

# **Iodine-mediated cross-dehydrogenative coupling of pyrazolones and alkenes**

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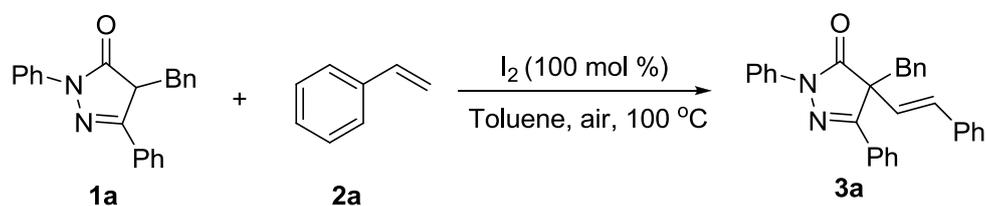
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## 1. Optimization of the reaction conditions

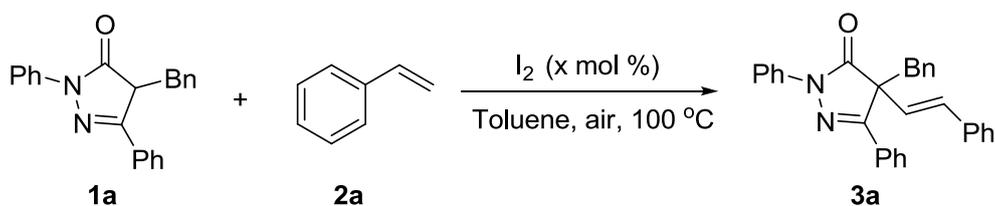
**Table 1.** Screening of the amount of **2a**<sup>a</sup>



entry	ratio (2a:1a)	yield <sup>b</sup> (%)
1	1	trace
2	2	20
3	3	22
4	5	36
5	8	52
<b>6</b>	<b>10</b>	<b>70</b>
7	12	69

<sup>a</sup> Reaction conditions: **1a** (0.1 mmol), **2a** (x mmol), and  $I_2$  (100 mol%) in PhMe (2.0 mL) at 100 °C were stirred under an air atmosphere for 12 h. <sup>b</sup> Isolated yields.

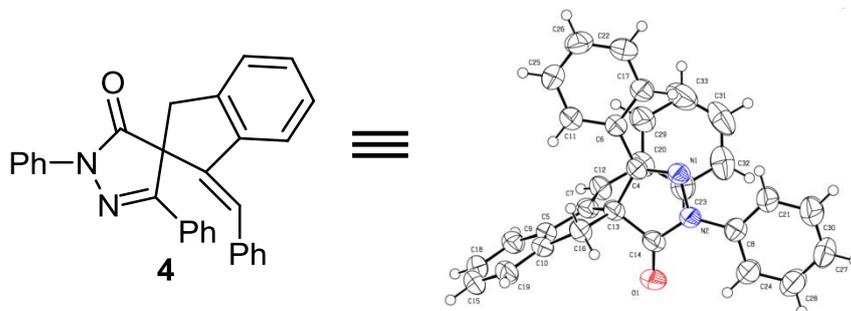
**Table 2.** Screening of the loading of iodine<sup>a</sup>



entry	iodine loading	yield <sup>b</sup> (%)
1	20 mol %	20
2	50 mol %	59
3	80 mol %	66
<b>4</b>	<b>100 mol %</b>	<b>70</b>
5	120 mol %	67
6	150 mol %	51
7	200 mol %	53
8	500 mol %	N.P. <sup>c</sup>

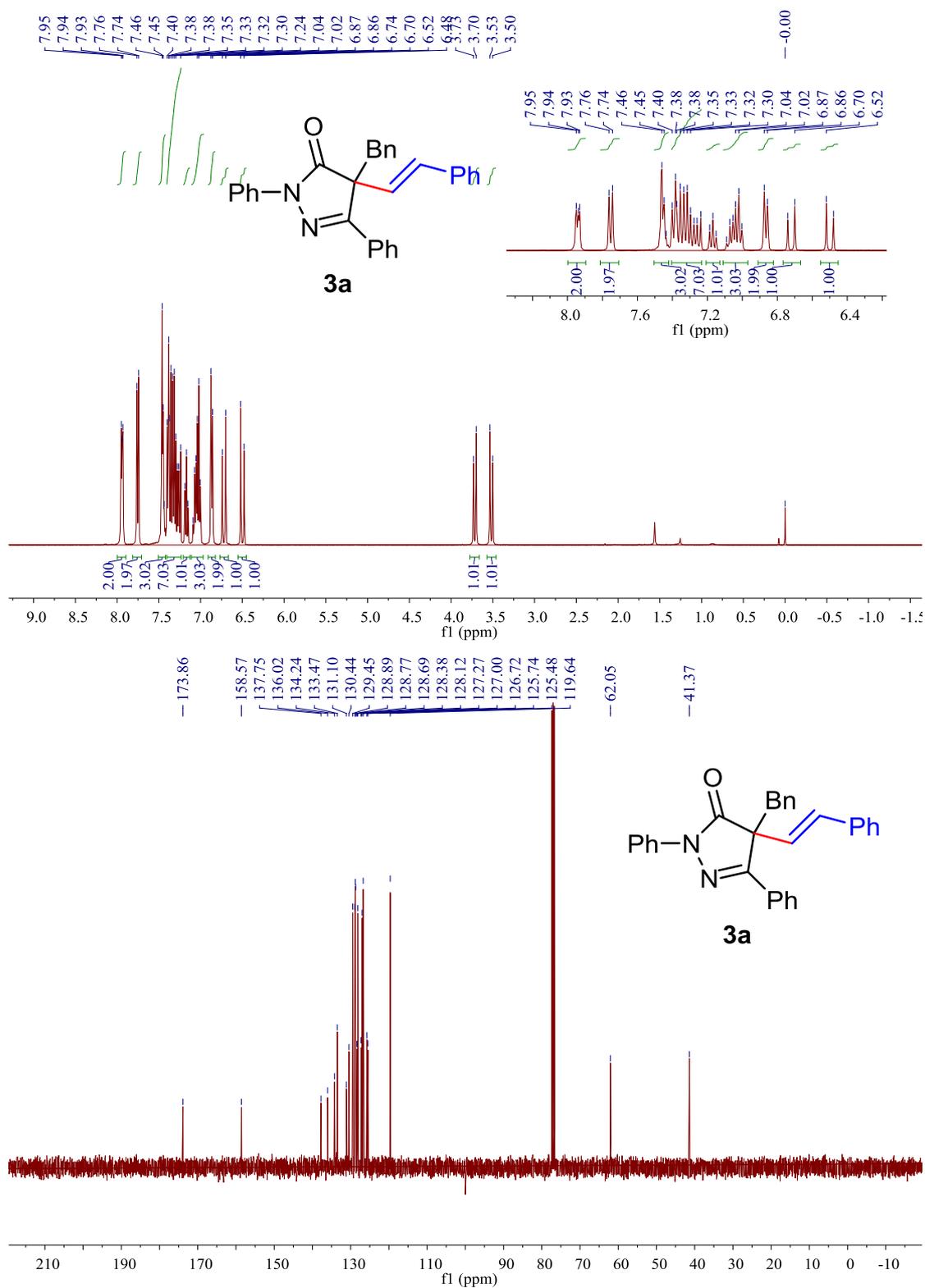
<sup>a</sup> Reaction conditions: **1a** (0.1 mmol), **2a** (1.0 mmol), and I<sub>2</sub> (x mol%) in PhMe (2.0 mL) at 100 °C were stirred under an air atmosphere for 12 h. <sup>b</sup> Isolated yields. <sup>c</sup> N.P. = no product.

