

# Supporting Information

## **Phragmalin-type limonoids from the fruits of *Chukrasia tabularis* and their anti-inflammatory activity**

Shu-Jun Dai <sup>1</sup>, Yu-Zhen Wu <sup>1</sup>, Xiu-Juan Xin <sup>1</sup> and Fa-Liang An <sup>1,2\*</sup>

<sup>1</sup> State Key Laboratory of Bioreactor Engineering, East China University of Science and Technology, 130 Meilong Road, Shanghai 200237, China

<sup>2</sup> Marine Biomedical Science and Technology Innovation Platform of Lin-gang Special Area, No.4, Lane 218, Haiji Sixth Road, Shanghai 201306, China

\*Correspondence: [flan2016@ecust.edu.cn](mailto:flan2016@ecust.edu.cn); Tel.: +86-21-6425-3823

# Contents

- Figure S1.  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) spectrum of compound **1**  
Figure S2.  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ ) spectrum of compound **1**  
Figure S3. HSQC spectrum of compound **1** in  $\text{CDCl}_3$   
Figure S4.  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of compound **1** in  $\text{CDCl}_3$   
Figure S5. HMBC spectrum of compound **1** in  $\text{CDCl}_3$   
Figure S6. ROESY spectrum of compound **1** in  $\text{CDCl}_3$   
Figure S7. HRESIMS spectrum of compound **1**  
Figure S8.  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) spectrum of compound **2**  
Figure S9.  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ ) spectrum of compound **2**  
Figure S10. HSQC spectrum of compound **2** in  $\text{CDCl}_3$   
Figure S11.  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of compound **2** in  $\text{CDCl}_3$   
Figure S12. HMBC spectrum of compound **2** in  $\text{CDCl}_3$   
Figure S13. ROESY spectrum of compound **2** in  $\text{CDCl}_3$   
Figure S14. HRESIMS spectrum of compound **2**  
Figure S15.  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) spectrum of compound **3**  
Figure S16.  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ ) spectrum of compound **3**  
Figure S17. HSQC spectrum of compound **3** in  $\text{CDCl}_3$   
Figure S18.  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of compound **3** in  $\text{CDCl}_3$   
Figure S19. HMBC spectrum of compound **3** in  $\text{CDCl}_3$   
Figure S20. ROESY spectrum of compound **3** in  $\text{CDCl}_3$   
Figure S21. HRESIMS spectrum of compound **3**  
Figure S22.  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) spectrum of compound **4**  
Figure S23.  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ ) spectrum of compound **4**  
Figure S24. HSQC spectrum of compound **4** in  $\text{CDCl}_3$   
Figure S25.  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of compound **4** in  $\text{CDCl}_3$   
Figure S26. HMBC spectrum of compound **4** in  $\text{CDCl}_3$   
Figure S27. ROESY spectrum of compound **4** in  $\text{CDCl}_3$   
Figure S28. HRESIMS spectrum of compound **4**  
Figure S29.  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) spectrum of compound **5**  
Figure S30.  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ ) spectrum of compound **5**  
Figure S31. HSQC spectrum of compound **5** in  $\text{CDCl}_3$   
Figure S32.  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of compound **5** in  $\text{CDCl}_3$   
Figure S33. HMBC spectrum of compound **5** in  $\text{CDCl}_3$   
Figure S34. ROESY spectrum of compound **5** in  $\text{CDCl}_3$   
Figure S35. HRESIMS spectrum of compound **5**

Figure S1.  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) spectrum of compound **1**

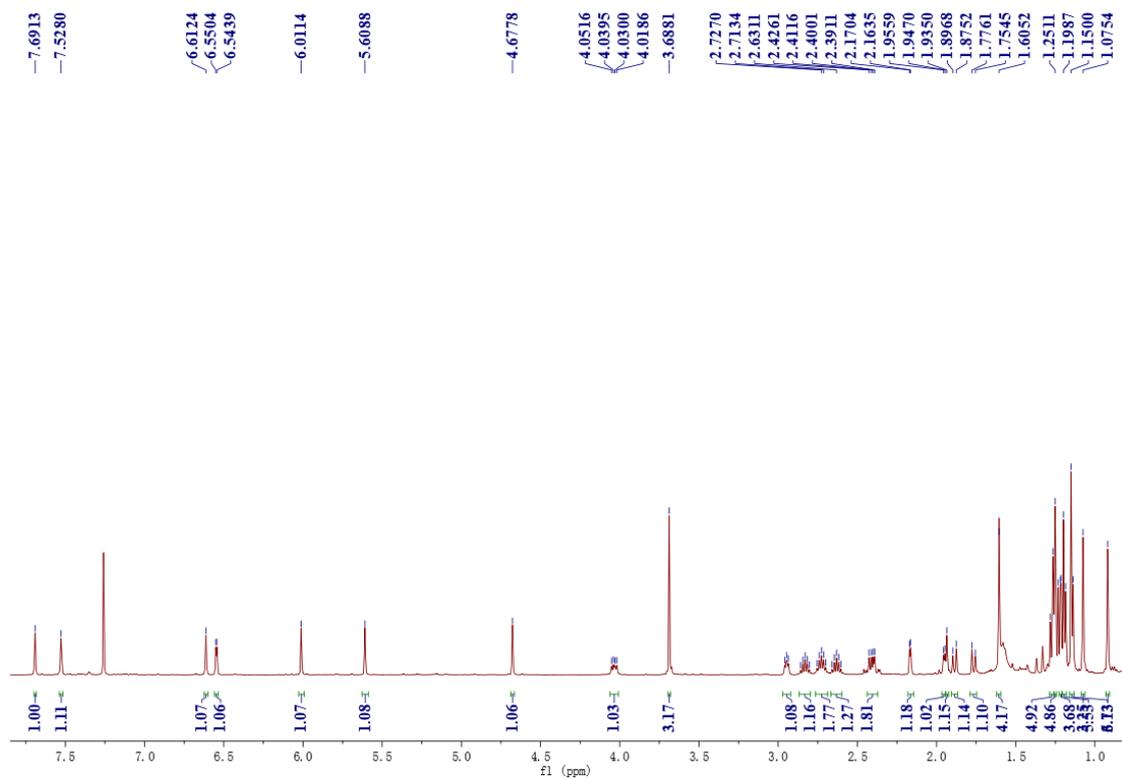


Figure S2.  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ ) spectrum of compound **1**

