

## Supporting Information

### **New Safrole Oxide Derivatives: Synthesis and *in vitro* Antiproliferative Activities on A549 Human Lung Cancer Cells**

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Liang Fang,<sup>†</sup> Hua Zuo,<sup>\*</sup> Gautam Dupati,<sup>‡</sup> Kiwan Jang,<sup>‡</sup> and Dong-Soo Shin<sup>\*,‡</sup>**

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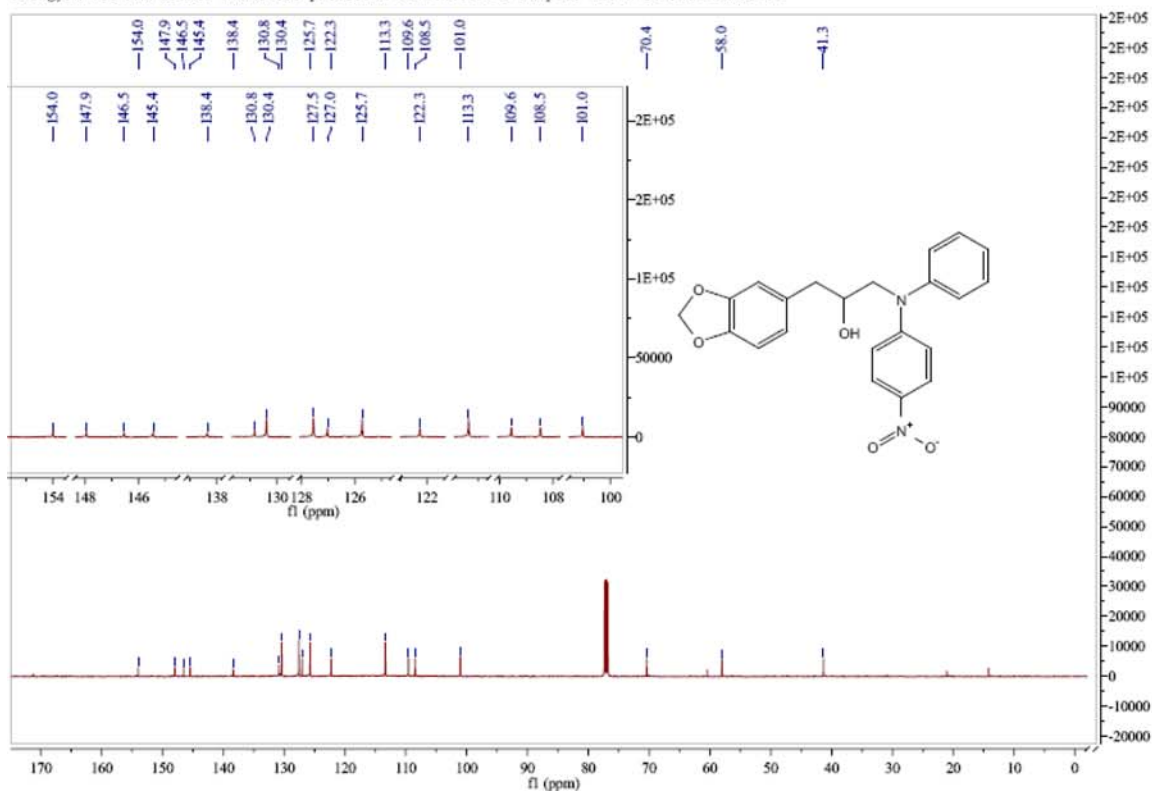
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*\*E-mail: dsshin@changwon.ac.kr*

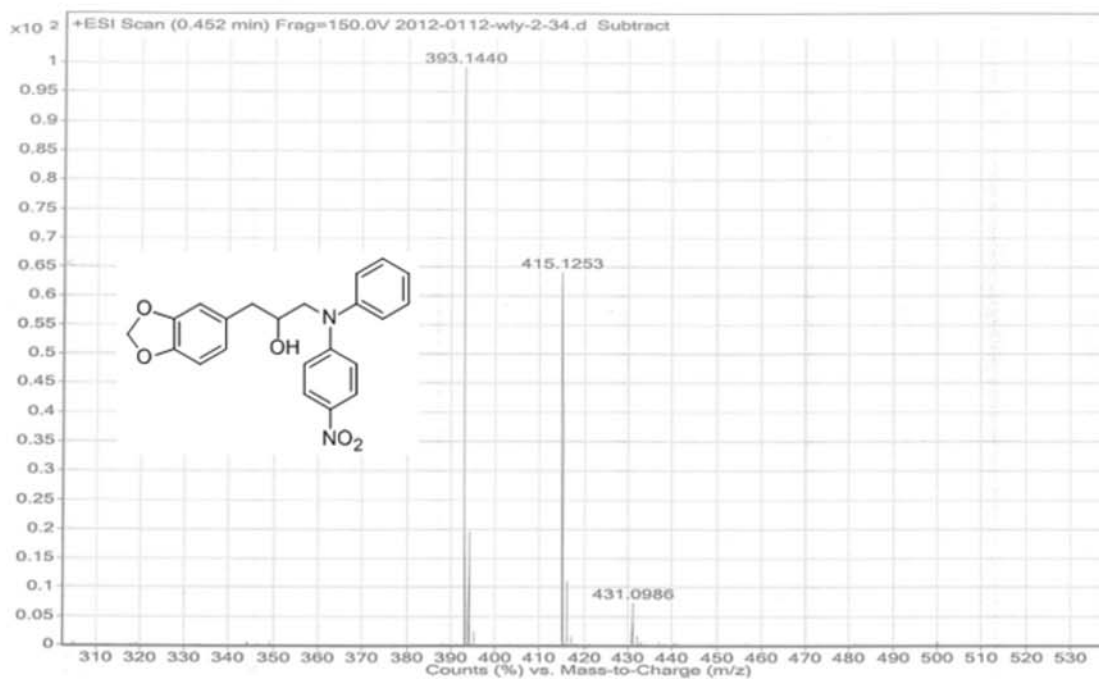
*Received May 29, 2012, Accepted August 1, 2012*

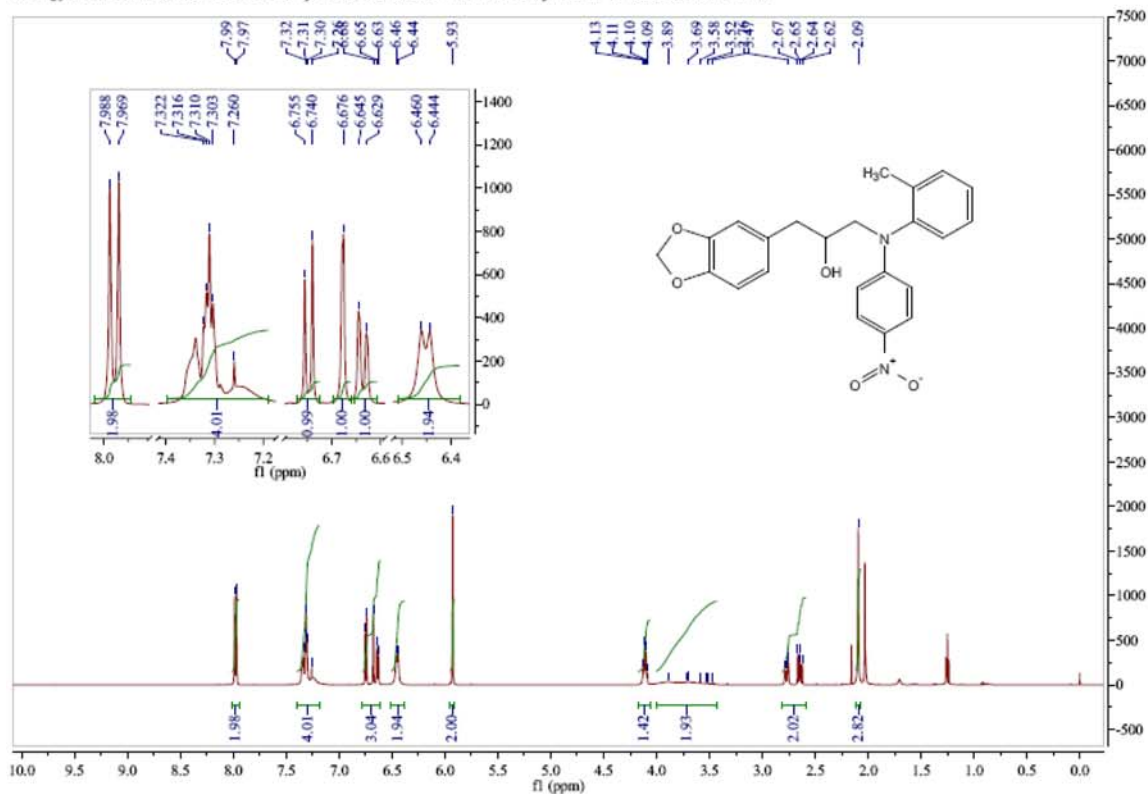
### Compound 2

xiongyan 13C NMR Bruker Avance500 probe:TXI solvent:CDCl3 sample: WLY-2-34 date:20110108