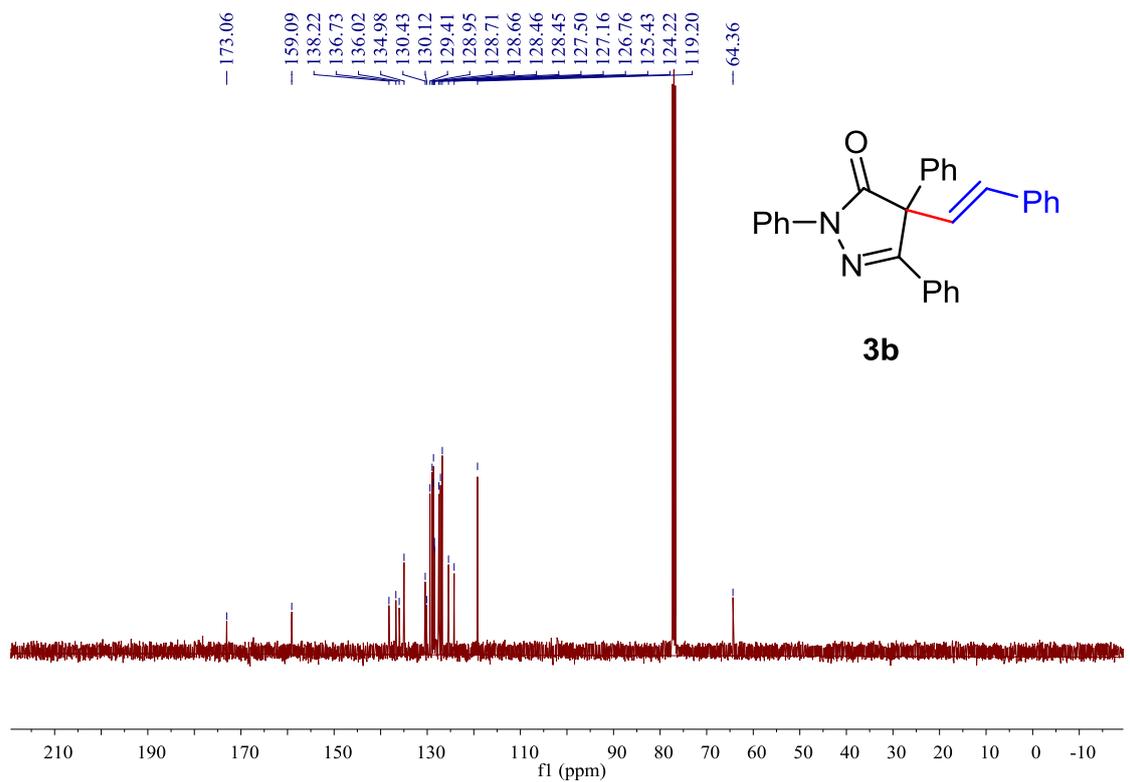
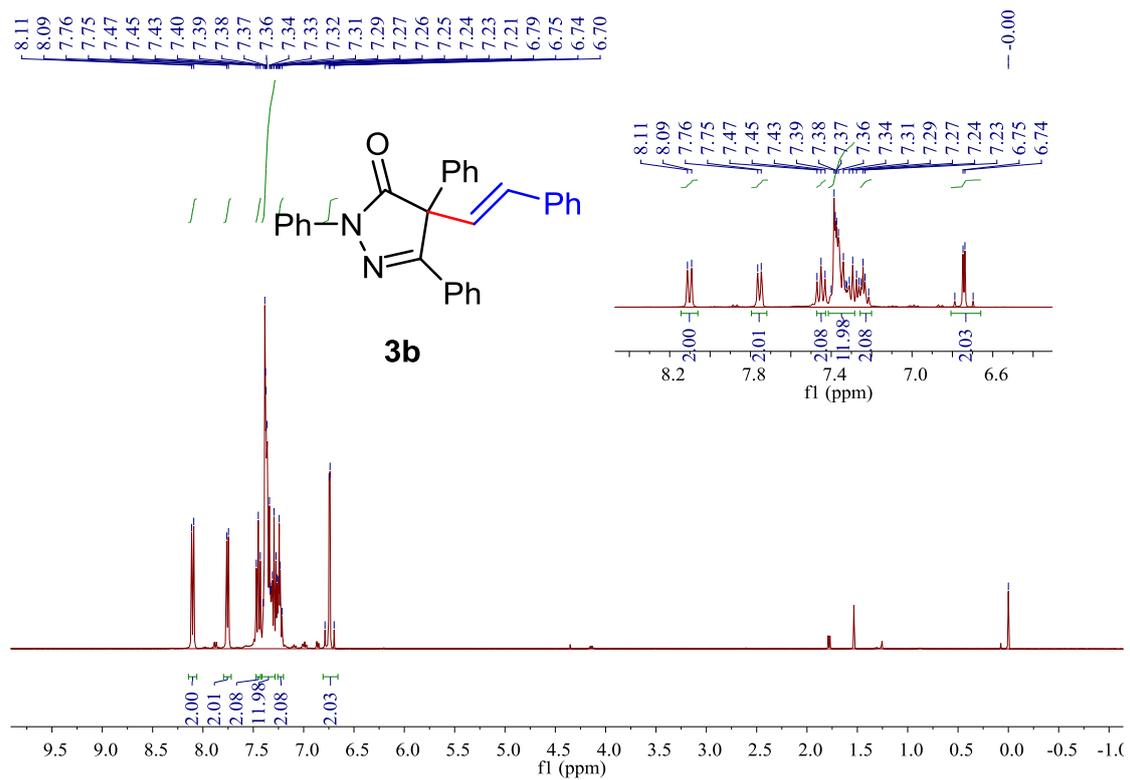
## 2. X-ray crystallography of compound **4**

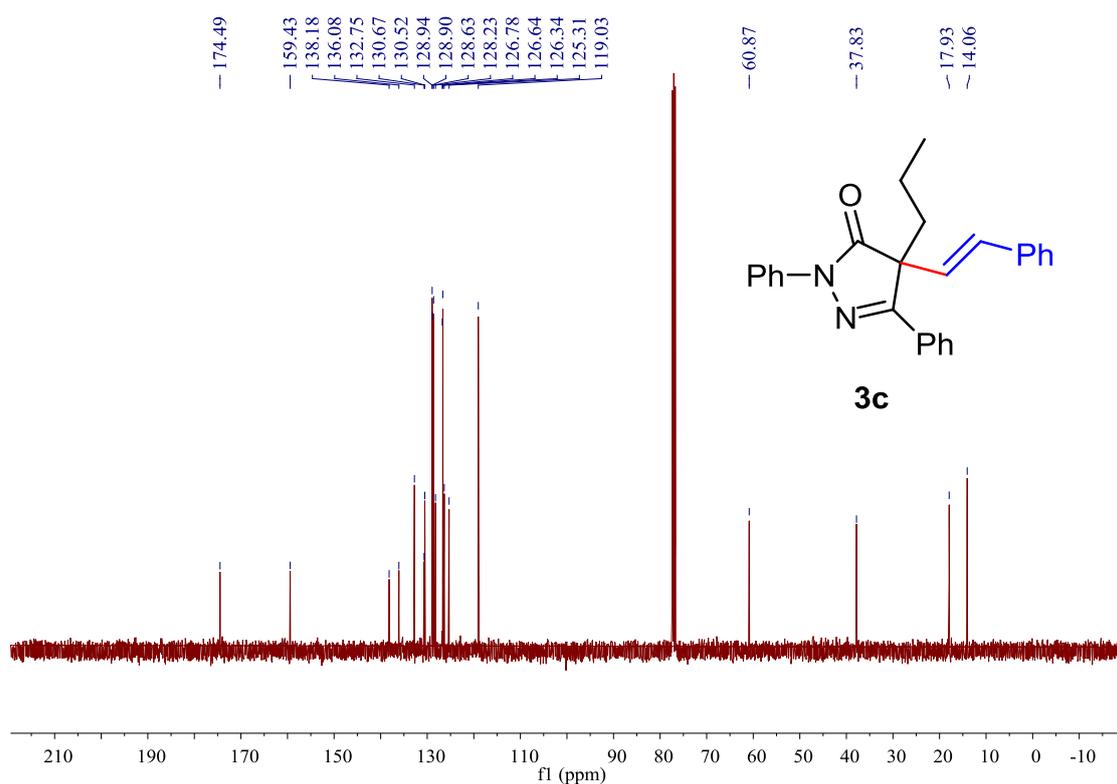
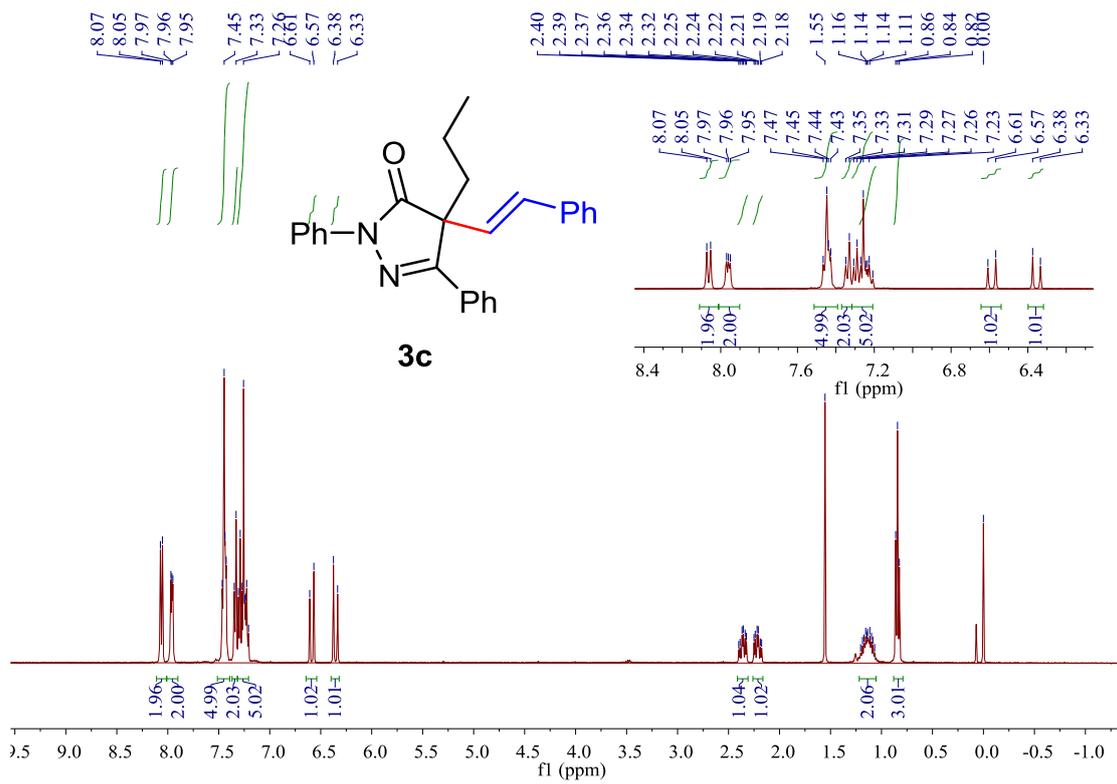


