

Supporting Information

**Aerobic alcoholization via aromatization driven C–C bond  
cleavage of unstrained ketones**

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**Table of Contents**

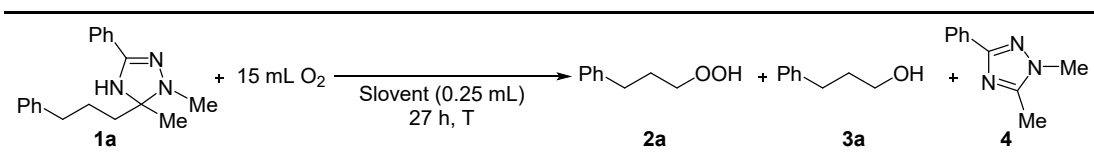
1. General Information .....	S1
2. Optimization of the Reaction Conditions .....	S1
3. General Procedures for Preparation of the dihydro-1,2,4-triazole substrates 1 .....	S3
4. General procedure for the Synthesis of compounds 3, 4, 5. ....	S4
5. Mechanism research .....	S5
6. Reaction of substrate 1am under standard conditions .....	S7
7. Analytical Data of the compounds 1, 2, 3, 4, 5, 6, 9, 14 .....	S7
8. Copies of <sup>1</sup> H, <sup>13</sup> C, and <sup>19</sup> F NMR Spectra .....	S36
9. References .....	S113

## 1. General Information

All reagents were purchased from commercial sources and used without further purification unless otherwise stated. All reactions were monitored by thin-layer chromatography (TLC). All reactions were carried out in oxygen atmosphere unless otherwise stated. Column chromatography was performed on silica gel (200-300 mesh) and visualized with ultraviolet light. Ethyl acetate and petroleum ether were used as eluents (unless otherwise stated).  $^1\text{H}$ ,  $^{13}\text{C}$  NMR and  $^{19}\text{F}$  NMR spectra were recorded on 400 MHz and 600 MHz NMR spectrometers in  $\text{CDCl}_3$  (unless otherwise stated) at room temperature. The chemical shifts are referenced to internal TMS. HRMS analyses were made by Lanzhou University by means of ESI. All solvents were purified and dried by standard techniques.

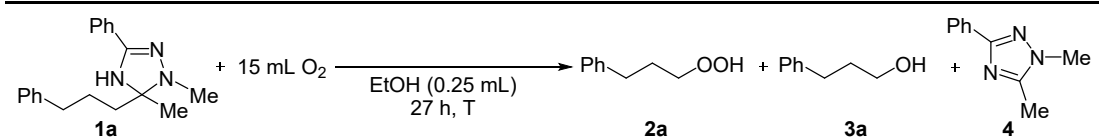
## 2. Optimization of the Reaction Conditions

### 1). Optimizing reaction temperature (T)<sup>a</sup>

				
Entry	T (°C)	Yield <sup>b</sup> <b>2a</b> (%)	Yield <sup>b</sup> <b>3a</b> (%)	Yield <sup>b</sup> ( <b>2a+3a</b> ) (%)
1	0	0	0	0
2	25	0	22	22
3	40	20	25	45
4	55	17	27	44
5	65	15	32	47
6	80	37	26	<b>53</b>

<sup>a</sup>General conditions: **1a** (0.1 mmol) and  $\text{O}_2$  (15.0 mL), in MeOH (0.25 mL) at T °C for 27 h. <sup>b</sup>Yields were determined by  $^1\text{H}$  NMR using dibromomethane as internal standard.

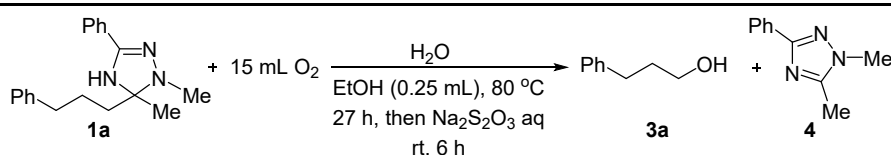
## 2). Optimizing reaction temperature in EtOH (T)<sup>a</sup>



Entry	T (°C)	Yield <sup>b</sup> <b>2a</b> (%)	Yield <sup>b</sup> <b>3a</b> (%)	Yield <sup>b</sup> ( <b>2a+3a</b> ) (%)
1	80	37	26	<b>63 (60)<sup>c</sup></b>
2	100	0	20	20

<sup>a</sup>General conditions: **1a** (0.1 mmol) and O<sub>2</sub> (15.0 mL,) in EtOH (0.25 mL) at T °C for 27 h. <sup>b</sup>Yields were determined by <sup>1</sup>H NMR using dibromomethane as internal standard. <sup>c</sup>After the reaction is completed, add saturated Na<sub>2</sub>S<sub>2</sub>O<sub>3</sub> aqueous solution and stir at room temperature for 6 h.

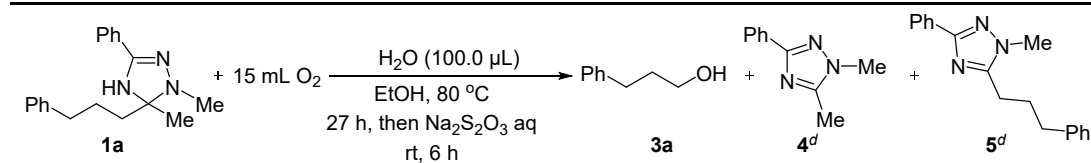
## 3). Screening the amount of H<sub>2</sub>O<sup>a</sup>



Entry	H <sub>2</sub> O (μL)	Yield <sup>b</sup> <b>3a</b> (%)
1	5	48
2	20	65
3	50	43
4	100	<b>78</b>
5	150	64
6	200	77

<sup>a</sup>General conditions: **1a** (0.1 mmol) and O<sub>2</sub> (15.0 mL,) in EtOH (0.25 mL) and H<sub>2</sub>O at 80 °C for 27 h, then add saturated Na<sub>2</sub>S<sub>2</sub>O<sub>3</sub> aq and stir at room temperature for 6 h. <sup>b</sup>Yields were determined by <sup>1</sup>H NMR using dibromomethane as internal standard.

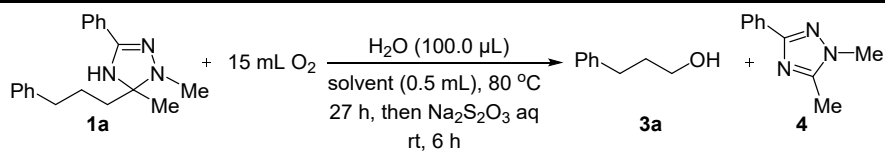
## 4). Screening the amount of EtOH<sup>a</sup>



Entry	EtOH (mL)	Yield <sup>b</sup> <b>3a</b> (%)
1	0.50	<b>82 (78)<sup>c</sup></b>
2	0.75	79
3	1.00	78
4	1.25	79
5	1.50	72
6 <sup>e</sup>	0.50	42

<sup>a</sup>General conditions: **1a** (0.1 mmol) and O<sub>2</sub> (15.0 mL,) in H<sub>2</sub>O (0.25 mL) and EtOH at 80 °C for 27 h, then add saturated Na<sub>2</sub>S<sub>2</sub>O<sub>3</sub> aq and stir at room temperature for 6 h. <sup>b</sup>Yields were determined by <sup>1</sup>H NMR using dibromomethane as internal standard. <sup>c</sup>Isolated yield. <sup>d</sup>The yield of **5** is 3% under standard conditions, and the yield of **4** is 96% under standard conditions (entry 1). <sup>e</sup>**1a** was replaced by 2-(1,5-dimethyl-5-(3-phenylpropyl)-4,5-dihydro-1H-1,2,4-triazol-3-yl)pyridine (**1ao**).

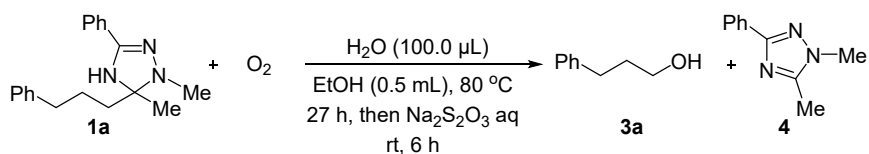
### 5). Screening the type of solvents<sup>a</sup>



Entry	Solvent	Yield <sup>b</sup> <b>3a</b> (%)
1	<sup>t</sup> BuOH	68
2	Toluene	63
3	DCE	61
4	DMSO	77
5	EA	54
6	$\text{CH}_3\text{CN}$	59

<sup>a</sup>General conditions: **1a** (0.1 mmol) and  $\text{O}_2$  (15.0 mL), in solvent (0.5 mL) and  $\text{H}_2\text{O}$  (100.0  $\mu\text{L}$ ) at 80 °C for 27 h, then add saturated  $\text{Na}_2\text{S}_2\text{O}_3$  aq and stir at room temperature for 6 h. <sup>b</sup>Yields were determined by  $^1\text{H}$  NMR using dibromomethane as internal standard.

### 6). Screening the amount of $\text{O}_2$ <sup>a</sup>



Entry	$\text{O}_2$ (mL)	Yield <sup>b</sup> <b>3a</b> (%)
1	Air	29
2	5	40
3	10	69
4	20	63
5	Ballon	57
6	Ar	0

<sup>a</sup>General conditions: **1a** (0.1 mmol) and  $\text{O}_2$  in EtOH (0.5 mL) and  $\text{H}_2\text{O}$  (100.0  $\mu\text{L}$ ) at 80 °C for 27 h, then add saturated  $\text{Na}_2\text{S}_2\text{O}_3$  aq and stir at room temperature for 6 h. <sup>b</sup>Yields were determined by  $^1\text{H}$  NMR using dibromomethane as internal standard.



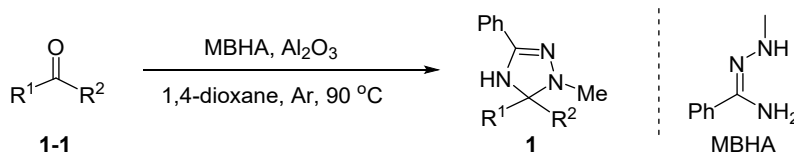
## 7). Screening the acid catalysts in one pot<sup>a</sup>

Entry	Acid catalysts (10 mol%)	Yield <sup>b</sup> <b>3a</b> (%)
1	TsOH	12
2	1-AdCOOH	12
3	CH <sub>3</sub> COOH	13
4	CF <sub>3</sub> COOH	15
5	<i>n</i> -PrCOOH	14
6 <sup>c</sup>	no	40 <sup>d</sup>

<sup>a</sup>General procedure: a mixture of **1-1** (0.5 mmol), MBHA (0.5 mmol), acid catalysts (10 mol%) and Al<sub>2</sub>O<sub>3</sub> (activated, neutral) (0.6 mmol) in 1,4-dioxane (1.0 mL) was combined in a 20-mL vial and sealed under argon. Then the reaction was stirred in oil bath pot at 90 °C for 29 hours. After cooled to room temperature, the reaction mixture was filtered through a short plug of Celite using EA as an eluent. The filtrate was concentrated under vacuum to provide the crude product. A reaction tube (25.0 mL) was charged with a magnetic stir-bar and crude product. Then remove the air from the reaction tube and fill it with oxygen using an oxygen balloon. H<sub>2</sub>O (500.0 μL) and absolute EtOH (2.5 mL) were added via syringe. The tube was stirred at 80 °C in the pre-heated oil bath for 27 h. After completion, the reaction mixture was cooled to room temperature, add saturated Na<sub>2</sub>S<sub>2</sub>O<sub>3</sub> aqueous solution and stir at room temperature for 6 h.

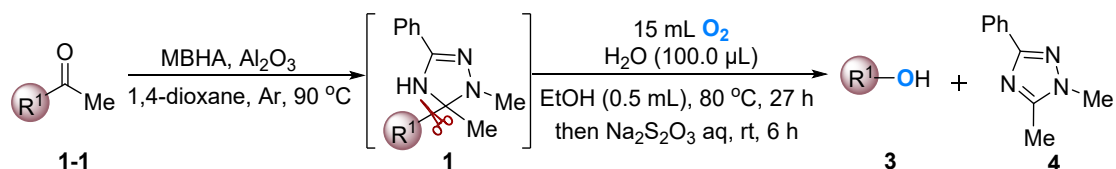
<sup>b</sup>Yields were determined by <sup>1</sup>H NMR using dibromomethane as internal standard. <sup>c</sup>General procedure see ESI part 4 for a one-pot procedure. <sup>d</sup>Isolated yield. Ad: adamantyl

## 3. General Procedures for Preparation of the dihydro-1,2,4-triazole substrates **1**



A mixture of **1-1**<sup>[1-6]</sup> (1.0 mmol), *N'*-methylbenzohydrazonamide (MBHA) (149.1 mg, 1.0 mmol), and aluminum oxide (activated, neutral) (122.3 mg, 1.2 mmol) in 1,4-dioxane (1.0 mL) was combined in a 20-mL vial and sealed under argon. Then the reaction was stirred in oil bath pot at 90 °C for 24 hours. After cooled to room temperature, the reaction mixture was filtered through a short plug of Celite using ethyl acetate (EA) as an eluent. The filtrate was concentrated under vacuum to provide the crude product. The residue was purified by preparative TLC or column chromatography over silica gel using petroleum ether (PE)/EA /triethyl amine as an eluent to afford substrate **1**.

## 4. General procedure for the Synthesis of compounds **3**.

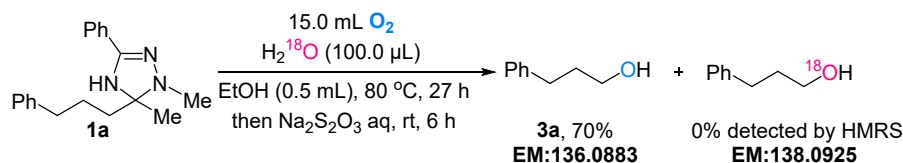


**For a one-pot procedure:** A mixture of 5-phenylpentan-2-one (0.5 mmol), MBHA (74.5mg, 0.5 mmol), and aluminum oxide (activated, neutral) (61.0 mg, 0.6 mmol) in 1,4-dioxane (1.0 mL) was combined in a 20-mL vial and sealed under argon. Then the reaction was stirred in oil bath pot at 90 °C for 52 hours. After cooled to room temperature, the reaction mixture was filtered through a short plug of Celite using EA as an eluent. The filtrate was concentrated under vacuum to provide the crude product. A reaction tube (25.0 mL) was charged with a magnetic stir-bar and crude product. Then remove the air from the reaction tube and fill it with oxygen using an oxygen balloon. H<sub>2</sub>O (500.0 µL) and absolute EtOH (2.5 mL) were added via syringe. The tube was stirred at 80 °C in the pre-heated oil bath for 27 h. After completion, the reaction mixture was cooled to room temperature, add saturated Na<sub>2</sub>S<sub>2</sub>O<sub>3</sub> aqueous solution and stir at room temperature for 6 h. The reaction mixture diluted with H<sub>2</sub>O (2.0 mL) and was extracted by EA (3 × 3.0 mL). The organic layers were combined and dried by Na<sub>2</sub>SO<sub>4</sub>. After filtration, evaporation of the solvent and purification by preparative TLC to give **3a** in 40% yield.

**Synthesis of compounds 3 from dihydro-1,2,4-triazole substrates 1:** a reacting tube (16.0 mL) was charged with a magnetic stir-bar and substrates **1** (0.1 mmol). Then remove the air from the reaction tube and fill it with oxygen using an oxygen balloon. H<sub>2</sub>O (100.0 µL) and absolute EtOH (0.5 mL) were added via syringe. The tube was stirred at 80 °C in the pre-heated oil bath for 27 h. After completion, the reaction mixture was cooled to room temperature, add saturated Na<sub>2</sub>S<sub>2</sub>O<sub>3</sub> aqueous solution and stir at room temperature for 6 h. The reaction mixture diluted with H<sub>2</sub>O (2.0 mL) and was extracted by EA (3 × 3.0 mL). The organic layers were combined and dried by Na<sub>2</sub>SO<sub>4</sub>. After filtration, evaporation of the solvent and purification by preparative TLC or flash column chromatograph, the desired products **3**, **4** were obtained.

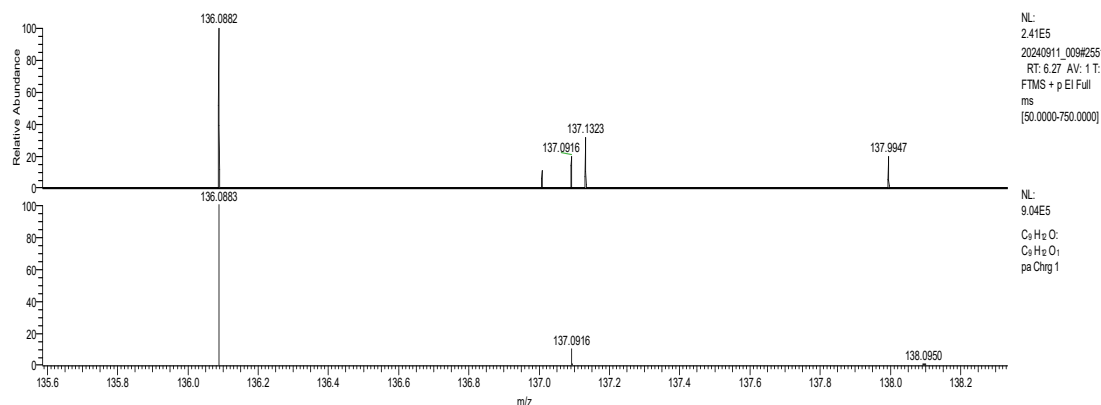
## 5. Mechanism research

### a) H<sub>2</sub><sup>18</sup>O labeling experiment

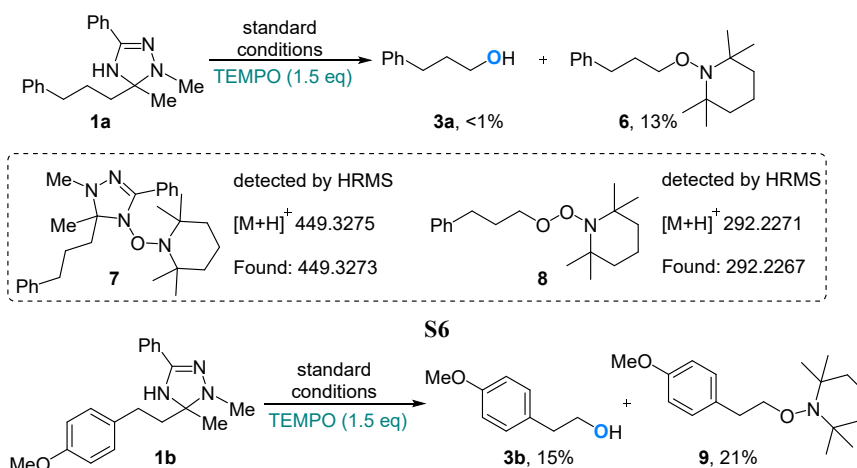


A reacting tube (16.0 mL) was charged with a magnetic stir-bar and dihydro-1,2,4-triazole substrates **1a** (0.1 mmol). Then remove the air from the reaction tube and fill it with oxygen using an oxygen balloon. H<sub>2</sub><sup>18</sup>O (100.0 μL) and absolute EtOH (0.5 mL) were added via syringe. The tube was stirred at 80 °C in the pre-heated oil bath for 27 h. After completion, the reaction mixture was cooled to room temperature, add saturated Na<sub>2</sub>S<sub>2</sub>O<sub>3</sub> aqueous solution and stir at room temperature for 6 h. The reaction mixture diluted with H<sub>2</sub>O (2.0 mL) and was extracted by EA (3 × 3.0 mL). The organic layer was dried over sodium sulfate and concentrated in vacuo. The reaction was purified by preparative TLC (25% EA/PE) to afford **3a** as a colorless oil (9.6 mg, 70%). *HRMS only detected a peak for 3a, thus no <sup>18</sup>O was incorporated.*

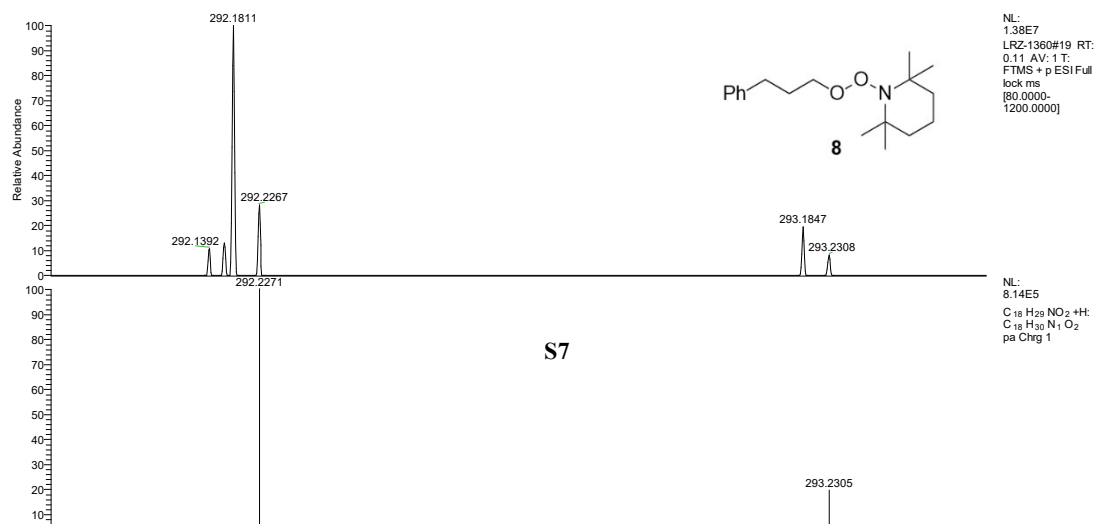
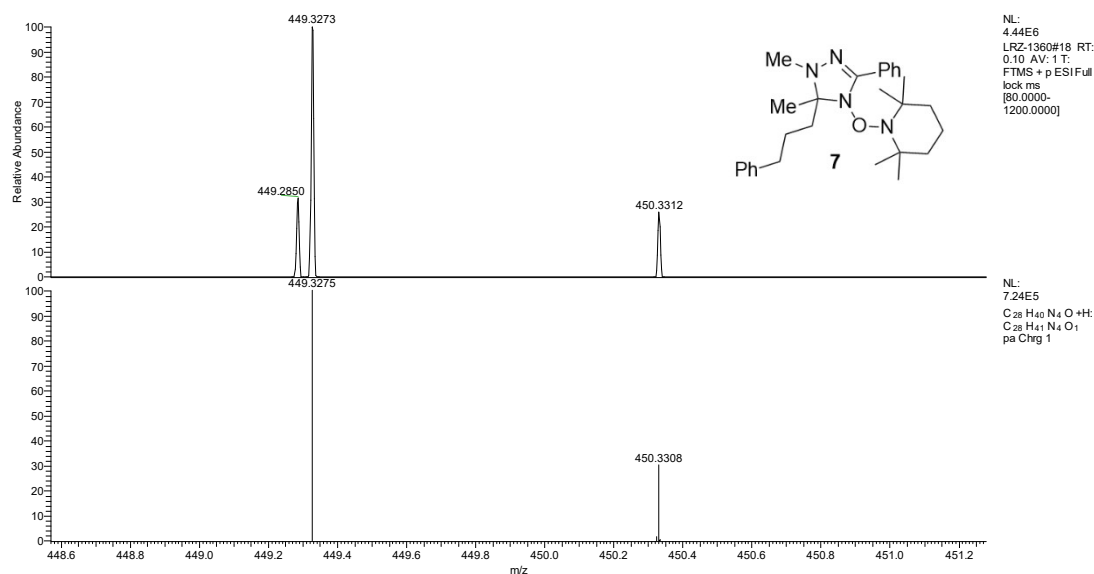
**HRMS (EI) Calcd. For C<sub>9</sub>H<sub>12</sub>O<sup>+</sup> [M]<sup>+</sup>: 136.0883; Found: 136.0882**



### b) Radical trapping experiments

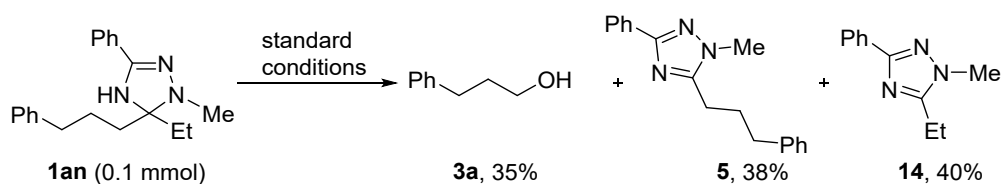


A reacting tube (16.0 mL) was charged with a magnetic stir-bar, dihydro-1,2,4-triazole substrates **1a** (0.1 mmol) and TEMPO (0.15 mmol). Then remove the air from the reaction tube and fill it with oxygen using an oxygen balloon. H<sub>2</sub>O (100.0  $\mu$ L) and absolute EtOH (0.5 mL) were added via syringe. The tube was stirred at 80 °C in the pre-heated oil bath for 27 h. After completion, the reaction mixture was cooled to room temperature, add saturated Na<sub>2</sub>S<sub>2</sub>O<sub>3</sub> aqueous solution and stir at room temperature for 6 h. The reaction mixture diluted with H<sub>2</sub>O (2.0 mL) and was extracted by EA (3  $\times$  3.0 mL). The organic layers were combined and dried by Na<sub>2</sub>SO<sub>4</sub>. After filtration, evaporation of the solvent and purification by preparative TLC or flash column chromatograph the desired products **6**, **9** were obtained. Compounds **7**, **8** were detected by HRMS.

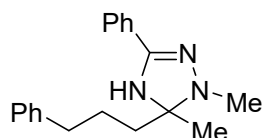


## 6. Reaction of substrate 1an under standard conditions

When substrate **1a** is replaced with **1an**, the yield of **3a** decreases to 35%, and the reaction selectivity cleavage ratio is 1:1 (**5:14**)



## 7. Analytical Data of the compounds 1, 2, 3, 4, 5, 6, 9, 14

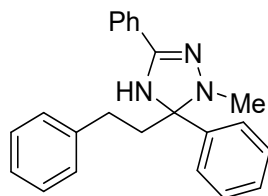


### 1,5-dimethyl-3-phenyl-5-(3-phenylpropyl)-4,5-dihydro-1H-1,2,4-triazole (**1a**)

White solid (50%, 147 mg), purified by flash column chromatograph (PE : EA = 3 : 1).

<sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>) δ 7.60 – 7.59 (m, 2H), 7.36 – 7.32 (m, 3H), 7.28 (t, *J* = 7.5 Hz, 2H), 7.21 – 7.17 (m, 3H), 4.13 (s, 1H), 2.78 (s, 3H), 2.72 – 2.64 (m, 2H), 1.88 – 1.77 (m, 3H), 1.75 – 1.69 (m, 1H), 1.24 (s, 3H).

<sup>13</sup>C NMR (151 MHz, CDCl<sub>3</sub>) δ 148.6, 142.2, 129.0, 128.8, 128.4, 128.3, 128.2, 125.7, 125.1, 85.0, 38.4, 35.9, 35.4, 26.1, 21.1.

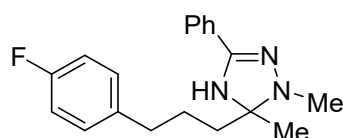


### 1-methyl-5-phenethyl-3,5-diphenyl-4,5-dihydro-1H-1,2,4-triazole (**1b**)

Yellow solid (50%, 170 mg), purified by flash column chromatograph (PE : EA = 3 : 1).

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.66 – 7.61 (m, 2H), 7.53 – 7.48 (m, 2H), 7.44 – 7.38 (m, 5H), 7.37 – 7.27 (m, 3H), 7.23 – 7.19 (m, 3H), 4.73 (s, 1H), 2.88 – 2.80 (m, 2H), 2.61 – 2.49 (m, 5H).

$^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  148.4, 142.1, 140.4, 129.2, 128.8, 128.5, 128.5, 128.4, 128.2, 128.2, 126.5, 125.9, 125.3, 87.5, 37.5, 36.5, 30.7.

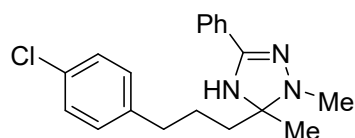


**5-(3-(4-fluorophenyl)propyl)-1,5-dimethyl-3-phenyl-4,5-dihydro-1H-1,2,4-triazole (1c)**

White solid (80%, 248 mg), purified by flash column chromatograph (PE : EA = 3 : 1).

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.62 – 7.57 (m, 2H), 7.38 – 7.33 (m, 3H), 7.17 – 7.11 (m, 2H), 6.99 – 6.93 (m, 2H), 4.12 (s, 1H), 2.77 (s, 3H), 2.68 – 2.59 (m, 2H), 1.88 – 1.65 (m, 4H), 1.24 (s, 3H).

$^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  161.2 (d,  $J = 243.2$  Hz), 148.5, 137.8 (d,  $J = 3.2$  Hz), 129.7 (d,  $J = 7.7$  Hz), 129.1, 128.8, 128.3, 125.1, 114.9 (d,  $J = 21.1$  Hz), 84.9, 38.3, 35.3, 35.1, 26.2, 21.2

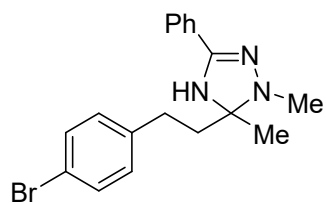


**5-(3-(4-chlorophenyl)propyl)-1,5-dimethyl-3-phenyl-4,5-dihydro-1H-1,2,4-triazole (1d)**

White solid (82%, 268 mg), purified by flash column chromatograph (PE : EA = 3 : 1).

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.62 – 7.57 (m, 2H), 7.38 – 7.32 (m, 3H), 7.26 – 7.22 (m, 2H), 7.13 – 7.11 (m, 2H), 4.11 (s, 1H), 2.77 (s, 3H), 2.68 – 2.59 (m, 2H), 1.88 – 1.64 (m, 4H), 1.24 (s, 3H).

$^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  148.5, 140.6, 131.4, 129.7, 129.1, 128.8, 128.3, 128.3, 125.1, 84.9, 38.2, 35.4, 35.2, 25.9, 21.2.

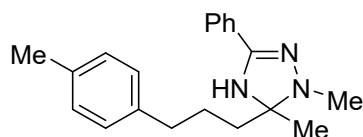


**5-(4-bromophenethyl)-1,5-dimethyl-3-phenyl-4,5-dihydro-1H-1,2,4-triazole (1e)**

Yellow solid (75%, 268 mg), purified by flash column chromatograph (PE : EA = 3 : 1).

$^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ )  $\delta$  7.59 (d,  $J$  = 5.5 Hz, 2H), 7.42 – 7.36 (m, 5H), 7.10 (d,  $J$  = 7.7 Hz, 2H), 4.14 (s, 1H), 2.81 (d,  $J$  = 10.9 Hz, 5H), 2.06 – 1.93 (m, 2H), 1.30 (s, 3H).

$^{13}\text{C}$  NMR (151 MHz,  $\text{CDCl}_3$ )  $\delta$  148.5, 141.4, 131.3, 130.1, 129.2, 128.6, 128.4, 125.1, 119.3, 84.9, 40.2, 35.3, 30.2, 21.4.

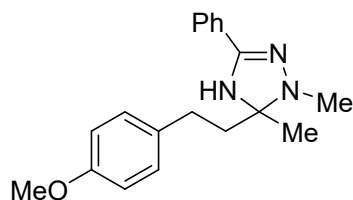


**1,5-dimethyl-3-phenyl-5-(3-(p-tolyl)propyl)-4,5-dihydro-1H-1,2,4-triazole (1f)**

White solid (85%, 260 mg), purified by flash column chromatograph (PE : EA = 3 : 1).

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.62 – 7.57 (m, 2H), 7.38 – 7.31 (m, 3H), 7.10 (s, 4H), 4.13 (s, 1H), 2.78 (s, 3H), 2.70 – 2.58 (m, 2H), 2.32 (s, 3H), 1.86 – 1.76 (m, 3H), 1.75 – 1.68 (m, 1H), 1.24 (s, 3H).

$^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  148.6, 139.1, 135.1, 129.0, 128.9, 128.8, 128.3, 128.2, 125.2, 85.0, 38.3, 35.5, 35.4, 26.3, 21.1, 20.9.

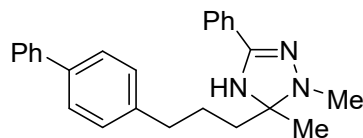


**5-(4-methoxyphenethyl)-1,5-dimethyl-3-phenyl-4,5-dihydro-1H-1,2,4-triazole (1g)**

White solid (82%, 253 mg), purified by flash column chromatograph (PE : EA = 3 : 1).

$^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ )  $\delta$  7.59 – 7.56 (m, 2H), 7.37 – 7.34 (m, 3H), 7.16 – 7.13 (m, 2H), 6.85 – 6.83 (m, 2H), 4.14 (s, 1H), 3.79 (s, 3H), 2.83 (s, 3H), 2.82 – 2.76 (m, 2H), 2.09 – 2.04 (m, 1H), 1.99 – 1.93 (m, 1H), 1.32 (s, 3H).

$^{13}\text{C}$  NMR (151 MHz,  $\text{CDCl}_3$ )  $\delta$  157.7, 148.6, 134.2, 129.2, 129.0, 128.8, 128.3, 125.1, 113.8, 84.9, 55.2, 40.4, 35.1, 29.8, 21.3.

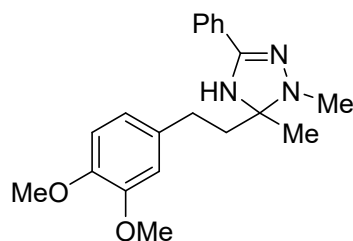


**5-(3-([1,1'-biphenyl]-4-yl)propyl)-1,5-dimethyl-3-phenyl-4,5-dihydro-1H-1,2,4-triazole (1h)**

White solid (80%, 295 mg), purified by flash column chromatograph (PE : EA = 3 : 1).

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.62 – 7.58 (m, 4H), 7.54 – 7.52 (m, 2H), 7.45 – 7.41 (m, 2H), 7.37 – 7.33 (m, 3H), 7.29 – 7.26 (m, 2H), 4.14 (s, 1H), 2.80 (s, 3H), 2.77 – 2.69 (m, 2H), 1.93 – 1.71 (m, 4H), 1.26 (s, 3H).

$^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  148.6, 141.4, 141.0, 138.7, 129.1, 128.9, 128.8, 128.6, 128.3, 127.0, 126.9, 126.9, 125.2, 85.0, 38.4, 35.6, 35.4, 26.1, 21.2.

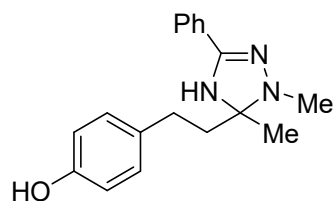


**5-(3,4-dimethoxyphenethyl)-1,5-dimethyl-3-phenyl-4,5-dihydro-1H-1,2,4-triazole (1i)**

White solid (78%, 264 mg), purified by flash column chromatograph (PE : EA = 3 : 1).

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.57 (d,  $J$  = 3.6 Hz, 2H), 7.39 – 7.31 (m, 3H), 6.78 – 6.72 (m, 3H), 4.31 (s, 1H), 3.82 (d,  $J$  = 8.7 Hz, 6H), 2.82 – 2.76 (m, 5H), 2.10 – 2.05 (m, 1H), 2.00 – 1.92 (m, 1H), 1.30 (s, 3H).

$^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  148.6, 146.9, 134.7, 129.0, 128.5, 128.3, 128.2, 125.0, 119.9, 111.5, 111.1, 84.9, 55.7, 55.6, 40.1, 35.2, 30.2, 21.1.



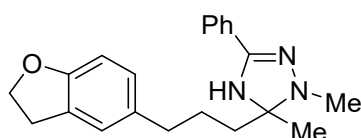
**4-(2-(1,5-dimethyl-3-phenyl-4,5-dihydro-1H-1,2,4-triazol-5-yl)ethyl)phenol (1j)**

White solid (60%, 177 mg), purified by flash column chromatograph (PE : EA = 1 : 1).



$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.57 (s, 2H), 7.34 (s, 3H), 7.04 (d,  $J = 7.7$  Hz, 2H), 6.78 (d,  $J = 7.8$  Hz, 2H), 4.27 (s, 1H), 2.81 (s, 3H), 2.77 – 2.73 (m, 2H), 2.12 – 1.91 (m, 2H), 1.32 (s, 3H).

$^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  154.4, 149.3, 133.4, 129.4, 129.3, 128.4, 128.3, 125.3, 115.4, 85.0, 40.3, 35.2, 29.8, 21.2.

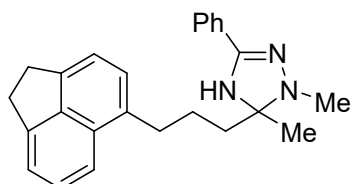


**5-(3-(2,3-dihydrobenzofuran-5-yl)propyl)-1,5-dimethyl-3-phenyl-4,5-dihydro-1H-1,2,4-triazole (1k)**

White solid (72%, 241 mg), purified by flash column chromatograph (PE : EA = 3 : 1).

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.62 – 7.58 (m, 2H), 7.38 – 7.33 (m, 3H), 7.03 (s, 1H), 6.92 (d,  $J = 8.2$  Hz, 1H), 6.69 (d,  $J = 8.1$  Hz, 1H), 4.53 (t,  $J = 8.7$  Hz, 2H), 4.15 (s, 1H), 3.16 (t,  $J = 8.7$  Hz, 2H), 2.78 (s, 3H), 2.64 – 2.55 (m, 2H), 1.83 – 1.67 (m, 4H), 1.25 (s, 3H).

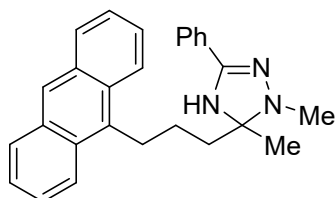
$^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  158.1, 148.6, 134.2, 129.0, 128.8, 128.3, 127.7, 126.9, 125.1, 124.8, 108.8, 85.0, 71.0, 38.3, 35.4, 35.4, 29.7, 26.7, 21.1.



**5-(3-(1,2-dihydroacenaphthylen-5-yl)propyl)-1,5-dimethyl-3-phenyl-4,5-dihydro-1H-1,2,4-triazole (1l)**

White solid (65%, 239 mg), purified by flash column chromatograph (PE : EA = 3 : 1).

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.71 (d,  $J = 8.3$  Hz, 1H), 7.57 – 7.55 (m, 2H), 7.44 (dd,  $J = 8.3, 7.0$  Hz, 1H), 7.35 – 7.32 (m, 3H), 7.29 – 7.27 (m, 2H), 7.20 (d,  $J = 7.0$  Hz, 1H), 4.09 (s, 1H), 3.41 – 3.35 (m, 4H), 3.12 – 3.00 (m, 2H), 2.79 (s, 3H), 1.99 – 1.86 (m, 3H), 1.85 – 1.77 (m, 1H), 1.24 (s, 3H).

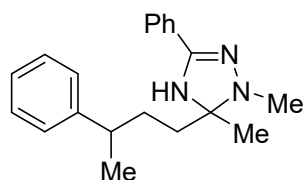


**5-(3-(anthracen-9-yl)propyl)-1,5-dimethyl-3-phenyl-4,5-dihydro-1H-1,2,4-triazole (1m)**

Yellow solid (65%, 255 mg), purified by flash column chromatograph (PE : EA = 3 : 1).

<sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>) δ 8.33 (s, 1H), 8.29 (d, *J* = 8.4 Hz, 2H), 8.00 (d, *J* = 7.6 Hz, 2H), 7.57 (dd, *J* = 6.3, 2.7 Hz, 2H), 7.48 – 7.42 (m, 4H), 7.38 – 7.33 (m, 3H), 4.11 (s, 1H), 3.75 – 3.64 (m, 2H), 2.82 (s, 3H), 2.12 – 1.95 (m, 4H), 1.24 (s, 3H).

<sup>13</sup>C NMR (151 MHz, CDCl<sub>3</sub>) δ 148.5, 134.8, 131.5, 129.4, 129.1, 129.0, 128.7, 128.3, 125.6, 125.4, 125.1, 124.7, 124.3, 85.0, 38.9, 35.3, 27.9, 26.1, 20.8.

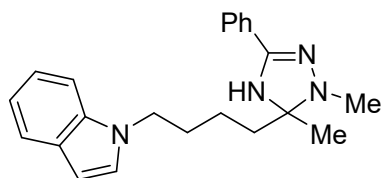


**1,5-dimethyl-3-phenyl-5-(3-phenylbutyl)-4,5-dihydro-1H-1,2,4-triazole (1n)**

Yellow oil (70%, 215 mg), purified by flash column chromatograph (PE : EA = 3 : 1).

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.61 – 7.59 (m, 3H), 7.45 – 7.40 (m, 1H), 7.36 – 7.32 (m, 5H), 7.30 – 7.27 (m, 4H), 7.23 – 7.16 (m, 7H), 4.10 (d, *J* = 13.1 Hz, 2H), 3.10 – 3.04 (m, 1H), 2.76 – 2.68 (m, 7H), 1.86 – 1.67 (m, 5H), 1.65 – 1.53 (m, 2H), 1.52 – 1.45 (m, 1H), 1.36 (t, *J* = 7.3 Hz, 1H), 1.28 (dd, *J* = 6.9, 2.5 Hz, 6H), 1.19 (d, *J* = 6.6 Hz, 6H).

<sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>) δ 148.6, 148.6, 147.3, 147.2, 129.0, 129.0, 128.8, 128.8, 128.7, 128.5, 128.4, 128.3, 126.9, 126.9, 126.2, 126.0, 125.9, 125.1, 85.0, 85.0, 40.2, 40.1, 36.8, 36.7, 35.3, 35.2, 32.7, 32.6, 22.7, 22.7, 21.1, 21.1.

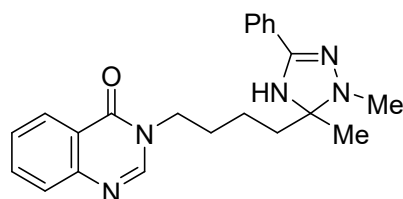


**1-(4-(1,5-dimethyl-3-phenyl-4,5-dihydro-1H-1,2,4-triazol-5-yl)butyl)-1H-indole (1o)**

Yellow oil (72%, 249 mg), purified by flash column chromatograph (PE : EA = 1 : 1).

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.62 (dd,  $J = 23.2, 5.8$  Hz, 3H), 7.43 – 7.36 (m, 4H), 7.21 (t,  $J = 7.5$  Hz, 1H), 7.13 – 7.04 (m, 2H), 6.49 (d,  $J = 2.2$  Hz, 1H), 4.21 – 4.10 (m, 3H), 2.78 (s, 3H), 1.94 – 1.87 (m, 2H), 1.81 – 1.72 (m, 1H), 1.69 – 1.61 (m, 1H), 1.60 – 1.51 (m, 2H), 1.20 (s, 3H).

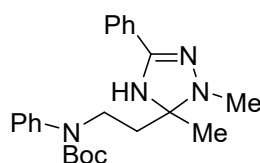
$^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  148.6, 135.8, 129.1, 128.7, 128.5, 128.3, 127.8, 125.1, 121.2, 120.9, 119.1, 109.3, 100.8, 84.9, 46.2, 38.3, 35.4, 30.3, 21.8, 21.0.



**3-(4-(1,5-dimethyl-3-phenyl-4,5-dihydro-1H-1,2,4-triazol-5-yl)butyl)quinazolin-4(3H)-one (1p)**

Yellow solid (58%, 217 mg), purified by flash column chromatograph (PE : EA = 1 : 1).

$^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ )  $\delta$  8.31 (d,  $J = 7.9$  Hz, 1H), 8.06 – 8.00 (m, 1H), 7.77 – 7.70 (m, 2H), 7.60 – 7.59 (m, 2H), 7.52 – 7.49 (m, 1H), 7.39 – 7.34 (m, 3H), 4.19 (s, 1H), 4.13 – 3.97 (m, 2H), 2.79 (s, 3H), 1.91 – 1.84 (m, 2H), 1.83 – 1.72 (m, 2H), 1.66 – 1.60 (m, 2H), 1.26 (s, 3H).

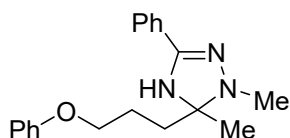


**tert-butyl(2-(1,5-dimethyl-3-phenyl-4,5-dihydro-1H-1,2,4-triazol-5-yl)ethyl)(phenyl)carbamate (1q)**

Yellow oil (74%, 291 mg), purified by flash column chromatograph (PE : EA = 3 : 1).

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.58 (dd,  $J = 6.6, 2.9$  Hz, 2H), 7.36 – 7.29 (m, 5H), 7.19 – 7.16 (t,  $J = 7.6$  Hz, 3H), 4.60 (s, 1H), 3.96 – 3.91 (m, 2H), 2.72 (s, 3H), 2.07 – 2.00 (m, 1H), 1.97 – 1.90 (m, 1H), 1.42 (s, 9H), 1.24 (s, 3H).

$^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  154.8, 148.8, 142.4, 129.0, 128.6, 128.6, 128.2, 126.8, 125.9, 125.1, 84.2, 80.0, 46.4, 36.2, 35.0, 28.2, 20.9.

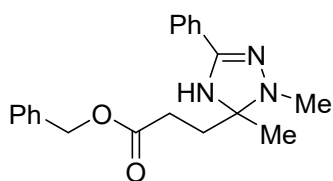


**1,5-dimethyl-5-(3-phenoxypropyl)-3-phenyl-4,5-dihydro-1H-1,2,4-triazole (1r)**

Yellow oil (68%, 210 mg), purified by flash column chromatograph (PE : EA = 3 : 1).

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.60 (dd,  $J$  = 6.4, 2.9 Hz, 2H), 7.39 – 7.32 (m, 3H), 7.30 – 7.26 (m, 2H), 6.96 – 6.90 (m, 3H), 4.26 (s, 1H), 4.09 – 4.00 (m, 2H), 2.81 (s, 3H), 2.07 – 2.00 (m, 2H), 1.97 – 1.87 (m, 2H), 1.30 (s, 3H).

$^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  158.8, 148.6, 129.4, 129.1, 128.7, 128.3, 125.1, 120.5, 114.4, 84.9, 67.7, 35.3, 35.1, 24.3, 21.3.

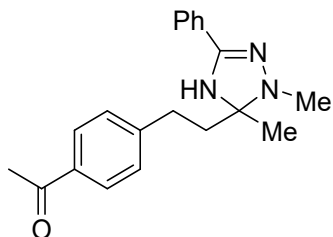


**benzyl 3-(1,5-dimethyl-3-phenyl-4,5-dihydro-1H-1,2,4-triazol-5-yl)propanoate (1s)**

Yellow oil (51%, 171 mg), purified by flash column chromatograph (PE : EA = 3 : 1).

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.59 – 7.52 (m, 2H), 7.38 – 7.29 (m, 8H), 5.12 – 5.05 (m, 2H), 4.15 (s, 1H), 2.75 – 2.55 (m, 5H), 2.07 (t,  $J$  = 7.1 Hz, 2H), 1.27 (s, 3H).

$^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  174.2, 148.3, 136.0, 129.1, 128.6, 128.4, 128.3, 128.0, 128.0, 125.1, 84.6, 66.1, 35.1, 33.0, 29.3, 21.5.

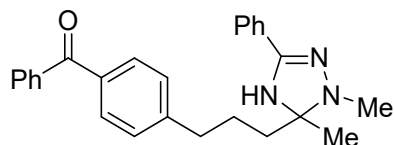


**1-(4-(2-(1,5-dimethyl-3-phenyl-4,5-dihydro-1H-1,2,4-triazol-5-yl)ethyl)phenyl)ethan-1-one (1t)**

Yellow solid (67%, 215 mg), purified by flash column chromatograph (PE : EA = 3 : 1).

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.88 (d,  $J$  = 8.2 Hz, 2H), 7.61 – 7.59 (m, 2H), 7.39 – 7.30 (m, 5H), 4.16 (s, 1H), 2.93 (t,  $J$  = 8.3 Hz, 2H), 2.82 (s, 3H), 2.58 (s, 3H), 2.12 – 1.95 (m, 2H), 1.31 (s, 3H).

$^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  197.8, 148.5, 134.9, 129.2, 128.7, 128.6, 128.5, 128.4, 126.0, 125.1, 84.9, 40.1, 35.3, 30.8, 26.5, 21.5.

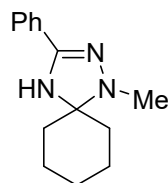


**(4-(3-(1,5-dimethyl-3-phenyl-4,5-dihydro-1H-1,2,4-triazol-5-yl)propyl)phenyl)(phenyl)methanone (1u)**

Yellow oil (60%, 238 mg), purified by flash column chromatograph (PE : EA = 3 : 1).

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.76 (dd,  $J$  = 17.7, 7.6 Hz, 4H), 7.61 – 7.56 (m, 3H), 7.47 (t,  $J$  = 7.6 Hz, 2H), 7.38 – 7.30 (m, 5H), 4.15 (s, 1H), 2.85 – 2.61 (m, 5H), 1.94 – 1.69 (m, 4H), 1.25 (s, 3H).

$^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  196.5, 148.6, 147.5, 137.8, 135.2, 132.1, 130.3, 129.9, 129.1, 128.7, 128.3, 128.3, 128.1, 125.1, 85.0, 38.3, 35.9, 35.4, 25.8, 21.2.

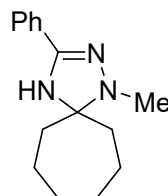


**1-methyl-3-phenyl-1,2,4-triazaspiro[4.5]dec-2-ene (1x)**

Yellow oil (54%, 123 mg), purified by flash column chromatograph (PE : EA = 3 : 1).

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.68 – 7.66 (m, 2H), 7.41 – 7.31 (m, 3H), 4.75 (s, 1H), 2.82 (s, 3H), 1.90 – 1.79 (m, 4H), 1.71 – 1.68 (m, 1H), 1.55 (td,  $J$  = 13.0, 3.7 Hz, 2H), 1.45 – 1.34 (m, 2H), 1.24 – 1.12 (m, 1H).

$^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  148.8, 128.8, 128.7, 128.1, 125.1, 84.0, 35.2, 32.5, 25.0, 23.1.

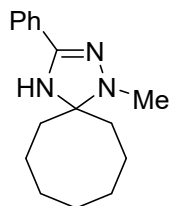


**1-methyl-3-phenyl-1,2,4-triazaspiro[4.6]undec-2-ene (1y)**

Yellow oil (77%, 187 mg), purified by flash column chromatograph (PE : EA = 3 : 1).

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.63 – 7.61 (m, 2H), 7.38 – 7.32 (m, 3H), 4.50 (s, 1H), 2.85 (s, 3H), 2.04 – 1.98 (m, 2H), 1.91 – 1.85 (m, 2H), 1.67 – 1.62 (m, 6H), 1.51 – 1.45 (m, 2H).

$^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  148.7, 129.1, 128.9, 128.3, 125.2, 87.9, 36.7, 35.6, 29.4, 22.8.

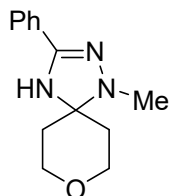


### 1-methyl-3-phenyl-1,2,4-triazaspiro[4.7]dodec-2-ene (1z)

Yellow oil (78%, 200 mg), purified by flash column chromatograph (PE : EA = 1 : 1).

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.63 – 7.61 (m, 2H), 7.43 – 7.34 (m, 3H), 4.43 (s, 1H), 2.85 (s, 3H), 2.08 (dd,  $J$  = 14.4, 8.8 Hz, 2H), 1.85 (dd,  $J$  = 14.2, 8.2 Hz, 2H), 1.70 – 1.46 (m, 10H).

$^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  148.6, 129.0, 129.0, 128.3, 125.2, 87.1, 36.4, 32.7, 28.0, 24.5, 22.6.

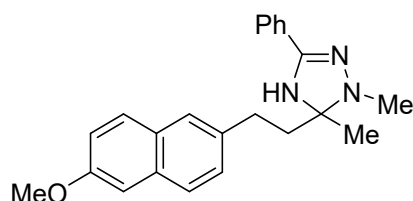


### 1-methyl-3-phenyl-8-oxa-1,2,4-triazaspiro[4.5]dec-2-ene (1aa)

Yellow solid (85%, 255 mg), purified by preparative TLC (PE : EA = 1 : 1).

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.69 – 7.64 (m, 2H), 7.40 – 7.35 (m, 3H), 4.73 (s, 1H), 4.05 (dd,  $J$  = 11.9, 5.0 Hz, 2H), 3.54 (td,  $J$  = 12.4, 1.8 Hz, 2H), 2.83 (s, 3H), 1.98 (td,  $J$  = 12.9, 5.2 Hz, 2H), 1.77 – 1.74 (m, 2H).

$^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  149.0, 129.4, 128.6, 128.4, 125.4, 81.2, 65.3, 35.5, 33.5.

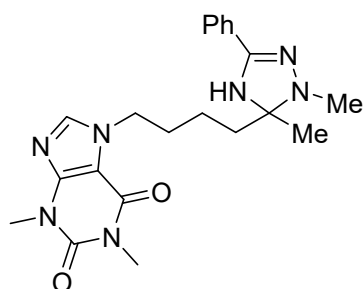


**5-(2-(6-methoxynaphthalen-2-yl)ethyl)-1,5-dimethyl-3-phenyl-4,5-dihydro-1H-1,2,4-triazole (1ac)**

White solid (84%, 301 mg), purified by flash column chromatograph (PE : EA = 3 : 1).

$^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ )  $\delta$  7.66 (t,  $J$  = 7.9 Hz, 2H), 7.60 – 7.56 (m, 3H), 7.38 – 7.33 (m, 4H), 7.13 – 7.10 (m, 2H), 4.16 (s, 1H), 3.92 (s, 3H), 3.02 – 2.94 (m, 2H), 2.86 (s, 3H), 2.20 – 2.14 (m, 1H), 2.09 – 2.04 (m, 1H), 1.35 (s, 3H).

$^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  157.1, 148.6, 137.4, 132.9, 129.1, 128.8, 128.7, 128.3, 127.8, 126.8, 126.0, 125.1, 118.6, 105.6, 85.0, 55.2, 40.1, 35.3, 30.7, 21.4.

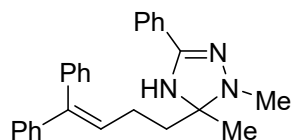


**7-(4-(1,5-dimethyl-3-phenyl-4,5-dihydro-1H-1,2,4-triazol-5-yl)butyl)-1,3-dimethyl-3,7-dihydro-1H-purine-2,6-dione (1ae)**

White solid (56%, 229 mg), purified by flash column chromatograph (PE : EA = 0 : 1).

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.62 – 7.56 (m, 2H), 7.53 (s, 1H), 7.40 – 7.32 (m, 3H), 4.36 – 4.24 (m, 2H), 4.14 (s, 1H), 3.58 (s, 3H), 3.41 (s, 3H), 2.77 (s, 3H), 2.00 – 1.93 (m, 2H), 1.83 – 1.69 (m, 2H), 1.59 – 1.56 (m, 2H), 1.24 (s, 3H).

$^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  155.0, 151.5, 148.8, 148.7, 140.8, 129.1, 128.5, 128.2, 125.1, 106.8, 84.8, 47.0, 37.8, 35.2, 30.8, 29.6, 27.8, 21.0, 14.0.

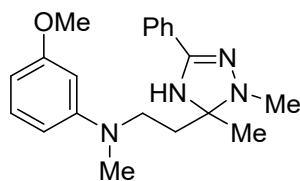


**5-(4,4-diphenylbut-3-en-1-yl)-1,5-dimethyl-3-phenyl-4,5-dihydro-1H-1,2,4-triazole (1ah)**

Yellow oil (48%, 182 mg), purified by flash column chromatograph (PE : EA = 3 : 1).

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.54 – 7.50 (m, 2H), 7.37 – 7.31 (m, 6H), 7.25 – 7.16 (m, 7H), 6.16 (t,  $J$  = 7.6 Hz, 1H), 4.08 (s, 1H), 2.75 (s, 3H), 2.33 (dd,  $J$  = 15.7, 7.8 Hz, 2H), 1.98 – 1.90 (m, 1H), 1.83 – 1.76 (m, 1H), 1.20 (s, 3H).

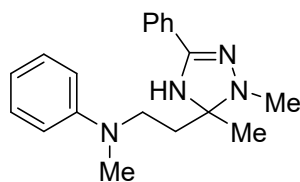
$^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  148.7, 142.5, 141.9, 139.9, 129.8, 129.4, 129.1, 128.8, 128.4, 128.3, 128.1, 127.2, 127.0, 126.9, 125.2, 85.1, 38.3, 35.2, 25.0, 21.1.



***N*-(2-(1,5-dimethyl-3-phenyl-4,5-dihydro-1*H*-1,2,4-triazol-5-yl)ethyl)-3-methoxy-*N*-methylaniline (1ai)**

Yellow oil (53%, 179 mg), purified by flash column chromatograph (PE : EA = 1 : 1).

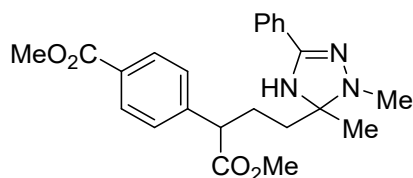
$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.59 – 7.52 (m, 2H), 7.38 – 7.34 (m, 3H), 7.16 (t,  $J$  = 8.1 Hz, 1H), 6.79 – 6.77 (m, 1H), 6.68 – 6.66 (m, 1H), 6.59 (s, 1H), 4.38 (s, 1H), 3.65 (s, 3H), 3.19 (s, 3H), 2.67 (s, 3H), 2.47 – 2.39 (m, 1H), 2.34 – 2.23 (m, 1H), 2.14 – 2.05 (m, 1H), 2.01 – 1.94 (m, 1H), 1.24 (s, 3H).



***N*-(2-(1,5-dimethyl-3-phenyl-4,5-dihydro-1*H*-1,2,4-triazol-5-yl)ethyl)-*N*-methylaniline (1aj)**

Yellow oil (65%, 200 mg), purified by flash column chromatograph (PE : EA = 1 : 1).

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.55 (dd,  $J$  = 6.4, 2.7 Hz, 2H), 7.37 – 7.34 (m, 3H), 7.26 – 7.22 (m, 3H), 7.08 (dd,  $J$  = 7.9, 1.2 Hz, 2H), 4.35 (s, 1H), 3.21 (s, 3H), 2.66 (s, 3H), 2.37 – 2.25 (m, 2H), 2.04 – 1.96 (m, 2H), 1.24 (s, 3H).



**methyl 4-(4-(1,5-dimethyl-3-phenyl-4,5-dihydro-1*H*-1,2,4-triazol-5-yl)-1-methoxy-1-oxobutan-2-yl)benzoate (1al)**

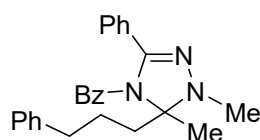
Yellow oil (76%, 310 mg), purified by flash column chromatograph (PE : EA = 3 : 1).

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.05 – 7.92 (m, 4H), 7.59 (d,  $J$  = 3.6 Hz, 3H), 7.39 – 7.34 (m, 11H), 4.20 – 4.16 (m, 2H), 3.89 (s, 6H), 3.70 – 3.57 (m, 8H), 2.72 (d,  $J$  = 14.6



Hz, 6H), 2.36 – 2.25 (m, 2H), 2.10 – 2.01 (m, 2H), 1.73 – 1.51 (m, 4H), 1.20 (d,  $J = 7.4$  Hz, 6H).

$^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  173.7, 173.7, 166.7, 148.5, 148.5, 144.0, 144.0, 129.9, 129.1, 128.6, 128.3, 128.1, 128.0, 126.2, 126.0, 125.1, 84.8, 84.8, 52.1, 52.0, 51.4, 51.3, 36.2, 36.1, 35.2, 35.2, 28.1, 28.1, 21.2, 21.1.

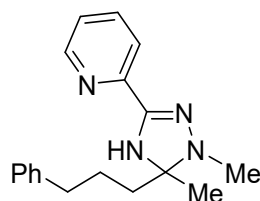


**(1,5-dimethyl-3-phenyl-5-(3-phenylpropyl)-1,5-dihydro-4H-1,2,4-triazol-4-yl)(phenyl)methanone (1am)**

Yellow oil (70%, 278 mg), purified by flash column chromatograph (PE : EA = 3 : 1).

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.72 (dd,  $J = 22.5, 7.3$  Hz, 4H), 7.47 – 7.34 (m, 6H), 7.25 – 7.20 (m, 2H), 7.16 – 7.12 (m, 1H), 7.03 (d,  $J = 7.3$  Hz, 2H), 2.59 (s, 3H), 2.53 – 2.40 (m, 2H), 1.70 – 1.41 (m, 7H).

$^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  170.9, 157.5, 142.0, 134.7, 131.2, 130.9, 130.5, 128.8, 128.5, 128.3, 128.2, 128.0, 127.8, 125.7, 91.5, 39.3, 37.6, 36.1, 26.6, 19.4.

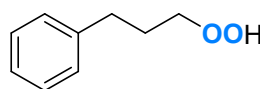


**2-(1,5-dimethyl-5-(3-phenylpropyl)-4,5-dihydro-1H-1,2,4-triazol-3-yl)pyridine (1ao)**

Yellow oil (90%, 264 mg), purified by flash column chromatograph (PE : EA = 1 : 1).

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.51 – 8.49 (m, 1H), 7.89 (d,  $J = 8.0$  Hz, 1H), 7.65 (td,  $J = 7.8, 1.7$  Hz, 1H), 7.29 – 7.25 (m, 2H), 7.23 – 7.15 (m, 4H), 5.18 (s, 1H), 2.80 (s, 3H), 2.73 – 2.62 (m, 2H), 1.92 – 1.69 (m, 4H), 1.24 (s, 3H).

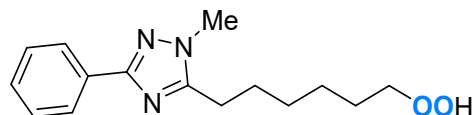
$^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  149.1, 148.6, 147.6, 142.2, 136.0, 128.4, 128.2, 125.7, 123.3, 120.6, 86.0, 38.4, 36.0, 35.2, 26.1, 20.7.



**(3-hydroperoxypropyl)benzene (2a)**

Colorless oil (37%, 5.6 mg), purified by preparative TLC (PE : EA = 3 : 1). Data was consistent with literature precedent.<sup>[7]</sup>

<sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>)  $\delta$  7.94 (s, 1H), 7.31 – 7.29 (m, 2H), 7.21 – 7.20 (m, 3H), 4.05 (t,  $J$  = 6.4 Hz, 2H), 4.05 (t,  $J$  = 7.92 Hz, 2H), 2.01 – 1.97 (m, 2H). <sup>13</sup>C NMR (151 MHz, CDCl<sub>3</sub>)  $\delta$  141.4, 128.4, 125.9, 76.2, 32.0, 29.1.



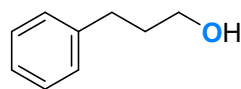
### 5-(6-hydroperoxyhexyl)-1-methyl-3-phenyl-1H-1,2,4-triazole (2b)

Colorless oil (20%, 5.5 mg), purified by preparative TLC (PE : EA = 3 : 1).

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  9.59 (s, 1H), 8.04 – 8.02 (m, 2H), 7.43 – 7.34 (m, 3H), 4.02 (t,  $J$  = 6.3 Hz, 2H), 3.85 (s, 3H), 2.82 – 2.75 (m, 2H), 1.84 – 1.74 (m, 2H), 1.69 – 1.62 (m, 2H), 1.48 – 1.43 (m, 4H).

<sup>13</sup>C NMR (151 MHz, CDCl<sub>3</sub>)  $\delta$  160.5, 156.6, 130.9, 129.0, 128.5, 126.2, 76.6, 35.1, 28.6, 27.3, 27.2, 25.6, 25.3.

HRMS (ESI,  $m/z$ ) Calcd. For C<sub>15</sub>H<sub>22</sub>N<sub>3</sub>O<sub>2</sub><sup>+</sup> [M+H]<sup>+</sup>: 276.1707; Found: 276.1706.

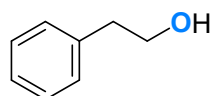


### 3-phenylpropan-1-ol (3a)

Colorless oil (78%, 10.6 mg), purified by preparative TLC (PE : EA = 3 : 1). Data was consistent with literature precedent.<sup>[8]</sup>

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.30 – 7.17 (m, 5H), 3.68 – 3.65 (m, 2H), 2.70 (t,  $J$  = 7.6 Hz, 2H), 1.93 – 1.86 (m, 2H), 1.60 (s, 1H).

<sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  141.8, 128.4, 128.4, 125.8, 62.2, 34.2, 32.0.

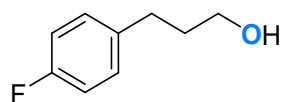


### 2-phenylethan-1-ol (3b)

Colorless oil (67%, 8.2 mg), purified by preparative TLC (PE : EA = 3 : 1). Data was consistent with literature precedent.<sup>[8]</sup>

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.34 – 7.30 (m, 2H), 7.25 – 7.22 (m, 3H), 3.86 (t,  $J$  = 6.6 Hz, 2H), 2.87 (t,  $J$  = 6.6 Hz, 2H).

$^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  138.4, 129.0, 128.5, 126.4, 63.6, 39.1.



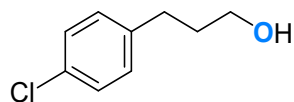
### 3-(4-fluorophenyl)propan-1-ol (3c)

Colorless oil (71%, 10.9 mg), purified by preparative TLC (PE : EA = 3 : 1). Data was consistent with literature precedent.<sup>[9]</sup>

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.16 – 7.13 (m, 2H), 6.99 – 6.94 (m, 2H), 3.66 (t,  $J$  = 6.4 Hz, 2H), 2.70 – 2.66 (m, 2H), 1.90 – 1.83 (m, 2H), 1.43 (s, 1H).

