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# Supporting Information

## New lignan from the rattan stems of *Schisandra chinensis*

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### ABSTRACT:

A new lignan named schilignan F (**1**), together with twelve known ones (**2-13**), were isolated from the rattan stems of *Schisandra chinensis*. Their chemical structures were elucidated by spectroscopic methods including one and two-dimensional NMR spectra referring to the literatures, as well as high-resolution mass spectrometric analysis. All compounds were evaluated for their cytotoxicities against human Hela cancer cell lines *in vitro*. The results showed that compounds **2**, **6** and **8** exhibited weak cytotoxic activity with IC<sub>50</sub> values of 30.6, 86.3 and 41.0 μM, and cisplatin showed cytotoxic activity with IC<sub>50</sub> value of 27.3 μM.

**Keywords:** *Magnoliaceae*, Lignan, *Schisandra chinensis*, Natural products, Cytotoxicity

**Table S1** <sup>13</sup>C-NMR Data of **2-13** (100 MHz in <sup>13</sup>C NMR, CD<sub>3</sub>OD)

NO.	2	3	4	5	6	7	8	9	10	11	12	13
1	139.1	138.4	138.8	133.2	134.7	128.5	129.1	133.7	138.8	146.3	146.4	130.6
2	111.3	111.3	111.2	109.3	110.8	114.0	112.7	111.6	112.7	150.8	150.8	111.9
3	152.1	150.9	152.1	147.6	149.0	148.4	149.1	148.8	148.9	118.4	118.3	153.4
4	146.4	147.6	146.6	146.0	147.4	147.5	147.5	147.6	145.6	136.5	136.5	149.1
5	119.1	118.0	119.6	114.6	116.1	115.2	116.0	115.8	116.1	122.2	122.1	115.8
6	119.6	119.4	119.1	118.3	119.8	122.4	121.6	120.7	121.5	114.1	114.2	124.7
7	88.3	88.5	88.6	87.8	89.2	90.0	89.3	74.1	67.3	40.8	40.8	199.7
8	55.9	55.6	55.7	51.5	52.9	99.2	92.8	87.7	37.3	139.0	139.0	41.7
9	65.2	65.1	62.2	70.9	72.3	73.1	76.1	61.8	9.9	115.9	115.9	58.9
1'	136.9	137.1	137.1	135.6	137.0	133.1	133.6	138.2	138.0	103.1	103.0	
2'	117.1	114.2	114.1	112.6	114.2	110.6	111.3	114.1	112.7	74.9	75.0	
3'	141.9	145.3	145.2	143.8	145.2	149.3	148.7	151.6	148.8	78.0	78.2	
4'	146.5	147.5	147.5	146.0	147.5	147.3	147.4	147.2	145.5	71.6	71.4	
5'	129.5	129.6	129.1	128.3	129.7	116.3	115.6	119.6	116.1	77.8	77.9	
6'	116.7	118.0	117.9	116.8	118.2	119.9	120.5	122.1	121.6	68.7	62.5	
7'	32.7	32.9	32.9	31.5	32.9	86.8	87.8	32.7	57.3			
8'	35.9	35.8	35.8	34.4	35.8	60.3	62.4	32.7	36.9			
9'	62.3	62.3	65.1	60.8	62.2	72.2	72.0	69.9	12.2			
OCH <sub>3</sub>	56.5	56.8	56.4	55.0	56.8	56.5	56.4	56.3	56.4	56.7	56.7	56.4
OCH <sub>3</sub>		56.8	56.7	56.3	56.5	56.6	56.4	56.5	56.4			
1''	101.3	102.8	101.4	102.8	104.3	100.1		104.5		111.0		
2''	72.1	74.9	72.2	73.7	75.2	74.8		75.2		77.0		
3''	72.2	78.2	72.1	76.8	78.2	78.3		77.9		80.5		
4''	73.9	71.4	73.9	70.2	71.7	71.1		71.7		75.0		
5''	70.8	77.8	70.8	76.6	78.1	78.0		78.1		65.6		
6''	17.9	62.5	18.0	61.3	62.8	62.4		62.8				

**Table S2** Cytotoxic activities of compounds (**1-13**) from the rattan stems of *S. chinensis*.

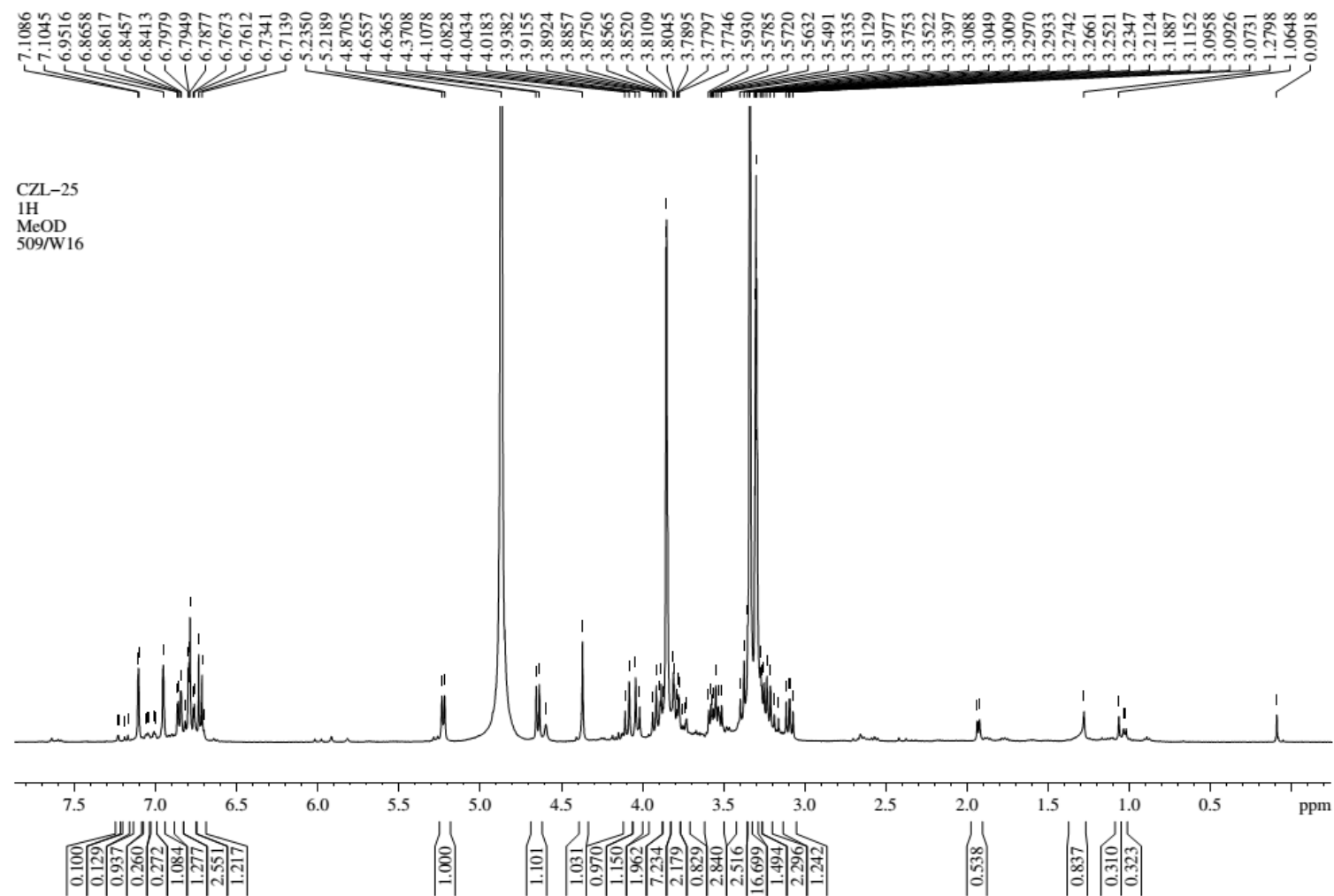
Growth Inhibition Constant (IC <sub>50</sub> in $\mu\text{M}$ ) <sup>a</sup>			
Drugs	IC <sub>50</sub> ( $\mu\text{M}$ )	Drugs	IC <sub>50</sub> ( $\mu\text{M}$ )
cisplatin <sup>b</sup>	27.3 $\pm$ 1.9	Compound <b>7</b>	>100
Compound <b>1</b>	>100	Compound <b>8</b>	>100
Compound <b>2</b>	30.6 $\pm$ 1.7	Compound <b>9</b>	41.0 $\pm$ 3.5
Compound <b>3</b>	>100	Compound <b>10</b>	>100
Compound <b>4</b>	>100	Compound <b>11</b>	>100
Compound <b>5</b>	>100	Compound <b>12</b>	>100
Compound <b>6</b>	86.3 $\pm$ 5.2	Compound <b>13</b>	>100

<sup>a</sup>IC<sub>50</sub> was defined as the concentration that resulted in a 50% decrease in cell number