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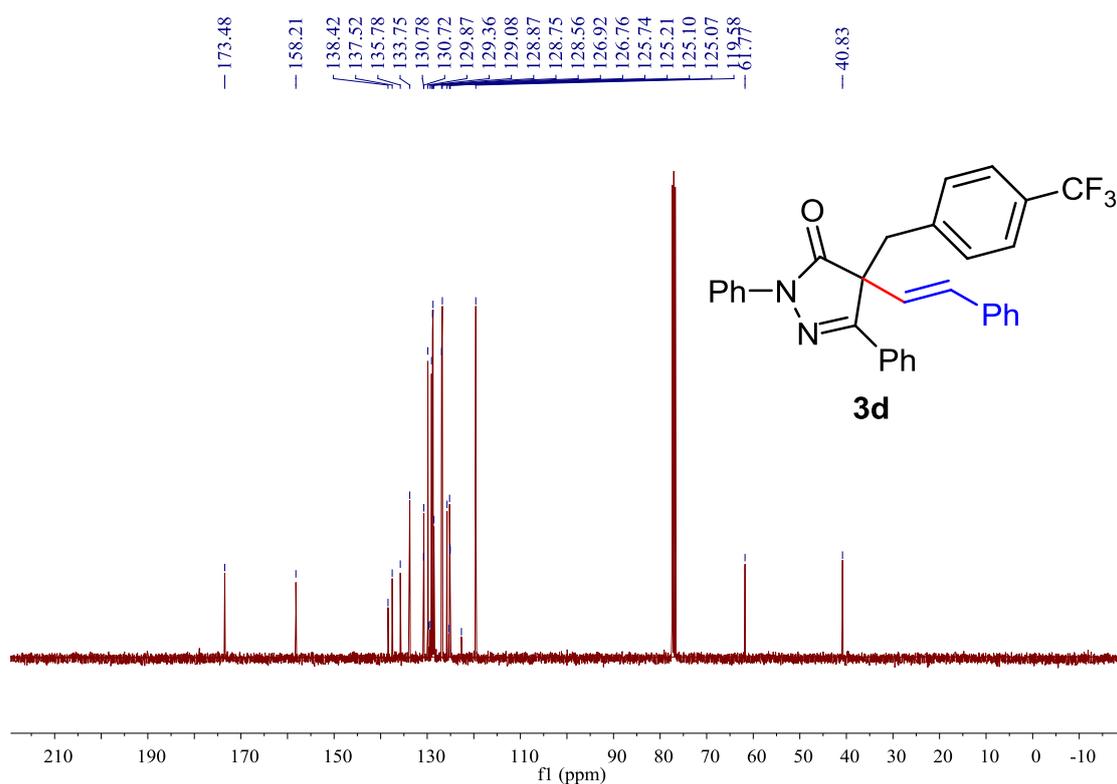
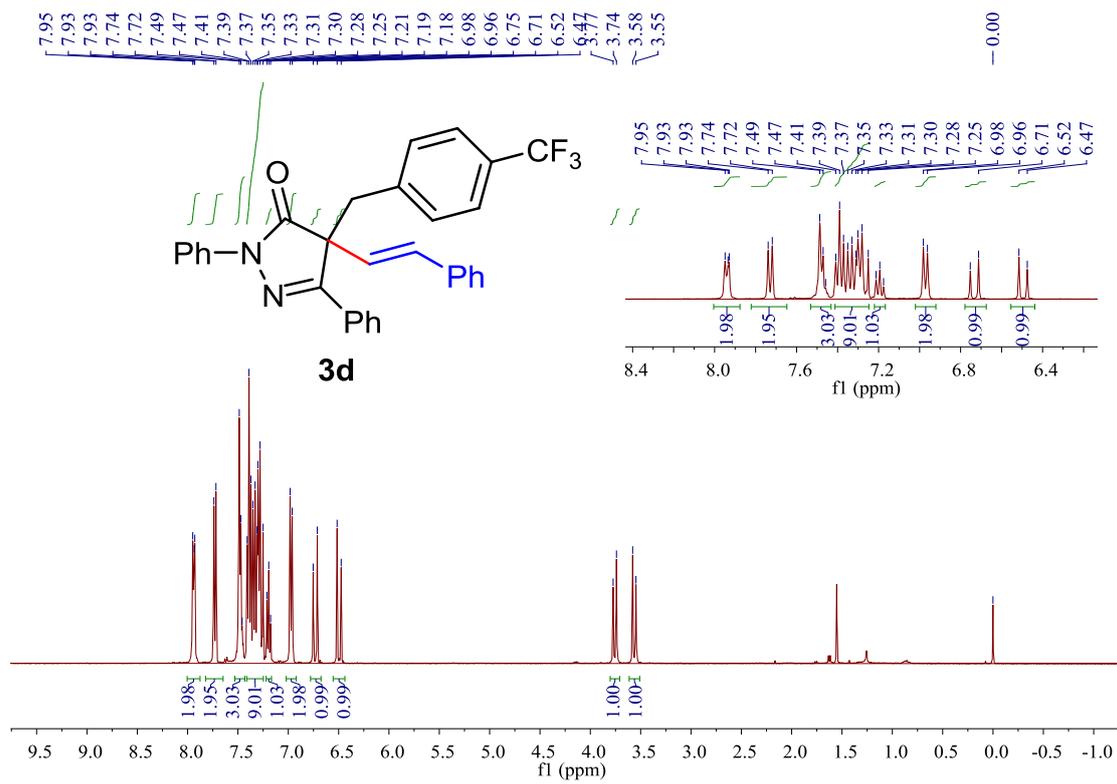
### 3. NMR Spectra