$^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  161.2 (d,  $J$  = 243.4 Hz), 137.3 (d,  $J$  = 3.2 Hz), 129.7 (d,  $J$  = 7.7 Hz), 115.0 (d,  $J$  = 21.1 Hz), 62.0, 34.2, 31.2.

$^{19}\text{F}$  NMR (565 MHz,  $\text{CDCl}_3$ )  $\delta$  -117.7.

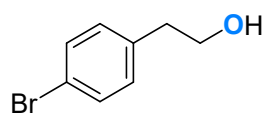


### 3-(4-chlorophenyl)propan-1-ol (3d)

Colorless oil (70%, 11.9 mg), purified by preparative TLC (PE : EA = 3 : 1). Data was consistent with literature precedent.<sup>[10]</sup>

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.26 – 7.24 (m, 2H), 7.13 (d,  $J$  = 8.3 Hz, 2H), 3.66 (t,  $J$  = 6.4 Hz, 2H), 2.70 – 2.66 (m, 2H), 1.90 – 1.83 (m, 2H), 1.47 (s, 1H).

$^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  140.2, 131.5, 129.7, 128.4, 61.9, 34.0, 31.3.

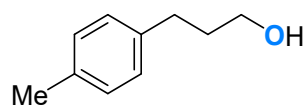


### 2-(4-bromophenyl)ethan-1-ol (3e)

Colorless oil (55%, 10.9 mg), purified by preparative TLC (PE : EA = 3 : 1). Data was consistent with literature precedent.<sup>[11]</sup>

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.43 (d,  $J$  = 8.3 Hz, 2H), 7.11 (d,  $J$  = 8.2 Hz, 2H), 3.84 (t,  $J$  = 6.5 Hz, 2H), 2.82 (t,  $J$  = 6.5 Hz, 2H), 1.43 (s, 1H).

$^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  137.5, 131.6, 130.7, 120.3, 63.3, 38.5.

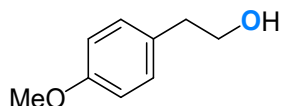


### 3-(p-tolyl)propan-1-ol (3f)

Colorless oil (67%, 10.1 mg), purified by preparative TLC (PE : EA = 3 : 1). Data was consistent with literature precedent.<sup>[12]</sup>

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.11 (s, 4H), 3.68 (t, *J* = 6.5 Hz, 2H), 2.70 – 2.66 (m, 2H), 2.33 (s, 3H), 1.96 – 1.85 (m, 3H).

<sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>) δ 138.6, 135.2, 129.0, 128.2, 62.2, 34.2, 31.5, 20.9.

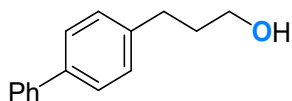


### 2-(4-methoxyphenyl)ethan-1-ol (3g)

Colorless oil (57%, 8.7 mg), purified by preparative TLC (PE : EA = 3 : 1). Data was consistent with literature precedent.<sup>[13]</sup>

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.16 – 7.12 (m, 2H), 6.87 – 6.83 (m, 2H), 3.82 – 3.80 (m, 2H), 3.78 (s, 3H), 2.80 (t, *J* = 6.6 Hz, 2H), 1.63 (s, 1H).

<sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>) δ 158.2, 130.4, 129.9, 113.9, 63.7, 55.2, 38.2.

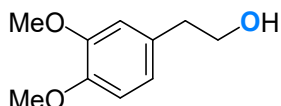


### 3-([1,1'-biphenyl]-4-yl)propan-1-ol (3h)

White solid (84%, 17.8 mg), purified by preparative TLC (PE : EA = 3 : 1). Data was consistent with literature precedent.<sup>[10]</sup>

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.59 – 7.57 (m, 2H), 7.53 – 7.51 (m, 2H), 7.44 – 7.40 (m, 2H), 7.34 – 7.30 (m, 1H), 7.28 – 7.24 (m, 2H), 3.70 (t, *J* = 6.4 Hz, 2H), 2.77 – 2.73 (m, 2H), 1.96 – 1.89 (m, 2H), 1.44 (s, 1H).

<sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>) δ 141.0, 140.9, 138.8, 128.8, 128.7, 127.1, 127.0, 126.9, 62.2, 34.1, 31.6.

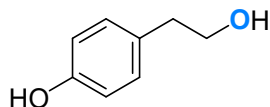


### 2-(3,4-dimethoxyphenyl)ethan-1-ol (3i)

Colorless oil (80%, 14.6 mg), purified by preparative TLC (PE : EA = 3 : 1). Data was consistent with literature precedent.<sup>[14]</sup>

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 6.93 – 6.75 (m, 3H), 3.89 – 3.81 (m, 8H), 2.81 (t, *J* = 6.5 Hz, 2H).

$^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  148.9, 147.6, 130.9, 120.8, 112.1, 111.2, 63.7, 55.8, 55.7, 38.6.

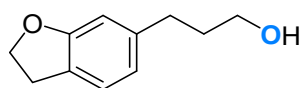


**4-(2-hydroxyethyl)phenol (3j)**

White solid (46%, 6.3 mg), purified by preparative TLC (PE : EA = 3 : 1). Data was consistent with literature precedent.<sup>[15]</sup>

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.10 – 7.08 (m, 2H), 6.80 – 6.76 (m, 2H), 5.10 (s, 1H), 3.83 (t,  $J$  = 6.5 Hz, 2H), 2.80 (t,  $J$  = 6.5 Hz, 2H), 1.50 (s, 1H).

$^{13}\text{C}$  NMR (151 MHz,  $\text{CDCl}_3$ )  $\delta$  154.2, 130.3, 130.1, 115.4, 63.8, 38.1.



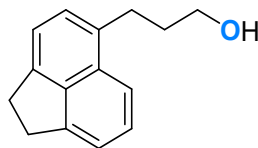
**3-(2,3-dihydrobenzofuran-6-yl)propan-1-ol (3k)**

White solid (67%, 11.9 mg), purified by preparative TLC (PE : EA = 3 : 1).

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.03 (s, 1H), 6.93 (d,  $J$  = 8.1 Hz, 1H), 6.70 (d,  $J$  = 8.1 Hz, 1H), 4.54 (t,  $J$  = 8.7 Hz, 2H), 3.67 (t,  $J$  = 6.4 Hz, 2H), 3.18 (t,  $J$  = 8.7 Hz, 2H), 2.65 – 2.22 (m, 2H), 1.89 – 1.82 (m, 2H), 1.69 (s, 1H).

$^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  158.2, 133.7, 127.7, 127.0, 124.8, 108.9, 71.1, 62.2, 34.6, 31.4, 29.7.

HRMS (EI,  $m/z$ ) Calcd. For  $\text{C}_{11}\text{H}_{14}\text{O}_2$   $[\text{M}]^{+}$ : 178.0988; Found: 178.0988.



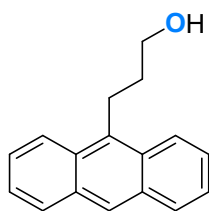
**3-(1,2-dihydroacenaphthylen-5-yl)propan-1-ol (3l)**

White solid (54%, 11.4 mg), purified by preparative TLC (PE : EA = 3 : 1).

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.72 (d,  $J$  = 8.3 Hz, 1H), 7.47 (dd,  $J$  = 8.2, 7.0 Hz, 1H), 7.29 (d,  $J$  = 7.0 Hz, 2H), 7.21 (d,  $J$  = 7.0 Hz, 1H), 3.74 (t,  $J$  = 6.4 Hz, 2H), 3.42 – 3.36 (m, 4H), 3.13 – 3.09 (m, 2H), 2.06 – 1.99 (m, 2H), 1.43 (s, 1H).

$^{13}\text{C}$  NMR (151 MHz,  $\text{CDCl}_3$ )  $\delta$  146.5, 144.1, 139.5, 133.6, 130.3, 127.5, 127.3, 119.2, 119.0, 118.9, 62.5, 33.6, 30.5, 29.8, 28.1.

HRMS (EI,  $m/z$ ) Calcd. For  $C_{15}H_{16}O^{+}$   $[M]^{+}$ : 212.1196; Found: 212.1194.

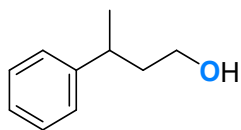


### 3-(anthracen-9-yl)propan-1-ol (3m)

Colorless oil (30%, 7.1 mg), purified by preparative TLC (PE : EA = 3 : 1). Data was consistent with literature precedent.<sup>[16]</sup>

$^1H$  NMR (400 MHz,  $CDCl_3$ )  $\delta$  8.35 – 8.30 (m, 3H), 8.01 (d,  $J$  = 8.1 Hz, 2H), 7.53 – 7.44 (m, 4H), 3.83 (t,  $J$  = 6.2 Hz, 2H), 3.76– 3.72 (m, 2H), 2.13 – 2.05 (m, 2H), 1.63 (s, 1H).

$^{13}C$  NMR (151 MHz,  $CDCl_3$ )  $\delta$  134.2, 131.6, 129.6, 129.2, 125.8, 125.5, 124.8, 124.3, 62.6, 33.9, 24.0.

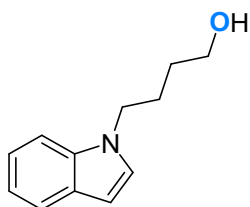


### 3-phenylbutan-1-ol (3n)

Colorless oil (78%, 11.7 mg), purified by preparative TLC (PE : EA = 3 : 1). Data was consistent with literature precedent.<sup>[17]</sup>

$^1H$  NMR (400 MHz,  $CDCl_3$ )  $\delta$  7.32 – 7.28 (m, 2H), 7.22 – 7.18 (m, 3H), 3.62 – 3.51 (m, 2H), 2.93 – 2.84 (m, 1H), 1.90 – 1.82 (m, 2H), 1.28 (d,  $J$  = 7.0 Hz, 3H).

$^{13}C$  NMR (101 MHz,  $CDCl_3$ )  $\delta$  146.8, 128.4, 126.9, 126.1, 61.2, 40.9, 36.4, 22.3.

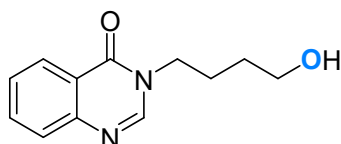


### 4-(1H-indol-1-yl)butan-1-ol (3o)

Colorless oil (75%, 14.2 mg), purified by preparative TLC (PE : EA = 3 : 1). Data was consistent with literature precedent.<sup>[18]</sup>

$^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ )  $\delta$  7.64 (d,  $J = 7.9$  Hz, 1H), 7.35 (d,  $J = 8.2$  Hz, 1H), 7.22 – 7.20 (m, 1H), 7.12 – 7.09 (m, 2H), 6.50 (d,  $J = 2.9$  Hz, 1H), 4.17 (t,  $J = 7.0$  Hz, 2H), 3.64 (t,  $J = 6.4$  Hz, 2H), 1.96 – 1.91 (m, 2H), 1.59 – 1.55 (m, 2H).

$^{13}\text{C}$  NMR (151 MHz,  $\text{CDCl}_3$ )  $\delta$  135.8, 128.5, 127.7, 121.3, 120.9, 119.2, 109.3, 101.0, 62.3, 46.1, 29.9, 26.6.

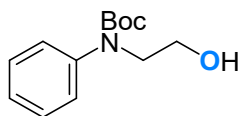


### 3-(4-hydroxybutyl)quinazolin-4(3H)-one (3p)

Colorless oil (70%, 15.3 mg), purified by preparative TLC (PE : EA = 1 : 1). Data was consistent with literature precedent.<sup>[19]</sup>

$^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ )  $\delta$  8.30 – 8.28 (m, 1H), 8.05 (s, 1H), 7.76 – 7.73 (m, 1H), 7.70 – 7.69 (m, 1H), 7.51 – 7.48 (m, 1H), 4.05 (t,  $J = 7.4$  Hz, 2H), 3.71 (t,  $J = 6.2$  Hz, 2H), 2.13 (s, 1H), 1.93 – 1.88 (m, 2H), 1.67 – 1.62 (m, 2H).

$^{13}\text{C}$  NMR (151 MHz,  $\text{CDCl}_3$ )  $\delta$  161.1, 148.0, 146.5, 134.2, 127.3, 127.2, 126.6, 122.0, 62.0, 46.7, 29.3, 26.0.

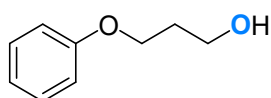


### tert-butyl (2-hydroxyethyl)(phenyl)carbamate (3q)

White solid (50%, 11.9 mg), purified by preparative TLC (PE : EA = 3 : 1). Data was consistent with literature precedent.<sup>[20]</sup>

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.36 – 7.32 (m, 2H), 7.24 – 7.19 (m, 3H), 3.82 – 3.78 (m, 4H), 1.41 (s, 9H).

$^{13}\text{C}$  NMR (151 MHz,  $\text{CDCl}_3$ )  $\delta$  156.2, 142.7, 128.8, 127.0, 126.3, 80.8, 61.9, 52.9, 28.2.

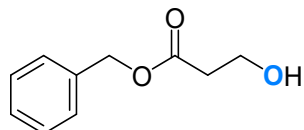


### 3-phenoxypropan-1-ol (3r)

Colorless oil (80%, 12.2 mg), purified by preparative TLC (PE : EA = 3 : 1). Data was consistent with literature precedent.<sup>[21]</sup>

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.31 – 7.25 (m, 2H), 6.97 – 6.90 (m, 3H), 4.12 (t,  $J$  = 5.9 Hz, 2H), 3.86 (t,  $J$  = 5.9 Hz, 2H), 2.04 (p,  $J$  = 5.9 Hz, 2H), 1.95 (s, 1H).

$^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  158.7, 129.4, 120.8, 114.4, 65.6, 60.5, 31.9.



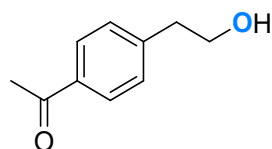
### benzyl 3-hydroxypropanoate (3s)

Colorless oil (35%, 6.3 mg), purified by preparative TLC (PE : EA = 3 : 1).

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.40 – 7.31 (m, 5H), 5.16 (s, 2H), 3.89 (t,  $J$  = 5.1 Hz, 2H), 2.63 (t,  $J$  = 5.6 Hz, 2H), 2.37 (s, 1H).

$^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  172.7, 135.5, 128.6, 128.3, 128.2, 66.5, 58.2, 36.7.

HRMS (EI,  $m/z$ ) Calcd. For  $\text{C}_{10}\text{H}_{12}\text{O}_3$  $^{*+}$  [M] $^{*+}$ : 180.0781; Found: 180.0779.

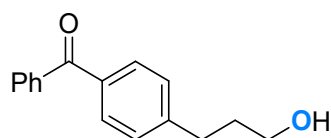


### 1-(4-(2-hydroxyethyl)phenyl)ethan-1-one (3t)

Colorless oil (67%, 11.0 mg), purified by preparative TLC (PE : EA = 1 : 1). Data was consistent with literature precedent.<sup>[22]</sup>

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.90 (d,  $J$  = 8.0 Hz, 2H), 7.33 (d,  $J$  = 7.9 Hz, 2H), 3.89 (t,  $J$  = 5.9 Hz, 2H), 2.93 (t,  $J$  = 6.5 Hz, 2H), 2.58 (s, 3H), 1.65 (s, 1H).

$^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  197.8, 144.4, 135.5, 129.2, 128.6, 63.1, 39.0, 26.5.



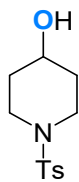
### (4-(3-hydroxypropyl)phenyl)(phenyl)methanone (3u)

Colorless oil (46%, 11.0 mg), purified by preparative TLC (PE : EA = 1 : 1).

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.80 – 7.74 (m, 4H), 7.58 (t,  $J$  = 7.4 Hz, 1H), 7.48 (t,  $J$  = 7.5 Hz, 2H), 7.31 (d,  $J$  = 8.0 Hz, 2H), 3.70 (t,  $J$  = 6.3 Hz, 2H), 2.82 – 2.78 (m, 2H), 1.97 – 1.90 (m, 2H), 1.54 (s, 1H).

$^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  196.4, 147.0, 137.8, 135.3, 132.2, 130.4, 129.9, 128.3, 128.2, 61.9, 33.8, 32.0.



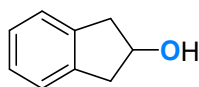


### 1-tosylpiperidin-4-ol (3v)

White solid (80%, 20.4 mg), purified by preparative TLC (PE : EA = 3 : 1). Data was consistent with literature precedent.<sup>[23]</sup>

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.62 (d, *J* = 7.7 Hz, 2H), 7.31 (d, *J* = 7.7 Hz, 2H), 3.78 – 3.68 (m, 1H), 3.36 – 3.24 (m, 2H), 2.87 – 2.75 (m, 2H), 2.42 (s, 3H), 2.96 – 1.84 (m, 2H), 1.67 – 1.62 (m, 2H).

<sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>) δ 143.5, 133.1, 129.6, 127.6, 65.8, 43.1, 33.2, 21.4.

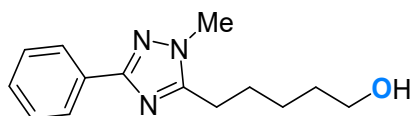


### 2,3-dihydro-1H-inden-2-ol (3w)

White solid (80%, 10.7 mg), purified by preparative TLC (PE : EA = 3 : 1). Data was consistent with literature precedent.<sup>[24]</sup>

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.31 – 7.29 (m, 2H), 7.26 – 7.22 (m, 2H), 4.75 – 4.71 (m, 1H), 3.26 (dd, *J* = 16.4, 5.9 Hz, 2H), 2.96 (dd, *J* = 16.3, 3.2 Hz, 2H), 2.02 (s, 1H).

<sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>) δ 140.7, 126.5, 124.9, 73.0, 42.5.



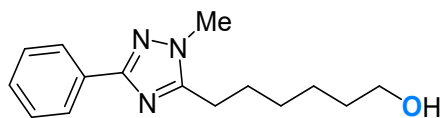
### 5-(1-methyl-3-phenyl-1H-1,2,4-triazol-5-yl)pentan-1-ol (3x)

Colorless oil (58%, 14.2 mg), purified by preparative TLC (PE : EA = 1 : 1).

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.04 (d, *J* = 7.9 Hz, 2H), 7.43 – 7.34 (m, 3H), 3.83 (s, 3H), 3.67 (t, *J* = 6.1 Hz, 2H), 2.77 (t, *J* = 7.5 Hz, 2H), 2.34 (s, 1H), 1.87 – 1.79 (m, 2H), 1.65 – 1.59 (m, 2H), 1.54 – 1.4 (m, 2H).

<sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>) δ 160.5, 156.4, 131.0, 128.9, 128.5, 126.1, 62.2, 35.0, 32.0, 26.9, 25.7, 25.2.

HRMS (EI, *m/z*) Calcd. For C<sub>14</sub>H<sub>19</sub>N<sub>3</sub>O<sup>+</sup> [*M*]<sup>+</sup>: 245.1523; Found: 245.1524.



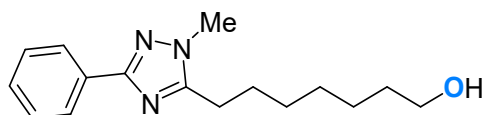
**6-(1-methyl-3-phenyl-1H-1,2,4-triazol-5-yl)hexan-1-ol (3y)**

White solid (55%, 14.2 mg), purified by preparative TLC (PE : EA = 1 : 1).

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.05 – 8.03 (m, 2H), 7.43 – 7.33 (m, 3H), 3.84 (s, 3H), 3.63 (t,  $J$  = 6.4 Hz, 2H), 2.84 – 2.71 (t,  $J$  = 7.8 Hz, 2H), 1.89 (s, 1H), 1.83 – 1.76 (m, 2H), 1.61 – 1.54 (m, 2H), 1.48 – 1.40 (m, 4H).

$^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  160.6, 156.5, 131.1, 128.9, 128.4, 126.1, 62.5, 35.1, 32.4, 28.7, 27.5, 25.7, 25.2.

HRMS (EI,  $m/z$ ) Calcd. For  $\text{C}_{15}\text{H}_{21}\text{N}_3\text{O}^{++}$   $[\text{M}]^{++}$ : 259.1679; Found: 259.1679.



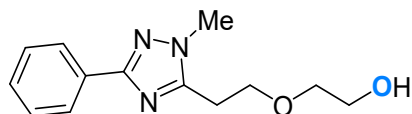
**7-(1-methyl-3-phenyl-1H-1,2,4-triazol-5-yl)heptan-1-ol (3z)**

Colorless oil (61%, 16.6 mg), purified by preparative TLC (PE : EA = 1 : 1).

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.05 – 8.03 (m, 2H), 7.42 – 7.33 (m, 3H), 3.84 (s, 3H), 3.61 (t,  $J$  = 6.6 Hz, 2H), 2.77 – 2.74 (m, 2H), 1.81 – 1.74 (m, 2H), 1.59 – 1.51 (m, 2H), 1.47 – 1.37 (m, 6H).

$^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  160.5, 156.6, 131.1, 128.8, 128.4, 126.1, 62.7, 35.1, 32.5, 29.1, 28.9, 27.6, 25.9, 25.5.

HRMS (EI,  $m/z$ ) Calcd. For  $\text{C}_{16}\text{H}_{23}\text{N}_3\text{O}^{++}$   $[\text{M}]^{++}$ : 273.1836; Found: 273.1838.



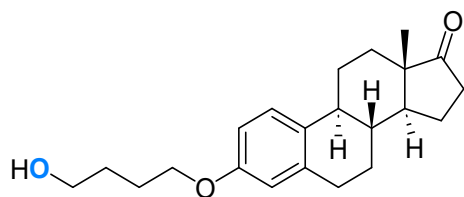
**2-(2-(1-methyl-3-phenyl-1H-1,2,4-triazol-5-yl)ethoxy)ethan-1-ol (3aa)**

White solid (51%, 12.6 mg), purified by preparative TLC (PE : EA = 3 : 1).

$^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ )  $\delta$  8.05 – 8.03 (m, 2H), 7.43 – 7.40 (m, 2H), 7.38 – 7.35 (m, 1H), 4.00 (t,  $J$  = 5.8 Hz, 2H), 3.85 (s, 3H), 3.75 – 3.74 (m, 2H), 3.64 – 3.63 (m, 2H), 3.02 (t,  $J$  = 5.8 Hz, 2H).

$^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  160.6, 154.3, 130.7, 129.0, 128.5, 126.1, 72.0, 67.1, 61.5, 35.2, 26.7.

HRMS (ESI,  $m/z$ ) Calcd. For  $\text{C}_{13}\text{H}_{18}\text{N}_3\text{O}_2^+$   $[\text{M}+\text{H}]^+$ : 248.1394; Found: 248.1394.



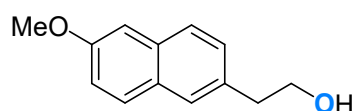
**(8*R*,9*S*,13*S*,14*S*)-3-(4-hydroxybutoxy)-13-methyl-6,7,8,9,11,12,13,14,15,16-decahydro-17*H*-cyclopenta[*a*]phenanthren-17-one (3ab)**

White solid (53%, 18.1 mg), purified by preparative TLC (PE : EA = 3 : 1).

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.19 (d,  $J$  = 8.6 Hz, 1H), 6.71 (dd,  $J$  = 8.5, 2.5 Hz, 1H), 6.65 (d,  $J$  = 2.3 Hz, 1H), 3.98 (t,  $J$  = 6.1 Hz, 2H), 3.72 (t,  $J$  = 6.3 Hz, 2H), 2.95 – 2.82 (m, 2H), 2.50 (dd,  $J$  = 18.8, 8.5 Hz, 1H), 2.44 – 2.36 (m, 1H), 2.27 – 2.22 (m, 1H), 2.19 – 1.94 (m, 4H), 1.91 – 1.84 (m, 2H), 1.78 – 1.72 (m, 2H), 1.67 – 1.38 (m, 6H), 0.91 (s, 3H).

$^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  220.9, 156.8, 137.7, 132.1, 126.3, 114.5, 112.0, 67.7, 62.5, 50.3, 48.0, 43.9, 38.3, 35.8, 31.5, 29.6, 29.5, 26.5, 25.9, 25.8, 21.5, 13.8.

HRMS (EI,  $m/z$ ) Calcd. For  $\text{C}_{22}\text{H}_{30}\text{O}_3$   $[\text{M}]^{+}$ : 342.2189; Found: 342.2189.

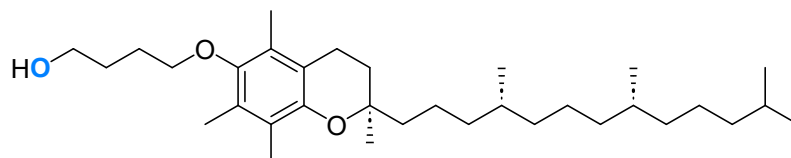


**2-(6-methoxynaphthalen-2-yl)ethan-1-ol (3ac)**

White solid (50%, 10.1 mg), purified by preparative TLC (PE : EA = 3 : 1). Data was consistent with literature precedent.<sup>[25]</sup>

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.73 – 7.68 (m, 2H), 7.61 (s, 1H), 7.33 (dd,  $J$  = 8.4, 1.4 Hz, 1H), 7.17 – 7.12 (m, 2H), 3.95 – 3.92 (m, 5H), 3.00 (t,  $J$  = 6.5 Hz, 2H), 1.47 (s, 1H).

$^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  157.3, 133.5, 133.3, 129.0, 128.9, 127.8, 127.3, 127.1, 118.8, 105.6, 63.6, 55.2, 39.1.



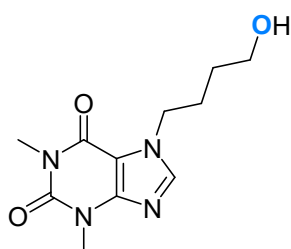
**4-(((*R*)-2,5,7,8-tetramethyl-2-((4*R*,8*R*)-4,8,12-trimethyltridecyl)chroman-6-yl)oxy)butan-1-ol (3ad)**

White solid (29%, 14.6 mg), purified by preparative TLC (PE : EA = 3 : 1).

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  3.75 (t,  $J = 5.6$  Hz, 2H), 3.68 (t,  $J = 5.8$  Hz, 2H), 2.57 (t,  $J = 6.6$  Hz, 2H), 2.17 – 2.08 (m, 9H), 1.91 – 1.71 (m, 7H), 1.59 – 1.49 (m, 3H), 1.47 – 1.34 (m, 4H), 1.31 – 1.23 (m, 10H), 1.16 – 1.07 (m, 6H), 0.87 – 0.83 (m, 12H).

$^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  148.1, 147.7, 127.7, 125.7, 122.8, 117.5, 74.7, 72.7, 62.9, 40.0, 39.3, 37.4, 37.4, 37.4, 37.2, 32.7, 32.6, 31.2, 29.9, 27.9, 27.0, 24.7, 24.4, 23.8, 22.7, 22.6, 21.0, 20.6, 19.7, 19.6, 12.7, 11.9, 11.7.

HRMS (ESI,  $m/z$ ) Calcd. For  $\text{C}_{33}\text{H}_{59}\text{O}_3^+$   $[\text{M}+\text{H}]^+$ : 503.4459; Found: 503.4458.



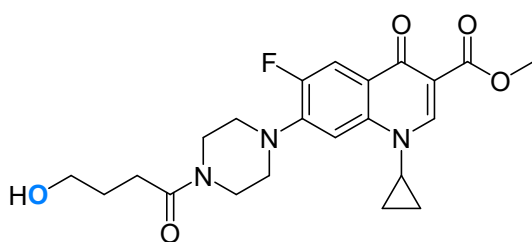
**7-(4-hydroxybutyl)-1,3-dimethyl-3,7-dihydro-1H-purine-2,6-dione (3ae)**

White solid (39%, 9.8 mg), purified by preparative TLC (PE : EA = 0 : 1).

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.57 (s, 1H), 4.38 – 4.28 (t,  $J = 7.5$  Hz, 2H), 3.72 (t,  $J = 6.1$  Hz, 2H), 3.59 (s, 3H), 3.41 (s, 3H), 2.03 – 1.96 (m, 2H), 1.63 – 1.56 (m, 2H).

$^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  155.2, 151.6, 149.0, 140.9, 106.9, 61.7, 46.7, 29.7, 28.8, 28.0, 27.6.

HRMS (EI,  $m/z$ ) Calcd. For  $\text{C}_{11}\text{H}_{16}\text{N}_4\text{O}_3^{*+}$   $[\text{M}]^{*+}$ : 252.1217; Found: 252.1217.



**methyl 1-cyclopropyl-6-fluoro-7-(4-(4-hydroxybutanoyl)piperazin-1-yl)-4-oxo-1,4-dihydroquinoline-3-carboxylate (3af)**

White solid (56%, 24.1 mg), purified by preparative TLC (dichloromethane : methanol = 8 : 1).

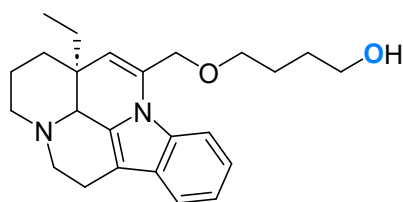
$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.53 (s, 1H), 8.03 (d,  $J = 13.1$  Hz, 1H), 7.24 (d,  $J = 1.6$  Hz, 1H), 3.89 – 3.84 (m, 5H), 3.71 (t,  $J = 5.7$  Hz, 4H), 3.44 – 3.39 (m, 1H), 3.27 – 3.19

(m, 4H), 2.56 (t,  $J = 6.8$  Hz, 2H), 2.28 (s, 1H), 1.97 – 1.91 (m, 2H), 1.31 (q,  $J = 6.7$  Hz, 2H), 1.12 (q,  $J = 6.5$  Hz, 2H).

$^{13}\text{C}$  NMR (151 MHz,  $\text{CDCl}_3$ )  $\delta$  173.0, 172.0, 166.3, 153.3 (d,  $J = 248.7$  Hz), 148.4, 144.0 (d,  $J = 10.8$  Hz), 137.9, 123.5 (d,  $J = 7.3$  Hz), 113.5 (d,  $J = 23.0$  Hz), 110.2, 105.1, 62.4, 52.0, 50.4 (d,  $J = 5.1$  Hz), 49.5, 45.5, 41.4, 34.5, 30.5, 27.5, 8.1.

$^{19}\text{F}$  NMR (565 MHz,  $\text{CDCl}_3$ )  $\delta$  -123.8.

HRMS (ESI,  $m/z$ ) Calcd. For  $\text{C}_{22}\text{H}_{27}\text{FN}_3\text{O}_5^+$   $[\text{M}+\text{H}]^+$ : 432.1929; Found: 432.1930.



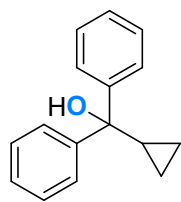
**4-(((13a*S*)-13a-ethyl-2,3,4<sup>1</sup>,5,6,13a-hexahydro-1*H*-indolo[3,2,1-*de*]pyrido[3,2,1-*ij*][1,5]naphthyridin-12-yl)methoxy)butan-1-ol (3ag)**

Yellow oil (35%, 13.4 mg), purified by preparative TLC (PE : EA = 0 : 1).

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.60 (d,  $J = 8.3$  Hz, 1H), 7.44 (d,  $J = 7.6$  Hz, 1H), 7.19 – 7.14 (m, 1H), 7.12 – 7.08 (m, 1H), 5.07 (s, 1H), 4.65 (d,  $J = 12.5$  Hz, 1H), 4.43 (d,  $J = 12.6$  Hz, 1H), 4.21 (s, 1H), 3.62 – 3.51 (m, 4H), 3.36 (dd,  $J = 13.6, 5.9$  Hz, 1H), 3.30 – 3.22 (m, 1H), 3.07 – 2.98 (m, 1H), 2.77 – 2.66 (m, 2H), 2.55 – 2.49 (m, 1H), 2.00 – 1.91 (m, 1H), 1.80 – 1.65 (m, 4H), 1.62 – 1.55 (m, 2H), 1.47 – 1.39 (m, 2H), 1.25 – 1.11 (m, 2H), 0.99 (t,  $J = 7.5$  Hz, 3H).

$^{13}\text{C}$  NMR (151 MHz,  $\text{CDCl}_3$ )  $\delta$  133.9, 132.1, 131.1, 128.8, 121.9, 119.8, 118.9, 118.1, 112.7, 107.9, 70.2, 69.2, 62.5, 56.0, 51.6, 45.1, 36.8, 29.9, 29.8, 27.3, 26.2, 20.5, 16.3, 8.8.

HRMS (EI,  $m/z$ ) Calcd. For  $\text{C}_{24}\text{H}_{32}\text{N}_2\text{O}_2^{*+}$   $[\text{M}]^{*+}$ : 380.2458; Found: 380.2458.

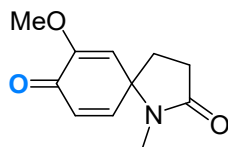


**Cyclopropyldiphenylmethanol (3ah)**

White solid (88%, 19.7 mg), purified by preparative TLC (PE : EA = 3 : 1). Data was consistent with literature precedent.<sup>[26]</sup>

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.45 – 7.43 (m, 4H), 7.33 – 7.22 (m, 6H), 1.91 (s, 1H), 1.66 – 1.59 (m, 1H), 0.61 – 0.55 (m, 2H), 0.50 – 0.46 (m, 2H).

<sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  147.1, 127.8, 126.9, 126.8, 77.0, 21.5, 1.7.



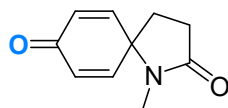
### 7-methoxy-1-methyl-1-azaspiro[4.5]deca-6,9-diene-2,8-dione (3ai)

Light yellow solid (60%, 12.4 mg), purified by preparative TLC (PE : EA = 3 : 1).

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  6.69 (dd,  $J$  = 9.9, 2.7 Hz, 1H), 6.34 (d,  $J$  = 9.9 Hz, 1H), 5.55 (d,  $J$  = 2.7 Hz, 1H), 3.68 (s, 3H), 2.64 (s, 3H), 2.61 – 2.56 (m, 2H), 2.27 – 2.14 (m, 2H).

<sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  179.7, 174.2, 152.0, 149.5, 129.6, 115.5, 63.6, 55.1, 30.7, 29.3, 25.9.

HRMS (EI,  $m/z$ ) Calcd. For C<sub>11</sub>H<sub>13</sub>NO<sub>3</sub><sup>+</sup> [M]<sup>+</sup>: 207.0890; Found: 207.0885.



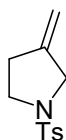
### 1-methyl-1-azaspiro[4.5]deca-6,9-diene-2,8-dione (3aj)

White solid (76%, 13.4 mg), purified by preparative TLC (PE : EA = 3 : 1).

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  6.70 (d,  $J$  = 9.6 Hz, 2H), 6.35 (d,  $J$  = 9.6 Hz, 2H), 2.66 (s, 3H), 2.58 (t,  $J$  = 7.9 Hz, 2H), 2.16 (t,  $J$  = 8.0 Hz, 2H).

<sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  184.1, 174.4, 148.9, 130.6, 61.9, 29.4, 29.1, 26.2.

HRMS (ESI,  $m/z$ ) Calcd. For C<sub>11</sub>H<sub>12</sub>NO<sub>2</sub><sup>+</sup> [M+H]<sup>+</sup>: 178.0863; Found: 178.0864.

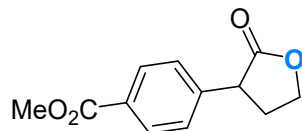


### 3-methylene-1-tosylpyrrolidine (3ak)

White solid (75%, 17.8 mg), purified by preparative TLC (PE : EA = 3 : 1). Data was consistent with literature precedent.<sup>[27]</sup>

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.70 (d,  $J$  = 8.2 Hz, 2H), 7.33 (d,  $J$  = 8.0 Hz, 2H), 4.93 – 4.89 (m, 2H), 3.76 (s, 2H), 3.27 (t,  $J$  = 7.1 Hz, 2H), 2.48 – 2.43 (m, 5H).

$^{13}\text{C}$  NMR (151 MHz,  $\text{CDCl}_3$ )  $\delta$  144.0, 143.6, 132.7, 129.6, 127.8, 107.3, 51.8, 48.0, 31.7, 21.5.

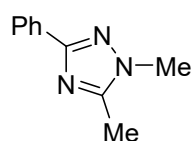


**methyl 4-(2-oxotetrahydrofuran-3-yl)benzoate (3al)**

Colorless oil (37%, 8.1 mg), purified by preparative TLC (PE : EA = 3 : 1). Data was consistent with literature precedent.<sup>[28]</sup>

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.05 – 8.02 (m, 2H), 7.39 – 7.37 (m, 2H), 4.53 – 4.47 (m, 1H), 4.40 – 4.34 (m, 1H), 3.91 – 3.85 (m, 4H), 2.79 – 2.71 (m, 1H), 2.51 – 2.41 (m, 1H).

$^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  176.5, 166.6, 141.5, 130.1, 129.5, 127.9, 66.4, 52.1, 45.3, 31.3.

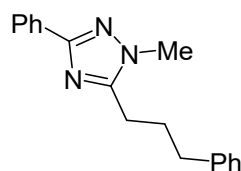


**1,5-dimethyl-3-phenyl-1H-1,2,4-triazole (4)**

White solid, purified by preparative TLC (PE : EA = 1 : 1). Data was consistent with literature precedent.<sup>[29]</sup>

$^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ )  $\delta$  8.04 (d,  $J$  = 7.4 Hz, 2H), 7.42 – 7.34 (m, 3H), 3.83 (s, 3H), 2.48 (s, 3H).

$^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  160.5, 152.8, 131.0, 128.9, 128.4, 126.0, 35.1, 11.8.



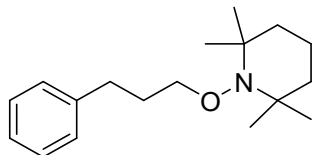
**1-methyl-3-phenyl-5-(3-phenylpropyl)-1H-1,2,4-triazole (5)**

White solid (3%, 0.8 mg) for substrate **1a**, (38%, 10.5 mg) for substrate **1al**, purified by preparative TLC (PE : EA = 3 : 1).

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.07 – 8.04 (m, 2H), 7.45 – 7.34 (m, 3H), 7.32 – 7.26 (m, 2H), 7.22 – 7.19 (m, 3H), 3.77 (s, 3H), 2.79 – 2.72 (m, 4H), 2.19 – 2.11 (m, 2H).

$^{13}\text{C}$  NMR (151 MHz,  $\text{CDCl}_3$ )  $\delta$  160.6, 156.2, 141.0, 131.1, 128.8, 128.4, 128.4, 126.1, 35.0, 35.0, 28.9, 25.1.

HRMS (ESI,  $m/z$ ) Calcd. For  $\text{C}_{18}\text{H}_{20}\text{N}_3^+$   $[\text{M}+\text{H}]^+$ : 278.1652; Found: 278.1651.



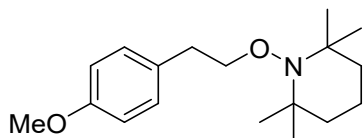
### 2,2,6,6-tetramethyl-1-(3-phenylpropoxy)piperidine (6)

Colorless oil (13%, 3.4 mg), purified by preparative TLC (PE : EA = 3 : 1). Data was consistent with literature precedent.<sup>[30]</sup>

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.29 – 7.26 (m, 2H), 7.22 – 7.15 (m, 3H), 3.77 (t,  $J$  = 6.5 Hz, 2H), 2.73 – 2.69 (m, 2H), 1.89 – 1.82 (m, 2H), 1.48 – 1.43 (m, 4H), 1.33 – 1.26 (m, 2H), 1.12 (d,  $J$  = 10.7 Hz, 12H).

$^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  142.4, 128.3, 128.2, 125.6, 76.0, 59.6, 39.6, 33.0, 32.7, 30.5, 20.0, 17.1.

HRMS (ESI,  $m/z$ ) Calcd. For  $\text{C}_{18}\text{H}_{30}\text{NO}^+$   $[\text{M}+\text{H}]^+$ : 276.2323; Found: 276.2323.



### 1-(4-methoxyphenethoxy)-2,2,6,6-tetramethylpiperidine (9)

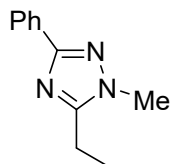
Colorless oil (21%, 6.1 mg), purified by preparative TLC (PE : EA = 3 : 1). Data was consistent with literature precedent.<sup>[31]</sup>

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.15 (d,  $J$  = 8.6 Hz, 2H), 6.82 (d,  $J$  = 8.6 Hz, 2H), 3.90 (t,  $J$  = 7.0 Hz, 1H), 3.79 (s, 3H), 2.76 (t,  $J$  = 7.0 Hz, 2H), 1.45 – 1.40 (m, 4H), 1.33 – 1.28 (m, 2H), 1.07 (s, 12H).

$^{13}\text{C}$  NMR (151 MHz,  $\text{CDCl}_3$ )  $\delta$  157.8, 131.7, 129.9, 113.5, 77.7, 59.6, 55.2, 39.6, 34.4, 32.9, 20.1, 17.1.

HRMS (ESI,  $m/z$ ) Calcd. For  $\text{C}_{18}\text{H}_{30}\text{NO}_2^+$   $[\text{M}+\text{H}]^+$ : 292.2271; Found: 292.2272.





### 5-ethyl-1-methyl-3-phenyl-1H-1,2,4-triazole (14)

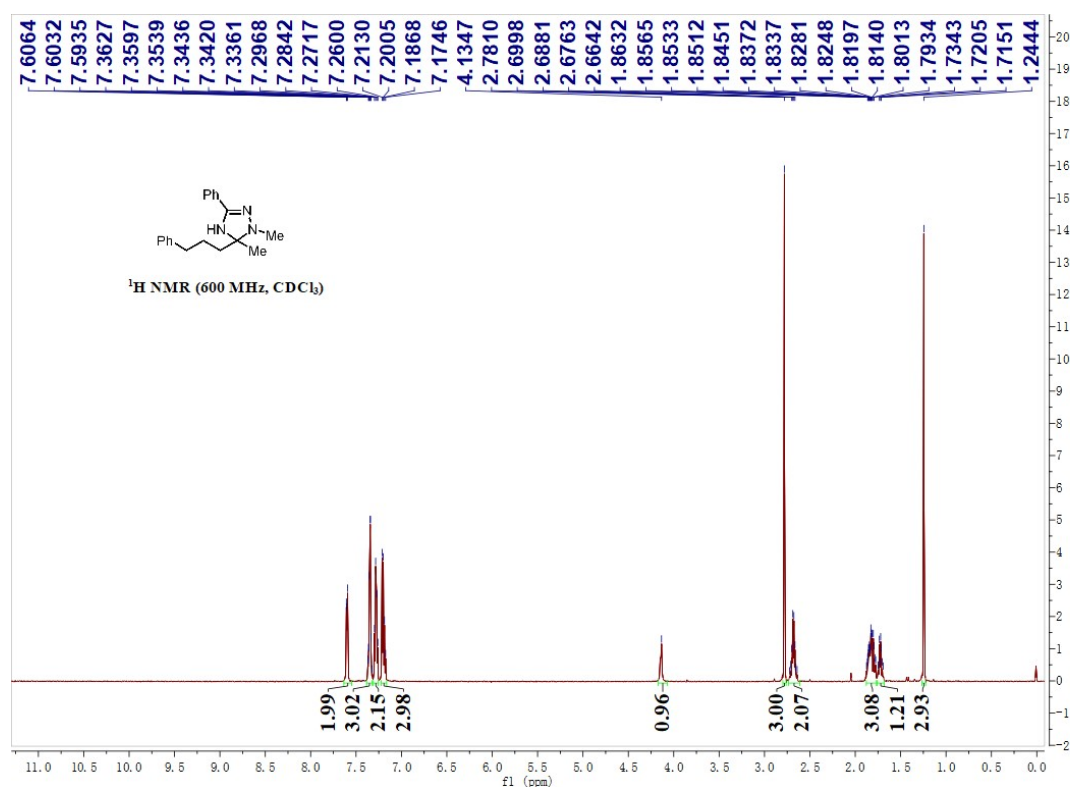
colorless oil (40%, 7.5 mg), purified by preparative TLC (PE : EA = 3 : 1). Data was consistent with literature precedent.<sup>[29]</sup>

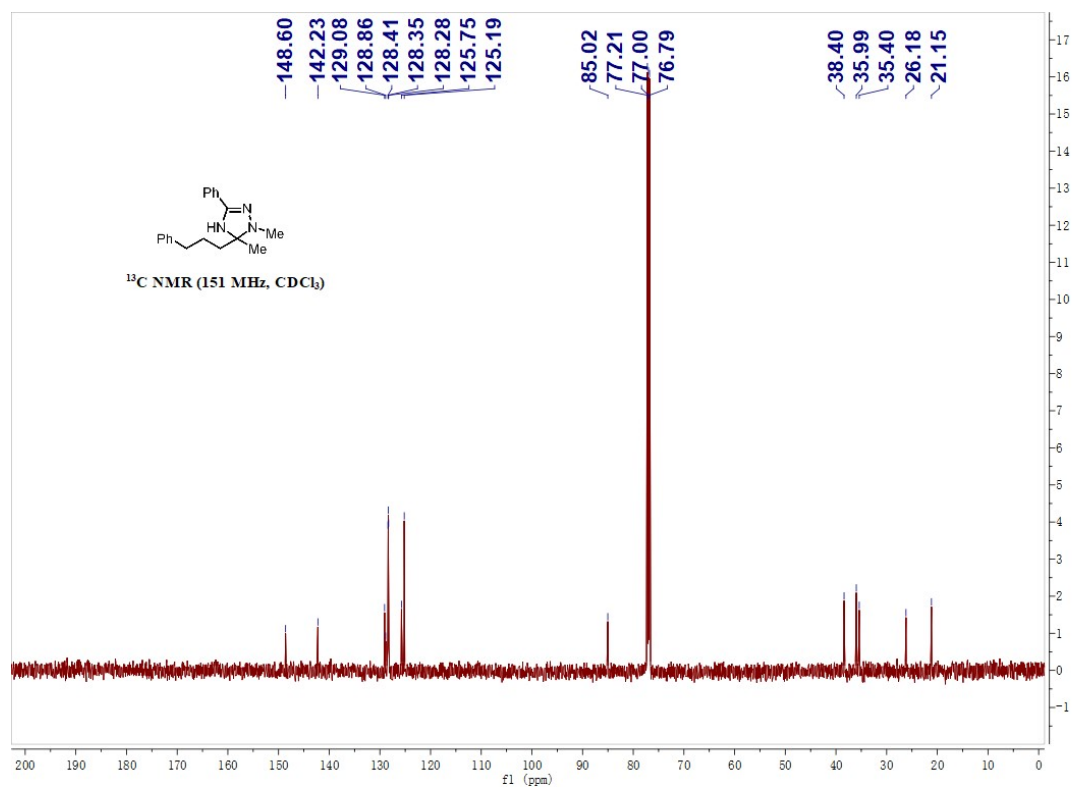
$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.06 – 8.04 (m, 2H), 7.43 – 7.33 (m, 3H), 3.86 (s, 3H), 2.81 (q,  $J = 7.6$  Hz, 2H), 1.39 (t,  $J = 7.6$  Hz, 3H).

$^{13}\text{C}$  NMR (151 MHz,  $\text{CDCl}_3$ )  $\delta$  160.6, 157.5, 131.1, 128.8, 128.4, 126.1, 35.0, 19.4, 12.0.

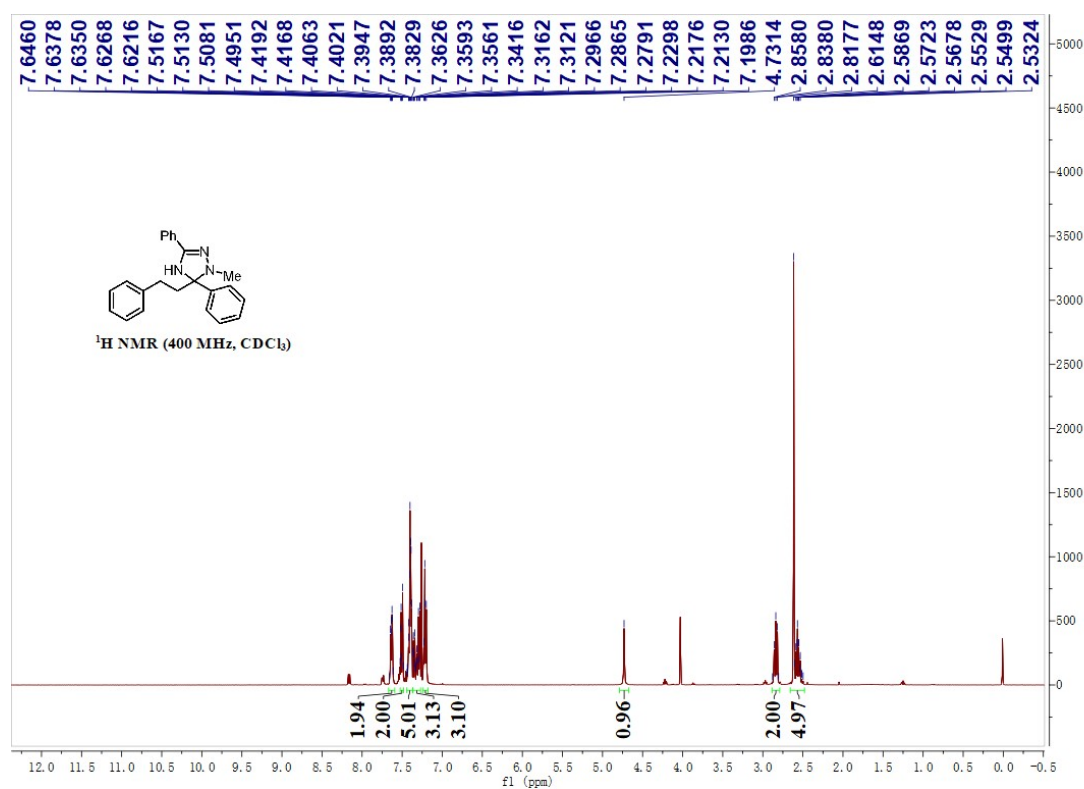
## 8. Copies of $^1\text{H}$ , $^{13}\text{C}$ , and $^{19}\text{F}$ NMR Spectra

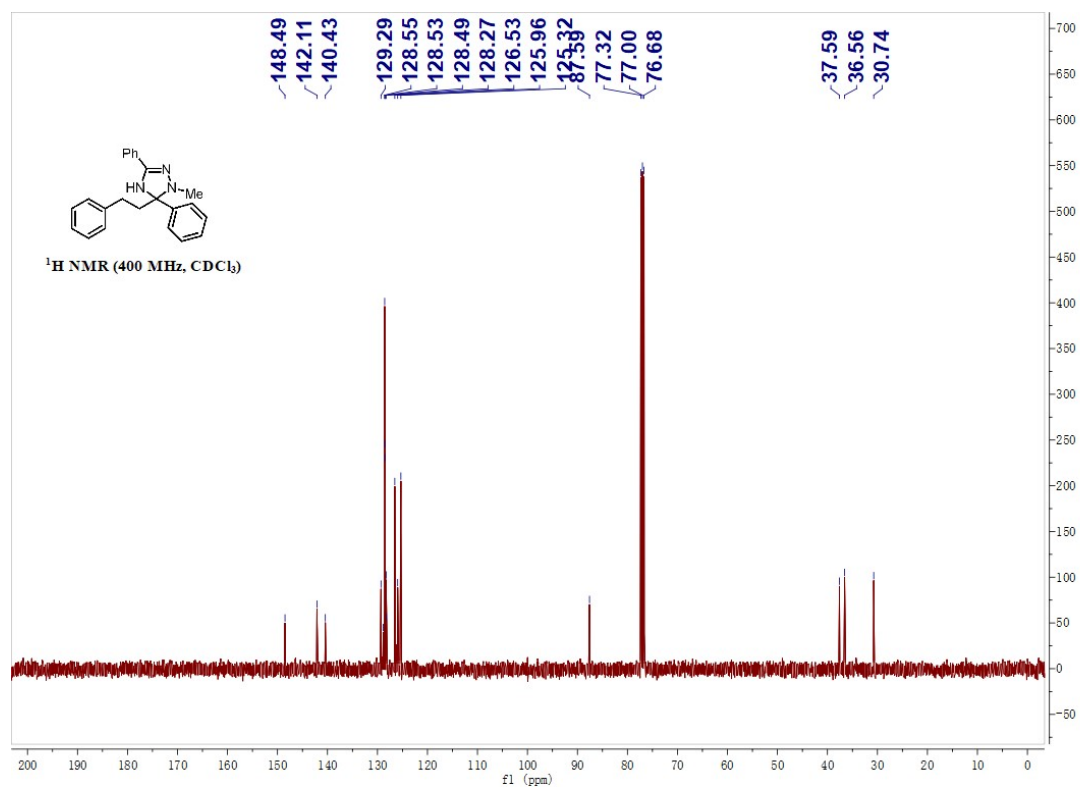
$^1\text{H}$  and  $^{13}\text{C}$  NMR spectra of compound **1a**



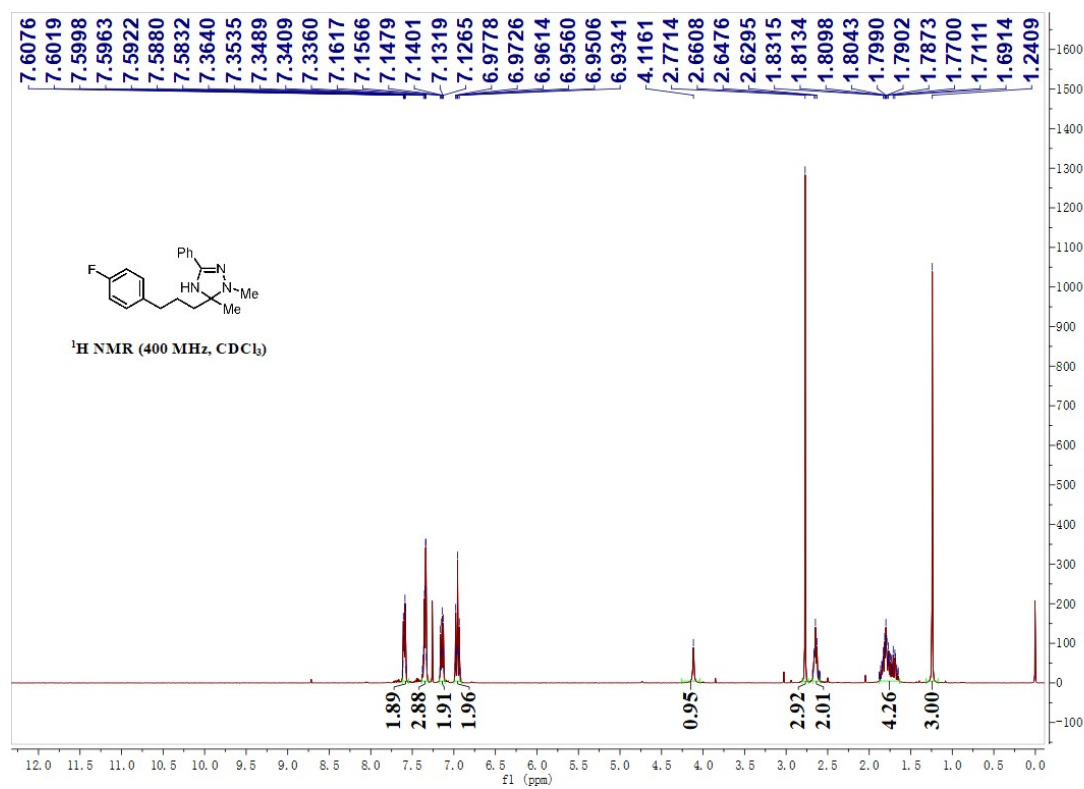


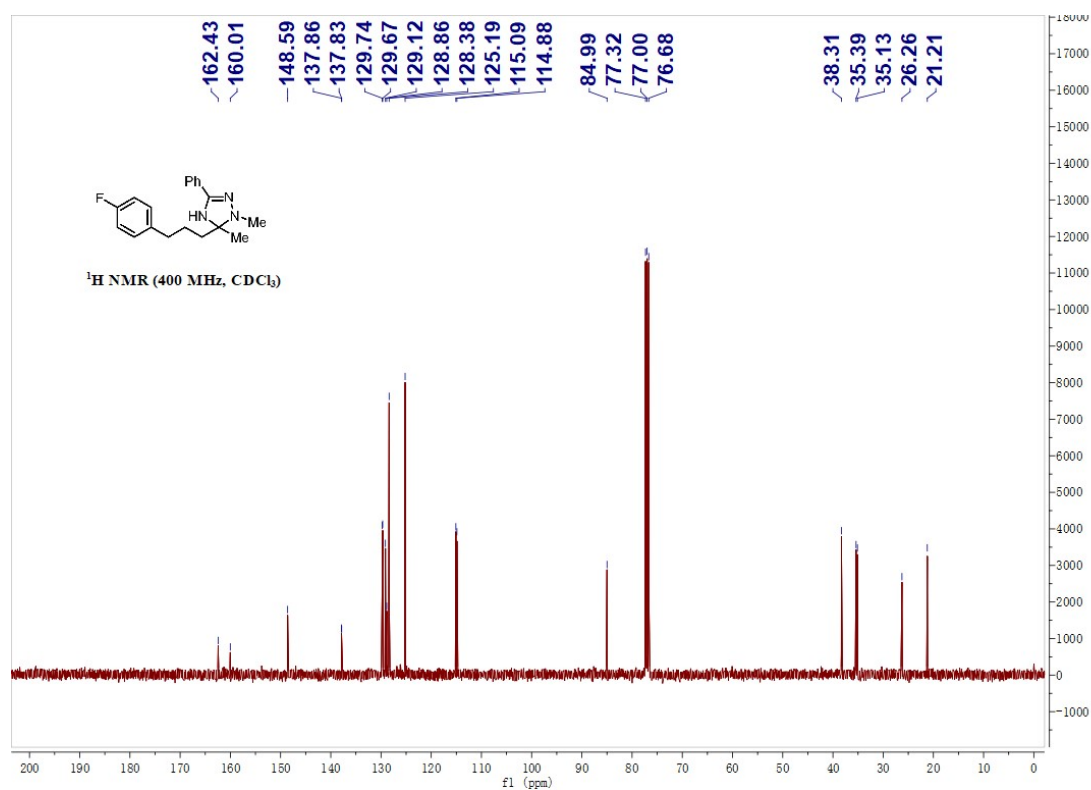
<sup>1</sup>H and <sup>13</sup>C NMR spectra of compound **1b**



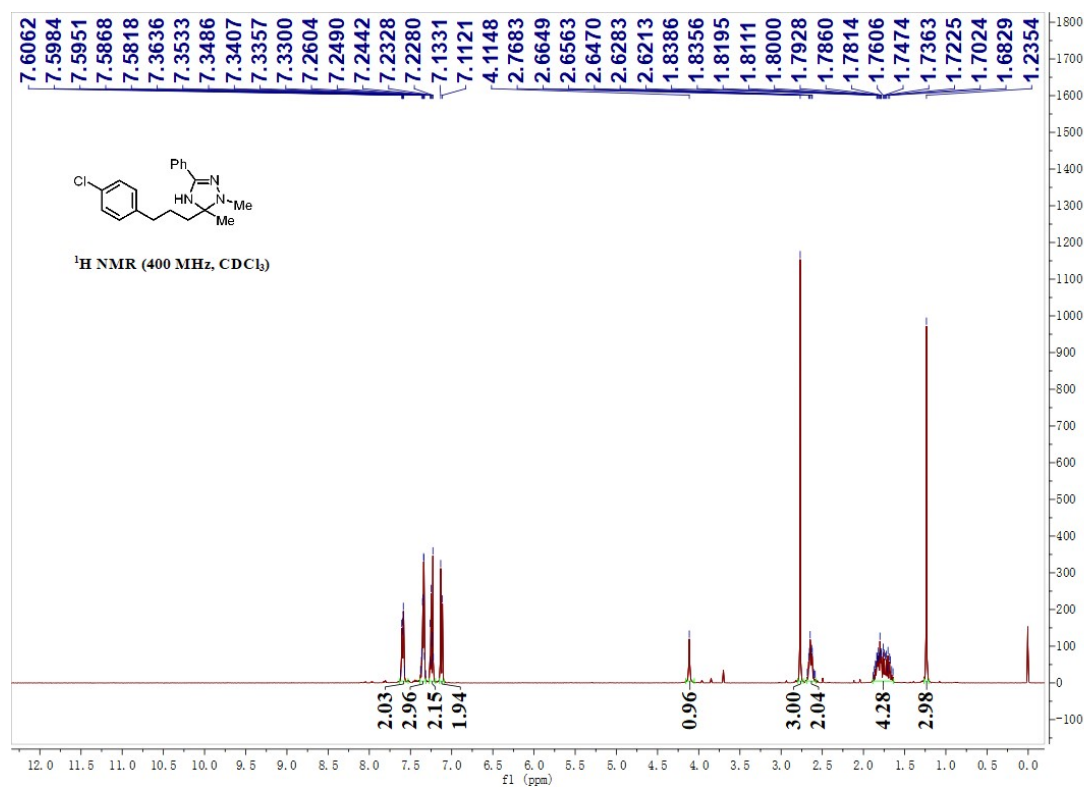


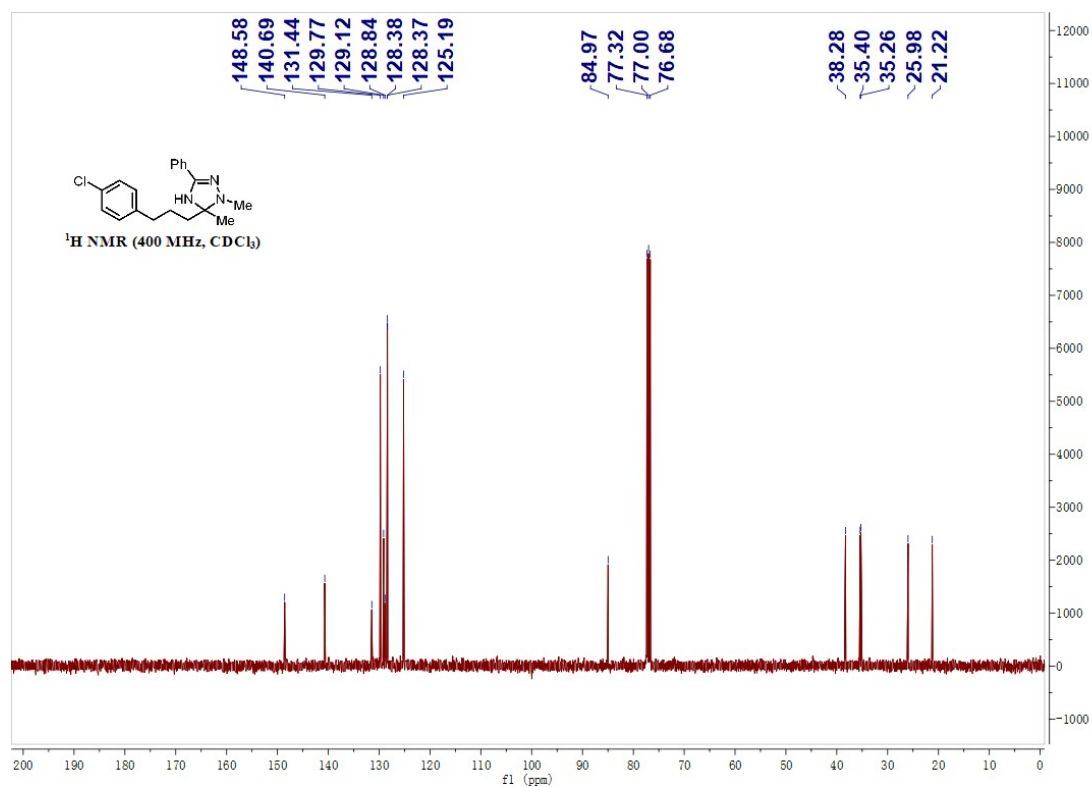
<sup>1</sup>H and <sup>13</sup>C NMR spectra of compound 1c