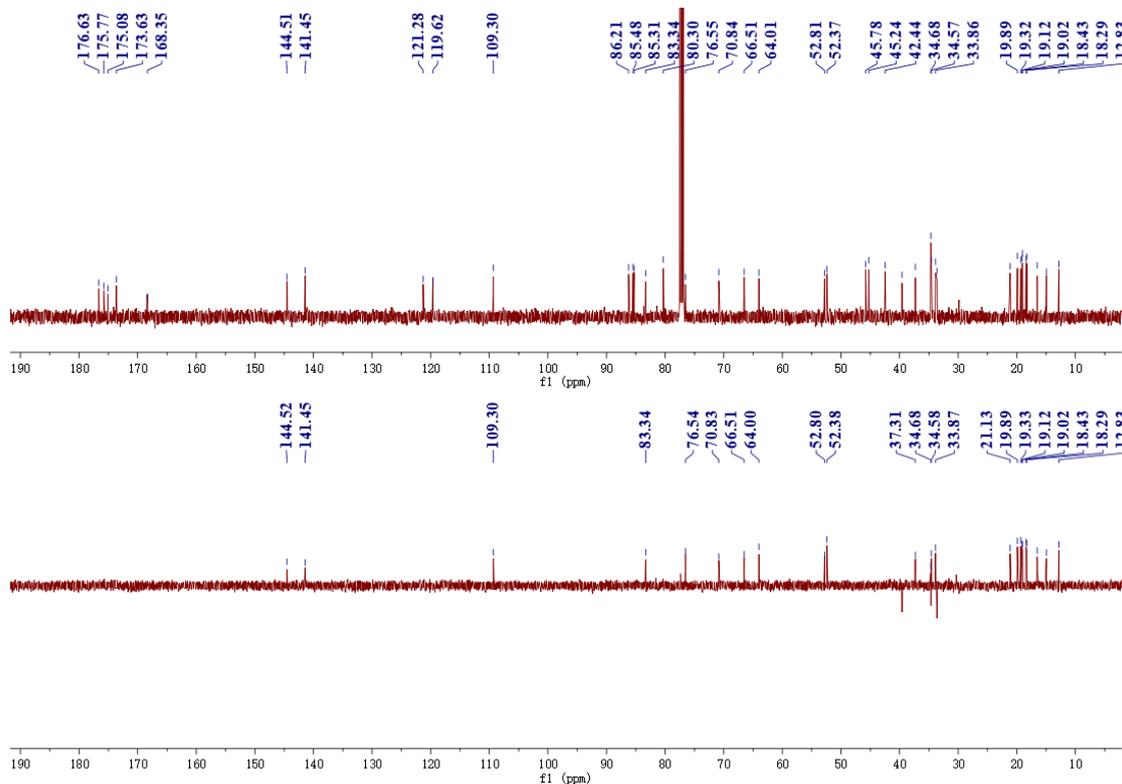


Figure S3. HSQC spectrum of compound **1** in CDCl<sub>3</sub>

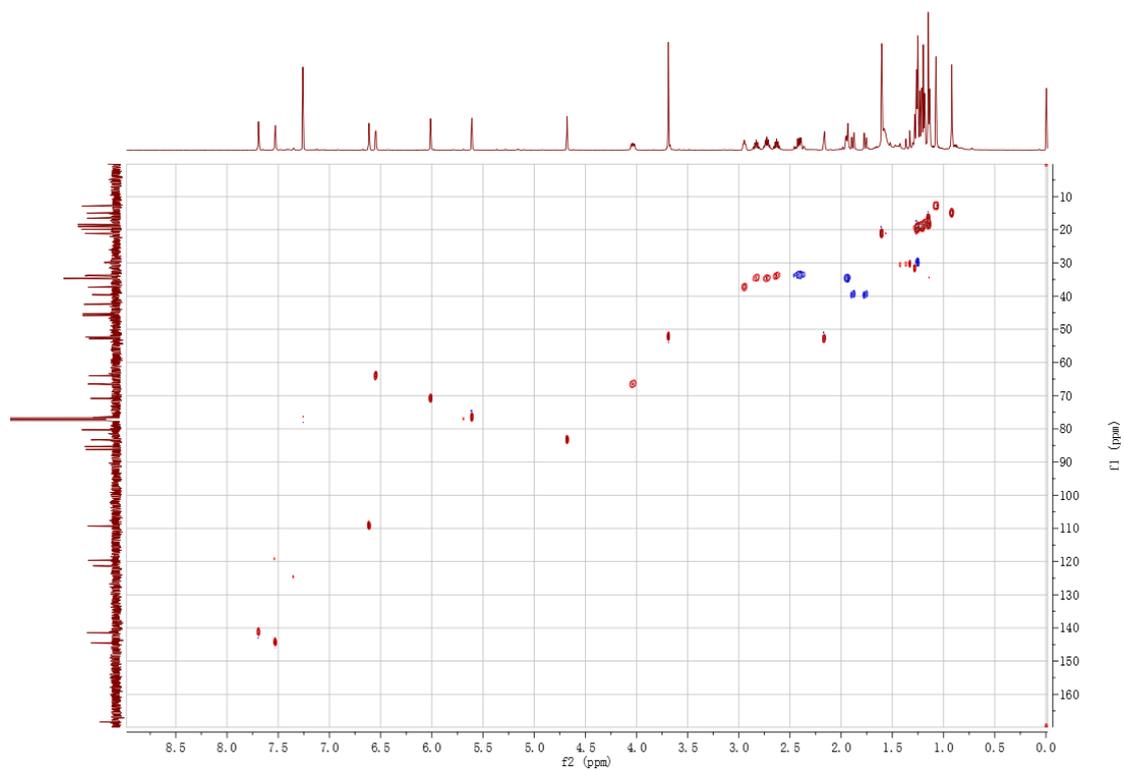


Figure S4. <sup>1</sup>H-<sup>1</sup>H COSY spectrum of compound **1** in CDCl<sub>3</sub>

