

# Supporting Information

## **Iron-catalyzed regioselective direct coupling of aromatic aldehydes with coumarins leading to 3-aroyl coumarins**

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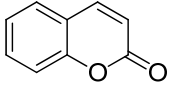
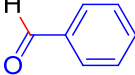
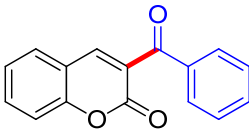
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**Table 1** Synthesis of 3-benzoyl coumarin using different oxidants

NMR Spectra of products

**Table 1** Synthesis of 3-benzoyl coumarin using different oxidants<sup>a</sup>

	+		$\xrightarrow[\text{PhCl, N}_2, 120^\circ\text{C}]{\text{[O] (4.0 equiv), FeCl}_2 \text{ (10 mol\%)}}$	
<b>1a</b>		<b>2a</b>		<b>3aa</b>
Entry	[O]	Yield <sup>b</sup> (%)		
1	H <sub>2</sub> O <sub>2</sub>	trace		
2 <sup>c</sup>	DTBP	15		
3	K <sub>2</sub> S <sub>2</sub> O <sub>8</sub>	nr <sup>d</sup>		
4	(NH <sub>4</sub> ) <sub>2</sub> S <sub>2</sub> O <sub>8</sub>	nr		
5 <sup>e</sup>	air	nr		

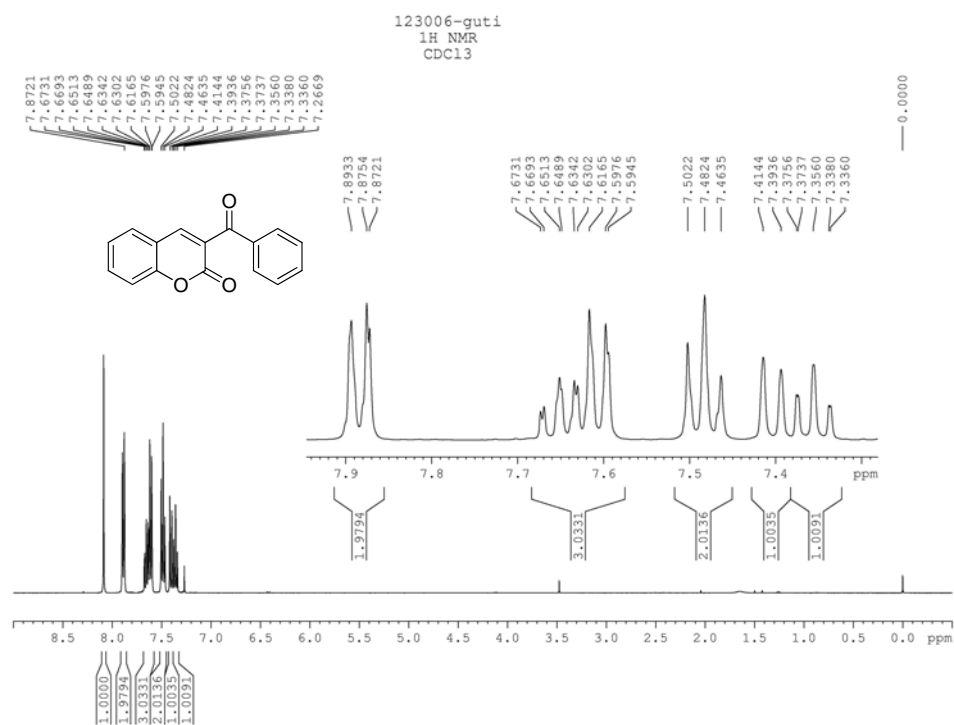
<sup>a</sup> Reaction conditions: **1a** (0.25 mmol), **2a** (1.0 mmol), FeCl<sub>2</sub> (10 mol%) as the catalyst, oxidant (4.0 equiv) in PhCl (2 mL) with stirring under nitrogen for 12 h.

<sup>b</sup> Isolated yield.

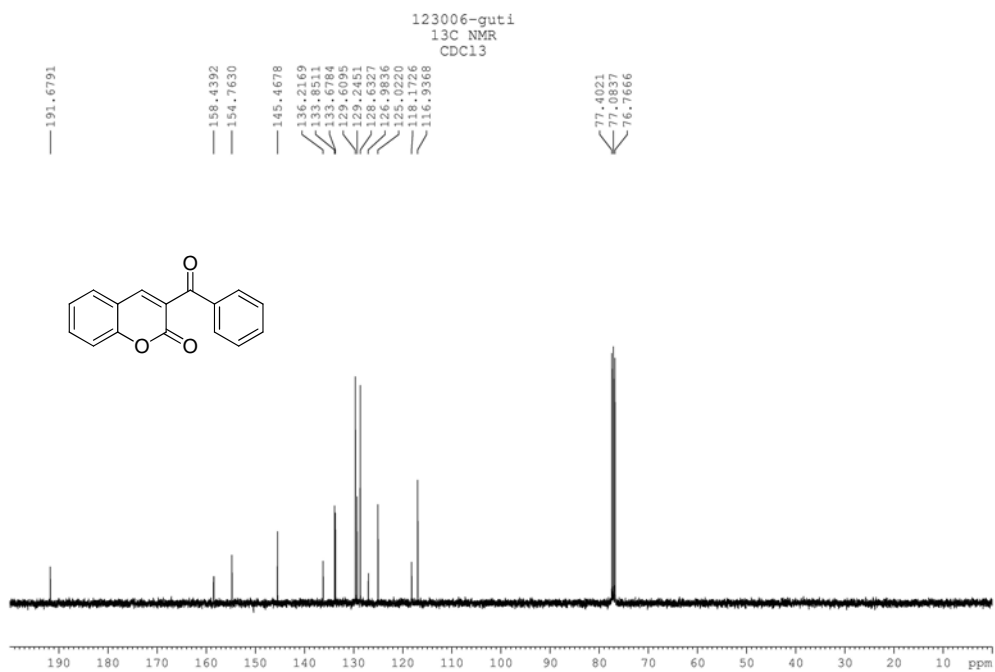
<sup>c</sup> DTBP: di-tert-butyl hydrogen peroxide.

<sup>d</sup> nr = no reaction

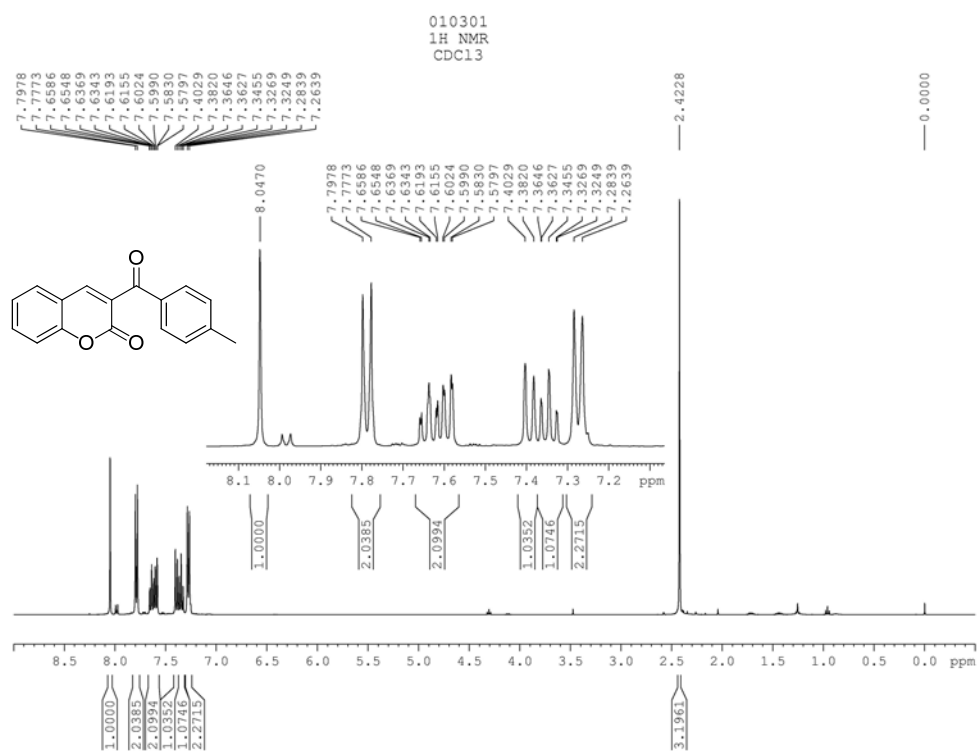
<sup>e</sup> No N<sub>2</sub>, using O<sub>2</sub> in the air as the oxidant.



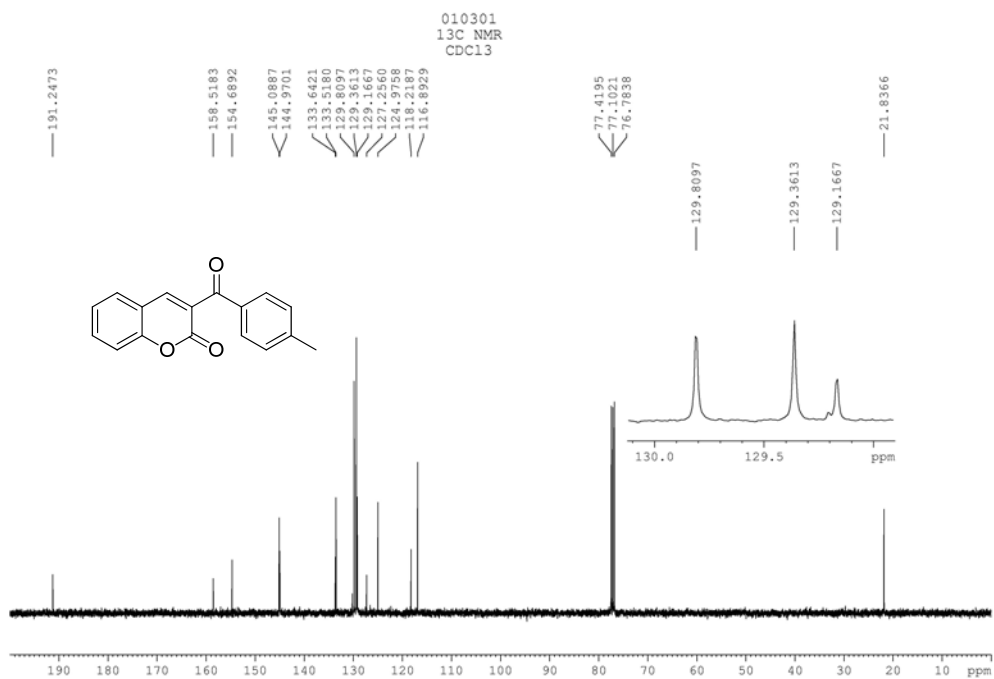
<sup>1</sup>H NMR spectrum of compound **3aa**



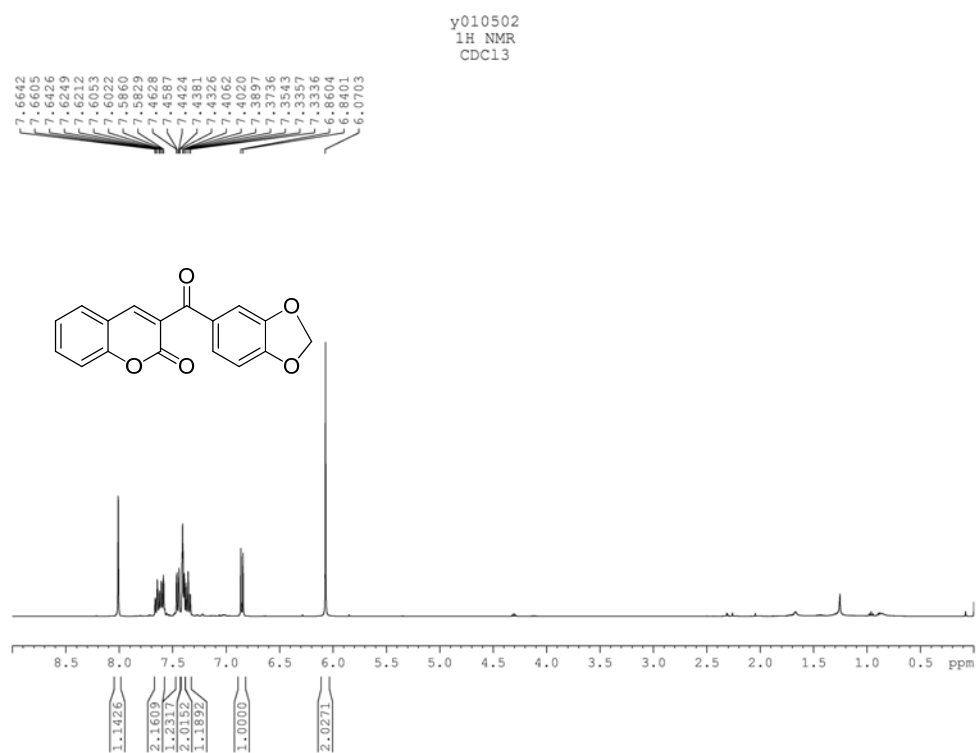
<sup>13</sup>C NMR spectrum of compound **3aa**



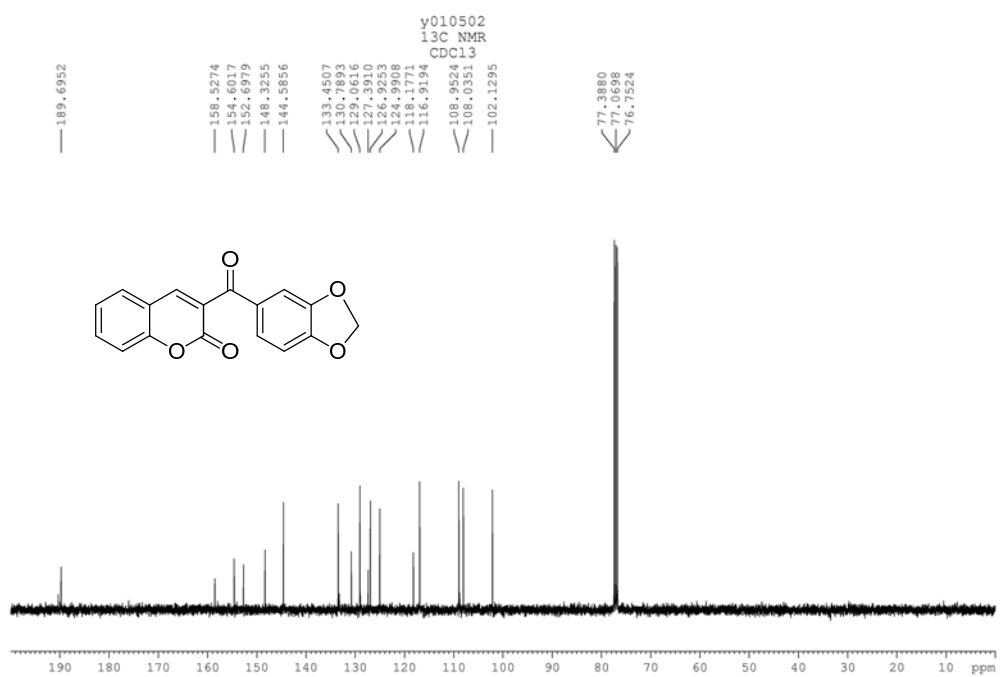
<sup>1</sup>H NMR spectrum of compound **3ab**



