

## Catalyst-free C-N Bond Formation under Biocompatible Reaction Conditions

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Contents	Pages
General information	2
Preparation of starting materials	2-5
Optimization of reaction condition	5-6
General procedure for the water-based amination of allenic carbonyls & Spectroscopic data obtained in this study	6-20
Synthetic transformations and utility of enamines	21-23
NMR Spectra	
HRMS Spectra	

## General Information:

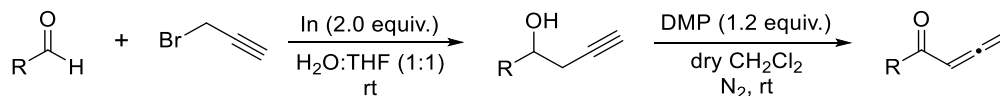
Unless otherwise stated, all commercial reagents and solvents were used without additional purification. Analytical thin layer chromatography (TLC) was performed on pre-coated silica gel 60 F254 plates. Visualization on TLC was achieved by the use of UV light (254 nm). Column chromatography was undertaken on silica gel (400-630 mesh) using a proper eluent system.  $^1\text{H}$  NMR,  $^{13}\text{C}$  NMR and  $^{19}\text{F}\{^1\text{H}\}$  NMR were recorded on Bruker Avance 400 MHz and 500 MHz.  $^{13}\text{C}$  NMR and  $^{19}\text{F}\{^1\text{H}\}$  NMR were fully decoupled by broad band proton decoupling. Chemical shifts were reported in ppm referenced to the center of a triplet at 77.0 ppm of chloroform-*d*. Chemical shifts were quoted in parts per million (ppm) referenced to the appropriate solvent peak or 0.0 ppm for tetramethylsilane. The following abbreviations were used to describe peak splitting patterns when appropriate: br = broad, s = singlet, d = doublet, t = triplet, q = quartet, dd = doublet of doublet, td = triplet of doublet, ddd = doublet of doublet of doublet, m = multiplet. Coupling constants, *J*, were reported in hertz unit (Hz). High resolution mass spectra were obtained on Waters Q-Tof Premier Spectrometer.

## II. General Procedure for the Preparation of Starting Materials

### II-1. Preparation of allenic ketones<sup>1</sup>

Allenic ketones (**1**) were prepared from the corresponding aldehydes according to the known procedures reported in the literature.<sup>1</sup> Allenic ketones **1w**, **1x**, **1ab**, **1ac**, **1ae-1ah** were prepared using reported procedures,<sup>1a</sup> **1z** was prepared using reported procedures,<sup>1b</sup> **1y** and **1ad** were prepared using *General Procedure 1a* and **1aa** was prepared using *General Procedure 1b*.

#### *General Procedure 1a*

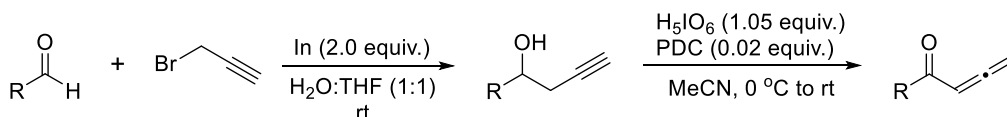


To a solution of propargyl bromide (20.0 mmol, 2.0 equiv.) and In powder (20.0 mmol, 2.0 equiv.) in H<sub>2</sub>O/THF (1:1, 20 mL), was added the aldehyde (10.0 mmol, 1.0 equiv.) and stirred overnight at room temperature. After the completion of the reaction (i.e. monitored by TLC), conc. HCl was added dropwise to quench the mixture (until a clear solution was obtained), followed by extraction with CH<sub>2</sub>Cl<sub>2</sub> (3x30 mL). The combined organic layers were washed with brine (30 mL) and dried over Na<sub>2</sub>SO<sub>4</sub>. The volatiles were evaporated under reduced pressure and the crude product was purified by flash column chromatography (silica gel, *n*-hexane/EtOAc) to afford the corresponding propargylic alcohol.

A solution of propargylic alcohol (1.0 equiv.) in anhydrous CH<sub>2</sub>Cl<sub>2</sub> (10 mL) was added dropwise to a solution of DMP (1.2 equiv.) in anhydrous CH<sub>2</sub>Cl<sub>2</sub> (20 mL) under nitrogen at room temperature. The reaction was allowed to stir overnight and upon the completion of the reaction (i.e. monitored by TLC), the mixture was diluted with Et<sub>2</sub>O (30 mL) and the layers were washed with 1M NaOH (40 mL). The aqueous layer was extracted with Et<sub>2</sub>O (3x30 mL) and the combined organic layers were washed with brine (30 mL), dried over Na<sub>2</sub>SO<sub>4</sub> and concentrated *in vacuo*. The residue was purified by flash column chromatography to yield the corresponding ketone allenic ketone **1**.

<sup>1</sup> (a) Goh, J.; Maraswami, M.; Loh, T. -P. Synthesis of Vinylic Sulfones in Aqueous Media. *Org. Lett.* **2021**, 23, 1060; (b) Melen, R. L.; Wilkins, L. C.; Kariuki, B. M.; Wadepohl, H.; Gade, L. H.; Hashmi, A. S. K.; Stephan, D. W.; Hasmann, M. M. Diverging Pathways in the Activation of Allenes with Lewis Acids and Bases: Addition, 1,2-Carboboration, and Cyclization. *Organometallics.* **2015**, 34, 4127.

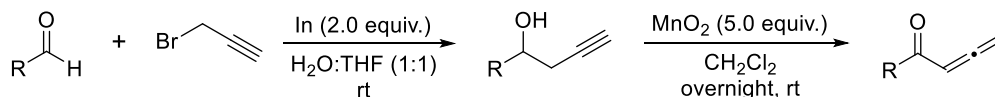
### General Procedure 1b



To a solution of propargyl bromide (20.0 mmol, 2.0 equiv.) and In powder (20.0 mmol, 2.0 equiv.) in H<sub>2</sub>O/THF (1:1, 20 mL), was added the aldehyde (10.0 mmol, 1.0 equiv.) and stirred overnight at room temperature. After the completion of the reaction (i.e. monitored by TLC), conc. HCl was added dropwise to quench the mixture (until a clear solution was obtained), followed by extraction with CH<sub>2</sub>Cl<sub>2</sub> (3x30 mL). The combined organic layers were washed with brine (30 mL) and dried over Na<sub>2</sub>SO<sub>4</sub>. The volatiles were evaporated under reduced pressure and the crude product was purified by flash column chromatography (silica gel, *n*-hexane/EtOAc) to afford the corresponding propargylic alcohol.

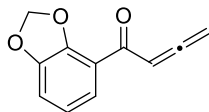
A solution of propargylic alcohol (1.0 equiv.) in MeCN (20 mL) was added dropwise to a solution of H<sub>5</sub>IO<sub>6</sub> (1.05 equiv.) at 0 °C. Subsequently, PDC (0.02 equiv.) was added portionwise to the reaction mixture. The mixture was allowed to warm to ambient conditions and stirred overnight until the completion of the reaction (i.e. monitored by TLC). The mixture was diluted with EtOAc (100 mL) and the mixture was washed with brine:H<sub>2</sub>O (1:1, 50 mL), saturated Na<sub>2</sub>S<sub>2</sub>O<sub>3</sub> (50 mL), brine (50 mL) and dried over Na<sub>2</sub>SO<sub>4</sub>. The volatiles were evaporated under reduced pressure and the crude product was purified by flash column chromatography to afford the corresponding ketone allenenes **1**.

### General Procedure 1c



To a solution of propargyl bromide (20.0 mmol, 2.0 equiv.) and In powder (20.0 mmol, 2.0 equiv.) in H<sub>2</sub>O/THF (1:1, 20 mL), was added the aldehyde (10.0 mmol, 1.0 equiv.) and stirred overnight at room temperature. After the completion of the reaction (i.e. monitored by TLC), conc. HCl was added dropwise to quench the mixture (until a clear solution was obtained), followed by extraction with CH<sub>2</sub>Cl<sub>2</sub> (3x30 mL). The combined organic layers were washed with brine (30 mL) and dried over Na<sub>2</sub>SO<sub>4</sub>. The volatiles were evaporated under reduced pressure and the crude product was purified by flash column chromatography (silica gel, *n*-hexane/EtOAc) to afford the corresponding propargylic alcohol.

A solution of MnO<sub>2</sub> (5.0 equiv.) in CH<sub>2</sub>Cl<sub>2</sub> was added dropwise to a solution of propargylic alcohol (1.0 equiv.) in CH<sub>2</sub>Cl<sub>2</sub> (0.1 M) and the reaction mixture was stirred overnight at room temperature. The mixture was filtered through celite and the filter cake was washed repeatedly with CH<sub>2</sub>Cl<sub>2</sub>. The volatiles were evaporated under reduced pressure and the crude product was purified by flash column chromatography to afford the corresponding ketone allenenes **1**.

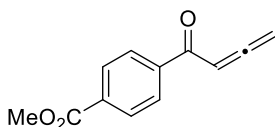


Following the general procedure 1a, **1y** was obtained as an orange solid (641.3 mg, 3.41 mmol, 34%). M.p. = 82 – 85 °C.

$^1\text{H NMR}$  (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.34 (d,  $J = 8.1$  Hz, 1H), 6.94 (d,  $J = 7.6$  Hz, 1H), 6.86 (t,  $J = 8.0$  Hz, 1H), 6.72 (t,  $J = 6.5$  Hz, 1H), 6.05 (s, 2H), 5.27 (d,  $J = 7.4$  Hz, 2H).

$^{13}\text{C NMR}$  (126 MHz,  $\text{CDCl}_3$ )  $\delta$  216.71, 187.22, 148.47, 147.27, 121.88, 121.52, 120.51, 112.40, 101.57, 94.68, 79.32.

HRMS (ESI):  $m/z$  calculated for  $\text{C}_{11}\text{H}_9\text{O}_3$   $[\text{M}+\text{H}]^+$ : 189.0552, found: 189.0552.

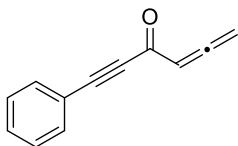


Following general procedure 1b, **1aa** was obtained as a reddish brown solid (1.08 g, 5.32 mmol, 53%). M.p. = 54 – 57 °C.

$^1\text{H NMR}$  (500 MHz,  $\text{CDCl}_3$ )  $\delta$  8.10 (d,  $J = 8.3$  Hz, 2H), 7.91 (d,  $J = 8.3$  Hz, 2H), 6.41 (t,  $J = 6.5$  Hz, 1H), 5.27 (d,  $J = 6.5$  Hz, 2H), 3.94 (s, 3H).

$^{13}\text{C NMR}$  (126 MHz,  $\text{CDCl}_3$ )  $\delta$  217.59, 190.88, 166.26, 140.89, 133.53, 129.57, 128.58, 93.66, 79.63, 52.45.

HRMS (ESI):  $m/z$  calculated for  $\text{C}_{12}\text{H}_{11}\text{O}_3$   $[\text{M}+\text{H}]^+$ : 203.0708, found: 203.0708.



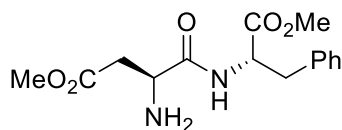
Following general procedure 1c, **1ad** was obtained as an orange oil (137 mg, 0.81 mmol, 8%).

$^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.56 – 7.51 (m, 2H), 7.42 (dd,  $J = 8.6, 6.3$  Hz, 1H), 7.35 (t,  $J = 7.4$  Hz, 2H), 5.99 (t,  $J = 6.3$  Hz, 1H), 5.40 (d,  $J = 6.3$  Hz, 2H).

$^{13}\text{C NMR}$  (101 MHz,  $\text{CDCl}_3$ )  $\delta$  218.90, 177.01, 133.05, 130.73, 128.63, 120.06, 99.06, 91.48, 86.43, 80.42.

HRMS (ESI):  $m/z$  calculated for  $\text{C}_{12}\text{H}_9\text{O}$   $[\text{M}+\text{H}]^+$ : 169.0653, found: 169.0653.

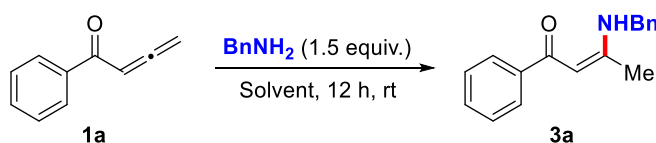
## II-2. Preparation of Asp-Phe dipeptide methyl ester<sup>2</sup>



The following Asp-Phe dipeptide methyl ester was synthesized from reported protocols.<sup>2</sup> The obtained dipeptide was neutralized with sat. Na<sub>2</sub>CO<sub>3</sub> to remove the HCl salt before use for reaction.

## III. Optimization Study

Table 1: Screening of solvents<sup>a</sup>

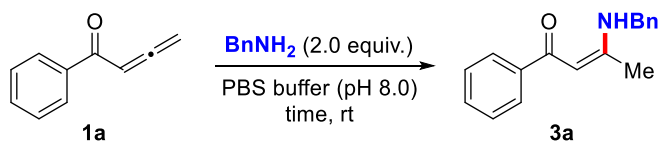


Entry	Solvent	Conversion (%) <sup>b</sup>	Yield (%) <sup>b</sup>
1	PhCF <sub>3</sub>	100	82
2	<i>p</i> -xylene	100	62
3	Et <sub>2</sub> O	100	70
4	MTBE	100	79
5	EtOH	100	67
6	<i>i</i> -PrOH	100	71
7	EtOAc	100	80
8	CH <sub>3</sub> CN	100	75
9	DMSO	100	71
10	H <sub>2</sub> O	100	35
11	H <sub>2</sub> O:EtOH (1:1)	100	50
12	H <sub>2</sub> O:CH <sub>3</sub> CN (1:1)	100	53
13	PBS buffer (pH 7)	100	51
14	PBS buffer (pH 8)	100	55
15	PBS buffer (pH 9)	100	52
16 <sup>c</sup>	PBS buffer (pH 8)	100	58
17 <sup>d</sup>	PBS buffer (pH 8)	100	57
18 <sup>e</sup>	PBS buffer (pH 8)	100	59

<sup>a</sup> Reaction Scale: **1a** (0.20 mmol) and BnNH<sub>2</sub> (0.30 mmol) in the specified solvent (2 mL) was stirred at room temperature overnight. <sup>b</sup> Conversion and yields were determined by <sup>1</sup>H NMR using CH<sub>2</sub>I<sub>2</sub> as the internal standard. <sup>c</sup> 1.0 equiv. of BnNH<sub>2</sub> was used. <sup>d</sup> 1.2 equiv. of BnNH<sub>2</sub> was used. <sup>e</sup> 2.0 equiv. of BnNH<sub>2</sub> was used.

<sup>2</sup> Ichitsuka, T.; Komatsuzaki, S.; Masuda, K.; Koumura, N.; Sato, K.; Kobayashi, S. Stereoretentive *N*-Arylation of Amino Acid Esters with Cyclohexanones Utilizing a Continuous-Flow System. *Chem. Eur. J.* **2021**, *27*, 10844.

**Table 2: Kinetics study of the reaction <sup>a</sup>**



Entry	Duration (mins)	Conversion (%) <sup>b</sup>	Yield (%) <sup>b</sup>
1	10	100	66
2	20	100	65
3	30	100	65
<b>4</b>	<b>40</b>	<b>100</b>	<b>81(70)<sup>c</sup></b>
5	50	100	77
6	60	100	79

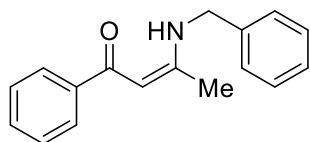
<sup>a</sup> Reaction Scale: **1a** (0.20 mmol) and BnNH<sub>2</sub> (0.40 mmol) in PBS buffer (pH 8.0) (2 mL) was stirred at room temperature at the specified duration. <sup>b</sup> Conversion and yields were determined by <sup>1</sup>H NMR using CH<sub>2</sub>I<sub>2</sub> as the internal standard. <sup>c</sup> Isolated yield.

#### IV. Experimental procedure for the water-based amination of allenic carbonyls & spectroscopic data of compounds obtained in this study

##### IV-1. General procedure for amination of **1a** with amines (Scheme 1)

An 8 mL vial was charged with allenic ketone **1a** (0.20 mmol, 1.0 equiv.), amine **2** (0.40 mmol, 2.0 equiv.) and PBS buffer (pH 8.0) (2 mL) under ambient conditions. The reaction was stirred at 25 °C for 40 mins and the mixture was diluted with CH<sub>2</sub>Cl<sub>2</sub> (5 mL) and the layers were separated. The aqueous layer was extracted with CH<sub>2</sub>Cl<sub>2</sub> (2 x 20 mL) and the combined organic layers were dried over Na<sub>2</sub>SO<sub>4</sub> and evaporated under reduced pressure. The crude product was purified by flash column chromatography (*n*-hexane/EtOAc) to afford the corresponding enaminone **3**. Unless otherwise stated, all products obtained have a *Z/E* ratio of >99:1.

##### (*Z*)-3-(benzylamino)-1-phenylbut-2-en-1-one



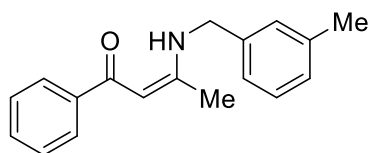
Following the general procedure, **3a** was obtained as a brown solid (34.5 mg, 0.137 mmol, 70%). M.p. = 58 – 59 °C.

<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.90 – 7.85 (m, 2H), 7.43 – 7.33 (m, 5H), 7.29 (dd, *J* = 15.8, 7.4 Hz, 3H), 5.75 (s, 1H), 4.55 (d, *J* = 6.3 Hz, 2H), 2.07 (s, 3H).

<sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 188.14, 164.91, 140.31, 137.76, 130.57, 128.91, 128.19, 127.57, 126.97, 126.90, 92.65, 47.07, 19.54.

HRMS (ESI): *m/z* calculated for C<sub>17</sub>H<sub>18</sub>NO [M+H]<sup>+</sup>: 252.1388, found: 252.1388.

**(Z)-3-((3-methylbenzyl)amino)-1-phenylbut-2-en-1-one**



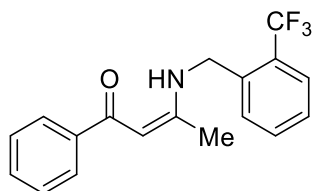
Following the general procedure, **3b** was obtained as an orange oil (45.4 mg, 0.171 mmol, 87%).

$^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.90 – 7.85 (m, 2H), 7.43 – 7.36 (m, 3H), 7.23 (dd,  $J$  = 10.3, 5.0 Hz, 1H), 7.12 – 7.06 (m, 3H), 5.74 (s, 1H), 4.49 (d,  $J$  = 6.3 Hz, 2H), 2.34 (s, 3H), 2.06 (s, 3H).

$^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  188.05, 164.95, 140.36, 138.62, 137.68, 130.55, 128.80, 128.34, 128.19, 127.67, 126.97, 124.02, 92.59, 47.07, 21.45, 19.56.

HRMS (ESI):  $m/z$  calculated for  $\text{C}_{18}\text{H}_{20}\text{NO}$   $[\text{M}+\text{H}]^+$ : 266.1545, found: 266.1536.

**(Z)-1-phenyl-3-((2-(trifluoromethyl)benzyl)amino)but-2-en-1-one**



Following the general procedure, **3c** was obtained as a brown solid (54.7 mg, 0.171 mmol, 85%). M.p. = 93 – 94 °C.

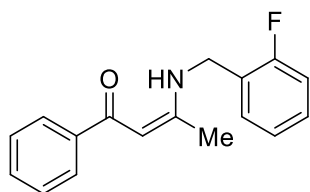
$^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.89 (dd,  $J$  = 7.9, 1.4 Hz, 2H), 7.68 (d,  $J$  = 7.8 Hz, 1H), 7.55 (dd,  $J$  = 10.7, 7.4 Hz, 2H), 7.47 – 7.36 (m, 4H), 5.81 (s, 1H), 4.74 (d,  $J$  = 6.5 Hz, 2H), 2.04 (s, 3H).

$^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  188.55, 164.84, 140.10, 136.64, 132.61, 130.76, 128.24, 128.08, 127.53, 127.03, 126.19, 126.14, 93.13, 43.33, 19.26.

$^{19}\text{F}\{^1\text{H}\}$  NMR (376 MHz,  $\text{CDCl}_3$ )  $\delta$  -60.48.

HRMS (ESI):  $m/z$  calculated for  $\text{C}_{18}\text{H}_{17}\text{F}_3\text{NO}$   $[\text{M}+\text{H}]^+$ : 320.1262, found: 320.1263.

**(Z)-3-((2-fluorobenzyl)amino)-1-phenylbut-2-en-1-one**



Following the general procedure, **3d** was obtained as an orange oil (42.7 mg, 0.159 mmol, 80%).

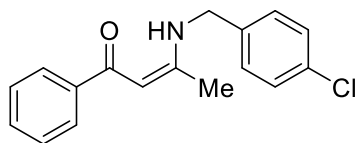
$^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.87 (d,  $J = 7.7$  Hz, 2H), 7.43 – 7.37 (m, 3H), 7.34 (t,  $J = 7.6$  Hz, 1H), 7.26 (m, 1H), 7.12-7.15 (m, 1H), 7.08 – 7.04 (m, 1H), 5.76 (s, 1H), 4.58 (d,  $J = 6.3$  Hz, 2H), 2.09 (s, 3H).

$^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  188.27, 164.80, 160.35 (d,  $J = 246.4$  Hz, 1H), 140.21, 130.64, 129.37 (d,  $J = 8.1$  Hz, 3H), 128.86 (d,  $J = 4.0$  Hz, 3H), 128.20, 126.99, 124.92 (d,  $J = 14.7$  Hz, 2H), 124.61 (d,  $J = 3.6$  Hz, 3H), 115.49 (d,  $J = 21.2$  Hz, 3H), 92.85, 40.76 (d,  $J = 4.7$  Hz, 3H), 19.35.

$^{19}\text{F}\{^1\text{H}\}$  NMR (376 MHz,  $\text{CDCl}_3$ )  $\delta$  -118.63.

HRMS (ESI):  $m/z$  calculated for  $\text{C}_{17}\text{H}_{17}\text{FNO}$   $[\text{M}+\text{H}]^+$ : 270.1294, found: 270.1294.

### (Z)-3-((4-chlorobenzyl)amino)-1-phenylbut-2-en-1-one



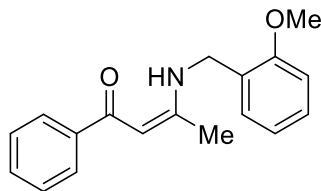
Following the general procedure, **3e** was obtained as an orange solid (40.3 mg, 0.141 mmol, 71%). M.p. = 123 – 125 °C.

$^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.87 (dd,  $J = 8.0, 1.5$  Hz, 2H), 7.44 – 7.37 (m, 3H), 7.32 (d,  $J = 8.4$  Hz, 2H), 7.23 (d,  $J = 8.4$  Hz, 2H), 5.76 (s, 1H), 4.50 (d,  $J = 6.3$  Hz, 2H), 2.05 (s, 3H).

$^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  188.35, 164.71, 140.15, 136.35, 133.39, 130.69, 129.06, 128.23, 126.98, 92.87, 46.38, 19.48.

HRMS (ESI):  $m/z$  calculated for  $\text{C}_{17}\text{H}_{17}\text{ClNO}$   $[\text{M}+\text{H}]^+$ : 286.0999, found: 286.0998.

### (Z)-3-((2-methoxybenzyl)amino)-1-phenylbut-2-en-1-one



Following the general procedure, **3f** was obtained as a beige solid (43.5 mg, 0.155 mmol, 79%). M.p. = 114 – 115 °C.

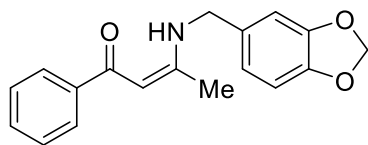
$^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.86 (dd,  $J = 7.8, 1.7$  Hz, 2H), 7.42 – 7.36 (m, 3H), 7.26 (m, 2H), 6.94 (t,  $J = 7.4$  Hz, 1H), 6.89 (d,  $J = 8.1$  Hz, 1H), 5.71 (s, 1H), 4.53 (d,  $J = 6.5$  Hz, 2H), 3.88 (s, 3H), 2.10 (s, 3H).

$^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  187.82, 164.97, 156.98, 140.56, 130.38, 128.80, 128.14, 128.10, 126.93, 126.00, 120.72, 110.35, 92.43, 55.39, 42.46, 19.39.

HRMS (ESI):  $m/z$  calculated for  $\text{C}_{18}\text{H}_{20}\text{NO}_2$   $[\text{M}+\text{H}]^+$ : 266.1545, found: 266.1545.



**(Z)-3-((benzo[d][1,3]dioxol-5-ylmethyl)amino)-1-phenylbut-2-en-1-one**



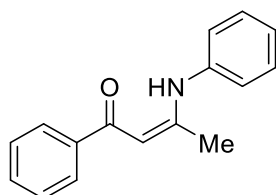
Following the general procedure, **3g** was obtained as an orange oil (32.7 mg, 0.111 mmol, 56%).

$^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.87 (dd,  $J = 8.0, 1.6$  Hz, 2H), 7.44 – 7.36 (m, 3H), 6.77 (dd,  $J = 7.4, 4.5$  Hz, 3H), 5.95 (s, 2H), 5.74 (s, 1H), 4.43 (d,  $J = 6.2$  Hz, 2H), 2.07 (s, 3H).

$^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  188.11, 164.74, 148.17, 147.09, 140.28, 131.55, 130.57, 128.18, 126.95, 120.26, 108.50, 107.62, 101.15, 92.64, 46.91, 19.52.

HRMS (ESI):  $m/z$  calculated for  $\text{C}_{18}\text{H}_{18}\text{NO}_3$   $[\text{M}+\text{H}]^+$ : 296.1287, found: 296.1286.

**(Z)-1-phenyl-3-(phenylamino)but-2-en-1-one**



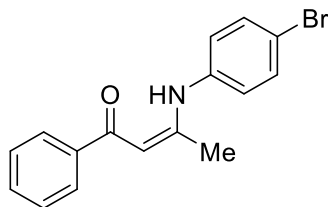
Following the general procedure, **3h** was obtained as a beige flaky solid (40.9 mg, 0.172 mmol, 86%). M.p. = 108 – 110 °C.

$^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.92 (d,  $J = 6.7$  Hz, 2H), 7.46 – 7.41 (m, 3H), 7.37 (m, 2H), 7.24 – 7.16 (m, 3H), 5.91 (s, 1H), 2.14 (s, 3H).

$^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  188.72, 162.24, 140.04, 138.68, 130.91, 129.18, 128.30, 127.09, 125.80, 124.81, 94.28, 20.45.

HRMS (ESI):  $m/z$  calculated for  $\text{C}_{16}\text{H}_{16}\text{NO}$   $[\text{M}+\text{H}]^+$ : 238.1232, found: 238.1232.

**(Z)-3-((4-bromophenyl)amino)-1-phenylbut-2-en-1-one**



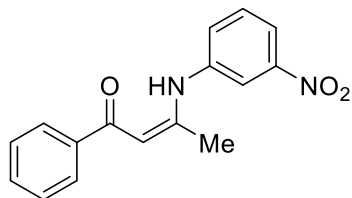
Following the general procedure, **3i** was obtained as a yellowish powder (53.6 mg, 0.170 mmol, 84%). M.p. = 125 – 126 °C.

$^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.91 (d,  $J = 7.4$  Hz, 2H), 7.50 – 7.41 (m, 5H), 7.06 (d,  $J = 7.7$  Hz, 2H), 5.91 (s, 1H), 2.14 (s, 3H).

$^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  189.05, 161.59, 139.79, 137.84, 132.30, 131.12, 128.35, 127.11, 126.21, 119.00, 94.82, 20.42.

HRMS (ESI):  $m/z$  calculated for  $\text{C}_{16}\text{H}_{15}\text{BrNO}$   $[\text{M}+\text{H}]^+$ : 316.0337, found: 316.0337.

### (Z)-3-((3-nitrophenyl)amino)-1-phenylbut-2-en-1-one



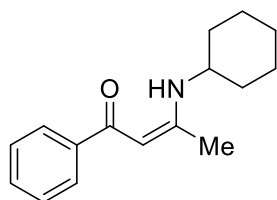
Following the general procedure, **3j** was obtained as an orange powder (40.1 mg, 0.142 mmol, 71%). M.p. = 110 – 111 °C.

$^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  8.04 (d,  $J$  = 9.3 Hz, 2H), 7.92 (d,  $J$  = 7.3 Hz, 2H), 7.56 – 7.52 (m, 1H), 7.50 – 7.42 (m, 4H), 6.00 (s, 1H), 2.25 (s, 3H).

$^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  189.71, 160.45, 148.79, 140.25, 139.40, 131.48, 130.10, 129.75, 128.44, 127.22, 119.81, 118.49, 96.09, 20.62.

HRMS (ESI):  $m/z$  calculated for  $\text{C}_{16}\text{H}_{15}\text{N}_2\text{O}_3$   $[\text{M}+\text{H}]^+$ : 283.1083, found: 283.1083.

### (Z)-3-(cyclohexylamino)-1-phenylbut-2-en-1-one



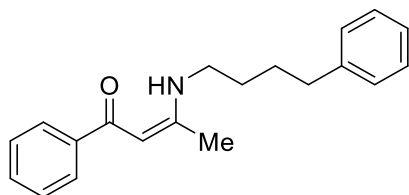
Following the general procedure, **3k** was obtained as a brown oil (28.0 mg, 0.115 mmol, 58%).

$^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  11.58 (s, 1H), 7.85 (dd,  $J$  = 7.6, 2.0 Hz, 2H), 7.41 – 7.36 (m, 3H), 5.62 (s, 1H), 3.50 – 3.42 (m, 1H), 2.09 (s, 3H), 1.97 – 1.90 (m, 2H), 1.84 – 1.77 (m, 2H), 1.47 – 1.24 (m, 6H).

$^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  187.30, 163.60, 140.56, 130.28, 128.11, 126.84, 91.82, 51.93, 33.83, 25.34, 24.52, 19.19.

HRMS (ESI):  $m/z$  calculated for  $\text{C}_{16}\text{H}_{22}\text{NO}$   $[\text{M}+\text{H}]^+$ : 244.1701, found: 244.1701.

**(Z)-1-phenyl-3-((4-phenylbutyl)amino)but-2-en-1-one**



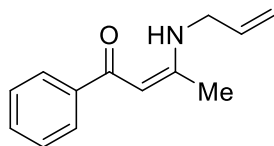
Following the general procedure, **3l** was obtained as a brown oil (33.7 mg, 0.115 mmol, 57%).

$^1\text{H NMR}$  (500 MHz,  $\text{CDCl}_3$ )  $\delta$  11.45 (s, 1H), 7.85 (dd,  $J = 7.8, 1.8$  Hz, 2H), 7.42 – 7.36 (m, 3H), 7.29 – 7.25 (m, 2H), 7.20 – 7.16 (m, 3H), 5.65 (s, 1H), 3.31 (q, 2H), 2.66 (t,  $J = 7.4$  Hz, 2H), 2.04 (s, 3H), 1.79 – 1.72 (m, 2H), 1.72 – 1.65 (m, 2H).

$^{13}\text{C NMR}$  (126 MHz,  $\text{CDCl}_3$ )  $\delta$  187.61, 164.87, 141.81, 140.50, 130.38, 128.44, 128.40, 128.15, 126.87, 125.92, 92.00, 43.24, 35.51, 29.64, 28.58, 19.42.

HRMS (ESI):  $m/z$  calculated for  $\text{C}_{20}\text{H}_{24}\text{NO}$   $[\text{M}+\text{H}]^+$ : 294.1858, found: 294.1858.

**(Z)-3-(allylamino)-1-phenylbut-2-en-1-one**



Following the general procedure, **3m** was obtained as a yellowish oil (30.4 mg, 0.151 mmol, 76%).

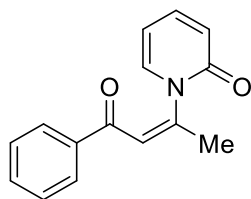
$^1\text{H NMR}$  (500 MHz,  $\text{CDCl}_3$ )  $\delta$  11.47 (s, 1H), 7.86 (d,  $J = 6.3$  Hz, 2H), 7.44 – 7.39 (m, 3H), 5.97 – 5.86 (m, 1H), 5.71 (s, 1H), 5.29 (dd,  $J = 18.3$  Hz, 1H), 5.21 (dd,  $J = 10.3$  Hz, 1H), 4.00 – 3.93 (m, 2H), 2.07 (s, 3H).

$^4\text{H NMR}$  (500 MHz,  $\text{CDCl}_3$ )  $\delta$  11.47 (s, 1H), 7.86 (d,  $J = 6.3$  Hz, 2H), 7.40 (d,  $J = 7.3$  Hz, 3H), 5.91 (ddd,  $J = 17.2, 10.2, 5.1$  Hz, 1H), 5.71 (s, 1H), 5.29 (d,  $J = 18.3$  Hz, 1H), 5.21 (d,  $J = 10.3$  Hz, 1H), 4.00 – 3.93 (m, 2H), 2.07 (s, 3H).

$^{13}\text{C NMR}$  (126 MHz,  $\text{CDCl}_3$ )  $\delta$  188.00, 165.02, 140.37, 133.75, 130.50, 128.17, 126.93, 116.56, 92.44, 45.43, 19.19.

HRMS (ESI):  $m/z$  calculated for  $\text{C}_{13}\text{H}_{16}\text{NO}$   $[\text{M}+\text{H}]^+$ : 202.1232, found: 202.1232.

**(Z)-1-(4-oxo-4-phenylbut-2-en-2-yl)pyridin-2(1H)-one**



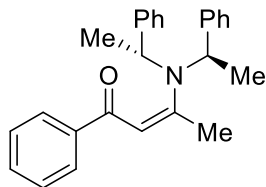
Following the general procedure, **3n** was obtained as a brown oil (36.5 mg, 0.153 mmol, 76%).

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.37 (dd,  $J = 4.9, 1.4$  Hz, 1H), 7.83 – 7.75 (m, 3H), 7.48 (t,  $J = 7.3$  Hz, 1H), 7.40 (t,  $J = 7.5$  Hz, 2H), 7.20 – 7.13 (m, 1H), 7.01 (d,  $J = 8.2$  Hz, 1H), 6.46 (s, 1H), 2.57 (s, 3H).

$^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  190.47, 170.16, 160.93, 148.46, 139.97, 139.56, 132.22, 128.40, 127.84, 120.66, 114.37, 106.11, 19.22.

HRMS (ESI):  $m/z$  calculated for  $\text{C}_{15}\text{H}_{14}\text{NO}_2$   $[\text{M}+\text{H}]^+$ : 240.1025, found: 240.1024.

**(Z)-3-(bis((R)-1-phenylethyl)amino)-1-phenylbut-2-en-1-one**



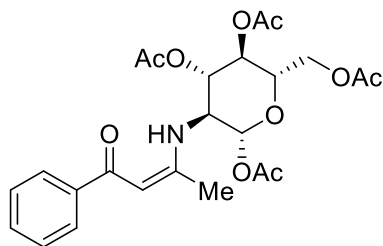
Following the general procedure, **3o** was obtained as an orange solid (54.2 mg, 0.147 mmol, 72%). M.p. = 90 – 93 °C.  $[\alpha]_D^{22} = +75.4^\circ$  ( $c = 1.0$ ,  $\text{CHCl}_3$ ).

$^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.28 – 7.24 (m, 5H), 7.23 – 7.15 (m, 10H), 5.54 (s, 1H), 5.23 (s, 2H), 2.88 (s, 3H), 1.80 (s, 3H), 1.78 (s, 3H).

$^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  188.30, 159.55, 142.82, 140.08, 130.21, 128.52, 127.77, 127.38, 127.25, 127.12, 98.81, 54.84, 17.91, 17.64.

HRMS (ESI):  $m/z$  calculated for  $\text{C}_{26}\text{H}_{28}\text{NO}$   $[\text{M}+\text{H}]^+$ : 370.2171, found: 370.2171.

**(2S,3R,4R,5S)-6-(acetoxymethyl)-3-(((Z)-4-oxo-4-phenylbut-2-en-2-yl)amino)tetrahydro-2H-pyran-2,4,5-triyl triacetate**



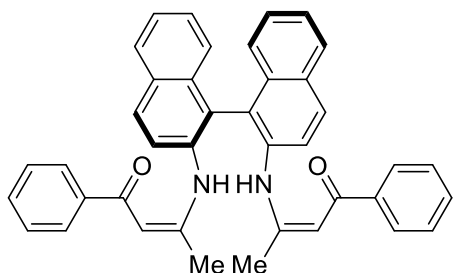
Following the general procedure, **3p** was obtained as a brown solid (72.6 mg, 0.148 mmol, 73%). M.p. = 145 – 147 °C.  $[\alpha]_D^{22} = +158.0^\circ$  ( $c = 1.0$ ,  $\text{CHCl}_3$ ).

$^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  11.32 (d,  $J = 10.6$  Hz, 1H), 7.84 (d,  $J = 6.8$  Hz, 2H), 7.40 (dt,  $J = 14.6, 7.0$  Hz, 3H), 5.71 (s, 1H), 5.68 (d,  $J = 8.6$  Hz, 1H), 5.31 – 5.21 (m, 1H), 5.11 (t,  $J = 9.5$  Hz, 1H), 4.37 (dd,  $J = 12.5, 4.5$  Hz, 1H), 4.11 (d,  $J = 12.6$  Hz, 1H), 3.87 (m, 2H), 2.13 (s, 3H), 2.08 (s, 6H), 2.04 (s, 3H), 1.98 (s, 3H).

$^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  188.88, 170.55, 169.77, 169.44, 168.37, 163.51, 139.56, 131.02, 128.21, 127.14, 93.99, 93.34, 73.42, 72.79, 67.98, 61.57, 56.58, 20.77, 20.70, 20.61, 20.46, 19.92.

HRMS (ESI):  $m/z$  calculated for  $\text{C}_{24}\text{H}_{30}\text{NO}_{10}$   $[\text{M}+\text{H}]^+$ : 492.1870, found: 492.1870.

**(2Z,2'Z)-3,3'-(((S)-[1,1'-binaphthalene]-2,2'-diyl)bis(azanediyl))bis(1-phenylbut-2-en-1-one)**



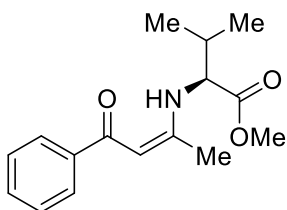
Following the general procedure, **3q** was obtained as a brown oil (74.0 mg, 0.129 mmol, 64%).  $[\alpha]_D^{22} = +384.8^\circ$  ( $c = 1.3$ ,  $\text{CHCl}_3$ ).

$^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  12.59 (s, 2H), 7.98 (dd,  $J = 13.6, 8.5$  Hz, 4H), 7.69 – 7.63 (m, 4H), 7.53 – 7.45 (m, 4H), 7.40 – 7.29 (m, 8H), 7.17 (d,  $J = 8.4$  Hz, 2H), 5.71 (s, 2H), 2.15 (s, 6H).

$^{13}\text{C NMR}$  (101 MHz,  $\text{CDCl}_3$ )  $\delta$  188.18, 161.50, 140.05, 135.69, 133.58, 131.67, 130.62, 129.27, 128.38, 128.07, 127.28, 126.94, 126.90, 125.85, 125.79, 124.35, 94.83, 20.68.

HRMS (ESI):  $m/z$  calculated for  $\text{C}_{40}\text{H}_{33}\text{N}_2\text{O}_2$   $[\text{M}+\text{H}]^+$ : 573.2524, found: 573.2524.

**Methyl (Z)-(4-oxo-4-phenylbut-2-en-2-yl)-L-valinate**



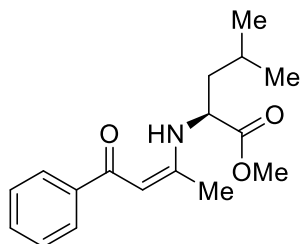
Following the general procedure, **3r** was obtained as a brown oil (38.3 mg, 0.139 mmol, 71%).  $[\alpha]_D^{22} = +115.5^\circ$  ( $c = 1.0$ ,  $\text{CHCl}_3$ ).

$^1\text{H NMR}$  (500 MHz,  $\text{CDCl}_3$ )  $\delta$  11.68 (d,  $J = 9.1$  Hz, 1H), 7.87 (dd,  $J = 8.0, 1.5$  Hz, 2H), 7.43 – 7.36 (m, 3H), 5.73 (s, 1H), 4.04 (dd,  $J = 9.5, 5.8$  Hz, 1H), 3.76 (s, 3H), 2.29 (dq,  $J = 13.5, 6.8$  Hz, 1H), 2.02 (s, 3H), 1.08 (d,  $J = 6.9$  Hz, 3H), 1.04 (d,  $J = 6.8$  Hz, 3H).

$^{13}\text{C NMR}$  (101 MHz,  $\text{CDCl}_3$ )  $\delta$  188.54, 171.59, 163.70, 140.13, 130.66, 128.15, 127.05, 93.26, 62.18, 52.34, 31.76, 19.59, 19.23, 18.01.

HRMS (ESI):  $m/z$  calculated for  $\text{C}_{16}\text{H}_{22}\text{NO}_3$   $[\text{M}+\text{H}]^+$ : 276.1600, found: 276.1608.

### Methyl (Z)-(4-oxo-4-phenylbut-2-en-2-yl)-L-leucinate



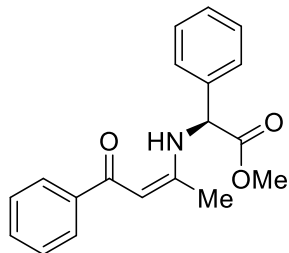
Following the general procedure, **3s** was obtained as a brown oil (44.0 mg, 0.152 mmol, 76%).  $[\alpha]_D^{22} = +104.7^\circ$  ( $c = 1.0$ ,  $\text{CHCl}_3$ ).

$^1\text{H NMR}$  (500 MHz,  $\text{CDCl}_3$ )  $\delta$  11.46 (d,  $J = 8.5$  Hz, 1H), 7.86 (dd,  $J = 8.1, 1.5$  Hz, 2H), 7.42 – 7.36 (m, 3H), 5.73 (s, 1H), 4.23 (td,  $J = 8.6, 5.8$  Hz, 1H), 3.75 (s, 3H), 2.03 (s, 3H), 1.80 (m, 3H), 0.98 (d,  $J = 6.3$  Hz, 3H), 0.94 (d,  $J = 6.3$  Hz, 3H).

$^{13}\text{C NMR}$  (126 MHz,  $\text{CDCl}_3$ )  $\delta$  188.60, 172.50, 163.50, 140.10, 130.71, 128.17, 127.04, 93.24, 54.89, 52.53, 41.85, 24.68, 22.81, 21.76, 19.60.

HRMS (ESI):  $m/z$  calculated for  $\text{C}_{17}\text{H}_{24}\text{NO}_3$   $[\text{M}+\text{H}]^+$ : 290.1756, found: 290.1760.

### Methyl (S,Z)-2-((4-oxo-4-phenylbut-2-en-2-yl)amino)-2-phenylacetate



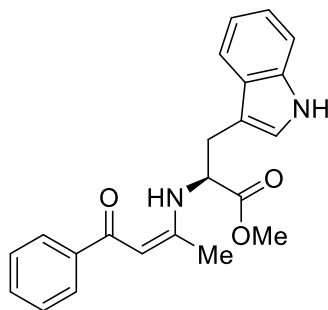
Following the general procedure, **3t** was obtained as an orange solid (50.6 mg, 0.164 mmol, 78%). M.p. = 105 – 108 °C.  $[\alpha]_D^{22} = -177.7^\circ$  ( $c = 1.0$ ,  $\text{CHCl}_3$ ).

$^1\text{H NMR}$  (500 MHz,  $\text{CDCl}_3$ )  $\delta$  12.19 (d,  $J = 7.4$  Hz, 1H), 7.91 (dd,  $J = 8.0, 1.4$  Hz, 2H), 7.48 – 7.32 (m, 8H), 5.79 (s, 1H), 5.32 (d,  $J = 7.8$  Hz, 1H), 3.77 (s, 3H), 1.95 (s, 3H).

$^{13}\text{C NMR}$  (126 MHz,  $\text{CDCl}_3$ )  $\delta$  188.86, 170.17, 162.52, 140.04, 136.77, 130.80, 129.18, 128.69, 128.19, 127.15, 126.96, 93.78, 60.47, 53.12, 19.78.

HRMS (ESI):  $m/z$  calculated for  $\text{C}_{19}\text{H}_{20}\text{NO}_3$   $[\text{M}+\text{H}]^+$ : 310.1443, found: 310.1444.

### Methyl (Z)-(4-oxo-4-phenylbut-2-en-2-yl)-L-tryptophanate



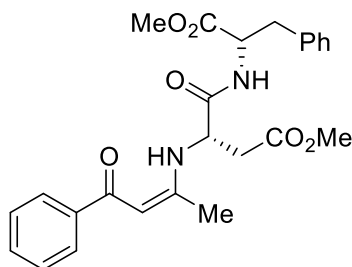
Following the general procedure, **3u** was obtained as a brown oil (55.4 mg, 0.153 mmol, 75%).  $[\alpha]_D^{22} = -190.5^\circ$  ( $c = 0.9$ ,  $\text{CHCl}_3$ ).

$^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  11.71 (d,  $J = 9.0$  Hz, 1H), 8.73 (s, 1H), 7.87 (d,  $J = 7.1$  Hz, 2H), 7.59 (d,  $J = 7.6$  Hz, 1H), 7.45 – 7.37 (m, 3H), 7.29 (d,  $J = 7.8$  Hz, 1H), 7.17 – 7.08 (m, 3H), 5.65 (s, 1H), 4.54 (td,  $J = 8.5, 4.7$  Hz, 1H), 3.70 (s, 3H), 3.42 (dd,  $J = 14.6, 4.5$  Hz, 1H), 3.27 (dd,  $J = 14.6, 8.1$  Hz, 1H), 1.78 (s, 3H).

$^{13}\text{C NMR}$  (101 MHz,  $\text{CDCl}_3$ )  $\delta$  188.65, 171.78, 163.77, 140.27, 136.29, 130.72, 128.24, 127.08, 126.99, 124.19, 121.97, 119.46, 118.15, 111.57, 109.24, 93.42, 57.18, 52.65, 29.76, 19.46.

HRMS (ESI):  $m/z$  calculated for  $\text{C}_{22}\text{H}_{23}\text{N}_2\text{O}_3$   $[\text{M}+\text{H}]^+$ : 363.1709, found: 363.1708.

### Methyl (S)-4-(((S)-1-methoxy-1-oxo-3-phenylpropan-2-yl)amino)-4-oxo-3-(((Z)-4-oxo-4-phenylbut-2-en-2-yl)amino)butanoate



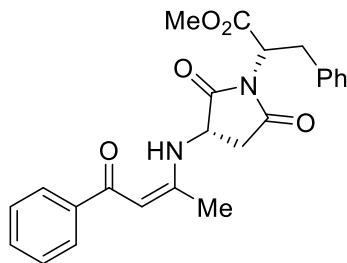
Following the general procedure, **3v** was obtained as a reddish-brown oil (63.5 mg, 0.140 mmol, 70%).  $[\alpha]_D^{22} = +87.2^\circ$  ( $c = 1.0$ ,  $\text{CHCl}_3$ ).

$^1\text{H NMR}$  (500 MHz,  $\text{CDCl}_3$ )  $\delta$  11.57 (d,  $J = 9.4$  Hz, 1H), 7.92 – 7.88 (m, 2H), 7.49 – 7.40 (m, 3H), 7.20 – 7.15 (m, 2H), 7.13 – 7.08 (m, 3H), 6.67 (d,  $J = 8.4$  Hz, 1H), 5.76 (s, 1H), 4.85 (dt,  $J = 8.4, 5.9$  Hz, 1H), 4.50 (ddd,  $J = 9.4, 7.7, 4.2$  Hz, 1H), 3.70 (s, 3H), 3.69 (s, 3H), 3.10 (m, 2H), 2.98 (dd,  $J = 17.1, 4.2$  Hz, 1H), 2.85 (dd,  $J = 17.1, 7.6$  Hz, 1H), 2.03 (s, 3H).

$^{13}\text{C NMR}$  (126 MHz,  $\text{CDCl}_3$ )  $\delta$  189.20, 171.42, 170.91, 170.15, 163.26, 139.68, 135.19, 131.13, 129.10, 128.89, 128.31, 127.24, 127.19, 94.41, 53.98, 52.91, 52.36, 52.22, 37.59, 37.14, 19.39.

HRMS (ESI):  $m/z$  calculated for  $\text{C}_{25}\text{H}_{29}\text{N}_2\text{O}_6$   $[\text{M}+\text{H}]^+$ : 453.2026, found: 453.2026.

**Methyl (S)-2-((S)-2,5-dioxo-3-(((Z)-4-oxo-4-phenylbut-2-en-2-yl)amino)pyrrolidin-1-yl)-3-phenylpropanoate**



Following the general procedure, **3v'** was obtained as a brown oil (18.5 mg, 0.153 mmol, 22%).  $[\alpha]_D^{22} = -102.4^\circ$  ( $c = 0.2$ ,  $\text{CHCl}_3$ ).

$^1\text{H NMR}$  (500 MHz,  $\text{CDCl}_3$ )  $\delta$  11.52 (d,  $J = 8.5$  Hz, 1H), 7.89 – 7.84 (m, 2H), 7.46 – 7.40 (m, 3H), 7.34 (t,  $J = 7.5$  Hz, 2H), 7.26 (s, 1H), 7.12 (d,  $J = 7.3$  Hz, 2H), 5.83 (s, 1H), 5.00 (dd,  $J = 11.6, 5.4$  Hz, 1H), 4.41 (td,  $J = 8.8, 6.3$  Hz, 1H), 3.81 (s, 3H), 3.49 (dd,  $J = 14.1, 5.3$  Hz, 1H), 3.40 (dd,  $J = 13.9, 11.8$  Hz, 1H), 3.08 (dd,  $J = 18.0, 9.1$  Hz, 1H), 2.52 (dd,  $J = 18.0, 6.2$  Hz, 1H), 2.15 (s, 3H).

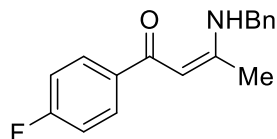
$^{13}\text{C NMR}$  (101 MHz,  $\text{CDCl}_3$ )  $\delta$  189.29, 174.32, 172.14, 168.31, 163.66, 139.66, 136.05, 131.10, 128.99, 128.89, 128.31, 127.09, 120.00, 94.55, 54.04, 53.04, 50.97, 36.00, 33.86, 19.85.

HRMS (ESI):  $m/z$  calculated for  $\text{C}_{24}\text{H}_{25}\text{N}_2\text{O}_5$   $[\text{M}+\text{H}]^+$ : 421.1763, found: 421.1764.

**IV-2. General procedure for various allenic ketones**

An 8 mL vial was charged with allenic ketone **1** (0.20 mmol, 1.0 equiv.), benzylamine **2a** (0.40 mmol, 2.0 equiv.) and PBS buffer (pH 8.0) (2 mL) under ambient conditions. The reaction was stirred at 25 °C for 40 mins and the mixture was diluted with  $\text{CH}_2\text{Cl}_2$  (5 mL) and the layers were separated. The aqueous layer was extracted with  $\text{CH}_2\text{Cl}_2$  (2 x 20 mL) and the combined organic layers were dried over  $\text{Na}_2\text{SO}_4$  and evaporated under reduced pressure. The crude product was purified by flash column chromatography ( $n$ -hexane/EtOAc) to afford the corresponding enaminone **3**. Unless otherwise stated, all products obtained have a  $Z/E$  ratio of >99:1.

**(Z)-3-(benzylamino)-1-(4-fluorophenyl)but-2-en-1-one**



Following the general procedure, **3w** was obtained as a brown oil (18.7 mg, 0.069 mmol, 31%).

$^1\text{H NMR}$  (500 MHz,  $\text{CDCl}_3$ )  $\delta$  11.70 (s, 1H), 7.91 – 7.85 (m, 2H), 7.38 – 7.34 (m, 2H), 7.33 – 7.27 (m, 3H), 7.07 (t,  $J = 8.8$  Hz, 2H), 5.69 (s, 1H), 4.55 (d,  $J = 6.3$  Hz, 2H), 2.08 (s, 3H).