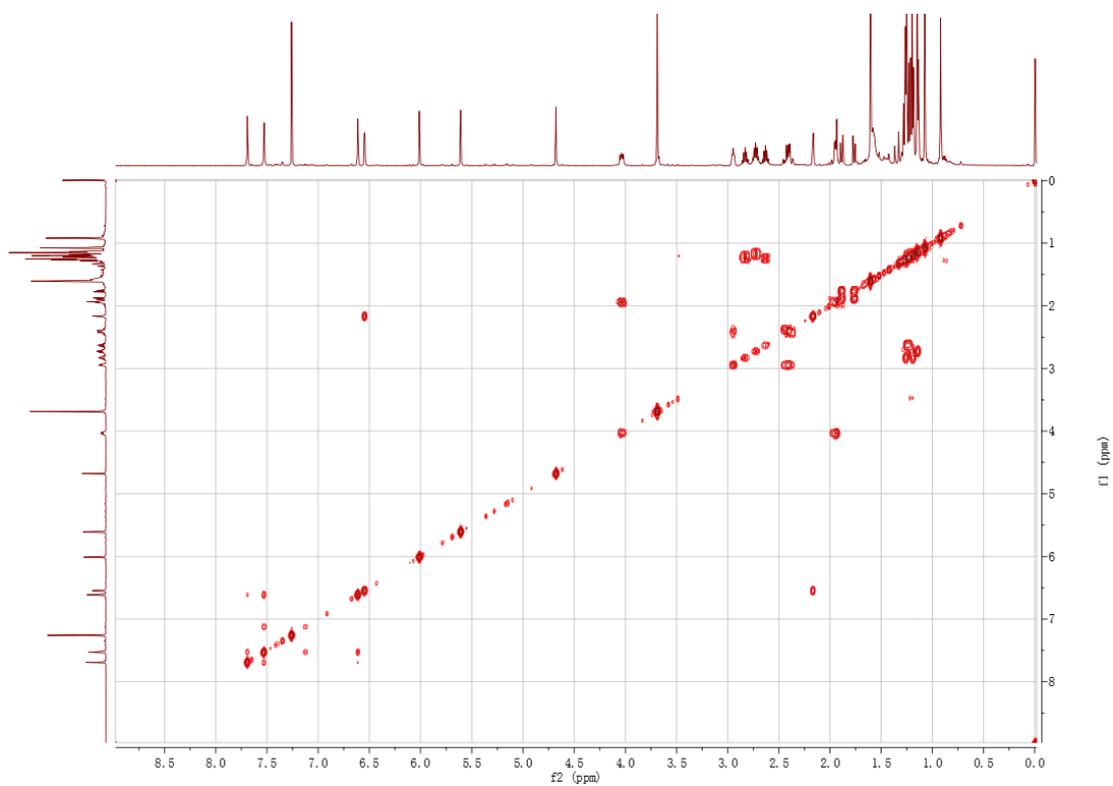


Figure S5. HMBC spectrum of compound **1** in CDCl<sub>3</sub>

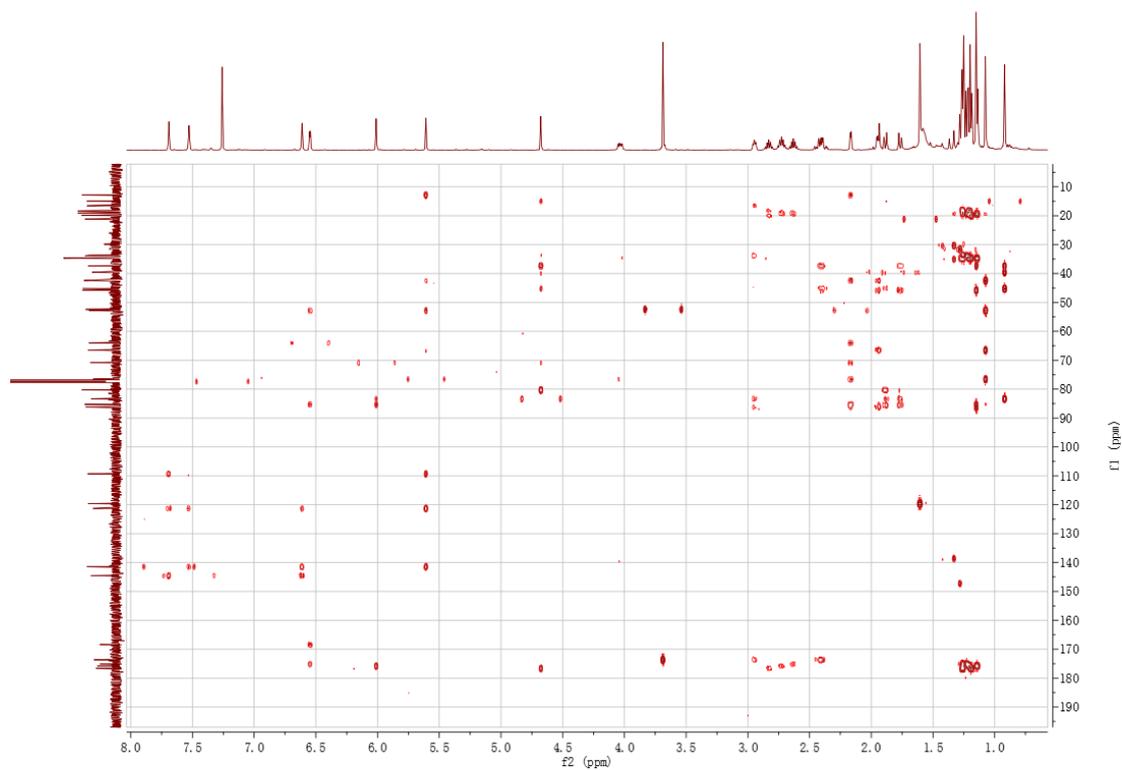


Figure S6. ROESY spectrum of compound **1** in CDCl<sub>3</sub>

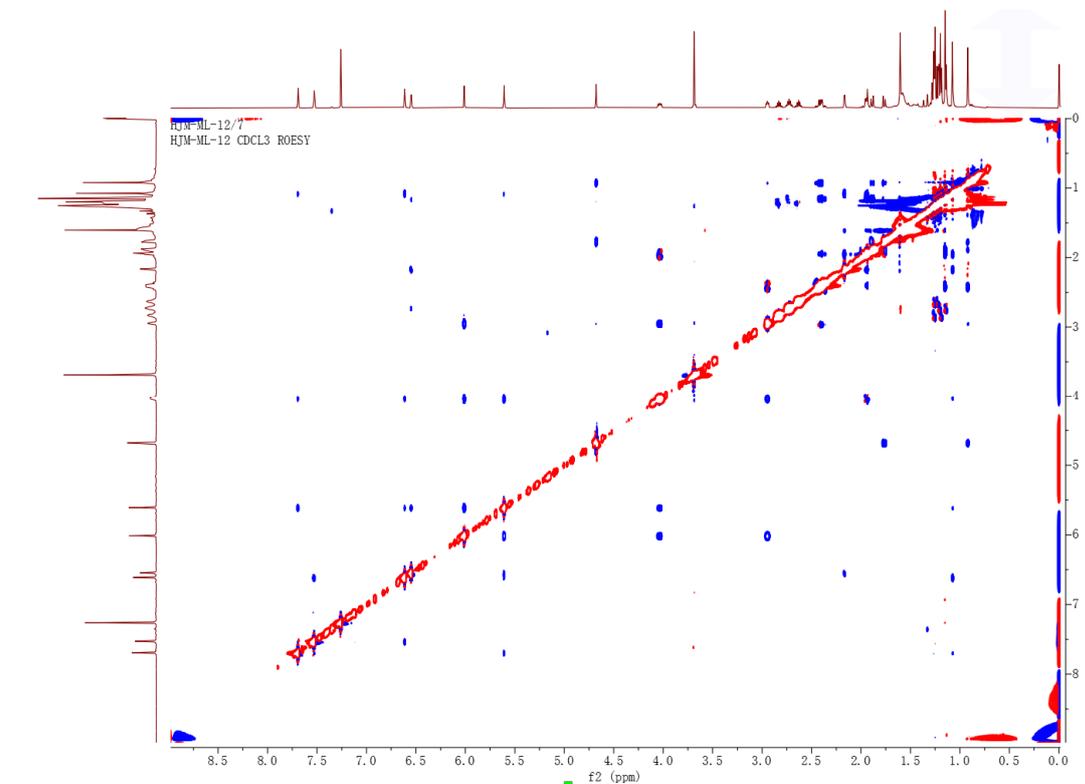


Figure S7. HRESIMS spectrum of compound 1

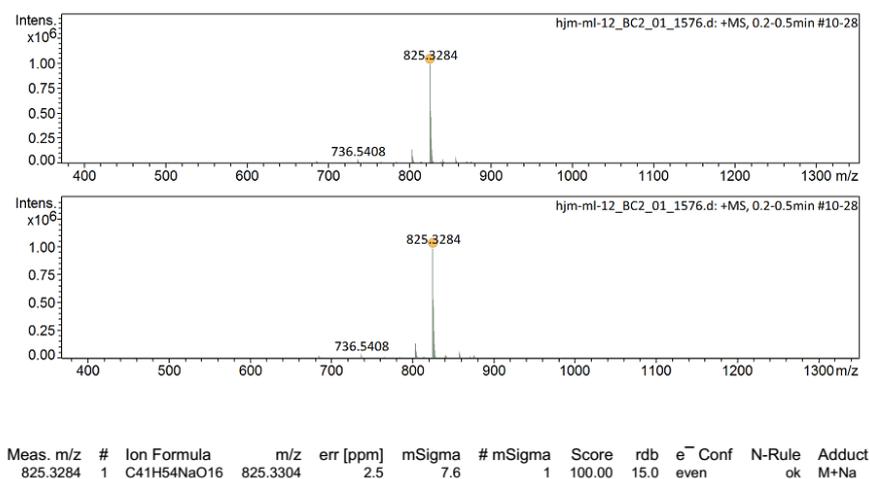


Figure S8. <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) spectrum of compound 2

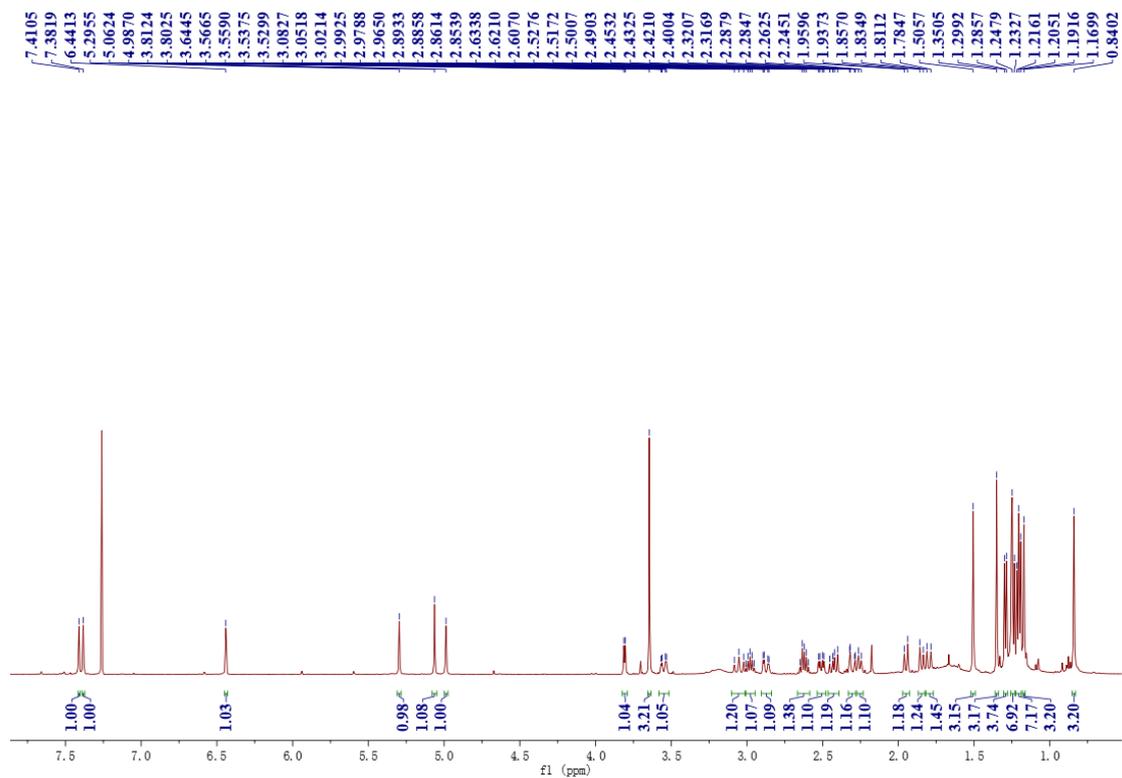


Figure S9.  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ ) spectrum of compound **2**

