

**Neuroprotective effects of 1,2-diarylpropane type phenylpropanoid  
enantiomers from red raspberry against H<sub>2</sub>O<sub>2</sub>-induced  
oxidative stress in human neuroblastoma SH-SY5Y cells**

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Xiao-Xiao Huang<sup>†,§,\*</sup>, Shao-Jiang Song<sup>†,\*</sup>

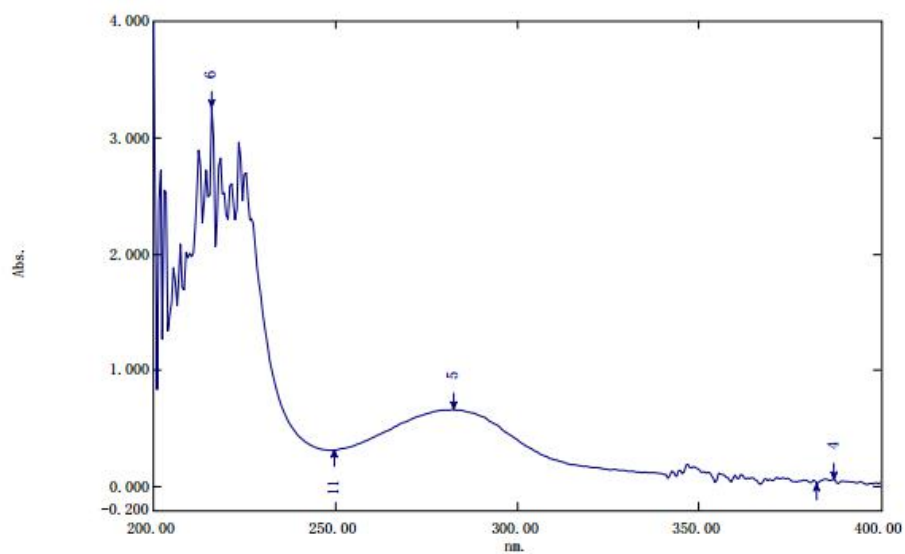
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University, Shenyang 110016, People's Republic of China*

<sup>‡</sup> *School of Pharmaceutical Engineering, Shenyang Pharmaceutical University,  
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of China*

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Huang).



测定属性  
 波长范围 (nm.): 200.00到500.00  
 扫描速度: 高速  
 采样间隔: 0.5  
 自动采样间隔: 停用  
 扫描模式: 单一的

试样准备属性  
 重量:

0.1mg  
 体积: 10ml  
 稀释:  
 光程长: 200-400  
 附加信息:

No.	P/V	Wavelength	Abs.	描述
1	●	483.00	.025	
2	●	469.00	.026	
3	●	421.00	.035	
4	●	387.00	.065	
5	●	282.50	.664	
6	●	216.00	3.257	
7	●	473.50	.020	
8	●	447.00	.019	
9	●	415.00	.022	
10	●	382.50	.028	
11	●	249.50	.314	

Figure S1.1 UV spectrum of compound 1

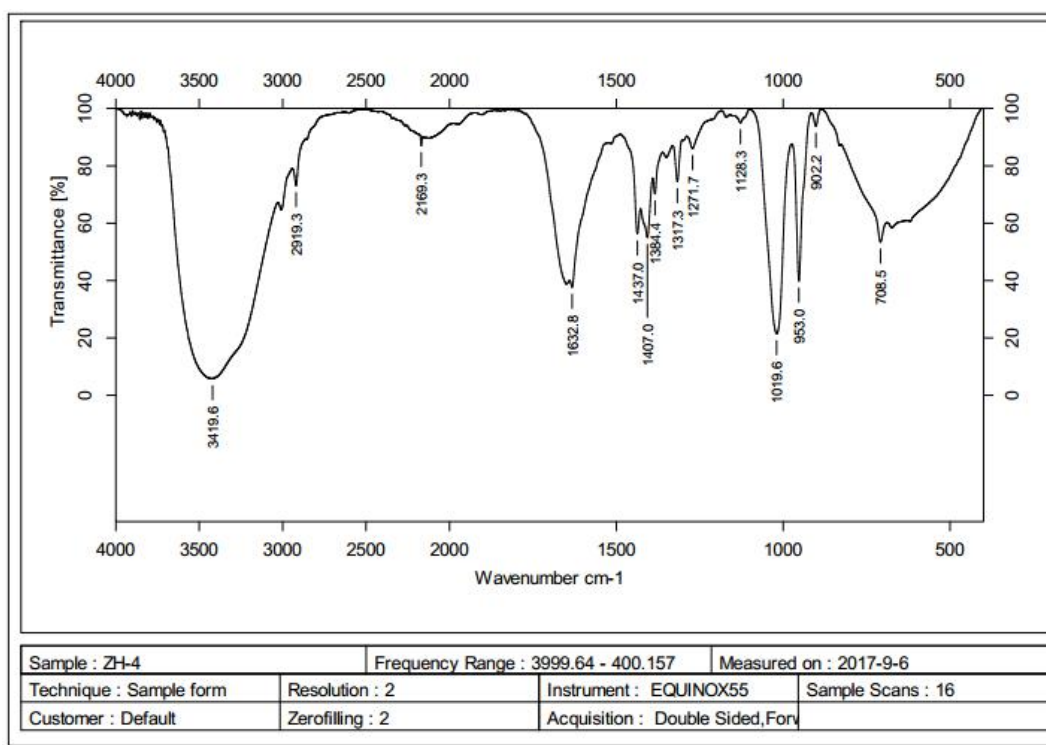


Figure S1.2 IR spectrum of compound 1

## Mass Spectrum Molecular Formula Report

### Analysis Info

Analysis Name D:\Data\20151015CEYANG\ZH-4\_1-C,5\_01\_5807.d  
 Method 20151019yezhi.m  
 Sample Name ZH-4  
 Comment

Acquisition Date 10/21/2015 11:15:17 AM

Instrument / Ser# Bruker Customer  
 Operator micrOTOF-Q 125

### Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.2 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	8.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	400.0 Vpp	Set Divert Valve	Source

### Generate Molecular Formula Parameter

Formula, min.		
Formula, max.		
Measured m/z	Tolerance	Charge
Check Valence	Minimum	Maximum
Nitrogen Rule	Electron Configuration	
Filter H/C Ratio	Minimum	Maximum
Estimate Carbon		

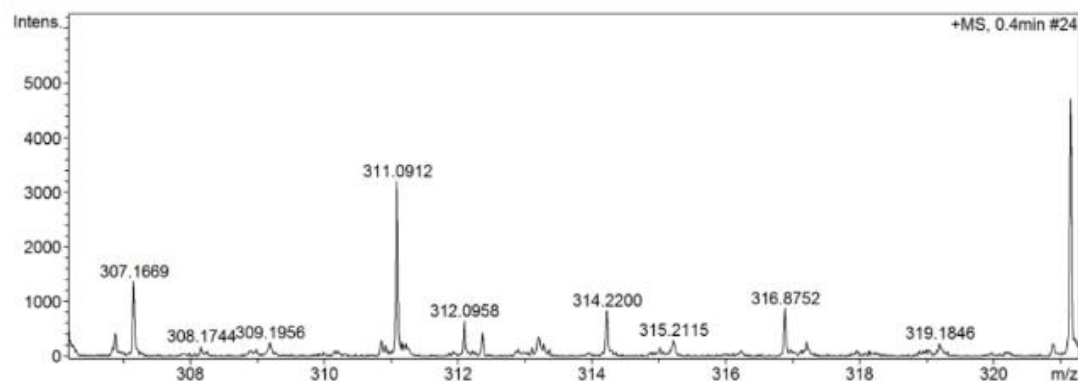


Figure S1.3 HRESIMS spectrum of compound 1

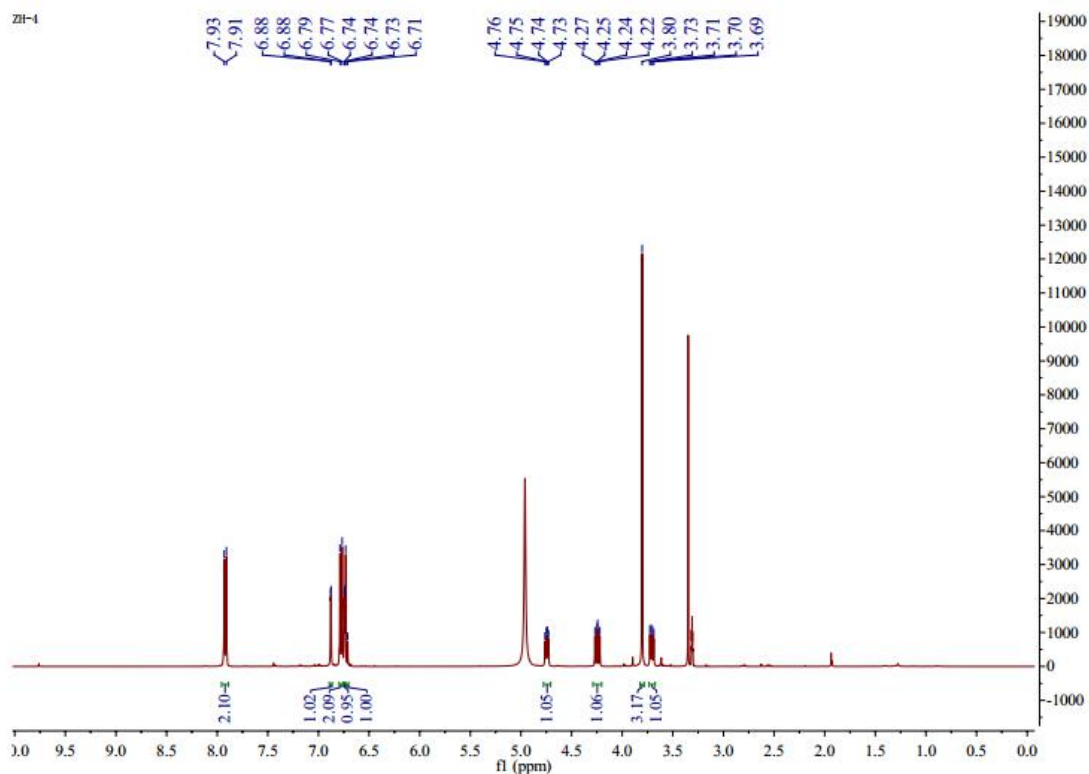
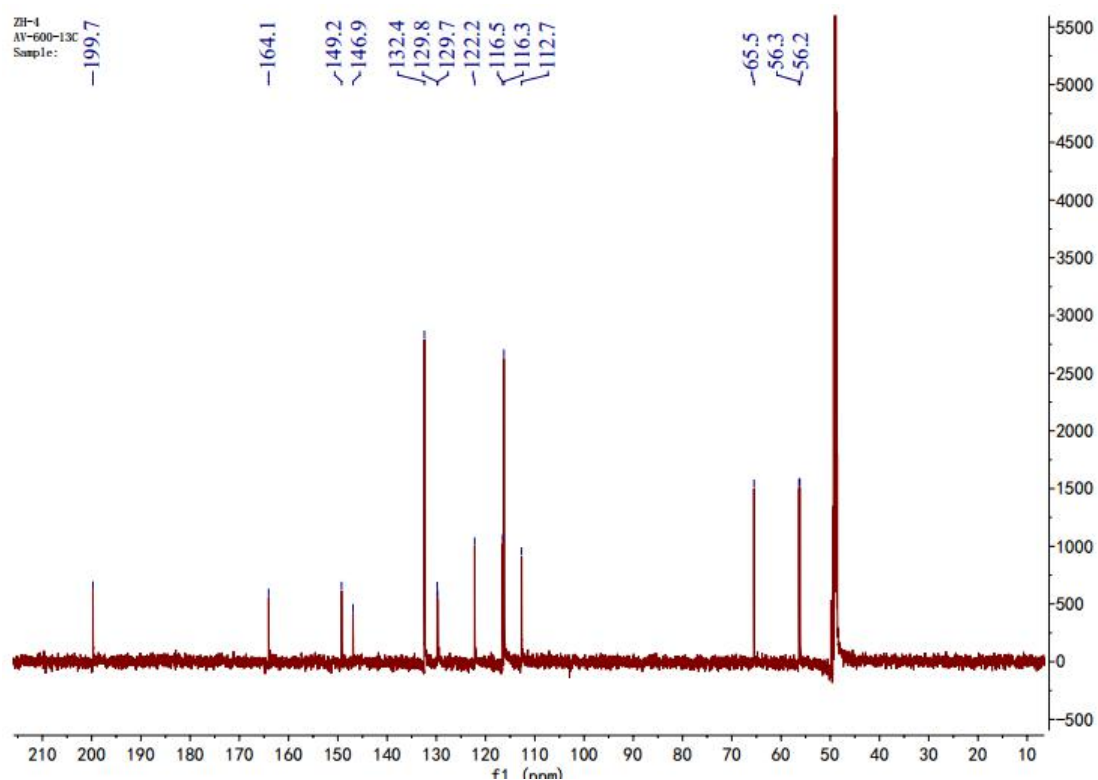
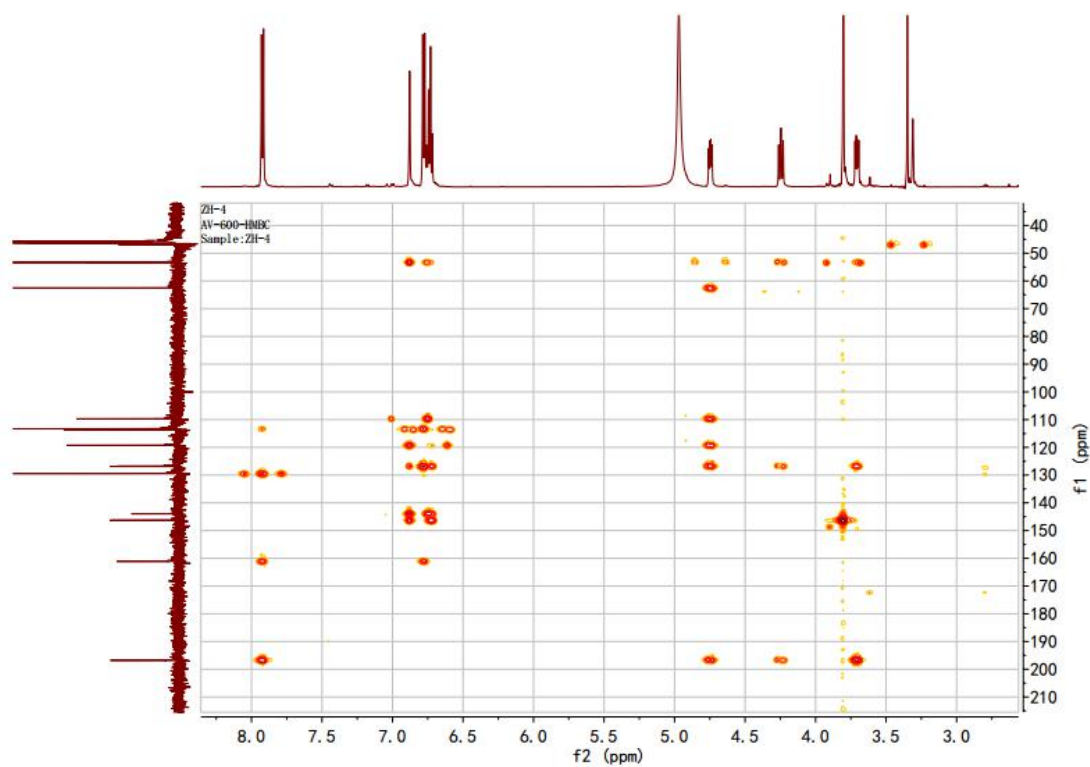