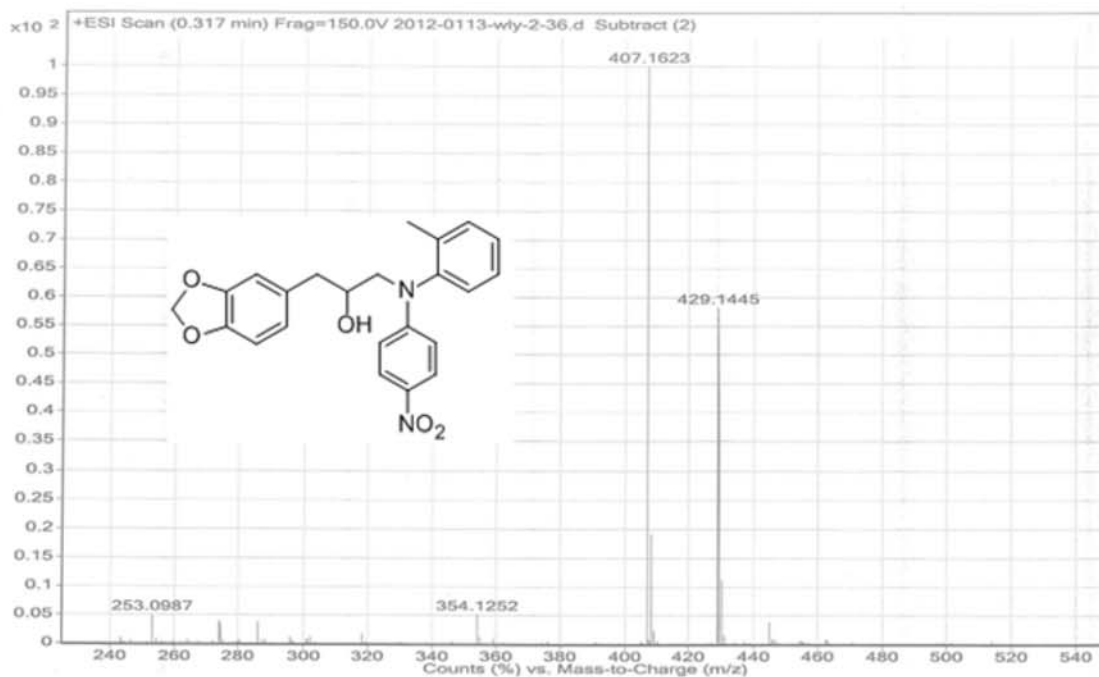


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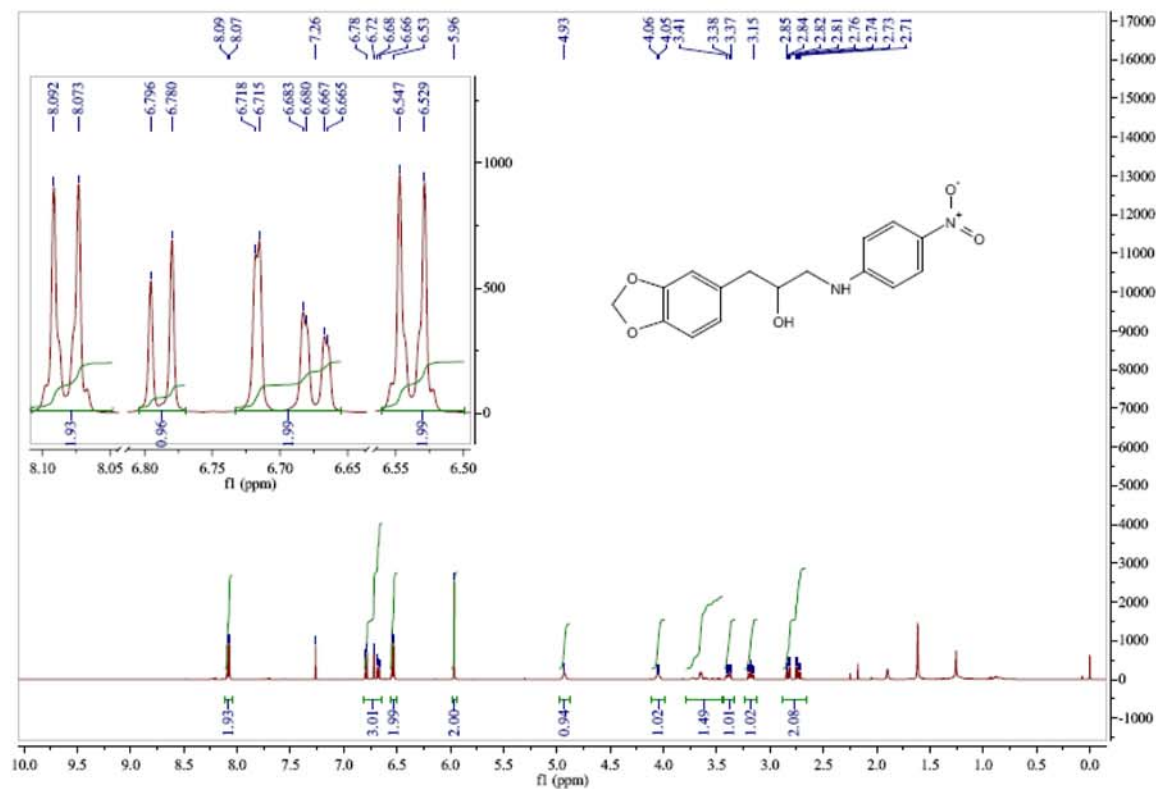
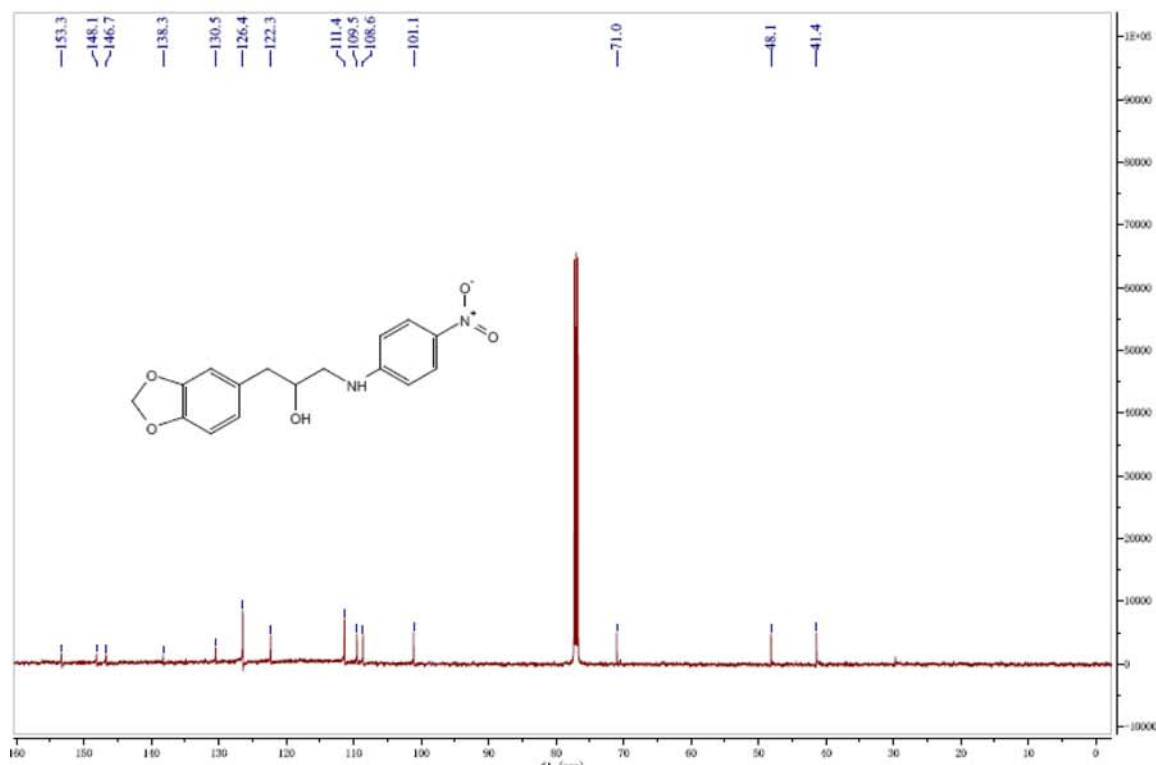


Compound **4b**xiongyan <sup>1</sup>H NMR Bruker Avance500 probe:TXI solvent:CDCl<sub>3</sub> sample:WLY-2-36 date:20110111

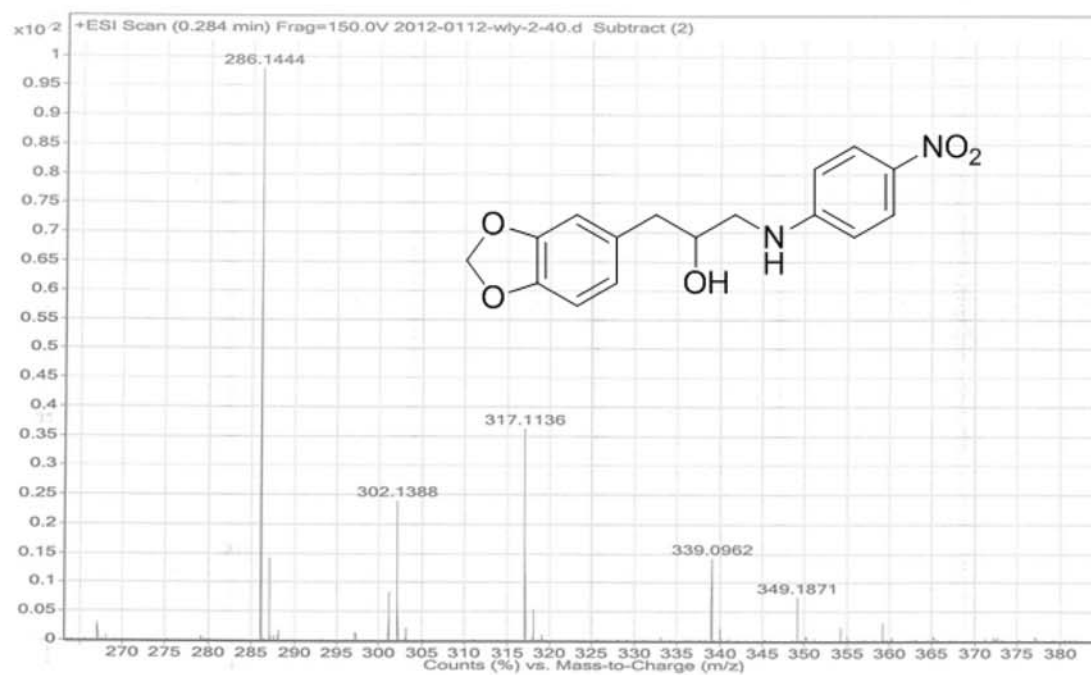
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## Compound 4c

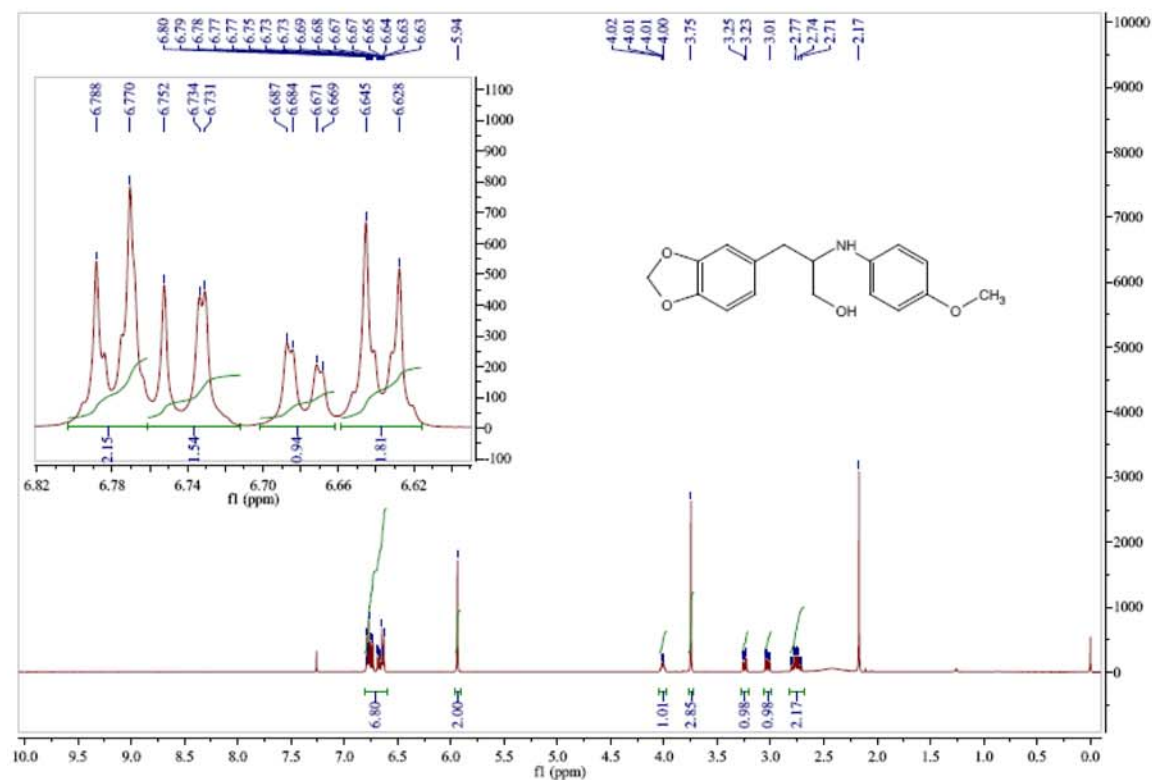
xiongyan <sup>1</sup>H NMR Bruker Avance500 probe:TXI solvent:CDCl<sub>3</sub> sample:WLY-2-40 date:20110109xiongyan <sup>13</sup>C NMR Bruker Avance500 probe:TXI solvent:CDCl<sub>3</sub> sample:WLY-2-40 date:20110109

Sample Name	2012-0112-wly-2-40	Position	P1-A2	Instrument Name	Instrument 1	User Name	
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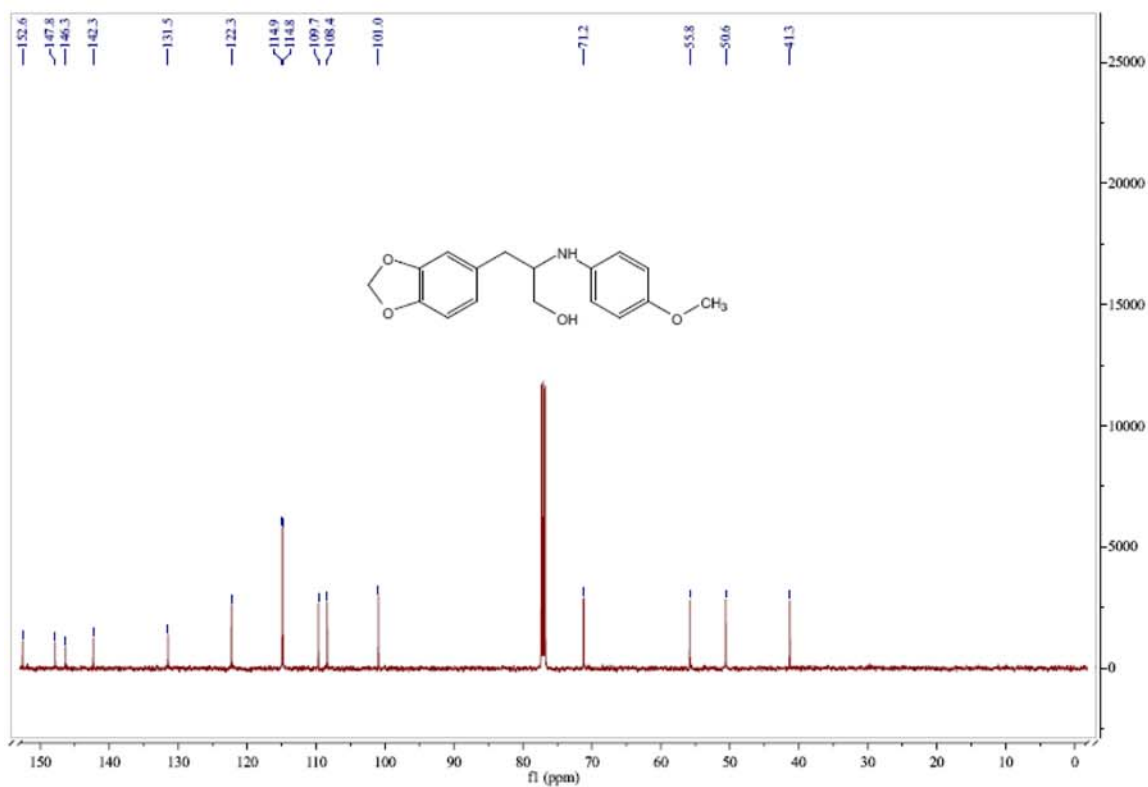


