

## Supporting Information

# Brønsted acid enabled metal-free remote oxygenation and amidation of unstrained C–C bonds *via* 1,4-heteroaryl migration chaperoned radical-polar crossover

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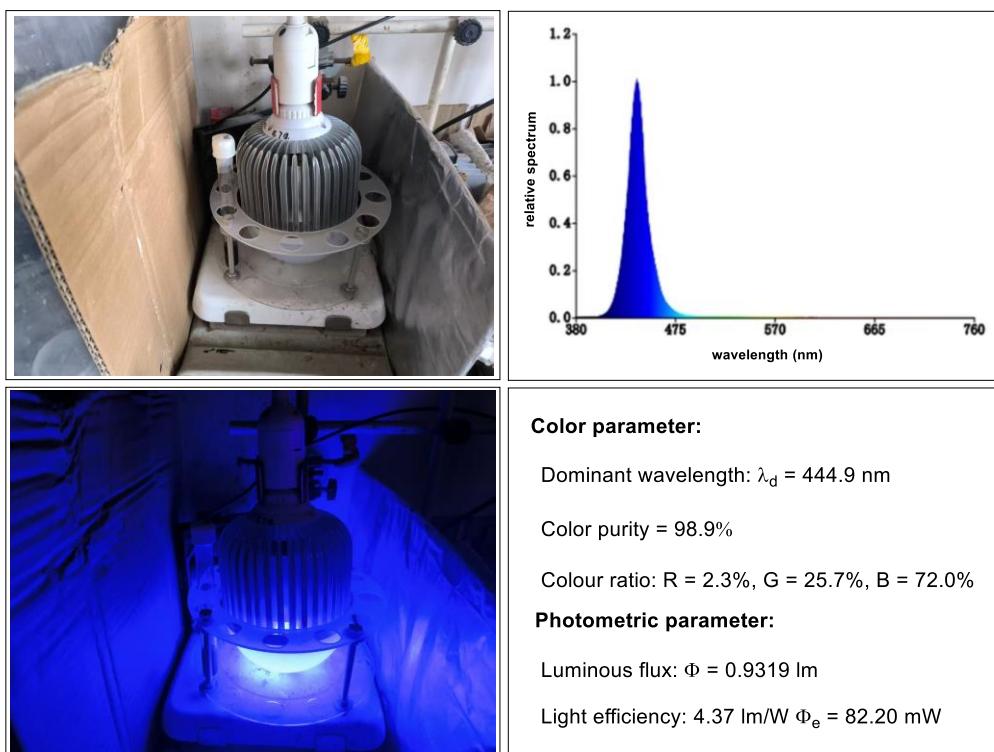
E-mail: [shiyun210@163.com](mailto:shiyun210@163.com); [ygzhu@njau.edu.cn](mailto:ygzhu@njau.edu.cn); [kchen@njau.edu.cn](mailto:kchen@njau.edu.cn)

## Table of Contents

1. General information.....	S2
2. General procedure for remote oxygenation and amidation of unstrained C–C bonds <i>via</i> 1,4-group migration.....	S3
3. X-Ray single crystal diffraction analysis of the products <b>2g</b> and <b>3i</b> .....	S9
4. Synthetic applications.....	S11
5. Mechanistic studies.....	S12
6. Characterization data.....	S17
7. References.....	S41
8. NMR spectra.....	S42

## 1.General information

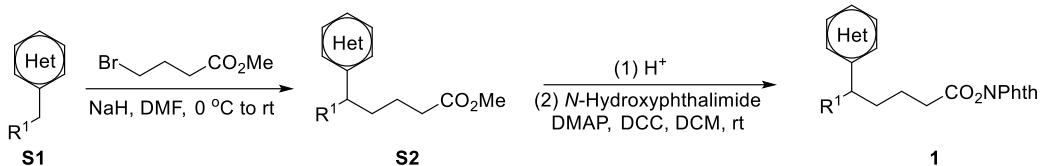
All commercially available reagents were used without further purification. Column chromatography was performed on silica gel (200-300 mesh).  $^1\text{H}$  NMR,  $^{13}\text{C}$  NMR, and  $^{19}\text{F}$  NMR spectra were recorded on Bruker 400 MHz and JOEL 500 MHz NMR spectrometers. Chemical shifts ( $\delta$ ) were reported in ppm, and coupling constants ( $J$ ) were given in Hertz (Hz). Data were reported as s = singlet, d = doublet, t = triplet, q = quartet, dd = doublet of doublets, br = broad, m = multiplet. High-resolution mass spectra (HRMS) were recorded on an AB SCIEX Triple ESI-TOF 5600+ mass spectrometer. The electrochemical measurements were carried out on a CS2350M electrochemical workstation (Wuhan Corrttest Instrument Co., Ltd). The 15W and 36 W blue LED lamp ( $\lambda_{\text{max}} = 445 \text{ nm}$ ) was manufactured by Hongye Photoelectricity Co., Ltd. Photo reactions were carried out in 20 mL reaction tubes at the distance of 2.0 cm from the LED lamp. An electronic fan is equipped to maintain the reaction temperature could in a range of  $30 \pm 2^\circ\text{C}$ .



**Figure S1.** The spectrum of the lamp and the visible-light irradiation instrument

## 2. General procedure for remote oxygenation and amidation of unstrained C–C bonds *via* 1,4-group migration

## 2.1 Procedure for the synthesis of substrates 1<sup>[1]</sup>



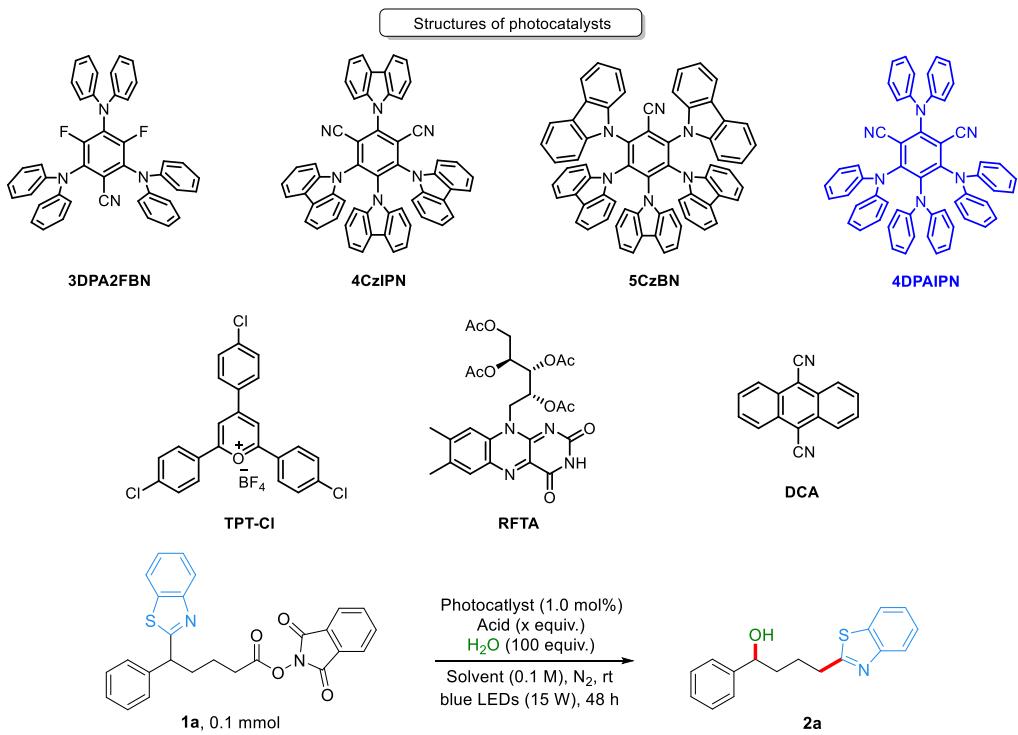
To a 100 mL oven-dried round-bottomed flask equipped with a stirring bar was charged with NaH (800 mg, 20 mmol, 60% suspension in mineral oil), DMF (20 mL) were added under N<sub>2</sub> atmosphere. The aryl acetonitrile and heteroaryl acetonitrile (10 mmol) were added dropwise after the mixture was cooled down by ice bath. Then the reaction mixture was warmed to room temperature and stirred 1 h, the **S1** (15 mmol) were added under the same conditions as above. After stirring at room temperature for 16 h, the reaction mixture was quenched with NH<sub>4</sub>Cl (20 mL), and extracted with EtOAc (20 mL × 3). The combined organic layers were washed with brine (20 mL), dried over Na<sub>2</sub>SO<sub>4</sub>, the crude product was further purified by flash chromatography to give the ester **S2**.

To a round-bottomed flask equipped with a magnetic stir bar were added **S2** (10.0 mmol) and EtOH (20 mL). Then the KOH solution (5.0 mL, 6.0 M) was added dropwise, and the reaction mixture was stirred at rt for 12 h. After that, the reaction mixture was brought to pH = 2 ~ 4 with HCl (6.0 M), and extracted with EtOAc (10 mL × 3). The combined organic layers were washed with brine (10 mL), dried over Na<sub>2</sub>SO<sub>4</sub>, and concentrated under reduced pressure. The crude product was further purified by flash chromatography to give corresponding acids.

To the acid (10 mmol) were added *N*-hydroxyphthalimide (15 mmol), *N,N*-dimethylpyridine (1.0 mmol), *N,N*-dicyclohexylcarbodiimide (15 mmol), and CH<sub>2</sub>Cl<sub>2</sub> (10 mL). The reaction mixture was stirred at rt for 12 h. After that, the mixture was filtered through a pad of silica gel and rinsed with CH<sub>2</sub>Cl<sub>2</sub>. The filtrate was concentrated under reduced pressure. The residue was purified by column chromatography on silica gel to afford substrates 1.

## 2.2 Optimization of reaction conditions

**Table S1.** Screening of photocatalysts, acids and solvents<sup>a</sup>

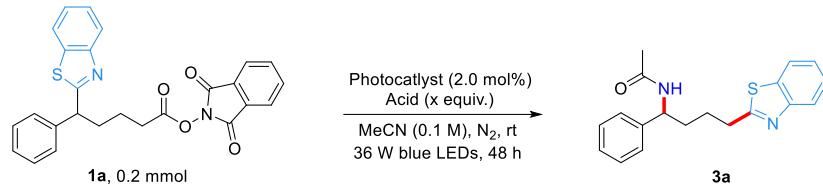


Entry	Photocatalysts	Acids (x equiv.)	Solvent	Yield (%) <sup>b</sup>
1	3DPA2FBN	TsOH•H <sub>2</sub> O (2.0)	MeCN	23
2	4CzIPN	TsOH•H <sub>2</sub> O (2.0)	MeCN	42
3	5CzBN	TsOH•H <sub>2</sub> O (2.0)	MeCN	n.d.
4	4DPAIPN	TsOH•H <sub>2</sub> O (2.0)	MeCN	60
5	TPT-Cl	TsOH•H <sub>2</sub> O (2.0)	MeCN	n.d.
6	RFTA	TsOH•H <sub>2</sub> O (2.0)	MeCN	n.d.
7	DCA	TsOH•H <sub>2</sub> O (2.0)	MeCN	n.d.
8	4DPAIPN	H <sub>3</sub> PO <sub>4</sub> (2.0)	MeCN	38
9	4DPAIPN	TFA (2.0)	MeCN	42
10	4DPAIPN	HBF <sub>4</sub> (2.0)	MeCN	48
11	4DPAIPN	TsOH•H <sub>2</sub> O (1.0)	MeCN	40
12	4DPAIPN	TsOH•H <sub>2</sub> O (3.0)	MeCN	77
13	4DPAIPN	TsOH•H <sub>2</sub> O (3.0)	DMSO	30
14	4DPAIPN	TsOH•H <sub>2</sub> O (3.0)	THF	34
15	4DPAIPN	TsOH•H <sub>2</sub> O (3.0)	EtOAC	53

16	4DPAIPN	TsOH•H <sub>2</sub> O (3.0)	DMF	47
17	4DPAIPN	TsOH•H <sub>2</sub> O (3.0)	Acetone	45
18	-	TsOH•H <sub>2</sub> O (3.0)	MeCN	n.d.
19	4DPAIPN	-	MeCN	n.d.
20 <sup>c</sup>	4DPAIPN	TsOH•H <sub>2</sub> O (3.0)	MeCN	n.d.
21 <sup>d</sup>	4DPAIPN	TsOH•H <sub>2</sub> O (3.0)	MeCN	n.d.

<sup>a</sup>Reaction conditions: **1a** (0.1 mmol), photocatalyst (1.0 mol%), acid (x equiv.), H<sub>2</sub>O (100 equiv.), solvent (1.0 mL), room temperature, N<sub>2</sub>, under blue LEDs (15 W) irradiation for 48 h. <sup>b</sup>Isolated yields were reported. <sup>c</sup>Without light. <sup>d</sup>Under air atmosphere. n.d.= not detected.

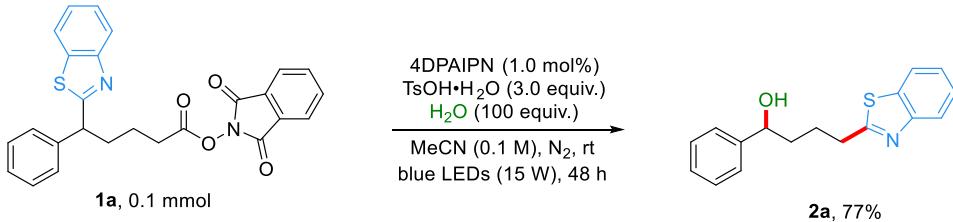
**Table S2.** Screening of photocatlysts and acids<sup>a</sup>



Entry	Photocatlysts	Acids (x equiv.)	Solvent	Yield (%) <sup>b</sup>
1 <sup>c</sup>	4DPAIPN	TsOH•H <sub>2</sub> O (2.0)	MeCN	49
2	4DPAIPN	TsOH•H <sub>2</sub> O (2.0)	MeCN	55
3	4DPAIPN	TsOH•H <sub>2</sub> O (1.0)	MeCN	37
4	4DPAIPN	TsOH•H <sub>2</sub> O (3.0)	MeCN	52
5	3DPA2FBN	TsOH•H <sub>2</sub> O (2.0)	MeCN	40
6	4CzIPN	TsOH•H <sub>2</sub> O (2.0)	MeCN	31
7	5CzBN	TsOH•H <sub>2</sub> O (2.0)	MeCN	39
8 <sup>d</sup>	4DPAIPN	TsOH•H <sub>2</sub> O (2.0)	MeCN	45
9 <sup>e</sup>	4DPAIPN	TsOH•H <sub>2</sub> O (2.0)	MeCN	51
10	4DPAIPN	TFA (2.0)	MeCN	46
11	4DPAIPN	H <sub>3</sub> PO <sub>4</sub> (2.0)	MeCN	54
12	4DPAIPN	HBF <sub>4</sub> (2.0)	MeCN	52
13	4DPAIPN	MeSO <sub>3</sub> H (2.0)	MeCN	60
14	-	MeSO <sub>3</sub> H (2.0)	MeCN	n.d.
15	4DPAIPN	-	MeCN	n.d.
16 <sup>f</sup>	4DPAIPN	MeSO <sub>3</sub> H (2.0)	MeCN	n.d.

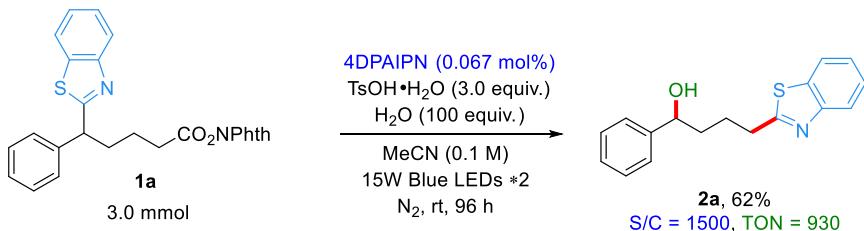
<sup>a</sup>Reaction conditions: **1a** (0.2 mmol), photocatalyst (2.0 mol%), acid (x equiv.), MeCN (0.1 M), room temperature, N<sub>2</sub>, under blue LEDs (36 W) irradiation for 48 h. <sup>b</sup>Isolated yields were reported. <sup>c</sup>Under blue LEDs (15 W) irradiation for 48 h. <sup>d</sup>MeCN (0.05 M). <sup>e</sup>MeCN (0.2 M). <sup>f</sup>In the dark. n.d.= not detected.

### 2.3 General procedure for remote oxygenation of NHPI esters *via* 1,4-group migration



To a 20 mL test tube flask equipped with a stirring bar was charged with **1a** (45.7 mg, 0.1 mmol), 4DPAIPN (0.8 mg, 1.0 mol%) and TsOH•H<sub>2</sub>O (57.1 mg, 3.0 equiv.) under N<sub>2</sub> atmosphere. Then, H<sub>2</sub>O (180 mg, 10 mmol, 0.18 mL) and MeCN (1.0 mL) were added *via* a syringe. The reaction vessel was exposed to blue LED (450-455 nm, 15 W) irradiation at room temperature stirring for 48 h. After completion of the reaction, the reaction mixture was diluted with EtOAc (10 mL), and washed with saturated aq. NaHCO<sub>3</sub> (10 mL). The aqueous layer was extracted by EtOAc (10 mL × 2). The combined organic phase was dried over anhydrous Na<sub>2</sub>SO<sub>4</sub> and then concentrated in *vacuo*. The residue was further purified by flash chromatography (silica gel, petroleum ether/ethyl acetate/triethylamine = 10:1:0.1, V/V/V) to give the product **2a** (21.8 mg, 77%).

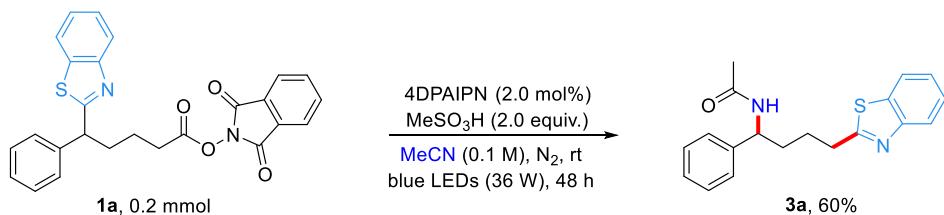
### 2.4 Procedure for a scale-up reaction of **1a**



To a 100 mL round bottom flask equipped with a stirring bar was charged with **1a** (1.370 g, 3.0 mmol), 4DPAIPN (1.6 mg, 0.02 mmol) and TsOH•H<sub>2</sub>O (1.712 g, 3.0 equiv.) under N<sub>2</sub> atmosphere. Then, H<sub>2</sub>O (5.4 g, 300 mmol, 5.4 mL) and MeCN (30 mL) were added *via* a syringe. The reaction vessel was exposed to blue LED (450-455 nm,

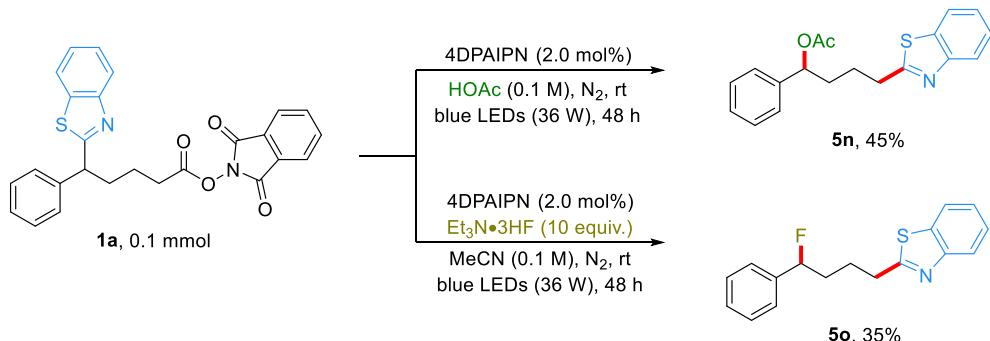
15 W×2) irradiation at room temperature stirring for 96 h. After completion of the reaction, MeCN was removed in *vacuo*, and the residue was diluted with EtOAc (30 mL), and washed with saturated aq. NaHCO<sub>3</sub> (15 mL). The aqueous layer was extracted by EtOAc (15 mL×2). The combined organic phase was dried over anhydrous Na<sub>2</sub>SO<sub>4</sub> and then concentrated in *vacuo*. The crude product was further purified by flash chromatography (silica gel, petroleum ether/ethyl acetate/triethylamine = 10:1:0.1, V/V/V) to give the product **2a** (527 mg, 62%).

## 2.5 General procedure for remote amidation of NHPI esters *via* 1,4-group migration



To a 20 mL test tube flask equipped with a stirring bar was charged with **1a** (91.3 mg, 0.2 mmol), 4DPAIPN (3.2 mg, 2.0 mol%) and MeSO<sub>3</sub>H (38.4 mg, 2.0 equiv.) dissolved in MeCN (2.0 mL) under N<sub>2</sub> atmosphere. The reaction vessel was exposed to blue LED (450-455 nm, 36 W) irradiation at room temperature stirring for 48 h. After completion of the reaction, the crude mixture was concentrated in *vacuo*. The residue was further purified by flash chromatography for two times (silica gel, petroleum ether/ethyl acetate/triethylamine = 2:1:0.02, V/V/V and afterwards DCM/MeOH = 100:1, V/V) to give the product **3a** (38.9 mg, 60%).

## 2.6 General procedure for remote functionalization of NHPI esters with HOAc and Et<sub>3</sub>N•3HF as nucleophiles



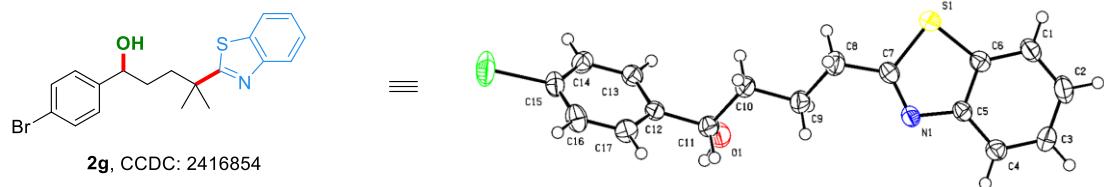
**HOAc as the nucleophile:**

To a 20 mL test tube flask equipped with a stirring bar were charged with **1a** (45.7 mg, 0.1 mmol) and 4DPAIPN (1.6 mg, 2.0 mol%) under N<sub>2</sub> atmosphere. Then HOAc (1.0 mL) was added *via* a syringe. The reaction vessel was exposed to blue LED (450-455 nm, 36 W) irradiation at room temperature stirring for 48 h. After completion of the reaction, the AcOH was removed in *vacuo*. The residue was further purified by flash chromatography (silica gel, petroleum ether/ethyl acetate = 20:1, V/V) to give the product **5n** (14.6 mg, 45%).

**Et<sub>3</sub>N•3HF as the nucleophile:**

To two 20 mL test tube flasks equipped with a stirring bar were charged with **1a** (45.7 mg, 0.1 mmol), 4DPAIPN (1.6 mg, 2.0 mol%) under N<sub>2</sub> atmosphere. Then Et<sub>3</sub>N•3HF (322.4 mg, 10 equiv.) and MeCN (2.0 mL) were added *via* a syringe. The reaction vessel was exposed to blue LED (450-455 nm, 36 W) irradiation at room temperature stirring for 48 h. After completion of the reaction, the crude mixture was concentrated in *vacuo*. The residue was further purified by flash chromatography (silica gel, petroleum ether/ethyl acetate = 20:1, V/V) to give the product **5o** (10.0 mg, 35%).

**3. X-Ray single crystal diffraction analysis of the products (CCDC: 2416854, 2416902)**



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Structure factors have been supplied for datablock(s) 1

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No syntax errors found. [CIF dictionary](#) [Interpreting this report](#)

## Datablock: 1

Bond precision: C-C = 0.0042 Å Wavelength=0.71073

```

Cell:           a=5.8254(11)      b=7.5174(14)      c=18.148(4)
                  alpha=87.425(3)    beta=84.849(3)    gamma=84.586(4)
Temperature:   296 K

```

	Calculated	Reported
Volume	787.5(3)	787.5(3)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C17 H16 Br N O S	?
Sum formula	C17 H16 Br N O S	C17 H16 Br N O S
Mr	362.27	362.28
Dx, g cm-3	1.528	1.528
Z	2	2
Mu (mm-1)	2.740	2.740
F000	368.0	368.0
F000'	367.80	
h, k, lmax	6, 8, 21	6, 8, 21
Nref	2769	2758
Tmin, Tmax	0.495, 0.518	
Tmin'	0.486	

Correction method= Not given

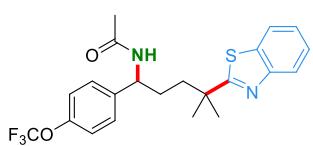
Data completeness= 0.996 Theta (max) = 24.999

R (reflections) = 0.0399 ( 2224)

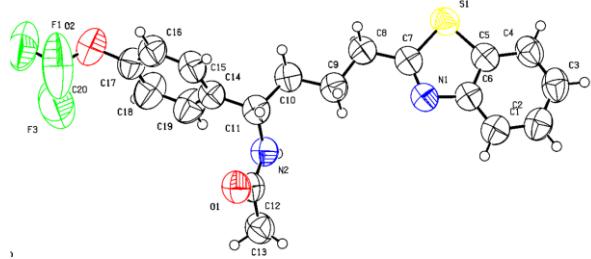
wR2 (reflections) =  
0.0985 ( 2758)

S = 1.022

Npar= 191



**3i**, CCDC: 2416902



## checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 1

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No syntax errors found. [CIF dictionary](#) [Interpreting this report](#)

### Datablock: 1

Bond precision:	C-C = 0.0050 Å	Wavelength=1.54178
Cell:	a=16.4672 (4) alpha=90	b=13.2488 (3) beta=107.031 (1)
Temperature:	273 K	c=9.8017 (2) gamma=90
	Calculated	Reported
Volume	2044.67 (8)	2044.66 (8)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C20 H19 F3 N2 O2 S	C20 H19 F3 N2 O2 S
Sum formula	C20 H19 F3 N2 O2 S	C20 H19 F3 N2 O2 S
Mr	408.43	408.43
Dx, g cm <sup>-3</sup>	1.327	1.327
Z	4	4
Mu (mm <sup>-1</sup> )	1.805	1.805
F000	848.0	848.0
F000'	852.18	
h, k, lmax	19, 15, 11	19, 15, 11
Nref	3757	3748
Tmin, Tmax	0.759, 0.791	0.567, 0.753
Tmin'	0.629	

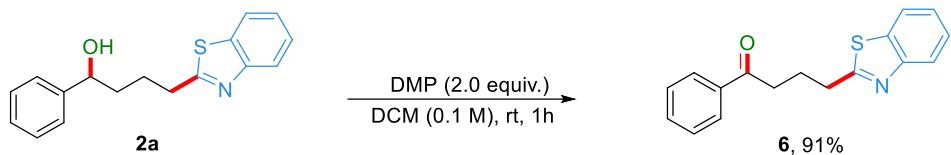
Correction method= # Reported T Limits: Tmin=0.567 Tmax=0.753  
AbsCorr = ?

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S = 1.075	Npar= 254

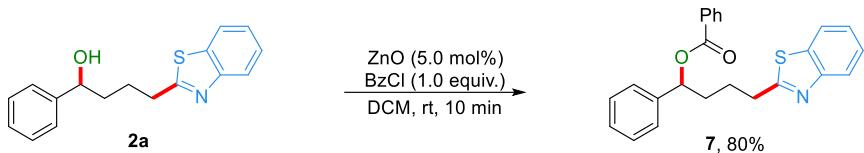
## 4. Synthetic applications

### 4.1 The synthesis of ketone **6**<sup>[2]</sup>



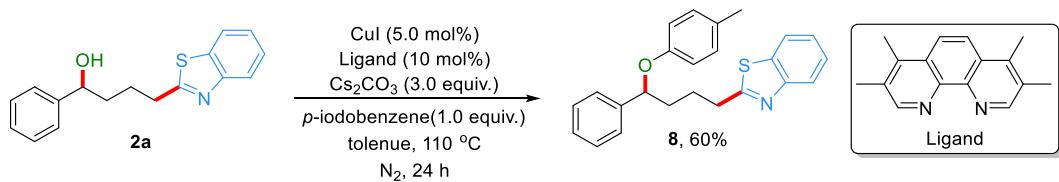
To a reaction tube equipped with a magnetic stir bar were added **2a** (56.7 mg, 0.2 mmol), Dess-Martin periodinane (77.7 mg, 2.0 equiv.) and DCM (2.0 mL). The reaction was stirred at room temperature for 1 h. Then the crude mixture was concentrated in *vacuo*. The residue was purified by column chromatography on silica gel (eluent: petroleum ether/ethyl acetate = 50:1, V/V) to give ketone **6** (51.2 mg, 91%).

### 4.2 The synthesis of benzyl benzoate **7**<sup>[3]</sup>



To a reaction tube equipped with a magnetic stir bar were added **2a** (56.7 mg, 0.2 mmol), BzCl (28.1 mg, 1.0 equiv.) ZnO (0.8 mg, 5.0 mol%) and DCM (2.0 mL). The reaction was stirred at room temperature for 10 min. Then the crude mixture was concentrated in *vacuo*. The residue was purified by column chromatography on silica gel (eluent: petroleum ether/ethyl acetate = 20:1, V/V) to give benzoate **7** (62.0 mg, 80%).

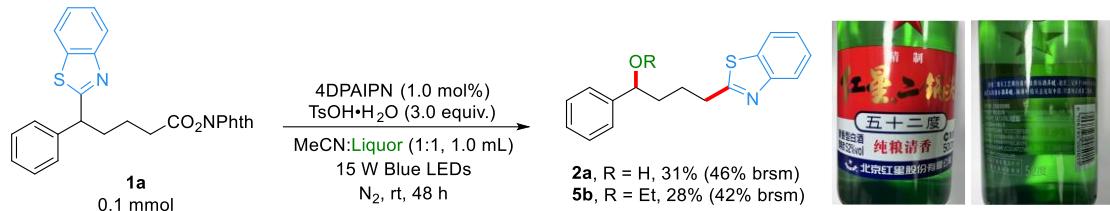
### 4.3 The synthesis of aryl ether **8**<sup>[4]</sup>



To a reaction tube equipped with a magnetic stir bar were added **2a** (56.7 mg, 0.2 mmol), *p*-iodobenzene (21.6 mg, 1.0 equiv.), CuI (1.9 mg, 5.0 mol%), Ligand (4.8 mg,

10 mol%), Cs<sub>2</sub>CO<sub>3</sub> (195.5 mg, 3.0 equiv.) and toluene (2.0 mL). The reaction was stirred at 110 °C for 24 h. The reaction mixture was concentrated in *vacuo*. The residue was purified by column chromatography on silica gel (eluent: petroleum ether/ethyl acetate = 20:1, V/V) to give aryl ether **8** (44.8 mg, 60%).

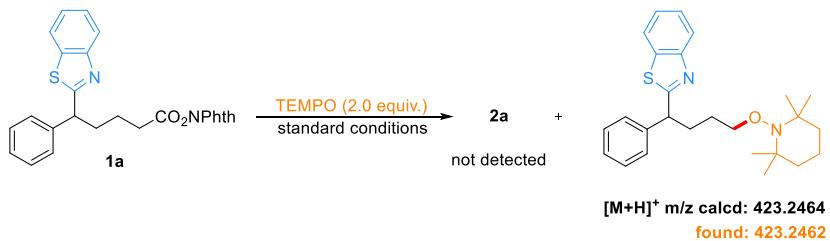
#### 4.4 The remote oxygenation of NHPI ester **1a** with Chinese liquor *Erguotou*



To a 20 mL test tube flask equipped with a stirring bar was charged with **1a** (45.7 mg, 0.1 mmol), 4DPAIPN (0.8 mg, 1.0 mol%) and TsOH•H<sub>2</sub>O (57.1 mg, 3.0 equiv.) under N<sub>2</sub> atmosphere. Then, Chinese liquor *Erguotou* (alc/vol: 52%vol) was added *via* a syringe. The reaction vessel was exposed to blue LED (450-455 nm, 15 W) irradiation at room temperature stirring for 48 h. After completion of the reaction, the reaction mixture was diluted with EtOAc (10 mL), and washed with saturated aq. NaHCO<sub>3</sub> (10 mL). The aqueous layer was extracted by EtOAc (10 mL×2). The combined organic phase was dried over anhydrous Na<sub>2</sub>SO<sub>4</sub> and then concentrated in *vacuo*. The residue was further purified by flash chromatography (silica gel, petroleum ether/ethyl acetate/triethylamine = 10:1:0.1, V/V/V) to give the recovered **1a** (15.1 mg, 33%), alcohol **2a** (8.8 mg, 31%) and ether **5b** (8.7 mg, 28%), respectively.

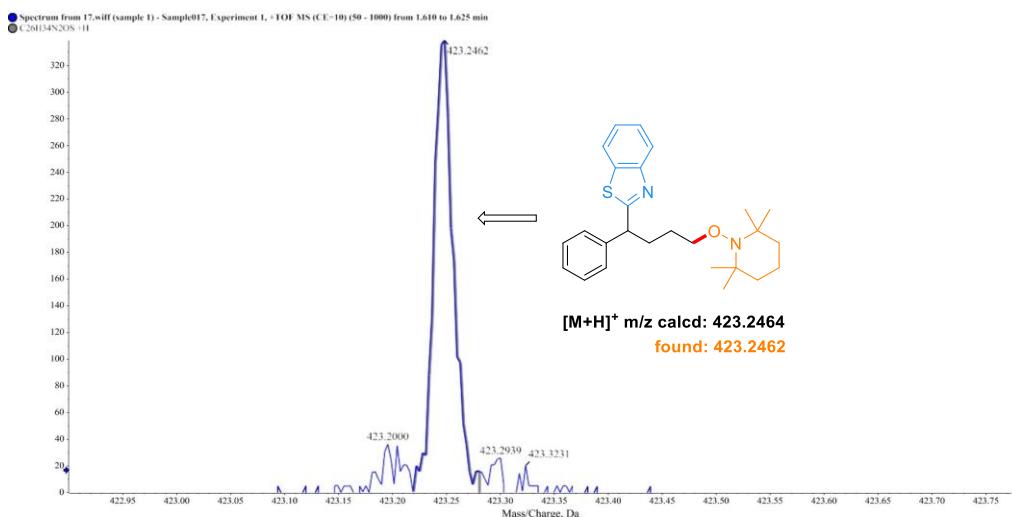
### 5. Mechanistic studies

#### 5.1 Radical-trapping experiment



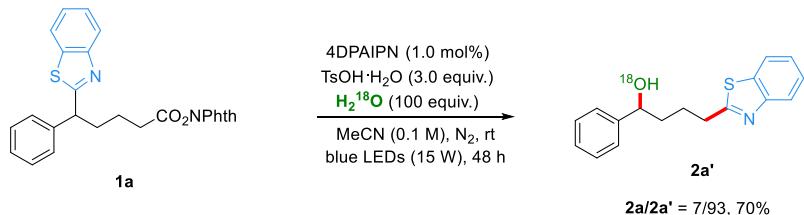
To a 20 mL test tube flask equipped with a stirring bar was charged with **1a** (45.7 mg, 0.1 mmol), 4DPAIPN (0.8 mg, 1.0 mol%), TsOH•H<sub>2</sub>O (57.1 mg, 3.0 equiv.) and TEMPO (93.8 mg, 0.6 mmol) under N<sub>2</sub> atmosphere. Then, H<sub>2</sub>O (180 mg, 10 mmol,

0.18 mL) and MeCN (1.0 mL) were added *via* a syringe. The reaction vessel was exposed to blue LED (450-455 nm, 15 W) irradiation at room temperature stirring for 48 h. Thin-layer chromatography (TLC) analysis indicated that the formation of product **2a** was not observed, and radical trapping adduct was detected by HRMS analysis (Figure S2).



**Figure S2.** HRMS analysis of the TEMPO trapping adduct.

## 5.2 Isotope labeling experiment



To a 20 mL test tube flask equipped with a stirring bar was charged with **1a** (45.7 mg, 0.1 mmol), 4DPAIPN (0.8 mg, 1.0 mol%) and TsOH•H<sub>2</sub>O (57.1 mg, 3.0 equiv.) under N<sub>2</sub> atmosphere. Then, H<sub>2</sub><sup>18</sup>O (200 mg, 10 mmol, 0.20 mL) and MeCN (1.0 mL) were added via a syringe. The reaction vessel was exposed to blue LED (450-455 nm, 15 W) irradiation at room temperature stirring for 48 h. Then, the reaction mixture was diluted with EtOAc (10 mL), and washed with saturated aq. NaHCO<sub>3</sub> (10 mL). The aqueous layer was extracted by EtOAc (10 mL × 2). The combined organic phase was dried over anhydrous Na<sub>2</sub>SO<sub>4</sub> and then concentrated in *vacuo*. The residue was purified by chromatography (silica gel, petroleum ether/ethyl acetate/triethylamine = 10:1:0.1, V/V/V) to afford the products **2a/2a'** (19.9 mg, 70%). The <sup>18</sup>O-labeled product **2a'** was

the dominant product detected by HRMS (abundance ratio: **2a**/**2a'** = 7:93), suggesting the hydroxyl group in product **2a** originated from H<sub>2</sub>O (Figure S3).

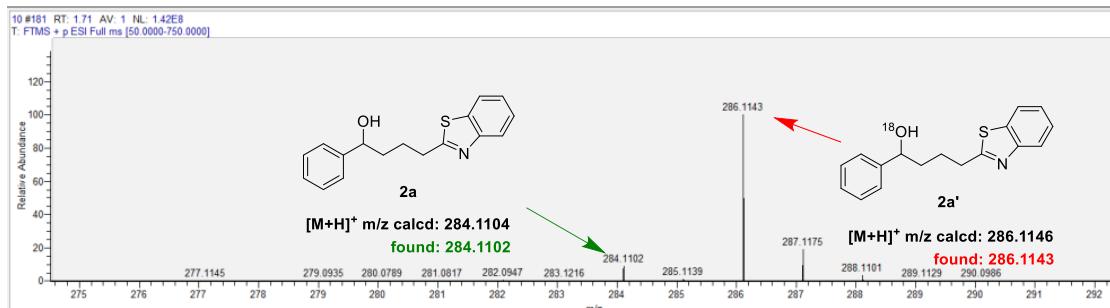
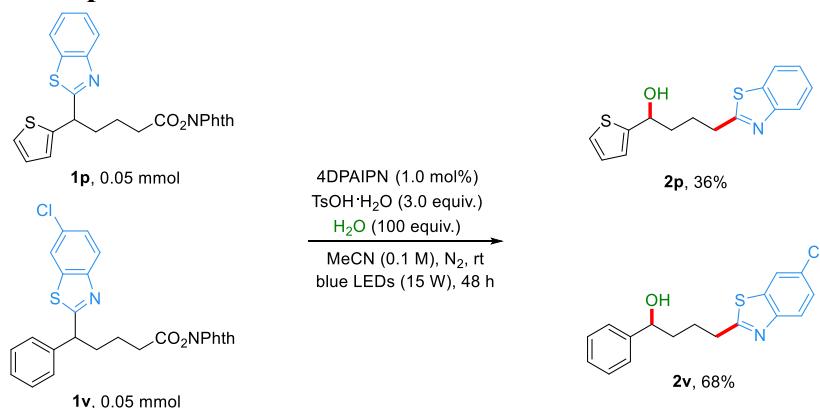


Figure S3. HRMS analysis of **2a** and the <sup>18</sup>O-labeled product **2a'**

### 5.3 Crossover experiment

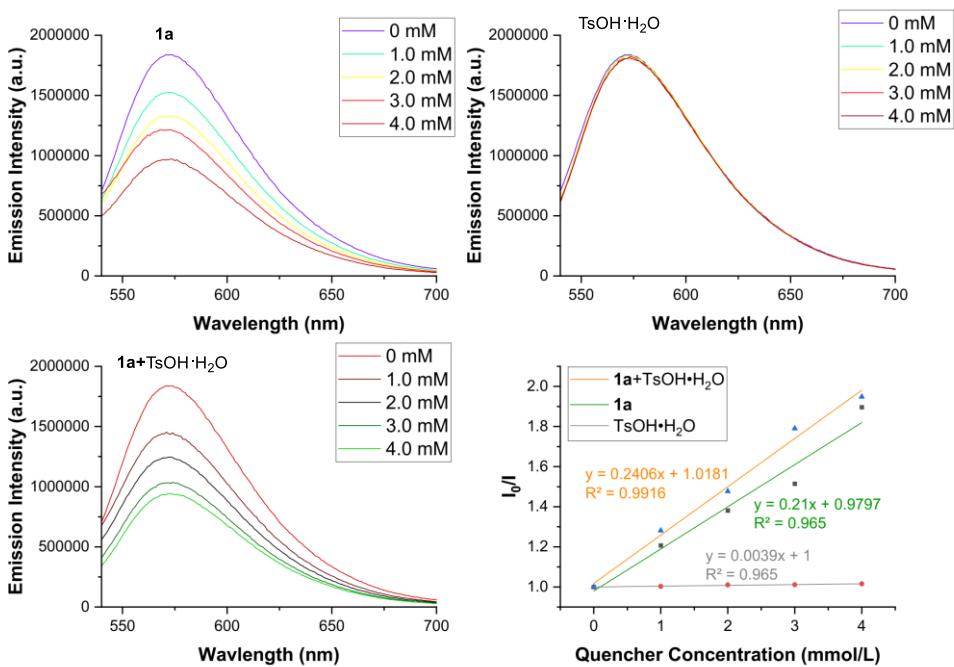


To a 20 mL test tube flask equipped with a stirring bar was charged with **1p** (23.1 mg, 0.05 mmol), **1v** (24.5 mg, 0.05 mmol), 4DPAIPN (0.8 mg, 1.0 mol%) and TsOH·H<sub>2</sub>O (57.1 mg, 3.0 equiv.) under N<sub>2</sub> atmosphere. Then, H<sub>2</sub>O (180 mg, 10 mmol, 0.18 mL) and MeCN (1.0 mL) were added *via* a syringe. The reaction vessel was exposed to blue LED (450–455 nm, 15 W) irradiation at room temperature stirring for 48 h. After completion of the reaction, the reaction mixture was diluted with EtOAc (10 mL), and washed with saturated aq. NaHCO<sub>3</sub> (10 mL). The aqueous layer was extracted by EtOAc (10 mL × 2). The combined organic phase was dried over anhydrous Na<sub>2</sub>SO<sub>4</sub> and then concentrated in *vacuo*. The residue was further purified by flash chromatography (silica gel, petroleum ether/ethyl acetate/triethylamine = 10:1:0.1, V/V/V) to give the product **2p** (5.2 mg, 36%) and **2v** (10.8 mg, 68%), respectively.

### 5.4 Stern-Volmer fluorescence quenching experiments

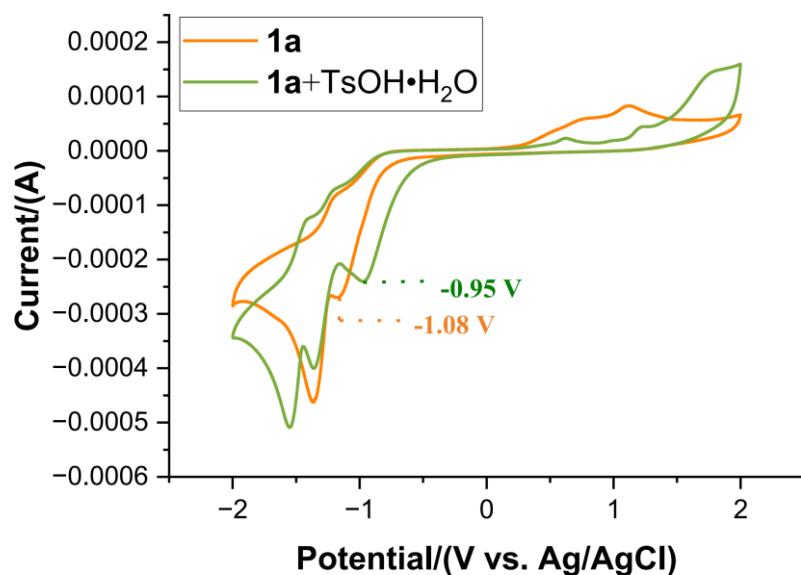
The luminescence quenching experiment was taken using a FluoroMax-4

Spectrophotometer. The experiments were carried out in  $3 \times 10^{-5}$  mol/L of 4DPAIPN in MeCN at rt. The excitation wavelength was 425 nm and the emission intensity was collected at 573 nm (Figure S4). The concentrations of quenchers in MeCN were 1.0 mM, 2.0 mM, 3.0 mM, and 4.0 mM.



**Figure S4** Stern-Volmer emission quenching experiments.

### 5.5 Cyclic voltammetry experiment



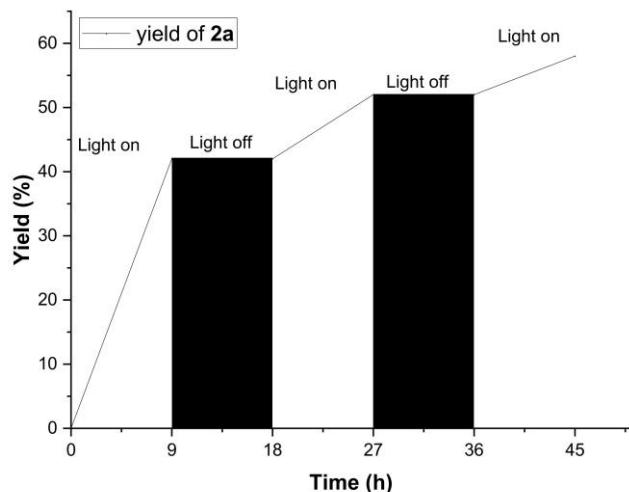
**Figure S5** Cyclic voltammetry measurements.