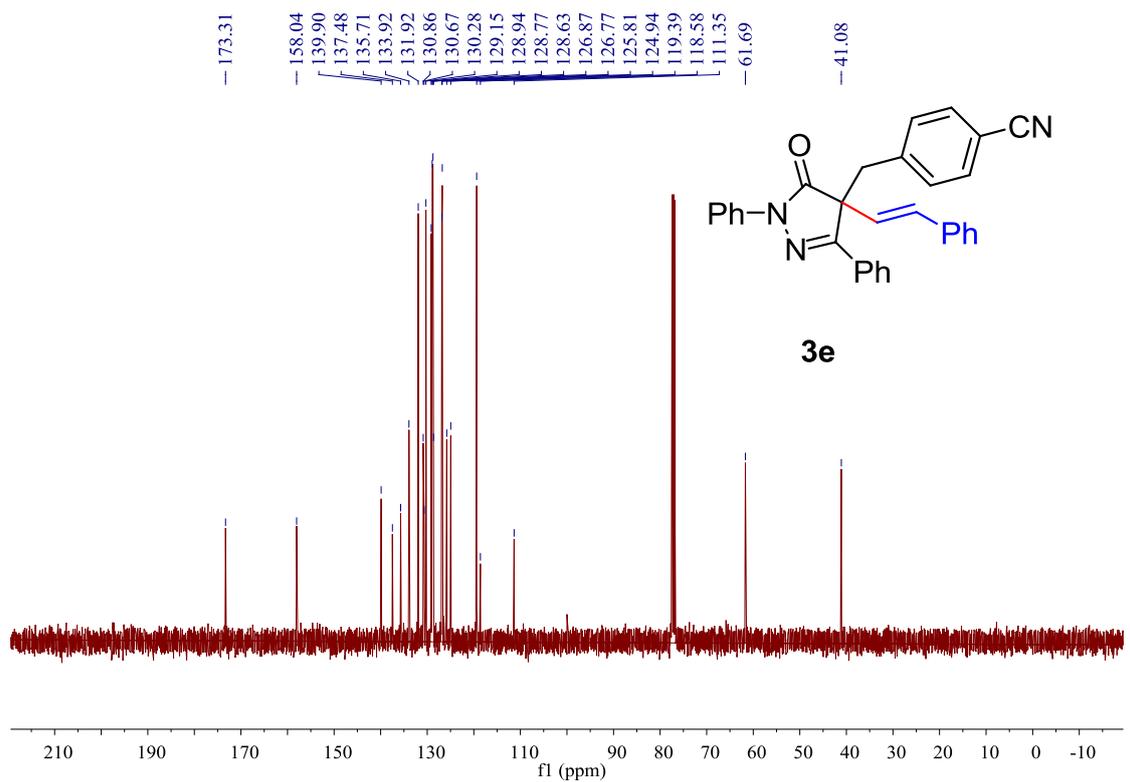
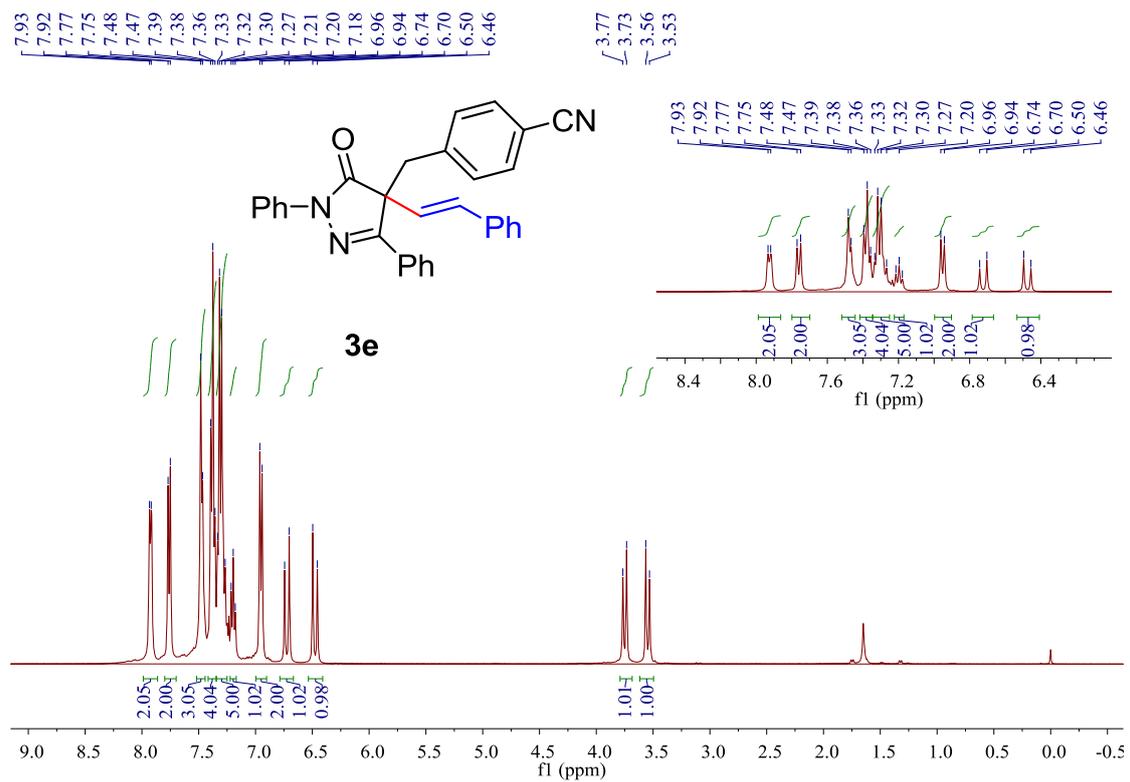


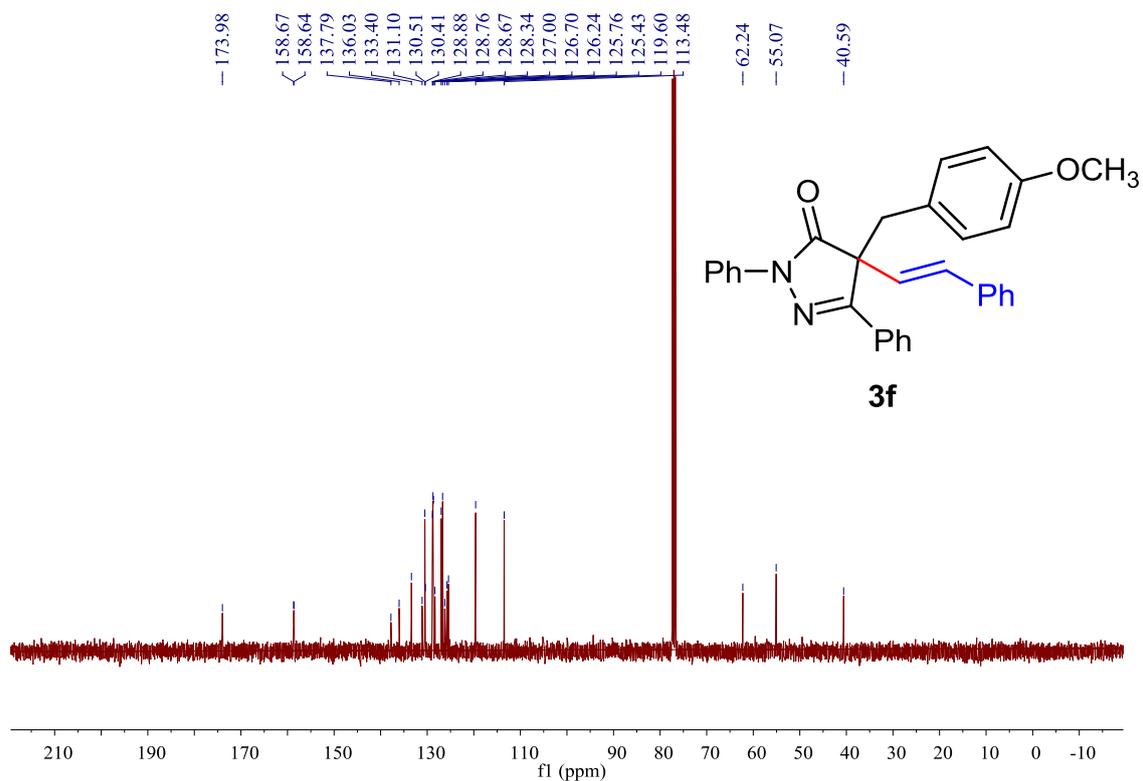
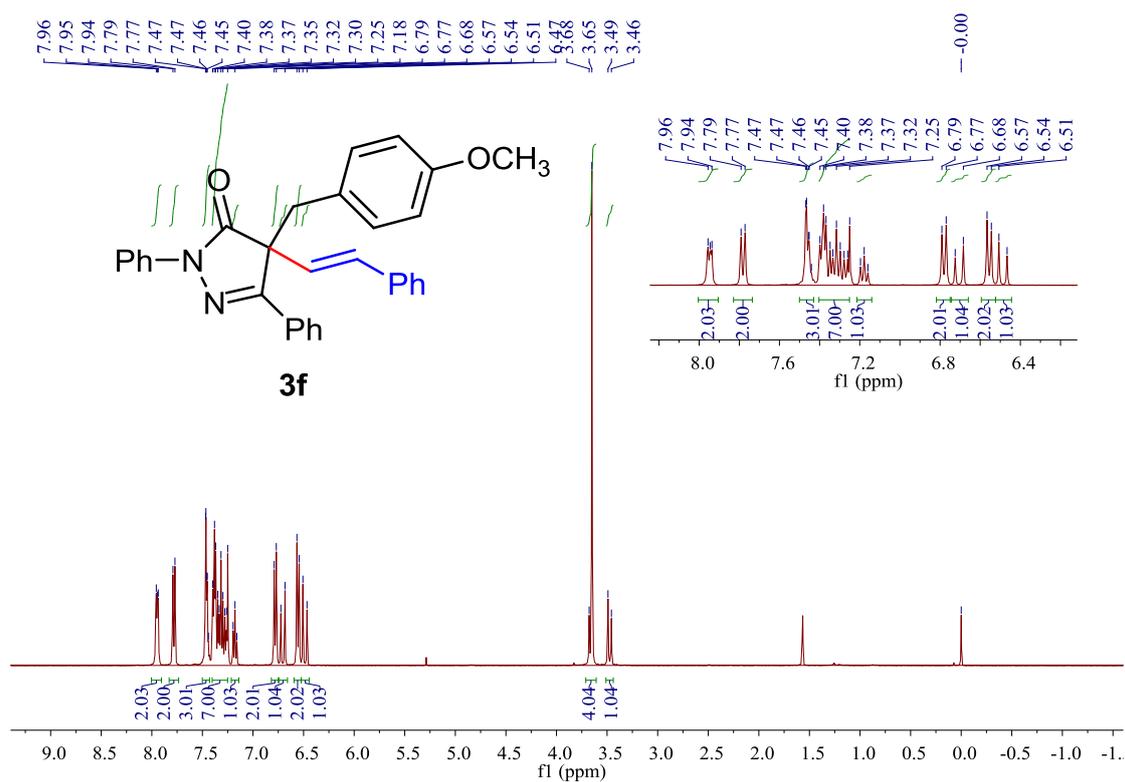