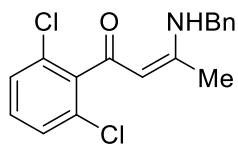
$^{13}\text{C NMR}$  (126 MHz,  $\text{CDCl}_3$ )  $\delta$  186.69, 165.08, 137.66, 136.51, 129.19, 129.12, 128.93, 127.61, 126.89, 115.15, 114.98, 92.28, 47.08, 19.55.

$^{19}\text{F}\{^1\text{H}\}$  NMR (376 MHz,  $\text{CDCl}_3$ )  $\delta$  -110.23.

HRMS (ESI):  $m/z$  calculated for  $\text{C}_{17}\text{H}_{17}\text{FNO}$   $[\text{M}+\text{H}]^+$ : 270.1294, found: 270.1294.



**(Z)-3-(benzylamino)-1-(2,6-dichlorophenyl)but-2-en-1-one**



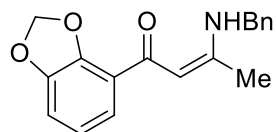
Following the general procedure, **3x** was obtained as a brown oil (39.8 mg, 0.124 mmol, 63%).

$^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  11.39 (s, 1H), 7.38 (t,  $J = 7.7$  Hz, 2H), 7.34 – 7.27 (m, 5H), 7.16 (t,  $J = 8.0$  Hz, 1H), 5.16 (s, 1H), 4.57 (d,  $J = 6.3$  Hz, 2H), 2.03 (s, 3H).

$^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  186.78, 165.88, 140.72, 137.28, 131.83, 129.24, 128.95, 127.94, 127.67, 126.86, 97.08, 47.18, 19.31.

HRMS (ESI):  $m/z$  calculated for  $\text{C}_{17}\text{H}_{16}\text{Cl}_2\text{NO}$   $[\text{M}+\text{H}]^+$ : 320.0609, found: 320.0609.

**(Z)-1-(benzo[*d*][1,3]dioxol-4-yl)-3-(benzylamino)but-2-en-1-one**



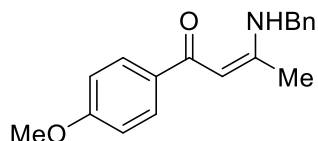
Following the general procedure, **3y** was obtained as an orange oil (40.5 mg, 0.137 mmol, 69%).

$^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  11.81 (s, 1H), 7.40 (dd,  $J = 5.5, 3.9$  Hz, 1H), 7.37 – 7.33 (m, 2H), 7.31 – 7.27 (m, 3H), 6.87 (s, 1H), 6.86 (d,  $J = 1.8$  Hz, 1H), 6.04 (s, 2H), 5.91 (s, 1H), 4.54 (d,  $J = 6.3$  Hz, 2H), 2.07 (s, 3H).

$^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  184.11, 165.38, 148.00, 145.71, 137.61, 128.89, 127.58, 126.95, 123.03, 121.29, 121.24, 110.30, 100.98, 95.78, 47.13, 19.53.

HRMS (ESI):  $m/z$  calculated for  $\text{C}_{18}\text{H}_{18}\text{NO}_3$   $[\text{M}+\text{H}]^+$ : 296.1287, found: 296.1287.

**(Z)-3-(benzylamino)-1-(4-methoxyphenyl)but-2-en-1-one**



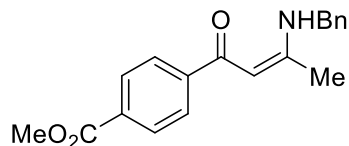
Following the general procedure, **3z** was obtained as a yellowish powder (32.0 mg, 0.114 mmol, 51%).  
M.p. = 92 – 93 °C.

$^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  11.65 (s, 1H), 7.86 (d,  $J = 9.0$  Hz, 2H), 7.38 – 7.25 (m, 5H), 6.90 (d,  $J = 9.0$  Hz, 2H), 5.71 (s, 1H), 5.29 (s, 1H), 4.52 (s, 2H), 3.84 (s, 3H), 2.05 (s, 3H).

$^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  187.38, 164.31, 161.69, 137.96, 132.97, 128.87, 128.80, 127.50, 126.89, 113.40, 92.10, 55.33, 53.45, 47.01, 19.56.

HRMS (ESI):  $m/z$  calculated for  $\text{C}_{18}\text{H}_{20}\text{NO}_2$   $[\text{M}+\text{H}]^+$ : 282.1494, found: 282.1494.

### Methyl (Z)-4-(3-(benzylamino)but-2-enoyl)benzoate



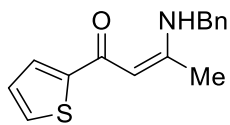
Following the general procedure, **3aa** was obtained as a brown solid (31.6 mg, 0.102 mmol, 51%). M.p. = 96 – 99 °C.

<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 11.84 (s, 1H), 8.06 (d, *J* = 8.5 Hz, 2H), 7.91 (d, *J* = 8.4 Hz, 2H), 7.36 (dd, *J* = 8.2, 6.7 Hz, 2H), 7.30 (dd, *J* = 7.8, 2.8 Hz, 3H), 5.75 (s, 1H), 4.55 (d, *J* = 6.3 Hz, 2H), 3.91 (s, 3H), 2.08 (s, 3H).

<sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 186.71, 166.79, 165.71, 144.25, 137.41, 131.59, 129.53, 128.96, 127.68, 126.91, 126.90, 93.04, 52.21, 47.16, 19.52.

HRMS (ESI): *m/z* calculated for C<sub>19</sub>H<sub>20</sub>NO<sub>3</sub> [M+H]<sup>+</sup>: 310.1443, found: 310.1443.

### (Z)-3-(benzylamino)-1-(thiophen-2-yl)but-2-en-1-one



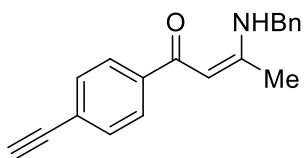
Following the general procedure, **3ab** was obtained as an orange oil (34.5 mg, 0.134 mmol, 67%).

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 11.38 (s, 1H), 7.55 (dd, *J* = 3.7, 1.0 Hz, 1H), 7.43 (dd, *J* = 5.0, 1.0 Hz, 1H), 7.38 – 7.32 (m, 2H), 7.29 (d, *J* = 7.3 Hz, 3H), 7.06 (dd, *J* = 4.9, 3.8 Hz, 1H), 5.63 (s, 1H), 4.52 (d, *J* = 6.3 Hz, 2H), 2.05 (s, 3H).

<sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>) δ 181.12, 164.62, 147.11, 137.64, 129.76, 128.90, 127.70, 127.59, 127.34, 126.93, 92.30, 47.12, 19.42.

HRMS (ESI): *m/z* calculated for C<sub>15</sub>H<sub>16</sub>NOS [M+H]<sup>+</sup>: 258.0953, found: 258.0952.

### (Z)-3-(benzylamino)-1-(4-ethynylphenyl)but-2-en-1-one



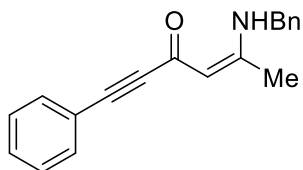
Following the general procedure, **3ac** was obtained as an orange solid (51.6 mg, 0.187 mmol, 90%). M.p. = 83 – 84 °C.

<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 11.79 (s, 1H), 7.83 (d, *J* = 8.4 Hz, 2H), 7.52 (d, *J* = 8.4 Hz, 2H), 7.39 – 7.34 (m, 2H), 7.32 – 7.27 (m, 3H), 5.73 (s, 1H), 4.55 (d, *J* = 6.3 Hz, 2H), 3.16 (s, 1H), 2.08 (s, 3H).

$^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  186.83, 165.34, 140.37, 137.55, 132.00, 128.94, 127.64, 126.90, 126.88, 124.14, 92.72, 83.47, 78.75, 47.13, 19.54.

HRMS (ESI):  $m/z$  calculated for  $\text{C}_{19}\text{H}_{18}\text{NO}$   $[\text{M}+\text{H}]^+$ : 276.1388, found: 276.1388.

**(Z)-5-(benzylamino)-1-phenylhex-4-en-1-yn-3-one**



Following the general procedure, **3ad** was obtained as a pale-orange solid (24.7 mg, 0.090 mmol, 45%).

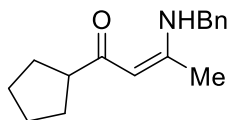
M.p. = 87 – 89 °C.

$^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  11.36 (s, 1H), 7.51 (d,  $J$  = 8.2 Hz, 2H), 7.36 – 7.27 (m, 6H), 7.24 (d,  $J$  = 6.8 Hz, 2H), 5.36 (s, 1H), 4.50 (d,  $J$  = 6.4 Hz, 2H), 1.97 (s, 3H).

$^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  172.82, 165.36, 137.26, 132.46, 129.34, 128.94, 128.37, 127.68, 126.72, 121.69, 99.83, 89.85, 86.18, 47.13, 18.93.

HRMS (ESI):  $m/z$  calculated for  $\text{C}_{19}\text{H}_{18}\text{NO}$   $[\text{M}+\text{H}]^+$ : 276.1388, found: 276.1388.

**(Z)-3-(benzylamino)-1-cyclopentylbut-2-en-1-one**



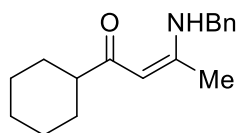
Following the general procedure, **3ae** was obtained as a yellowish solid (42.1 mg, 0.173 mmol, 91%). M.p. = 51 – 52 °C.

$^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  11.15 (s, 1H), 7.37 – 7.30 (m, 2H), 7.29 – 7.24 (m, 3H), 5.06 (s, 1H), 4.44 (d,  $J$  = 6.3 Hz, 2H), 2.68 (dd,  $J$  = 16.1, 8.0 Hz, 1H), 1.94 (s, 3H), 1.82 – 1.69 (m, 6H), 1.60 – 1.51 (m, 2H).

$^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  201.35, 162.99, 138.02, 128.81, 127.43, 126.93, 94.93, 50.71, 46.90, 30.53, 26.20, 19.11.

HRMS (ESI):  $m/z$  calculated for  $\text{C}_{16}\text{H}_{22}\text{NO}$   $[\text{M}+\text{H}]^+$ : 244.1701, found: 244.1701.

**(Z)-3-(benzylamino)-1-cyclohexylbut-2-en-1-one**



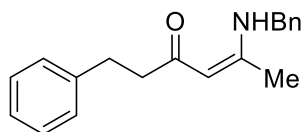
Following the general procedure, **3af** was obtained as a beige solid (45.4 mg, 0.176 mmol, 88%). M.p. = 82 – 85 °C.

<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 11.21 (s, 1H), 7.35 – 7.31 (m, 2H), 7.27 – 7.24 (m, 3H), 5.04 (s, 1H), 4.44 (d, *J* = 6.2 Hz, 2H), 2.17 – 2.11 (m, 1H), 1.94 (s, 3H), 1.82 – 1.75 (m, 4H), 1.68 – 1.63 (m, 1H), 1.42 – 1.34 (m, 2H), 1.28 – 1.18 (m, 3H).

<sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 201.78, 163.49, 137.99, 128.81, 127.43, 126.93, 94.06, 50.09, 46.90, 30.01, 26.18, 26.12, 19.15.

HRMS (ESI): *m/z* calculated for C<sub>17</sub>H<sub>24</sub>NO [M+H]<sup>+</sup>: 258.1858, found: 258.1858.

#### (Z)-5-(benzylamino)-1-phenylhex-4-en-3-one



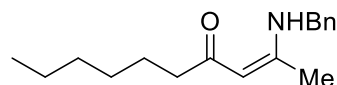
Following the general procedure, **3ag** was obtained as a beige powder (31.9 mg, 0.114 mmol, 58%). M.p. = 69 – 72 °C.

<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 11.21 (s, 1H), 7.35 (t, *J* = 7.4 Hz, 2H), 7.30 – 7.25 (m, 5H), 7.22 (d, *J* = 7.1 Hz, 2H), 7.18 (t, *J* = 7.2 Hz, 1H), 5.05 (s, 1H), 4.47 (d, *J* = 6.3 Hz, 2H), 2.98 – 2.88 (m, 2H), 2.59 (m, 2H), 1.93 (s, 3H).

<sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>) δ 196.94, 163.43, 142.10, 137.94, 128.84, 128.34, 128.32, 127.48, 126.80, 125.77, 95.44, 46.86, 43.51, 31.98, 18.98.

HRMS (ESI): *m/z* calculated for C<sub>19</sub>H<sub>22</sub>NO [M+H]<sup>+</sup>: 280.1701, found: 280.1701.

#### (Z)-2-(benzylamino)dec-2-en-4-one



Following the general procedure, **3ah** was obtained as yellowish oil (54.3 mg, 0.209 mmol, 99%).

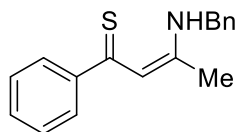
<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 11.19 (s, 1H), 7.37 – 7.30 (m, 2H), 7.27 – 7.22 (m, 3H), 5.03 (s, 1H), 4.45 (d, *J* = 6.3 Hz, 2H), 2.28 – 2.23 (m, 2H), 1.92 (s, 3H), 1.58 (q, *J* = 7.3 Hz, 2H), 1.29 (q, *J* = 5.8 Hz, 6H), 0.89 – 0.85 (m, 3H).

<sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 198.72, 163.04, 138.05, 128.81, 127.42, 126.81, 95.46, 46.81, 42.16, 31.77, 29.28, 26.15, 22.58, 19.01, 14.10.

HRMS (ESI): *m/z* calculated for C<sub>17</sub>H<sub>26</sub>NO [M+H]<sup>+</sup>: 260.2014, found: 260.2014.

## V. Synthetic Transformations and Utility of Enaminones

### (Z)-3-(benzylamino)-1-phenylbut-2-ene-1-thione



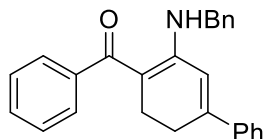
Following a modified procedure reported in the literature,<sup>3</sup> enaminothione **4** was obtained as an orange solid (31.6 mg, 0.118 mmol, 59%). M.p. = 54 – 56 °C.

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 11.75 (s, 1H), 7.87 (dd, *J* = 7.6, 1.8 Hz, 2H), 7.41 – 7.25 (m, 8H), 5.75 (s, 1H), 4.53 (d, *J* = 6.3 Hz, 2H), 2.06 (s, 3H).

<sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>) δ 188.11, 164.94, 140.31, 137.77, 130.57, 128.91, 128.20, 127.57, 126.98, 126.91, 92.66, 47.06, 19.53.

HRMS (ESI): *m/z* calculated for C<sub>17</sub>H<sub>18</sub>NS [M+H]<sup>+</sup>: 268.1160, found: 268.1158.

### (5-(benzylamino)-2,3-dihydro-[1,1'-biphenyl]-4-yl)(phenyl)methanone



Following a modified procedure reported in the literature,<sup>4</sup> compound **5** was obtained as a brown solid (40.7 mg, 0.111 mmol, 56%). M.p. = 90 – 95 °C.

<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 12.26 (s, 1H), 7.50 – 7.35 (m, 15H), 6.69 (s, 1H), 4.67 (d, *J* = 6.0 Hz, 2H), 2.59 (m, 4H).

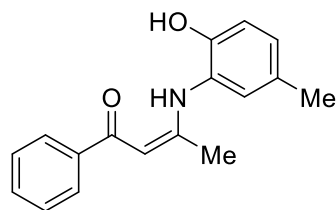
<sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 139.58, 138.24, 129.18, 128.90, 128.76, 128.72, 127.91, 127.50, 127.10, 127.07, 125.96, 116.02, 46.93, 28.15, 25.41.

HRMS (ESI): *m/z* calculated for C<sub>26</sub>H<sub>24</sub>NO [M+H]<sup>+</sup>: 366.1858, found: 366.1858.

<sup>3</sup> Liu, Z.; Wu, P.; He, Y.; Yang, T.; Yu, Z. [4+1] Cycloaddition of Enaminothiones and Aldehyde *N*-Tosylhydrazones Toward 3-Aminothiophenes. *Adv. Synth. Catal.* **2018**, 360, 4381.

<sup>4</sup> Feng, T.; Tian, M.; Zhang, X.; Fan, X. Tunable Synthesis of Functionalized Cyclohexa-1,3-dienes and 2-Aminobenzophenones/Benzoate from the Cascade Reactions of Allenic Ketones/Allenolate with Amines and Enones. *J. Org. Chem.* **2018**, 83, 5313.

**(Z)-3-((2-hydroxy-5-methylphenyl)amino)-1-phenylbut-2-en-1-one**



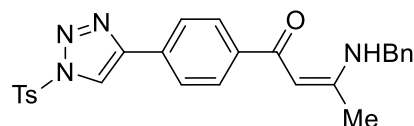
To a solution of 2-amino-4-methylphenol (1.10 g, 8.96 mmol, 1.0 equiv.) in EtOH (50 mL) was added a solution of allenic ketone **1a** (1.29 g, 8.96 mmol, 1.0 equiv.) in EtOH (40 mL) dropwise. The reaction mixture was stirred overnight under ambient conditions. After TLC showed the complete consumption of the allenic ketone, the volatiles were evaporated under reduced pressure to afford the pure anti-microbial agent **6** as yellowish-orange flakes (2.15 g, 8.04 mmol, 90%). M.p. = 140 – 143 °C.

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 12.33 (s, 1H), 8.33 (s, 1H), 7.87 (dd, *J* = 7.6, 1.8 Hz, 2H), 7.49 – 7.39 (m, 3H), 6.98 (d, *J* = 8.2, 1H), 6.92 (d, *J* = 8.3 Hz, 1H), 6.83 (s, 1H), 5.67 (s, 1H), 2.25 (s, 3H), 1.66 (s, 3H).

<sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>) δ 188.43, 165.32, 149.91, 139.90, 130.88, 129.36, 129.19, 128.23, 127.90, 127.27, 124.77, 116.90, 94.36, 20.39, 19.72.

HRMS (ESI): *m/z* calculated for C<sub>17</sub>H<sub>18</sub>NO<sub>2</sub> [M+H]<sup>+</sup>: 268.1338, found: 268.1338.

**(Z)-3-(benzylamino)-1-(4-(1-tosyl-1*H*-1,2,3-triazol-4-yl)phenyl)but-2-en-1-one**



Following a modified procedure reported in the literature,<sup>5</sup> **7** was obtained as a beige powder (55.0 mg, 0.116 mmol, 88%). M.p. = 161 – 163 °C.

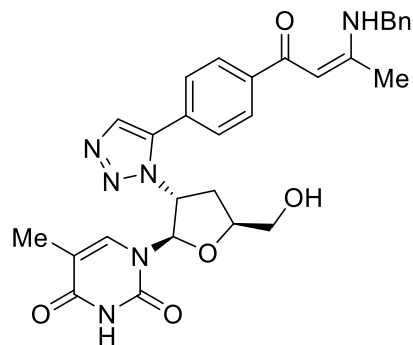
<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 11.80 (t, *J* = 5.9 Hz, 1H), 8.38 (s, 1H), 8.01 (d, *J* = 8.3 Hz, 2H), 7.94 (d, *J* = 8.3 Hz, 2H), 7.86 (d, *J* = 8.3 Hz, 2H), 7.41 – 7.32 (m, 4H), 7.28 (m, 3H), 5.76 (s, 1H), 4.54 (d, *J* = 6.2 Hz, 2H), 2.42 (s, 3H), 2.08 (s, 3H).

<sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>) δ 186.84, 165.36, 147.45, 146.90, 140.73, 137.59, 133.01, 130.75, 130.51, 128.92, 128.70, 127.66, 127.61, 126.91, 125.84, 119.46, 92.64, 47.11, 21.83, 19.53.

HRMS (ESI): *m/z* calculated for C<sub>26</sub>H<sub>25</sub>N<sub>4</sub>O<sub>3</sub>S [M+H]<sup>+</sup>: 473.1647, found: 473.1647.

<sup>5</sup> Miura, T.; Nakamuro, T.; Hiraga, K.; Murakami, M. The stereoselective synthesis of  $\alpha$ -amino aldols starting from terminal alkynes. *Chem. Commun.* **2014**, 50, 10474.

**1-((2R,3R,5S)-3-(5-(4-((Z)-3-(benzylamino)but-2-enoyl)phenyl)-1H-1,2,3-triazol-1-yl)-5-(hydroxymethyl)tetrahydrofuran-2-yl)-5-methylpyrimidine-2,4(1H,3H)-dione**



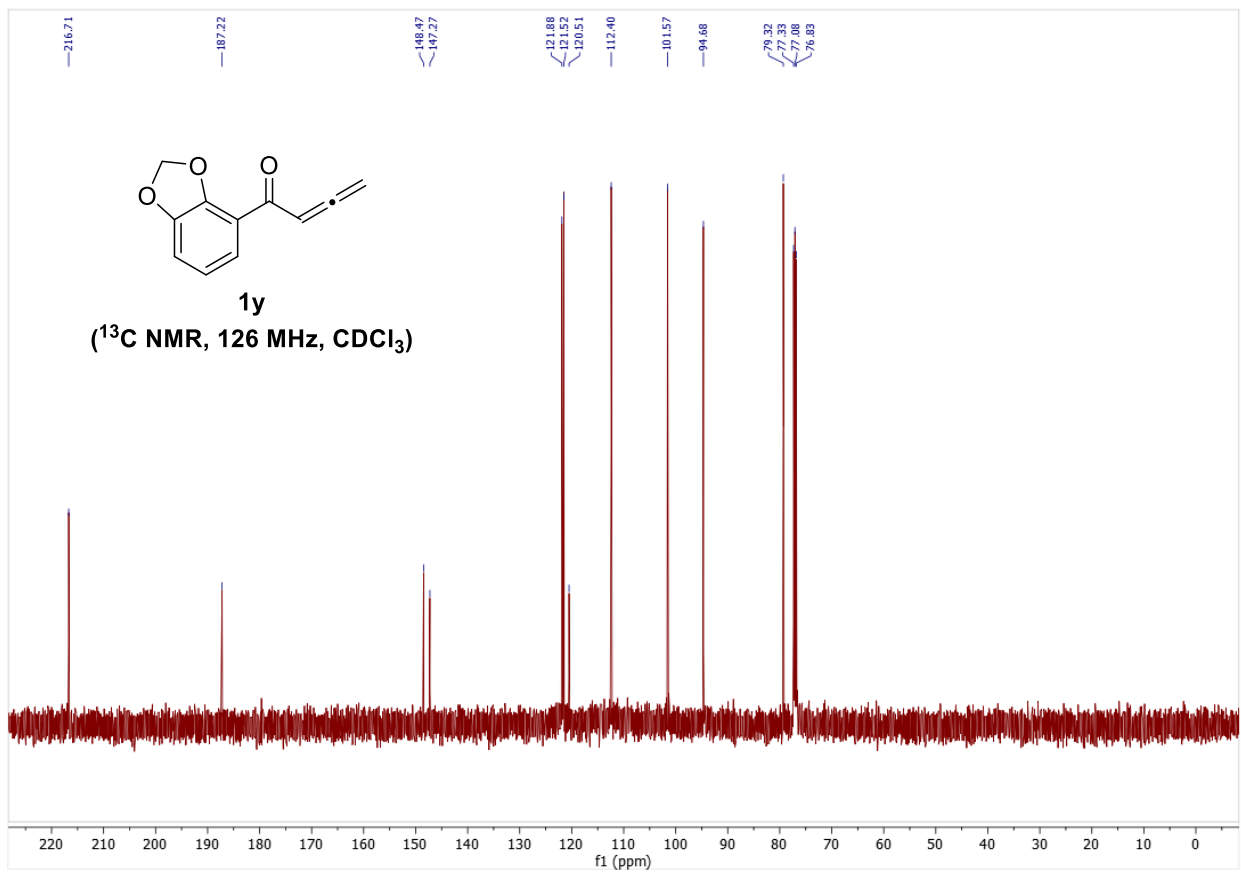
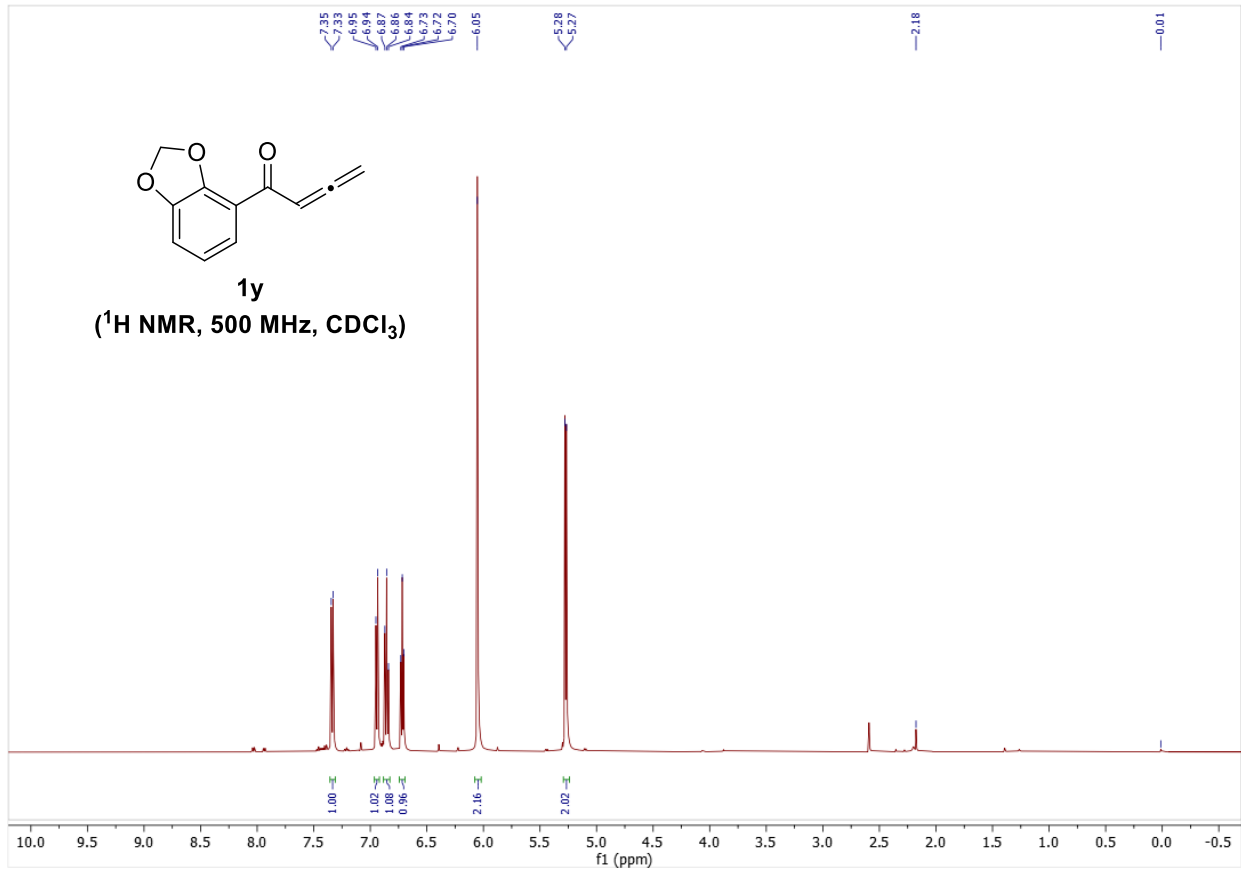
Following a modified procedure reported in the literature,<sup>6</sup> **8** was obtained as a beige paste (30.4 mg, 0.056 mmol, 27%). M.p. = 109 – 112 °C.  $[\alpha]_D^{22} = +136.6^\circ$  ( $c = 0.6$ ,  $\text{CHCl}_3$ ).

<sup>1</sup>H NMR (500 MHz, DMSO)  $\delta$  11.61 (t,  $J = 6.1$  Hz, 1H), 11.33 (s, 1H), 8.84 (s, 1H), 7.91 (q,  $J = 8.5$  Hz, 4H), 7.38 (t,  $J = 7.4$  Hz, 2H), 7.34 – 7.28 (m, 3H), 6.44 (t,  $J = 6.6$  Hz, 1H), 5.87 (s, 1H), 4.59 (d,  $J = 6.1$  Hz, 2H), 4.27 (d,  $J = 5.5$  Hz, 1H), 3.76 – 3.63 (m, 2H), 2.83 – 2.65 (m, 2H), 2.48 (s, 1H), 2.10 (s, 3H), 1.80 (s, 3H), 1.14 (d,  $J = 7.1$  Hz, 2H).

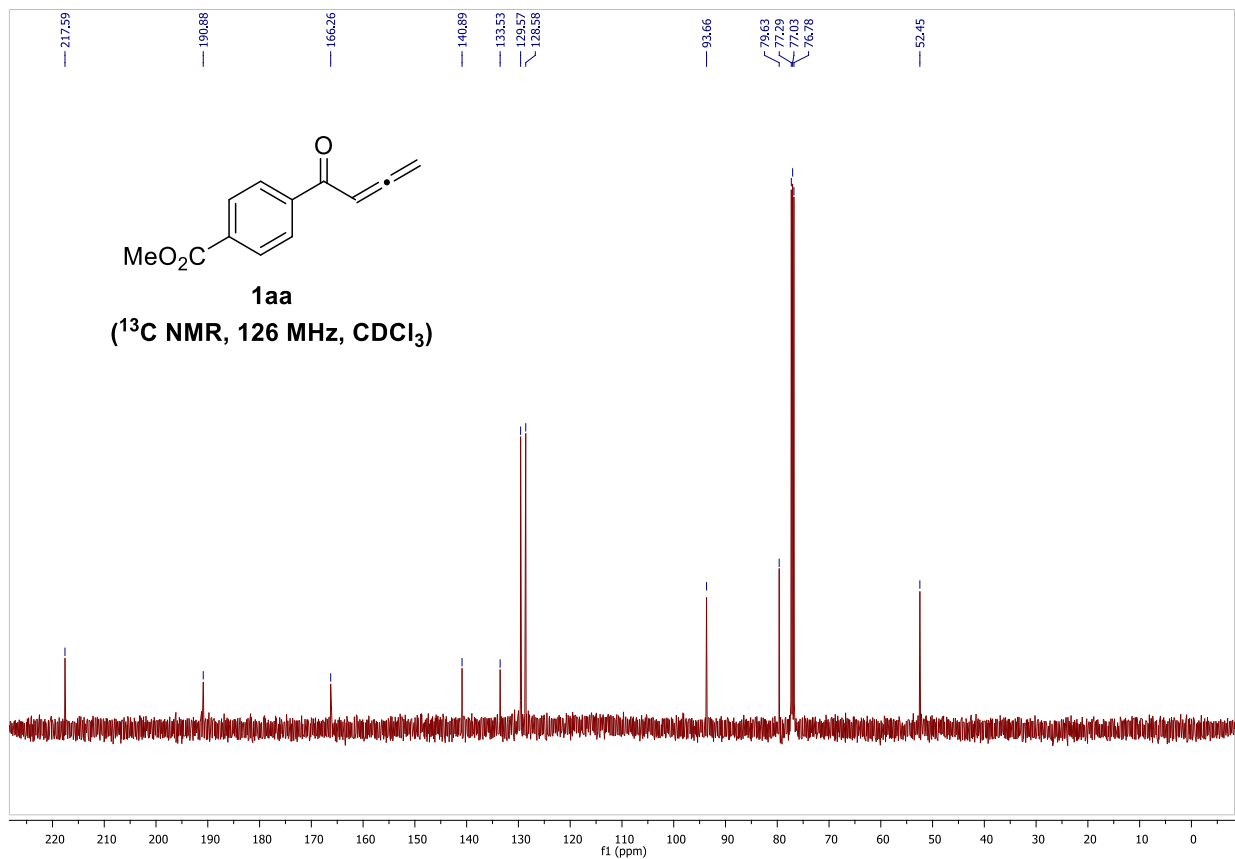
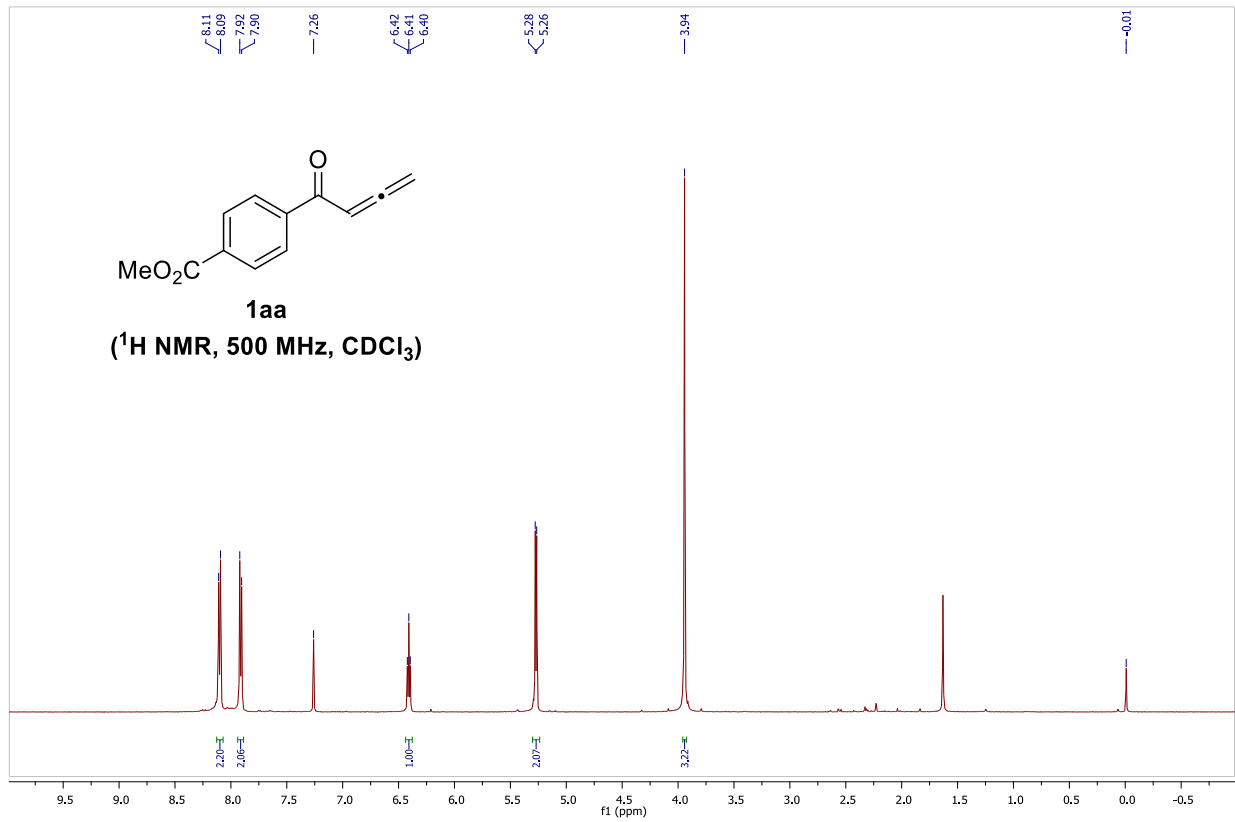
<sup>13</sup>C NMR (126 MHz, DMSO)  $\delta$  185.59, 165.87, 164.22, 150.93, 146.54, 139.69, 138.80, 136.74, 132.98, 129.24, 127.86, 127.71, 125.40, 122.10, 110.14, 92.05, 84.92, 84.39, 61.24, 59.92, 46.72, 37.63, 29.47, 22.57, 19.59, 14.55, 12.74.

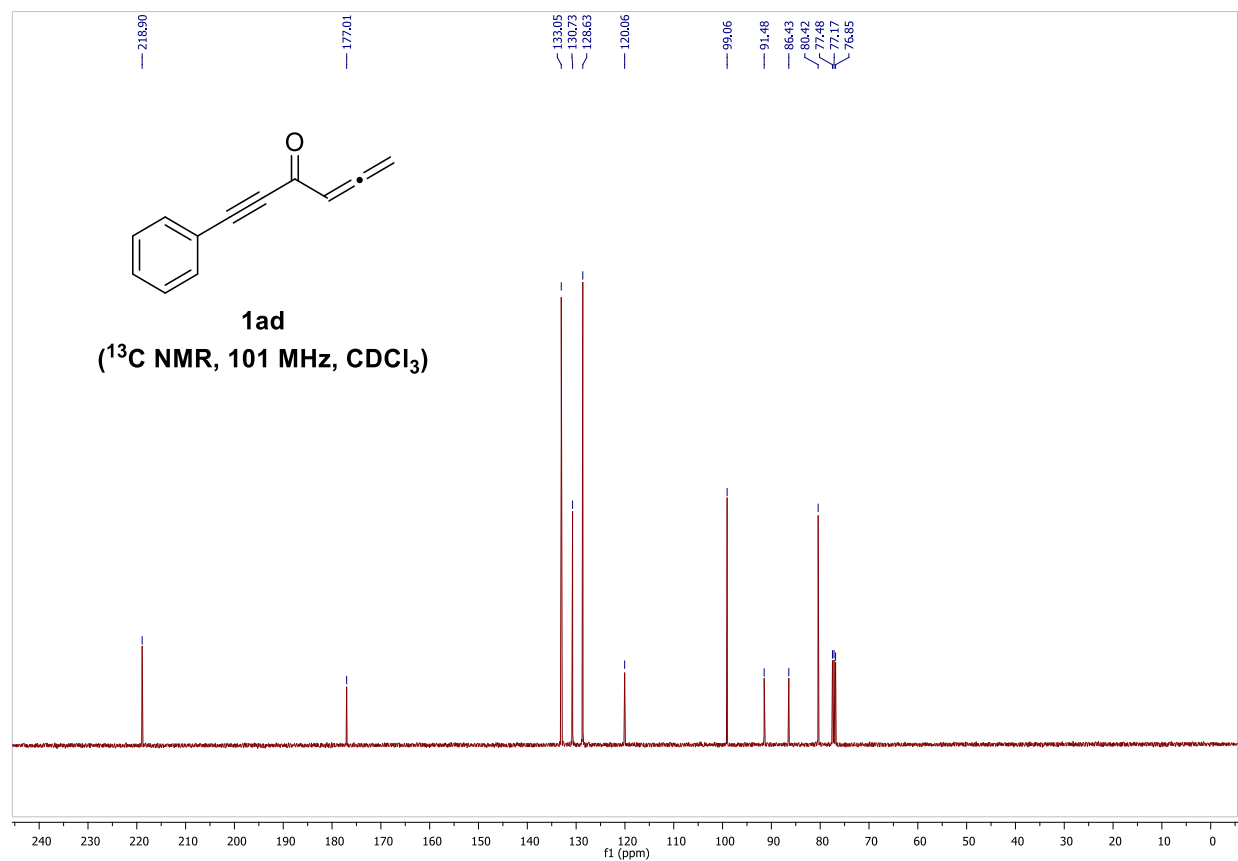
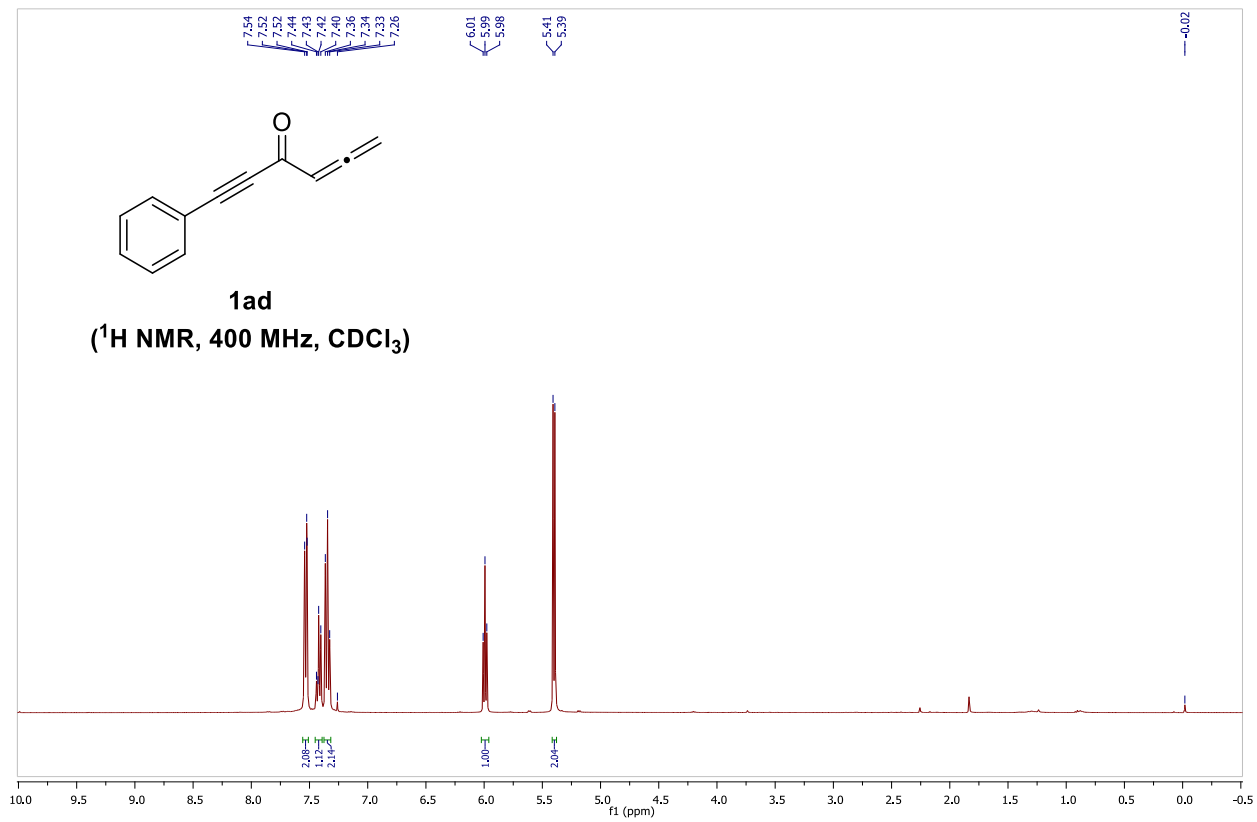
HRMS (ESI):  $m/z$  calculated for  $\text{C}_{29}\text{H}_{31}\text{N}_6\text{O}_5$   $[\text{M}+\text{H}]^+$ : 543.2356, found: 543.2356.

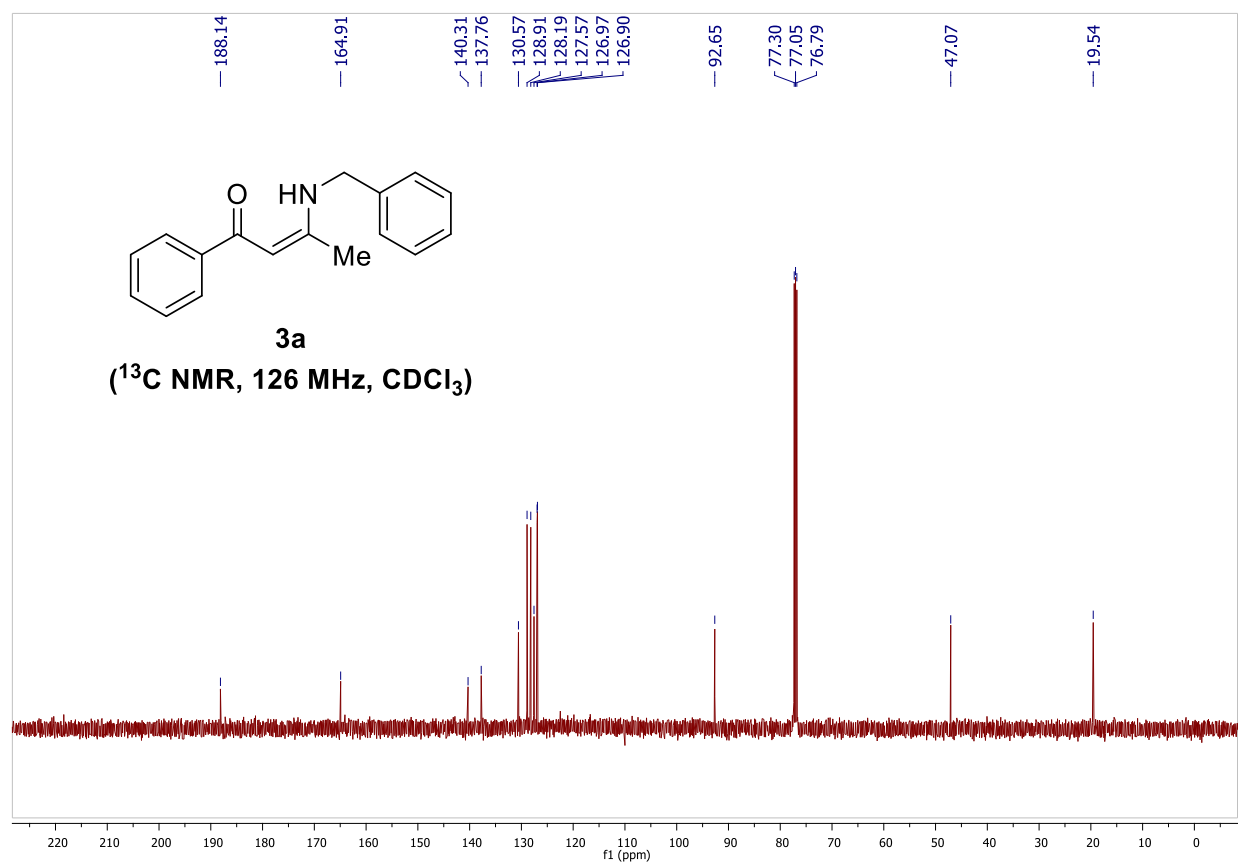
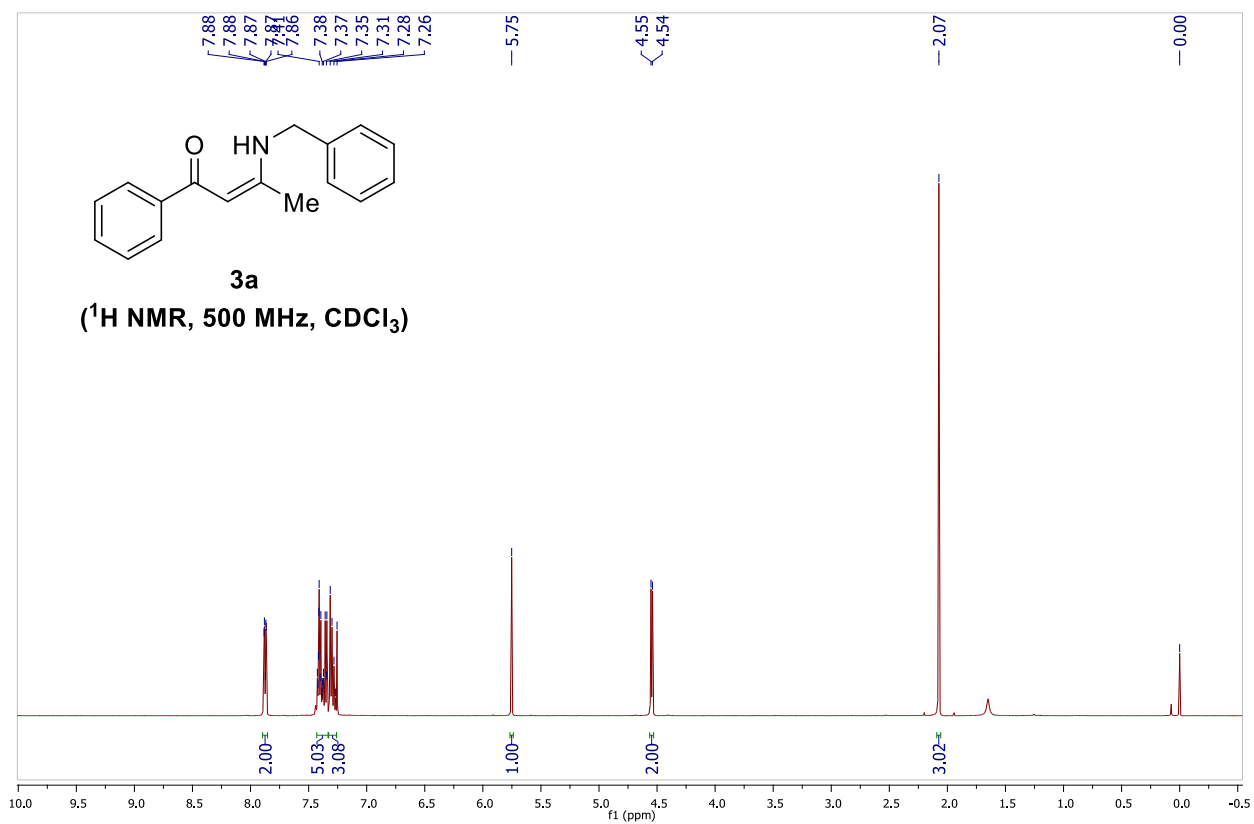
<sup>6</sup> Goh, J.; Maraswami, M.; Loh, T. –P. Synthesis of Vinylic Sulfones in Aqueous Media. *Org. Lett.* **2021**, 23, 1060.

