

---

## Supplementary Materials: Bioactive Diphenyl Ether Derivatives and Isocoumarin Derivatives from Gorgonian-Derived Fungus *Phoma* sp.

Ting Shi, Jun Qi, Chang-lun Shao, Dong-lin Zhao, Xue-mei Hou and Chang-yun Wang\*

**Figure S1.**  $^1\text{H}$  NMR spectrum of compound **1** (DMSO- $d_6$ ).

**Figure S2.**  $^{13}\text{C}$  NMR spectrum of compound **1** (DMSO- $d_6$ ).

**Figure S3.** COSY spectrum of compound **1** (DMSO- $d_6$ ).

**Figure S4.** HMQC spectrum of compound **1** (DMSO- $d_6$ ).

**Figure S5.** HMBC spectrum of compound **1** (DMSO- $d_6$ ).

**Figure S6.** ESIMS spectrum of compound **1**.

**Figure S7.** HRESIMS spectrum of compound **1**.

**Figure S8.**  $^1\text{H}$  NMR spectrum of compound **2** (CD<sub>3</sub>OD).

**Figure S9.**  $^{13}\text{C}$  NMR spectrum of compound **2** (CD<sub>3</sub>OD).

**Figure S10.** COSY spectrum of compound **2** (CD<sub>3</sub>OD).

**Figure S11.** HMQC spectrum of compound **2** (CD<sub>3</sub>OD).

**Figure S12.** HMBC spectrum of compound **2** (CD<sub>3</sub>OD).

**Figure S13.** ESIMS spectrum of compound **2**.

**Figure S14.** HRESIMS spectrum of compound **2**.

**Figure S15.**  $^1\text{H}$  NMR spectrum of compound **3** (CD<sub>3</sub>OD).

**Figure S16.**  $^{13}\text{C}$  NMR spectrum of compound **3** (CD<sub>3</sub>OD).

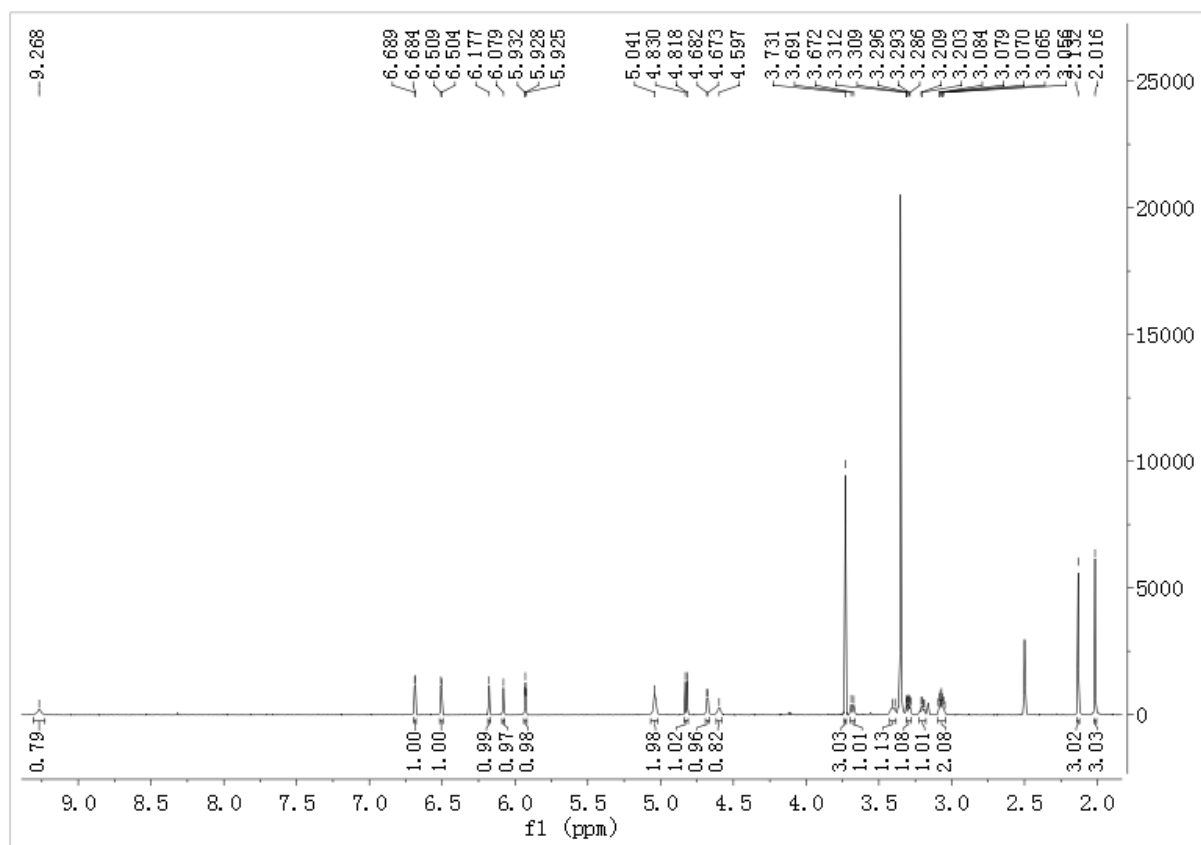
**Figure S17.** COSY spectrum of compound **3** (CD<sub>3</sub>OD).

**Figure S18.** HMQC spectrum of compound **3** (CD<sub>3</sub>OD).

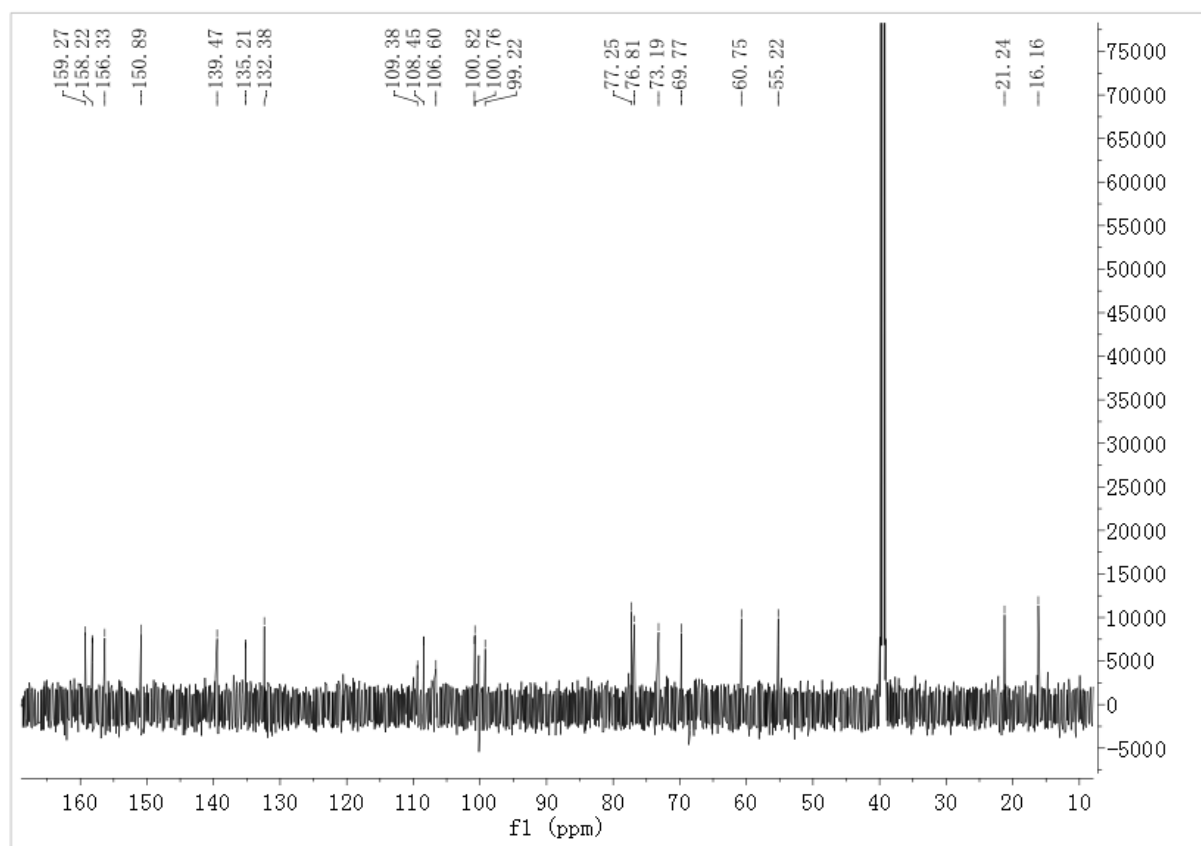
**Figure S19.** HMBC spectrum of compound **3** (CD<sub>3</sub>OD).