## Compound 6a

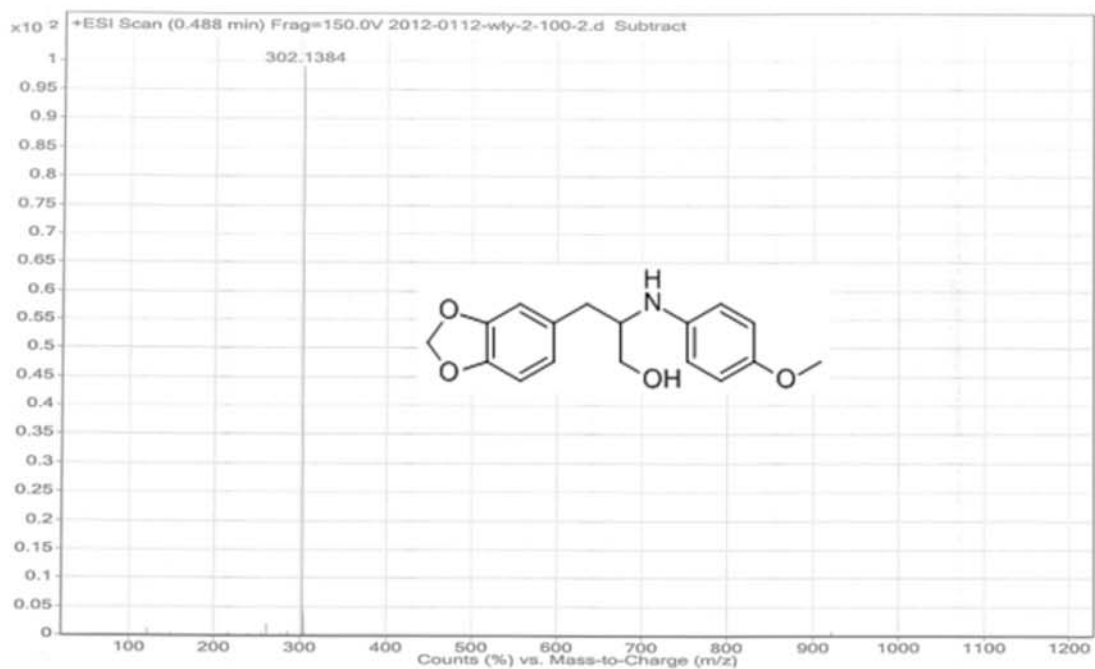
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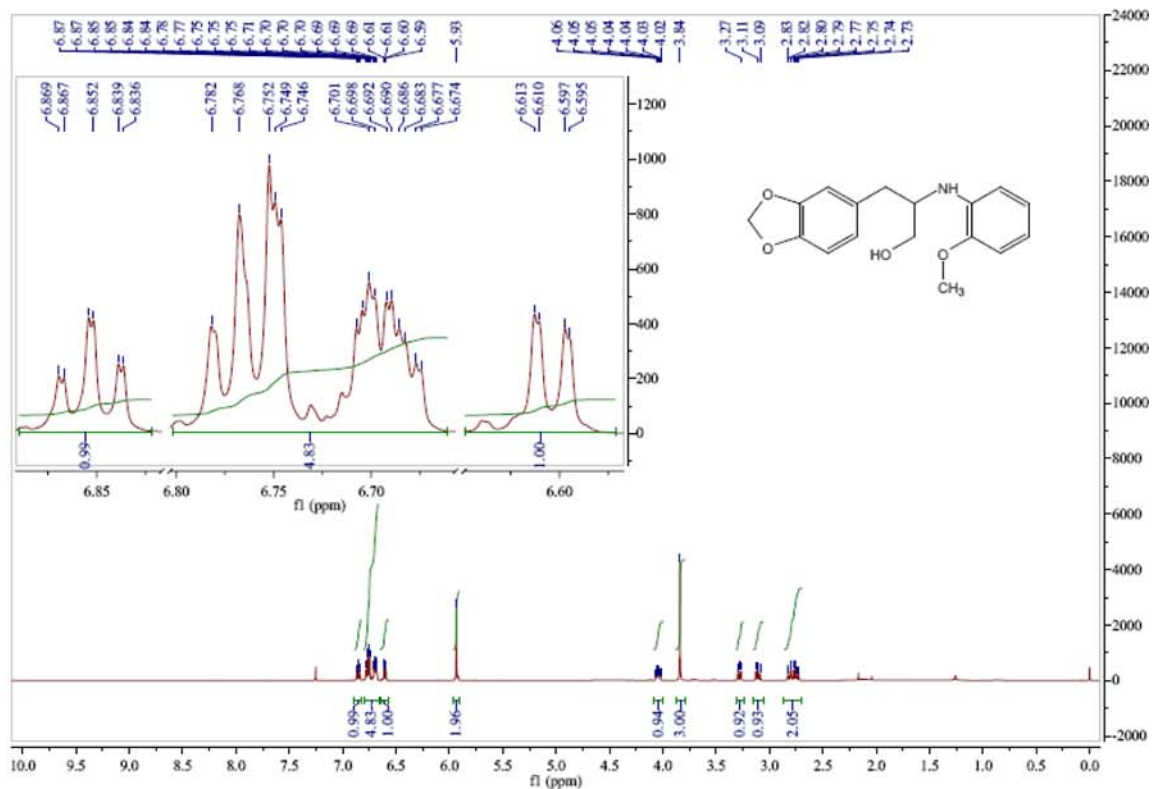
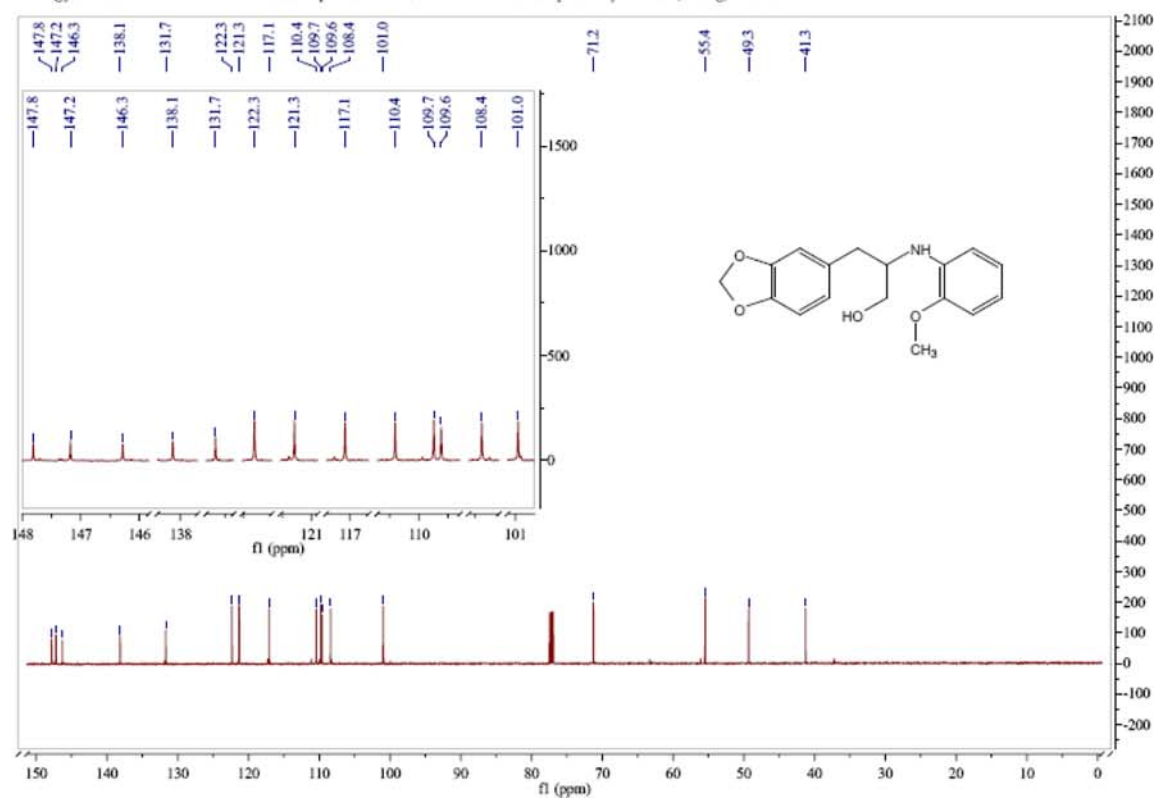


xiongyan 13C NMR Bruker Avance500 probe:BB0 solvent:CDCl3 sample:wly-2-100(1) date:20120104

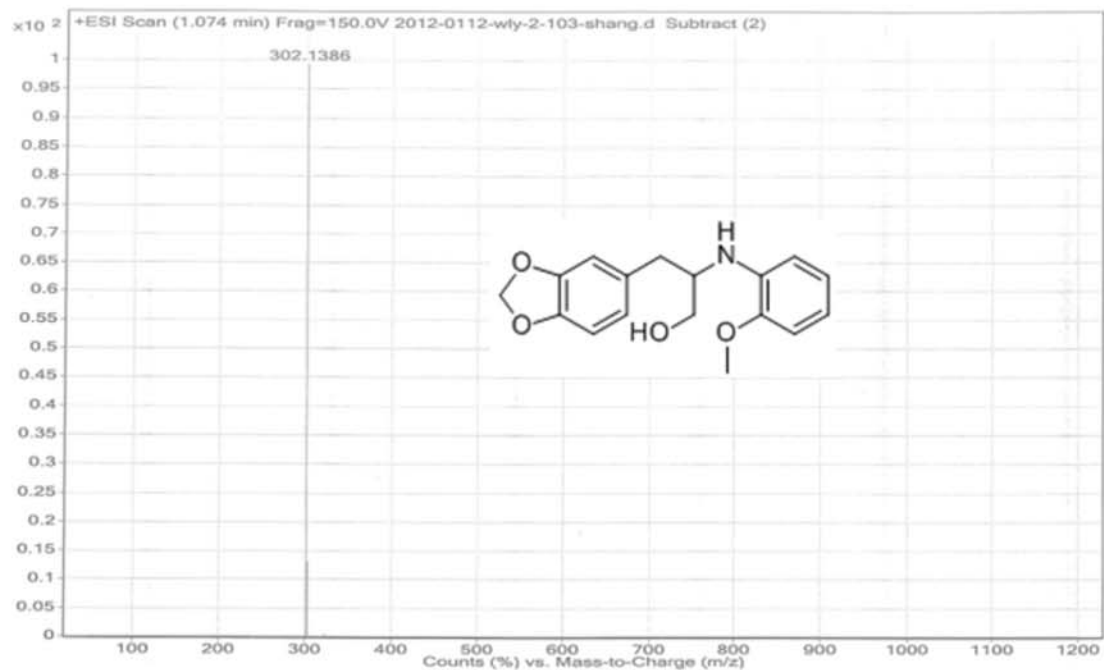


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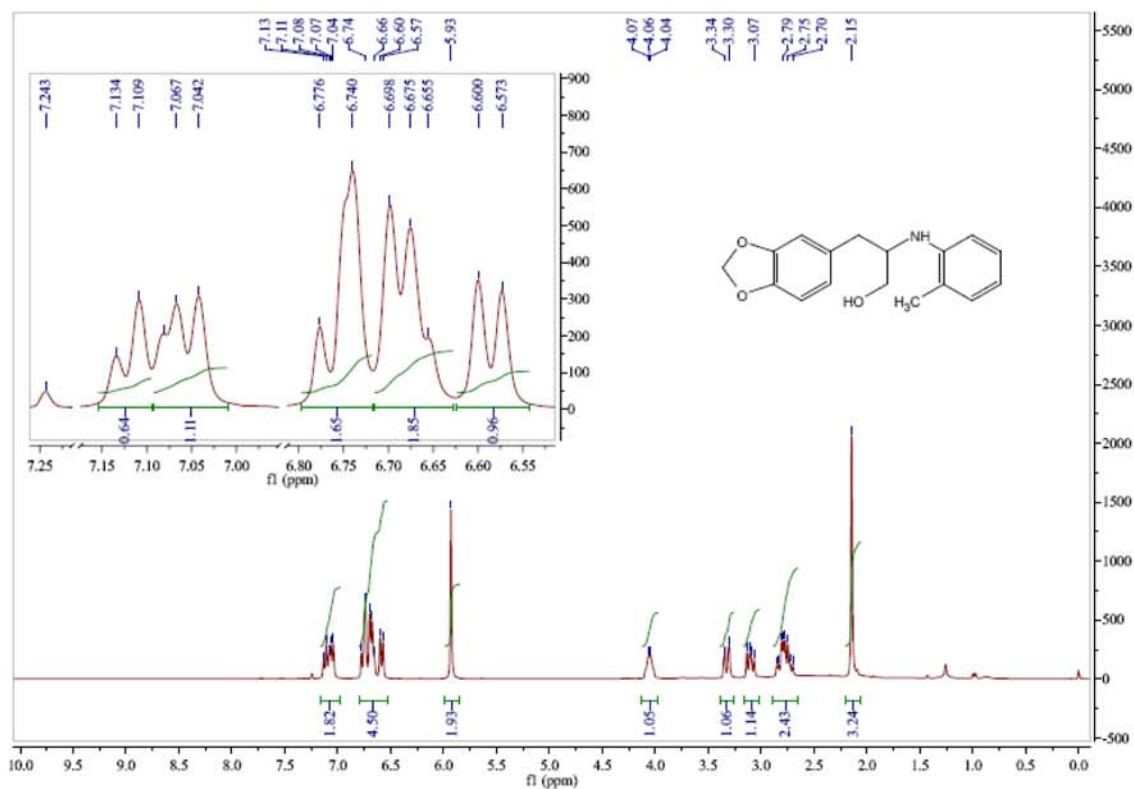


**Compound 6b**xiongyan <sup>1</sup>H NMR Bruker Avance500 probe:BBO solvent:CDCl<sub>3</sub> sample:wly-2-103(shang) date:20110930xiongyan <sup>13</sup>C NMR Bruker Avance500 probe:BBO solvent:CDCl<sub>3</sub> sample:wly-2-103(shang) date:20120104