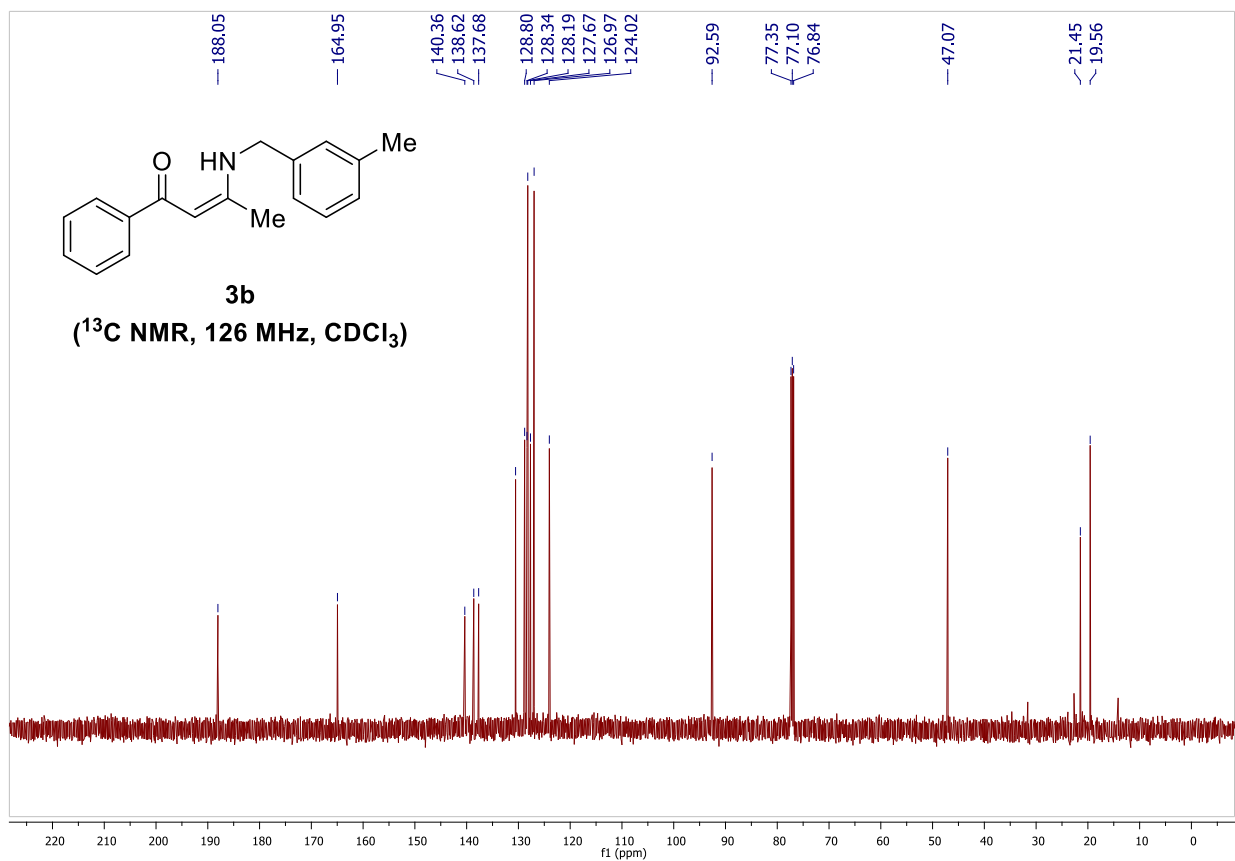
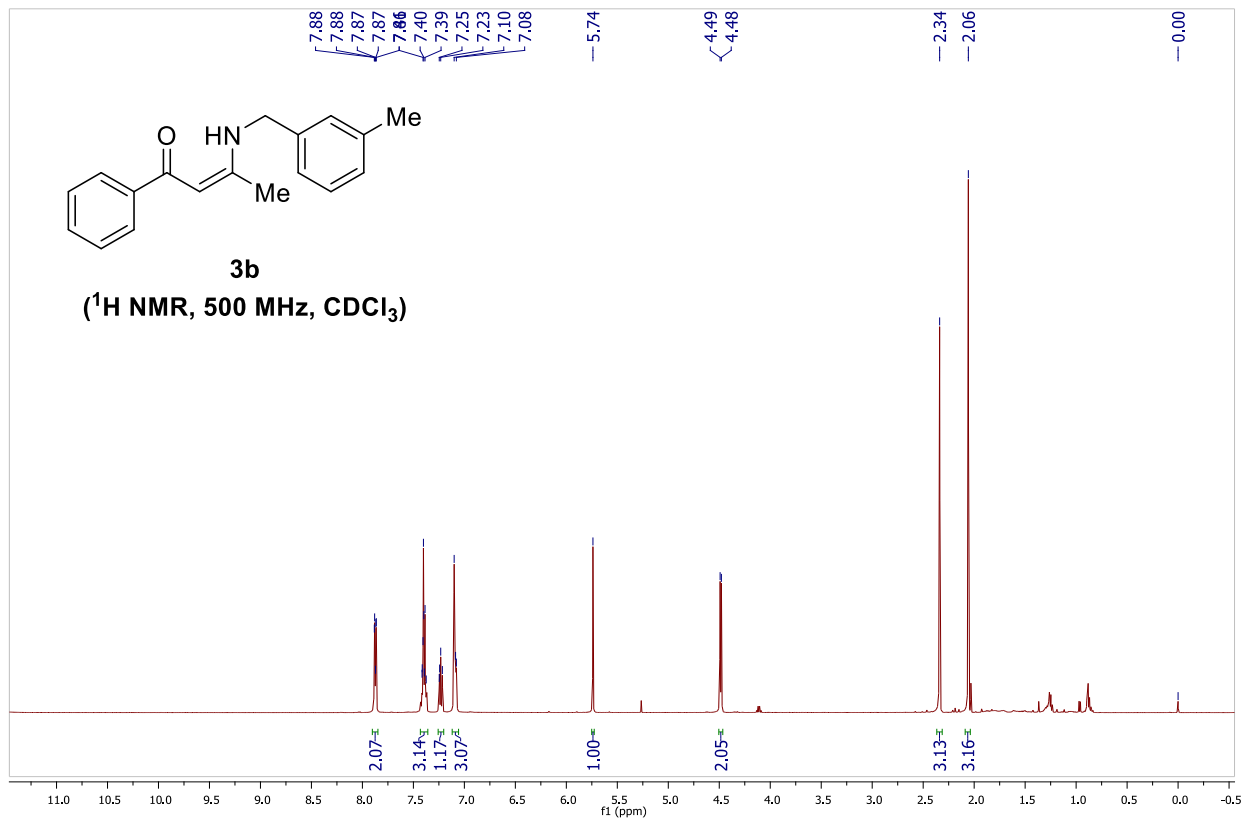


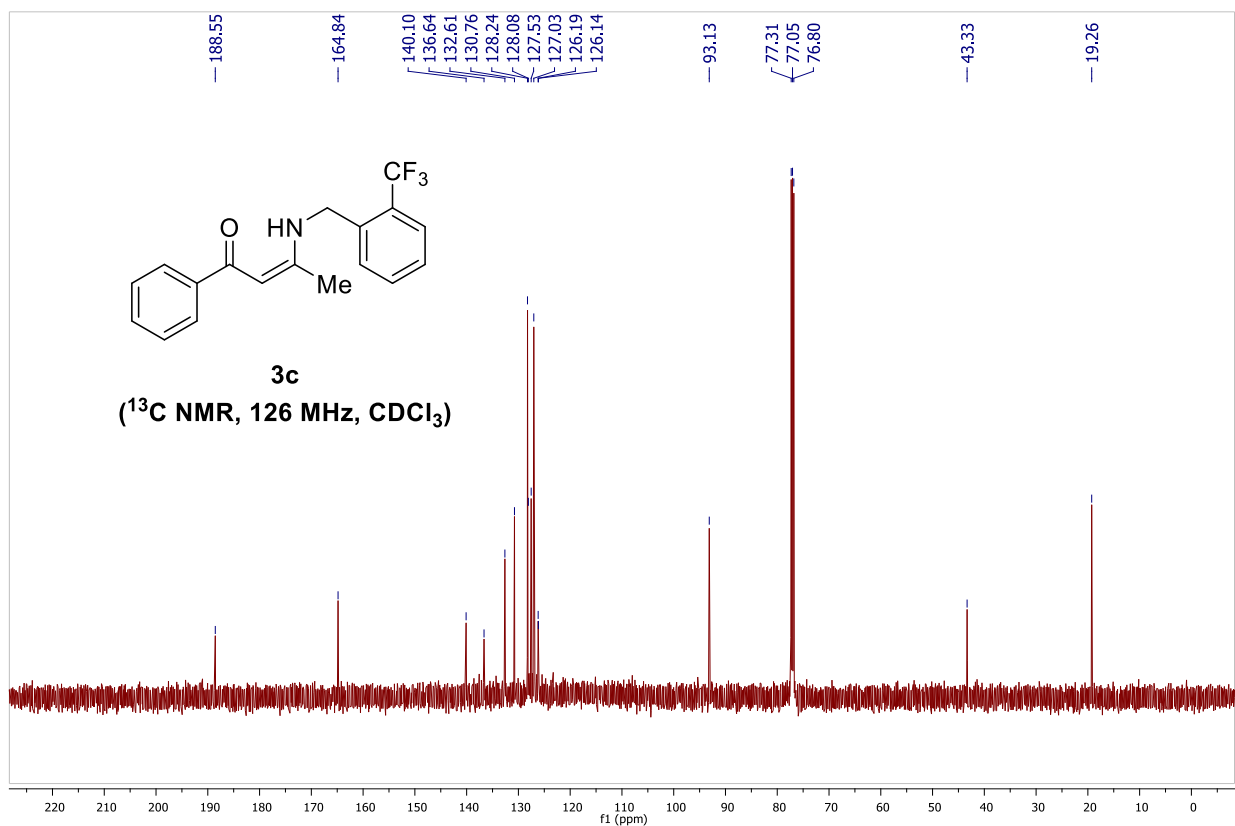
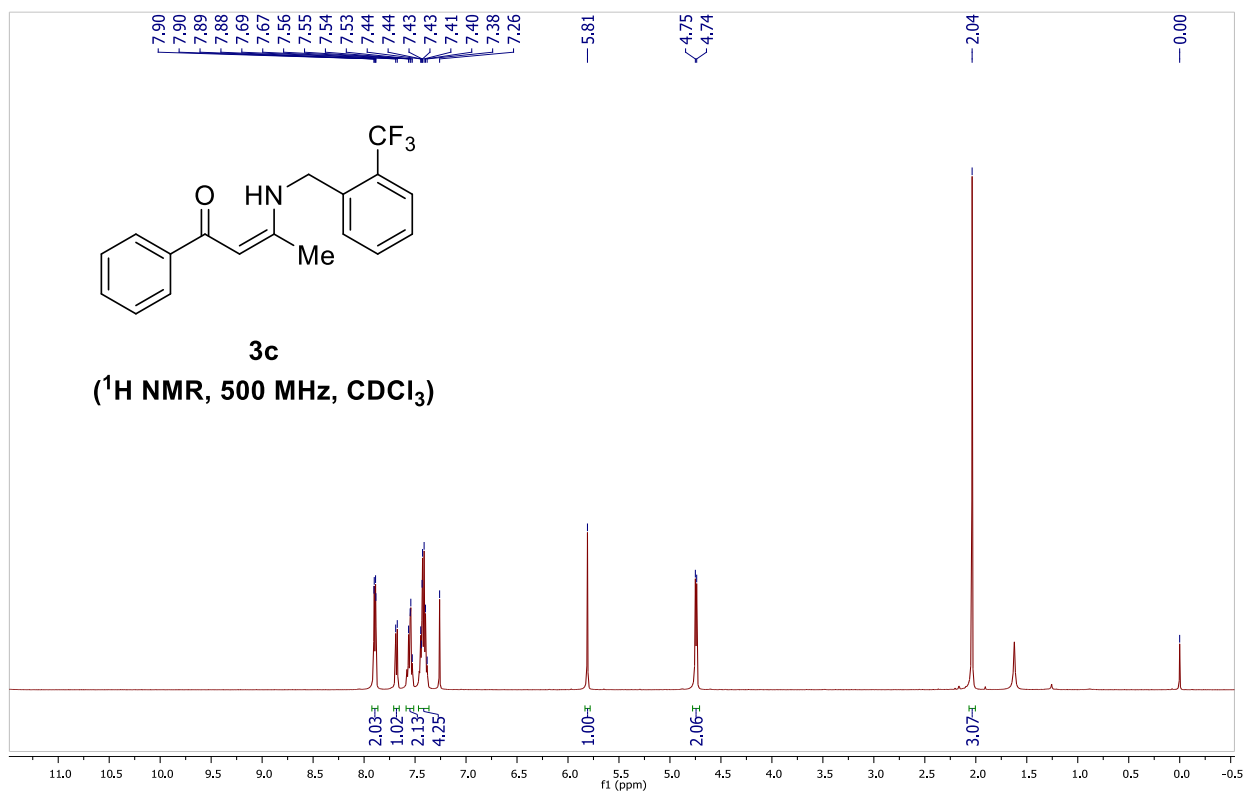


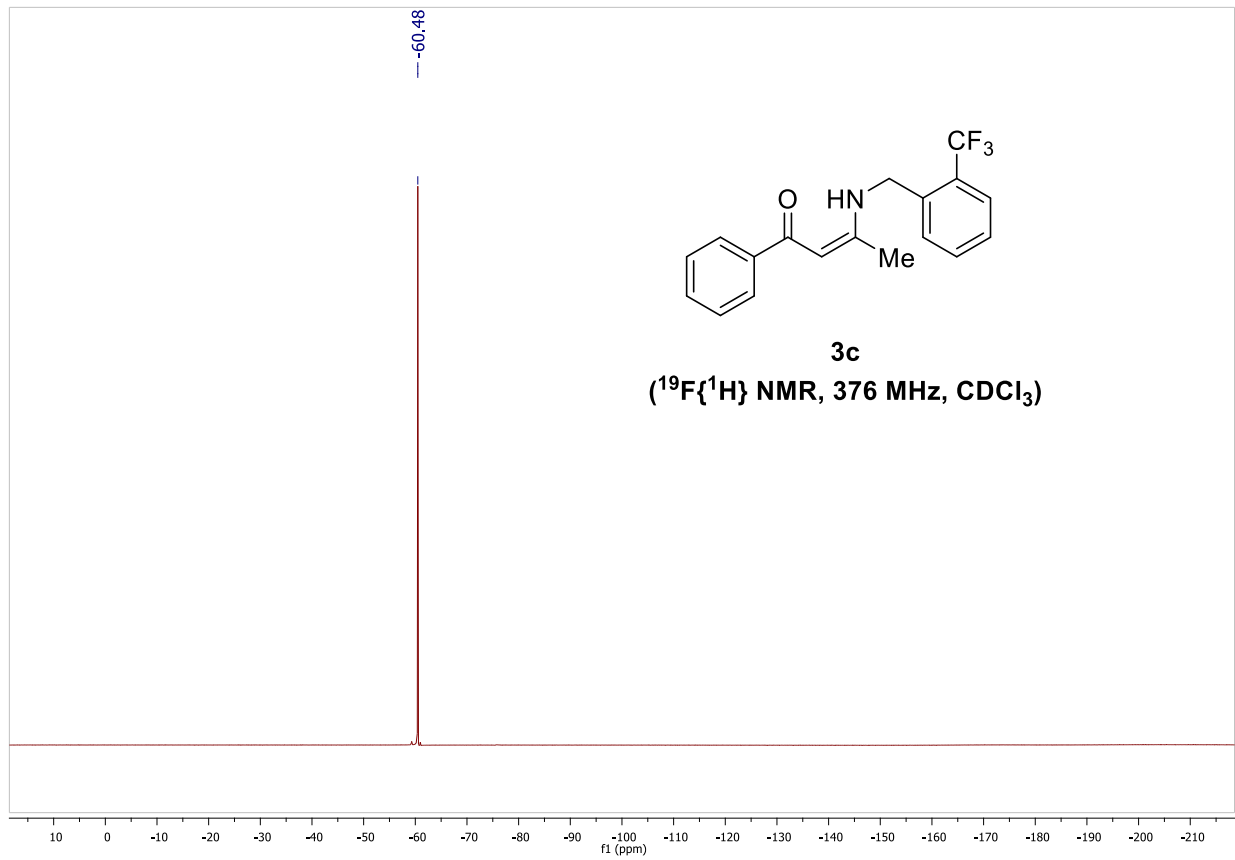


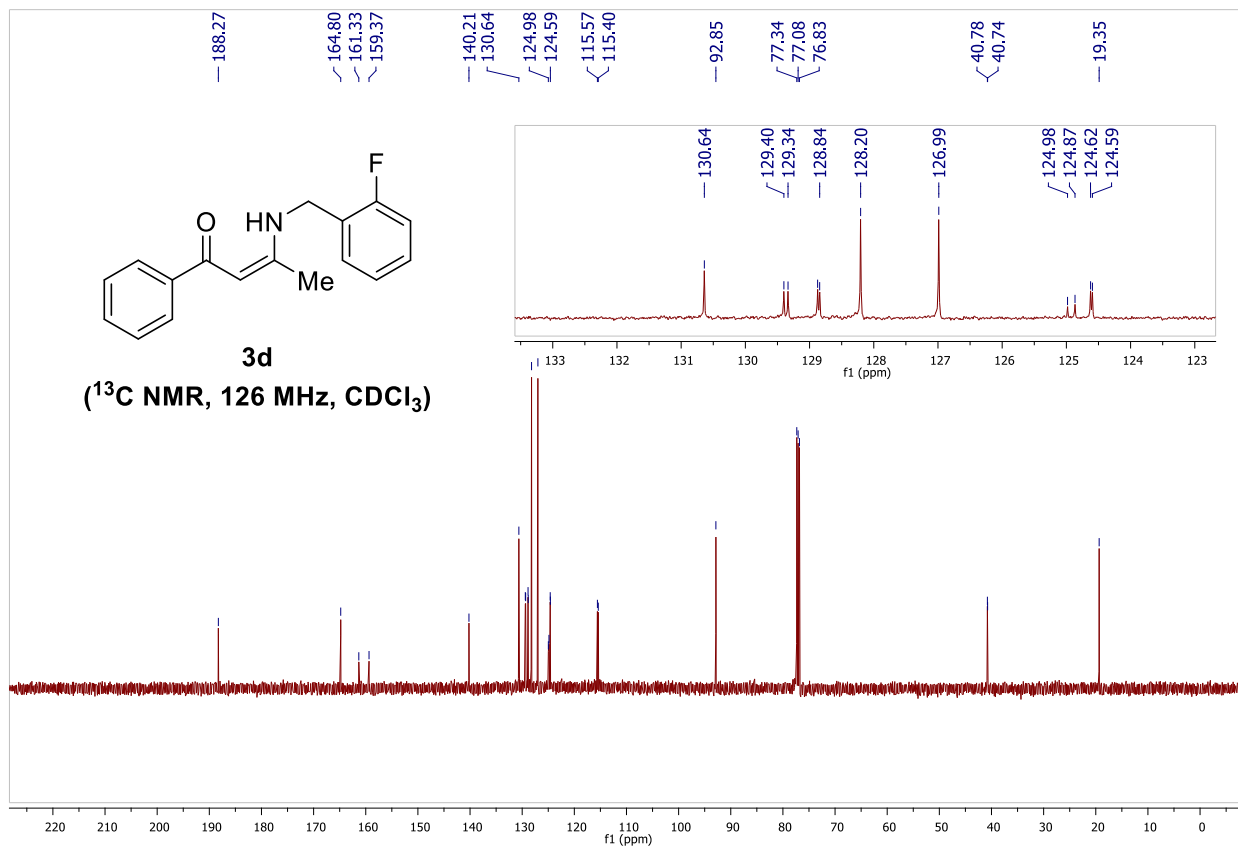
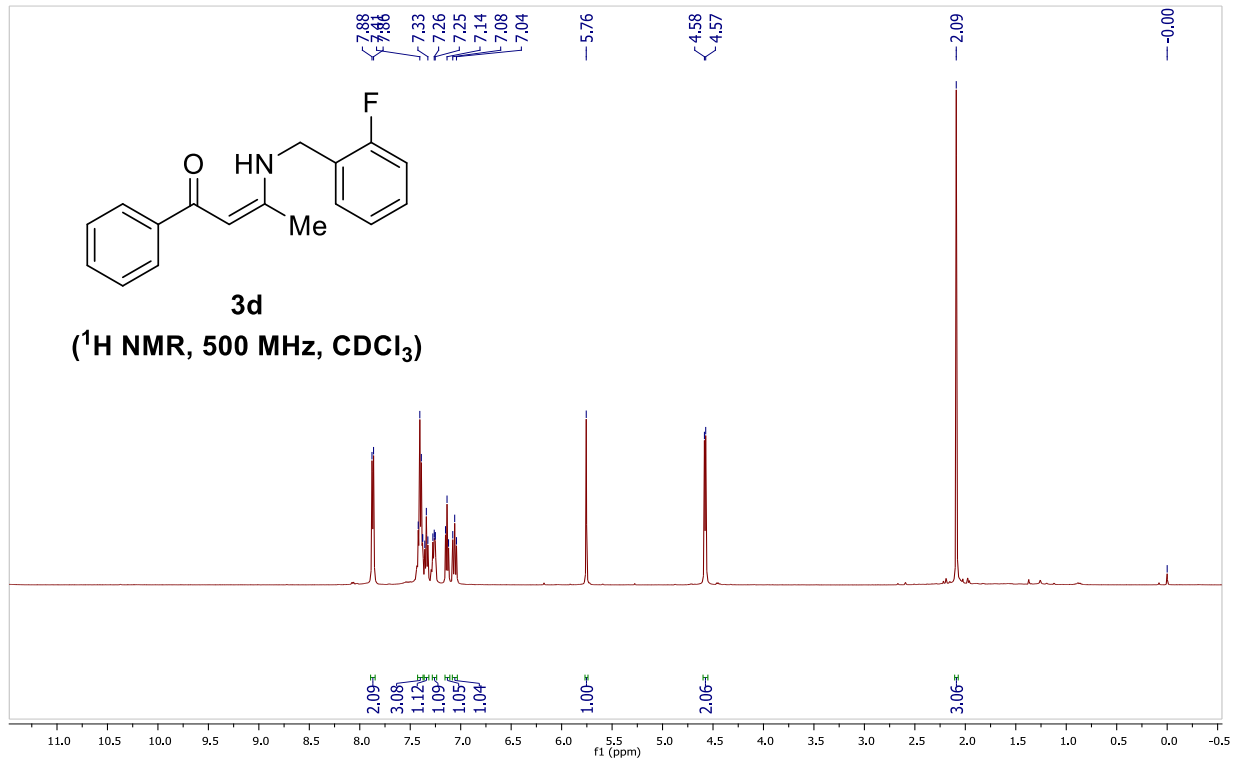


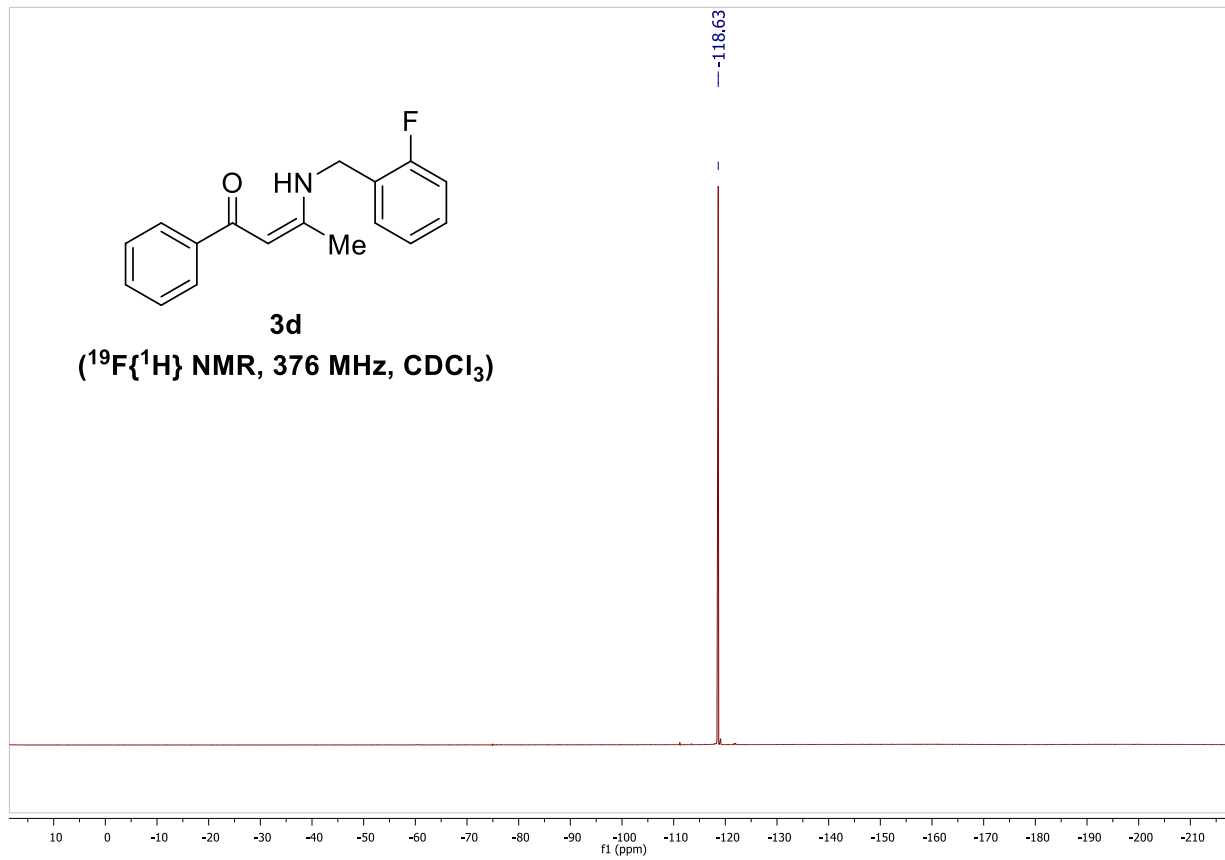




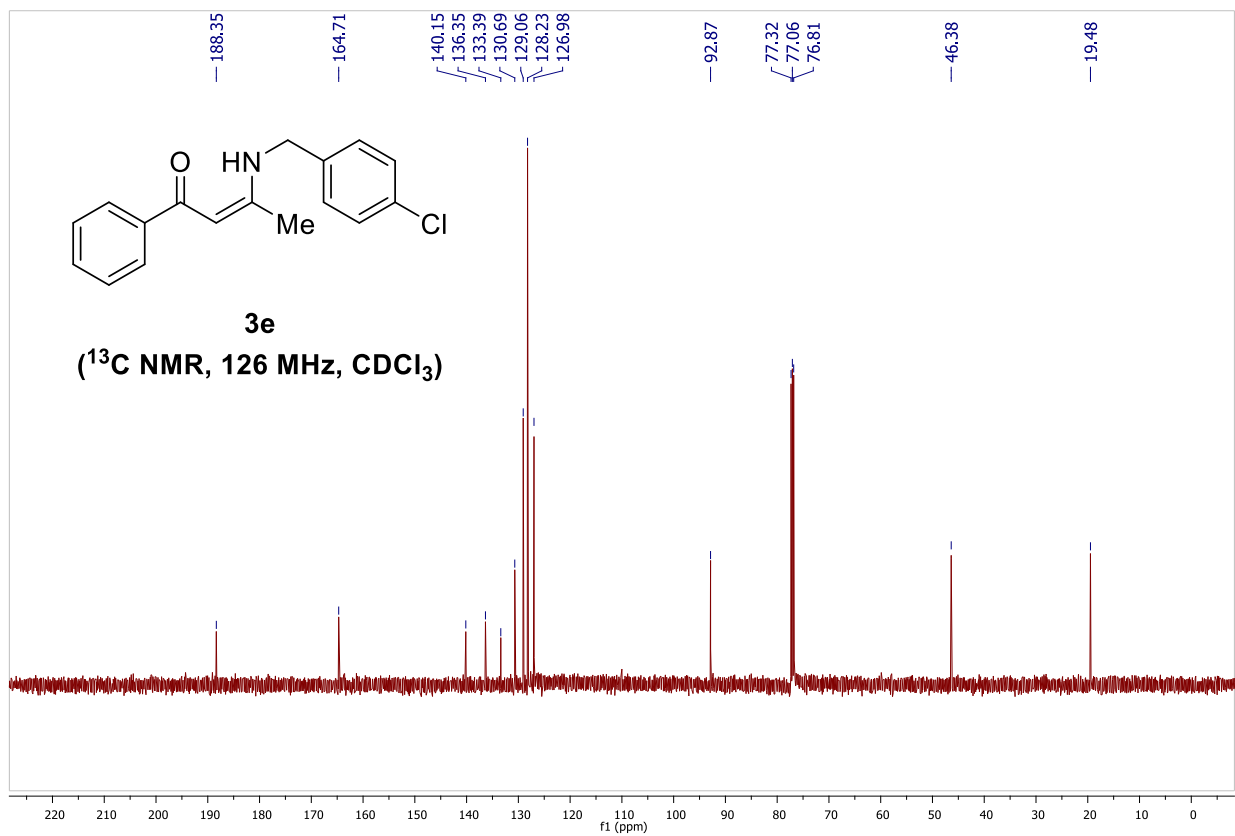
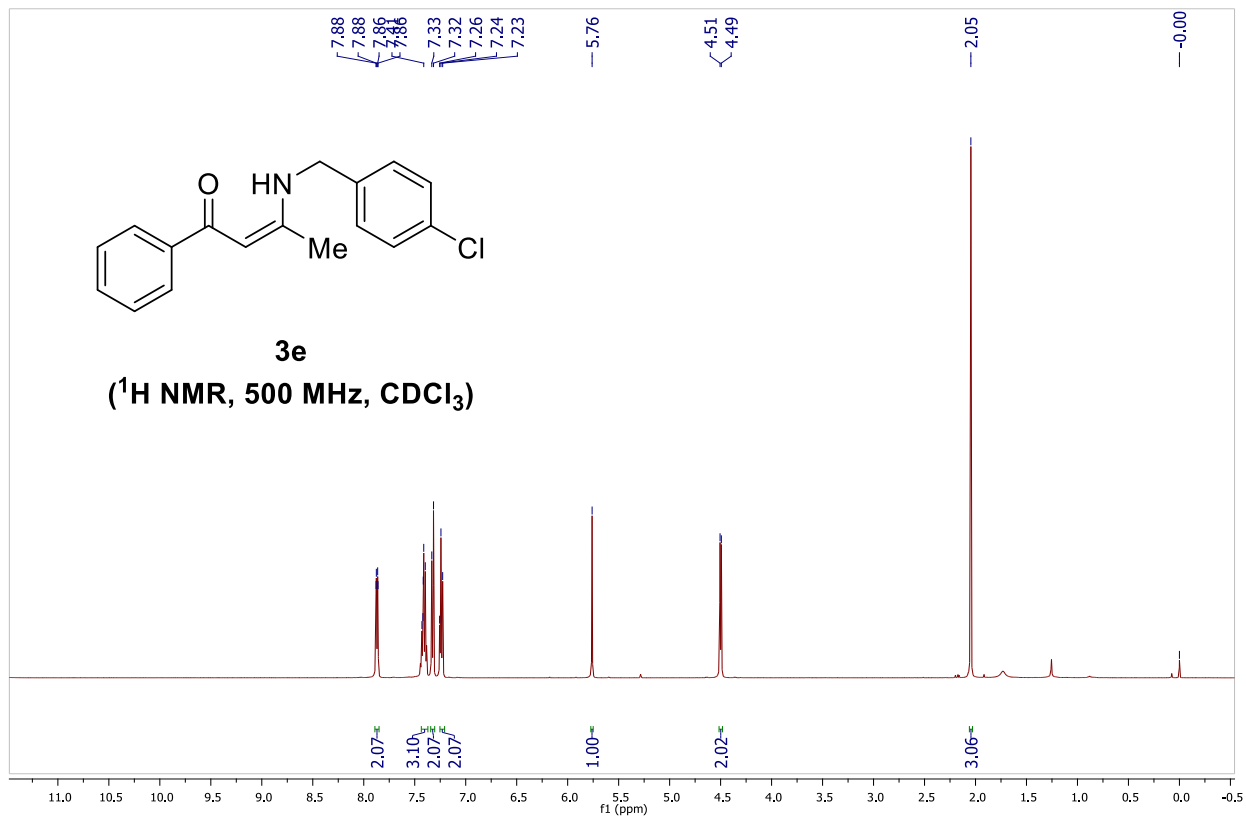


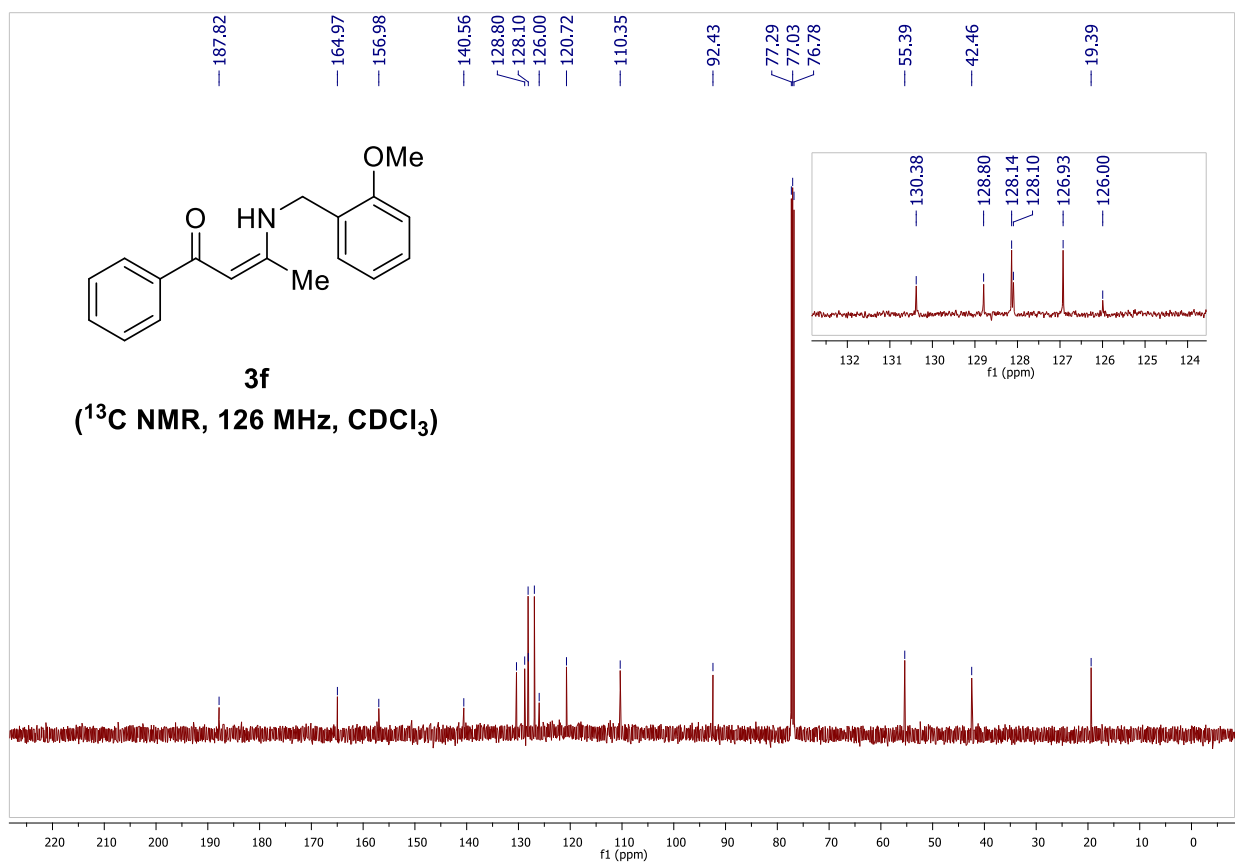
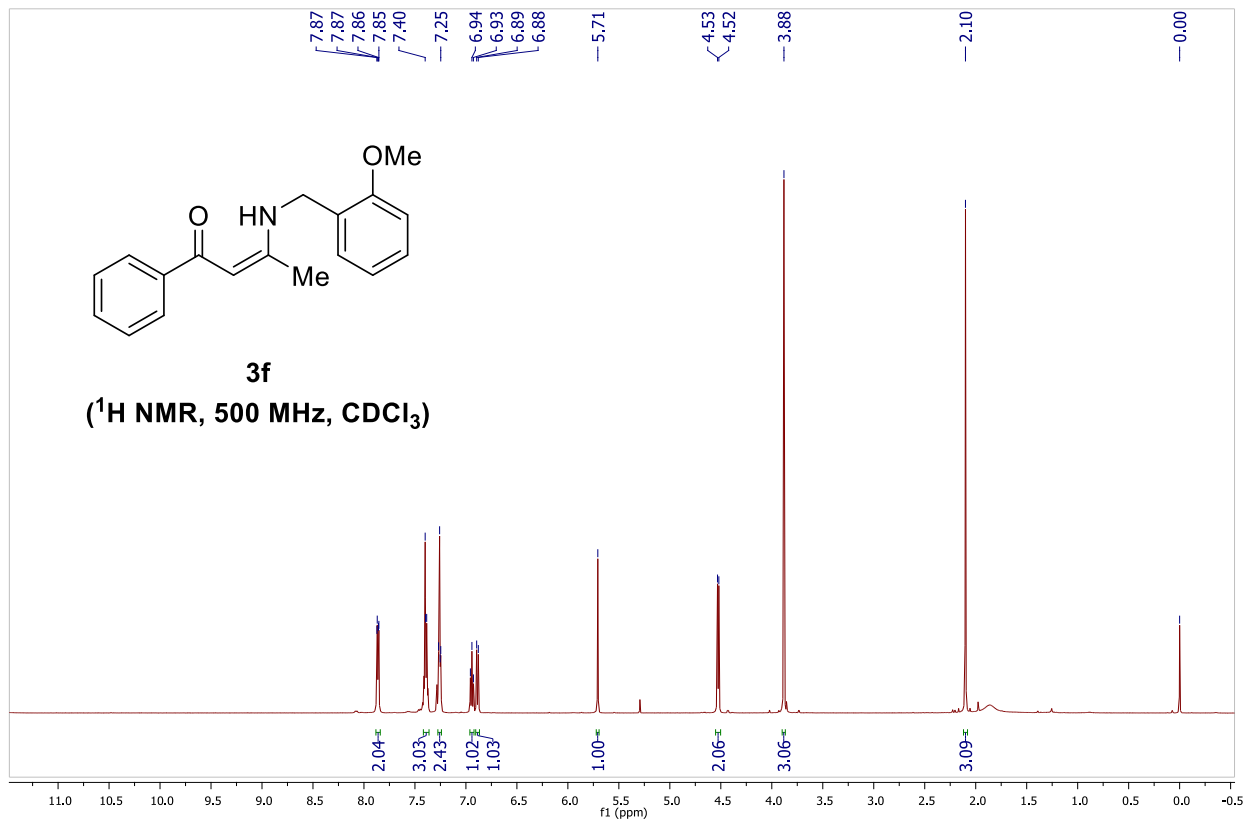


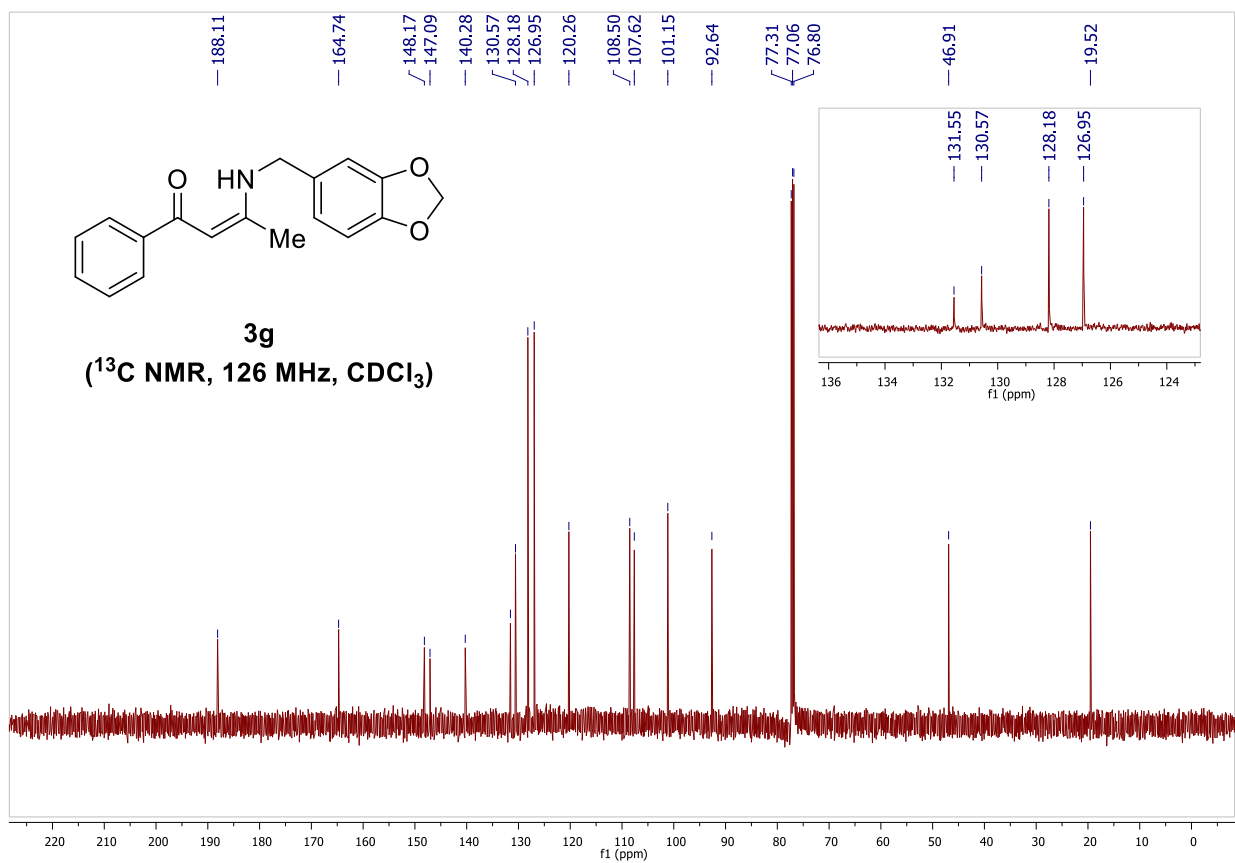
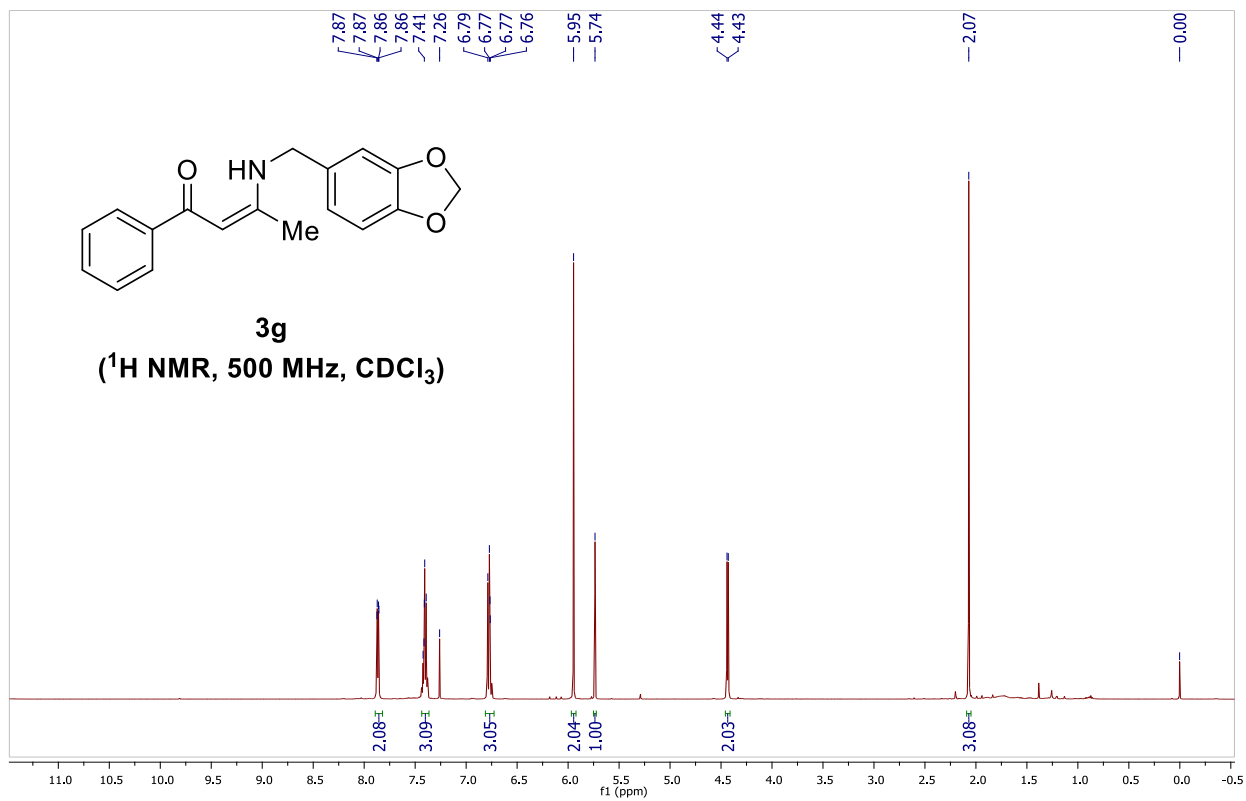


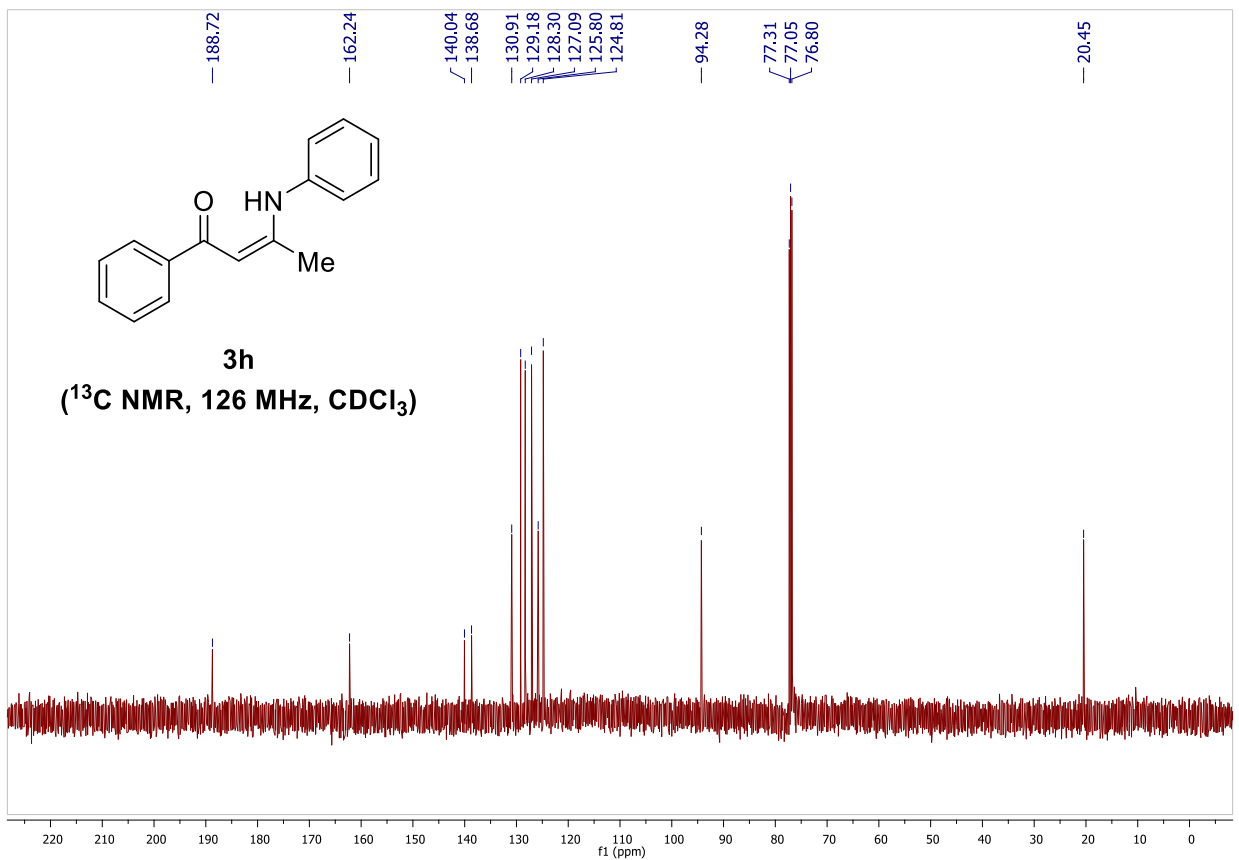
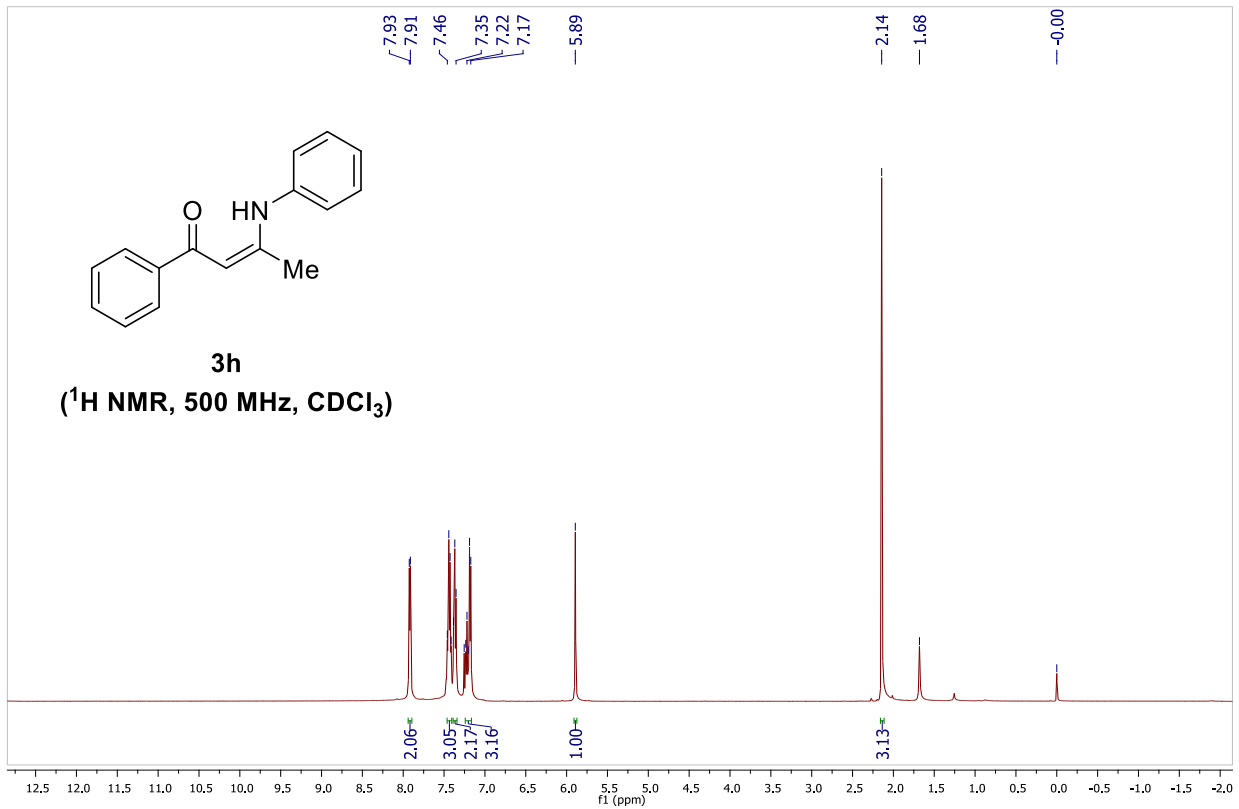


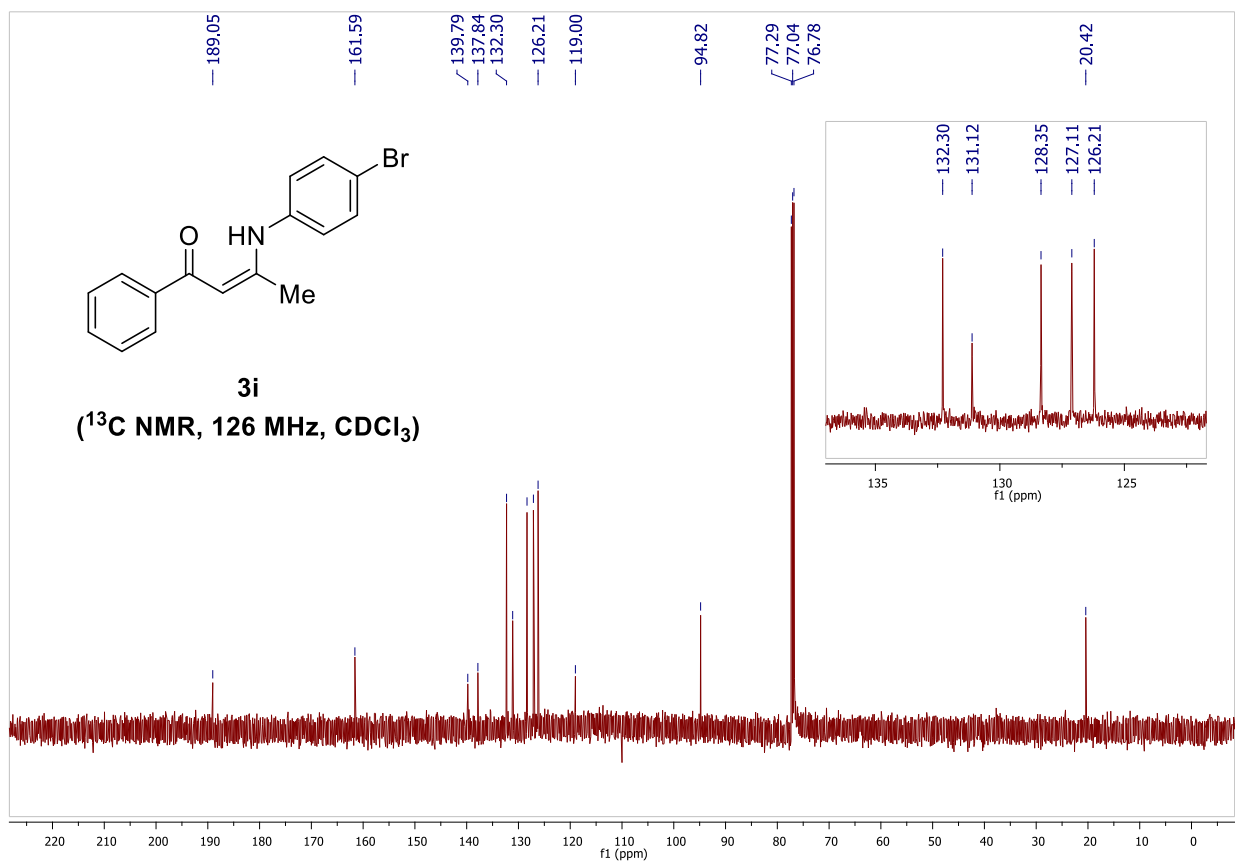
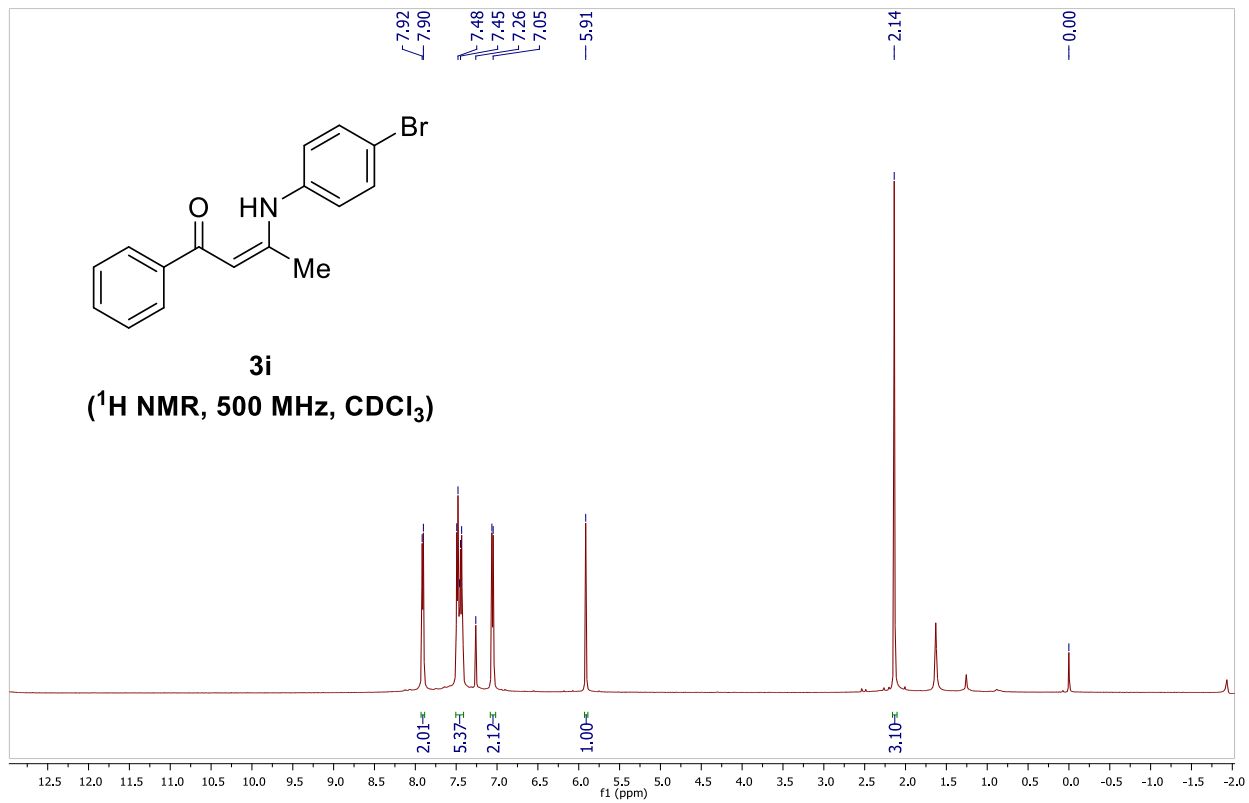


