

## Supporting Information

**Pestalotiopsis E-J, Six New Polyketide Derivatives from a Marine Derived Fungus**

***Pestalotiopsis* sp. SWMU-WZ04-1**

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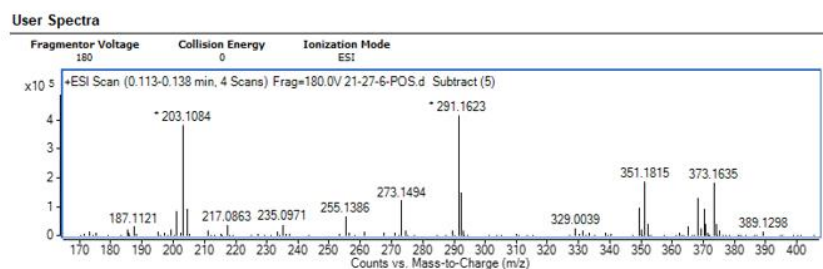
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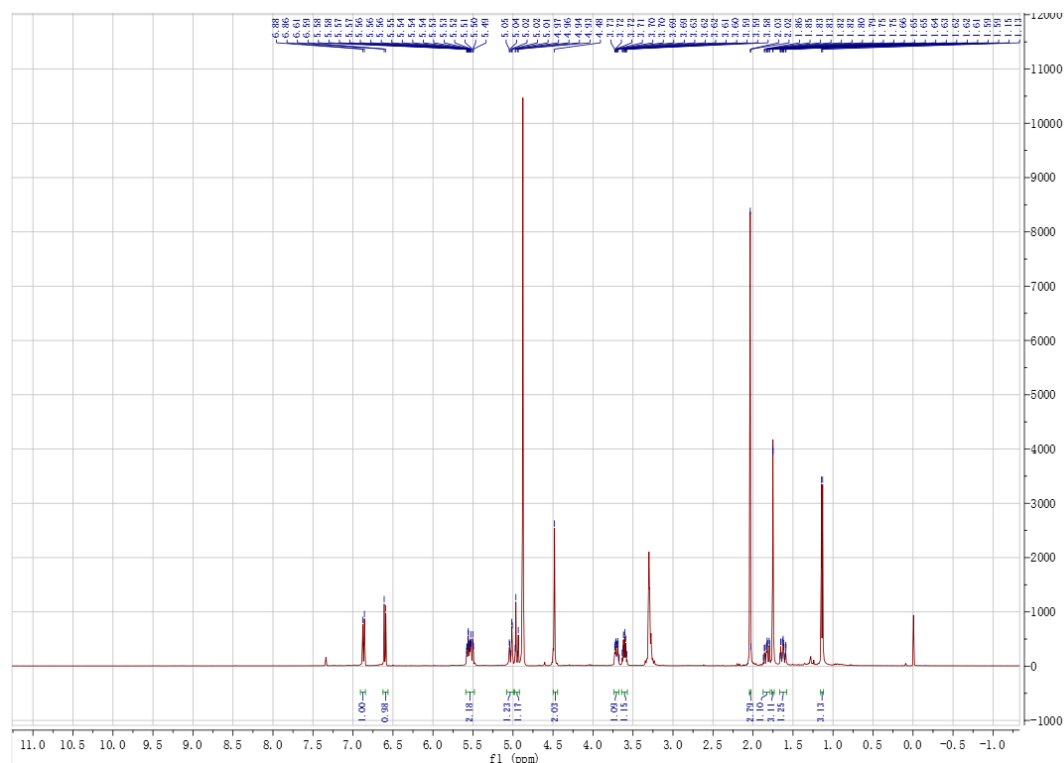
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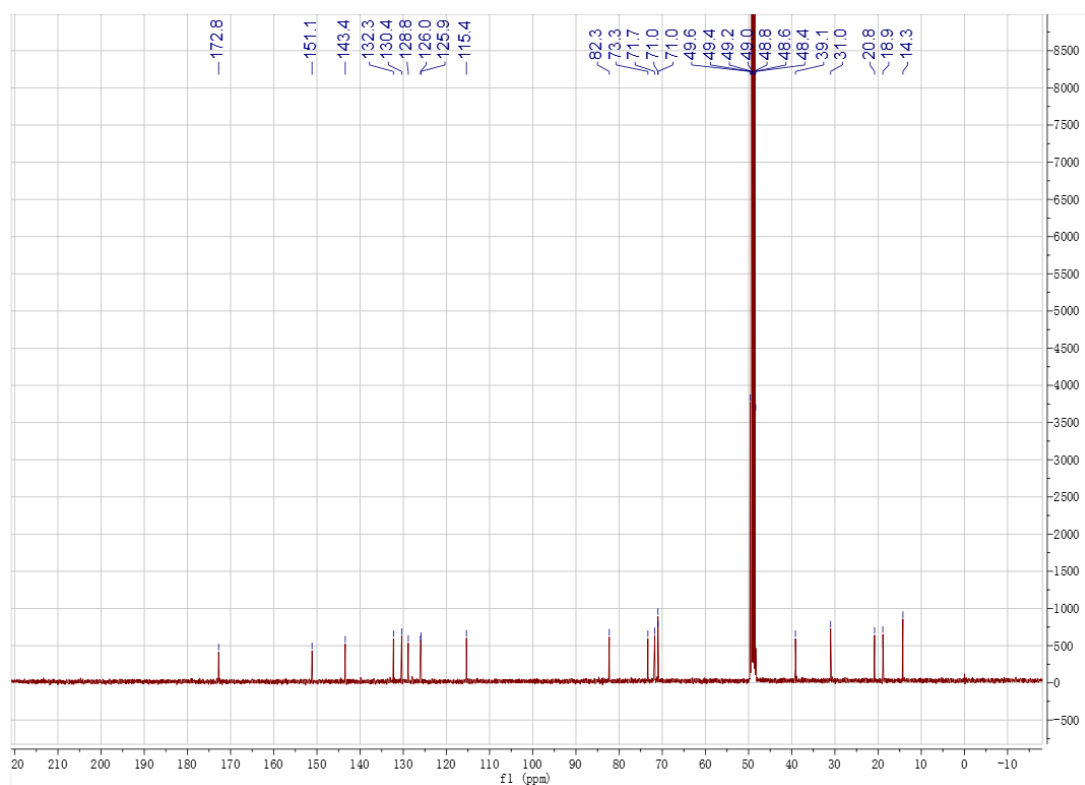
<b>Sample Type</b>	Sample	<b>Position</b>	P1-A4
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<b>Acq Method</b>	default-20211008-pos.m	<b>Acquired Time</b>	9/11/2023 8:48:22 AM
<b>IRM Calibration Status</b>	Some Ions Missed	<b>DA Method</b>	2023.m
<b>Comment</b>			
<b>Sample Group</b>	<b>Info.</b>		
<b>Acquisition SW</b>	6200 series TOF/6500		
<b>Version</b>	series Q-TOF B.05.00 (B5042.0)		



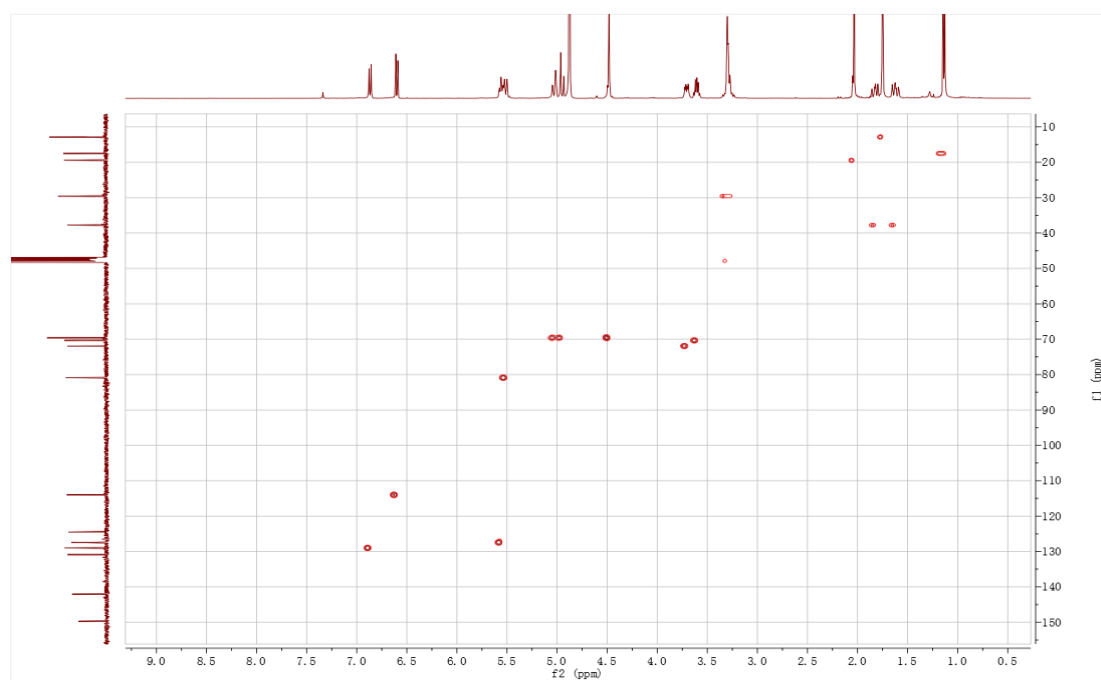
**Figure S1** HRESI-MS spectrum of the compound **1**



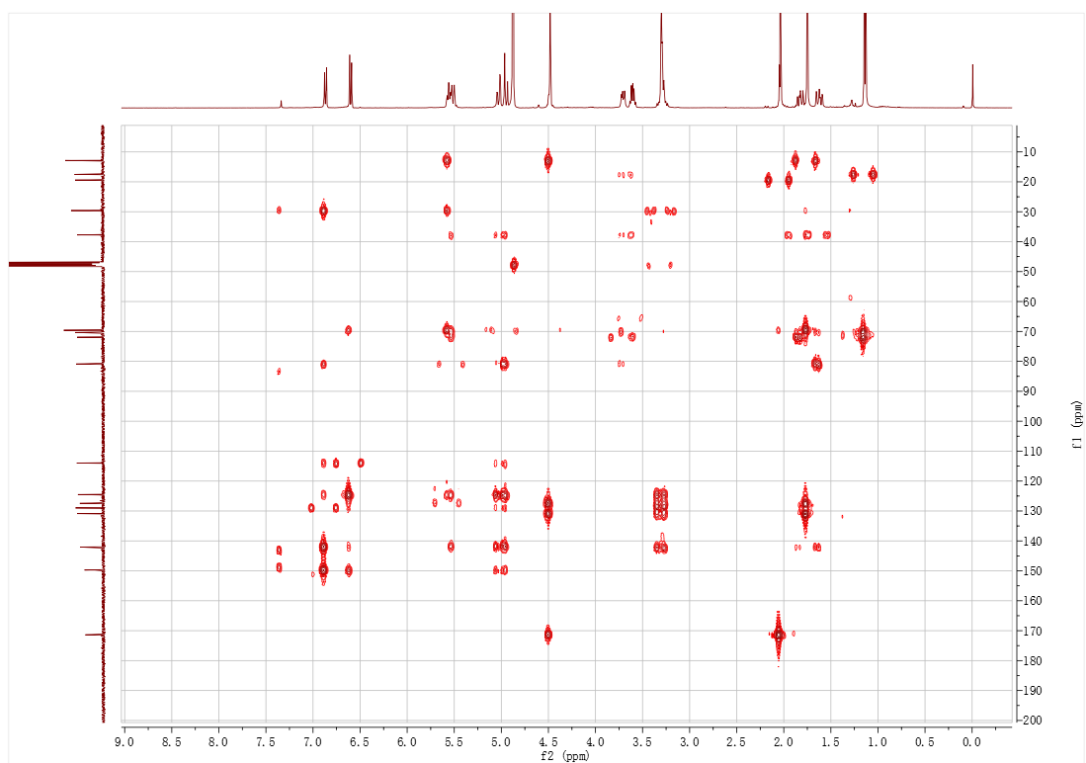
**Figure S2**  $^1\text{H}$  NMR (600 MHz,  $\text{CD}_3\text{OD}$ ) spectrum of the compound **1**