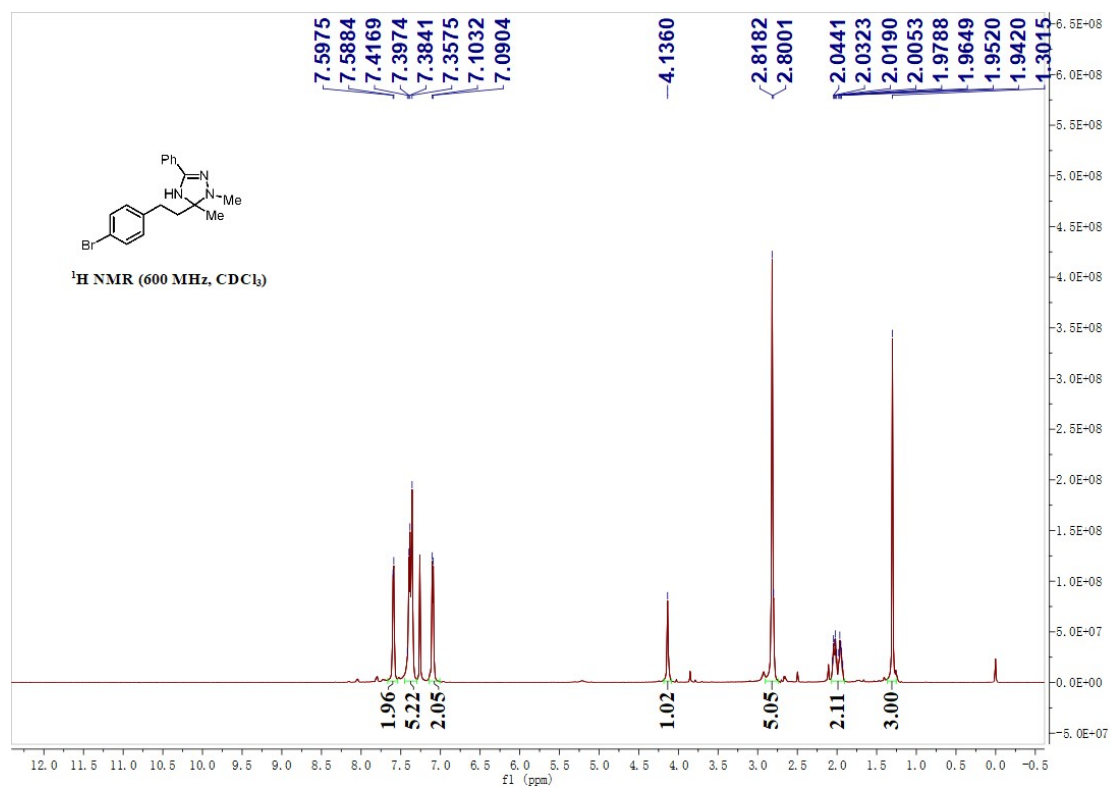


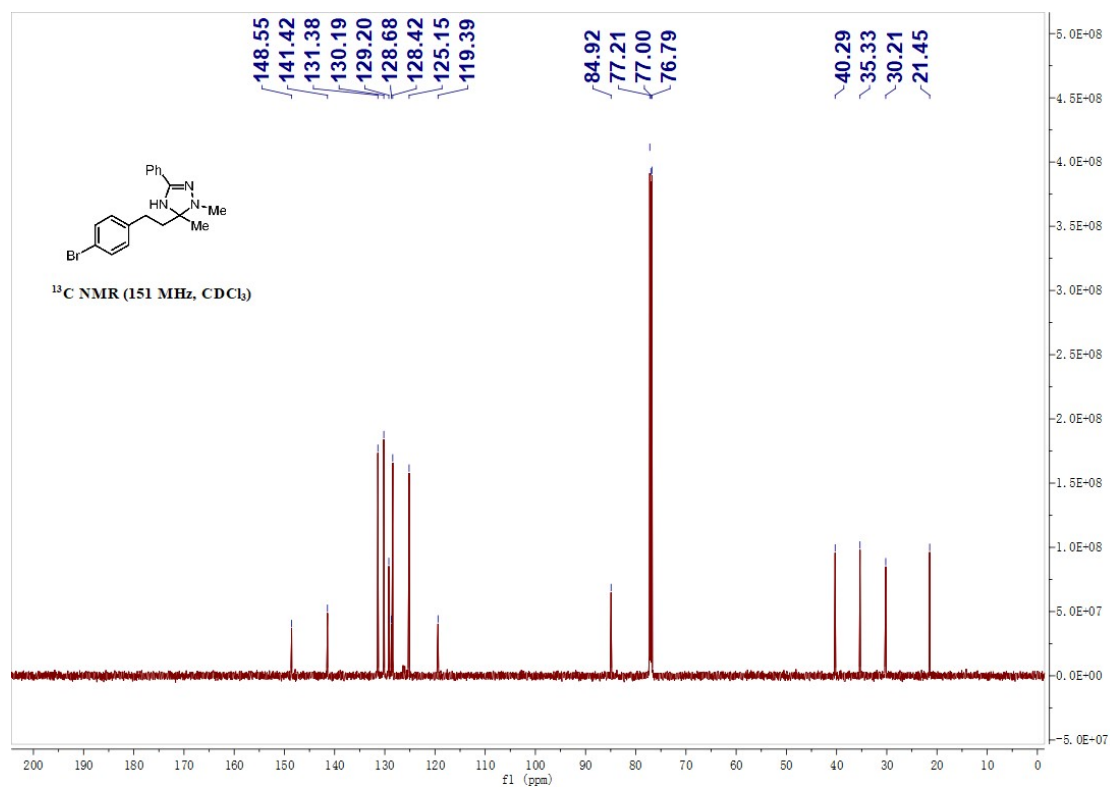
<sup>1</sup>H and <sup>13</sup>C NMR spectra of compound **1d**



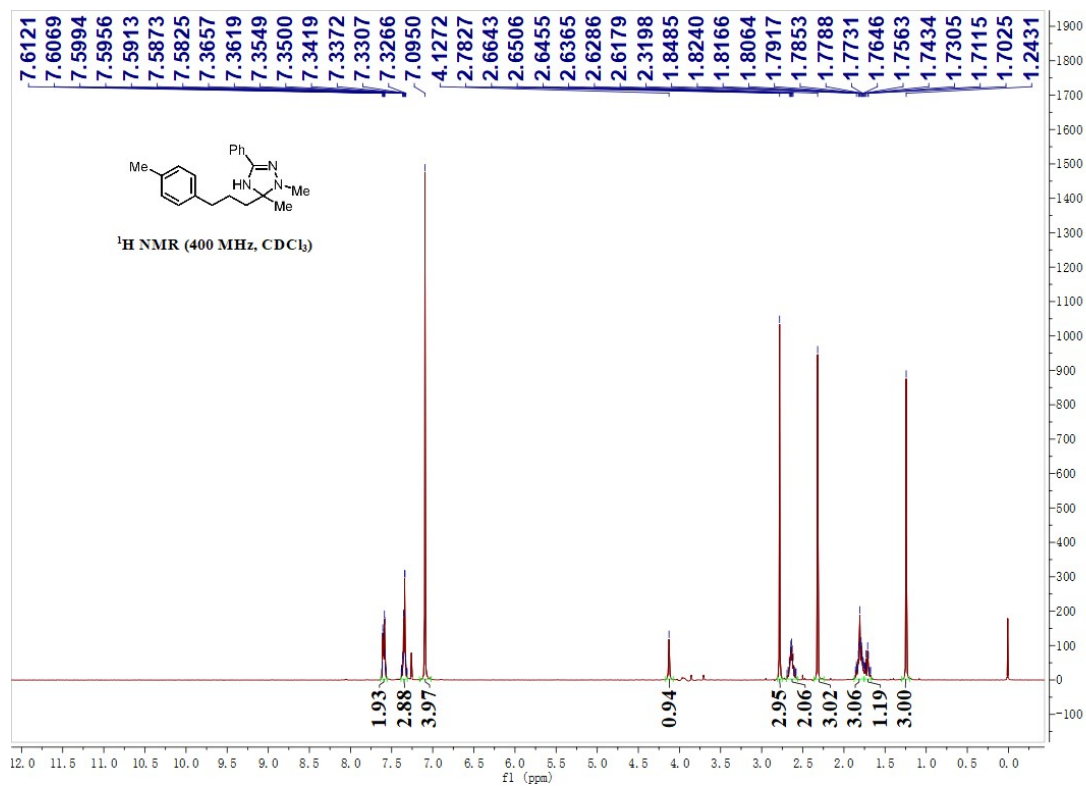


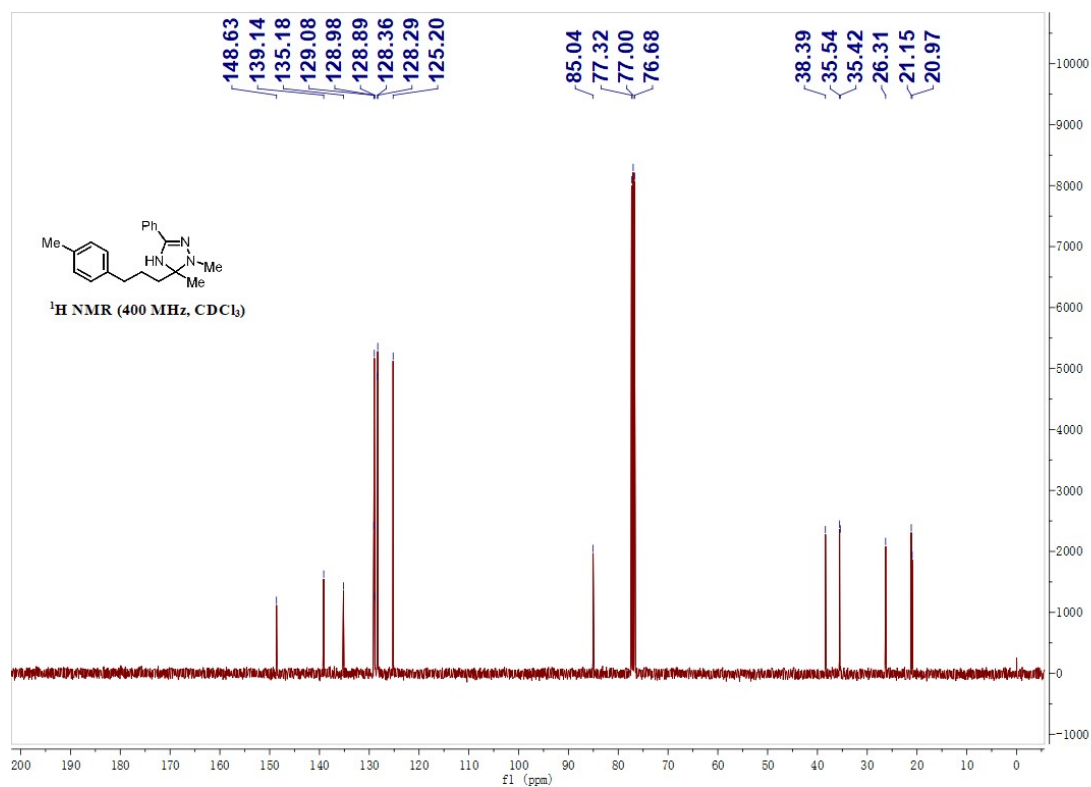
<sup>1</sup>H and <sup>13</sup>C NMR spectra of compound 1e



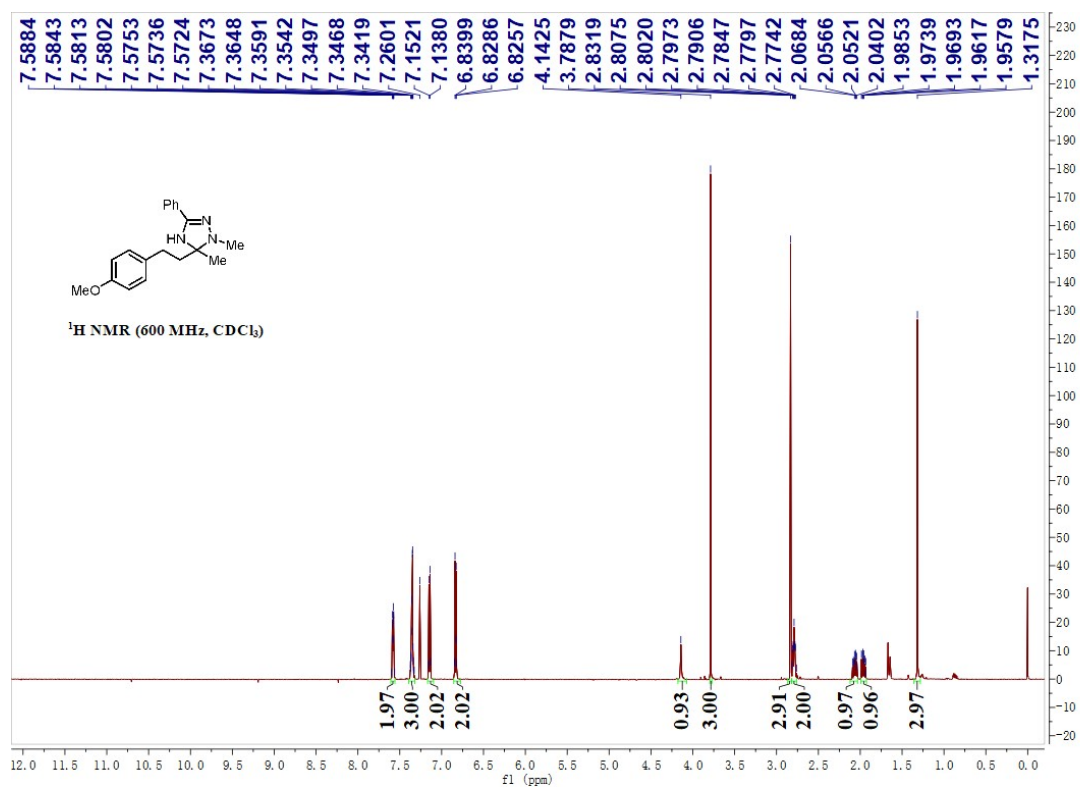


**<sup>1</sup>H and <sup>13</sup>C NMR spectra of compound **1f****

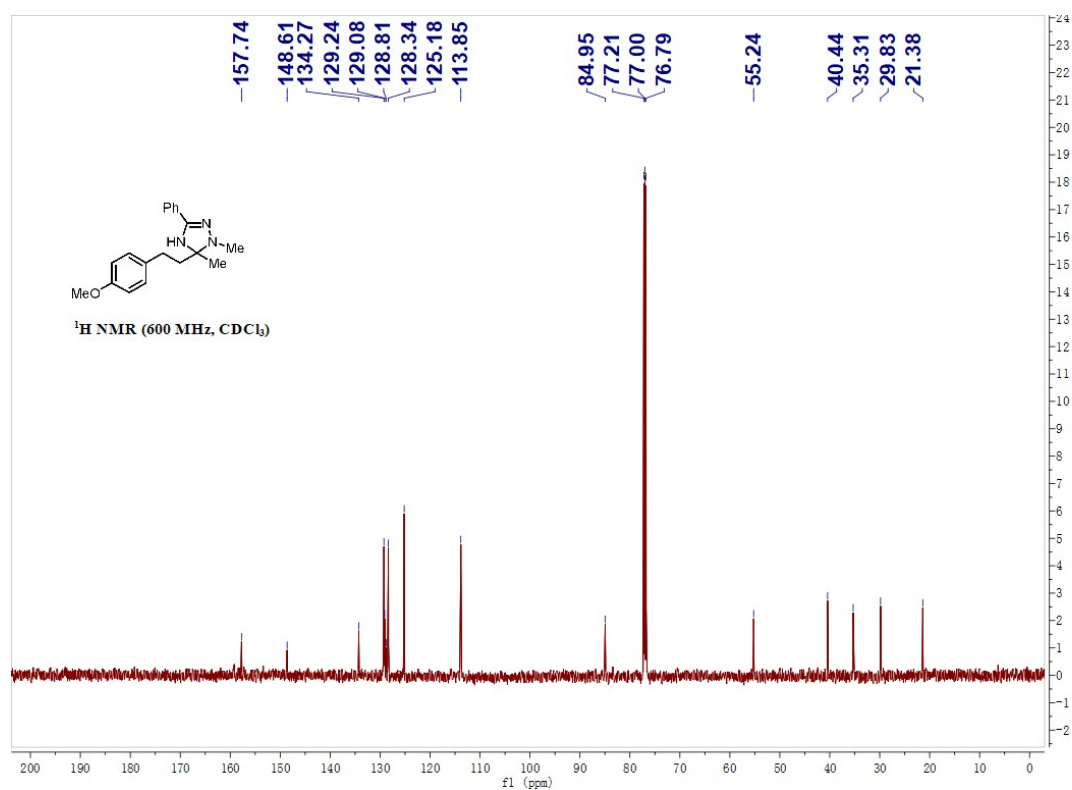




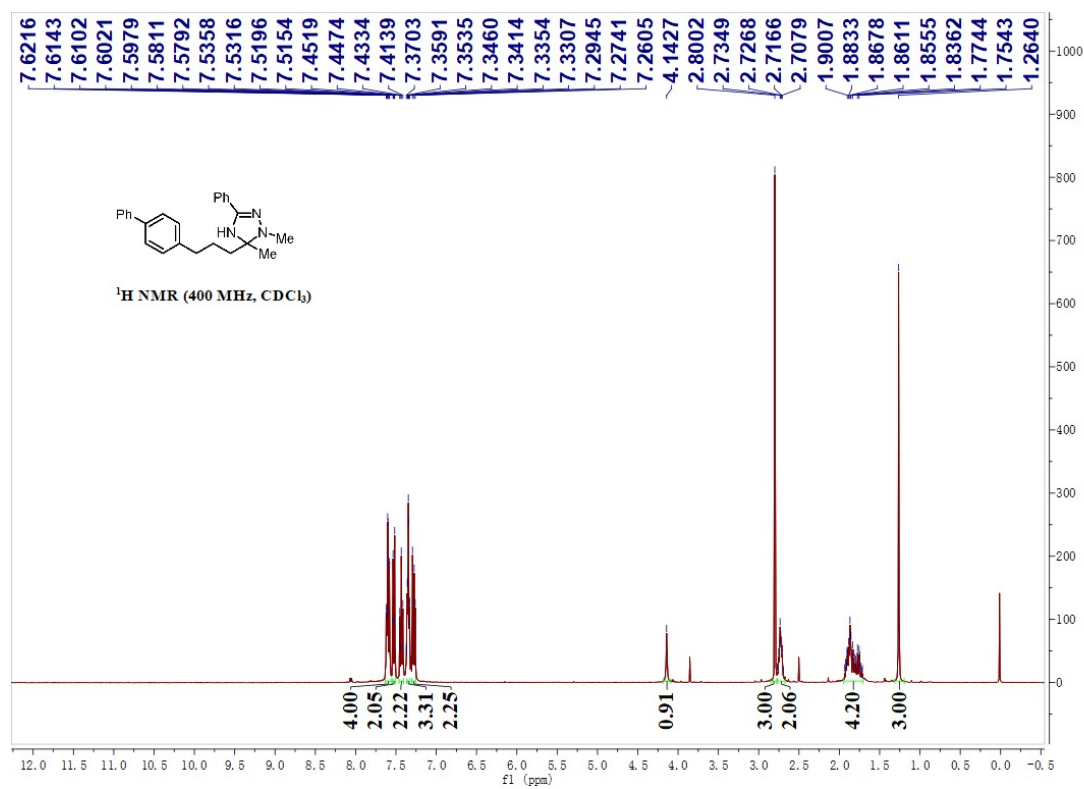
<sup>1</sup>H and <sup>13</sup>C NMR spectra of compound **1g**



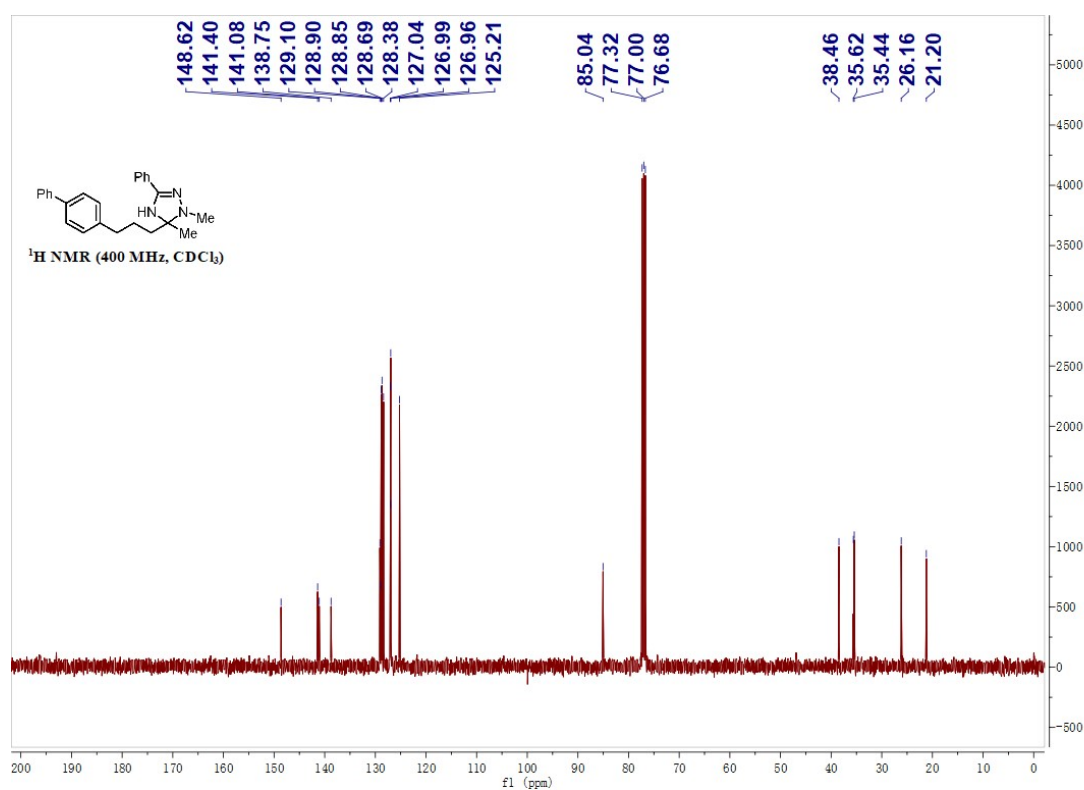




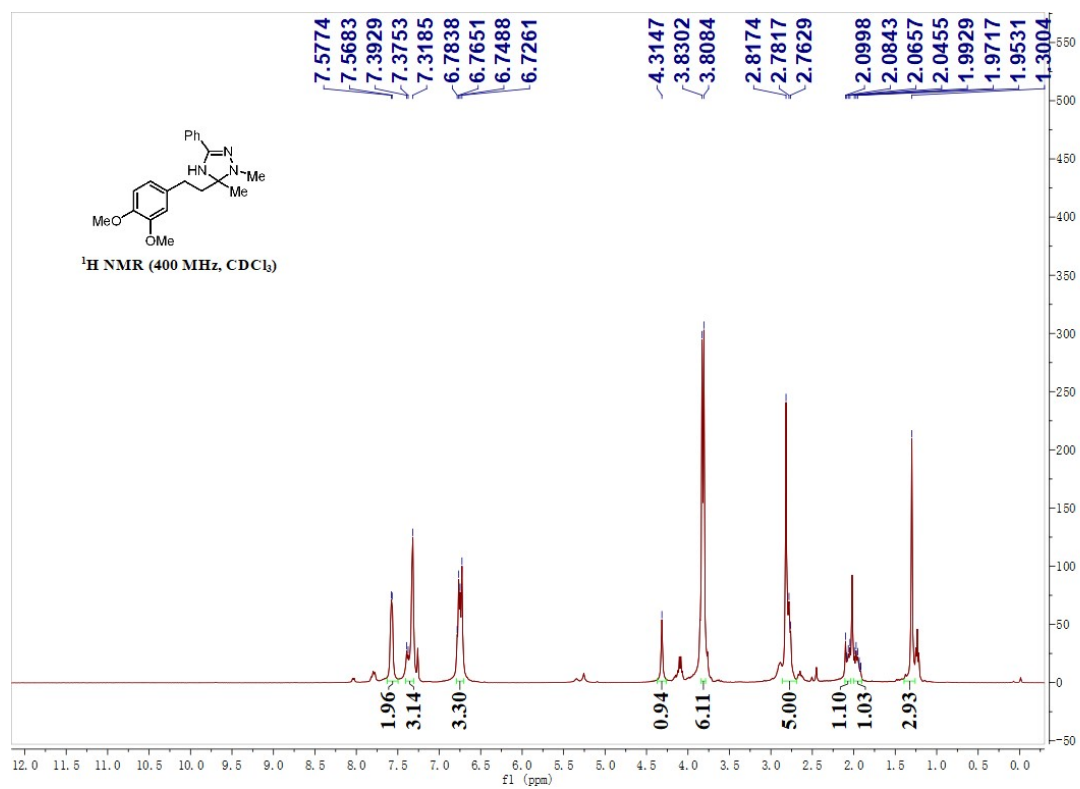
<sup>1</sup>H and <sup>13</sup>C NMR spectra of compound **1h**

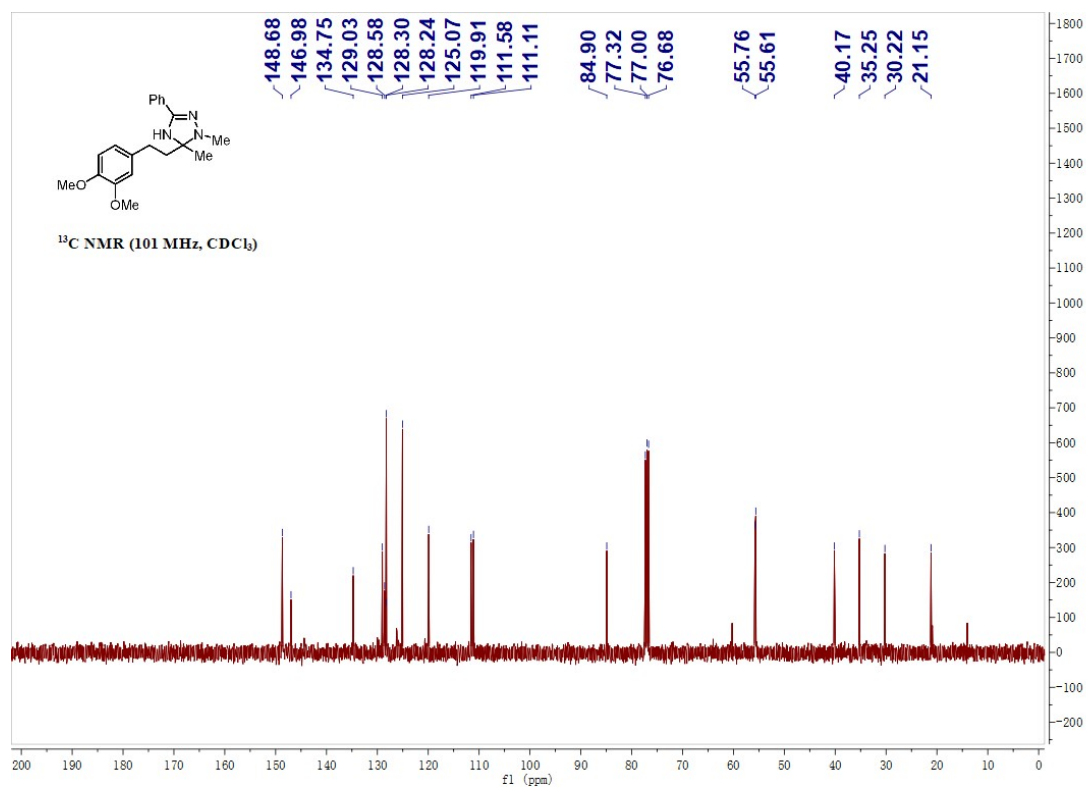




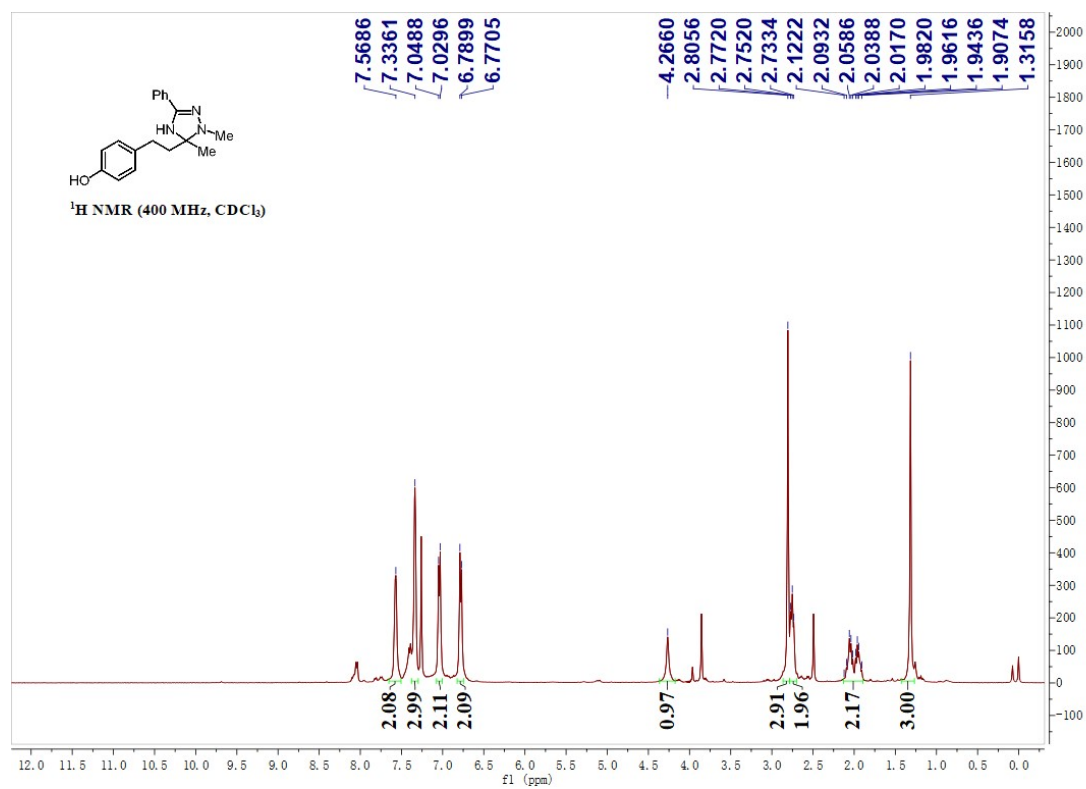


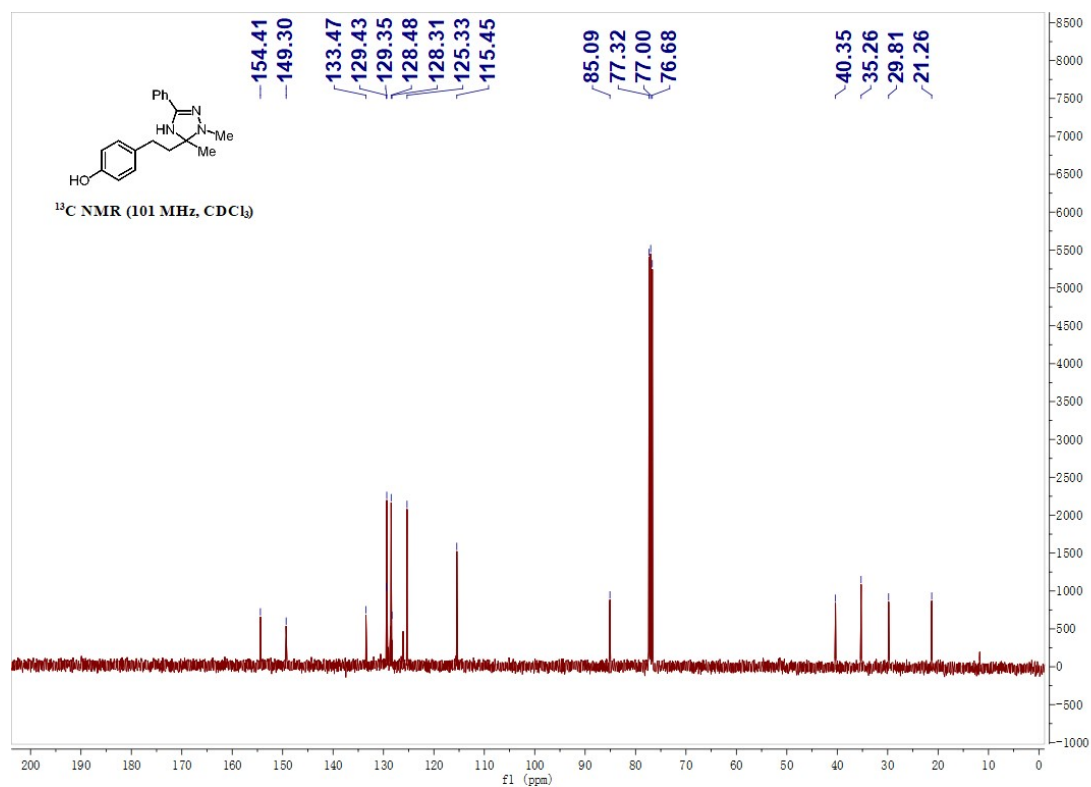
<sup>1</sup>H and <sup>13</sup>C NMR spectra of compound **1i**



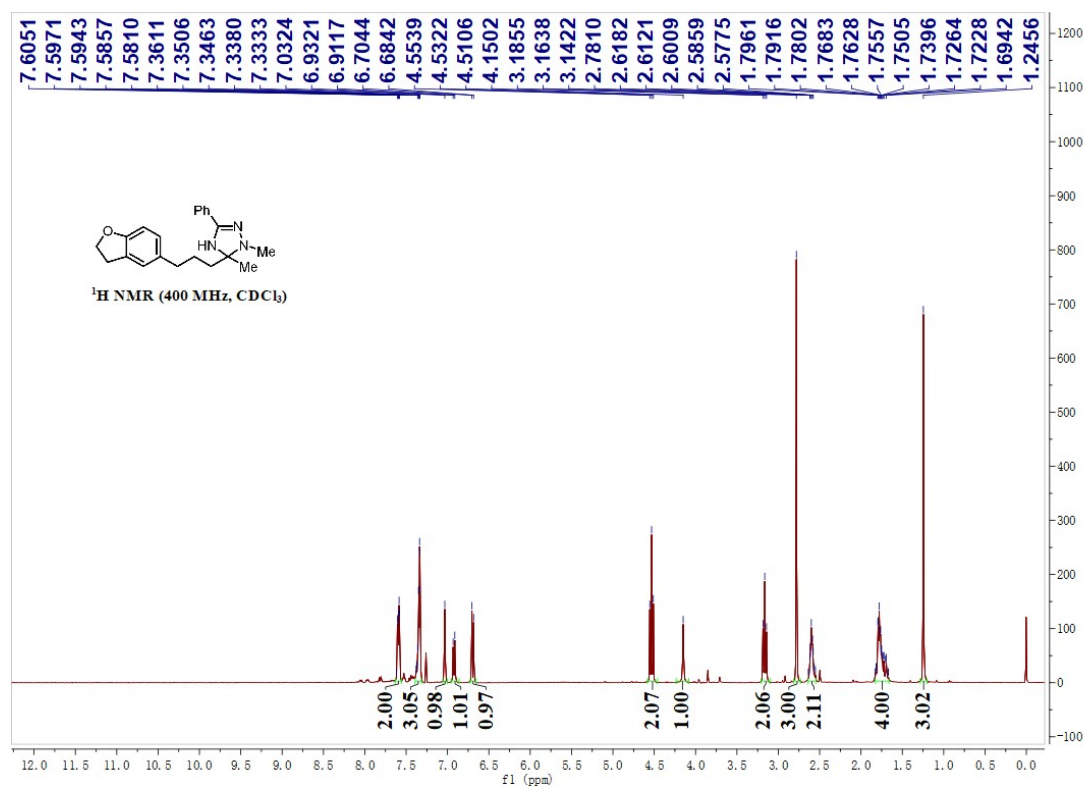


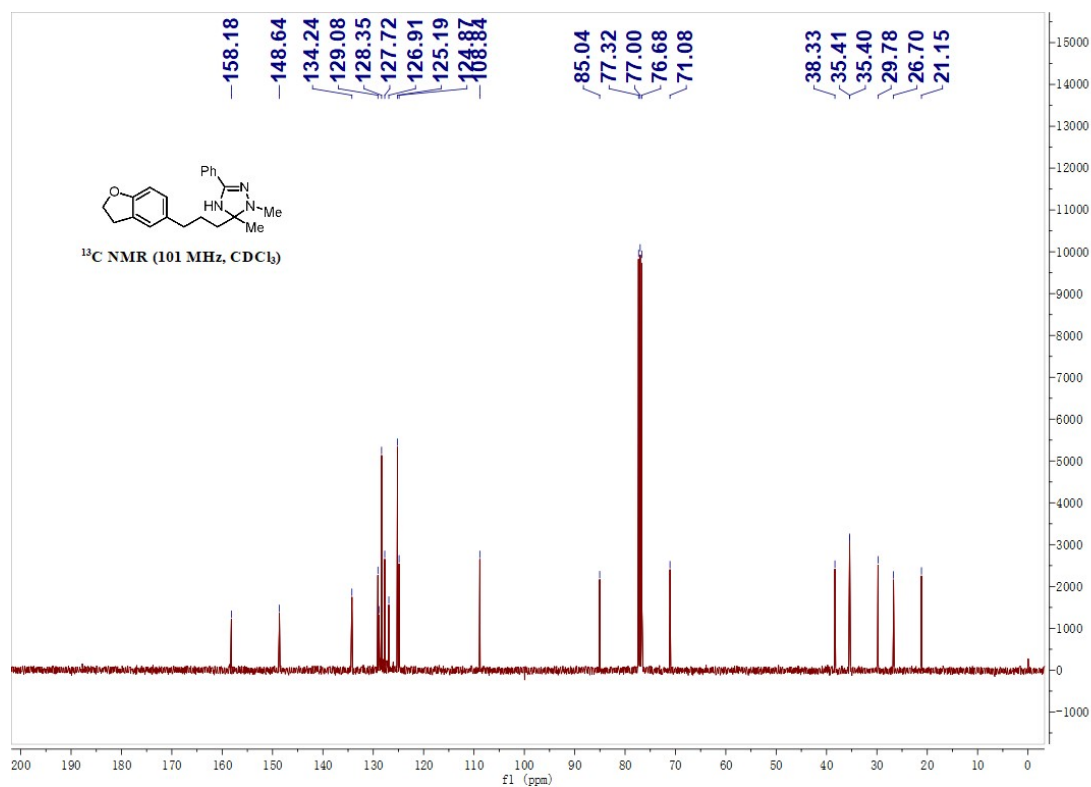
$^1\text{H}$  and  $^{13}\text{C}$  NMR spectra of compound **1j**



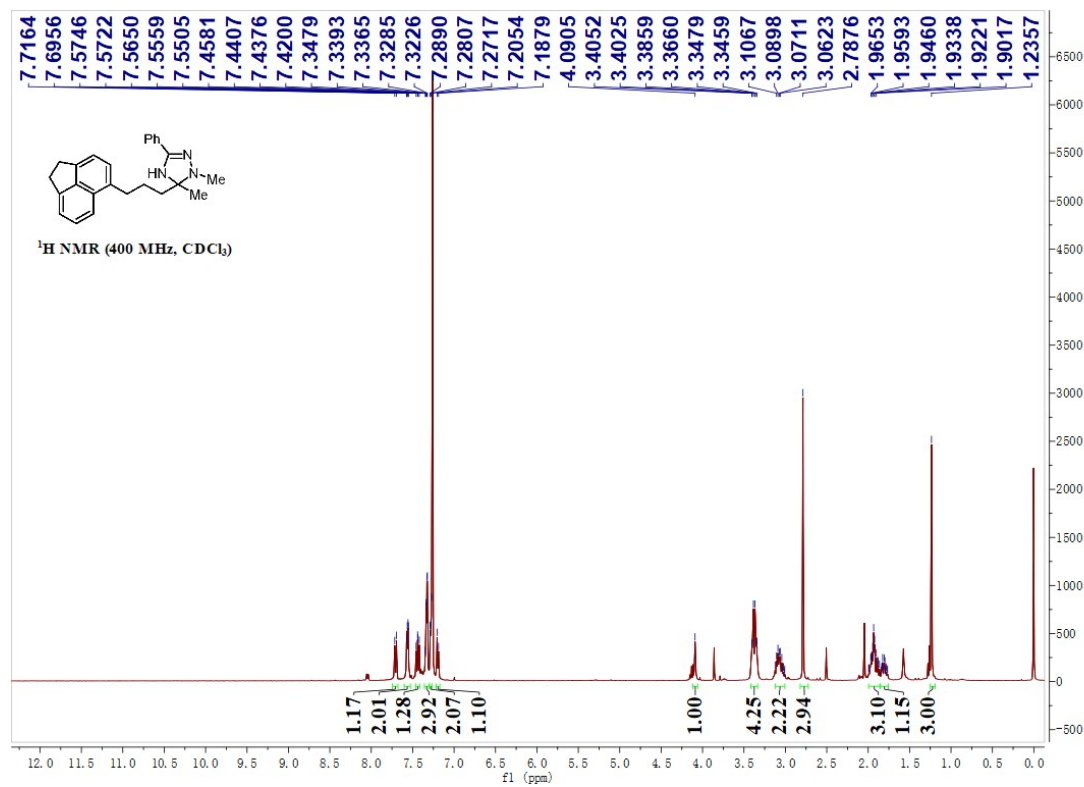


<sup>1</sup>H and <sup>13</sup>C NMR spectra of compound **1k**

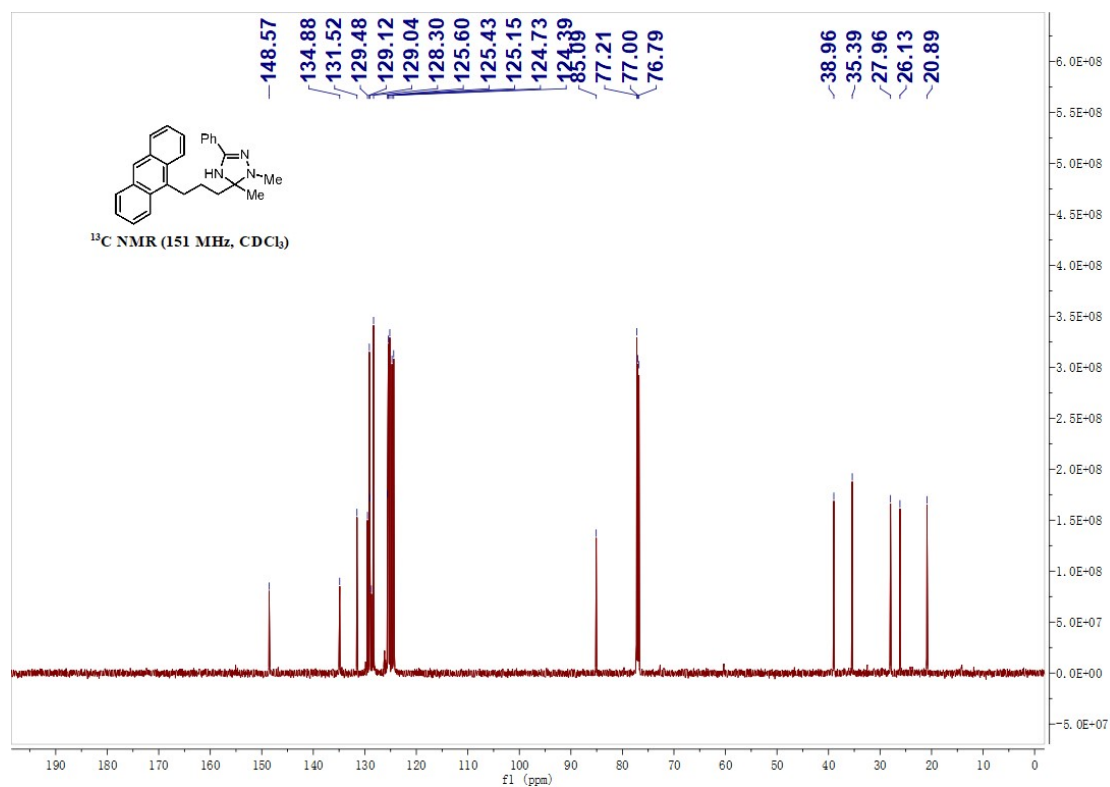
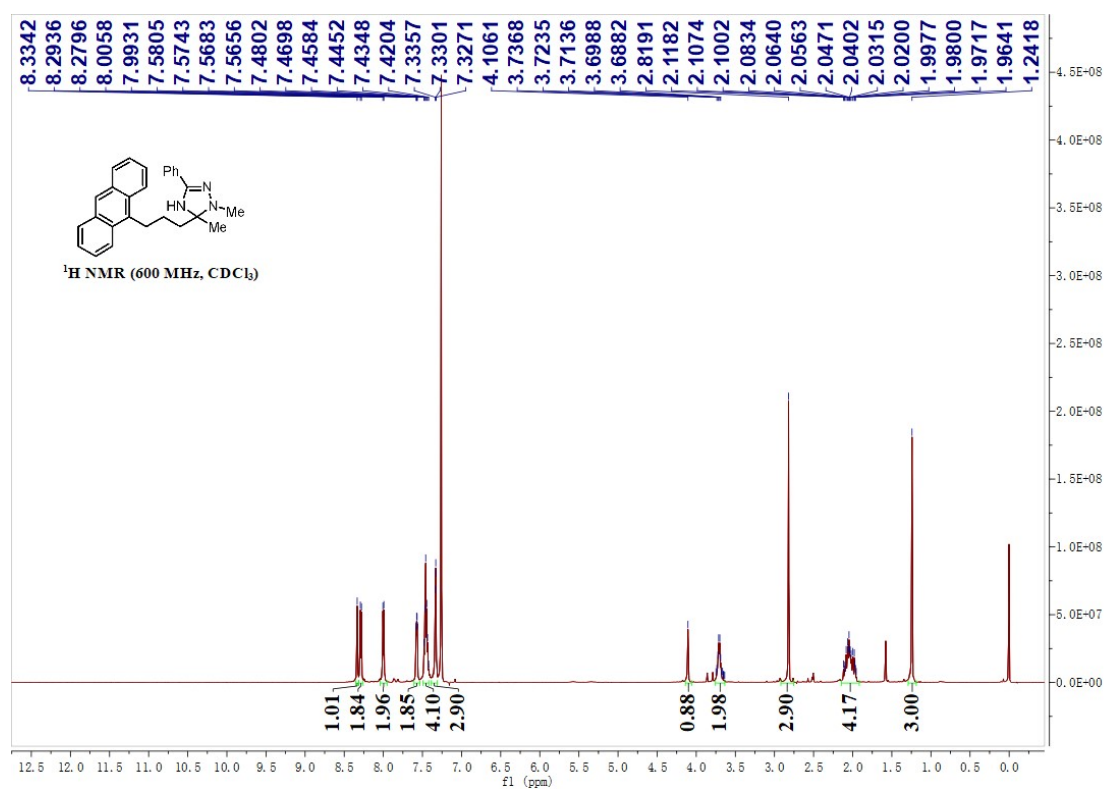




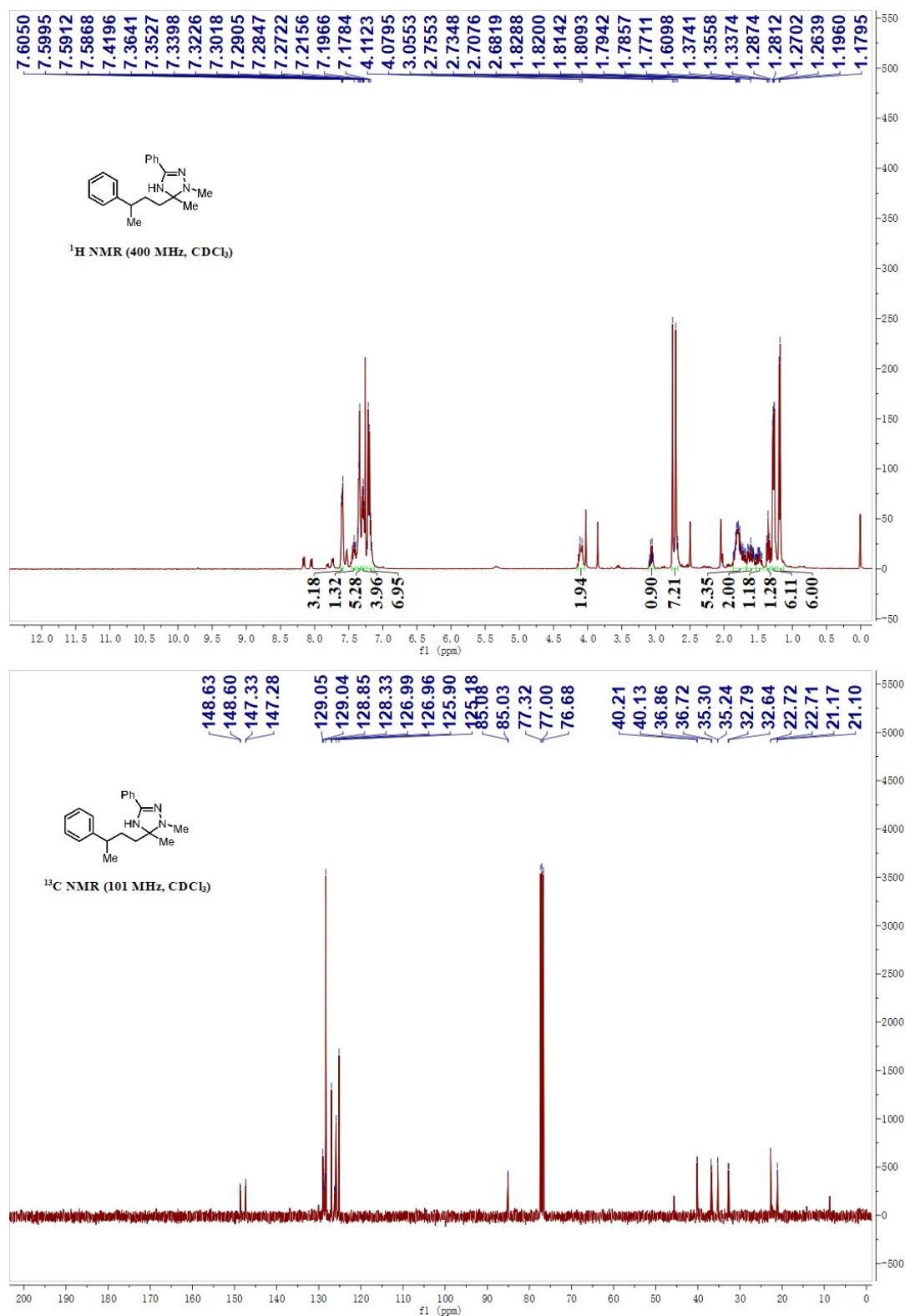
# <sup>1</sup>H NMR spectra of compound **11**



$^1\text{H}$  and  $^{13}\text{C}$  NMR spectra of compound **1m**

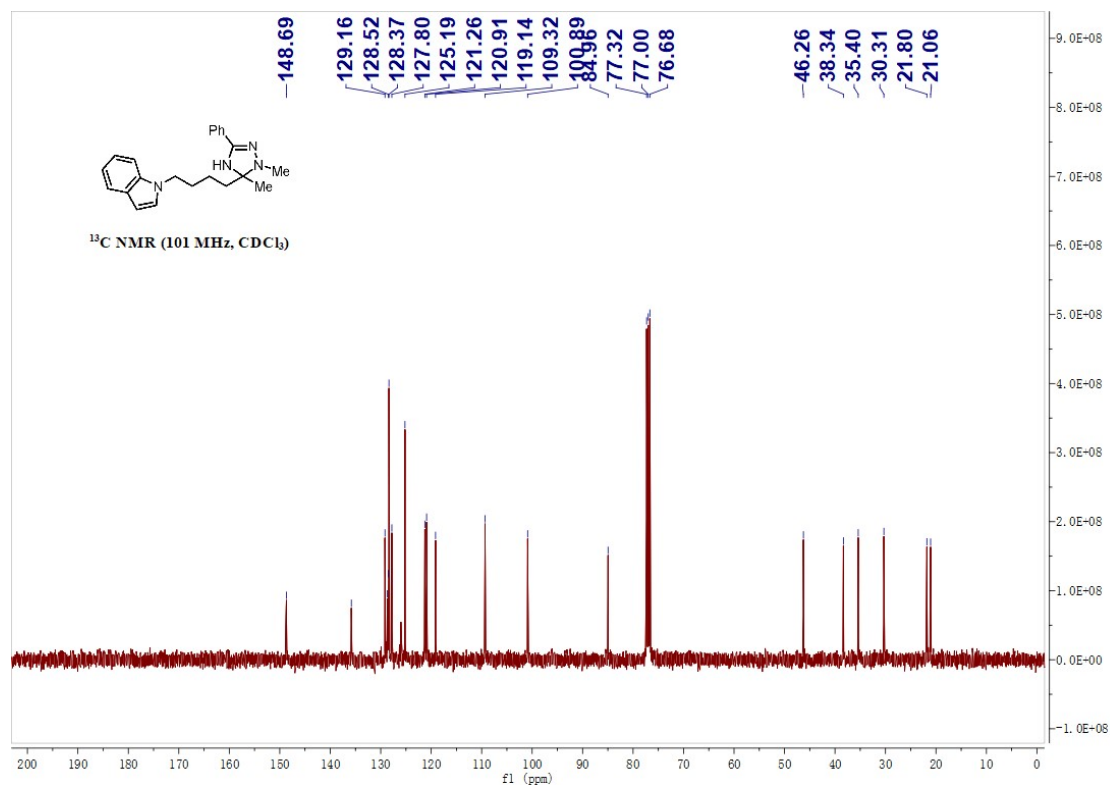
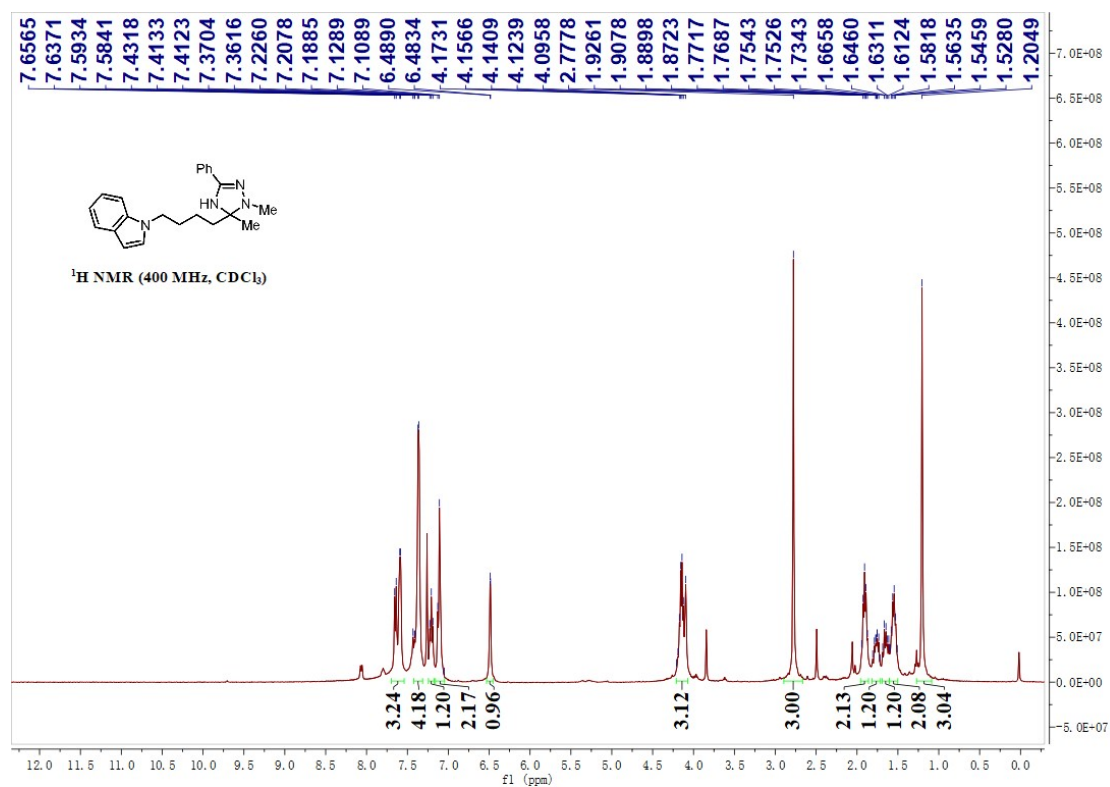


$^1\text{H}$  and  $^{13}\text{C}$  NMR spectra of compound **1n**

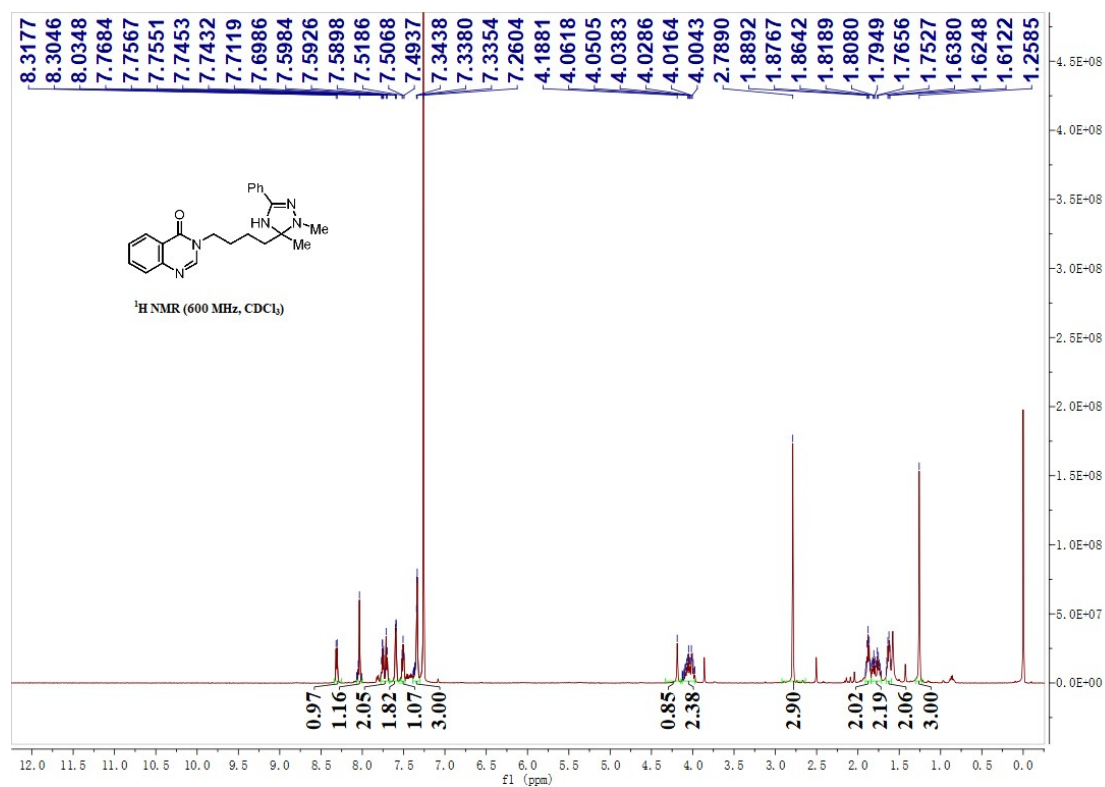


<sup>1</sup>H and <sup>13</sup>C NMR spectra of compound **10**

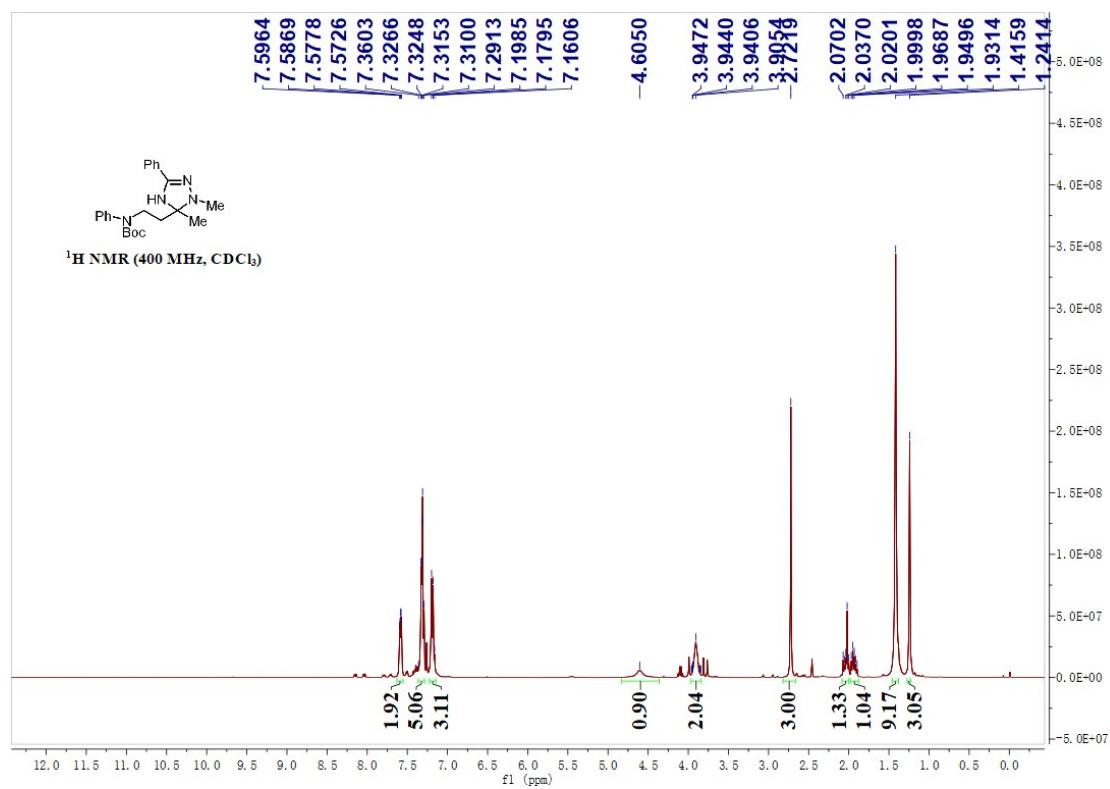




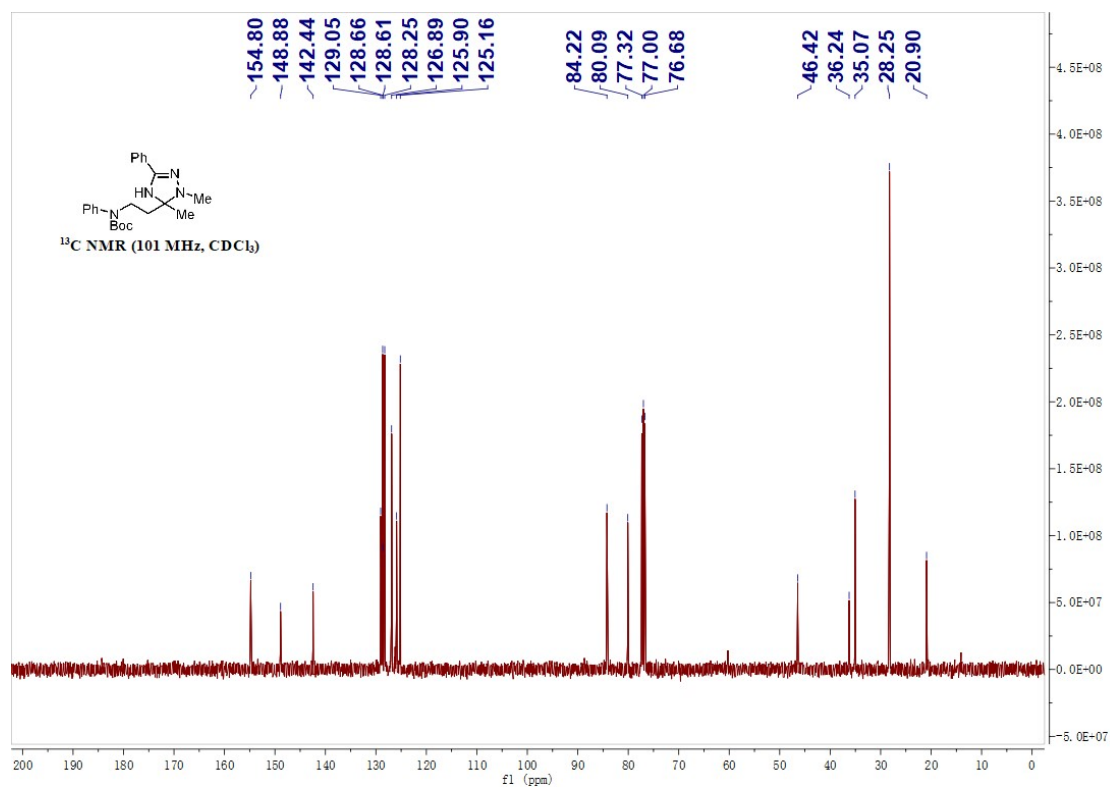
<sup>1</sup>H NMR spectra of compound **1p**



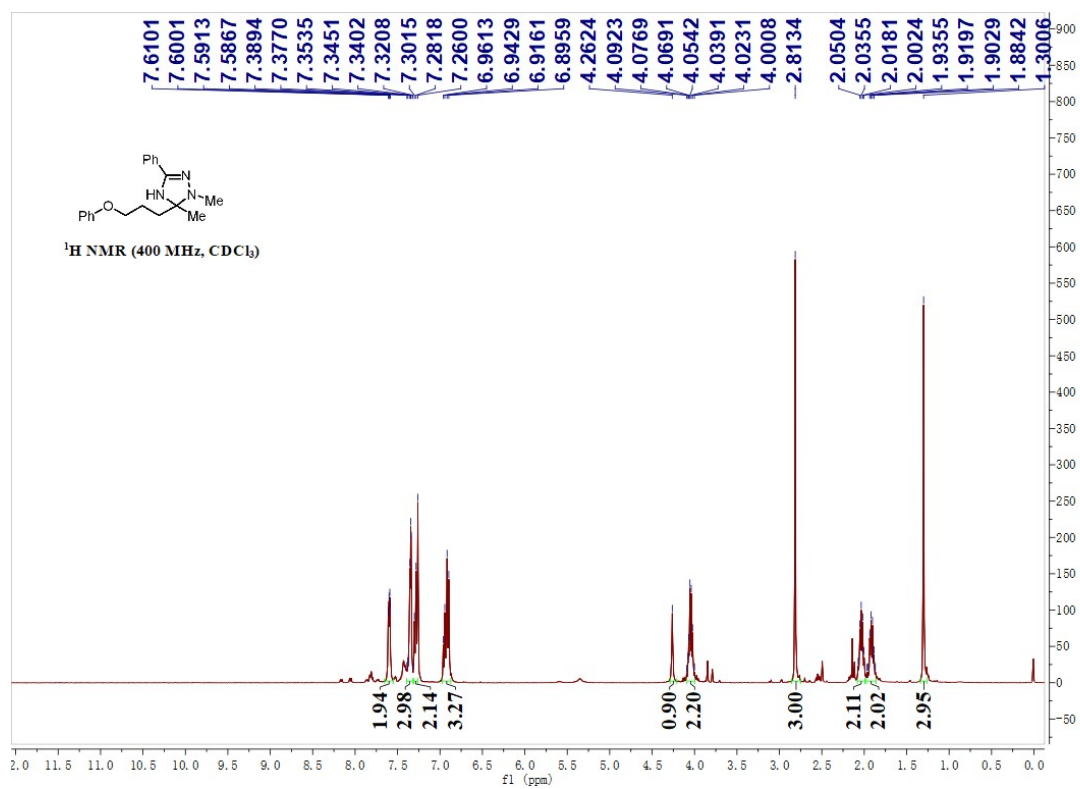
<sup>1</sup>H and <sup>13</sup>C NMR spectra of compound 1q