Figure S1.4 <sup>1</sup>H NMR spectrum (400 MHz, CD<sub>3</sub>OD) of compound 1

36



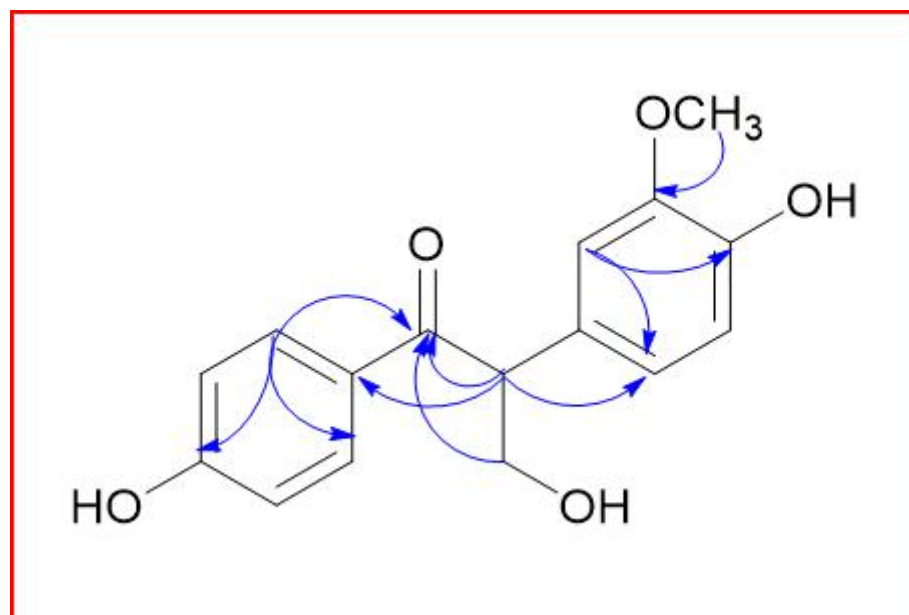
**Figure S1.5**  $^{13}\text{C}$  NMR spectrum (100 MHz,  $\text{CD}_3\text{OD}$ ) of compound **1**



**Figure S1.6** HMBC spectrum (600 MHz,  $\text{CD}_3\text{OD}$ ) of compound **1**

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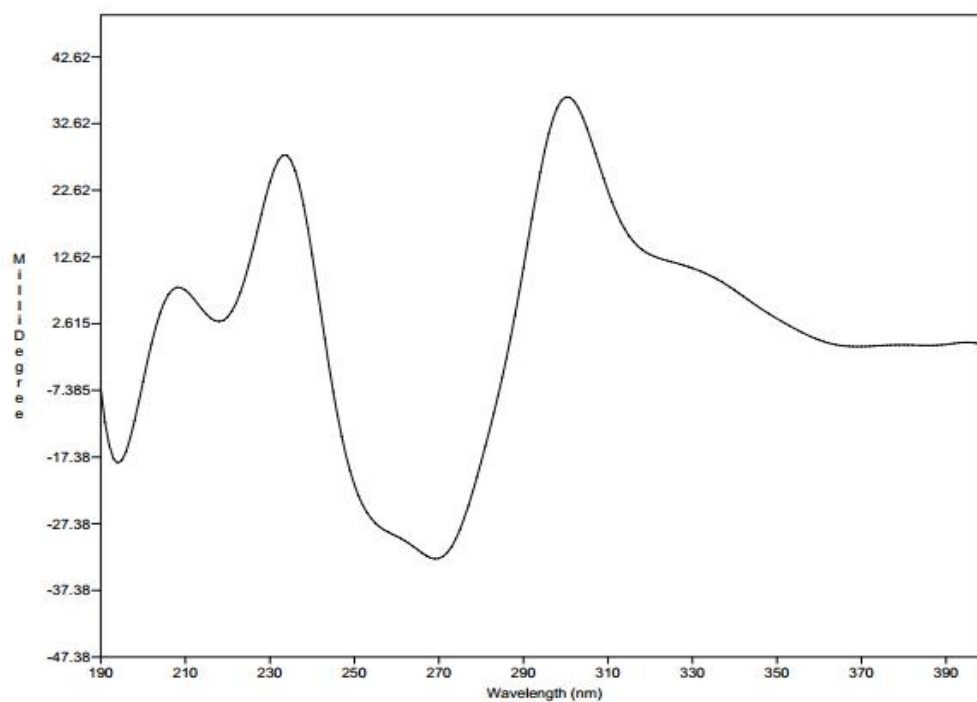
47

48 **Figure S1.7** Key HMBC correlations of compound **1**.

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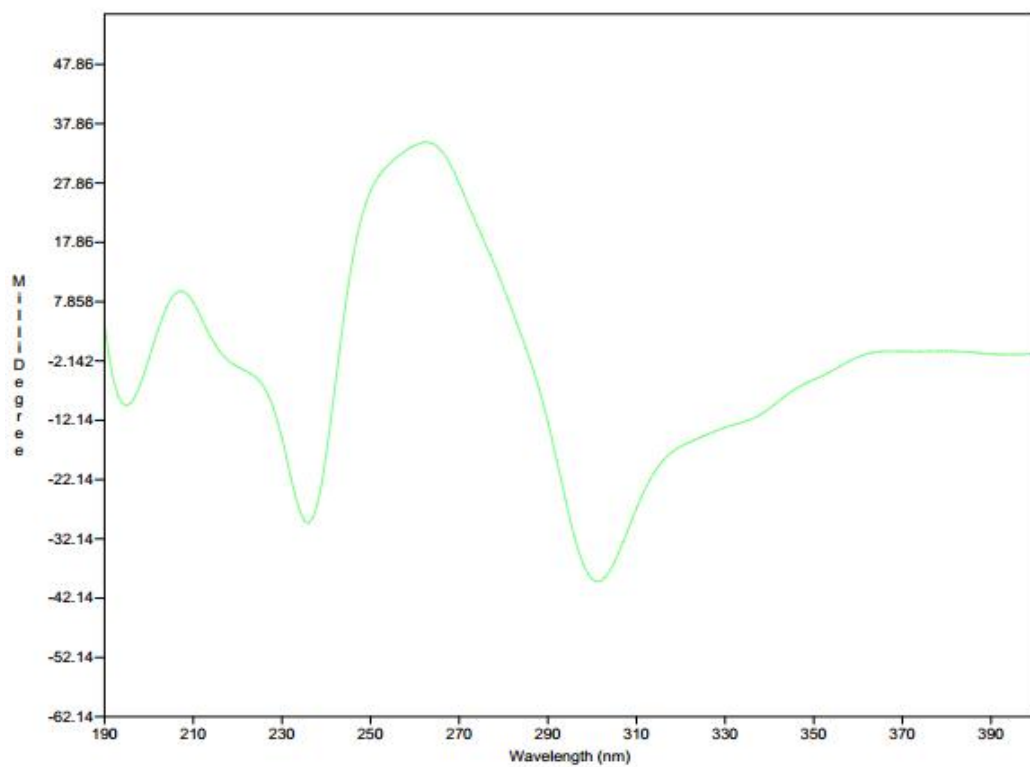
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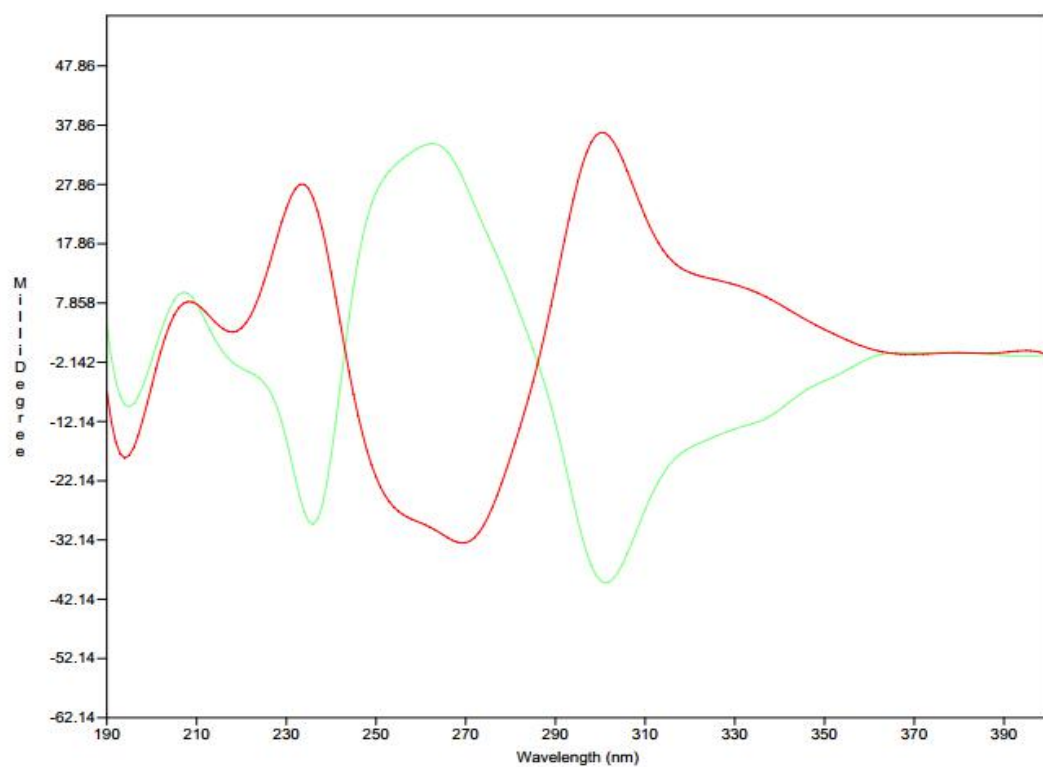