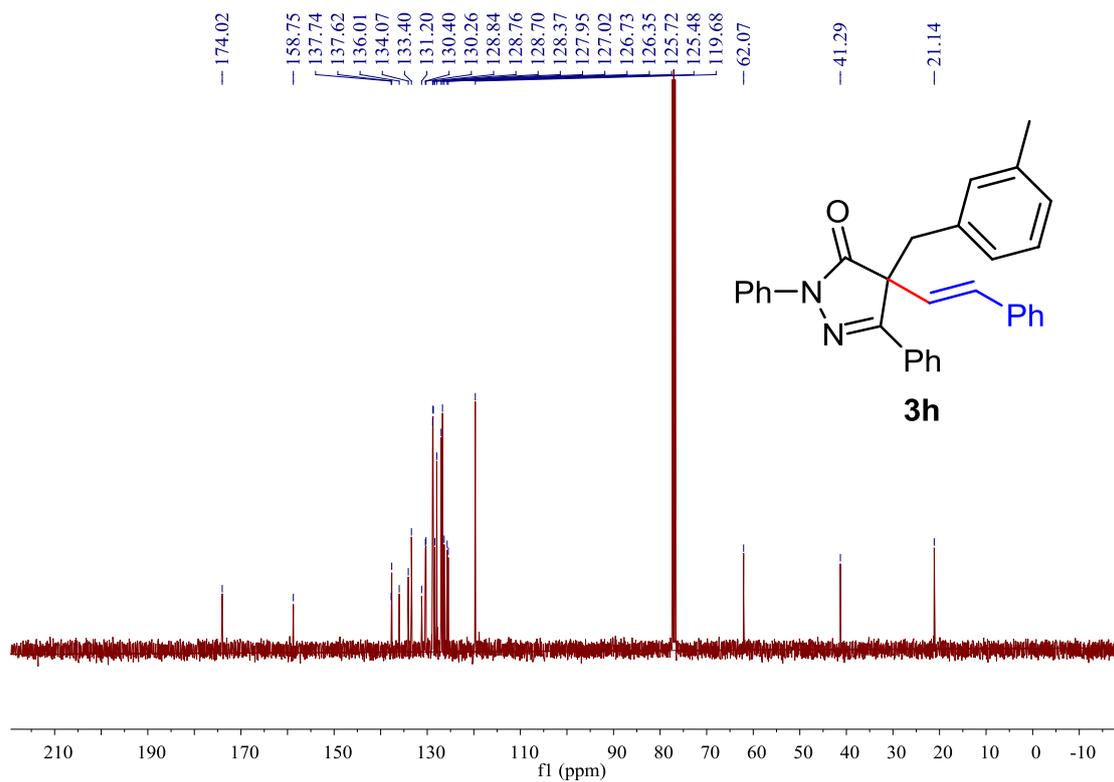
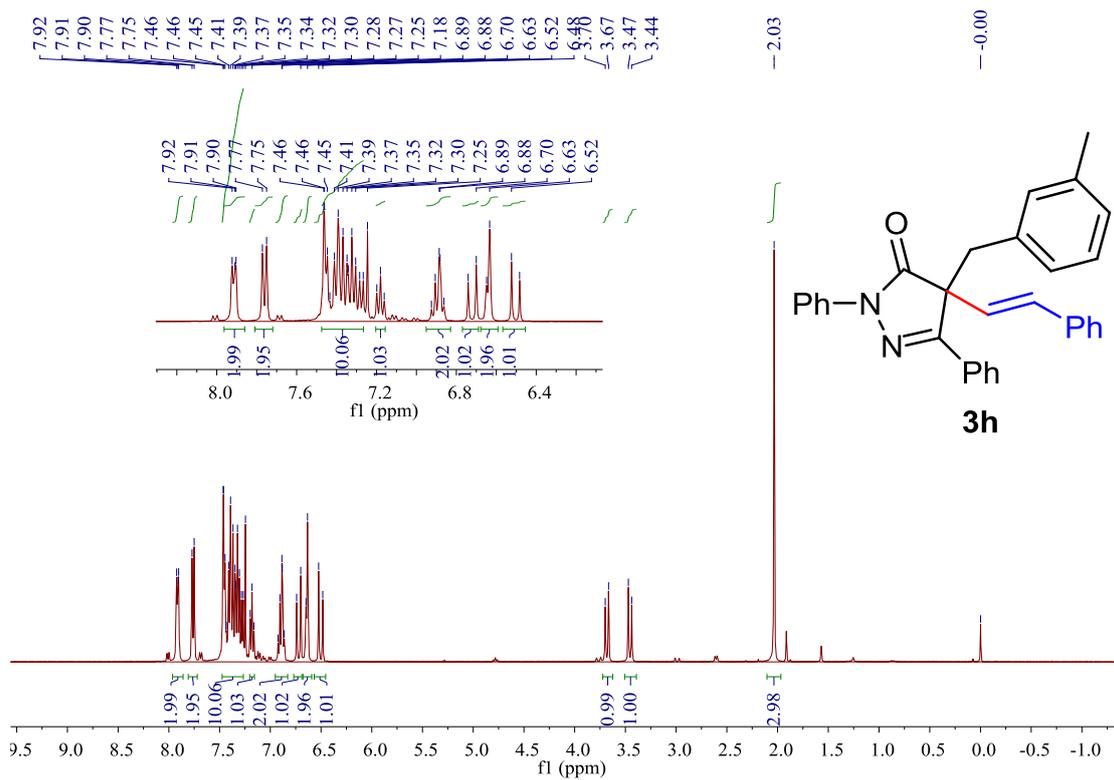
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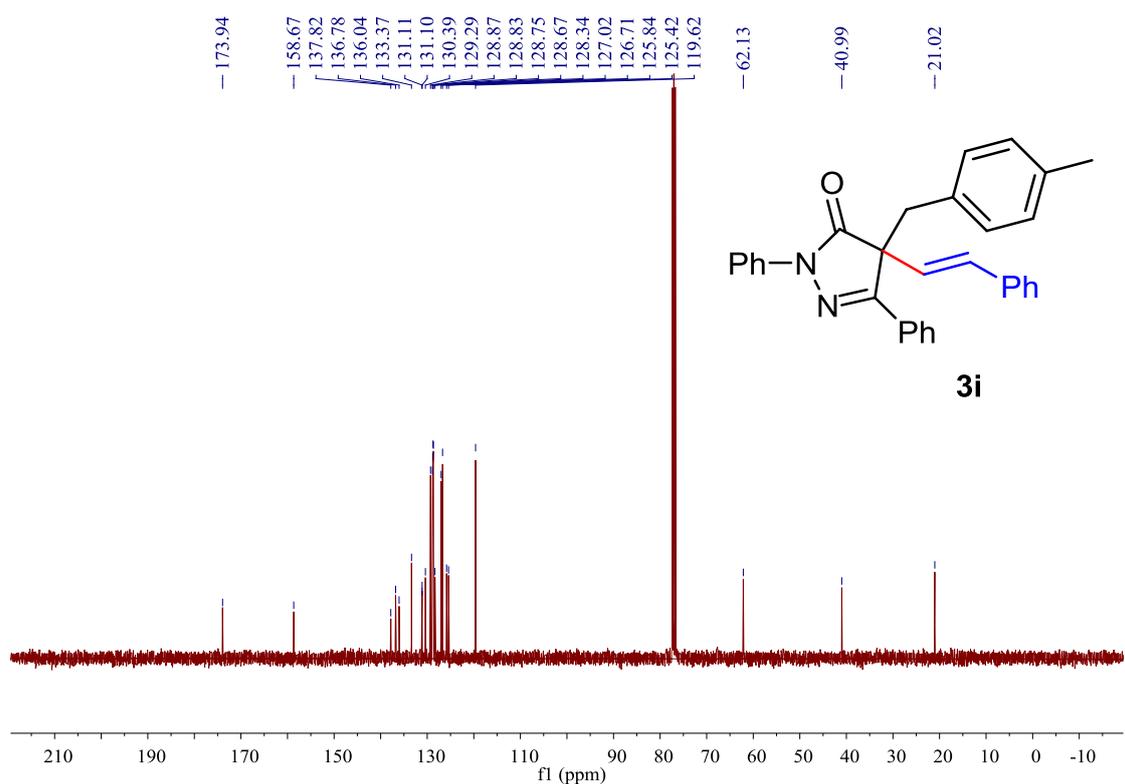
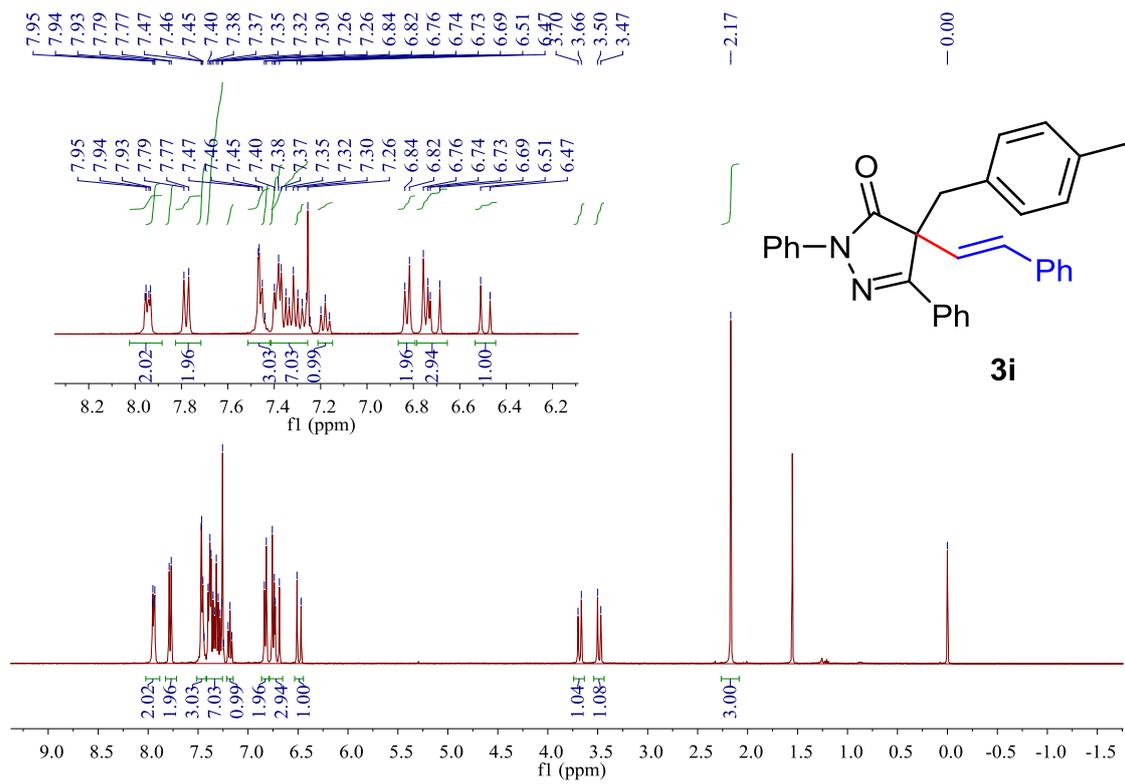


