

## **Bismuth-Catalyzed Allylation of *para*-Quinone Methides**

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## Electronic Supplementary Information

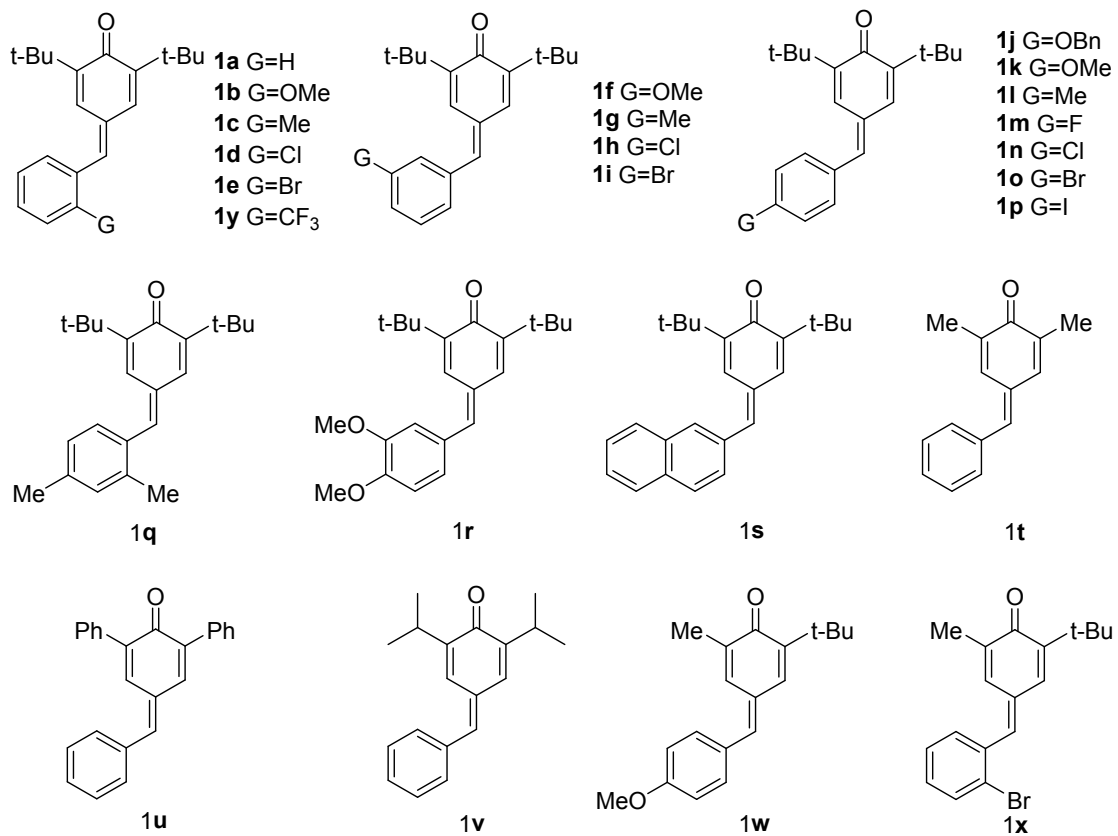
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**1. General information:** Commercial reagents were used as received, unless otherwise stated.  $^1\text{H}$  and  $^{13}\text{C}$  NMR were recorded on 400 MHz spectrometer. Chemical shifts are reported in ppm from tetramethylsilane with the solvent resonance as the internal standard. The following abbreviations were used to designate chemical shift multiplicities: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet. All first-order splitting patterns were assigned on the basis of the appearance of the multiplet. Splitting patterns that could not be easily interpreted are designated as multiplet (m). Mass spectra were obtained using electrospray ionization (ESI) mass spectrometer.

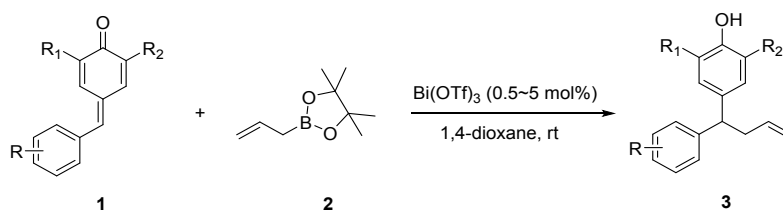
## 2. The synthesis of *para*-quinone methides (*p*-QMs)

The *para*-quinone methides (*p*-QMs) **1a-1s**<sup>1a</sup>, **1w-1y**<sup>1a</sup>, **1t**<sup>1c</sup>, **1u**<sup>1b</sup>, **1v**<sup>1c</sup> were prepared according to the reported literature procedures.



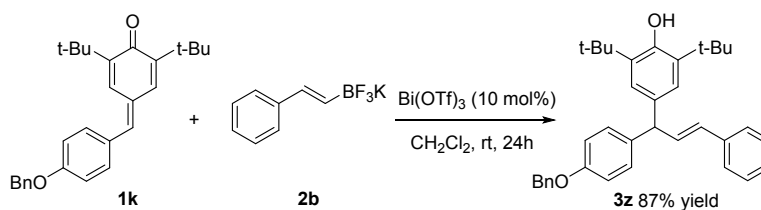
### 3. General experimental 1,6-addition reaction procedure

#### 3.1 1,6-addition of *p*-QMs



To a stirred solution of cyclohexa-2,5-dien-1-one **1** (0.05 mmol) and allylboronic acid pinacol ester **2** (0.1 mmol) in dry 1,4-dioxane (0.5 mL) at room temperature were added  $\text{Bi}(\text{OTf})_3$ . The reactions were monitored by TLC. After **1** were consumed completely, the reaction solution were concentrated *in vacuo* and the crude products were purified by flash chromatography eluting with (petroleum ether/ethyl acetate 30:1) to afford the products **3**.

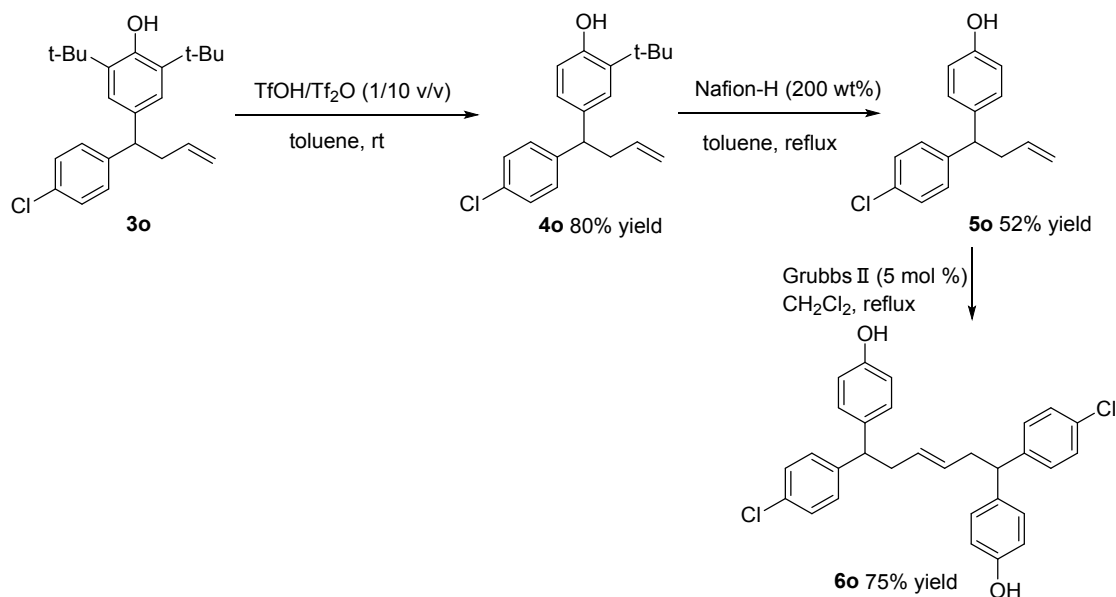
#### 3.2 The synthesis of **3z**



To a stirred solution of 4-(4-(benzyloxy)benzylidene)-2,6-di-tert-butylcyclohexa-2,5-dien-1-one **1k** (0.05 mmol) and *beta*-styryltrifluoroboric acid potassium **2z** (0.1 mmol) in dry  $\text{CH}_2\text{Cl}_2$  (0.5 mL) at room temperature was added  $\text{Bi}(\text{OTf})_3$ . The reaction was monitored by TLC. After **1k** was consumed completely, the reaction solution was concentrated *in vacuo* and the crude product was purified by flash chromatography eluting with (petroleum ether/ethyl acetate 30:1) to afford the product **3z**.

## 4. The transformation of the products

### 4.1 The transformation of **3o**<sup>2</sup>



#### The synthesis of **4o**

Under Ar atmosphere, to a stirred solution of **3o** (450 mg, 1.2 mmol) in 10.0 mL anhydrous toluene was added 10:1 Tf<sub>2</sub>O/TfOH (10:1 v/v) 400  $\mu$ L dropwise. The resulting mixture was stirred for 5h at room temperature. Then 10 mL H<sub>2</sub>O was added to quench the reaction and extracted with ethyl acetate. The organic phase was dried over Na<sub>2</sub>SO<sub>4</sub> and concentrated under reduced pressure. The crude residue was purified with silica gel by column chromatography (petroleum ether/ethyl acetate 10/1) to afford **4o** 301 mg as a colorless oil in 80 % yield.

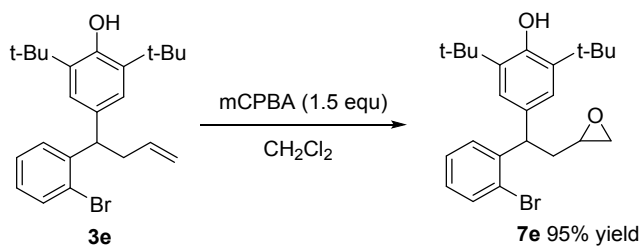
#### The synthesis of **5o**

A mixture of **4o** (251mg, 0.8 mmol) and Nafion-H (200 wt %) in toluene (5 mL) was refluxed 3 h until completion of the reaction. The solid resinsulfonic acid was then filtered off and the solvent was concentrated under reduced pressure. The crude residue was purified with silica gel by column chromatography (petroleum ether/ethyl acetate 3/1) to afford **5o** 134 mg as a colorless oil in 52 % yield.

#### The synthesis of **6o**

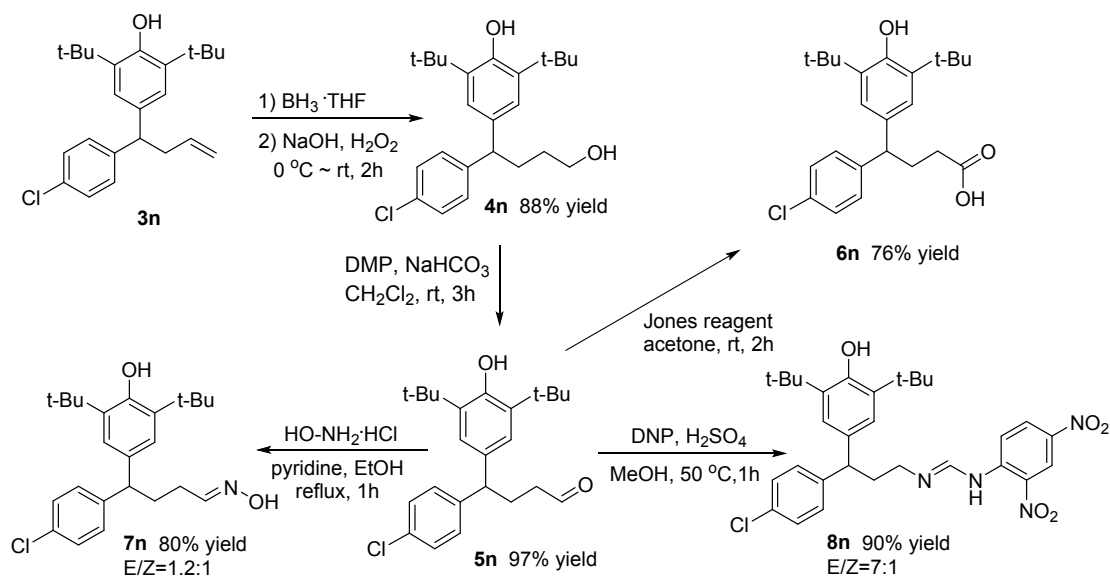
Under Ar atmosphere, **5o** (129 mg, 0.5 mmol) was added to a solution of Grubbs II catalyst (5 mol %) in 5ml CH<sub>2</sub>Cl<sub>2</sub>. The resulting mixture was heated to reflux for 3h. The solvent was concentrated under reduced pressure. Then the crude residue was purified with silica gel by column chromatography (petroleum ether /ethyl acetate 2/1) to afford **6o** 92 mg as a white solid in 75 % yield.

#### 4.2 The transformation of **3e**



m-CPBA (77.6mg, 1.5 equiv) was added to a solution of **3e** (111.3, 0.3 mmol) in  $\text{CH}_2\text{Cl}_2$  (5mL) at 0 °C. The resulting solution was stirred at room temperature for 24 h. Next, the reaction mixture was cooled to 0 °C and quenched with saturated  $\text{NaHCO}_3$  (10 mL). The organic layer was separated and the aqueous layer was extracted with  $\text{CH}_2\text{Cl}_2$ . The organic layer was separated, dried over  $\text{Na}_2\text{SO}_4$ , and concentrated under reduced pressure. The crude residue was purified with silica gel by column chromatography (petroleum ether /ethyl acetate 50/1) to afford **7e** 110 mg as a white solid in 95 % yield.

### 4.3 The transformation of **3n**<sup>4</sup>



#### The synthesis of **4n**

$\text{BH}_3 \cdot \text{THF}$  (1.0 M solution in THF, 1.16 mmol) was added to a solution of **3n** (430 mg, 1.16 mmol) in THF (5 mL) at  $0^\circ\text{C}$ . The mixture was stirred for 10 min at  $0^\circ\text{C}$  and for 1 h at room temperature. 15% NaOH (aq) (1.5 eq) and 30%  $\text{H}_2\text{O}_2$  (aq) (2.0 eq) were successively added at  $0^\circ\text{C}$ , and the resulting mixture was stirred for 1 h at room temperature. The reaction was quenched with saturated NaCl (aq) and the mixture was extracted with  $\text{Et}_2\text{O}$ . The organic layer was dried over  $\text{MgSO}_4$ , filtered, and concentrated under vacuum. The crude residue was purified with silica gel by column chromatography (petroleum ether/ethyl acetate 5/1) to afford **4n** 395 mg as a white oil in 88 % yield.

#### The synthesis of **5n**

To a stirred solution of **4n** (375 mg, 0.96 mmol) in  $\text{CH}_2\text{Cl}_2$  (10.0 mL) was added  $\text{NaHCO}_3$  (1.2 g, 14.5 mmol) and Dess-Martin periodinane (1.0 g, 2.4 mmol). The resulting slurry was stirred at room temperature for 3 h before filtrated through celite and concentrated under reduced pressure. The crude residue was purified with silica gel by column chromatography (petroleum ether/ethyl acetate 20/1) to afford **5n** 360 mg as a white oil in 97 % yield.

#### The synthesis of **6n**

To a stirred solution of **5n** (136 mg, 0.35 mmol) at  $0^\circ\text{C}$  in acetone (5 mL) was added Jones reagent ( $\text{CrO}_3/\text{H}_2\text{SO}_4 = 1 \text{ mmol}/4 \text{ mL}$ , 0.08 mol). The solution was stirred at room temperature for 2 h and quenched with *i*PrOH. The reaction was quenched with  $\text{H}_2\text{O}$  and the mixture was extracted with ethyl acetate, and concentrated under reduced pressure. The crude residue was purified with silica gel by column chromatography (petroleum ether/ethyl acetate 3/1) to afford **6n** 107 mg as a white solid in 76 % yield.

#### The synthesis of **7n**

To a stirred solution of **5n** (98 mg, 0.25 mmol) in EtOH (3 mL) was added hydroxyamine hydrochloride (52 mg, 0.75 mmol) and pyridine (0.04 mL). The resulting mixture was heated to reflux for 1 h. The solvent was concentrated under reduced pressure, EtOAc (5 mL) and water (5



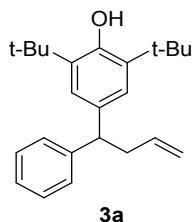
mL) were added, the organic layer was washed with 5% HCl and concentrated under reduced pressure. Then the crude residue was purified with silica gel by column chromatography (petroleum ether /ethyl acetate 5/1) to afford **7o** 80 mg as a white oil in 80 % yield.

#### **The synthesis of 8n**

To a stirred solution of 1-(2,4-dinitrophenyl)hydrazine (55mg, 0.28 mmol) and concentrated sulfuric acid (40 uL) in MeOH (3mL) at 50 °C was added a solution of **5n** (98mg, 0.25 mmol) in MeOH(2 mL). The resulting reaction mixture was stirred at 50 °C for additional 1h. Then the reaction mixture was concentrated to 1/4 of its original volume under vacuo and diluted with water (5 mL). The precipitates were separated by filtration and washed with 3% aqueous NaHCO<sub>3</sub> (3×1 mL) and water (3×1 mL). Products were recrystallized from EtOH to give **8n** 128mg as a yellow solid in 90 % yield

## 5. Analytical data of all compounds

**Compound 3a:** 2,6-di-tert-butyl-4-(1-phenylbut-3-en-1-yl)phenol.



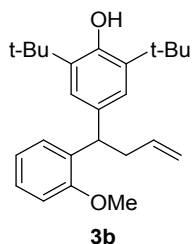
**Compound 3a:** colorless oil, 99% isolated yield.

**<sup>1</sup>H NMR** (400 MHz, CDCl<sub>3</sub>) δ 7.29 – 7.21 (m, 3H), 7.16 (d, *J* = 8.4 Hz, 2H), 6.99 (s, 2H), 5.75 – 5.62 (m, 1H), 5.06 (s, 1H), 5.04 – 4.92 (m, 2H), 3.89 (t, *J* = 7.9 Hz, 1H), 2.79 – 2.70 (m, 2H), 1.40 (s, 18H).

**<sup>13</sup>C NMR** (100 MHz, CDCl<sub>3</sub>) δ 152.11, 145.15, 137.52, 135.63, 135.25, 128.42, 128.14, 126.07, 124.45, 116.03, 51.45, 40.82, 34.51, 30.49.

**HRMS (ESI)** calcd for C<sub>24</sub>H<sub>32</sub>O (M+NH<sub>4</sub>)<sup>+</sup>: 354.2791, found: 354.2794.

**Compound 3b:** 2,6-di-tert-butyl-4-(1-(2-methoxyphenyl)but-3-en-1-yl)phenol.



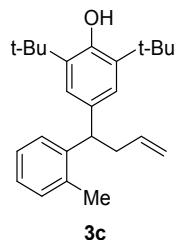
**Compound 3b:** colorless oil, 99% isolated yield.

**<sup>1</sup>H NMR** (400 MHz, CDCl<sub>3</sub>) δ 7.21 – 7.07 (m, 4H), 6.94 – 6.81 (m, 2H), 5.81 – 5.65 (m, 1H), 5.07 – 4.85 (m, 3H), 4.42 (t, *J* = 7.9 Hz, 1H), 3.80 (s, 3H), 2.77 (dt, *J* = 14.8, 7.7 Hz, 2H), 1.40 (s, 18H).

**<sup>13</sup>C NMR** (100 MHz, CDCl<sub>3</sub>) δ 157.07, 151.88, 137.92, 135.26, 134.93, 133.69, 128.08, 126.90, 124.82, 120.58, 115.60, 110.76, 55.55, 43.19, 39.58, 34.48, 30.52.

**HRMS (ESI)** calcd for C<sub>25</sub>H<sub>34</sub>O<sub>2</sub> (M+NH<sub>4</sub>)<sup>+</sup>: 384.2897, found: 384.2899.

**Compound 3c:** 2,6-di-tert-butyl-4-(1-(o-tolyl)but-3-en-1-yl)phenol.



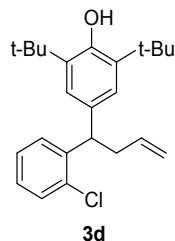
**Compound 3c:** colorless oil, 99% isolated yield.

**<sup>1</sup>H NMR** (400 MHz, CDCl<sub>3</sub>) δ 7.28 (d, *J* = 7.7 Hz, 1H), 7.21 – 7.05 (m, 3H), 6.98 (s, 2H), 5.79 – 5.65 (m, 1H), 5.06 – 4.88 (m, 3H), 4.12 (t, *J* = 7.7 Hz, 1H), 2.75 (d, *J* = 5.8 Hz, 2H), 2.31 (s, 3H), 1.38 (s, 18H).

$^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  151.96, 143.03, 137.59, 136.18, 135.50, 134.79, 130.48, 126.89, 126.04, 125.87, 124.70, 115.94, 46.65, 40.85, 34.47, 30.48, 20.21.

HRMS (ESI) calcd for  $\text{C}_{25}\text{H}_{34}\text{O}$  (M-H) $^-$ : 349.2537, found: 349.2543.

**Compound 3d:** 2,6-di-tert-butyl-4-(1-(2-chlorophenyl)but-3-en-1-yl)phenol.



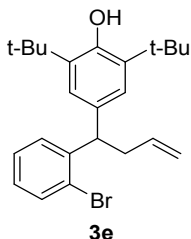
**Compound 3d:** colorless oil, 99% isolated yield.

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.33 (d,  $J = 8.0$  Hz, 1H), 7.28 (s, 1H), 7.23 – 7.17 (m, 1H), 7.10 (d,  $J = 7.8$  Hz, 1H), 7.07 (s, 2H), 5.81 – 5.63 (m, 1H), 5.10 – 4.89 (m, 3H), 4.53 (t,  $J = 7.9$  Hz, 1H), 2.78 (t,  $J = 7.0$  Hz, 2H), 1.40 (s, 18H).

$^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  142.63, 136.91, 135.60, 133.70, 129.70, 128.78, 127.17, 126.92, 124.76, 116.34, 46.34, 39.87, 34.50, 30.48.

HRMS (ESI) calcd for  $\text{C}_{24}\text{H}_{31}\text{ClO}$  (M+ $\text{NH}_4$ ) $^+$ : 388.2402, found: 388.2393.

**Compound 3e:** 4-(1-(2-bromophenyl)but-3-en-1-yl)-2,6-di-tert-butylphenol.



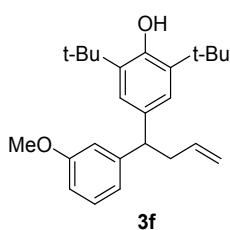
**Compound 3e:** colorless oil, 96% isolated yield.

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.53 (d,  $J = 7.4$  Hz, 1H), 7.24 (d,  $J = 3.2$  Hz, 2H), 7.09 (s, 2H), 7.02 (dd,  $J = 8.4, 2.7$  Hz, 1H), 5.81 – 5.64 (m, 1H), 5.12 – 4.91 (m, 3H), 4.52 (t,  $J = 7.8$  Hz, 1H), 2.77 (dd,  $J = 8.6, 5.8$  Hz, 2H), 1.40 (s, 18H).

$^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  152.24, 144.31, 136.83, 135.60, 133.68, 133.02, 128.97, 127.59, 127.52, 125.27, 124.78, 116.39, 48.92, 40.03, 34.52, 30.49.

HRMS (ESI) calcd for  $\text{C}_{24}\text{H}_{31}\text{BrO}$  (M-H) $^-$ : 413.1486, found: 413.1477.

**Compound 3f:** 2,6-di-tert-butyl-4-(1-(3-methoxyphenyl)but-3-en-1-yl)phenol.



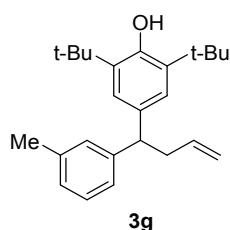
**Compound 3f:** colorless oil, 99% isolated yield.

**<sup>1</sup>H NMR** (400 MHz, CDCl<sub>3</sub>) δ 7.19 (d, *J* = 7.9 Hz, 1H), 7.04 (s, 2H), 6.90 – 6.69 (m, 3H), 5.80 – 5.65 (m, 1H), 5.09 – 4.89 (m, 3H), 3.88 (t, *J* = 7.9 Hz, 1H), 3.78 (s, 3H), 2.77 (dd, *J* = 11.4, 6.9 Hz, 2H), 1.41 (s, 18H).

**<sup>13</sup>C NMR** (100 MHz, CDCl<sub>3</sub>) δ 159.62, 152.15, 146.85, 137.47, 135.60, 135.04, 129.34, 124.40, 120.56, 116.05, 114.19, 111.05, 55.25, 51.49, 40.77, 34.50, 30.48.

**HRMS (ESI)** calcd for C<sub>25</sub>H<sub>34</sub>O<sub>2</sub>(M+NH<sub>4</sub>)<sup>+</sup>: 384.2897, found: 384.2894.

**Compound 3g:** 2,6-di-tert-butyl-4-(1-(*m*-tolyl)but-3-en-1-yl)phenol.



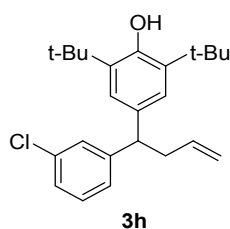
**Compound 3g:** colorless oil, 97% isolated yield.

**<sup>1</sup>H NMR** (400 MHz, CDCl<sub>3</sub>) δ 7.17 (t, *J* = 7.8 Hz, 1H), 7.09 – 6.95 (m, 5H), 5.78 – 5.64 (m, 1H), 5.08 – 4.89 (m, 3H), 3.86 (t, *J* = 7.9 Hz, 1H), 2.83 – 2.70 (m, 2H), 2.31 (s, 3H), 1.40 (s, 18H).

**<sup>13</sup>C NMR** (100 MHz, CDCl<sub>3</sub>) δ 152.08, 145.01, 137.87, 137.62, 135.55, 135.34, 129.05, 128.29, 126.85, 124.94, 124.42, 115.93, 51.48, 40.87, 34.50, 30.48, 21.71.

**HRMS (ESI)** calcd for C<sub>25</sub>H<sub>34</sub>O (M+NH<sub>4</sub>)<sup>+</sup>: 368.2948, found: 368.2949.

**Compound 3h:** 2,6-di-tert-butyl-4-(1-(3-chlorophenyl)but-3-en-1-yl)phenol.



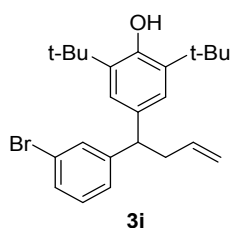
**Compound 3h:** colorless oil, 99% isolated yield.

**<sup>1</sup>H NMR** (400 MHz, CDCl<sub>3</sub>) δ 7.24 – 7.18 (m, 2H), 7.17 – 7.10 (m, 2H), 7.00 (s, 2H), 5.77 – 5.59 (m, 1H), 5.07 (s, 1H), 5.06 – 4.92 (m, 2H), 3.88 (t, *J* = 7.8 Hz, 1H), 2.81 – 2.69 (m, 2H), 1.41 (s, 18H).

**<sup>13</sup>C NMR** (100 MHz, CDCl<sub>3</sub>) δ 152.31, 147.24, 136.94, 135.78, 134.44, 134.15, 129.67, 128.37, 126.28, 124.37, 116.46, 51.13, 40.56, 34.52, 30.45.

**HRMS (ESI)** calcd for C<sub>24</sub>H<sub>31</sub>ClO (M-H)<sup>-</sup>: 369.1991, found: 369.1992.

**Compound 3i:** 4-(1-(3-bromophenyl)but-3-en-1-yl)-2,6-di-tert-butylphenol.



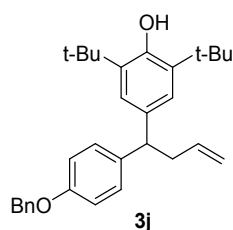
**Compound 3i:** colorless oil, 82% isolated yield.

**<sup>1</sup>H NMR** (400 MHz, CDCl<sub>3</sub>) δ 7.38 (s, 1H), 7.33 – 7.25 (m, 2H), 7.15 (d, *J* = 7.0 Hz, 2H), 6.99 (s, 2H), 5.75 – 5.60 (m, 1H), 5.07 (s, 1H), 5.06 – 4.92 (m, 2H), 3.87 (t, *J* = 7.8 Hz, 1H), 2.74 (t, *J* = 7.4 Hz, 2H), 1.41 (s, 18H).

**<sup>13</sup>C NMR** (100 MHz, CDCl<sub>3</sub>) δ 152.33, 147.57, 136.93, 135.82, 134.40, 131.32, 130.00, 129.22, 126.73, 124.38, 122.54, 116.48, 77.48, 77.16, 76.84, 51.14, 40.60, 34.53, 30.46.

**HRMS (ESI)** calcd for C<sub>24</sub>H<sub>31</sub>BrO (M+H)<sup>+</sup>: 415.1631, found: 415.1638.

**Compound 3j:** 4-(1-(4-(benzyloxy)phenyl)but-3-en-1-yl)-2,6-di-tert-butylphenol.



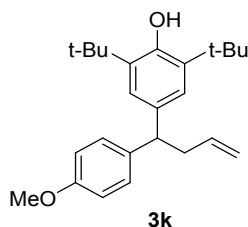
**Compound 3j:** colorless oil, 99% isolated yield.

**<sup>1</sup>H NMR** (400 MHz, CDCl<sub>3</sub>) δ 7.47 – 7.28 (m, 5H), 7.15 (d, *J* = 8.6 Hz, 2H), 7.01 (s, 2H), 6.90 (d, *J* = 8.6 Hz, 2H), 5.71 (m, *J* = 17.0, 10.1, 6.8 Hz, 1H), 5.09 – 4.90 (m, 5H), 3.87 (t, *J* = 7.9 Hz, 1H), 2.82 – 2.69 (m, 2H), 1.40 (s, 18H).

**<sup>13</sup>C NMR** (100 MHz, CDCl<sub>3</sub>) δ 157.12, 152.03, 137.61, 137.58, 137.31, 135.59, 135.56, 129.03, 128.68, 128.03, 127.65, 124.35, 115.97, 114.72, 70.11, 50.58, 41.00, 34.49, 30.48.

**HRMS (ESI)** calcd for C<sub>31</sub>H<sub>38</sub>O<sub>2</sub> (M+NH<sub>4</sub>)<sup>+</sup>: 460.3210, found: 460.3219.

**Compound 3k:** 2,6-di-tert-butyl-4-(1-(4-methoxyphenyl)but-3-en-1-yl)phenol.



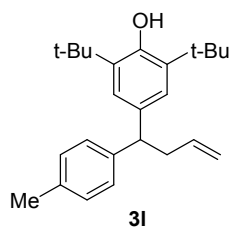
**Compound 3k:** colorless oil, 99% isolated yield.

**<sup>1</sup>H NMR** (400 MHz, CDCl<sub>3</sub>) δ 7.15 (d, *J* = 8.7 Hz, 2H), 7.01 (s, 2H), 6.82 (d, *J* = 8.7 Hz, 2H), 5.80 – 5.63 (m, 1H), 5.08 – 4.89 (m, 3H), 3.87 (t, *J* = 7.9 Hz, 1H), 3.77 (s, 3H), 2.74 (t, *J* = 7.4 Hz, 2H), 1.40 (s, 18H).

**<sup>13</sup>C NMR** (100 MHz, CDCl<sub>3</sub>) δ 157.83, 152.02, 137.62, 137.27, 135.64, 135.56, 129.00, 124.33, 115.95, 113.76, 55.32, 50.56, 41.01, 34.49, 30.48.

**HRMS (ESI)** calcd for C<sub>25</sub>H<sub>34</sub>O<sub>2</sub> (M+NH<sub>4</sub>)<sup>+</sup>: 384.2897, found: 384.2897.

**Compound 3l:** 2,6-di-tert-butyl-4-(1-(p-tolyl)but-3-en-1-yl)phenol.



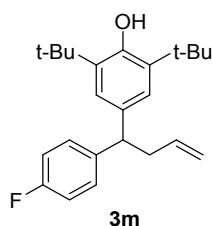
**Compound 3l:** colorless oil, 99% isolated yield.

**<sup>1</sup>H NMR** (400 MHz, CDCl<sub>3</sub>) δ 7.17 – 7.05 (m, 4H), 7.02 (s, 2H), 5.83 – 5.64 (m, 1H), 5.10 – 4.86 (m, 3H), 3.87 (t, *J* = 7.9 Hz, 1H), 2.76 (t, *J* = 7.4 Hz, 2H), 2.30 (s, 3H), 1.40 (s, 18H).