**Figure S20.** ESIMS spectrum of compound **3**.

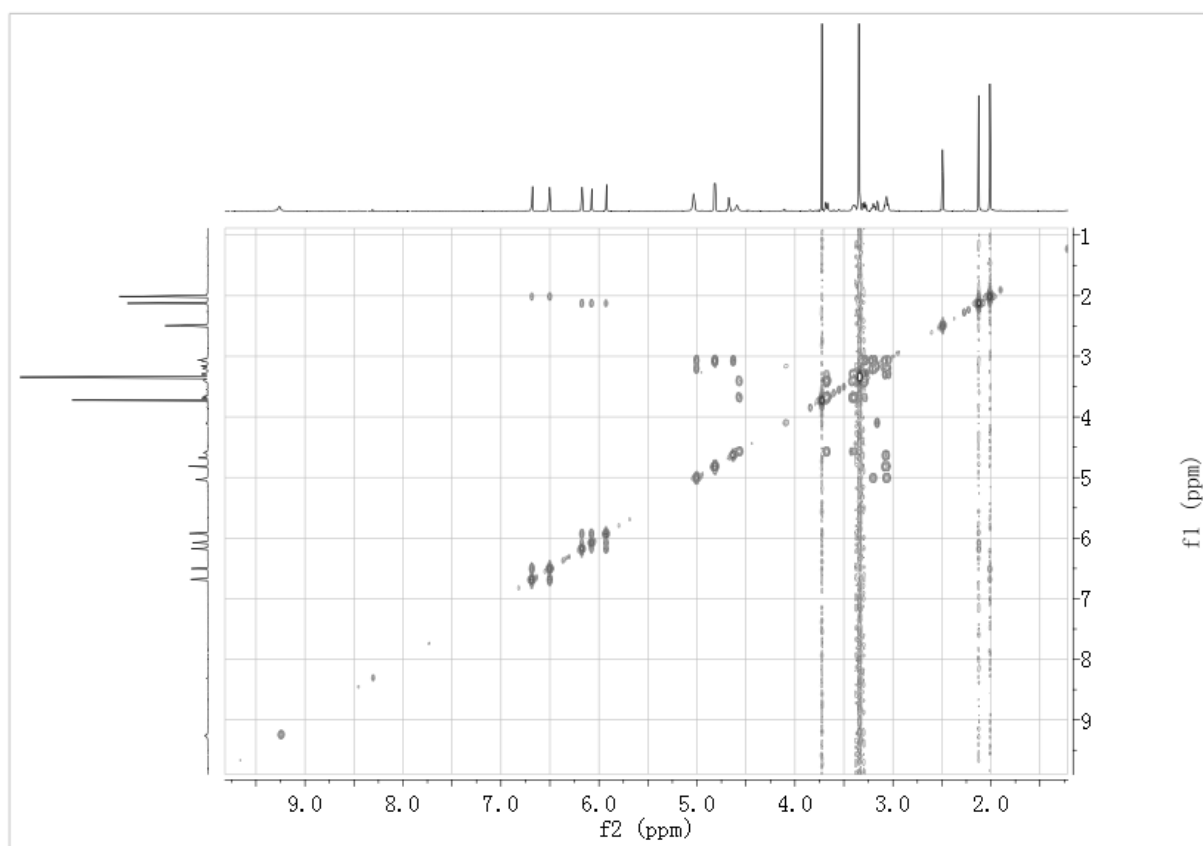
**Figure S21.** HRESIMS spectrum of compound **3**.



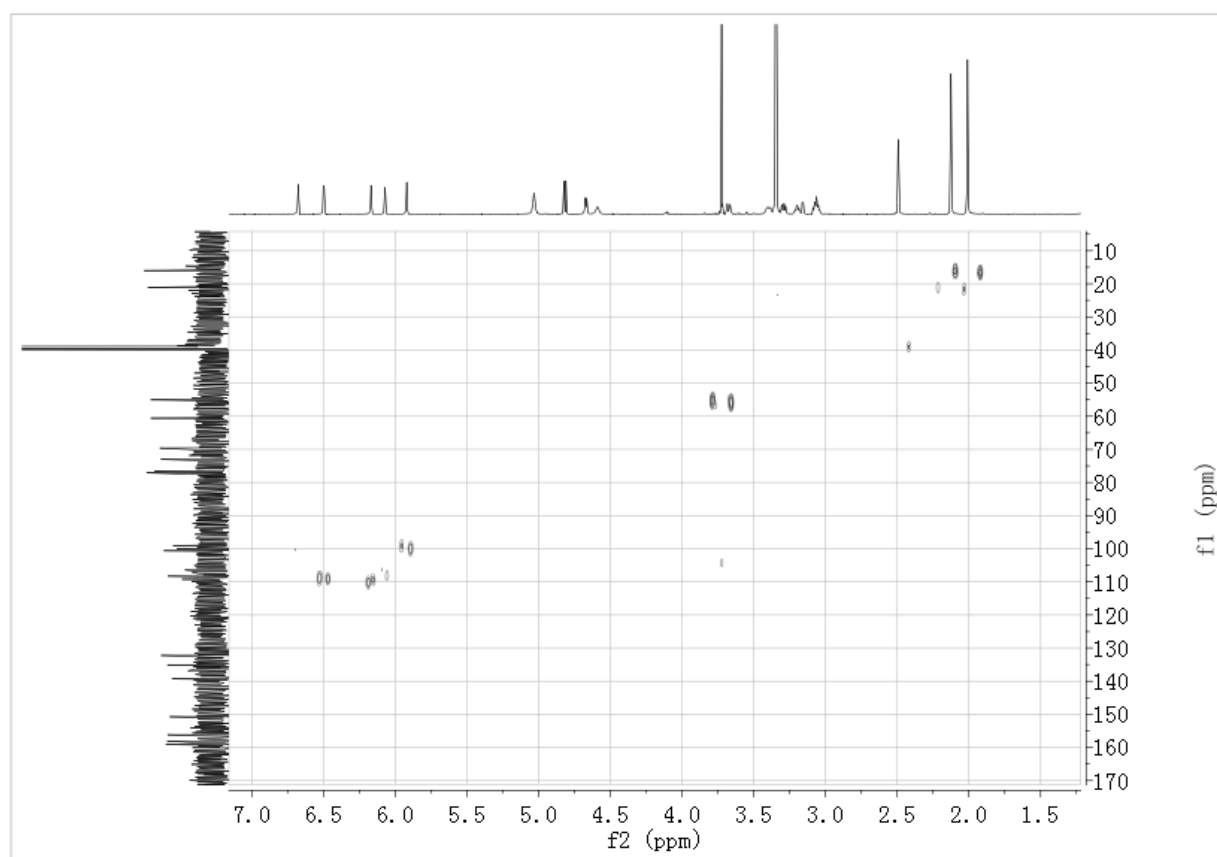
**Figure S1.**  $^1\text{H}$  NMR spectrum of compound 1 (DMSO- $d_6$ ).