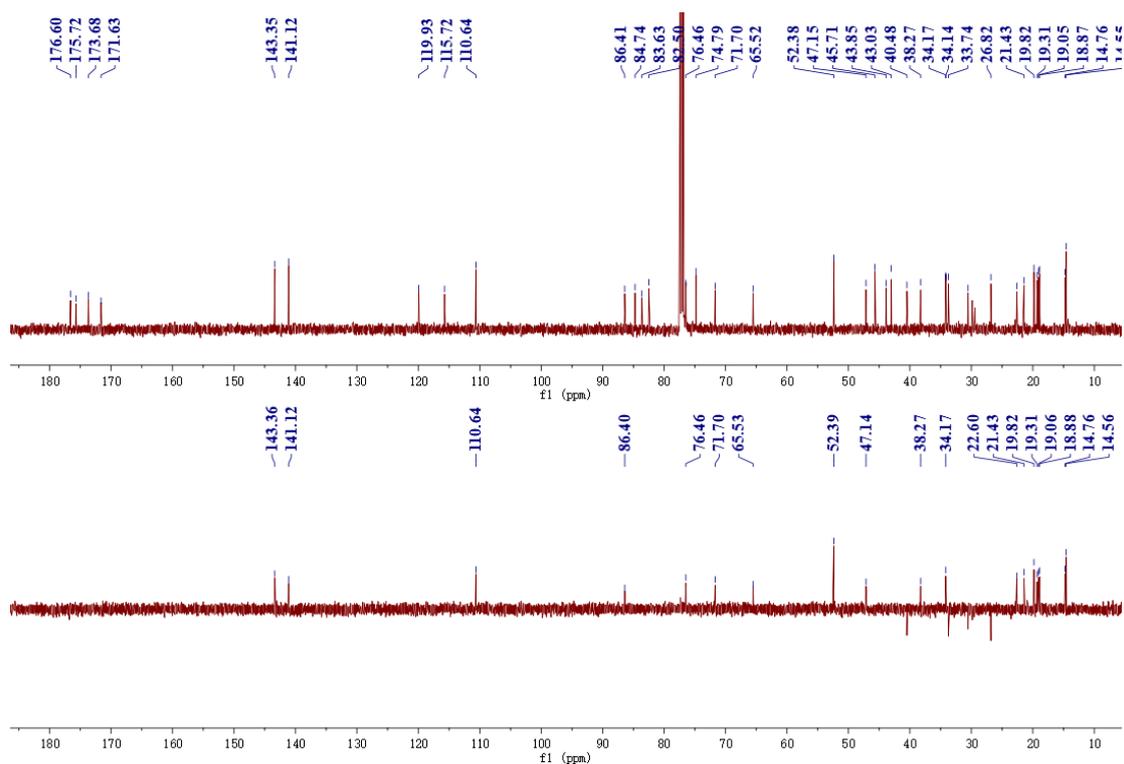


Figure S10. HSQC spectrum of compound **2** in  $\text{CDCl}_3$

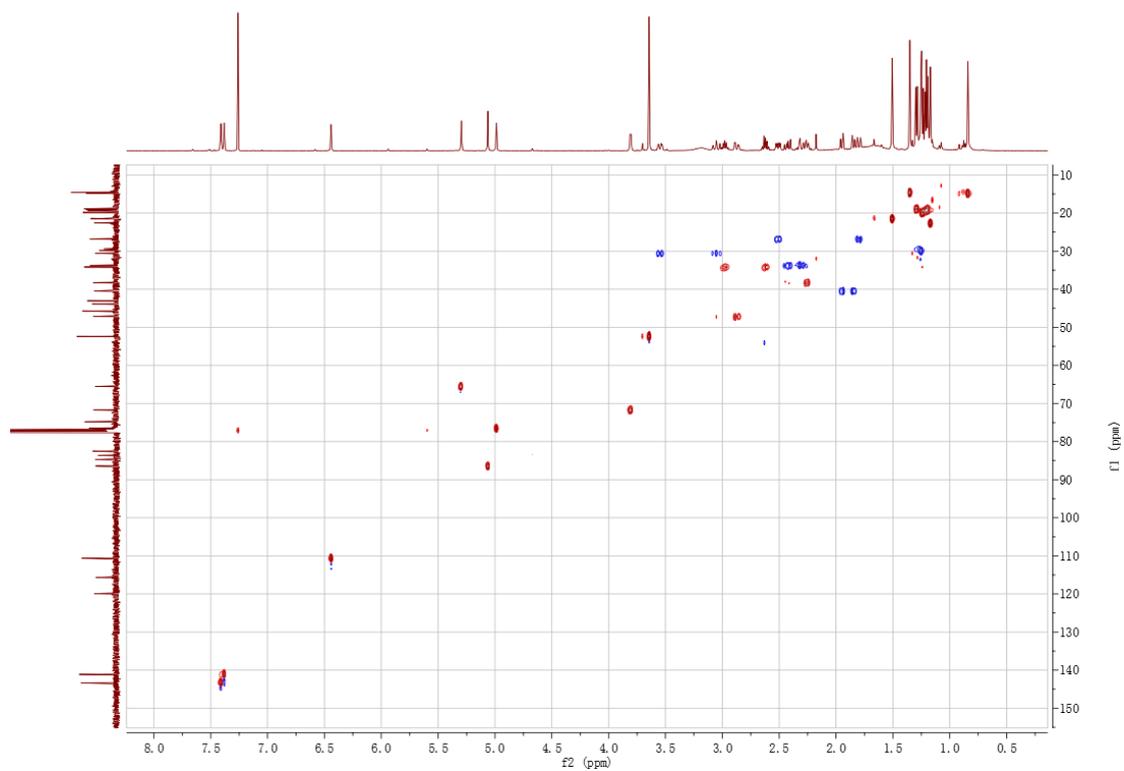


Figure S11.  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of compound **2** in  $\text{CDCl}_3$