52

53 **Figure S1.8** Experimental ECD spectra of **1a**



**Figure S1.9** Experimental ECD spectra of **1b**



**Figure S1.10** Experimental ECD spectra of **1a/1b**

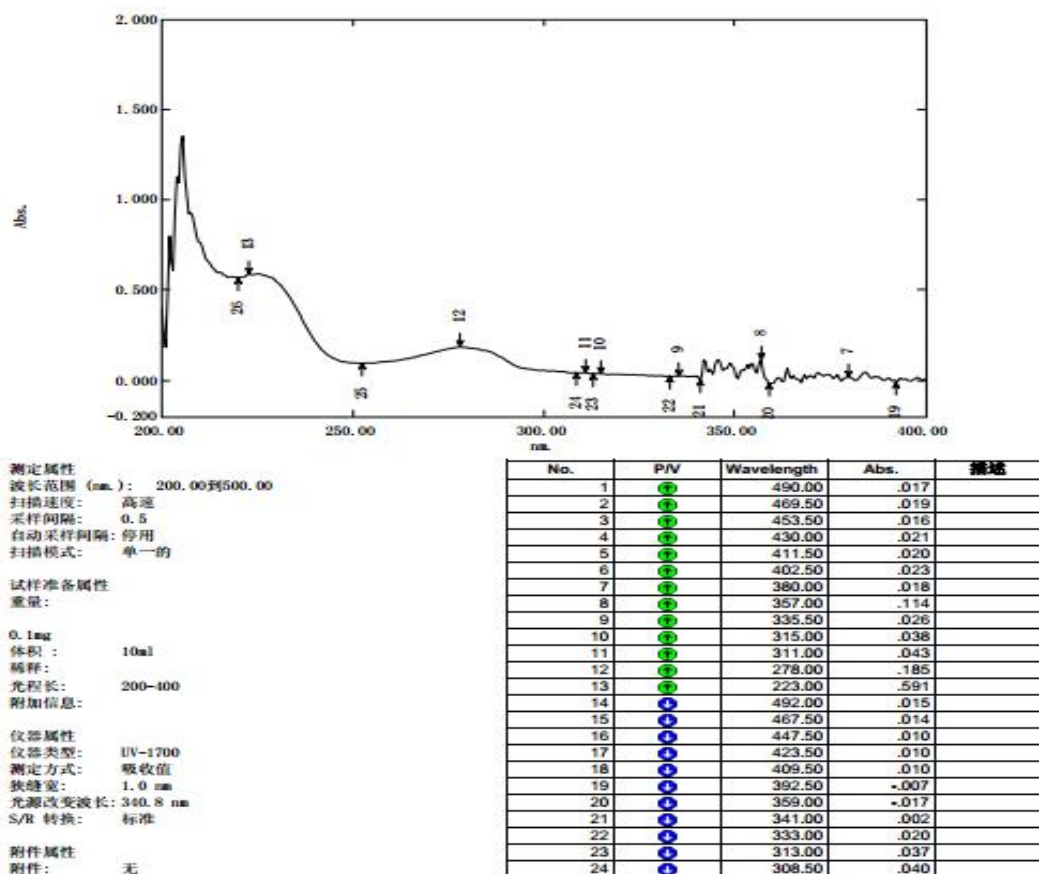


Figure S2.1 UV spectrum of compound 2

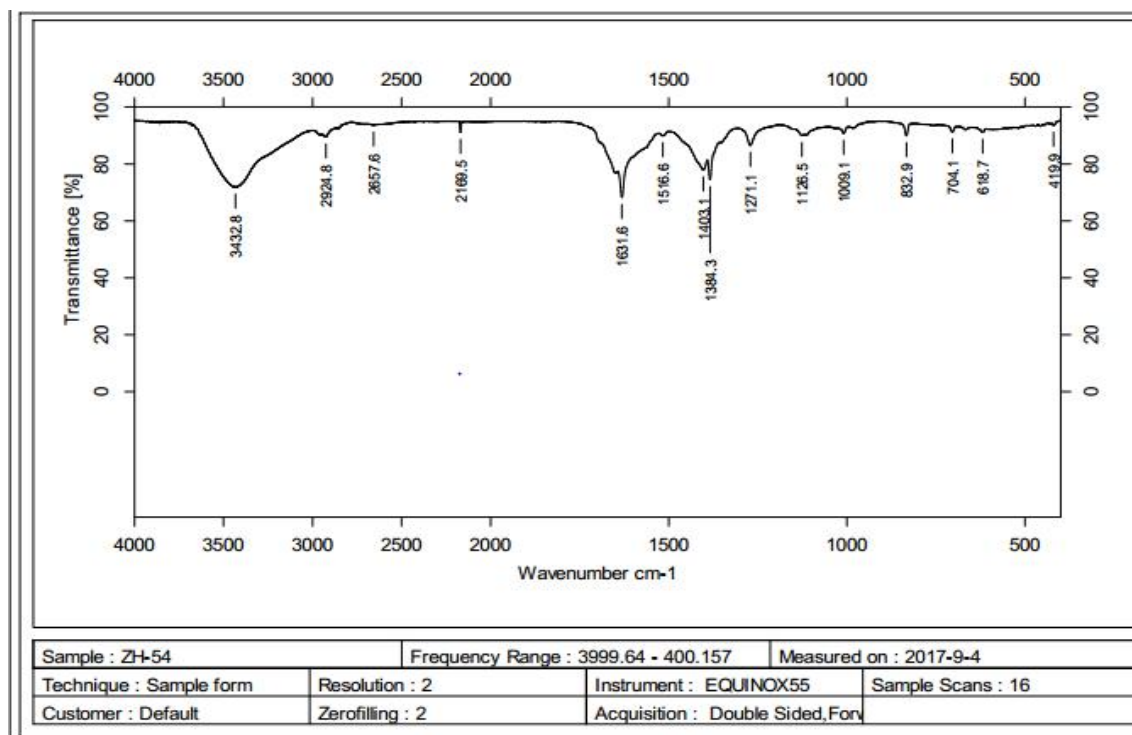


Figure S2.2 IR spectrum of compound 2



## Mass Spectrum Molecular Formula Report

### Analysis Info

Analysis Name D:\Data\20160331CEYANG\ZH-54\_1-A,2\_01\_6921.d  
 Method 20131026\_ceyang.m  
 Sample Name ZH-54  
 Comment

Acquisition Date 3/31/2016 2:57:07 PM

Instrument / Ser# Bruker Customer  
 Operator micrOTOF-Q 125

### Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.2 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	8.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	400.0 Vpp	Set Divert Valve	Source

### Generate Molecular Formula Parameter

Formula, min.		
Formula, max.		
Measured m/z		
Check Valence	Tolerance	Charge
Nitrogen Rule	Minimum	Maximum
Filter H/C Ratio	Electron Configuration	
Estimate Carbon	Minimum	Maximum

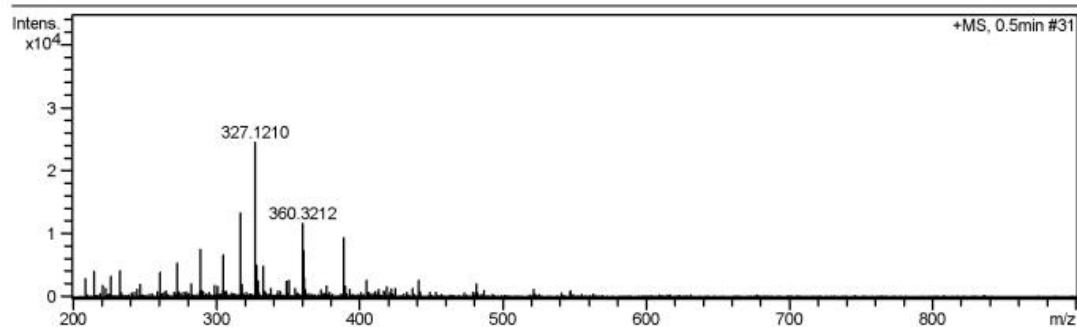


Figure S2.3 HRESIMS spectrum of compound 2

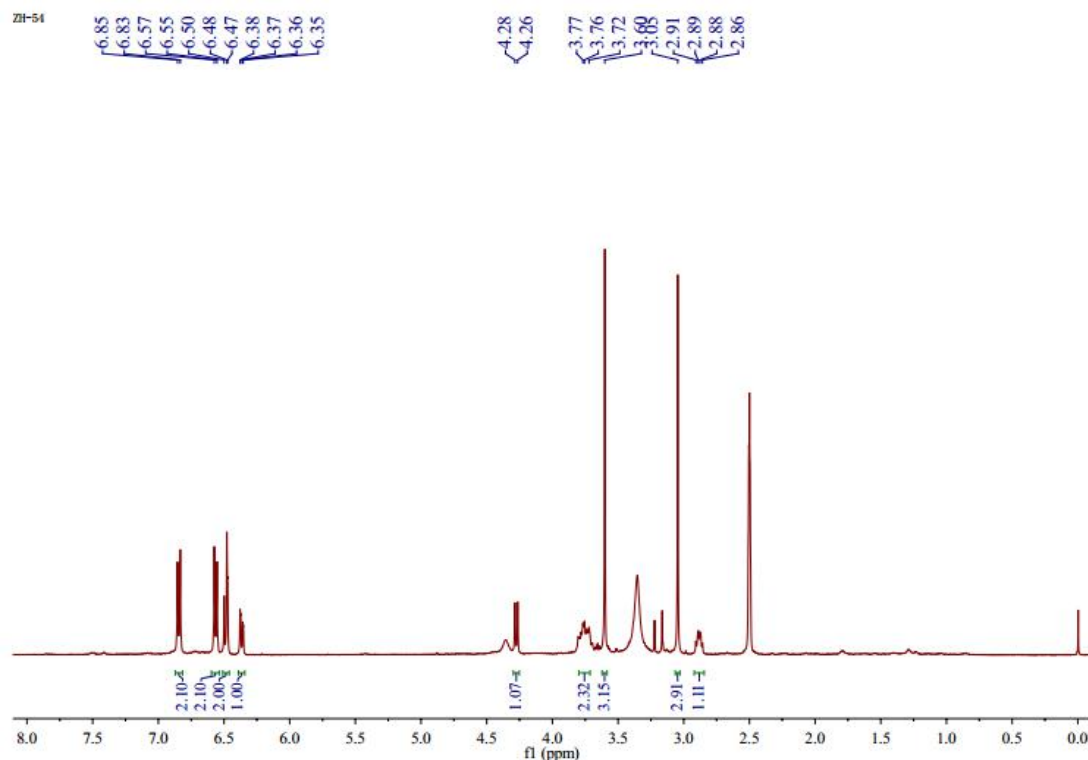
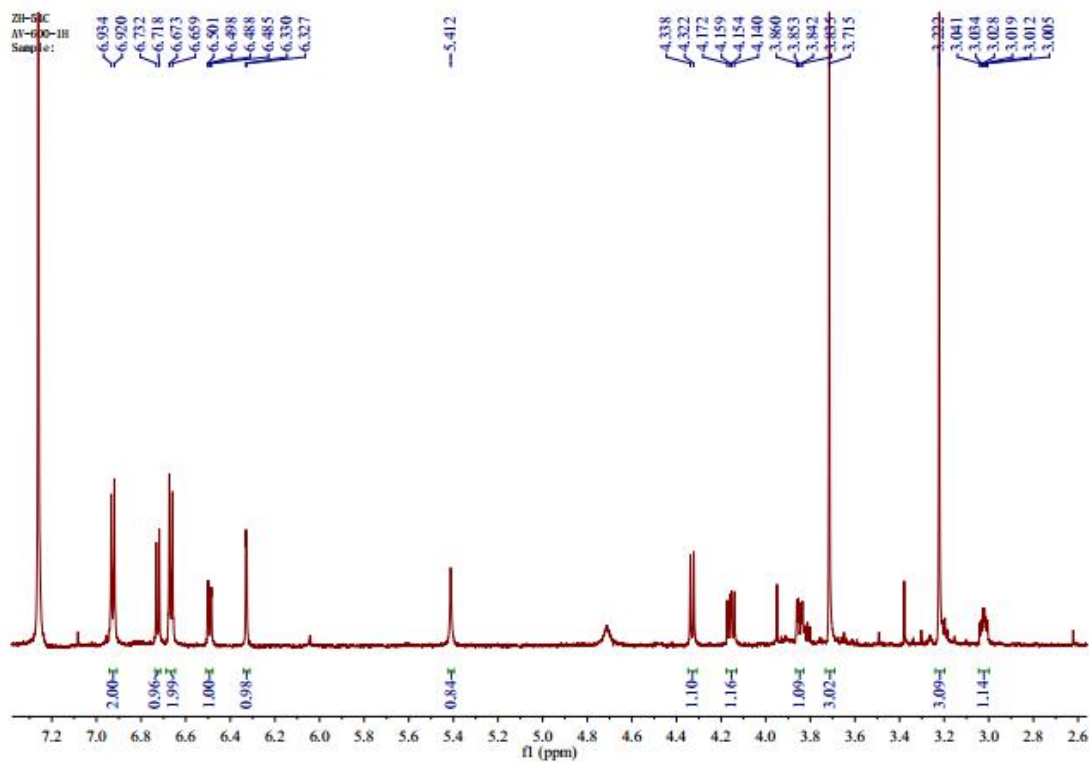
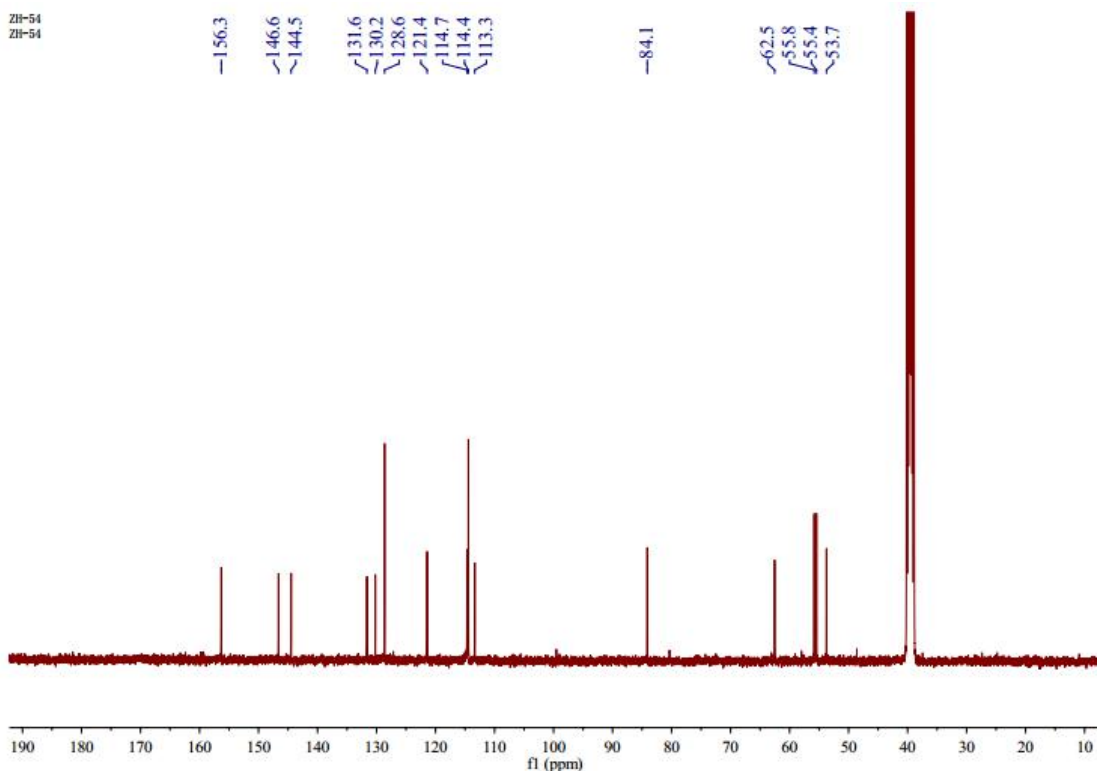