**Figure S2.**  $^{13}\text{C}$  NMR spectrum of compound 1 (DMSO- $d_6$ ).



**Figure S3.** COSY spectrum of compound 1 (DMSO-*d*<sub>6</sub>).



**Figure S4.** HMQC spectrum of compound 1 (DMSO-*d*<sub>6</sub>).

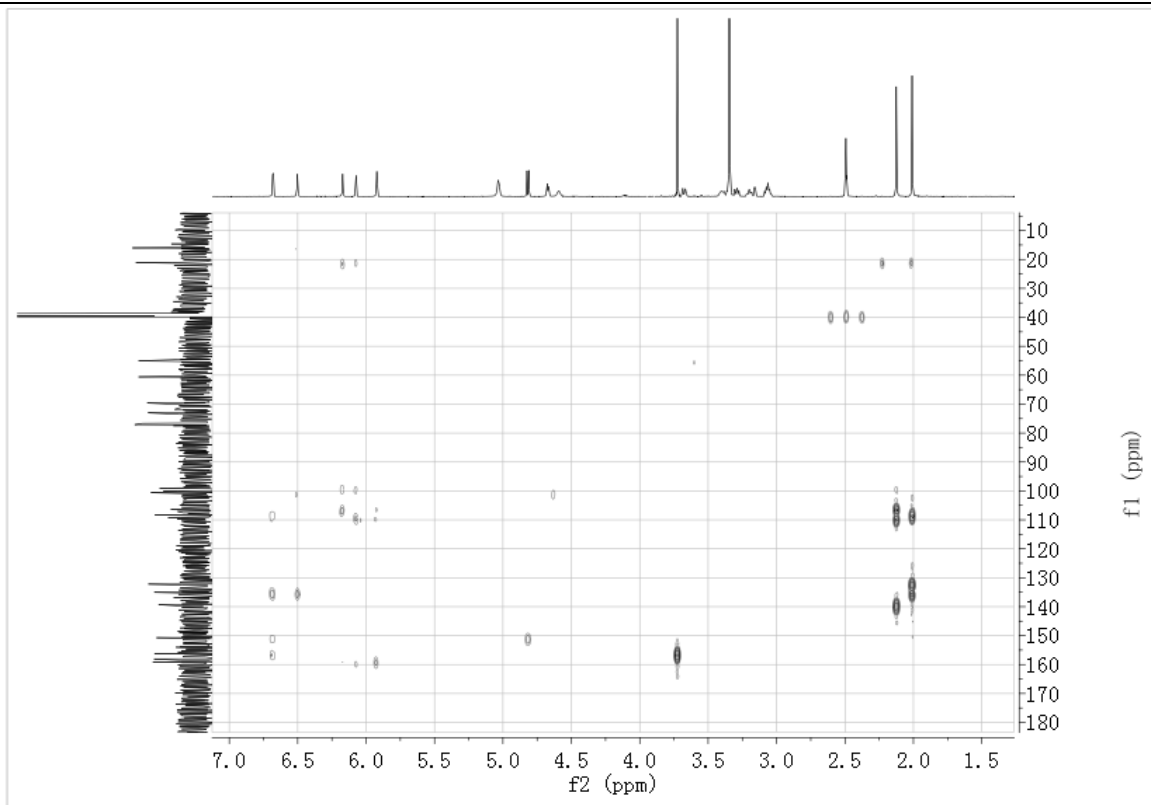


Figure S5. HMBC spectrum of compound 1 (DMSO-*d*<sub>6</sub>).

Display Report

<b>Analysis Info</b>		Acquisition Date	4/10/2012 9:07:25 AM
Analysis Name	D:\Data\ZHENGJUANJUAN\20120410\LH424D.d	Operator	OUC
Method	20120331-zz2-NEIBIAO-lcms.m	Instrument	amaZon SL
Sample Name	LH424D		
Comment			

<b>Acquisition Parameter</b>					
Ion Source Type	ESI	Ion Polarity	Positive	Alternating Ion Polarity	off
Mass Range Mode	Enhanced Resolution	Scan Begin	200 m/z	Scan End	1000 m/z
Capillary Exit	140.0 V	n/a	n/a	Trap Drive	56.6
Accumulation Time	75 µs	Averages	3 Spectra	Auto MS/MS	off

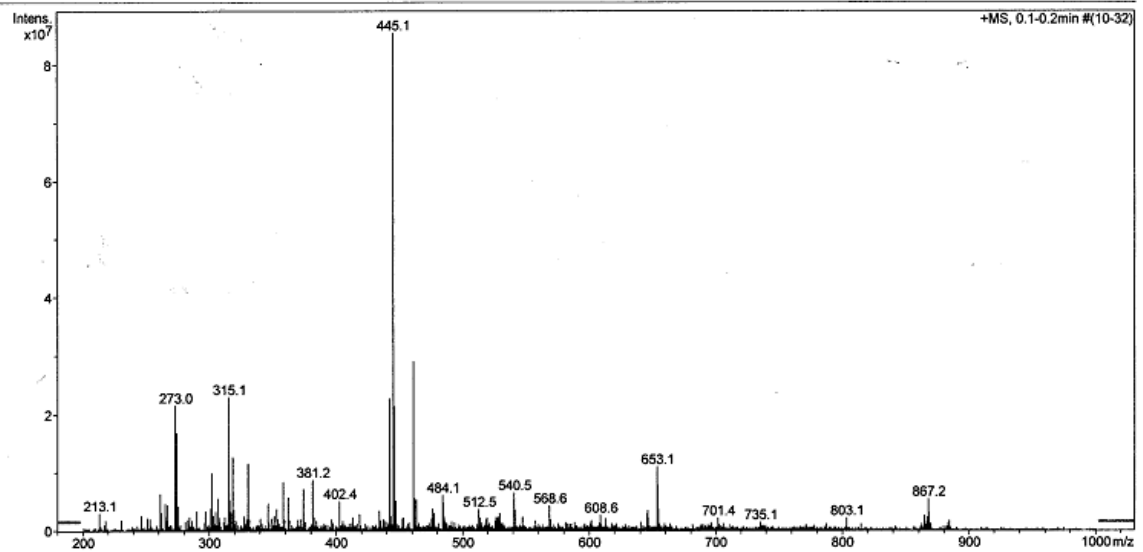


Figure S6. ESIMS spectrum of compound 1.