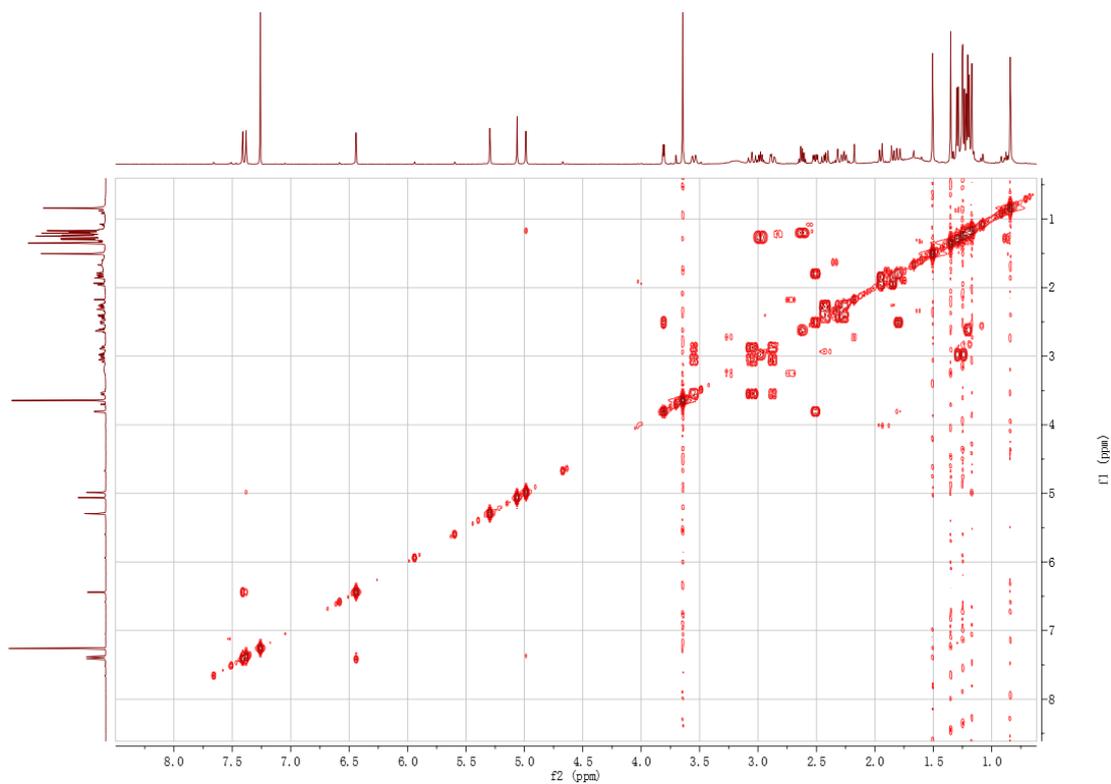


Figure S12. HMBC spectrum of compound **2** in  $\text{CDCl}_3$

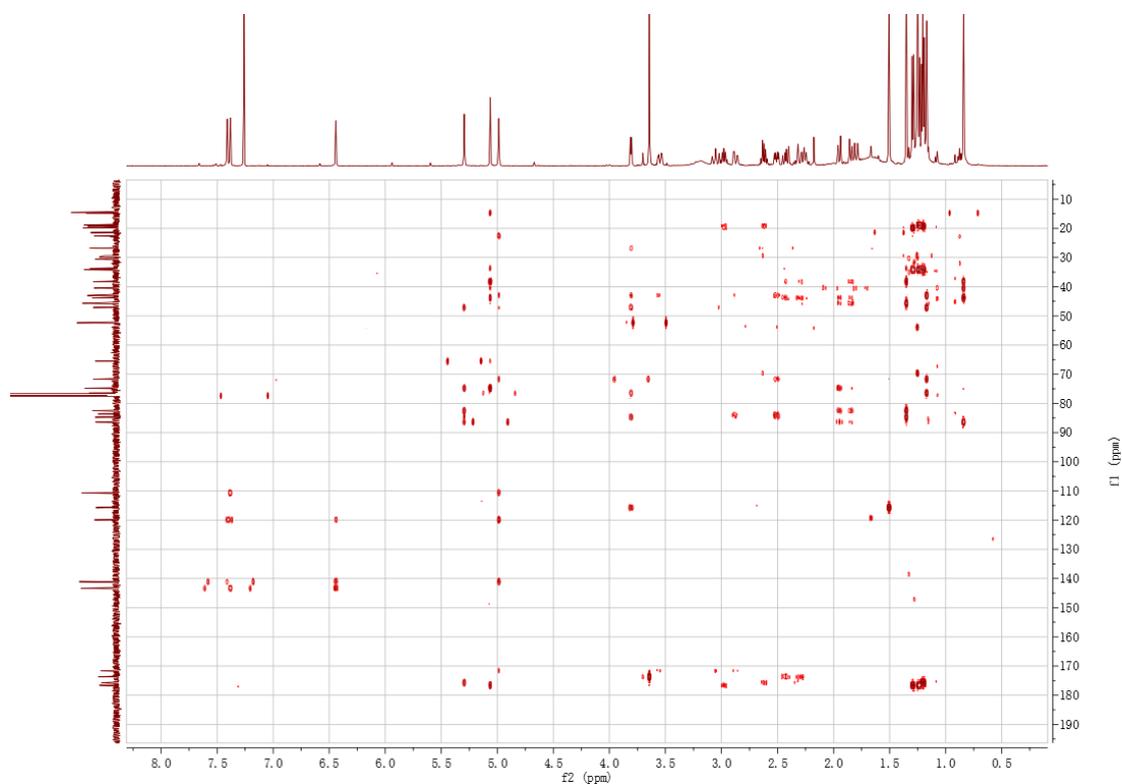


Figure S13. ROESY spectrum of compound 2 in CDCl<sub>3</sub>

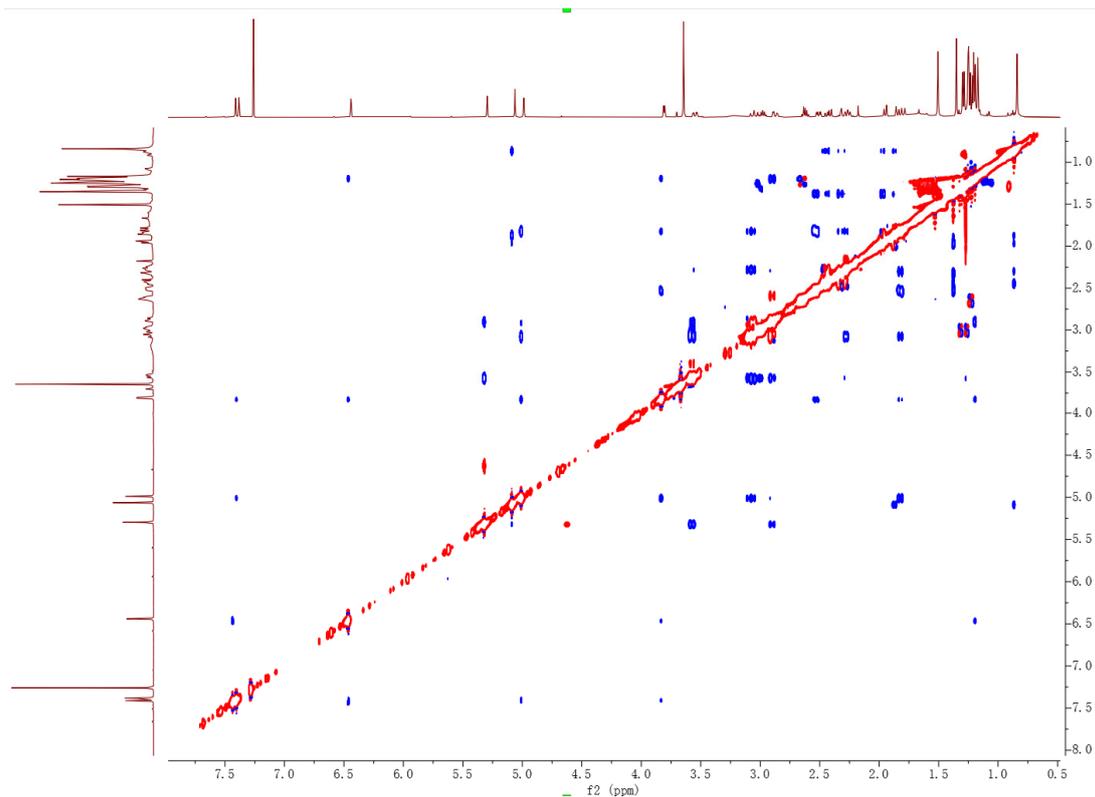
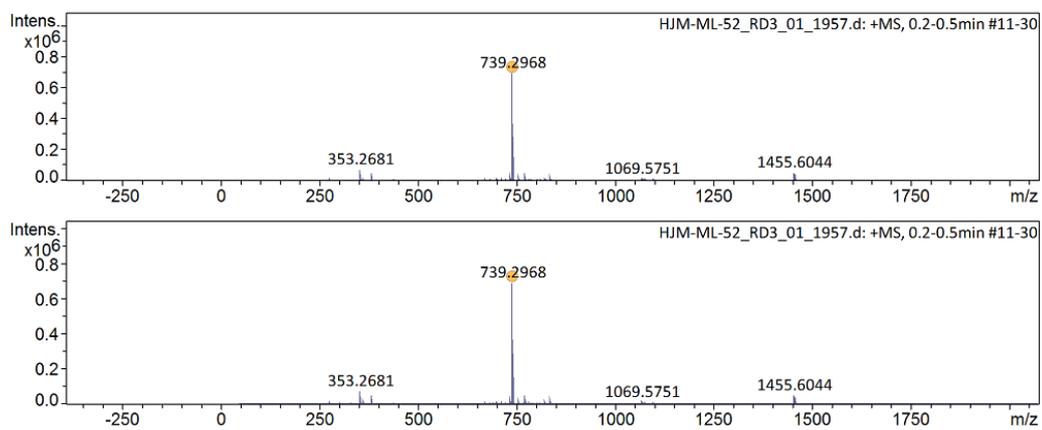


Figure S14. HRESI-MS spectrum of compound 2



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e <sup>-</sup> Conf	N-Rule	Adduct
739.2968	1	C <sub>37</sub> H <sub>48</sub> NaO <sub>14</sub>	739.2936	-4.2	3.1	1	100.00	14.0	even	ok	M+Na

Figure S15. <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) spectrum of compound 3