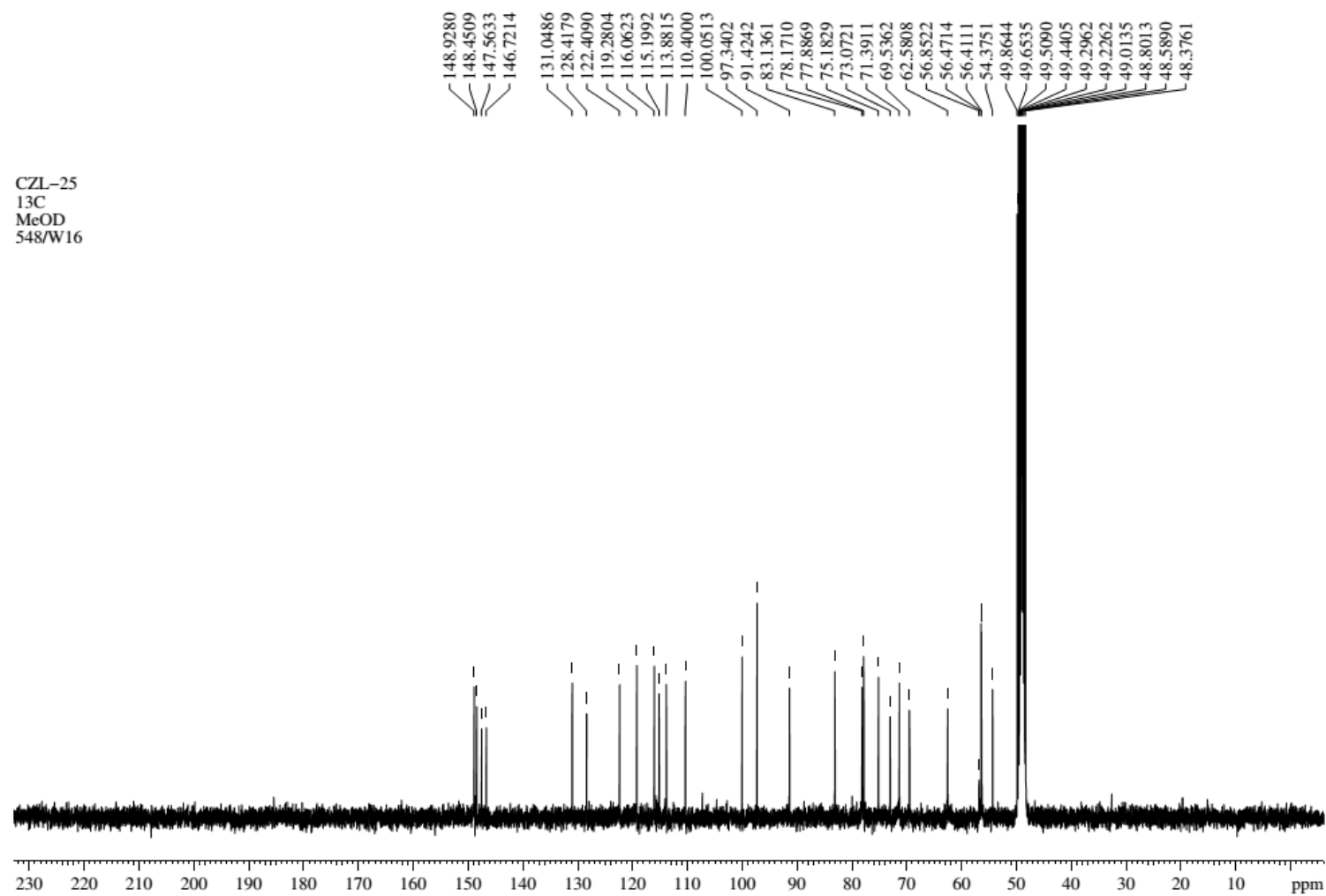
The IC<sub>50</sub> greater than 100  $\mu\text{M}$  was deemed inactive.

<sup>b</sup>Positive control.

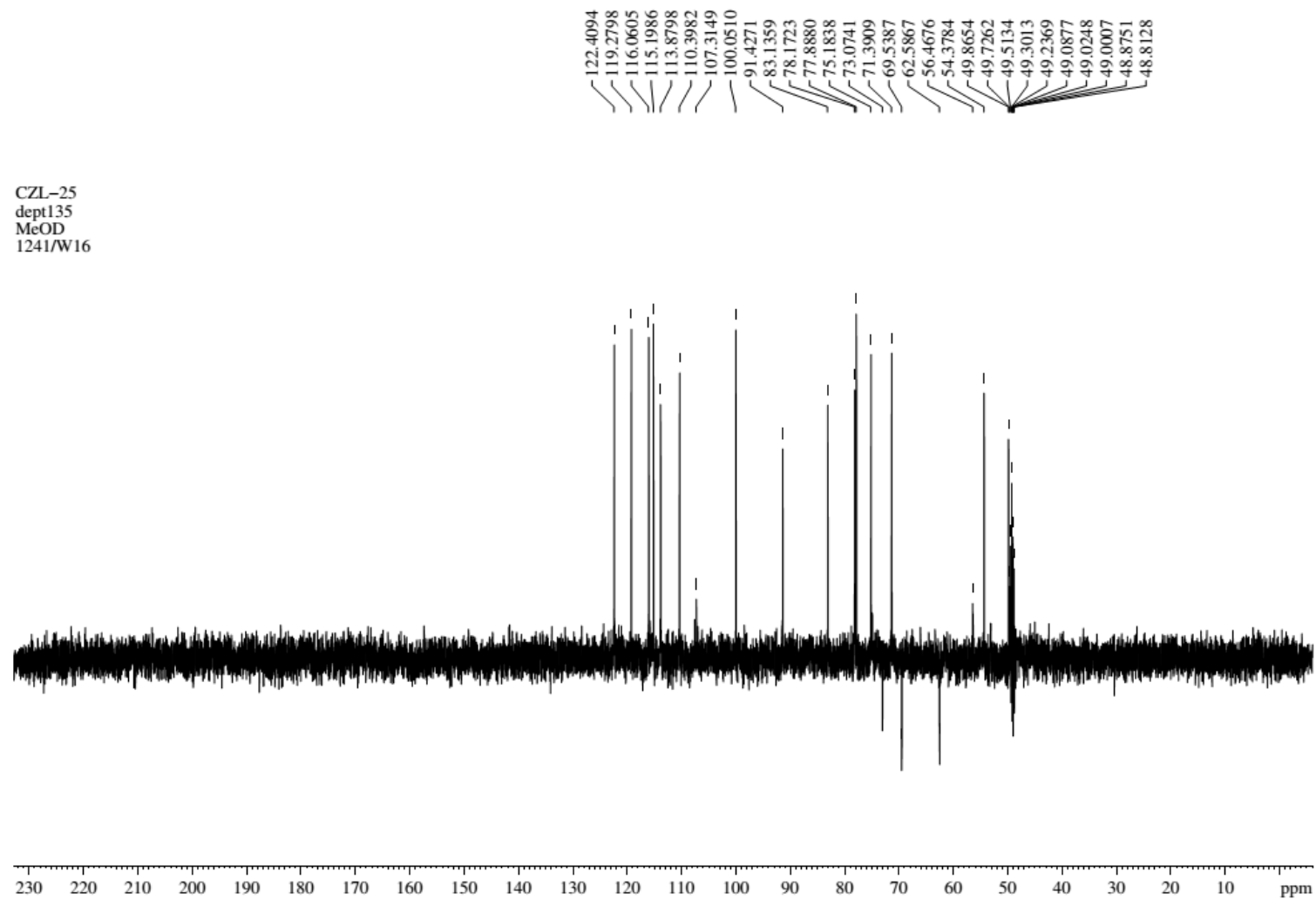
**Fig.S1.**  $^1\text{H}$ -NMR (400 MHz) Spectrum of compound **1** in  $\text{CD}_3\text{OD}$