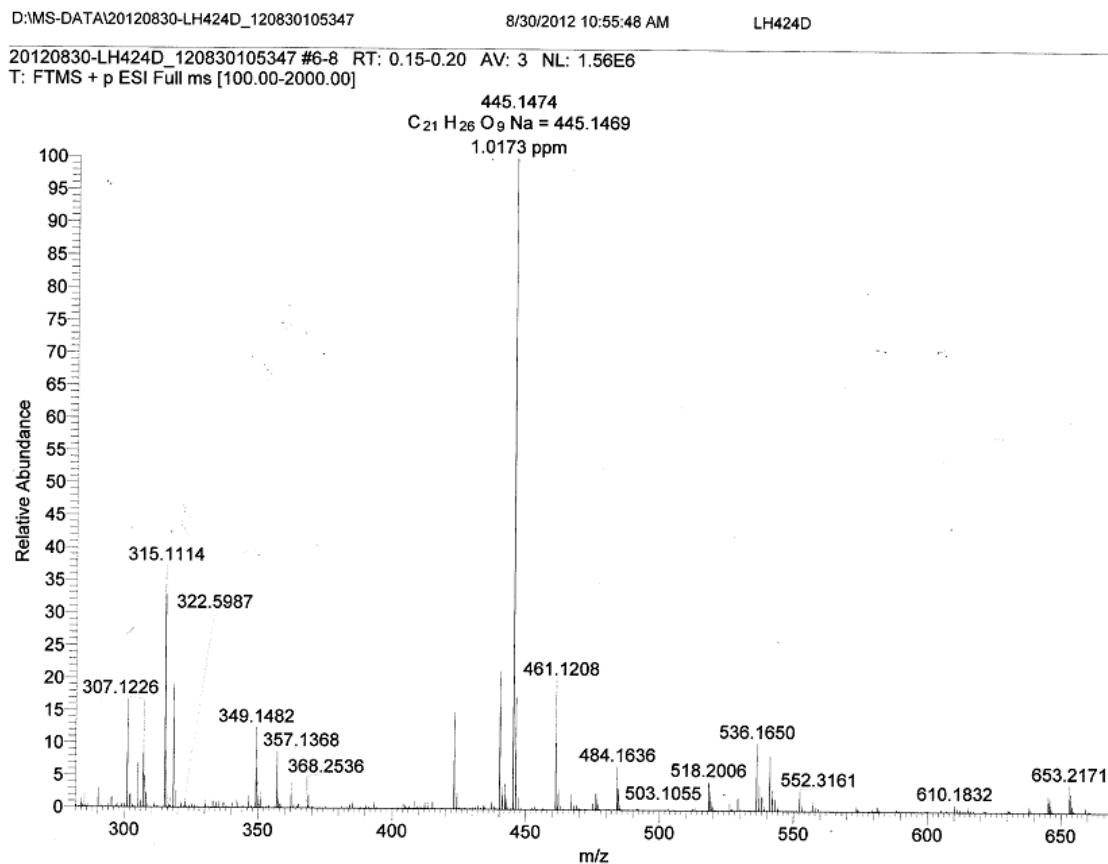
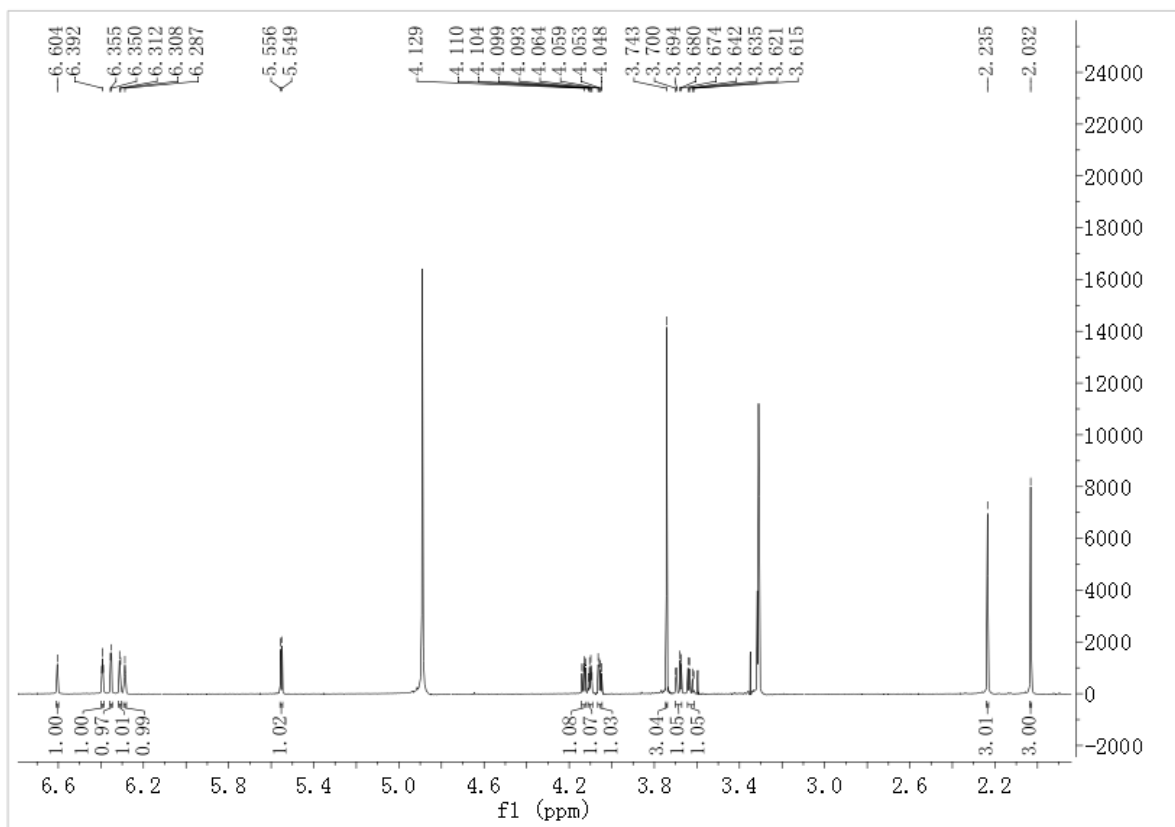
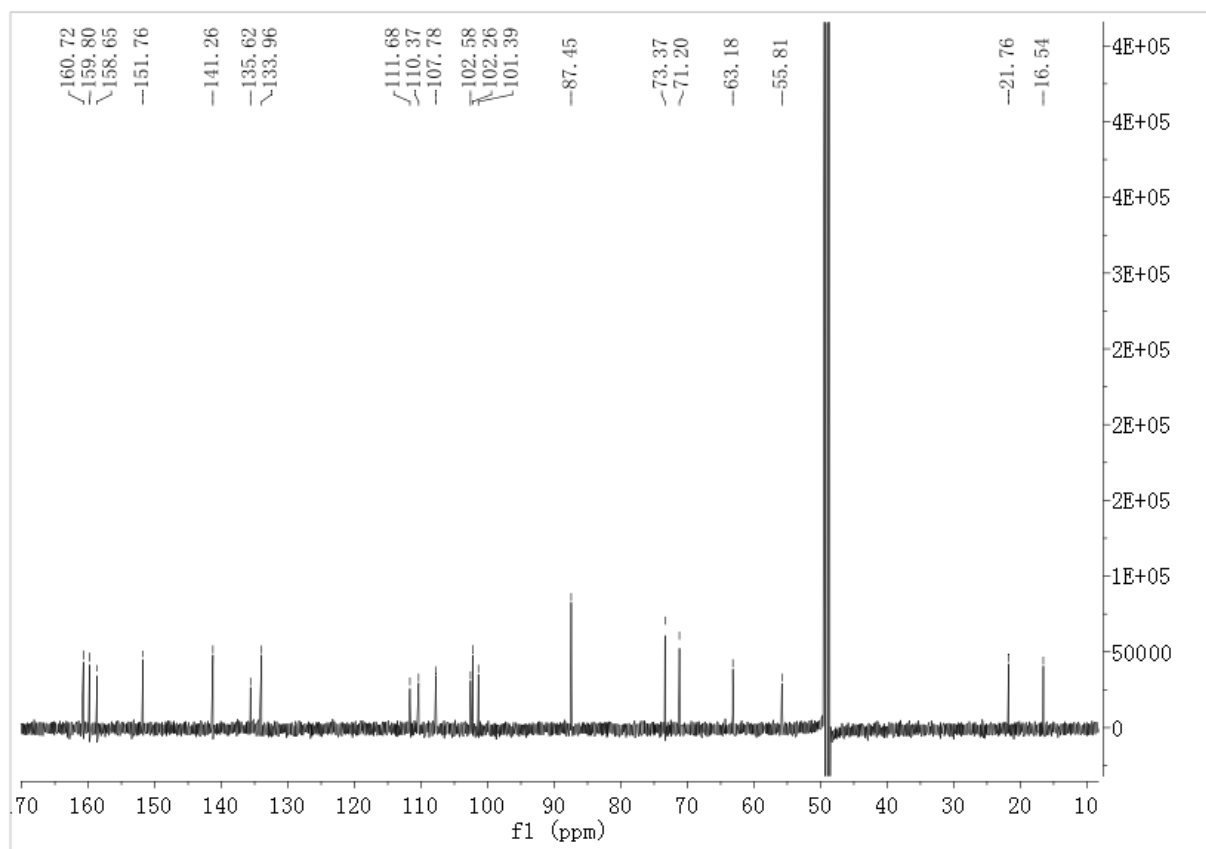
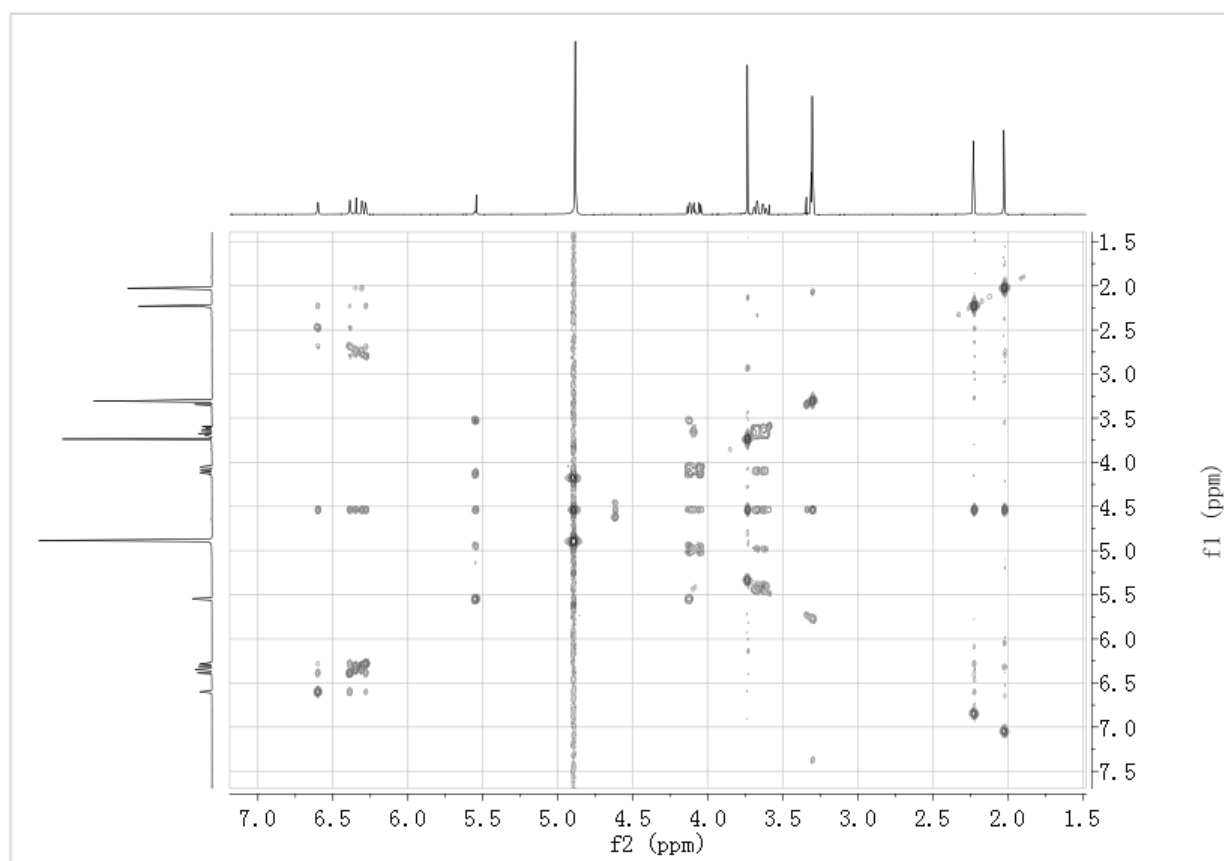


Figure S7. HRESIMS spectrum of compound 1.