Cyclic Voltammetry was performed on a CS2350M electrochemical workstation

(Wuhan Corrtest Instrument Co., Ltd). CV measurements of **1a** (1.0 mM) and **1a** (1.0 mM) + TsOH•H<sub>2</sub>O (3.0 mM) were carried out in MeCN solutions with Bu<sub>4</sub>NPF<sub>6</sub> (0.10 M) as the electrolyte at a scan rate of 50 mV/s under N<sub>2</sub> atmosphere. The working electrode is a glassy carbon, the counter electrode is a Pt wire, and the reference electrode is Ag/AgCl (3.5 M KCl). The reduction peak of **1a** and **1a** + TsOH•H<sub>2</sub>O was shown in Figure S5.

### 5.6 Light on/off experiment

To a reaction tube equipped with a magnetic stir bar were added substrate **1a** (0.1 mmol), 4DPAIPN (0.8 mg, 1.0 mol%) and TsOH•H<sub>2</sub>O (57.1 mg, 3.0 equiv.) under N<sub>2</sub> atmosphere. Then, H<sub>2</sub>O (180 mg, 10 mmol, 0.18 mL) and MeCN (1.0 mL) were added *via* a syringe. The yields of **2a** were determined by <sup>1</sup>H NMR with 1,3,5-trimethoxybenzene as an internal standard with the light turned on and off at intervals (Figure S6).

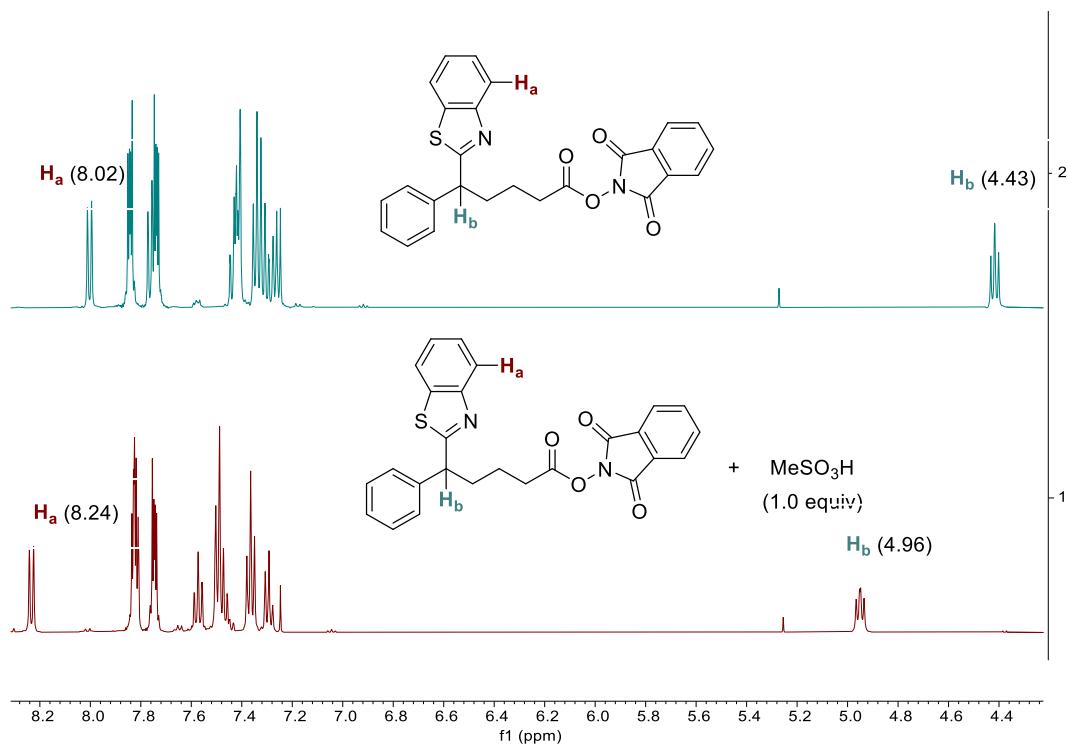


**Figure S6** Reaction profile with the light on/off over time.

### 5.6 NMR analysis of NHPI ester and Brønsted acid mixture

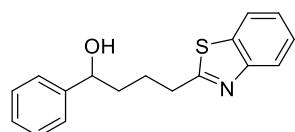
The mixture of NHPI ester **1a** (22.8 mg, 0.05 mmol) and MeSO<sub>3</sub>H (4.8 mg, 0.05 mmol, 1.0 equiv) was dissolved in CDCl<sub>3</sub> (1.0 mL), and the sample was analyzed by a 500 MHz NMR spectrometer. The spectrum was then compared with that of **1a** alone. Upon the addition of 1.0 equiv of MeSO<sub>3</sub>H, the signal of H<sub>a</sub> which were adjacent to N

atom shifted from 8.02 to 8.24. And the signal of H<sub>b</sub> at the benzylic position shifted from 4.43 to 4.96. These observations revealed the interaction between MeSO<sub>3</sub>H and the benzothiazole moiety.



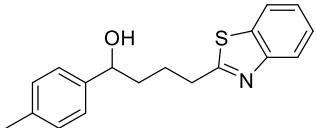
**Figure S7** NMR spectra for the coordination of MeSO<sub>3</sub>H with benzothiazole moiety

## 6. Characterization data

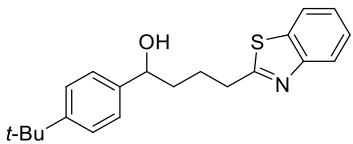


**4-(Benzo[d]thiazol-2-yl)-1-phenylbutan-1-ol (2a,** white solid, 21.8 mg, 77%). <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.94 (d, *J* = 8.1 Hz, 1H), 7.83 (d, *J* = 7.9 Hz, 1H), 7.46 – 7.43 (m, 1H), 7.36 – 7.33 (m, 5H), 7.28 – 7.25 (m, 1H), 4.74 (t, *J* = 6.3 Hz, 1H), 3.15 (t, *J* = 6.7 Hz, 2H), 2.43 (br, 1H), 2.08 – 2.01 (m, 1H), 1.96 – 1.91 (m, 2H), 1.88 – 1.84 (m, 1H); <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 171.9, 153.0, 144.5, 135.0, 128.5, 127.6, 125.9, 125.8, 124.7, 122.4, 121.5, 73.9, 38.3, 33.9, 25.6. HRMS(ESI) m/z: [M+H]<sup>+</sup> cacl. for

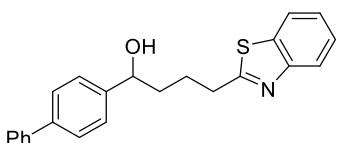
$C_{17}H_{18}NOS$  284.1104, found 284.1098.



**4-(benzo[d]thiazol-2-yl)-1-(*p*-tolyl)butan-1-ol (2b)**, white solid, 24.7 mg, 83%;  $^1H$  NMR (500 MHz, CDCl<sub>3</sub>)  $\delta$  7.95 (d,  $J$  = 8.1 Hz, 1H), 7.83 (d,  $J$  = 8.1 Hz, 1H), 7.46 – 7.43 (m, 1H), 7.36 – 7.33 (m, 1H), 7.24 – 7.23 (m, 2H), 7.15 – 7.14 (m, 2H), 4.71 (t,  $J$  = 6.3 Hz, 1H), 3.15 (t,  $J$  = 6.5 Hz, 2H), 2.33 (s, 3H), 2.21 (br, 1H), 2.05 – 2.02 (m, 1H), 1.94 – 1.91 (m, 2H), 1.86 – 1.82 (m, 1H);  $^{13}C$  NMR (126 MHz, CDCl<sub>3</sub>)  $\delta$  171.9, 153.0, 141.5, 137.3, 135.0, 129.2, 125.9, 125.8, 124.7, 122.5, 121.5, 73.8, 38.2, 33.9, 25.7, 21.1. HRMS(ESI) m/z: [M+H]<sup>+</sup> caclcd. for C<sub>18</sub>H<sub>20</sub>NOS 298.1260, found 298.1289.

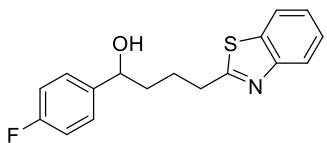


**4-(Benzo[d]thiazol-2-yl)-1-(4-(tert-butyl)phenyl)butan-1-ol (2c)**, colorless oil, 22.7 mg, 67%;  $^1H$  NMR (500 MHz, CDCl<sub>3</sub>)  $\delta$  7.93 (d,  $J$  = 8.1 Hz, 1H), 7.82 (d,  $J$  = 7.9 Hz, 1H), 7.46 – 7.42 (m, 1H), 7.37 – 7.34 (m, 3H), 7.29 – 7.27 (m, 2H), 4.72 (t,  $J$  = 6.2 Hz, 1H), 3.15 (t,  $J$  = 7.1 Hz, 2H), 2.39 (br, 1H), 2.08 – 2.04 (m, 1H), 1.99 – 1.90 (m, 2H), 1.88 – 1.82 (m, 1H), 1.31 (s, 9H);  $^{13}C$  NMR (126 MHz, CDCl<sub>3</sub>)  $\delta$  172.0, 153.1, 150.5, 141.5, 135.0, 125.9, 125.5, 125.4, 124.7, 122.5, 121.5, 73.8, 38.1, 34.5, 33.9, 31.3, 25.8. HRMS(ESI) m/z: [M+H]<sup>+</sup> caclcd. for C<sub>21</sub>H<sub>26</sub>NOS 340.1730, found 340.1727.

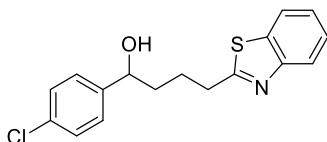


**1-([1,1'-Biphenyl]-4-yl)-4-(benzo[d]thiazol-2-yl)butan-1-ol (2d)**, white solid, 26.6 mg, 74%;  $^1H$  NMR (500 MHz, CDCl<sub>3</sub>)  $\delta$  7.96 (d,  $J$  = 8.1 Hz, 1H), 7.83 (d,  $J$  = 8.0 Hz, 1H), 7.59 – 7.56 (m, 4H), 7.47 – 7.41 (m, 5H), 7.37 – 7.33 (m, 2H), 4.83 – 4.77 (m, 1H), 3.19 (t,  $J$  = 6.7 Hz, 2H), 2.12 – 2.05 (m, 1H), 2.03 – 1.94 (m, 2H), 1.91 – 1.87 (m, 1H),

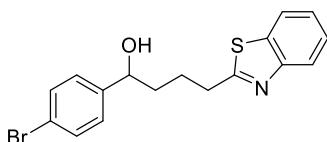
1.81 (br, 1H);  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  170.4, 152.0, 143.5, 140.8, 140.5, 137.1, 135.0, 128.7, 127.2, 127.1, 126.3, 126.0, 124.8, 122.5, 121.5, 73.7, 38.2, 33.9, 25.6. HRMS(ESI) m/z:  $[\text{M}+\text{H}]^+$  caclcd. for  $\text{C}_{23}\text{H}_{22}\text{NOS}$  360.1417, found 360.1412.



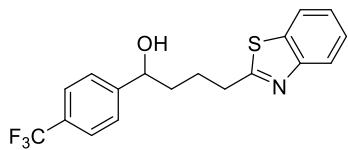
**4-(Benzo[d]thiazol-2-yl)-1-(4-fluorophenyl)butan-1-ol (2e)**, pale yellow solid, 18.4 mg, 61%).  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.93 (d,  $J = 8.1$  Hz, 1H), 7.82 (d,  $J = 8.0$  Hz, 1H), 7.45 – 7.42 (m, 1H), 7.36 – 7.33 (m, 1H), 7.31 – 7.28 (m, 2H), 7.02 – 6.98 (m, 2H), 4.72 (t,  $J = 6.4$  Hz, 1H), 3.14 (t,  $J = 7.1$  Hz, 2H), 2.56 (br, 1H), 2.04 – 1.99 (m, 1H), 1.92 – 1.89 (m, 2H), 1.84 – 1.79 (m, 1H);  $^{19}\text{F}$  NMR (471 MHz,  $\text{CDCl}_3$ )  $\delta$  -114.98 – -115.05 (m, 1F);  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  171.8, 162.1 (d,  $J = 250.7$  Hz), 153.0, 140.3 (d,  $J = 3.0$  Hz), 135.0, 127.4 (d,  $J = 7.9$  Hz), 126.0, 124.8, 122.4, 121.5, 115.2 (d,  $J = 21.3$  Hz), 73.2, 38.3, 33.8, 25.5. HRMS(ESI) m/z:  $[\text{M}+\text{H}]^+$  caclcd. for  $\text{C}_{17}\text{H}_{17}\text{FNOS}$  302.1009, found 302.1009.



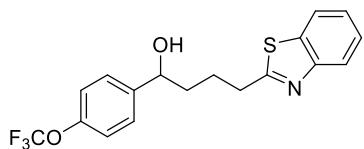
**4-(Benzo[d]thiazol-2-yl)-1-(4-chlorophenyl)butan-1-ol (2f)**, white solid, 18.7 mg, 59%).  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.93 (d,  $J = 8.1$  Hz, 1H), 7.83 (d,  $J = 7.9$  Hz, 1H), 7.46 – 7.43 (m, 1H), 7.36 – 7.33 (m, 1H), 7.30 – 7.28 (m, 4H), 4.72 (t,  $J = 6.3$  Hz, 1H), 3.17 – 3.13 (m, 2H), 2.67 (br, 1H), 2.04 – 2.00 (m, 1H), 1.96 – 1.87 (m, 2H), 1.83 – 1.79 (m, 1H);  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  171.8, 153.0, 143.0, 135.0, 133.2, 128.6, 127.2, 126.0, 124.8, 122.5, 121.5, 73.2, 38.3, 33.7, 25.3. HRMS(ESI) m/z:  $[\text{M}+\text{H}]^+$  caclcd. for  $\text{C}_{17}\text{H}_{17}\text{ClNOS}$  318.0714, found 318.0712.



**4-(Benzo[d]thiazol-2-yl)-1-(4-bromophenyl)butan-1-ol (2g)**, white solid, 22.7 mg, 63%).  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.93 (d,  $J = 8.1$  Hz, 1H), 7.83 (d,  $J = 7.9$  Hz, 1H), 7.46 – 7.43 (m, 3H), 7.37 – 7.34 (m, 1H), 7.22 – 7.21 (m, 2H), 4.72 – 4.70 (m, 1H), 3.16 – 3.13 (m, 2H), 2.61 (br, 1H), 2.04 – 2.00 (m, 1H), 1.94 – 1.89 (m, 2H), 1.83 – 1.81 (m, 1H);  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  171.8, 152.9, 143.6, 135.0, 131.5, 127.5, 126.0, 124.8, 122.4, 121.5, 121.2, 73.1, 38.2, 33.7, 25.3. HRMS(ESI) m/z: [M+H] $^+$  caclcd. for  $\text{C}_{17}\text{H}_{17}\text{BrNOS}$  362.0209, found 362.0211.

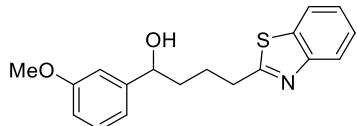


**4-(Benzo[d]thiazol-2-yl)-1-(4-(trifluoromethyl)phenyl)butan-1-ol (2h)**, white solid, 14.4 mg, 41%),  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.95 (d,  $J = 8.2$  Hz, 1H), 7.83 (d,  $J = 8.0$  Hz, 1H), 7.60 – 7.58 (m, 2H), 7.47 – 7.46 (m, 3H), 7.37 – 7.34 (m, 1H), 4.83 (dd,  $J = 7.7, 5.0$  Hz, 1H), 3.20 – 3.16 (m, 2H), 2.82 (br, 1H), 2.06 – 1.99 (m, 2H), 1.92 – 1.86 (m, 2H);  $^{19}\text{F}$  NMR (471 MHz,  $\text{CDCl}_3$ )  $\delta$  -62.3 (s, 3F);  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  171.7, 152.9, 148.5, 134.9, 129.6 (q,  $J = 32.4$  Hz), 126.04, 126.02, 125.4 (q,  $J = 4.0$  Hz), 124.9, 124.1 (q,  $J = 272.5$  Hz), 122.4, 121.5, 73.1, 38.3, 33.6, 25.1. HRMS(ESI) m/z: [M+H] $^+$  caclcd. for  $\text{C}_{18}\text{H}_{17}\text{F}_3\text{NOS}$  352.0977, found 352.0979.

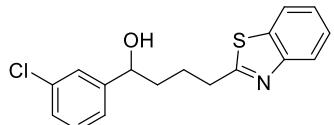


**4-(Benzo[d]thiazol-2-yl)-1-(4-(trifluoromethoxy)phenyl)butan-1-ol (2i)**, colorless oil, 12.8 mg, 35%),  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.91 (d,  $J = 8.2$  Hz, 1H), 7.82 (d,  $J = 8.0$  Hz, 1H), 7.45 – 7.42 (m, 1H), 7.37 – 7.33 (m, 3H), 7.17 – 7.16 (m, 2H), 4.76 (t,  $J = 6.1$  Hz, 1H), 3.15 (t,  $J = 7.2$  Hz, 2H), 3.03 (br, 1H), 2.06 – 2.02 (m, 1H), 1.98 – 1.88 (m, 2H), 1.84 – 1.81 (m, 1H);  $^{19}\text{F}$  NMR (471 MHz,  $\text{CDCl}_3$ )  $\delta$  -57.7 (s, 3F);  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  171.8, 152.9, 148.4, 143.4, 134.9, 127.2, 126.0, 124.8, 122.4, 121.5, 120.9, 120.4 (q,  $J = 322.1$  Hz), 73.0, 38.3, 33.7, 25.4. HRMS(ESI) m/z: [M+H] $^+$

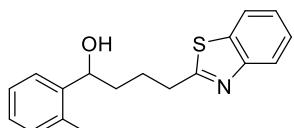
cacl. for  $C_{18}H_{17}F_3NO_2S$  368.0927, found 368.0930.



**4-(Benzo[d]thiazol-2-yl)-1-(3-methoxyphenyl)butan-1-ol (2j)**, colorless oil. 20.7 mg, 66%).  $^1H$  NMR (500 MHz,  $CDCl_3$ )  $\delta$  7.95 (d,  $J = 8.1$  Hz, 1H), 7.84 (d,  $J = 8.4$  Hz, 1H), 7.47 – 7.44 (m, 1H), 7.38 – 7.35 (m, 1H), 7.29 – 7.24 (m, 1H), 6.94 – 6.93 (m, 2H), 6.83 – 6.81 (m, 1H), 4.73 (t,  $J = 6.3$  Hz, 1H), 3.81 (s, 3H), 3.15 (t,  $J = 7.1$  Hz, 2H), 2.75 (br, 1H), 2.08 – 2.02 (m, 1H), 1.97 – 1.92 (m, 2H), 1.88 – 1.85 (m, 1H);  $^{13}C$  NMR (126 MHz,  $CDCl_3$ )  $\delta$  173.1, 141.2, 135.0, 128.9, 128.0, 127.5, 125.9, 124.8, 122.8, 121.5, 119.3, 61.1, 50.6, 41.2, 34.9, 33.8, 31.5, 23.1. HRMS(ESI) m/z: [M+H]<sup>+</sup> cacl. for  $C_{18}H_{20}NO_2S$  314.1209, found 314.1209.

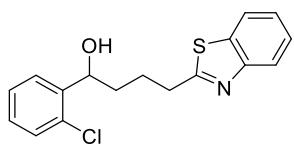


**4-(Benzo[d]thiazol-2-yl)-1-(3-chlorophenyl)butan-1-ol (2k)**, yellow oil, 14.9 mg, 47%).  $^1H$  NMR (500 MHz,  $CDCl_3$ )  $\delta$  7.92 (d,  $J = 8.2$  Hz, 1H), 7.82 (d,  $J = 8.0$  Hz, 1H), 7.45 – 7.42 (m, 1H), 7.36 – 7.32 (m, 2H), 7.24 – 7.20 (m, 3H), 4.71 (dd,  $J = 7.7, 4.9$  Hz, 1H), 3.18 (br, 1H), 3.14 (t,  $J = 7.4$  Hz, 2H), 2.05 – 1.99 (m, 1H), 1.95 – 1.86 (m, 2H), 1.84 – 1.78 (m, 1H);  $^{13}C$  NMR (126 MHz,  $CDCl_3$ )  $\delta$  171.9, 152.9, 146.8, 134.9, 134.3, 129.7, 127.5, 126.0, 124.8, 123.9, 122.4, 121.5, 73.1, 38.2, 33.7, 25.3. HRMS(ESI) m/z: [M+H]<sup>+</sup> cacl. for  $C_{17}H_{17}ClNOS$  318.0714, found 318.0712.

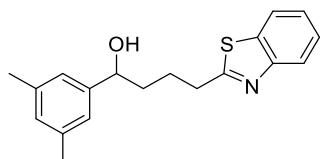


**4-(Benzo[d]thiazol-2-yl)-1-(o-tolyl)butan-1-ol (2l)**, colorless oil, 25.6 mg, 86%).  $^1H$  NMR (500 MHz,  $CDCl_3$ )  $\delta$  7.95 (d,  $J = 8.1$  Hz, 1H), 7.84 (d,  $J = 8.0$  Hz, 1H), 7.49 – 7.43 (m, 2H), 7.37 – 7.33 (m, 1H), 7.24 – 7.20 (m, 1H), 7.17 – 7.15 (m, 1H), 7.12 –

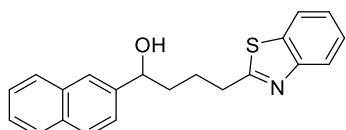
7.11 (m, 1H), 5.00 (dd,  $J = 7.9, 4.7$  Hz, 1H), 3.18 (t,  $J = 7.5$  Hz, 2H), 2.34 (br, 1H), 2.31 (s, 3H), 2.16 – 2.09 (m, 1H), 2.05 – 2.01 (m, 1H), 1.88 – 1.83 (m, 2H);  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  172.0, 152.9, 142.7, 134.8, 134.3, 130.4, 127.2, 126.3, 125.9, 125.1, 124.7, 122.5, 121.5, 70.1, 37.2, 33.9, 25.8, 19.0. HRMS(ESI) m/z: [M+H]<sup>+</sup> caclcd. for  $\text{C}_{18}\text{H}_{20}\text{NOS}$  298.1260, found 298.1257.



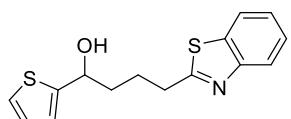
**4-(Benzo[d]thiazol-2-yl)-1-(2-chlorophenyl)butan-1-ol (2m)**, pale yellow oil, 17.2 mg, 54%),  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.95 (d,  $J = 8.1$  Hz, 1H), 7.83 (d,  $J = 8.0$  Hz, 1H), 7.60 – 7.58 (m, 1H), 7.46 – 7.43 (m, 1H), 7.36 – 7.33 (m, 1H), 7.31 – 7.28 (m, 2H), 7.20 – 7.17 (m, 1H), 5.19 (dd,  $J = 8.4, 4.0$  Hz, 1H), 3.20 (td,  $J = 7.5, 2.5$  Hz, 2H), 2.83 (br, 1H), 2.14 – 2.05 (m, 2H), 1.97 – 1.91 (m, 1H), 1.87 – 1.83 (m, 1H);  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  172.0, 153.0, 142.0, 135.0, 131.7, 129.3, 128.4, 127.1, 127.0, 125.9, 124.7, 122.5, 121.5, 70.0, 36.8, 33.7, 25.4. HRMS(ESI) m/z: [M+H]<sup>+</sup> caclcd. for  $\text{C}_{17}\text{H}_{17}\text{ClNOS}$  318.0714, found 318.0713.



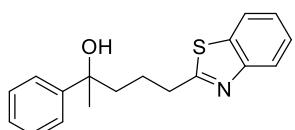
**4-(Benzo[d]thiazol-2-yl)-1-(3,5-dimethylphenyl)butan-1-ol (2n)**, white solid, 28.3 mg, 91%).  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.95 (d,  $J = 8.1$  Hz, 1H), 7.83 (d,  $J = 7.9$  Hz, 1H), 7.46 – 7.42 (m, 1H), 7.36 – 7.32 (m, 1H), 6.95 (s, 2H), 6.90 (s, 1H), 4.66 (dd,  $J = 7.3, 5.2$  Hz, 1H), 3.15 (t,  $J = 7.1$  Hz, 2H), 2.46 (br, 1H), 2.30 (s, 6H), 2.07 – 2.00 (m, 1H), 1.97 – 1.89 (m, 2H), 1.87 – 1.80 (m, 1H);  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  172.0, 153.1, 144.5, 138.0, 135.0, 129.2, 125.9, 124.7, 123.6, 122.5, 121.4, 74.0, 38.2, 33.9, 25.8, 21.3. HRMS(ESI) m/z: [M+H]<sup>+</sup> caclcd. for  $\text{C}_{19}\text{H}_{22}\text{NOS}$  312.1417, found 312.1410.



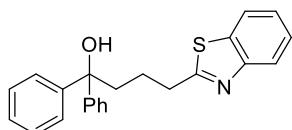
**4-(Benzo[*d*]thiazol-2-yl)-1-(naphthalen-2-yl)butan-1-ol (2o)**, white solid, 23.3 mg, 70%).  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.92 (d,  $J = 8.1$  Hz, 1H), 7.82 – 7.76 (m, 5H), 7.48 – 7.43 (m, 3H), 7.41 – 7.39 (m, 1H), 7.34 – 7.31 (m, 1H), 4.87 (t,  $J = 5.7$  Hz, 1H), 3.29 (br, 1H), 3.11 (t,  $J = 6.8$  Hz, 2H), 2.07 – 1.88 (m, 4H);  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  172.0, 152.9, 141.9, 134.9, 133.2, 132.9, 128.2, 127.9, 127.6, 126.0, 125.9, 125.7, 124.7, 124.5, 124.0, 122.4, 121.4, 76.7, 38.1, 33.8, 25.6. HRMS(ESI) m/z: [M+H]<sup>+</sup> caclcd. for  $\text{C}_{21}\text{H}_{20}\text{NOS}$  334.1260, found 334.1252.



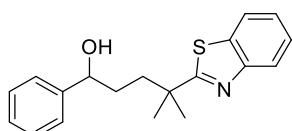
**4-(Benzo[*d*]thiazol-2-yl)-1-(thiophen-2-yl)butan-1-ol (2p)**, yellow oil, 13.6 mg, 47%).  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.66 – 7.63 (m, 1H), 7.48 – 7.45 (m, 1H), 7.35 – 7.34 (m, 3H), 7.30 – 7.28 (m, 2H), 4.78 – 4.71 (m, 1H), 2.97 (td,  $J = 7.0, 3.0$  Hz, 2H), 2.42 (br, 1H), 2.07 – 1.82 (m, 4H);  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  167.0, 150.7, 144.5, 141.2, 128.5, 127.6, 125.8, 124.5, 124.1, 119.5, 110.3, 73.9, 38.3, 28.3, 22.8. HRMS(ESI) m/z: [M+H]<sup>+</sup> caclcd. for  $\text{C}_{15}\text{H}_{16}\text{NOS}_2$  290.0668, found 290.0667.



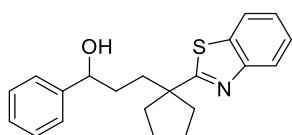
**5-(Benzo[*d*]thiazol-2-yl)-2-phenylpentan-2-ol (2q)**, colorless oil, 24.4 mg, 82%).  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.95 (d,  $J = 8.2$  Hz, 1H), 7.82 (d,  $J = 8.0$  Hz, 1H), 7.46 – 7.43 (m, 3H), 7.36 – 7.32 (m, 3H), 7.25 – 7.22 (m, 1H), 3.08 (t,  $J = 7.2$  Hz, 2H), 2.22 (br, 1H), 1.98 – 1.89 (m, 3H), 1.78 – 1.73 (m, 1H), 1.57 (s, 3H);  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  172.0, 153.0, 147.6, 135.0, 128.2, 126.6, 125.9, 124.73, 124.69, 122.5, 121.5, 74.4, 43.1, 34.1, 30.5, 24.0. HRMS(ESI) m/z: [M+H]<sup>+</sup> caclcd. for  $\text{C}_{18}\text{H}_{20}\text{NOS}$  298.1260, found 298.1253.



**4-(Benzo[d]thiazol-2-yl)-1,1-diphenylbutan-1-ol (2r)**, white solid, 30.2 mg, 84%). <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.90 – 7.89 (m, 1H), 7.80 – 7.78 (m, 1H), 7.43 – 7.41 (m, 5H), 7.37 – 7.34 (m, 5H), 7.29 – 7.27 (m, 2H), 2.48 – 2.45 (m, 2H), 2.37 (t, *J* = 7.0 Hz, 2H), 2.24 (br, 1H), 1.71 – 1.68 (m, 2H); <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 168.0, 146.3, 134.3, 132.6, 128.3, 128.1, 127.2, 126.0, 125.9, 123.6, 119.7, 77.8, 40.5, 20.1, 17.4. HRMS(ESI) m/z: [M+H]<sup>+</sup> caclcd. for C<sub>23</sub>H<sub>22</sub>NOS 360.1417, found 360.1414.

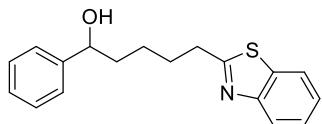


**4-(Benzo[d]thiazol-2-yl)-4-methyl-1-phenylpentan-1-ol (2s)**, colorless oil, 13.4 mg, 43%). <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.95 (d, *J* = 8.1 Hz, 1H), 7.84 – 7.80 (m, 2H), 7.73 – 7.71 (m, 1H), 7.43 – 7.39 (m, 1H), 7.32 – 7.29 (m, 1H), 7.27 – 7.26 (m, 2H), 7.22 – 7.19 (m, 1H), 4.60 (dd, *J* = 7.4, 5.5 Hz, 1H), 2.61 (br, 1H), 2.05 – 1.99 (m, 1H), 1.83 – 1.79 (m, 1H), 1.74 – 1.69 (m, 2H), 1.45 (s, 3H), 1.44 (s, 3H); <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 181.0, 152.8, 144.5, 134.3, 128.4, 127.4, 125.8, 124.6, 123.6, 122.6, 121.4, 74.4, 41.3, 39.2, 34.3, 28.9, 28.8. HRMS(ESI) m/z: [M+H]<sup>+</sup> caclcd. for C<sub>19</sub>H<sub>22</sub>NOS 312.1417, found 312.1446.



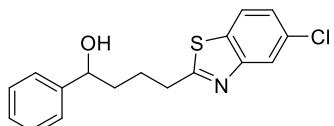
**3-(1-(Benzo[d]thiazol-2-yl)cyclopentyl)-1-phenylpropan-1-ol (2t)**, white solid, 10.8 mg, 32%). <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.96 (d, *J* = 8.2 Hz, 1H), 7.82 (d, *J* = 8.1 Hz, 1H), 7.44 – 7.41 (m, 1H), 7.34 – 7.31 (m, 1H), 7.28 – 7.22 (m, 5H), 4.58 (t, *J* = 6.7 Hz, 1H), 2.30 – 2.25 (m, 2H), 2.10 – 2.04 (m, 1H), 1.87 – 1.82 (m, 4H), 1.73 – 1.72 (m, 6H); <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 180.6, 152.9, 144.5, 135.0, 128.4, 127.4, 125.8,

125.7, 124.6, 123.6, 122.6, 121.4, 74.5, 53.3, 39.7, 39.5, 37.5, 35.0, 24.4. HRMS(ESI) m/z: [M+H]<sup>+</sup> caclcd. for C<sub>21</sub>H<sub>24</sub>NOS 338.1573, found 338.1578.

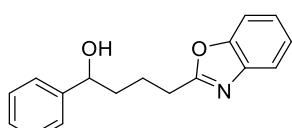


**5-(Benzo[d]thiazol-2-yl)-1-phenylpentan-1-ol (2u)**, pale yellow oil, 10.7 mg, 36%.

<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.87 (d, *J* = 8.1 Hz, 1H), 7.75 (d, *J* = 8.0 Hz, 1H), 7.38 – 7.35 (m, 1H), 7.28 – 7.23 (m, 5H), 7.20 – 7.18 (m, 1H), 4.61 (dd, *J* = 7.7, 5.5 Hz, 1H), 3.01 (t, *J* = 7.7 Hz, 2H), 2.26 (br, 1H), 1.86 – 1.77 (m, 3H), 1.73 – 1.67 (m, 1H), 1.55 – 1.48 (m, 1H), 1.42 – 1.35 (m, 1H); <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 172.1, 153.1, 144.7, 135.0, 128.4, 127.5, 125.9, 125.8, 124.6, 122.4, 121.4, 74.2, 38.6, 34.0, 29.3, 25.3. HRMS(ESI) m/z: [M+H]<sup>+</sup> caclcd. for C<sub>18</sub>H<sub>20</sub>NOS 298.1260, found 298.1258.

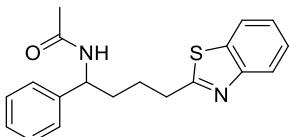


**4-(5-Chlorobenzo[d]thiazol-2-yl)-1-phenylbutan-1-ol (2v)**, white solid, 25.1 mg, 79%. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.89 (d, *J* = 2.0 Hz, 1H), 7.72 (d, *J* = 8.5 Hz, 1H), 7.34 – 7.27 (m, 6H), 4.74 (dd, *J* = 7.1, 5.1 Hz, 1H), 3.13 (t, *J* = 7.1 Hz, 2H), 2.52 (br, 1H), 2.06 – 1.82 (m, 4H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>) δ 174.0, 153.9, 144.5, 133.3, 131.9, 128.5, 127.6, 125.8, 125.2, 122.4, 122.1, 73.9, 38.2, 33.9, 25.6. HRMS(ESI) m/z: [M+H]<sup>+</sup> caclcd. for C<sub>17</sub>H<sub>17</sub>ClNOS 318.0714, found 318.0713.

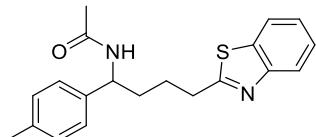


**4-(Benzo[d]oxazol-2-yl)-1-phenylbutan-1-ol (2w)**, pale yellow oil, 11.2 mg, 42%. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.66 – 7.63 (m, 1H), 7.48 – 7.44 (m, 1H), 7.36 – 7.31 (m, 4H), 7.30 – 7.28 (m, 3H), 4.76 – 4.73 (m, 1H), 3.00 – 2.95 (m, 2H), 2.43 (br, 1H), 2.08 – 2.02 (m, 1H), 1.99 – 1.91 (m, 2H), 1.89 – 1.82 (m, 1H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)

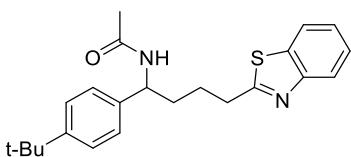
$\delta$  167.0, 150.7, 144.5, 141.2, 128.5, 127.6, 125.8, 124.5, 124.1, 119.5, 110.3, 73.9, 38.3, 28.3, 22.8. HRMS(ESI) m/z: [M+H]<sup>+</sup> caclcd. for C<sub>17</sub>H<sub>18</sub>NO<sub>2</sub> 268.1332, found 268.1331.



**N-(4-(benzo[d]oxazol-2-yl)-1-phenylbutyl)acetamide (3a)** white solid, 38.9 mg, 60%). <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>)  $\delta$  7.96 – 7.94 (m, 1H), 7.84 – 7.82 (m, 1H), 7.47 – 7.43 (m, 1H), 7.37 – 7.31 (m, 3H), 7.28 – 7.25 (m, 3H), 5.95 (d, *J* = 8.0 Hz, 1H), 5.02 (q, *J* = 7.3 Hz, 1H), 3.19 – 3.09 (m, 2H), 1.99 (s, 3H), 1.97 – 1.83 (m, 4H); <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>)  $\delta$  171.5, 169.3, 153.0, 141.8, 135.0, 128.8, 127.5, 126.5, 126.0, 124.8, 122.4, 121.5, 53.3, 35.1, 33.7, 26.1, 23.5. HRMS(ESI) m/z: [M+H]<sup>+</sup> caclcd. for C<sub>19</sub>H<sub>21</sub>N<sub>2</sub>OS 325.1369, found 325.1371.

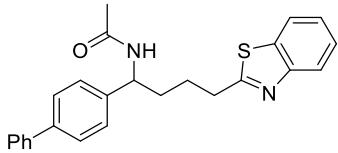


**N-(4-(benzo[d]thiazol-2-yl)-1-(p-tolyl)butyl)acetamide (3b)** yellow solid, 39.9 mg, 59%). <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>)  $\delta$  7.95 – 7.83 (m, 2H), 7.44 – 7.34 (m, 2H), 7.15 – 7.13 (m, 4H), 5.97 (br, 1H), 4.98 (s, 1H), 3.13 (s, 2H), 2.31 (s, 3H), 1.97 (s, 3H), 1.95 – 1.71 (m, 4H); <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>)  $\delta$  171.5, 169.2, 153.1, 138.8, 137.2, 135.1, 129.4, 126.5, 125.9, 124.7, 122.4, 121.5, 53.0, 35.1, 33.7, 26.2, 23.4, 21.0. HRMS(ESI) m/z: [M+H]<sup>+</sup> caclcd. for C<sub>20</sub>H<sub>23</sub>N<sub>2</sub>OS 339.1526, found 339.1528.

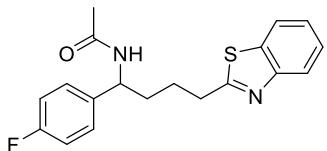


**N-(4-(benzo[d]thiazol-2-yl)-1-(4-(tert-butyl)phenyl)butyl)acetamide (3c)** brown oil, 51.8 mg, 68%), <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>)  $\delta$  7.93 (d, *J* = 8.0 Hz, 1H), 7.81 (d, *J* = 7.7 Hz, 1H), 7.44 – 7.42 (m, 1H), 7.35 – 7.31 (m, 3H), 7.20 – 7.18 (m, 2H), 6.11 (d, *J* = 8.0 Hz, 1H), 5.00 (q, *J* = 7.1 Hz, 1H), 3.15 – 3.08 (m, 2H), 1.95 (s, 3H), 1.94 – 1.83 (m,

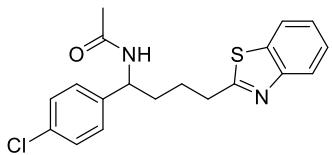
4H), 1.28 (s, 9H);  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  171.5, 169.3, 153.1, 150.3, 138.7, 135.0, 126.2, 125.9, 125.6, 124.7, 122.4, 121.5, 52.8, 35.1, 34.4, 33.7, 31.2, 26.2, 23.4. HRMS(ESI) m/z:  $[\text{M}+\text{H}]^+$  caclcd. for  $\text{C}_{23}\text{H}_{29}\text{N}_2\text{OS}$  381.1995, found 381.1993.



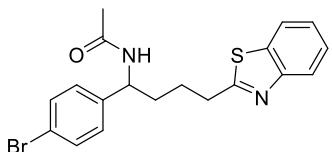
**N-(1-([1,1'-biphenyl]-4-yl)-4-(benzo[d]thiazol-2-yl)butyl)acetamide (3d)** (white solid, 49.7 mg, 62%).  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.95 (d,  $J = 8.1$  Hz, 1H), 7.83 (d,  $J = 7.9$  Hz, 1H), 7.56 – 7.53 (m, 4H), 7.47 – 7.41 (m, 3H), 7.37 – 7.32 (m, 4H), 6.15 (dd,  $J = 7.5, 4.4$  Hz, 1H), 5.06 (q,  $J = 7.2$  Hz, 1H), 3.19 – 3.12 (m, 2H), 2.01 (s, 3H), 1.98 – 1.88 (m, 4H);  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  171.4, 169.4, 153.1, 140.8, 140.6, 140.4, 135.0, 128.7, 127.4, 127.3, 127.0, 126.9, 125.9, 124.8, 122.4, 121.5, 53.0, 35.1, 33.7, 26.1, 23.4. HRMS(ESI) m/z:  $[\text{M}+\text{H}]^+$  caclcd. for  $\text{C}_{25}\text{H}_{25}\text{N}_2\text{OS}$  401.1682, found 401.1690.



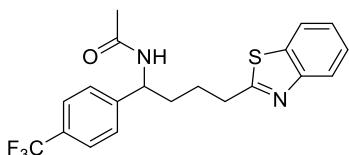
**N-(4-(benzo[d]thiazol-2-yl)-1-(4-fluorophenyl)butyl)acetamide (3e)** (white solid, 52.7 mg, 77%).  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.94 (d,  $J = 8.1$  Hz, 1H), 7.83 (d,  $J = 7.9$  Hz, 1H), 7.46 – 7.43 (m, 1H), 7.37 – 7.34 (m, 1H), 7.24 – 7.21 (m, 2H), 7.00 – 6.97 (m, 2H), 6.17 (d,  $J = 7.7$  Hz, 1H), 4.97 (q,  $J = 7.3$  Hz, 1H), 3.18 – 3.08 (m, 2H), 1.97 (s, 3H), 1.95 – 1.77 (m, 4H);  $^{19}\text{F}$  NMR (471 MHz,  $\text{CDCl}_3$ )  $\delta$  -114.94 (dt,  $J = 13.5, 6.0$  Hz, 1F);  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  171.5, 169.6, 162.1 (d,  $J = 245.5$  Hz), 153.1, 137.9 (d,  $J = 3.1$  Hz), 135.1, 128.3 (d,  $J = 8.0$  Hz), 126.1, 125.0, 122.5, 121.7, 115.6 (d,  $J = 21.4$  Hz), 52.8, 35.2, 33.7, 26.1, 23.5. HRMS(ESI) m/z:  $[\text{M}+\text{H}]^+$  caclcd. for  $\text{C}_{19}\text{H}_{20}\text{FN}_2\text{OS}$  343.1275, found 343.1281.



**N-(4-(benzo[d]thiazol-2-yl)-1-(4-chlorophenyl)butyl)acetamide (3f)** (white solid, 50.2 mg, 70%).  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.94 (d,  $J = 8.1$  Hz, 1H), 7.83 (d,  $J = 7.9$  Hz, 1H), 7.46 – 7.43 (m, 1H), 7.36 – 7.33 (m, 1H), 7.26 – 7.25 (m, 2H), 7.19 – 7.17 (m, 2H), 6.31 (d,  $J = 7.7$  Hz, 1H), 4.95 (q,  $J = 7.4$  Hz, 1H), 3.17 – 3.06 (m, 2H), 1.97 (s, 3H), 1.93 – 1.82 (m, 4H);  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  171.4, 169.6, 153.1, 140.7, 135.1, 133.2, 128.9, 128.0, 126.1, 125.0, 122.5, 121.7, 52.8, 35.1, 33.7, 26.0, 23.4. HRMS(ESI) m/z:  $[\text{M}+\text{H}]^+$  caclcd. for  $\text{C}_{19}\text{H}_{20}\text{ClN}_2\text{OS}$  359.0979, found 359.0977.

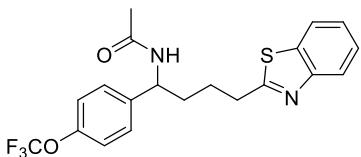


**N-(4-(benzo[d]thiazol-2-yl)-1-(4-bromophenyl)butyl)acetamide (3g)** (white solid, 54.0 mg, 67%).  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.95 (d,  $J = 8.1$  Hz, 1H), 7.84 (d,  $J = 7.9$  Hz, 1H), 7.47 – 7.42 (m, 3H), 7.38 – 7.35 (m, 1H), 7.15 – 7.13 (m, 2H), 6.14 (d,  $J = 7.6$  Hz, 1H), 4.95 (q,  $J = 7.4$  Hz, 1H), 3.17 – 3.08 (m, 2H), 1.99 (s, 3H), 1.93 – 1.85 (m, 4H);  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  171.2, 169.4, 152.8, 141.0, 135.1, 131.8, 128.2, 126.0, 124.9, 122.4, 121.6, 121.2, 52.8, 34.9, 33.5, 25.9, 23.4. HRMS(ESI) m/z:  $[\text{M}+\text{H}]^+$  caclcd. for  $\text{C}_{19}\text{H}_{20}\text{BrN}_2\text{OS}$  403.0474, found 403.0475.

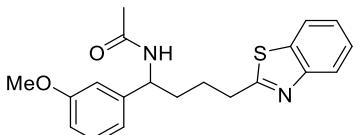


**N-(4-(benzo[d]thiazol-2-yl)-1-(4-(trifluoromethyl)phenyl)butyl)acetamide (3h)** (white solid, 24.3 mg, 31%).  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.94 (d,  $J = 8.0$  Hz, 1H), 7.83 (d,  $J = 8.0$  Hz, 1H), 7.55 – 7.53 (m, 2H), 7.46 – 7.43 (m, 1H), 7.37 – 7.33 (m, 3H), 6.55 (d,  $J = \text{Hz}$ , 1H), 5.02 (q,  $J = \text{Hz}$ , 1H), 3.18 – 3.06 (m, 2H), 1.99 (s, 3H), 1.98 – 1.82 (m, 4H);  $^{19}\text{F}$  NMR (471 MHz,  $\text{CDCl}_3$ )  $\delta$  -62.4 (s, 3F);  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  171.1, 169.6, 153.0, 146.3, 135.0, 129.5 (q,  $J = 32.4$  Hz), 126.8, 126.0, 125.6 (q,  $J =$

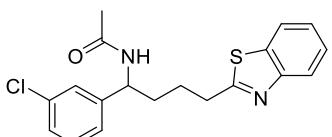
3.9 Hz), 124.9, 124.0 (q,  $J = 272.7$  Hz), 122.4, 121.5, 53.0, 34.9, 33.4, 25.7, 23.2. HRMS(ESI) m/z: [M+H]<sup>+</sup> caclcd. for C<sub>20</sub>H<sub>20</sub>F<sub>3</sub>N<sub>2</sub>OS 393.1243, found 393.1242.