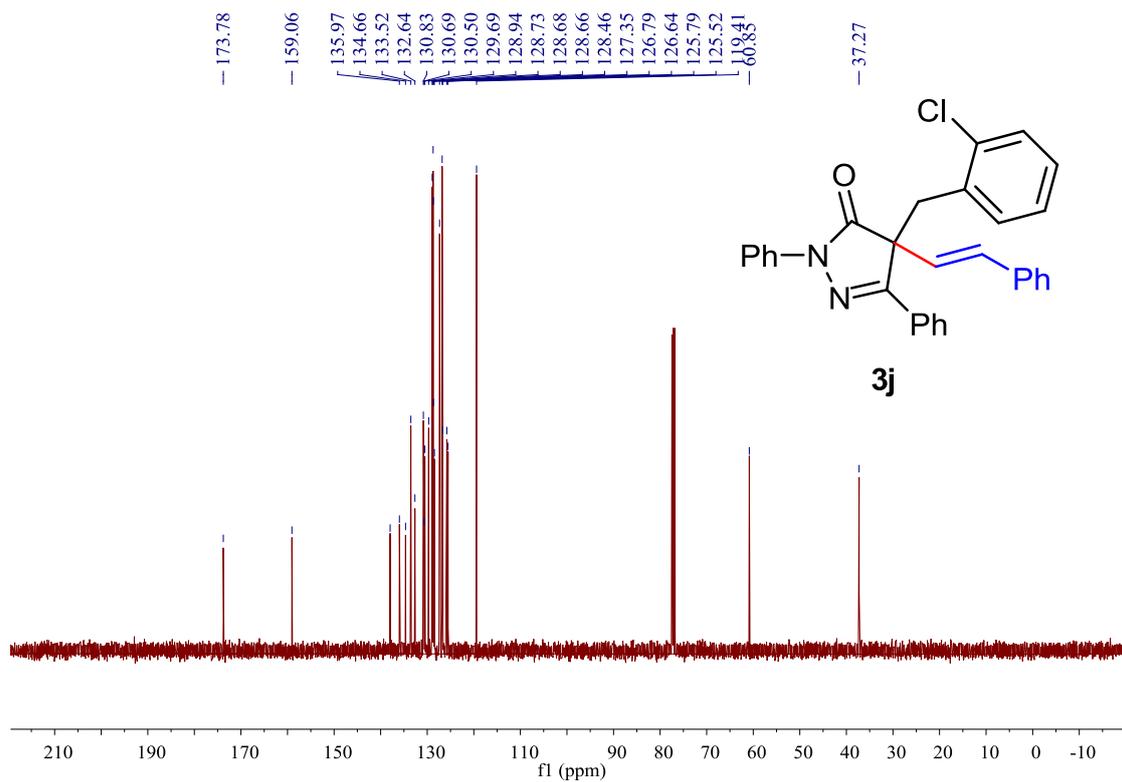
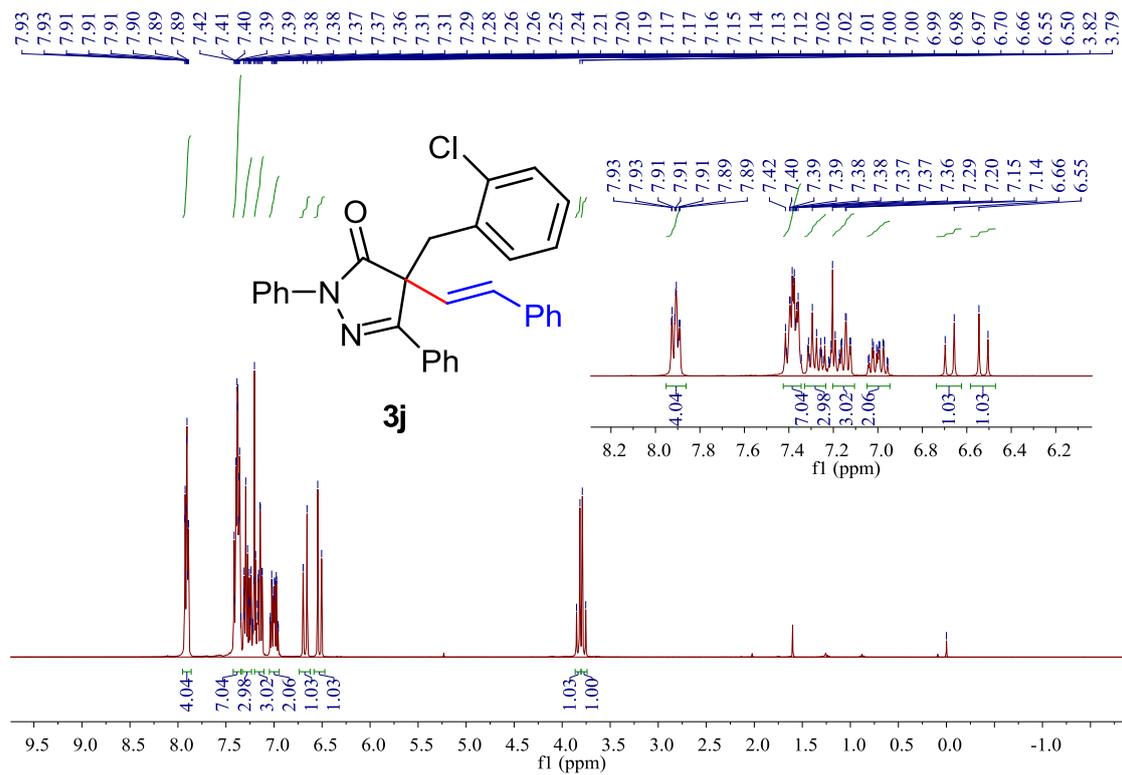