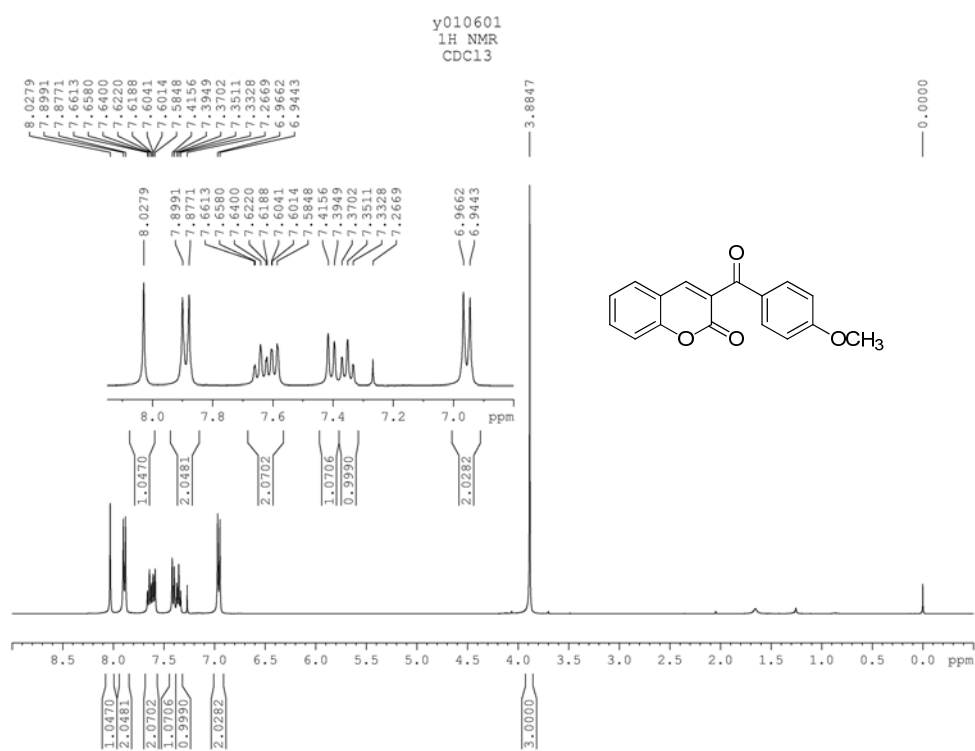
<sup>13</sup>C NMR spectrum of compound **3ab**



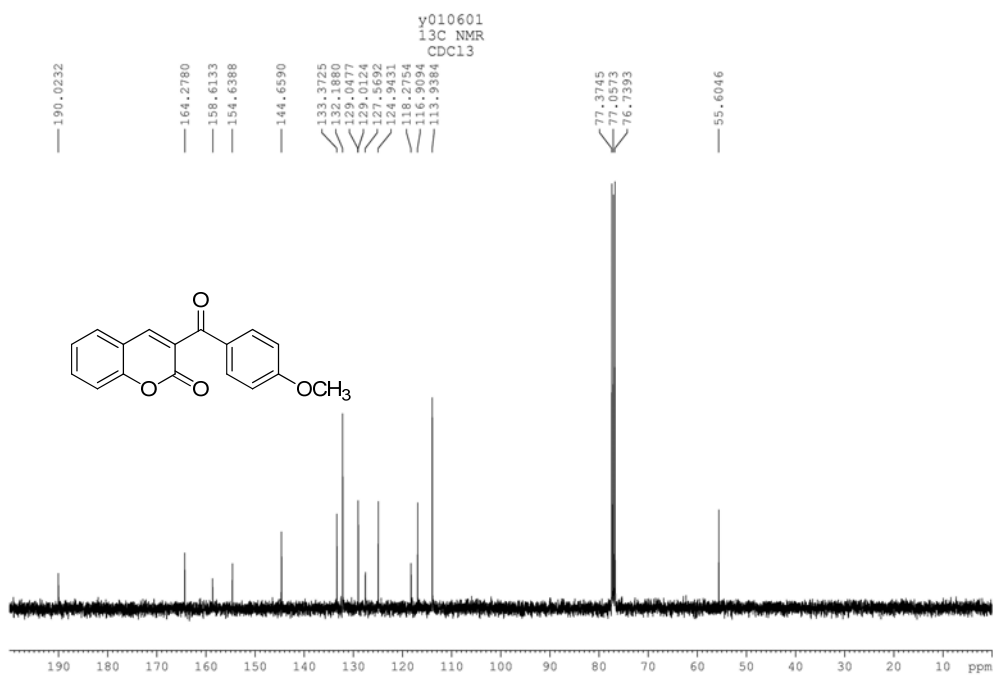
<sup>1</sup>H NMR spectrum of compound **3ac**



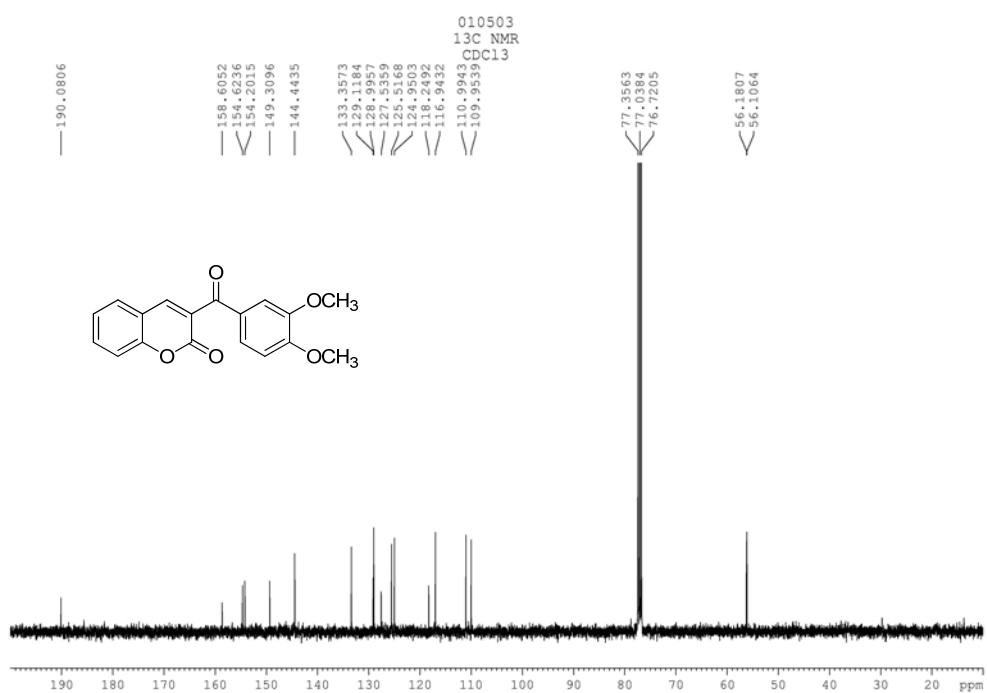
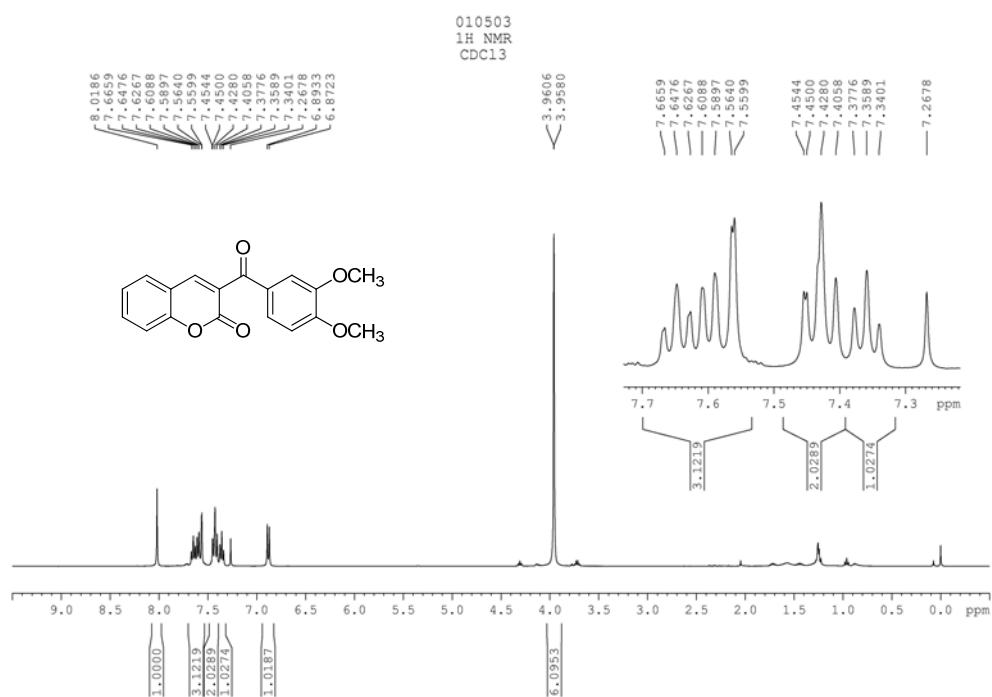
<sup>13</sup>C NMR spectrum of compound **3ac**