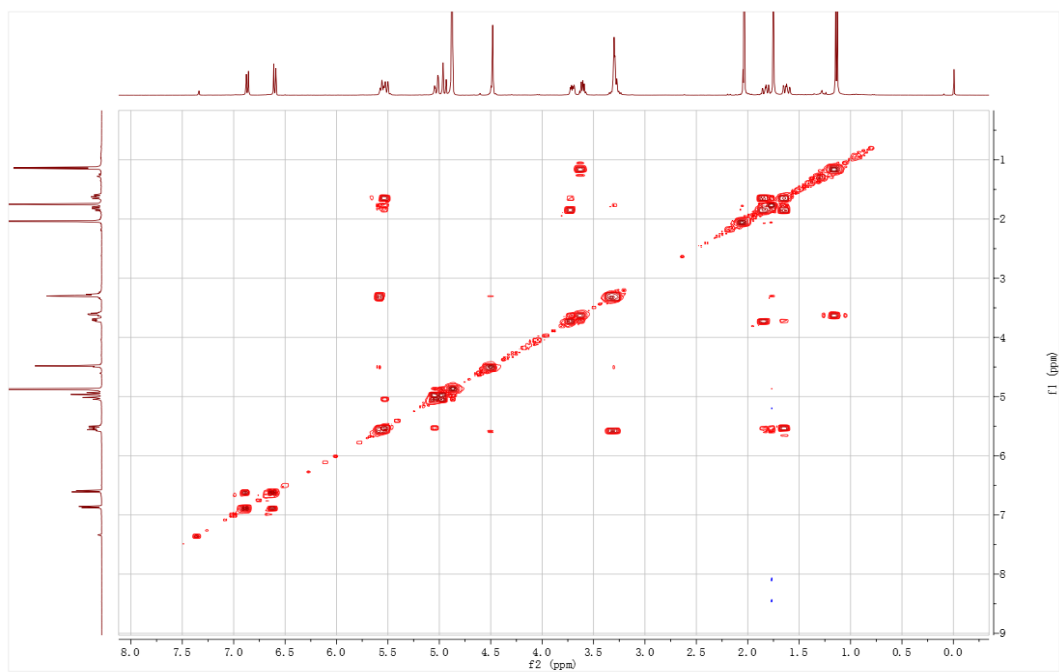
**Figure S3** <sup>13</sup>C NMR (150 MHz, CD<sub>3</sub>OD) spectrum of the compound **1**



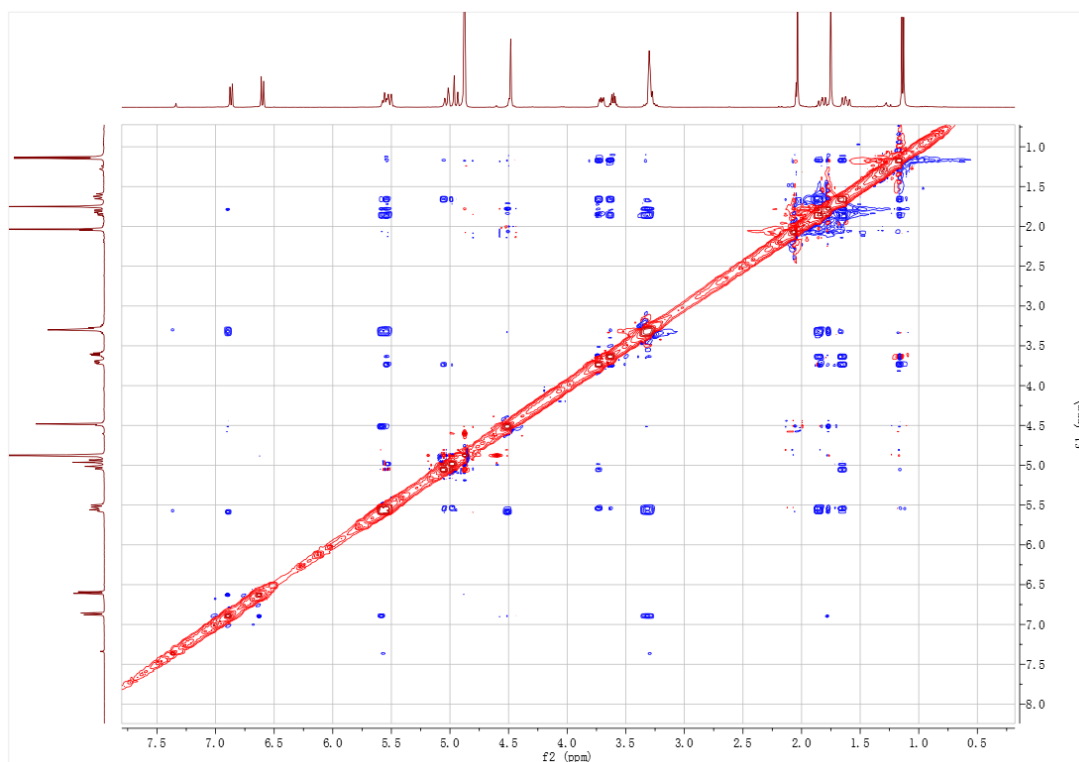
**Figure S4** HSQC spectrum of the compound **1** (CD<sub>3</sub>OD)



**Figure S5** HMBC spectrum of the compound **1**(CD<sub>3</sub>OD)



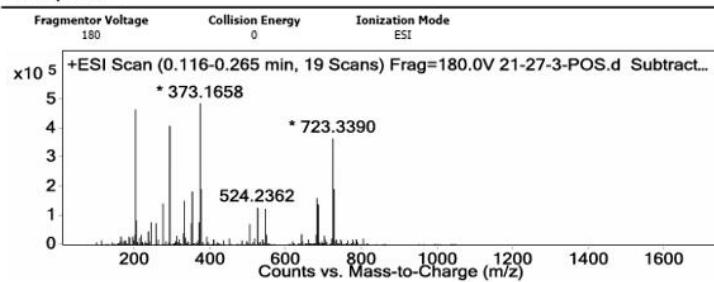
**Figure S6** COSY spectrum of the compound **1**(CD<sub>3</sub>OD)



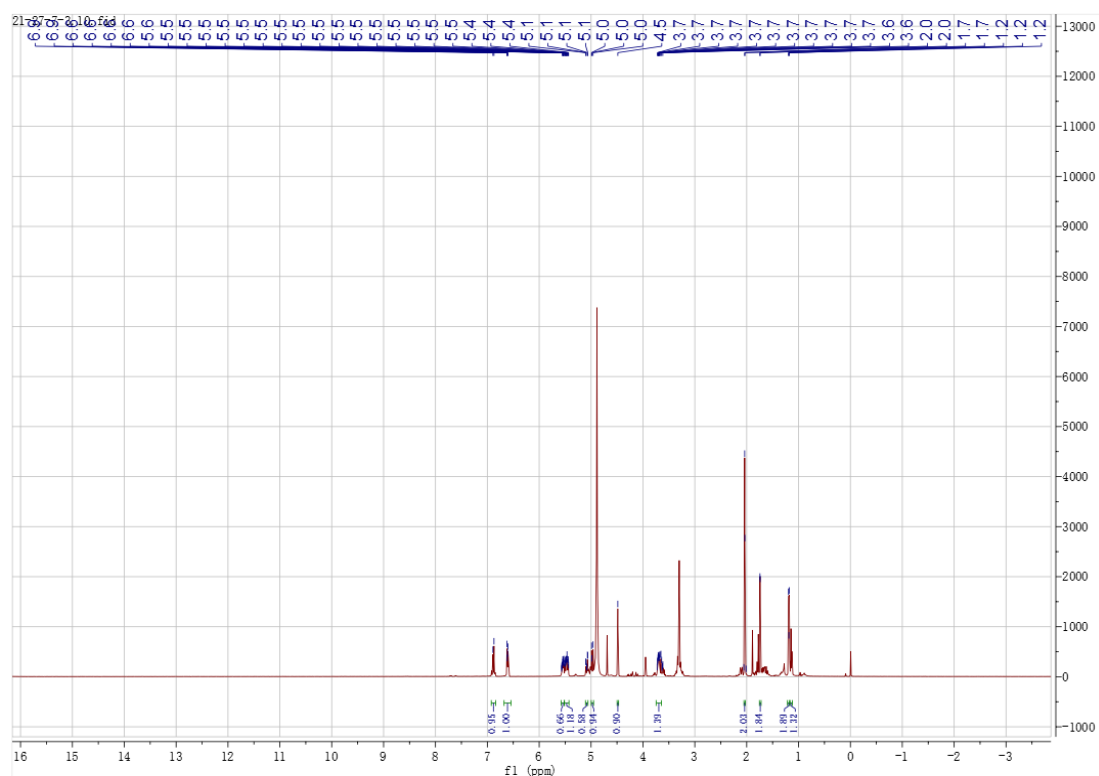
**Figure S7** NOESY spectrum of the compound **1**(CD<sub>3</sub>OD)

<b>Sample Type</b>	Sample	<b>Position</b>	P1-A3
<b>Instrument Name</b>	Instrument 1	<b>User Name</b>	
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<b>Comment</b>			
<b>Sample Group</b>		<b>Info.</b>	
<b>Acquisition SW</b>	6200 series TOF/6500 series		
<b>Version</b>	Q-TOF B.05.00 (B5042.0)		

