

**Synthesis of Casimiroin and Optimization of Its Quinone Reductase 2 and  
Aromatase Inhibitory Activity**

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Title Page	S1
Elemental Analyses	S2
<sup>1</sup> H NMR and <sup>13</sup> C NMR Spectrum of compounds <b>1, 1a-r, 2, 3a-b, 3g-h, 3i-j, 3m-q,</b> <b>6a, 6g, 6i, 6m, 6o, 7a, 7g, 7i, 7m, 7o, 8 and 9</b>	S3-S63

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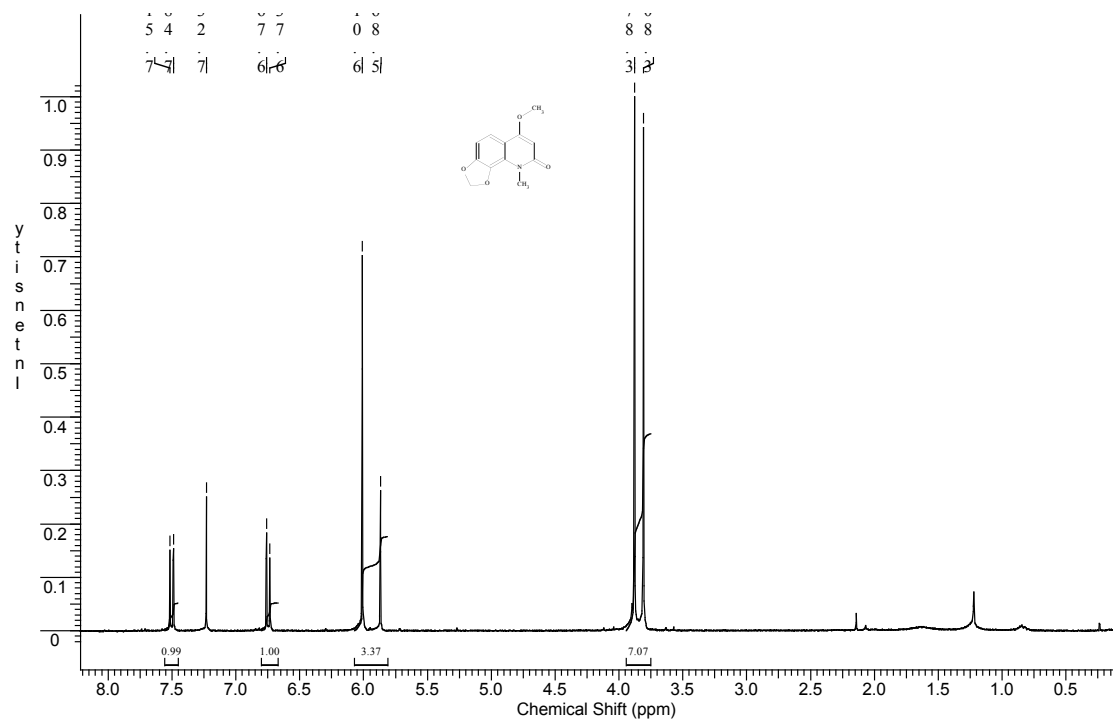
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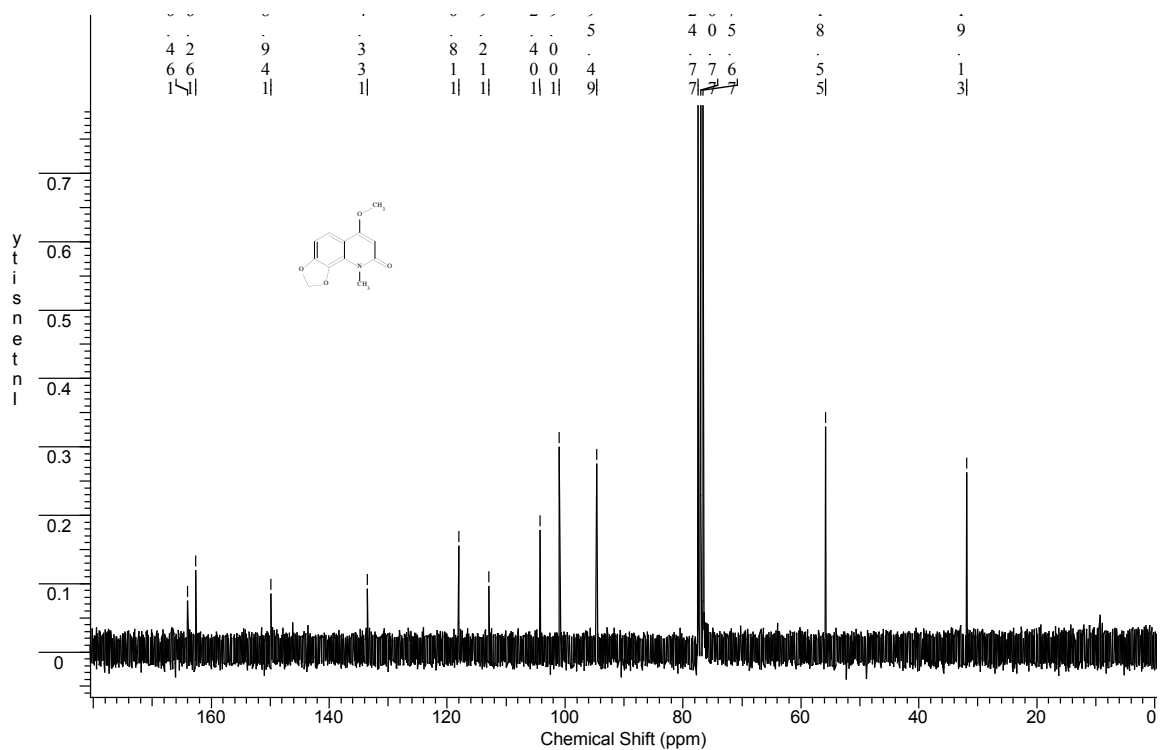
<sup>§</sup>University of Hawaii at Hilo

### Elemental Analyses

Compound	Formula	Calcd.	Found
<b>1</b>	$C_{12}H_{11}NO_4$	C, 61.80; H, 4.75; N, 6.01	C, 61.65; H, 4.58; N, 5.96
<b>1a</b>	$C_{11}H_9NO_3$	C, 65.02; H, 4.46; N, 6.89	C, 64.65; H, 4.30; N, 6.86
<b>1b</b>	$C_{12}H_{11}NO_3$	C, 66.35; H, 5.10; N, 6.45	C, 66.10; H, 5.04; N, 6.36
<b>1c</b>	$C_{10}H_9NO \cdot 0.1 H_2O$	C, 74.61; H, 5.76; N, 8.70	C, 74.50; H, 5.40; N, 8.64
<b>1d</b>	$C_{11}H_{11}NO \cdot 1.0 H_2O$	C, 69.09; H, 6.85; N, 7.32	C, 68.79; H, 6.94; N, 6.91
<b>1e</b>	$C_{11}H_{11}NO_2$	C, 69.83; H, 5.86; N, 7.40	C, 69.94; H, 5.75; N, 7.47
<b>1f</b>	$C_{12}H_{13}NO_2$	C, 70.92; H, 6.45; N, 6.89	C, 70.94; H, 6.48; N, 6.75
<b>1g</b>	$C_{12}H_{13}NO_3$	C, 65.74; H, 5.98; N, 6.39	C, 65.65; H, 5.67; N, 6.27
<b>1h</b>	$C_{13}H_{15}NO_3$	C, 66.94; H, 6.48; N, 6.00	C, 66.85; H, 6.35; N, 5.71
<b>1i</b>	$C_{12}H_{13}NO_3$	C, 65.74; H, 5.98; N, 6.39	C, 65.37; H, 5.80; N, 6.23
<b>1j</b>	$C_{13}H_{15}NO_3$	C, 66.94; H, 6.48; N, 6.00	C, 67.11; H, 6.56; N, 5.99
<b>1k</b>	$C_{12}H_{13}NO_3 \cdot 0.75 H_2O$	C, 61.93; H, 6.28; N, 6.02	C, 61.85; H, 6.74; N, 5.79
<b>1l</b>	$C_{13}H_{15}NO_3$	C, 66.94; H, 6.48; N, 6.00	C, 66.85; H, 6.50; N, 5.91
<b>1m</b>	$C_{13}H_{15}NO_4$	C, 62.64; H, 6.07; N, 5.62	C, 62.39; H, 5.88; N, 5.37
<b>1n</b>	$C_{14}H_{17}NO_4$	C, 63.87; H, 6.51; N, 5.32	C, 64.13; H, 6.62; N, 5.11
<b>1o</b>	$C_{13}H_{15}NO_4$	C, 62.64; H, 6.07; N, 5.62	C, 62.69; H, 6.26; N, 5.66
<b>1p</b>	$C_{14}H_{17}NO_4$	C, 63.87; H, 6.51; N, 5.32	C, 63.91; H, 6.60; N, 5.16
<b>1q</b>	$C_{14}H_{17}NO_5$	C, 60.21; H, 6.14; N, 5.02	C, 60.26; H, 6.10; N, 4.99
<b>1r</b>	$C_{15}H_{19}NO_5$	C, 61.42; H, 6.53; N, 4.78	C, 61.37; H, 6.48; N, 4.71

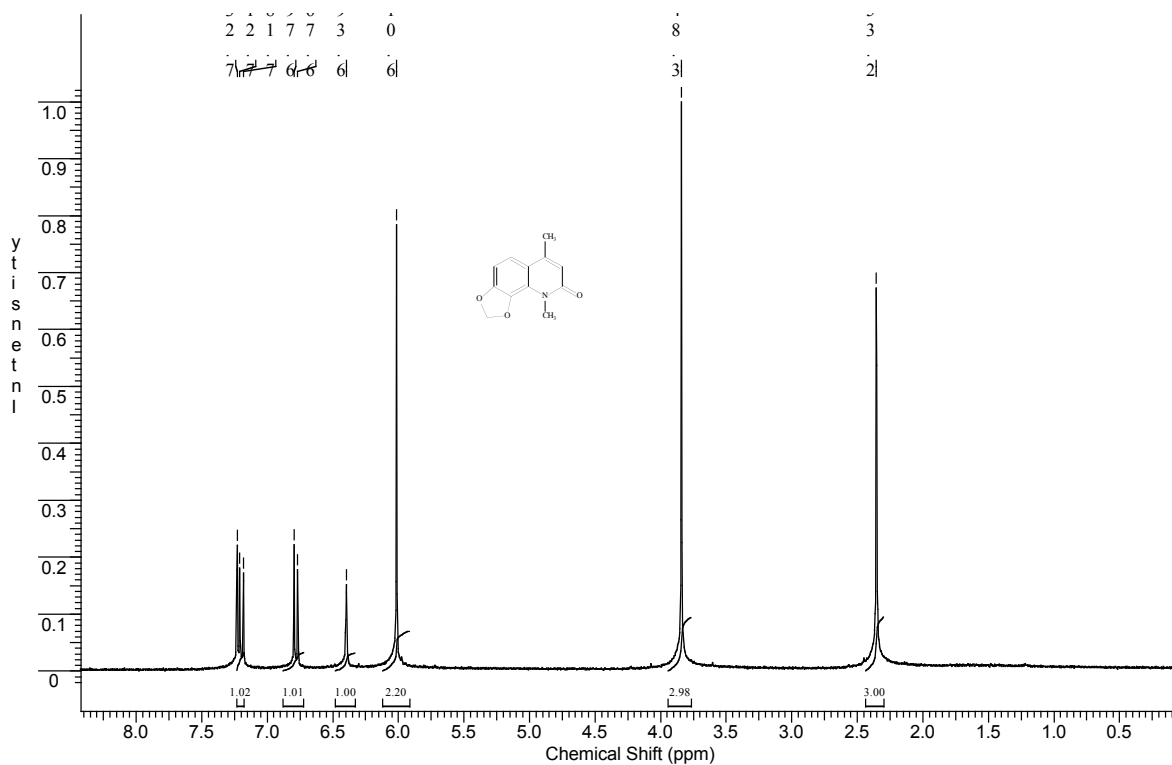


**<sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz) of Compound 1**

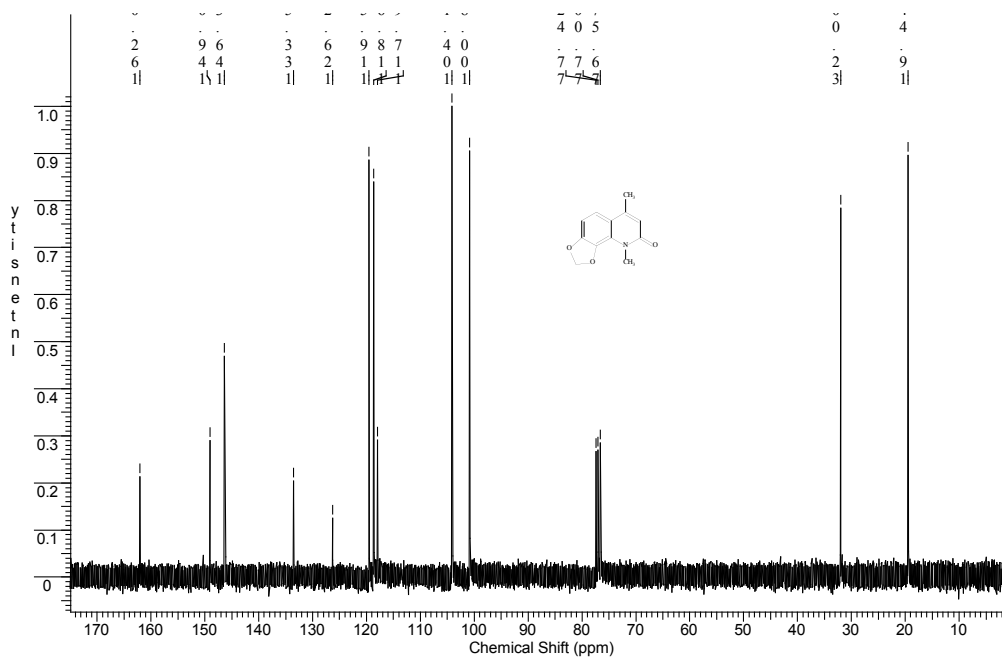


**<sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz) of Compound 1**

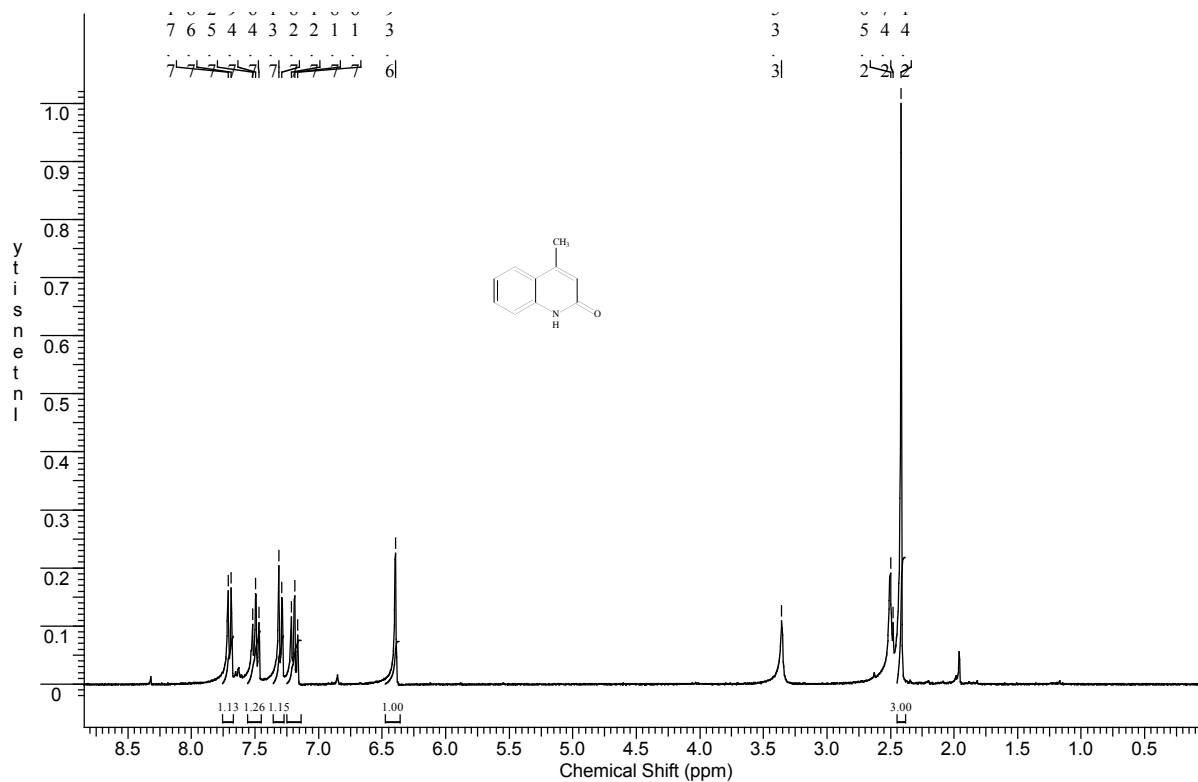




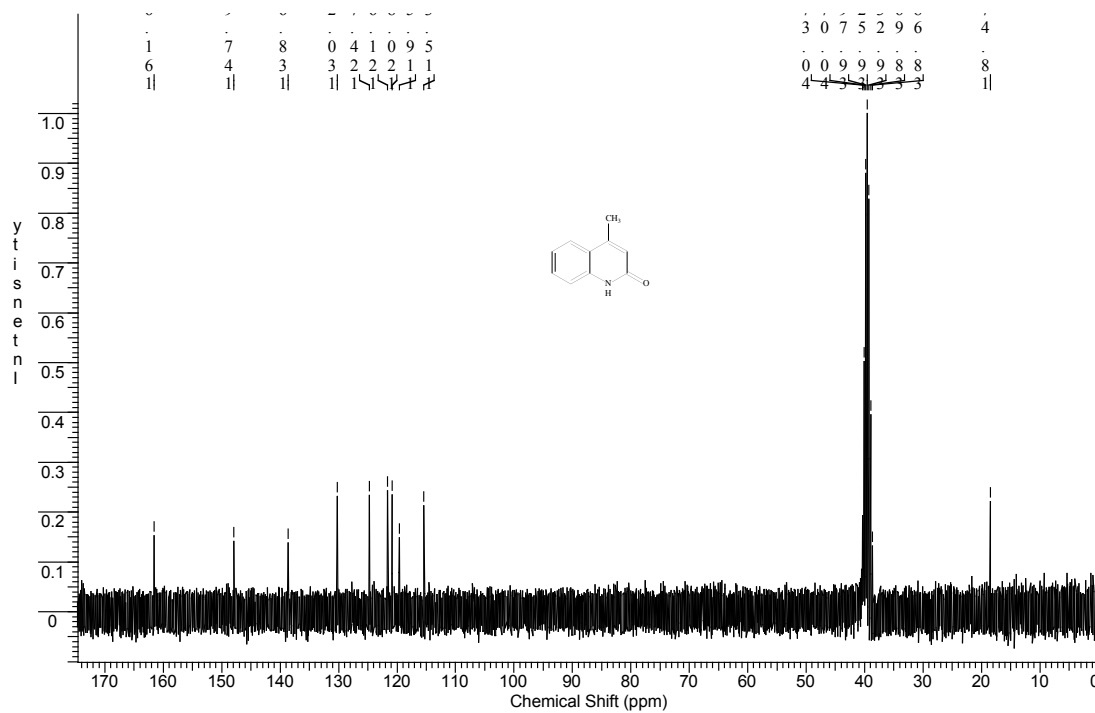
**<sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz) of Compound 1b**



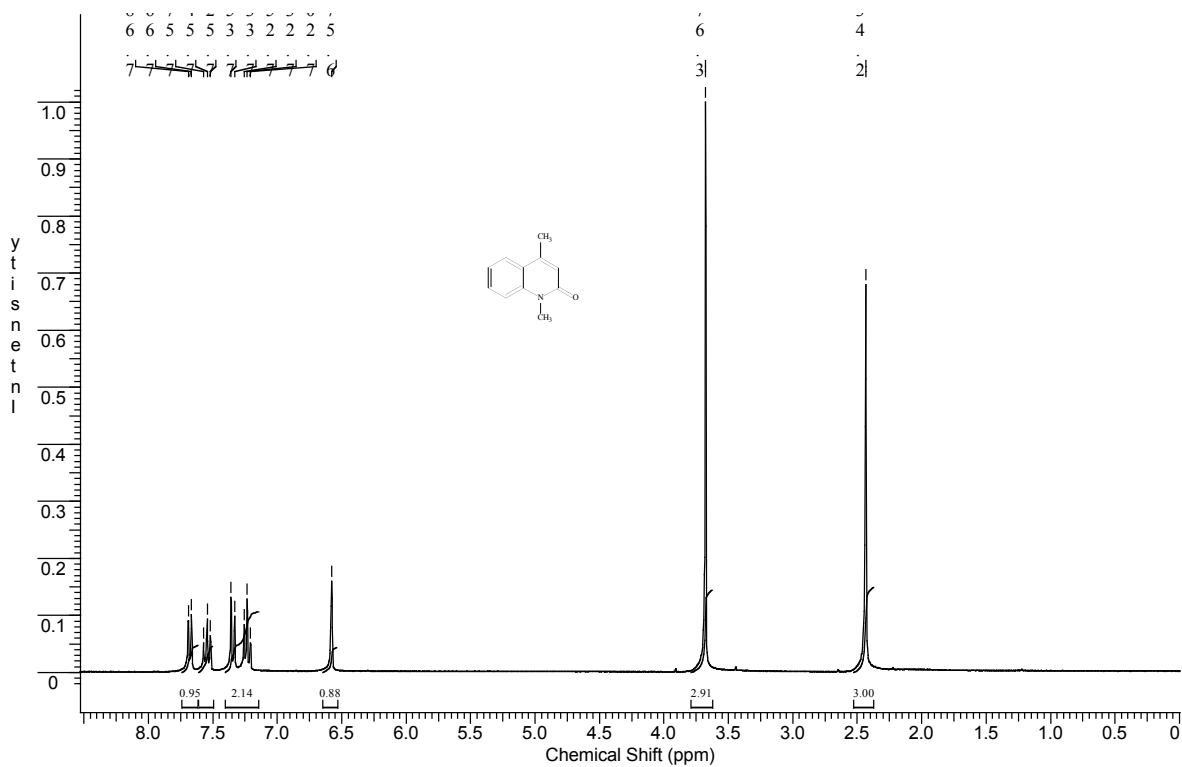
**<sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz) of Compound 1b**



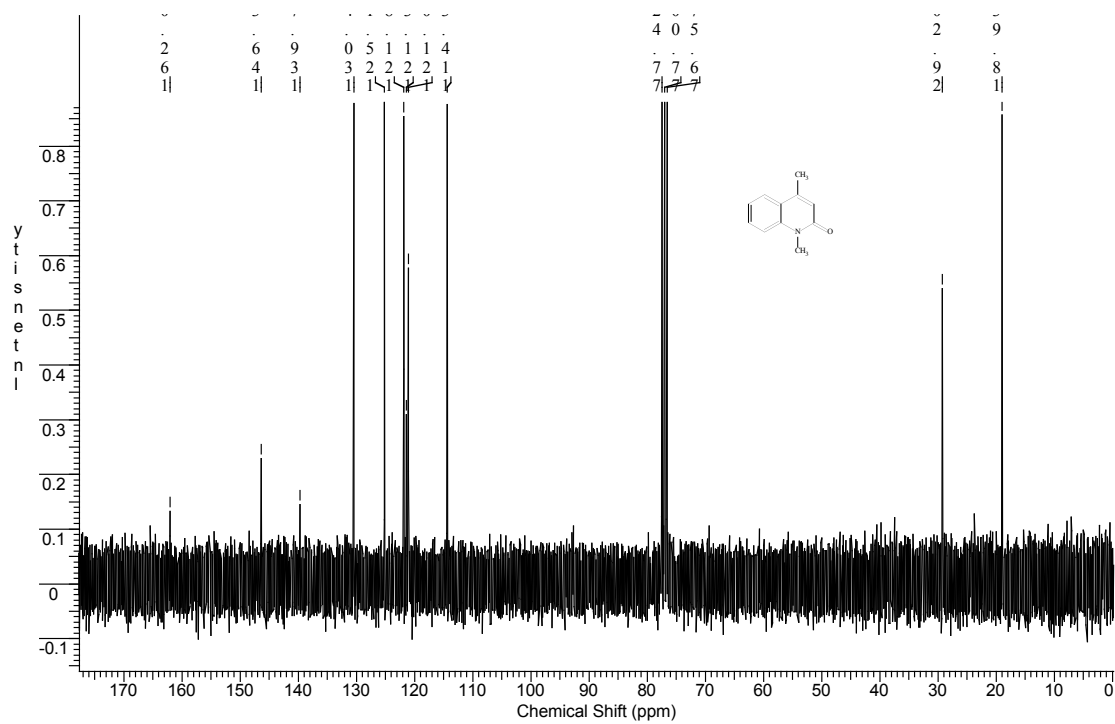
**<sup>1</sup>H NMR (DMSO-d<sub>6</sub>, 300 MHz) of Compound 1c**



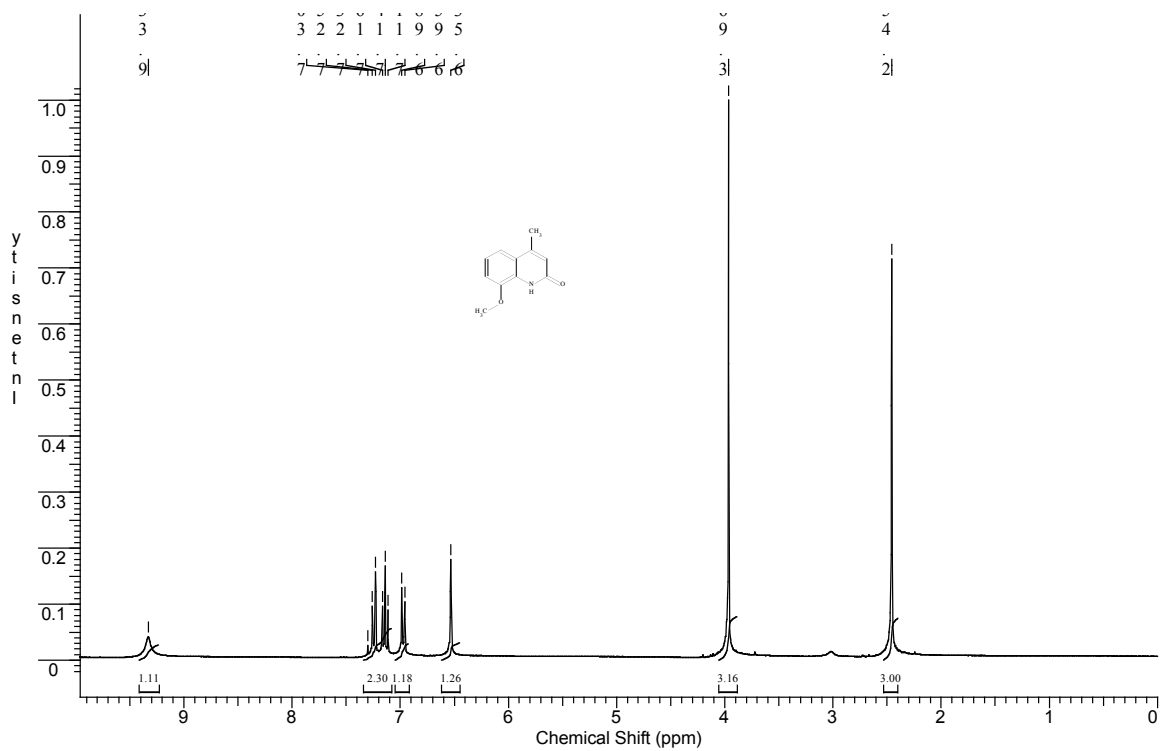
**<sup>13</sup>C NMR (DMSO-d<sub>6</sub>, 75 MHz) of Compound 1c**



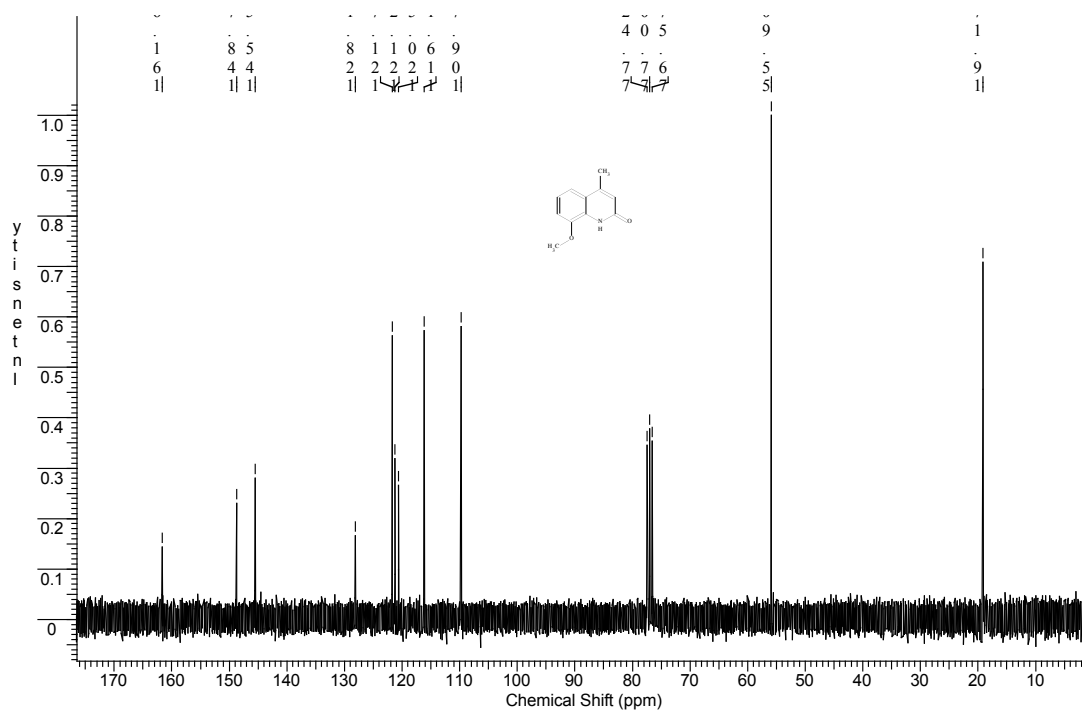
**<sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz) of Compound 1d**



**<sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz) of Compound 1d**

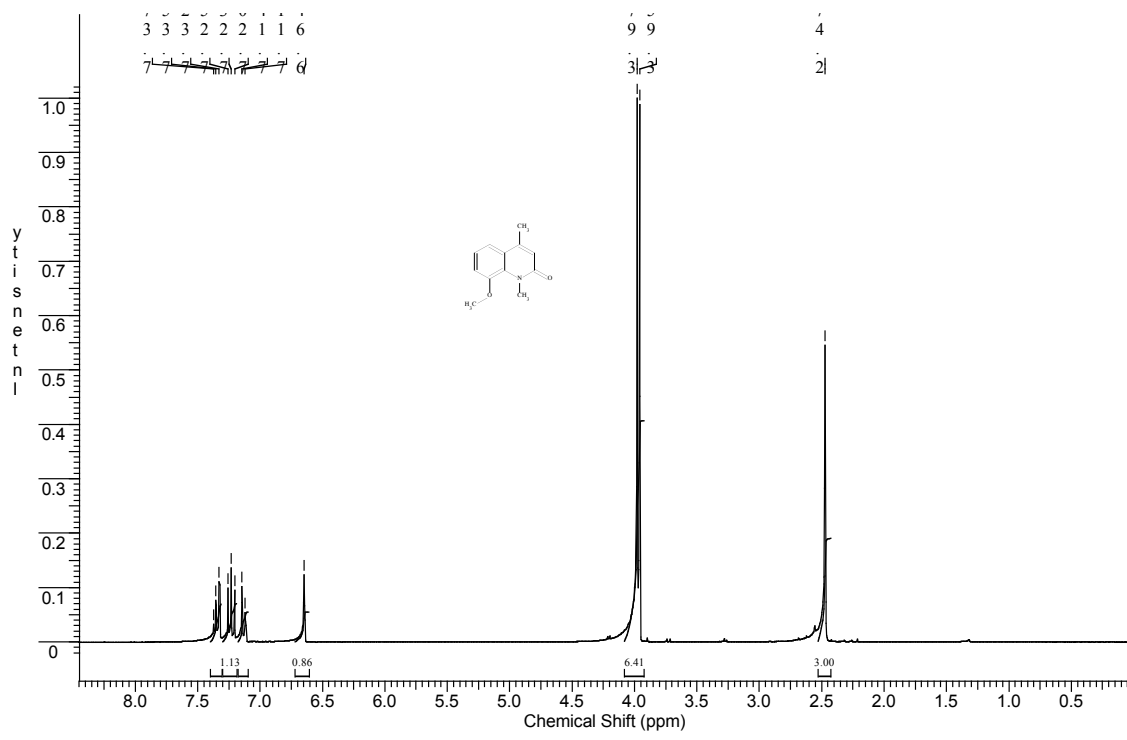


**<sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz) of Compound 1e**

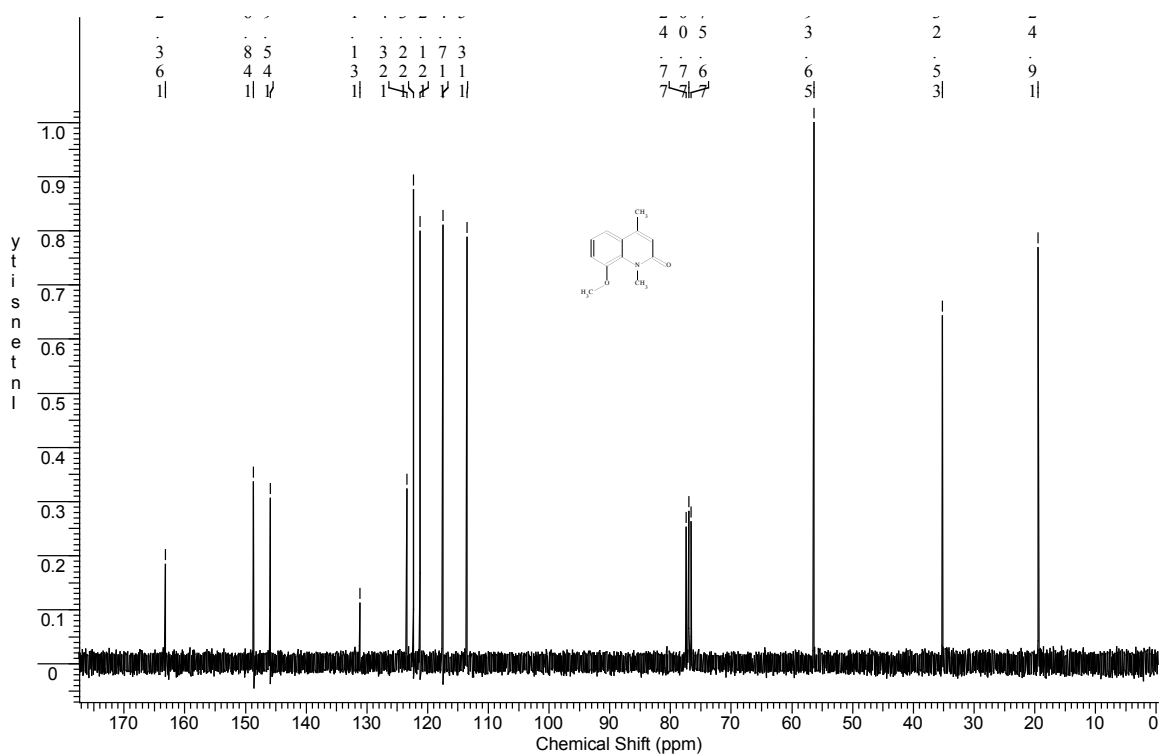


**<sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz) of Compound 1e**

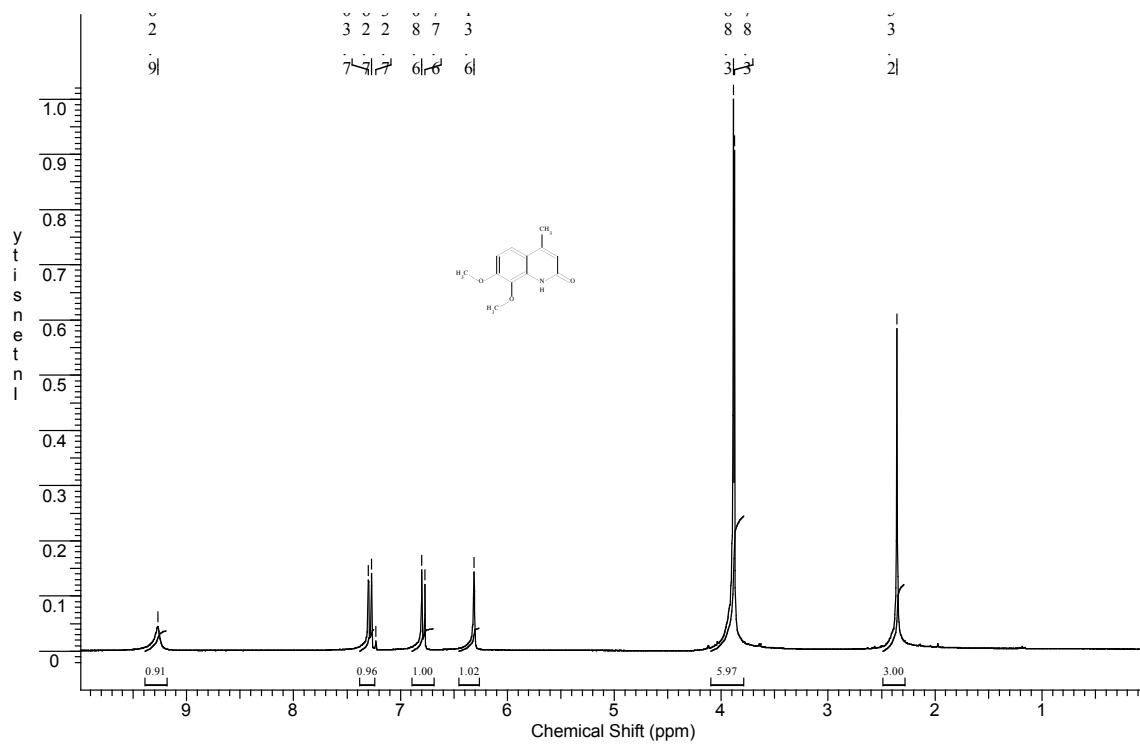




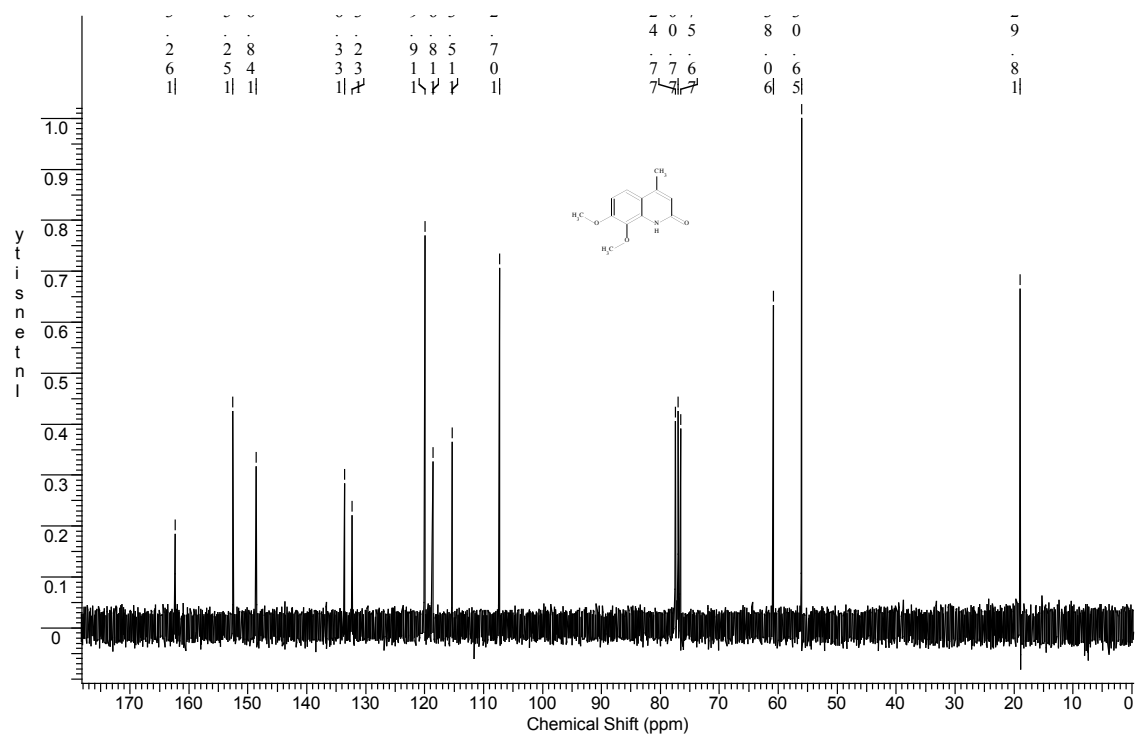
**<sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz) of Compound 1f**