**N-(4-(benzo[d]thiazol-2-yl)-1-(4-(trifluoromethoxy)phenyl)butyl)acetamide (3i)** (3i, white solid, 56.4 mg, 69%). <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.95 (d,  $J = 8.0$  Hz, 1H), 7.83 (d,  $J = 7.9$  Hz, 1H), 7.47 – 7.44 (m, 1H), 7.37 – 7.34 (m, 1H), 7.29 – 7.28 (m, 2H), 7.15 – 7.13 (m, 2H), 6.24 (d,  $J = 7.6$  Hz, 1H), 5.00 (q,  $J = 7.0$  Hz, 1H), 3.19 – 3.07 (m, 2H), 1.99 (s, 3H), 1.97 – 1.88 (m, 4H); <sup>19</sup>F NMR (471 MHz, CDCl<sub>3</sub>) δ -57.7 (s, 3F); <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 171.2, 169.5, 153.0, 148.3, 140.8, 135.0, 127.9, 126.0, 124.9, 122.4, 121.6, 121.1, 120.4 (q,  $J = 257.9$  Hz), 52.7, 35.0, 33.5, 25.9, 23.3. HRMS(ESI) m/z: [M+H]<sup>+</sup> caclcd. for C<sub>20</sub>H<sub>20</sub>F<sub>3</sub>N<sub>2</sub>O<sub>2</sub>S 409.1192, found 409.1196.

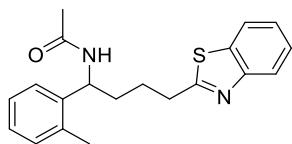


**N-(4-(benzo[d]thiazol-2-yl)-1-(3-methoxyphenyl)butyl)acetamide (3j)** (3j, white solid, 44.0 mg, 62%). <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.93 (d,  $J = 8.1$  Hz, 1H), 7.81 (d,  $J = 7.9$  Hz, 1H), 7.44 – 7.41 (m, 1H), 7.34 – 7.31 (m, 1H), 7.23 – 7.20 (m, 1H), 6.85 – 6.76 (m, 3H), 6.25 (d,  $J = 7.6$  Hz, 1H), 4.97 (d,  $J = 7.0$  Hz, 1H), 3.75 (s, 3H), 3.14 – 3.07 (m, 2H), 1.95 (s, 3H), 1.92 – 1.82 (m, 4H); <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 171.4, 169.3, 159.8, 153.2, 143.5, 135.0, 133.3, 129.8, 125.9, 124.8, 122.4, 121.5, 118.7, 112.6, 55.2, 53.2, 35.2, 33.7, 26.1, 23.4. HRMS(ESI) m/z: [M+H]<sup>+</sup> caclcd. for C<sub>20</sub>H<sub>23</sub>N<sub>2</sub>O<sub>2</sub>S 355.1475, found 355.1477.

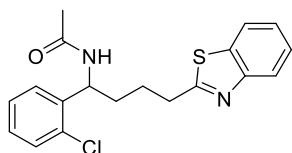


**N-(4-(benzo[d]thiazol-2-yl)-1-(3-chlorophenyl)butyl)acetamide (3k)** (3k, white solid,

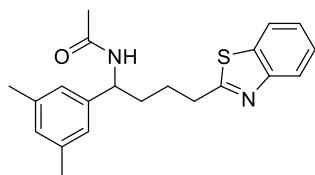
35.9 mg, 50%),  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.96 (d,  $J = 8.1$  Hz, 1H), 7.83 (d,  $J = 7.9$  Hz, 1H), 7.47 – 7.44 (m, 1H), 7.37 – 7.34 (m, 1H), 7.25 – 7.22 (m, 3H), 7.15 – 7.14 (m, 1H), 6.27 (d,  $J = 8.0$  Hz, 1H), 4.97 (q,  $J = 7.3$  Hz, 1H), 3.18 – 3.09 (m, 2H), 2.00 (s, 3H), 1.99 – 1.83 (m, 4H);  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  171.3, 169.6, 152.9, 144.2, 134.9, 134.5, 130.0, 127.6, 126.5, 126.0, 124.88, 124.86, 122.4, 121.6, 52.9, 35.0, 33.5, 25.8, 23.3. HRMS(ESI) m/z:  $[\text{M}+\text{H}]^+$  caclcd. for  $\text{C}_{19}\text{H}_{20}\text{ClN}_2\text{OS}$  359.0979, found 359.0983.



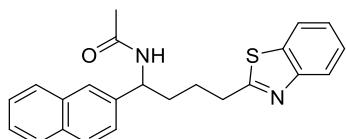
**N-(4-(benzo[d]thiazol-2-yl)-1-(o-tolyl)butyl)acetamide (3l)** brown oil, 46.0 mg, 68%).  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.94 (d,  $J = 7.9$  Hz, 1H), 7.83 (d,  $J = 7.8$  Hz, 1H), 7.46 – 7.43 (m, 1H), 7.36 – 7.33 (m, 1H), 7.20 – 7.15 (m, 4H), 5.98 (d,  $J = 7.7$  Hz, 1H), 5.25 (q,  $J = 7.6$  Hz, 1H), 3.18 – 3.08 (m, 2H), 2.39 (s, 3H), 1.96 (s, 3H), 1.94 – 1.82 (m, 4H);  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  171.5, 169.2, 153.0, 140.0, 136.1, 135.0, 130.7, 127.3, 126.3, 125.9, 124.8, 124.7, 122.4, 121.5, 49.2, 34.8, 33.8, 26.2, 23.3, 19.4. HRMS(ESI) m/z:  $[\text{M}+\text{H}]^+$  caclcd. for  $\text{C}_{20}\text{H}_{23}\text{N}_2\text{OS}$  339.1526, found 339.1532.



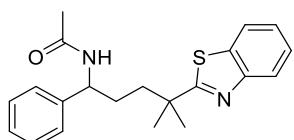
**N-(4-(benzo[d]thiazol-2-yl)-1-(2-chlorophenyl)butyl)acetamide (3m)** white solid, 33.0 mg, 46%).  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.94 (d,  $J = 8.0$  Hz, 1H), 7.82 (d,  $J = 7.8$  Hz, 1H), 7.46 – 7.43 (m, 1H), 7.36 – 7.31 (m, 2H), 7.27 – 7.26 (m, 1H), 7.21 – 7.14 (m, 2H), 6.60 (d,  $J = 7.1$  Hz, 1H), 5.33 (q,  $J = 5.8$  Hz, 1H), 3.18 – 3.09 (m, 2H), 2.00 (s, 3H), 1.95 – 1.86 (m, 4H);  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  171.4, 169.5, 153.0, 139.3, 135.0, 132.8, 130.1, 128.4, 127.7, 127.0, 125.9, 124.8, 122.3, 121.5, 51.3, 34.0, 33.5, 26.0, 23.2. HRMS(ESI) m/z:  $[\text{M}+\text{H}]^+$  caclcd. for  $\text{C}_{19}\text{H}_{20}\text{ClN}_2\text{OS}$  359.0979, found 359.0977.



**N-(4-(benzo[d]thiazol-2-yl)-1-(3,5-dimethylphenyl)butyl)acetamide (3n)** (white solid, 47.9 mg, 68%). <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.94 (d, *J* = 8.2 Hz, 1H), 7.83 (d, *J* = 8.0 Hz, 1H), 7.46 – 7.43 (m, 1H), 7.36 – 7.33 (m, 1H), 6.88 – 6.87 (m, 3H), 5.95 (d, *J* = 8.2 Hz, 1H), 4.93 (q, *J* = 7.4 Hz, 1H), 3.17 – 3.07 (m, 2H), 2.28 (s, 6H), 1.97 (s, 3H), 1.95 – 1.78 (m, 4H); <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 171.6, 169.2, 153.1, 141.6, 138.3, 135.1, 129.2, 125.9, 124.7, 124.3, 122.4, 121.5, 53.2, 35.2, 33.8, 26.2, 23.5, 21.3. HRMS(ESI) m/z: [M+H]<sup>+</sup> caclcd. for C<sub>21</sub>H<sub>25</sub>N<sub>2</sub>OS 353.1682, found 353.1685.

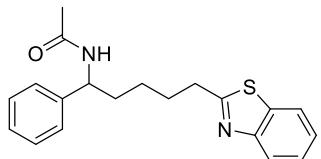


**N-(4-(benzo[d]thiazol-2-yl)-1-(naphthalen-2-yl)butyl)acetamide (3o)** (white solid, 48.7 mg, 65%). <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.95 (d, *J* = 8.0 Hz, 1H), 7.83 – 7.72 (m, 5H), 7.48 – 7.43 (m, 3H), 7.39 – 7.33 (m, 2H), 6.18 (d, *J* = 8.3 Hz, 1H), 5.18 (q, *J* = 7.3 Hz, 1H), 3.19 – 3.09 (m, 2H), 2.05 – 1.82 (m, 4H), 2.00 (s, 3H); <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 171.5, 169.5, 153.0, 139.1, 135.0, 133.3, 132.7, 128.6, 127.8, 127.6, 126.2, 125.93, 125.88, 125.3, 124.8, 124.6, 122.4, 121.5, 53.3, 35.0, 33.7, 26.1, 23.4. HRMS(ESI) m/z: [M+H]<sup>+</sup> caclcd. for C<sub>23</sub>H<sub>23</sub>N<sub>2</sub>OS 375.1526, found 375.1533.

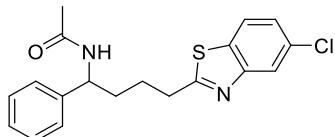


**N-(4-(benzo[d]thiazol-2-yl)-4-methyl-1-phenylpentyl)acetamide (3p)** (brown wax, 45.1 mg, 64%). <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.98 (d, *J* = 8.2 Hz, 1H), 7.85 (d, *J* = 7.9 Hz, 1H), 7.48 – 7.45 (m, 1H), 7.37 – 7.34 (m, 1H), 7.29 – 7.26 (m, 2H), 7.23 – 7.19 (m, 3H), 6.17 (d, *J* = 7.8 Hz, 1H), 4.90 (q, *J* = 7.2 Hz, 1H), 1.99 (s, 3H), 1.96 – 1.93 (m,

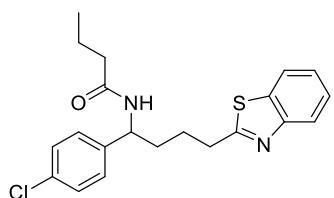
1H), 1.78 – 1.71 (m, 3H), 1.47 (s, 3H), 1.45 (s, 3H);  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  180.7, 169.4, 152.9, 142.2, 134.9, 128.5, 127.2, 126.4, 125.8, 124.7, 122.5, 121.5, 53.6, 41.4, 39.5, 31.4, 29.3, 28.5, 23.4. HRMS(ESI) m/z:  $[\text{M}+\text{H}]^+$  cacl. for  $\text{C}_{21}\text{H}_{25}\text{N}_2\text{OS}$  353.1682, found 353.1688.



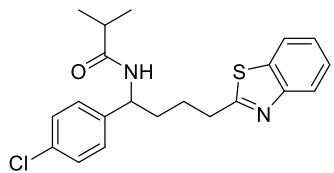
**N-(5-(benzo[d]thiazol-2-yl)-1-phenylpentyl)acetamide (3q)**, brown wax, 42.0 mg, 62%).  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.94 (d,  $J = 8.1$  Hz, 1H), 7.82 (d,  $J = 7.9$  Hz, 1H), 7.46 – 7.42 (m, 1H), 7.36 – 7.33 (m, 1H), 7.31 – 7.28 (m, 2H), 7.25 – 7.22 (m, 3H), 5.96 (d,  $J = 8.2$  Hz, 1H), 4.95 (q,  $J = 7.6$  Hz, 1H), 3.07 (t,  $J = 7.7$  Hz, 2H), 1.94 (s, 3H), 1.92 – 1.78 (m, 4H), 1.51 – 1.47 (m, 1H), 1.43 – 1.33 (m, 1H);  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  171.8, 169.3, 153.0, 142.0, 135.0, 128.6, 127.4, 126.5, 125.9, 124.7, 122.4, 121.5, 53.2, 35.5, 33.9, 29.2, 25.5, 23.4. HRMS(ESI) m/z:  $[\text{M}+\text{H}]^+$  cacl. for  $\text{C}_{20}\text{H}_{23}\text{N}_2\text{OS}$  339.1526, found 339.1540.



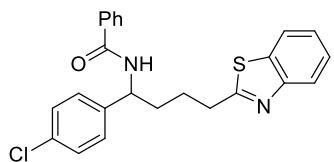
**N-(4-(5-chlorobenzo[d]thiazol-2-yl)-1-phenylbutyl)acetamide (3r)**, white solid, 23.7 mg, 33%).  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.92 (s, 1H), 7.72 (d,  $J = 8.4$  Hz, 1H), 7.32 – 7.26 (m, 6H), 5.97 (d,  $J = 8.2$  Hz, 1H), 5.01 (q,  $J = 7.2$  Hz, 1H), 3.16 – 3.07 (m, 2H), 1.98 (s, 3H), 1.93 – 1.80 (m, 4H);  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  171.7, 169.3, 154.0, 141.7, 136.5, 131.9, 128.8, 127.6, 126.5, 125.2, 122.4, 122.2, 53.2, 35.1, 33.8, 26.0, 23.4. HRMS(ESI) m/z:  $[\text{M}+\text{H}]^+$  cacl. for  $\text{C}_{19}\text{H}_{20}\text{ClN}_2\text{OS}$  359.0979, found 359.0987.



**N-(4-(benzo[d]thiazol-2-yl)-1-(4-chlorophenyl)butyl)butyramide (3s,** white solid, 37.1 mg, 48%).  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.95 (d,  $J = 8.1$  Hz, 1H), 7.83 (d,  $J = 8.0$  Hz, 1H), 7.47 – 7.44 (m, 1H), 7.37 – 7.34 (m, 1H), 7.27 – 7.26 (m, 2H), 7.20 – 7.18 (m, 2H), 6.10 (d,  $J = 7.6$  Hz, 1H), 4.98 (q,  $J = 7.2$  Hz, 1H), 3.19 – 3.09 (m, 2H), 2.18 – 2.14 (m, 2H), 1.97 – 1.83 (m, 4H), 1.68 – 1.60 (m, 2H), 0.90 (t,  $J = 7.4$  Hz, 3H);  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  172.4, 171.3, 153.0, 140.7, 135.0, 133.0, 128.8, 127.8, 126.0, 124.8, 122.4, 121.5, 52.5, 38.6, 34.9, 33.5, 25.9, 19.1, 13.7. HRMS(ESI) m/z: [M+Na] $^+$  caclcd. for  $\text{C}_{21}\text{H}_{23}\text{ClN}_2\text{NaOS}$  409.1112, found 409.1121.

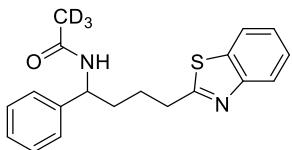


**N-(4-(benzo[d]thiazol-2-yl)-1-(4-chlorophenyl)butyl)isobutyramide (3t,** white solid, 34.1 mg, 44%).  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.96 (d,  $J = 7.6$  Hz, 1H), 7.84 (d,  $J = 7.3$  Hz, 1H), 7.48 – 7.45 (m, 1H), 7.38 – 7.35 (m, 1H), 7.28 – 7.26 (m, 2H), 7.20 – 7.19 (m, 2H), 5.93 (d,  $J = 7.5$  Hz, 1H), 4.97 (q,  $J = 7.0$  Hz, 1H), 3.19 – 3.08 (m, 2H), 2.40 – 2.34 (m, 1H), 1.96 – 1.88 (m, 4H), 1.16 (d,  $J = 6.9$  Hz, 3H), 1.13 (d,  $J = 6.9$  Hz, 3H);  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  176.4, 171.3, 159.2, 140.7, 135.0, 133.0, 128.8, 127.8, 126.0, 124.9, 122.4, 121.6, 52.4, 35.6, 35.0, 33.5, 26.0, 19.58, 19.55. HRMS(ESI) m/z: [M+H] $^+$  caclcd. for  $\text{C}_{21}\text{H}_{24}\text{ClN}_2\text{OS}$  387.1292, found 387.1302.

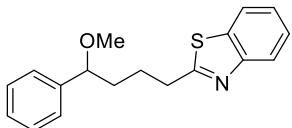


**N-(4-(benzo[d]thiazol-2-yl)-1-(4-chlorophenyl)butyl)benzamide (3u,** white solid, 33.7 mg, 40%).  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.92 – 7.90 (m, 1H), 7.83 – 7.80 (m, 3H), 7.47 – 7.33 (m, 6H), 7.26 – 7.24 (m, 3H), 6.90 – 6.89 (m, 1H), 5.16 – 5.15 (m, 1H), 3.21 – 3.12 (m, 2H), 2.03 – 1.90 (m, 4H);  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  171.2, 167.0, 153.0, 140.7, 135.0, 134.2, 133.1, 131.6, 128.8, 128.5, 127.9, 127.0, 126.0, 124.9, 122.4, 121.6, 53.3, 34.9, 33.4, 25.8. HRMS(ESI) m/z: [M+H] $^+$  caclcd. for  $\text{C}_{24}\text{H}_{22}\text{ClN}_2\text{OS}$

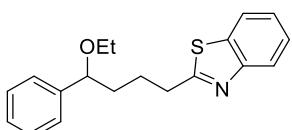
421.1136, found 421.1145.



**N-(4-(benzo[d]thiazol-2-yl)-1-phenylbutyl)acetamide-2,2,2-d<sub>3</sub> (3v)** (white solid, 41.9 mg, 64%), <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.95 (d, *J* = 8.1 Hz, 1H), 7.83 (d, *J* = 7.9 Hz, 1H), 7.46 – 7.43 (m, 1H), 7.36 – 7.30 (m, 3H), 7.27 – 7.23 (m, 3H), 5.97 (d, *J* = 8.1 Hz, 1H), 5.02 (q, *J* = 7.3 Hz, 1H), 3.18 – 3.08 (m, 2H), 1.99 – 1.84 (m, 4H); <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 171.4, 169.4, 153.1, 141.8, 135.0, 128.7, 127.4, 126.5, 125.9, 124.7, 122.4, 121.5, 53.2, 35.2, 33.7, 26.1, 22.4. HRMS(ESI) m/z: [M+H]<sup>+</sup> cacl. for C<sub>19</sub>H<sub>18</sub>D<sub>3</sub>N<sub>2</sub>OS 328.1557, found 328.1560.

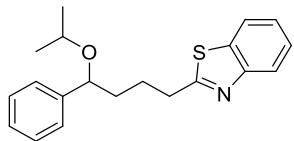


**2-(4-Methoxy-4-phenylbutyl)benzo[d]thiazole (5a)** (colorless oil, 22.9 mg, 77%). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.95 (d, *J* = 8.1 Hz, 1H), 7.82 (d, *J* = 7.9 Hz, 1H), 7.46 – 7.42 (m, 1H), 7.36 – 7.32 (m, 3H), 7.29 – 7.27 (m, 3H), 4.15 (dd, *J* = 7.3, 5.3 Hz, 1H), 3.21 (s, 3H), 3.12 (t, *J* = 7.5 Hz, 2H), 2.05 – 2.00 (m, 1H), 1.96 – 1.86 (m, 2H), 1.82 – 1.76 (m, 1H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>) δ 171.8, 153.2, 141.9, 135.1, 128.4, 127.6, 126.6, 125.8, 124.6, 122.5, 121.4, 83.5, 56.6, 37.5, 34.1, 26.0. HRMS(ESI) m/z: [M+H]<sup>+</sup> cacl. for C<sub>18</sub>H<sub>20</sub>NOS 298.1260, found 298.1260.

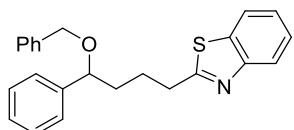


**2-(4-Ethoxy-4-phenylbutyl)benzo[d]thiazole (5b)** (colorless oil, 23.0 mg, 74%). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.96 (d, *J* = 8.2 Hz, 1H), 7.82 (d, *J* = 8.0 Hz, 1H), 7.46 – 7.42 (m, 1H), 7.35 – 7.28 (m, 6H), 4.26 (dd, *J* = 7.4, 5.3 Hz, 1H), 3.42 – 3.27 (m, 2H), 3.12 (t, *J* = 7.4 Hz, 2H), 2.08 – 2.02 (m, 1H), 1.99 – 1.85 (m, 2H), 1.81 – 1.75 (m, 1H),

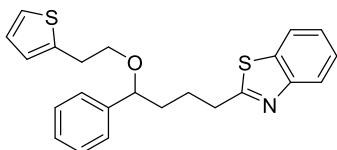
1.18 (t,  $J = 7.0$  Hz, 3H);  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  171.9, 153.2, 142.7, 135.1, 128.3, 127.4, 126.5, 125.8, 124.6, 122.4, 121.4, 81.6, 64.1, 37.7, 34.1, 26.1, 15.3. HRMS(ESI) m/z:  $[\text{M}+\text{H}]^+$  caclcd. for  $\text{C}_{19}\text{H}_{22}\text{NOS}$  312.1417, found 312.1417.



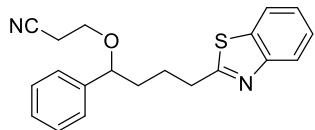
**2-(4-Isopropoxy-4-phenylbutyl)benzo[d]thiazole (5c)**, colorless oil, 23.4 mg, 72%).  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.96 (d,  $J = 8.2$  Hz, 1H), 7.82 (d,  $J = 8.0$  Hz, 1H), 7.46 – 7.43 (m, 1H), 7.35 – 7.31 (m, 5H), 7.27 – 7.24 (m, 1H), 4.40 – 4.37 (m, 1H), 3.50 – 3.46 (m, 1H), 3.14 – 3.11 (m, 2H), 2.08 – 2.02 (m, 1H), 1.91 – 1.85 (m, 2H), 1.77 – 1.71 (m, 1H), 1.16 (d,  $J = 6.0$  Hz, 3H), 1.09 (d,  $J = 6.2$  Hz, 3H);  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  171.9, 153.2, 143.4, 135.1, 128.2, 127.3, 126.4, 125.8, 124.6, 122.4, 121.4, 78.6, 68.7, 38.1, 34.1, 26.3, 23.4, 21.1. HRMS(ESI) m/z:  $[\text{M}+\text{H}]^+$  caclcd. for  $\text{C}_{20}\text{H}_{24}\text{NOS}$  326.1573, found 326.1568.



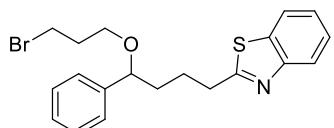
**2-(4-(Benzyl)-4-phenylbutyl)benzo[d]thiazole (5d)**, colorless oil, 22.0 mg, 59%).  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.95 (d,  $J = 8.2$  Hz, 1H), 7.83 (d,  $J = 8.0$  Hz, 1H), 7.46 – 7.43 (m, 1H), 7.37 – 7.30 (m, 11H), 4.48 – 4.45 (m, 1H), 4.37 (dd,  $J = 7.8, 5.2$  Hz, 1H), 4.27 – 4.24 (m, 1H), 3.12 – 3.08 (m, 2H), 2.09 – 1.98 (m, 2H), 1.93 – 1.86 (m, 1H), 1.83 – 1.79 (m, 1H);  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  171.8, 153.2, 142.2, 138.5, 135.1, 128.5, 128.3, 127.8, 127.7, 127.5, 126.7, 125.8, 124.6, 122.5, 121.5, 80.9, 70.4, 37.7, 34.1, 26.1. HRMS(ESI) m/z:  $[\text{M}+\text{H}]^+$  caclcd. for  $\text{C}_{24}\text{H}_{24}\text{NOS}$  374.1573, found 374.1566.



**2-(4-Phenyl-4-(2-(thiophen-2-yl)ethoxy)butyl)benzo[d]thiazole (5e)** (colorless oil, 13.0 mg, 33%). <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.96 (d, *J* = 7.9 Hz, 1H), 7.83 (d, *J* = 8.0 Hz, 1H), 7.46 – 7.43 (m, 1H), 7.36 – 7.30 (m, 3H), 7.27 – 7.25 (m, 3H), 7.11 – 7.10 (m, 1H), 6.90 – 6.88 (m, 1H), 6.81 – 6.80 (m, 1H), 4.29 (dd, *J* = 7.5, 5.3 Hz, 1H), 3.59 – 3.54 (m, 1H), 3.48 – 3.43 (m, 1H), 3.13 – 3.05 (m, 4H), 2.05 – 2.00 (m, 1H), 1.97 – 1.91 (m, 1H), 1.90 – 1.84 (m, 1H), 1.80 – 1.75 (m, 1H); <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 171.9, 153.3, 142.2, 141.4, 135.1, 133.5, 128.4, 127.6, 126.6, 125.9, 125.1, 124.7, 123.5, 122.4, 121.5, 82.1, 69.4, 37.6, 34.0, 30.6, 26.0. HRMS(ESI) m/z: [M+H]<sup>+</sup> caclcd. for C<sub>23</sub>H<sub>24</sub>NOS<sub>2</sub> 394.1294, found 394.1302.

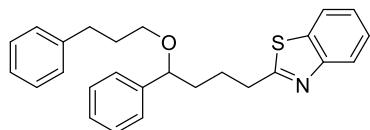


**3-(4-(Benzo[d]thiazol-2-yl)-1-phenylbutoxy)propanenitrile (5f)** (colorless oil, 15.5 mg, 46%). <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 8.01 (d, *J* = 8.1 Hz, 1H), 7.78 (d, *J* = 8.0 Hz, 1H), 7.46 – 7.43 (m, 1H), 7.41 – 7.39 (m, 2H), 7.36 – 7.33 (m, 3H), 7.29 – 7.27 (m, 1H), 4.39 (dd, *J* = 8.4, 7.1 Hz, 1H), 4.25 (t, *J* = 6.4 Hz, 2H), 2.68 (t, *J* = 6.4 Hz, 2H), 2.50 – 2.42 (m, 3H), 2.27 – 2.21 (m, 1H), 1.76 – 1.67 (m, 2H); <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 174.8, 172.6, 152.9, 141.1, 135.1, 128.9, 127.5, 126.0, 124.9, 122.8, 121.5, 116.7, 58.6, 50.6, 34.8, 33.5, 22.9, 18.0. HRMS(ESI) m/z: [M+Na]<sup>+</sup> caclcd. for C<sub>20</sub>H<sub>20</sub>N<sub>2</sub>NaOS 359.1189, found 359.1179.

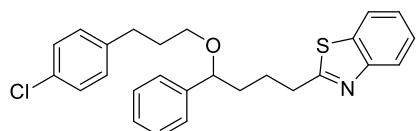


**2-(4-(3-Bromopropoxy)-4-phenylbutyl)benzo[d]thiazole (5g)** (colorless oil, 24.6 mg, 61%). <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.96 (d, *J* = 8.1 Hz, 1H), 7.83 (d, *J* = 8.0 Hz, 1H), 7.46 – 7.43 (m, 1H), 7.36 – 7.32 (m, 3H), 7.28 – 7.27 (m, 3H), 4.26 (dd, *J* = 7.5, 5.1

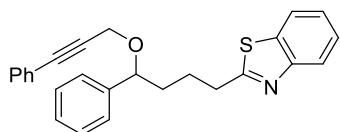
Hz, 1H), 3.56 – 3.48 (m, 2H), 3.43 – 3.36 (m, 2H), 3.14 – 3.11 (m, 2H), 2.08 – 2.05 (m, 3H), 1.94 – 1.87 (m, 2H), 1.79 – 1.74 (m, 1H);  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  171.7, 153.2, 141.9, 134.9, 128.4, 127.6, 126.5, 125.9, 124.7, 122.5, 121.5, 82.1, 66.1, 37.6, 34.1, 33.0, 30.8, 26.0. HRMS(ESI) m/z:  $[\text{M}+\text{H}]^+$  cacl. for  $\text{C}_{20}\text{H}_{23}\text{BrNOS}$  404.0678, found 404.0672.



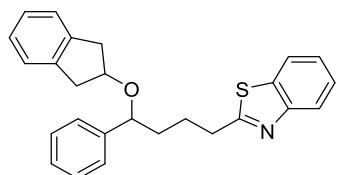
**2-(4-Phenyl-4-(3-phenylpropoxy)butyl)benzo[d]thiazole (5h)**, colorless oil, 14.9 mg, 37%).  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  8.06 (d,  $J = 8.1$  Hz, 1H), 7.93 (d,  $J = 8.0$  Hz, 1H), 7.56 – 7.53 (m, 1H), 7.46 – 7.42 (m, 3H), 7.40 – 7.34 (m, 6H), 7.28 – 7.25 (m, 2H), 4.34 (dd,  $J = 7.6, 5.2$  Hz, 1H), 3.48 – 3.34 (m, 2H), 3.29 – 3.20 (m, 2H), 2.84 – 2.72 (m, 2H), 2.21 – 2.14 (m, 1H), 2.07 – 1.96 (m, 4H), 1.92 – 1.86 (m, 1H);  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  171.9, 153.2, 142.6, 142.0, 135.1, 128.41, 128.35, 128.2, 127.5, 126.5, 125.8, 125.7, 124.6, 122.5, 121.4, 81.9, 68.0, 37.7, 34.1, 32.4, 31.5, 26.1. HRMS(ESI) m/z:  $[\text{M}+\text{H}]^+$  cacl. for  $\text{C}_{26}\text{H}_{28}\text{NOS}$  402.1886, found 402.1890.



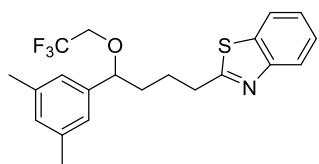
**2-(4-(3-(4-Chlorophenyl)propoxy)-4-phenylbutyl)benzo[d]thiazole (5i)**, colorless oil, 14.8 mg, 34%).  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  8.01 (d,  $J = 8.3$  Hz, 1H), 7.78 (d,  $J = 8.0$  Hz, 1H), 7.46 – 7.43 (m, 1H), 7.39 – 7.38 (m, 2H), 7.36 – 7.32 (m, 3H), 7.29 – 7.27 (m, 1H), 7.23 – 7.21 (m, 2H), 7.11 – 7.09 (m, 2H), 4.38 (t,  $J = 7.7$  Hz, 1H), 4.23 (t,  $J = 6.9$  Hz, 2H), 2.87 (t,  $J = 6.9$  Hz, 2H), 2.46 – 2.40 (m, 1H), 2.37 – 2.33 (m, 2H), 2.22 – 2.18 (m, 1H), 1.69 – 1.62 (m, 4H);  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  173.1, 153.9, 142.9, 141.2, 139.0, 132.3, 130.2, 128.9, 128.6, 128.0, 127.5, 126.0, 124.9, 122.8, 121.5, 64.5, 50.6, 34.9, 34.4, 33.9, 29.7, 23.1. HRMS(ESI) m/z:  $[\text{M}+\text{H}]^+$  cacl. for  $\text{C}_{26}\text{H}_{27}\text{ClNOS}$  436.1496, found 436.1498.



**2-(4-Phenyl-4-((3-phenylprop-2-yn-1-yl)oxy)butyl)benzo[d]thiazole (5j,** colorless oil, 19.9 mg, 50%).  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.95 (d,  $J = 8.1$  Hz, 1H), 7.81 (d,  $J = 8.0$  Hz, 1H), 7.46 – 7.42 (m, 3H), 7.38 – 7.34 (m, 5H), 7.32 – 7.27 (m, 4H), 4.61 (dd,  $J = 7.8, 5.4$  Hz, 1H), 4.35 – 4.32 (m, 1H), 4.11 – 4.08 (m, 1H), 3.17 – 3.14 (m, 2H), 2.14 – 2.07 (m, 1H), 2.06 – 1.99 (m, 1H), 1.97 – 1.88 (m, 1H), 1.86 – 1.80 (m, 1H);  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  171.9, 153.2, 141.2, 135.1, 131.7, 128.5, 128.3, 128.2, 127.9, 126.9, 125.8, 124.6, 122.9, 122.5, 121.5, 86.0, 85.3, 80.4, 56.5, 37.2, 34.0, 26.0. HRMS(ESI) m/z:  $[\text{M}+\text{H}]^+$  caclcd. for  $\text{C}_{26}\text{H}_{24}\text{NOS}$  398.1573, found 398.1567.

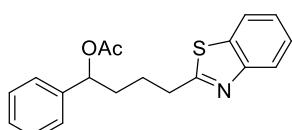


**2-((2,3-Dihydro-1H-inden-2-yl)oxy)-4-phenylbutylbenzo[d]thiazole (5k,** white solid, 12.0 mg, 30%).  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  8.00 (d,  $J = 8.2$  Hz, 1H), 7.78 (d,  $J = 8.0$  Hz, 1H), 7.46 – 7.43 (m, 1H), 7.38 – 7.31 (m, 5H), 7.27 – 7.25 (m, 1H), 7.23 – 7.17 (m, 4H), 5.52 – 5.50 (m, 1H), 4.37 (t,  $J = 7.7$  Hz, 1H), 3.29 (dd,  $J = 16.9, 6.5$  Hz, 2H), 2.98 (dd,  $J = 16.9, 3.1$  Hz, 2H), 2.45 – 2.40 (m, 1H), 2.35 – 2.32 (m, 2H), 2.24 – 2.18 (m, 1H), 1.70 – 1.65 (m, 2H);  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  173.2, 153.0, 141.3, 140.4, 135.2, 128.8, 128.0, 127.4, 126.7, 125.9, 124.8, 124.6, 122.8, 121.5, 75.2, 50.7, 39.6, 34.9, 34.1, 23.1. HRMS(ESI) m/z:  $[\text{M}+\text{H}]^+$  caclcd. for  $\text{C}_{26}\text{H}_{26}\text{NOS}$  400.1730, found 400.1732.

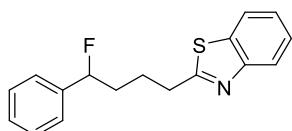


**2-(4-(3,5-Dimethylphenyl)-4-(2,2,2-trifluoroethoxy)butyl)benzo[d]thiazole (5l,**

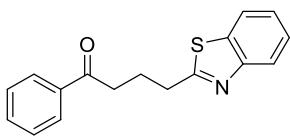
yellow oil, 11.0 mg, 28%).  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.96 (d,  $J = 8.1$  Hz, 1H), 7.83 (d,  $J = 7.9$  Hz, 1H), 7.46 – 7.43 (m, 1H), 7.36 – 7.33 (m, 1H), 6.94 (br, 1H), 6.88 (br, 2H), 4.36 (dd,  $J = 8.0, 5.2$  Hz, 1H), 3.74 – 3.55 (m, 2H), 3.16 – 3.12 (m, 2H), 2.31 (s, 6H), 2.09 – 2.05 (m, 1H), 2.01 – 1.95 (m, 1H), 1.91 – 1.86 (m, 1H), 1.80 – 1.76 (m, 1H);  $^{19}\text{F}$  NMR (471 MHz,  $\text{CDCl}_3$ )  $\delta$  -73.8 (t,  $J = 8.3$  Hz, 3F);  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  171.7, 153.1, 140.2, 138.3, 135.1, 129.9, 125.9, 124.7, 124.42 (q,  $J = 213.4$  Hz), 124.4, 122.5, 121.5, 83.4, 65.8 (q,  $J = 34.0$  Hz), 37.2, 33.9, 25.9, 21.3. HRMS(ESI) m/z:  $[\text{M}+\text{H}]^+$  caclcd. for  $\text{C}_{21}\text{H}_{23}\text{F}_3\text{NOS}$  394.1447, found 394.1452.



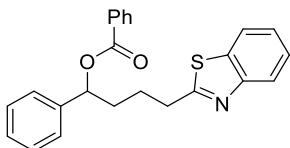
**4-(Benzo[d]thiazol-2-yl)-1-phenylbutyl acetate (5m)**, colorless oil, 14.6 mg, 45%).  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.96 (d,  $J = 8.1$  Hz, 1H), 7.83 (d,  $J = 8.0$  Hz, 1H), 7.46 – 7.43 (m, 1H), 7.36 – 7.28 (m, 6H), 5.80 – 5.77 (m, 1H), 3.13 (t,  $J = 6.8$  Hz, 2H), 2.07 (s, 3H), 2.05 – 1.82 (m, 4H);  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  171.4, 170.4, 153.1, 140.2, 135.0, 128.5, 128.0, 126.4, 125.9, 124.8, 122.5, 121.5, 75.5, 35.6, 33.8, 25.6, 21.2. HRMS(ESI) m/z:  $[\text{M}+\text{H}]^+$  caclcd. for  $\text{C}_{19}\text{H}_{20}\text{NO}_2\text{S}$  326.1209, found 326.1211.



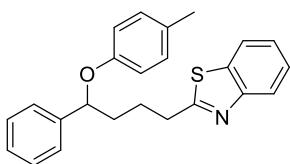
**2-(4-Fluoro-4-phenylbutyl)benzo[d]thiazole (5n)**, colorless oil, 10.0 mg, 35%).  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.97 – 7.96 (m, 1H), 7.85 – 7.83 (m, 1H), 7.47 – 7.44 (m, 1H), 7.38 – 7.32 (m, 6H), 5.50 (ddd,  $J = 47.7, 7.7, 4.1$  Hz, 1H), 3.23 – 3.14 (m, 2H), 2.17 – 2.06 (m, 2H), 2.05 – 1.92 (m, 2H);  $^{19}\text{F}$  NMR (471 MHz,  $\text{CDCl}_3$ )  $\delta$  -175.2 (ddd,  $J = 45.9, 29.0, 16.4$  Hz, 1F);  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  171.3, 153.1, 140.0 (d,  $J = 19.7$  Hz), 135.1, 128.5, 128.3 (d,  $J = 1.3$  Hz), 126.0, 125.5 (d,  $J = 6.9$  Hz), 124.8, 122.5, 121.5, 94.10 (d,  $J = 171.1$  Hz), 36.4 (d,  $J = 23.9$  Hz), 33.8, 25.2 (d,  $J = 4.2$  Hz). HRMS(ESI) m/z:  $[\text{M}+\text{H}]^+$  caclcd. for  $\text{C}_{17}\text{H}_{17}\text{FNS}$  286.1060, found 286.1059.



**4-(benzo[d]thiazol-2-yl)-1-phenylbutan-1-one (6,** white solid, 51.2 mg, 91%).  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.97 – 7.93 (m, 3H), 7.83 – 7.82 (m, 1H), 7.53 – 7.34 (m, 5H), 3.25 – 3.22 (m, 2H), 3.14 – 3.11 (m, 2H), 2.37 – 2.31 (m, 2H);  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  199.2, 171.2, 153.1, 136.7, 135.1, 133.0, 128.5, 128.0, 125.9, 124.7, 122.5, 121.5, 37.3, 33.4, 23.7. HRMS(ESI) m/z:  $[\text{M}+\text{H}]^+$  caclcd. for  $\text{C}_{17}\text{H}_{16}\text{NOS}$  282.0947, found 282.0950.



**4-(Benzo[d]thiazol-2-yl)-1-phenylbutyl benzoate (7,** white solid, 62.0 mg, 80%).  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  8.09 – 8.07 (m, 2H), 8.00 – 7.95 (m, 1H), 7.83 – 7.82 (m, 1H), 7.57 – 7.54 (m, 1H), 7.46 – 7.41 (m, 5H), 7.36 – 7.33 (m, 3H), 7.30 – 7.27 (m, 1H), 6.06 (dd,  $J = 7.6, 5.2$  Hz, 1H), 3.17 (t,  $J = 7.3$  Hz, 2H), 2.26 – 2.18 (m, 1H), 2.11 – 2.02 (m, 2H), 1.99 – 1.92 (m, 1H);  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  171.3, 165.8, 153.1, 140.3, 135.1, 133.0, 130.3, 129.7, 128.6, 128.4, 128.0, 126.4, 125.9, 124.8, 122.5, 121.5, 76.1, 35.8, 33.9, 25.6. HRMS(ESI) m/z:  $[\text{M}+\text{H}]^+$  caclcd. for  $\text{C}_{24}\text{H}_{22}\text{NO}_2\text{S}$  388.1366, found 388.1362.



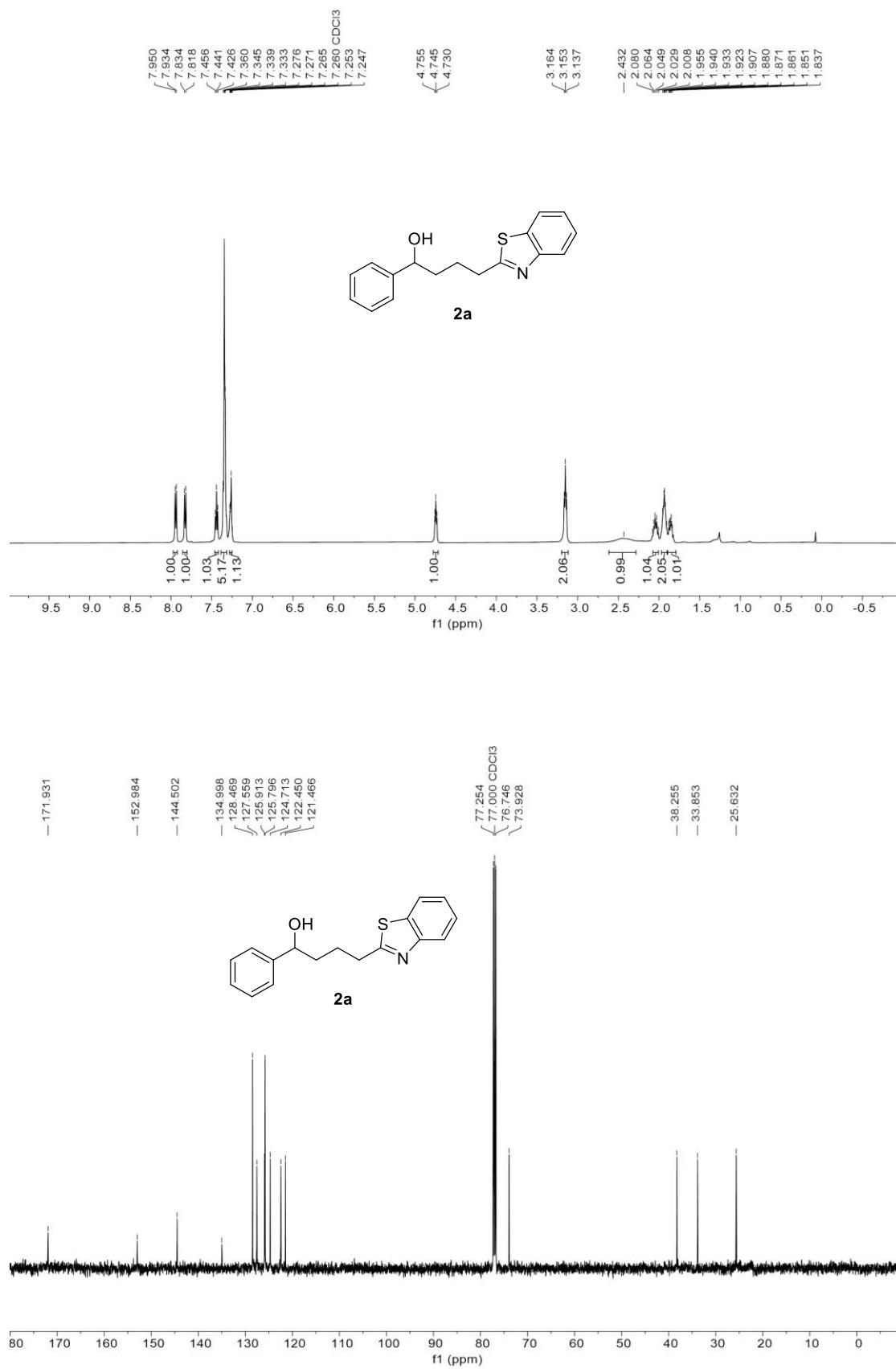
**2-(4-Phenyl-4-(p-tolyloxy)butyl)benzo[d]thiazole (8,** white solid, 44.8 mg, 60%).  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.97 – 7.95 (m, 1H), 7.84 – 7.82 (m, 1H), 7.46 – 7.43 (m, 1H), 7.36 – 7.29 (m, 5H), 7.24 – 7.22 (m, 1H), 6.97 – 6.95 (m, 2H), 6.74 – 6.72 (m, 2H), 5.11 (dd,  $J = 7.7, 4.5$  Hz, 1H), 3.19 – 3.15 (m, 2H), 2.21 (s, 3H), 2.18 – 2.08 (m, 2H), 2.06 – 1.93 (m, 2H);  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  171.7, 156.0, 153.1, 141.9,

135.1, 129.9, 129.7, 128.6, 127.9, 127.5, 125.9, 124.7, 122.5, 121.5, 115.7, 79.7, 38.0, 34.0, 25.9, 20.4. HRMS(ESI) m/z: [M+H]<sup>+</sup> caclcd. for C<sub>24</sub>H<sub>24</sub>NOS 374.1573, found 374.1570.