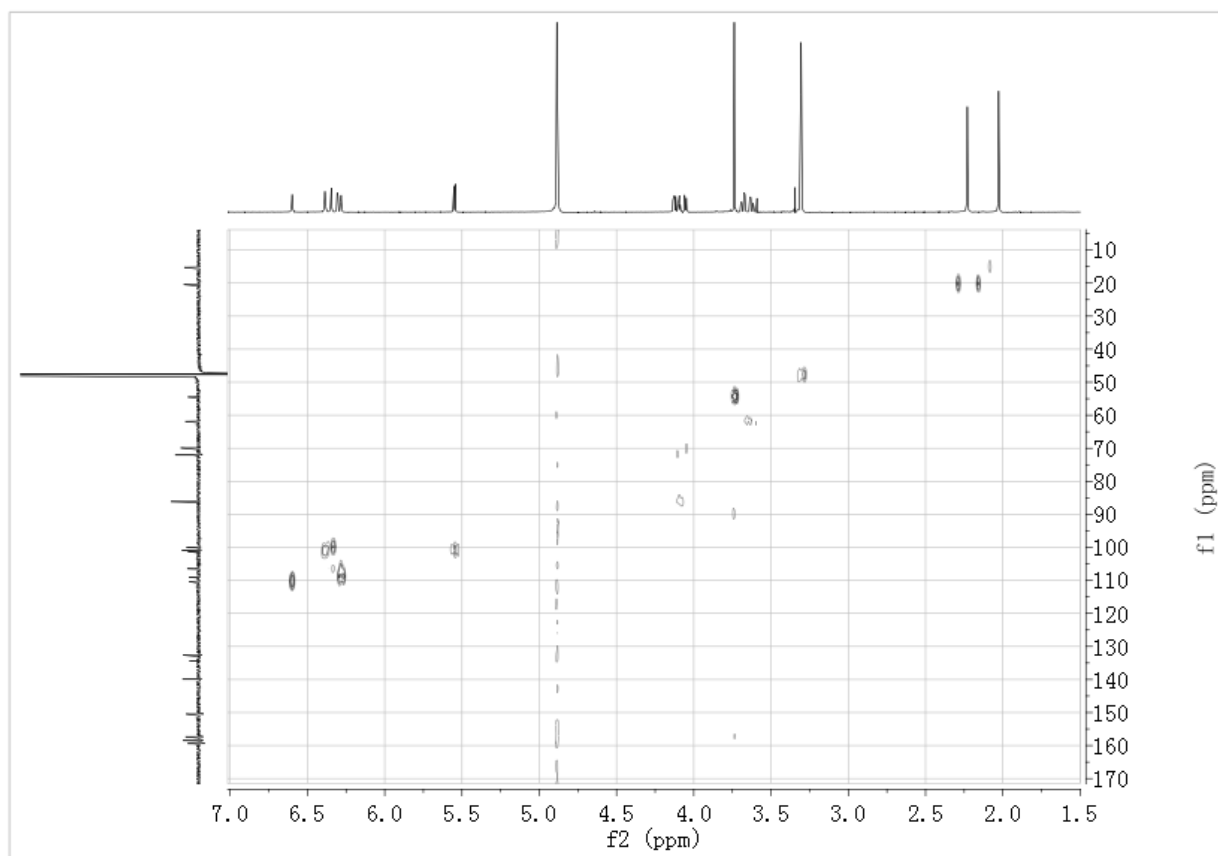
Figure S8.  $^1H$  NMR spectrum of compound 2 ( $CD_3OD$ ).



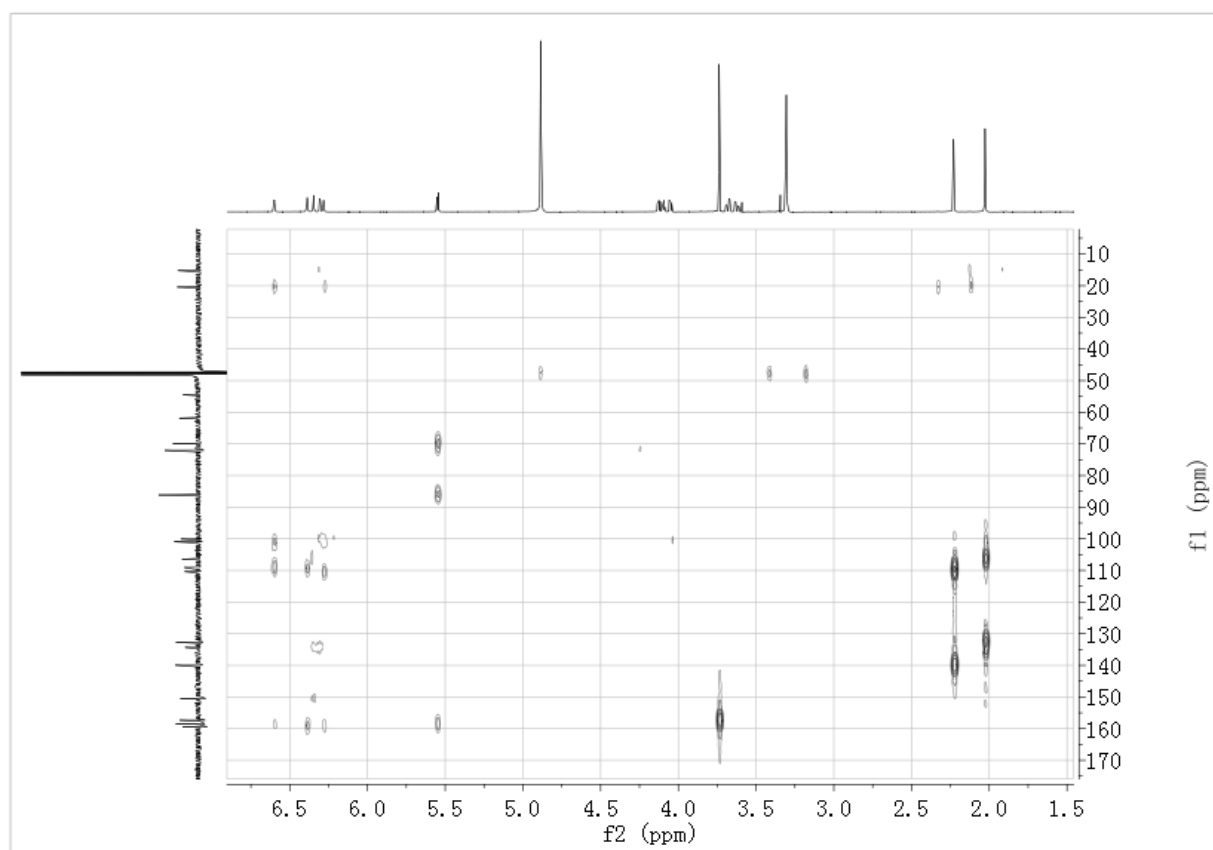
**Figure S9.**  $^{13}\text{C}$  NMR spectrum of compound **2** ( $\text{CD}_3\text{OD}$ ).



**Figure S10.** COSY spectrum of compound **2** ( $\text{CD}_3\text{OD}$ ).



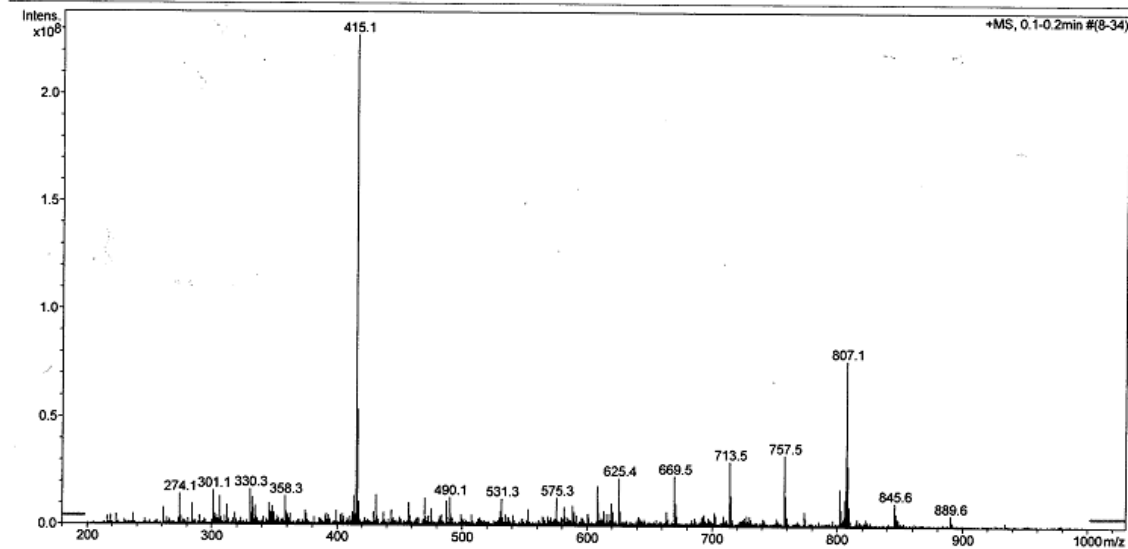
**Figure S11.** HMQC spectrum of compound **2** (CD<sub>3</sub>OD).



