

## Supporting Information

### Cytotoxic polyketides from the marine sponge-derived fungus *Pestalotiopsis heterocornis* XWS03F09

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Figure S1. HRESI-MS spectrum of the new compound **1**

Figure S2. <sup>1</sup>H NMR (600 MHz, CD<sub>3</sub>OD) spectrum of the new compound **1**

Figure S3. <sup>13</sup>C NMR (150 MHz, CD<sub>3</sub>OD) spectrum of the new compound **1**

Figure S4. HSQC spectrum of the new compound **1**

Figure S5. HMBC spectrum of the new compound **1**

Figure S6. COSY spectrum of the new compound **1**

Figure S7. NOESY spectrum of the new compound **1**

Figure S8. HRESI-MS spectrum of the new compound **2**

Figure S9. <sup>1</sup>H NMR (600 MHz, CD<sub>3</sub>OD) spectrum of the new compound **2**

Figure S10. <sup>13</sup>C NMR (150 MHz, CD<sub>3</sub>OD) spectrum of the new compound **2**

Figure S11. HSQC spectrum of the new compound **2**

Figure S12. HMBC spectrum of the new compound **2**

Figure S13. COSY spectrum of the new compound **2**

Figure S14. NOESY spectrum of the new compound **2**

Figure S15. HRESI-MS spectrum of the new compound **3/4**

Figure S16.  $^1\text{H}$  NMR (600 MHz,  $\text{CD}_3\text{OD}$ ) spectrum of the new compound **3/4**

Figure S17.  $^{13}\text{C}$  NMR (150 MHz,  $\text{CD}_3\text{OD}$ ) spectrum of the new compound **3/4**

Figure S18. HSQC spectrum of the new compound **3/4**

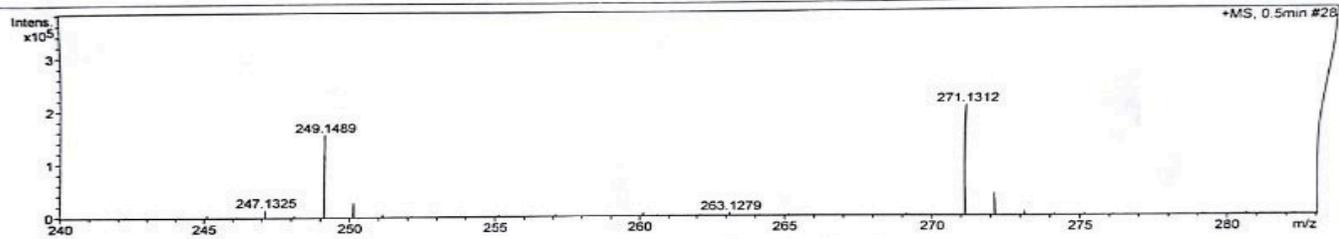
Figure S19. HMBC spectrum of the new compound **3/4**

Figure S20. COSY spectrum of the new compound **3/4**

Figure S21. NOESY spectrum of the new compound **3/4**

## Mass Spectrum SmartFormula Report

<b>Analysis Info</b>			Acquisition Date		6/25/2018 10:44:40 AM
Analysis Name	D:\Data\MS\data\201806\yangbin_L9_pos_31_01_5004.d			Operator	SCSIO
Method	LC_Direct Infusion_pos_100-1000mz.m			Instrument	maXis
Sample Name	yangbin_L9_pos				255552.00029
Comment					
<b>Acquisition Parameter</b>					
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	2000 m/z	Set Charging Voltage	0 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	Score	m/z	err [ppm]	err [mDa]	mSigma	rdb	e <sup>-</sup> Conf	N-Rule
249.1489	1	C15H21O3	100.00	249.1485	1.4	0.4	3.9	5.5	even	ok
271.1312	1	C15H20NaO3	100.00	271.1305	-2.8	-0.8	20.2	5.5	even	ok
497.2886	1	C30H41O6	100.00	497.2898	2.3	1.1	21.6	10.5	even	ok
519.2712	1	C30H40NaO6	100.00	519.2717	0.9	0.5	26.7	10.5	even	ok

Figure 1. HRESI-MS spectrum of the new compound 1.

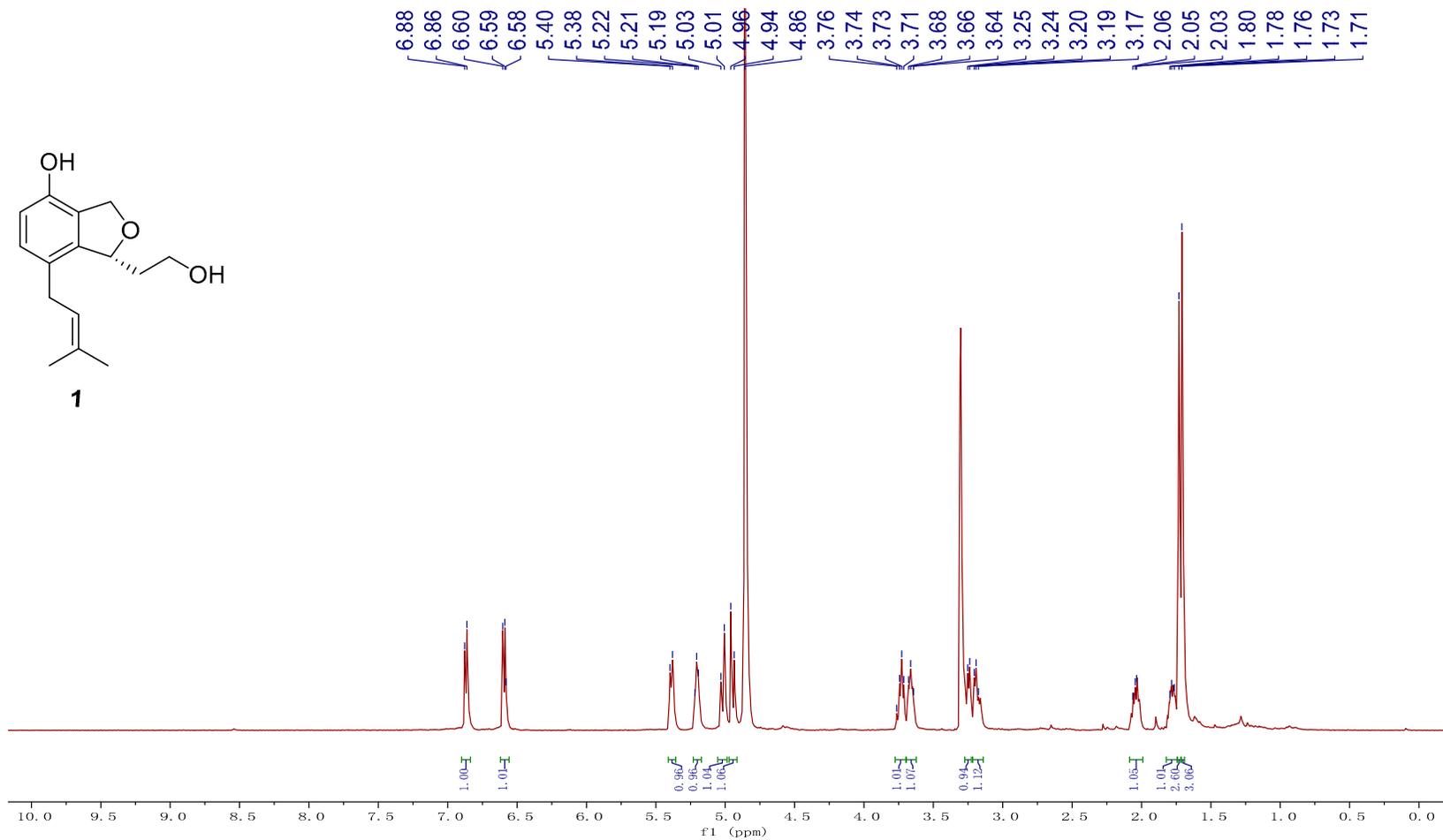


Figure S2. <sup>1</sup>H NMR (600 MHz, CD<sub>3</sub>OD) spectrum of the new compound **1**