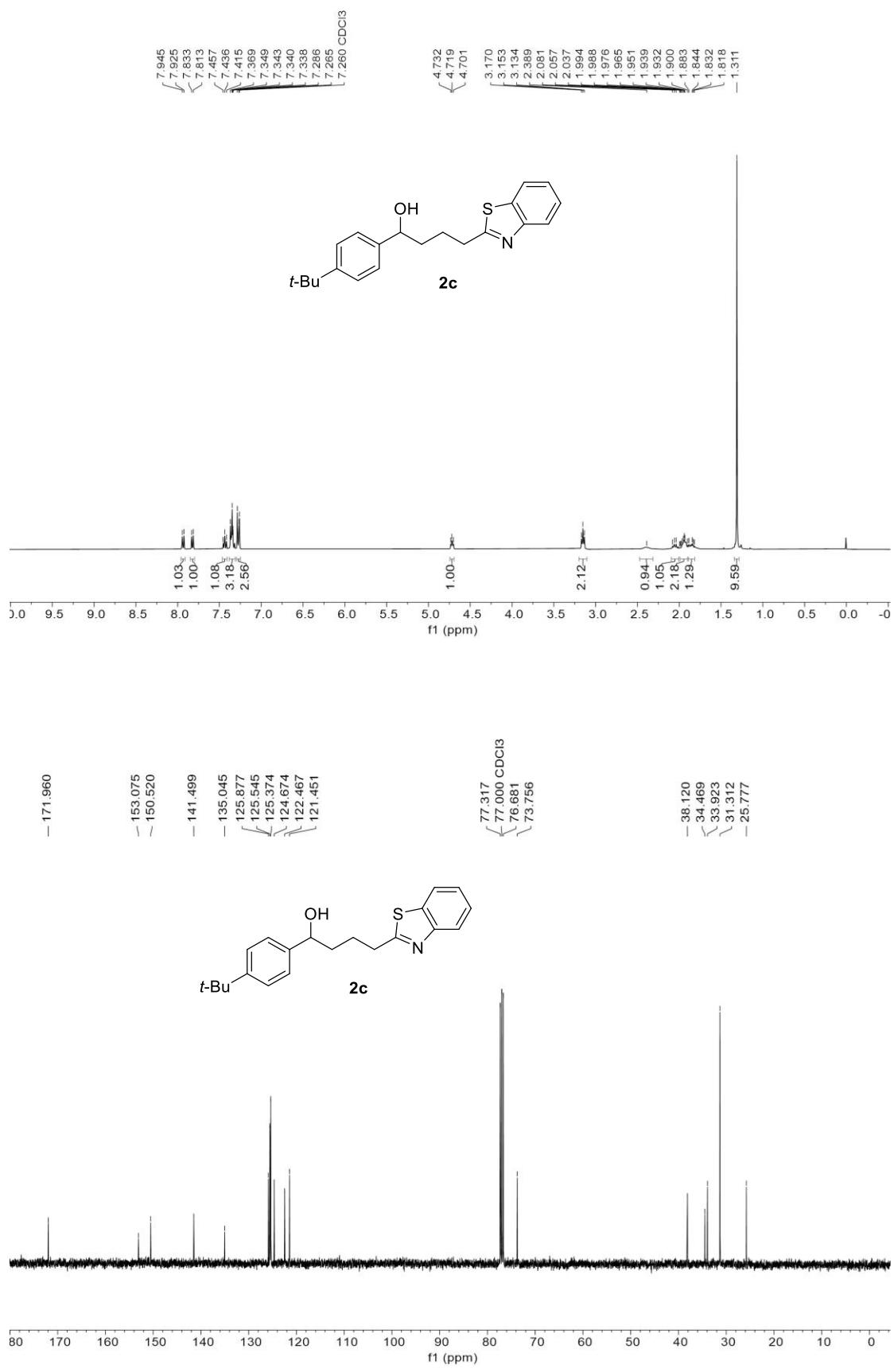
## 7. References

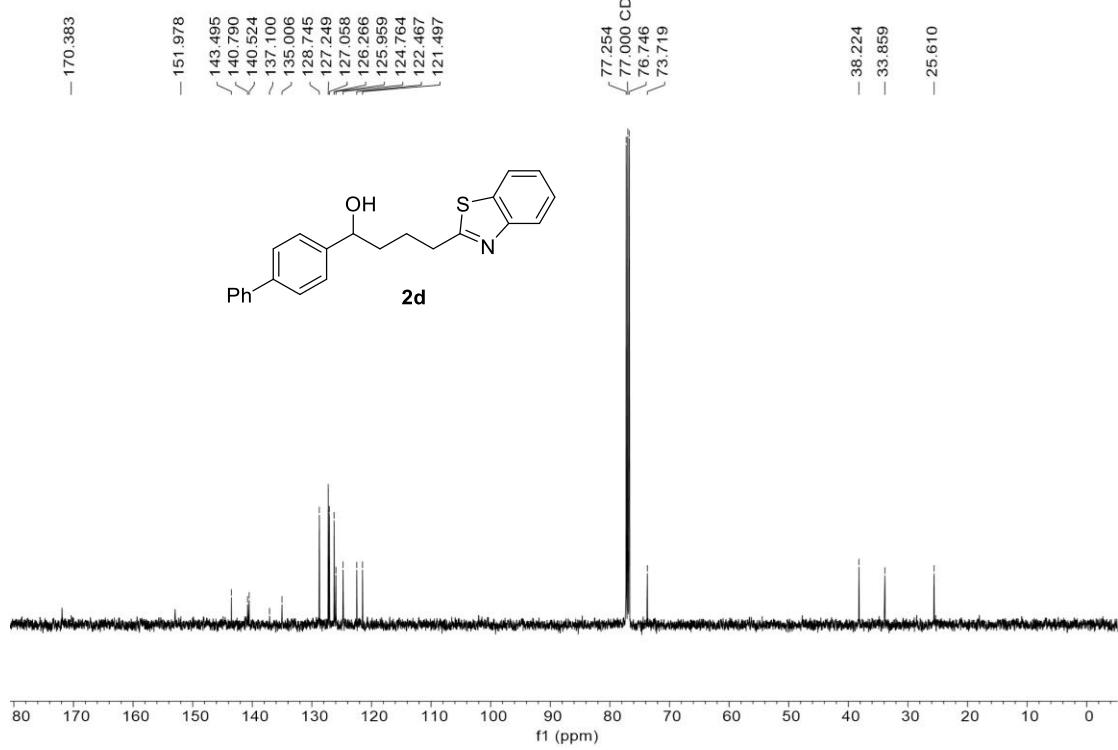
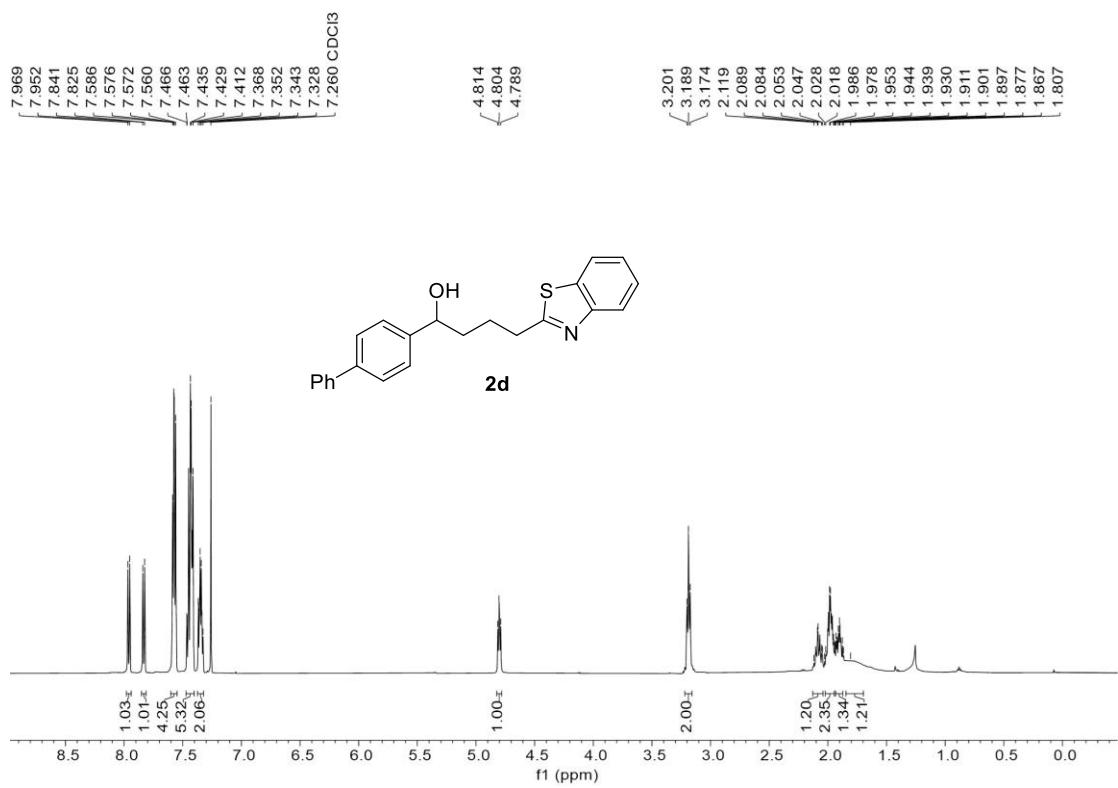
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4. R. A. Altman, A. Shafir, A. Choi, P. A. Lichtor and S. L. Buchwald, *J. Org. Chem.*, 2008, **73**, 284–286.

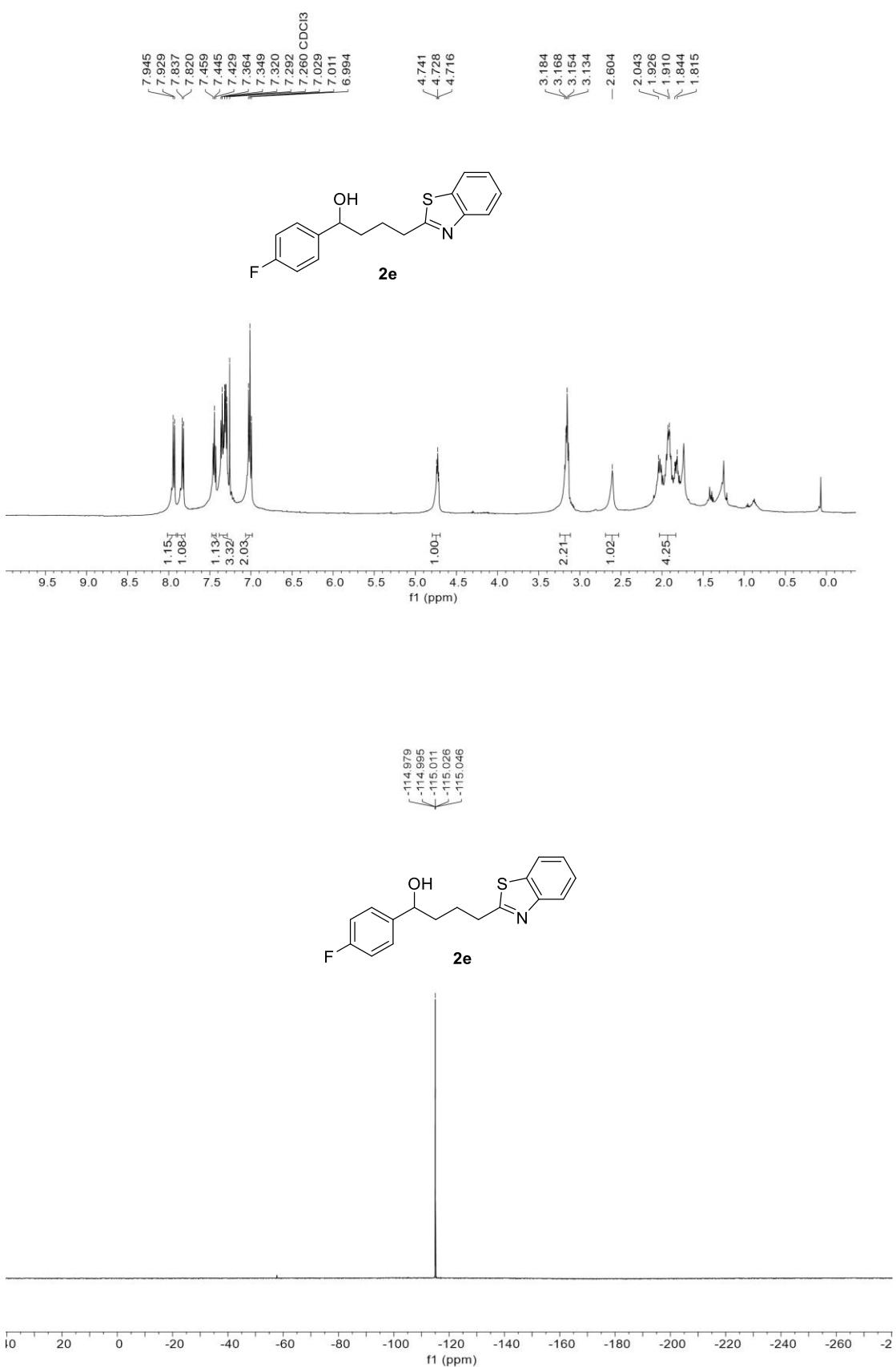
## 8. NMR spectra

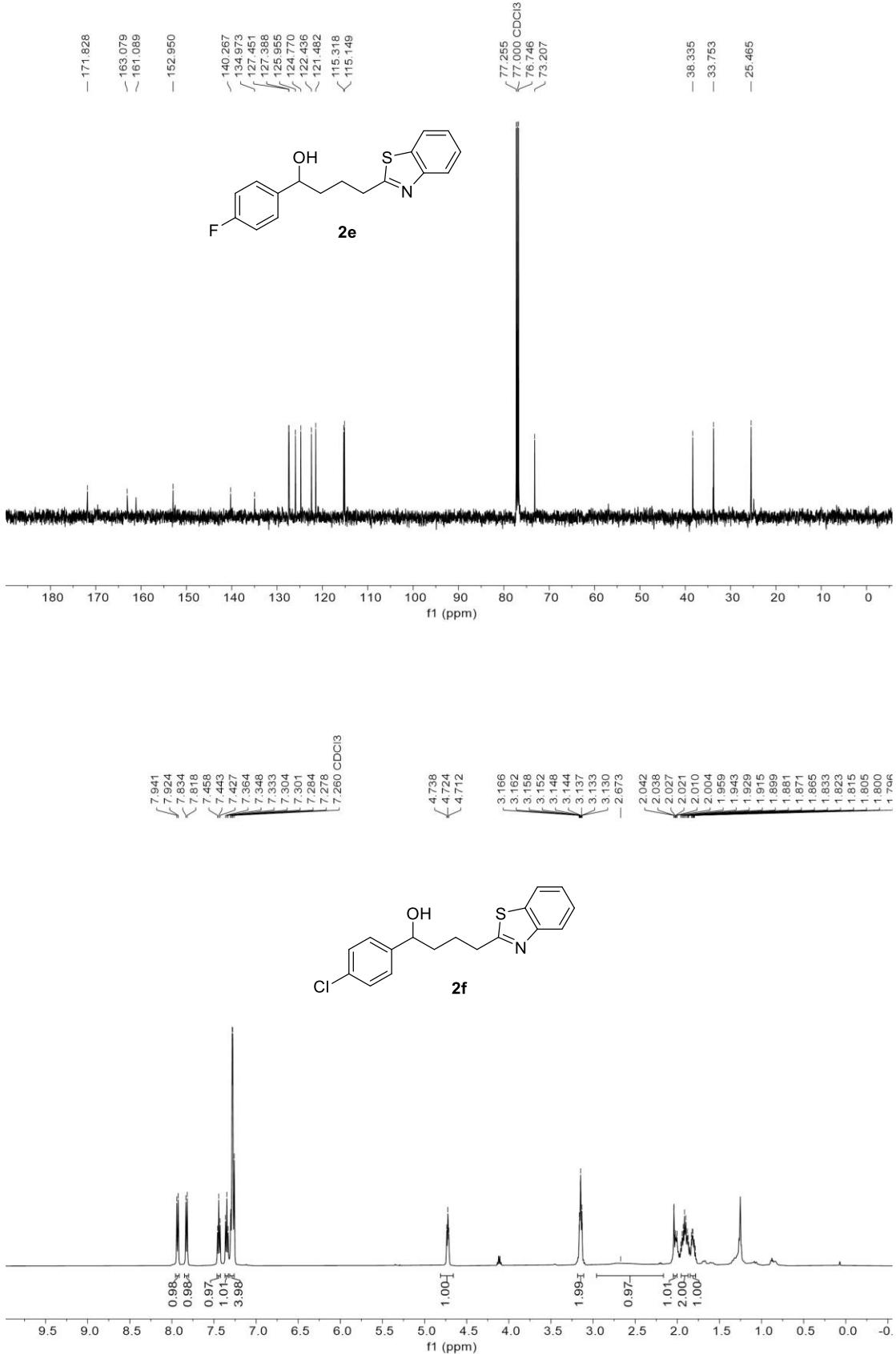


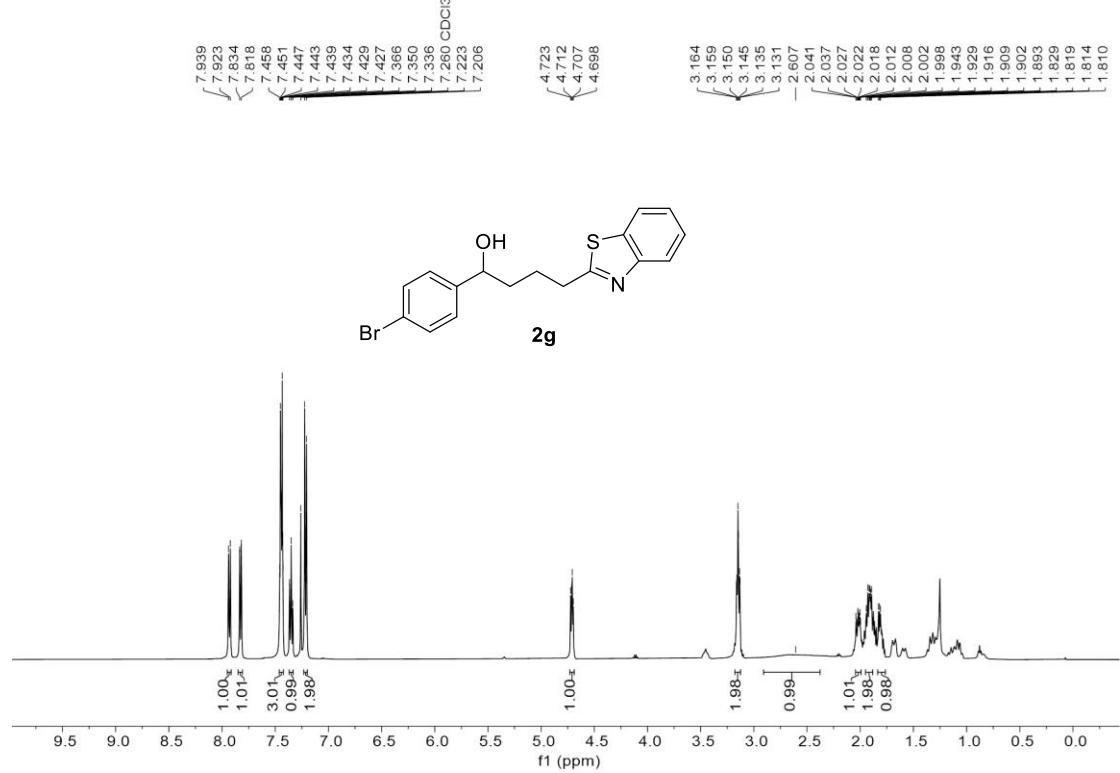
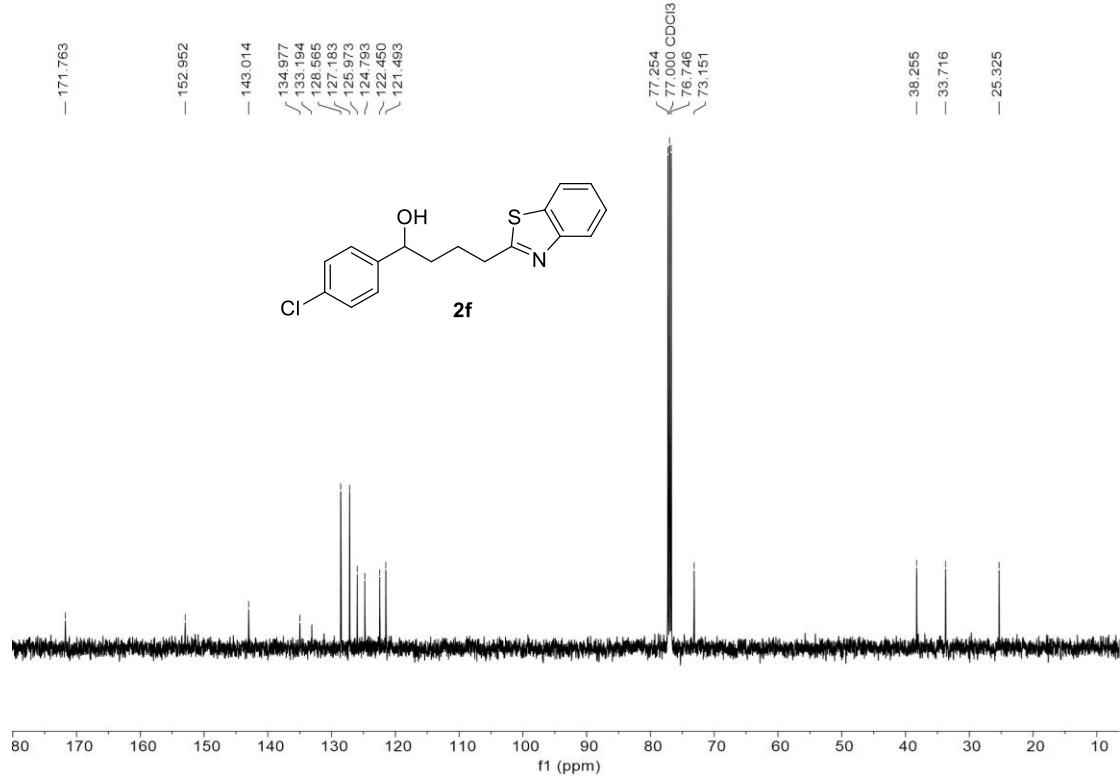


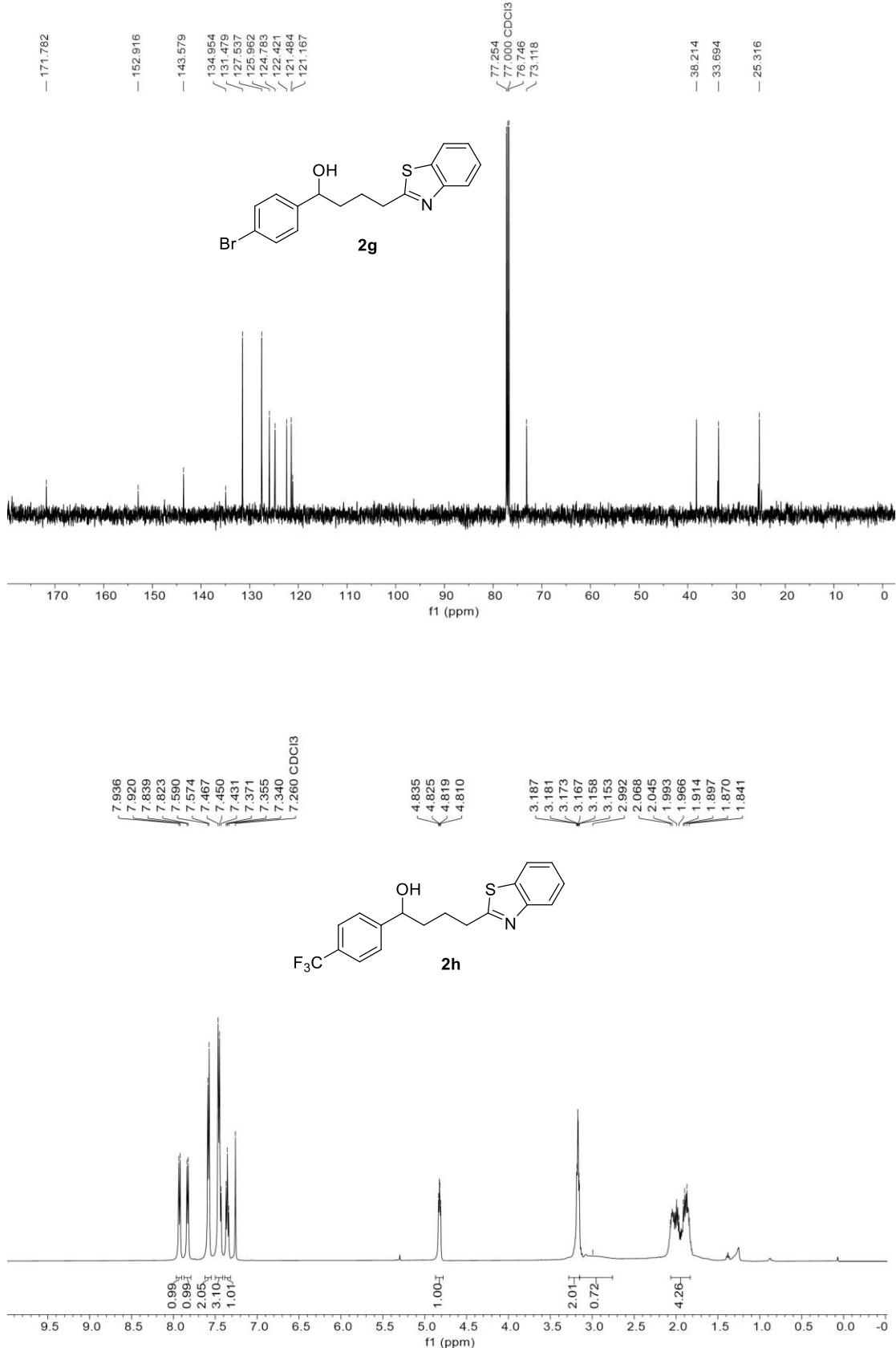


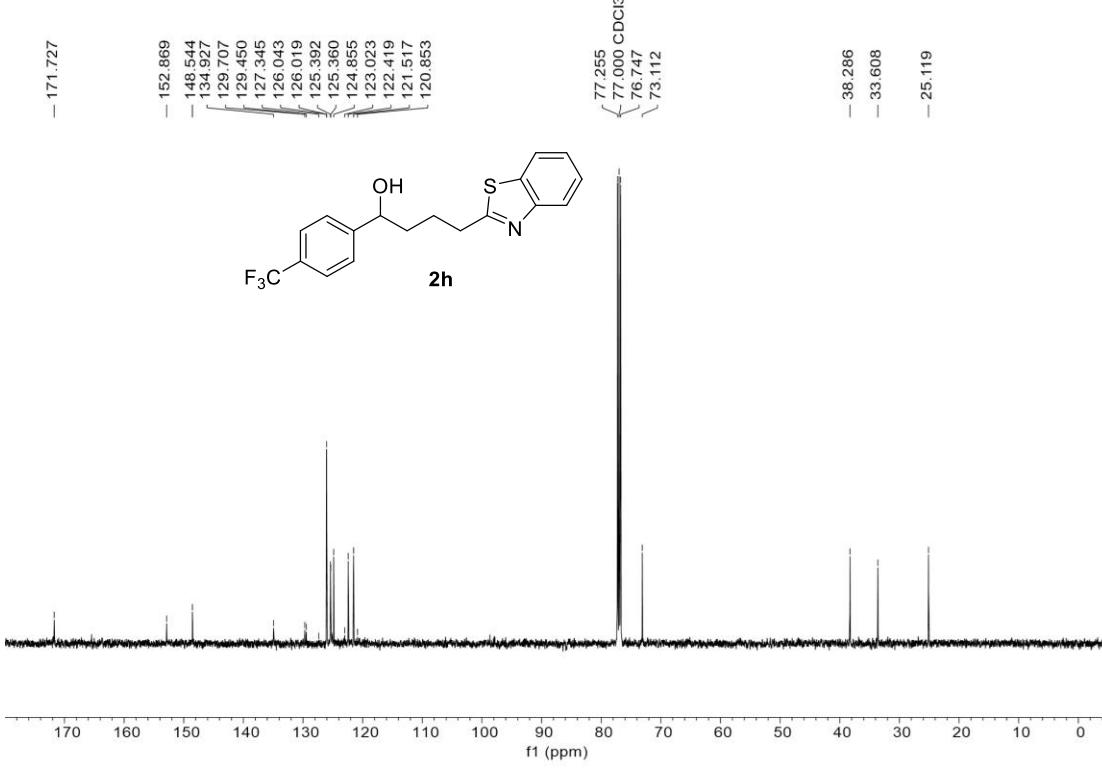
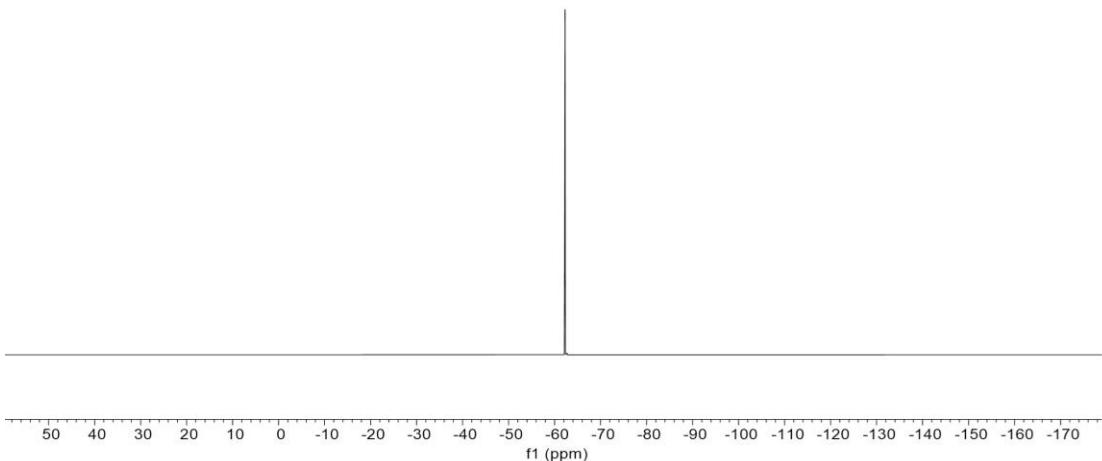
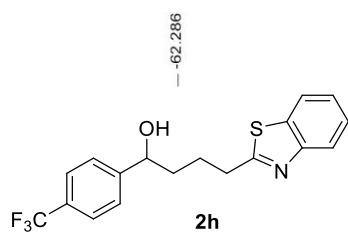


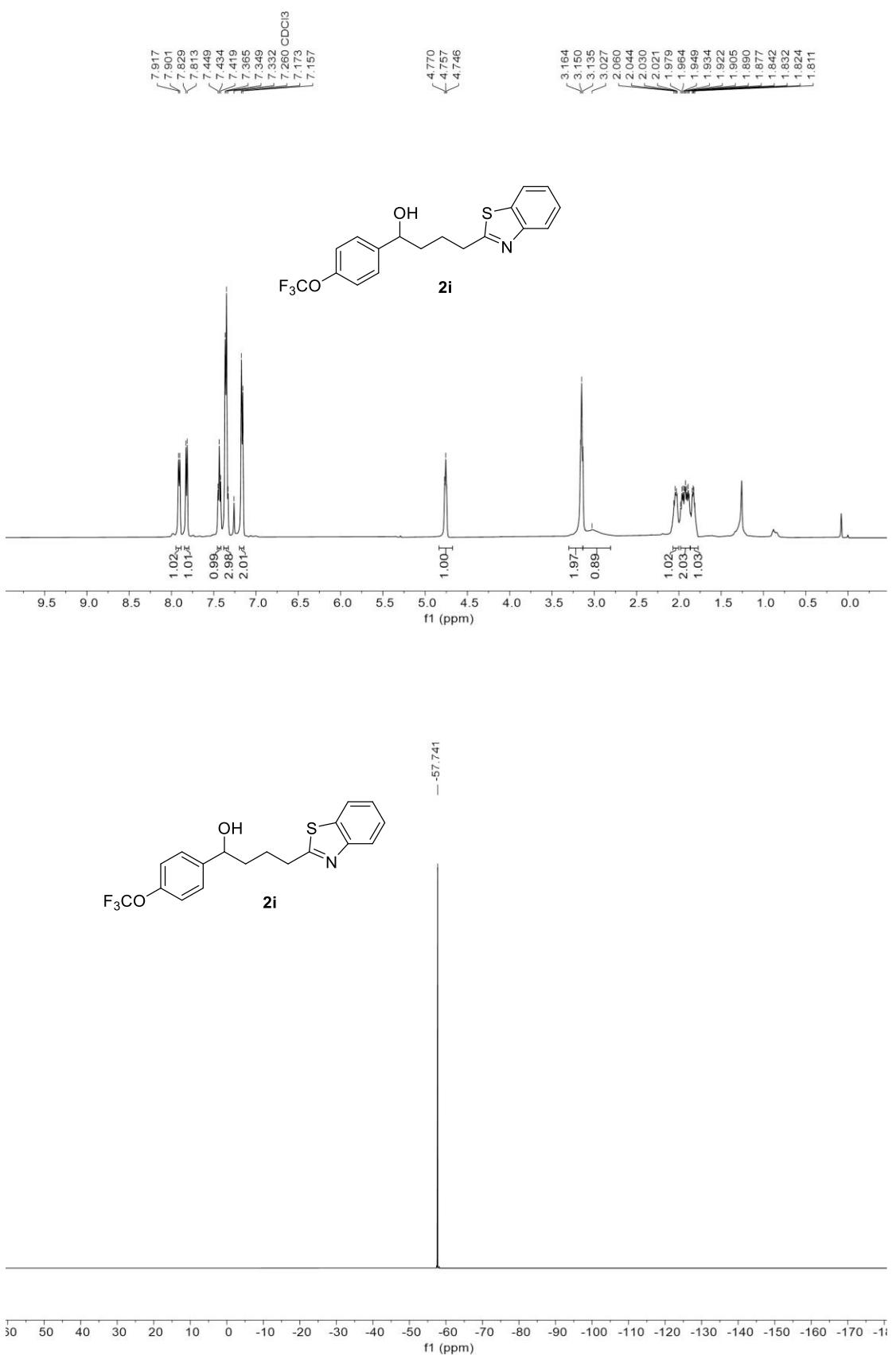


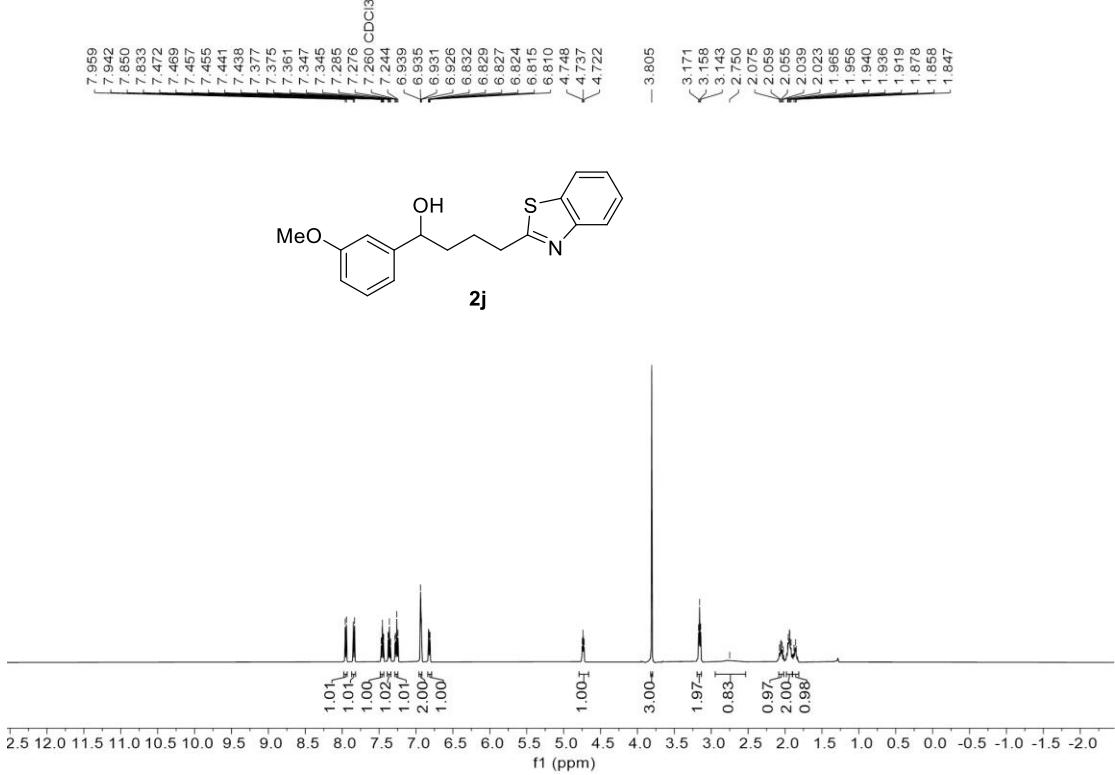
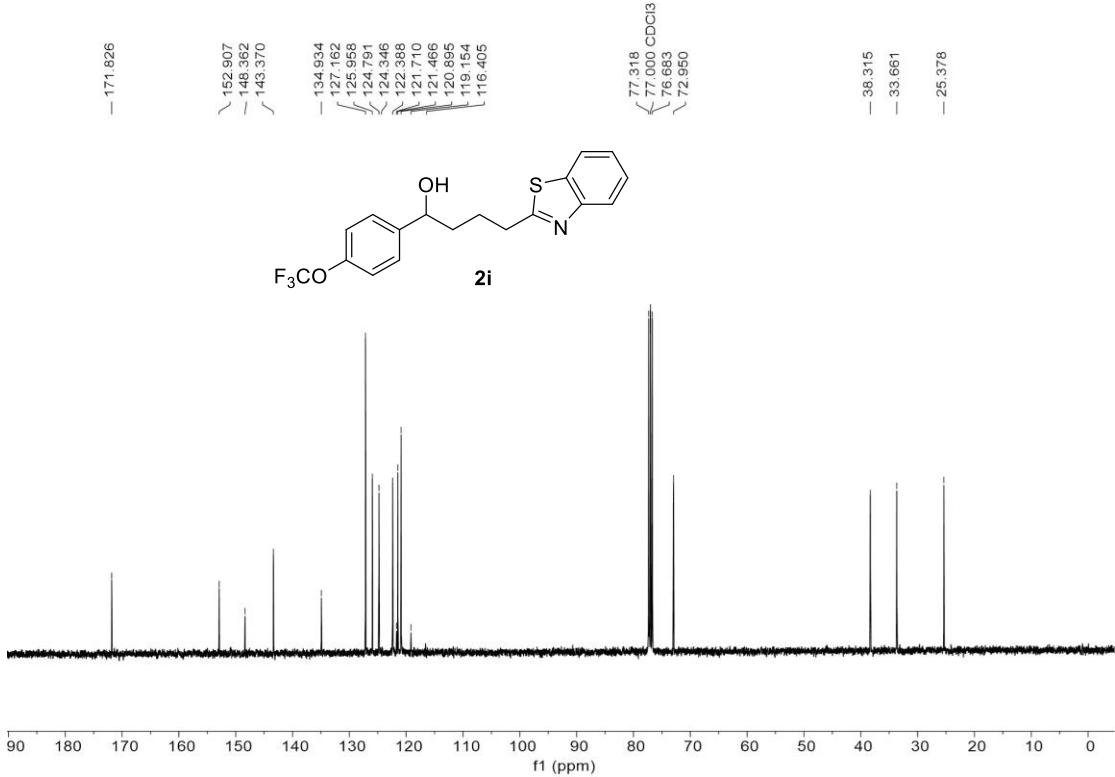