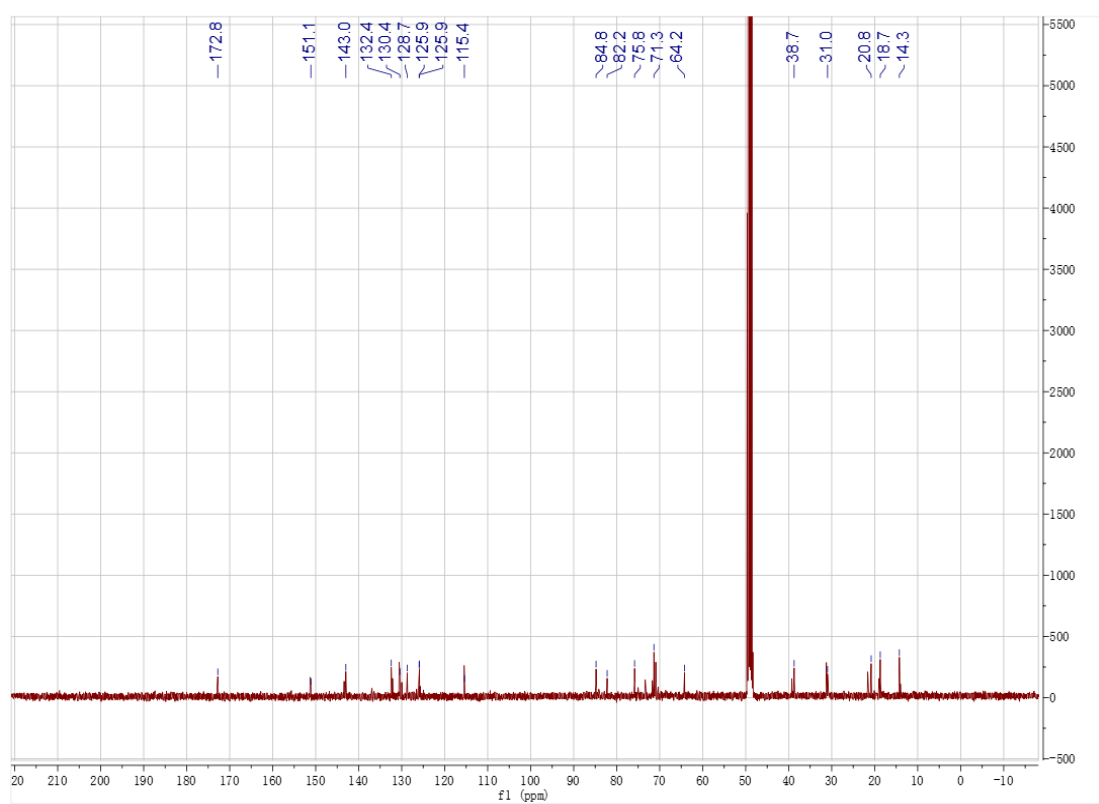
#### User Spectra



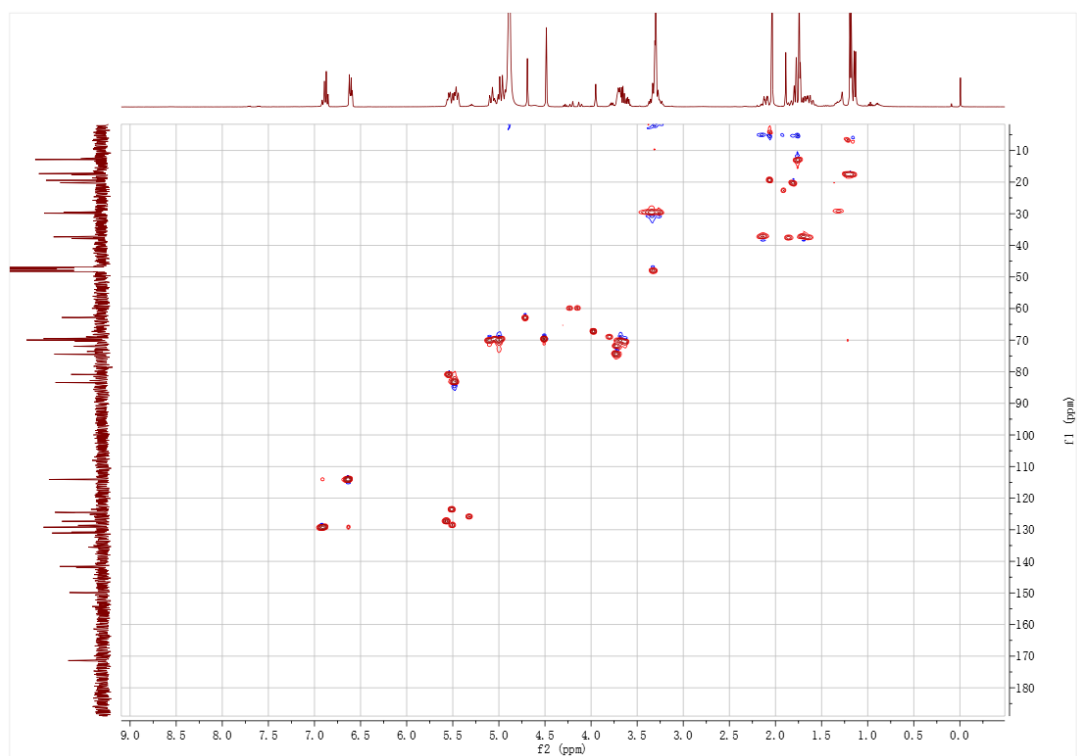
**Figure S8** HRESI-MS spectrum of the compound **2**



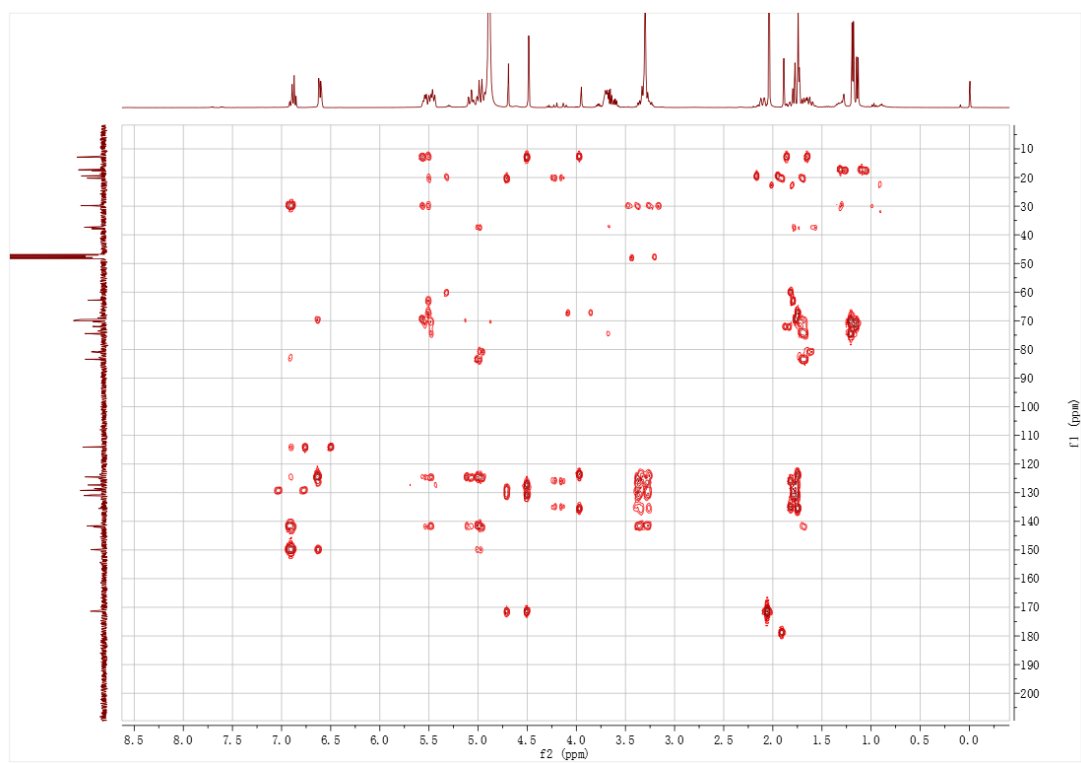
**Figure S9** <sup>1</sup>H NMR (600 MHz, CD<sub>3</sub>OD) spectrum of the compound **2**



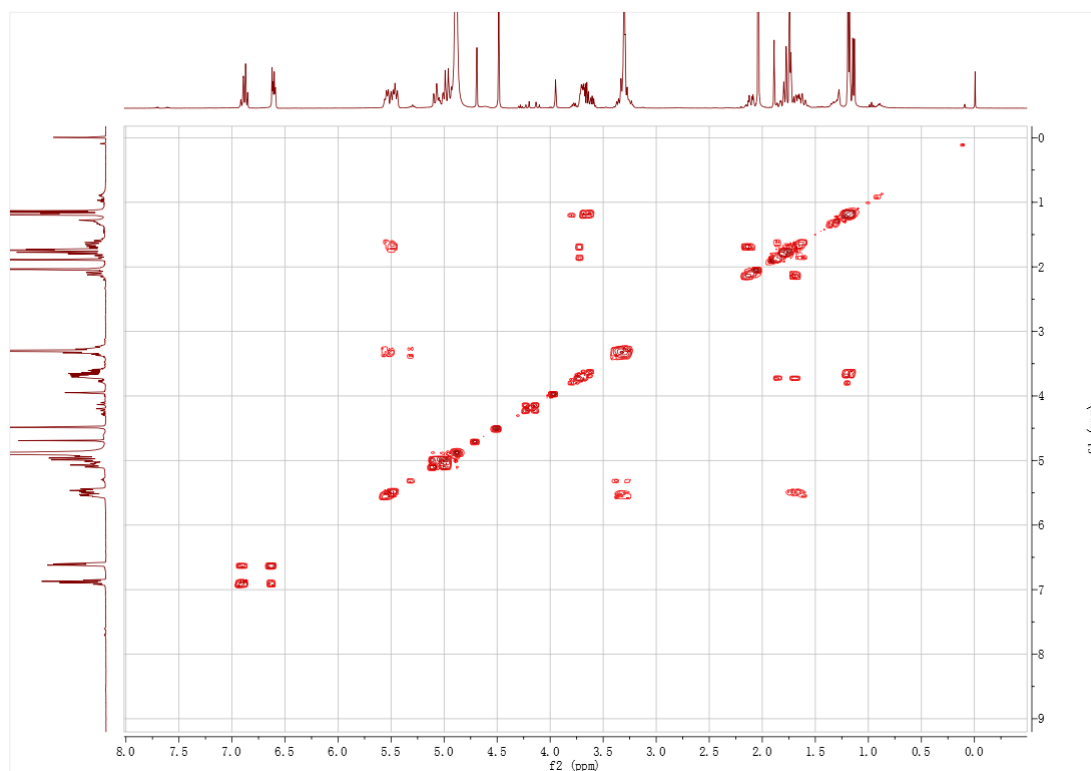
**Figure S10** <sup>13</sup>C NMR (150 MHz, CD<sub>3</sub>OD) spectrum of the compound **2**



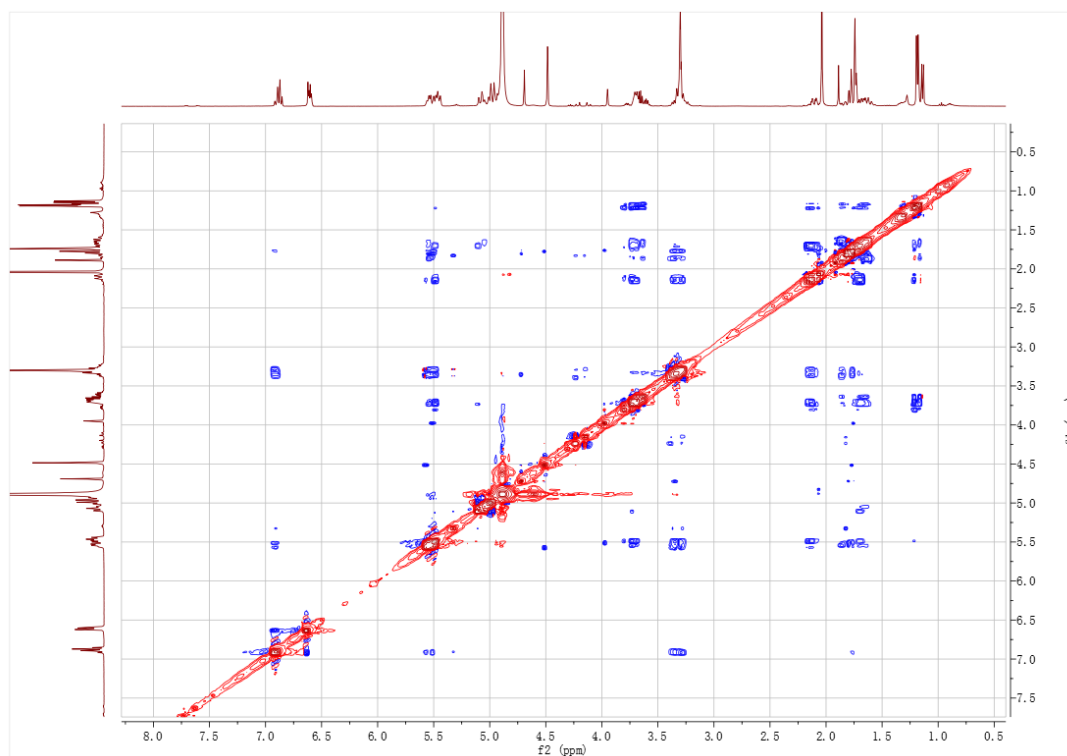
**Figure S11** HSQC spectrum of the compound **2** (CD<sub>3</sub>OD)



