-ol(1k)^[1]: Purified by silica-gel column chromatography (PE/EA=3/1). White solid. yiled: 320 mg, 64 %; ¹H NMR (400 MHz, Chloroform-*d*) δ 8.22 – 8.10 (m, 1H), 7.93 – 7.84 (m, 1H), 7.79 (d, J = 8.2 Hz, 1H), 7.60 (d, J = 7.1 Hz, 1H), 7.55 – 7.49 (m, 2H), 7.49 – 7.43 (m, 1H), 7.39 (d, J = 15.9 Hz, 1H), 6.40 (dt, J = 15.6, 5.6 Hz, 1H), 4.44 (d, J = 4.2 Hz, 2H), 1.85 (s, 1H). ¹³C NMR (100 MHz, Chloroform-*d*) δ 134.6, 133.7, 131.9, 131.3, 128.7, 128.3, 128.2, 126.2, 125.9, 125.7, 124.0, 123.9, 64.0.

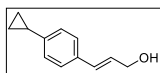


(E)-3-(furan-3-yl)prop-2-en-1-ol(1l)^[2]: Purified by silica-gel column chromatography (PE/EA=5/1).



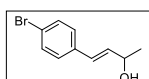
Yellow liquid. Yield: 1.2 g, 59 %; ¹H NMR (400 MHz, Chloroform-*d*) δ 7.33 (d, *J* = 1.8 Hz, 1H), 6.42 (dt, *J* = 15.9, 1.6 Hz, 1H), 6.35 (dd, *J* = 3.4, 1.8 Hz, 1H), 6.27 (dt, *J* = 15.9, 5.6 Hz, 1H), 6.22 (d, *J* = 3.3 Hz, 1H), 4.26 (dd, *J* = 5.5, 1.6 Hz, 2H), 2.36 (s, 1H). ¹³C NMR (100 MHz, Chloroform-*d*) δ 152.4, 142.0, 127.3, 119.2, 111.3, 108.0, 63.1.

(E)-3-(4-cyclopropylphenyl)prop-2-en-1-ol(1m)^[1]: Purified by silica-gel column chromatography



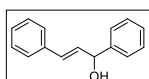
(PE/EA=5/1). White solid. Yield: 180 mg, 68 %. ¹H NMR (400 MHz, Chloroform-*d*) δ 7.35 – 7.21 (m, 2H), 7.01 (d, *J* = 1.8 Hz, 2H), 6.66 – 6.48 (m, 1H), 6.30 (dt, *J* = 15.8, 5.8 Hz, 1H), 4.30 (d, *J* = 5.8 Hz, 2H), 1.92–1.85 (m, 1H), 1.61 (s, 1H), 1.00 – 0.93 (m, 2H), 0.83 – 0.60 (m, 2H). ¹³C NMR (100 MHz, Chloroform-*d*) δ 143.8, 133.9, 131.2, 127.4, 126.4, 125.8, 63.9, 15.3, 9.4.

(E)-4-(4-bromophenyl)but-3-en-2-ol(1n)^[17]: Purified by silica-gel column chromatography



(PE/EA=3/1). Yellow solid. Yield: 640 mg, 60 %. ¹H NMR (400 MHz, Chloroform-*d*) δ 7.50 – 7.40 (m, 2H), 7.33 – 7.14 (m, 2H), 6.53 (d, *J* = 15.9 Hz, 1H), 6.29 (d, *J* = 6.2 Hz, 1H), 4.50 (td, *J* = 6.3, 1.3 Hz, 1H), 1.83 (s, 1H), 1.39 (d, *J* = 6.4 Hz, 3H). ¹³C NMR (100 MHz, Chloroform-*d*) δ 135.7, 134.3, 131.7, 128.2, 128.0, 121.4, 68.8, 23.4.

(E)-1,3-diphenylprop-2-en-1-ol(1o)^[3]: Purified by silica-gel column chromatography (PE/EA=5/1).



yellow oil. Yield: 950 mg, 94 %. ¹H NMR (400 MHz, Chloroform-*d*) δ 7.47 – 7.43 (m, 2H), 7.42 – 7.36 (m, 4H), 7.35 – 7.29 (m, 3H), 7.28 – 7.23 (m, 1H), 6.70 (dd, *J* = 15.9, 1.2 Hz, 1H), 6.40 (dd, *J* = 15.9, 6.5 Hz, 1H), 5.39 (dd, *J* = 6.7, 3.0 Hz, 1H), 2.24 (d, *J* = 3.5 Hz, 1H). ¹³C NMR (100 MHz, Chloroform-*d*) δ 142.9, 136.6, 131.6, 130.7, 128.8, 128.7, 127.9, 126.7, 126.5, 75.2.

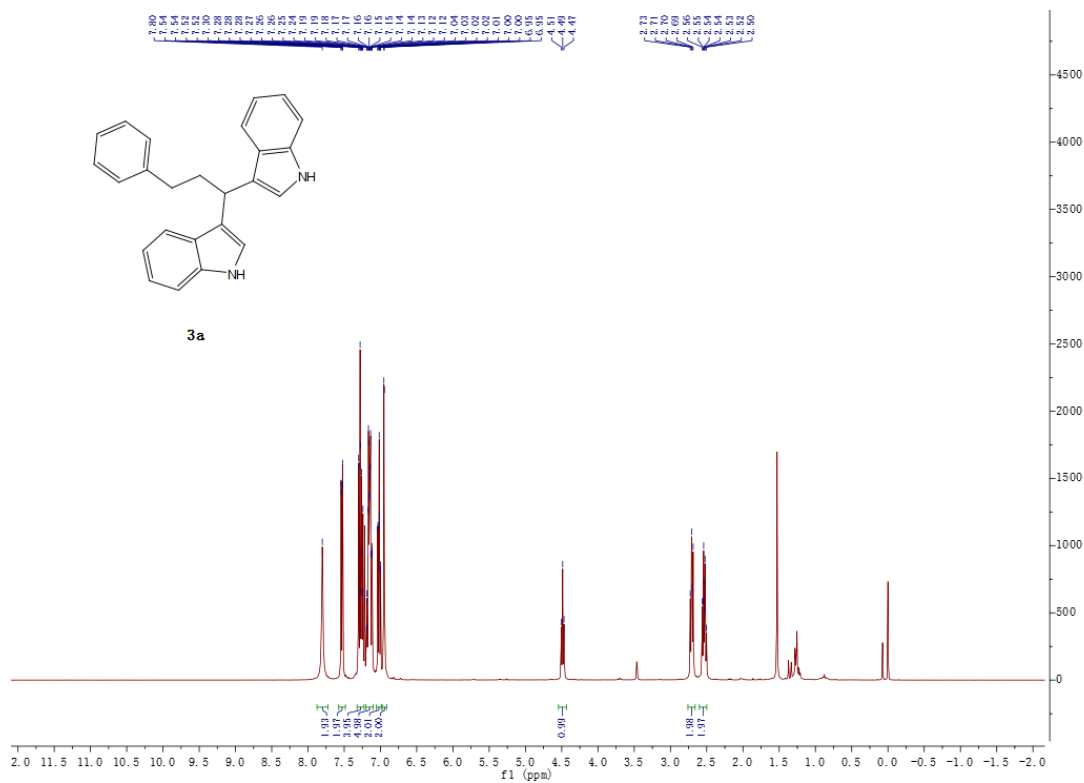
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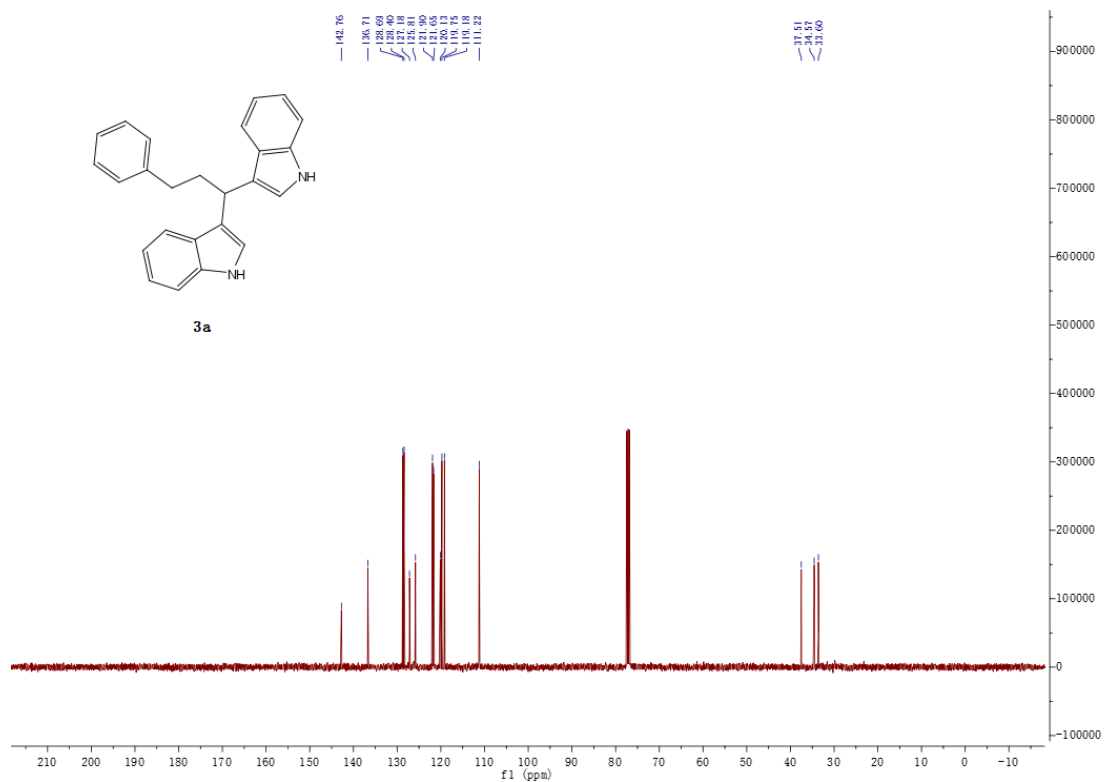
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9. ^1H and ^{13}C NMR spectra of all products

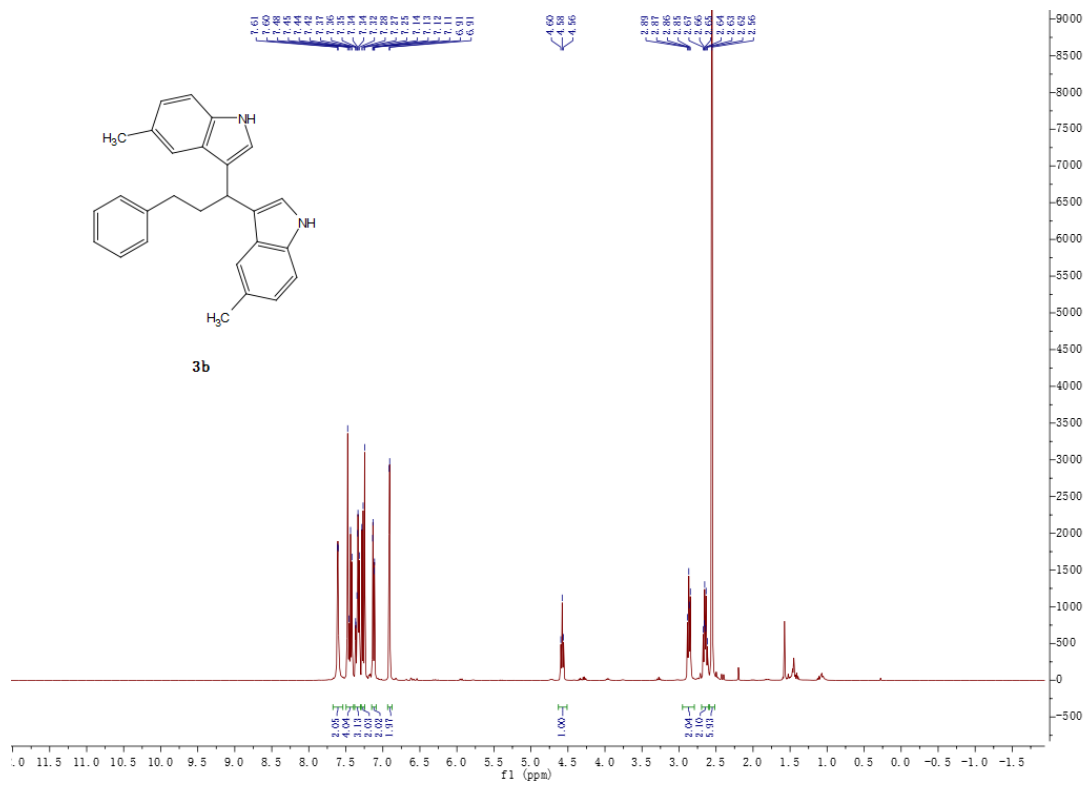
^1H NMR of 3a



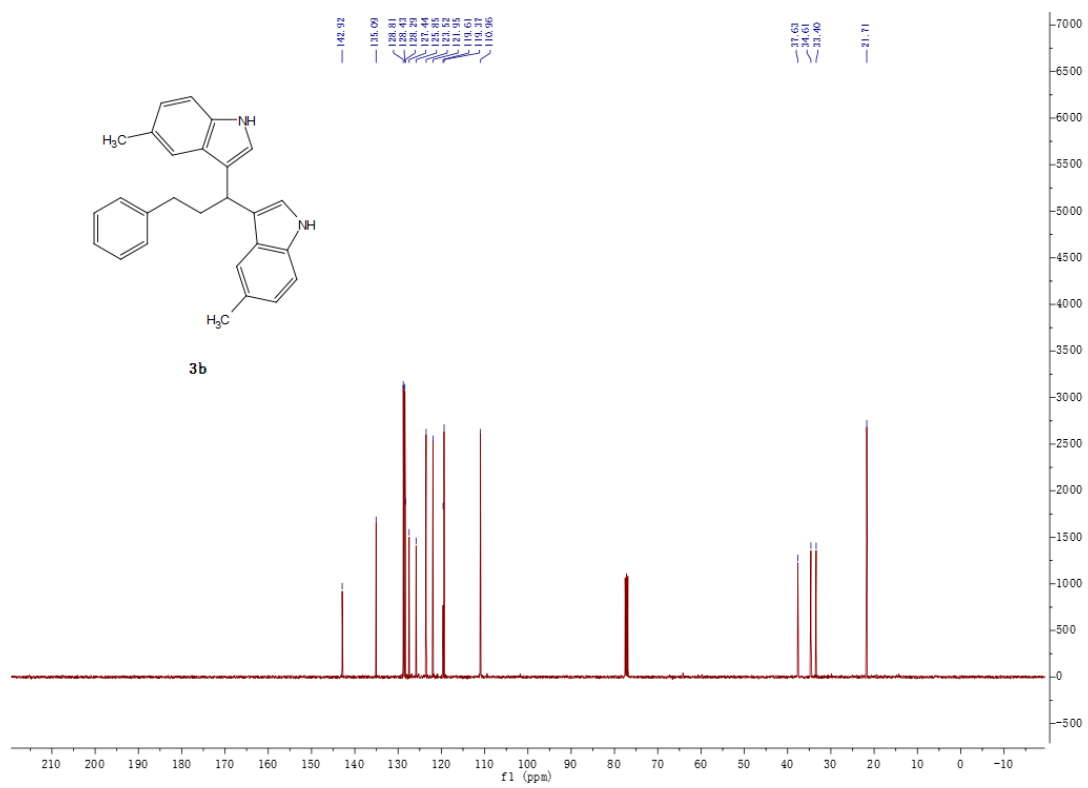
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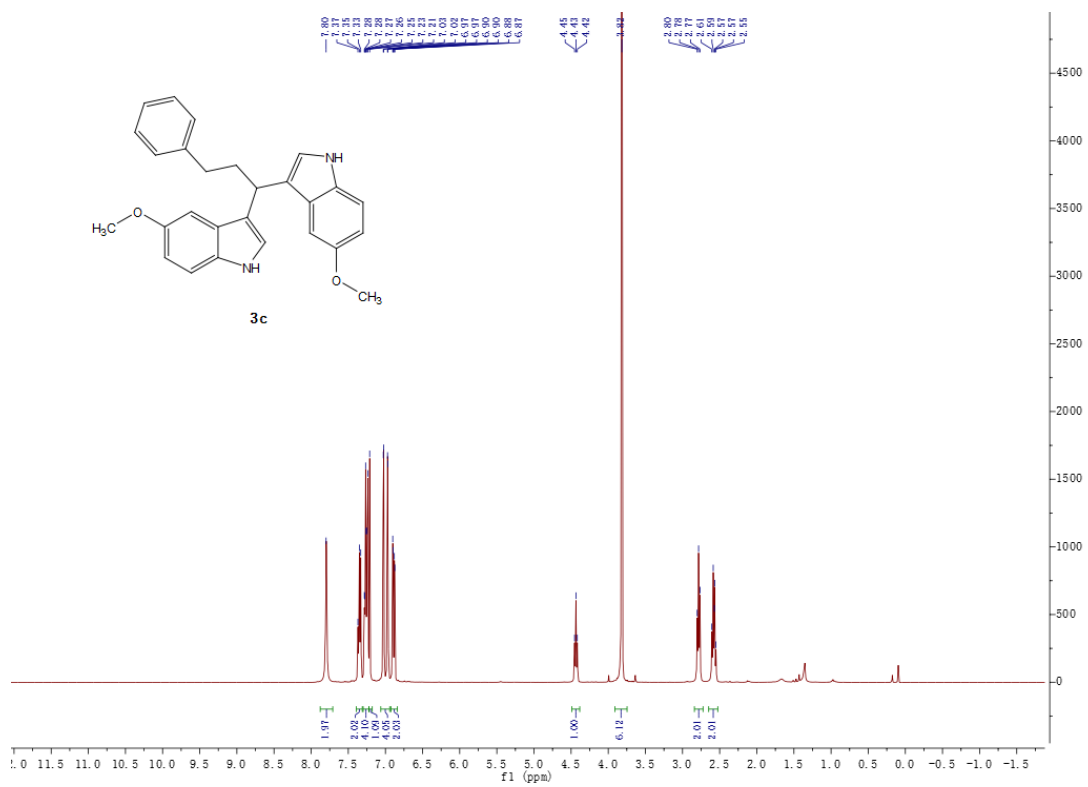
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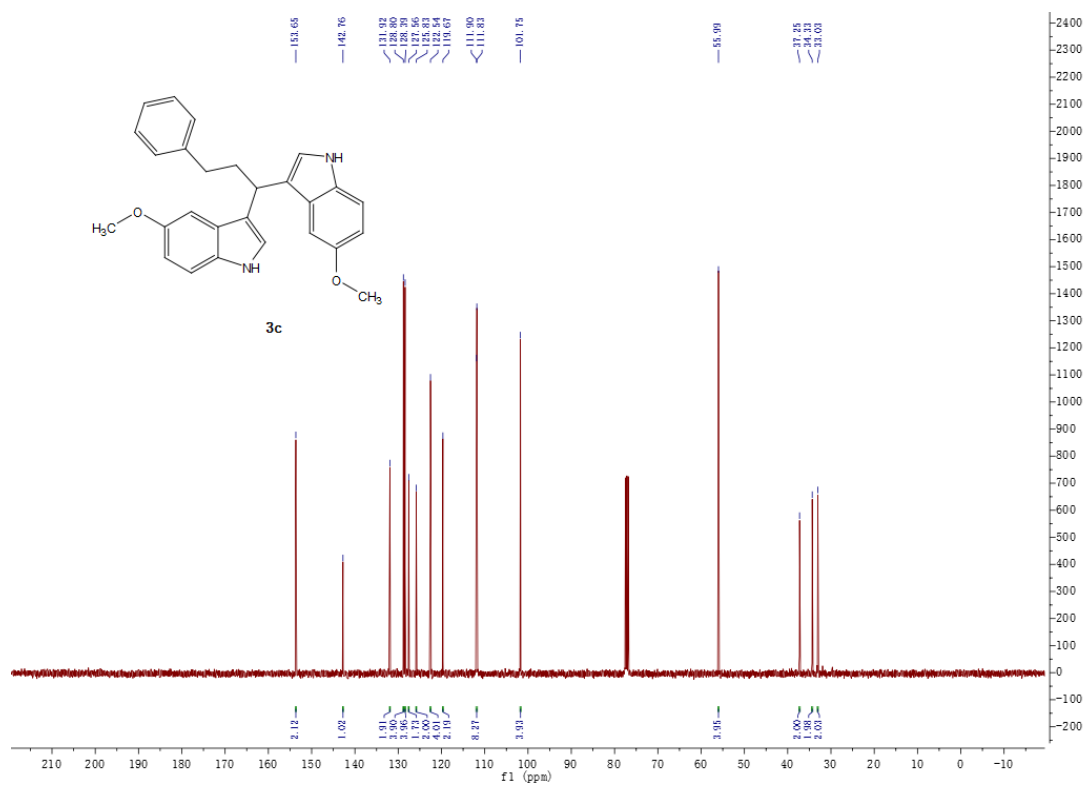
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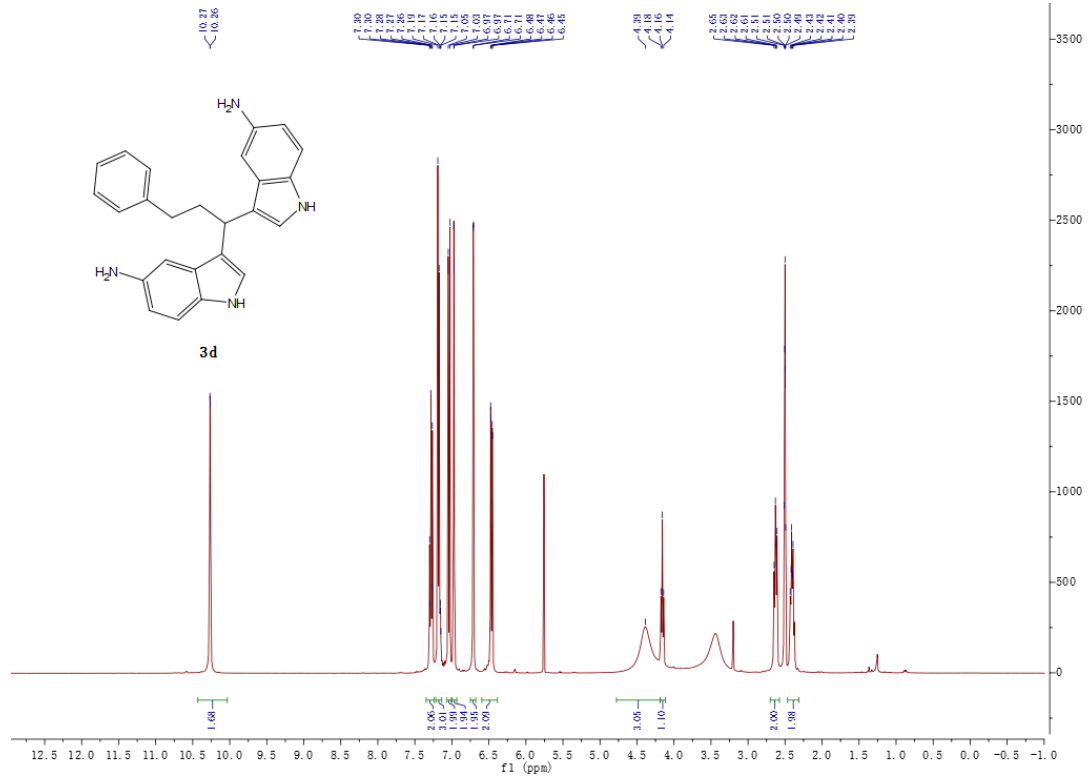
¹H NMR of 3c



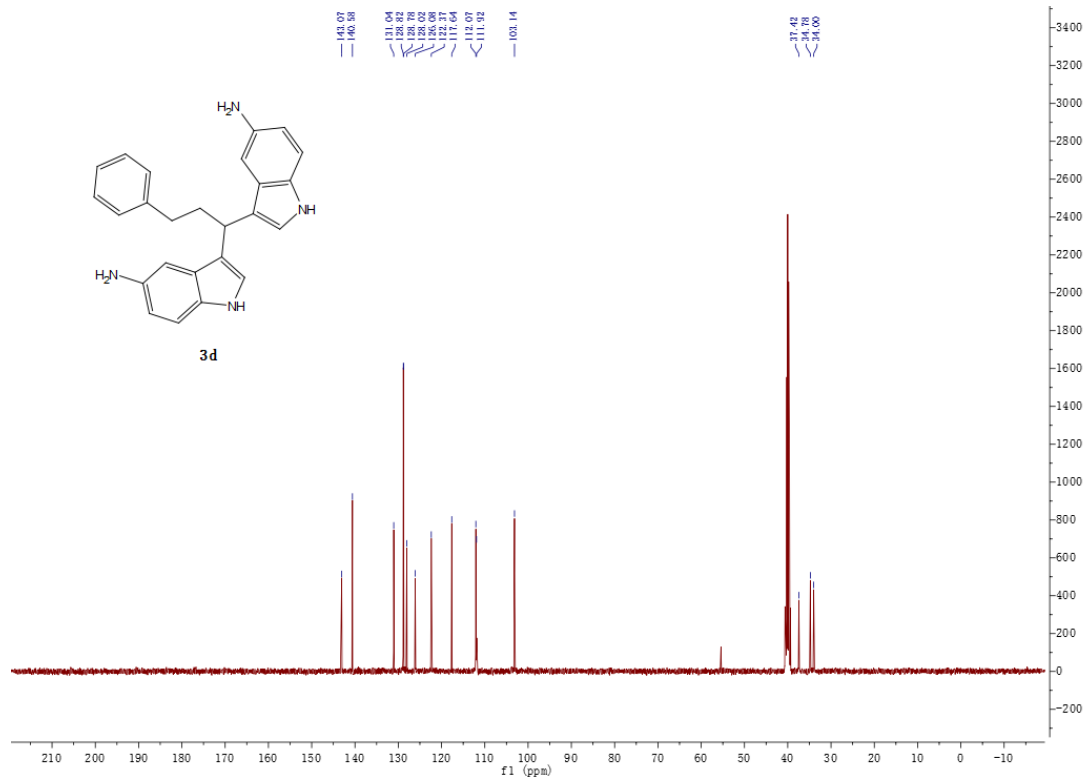
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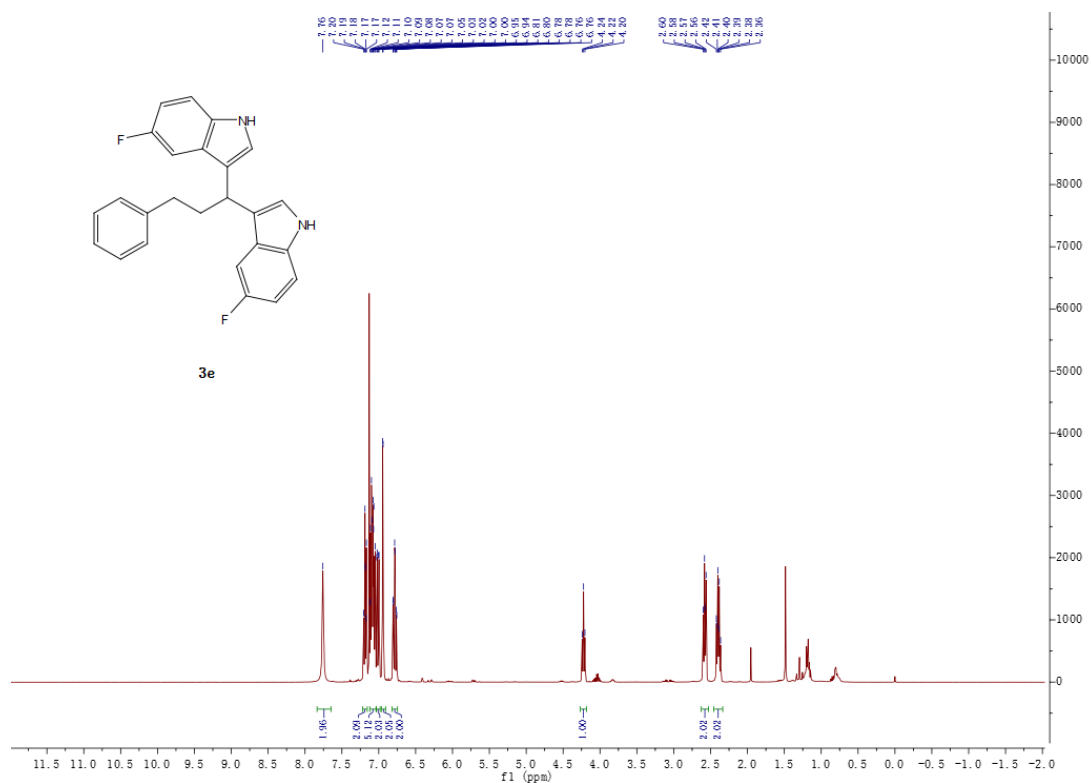
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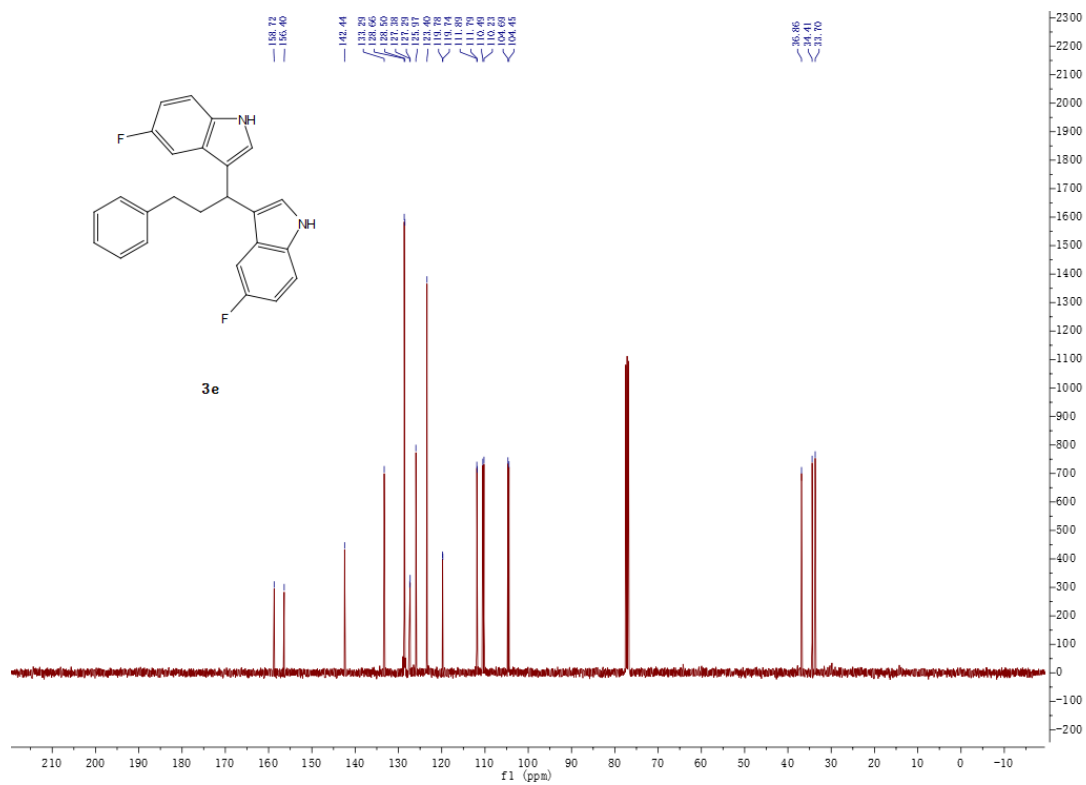
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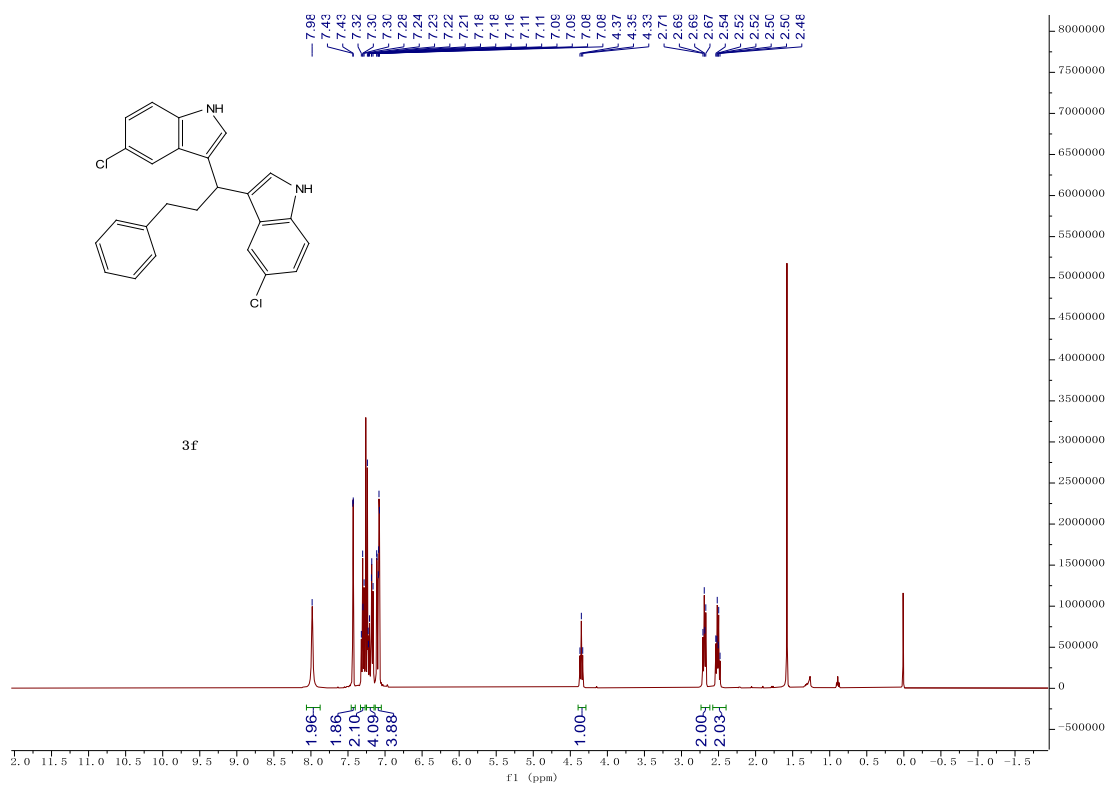
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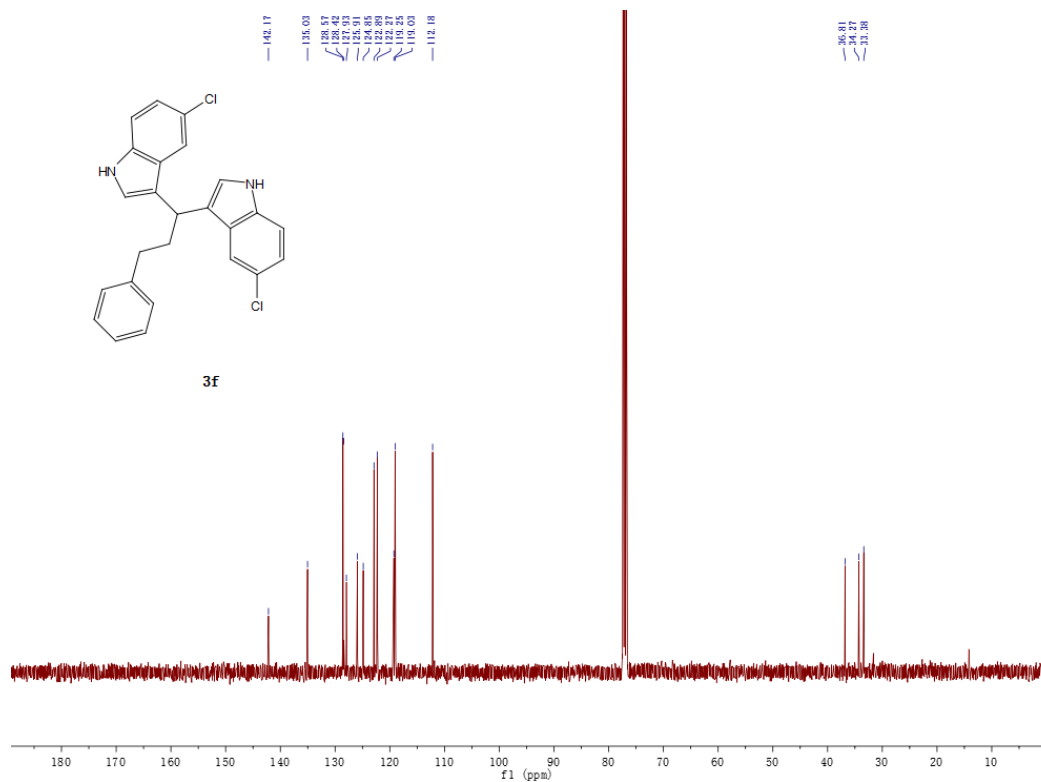
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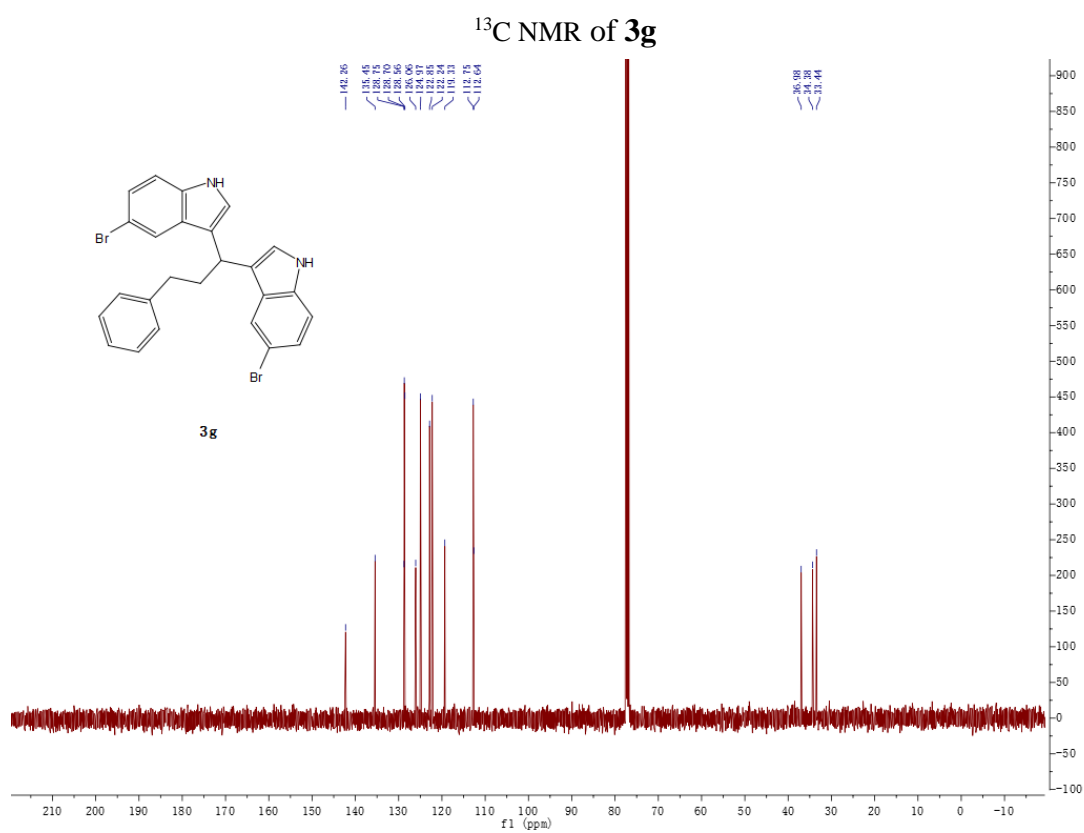
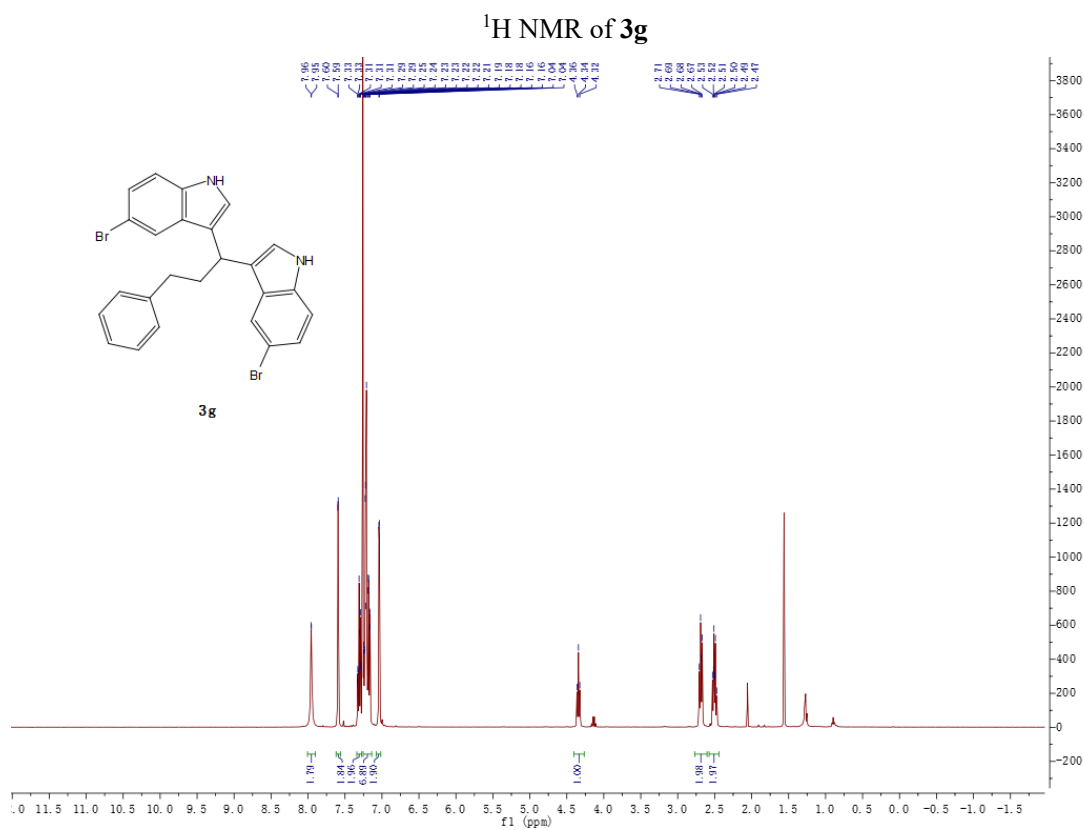


¹H NMR of 3f

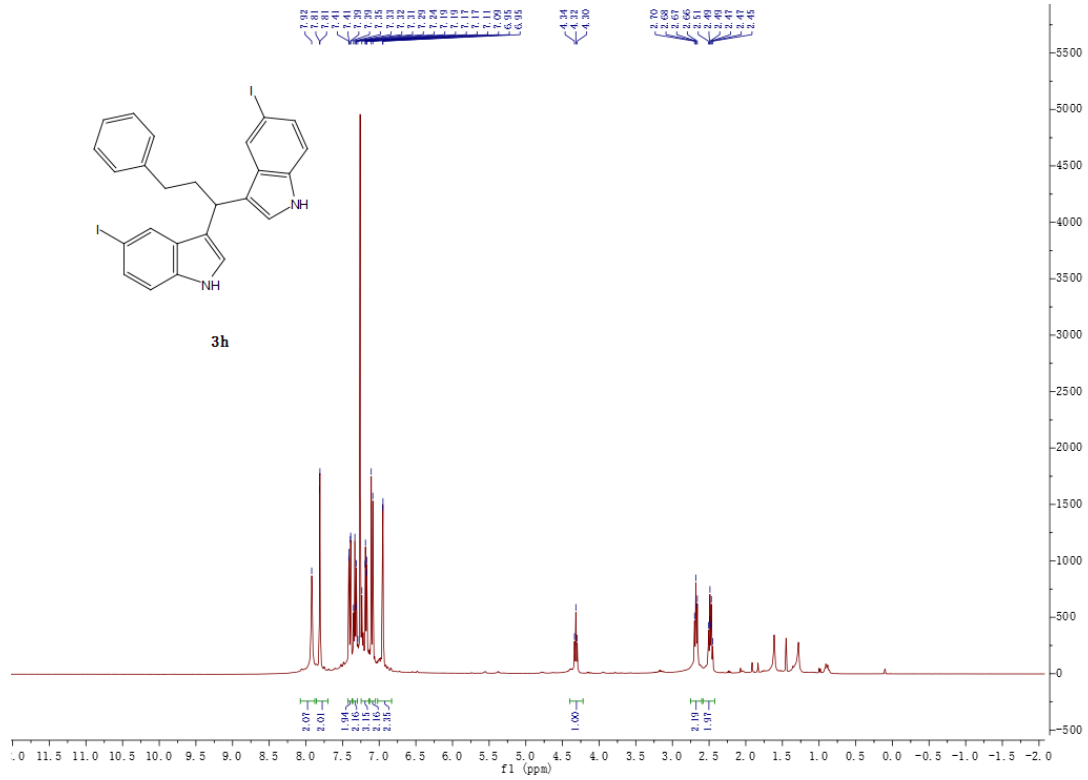


¹³C NMR of 3f

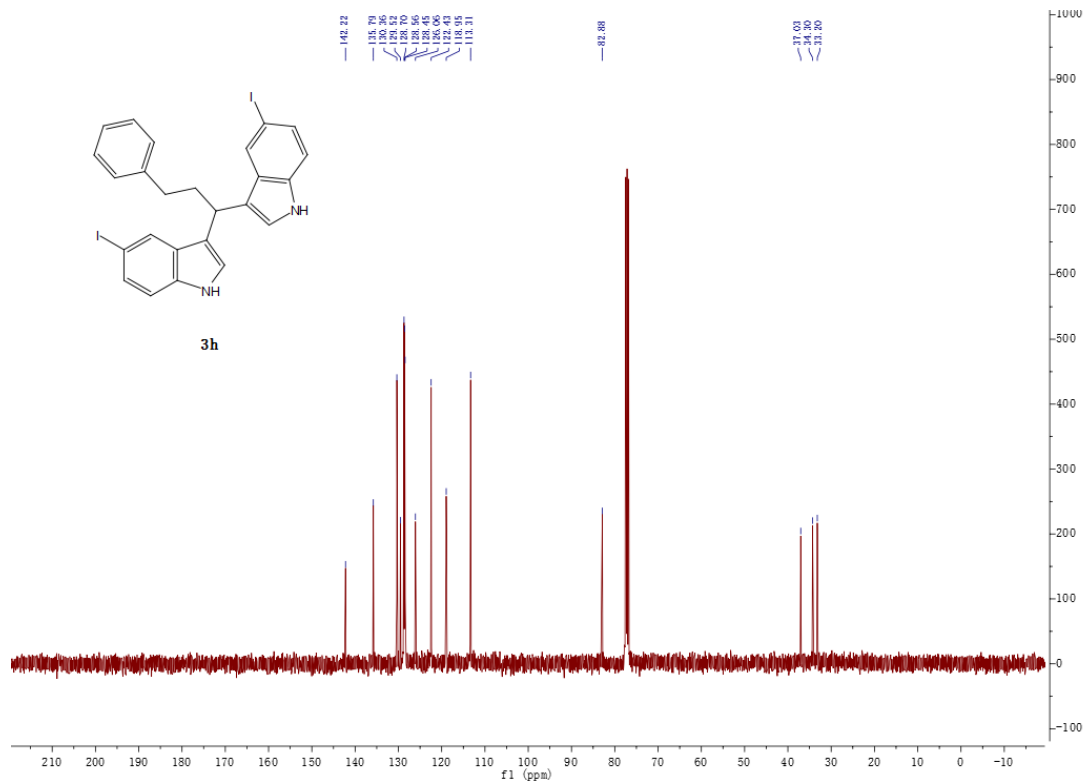




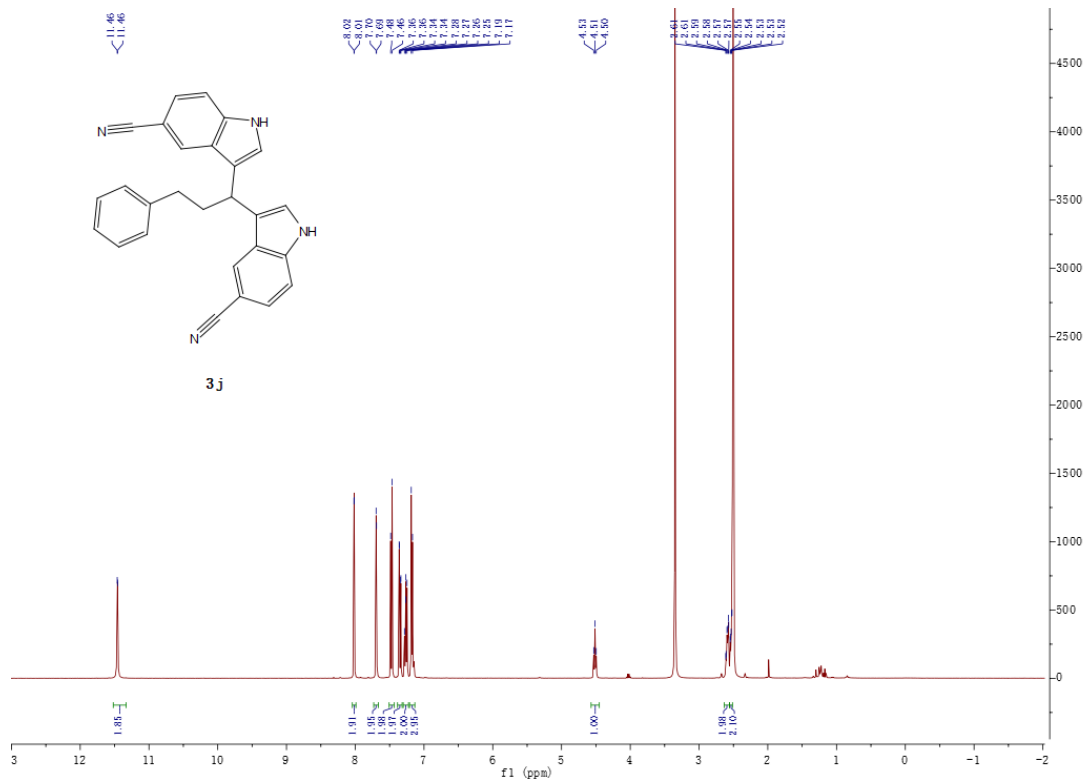
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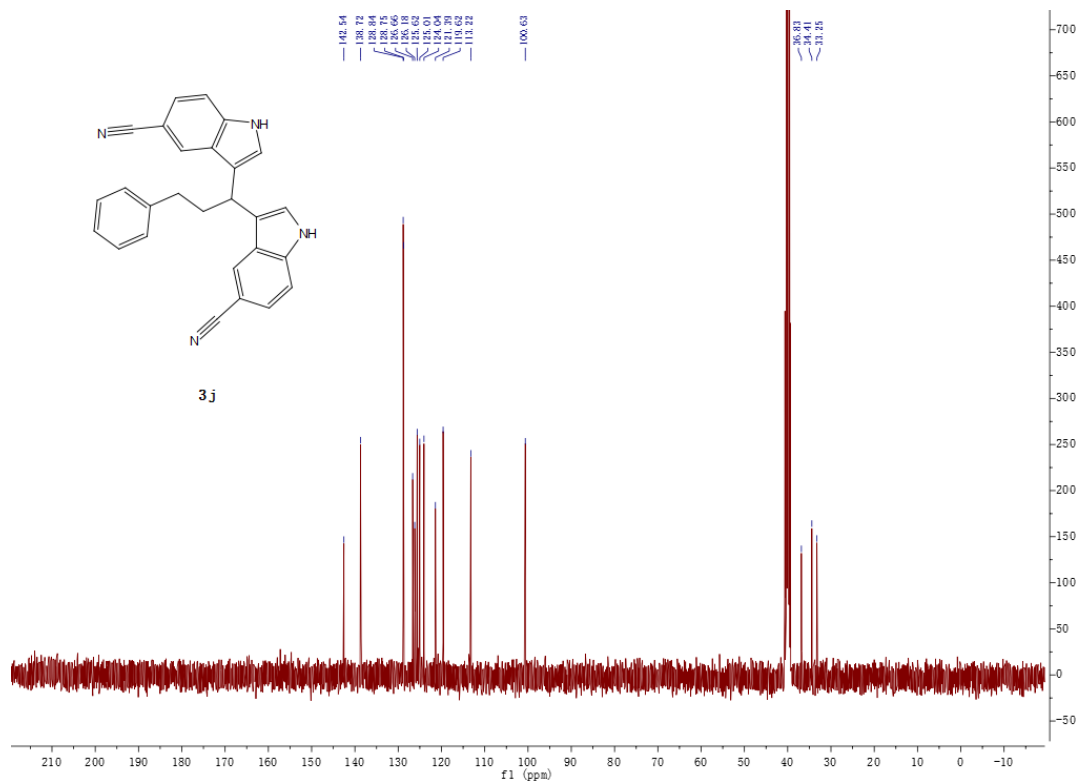
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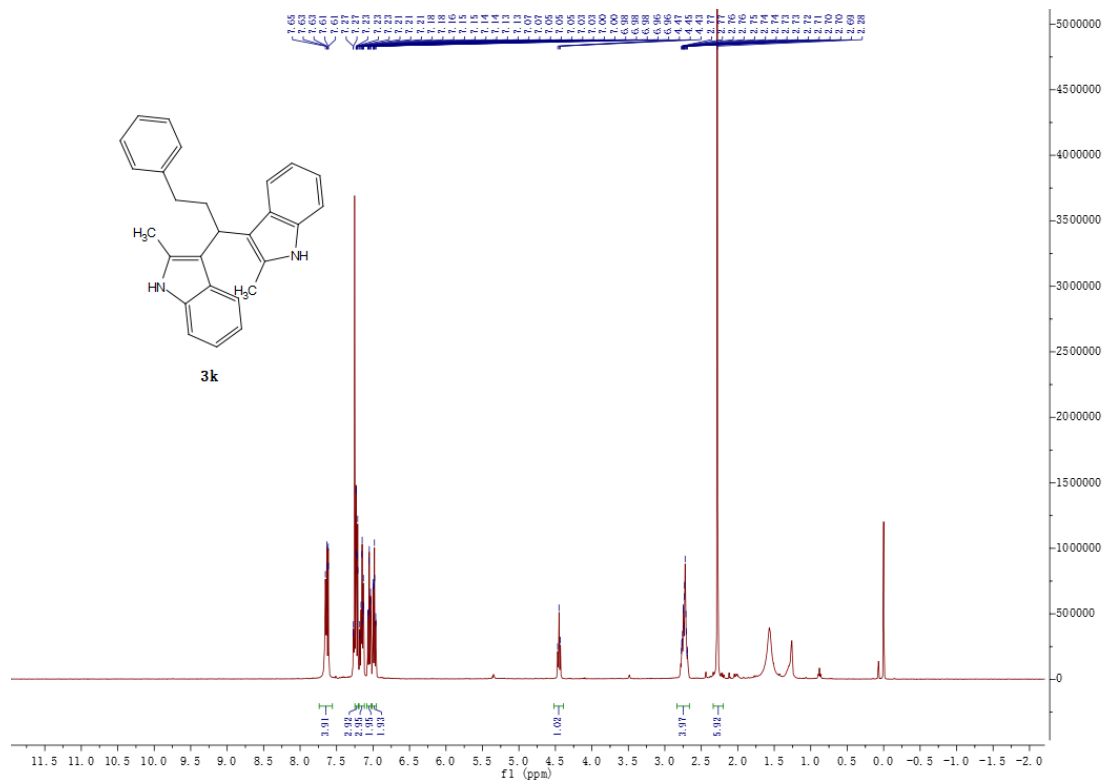
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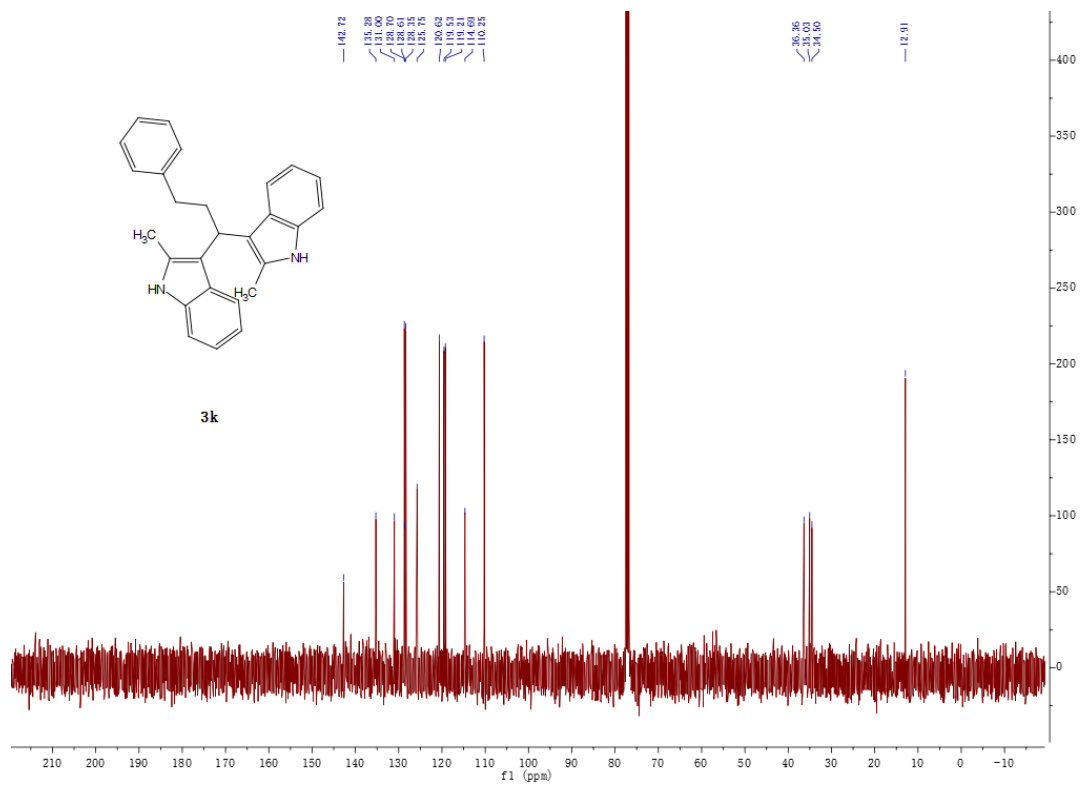
¹³C NMR of 3h