**<sup>13</sup>C NMR** (100 MHz, CDCl<sub>3</sub>) δ 152.05, 142.14, 137.64, 135.55, 135.47, 129.13, 127.92, 124.36, 115.93, 51.08, 40.86, 34.49, 30.48, 21.16.

**HRMS (ESI)** calcd for C<sub>25</sub>H<sub>34</sub>O (M+NH<sub>4</sub>)<sup>+</sup>: 368.2948, found: 368.2944.

**Compound 3m:** 2,6-di-tert-butyl-4-(1-(4-fluorophenyl)but-3-en-1-yl)phenol.



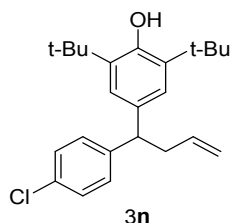
**Compound 3m:** colorless oil, 96% isolated yield.

**<sup>1</sup>H NMR** (400 MHz, CDCl<sub>3</sub>) δ 7.18 (dd, *J* = 8.6, 5.5 Hz, 2H), 7.02 – 6.92 (m, 4H), 5.79 – 5.63 (m, 1H), 5.05 (s, 1H), 5.05 – 4.91 (m, 2H), 3.90 (t, *J* = 7.8 Hz, 1H), 2.74 (t, *J* = 8.1 Hz, 2H), 1.40 (s, 18H).

**<sup>13</sup>C NMR** (100 MHz, CDCl<sub>3</sub>) δ 152.17, 137.23, 135.72, 135.12, 129.54, 129.47, 124.34, 116.27, 115.25, 115.04, 50.56, 40.90, 34.52, 30.47.

**HRMS (ESI)** calcd for C<sub>24</sub>H<sub>31</sub>FO (M-H)<sup>-</sup>: 353.2286, found: 353.2292.

**Compound 3n:** 2,6-di-tert-butyl-4-(1-(4-chlorophenyl)but-3-en-1-yl)phenol.



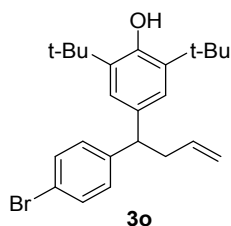
**Compound 3n:** colorless oil, 99% isolated yield.

**<sup>1</sup>H NMR** (400 MHz, CDCl<sub>3</sub>) δ 7.24 (d, *J* = 8.0 Hz, 2H), 7.16 (d, *J* = 8.2 Hz, 2H), 6.99 (s, 2H), 5.83 – 5.61 (m, 1H), 5.06 (s, 1H), 5.05 – 4.92 (m, 2H), 3.89 (t, *J* = 7.8 Hz, 1H), 2.74 (t, *J* = 7.4 Hz, 2H), 1.40 (s, 18H).

**<sup>13</sup>C NMR** (100 MHz, CDCl<sub>3</sub>) δ 152.24, 143.62, 137.05, 135.75, 134.75, 131.70, 129.50, 128.53, 124.31, 116.40, 50.71, 40.64, 34.51, 30.45.

**HRMS (ESI)** calcd for C<sub>24</sub>H<sub>31</sub>ClO (M-H)<sup>-</sup>: 369.1991, found: 369.1991.

**Compound 3o:** 4-(1-(4-bromophenyl)but-3-en-1-yl)-2,6-di-tert-butylphenol.



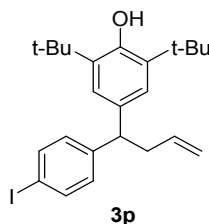
**Compound 3o:** colorless oil, 92% isolated yield.

**<sup>1</sup>H NMR** (400 MHz, CDCl<sub>3</sub>) δ 7.39 (d, *J* = 8.3 Hz, 2H), 7.10 (d, *J* = 8.3 Hz, 2H), 6.98 (s, 2H), 5.76 – 5.61 (m, 1H), 5.06 (s, 1H), 5.05 – 4.91 (m, 2H), 3.87 (t, *J* = 7.9 Hz, 1H), 2.74 (t, *J* = 7.1 Hz, 2H), 1.40 (s, 18H).

**<sup>13</sup>C NMR** (100 MHz, CDCl<sub>3</sub>) δ 152.26, 144.16, 137.01, 135.77, 134.65, 131.47, 129.91, 124.30, 119.81, 116.42, 50.79, 40.56, 34.51, 30.45.

**HRMS (ESI)** calcd for C<sub>24</sub>H<sub>31</sub>BrO (M+H)<sup>+</sup>: 413.1486, found: 413.1487.

**Compound 3p:** 2,6-di-tert-butyl-4-(1-(4-iodophenyl)but-3-en-1-yl)phenol.



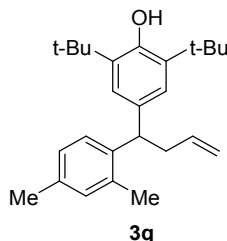
**Compound 3p:** colorless oil, 99% isolated yield.

**<sup>1</sup>H NMR** (400 MHz, CDCl<sub>3</sub>) δ 7.59 (d, *J* = 8.3 Hz, 2H), 7.03 – 6.96 (m, 4H), 5.76 – 5.58 (m, 1H), 5.06 (s, 1H), 5.05 – 4.91 (m, 2H), 3.85 (t, *J* = 7.9 Hz, 1H), 2.79 – 2.68 (m, 2H), 1.40 (s, 18H).

**<sup>13</sup>C NMR** (100 MHz, CDCl<sub>3</sub>) δ 152.26, 144.89, 137.45, 137.01, 135.77, 134.59, 130.25, 124.29, 116.43, 50.90, 40.48, 34.51, 30.45.

**HRMS (ESI)** calcd for C<sub>24</sub>H<sub>31</sub>IO (M-H)<sup>-</sup>: 461.1347, found: 461.1343.

**Compound 3q:** 2,6-di-tert-butyl-4-(1-(2,4-dimethylphenyl)but-3-en-1-yl)phenol.



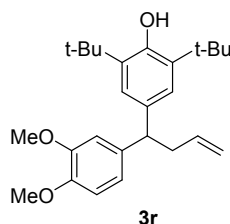
**Compound 3q:** colorless oil, 99% isolated yield.

**<sup>1</sup>H NMR** (400 MHz, CDCl<sub>3</sub>) δ 7.17 (d, *J* = 7.8 Hz, 1H), 7.02 – 6.91 (m, 4H), 5.81 – 5.64 (m, 1H), 5.09 – 4.87 (m, 3H), 4.08 (t, *J* = 7.8 Hz, 1H), 2.82 – 2.66 (m, 2H), 2.27 (d, *J* = 2.9 Hz, 6H), 1.38 (s, 18H).

**<sup>13</sup>C NMR** (100 MHz, CDCl<sub>3</sub>) δ 151.91, 140.03, 137.73, 135.91, 135.45, 135.16, 135.04, 131.30, 126.76, 126.73, 124.62, 115.85, 46.37, 40.91, 34.46, 30.49, 21.05, 20.14.

**HRMS (ESI)** calcd for C<sub>26</sub>H<sub>36</sub>O (M+NH<sub>4</sub>)<sup>+</sup>: 382.3104, found: 382.3108.

**Compound 3r:** 2,6-di-tert-butyl-4-(1-(3,4-dimethoxyphenyl)but-3-en-1-yl)phenol.



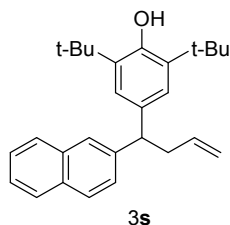
**Compound 3r:** colorless oil, 99% isolated yield.

**<sup>1</sup>H NMR** (400 MHz, CDCl<sub>3</sub>) δ 7.03 (s, 2H), 6.78 (d, *J* = 7.9 Hz, 3H), 5.84 – 5.63 (m, 1H), 5.13 – 4.88 (m, 3H), 3.85 (s, 7H), 2.75 (t, *J* = 7.4 Hz, 2H), 1.40 (s, 18H).

**<sup>13</sup>C NMR** (100 MHz, CDCl<sub>3</sub>) δ 152.10, 148.83, 147.36, 137.76, 137.58, 135.66, 135.47, 124.33, 120.06, 115.97, 111.66, 111.21, 56.00, 55.94, 53.56, 51.01, 41.17, 34.52, 30.51.

**HRMS (ESI)** calcd for C<sub>26</sub>H<sub>36</sub>O<sub>3</sub> (M+NH<sub>4</sub>)<sup>+</sup>: 414.3003, found: 414.3004.

**Compound 3s:** 2,6-di-tert-butyl-4-(1-(naphthalen-2-yl)but-3-en-1-yl)phenol.



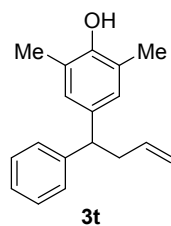
**Compound 3s:** colorless oil, 94% isolated yield.

**<sup>1</sup>H NMR** (400 MHz, CDCl<sub>3</sub>) δ 7.84 – 7.72 (m, 3H), 7.68 (d, *J* = 1.7 Hz, 1H), 7.49 – 7.33 (m, 3H), 7.08 (s, 2H), 5.84 – 5.68 (m, 1H), 5.15 – 4.86 (m, 3H), 4.08 (t, *J* = 7.8 Hz, 1H), 2.87 (q, *J* = 7.9, 7.3 Hz, 2H), 1.40 (s, 18H).

**<sup>13</sup>C NMR** (100 MHz, CDCl<sub>3</sub>) δ 152.18, 142.65, 137.44, 135.73, 135.12, 133.70, 132.27, 128.02, 127.88, 127.69, 126.92, 126.32, 125.92, 125.35, 124.54, 116.13, 51.52, 40.62, 34.52, 30.50.

**HRMS (ESI)** calcd for C<sub>28</sub>H<sub>34</sub>O (M+NH<sub>4</sub>)<sup>+</sup>: 404.2948, found: 404.2949.

**Compound 3t:** 2,6-dimethyl-4-(1-phenylbut-3-en-1-yl)phenol.



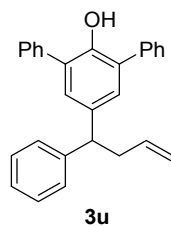
**Compound 3t:** colorless oil, 95% isolated yield.

**<sup>1</sup>H NMR** (400 MHz, CDCl<sub>3</sub>) δ 7.31 – 7.13 (m, 5H), 6.84 (s, 2H), 5.81 – 5.62 (m, 1H), 5.12 – 4.88 (m, 2H), 4.45 (s, 1H), 3.87 (t, *J* = 7.9 Hz, 1H), 2.81 – 2.72 (m, 2H), 2.20 (s, 6H).

**<sup>13</sup>C NMR** (100 MHz, CDCl<sub>3</sub>) δ 150.60, 145.21, 137.27, 136.27, 128.49, 128.09, 127.92, 126.14, 122.93, 116.19, 50.65, 40.28, 16.21.

**HRMS (ESI)** calcd for C<sub>18</sub>H<sub>20</sub>O (M+H)<sup>+</sup>: 251.1441, found: 251.1446.

**Compound 3u:** 5'-(1-phenylbut-3-en-1-yl)-[1,1':3',1''-terphenyl]-2'-ol.



**Compound 3u:** colorless oil, 96% isolated yield.

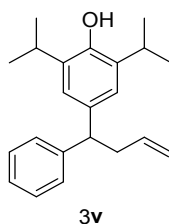


**<sup>1</sup>H NMR** (400 MHz, CDCl<sub>3</sub>) δ 7.52 (d, *J* = 7.9 Hz, 4H), 7.48 – 7.40 (m, 4H), 7.40 – 7.33 (m, 2H), 7.27 (d, *J* = 4.4 Hz, 4H), 7.15 (s, 3H), 5.85 – 5.67 (m, 1H), 5.28 (s, 1H), 5.13 – 4.92 (m, 2H), 4.01 (t, *J* = 7.9 Hz, 1H), 2.84 (t, *J* = 7.4 Hz, 2H).

**<sup>13</sup>C NMR** (100 MHz, CDCl<sub>3</sub>) δ 147.74, 144.80, 137.87, 137.03, 136.83, 129.48, 128.93, 128.68, 128.59, 127.96, 127.71, 126.32, 116.47, 50.79, 40.31.

**HRMS (ESI)** calcd for C<sub>28</sub>H<sub>24</sub>O (M+NH<sub>4</sub>)<sup>+</sup>: 394.2165, found: 394.2173.

**Compound 3v:** 2,6-diisopropyl-4-(1-phenylbut-3-en-1-yl)phenol.



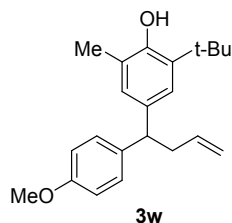
**Compound 3v:** colorless oil, 99% isolated yield.

**<sup>1</sup>H NMR** (400 MHz, CDCl<sub>3</sub>) δ 7.30 – 7.20 (m, 4H), 7.16 (t, *J* = 7.0 Hz, 1H), 6.91 (s, 2H), 5.81 – 5.62 (m, 1H), 5.08 – 4.88 (m, 2H), 4.63 (s, 1H), 3.93 (t, *J* = 7.9 Hz, 1H), 3.10 (p, *J* = 6.9 Hz, 2H), 2.82 – 2.74 (m, 2H), 1.23 (dd, *J* = 6.8, 2.9 Hz, 12H).

**<sup>13</sup>C NMR** (100 MHz, CDCl<sub>3</sub>) δ 148.38, 145.25, 137.41, 136.38, 133.47, 128.44, 128.01, 126.07, 123.05, 116.11, 51.22, 40.69, 27.46, 22.90.

**HRMS (ESI)** calcd for C<sub>22</sub>H<sub>28</sub>O (M-H)<sup>-</sup>: 307.2067, found: 307.2070.

**Compound 3w:** 2-(tert-butyl)-4-(1-(4-methoxyphenyl)but-3-en-1-yl)-6-methylphenol.



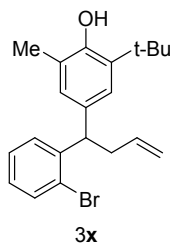
**Compound 3w:** colorless oil, 96% isolated yield.

**<sup>1</sup>H NMR** (400 MHz, CDCl<sub>3</sub>) δ 7.14 (d, *J* = 8.7 Hz, 2H), 7.01 (d, *J* = 2.2 Hz, 1H), 6.85 – 6.74 (m, 3H), 5.79 – 5.63 (m, 1H), 5.08 – 4.89 (m, 2H), 4.60 (s, 1H), 3.89 – 3.80 (m, 1H), 3.76 (s, 3H), 2.82 – 2.64 (m, 2H), 2.17 (s, 3H), 1.38 (s, 9H).

**<sup>13</sup>C NMR** (100 MHz, CDCl<sub>3</sub>) δ 164.33, 157.87, 150.96, 137.49, 137.38, 136.22, 135.41, 129.84, 128.88, 127.75, 124.63, 122.92, 116.03, 113.83, 55.33, 50.14, 40.73, 34.68, 29.93, 16.30.

**HRMS (ESI)** calcd for C<sub>22</sub>H<sub>28</sub>O<sub>2</sub> (M+NH<sub>4</sub>)<sup>+</sup>: 342.2428, found: 342.3420.

**Compound 3x:** 4-(1-(2-bromophenyl)but-3-en-1-yl)-2-(tert-butyl)-6-methylphenol.



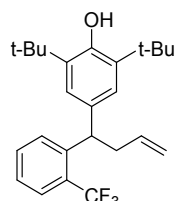
**Compound 3x:** colorless oil, 96% isolated yield.

**<sup>1</sup>H NMR** (400 MHz, CDCl<sub>3</sub>) δ 7.52 (d, *J* = 7.7 Hz, 1H), 7.24 (d, *J* = 3.9 Hz, 2H), 7.10 (d, *J* = 2.3 Hz, 1H), 7.05 – 6.98 (m, 1H), 6.85 (d, *J* = 2.4 Hz, 1H), 5.81 – 5.66 (m, 1H), 5.09 – 4.90 (m, 2H), 4.62 (s, 1H), 4.48 (t, *J* = 7.8 Hz, 1H), 2.84 – 2.71 (m, 2H), 2.19 (s, 3H), 1.39 (s, 9H).

**<sup>13</sup>C NMR** (100 MHz, CDCl<sub>3</sub>) δ 151.16, 144.20, 136.73, 135.39, 134.21, 133.07, 128.98, 128.11, 127.60, 125.30, 125.22, 122.95, 116.47, 48.73, 40.00, 34.70, 29.93, 16.31.

**HRMS (ESI)** calcd for C<sub>21</sub>H<sub>25</sub>BrO (M-H)<sup>-</sup>: 371.1016, found: 371.1018.

**Compound 3y:** 2,6-di-tert-butyl-4-(1-(2-(trifluoromethyl)phenyl)but-3-en-1-yl)phenol.



**3y**

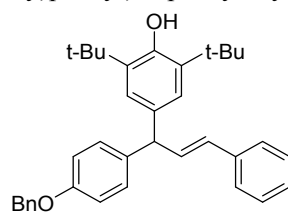
**Compound 3y:** colorless oil, 96% isolated yield.

**<sup>1</sup>H NMR** (400 MHz, CDCl<sub>3</sub>) δ 7.65 – 7.58 (m, 1H), 7.49 – 7.38 (m, 2H), 7.25 (d, *J* = 5.3 Hz, 1H), 7.11 (s, 2H), 5.77 – 5.62 (m, 1H), 5.06 (s, 1H), 5.05 – 4.86 (m, 2H), 4.43 (t, *J* = 7.8 Hz, 1H), 3.07 – 2.61 (m, 2H), 1.40 (s, 18H).

**<sup>13</sup>C NMR** (100 MHz, CDCl<sub>3</sub>) δ 152.24, 144.83, 136.68, 135.59, 133.77, 131.99, 129.64, 125.88, 125.78, 124.69, 116.47, 45.23, 41.13, 34.53, 30.44.

**HRMS (ESI)** calcd for C<sub>25</sub>H<sub>31</sub>F<sub>3</sub>O (M-H)<sup>-</sup>: 403.2254, found: 403.2258.

**Compound 3z:** (E)-4-(1-(4-(benzyloxy)phenyl)-3-phenylallyl)-2,6-di-tert-butylphenol



**3z**

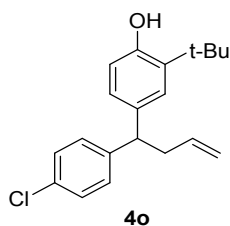
**Compound 3z:** colorless oil, 87% isolated yield.

**<sup>1</sup>H NMR** (400 MHz, CDCl<sub>3</sub>) δ 7.45 – 7.26 (m, 9H), 7.15 (d, *J* = 8.5 Hz, 3H), 7.03 (s, 2H), 6.92 (d, *J* = 8.8 Hz, 2H), 6.63 (dd, *J* = 15.7, 7.6 Hz, 1H), 6.33 (d, *J* = 15.8 Hz, 1H), 5.09 (s, 1H), 5.05 (s, 2H), 4.74 (d, *J* = 7.6 Hz, 1H), 1.40 (s, 18H).

**<sup>13</sup>C NMR** (100 MHz, CDCl<sub>3</sub>) δ 157.33, 152.36, 137.74, 137.27, 136.61, 135.81, 134.26, 133.90, 130.62, 129.70, 128.69, 128.60, 128.05, 127.64, 127.20, 126.41, 125.23, 114.81, 70.17, 53.58, 34.52, 30.47.

**HRMS (ESI)** calcd for C<sub>36</sub>H<sub>40</sub>O<sub>2</sub> (M-H)<sup>-</sup>: 503.2956, found: 503.2951.

**Compound 4o:** 2-(tert-butyl)-4-(1-(4-chlorophenyl)but-3-en-1-yl)phenol



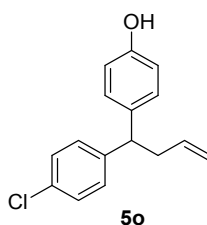
**Compound 4o:** colorless oil, 80% isolated yield.

**<sup>1</sup>H NMR** (400 MHz, CDCl<sub>3</sub>) δ 7.24 (d, *J* = 8.5 Hz, 2H), 7.14 (d, *J* = 8.5 Hz, 2H), 7.09 (d, *J* = 2.2 Hz, 1H), 6.87 (dd, *J* = 8.1, 2.3 Hz, 1H), 6.57 (d, *J* = 8.1 Hz, 1H), 5.81 – 5.58 (m, 1H), 5.14 – 4.89 (m, 2H), 4.64 (s, 1H), 3.91 (t, *J* = 7.9 Hz, 1H), 2.82 – 2.66 (m, 2H), 1.37 (s, 9H).

**<sup>13</sup>C NMR** (100 MHz, CDCl<sub>3</sub>) δ 152.66, 143.59, 136.84, 136.07, 131.82, 129.40, 128.58, 126.89, 125.95, 116.61, 116.54, 50.23, 40.41, 34.71, 29.72.

**HRMS (ESI)** calcd for C<sub>20</sub>H<sub>23</sub>ClO (M-H)<sup>+</sup>: 313.1365, found:313.1366.

**Compound 5o:** 4-(1-(4-chlorophenyl)but-3-en-1-yl)phenol



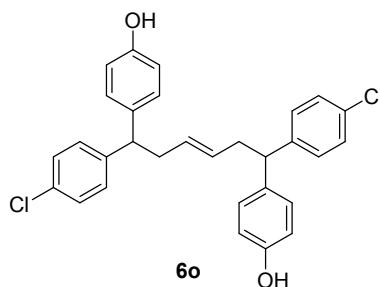
**Compound 5o:** colorless oil, 52% isolated yield.

**<sup>1</sup>H NMR** (400 MHz, CDCl<sub>3</sub>) δ 7.22 (d, *J* = 8.4 Hz, 2H), 7.11 (d, *J* = 8.5 Hz, 2H), 7.04 (d, *J* = 8.5 Hz, 2H), 6.72 (d, *J* = 8.6 Hz, 2H), 5.80 – 5.58 (m, 1H), 5.31 (s, 1H), 5.10 – 4.83 (m, 2H), 3.90 (t, *J* = 7.9 Hz, 1H), 2.90 – 2.63 (m, 2H).

**<sup>13</sup>C NMR** (100 MHz, CDCl<sub>3</sub>) δ 153.81, 143.38, 136.57, 136.51, 131.86, 129.31, 129.09, 128.58, 116.70, 115.46, 49.74, 40.08.

**HRMS (ESI)** calcd for C<sub>16</sub>H<sub>15</sub>ClO (M-H)<sup>+</sup>: 257.0739, found:257.0744.

**Compound 6o:** (E)-4,4'-(1,6-bis(4-chlorophenyl)hex-3-ene-1,6-diyl)diphenol



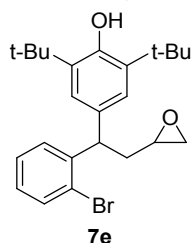
**Compound 6o:** white solid, 75% isolated yield.

**<sup>1</sup>H NMR** (400 MHz, CDCl<sub>3</sub>) δ 7.25 – 7.16 (m, 4H), 6.99 (ddd, *J* = 27.2, 8.4, 3.5 Hz, 8H), 6.72 (t, *J* = 9.1 Hz, 4H), 5.27 (t, *J* = 3.8 Hz, 2H), 4.75 (d, *J* = 10.5 Hz, 2H), 3.74 (t, *J* = 7.8 Hz, 2H), 2.58 (t, *J* = 6.2 Hz, 4H).

**<sup>13</sup>C NMR** (100 MHz, CDCl<sub>3</sub>) δ 153.91, 143.59, 136.44, 131.78, 130.16, 129.29, 129.08, 128.53, 115.39, 50.04, 38.85.

**HRMS (ESI)** calcd for C<sub>30</sub>H<sub>26</sub>Cl<sub>2</sub>O<sub>2</sub> (M-H)<sup>+</sup>: 487.1237, found:487.1234.

**Compound 7e:** 4-(1-(2-bromophenyl)-2-(oxiran-2-yl)ethyl)-2,6-di-tert-butylphenol



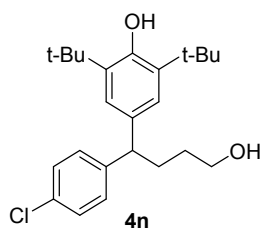
**Compound 7e:** white solid, 95% isolated yield.

**<sup>1</sup>H NMR** (400 MHz, CDCl<sub>3</sub>) δ 7.58 – 7.51 (m, 1H), 7.34 – 7.27 (m, 1H), 7.24 (d, *J* = 3.2 Hz, 1H), 7.14 – 7.00 (m, 3H), 5.07 (s, 1H), 4.73 – 4.60 (m, 1H), 2.94 – 2.81 (m, 1H), 2.67 (dt, *J* = 8.3, 4.5 Hz, 1H), 2.48 – 2.25 (m, 2H), 2.22 – 2.05 (m, 1H), 1.40 (d, *J* = 2.0 Hz, 18H).

**<sup>13</sup>C NMR** (100 MHz, CDCl<sub>3</sub>) δ 144.00, 135.84, 133.50, 133.18, 128.86, 128.68, 127.80, 124.67, 124.45, 51.14, 47.88, 46.40, 38.92, 34.52, 30.46.

**HRMS (ESI)** calcd for C<sub>24</sub>H<sub>31</sub>BrO<sub>2</sub> (M-H)<sup>-</sup>: 430.1435, found:429.1444.

**Compound 4n:** 2,6-di-tert-butyl-4-(1-(4-chlorophenyl)-4-hydroxybutyl)phenol



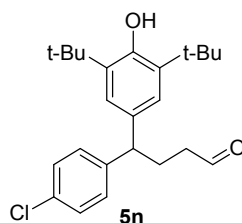
**Compound 4n:** white oil, 88% isolated yield.

**<sup>1</sup>H NMR** (400 MHz, CDCl<sub>3</sub>) δ 7.24 (d, *J* = 8.7 Hz, 2H), 7.17 (d, *J* = 8.5 Hz, 2H), 6.98 (s, 2H), 5.05 (s, 1H), 3.78 (t, *J* = 7.8 Hz, 1H), 3.63 (q, *J* = 6.0 Hz, 2H), 2.04 (q, *J* = 7.8 Hz, 2H), 1.57 – 1.45 (m, 3H), 1.40 (s, 18H).

**<sup>13</sup>C NMR** (100 MHz, CDCl<sub>3</sub>) δ 152.23, 144.11, 135.85, 135.16, 131.70, 129.32, 128.60, 124.15, 63.01, 50.75, 34.51, 32.49, 31.49, 30.47.

**HRMS (ESI)** calcd for C<sub>24</sub>H<sub>33</sub>ClO<sub>2</sub> (M+NH<sub>4</sub>)<sup>+</sup>: 406.2507, found:406.2515.

**Compound 5n:** 4-(4-chlorophenyl)-4-(3,5-di-tert-butyl-4-hydroxyphenyl)butanal



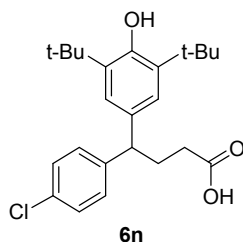
**Compound 5n:** white oil, 97% isolated yield.

**<sup>1</sup>H NMR** (400 MHz, CDCl<sub>3</sub>) δ 9.71 (t, *J* = 1.3 Hz, 1H), 7.25 (d, *J* = 8.4 Hz, 2H), 7.17 (d, *J* = 8.5 Hz, 2H), 6.97 (s, 2H), 5.09 (s, 1H), 3.79 (t, *J* = 7.8 Hz, 1H), 2.44 – 2.36 (m, 2H), 2.34 – 2.26 (m, 2H), 1.40 (s, 18H).

**<sup>13</sup>C NMR** (100 MHz, CDCl<sub>3</sub>) δ 202.09, 152.45, 143.23, 136.02, 134.12, 132.02, 129.25, 128.74, 124.17, 49.97, 42.65, 34.49, 30.42, 28.32.

**HRMS (ESI)** calcd for  $C_{24}H_{31}ClO_2$  ( $M+H$ )<sup>+</sup>: 387.2085, found:387.2089.

**Compound 6n:** 4-(4-chlorophenyl)-4-(3,5-di-tert-butyl-4-hydroxyphenyl)butanoic acid



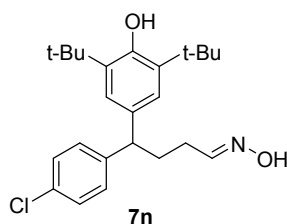
**Compound 6n:** white solid, 76% isolated yield.

**<sup>1</sup>H NMR** (400 MHz,  $CDCl_3$ )  $\delta$  7.24 (d,  $J = 2.4$  Hz, 2H), 7.22 – 7.12 (m, 2H), 6.97 (d,  $J = 2.3$  Hz, 2H), 5.08 (s, 1H), 3.82 (d,  $J = 7.3$  Hz, 1H), 2.30 (d,  $J = 4.1$  Hz, 4H), 1.39 (d,  $J = 2.3$  Hz, 18H).

**<sup>13</sup>C NMR** (100 MHz,  $CDCl_3$ )  $\delta$  179.76, 152.44, 143.16, 135.98, 134.07, 132.02, 129.31, 128.73, 124.20, 49.98, 34.50, 32.68, 30.90, 30.42.

**HRMS (ESI)** calcd for  $C_{24}H_{31}ClO_3$  ( $M+NH_4$ )<sup>+</sup>: 420.2300, found:420.2298.

**Compound 7n:** (E)-4-(4-chlorophenyl)-4-(3,5-di-tert-butyl-4-hydroxyphenyl)butanal oxime



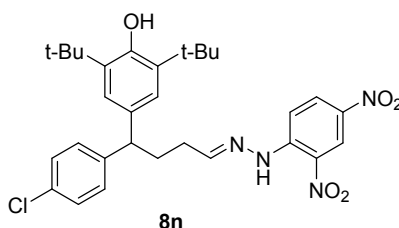
**Compound 7n:** white oil, 80% isolated yield.

**<sup>1</sup>H NMR** (400 MHz,  $CDCl_3$ )  $\delta$  7.42 (d,  $J = 5.5$  Hz, 1H), 7.29 – 7.12 (m, 4H), 6.97 (d,  $J = 4.6$  Hz, 2H), 5.07 (s, 1H), 3.89 – 3.72 (m, 1H), 2.42 – 2.26 (m, 1H), 2.26 – 2.09 (m, 3H), 1.40 (d,  $J = 1.5$  Hz, 18H).

**<sup>13</sup>C NMR** (100 MHz,  $CDCl_3$ )  $\delta$  152.38, 151.77, 143.36, 135.95, 134.43, 131.93, 129.30, 128.72, 124.16, 50.17, 34.50, 32.85, 30.44, 28.22.