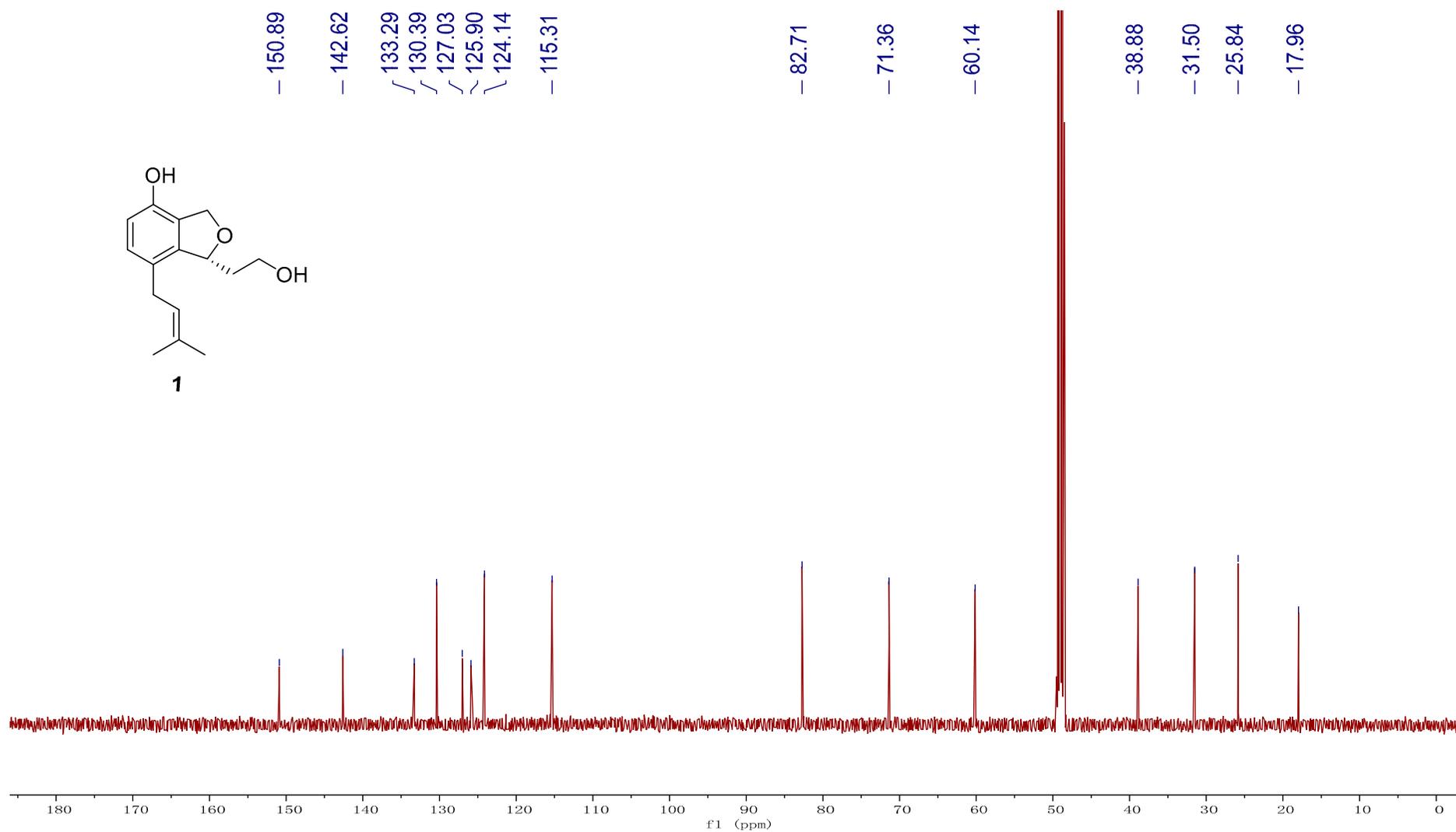


Figure S3. <sup>13</sup>C NMR (150 MHz, CD<sub>3</sub>OD) spectrum of the new compound **1**