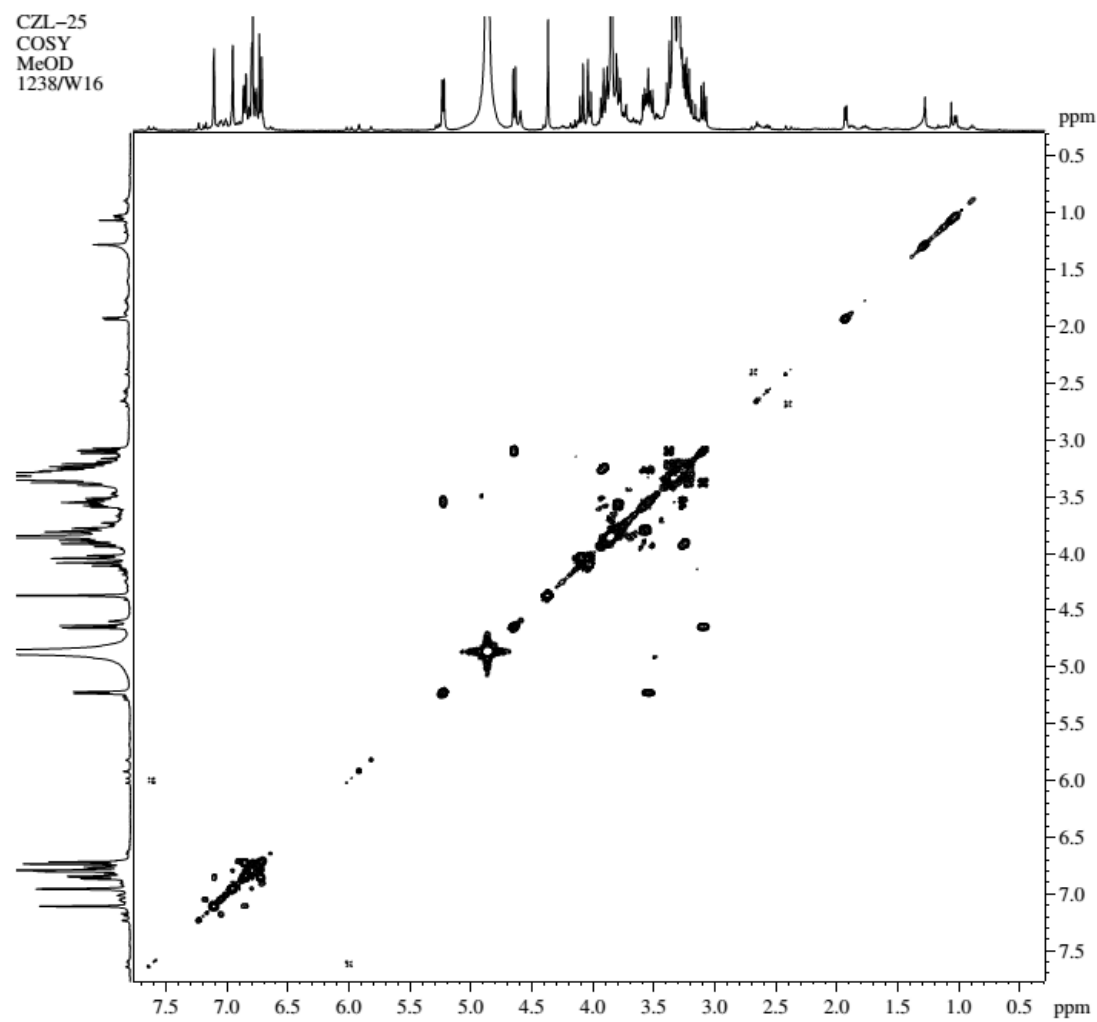
**Fig.S2.**  $^{13}\text{C}$ -NMR (100 MHz) Spectrum of compound **1** in  $\text{CD}_3\text{OD}$



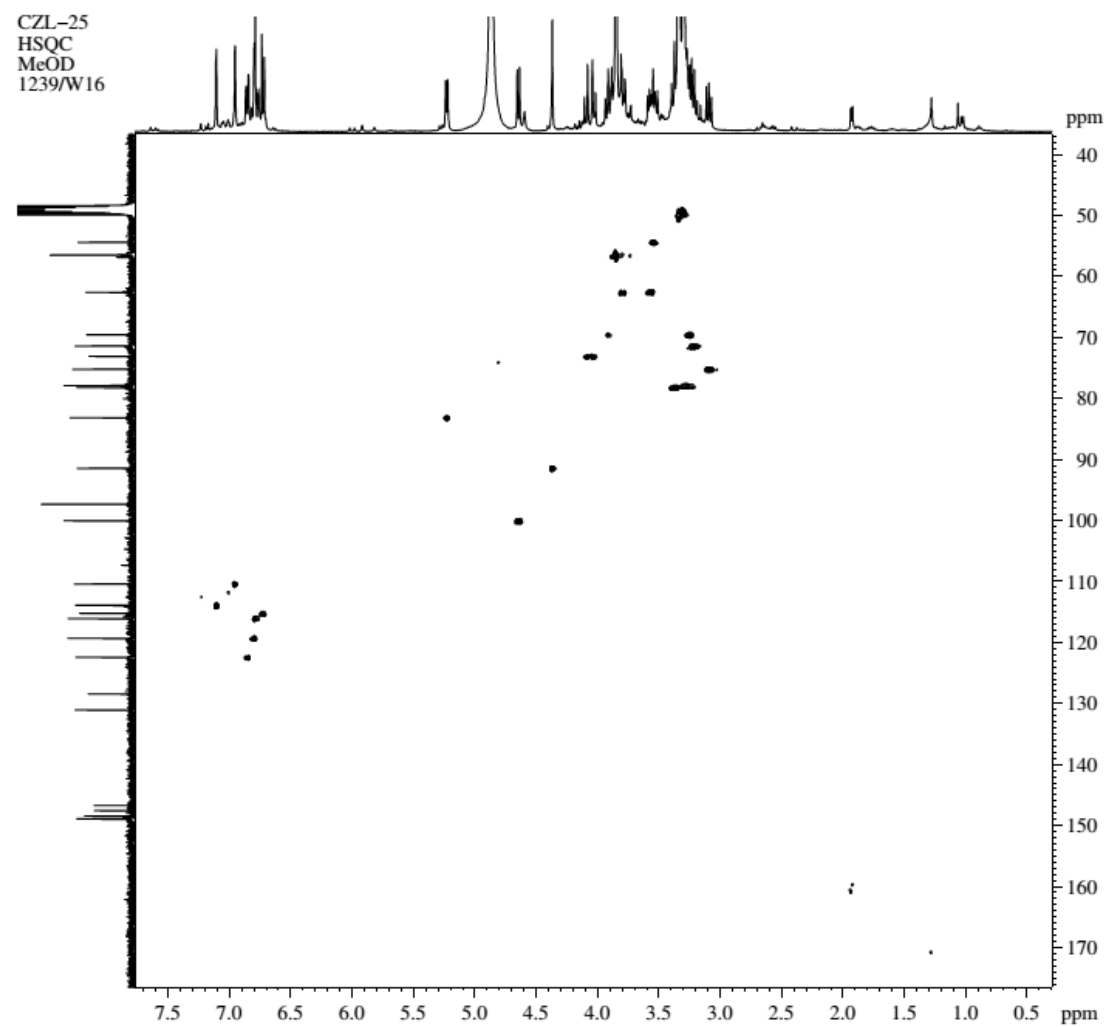
**Fig.S3.** DEPT Spectrum of compound **1** in CD<sub>3</sub>OD