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



**Figure S13** COSY spectrum of the compound **2** (CD<sub>3</sub>OD)

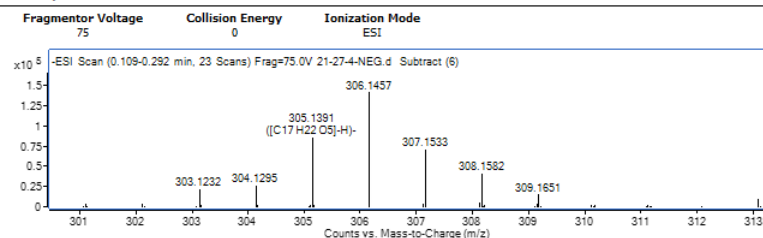


**Figure S14** NOESY spectrum of the compound **2** (CD<sub>3</sub>OD)

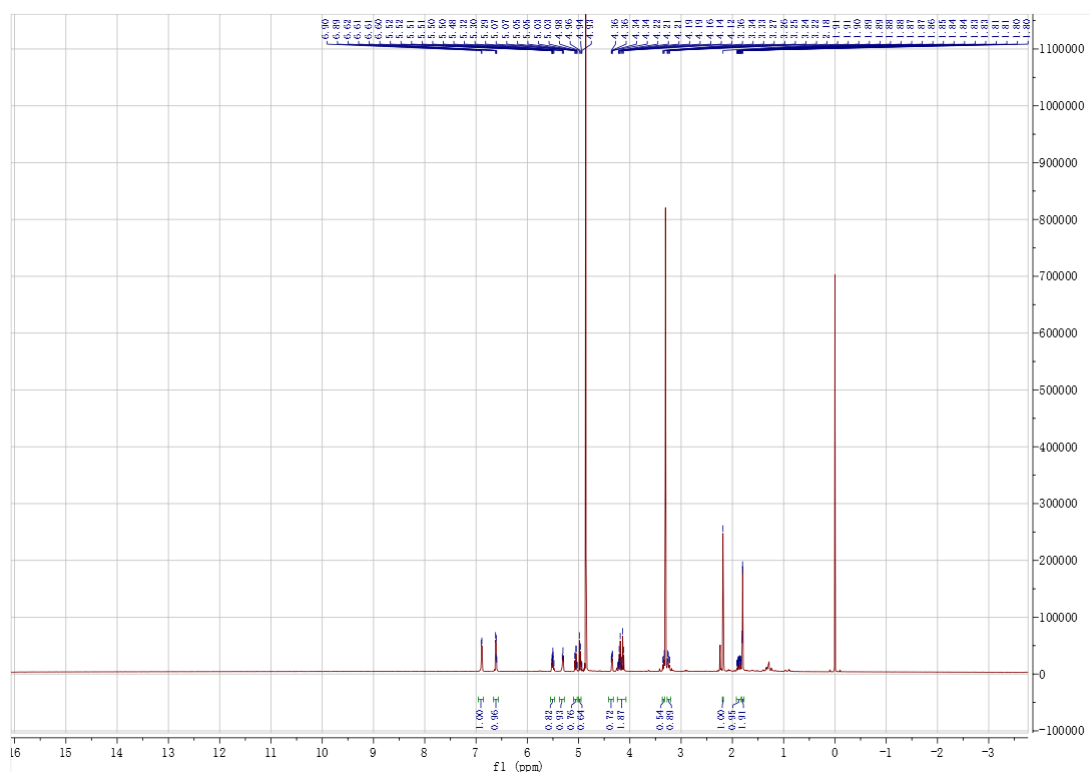


<b>Instrument Name</b>	Instrument 1	<b>User Name</b>	
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<b>IRM Calibration Status</b>	Some Ions Missed	<b>DA Method</b>	2023.m
<b>Comment</b>			
<b>Sample Group</b>		<b>Info.</b>	
<b>Acquisition SW</b>	6200 series TOF/6500		
<b>Version</b>	series Q-TOF B.05.00 (B5042.0)		

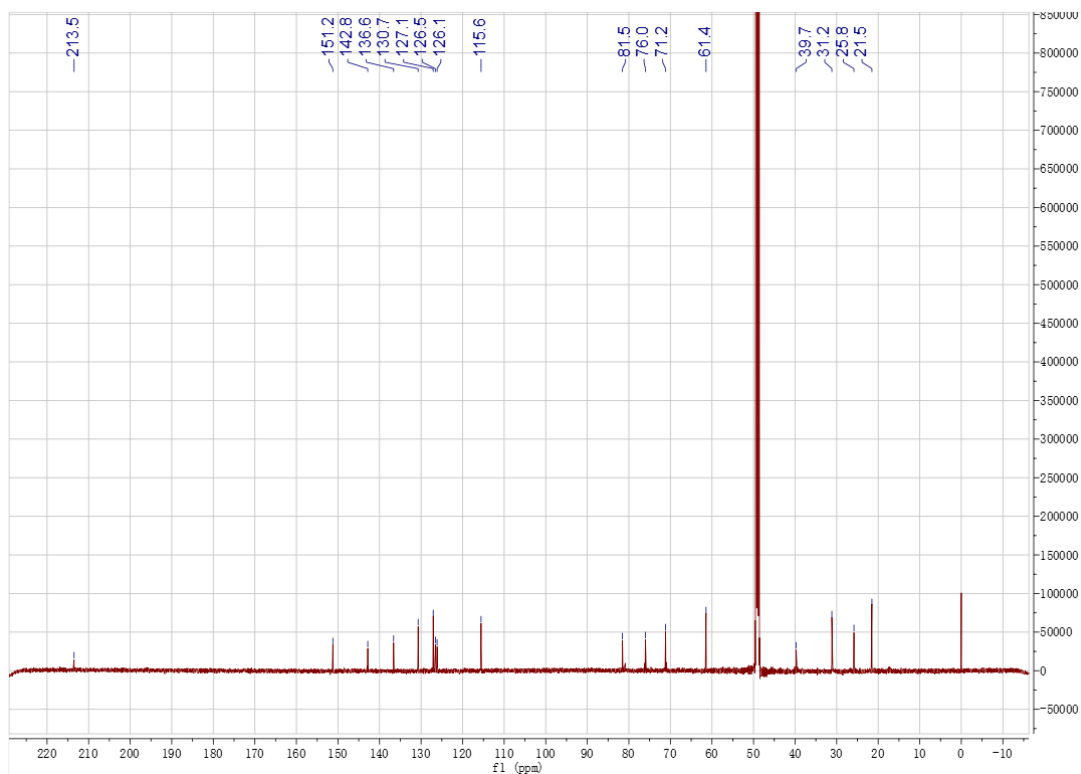
#### User Spectra



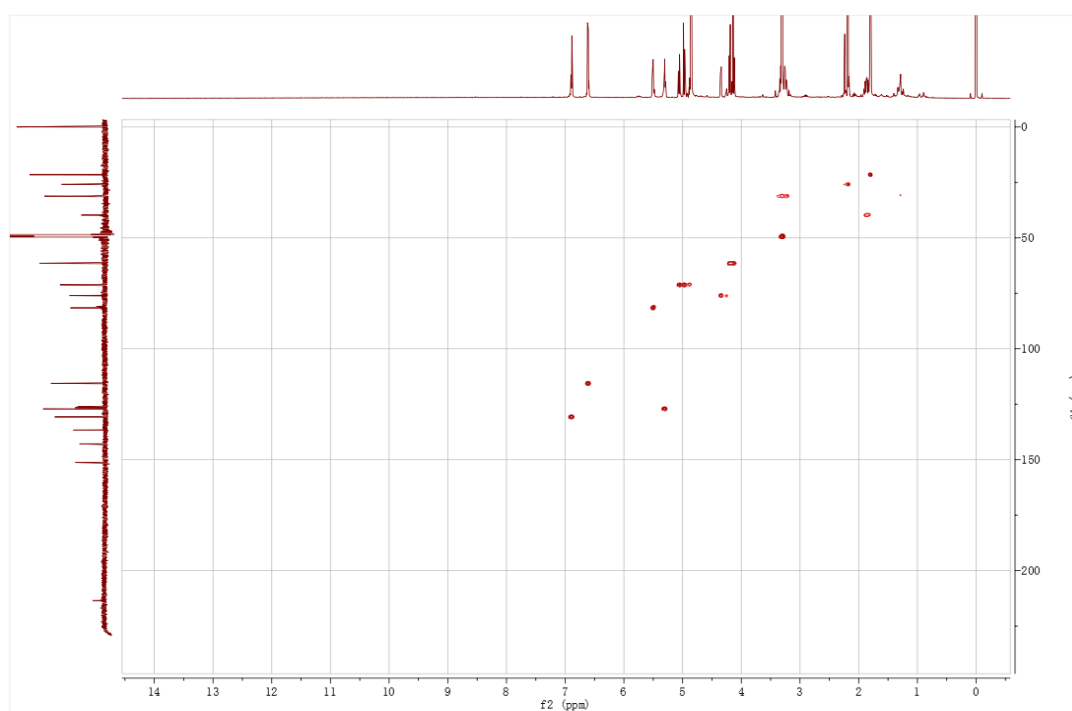
**Figure S15** HRESI-MS spectrum of the compound **3**



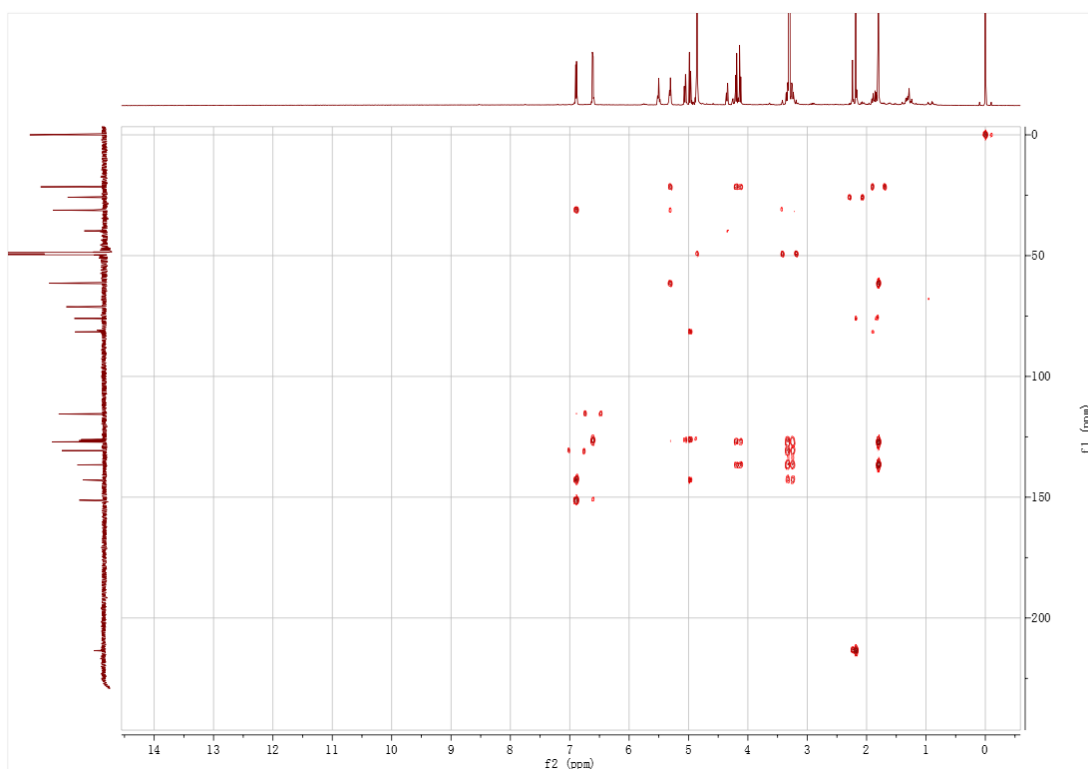
**Figure S16**  $^1\text{H}$  NMR (600 MHz,  $\text{CD}_3\text{OD}$ ) spectrum of the compound **3**