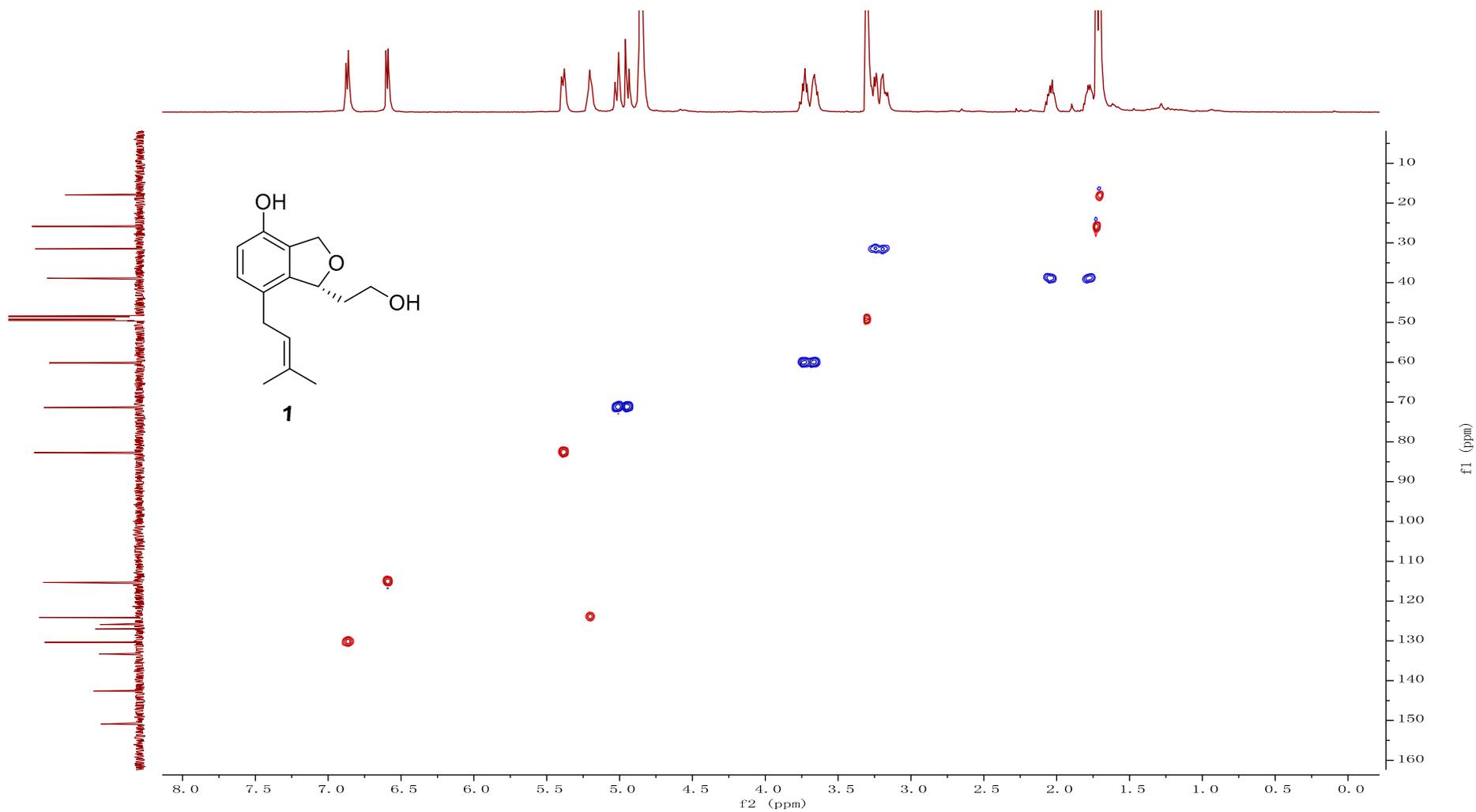


Figure S4. HSQC spectrum of the new compound **1**

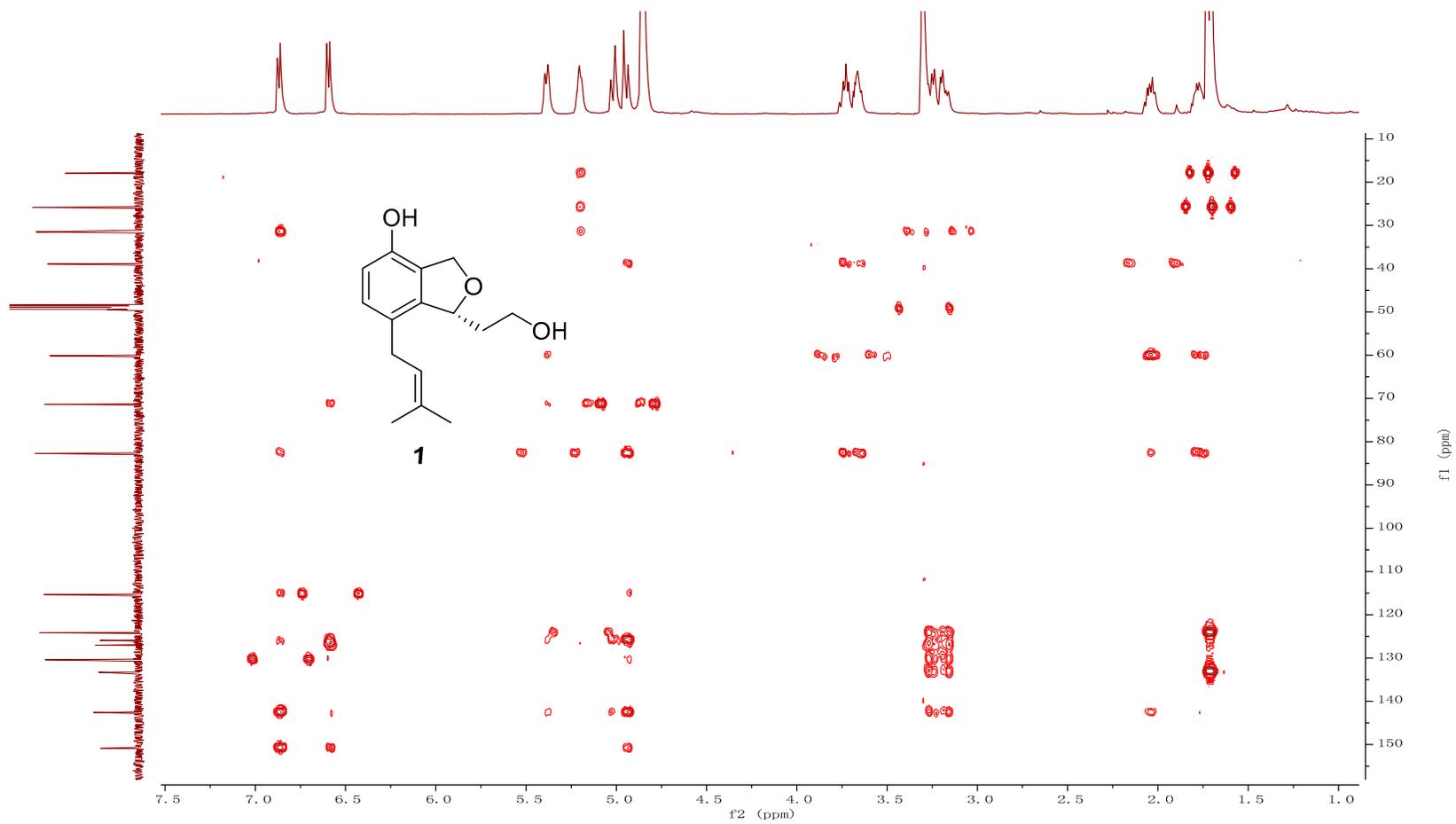


Figure S5. HMBC spectrum of the new compound **1**

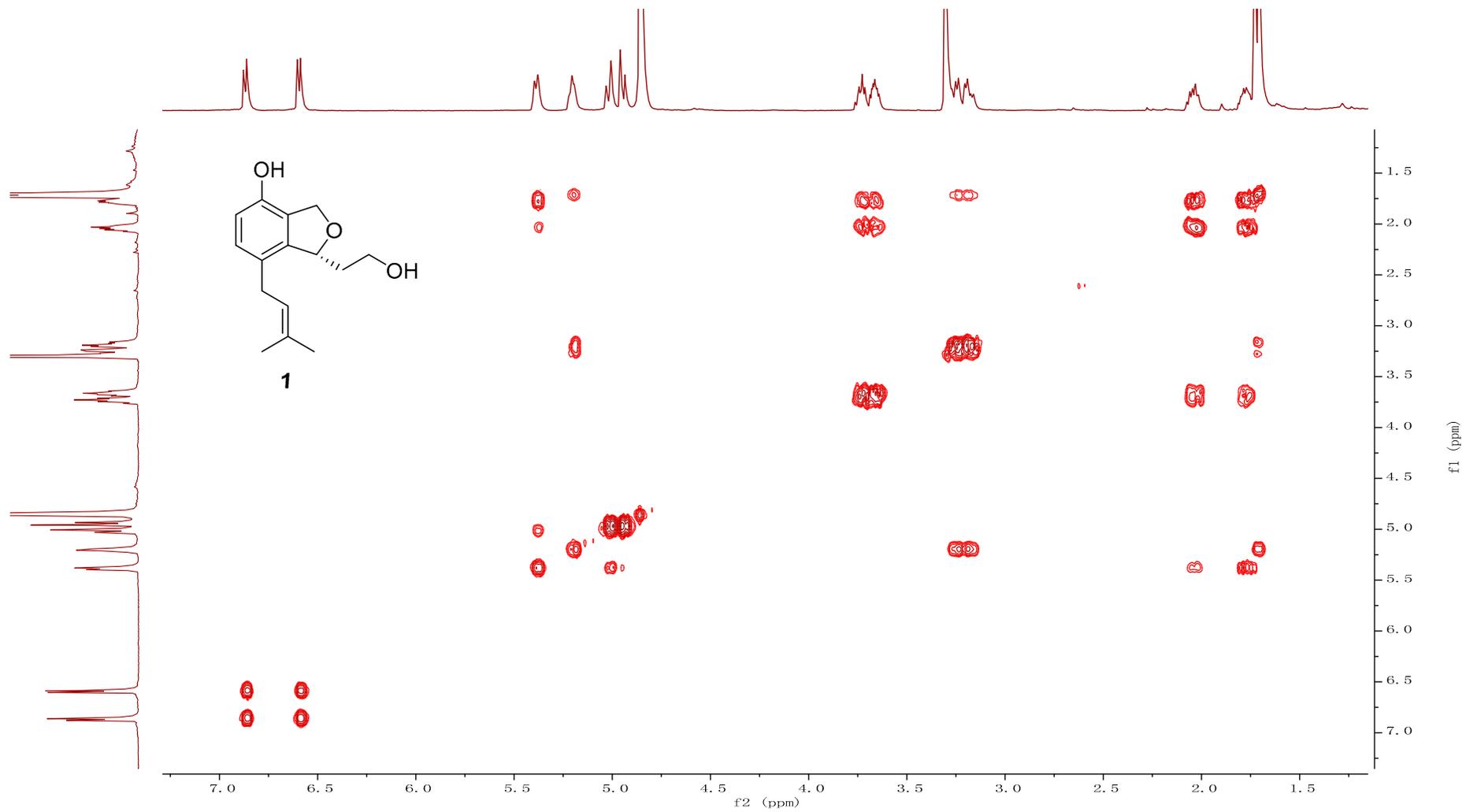


Figure S6. COSY spectrum of the new compound **1**

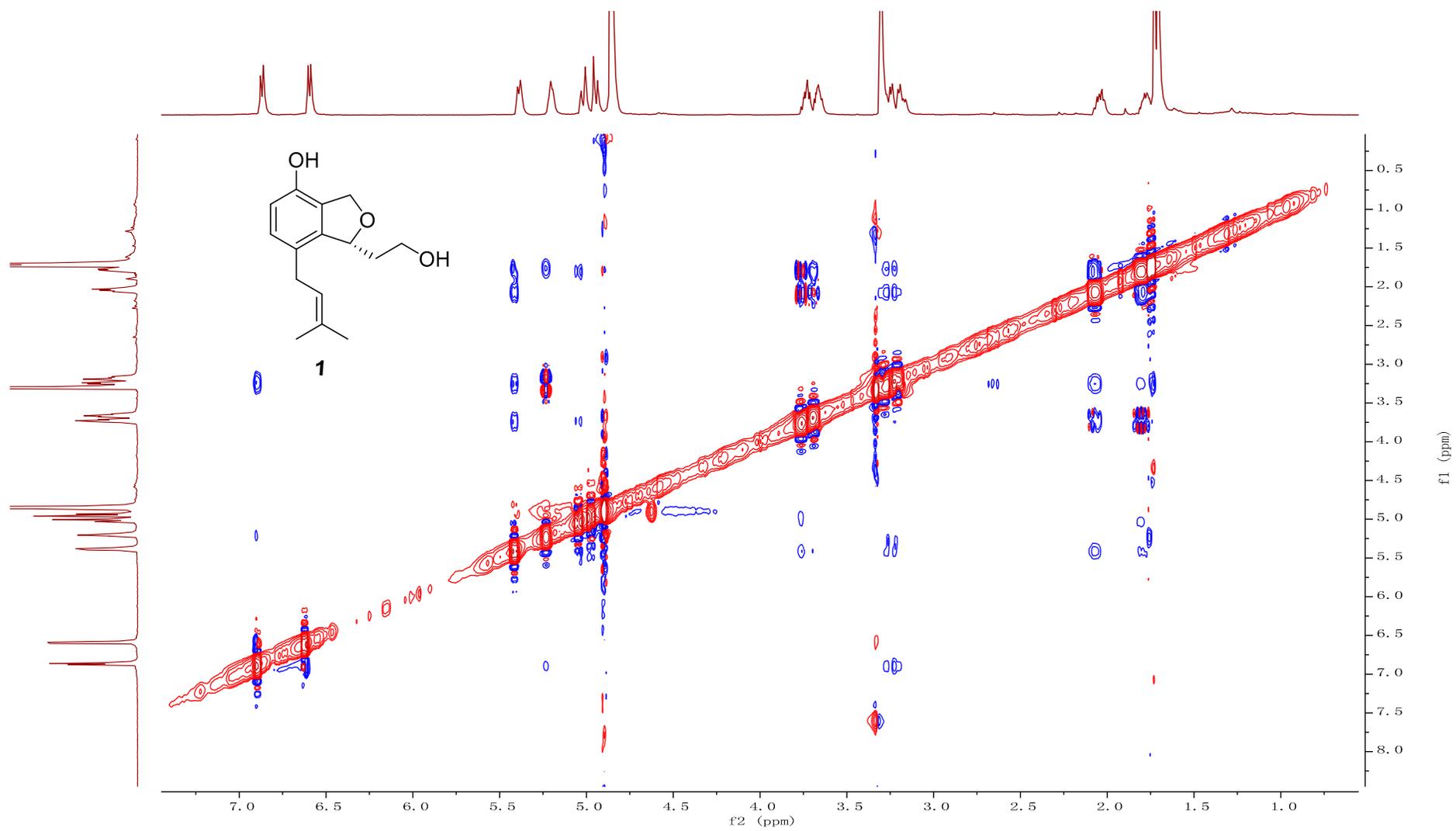
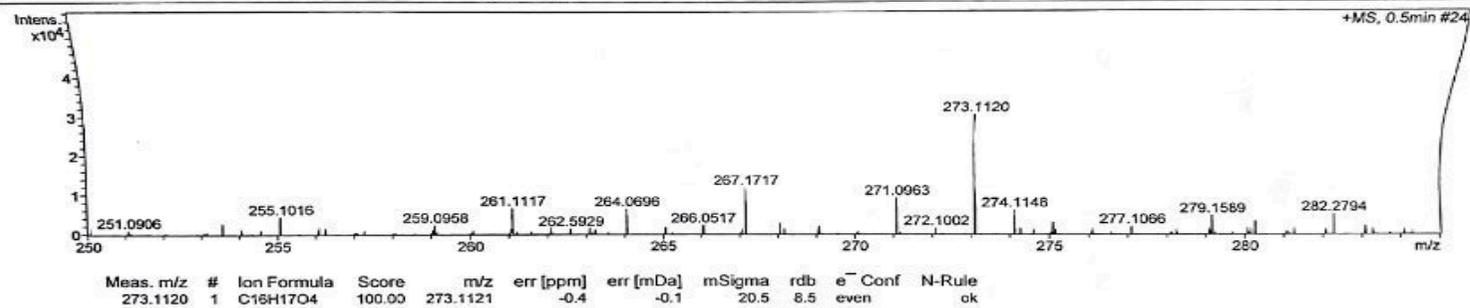


Figure S7. NOESY spectrum of the new compound **1**

### Mass Spectrum SmartFormula Report

<b>Analysis Info</b>		Acquisition Date	6/25/2018 10:48:06 AM	
Analysis Name	D:\Data\MS\data\201806\yangbin_L15_pos_32_01_5005.d	Operator	SCSIO	
Method	LC_Direct Infusion_pos_100-1000mz.m	Instrument	maXis	255552.00029
Sample Name	yangbin_L15_pos			
Comment				

<b>Acquisition Parameter</b>					
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	2000 m/z	Set Charging Voltage	0 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



yangbin\_L15\_pos\_32\_01\_5005.d  
Bruker Compass DataAnalysis 4.1

printed: 6/25/2018 10:52:36 AM

by: SCSIO

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Figure S8. HRESI-MS spectrum of the new compound 2