**Figure S12.** HMBC spectrum of compound **2** (CD<sub>3</sub>OD).

Display Report

<b>Analysis Info</b>		Acquisition Date	4/10/2012 9:16:58 AM		
Analysis Name	D:\Data\ZHENGJUANJUAN\20120410\LH246.d		Operator	OUC	
Method	20120331-zz2-NEIBIAO-lcms.m		Instrument	amaZon SL	
Sample Name	LH246				
Comment					
<b>Acquisition Parameter</b>					
Ion Source Type	ESI	Ion Polarity	Positive	Alternating Ion Polarity	off
Mass Range Mode	Enhanced Resolution	Scan Begin	200 m/z	Scan End	1000 m/z
Capillary Exit	140.0 V	n/a	n/a	Trap Drive	56.6
Accumulation Time	29 $\mu$ s	Averages	3 Spectra	Auto MS/MS	off



Bruker Compass DataAnalysis 4.0

printed: 4/10/2012 10:17:08 AM

Page 1 of 1

Figure S13. ESIMS spectrum of compound 2.

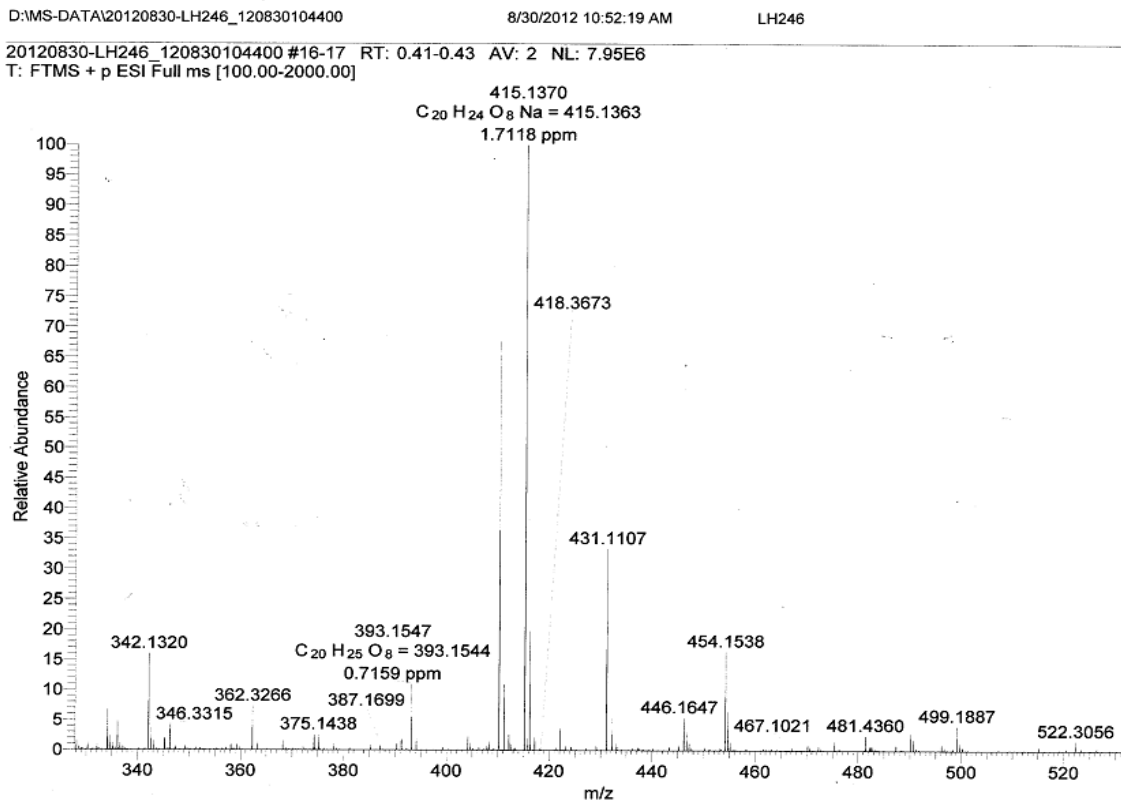


Figure S14. HRESIMS spectrum of compound 2.



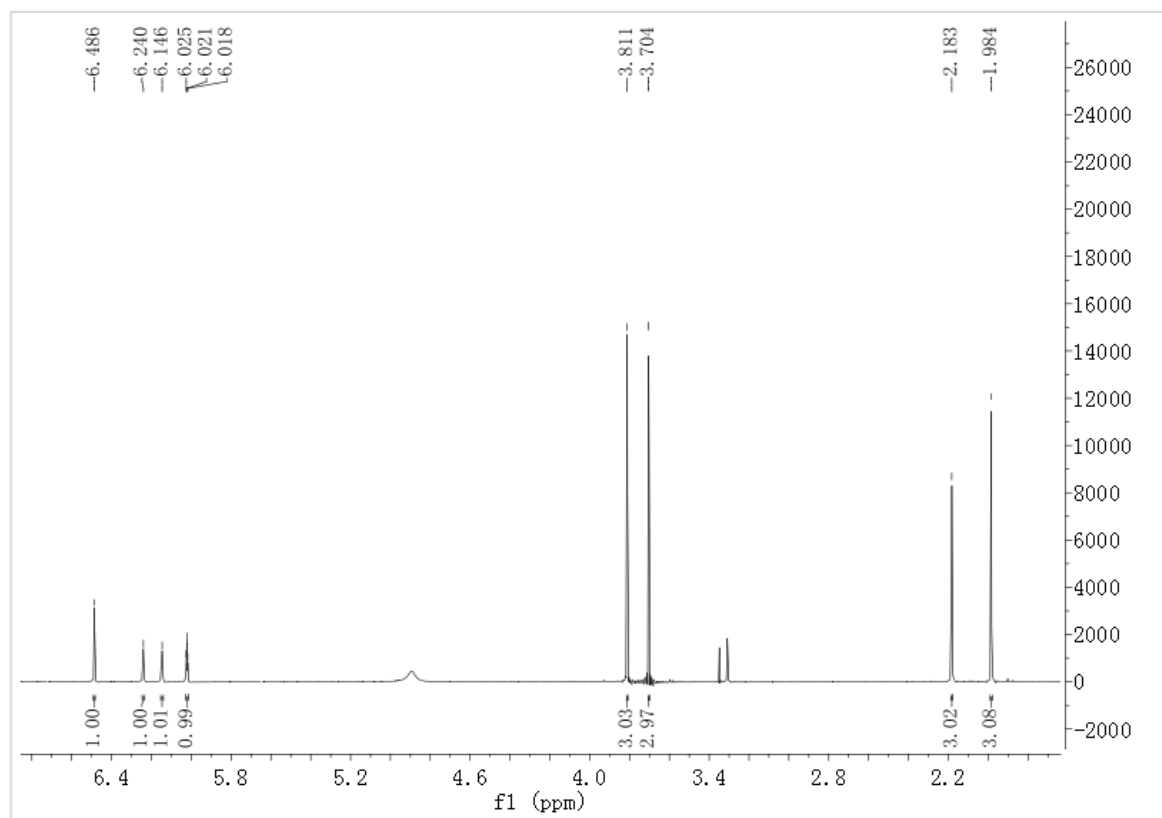


Figure S15.  $^1\text{H}$  NMR spectrum of compound 3 ( $\text{CD}_3\text{OD}$ ).