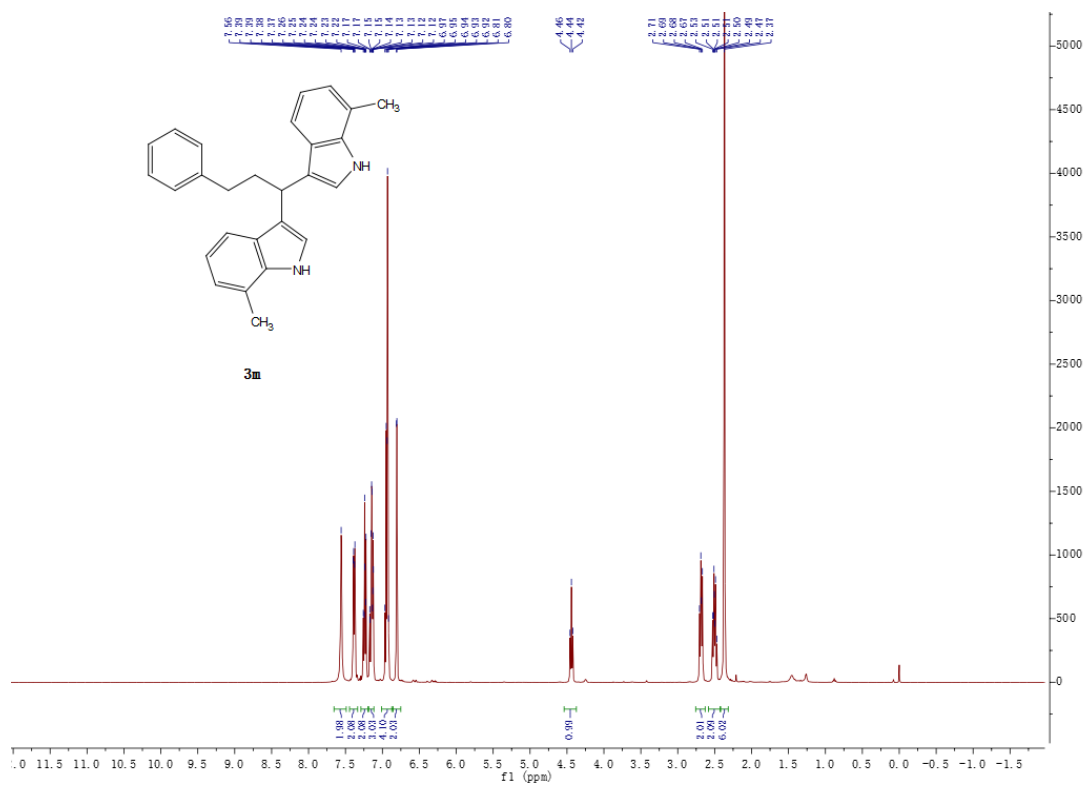
¹H NMR of 3k



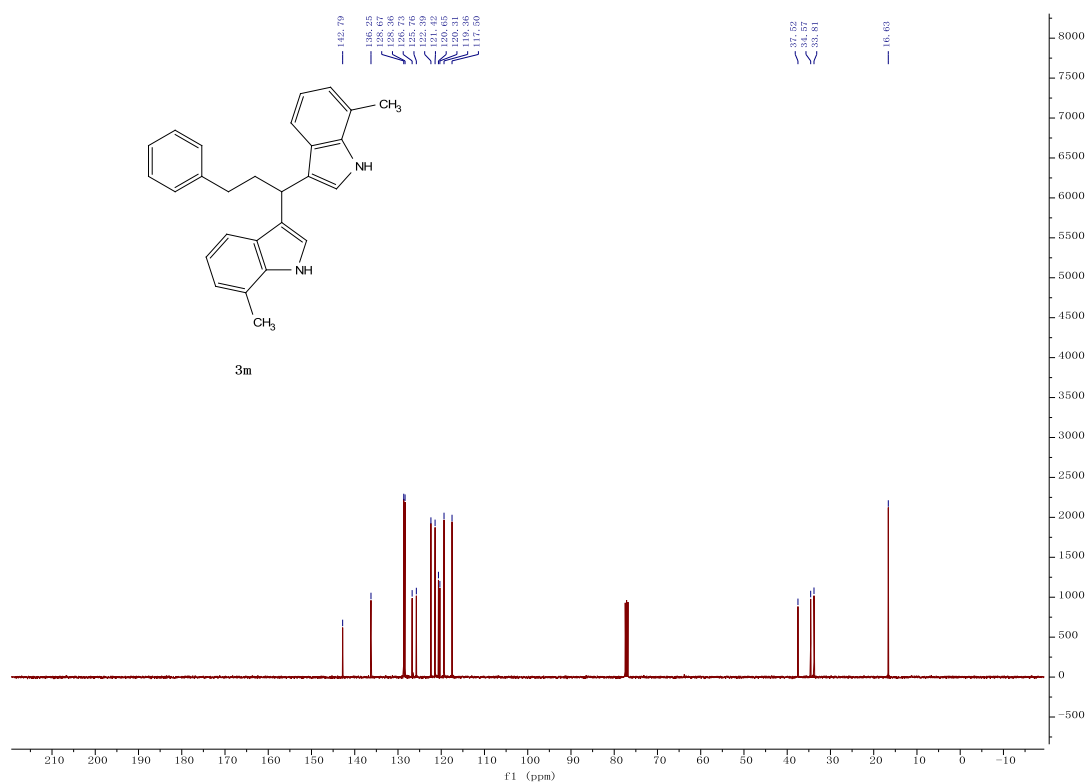
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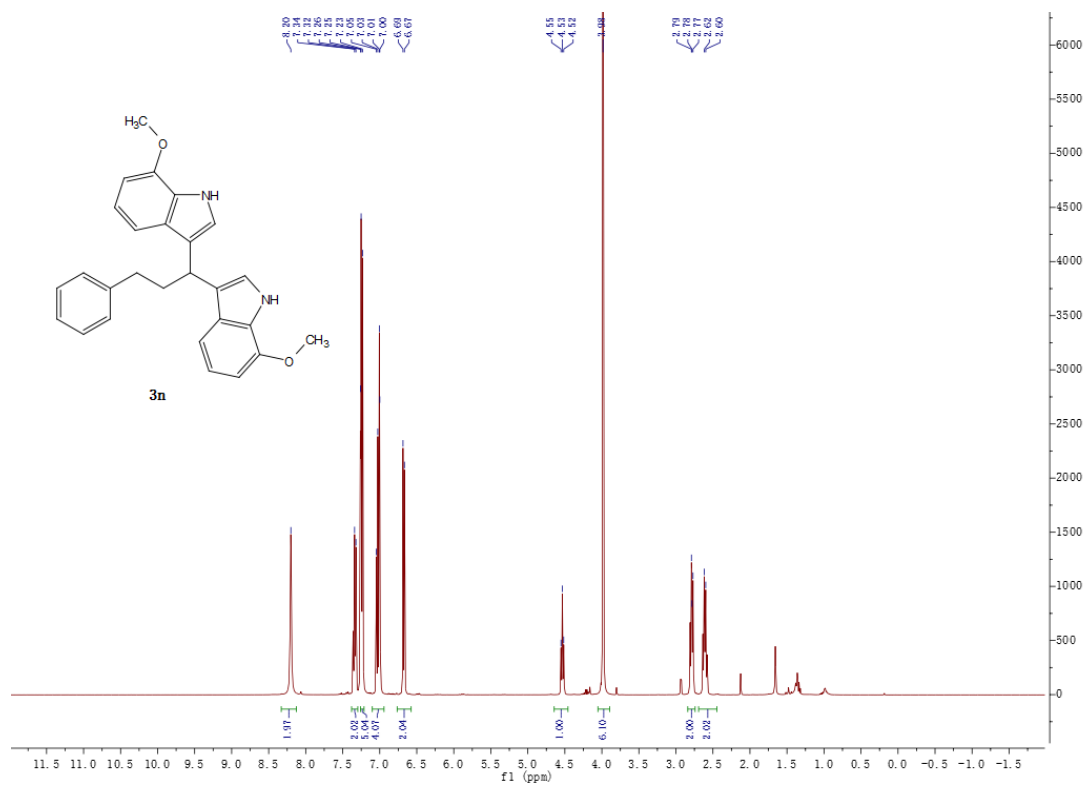
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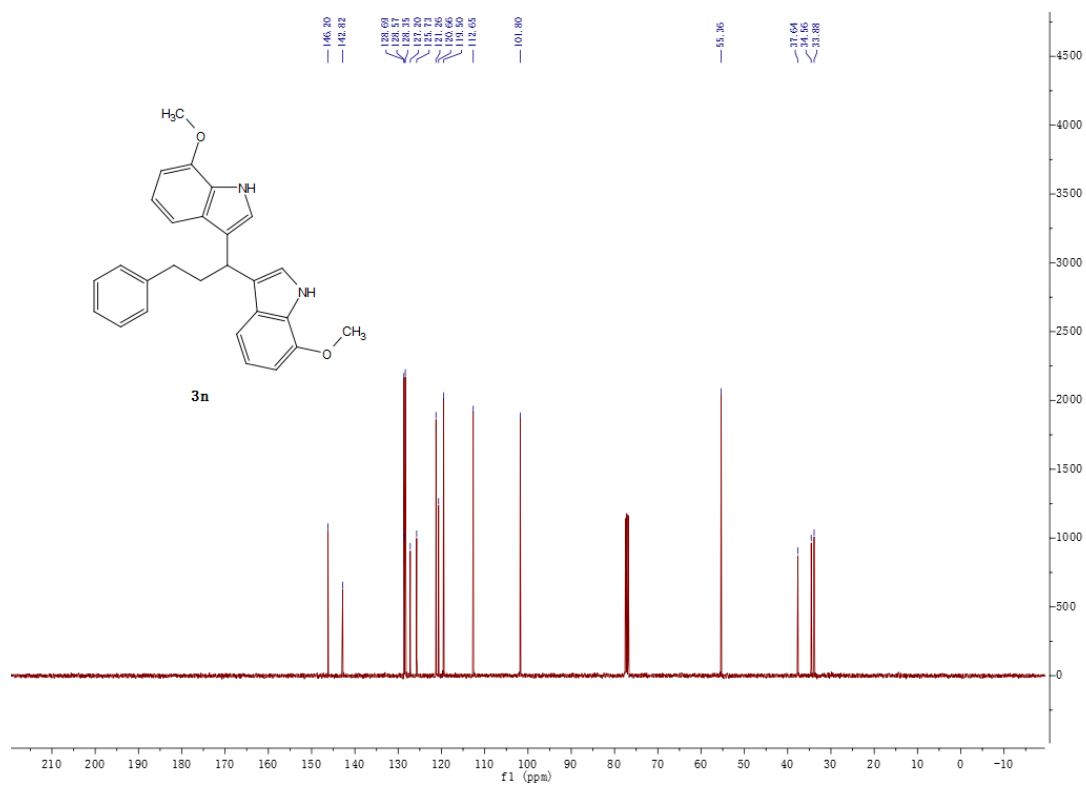
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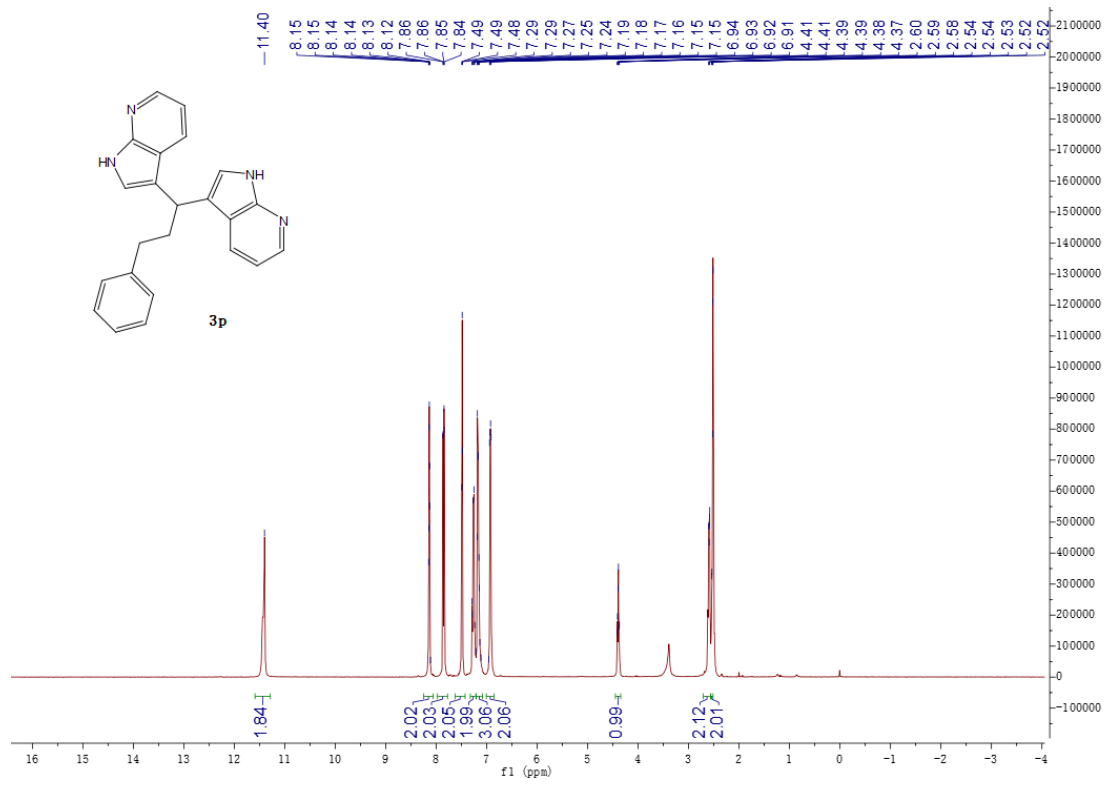
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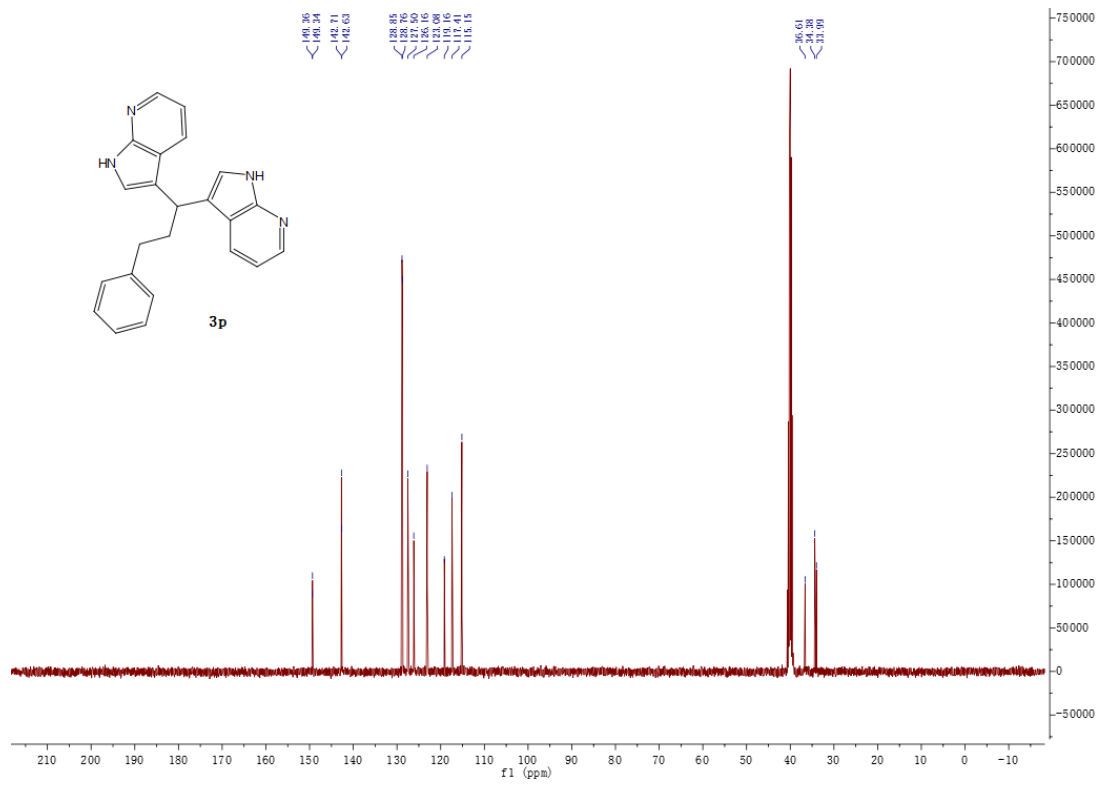
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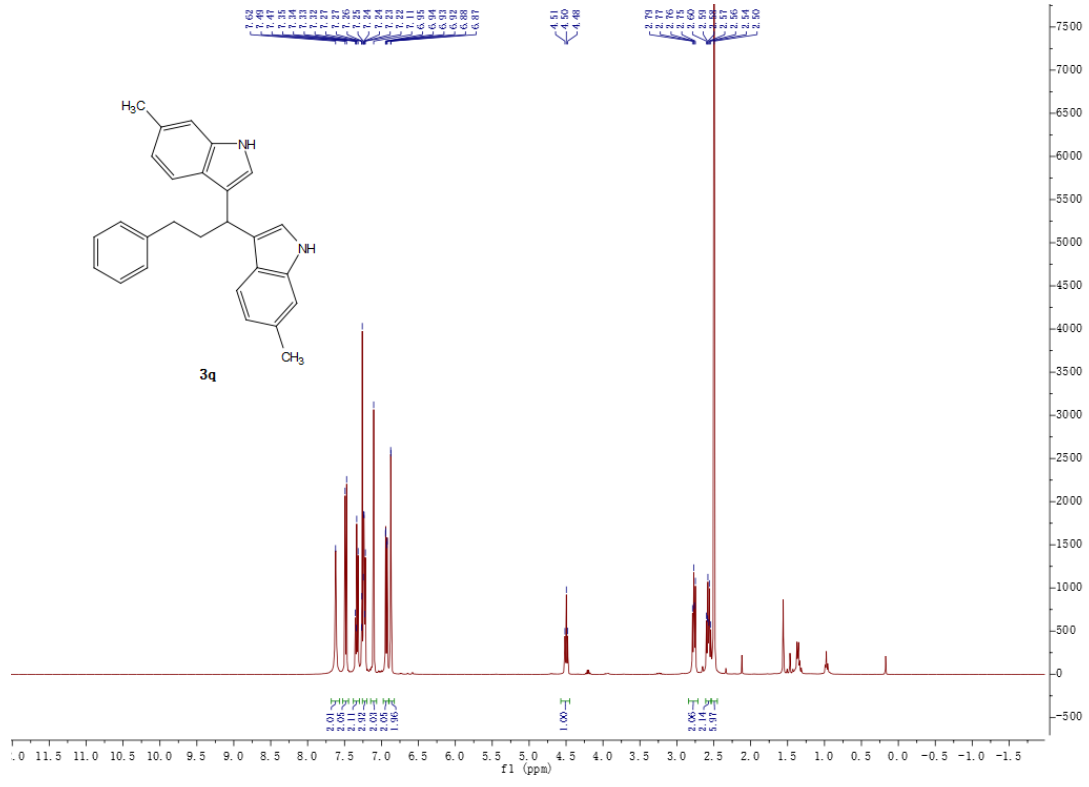
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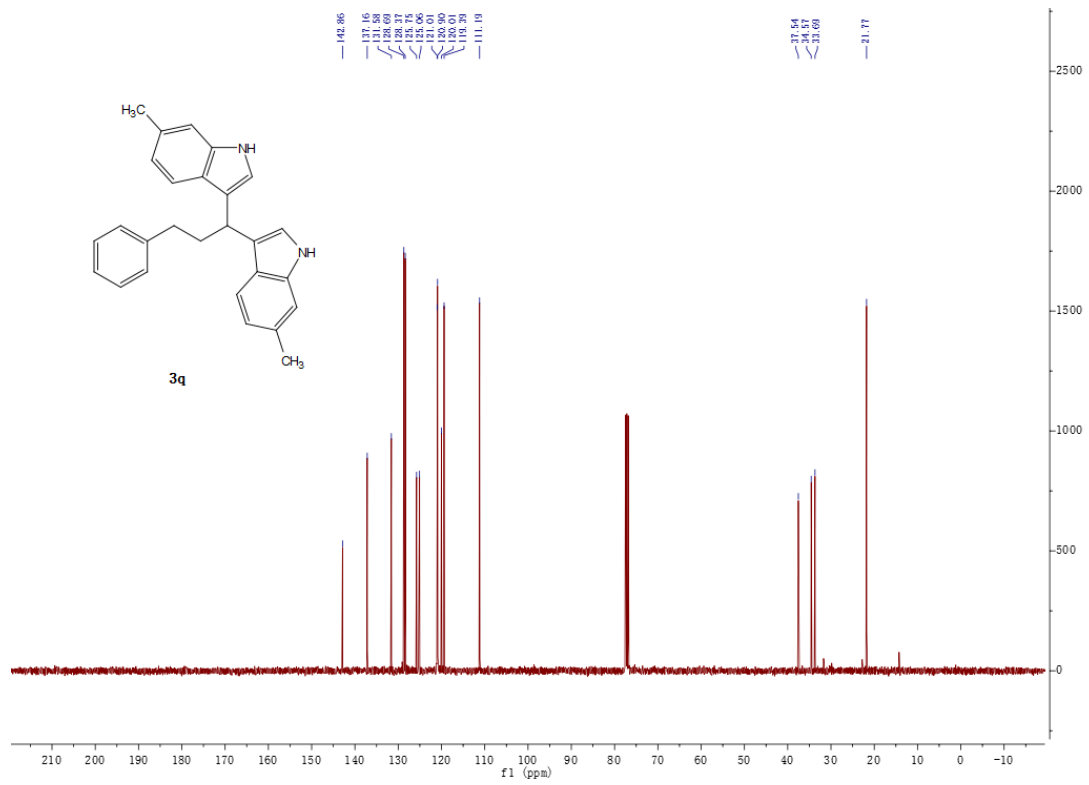
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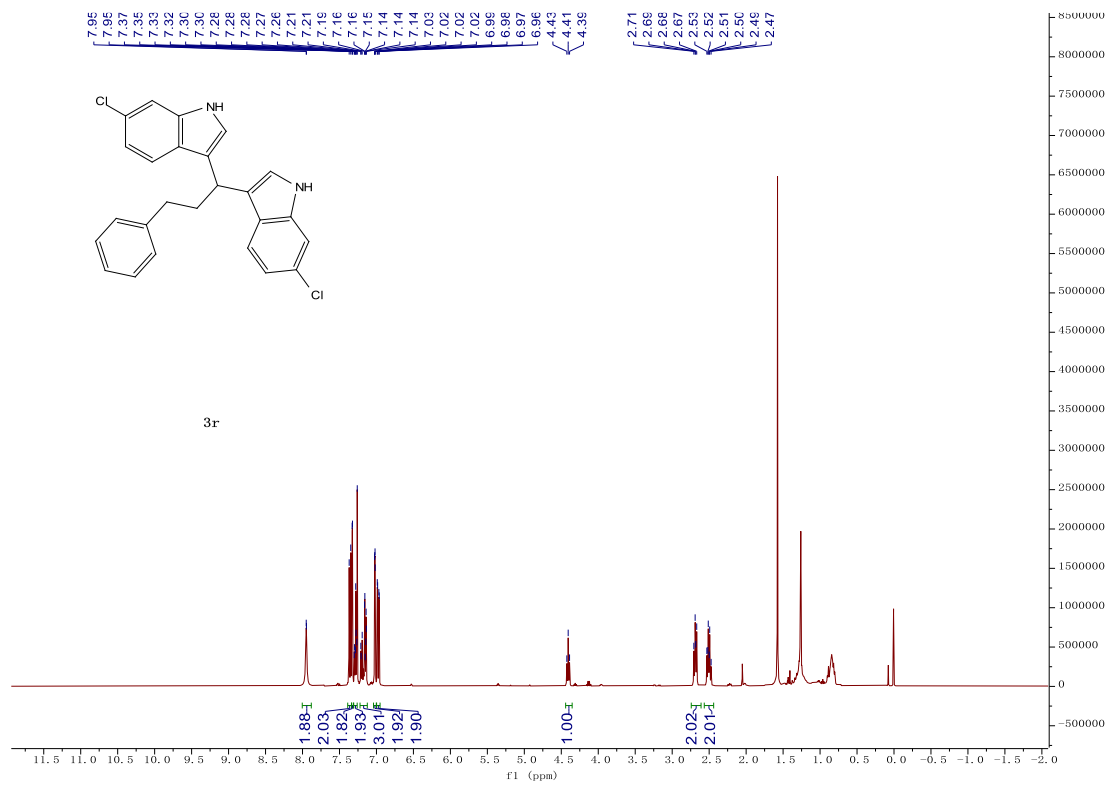
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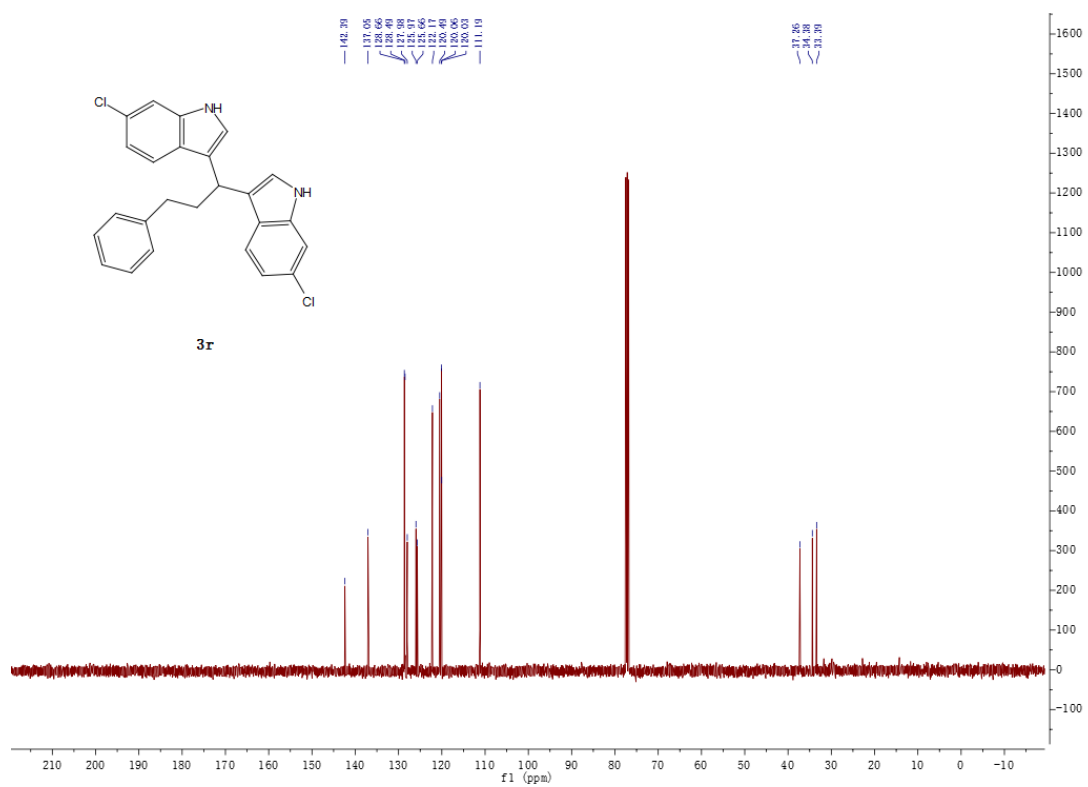
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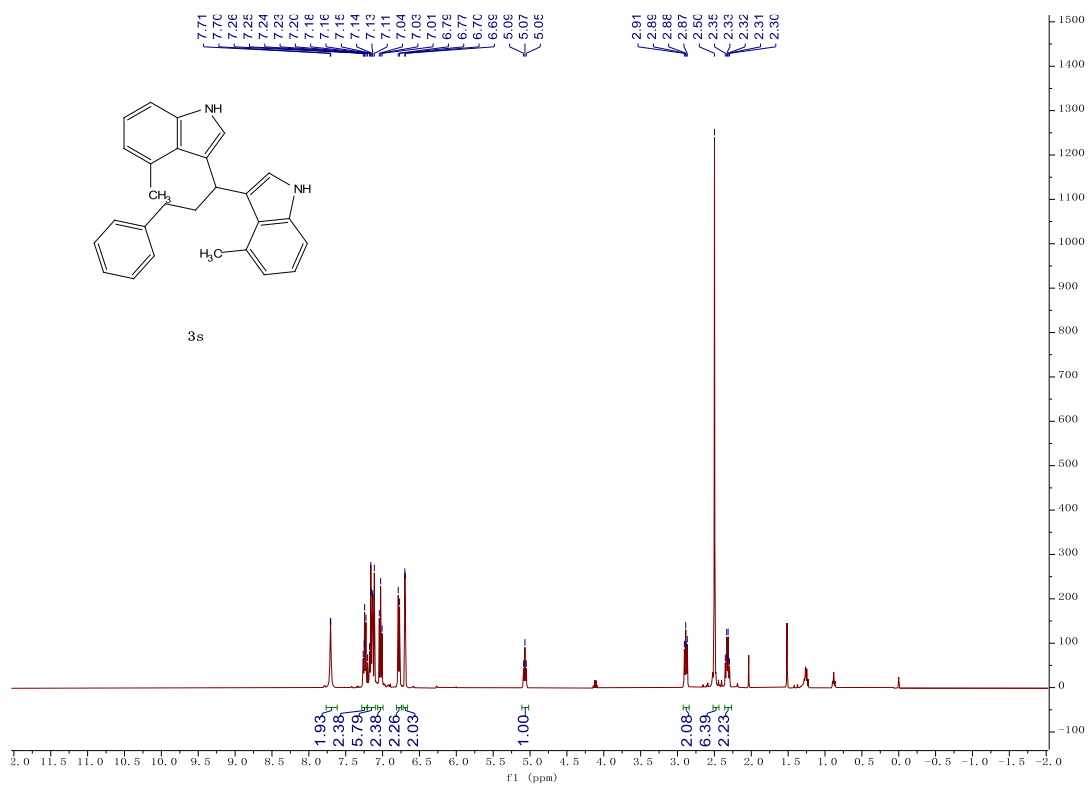
¹H NMR of 3r



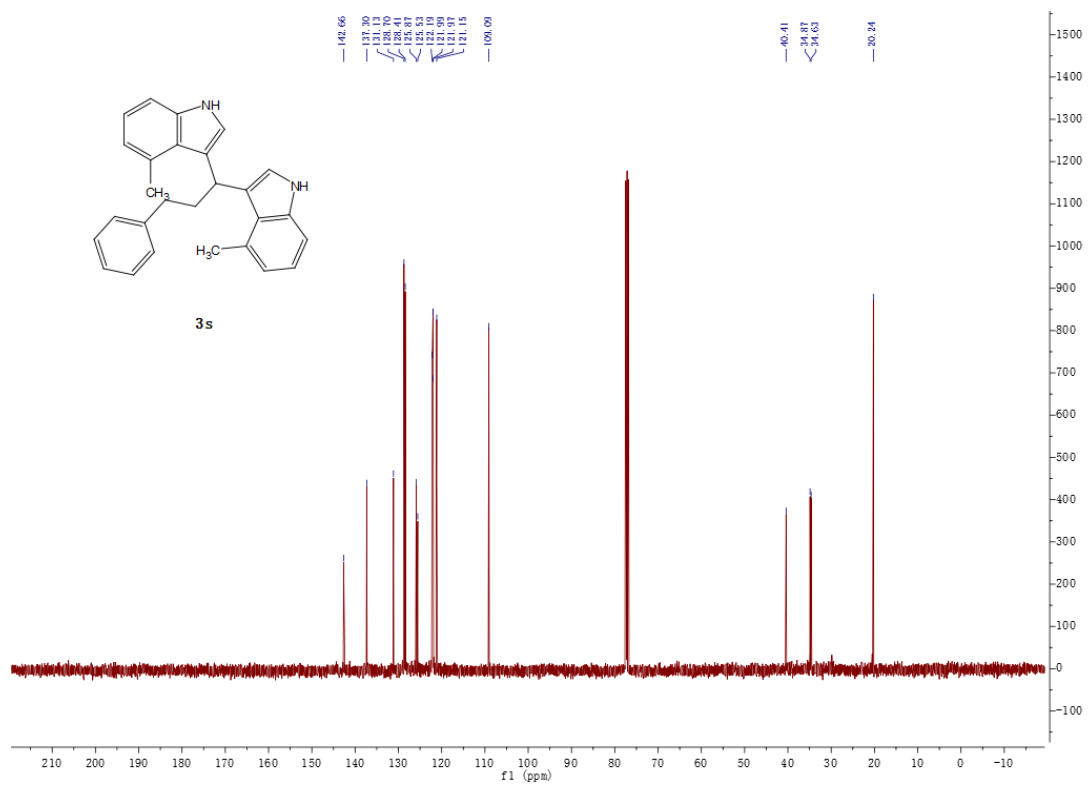
¹³C NMR of 3r



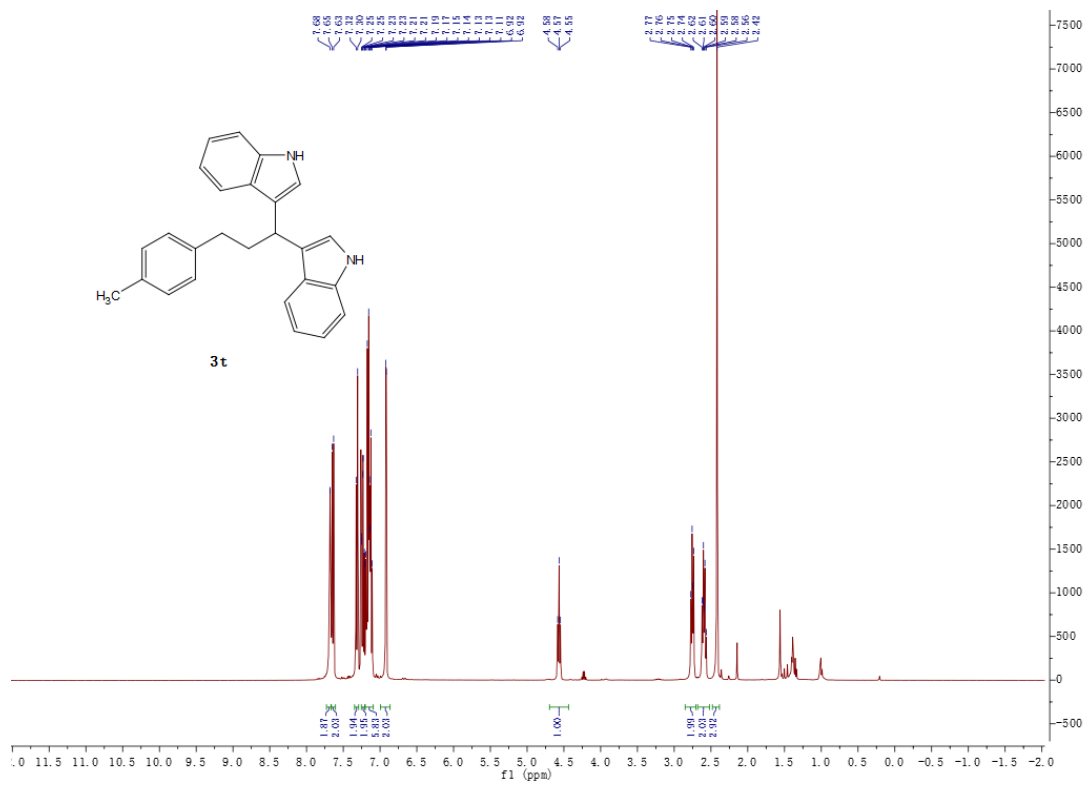
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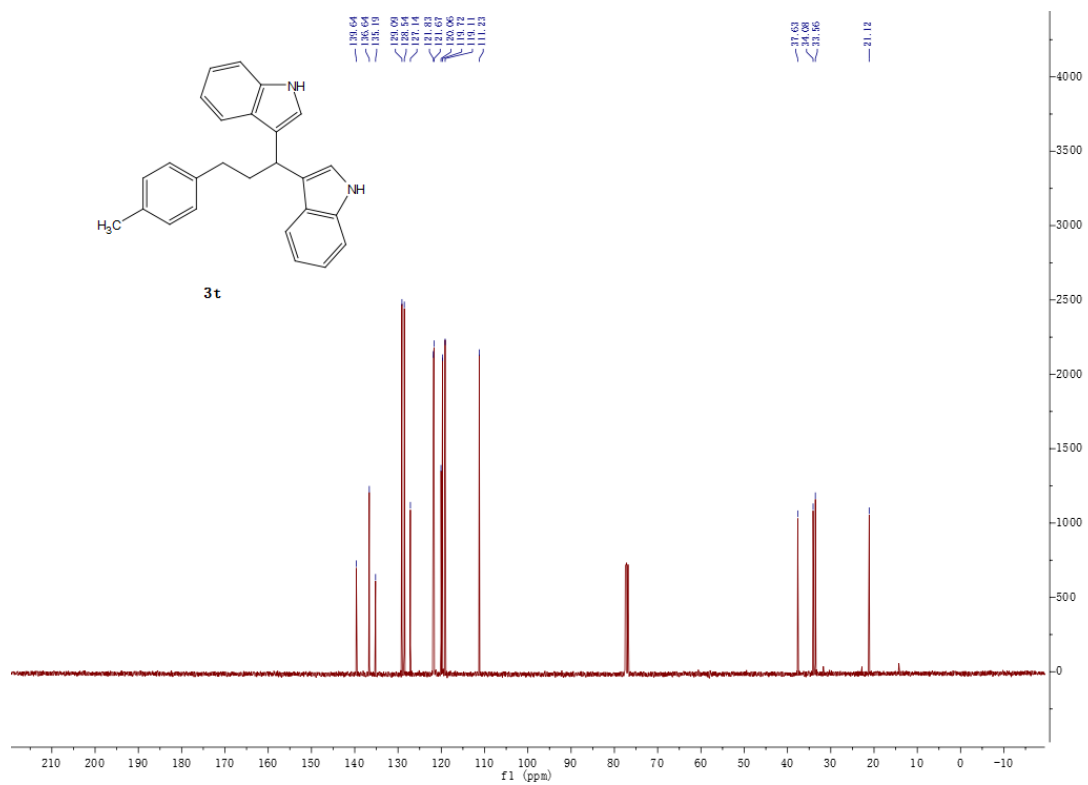
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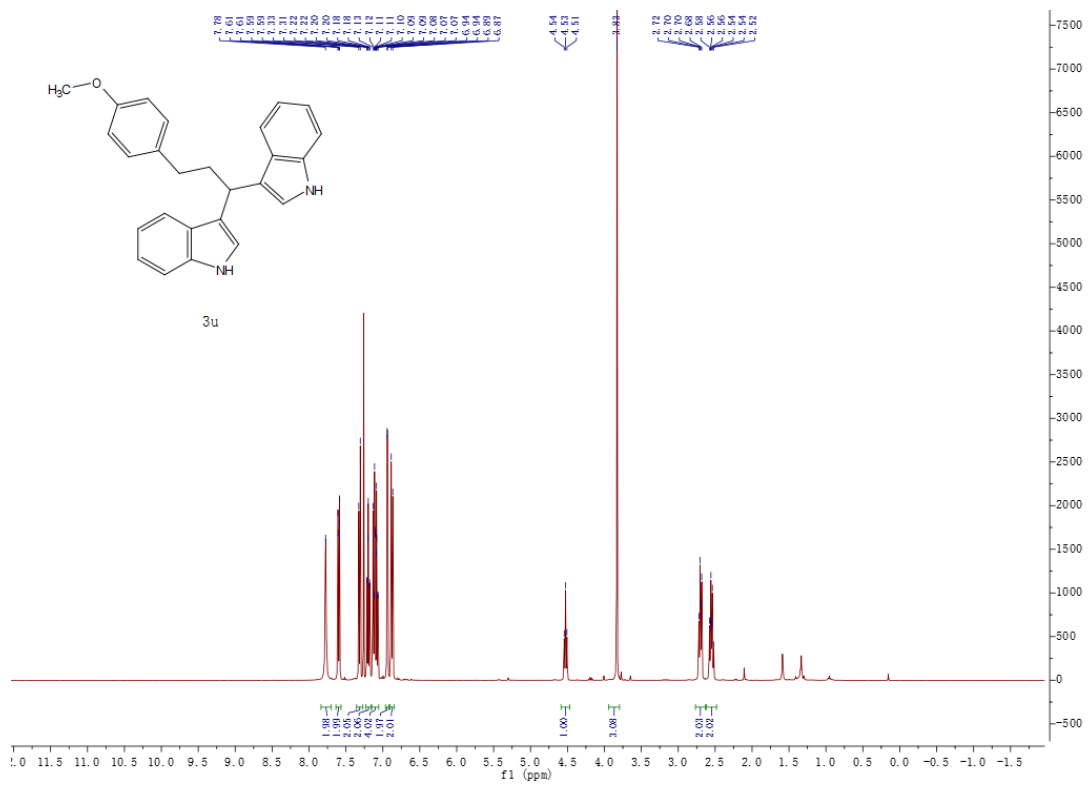
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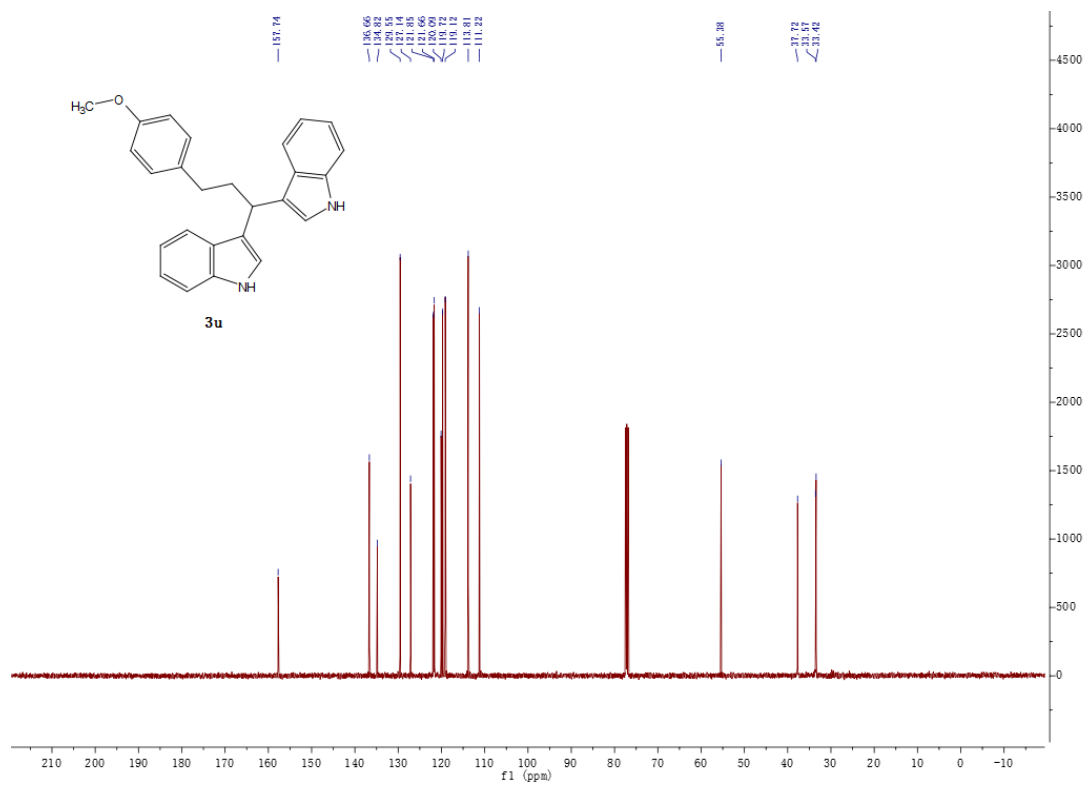
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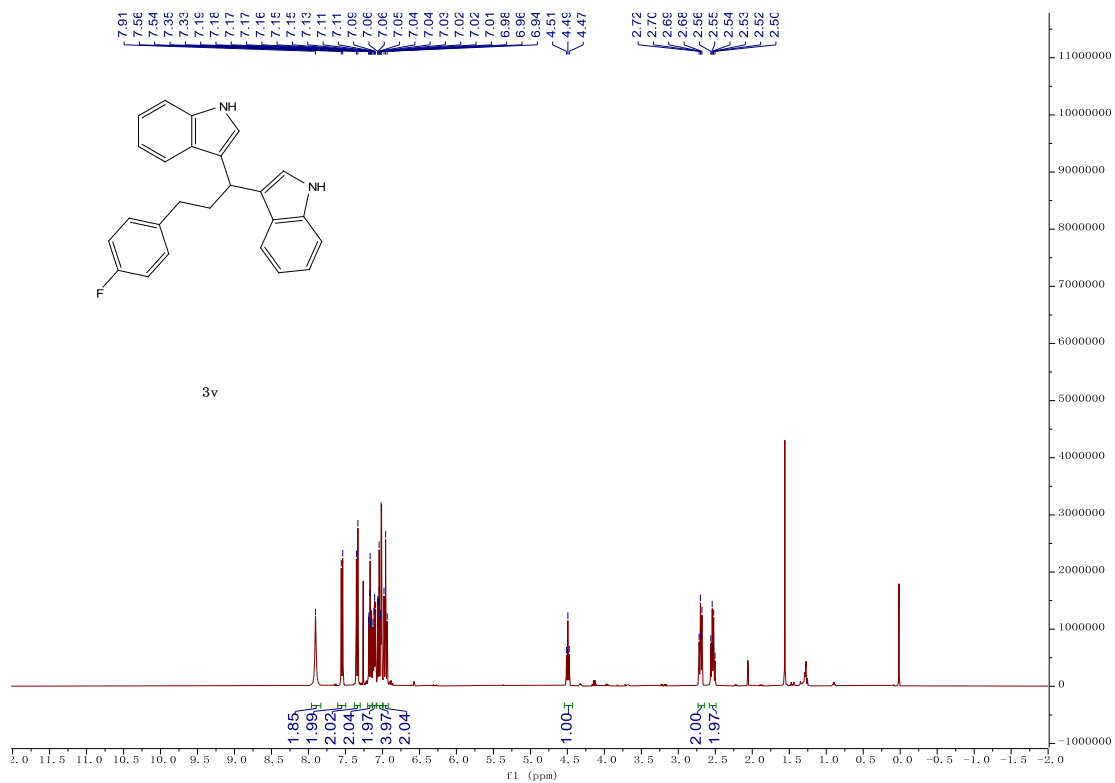
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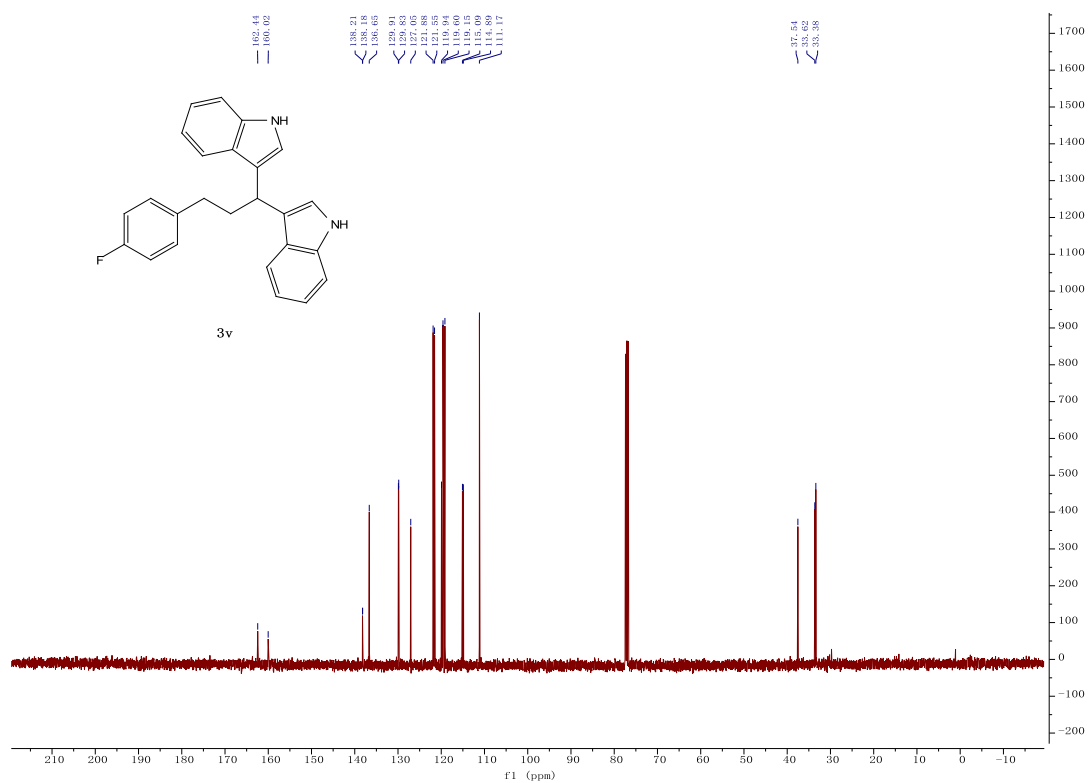
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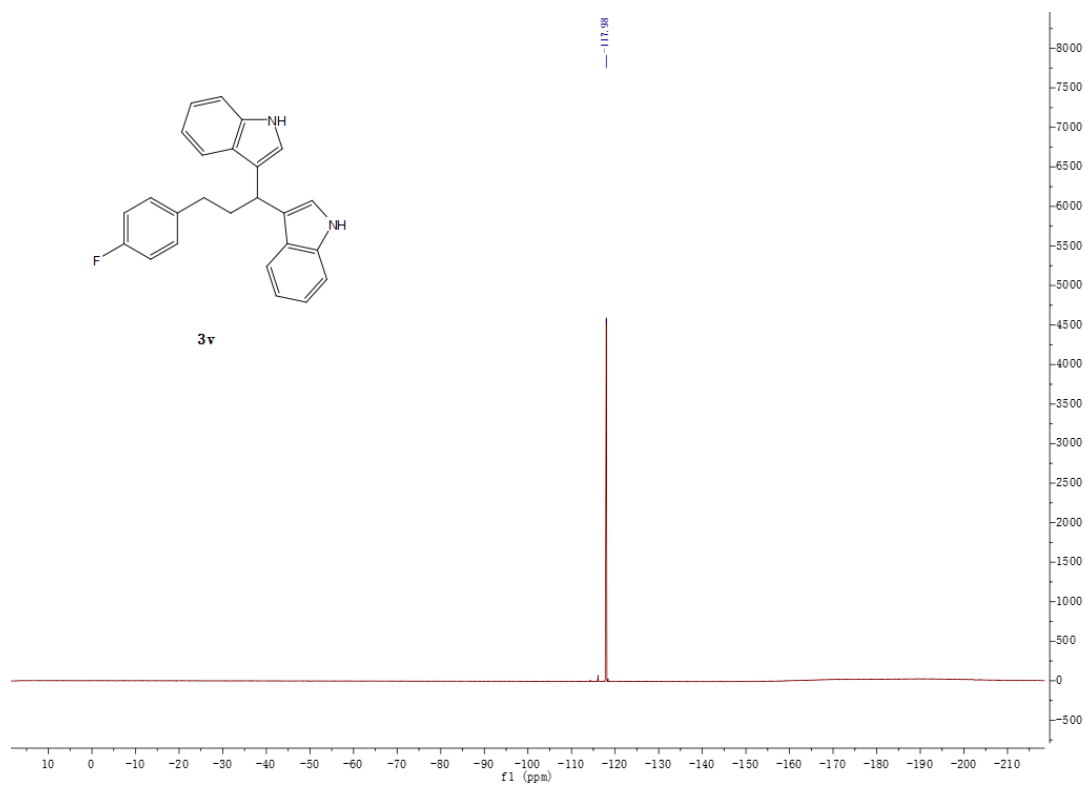
¹H NMR of 3v



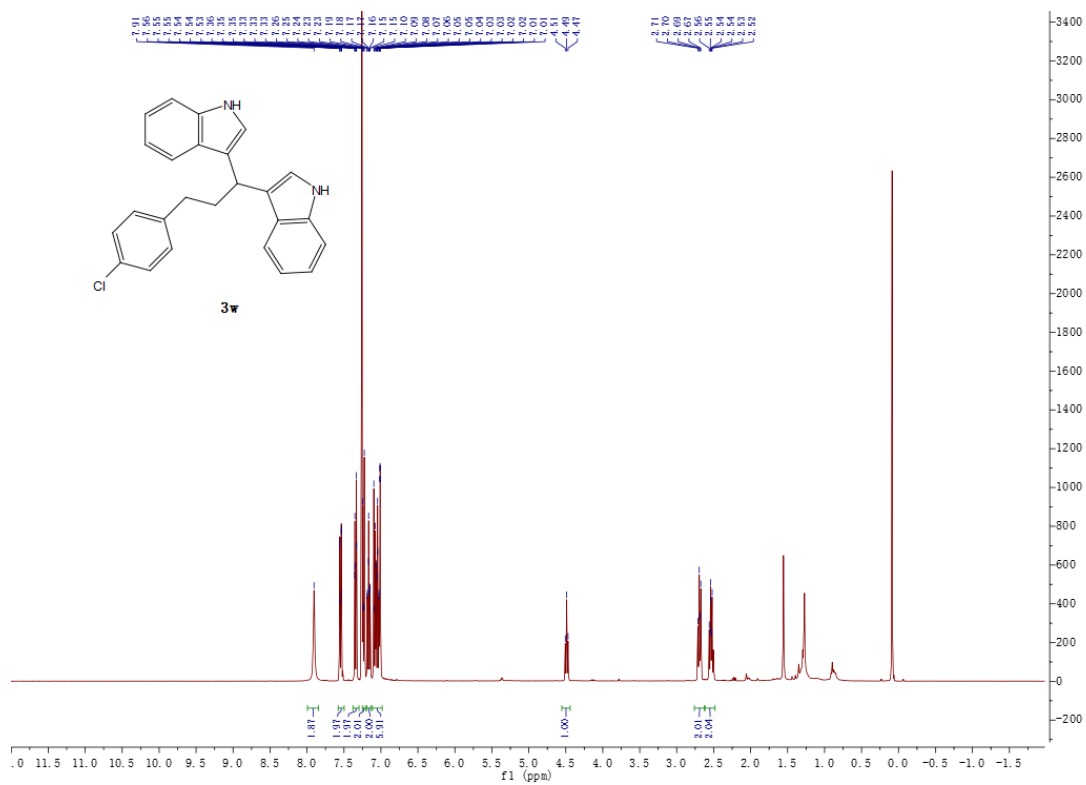
¹³C NMR of 3v



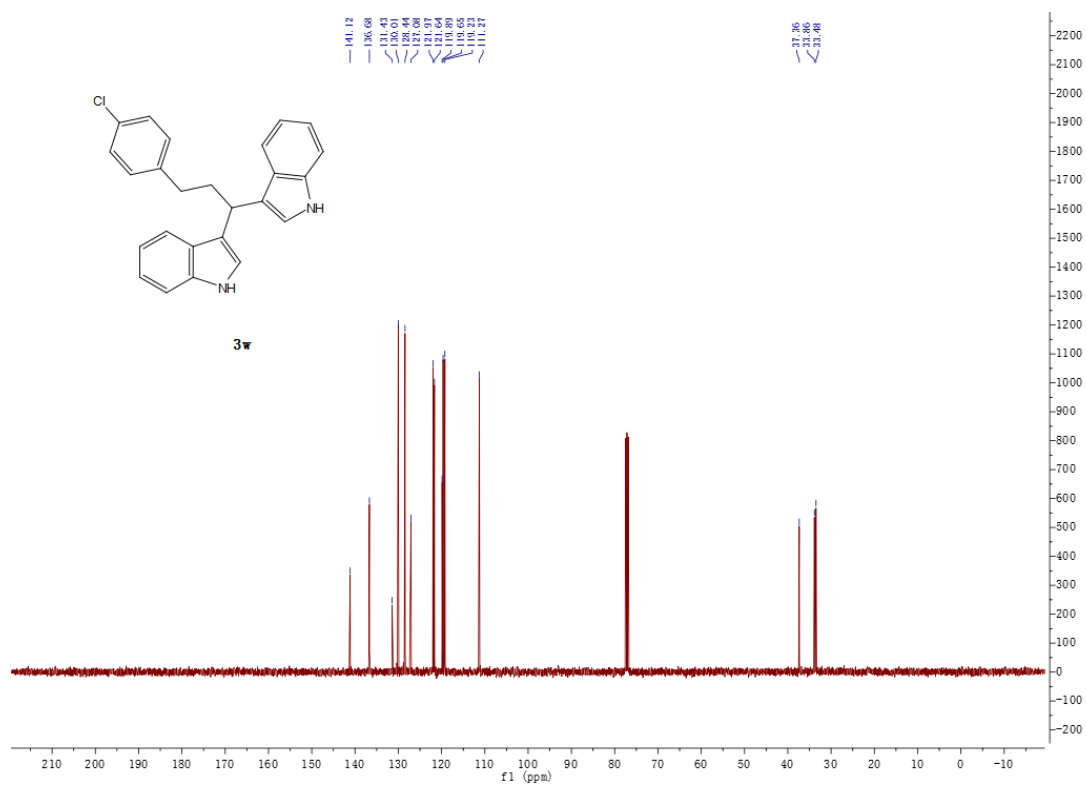
¹⁹F NMR of **3v**



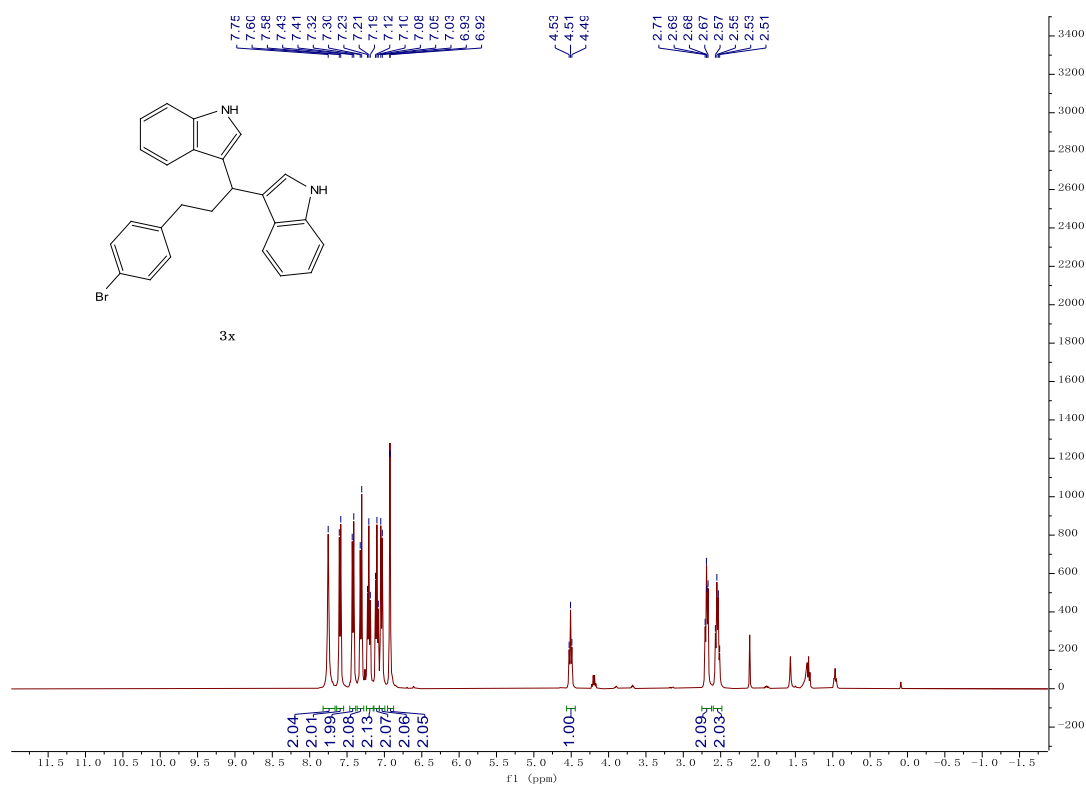
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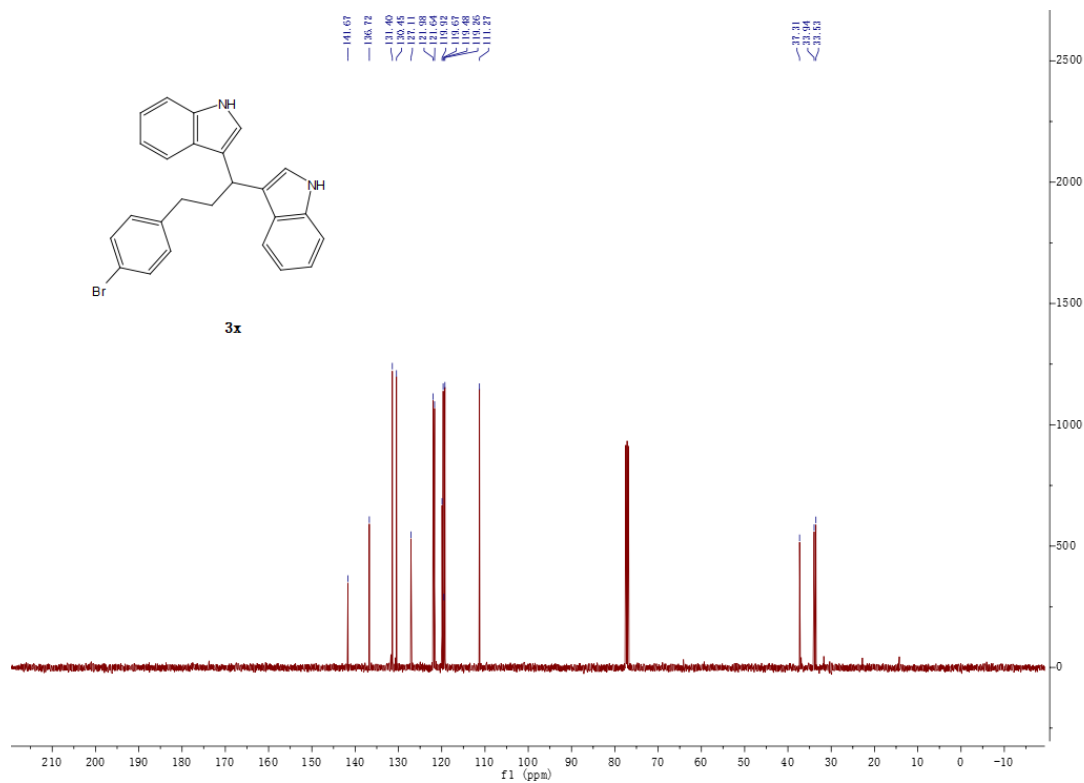
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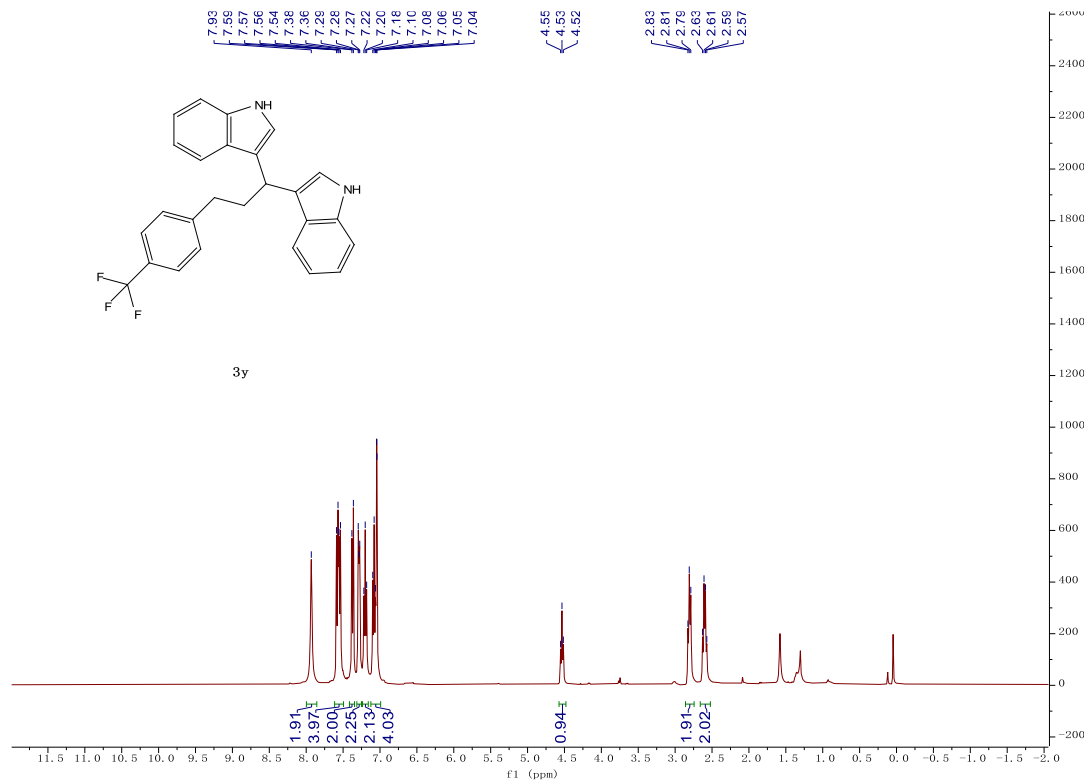
¹H NMR of 3x