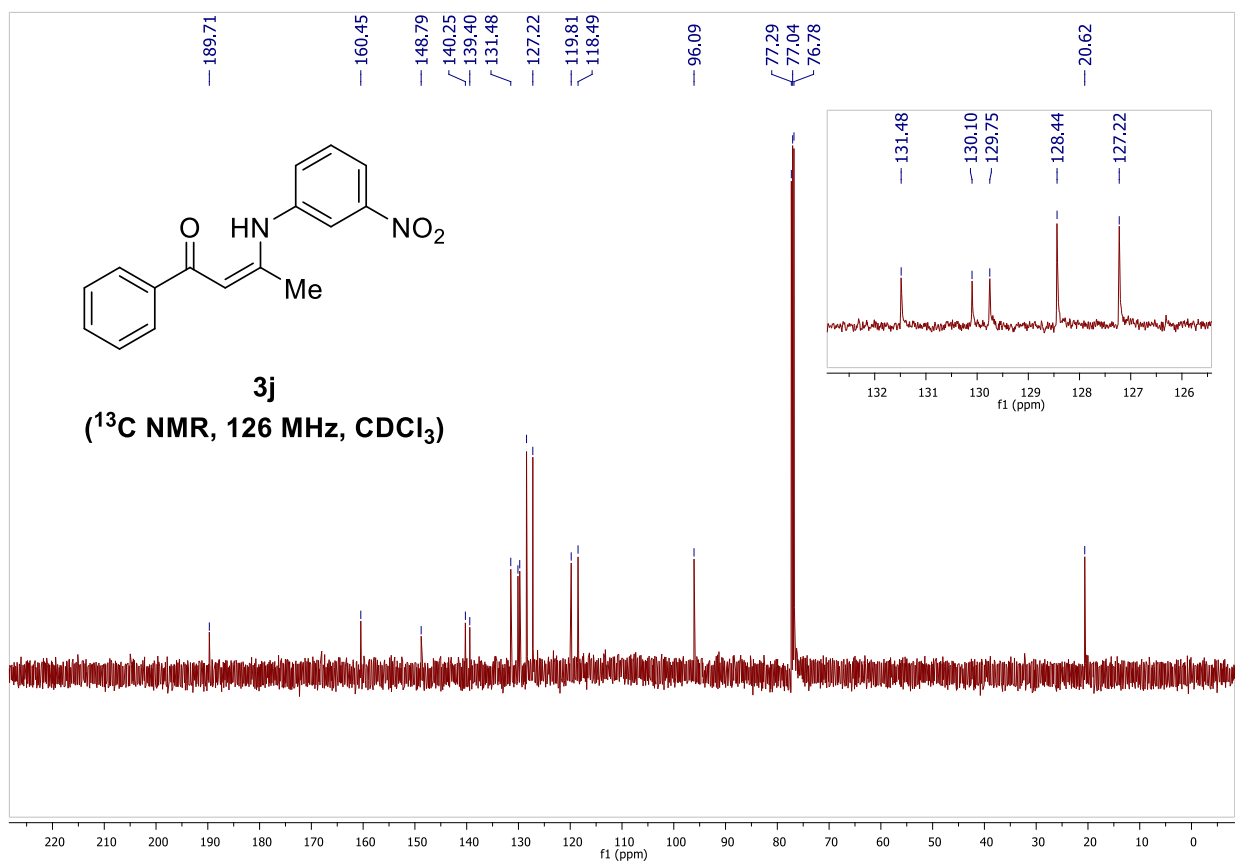
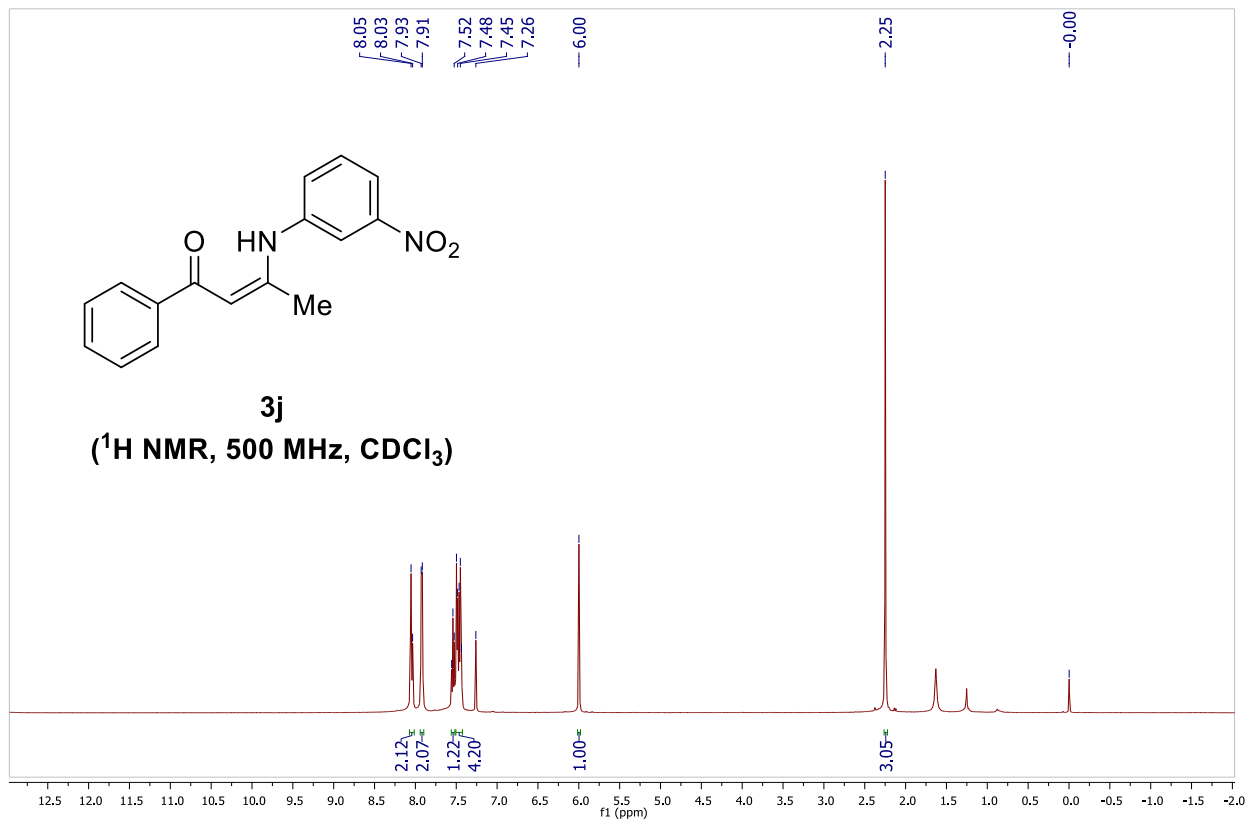


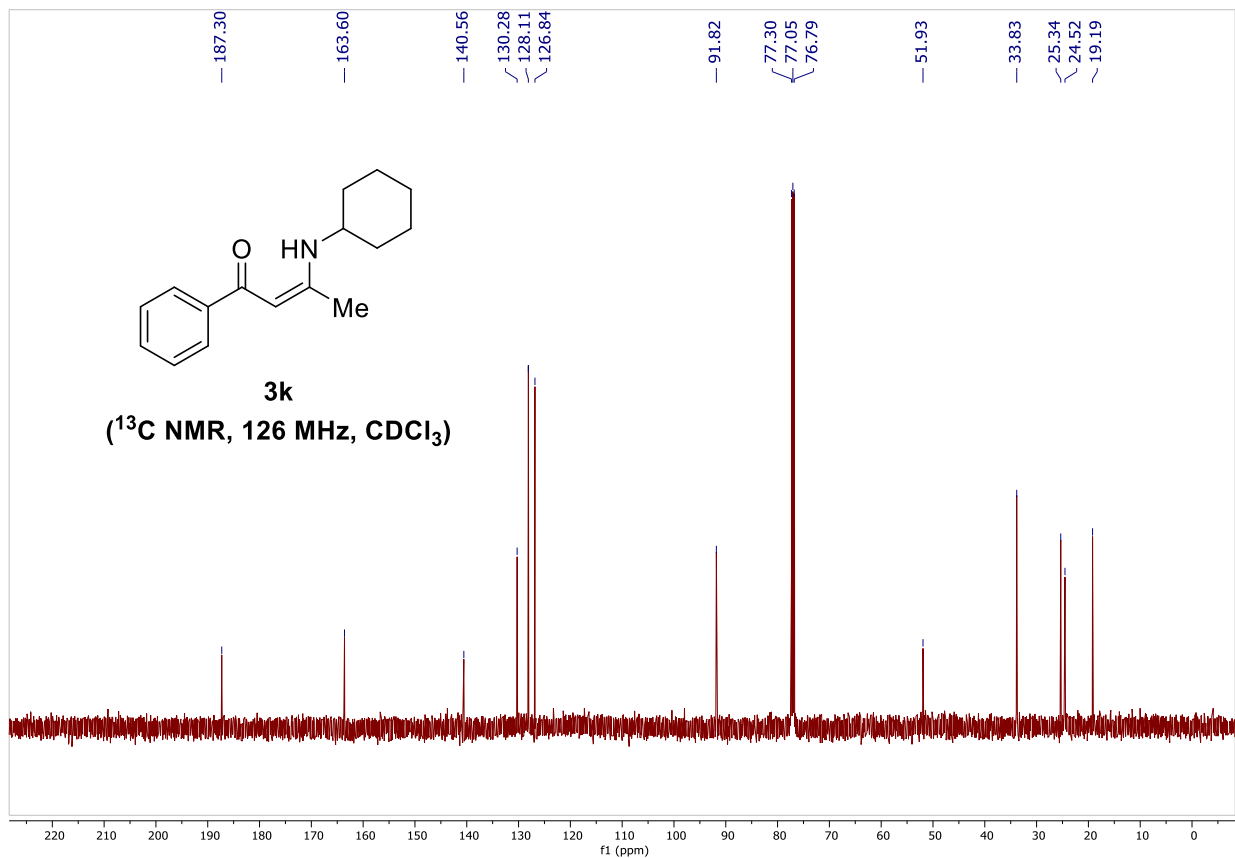
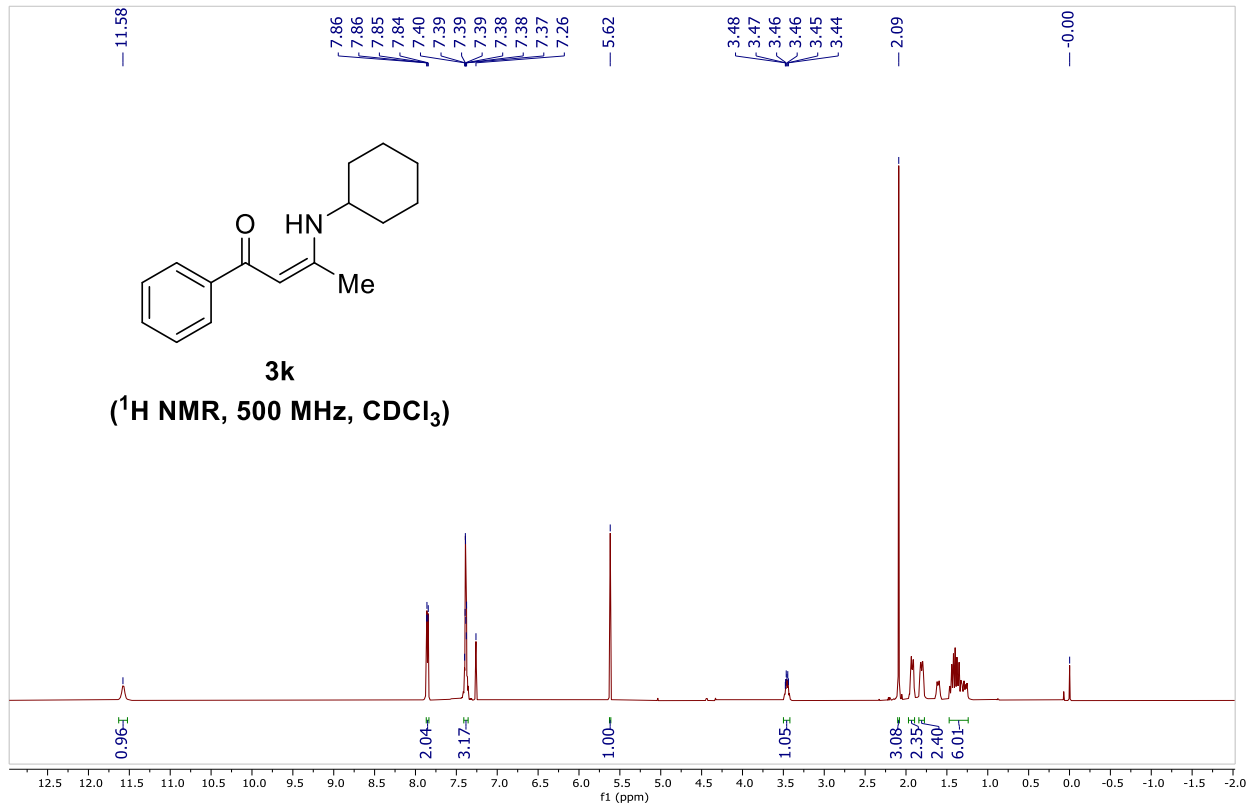


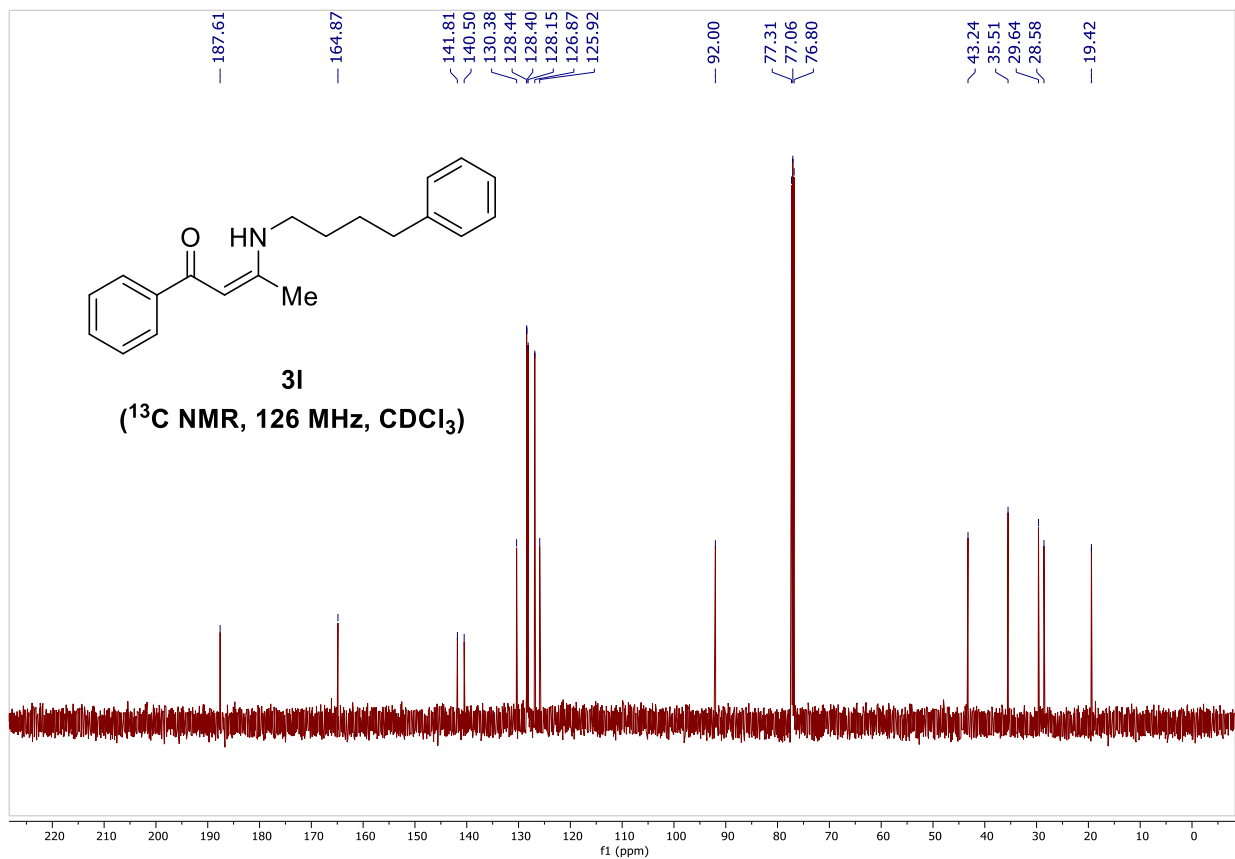
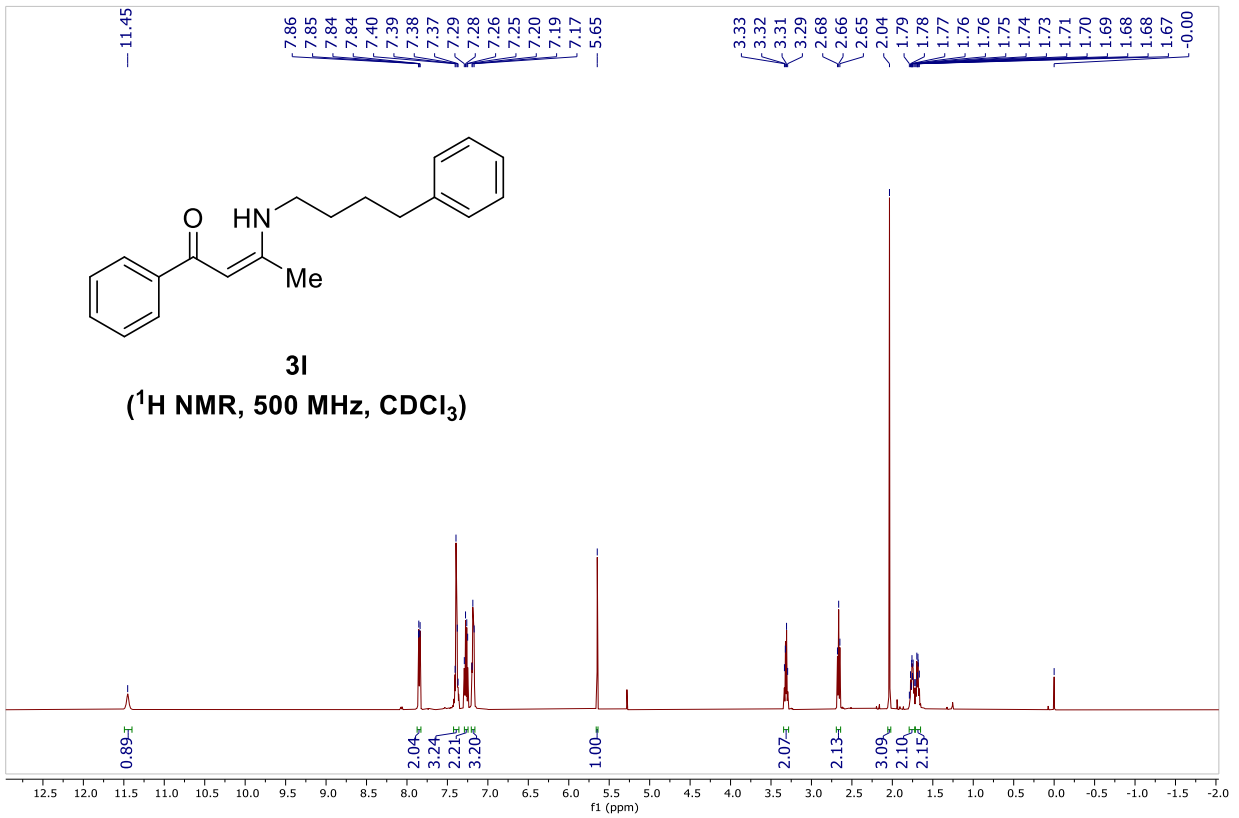




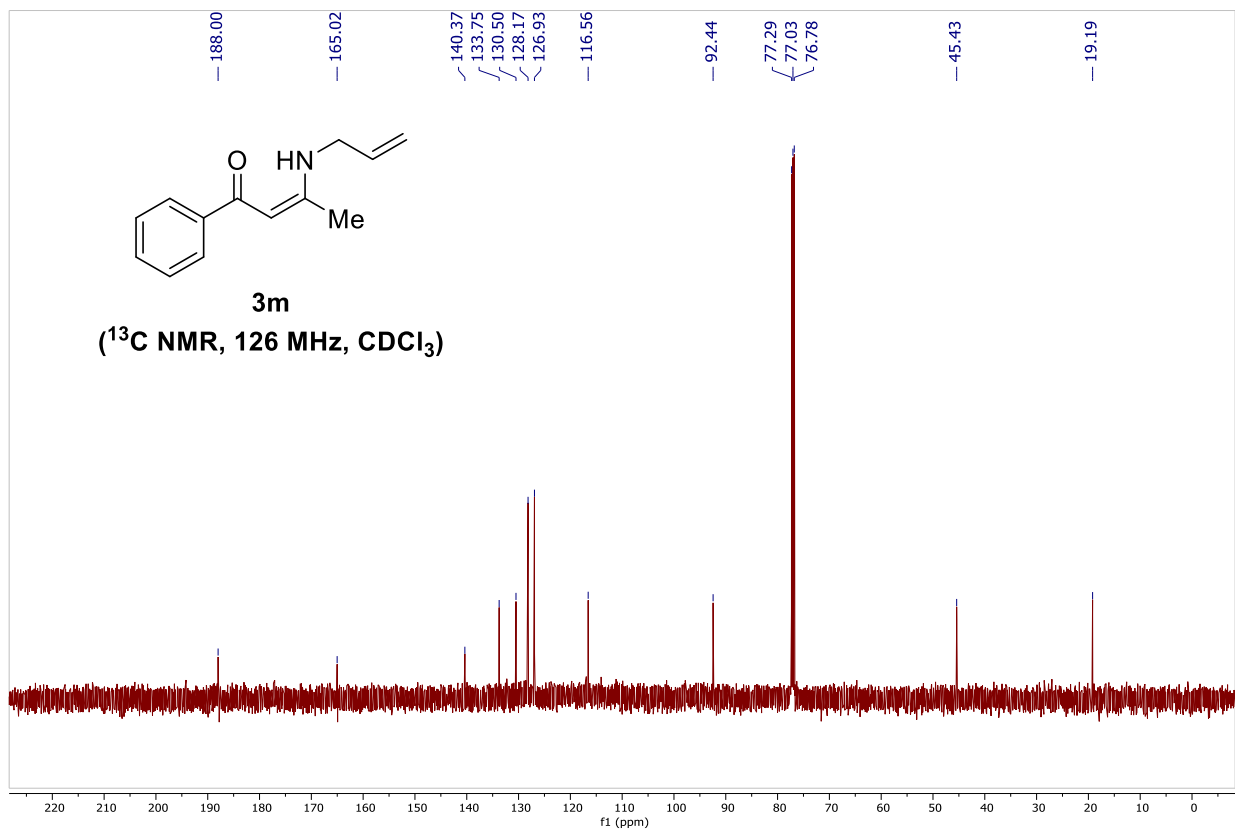
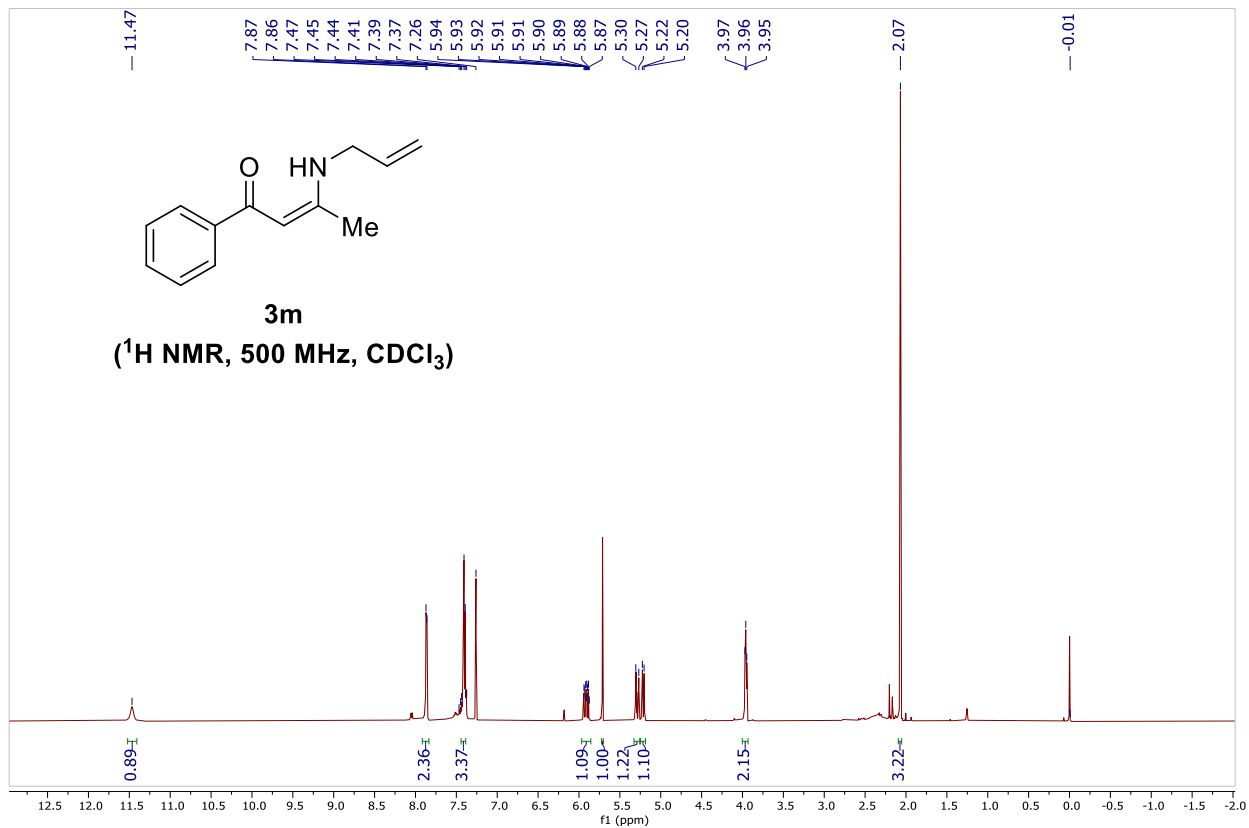


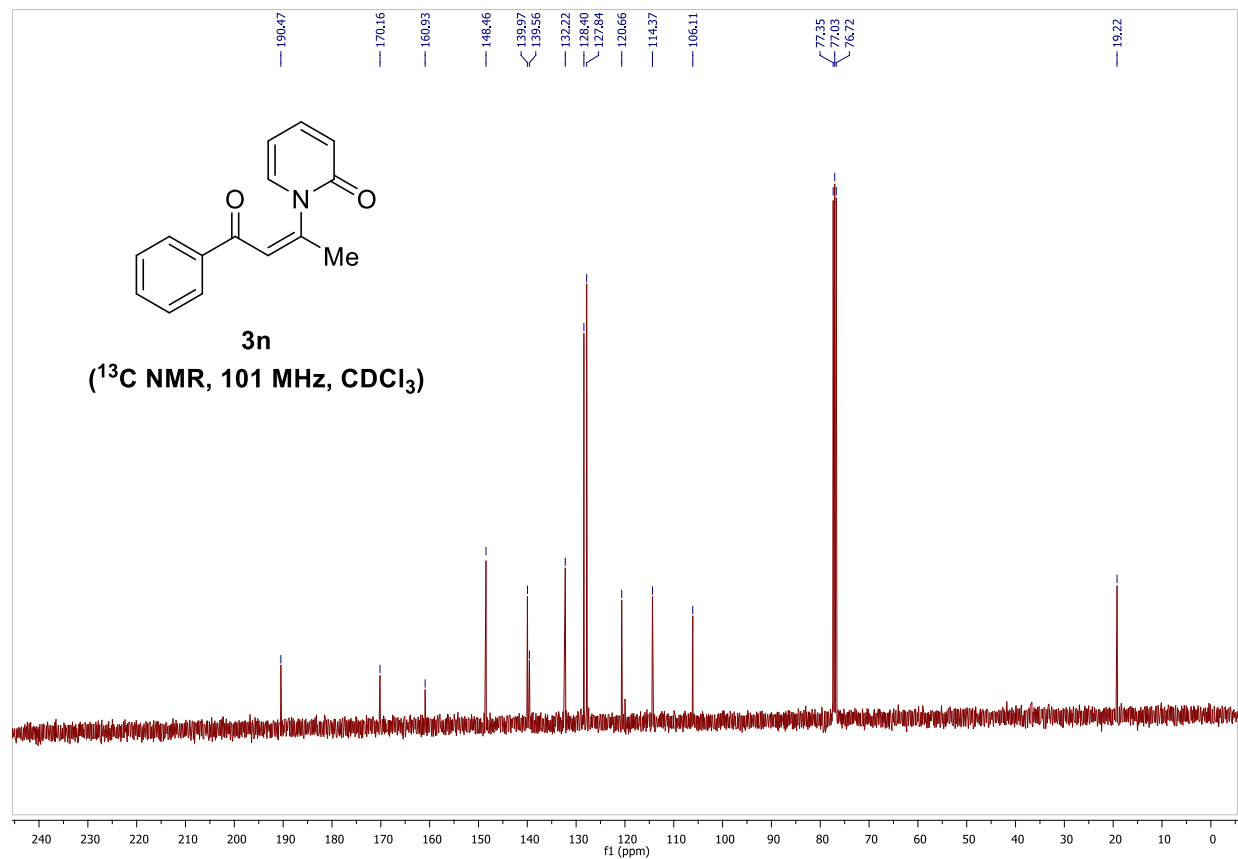
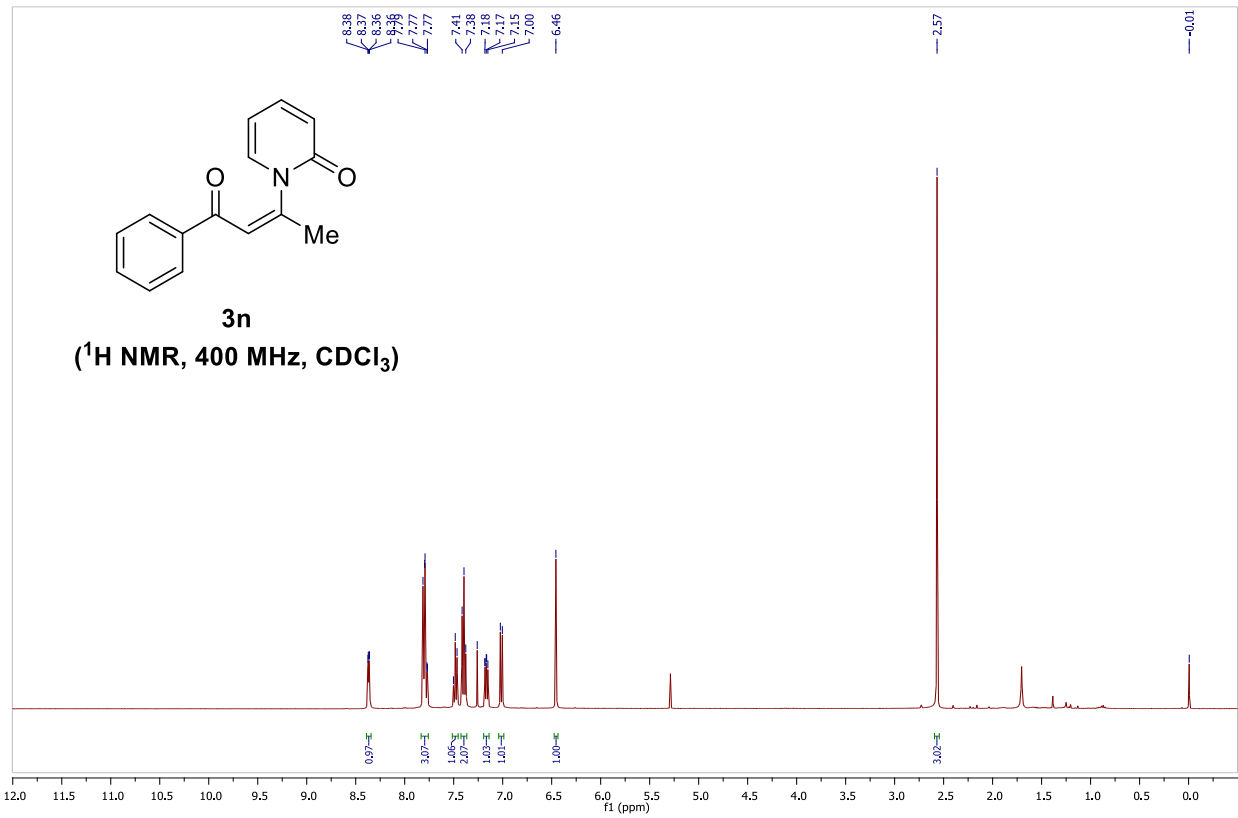


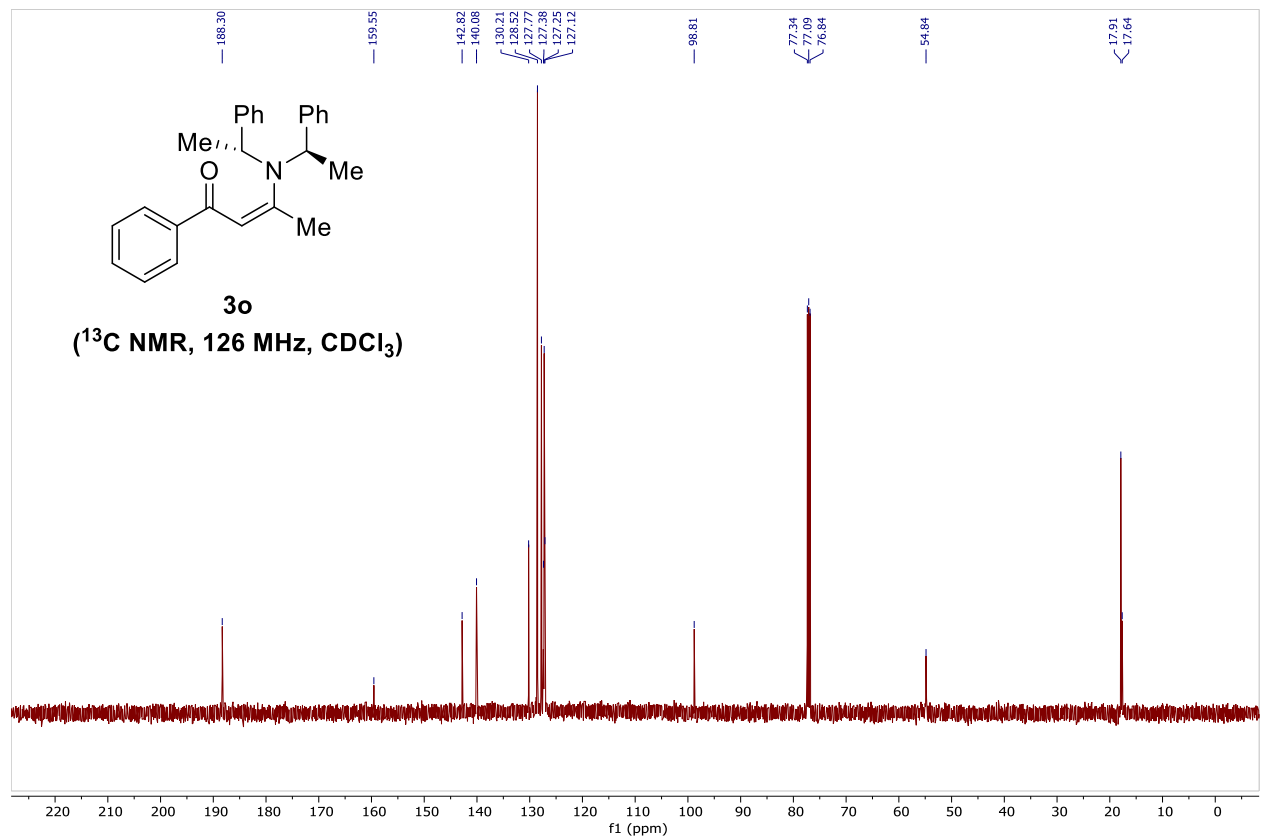
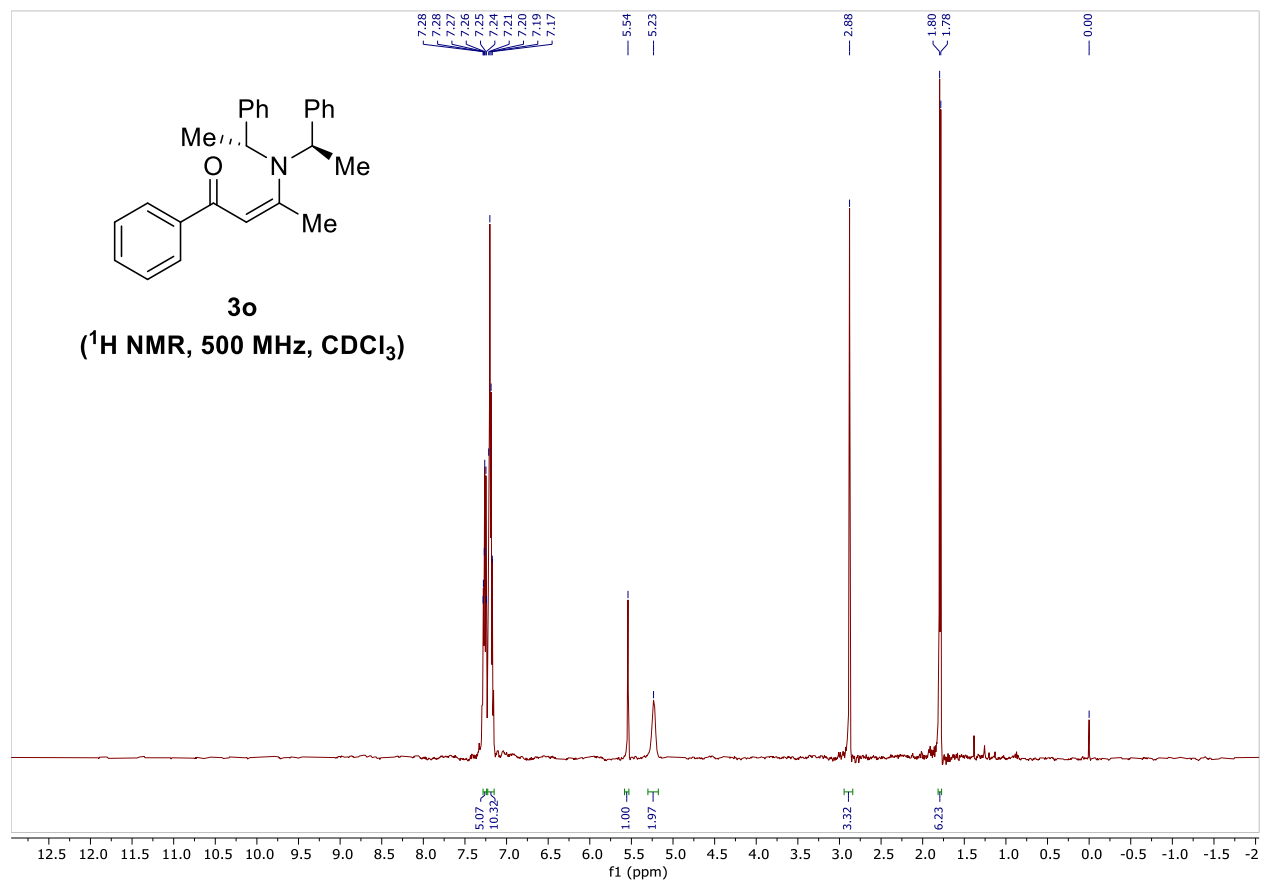


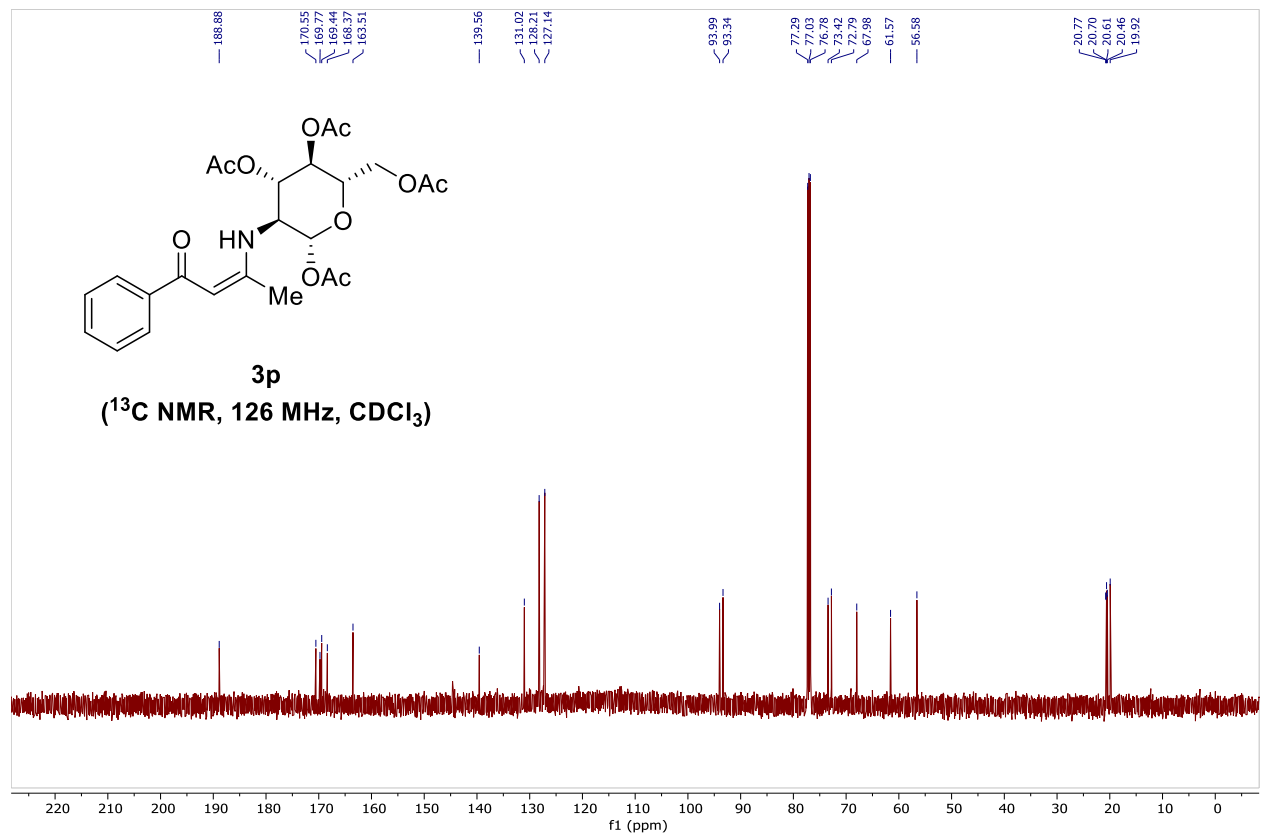
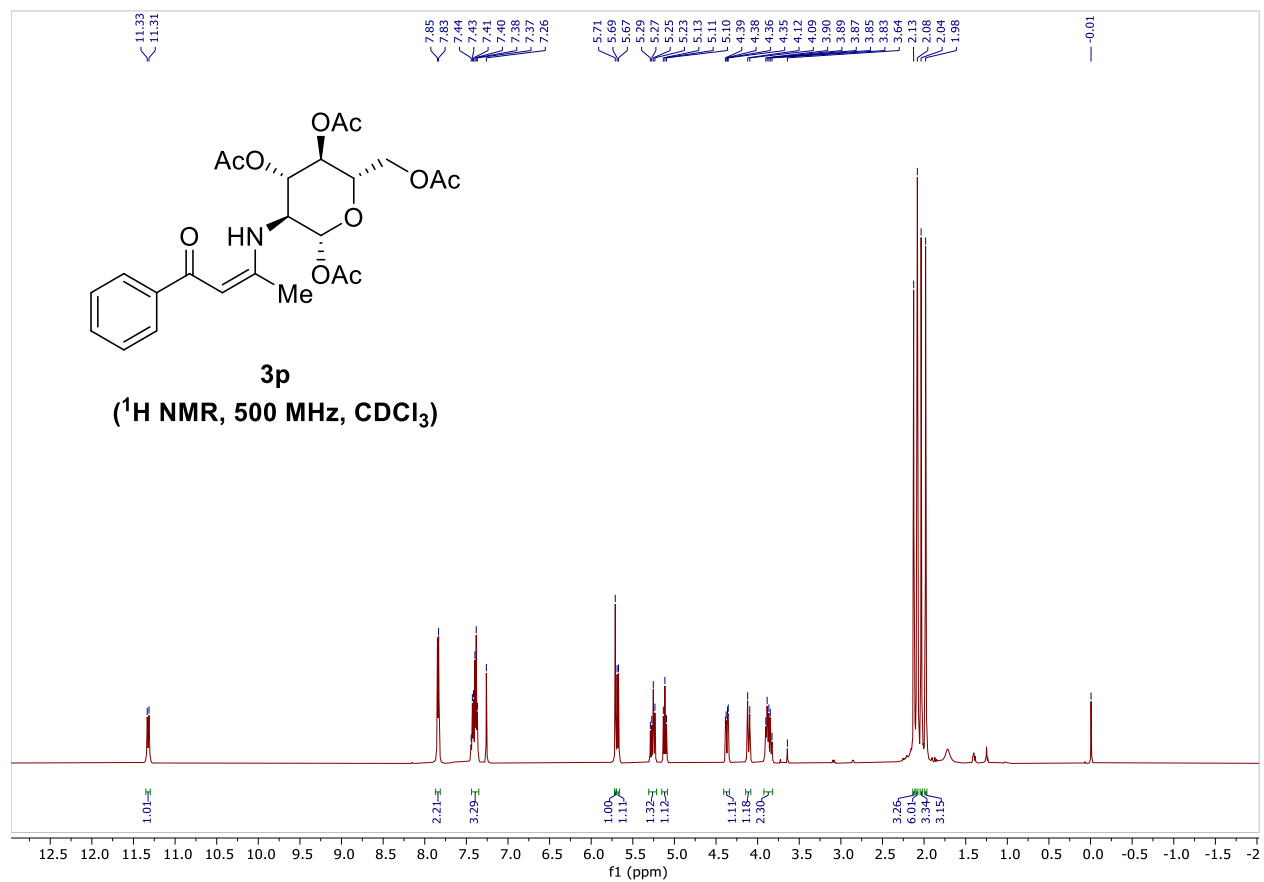