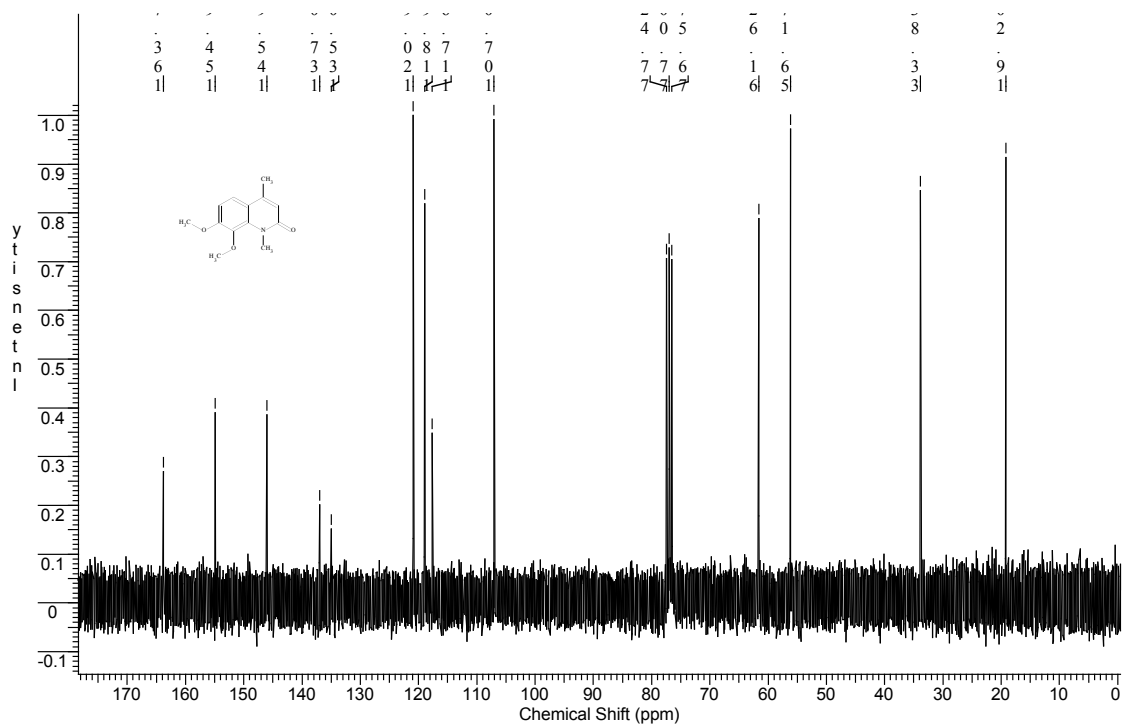
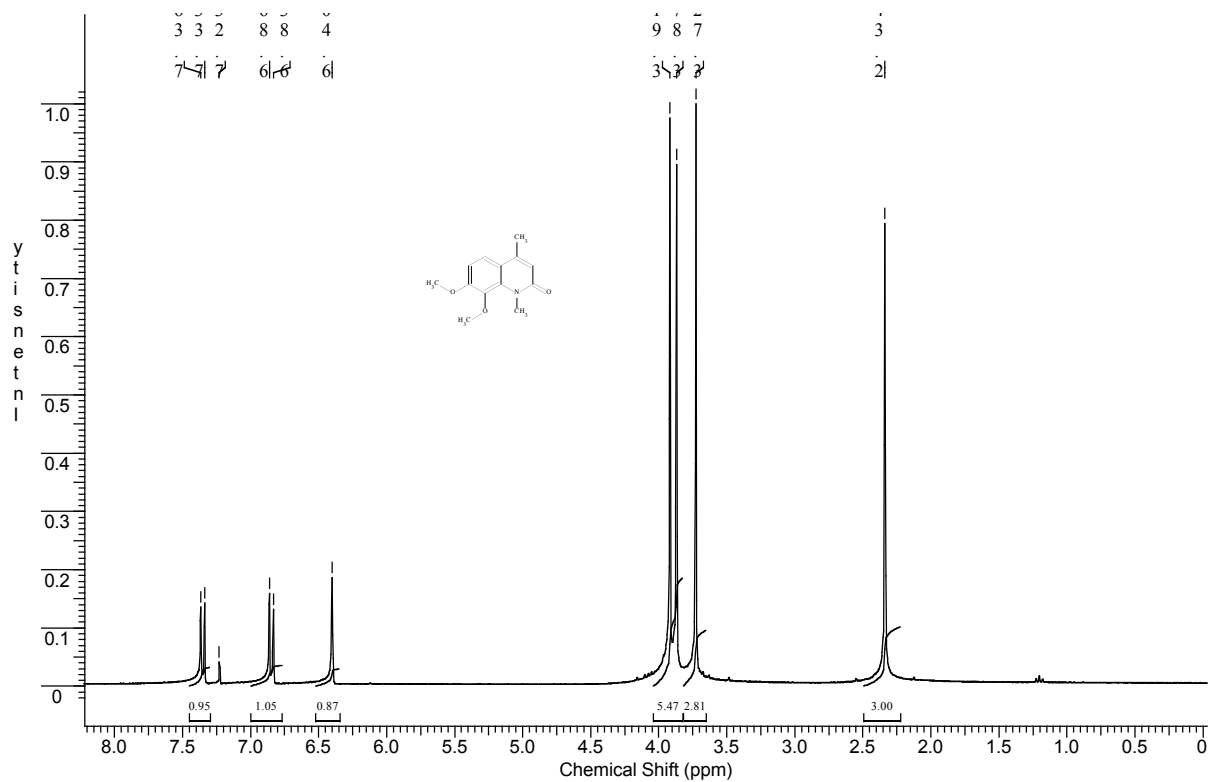
**<sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz) of Compound 1f**

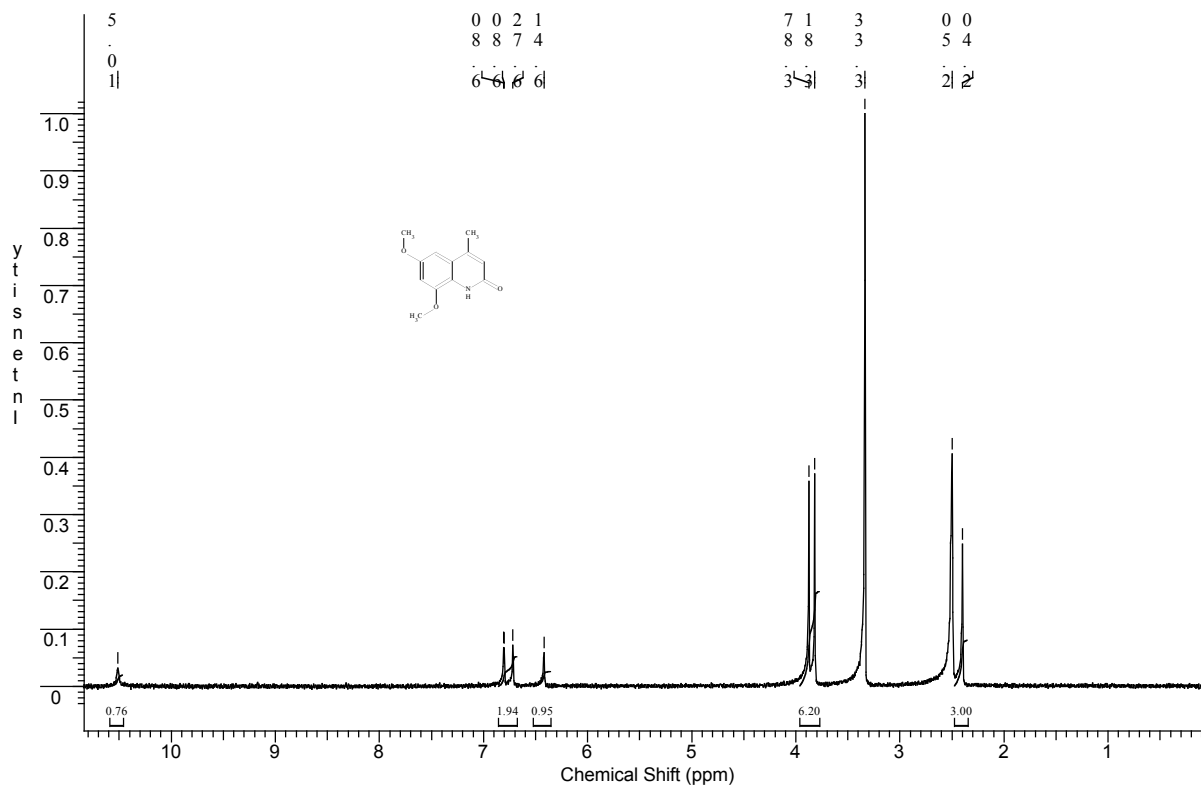


**<sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz) of Compound 1g**

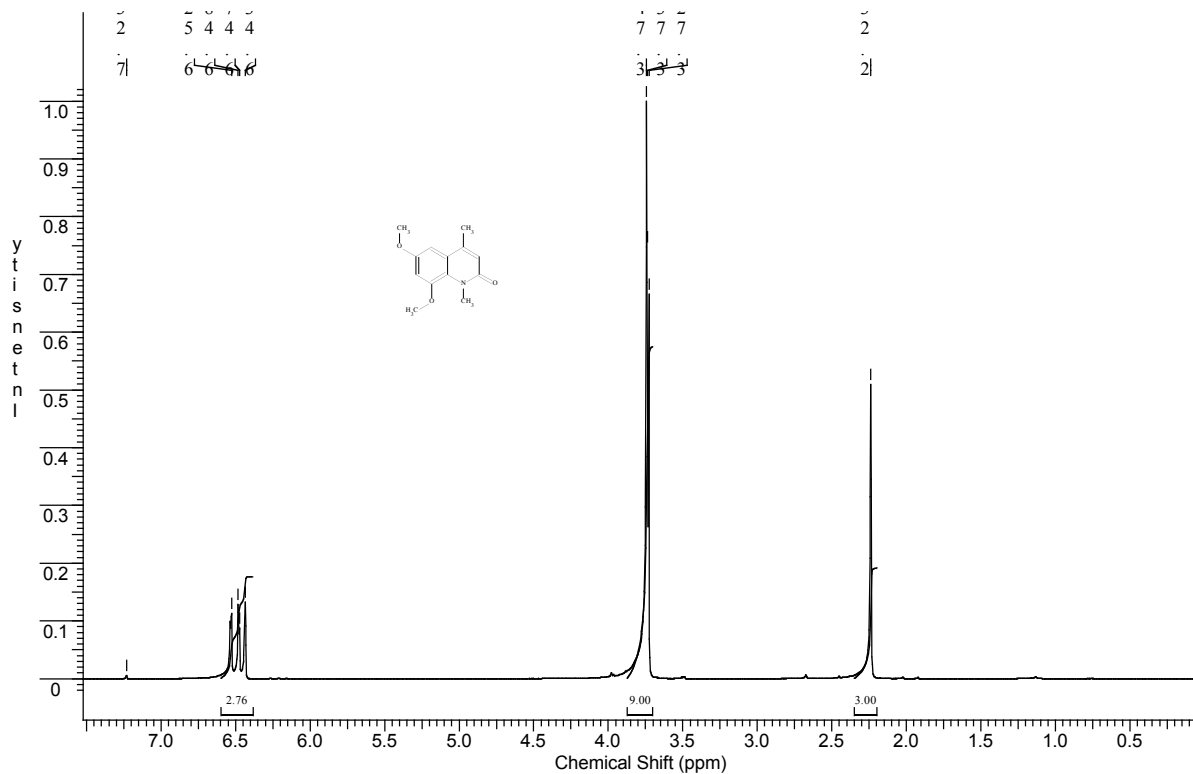


**<sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz) of Compound 1g**

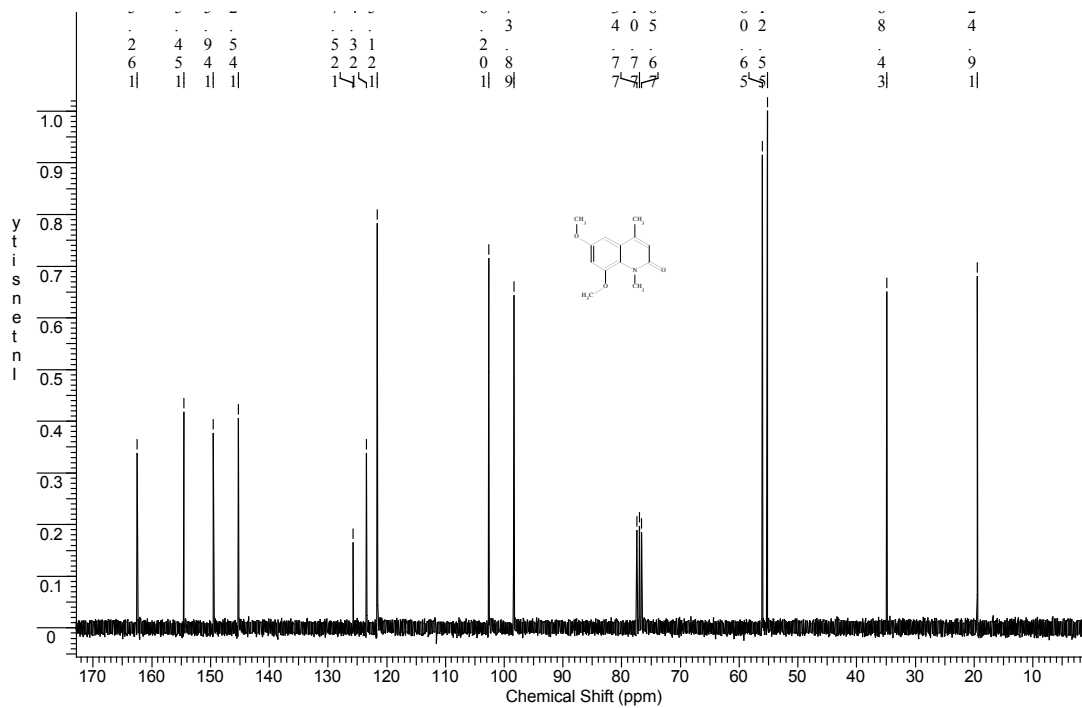




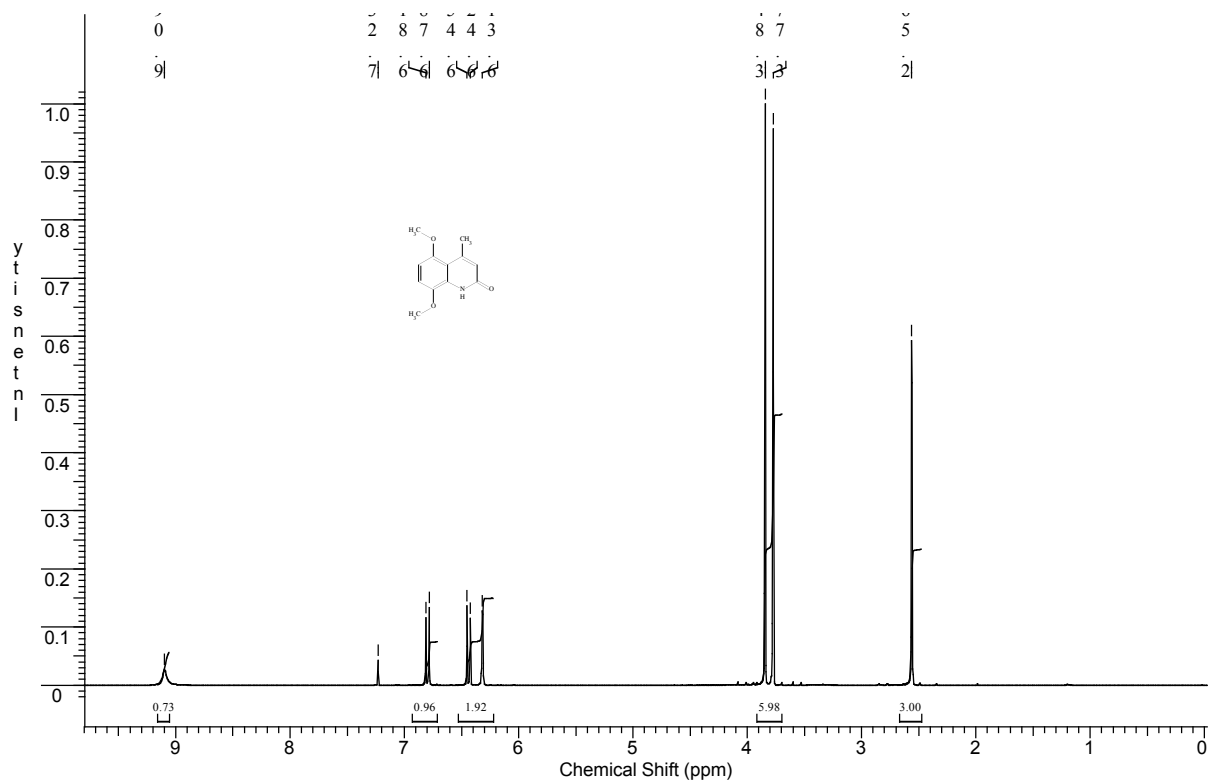
**<sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz) of Compound 1i**



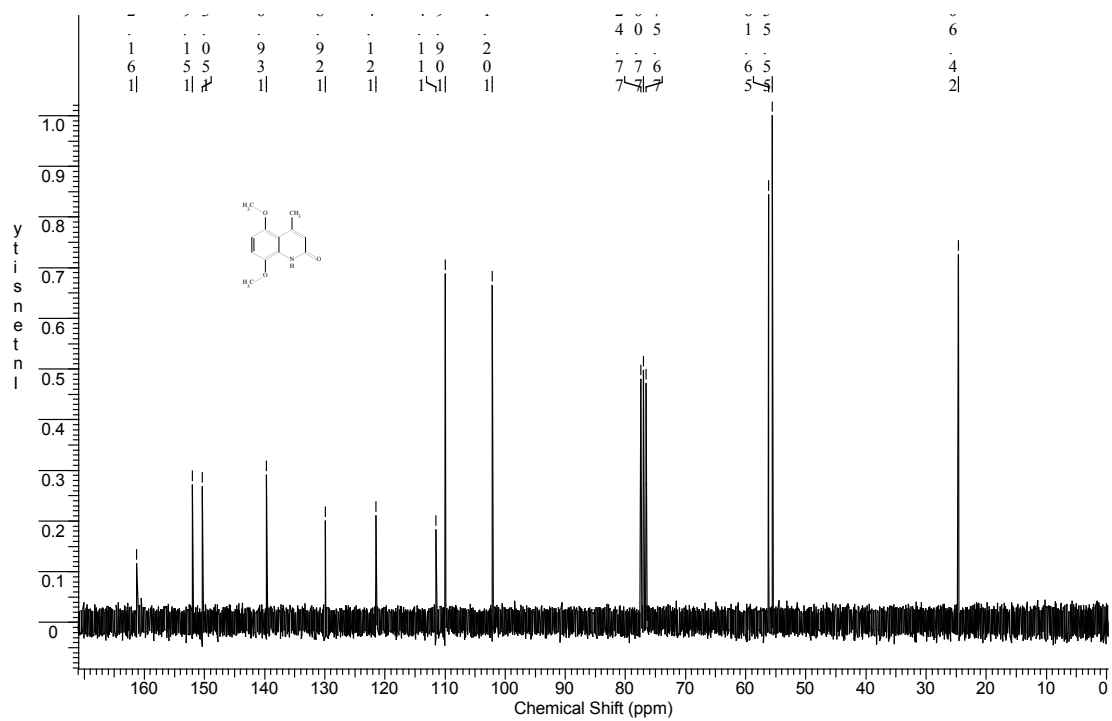
**<sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz) of Compound 1j**



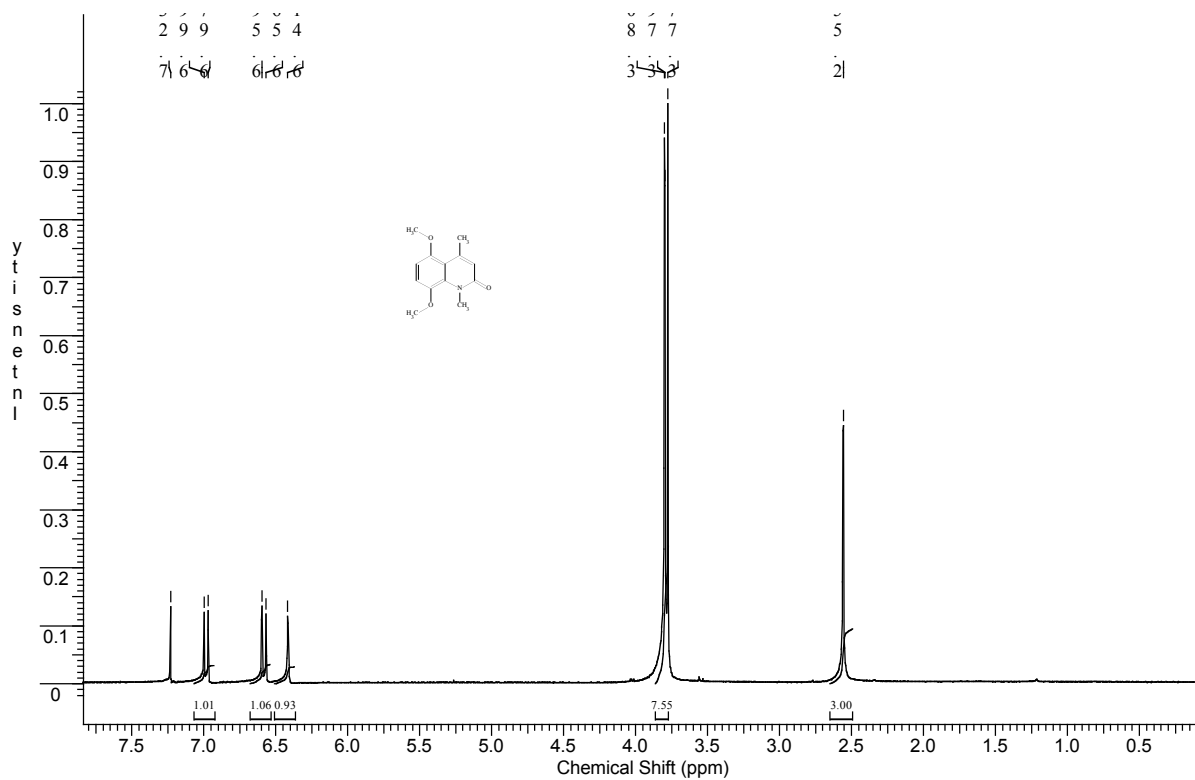
**<sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz) of Compound 1j**



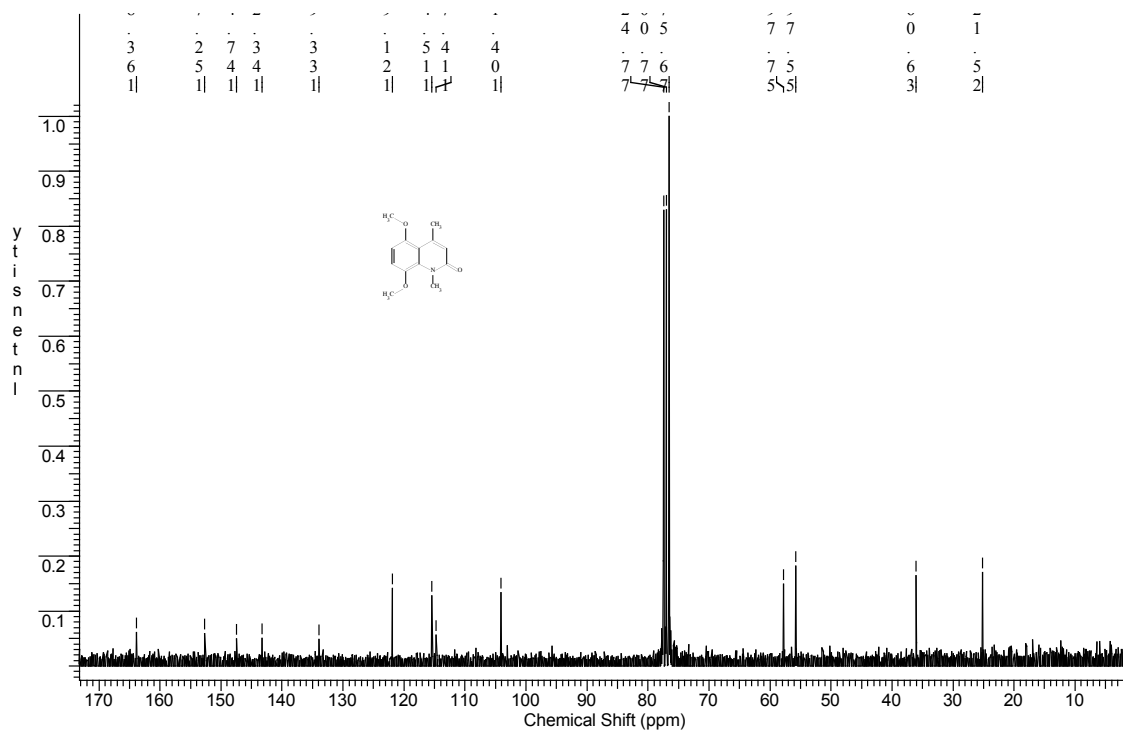
**<sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz) of Compound 1k**



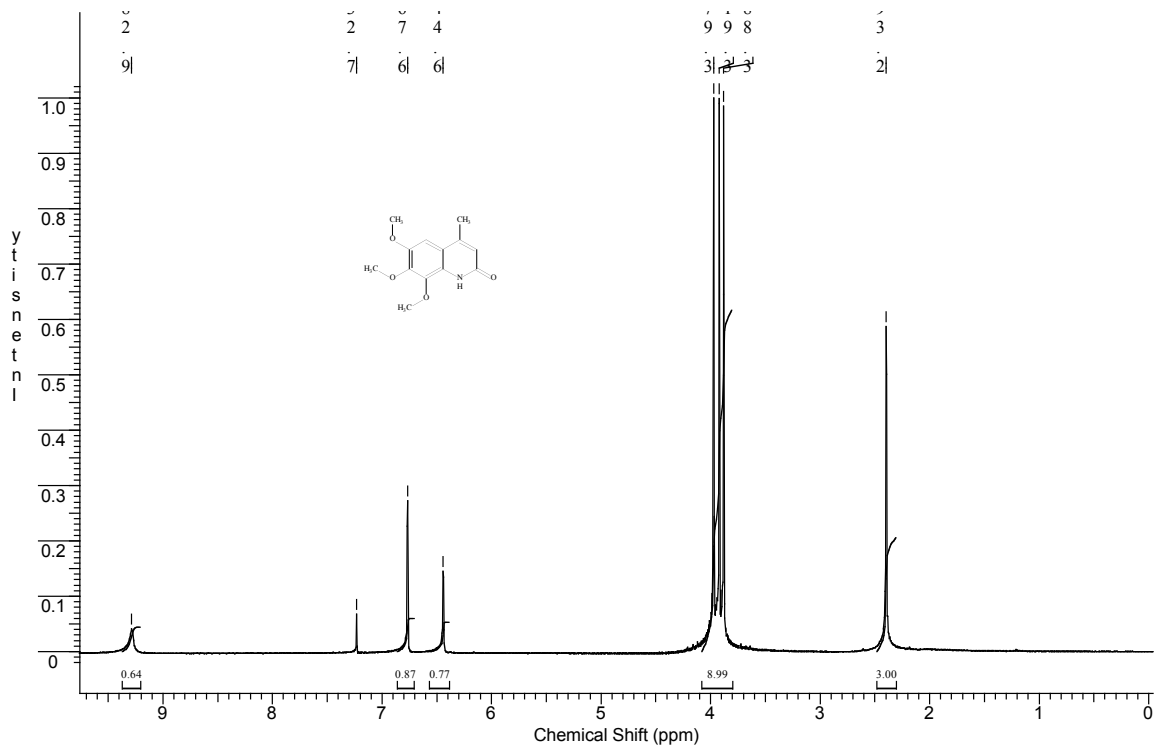
**<sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz) of Compound 1k**



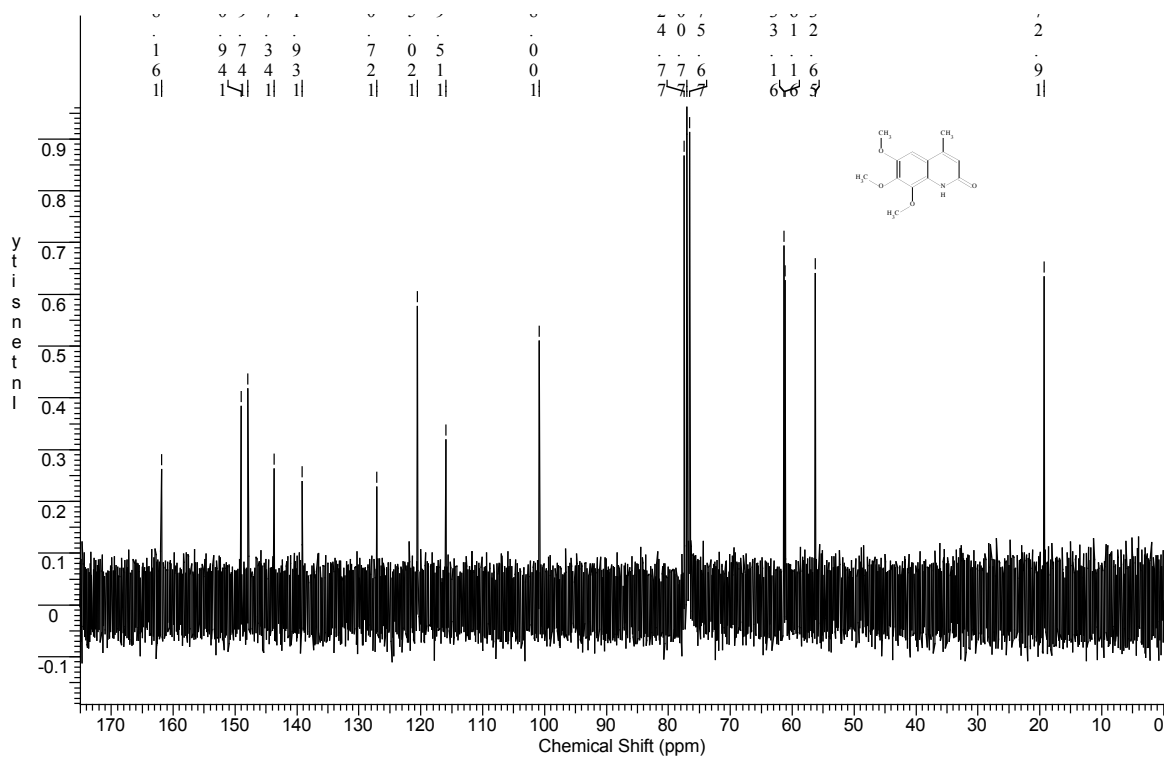
**<sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz) of Compound 11**



**<sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz) of Compound 11**

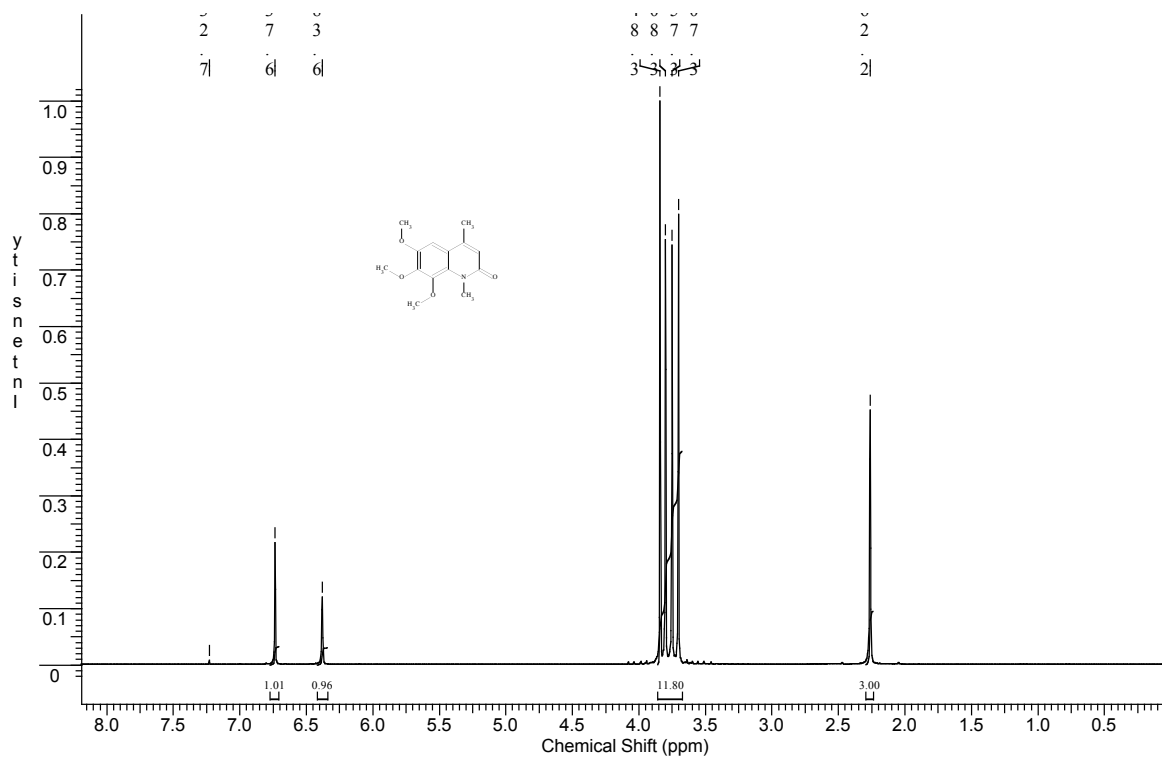


**<sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz) of Compound 1m**

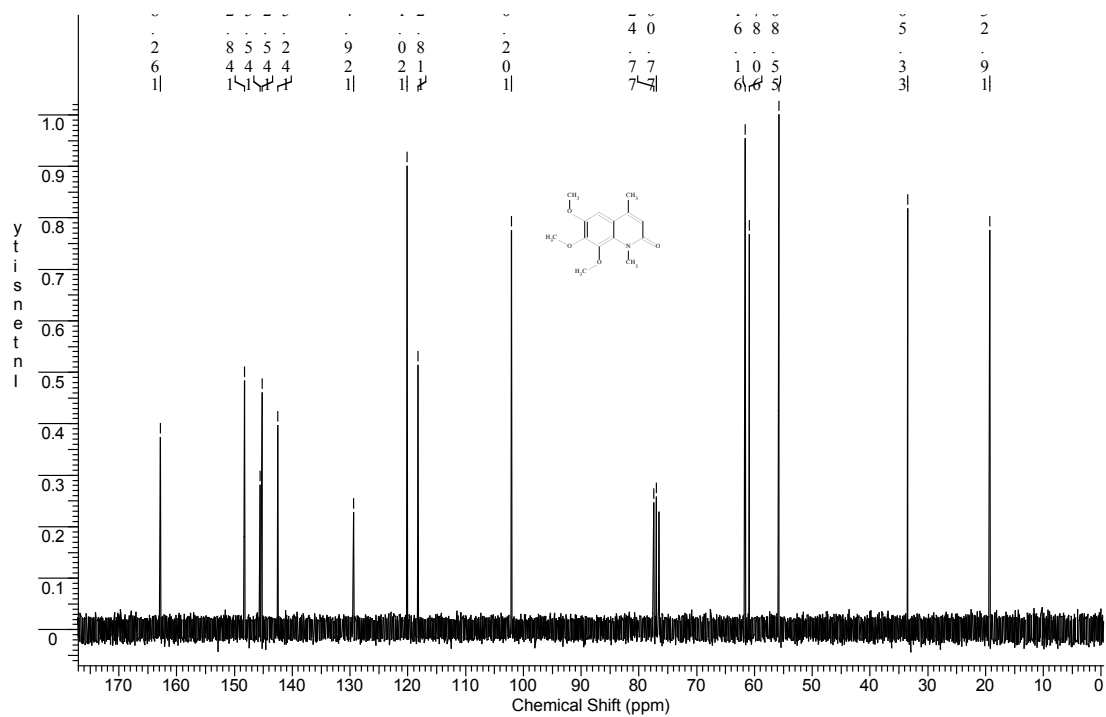


**<sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz) of Compound 1m**

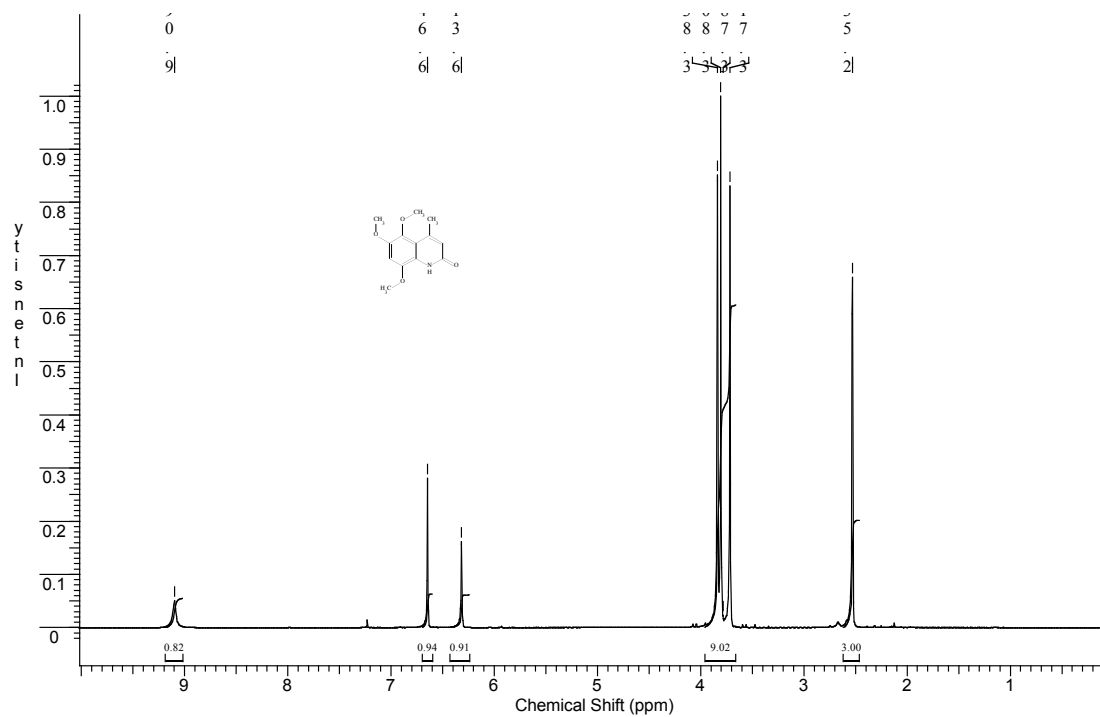




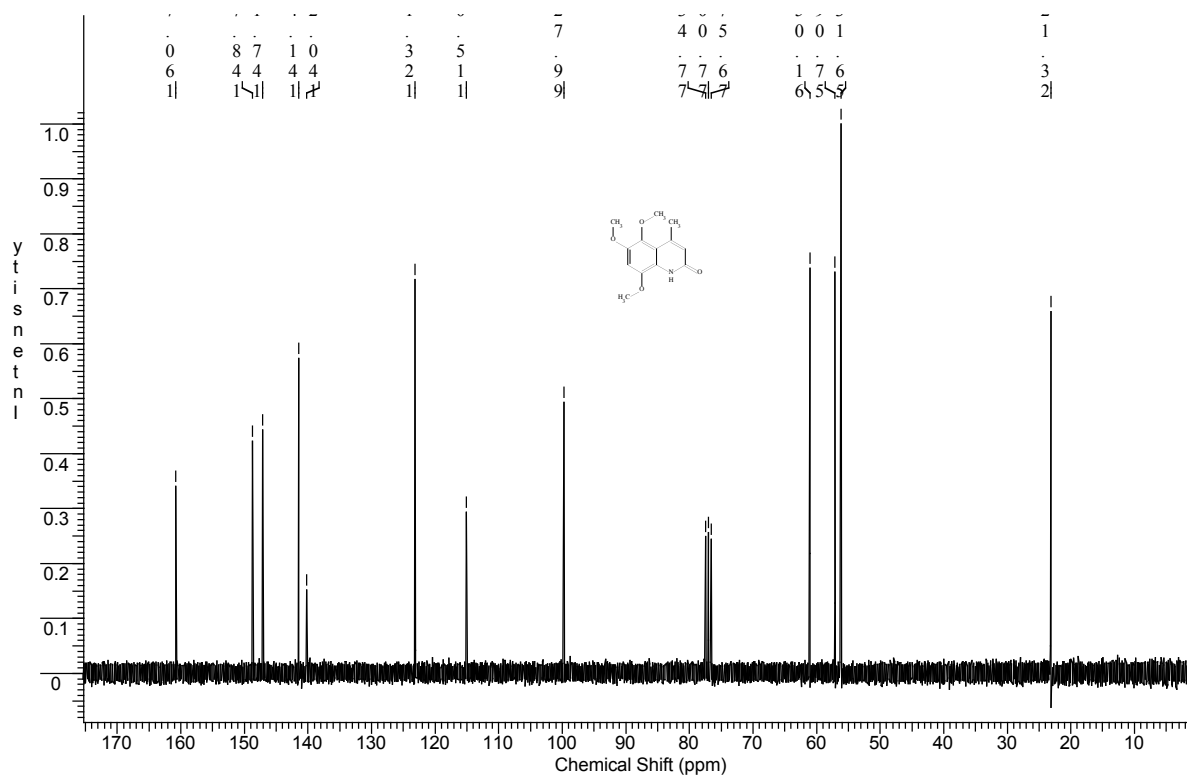
**<sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz) of Compound 1n**