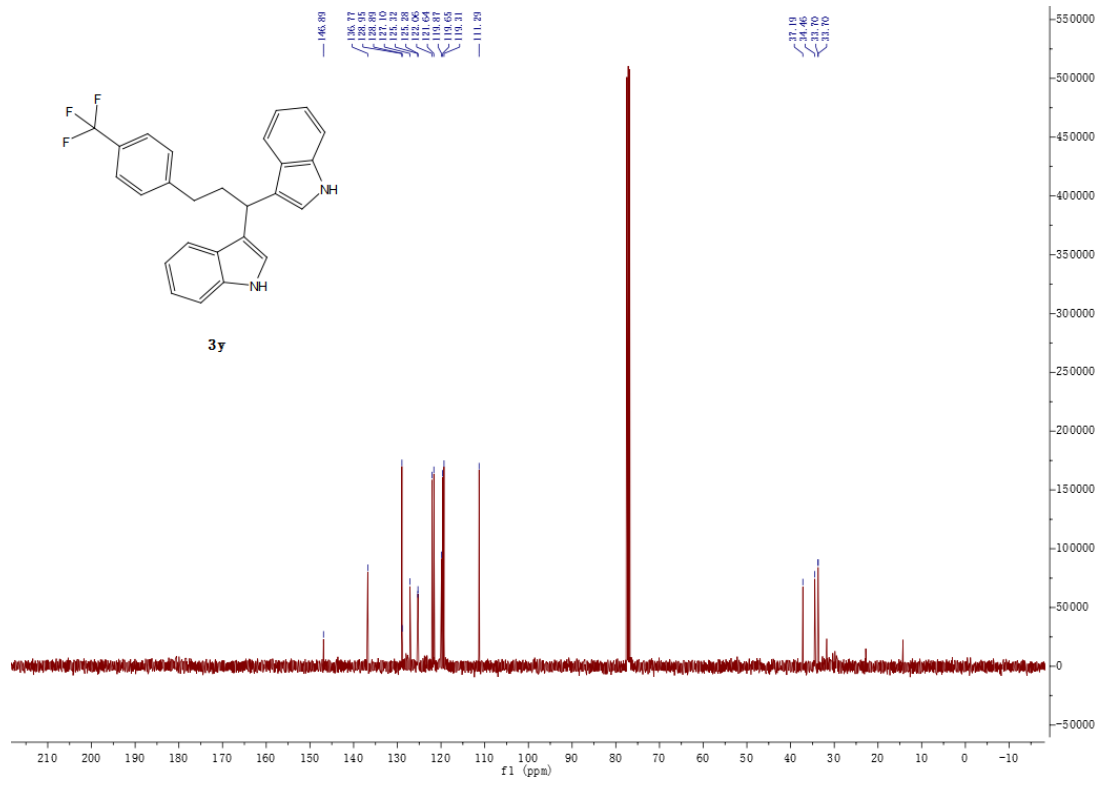
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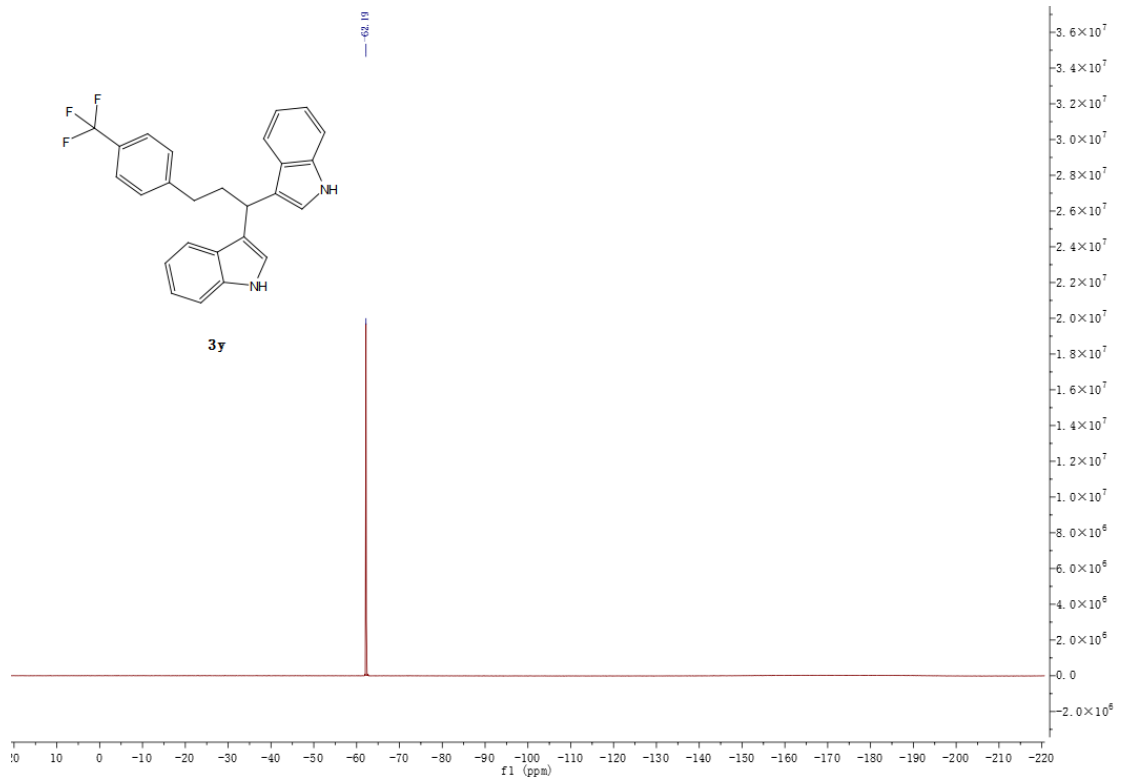
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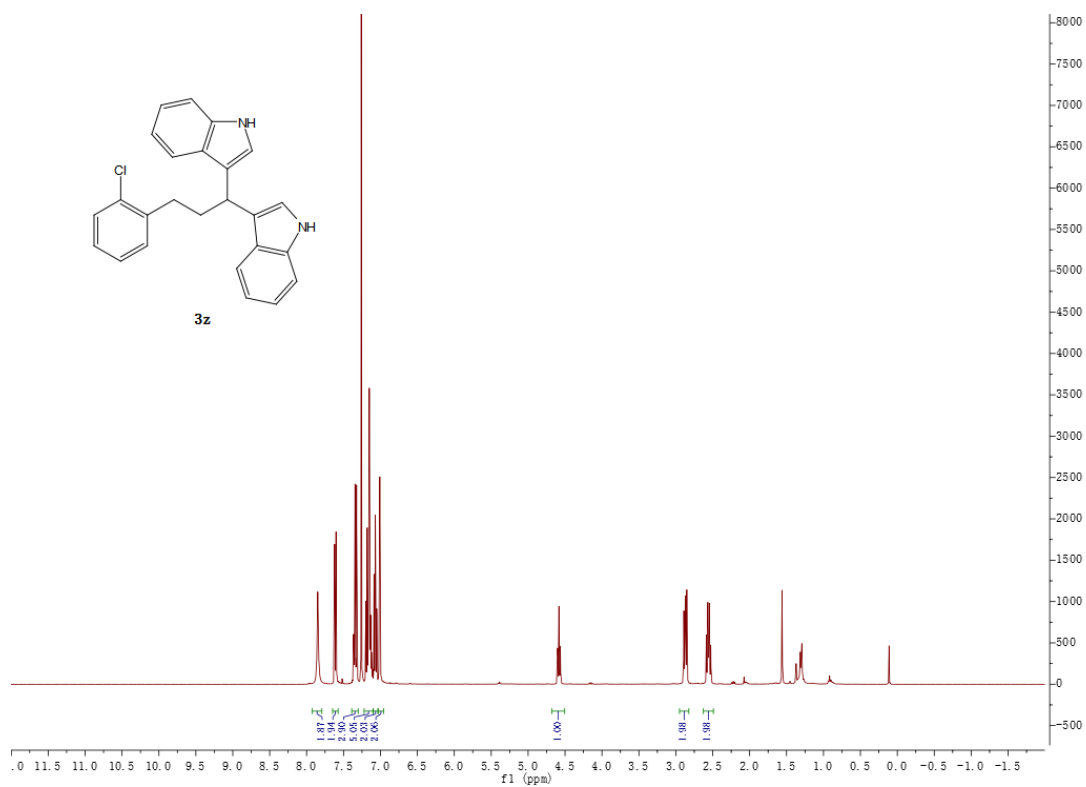
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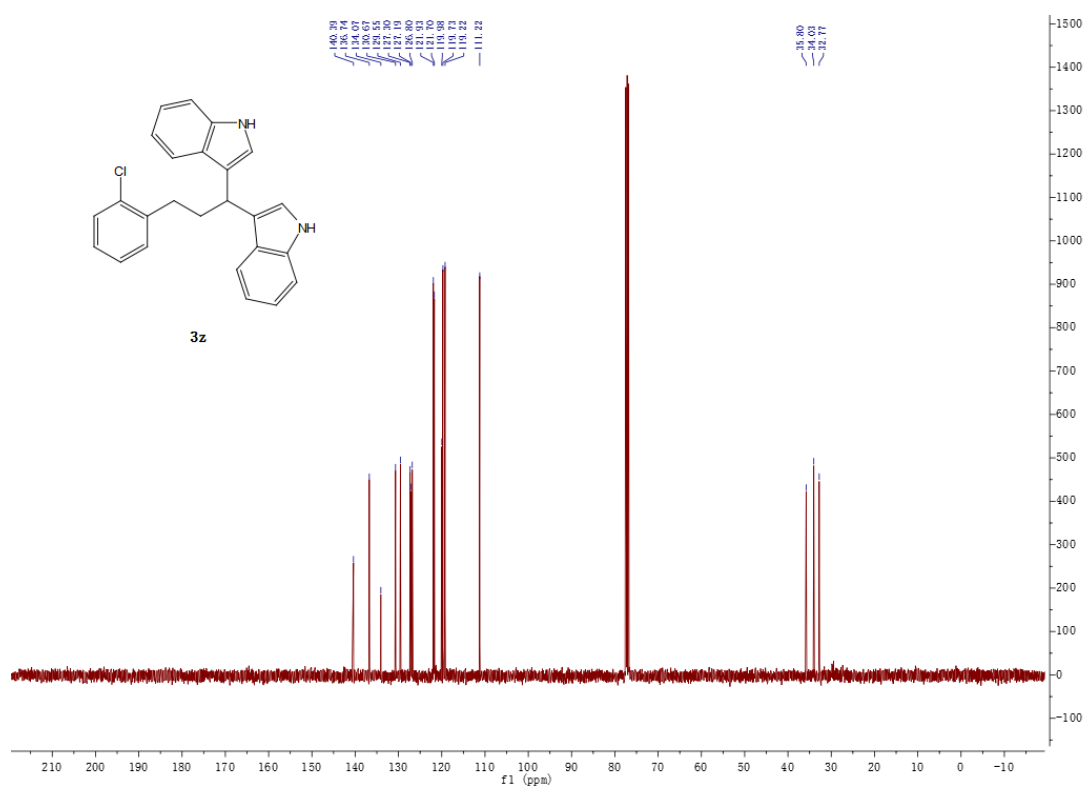
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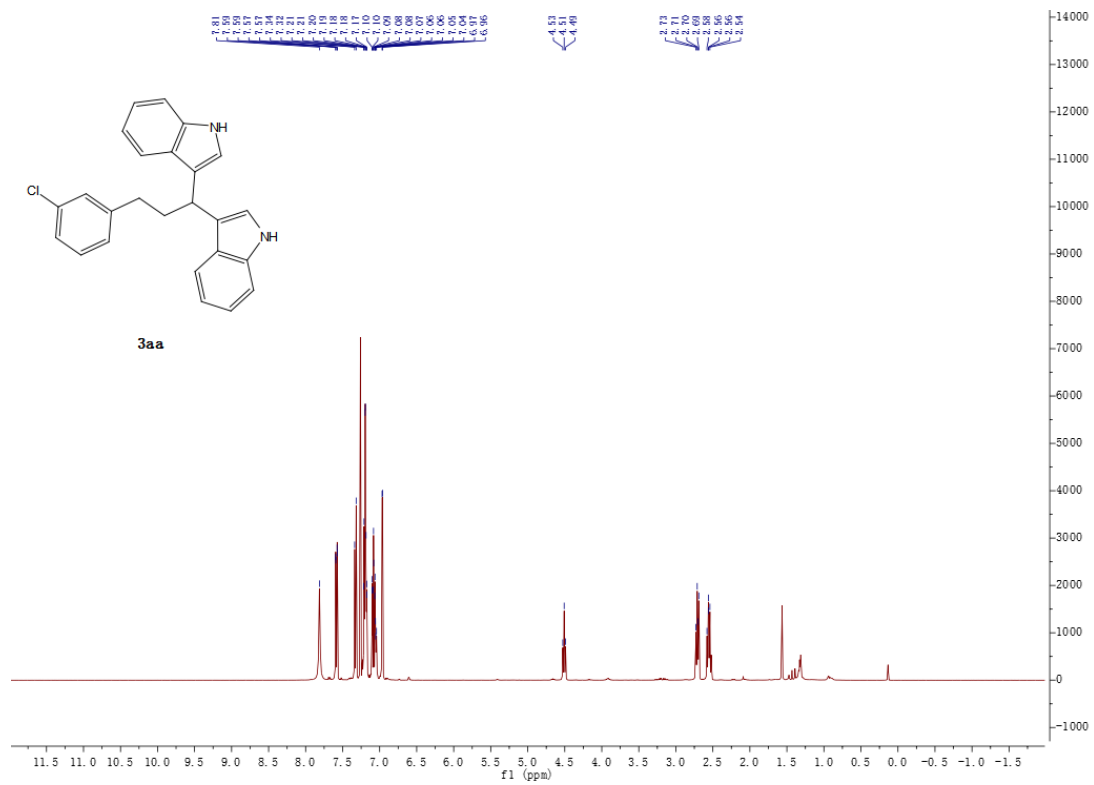
^1H NMR of **3z**



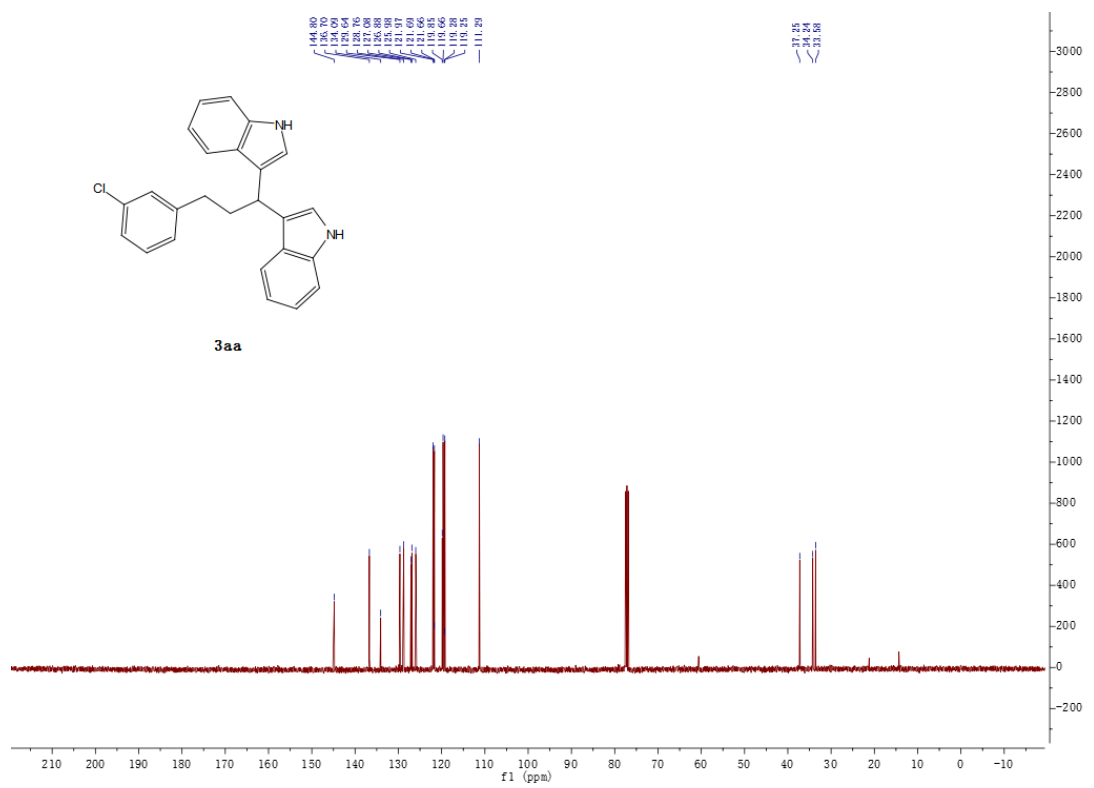
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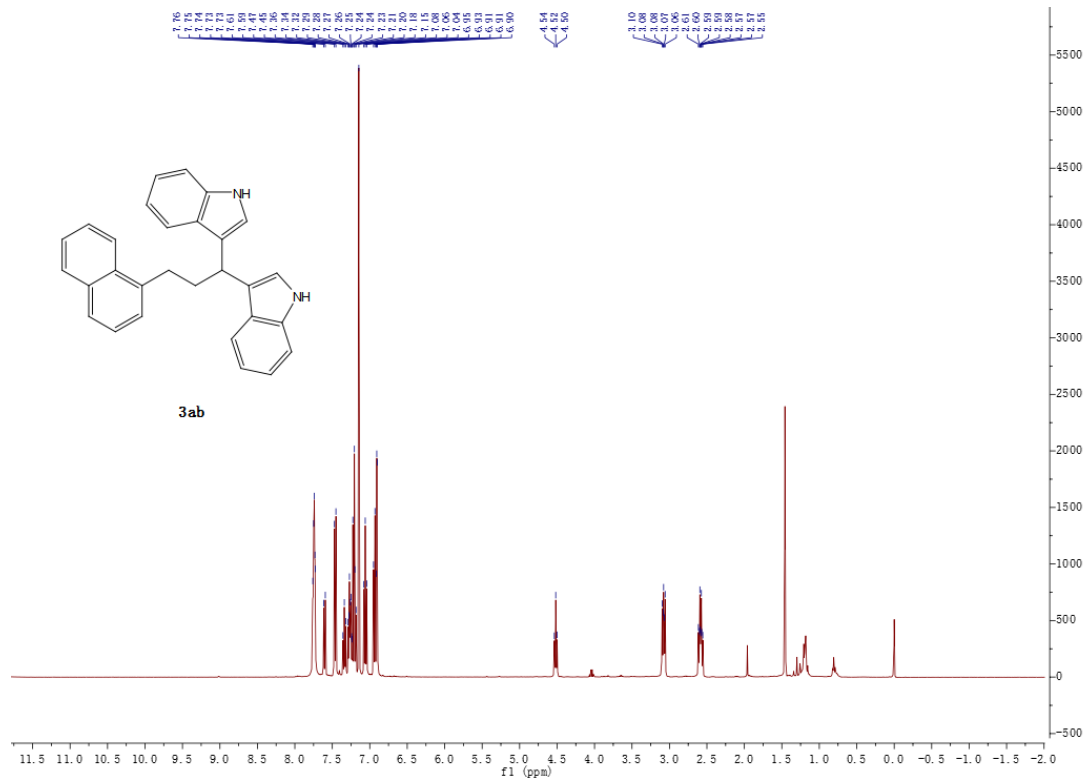
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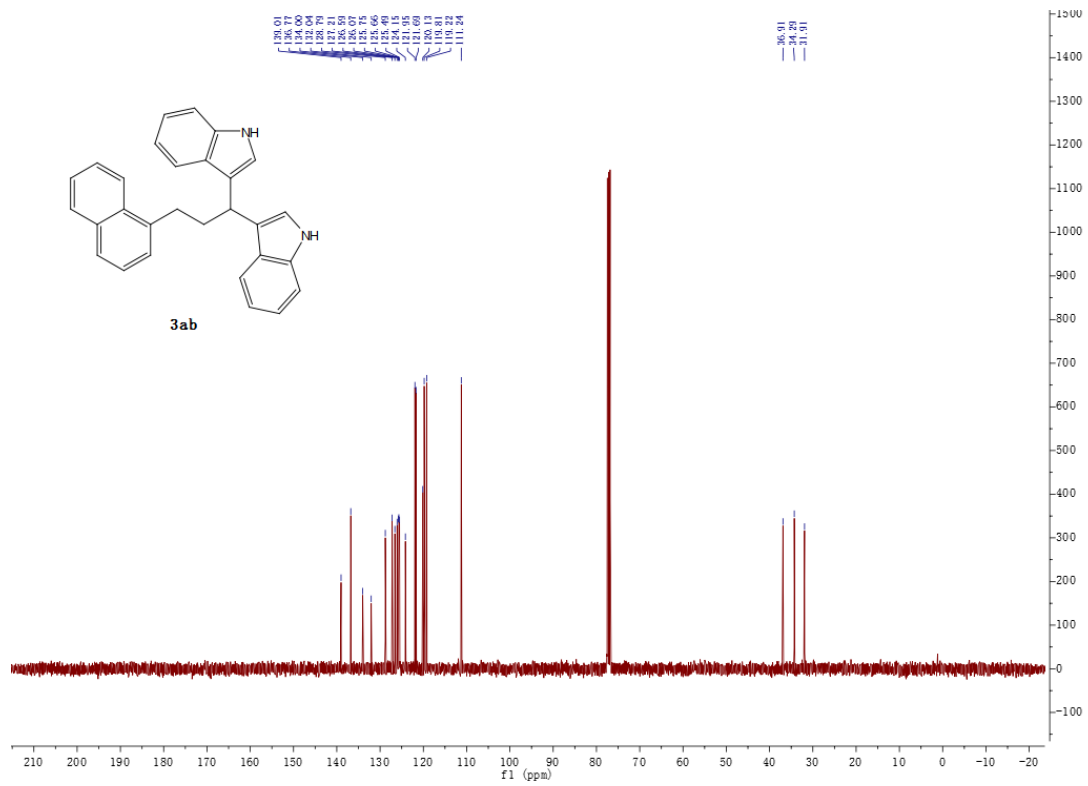
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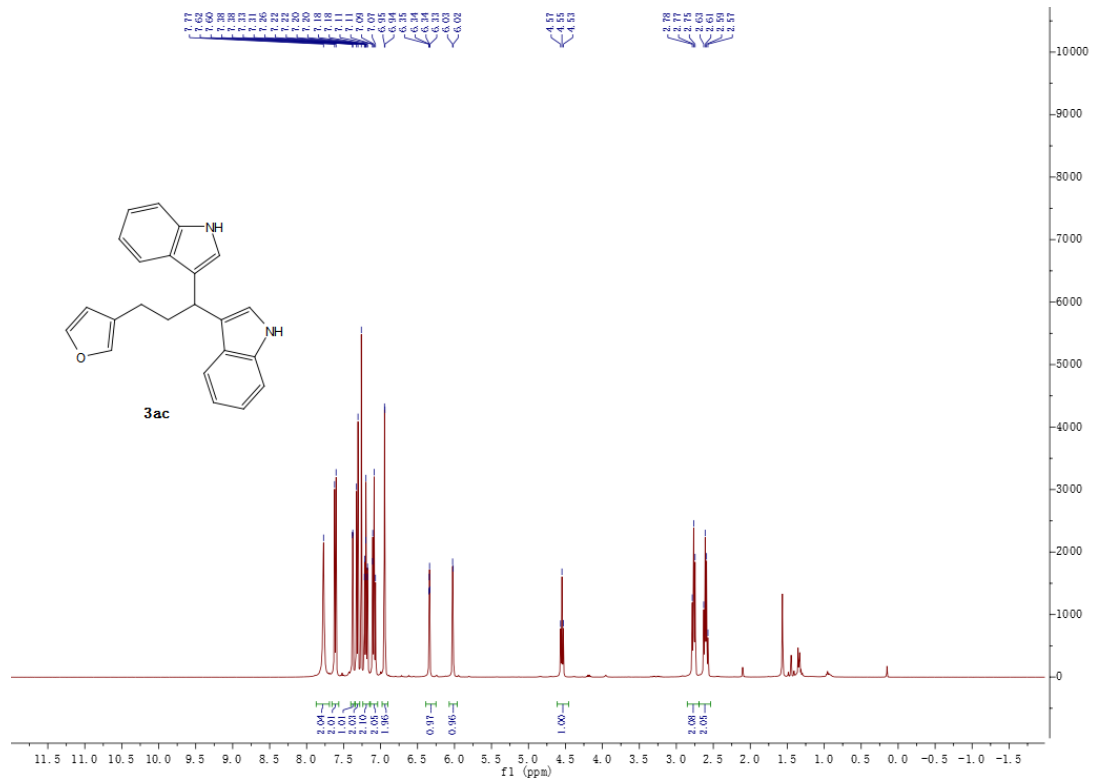
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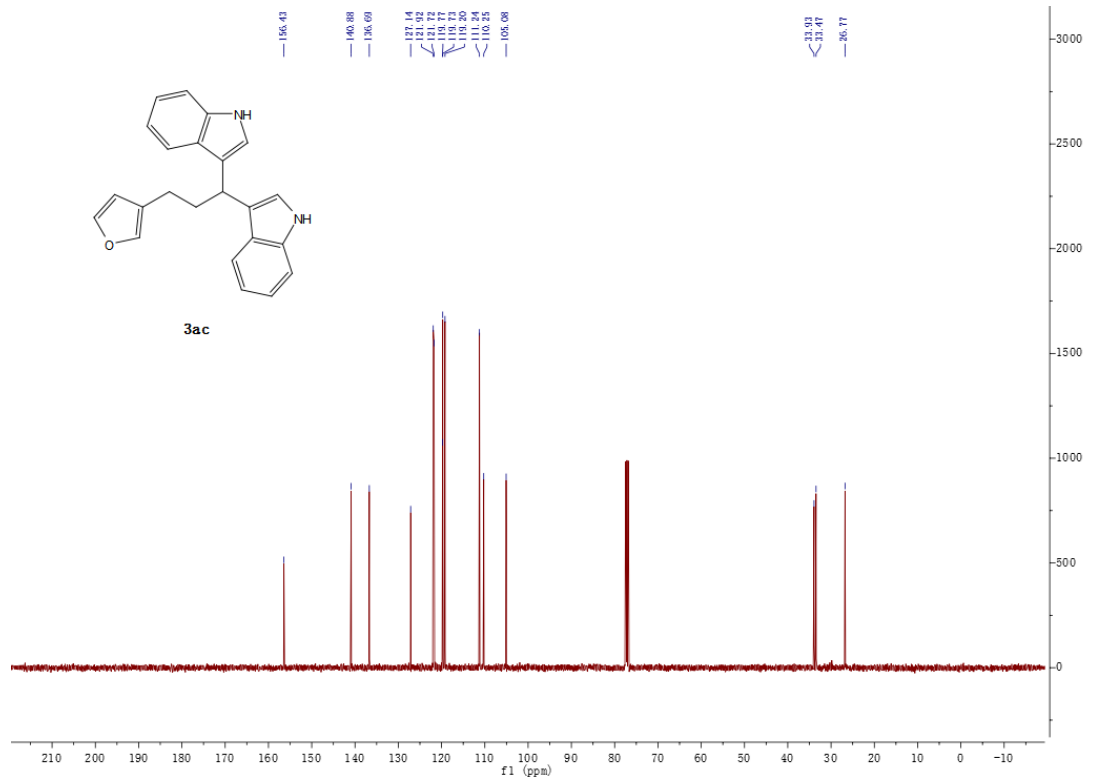
¹³C NMR of 3ab

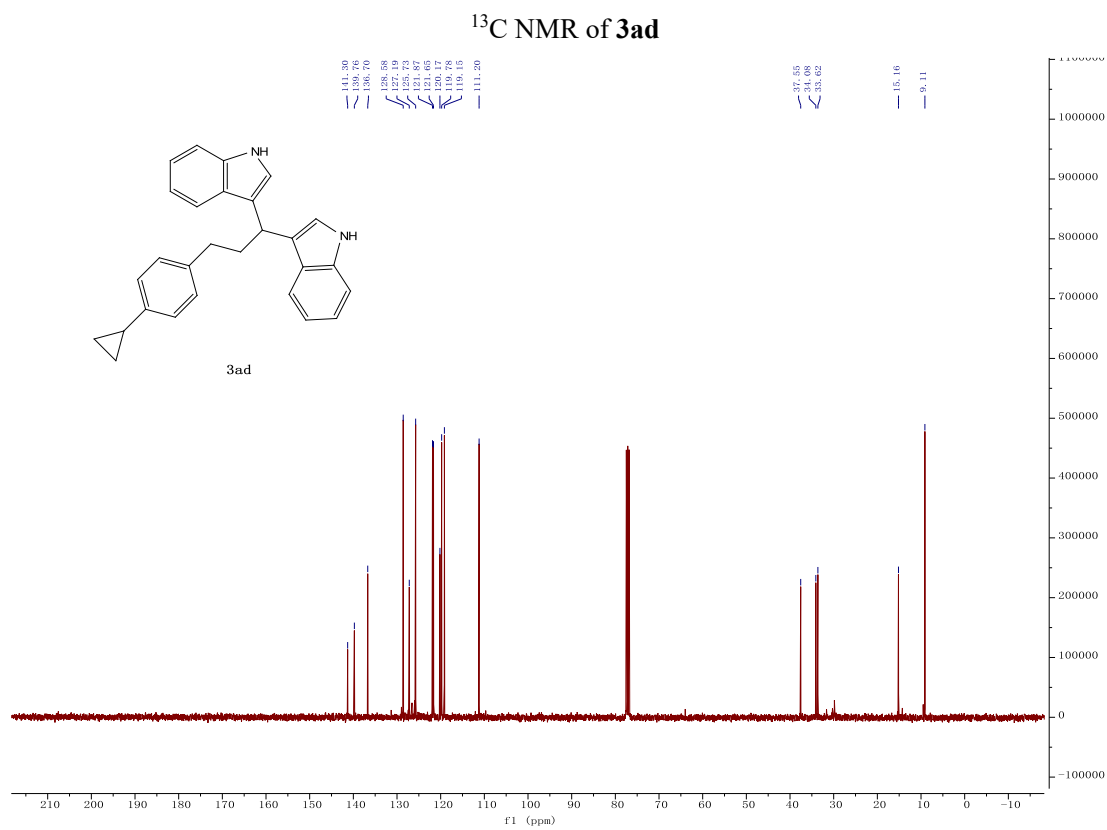
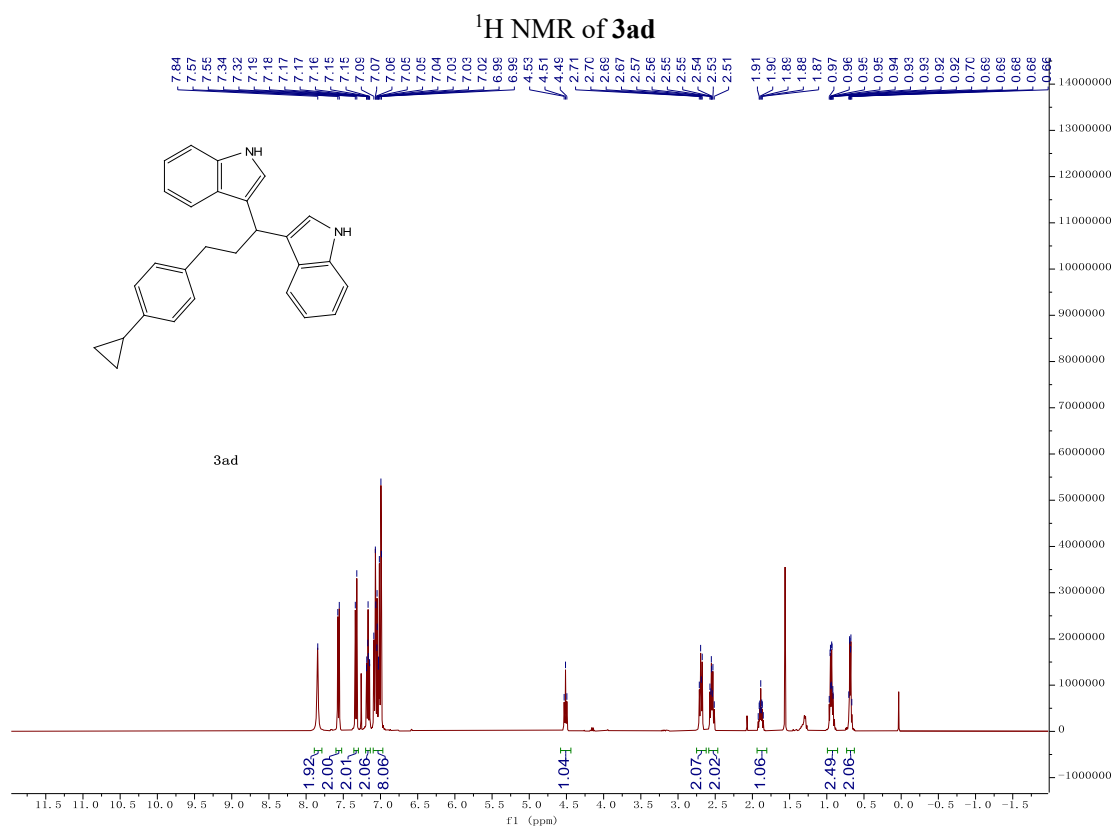