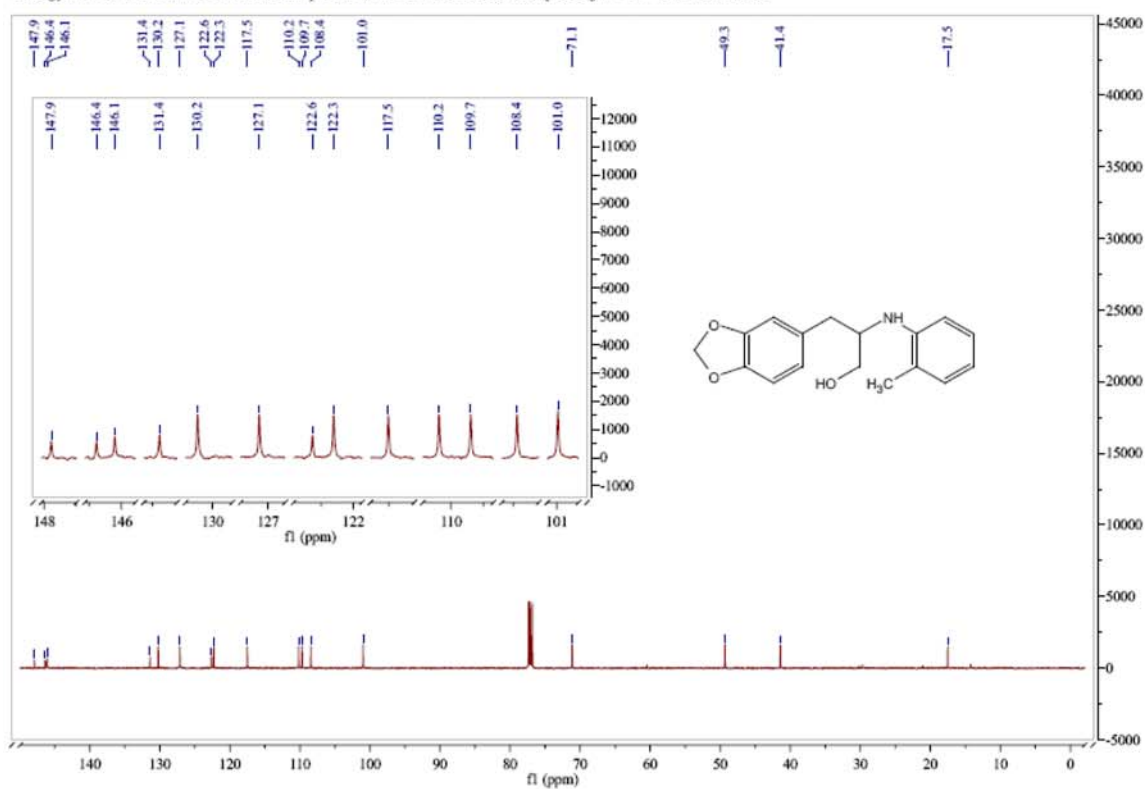
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Compound **6c**

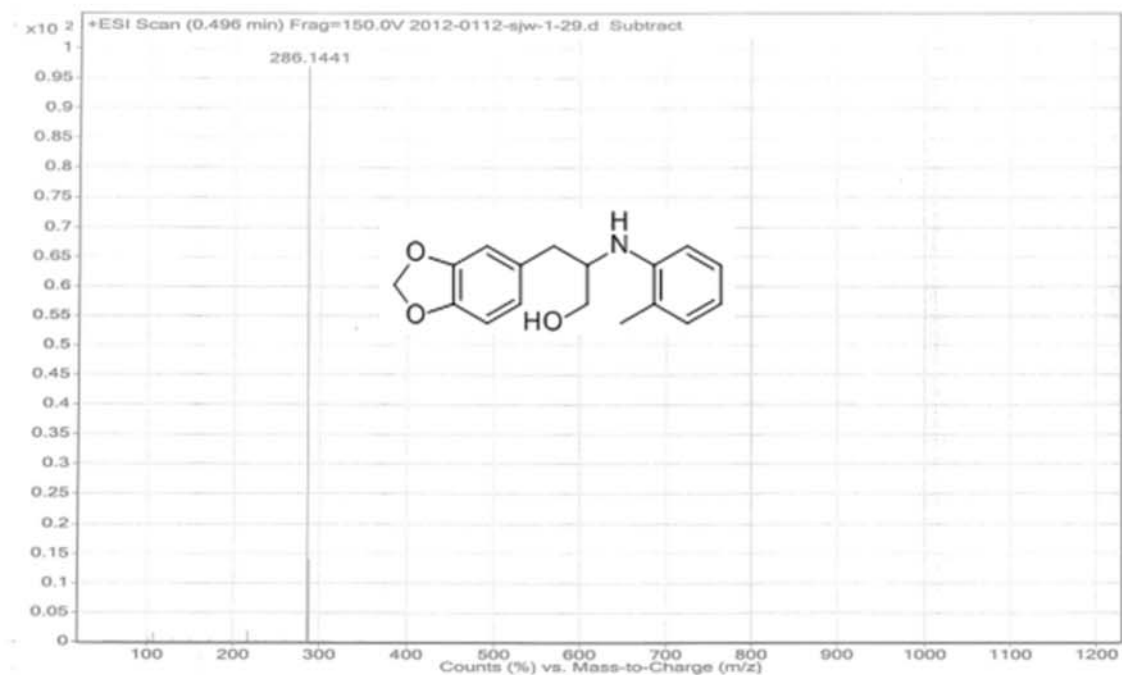
<sup>1</sup>H NMR Bruker Avance300 probe:BBO solvent:CDCl<sub>3</sub> sample:SHZ-1-4-A



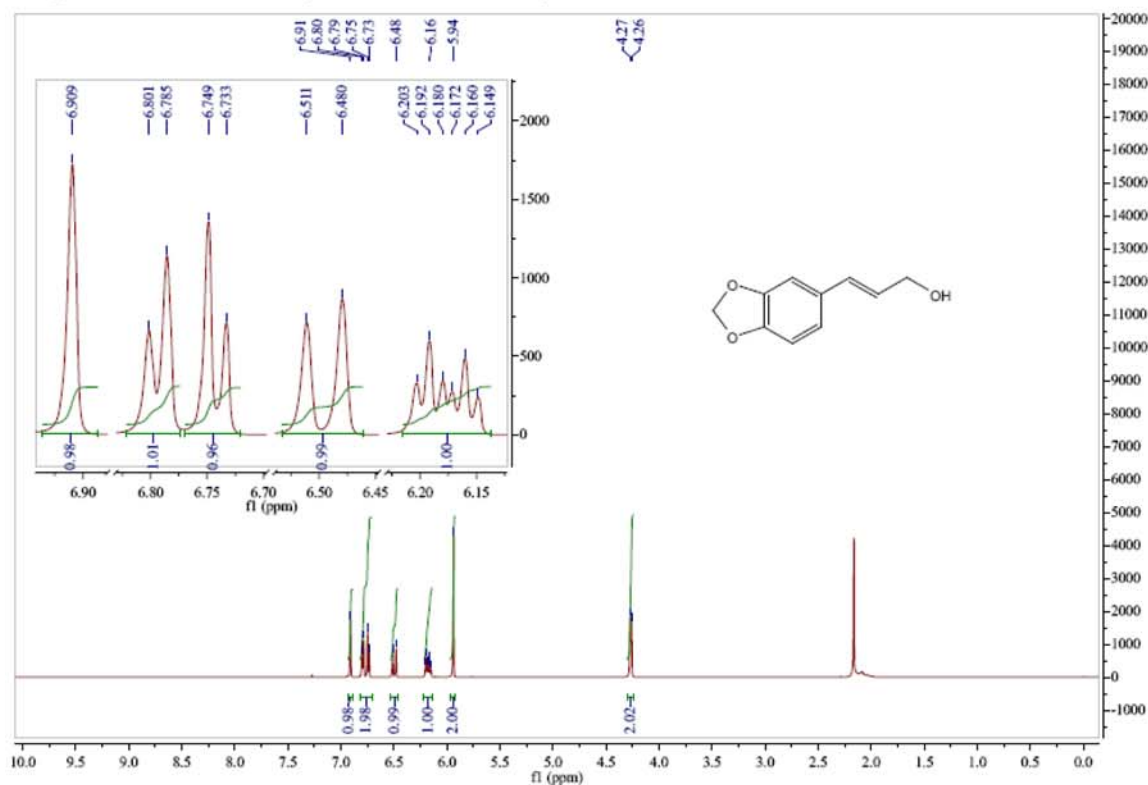
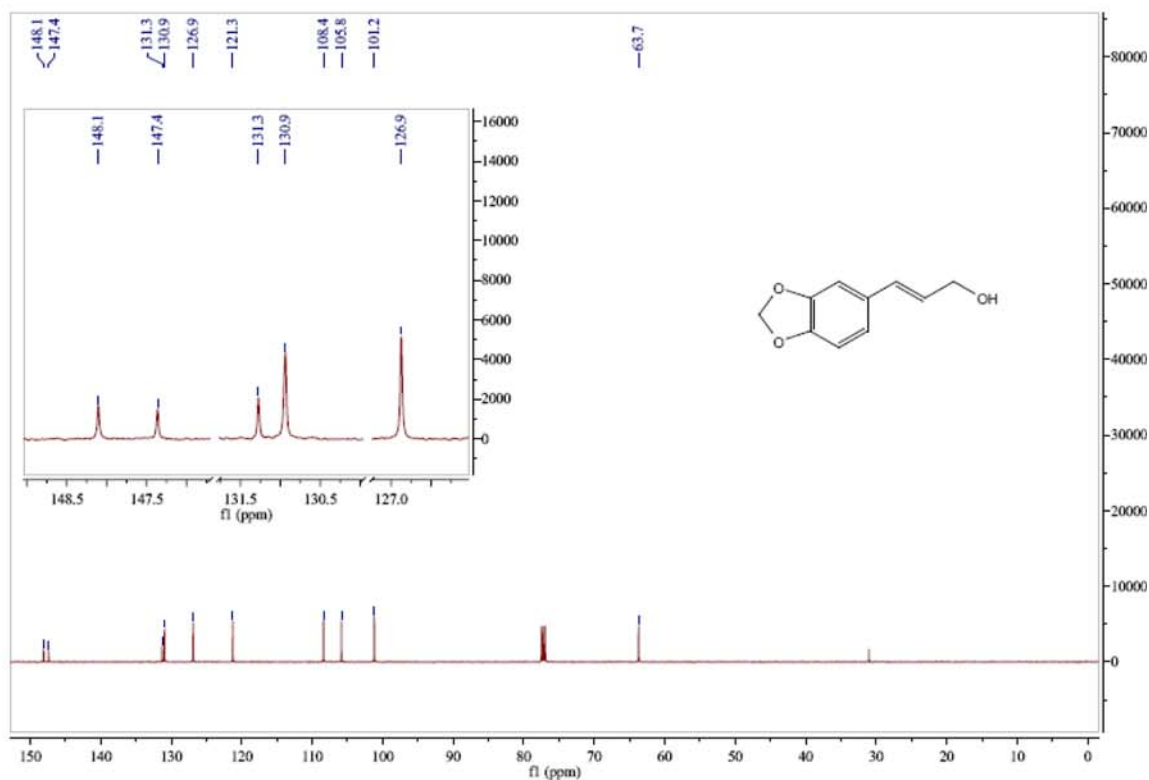
xiongyan 13C NMR Bruker Avance500 probe:BB0 solvent:CDCl3 sample:sjw-1-29 date:20111212