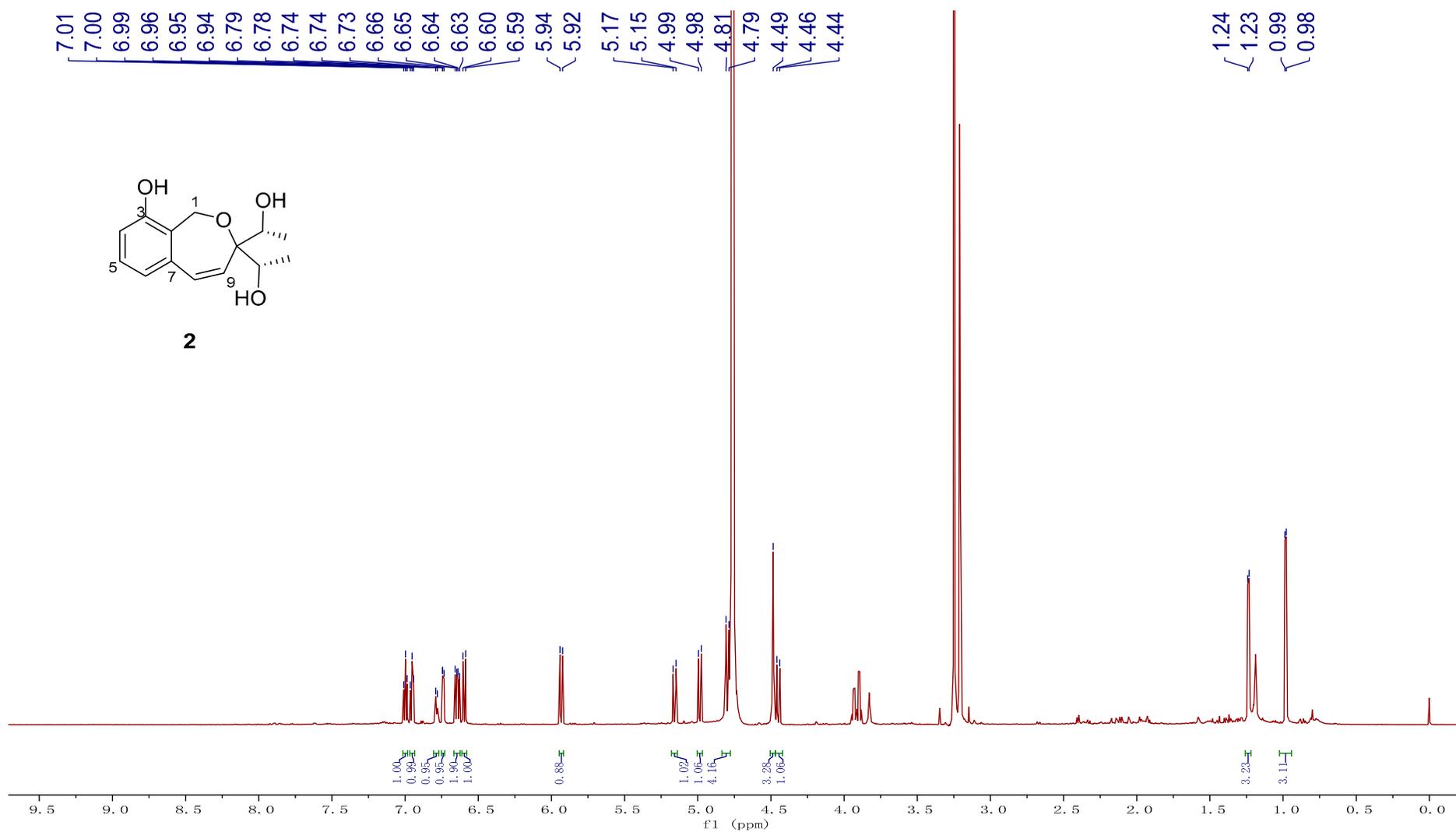


Figure S9. <sup>1</sup>H NMR (600 MHz, CD<sub>3</sub>OD) spectrum of the new compound **2**

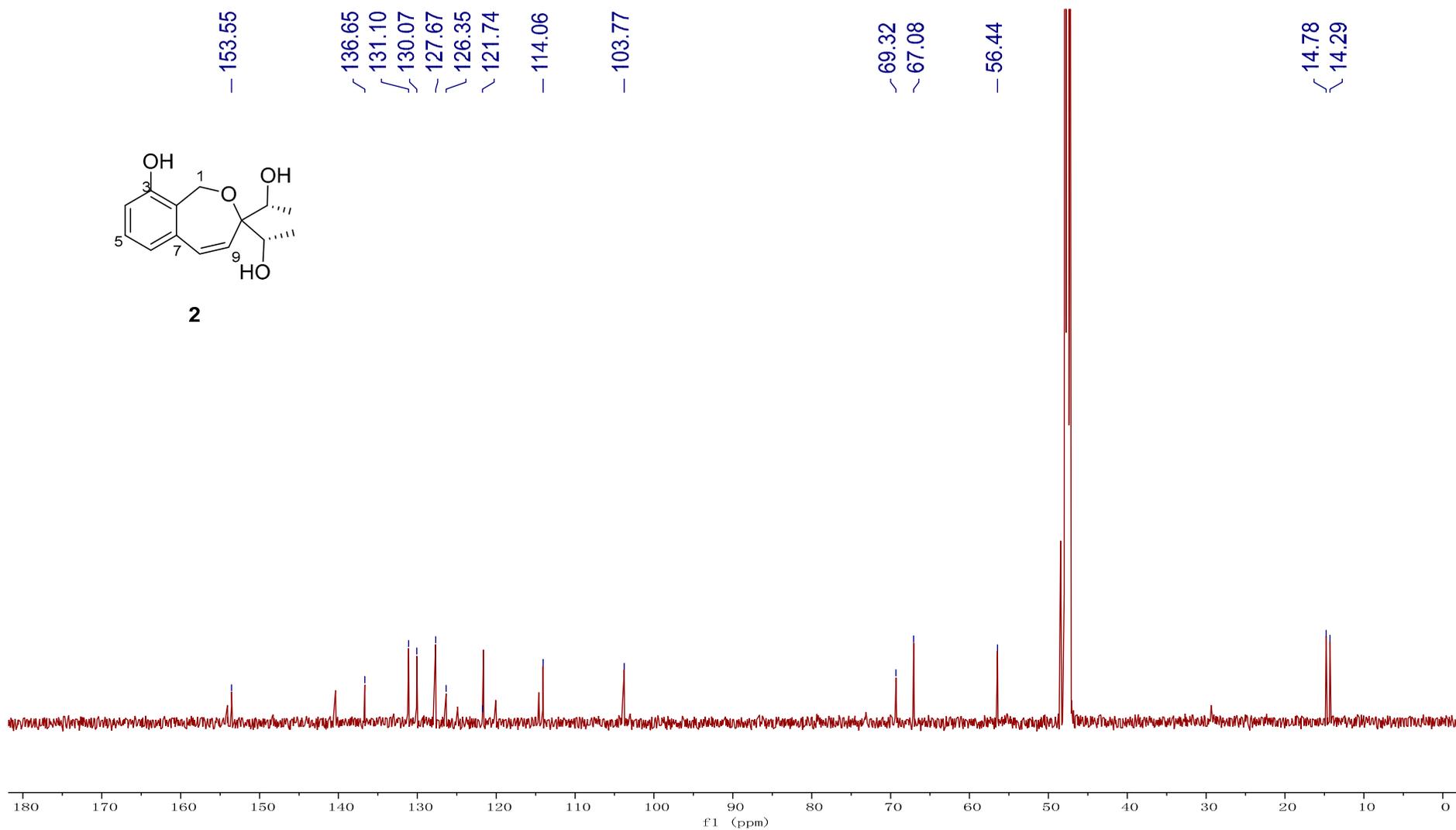


Figure S10. <sup>13</sup>C NMR (150 MHz, CD<sub>3</sub>OD) spectrum of the newcompound **2**