¹H NMR of 3ac

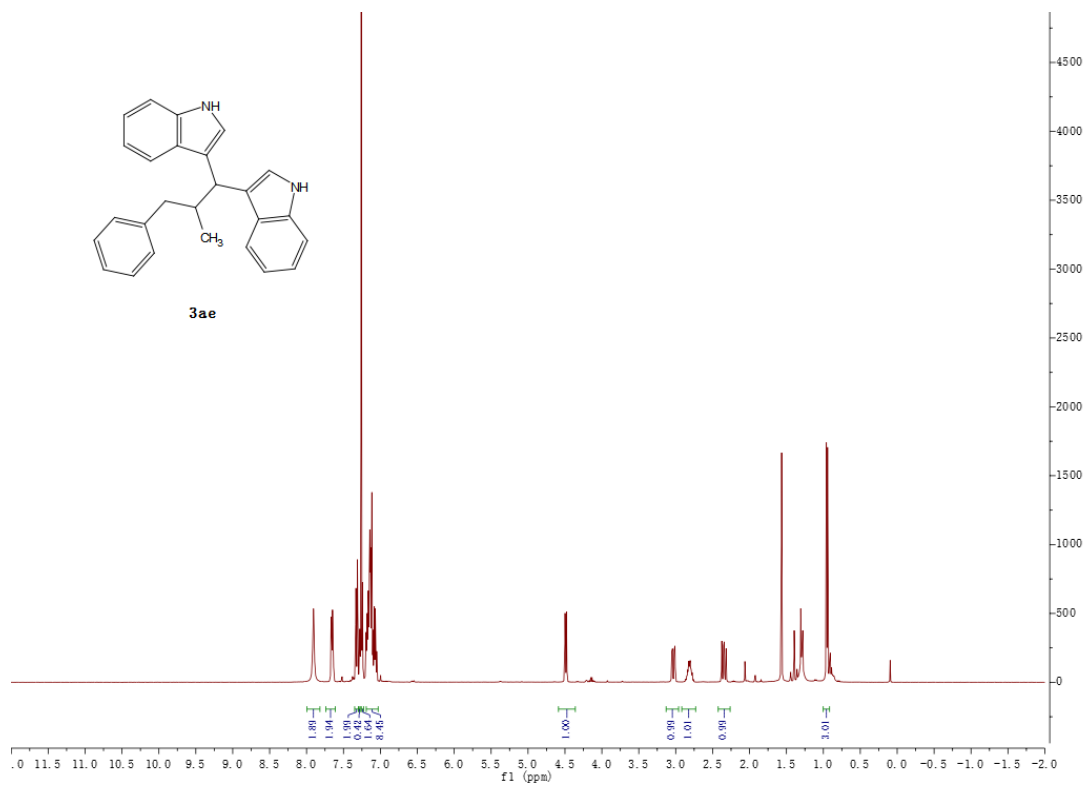


¹³C NMR of 3ac

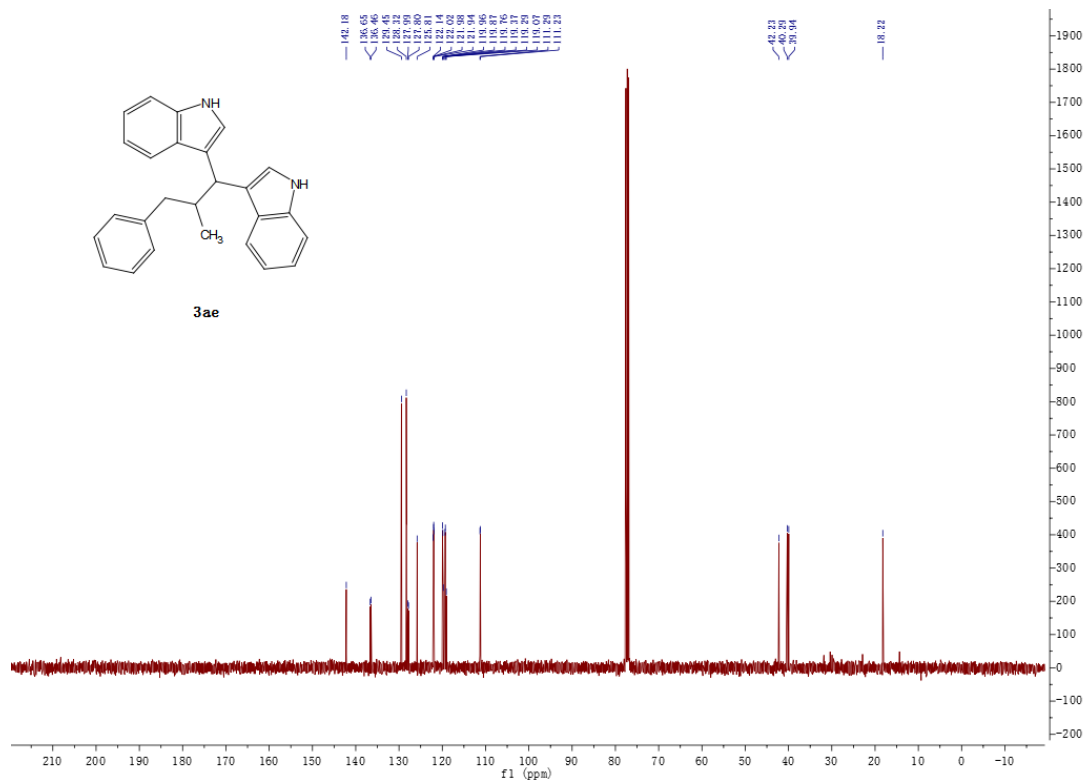




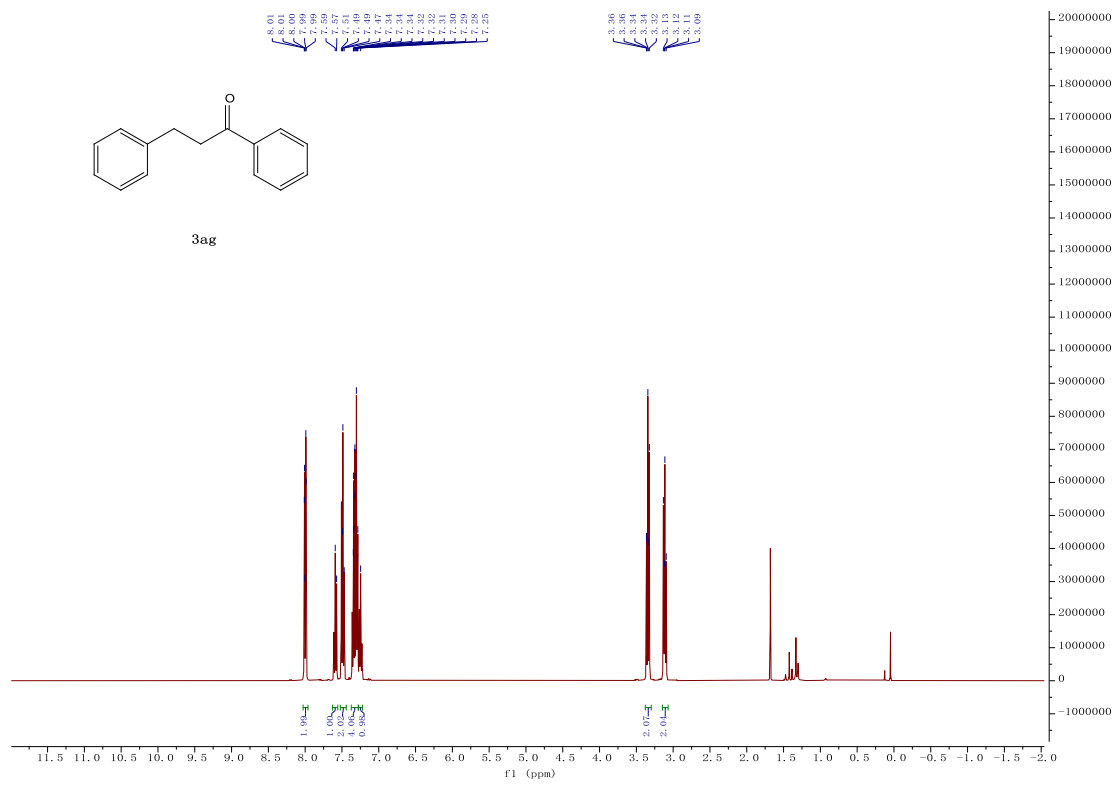
¹H NMR of 3ae



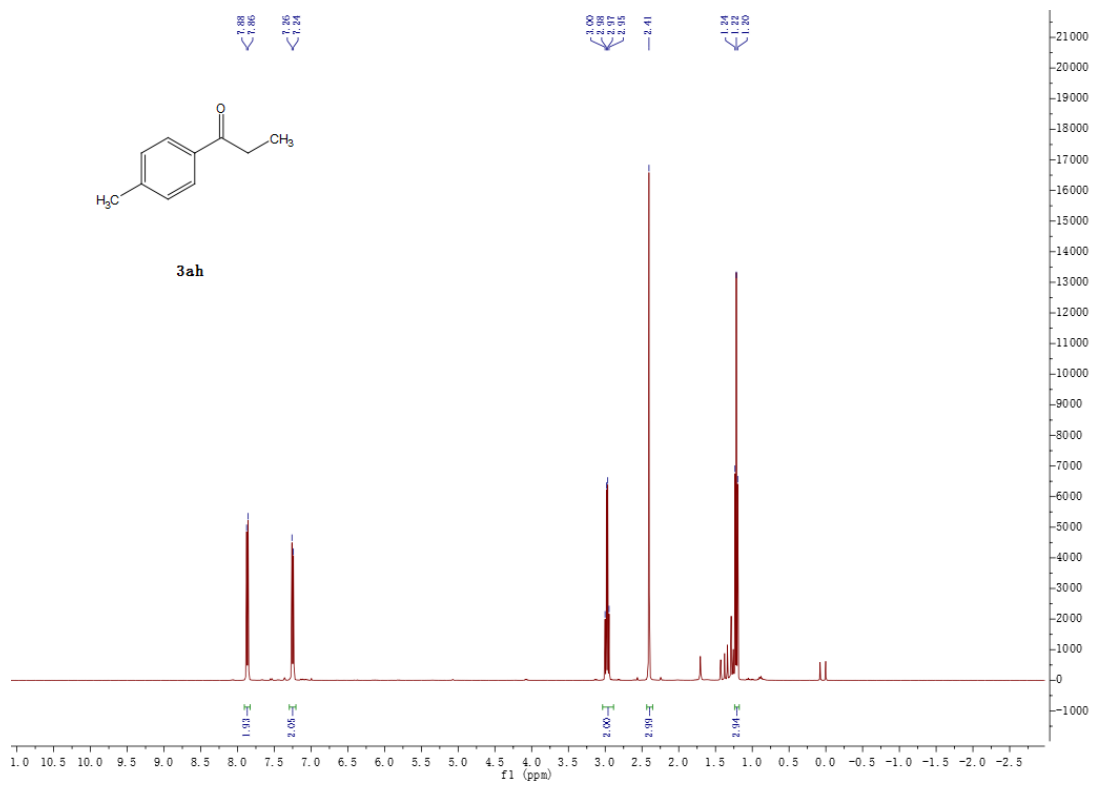
¹³C NMR of 3ae



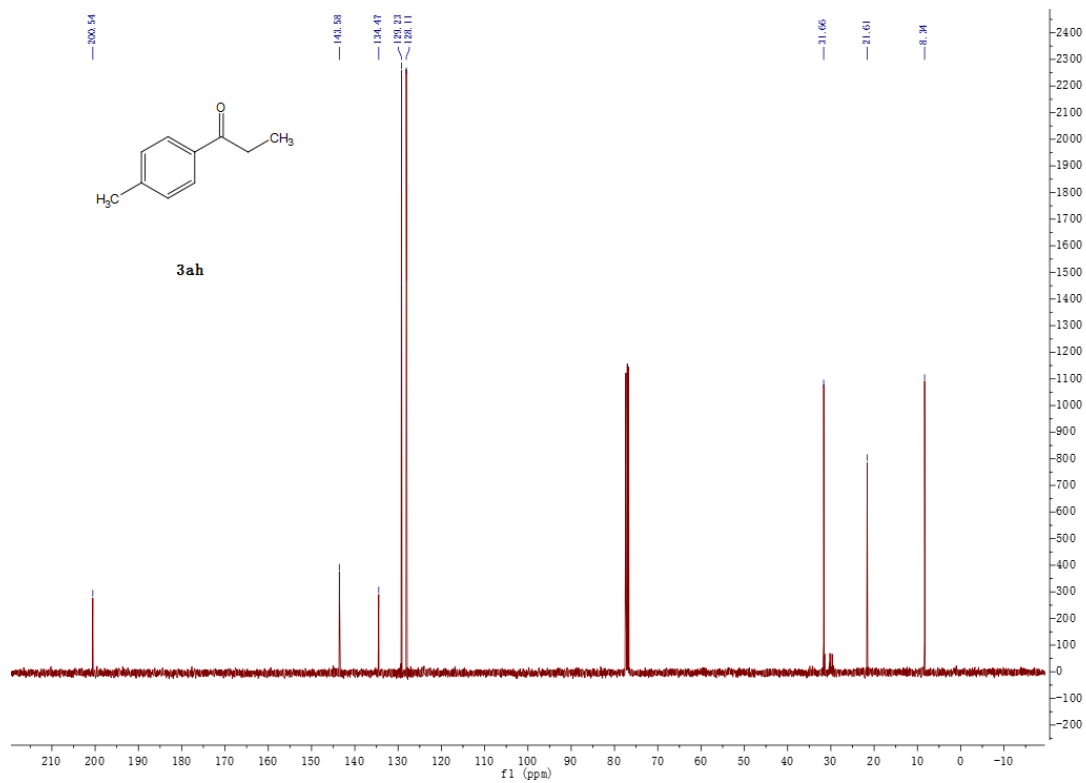
¹H NMR of 3ag



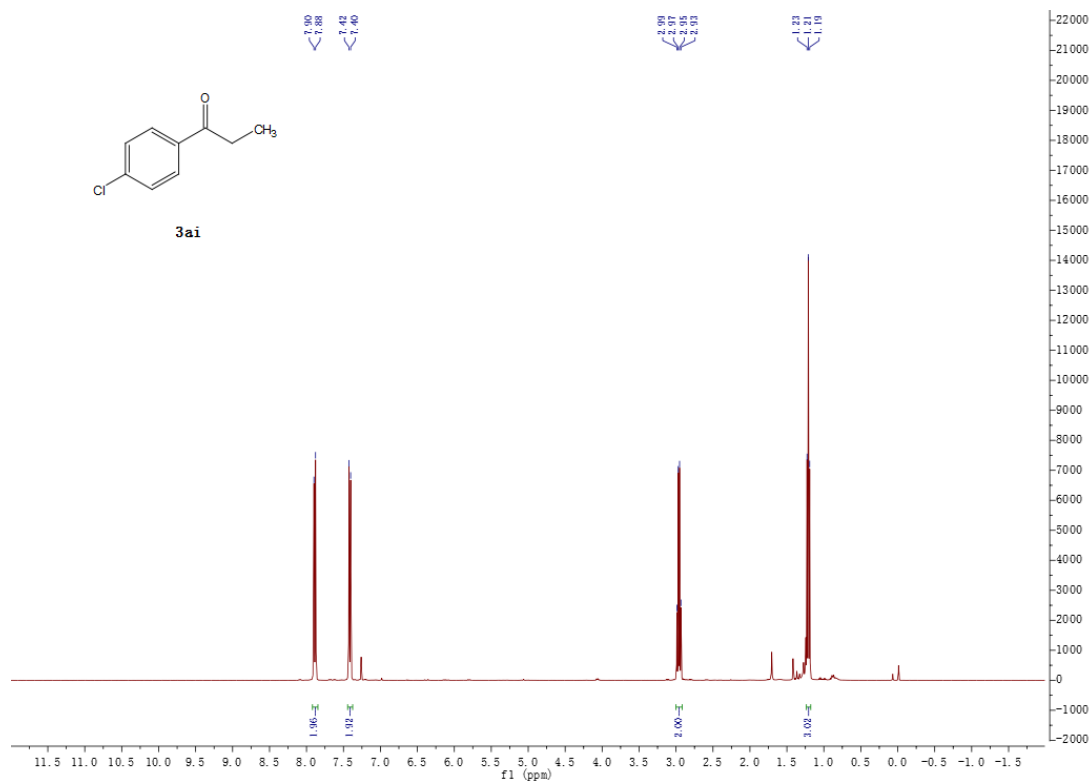
¹H NMR of 3ah



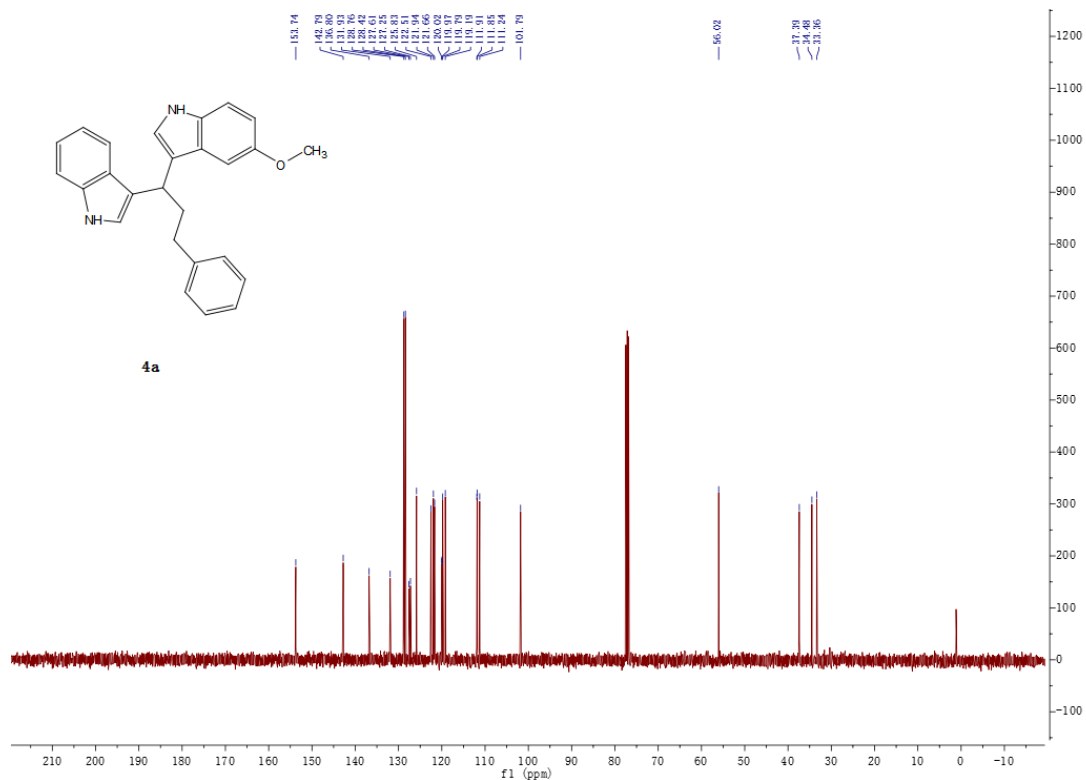
^{13}C NMR of **3ah**



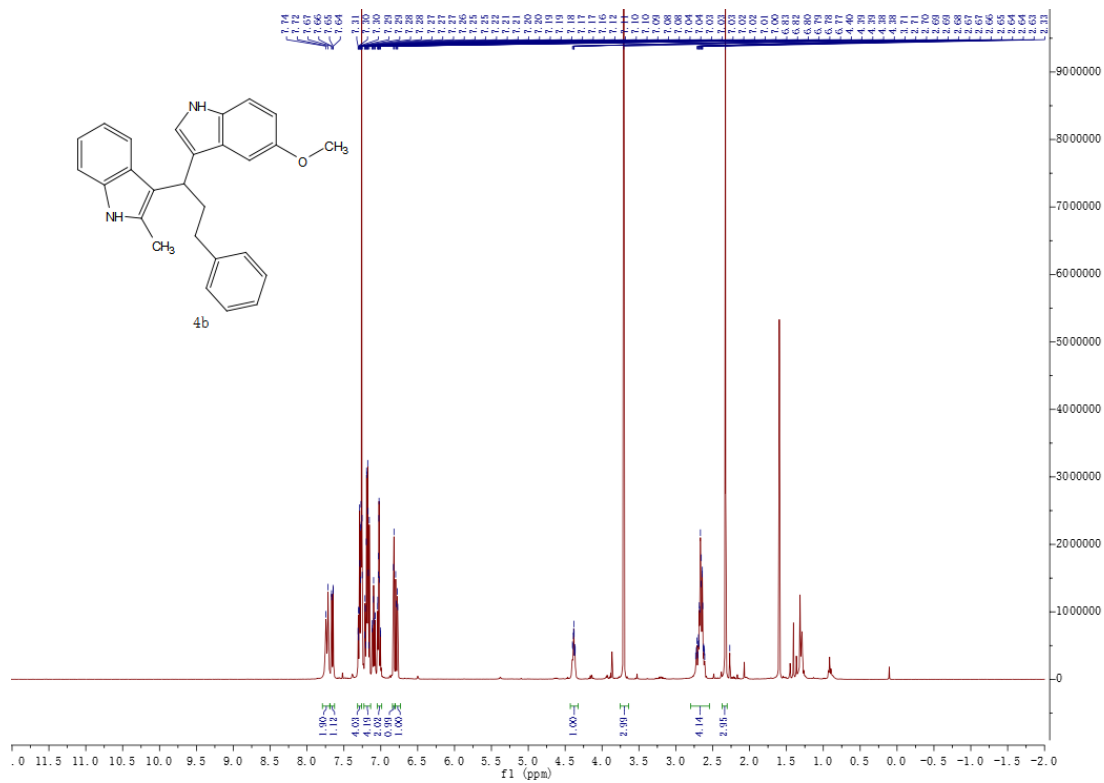
^1H NMR of **3ai**



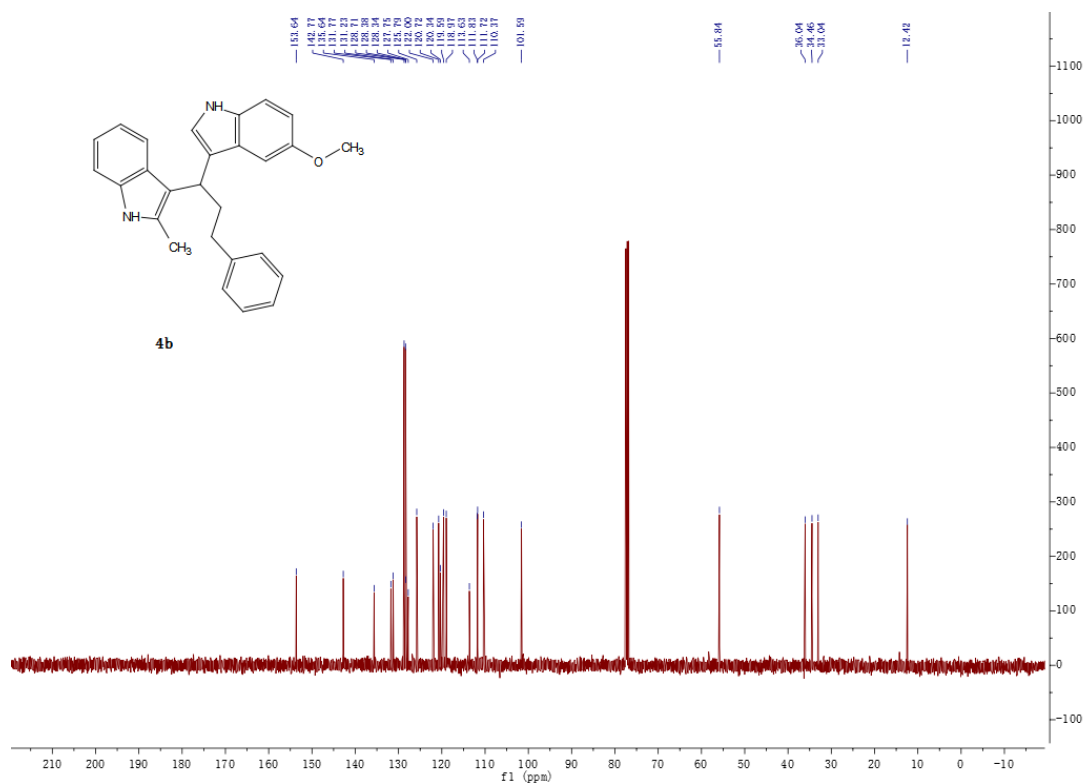
¹³C NMR of 4a



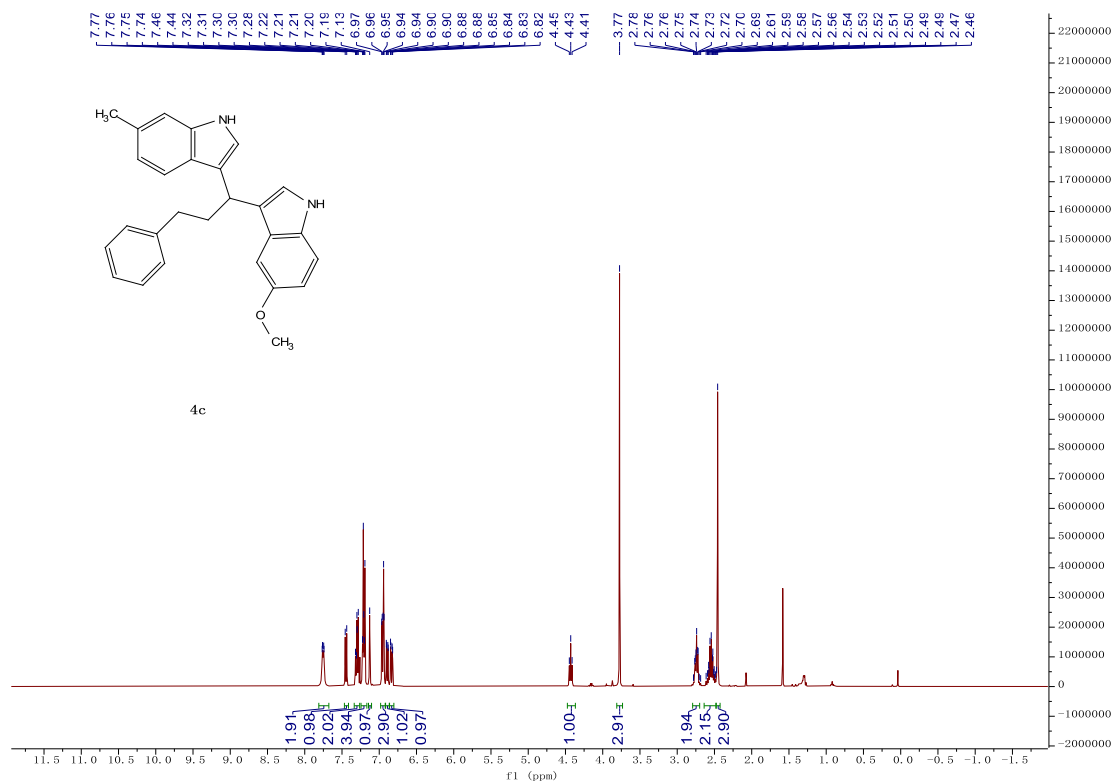
¹H NMR of 4b



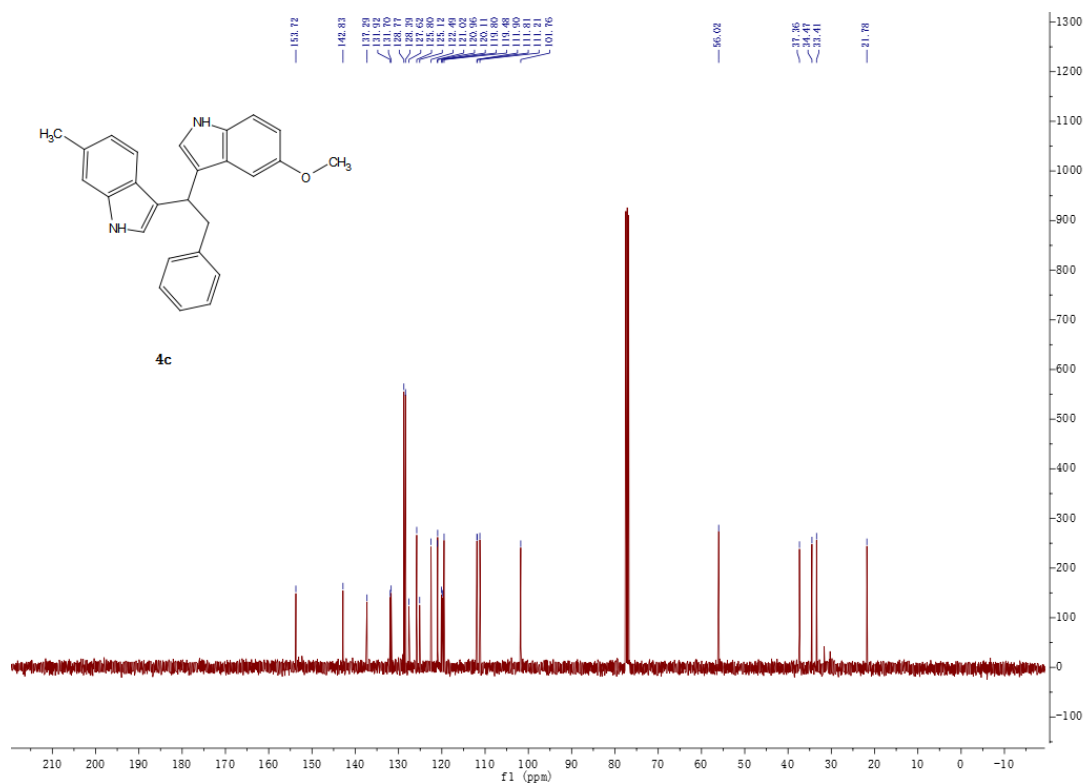
¹³C NMR of 4b



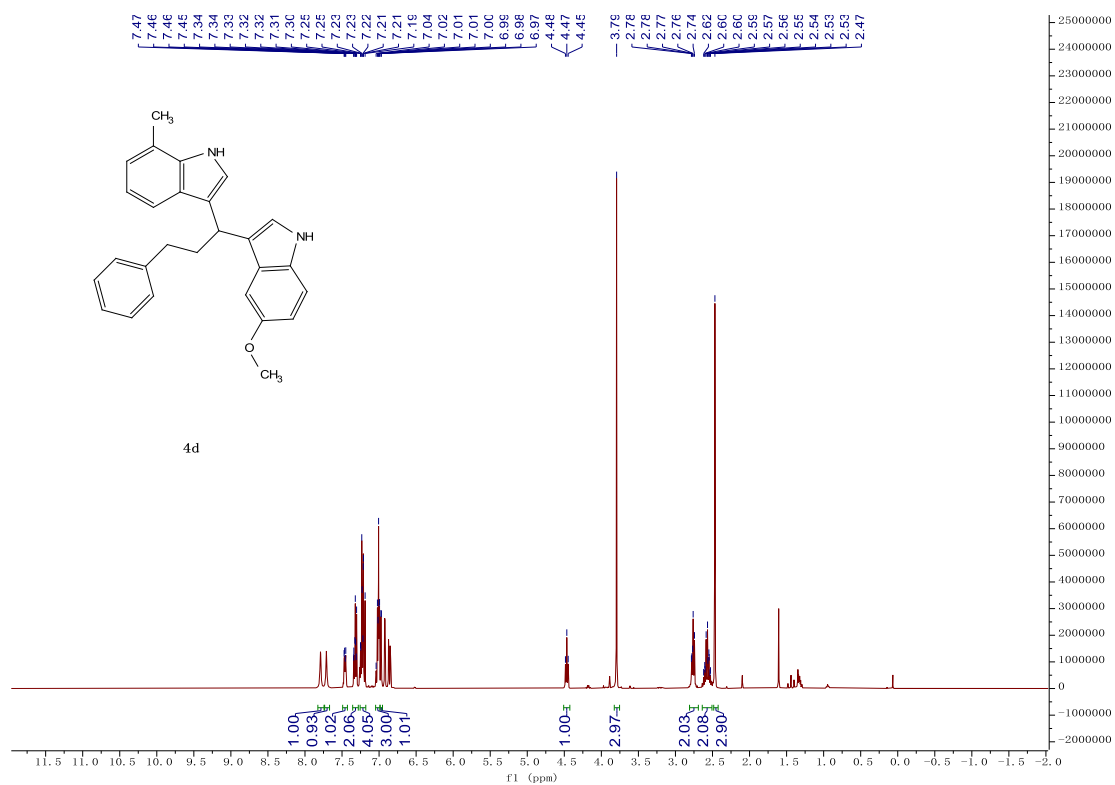
¹H NMR of 4c



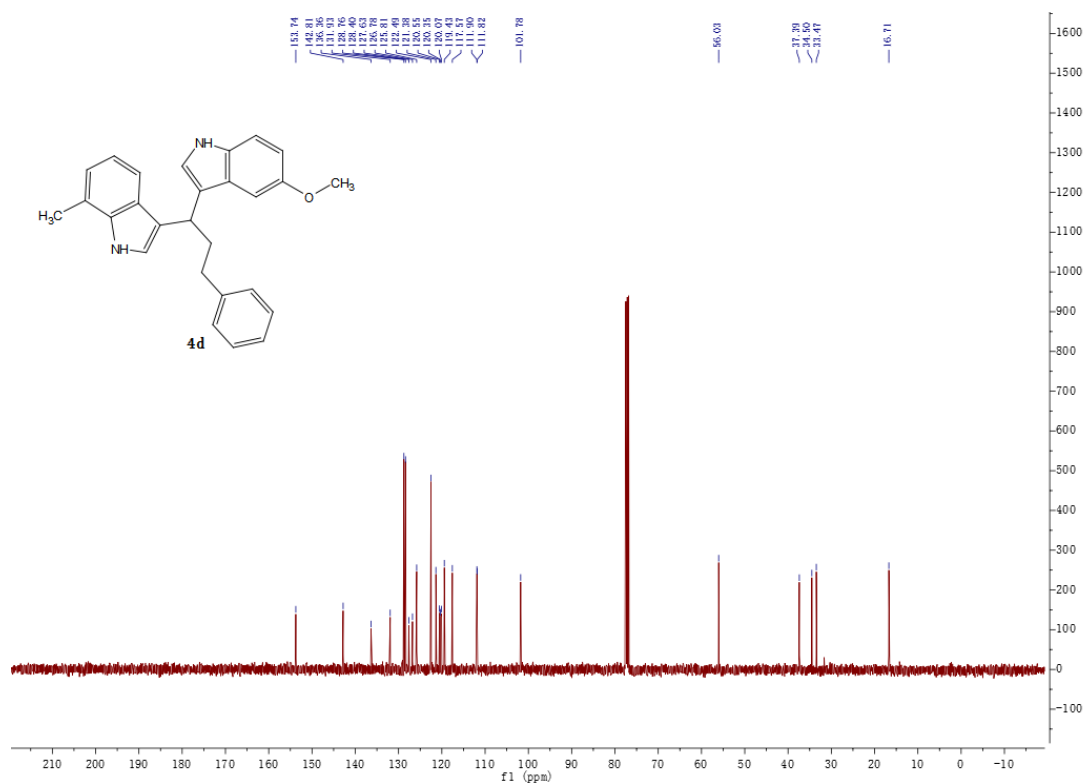
^{13}C NMR of 4c



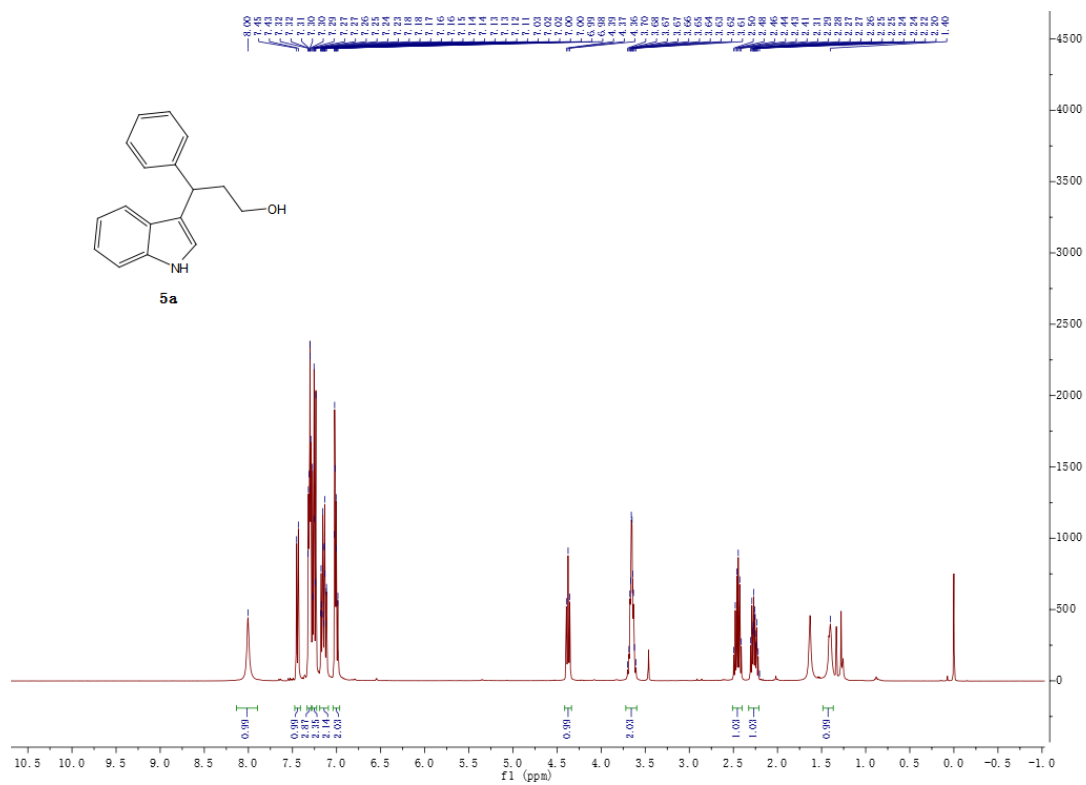
^1H NMR of 4d



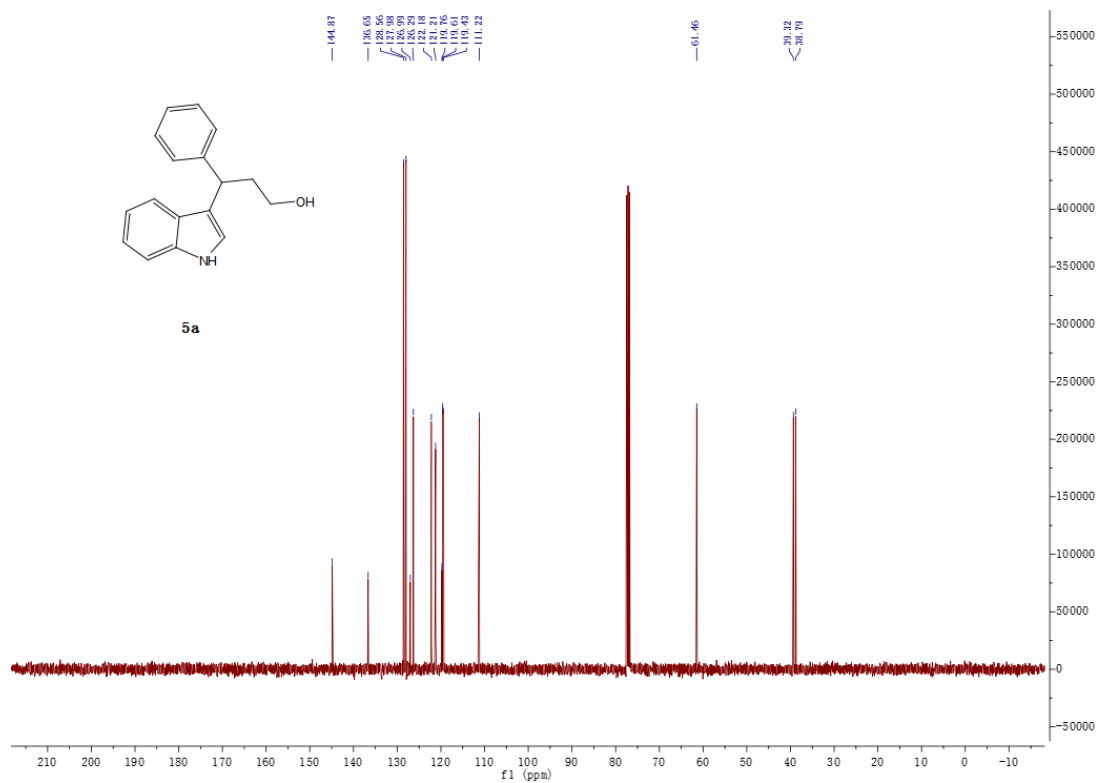
¹³C NMR of 4d



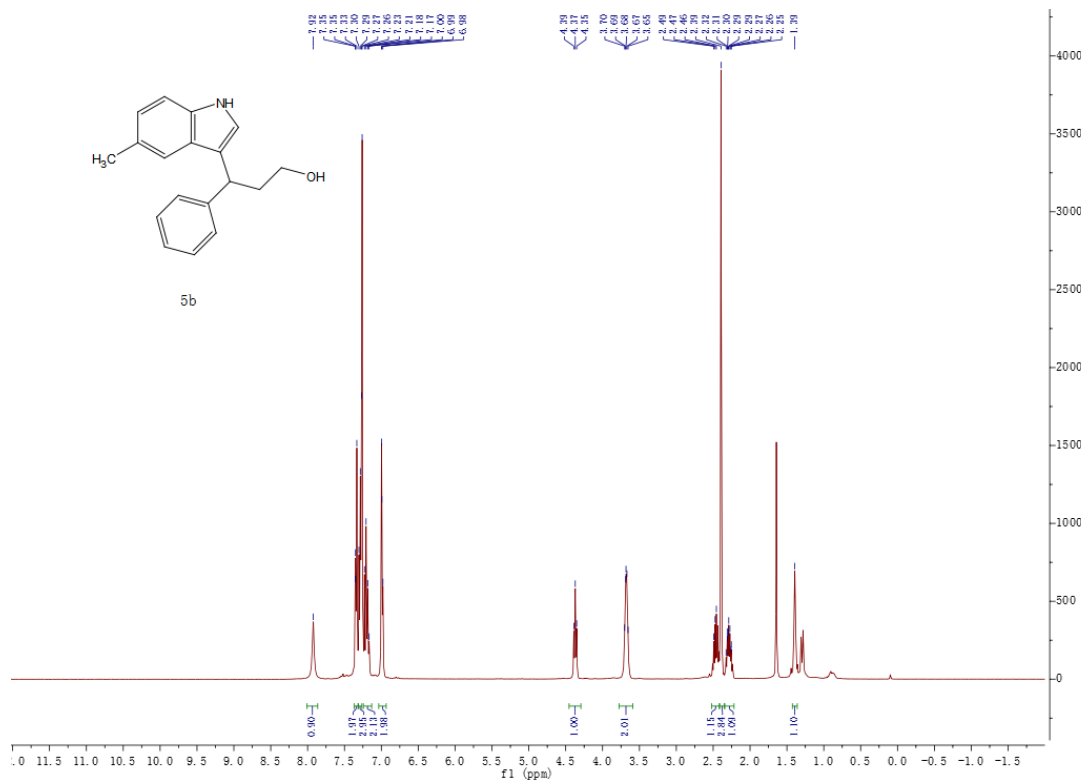
¹H NMR of 5a



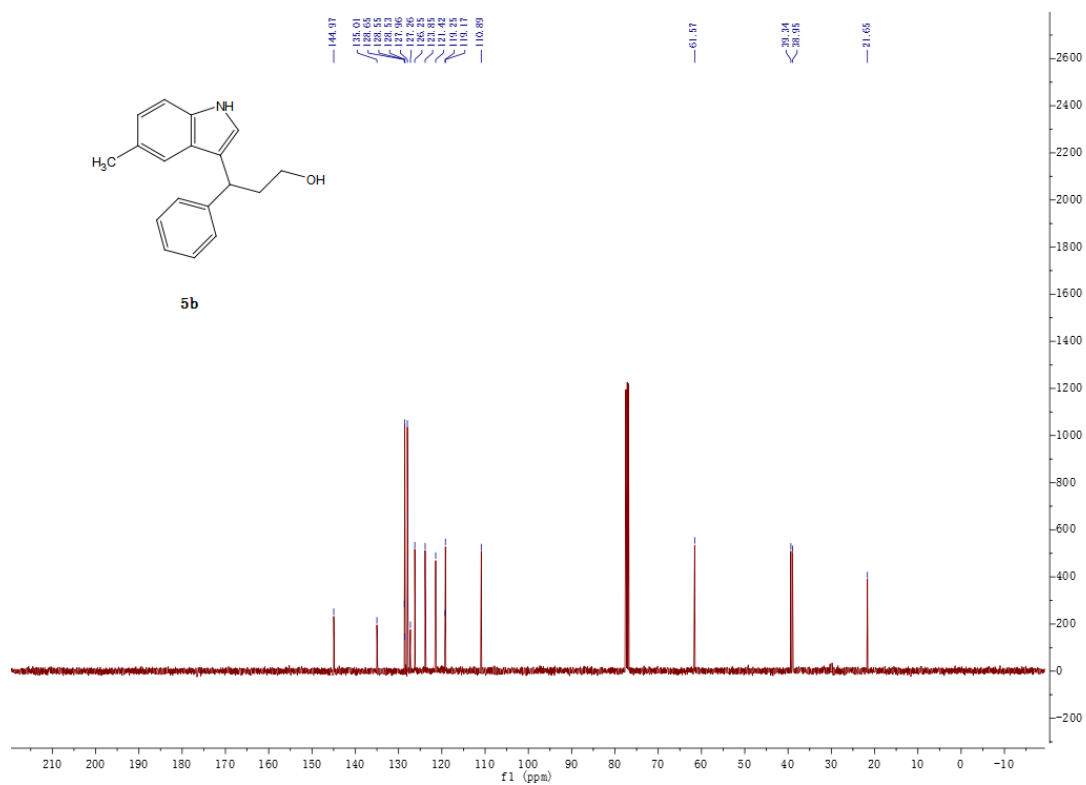
^{13}C NMR of 5a



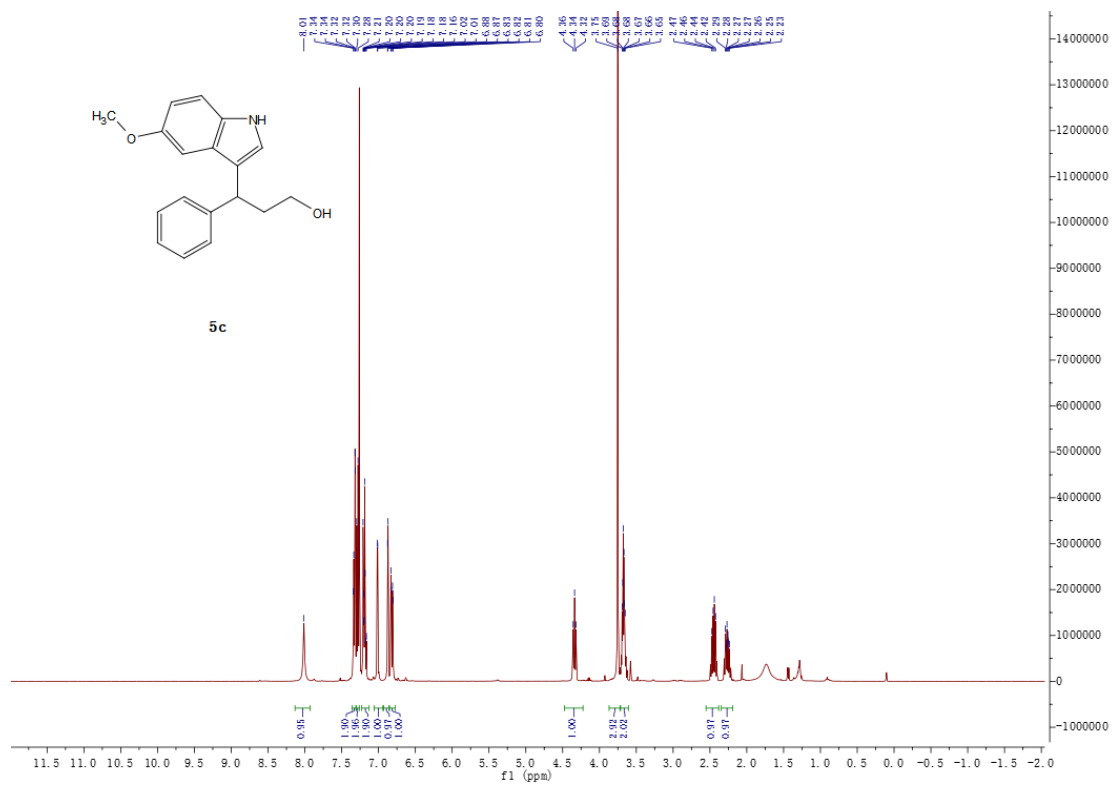
^1H NMR of 5b



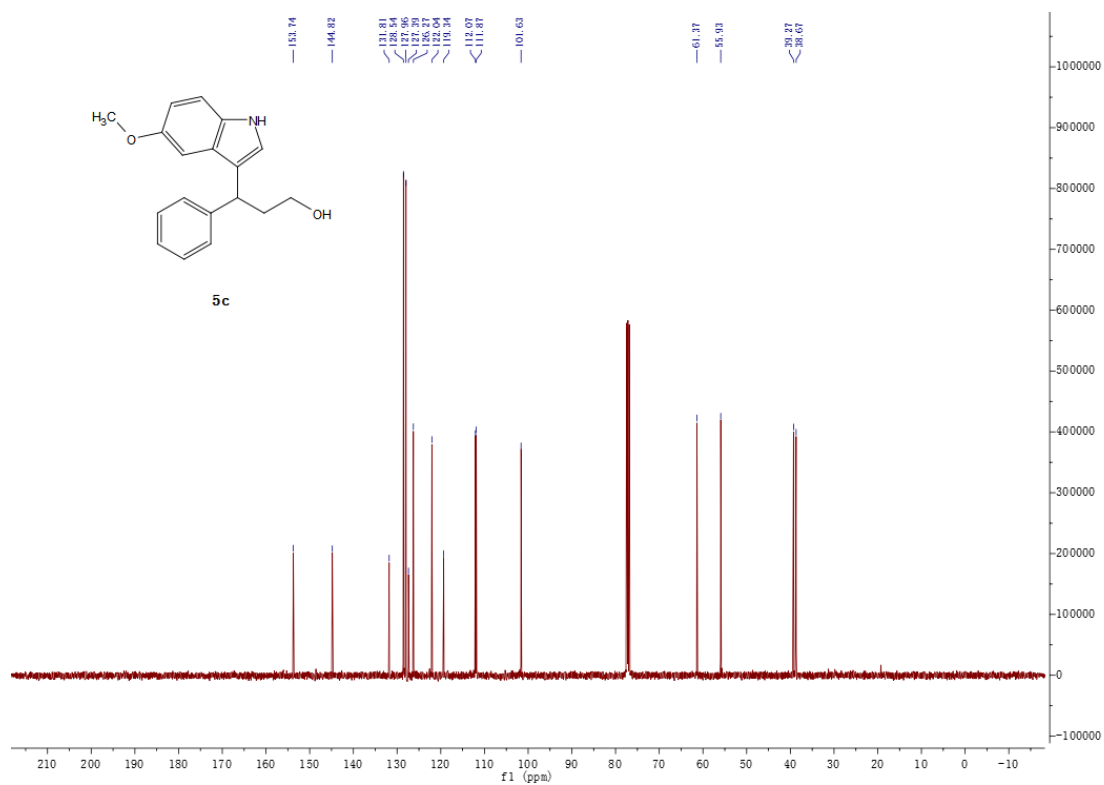
¹³C NMR of **5b**



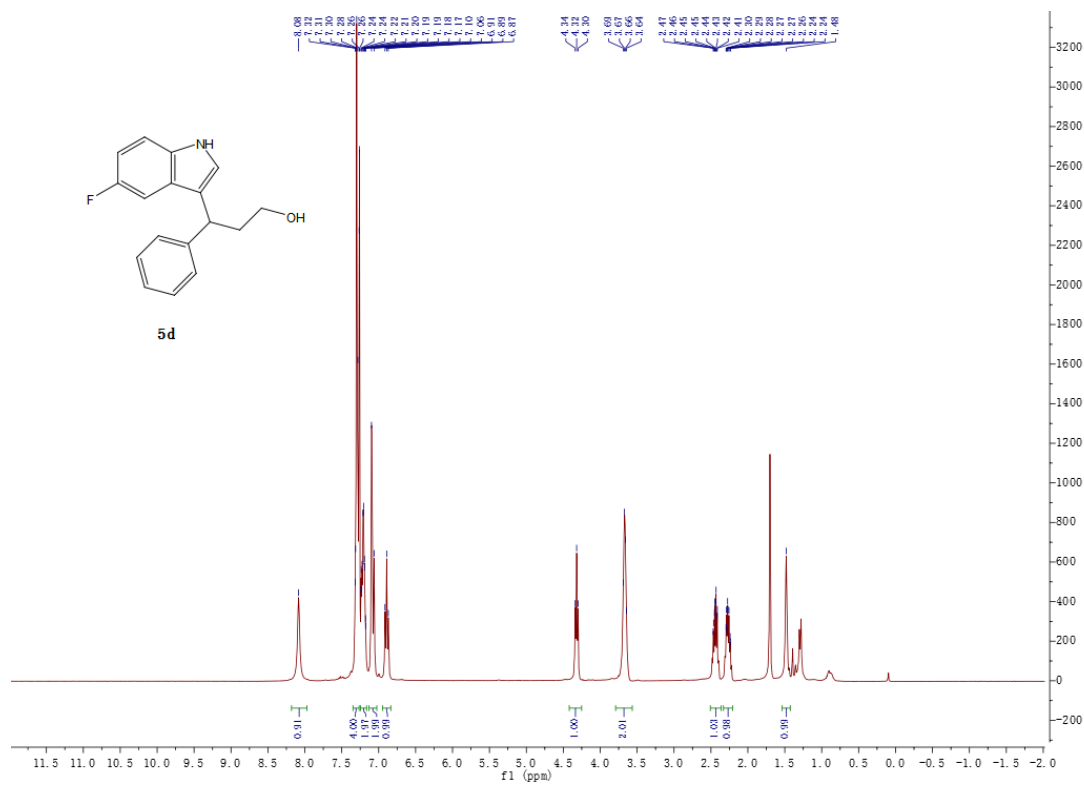
¹H NMR of **5c**



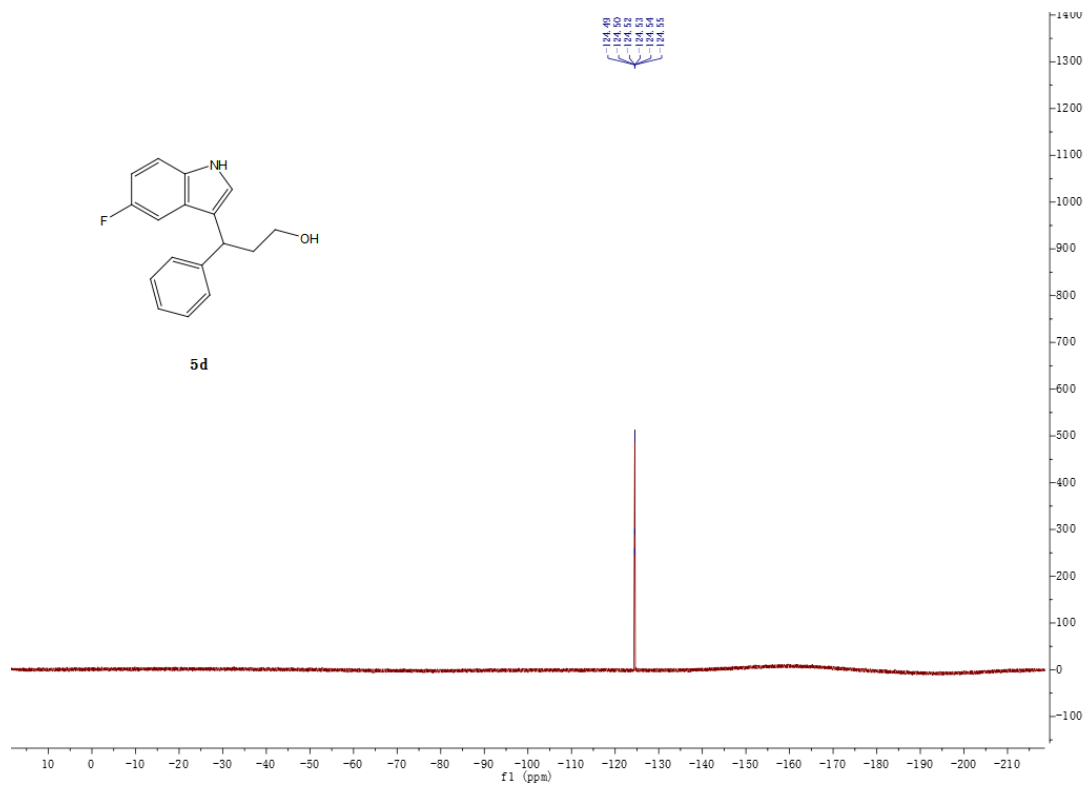
¹³C NMR of 5c



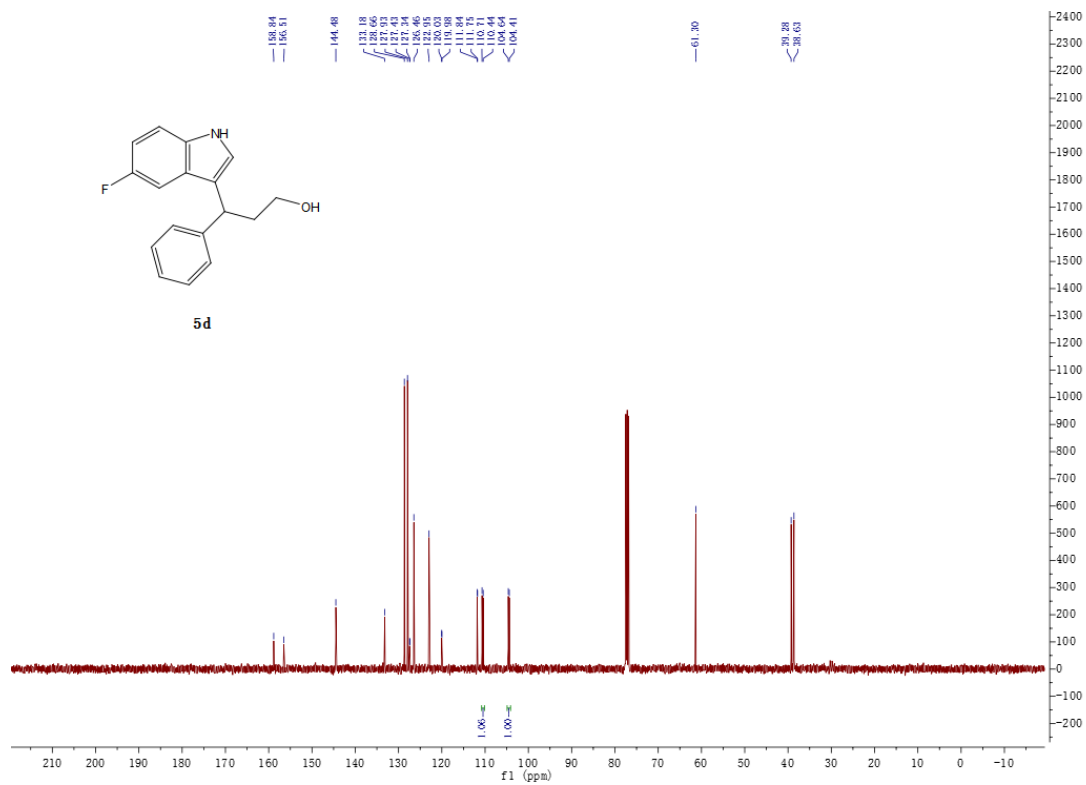
¹H NMR of 5d

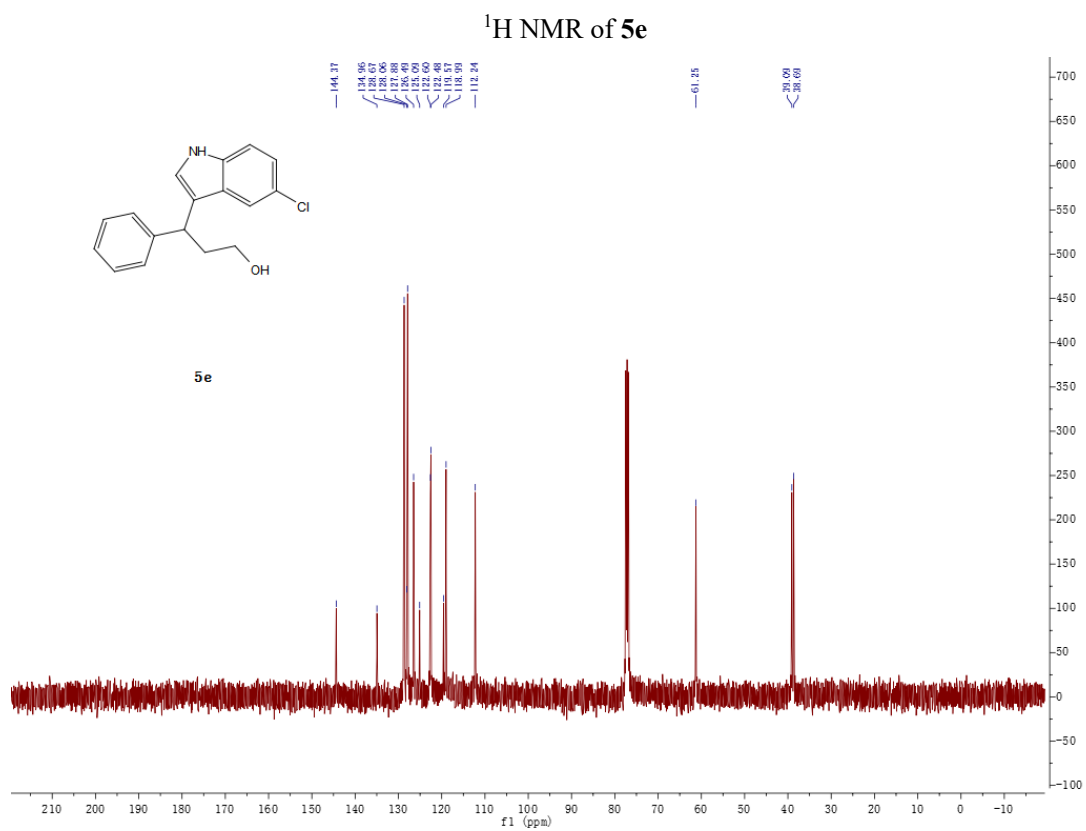
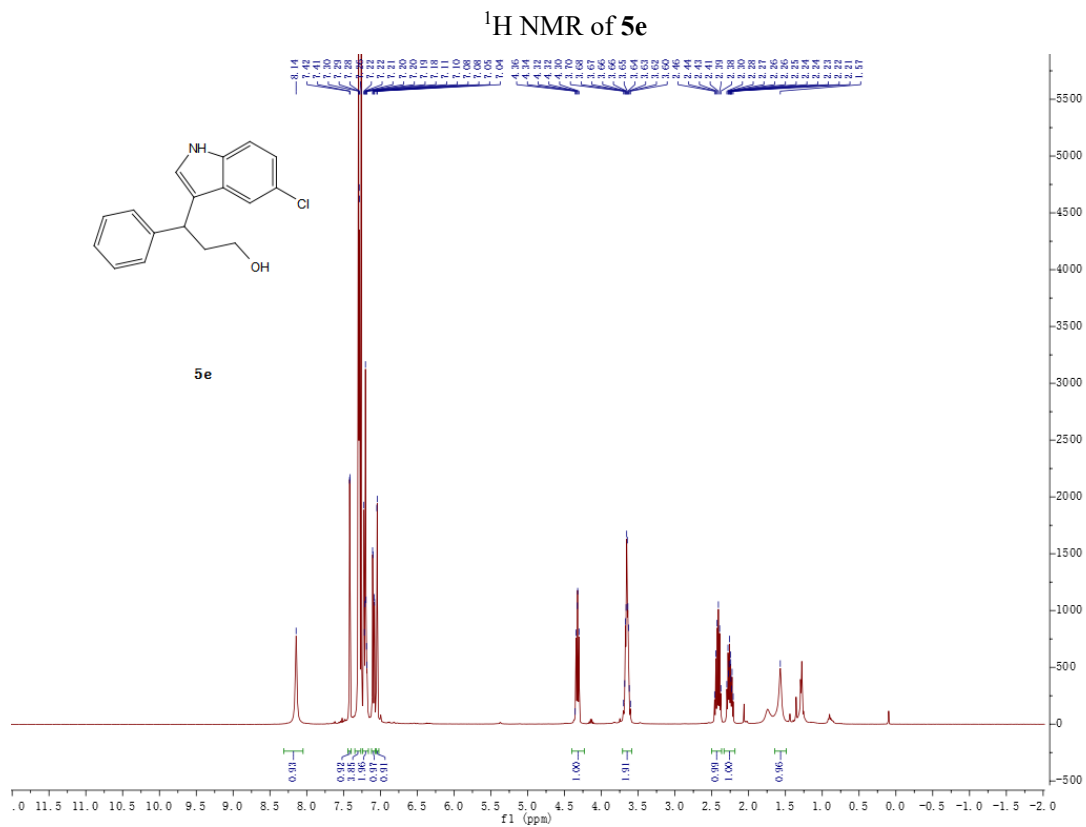