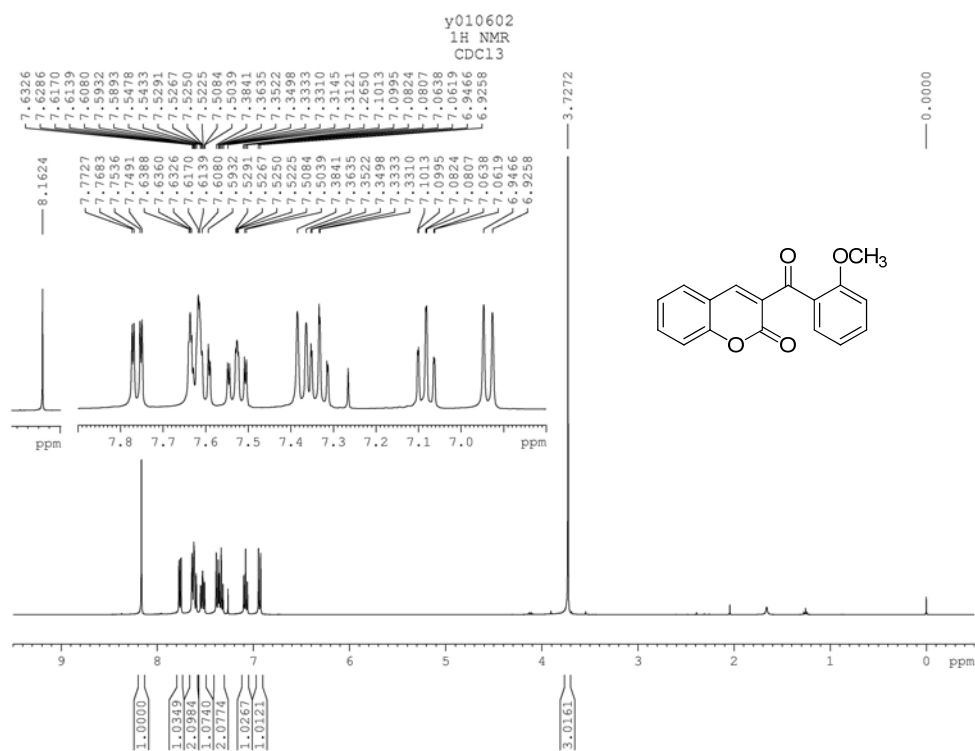


<sup>1</sup>H NMR spectrum of compound **3ad**

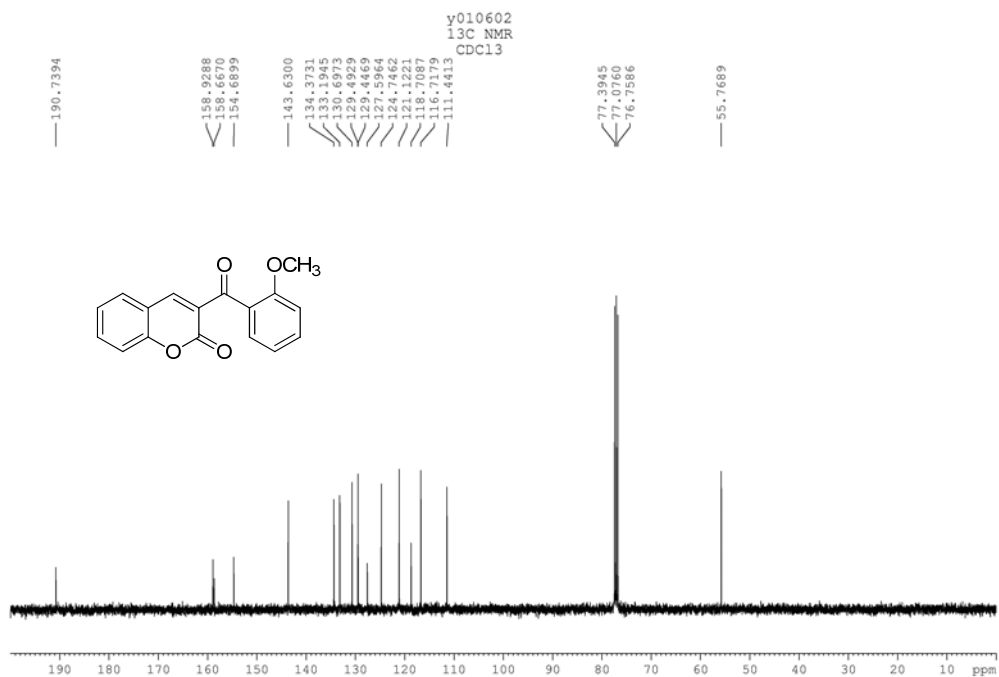


<sup>13</sup>C NMR spectrum of compound **3ad**



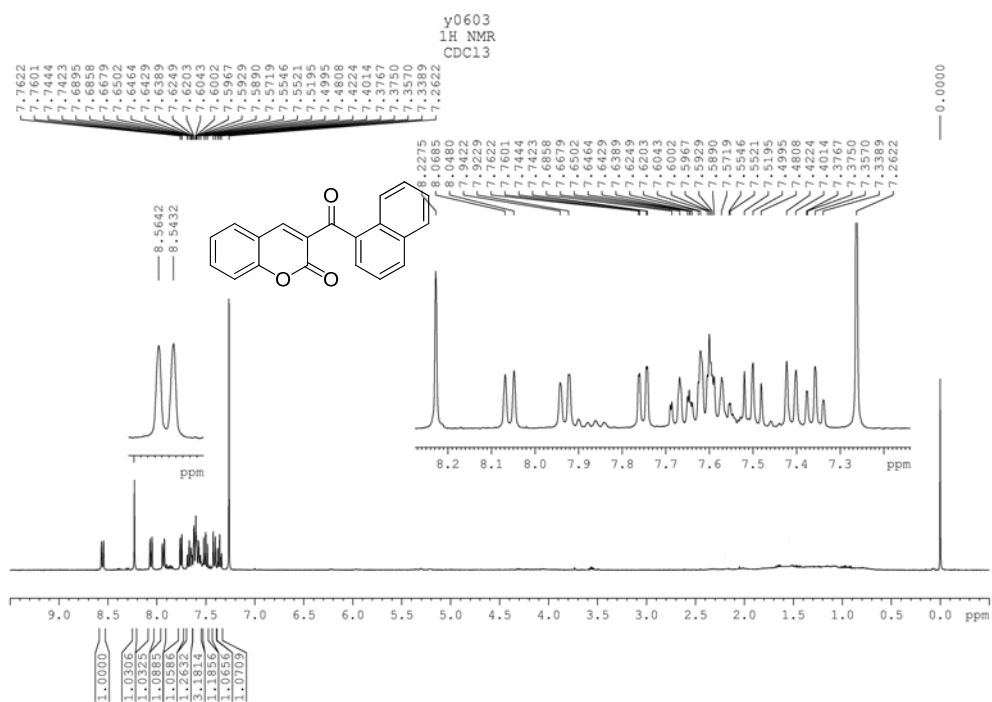


<sup>1</sup>H NMR spectrum of compound **3af**

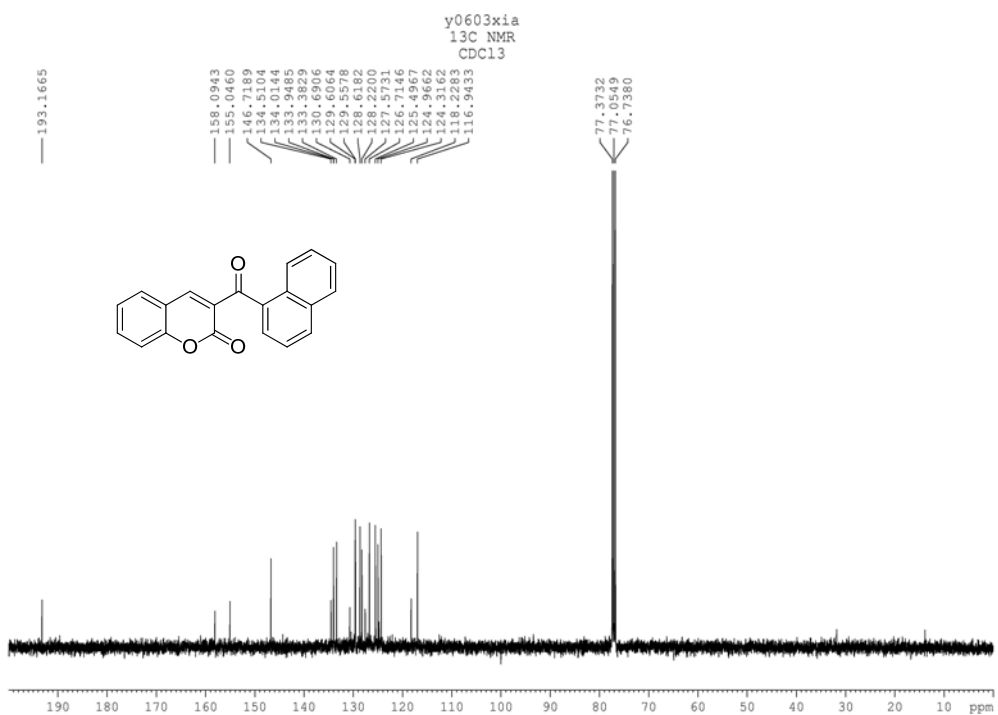


<sup>13</sup>C NMR spectrum of compound **3af**

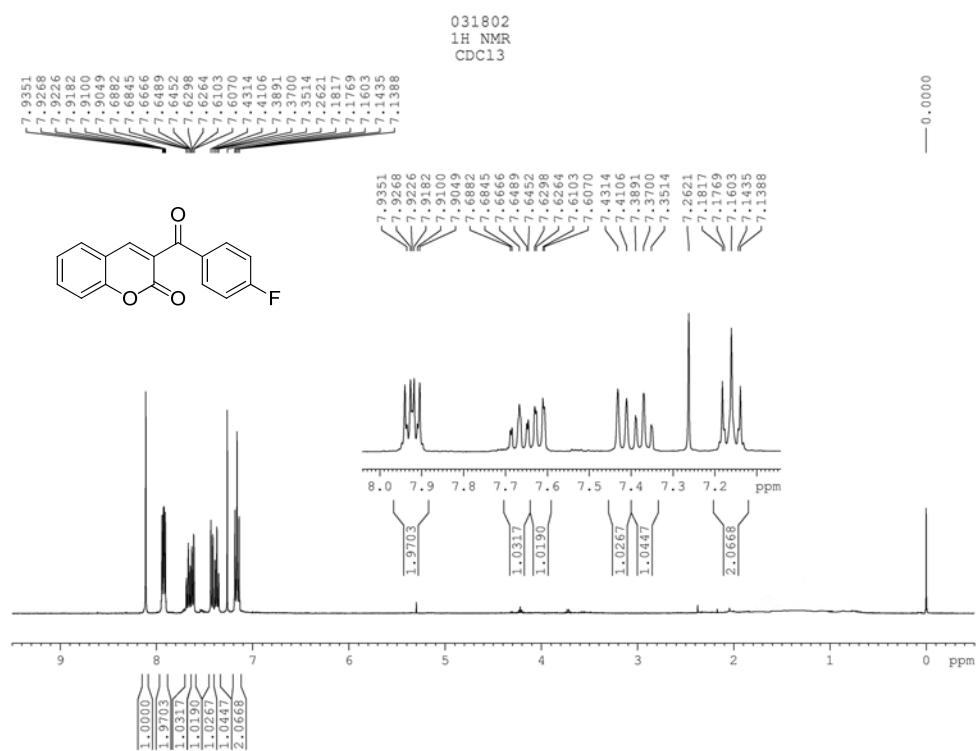




<sup>1</sup>H NMR spectrum of compound **3ag**



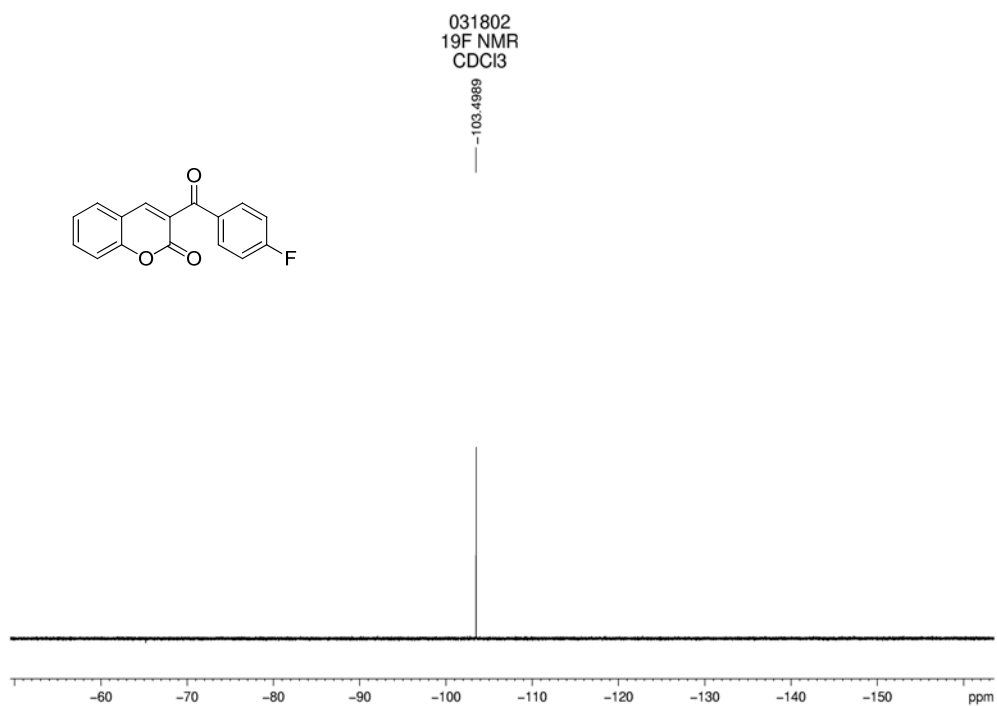
<sup>13</sup>C NMR spectrum of compound **3ag**



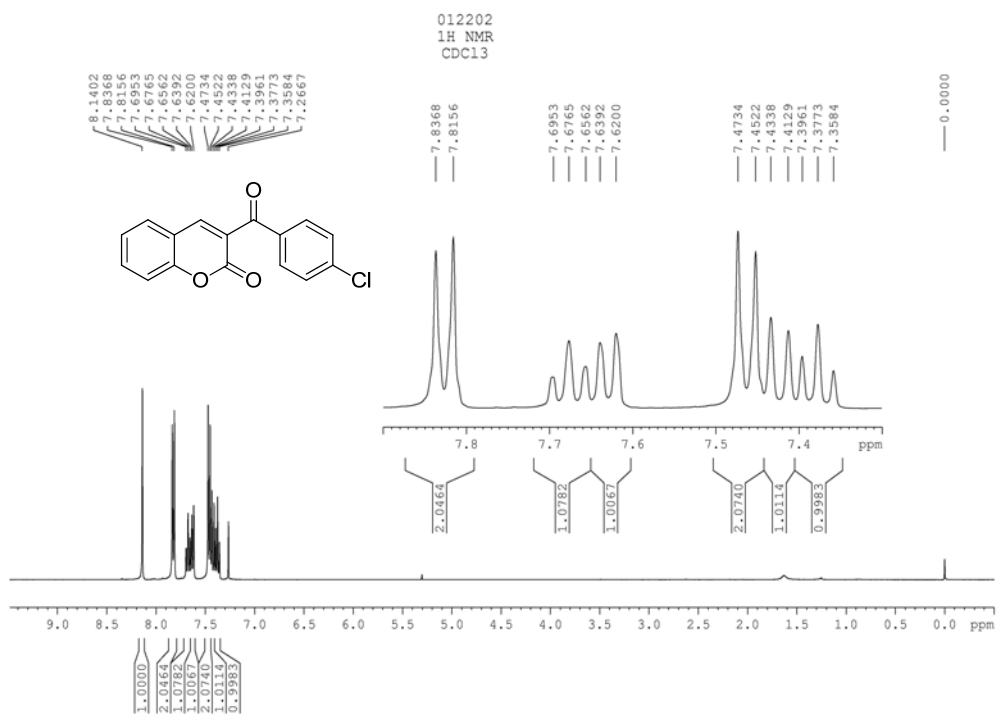
<sup>1</sup>H NMR spectrum of compound **3ah**



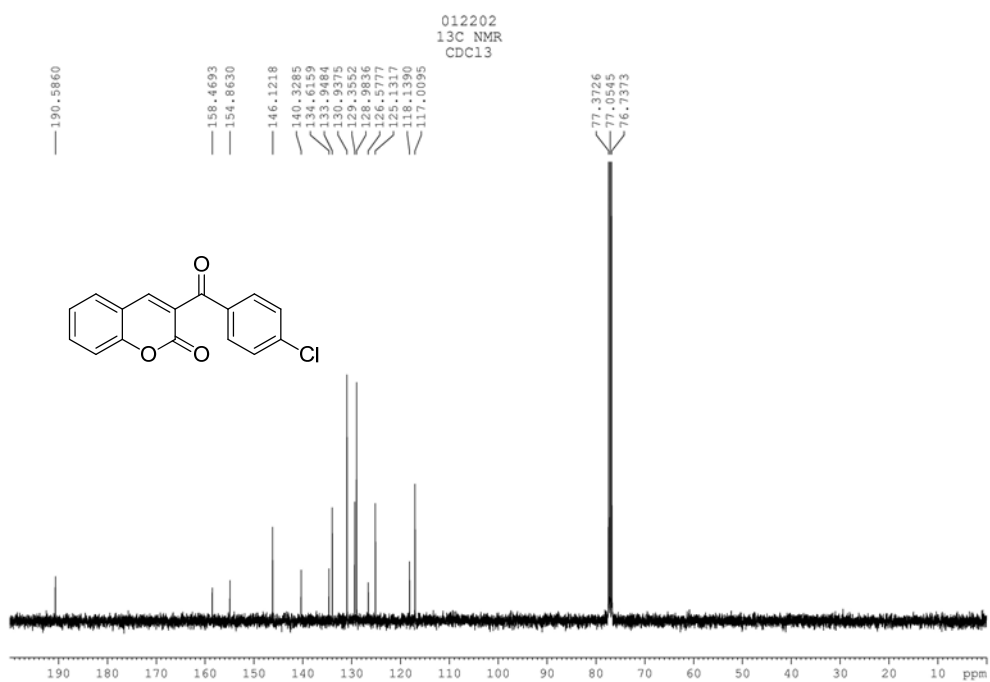
<sup>13</sup>C NMR spectrum of compound **3ah**