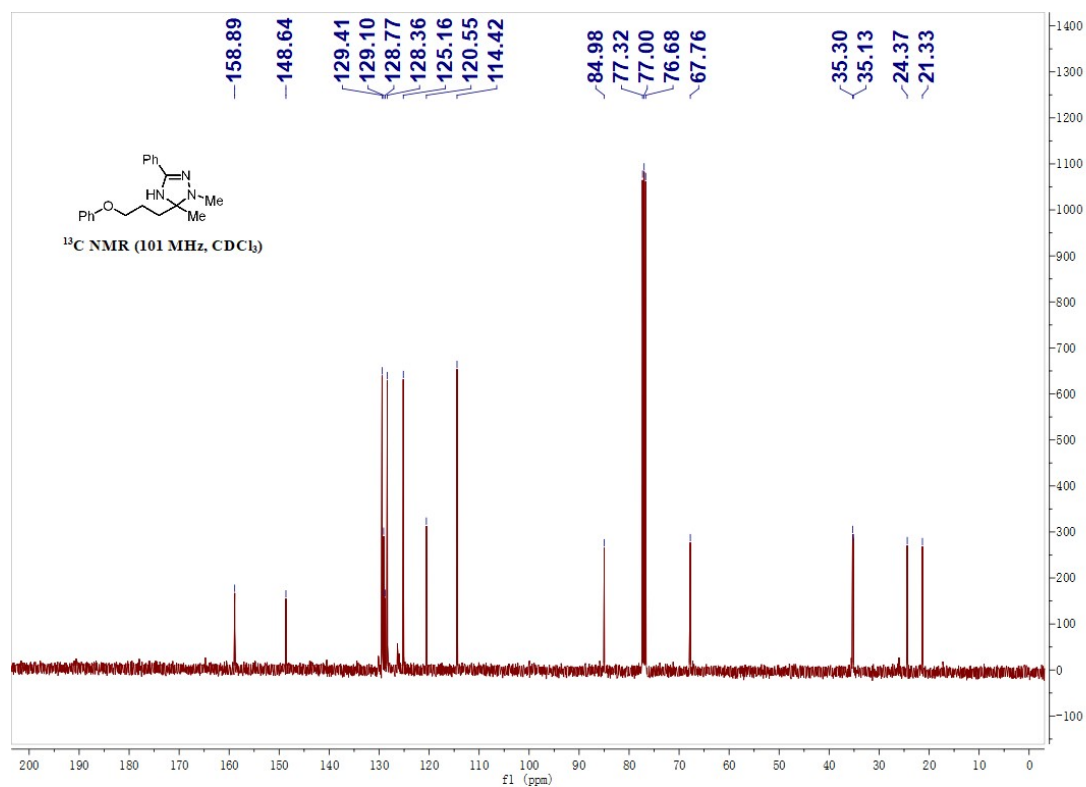




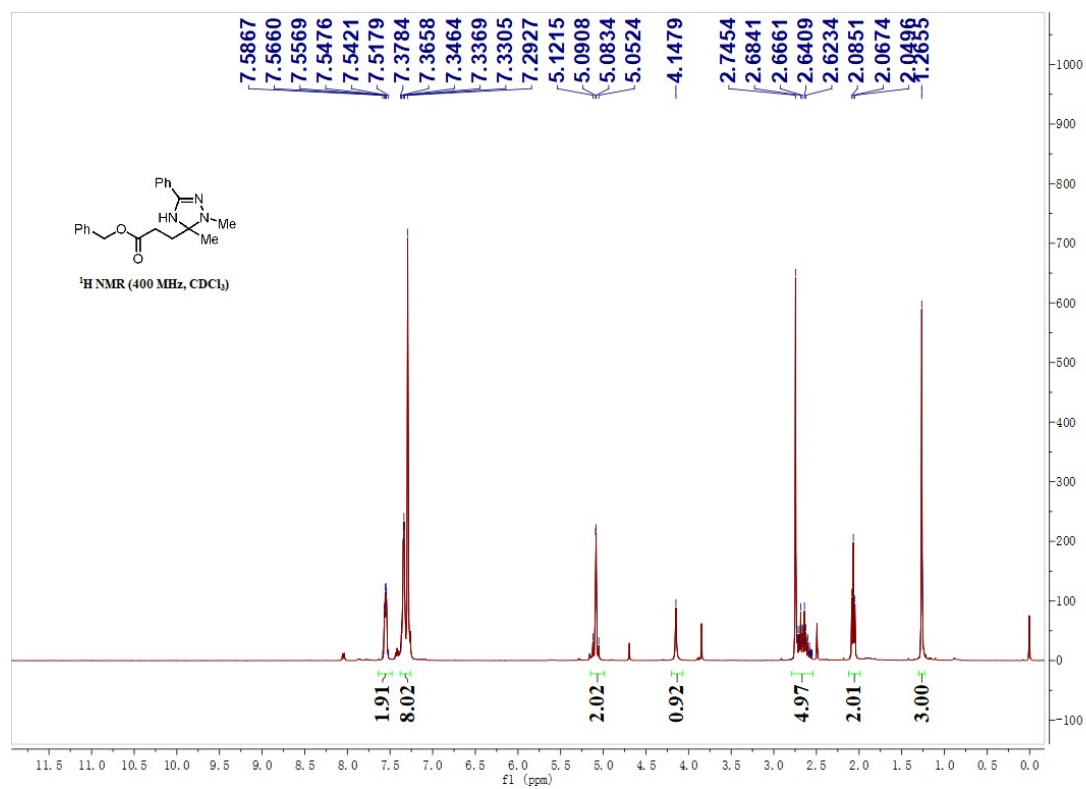


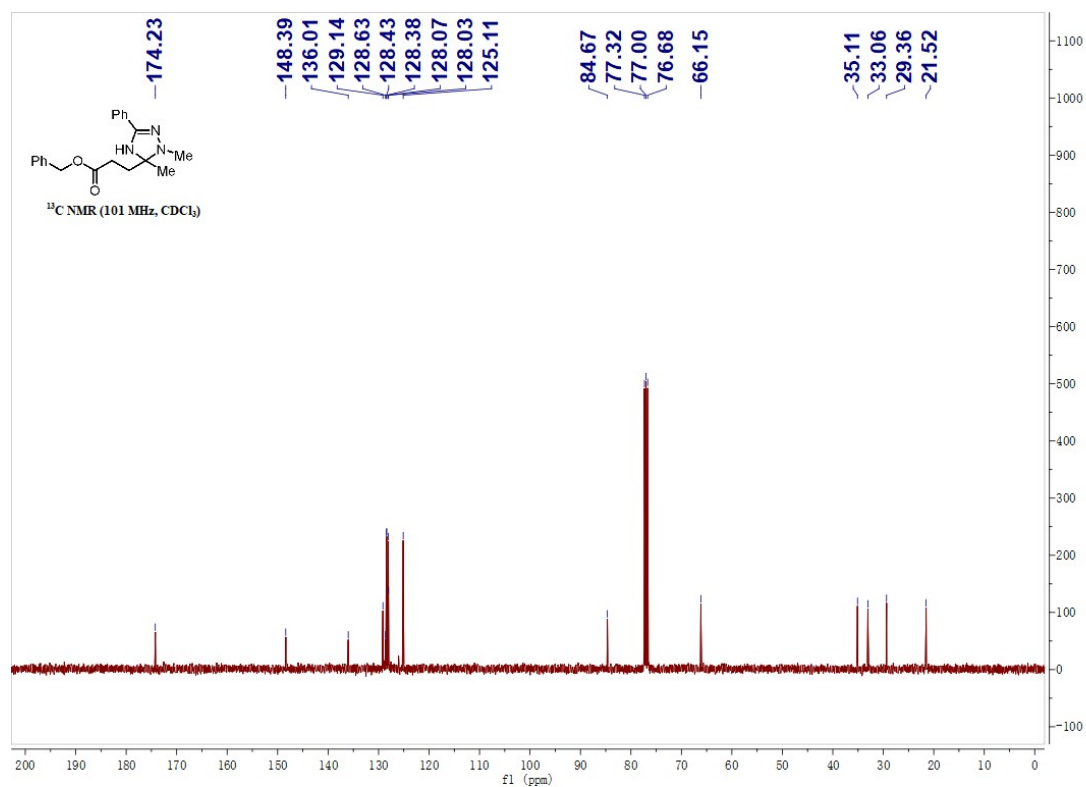
**<sup>1</sup>H and <sup>13</sup>C NMR spectra of compound **1r****



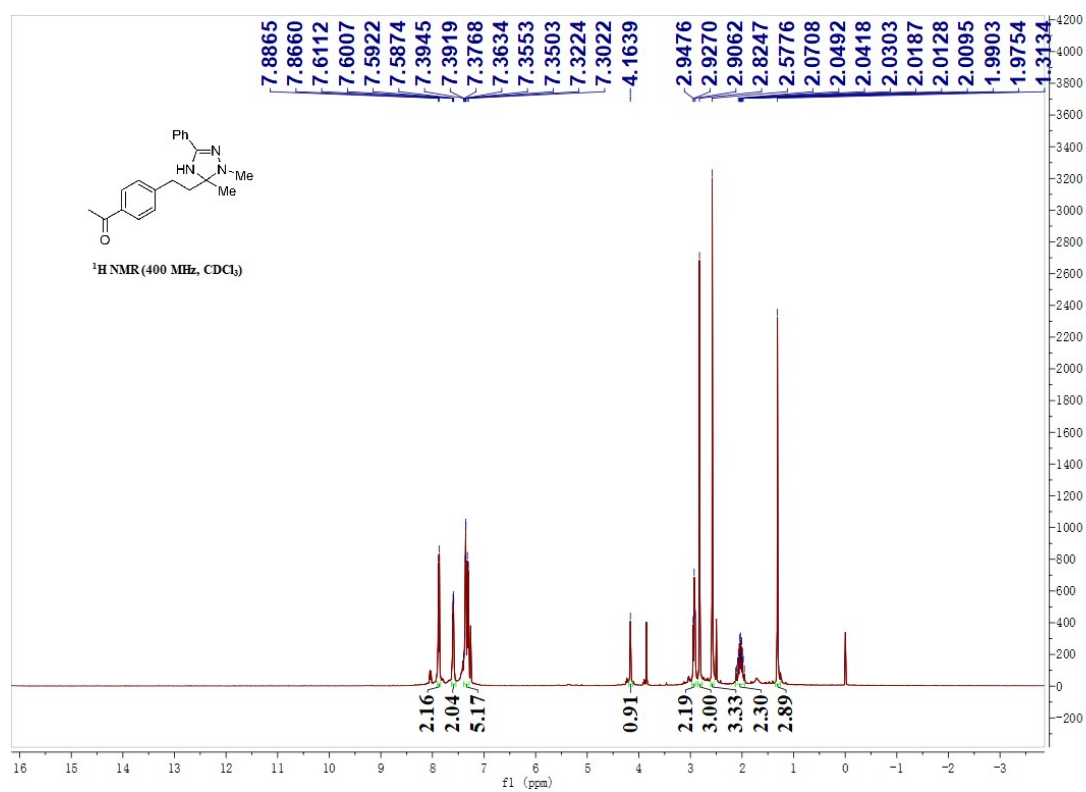


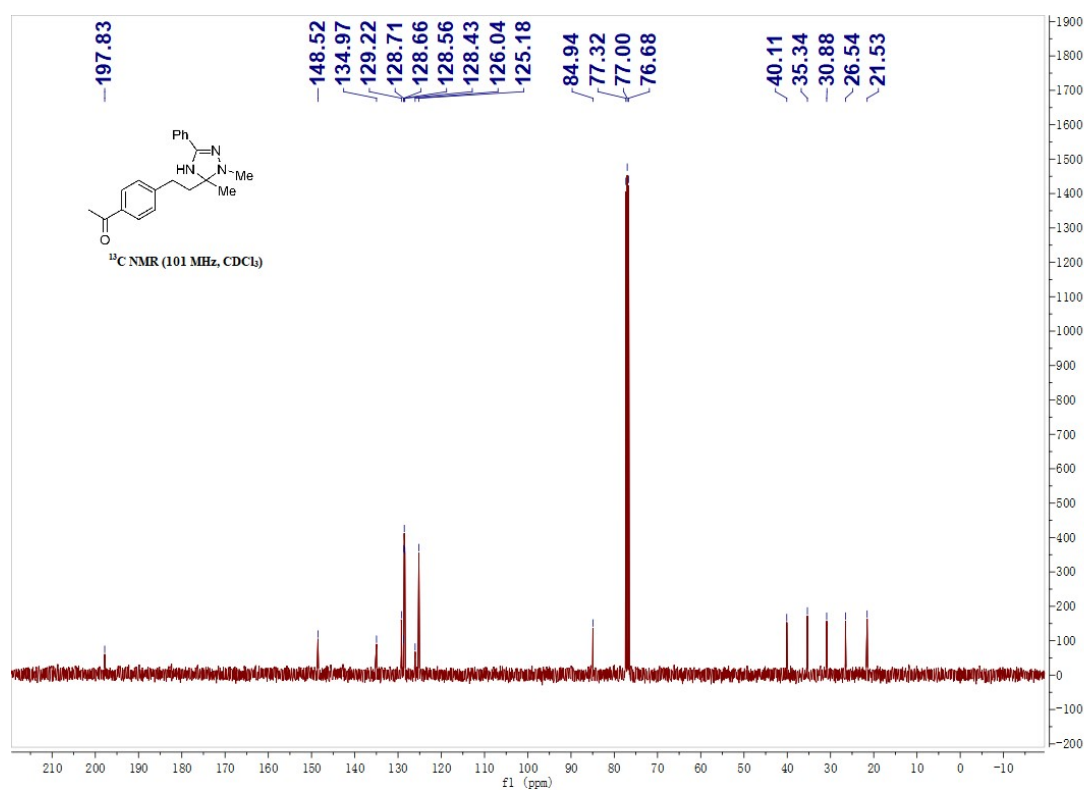
<sup>1</sup>H and <sup>13</sup>C NMR spectra of compound **1s**



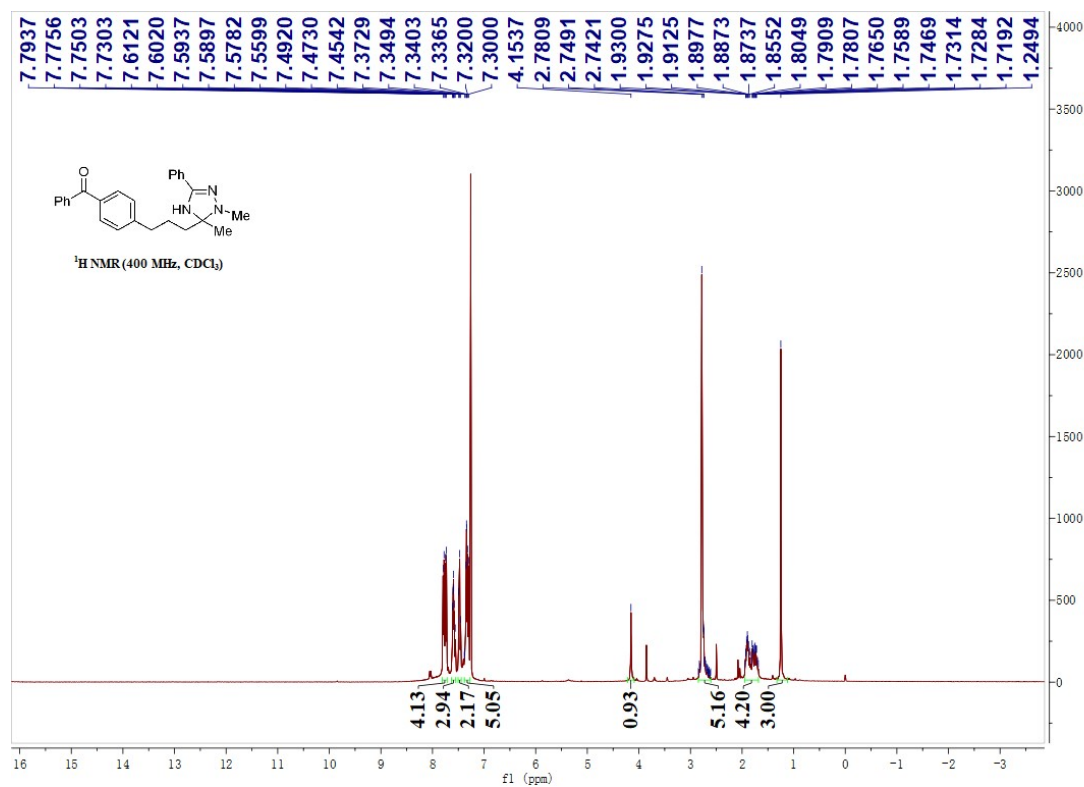


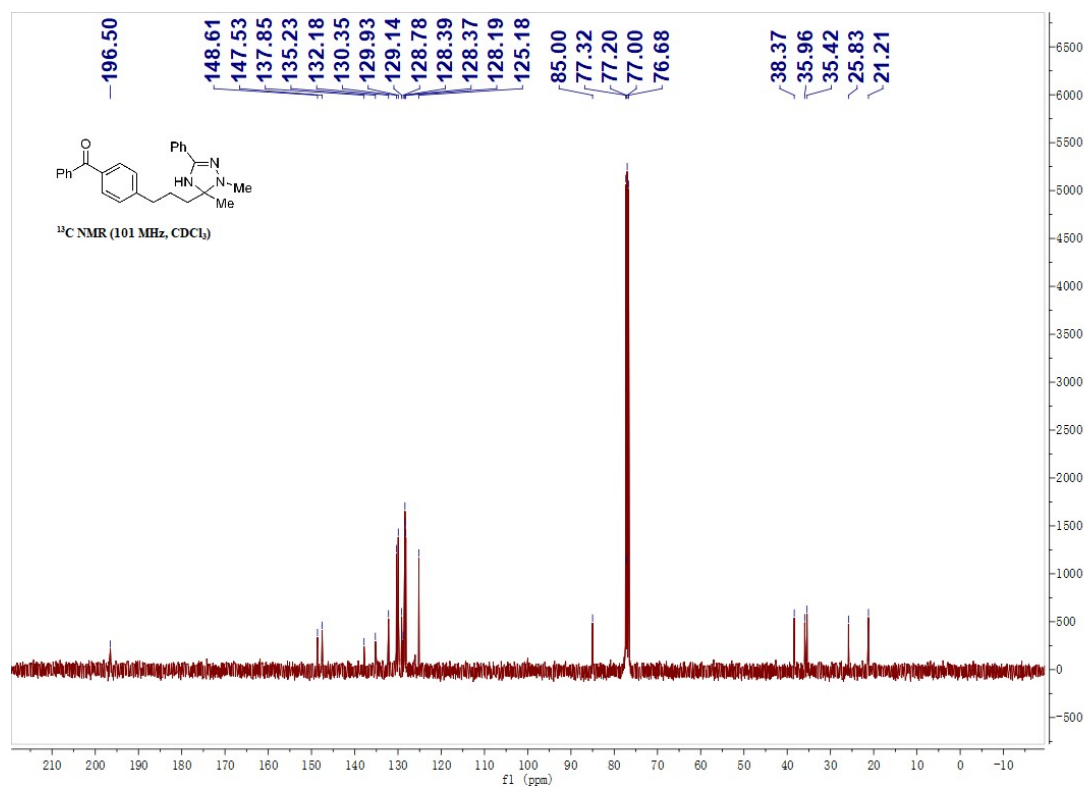
**<sup>1</sup>H and <sup>13</sup>C NMR spectra of compound **1t****



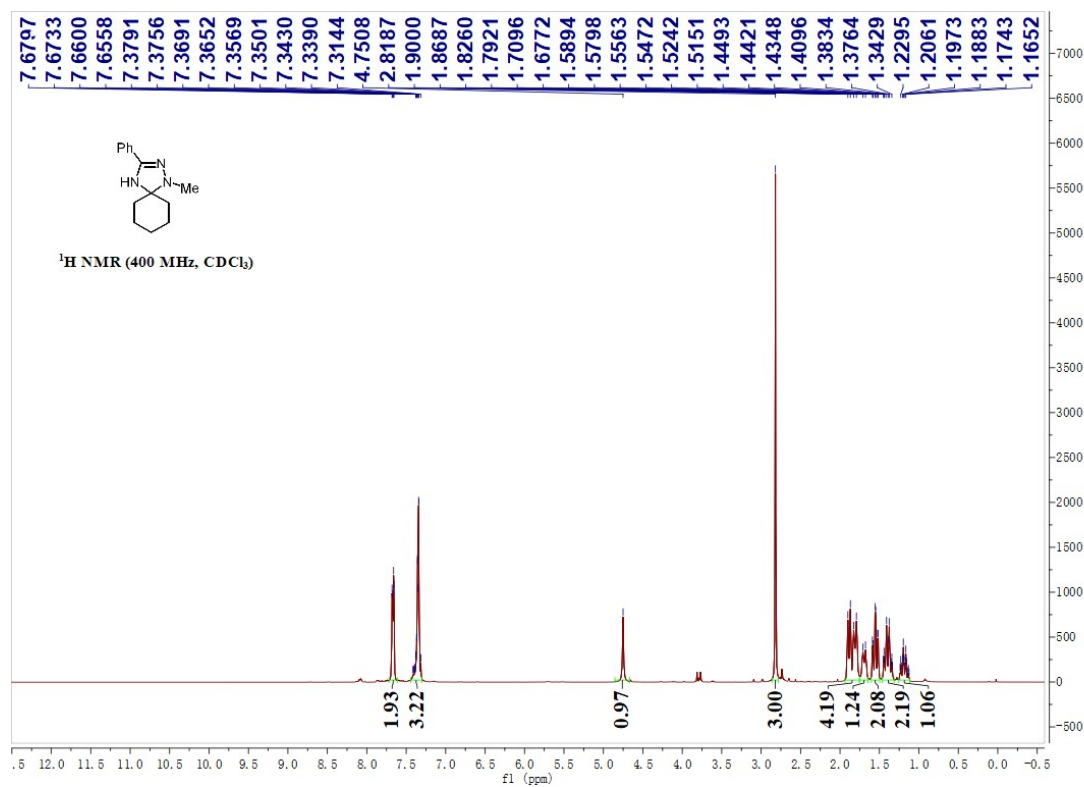


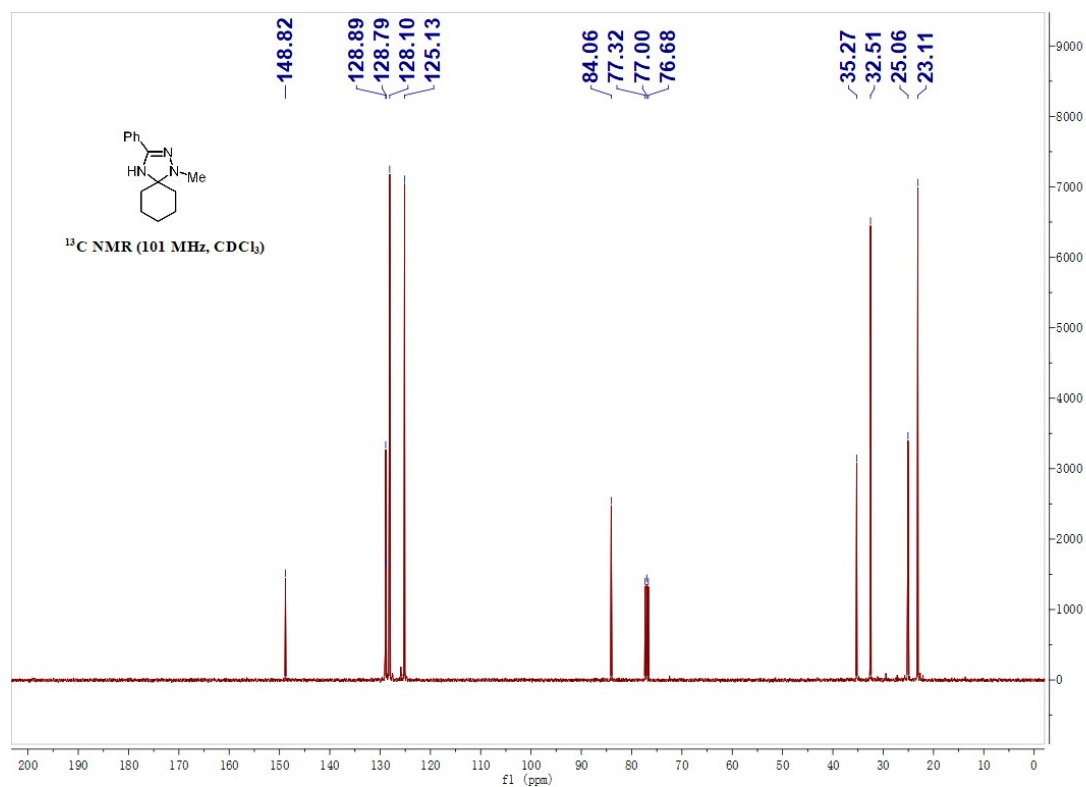
<sup>1</sup>H and <sup>13</sup>C NMR spectra of compound **1u**



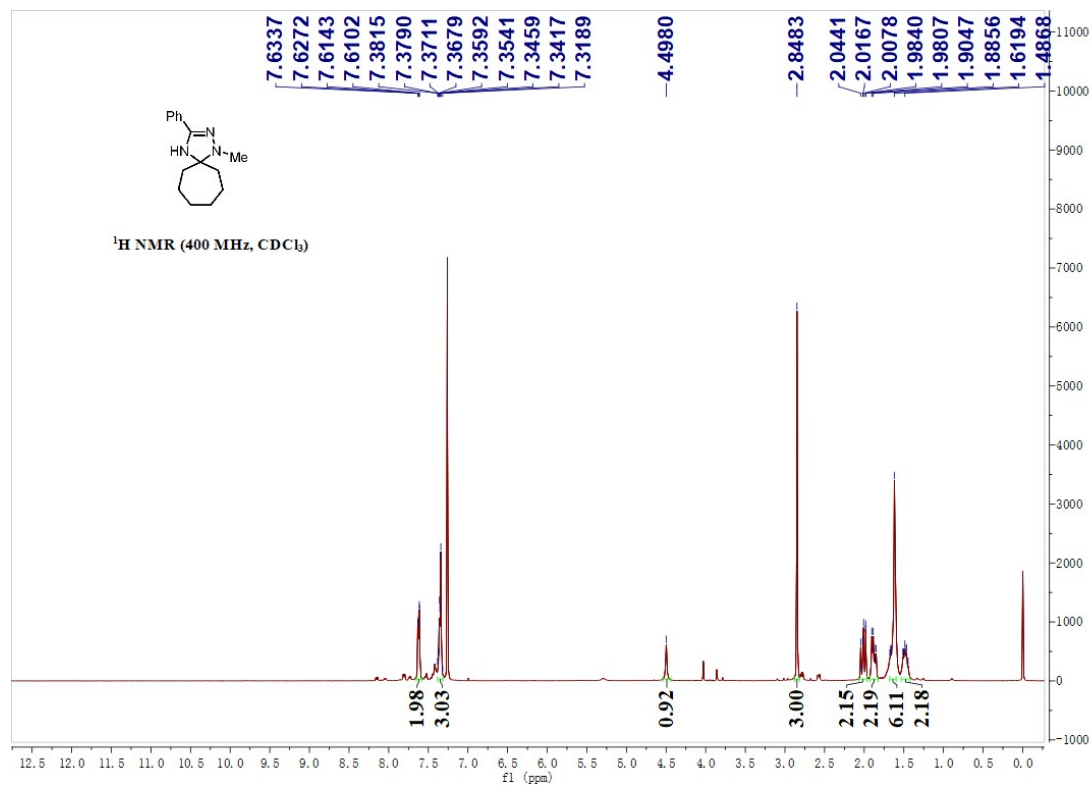


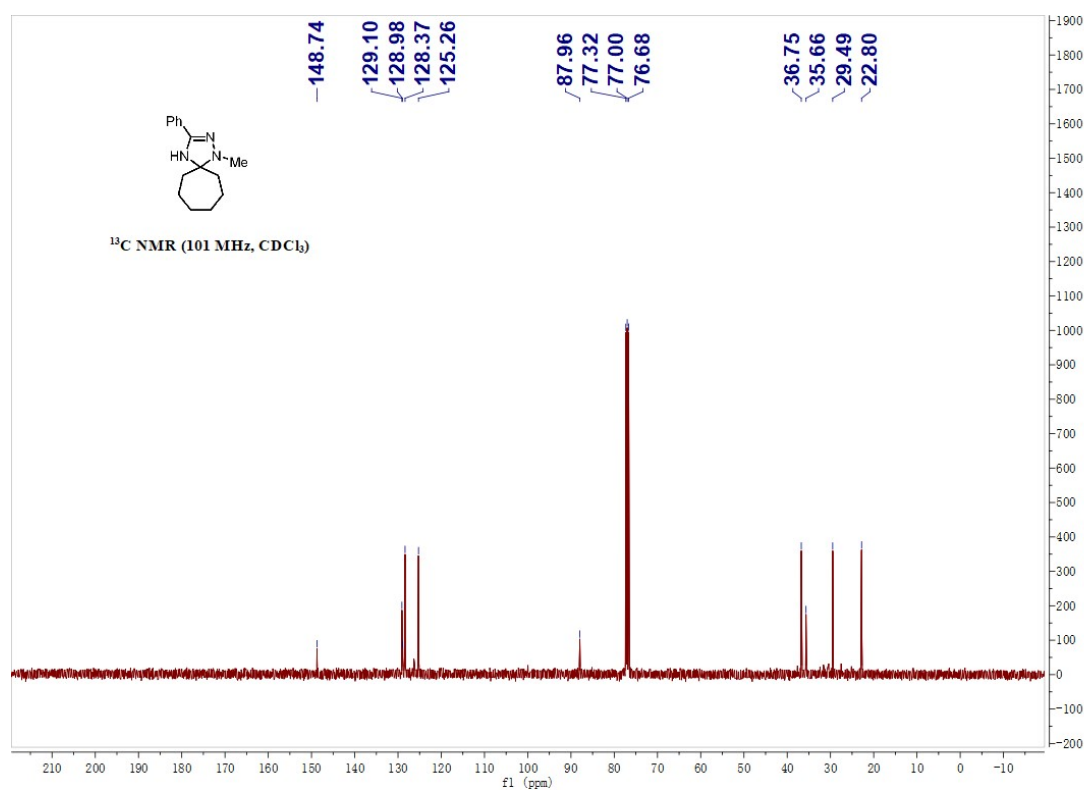
<sup>1</sup>H and <sup>13</sup>C NMR spectra of compound 1x



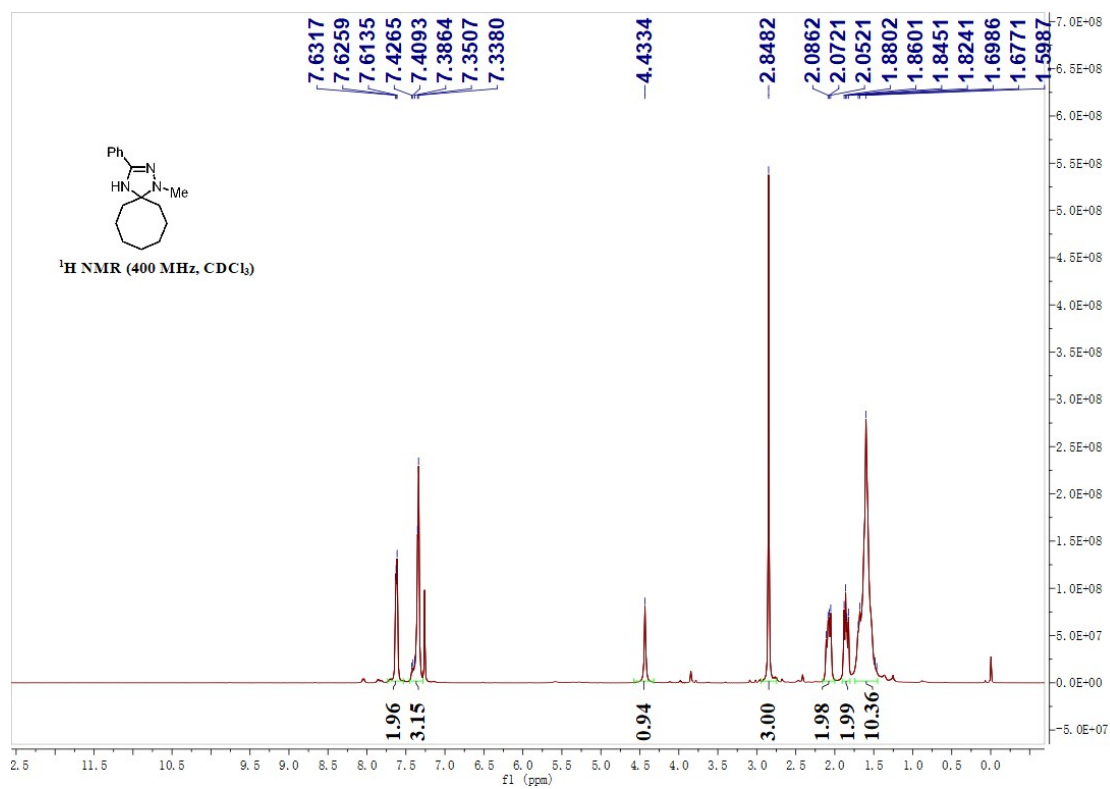


**<sup>1</sup>H and <sup>13</sup>C NMR spectra of compound **1y****

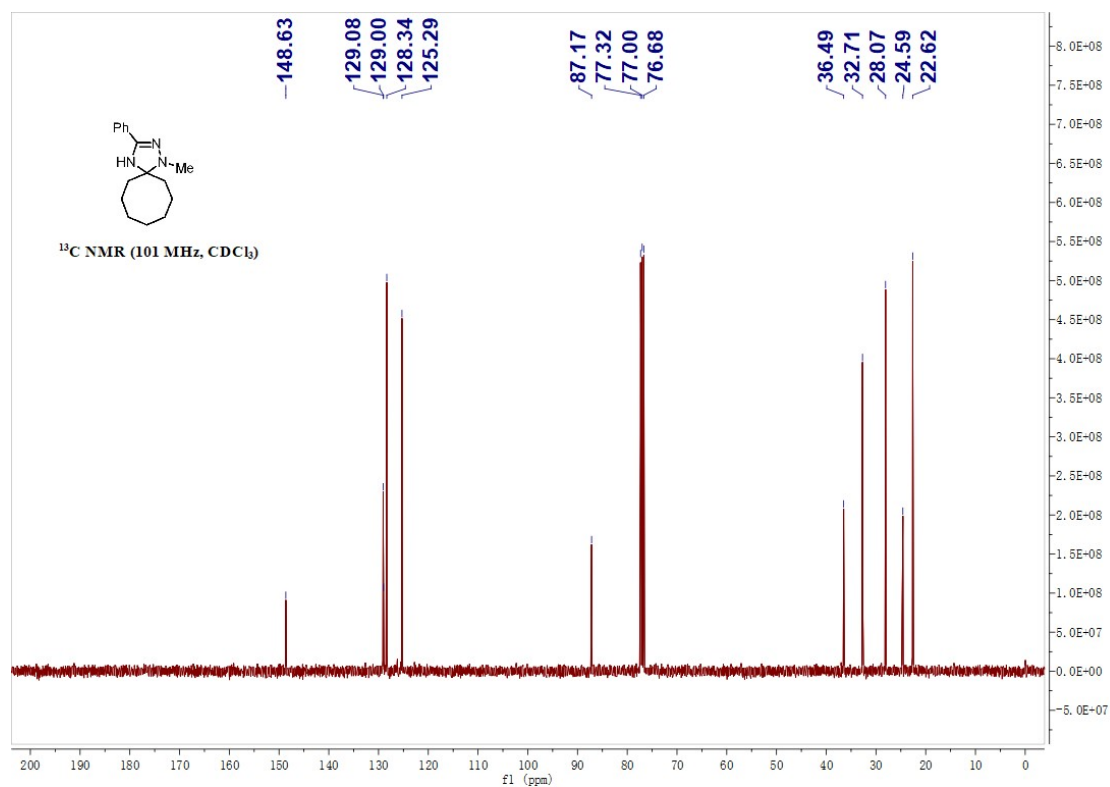




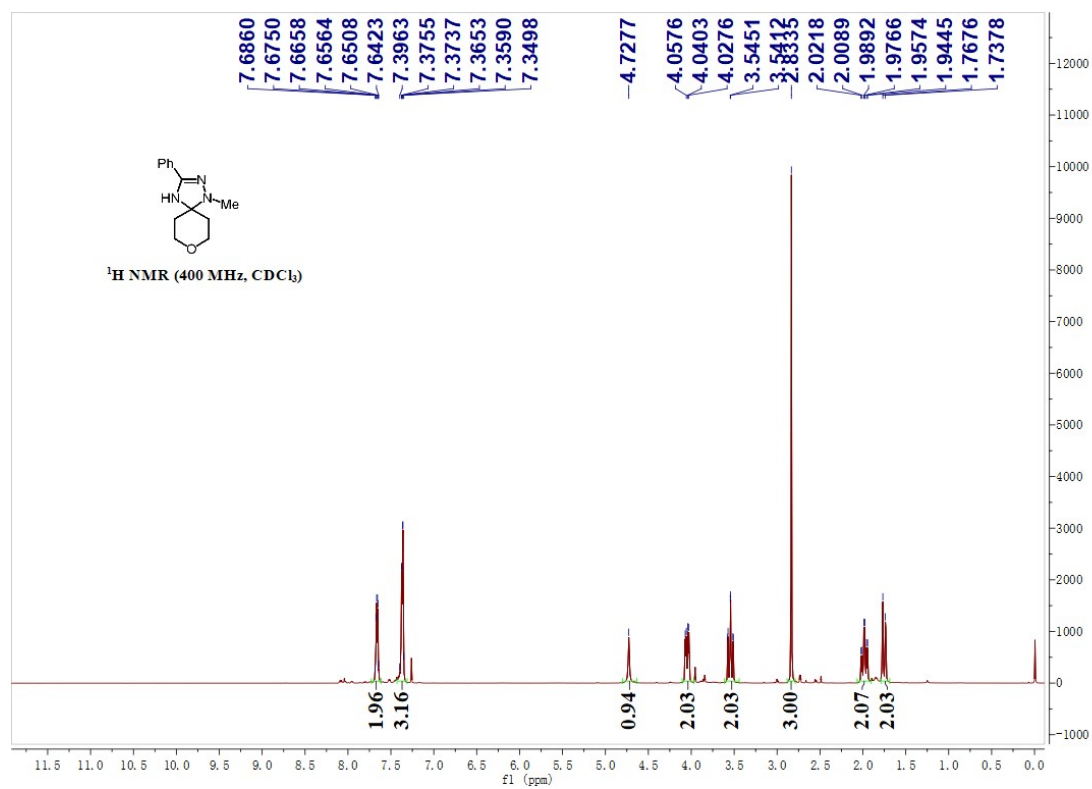
<sup>1</sup>H and <sup>13</sup>C NMR spectra of compound **1z**



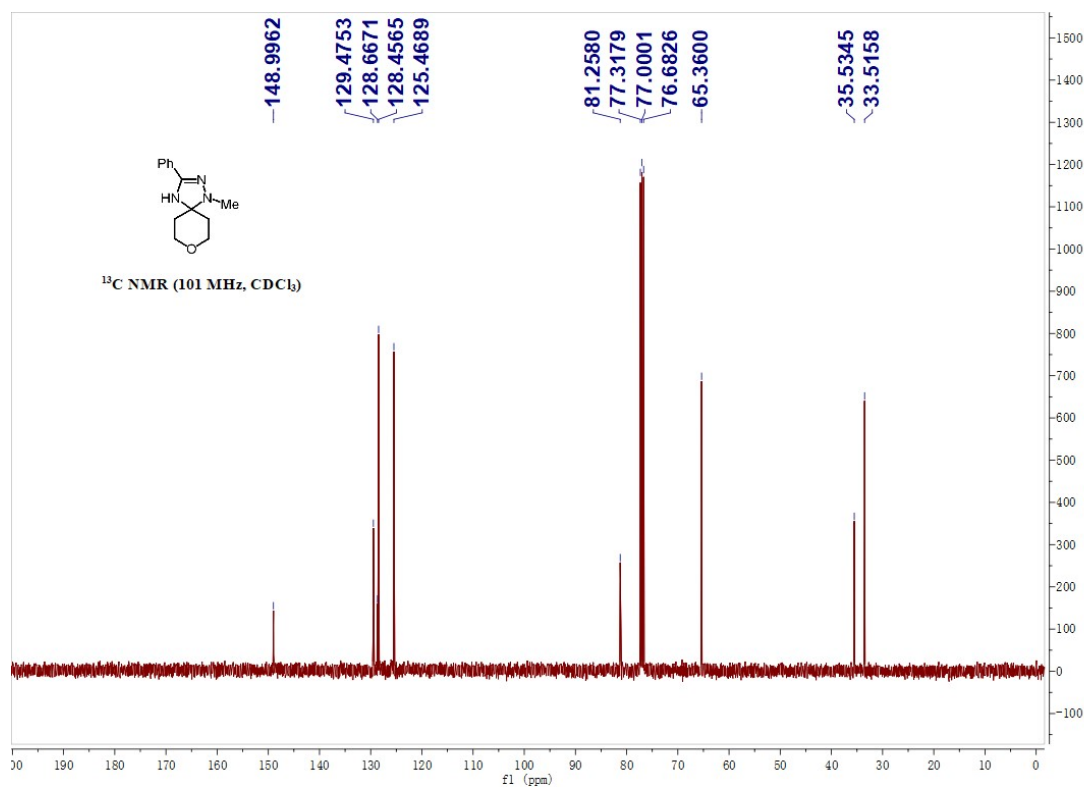




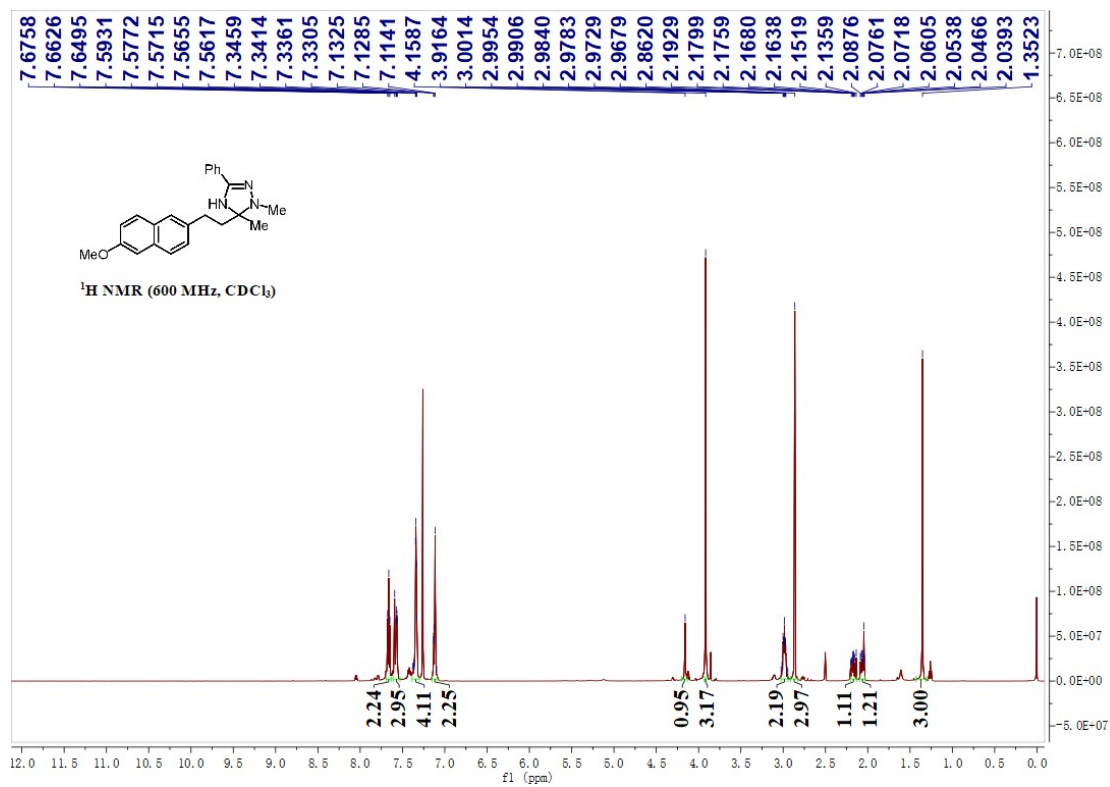
<sup>1</sup>H and <sup>13</sup>C NMR spectra of compound **1aa**

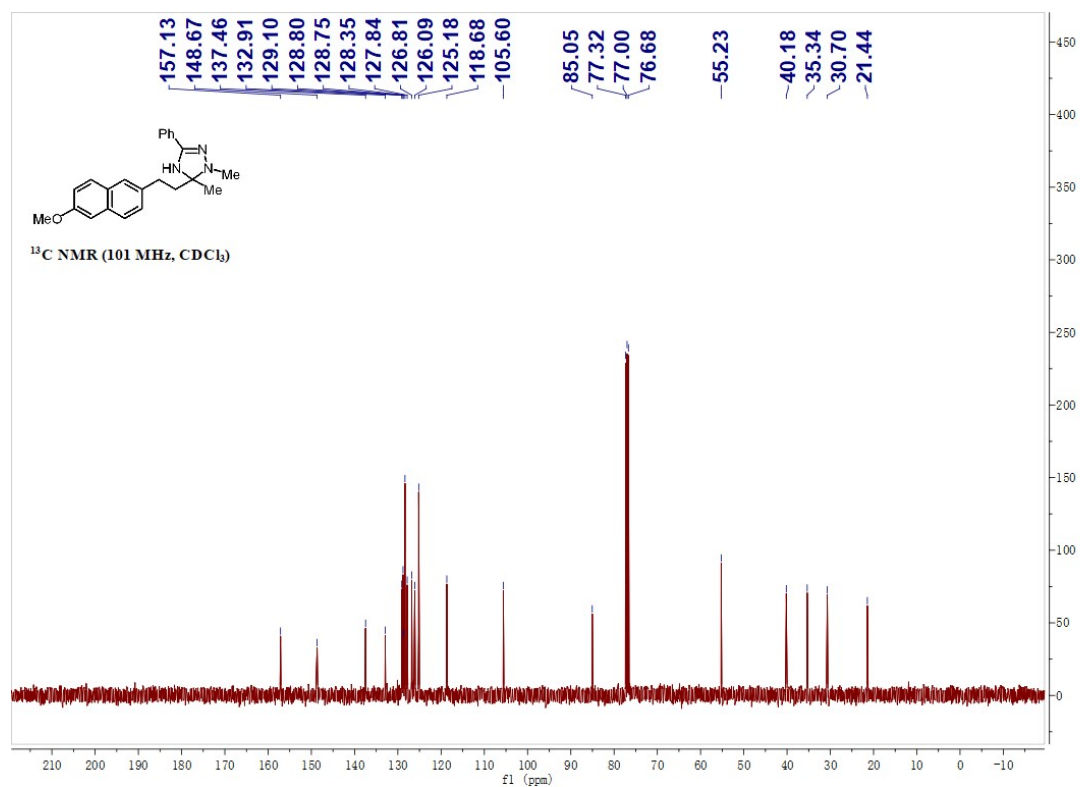




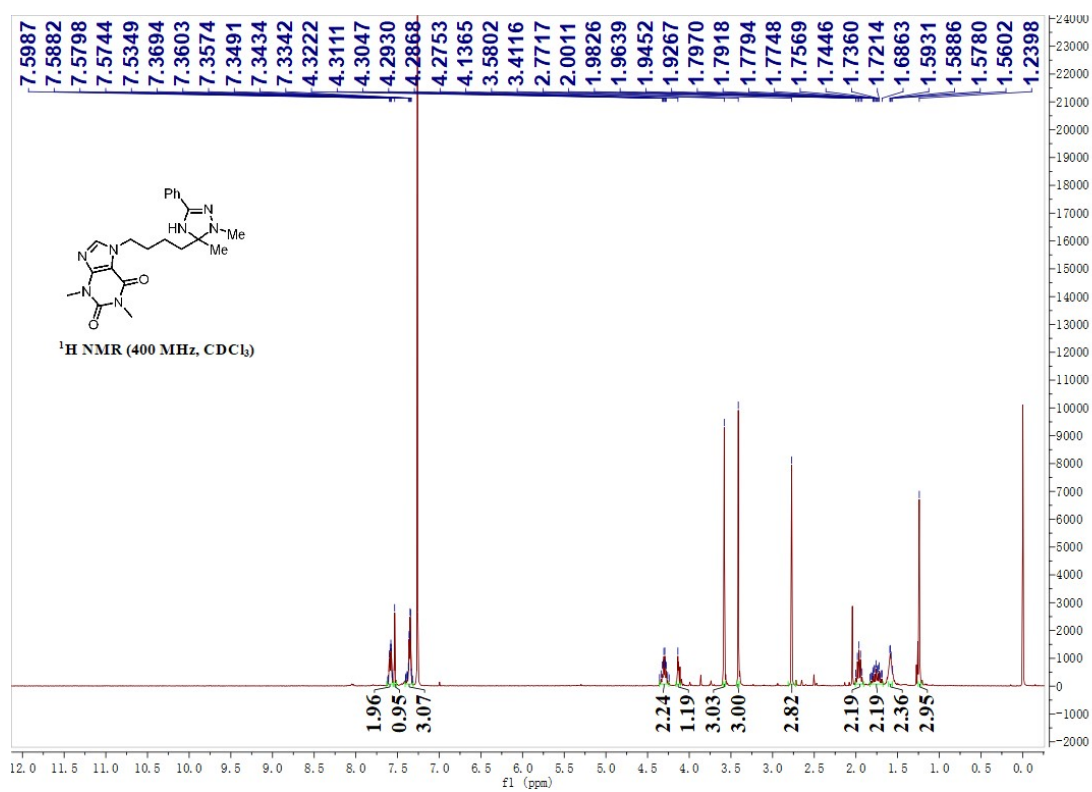


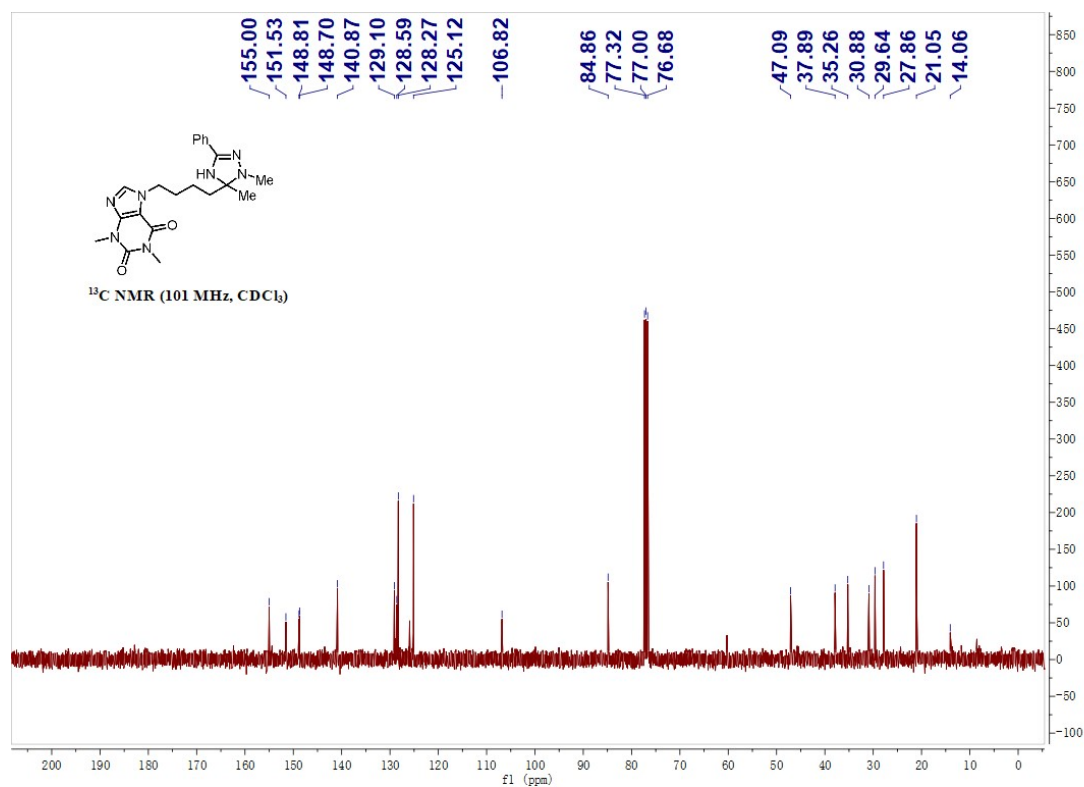
**<sup>1</sup>H and <sup>13</sup>C NMR spectra of compound **1ac****



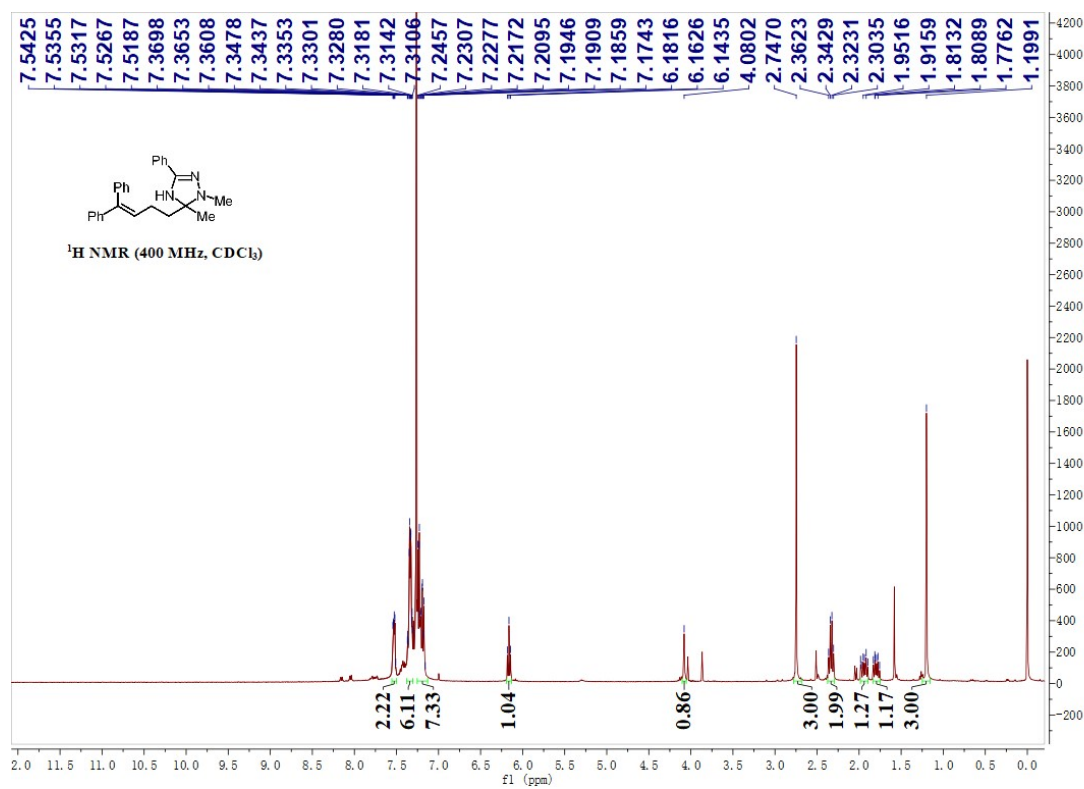


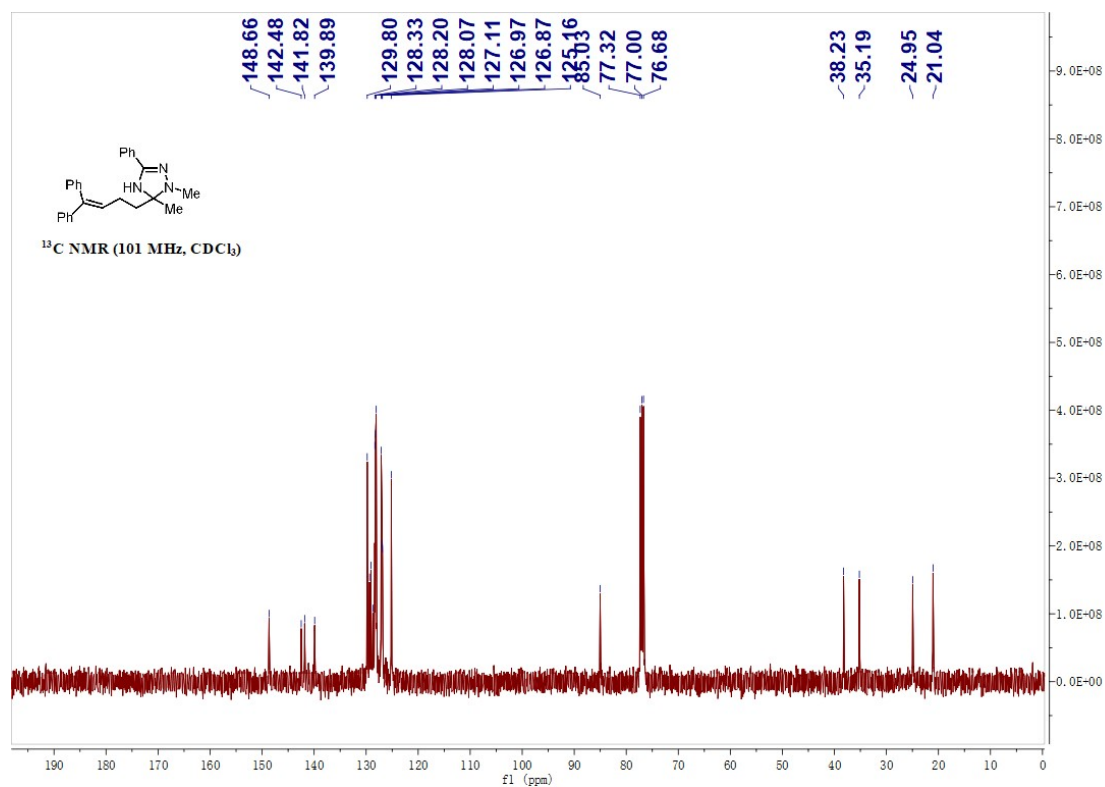
**<sup>1</sup>H and <sup>13</sup>C NMR spectra of compound **1ae****



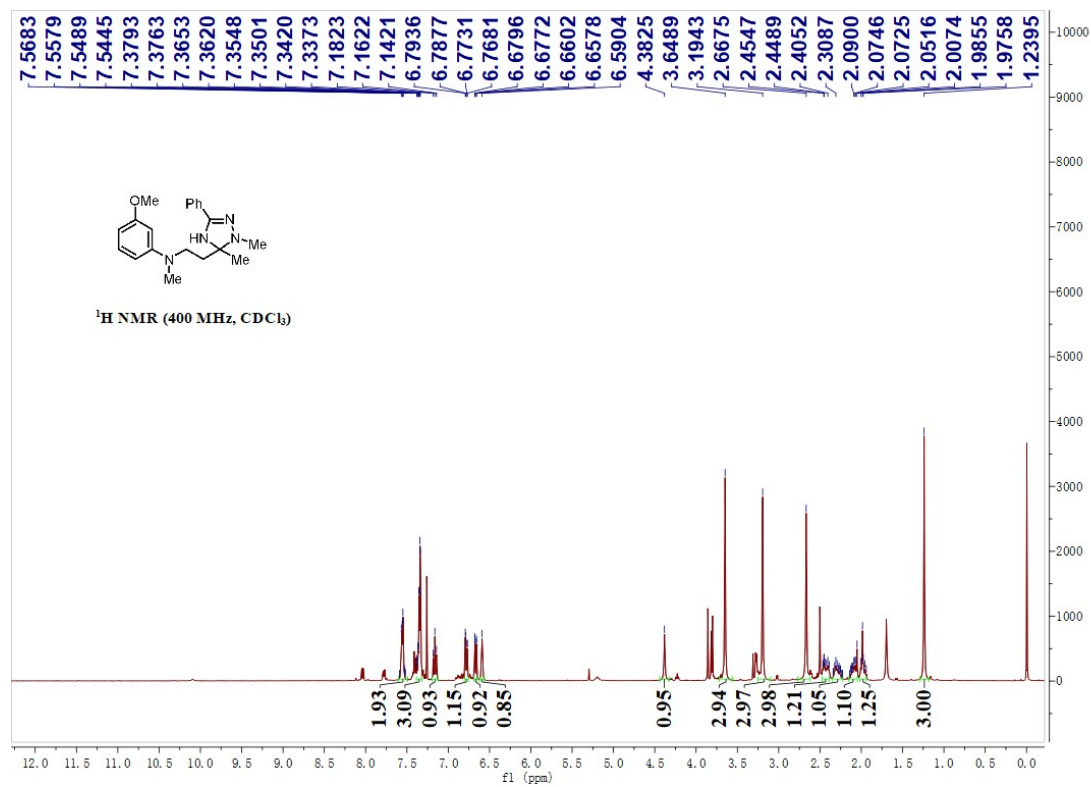


**<sup>1</sup>H and <sup>13</sup>C NMR spectra of compound **1ah****

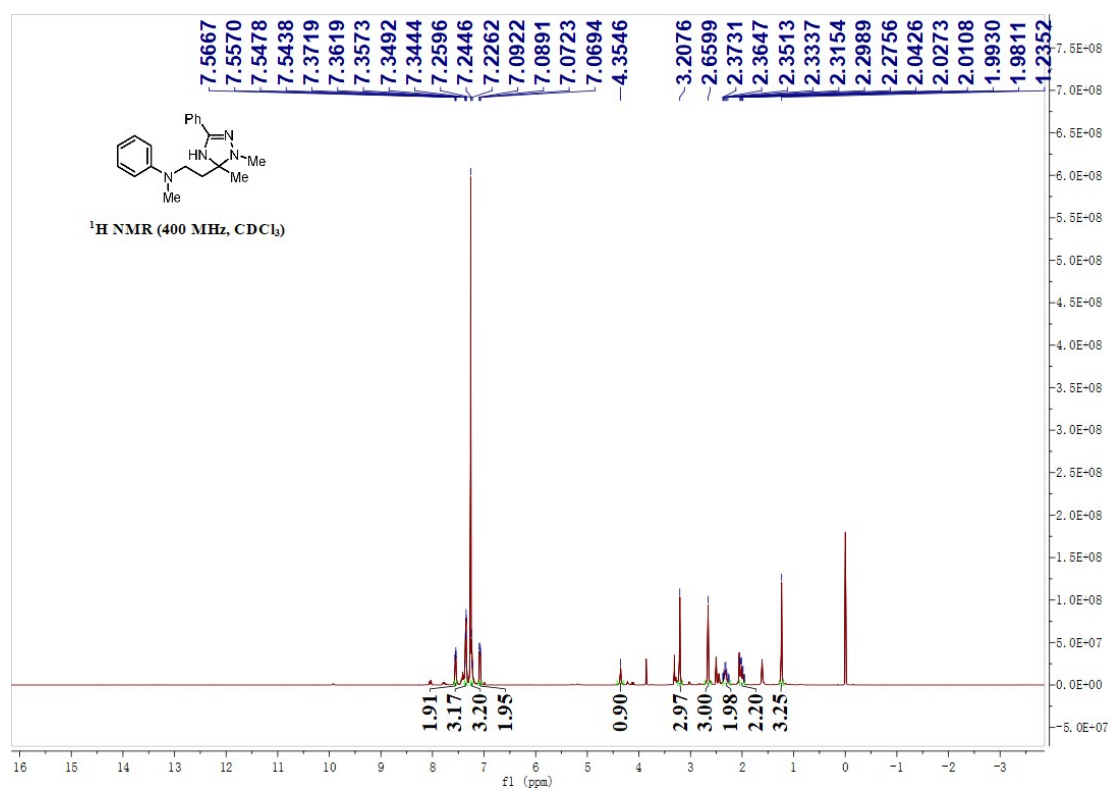




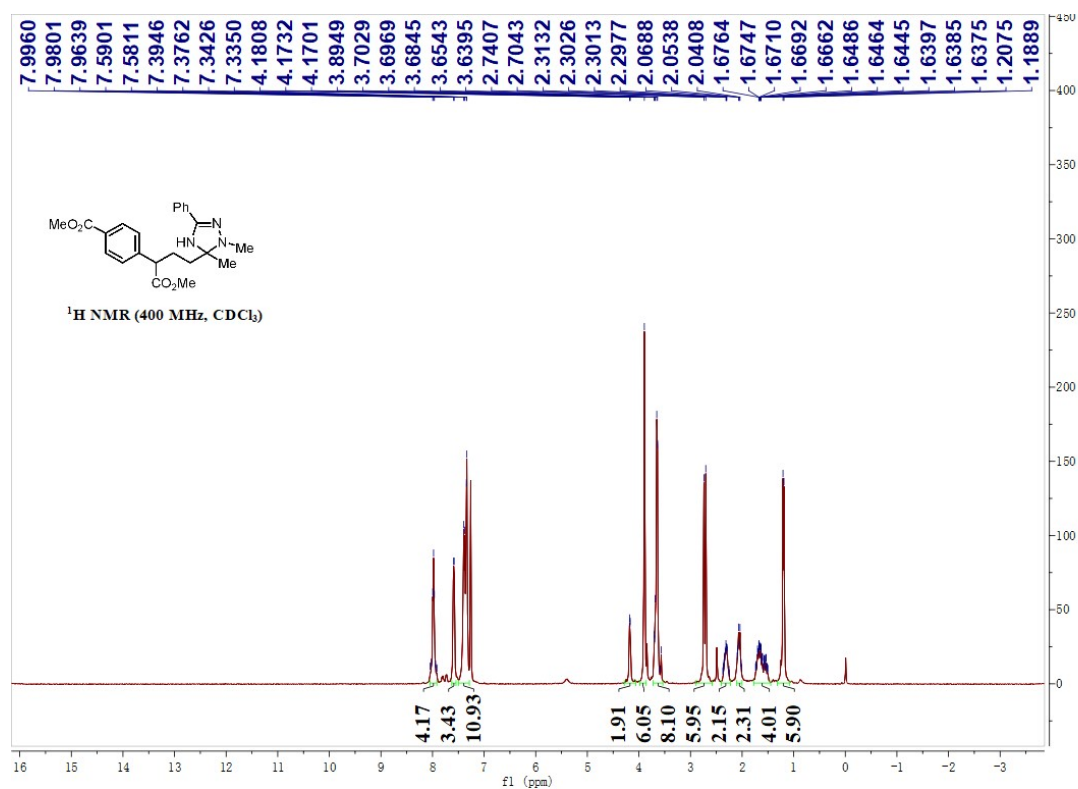
**<sup>1</sup>H NMR spectra of compound **1ai****