¹⁹F NMR of 5d

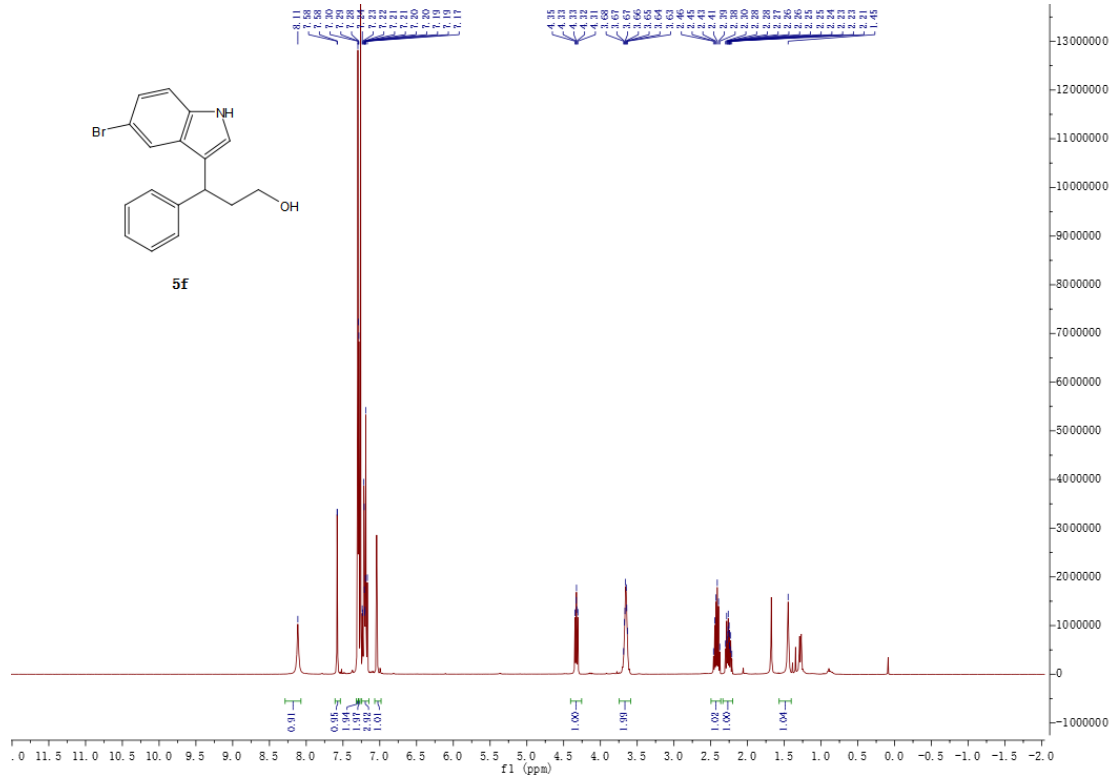


¹³C NMR of 5d

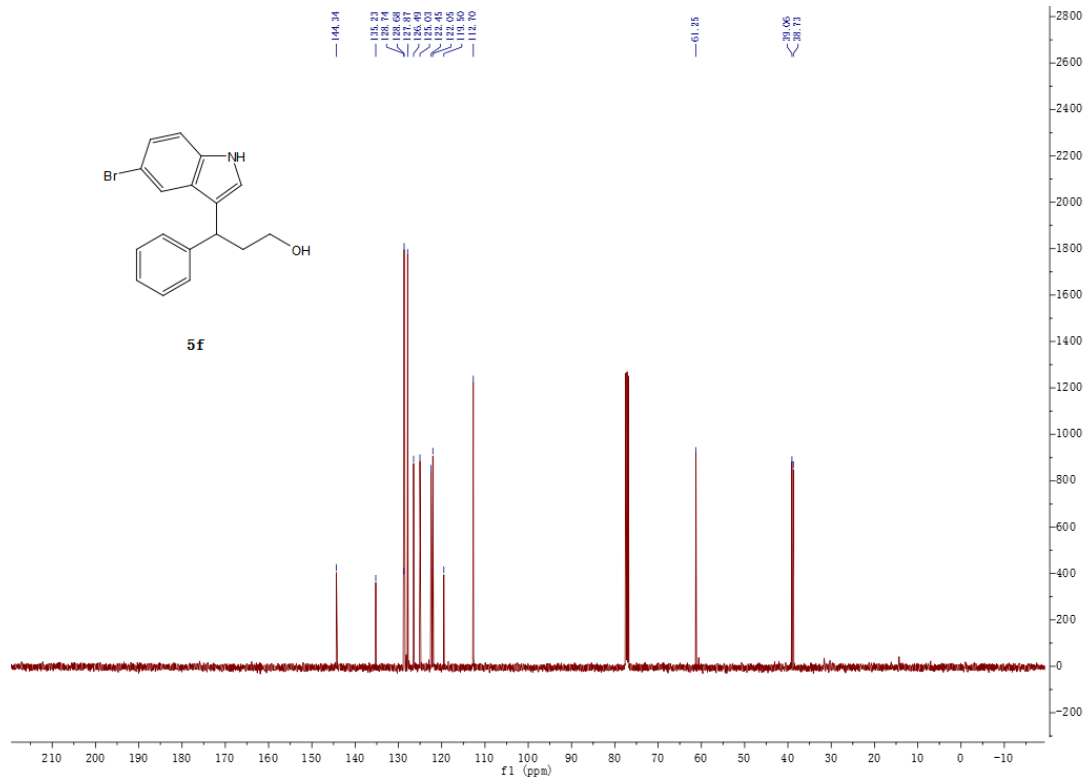




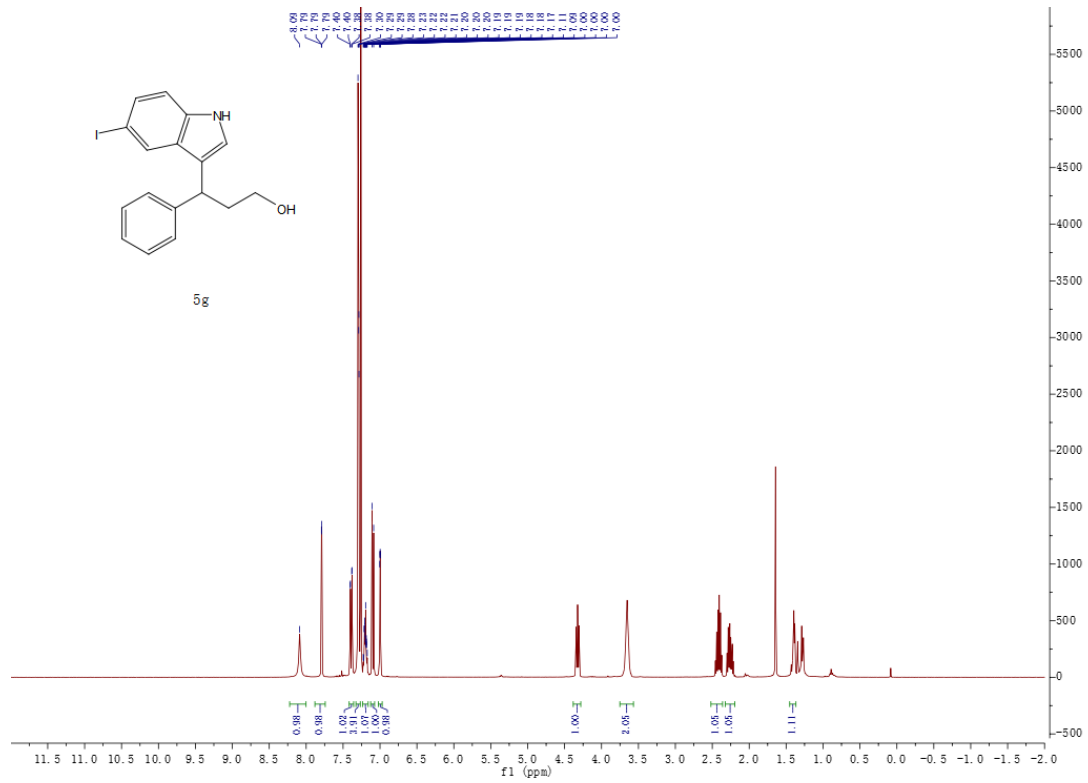
$^1\text{H NMR}$ of **5f**



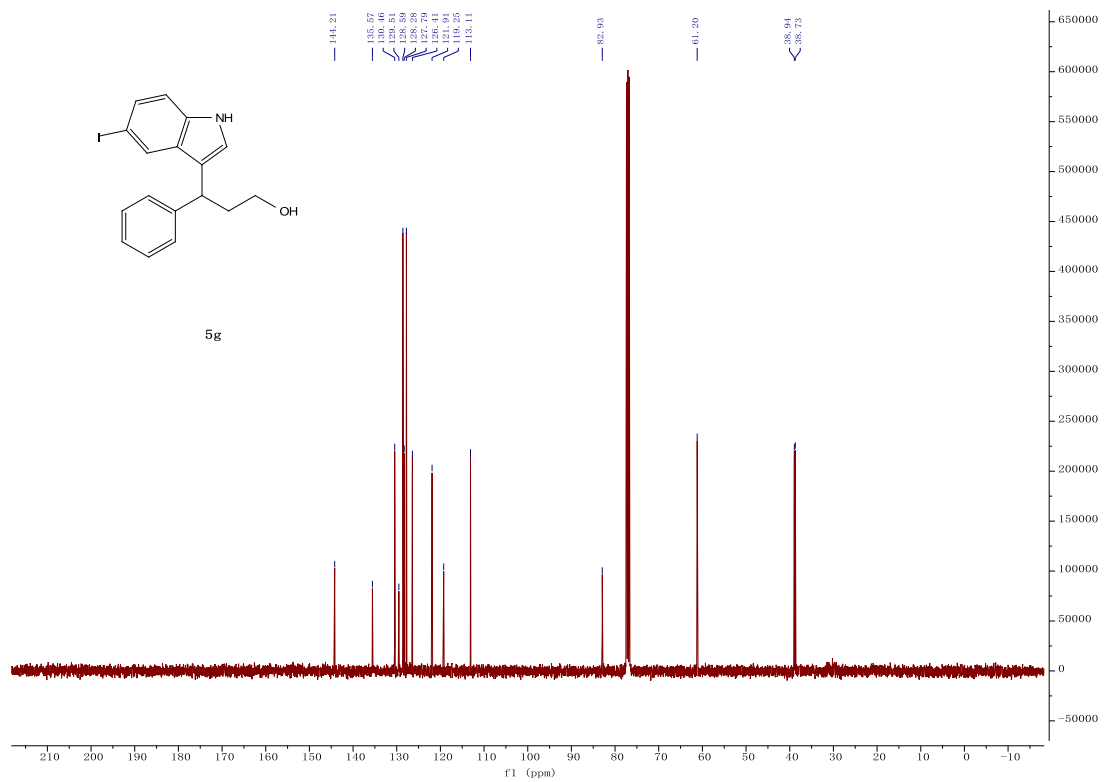
$^{13}\text{C NMR}$ of **5f**



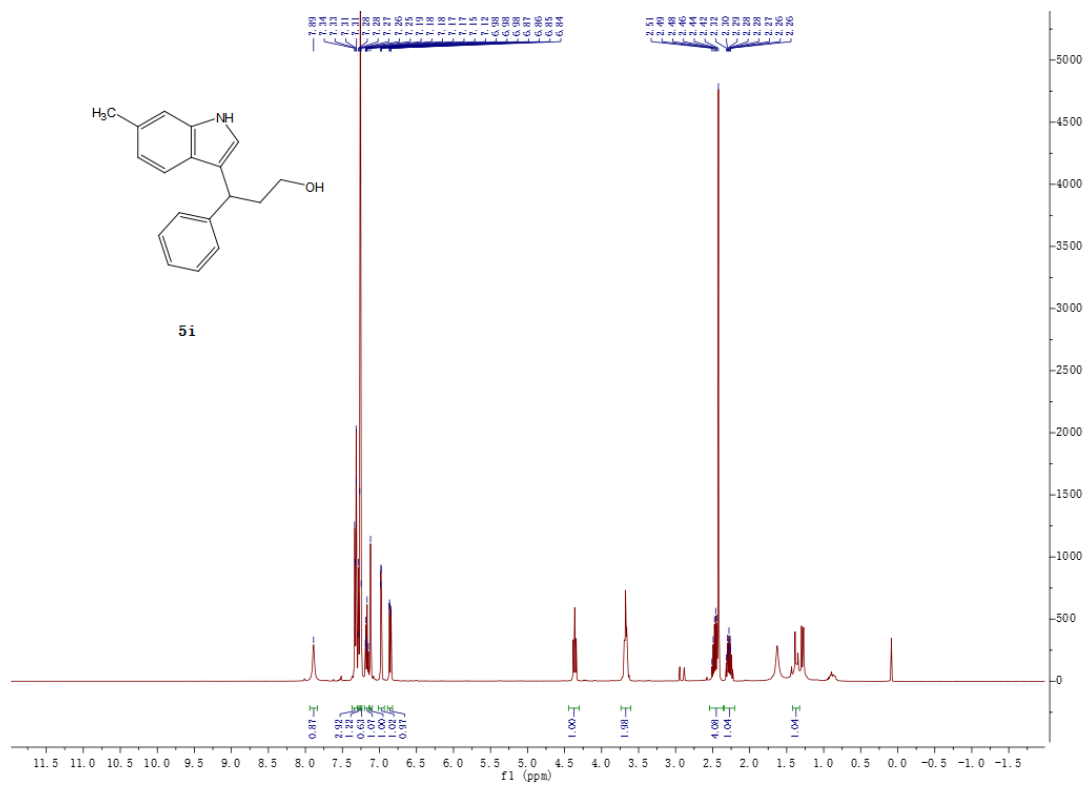
^1H NMR of **5g**



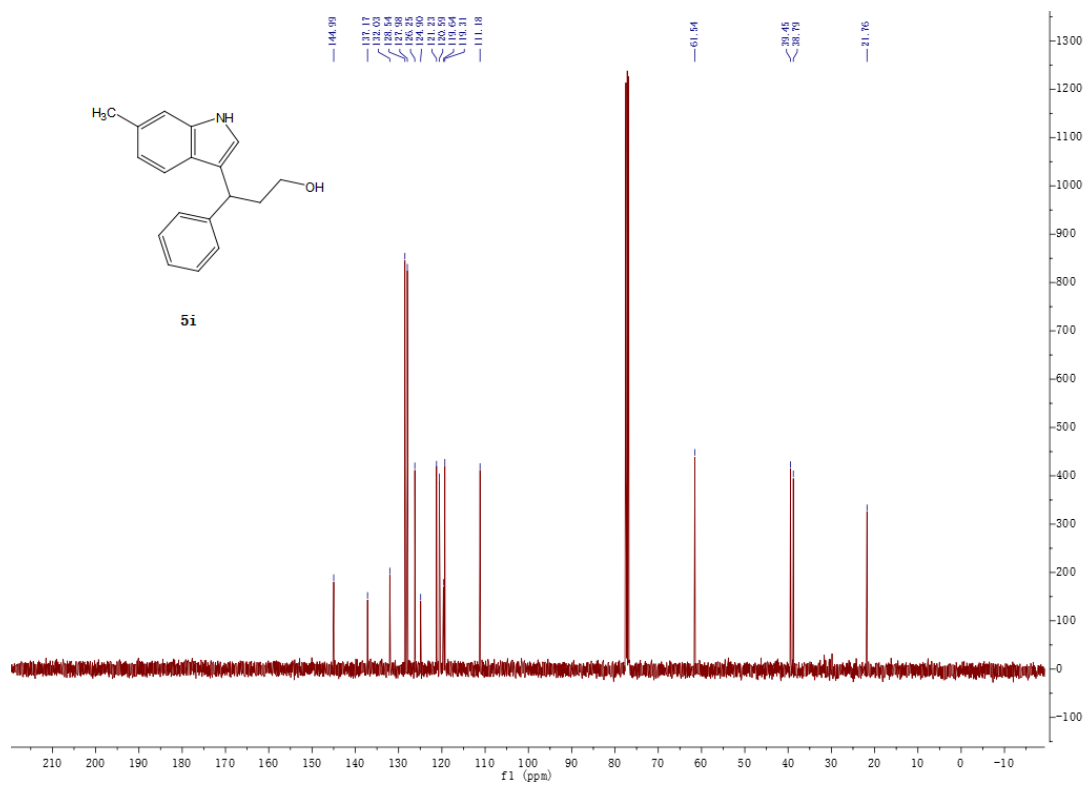
^{13}C NMR of **5g**



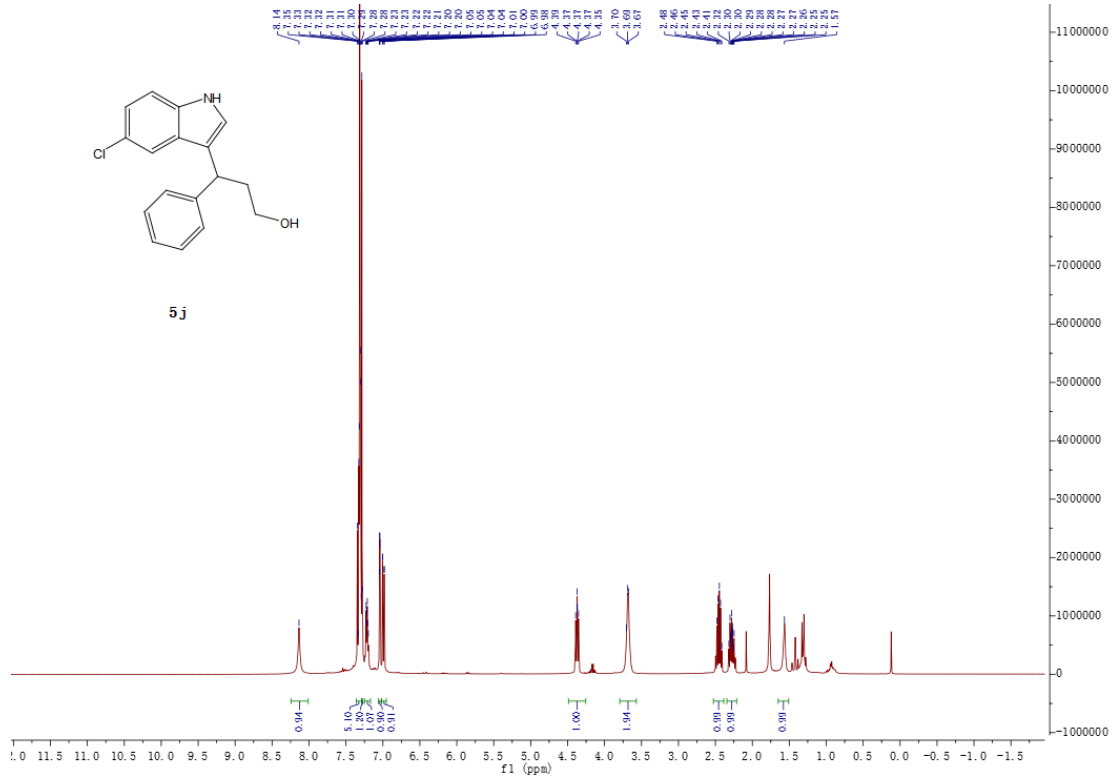
^1H NMR of **5i**



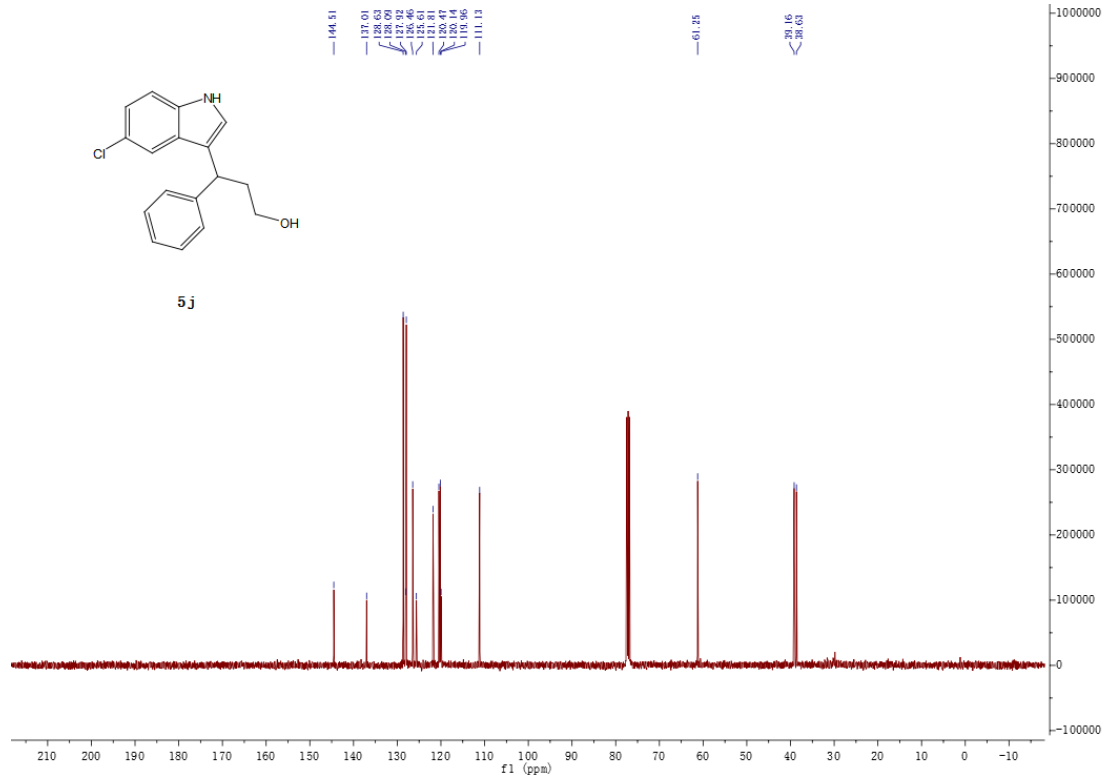
^{13}C NMR of **5i**



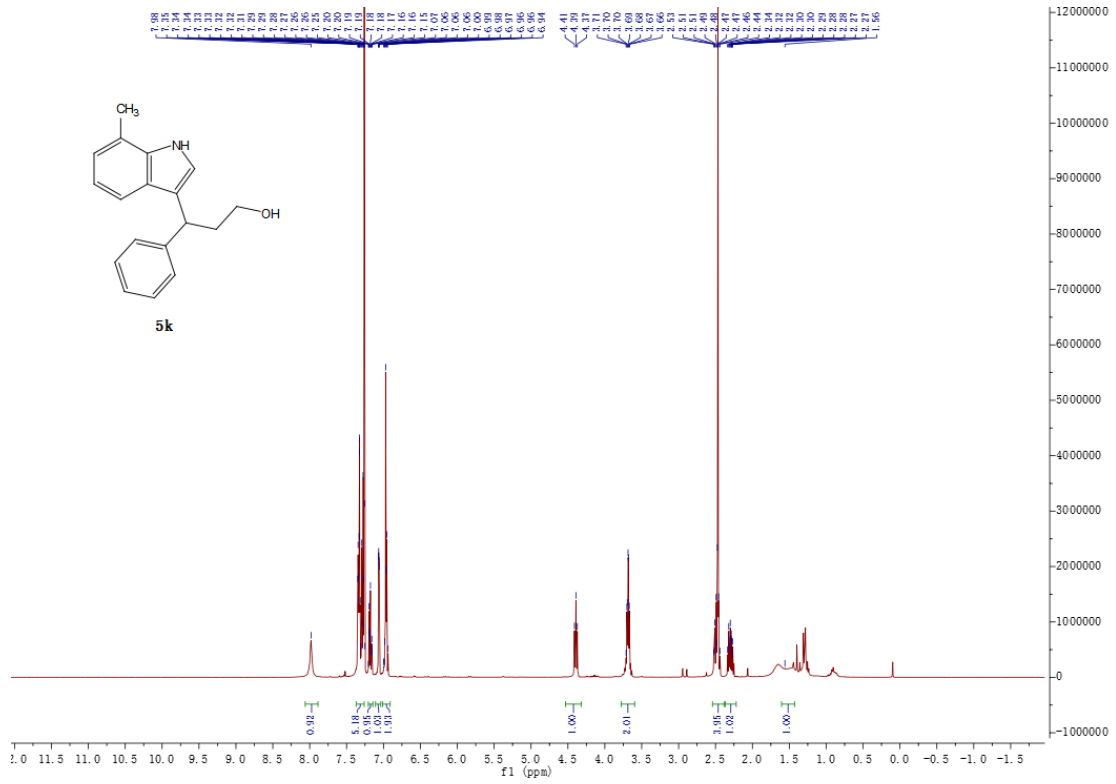
¹H NMR of 5j



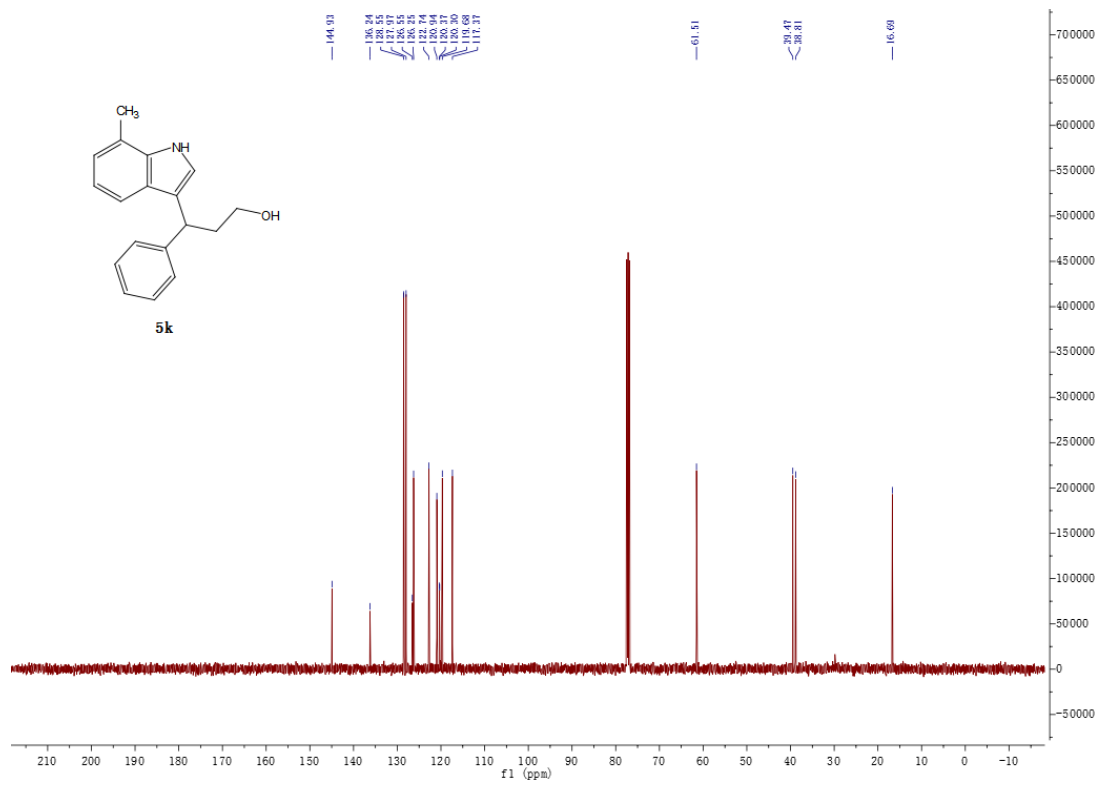
¹³C NMR of 5j



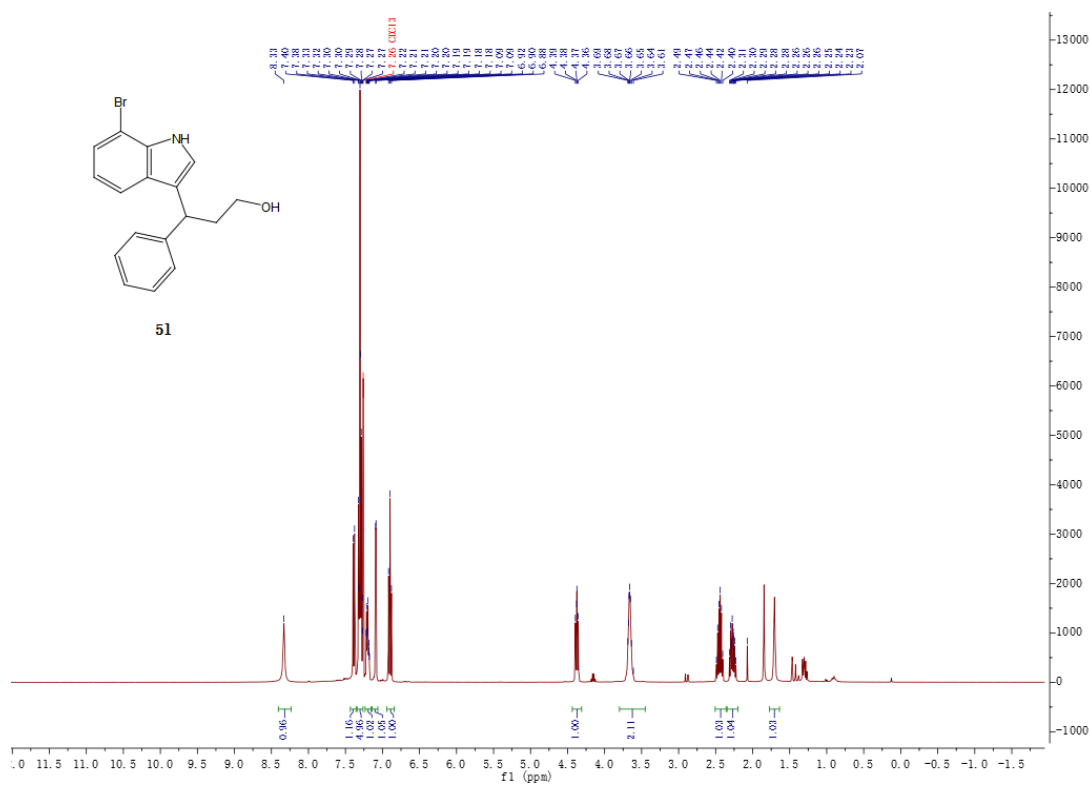
¹H NMR of 5k



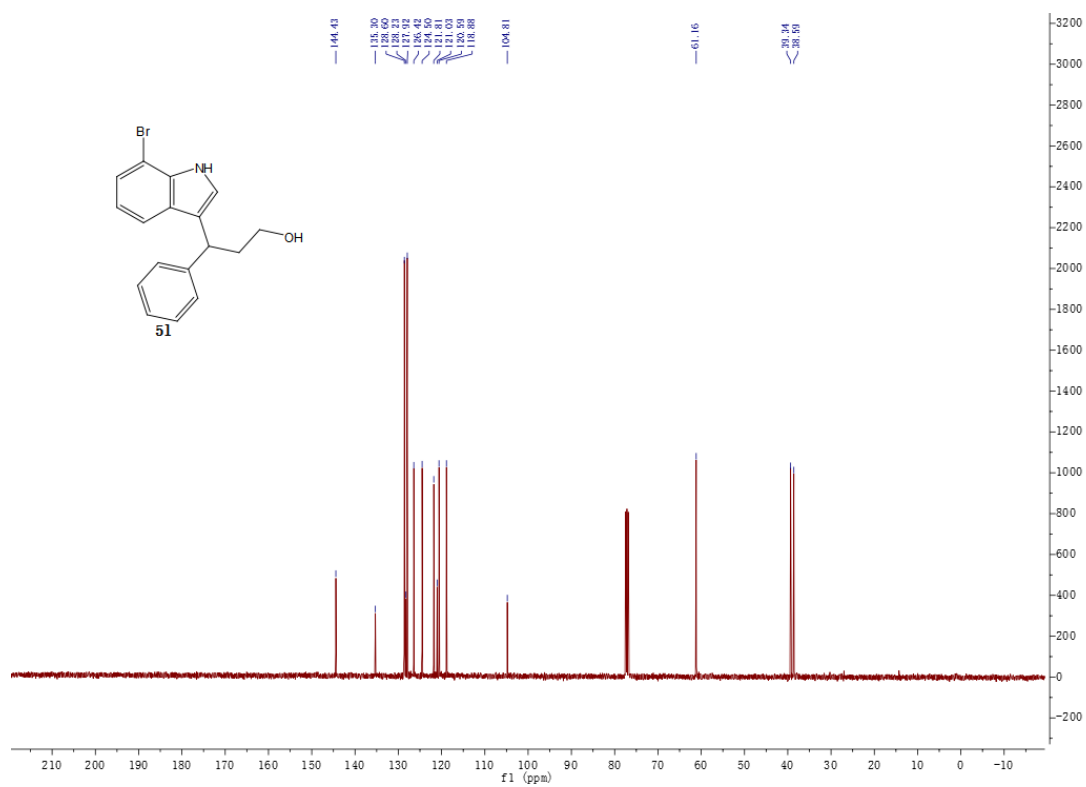
¹³C NMR of 5k



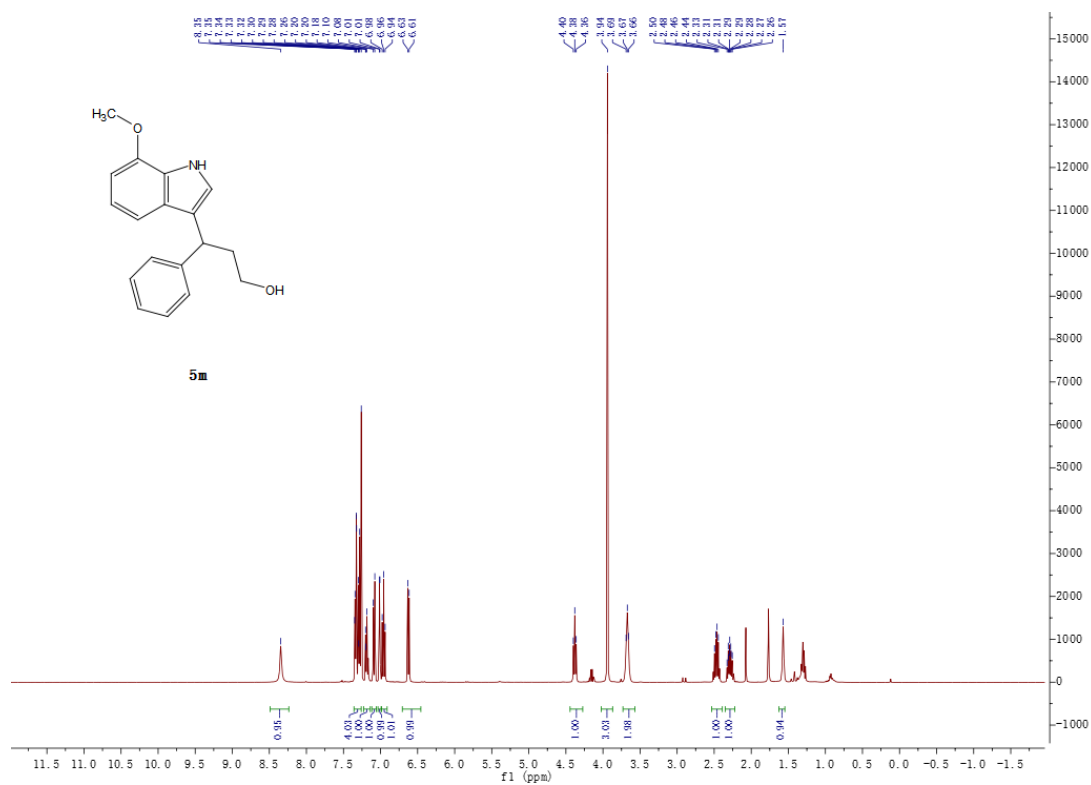
¹H NMR of 51



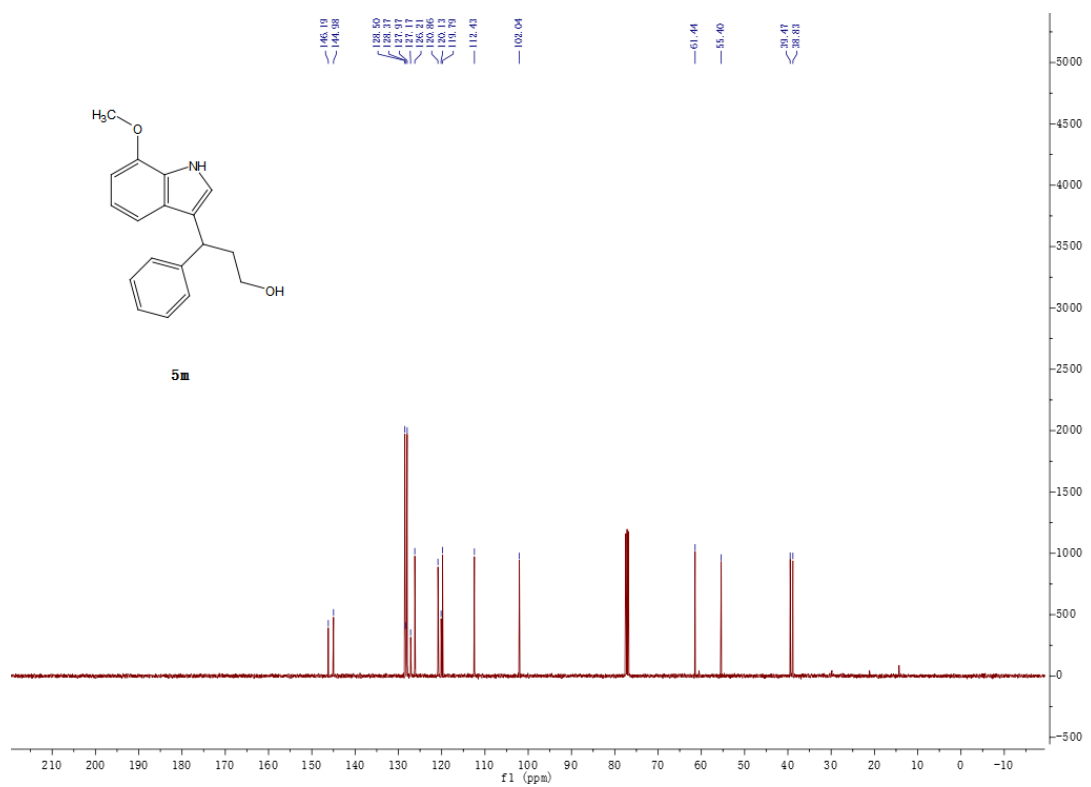
¹³C NMR of 51



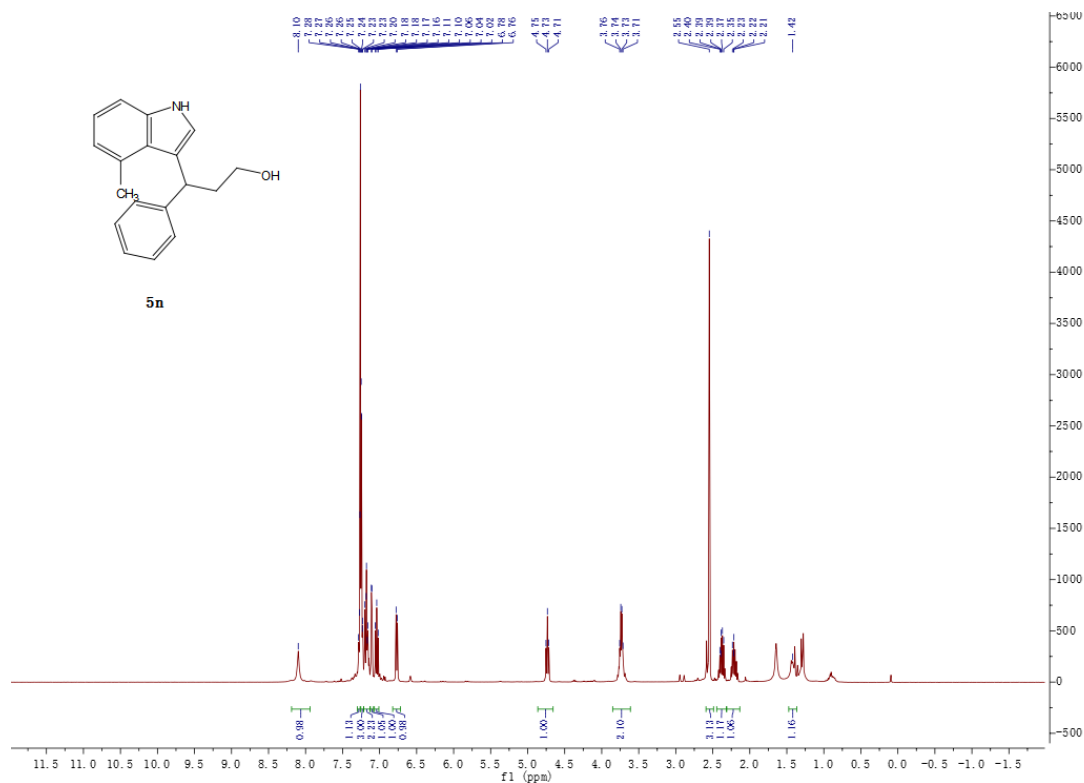
¹H NMR of 5m



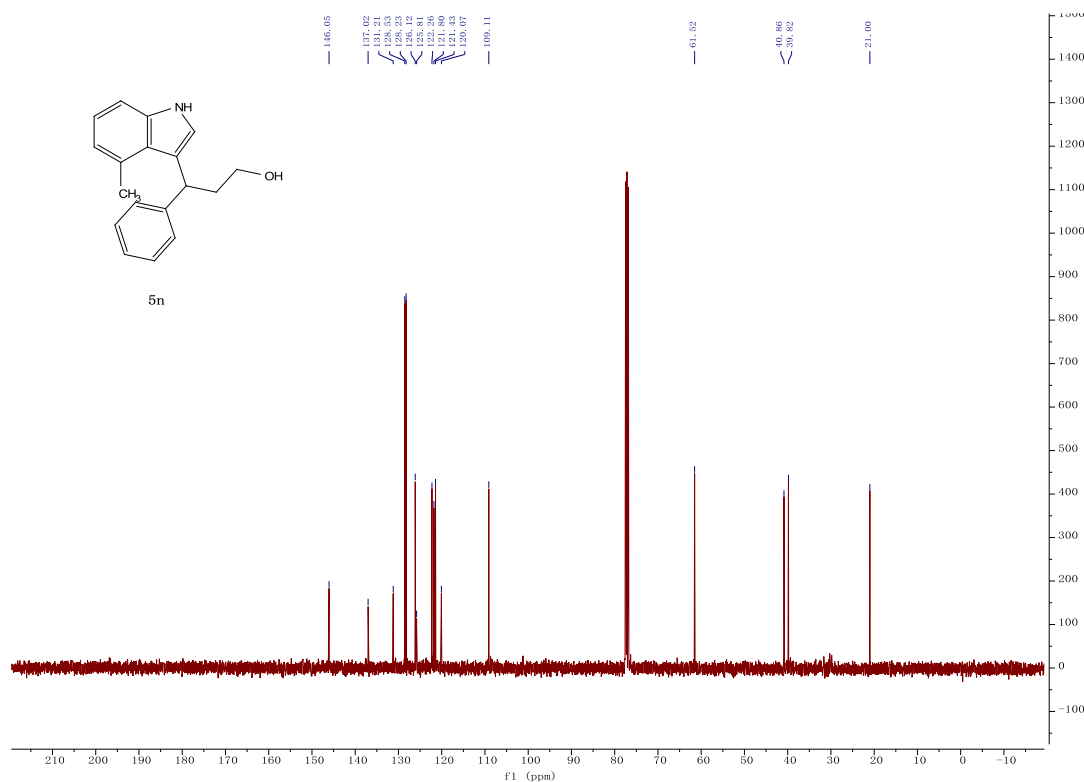
¹³C NMR of 5m



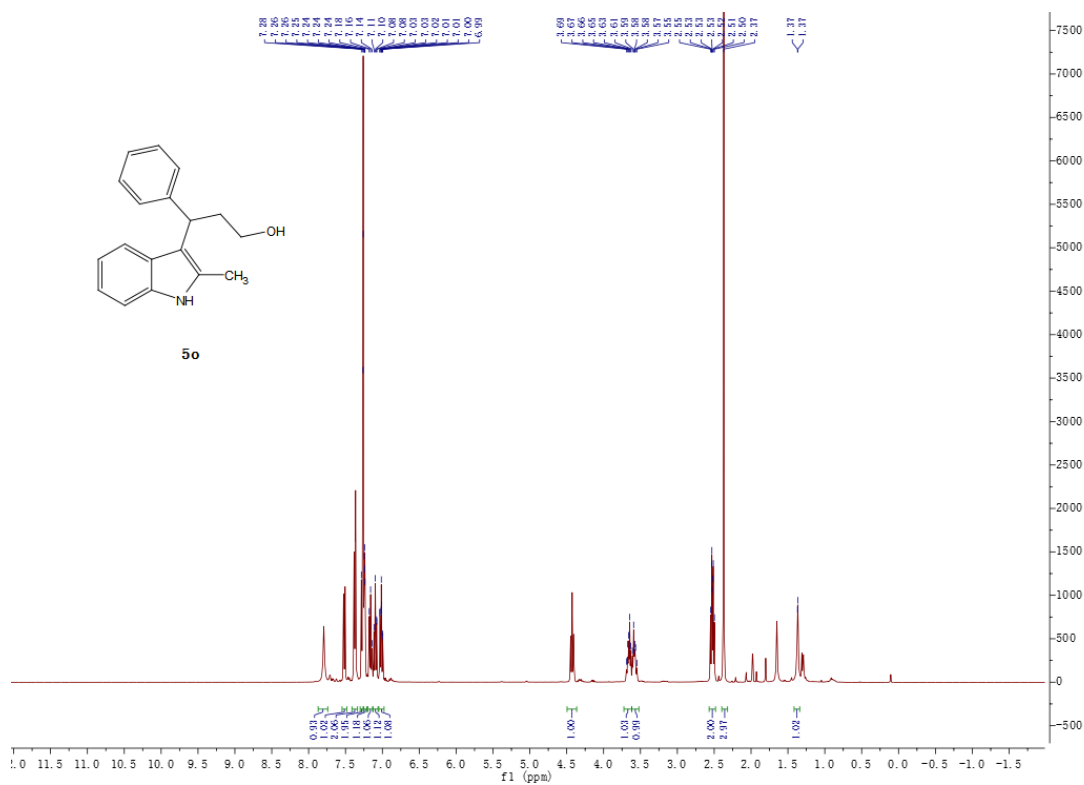
¹H NMR of 5n



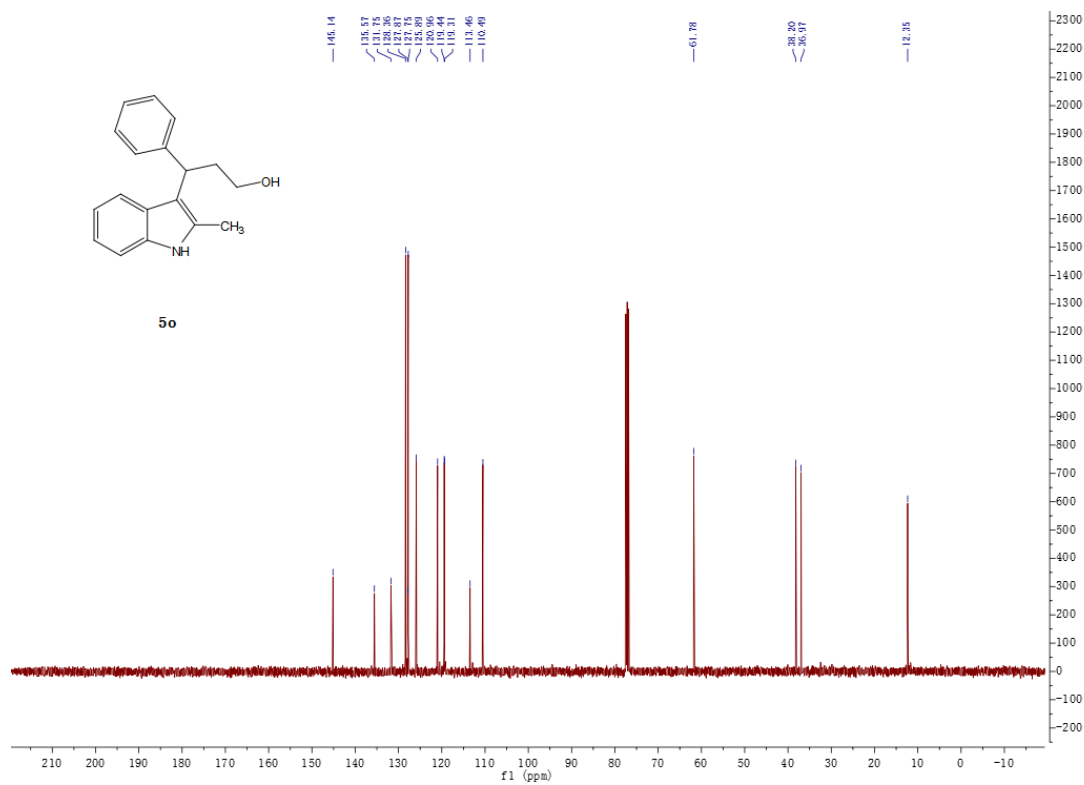
¹³C NMR of 5n



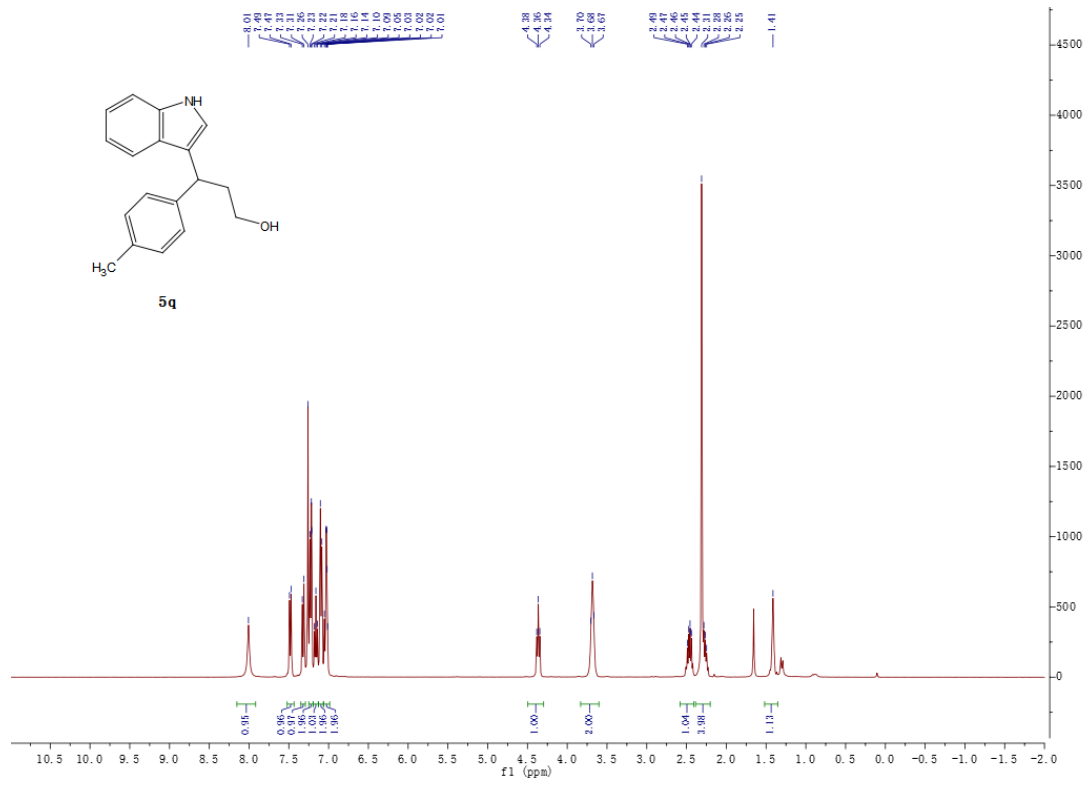
¹H NMR of **5o**



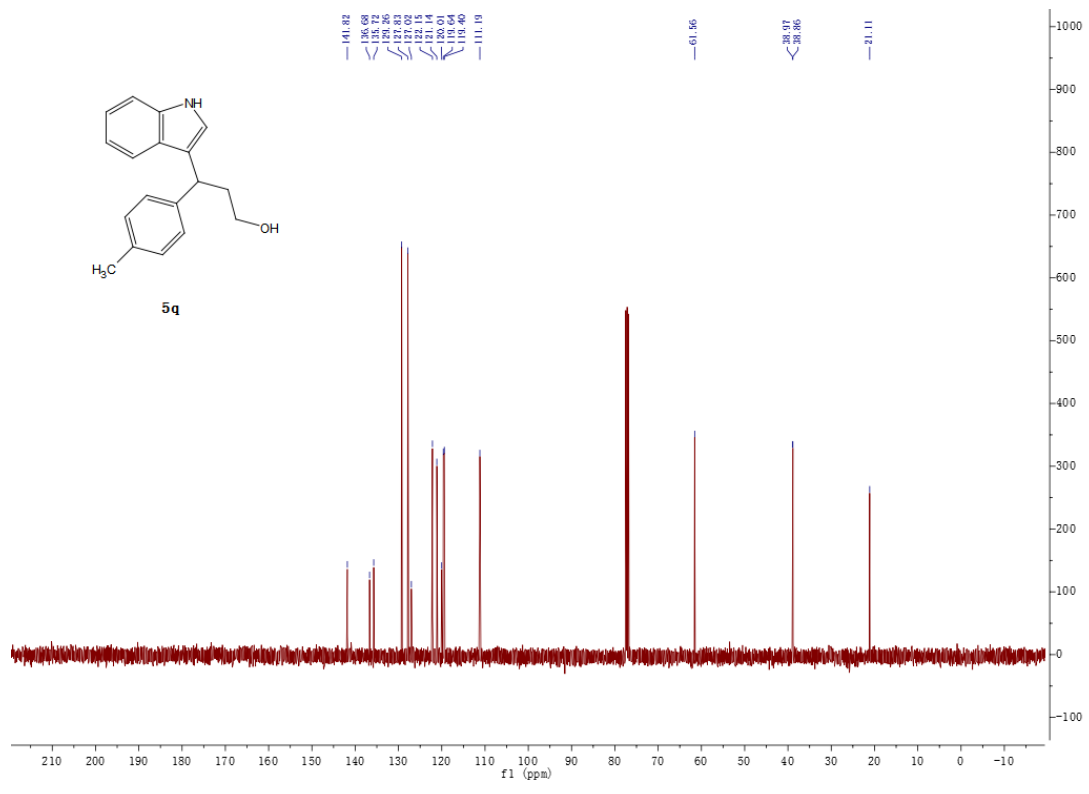
¹³C NMR of **5o**



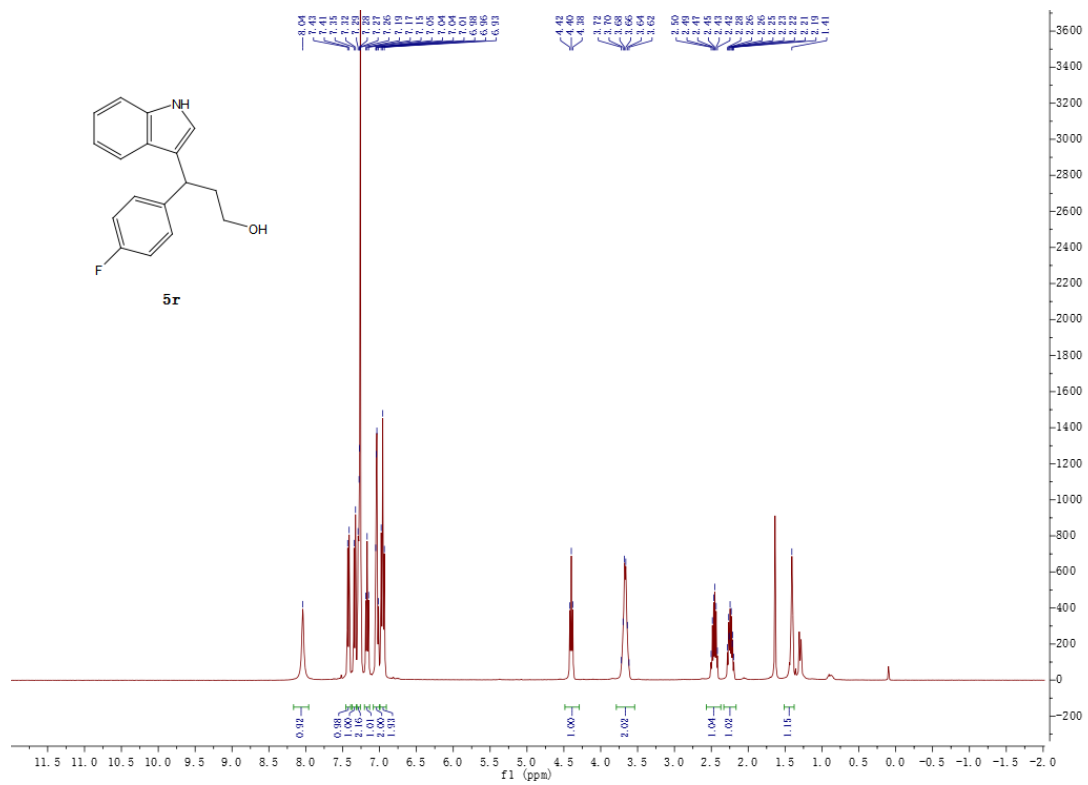
¹H NMR of 5q



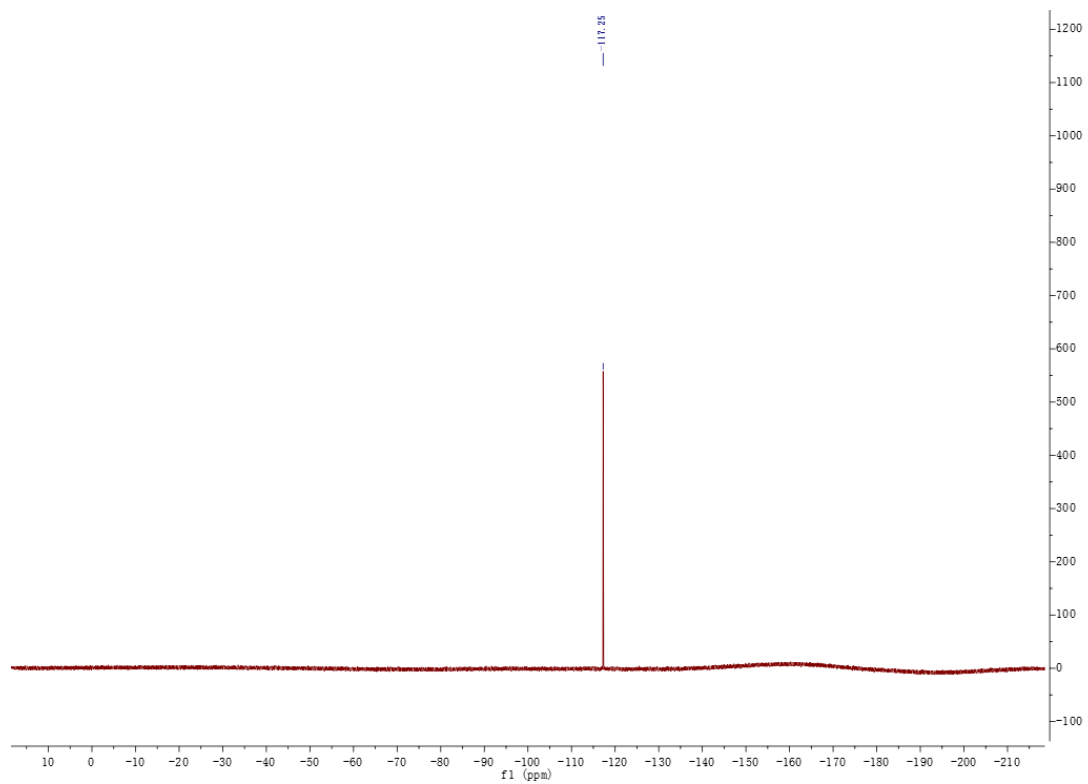
¹³C NMR of 5q



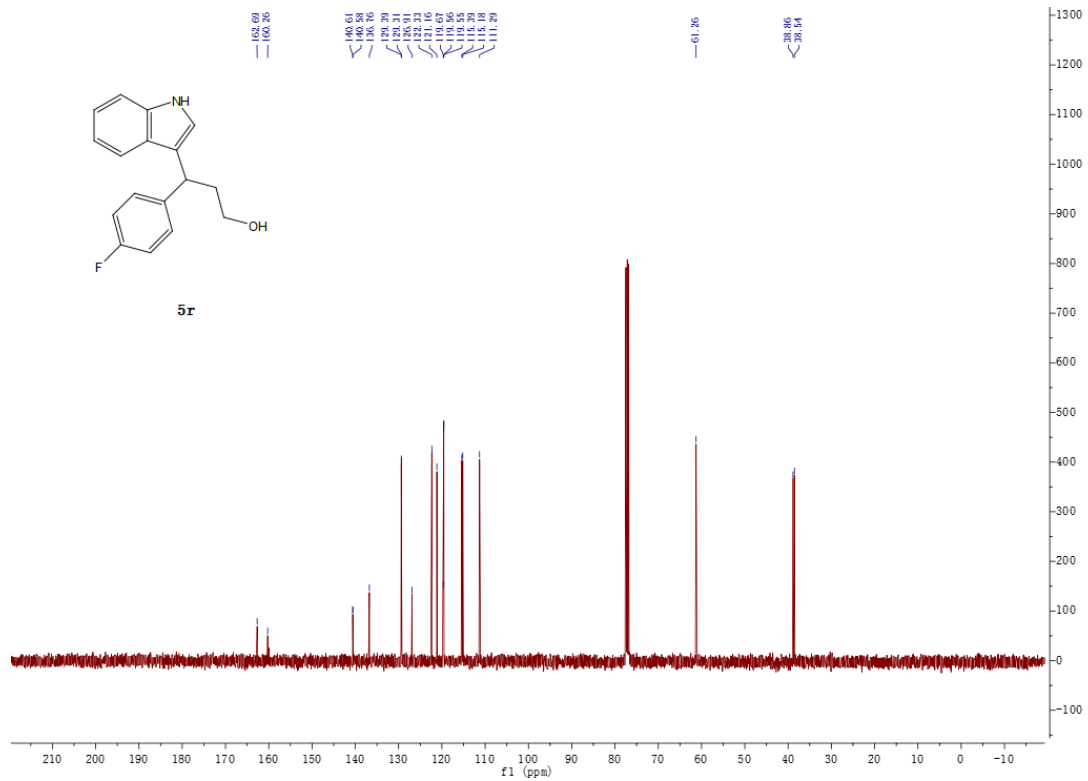
¹H NMR of 5r



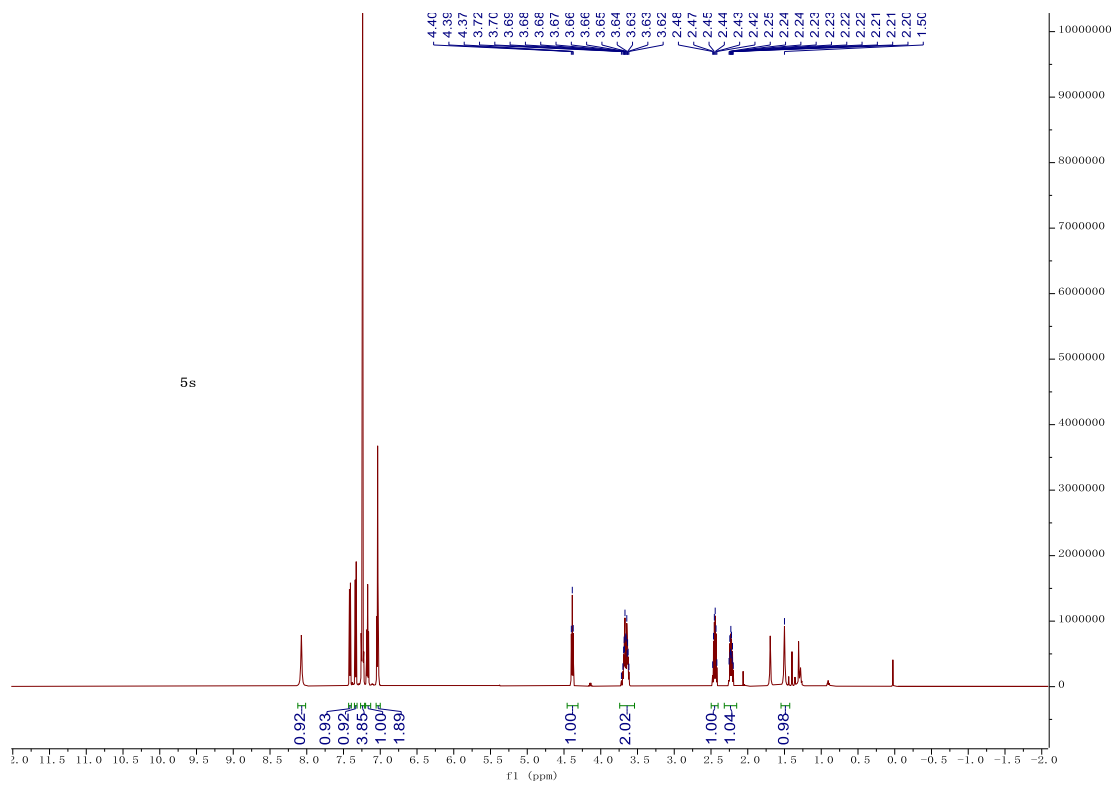
¹⁹F NMR of 5r



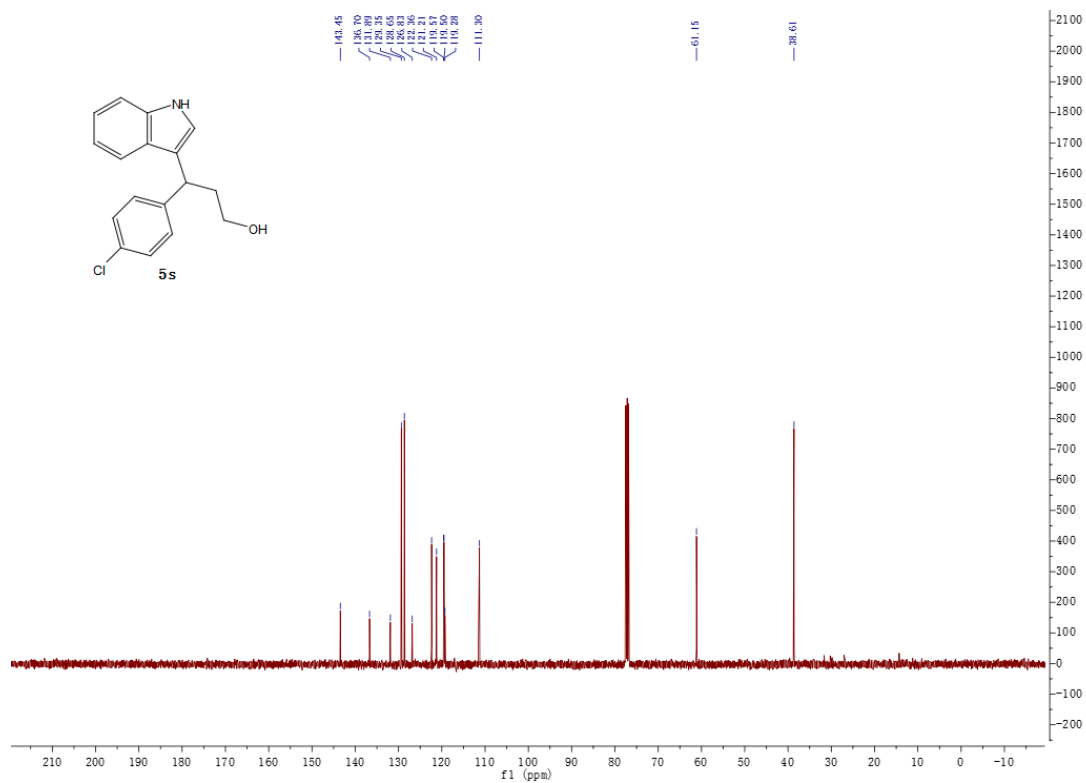
¹³C NMR of 5r



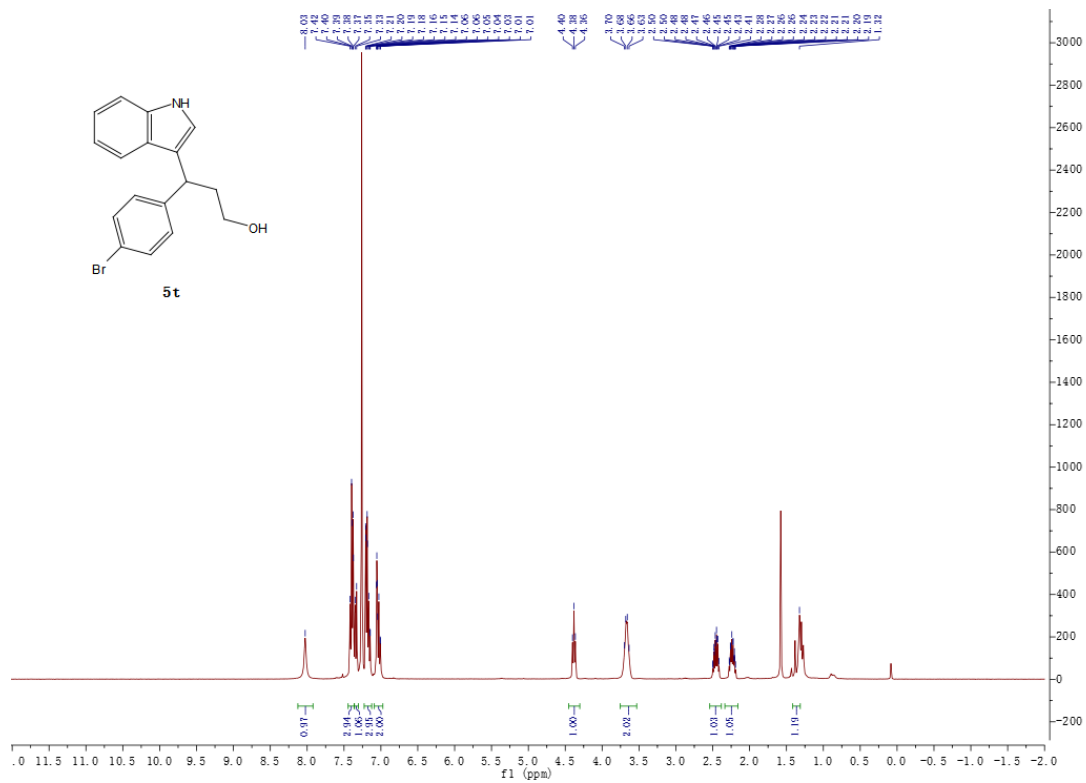
¹H NMR of 5s

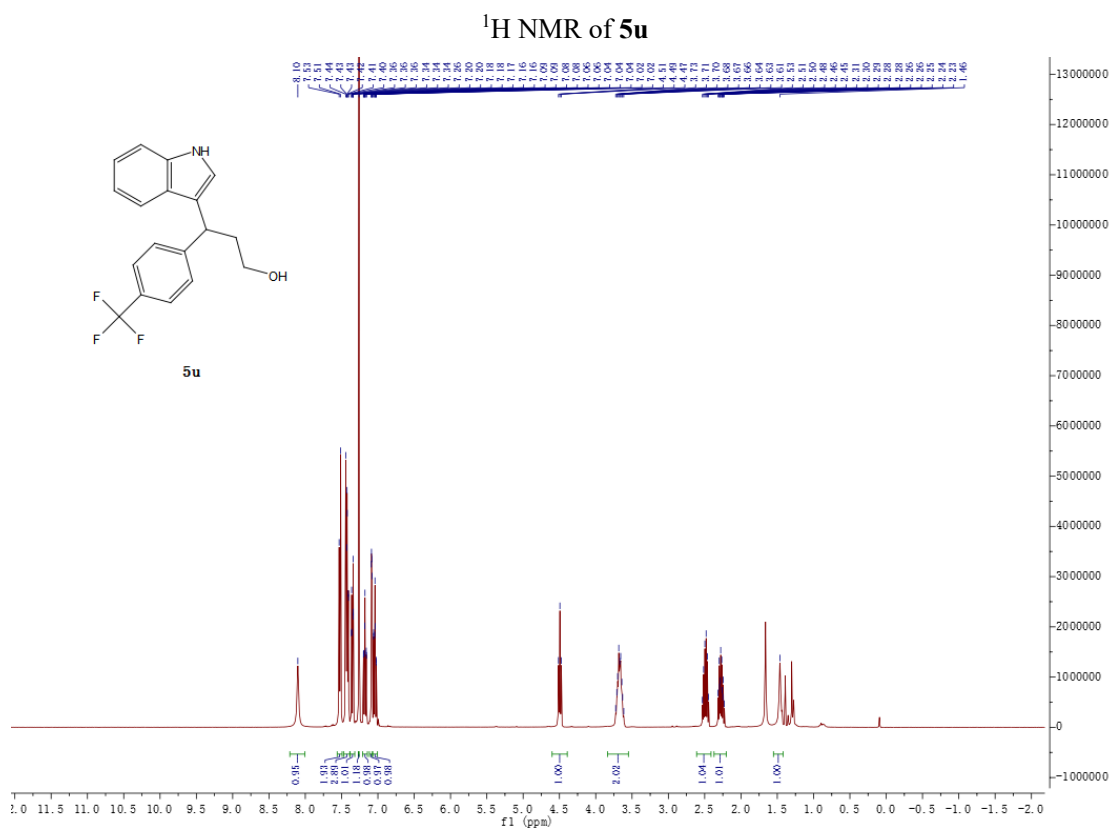
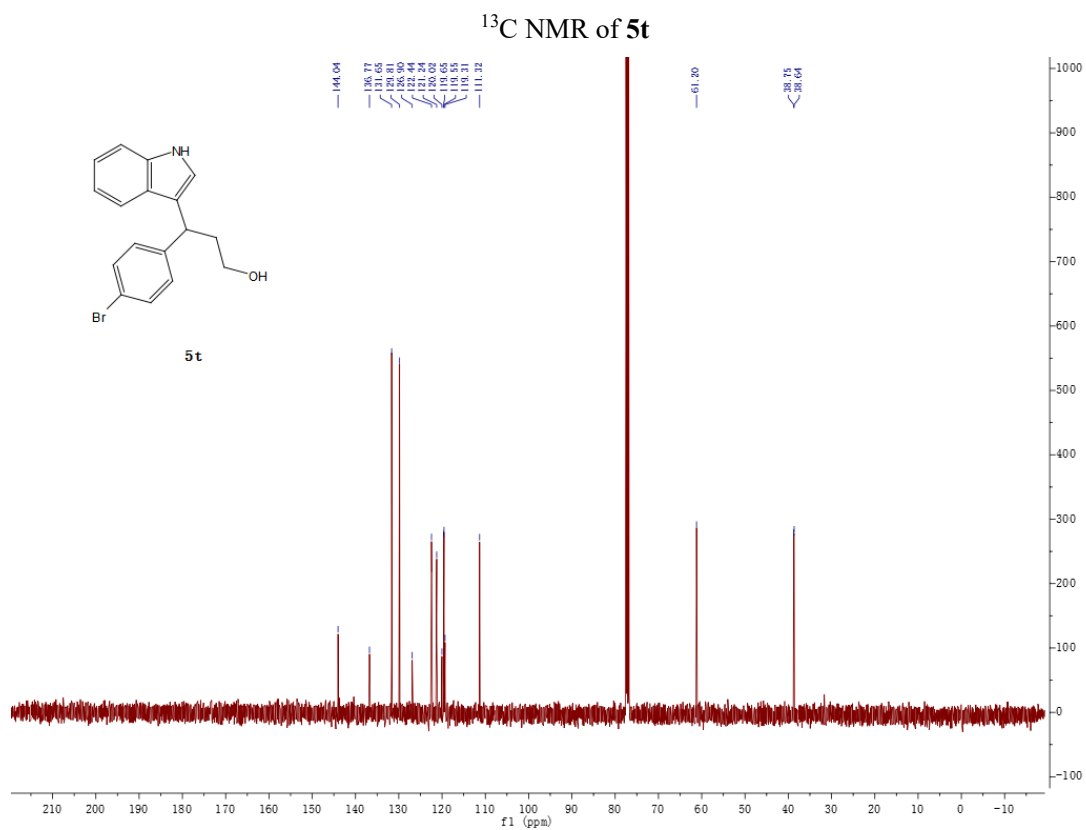