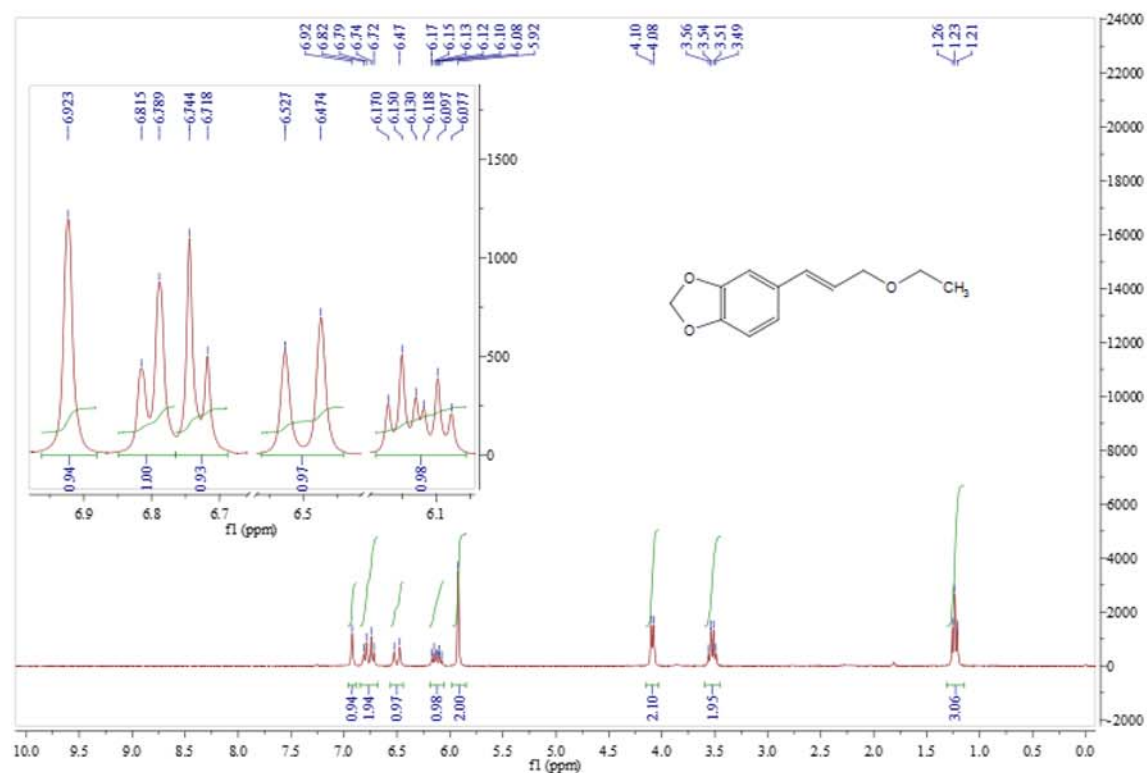
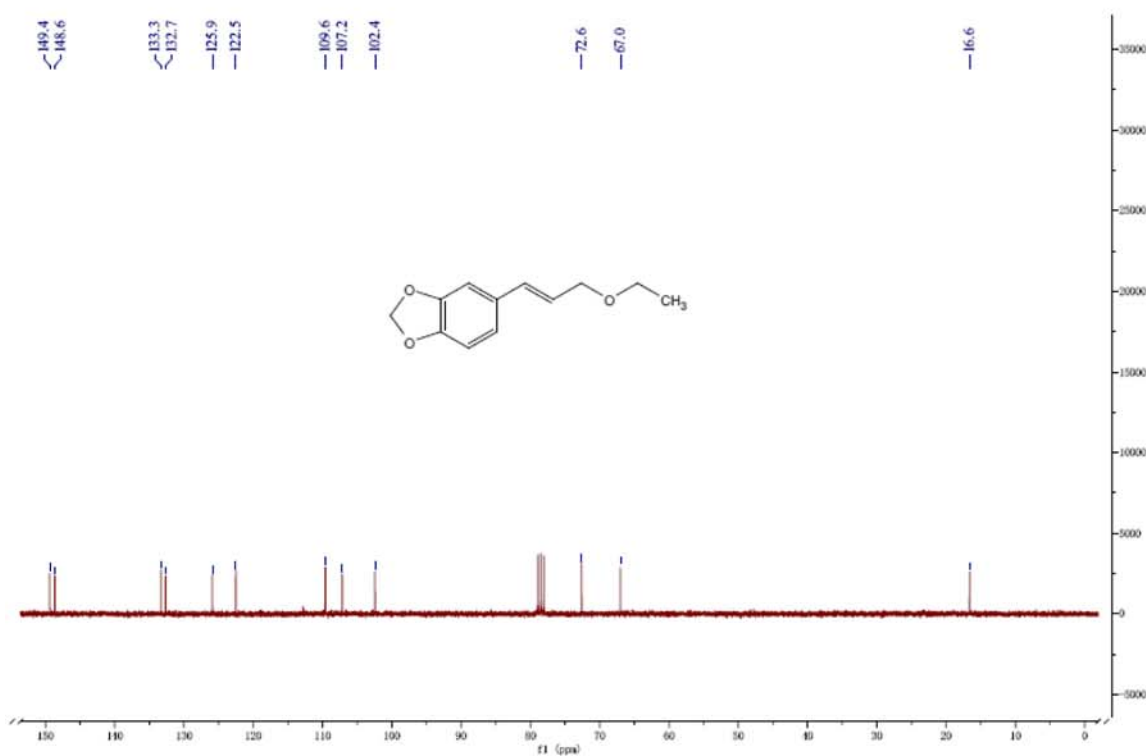


Sample Name	2012-0112-sjw-1-29	Position	P1-02	Instrument Name	Instrument 1	User Name	
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## Compound 7

xiongyan <sup>1</sup>H NMR Bruker Avance500 probe:BBO solvent:CDCl<sub>3</sub> sample:ZHY-1-5 date:20110510xiongyan <sup>13</sup>C NMR Bruker Avance500 probe:BBO solvent:CDCl<sub>3</sub> sample:ZHY-1-5 date:20110510

**Compound 9a**<sup>1</sup>H NMR Bruker Avance300 Solvent:CDCl<sub>3</sub> sample:TJL-1-23<sup>13</sup>C NMR Bruker Avance300 Solvent:CDCl<sub>3</sub> sample:TJL-1-23

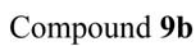


Figure 1 displays the  $^1\text{H}$  NMR spectra of compound **1**. The top spectrum is recorded in  $\text{CDCl}_3$ , and the bottom spectrum is recorded in  $\text{DMSO}-d_6$ . The chemical structure of compound **1** is shown in the center.

**Chemical Structure of Compound 1:**

CCCCOCC/C=C/c1ccc2c(c1)OCO2

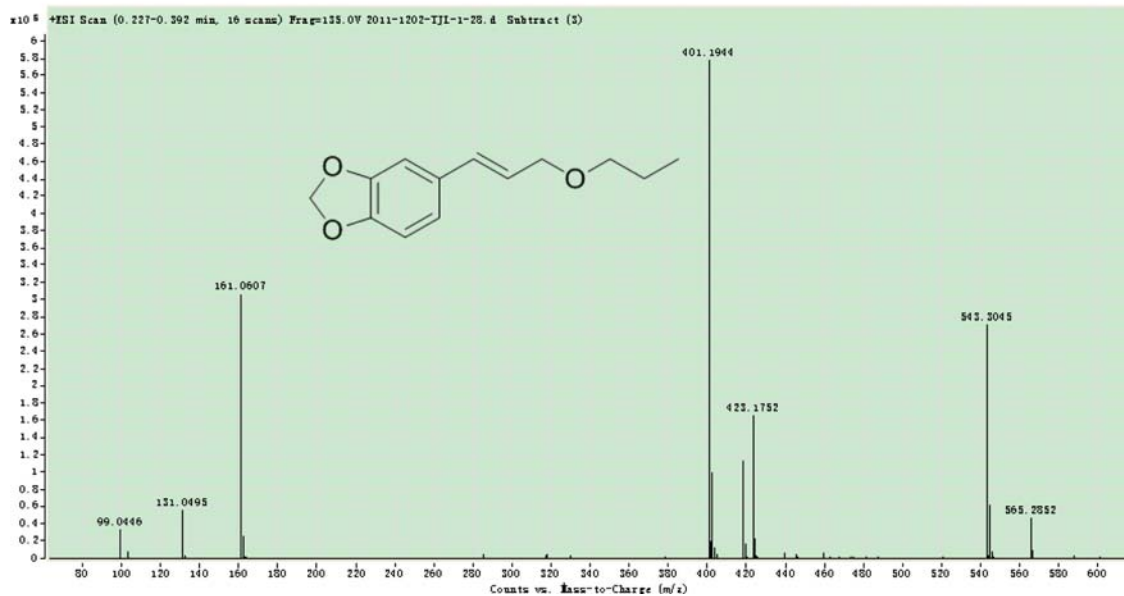
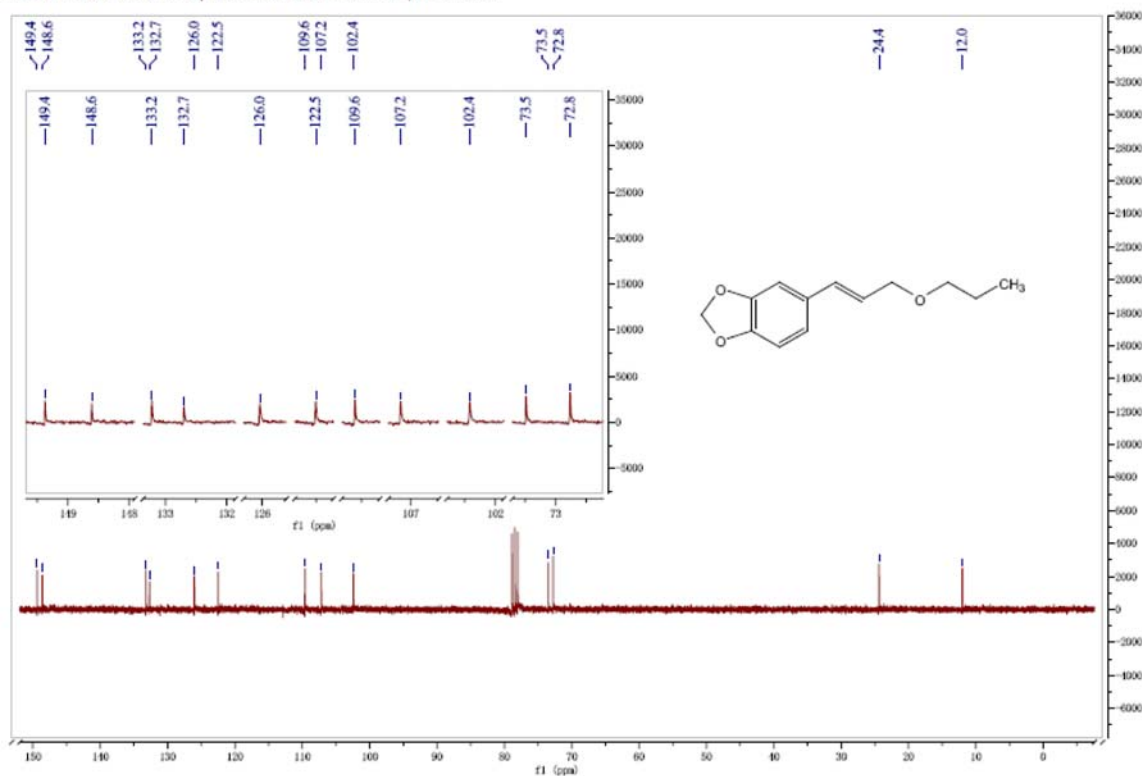
**$^1\text{H}$  NMR Data (Top Spectrum,  $\text{CDCl}_3$ ):**

Chemical Shift (ppm)	Integration
6.94, 6.83, 6.81, 6.80, 6.76, 6.73	0.94
6.54, 6.49	1.00
6.16, 6.13, 6.11, 6.11, 6.09, 6.09	0.92
4.1, 4.0, 3.5, 3.46, 3.43, 3.41	0.99
2.12, 2.05	2.12
1.67, 1.65, 1.63, 1.60, 1.58	1.95
0.97, 0.95, 0.92	3.01

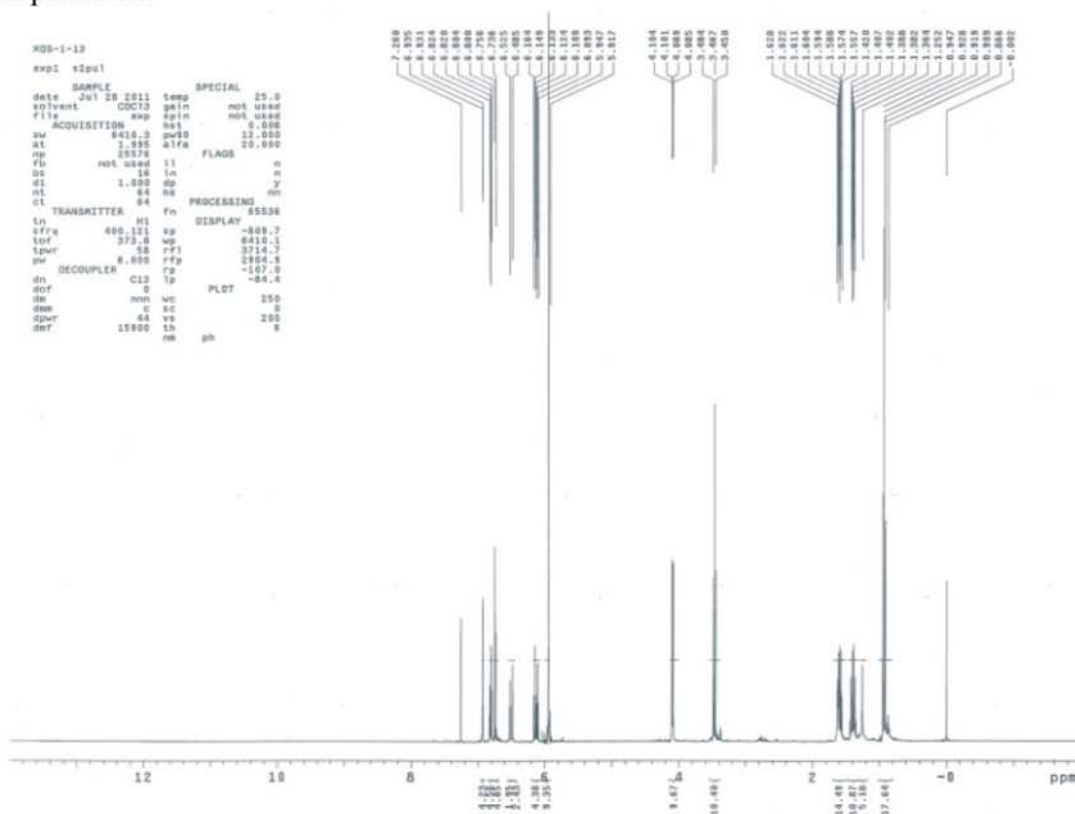
**$^1\text{H}$  NMR Data (Bottom Spectrum,  $\text{DMSO}-d_6$ ):**

Chemical Shift (ppm)	Integration
6.94, 6.83, 6.81, 6.80, 6.76, 6.73	0.94
6.54, 6.49	1.93
6.16, 6.13, 6.11, 6.11, 6.09, 6.09	0.99
4.1, 4.0, 3.5, 3.46, 3.43, 3.41	0.99
2.12, 2.05	2.00
1.67, 1.65, 1.63, 1.60, 1.58	2.12
0.97, 0.95, 0.92	2.05