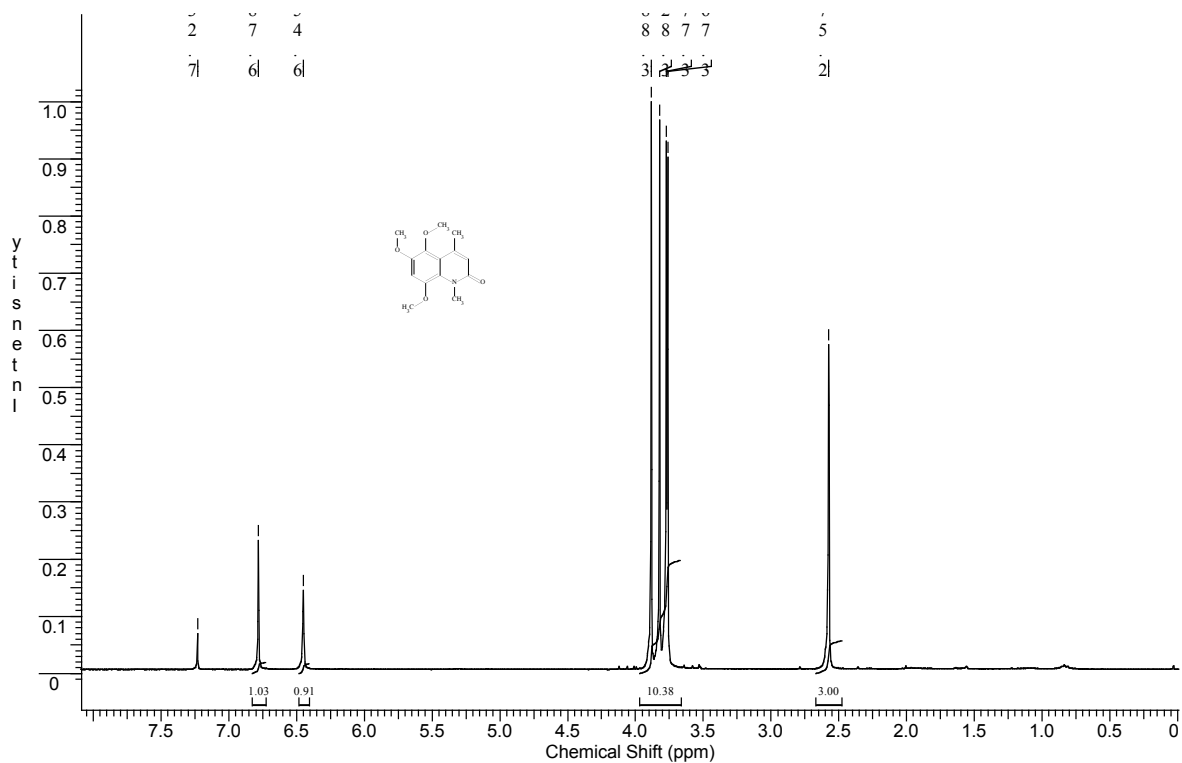
**<sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz) of Compound 1n**



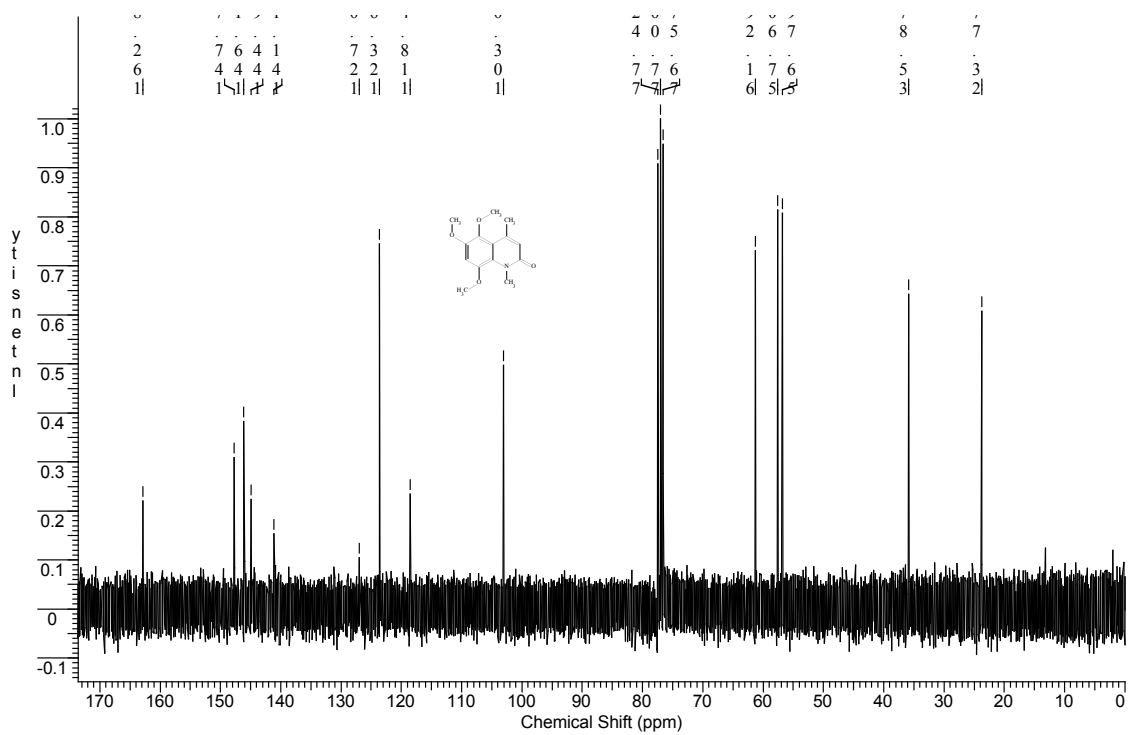
**<sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz) of Compound 1o**



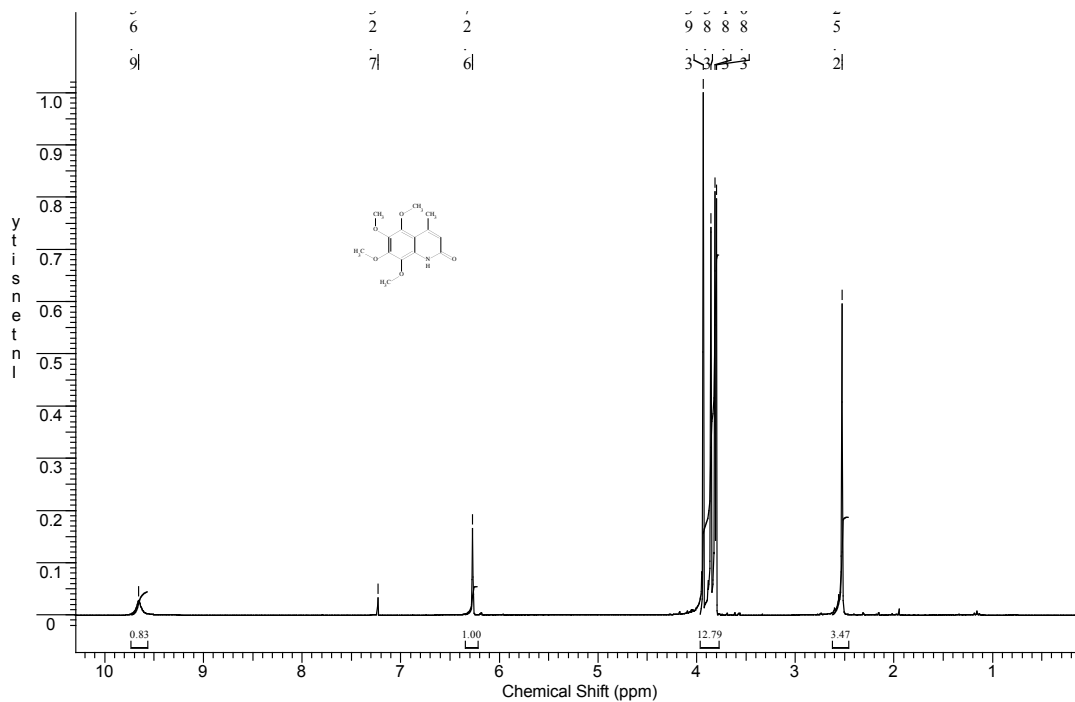
**<sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz) of Compound 1o**



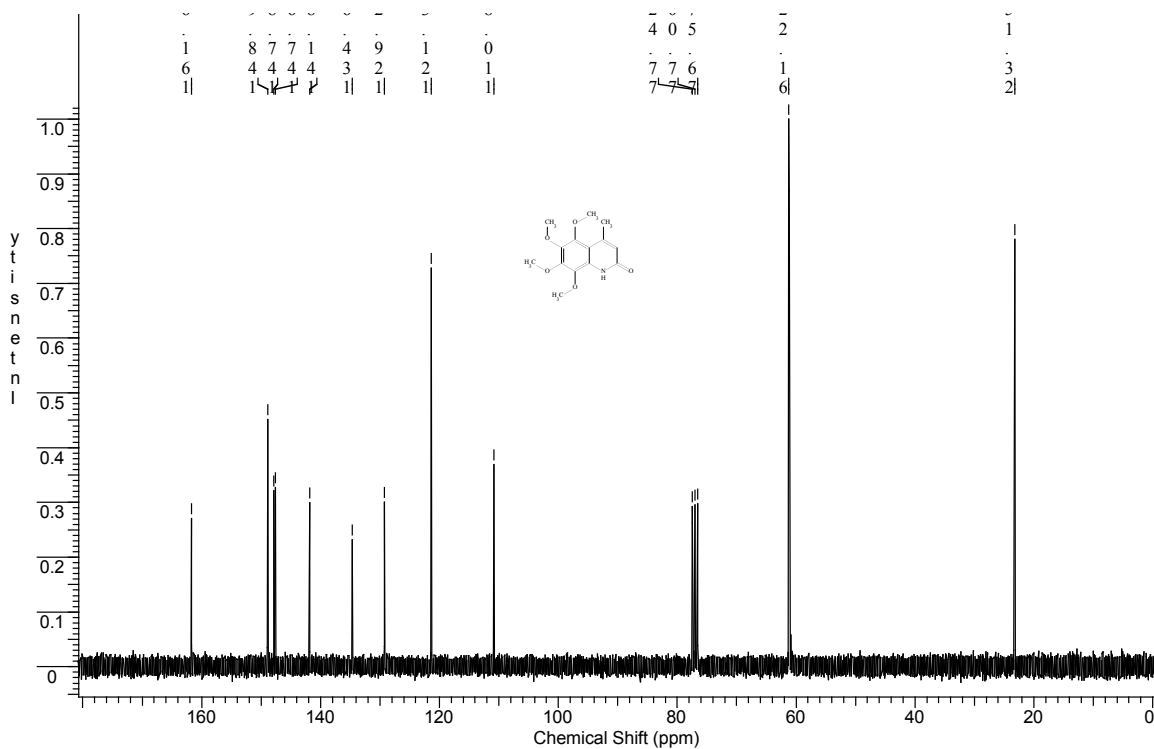
**<sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz) of Compound 1p**



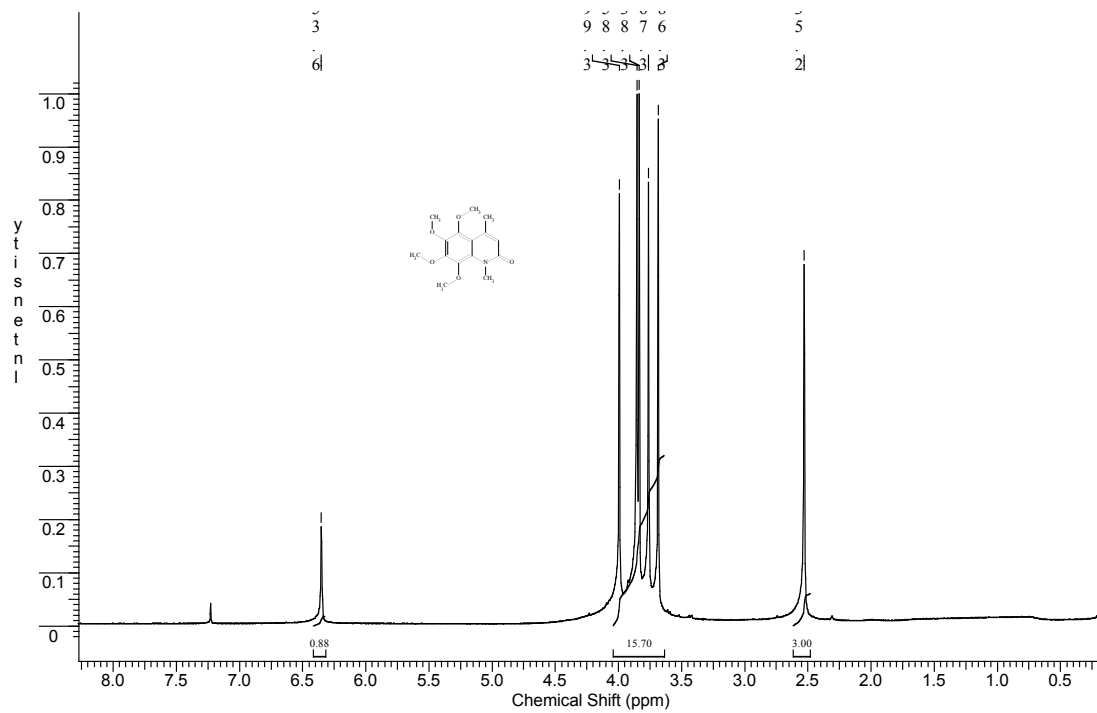
**<sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz) of Compound 1p**



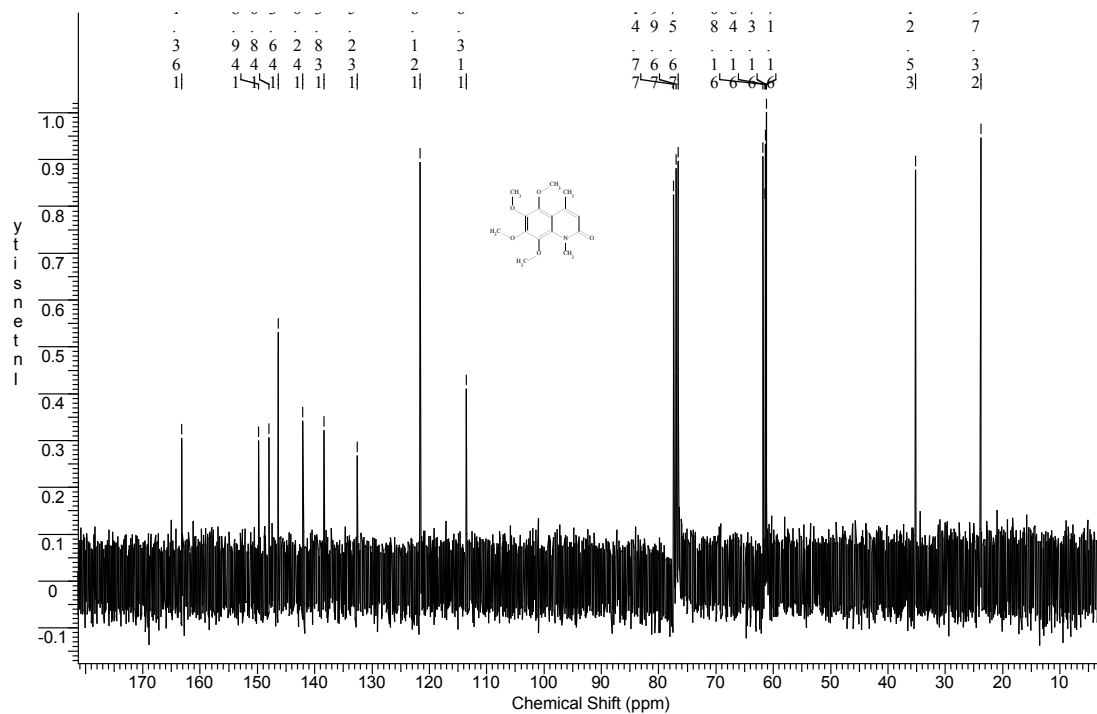
**<sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz) of Compound 1q**



**<sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz) of Compound 1q**

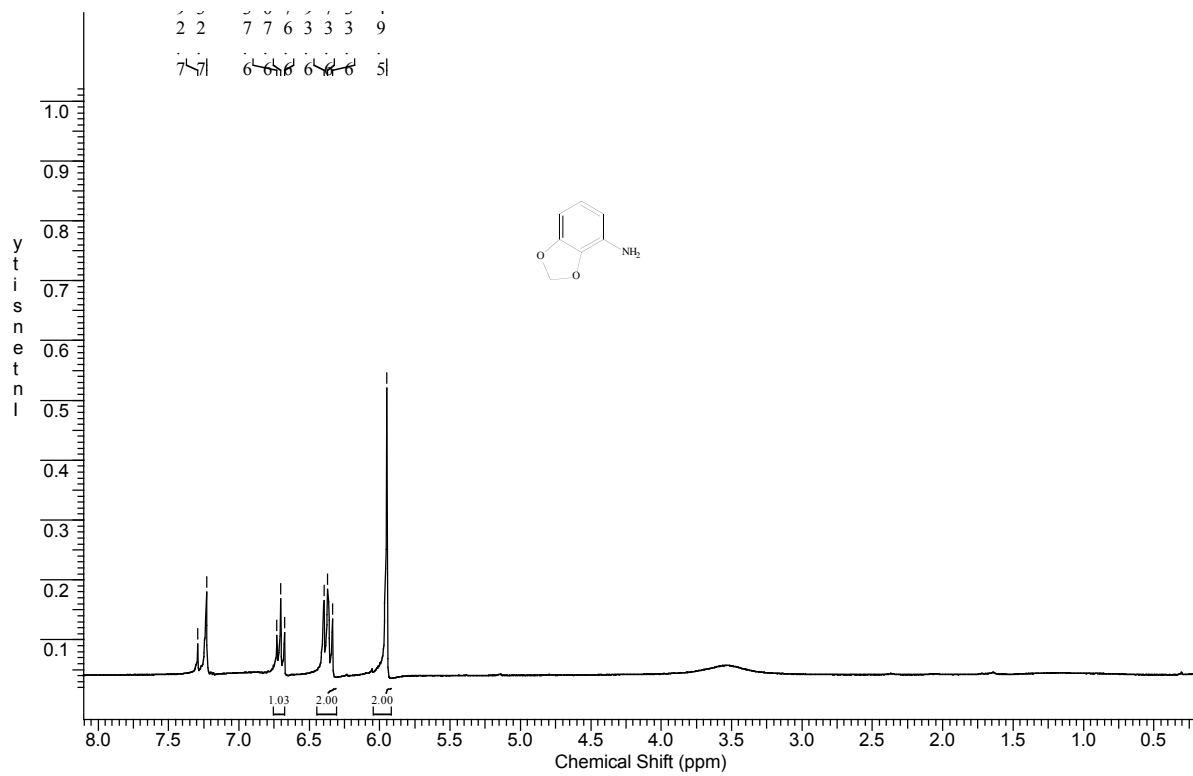


**<sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz) of Compound 1r**

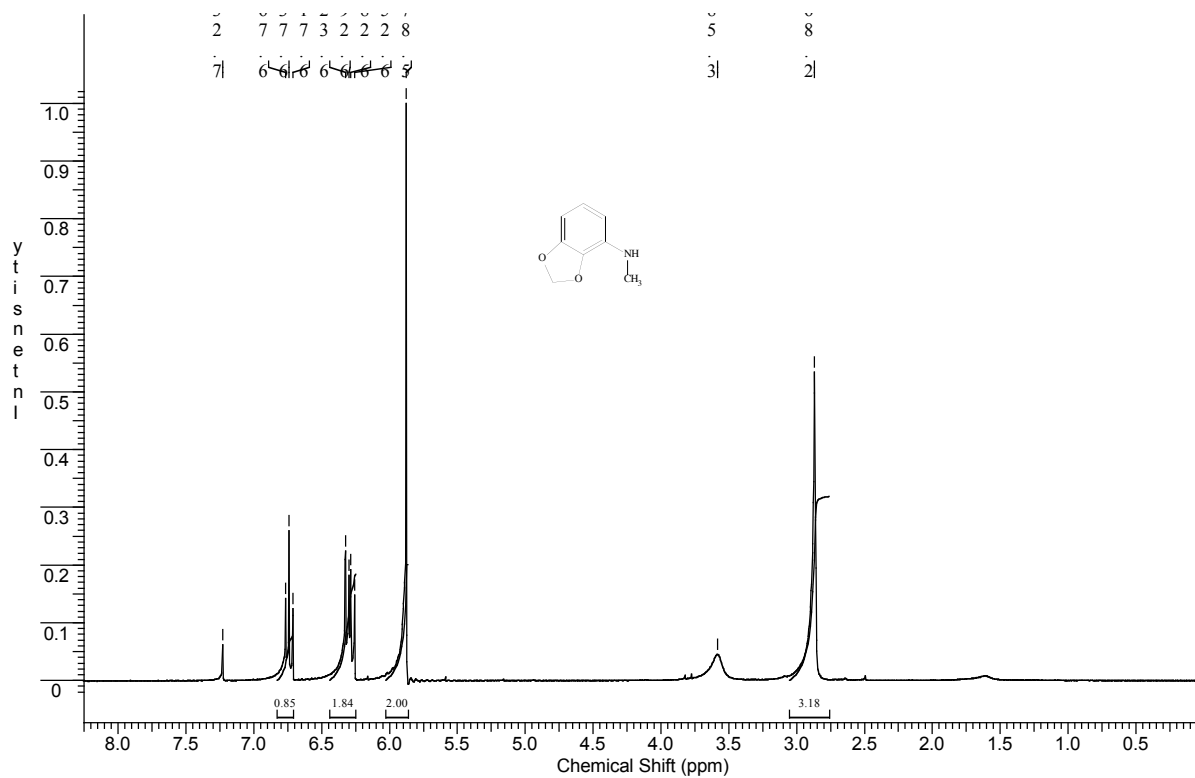


**<sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz) of Compound 1r**

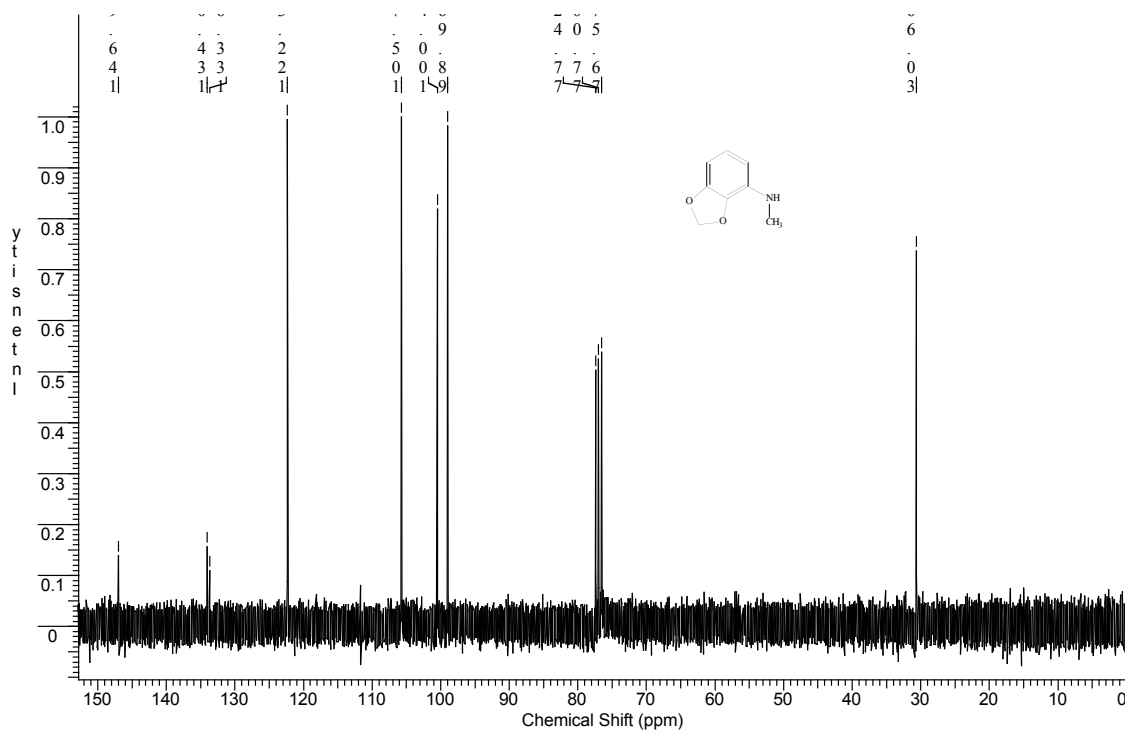




**$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300 MHz) of Compound 3a**

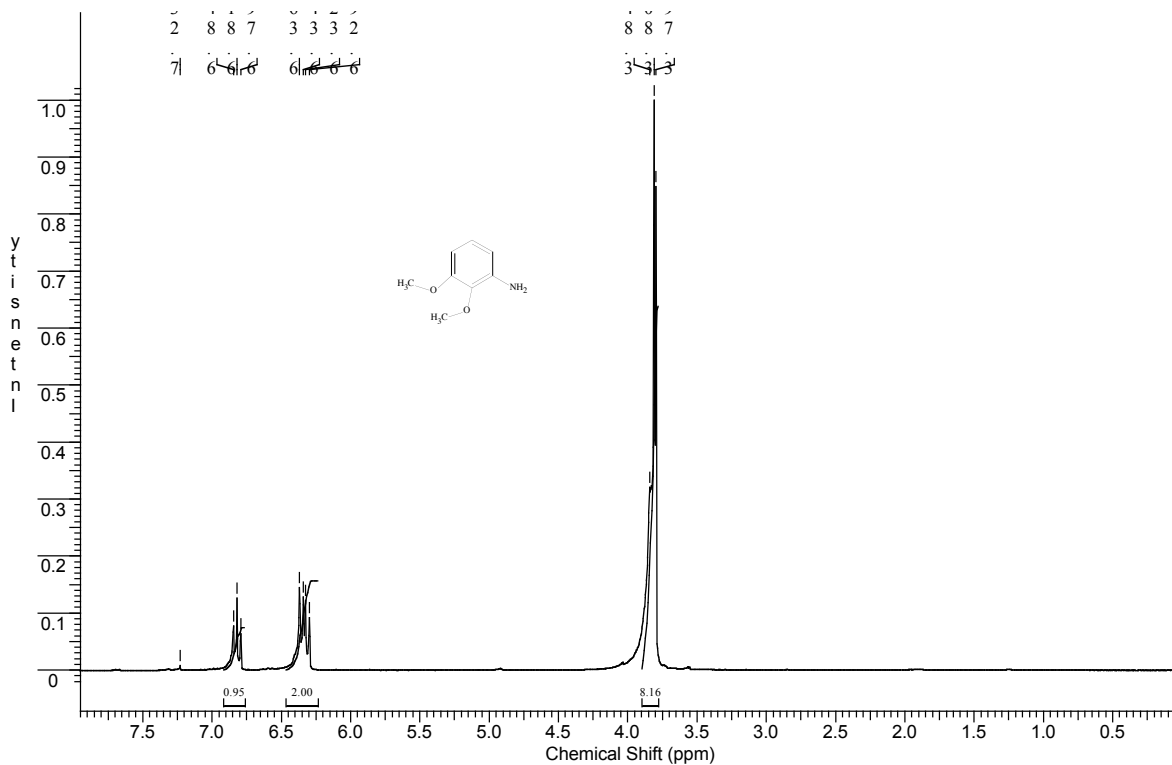


**<sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz) of Compound 3b**

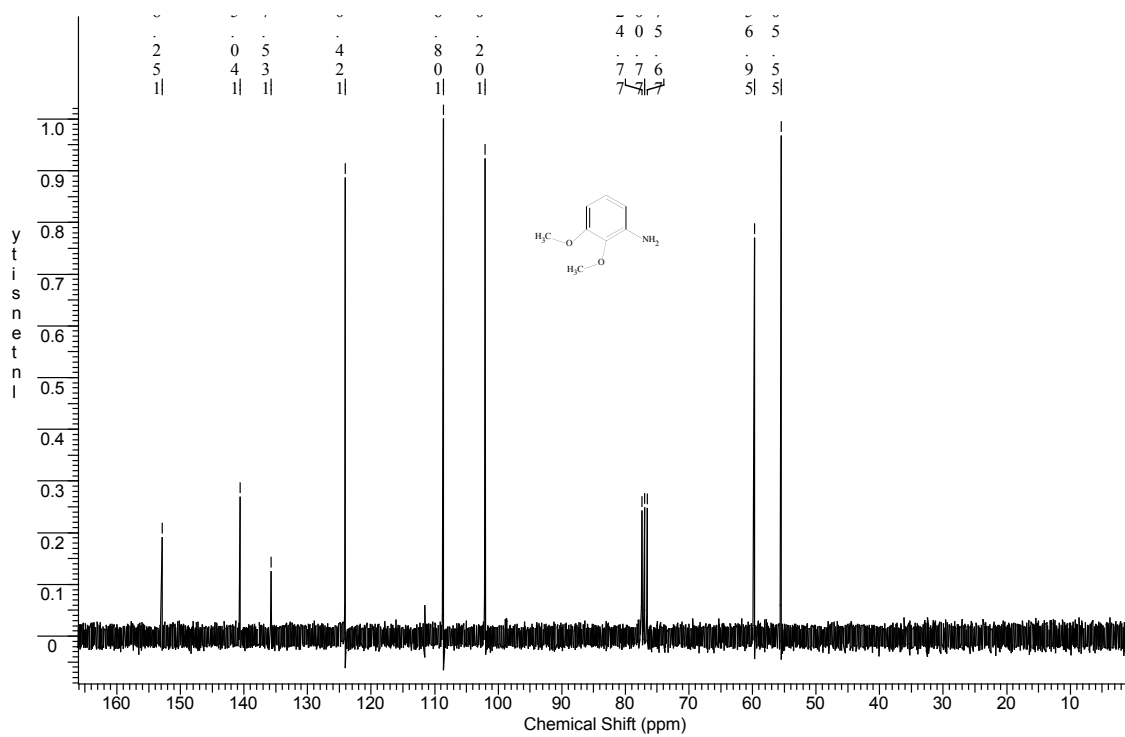


**<sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz) of Compound 3b**

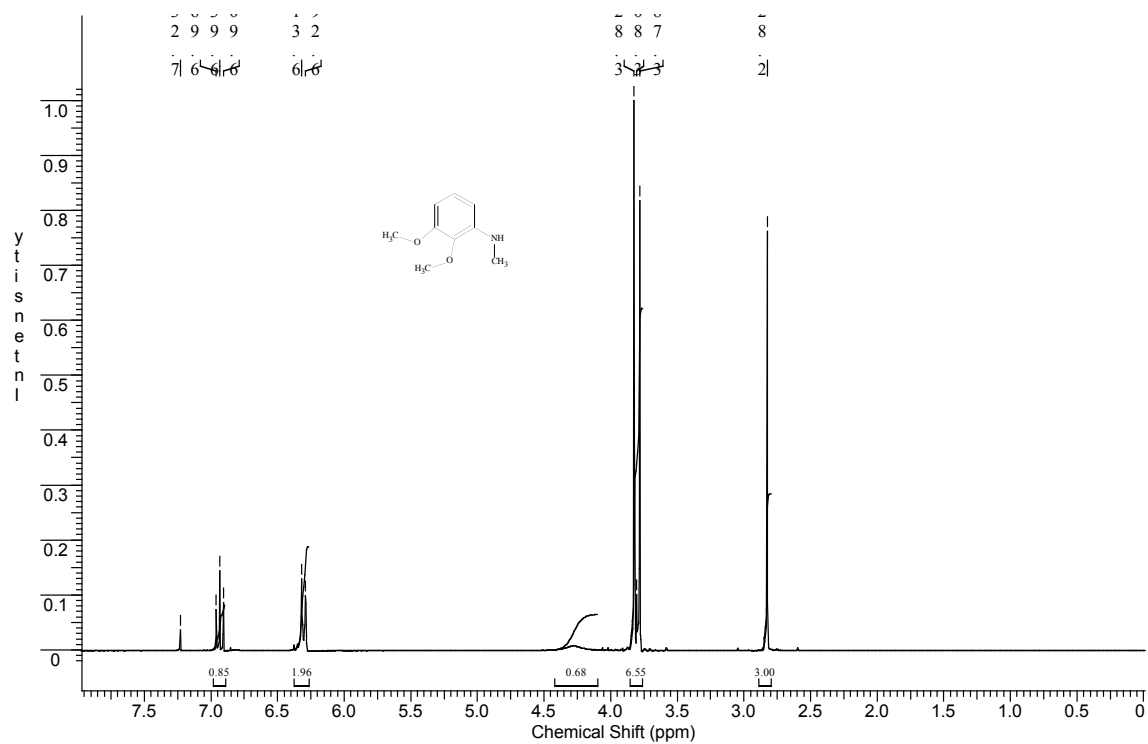




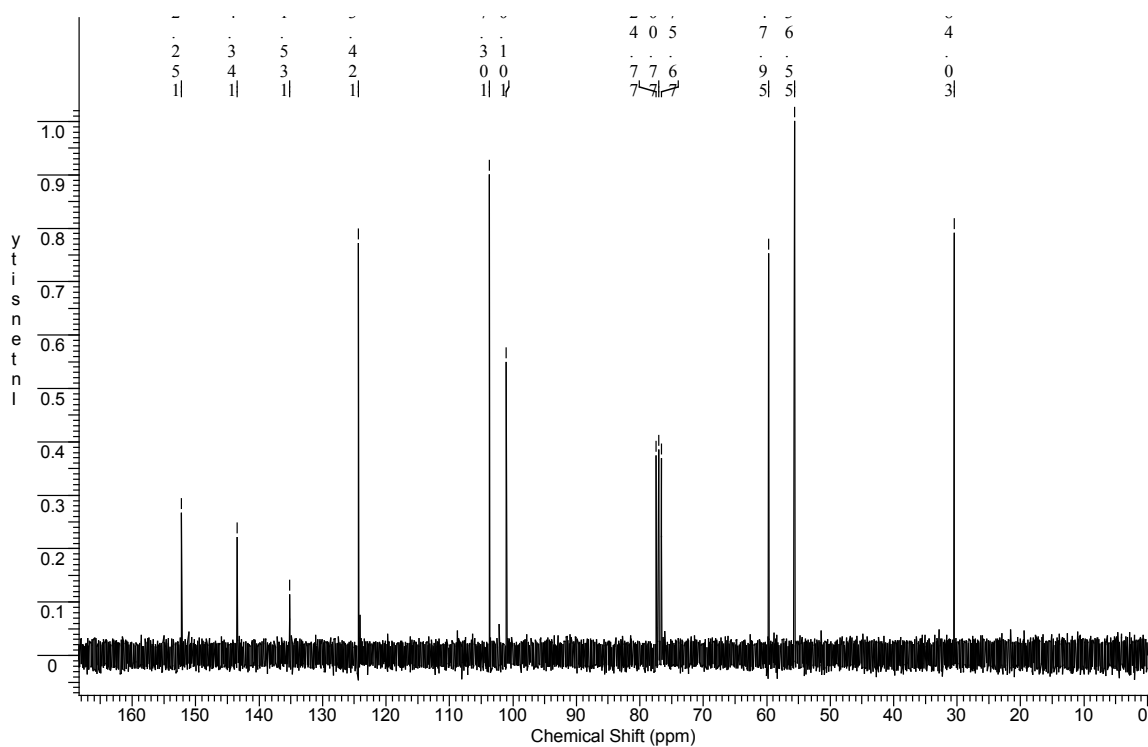
**<sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz) of Compound 3g**