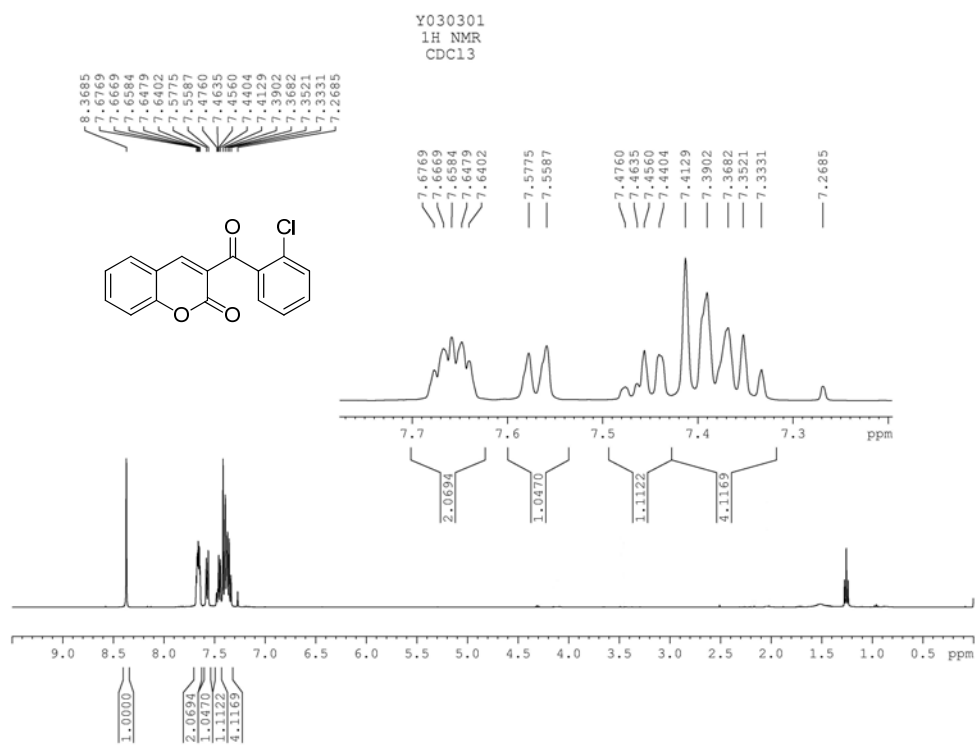
<sup>19</sup>F NMR spectrum of compound **3ah**



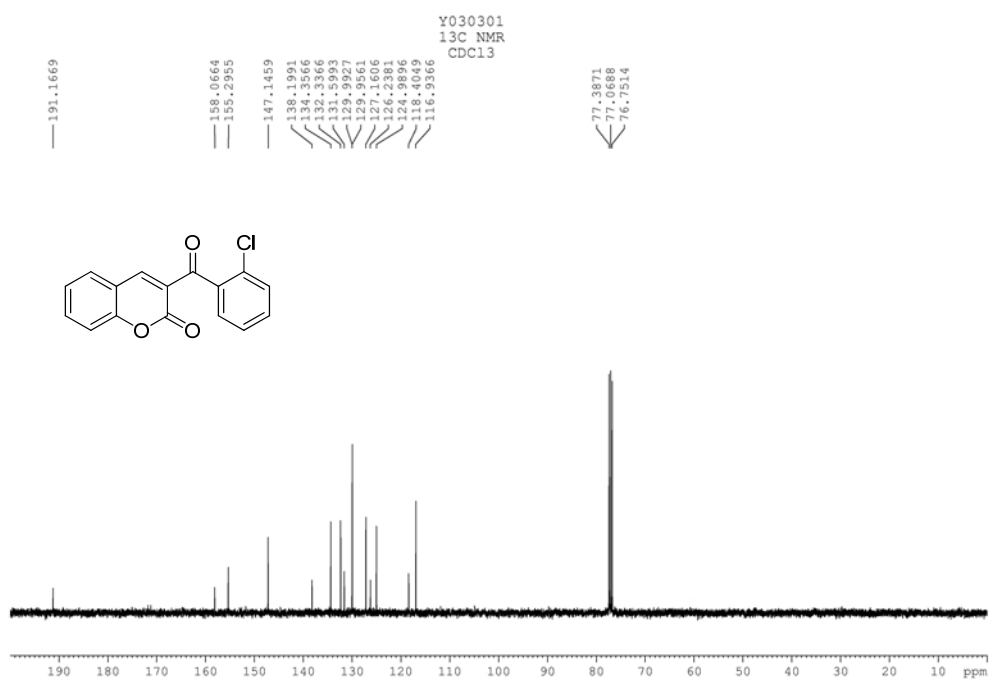
<sup>1</sup>H NMR spectrum of compound **3ai**



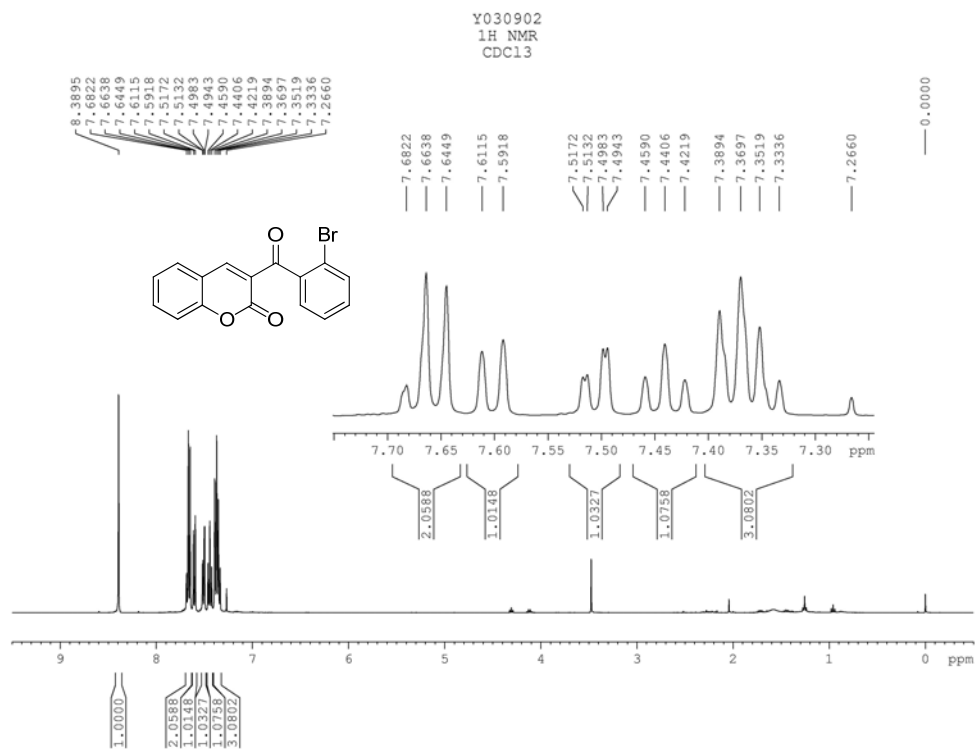
<sup>13</sup>C NMR spectrum of compound **3ai**



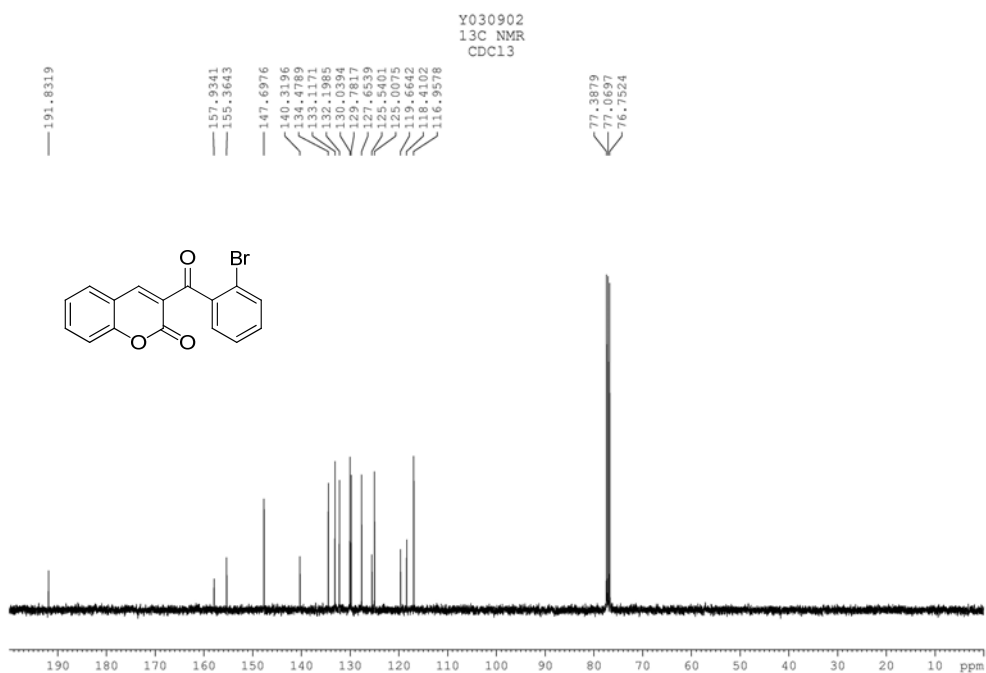
<sup>1</sup>H NMR spectrum of compound **3aj**



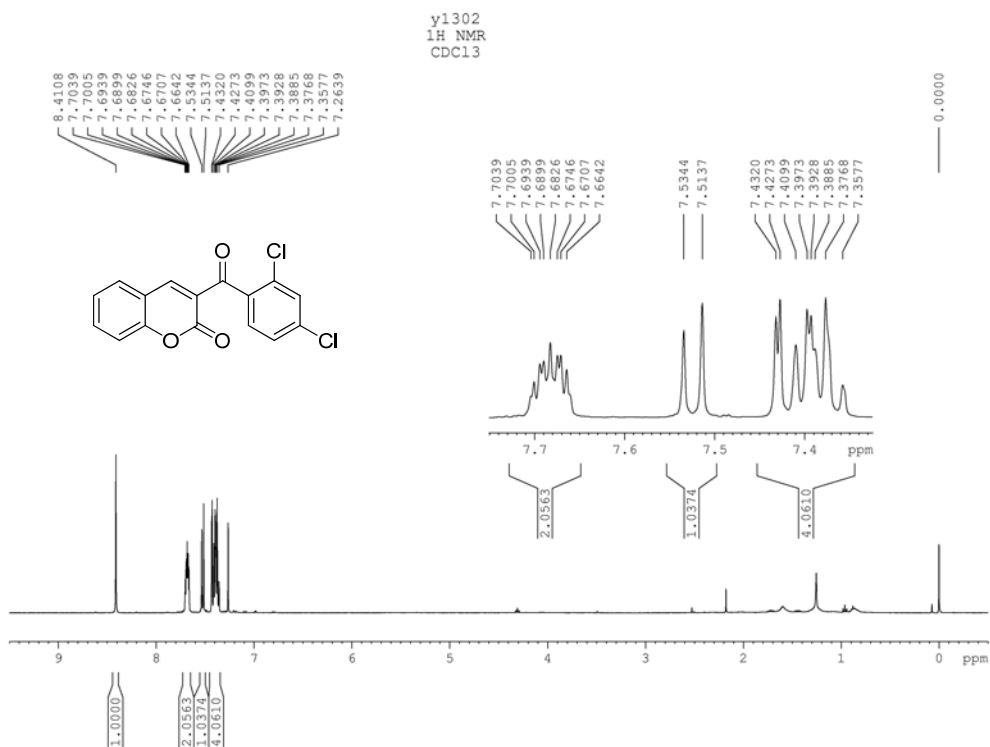
<sup>13</sup>C NMR spectrum of compound **3aj**



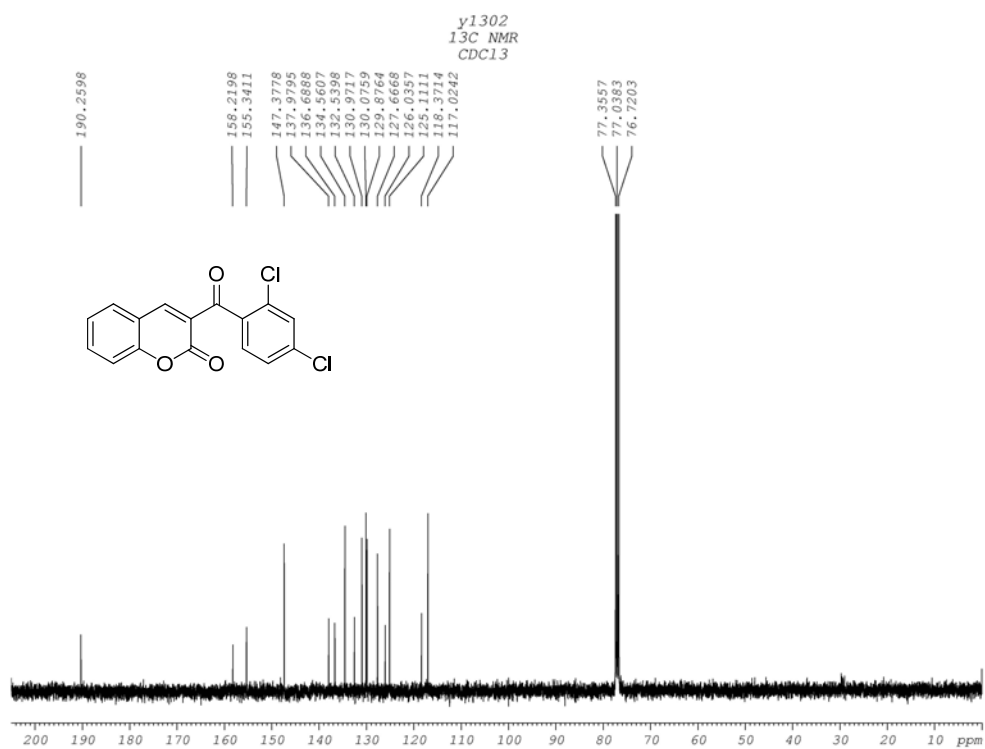
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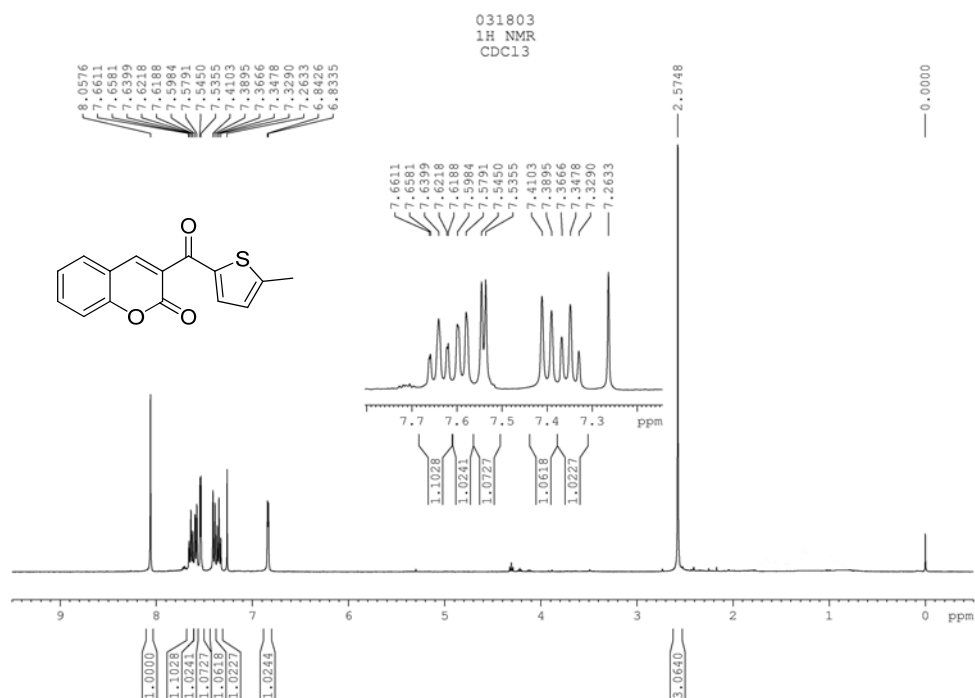
<sup>13</sup>C NMR spectrum of compound **3ak**