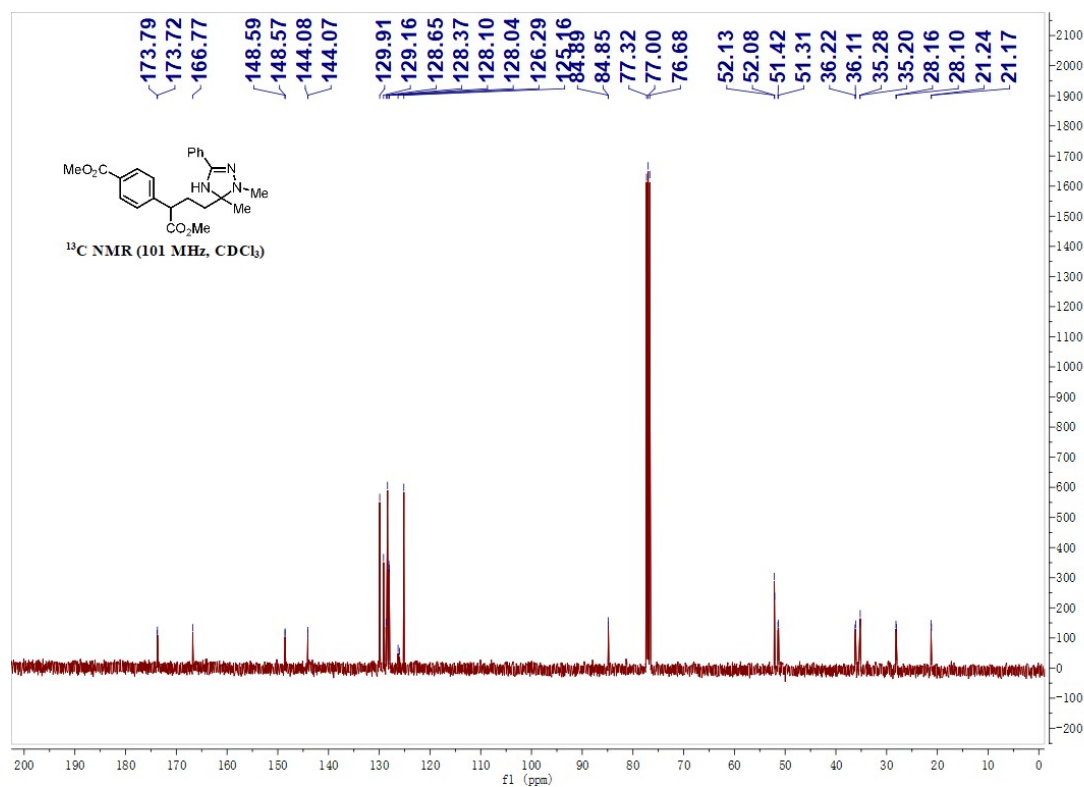


<sup>1</sup>H NMR spectra of compound **1aj**

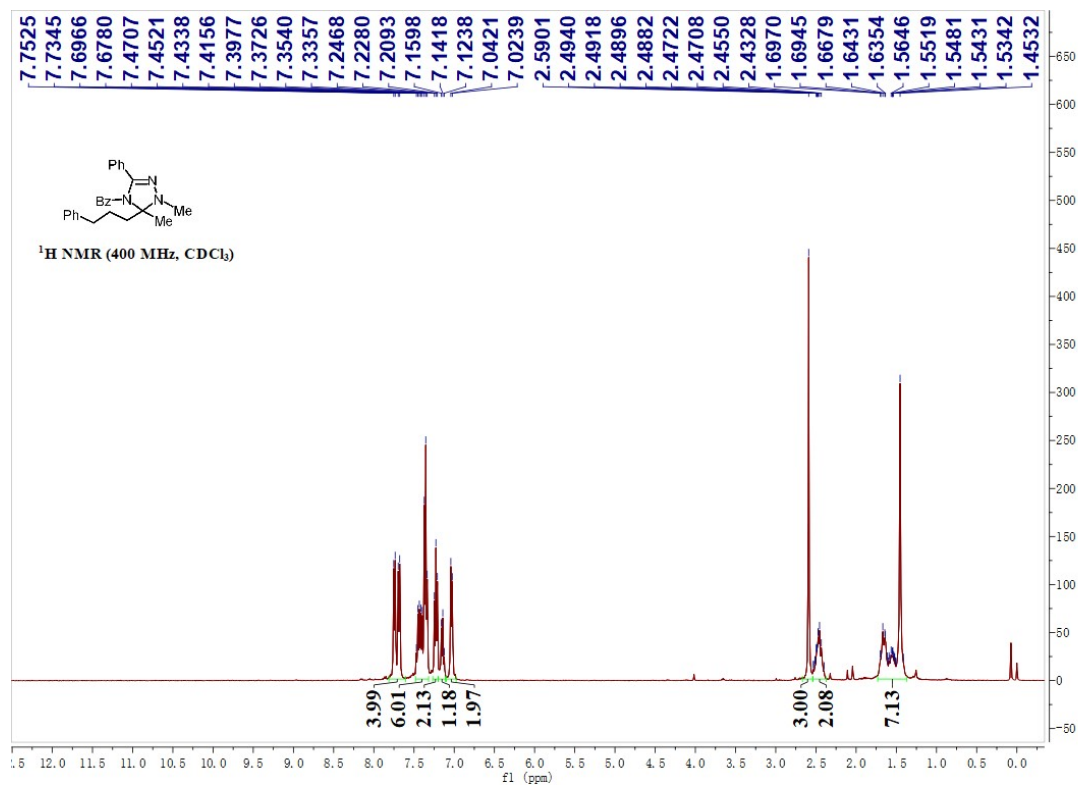


<sup>1</sup>H and <sup>13</sup>C NMR spectra of compound **1al**

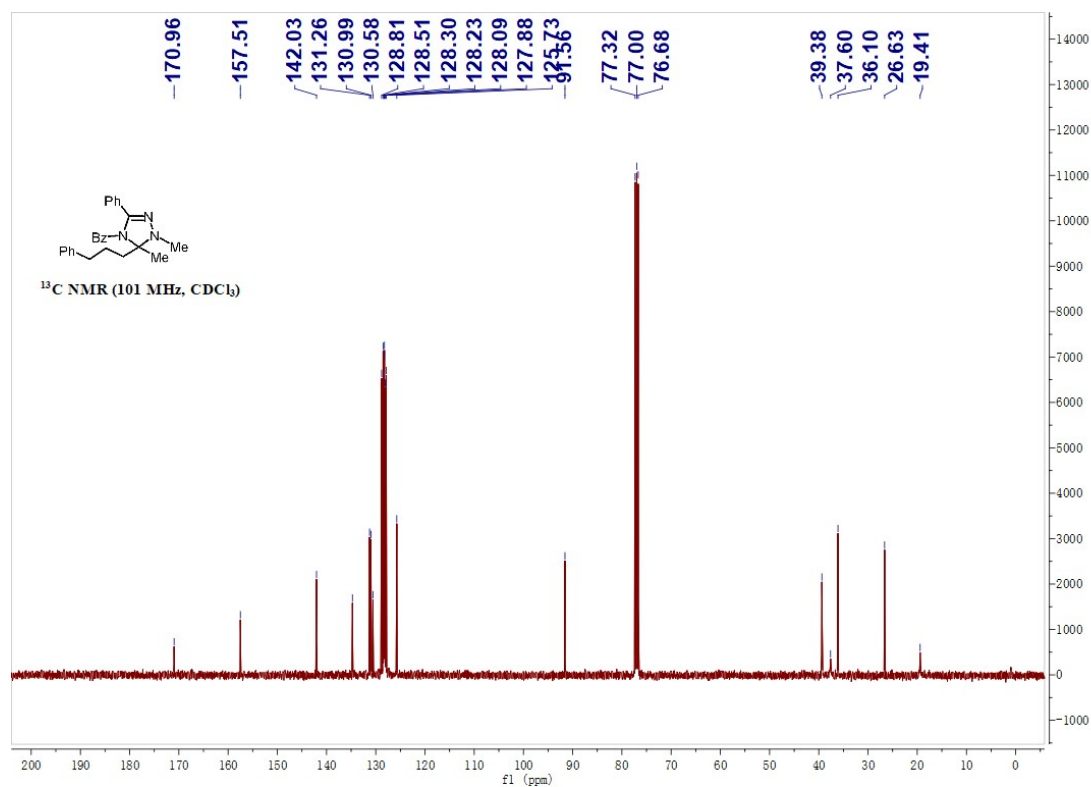




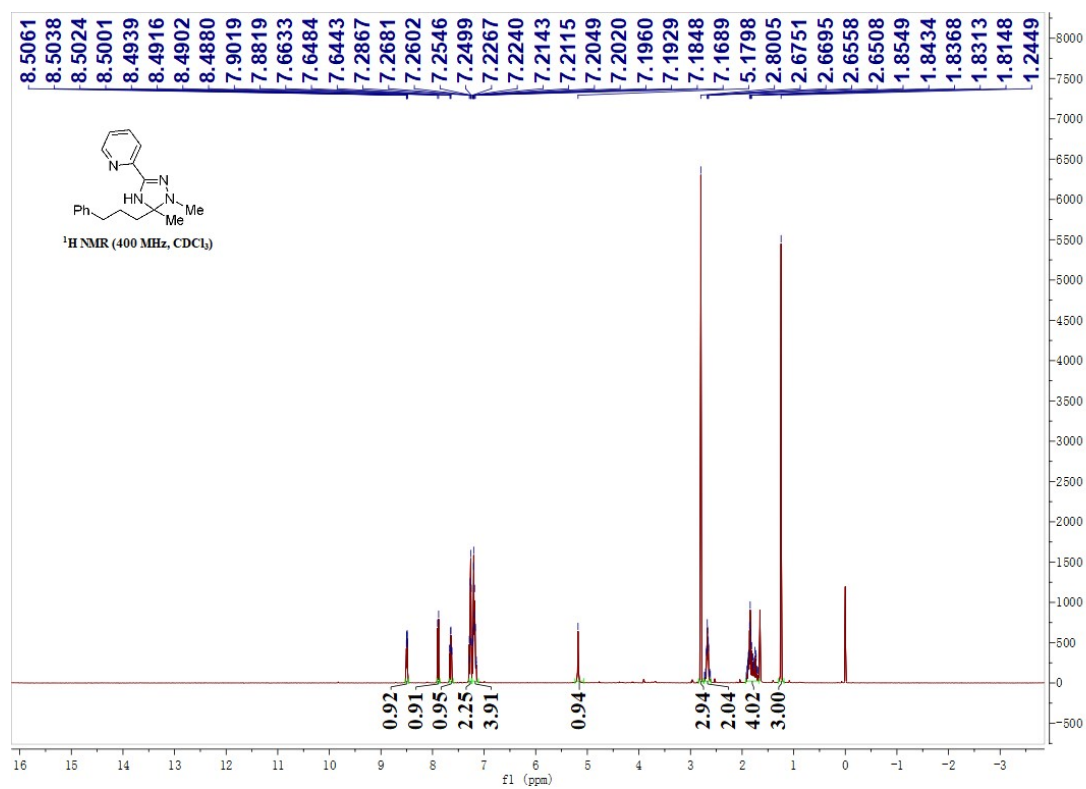
**<sup>1</sup>H and <sup>13</sup>C NMR spectra of compound **1am****

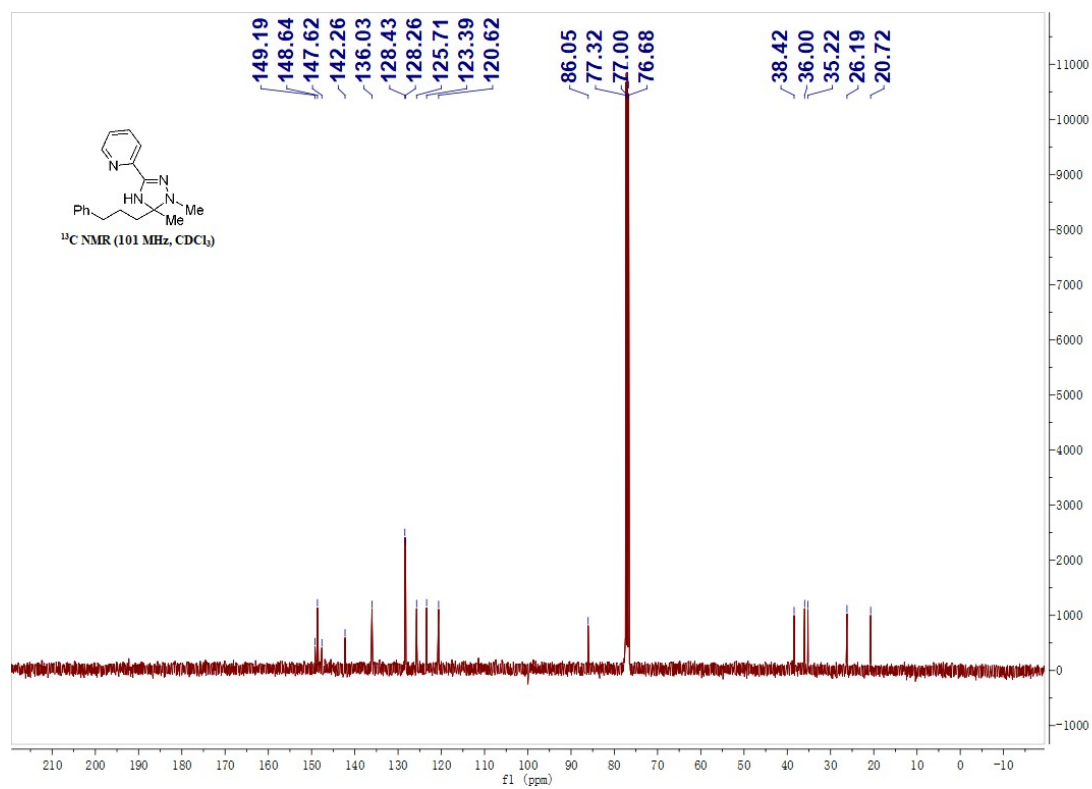




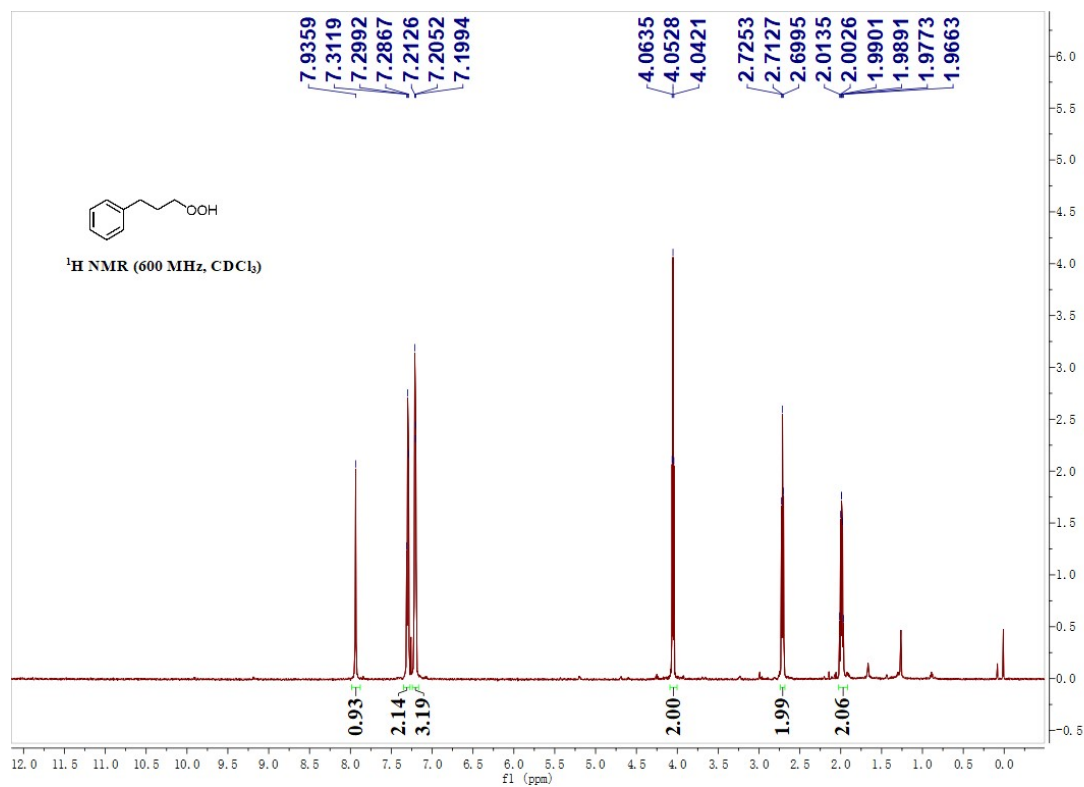


**<sup>1</sup>H and <sup>13</sup>C NMR spectra of compound **1ao****

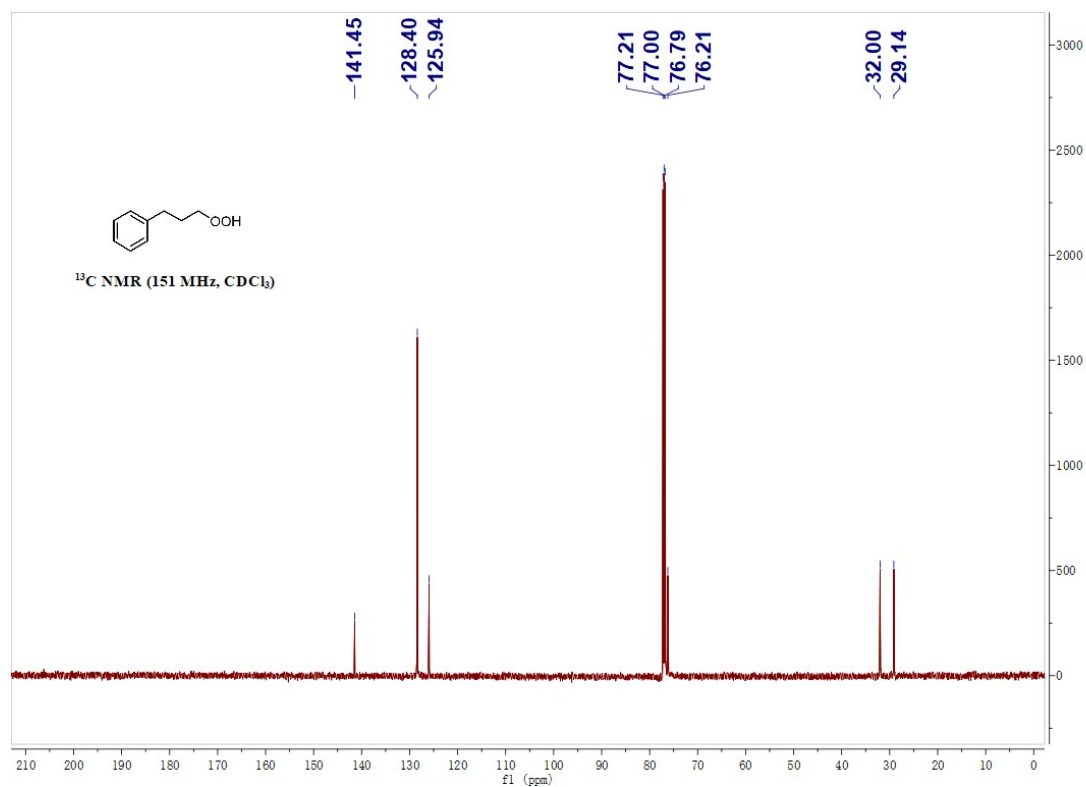




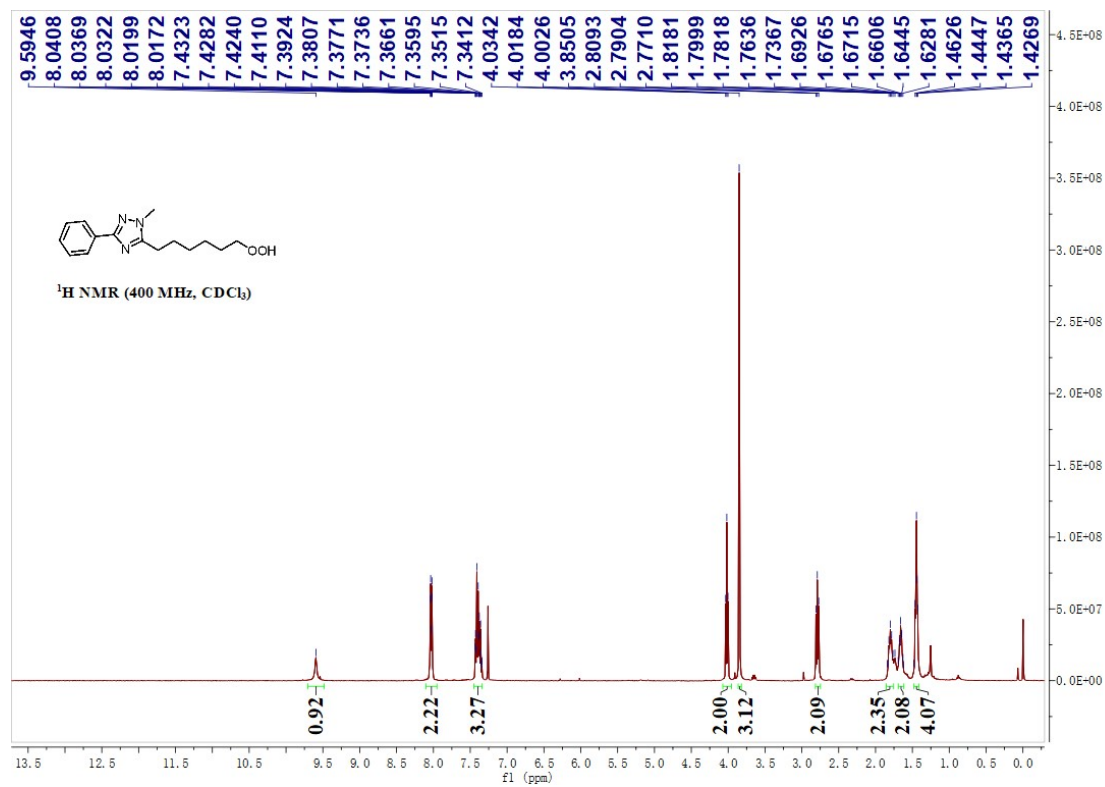
<sup>1</sup>H and <sup>13</sup>C NMR spectra of compound **2a**

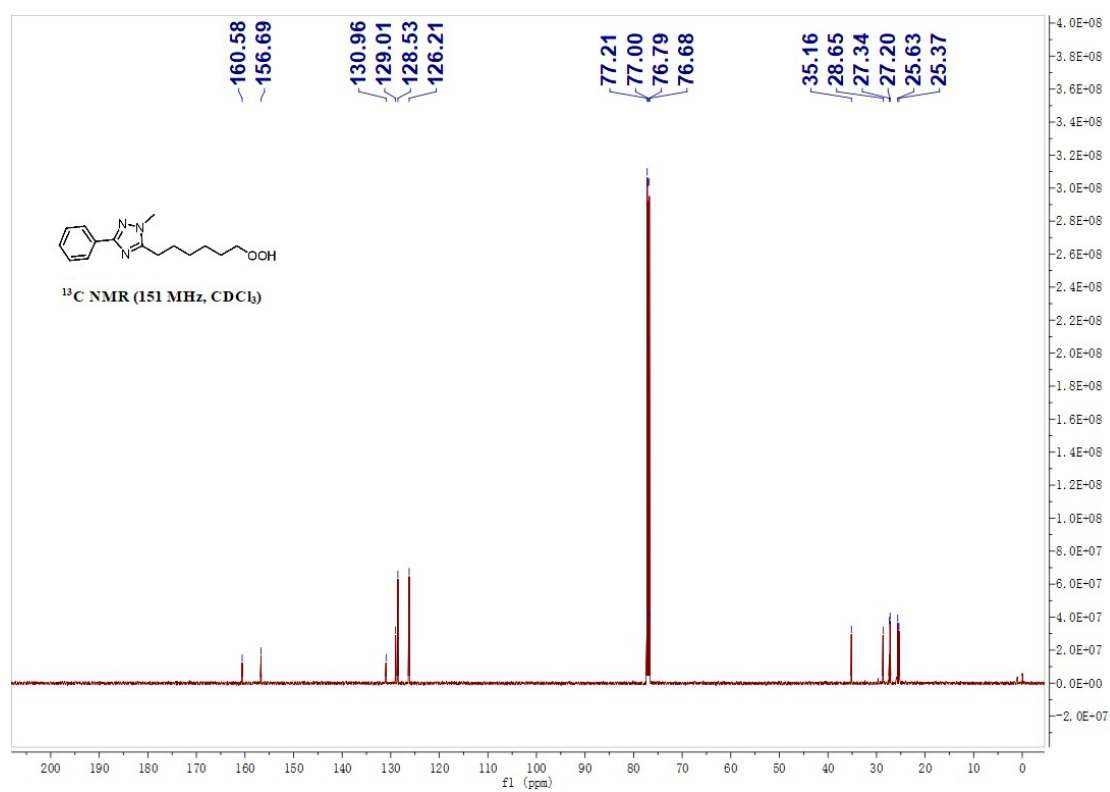




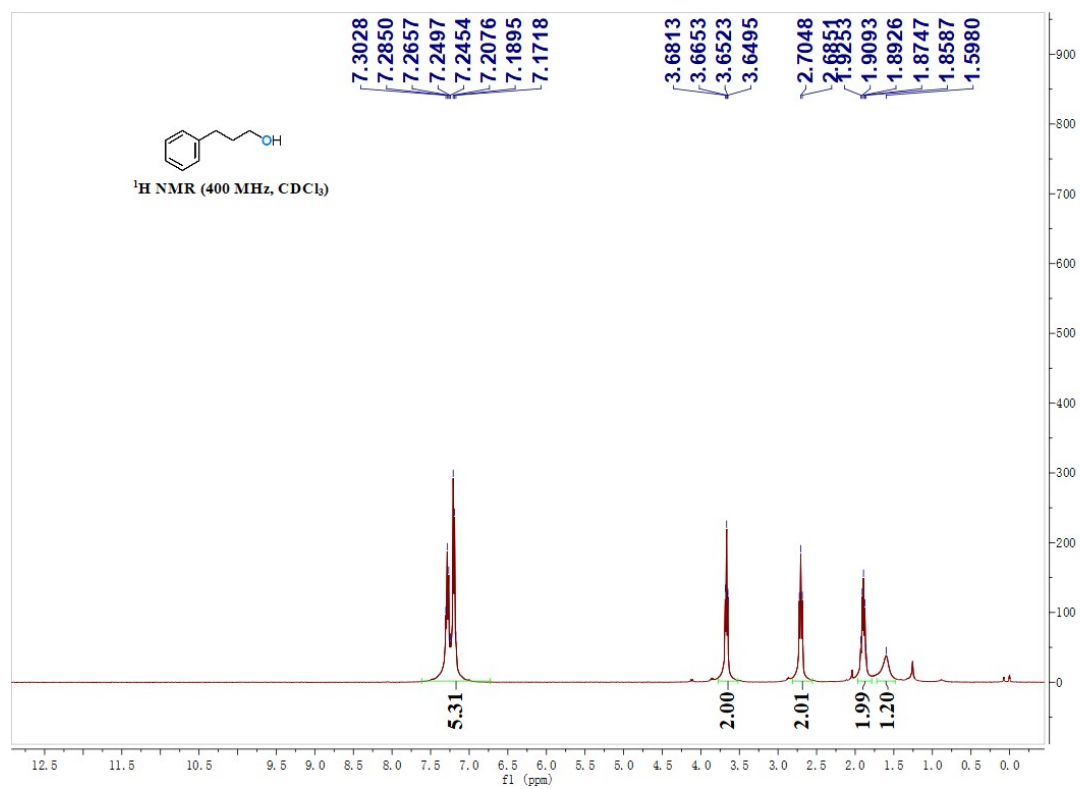


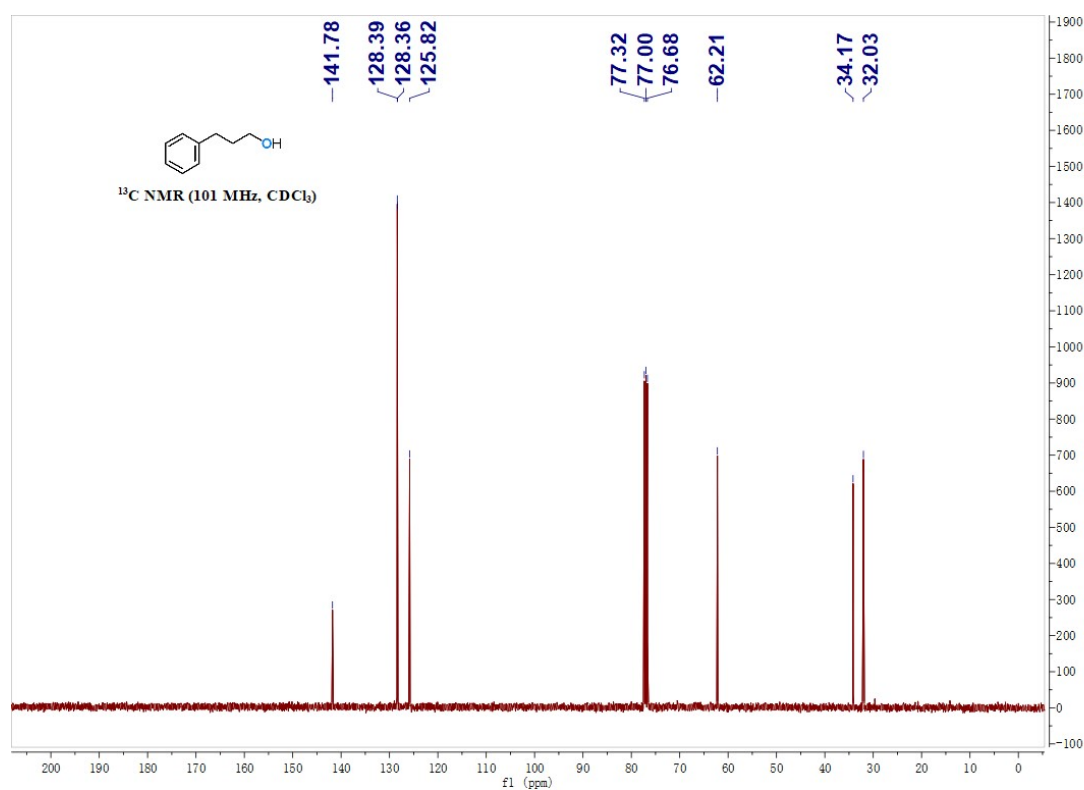
<sup>1</sup>H and <sup>13</sup>C NMR spectra of compound **2b**



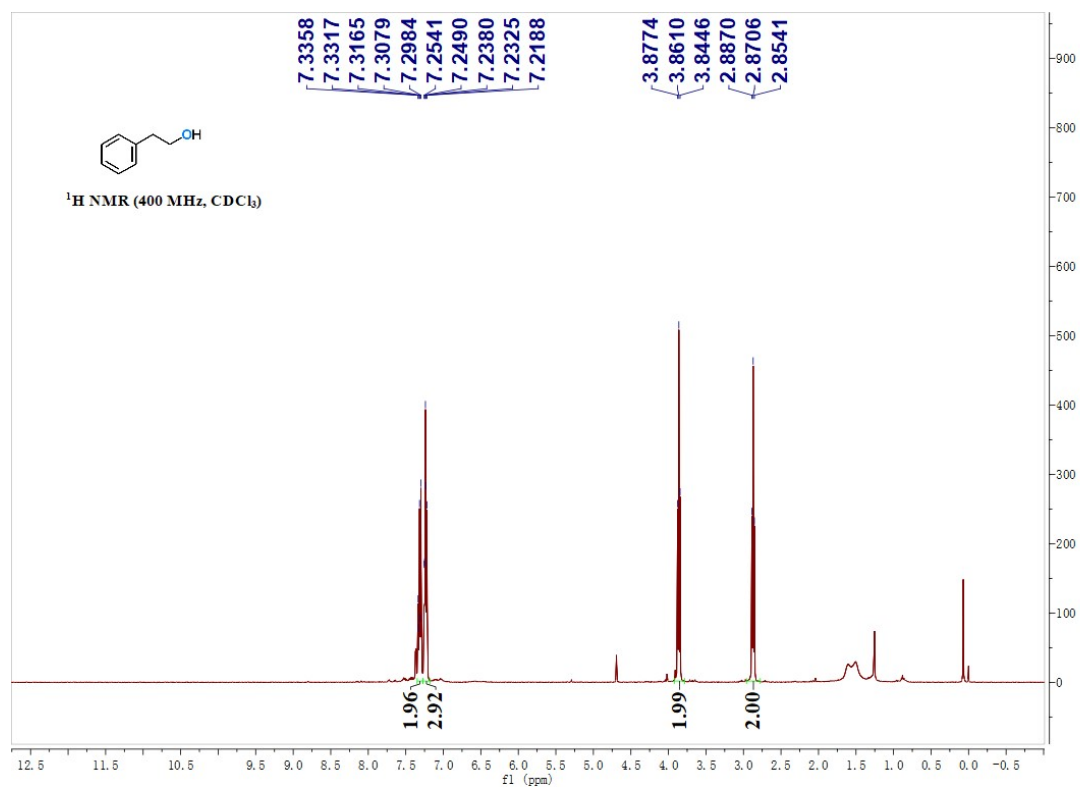


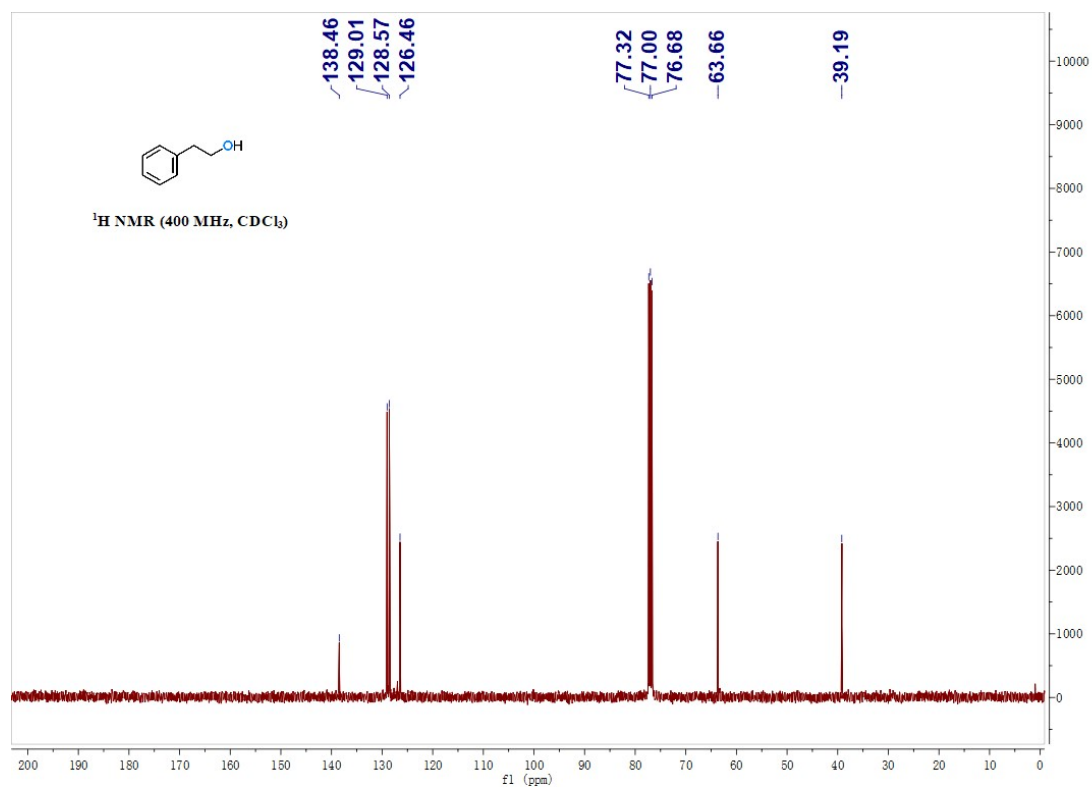
<sup>1</sup>H and <sup>13</sup>C NMR spectra of compound **3a**



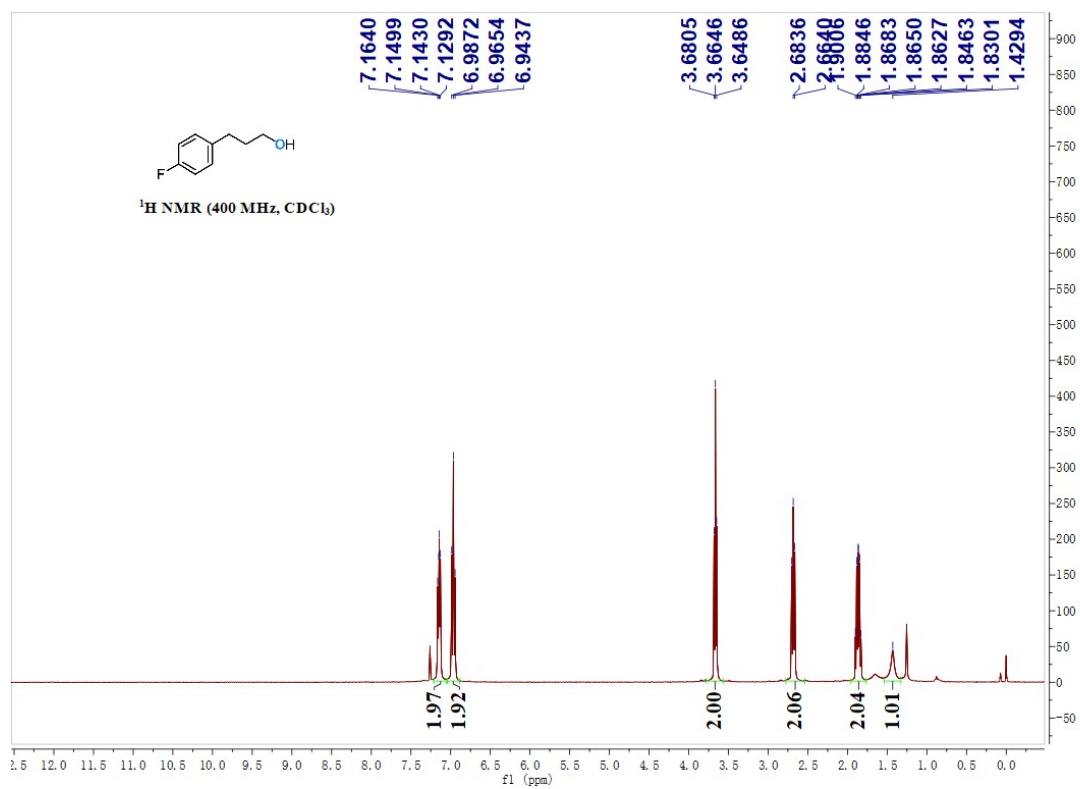


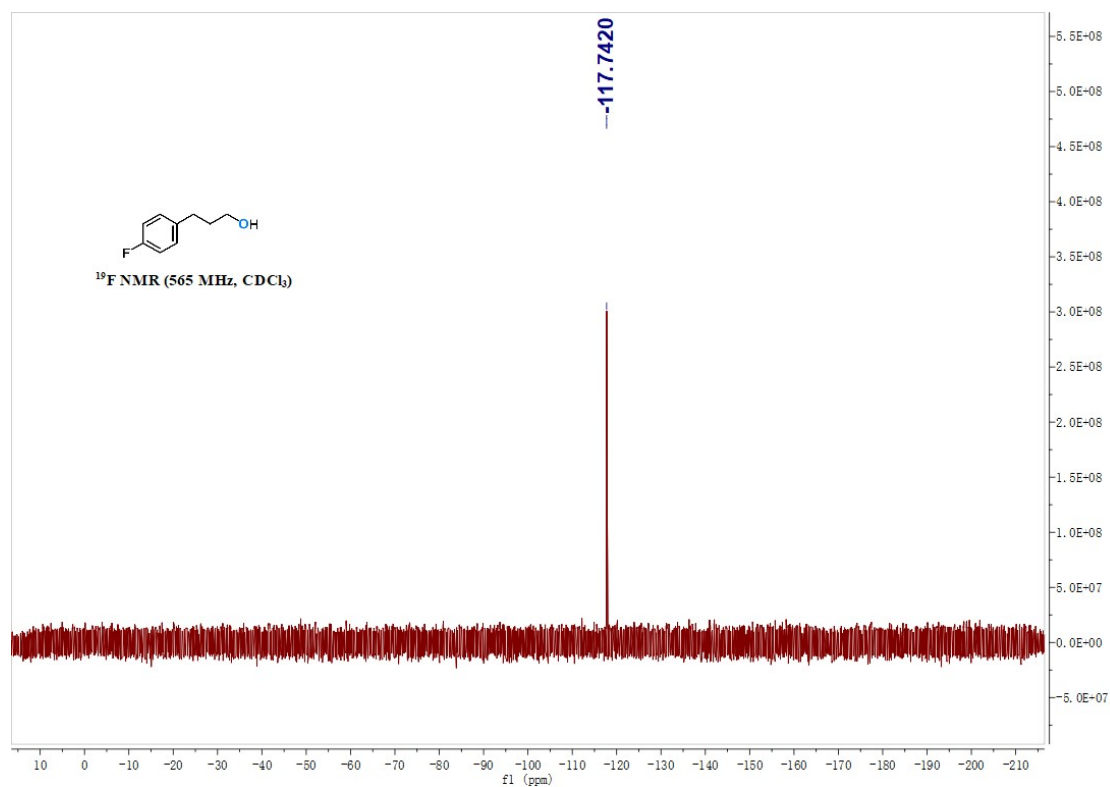
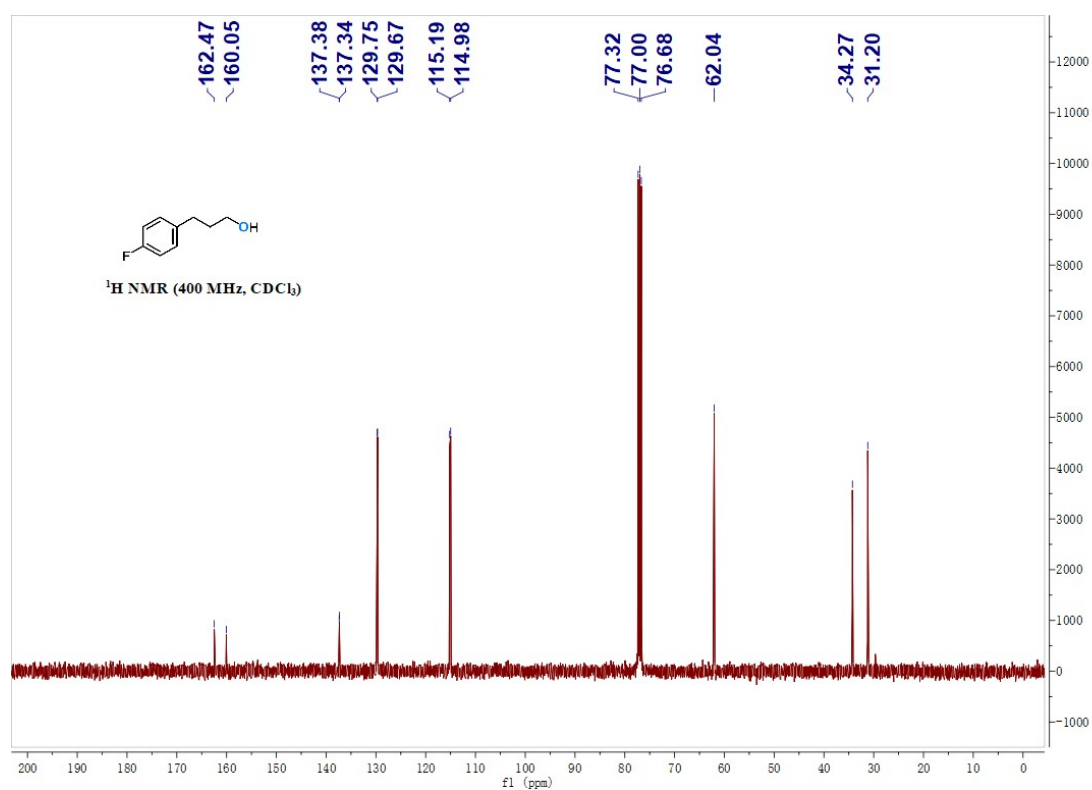
<sup>1</sup>H and <sup>13</sup>C NMR spectra of compound **3b**



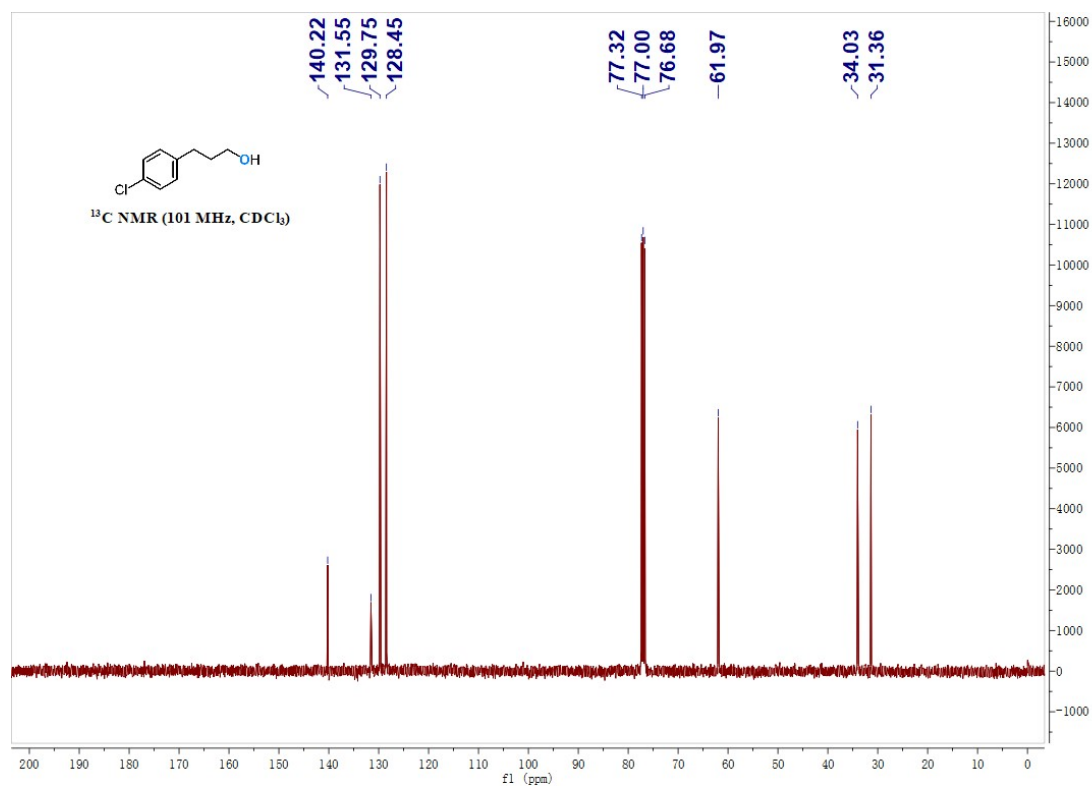
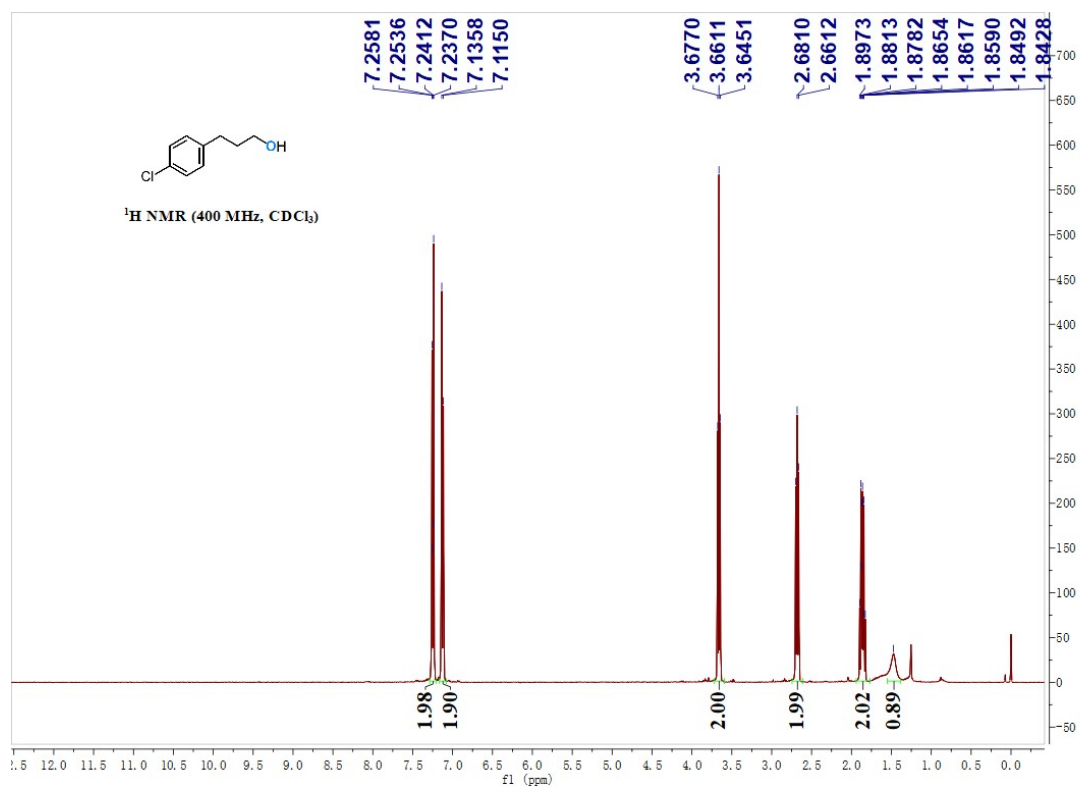


<sup>1</sup>H, <sup>13</sup>C and <sup>19</sup>F NMR spectra of compound **3c**

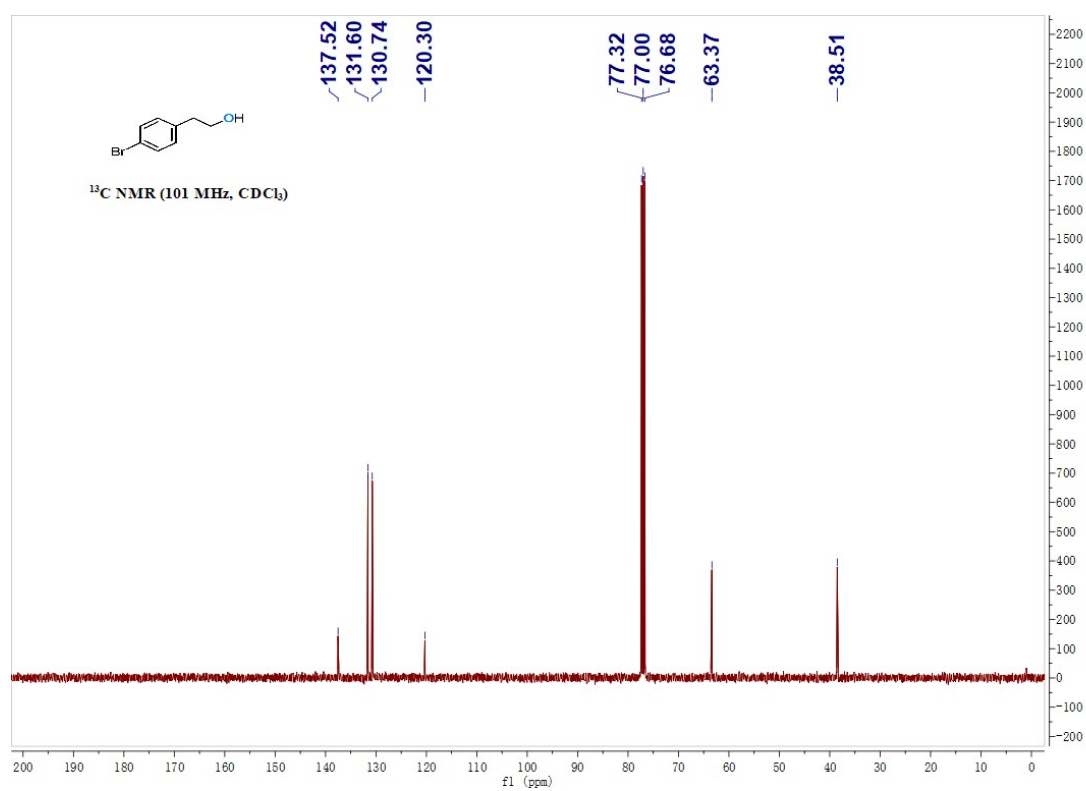
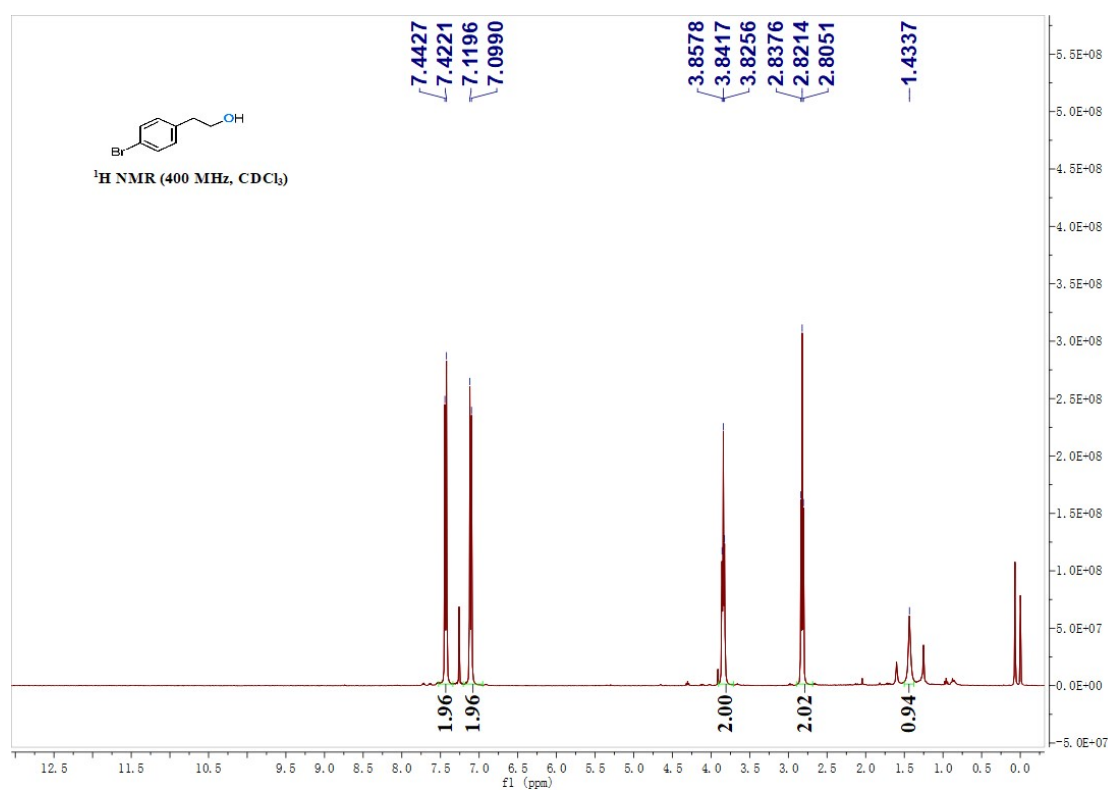




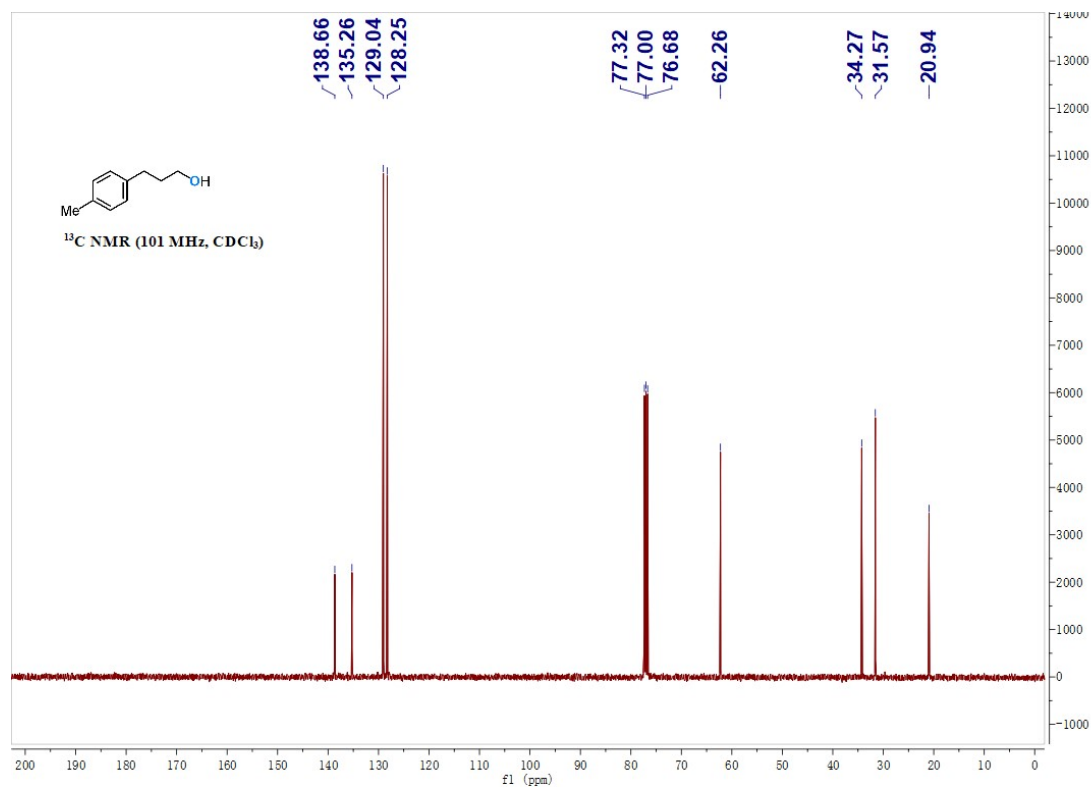
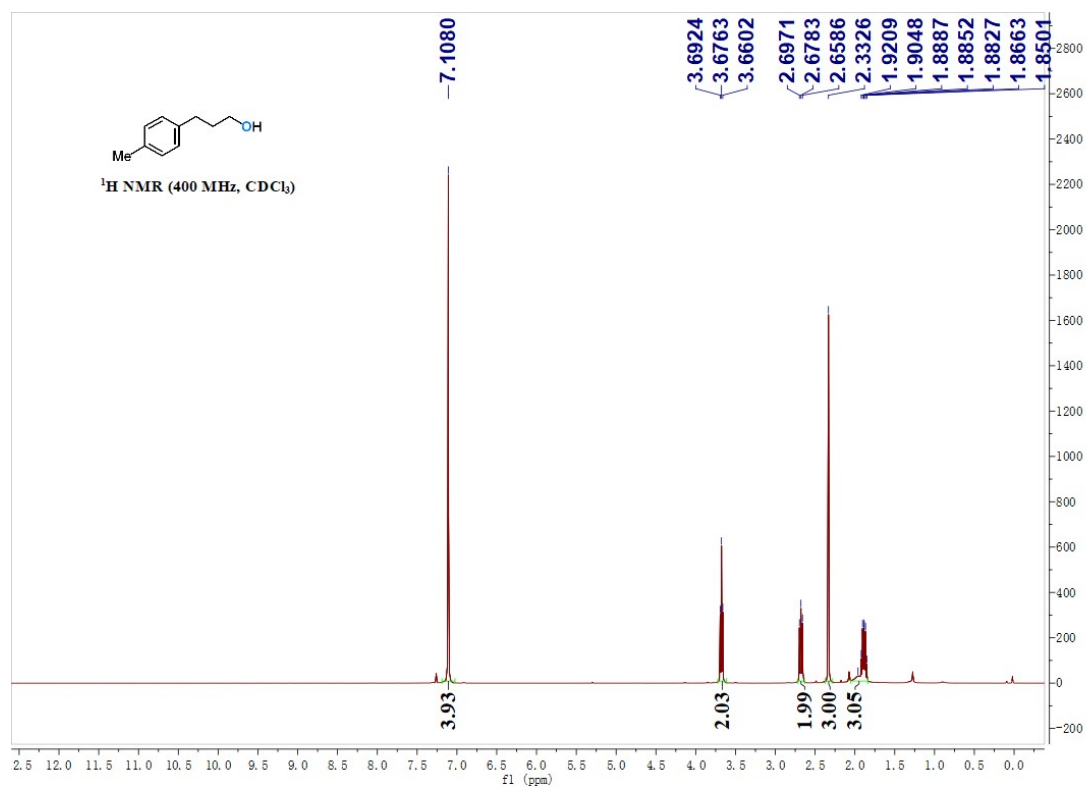
<sup>1</sup>H and <sup>13</sup>C NMR spectra of compound **3d**



<sup>1</sup>H and <sup>13</sup>C NMR spectra of compound **3e**

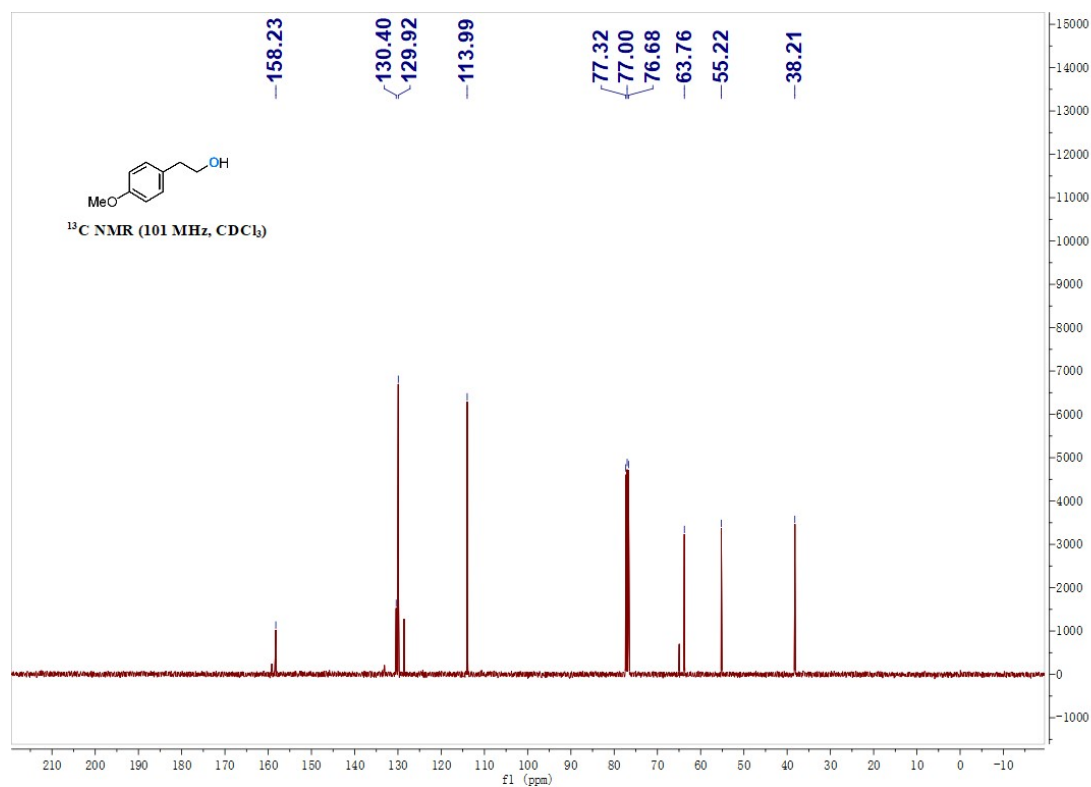
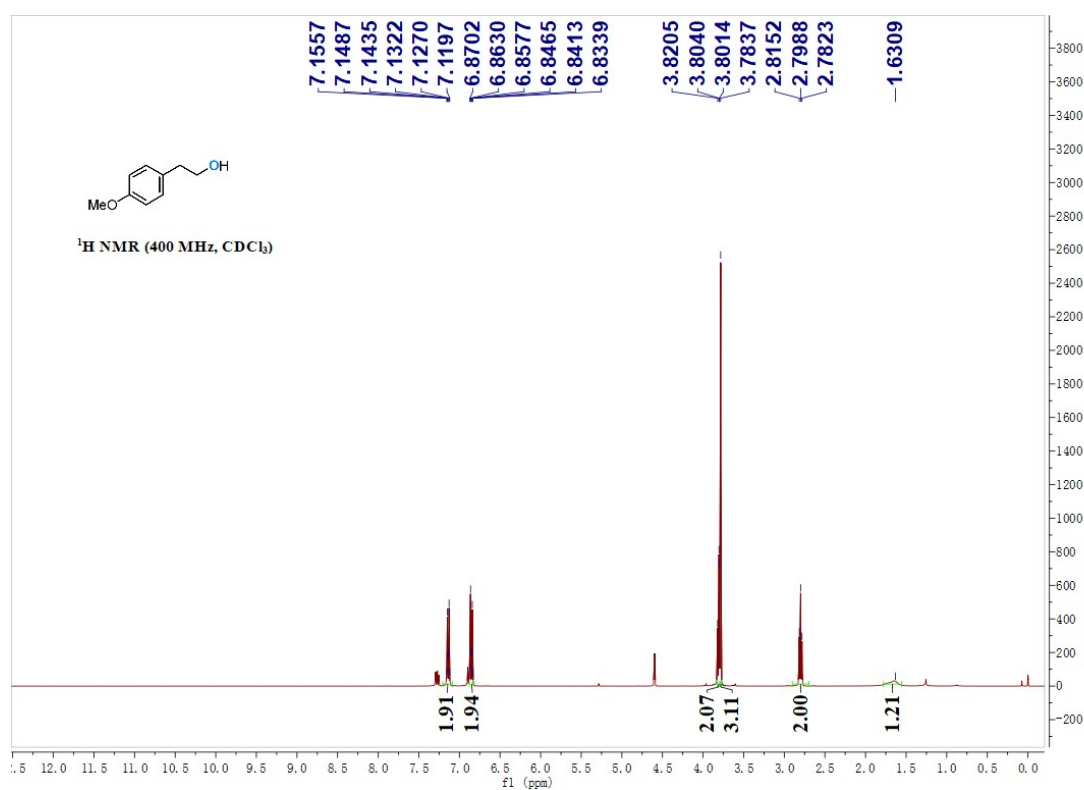