**HRMS (ESI)** calcd for  $C_{24}H_{32}ClNO_2$  ( $M+H$ )<sup>+</sup>: 402.2194, found: 402.2192.

**Compound 8n:** (E)-2,6-di-tert-butyl-4-(1-(4-chlorophenyl)-4-(2-(2,4-dinitrophenyl)hydrazono)butyl)phenol



**Compound 8n:** yellow solid, 90% isolated yield.

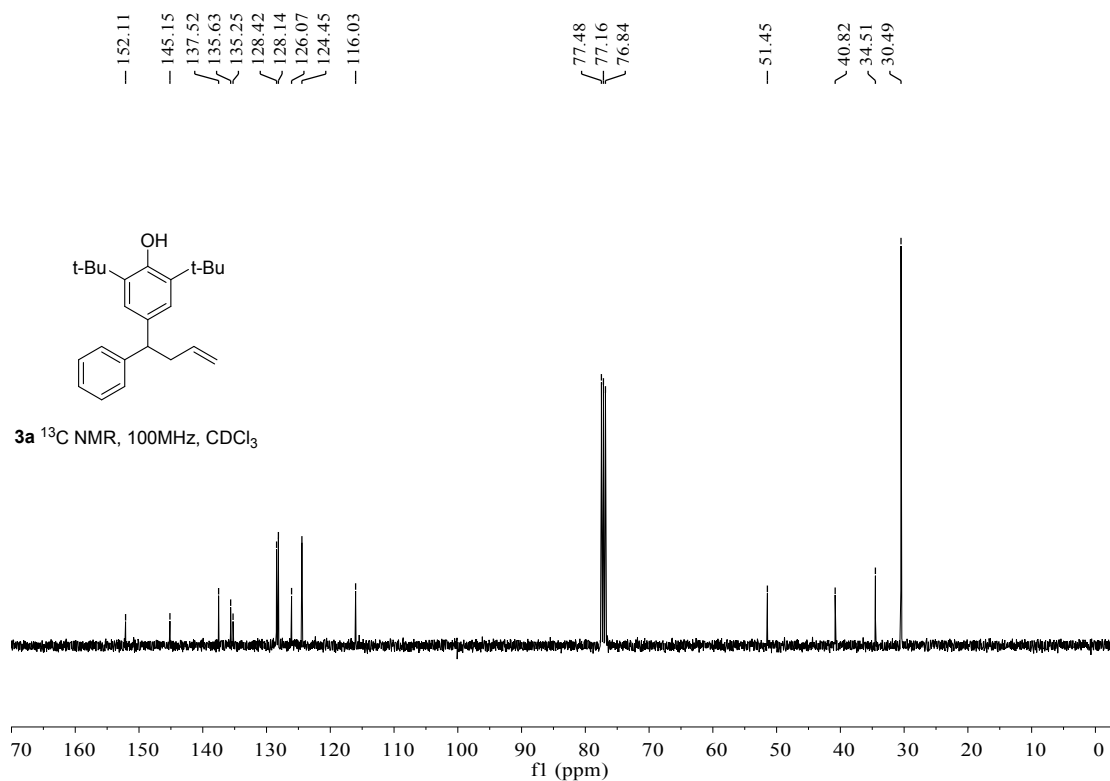
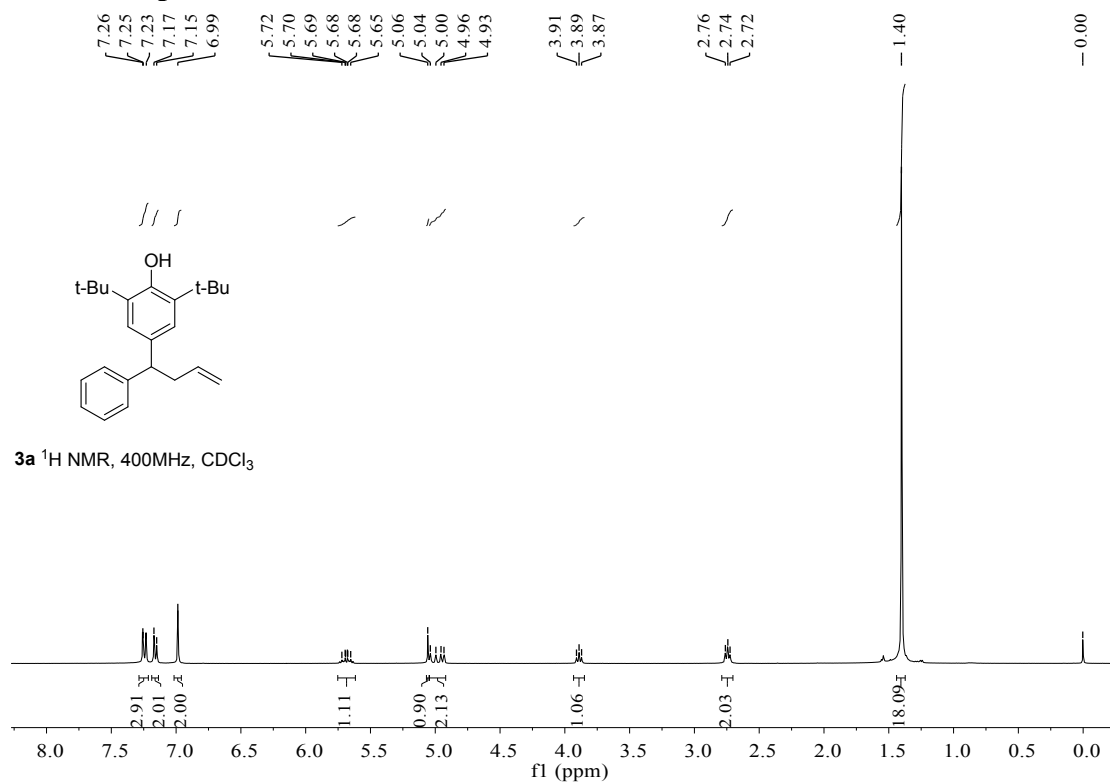
**<sup>1</sup>H NMR** (400 MHz,  $CDCl_3$ )  $\delta$  10.97 (s, 1H), 9.09 (d,  $J = 2.6$  Hz, 1H), 8.27 (dd,  $J = 9.5, 2.6$  Hz, 1H), 7.88 (d,  $J = 9.6$  Hz, 1H), 7.49 (t,  $J = 4.9$  Hz, 1H), 7.30 – 7.19 (m, 4H), 7.02 (s, 2H), 5.11 (s, 1H), 3.88 (t,  $J = 7.6$  Hz, 1H), 2.49 – 2.27 (m, 4H), 1.41 (s, 18H).

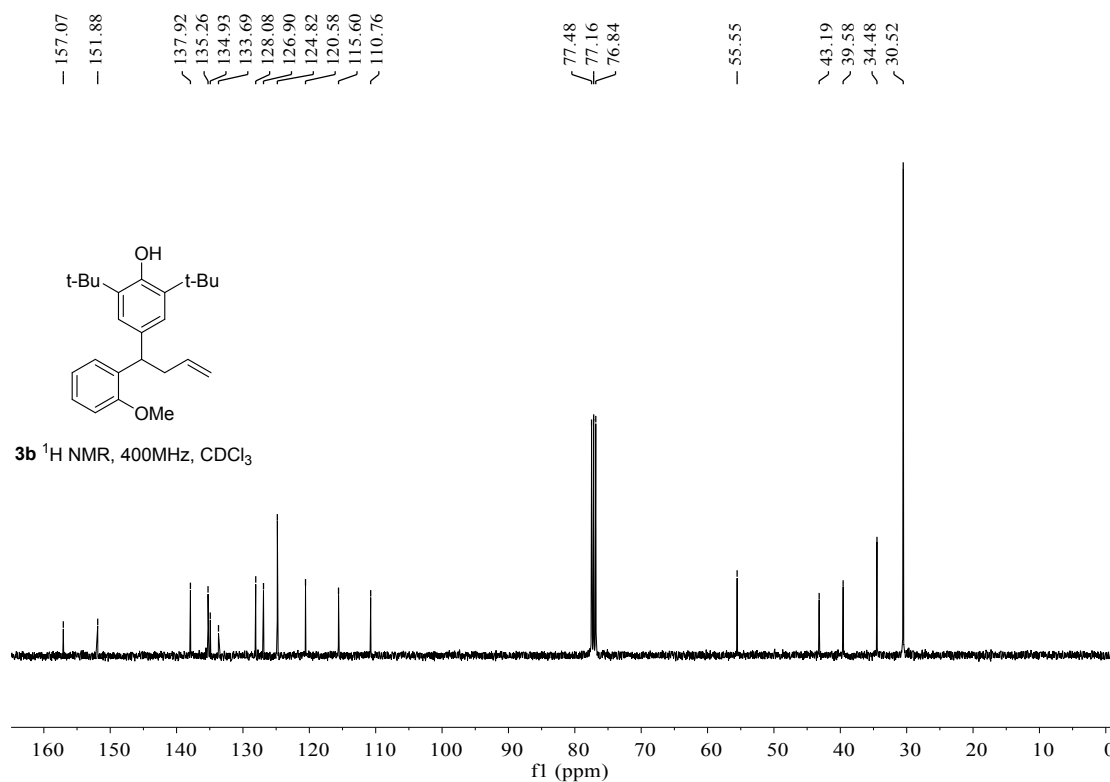
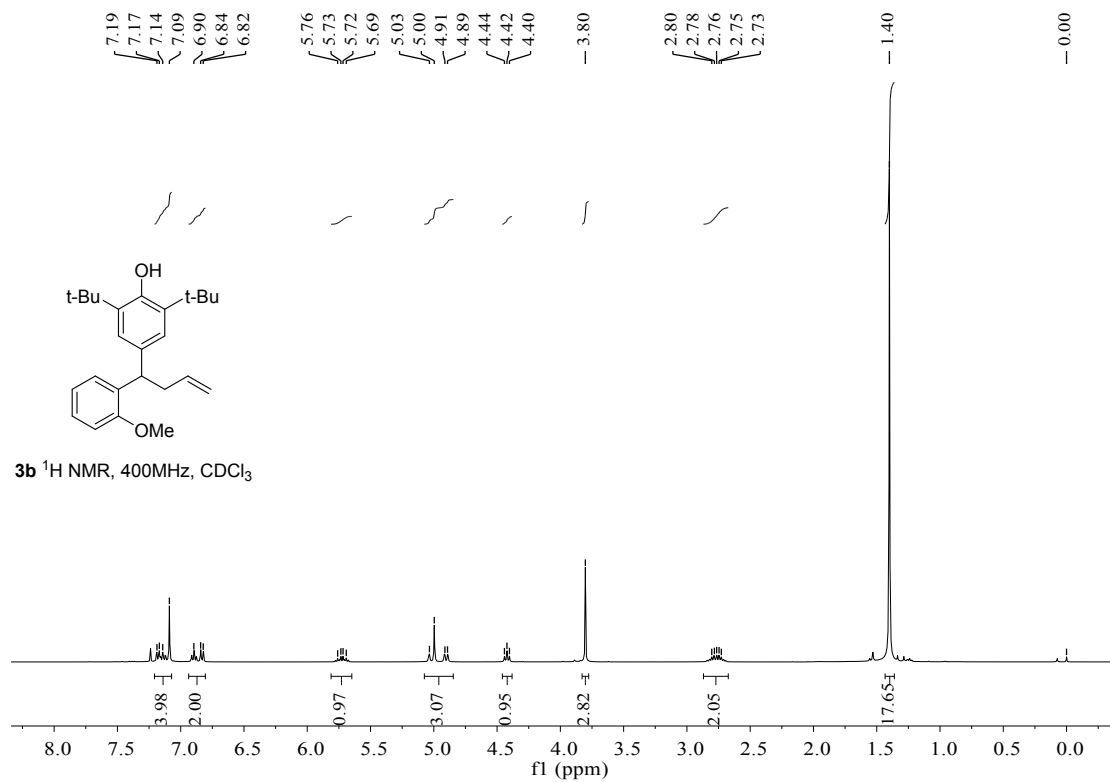
**<sup>13</sup>C NMR** (100 MHz,  $CDCl_3$ )  $\delta$  152.45, 152.07, 145.12, 143.25, 137.84, 136.06, 134.24, 132.04,

130.02, 129.27, 128.84, 128.75, 124.14, 123.58, 116.56, 50.32, 34.50, 32.64, 31.32, 30.41.

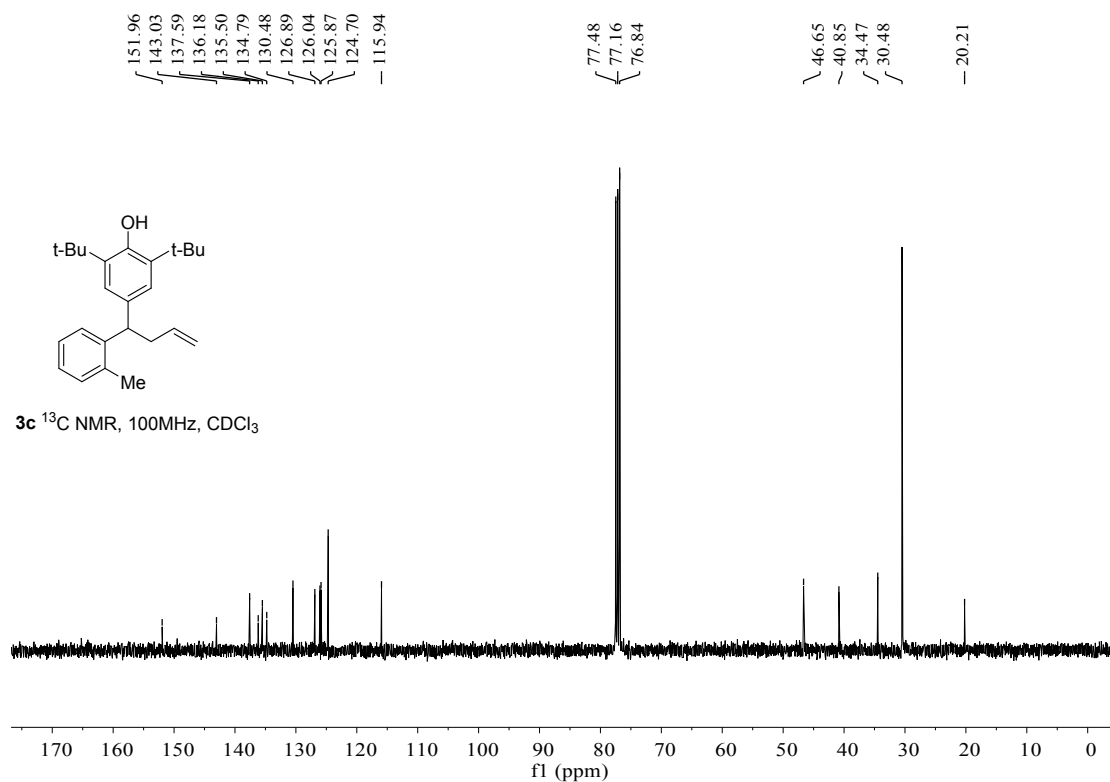
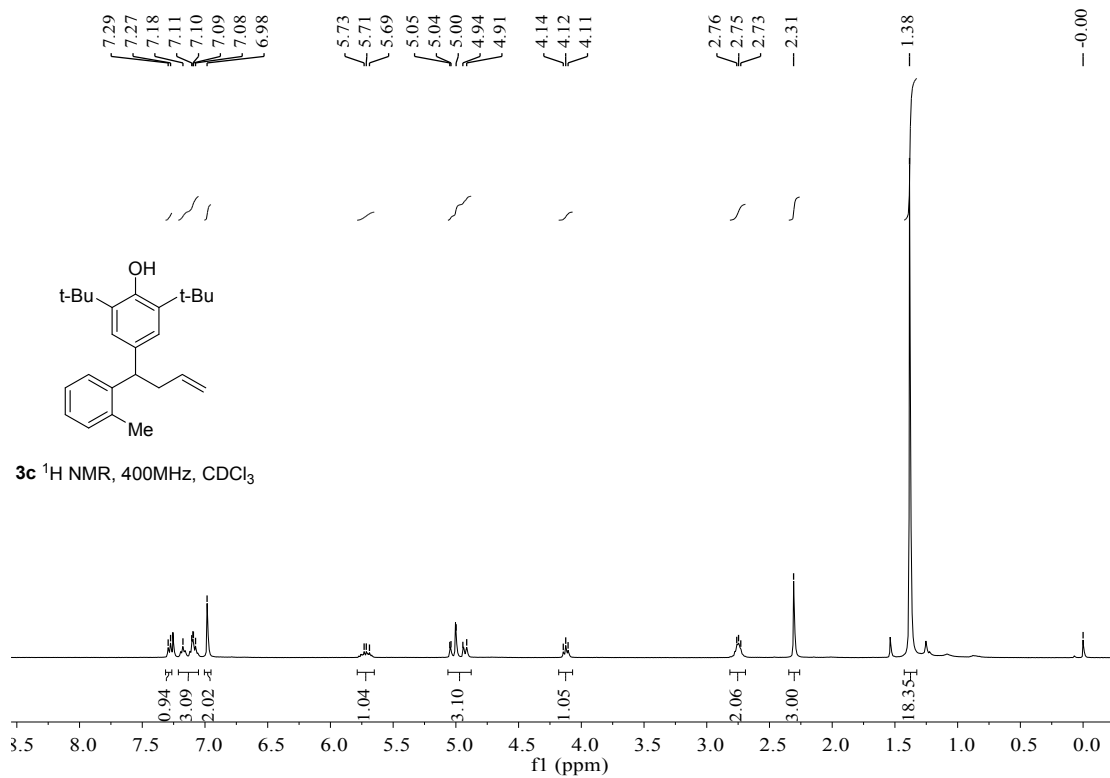
**HRMS (ESI)** calcd for  $C_{30}H_{35}ClN_4O_5$  (M+H)<sup>+</sup>: 567.2369, found:567.2356.

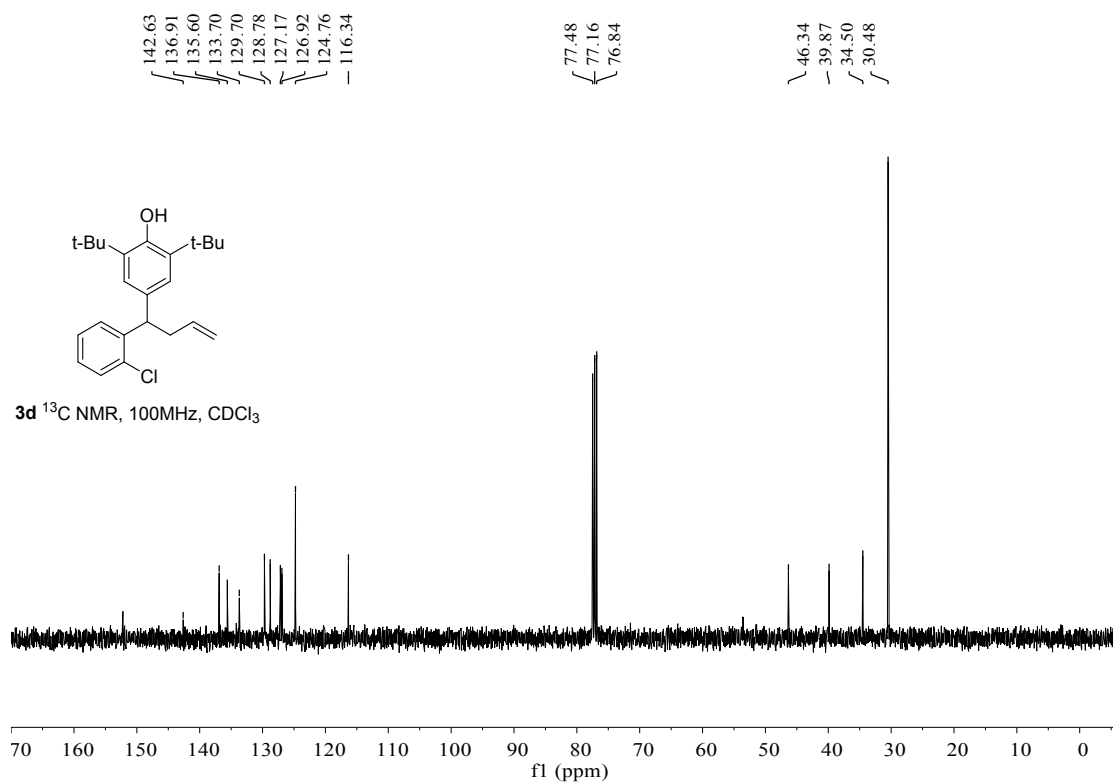
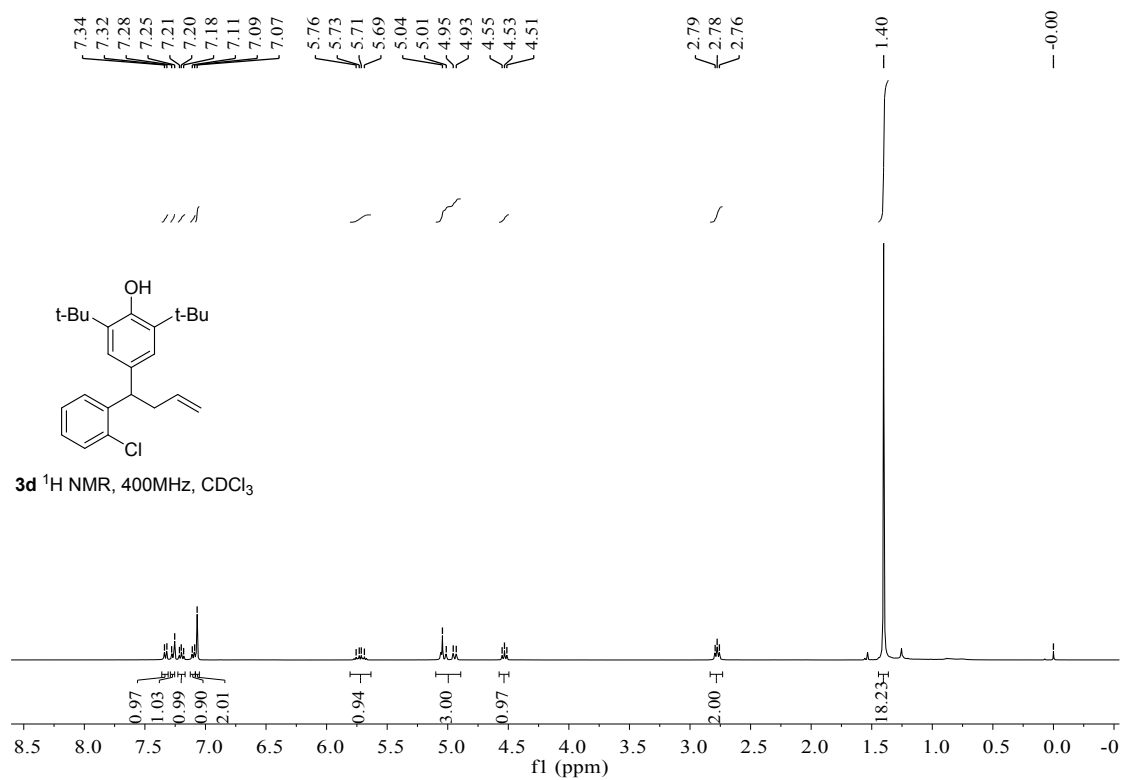
## 6. NMR copies

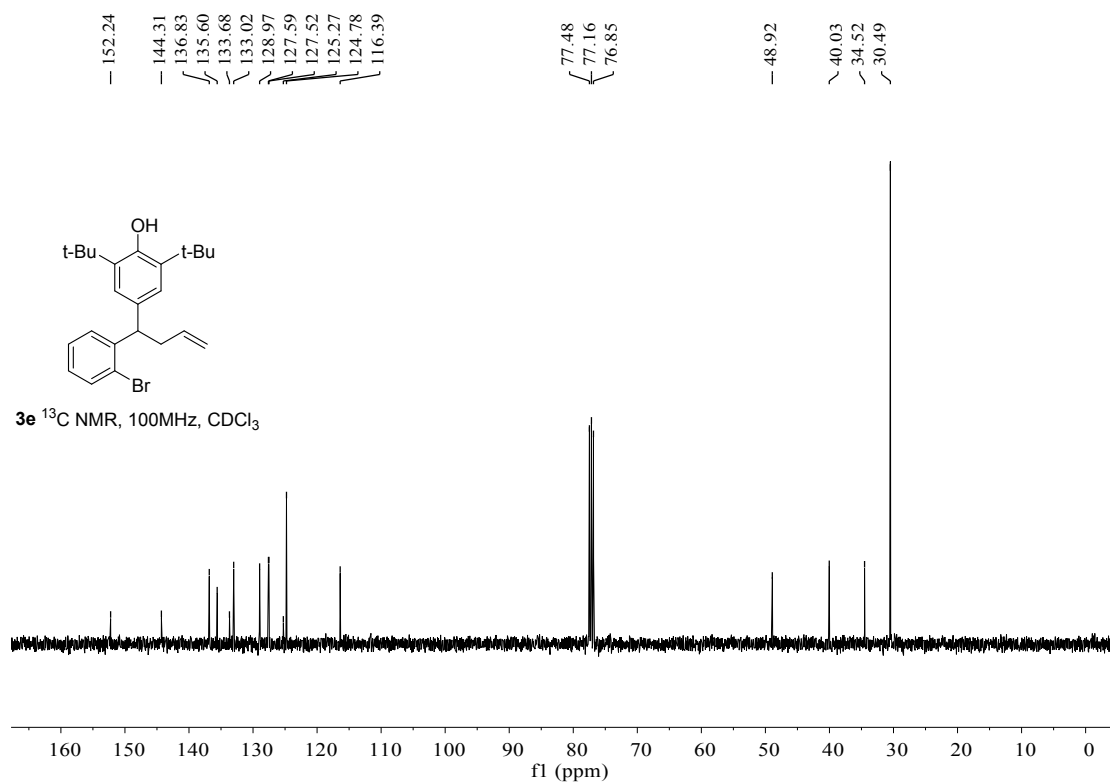
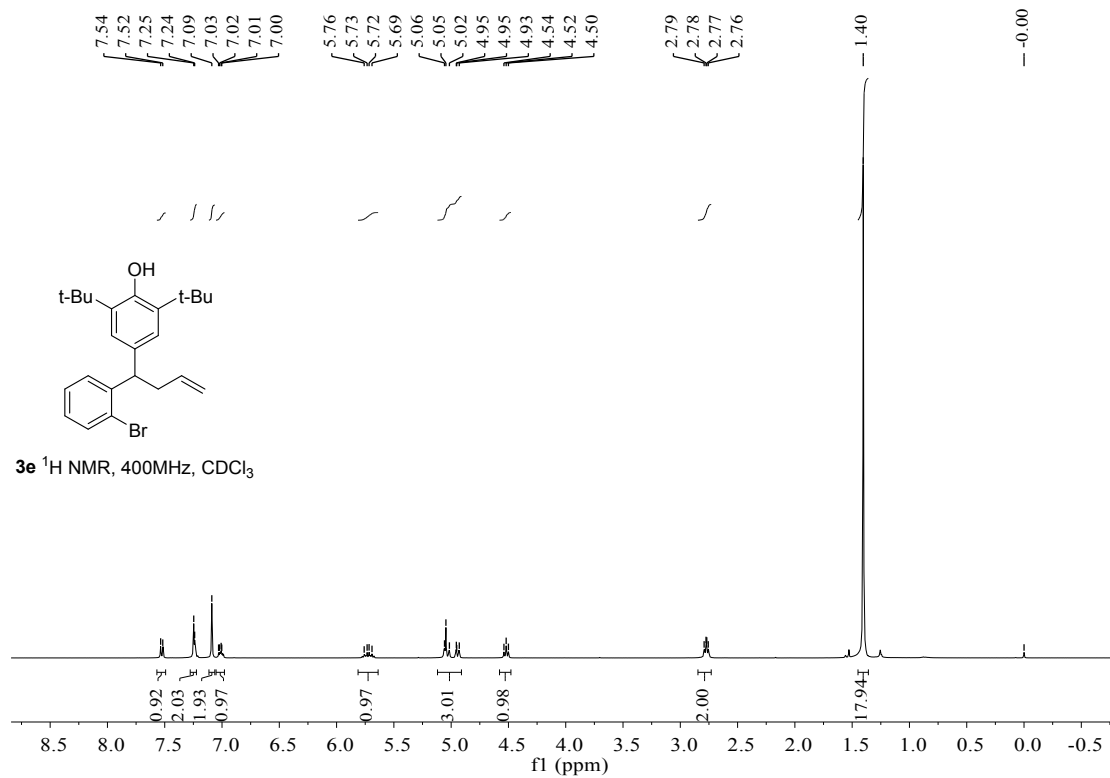


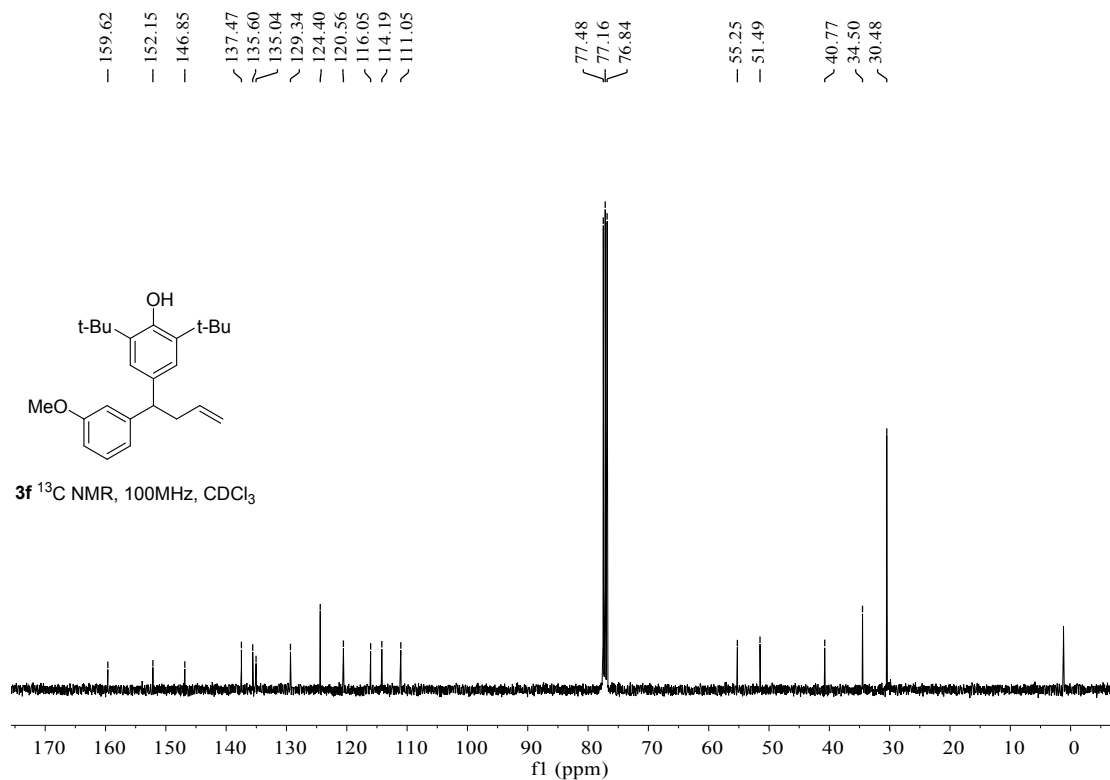
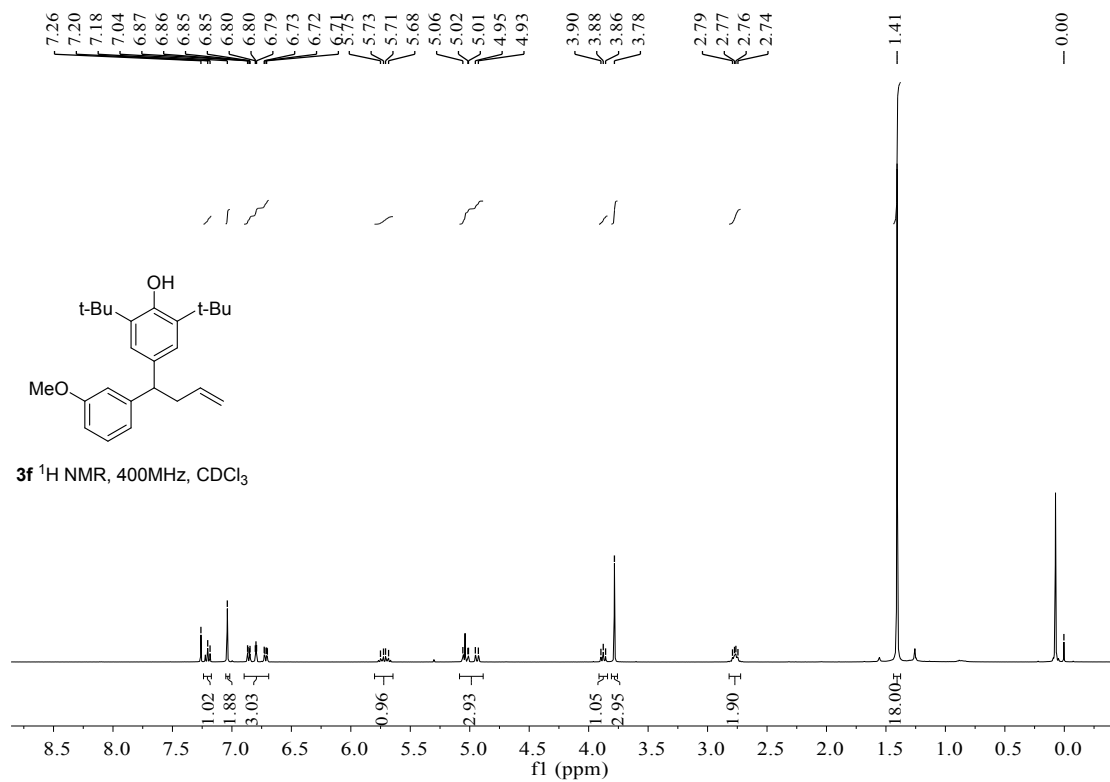