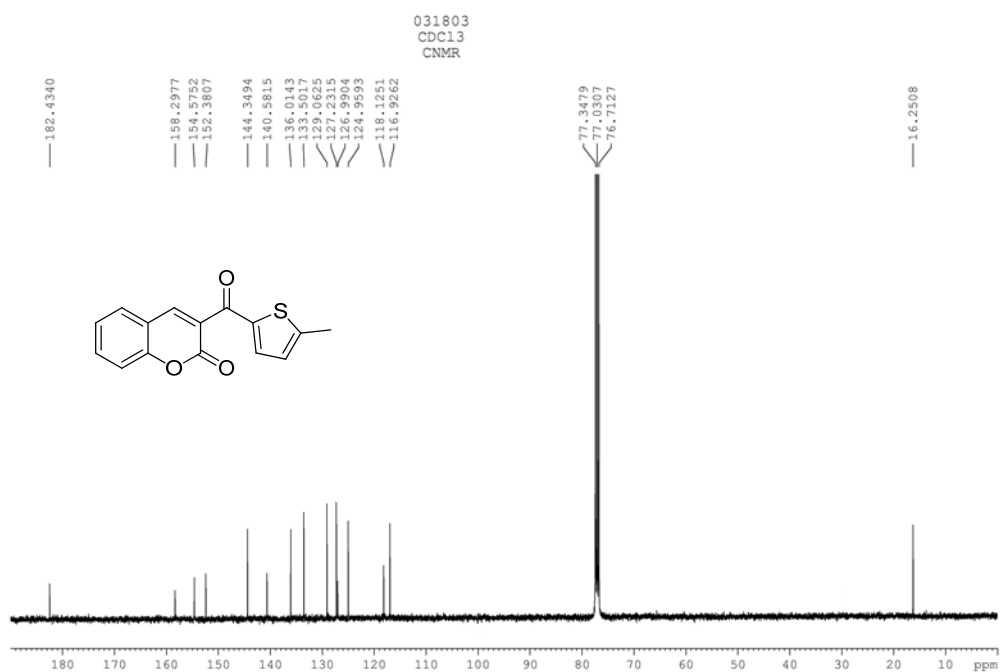
<sup>1</sup>H NMR spectrum of compound **3al**



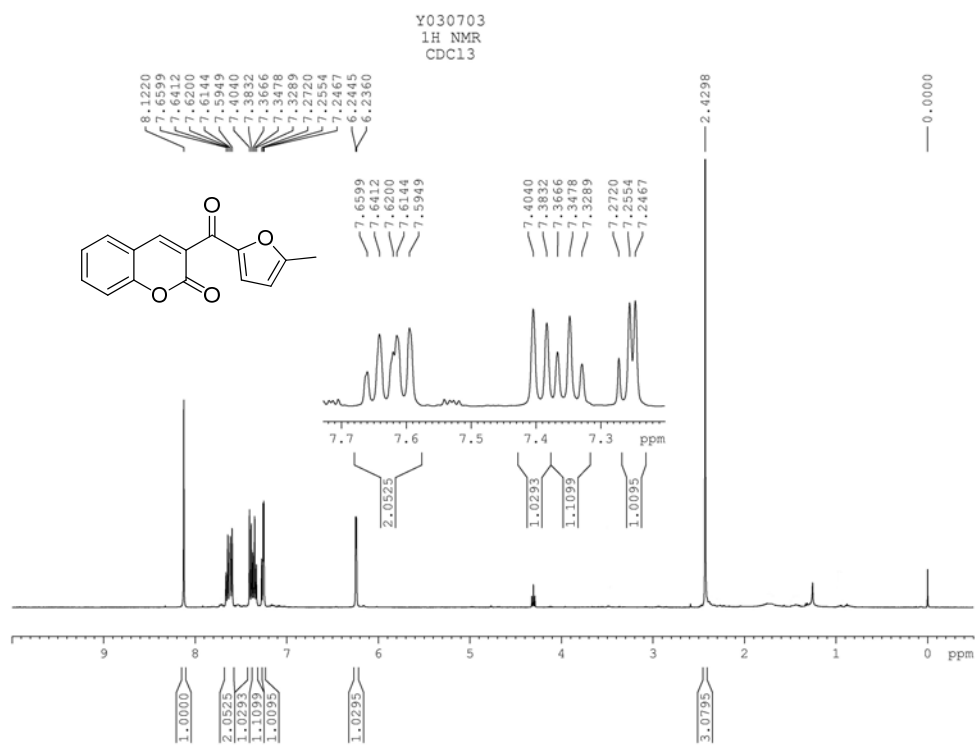
<sup>13</sup>C NMR spectrum of compound **3al**



<sup>1</sup>H NMR spectrum of compound **3am**

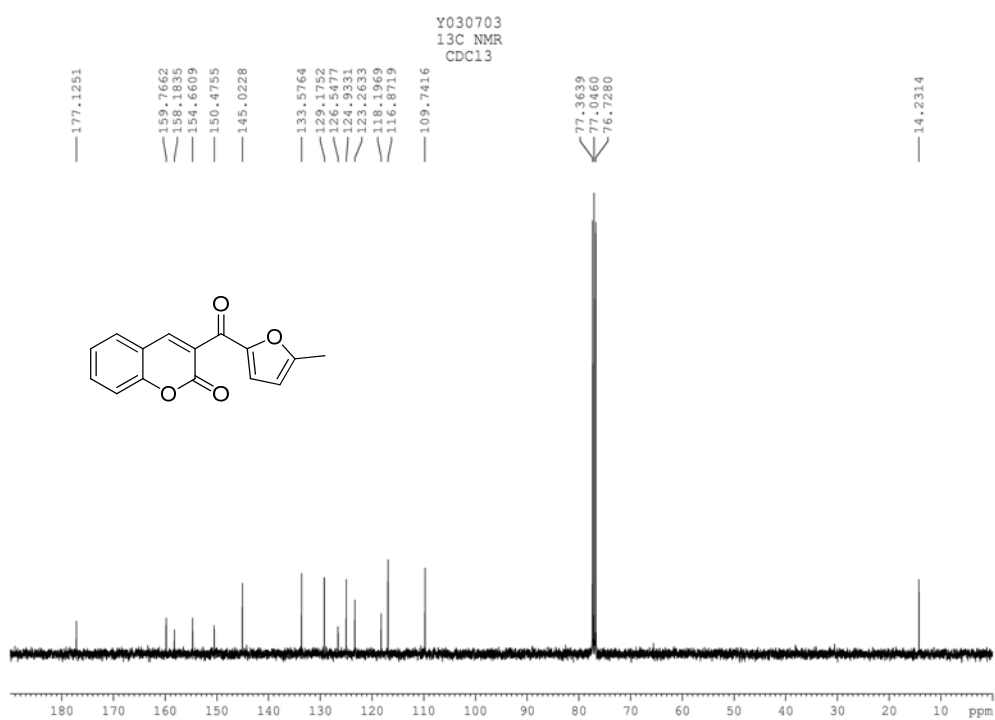


<sup>13</sup>C NMR spectrum of compound **3am**

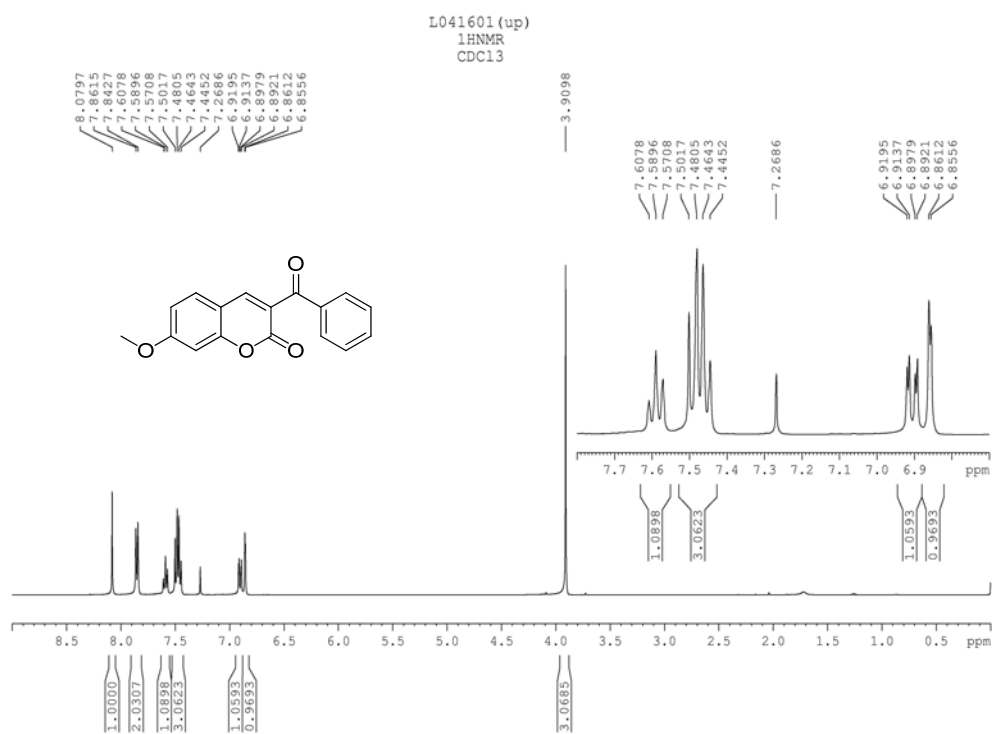


<sup>1</sup>H NMR spectrum of compound **3an**

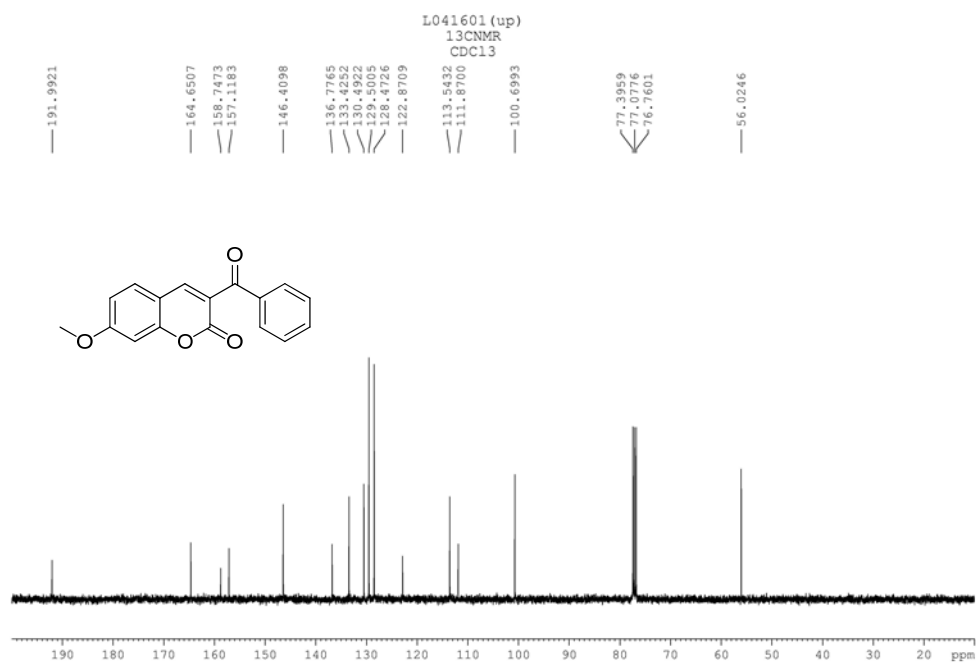




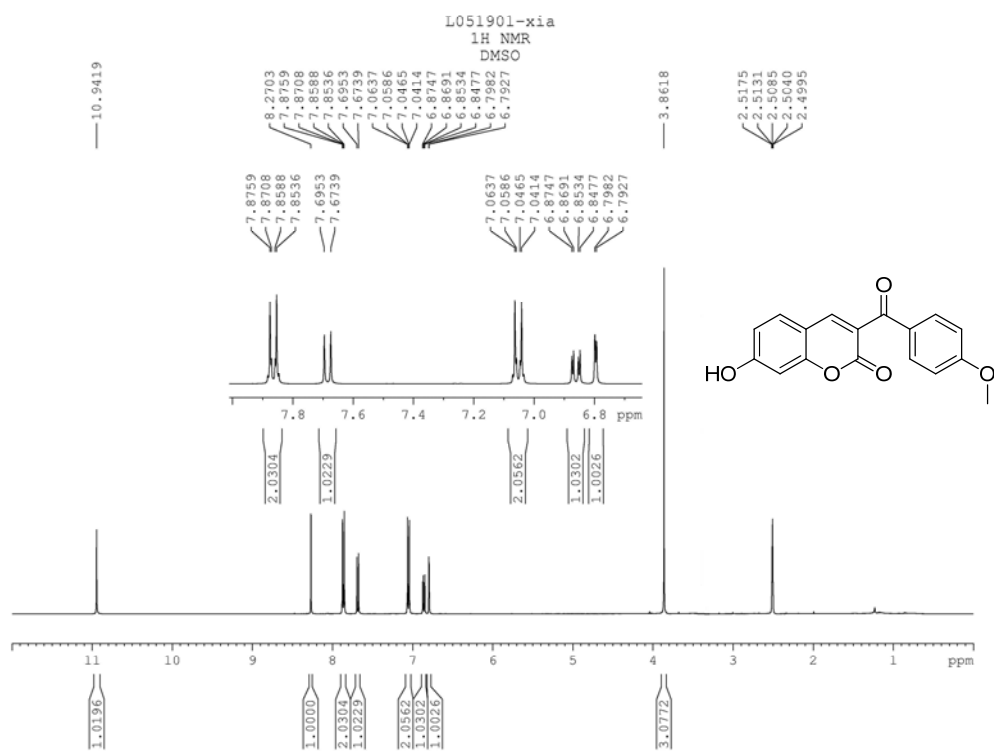
$^{13}\text{C}$  NMR spectrum of compound **3an**