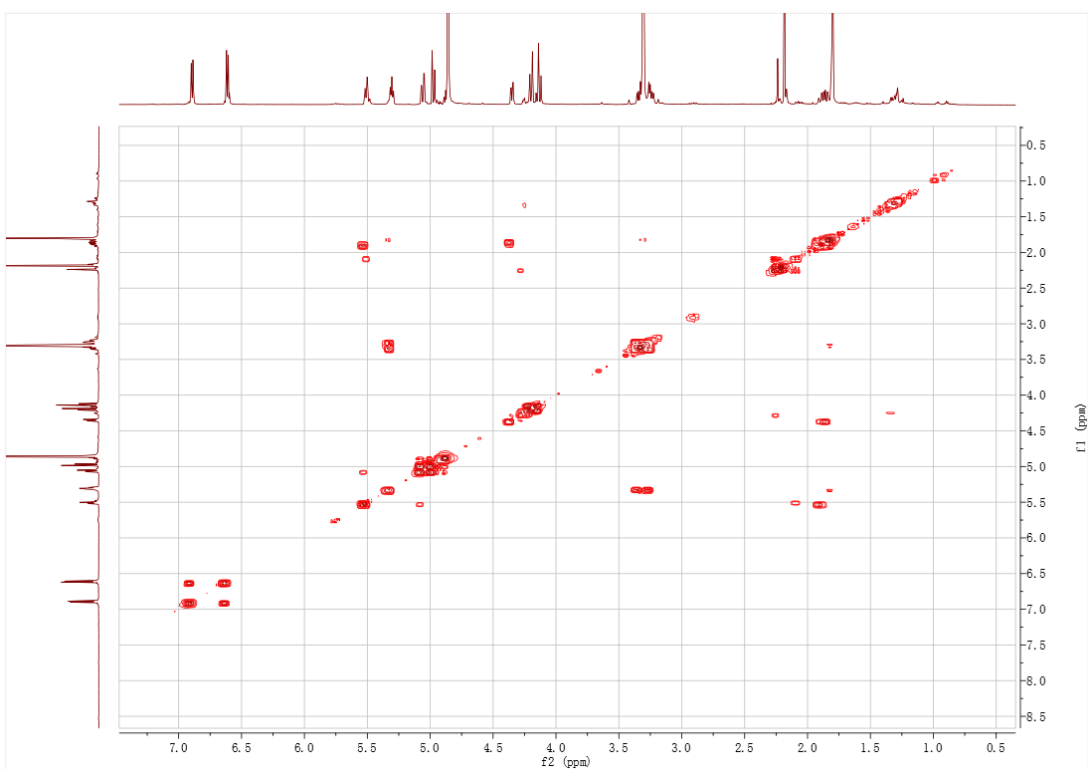
**Figure S17**  $^{13}\text{C}$  NMR (150 MHz,  $\text{CD}_3\text{OD}$ ) spectrum of the compound **3**



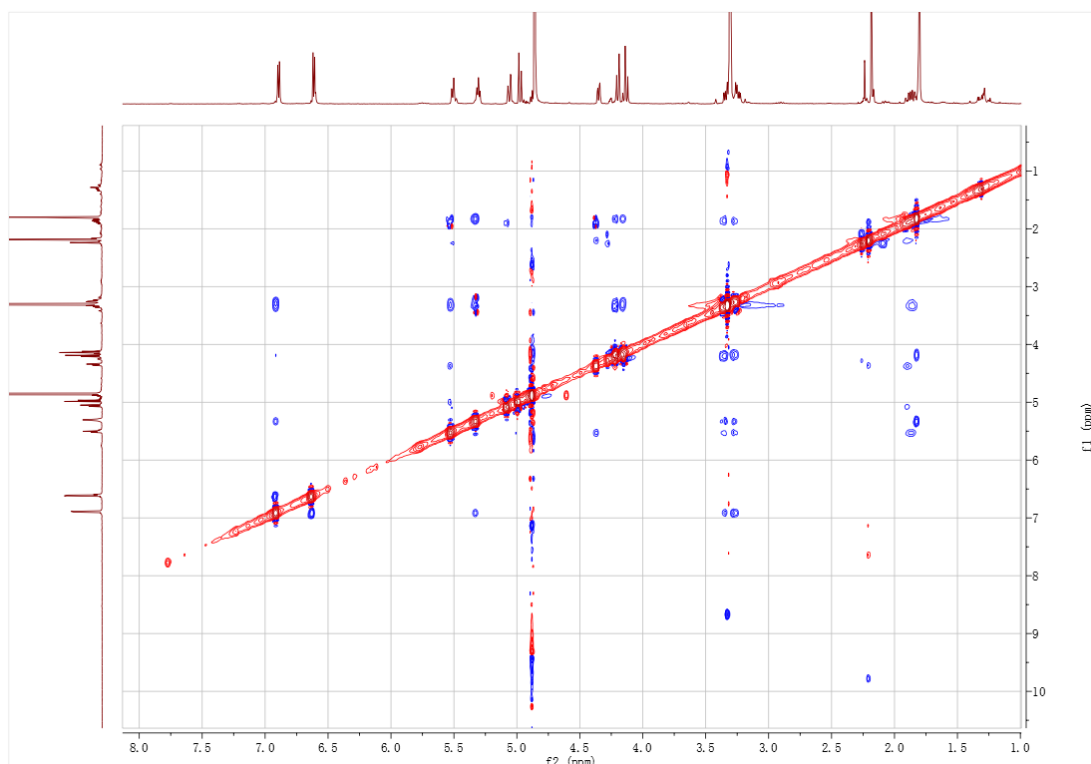
**Figure S18** HSQC spectrum of the compound **3** ( $\text{CD}_3\text{OD}$ )



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



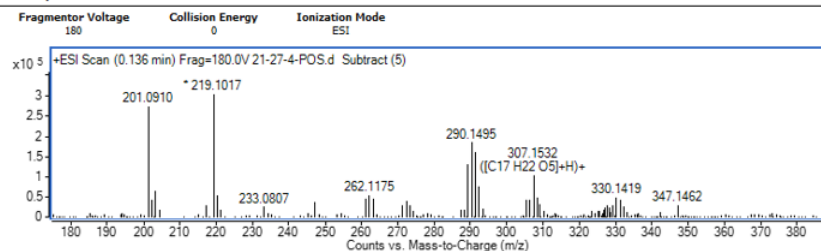
**Figure S20** COSY spectrum of the compound **3** (CD<sub>3</sub>OD)



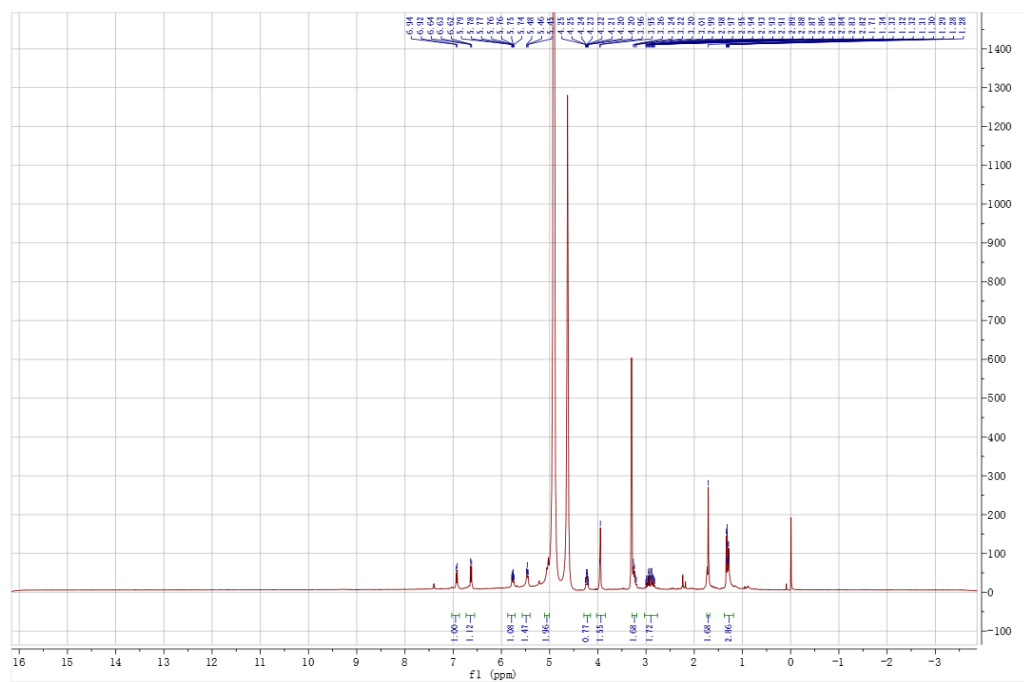
**Figure S21** NOESY spectrum of the compound **3** (CD<sub>3</sub>OD)

Sample Type	Unavailable	Position	Unavailable
Instrument Name	Unavailable	User Name	Unavailable
Acq Method		Acquired Time	Unavailable
IRM Calibration Status	Some Ions Missed	DA Method	2023.m
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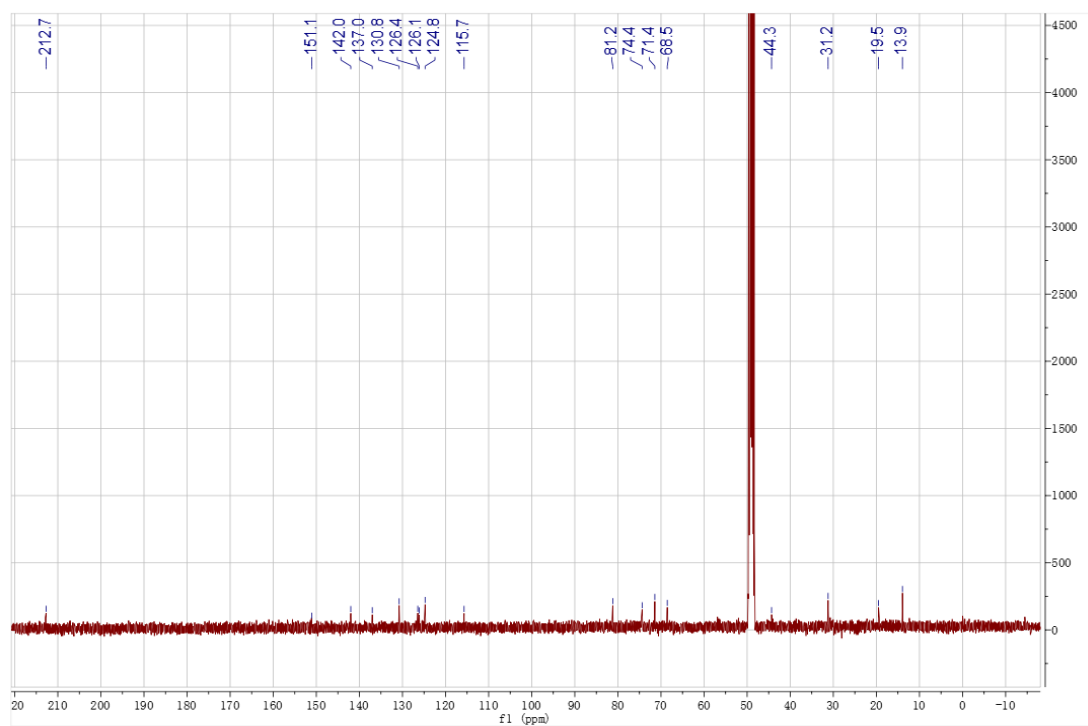
#### User Spectra