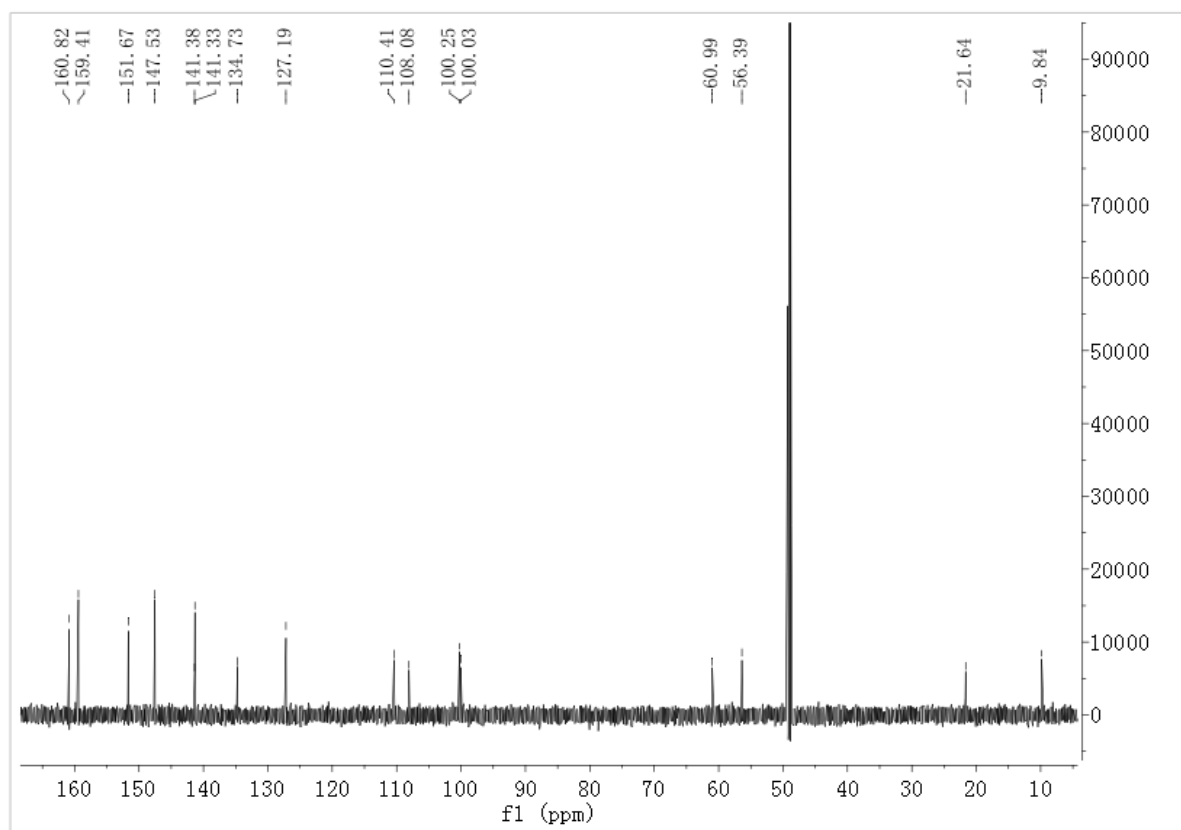
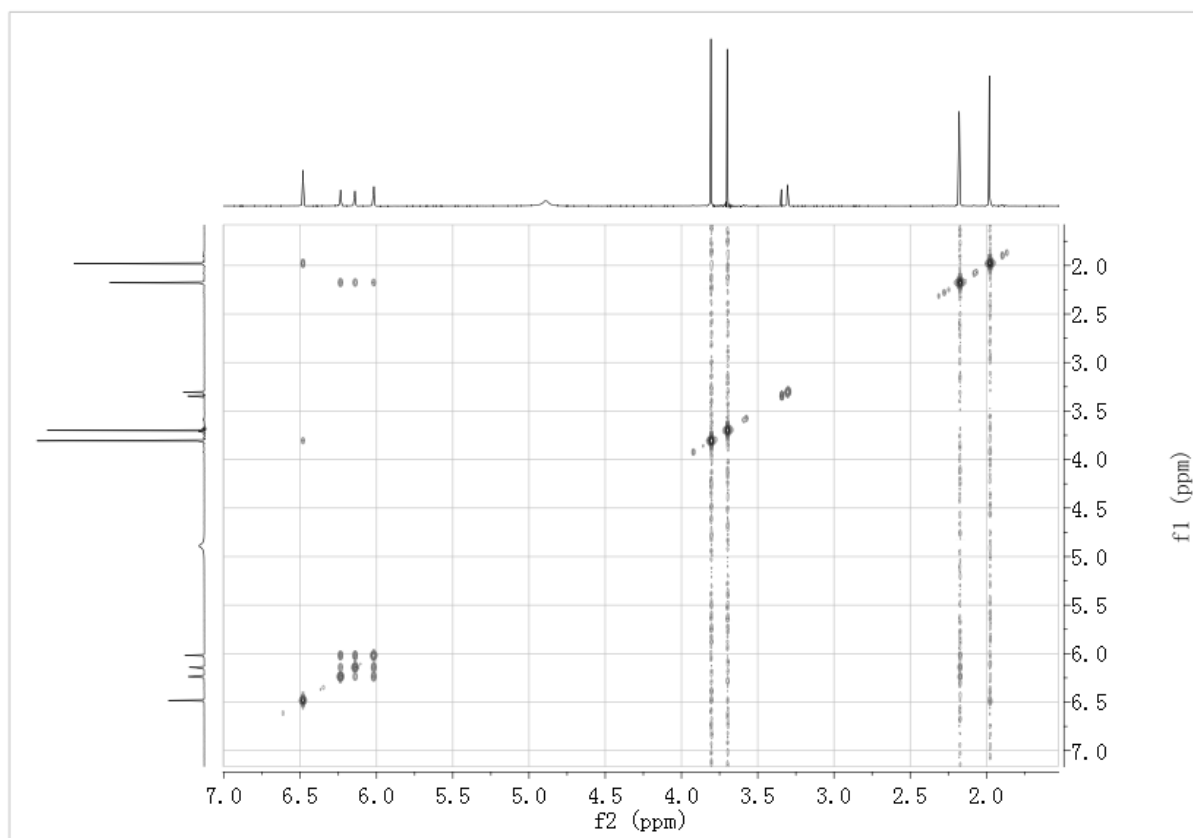
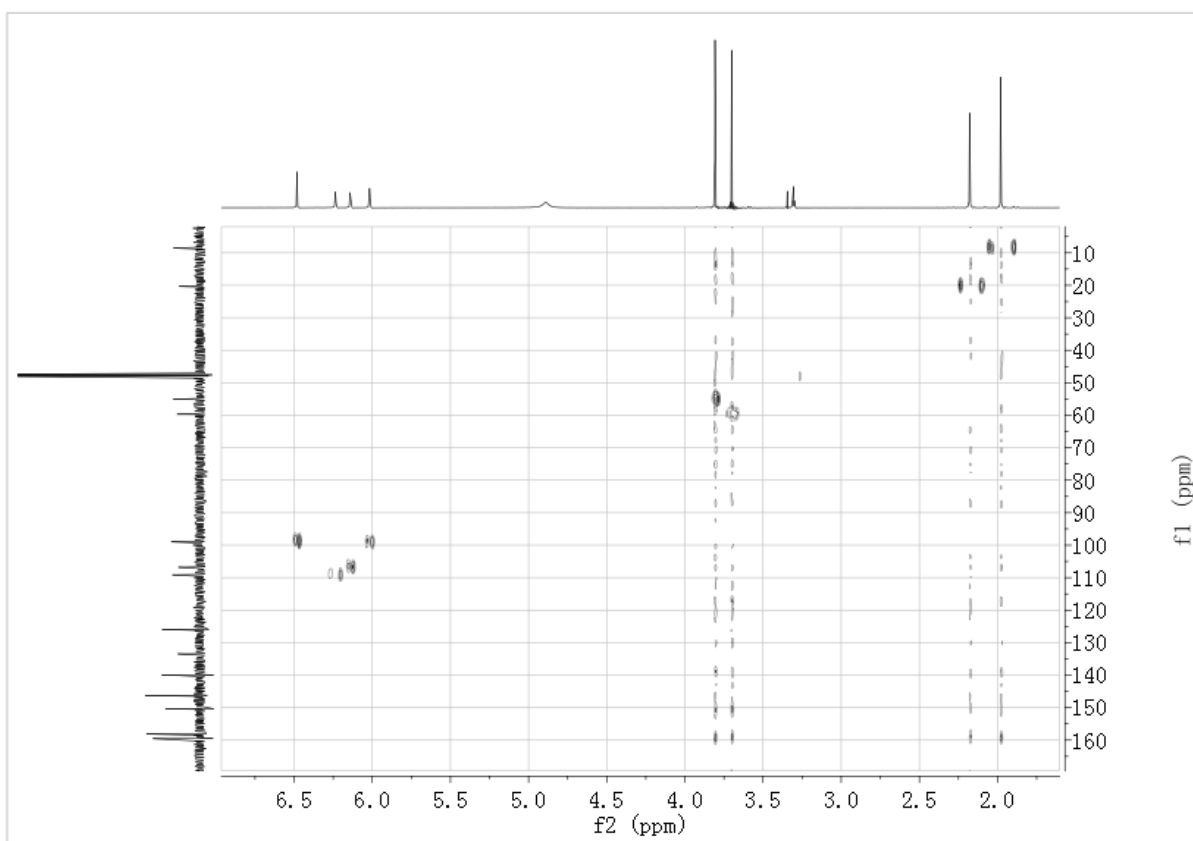


Figure S16.  $^{13}\text{C}$  NMR spectrum of compound 3 ( $\text{CD}_3\text{OD}$ ).