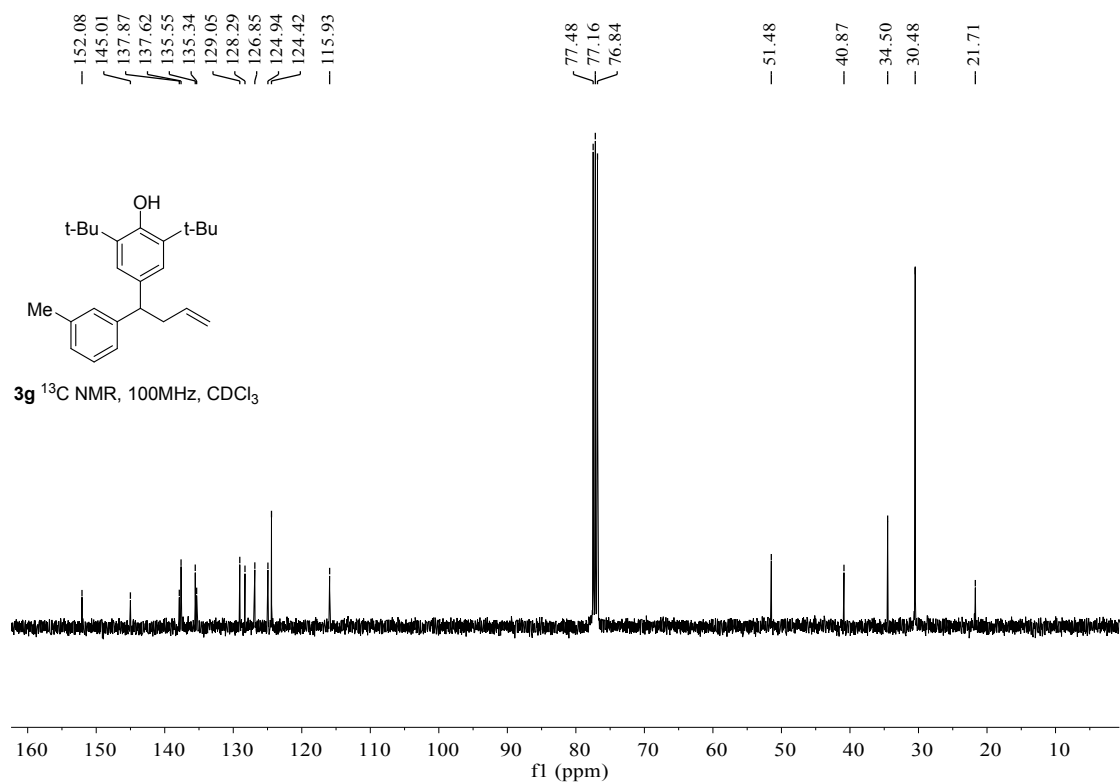
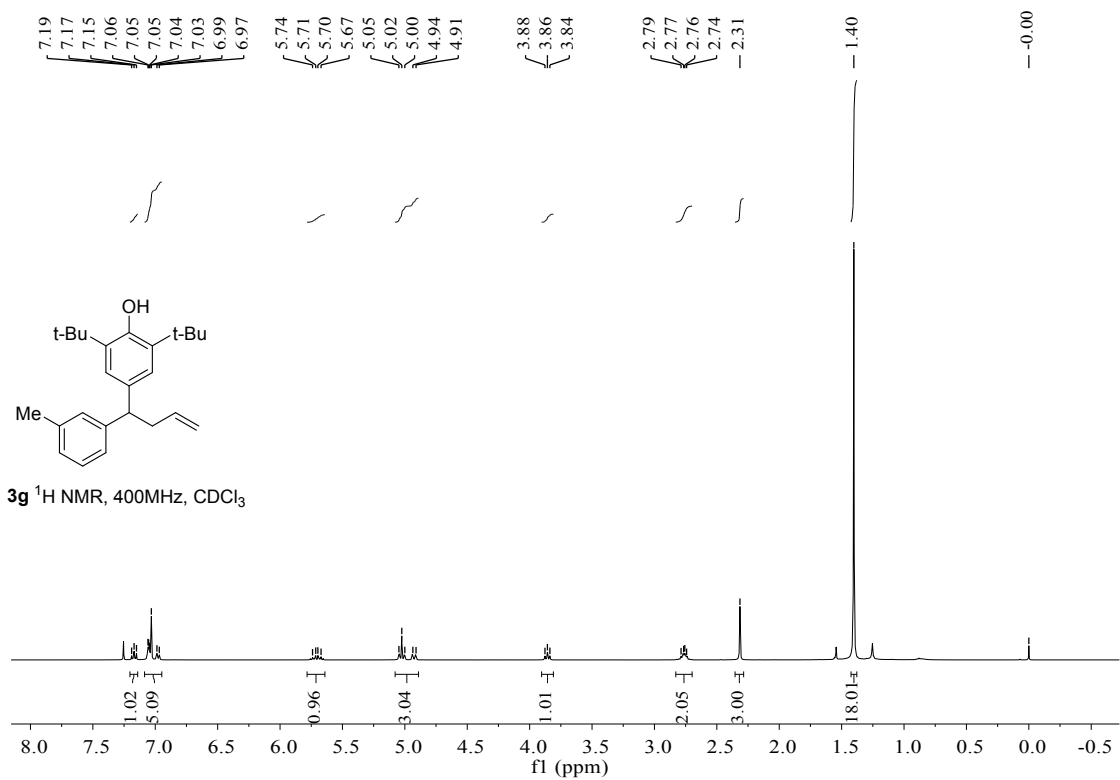


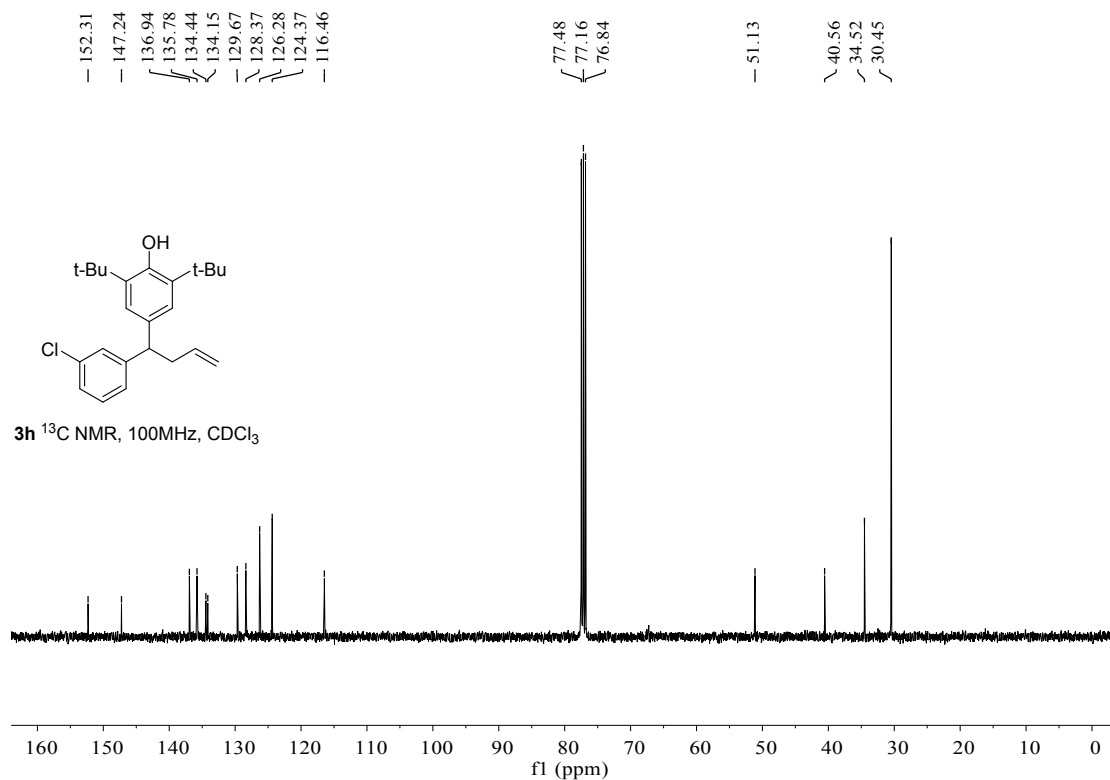
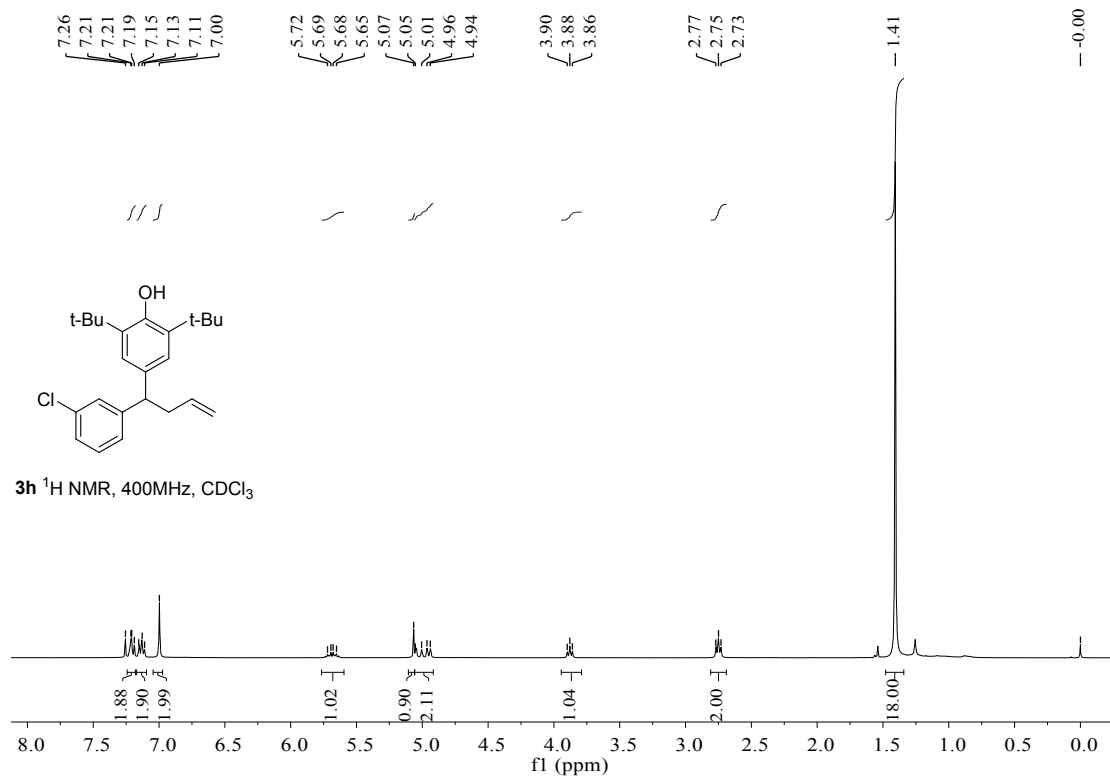


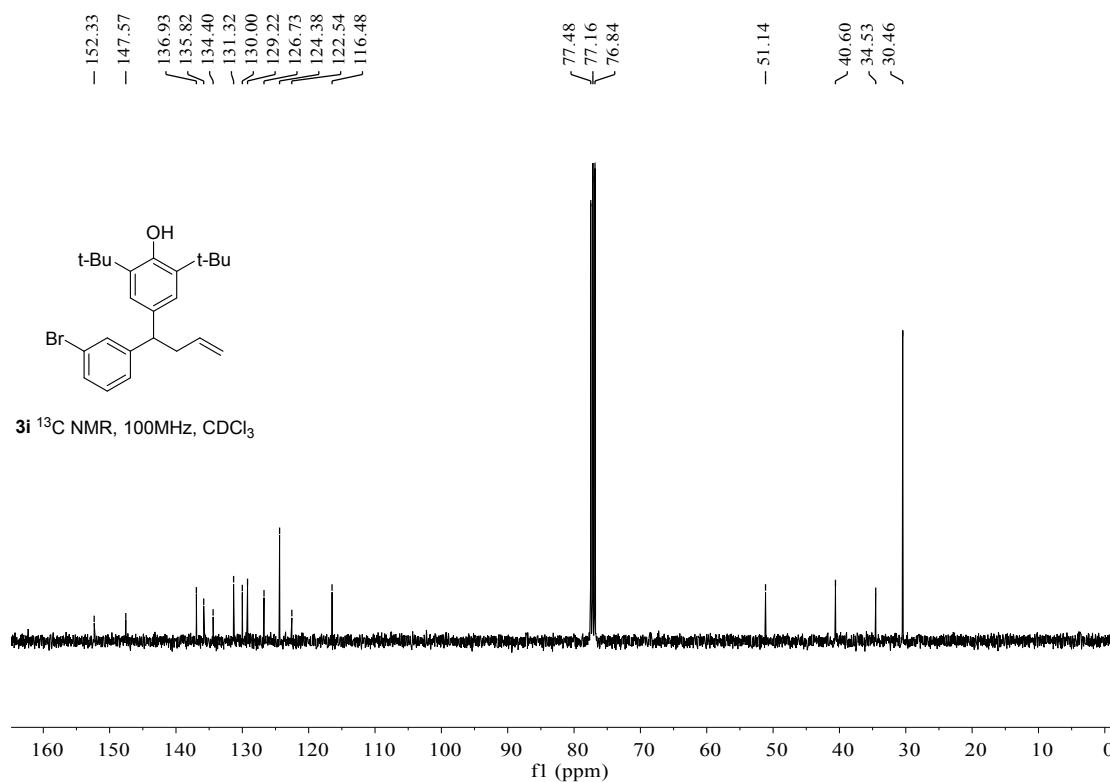
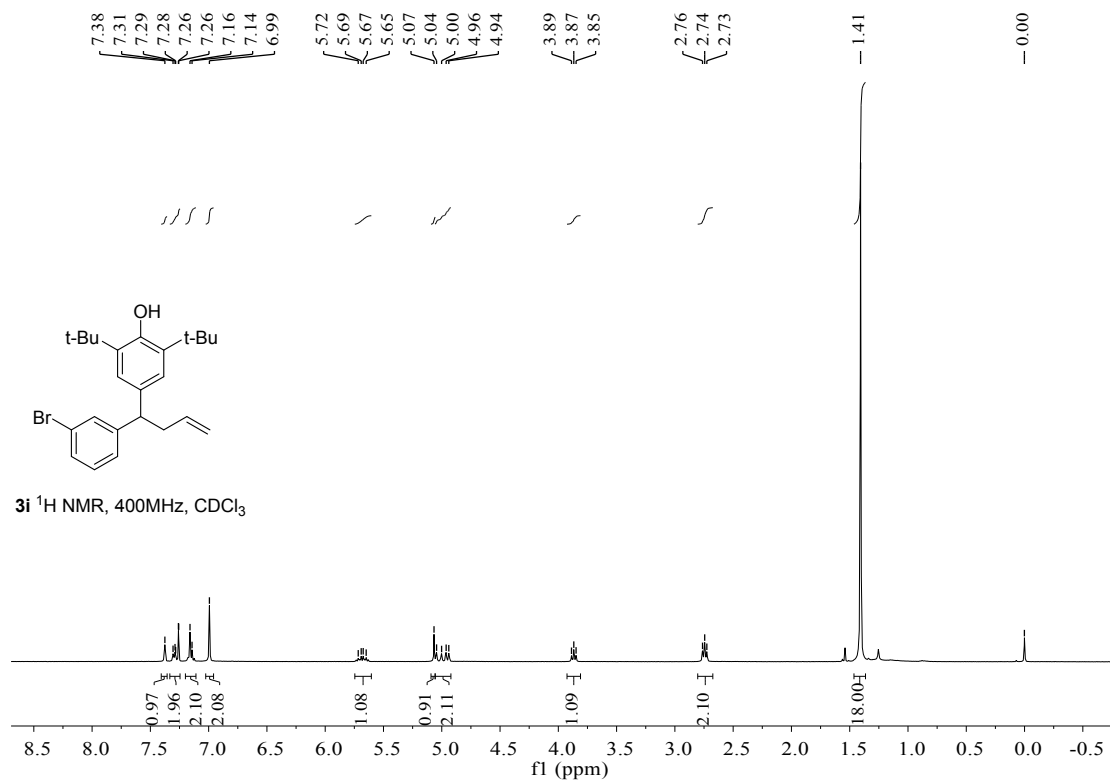


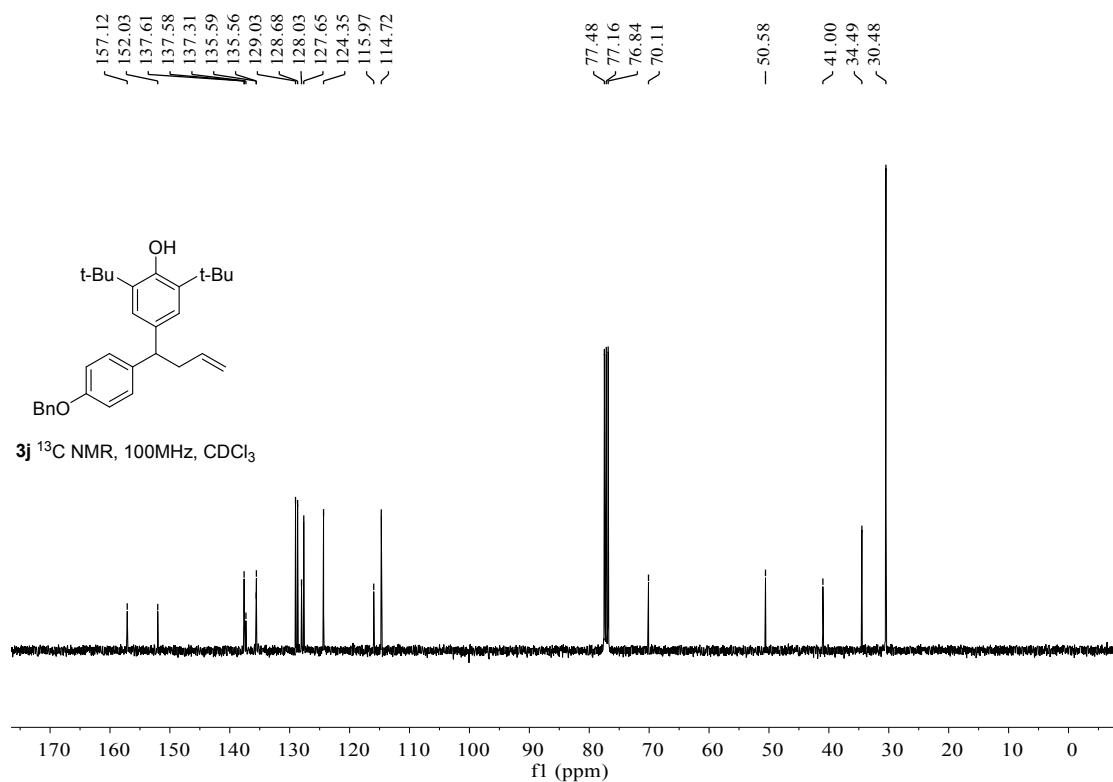
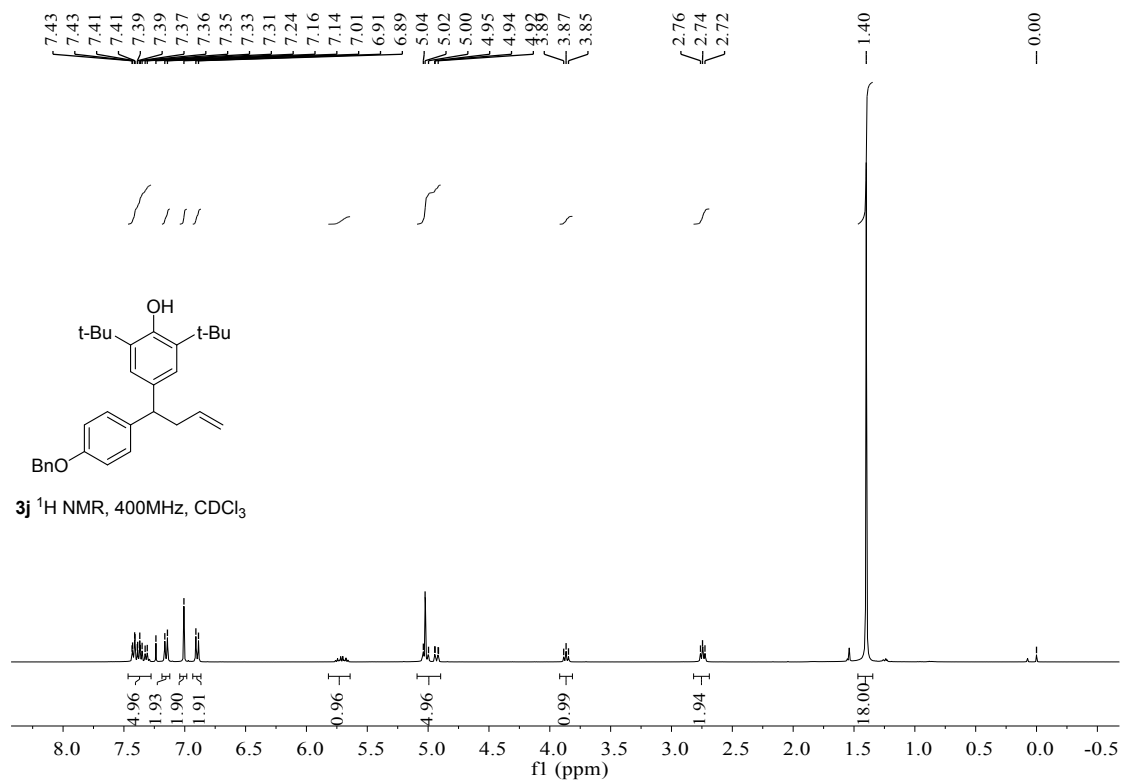




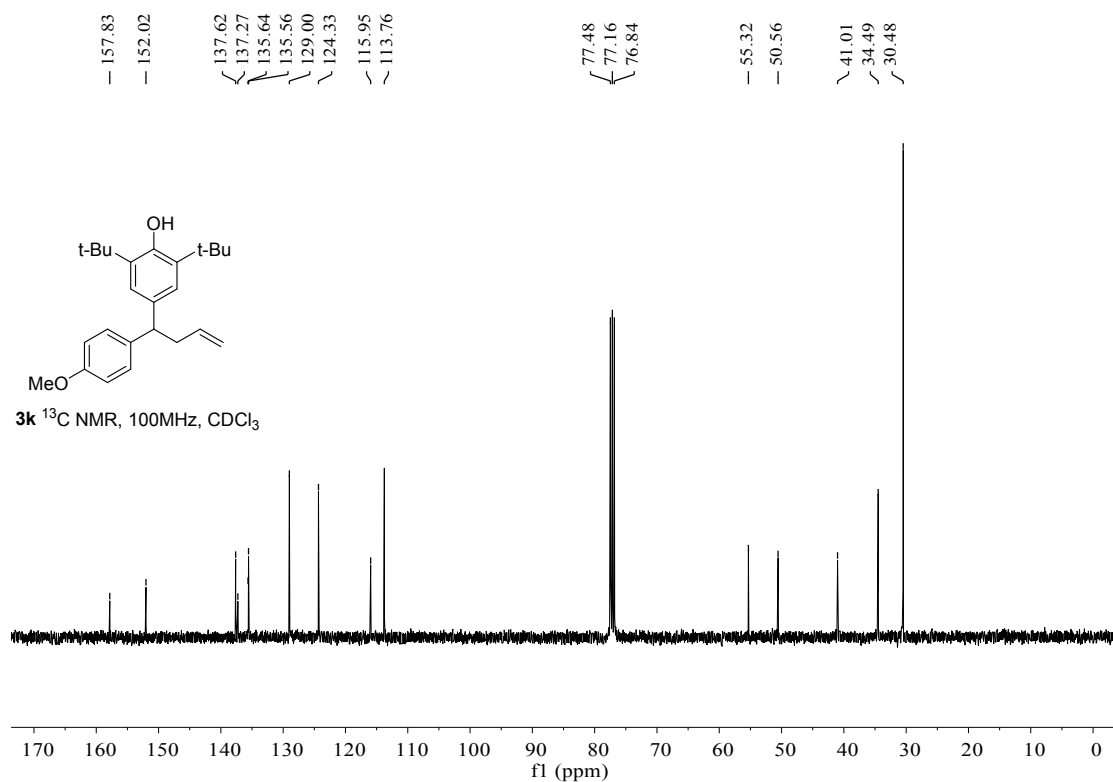
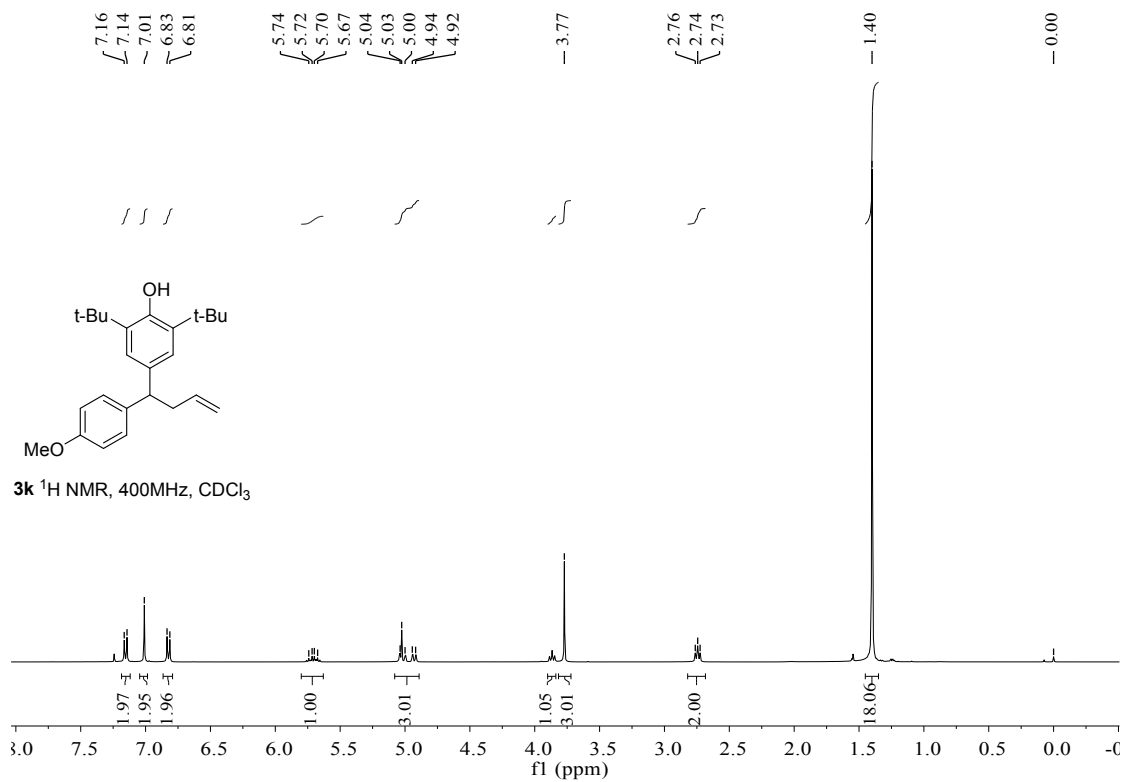


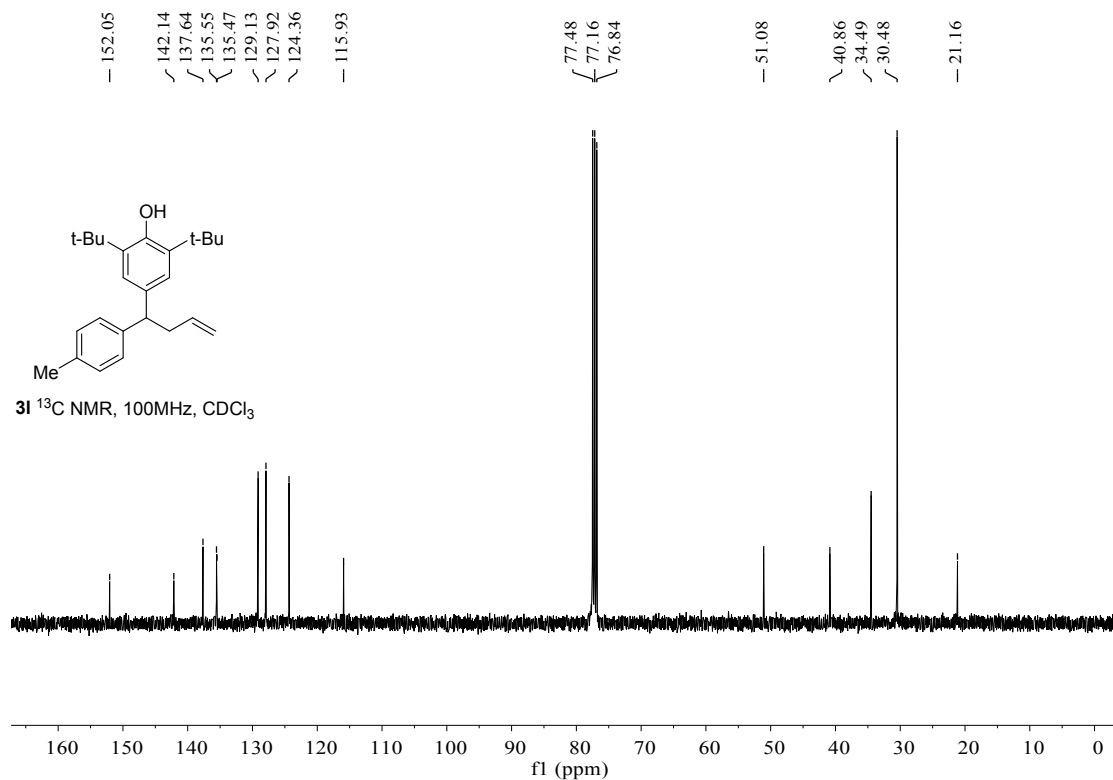
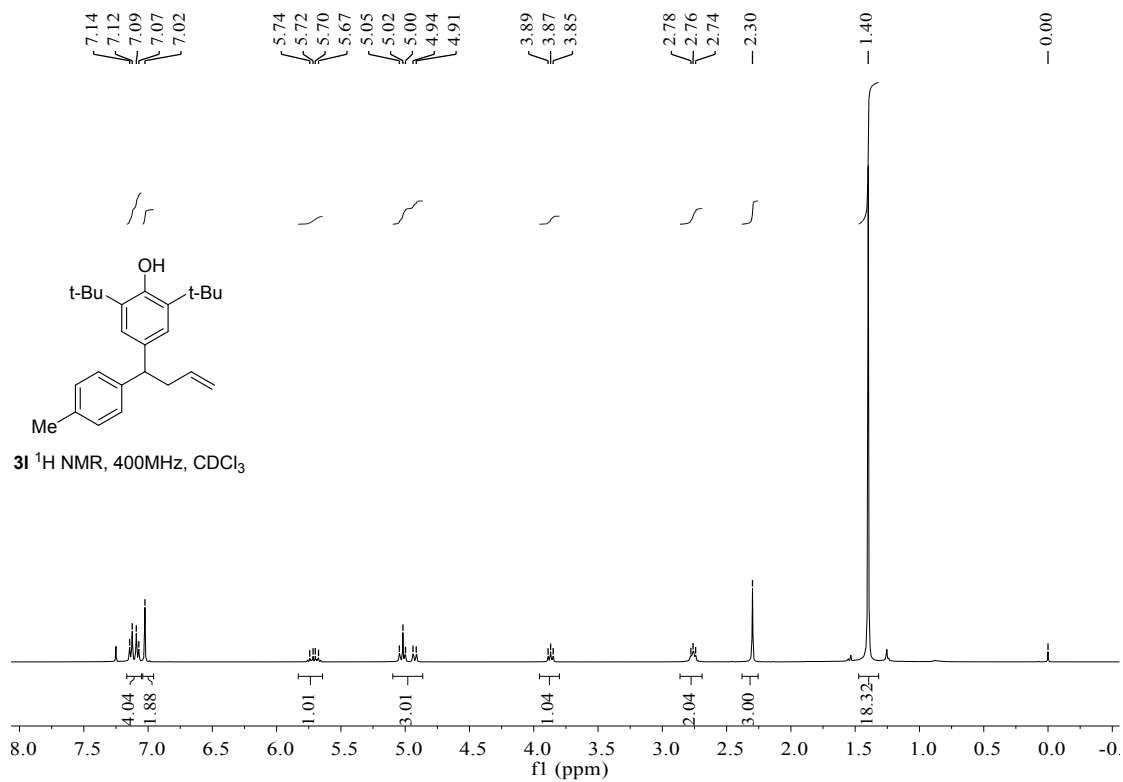