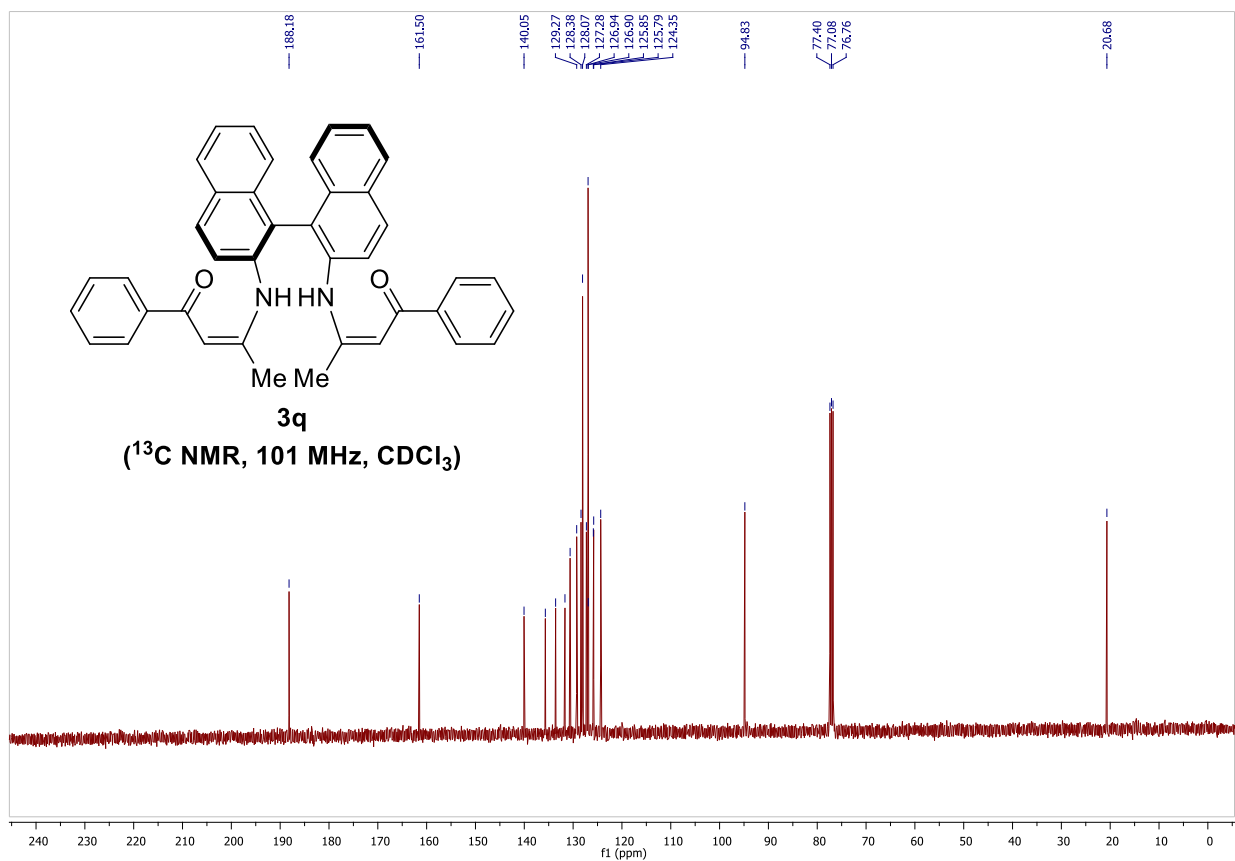
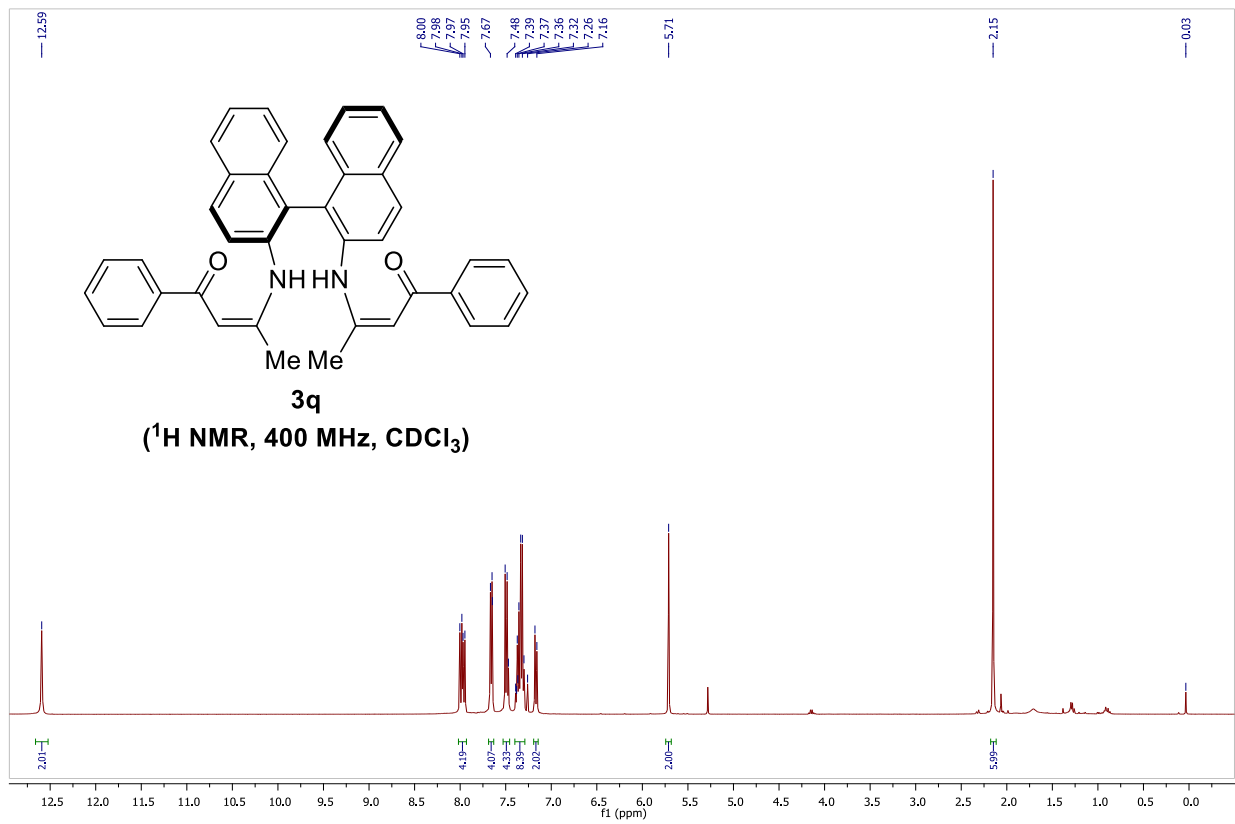


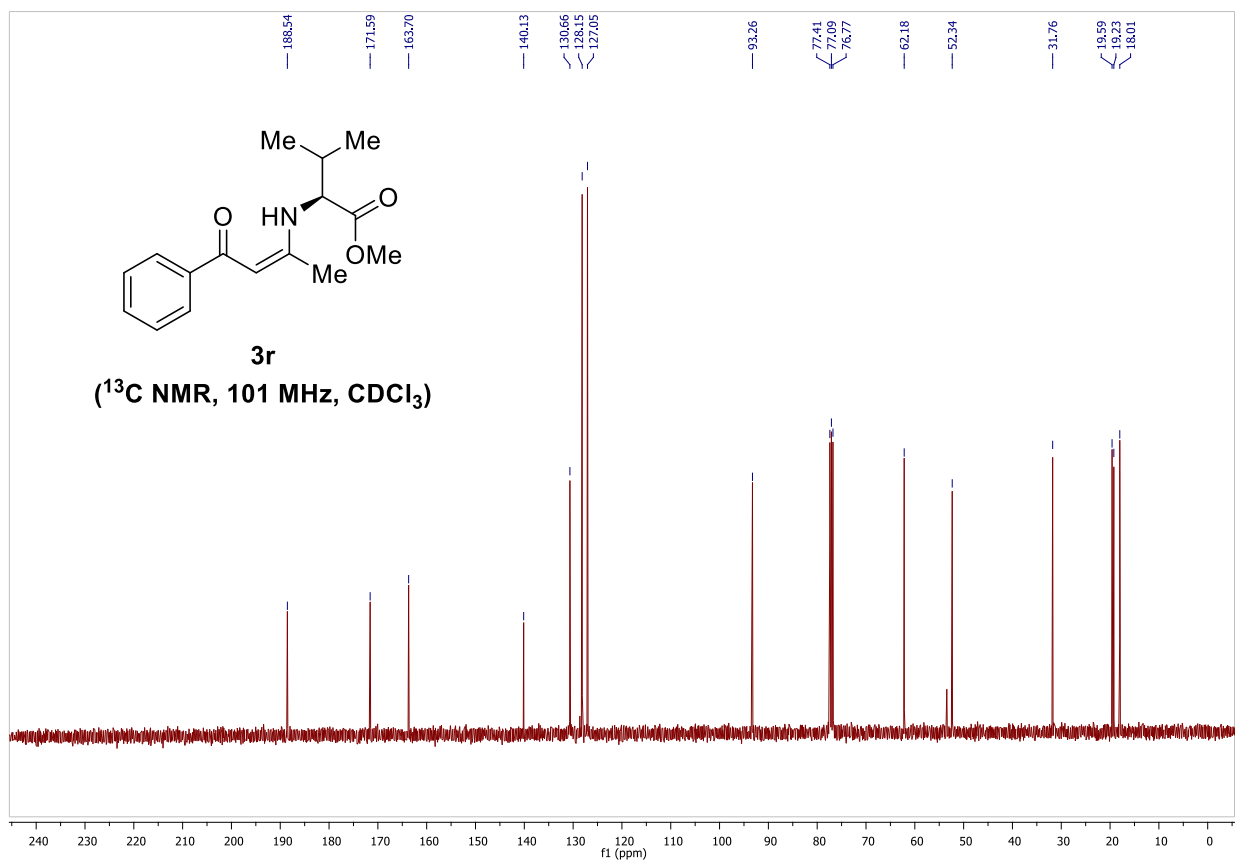
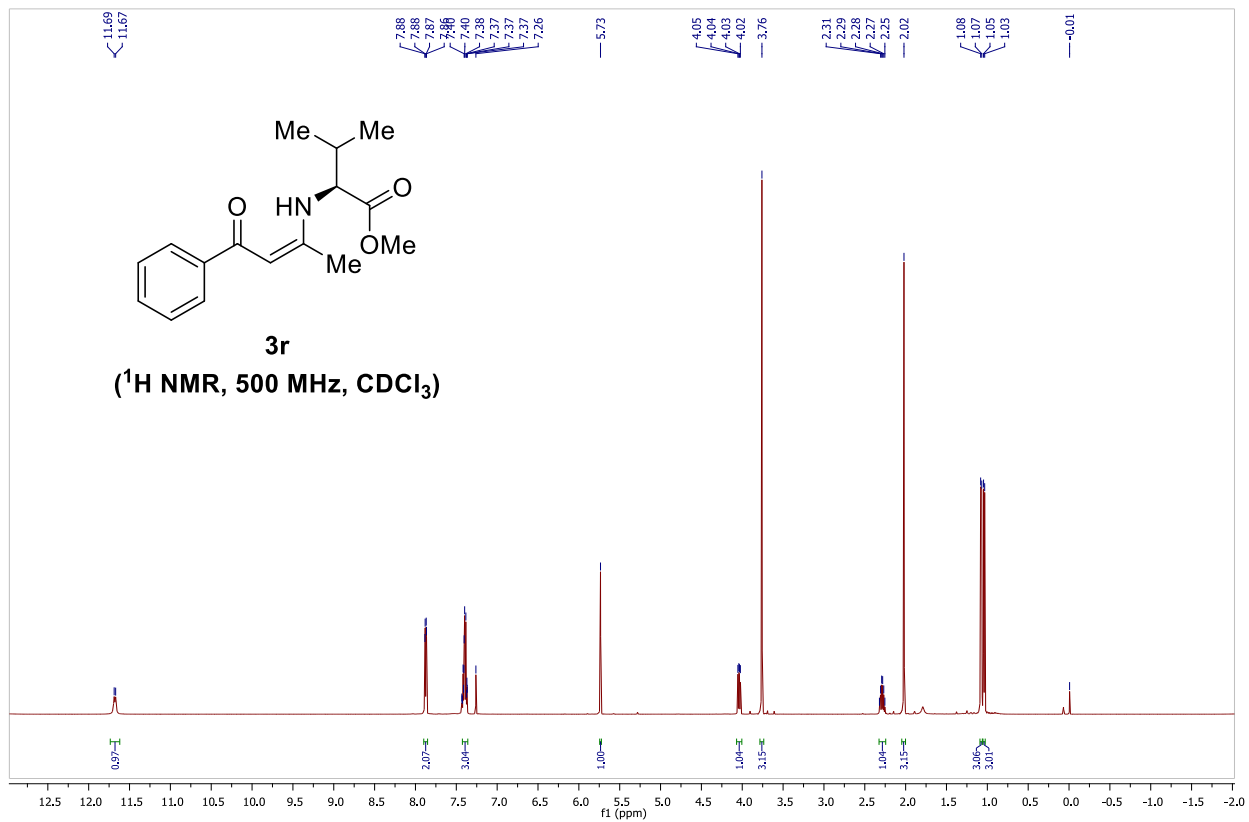


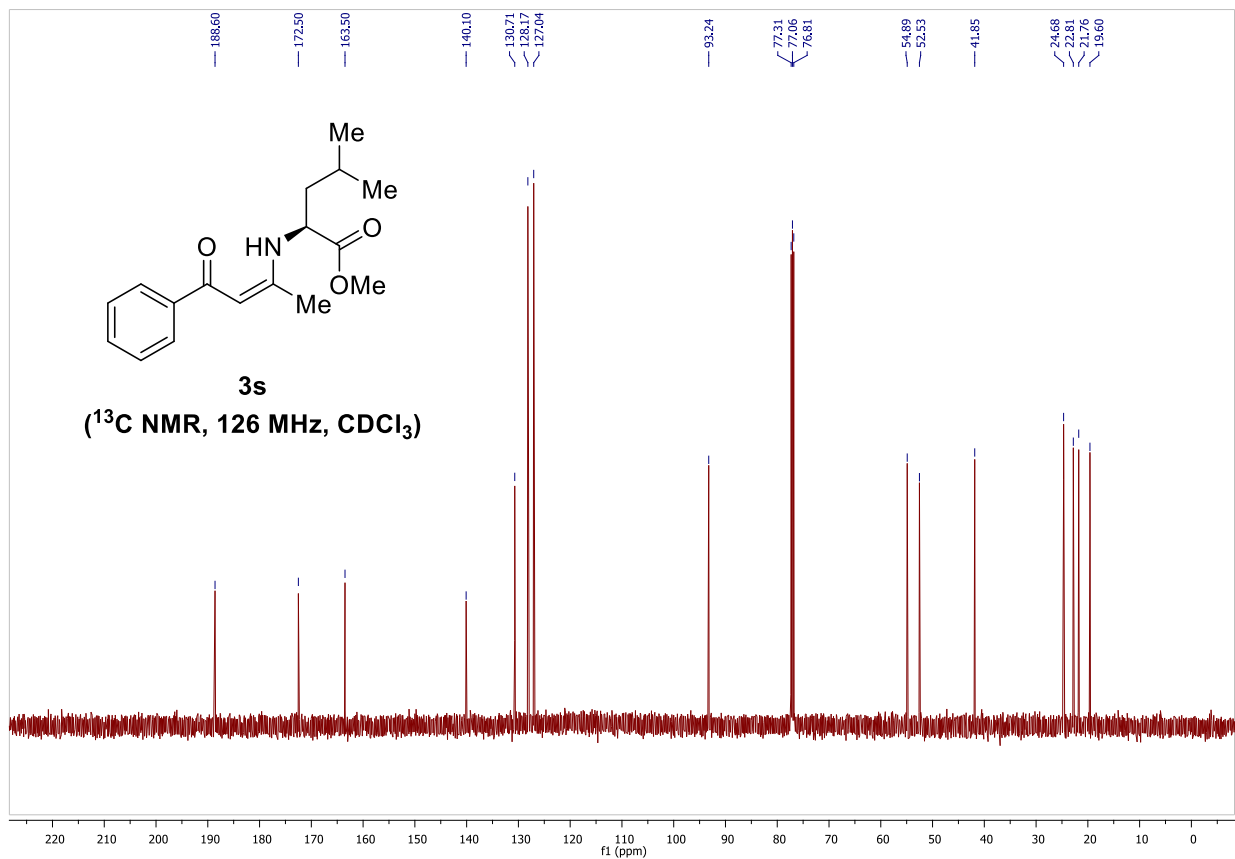
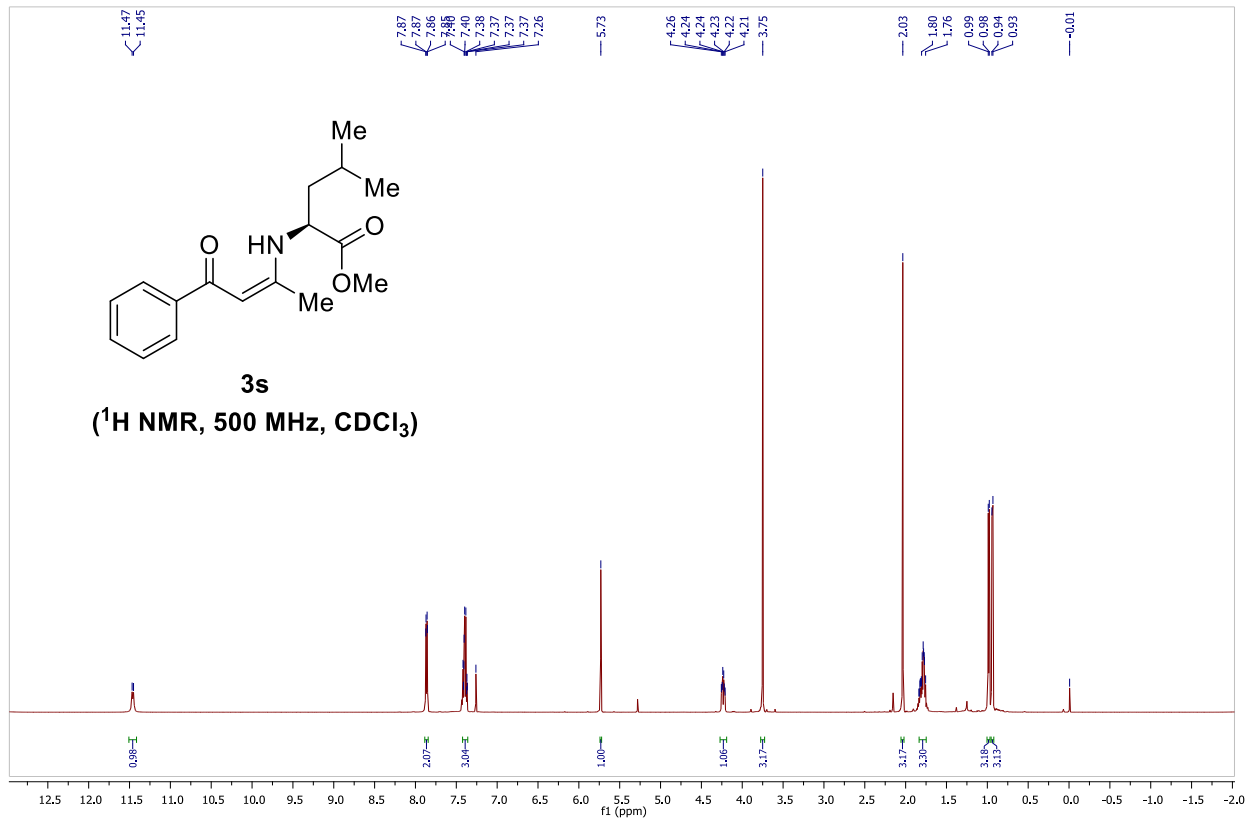


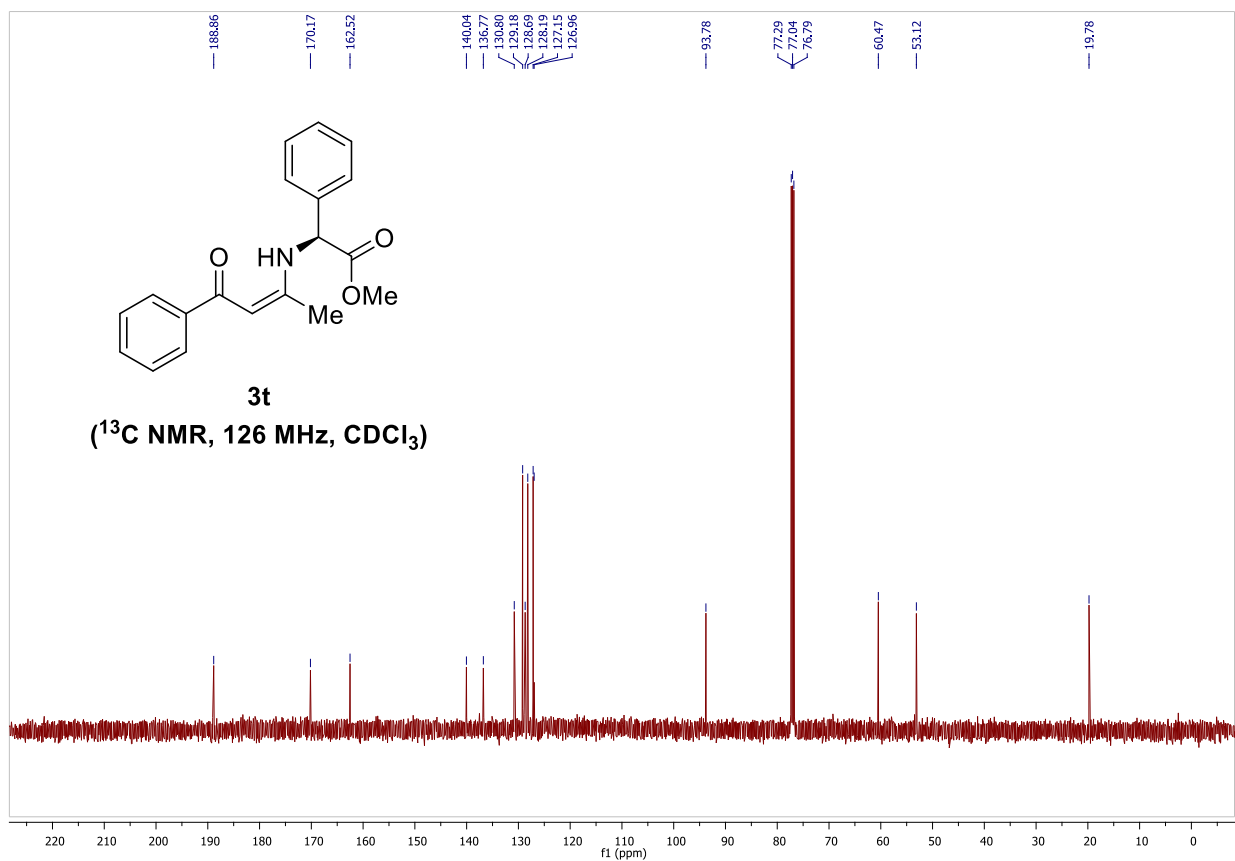
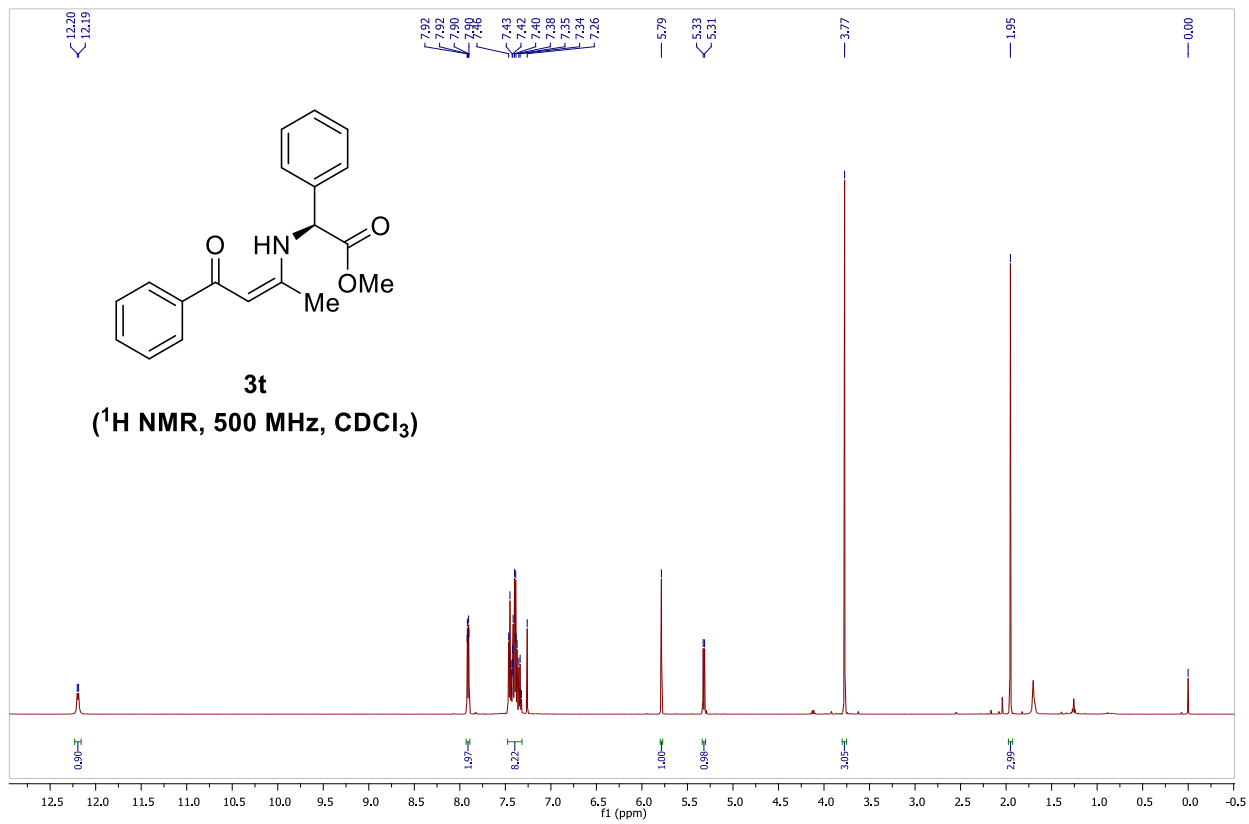




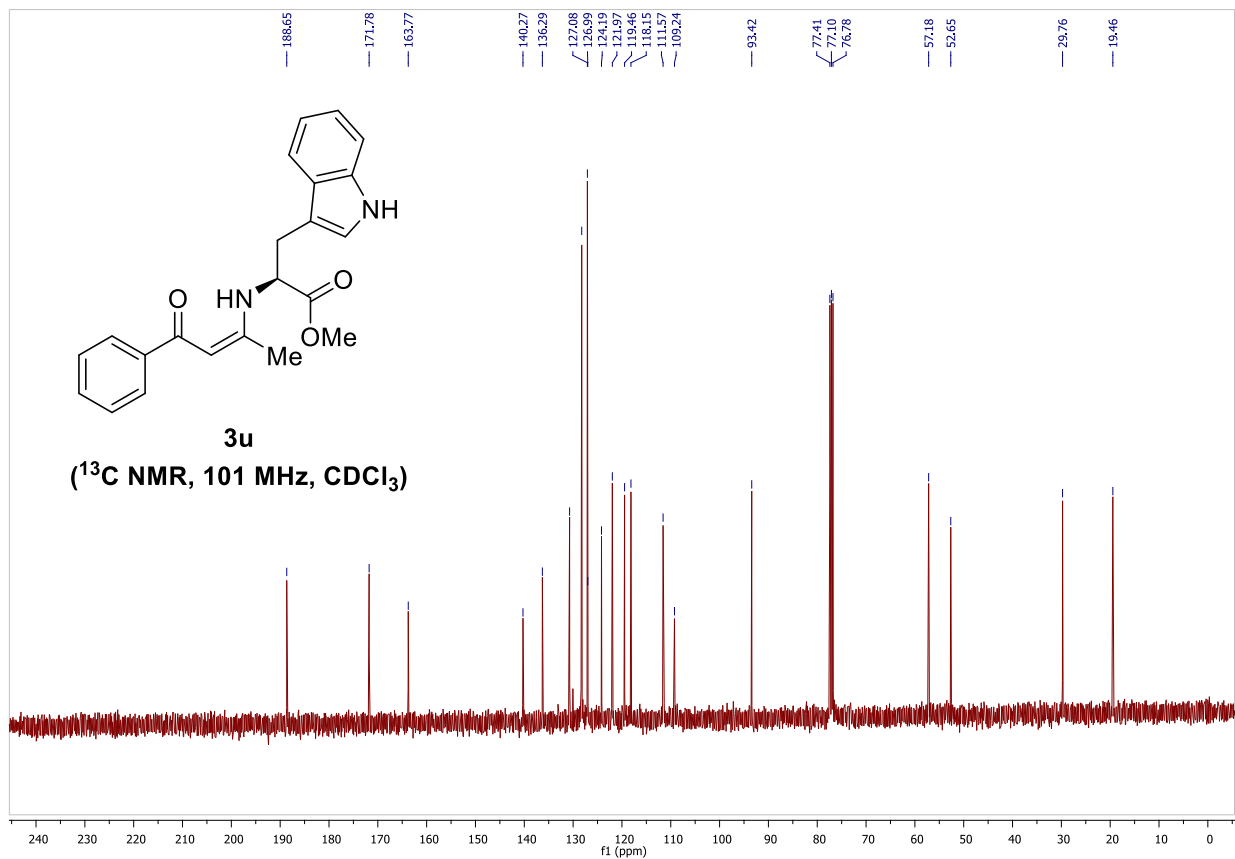
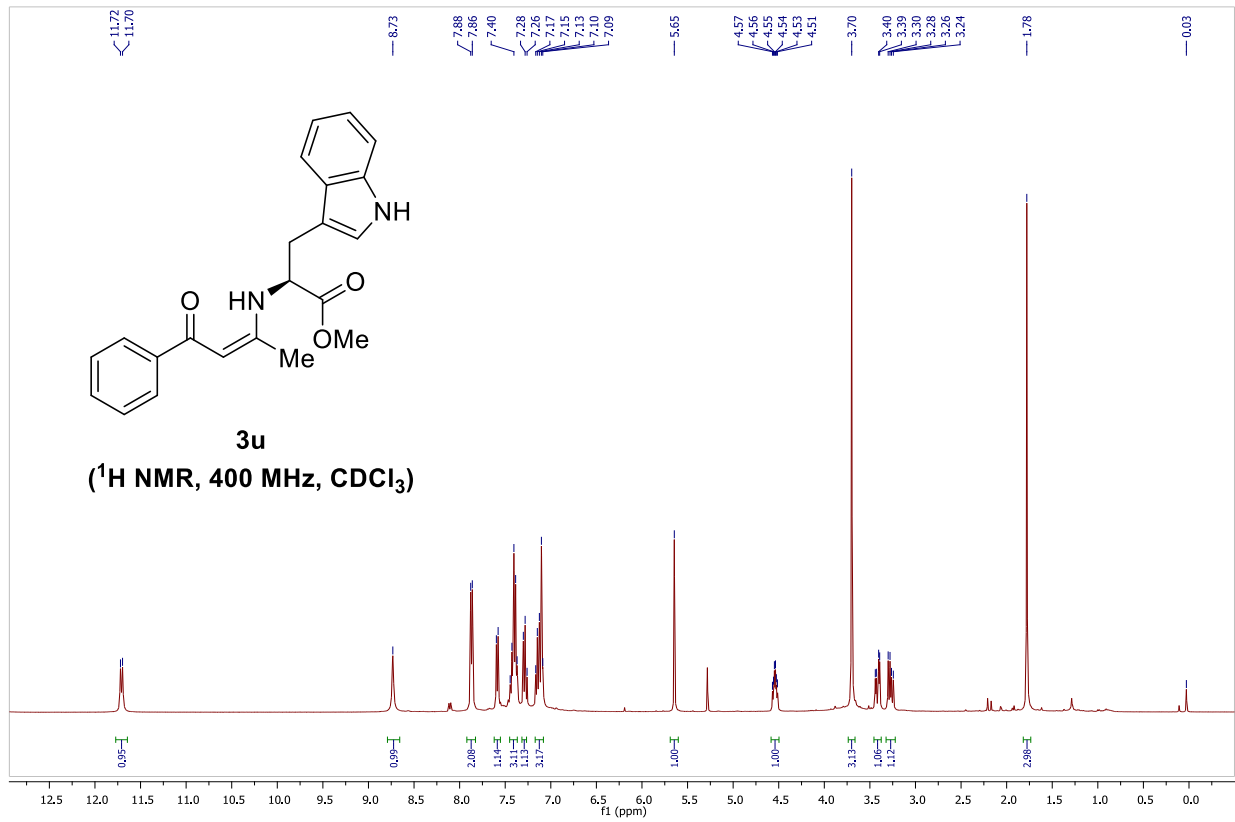


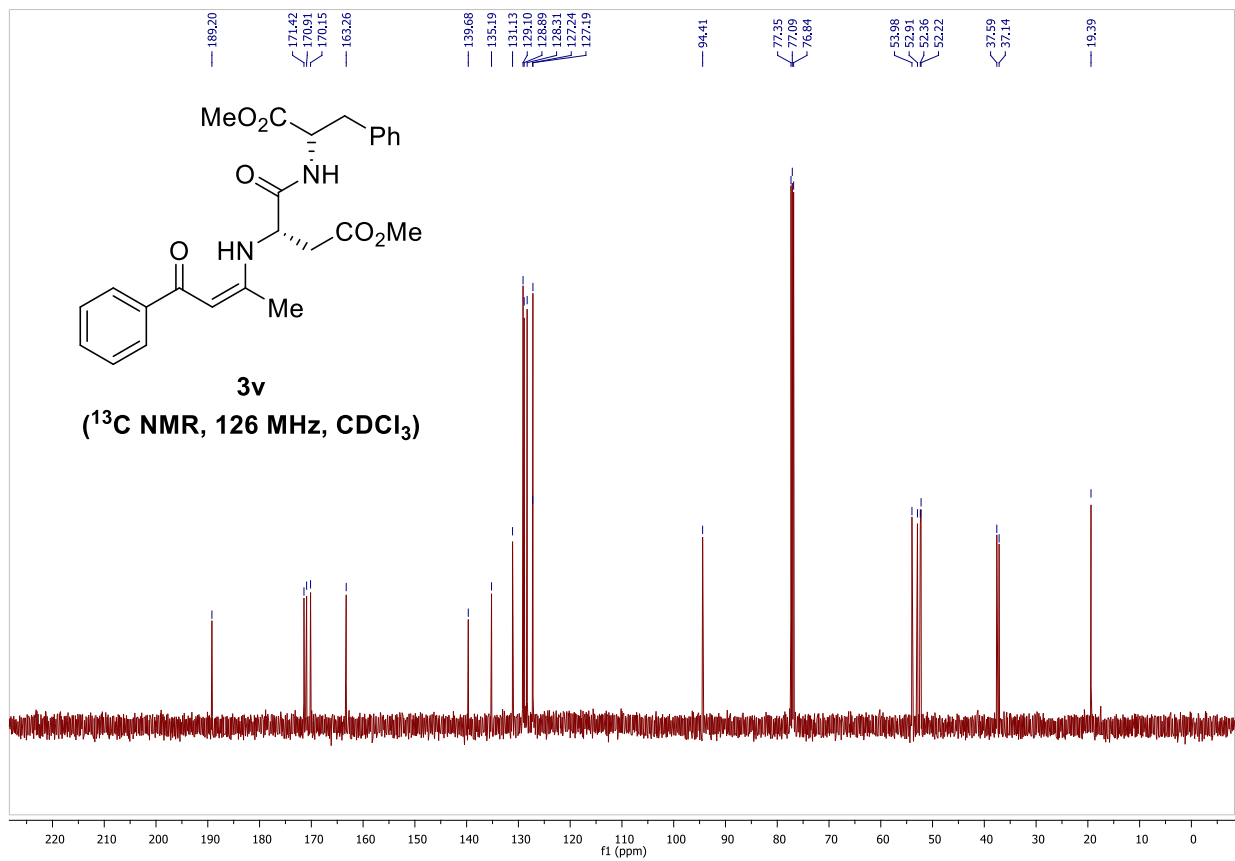
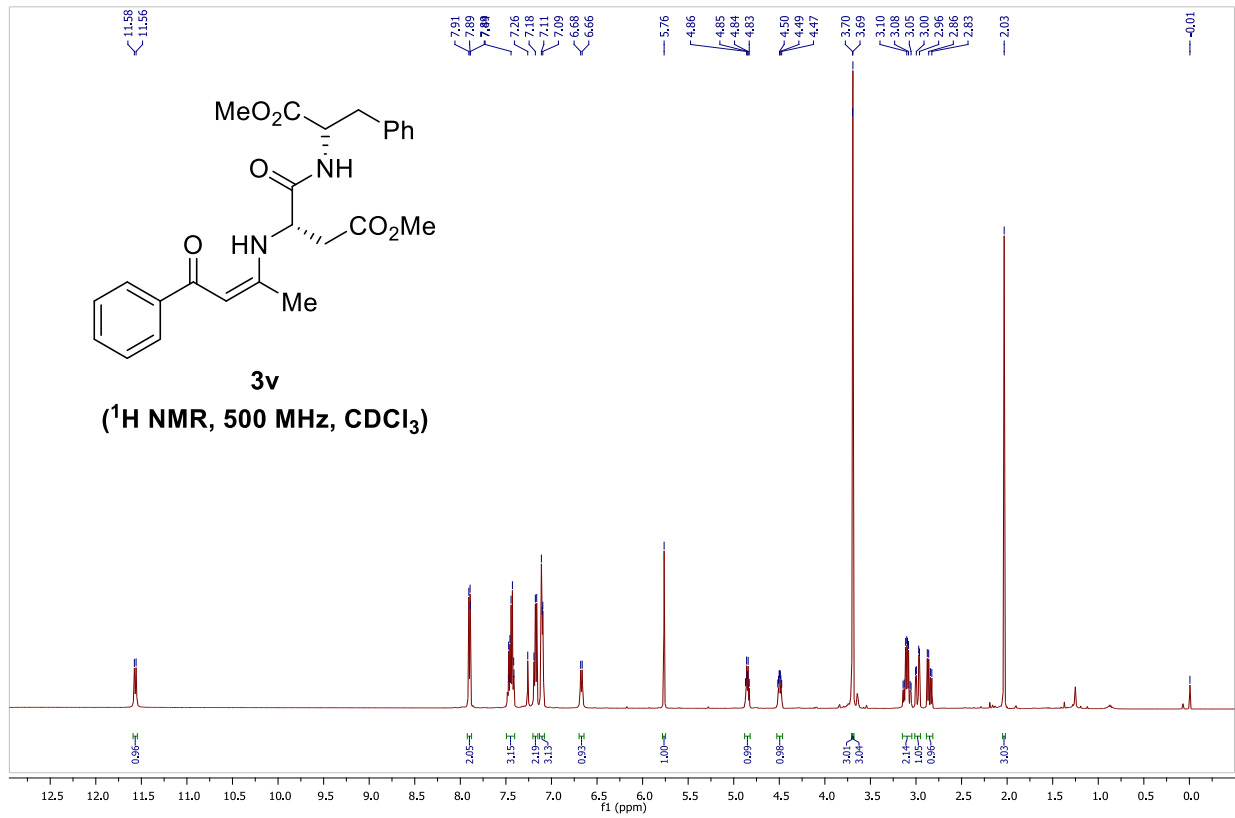


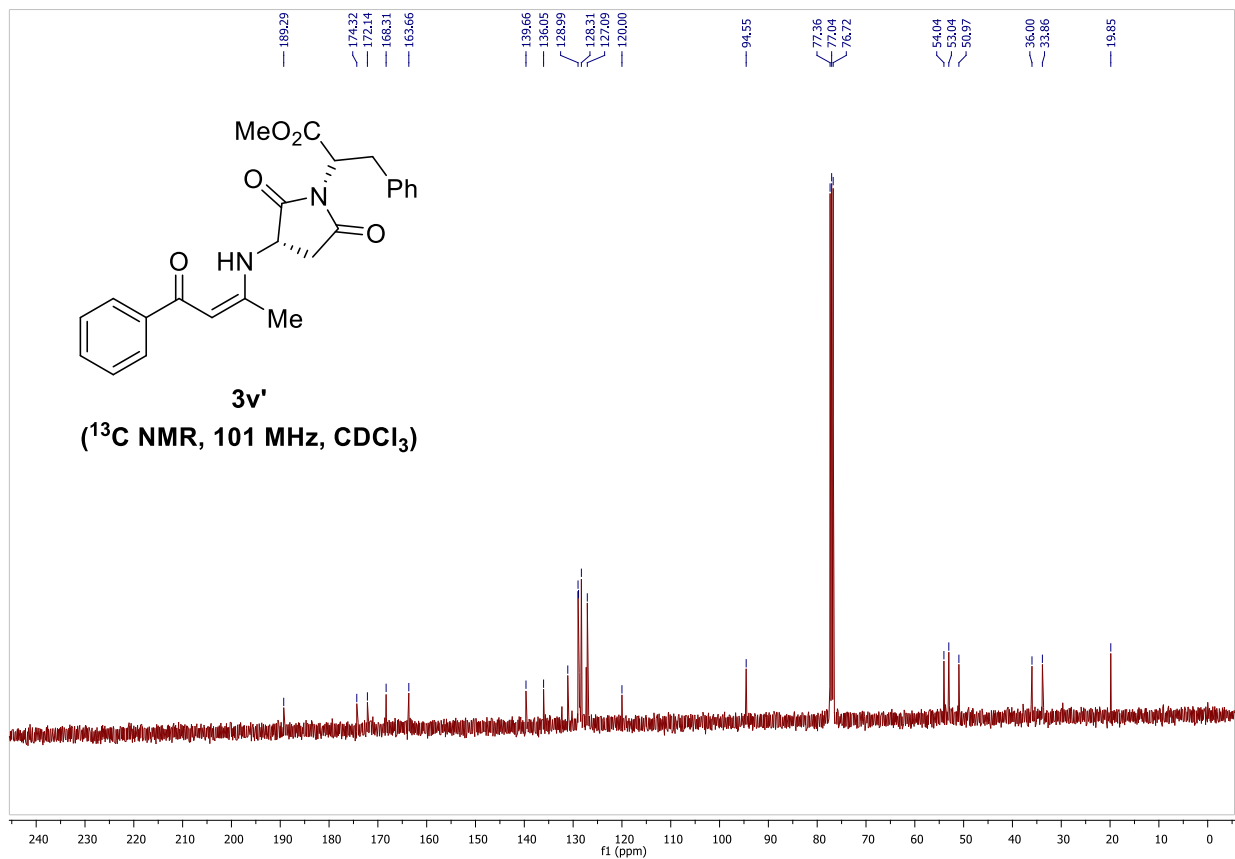
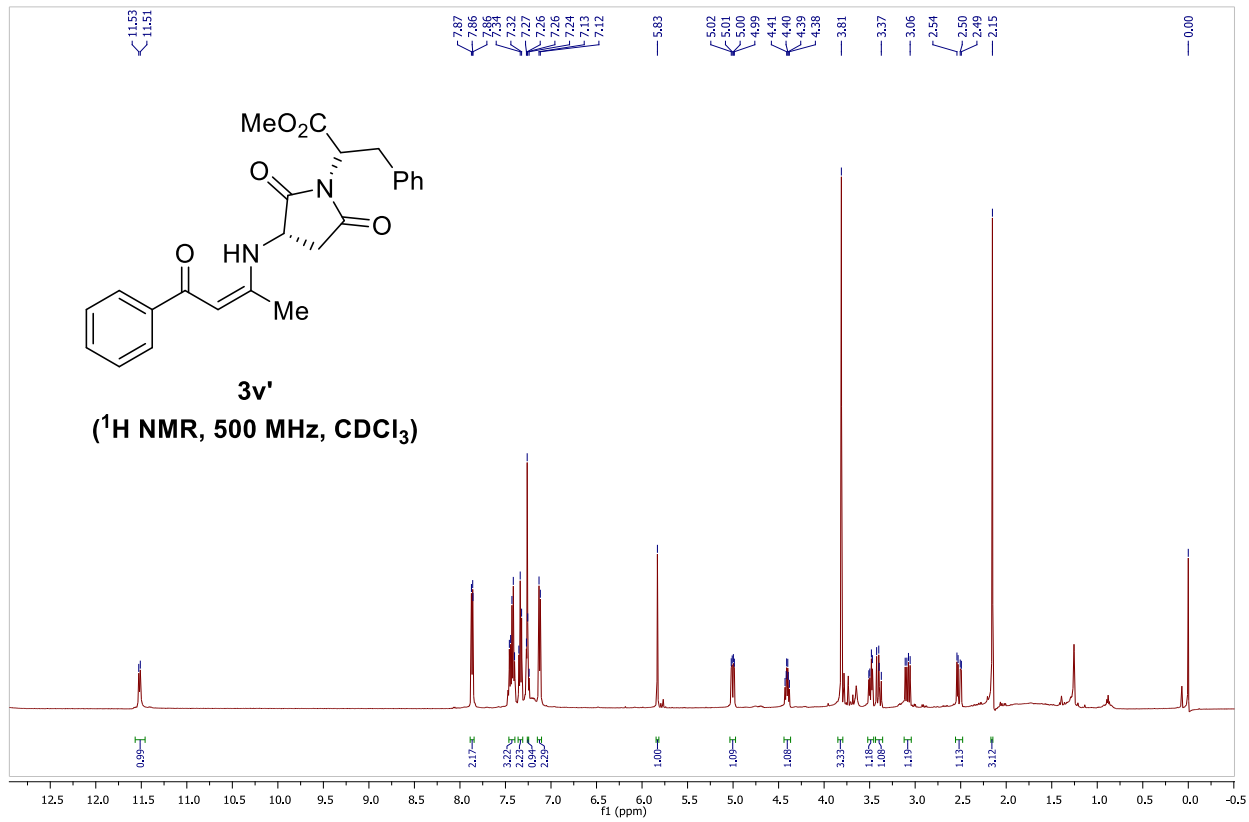


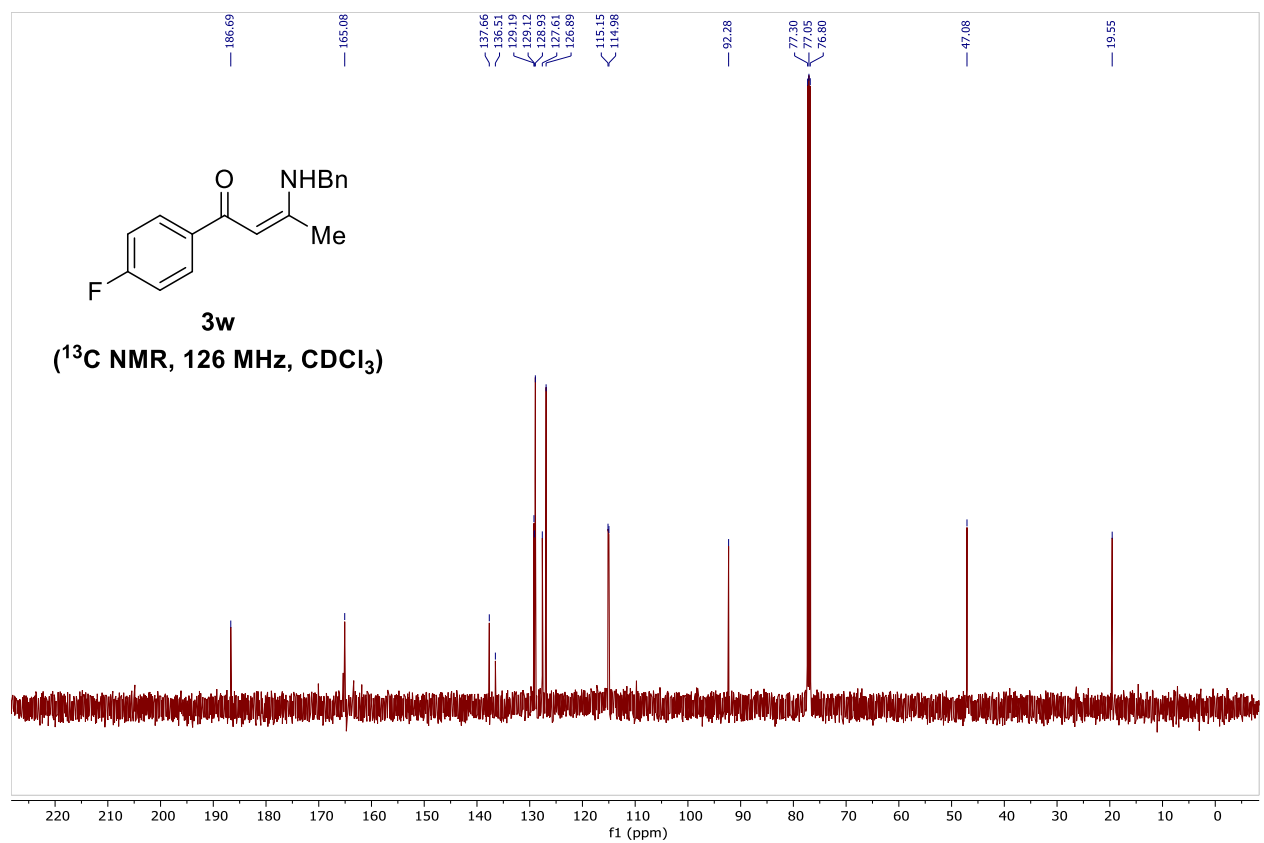
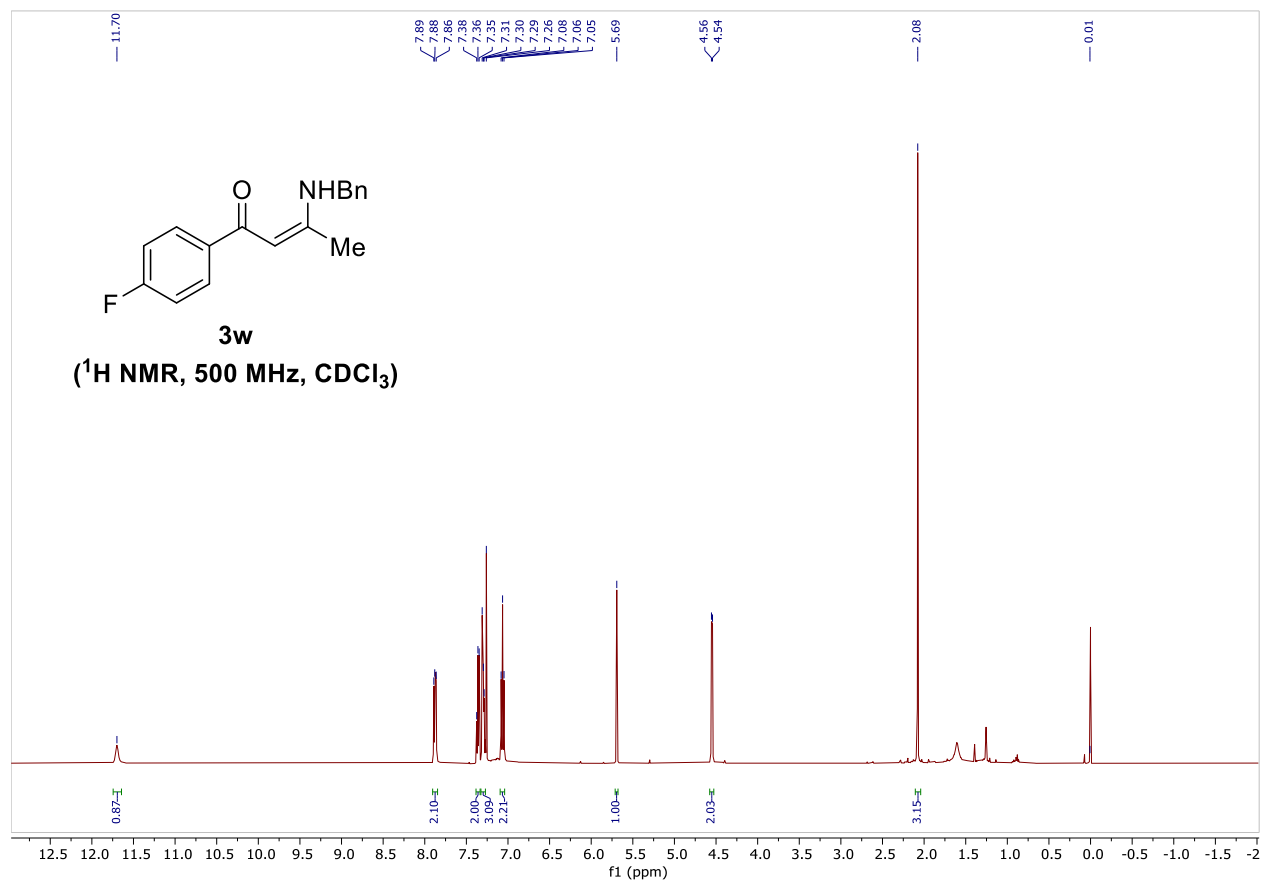