**Figure S17.** COSY spectrum of compound **3** (CD<sub>3</sub>OD).



**Figure S18.** HMBC spectrum of compound **3** (CD<sub>3</sub>OD).

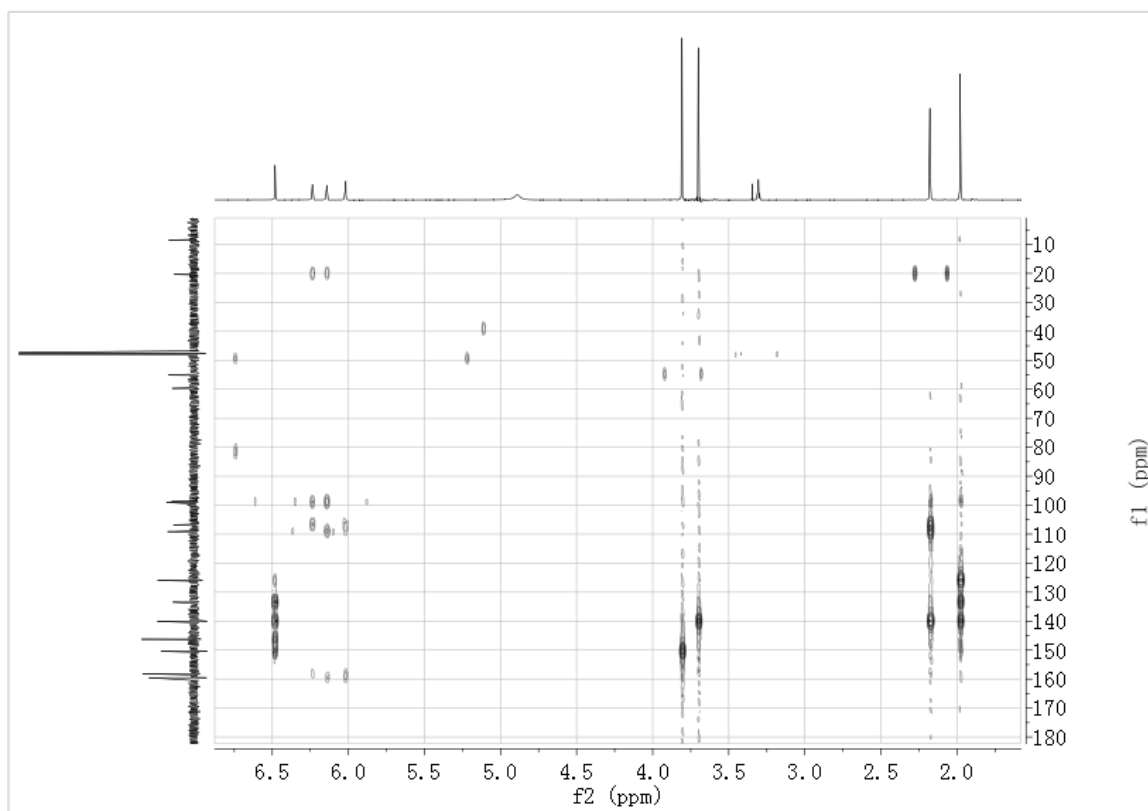


Figure S19. HMBC spectrum of compound 3 (CD<sub>3</sub>OD).

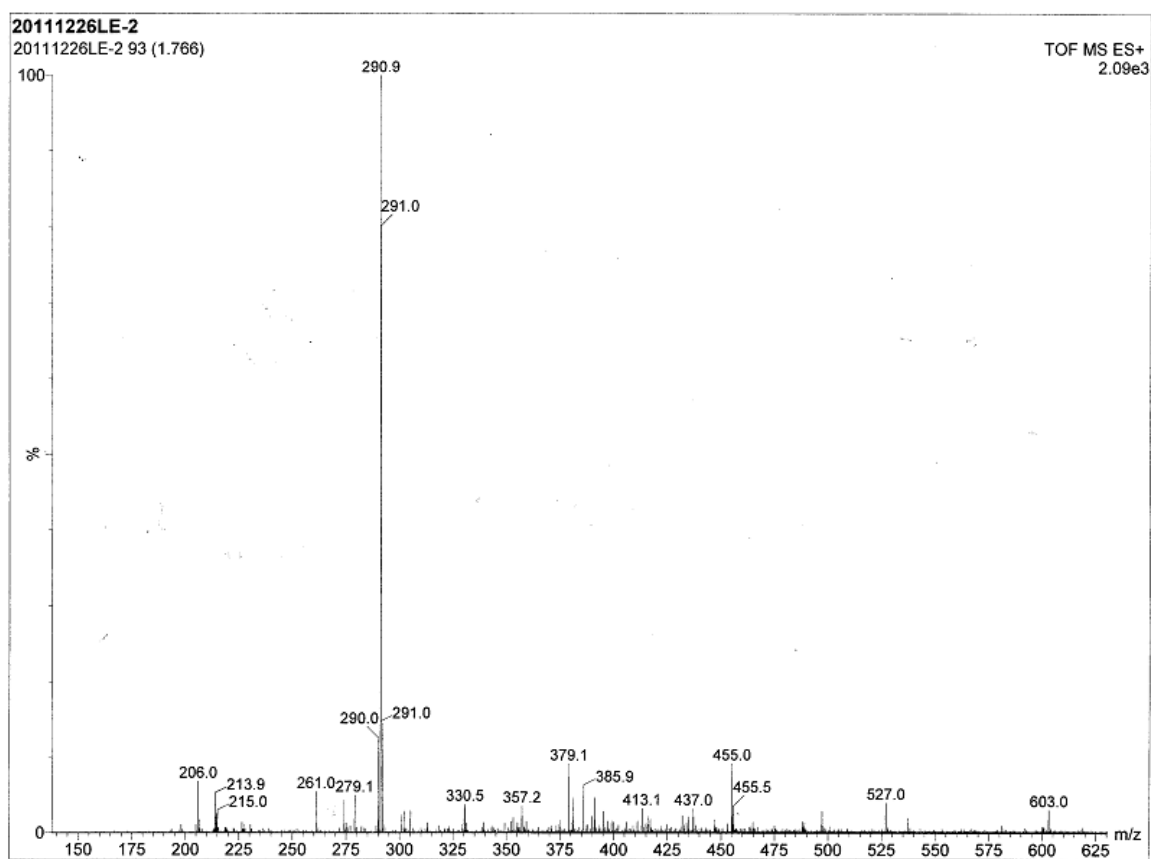


Figure S20. ESIMS spectrum of compound 3.

D:\MS-DATA\20120830-LE-2\_120830110153

8/30/2012 11:05:13 AM

LE-2

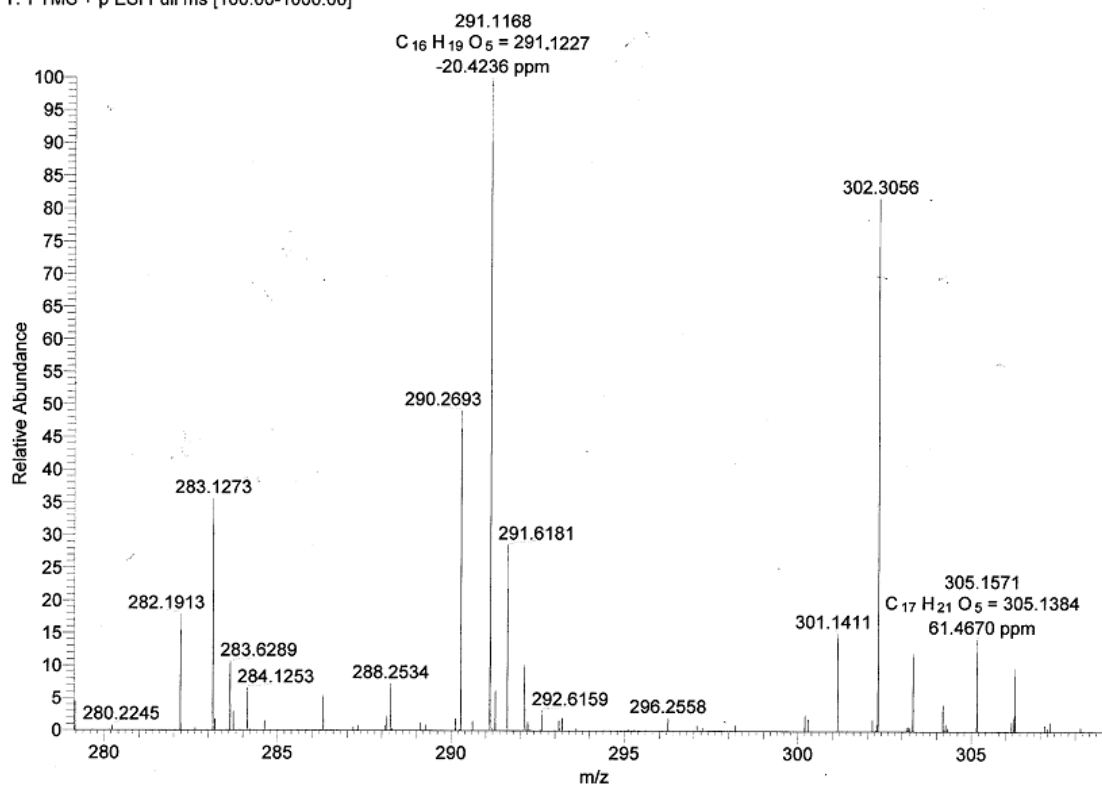
20120830-LE-2\_120830110153 #22-26 RT: 0.58-0.68 AV: 5 NL: 6.76E5  
T: FTMS + p ESI Full ms [100.00-1000.00]

Figure S21. HRESIMS spectrum of compound 3.