$^1\text{H}$  and  $^{13}\text{C}$  NMR spectra of compound **3f**

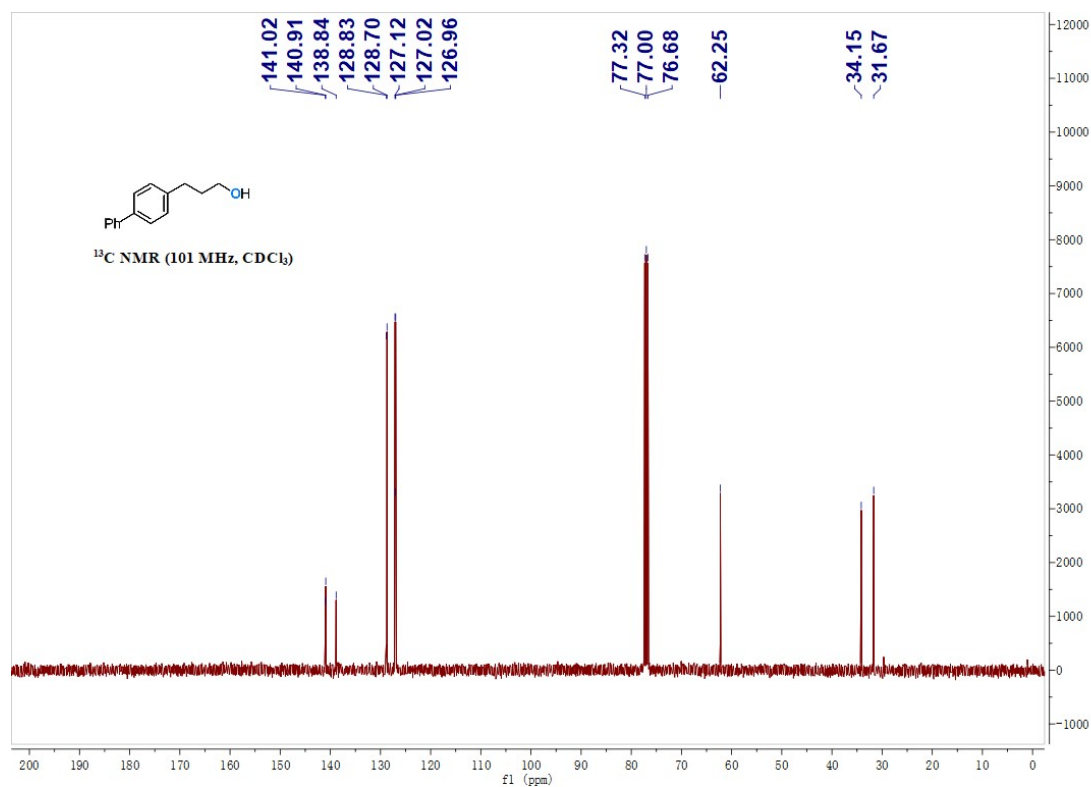
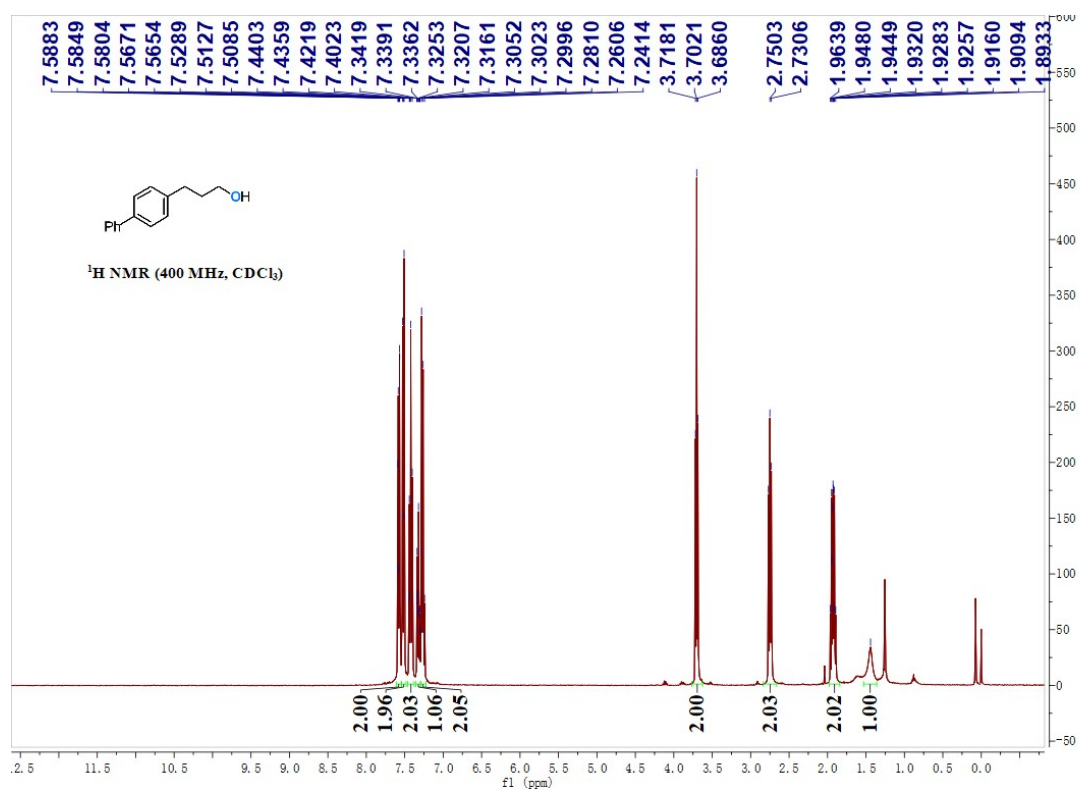


$^1\text{H}$  and  $^{13}\text{C}$  NMR spectra of compound **3g**

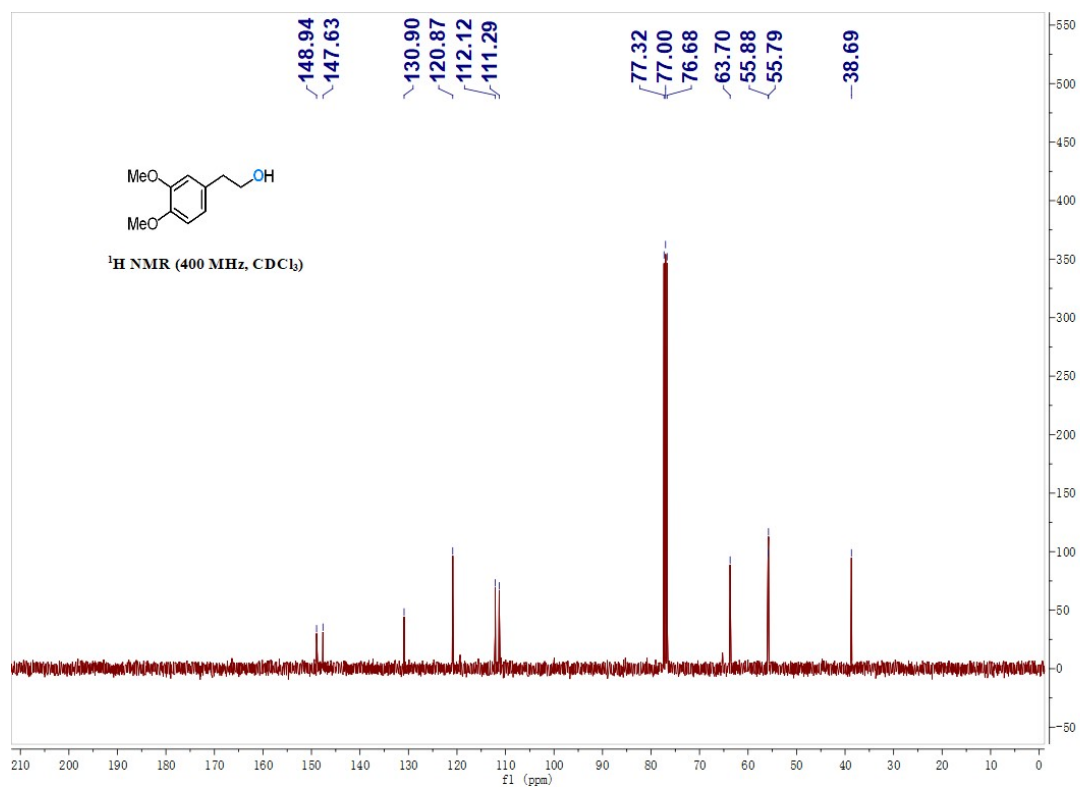
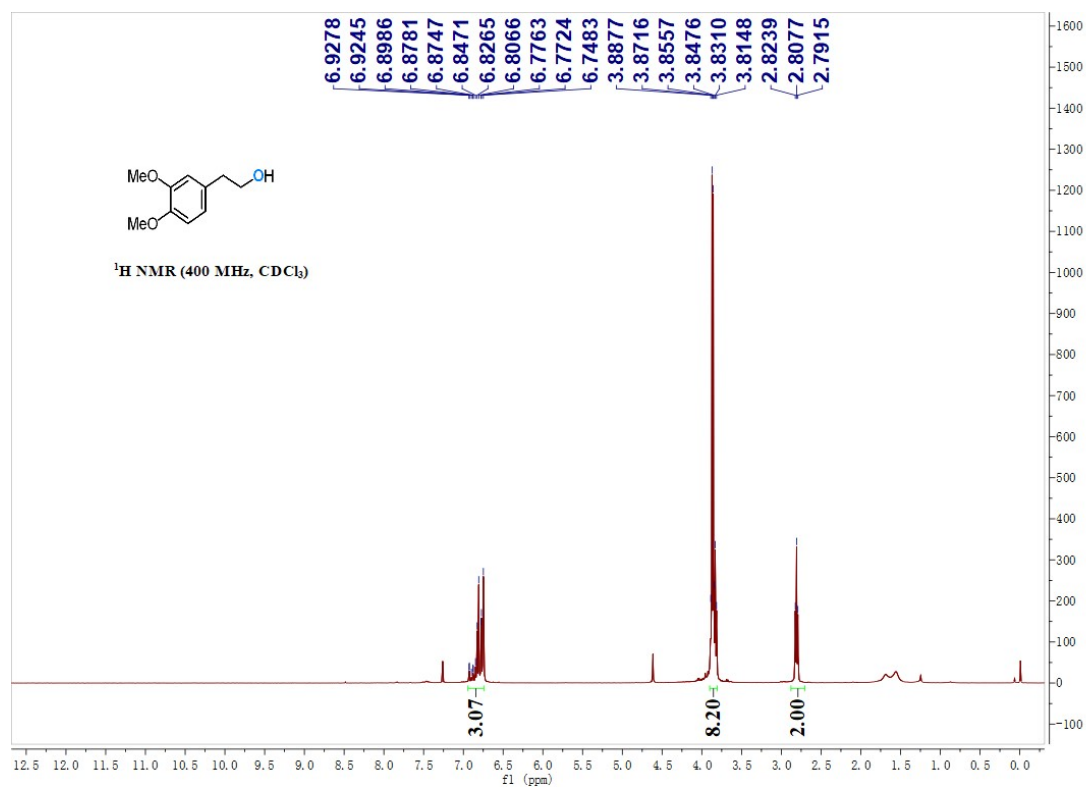




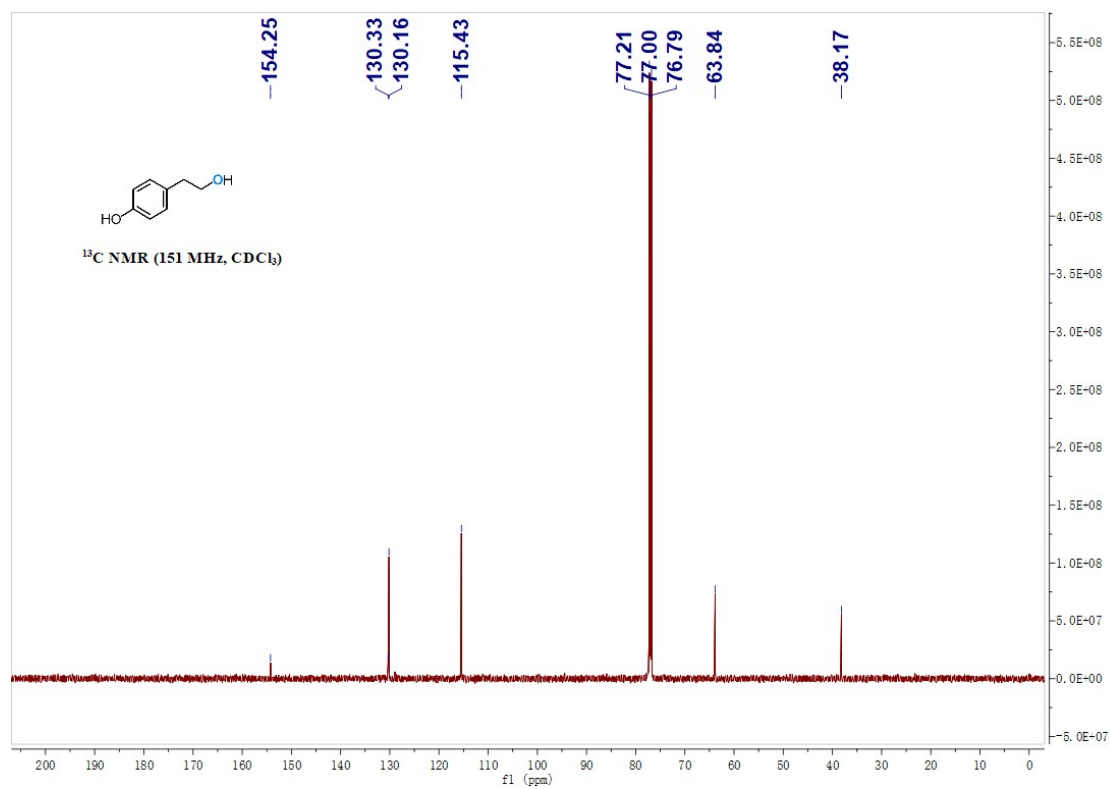
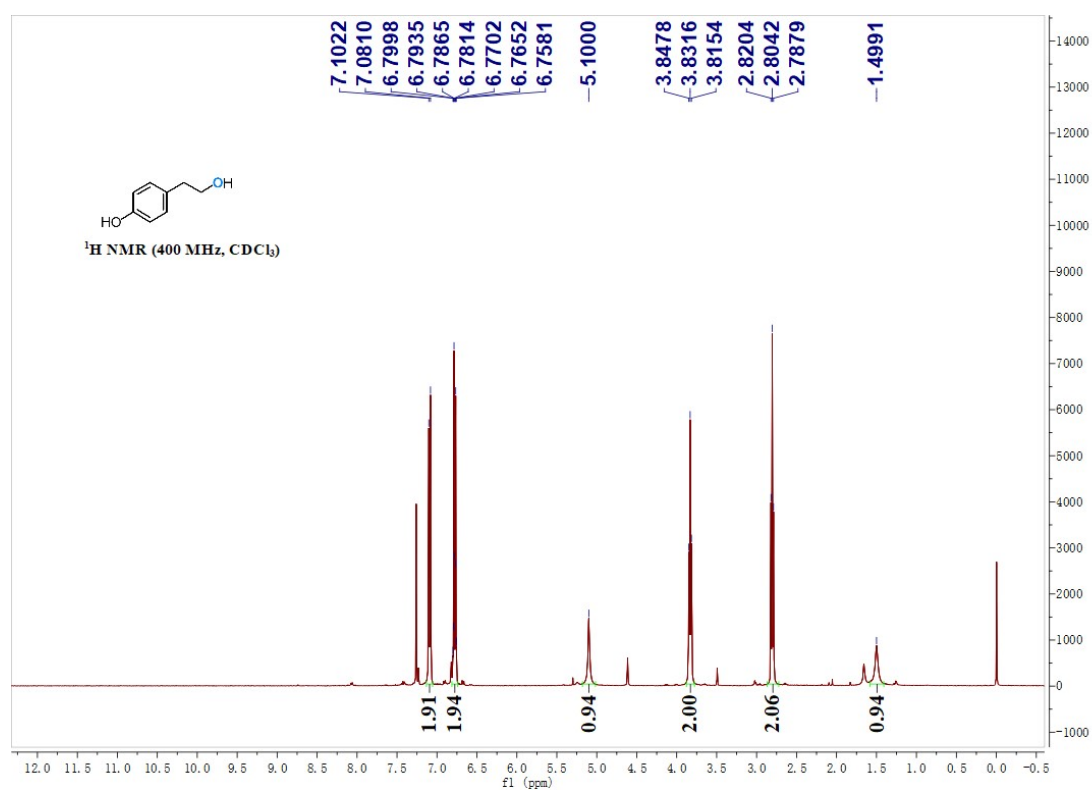
$^1\text{H}$  and  $^{13}\text{C}$  NMR spectra of compound **3h**



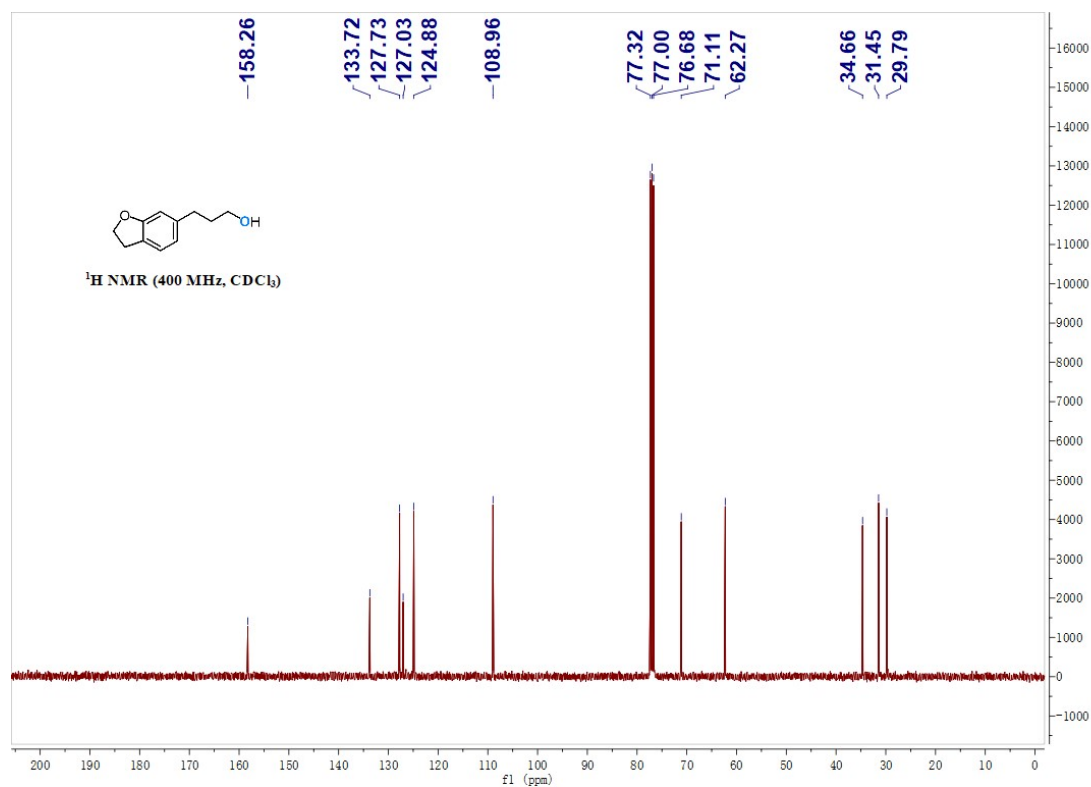
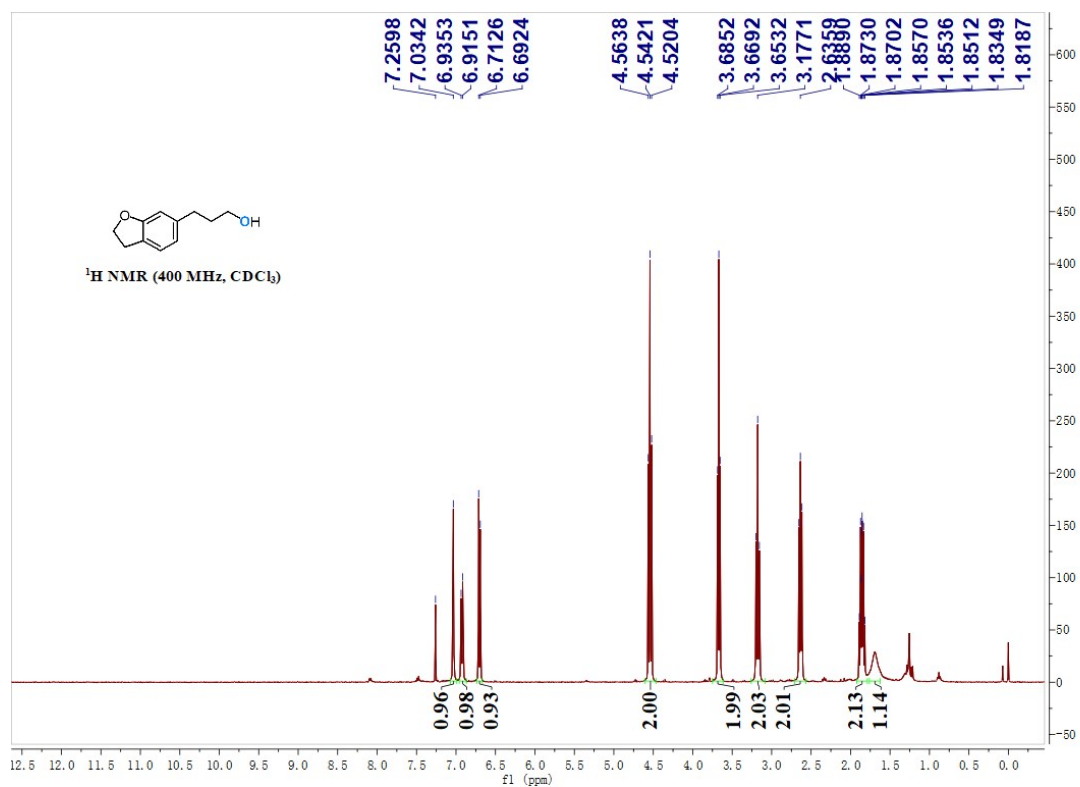
<sup>1</sup>H and <sup>13</sup>C NMR spectra of compound **3i**



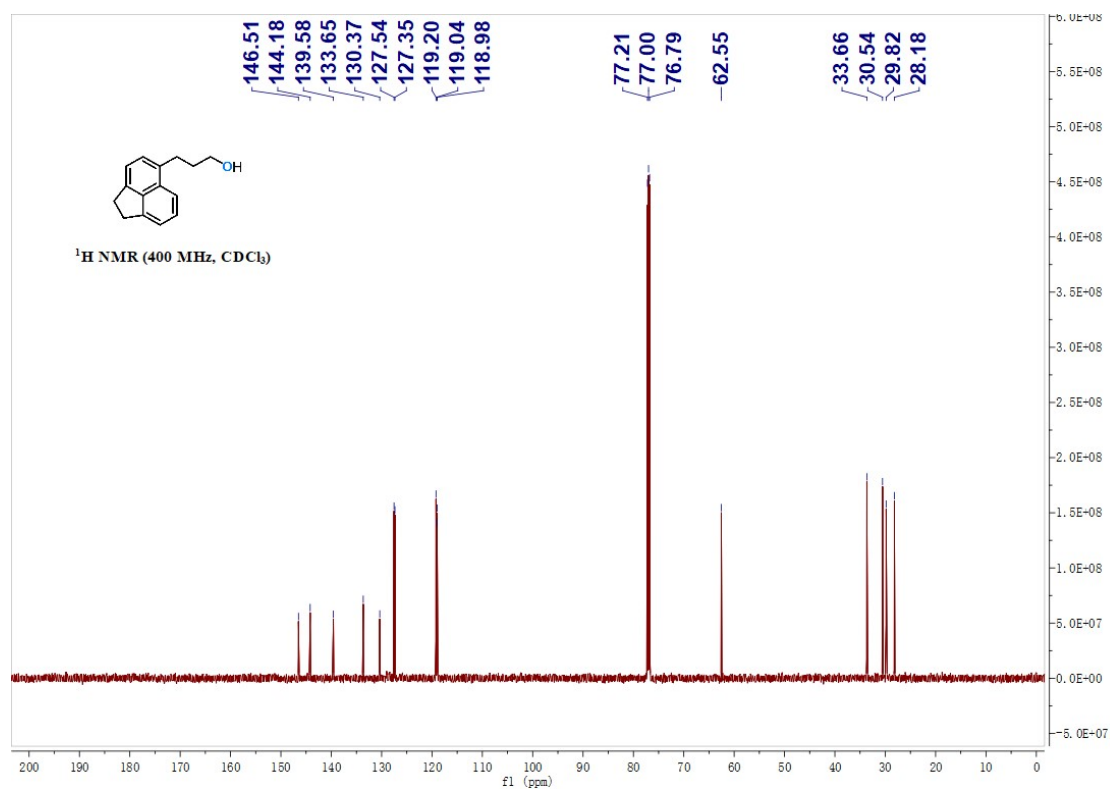
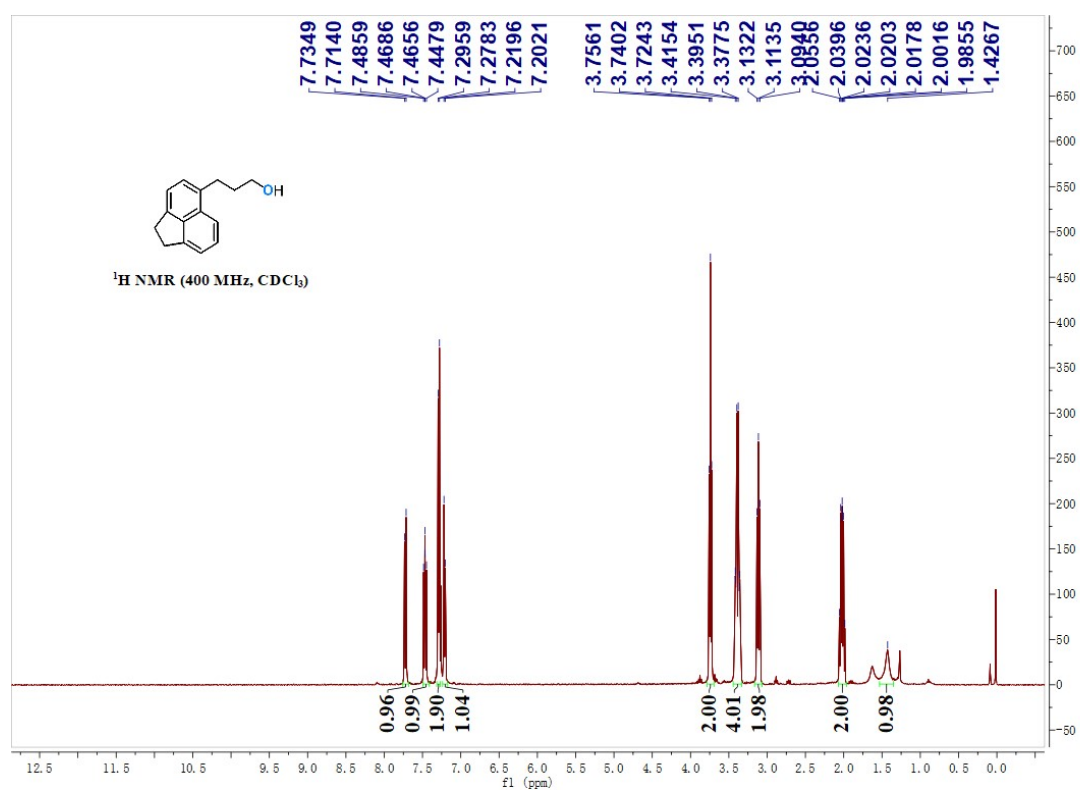
$^1\text{H}$  and  $^{13}\text{C}$  NMR spectra of compound **3j**



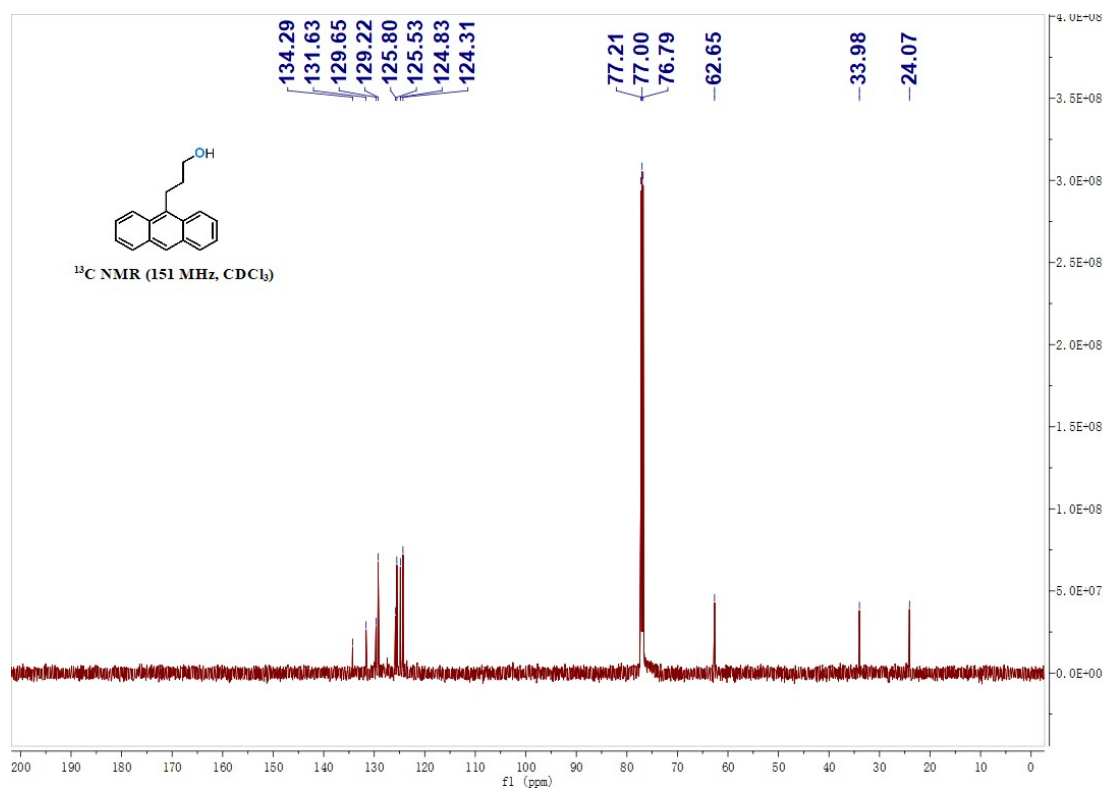
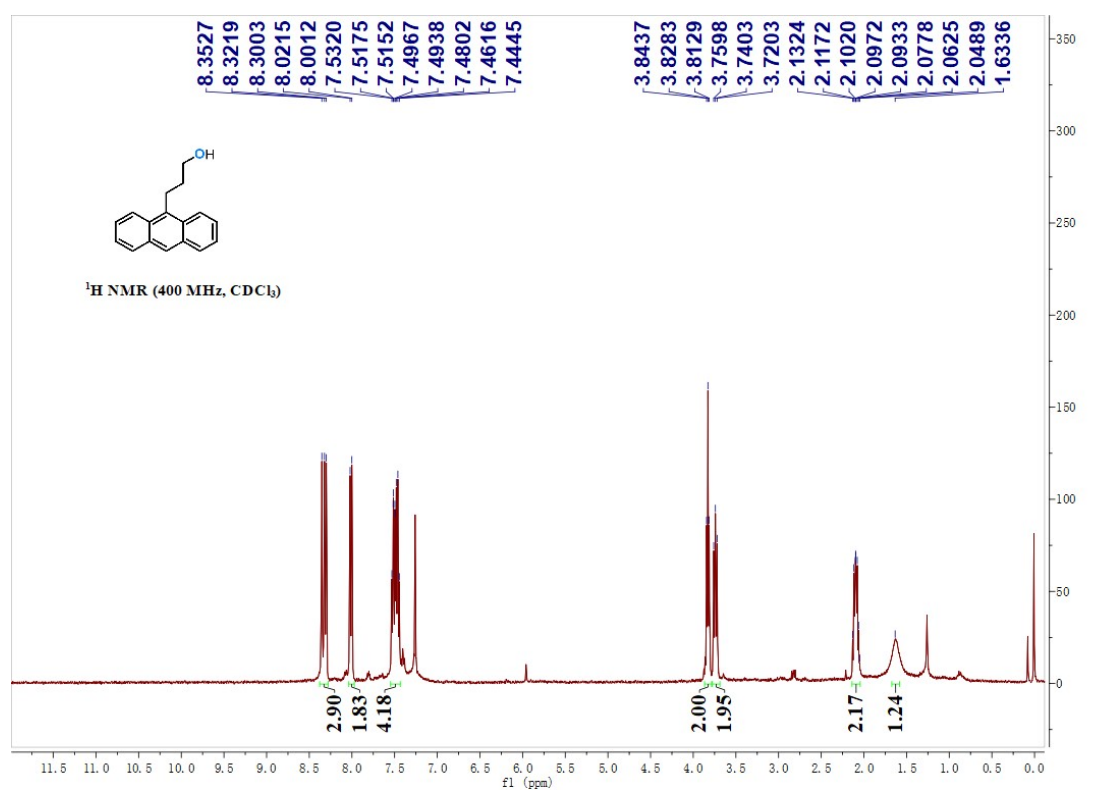
<sup>1</sup>H and <sup>13</sup>C NMR spectra of compound **3k**



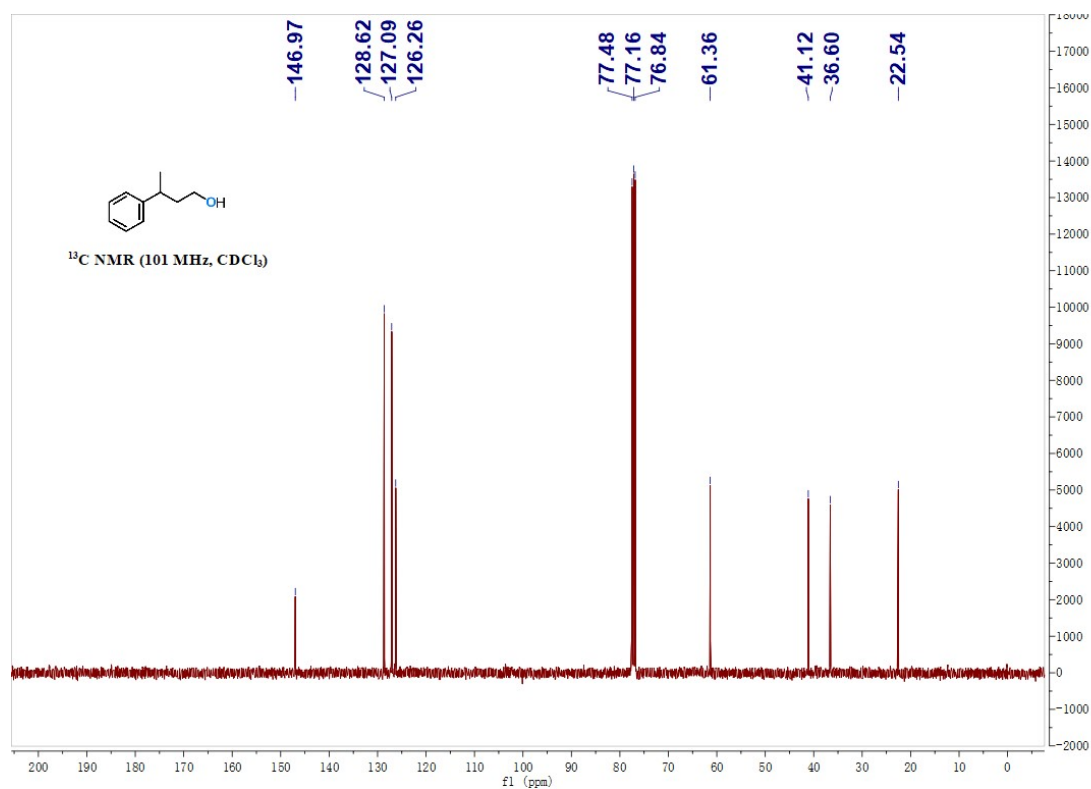
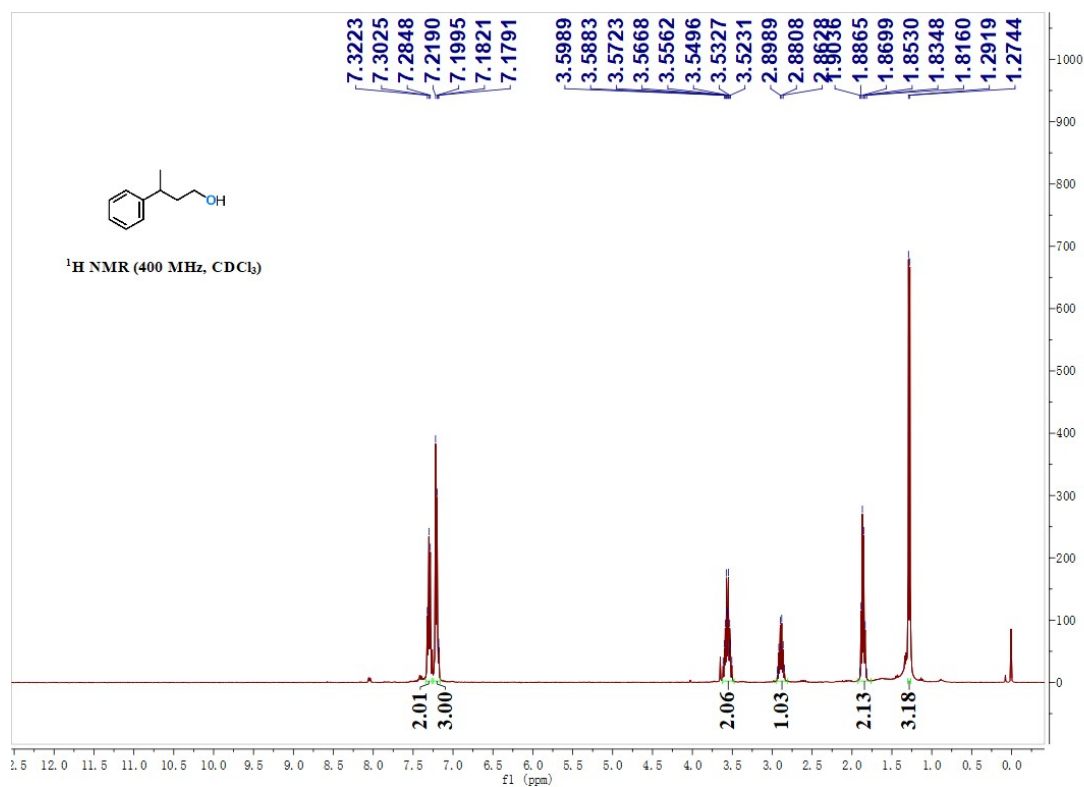
$^1\text{H}$  and  $^{13}\text{C}$  NMR spectra of compound **31**



<sup>1</sup>H and <sup>13</sup>C NMR spectra of compound **3m**

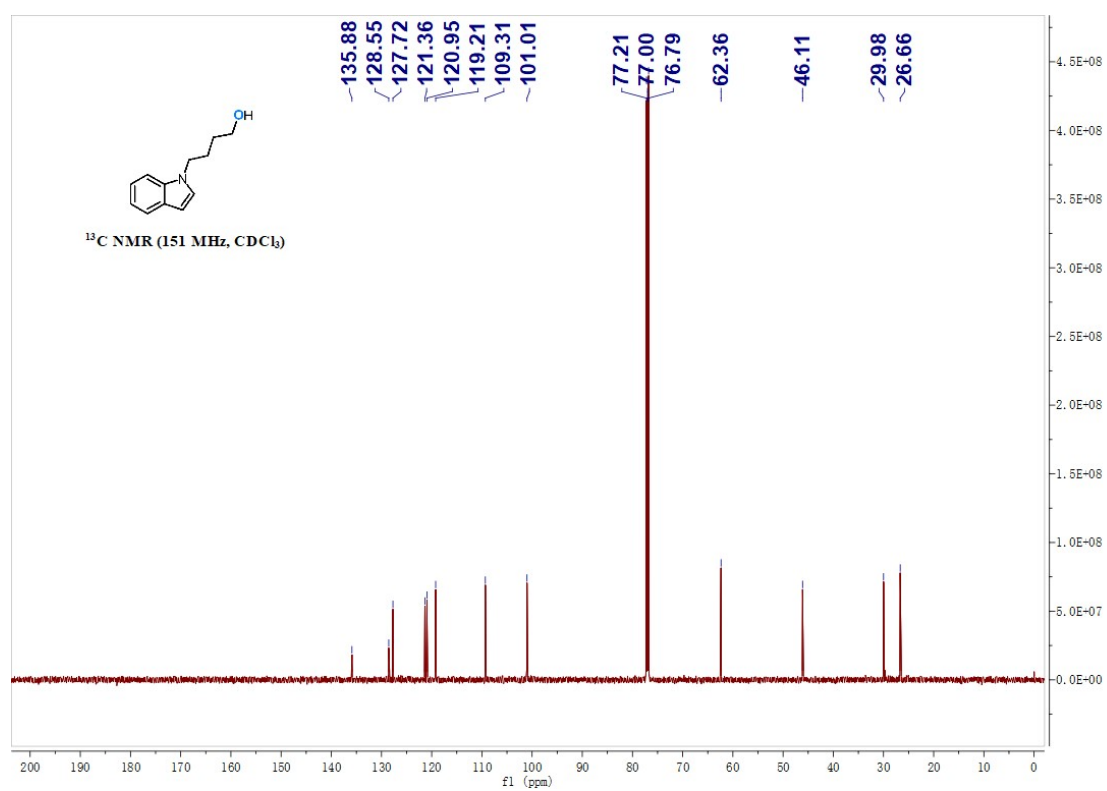
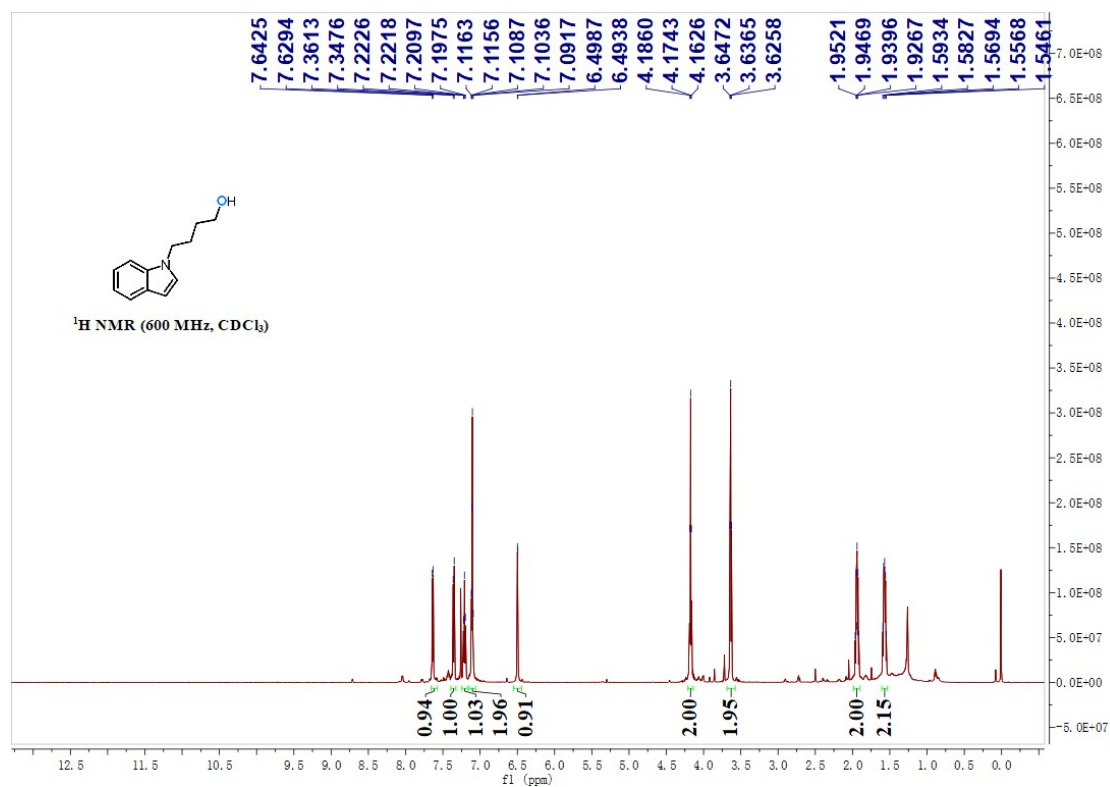


<sup>1</sup>H and <sup>13</sup>C NMR spectra of compound **3n**

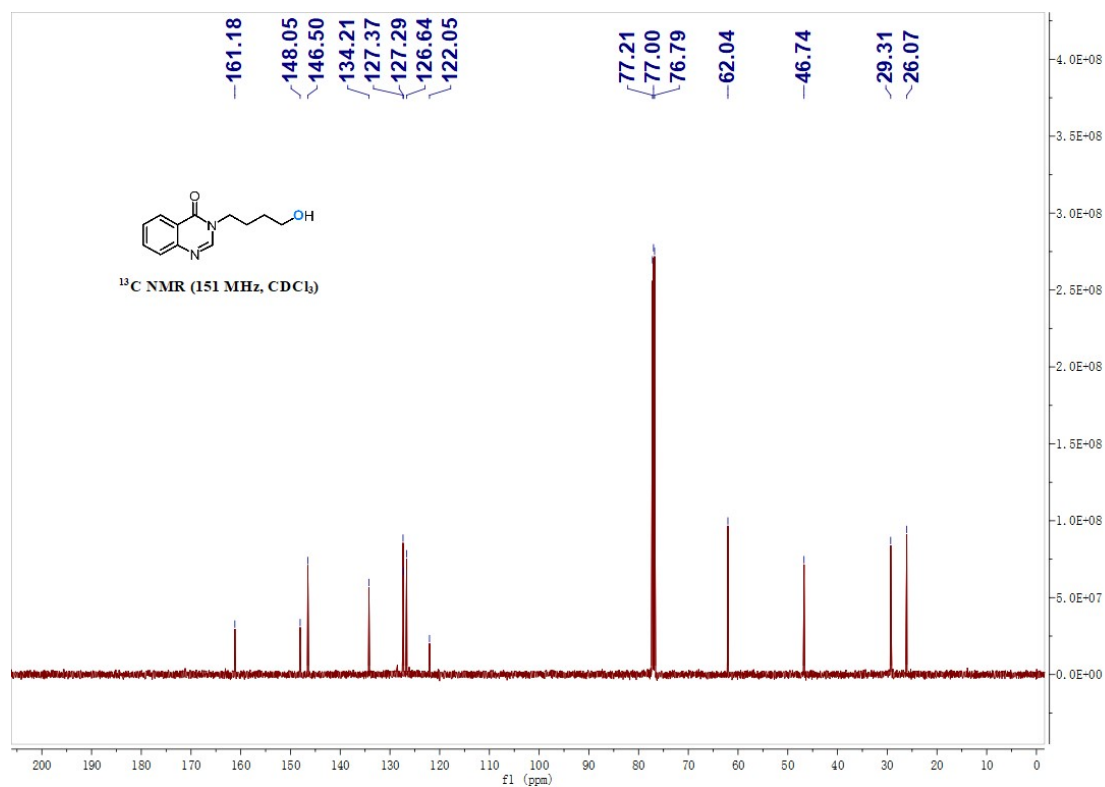
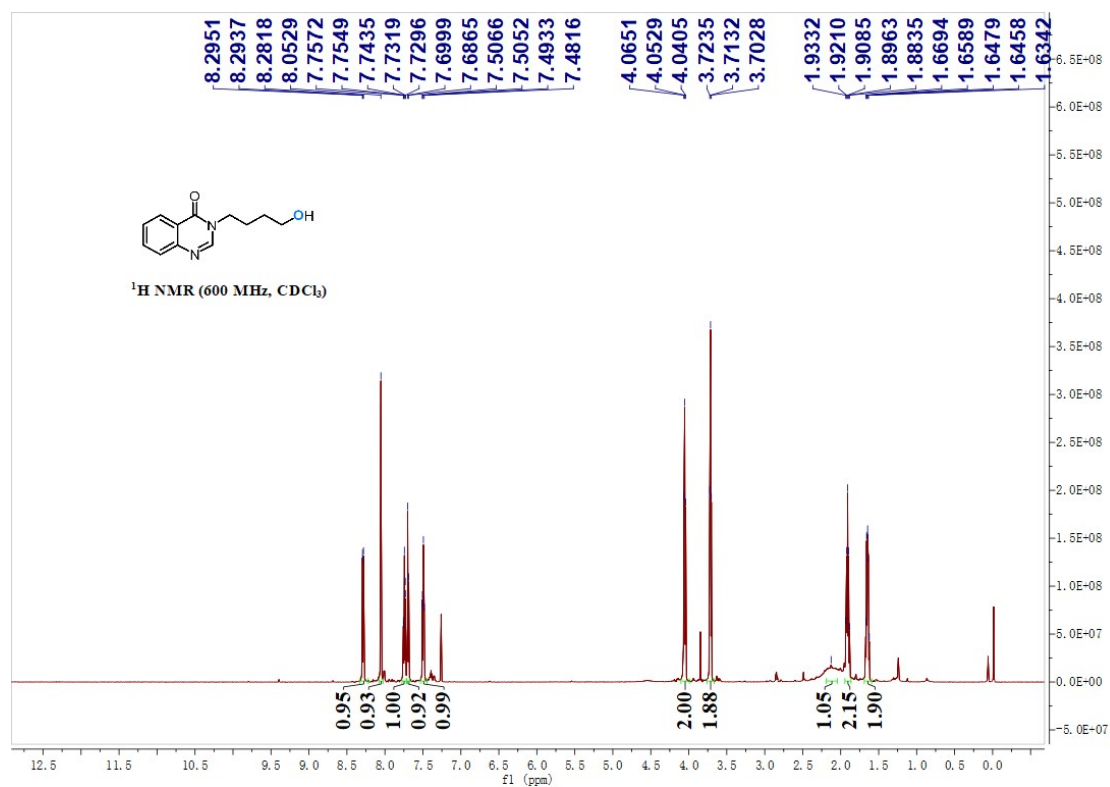


$^1\text{H}$  and  $^{13}\text{C}$  NMR spectra of compound **3o**

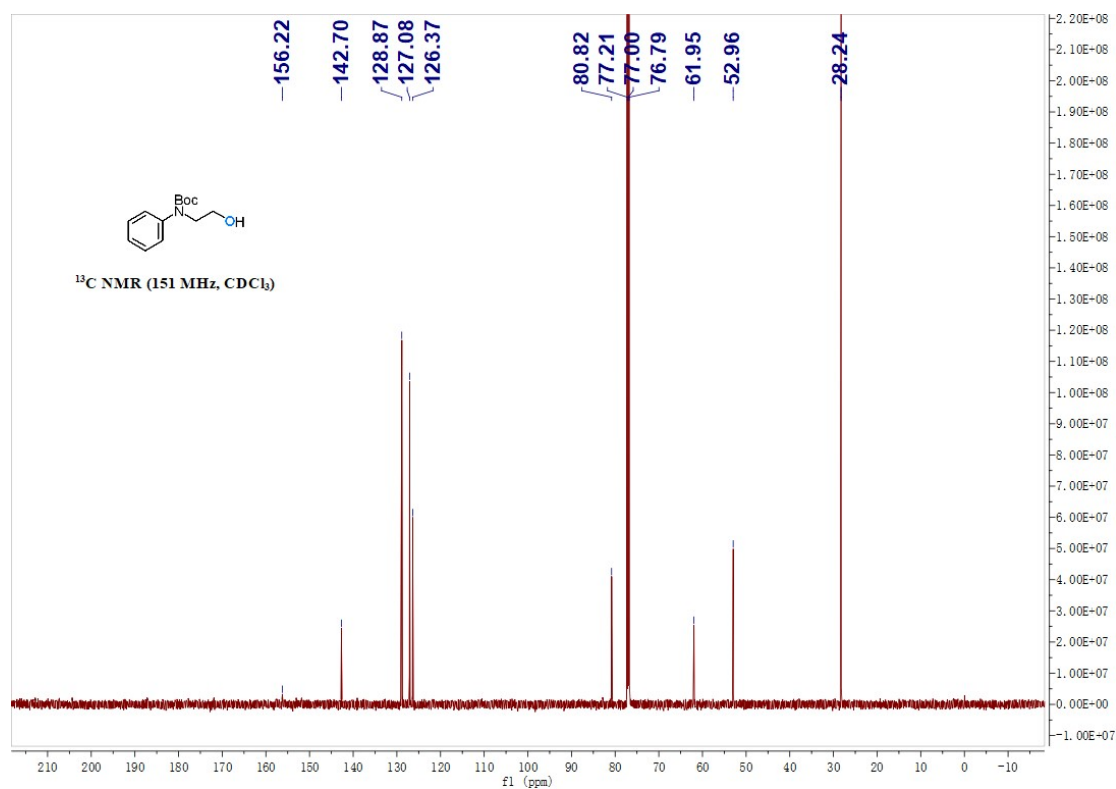
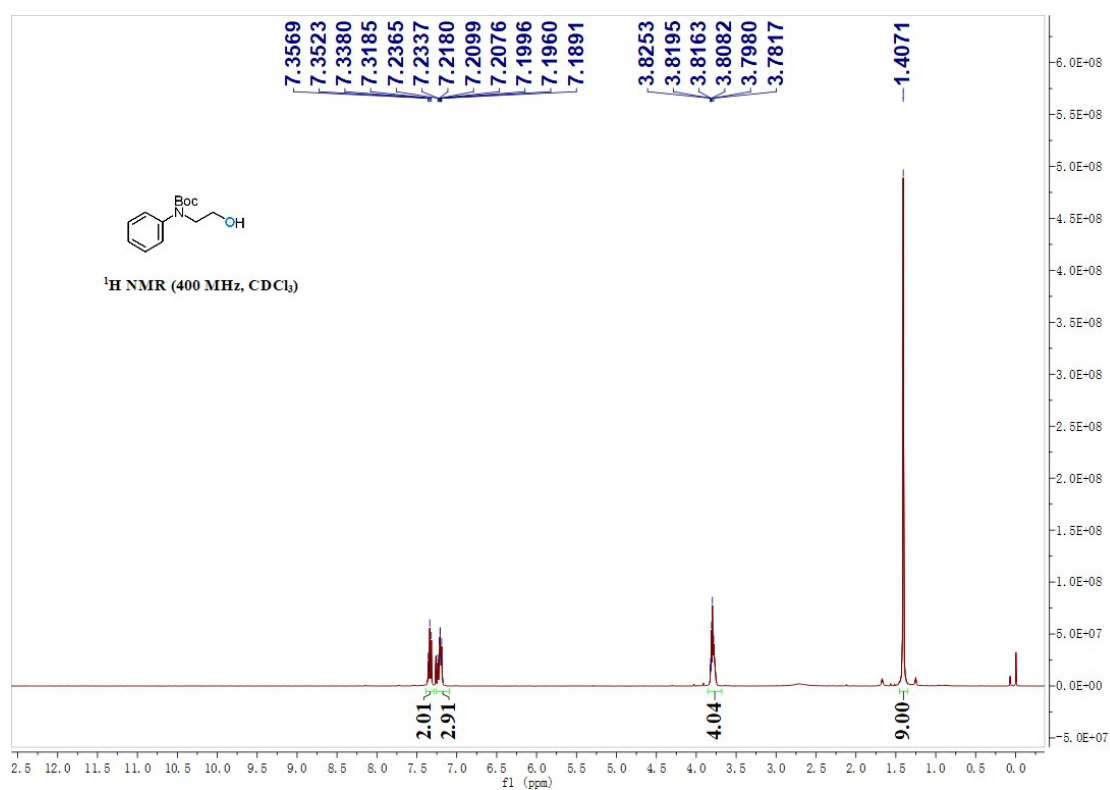




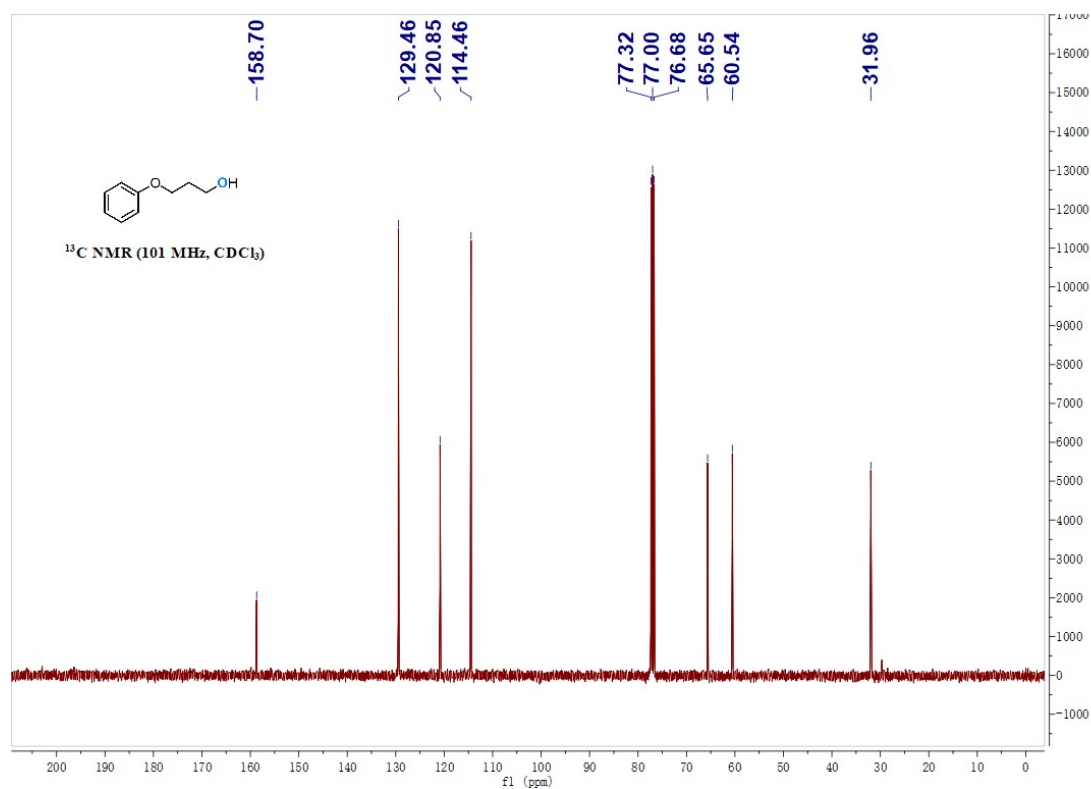
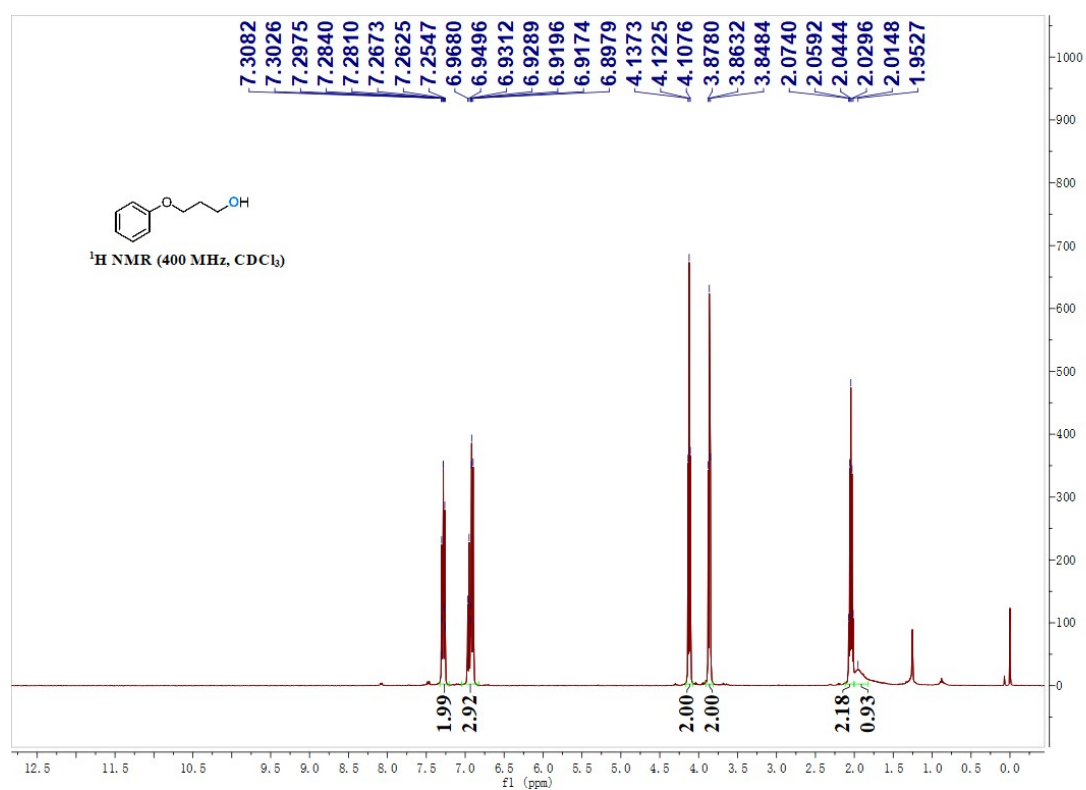
$^1\text{H}$  and  $^{13}\text{C}$  NMR spectra of compound **3p**



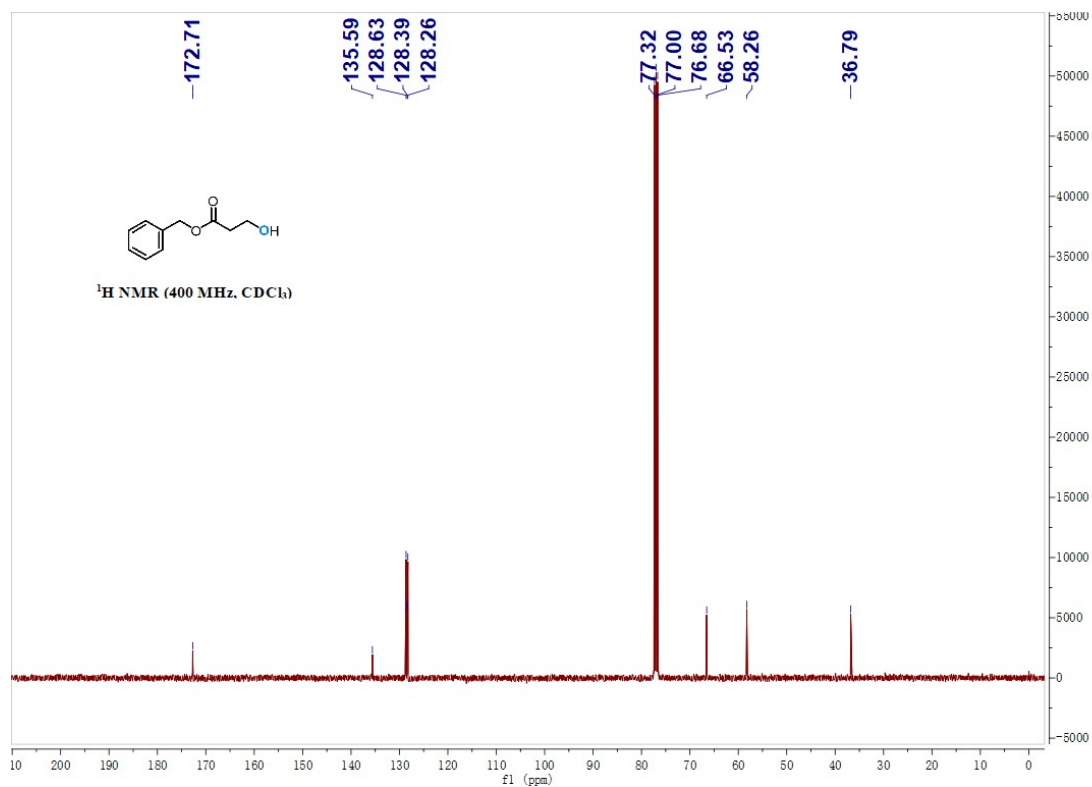
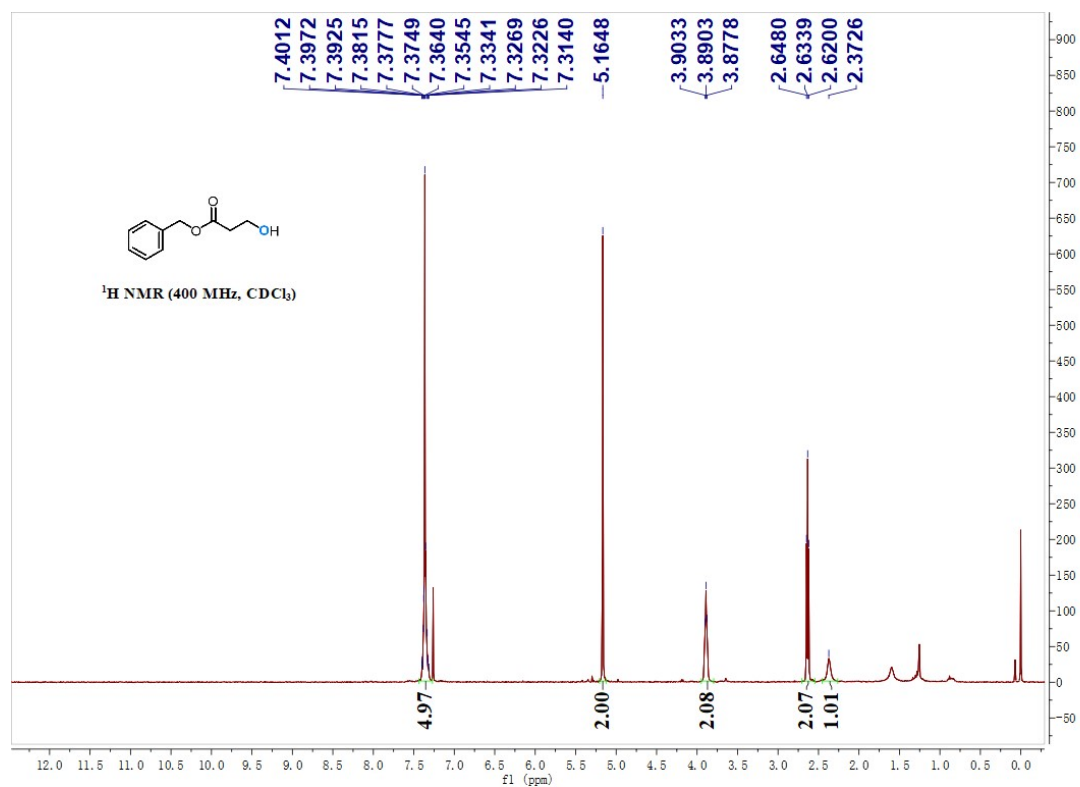
<sup>1</sup>H and <sup>13</sup>C NMR spectra of compound **3q**