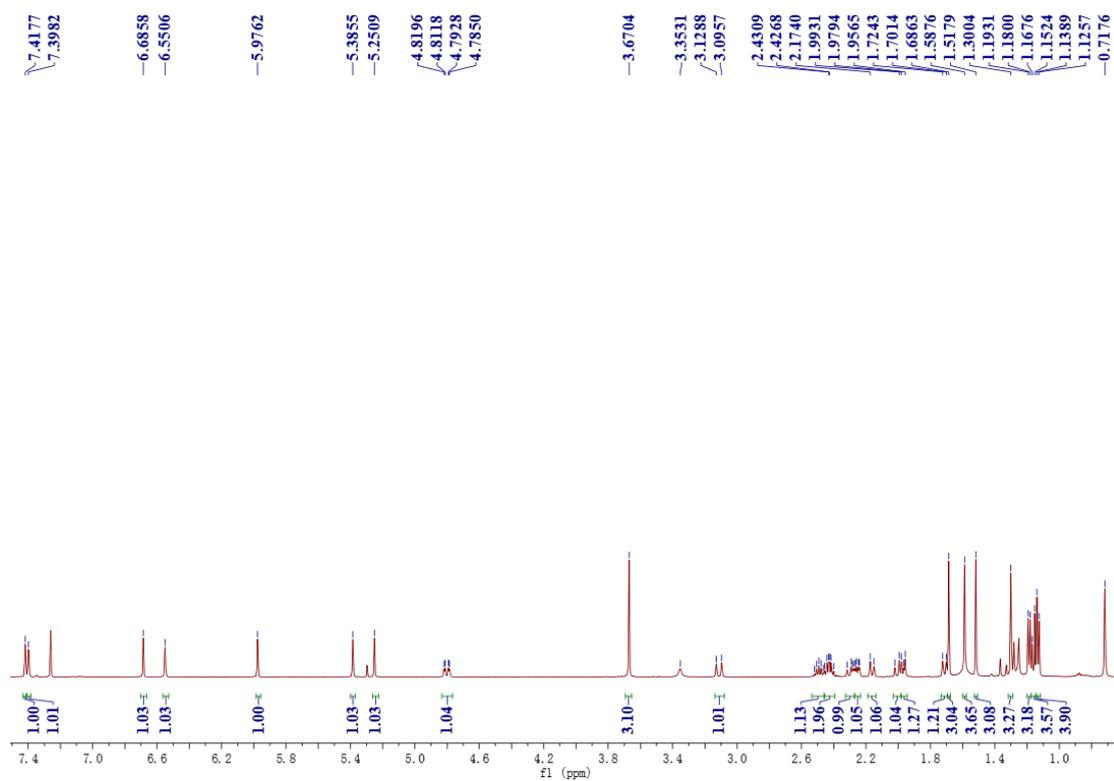


Figure S16. <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) spectrum of compound 3

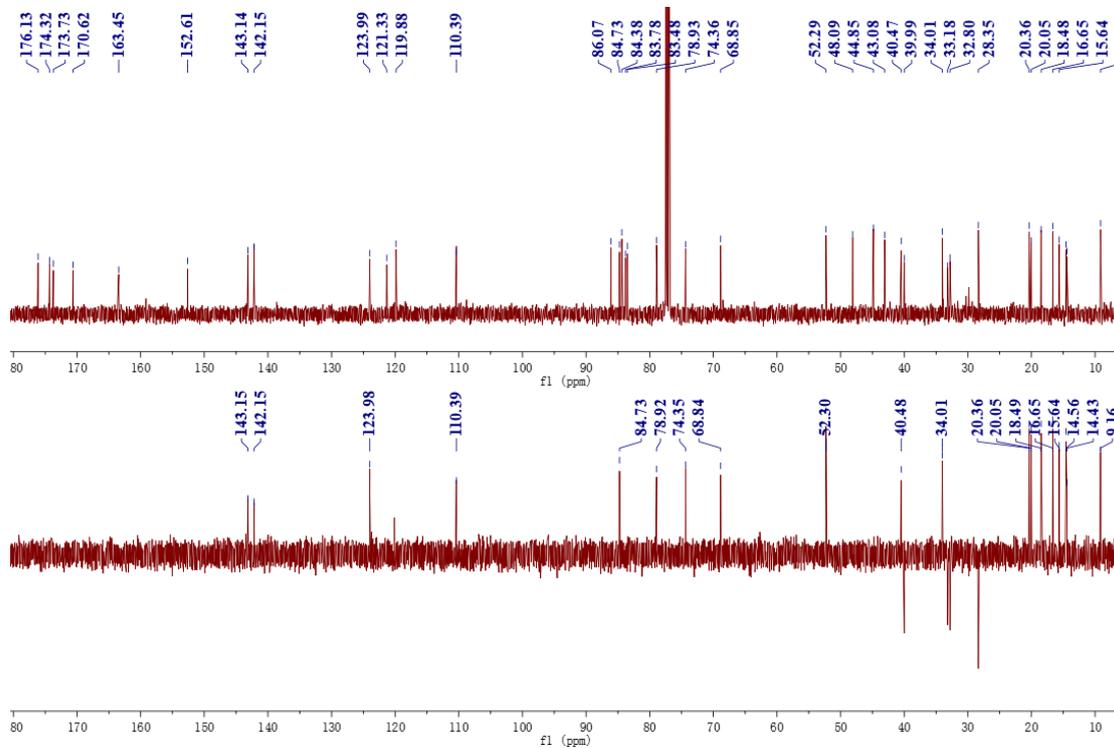


Figure S17. HSQC spectrum of compound 3 in CDCl<sub>3</sub>

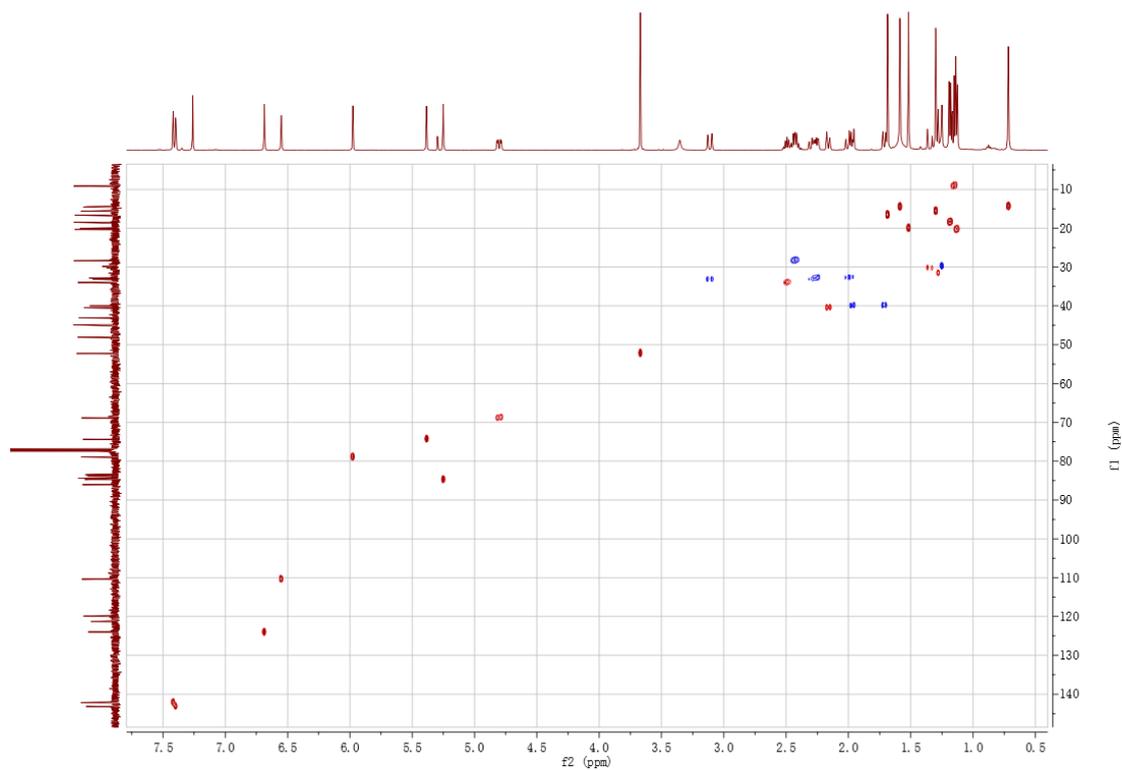


Figure S18. <sup>1</sup>H-<sup>1</sup>H COSY spectrum of compound 3 in CDCl<sub>3</sub>