**Fig.S4.**  $^1\text{H}$ - $^1\text{H}$  COSY Spectrum of compound **1** in  $\text{CD}_3\text{OD}$

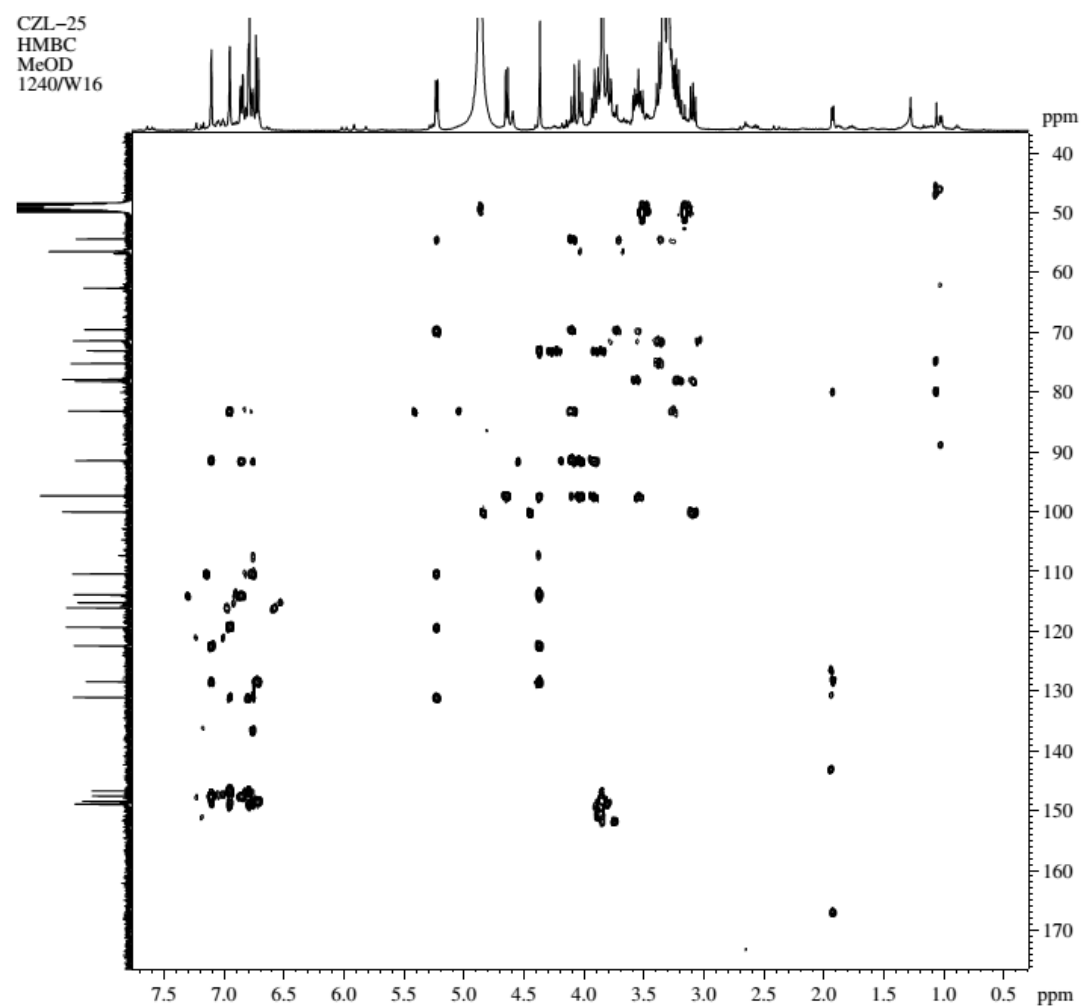


**Fig.S5.** HSQC Spectrum of compound **1** in CD<sub>3</sub>OD





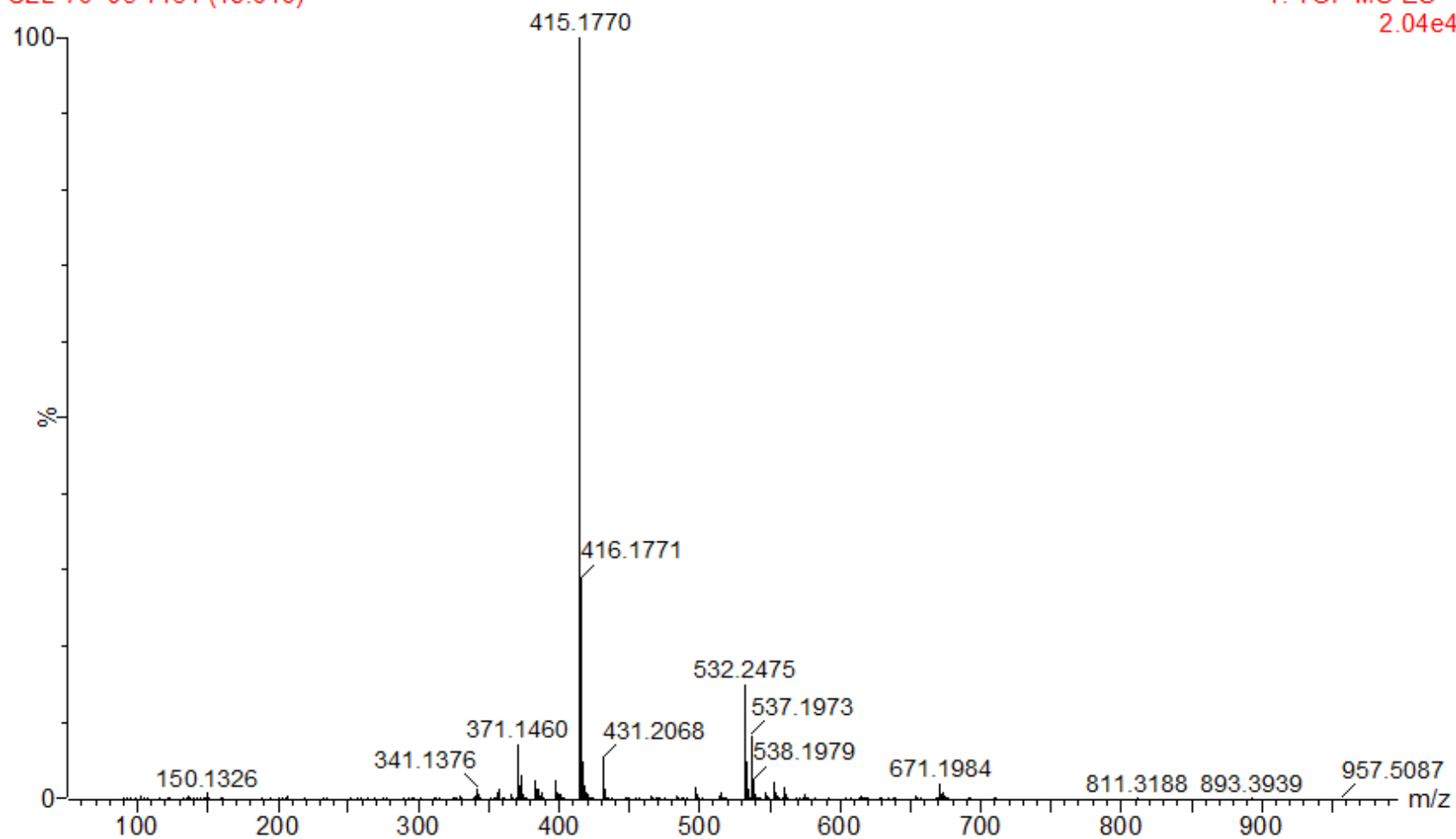
**Fig.S6.** HMBC Spectrum of compound **1** in CD<sub>3</sub>OD



**Fig.S7.** MS Spectrum of compound **1**

CZL-70+95 1164 (18.040)

1: TOF MS ES+  
2.04e4



**Fig.S8.** Key HMBC and  $^1\text{H}$ - $^1\text{H}$  COSY correlations of compound **1**

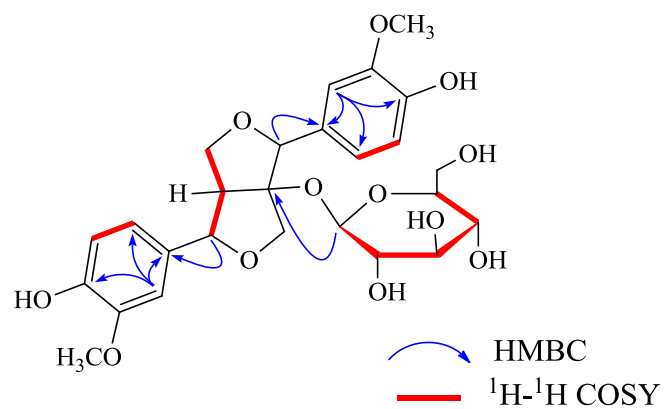
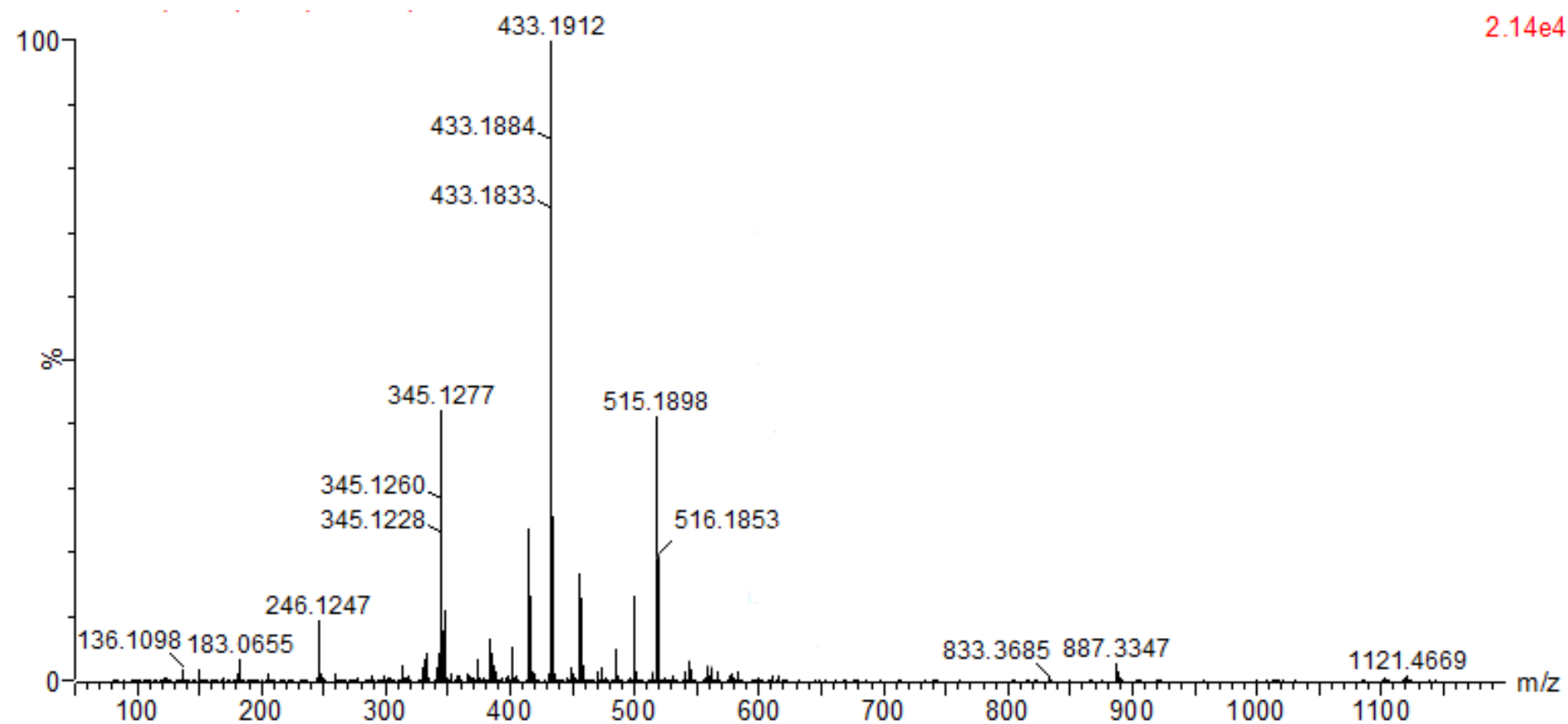