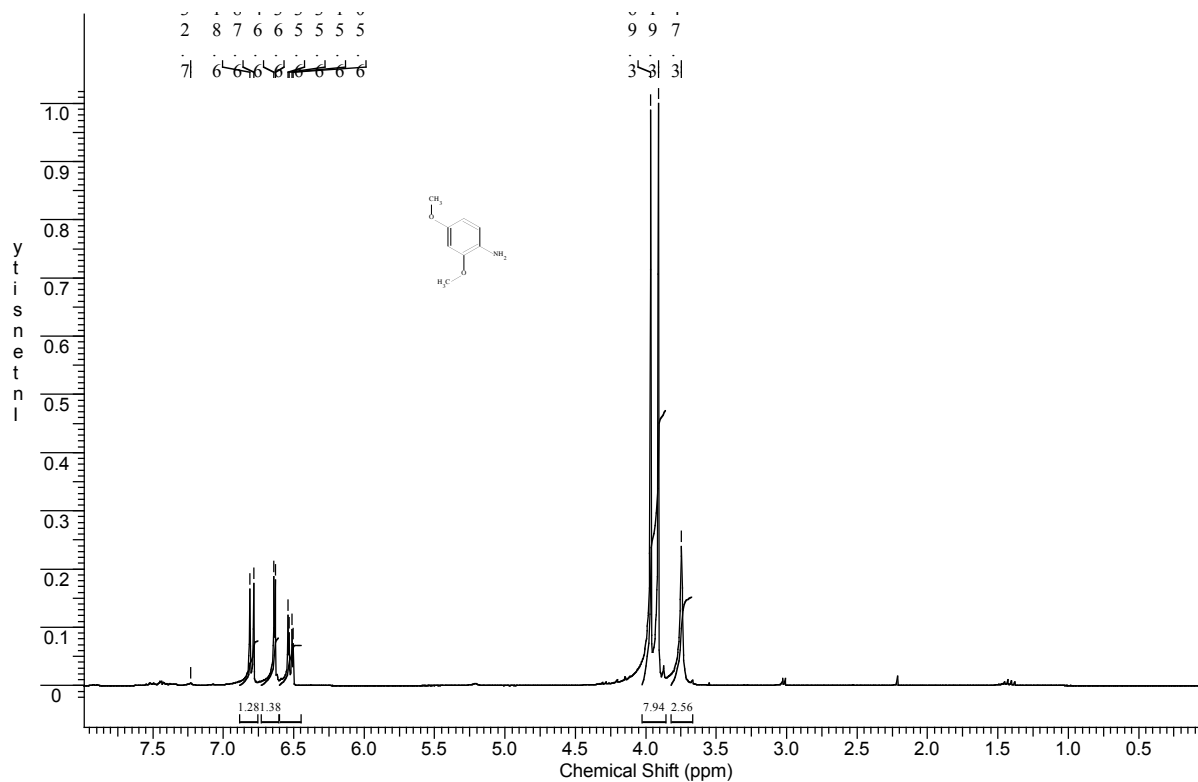
**<sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz) of Compound 3g**



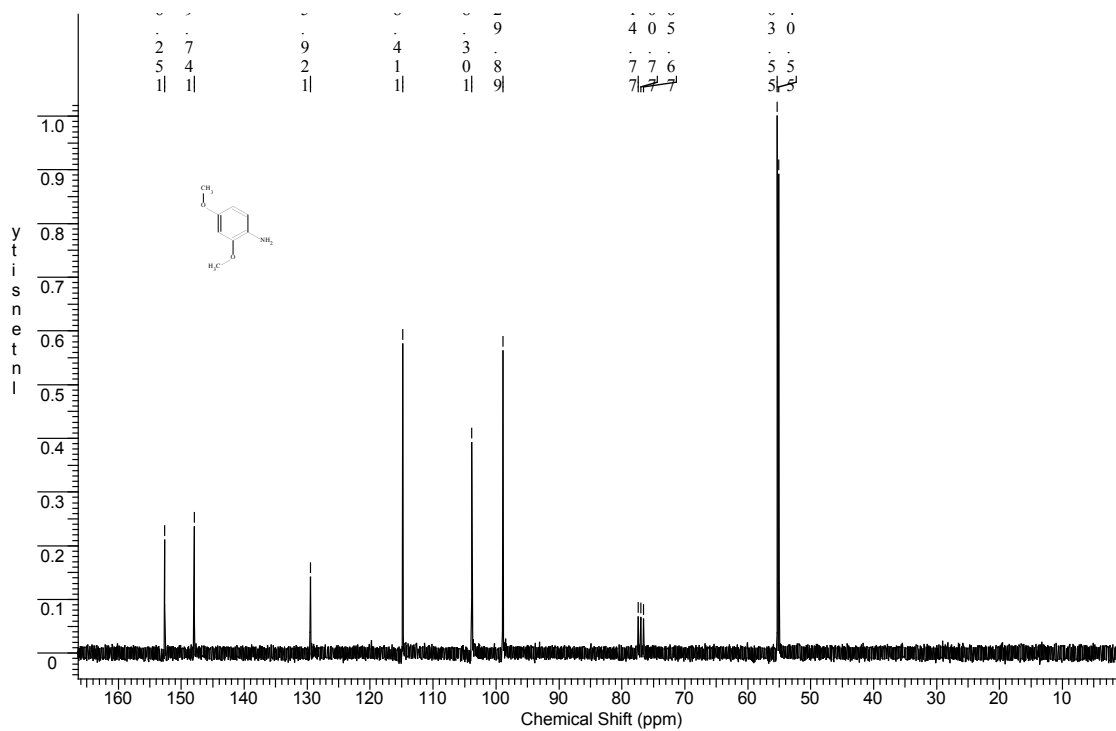
**<sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz) of Compound 3h**



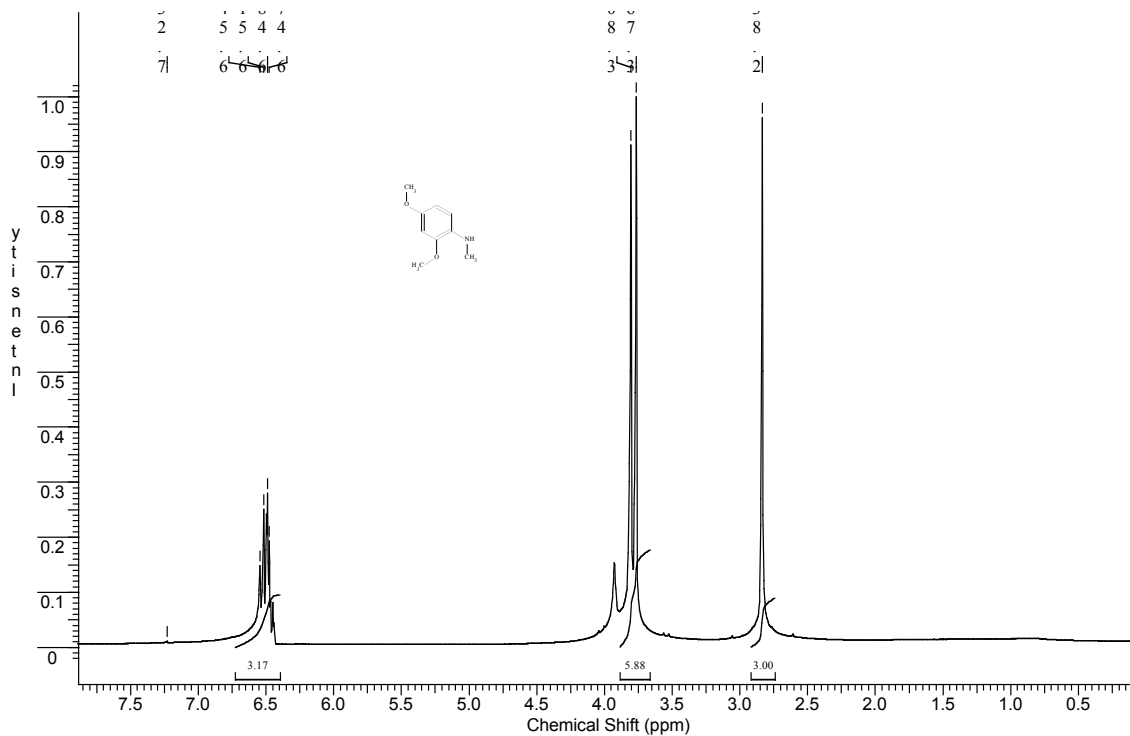
**<sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz) of Compound 3h**



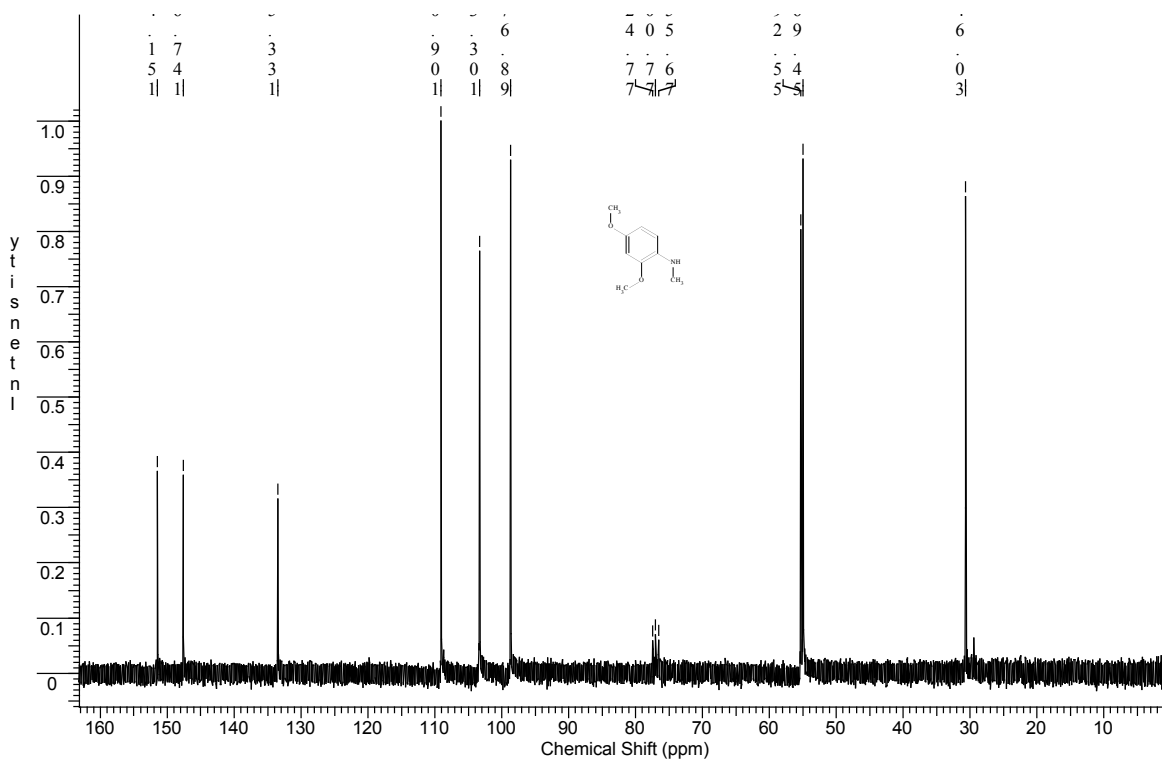
**<sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz) of Compound 3i**



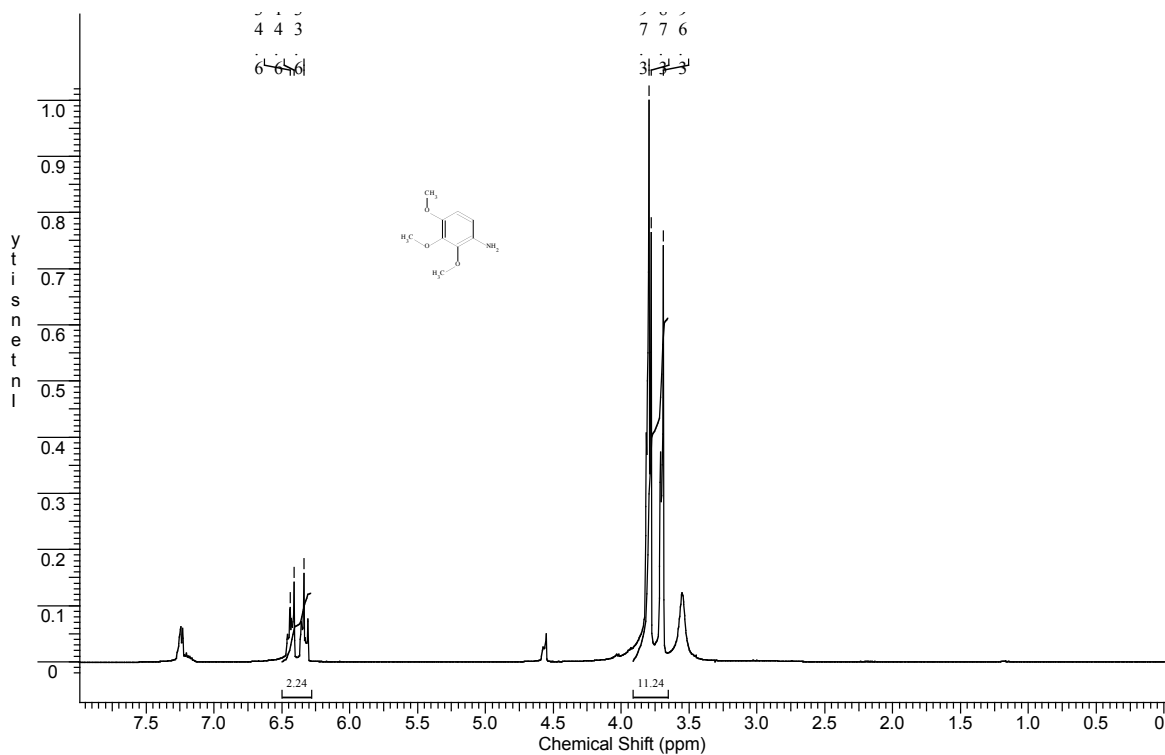
**<sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz) of Compound 3i**



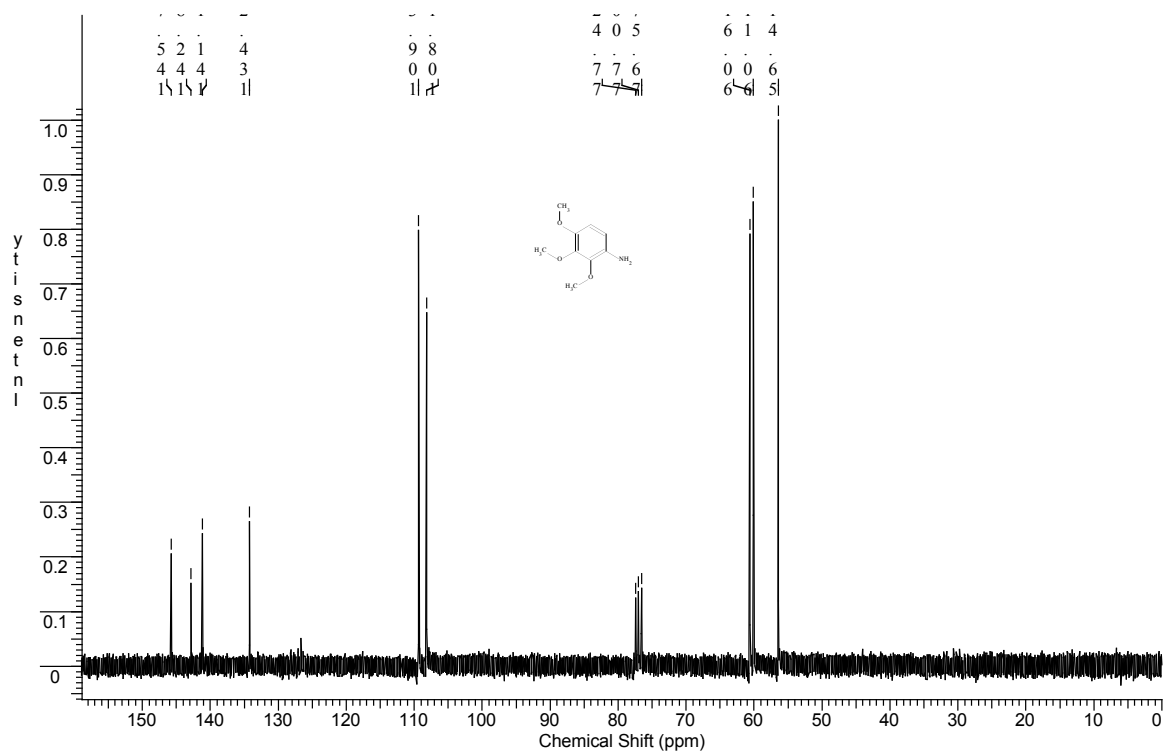
**<sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz) of Compound 3j**



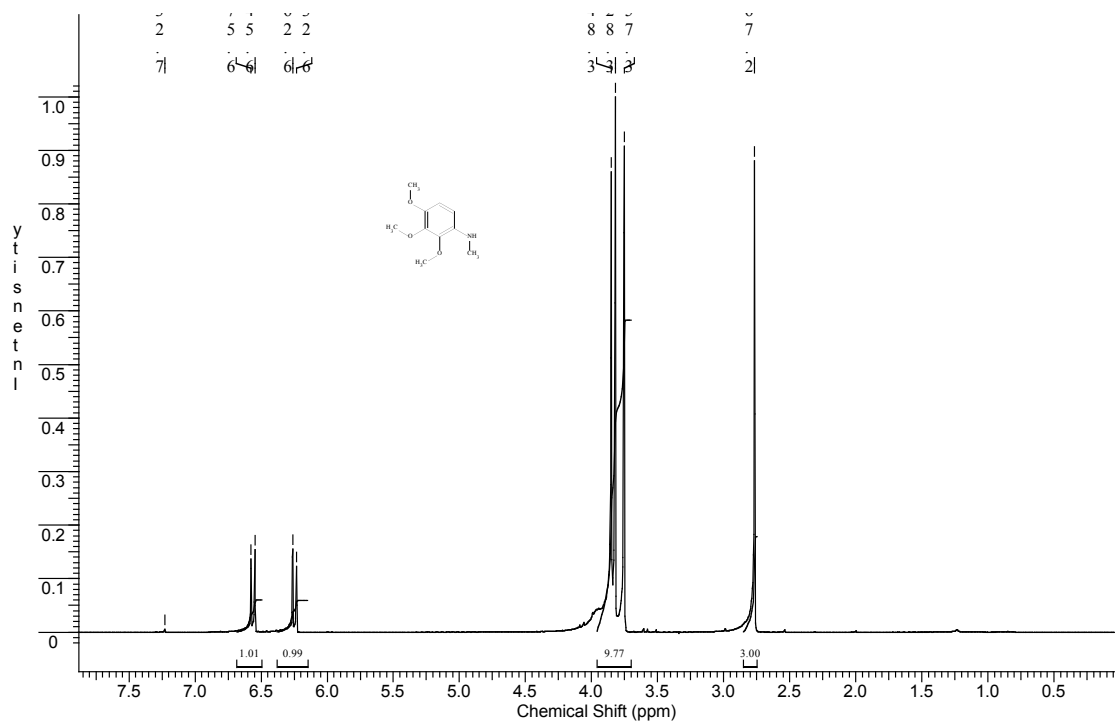
**<sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz) of Compound 3j**



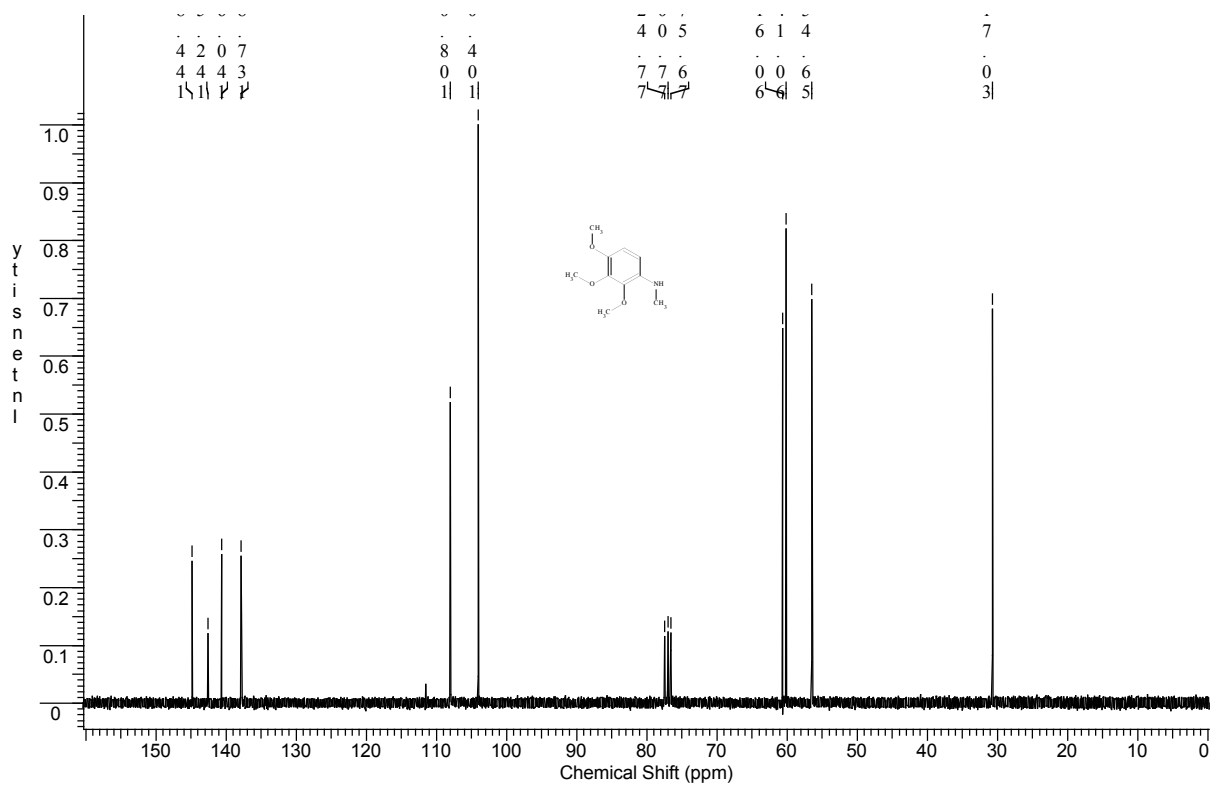
**<sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz) of Compound 3m**



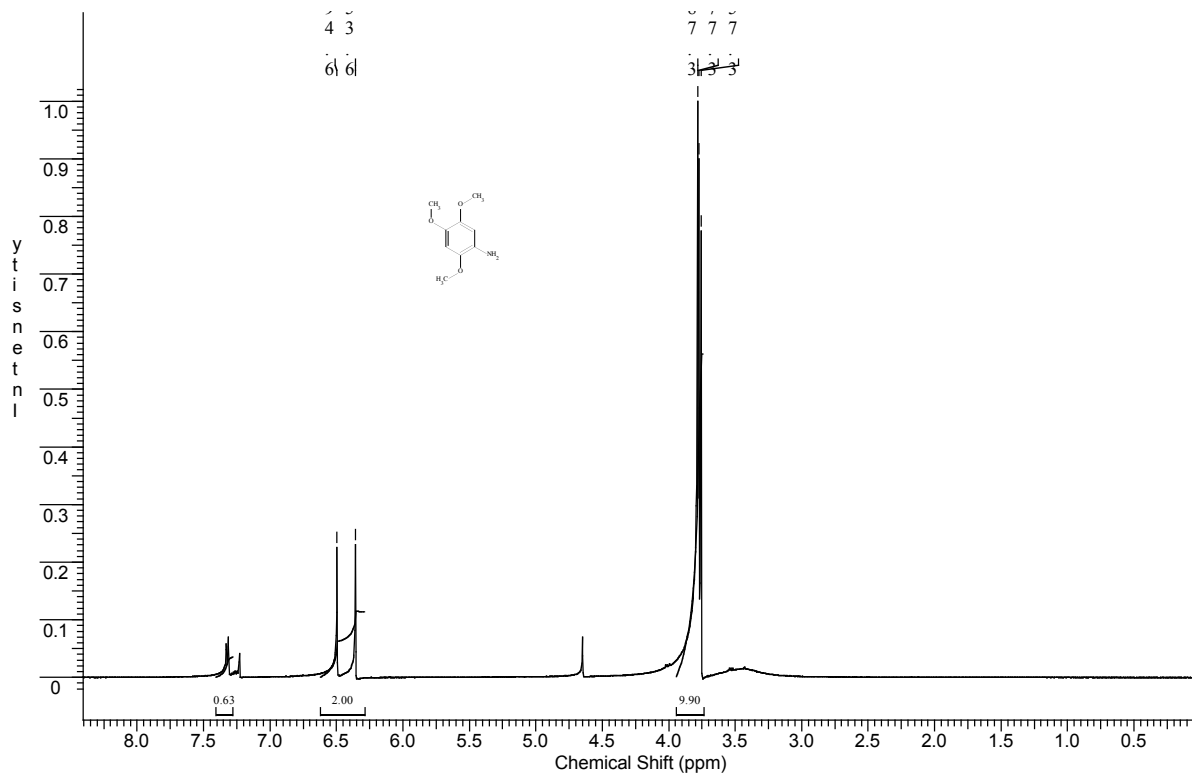
**<sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz) of Compound 3m**



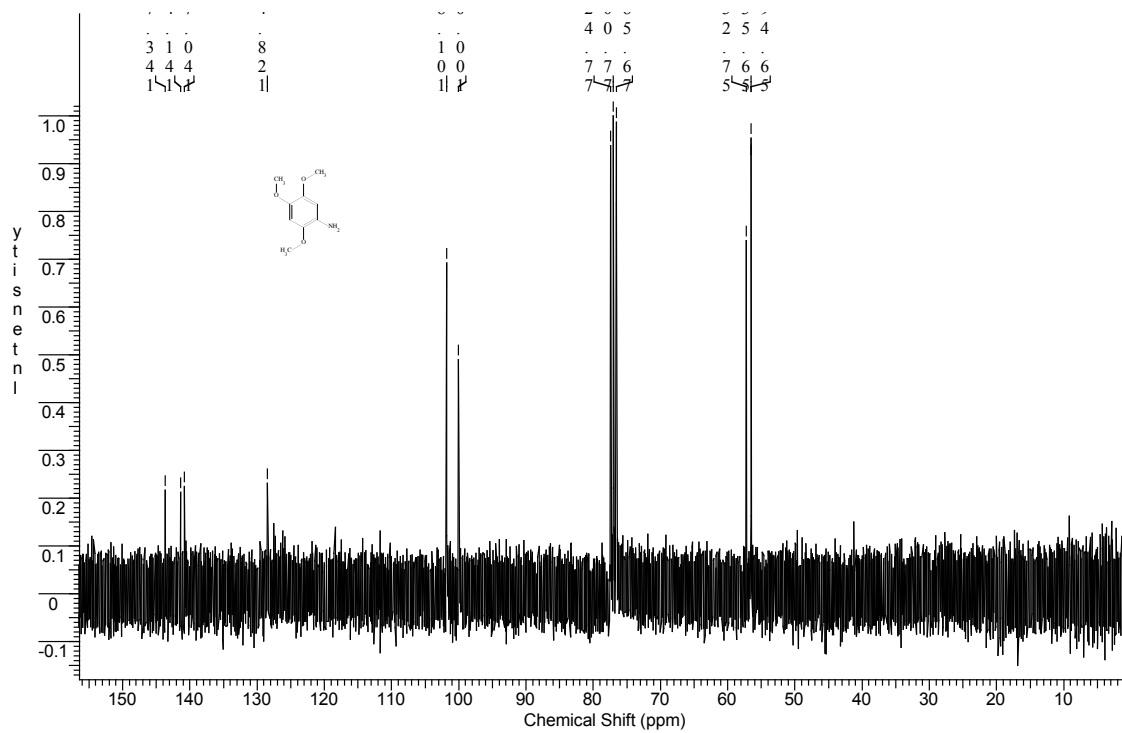
**<sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz) of Compound 3n**



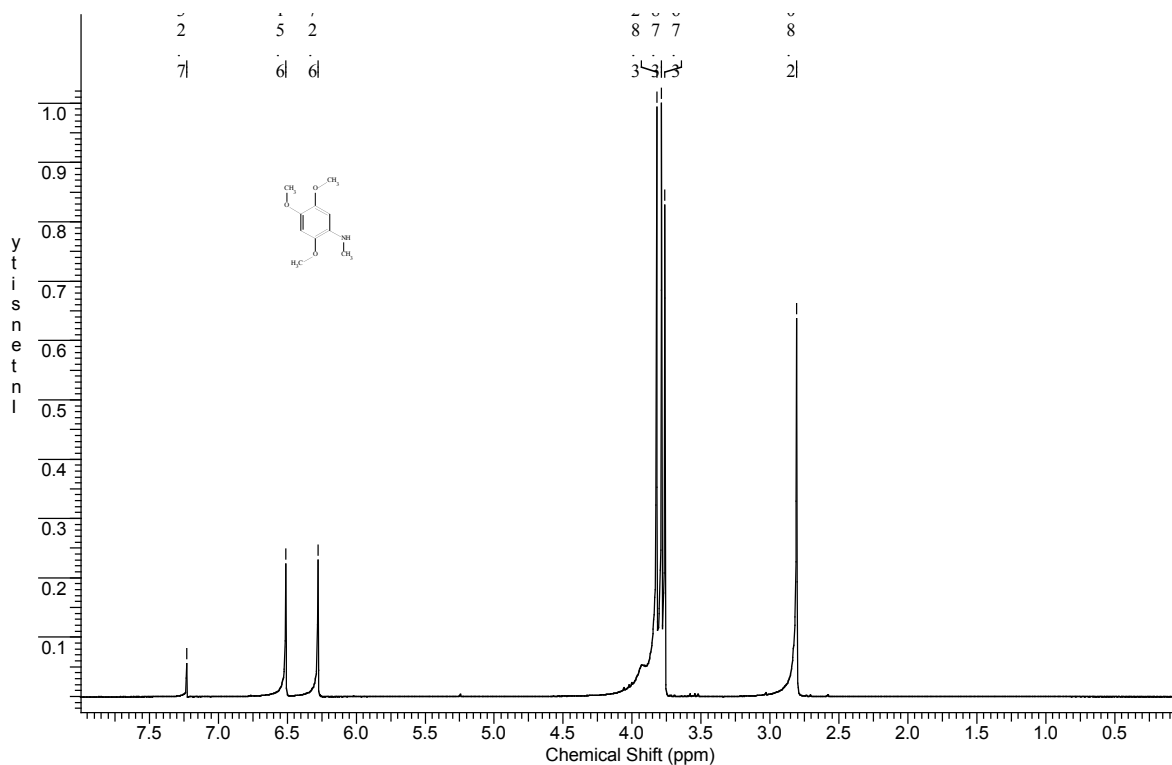
**<sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz) of Compound 3n**



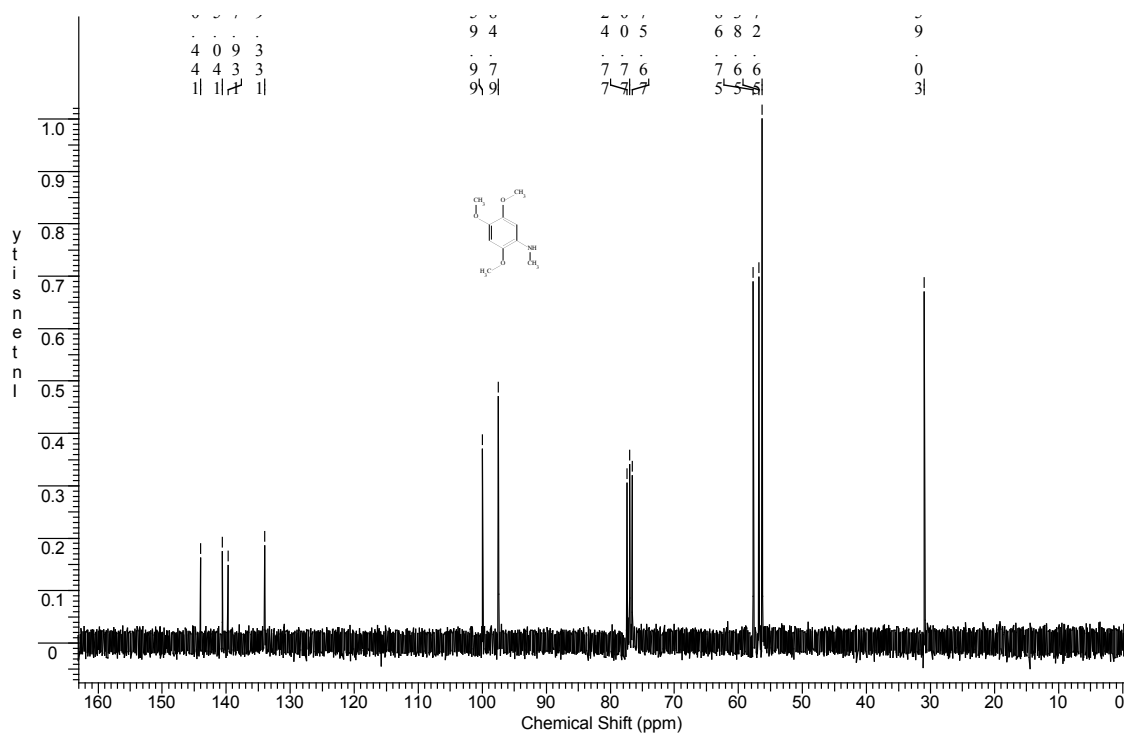
**<sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz) of Compound 3o**