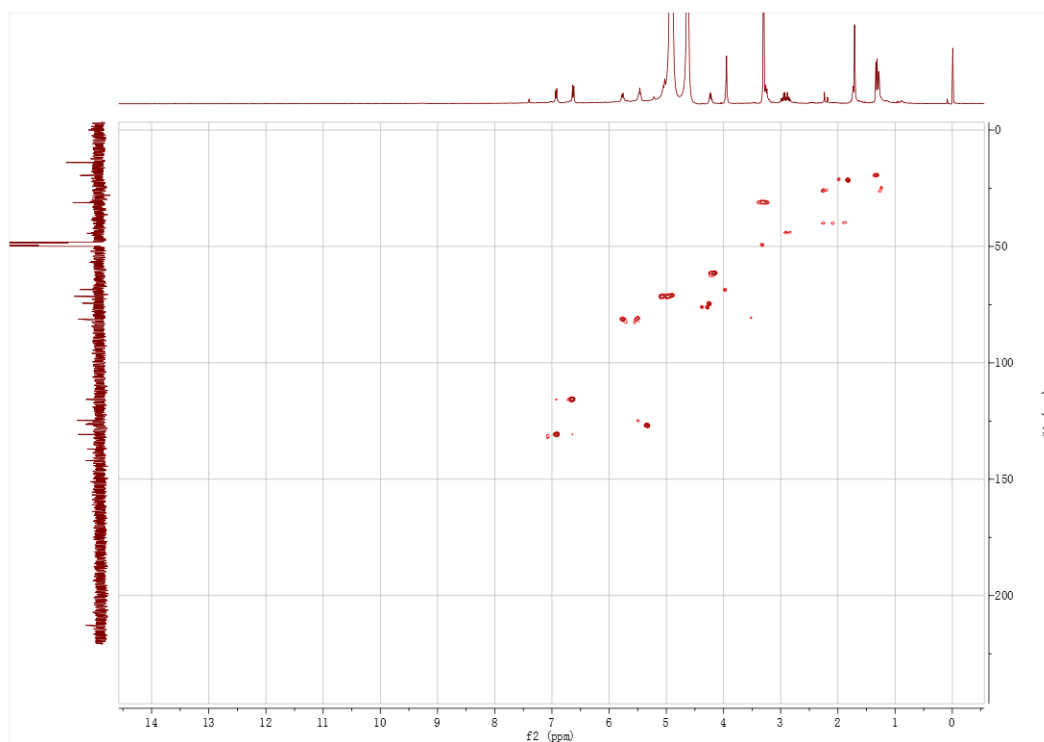
**Figure S22** HRESI-MS spectrum of the compound **4**



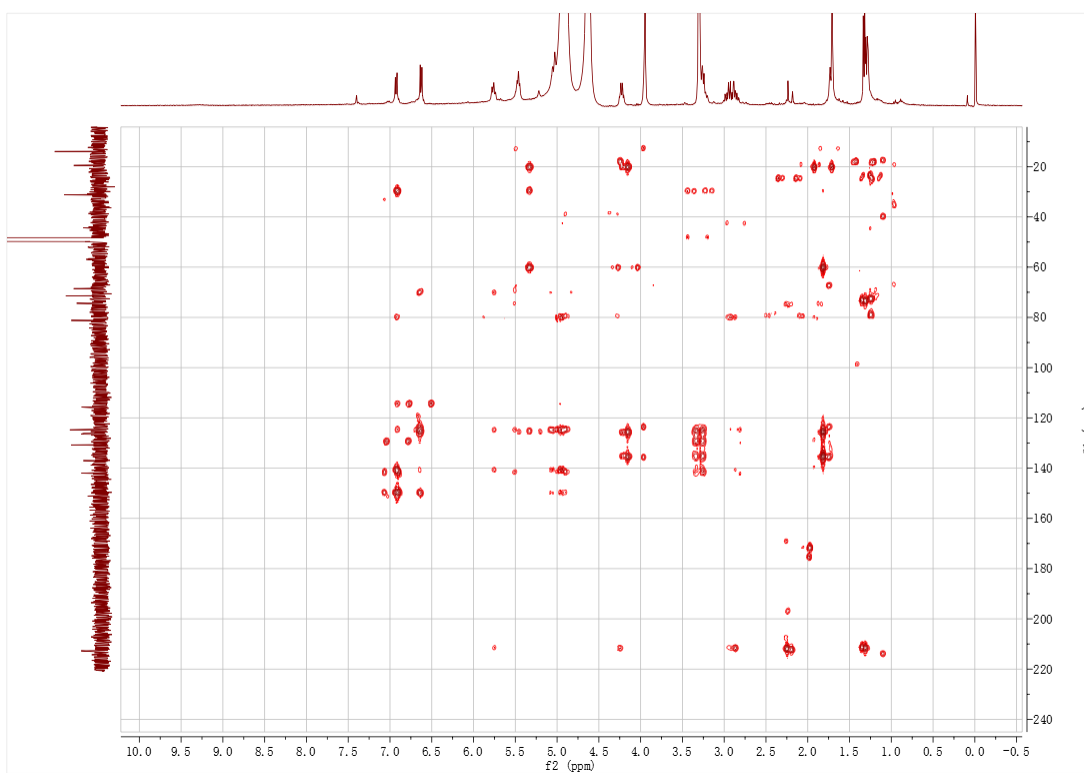
**Figure S23** <sup>1</sup>H NMR (600 MHz, CD<sub>3</sub>OD) spectrum of the compound **4**



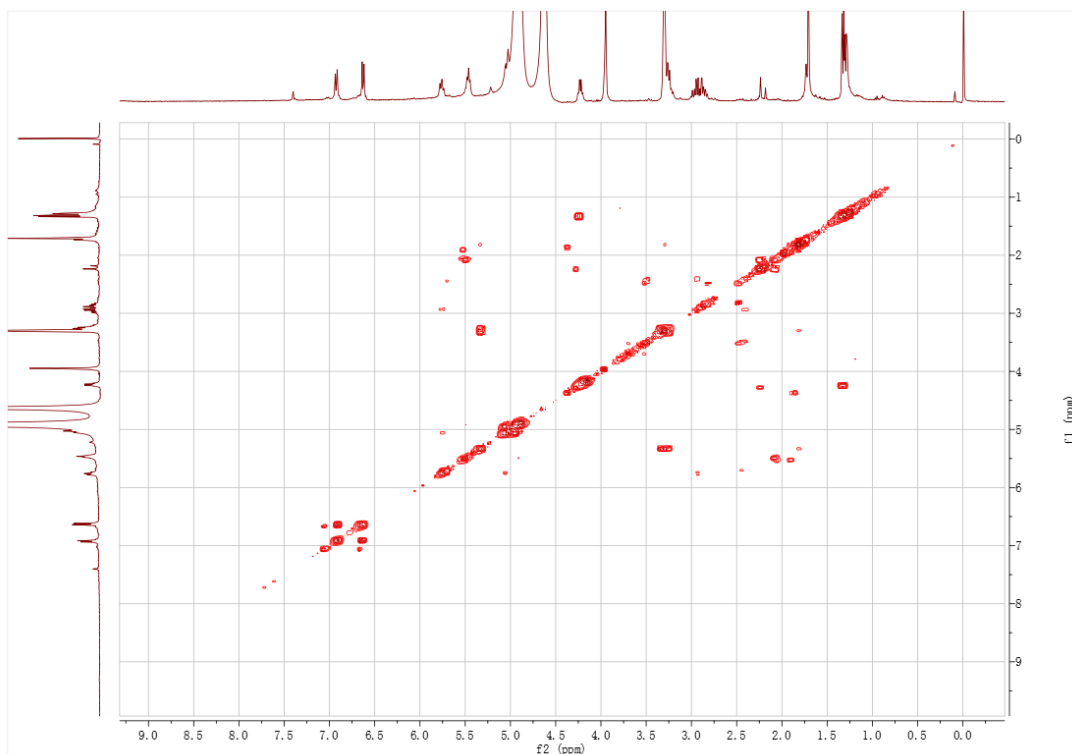
**Figure S24** <sup>13</sup>C NMR (150 MHz, CD<sub>3</sub>OD) spectrum of the compound **4**



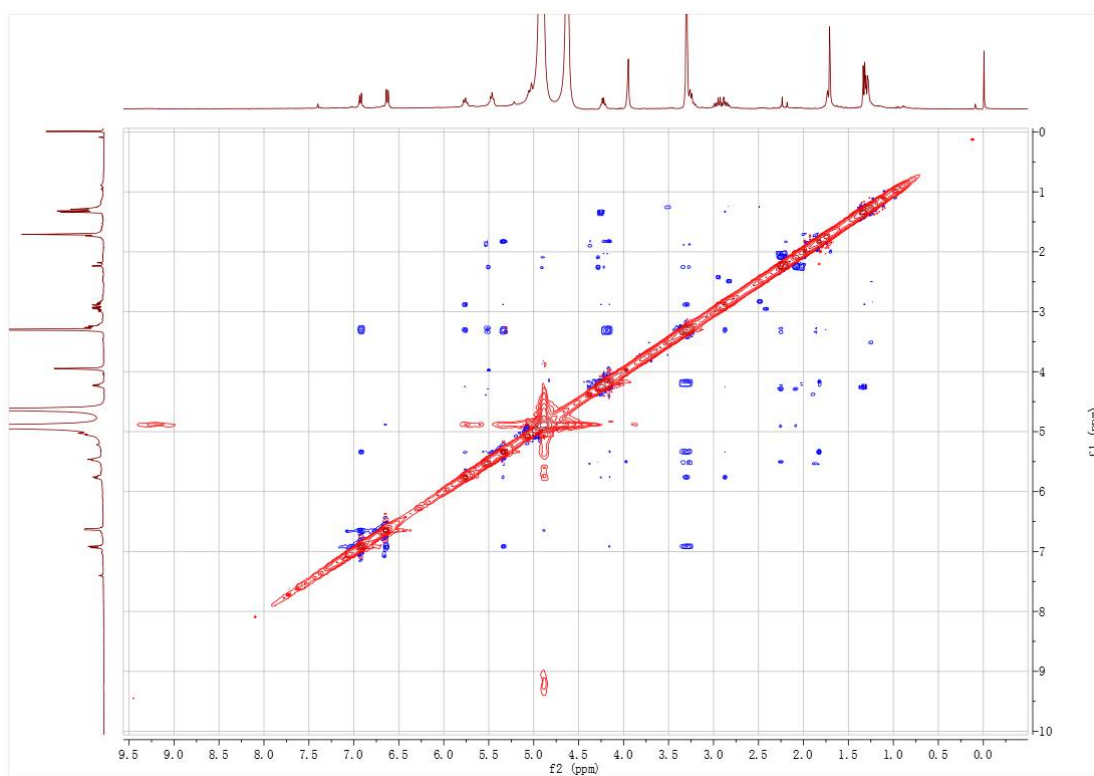
**Figure S25** HSQC spectrum of the compound **4** (CD<sub>3</sub>OD)



**Figure S26** HMBC spectrum of the compound **4** (CD<sub>3</sub>OD)



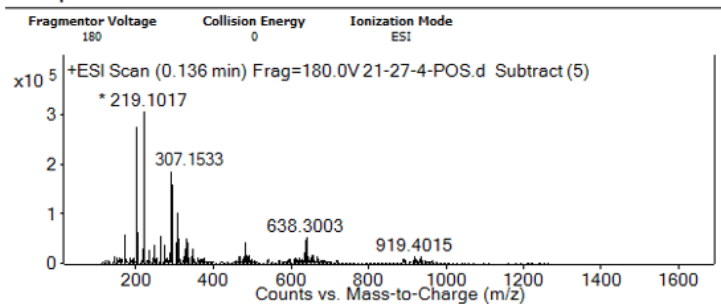
**Figure S27** COSY spectrum of the compound **4** (CD<sub>3</sub>OD)