Fig.S9. MS Spectrum of compound 2



**Fig.S10.** MS Spectrum of compound **3**

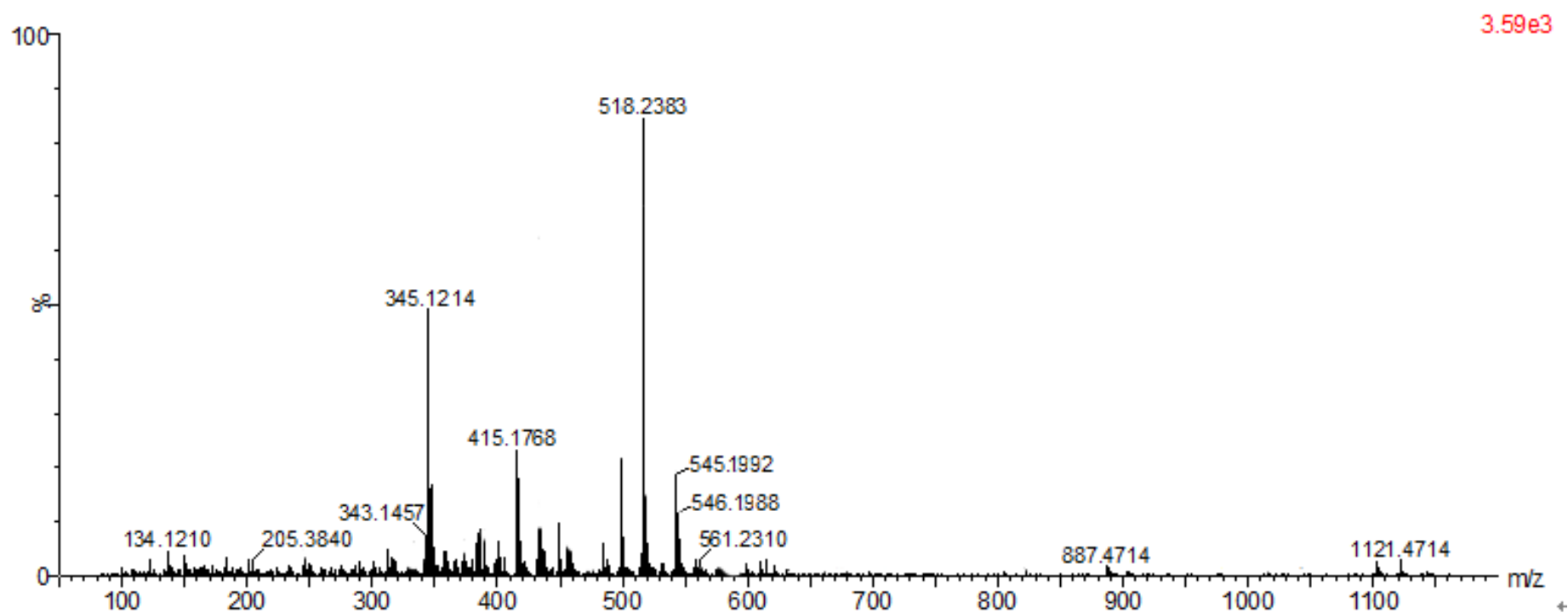


Fig.S11. MS Spectrum of compound 4