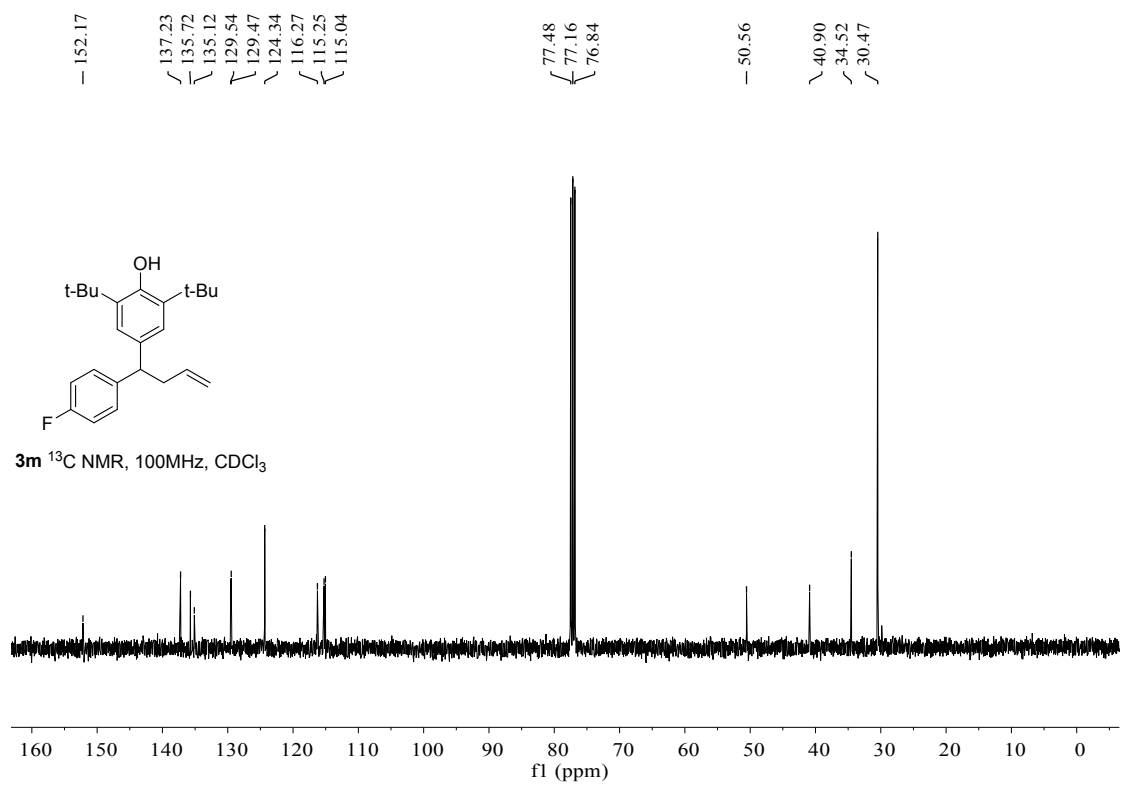
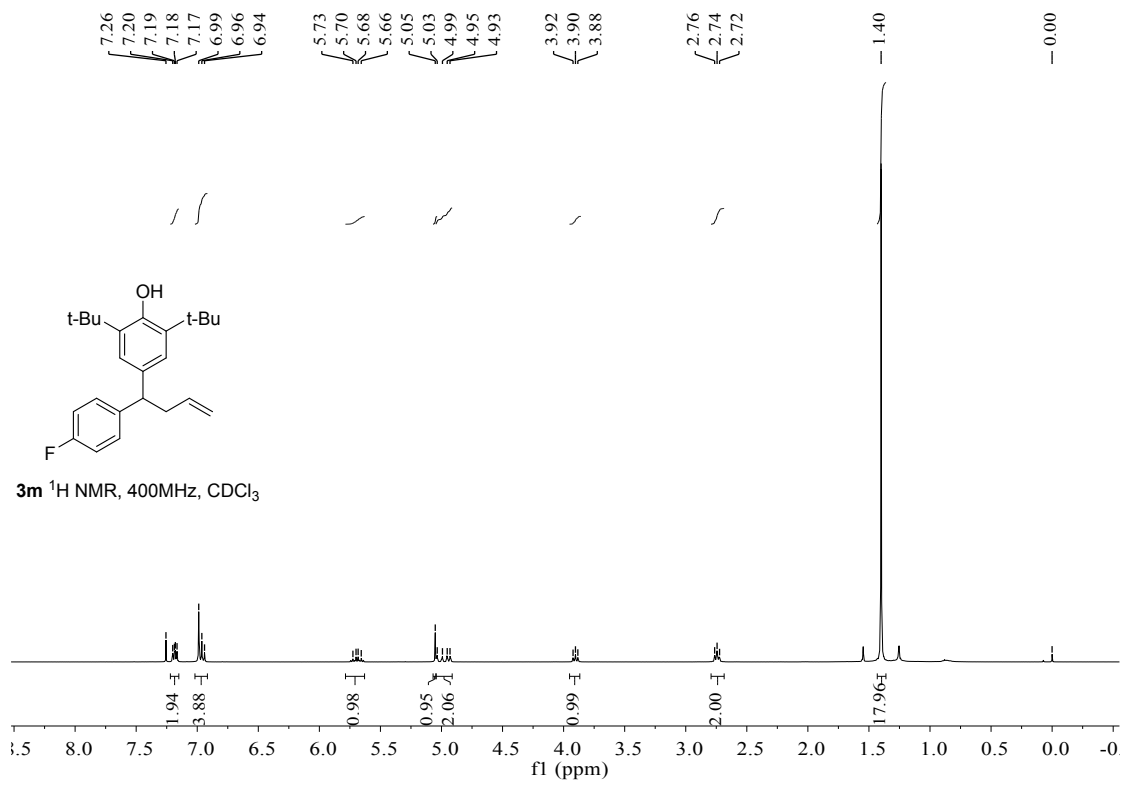


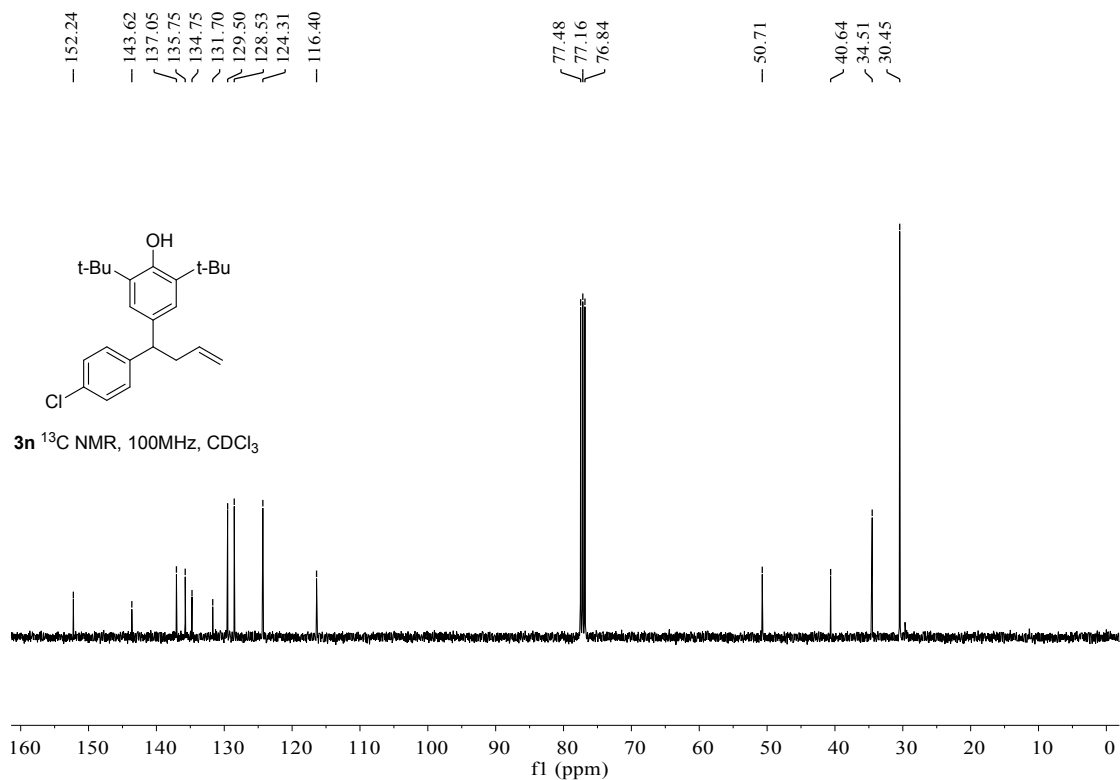
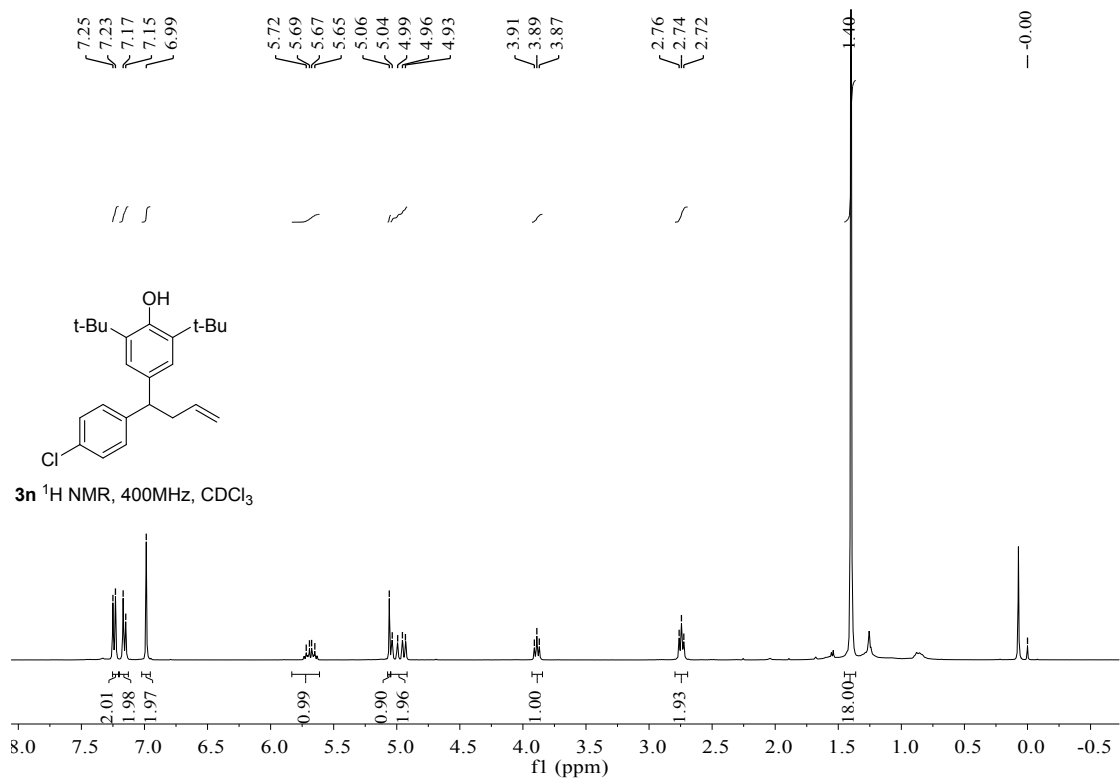


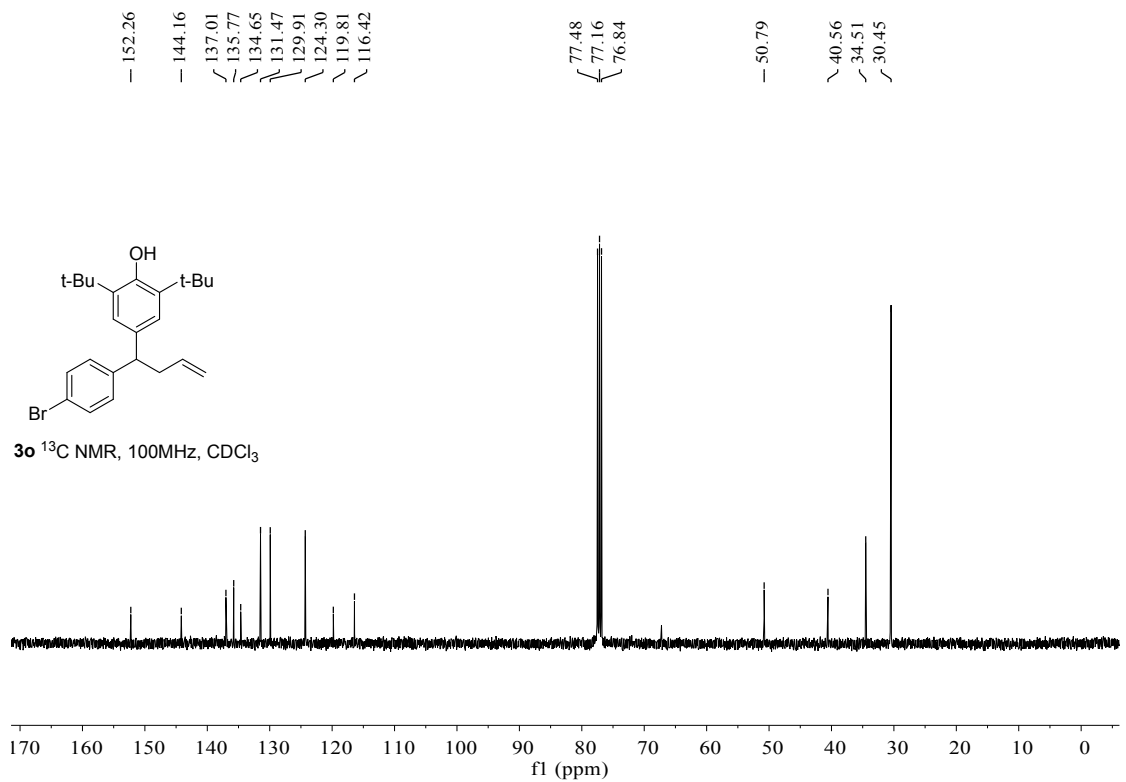
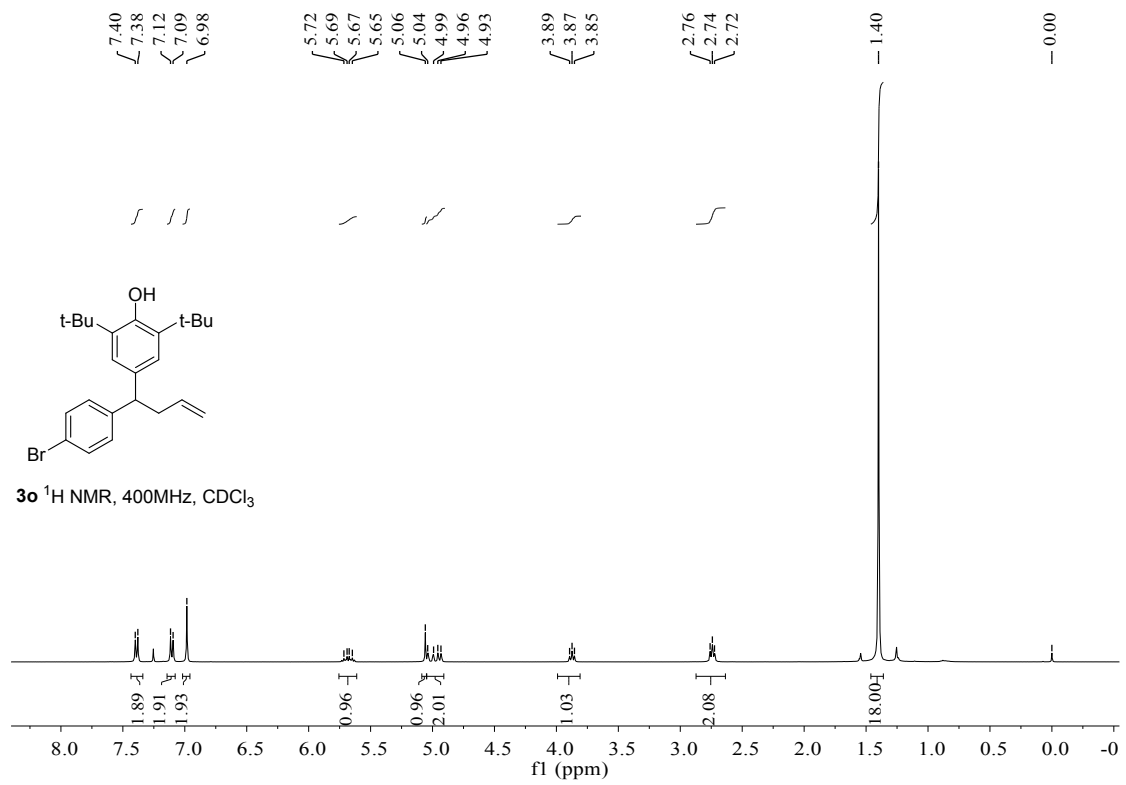


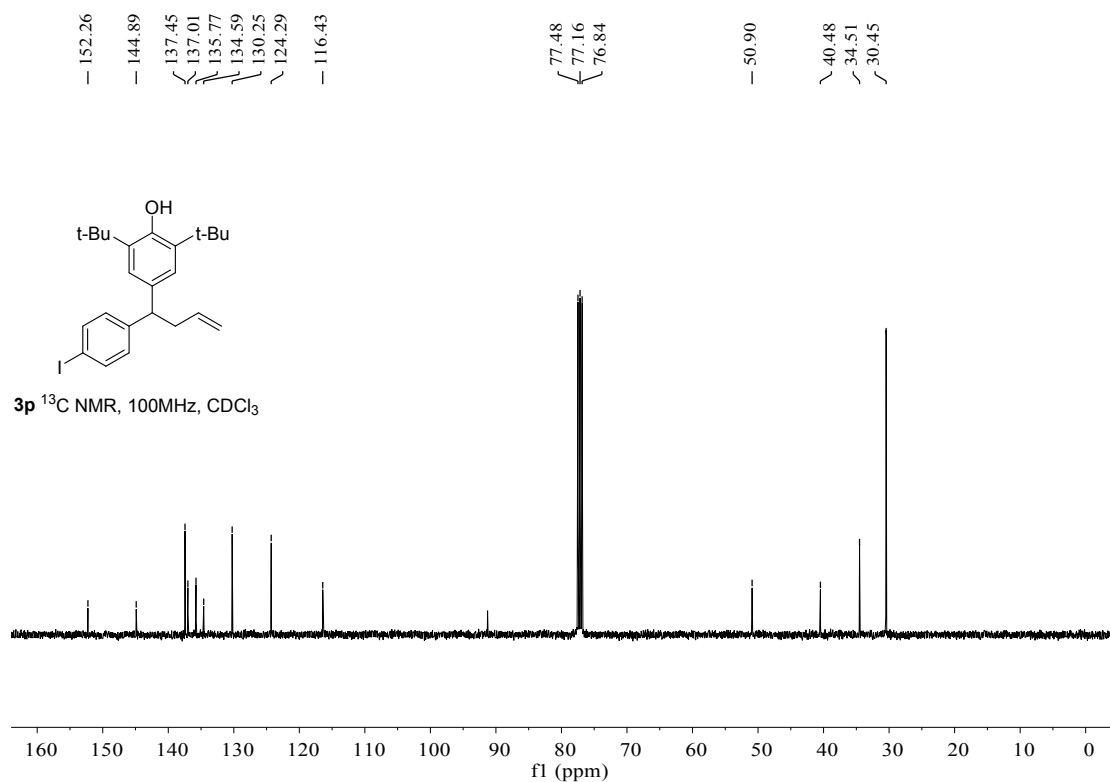
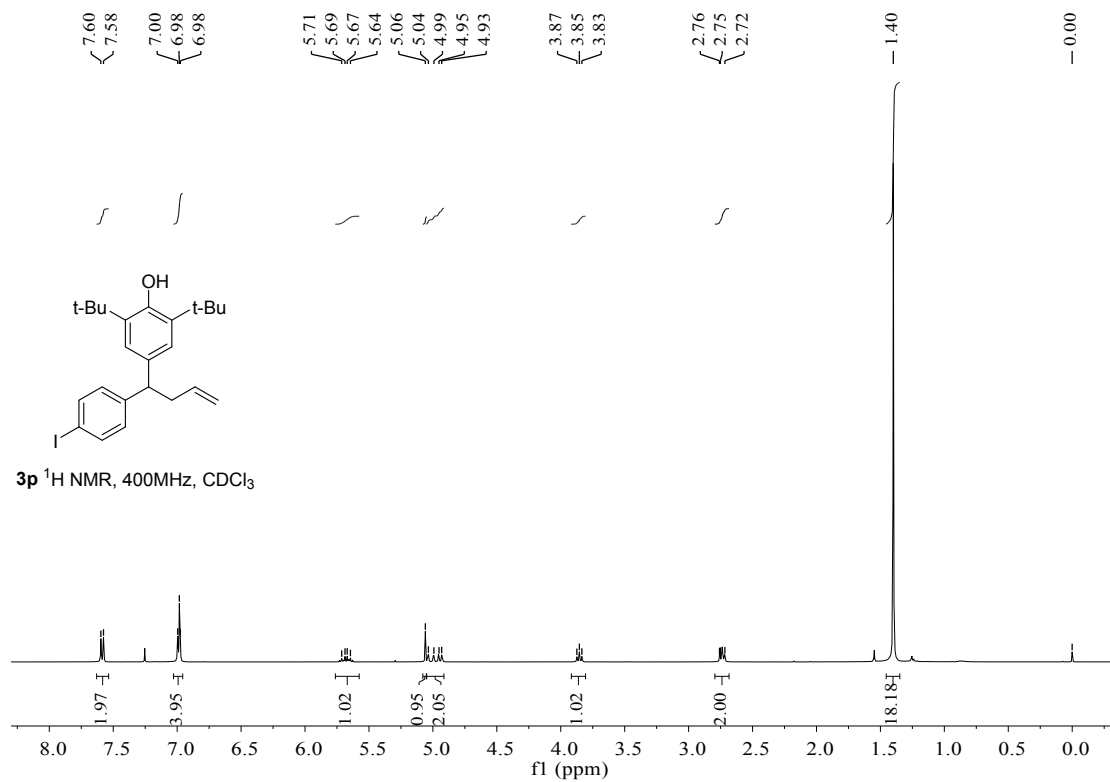


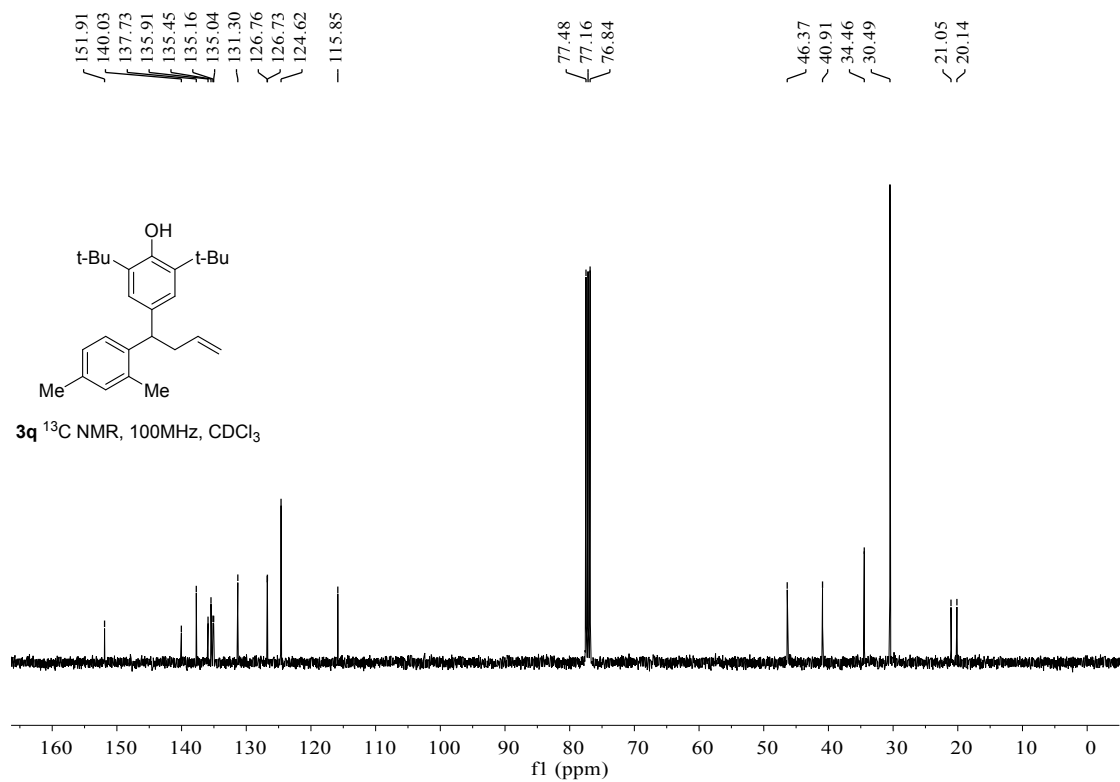
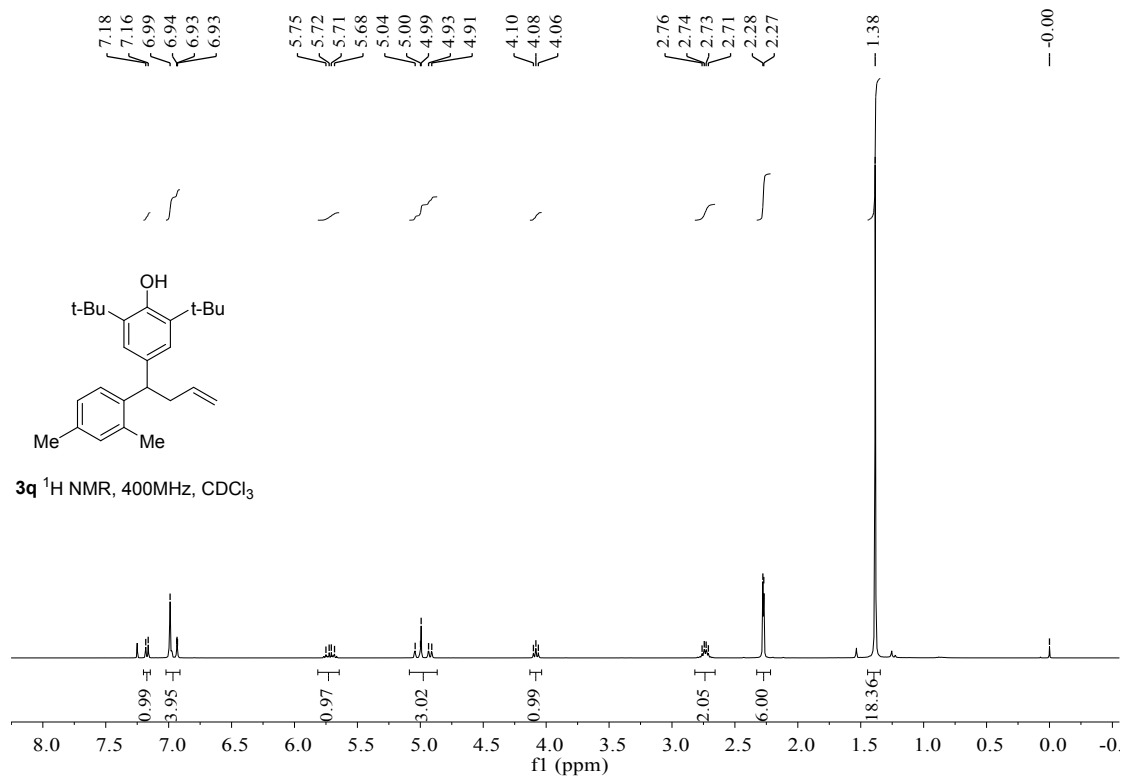


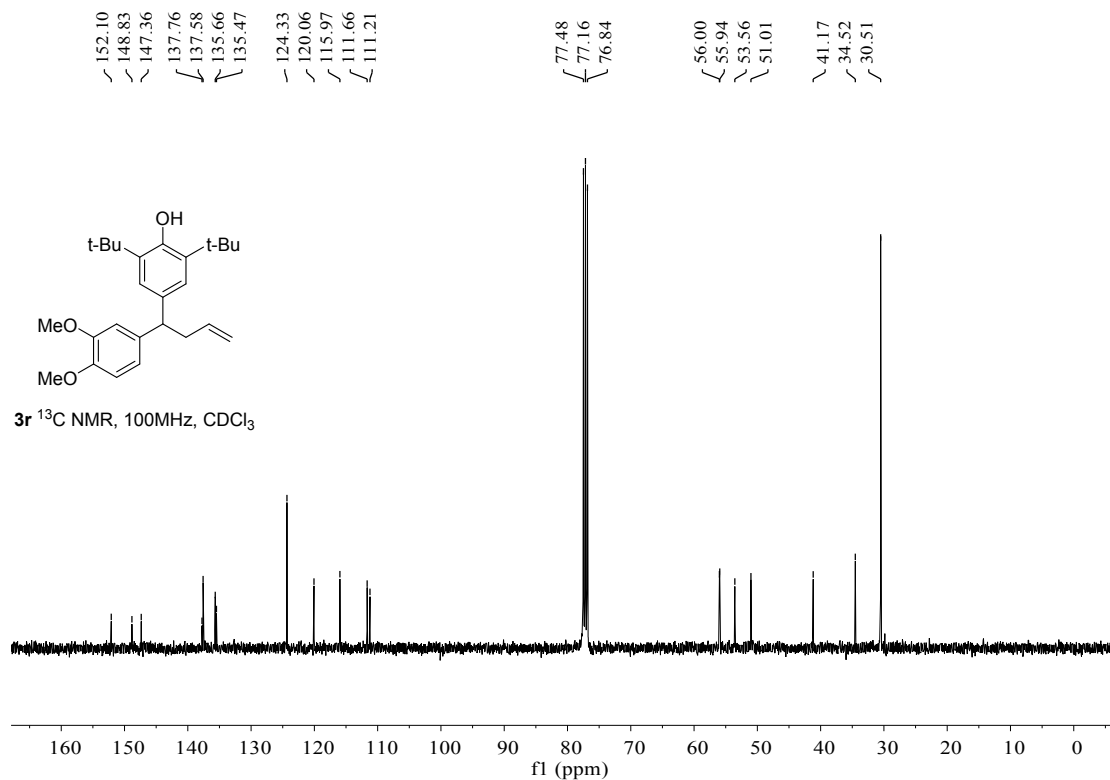
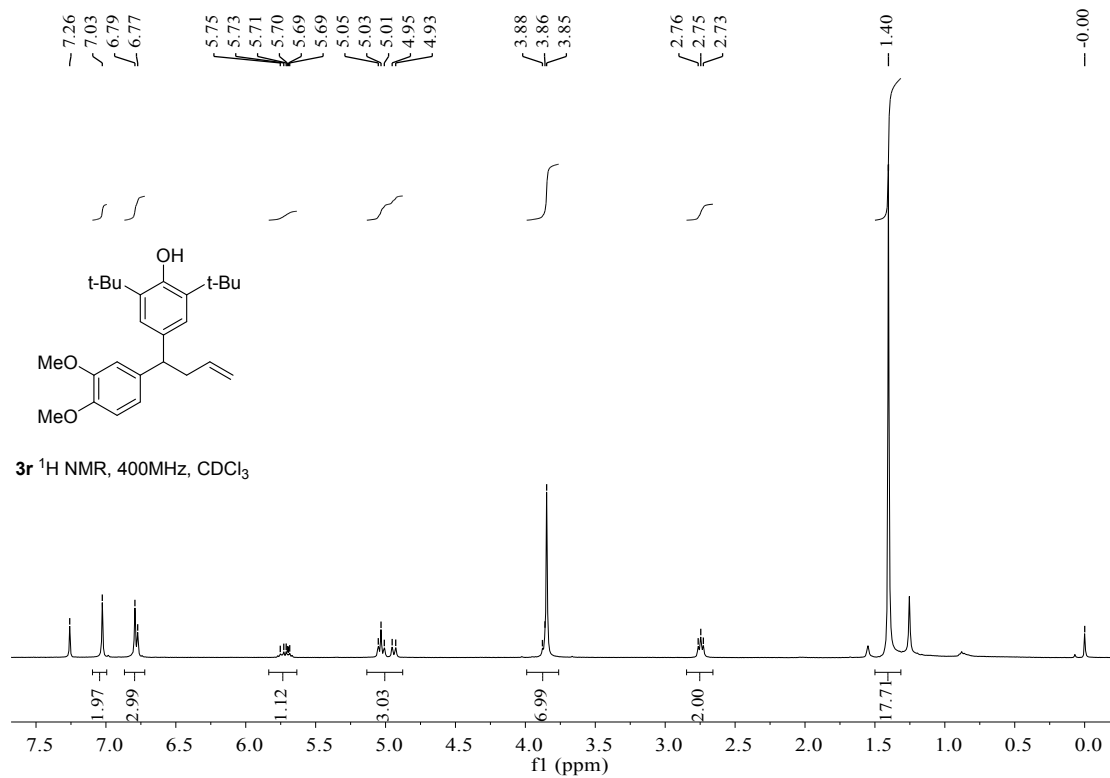