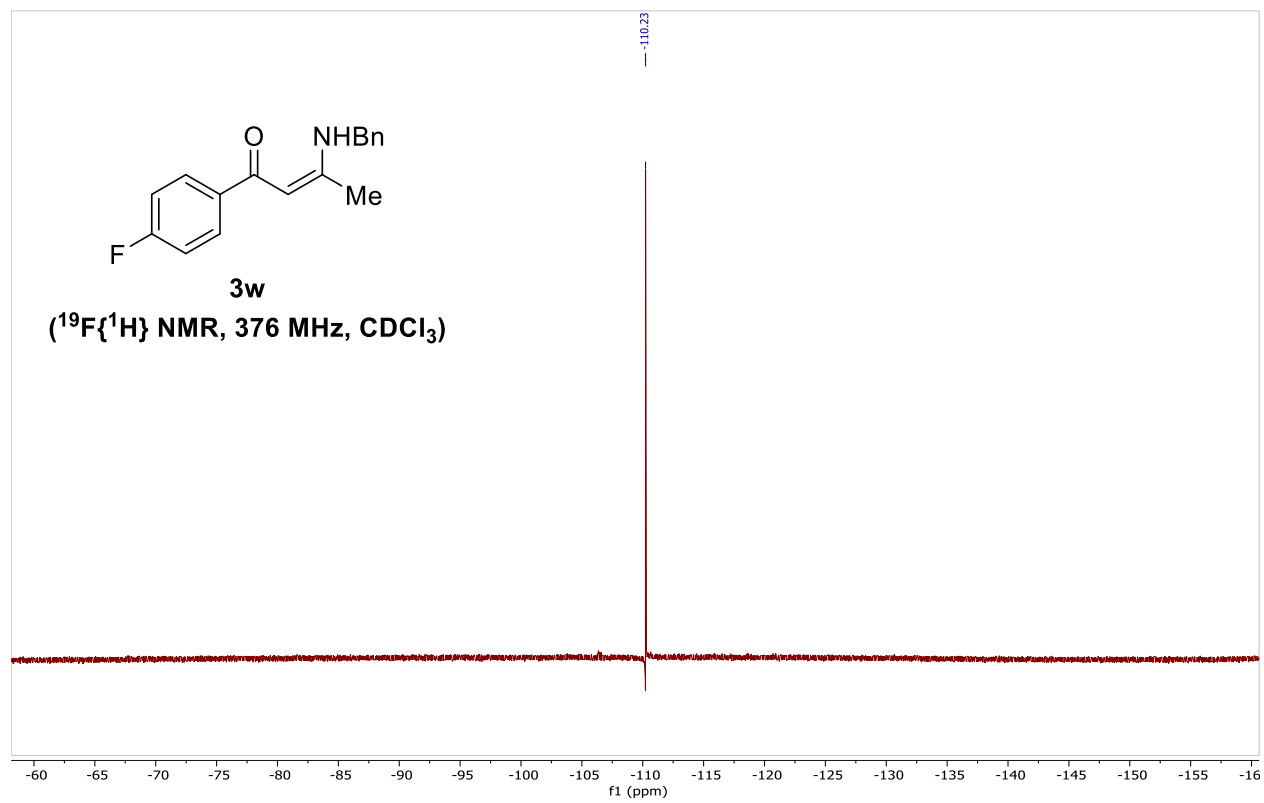


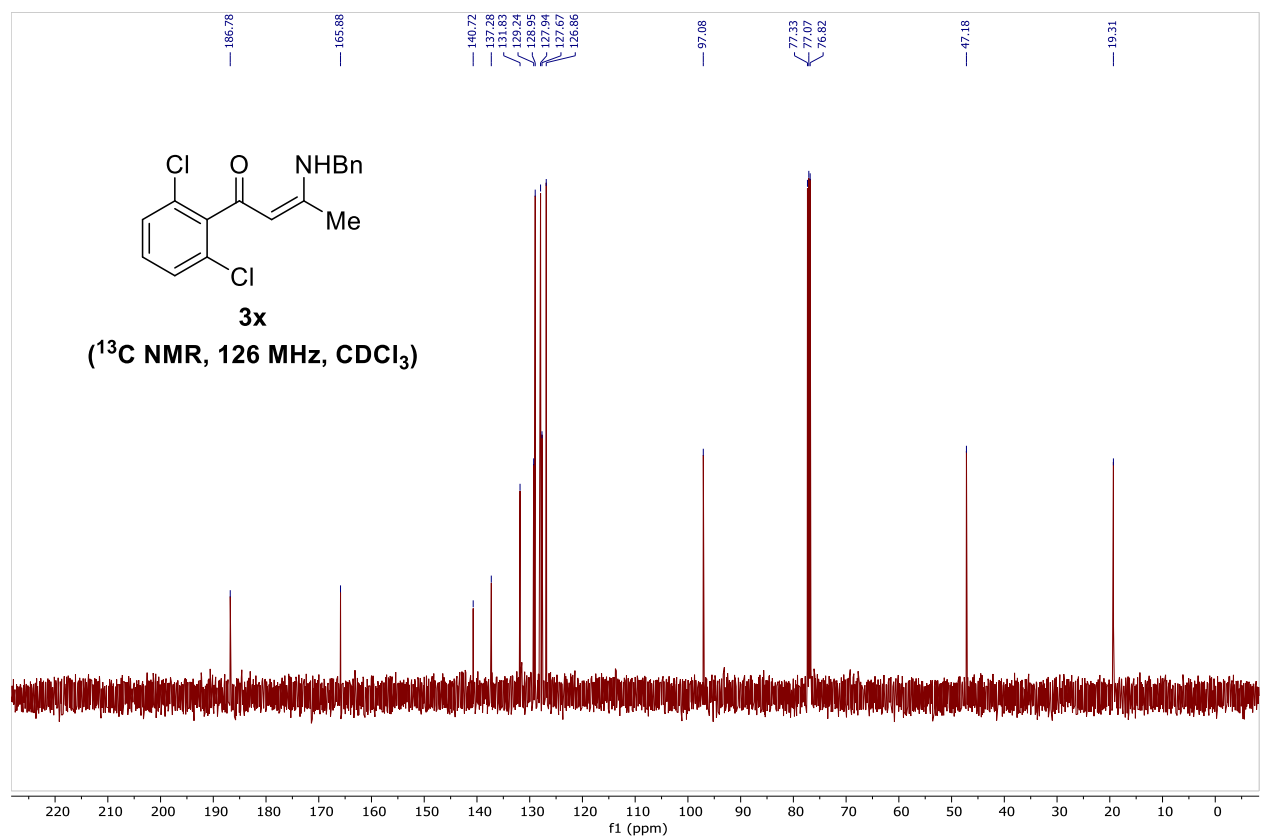
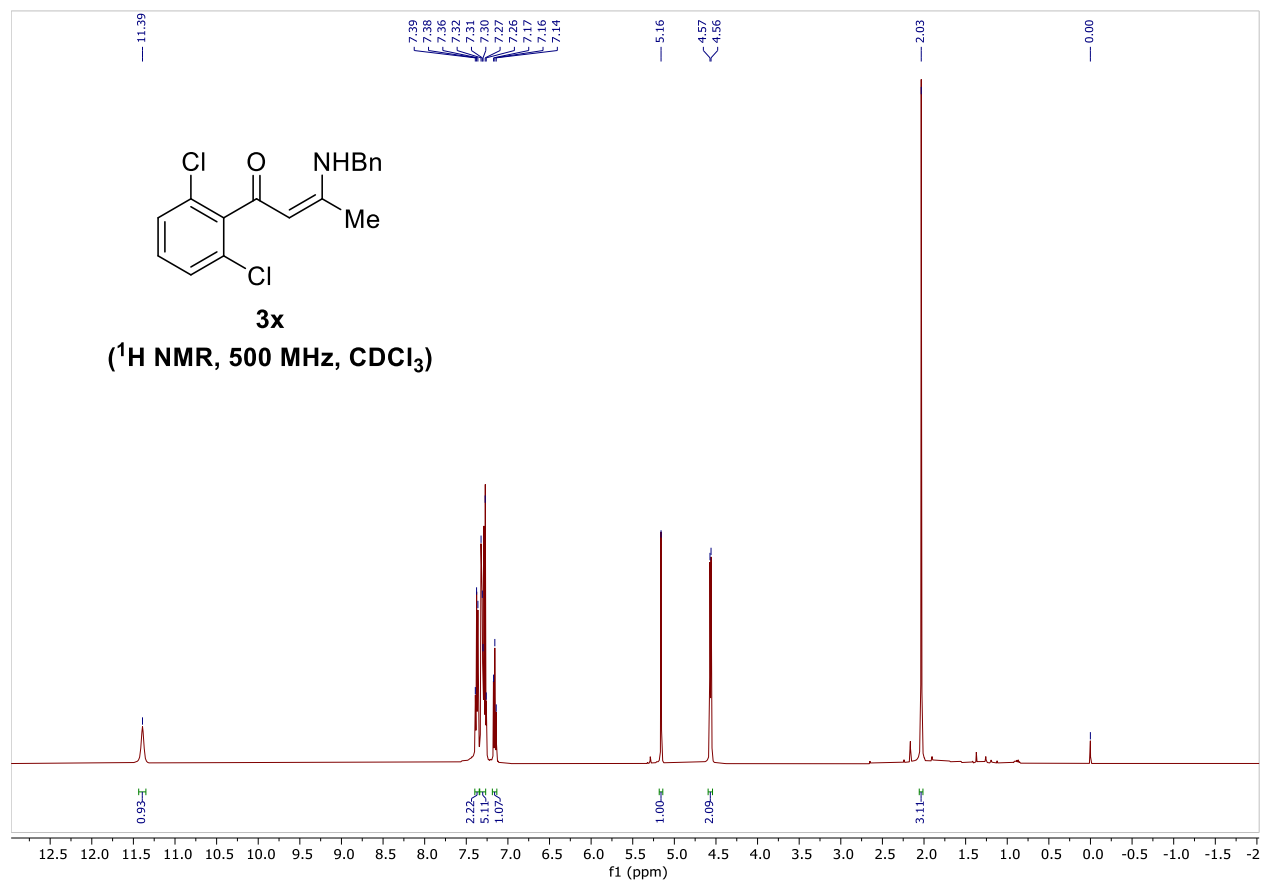


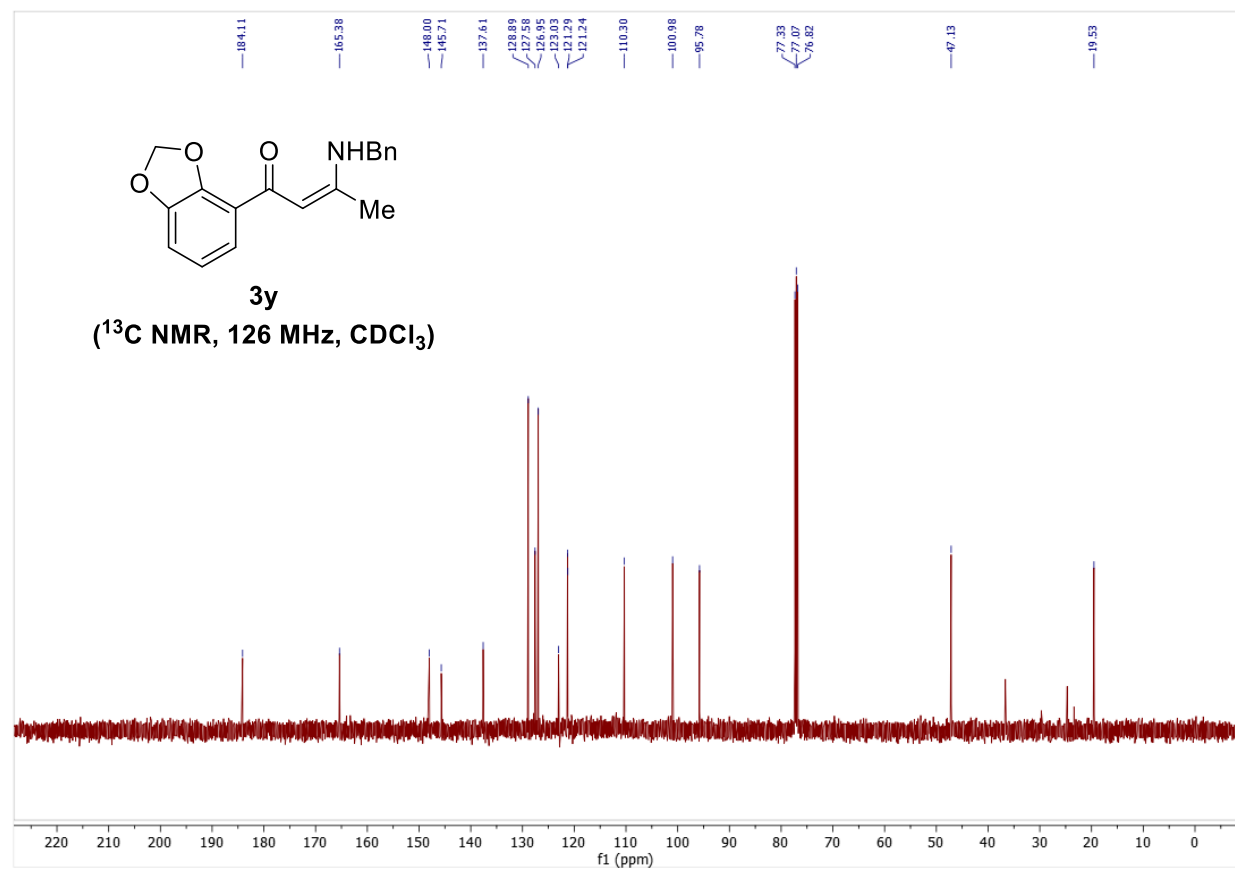
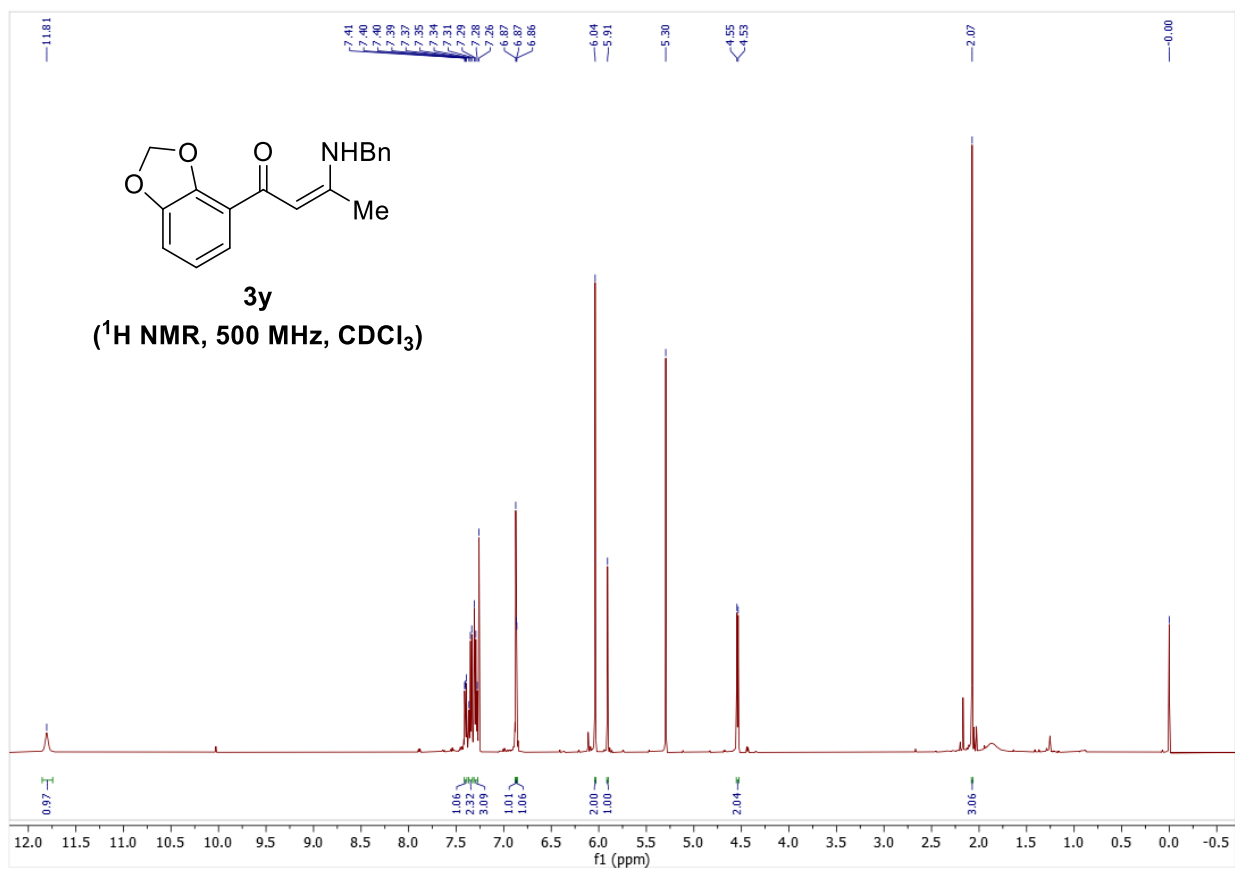


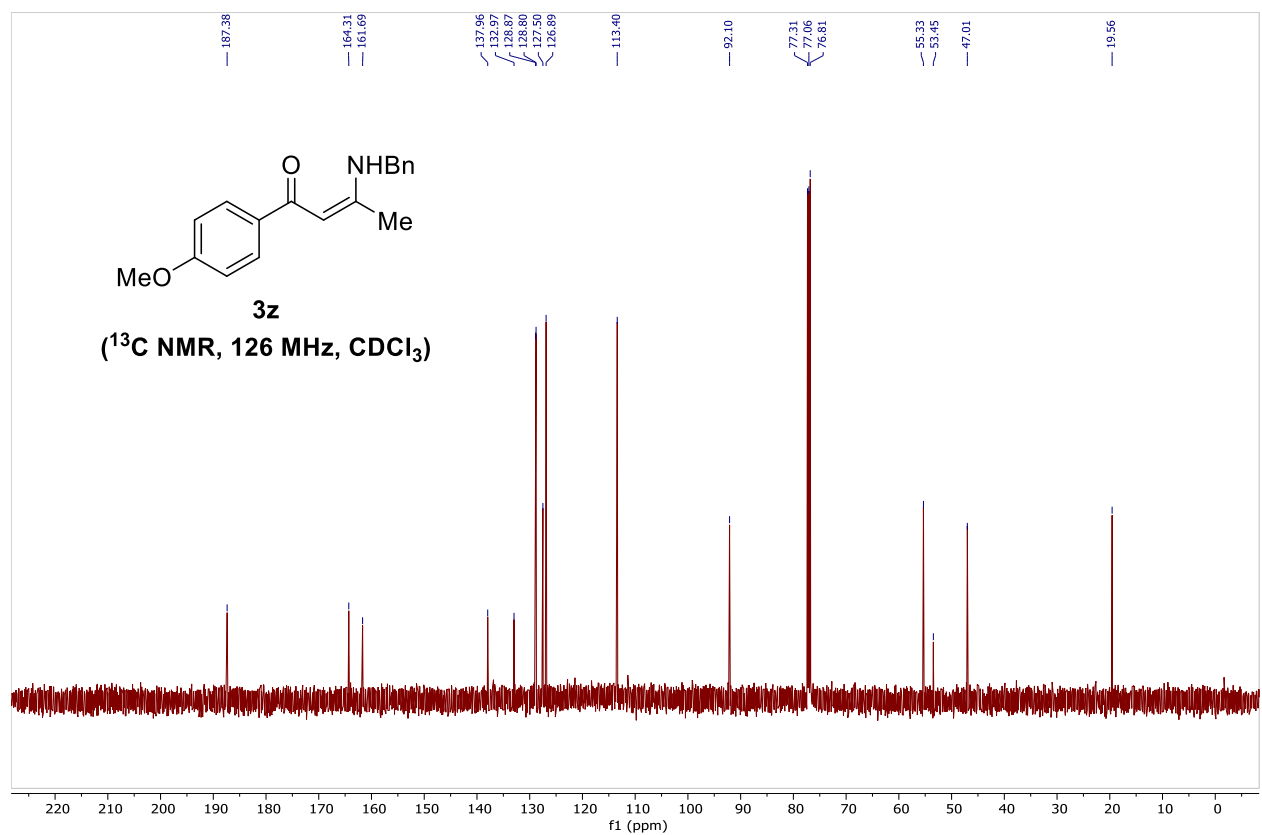
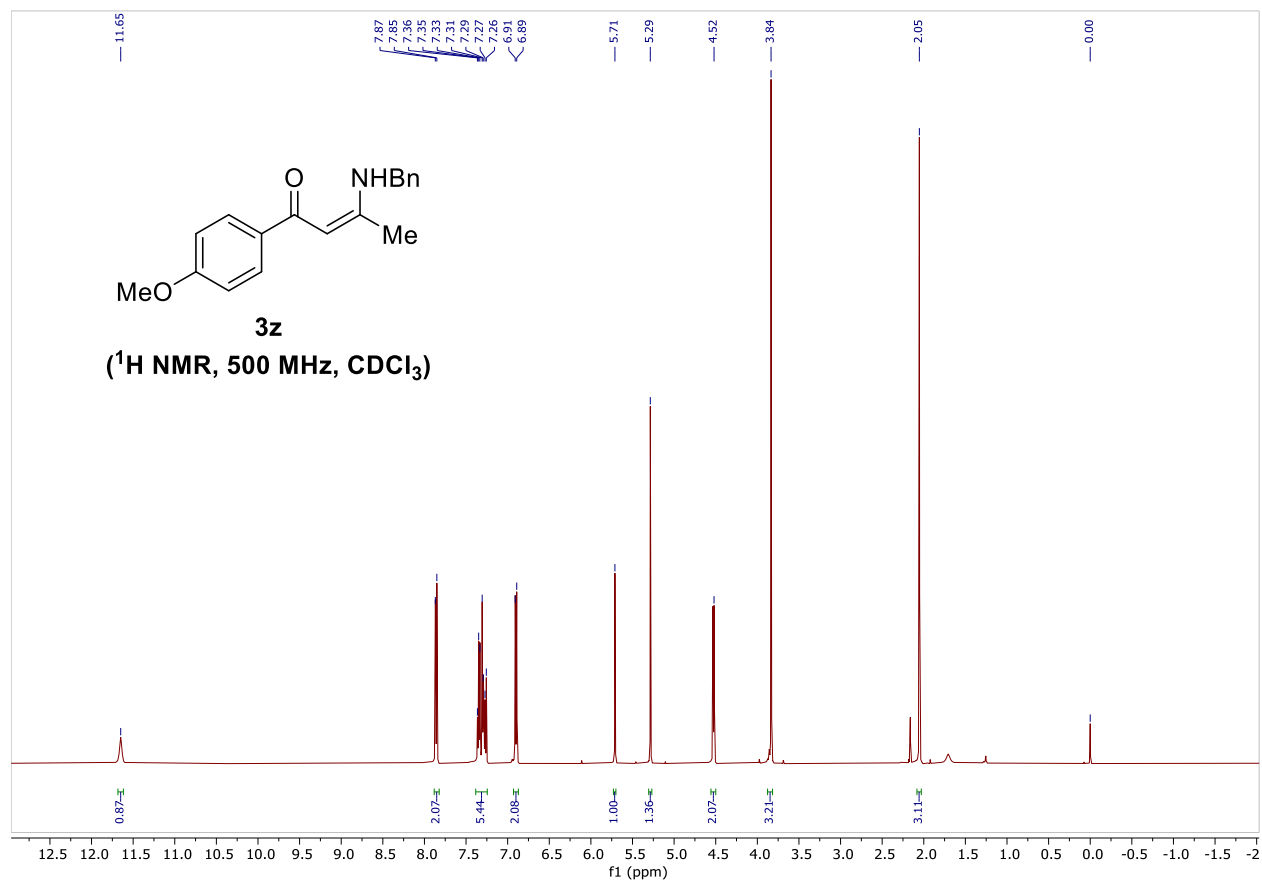




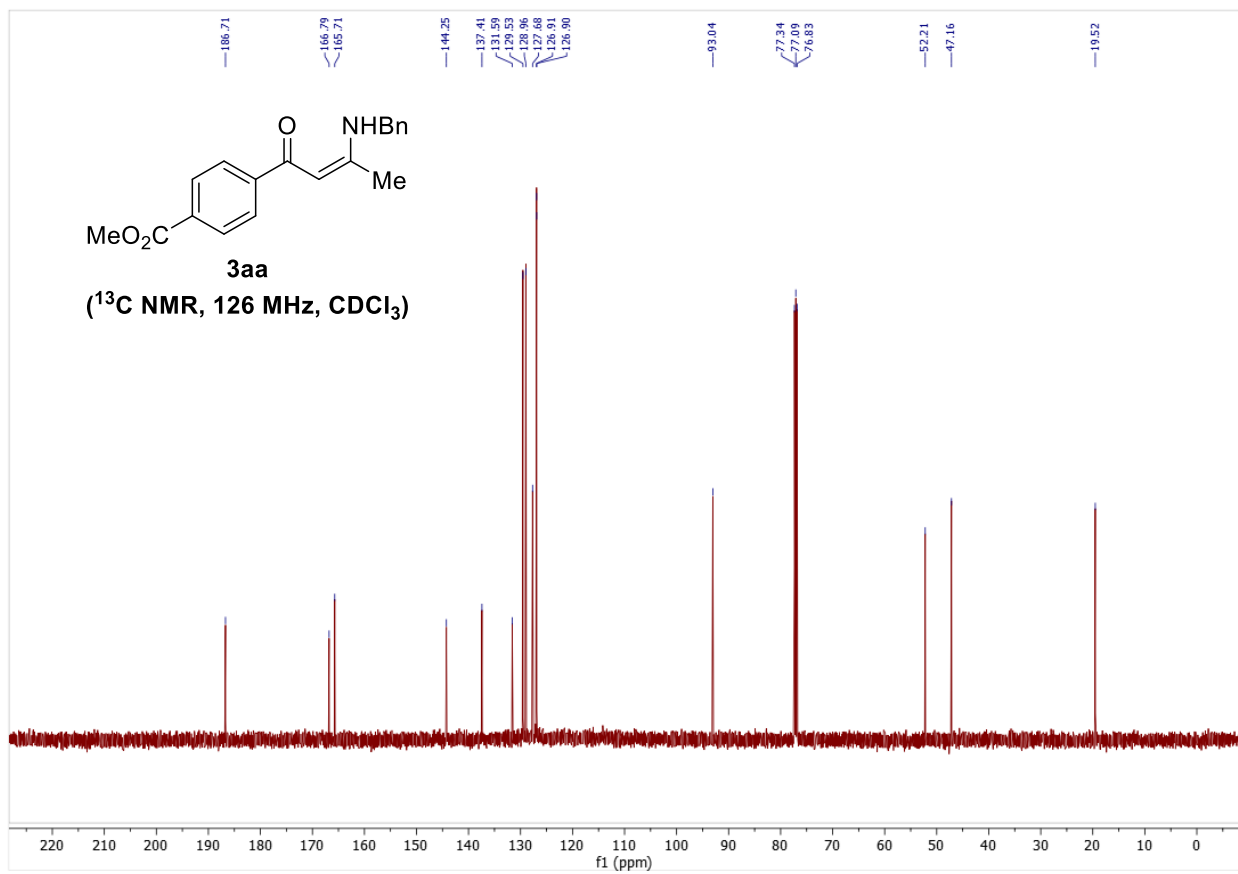
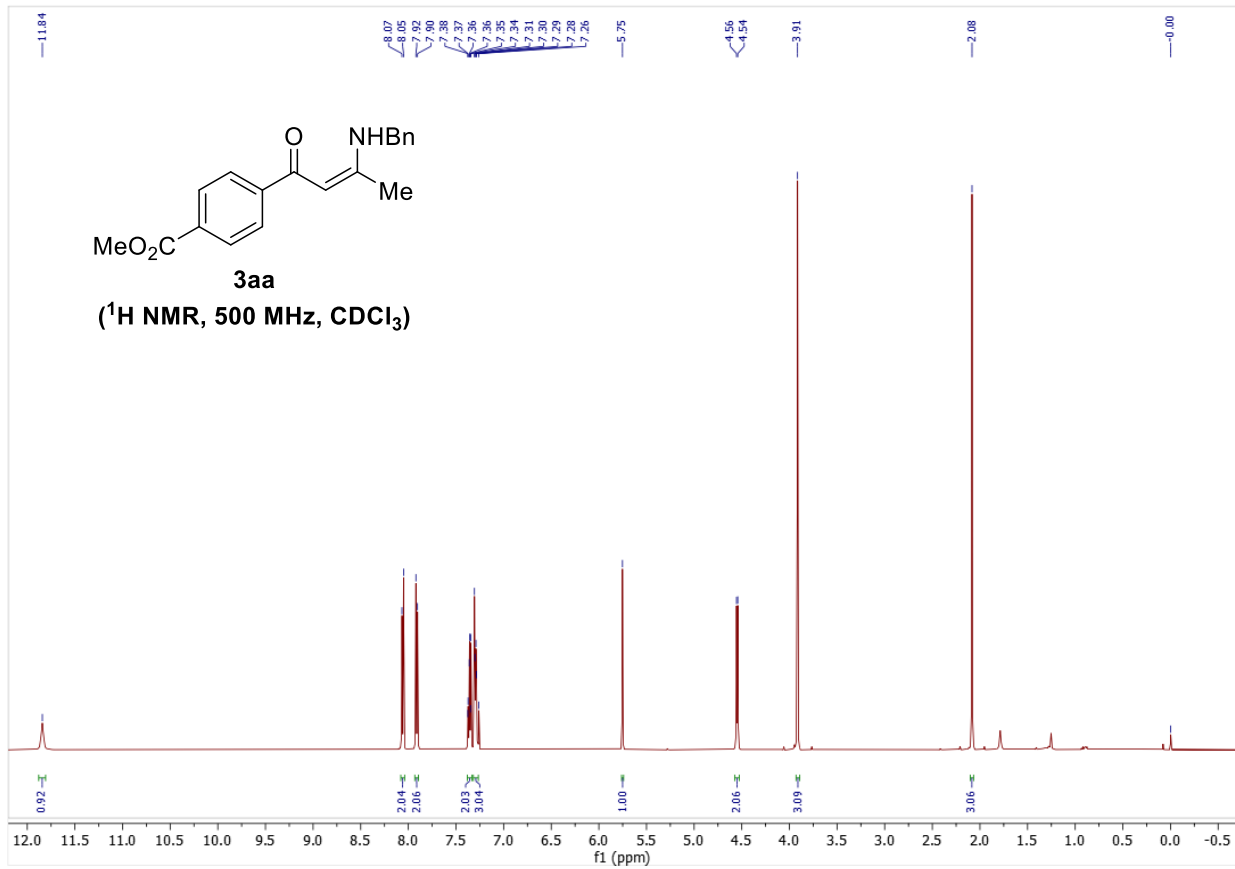


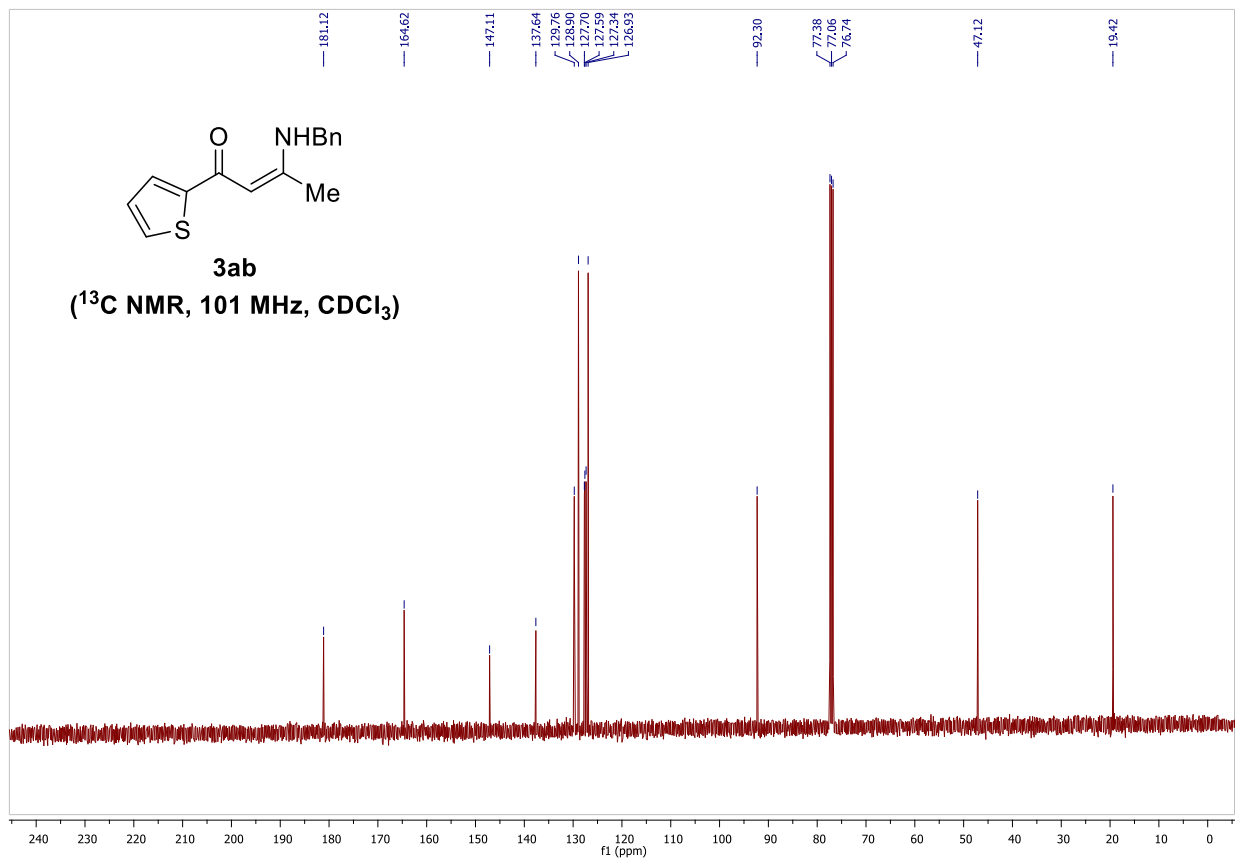
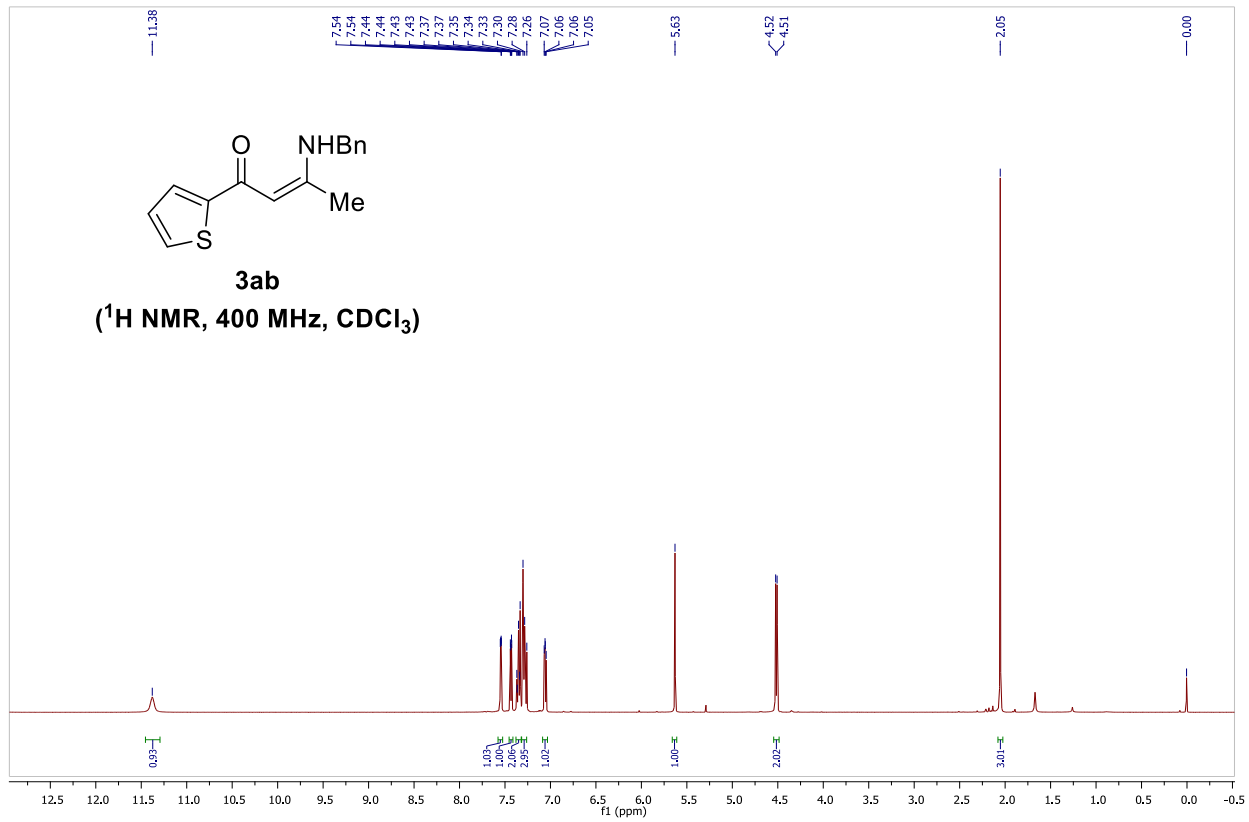


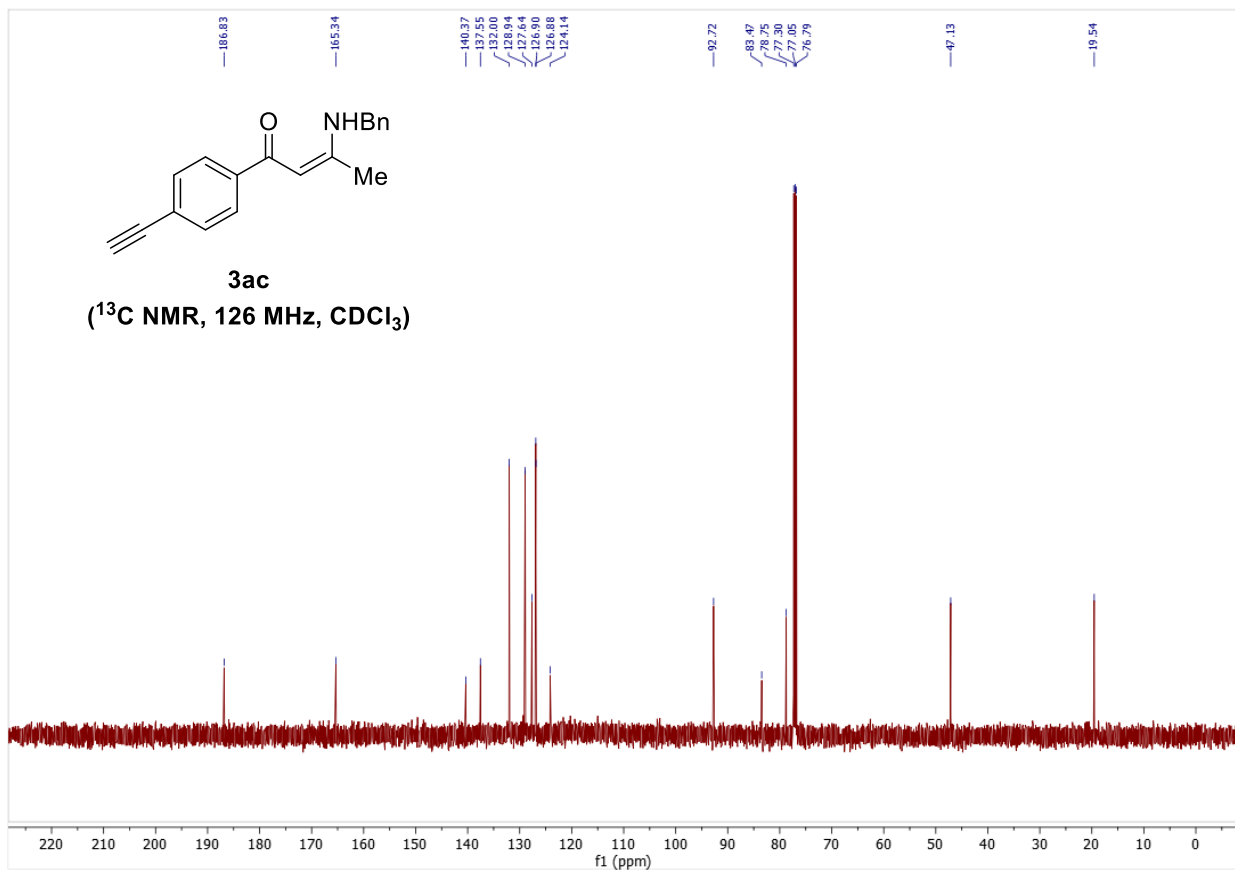
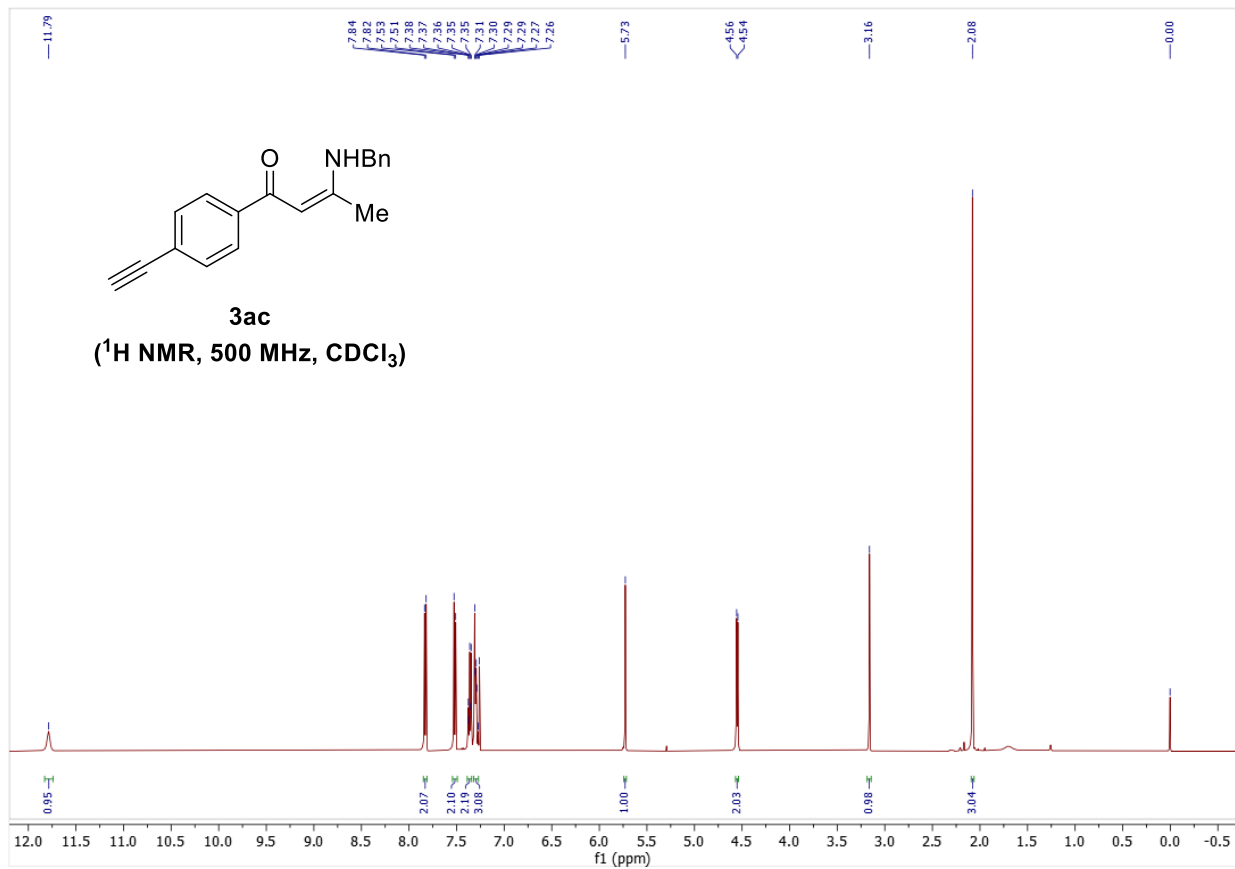


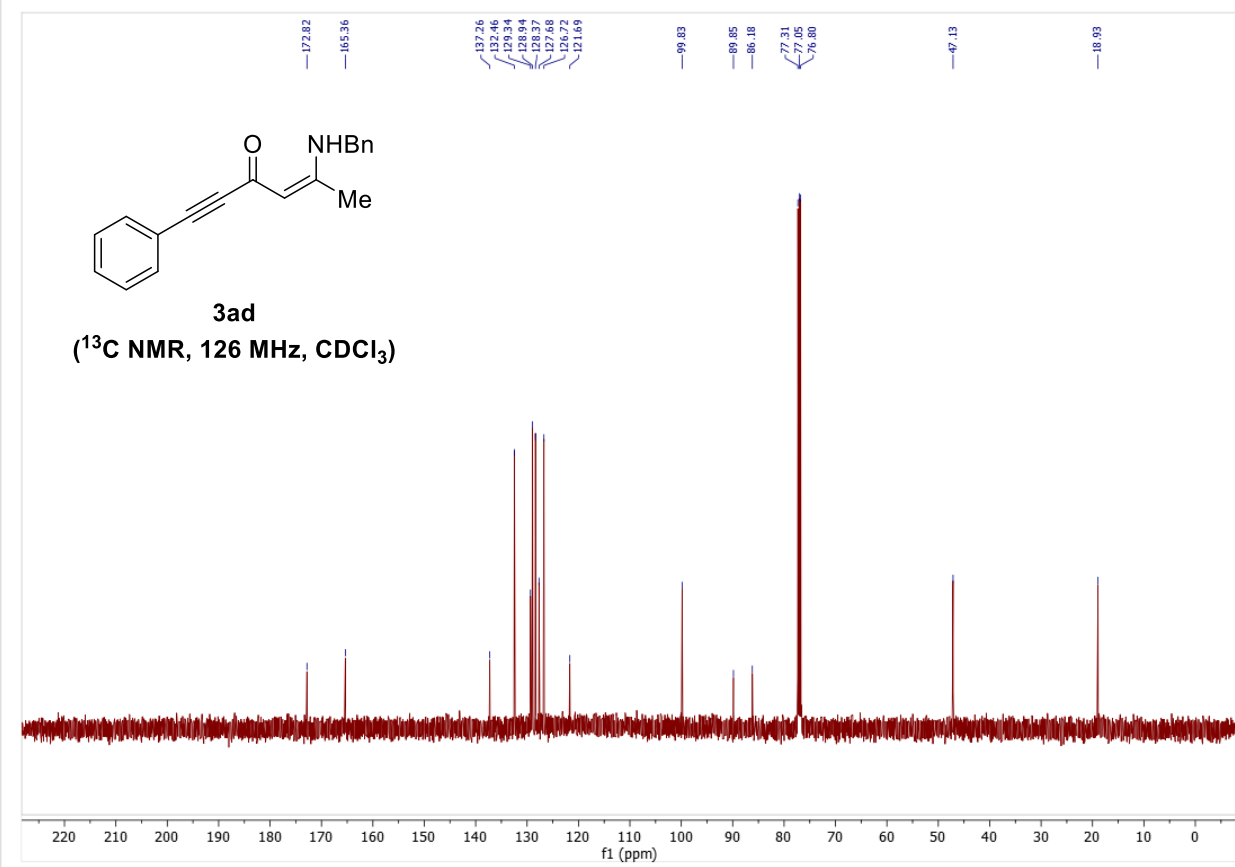
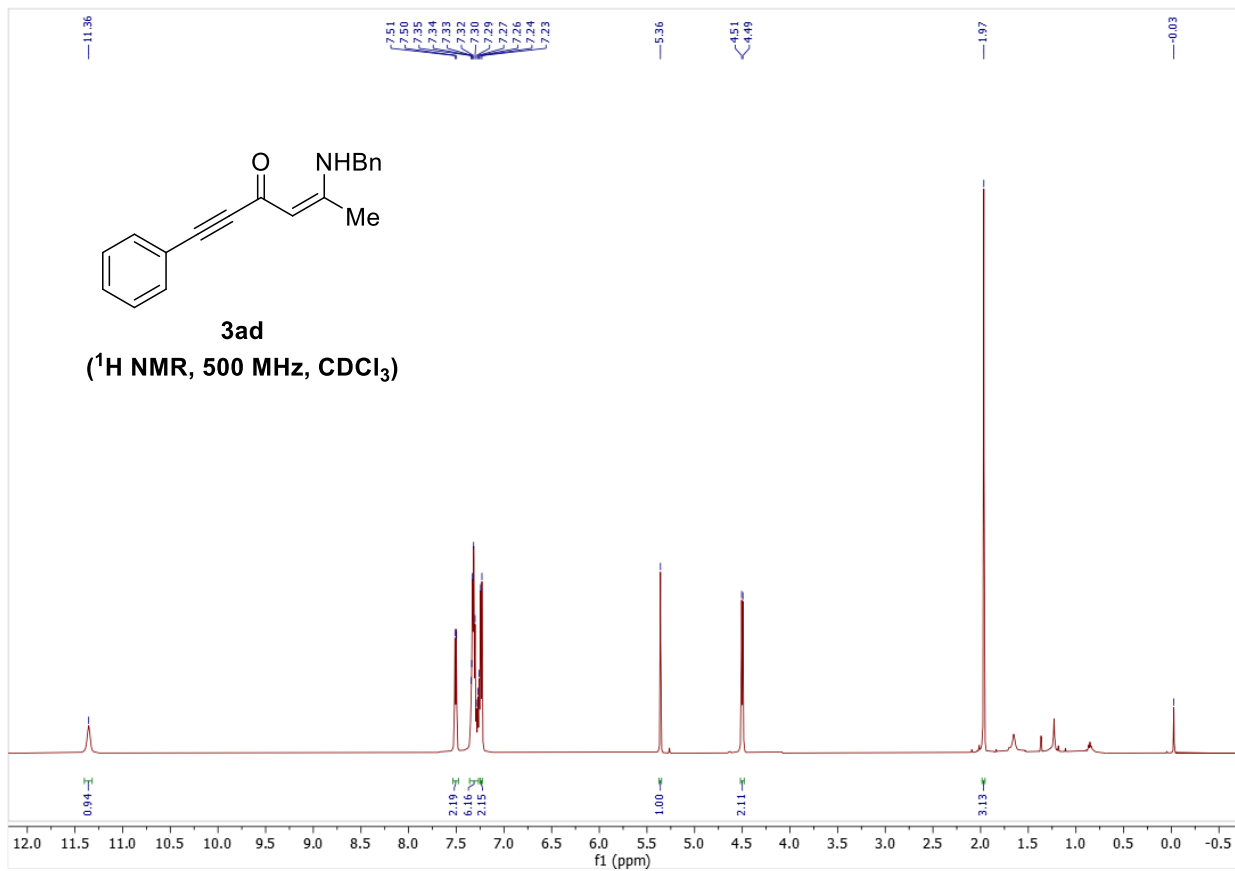


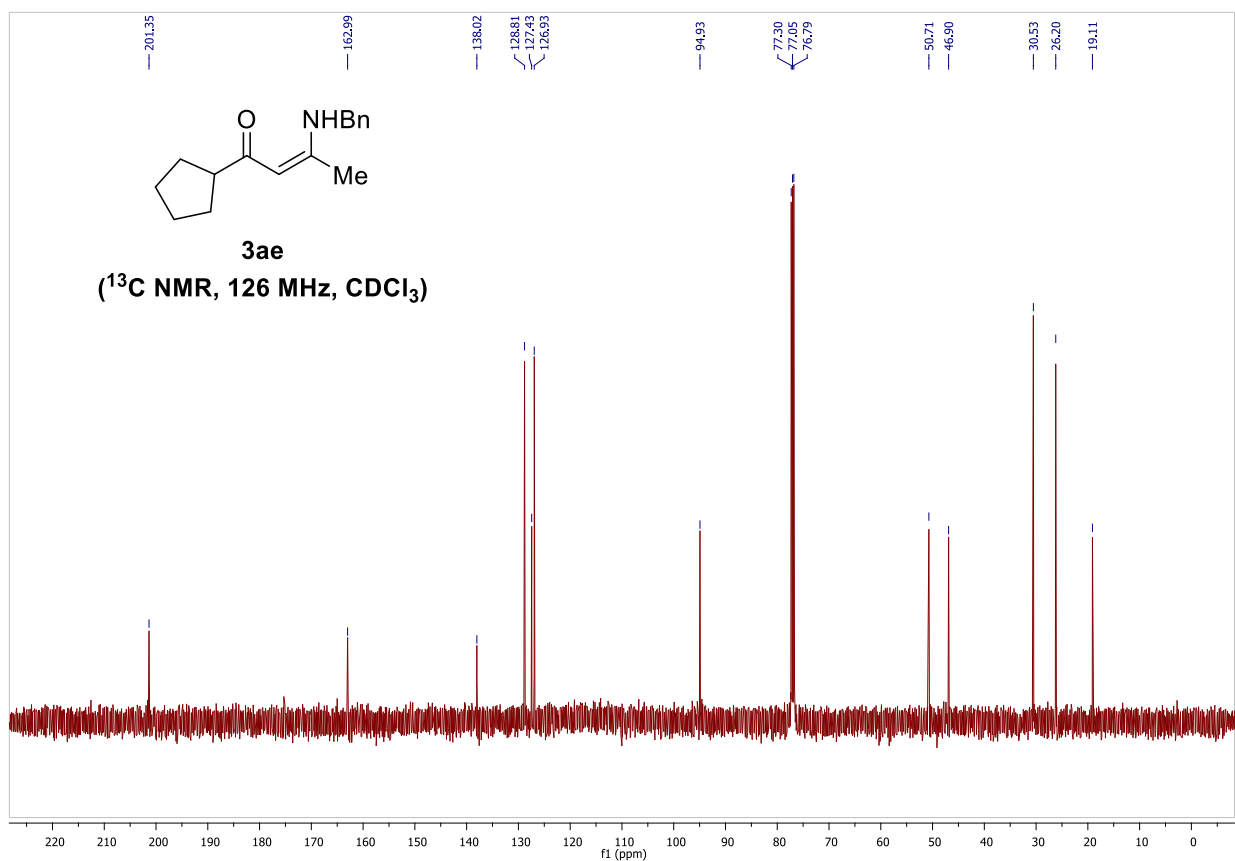
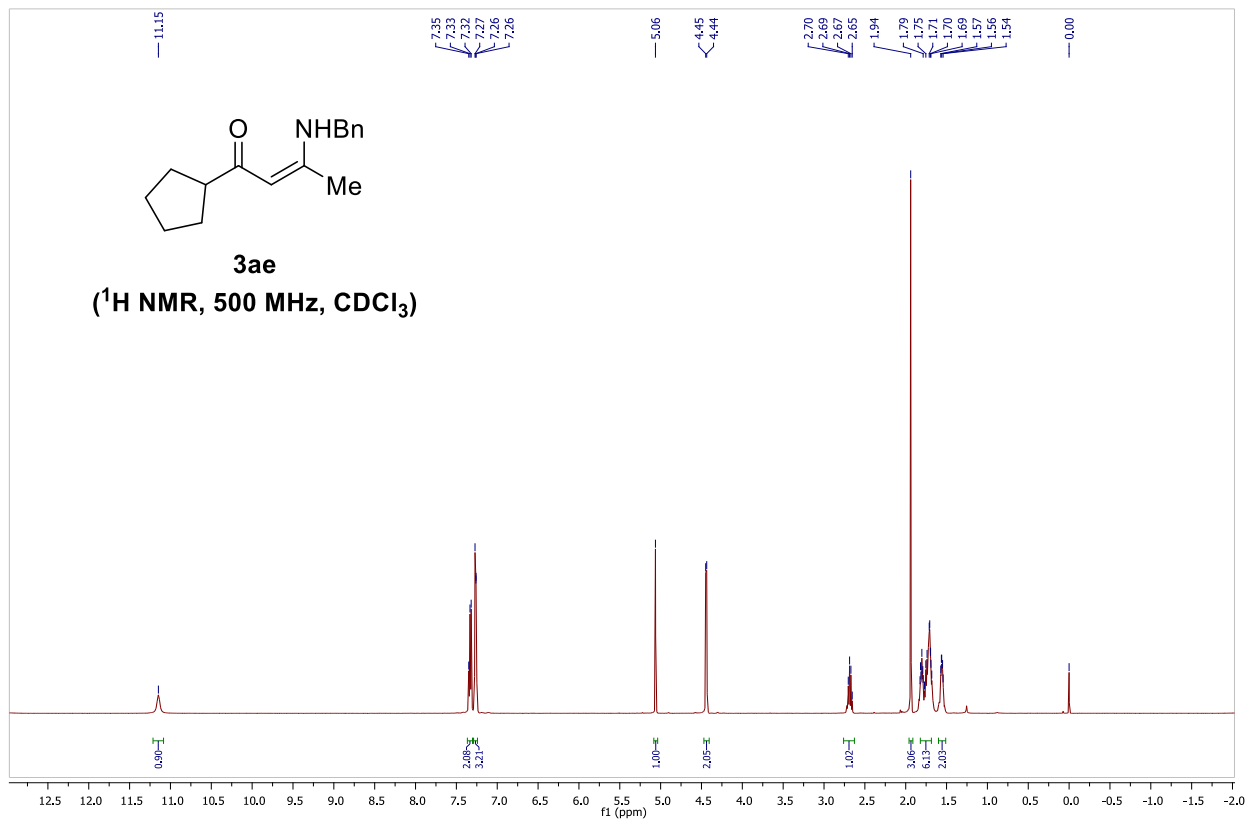