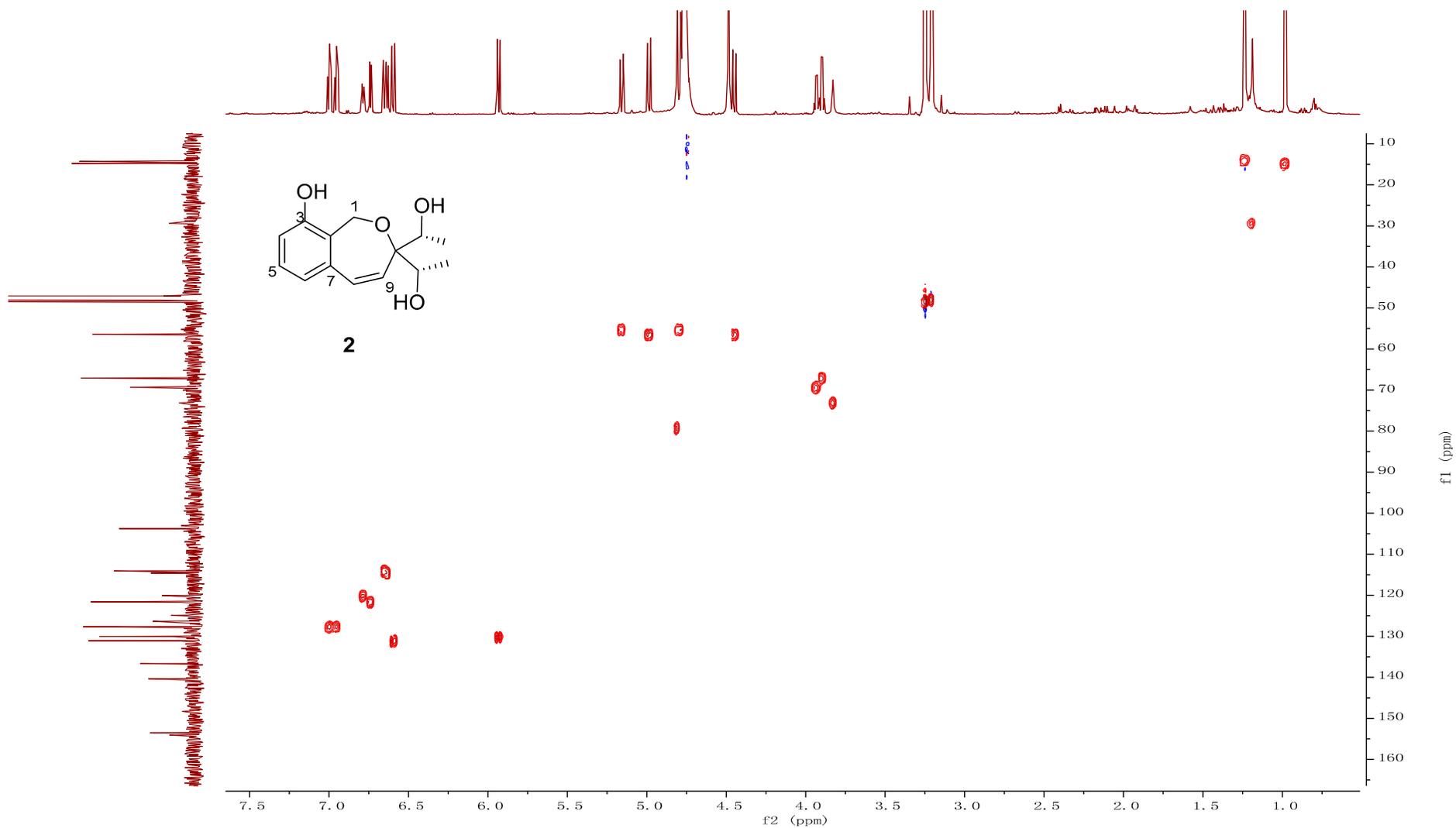


Figure S11. HSQC spectrum of the new compound 2

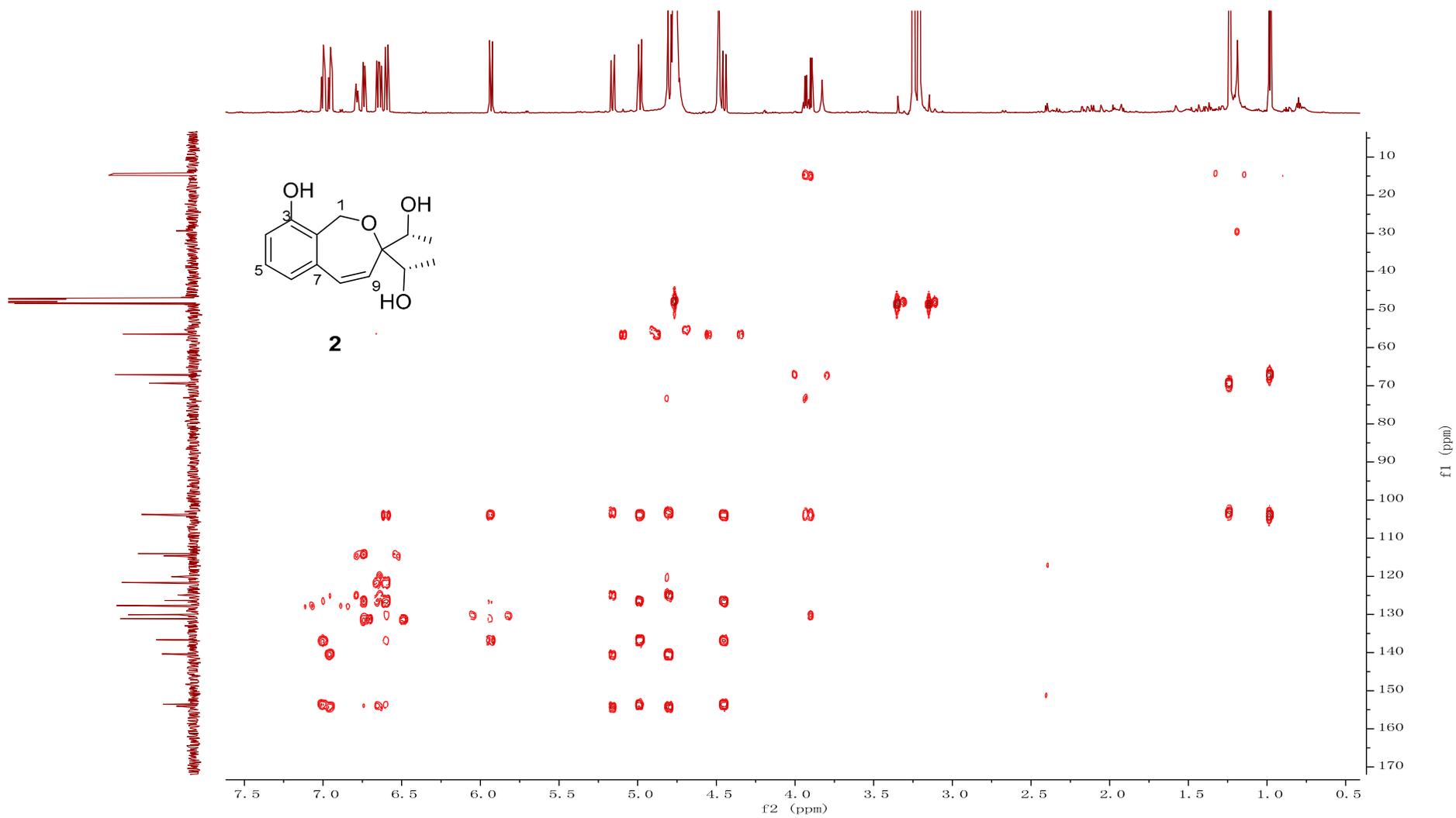


Figure S12. HMBC spectrum of the new compound **2**

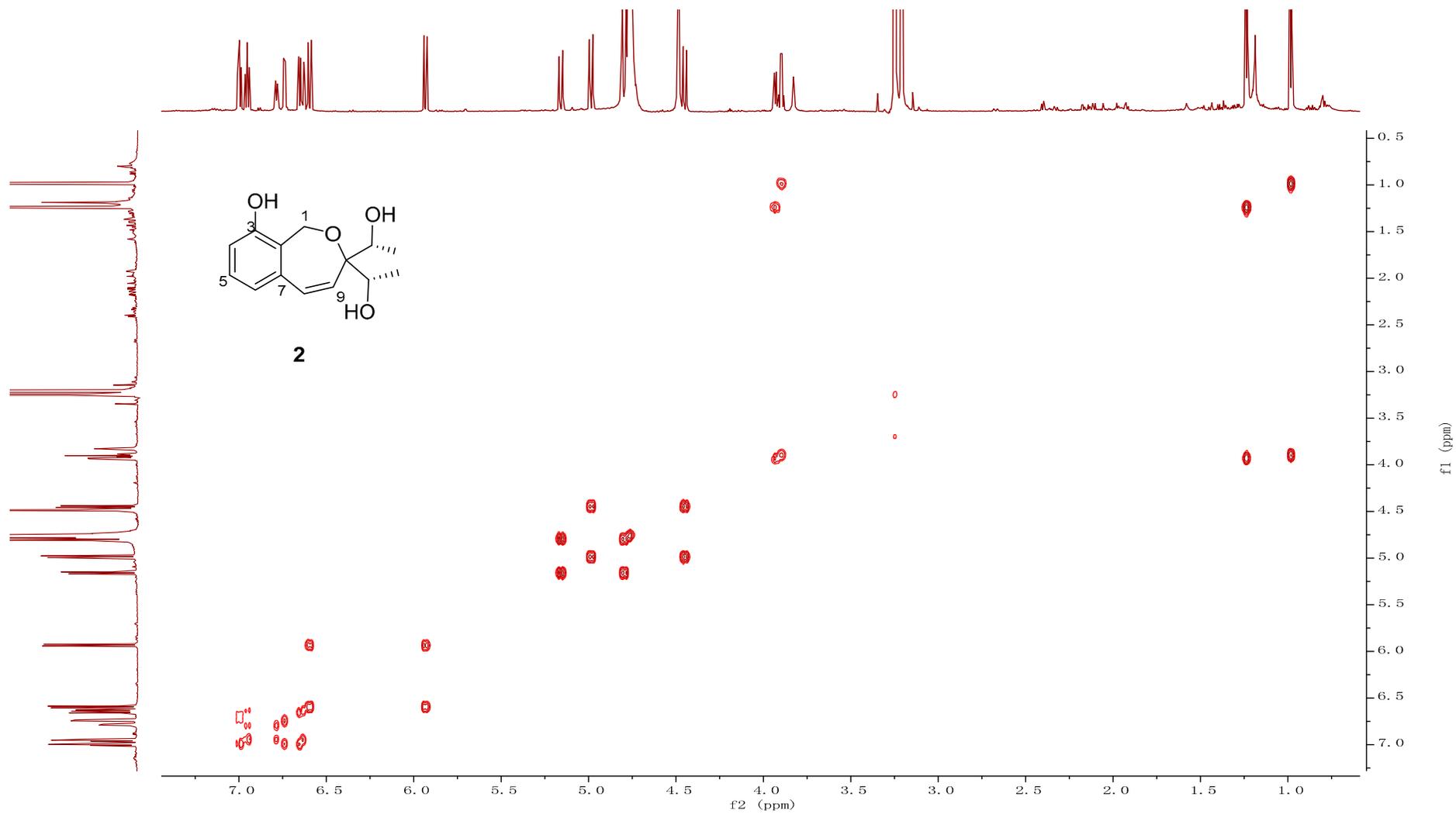


Figure S13. COSY spectrum of the new compound **2**

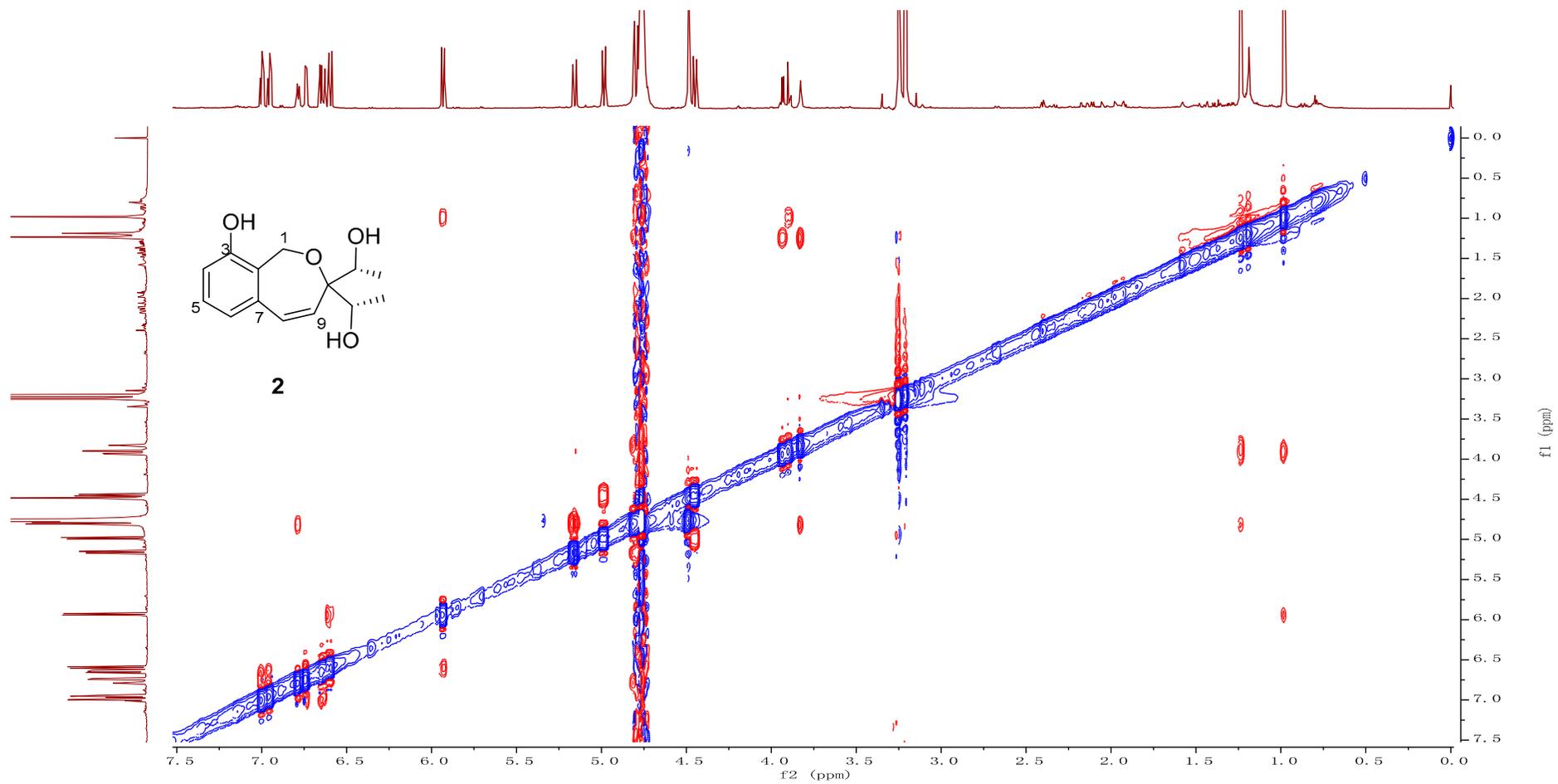


Figure S14. NOESY spectrum of the new compound 2

## Mass Spectrum Molecular Formula Report

### Analysis Info

Analysis Name D:\Data\20151216CEYANG\new folder\NEU-19\_1-C,1\_01\_6265.d  