Figure S2.4  $^1\text{H}$  NMR spectrum (400 MHz,  $\text{DMSO}-d_6$ ) of compound 2

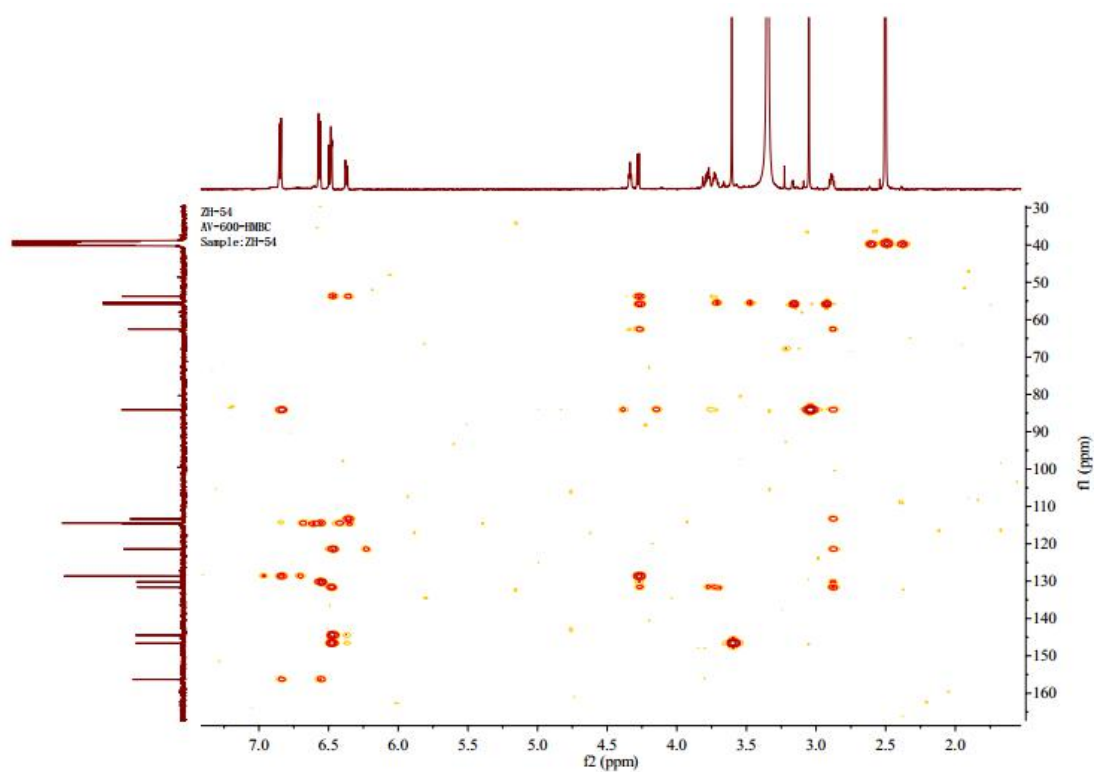




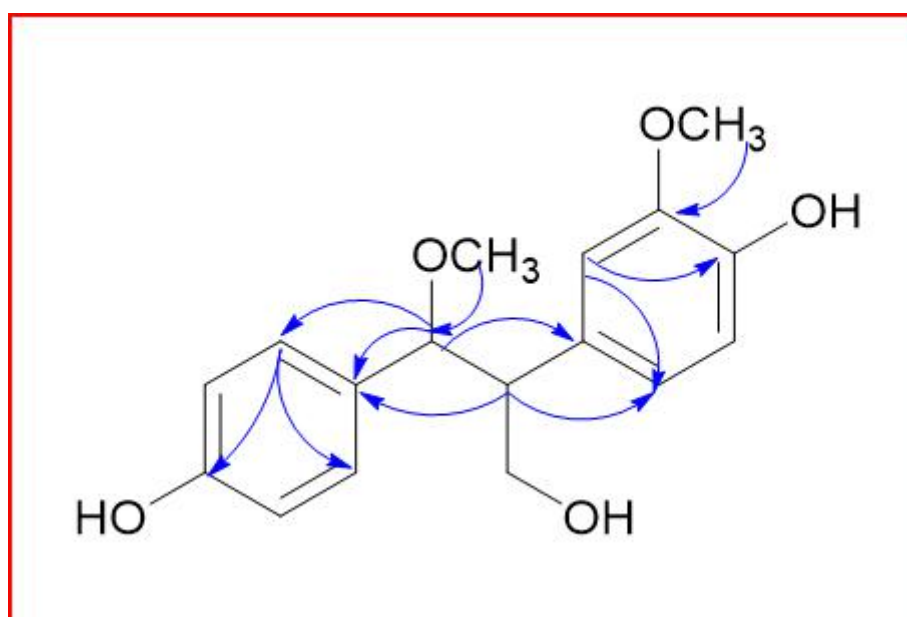
**Figure S2.5**  $^1\text{H}$  NMR spectrum (600 MHz,  $\text{CDCl}_3$ ) of compound **2**



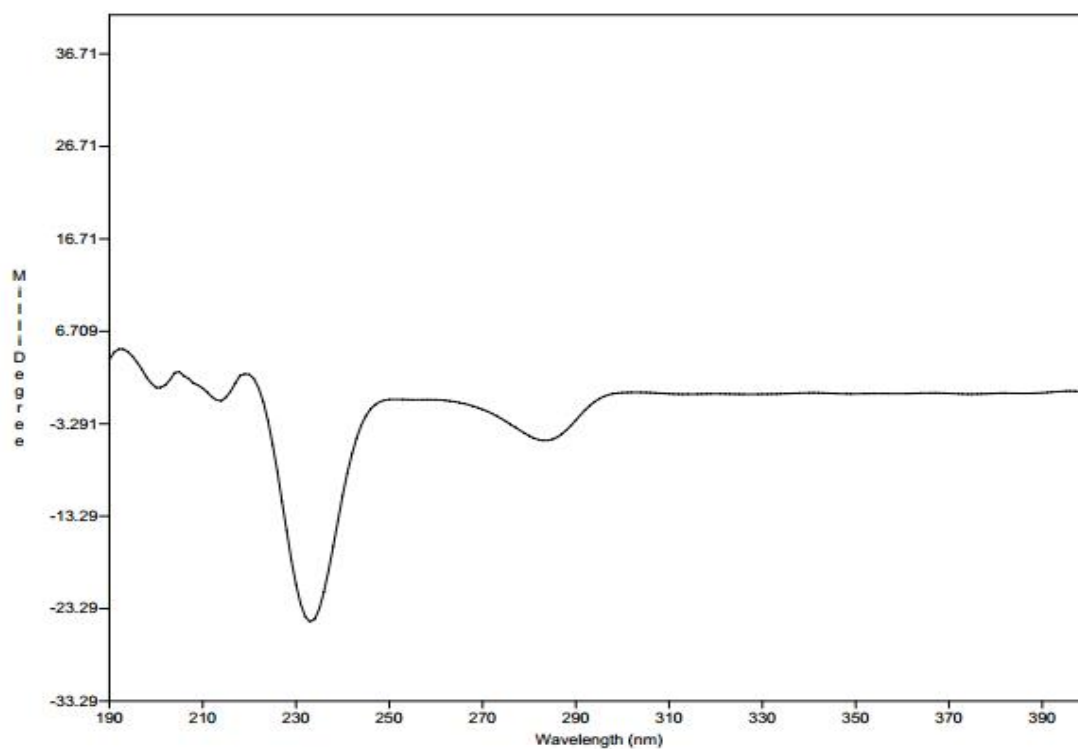
**Figure S2.6**  $^{13}\text{C}$  NMR spectrum (100 MHz,  $\text{DMSO}-d_6$ ) of compound **2**



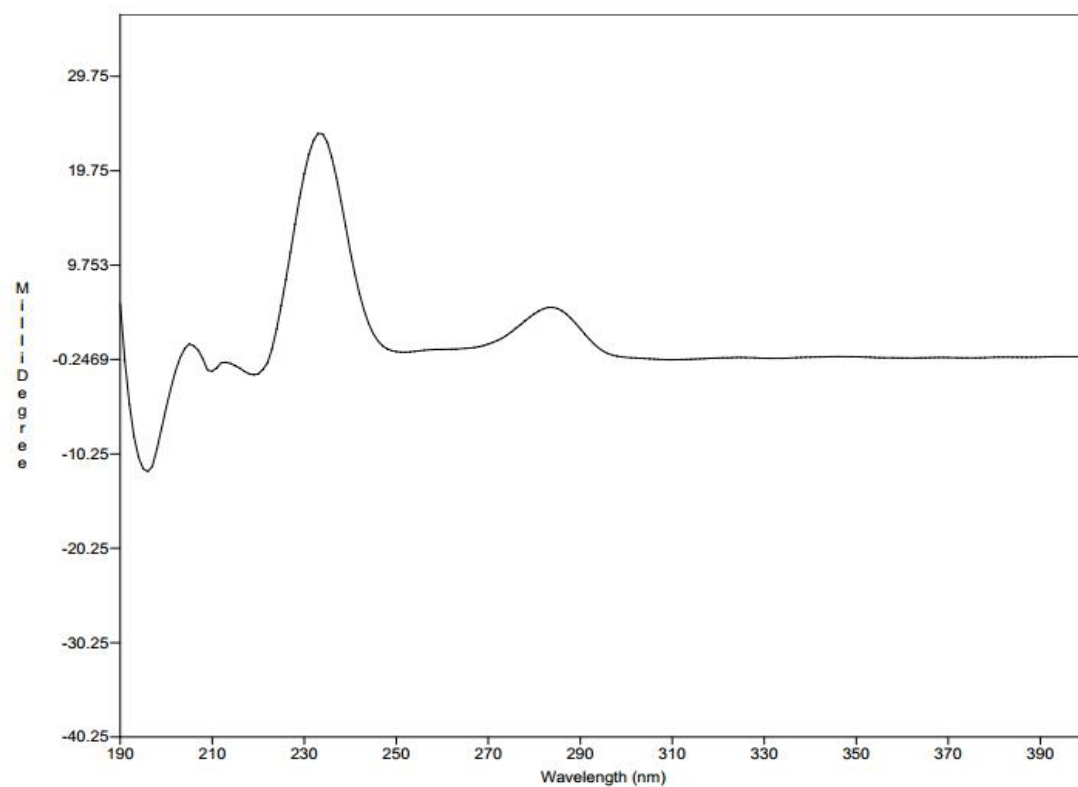
**Figure S2.7** HMBC spectrum (600 MHz, DMSO- $d_6$ ) of compound **2**