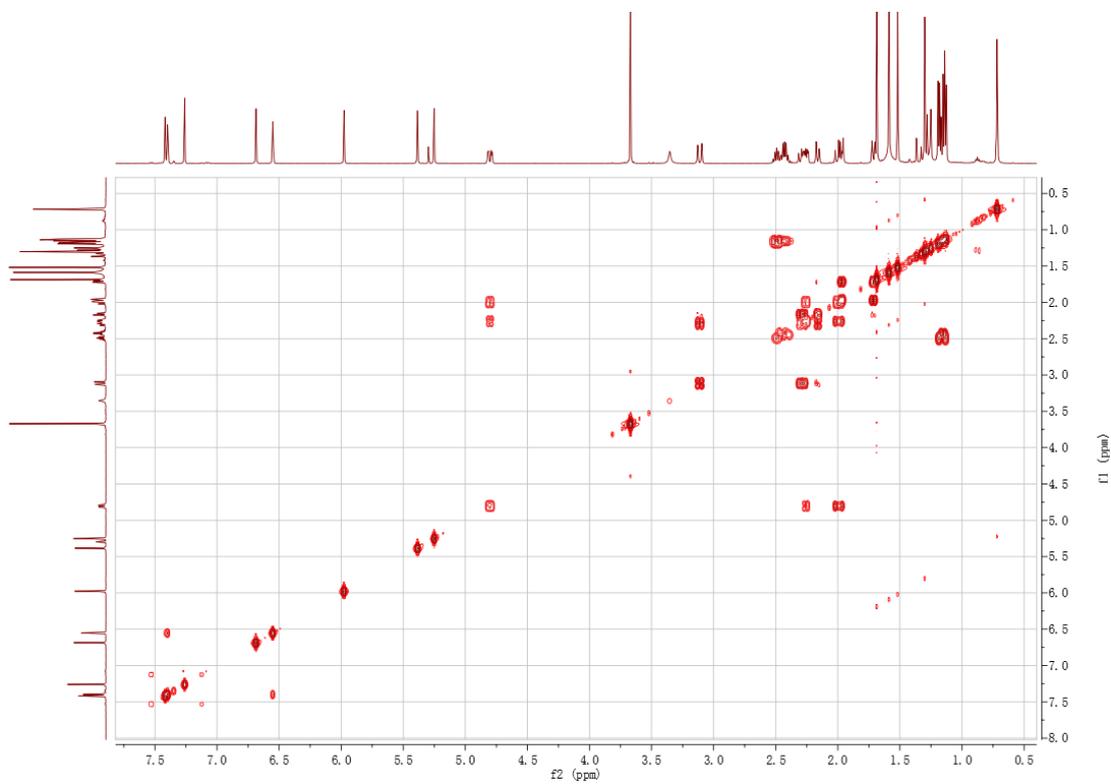


Figure S19. HMBC spectrum of compound 3 in CDCl<sub>3</sub>

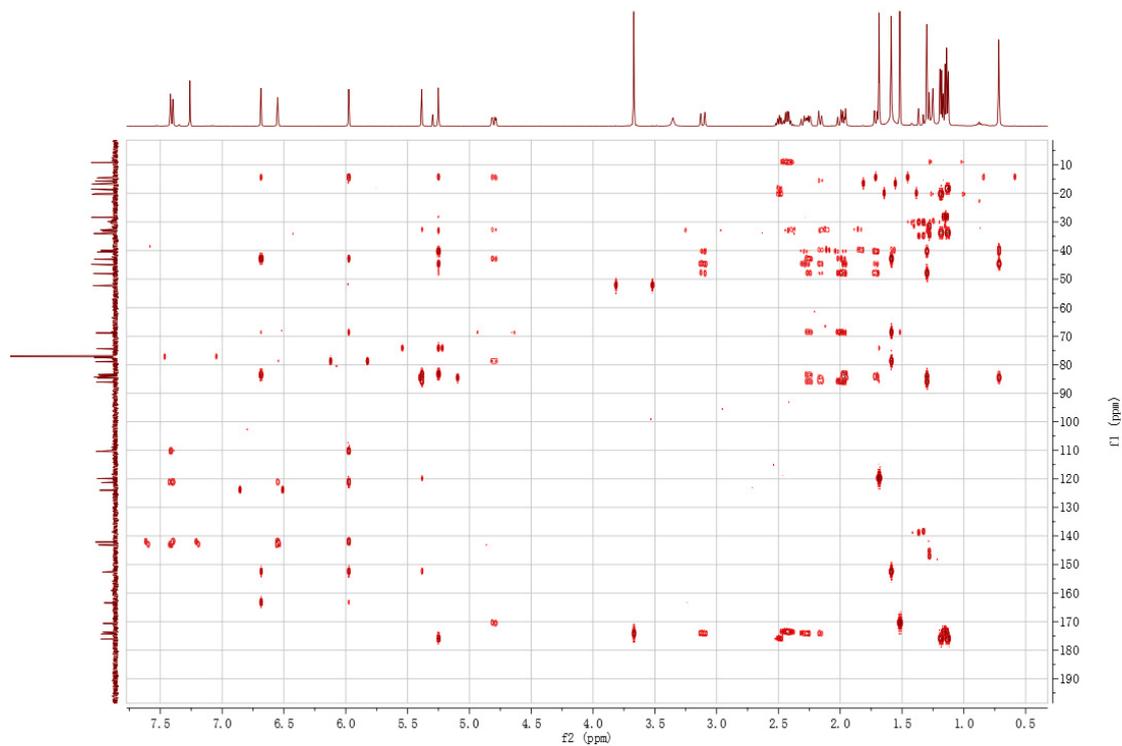


Figure S20. ROESY spectrum of compound 3 in CDCl<sub>3</sub>

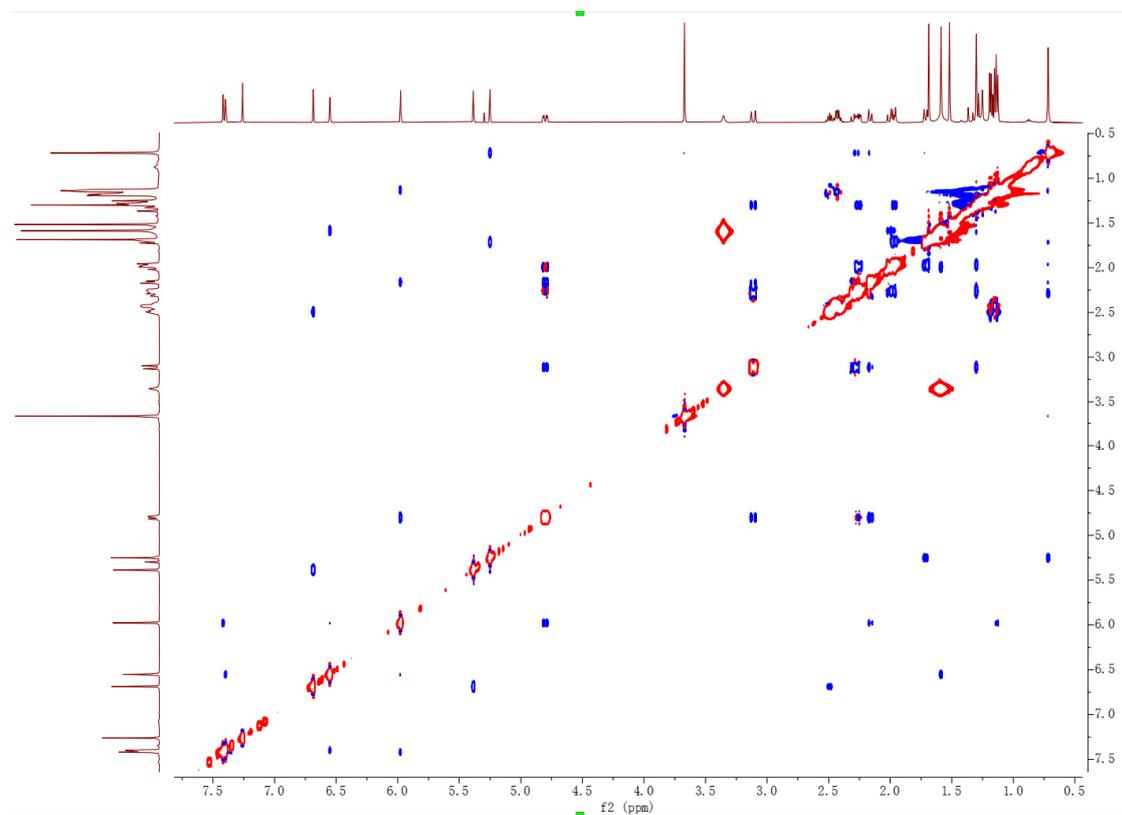
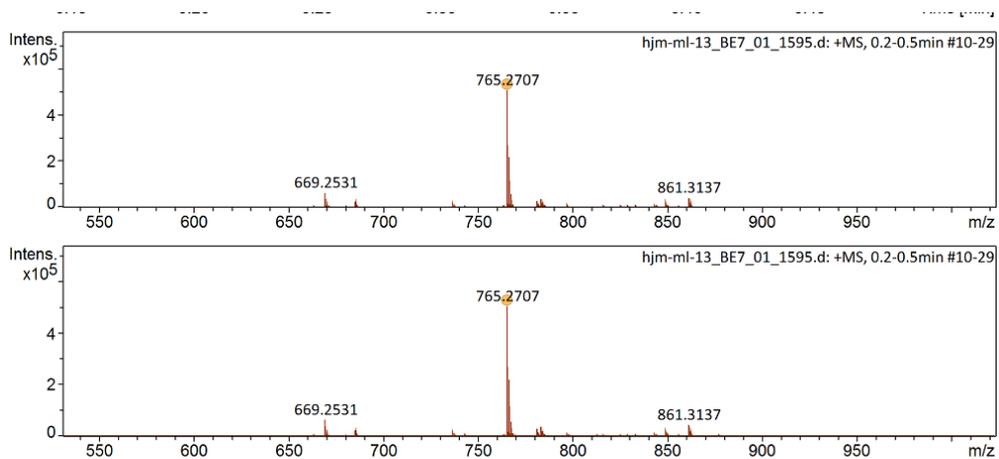