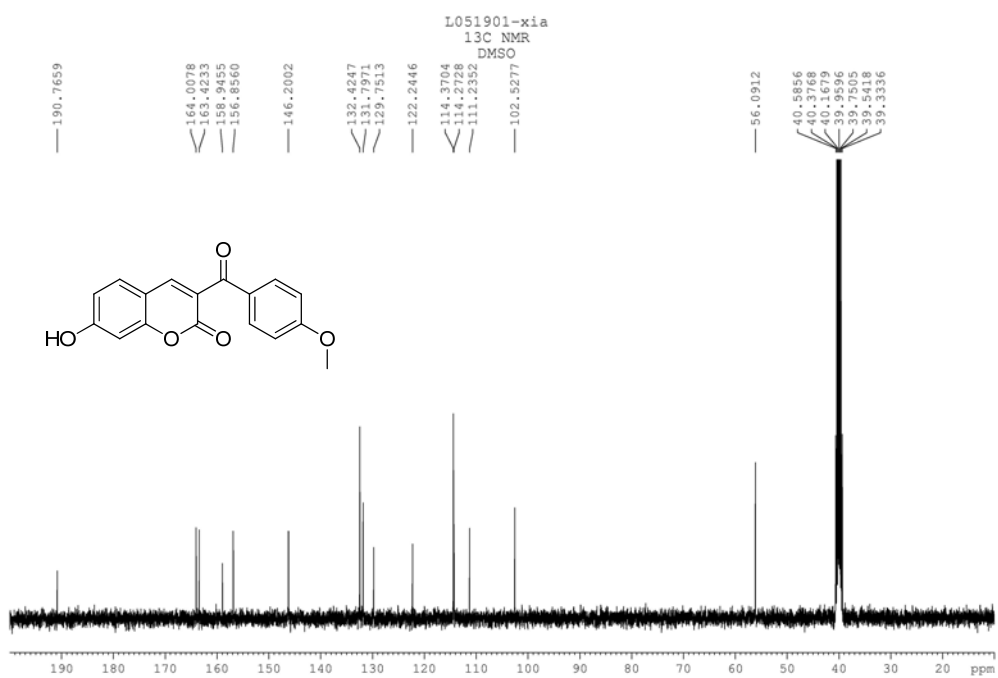
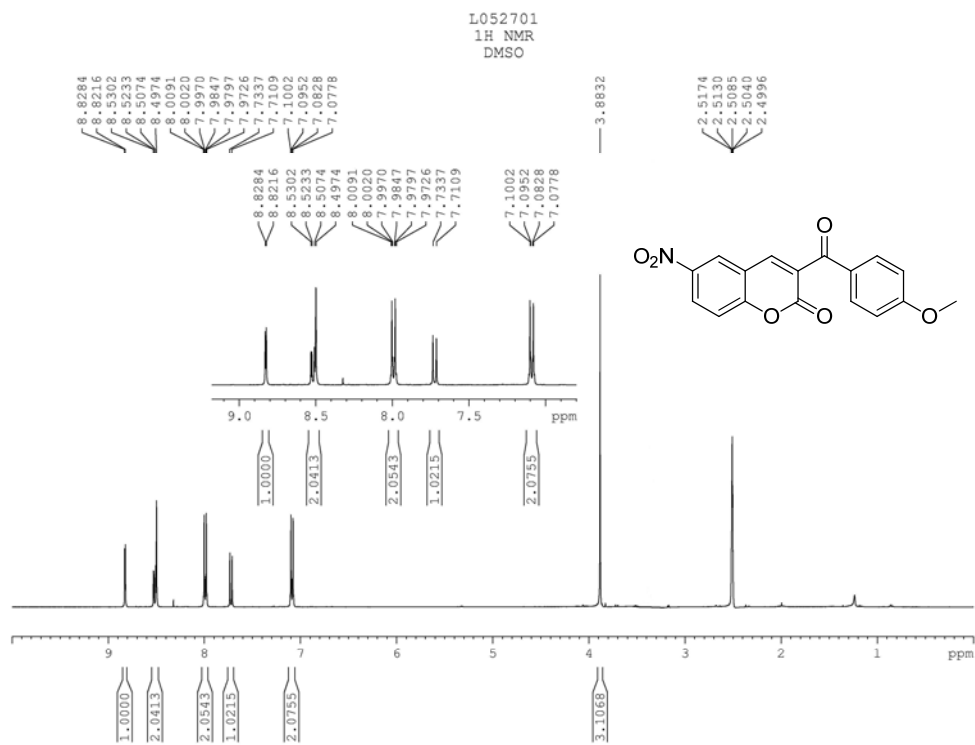
$^1\text{H}$  NMR spectrum of compound **3ba**

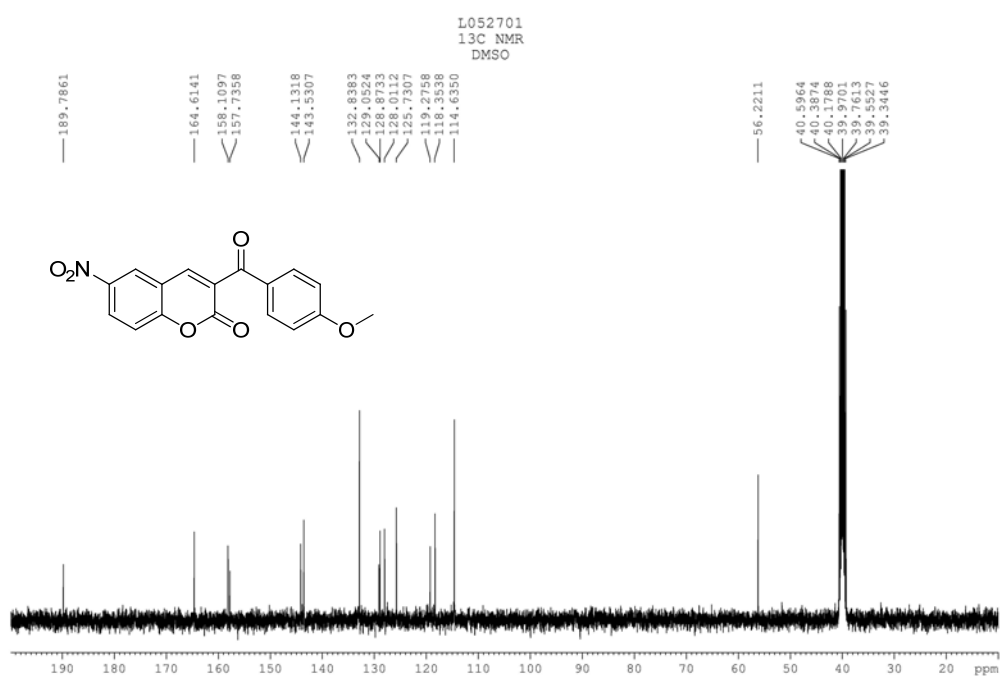


<sup>13</sup>C NMR spectrum of compound **3ba**

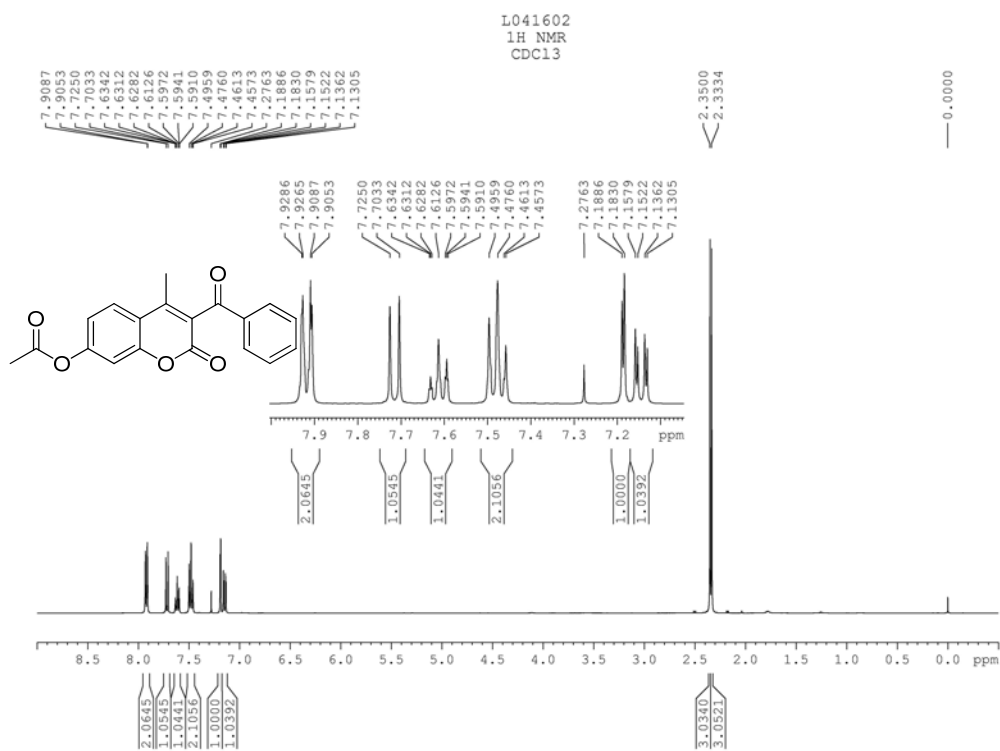


<sup>1</sup>H NMR spectrum of compound **3ce**

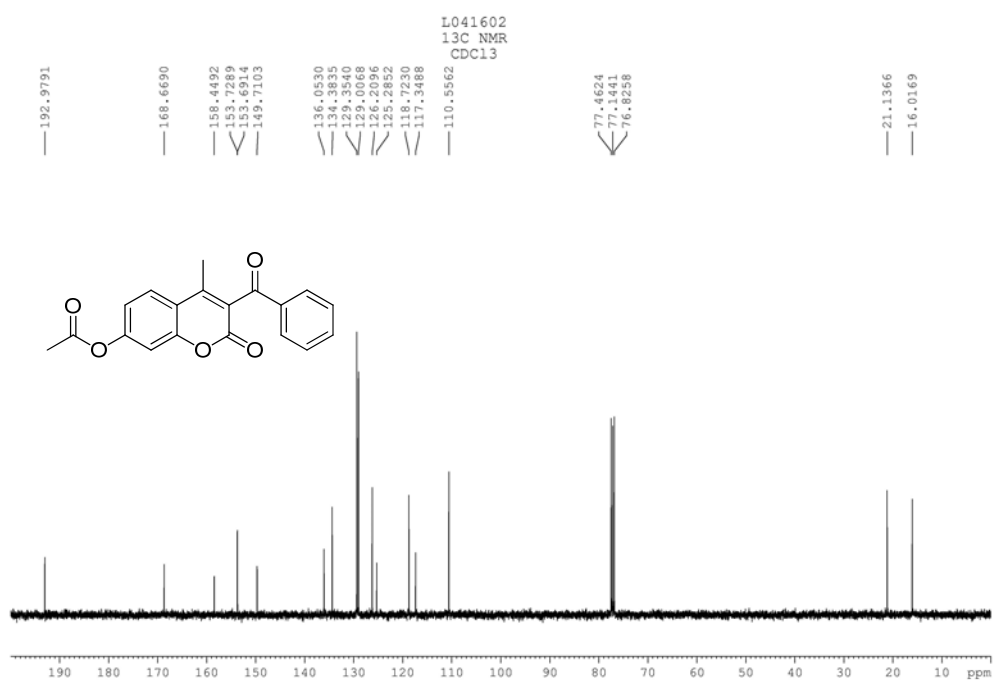
 $^{13}\text{C}$  NMR spectrum of compound **3ce**<sup>1</sup>H NMR spectrum of compound **3de**