**Figure S2.8** Key HMBC correlations of compound **2**



**Figure S2.9** Experimental ECD spectra of **2a**



**Figure S2.10** Experimental ECD spectra of **2b**

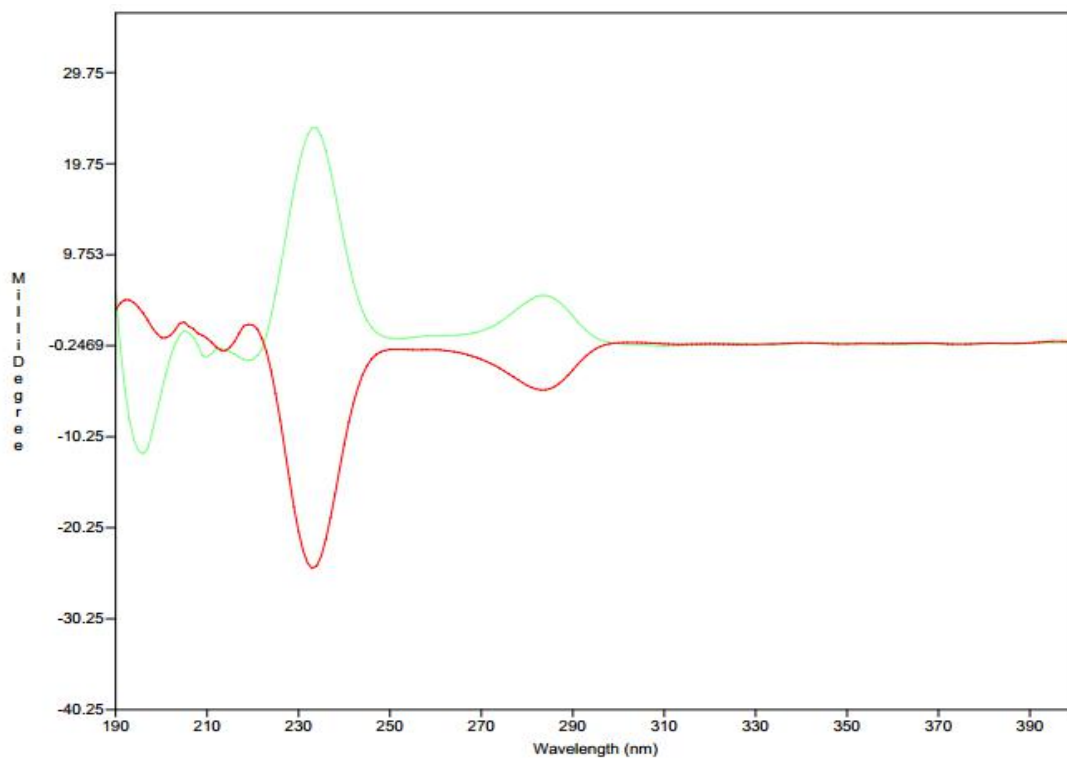


Figure S2.11 Experimental ECD spectra of 2a/2b

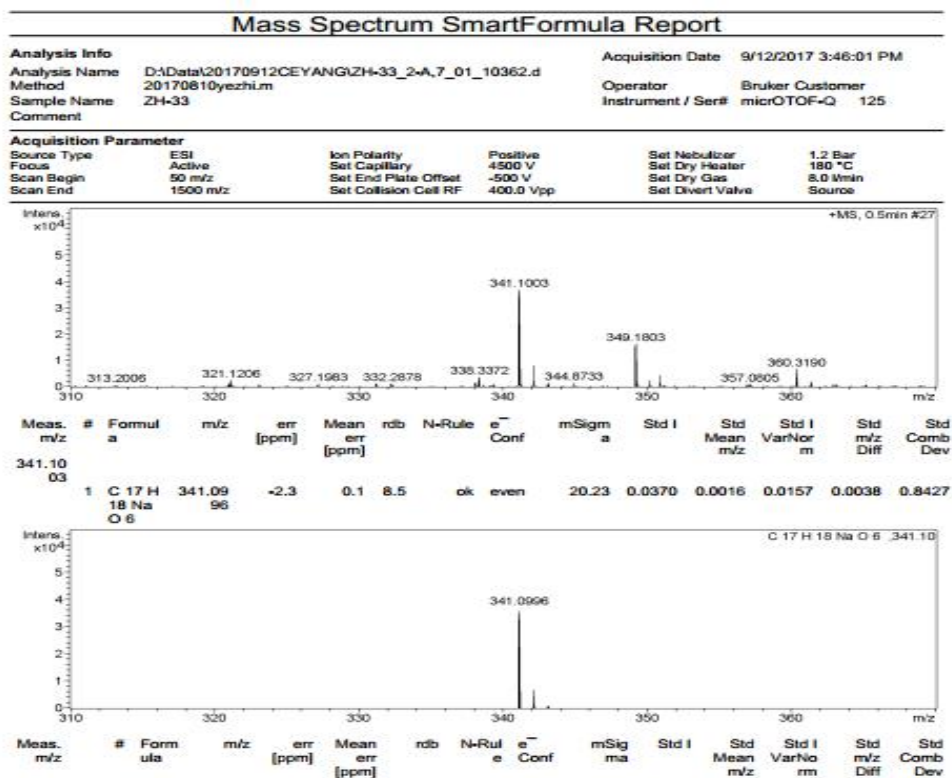
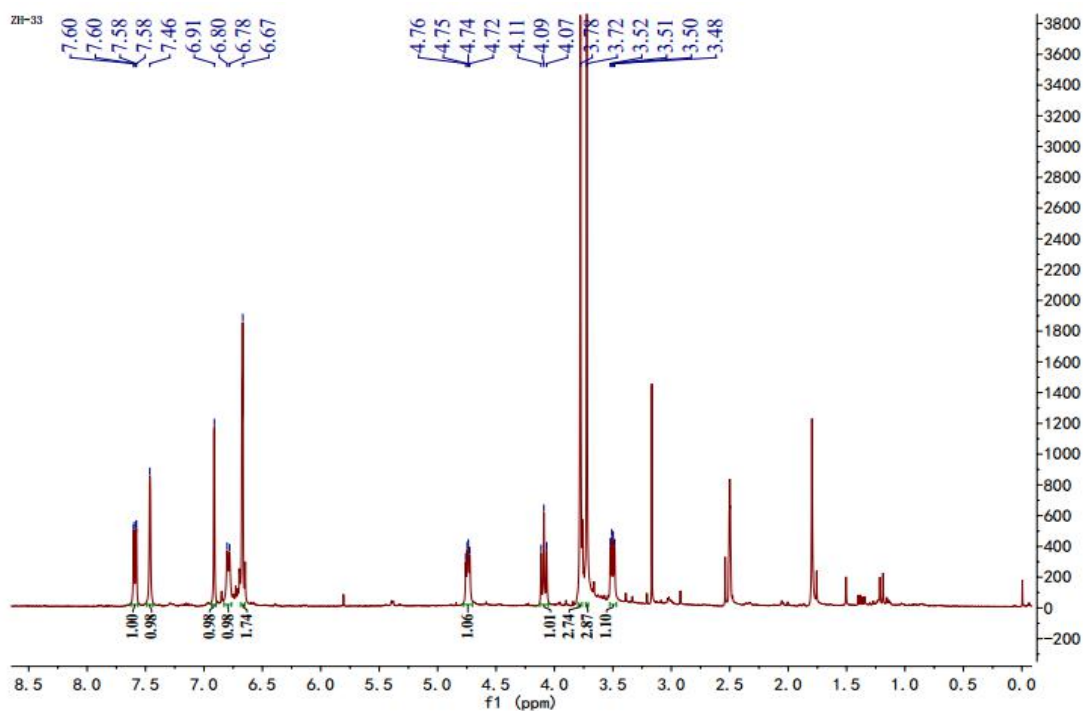


Figure S3.1 HRESIMS spectrum of compound 3

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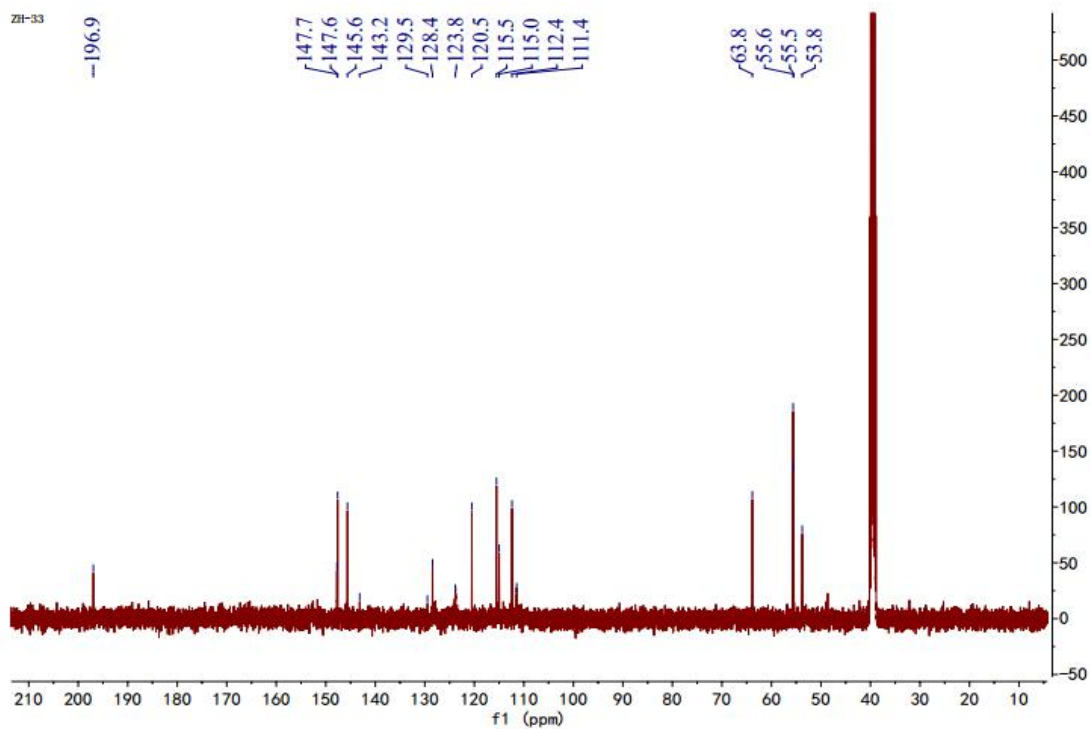
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**Figure S3.2** <sup>1</sup>H NMR spectrum (400 MHz, DMSO-*d*<sub>6</sub>) of compound **3**