Method 20131026\_ceyang.m  
Sample Name NEU-19  
Comment

Acquisition Date 12/16/2015 3:33:42 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	100.0 Vpp	Set Divert Valve	Source

### Generate Molecular Formula Parameter

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

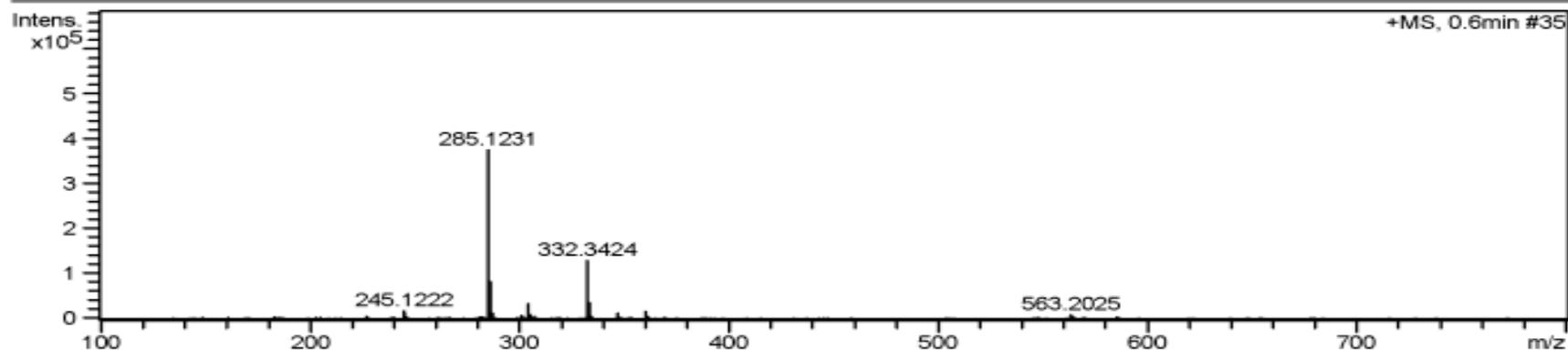


Figure S15. HRESI-MS spectrum of the new compound 3/4

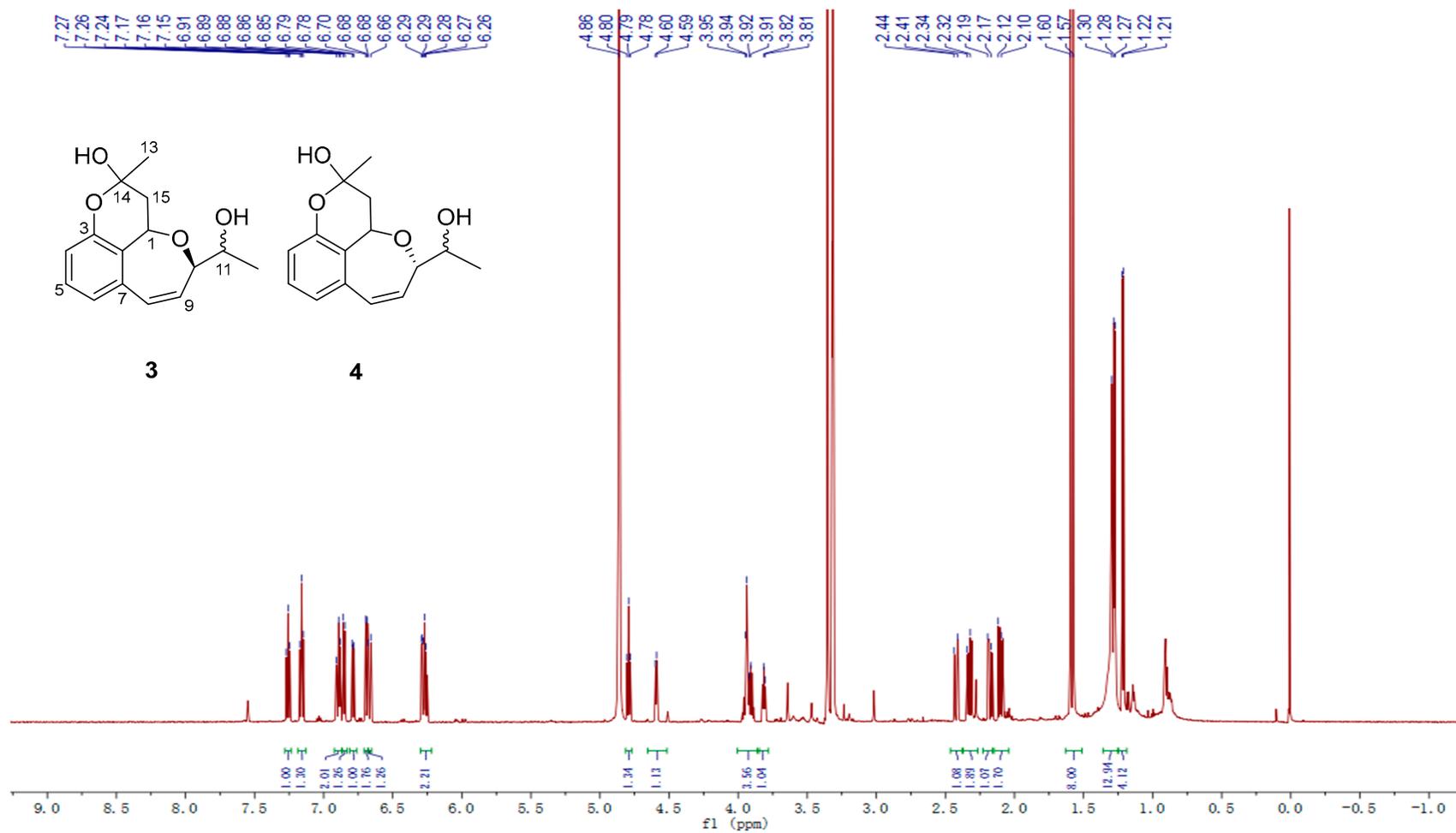


Figure S16.  $^1\text{H}$  NMR (600 MHz,  $\text{CD}_3\text{OD}$ ) spectrum of the new compound 3/4