**<sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz) of Compound 3o**

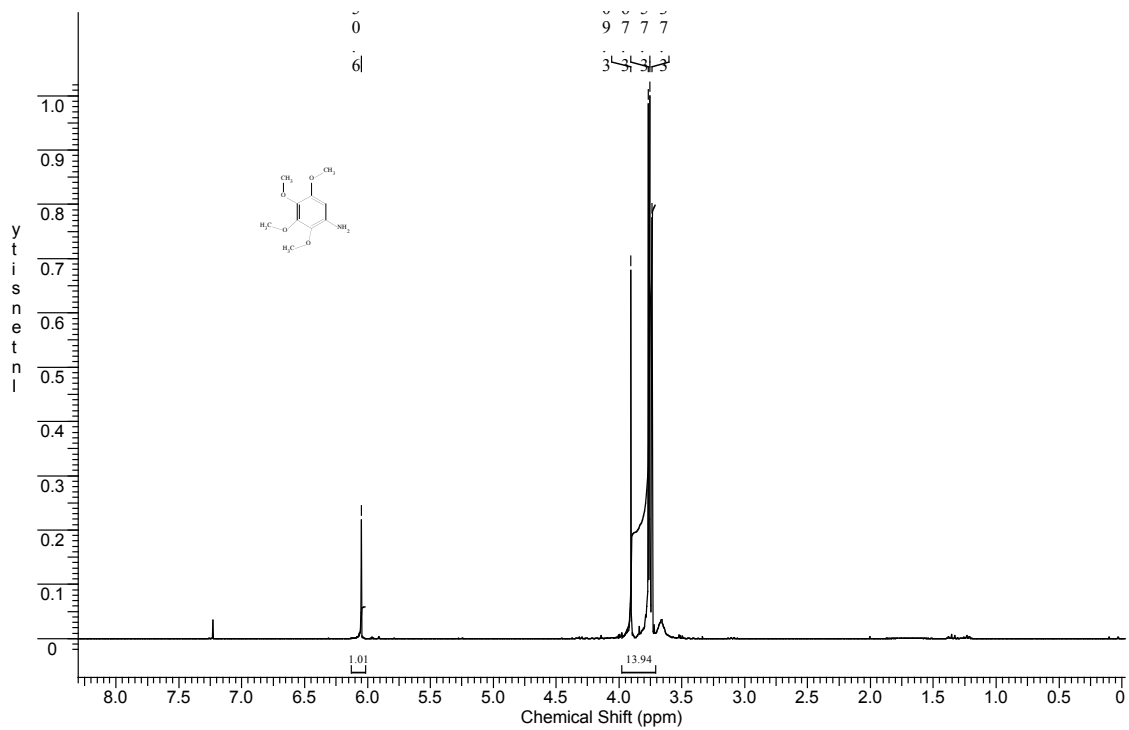


**<sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz) of Compound 3p**

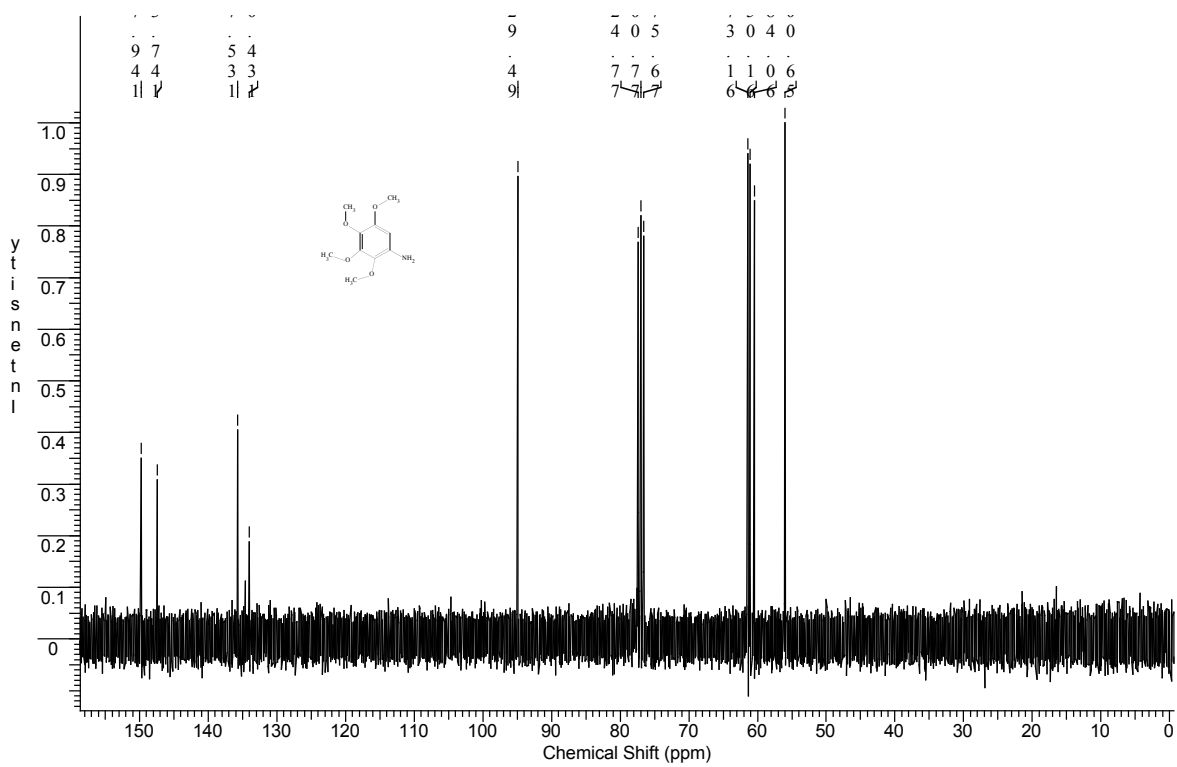


**<sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz) of Compound 3p**

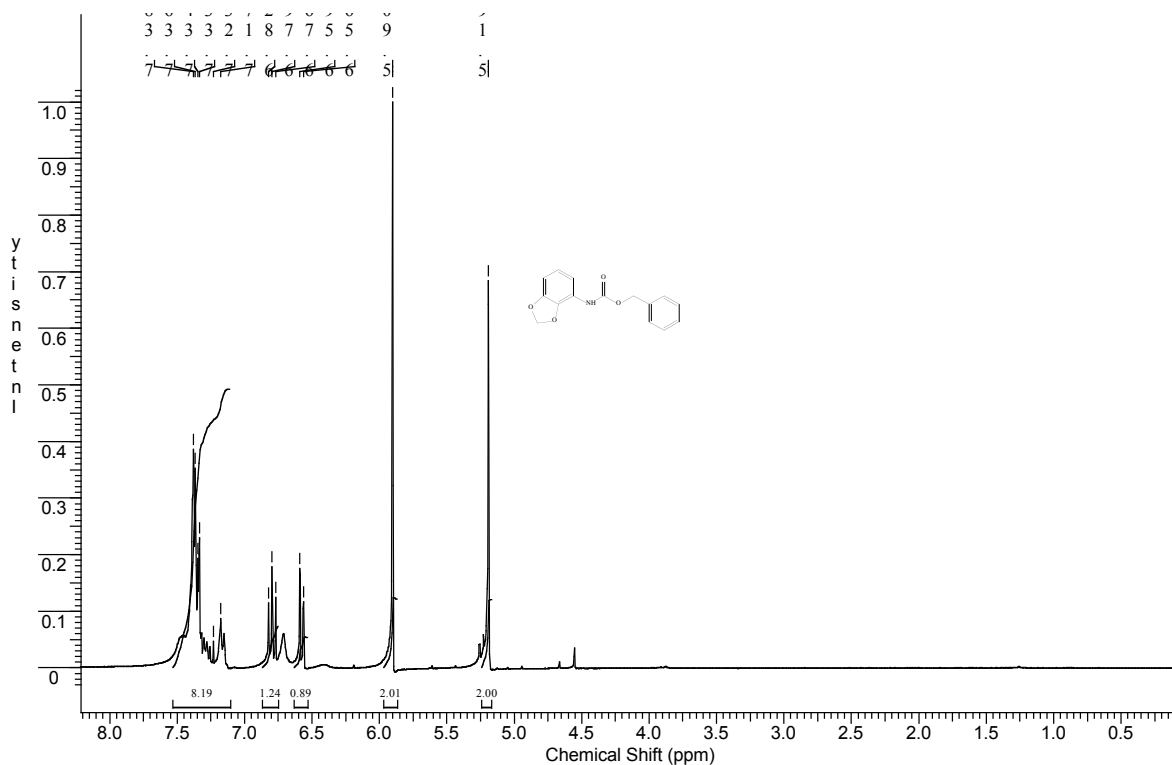




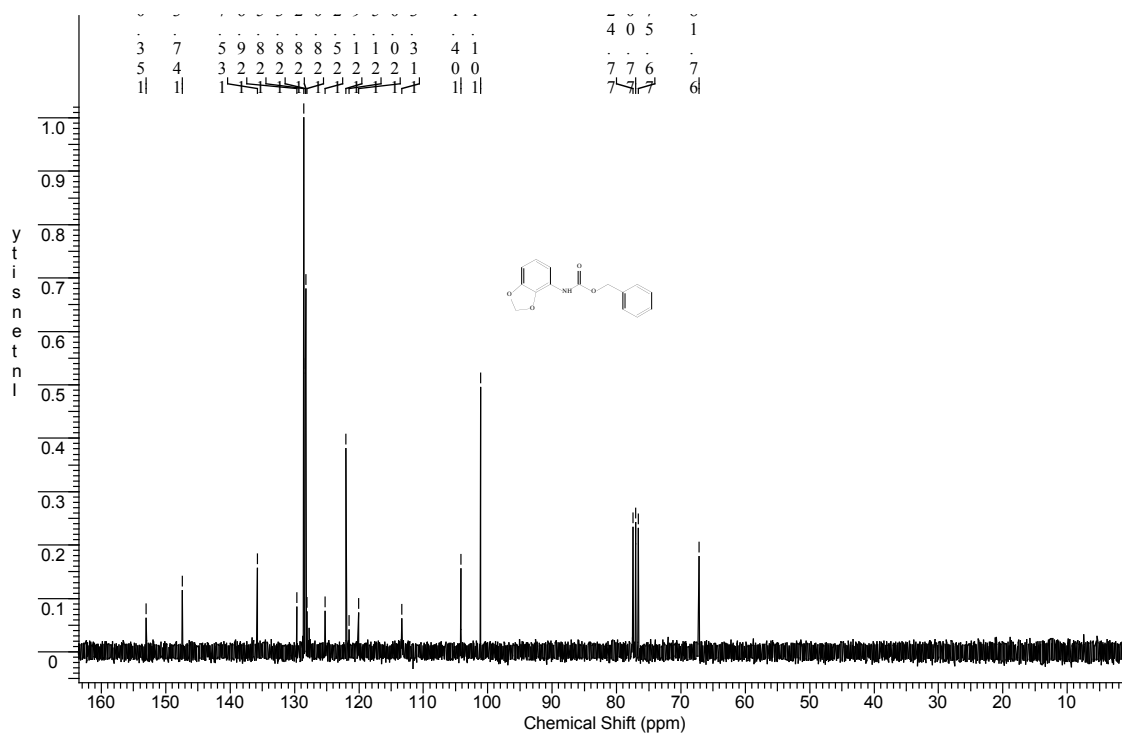
**<sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz) of Compound 3q**



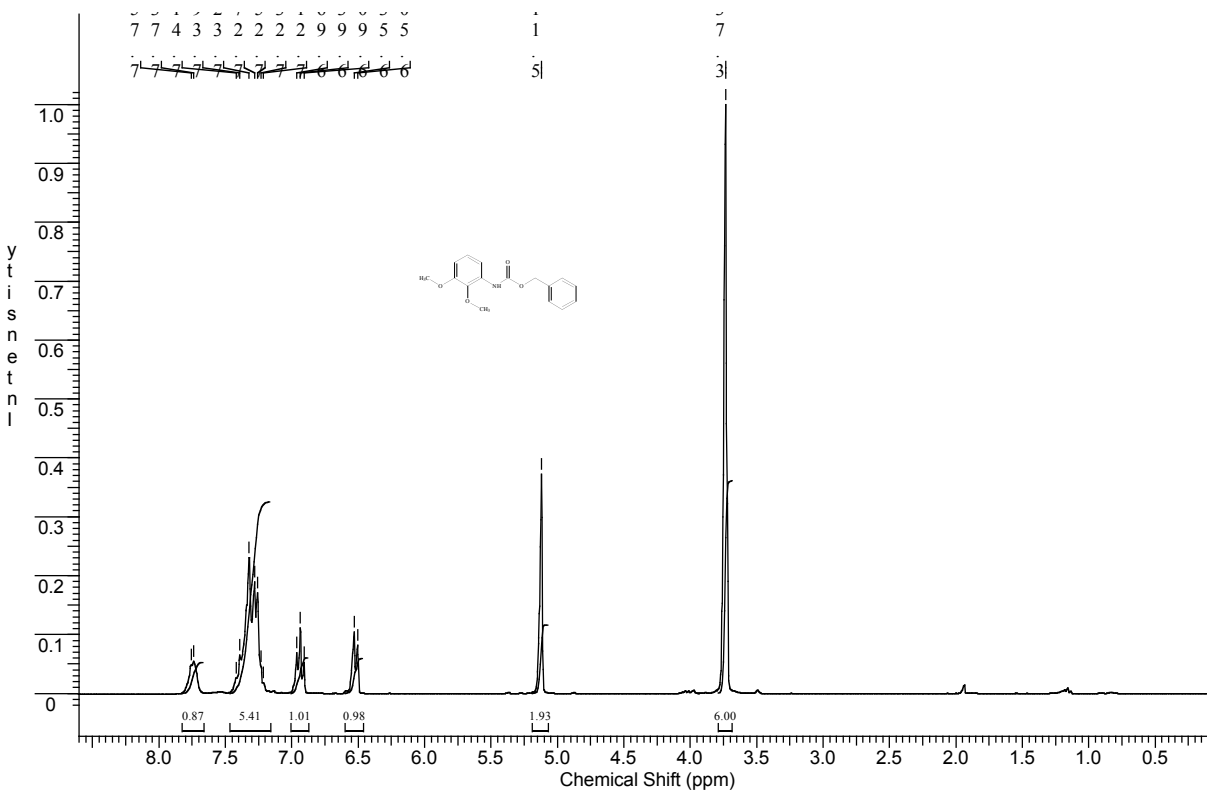
**<sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz) of Compound 3q**



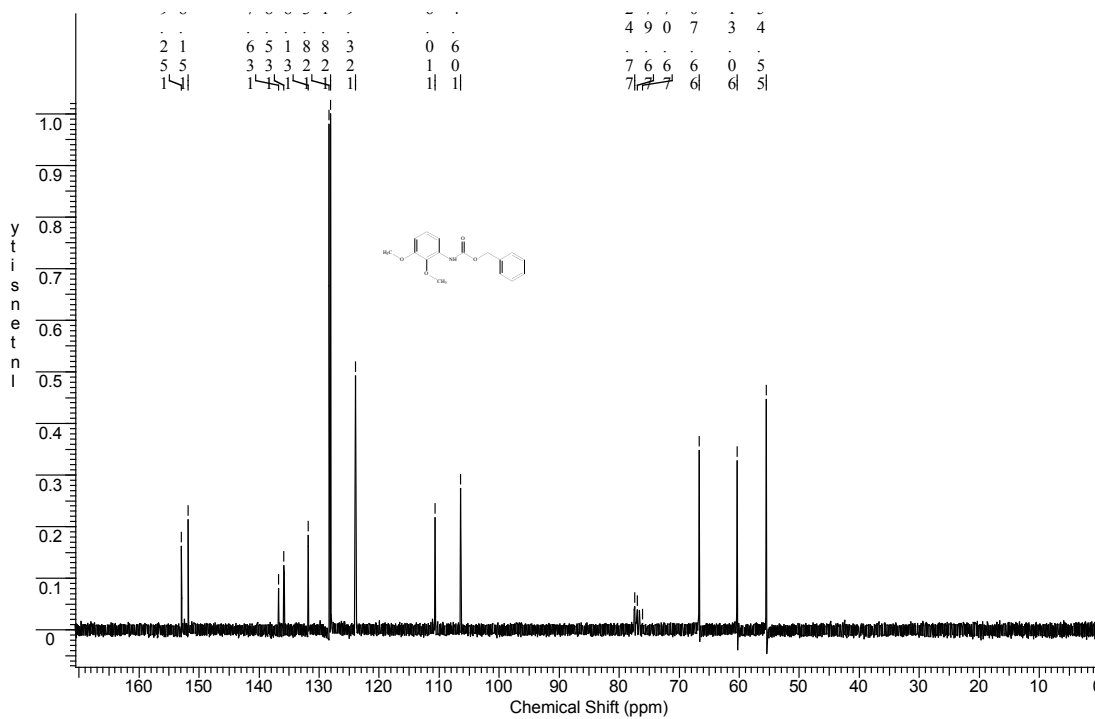
**<sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz) of Compound 6a**



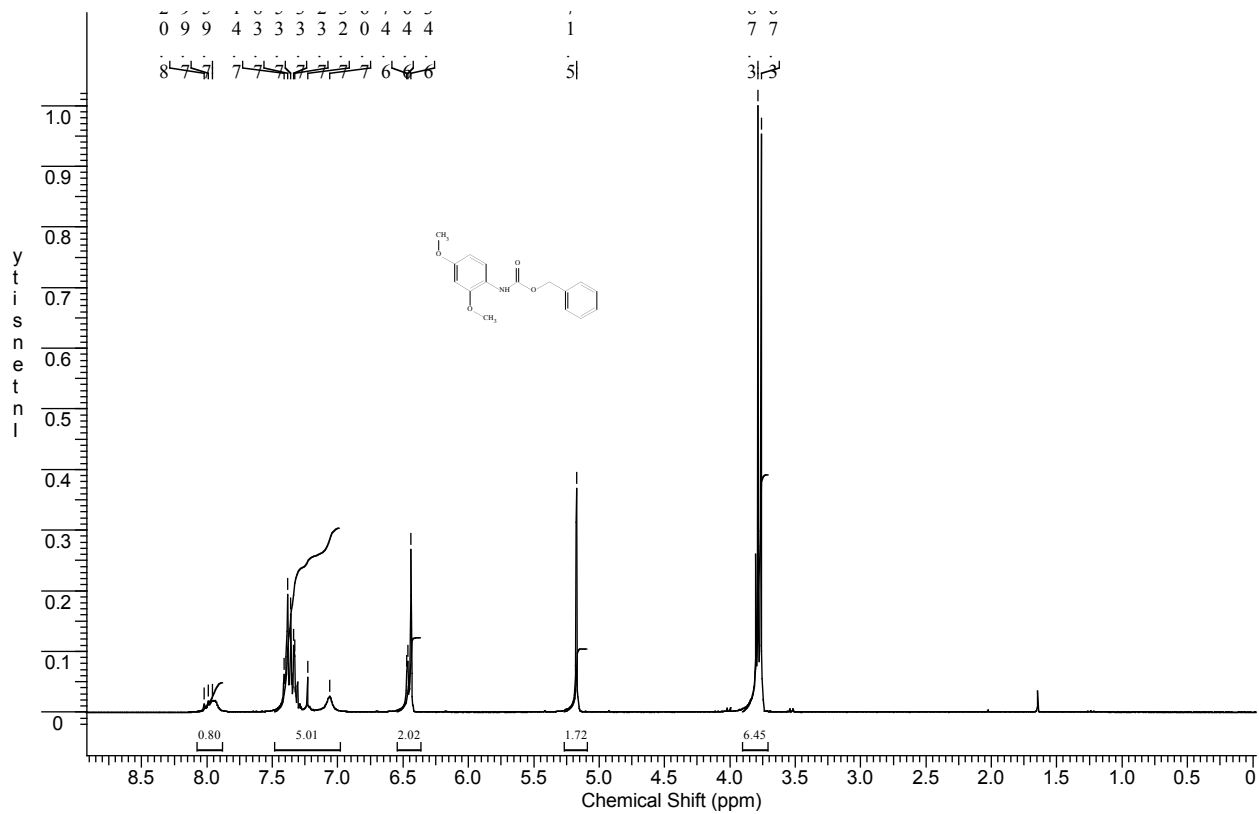
**<sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz) of Compound 6a**



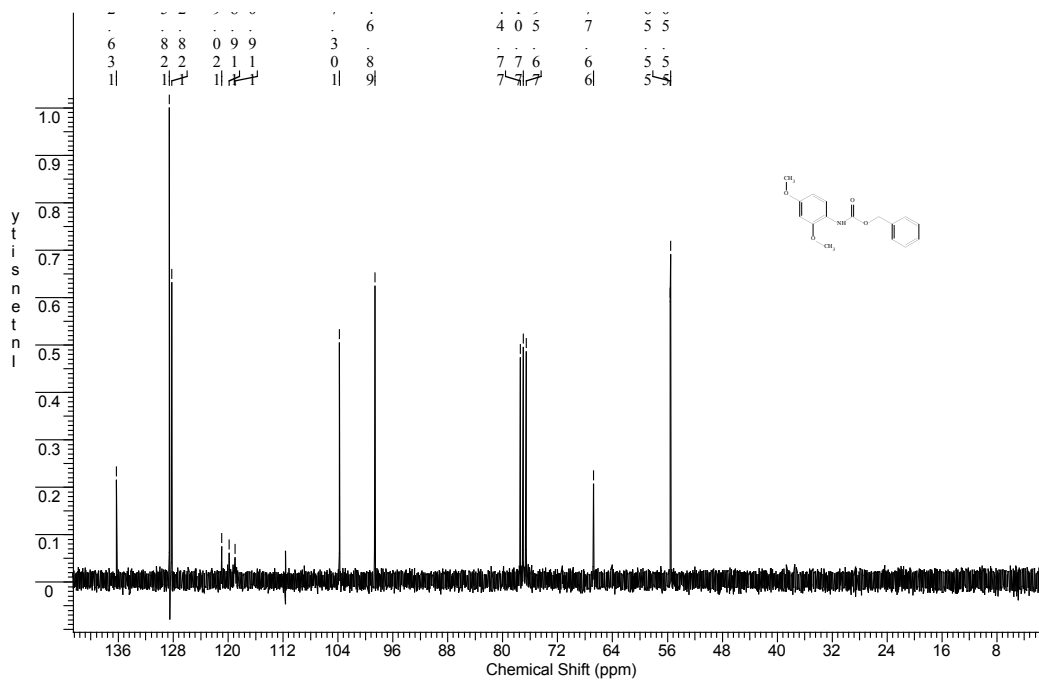
**<sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz) of Compound 6g**



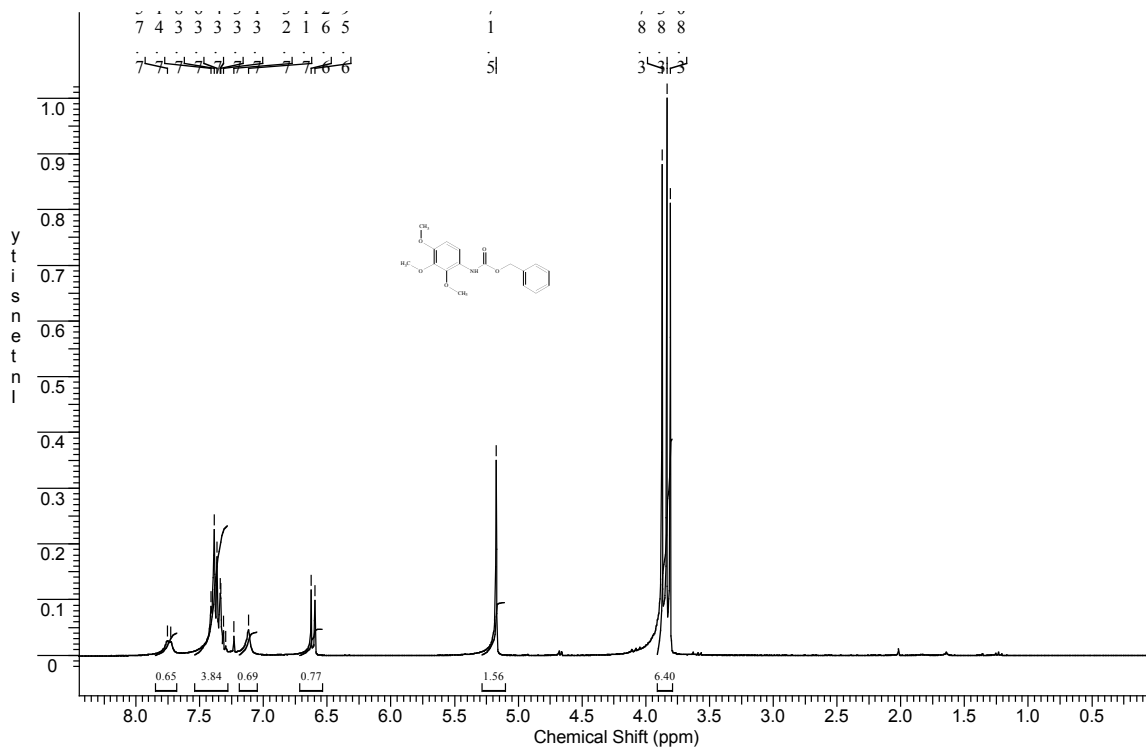
**<sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz) of Compound 6g**



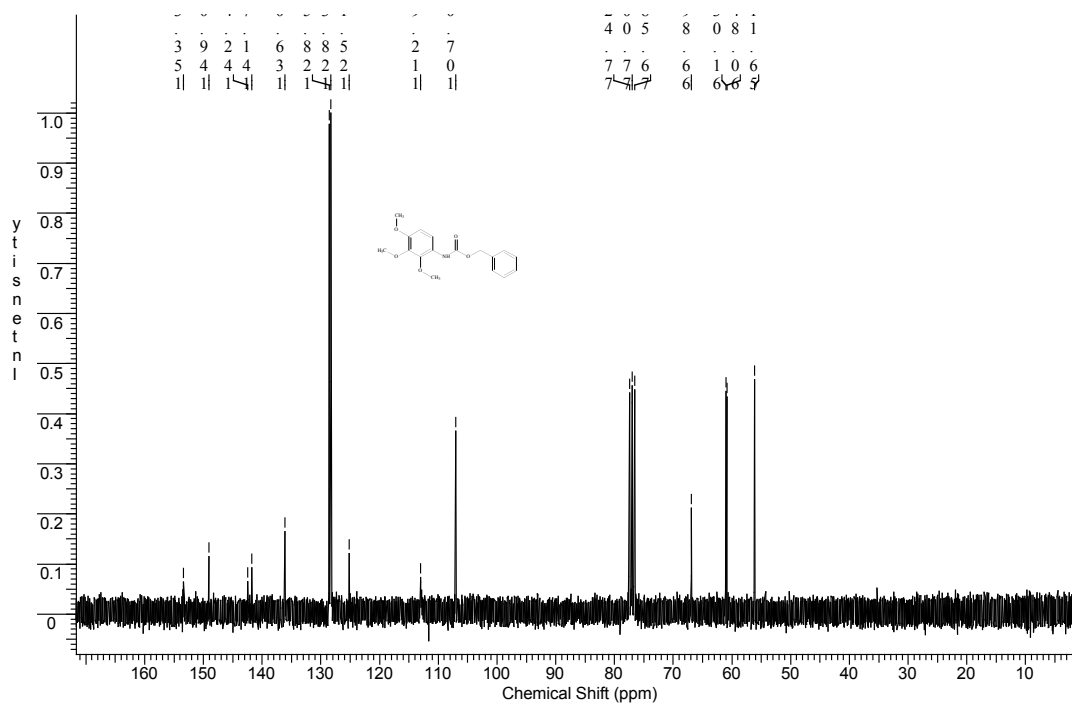
**<sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz) of Compound 6i**



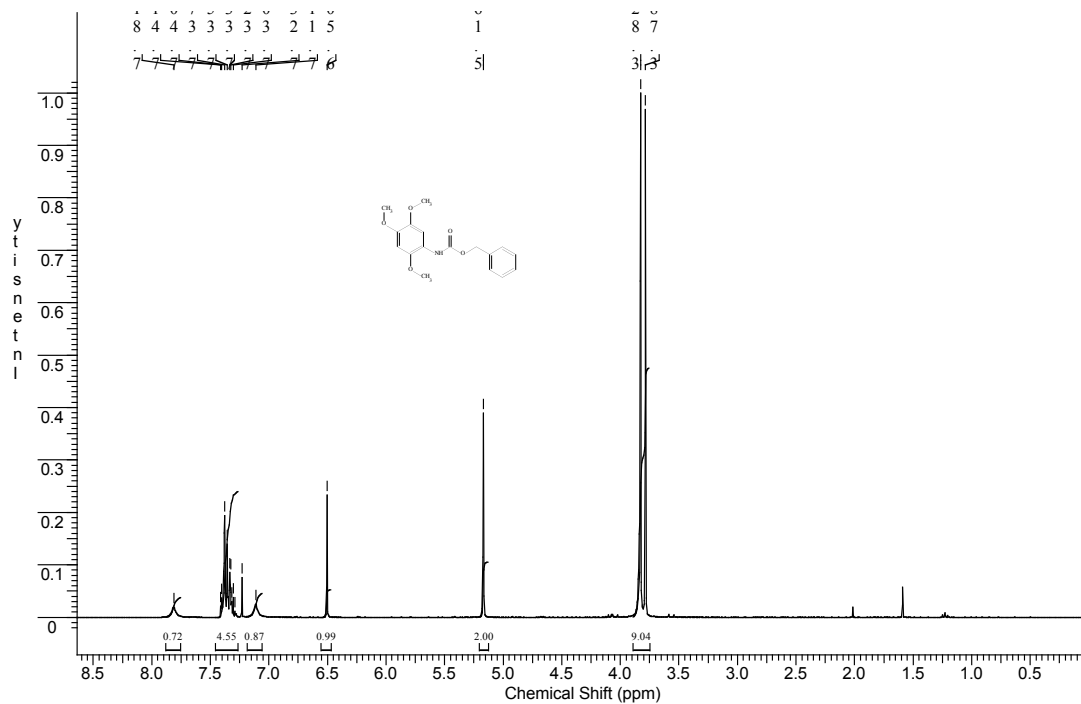
**<sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz) of Compound 6i**



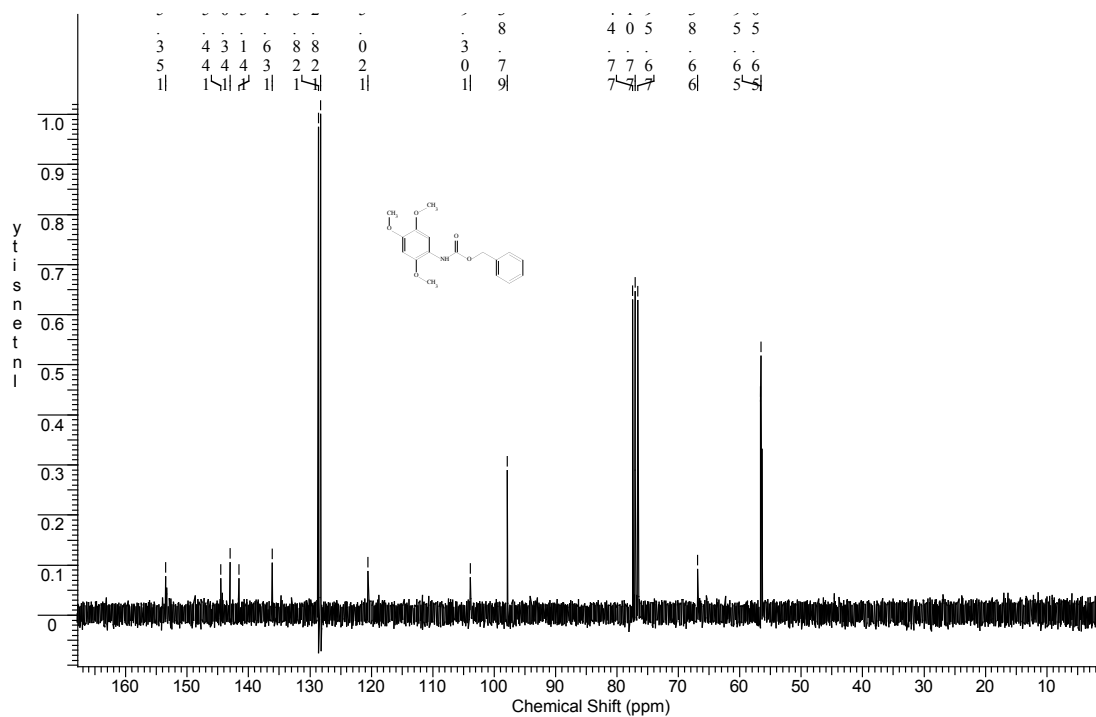
**<sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz) of Compound 6m**



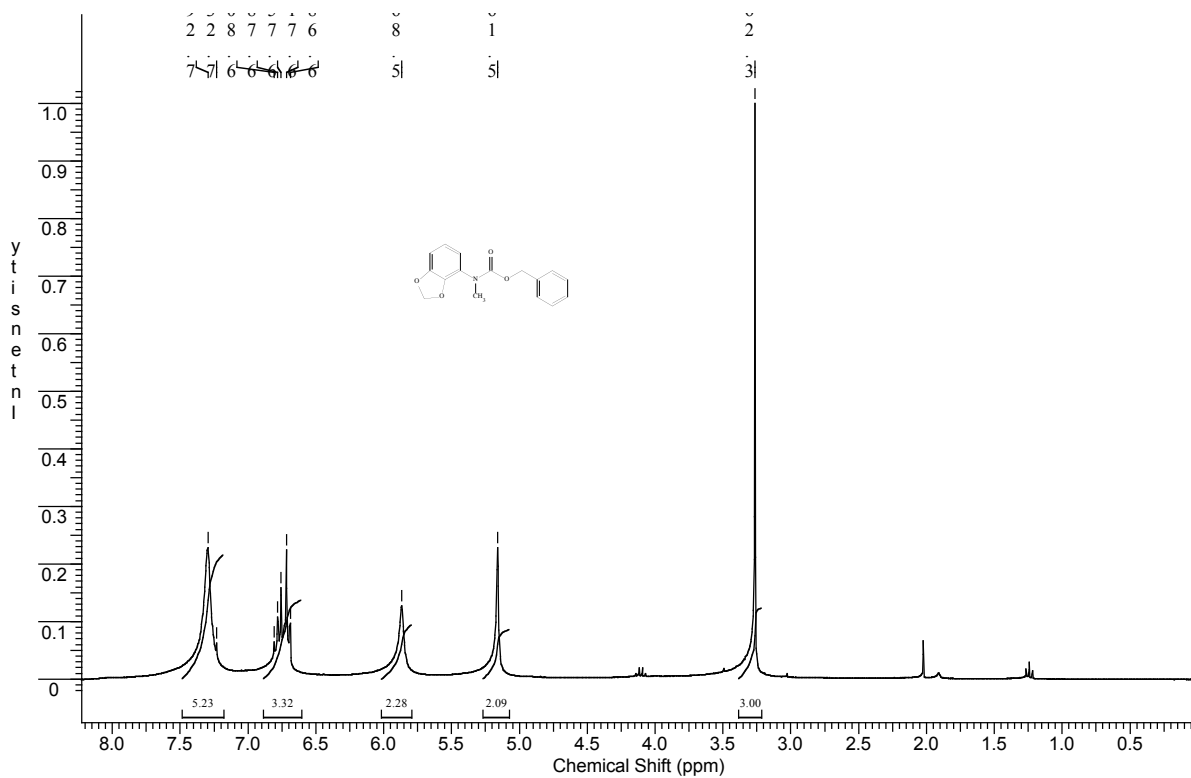
**<sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz) of Compound 6m**



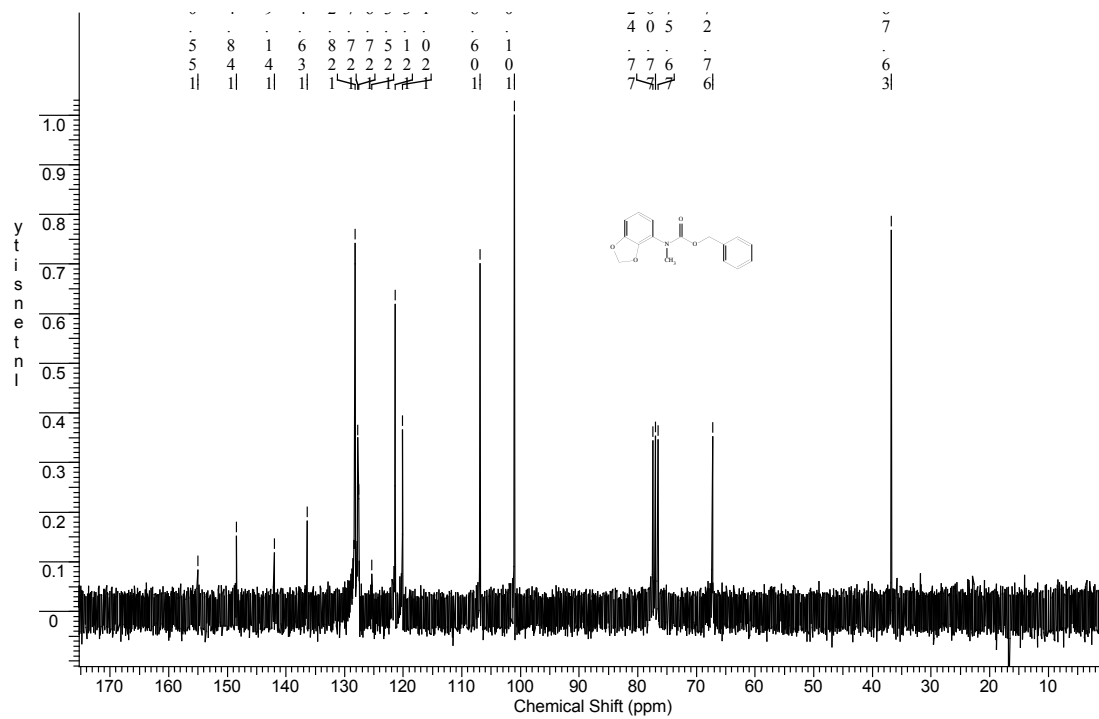
**<sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz) of Compound 60**



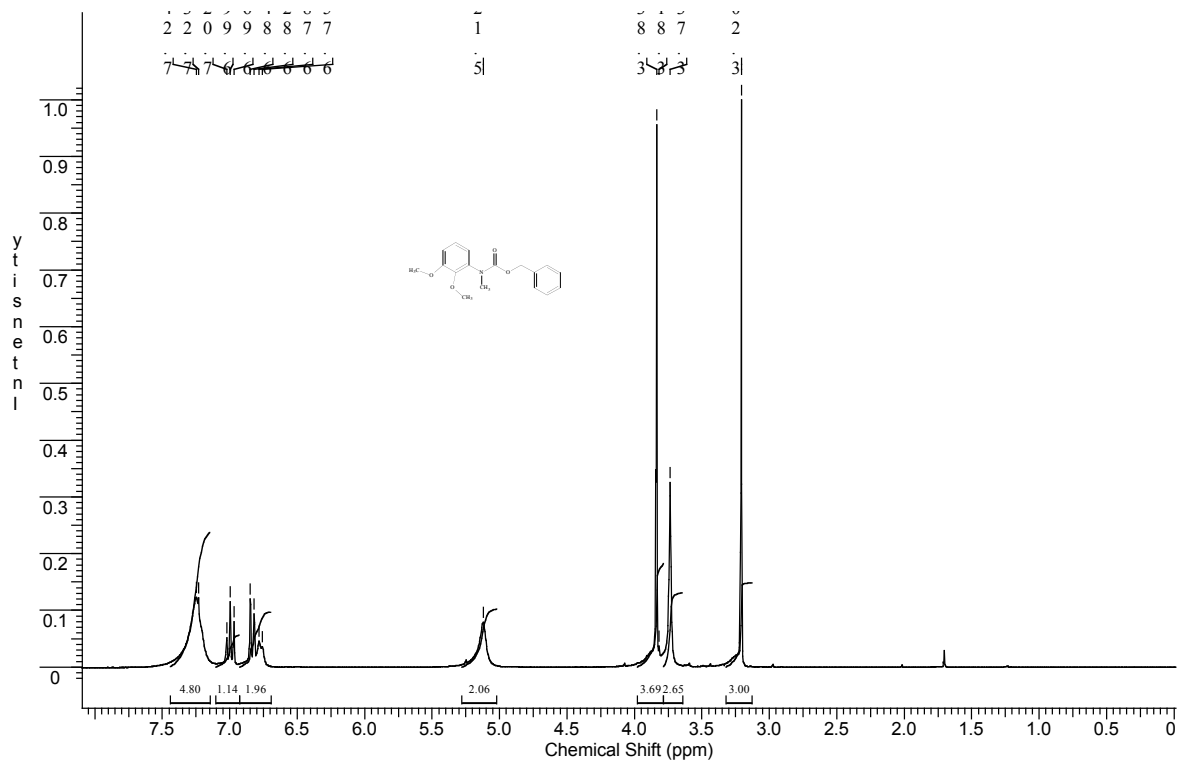
**<sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz) of Compound 60**



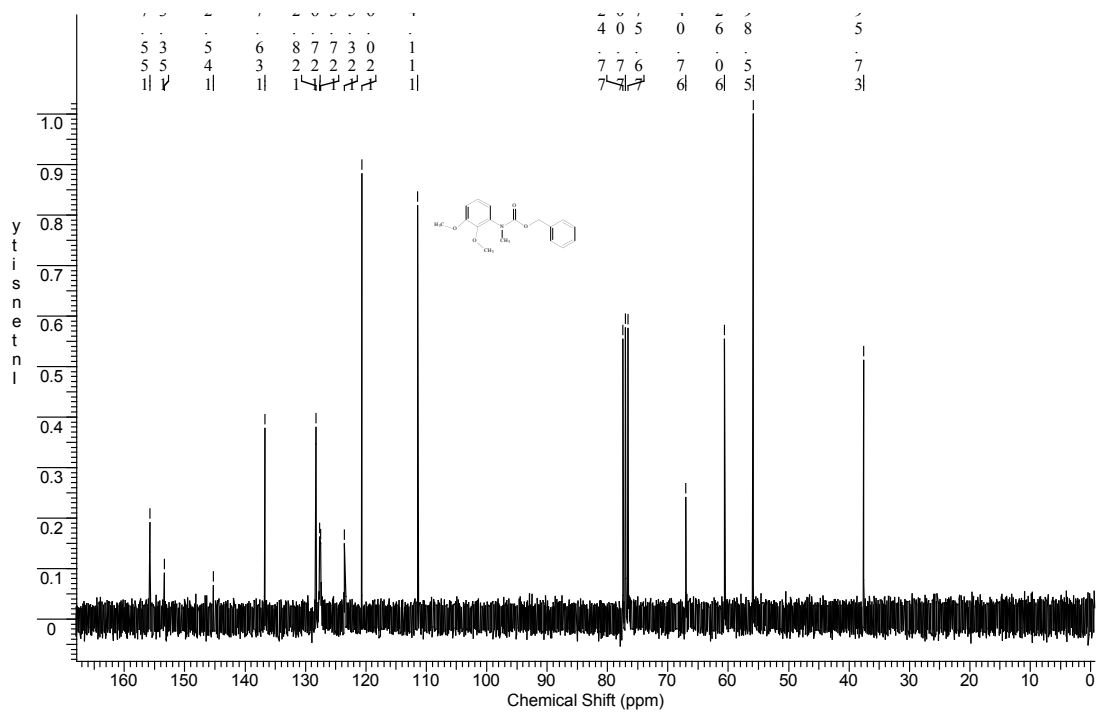
**<sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz) of Compound 7a**