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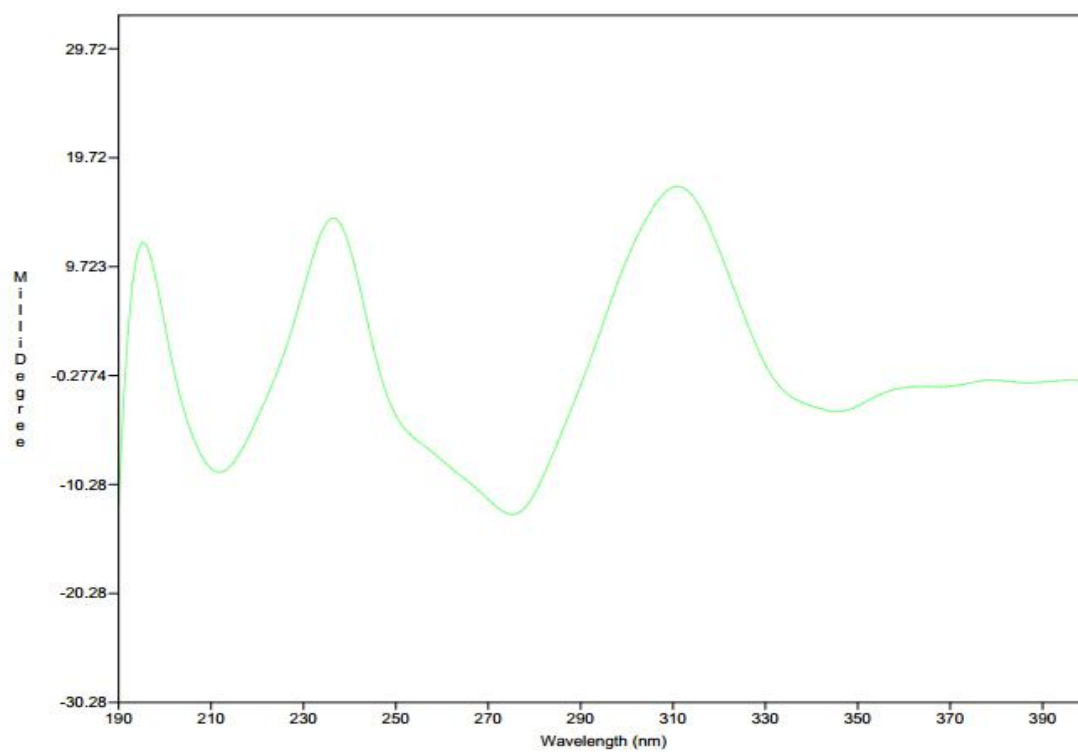
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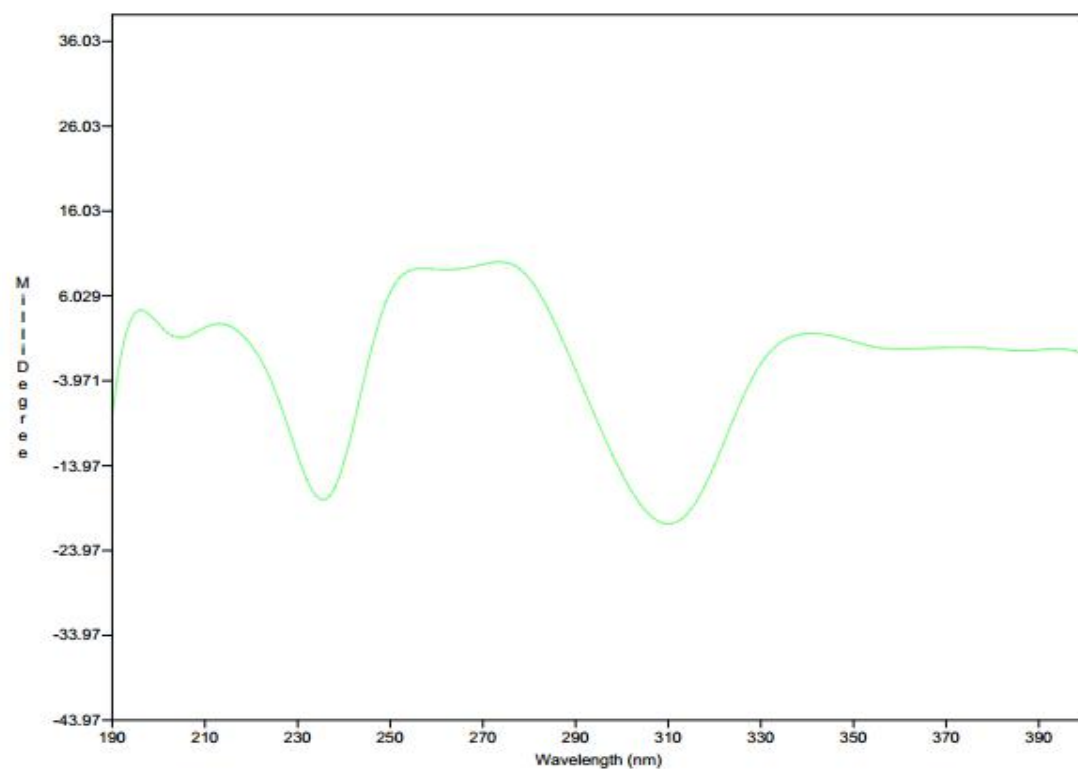
109

**Figure S3.3** <sup>13</sup>C NMR spectrum (100 MHz, DMSO-*d*<sub>6</sub>) of compound **3**

110



**Figure S3.4** Experimental ECD spectra of **3a**



**Figure S3.5** Experimental ECD spectra of **3b**

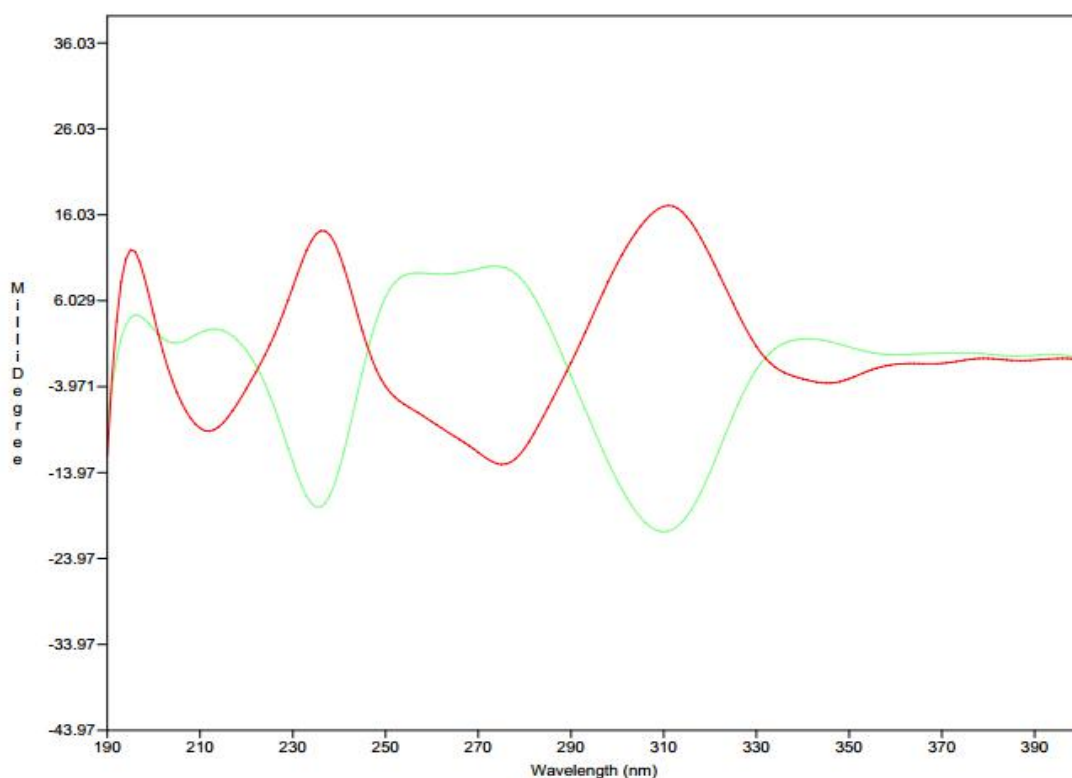


Figure S3.6 Experimental ECD spectra of 3a/3b

### Mass Spectrum SmartFormula Report

#### Analysis Info

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 Method 20170323yezhi.m  
 Sample Name ZH-51  
 Comment

Acquisition Date 3/30/2017 3:38:04 PM

Operator Bruker Customer  
 Instrument / Ser# micrOTOF-Q 125

#### Acquisition Parameter

Source Type ESI  
 Focus Active  
 Scan Begin 50 m/z  
 Scan End 1500 m/z

Ion Polarity Positive  
 Set Capillary 4500 V  
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Set Nebulizer 1.2 Bar  
 Set Dry Heater 180 °C  
 Set Dry Gas 8.0 l/min  
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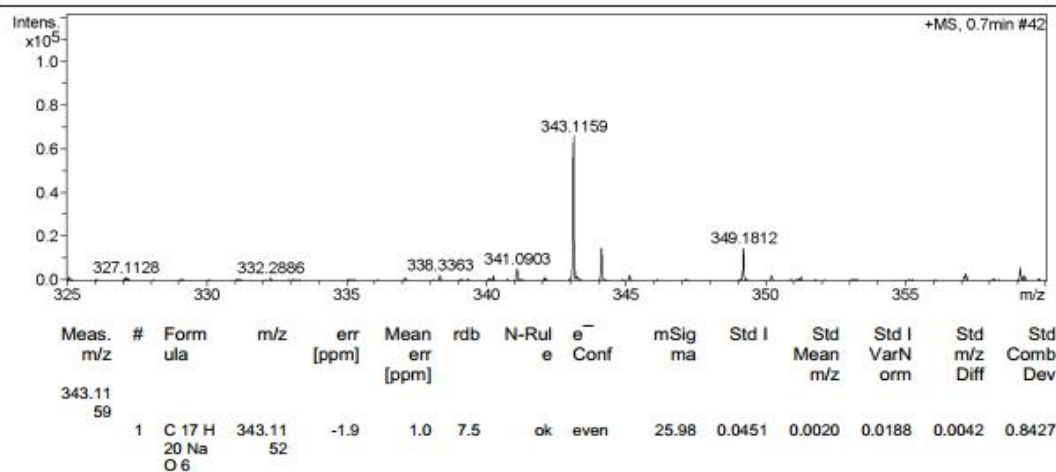
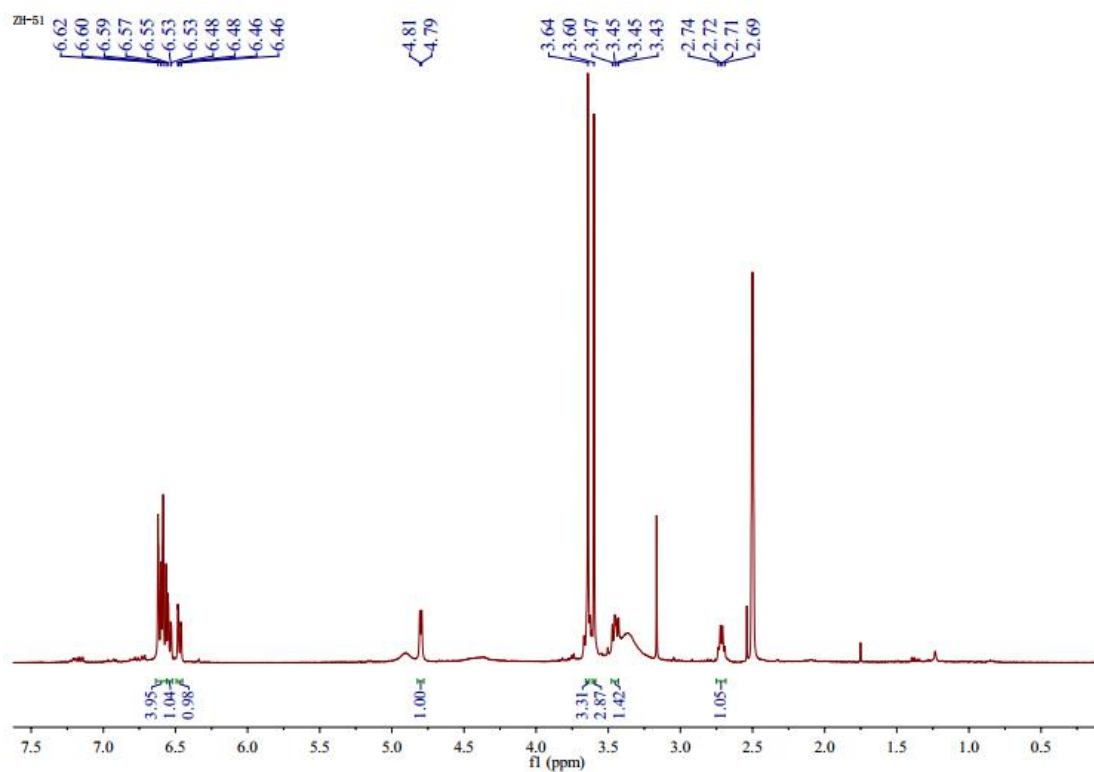
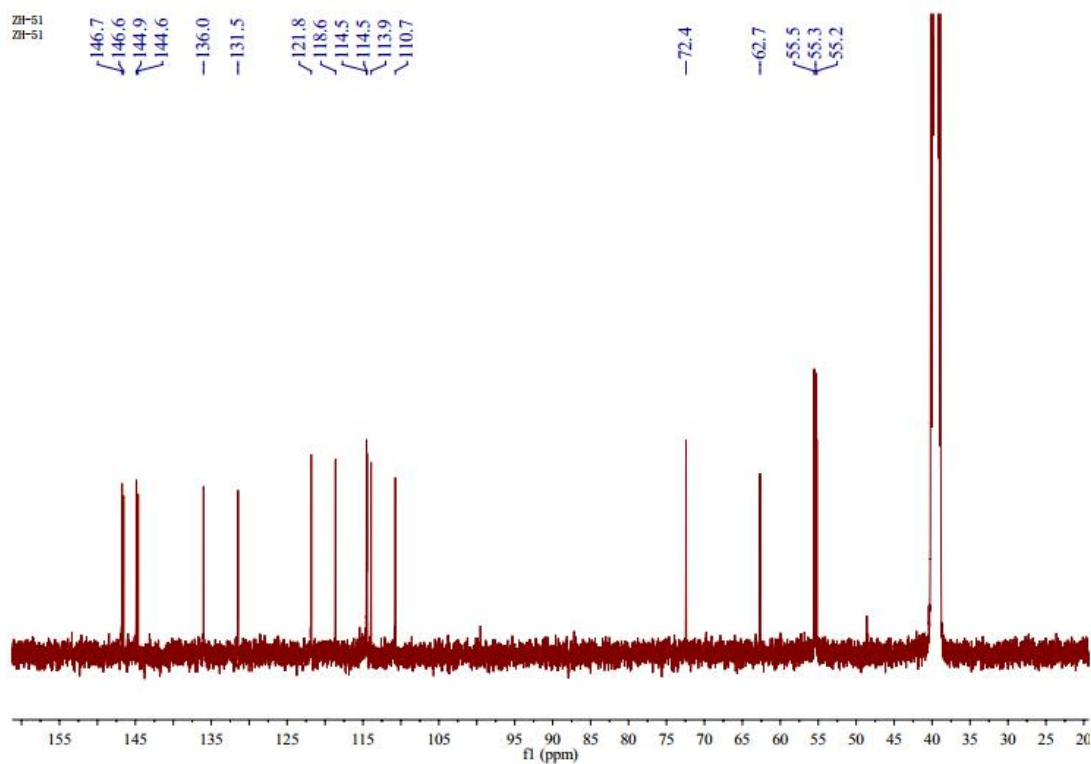