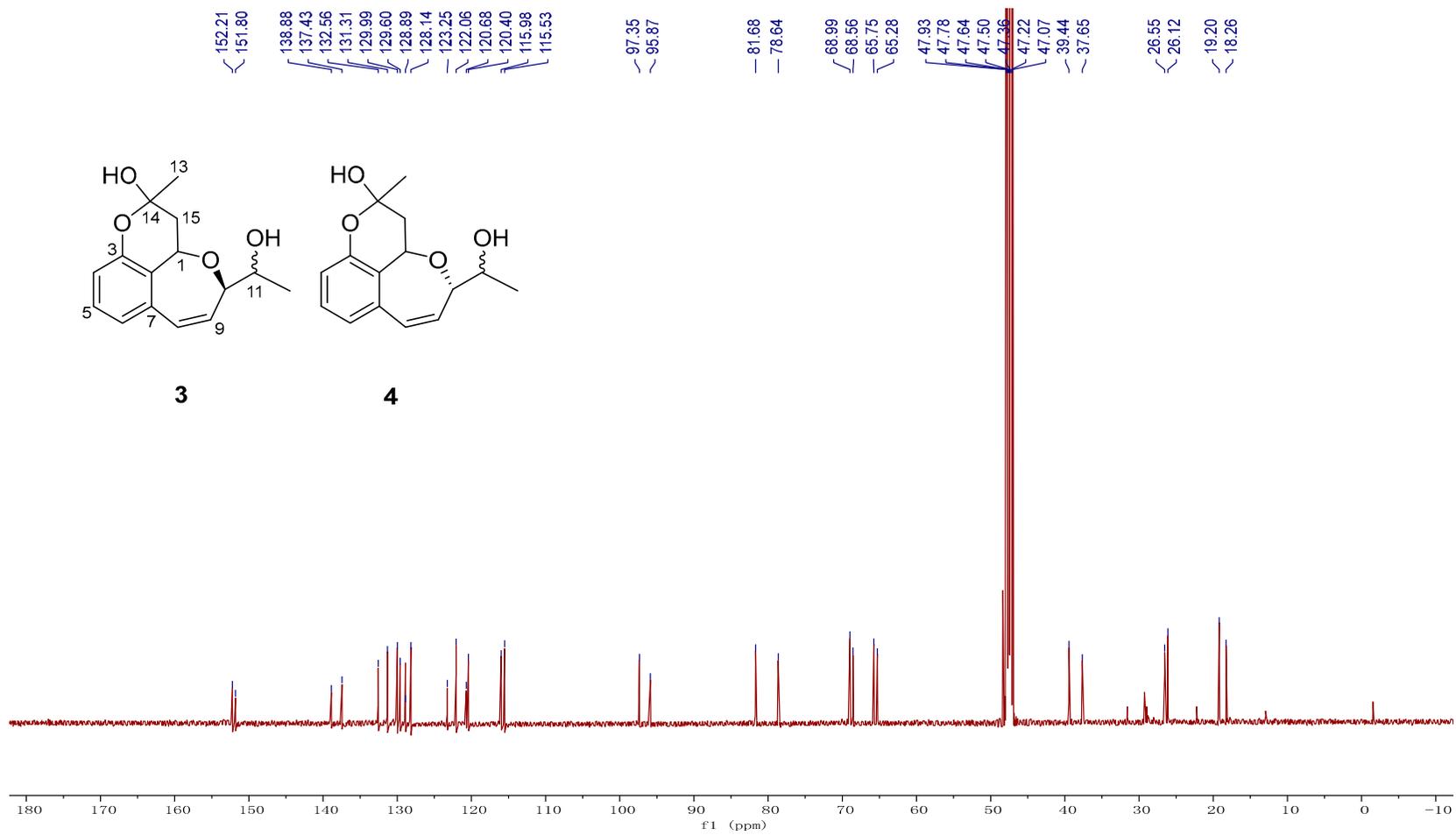


Figure S17. <sup>13</sup>C NMR (150 MHz, CD<sub>3</sub>OD) spectrum of the new compound 3/4