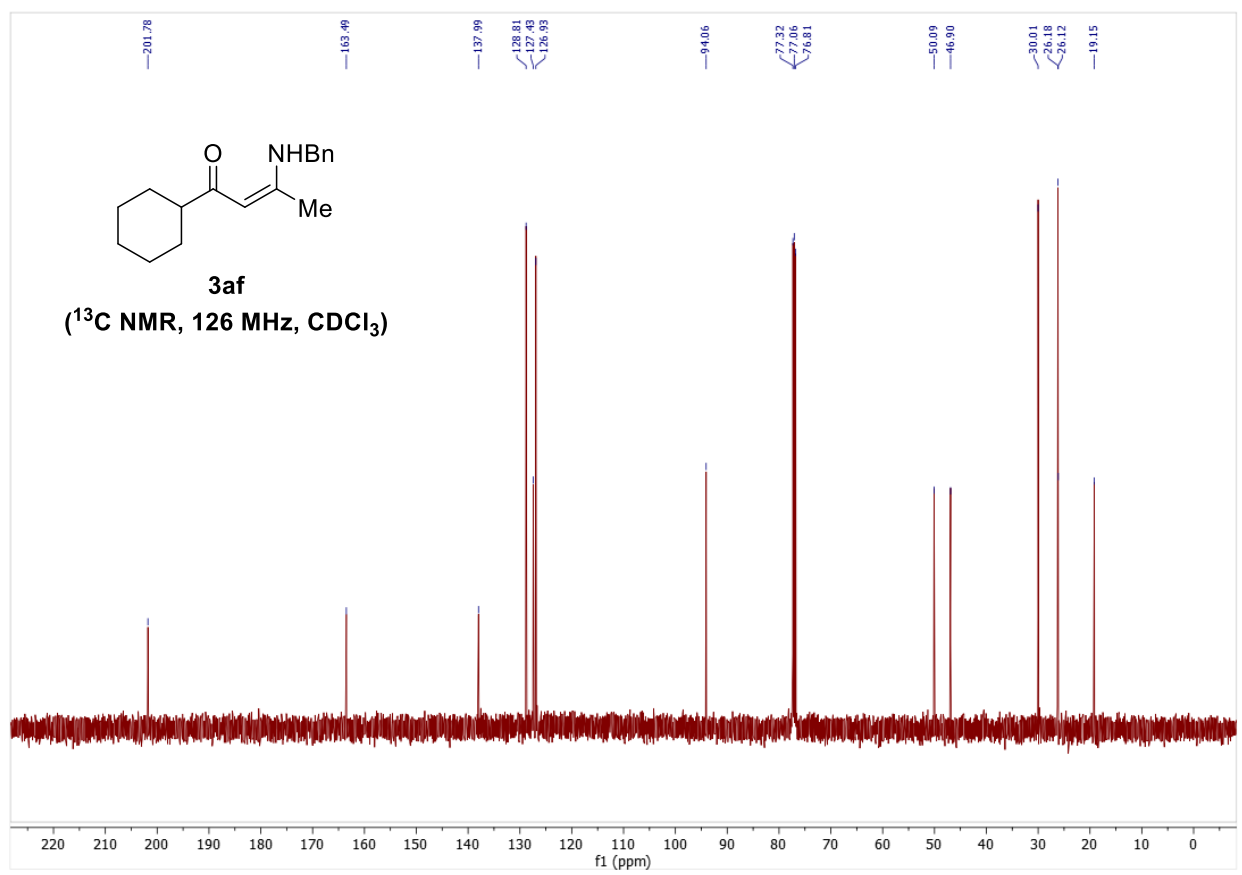
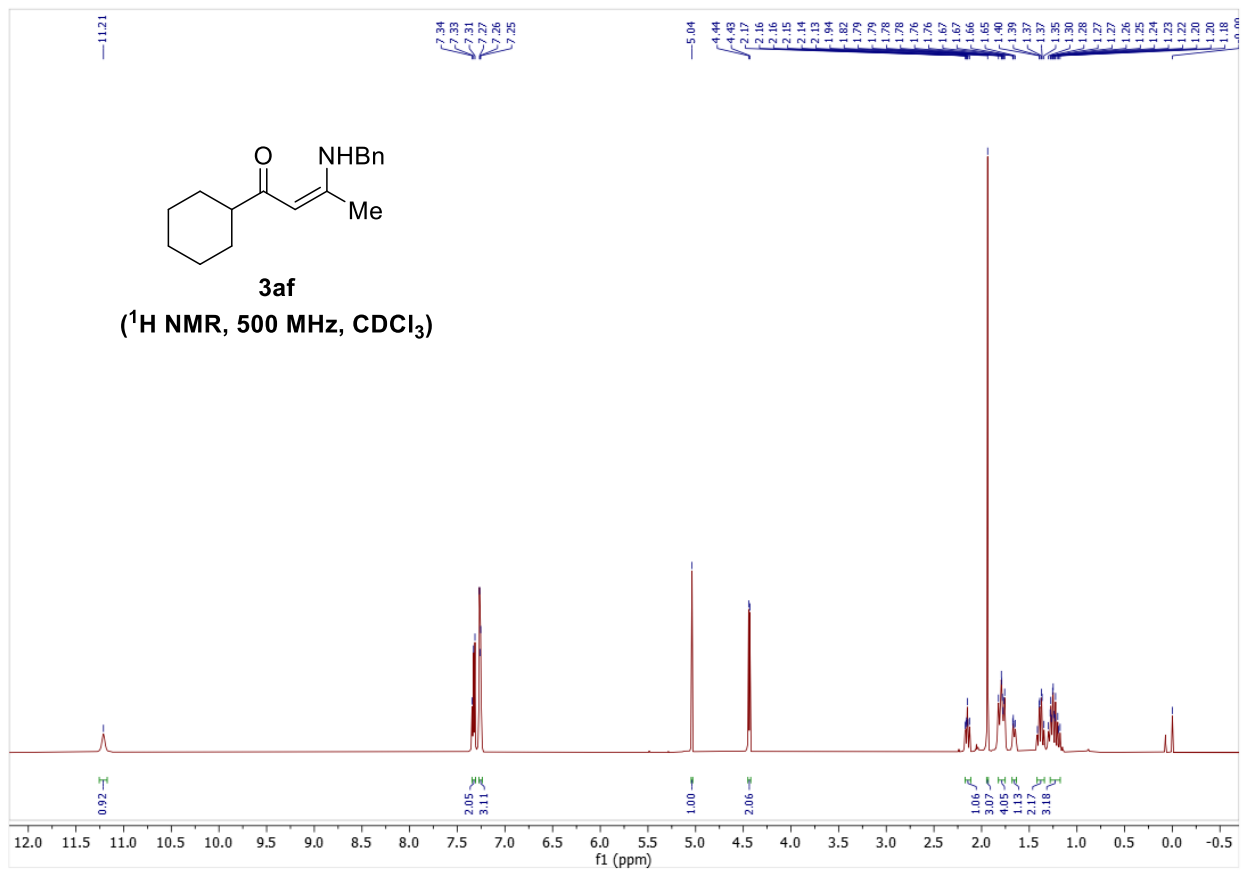


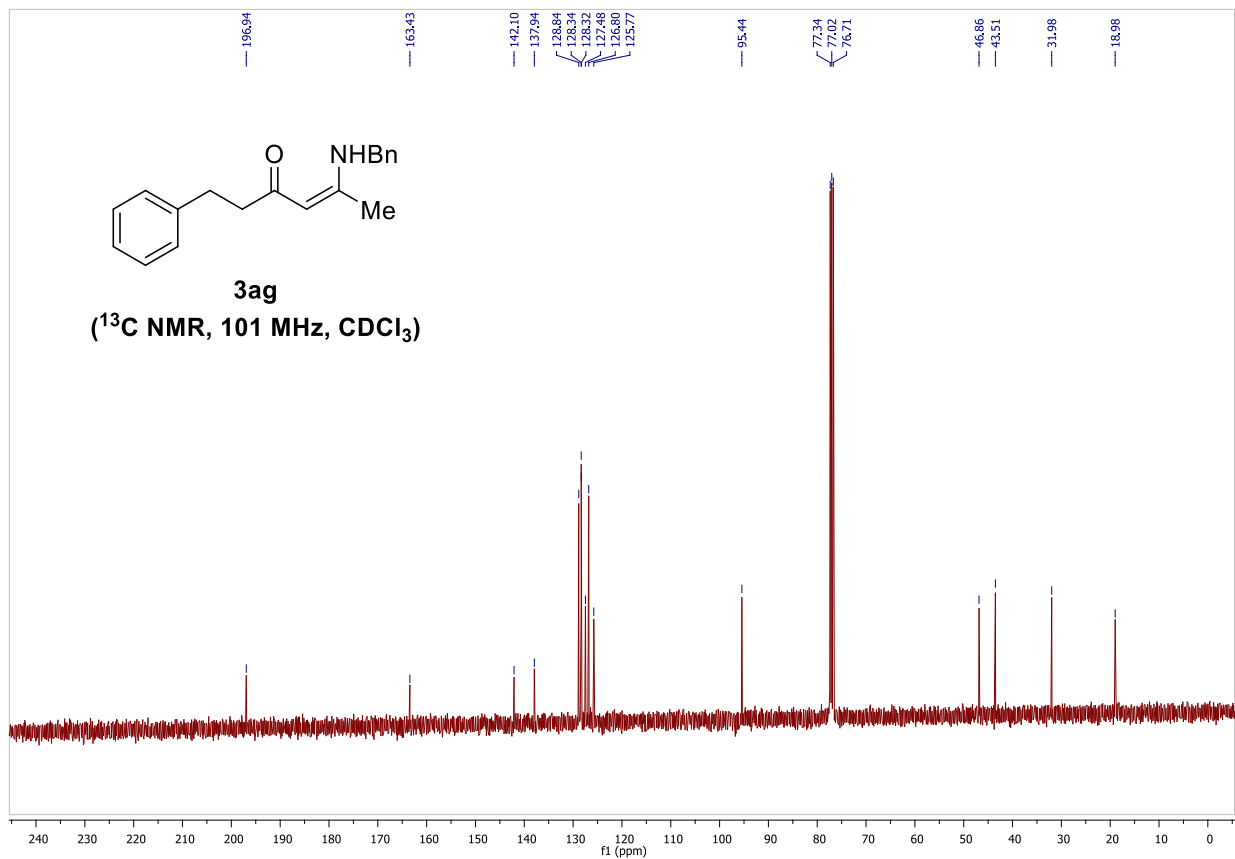
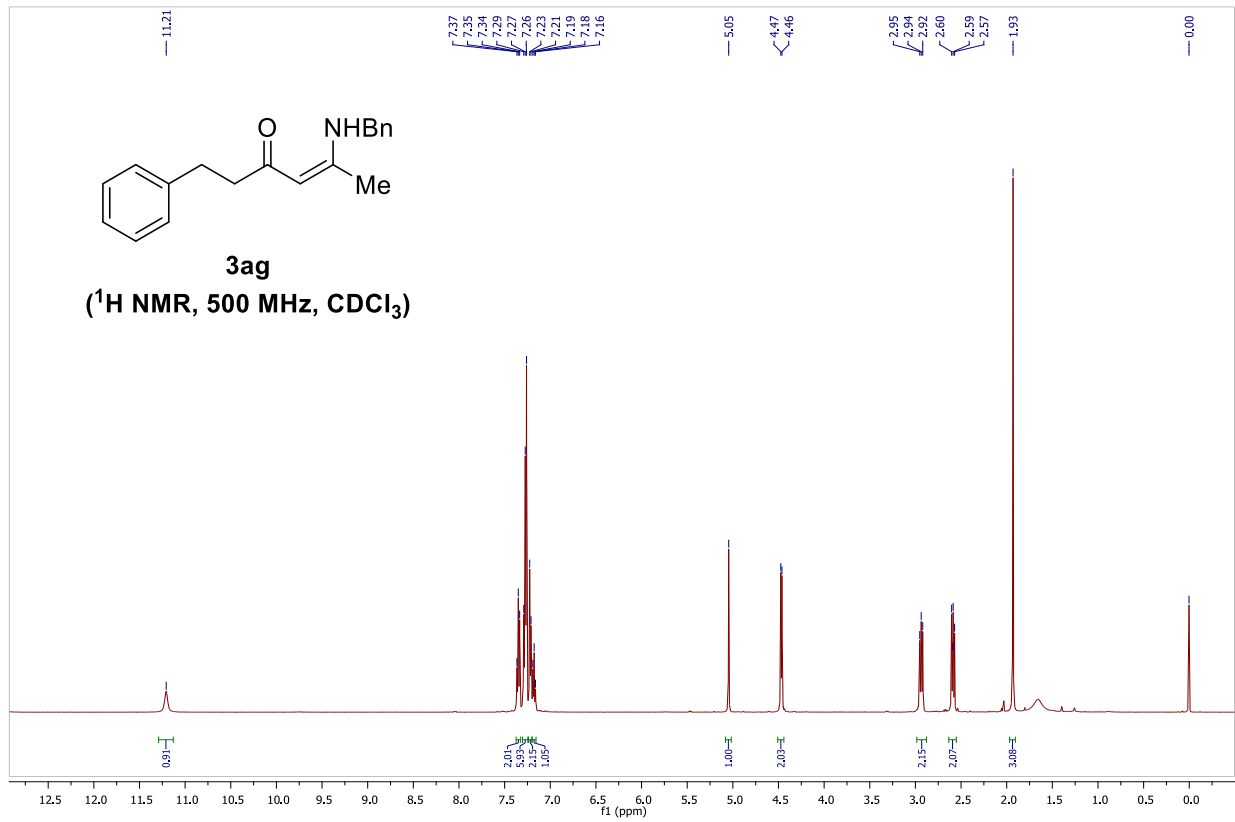


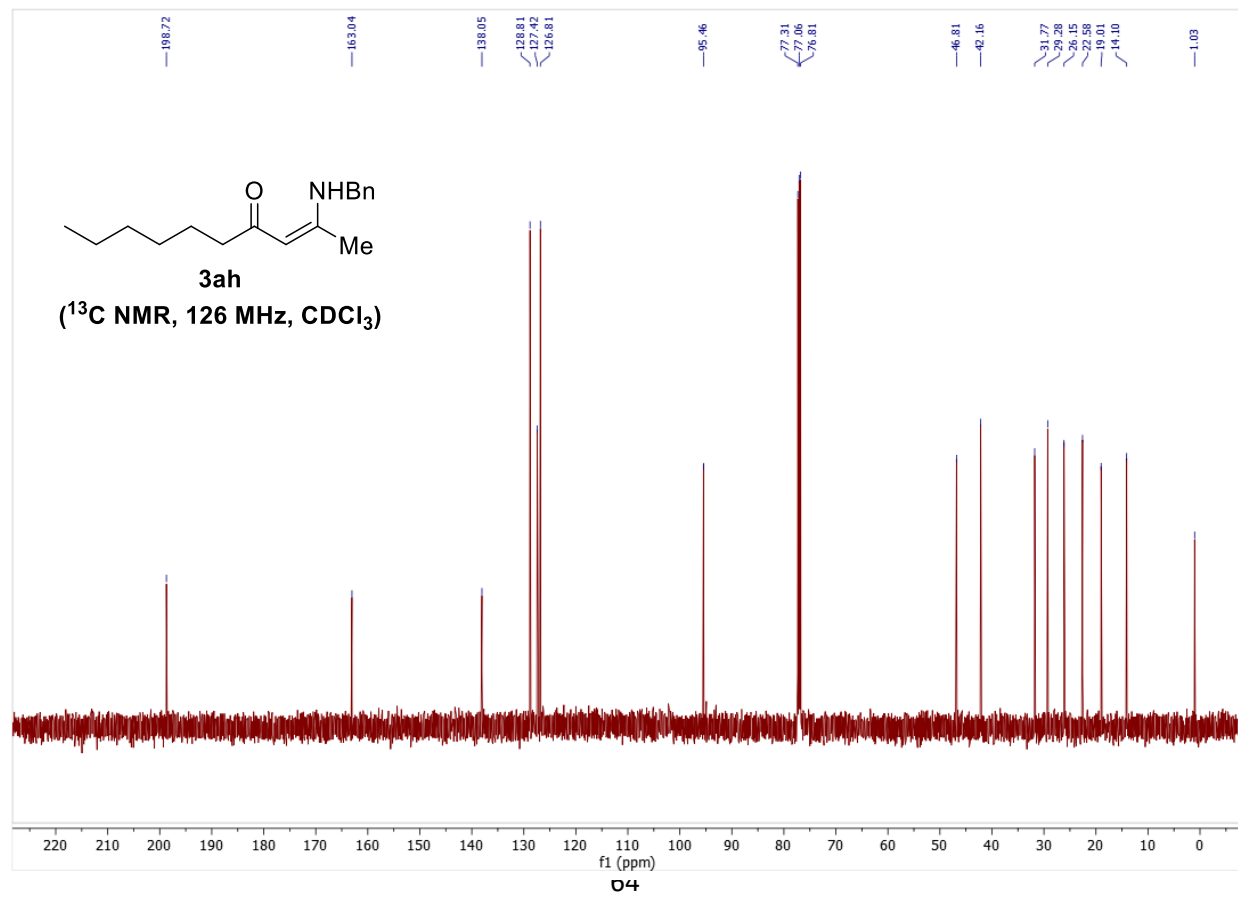
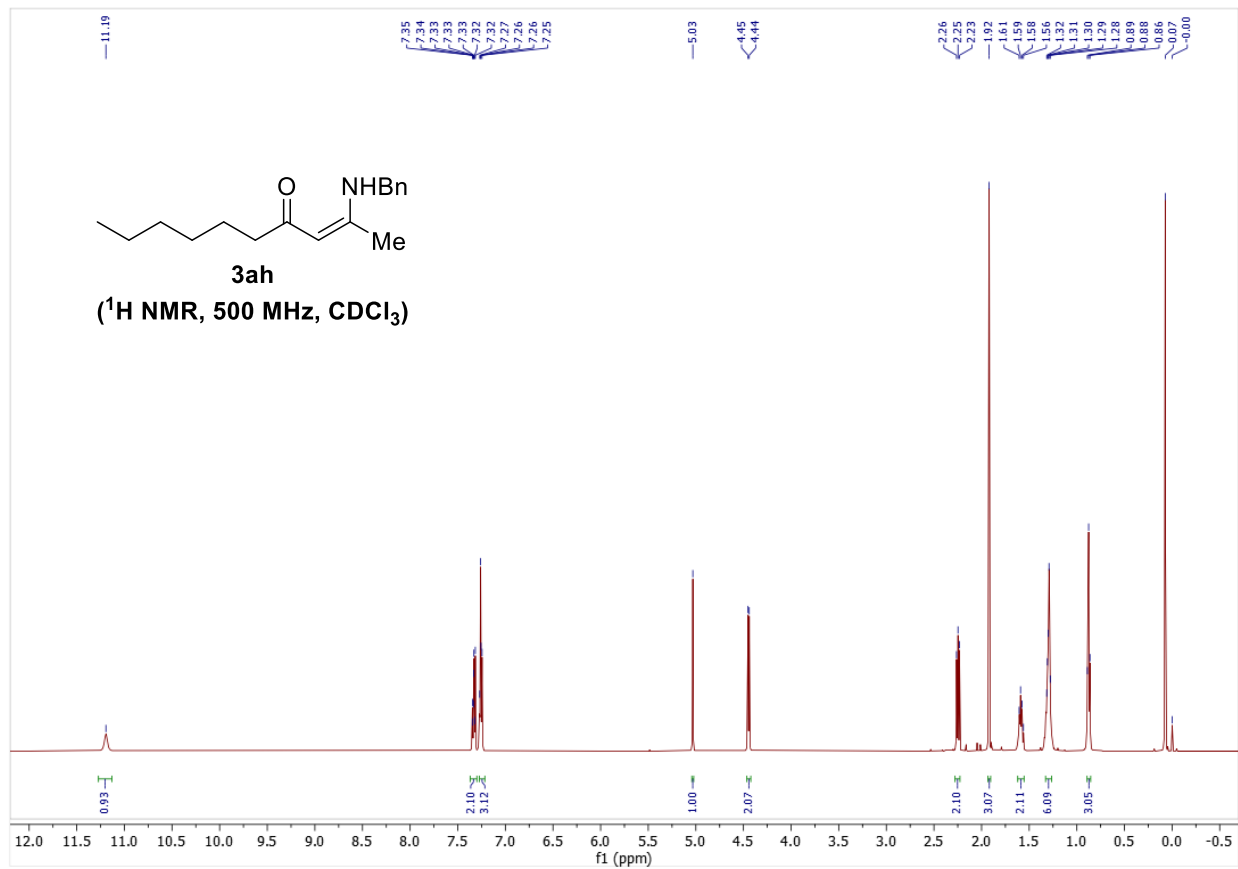




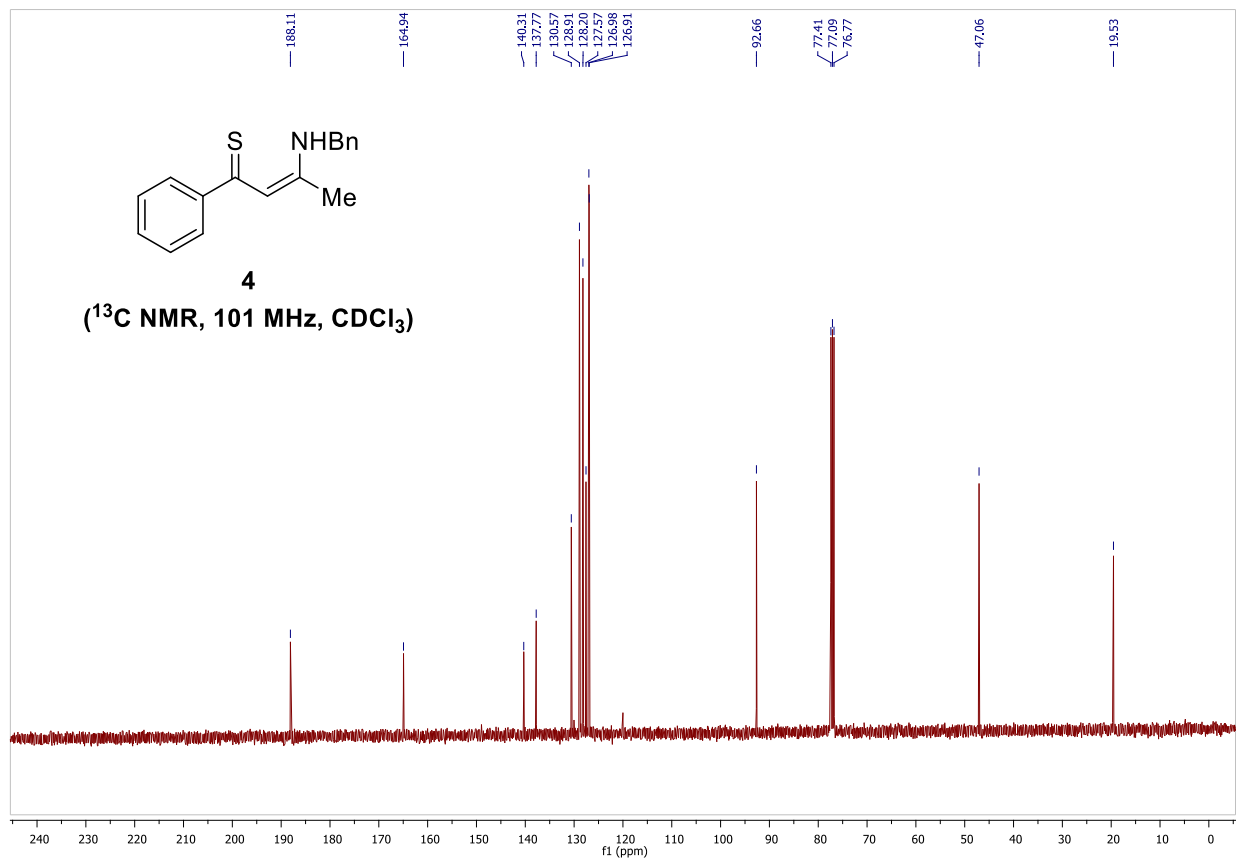
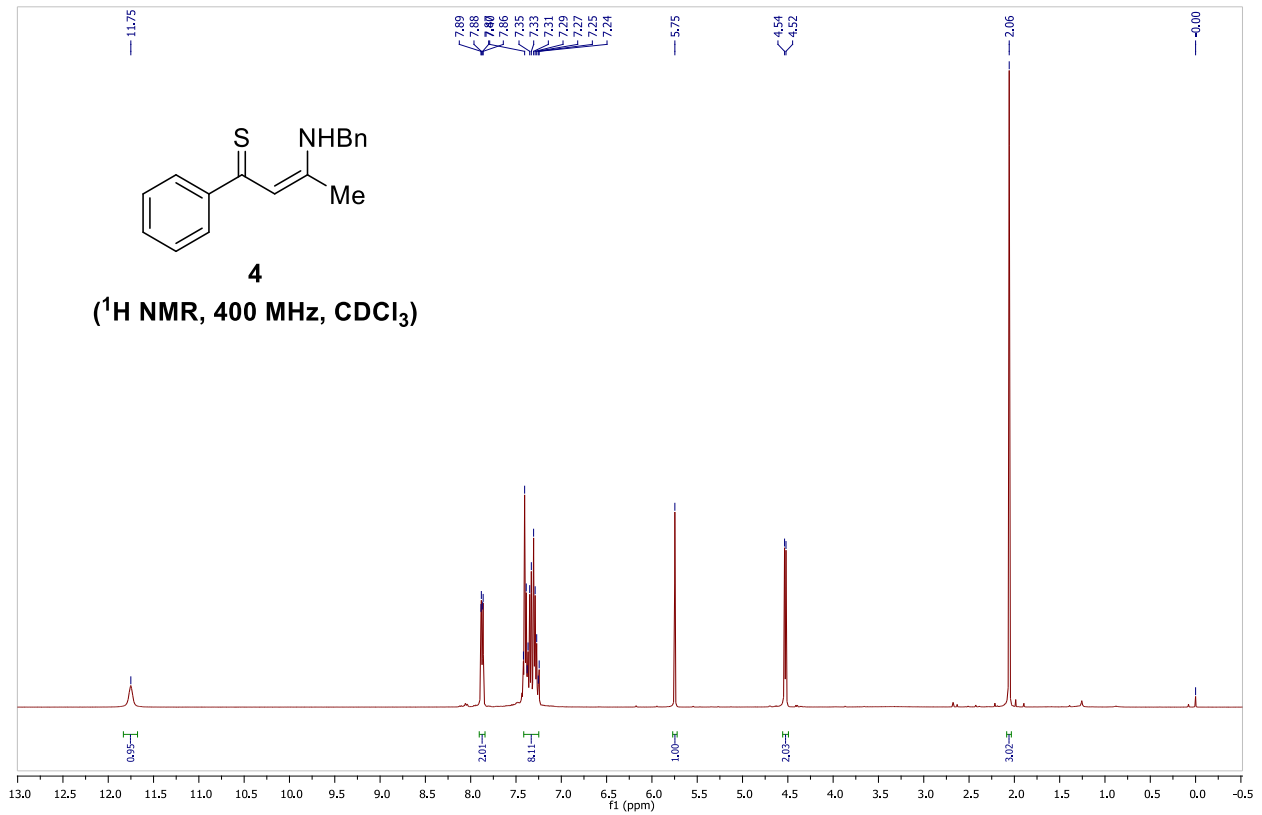


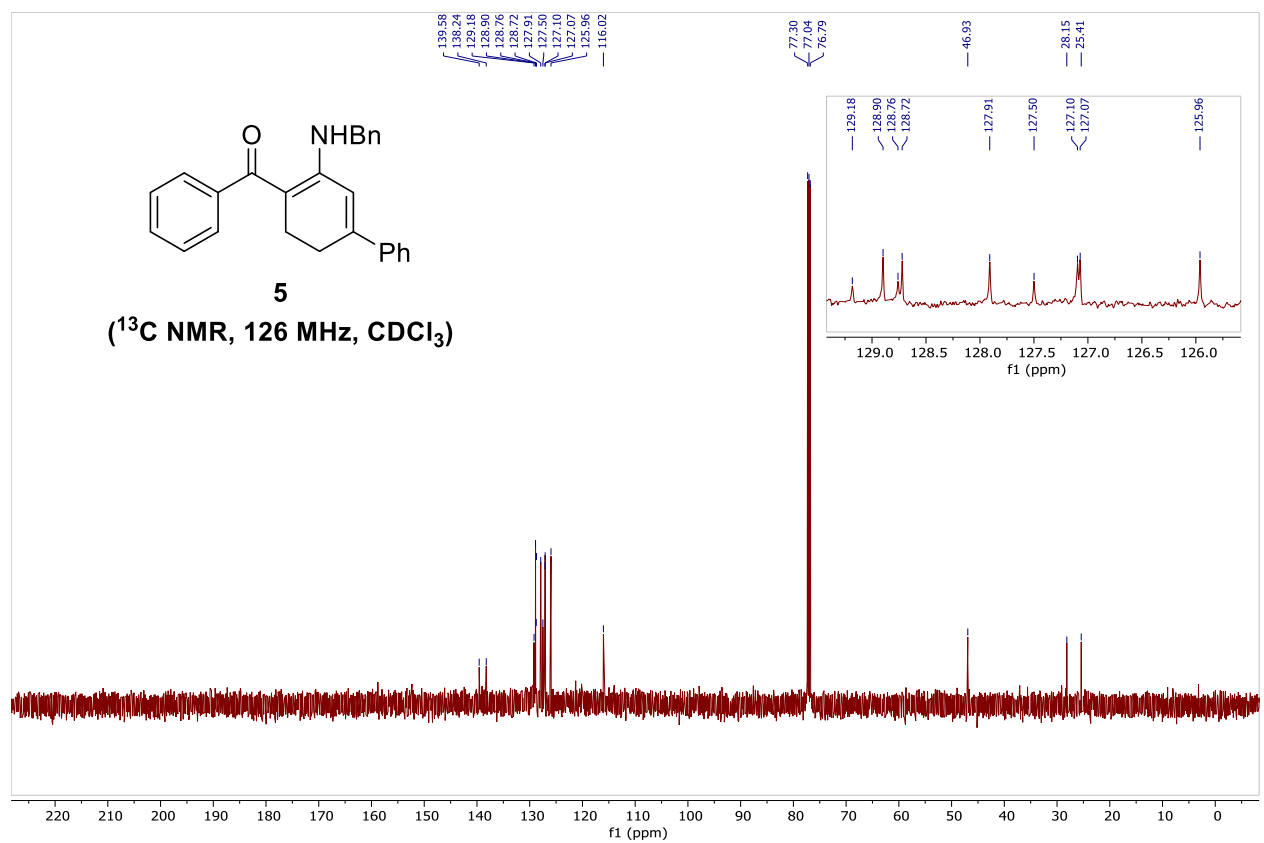
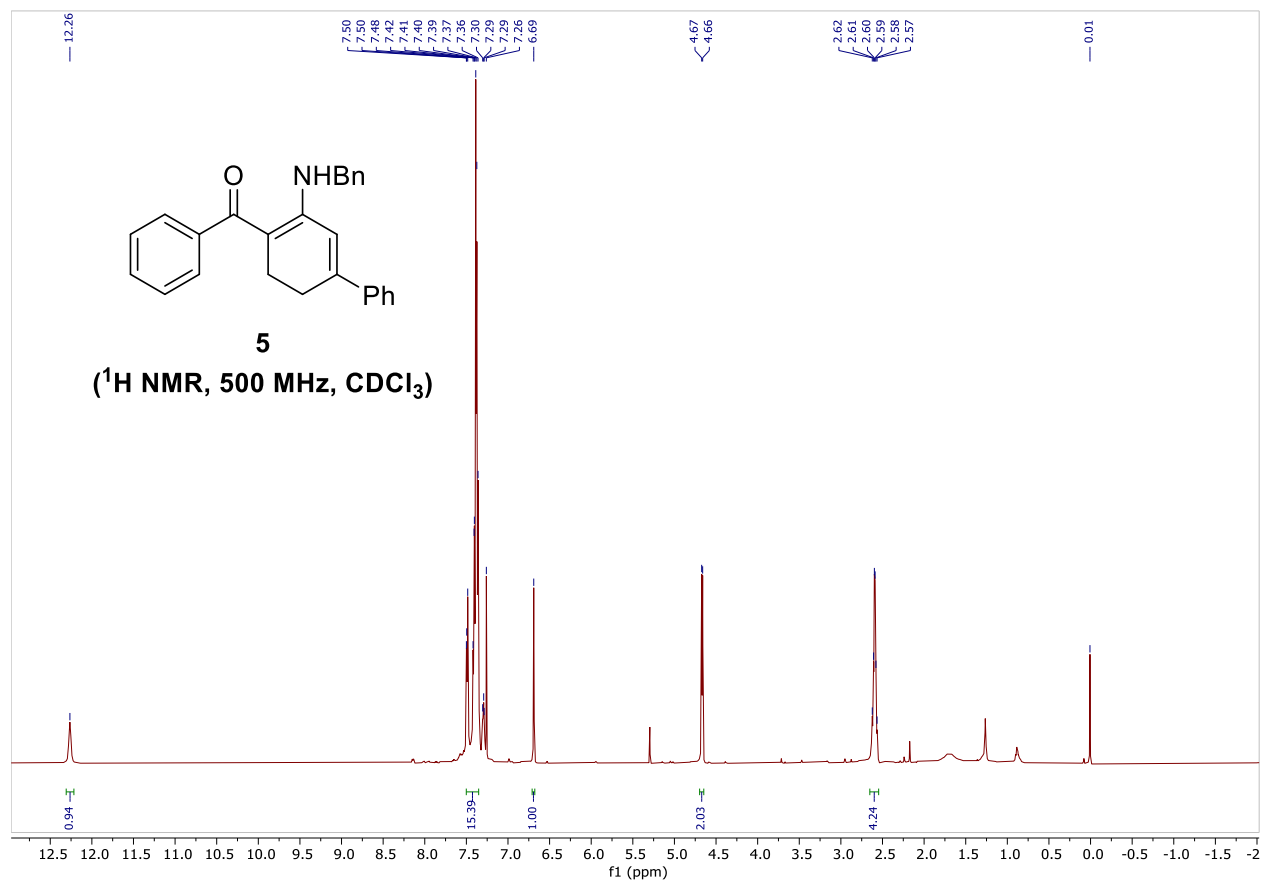


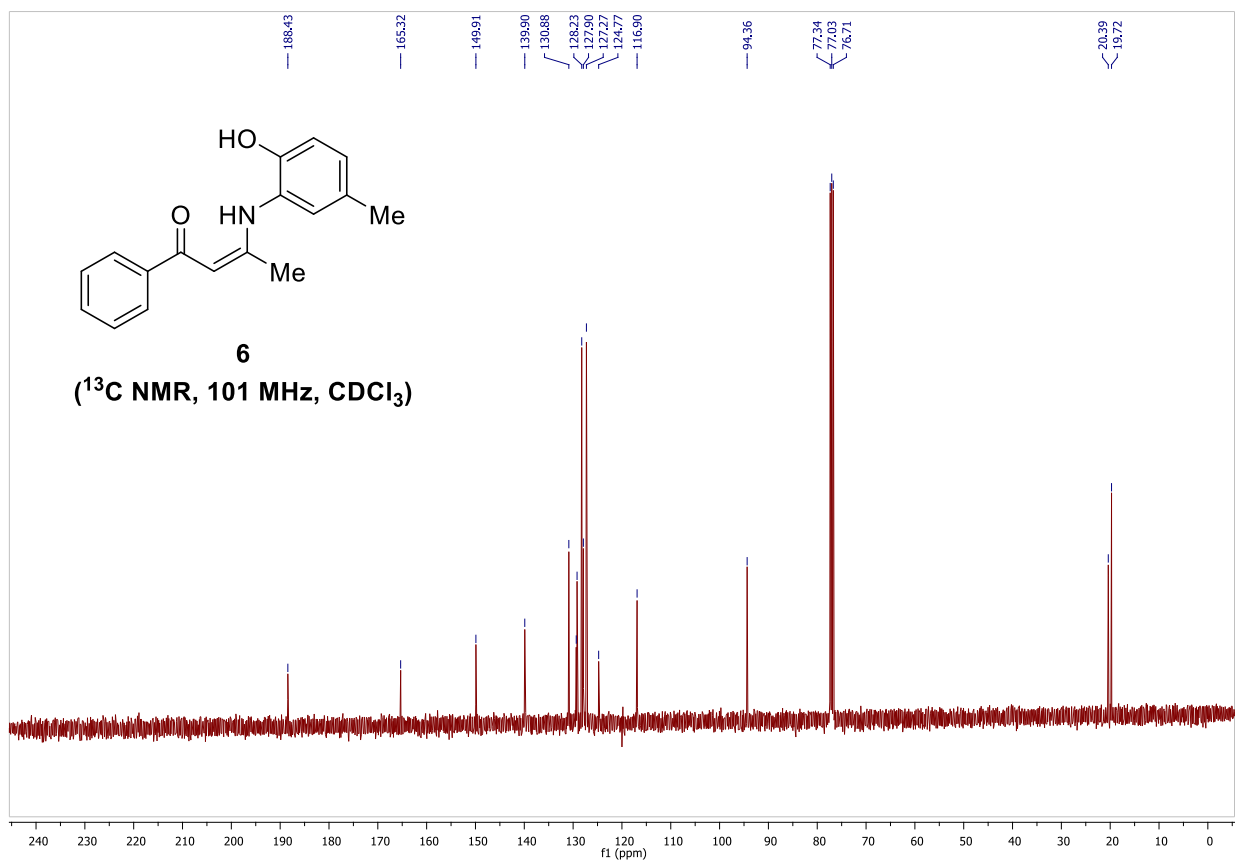
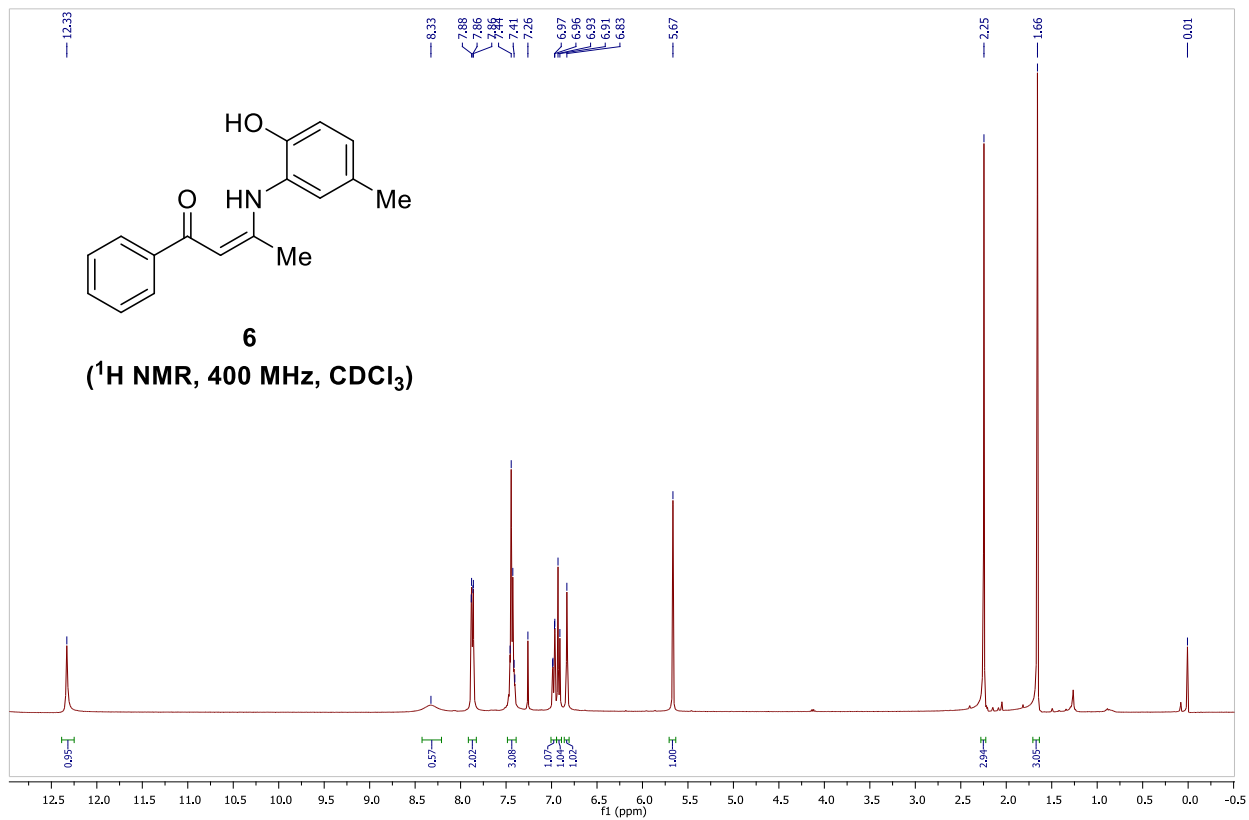


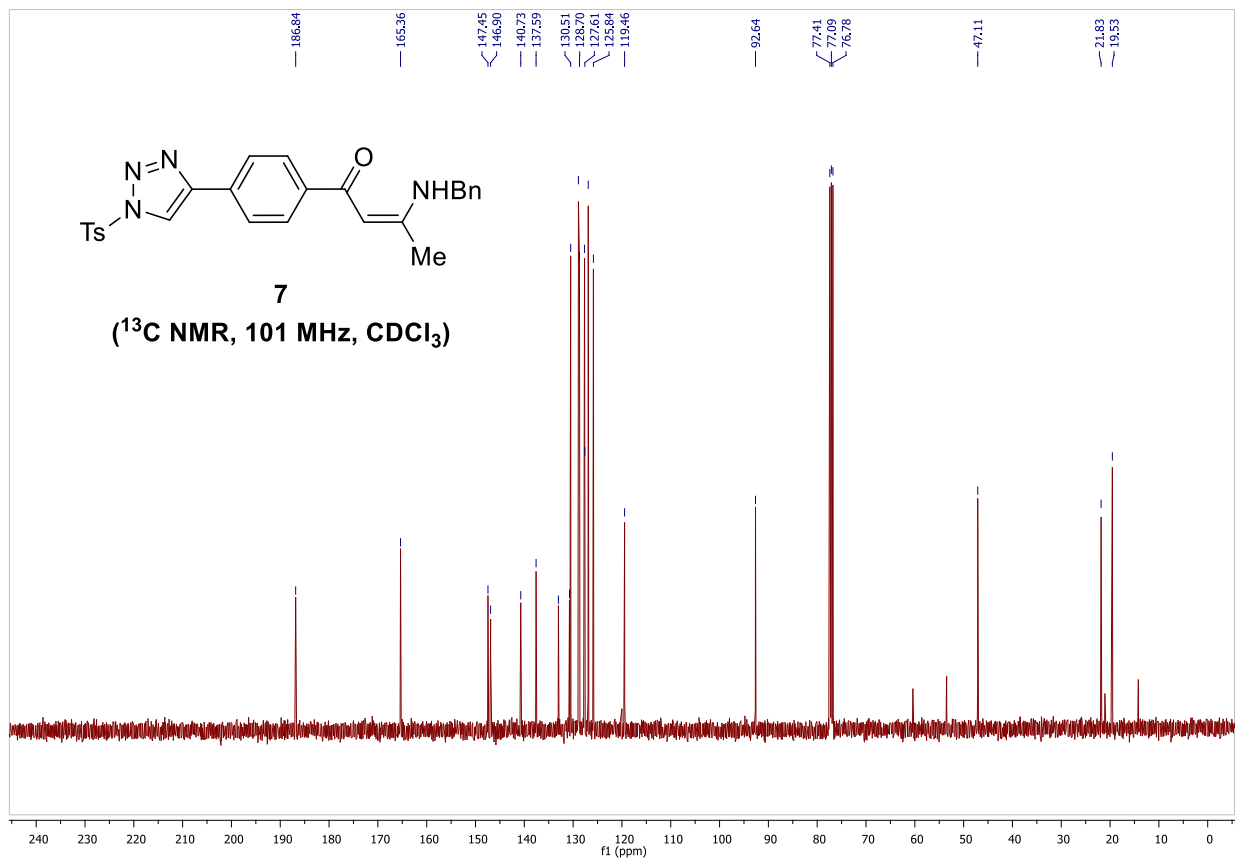
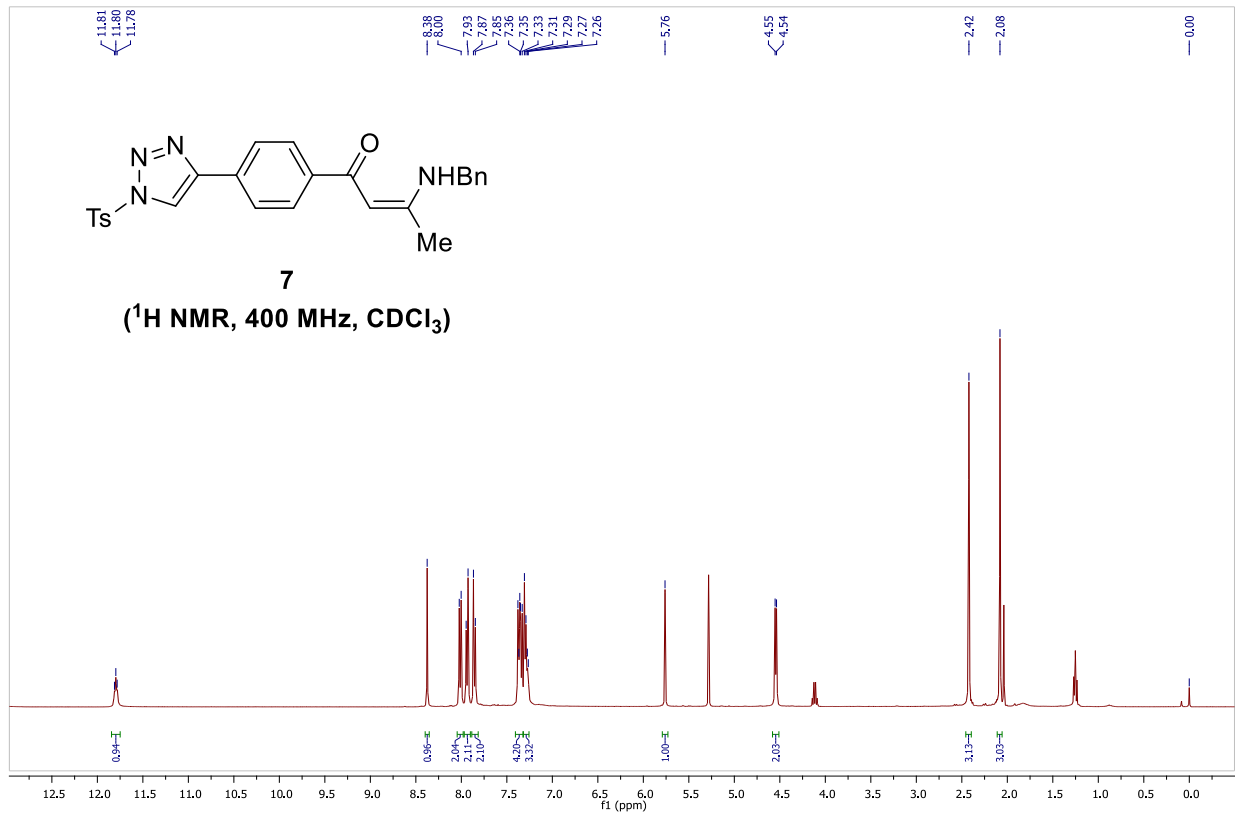