^{13}C NMR of **5s**

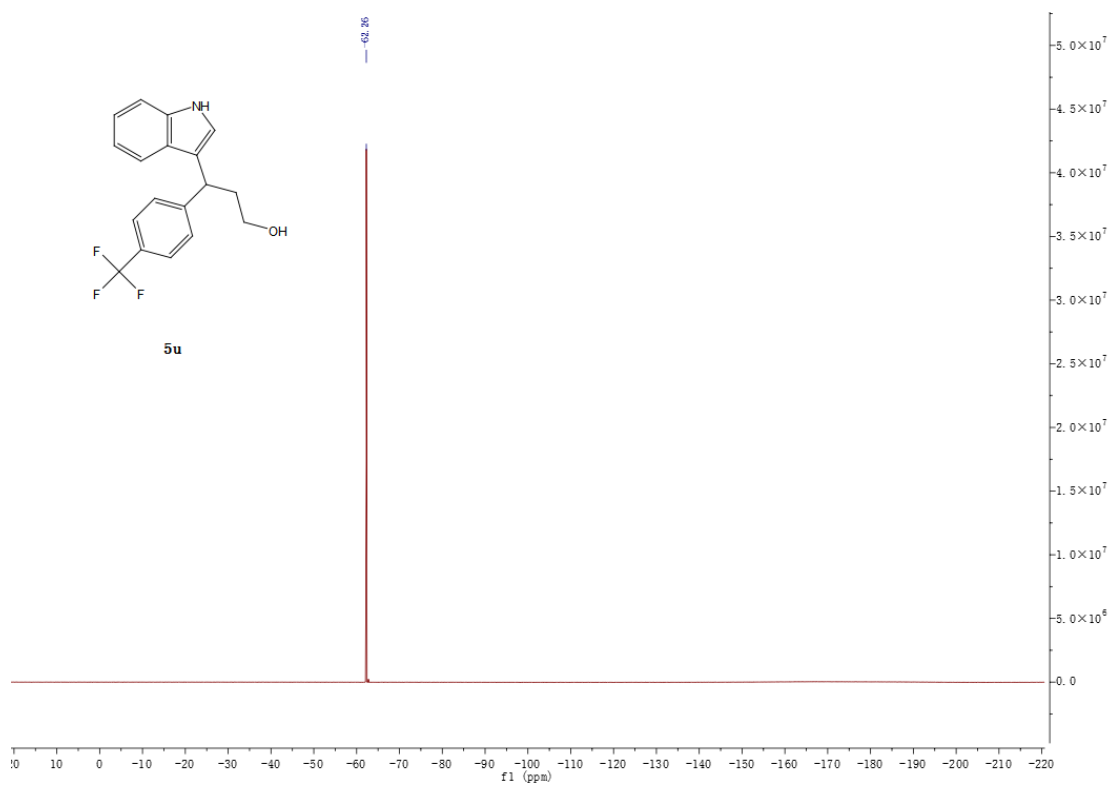


^1H NMR of **5t**

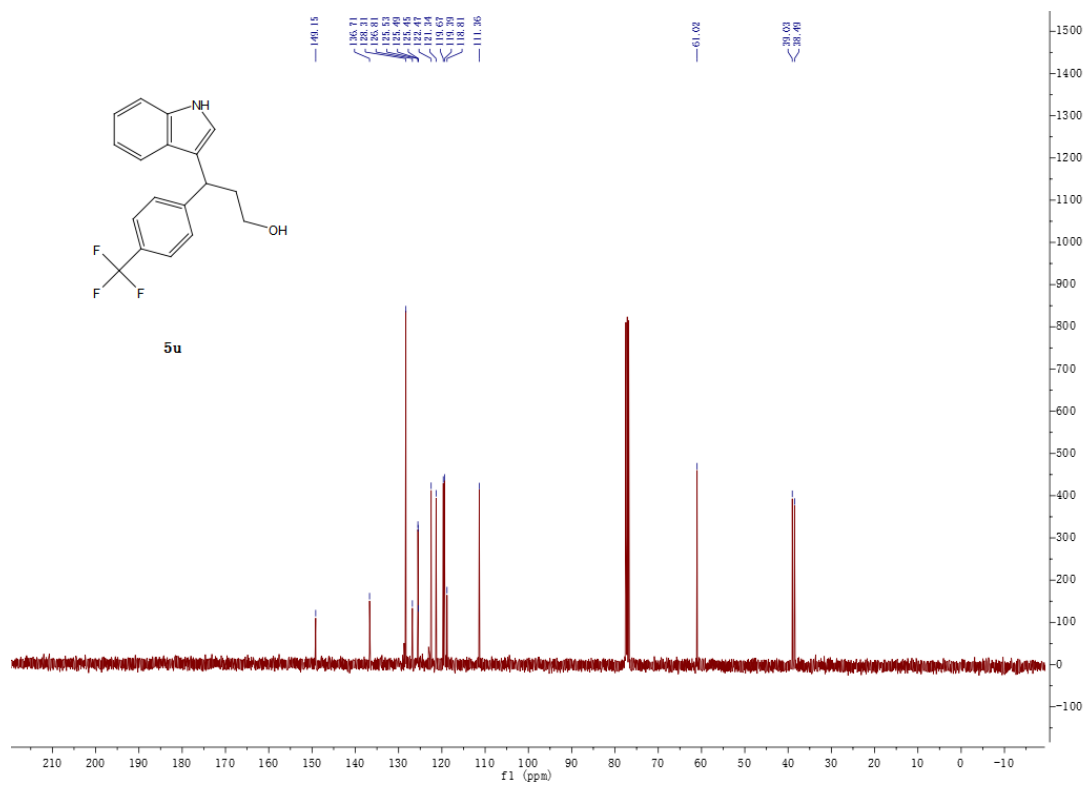




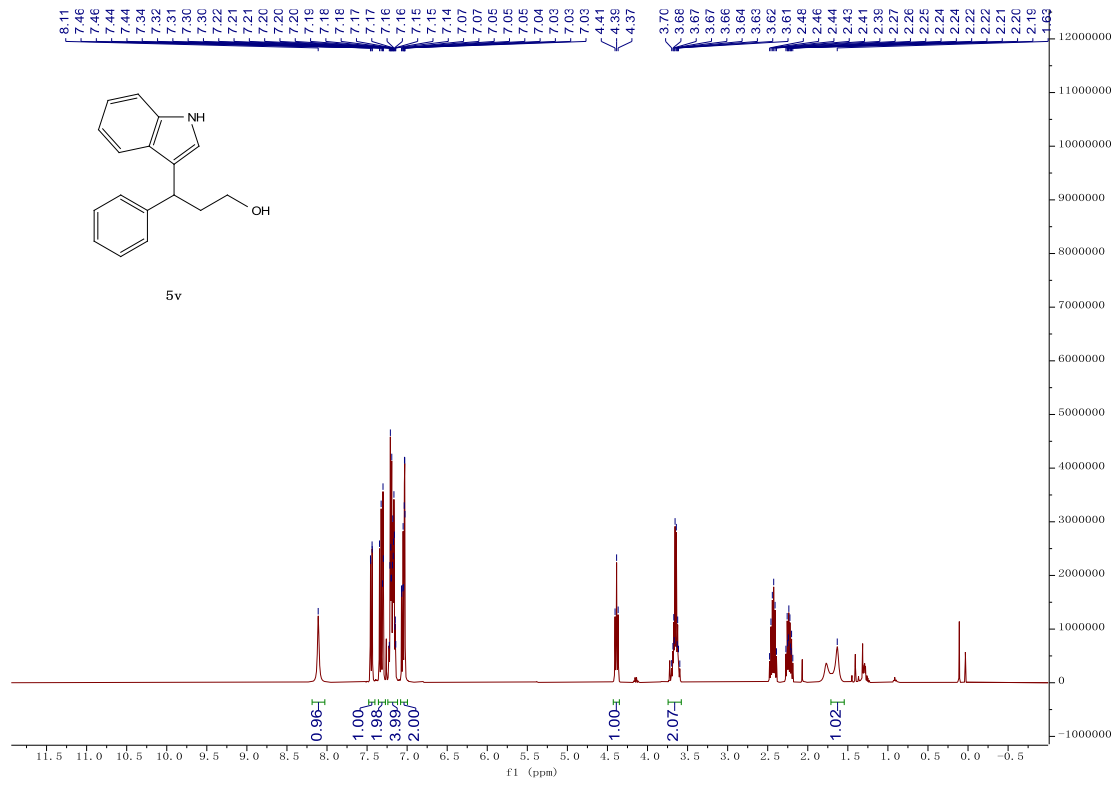
¹⁹F NMR of **5u**



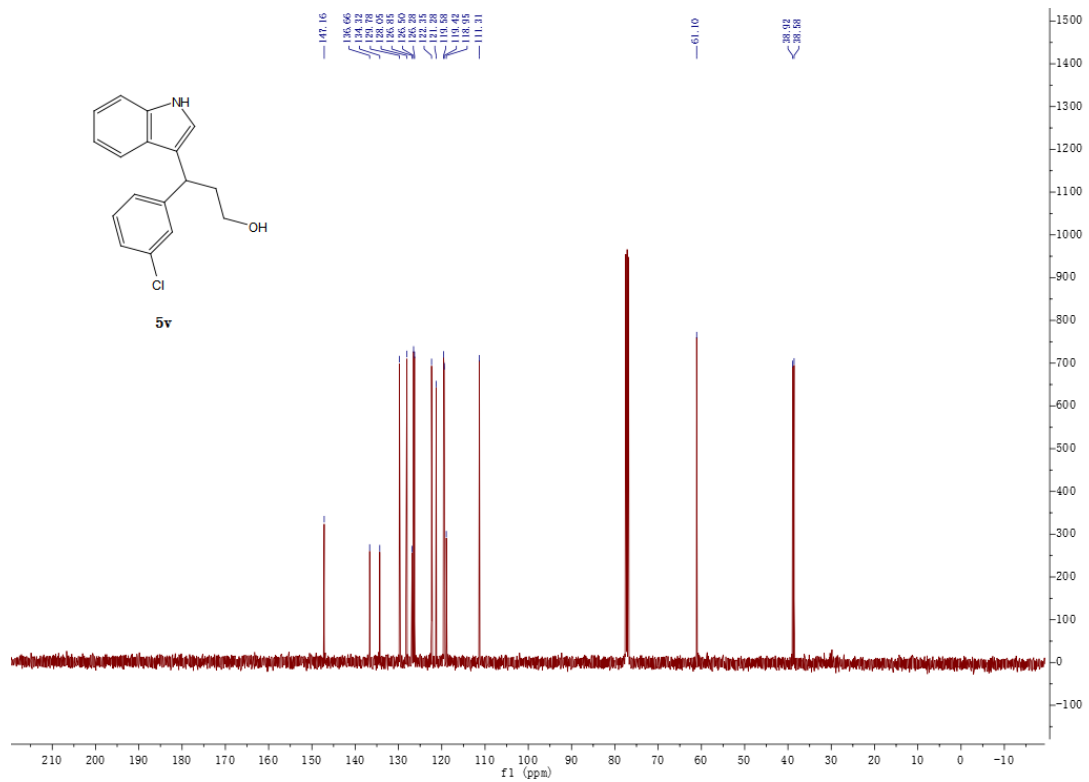
¹³C NMR of **5u**



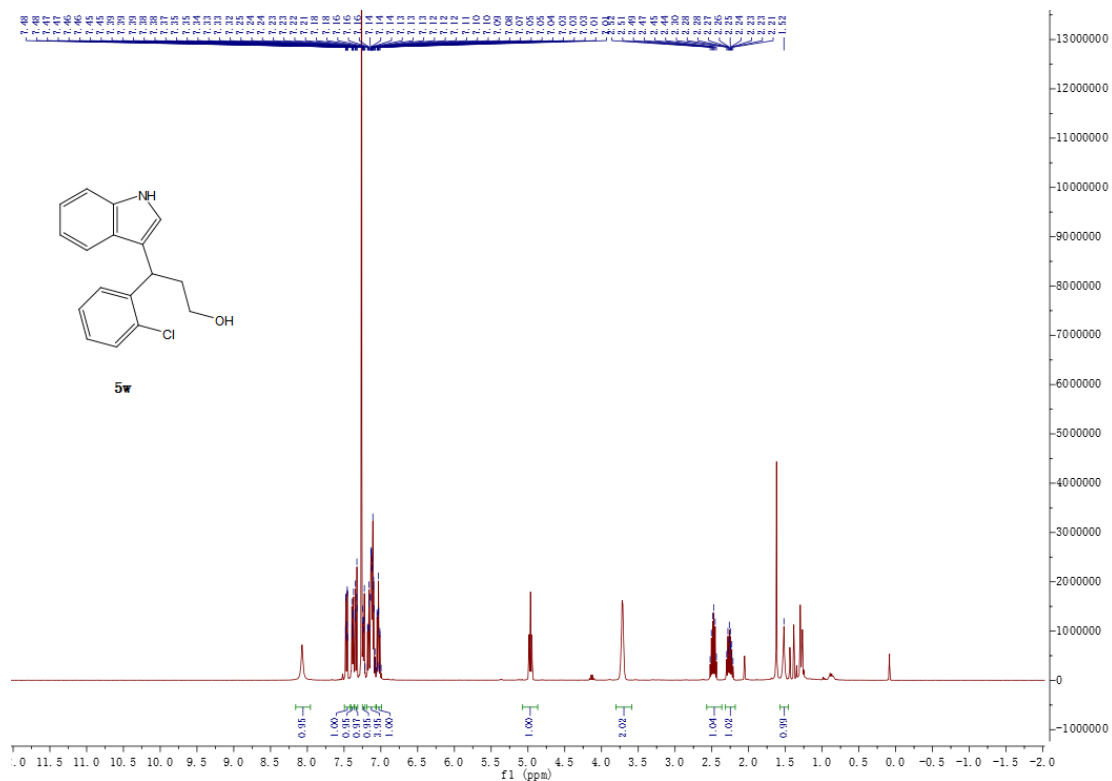
¹H NMR of 5v



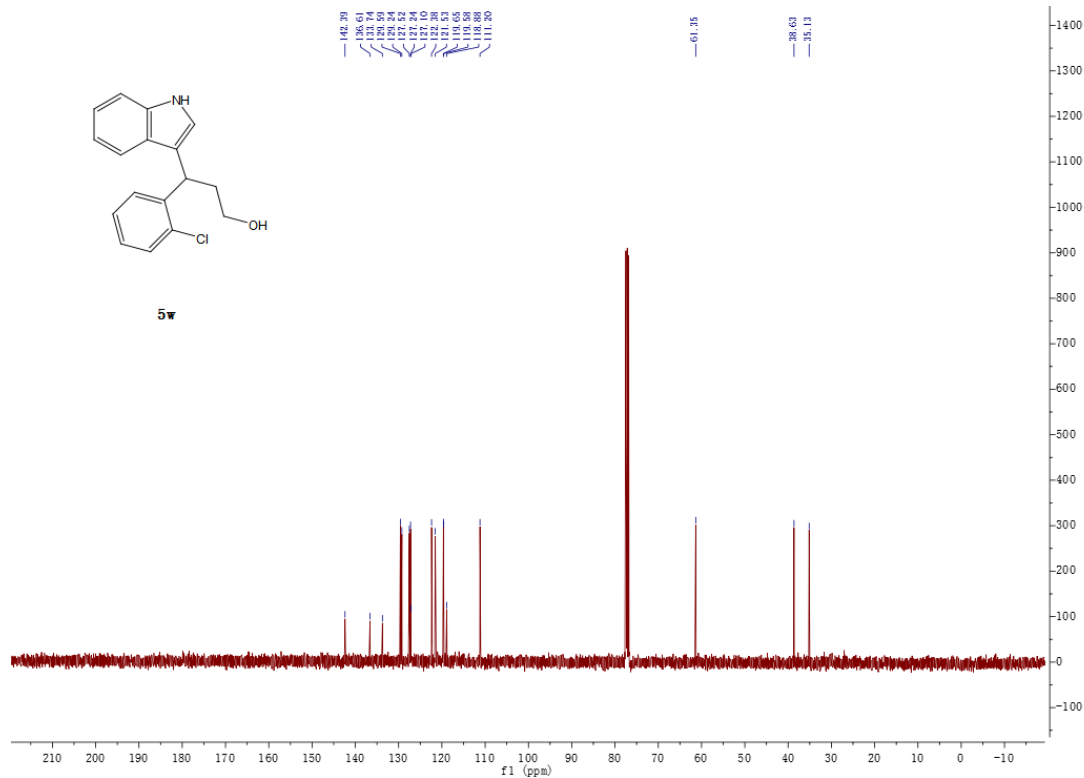
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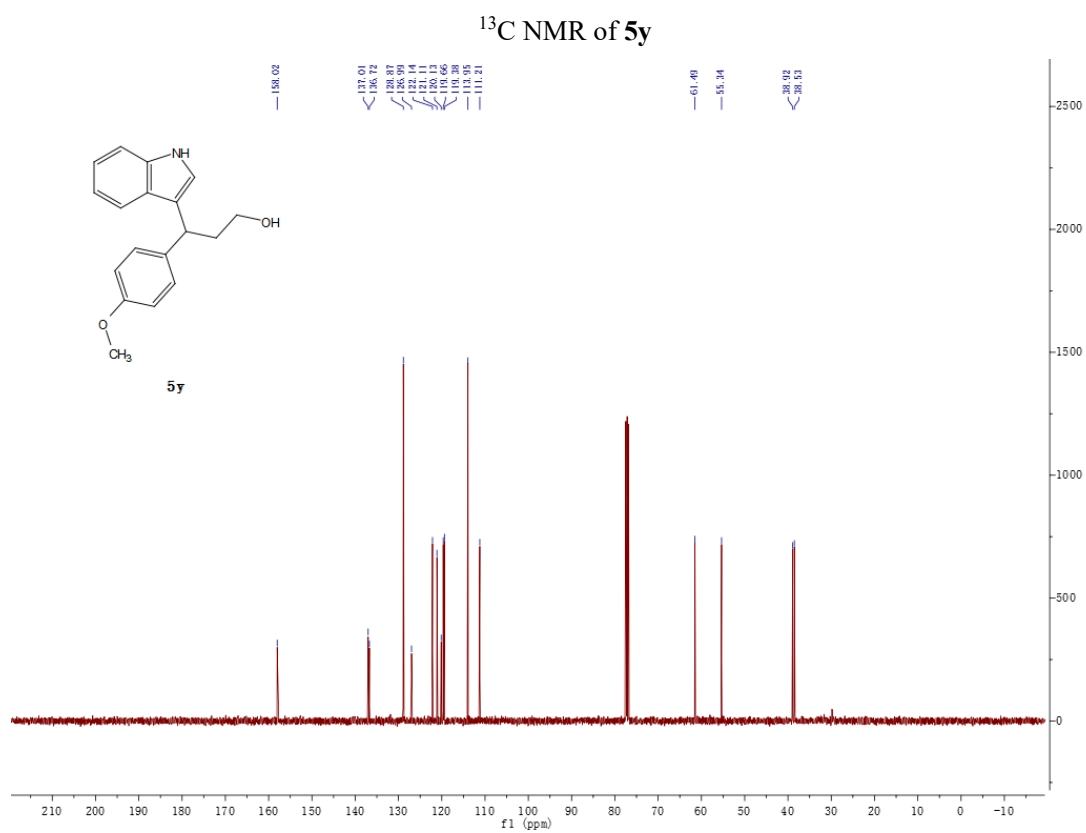
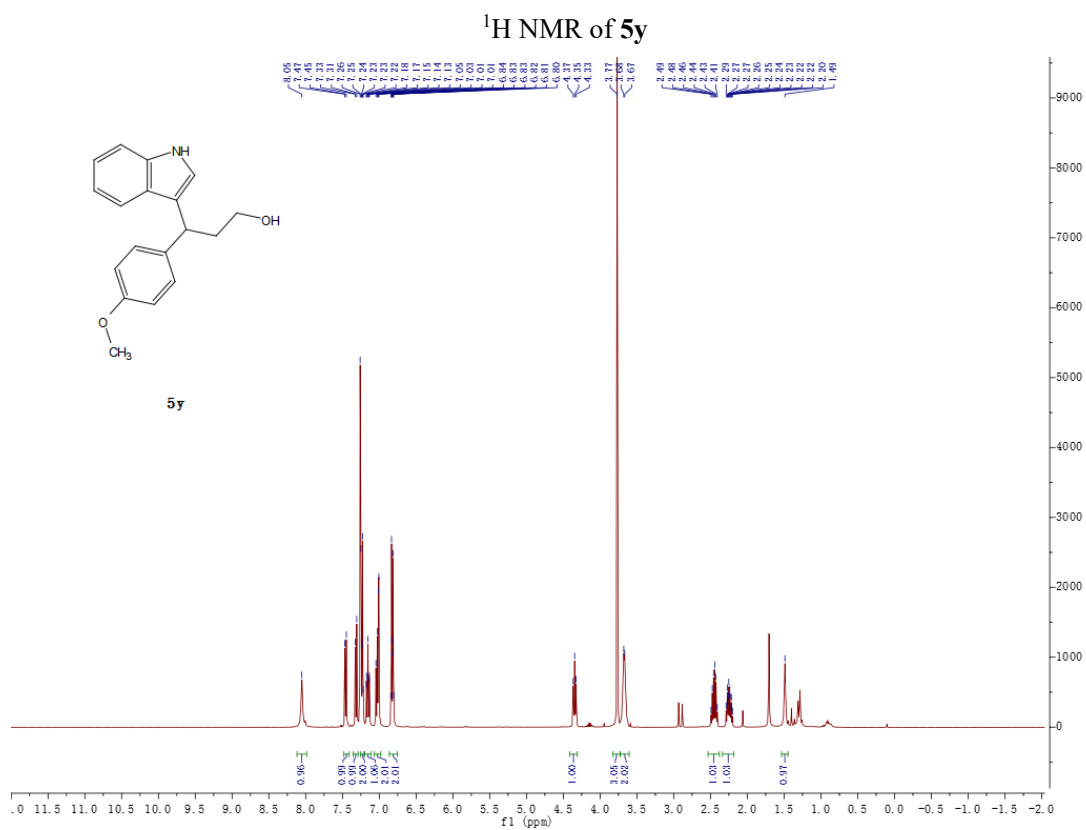


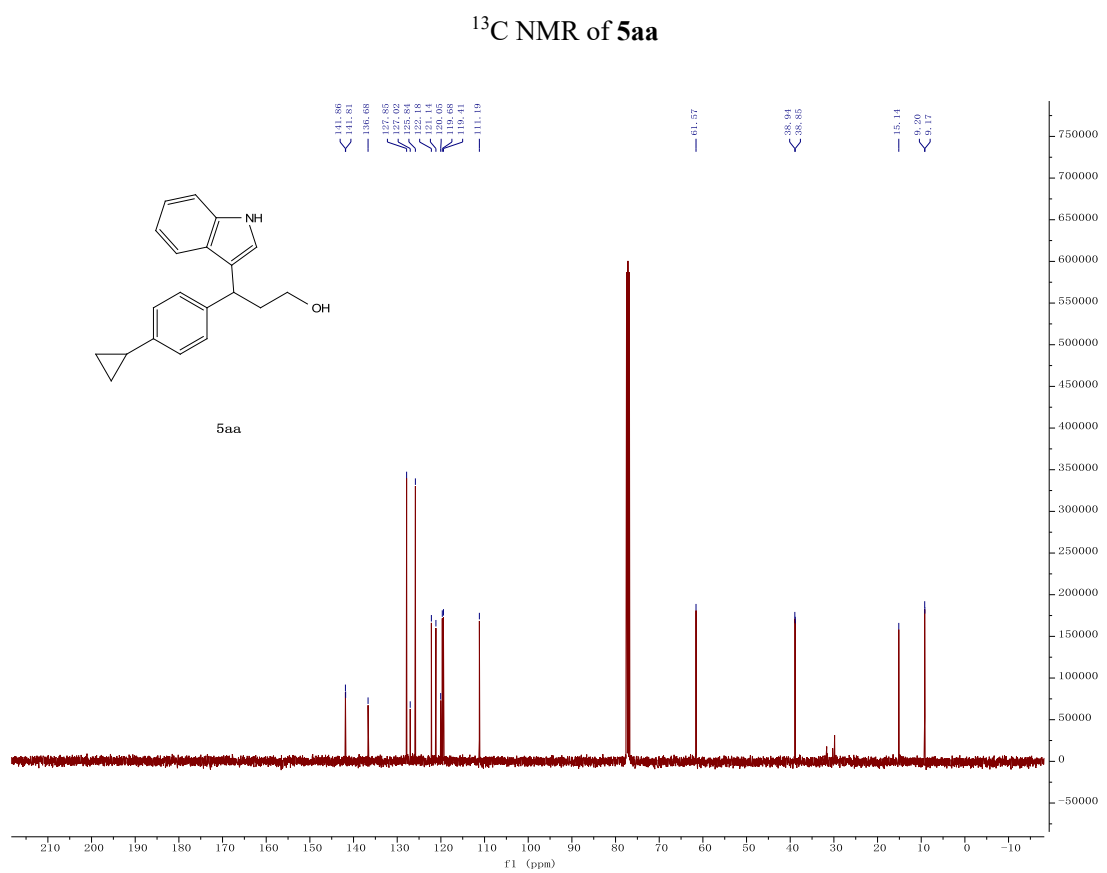
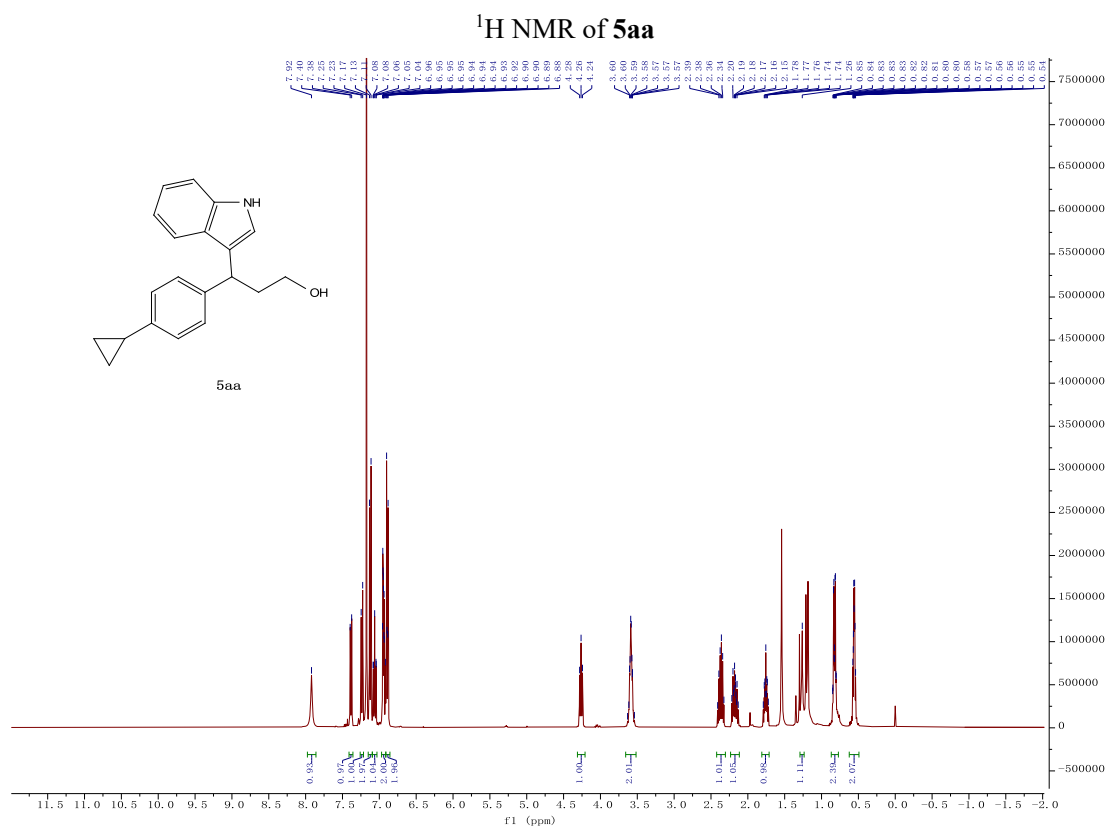
¹H NMR of 5w



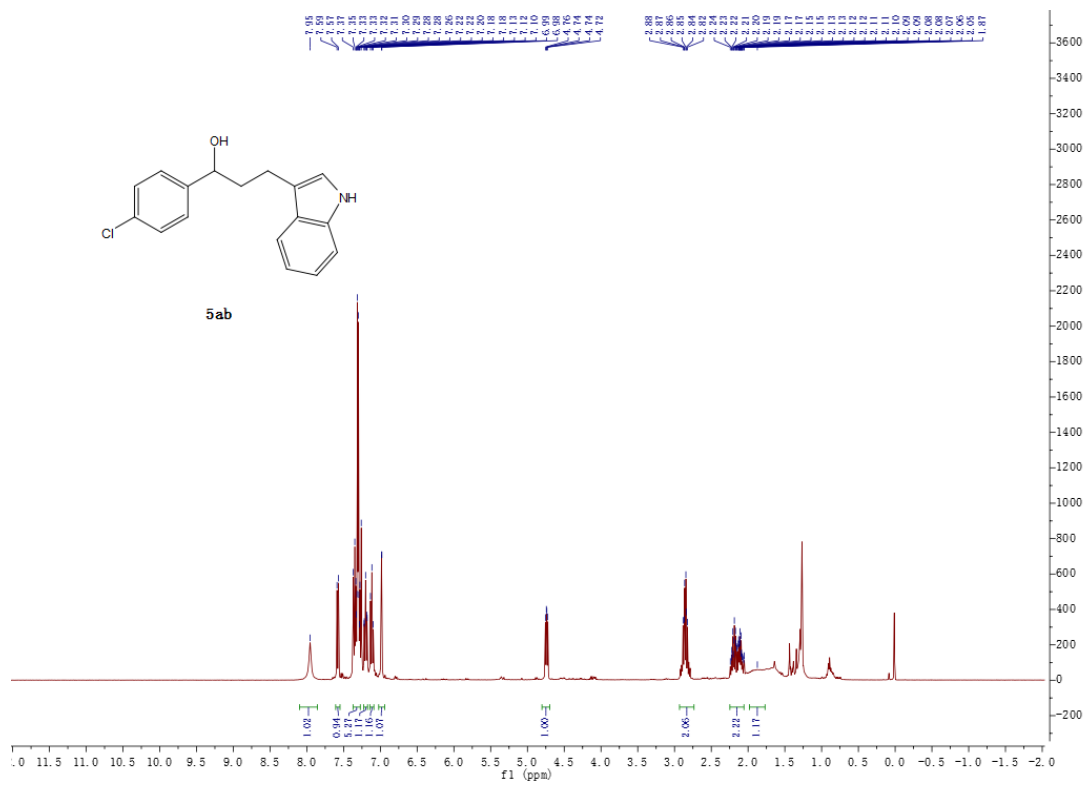
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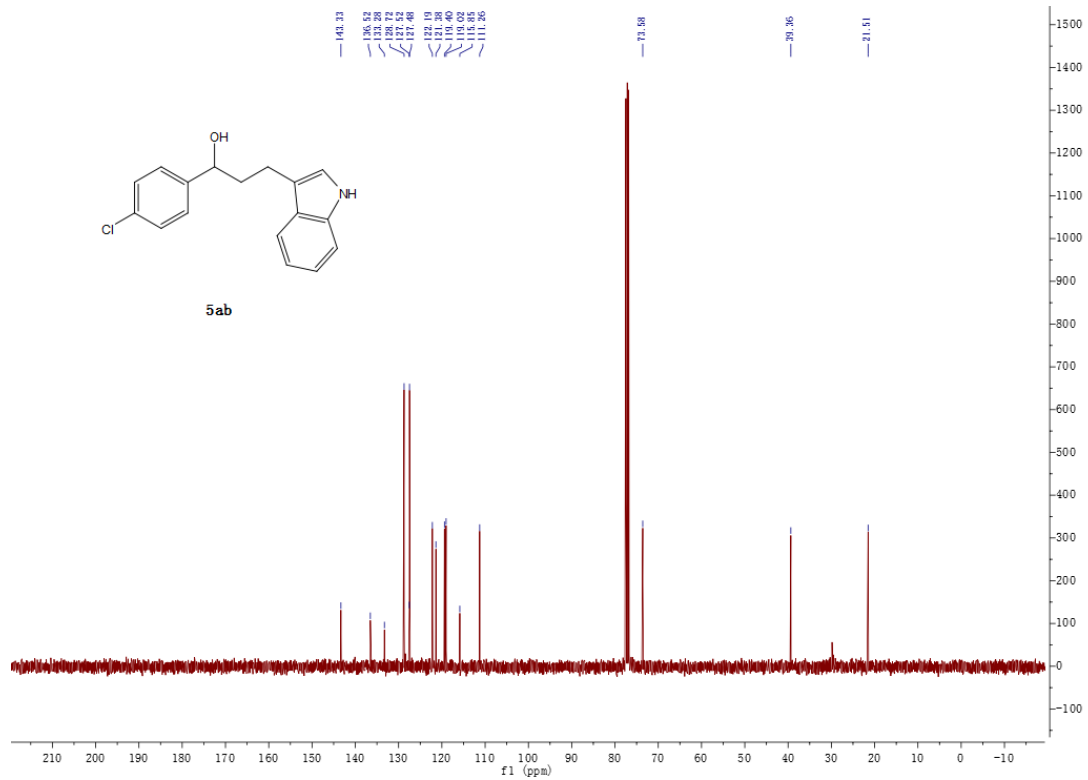




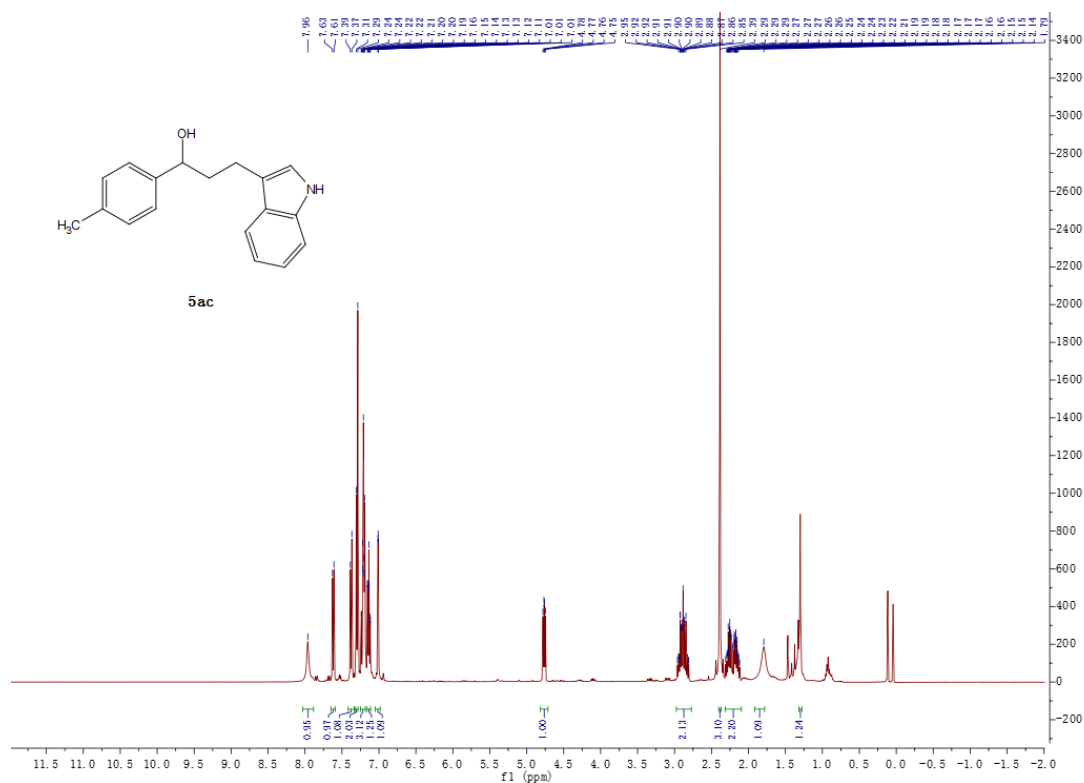
¹H NMR of 5ab



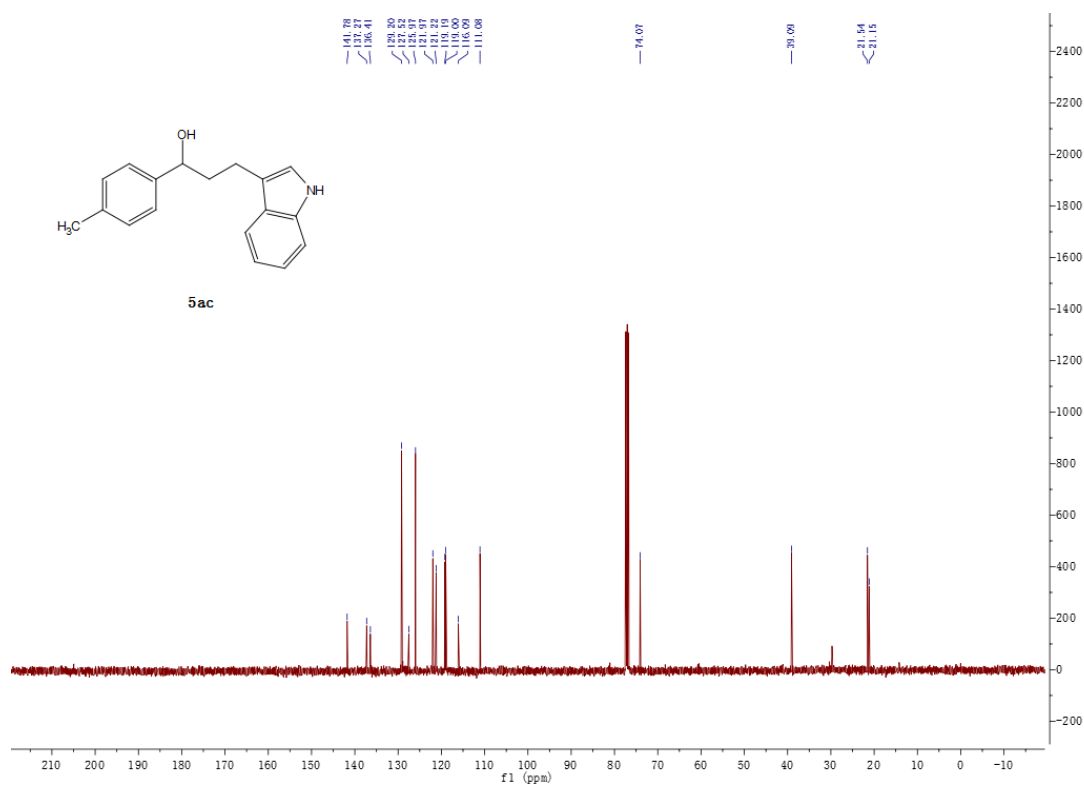
¹³C NMR of 5ab



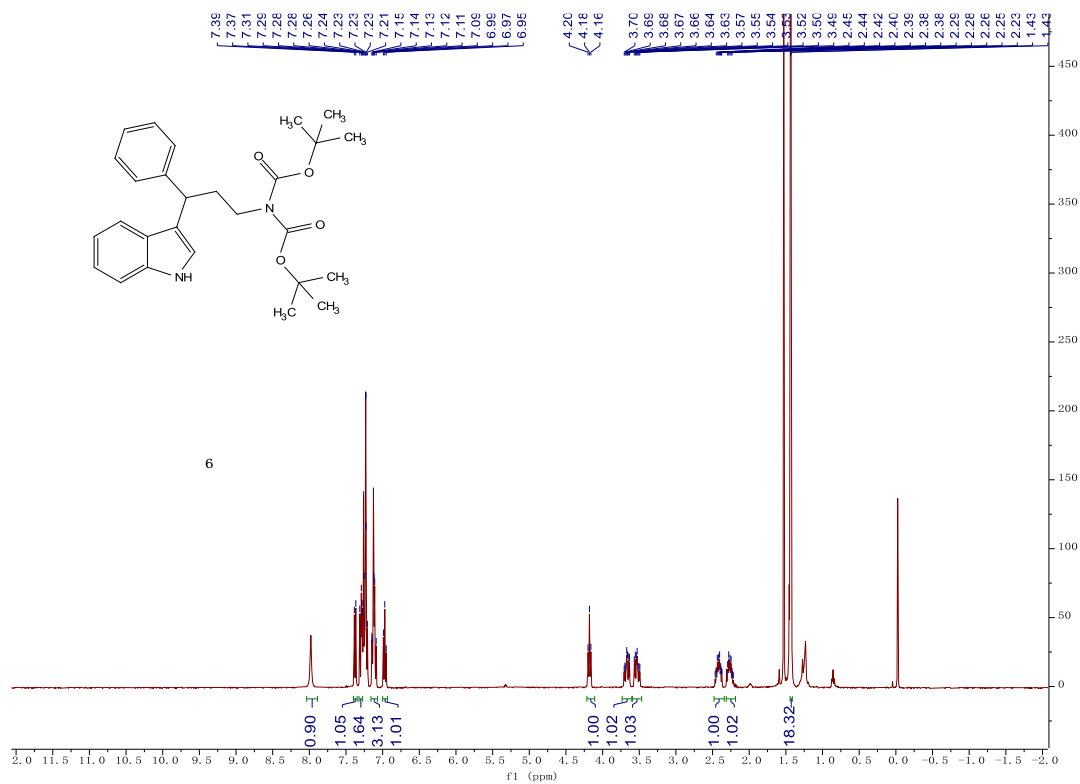
¹H NMR of 5ac



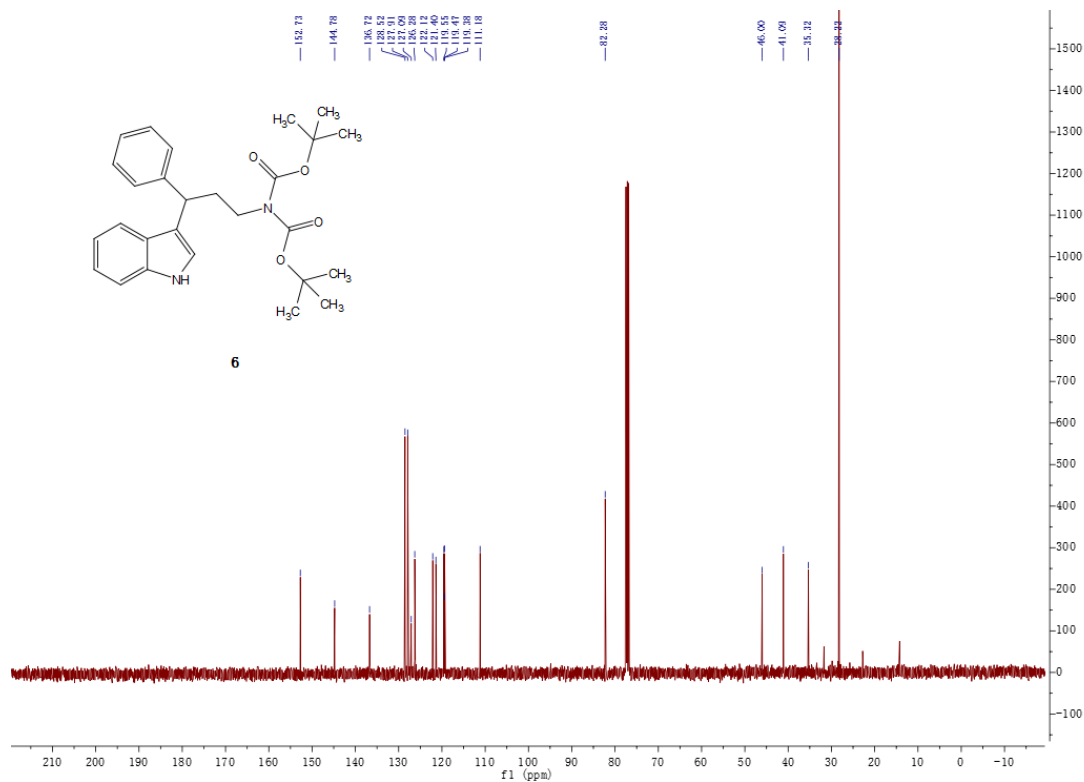
¹³C NMR of 5ac



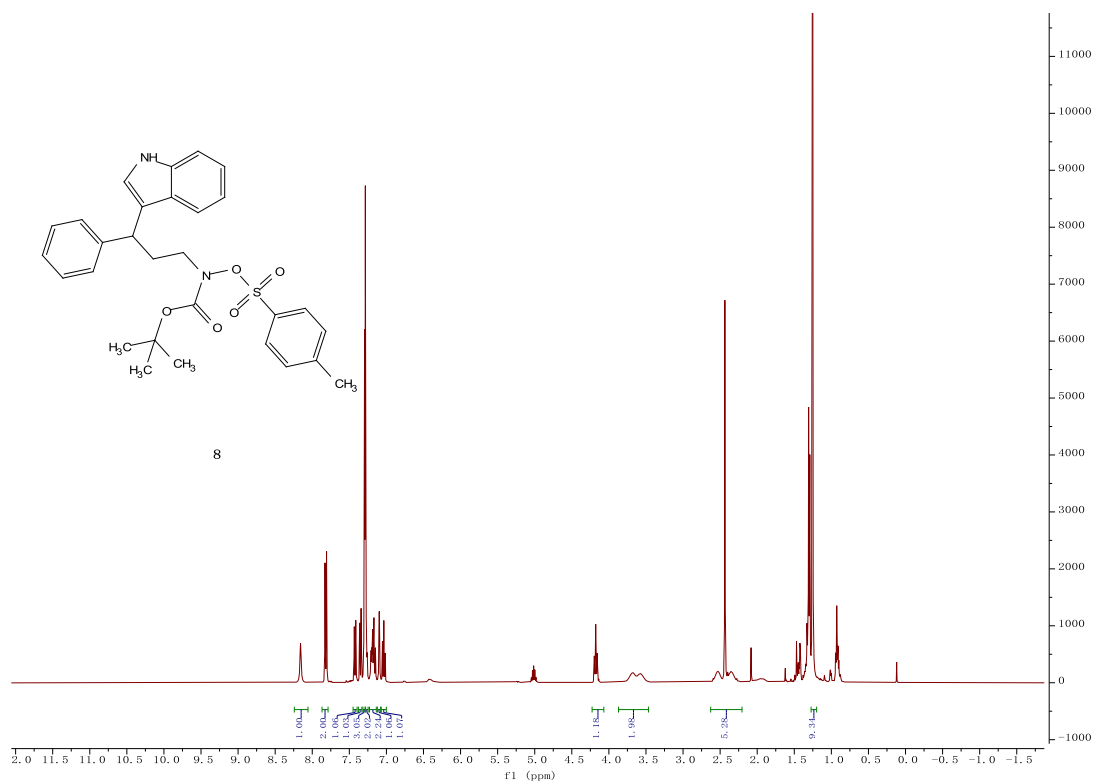
¹H NMR of 6



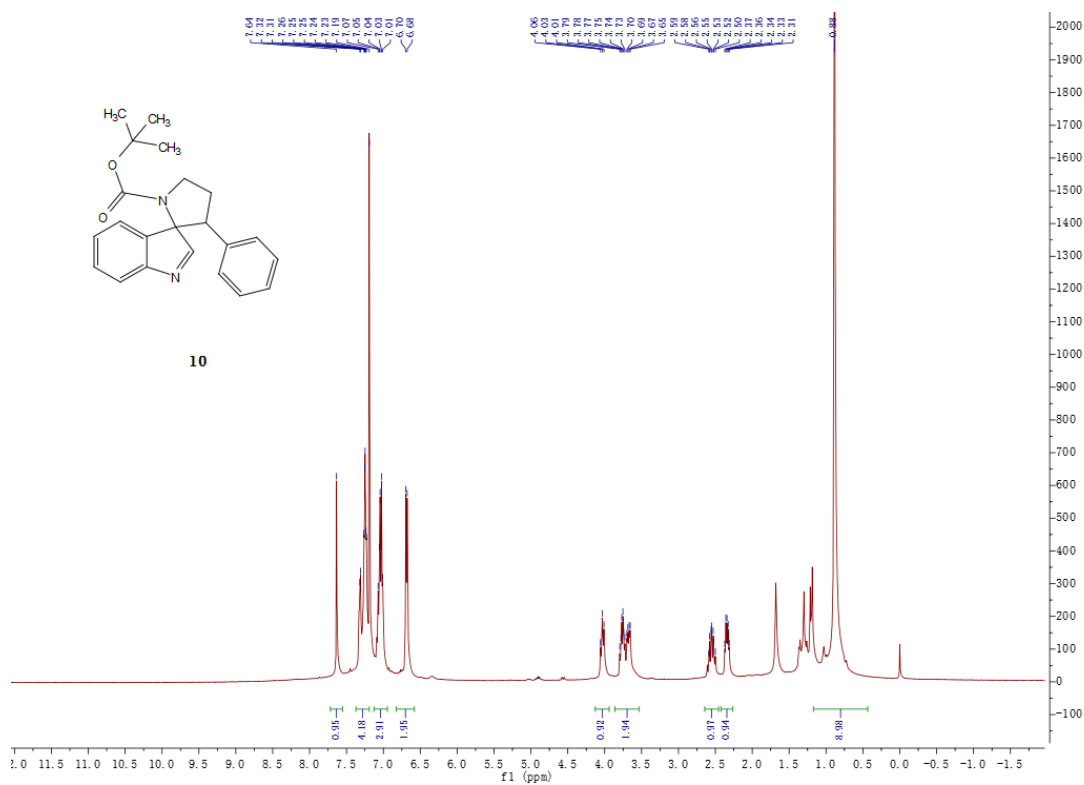
¹³C NMR of 6



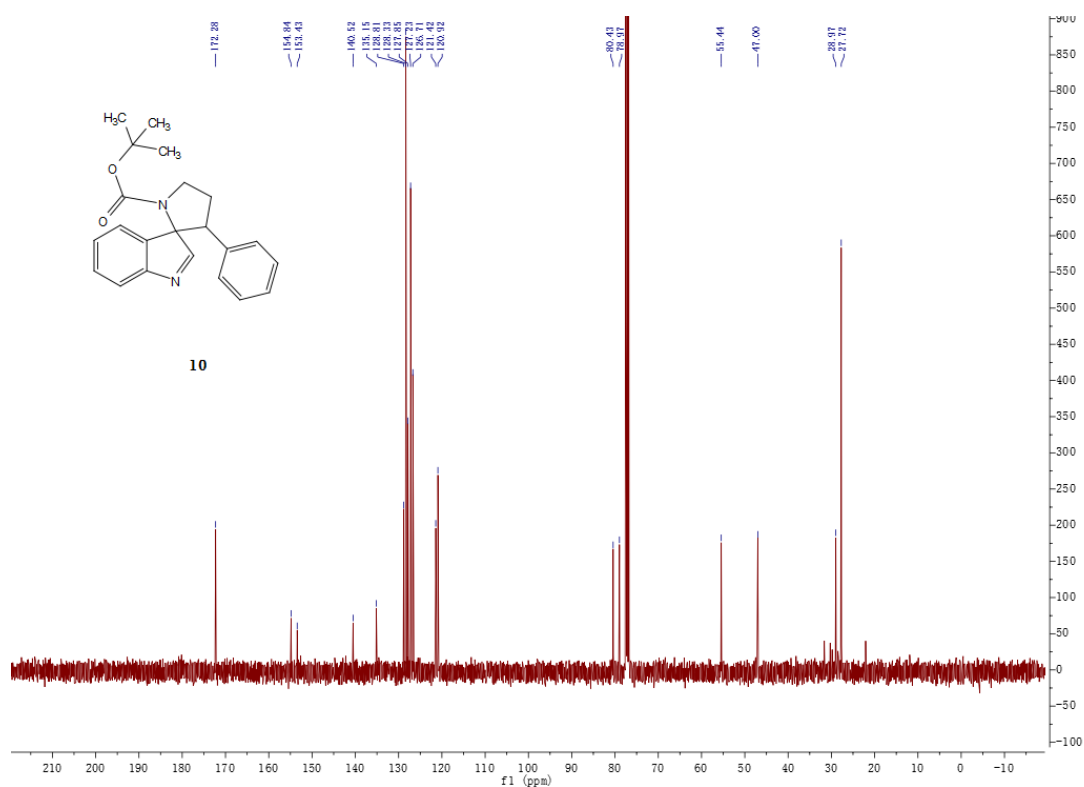
¹H NMR of 8



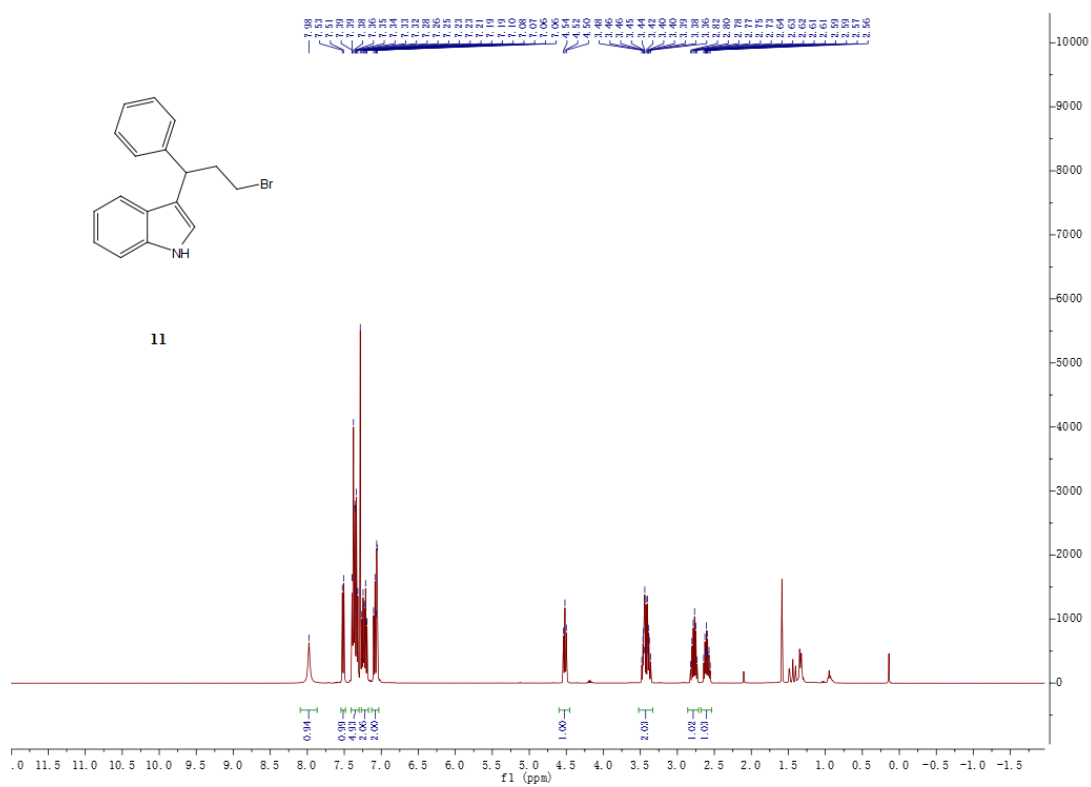
¹H NMR of 10



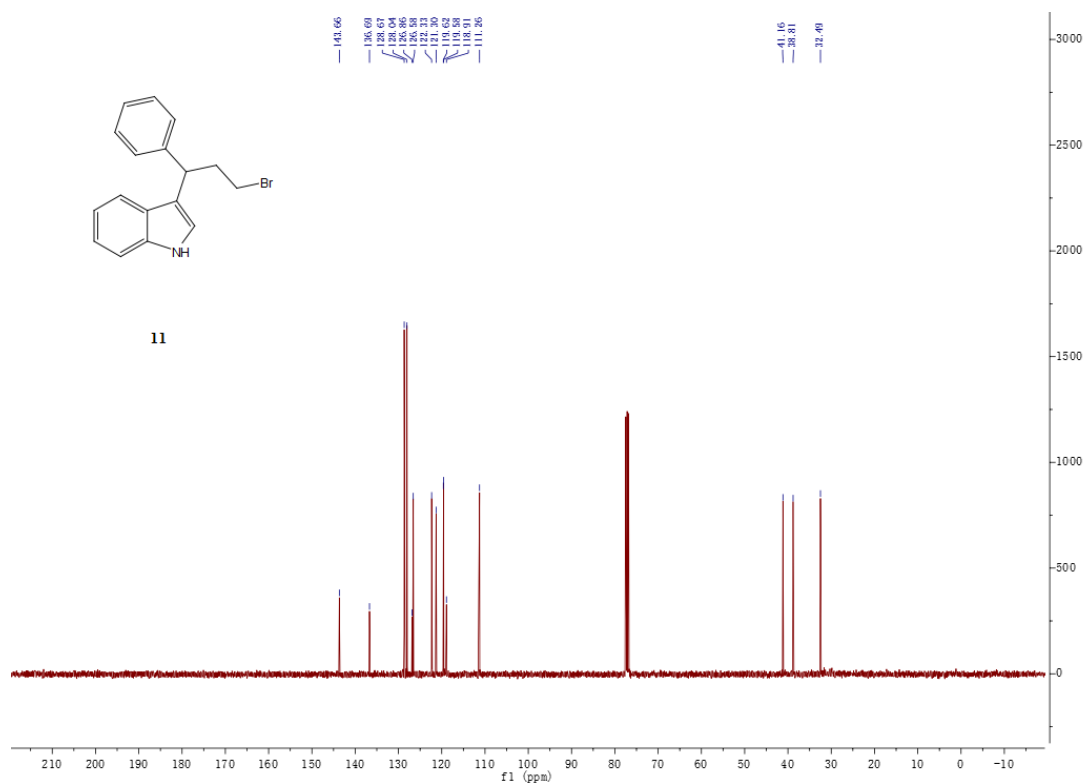
^{13}C NMR of 10



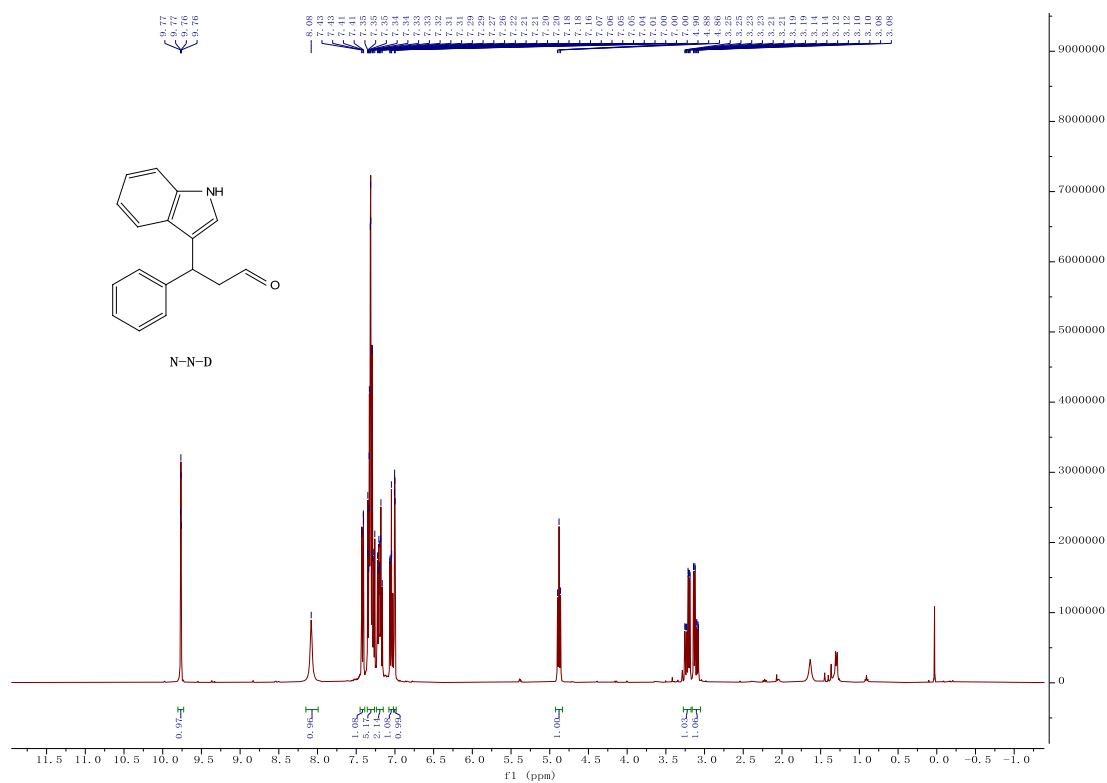
^1H NMR of 11



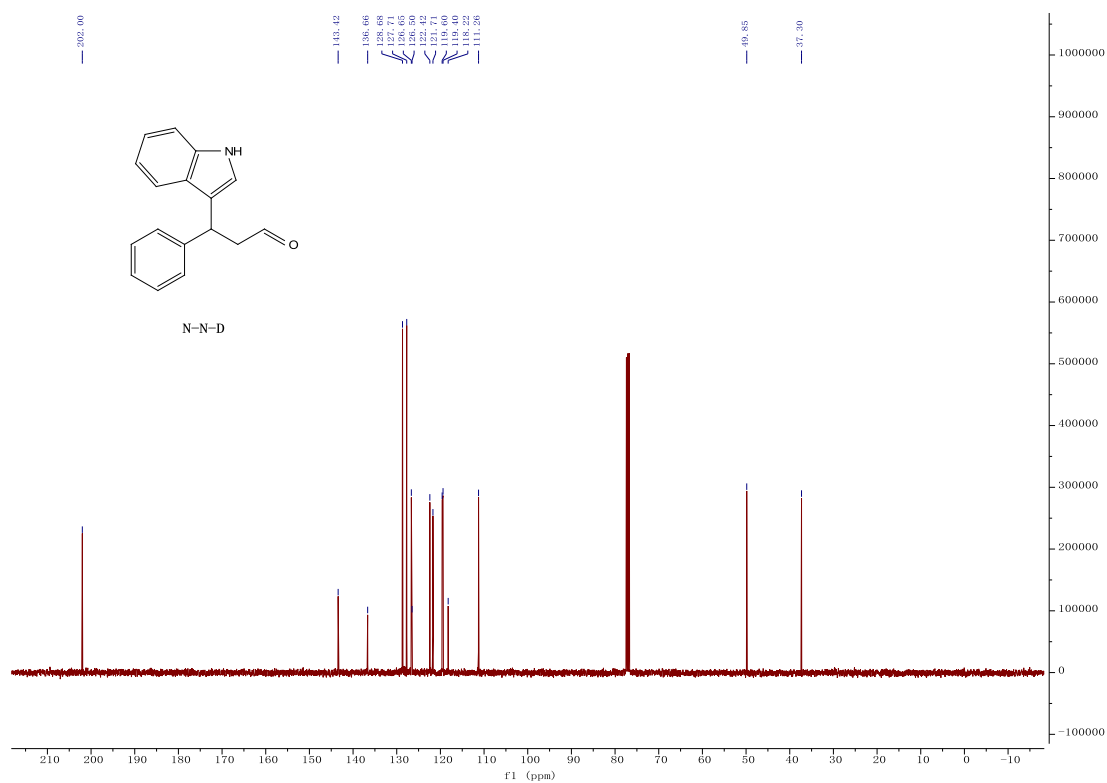
¹³C NMR of 11



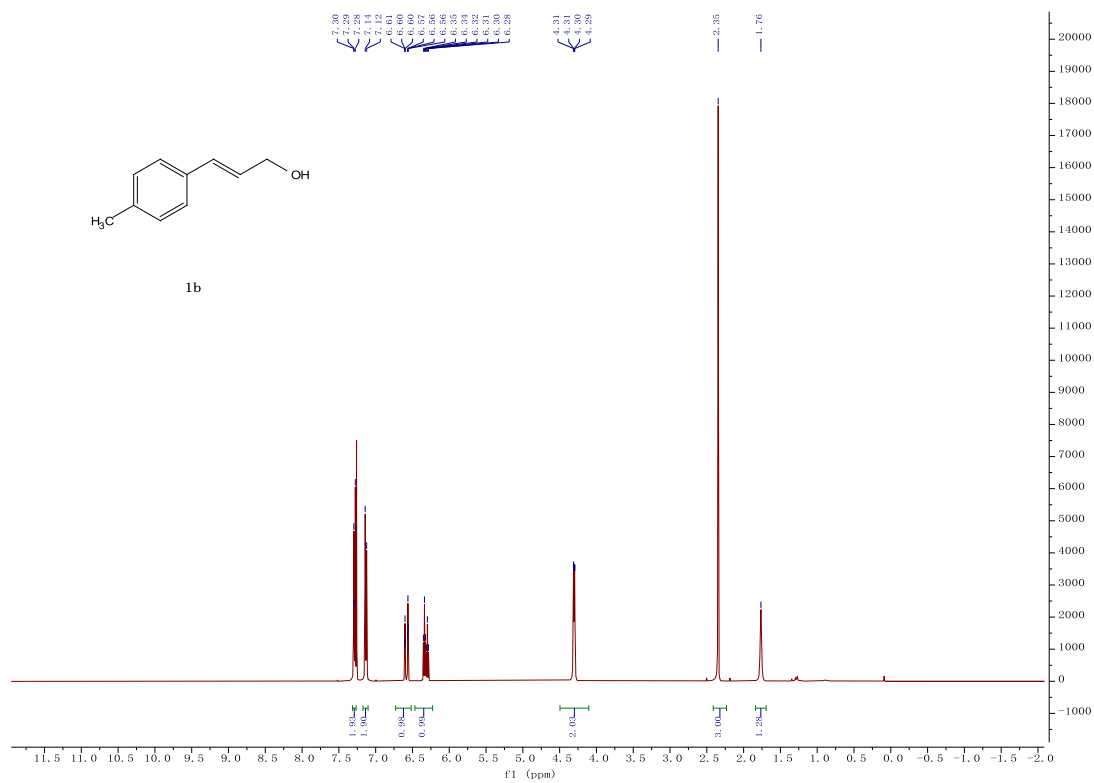
¹H NMR of N-N-D



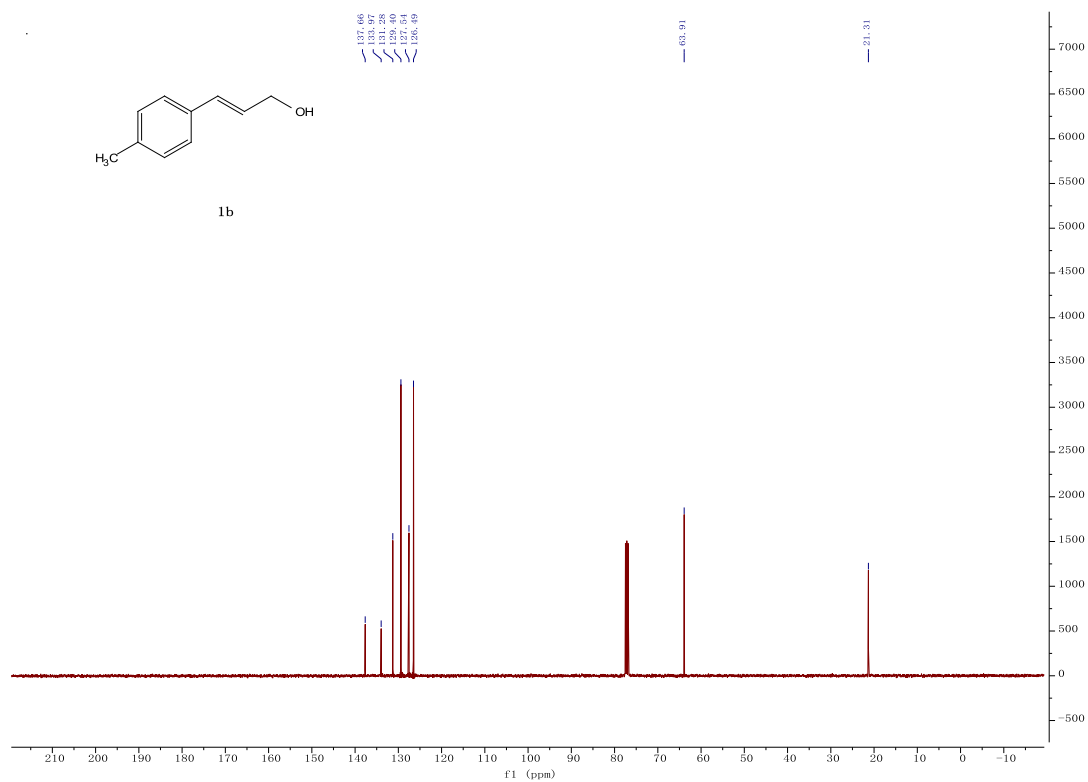
¹³C NMR of N-N-D



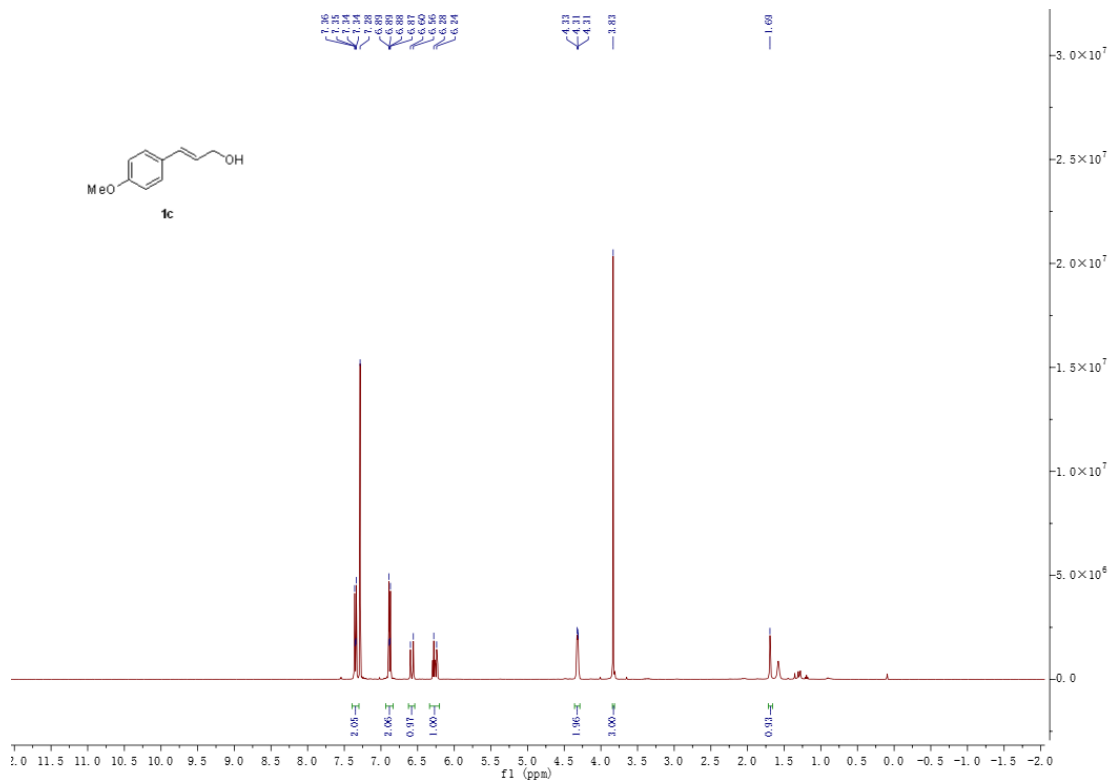
¹H NMR of 1b



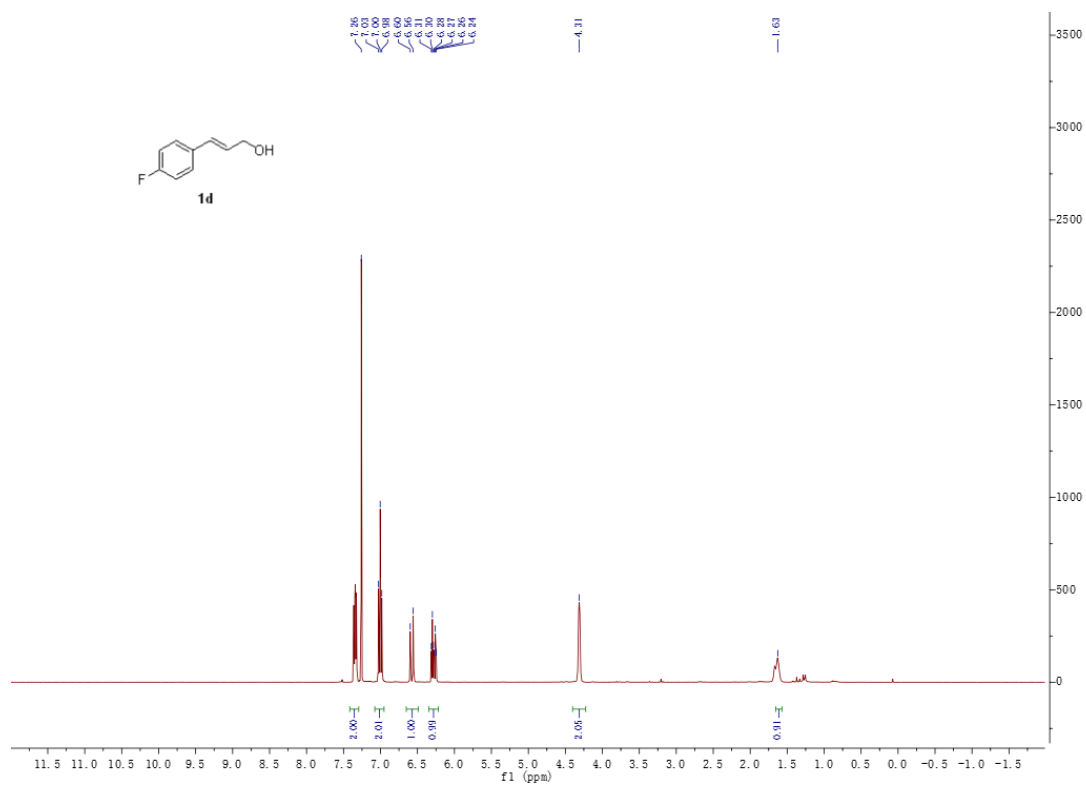
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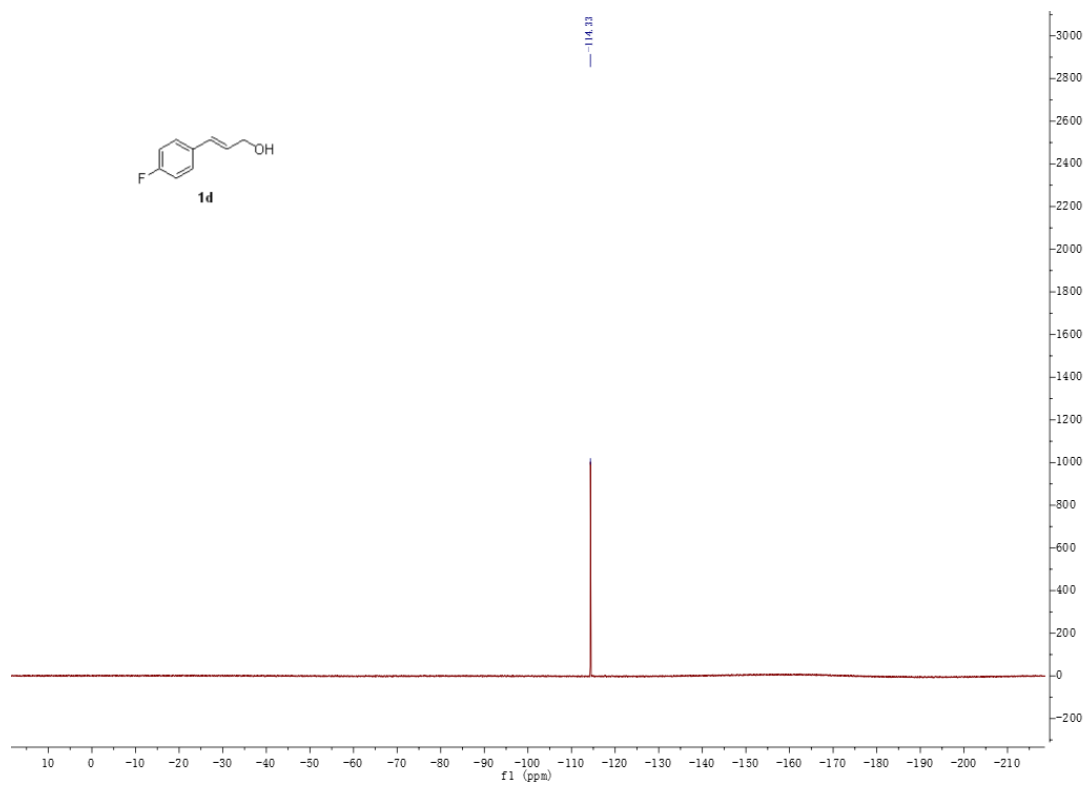
¹H NMR of 1c