**<sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz) of Compound 7a**

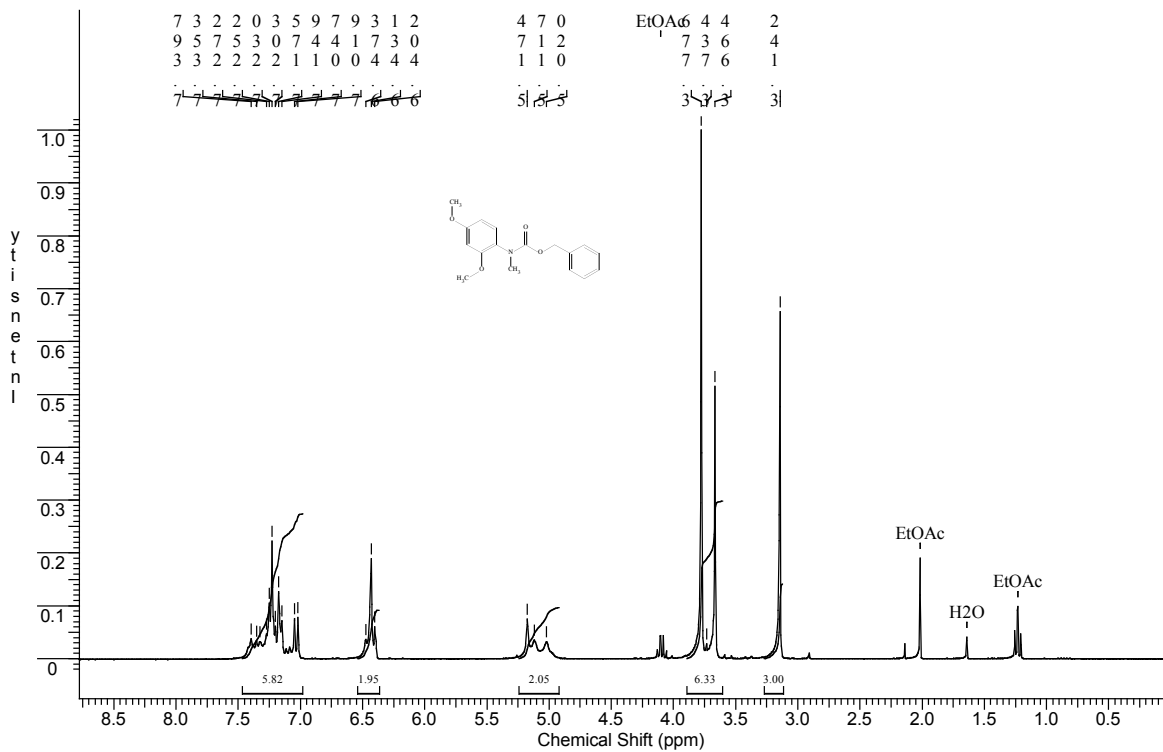


**<sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz) of Compound 7g**

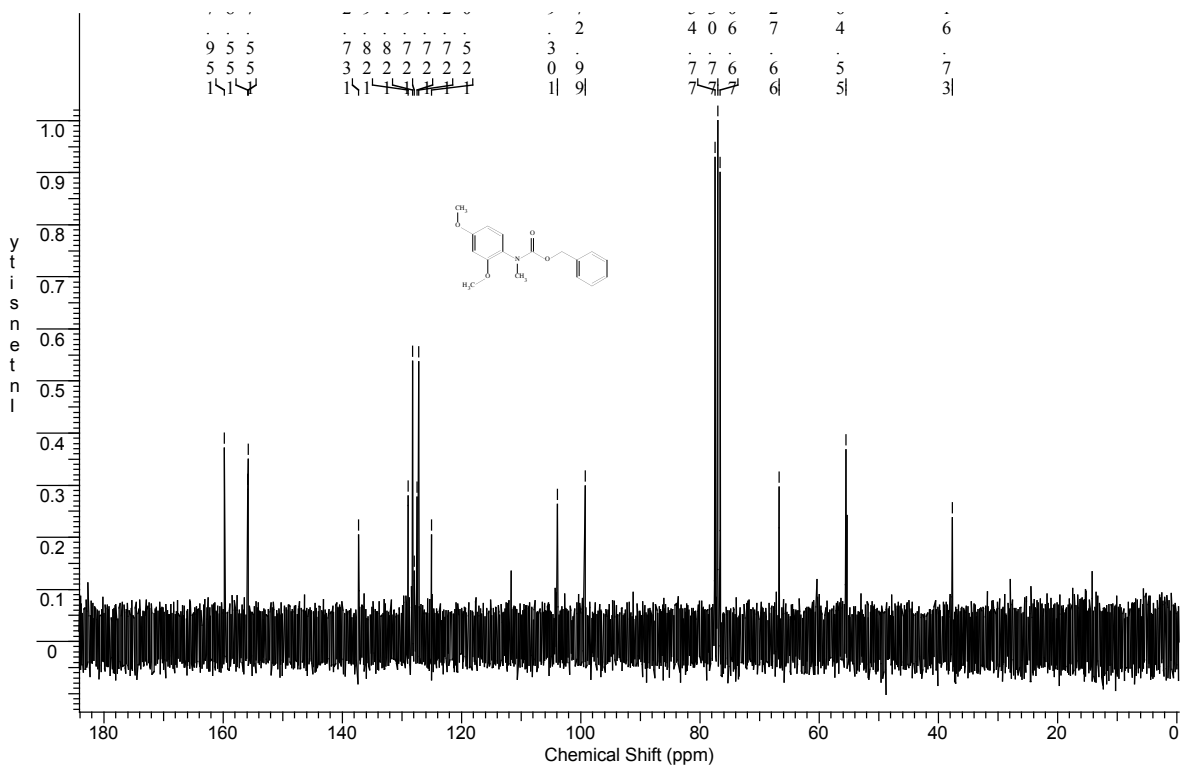


**<sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz) of Compound 7g**

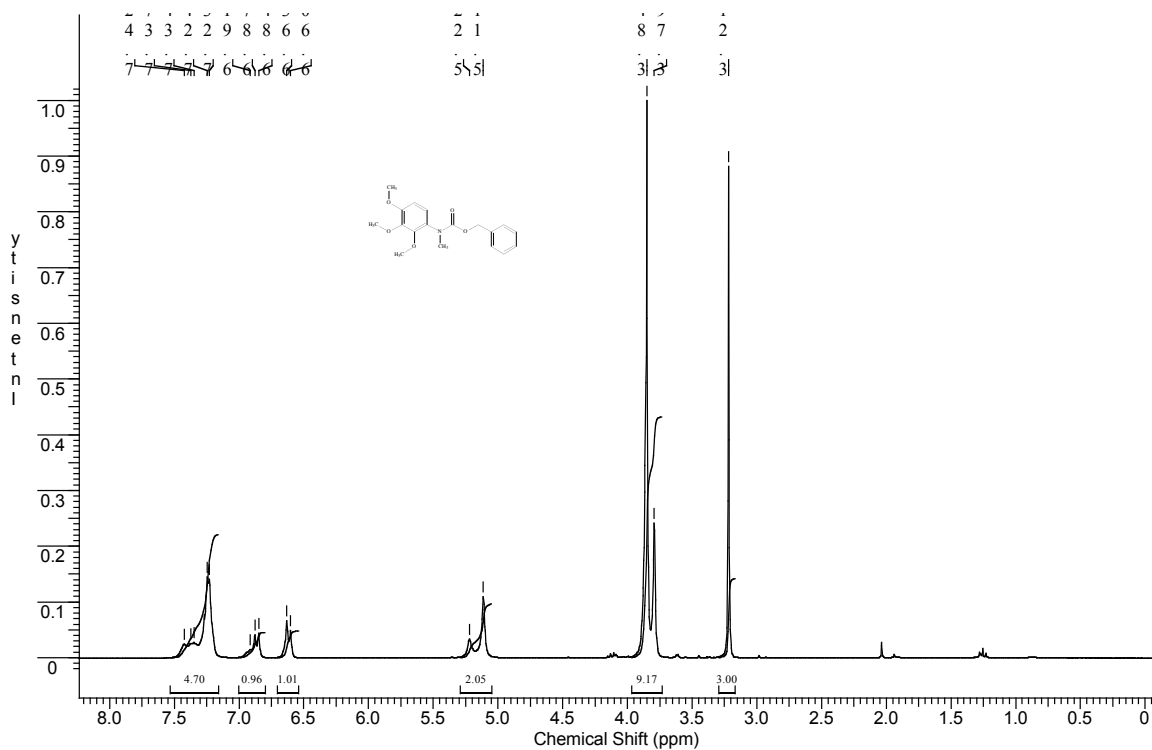




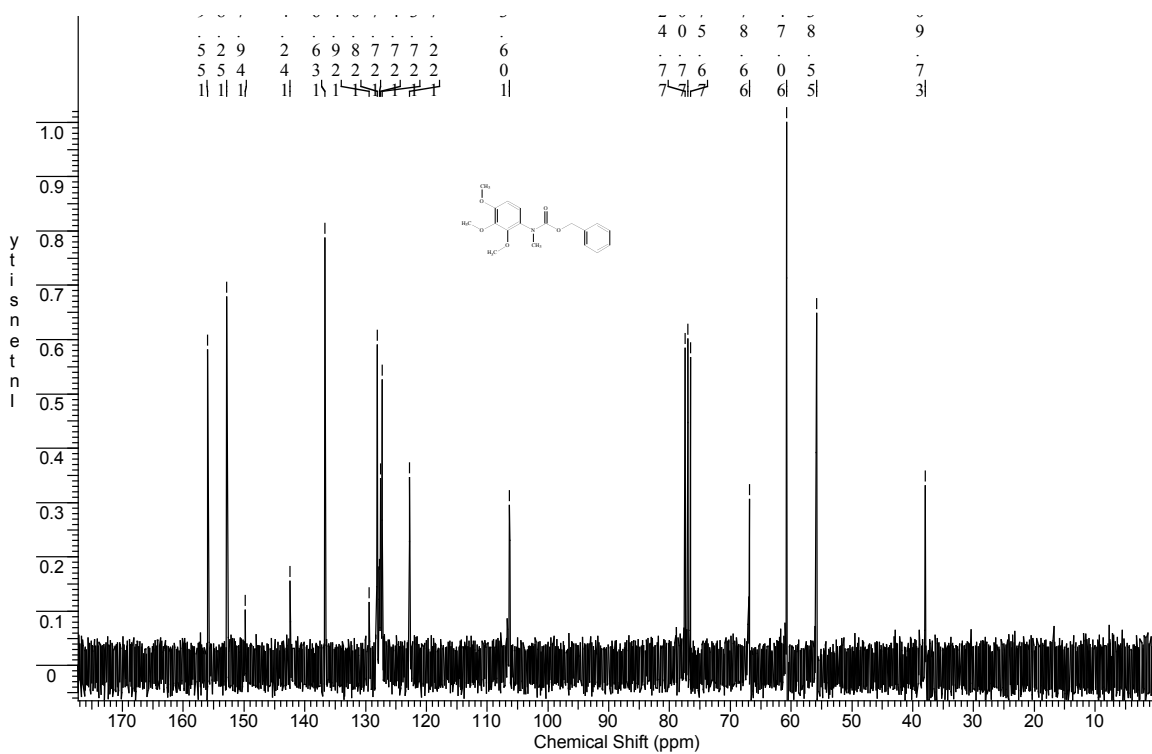
**<sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz) of Compound 7i**



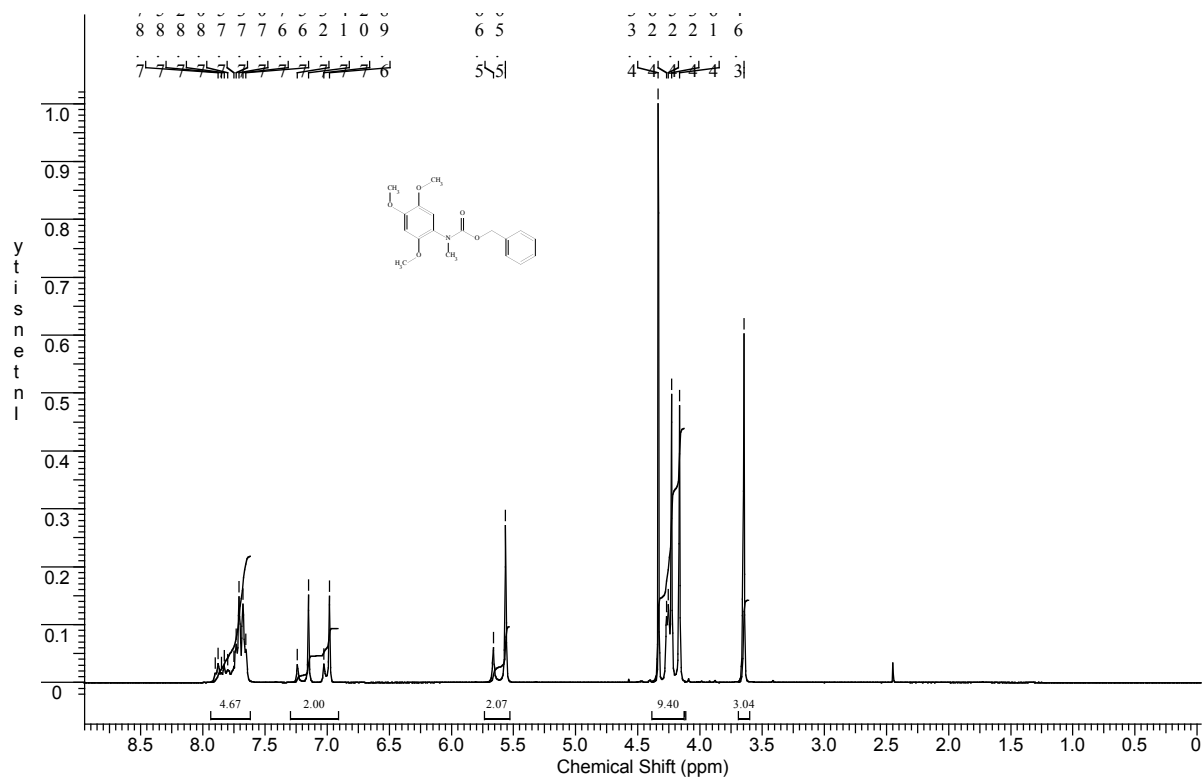
**<sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz) of Compound 7i**



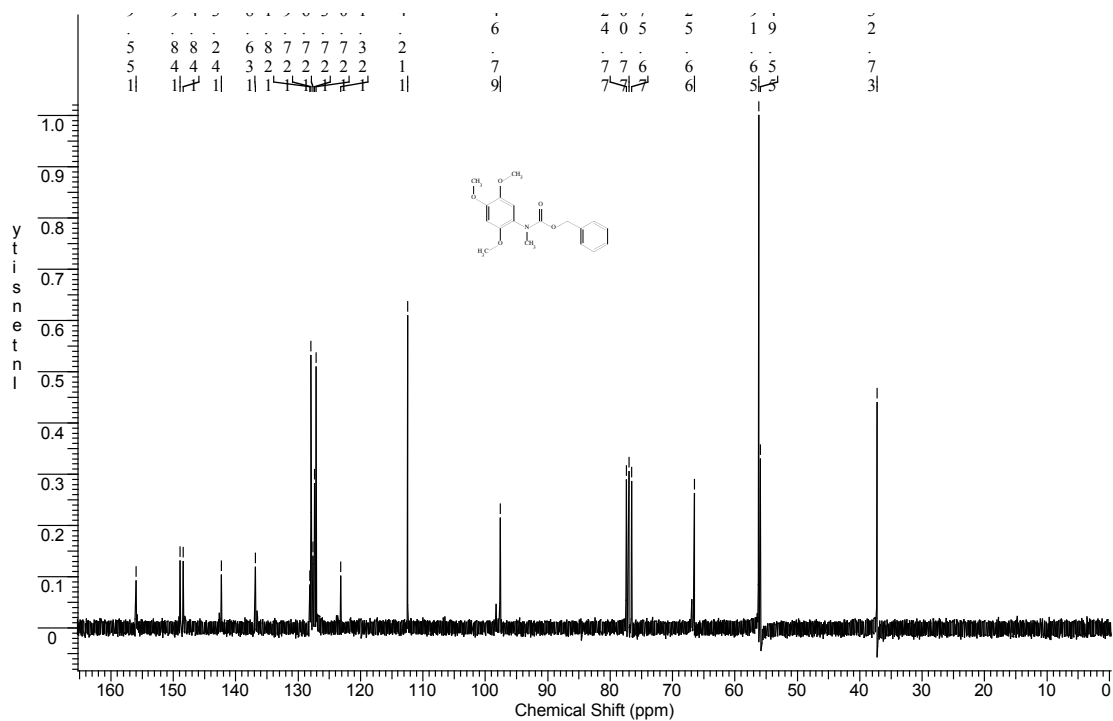
**<sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz) of Compound 7m**



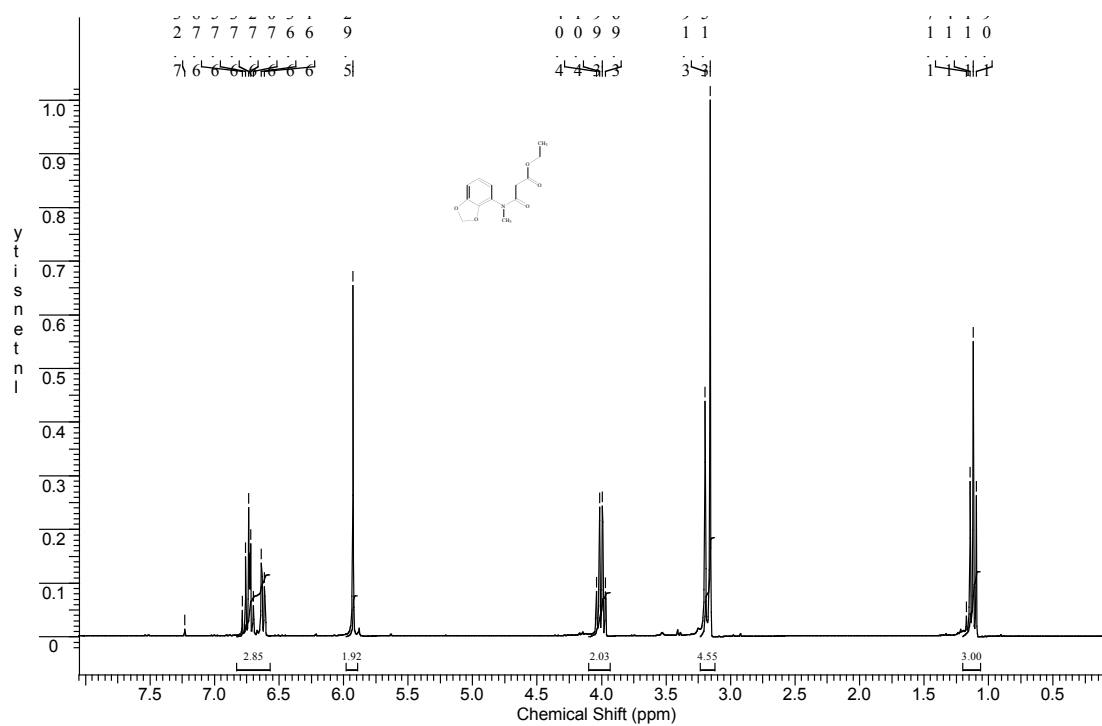
**<sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz) of Compound 7m**



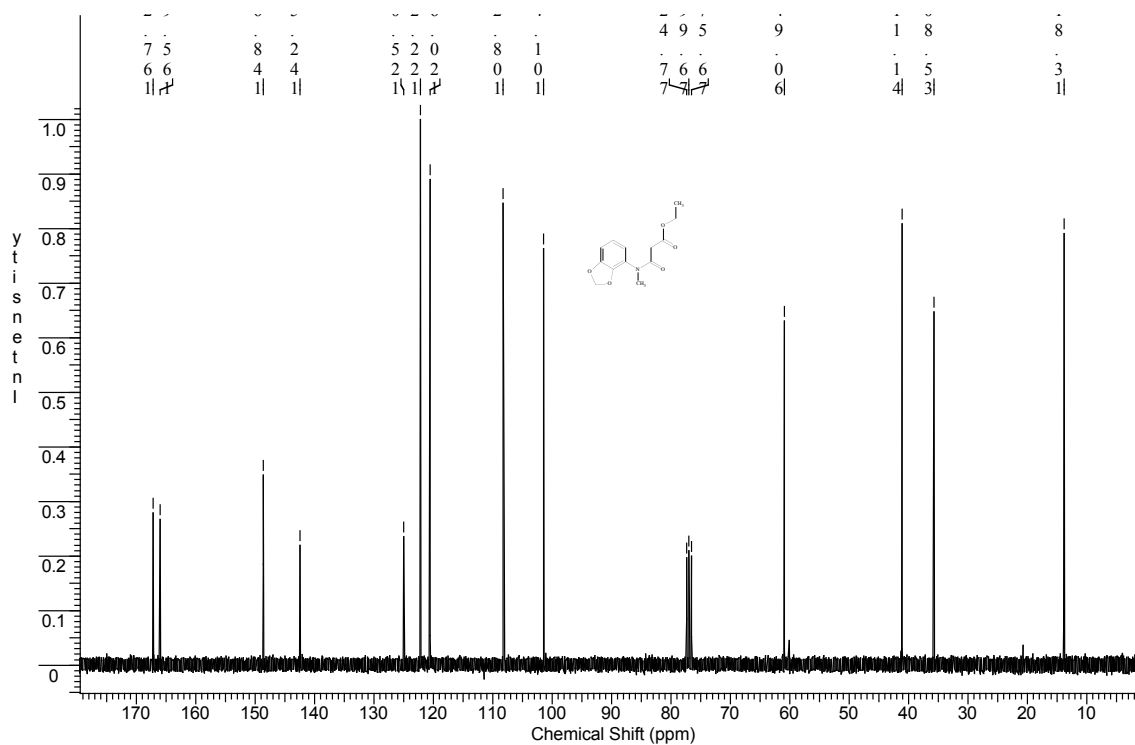
**<sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz) of Compound 7o**



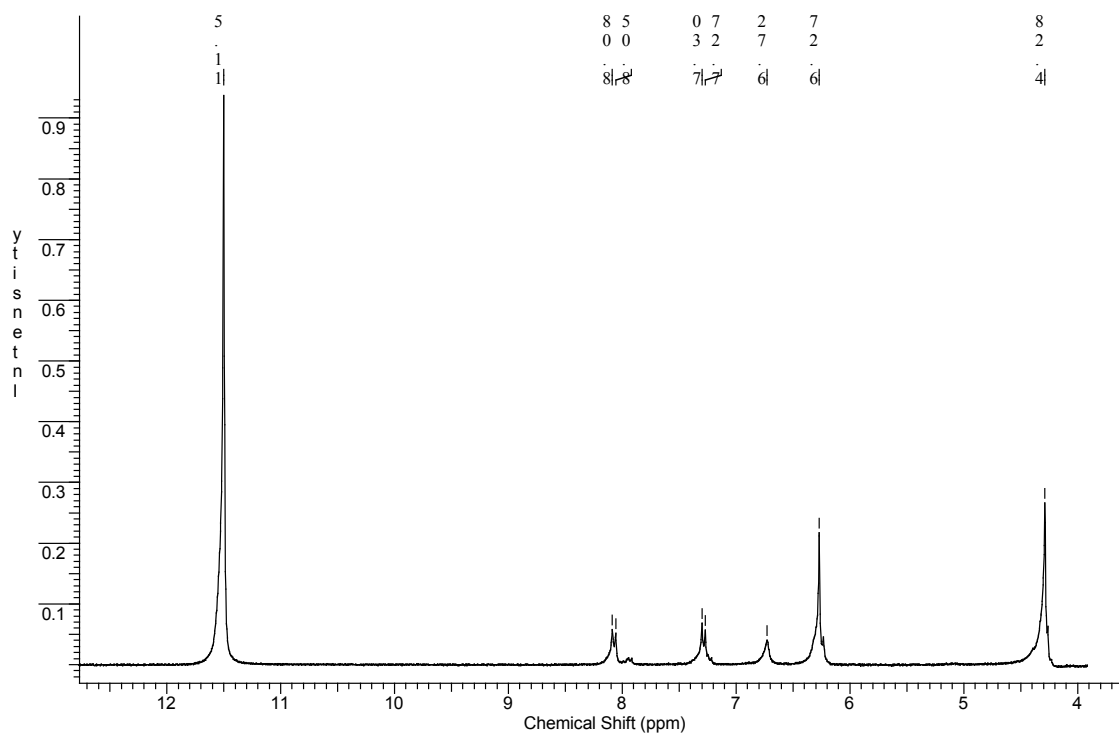
**$^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 75 MHz) of Compound 7o**



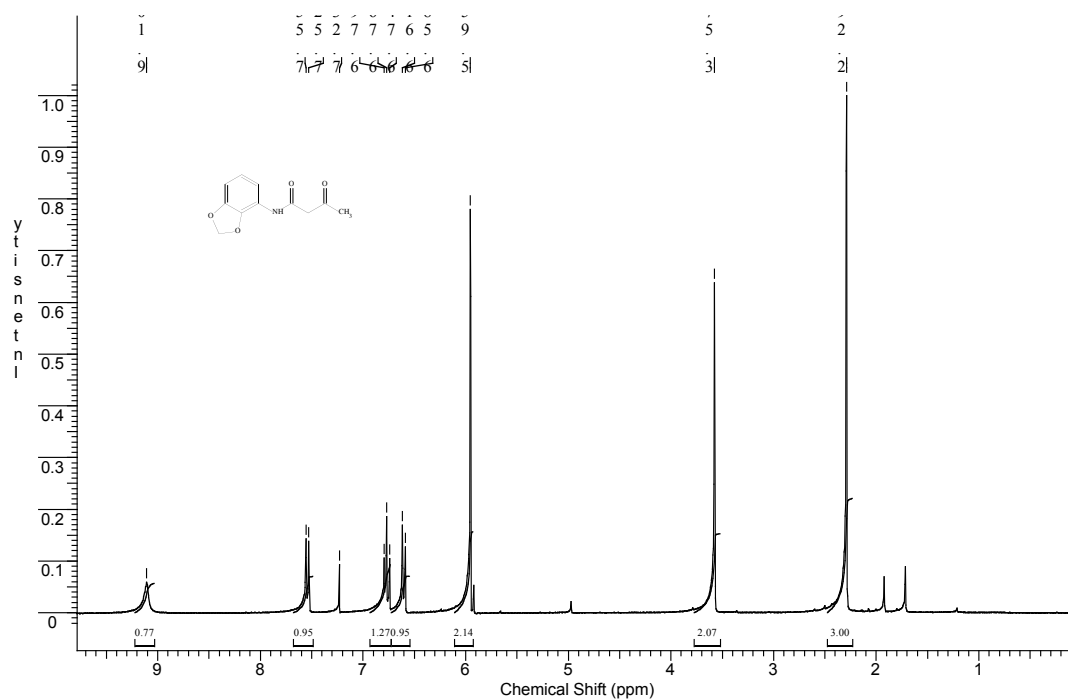
**$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300 MHz) of Compound 8**



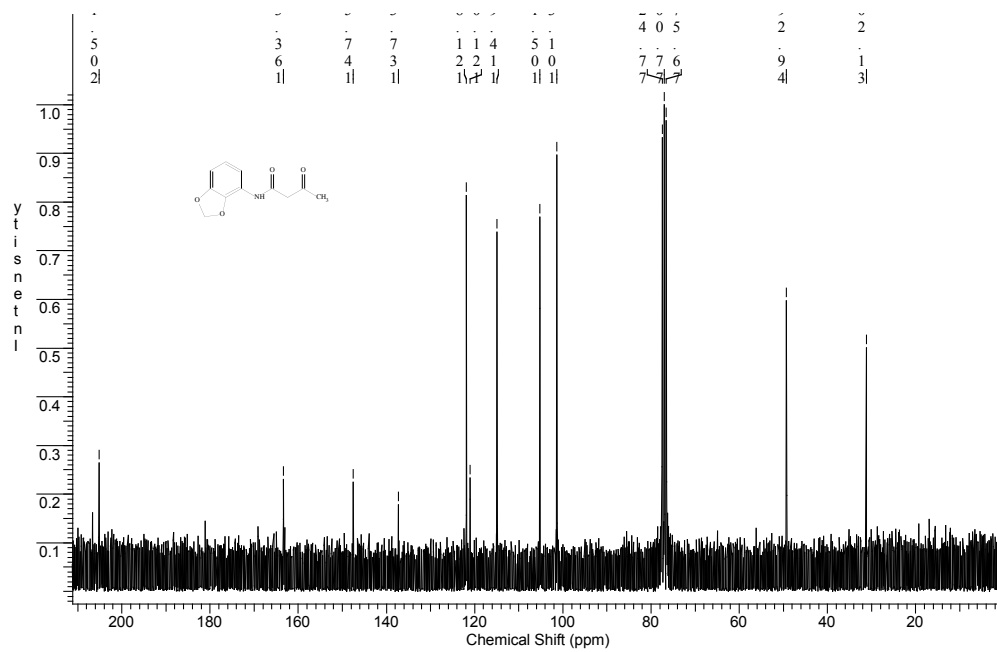
**$^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 75 MHz) of Compound 8**



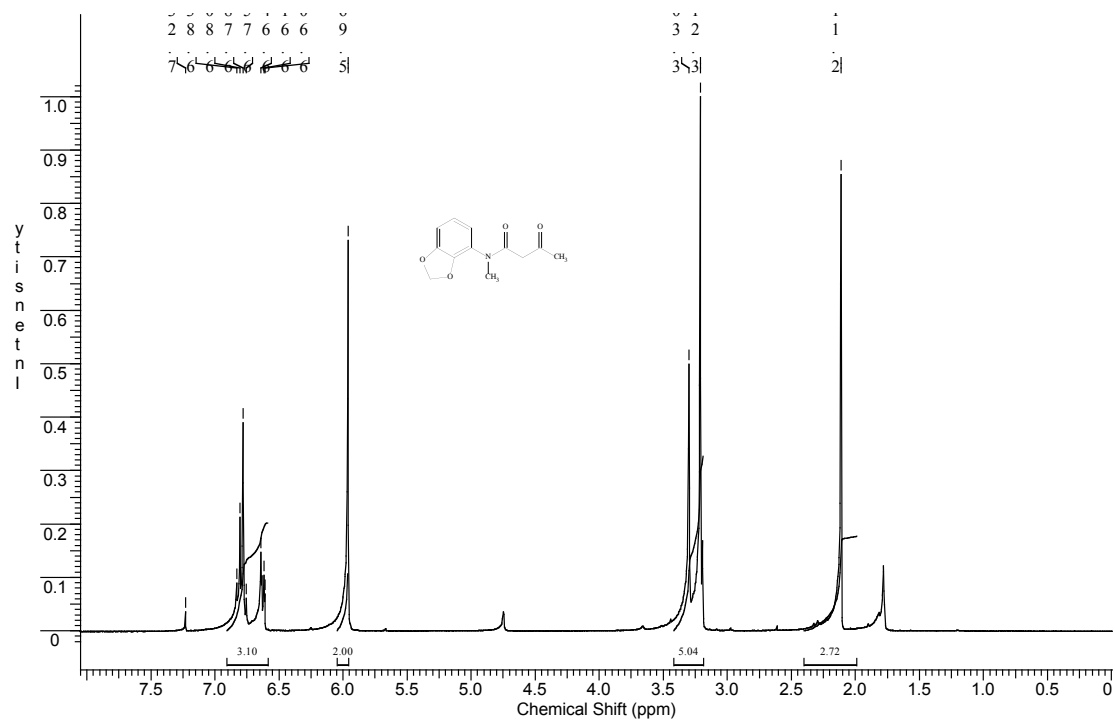
**$^1\text{H}$  NMR ( $\text{CF}_3\text{CO}_2\text{D}$ , 300 MHz) of Compound 9**



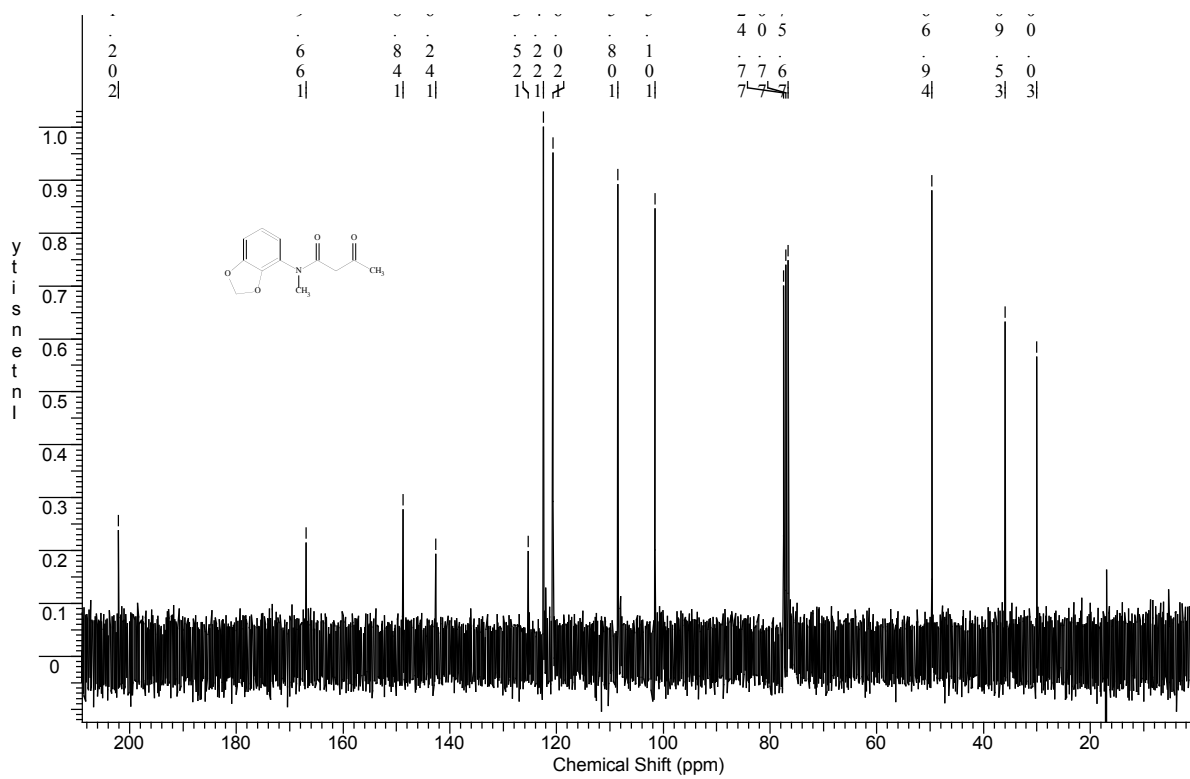
**<sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz) of Compound 10a**



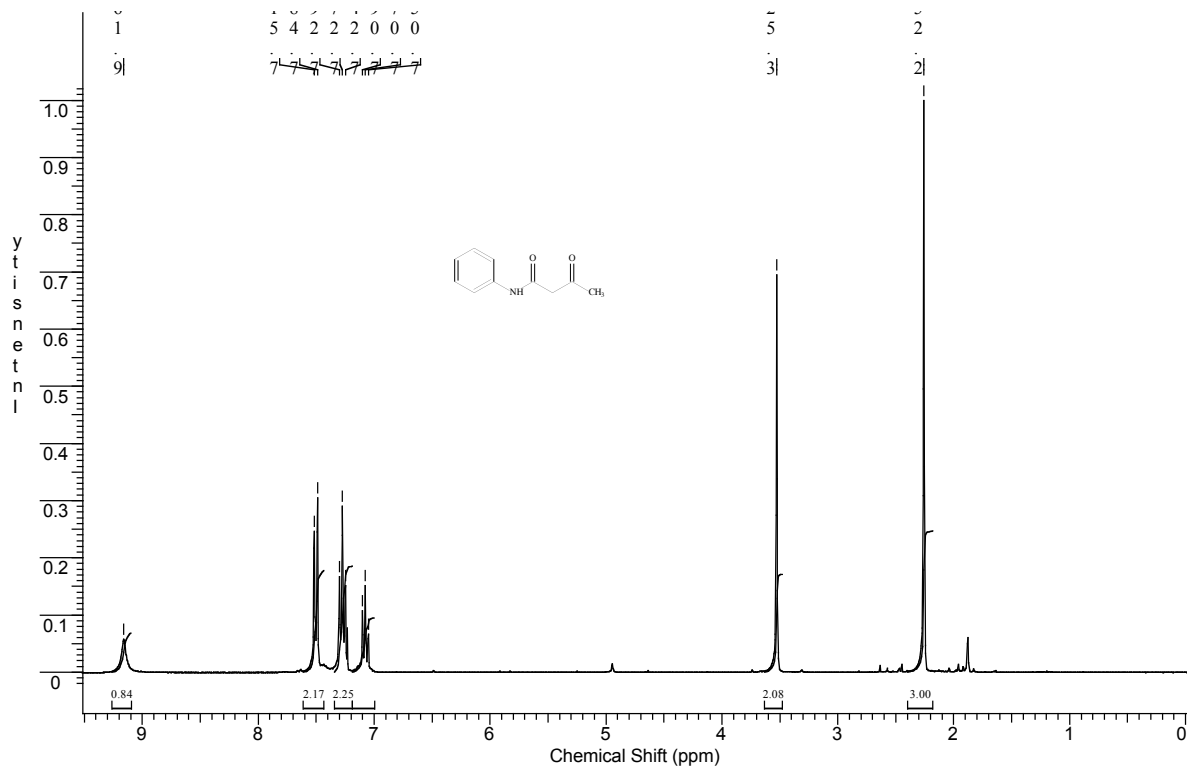
**<sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz) of Compound 10a**



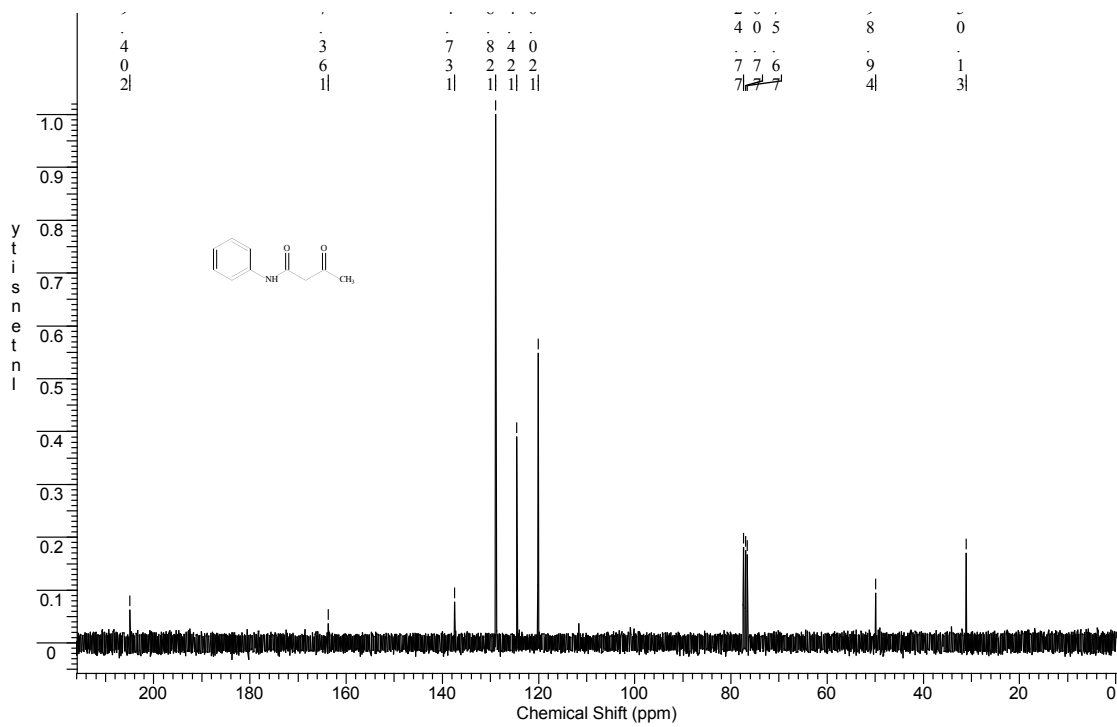
**<sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz) of Compound 10b**