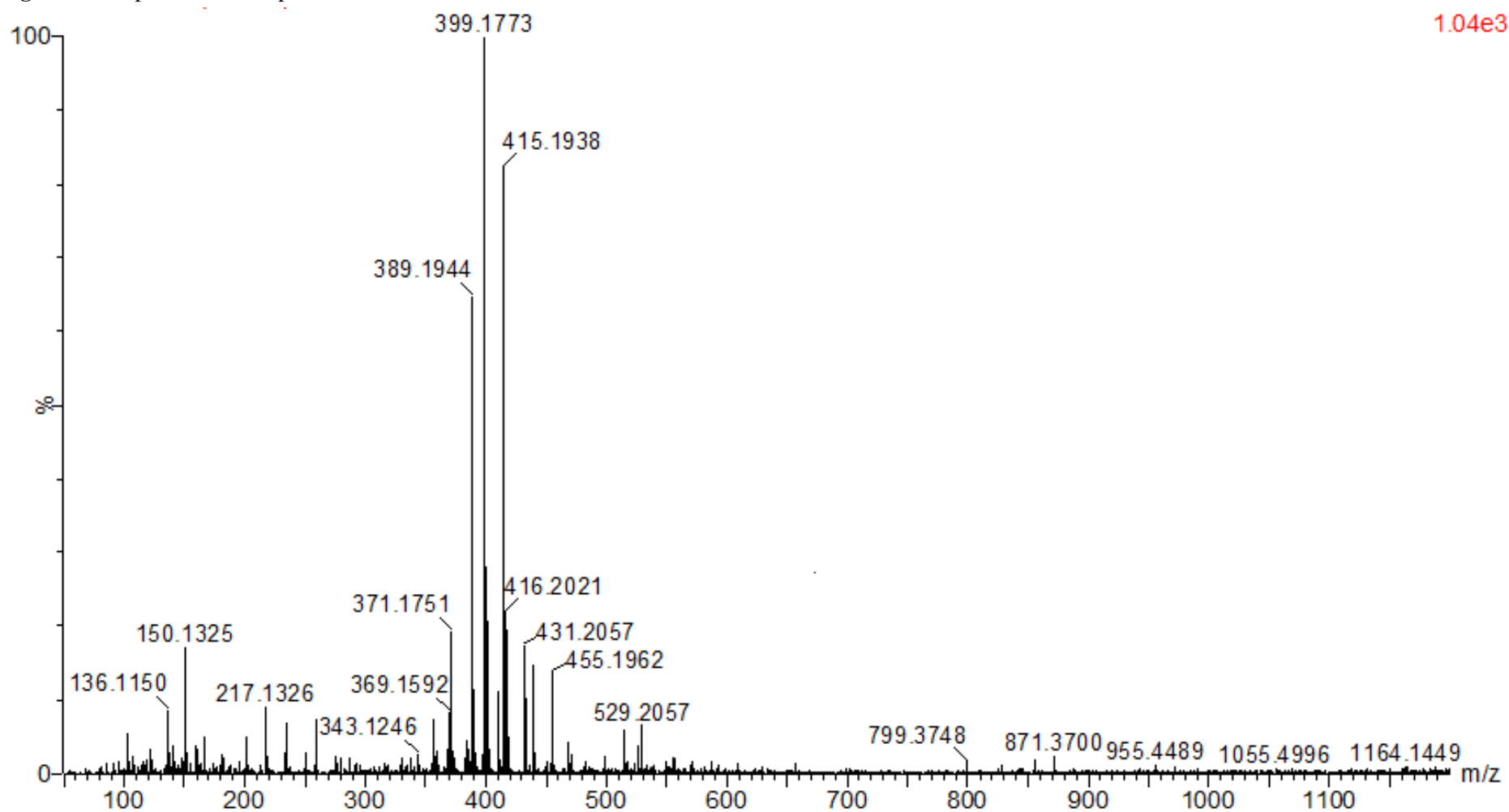


Fig.S12. MS Spectrum of compound 5

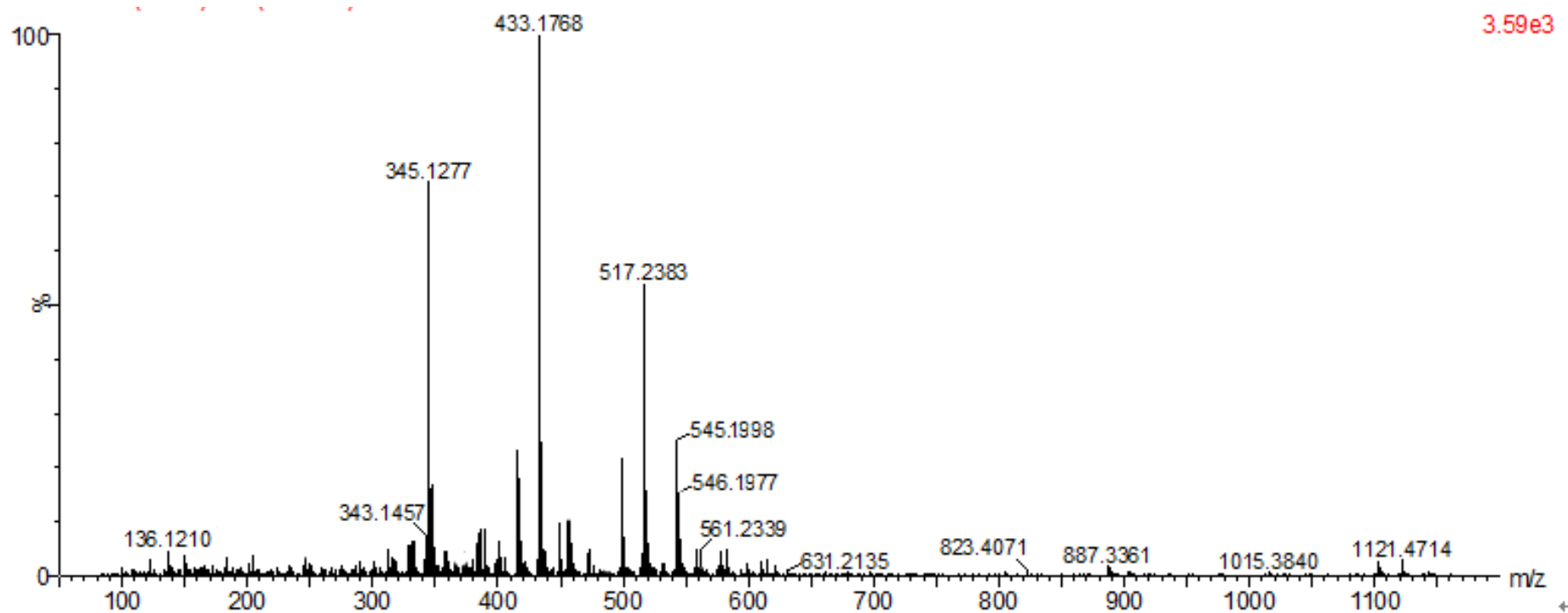
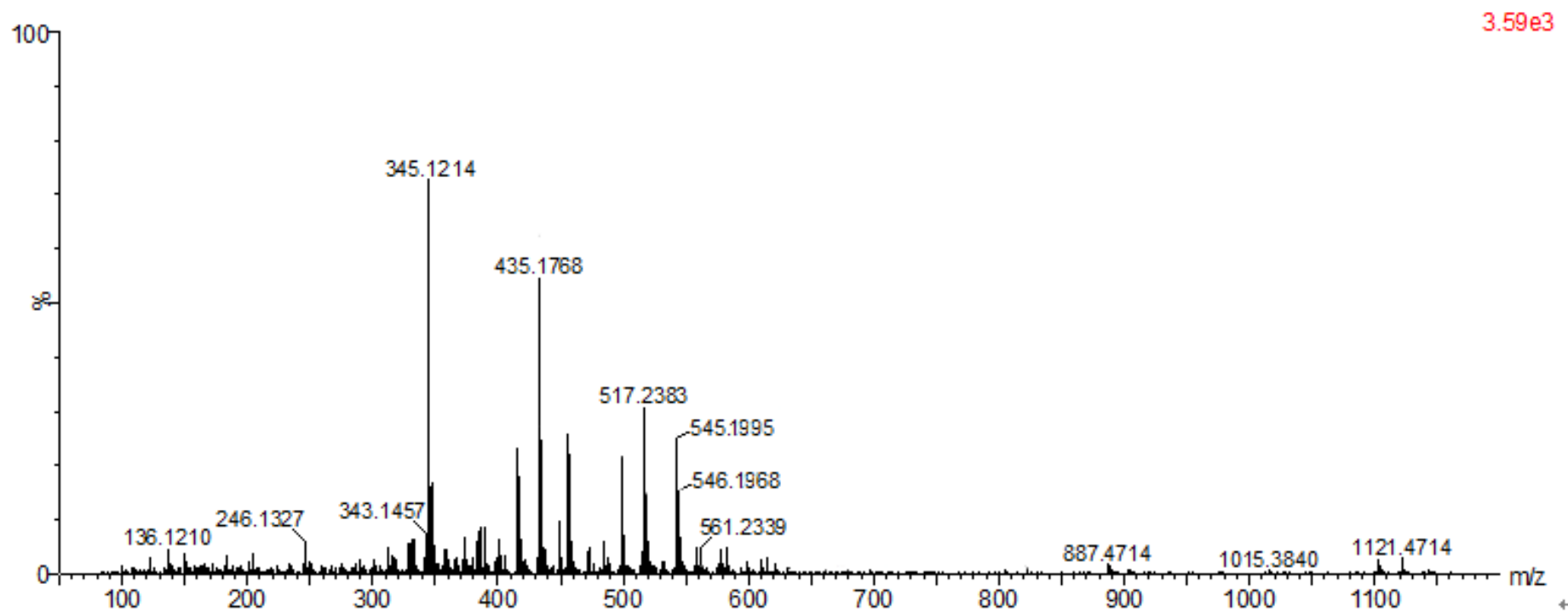