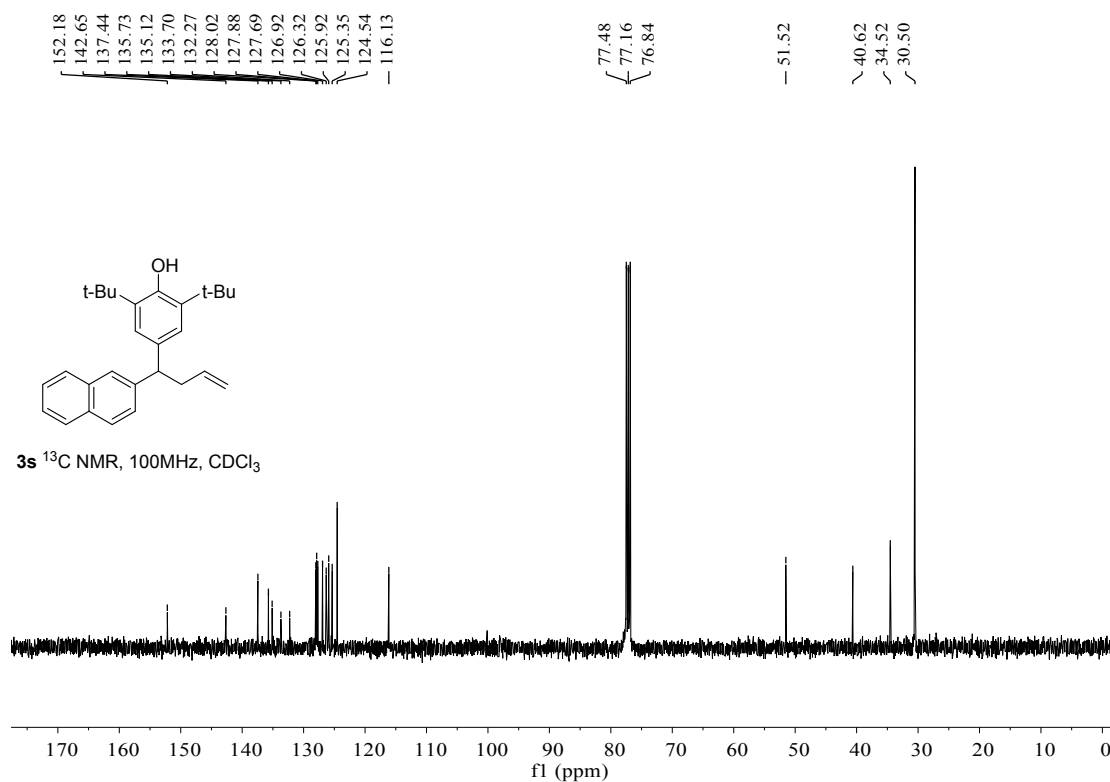
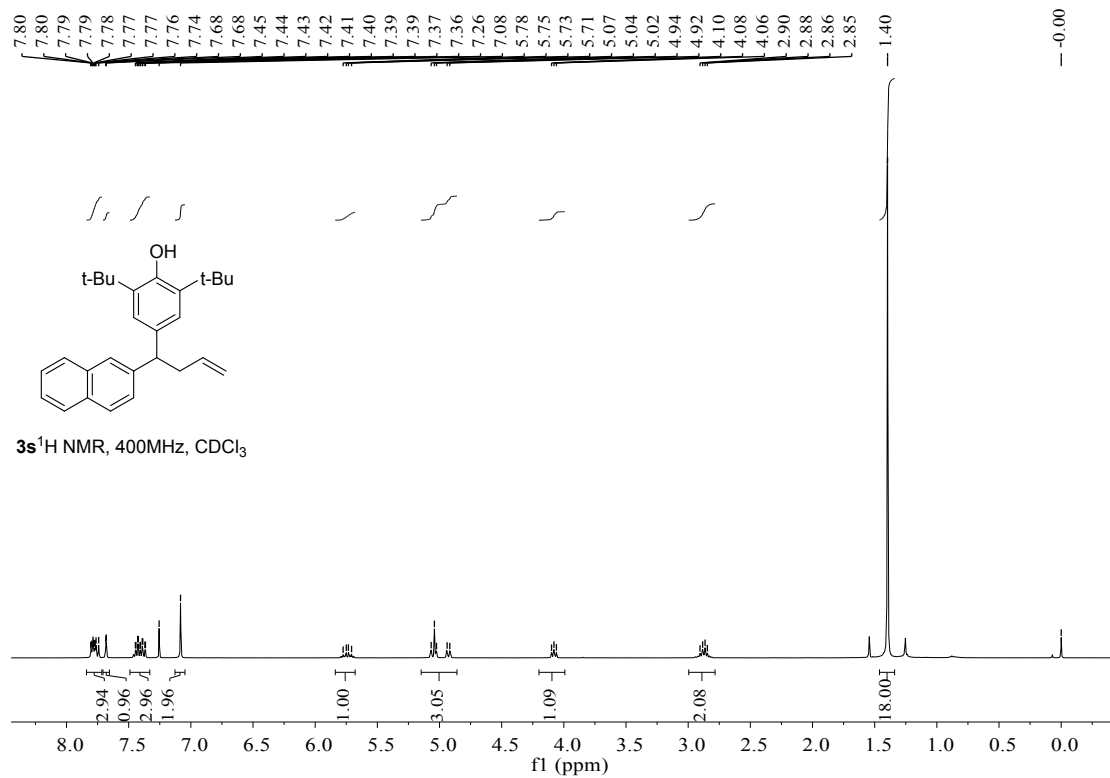


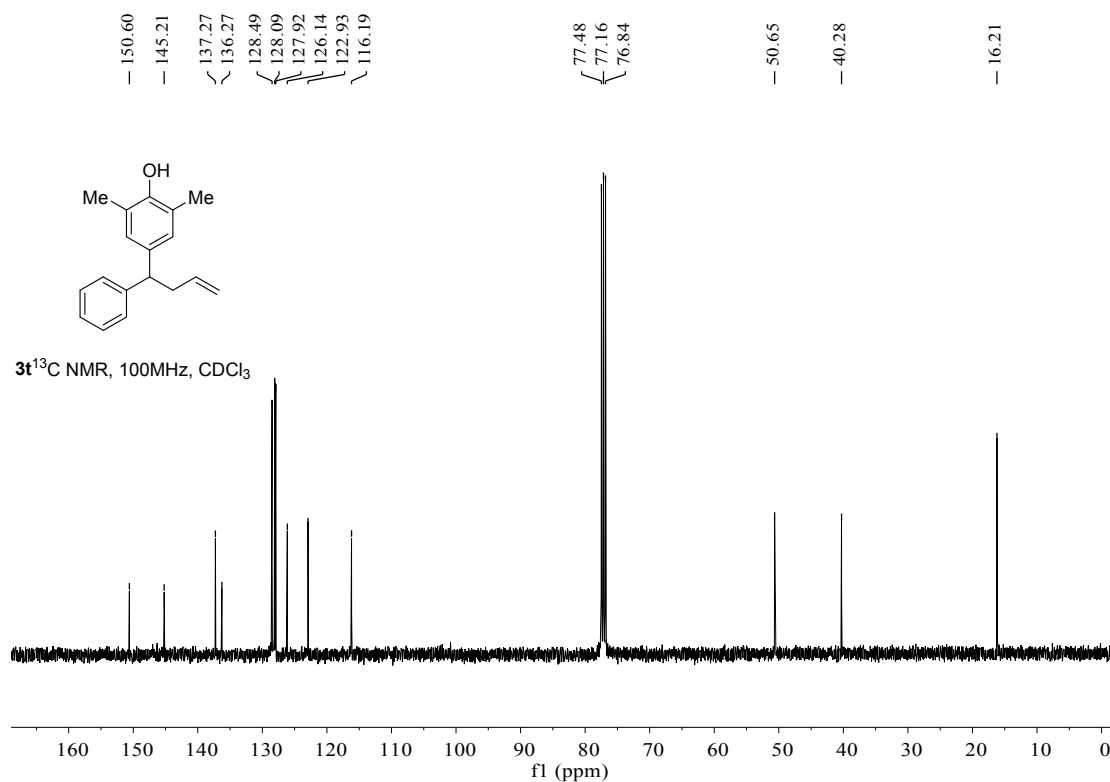
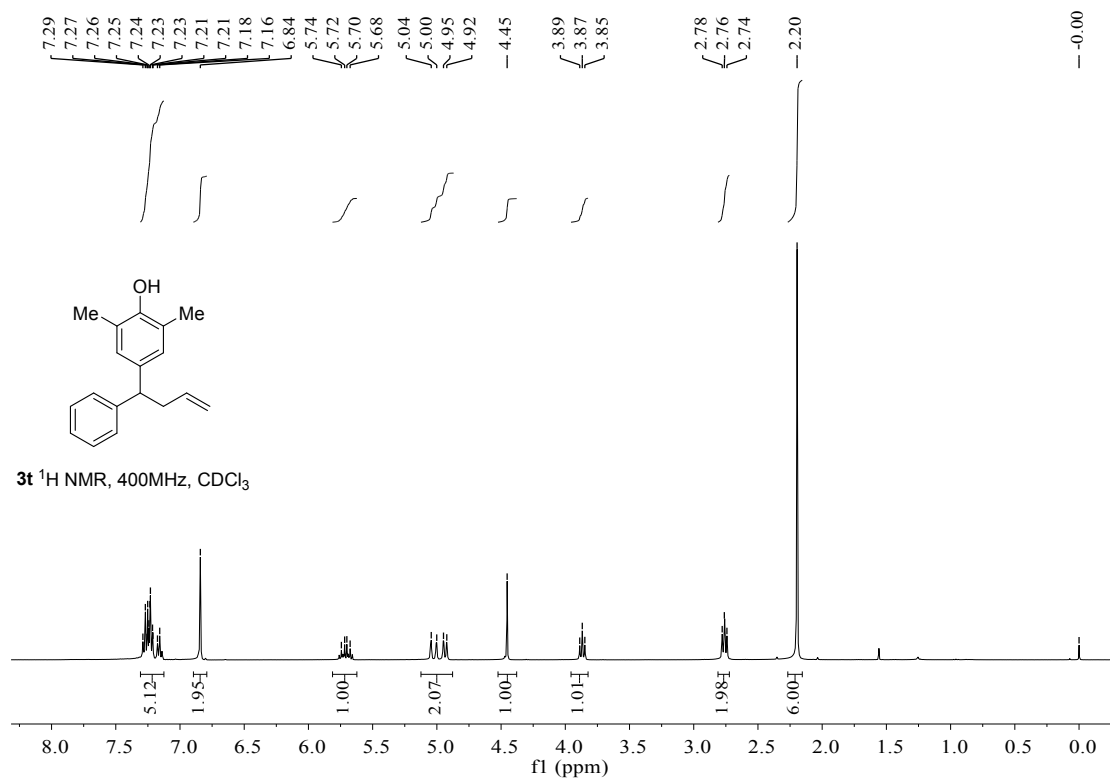


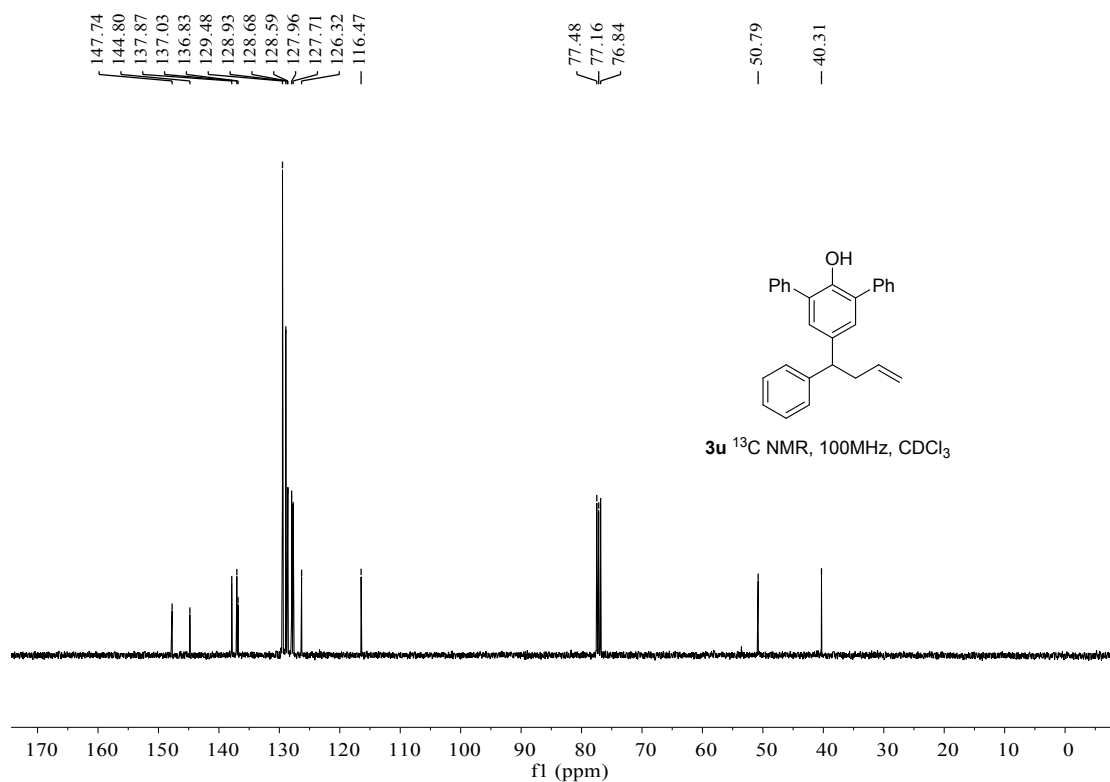
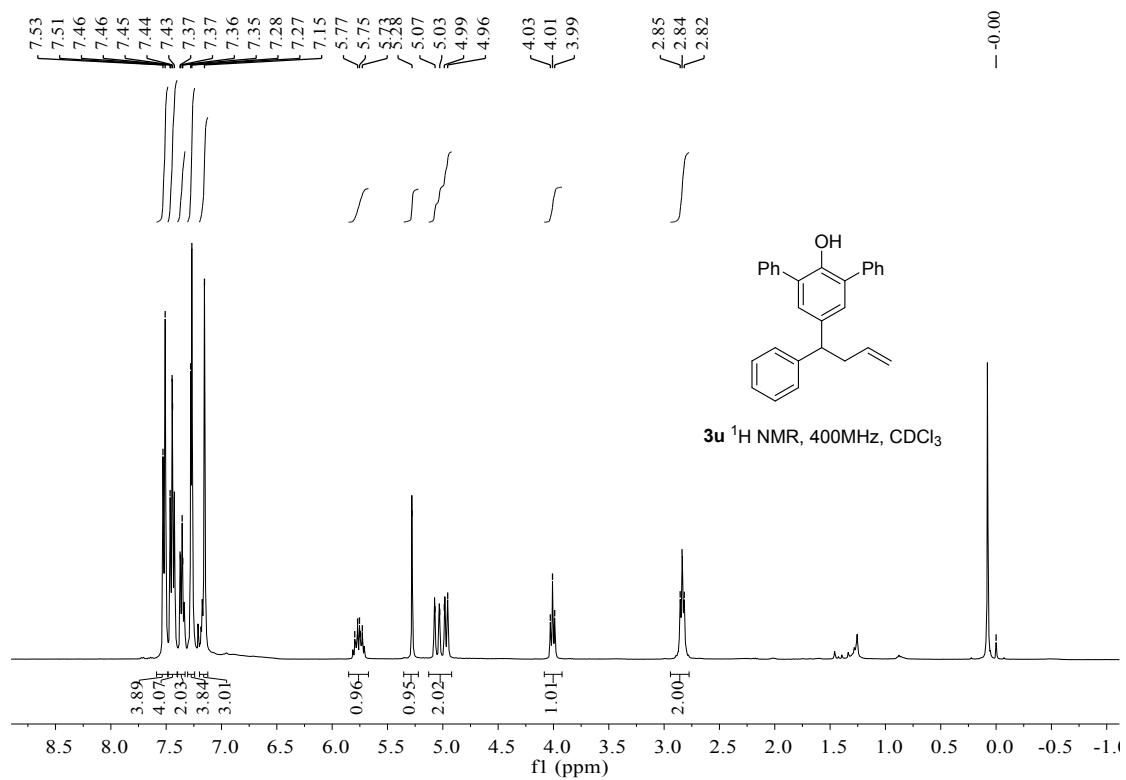


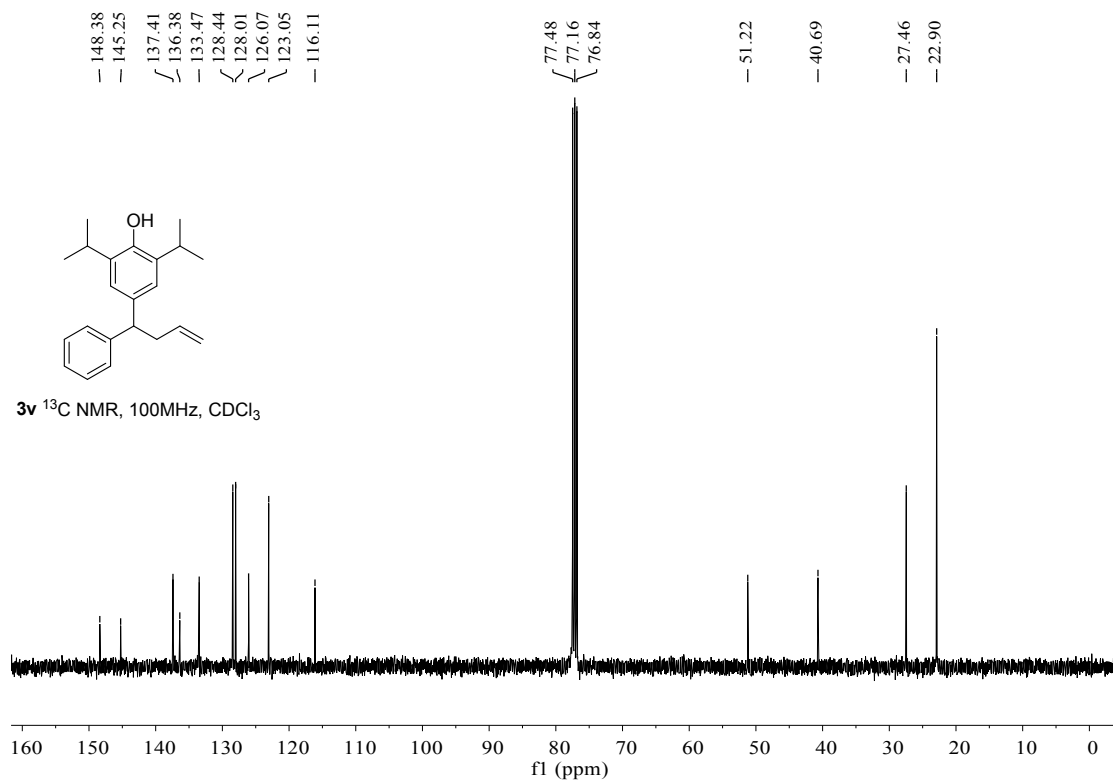
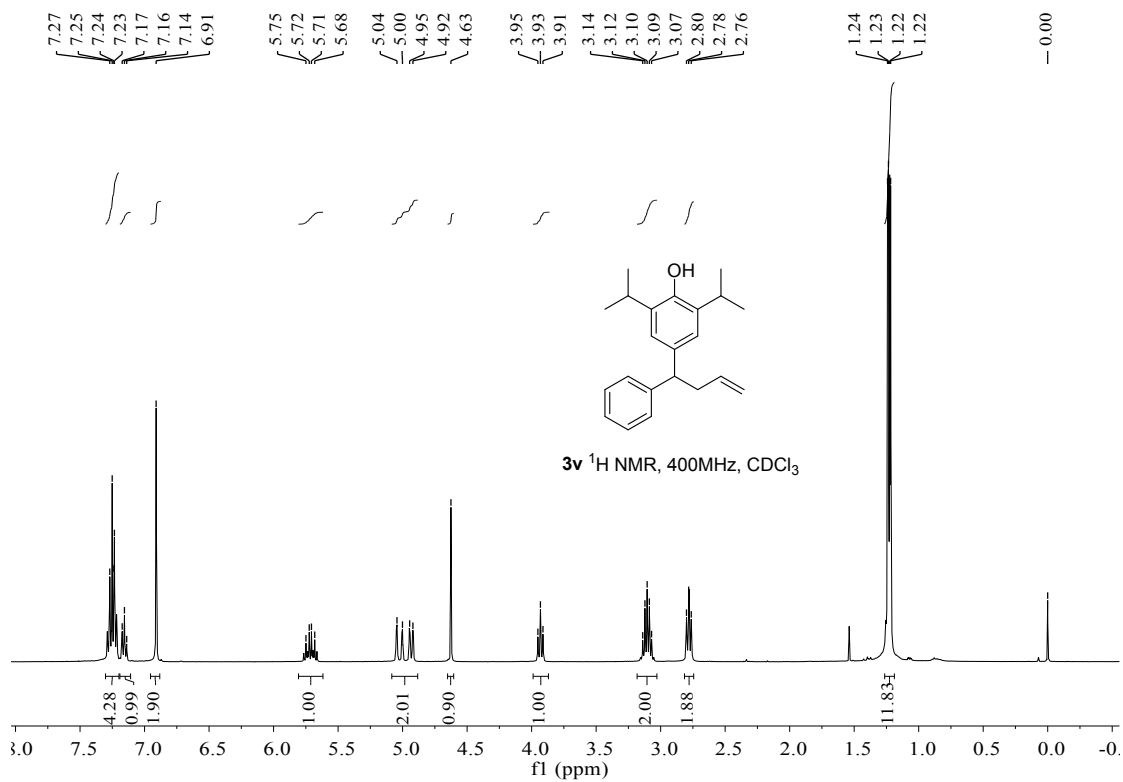


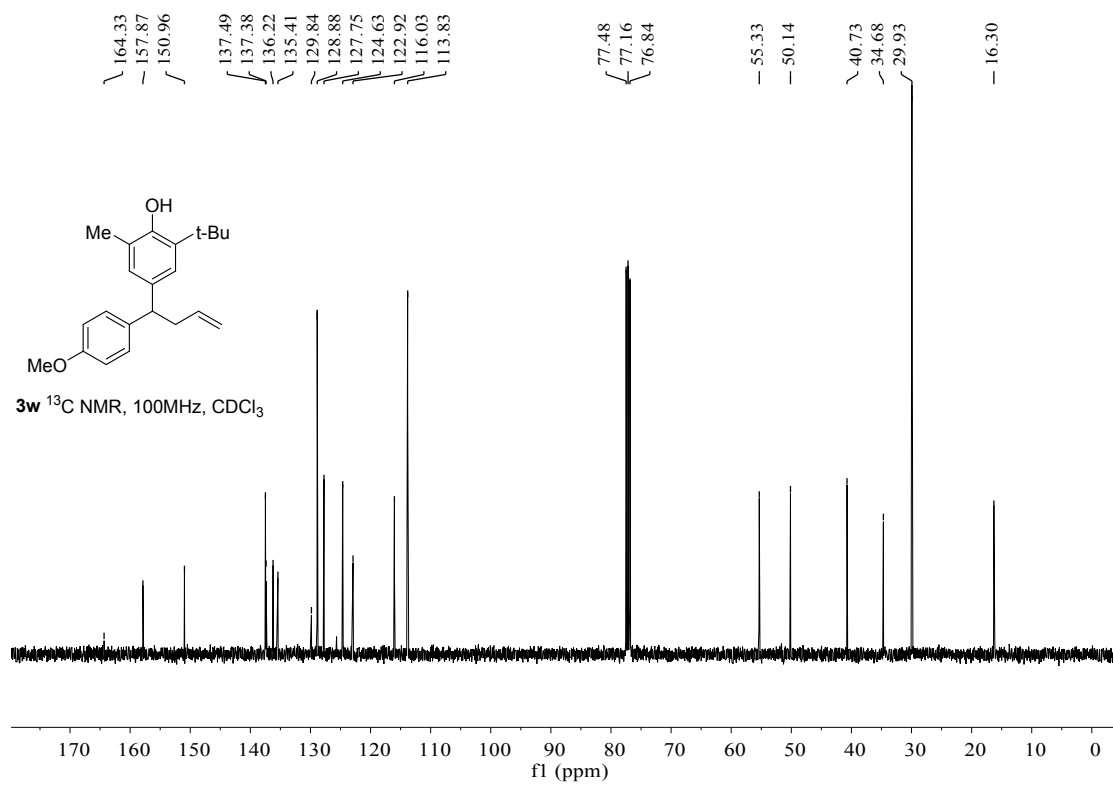
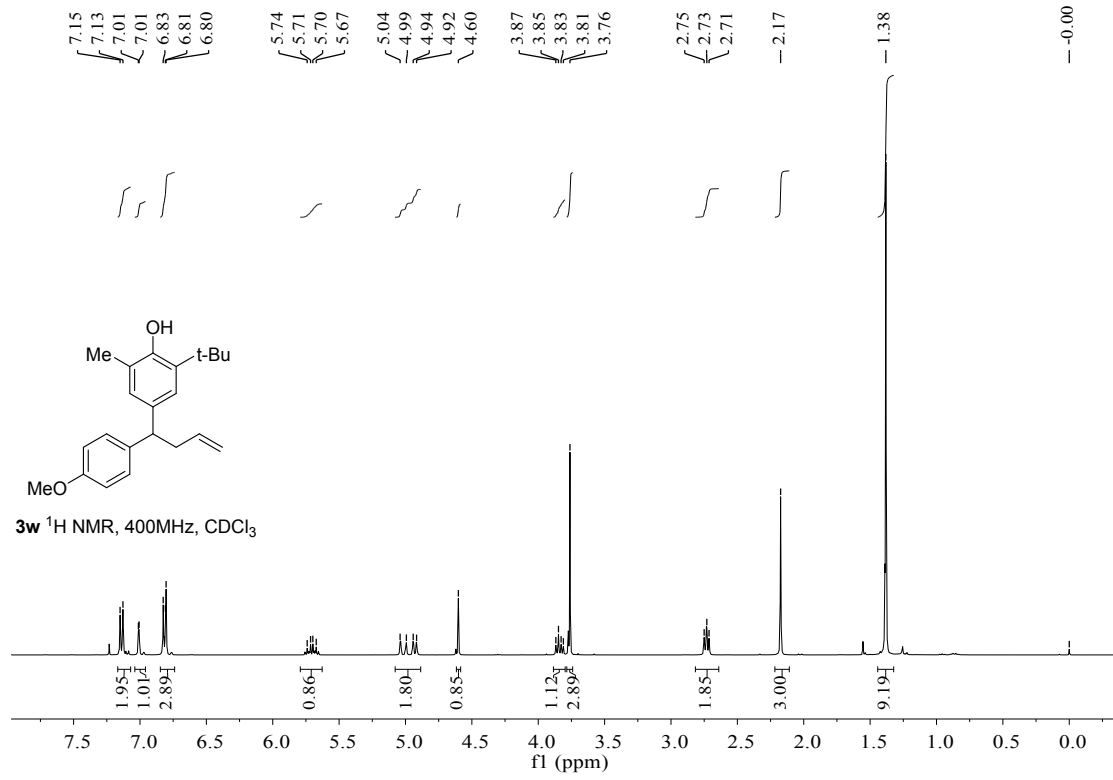


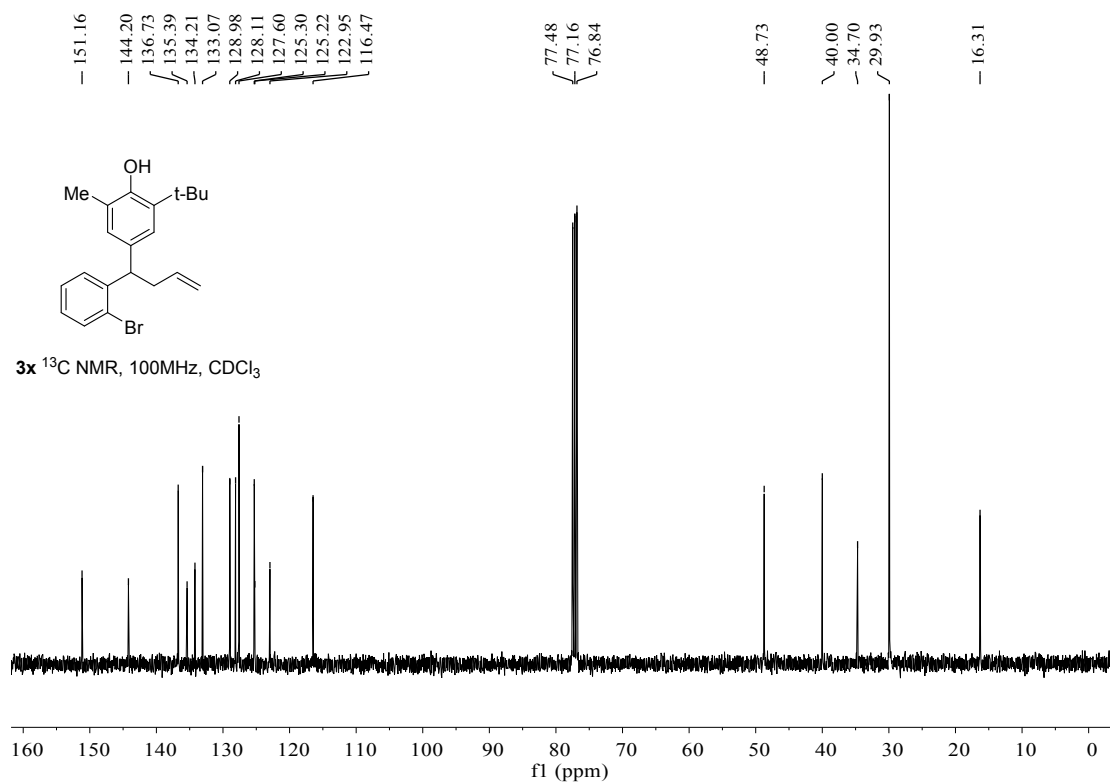
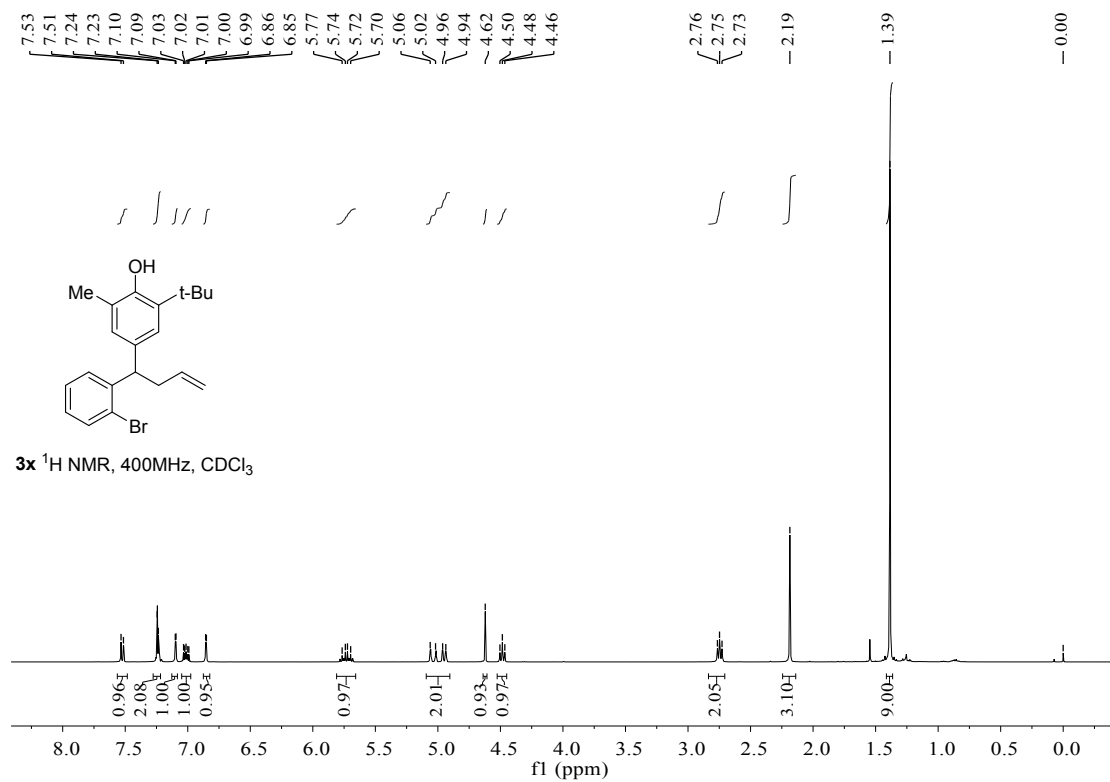