Figure S4.1 HRESIMS spectrum of compound 4

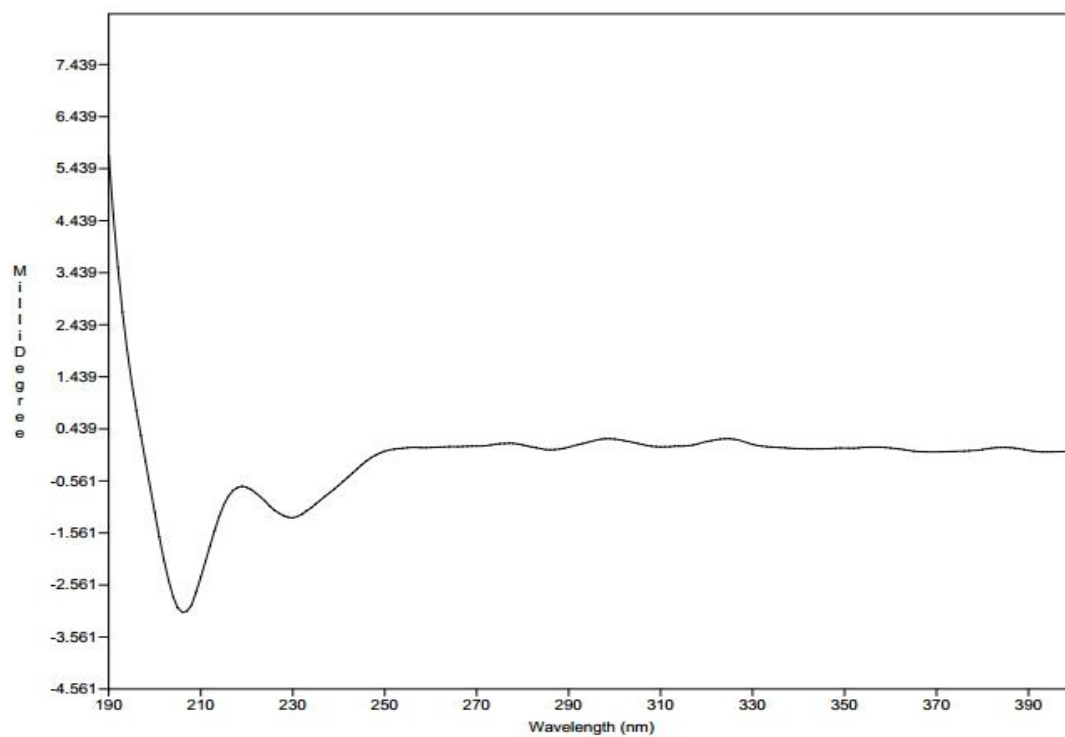




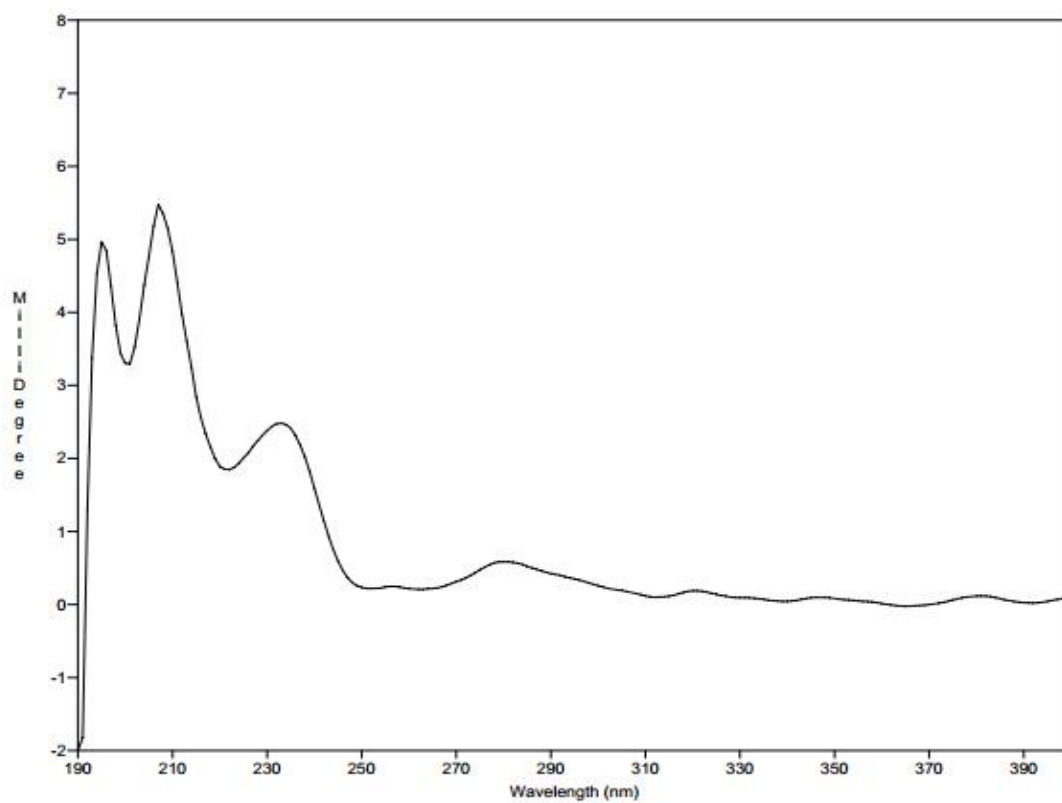
**Figure S4.2** <sup>1</sup>H NMR spectrum (400 MHz, DMSO-*d*<sub>6</sub>) of compound 4



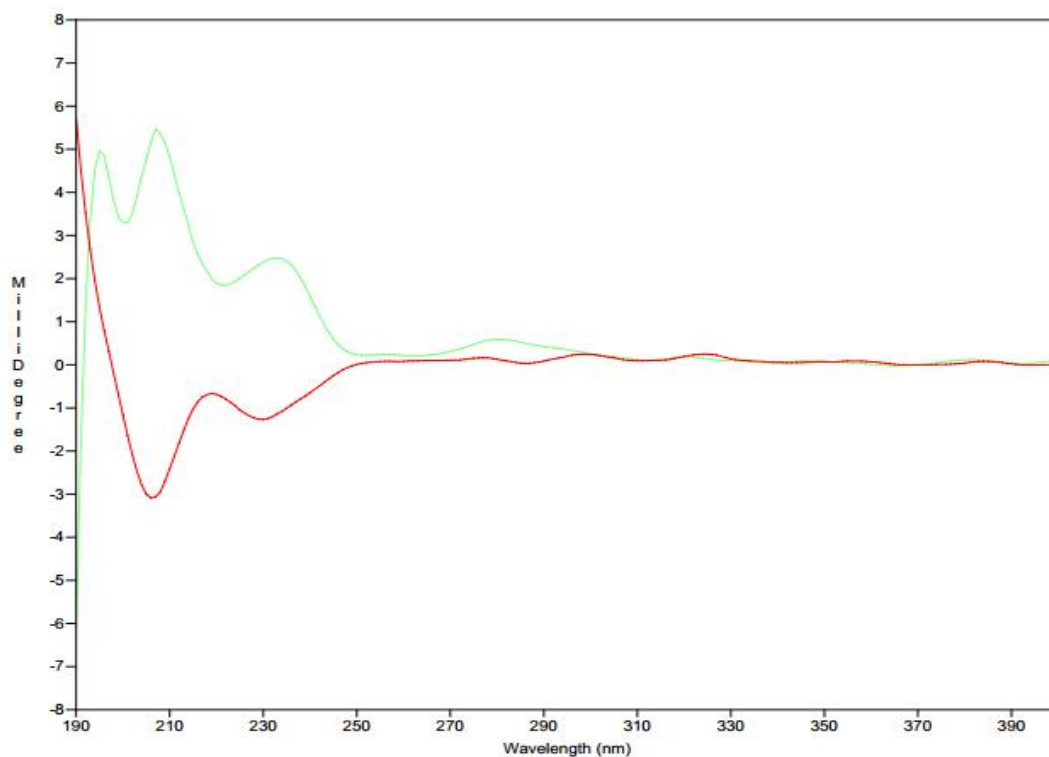
**Figure S4.3** <sup>13</sup>C NMR spectrum (100 MHz, DMSO-*d*<sub>6</sub>) of compound 4



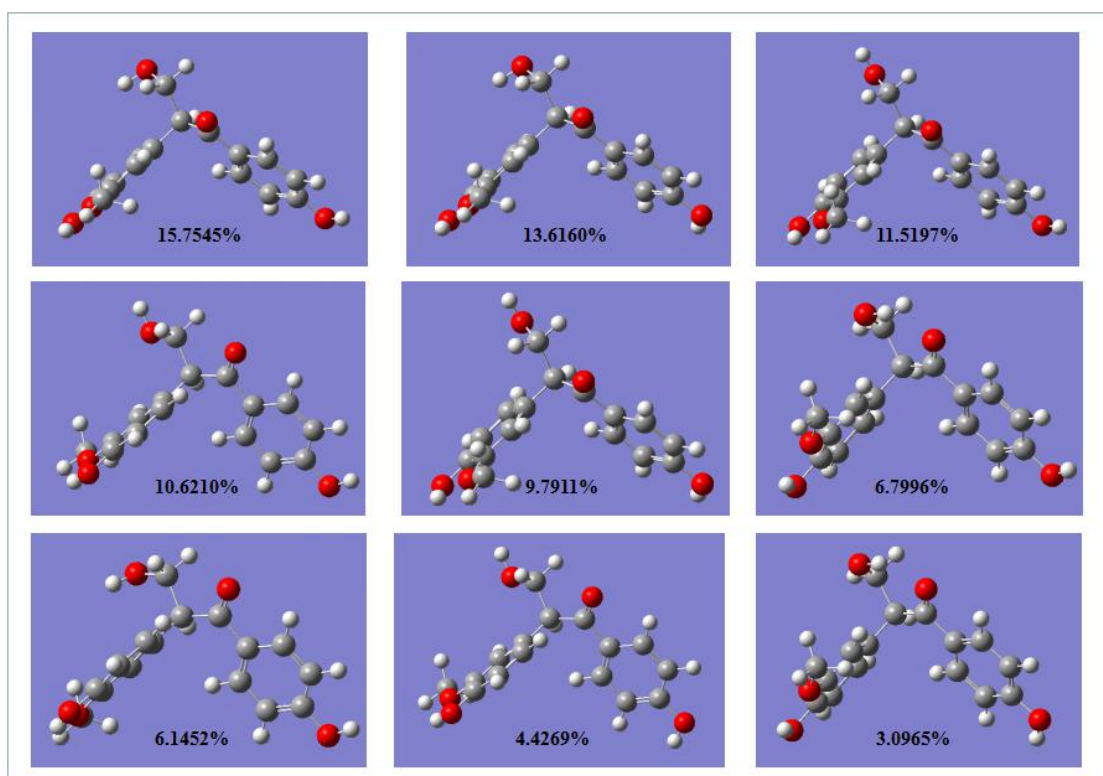
**Figure S4.4** Experimental ECD spectra of **4a**