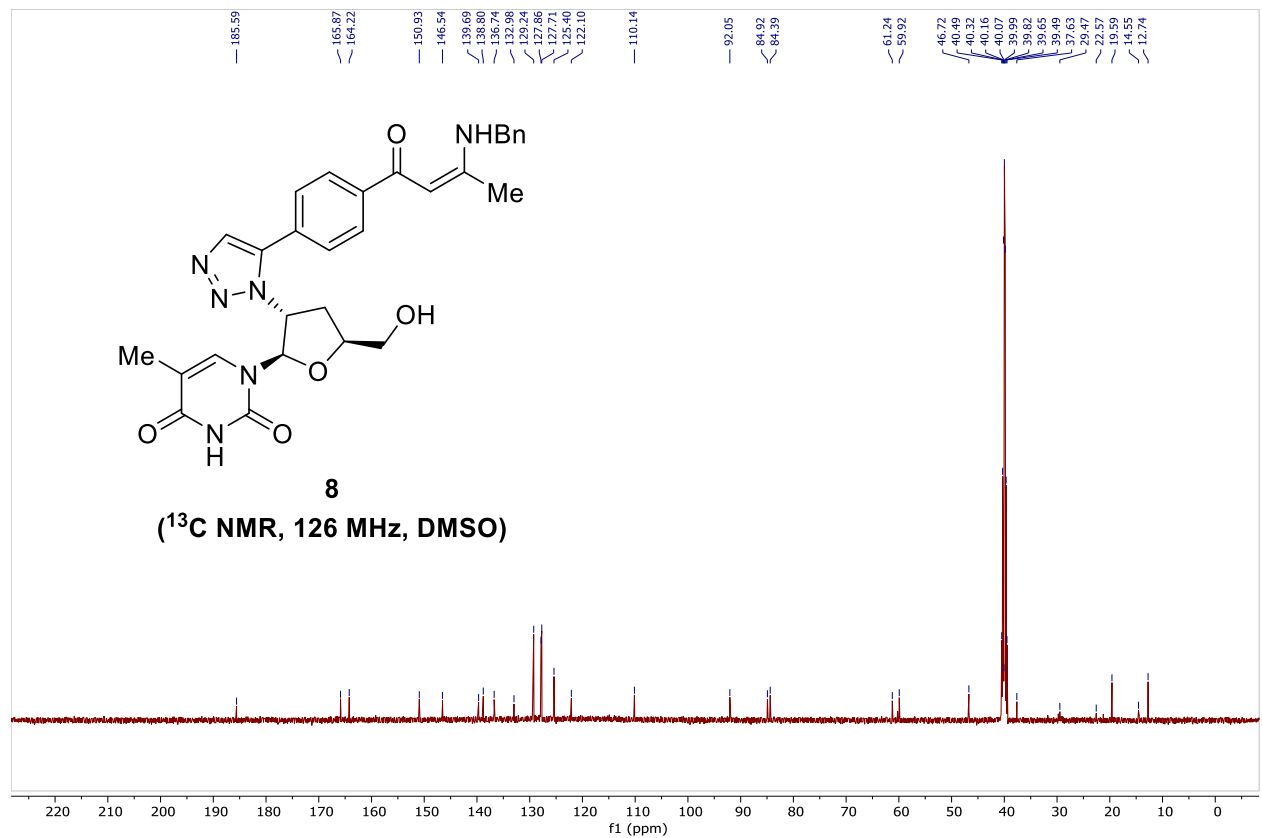
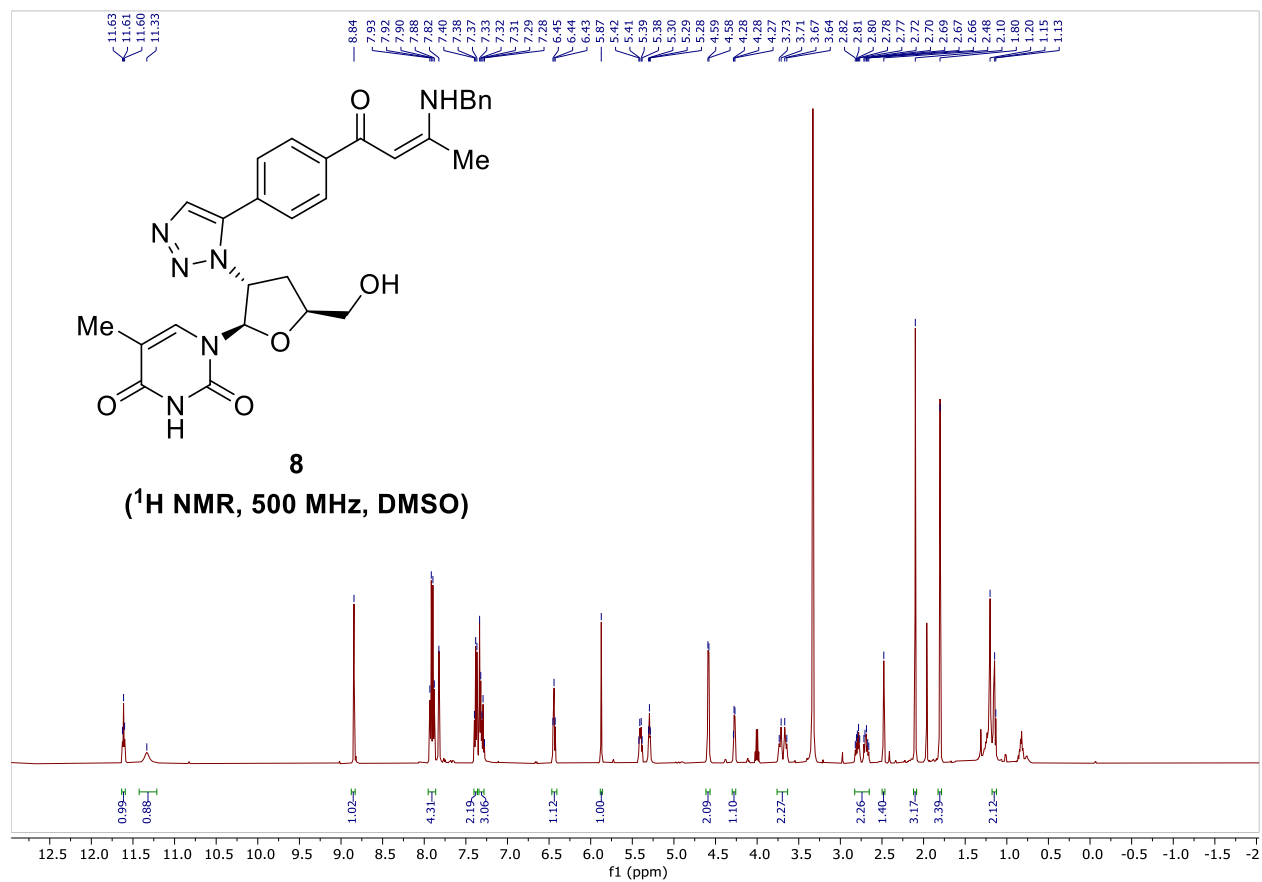












Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

8 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

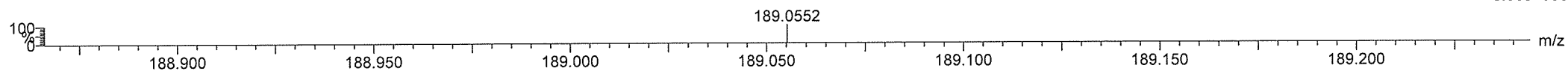
Elements Used:

C: 0-15 H: 0-15 O: 0-5

C<sub>11</sub>H<sub>8</sub>O<sub>3</sub>

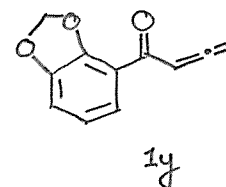
OSK1004 5 (0.121) Cm (1:16)

1: TOF MS ES+  
3.36e+005



Minimum: -1.5  
Maximum: 10.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
189.0552	189.0552	0.0	0.0	7.5	37.1	n/a	n/a	C <sub>11</sub> H <sub>9</sub> O <sub>3</sub>



## Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

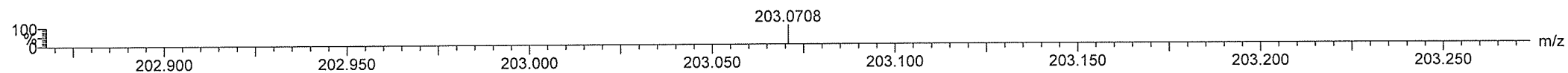
8 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 0-15 H: 0-15 O: 0-5

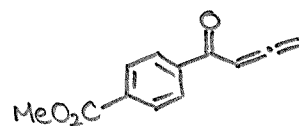
C<sub>12</sub>H<sub>10</sub>O<sub>3</sub>

JJG4100 6 (0.138)

1: TOF MS ES+  
1.86e+005

Minimum: -1.5  
Maximum: 10.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
203.0708	203.0708	0.0	0.0	7.5	35.8	n/a	n/a	C <sub>12</sub> H <sub>11</sub> O <sub>3</sub>



1aa

## Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron Ions

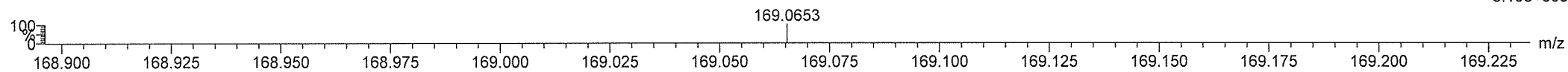
6 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 0-15 H: 0-15 O: 0-3

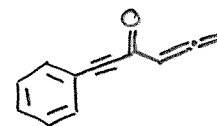
C12H8O

S12 65 (1.176)

1: TOF MS ES+  
3.19e+003

Minimum: -1.5  
Maximum: 5.0 5.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
169.0653	169.0653	0.0	0.0	8.5	21.1	n/a	n/a	C12 H9 O



1ad



## Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

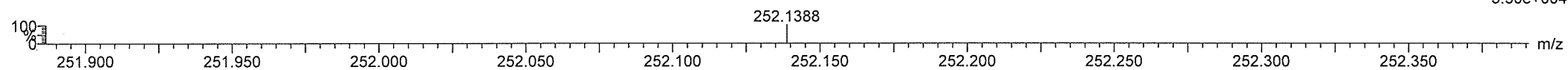
16 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 0-20 H: 0-20 N: 0-2 O: 0-2

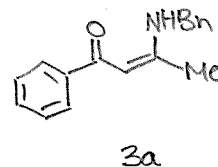
C17H17NO

JJG4026-3 263 (4.663)

1: TOF MS ES+  
3.50e+004

Minimum: -1.5  
Maximum: 5.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
252.1388	252.1388	0.0	0.0	9.5	32.2	n/a	n/a	C17 H18 N O



# Elemental Composition Report

## Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

13 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

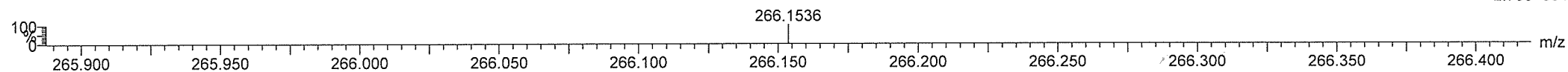
Elements Used:

C: 0-20 H: 0-20 N: 0-2 O: 0-2

C<sub>18</sub>H<sub>19</sub>NO

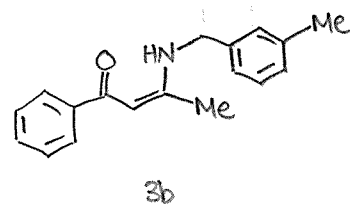
JJG4066-2 309 (5.481)

1: TOF MS ES+  
2.73e+004



Minimum: -1.5  
Maximum: 5.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
266.1536	266.1545	-0.9	-3.4	9.5	32.0	n/a	n/a	C <sub>18</sub> H <sub>20</sub> N O



# Elemental Composition Report

## Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

32 formula(e) evaluated with 1 results within limits (up to 1000) for each mass

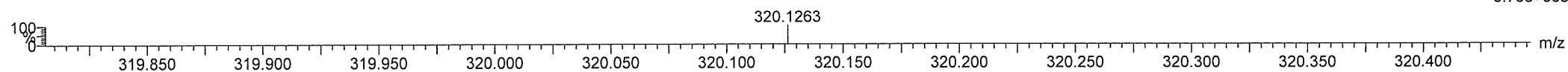
Elements Used:

C: 0-20 H: 0-20 N: 0-2 O: 0-2 F: 0-3

C<sub>18</sub>H<sub>16</sub>F<sub>3</sub>NO

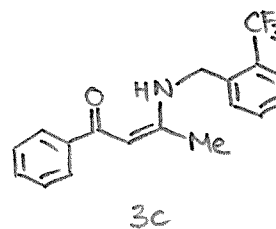
JJG4066-3 410 (7.249)

1: TOF MS ES+  
3.75e+003



Minimum: -1.5  
Maximum: 5.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
320.1263	320.1262	0.1	0.3	9.5	26.9	n/a	n/a	C <sub>18</sub> H <sub>17</sub> N O F <sub>3</sub>



## Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

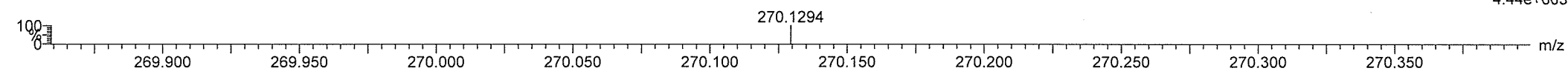
23 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 0-19 H: 0-20 N: 0-2 O: 0-2 F: 0-1

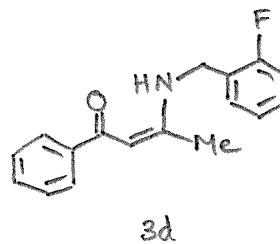
C<sub>17</sub>H<sub>16</sub>FNO

JJG4066-4 434 (7.675)

1: TOF MS ES+  
4.44e+003

Minimum: -1.5  
Maximum: 5.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
270.1294	270.1294	0.0	0.0	9.5	27.1	n/a	n/a	C <sub>17</sub> H <sub>17</sub> N O F



# Elemental Composition Report

## Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

36 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

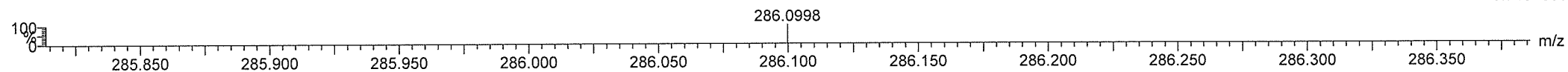
Elements Used:

C: 0-19 H: 0-20 N: 0-2 O: 0-2 Cl: 0-2

C<sub>17</sub>H<sub>16</sub>ClNO

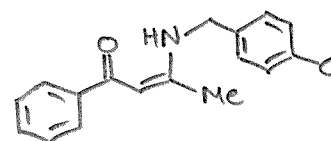
JJG4066-5 341 (6.042)

1: TOF MS ES+  
9.71e+003



Minimum: -1.5  
Maximum: 5.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
286.0998	286.0999	-0.1	-0.3	9.5	29.6	n/a	n/a	C <sub>17</sub> H <sub>17</sub> N O Cl



3e

## Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

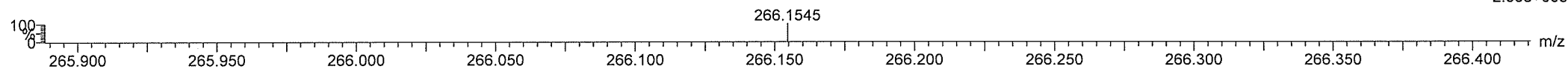
13 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 0-20 H: 0-20 N: 0-2 O: 0-2

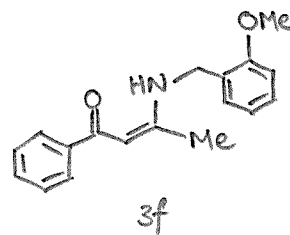
C18H19NO

JJG4066-6 125 (2.230)

1: TOF MS ES+  
2.33e+003

Minimum: -1.5  
Maximum: 5.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
266.1545	266.1545	0.0	0.0	9.5	25.5	n/a	n/a	C18 H20 N O



# Elemental Composition Report

## Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

22 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

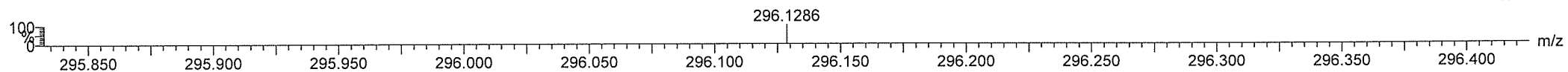
Elements Used:

C: 0-20 H: 0-20 N: 0-2 O: 0-5

C<sub>18</sub>H<sub>17</sub>NO<sub>3</sub>

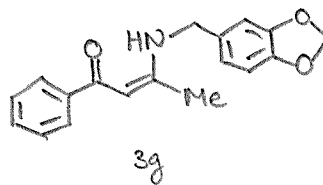
JJG4066-7 329 (5.819)

1: TOF MS ES+  
2.67e+003



Minimum: -1.5  
Maximum: 5.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
296.1286	296.1287	-0.1	-0.3	10.5	25.9	n/a	n/a	C <sub>18</sub> H <sub>18</sub> N O <sub>3</sub>



# Elemental Composition Report

## Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

29 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

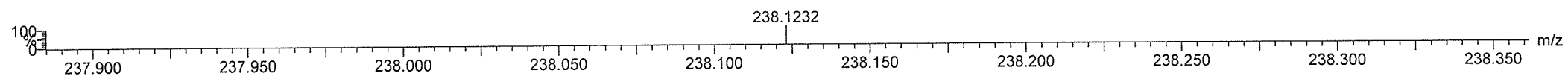
Elements Used:

C: 0-20 H: 0-20 N: 0-3 O: 0-3

C<sub>16</sub>H<sub>15</sub>NO

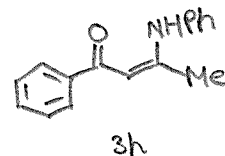
JJG4066-8 50 (0.902)

1: TOF MS ES+  
2.31e+006



Minimum: -1.5  
Maximum: 10.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
238.1232	238.1232	0.0	0.0	9.5	42.5	n/a	n/a	C <sub>16</sub> H <sub>16</sub> N O





## Elemental Composition Report

## Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

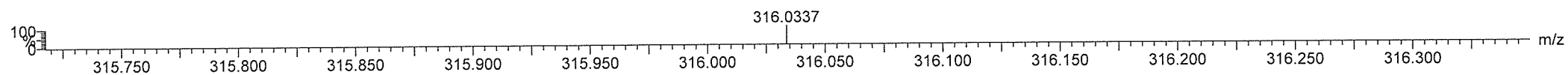
91 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 0-20 H: 0-20 N: 0-3 O: 0-3 Br: 0-3

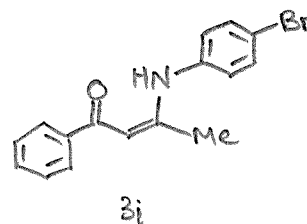
C16H14BrNO

JJG4066-9 17 (0.324)

1: TOF MS ES+  
4.46e+005

Minimum: -1.5  
Maximum: 10.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
316.0337	316.0337	0.0	0.0	9.5	39.8	n/a	n/a	C16 H15 N O Br



# Elemental Composition Report

## Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

57 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

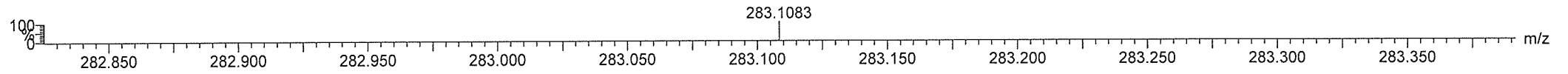
Elements Used:

C: 0-20 H: 0-20 N: 0-5 O: 0-5

C<sub>16</sub>H<sub>14</sub>N<sub>2</sub>O<sub>3</sub>

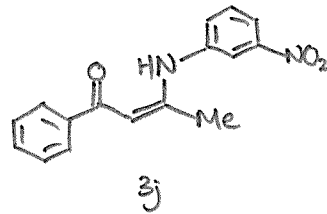
JJG4066-10 5 (0.121) Cm (1:12)

1: TOF MS ES+  
2.36e+007



Minimum: -1.5  
Maximum: 10.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
283.1083	283.1083	0.0	0.0	10.5	48.5	n/a	n/a	C <sub>16</sub> H <sub>15</sub> N <sub>2</sub> O <sub>3</sub>



# Elemental Composition Report

## Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

35 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

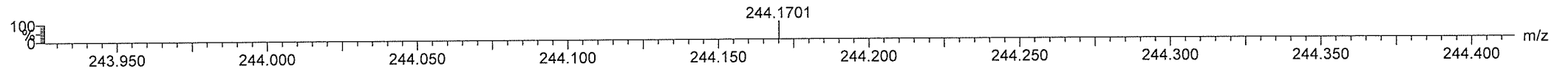
Elements Used:

C: 0-20 H: 0-25 N: 0-3 O: 0-3

C<sub>16</sub>H<sub>21</sub>NO

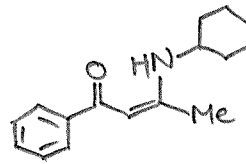
JJG4066-12 76 (1.362)

1: TOF MS ES+  
3.10e+006



Minimum: -1.5  
Maximum: 10.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
244.1701	244.1701	0.0	0.0	6.5	43.3	n/a	n/a	C <sub>16</sub> H <sub>22</sub> N O



3k

# Elemental Composition Report

## Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

24 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

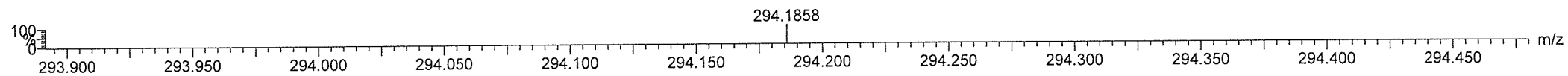
Elements Used:

C: 0-20 H: 0-25 N: 0-3 O: 0-3

C<sub>20</sub>H<sub>23</sub>NO

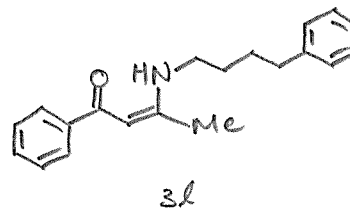
JJG4066-13 30 (0.564)

1: TOF MS ES+  
1.44e+007



Minimum: -1.5  
Maximum: 10.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
294.1858	294.1858	0.0	0.0	9.5	47.5	n/a	n/a	C <sub>20</sub> H <sub>24</sub> N O



# Elemental Composition Report

## Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

29 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

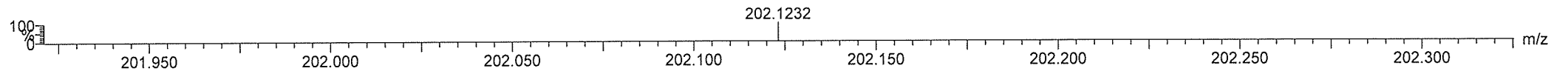
Elements Used:

C: 0-20 H: 0-20 N: 0-3 O: 0-3

C<sub>13</sub>H<sub>15</sub>NO

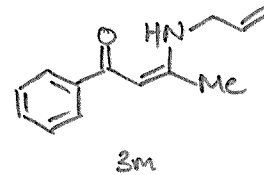
JJG4066-14 17 (0.324)

1: TOF MS ES+  
2.77e+006



Minimum: -1.5  
Maximum: 10.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
202.1232	202.1232	0.0	0.0	6.5	42.7	n/a	n/a	C <sub>13</sub> H <sub>16</sub> N O



# Elemental Composition Report

## Single Mass Analysis

Tolerance = 20.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron Ions

21 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

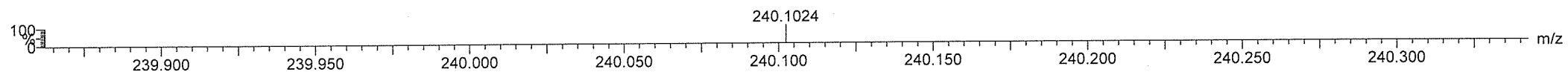
Elements Used:

C: 0-20 H: 0-15 N: 0-3 O: 0-3

C<sub>15</sub>H<sub>13</sub>NO<sub>2</sub>

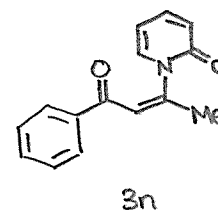
S1 469 (8.287)

1: TOF MS ES+  
2.08e+003



Minimum: -1.5  
Maximum: 5.0 20.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
240.1024	240.1025	-0.1	-0.4	9.5	20.6	n/a	n/a	C <sub>15</sub> H <sub>14</sub> N O <sub>2</sub>



# Elemental Composition Report

## Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

42 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

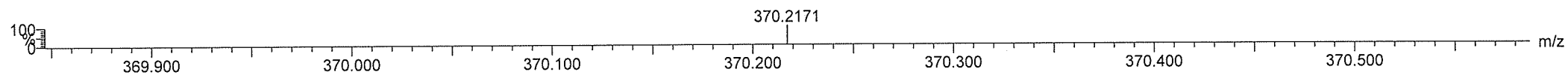
Elements Used:

C: 0-30 H: 0-30 N: 0-3 O: 0-3

C<sub>26</sub>H<sub>27</sub>N<sub>1</sub>O

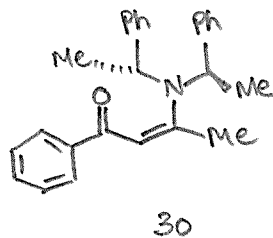
JJG4090-3 28 (0.510)

1: TOF MS ES+  
1.86e+006



Minimum: -1.5  
Maximum: 10.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
370.2171	370.2171	0.0	0.0	13.5	42.8	n/a	n/a	C <sub>26</sub> H <sub>28</sub> N O



# Elemental Composition Report

## Single Mass Analysis

Tolerance = 20.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron Ions

68 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

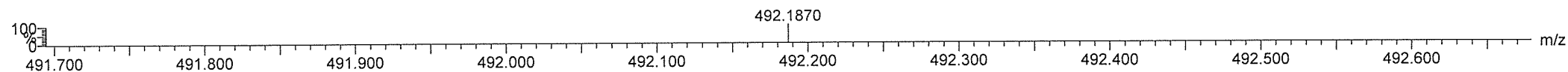
Elements Used:

C: 0-30 H: 0-35 N: 0-2 O: 0-12

C<sub>24</sub>H<sub>29</sub>NO<sub>10</sub>

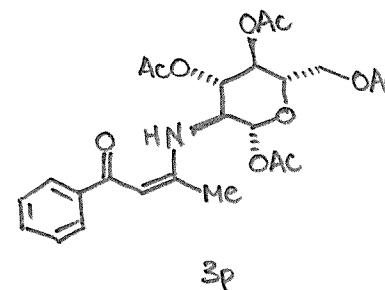
S2 87 (1.568)

1: TOF MS ES+  
2.16e+004



Minimum: -1.5  
Maximum: 5.0 20.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
492.1870	492.1870	0.0	0.0	10.5	26.5	n/a	n/a	C <sub>24</sub> H <sub>30</sub> N O <sub>10</sub>





## Elemental Composition Report

## Single Mass Analysis

Tolerance = 20.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron Ions

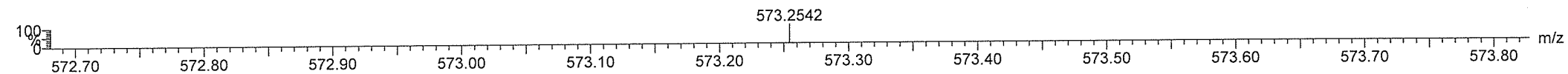
13 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 0-42 H: 0-35 N: 0-3 O: 0-2

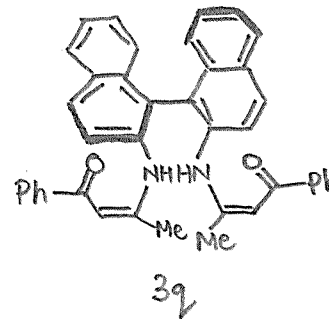
C<sub>40</sub>H<sub>32</sub>N<sub>2</sub>O<sub>2</sub>

S3 7 (0.155)

1: TOF MS ES+  
1.14e+004

Minimum: -1.5  
Maximum: 5.0 20.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
573.2542	573.2542	0.0	0.0	25.5	25.7	n/a	n/a	C <sub>40</sub> H <sub>33</sub> N <sub>2</sub> O <sub>2</sub>



Single Mass Analysis

Tolerance = 20.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron Ions

38 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

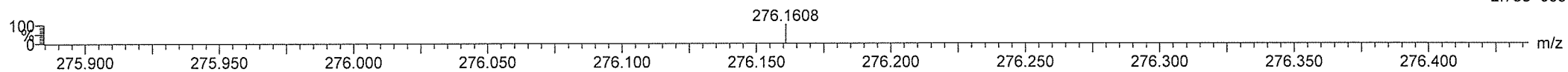
Elements Used:

C: 0-20 H: 0-25 N: 0-3 O: 0-4

C16H21NO3

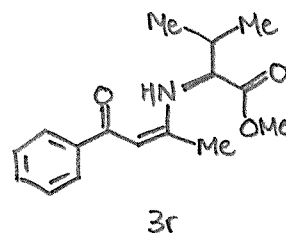
S4 1 (0.053)

1: TOF MS ES+  
2.75e+003



Minimum: -1.5  
Maximum: 5.0 20.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
276.1608	276.1600	0.8	2.9	6.5	21.5	n/a	n/a	C16 H22 N O3



# Elemental Composition Report

## Single Mass Analysis

Tolerance = 20.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron Ions

33 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

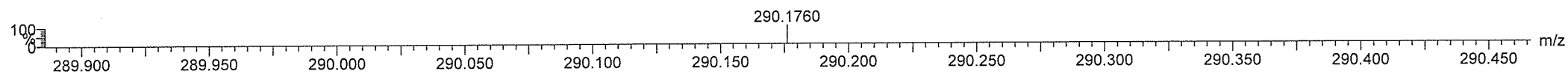
Elements Used:

C: 0-20 H: 0-25 N: 0-3 O: 0-4

C<sub>17</sub>H<sub>23</sub>NO<sub>3</sub>

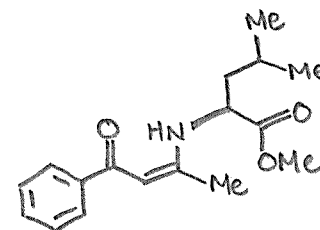
S5 466 (8.236)

1: TOF MS ES+  
4.14e+003



Minimum: -1.5  
Maximum: 5.0 20.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
290.1760	290.1756	0.4	1.4	6.5	22.4	n/a	n/a	C <sub>17</sub> H <sub>24</sub> N O <sub>3</sub>



3s

# Elemental Composition Report

## Single Mass Analysis

Tolerance = 20.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron Ions

26 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

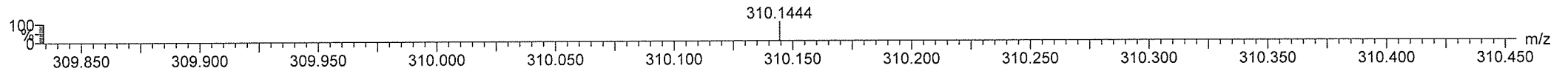
Elements Used:

C: 0-20 H: 0-25 N: 0-3 O: 0-4

C<sub>19</sub>H<sub>19</sub>NO<sub>3</sub>

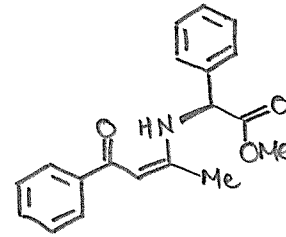
S6 489 (8.645)

1: TOF MS ES+  
1.52e+003



Minimum: -1.5  
Maximum: 5.0 20.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
310.1444	310.1443	0.1	0.3	10.5	20.5	n/a	n/a	C <sub>19</sub> H <sub>20</sub> N O <sub>3</sub>



3t

# Elemental Composition Report

## Single Mass Analysis

Tolerance = 20.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron Ions

29 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

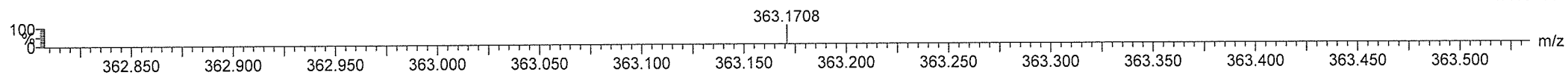
Elements Used:

C: 0-25 H: 0-25 N: 0-3 O: 0-4

C<sub>22</sub>H<sub>22</sub>N<sub>2</sub>O<sub>3</sub>

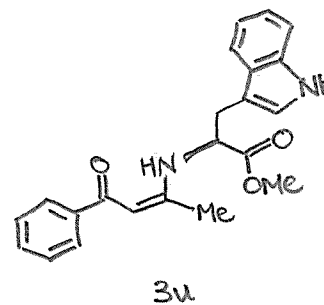
S7 339 (6.008)

1: TOF MS ES+  
4.41e+003



Minimum: -1.5  
Maximum: 5.0 20.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
363.1708	363.1709	-0.1	-0.3	12.5	22.9	n/a	n/a	C <sub>22</sub> H <sub>23</sub> N <sub>2</sub> O <sub>3</sub>



# Elemental Composition Report

## Single Mass Analysis

Tolerance = 20.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron Ions

50 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

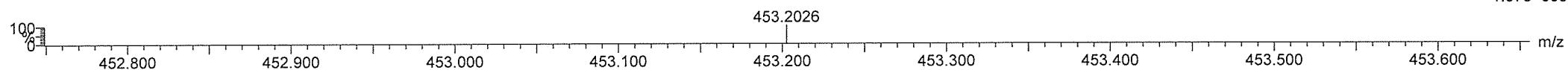
Elements Used:

C: 0-28 H: 0-30 N: 0-3 O: 0-8

C<sub>25</sub>H<sub>28</sub>N<sub>2</sub>O<sub>6</sub>

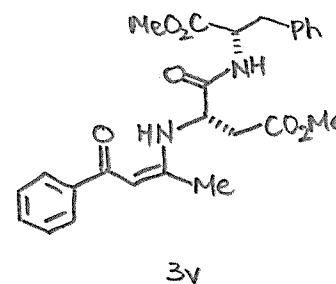
S8 253 (4.494)

1: TOF MS ES+  
1.97e+003



Minimum: -1.5  
Maximum: 5.0 20.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
453.2026	453.2026	0.0	0.0	12.5	21.6	n/a	n/a	C <sub>25</sub> H <sub>29</sub> N <sub>2</sub> O <sub>6</sub>



# Elemental Composition Report

## Single Mass Analysis

Tolerance = 20.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron Ions

65 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

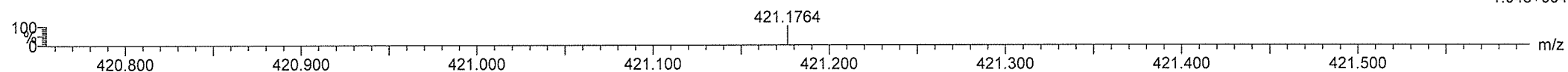
Elements Used:

C: 0-28 H: 0-30 N: 0-3 O: 0-8

C<sub>24</sub>H<sub>24</sub>N<sub>2</sub>O<sub>5</sub>

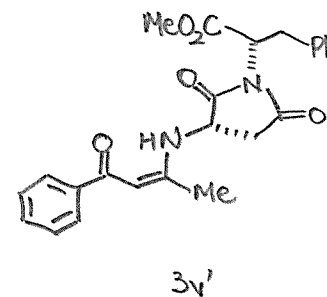
S9 166 (2.943)

1: TOF MS ES+  
1.04e+004



Minimum: -1.5  
Maximum: 5.0 20.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
421.1764	421.1763	0.1	0.2	13.5	24.8	n/a	n/a	C <sub>24</sub> H <sub>25</sub> N <sub>2</sub> O <sub>5</sub>



# Elemental Composition Report

## Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

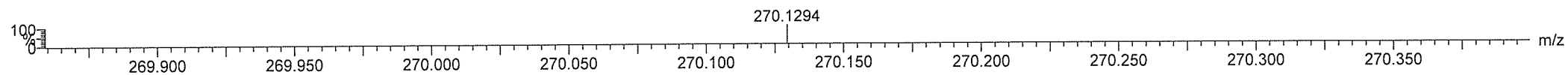
49 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 0-19 H: 0-20 N: 0-3 O: 0-3 F: 0-1

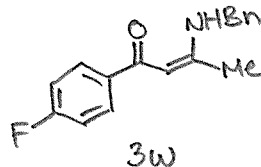
C17H16FNO  
JJG4070-3 34 (0.631)

1: TOF MS ES+  
8.09e+006



Minimum: -1.5  
Maximum: 10.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
270.1294	270.1294	0.0	0.0	9.5	45.8	n/a	n/a	C17 H17 N O F





# Elemental Composition Report

## Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

106 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

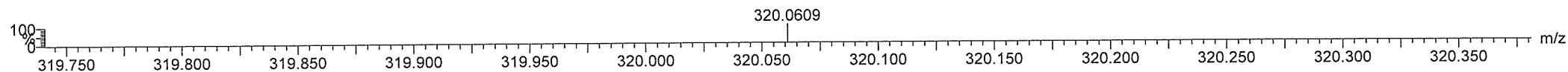
Elements Used:

C: 0-20 H: 0-20 N: 0-2 O: 0-3 Cl: 0-5

C<sub>17</sub>H<sub>15</sub>Cl<sub>2</sub>NO

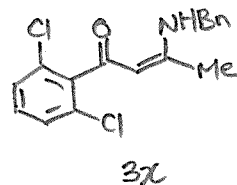
JJG4070-4 29 (0.547)

1: TOF MS ES+  
1.20e+007



Minimum: -1.5  
Maximum: 10.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
320.0609	320.0609	0.0	0.0	9.5	47.8	n/a	n/a	C <sub>17</sub> H <sub>16</sub> N O Cl <sub>2</sub>



# Elemental Composition Report

## Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

31 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

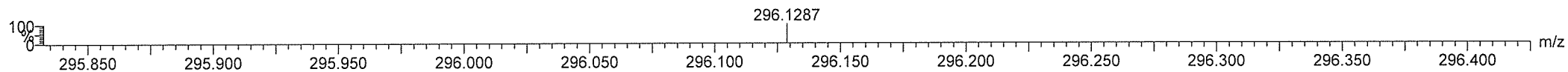
Elements Used:

C: 0-20 H: 0-20 N: 0-3 O: 0-5

C<sub>18</sub>H<sub>17</sub>NO<sub>3</sub>

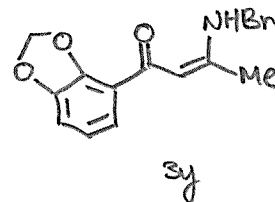
OSK1022 36 (0.665)

1: TOF MS ES+  
1.54e+006



Minimum: -1.5  
Maximum: 10.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
296.1287	296.1287	0.0	0.0	10.5	41.8	n/a	n/a	C <sub>18</sub> H <sub>18</sub> N O <sub>3</sub>



# Elemental Composition Report

## Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

35 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

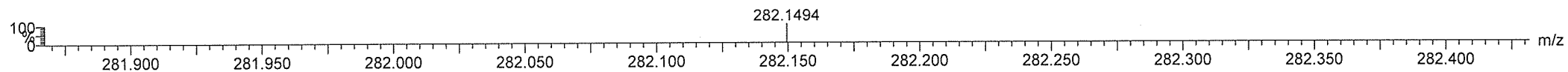
Elements Used:

C: 0-25 H: 0-25 N: 0-3 O: 0-3

C<sub>18</sub>H<sub>19</sub>NO<sub>2</sub>

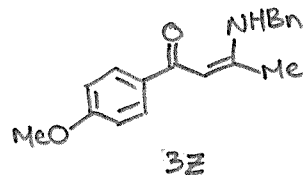
JJG4070-11 110 (1.957)

1: TOF MS ES+  
1.06e+007



Minimum: -1.5  
Maximum: 10.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
282.1494	282.1494	0.0	0.0	9.5	46.6	n/a	n/a	C <sub>18</sub> H <sub>20</sub> N O <sub>2</sub>



# Elemental Composition Report

## Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

52 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

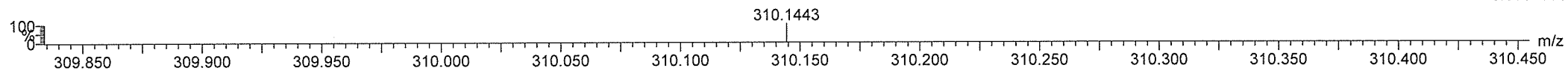
Elements Used:

C: 0-25 H: 0-25 N: 0-3 O: 0-5

C<sub>19</sub>H<sub>19</sub>NO<sub>3</sub>

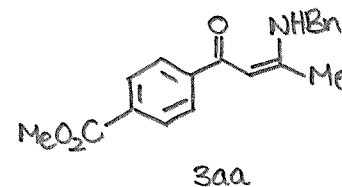
OSK1006 9 (0.189)

1: TOF MS ES+  
8.39e+005



Minimum: -1.5  
Maximum: 10.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
310.1443	310.1443	0.0	0.0	10.5	40.4	n/a	n/a	C <sub>19</sub> H <sub>20</sub> N O <sub>3</sub>



# Elemental Composition Report

## Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

85 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

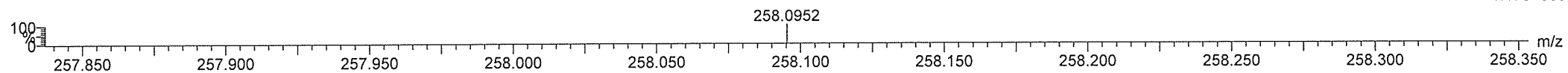
Elements Used:

C: 0-20 H: 0-20 N: 0-2 O: 0-3 S: 0-3

C15H15NOS

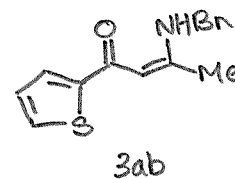
OSK1020 5 (0.121) Cm (1:13)

1: TOF MS ES+  
1.17e+008



Minimum: -1.5  
Maximum: 10.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
258.0952	258.0953	-0.1	-0.4	8.5	52.4	n/a	n/a	C15 H16 N O S



## Elemental Composition Report

## Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

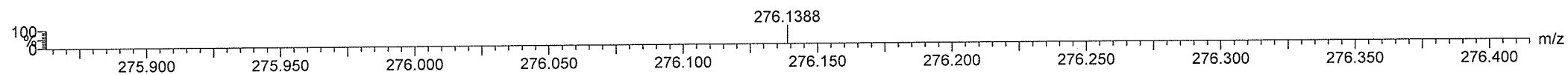
35 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 0-25 H: 0-25 N: 0-3 O: 0-3

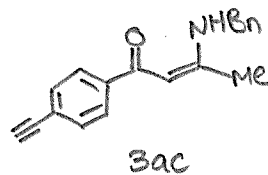
C<sub>19</sub>H<sub>17</sub>NO

JJG4070-1 42 (0.767)

1: TOF MS ES+  
1.05e+007

Minimum: -1.5  
Maximum: 10.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
276.1388	276.1388	0.0	0.0	11.5	46.6	n/a	n/a	C <sub>19</sub> H <sub>18</sub> N O



# Elemental Composition Report

## Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

35 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

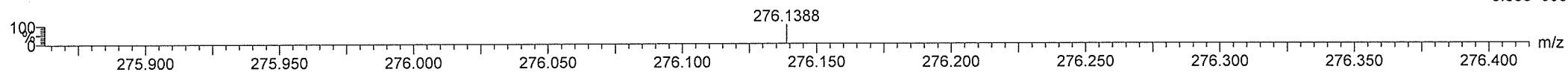
Elements Used:

C: 0-25 H: 0-25 N: 0-3 O: 0-3

C<sub>19</sub>H<sub>17</sub>NO

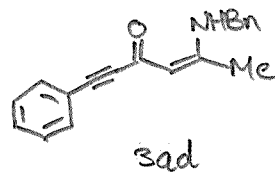
JJG4070-10 6 (0.138)

1: TOF MS ES+  
5.83e+006



Minimum: -1.5  
Maximum: 10.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
276.1388	276.1388	0.0	0.0	11.5	45.1	n/a	n/a	C <sub>19</sub> H <sub>18</sub> N O



# Elemental Composition Report

## Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

35 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

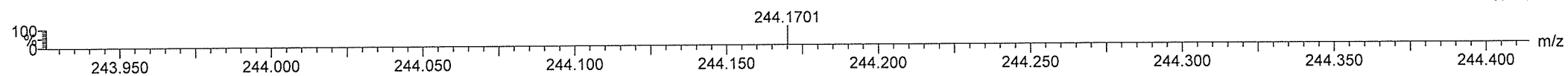
Elements Used:

C: 0-20 H: 0-25 N: 0-3 O: 0-3

C<sub>16</sub>H<sub>21</sub>NO

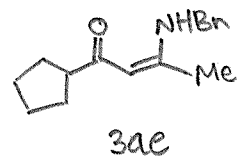
JJG4070-6 86 (1.551)

1: TOF MS ES+  
9.74e+006



Minimum: -1.5  
Maximum: 10.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
244.1701	244.1701	0.0	0.0	6.5	46.2	n/a	n/a	C <sub>16</sub> H <sub>22</sub> N O





# Elemental Composition Report

## Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

34 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

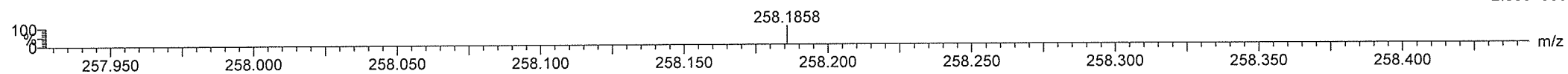
Elements Used:

C: 0-20 H: 0-25 N: 0-3 O: 0-3

C<sub>17</sub>H<sub>23</sub>NO

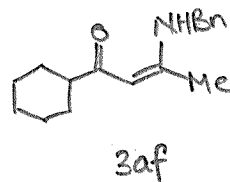
JJG4070-5 50 (0.902)

1: TOF MS ES+  
2.33e+006



Minimum: -1.5  
Maximum: 10.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
258.1858	258.1858	0.0	0.0	6.5	42.7	n/a	n/a	C <sub>17</sub> H <sub>24</sub> N O



# Elemental Composition Report

## Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

35 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

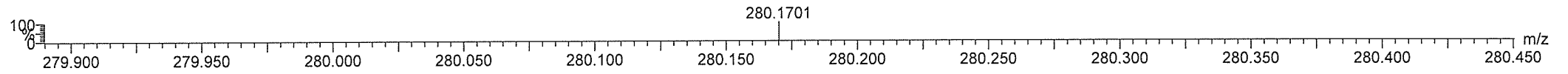
Elements Used:

C: 0-25 H: 0-25 N: 0-3 O: 0-3

C<sub>19</sub>H<sub>21</sub>NO

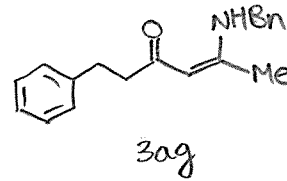
JJG4070-7 8 (0.172)

1: TOF MS ES+  
7.81e+006



Minimum: -1.5  
Maximum: 10.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
280.1701	280.1701	0.0	0.0	9.5	45.9	n/a	n/a	C <sub>19</sub> H <sub>22</sub> N O



Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

42 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

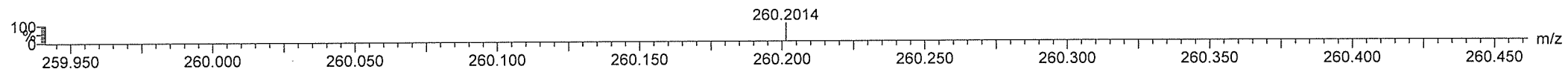
Elements Used:

C: 0-20 H: 0-30 N: 0-3 O: 0-3

C17H25NO

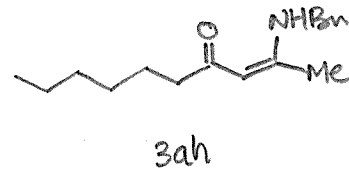
JJG4070-9 39 (0.716)

1: TOF MS ES+  
1.18e+007



Minimum: -1.5  
Maximum: 10.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
260.2014	260.2014	0.0	0.0	5.5	46.7	n/a	n/a	C17 H26 N O



Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

26 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

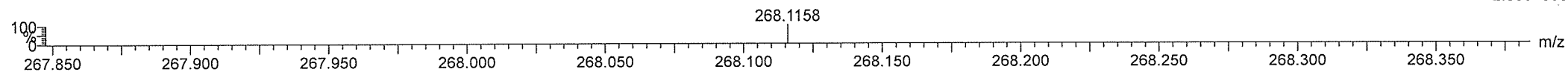
Elements Used:

C: 0-20 H: 0-20 N: 0-3 S: 0-3

C17H17NS

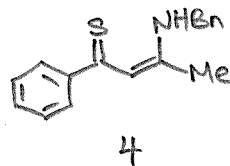
JJG4078-3 409 (7.232)

1: TOF MS ES+  
2.86e+003



Minimum: -1.5  
Maximum: 10.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
268.1158	268.1160	-0.2	-0.7	9.5	26.0	n/a	n/a	C17 H18 N S



# Elemental Composition Report

## Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

44 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

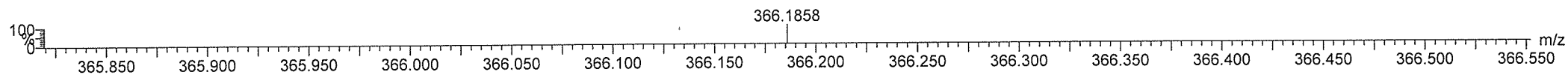
Elements Used:

C: 0-30 H: 0-30 N: 0-3 O: 0-3

C<sub>26</sub>H<sub>23</sub>NO

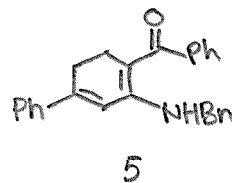
JJG4078-4 6 (0.138)

1: TOF MS ES+  
2.63e+006



Minimum: -1.5  
Maximum: 10.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
366.1858	366.1858	0.0	0.0	15.5	43.7	n/a	n/a	C <sub>26</sub> H <sub>24</sub> N O



## Single Mass Analysis

Tolerance = 20.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron Ions

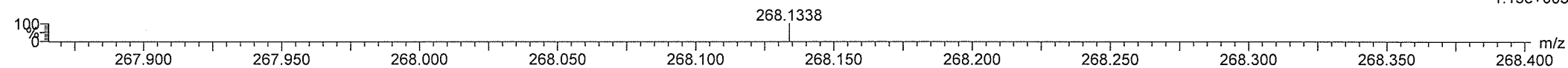
25 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 0-20 H: 0-20 N: 0-3 O: 0-3

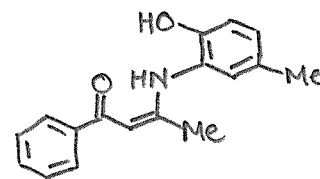
C17H17NO2

S10 441 (7.793)

1: TOF MS ES+  
1.15e+003

Minimum: -1.5  
Maximum: 5.0 20.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
268.1338	268.1338	0.0	0.0	9.5	19.7	n/a	n/a	C17 H18 N O2



6

Single Mass Analysis

Tolerance = 20.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron Ions

74 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

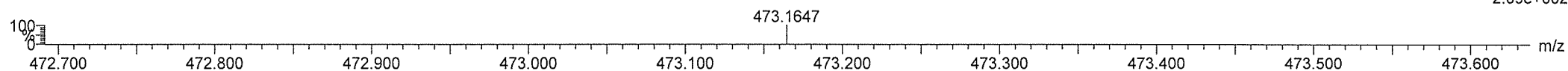
Elements Used:

C: 0-28 H: 0-30 N: 0-5 O: 0-5 S: 0-1

C<sub>26</sub>H<sub>24</sub>N<sub>4</sub>O<sub>3</sub>S

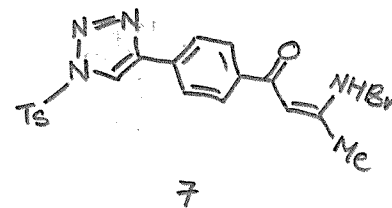
S11 56 (1.004)

1: TOF MS ES+  
2.09e+002



Minimum: -1.5  
Maximum: 5.0 20.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
473.1647	473.1647	0.0	0.0	16.5	17.2	n/a	n/a	C <sub>26</sub> H <sub>25</sub> N <sub>4</sub> O <sub>3</sub> S



# Elemental Composition Report

## Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

65 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

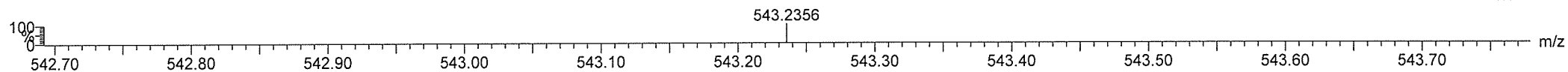
Elements Used:

C: 0-30 H: 0-35 N: 0-7 O: 0-7

C<sub>29</sub>H<sub>30</sub>N<sub>6</sub>O<sub>5</sub>

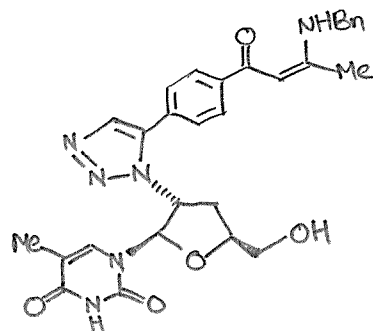
JJG4078-5 16 (0.307)

1: TOF MS ES+  
1.97e+005



Minimum: -1.5  
Maximum: 10.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
543.2356	543.2356	0.0	0.0	17.5	37.7	n/a	n/a	C <sub>29</sub> H <sub>31</sub> N <sub>6</sub> O <sub>5</sub>



8