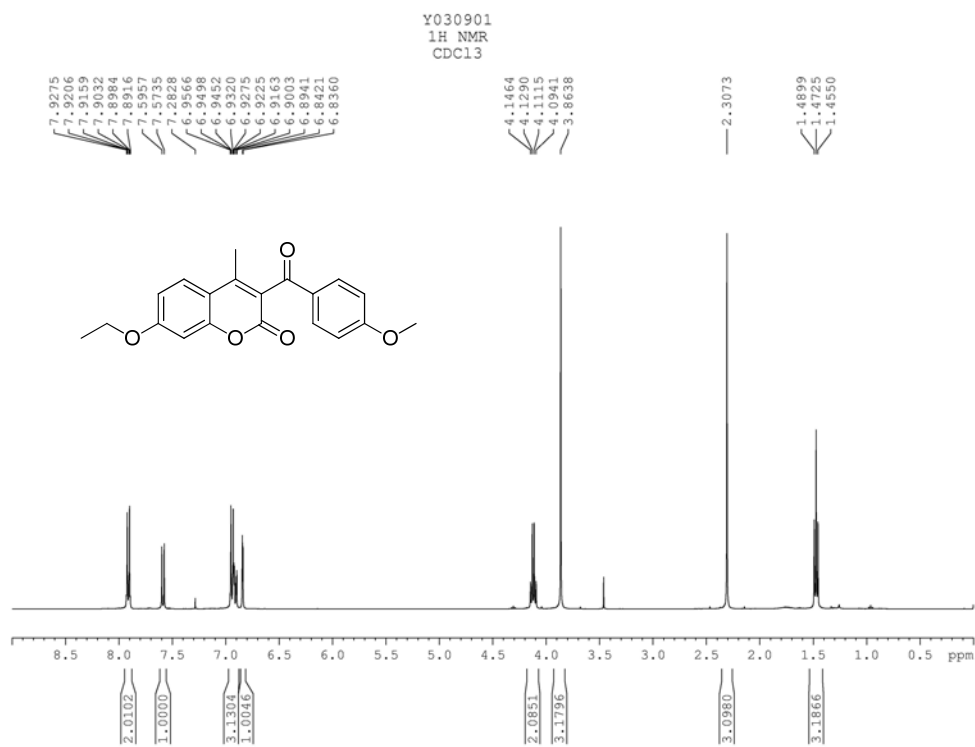
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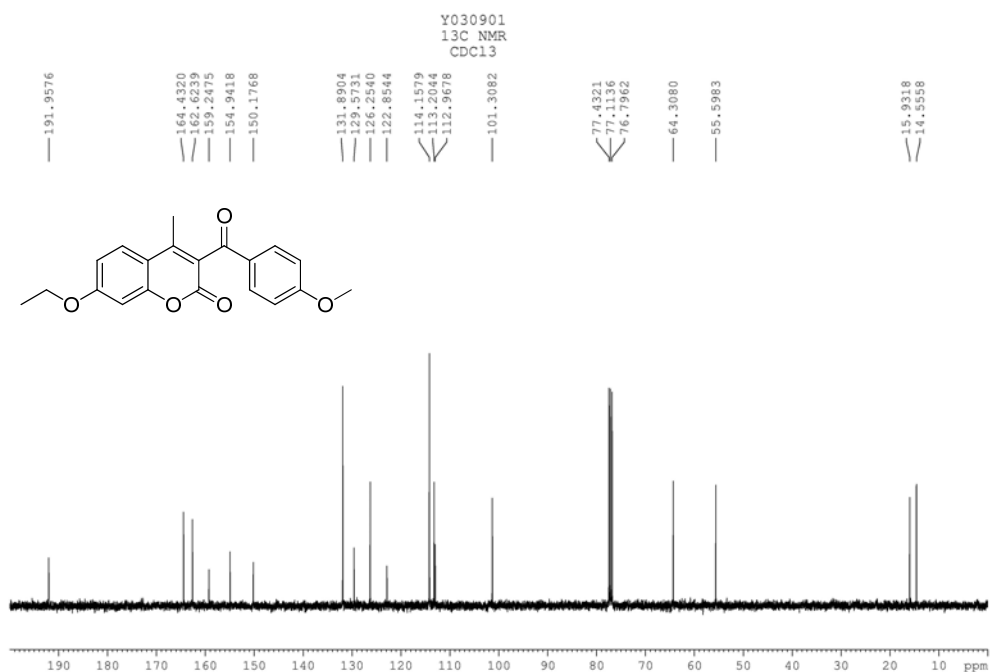
<sup>1</sup>H NMR spectrum of compound **3ea**



<sup>13</sup>C NMR spectrum of compound **3ea**



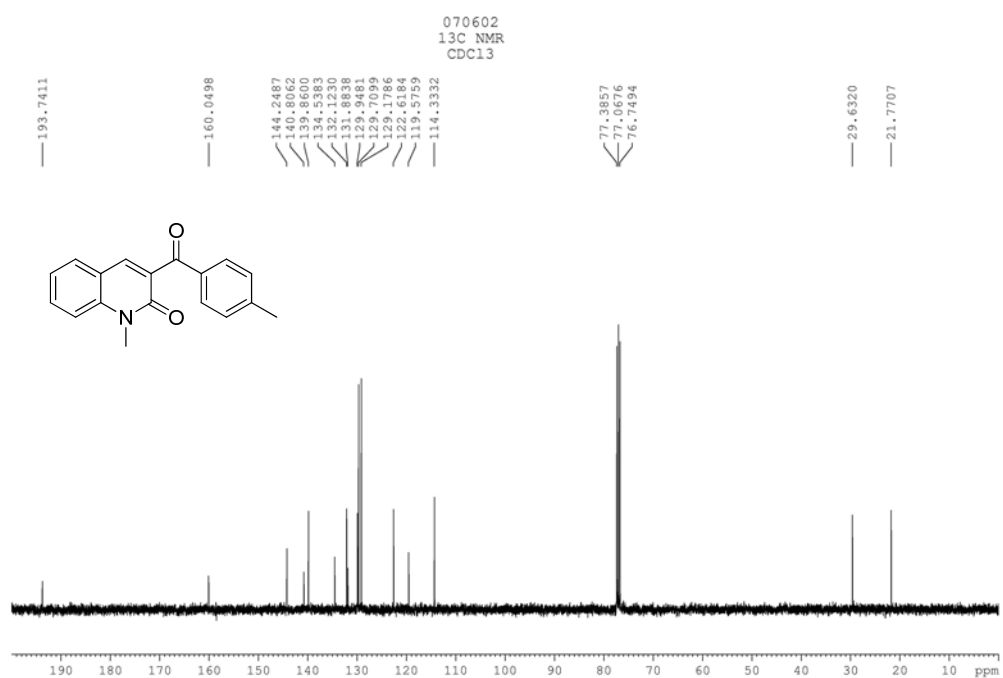
<sup>1</sup>H NMR spectrum of compound **3fe**



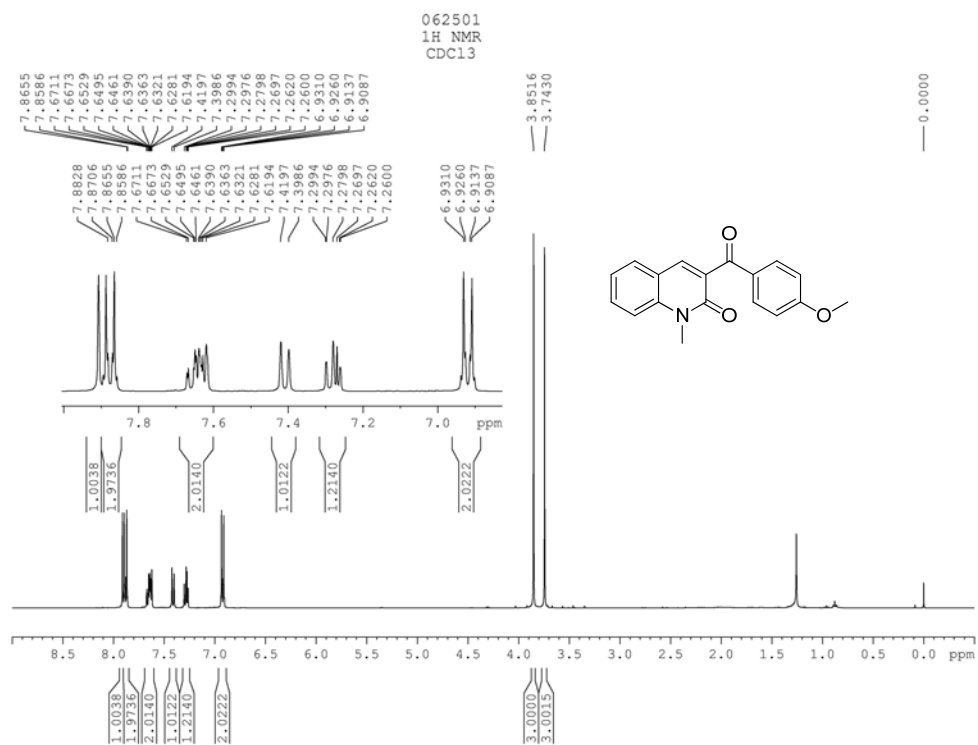
<sup>13</sup>C NMR spectrum of compound **3fe**



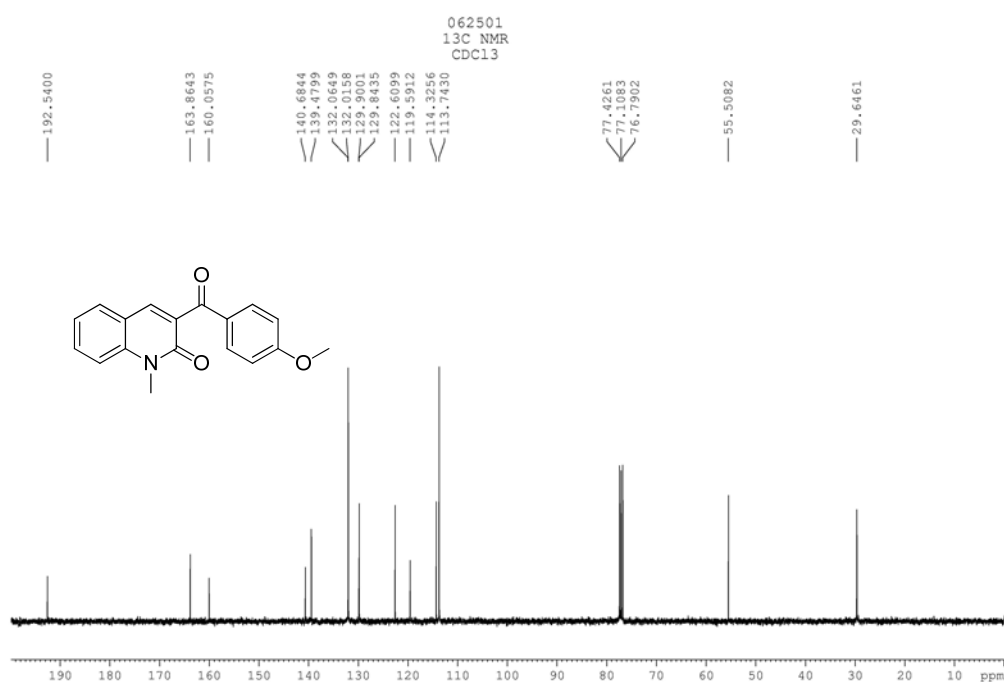
<sup>1</sup>H NMR spectrum of compound **5ab**



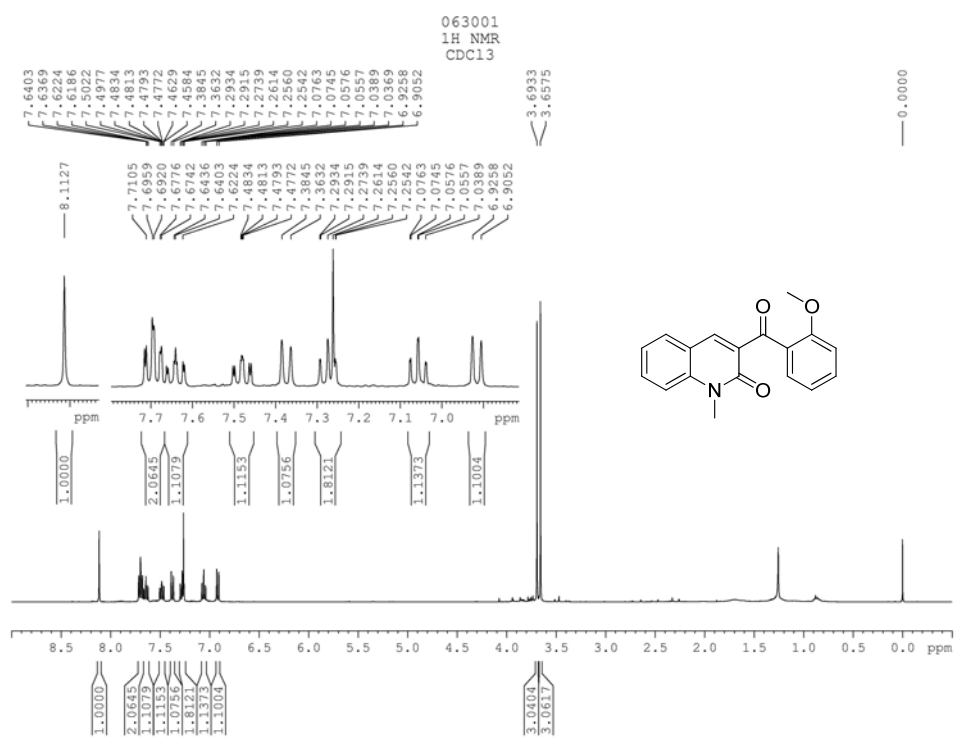
<sup>13</sup>C NMR spectrum of compound **5ab**