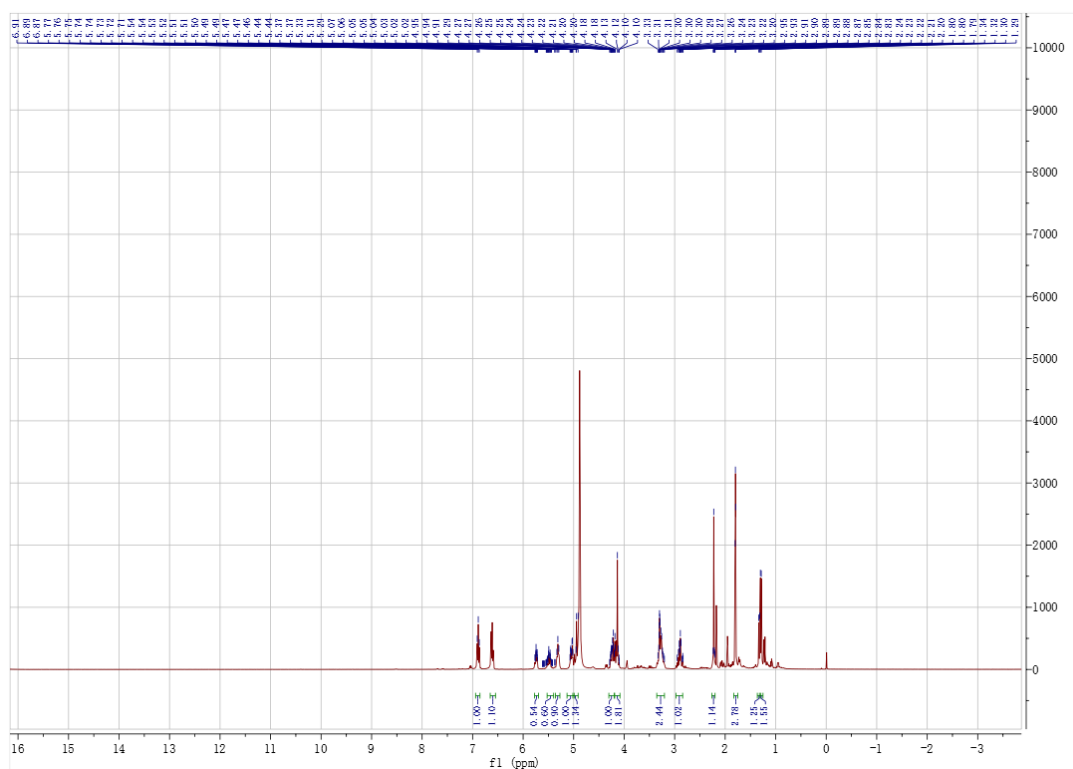
**Figure S28** NOESY spectrum of the compound **4** (CD<sub>3</sub>OD)

Sample Type	Unavailable	Position	Unavailable
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Acq Method		Acquired Time	Unavailable
IRM Calibration Status	Some Ions Missed	DA Method	2023.m
Comment	Sample information is unavailable		