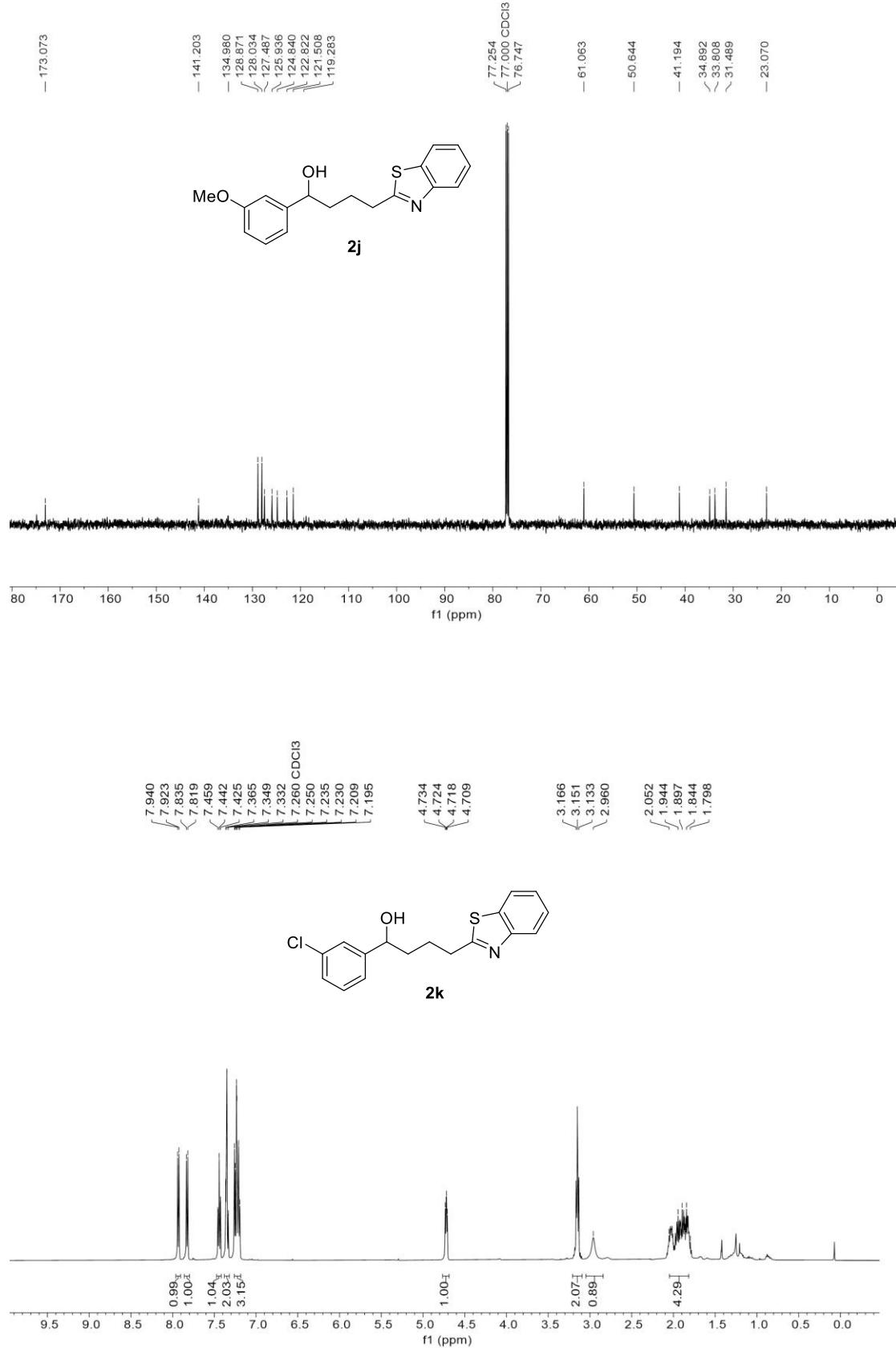


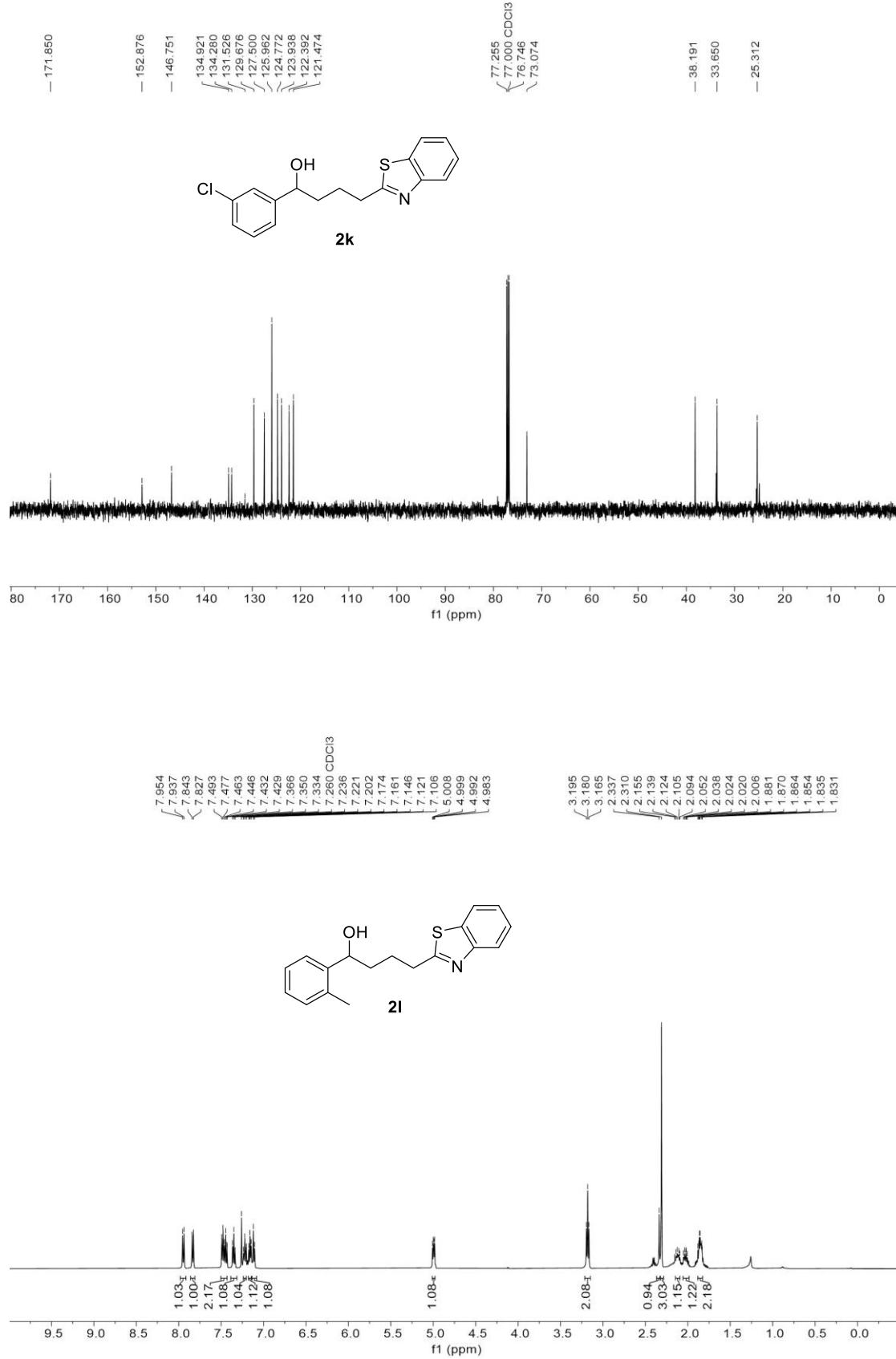


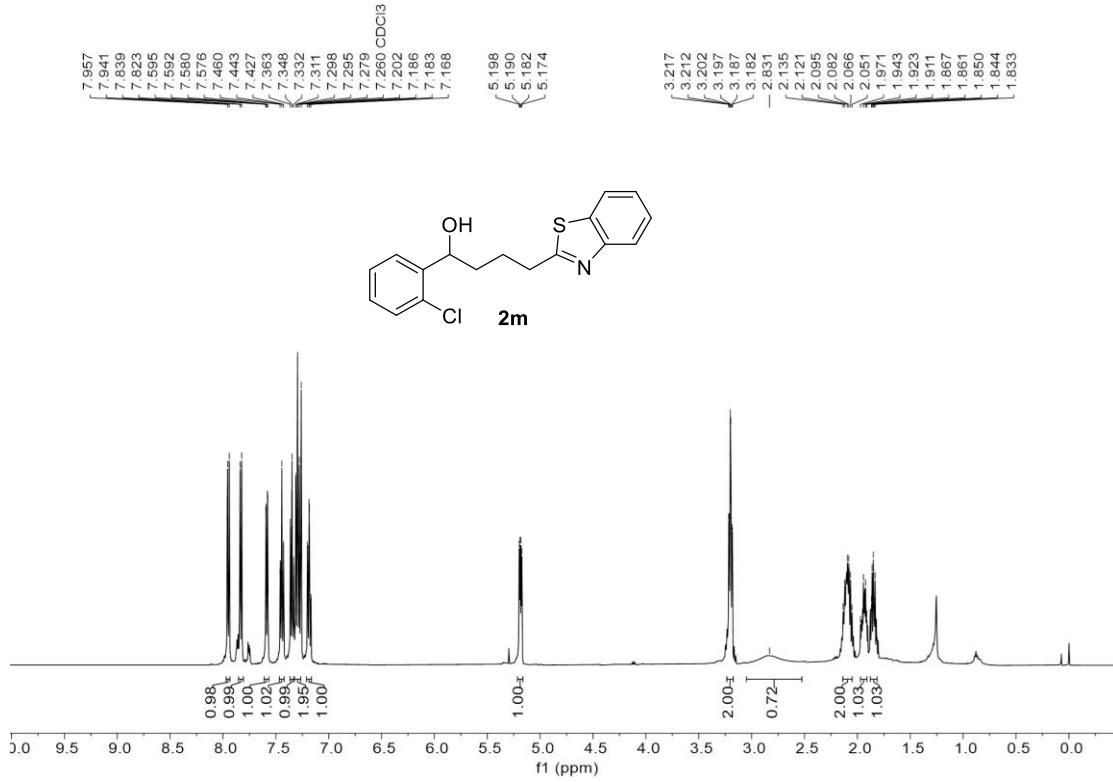
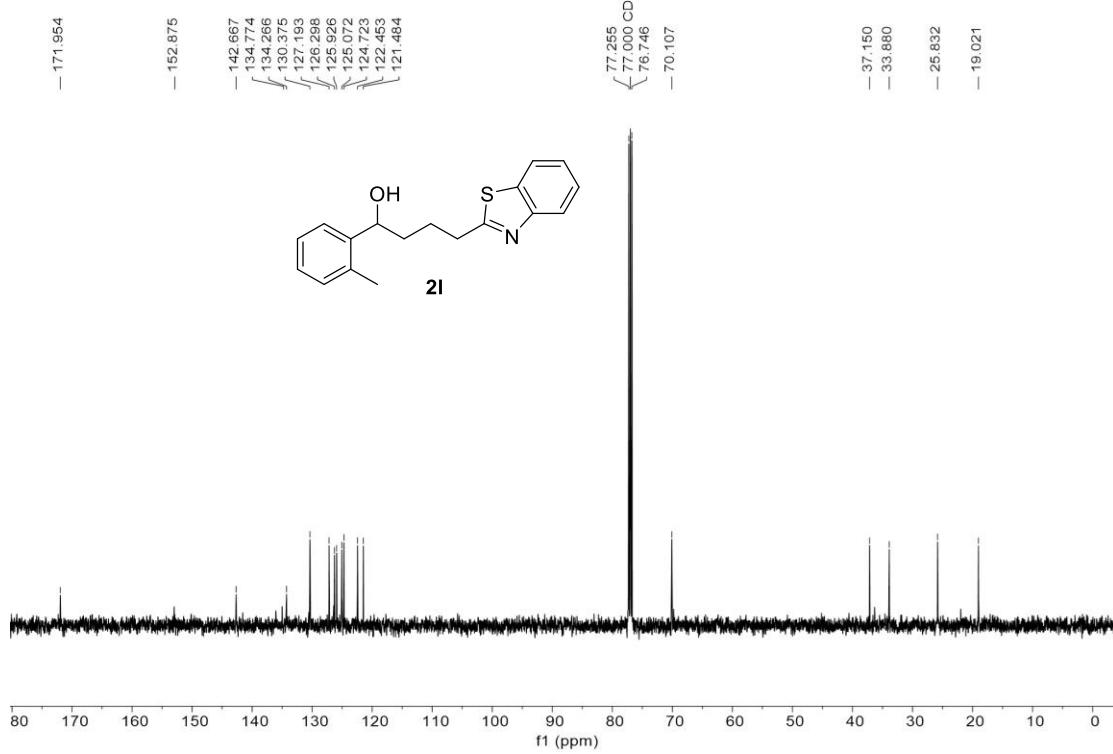


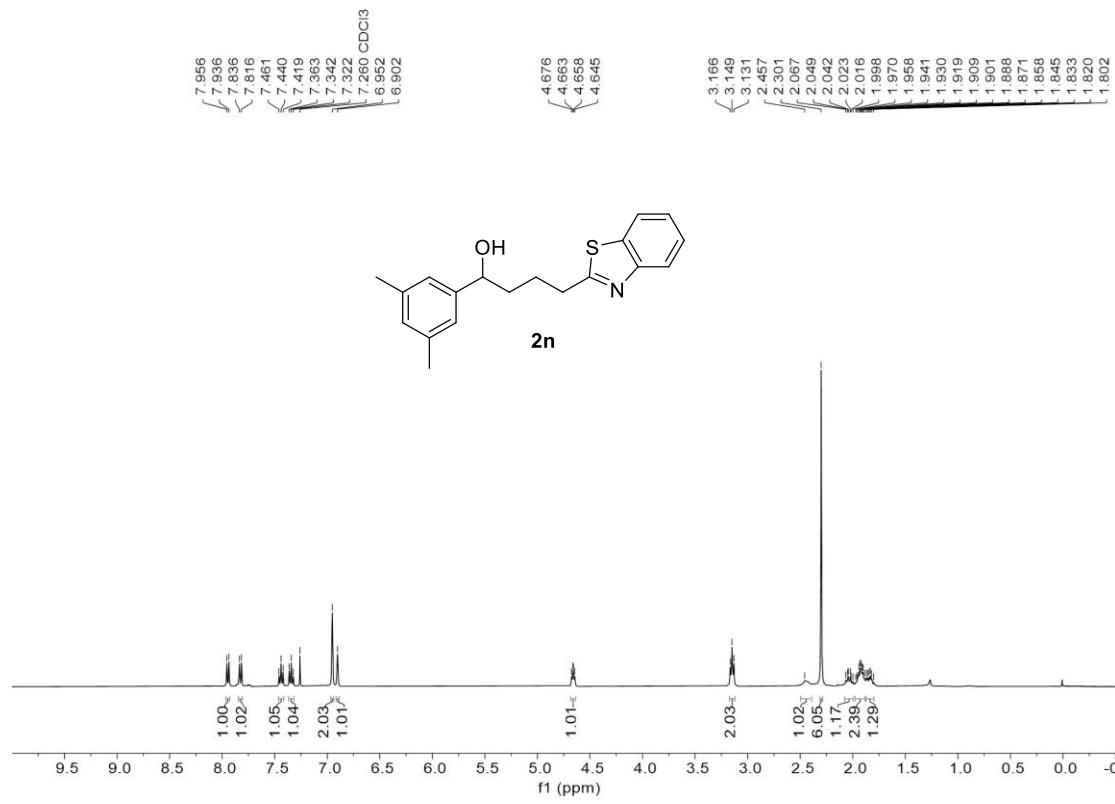
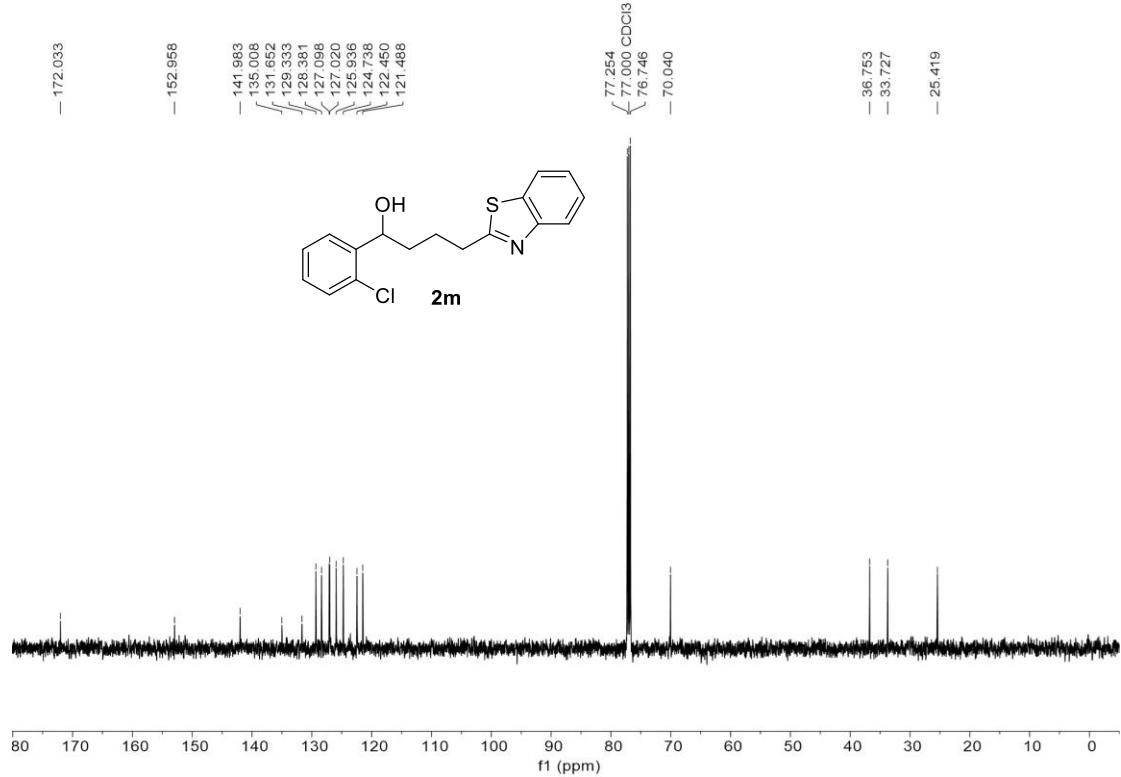












— 172.007

— 153.051

— 144.482

— 137.987

— 135.033

— 129.156

— 125.864

— 124.661

— 123.590

— 122.451

— 121.431

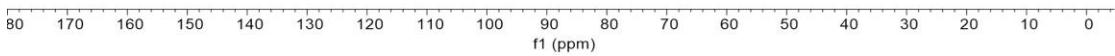
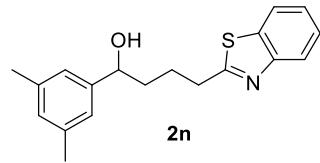
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77.000 CDCl<sub>3</sub>  
76.682  
73.965

— 38.169

— 33.889

— 25.757

— 21.264



7.928

7.907

7.819

7.796

7.785

7.760

7.747

7.743

7.454

7.442

7.429

7.408

7.388

7.343

7.324

7.305

7.260 CDCl<sub>3</sub>

4.885

4.872

4.856

3.291

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3.113

3.097

3.097

2.069

2.063

2.055

2.049

2.043

2.038

2.015

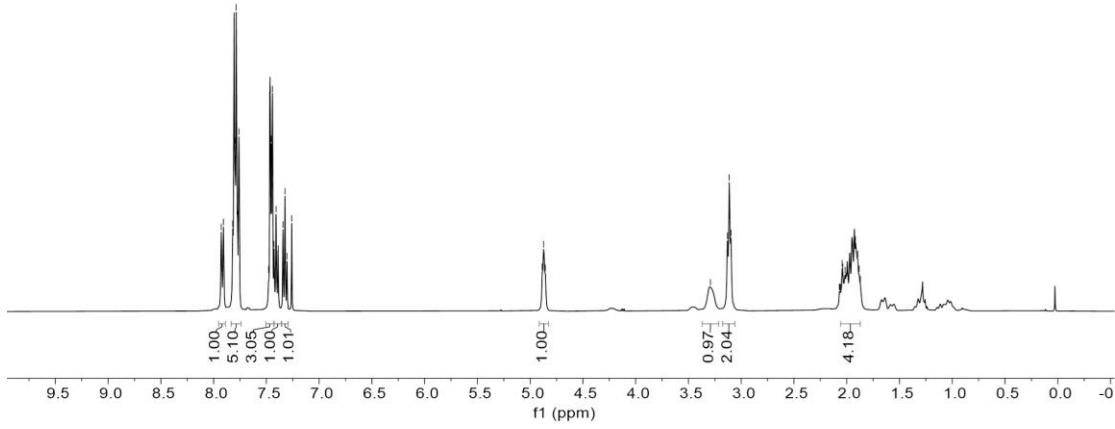
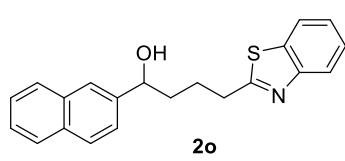
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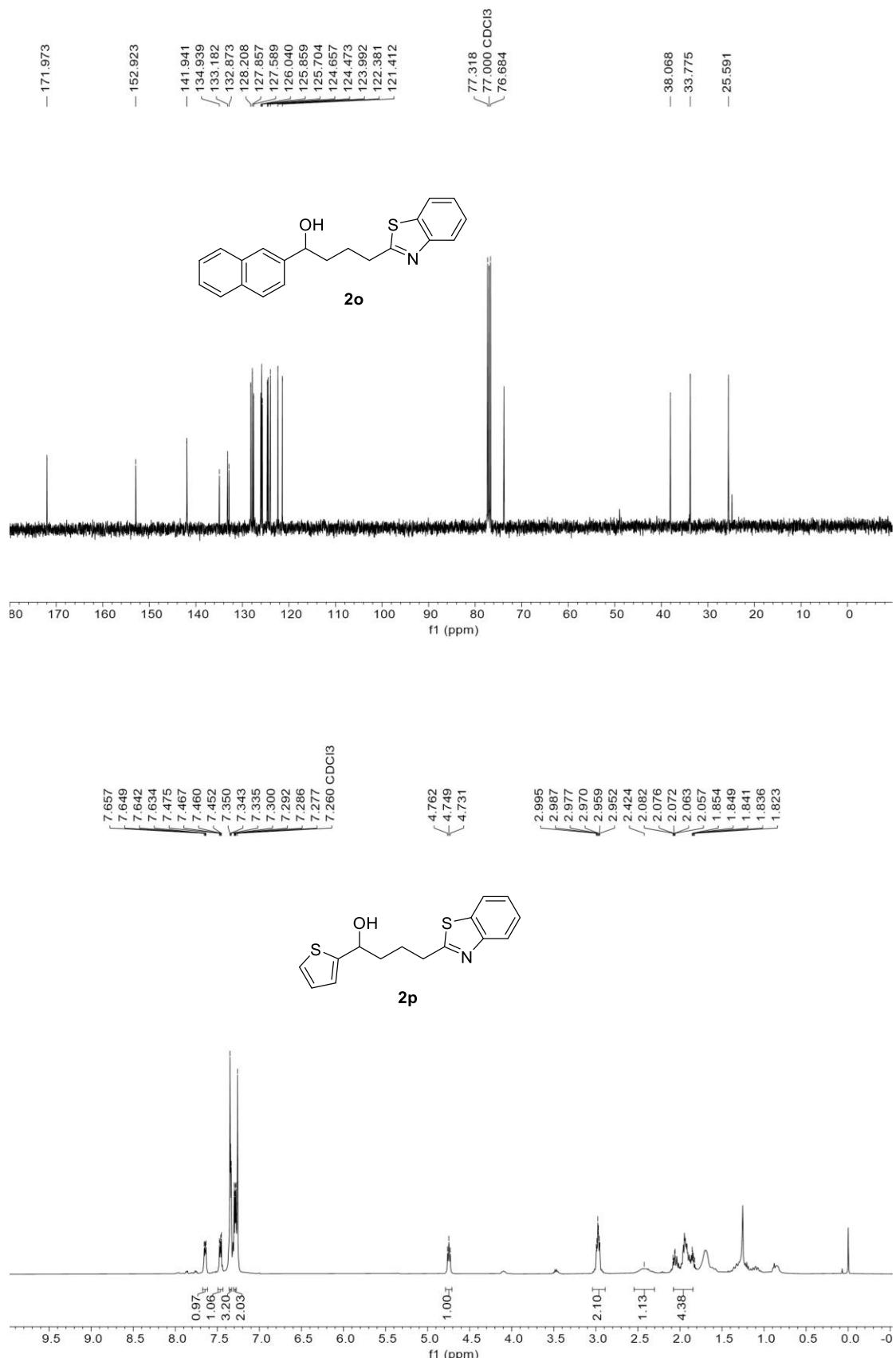
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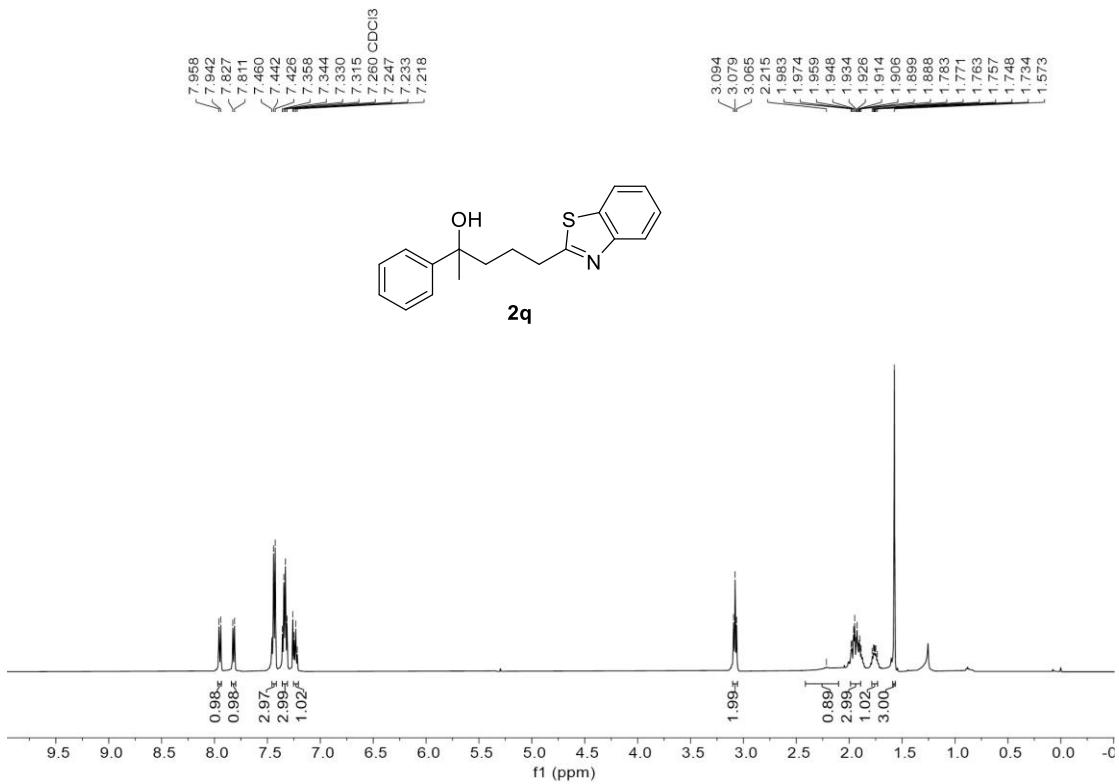
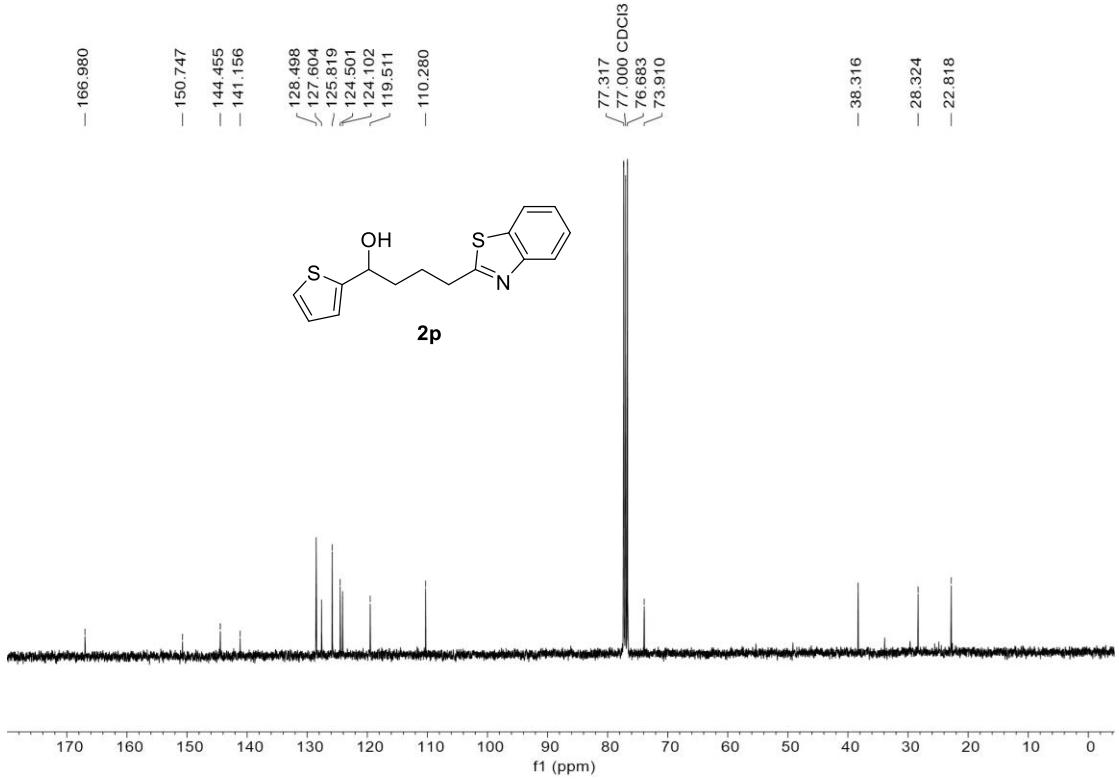
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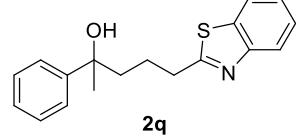
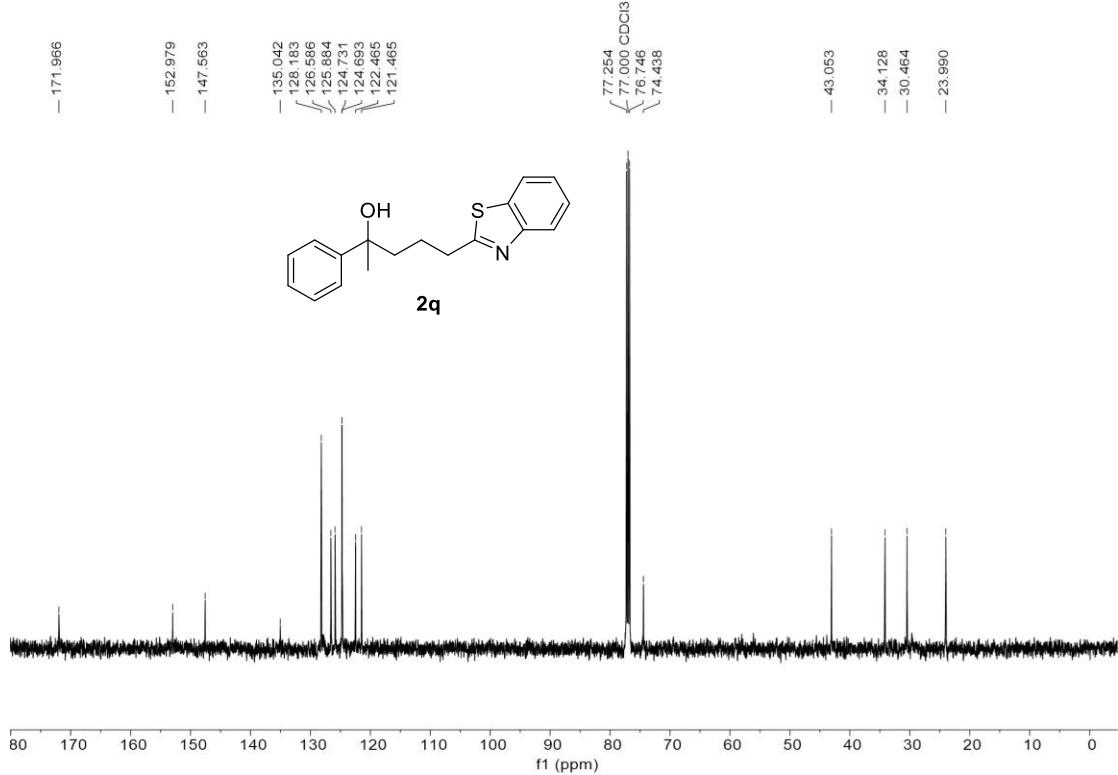
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1.871

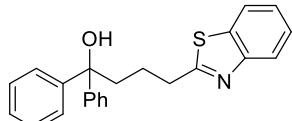
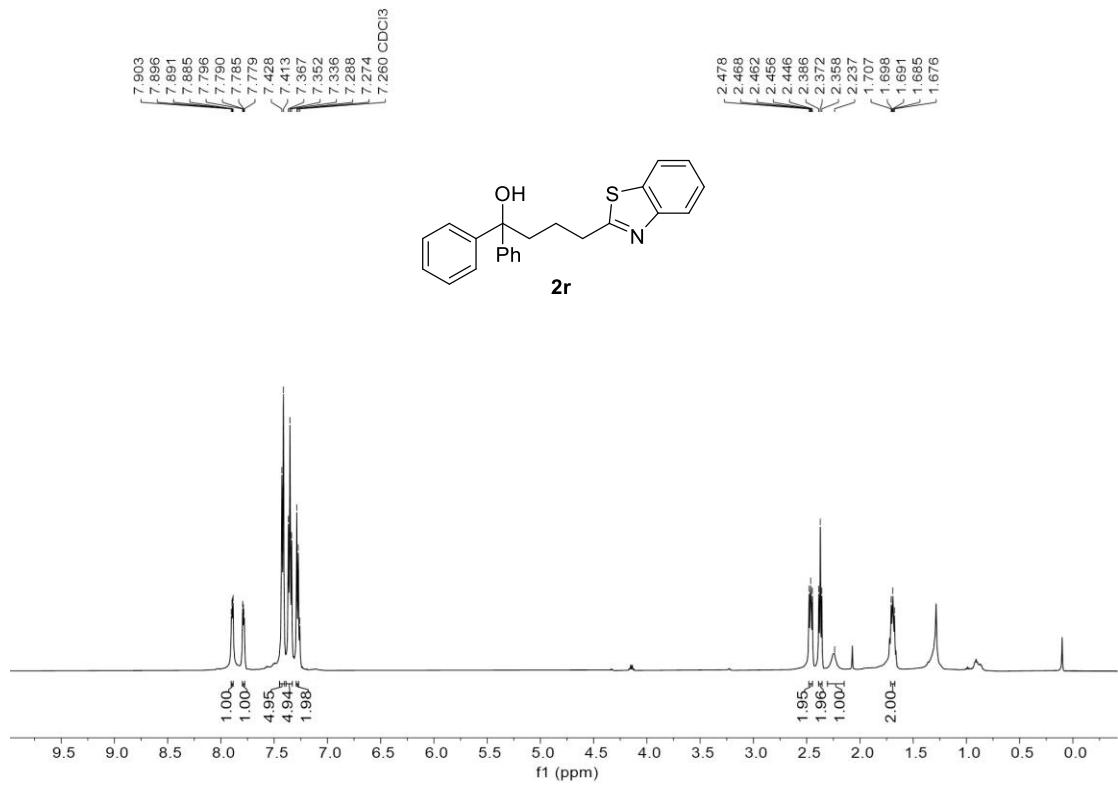




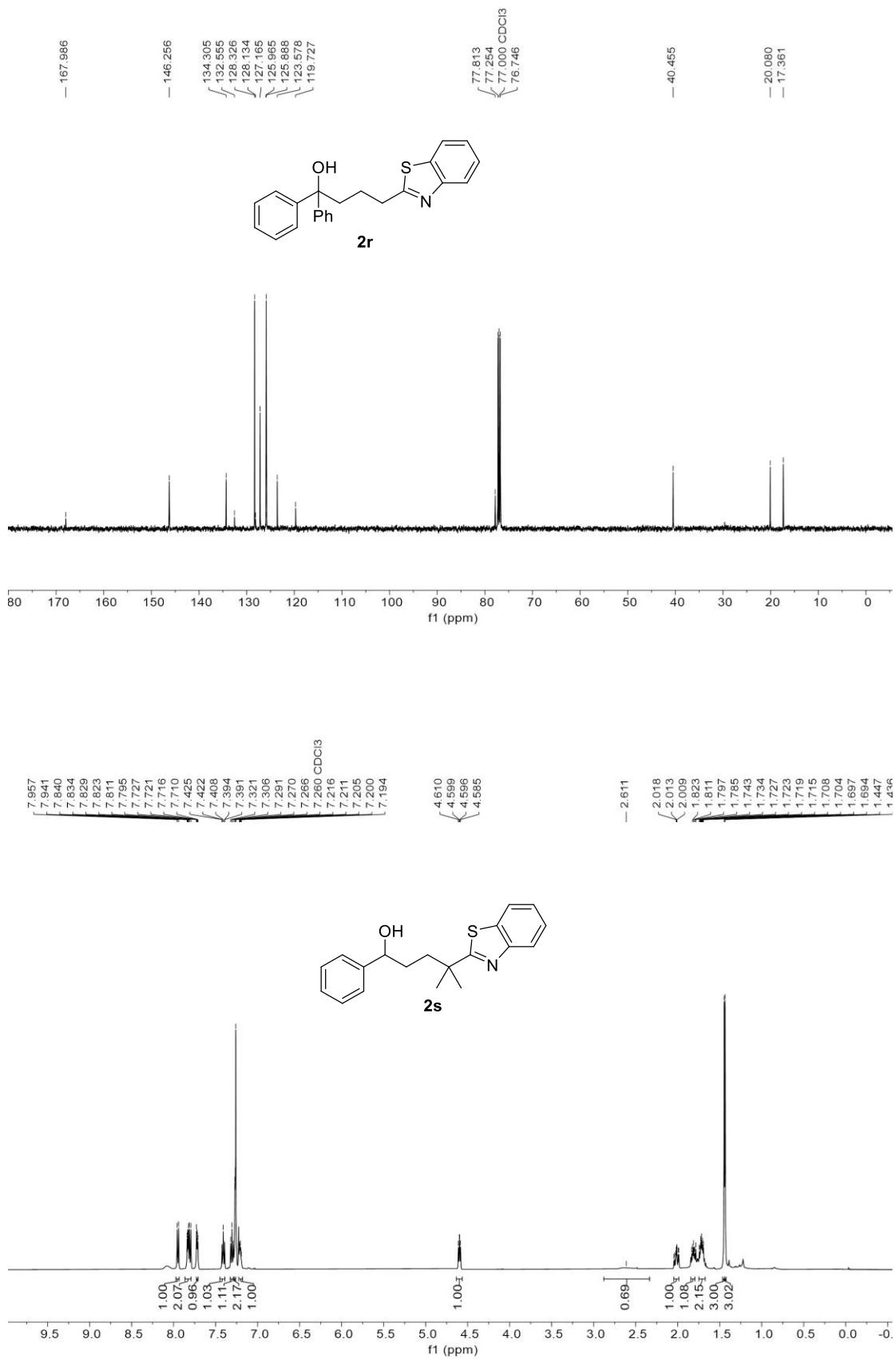


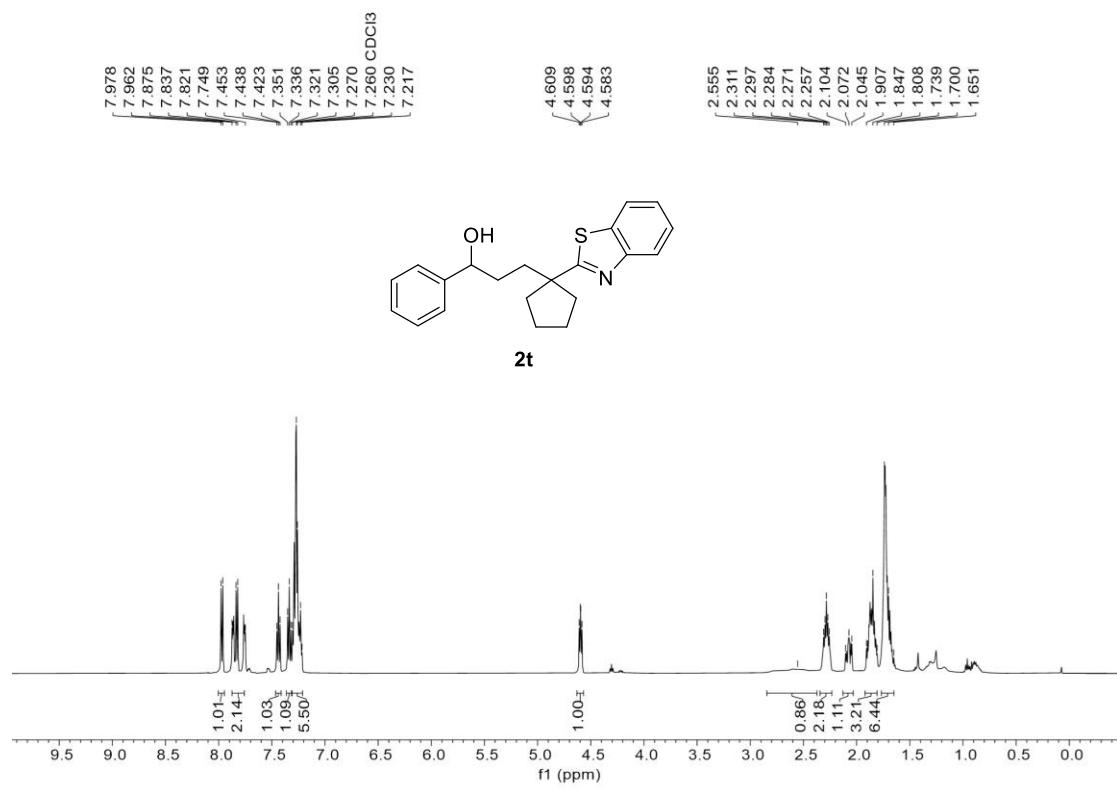
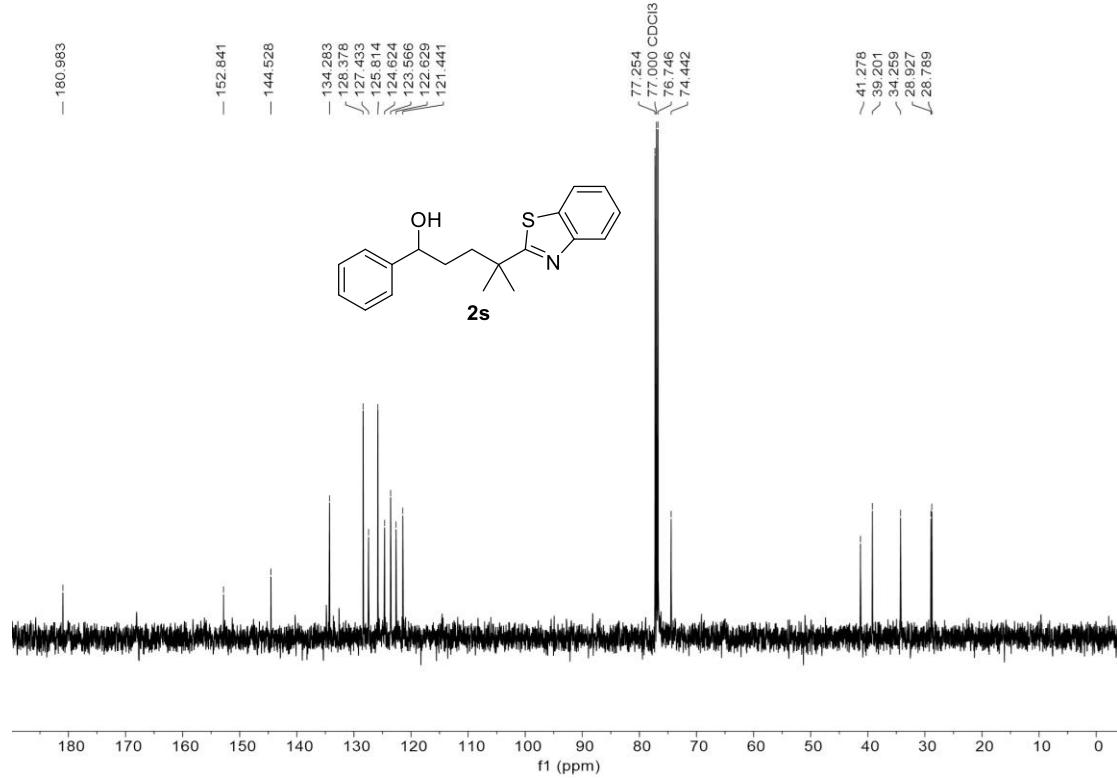


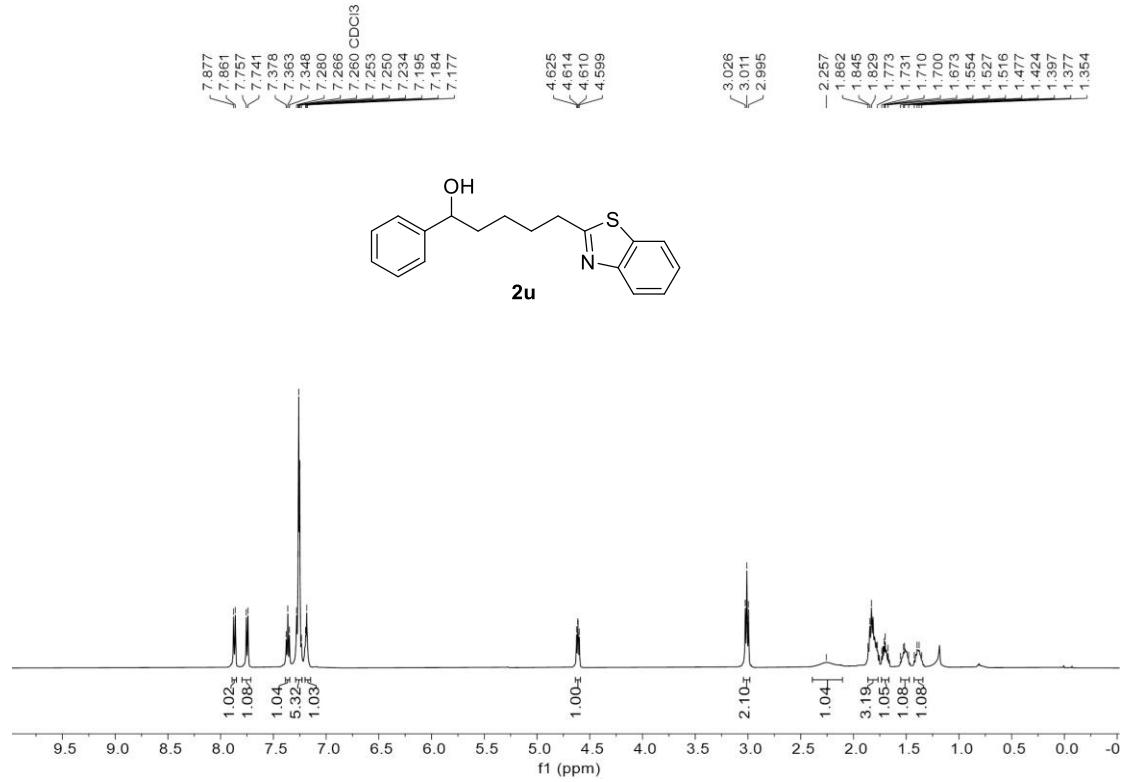
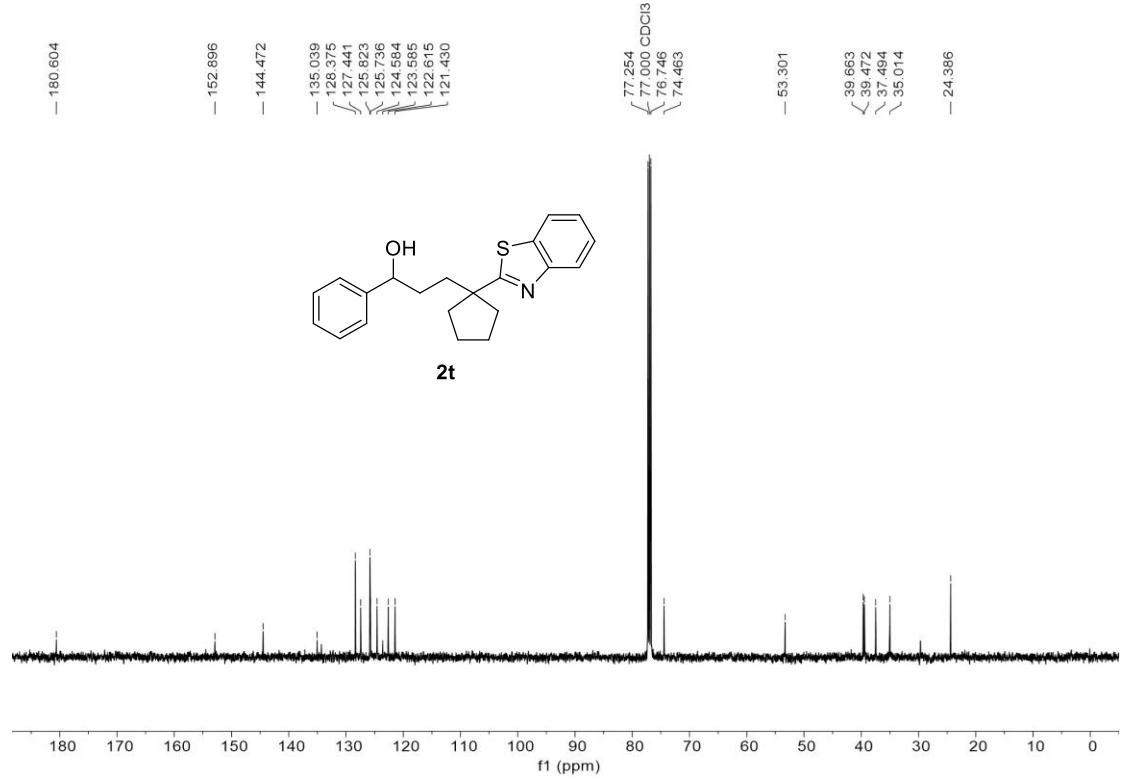
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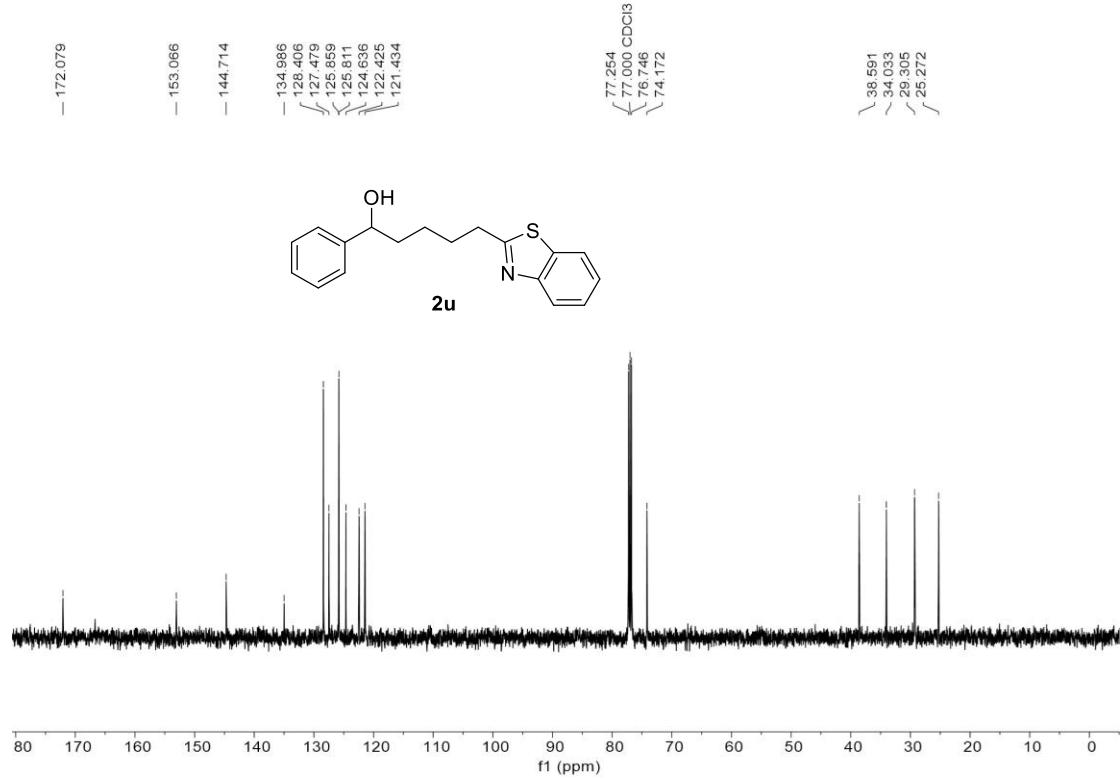