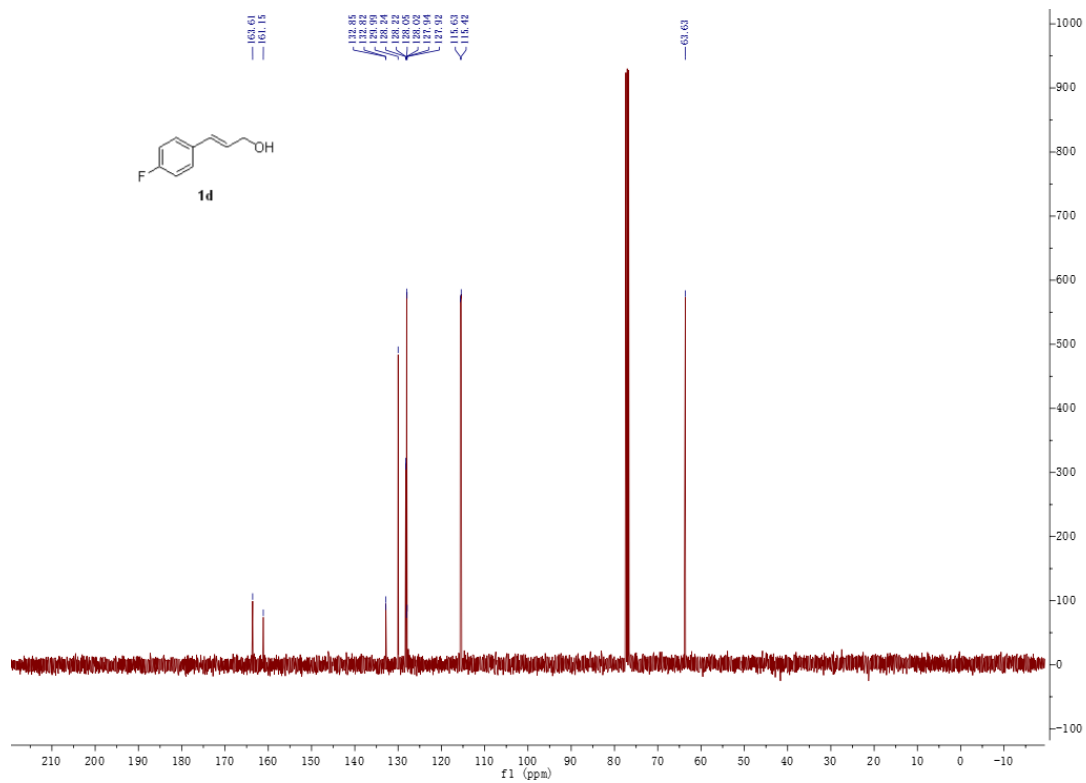
¹H NMR of **1d**



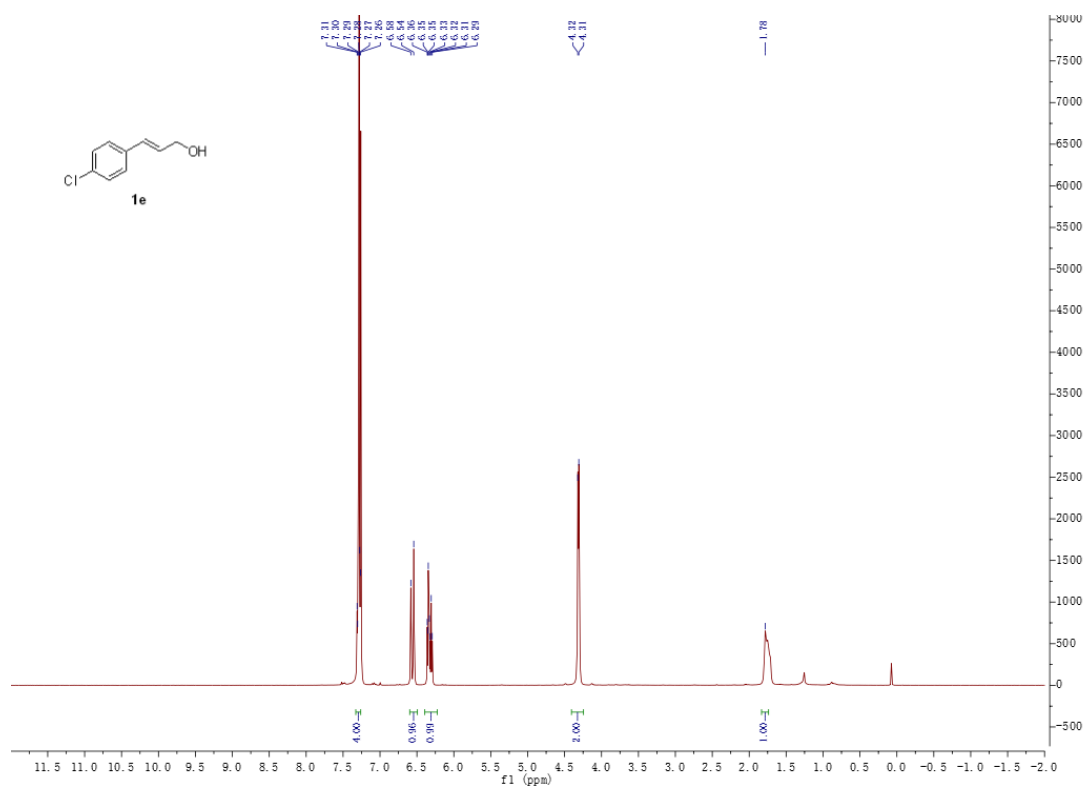
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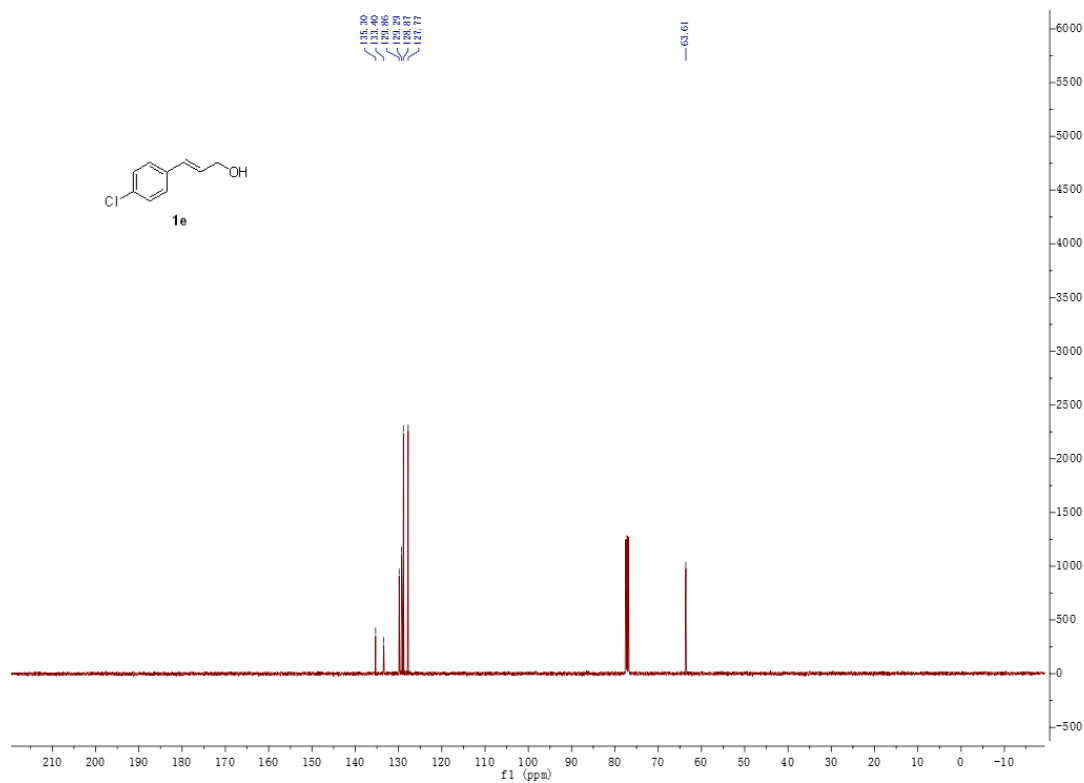
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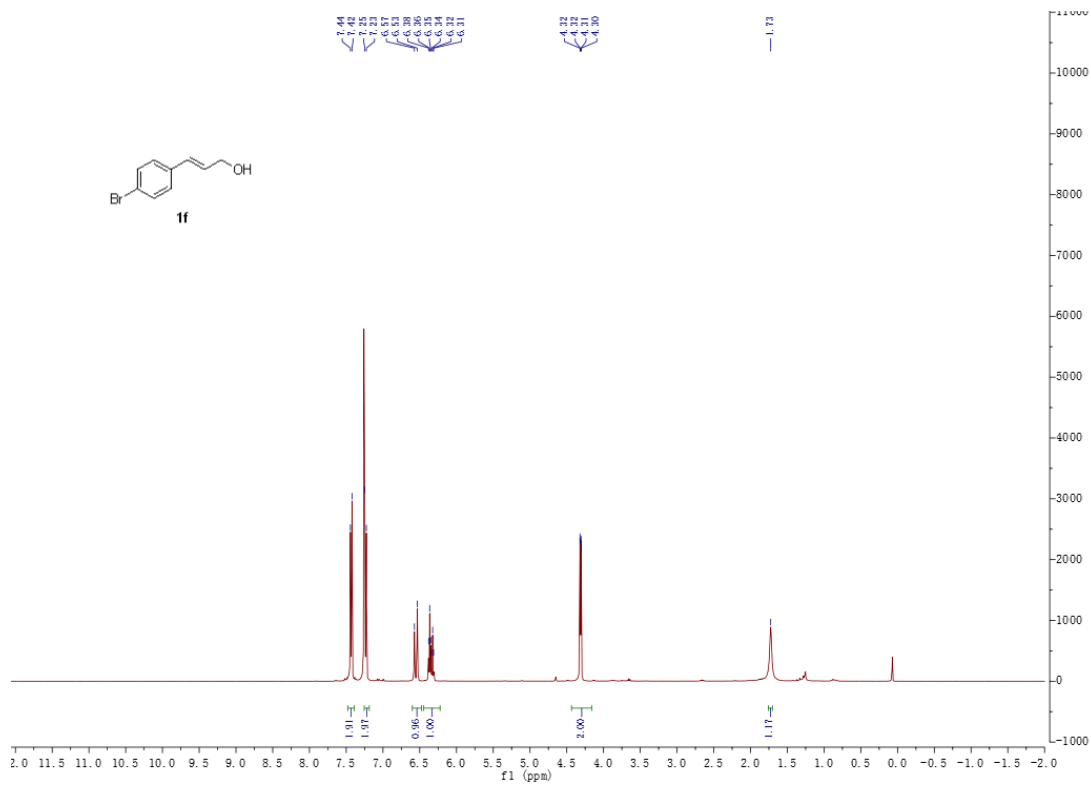
^1H NMR of **1e**



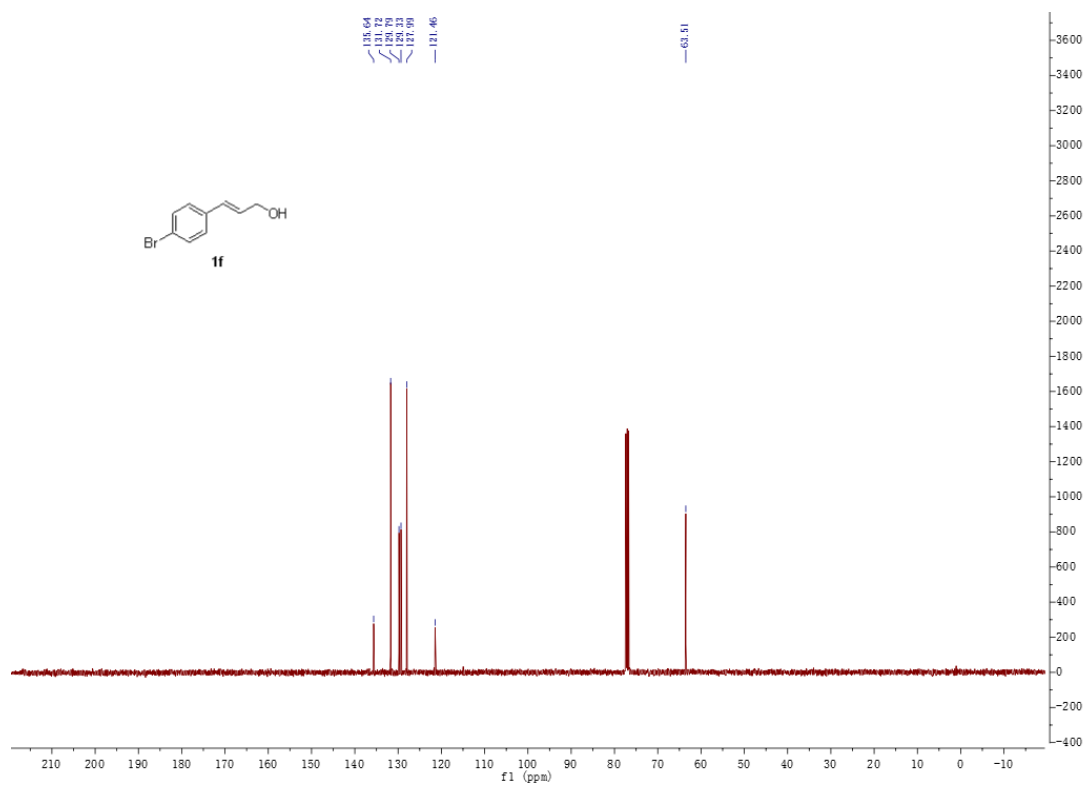
¹³C NMR of 1e



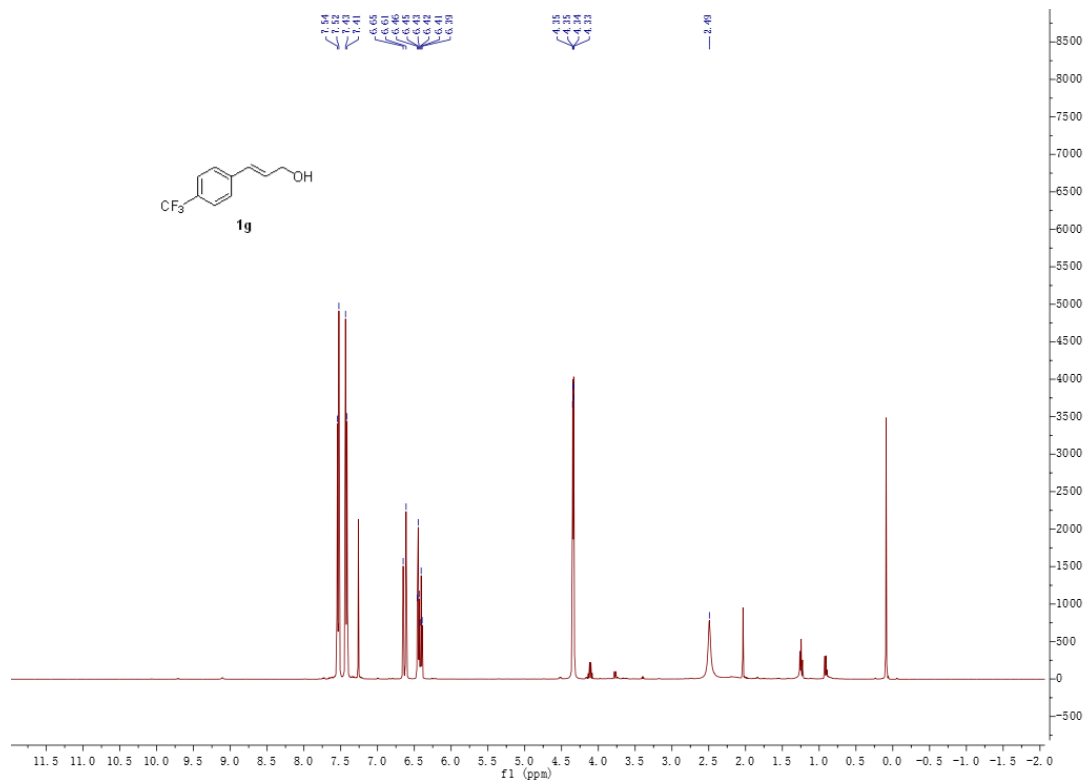
¹H NMR of 1f



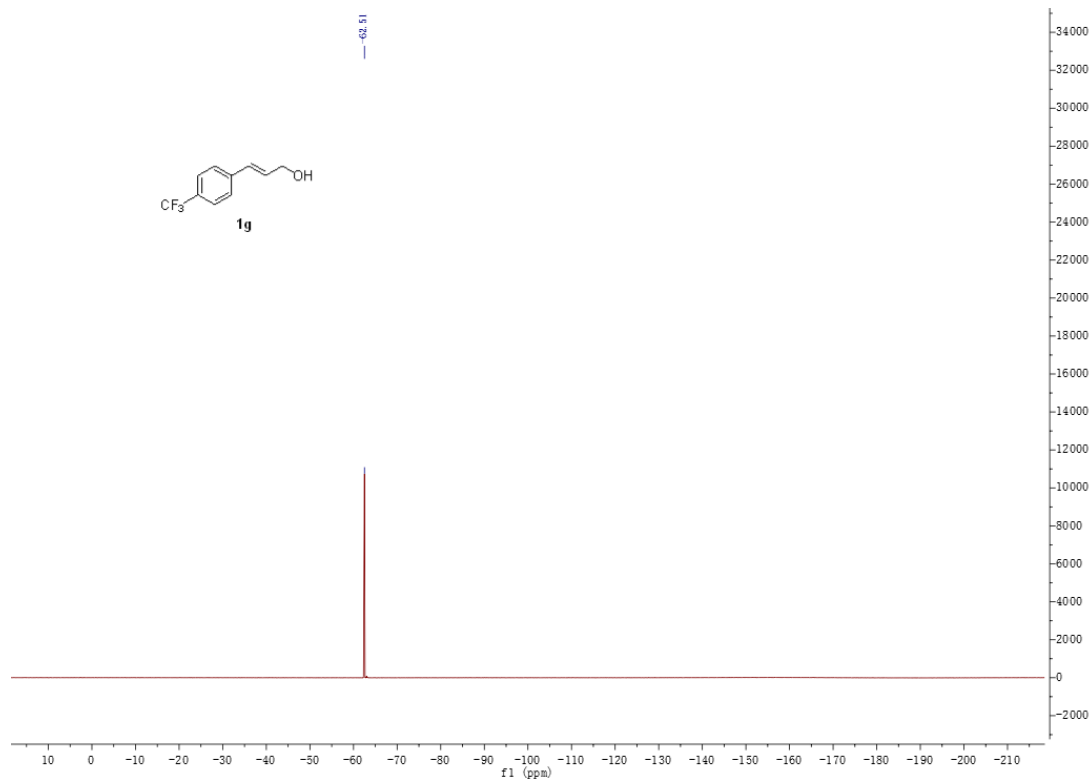
^{13}C NMR of **1f**



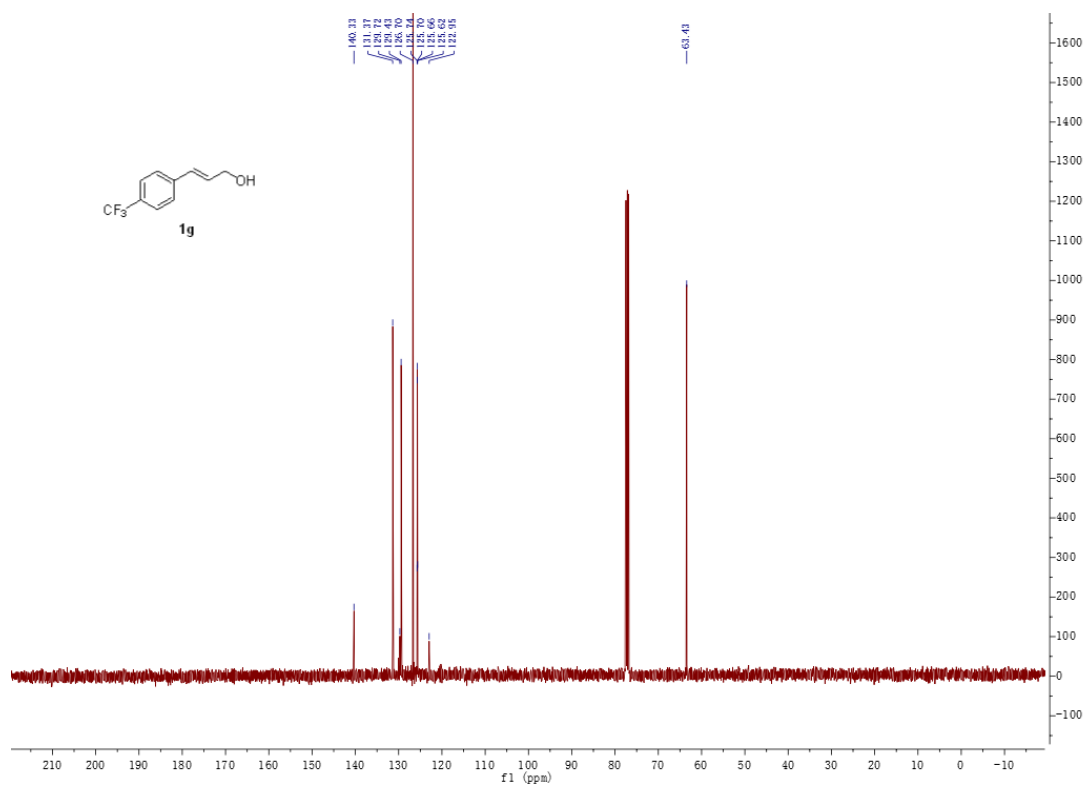
^1H NMR of **1g**



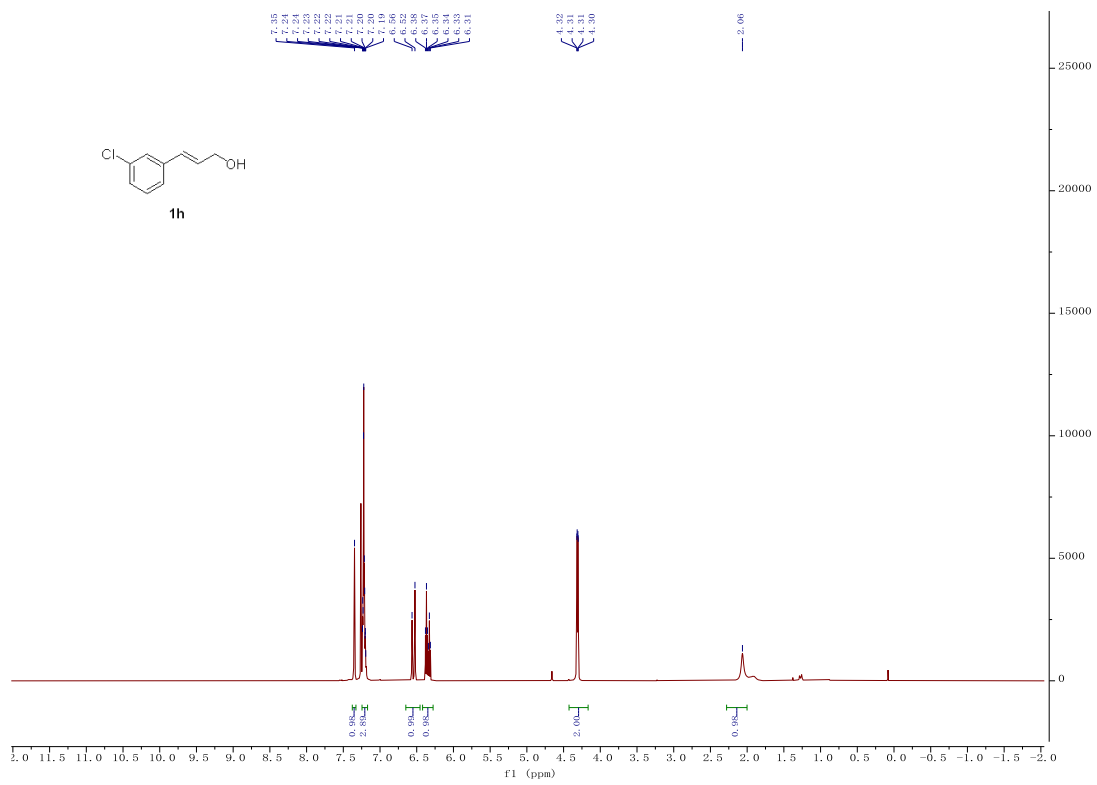
¹⁹F NMR of **1g**



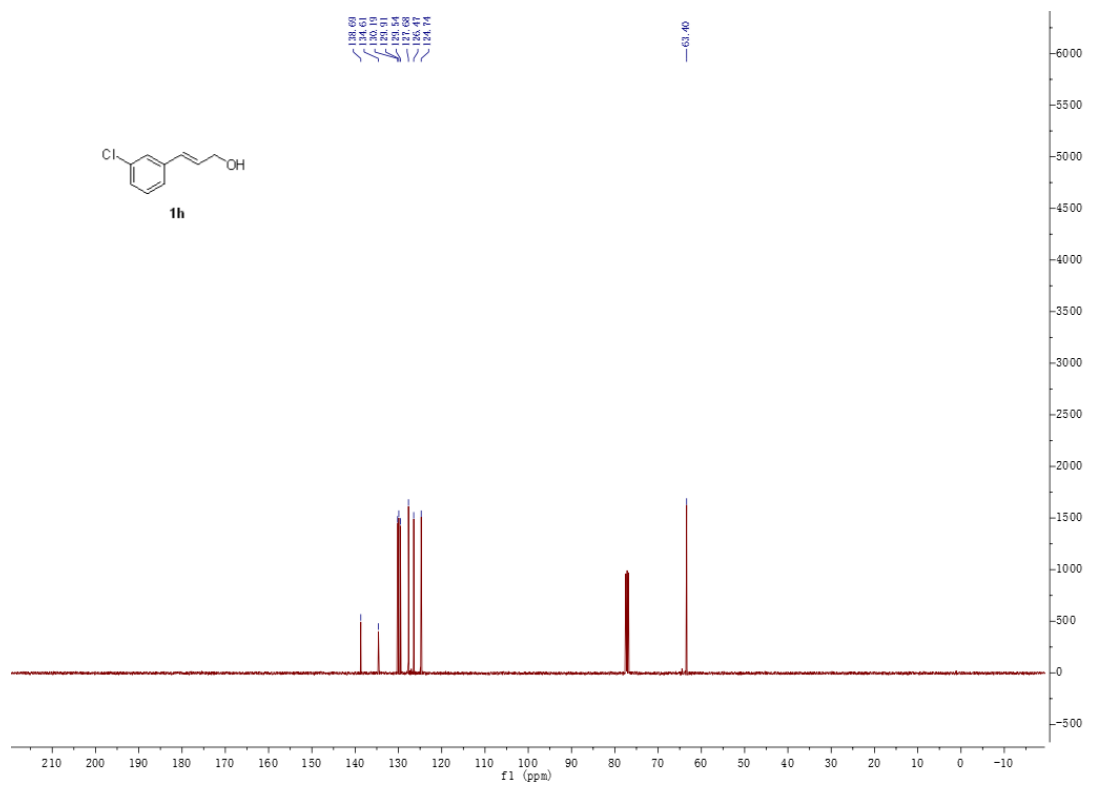
¹³C NMR of **1g**



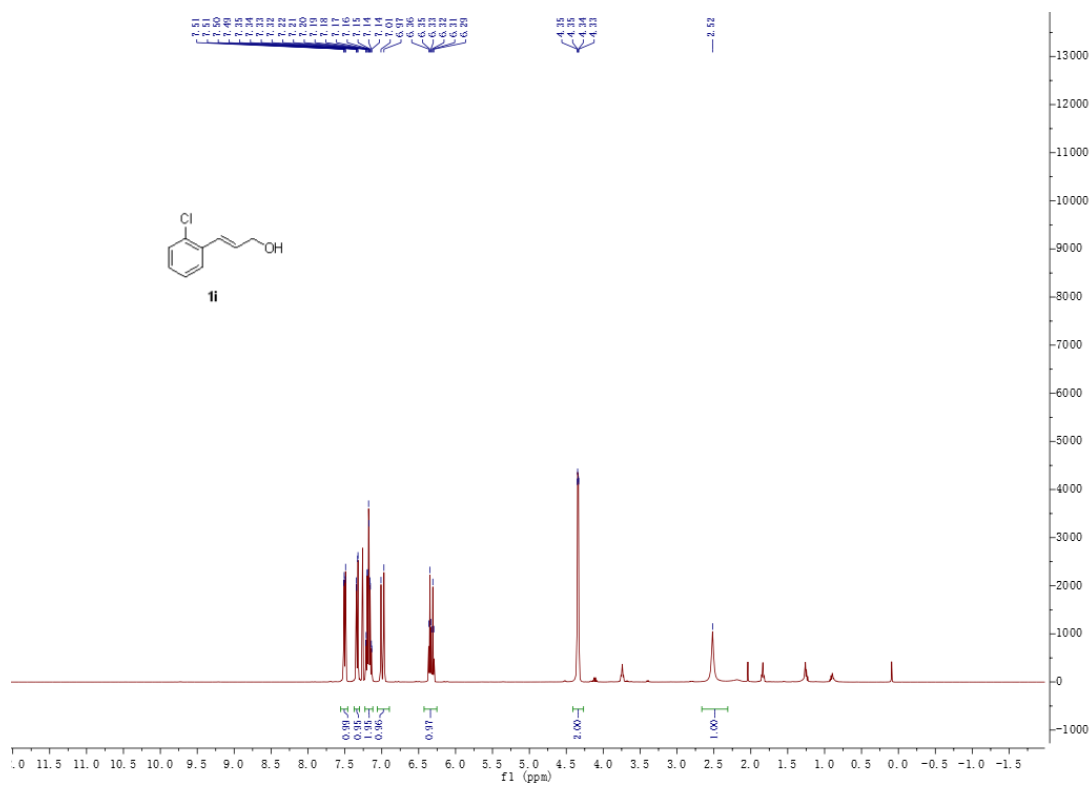
¹H NMR of **1h**



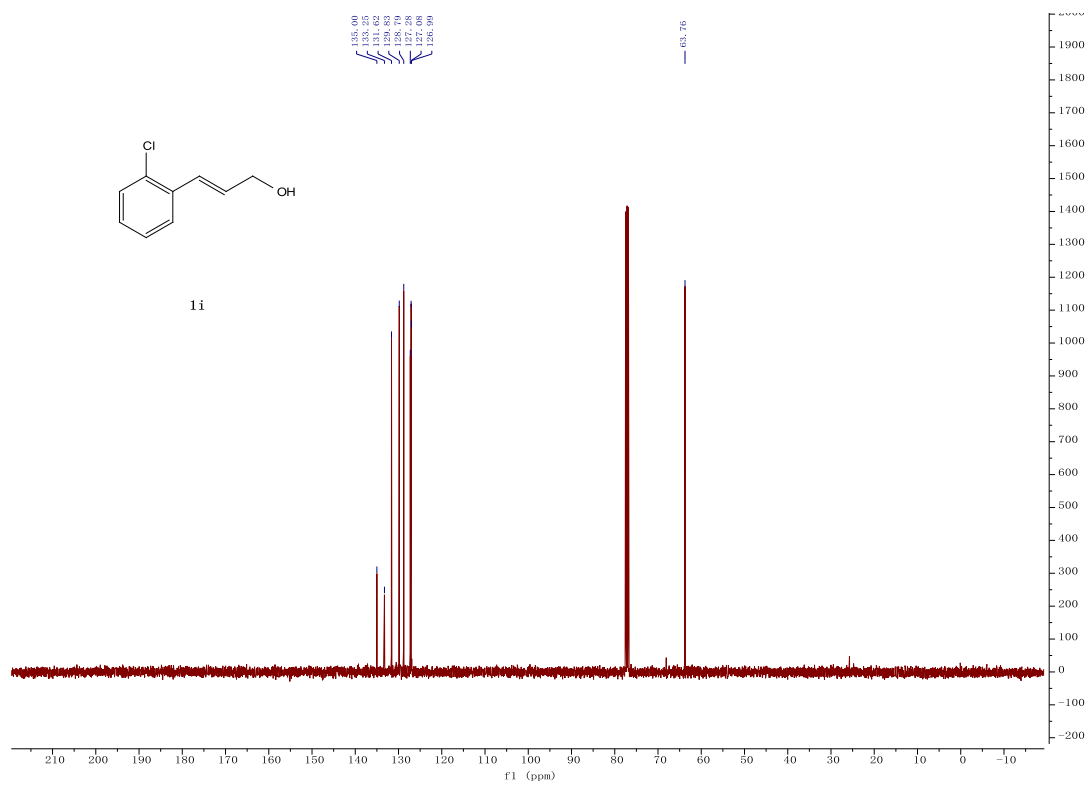
¹³C NMR of **1h**



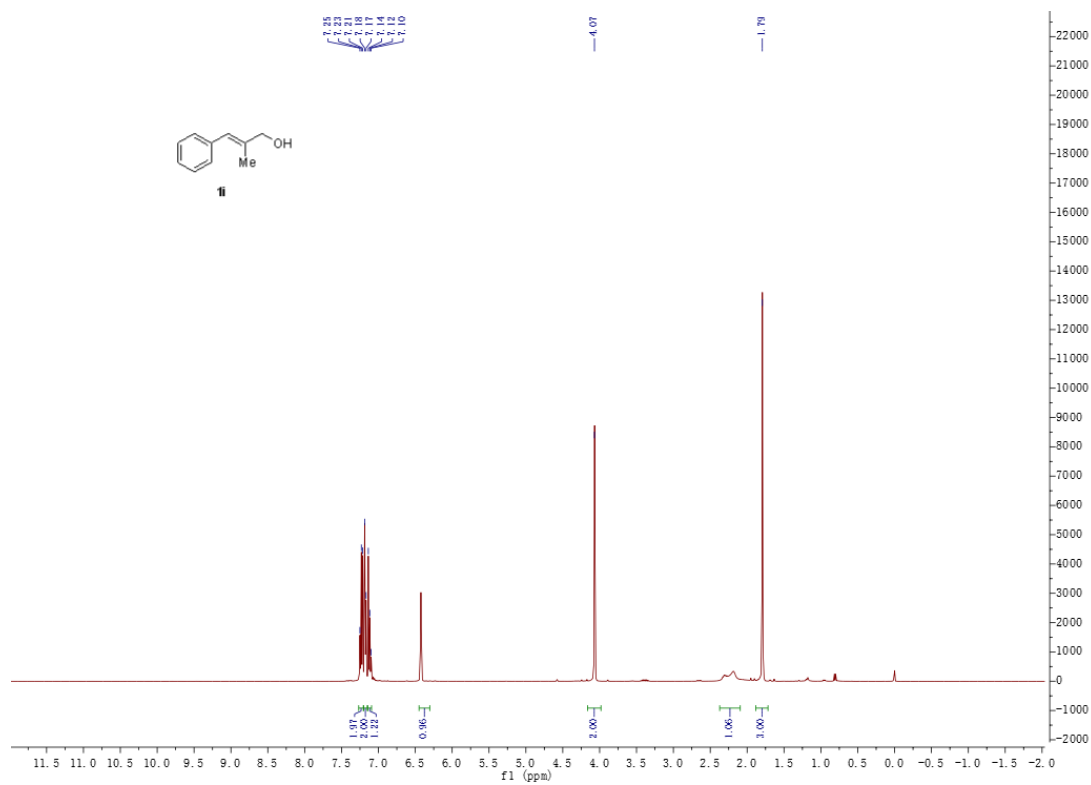
^1H NMR of **1i**



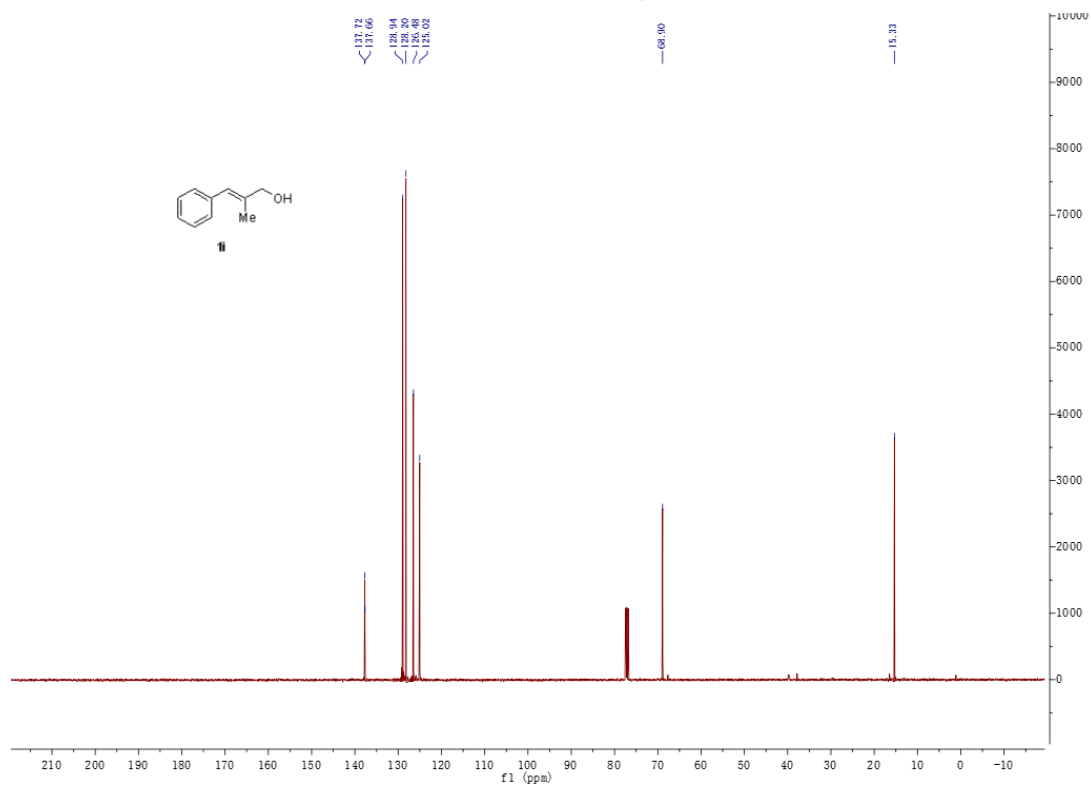
^{13}C NMR of **1i**



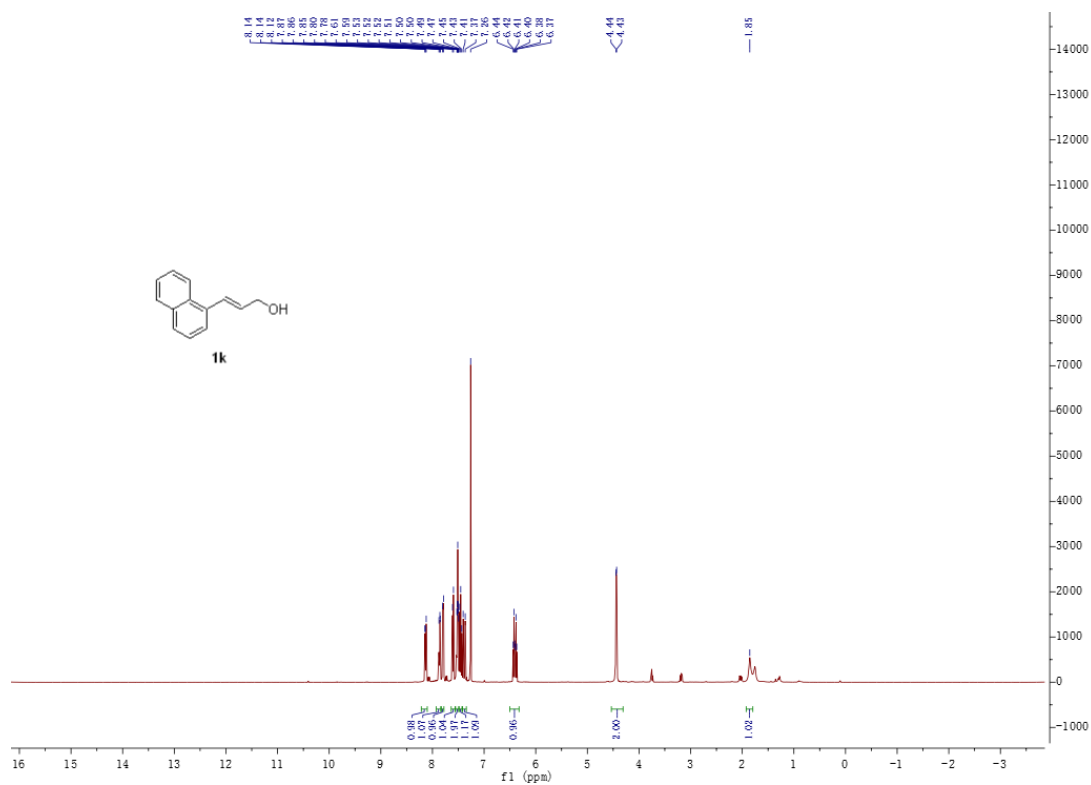
¹H NMR of 1j



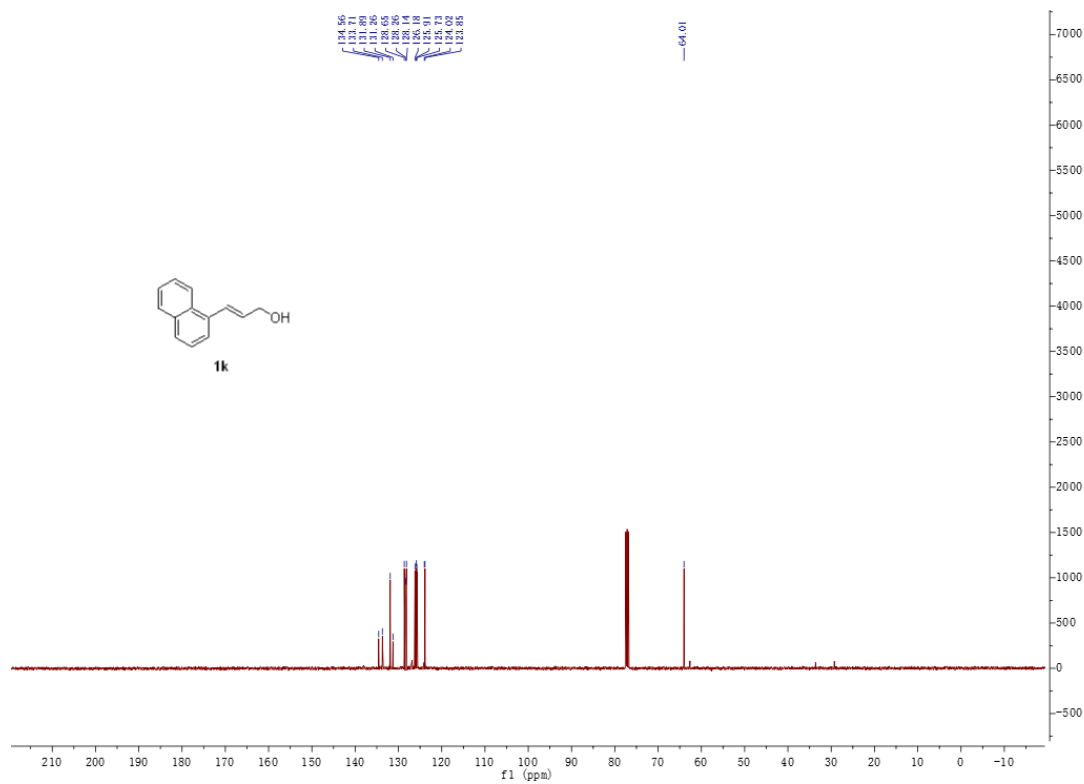
¹³C NMR of 1j



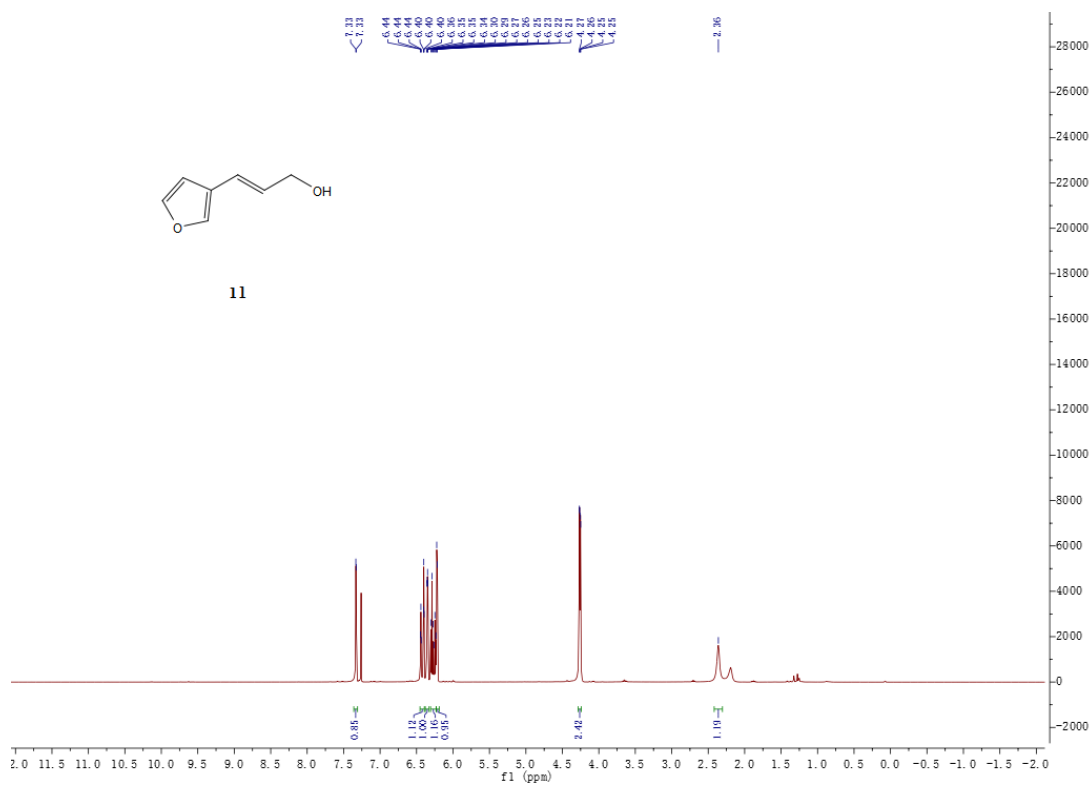
¹H NMR of **1k**



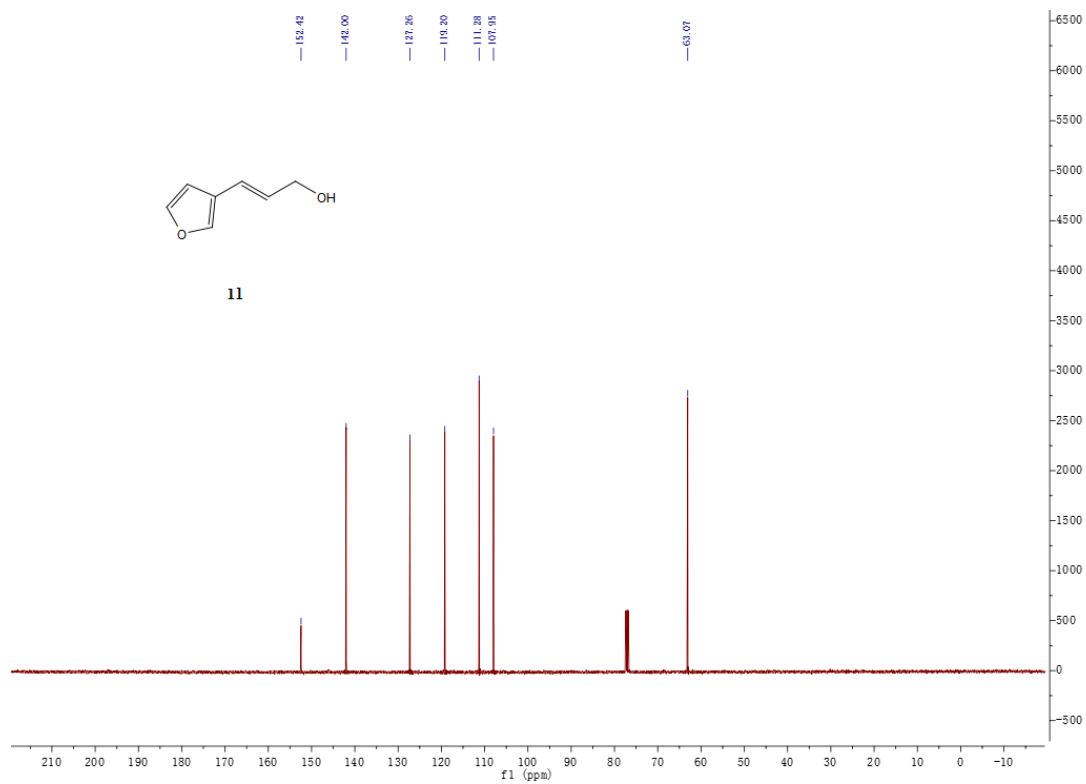
¹³C NMR of **1k**



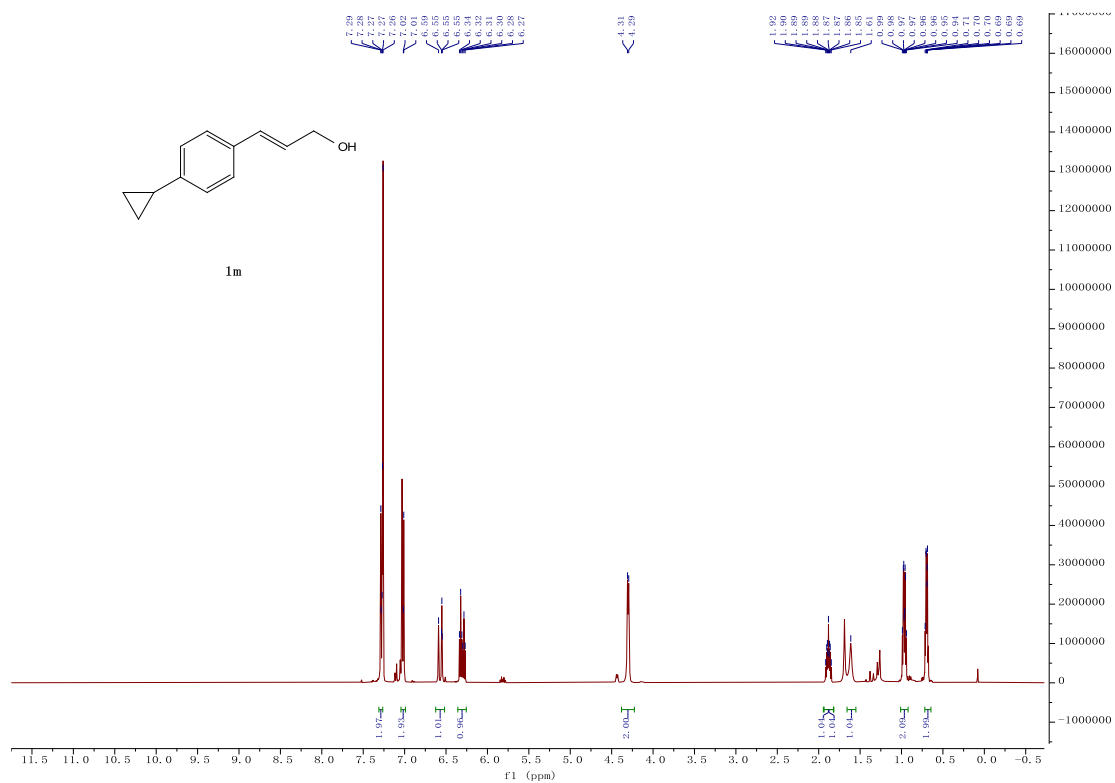
¹H NMR of **11**



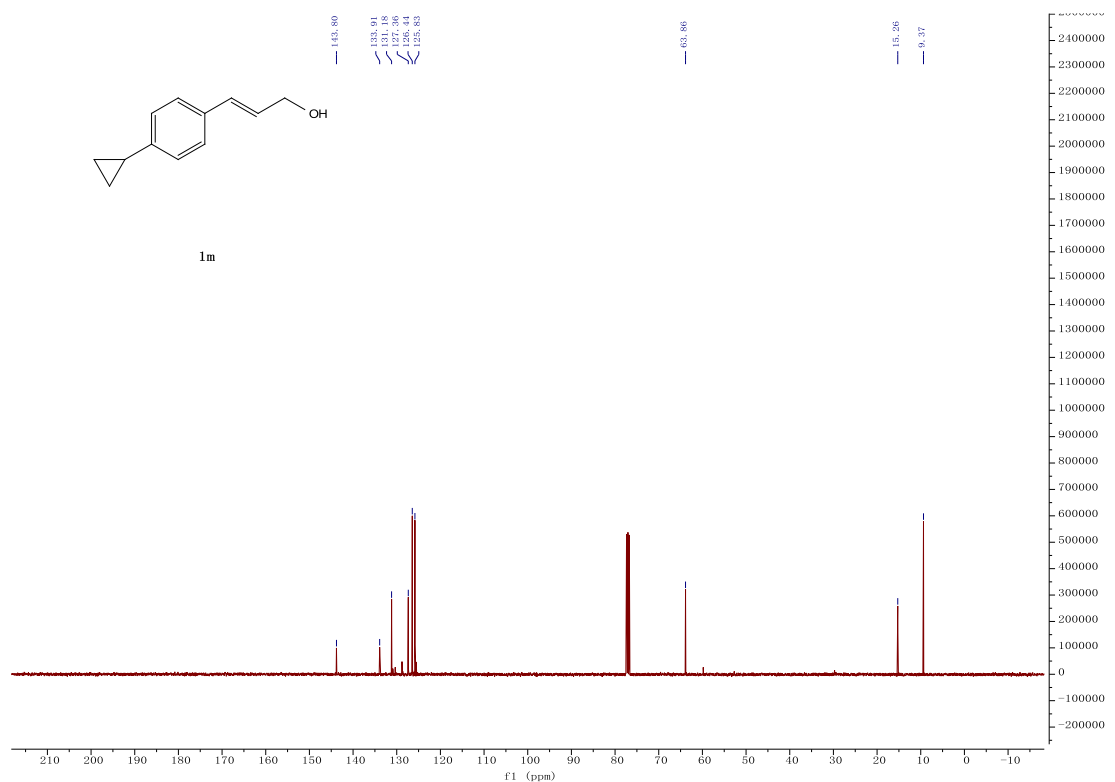
¹³C NMR of **11**



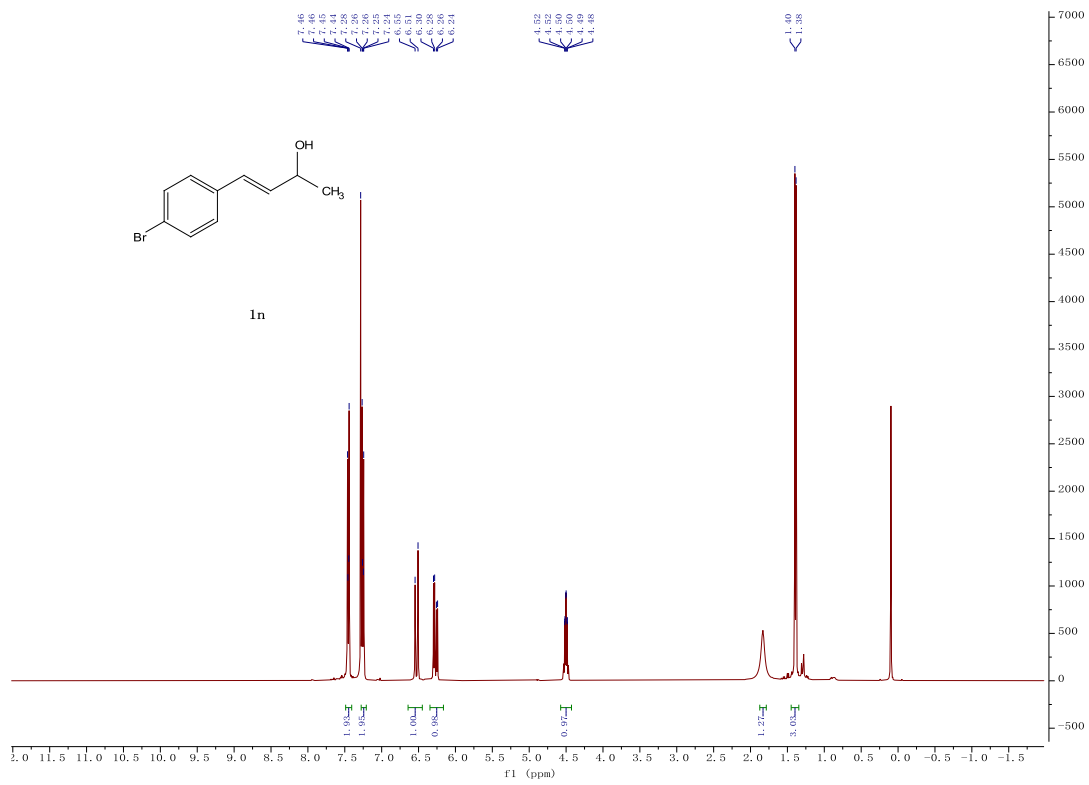
¹H NMR of 1m



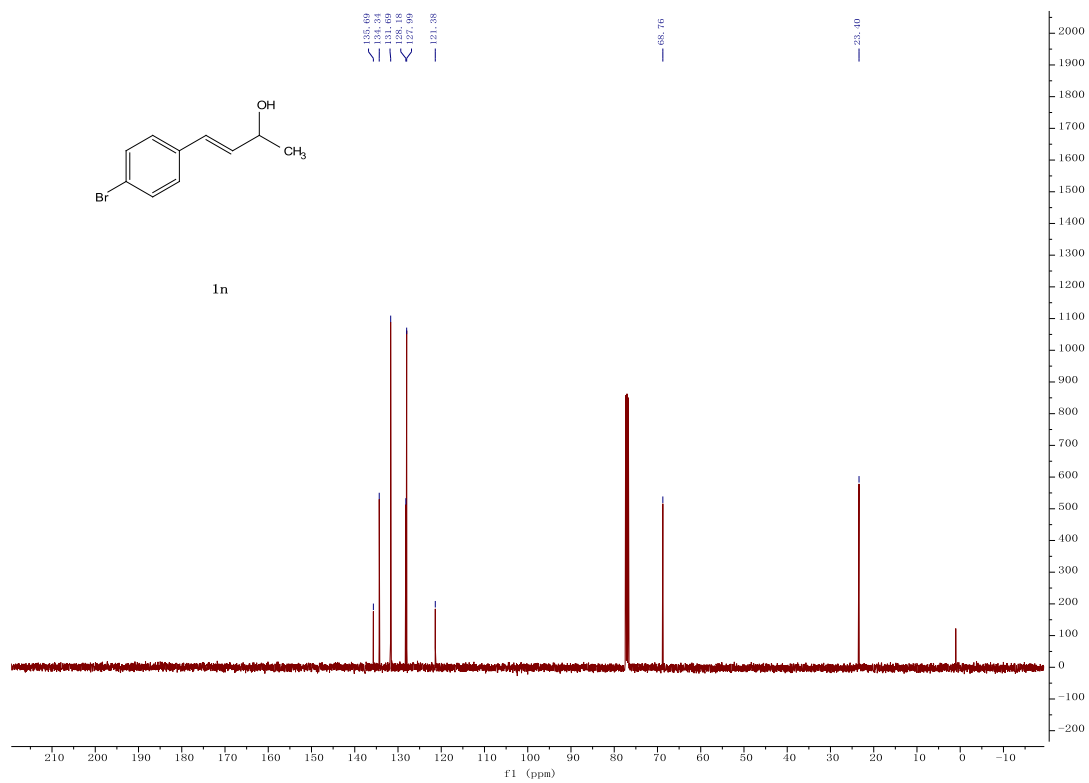
¹³C NMR of 1m



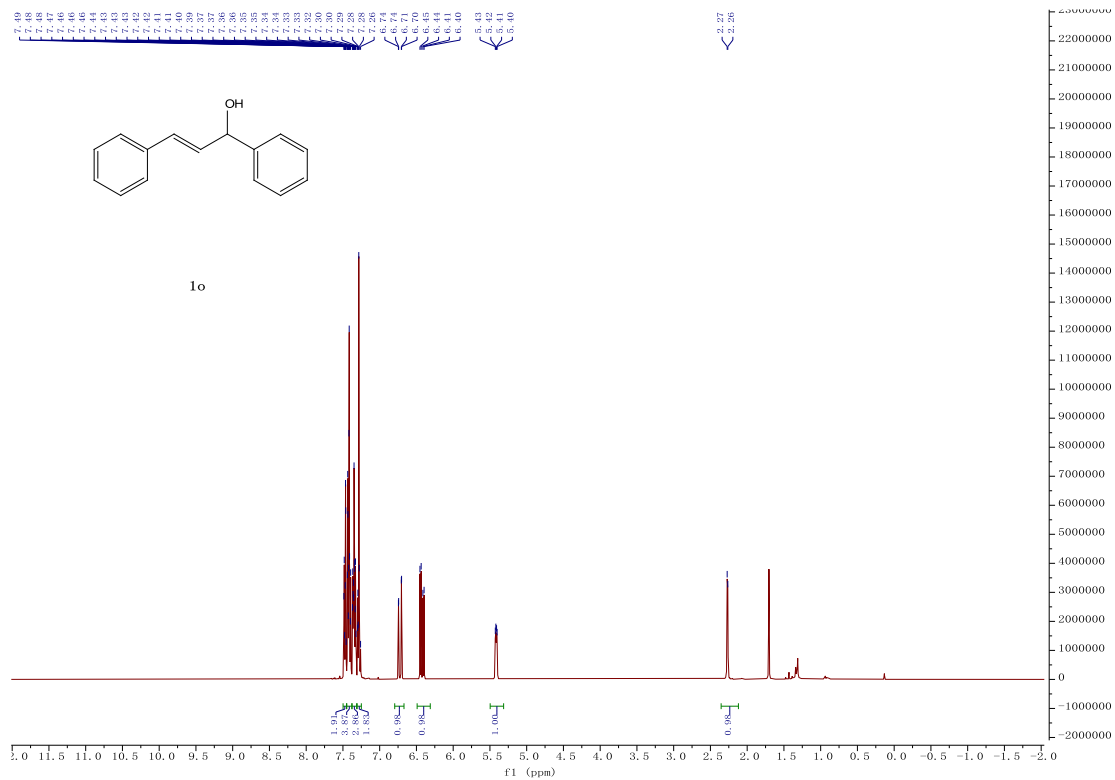
¹H NMR of **1n**



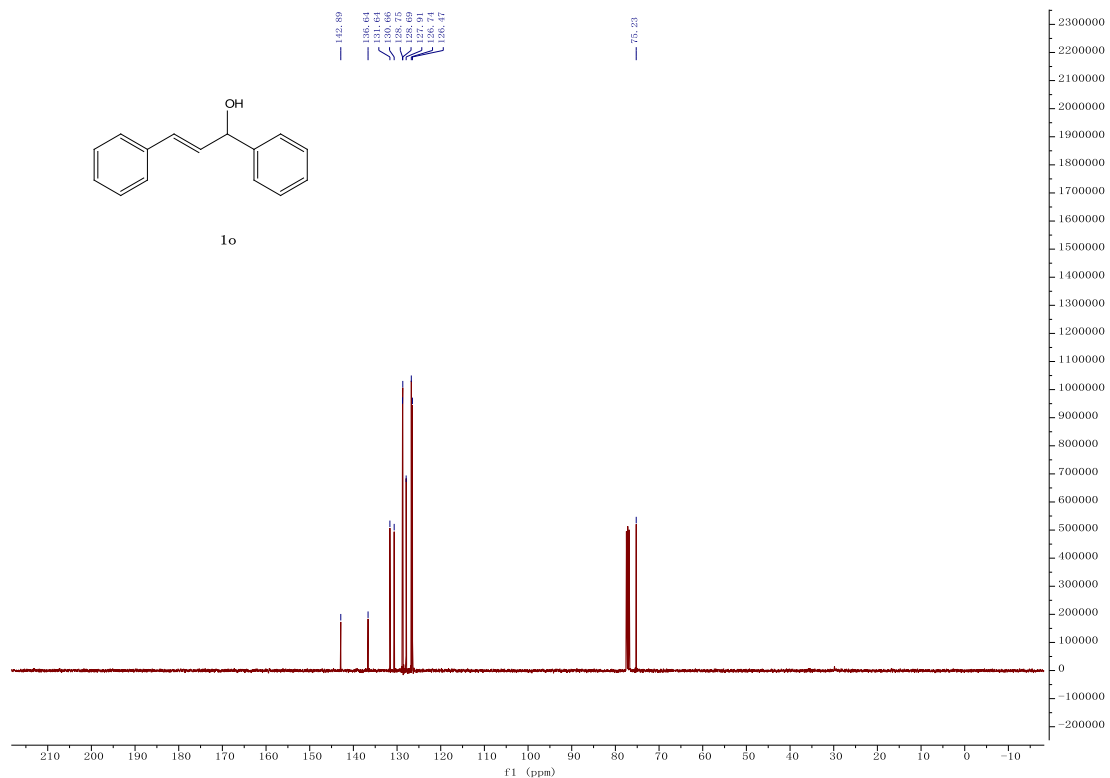
¹³C NMR of **1n**



¹H NMR of 1o

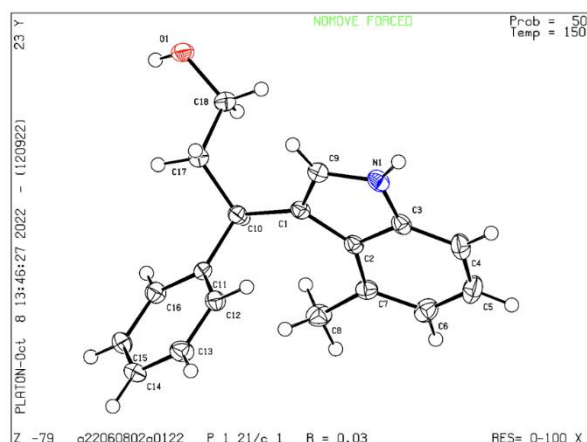


¹³C NMR of 1o



10. Crystallographic details of 5n

Identification code:	2265350
Empirical formula:	C ₁₈ H ₁₉ NO
Formula weight:	265.34
Temperature/K:	150
Crystal system:	monoclinic
Space group:	P2 ₁ /c
a/Å:	7.4178(1)
b/Å:	10.2857(1)
c/Å:	18.5504(2)
α/°:	90
β/°:	94.816(1)
γ/°:	90
Volume/Å ³ :	1410.35(3)
Z:	4
ρ _{calc} /cm ³ :	1.250
μ/mm ⁻¹ :	0.598
F(000):	568.0
Theta range [°]	4.2430-74.0430
Reflections collected	13805