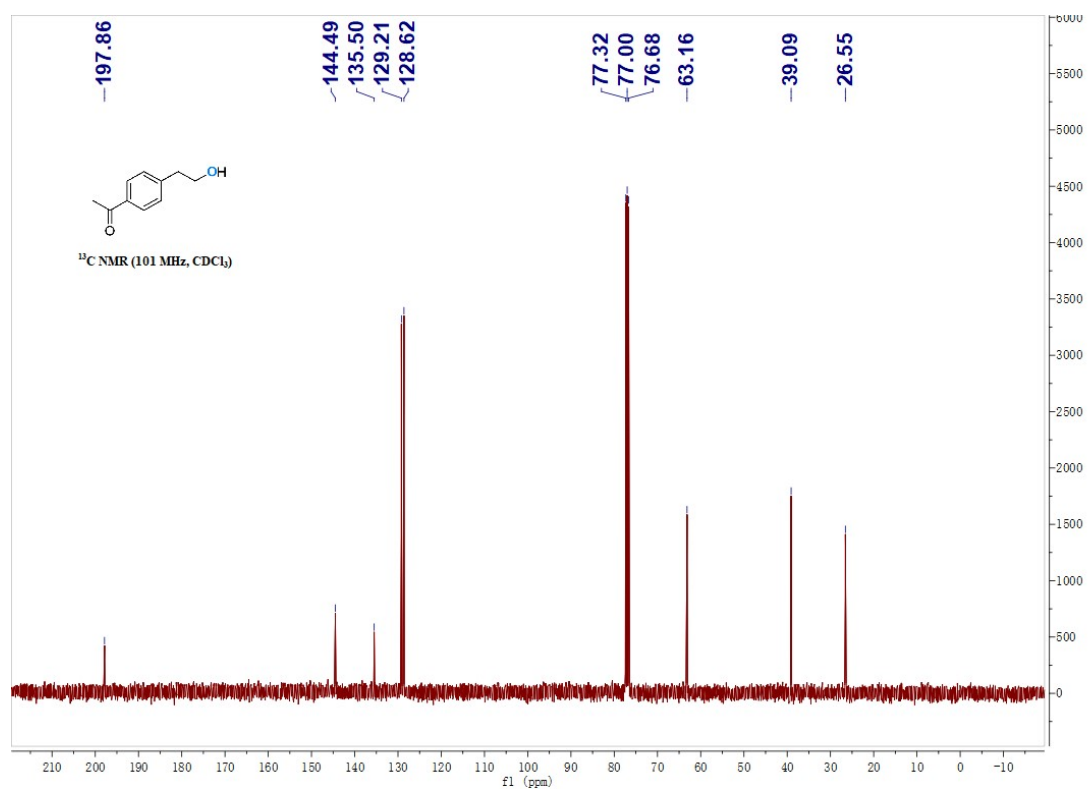
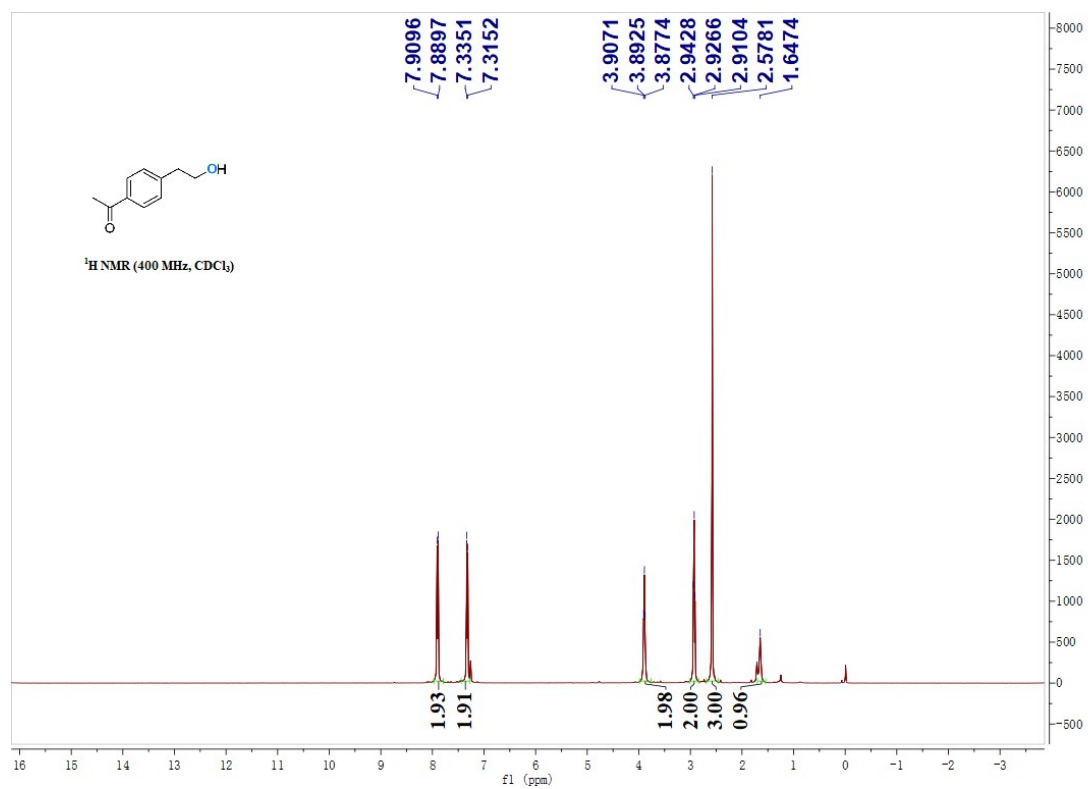
$^1\text{H}$  and  $^{13}\text{C}$  NMR spectra of compound **3r**



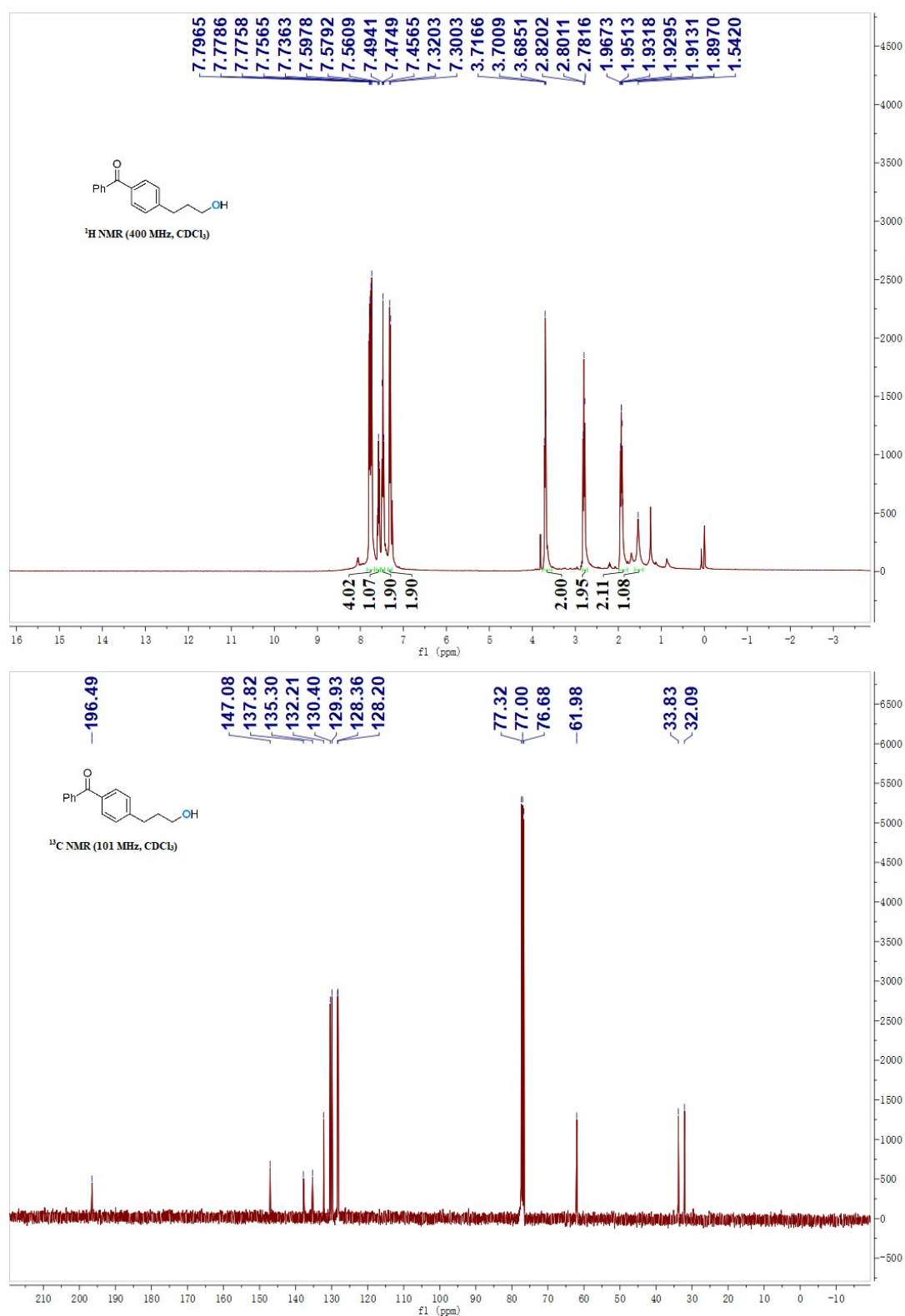
$^1\text{H}$  and  $^{13}\text{C}$  NMR spectra of compound **3s**



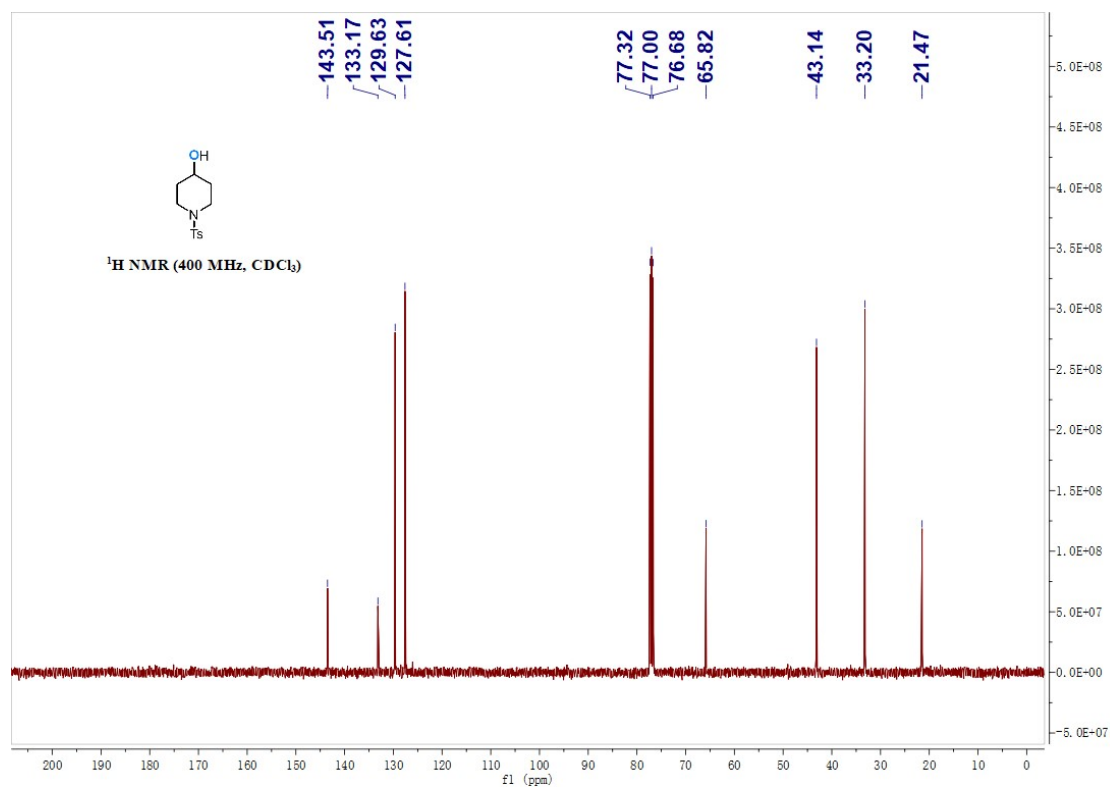
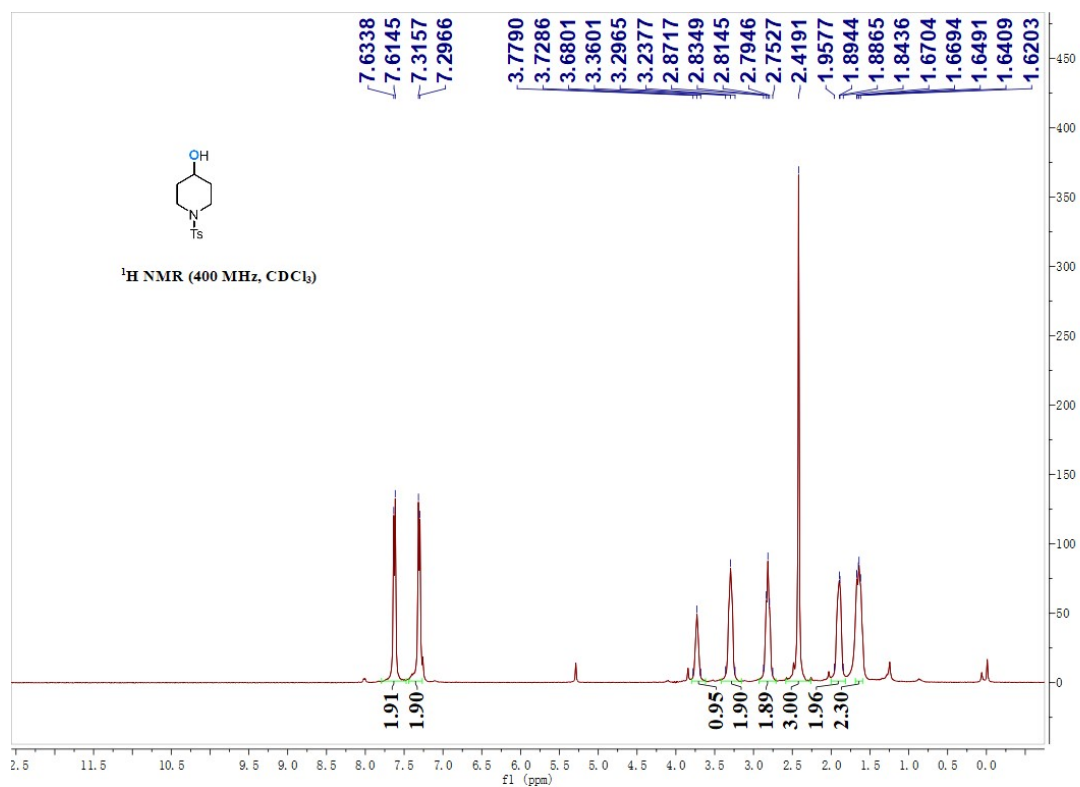
<sup>1</sup>H and <sup>13</sup>C NMR spectra of compound **3t**



$^1\text{H}$  and  $^{13}\text{C}$  NMR spectra of compound **3u**

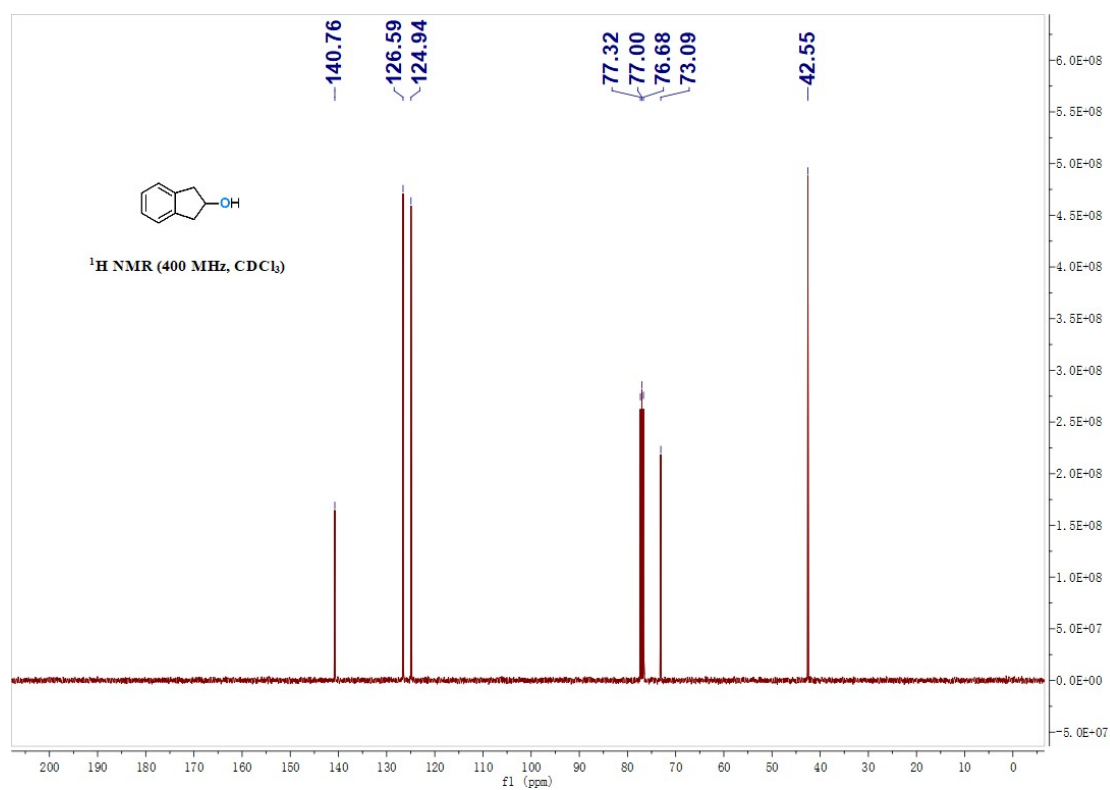
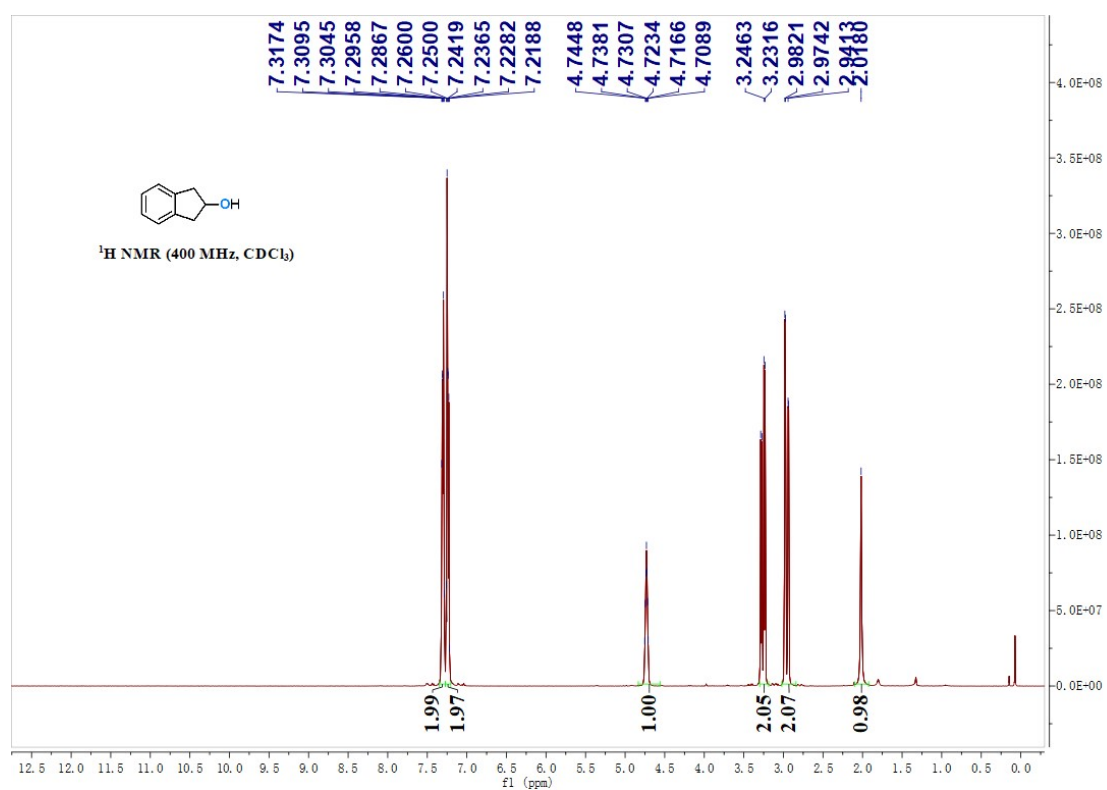


<sup>1</sup>H and <sup>13</sup>C NMR spectra of compound **3v**

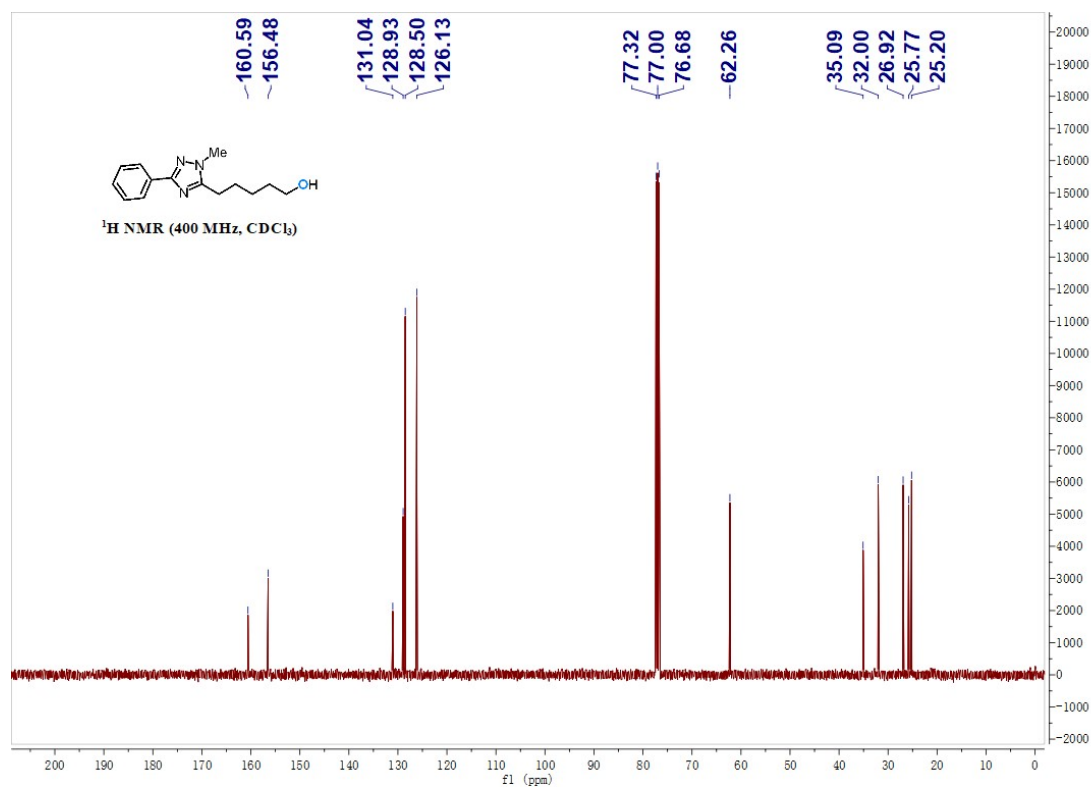
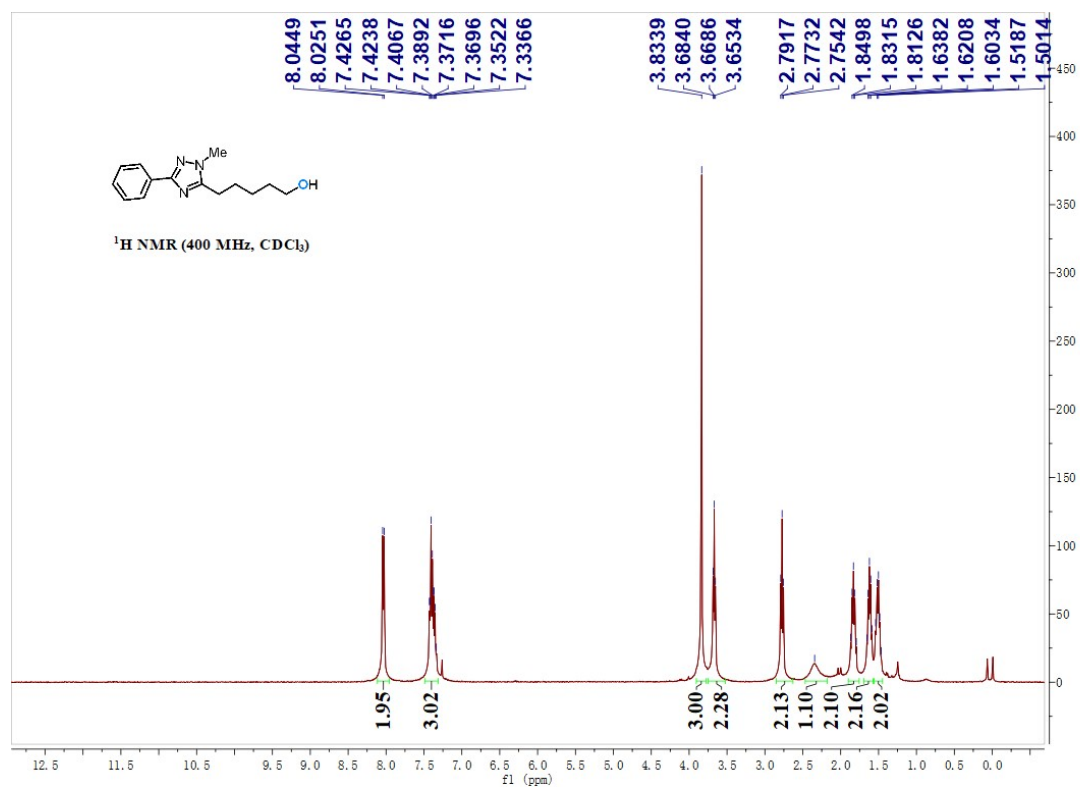


<sup>1</sup>H and <sup>13</sup>C NMR spectra of compound **3w**

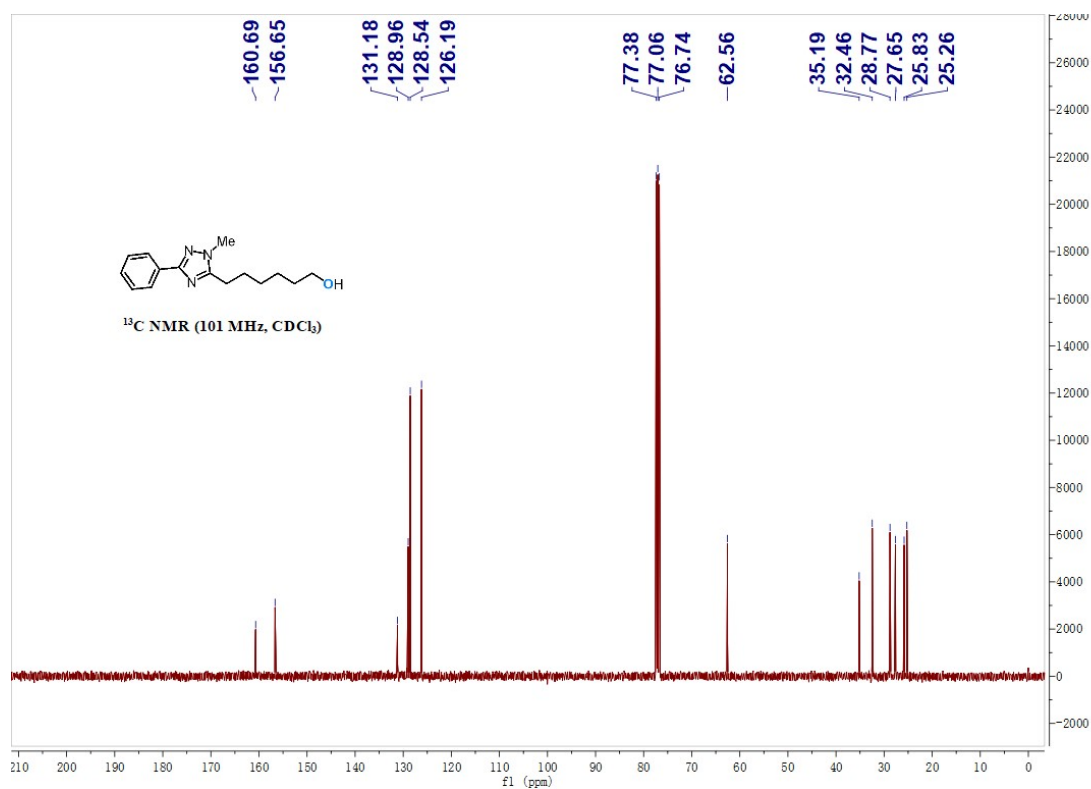
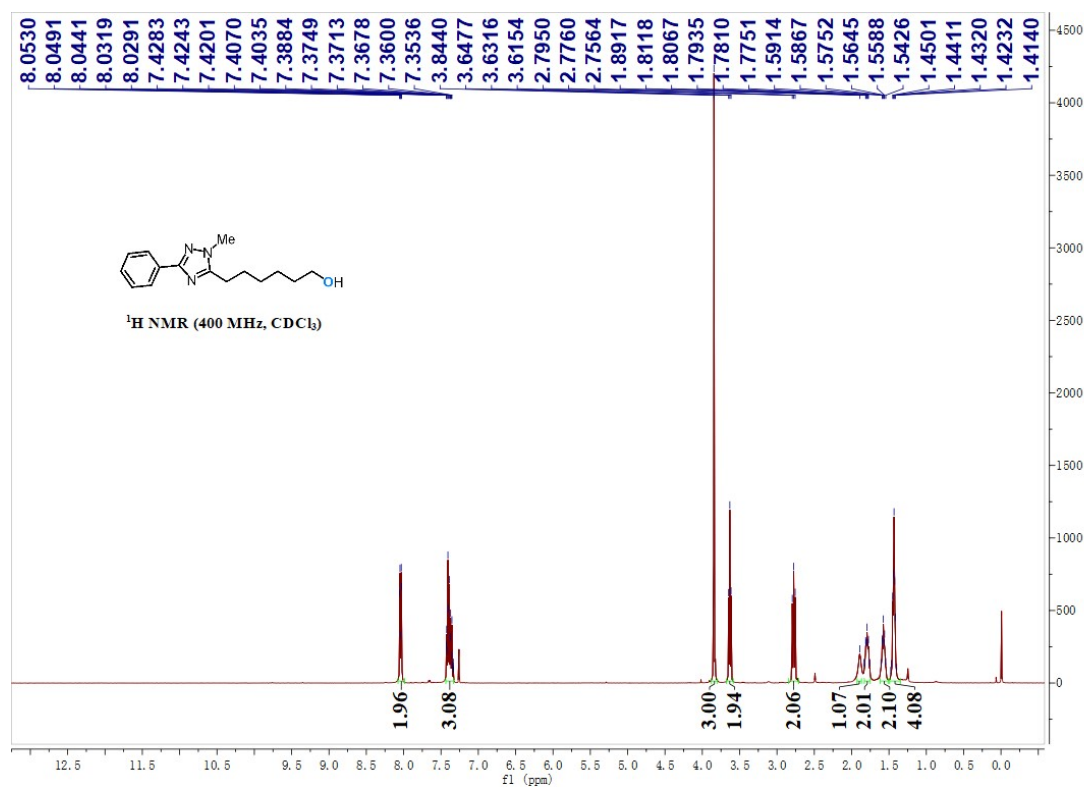




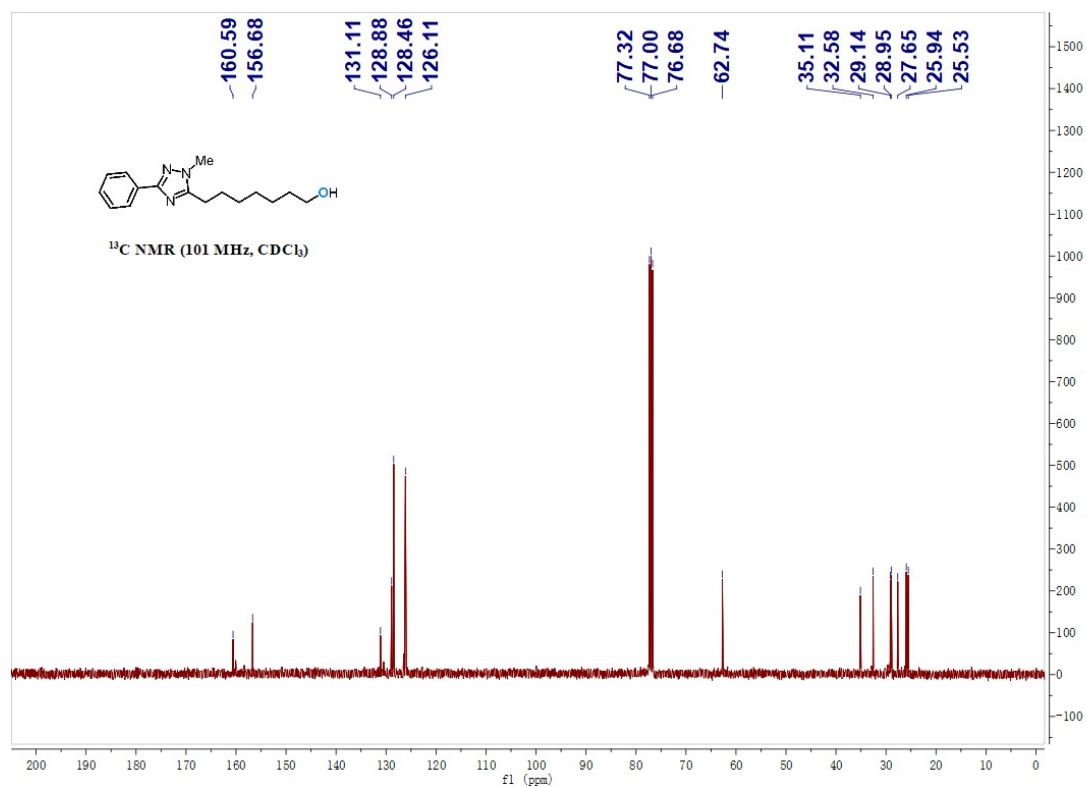
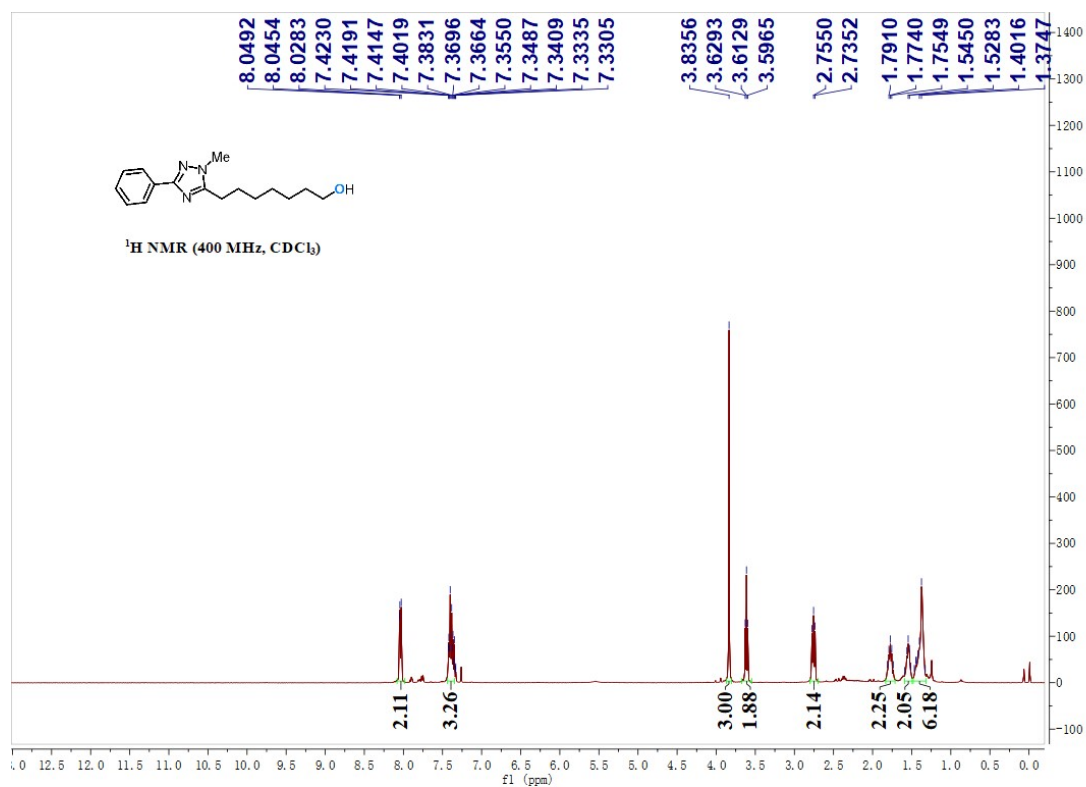
$^1\text{H}$  and  $^{13}\text{C}$  NMR spectra of compound **3x**



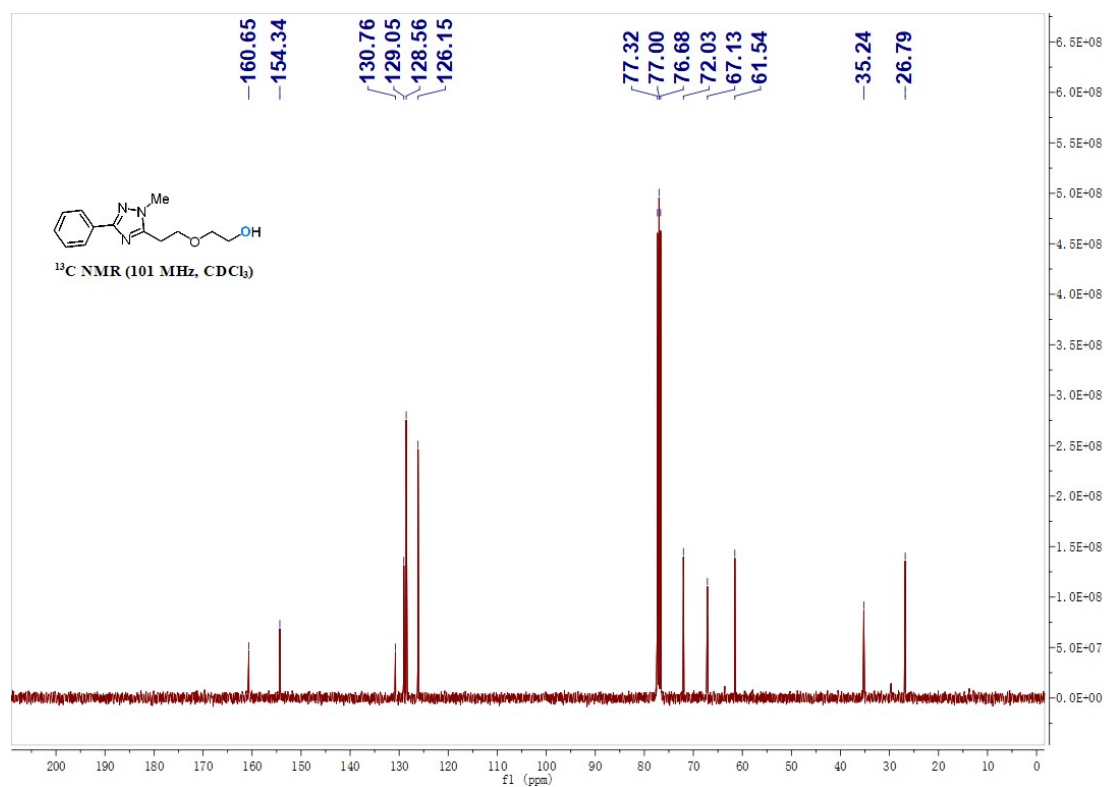
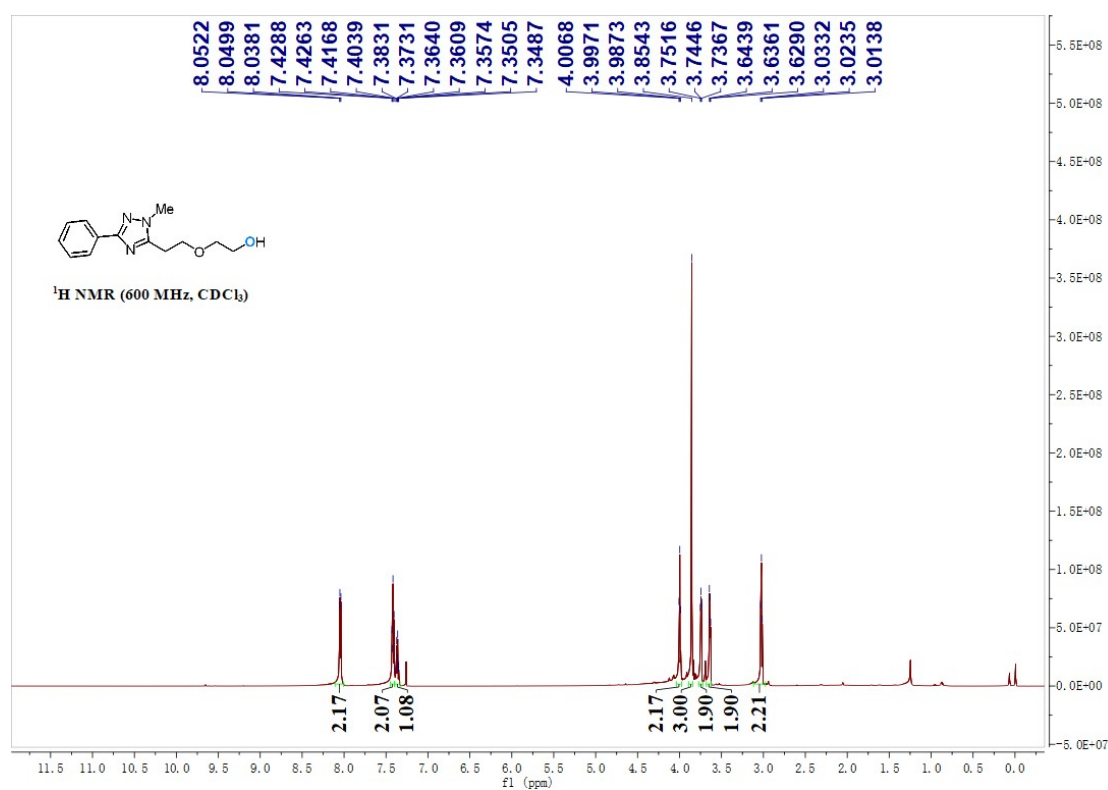
<sup>1</sup>H and <sup>13</sup>C NMR spectra of compound **3y**



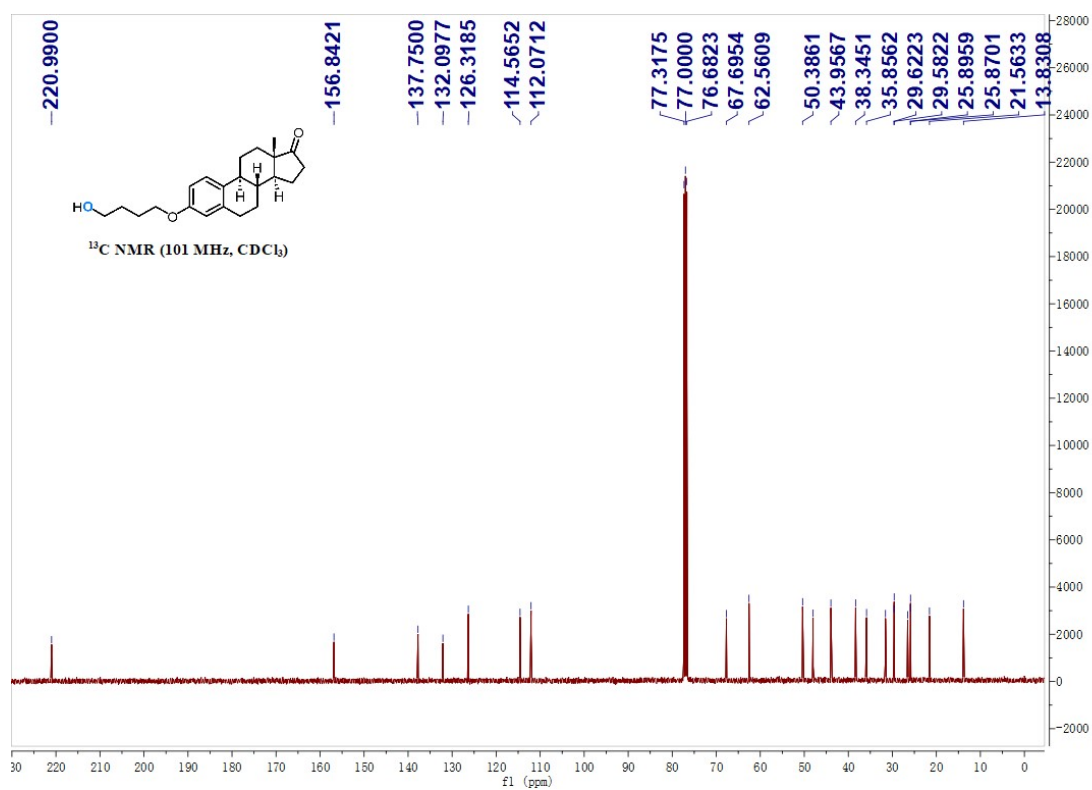
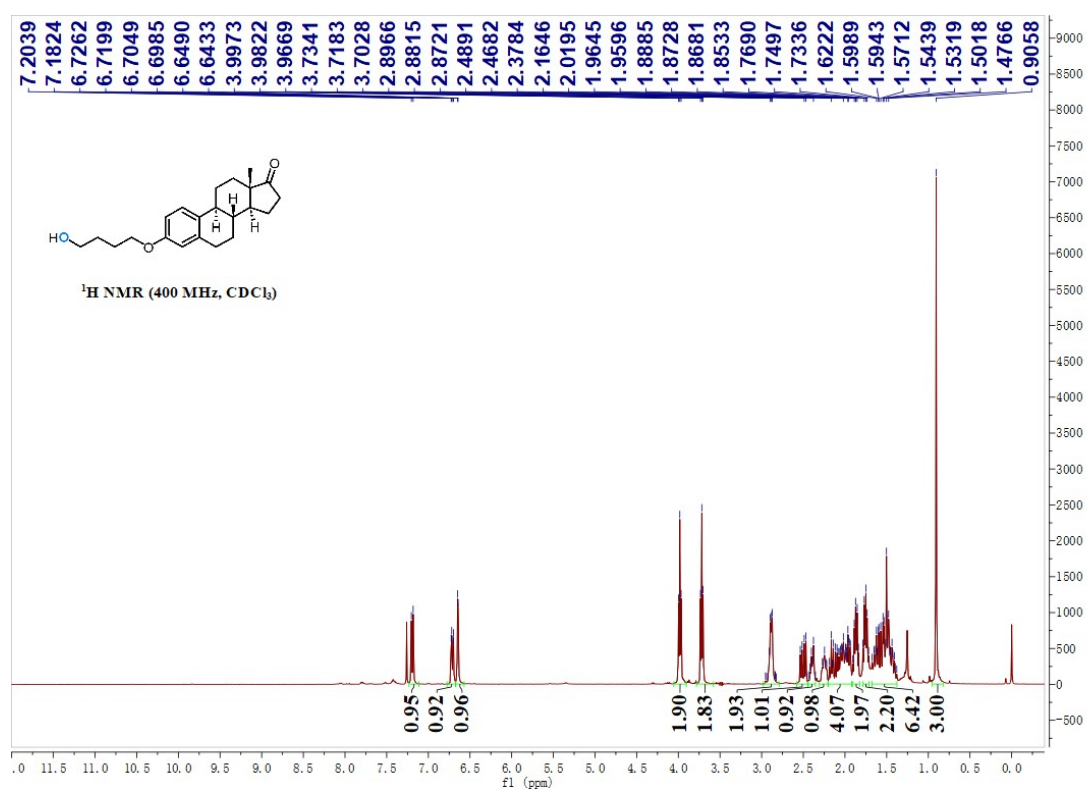
<sup>1</sup>H and <sup>13</sup>C NMR spectra of compound **3z**



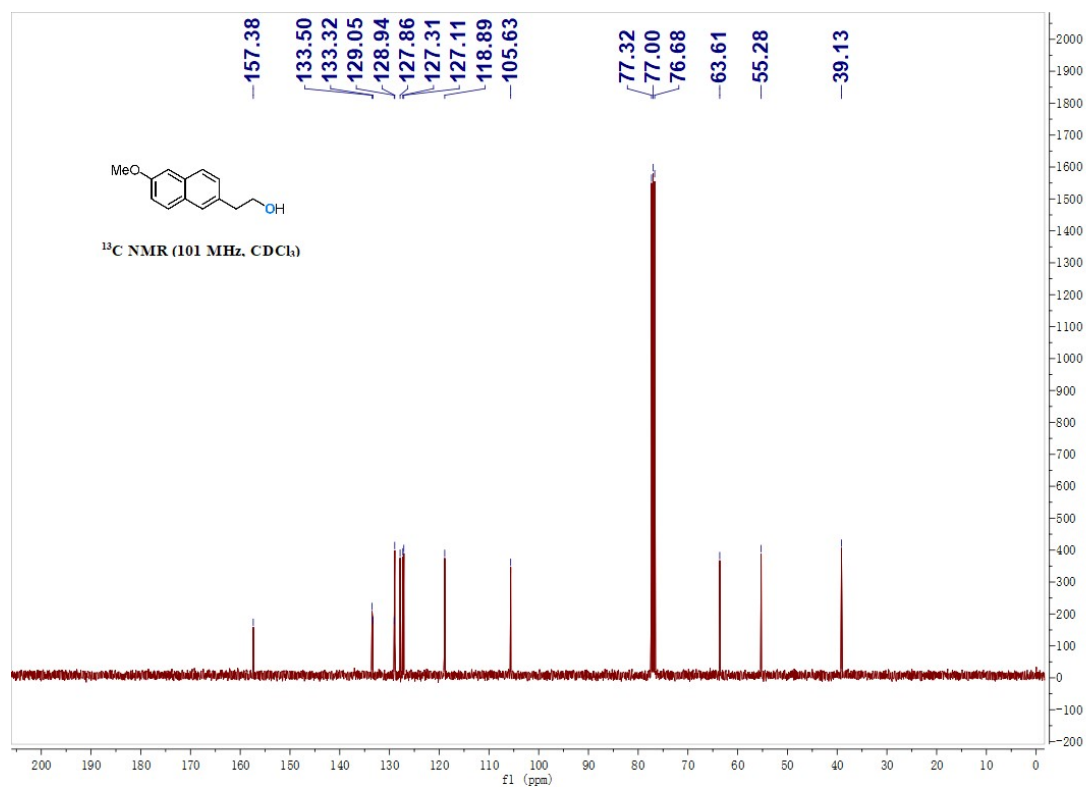
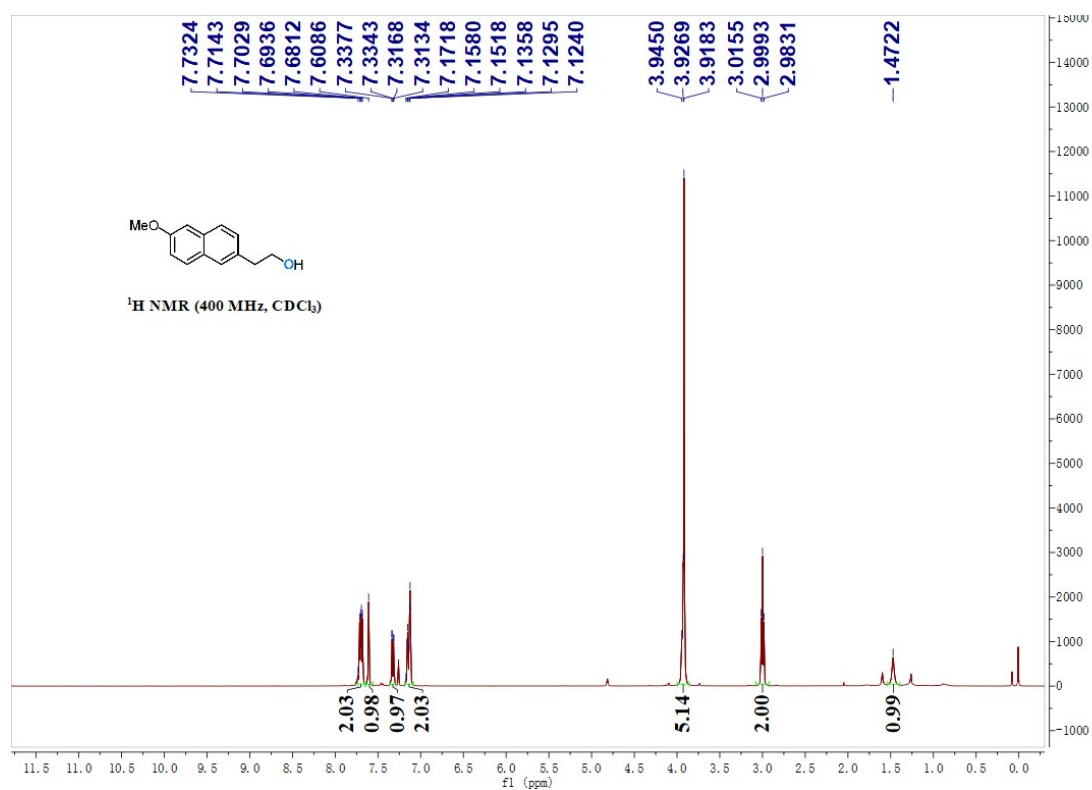
<sup>1</sup>H and <sup>13</sup>C NMR spectra of compound **3aa**



<sup>1</sup>H and <sup>13</sup>C NMR spectra of compound **3ab**

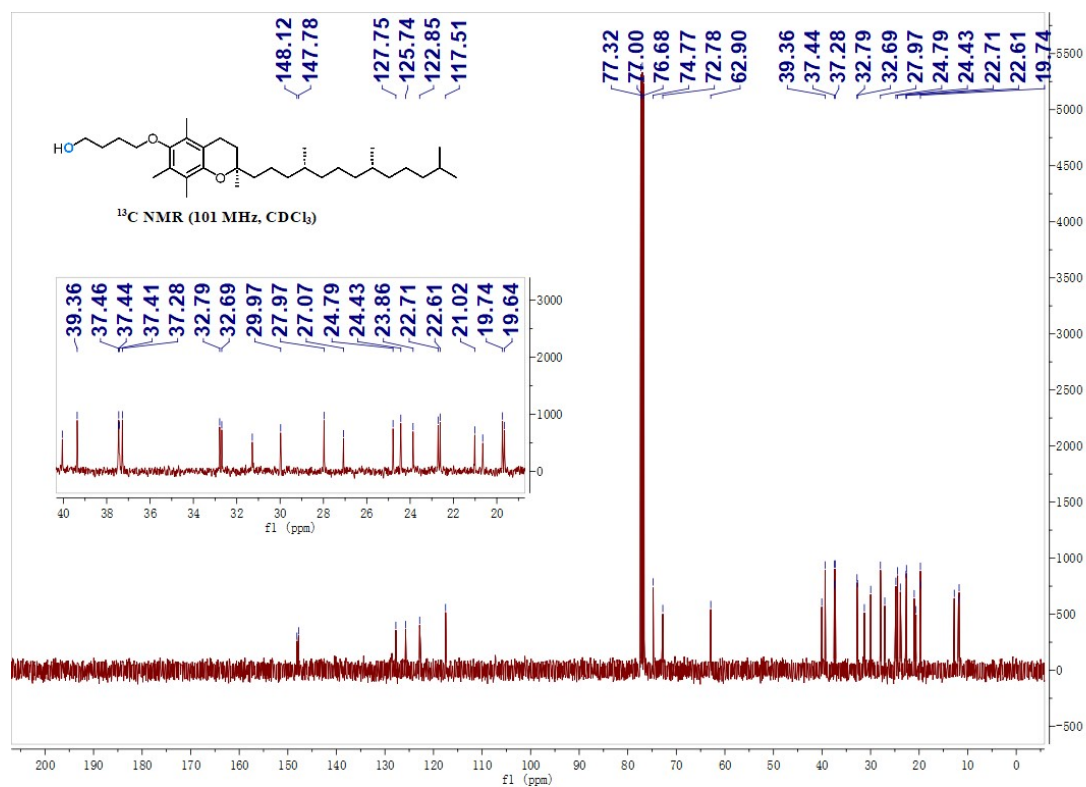
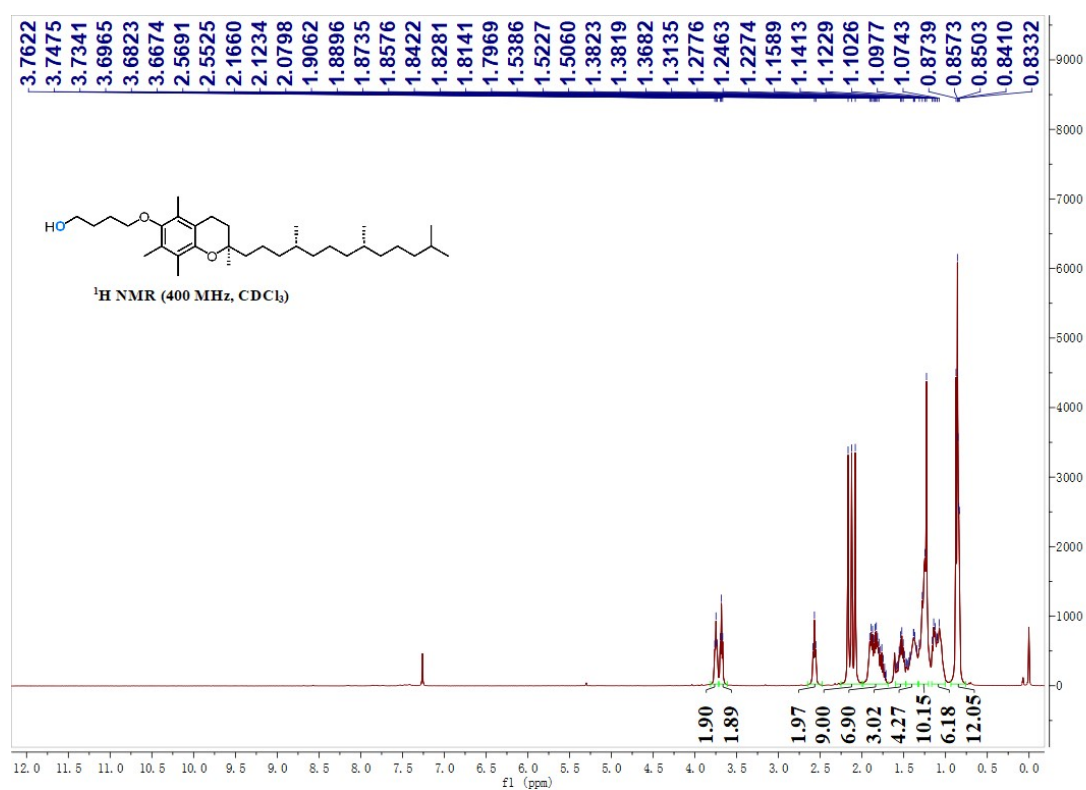


<sup>1</sup>H and <sup>13</sup>C NMR spectra of compound **3ac**



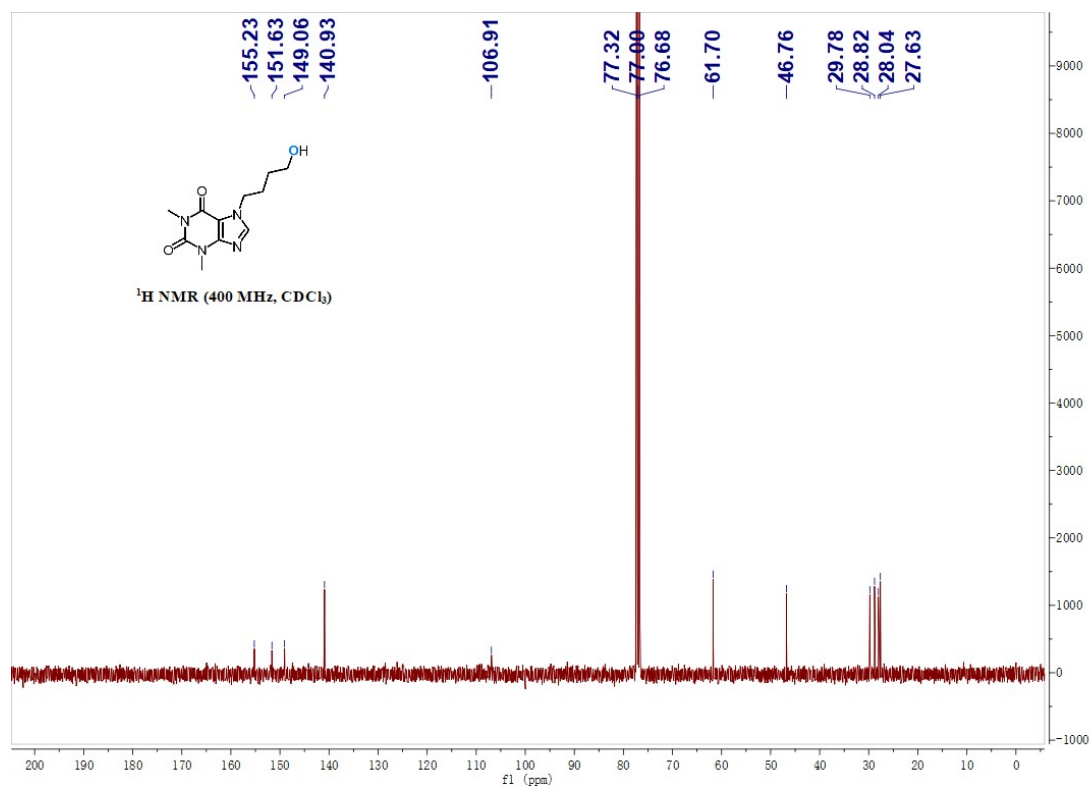
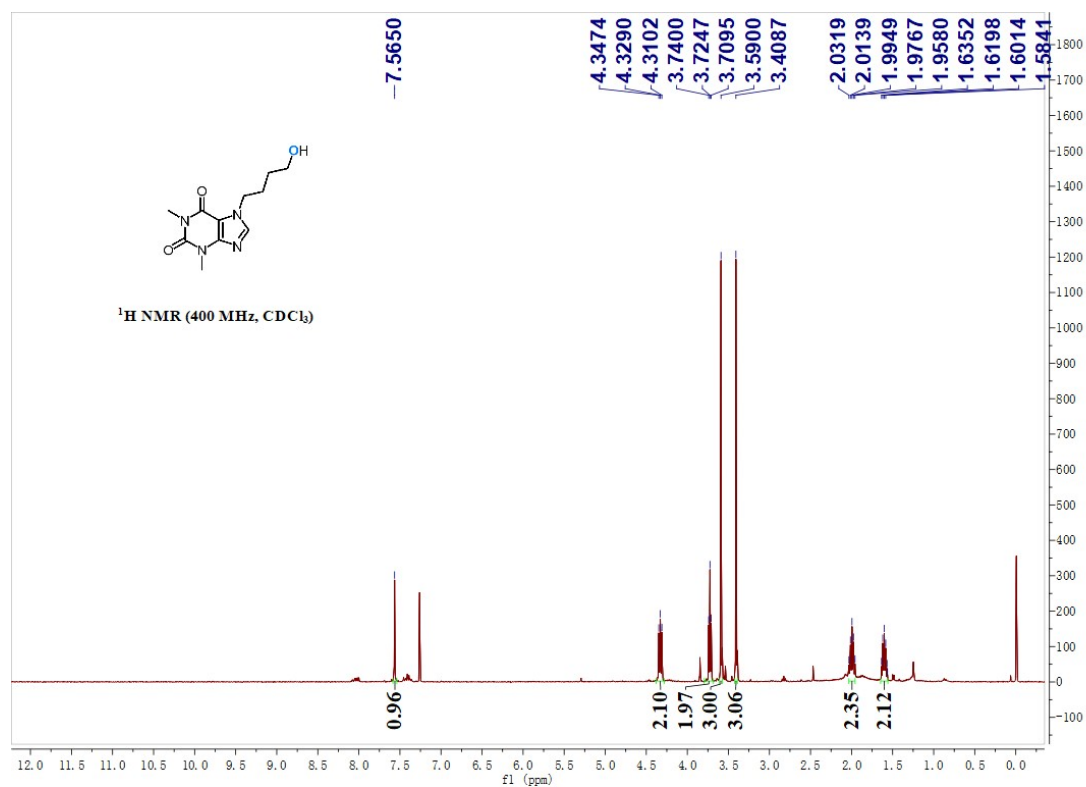
$^1\text{H}$  and  $^{13}\text{C}$  NMR spectra of compound **3ad**