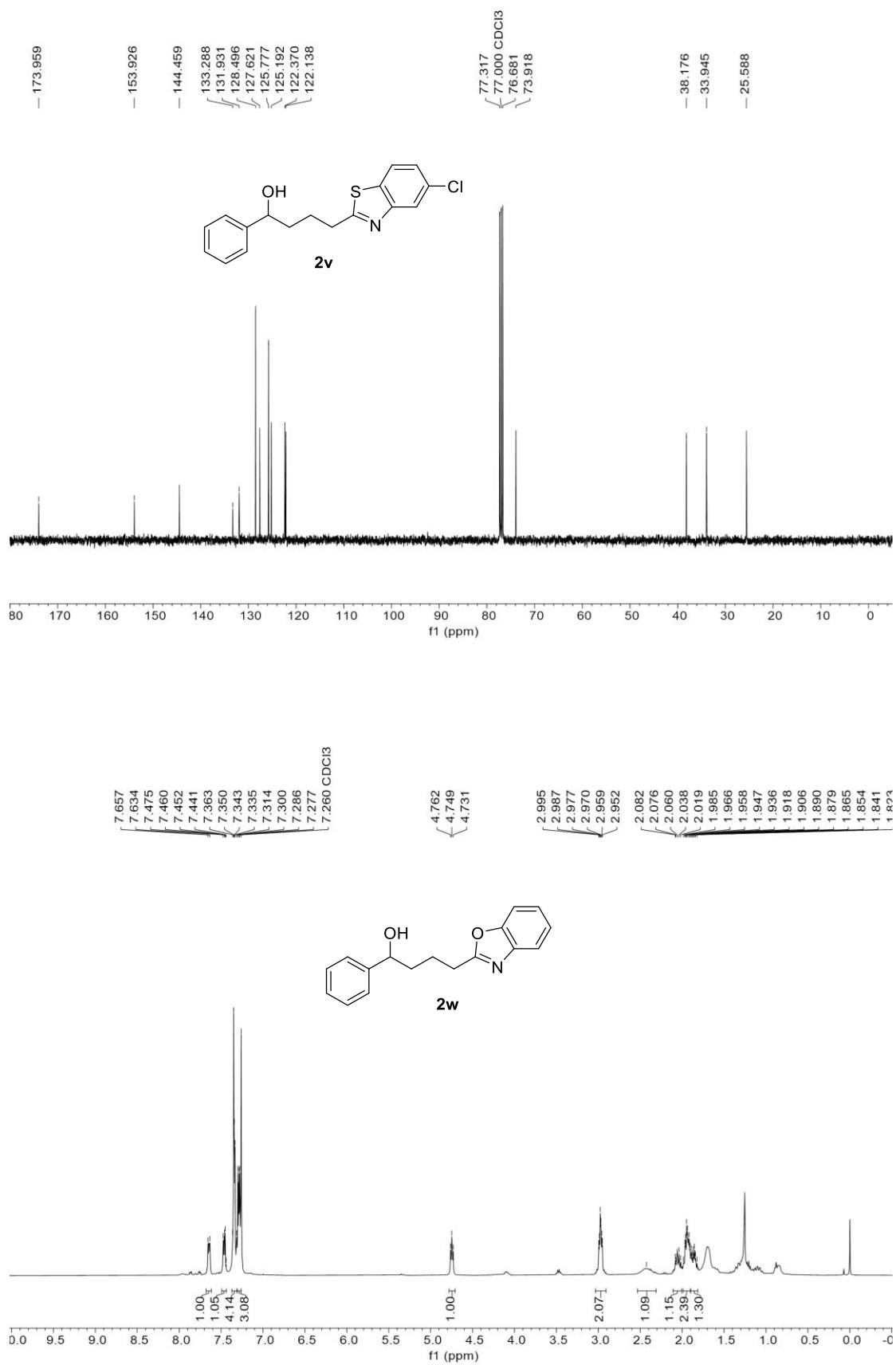
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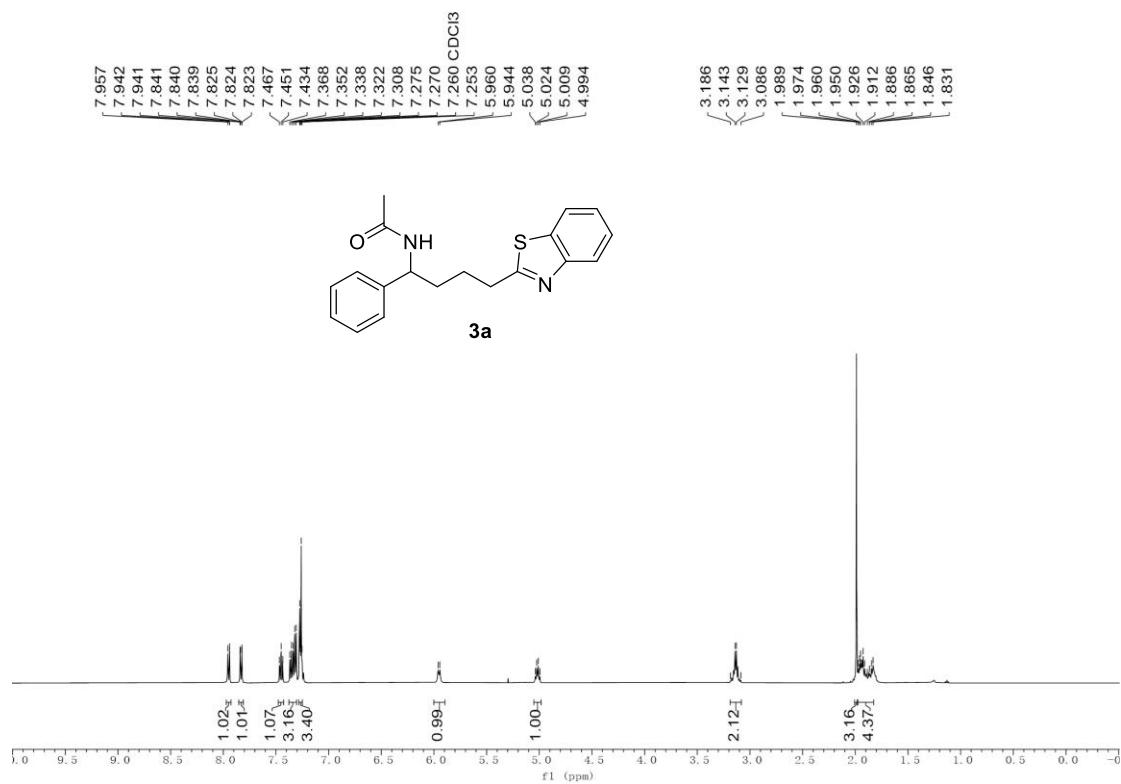
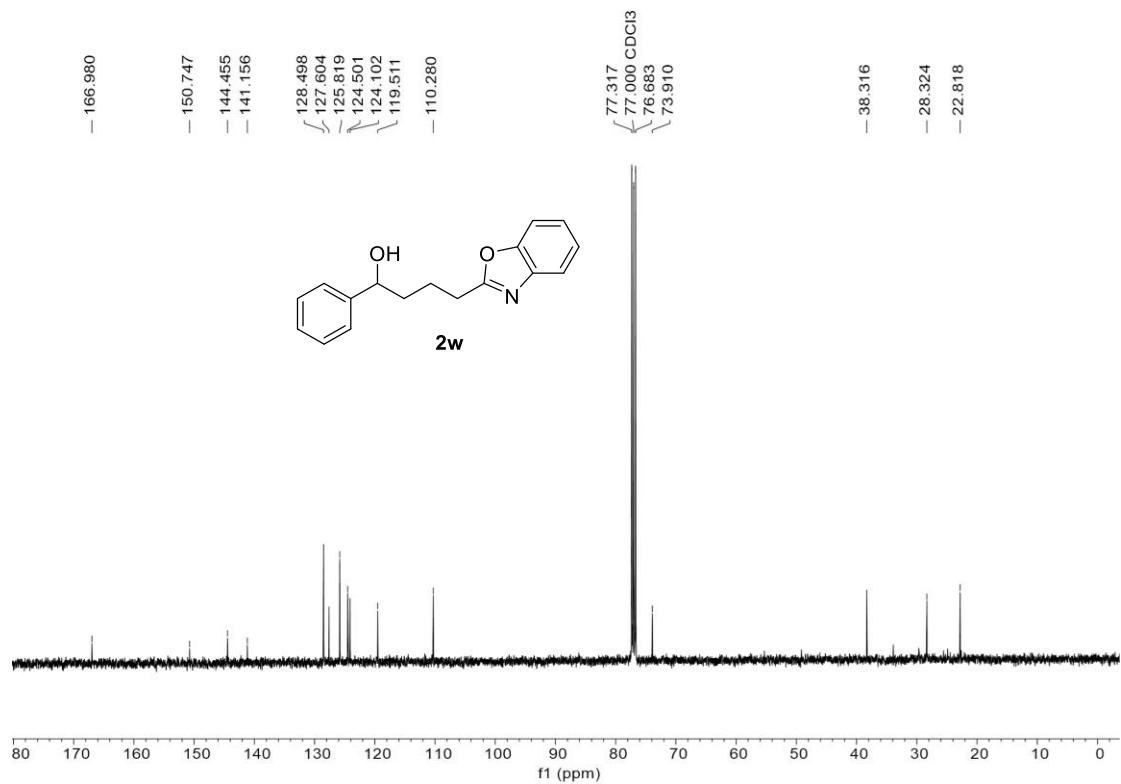


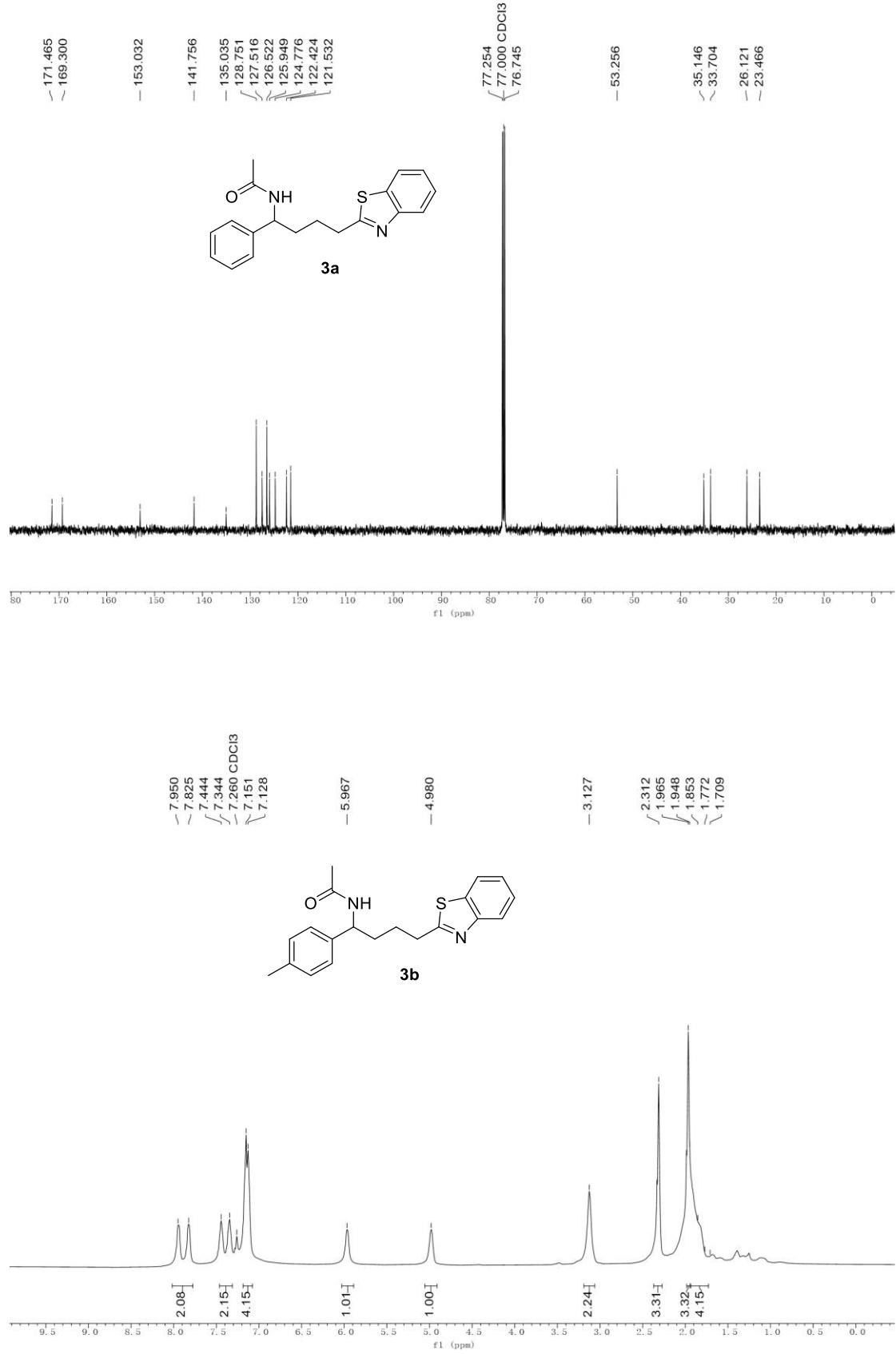


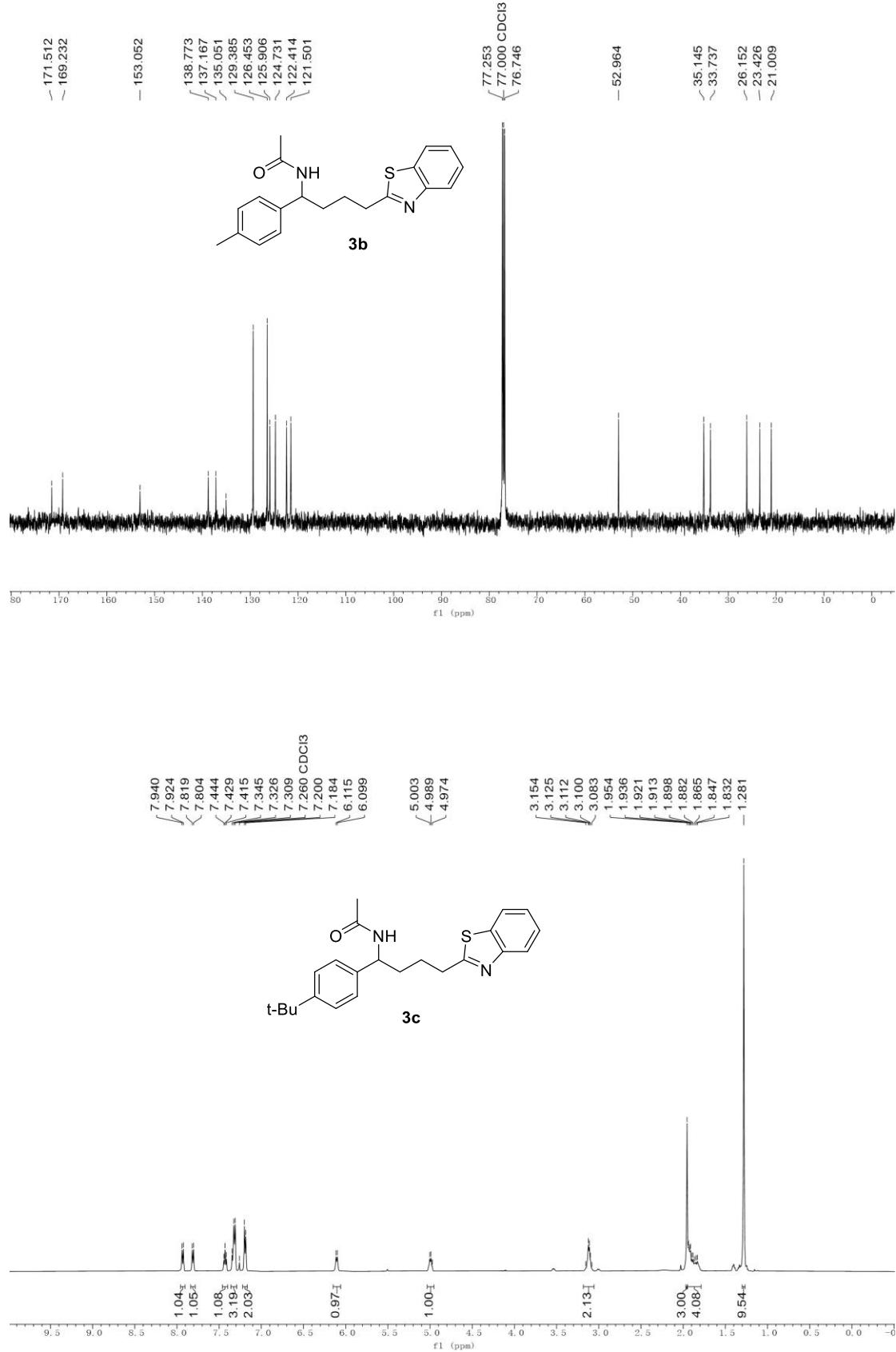


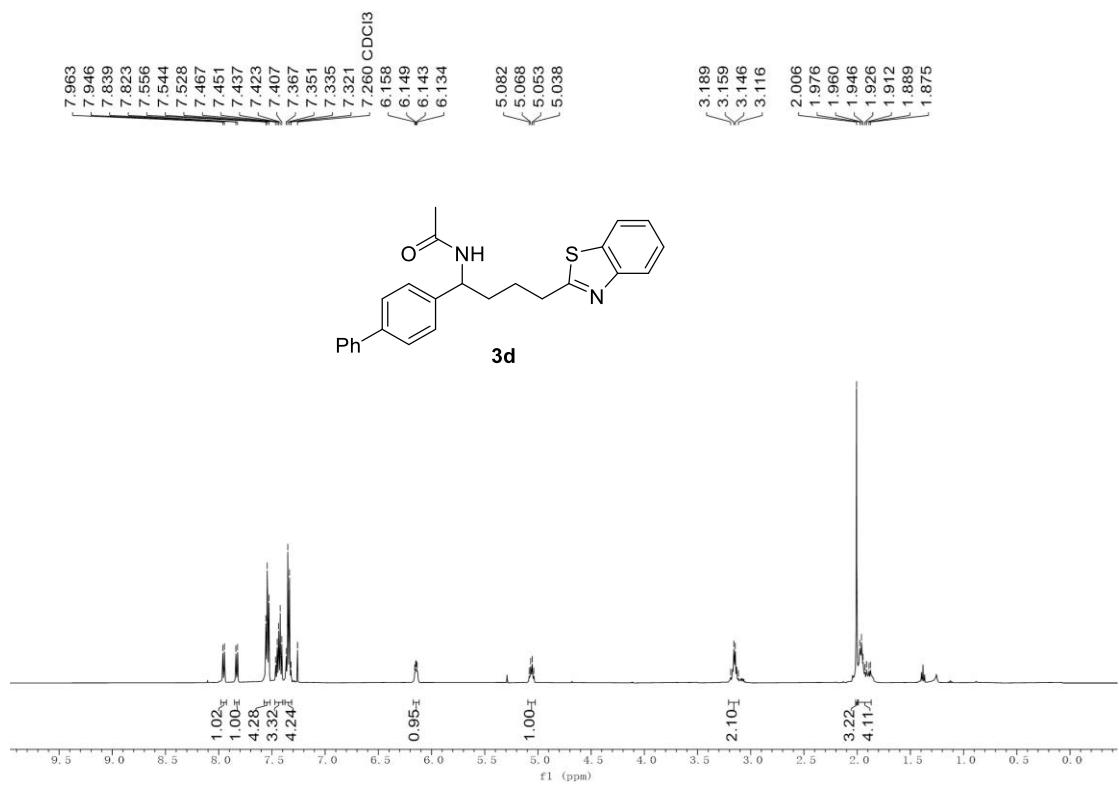
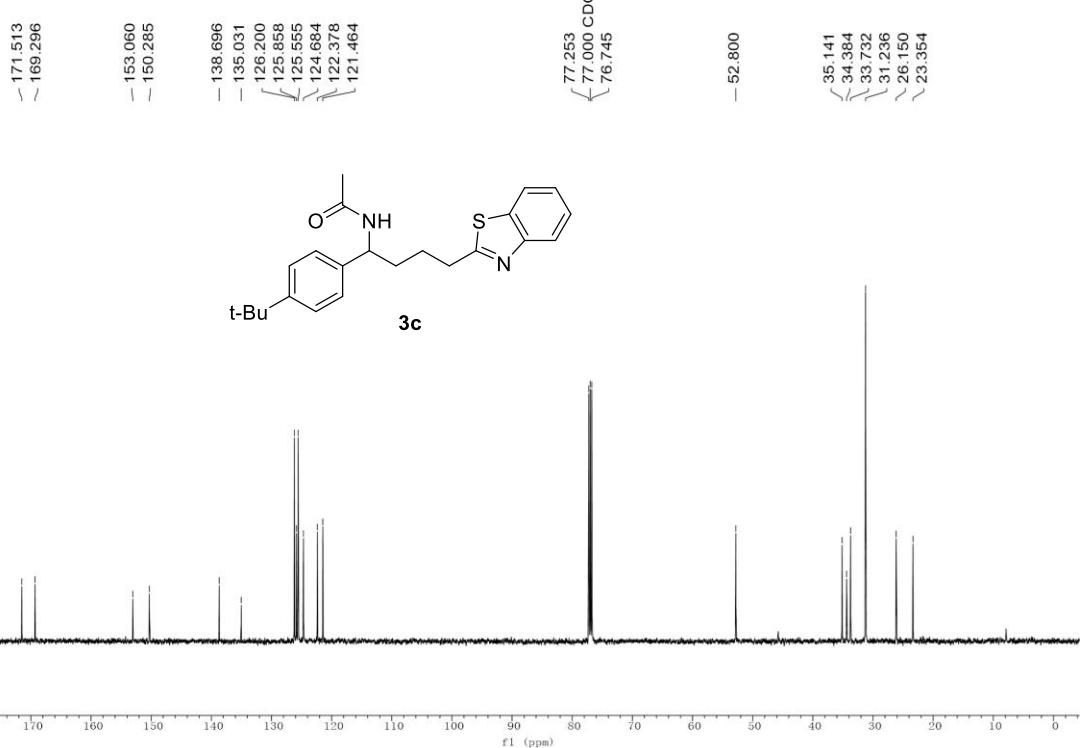


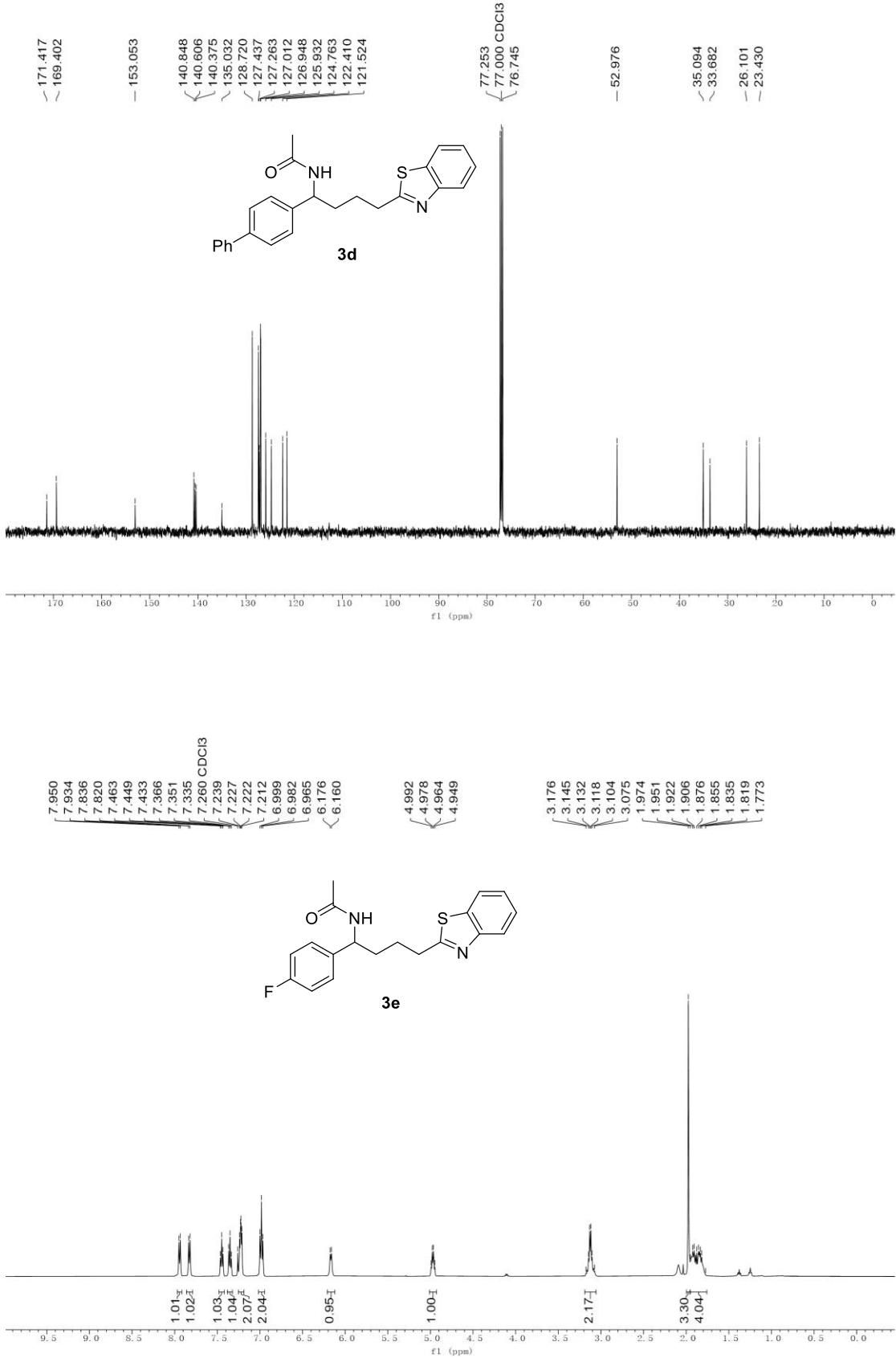


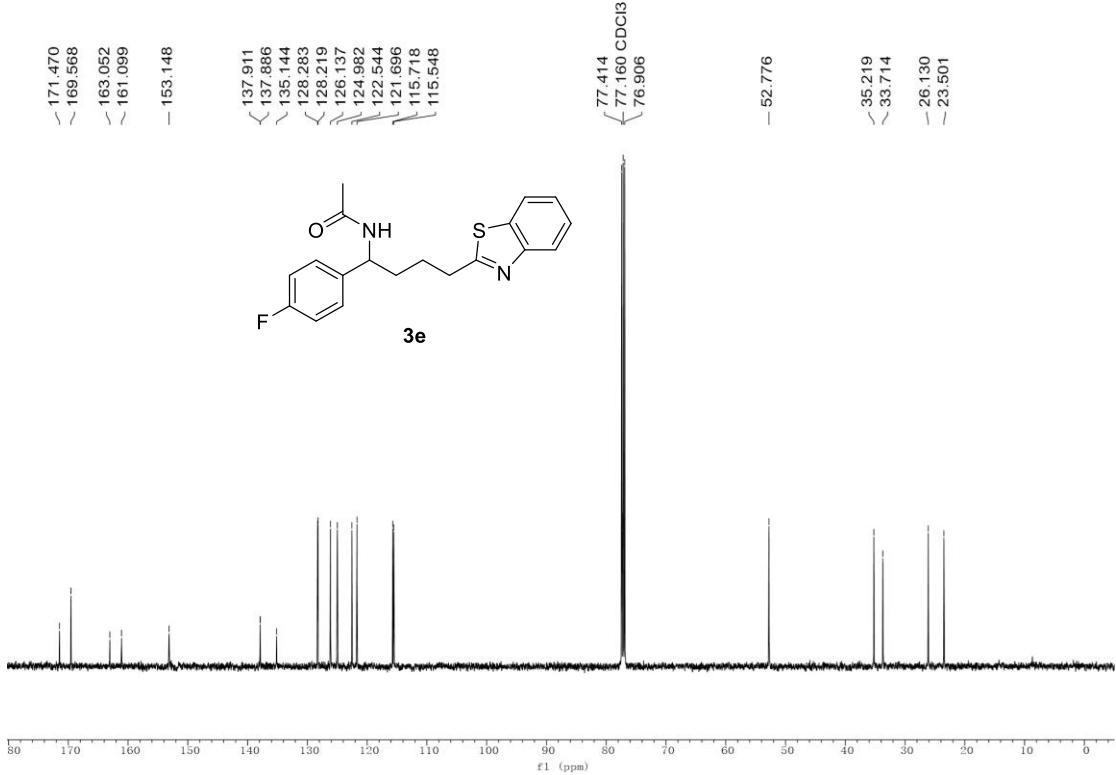
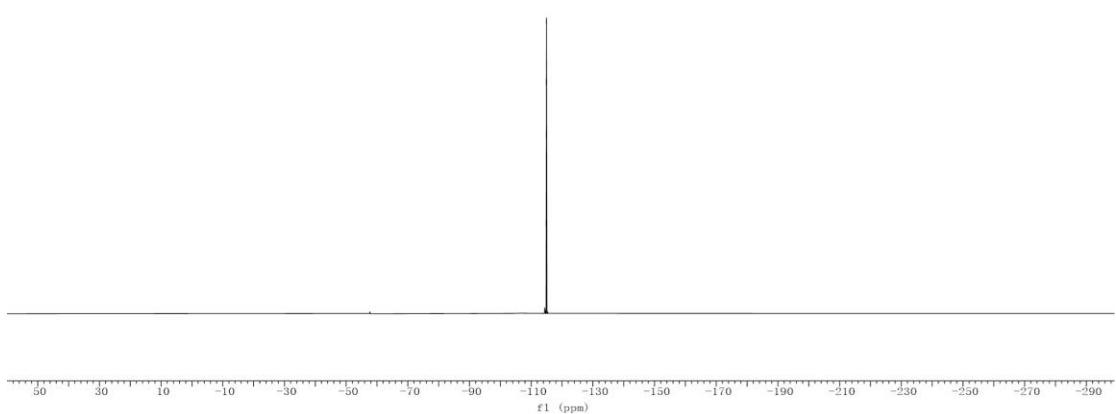
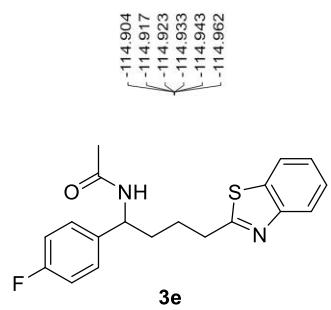


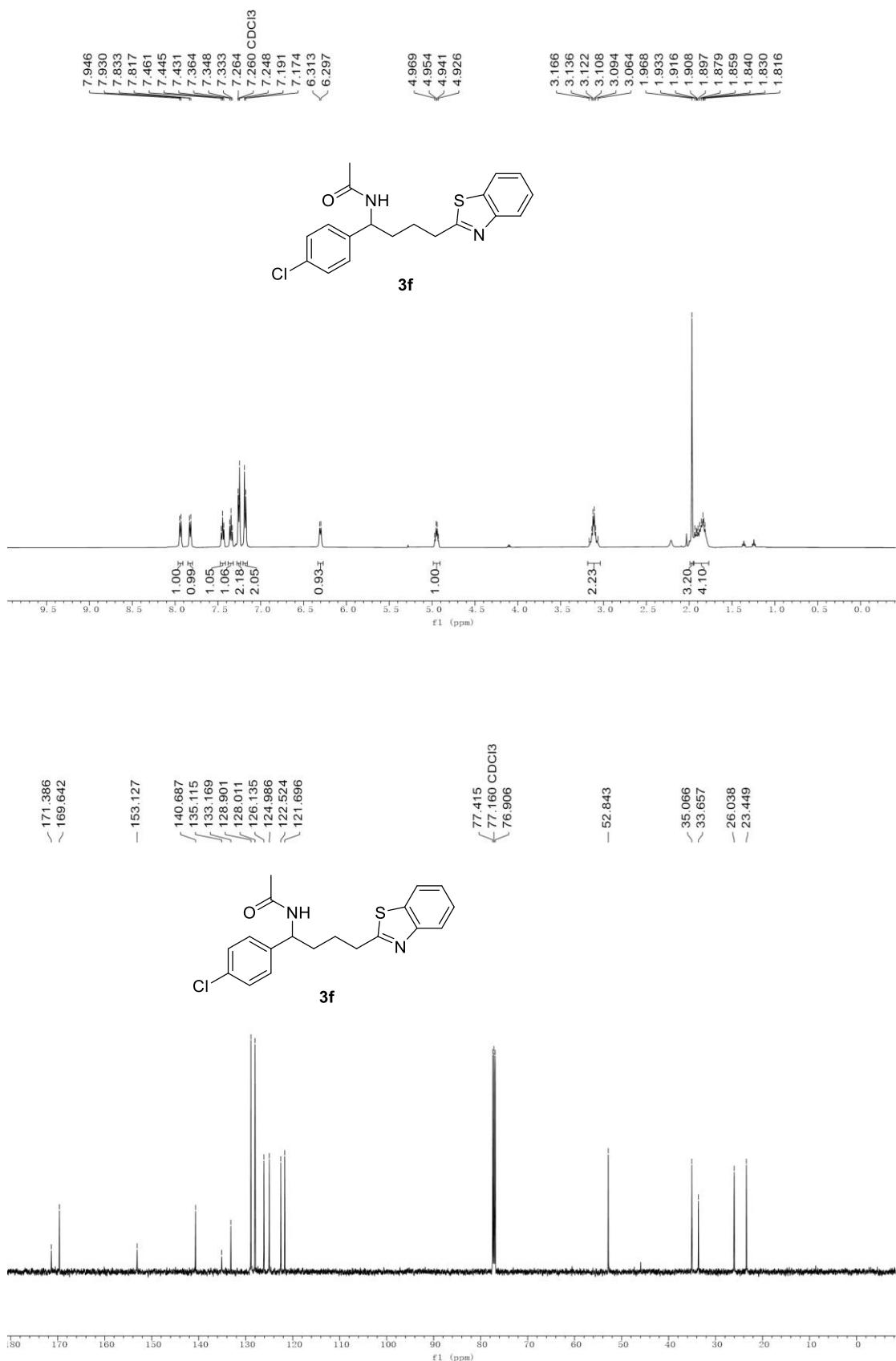


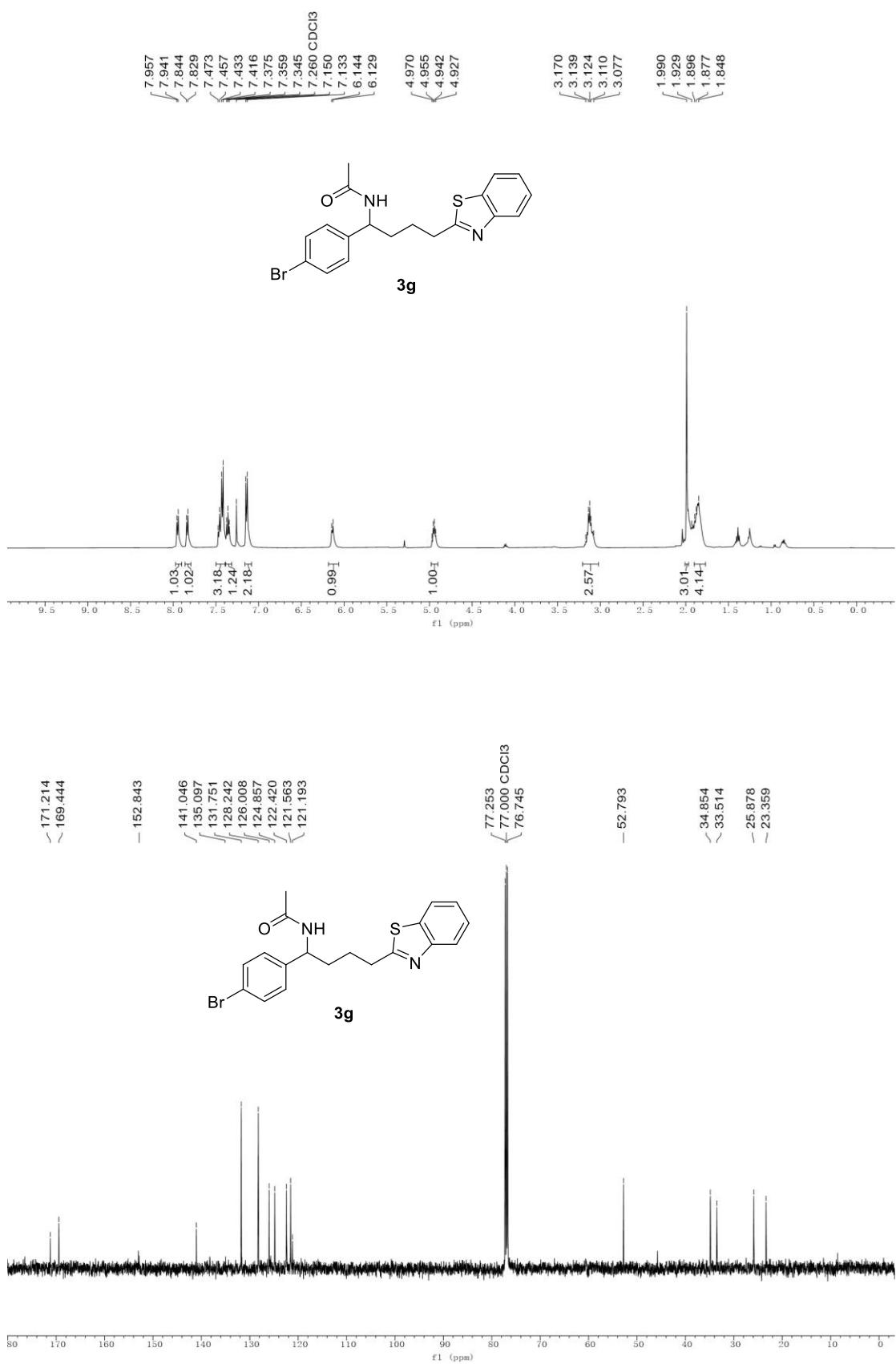


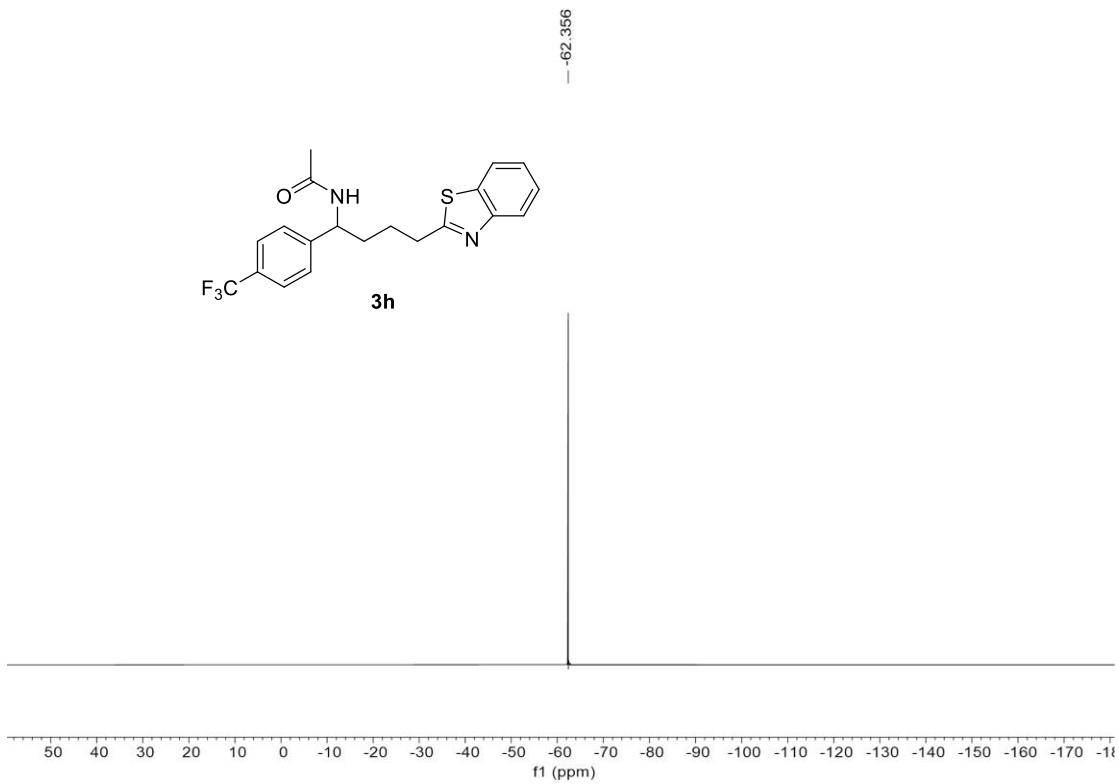
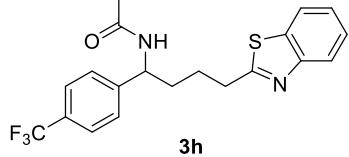
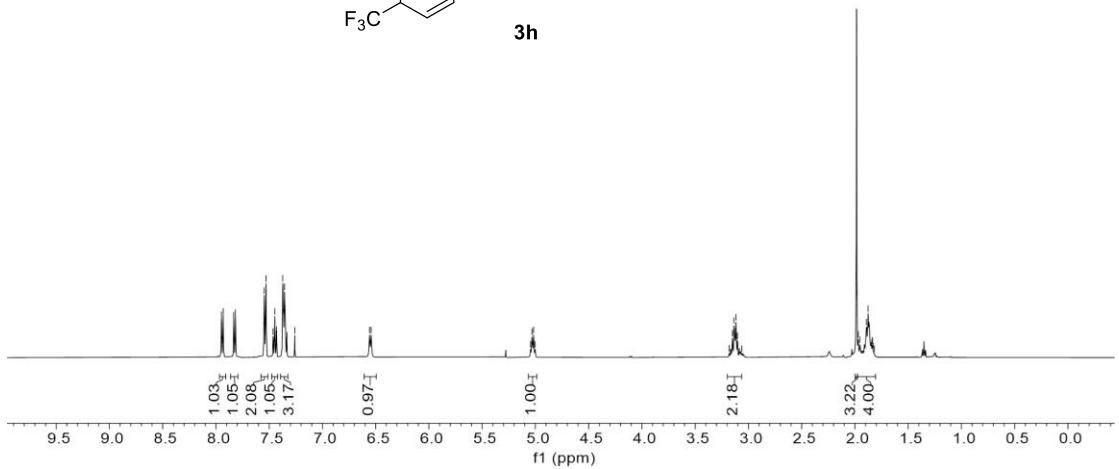
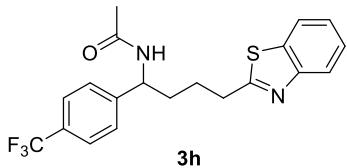