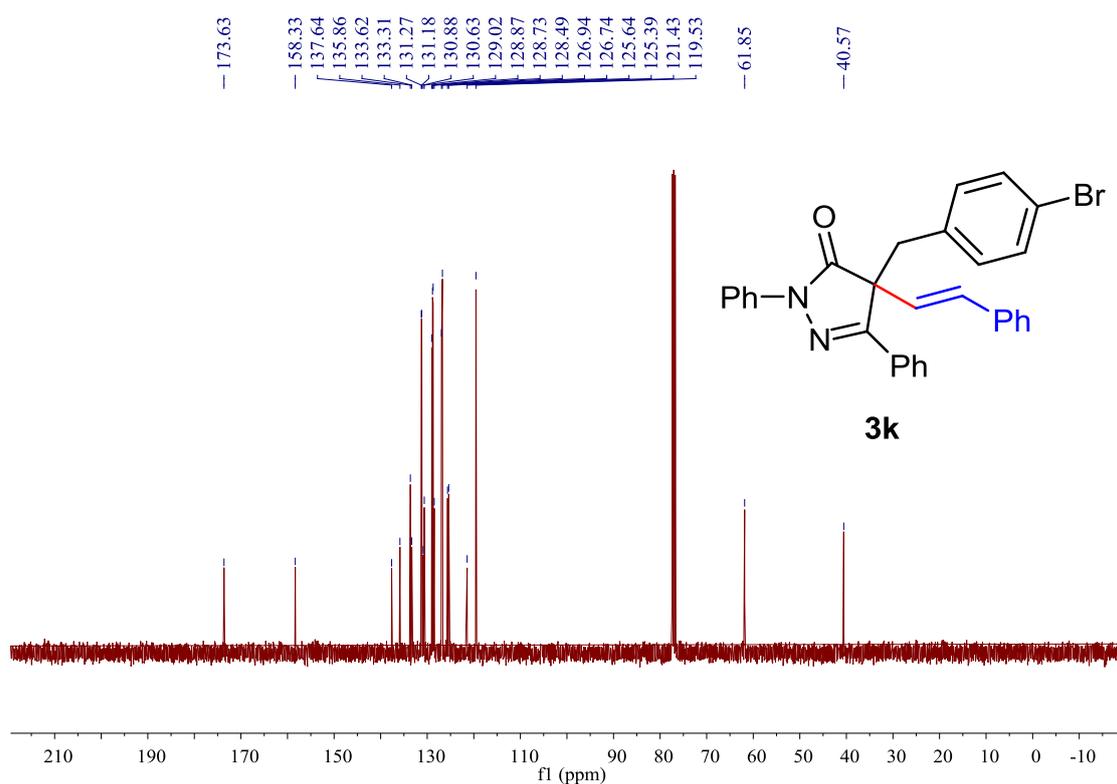
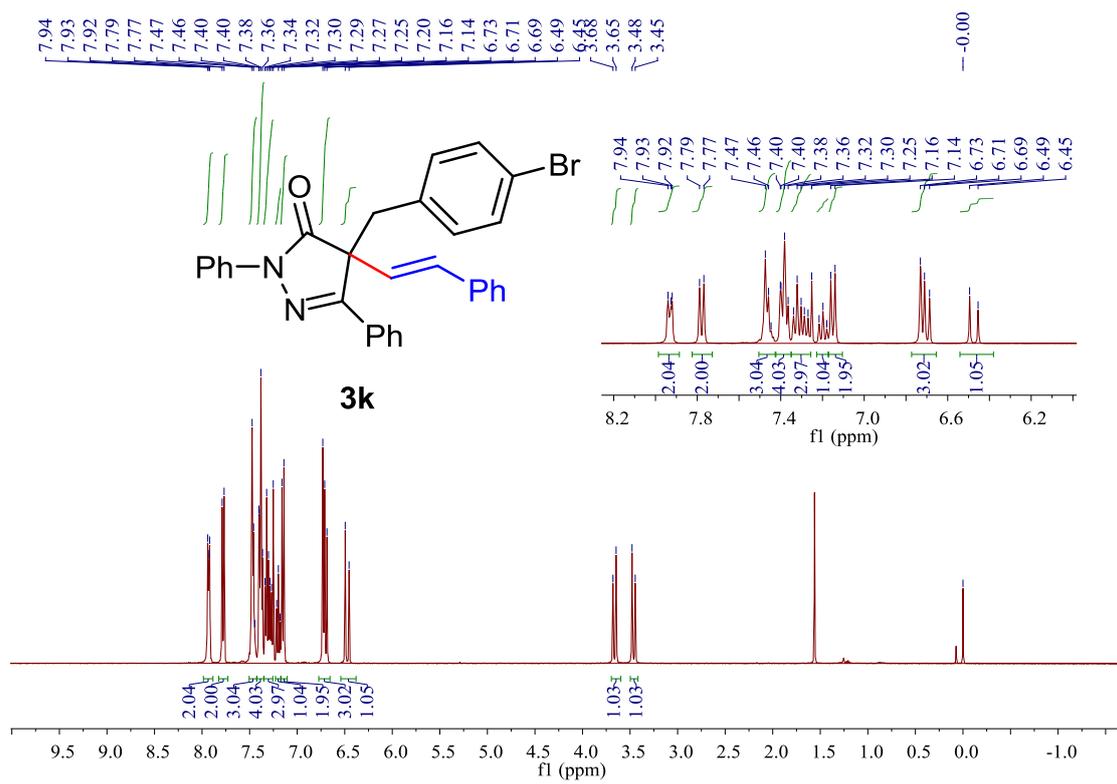




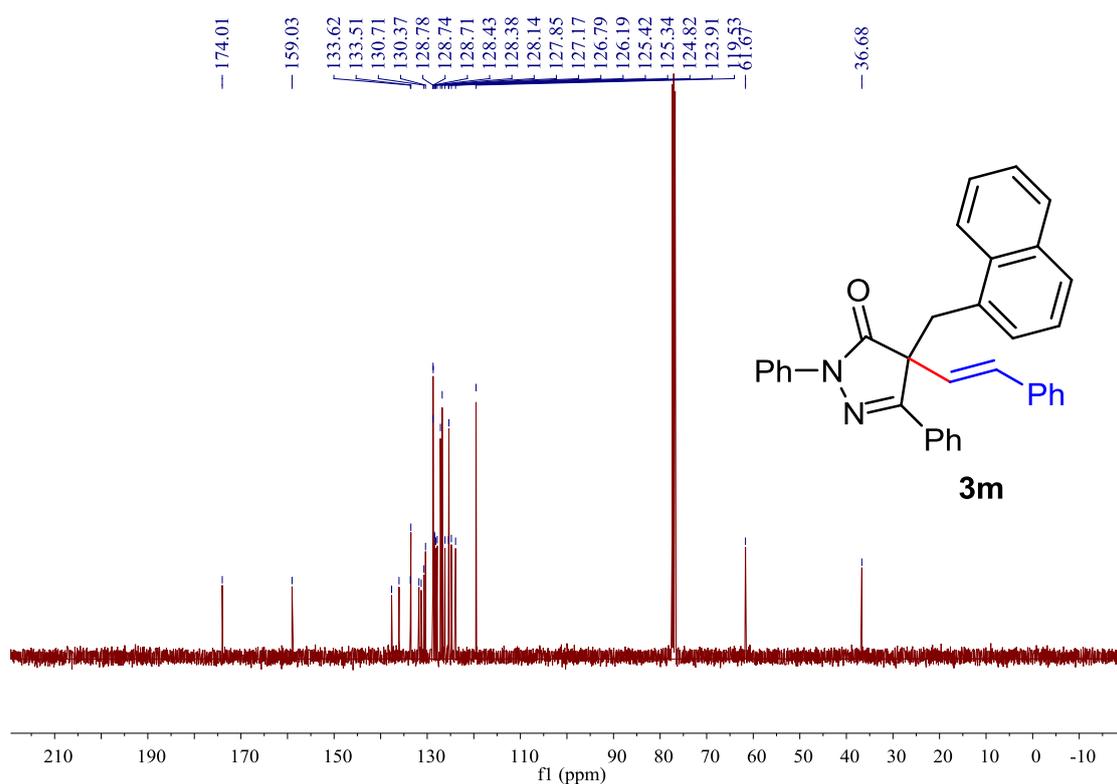
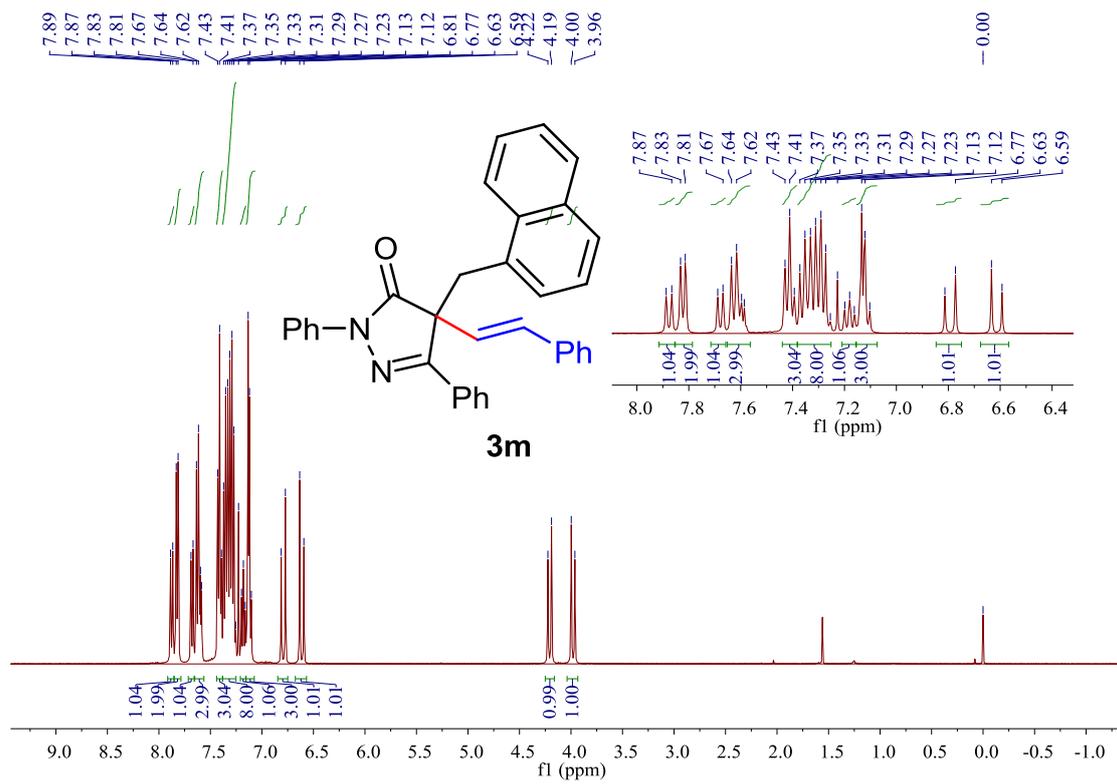