11. Cartesian coordinates

CsOH sol_energy=-96.059062933

Coordinates (Angstroms)			
ATOM	X	Y	Z
O	0.011901	2.265740	0.000000
H	-0.749765	2.867666	0.000000
Cs	0.011901	-0.381702	0.000000

H2O sol_energy=-76.4594743887

Coordinates (Angstroms)			
ATOM	X	Y	Z
O	0.000000	0.000000	0.119419
H	0.000000	0.762666	-0.477675
H	0.000000	-0.762666	-0.477675

iButOH sol_energy=-233.661520971

Coordinates (Angstroms)			
ATOM	X	Y	Z
C	-0.005096	-0.000001	0.015171
C	-1.488422	-0.000232	-0.360458
H	-1.614666	-0.000231	-1.448360
H	-1.981353	-0.887094	0.051070
H	-1.981632	0.886461	0.051103
C	0.691120	1.264786	-0.509100
H	0.211169	2.157605	-0.095234
H	1.748496	1.275614	-0.212635
H	0.651742	1.319946	-1.603231
C	0.691529	-1.264545	-0.509142
H	1.748918	-1.275020	-0.212707
H	0.211893	-2.157537	-0.095282
H	0.652143	-1.319696	-1.603272
O	0.009960	-0.000021	1.451996
H	0.938819	0.000069	1.733758

iButOK sol_energy=-261.41943801

Coordinates (Angstroms)			
ATOM	X	Y	Z
C	1.039446	0.000000	-0.030029
C	2.163951	-0.000220	-1.102100
H	3.175389	-0.000250	-0.670527
H	2.055201	-0.886180	-1.738991
H	2.055339	0.885607	-1.739197
C	1.219902	1.259738	0.864120
H	1.083877	2.159869	0.251680
H	0.448211	1.265553	1.649281
H	2.201891	1.317958	1.355282
C	1.219793	-1.259479	0.864507
H	0.448151	-1.264932	1.649718
H	1.083609	-2.159791	0.252369
H	2.201805	-1.317672	1.355627

O	-0.186342	-0.000040	-0.632894
K	-2.480068	-0.000004	-0.046373

iButONa sol_energy=-395.38797907500003

Coordinates (Angstroms)			
ATOM	X	Y	Z
C	0.613022	-0.000001	-0.007552
C	1.405366	-0.001763	-1.337906
H	2.493671	-0.001914	-1.186016
H	1.135558	-0.889012	-1.923397
H	1.136078	0.884330	-1.925379
C	0.997300	1.260654	0.804675
H	0.719829	2.158411	0.238494
H	0.438539	1.270323	1.749888
H	2.070054	1.313494	1.036503
C	0.996883	-1.258797	0.807751
H	0.438365	-1.265786	1.753132
H	0.718817	-2.157857	0.243931
H	2.069672	-1.311587	1.039436
O	-0.737309	-0.000102	-0.272088
Na	-2.672504	-0.000014	-0.041063

RC sol_energy=-424.192316223

Coordinates (Angstroms)			
ATOM	X	Y	Z
C	2.881451	-1.003936	-0.174886
C	1.519588	-1.276305	-0.048300
C	0.579589	-0.241378	0.103548
C	1.055730	1.083477	0.131596
C	2.414519	1.357009	0.004285
C	3.335457	0.315443	-0.150405
H	3.586752	-1.822440	-0.292028
H	1.173075	-2.307302	-0.069037
H	0.358316	1.906053	0.259521
H	2.759197	2.387488	0.029267
H	4.395635	0.532579	-0.247611

C	-1.890922	0.250115	0.297796
H	-1.754829	1.329828	0.253335
C	-3.318367	-0.203518	0.404208
H	-3.778449	0.179628	1.323391
O	-4.126641	0.317233	-0.652399
C	-0.844517	-0.587229	0.223497
H	-3.367063	-1.304500	0.448289
H	-1.051987	-1.658665	0.251945
H	-3.702698	0.057401	-1.485922

N-C-1 sol_energy=-443.800490095

Coordinates (Angstroms)			
ATOM	X	Y	Z
C	-3.692007	-0.423980	0.992830
C	-2.582891	0.380817	1.249469
C	-1.742777	0.839593	0.211324
C	-2.072343	0.437302	-1.104407
C	-3.181290	-0.366155	-1.360168
C	-4.001236	-0.806118	-0.315253
H	-4.320235	-0.751262	1.818186
H	-2.359373	0.677042	2.272784
H	-1.456298	0.772077	-1.935014
H	-3.411213	-0.648363	-2.385385
H	-4.866705	-1.430761	-0.518613
C	-0.556950	1.638165	0.536735
H	-0.369921	1.770978	1.606193
C	0.350093	2.162637	-0.321355
H	0.198022	2.075628	-1.398785
C	1.765796	2.572336	0.050204
H	1.789142	2.798806	1.149698
H	2.020991	3.537977	-0.447337
O	2.520850	1.507606	-0.348362
Cs	1.579826	-1.081283	0.054344

N-K-1 sol_energy=-451.953934664

Coordinates (Angstroms)			
ATOM	X	Y	Z

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-----
C      3.199842   -0.109729    0.985410
C      1.915196   -0.617732    1.173119
C      0.967989   -0.638508    0.127244
C      1.374662   -0.112284   -1.120462
C      2.659310    0.394076   -1.307702
C      3.582777    0.401498   -0.257251
H      3.905662   -0.115485    1.812569
H      1.632632   -1.019294    2.144385
H      0.679524   -0.116716   -1.956245
H      2.943404    0.782997   -2.282880
H      4.583718    0.796673   -0.406637
C     -0.389376   -1.135028    0.387620
H     -0.595579   -1.388766    1.431535
C     -1.409768   -1.259475   -0.493545
H     -1.247086   -1.047502   -1.552344
C     -2.878787   -1.338719   -0.110043
H     -2.950634   -1.755502    0.926561
H     -3.393158   -2.082183   -0.760445
O     -3.335936   -0.054794   -0.255229
K     -1.736951    1.730501    0.335736
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N-N-1 sol_energy=-585.920347874

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                        Coordinates (Angstroms)
ATOM      X          Y          Z
-----
C      3.110141   -0.784236    0.613358
C      1.780548   -1.194766    0.524621
C      0.817633   -0.420477   -0.151526
C      1.244364    0.795040   -0.726847
C      2.572850    1.205162   -0.638734
C      3.515346    0.418892    0.031498
H      3.831322   -1.406420    1.137231
H      1.476484   -2.136689    0.976401
H      0.529497    1.420256   -1.255697
H      2.875143    2.144282   -1.095585
H      4.550528    0.741538    0.099532
C     -0.579275   -0.883902   -0.199134
H     -0.798839   -1.756093    0.423697
C     -1.602762   -0.364823   -0.915905
H     -1.428960    0.481367   -1.584776
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C	-3.070683	-0.677247	-0.664474
H	-3.141794	-1.698227	-0.221174
H	-3.593813	-0.738439	-1.642164
O	-3.562499	0.326886	0.146112
Na	-2.048050	1.070134	1.341500

N-C-2 sol_energy=-867.999967287

Coordinates (Angstroms)			
ATOM	X	Y	Z
C	4.731596	-2.399096	-1.027781
C	3.448988	-1.856415	-1.107210
C	2.440221	-2.219014	-0.193750
C	2.767251	-3.165687	0.796866
C	4.046588	-3.710064	0.875874
C	5.039486	-3.329024	-0.032781
H	5.489836	-2.096868	-1.746462
H	3.220864	-1.124718	-1.878962
H	2.006076	-3.482650	1.503743
H	4.271096	-4.440421	1.649601
H	6.036716	-3.756135	0.032042
C	1.115487	-1.588976	-0.301031
H	0.956231	-1.015245	-1.216807
C	0.119358	-1.606552	0.600173
H	0.213680	-2.157891	1.536046
C	-1.222949	-0.917799	0.424949
H	-1.194598	-0.428462	-0.602649
H	-1.152132	0.012132	1.108053
O	-2.279778	-1.693477	0.670622
C	4.252400	1.603446	-0.334129
C	3.008044	1.410247	0.269648
C	2.160287	2.493881	0.529468
C	2.589334	3.780727	0.174175
C	3.832065	3.978993	-0.429003
C	4.668153	2.888740	-0.686653
H	4.888143	0.742750	-0.524099
H	2.690193	0.408175	0.537849
H	1.944951	4.634812	0.376073
H	4.150093	4.984381	-0.694110
H	5.637129	3.042839	-1.154596
C	-1.716059	2.167878	0.703208
H	-1.782286	2.174143	1.812689

O	-2.734065	2.073408	0.027236
Cs	-4.518684	-0.418187	-0.326819
C	0.796278	2.274326	1.147389
H	0.753315	1.280695	1.607063
H	0.625394	3.008186	1.947866
C	-0.339820	2.384003	0.115744
H	-0.201797	1.659119	-0.695988
H	-0.334807	3.378325	-0.356130

N-K-2 sol_energy=-876.165270389

Coordinates (Angstroms)			
ATOM	X	Y	Z
C	-2.135433	2.732418	-1.411068
C	-2.721145	1.670338	-0.721298
C	-2.441422	1.457101	0.634624
C	-1.564239	2.334773	1.285612
C	-0.972919	3.397258	0.597667
C	-1.256183	3.597474	-0.755203
H	-2.354110	2.873896	-2.465905
H	-3.367590	0.972607	-1.247059
H	-1.337237	2.178987	2.338656
H	-0.290956	4.065553	1.117167
H	-0.792352	4.418529	-1.294793
C	-2.434850	-2.260004	1.679405
H	-3.492835	-2.364810	2.005381
H	-1.426877	0.074049	-2.852888
O	-1.691193	-3.236062	1.745254
C	4.868614	0.089532	0.332200
C	3.918929	-0.266092	-0.626281
C	2.579596	0.157731	-0.527770
C	2.230672	0.965358	0.576362
C	3.178808	1.319798	1.532130
C	4.503826	0.883540	1.420665
H	5.895421	-0.252018	0.225633
H	4.217031	-0.878564	-1.475708
H	1.212032	1.328595	0.678419
H	2.883119	1.946250	2.370536
H	5.240016	1.163941	2.169102
C	1.605926	-0.273072	-1.544046
H	2.019349	-0.880945	-2.355198

C	0.283100	-0.013675	-1.558969
H	-0.154761	0.602323	-0.775755
C	-0.740728	-0.699576	-2.442711
H	-0.216151	-1.123797	-3.332352
O	-1.382496	-1.650466	-1.669898
K	0.162323	-3.151642	-0.324437
C	-2.976580	0.232829	1.345722
H	-3.970392	-0.024422	0.957468
H	-3.092998	0.437718	2.418301
C	-2.020725	-0.948874	1.115256
H	-1.014509	-0.707961	1.488558
H	-1.882311	-1.117664	-0.001899

N-N-2 sol_energy=-1010.12322654

Coordinates (Angstroms)

ATOM	X	Y	Z
C	1.706336	2.970288	-0.312936
C	0.811885	2.063231	0.258901
C	-0.518220	2.425033	0.509052
C	-0.930875	3.723504	0.177496
C	-0.040709	4.632380	-0.396064
C	1.282499	4.257875	-0.645592
H	2.733408	2.663641	-0.493604
H	1.152307	1.064196	0.513683
H	-1.956617	4.030184	0.372217
H	-0.379457	5.634600	-0.646209
H	1.975662	4.965819	-1.092168
C	-3.569385	0.026853	0.818135
H	-3.423012	-0.220591	1.889247
H	-1.984111	-1.300356	0.480362
O	-4.467038	-0.530999	0.182362
Na	-4.406664	-2.614424	-0.614030
C	4.518545	-0.575363	-0.495465
C	3.155374	-0.571969	-0.790664
C	2.280432	-1.520553	-0.226823
C	2.830357	-2.482109	0.643052
C	4.191613	-2.489212	0.934937
C	5.045136	-1.534997	0.370611
H	5.169489	0.170527	-0.945093
H	2.751990	0.178929	-1.466651

H	2.184663	-3.232116	1.090641
H	4.591487	-3.243884	1.607803
H	6.106665	-1.542947	0.602947
C	0.849916	-1.448464	-0.555023
H	0.592757	-0.671955	-1.278187
C	-0.160022	-2.183692	-0.061693
H	0.007097	-2.988934	0.653467
C	-1.611972	-1.932037	-0.409064
H	-1.624250	-1.178773	-1.242558
O	-2.370212	-3.024576	-0.618233
C	-1.474460	1.426875	1.128452
H	-0.945305	0.480307	1.285158
H	-1.792907	1.778022	2.120816
C	-2.726710	1.154622	0.273348
H	-2.458508	0.915260	-0.761785
H	-3.368492	2.047731	0.227253

N-C-TS2-3 sol_energy=-867.993556281

	Coordinates (Angstroms)		
ATOM	X	Y	Z
C	4.742320	-2.466324	-1.052950
C	3.427879	-2.057705	-1.275122
C	2.436367	-2.207800	-0.286724
C	2.815897	-2.792421	0.937713
C	4.127422	-3.203131	1.159951
C	5.100284	-3.041557	0.167854
H	5.487114	-2.333069	-1.833552
H	3.160275	-1.598014	-2.223694
H	2.077798	-2.918486	1.724287
H	4.395114	-3.648047	2.115069
H	6.124035	-3.358749	0.346997
C	1.081230	-1.712754	-0.557931
H	0.950076	-1.259388	-1.542362
C	0.013463	-1.732384	0.258841
H	0.051652	-2.177687	1.252135
C	-1.318213	-1.139048	-0.103976
H	-1.315560	-0.787706	-1.173664
H	-1.166552	0.069942	0.363965
O	-2.392142	-1.685783	0.354944
C	4.594241	1.651555	-0.275873

C	3.346649	1.264562	0.218259
C	2.359191	2.214472	0.507541
C	2.657259	3.569193	0.297547
C	3.902975	3.961814	-0.192986
C	4.877210	3.002346	-0.484810
H	5.339141	0.890653	-0.495519
H	3.138597	0.212526	0.380991
H	1.903565	4.321687	0.521694
H	4.115193	5.017271	-0.346419
H	5.847728	3.307760	-0.867810
C	-1.482314	1.486292	0.428438
H	-1.572006	1.437384	1.544350
O	-2.521948	1.710730	-0.257271
Cs	-4.768458	-0.154270	-0.121921
C	0.994071	1.788467	1.002280
H	1.021021	0.730274	1.286564
H	0.731982	2.353486	1.908502
C	-0.115278	1.993235	-0.043219
H	0.147509	1.491845	-0.983842
H	-0.222668	3.060730	-0.282391

N-K-TS2-3 sol_energy=-876.151995659

Coordinates (Angstroms)			
ATOM	X	Y	Z
C	3.460058	1.451239	-0.643304
C	2.185936	1.341493	-1.195830
C	1.065674	1.899789	-0.562288
C	1.263973	2.576147	0.648249
C	2.539839	2.689704	1.207941
C	3.642712	2.127171	0.565331
H	4.305248	0.984611	-1.141384
H	2.049856	0.789944	-2.123017
H	0.416080	3.016055	1.165637
H	2.668059	3.215908	2.150956
H	4.633407	2.204454	1.005630
C	-2.794514	1.285505	-0.862828
H	-2.852781	1.454043	-1.963073
H	-2.373459	-0.102283	-1.019127
O	-3.866607	1.292608	-0.189931
C	3.844992	-2.399800	-0.430594
C	2.539605	-2.370901	-0.920850

C	1.489062	-1.816749	-0.167806
C	1.798691	-1.276956	1.095343
C	3.099472	-1.305356	1.586040
C	4.131332	-1.868586	0.827958
H	4.638241	-2.835287	-1.033224
H	2.323617	-2.783696	-1.904128
H	1.020669	-0.794047	1.678016
H	3.315951	-0.864423	2.555400
H	5.148491	-1.880673	1.210549
C	0.136474	-1.781187	-0.737294
H	0.077464	-2.016347	-1.802284
C	-1.009898	-1.487662	-0.101558
H	-1.029334	-1.284285	0.968734
C	-2.350898	-1.387478	-0.771573
H	-2.296793	-1.718609	-1.836721
O	-3.397452	-1.712216	-0.088098
K	-5.245031	-0.461231	0.979828
C	-0.304007	1.753167	-1.198903
H	-0.327380	0.798677	-1.738101
H	-0.436846	2.532887	-1.964340
C	-1.494979	1.799113	-0.233942
H	-1.684377	2.826427	0.108417
H	-1.289188	1.204969	0.665013

N-N-TS2-3 sol_energy=-1010.11871547

	Coordinates (Angstroms)		
ATOM	X	Y	Z
C	-1.942794	-3.109996	-0.283667
C	-1.134680	-2.162674	0.346758
C	0.236830	-2.389829	0.533282
C	0.777152	-3.598148	0.071977
C	-0.027800	-4.549214	-0.558939
C	-1.391311	-4.308778	-0.741183
H	-3.002403	-2.906885	-0.419159
H	-1.572754	-1.230242	0.692943
H	1.837598	-3.798373	0.202112
H	0.412676	-5.478762	-0.910983
H	-2.016442	-5.047429	-1.235950
C	3.096800	0.193984	1.025373
H	2.709277	0.614448	1.980322

H	2.148547	0.973019	0.228825
O	4.271583	0.513196	0.660516
Na	4.663005	2.209155	-0.583787
C	-4.435632	0.893918	-0.348773
C	-3.100022	0.701902	-0.700904
C	-2.094183	1.582266	-0.257954
C	-2.478969	2.666282	0.554993
C	-3.812326	2.860304	0.903771
C	-4.799053	1.975505	0.455213
H	-5.192053	0.198625	-0.703660
H	-2.822306	-0.144165	-1.325143
H	-1.726323	3.359782	0.918380
H	-4.085455	3.704287	1.532074
H	-5.838476	2.128712	0.732432
C	-0.703711	1.324012	-0.650195
H	-0.558367	0.411237	-1.230774
C	0.388659	2.057132	-0.372162
H	0.340813	2.988633	0.189369
C	1.765741	1.647266	-0.801154
H	1.720959	0.772461	-1.495868
O	2.640086	2.573563	-1.067390
C	1.084721	-1.341707	1.225338
H	0.562207	-0.380293	1.156774
H	1.147886	-1.569581	2.299535
C	2.509951	-1.170747	0.668893
H	2.521988	-1.281200	-0.422753
H	3.189990	-1.937906	1.064184

N-C-3 sol_energy=-868.0097216309999

Coordinates (Angstroms)			
ATOM	X	Y	Z
C	4.114240	-2.095840	-0.292380
C	2.795608	-1.653471	-0.375473
C	1.720084	-2.539255	-0.173472
C	2.006468	-3.889375	0.109944
C	3.323213	-4.331582	0.188132
C	4.382068	-3.437084	-0.011552
H	4.924282	-1.388076	-0.444507
H	2.593675	-0.607447	-0.587923
H	1.193177	-4.591292	0.269814

H	3.529107	-5.375958	0.407222
H	5.408771	-3.787560	0.053266
C	0.364348	-2.005687	-0.256151
H	0.303296	-0.944953	-0.494488
C	-0.816673	-2.637626	-0.062632
H	-0.907294	-3.692643	0.188506
C	-2.031272	-1.835271	-0.162283
H	-1.876580	-0.755551	-0.425702
H	-0.753067	0.579593	1.228097
O	-3.170734	-2.271201	0.053183
C	5.182730	1.579012	0.296854
C	3.897878	1.418064	0.823227
C	2.871266	2.325692	0.525780
C	3.175637	3.409589	-0.312952
C	4.455929	3.576305	-0.840474
C	5.467396	2.659117	-0.539772
H	5.961752	0.862842	0.548952
H	3.685963	0.571024	1.471409
H	2.394509	4.126152	-0.556300
H	4.666299	4.424159	-1.488081
H	6.465345	2.788545	-0.950593
C	-0.968271	1.452742	0.539962
H	-1.275246	2.275399	1.246730
O	-1.883328	1.167649	-0.421427
Cs	-4.554710	0.548676	-0.047076
C	1.471825	2.129879	1.065912
H	1.471781	1.282526	1.765431
H	1.173498	3.010810	1.652954
C	0.412010	1.876699	-0.022407
H	0.760685	1.090620	-0.707112
H	0.274682	2.771589	-0.644107

N-K-3 sol_energy=-876.173007808

Coordinates (Angstroms)			
ATOM	X	Y	Z
C	4.963926	-0.687928	0.190189
C	3.706951	-0.355974	-0.316141
C	3.376178	0.974274	-0.618381
C	4.344980	1.962354	-0.398685
C	5.605212	1.636108	0.107230

C	5.920126	0.308489	0.404382
H	5.200123	-1.725837	0.413422
H	2.964963	-1.134631	-0.481464
H	4.106344	2.998914	-0.628563
H	6.342689	2.419274	0.266525
H	6.901345	0.052055	0.795547
C	-0.484151	1.608920	-0.423421
H	-0.548486	2.517647	-1.084142
H	-0.649065	0.751160	-1.129197
O	-1.377949	1.607673	0.616295
C	-0.216553	-4.290543	-0.056542
C	-1.450277	-3.716724	-0.354138
C	-1.718092	-2.372296	-0.029838
C	-0.721175	-1.612926	0.622599
C	0.507113	-2.196058	0.921344
C	0.766562	-3.528980	0.581168
H	-0.021790	-5.326800	-0.319233
H	-2.216373	-4.308233	-0.851277
H	-0.914678	-0.573329	0.891010
H	1.271741	-1.606140	1.418832
H	1.730407	-3.972740	0.817152
C	-3.012963	-1.798928	-0.376013
H	-3.751140	-2.503423	-0.769411
C	-3.360431	-0.493530	-0.253034
H	-2.646964	0.269030	0.112955
C	-4.698839	-0.061356	-0.590029
H	-5.385780	-0.834086	-0.997755
O	-5.119425	1.093873	-0.445145
K	-3.440886	2.965518	0.645551
C	1.990673	1.321078	-1.110838
H	1.625814	0.516332	-1.764358
H	2.023988	2.231544	-1.724459
C	0.984043	1.507470	0.040441
H	1.243318	2.396573	0.632127
H	1.059674	0.654784	0.725856

N-N-3 sol_energy=-1010.1426131000001

Coordinates (Angstroms)			
ATOM	X	Y	Z
C	-2.625729	-2.488318	1.209607

C	-1.249840	-2.726534	1.208359
C	-0.539009	-2.870708	0.006989
C	-1.248430	-2.743714	-1.197188
C	-2.624375	-2.505711	-1.203456
C	-3.321310	-2.385336	0.001895
H	-3.155823	-2.389624	2.153547
H	-0.716261	-2.813258	2.152483
H	-0.713742	-2.843954	-2.139348
H	-3.153418	-2.420789	-2.149334
H	-4.395143	-2.216343	0.000070
C	3.294641	-1.960848	-0.002900
H	3.548000	-2.602914	-0.881779
H	3.550489	-2.588987	0.885383
O	3.929855	-0.752793	-0.013643
Na	5.099387	0.872629	0.012205
C	-3.550988	1.252578	-0.008148
C	-2.180190	1.006001	-0.015018
C	-1.258983	2.071569	-0.009001
C	-1.750143	3.392874	0.003546
C	-3.119115	3.635376	0.009997
C	-4.024062	2.566120	0.004305
H	-4.241559	0.414780	-0.012415
H	-1.818385	-0.018036	-0.024471
H	-1.056456	4.228498	0.007766
H	-3.486481	4.657885	0.019440
H	-5.093176	2.761006	0.009514
C	0.159966	1.746701	-0.015429
H	0.377458	0.679387	-0.030364
C	1.229471	2.581208	-0.003372
H	1.150957	3.665575	0.013635
C	2.548295	1.981287	-0.009407
H	2.599046	0.873655	-0.027332
O	3.616192	2.618746	0.007005
C	0.954338	-3.108451	0.009295
H	1.235524	-3.693830	0.894959
H	1.235690	-3.709039	-0.866087
C	1.757204	-1.795362	-0.002219
H	1.481548	-1.194014	0.876716
H	1.479669	-1.208942	-0.890679

C-N-1 sol_energy=-819.58426788

Coordinates (Angstroms)			
ATOM	X	Y	Z
C	-0.859005	1.888148	-1.283273
C	0.391266	1.070571	-1.194858
H	0.504750	0.348050	-2.001404
O	-0.982360	2.872370	-0.225219
C	1.297666	1.128275	-0.208172
H	1.169893	1.877761	0.574338
C	2.483617	0.270554	-0.059873
C	3.545146	0.694313	0.758652
C	2.595558	-0.980375	-0.695442
C	4.689580	-0.086485	0.917558
H	3.472943	1.653512	1.267641
C	3.738537	-1.760341	-0.537963
H	1.769326	-1.354644	-1.292885
C	4.793307	-1.316742	0.265768
H	5.499208	0.265330	1.551674
H	3.801439	-2.725409	-1.033839
H	5.681373	-1.930097	0.391094
H	-1.728863	1.219319	-1.138205
H	-0.219042	3.468907	-0.272429
C	-3.176434	-1.816826	1.496794
C	-3.002477	-1.173258	0.098466
H	-2.295183	-1.594062	2.115359
H	-4.057700	-1.385755	1.988952
H	-3.299967	-2.908051	1.460566
C	-4.236380	-1.522979	-0.767752
C	-1.735637	-1.773291	-0.564356
H	-4.129153	-1.060909	-1.756395
H	-4.373545	-2.605334	-0.900306
H	-5.139501	-1.110944	-0.301737
H	-1.769777	-2.868578	-0.643810
H	-1.616519	-1.361848	-1.575166
H	-0.849036	-1.492507	0.018432
O	-2.877296	0.196095	0.205954
H	-0.941906	2.389442	-2.258674
Na	-2.159086	1.718065	1.327964

C-N-TS1-2 sol_energy=-819.563755961

Coordinates (Angstroms)

ATOM	X	Y	Z
C	1.062194	1.723757	1.101052
C	-0.187446	1.007797	1.125971
H	-0.219679	0.185401	1.841640
O	1.080878	2.831401	0.160963
C	-1.237335	1.157187	0.255321
H	-1.282600	2.069792	-0.346206
C	-2.399069	0.274745	0.135186
C	-3.568187	0.735275	-0.505536
C	-2.406037	-1.051810	0.618226
C	-4.692714	-0.076572	-0.640585
H	-3.593114	1.754632	-0.887566
C	-3.533500	-1.859408	0.490750
H	-1.511003	-1.457562	1.082509
C	-4.686721	-1.380267	-0.138548
H	-5.579255	0.312555	-1.135696
H	-3.507459	-2.876525	0.874581
H	-5.561920	-2.015491	-0.242916
H	1.988335	0.828199	0.424595
H	0.390063	3.469374	0.415164
C	3.599064	-1.671107	-1.386662
C	3.108058	-0.980963	-0.105721
H	2.755346	-1.851948	-2.065302
H	4.322918	-1.030375	-1.902460
H	4.076770	-2.634962	-1.171479
C	4.291507	-0.721345	0.843806
C	2.054073	-1.863320	0.593246
H	3.942260	-0.209905	1.748377
H	4.786916	-1.652972	1.144468
H	5.026262	-0.074559	0.352644
H	2.458745	-2.848238	0.856050
H	1.702336	-1.384928	1.514217
H	1.187585	-2.010950	-0.063590
O	2.538226	0.257978	-0.484184
H	1.494948	1.996547	2.068372
Na	0.886035	1.177553	-1.476425

C-N-2 sol_energy=-819.573877144

Coordinates (Angstroms)

ATOM	X	Y	Z
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C      -3.663410      0.022270      0.648150
C      -2.584398     -0.822792      0.724681
H      -2.385022     -1.214407      1.722670
O      -3.961194      0.675950     -0.588100
C      -1.692703     -1.153377     -0.329054
H      -2.021856     -0.969057     -1.354483
C      -0.363442     -1.670762     -0.182366
C      0.481462      -1.813499     -1.325561
C      0.245895      -1.983605      1.069974
C      1.804759     -2.237069     -1.224426
H      0.063534     -1.599939     -2.308867
C      1.566249     -2.408946      1.158268
H      -0.335465     -1.891046      1.983439
C      2.373074     -2.537396      0.018154
H      2.399794     -2.331175     -2.130787
H      1.978903     -2.640807      2.138449
H      3.404341     -2.867913      0.097297
H      0.631389      0.399889     -0.738501
H      -4.234740      0.007164     -1.241289
C      1.425013      1.533619      1.580640
C      1.594048      1.924334      0.107481
H      0.488744      1.941262      1.983714
H      1.397400      0.443928      1.681293
H      2.251122      1.921671      2.187125
C      2.907174      1.373158     -0.457945
C      1.495774      3.437118     -0.084624
H      2.988701      1.607430     -1.524629
H      3.765566      1.811912      0.062737
H      2.951601      0.284860     -0.335335
H      2.289839      3.947790      0.469866
H      1.585501      3.696639     -1.144580
H      0.533018      3.813953      0.284531
O      0.488491      1.367812     -0.656475
H      -4.407993      0.169382      1.421836
Na     -1.736338      1.376367     -0.319828
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C-N-TS2-3 sol_energy=-819.567333171

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                          Coordinates (Angstroms)
ATOM      X           Y           Z
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C	-1.740261	-2.842337	0.432206
C	-0.555986	-2.203704	0.569740
H	-0.026970	-2.425761	1.495737
O	-2.574227	-2.654993	-0.707613
C	0.039204	-1.248172	-0.361049
H	-0.181546	-1.478405	-1.413388
C	1.451131	-0.846169	-0.175472
C	2.251695	-0.520189	-1.289776
C	2.034330	-0.677766	1.098153
C	3.558544	-0.058019	-1.143145
H	1.833460	-0.635781	-2.287982
C	3.345227	-0.224673	1.245650
H	1.448449	-0.888886	1.989710
C	4.120765	0.090371	0.127532
H	4.143587	0.181104	-2.028452
H	3.760106	-0.109722	2.244646
H	5.140238	0.447665	0.243854
H	-0.729559	-0.050798	-0.254048
H	-2.009286	-2.661541	-1.500886
C	-0.393532	2.164838	1.389109
C	-1.090891	2.127665	0.017503
H	-1.093349	1.845907	2.172568
H	0.466174	1.487103	1.398151
H	-0.036970	3.172594	1.635797
C	-0.098888	2.516892	-1.093040
C	-2.291368	3.086403	0.011706
H	-0.593457	2.459460	-2.069600
H	0.281342	3.536537	-0.954038
H	0.754632	1.830868	-1.099594
H	-1.983799	4.124640	0.186554
H	-2.808107	3.036091	-0.953947
H	-3.002860	2.806525	0.800571
O	-1.589968	0.824373	-0.231836
H	-2.132865	-3.591564	1.110496
Na	-3.063226	-0.602901	0.165886

C-N-3 sol_energy=-819.618170316

Coordinates (Angstroms)			
ATOM	X	Y	Z
C	-0.310781	2.525084	0.666123
C	-1.160347	2.703232	-0.377948

H	-1.607696	3.681958	-0.525906
O	0.330389	1.419991	0.985172
C	-1.473973	1.611285	-1.375574
H	-2.205798	1.984675	-2.106053
C	-2.030317	0.323047	-0.776734
C	-1.682551	-0.930131	-1.309839
C	-2.875300	0.348098	0.347000
C	-2.140362	-2.120295	-0.729676
H	-1.013656	-0.973192	-2.165483
C	-3.338633	-0.835375	0.930103
H	-3.120330	1.312953	0.781875
C	-2.967240	-2.079599	0.399569
H	-1.845706	-3.075725	-1.156496
H	-3.987402	-0.788995	1.801460
H	-3.325909	-3.000103	0.852415
H	-0.583909	1.337065	-1.963579
H	1.202073	0.463650	-0.069996
C	3.498527	-1.790592	-0.545080
C	2.979560	-0.425880	-0.093135
H	3.008968	-2.590267	0.023688
H	3.283840	-1.945870	-1.607725
H	4.580378	-1.869724	-0.390678
C	3.593912	0.705159	-0.929981
C	3.249065	-0.193165	1.403002
H	3.189939	1.672925	-0.610782
H	4.684318	0.734100	-0.821023
H	3.350741	0.563192	-1.988259
H	4.321712	-0.104762	1.610259
H	2.744369	0.722472	1.729760
H	2.862226	-1.034737	1.994757
O	1.558018	-0.444186	-0.321766
H	-0.138836	3.387914	1.330837
Na	-0.232358	-0.666289	1.120609

C-K-1 sol_energy=-685.612347095

Coordinates (Angstroms)			
ATOM	X	Y	Z
C	-0.865939	1.564279	-1.607616
C	0.367952	0.749726	-1.371937
H	0.386622	-0.194316	-1.914519
O	-0.887363	2.803242	-0.864418

C	1.360465	1.060594	-0.522867
H	1.325087	2.029295	-0.021423
C	2.529058	0.230414	-0.193530
C	3.656708	0.827892	0.397302
C	2.563121	-1.157714	-0.427207
C	4.786831	0.077101	0.719999
H	3.647885	1.898474	0.593511
C	3.691710	-1.907920	-0.106314
H	1.690434	-1.654936	-0.840456
C	4.811175	-1.295413	0.465715
H	5.647920	0.564381	1.170194
H	3.693439	-2.978811	-0.291997
H	5.688174	-1.884649	0.719286
H	-1.731725	0.973227	-1.230859
H	-0.160634	3.357019	-1.190490
C	-1.536273	-1.921220	0.731046
C	-2.794460	-1.350615	0.012429
H	-0.632165	-1.477683	0.293776
H	-1.563391	-1.649552	1.797951
H	-1.448967	-3.015286	0.670663
C	-4.054566	-1.946426	0.691745
C	-2.760775	-1.827729	-1.464552
H	-4.951891	-1.567846	0.188300
H	-4.080536	-3.045757	0.675771
H	-4.093598	-1.615548	1.738669
H	-2.785962	-2.921769	-1.568746
H	-3.619518	-1.404590	-1.998344
H	-1.848920	-1.460460	-1.954328
O	-2.815791	0.020664	0.073152
H	-1.011942	1.763192	-2.680276
K	-1.845006	1.740871	1.485693

C-K-TS1-2 sol_energy=-685.60087933

Coordinates (Angstroms)			
ATOM	X	Y	Z
C	0.989647	-1.301174	-1.454056
C	-0.257865	-0.584363	-1.336987
H	-0.255541	0.399474	-1.808846
O	0.958535	-2.637101	-0.896545
C	-1.352845	-0.957658	-0.605579

H	- 1.396877	-1.989694	-0.249028
C	-2.529361	-0.145972	-0.304300
C	-3.691352	-0.760324	0.211404
C	-2.566744	1.256198	-0.475819
C	-4.831937	-0.022694	0.522410
H	-3.696496	-1.840311	0.352146
C	-3.709539	1.991237	-0.172213
H	-1.683466	1.775119	-0.838777
C	-4.853063	1.360863	0.329697
H	-5.710306	-0.531788	0.912590
H	-3.704558	3.068941	-0.318541
H	-5.740705	1.938930	0.571294
H	1.942184	-0.642393	-0.616890
H	0.288063	-3.151212	-1.380784
C	2.034457	2.073270	0.149766
C	3.172402	1.031385	0.065333
H	1.263475	1.857775	-0.598370
H	1.561871	2.036050	1.141054
H	2.392997	3.097447	-0.013694
C	4.217879	1.322849	1.154907
C	3.838183	1.101573	-1.324032
H	5.021767	0.580234	1.106416
H	4.656268	2.323380	1.047278
H	3.753222	1.256486	2.147364
H	4.287565	2.084345	-1.515083
H	4.619856	0.337562	-1.395883
H	3.101144	0.904121	-2.111215
O	2.668425	-0.262813	0.293875
H	1.444165	-1.285969	-2.452593
K	0.846343	-1.432122	1.593670

C-K-2 sol_energy=-685.609524042

Coordinates (Angstroms)			
ATOM	X	Y	Z
C	3.822326	-0.045776	-0.665758
C	2.714744	-0.845222	-0.734659
H	2.516878	-1.267309	-1.721928
O	4.154052	0.629161	0.542854
C	1.805562	-1.145705	0.317507
H	2.146564	-0.998284	1.344267

C	0.498859	-1.692302	0.154999
C	-0.268000	-2.117476	1.285729
C	-0.173579	-1.795528	-1.106427
C	-1.555630	-2.617657	1.164721
H	0.192037	-2.058526	2.271277
C	-1.463205	-2.319523	-1.215572
H	0.344571	-1.488383	-2.012267
C	-2.181904	-2.730223	-0.089338
H	-2.085922	-2.934145	2.061413
H	-1.917687	-2.390328	-2.202474
H	-3.186920	-3.131202	-0.179874
H	-0.867361	0.251936	-0.736048
H	4.386496	-0.040093	1.209811
C	-3.296510	0.928083	-0.754005
C	-2.132965	1.609593	-0.023302
H	-3.272094	1.181193	-1.819374
H	-3.224060	-0.160310	-0.651801
H	-4.259106	1.249141	-0.339942
C	-2.101290	1.194338	1.454124
C	-2.212806	3.130504	-0.168222
H	-1.289188	1.711693	1.983096
H	-3.041661	1.446715	1.957539
H	-1.935038	0.115981	1.542027
H	-3.131349	3.516039	0.286198
H	-1.363612	3.614831	0.332934
H	-2.197751	3.415802	-1.225389
O	-0.887078	1.231358	-0.650781
H	4.568450	0.050312	-1.448417
K	1.618282	1.774324	0.131242

C-K-TS2-3 sol_energy=-685.602517969

Coordinates (Angstroms)			
ATOM	X	Y	Z
C	-1.626117	-2.859078	0.258771
C	-0.463700	-2.217408	0.497365
H	0.047233	-2.513077	1.412768
O	-2.419677	-2.609408	-0.887832
C	0.149316	-1.169895	-0.327609
H	-0.101291	-1.271914	-1.394640
C	1.593407	-0.895295	-0.143597

C	2.424524	-0.616633	-1.247661
C	2.182210	-0.802370	1.135478
C	3.765355	-0.267917	-1.087177
H	2.004401	-0.681230	-2.249780
C	3.525399	-0.466451	1.297212
H	1.570216	-0.974267	2.018060
C	4.331122	-0.194705	0.187746
H	4.373289	-0.060900	-1.965288
H	3.943481	-0.405062	2.299756
H	5.376477	0.073065	0.315599
H	-0.508883	0.034086	-0.026050
H	-1.809275	-2.482215	-1.635546
C	0.424088	2.528110	1.035700
C	-0.650069	2.256621	-0.035590
H	-0.031309	2.494742	2.033037
H	1.202381	1.759823	0.991923
H	0.898070	3.509262	0.902471
C	-0.010655	2.294874	-1.438833
C	-1.753141	3.328054	0.055165
H	-0.763447	2.042989	-2.196905
H	0.400444	3.284789	-1.674290
H	0.802537	1.564925	-1.506077
H	-1.359532	4.341616	-0.092908
H	-2.519650	3.146172	-0.710768
H	-2.232507	3.288386	1.042025
O	-1.255944	1.006584	0.191054
H	-2.030012	-3.660139	0.869566
K	-3.326741	-0.325048	0.316813

C-K-3 sol_energy=-685.654406072

Coordinates (Angstroms)			
ATOM	X	Y	Z
C	0.056889	-2.442487	-0.911166
C	-0.590724	-2.747536	0.244459
H	-0.913586	-3.771838	0.408584
O	0.526300	-1.269066	-1.268948
C	-0.860244	-1.720208	1.319281
H	-1.316195	-2.214276	2.189505
C	-1.776799	-0.567089	0.916005
C	-2.826249	-0.752463	0.001004

C	-1.590955	0.717860	1.453263
C	-3.660654	0.307458	-0.367130
H	-2.954644	-1.738143	-0.438145
C	-2.421783	1.784094	1.089460
H	-0.762774	0.886835	2.136042
C	-3.462169	1.585228	0.173652
H	-4.473334	0.136065	-1.069903
H	-2.258190	2.768176	1.523585
H	-4.118396	2.407446	-0.101662
H	0.073998	-1.272937	1.688617
H	1.114389	-0.260397	-0.132053
C	3.420138	1.707828	1.035452
C	2.891158	0.462094	0.323359
H	3.116771	2.612926	0.495039
H	3.011885	1.763543	2.050385
H	4.514166	1.693078	1.097765
C	3.263813	-0.813286	1.095955
C	3.416736	0.382144	-1.121091
H	2.829763	-1.690580	0.603536
H	4.350918	-0.946520	1.152381
H	2.864683	-0.761338	2.114948
H	4.503878	0.242806	-1.152034
H	2.933871	-0.455235	-1.636438
H	3.182790	1.311211	-1.660397
O	1.463677	0.587036	0.298532
H	0.206218	-3.262264	-1.635963
K	-0.367419	1.083466	-1.651868

C-C-1 sol_energy=-520.248979801

ATOM	Coordinates (Angstroms)		
	X	Y	Z
C	0.892978	2.305363	-0.263439
C	-0.473115	1.833102	0.085411
H	-0.870973	2.258564	1.006930
O	1.384696	1.768342	-1.509660
C	-1.179381	0.900590	-0.587009
H	-0.764939	0.532616	-1.527228
C	-2.476764	0.323956	-0.214318
C	-3.206398	-0.410089	-1.169691
C	-3.032826	0.448376	1.075225
C	-4.441709	-0.978778	-0.862223

H	-2.798031	-0.522346	-2.172598
C	-4.267624	-0.117329	1.382636
H	-2.483865	0.981181	1.846594
C	-4.982302	-0.833833	0.417078
H	-4.983491	-1.534428	-1.623789
H	-4.672038	-0.006250	2.385765
H	-5.943700	-1.277116	0.661815
H	1.631937	1.938011	0.551722
H	0.790802	2.074430	-2.214487
O	2.662614	1.153213	1.615007
H	3.377683	1.805719	1.683032
Cs	2.225565	-0.979238	-0.006398
H	0.934893	3.407108	-0.270644

C-C-TS1-2 sol_energy=-520.244455612

Coordinates (Angstroms)			
ATOM	X	Y	Z
C	1.273186	2.328077	-0.146124
C	-0.108242	1.957229	0.130400
H	-0.493826	2.345836	1.074078
O	1.762331	1.871785	-1.424417
C	-0.870482	1.094185	-0.598124
H	-0.484071	0.783586	-1.570909
C	-2.163886	0.519987	-0.237188
C	-2.871889	-0.250339	-1.185837
C	-2.747244	0.654393	1.043110
C	-4.095666	-0.843726	-0.881707
H	-2.451791	-0.369480	-2.183681
C	-3.972207	0.065706	1.344657
H	-2.228798	1.221801	1.811174
C	-4.658579	-0.689882	0.387640
H	-4.613768	-1.425675	-1.640671
H	-4.393746	0.192182	2.339308
H	-5.612454	-1.150752	0.628980
H	2.031093	1.720685	0.731357
H	1.205907	2.273609	-2.114211
O	2.806049	0.946937	1.513116
H	3.615048	1.475168	1.592735
Cs	1.758235	-1.127852	-0.009505
H	1.466514	3.401380	0.004049

C-C-2 sol_energy=-520.249233277

Coordinates (Angstroms)			
ATOM	X	Y	Z
C	1.764085	2.313554	-0.025714
C	0.404785	2.122616	0.208767
H	0.046512	2.508222	1.165047
O	2.317606	1.834772	-1.247294
C	-0.488020	1.428602	-0.614708
H	-0.158274	1.215210	-1.633569
C	-1.759489	0.866969	-0.242614
C	-2.550320	0.181010	-1.209352
C	-2.268162	0.860984	1.088502
C	-3.746584	-0.446405	-0.877381
H	-2.209676	0.171218	-2.244940
C	-3.470438	0.238987	1.409384
H	-1.704110	1.355427	1.875842
C	-4.226847	-0.428755	0.437770
H	-4.317554	-0.949312	-1.656260
H	-3.821788	0.269377	2.439497
H	-5.162523	-0.915958	0.697080
H	2.544105	1.058805	1.219122
H	1.901631	2.327803	-1.978962
O	2.993616	0.266857	1.652277
H	3.932080	0.507305	1.638268
Cs	1.131088	-1.279058	-0.113085
H	2.295898	3.161687	0.410729

C-C-TS2-3 sol_energy=-520.239971429

Coordinates (Angstroms)			
ATOM	X	Y	Z
C	-0.641853	2.419095	-0.191232
C	0.394466	1.629290	-0.530919
H	0.845670	1.833930	-1.501643
O	-1.345847	2.291402	1.022899
C	0.904619	0.472150	0.219276

C	2.362136	0.152246	0.131238
C	3.331282	1.018802	-0.403972
C	2.800720	-1.110060	0.584291
C	4.674356	0.642234	-0.489228
H	3.034220	2.009214	-0.739836
C	4.141242	-1.480546	0.515190
H	2.054373	-1.806200	0.960887
C	5.090839	-0.606728	-0.026349
H	5.400292	1.336793	-0.907347
H	4.447859	-2.461304	0.873299
H	-0.687015	2.052260	1.698893
H	0.301192	-0.671271	-0.169712
O	-0.280955	-1.816534	-0.349016
H	0.397686	-2.319362	-0.822255
H	0.587849	0.479389	1.275957
H	6.136900	-0.896693	-0.086501
Cs	-2.669424	-0.461844	-0.073107
H	-1.033120	3.226823	-0.801702

C-C-3 sol_energy=-520.296629789

Coordinates (Angstroms)			
ATOM	X	Y	Z
C	4.747158	-1.141730	-1.058927
C	3.476639	-1.393454	-0.541232
C	2.813260	-0.440188	0.251022
C	3.460755	0.785309	0.482445
C	4.732126	1.039729	-0.032038
C	5.384743	0.076386	-0.805516
H	5.237588	-1.894894	-1.671794
H	2.982177	-2.332642	-0.771740
H	2.938859	1.525761	1.080200
H	5.217190	1.992236	0.172035
H	6.373751	0.273661	-1.212008
C	1.434509	-0.645013	0.816930
C	0.938411	-1.908510	0.994335
H	1.562585	-2.774050	0.800964
O	0.784022	0.457303	1.102671
C	-0.464699	-2.137985	1.492149
C	-1.572365	-1.870155	0.472389
C	-1.376451	-2.114768	-0.896170

C	-2.820137	-1.371394	0.880550
C	-2.391283	-1.873791	-1.827248
H	-0.403345	-2.473874	-1.220796
C	-3.840090	-1.127903	-0.045494
H	-2.971070	-1.130315	1.928671
C	-3.631156	-1.377224	-1.406663
H	-2.218119	-2.081911	-2.881201
H	-4.798420	-0.742420	0.296802
H	-0.478268	0.670160	2.130749
H	-0.677086	-1.512237	2.369383
O	-1.337388	1.023578	2.526330
H	-1.148236	1.123463	3.469563
H	-0.571714	-3.179857	1.828175
H	-4.426013	-1.199095	-2.127385
Cs	-1.228027	1.725329	-0.470597

P-C-TS1-2 sol_energy=-443.756732779

Coordinates (Angstroms)			
ATOM	X	Y	Z
C	-4.079271	-0.851202	0.872826
C	-2.884065	-0.259830	1.266111
C	-2.081336	0.485086	0.363017
C	-2.589930	0.628675	-0.954540
C	-3.781744	0.024239	-1.346410
C	-4.540198	-0.728453	-0.443815
H	-4.660983	-1.413889	1.600728
H	-2.541619	-0.374828	2.293908
H	-2.050958	1.244950	-1.669973
H	-4.134631	0.160620	-2.367195
H	-5.474757	-1.189530	-0.751349
C	-0.802624	1.008980	0.786624
H	-0.631847	1.082573	1.862254
C	0.127636	1.638140	-0.062611
H	0.116158	1.400131	-1.131420
C	1.379137	2.277915	0.355878
H	1.331541	2.715464	1.376266
H	0.249669	3.040705	-0.198589
O	2.483416	2.164582	-0.247841
Cs	2.062627	-0.896803	-0.073716

P-K-TS1-2 sol_energy=-451.90505684199996

Coordinates (Angstroms)			
ATOM	X	Y	Z
C	3.434504	0.721898	0.745761
C	2.123598	0.528579	1.167375
C	1.192629	-0.214699	0.398984
C	1.680172	-0.784716	-0.803845
C	2.990832	-0.578019	-1.228524
C	3.883177	0.180131	-0.464617
H	4.115658	1.300134	1.366995
H	1.792430	0.965135	2.108624
H	1.027046	-1.419173	-1.398012
H	3.325432	-1.032725	-2.158996
H	4.907438	0.330806	-0.794339
C	-0.184958	-0.329298	0.834809
H	-0.380088	-0.144539	1.892802
C	-1.209176	-0.952971	0.090305
H	-1.146883	-0.945270	-1.004002
C	-2.564531	-1.219180	0.578397
H	-2.617458	-1.474610	1.655523
H	-1.598920	-2.290428	0.219491
O	-3.616032	-0.963218	-0.078483
K	-2.556520	1.489793	-0.482742

P-N-TS1-2 sol_energy=-585.861628687

Coordinates (Angstroms)			
ATOM	X	Y	Z
C	3.209291	1.006335	0.120415
C	1.868638	1.208805	0.430797
C	0.914228	0.170547	0.313550
C	1.394338	-1.094136	-0.101208
C	2.736011	-1.290450	-0.422506
C	3.657071	-0.244460	-0.319286
H	3.912681	1.829813	0.222875
H	1.535952	2.190534	0.763755
H	0.711417	-1.938833	-0.145726

H	3.069070	-2.276978	-0.737822
H	4.704310	-0.403483	-0.561011
C	-0.488656	0.437397	0.585759
H	-0.704234	1.293417	1.227774
C	-1.528873	-0.507429	0.411712
H	-1.449538	-1.230007	-0.410172
C	-2.903809	-0.287978	0.859519
H	-3.013668	0.183282	1.851511
H	-2.016365	-1.408146	1.347509
O	-3.898721	-0.391854	0.076630
Na	-2.609936	0.773041	-1.404023

P-C-2 sol_energy=-443.803518369

Coordinates (Angstroms)			
ATOM	X	Y	Z
C	0.026595	2.791481	0.785408
C	0.918707	1.816990	1.209153
C	1.521928	0.872098	0.302776
C	1.135397	1.030466	-1.076647
C	0.246052	2.022691	-1.482606
C	-0.344884	2.910062	-0.569042
H	-0.385018	3.484236	1.519023
H	1.191737	1.763524	2.262603
H	1.543611	0.353502	-1.819491
H	0.006756	2.105971	-2.542954
H	-1.022566	3.691960	-0.899932
C	2.383910	-0.138124	0.768733
H	2.632206	-0.157153	1.826868
C	2.979633	-1.216208	-0.099314
H	3.175111	-0.925504	-1.137449
C	1.782336	-2.104317	0.028710
H	1.719832	-2.632086	1.006866
H	3.886151	-1.651489	0.337074
O	0.839625	-2.186357	-0.786039
Cs	-1.515688	-0.662781	0.118776

P-K-2 sol_energy=-451.952403323

Coordinates (Angstroms)			
ATOM	X	Y	Z
C	2.751037	-0.247914	0.613814
C	1.566744	-0.695243	1.176498
C	0.363529	-0.888401	0.400492
C	0.543155	-0.714169	-1.021221
C	1.746420	-0.274103	-1.568783
C	2.862768	0.011157	-0.768702
H	3.618488	-0.105051	1.257643
H	1.517860	-0.879727	2.249728
H	-0.293871	-0.907877	-1.689022
H	1.814656	-0.152112	-2.649695
H	3.798680	0.347339	-1.204459
C	-0.888950	-1.087861	1.012870
H	-0.891189	-1.378039	2.061665
C	-2.115693	-1.441338	0.230685
H	-1.959966	-2.229168	-0.543545
C	-2.830656	-0.350337	-0.539608
H	-3.718827	-0.700207	-1.115747
H	-2.894720	-1.879180	0.878315
O	-2.520815	0.830503	-0.609459
K	-0.253406	1.861540	0.442869

P-N-2 sol_energy=-585.914724393

Coordinates (Angstroms)			
ATOM	X	Y	Z
C	-2.852549	0.598299	0.229520
C	-1.640748	1.265439	0.151081
C	-0.436938	0.619463	-0.284024
C	-0.589360	-0.754539	-0.660610
C	-1.820828	-1.412098	-0.580552
C	-2.965445	-0.758260	-0.125068
H	-3.734304	1.142275	0.564111
H	-1.586260	2.317006	0.429783
H	0.268886	-1.305924	-1.039831
H	-1.878898	-2.454856	-0.888612
H	-3.918499	-1.274745	-0.061124
C	0.835225	1.290745	-0.224277
H	0.778255	2.376856	-0.177340

C	1.997262	0.772127	-1.030975
H	1.729585	0.441800	-2.062111
C	2.790288	-0.397624	-0.496831
H	3.611285	-0.753607	-1.155219
H	2.749308	1.561265	-1.201405
O	2.596090	-0.991659	0.558911
Na	0.846406	-0.132556	1.750079