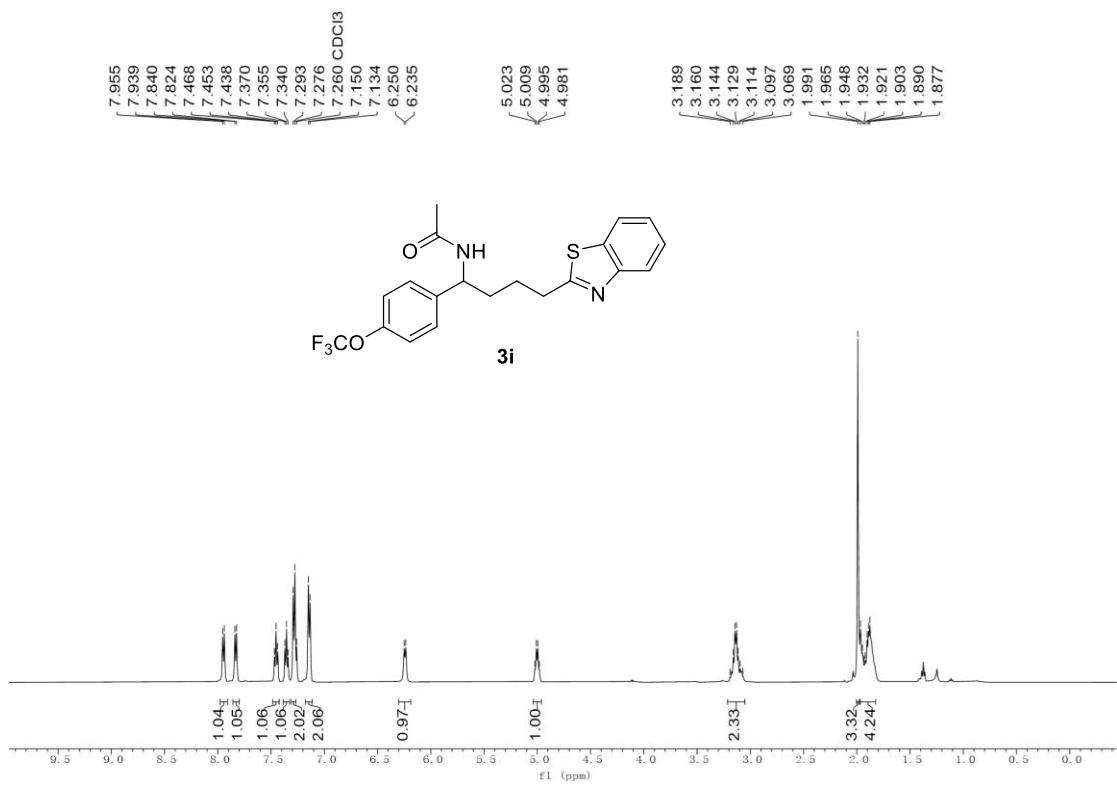
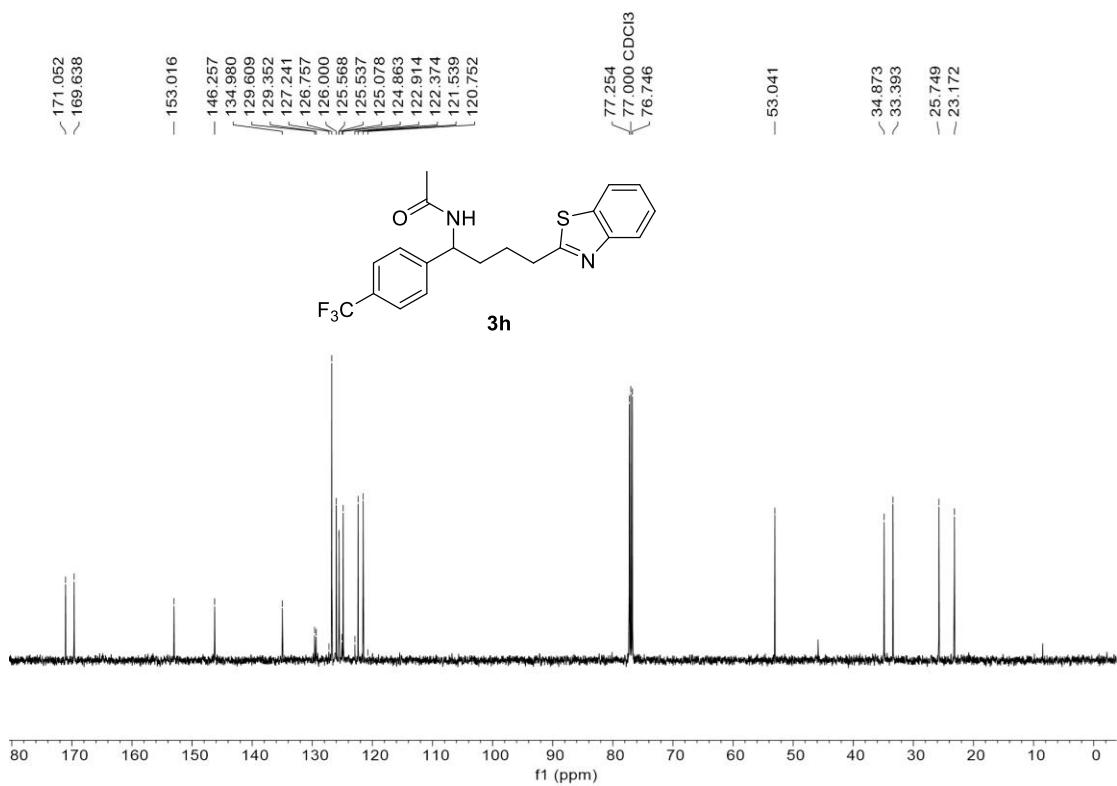


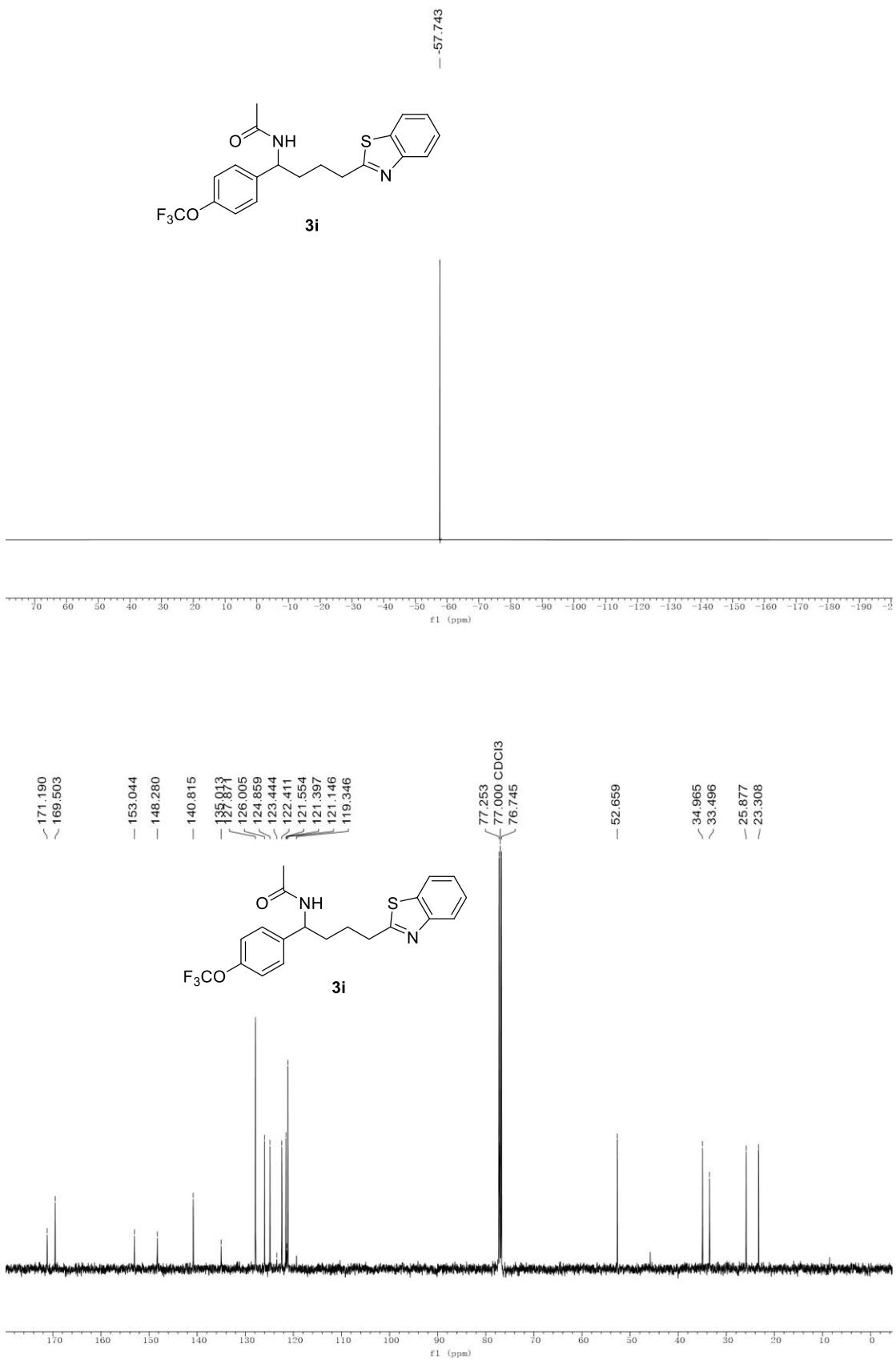


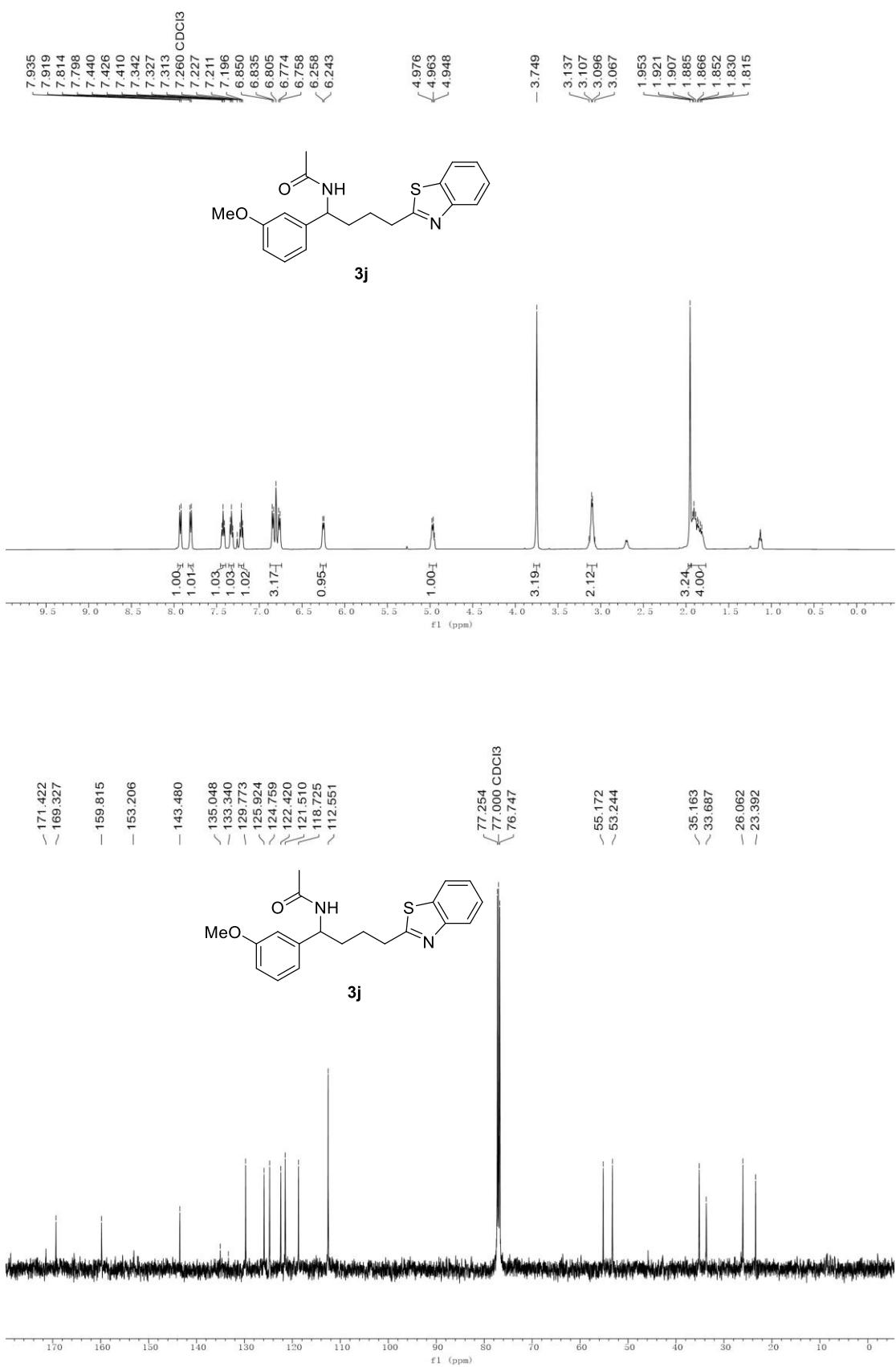


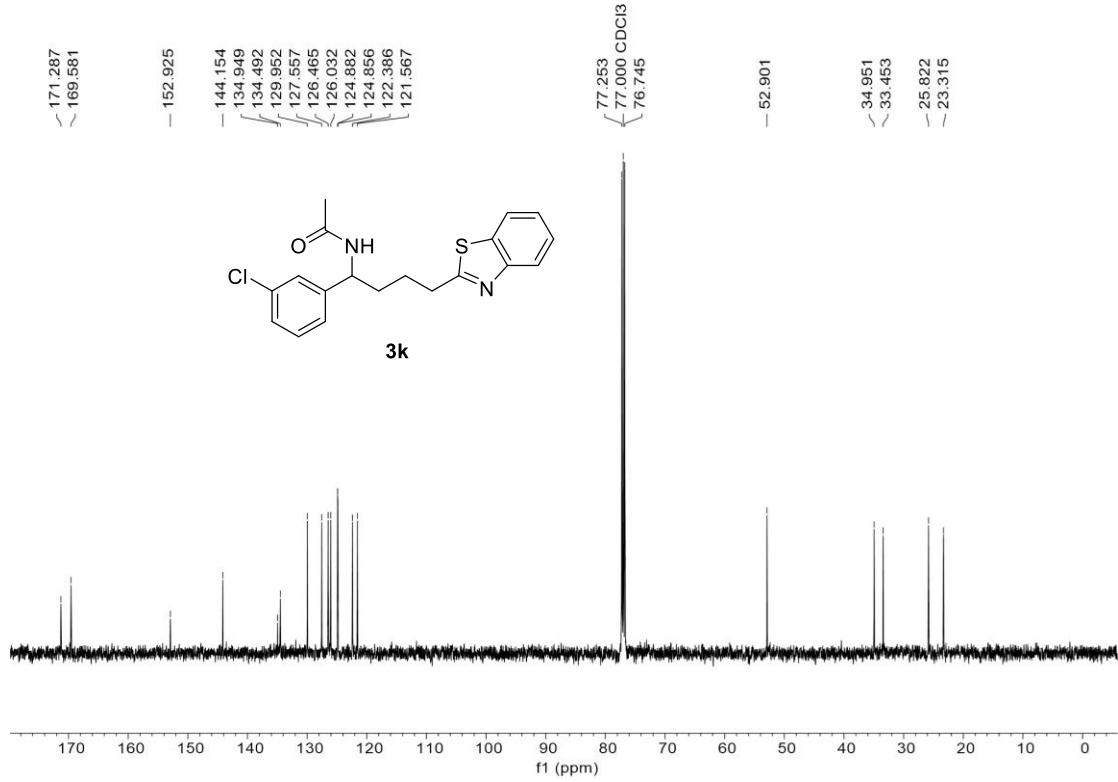
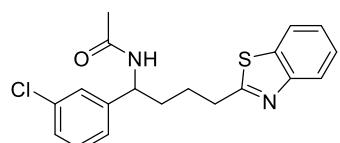
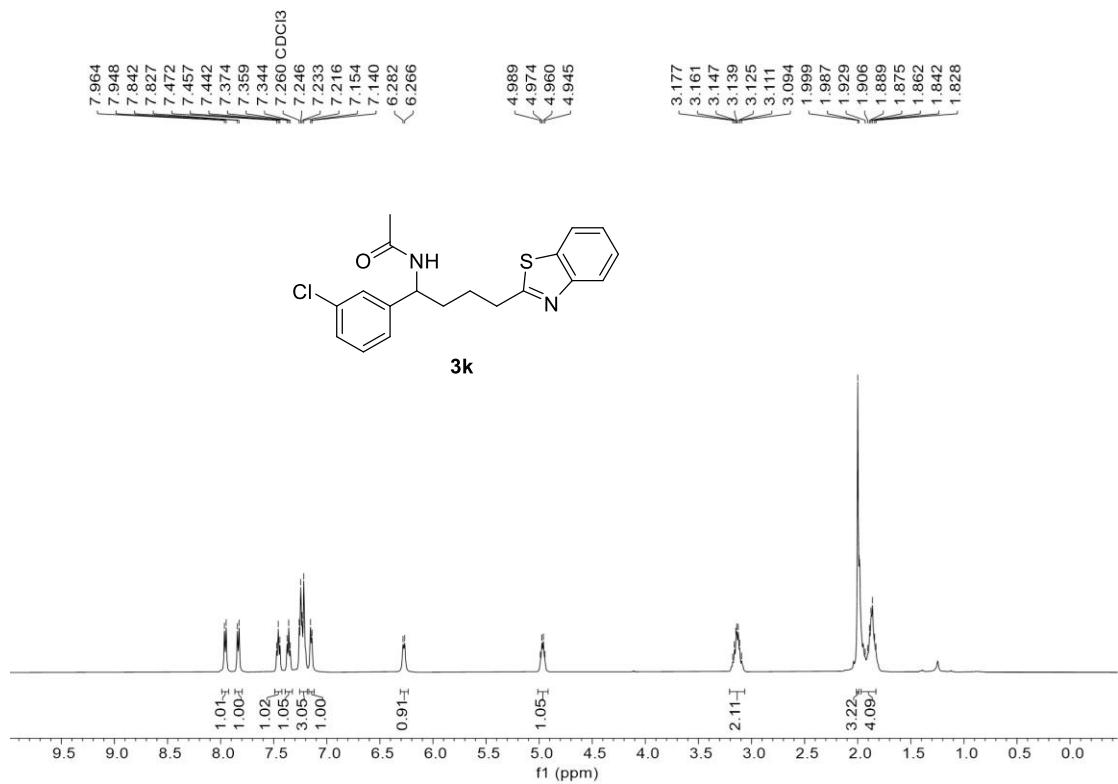
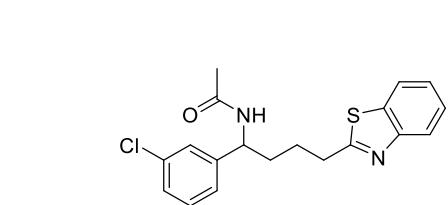


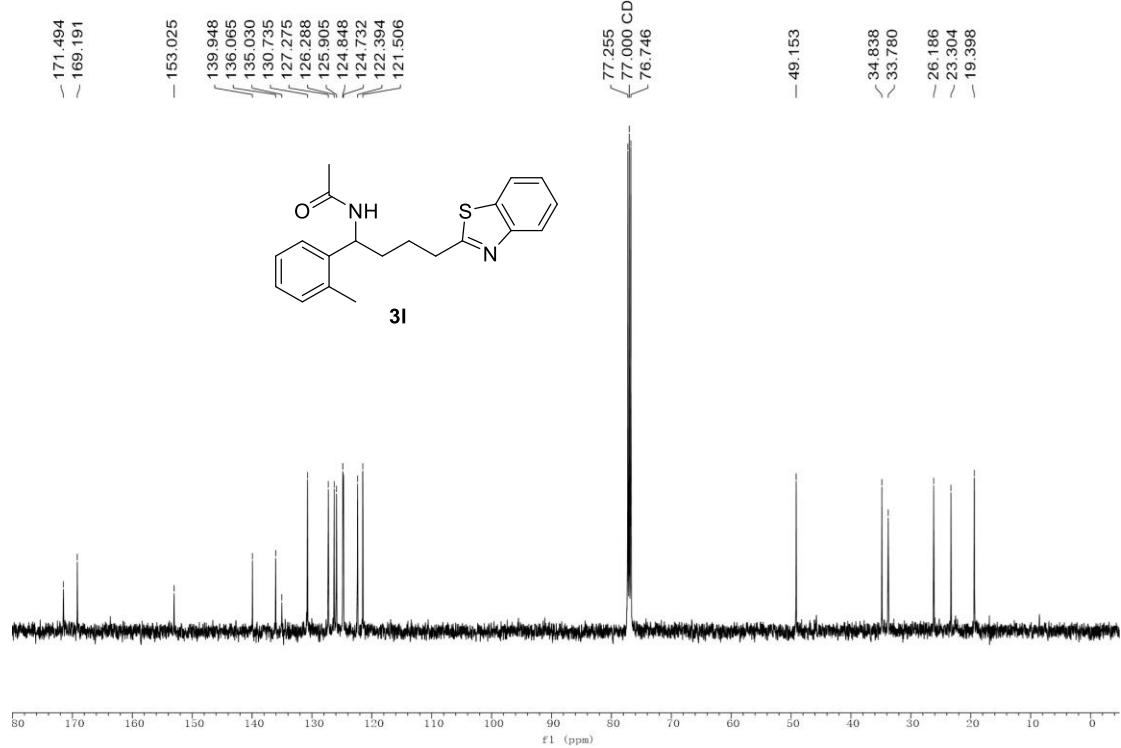
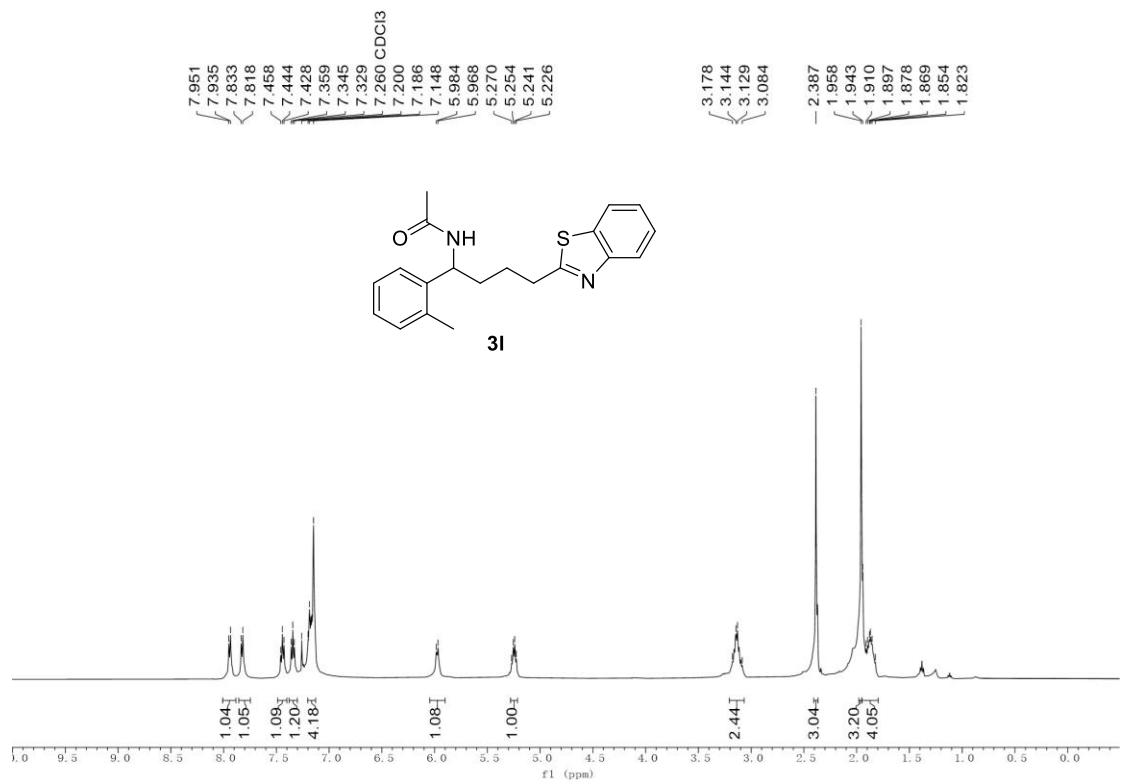