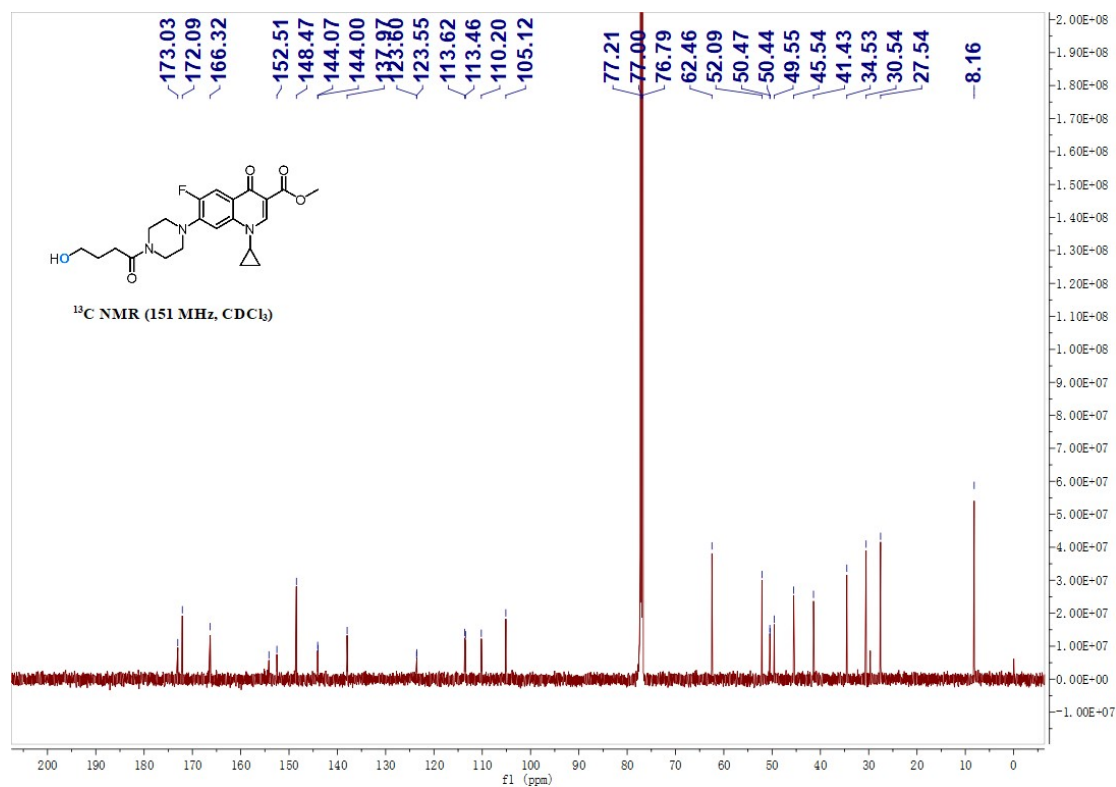
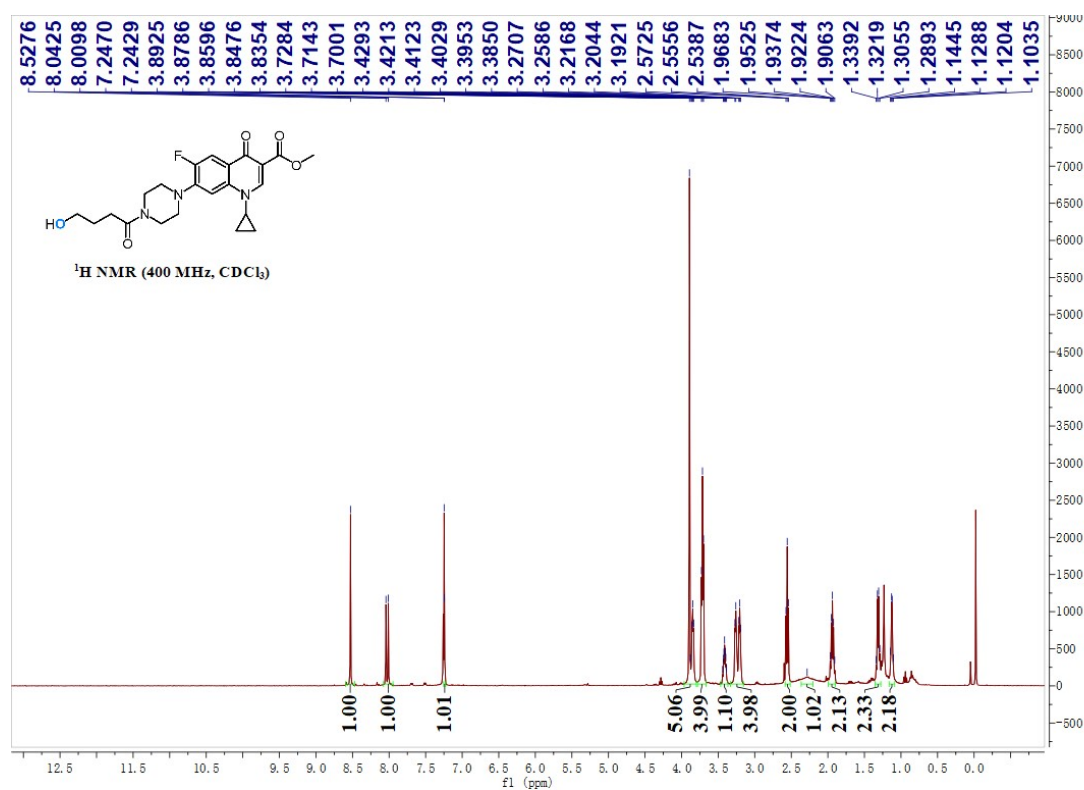


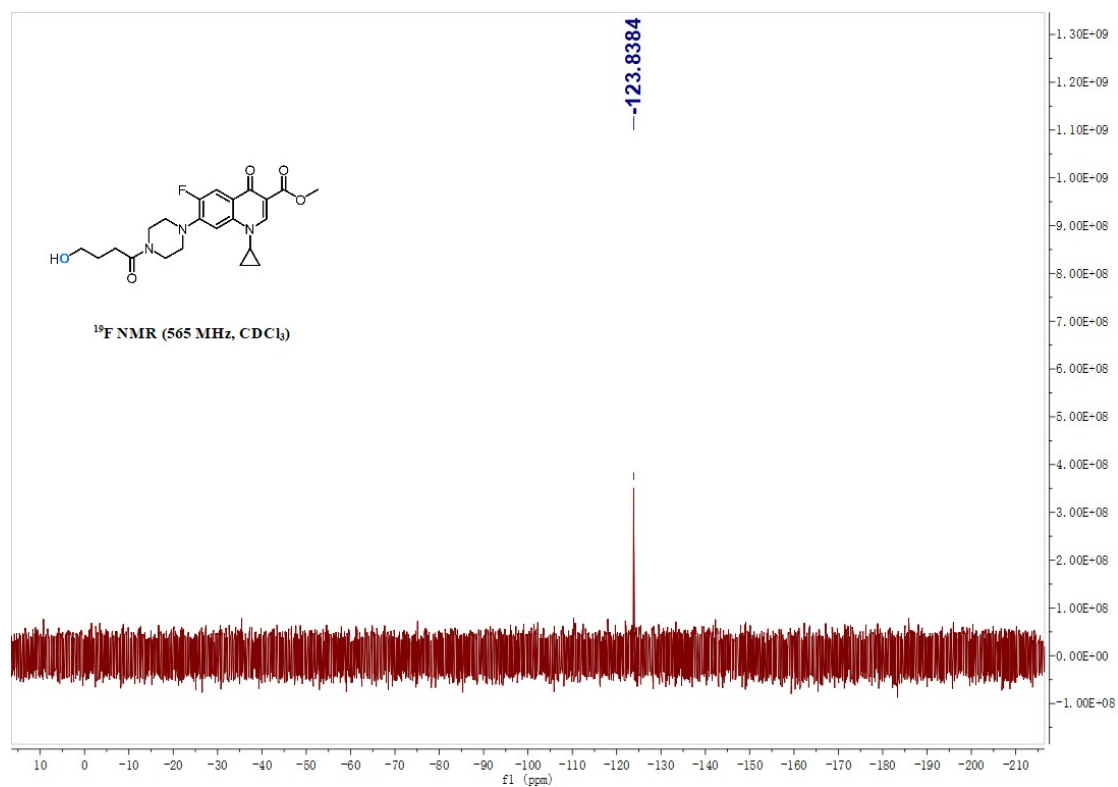
<sup>1</sup>H and <sup>13</sup>C NMR spectra of compound 3ae



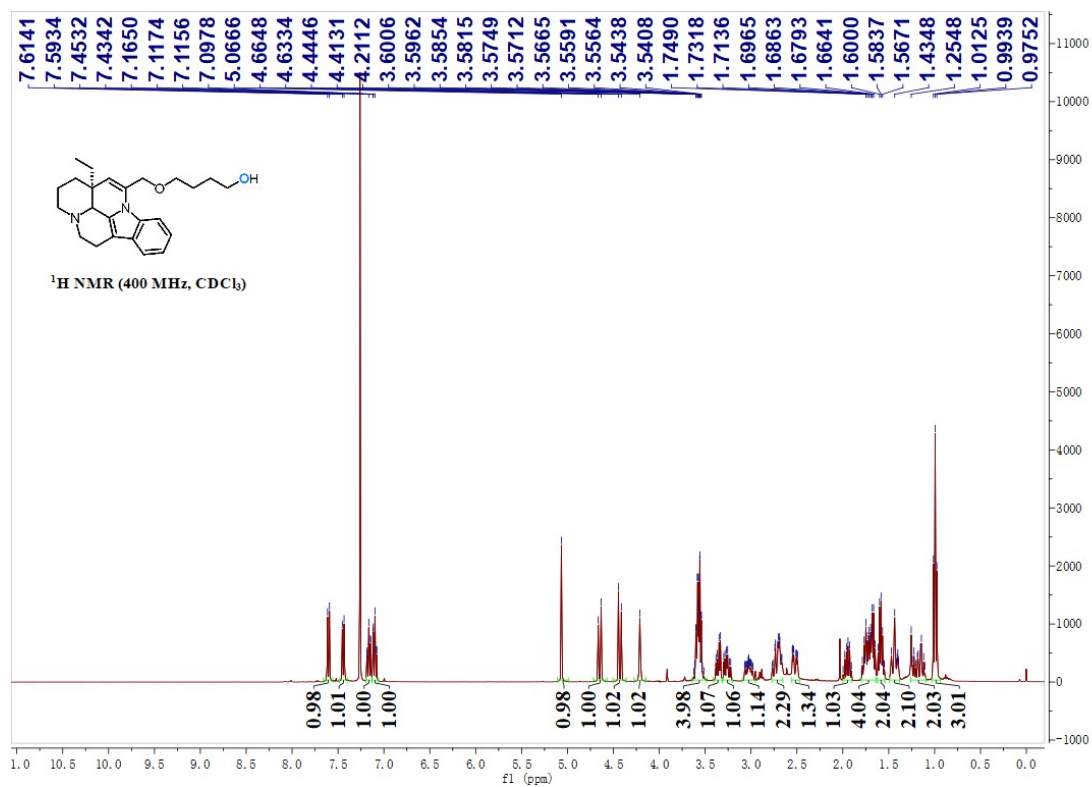


<sup>1</sup>H, <sup>13</sup>C and <sup>19</sup>F NMR spectra of compound **3af**

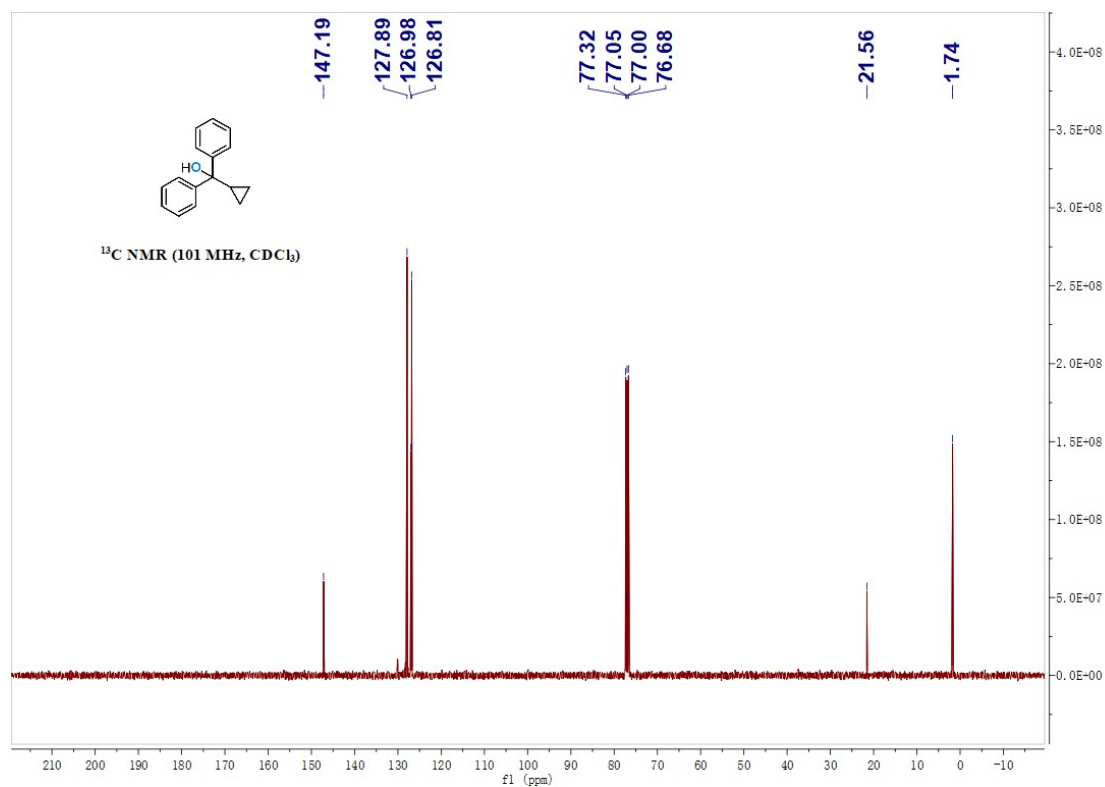




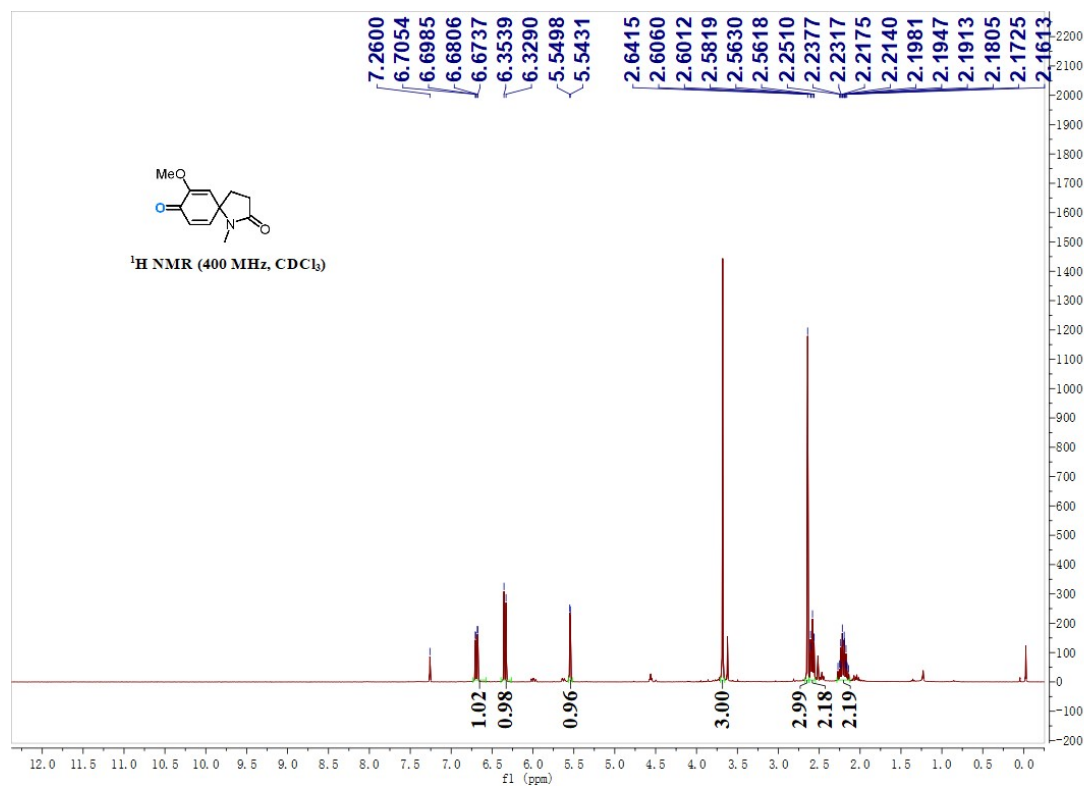
**<sup>1</sup>H and <sup>13</sup>C NMR spectra of compound **3ag****

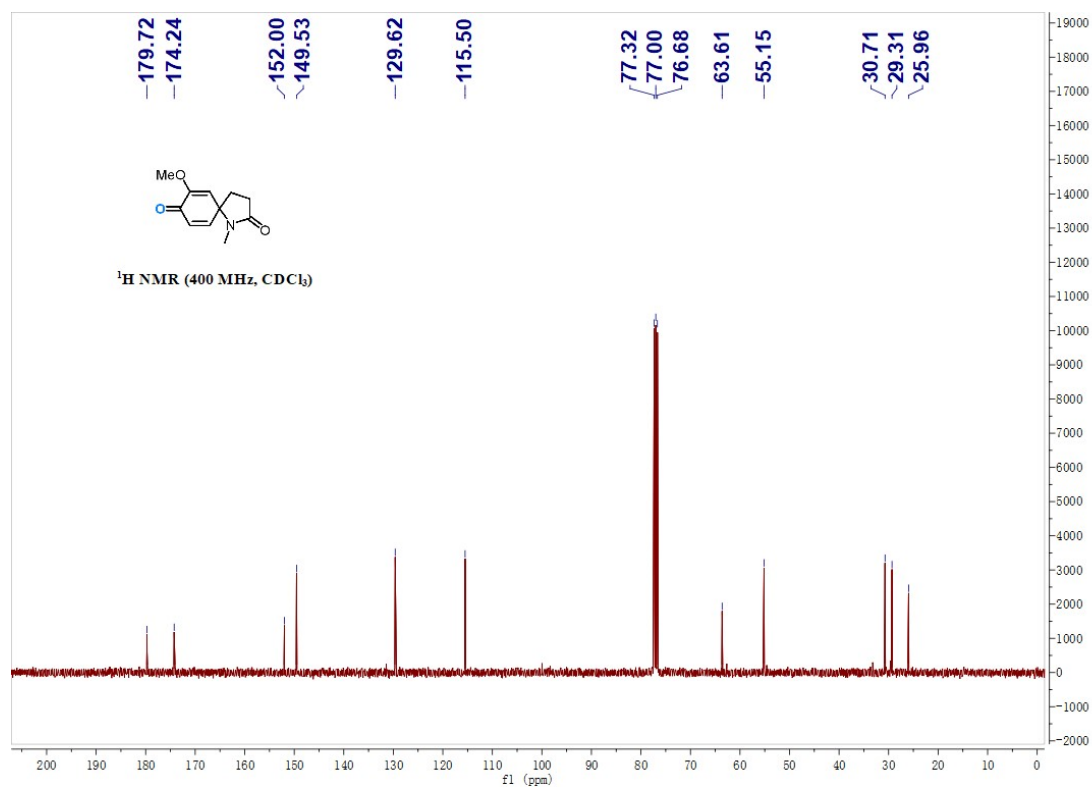




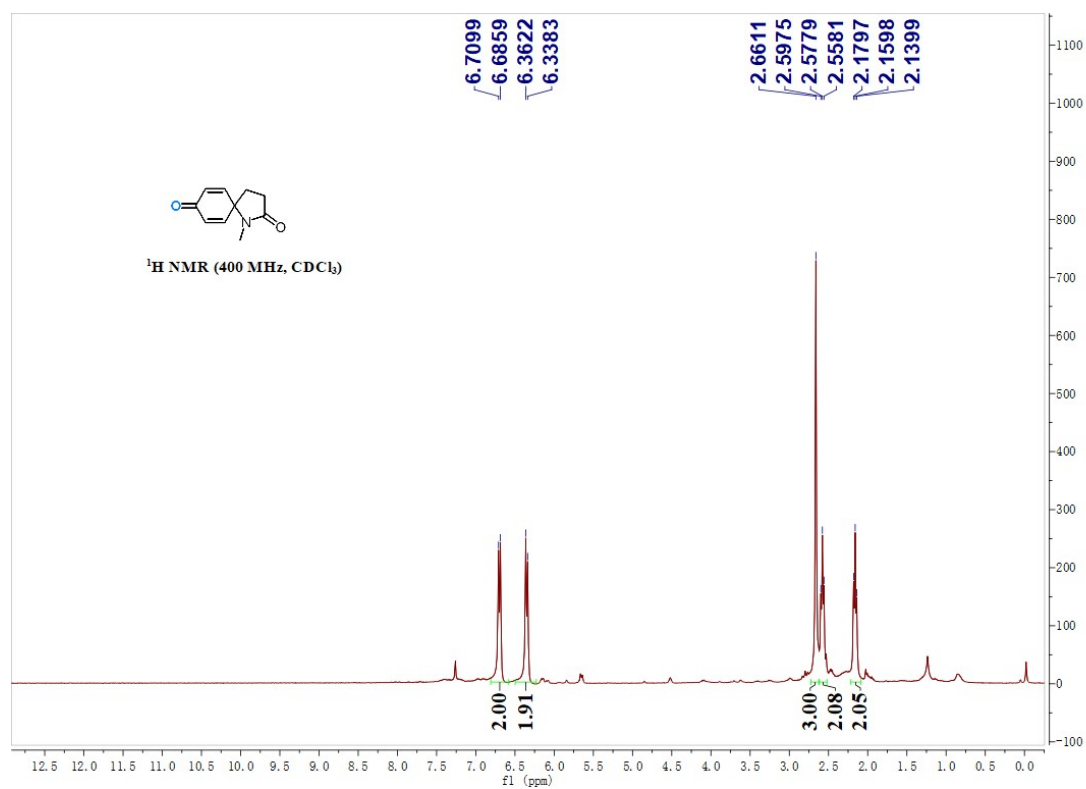


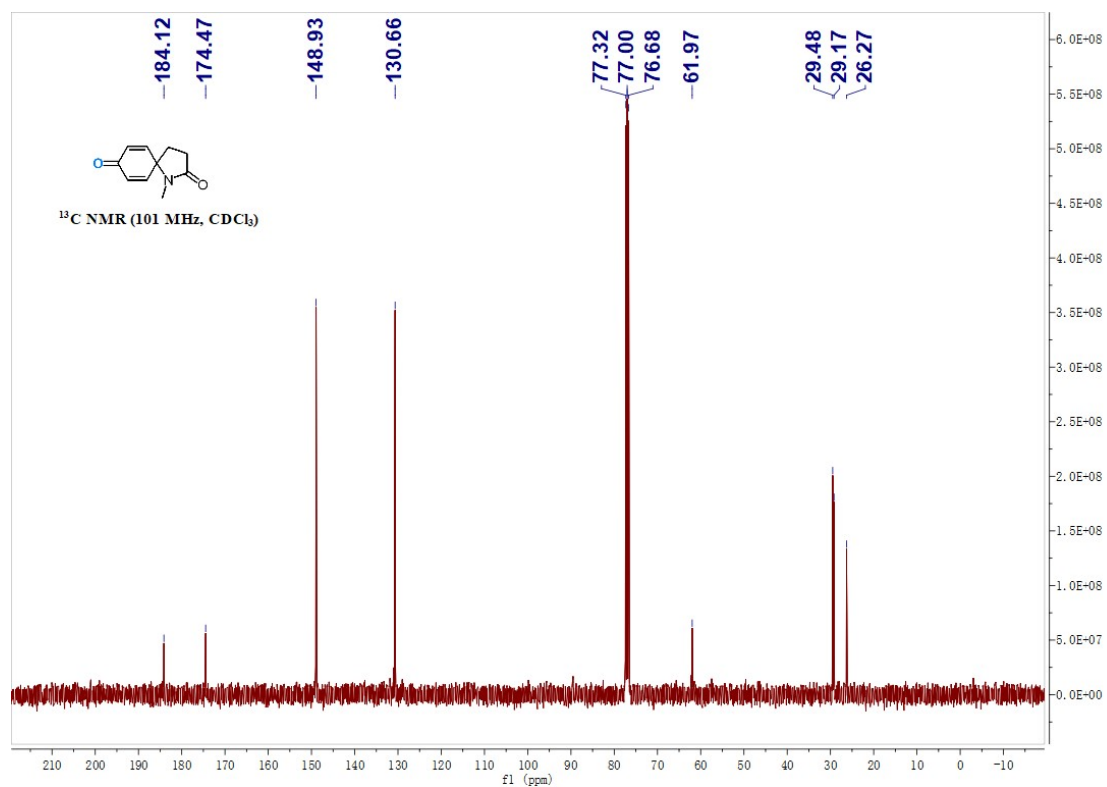
<sup>1</sup>H and <sup>13</sup>C NMR spectra of compound **3ai**



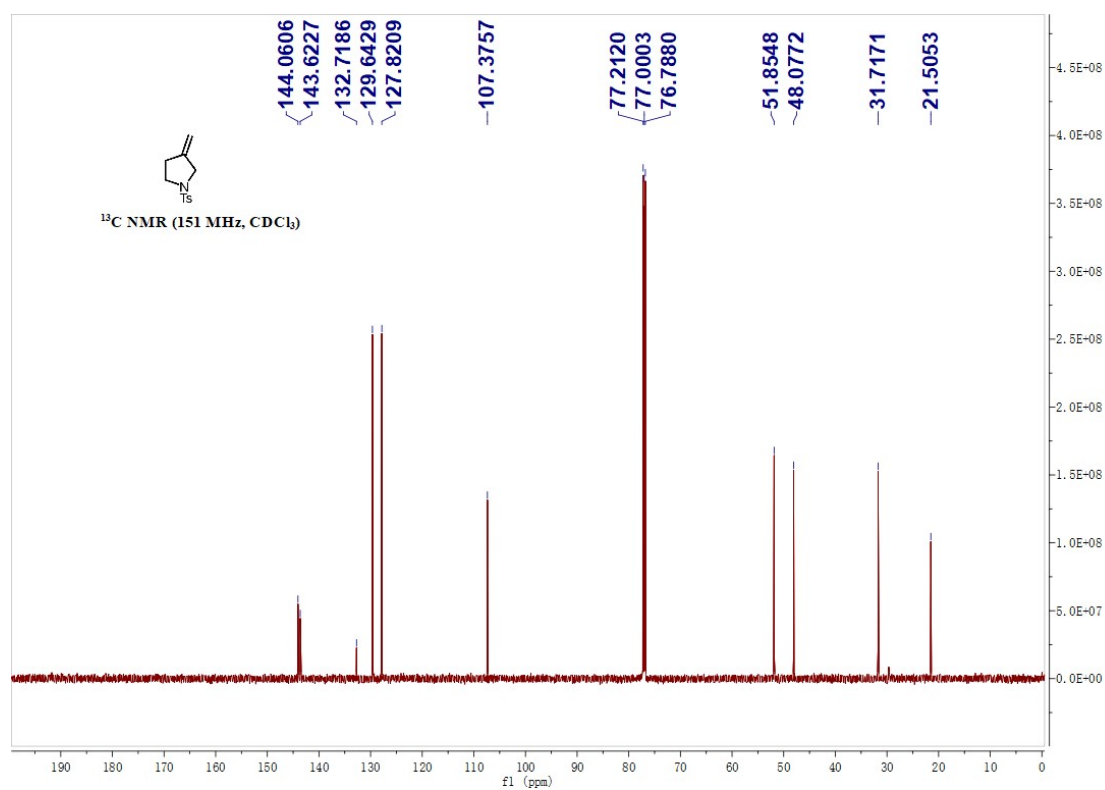
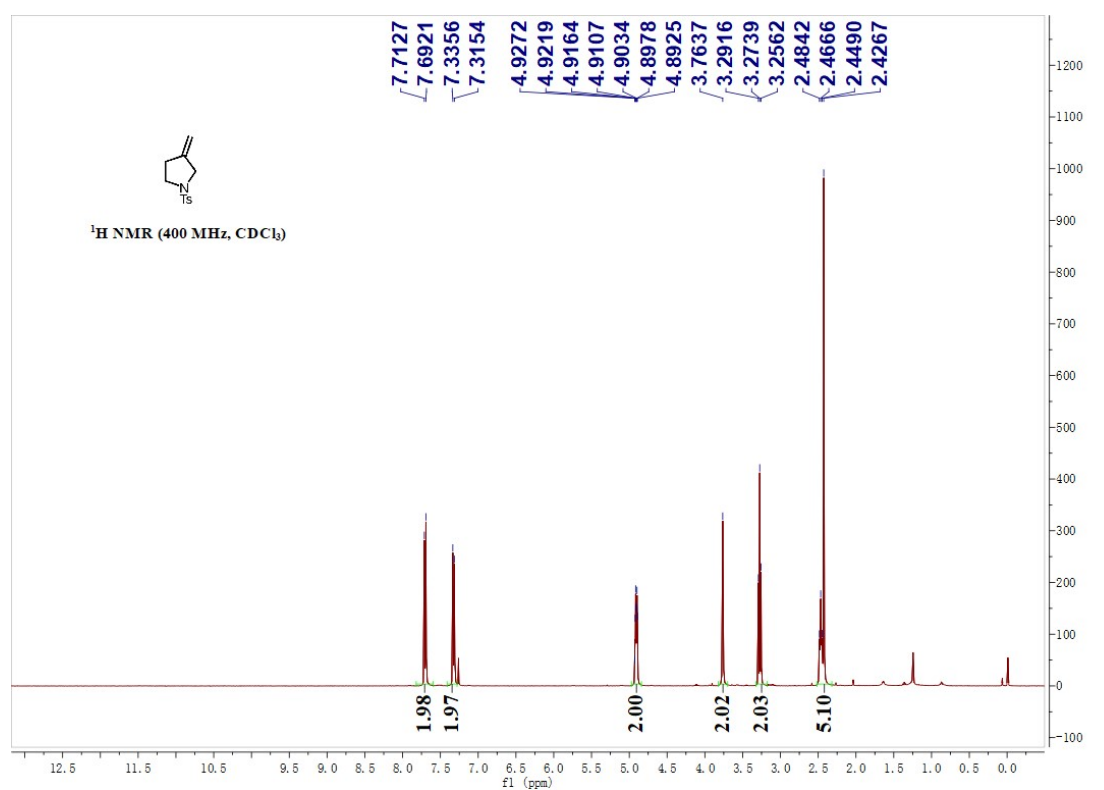


$^1\text{H}$  and  $^{13}\text{C}$  NMR spectra of compound **3aj**



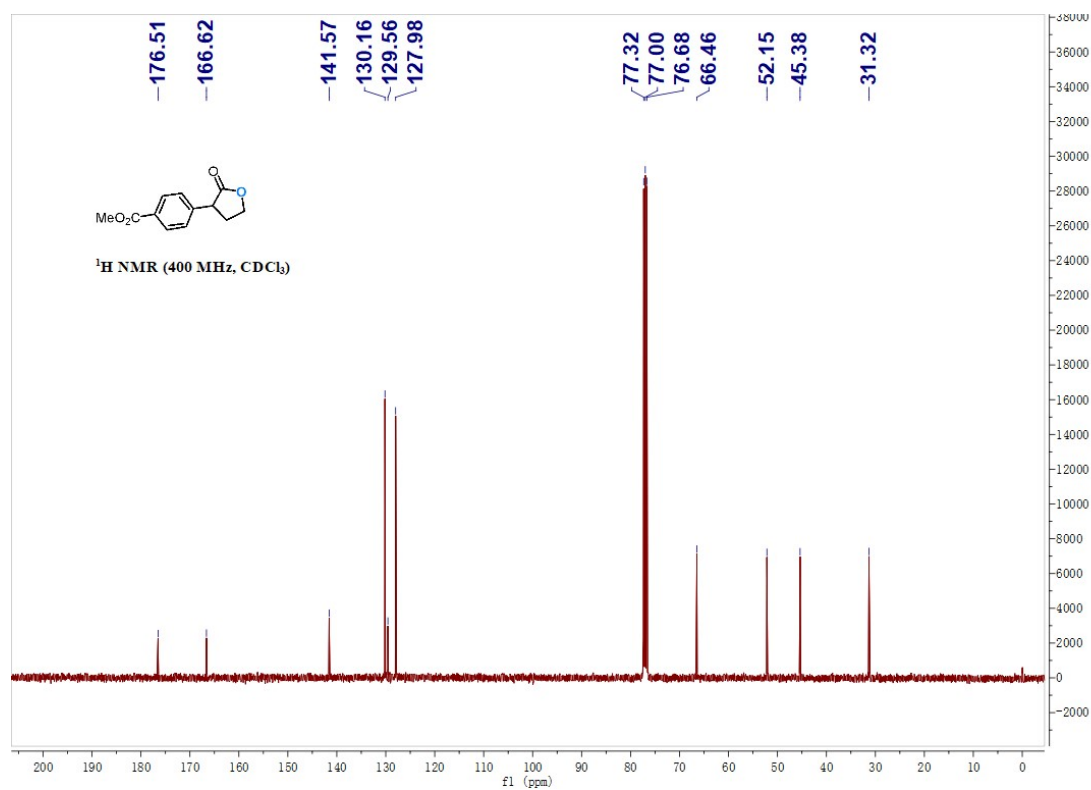
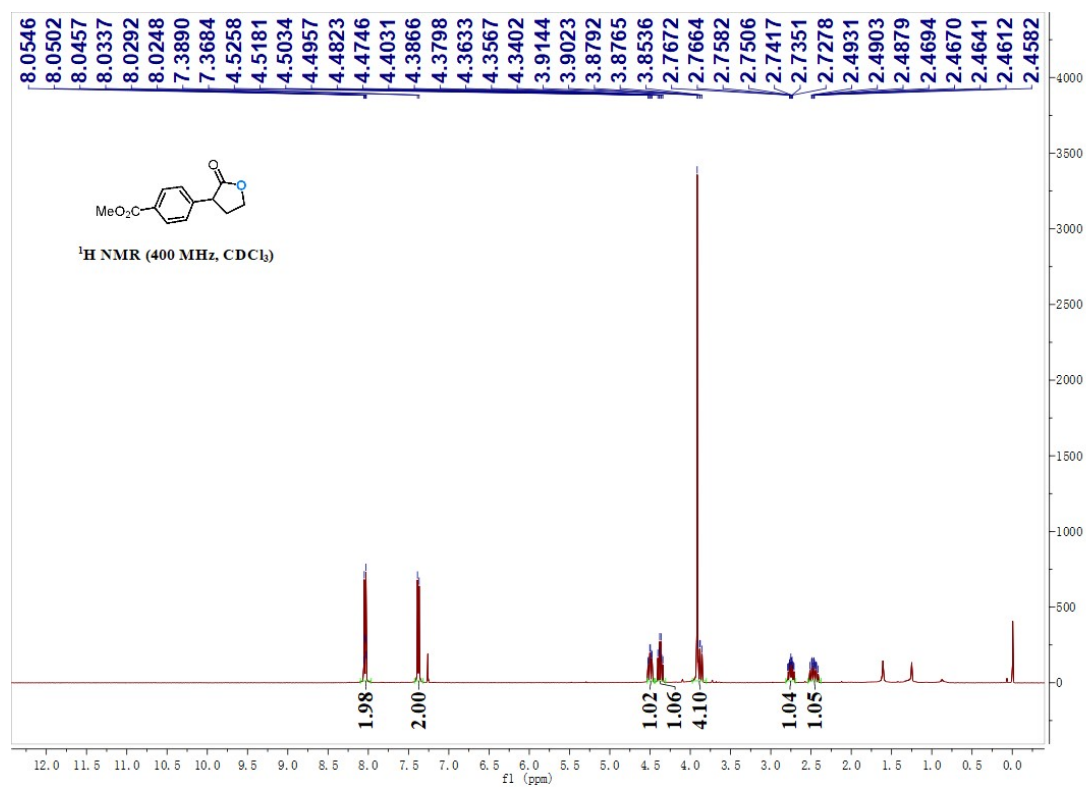


<sup>1</sup>H and <sup>13</sup>C NMR spectra of compound **3ak**

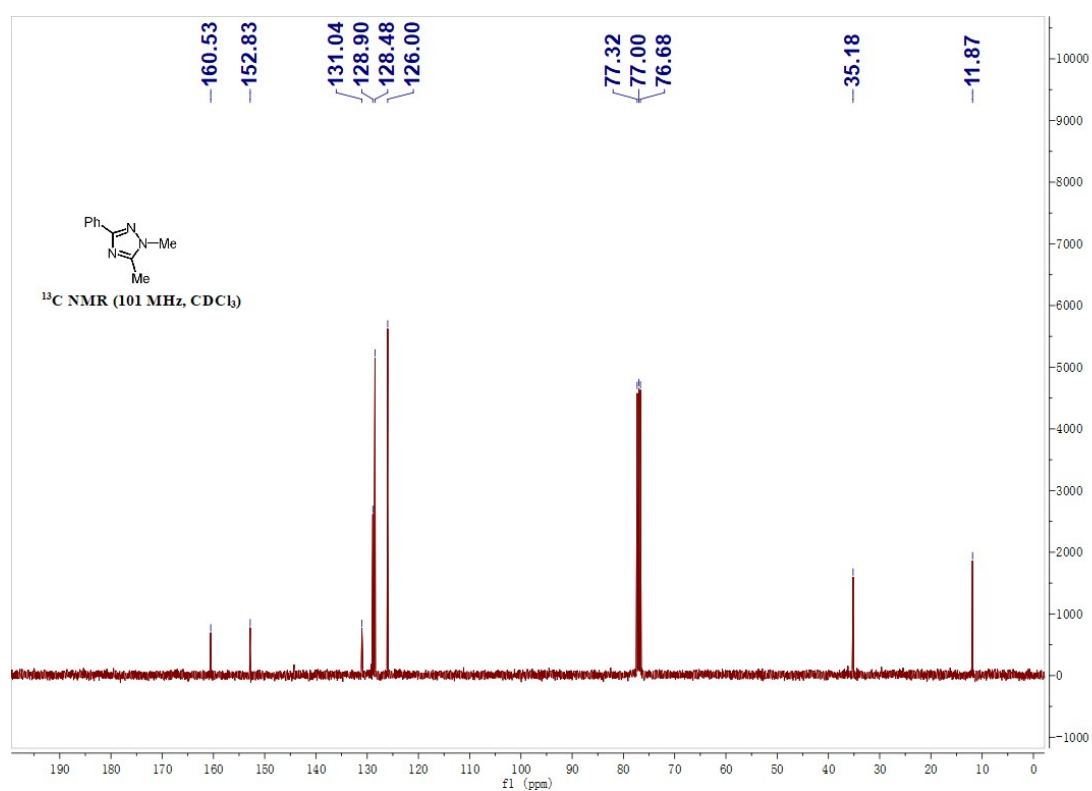
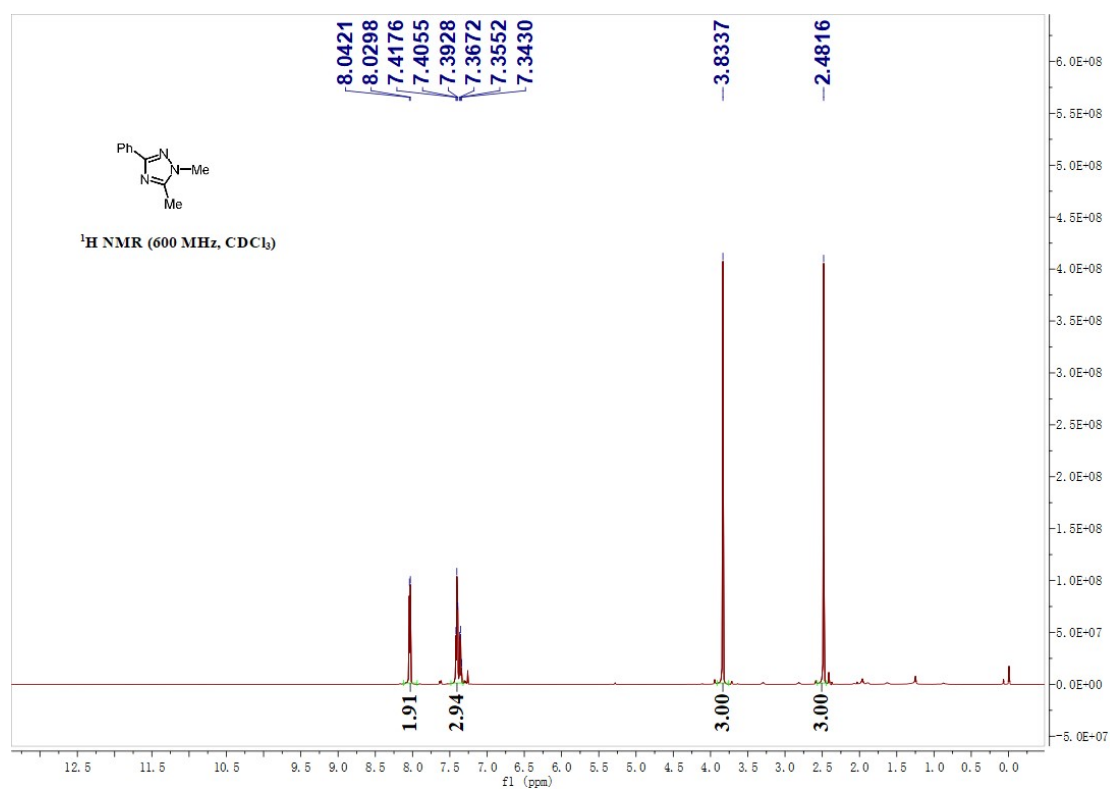


$^1\text{H}$  and  $^{13}\text{C}$  NMR spectra of compound **3al**

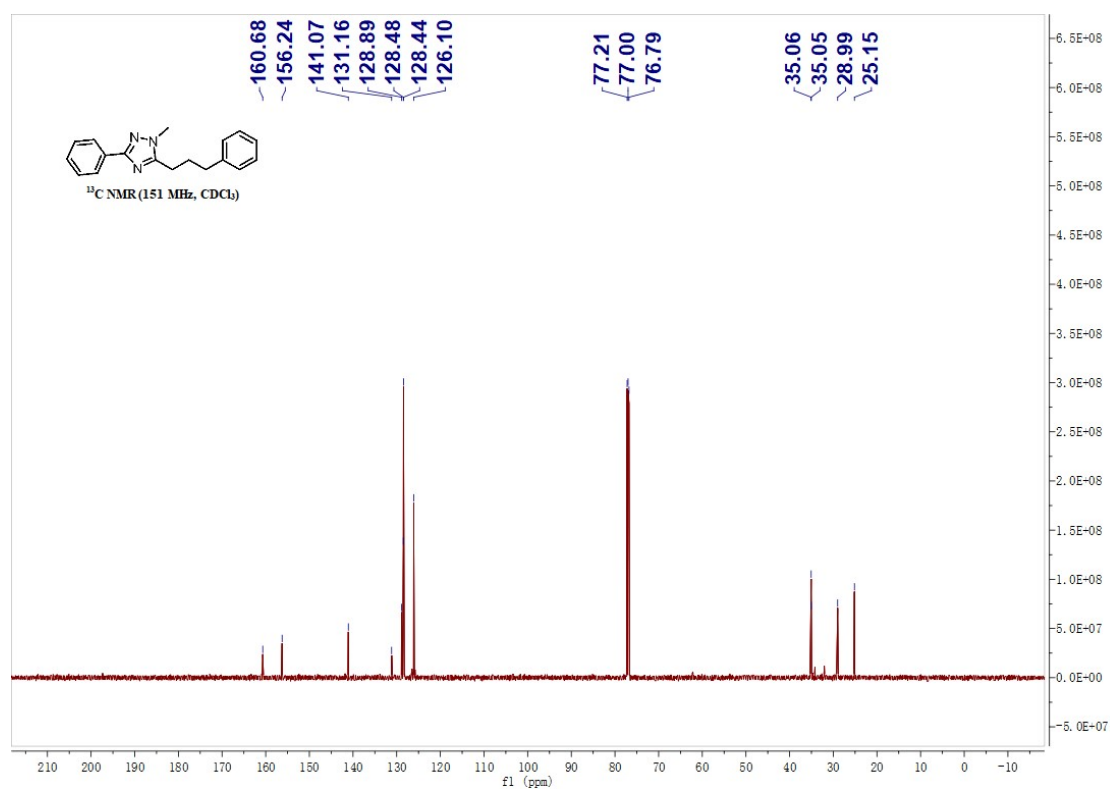
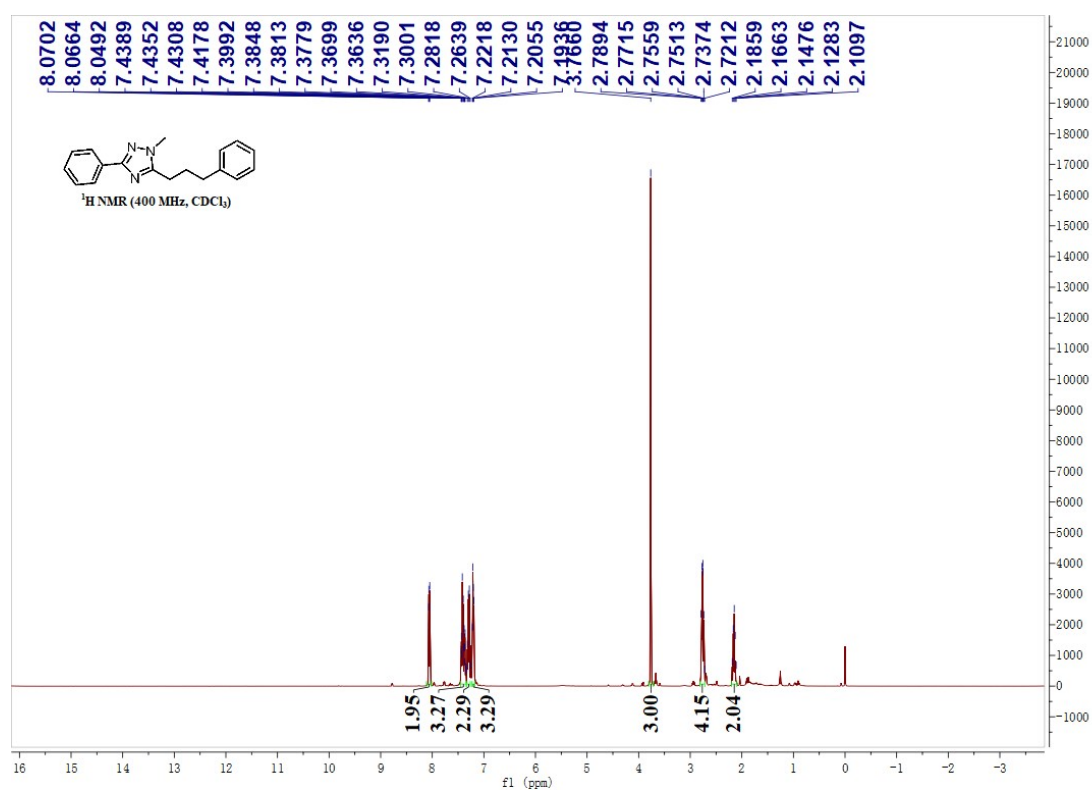




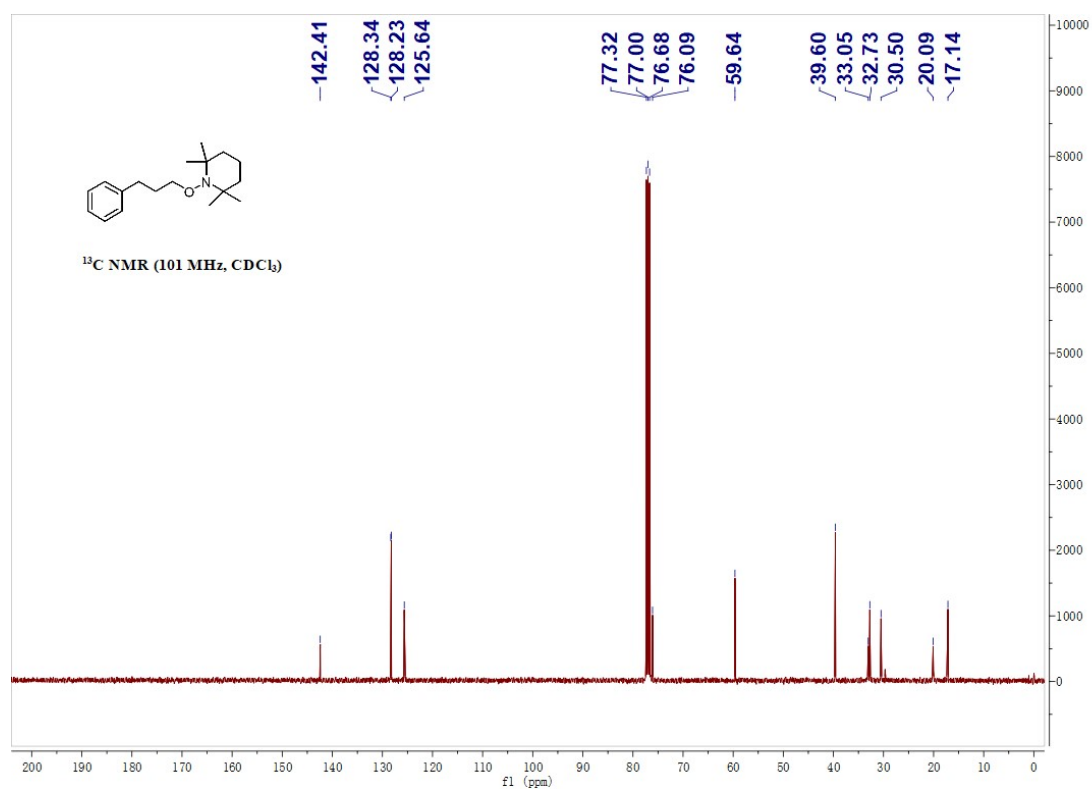
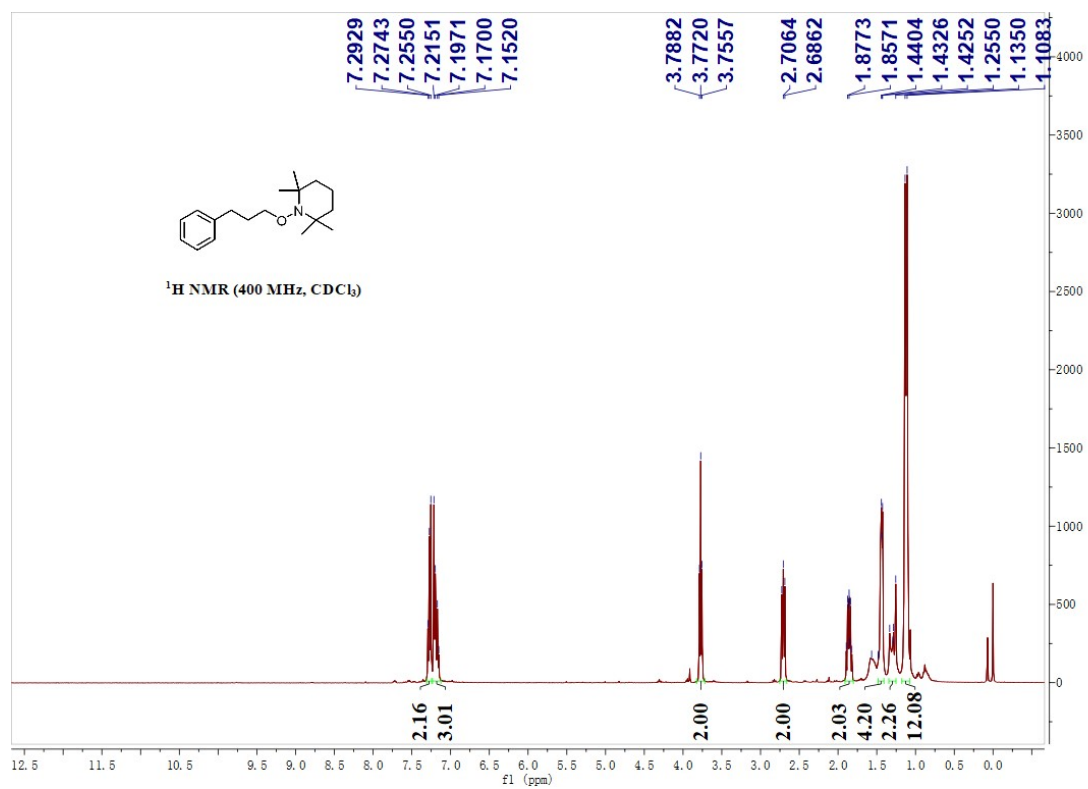
# <sup>1</sup>H and <sup>13</sup>C NMR spectra of compound 4



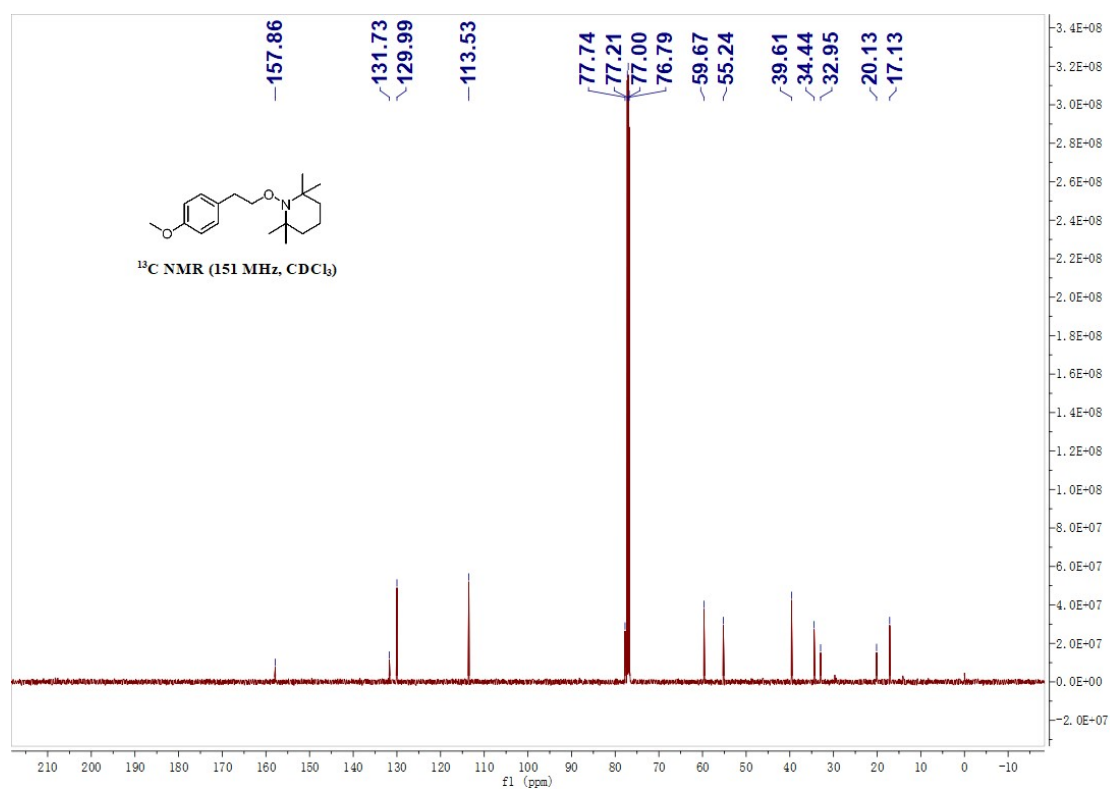
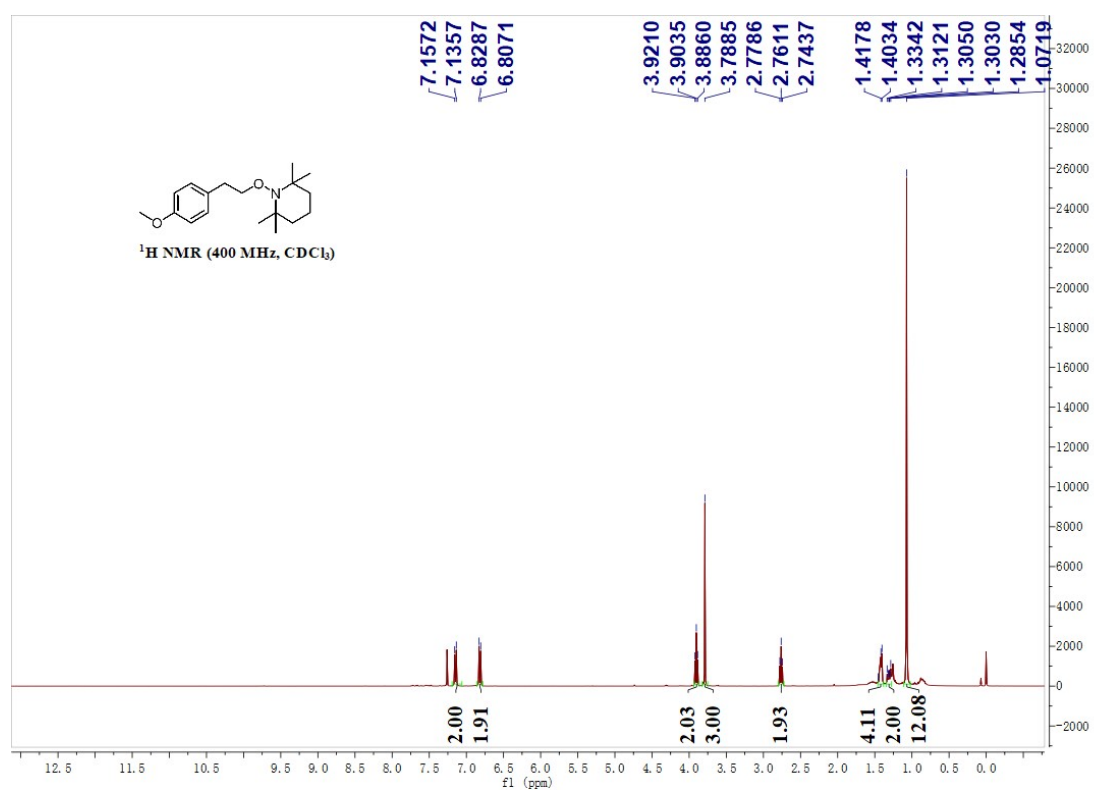
# <sup>1</sup>H and <sup>13</sup>C NMR spectra of compound 5



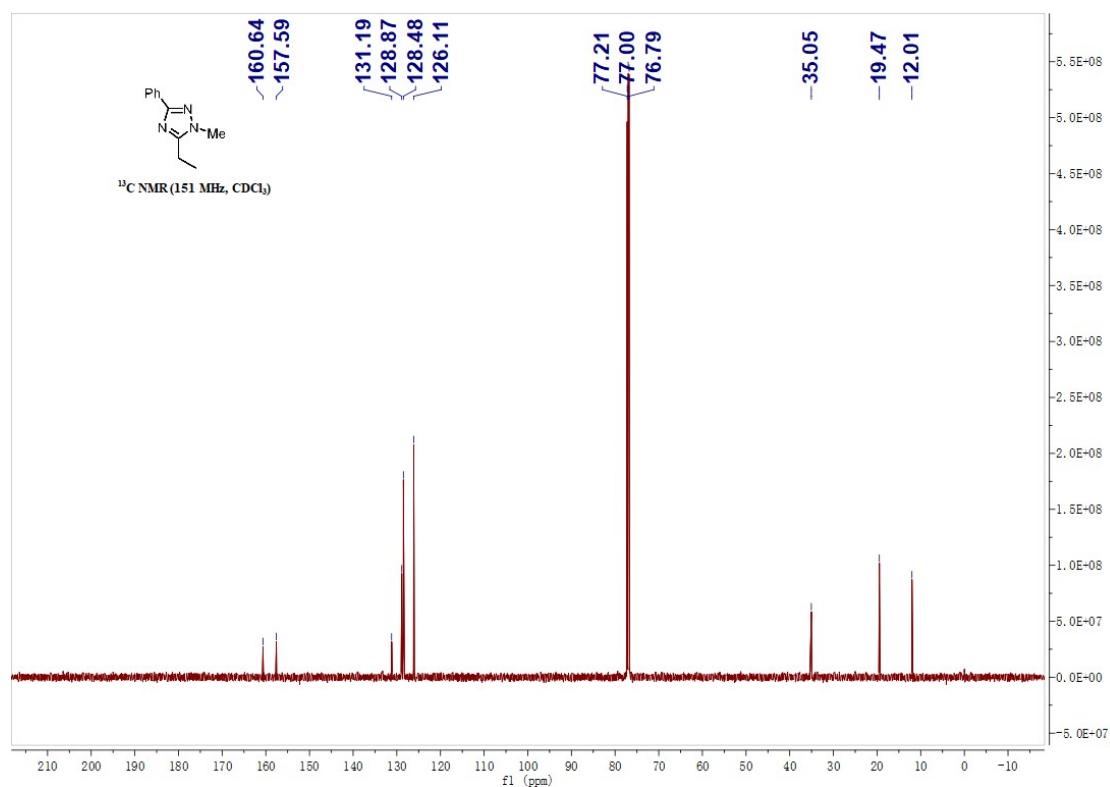
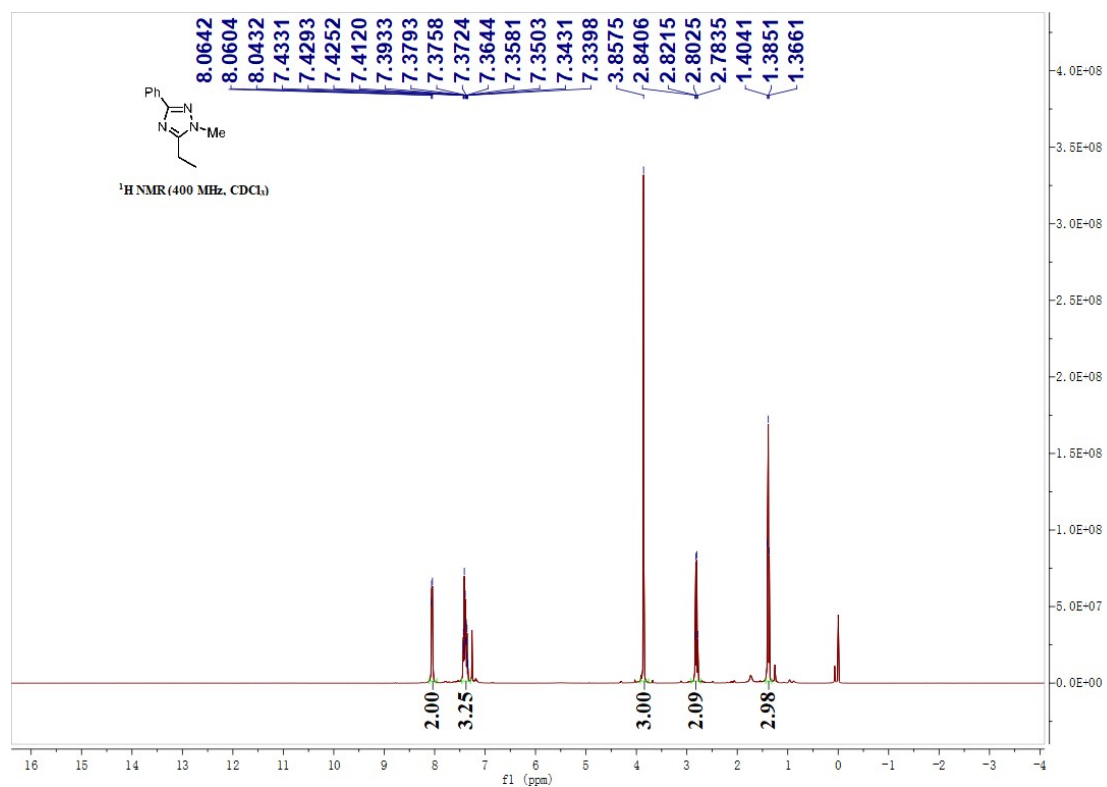
<sup>1</sup>H and <sup>13</sup>C NMR spectra of compound 6



<sup>1</sup>H and <sup>13</sup>C NMR spectra of compound **9**



<sup>1</sup>H and <sup>13</sup>C NMR spectra of compound 14



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