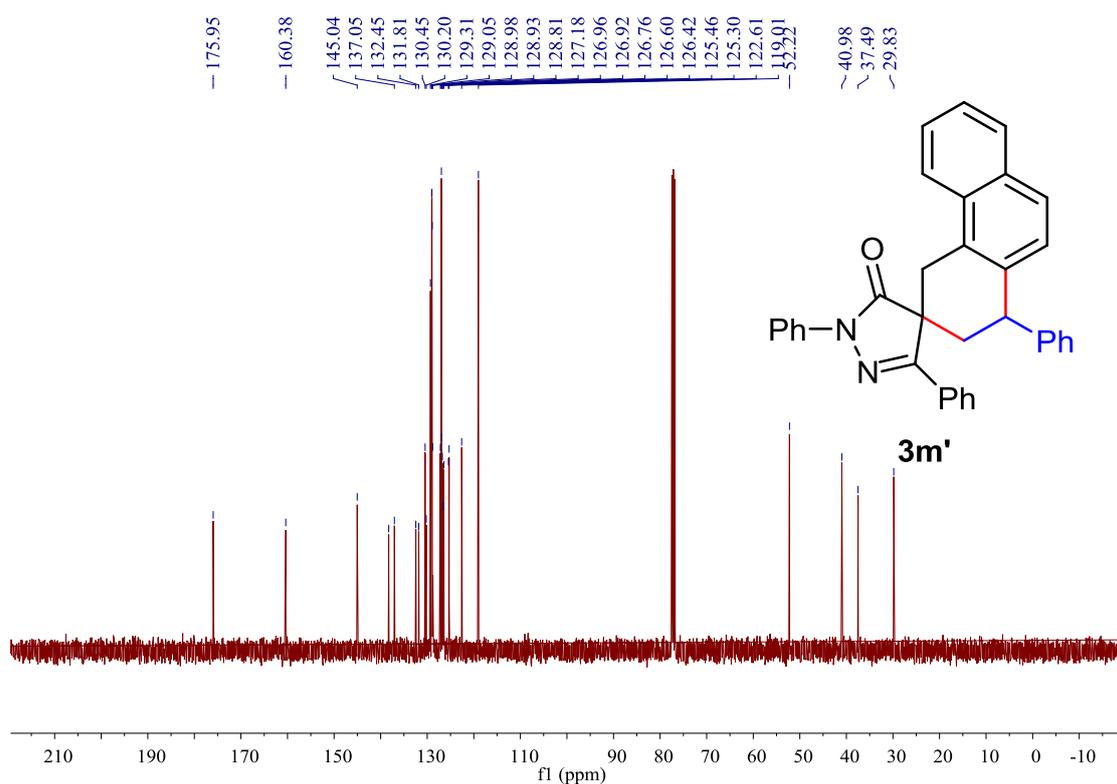
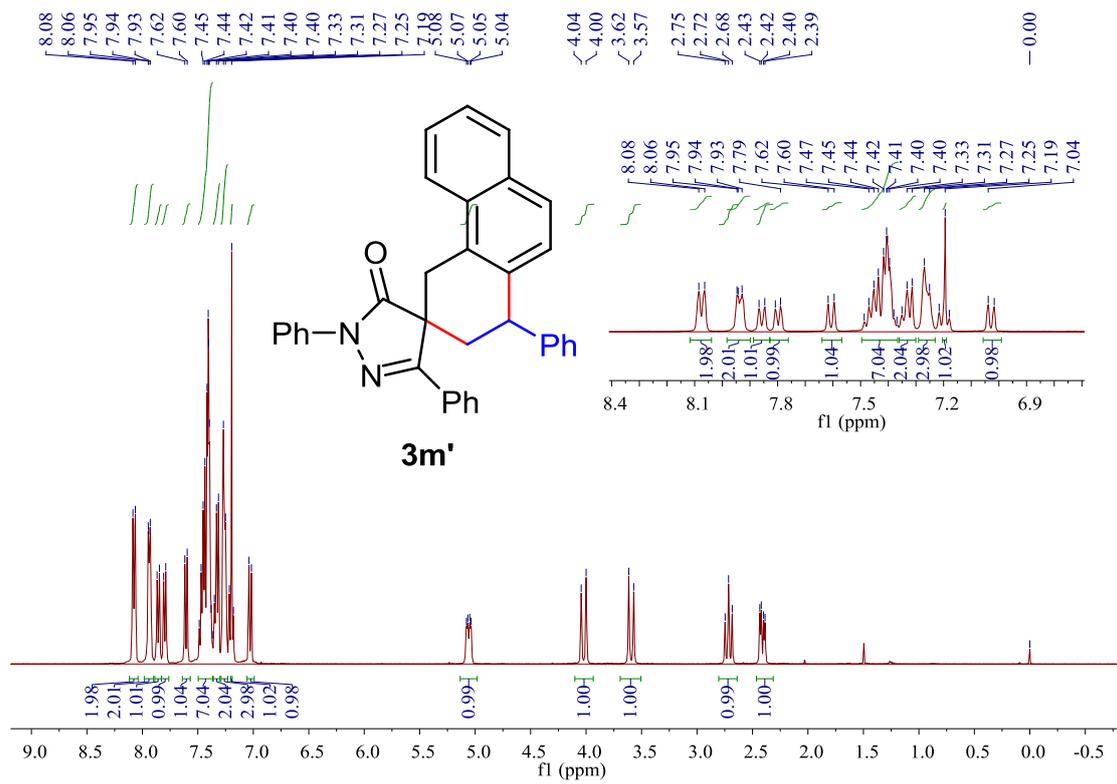


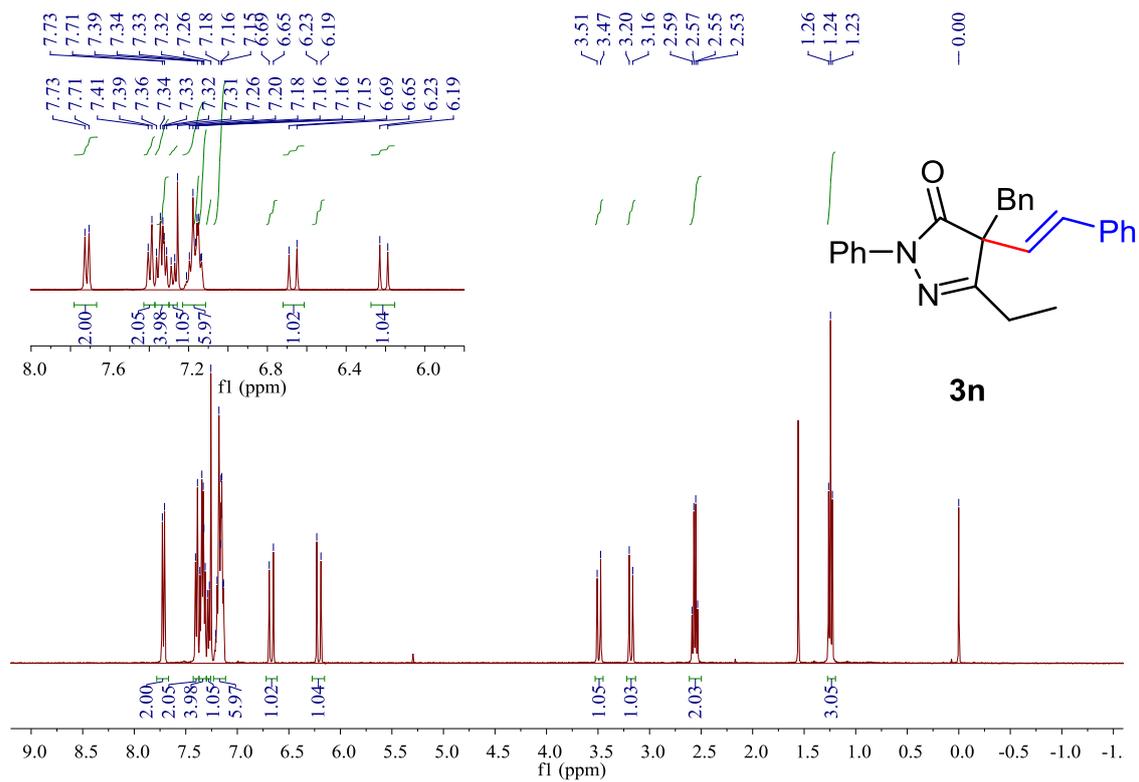












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