Fig.S13. MS Spectrum of compound 6





**Fig.S14.** MS Spectrum of compound **7**

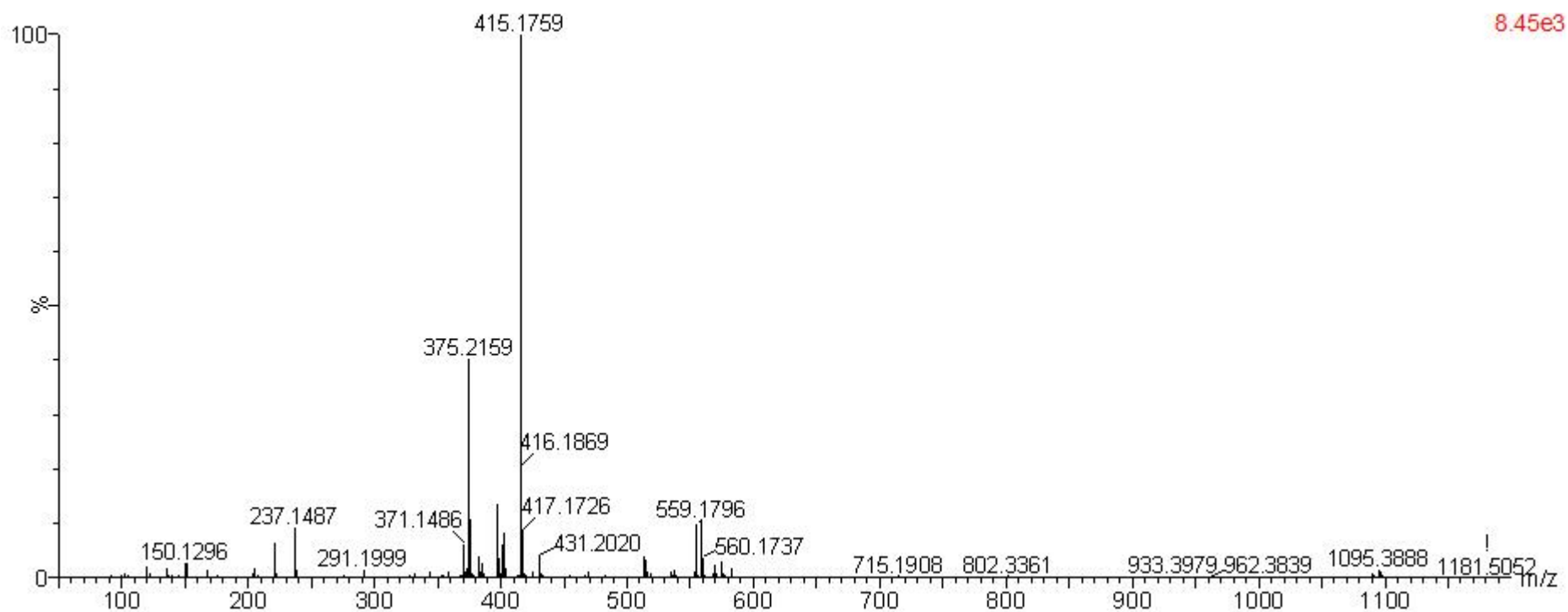


Fig.S15. MS Spectrum of compound 8

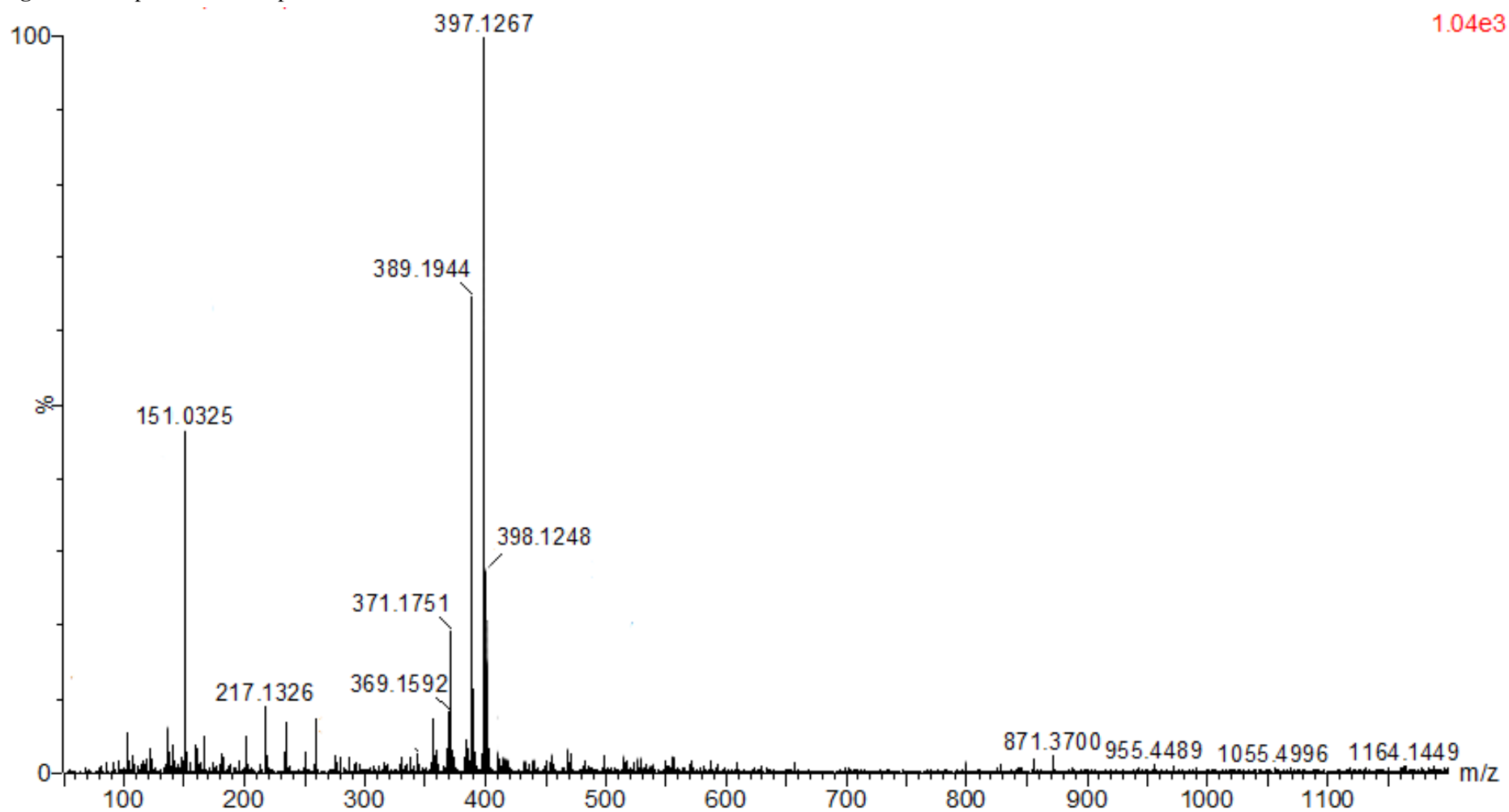


Fig.S16. MS Spectrum of compound 9

2.14e4

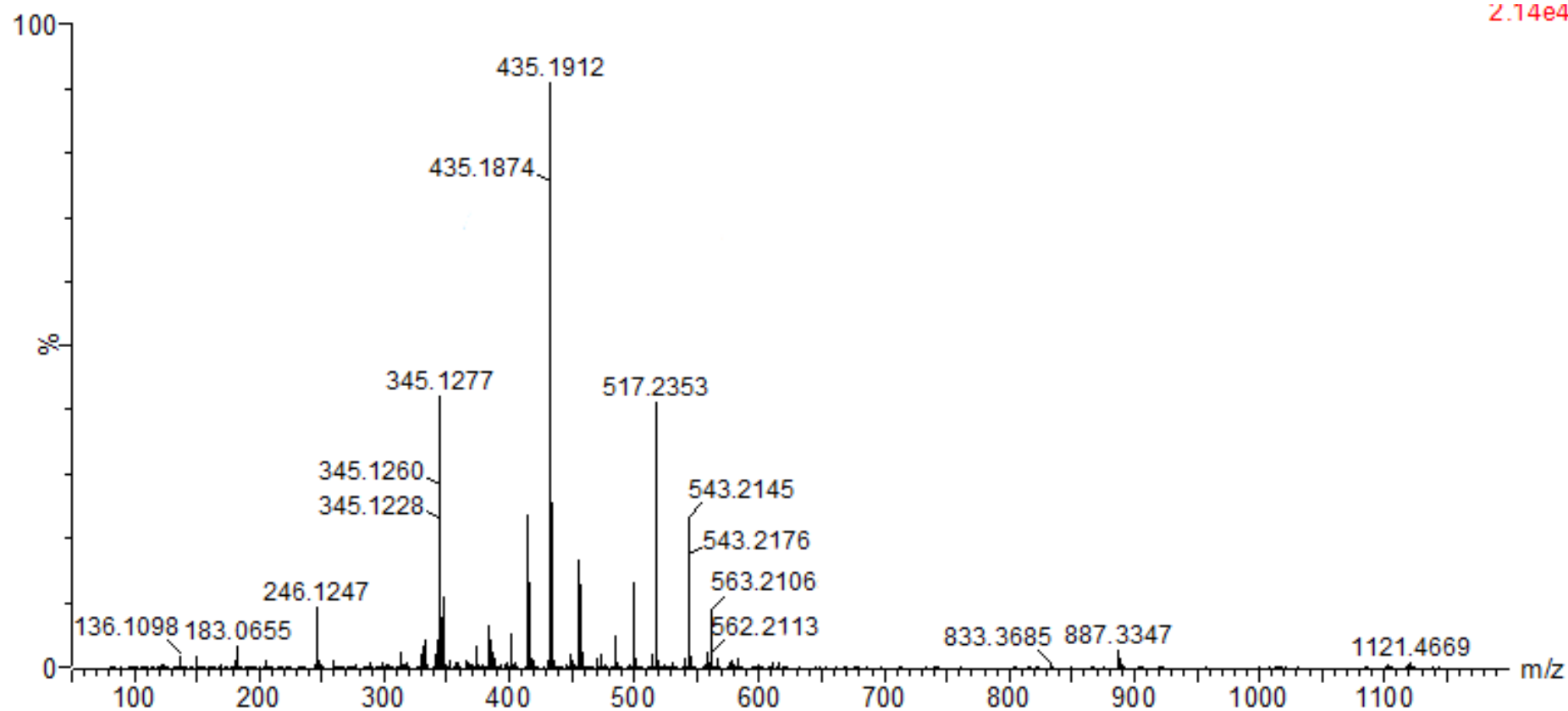