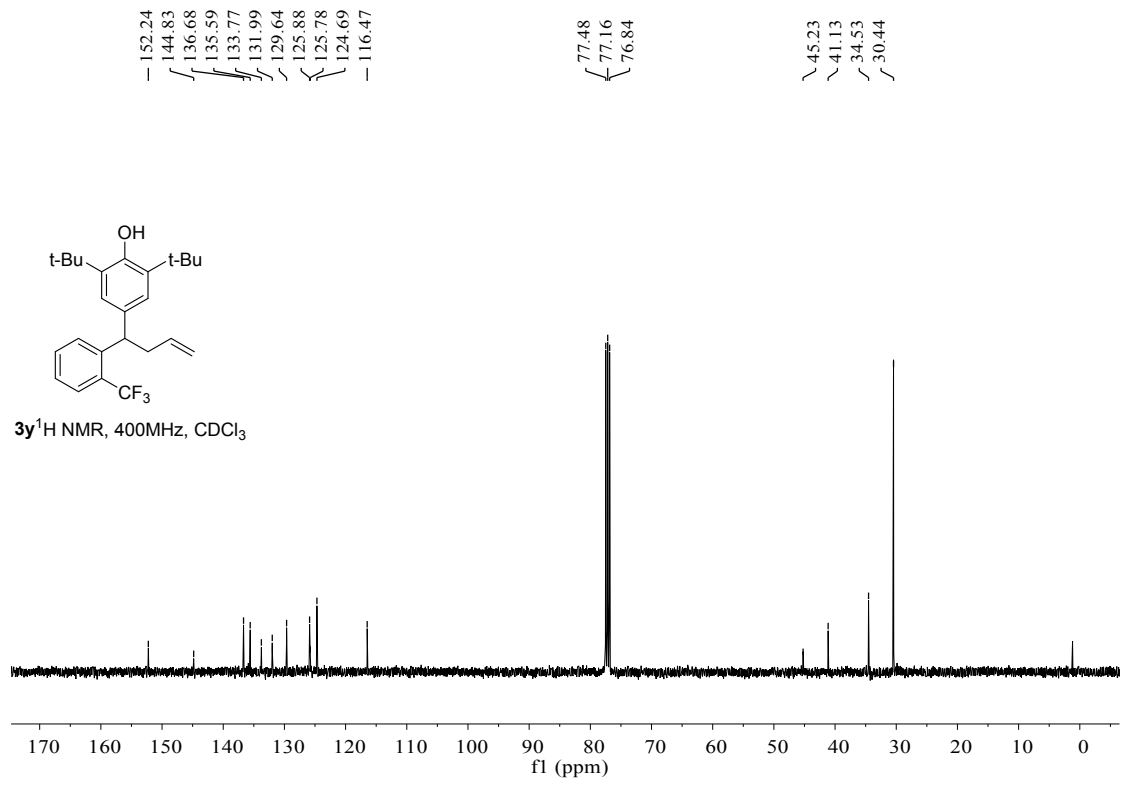
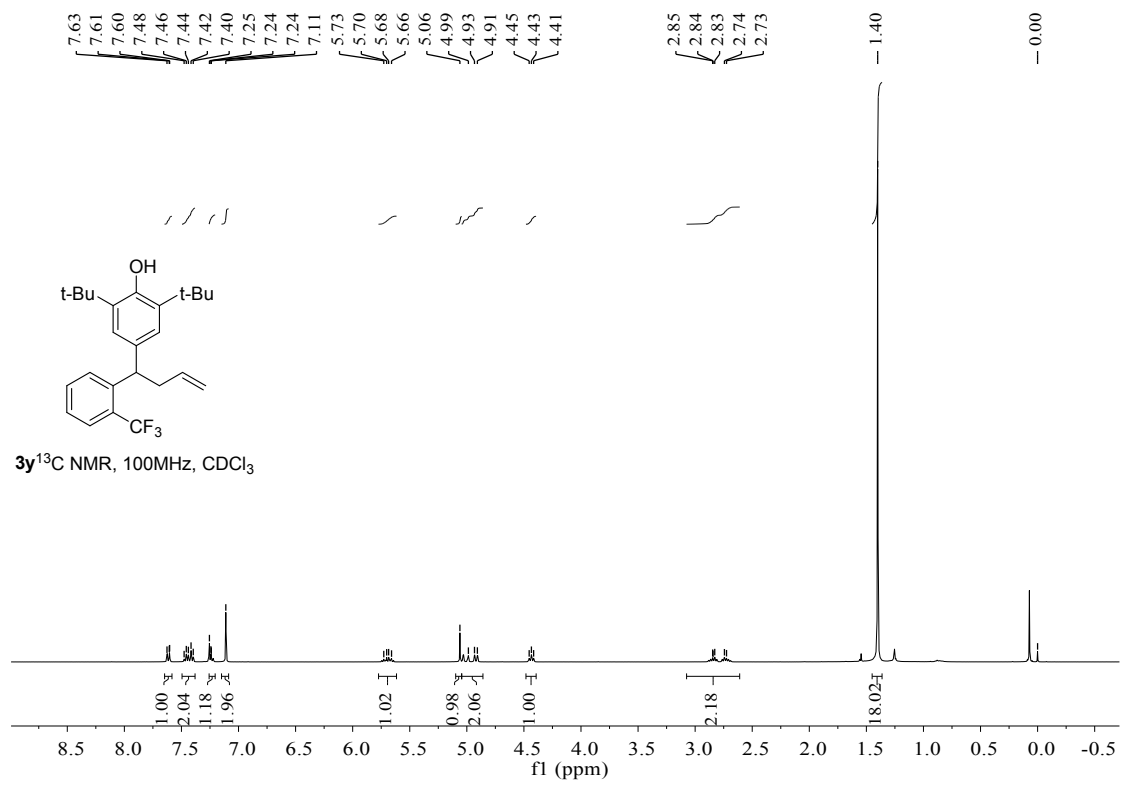


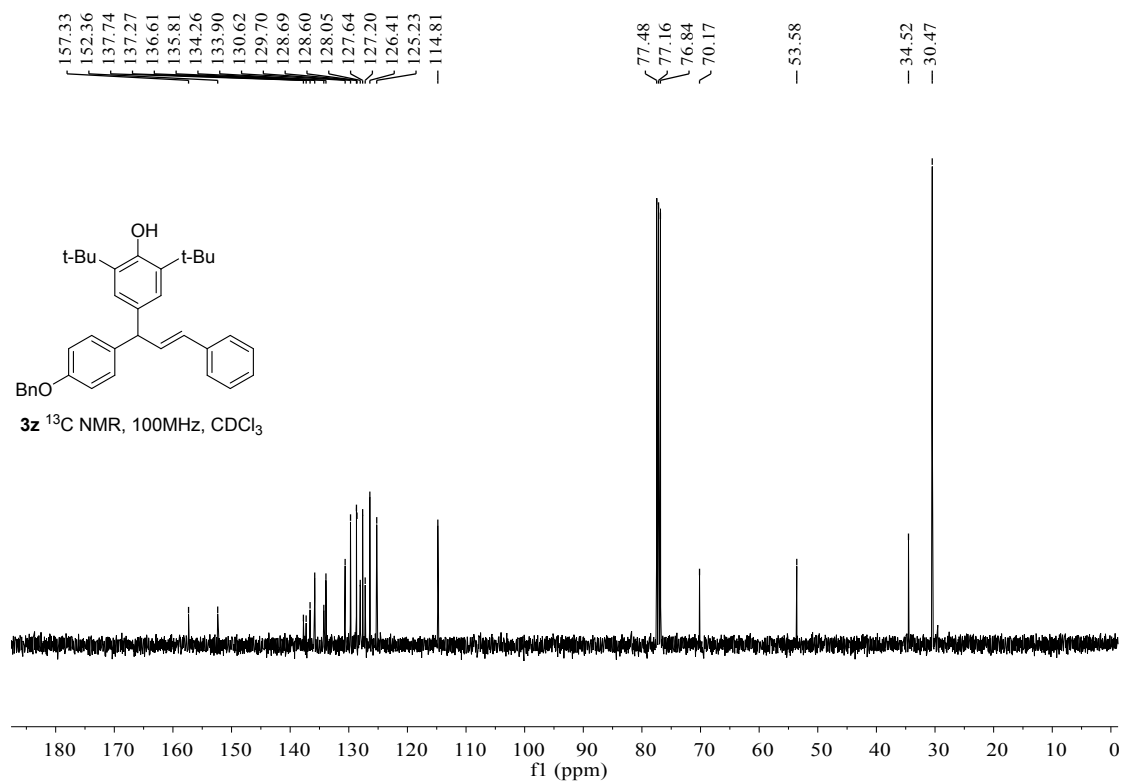
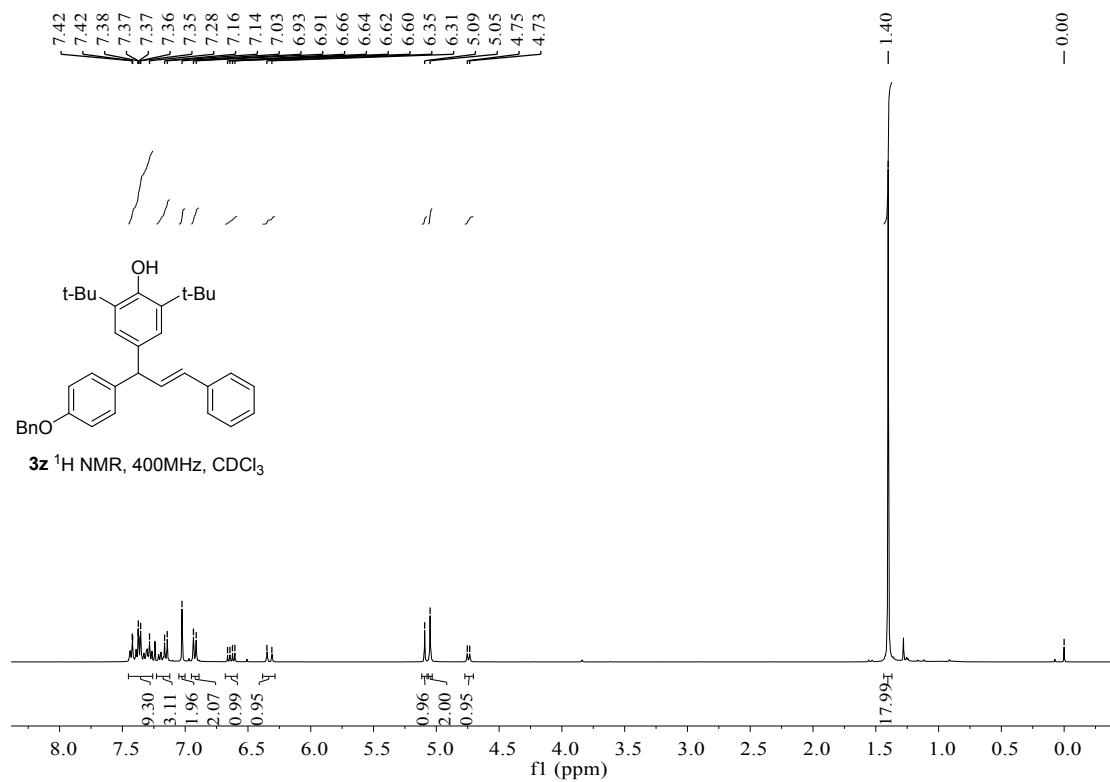




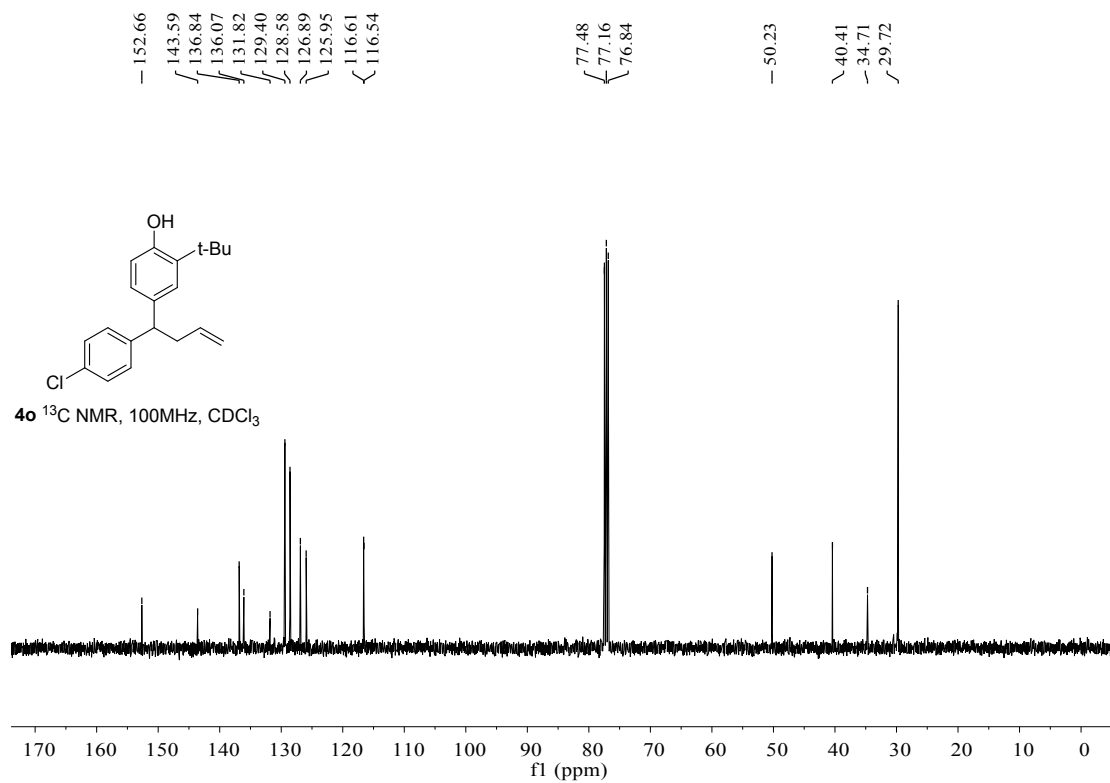
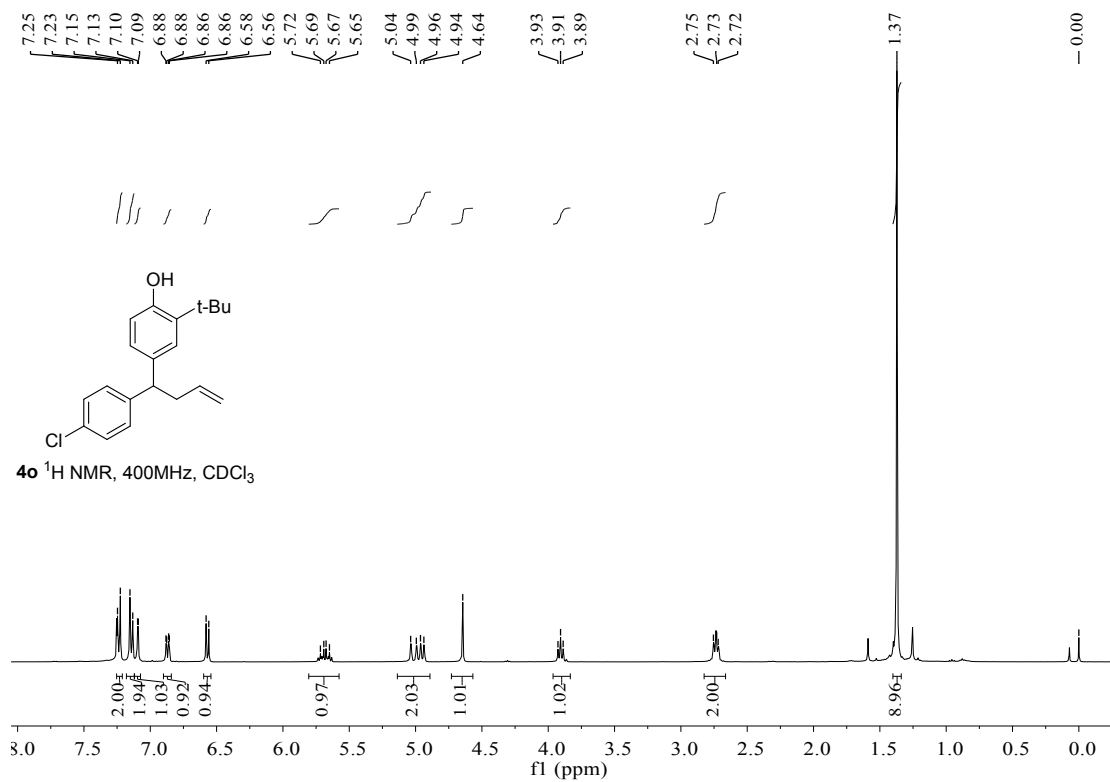


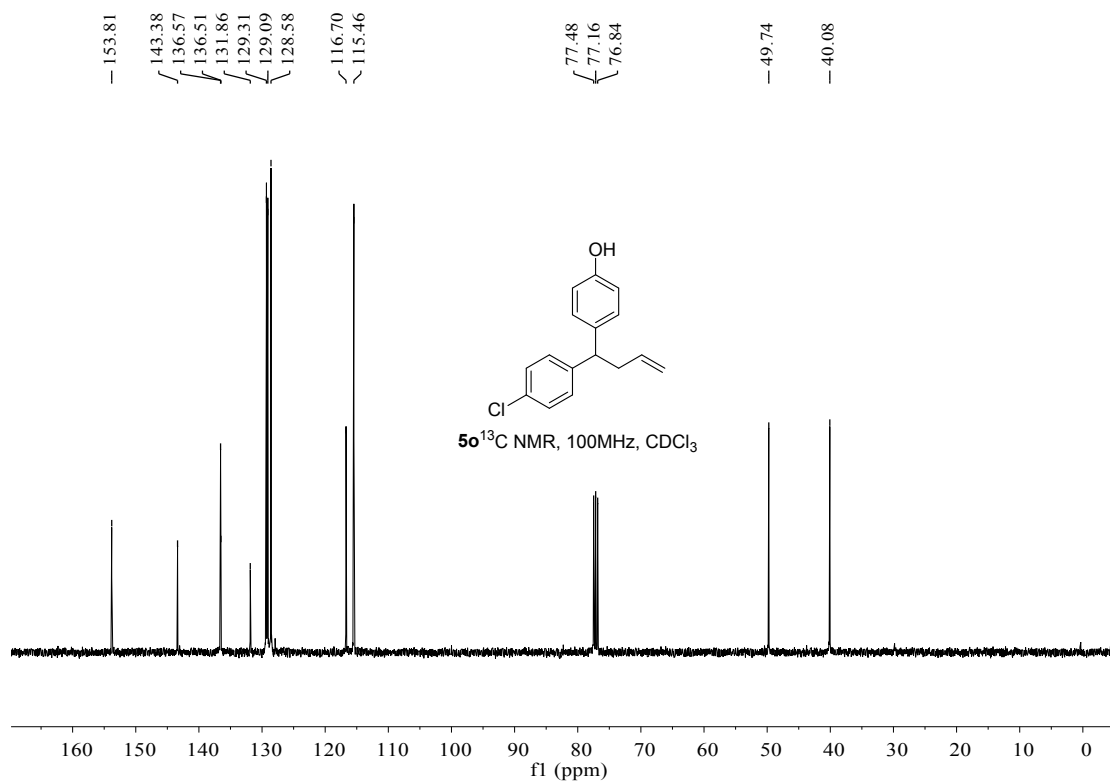
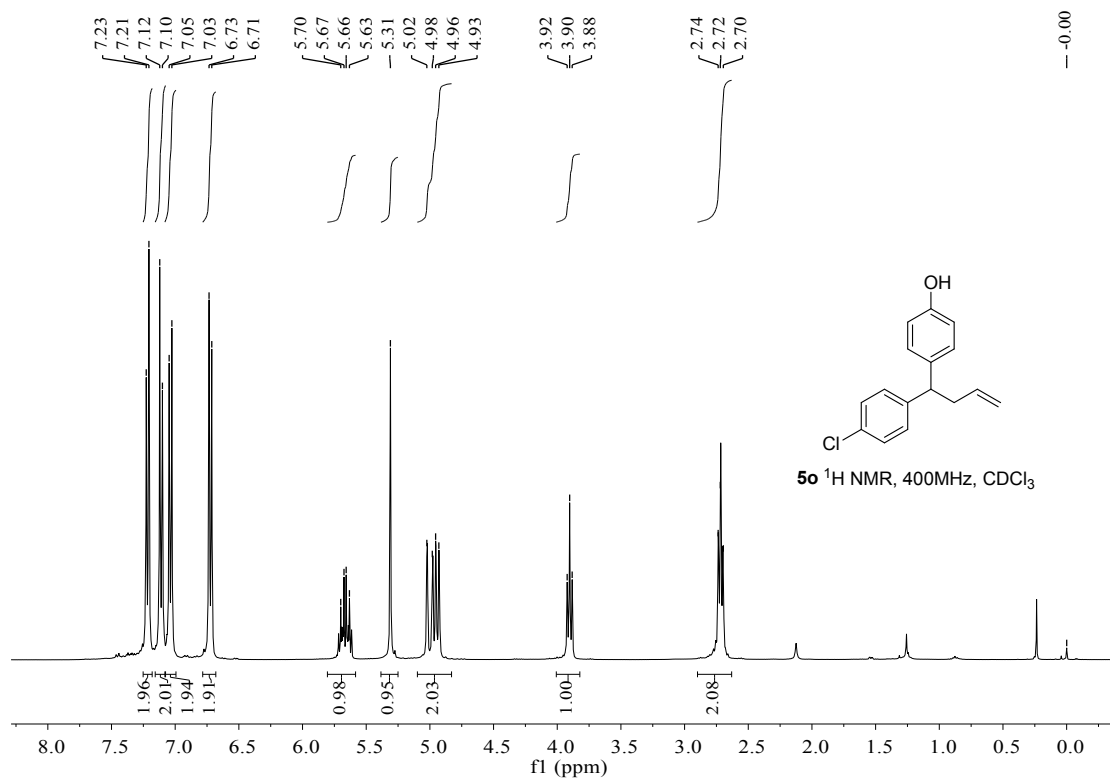


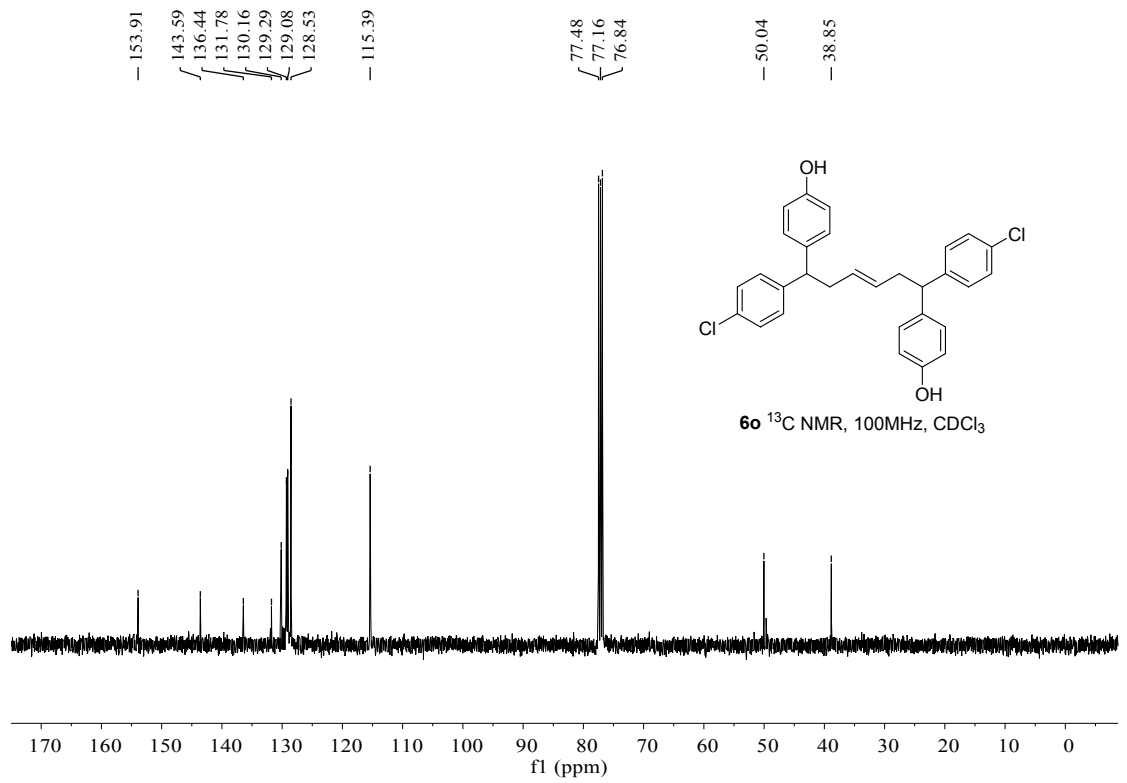
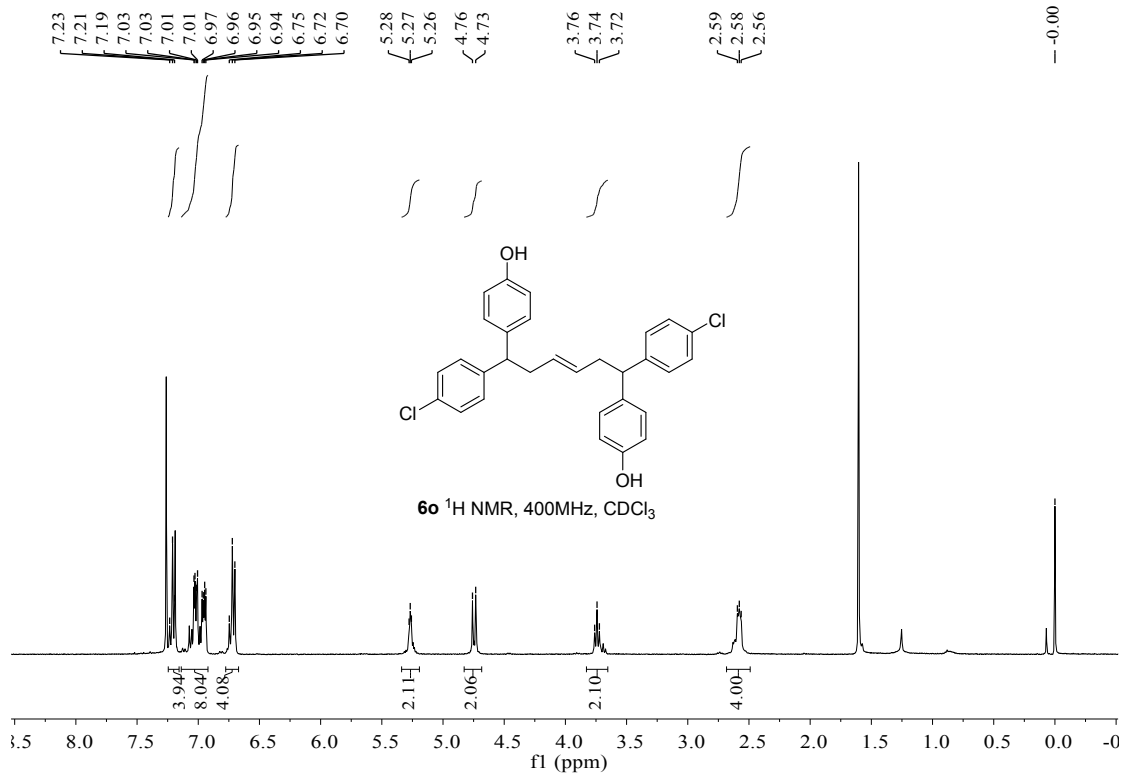


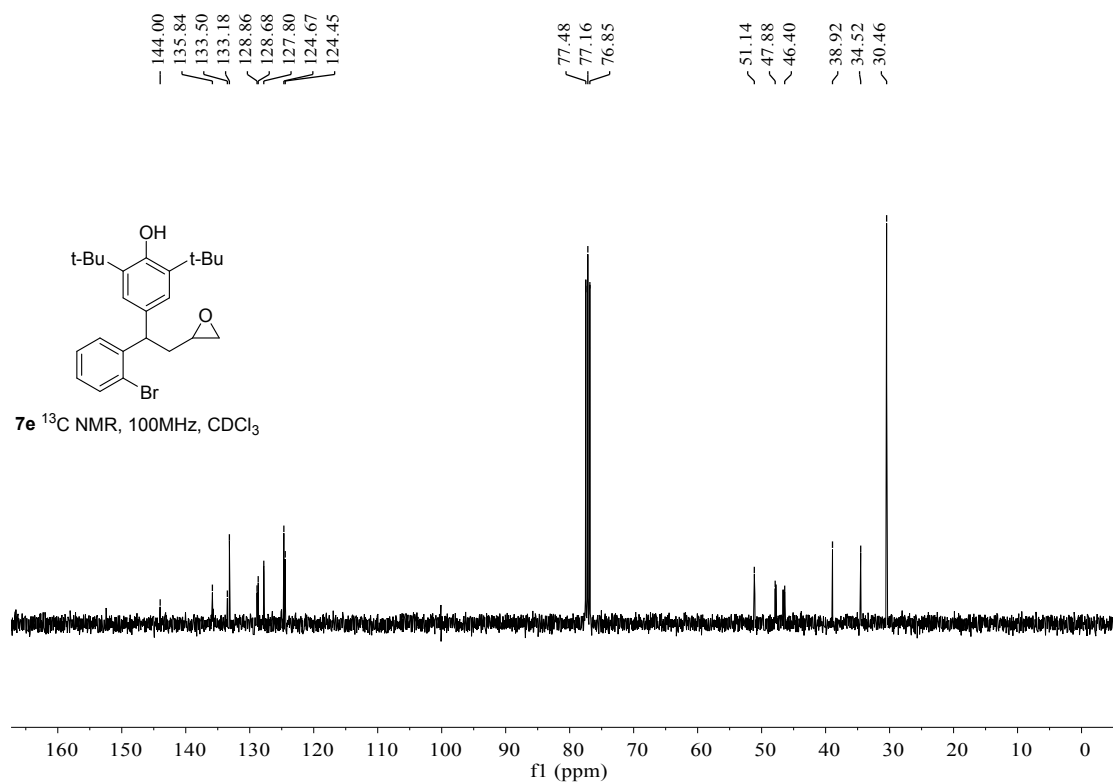
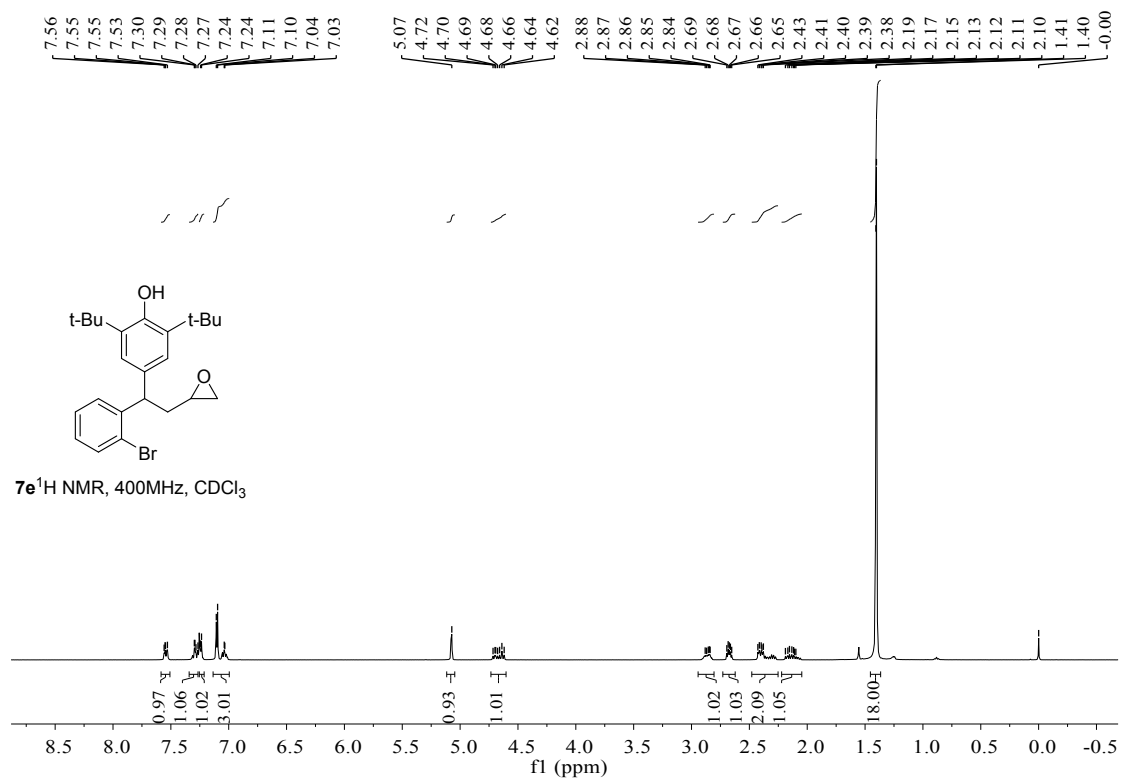