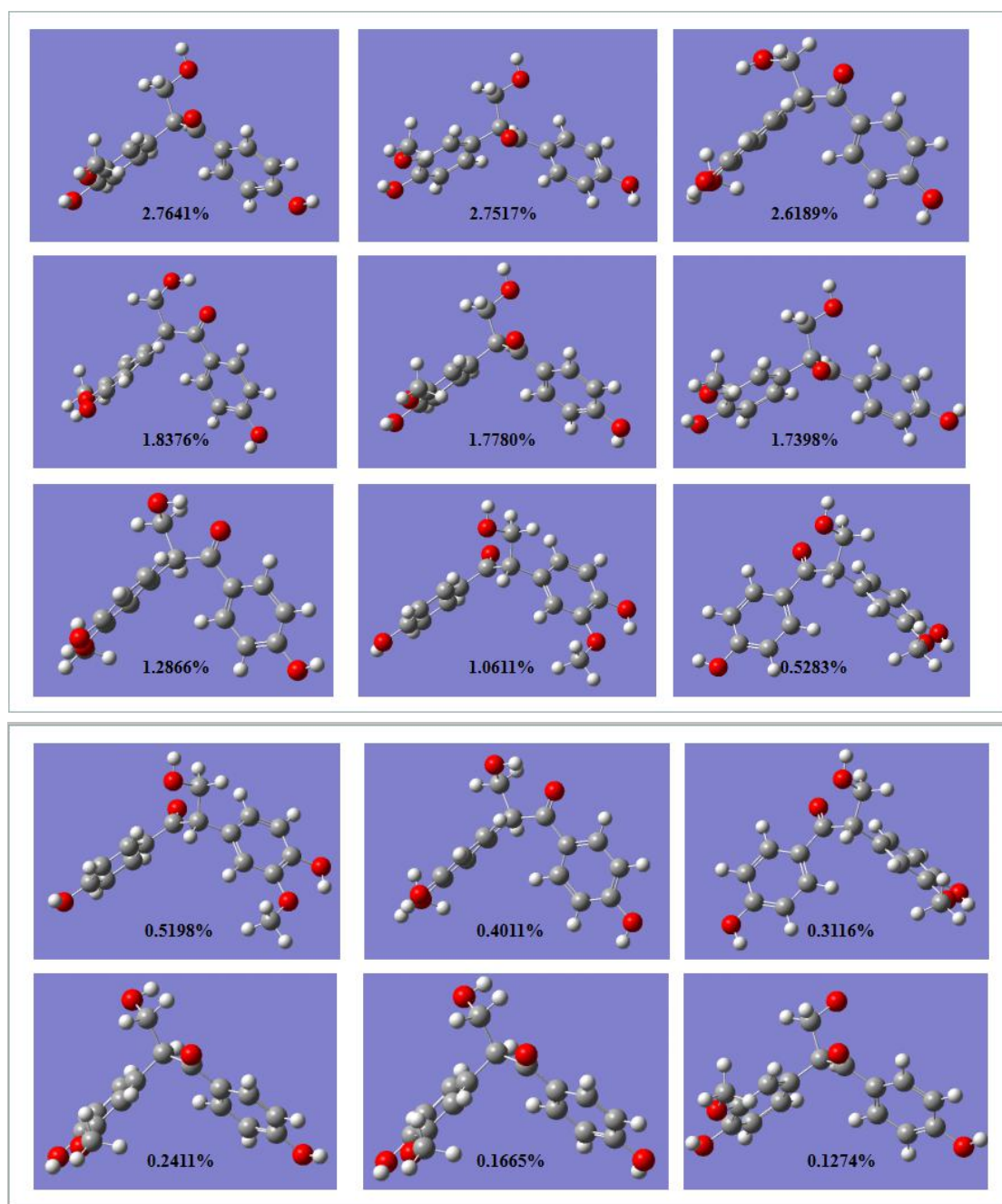


**Figure S4.5** Experimental ECD spectra of **4b**

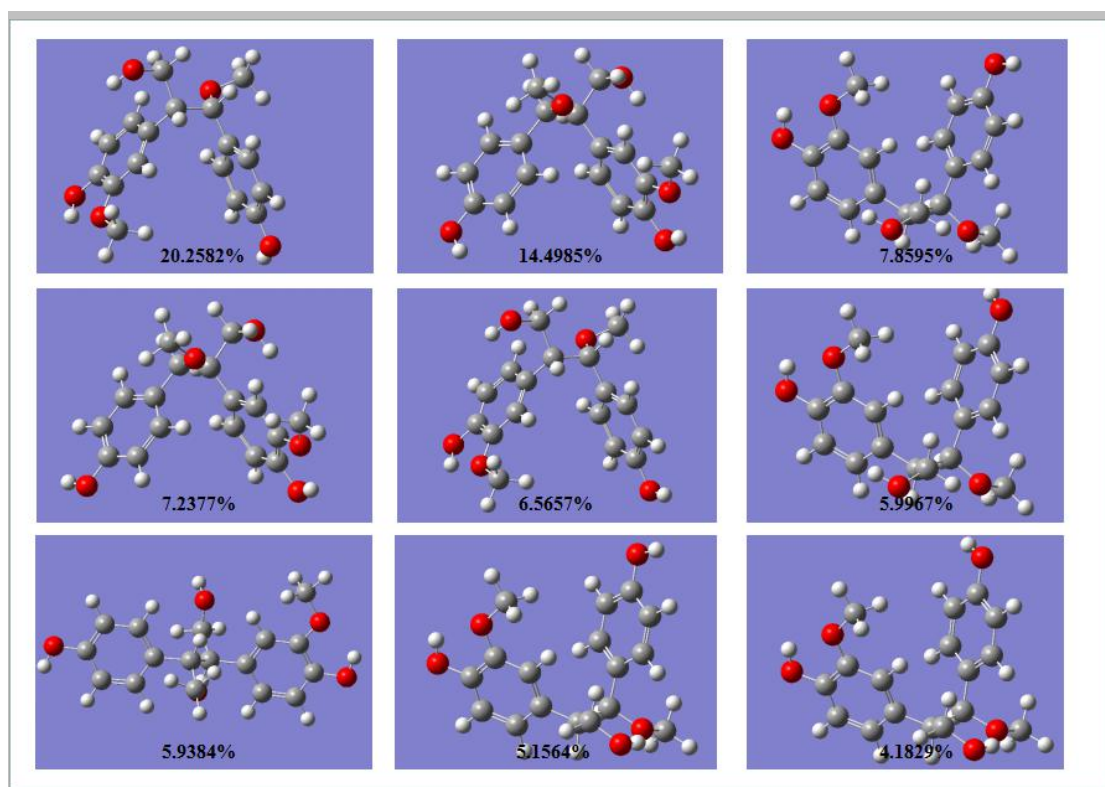


**Figure S4.6** Experimental ECD spectra of **4a/4b**

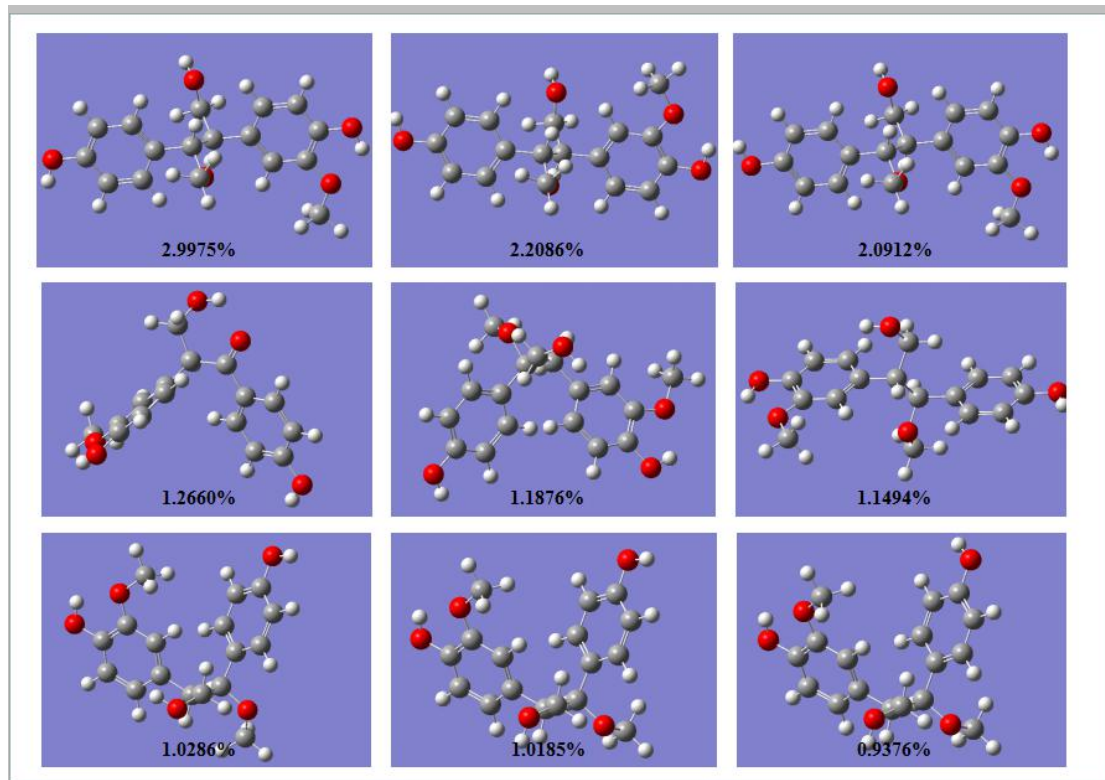




**Figure S5.** low-energy conformers and their boltzmann distribution ratios of compound **1**

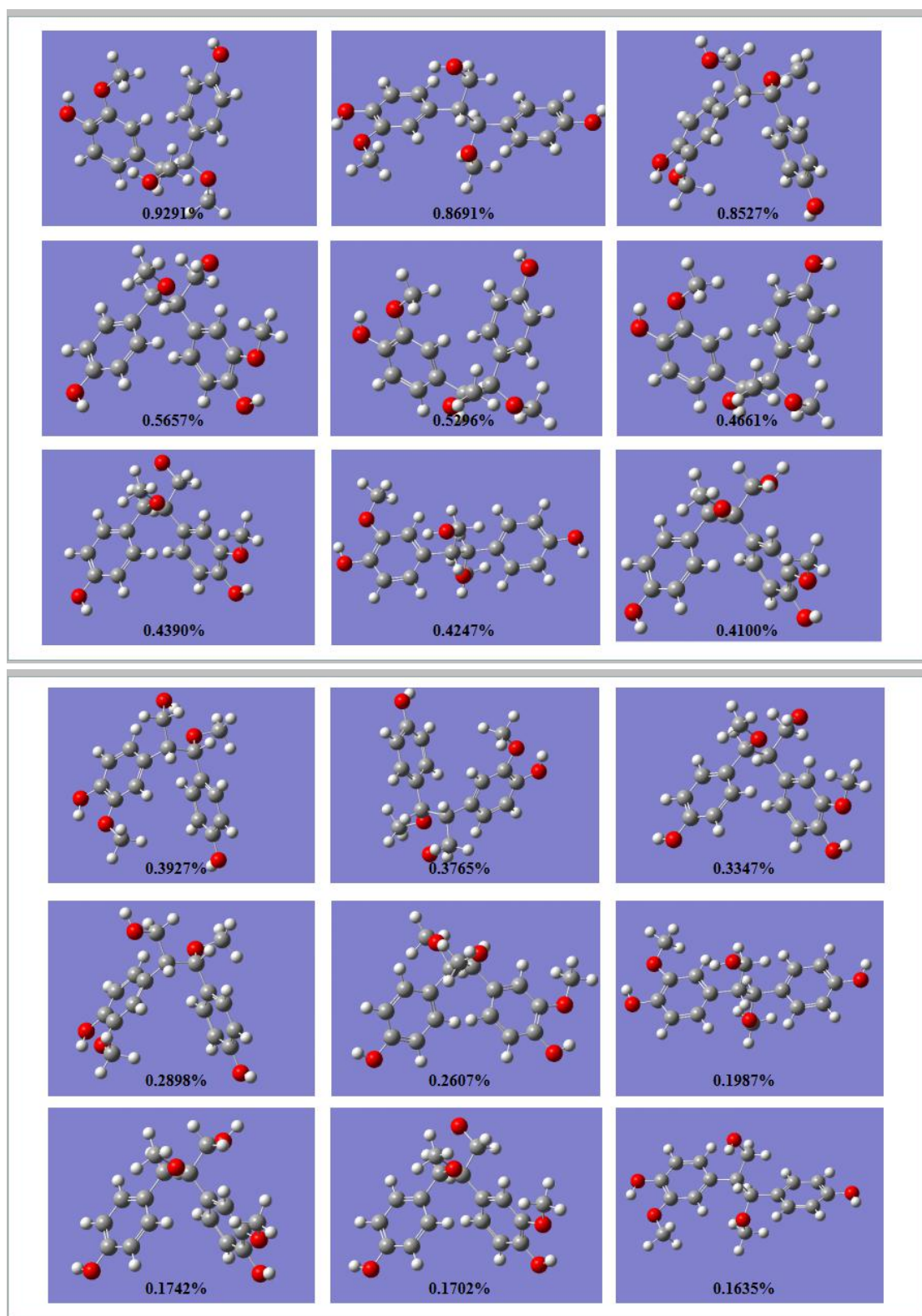


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**Figure S6.** low-energy conformers and their boltzmann distribution ratios of compound **2**