#### User Spectra

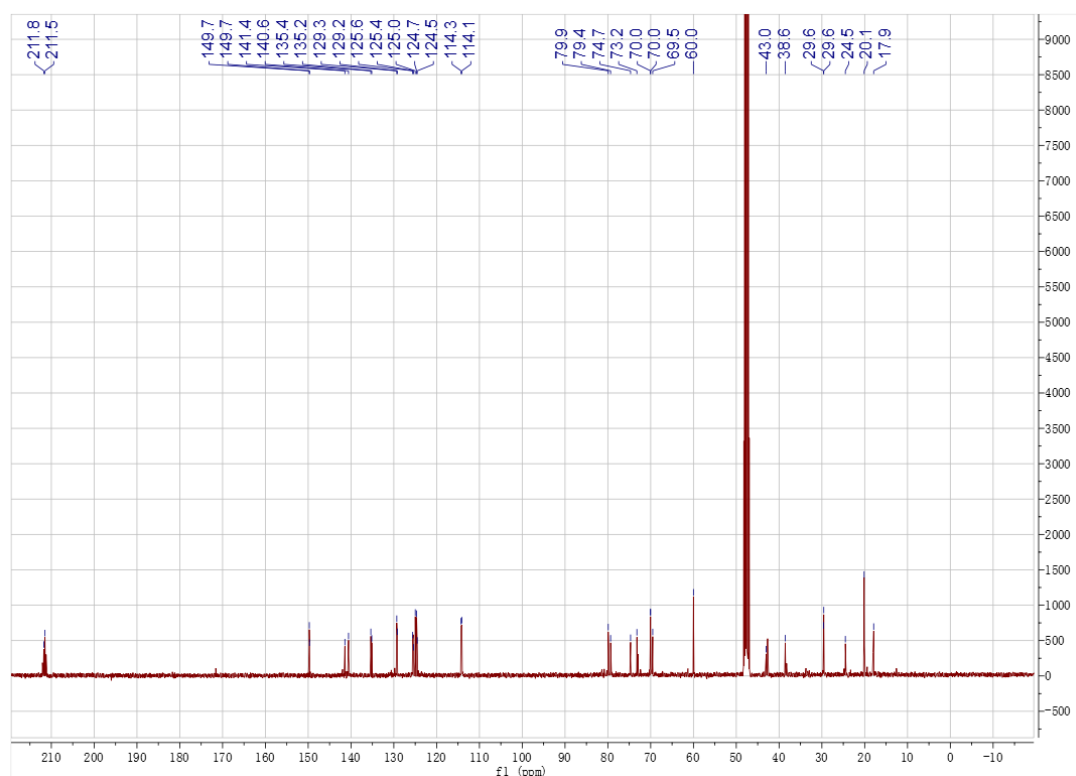


**Figure S29** HRESI-MS spectrum of the compounds **5/6**

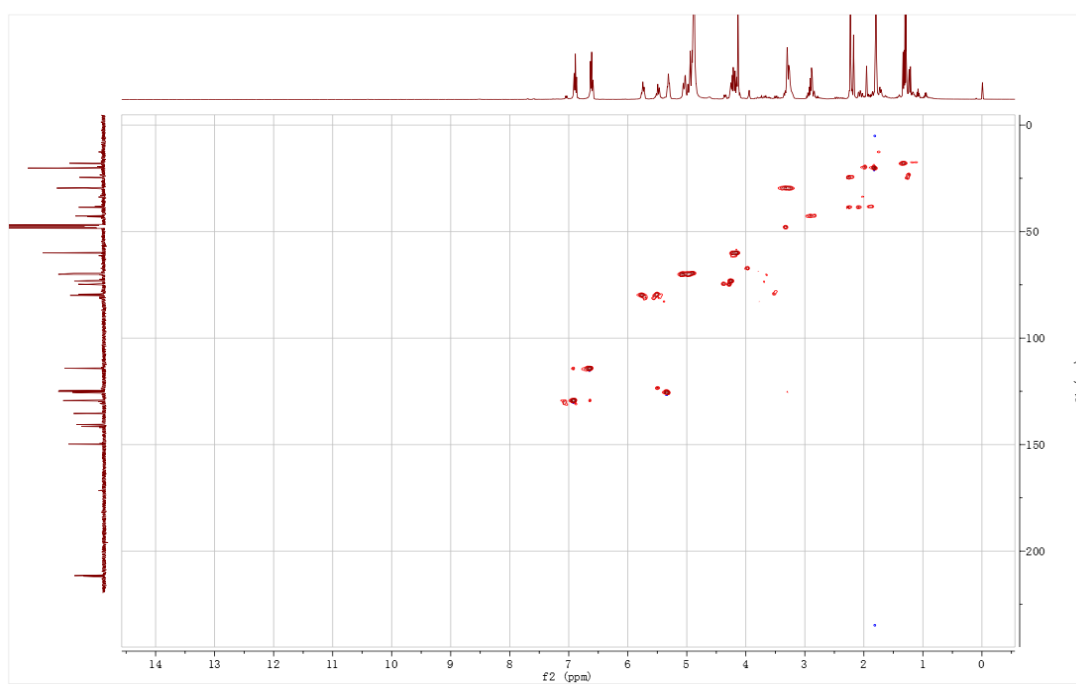


**Figure S30**  $^1\text{H}$  NMR (600 MHz,  $\text{CD}_3\text{OD}$ ) spectrum of the compounds **5/6**

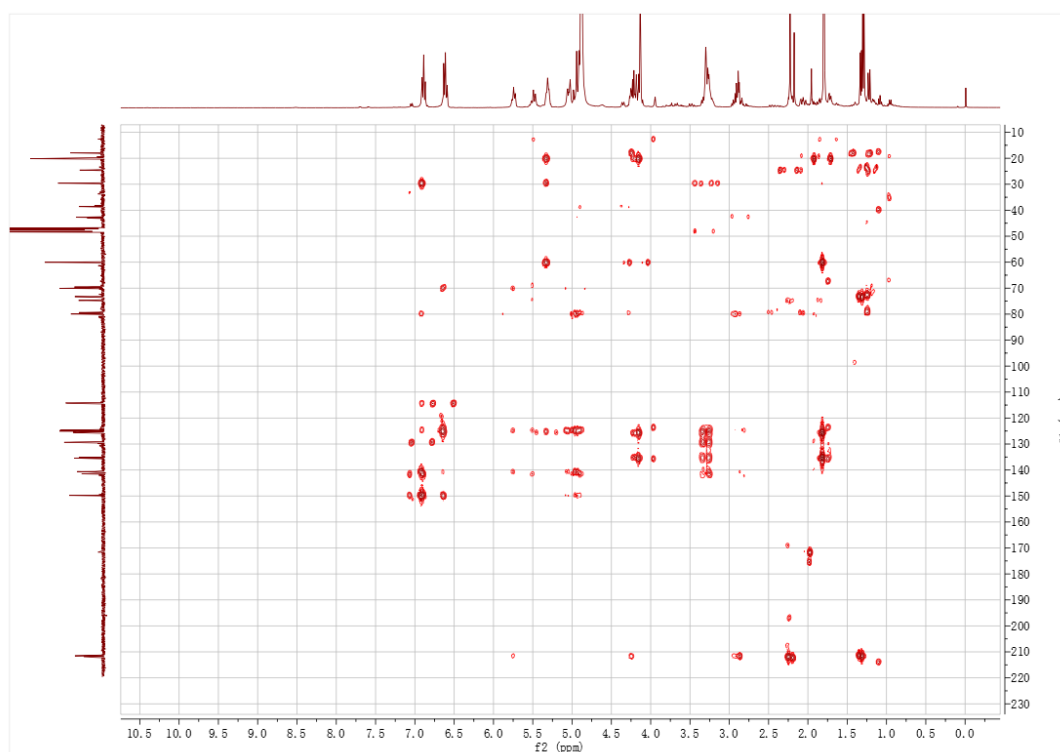




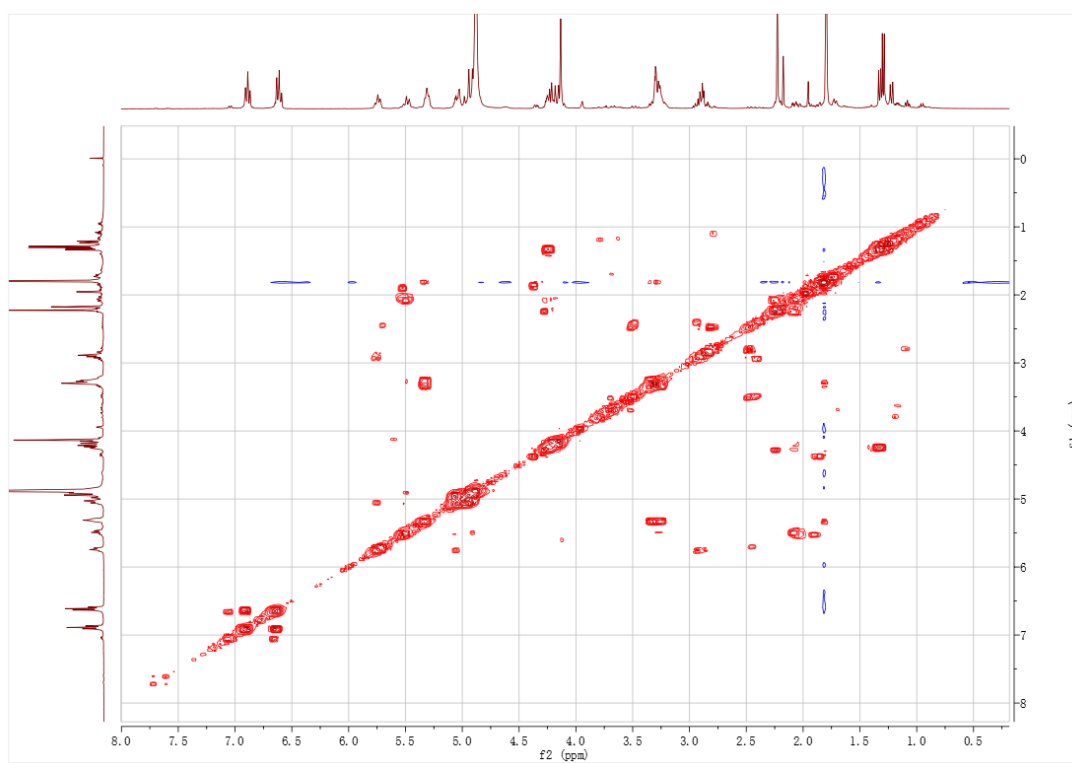
**Figure S31**  $^{13}\text{C}$  NMR (150 MHz,  $\text{CD}_3\text{OD}$ ) spectrum of the compounds **5/6**



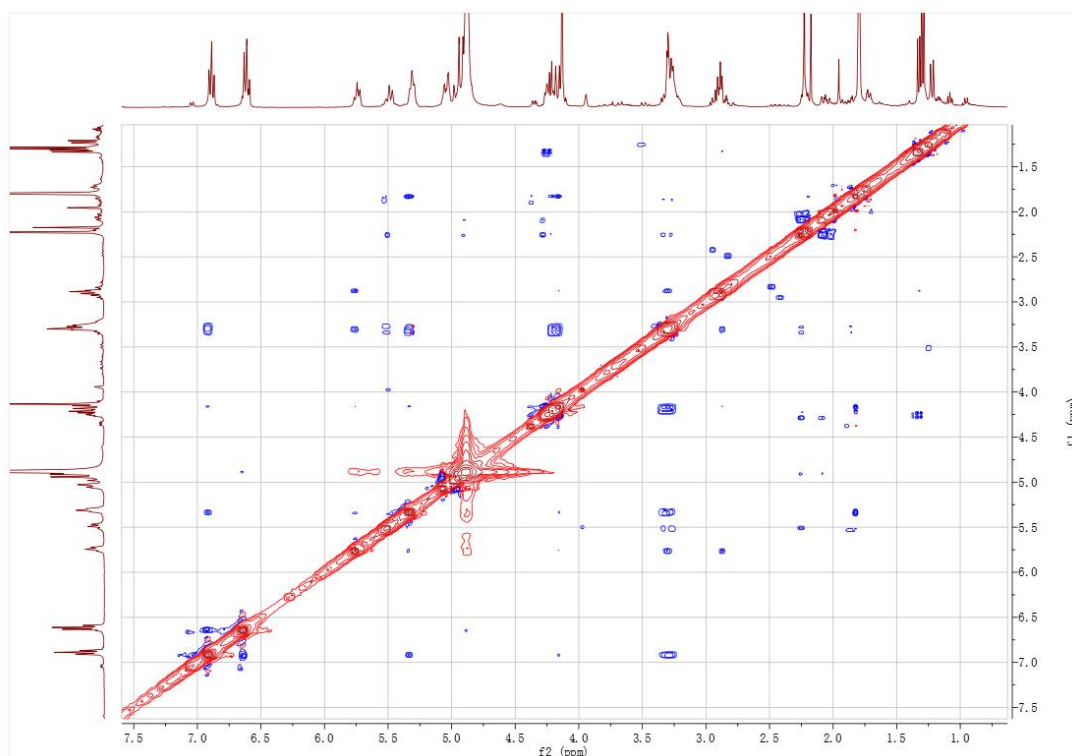
**Figure S32** HSQC spectrum of the compounds **5/6** ( $\text{CD}_3\text{OD}$ )



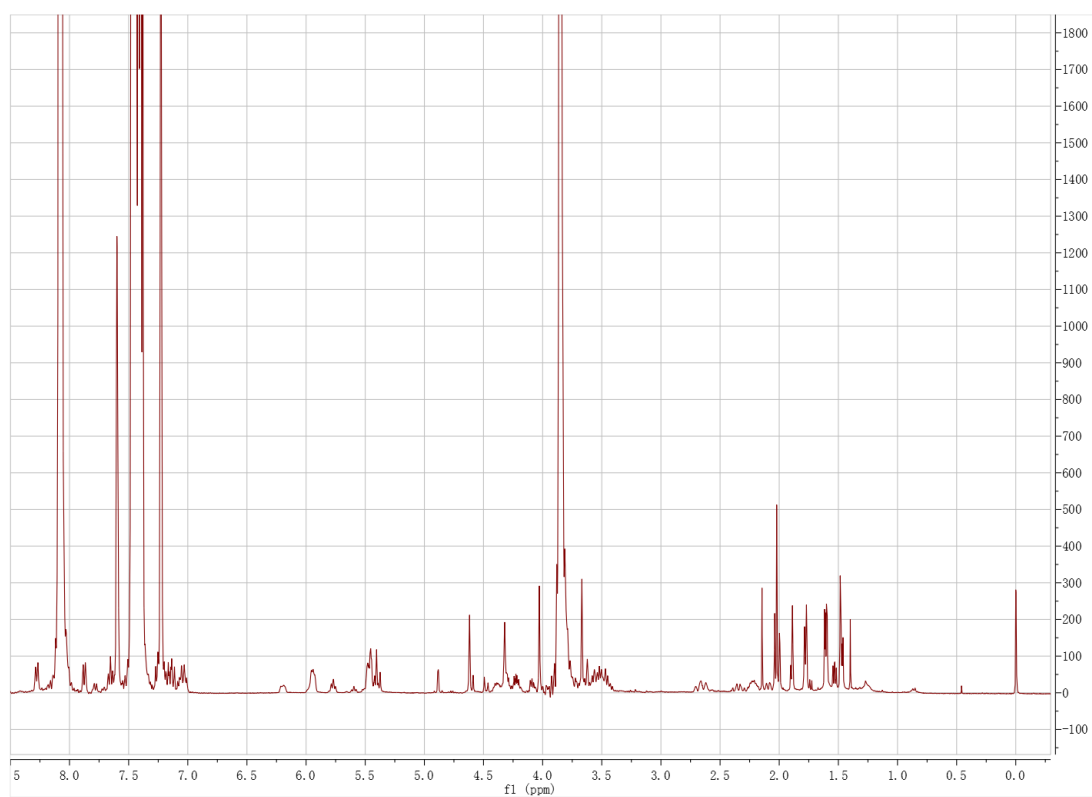
**Figure S33** HMBC spectrum of the compounds **5/6** (CD<sub>3</sub>OD)



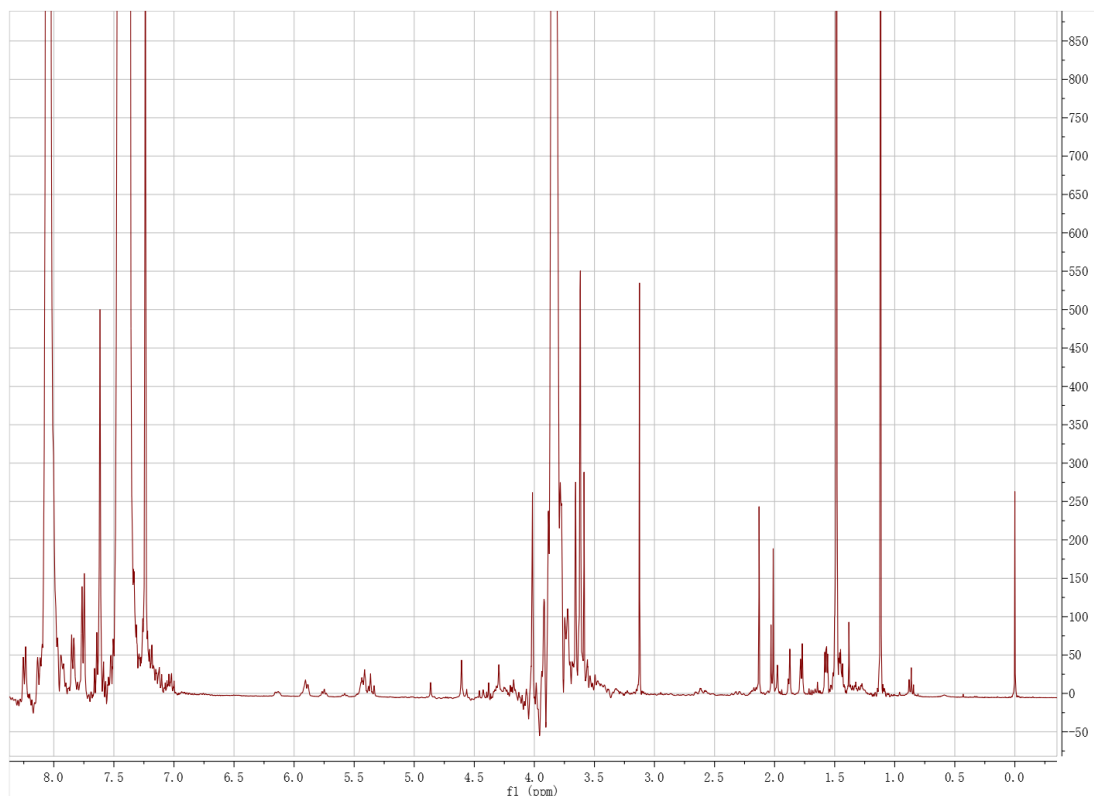
**Figure S34** COSY spectrum of the compounds **5/6** (CD<sub>3</sub>OD)



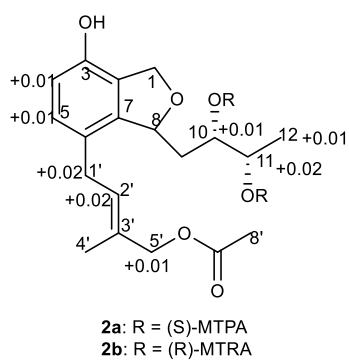
**Figure S35** NOESY spectrum of the compounds **5/6** ( $\text{CD}_3\text{OD}$ )



**Figure S36**  $^1\text{H}$  NMR spectrum of the compounds **2a** (400 MHz) ( $\text{pyridine-d}_6$ )



**Figure S37**  $^1\text{H}$  NMR spectrum of the compounds **2b** (400 MHz) (pyridine- $\text{d}_6$ )



**Figure S38.** The  $\Delta\delta$  ( $\delta S - \delta R$ ) values from the (*S*)- and (*R*)-MTPA esters of **2**.