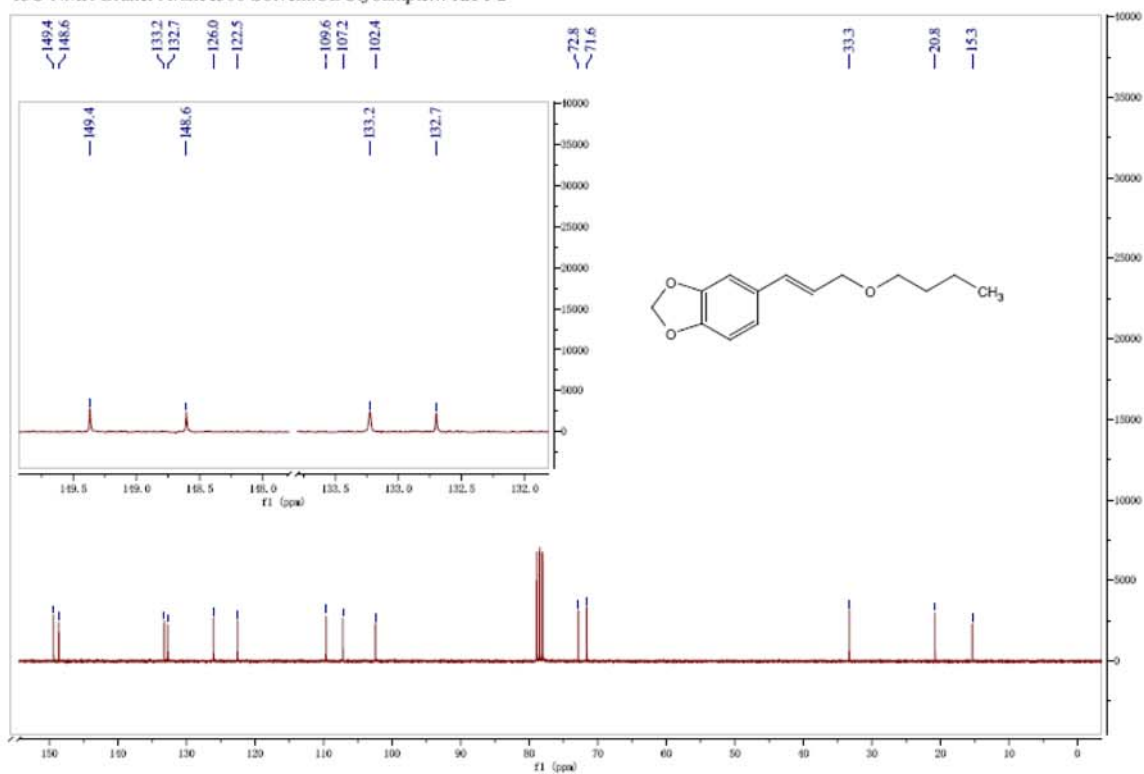
<sup>13</sup>C NMR Bruker Avance300 probe:BBO solvent:CDCl<sub>3</sub> sample:TJL-1-28

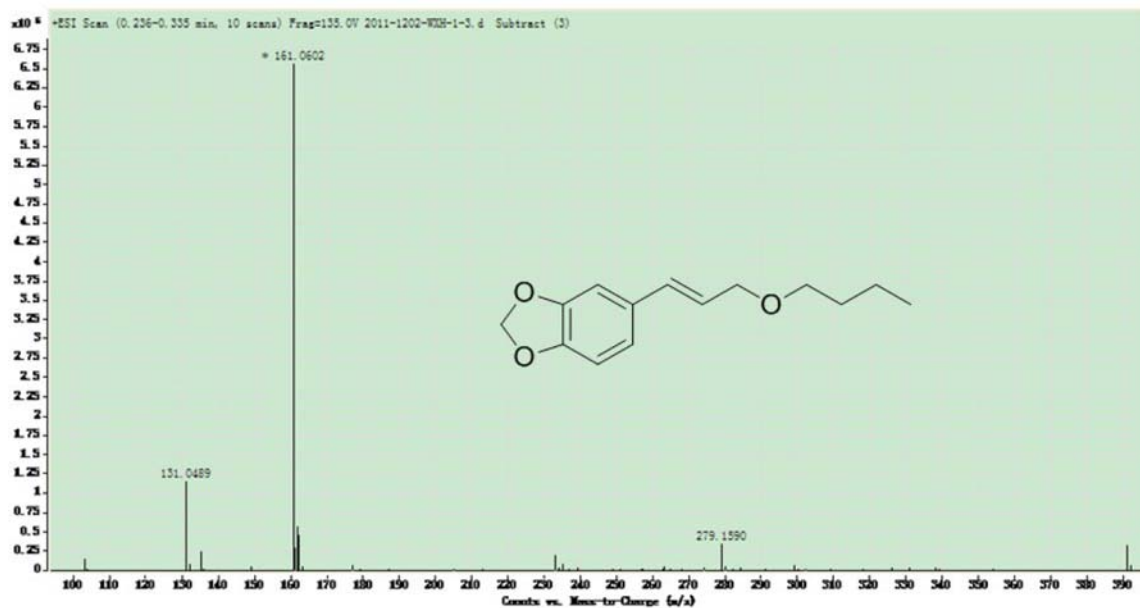


### Compound 9c



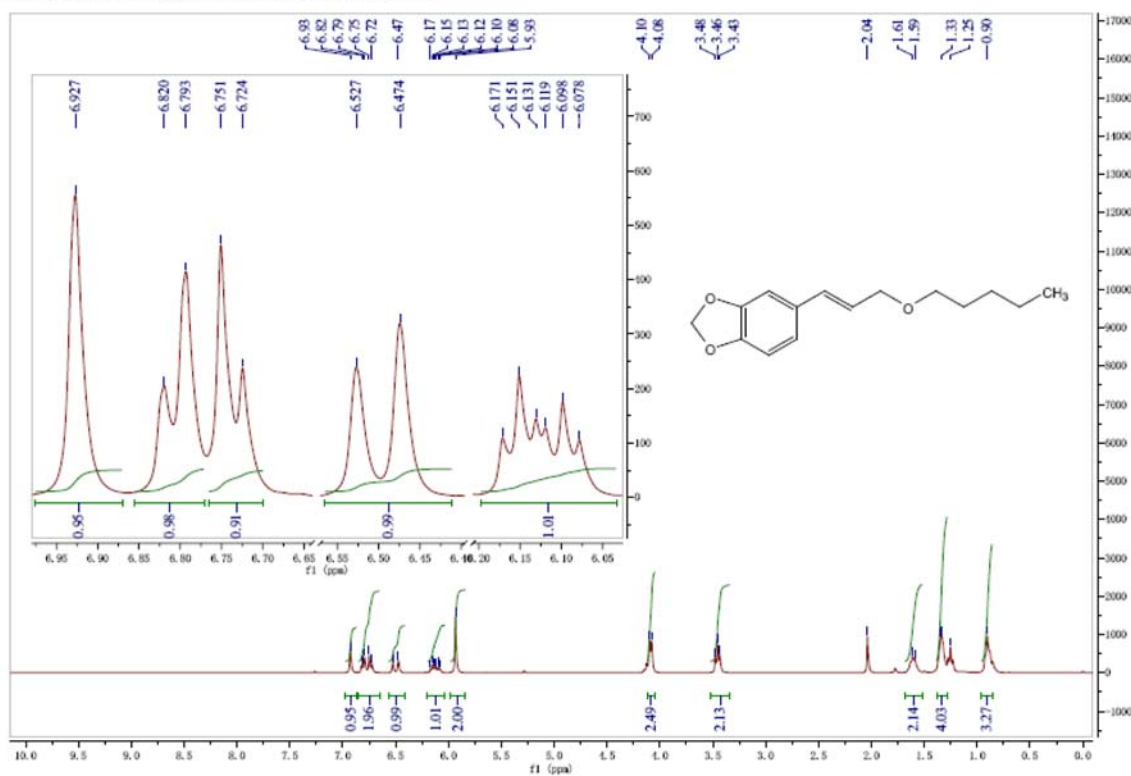
<sup>13</sup>C NMR Bruker Avance300 Solvent:CDCl<sub>3</sub> sample:W XH-1-2



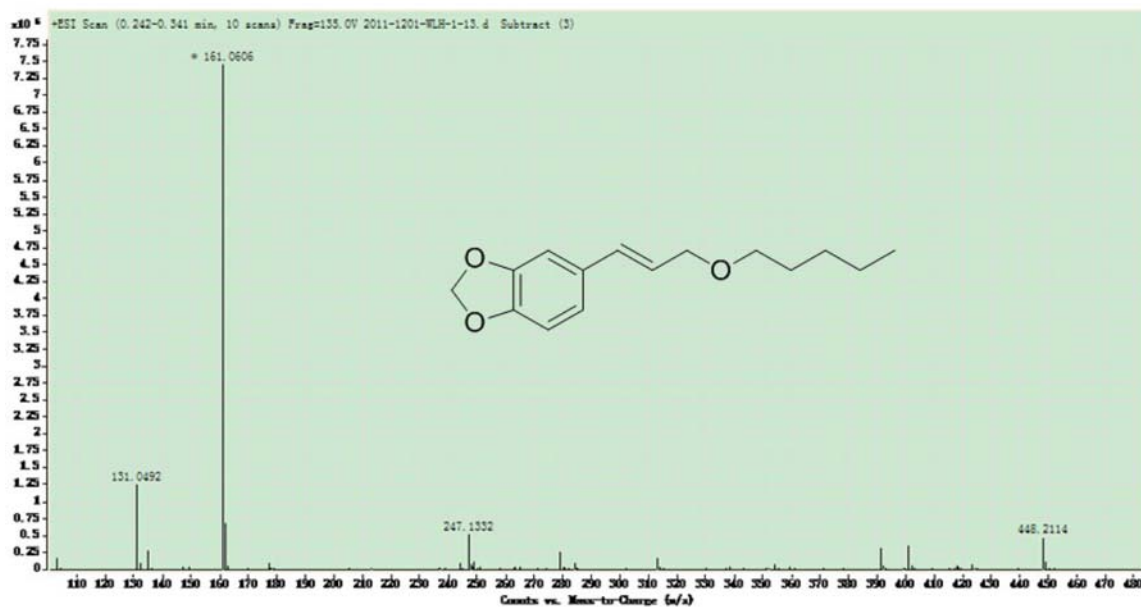
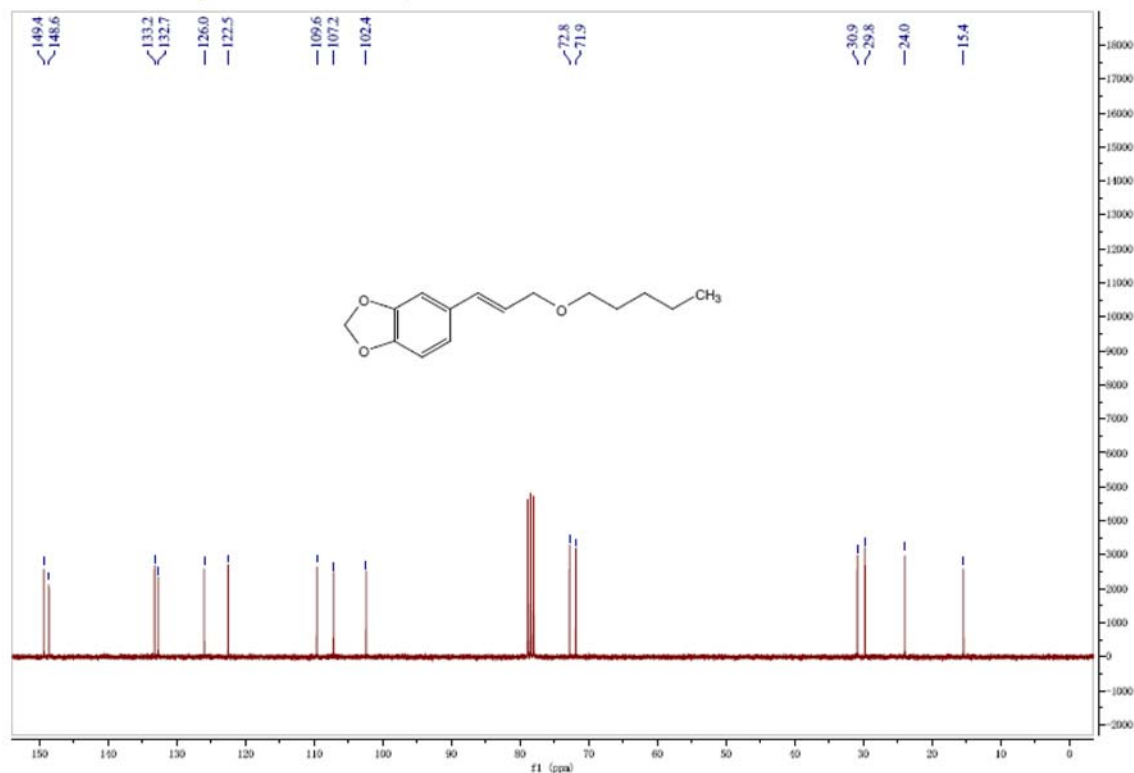