**<sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz) of Compound 10b**

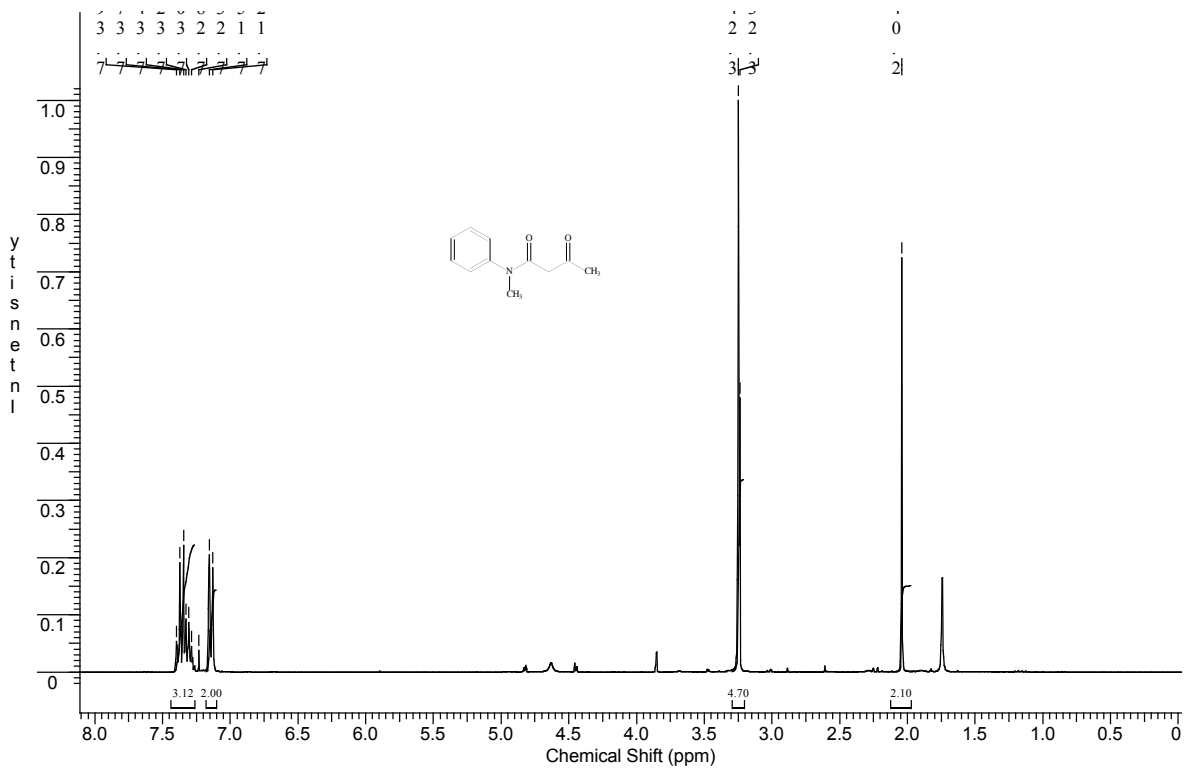


**<sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz) of Compound 10c**

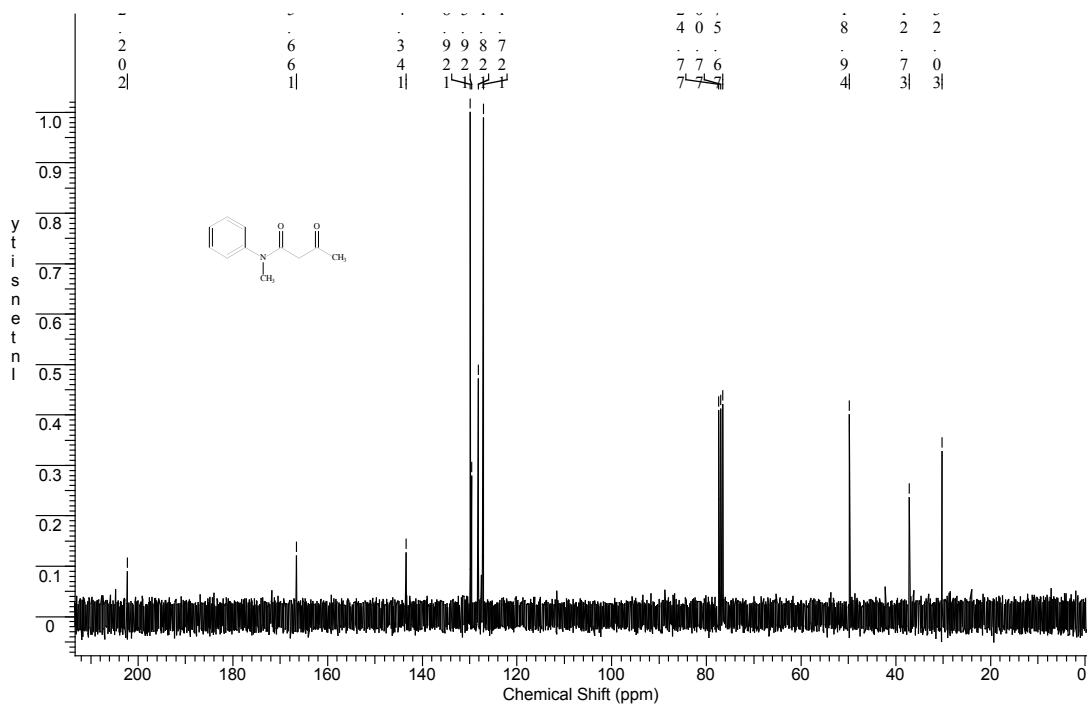


**<sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz) of Compound 10c**

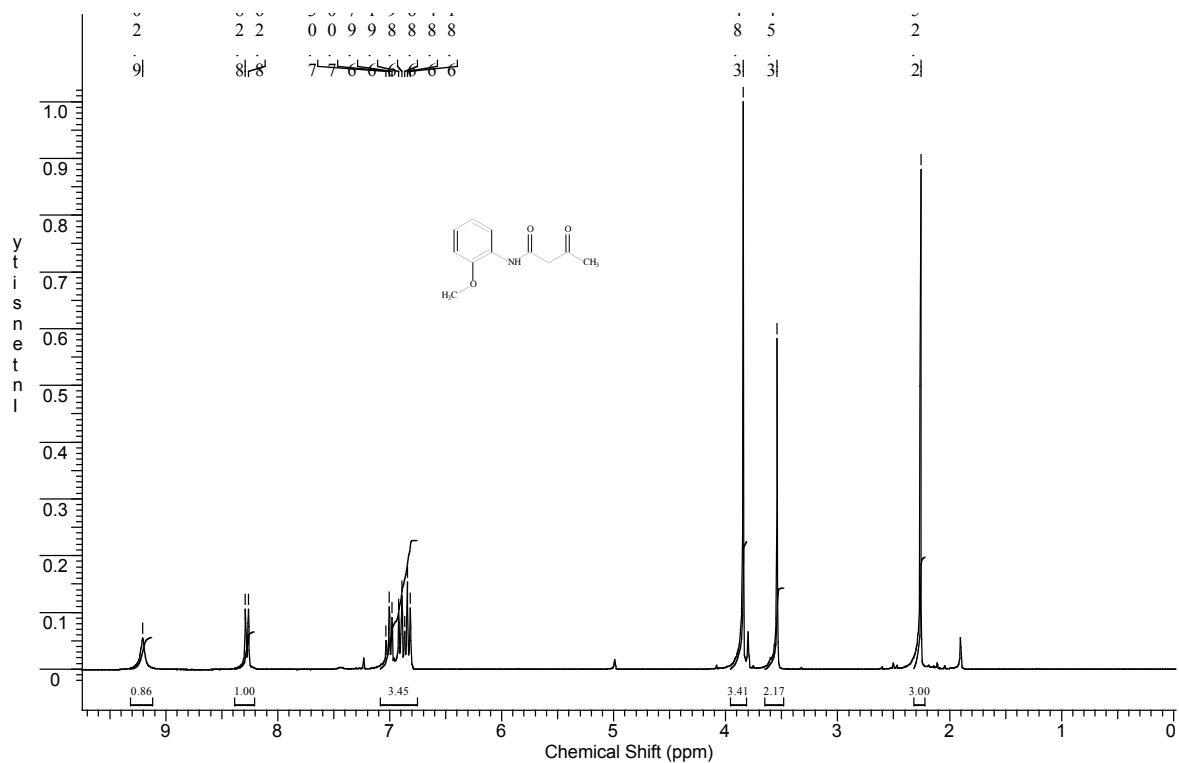




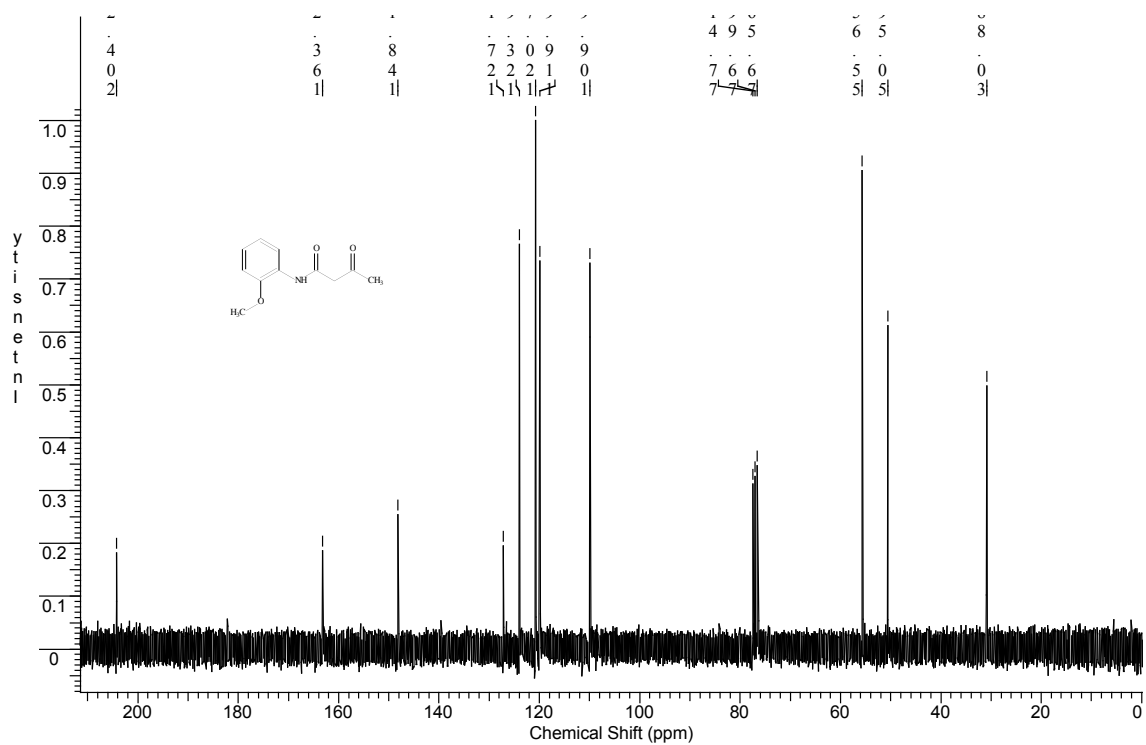
**<sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz) of Compound 10d**



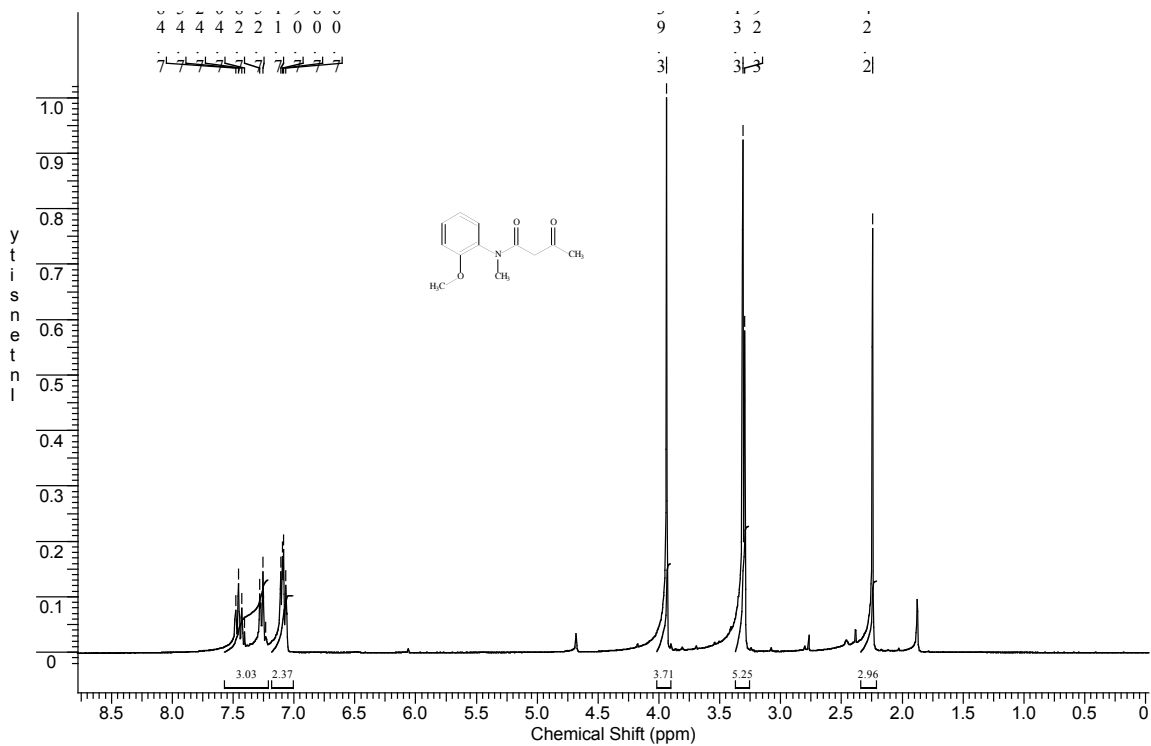
**<sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz) of Compound 10d**



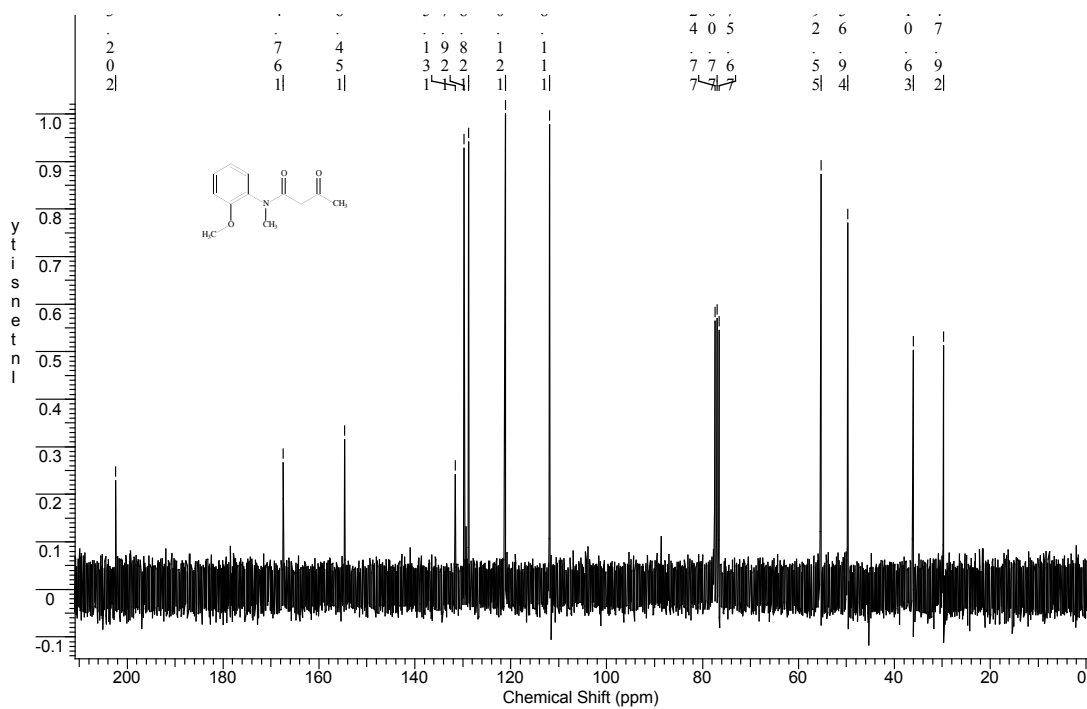
**<sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz) of Compound 10e**



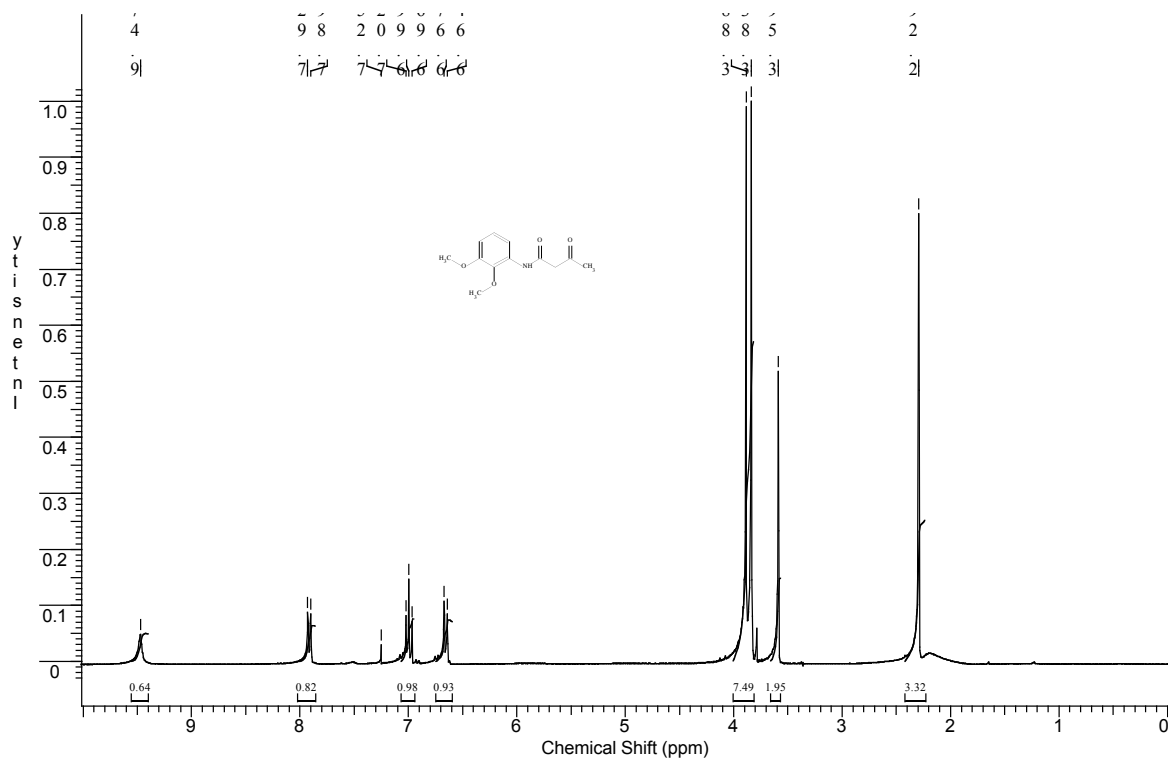
**<sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz) of Compound 10e**



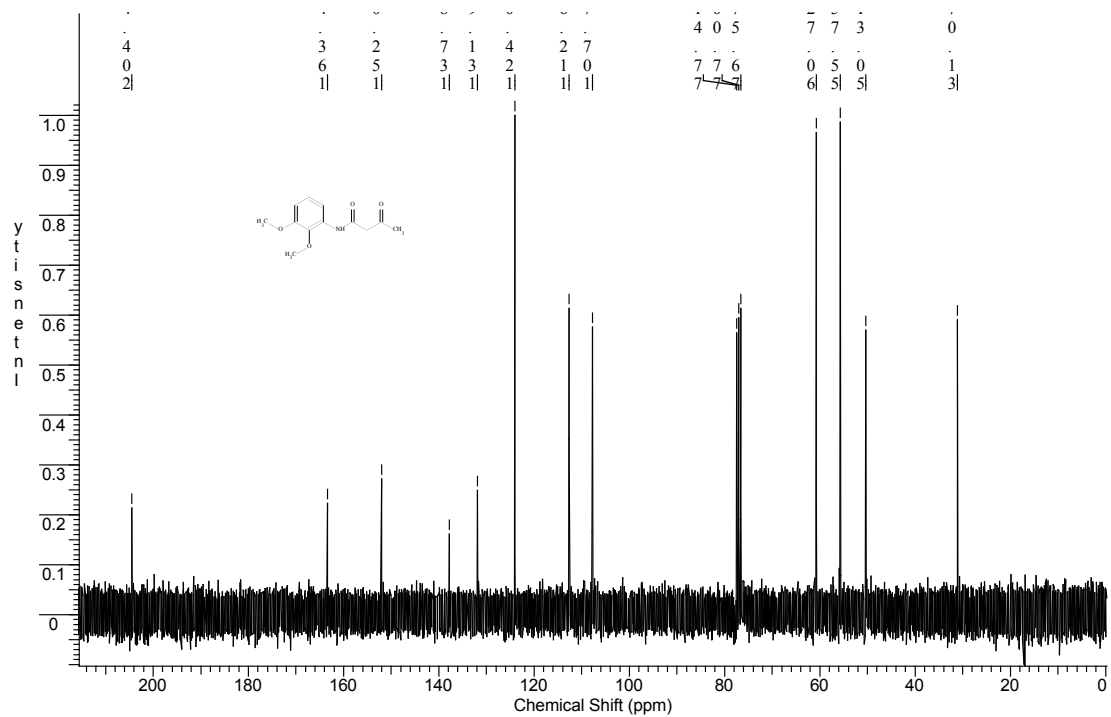
**<sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz) of Compound 10f**



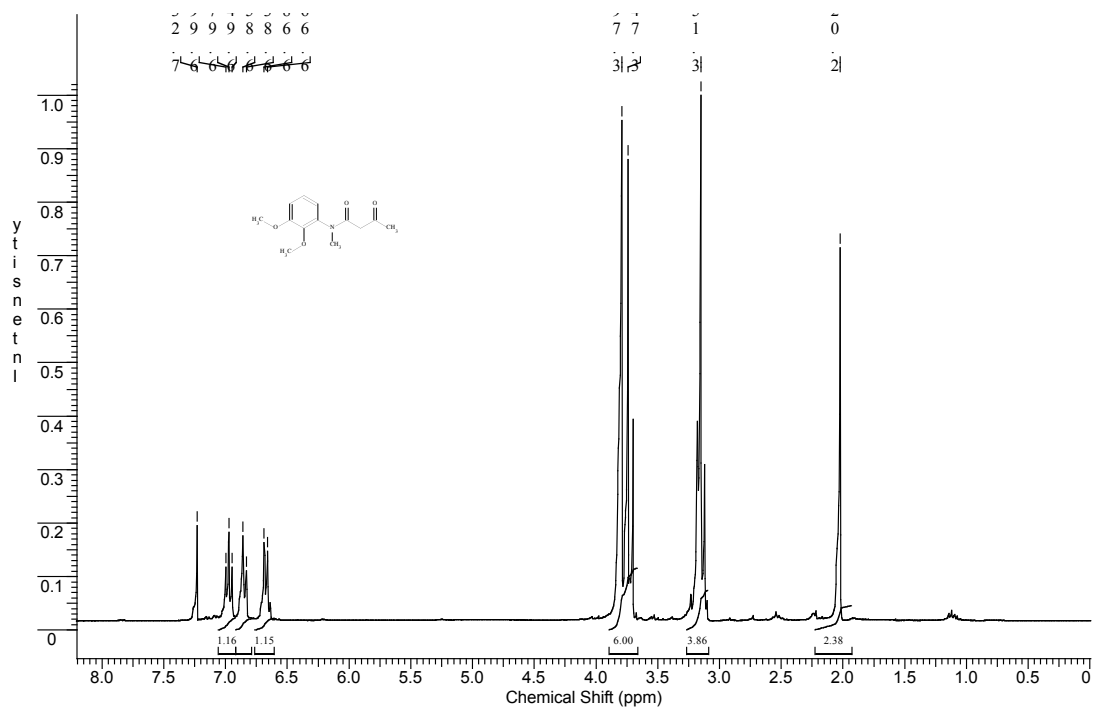
**<sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz) of Compound 10f**



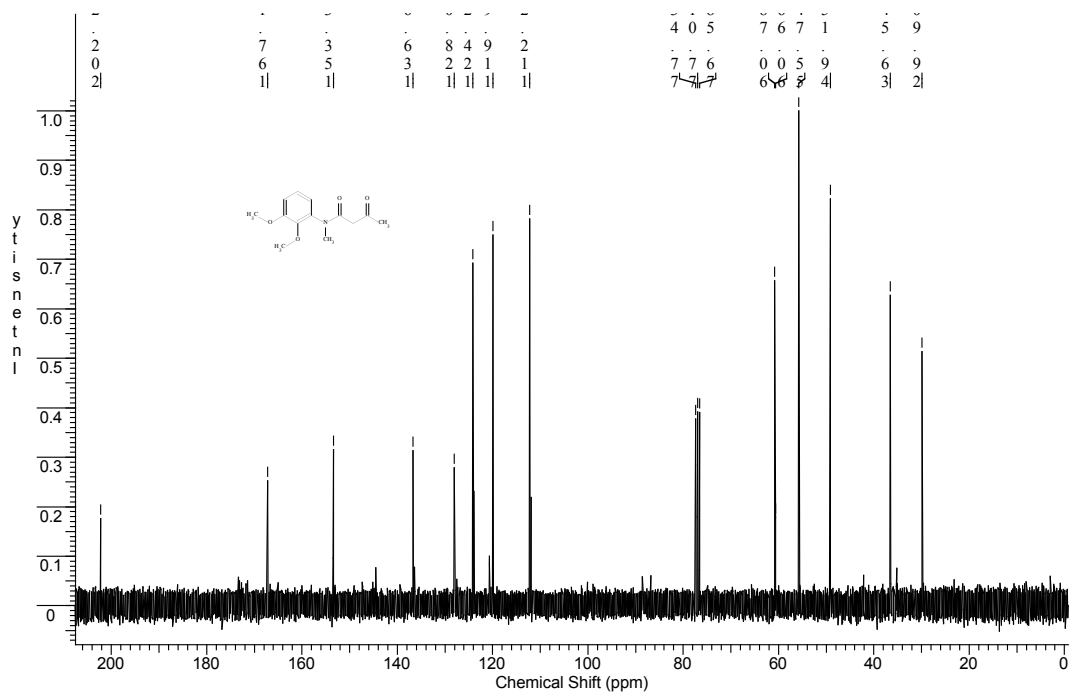
**<sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz) of Compound 10g**



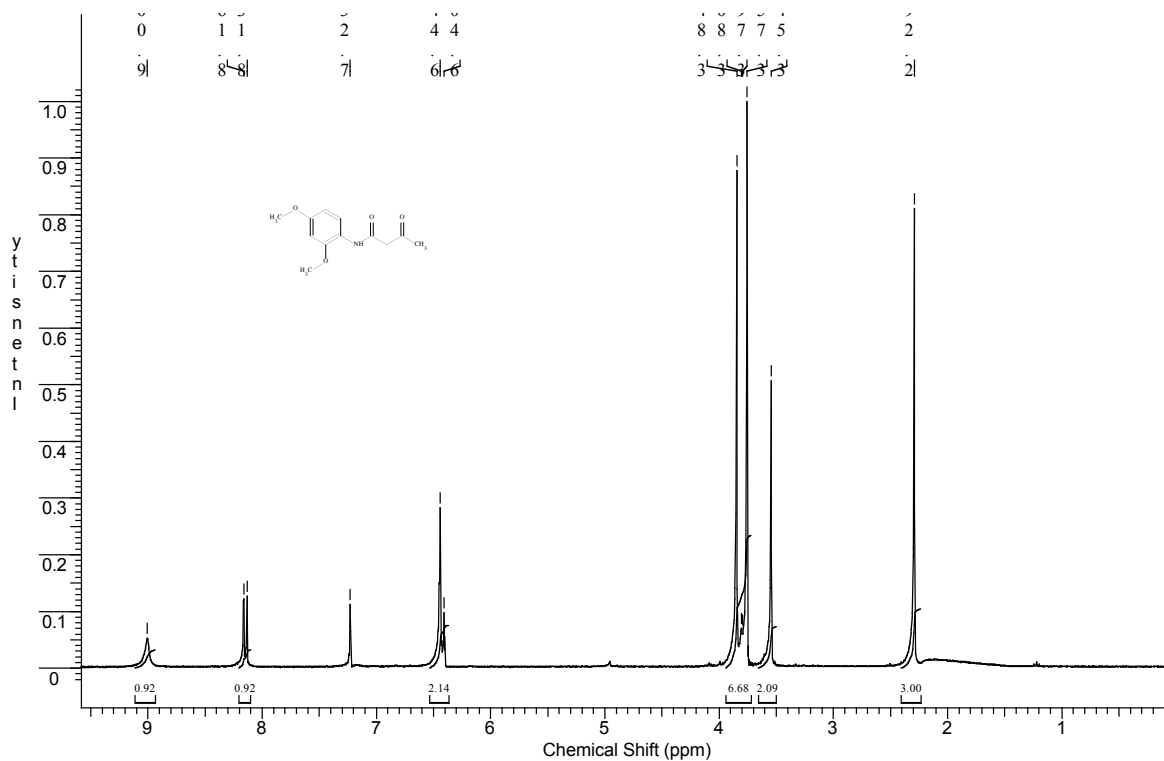
**<sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz) of Compound 10g**



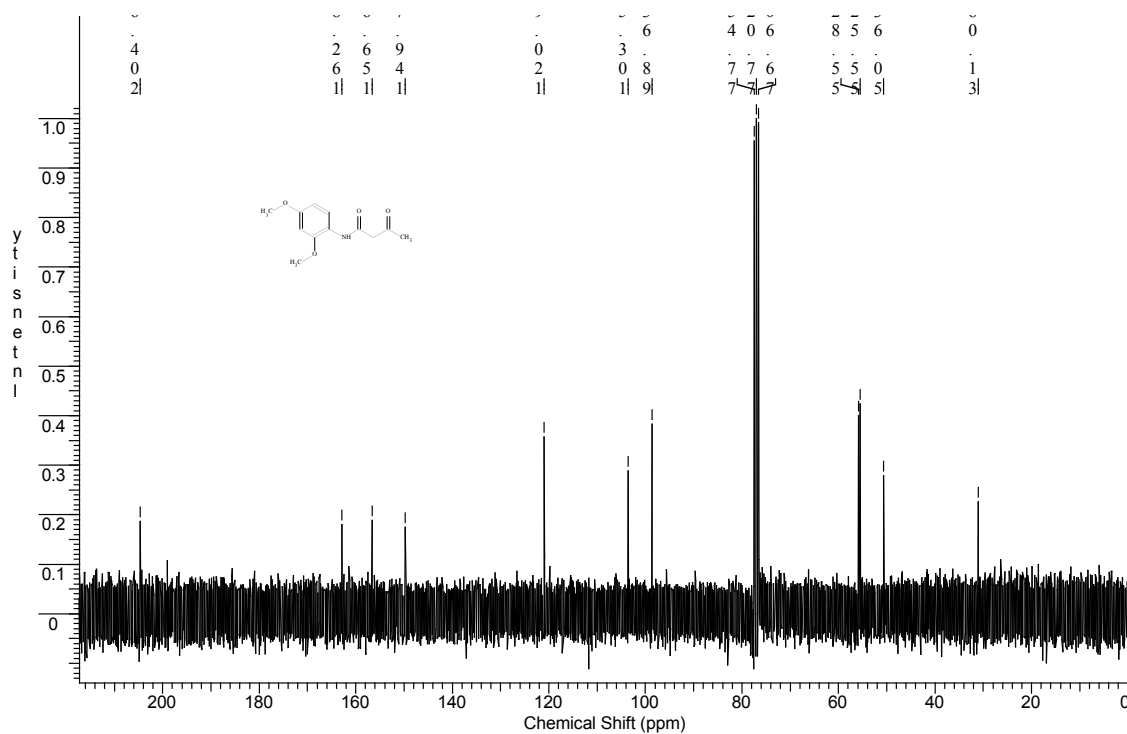
**<sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz) of Compound 10h**



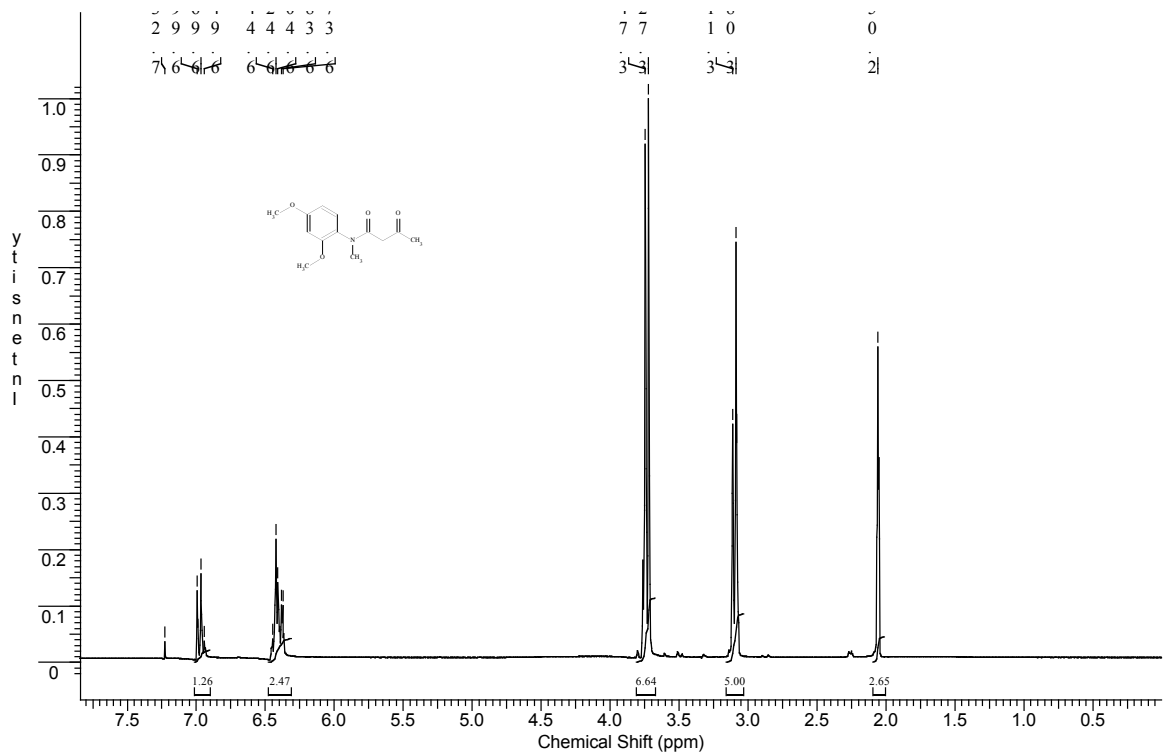
**<sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz) of Compound 10h**



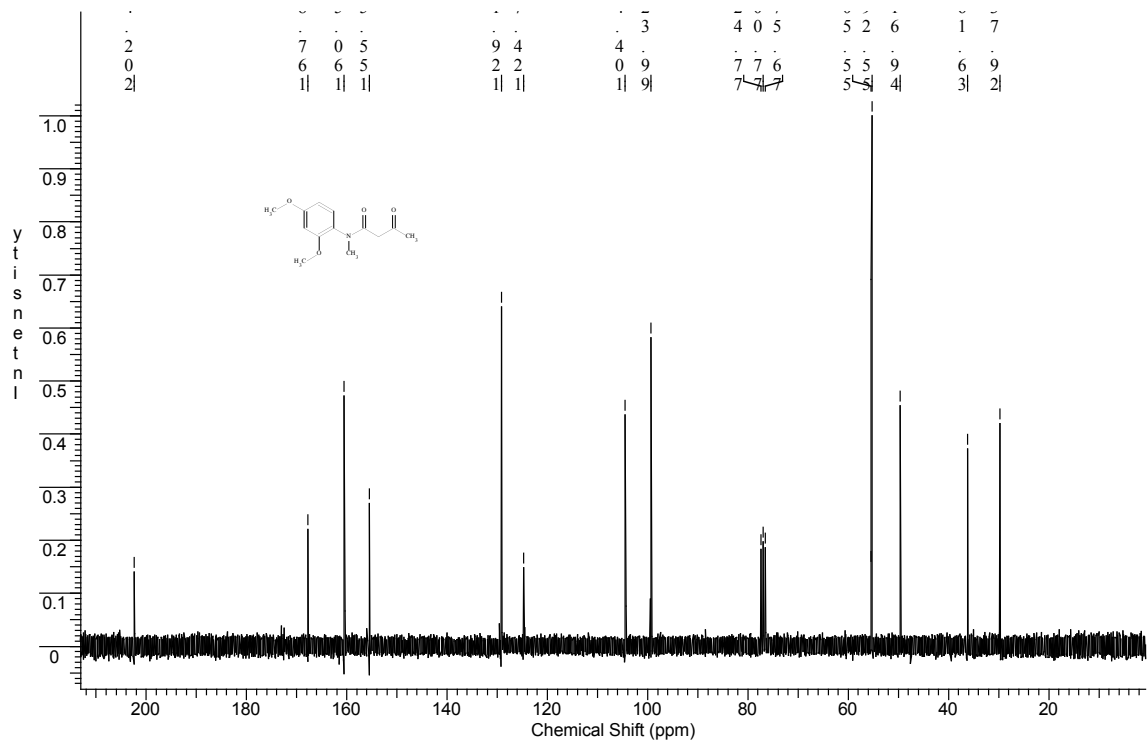
**<sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz) of Compound 10i**