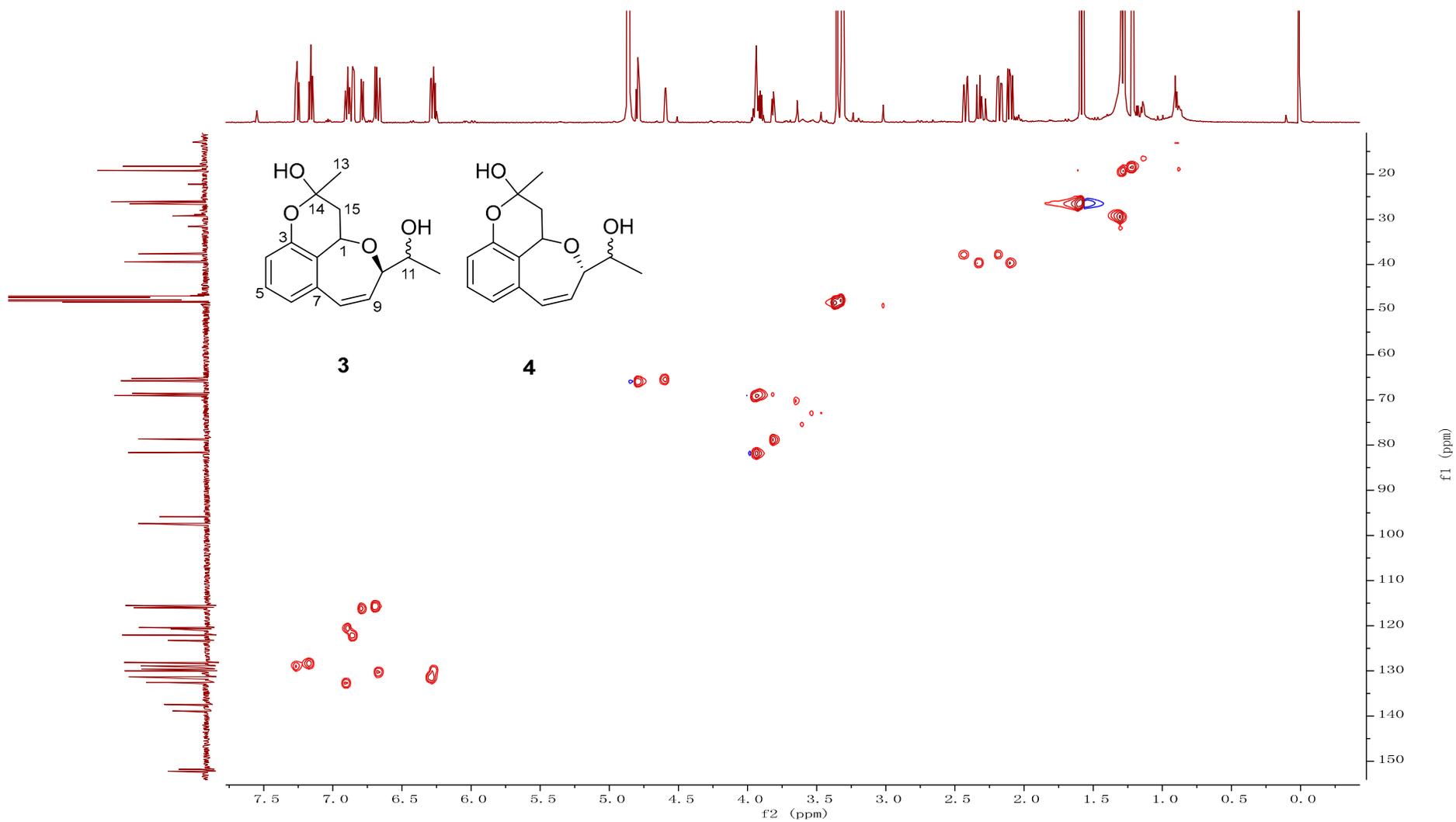


Figure S18. HSQC spectrum of the new compound 3/4

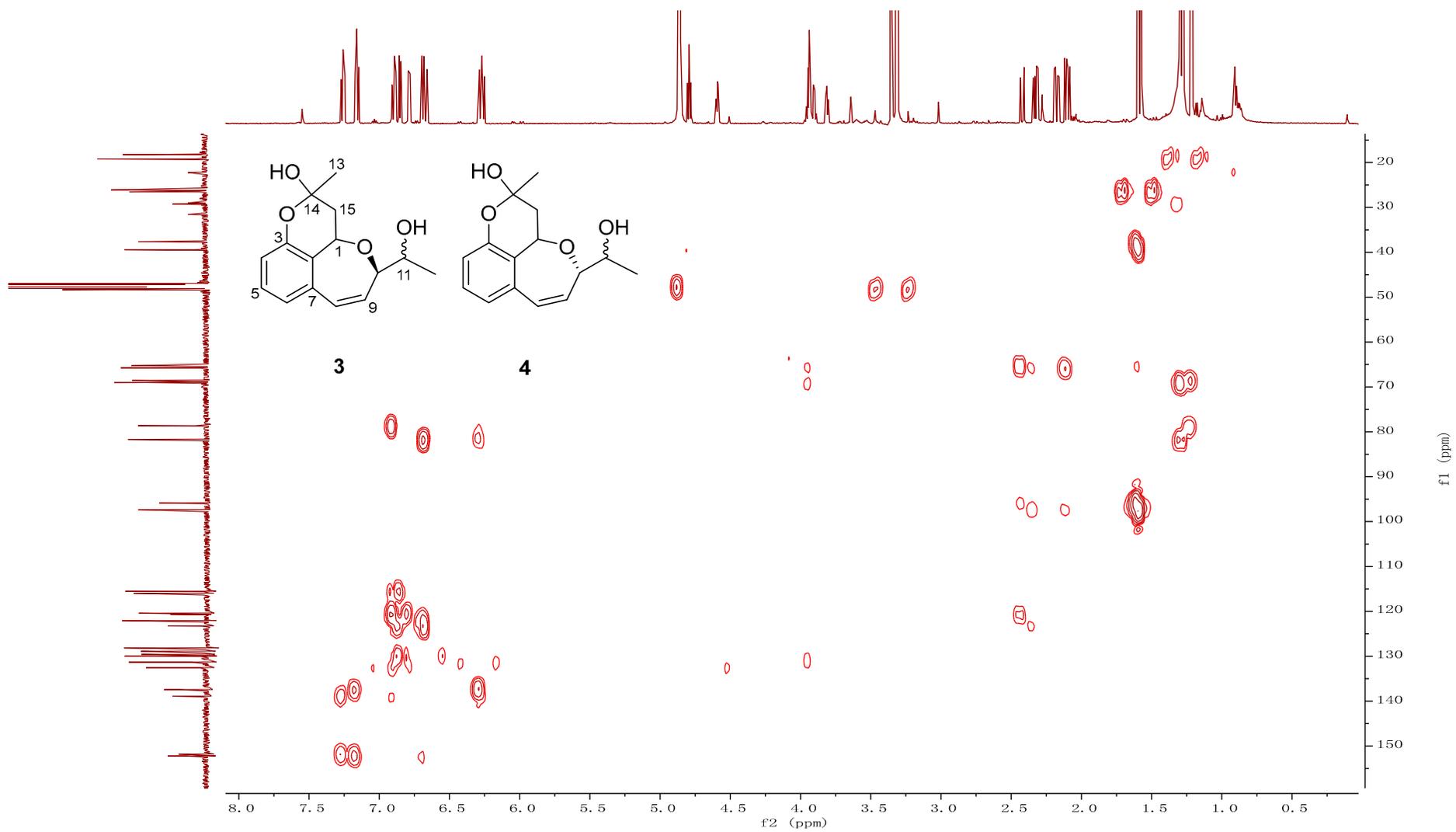


Figure S19. HMBC spectrum of the new compound 3/4

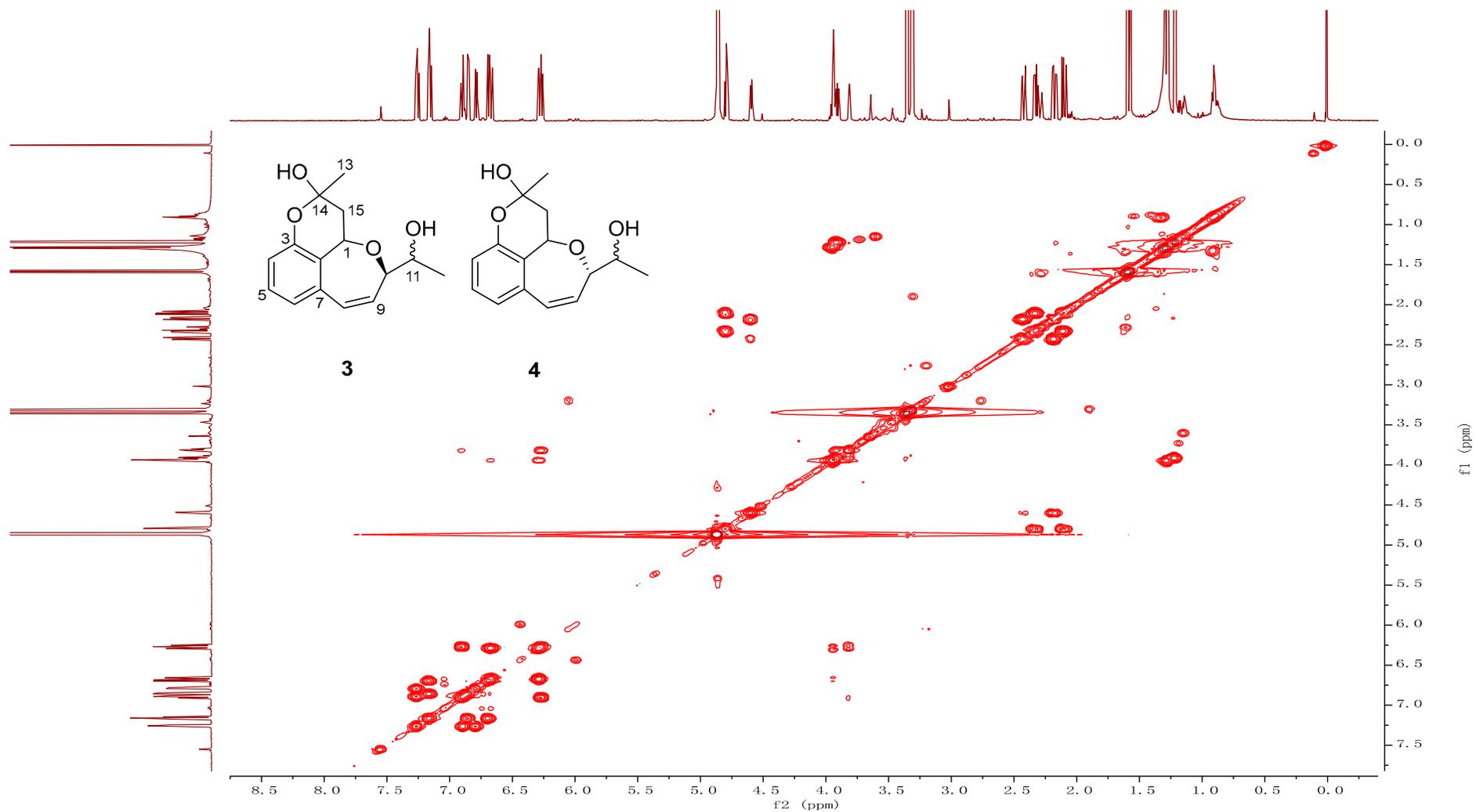


Figure S20. COSY spectrum of the new compound 3/4

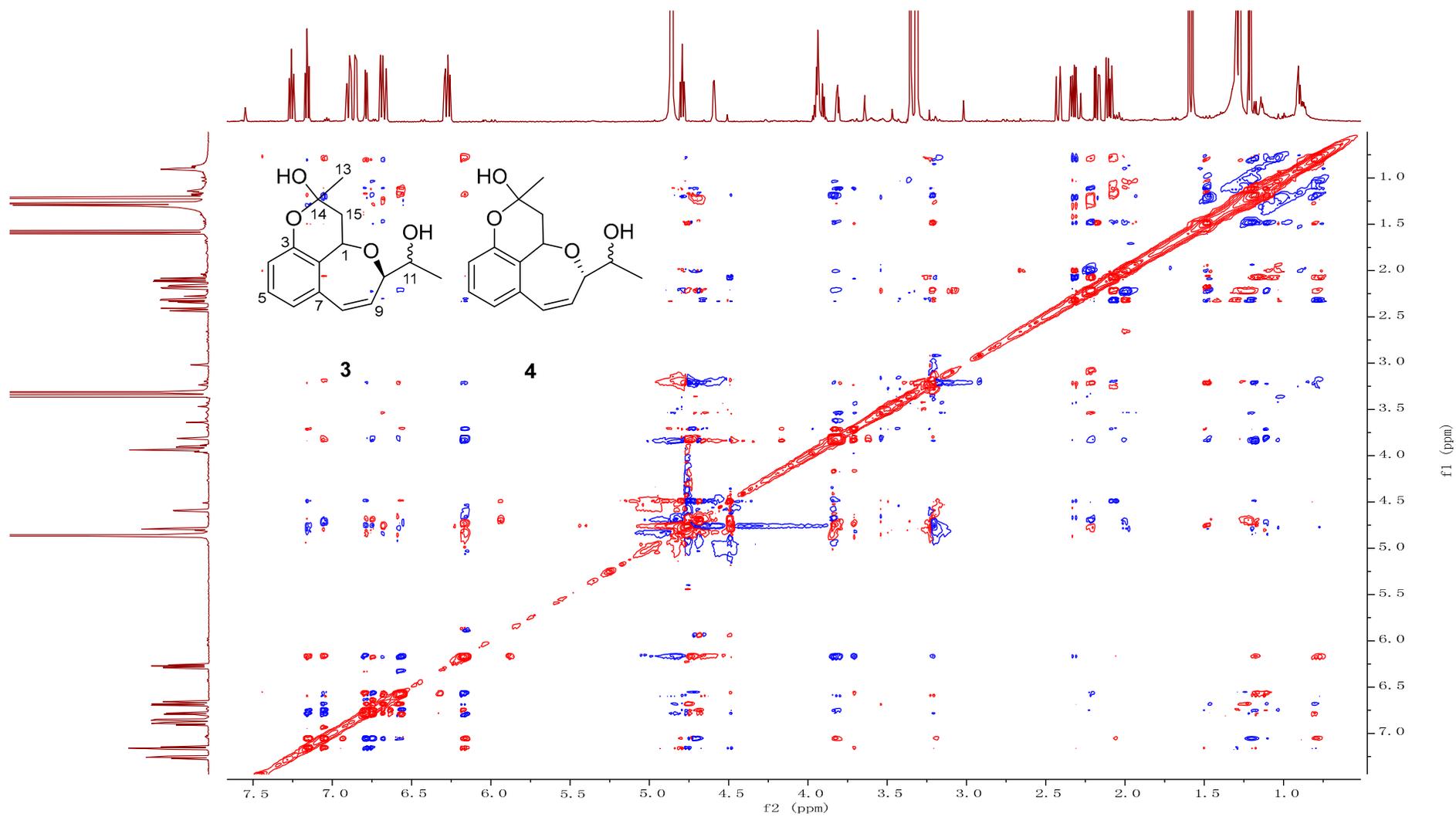


Figure S21. NOESY spectrum of the new compound 3/4