Fig.S17. MS Spectrum of compound 10

2.14e4

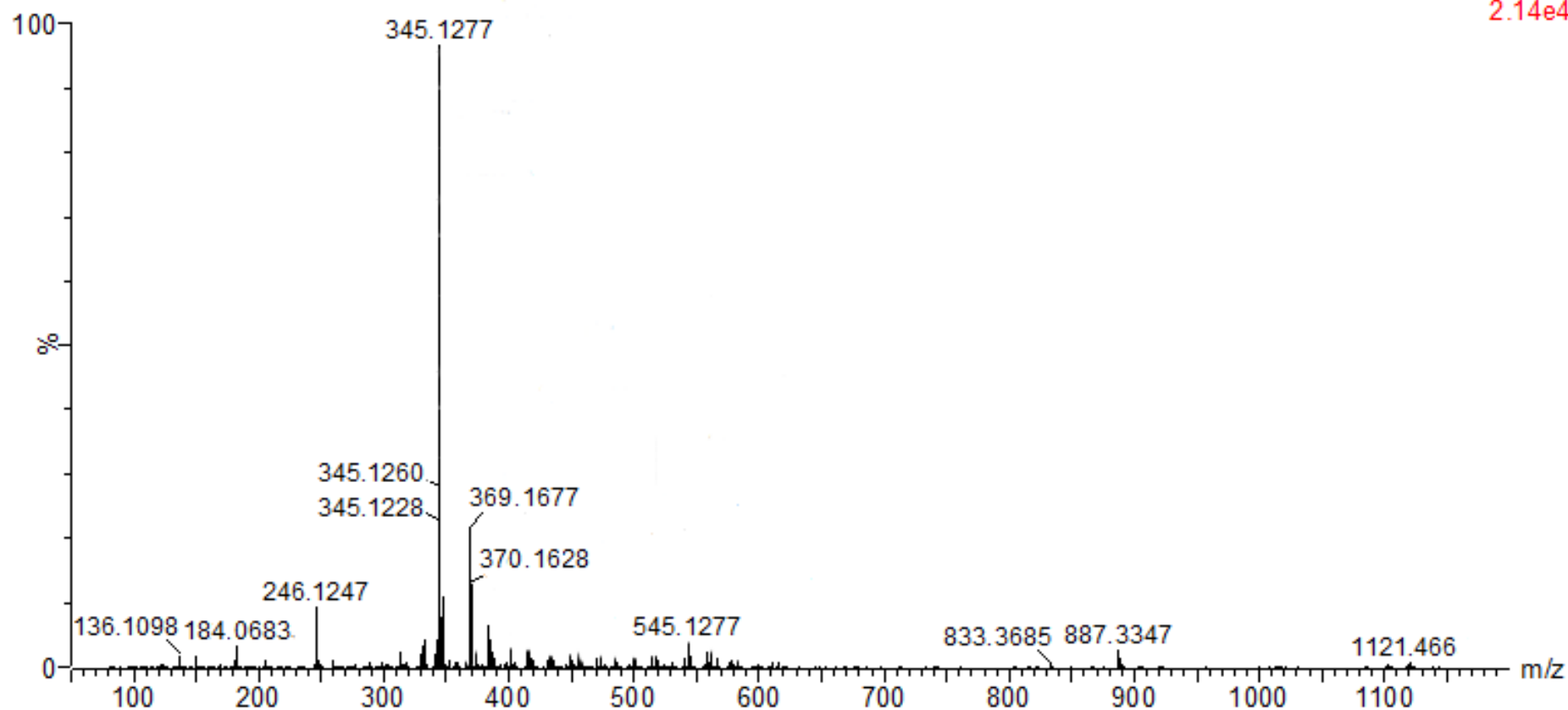
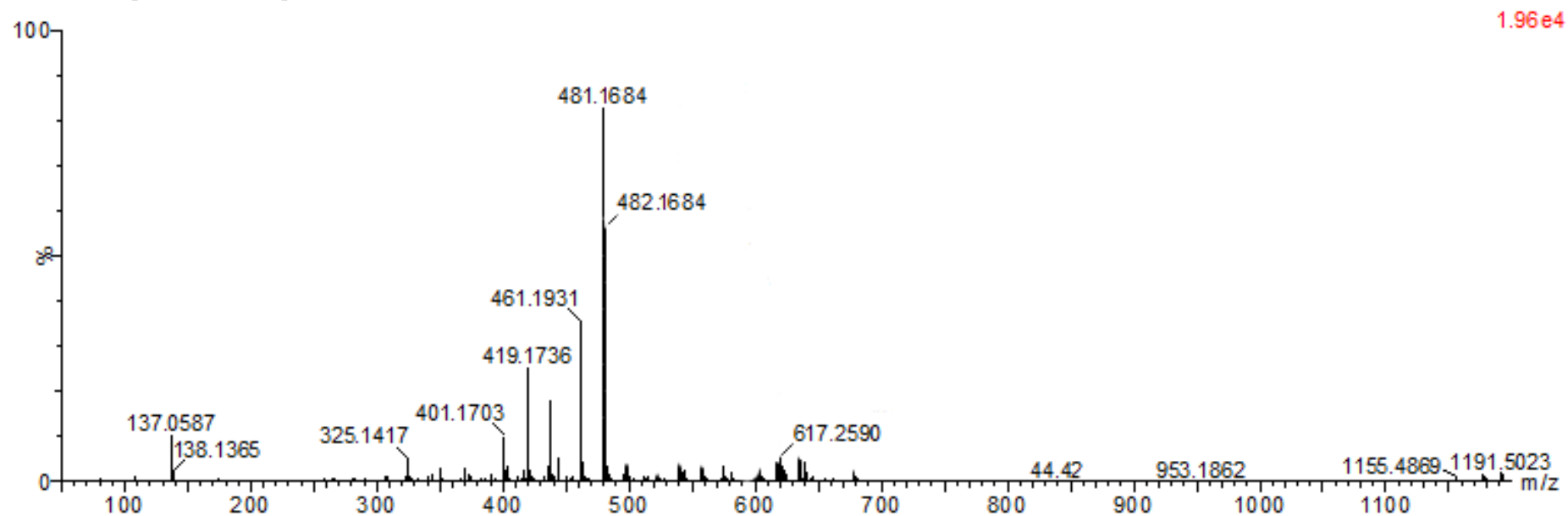


Fig.S18. MS Spectrum of compound 11



**Fig.S19.** MS Spectrum of compound **12**

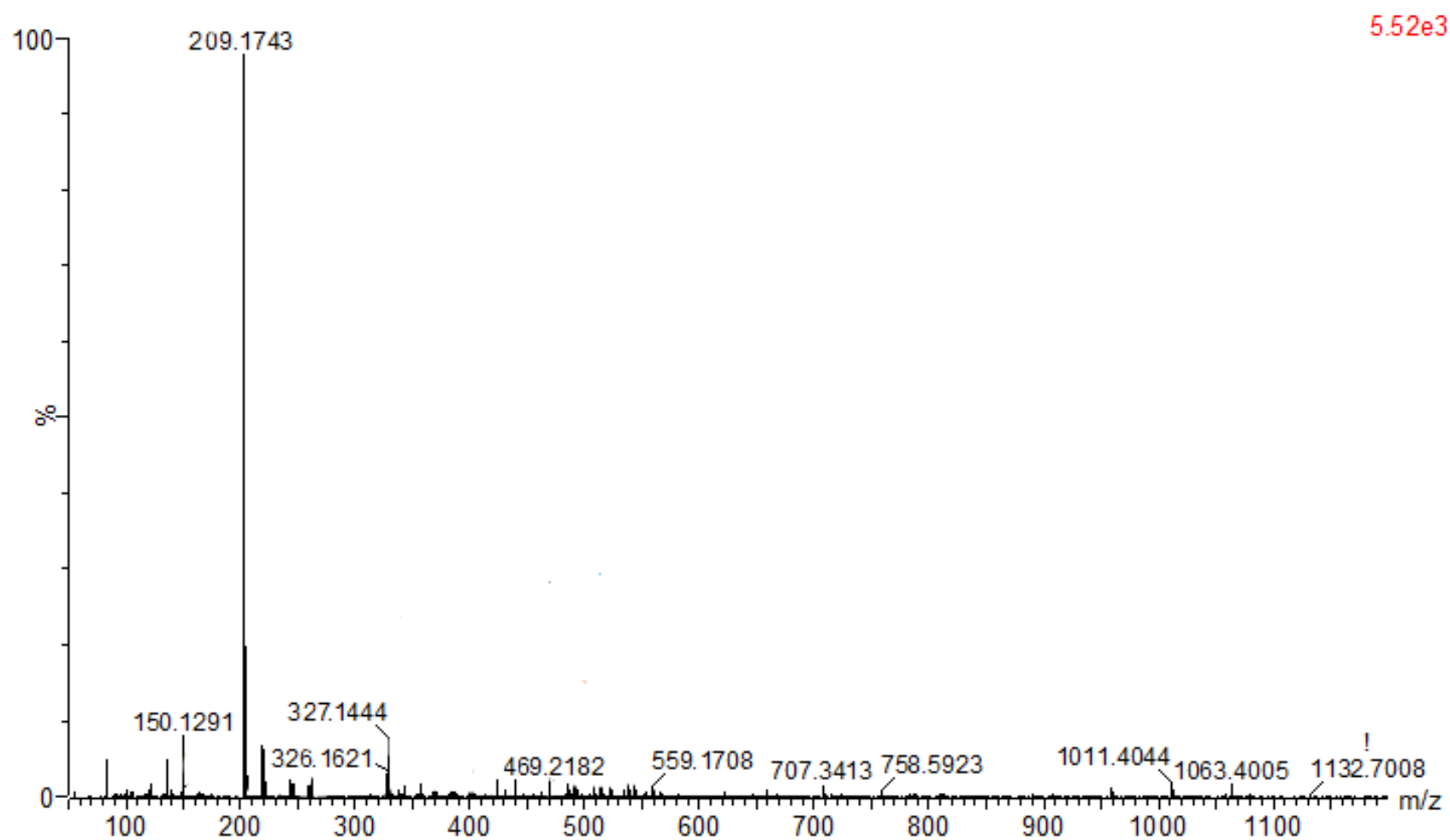


Fig.S20. MS Spectrum of compound 13