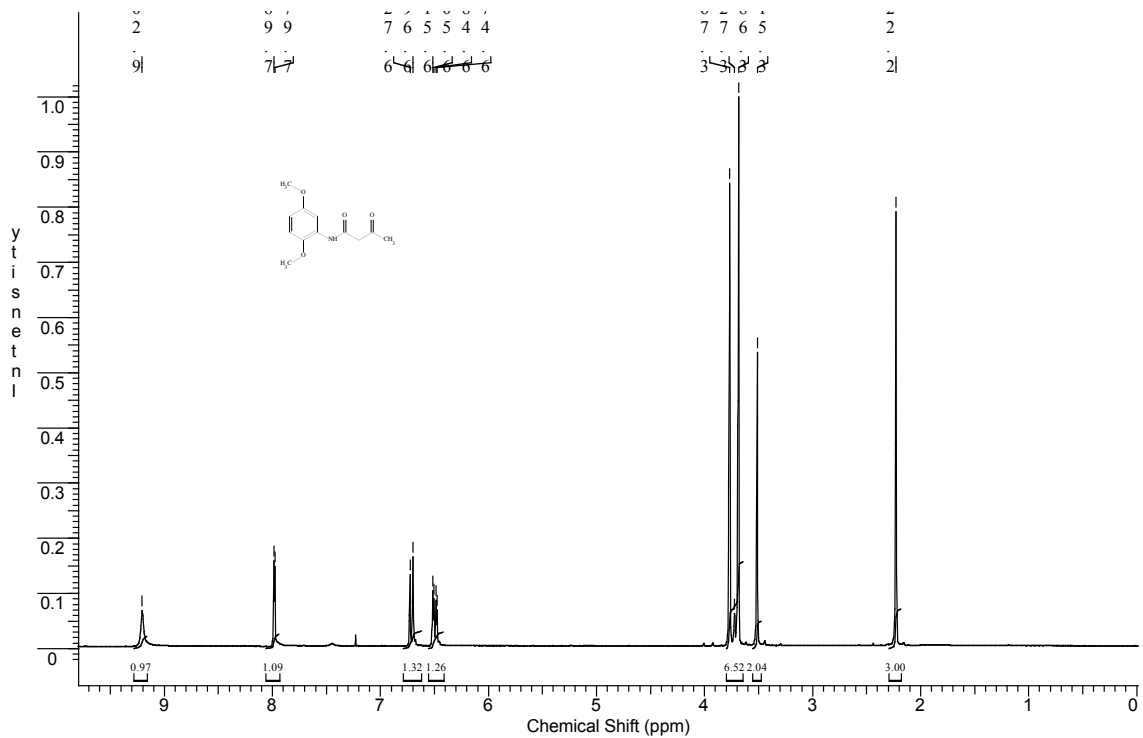
**<sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz) of Compound 10i**



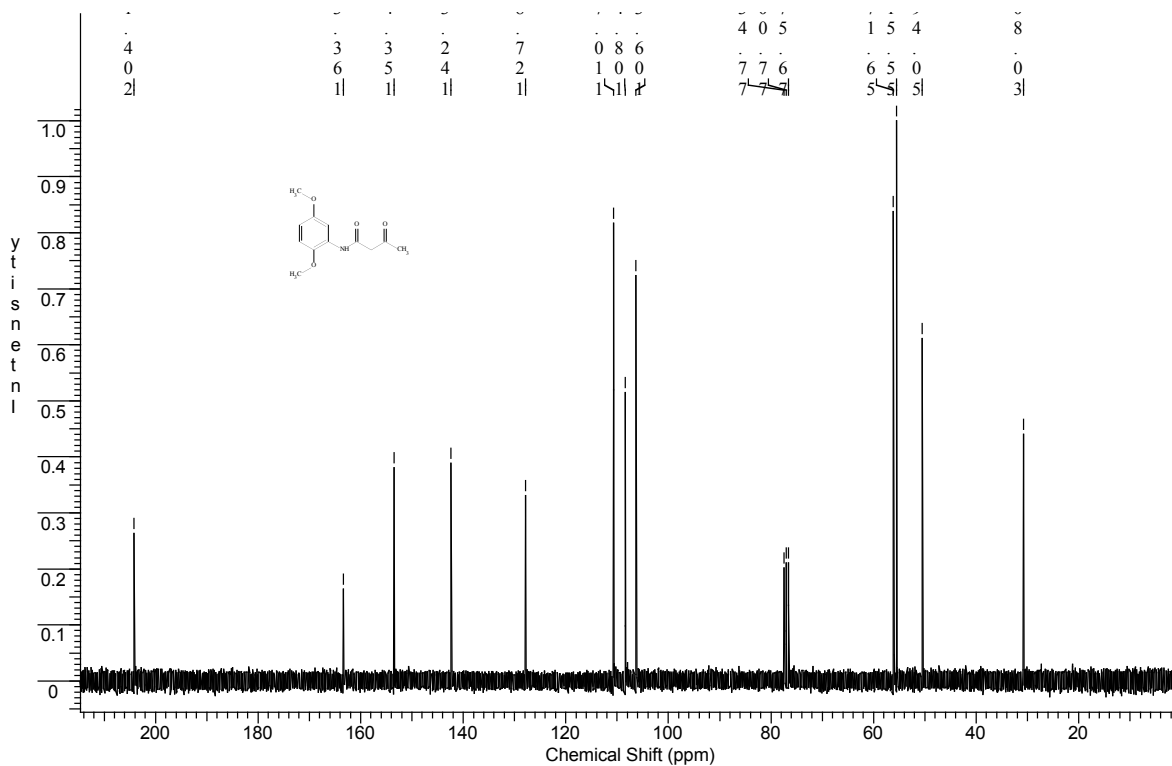
**<sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz) of Compound 10j**



**<sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz) of Compound 10j**

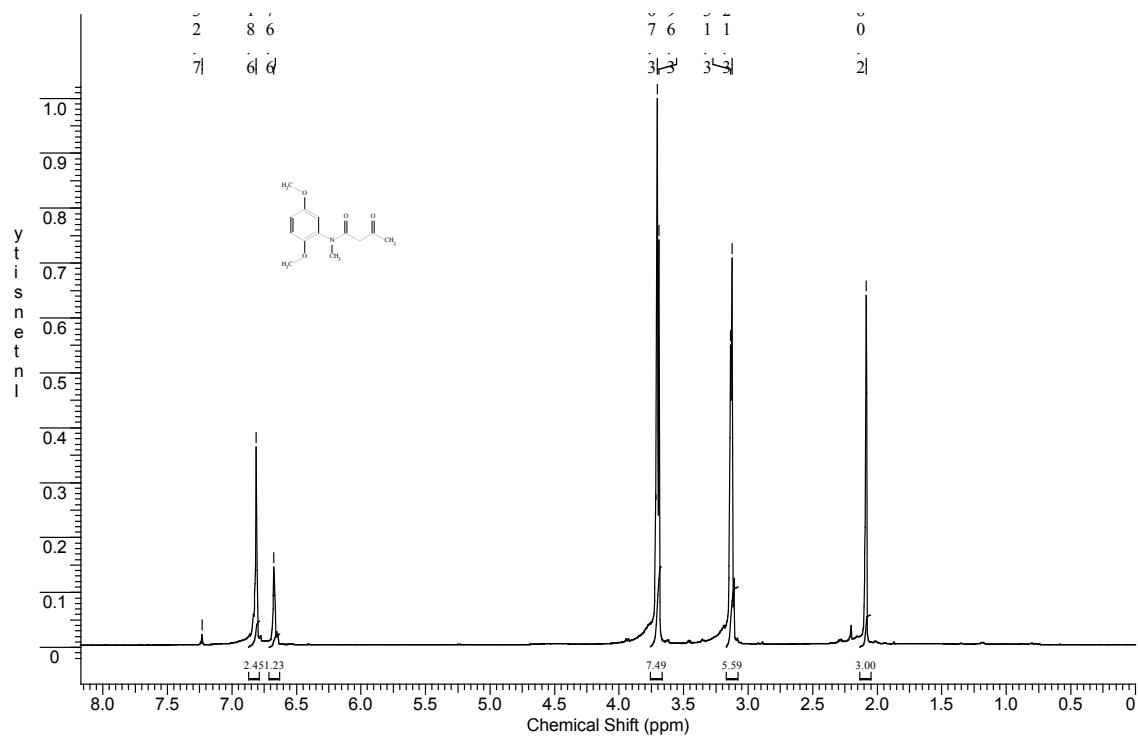


**<sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz) of Compound 10k**

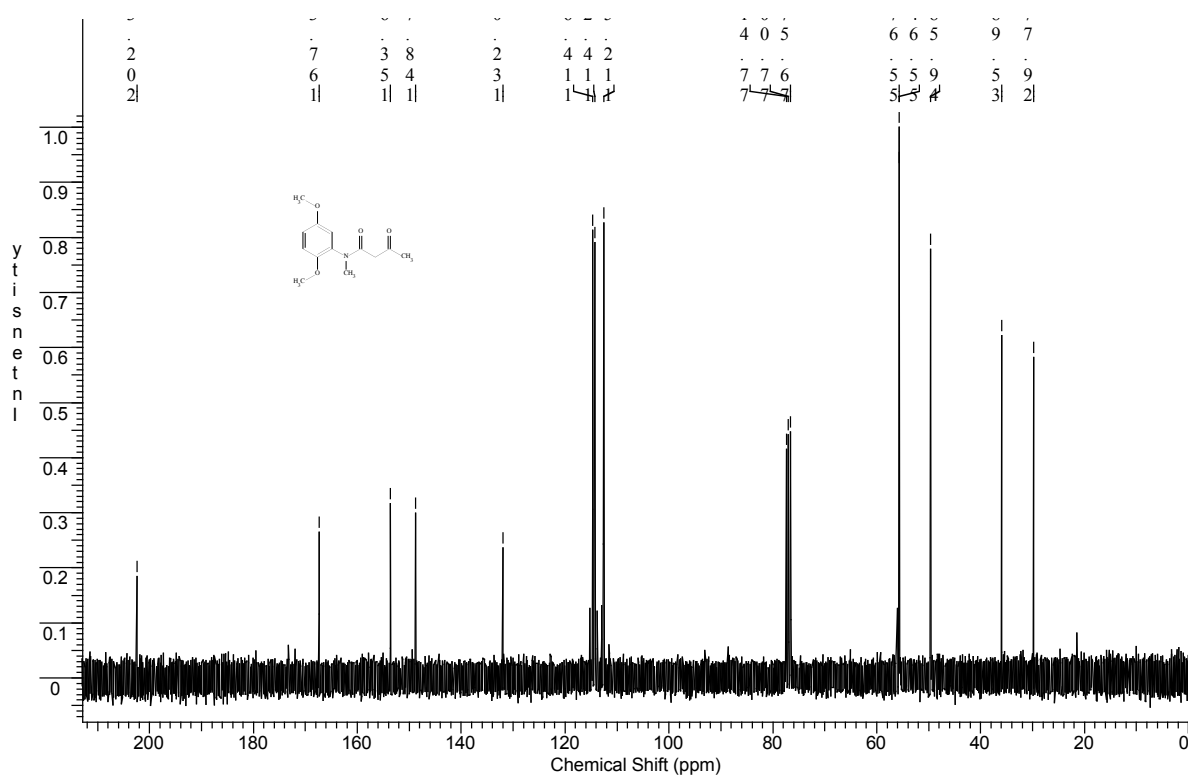


**<sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz) of Compound 10k**

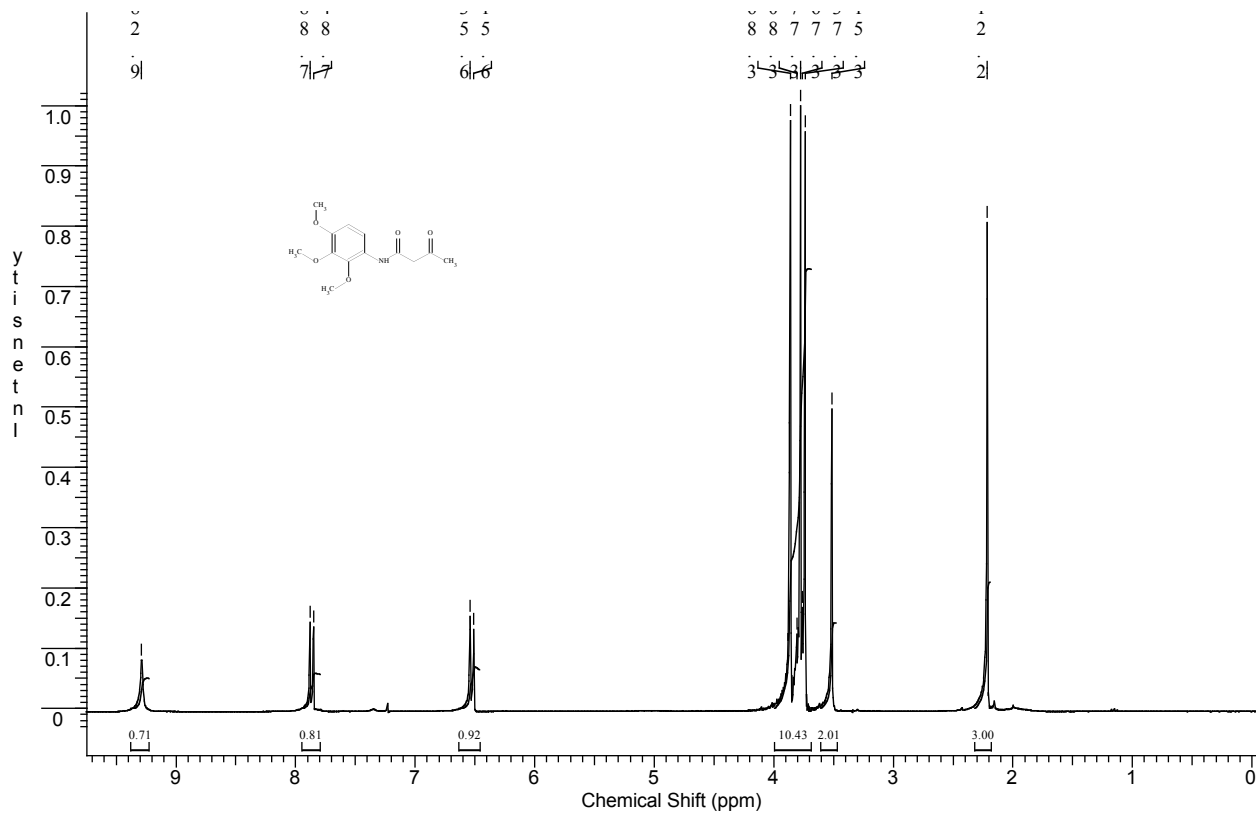




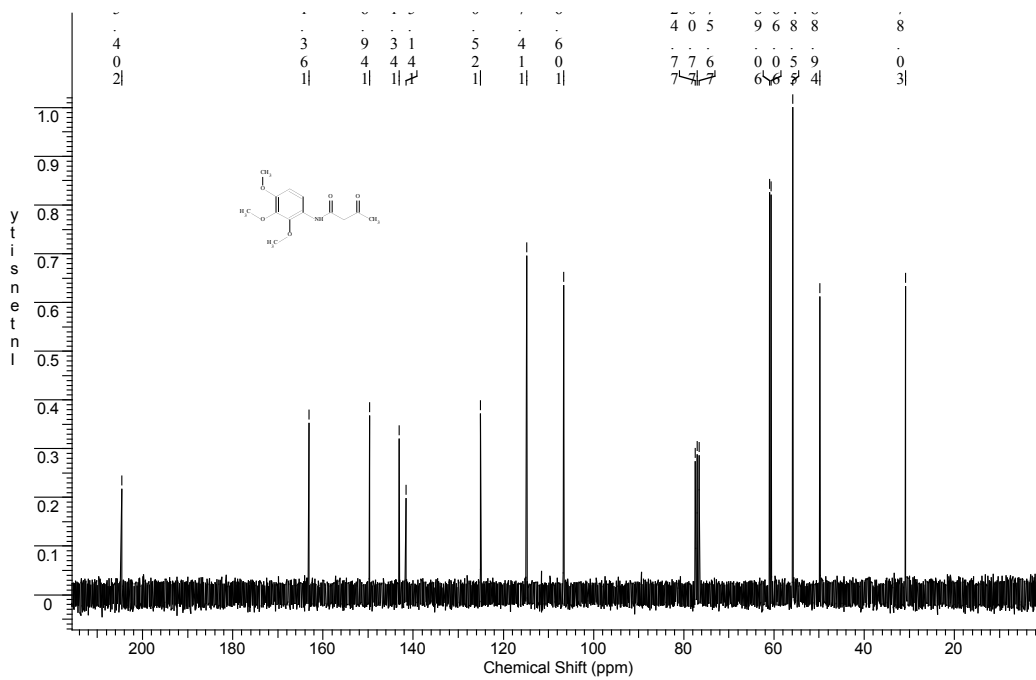
**<sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz) of Compound 10l**



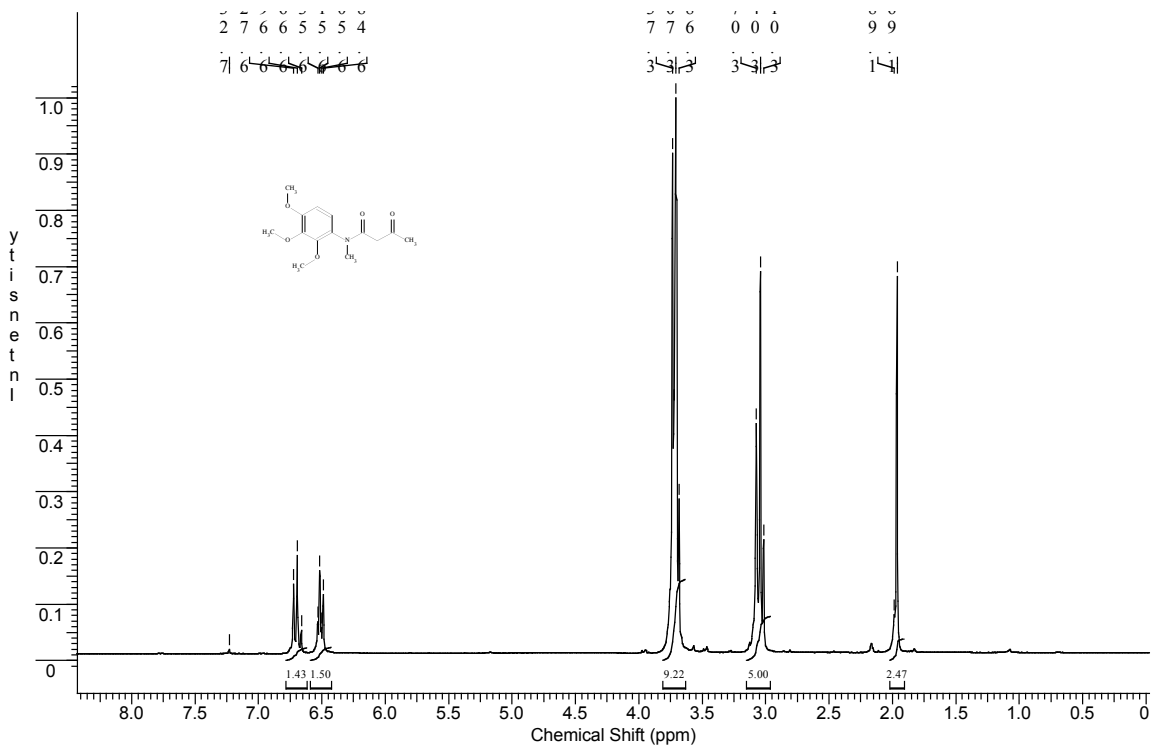
**<sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz) of Compound 10l**



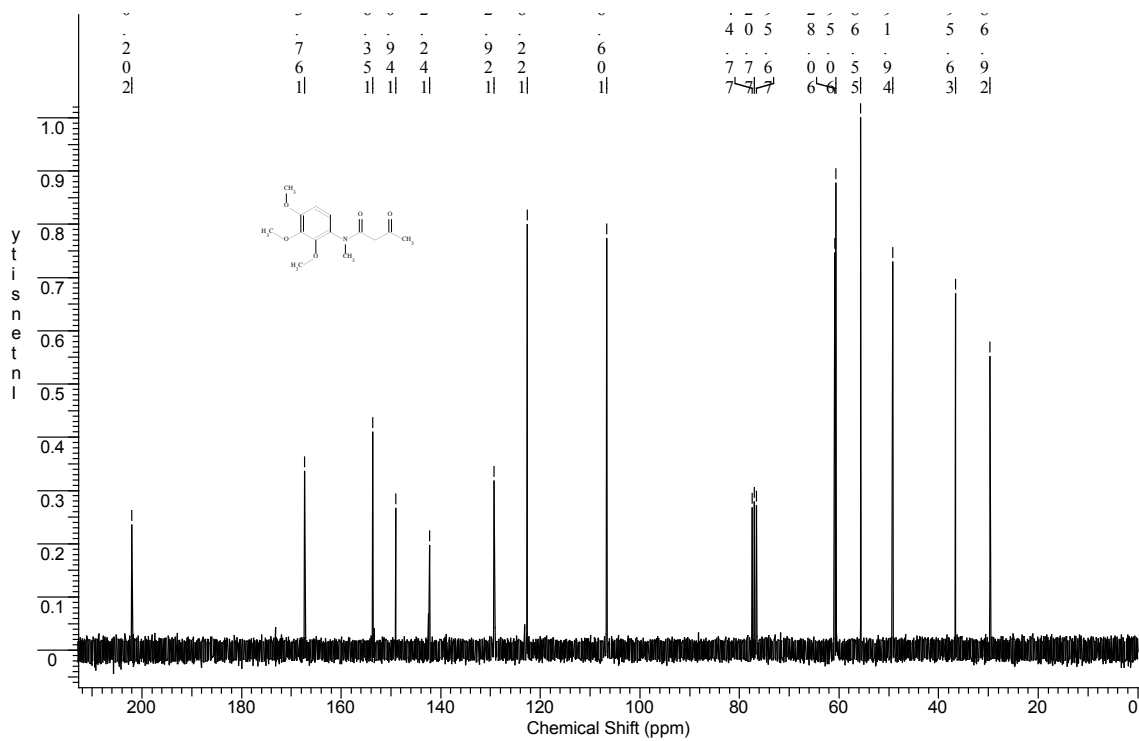
**<sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz) of Compound 10m**



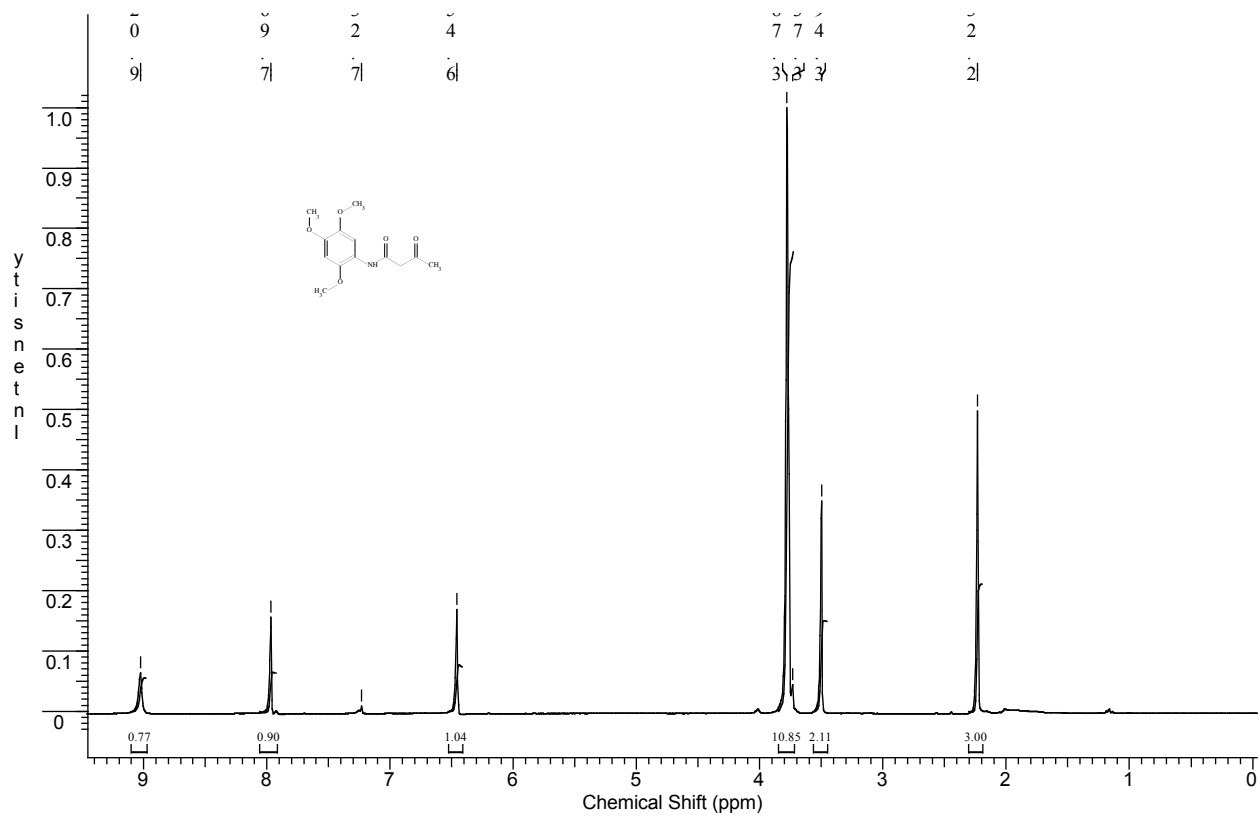
**<sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz) of Compound 10m**



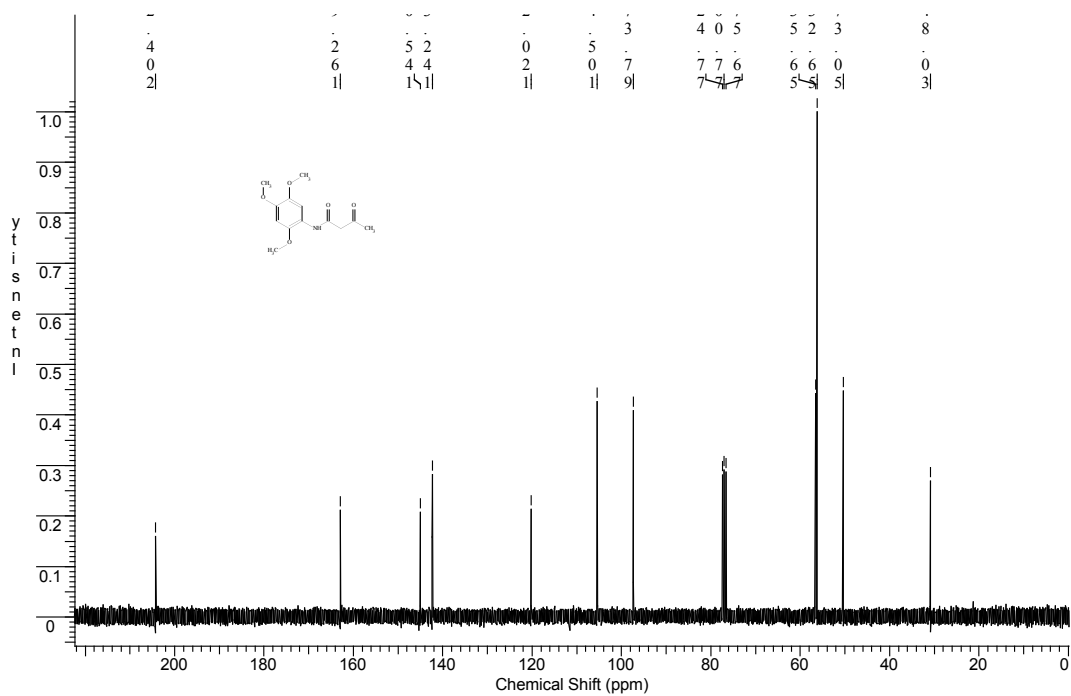
**<sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz) of Compound 10n**



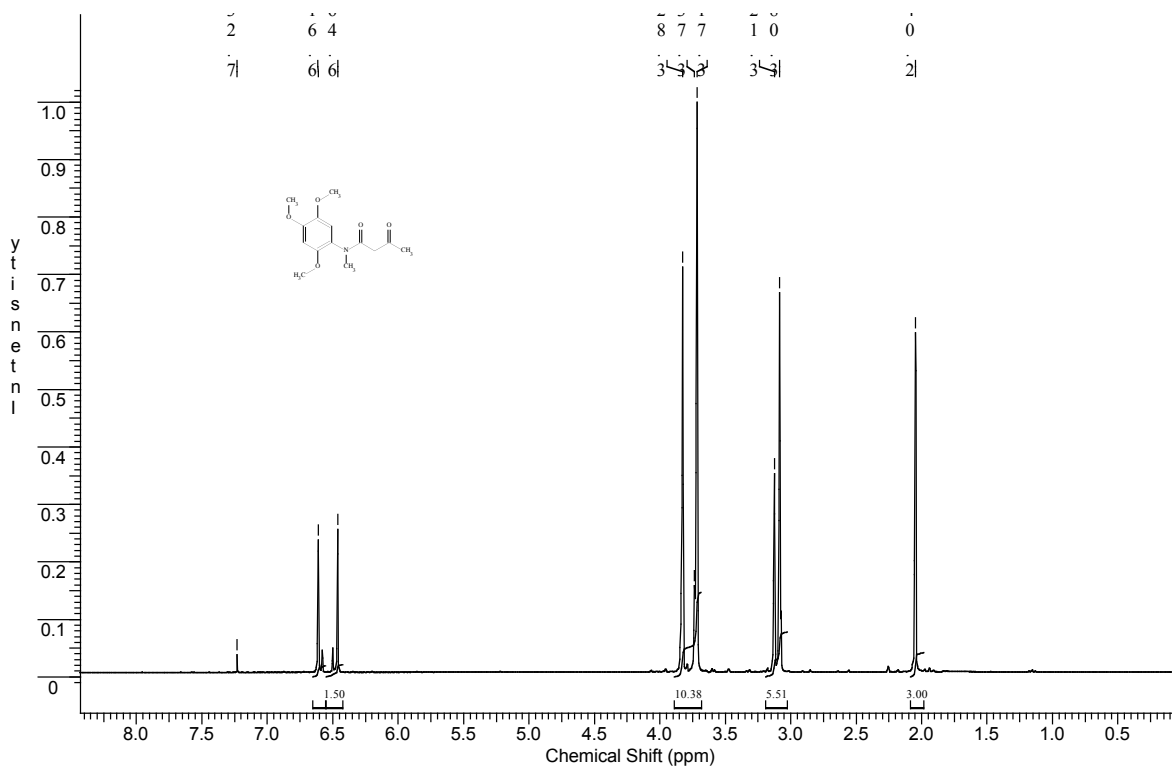
**<sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz) of Compound 10n**



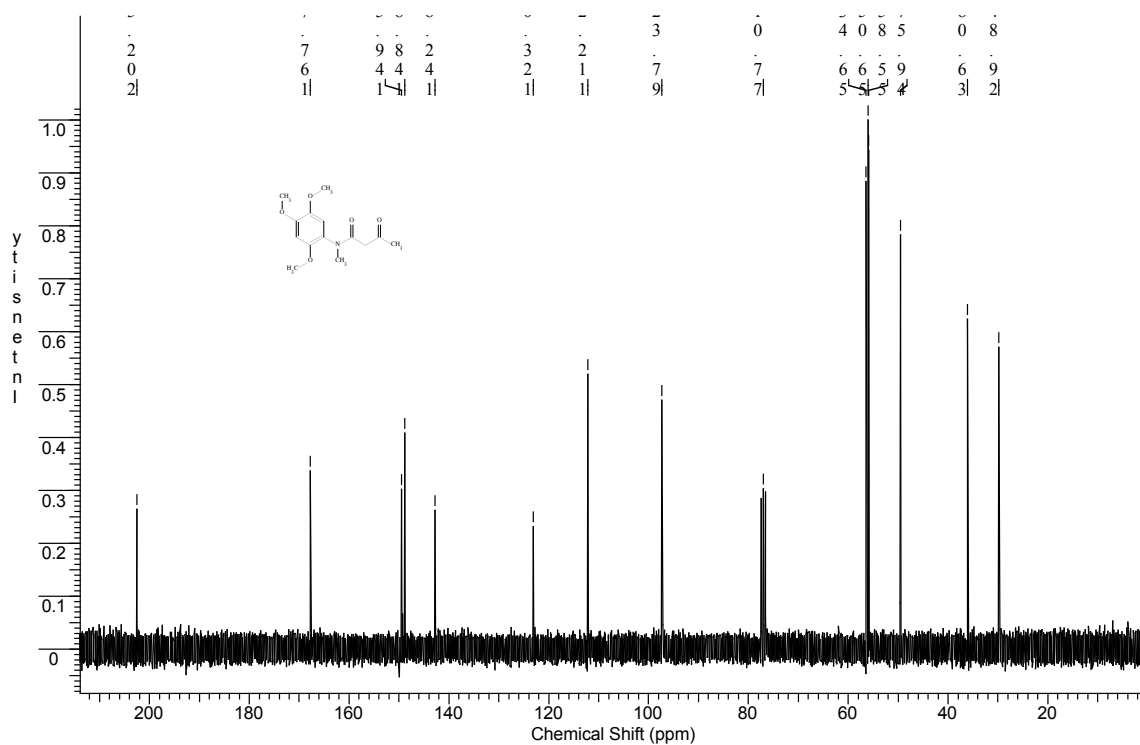
**<sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz) of Compound 10o**



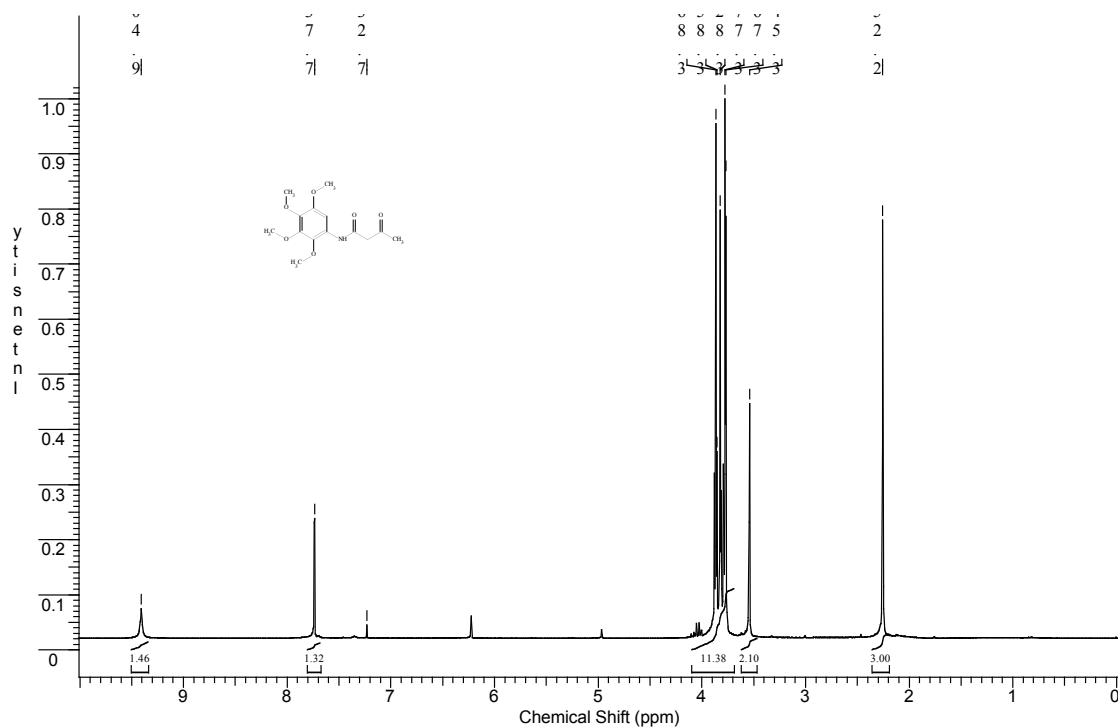
**<sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz) of Compound 10o**



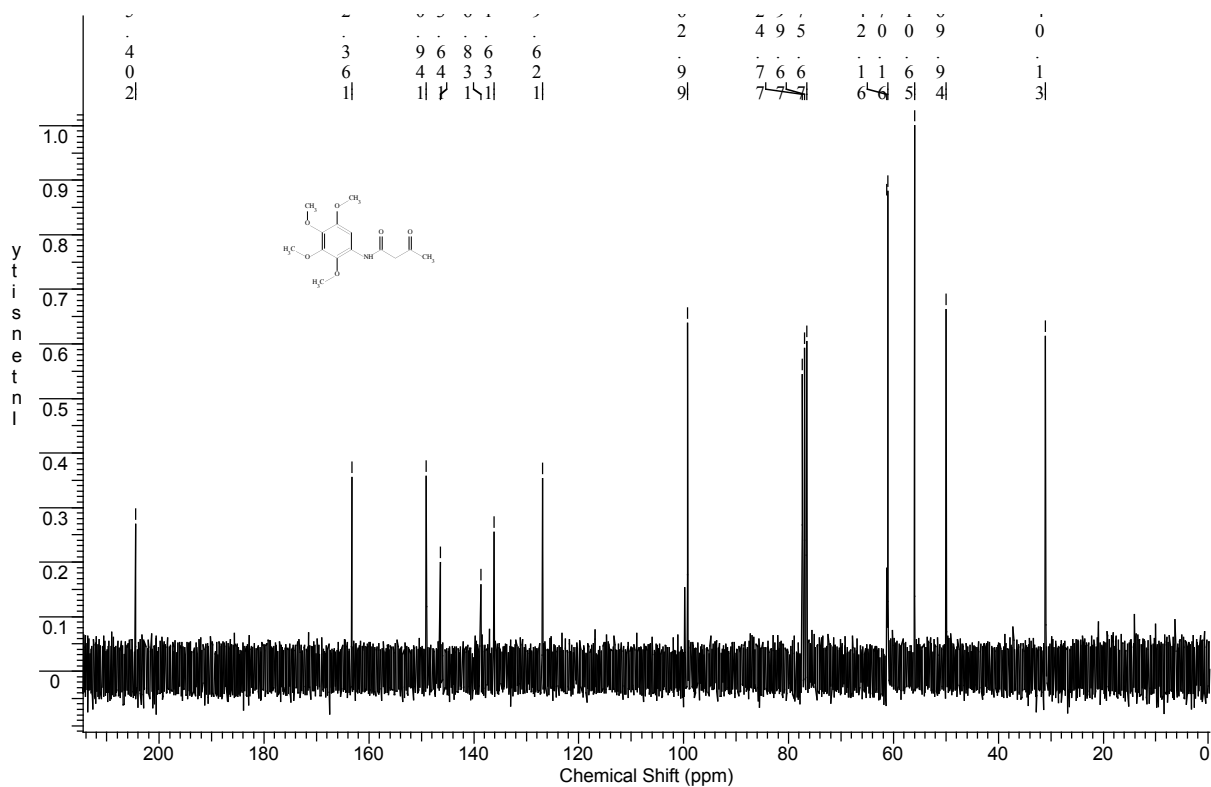
**<sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz) of Compound 10p**



**<sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz) of Compound 10p**



**<sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz) of Compound 10q**



**<sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz) of Compound 10q**