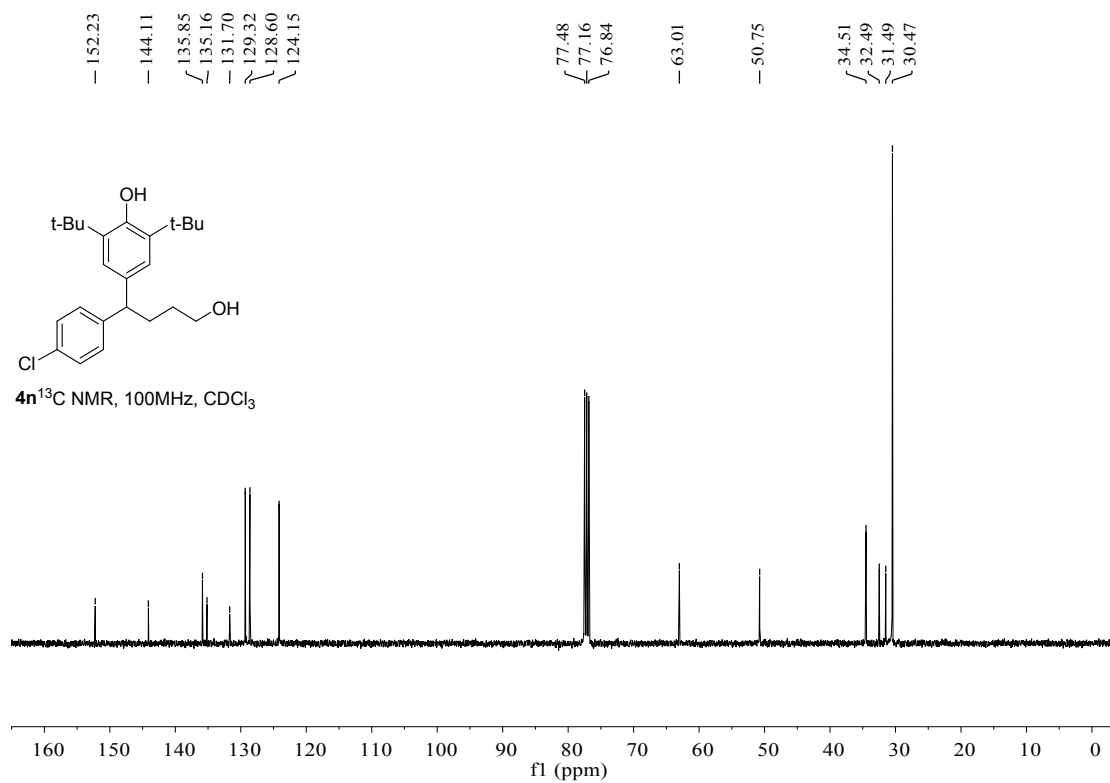
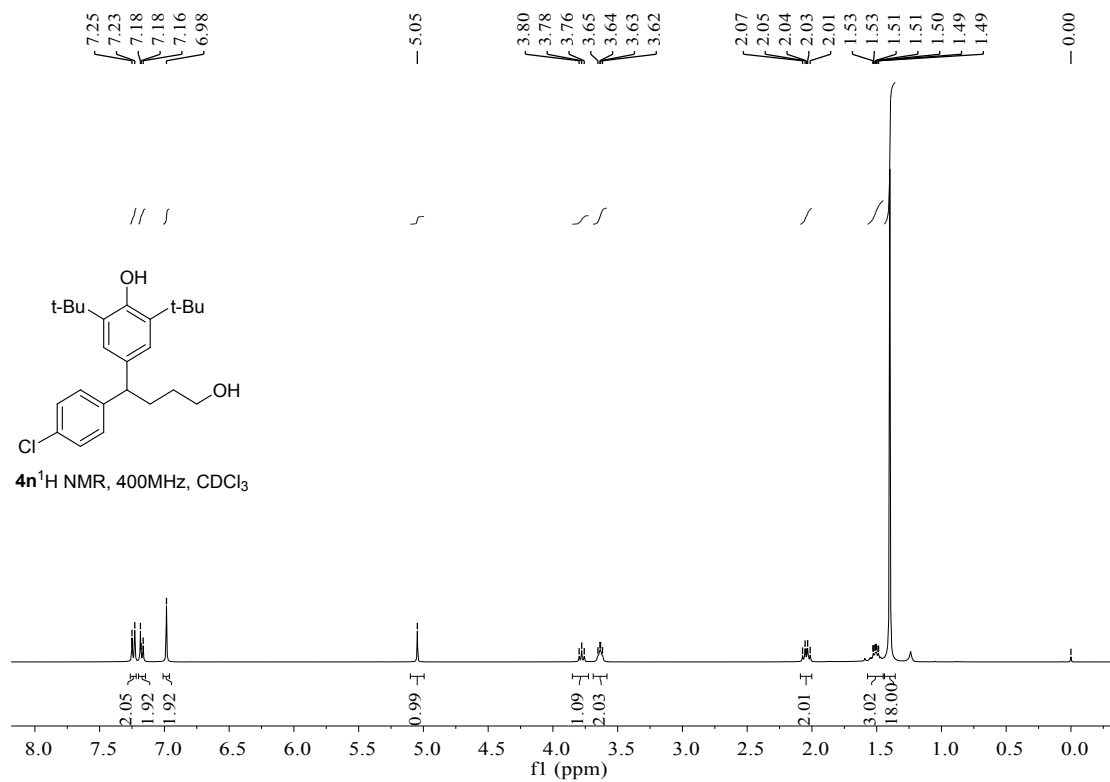


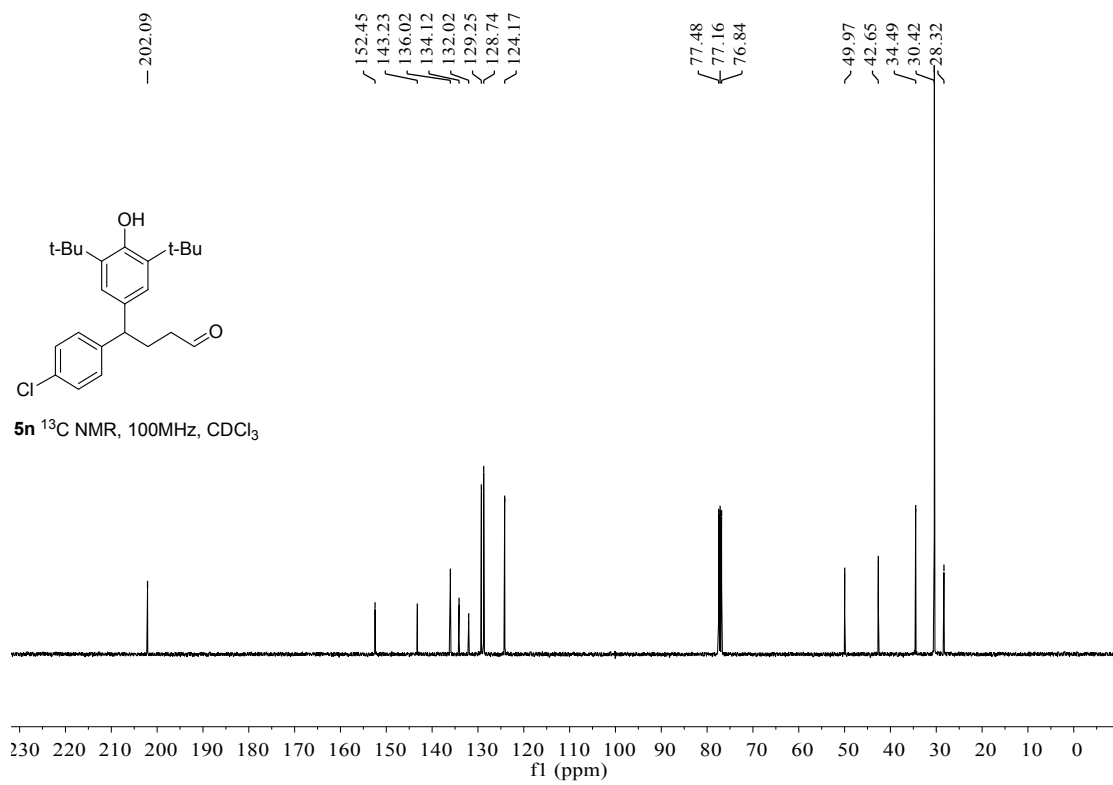
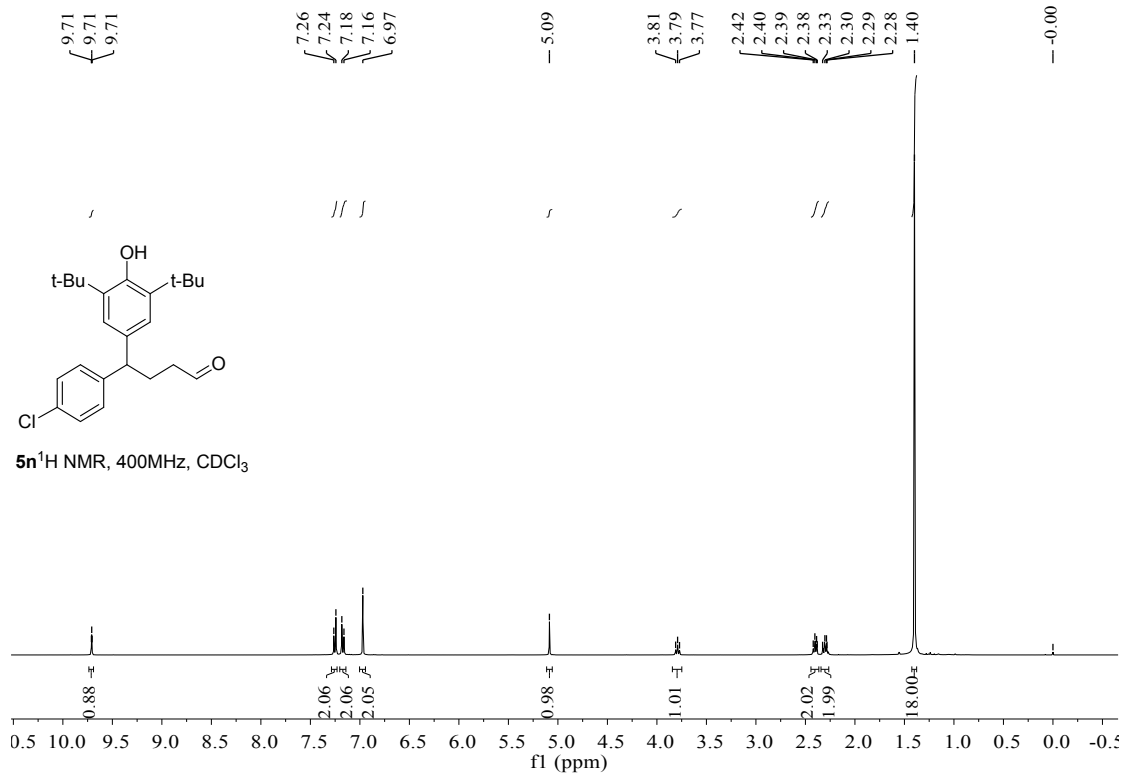


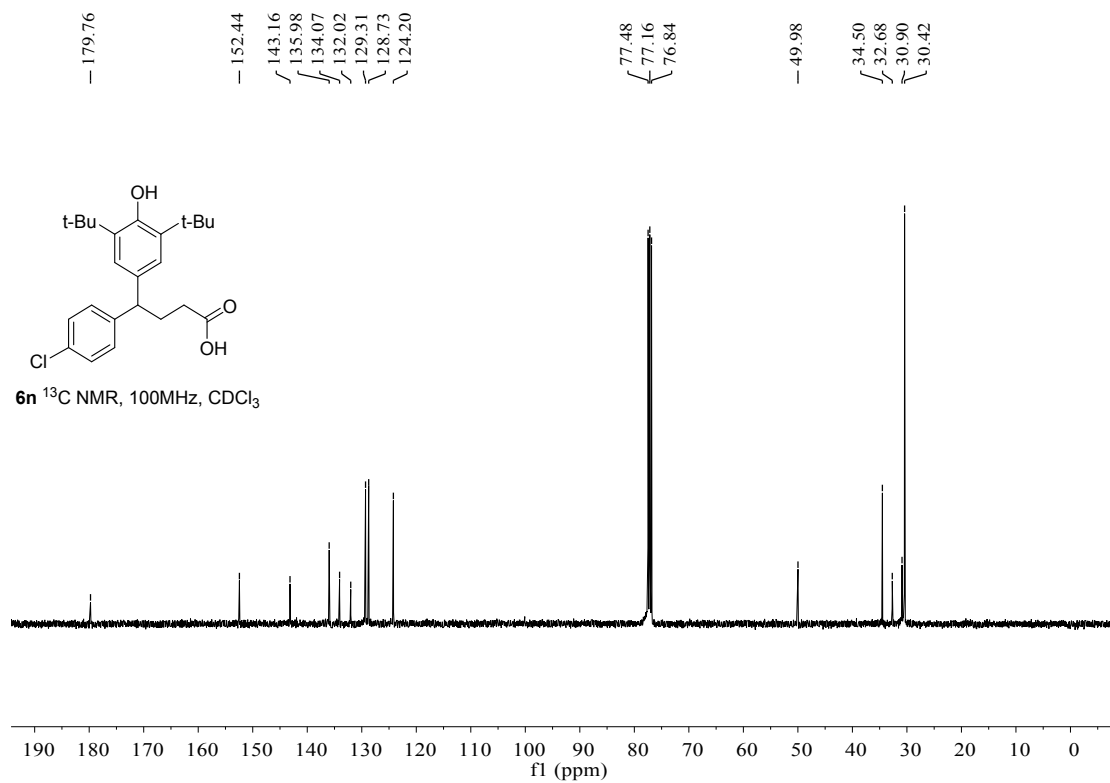
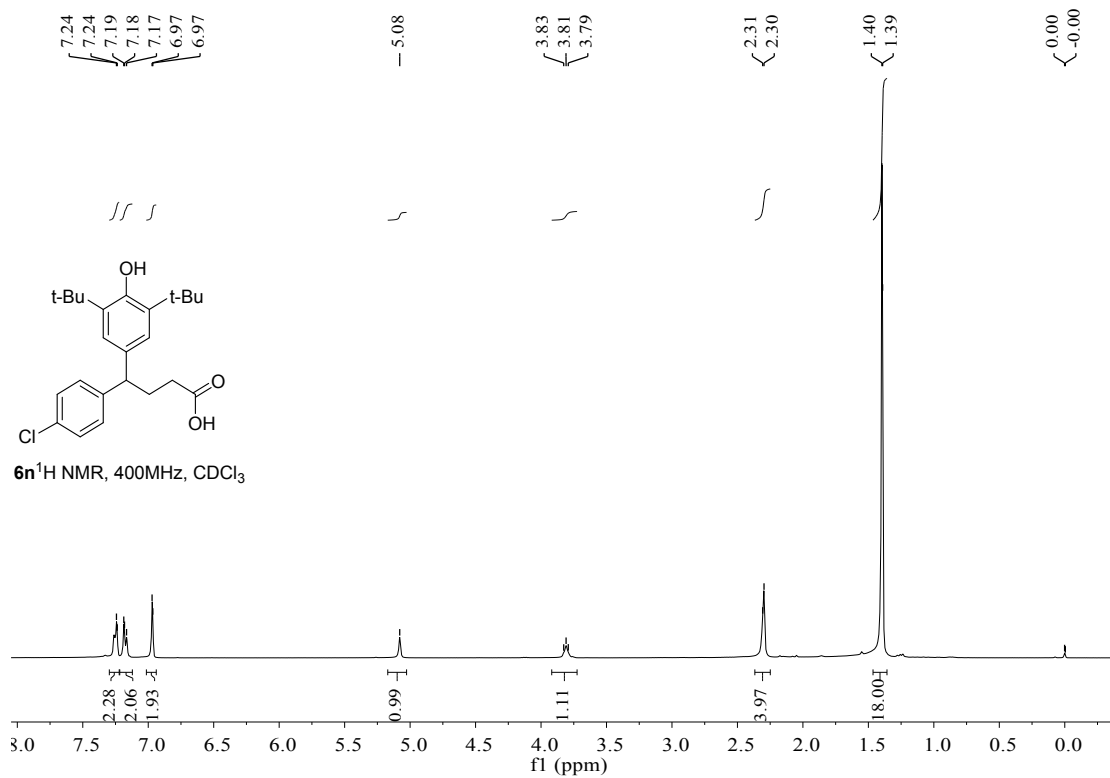


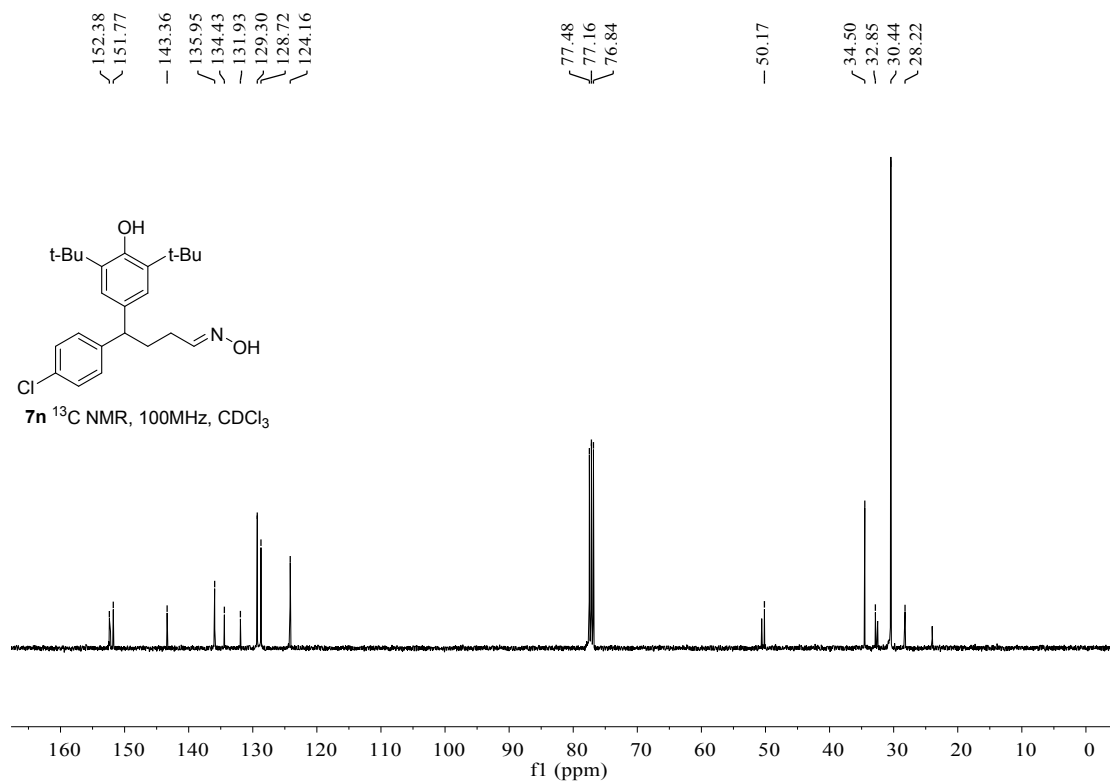
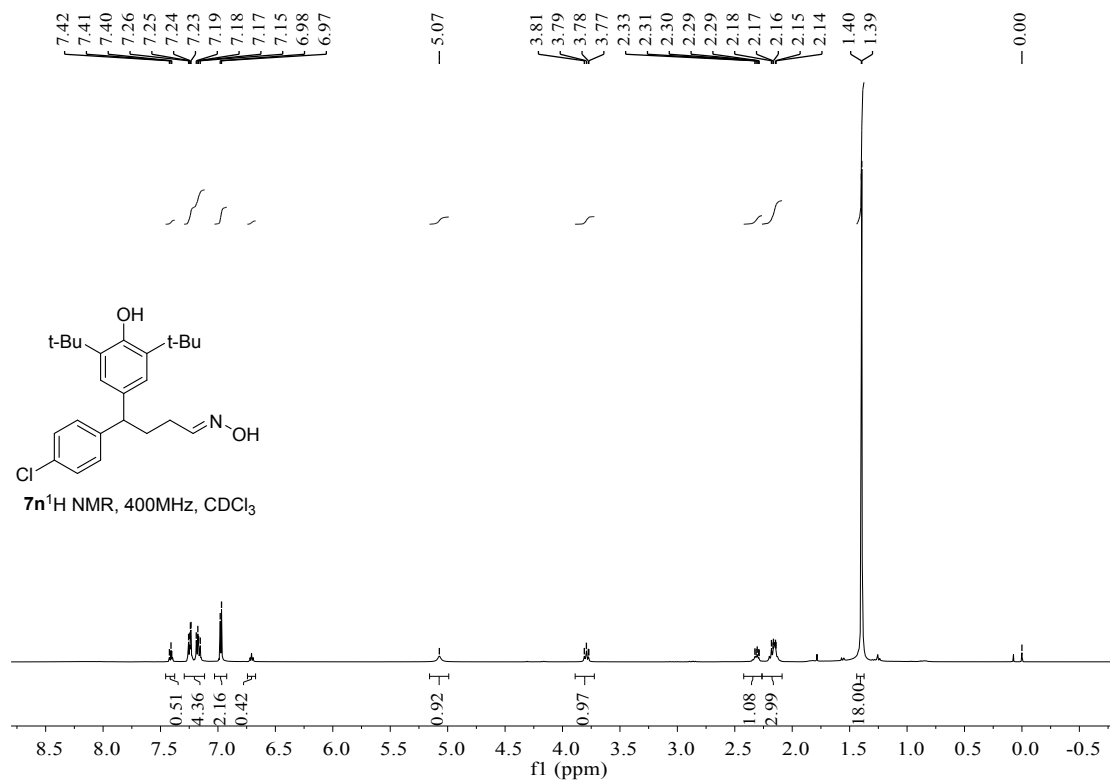




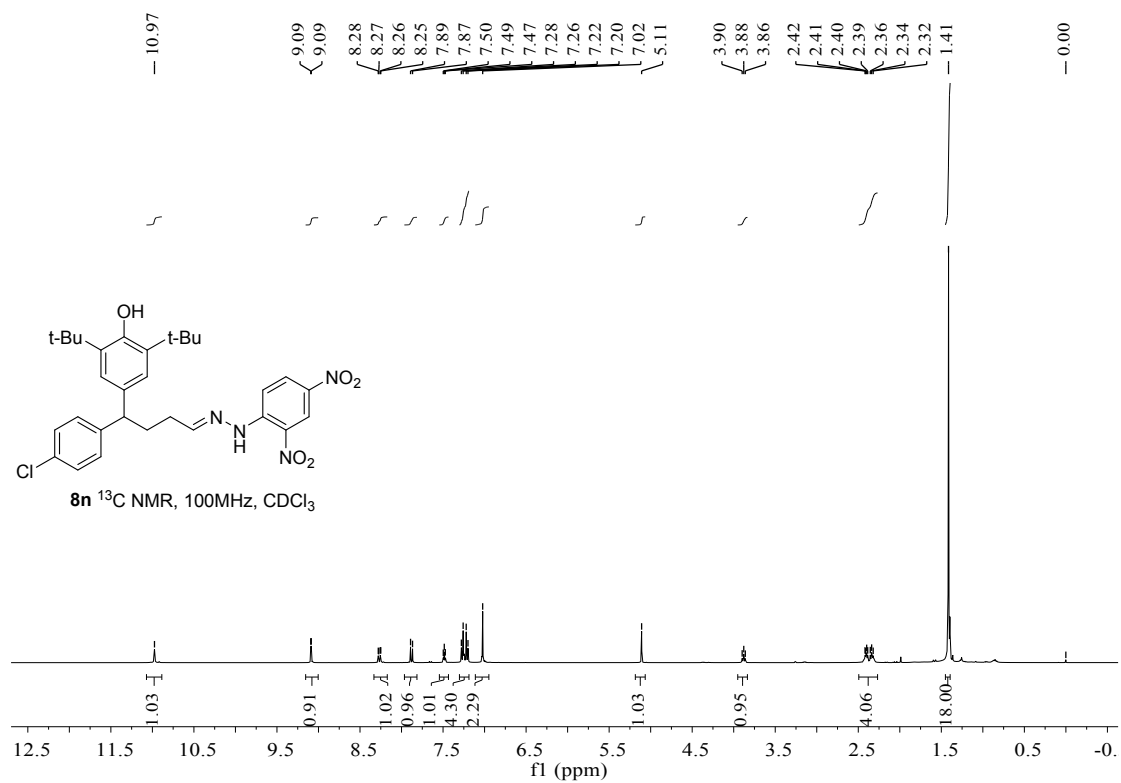
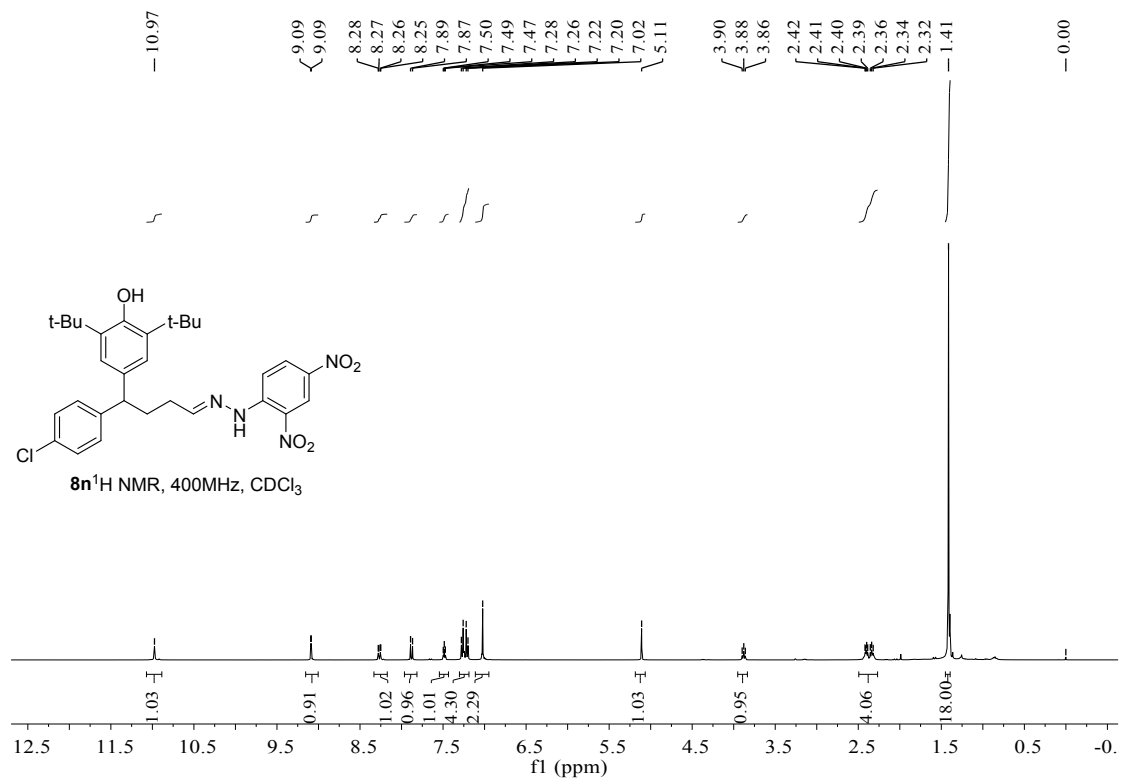




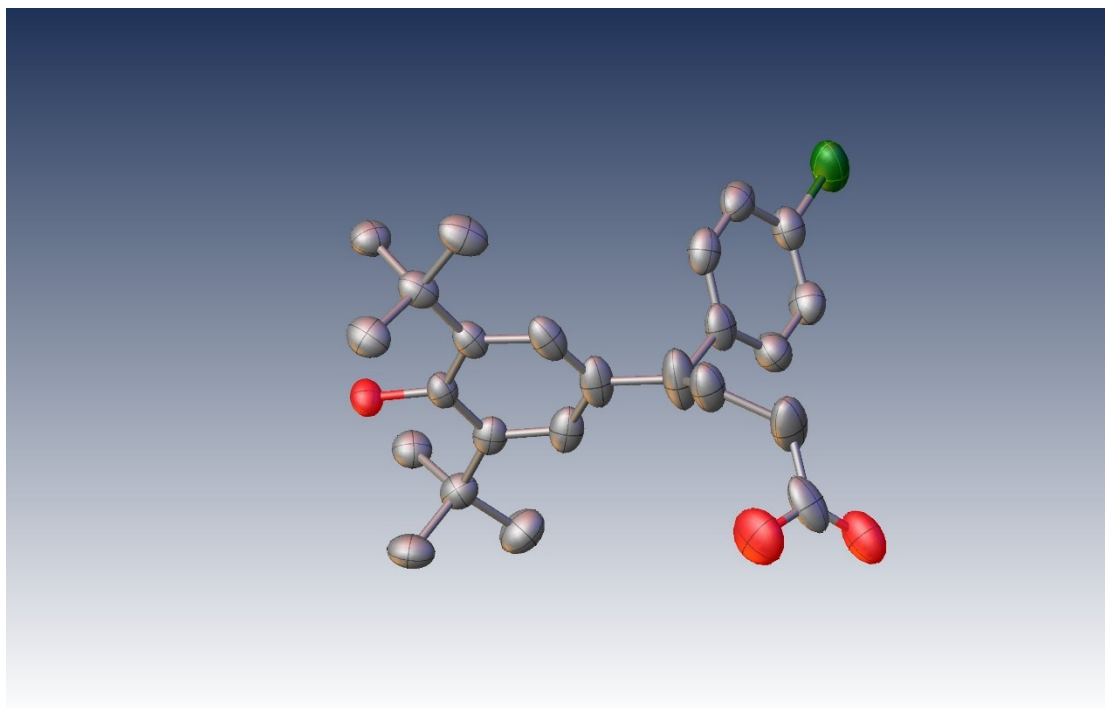








## 7. X-ray crystallography data of 6n



**Figure 1** X-ray crystallography data of **6n**.

Table 1 Crystal data and structure refinement for CCDC 1521335

Identification code	CCDC 1521335
Empirical formula	C <sub>24</sub> H <sub>31</sub> Cl O <sub>3</sub>
Formula weight	402.94
Temperature	113(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, P2(1)/c
Unit cell dimensions	a = 10.500(4) Å    alpha = 90 deg. b = 9.336(4) Å    beta = 100.864(9) deg.
	c = 22.910(10) Å    gamma = 90 deg.
Volume	2205.7(15) Å <sup>3</sup>
Z, Calculated density	4, 1.213 Mg/m <sup>3</sup>
Absorption coefficient	0.194 mm <sup>-1</sup>
F(000)	864
Crystal size	0.20 x 0.18 x 0.12 mm
Theta range for data collection	3.19 to 25.02 deg.
Limiting indices	-12 ≤ h ≤ 12, -11 ≤ k ≤ 10, -27 ≤ l ≤ 27
Reflections collected / unique	17912 / 3869 [R(int) = 0.1143]
Completeness to theta = 25.02	99.6 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9771 and 0.9622
Refinement method	Full-matrix least-squares on F <sup>2</sup>

Data / restraints / parameters	3869 / 106 / 270
Goodness-of-fit on $F^2$	1.002
Final R indices [ $I > 2\sigma(I)$ ]	R1 = 0.0799, wR2 = 0.2117
R indices (all data)	R1 = 0.1257, wR2 = 0.2432
Largest diff. peak and hole	0.634 and -0.365 e.A <sup>-3</sup>

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