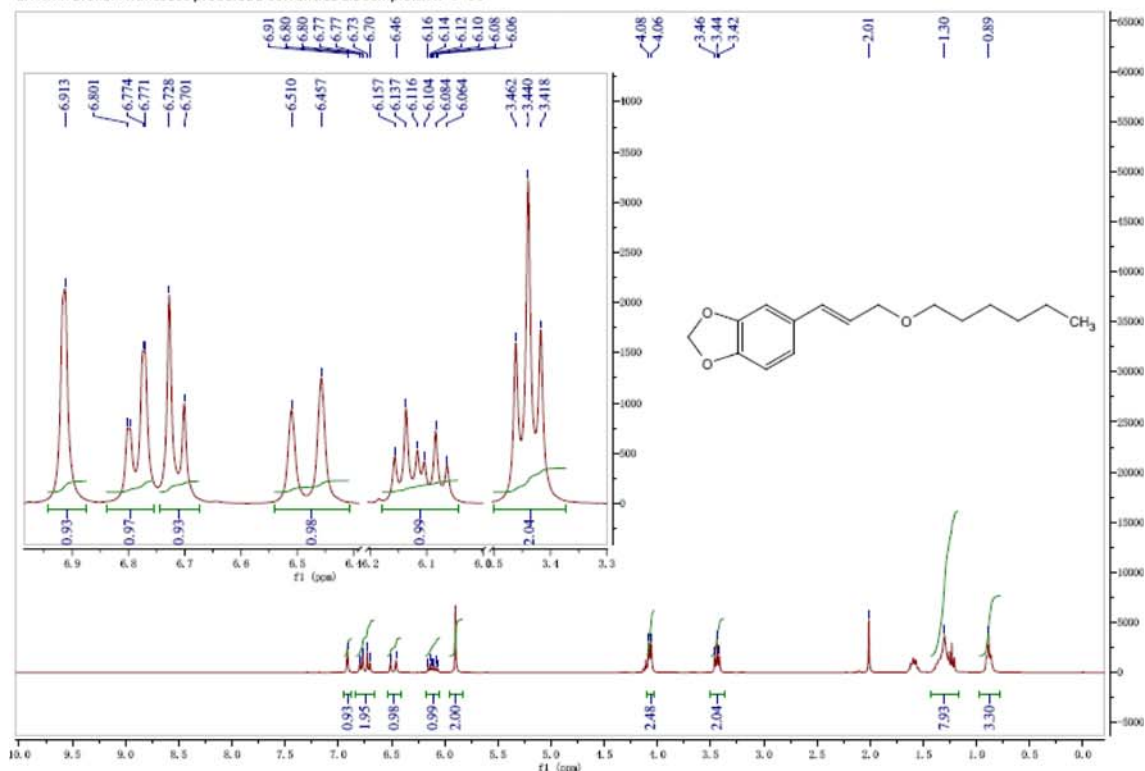
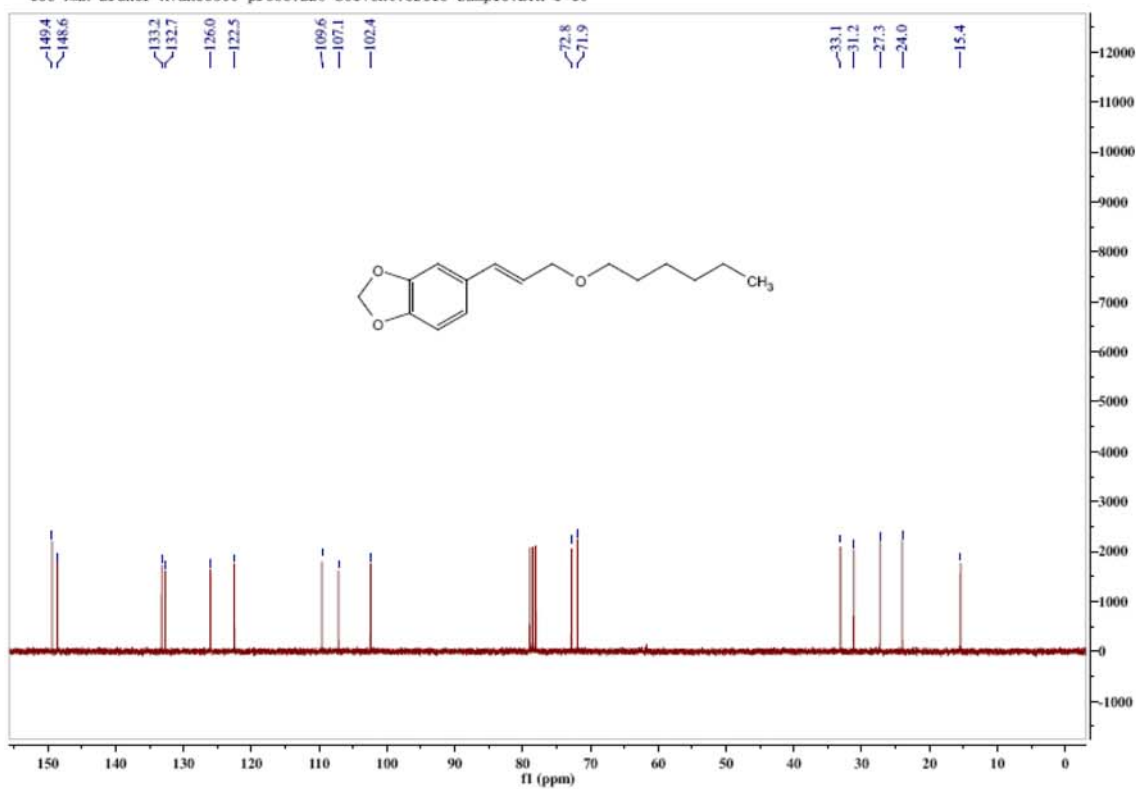
## Compound 9d

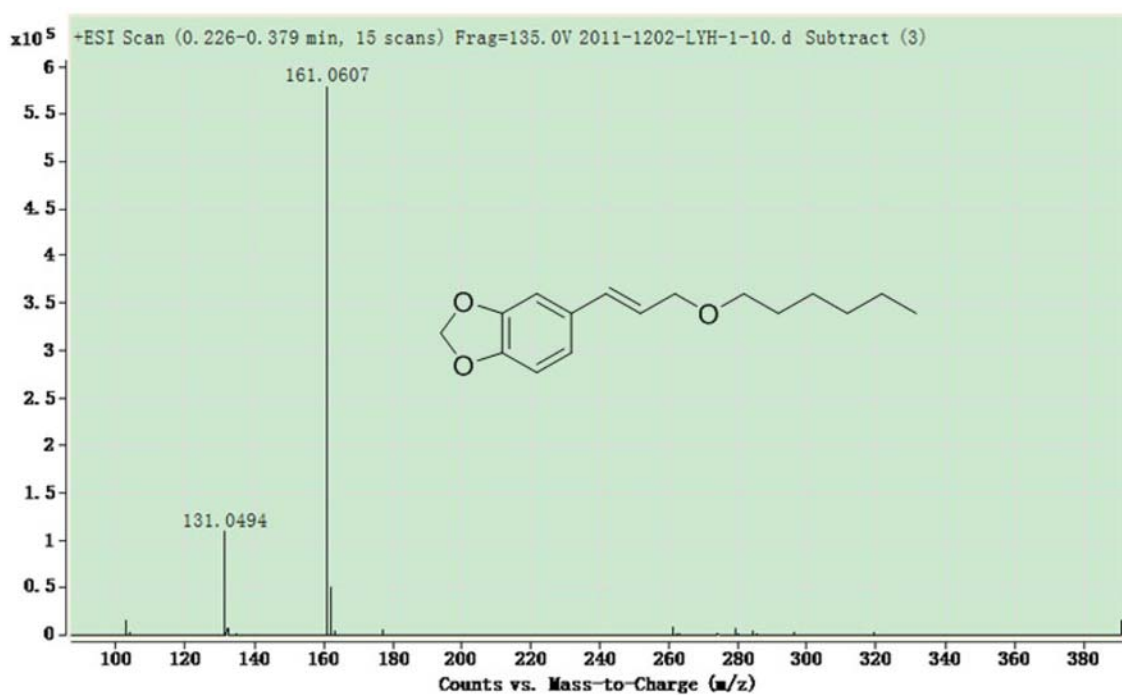
<sup>1</sup>H NMR: Bruker Avance300 probe:BBO solvent:CDCl<sub>3</sub> sample: WLH-1-13



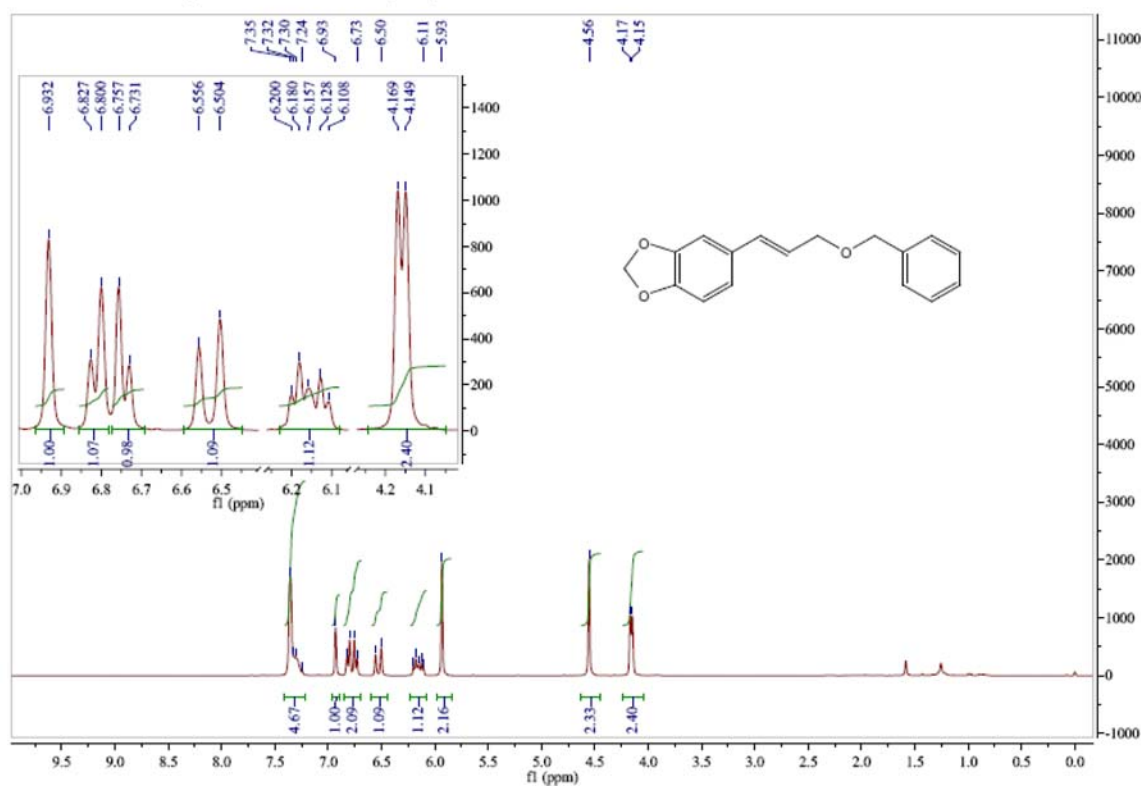
<sup>13</sup>C NMR Bruker Avance300 probe:BBO solvent:CDCl<sub>3</sub> sample: WLH-1-13

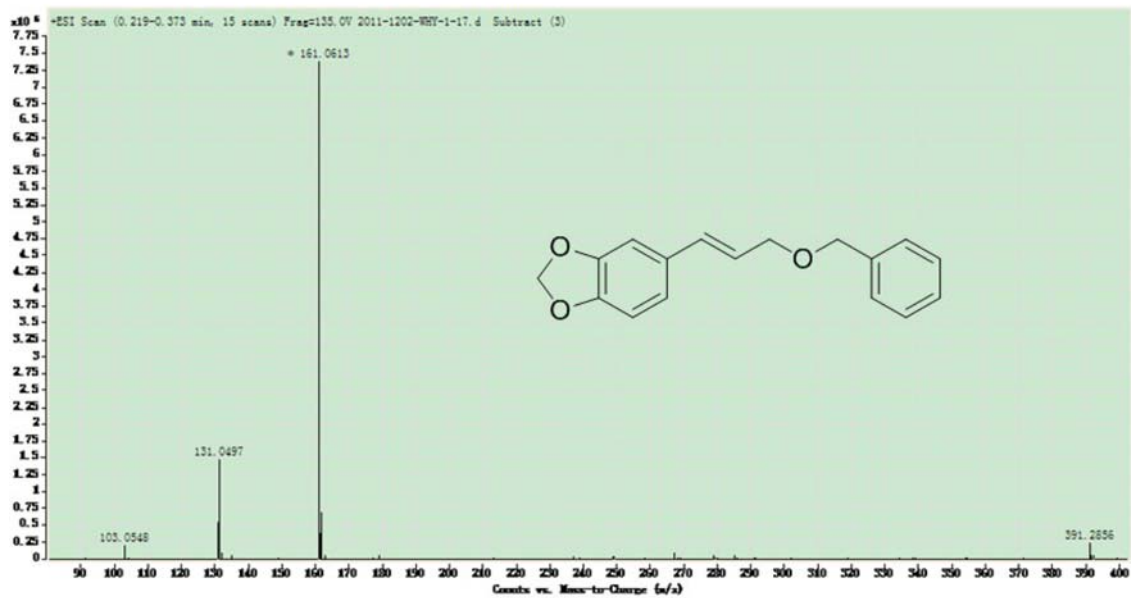
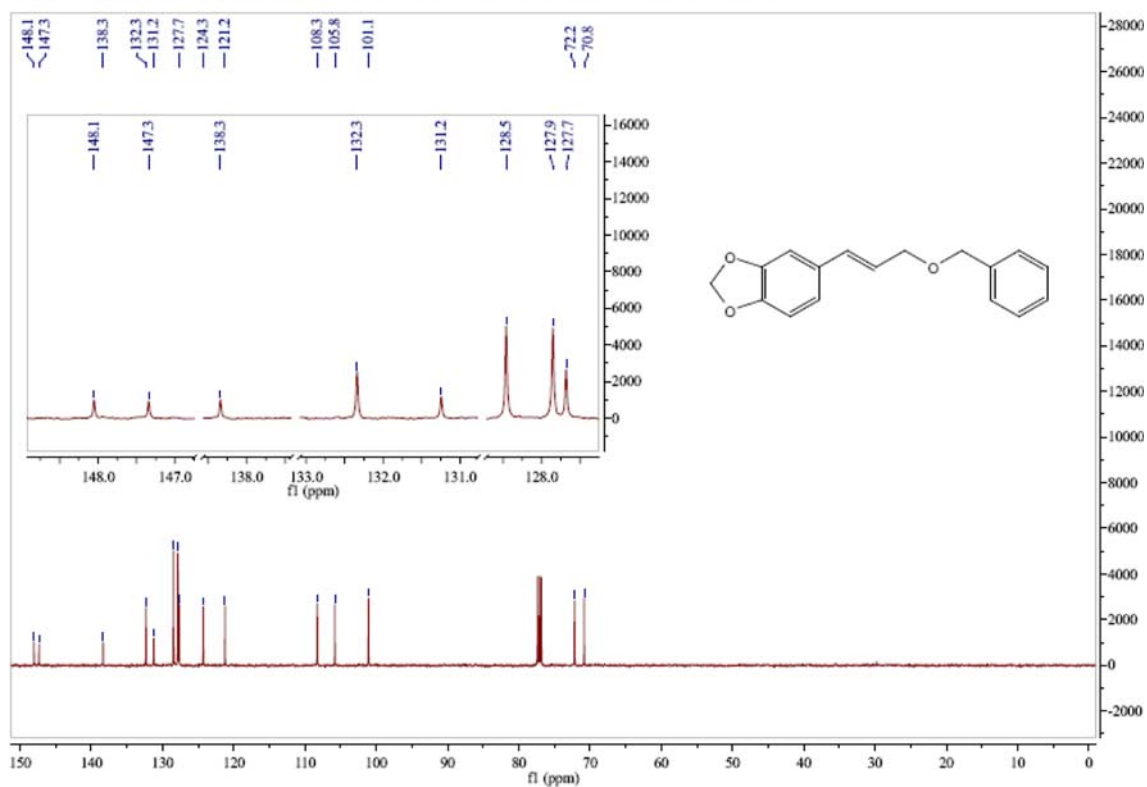