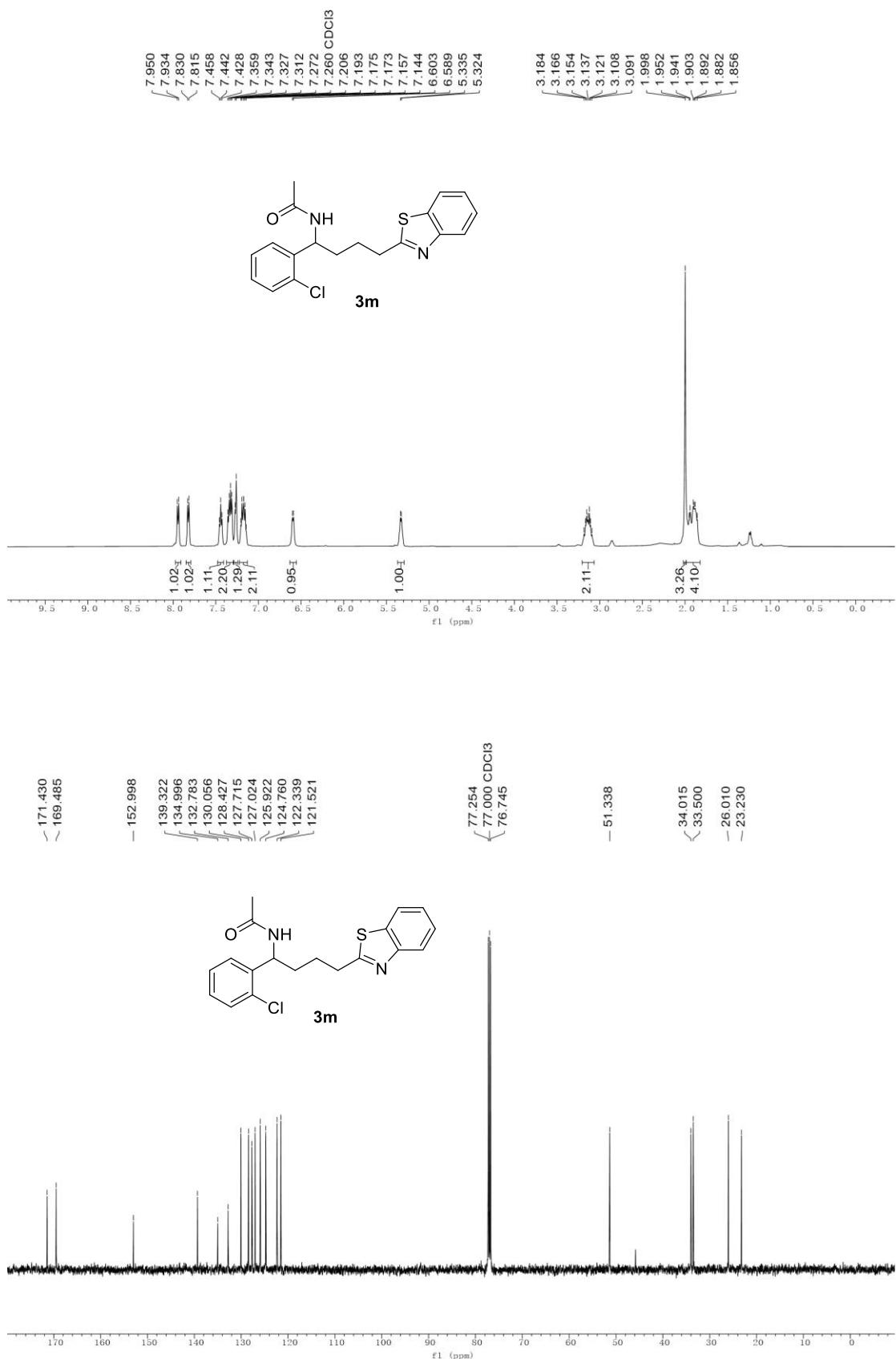


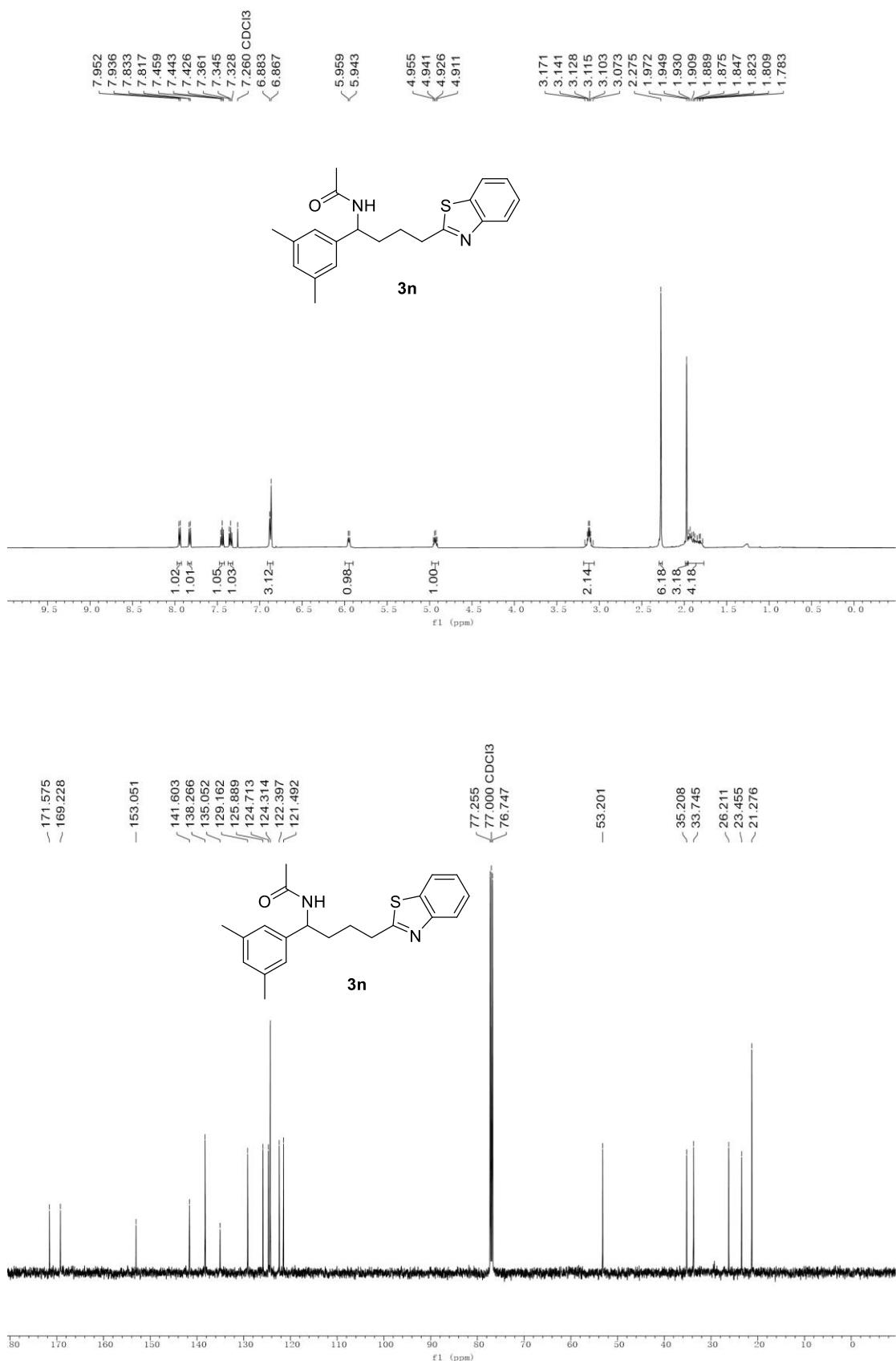


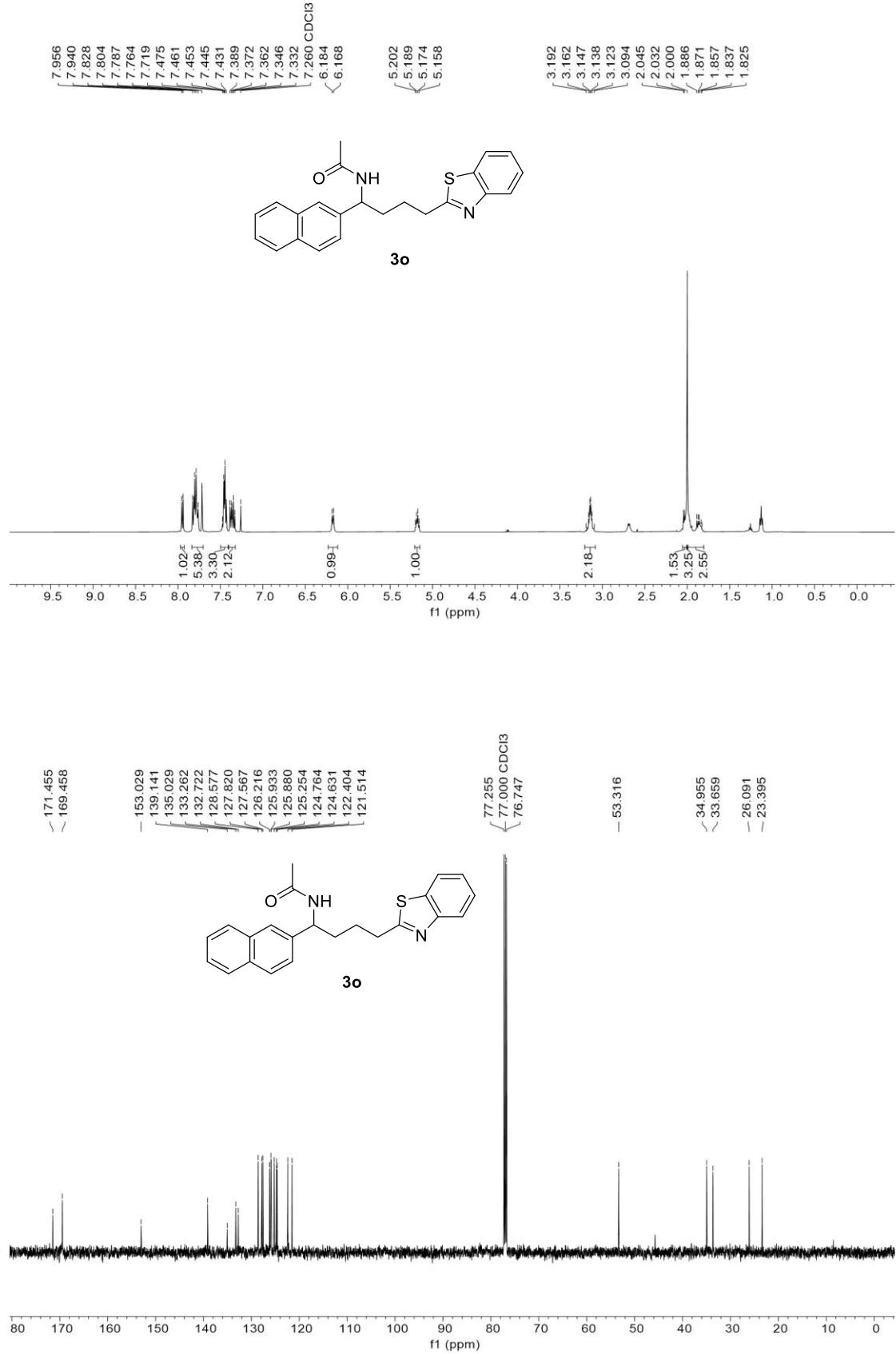


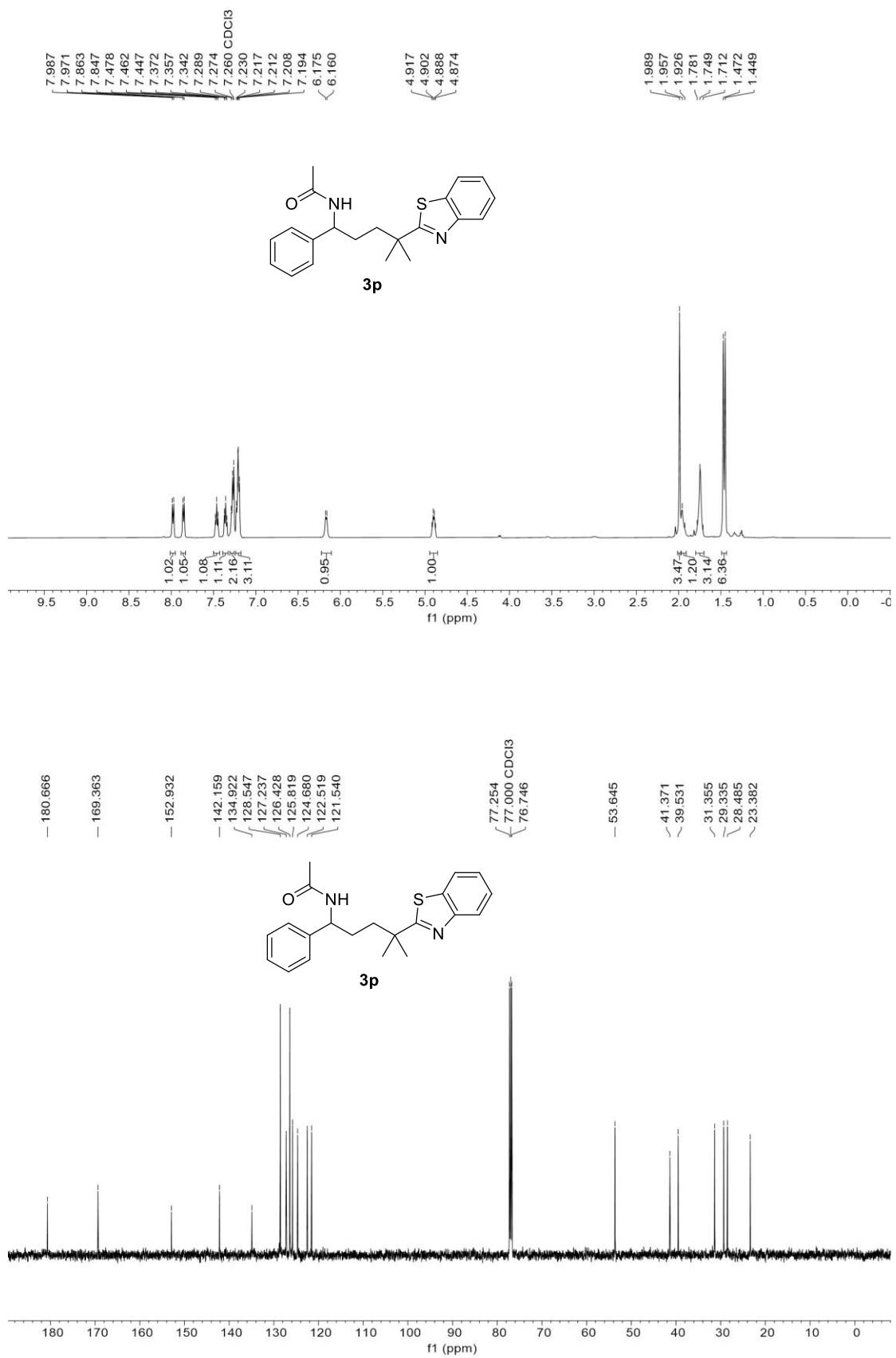


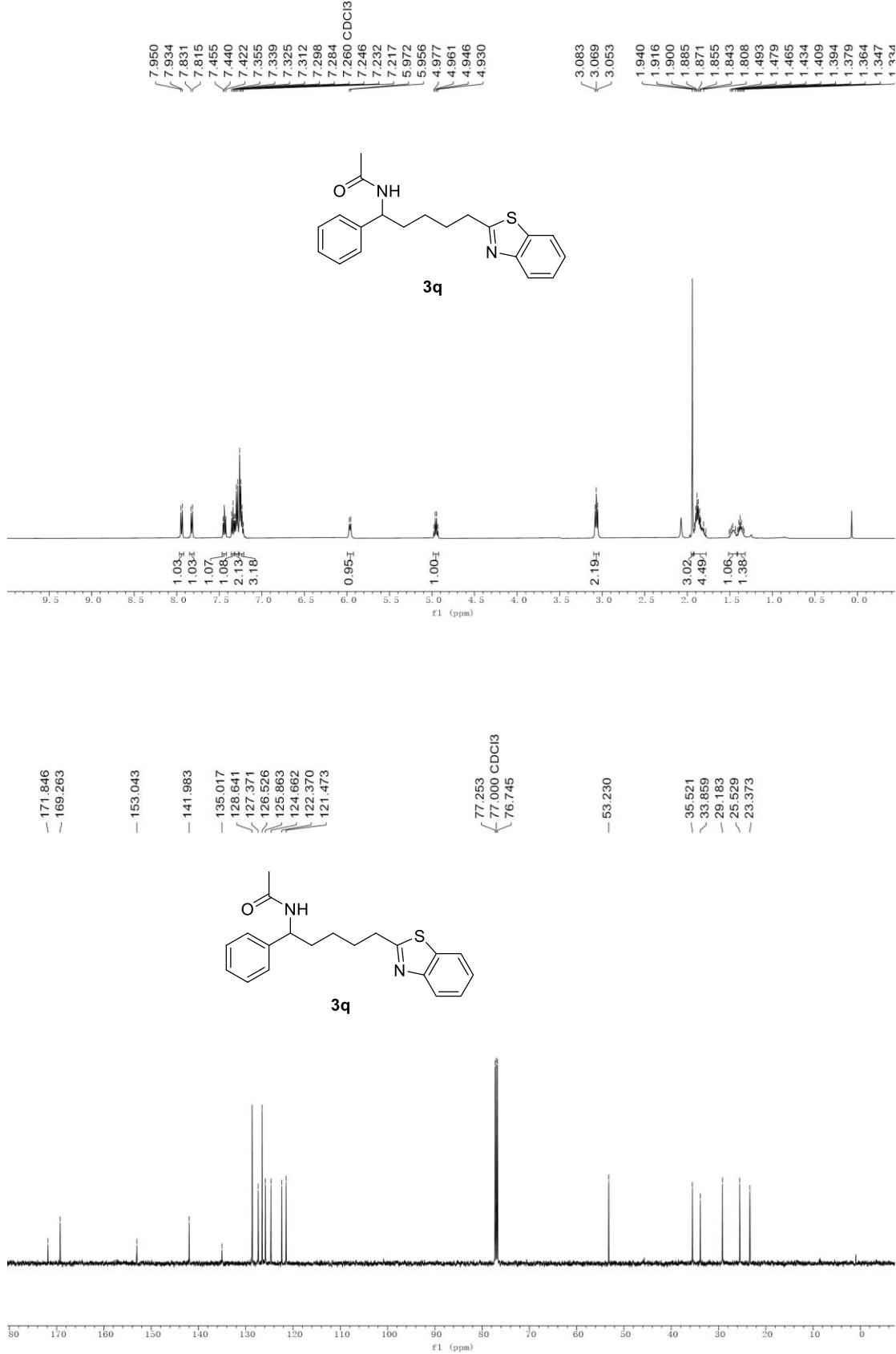


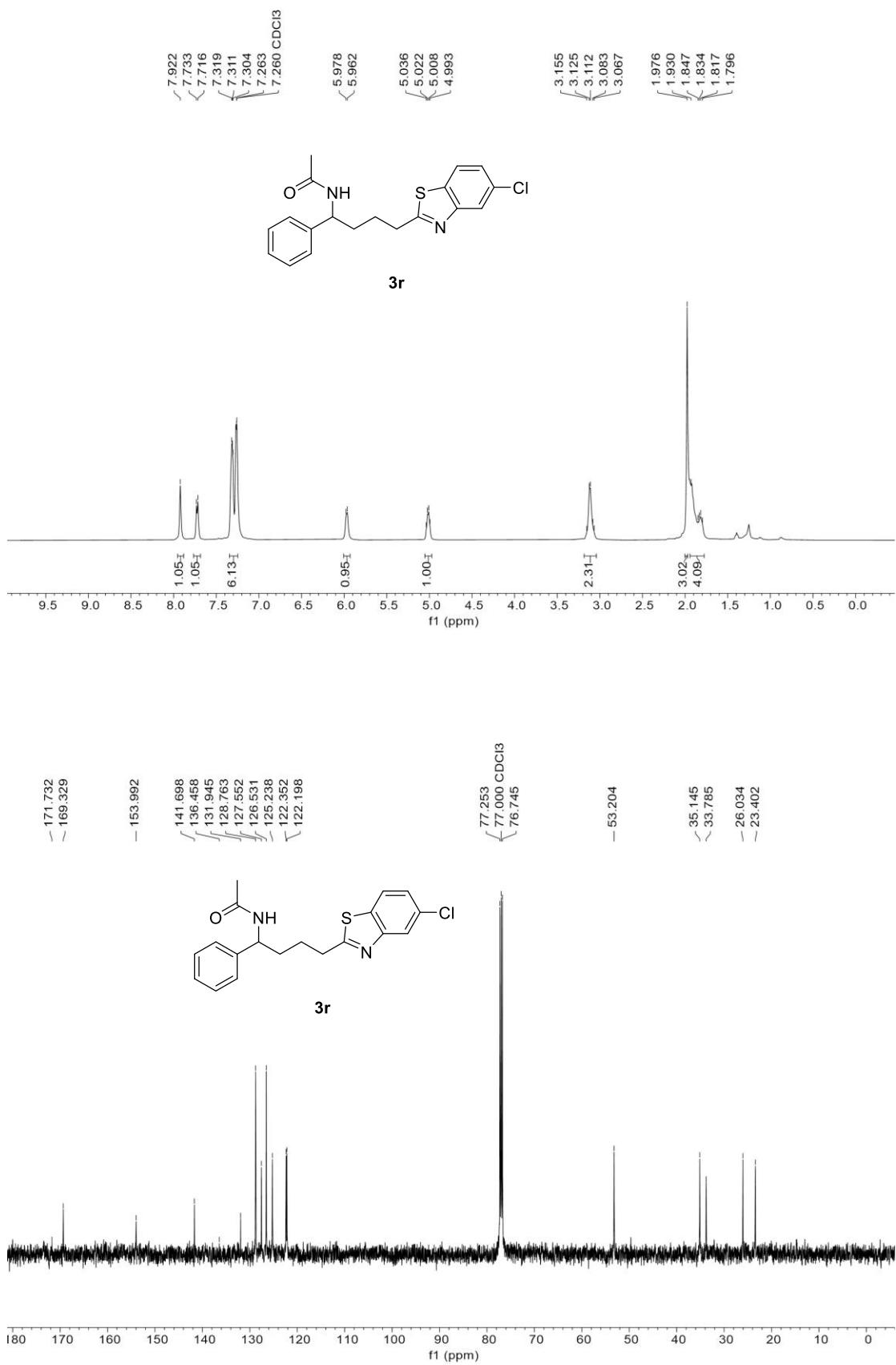


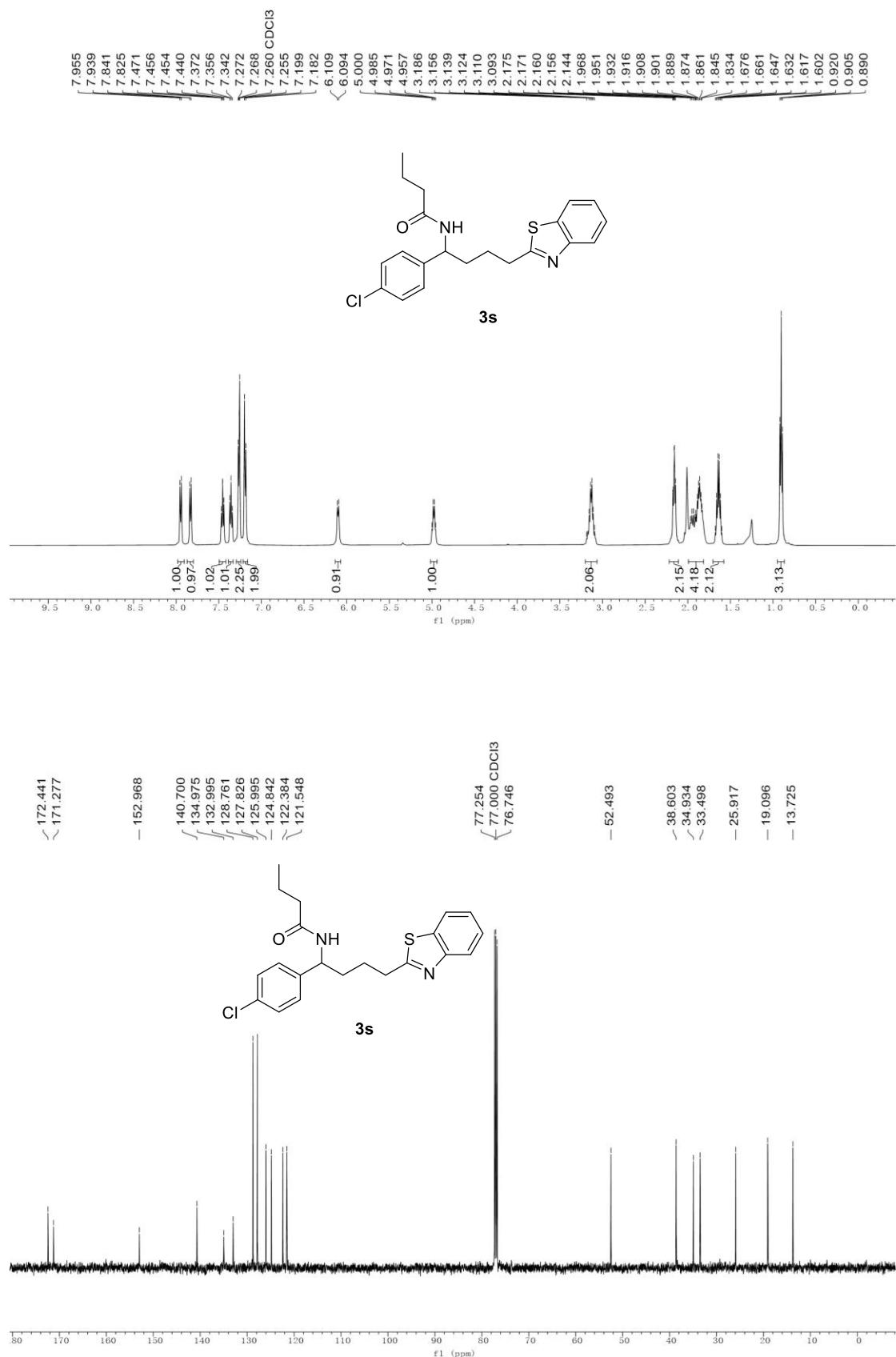


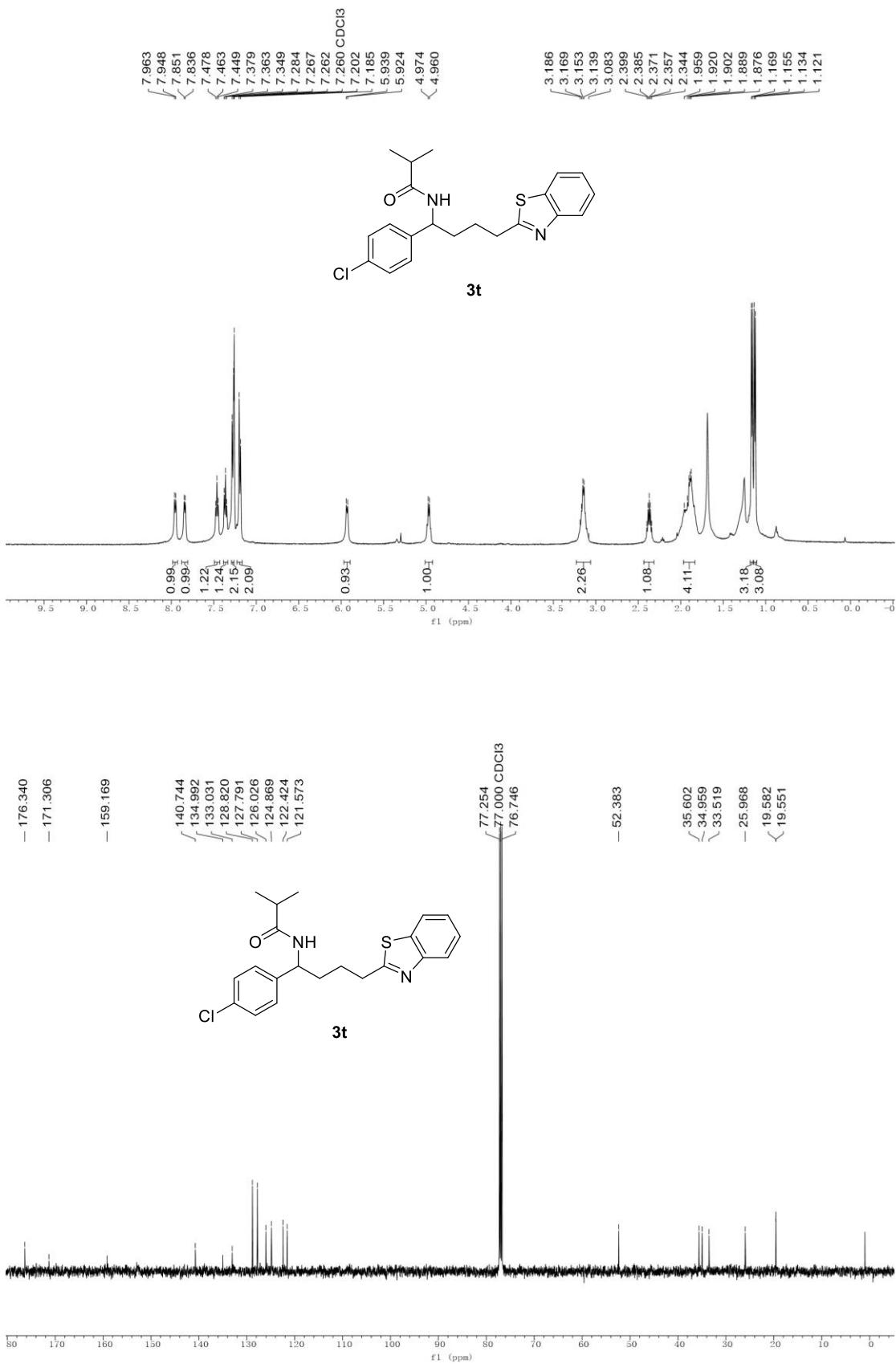


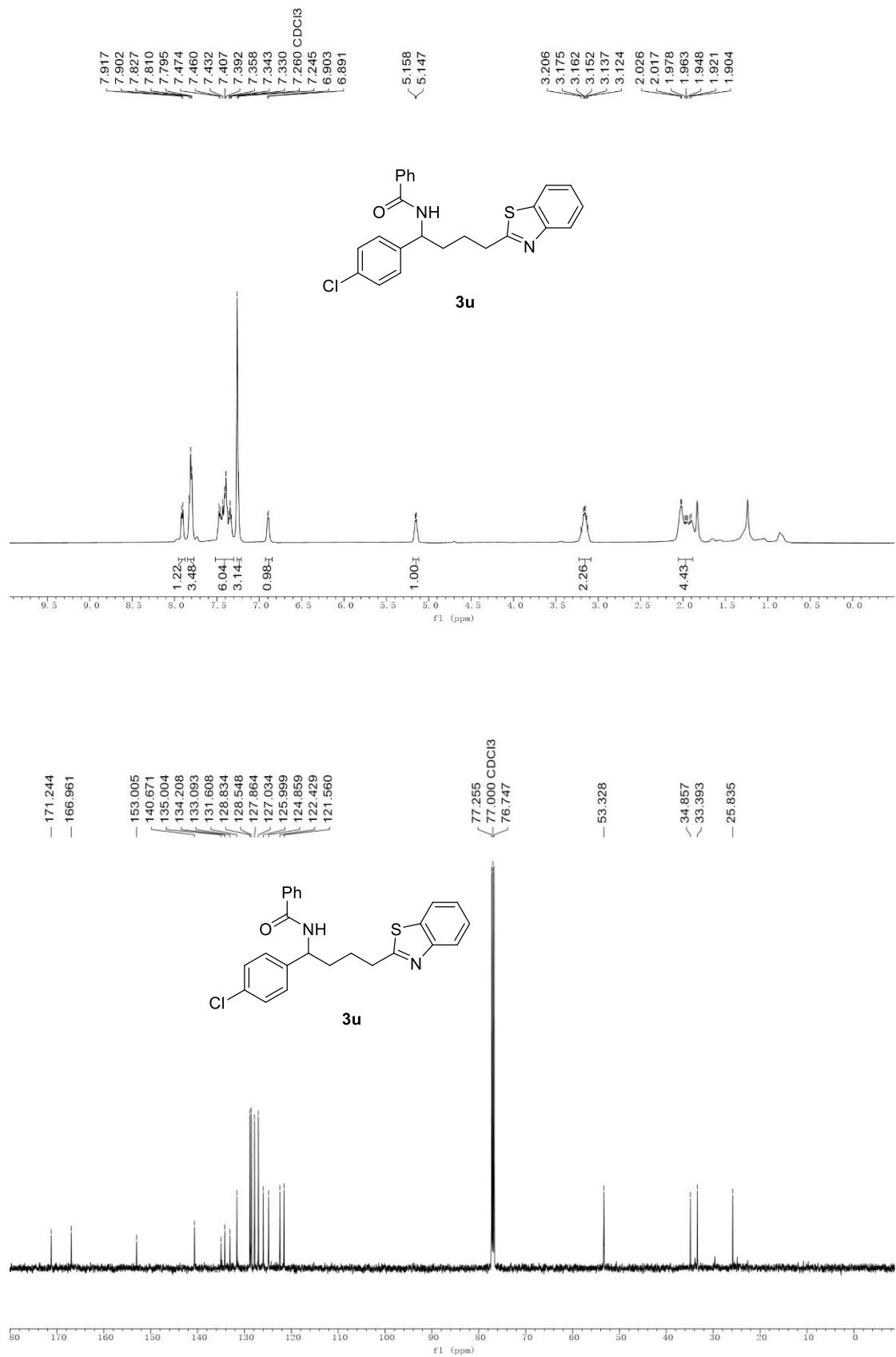


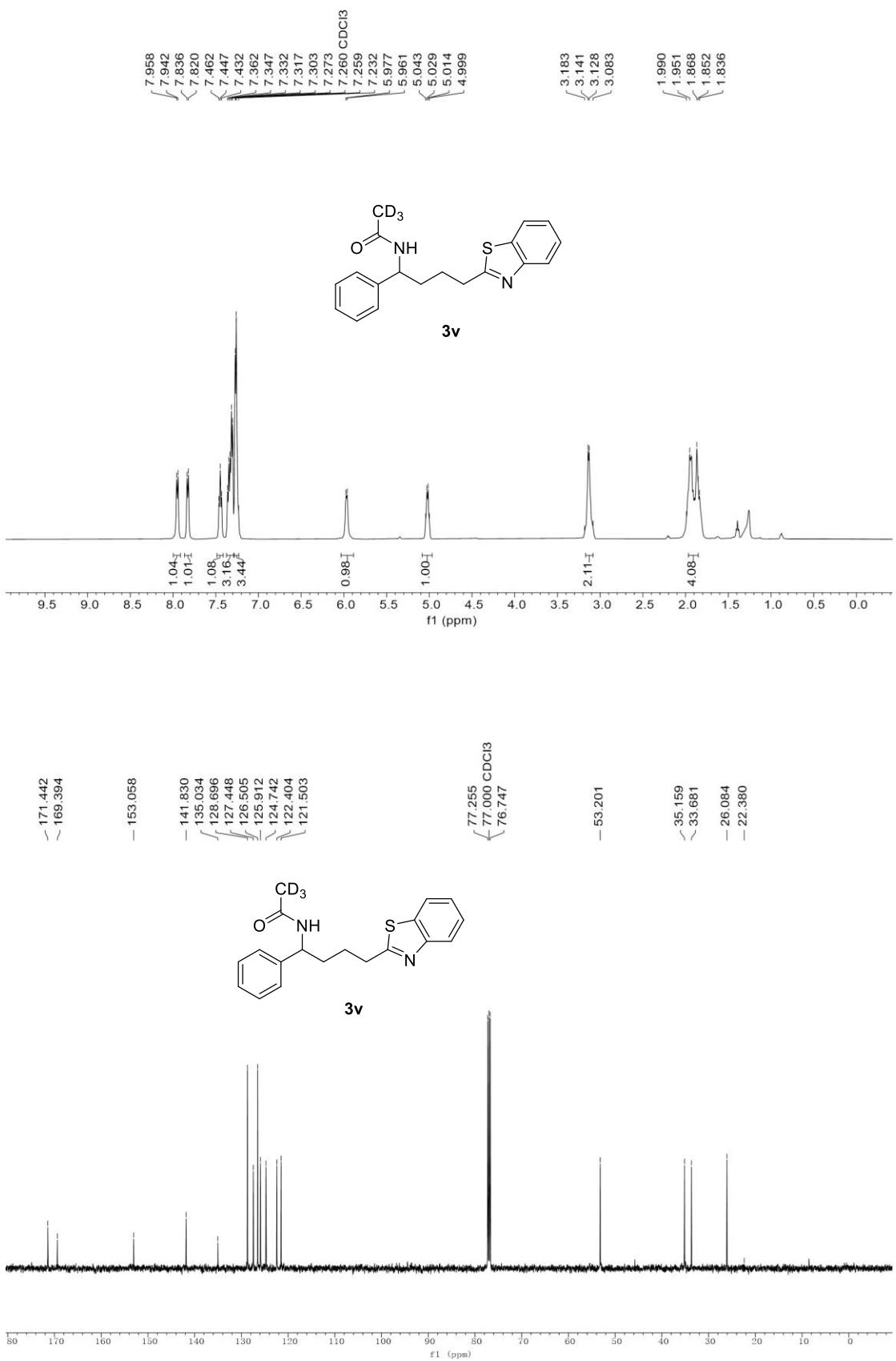




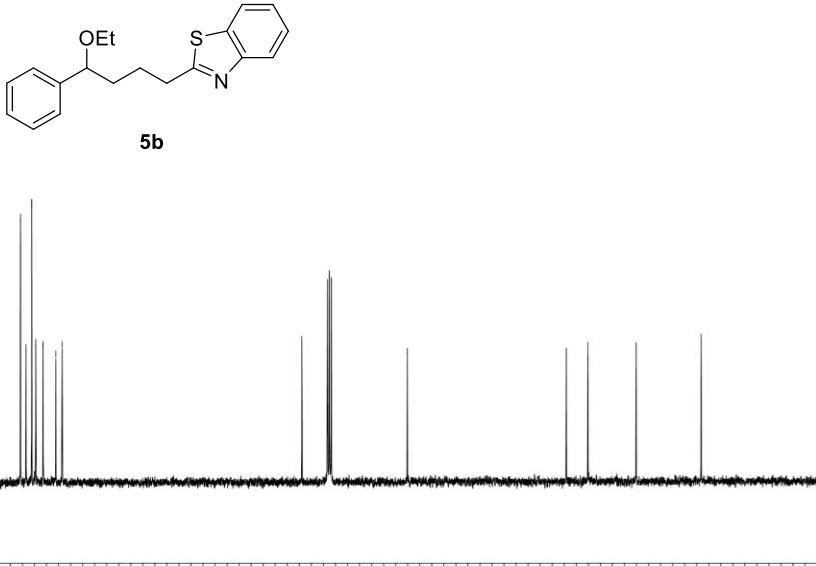
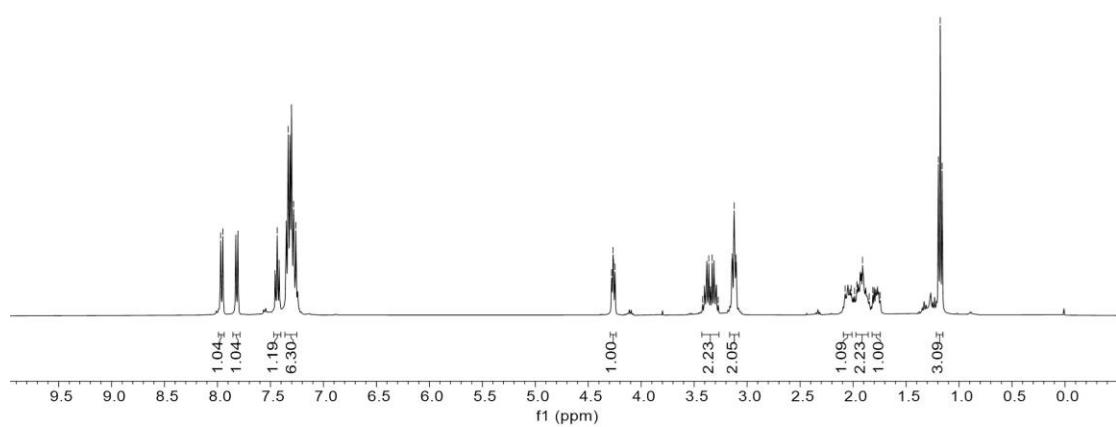
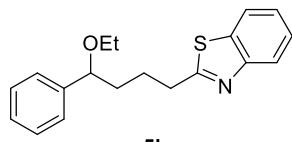


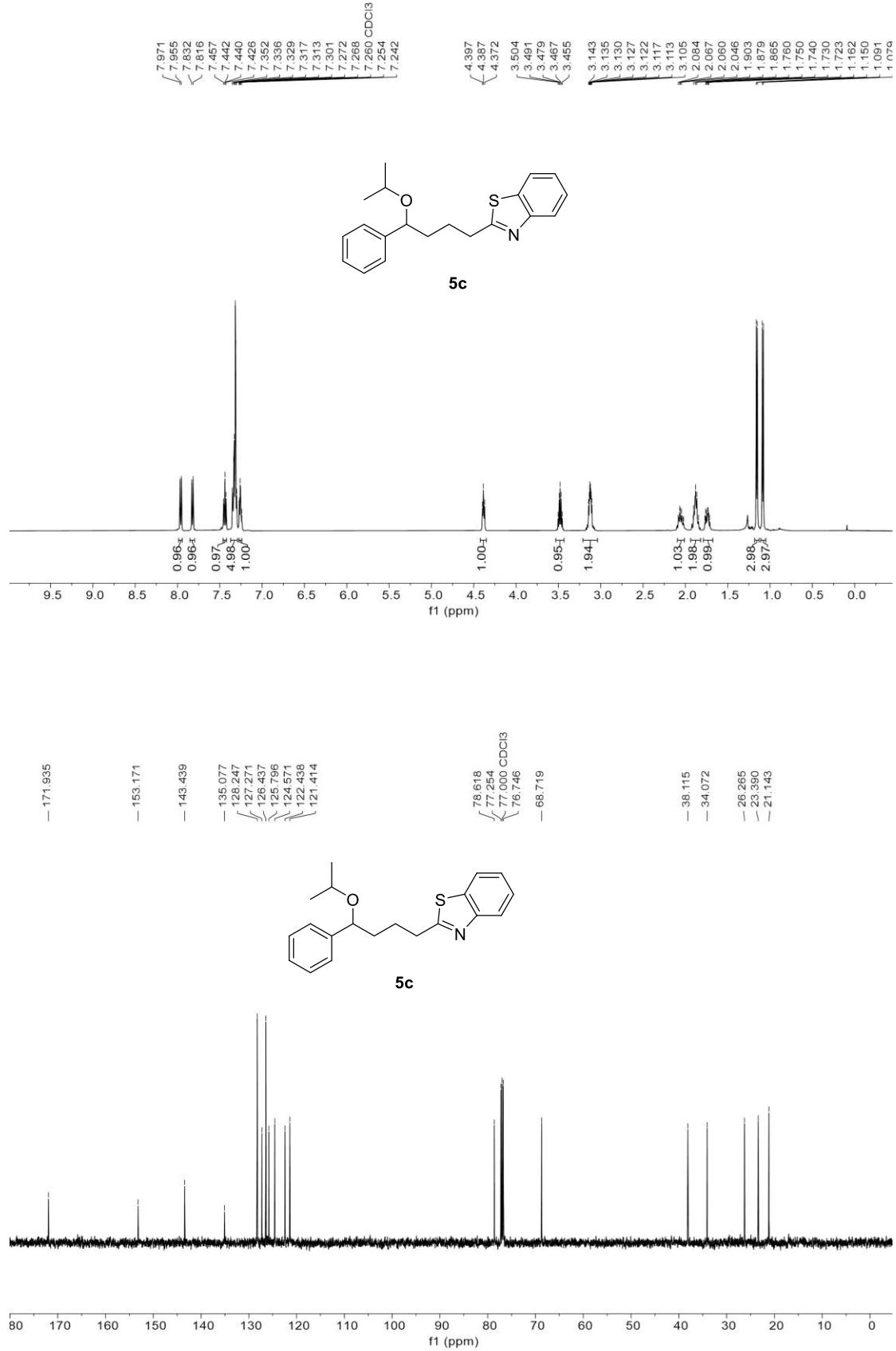


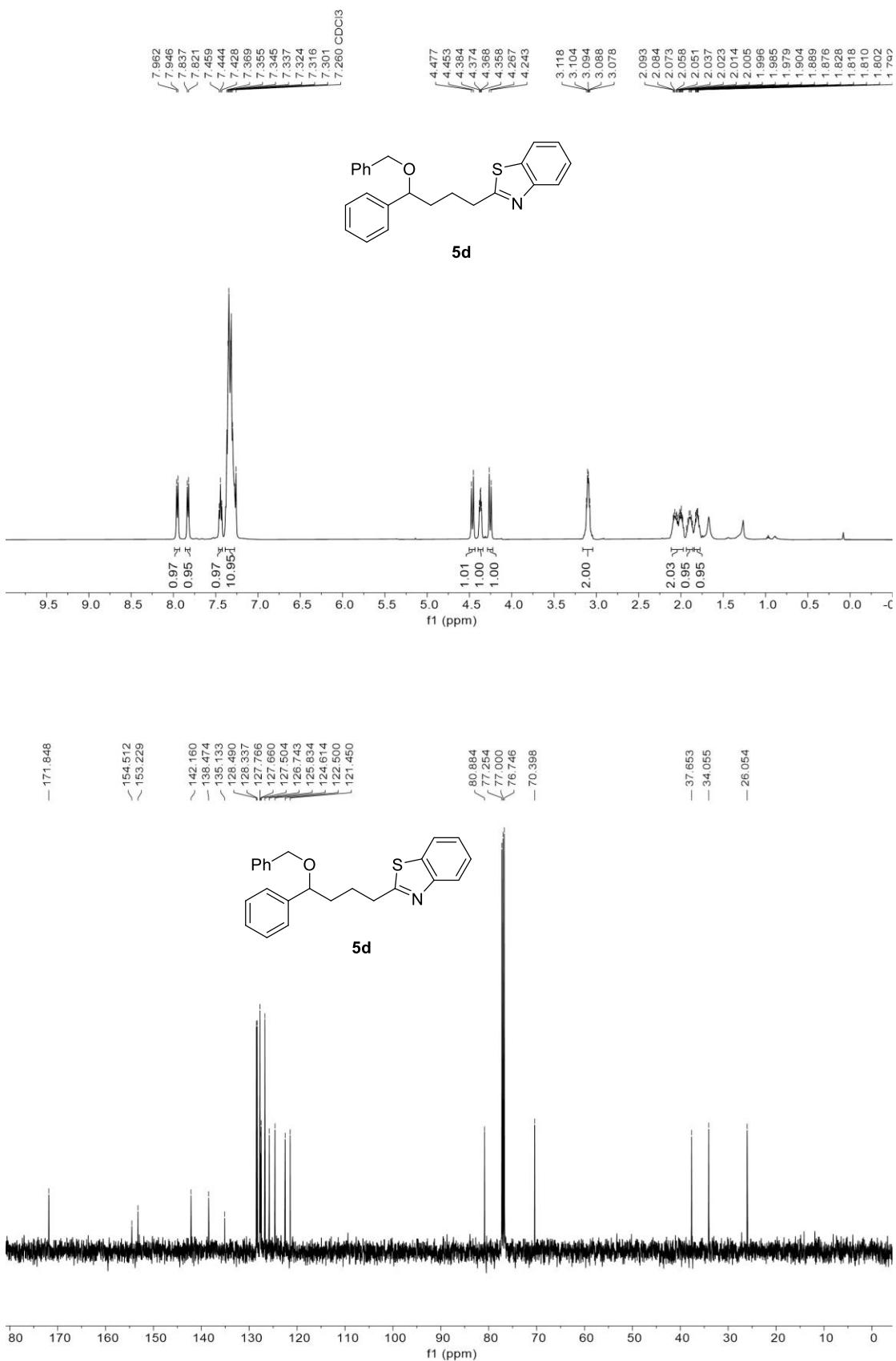


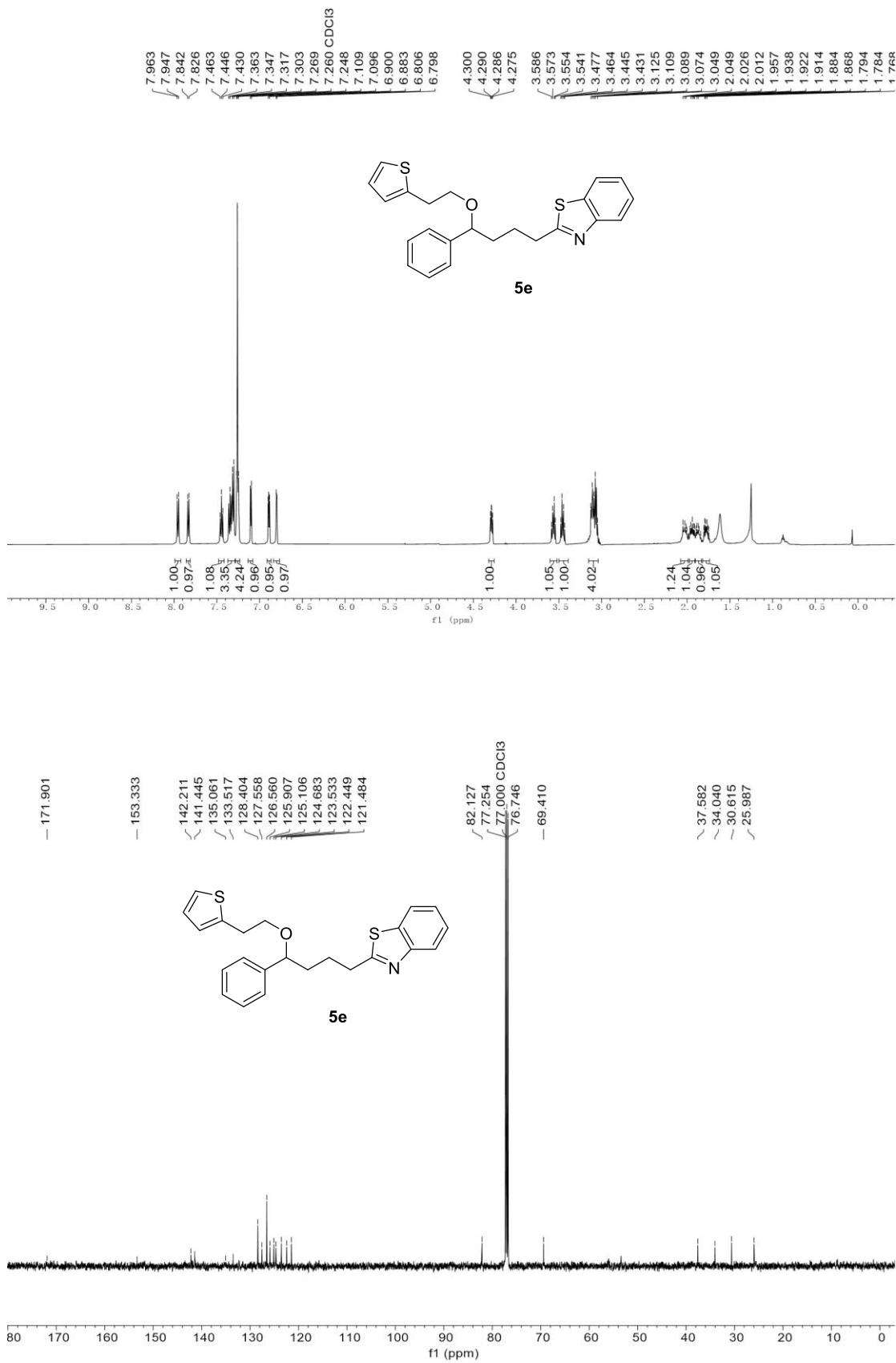


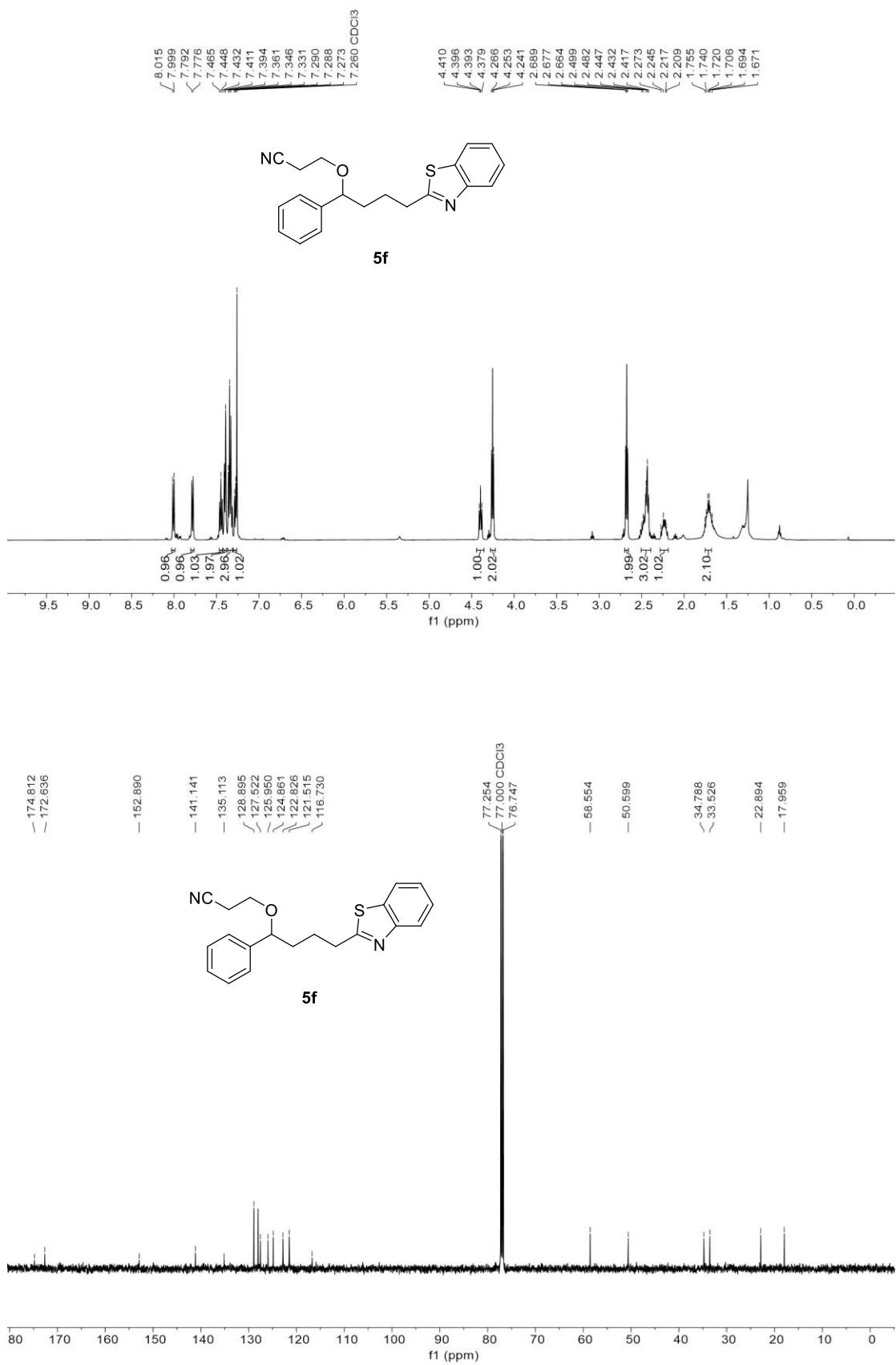


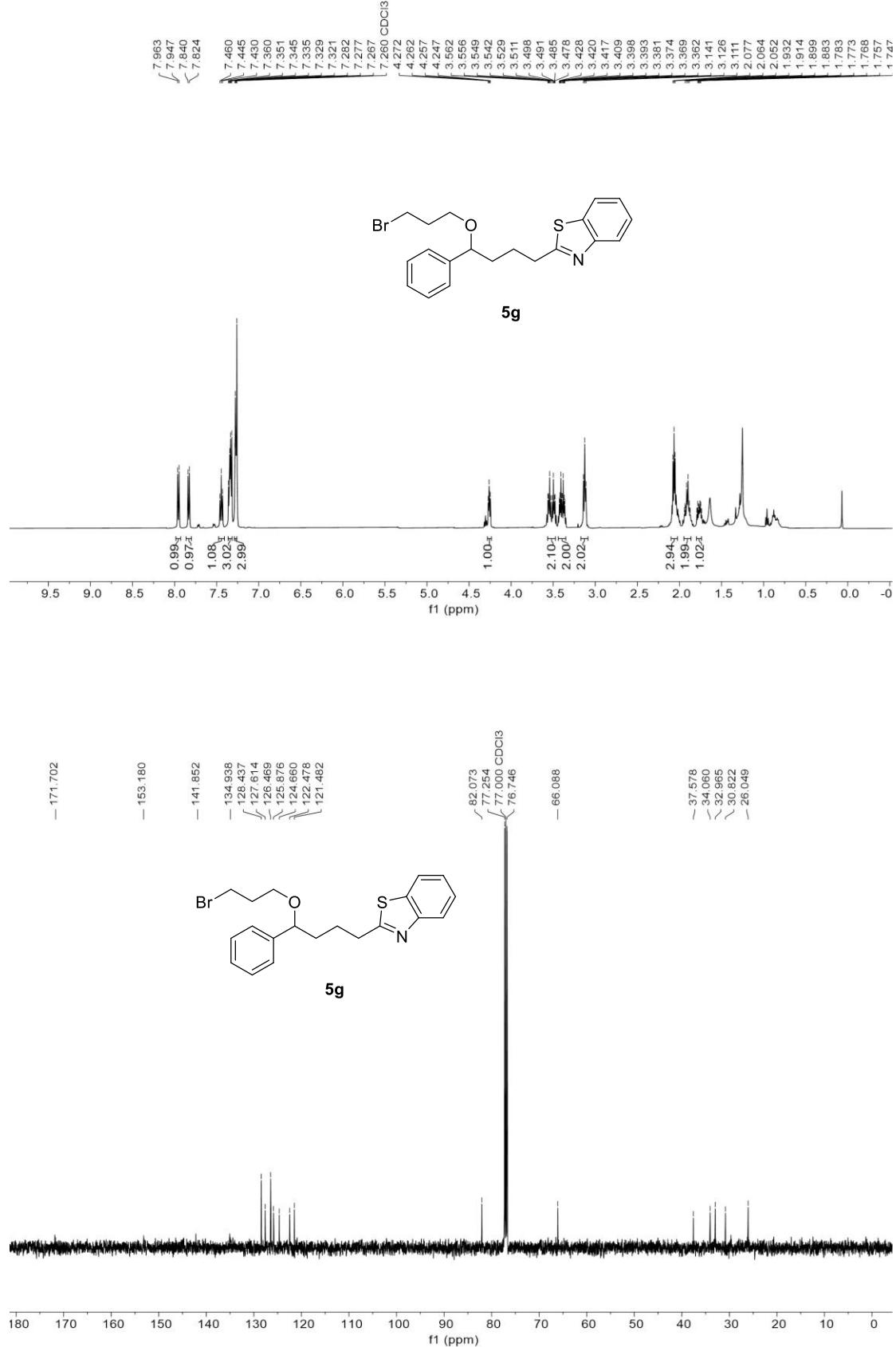


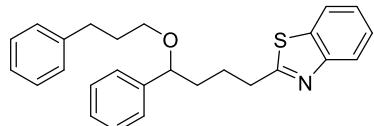
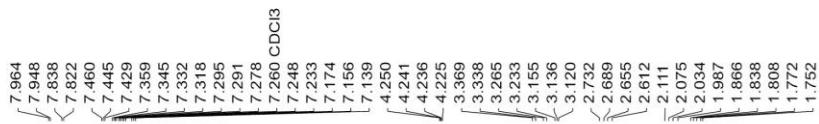




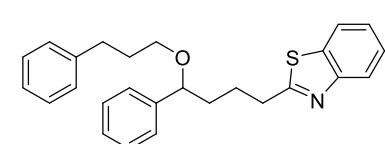
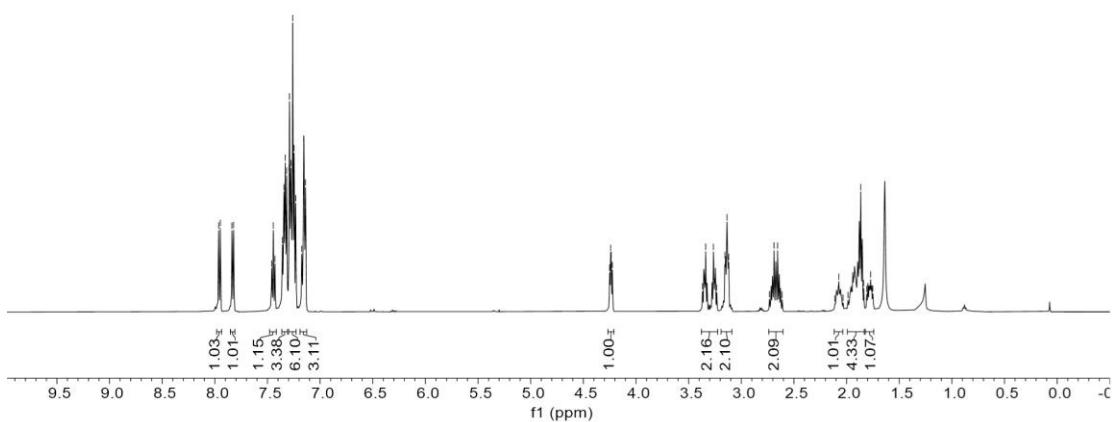




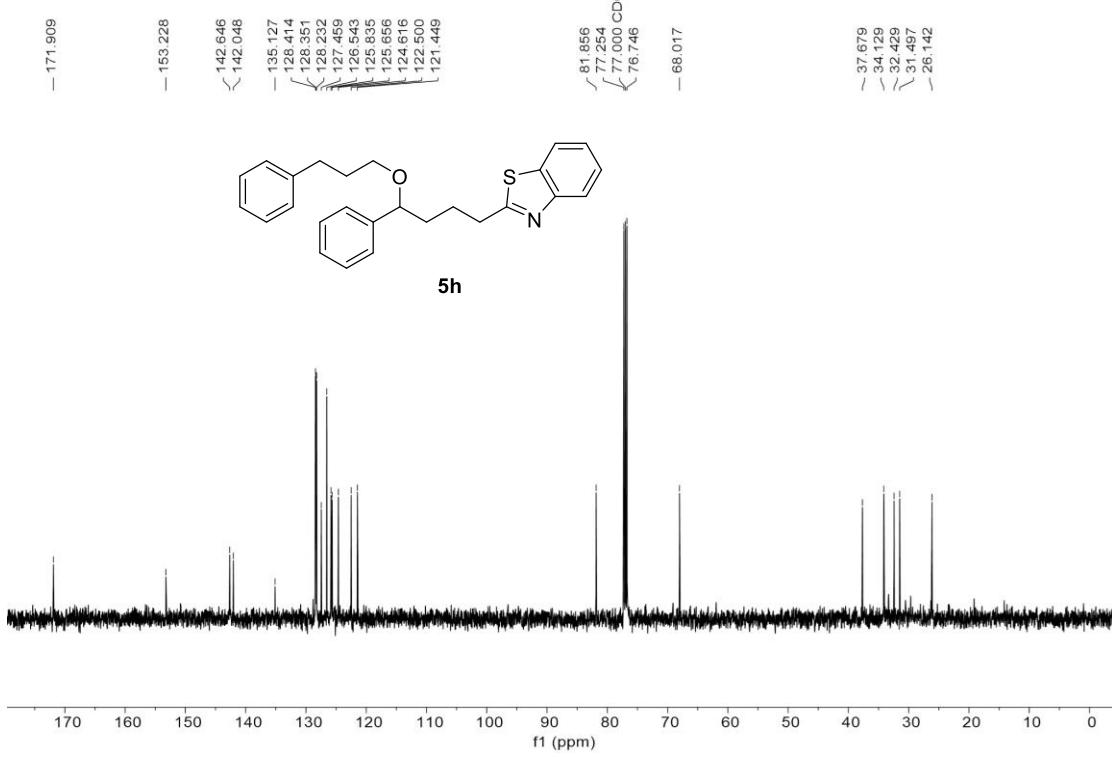


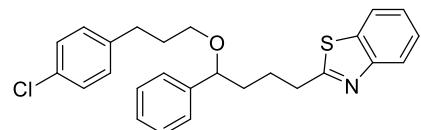
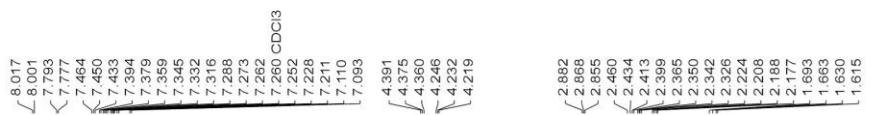


5h

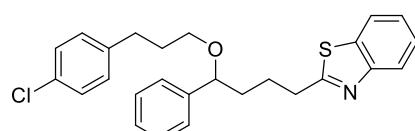
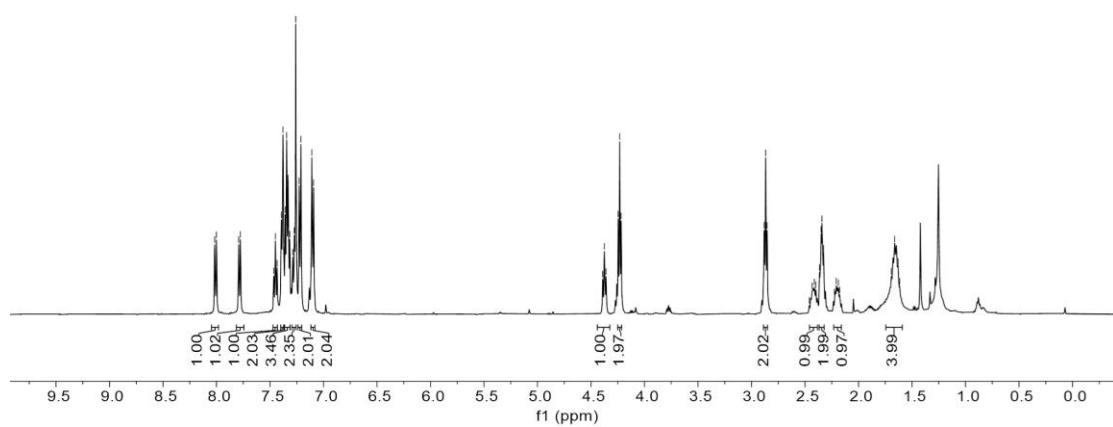


5h





5i



5i