<sup>1</sup>H NMR spectrum of compound **5ad**

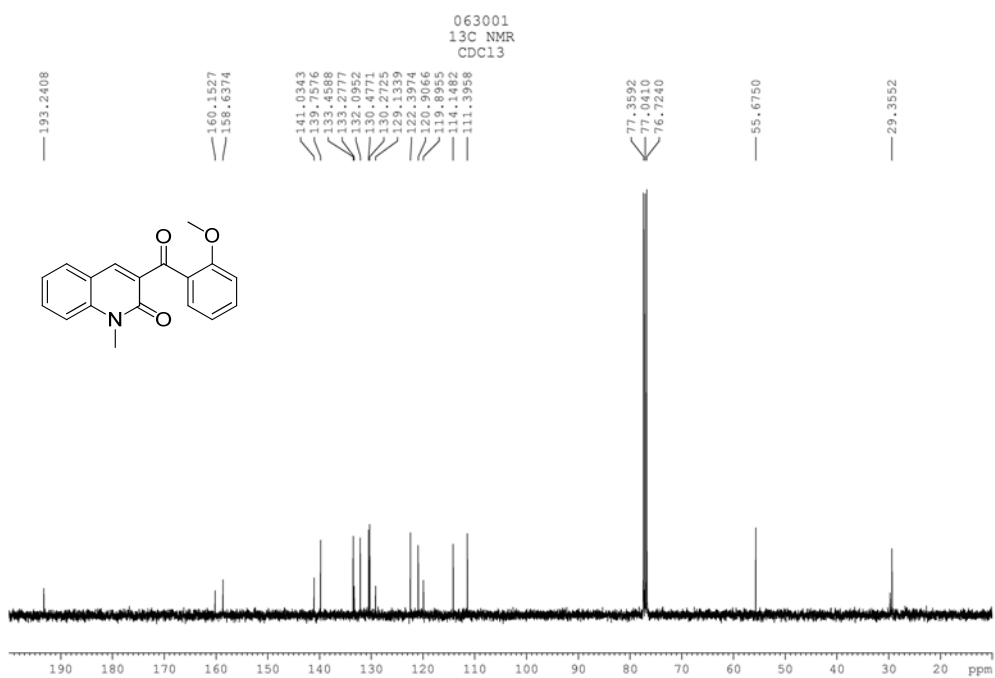


<sup>13</sup>C NMR spectrum of compound **5ad**

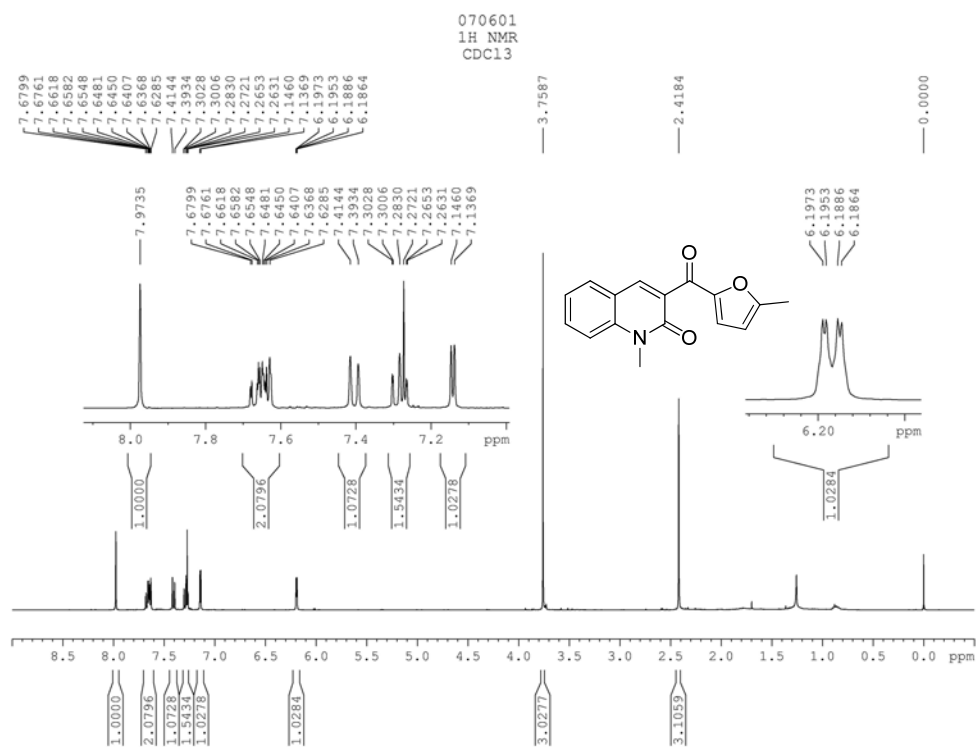


<sup>1</sup>H NMR spectrum of compound **5af**

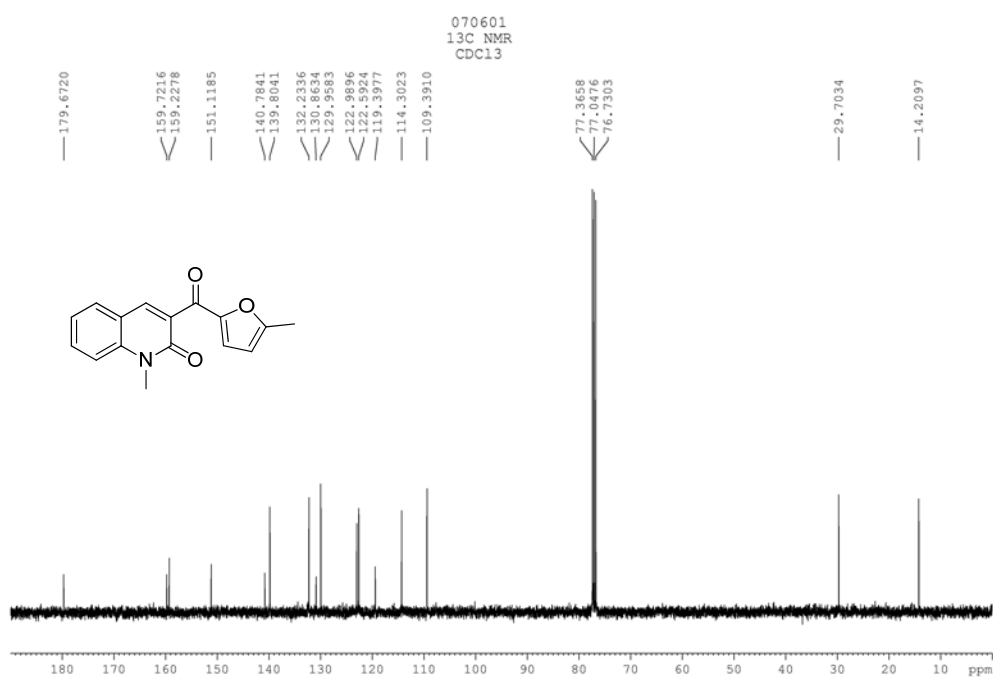




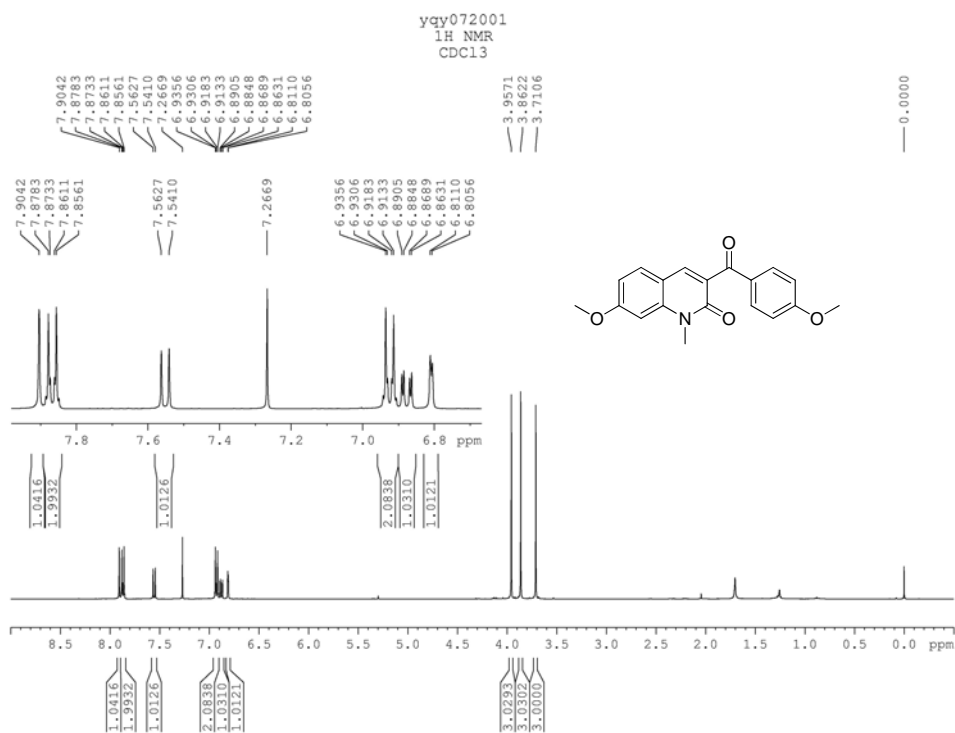
<sup>13</sup>C NMR spectrum of compound **5af**



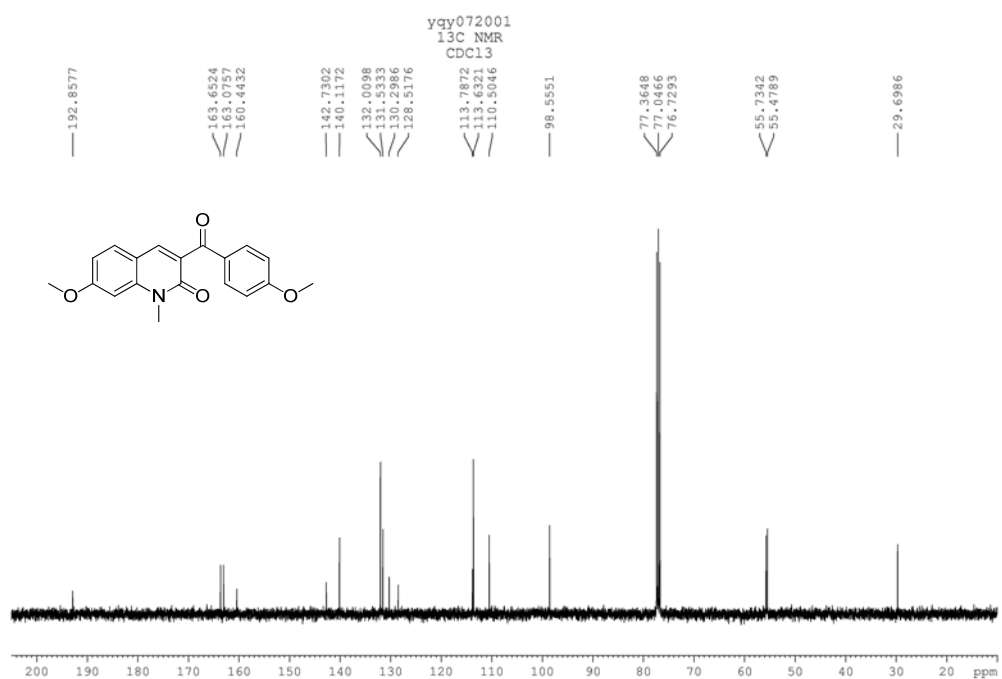
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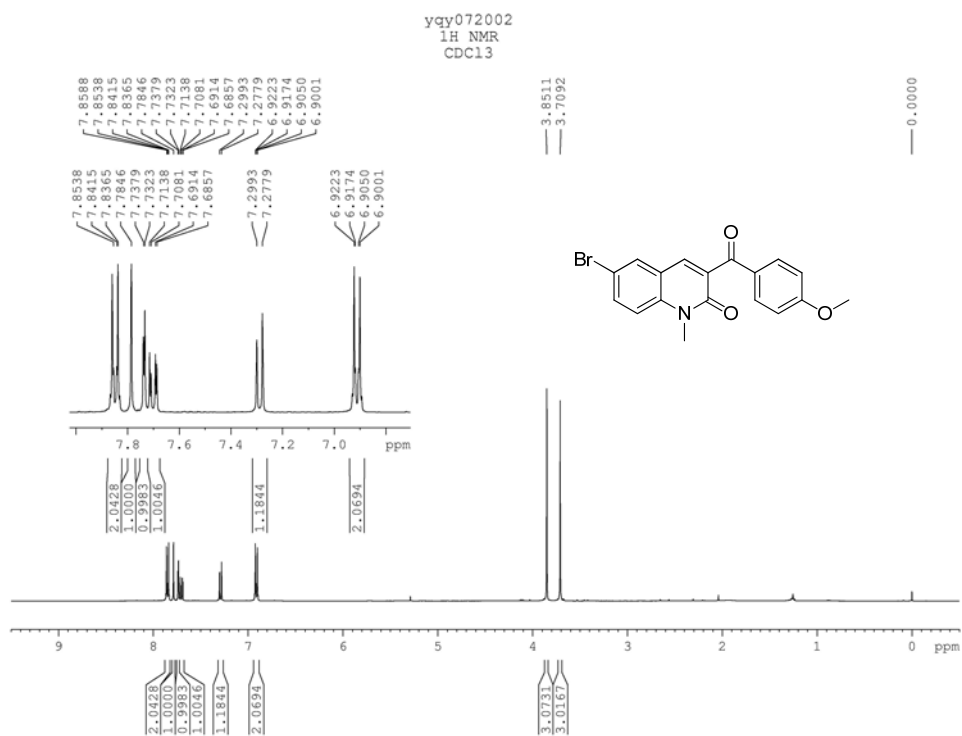
$^{13}\text{C}$  NMR spectrum of compound **5an**



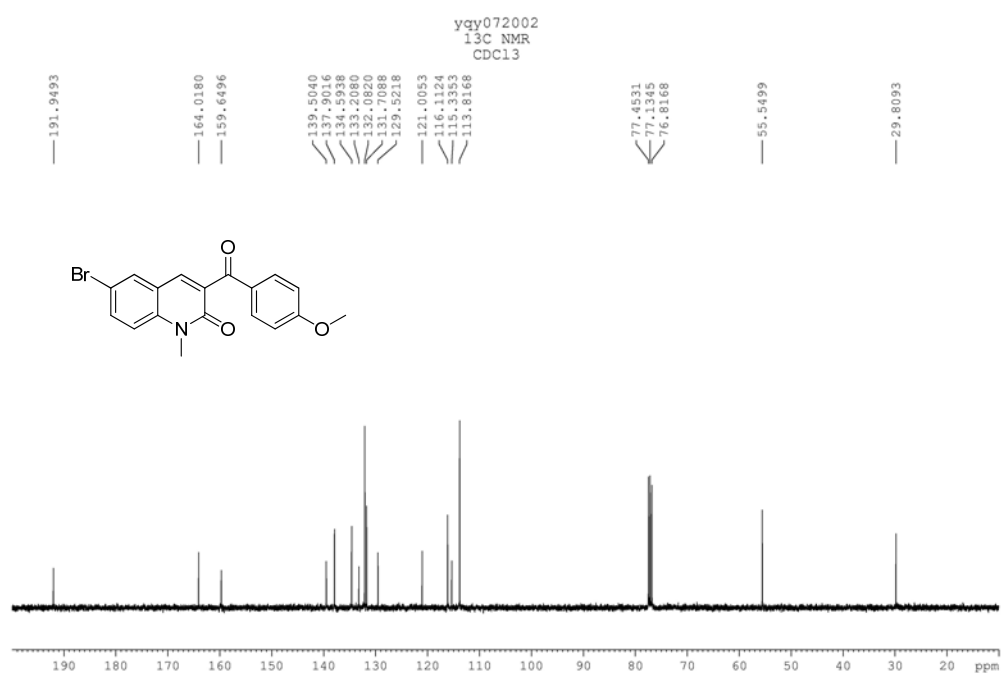
$^1\text{H}$  NMR spectrum of compound **5bd**



<sup>13</sup>C NMR spectrum of compound **5bd**



<sup>1</sup>H NMR spectrum of compound **5cd**



<sup>13</sup>C NMR spectrum of compound **5cd**