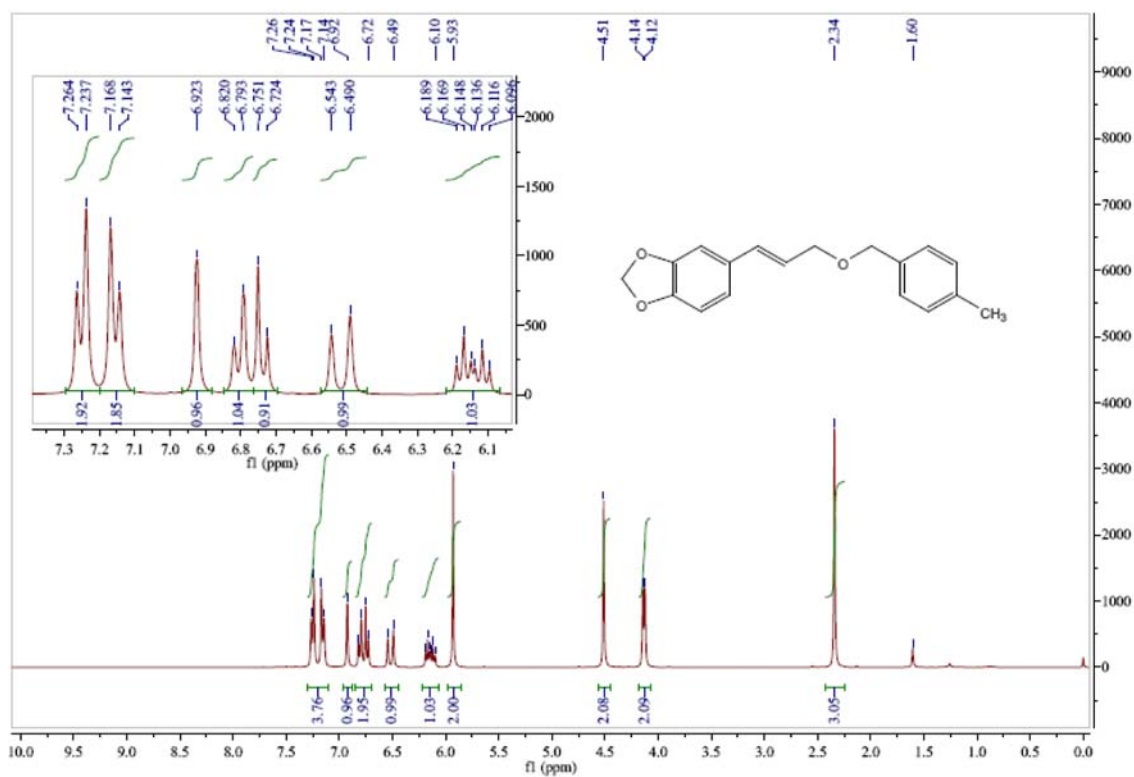
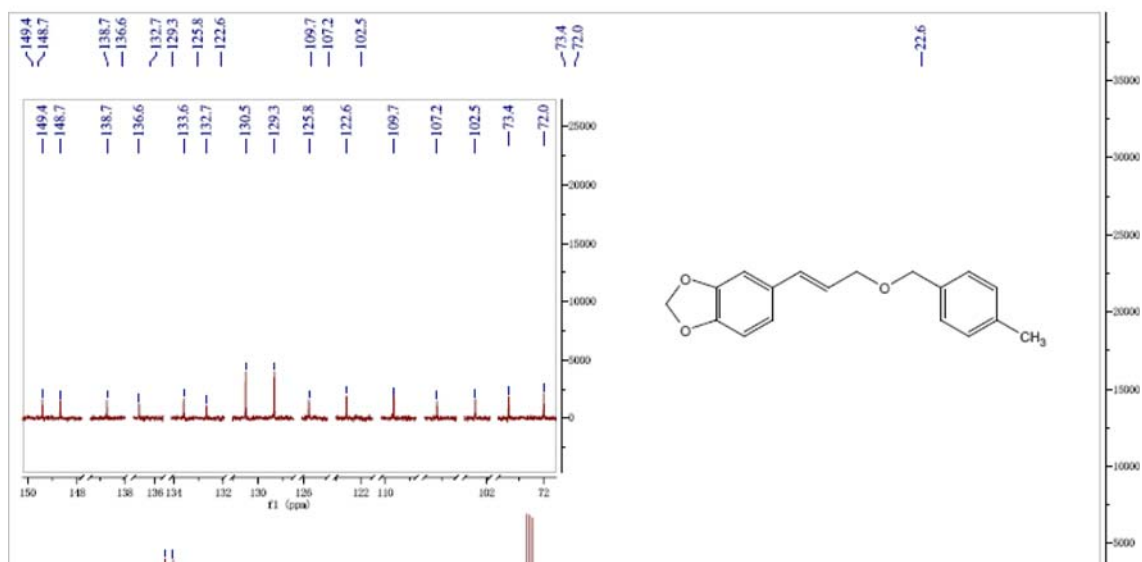
Compound **9e**<sup>1</sup>H NMR Bruker Avance300 probe:BBO solvent:CDCl<sub>3</sub> sample:LYH-1-10<sup>13</sup>C NMR Bruker Avance300 probe:BBO solvent:CDCl<sub>3</sub> sample:LYH-1-10

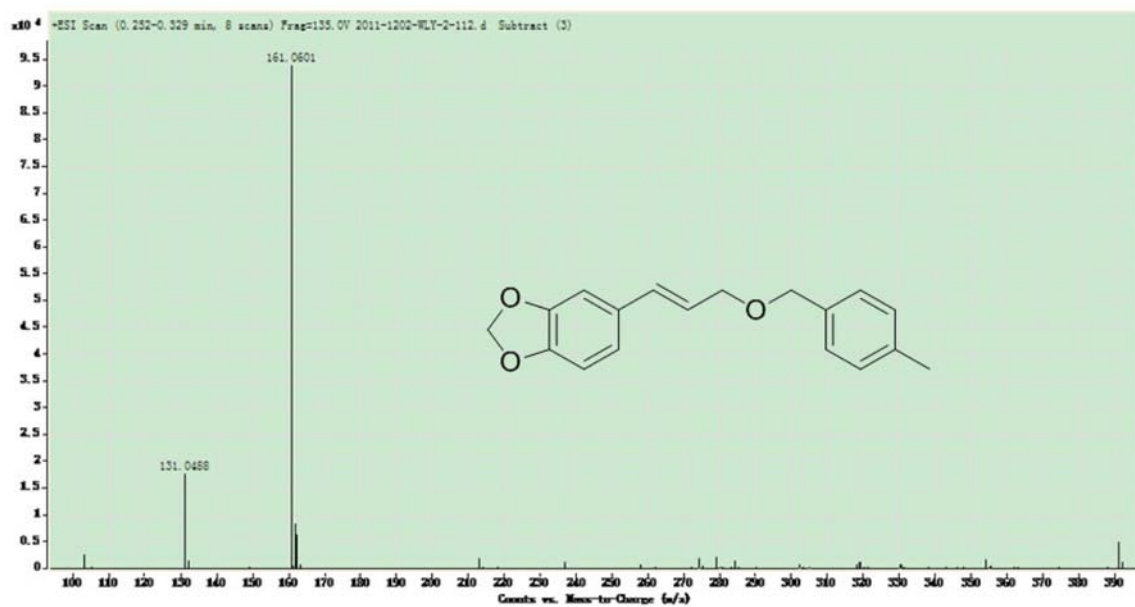


## Compound 9f

<sup>1</sup>HNMR Bruker Avance300 probe:BBO solvent:CDCl<sub>3</sub> sample:wly-2-94

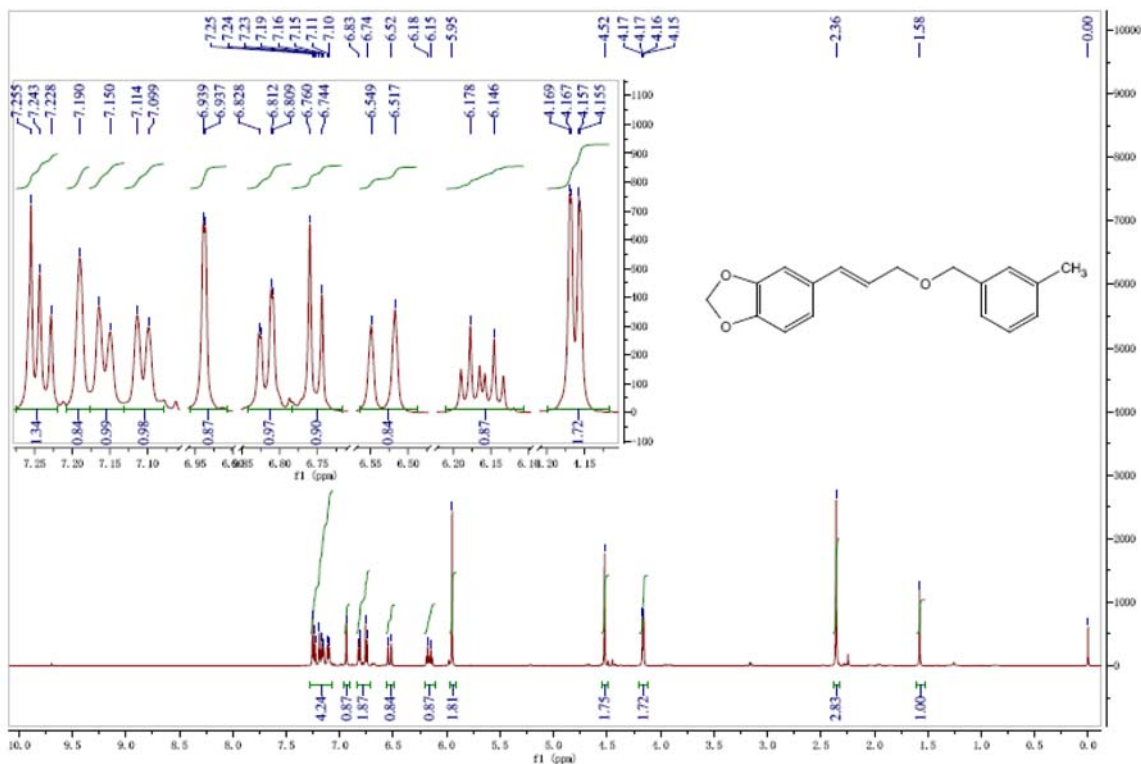
xiongyan <sup>13</sup>C NMR Bruker Avance500 probe:BBO solvent:CDCl<sub>3</sub> sample:wly-2-94 date:20110930

Compound **9g**<sup>1</sup>H NMR Bruker Avance300 Solvent:CDCl<sub>3</sub> sample:Wly-2-112<sup>13</sup>C NMR Bruker Avance300 Solvent:CDCl<sub>3</sub> sample:Wly-2-112



## Compound 9h

xiongyan  $^1\text{H}$  NMR Bruker Avance500 probe:BB0 solvent:CDCl<sub>3</sub> sample:WLY-2-113 date:20111212



xiongyan <sup>13</sup>C NMR Bruker Avance500 probe:BBO solvent:CDCl<sub>3</sub> sample:wly-2-113 date:20120104