Figure S21. HRESI-MS spectrum of compound 3



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e <sup>-</sup> Conf	N-Rule	Adduct
765.2707	1	C38H46NaO15	765.2729	2.8	4.8	1	100.00	16.0	even	ok	M+Na

Figure S22. <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) spectrum of compound 4

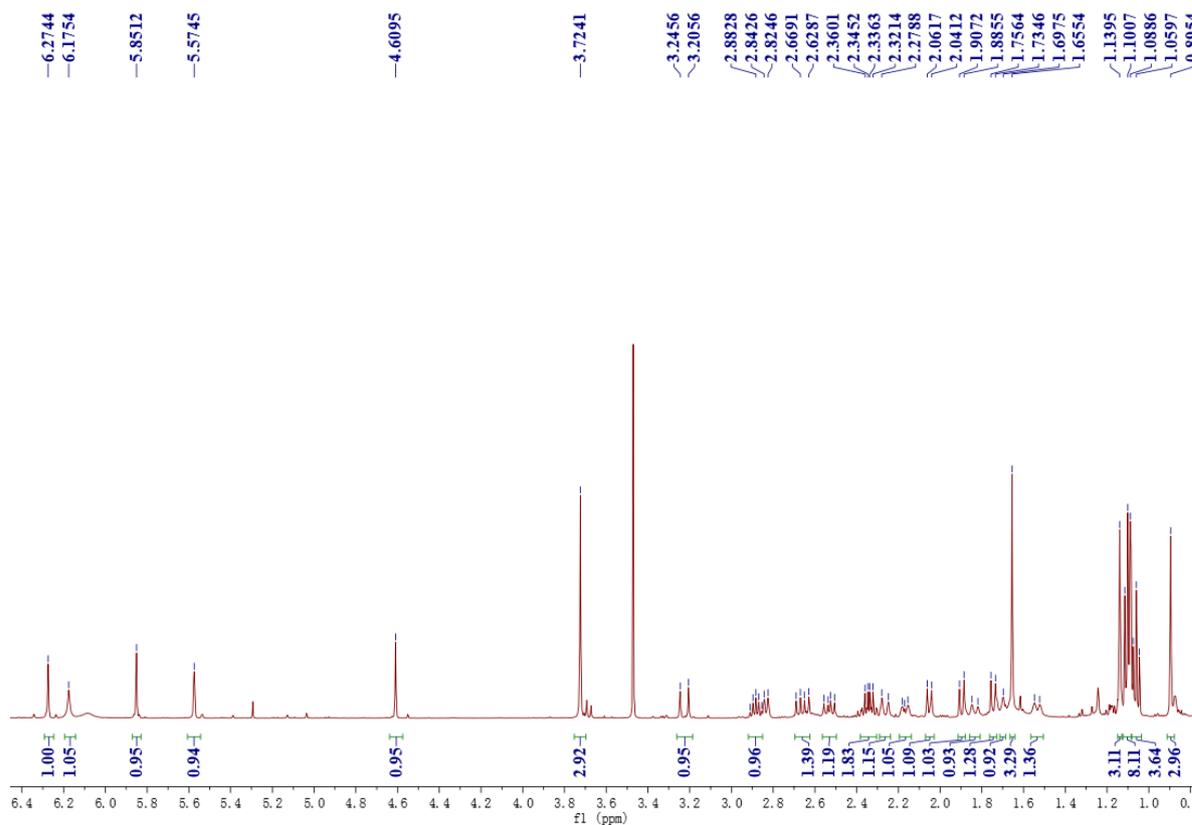


Figure S23.  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ ) spectrum of compound 4

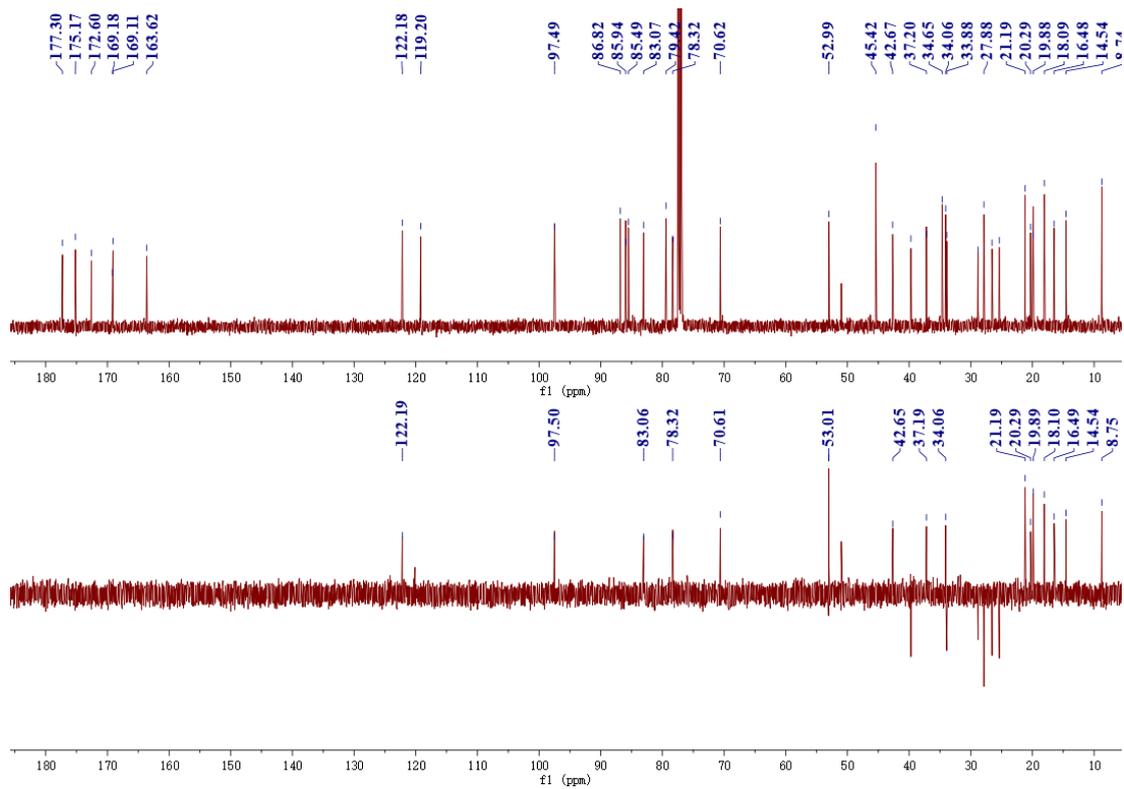


Figure S24. HSQC spectrum of compound 4 in  $\text{CDCl}_3$

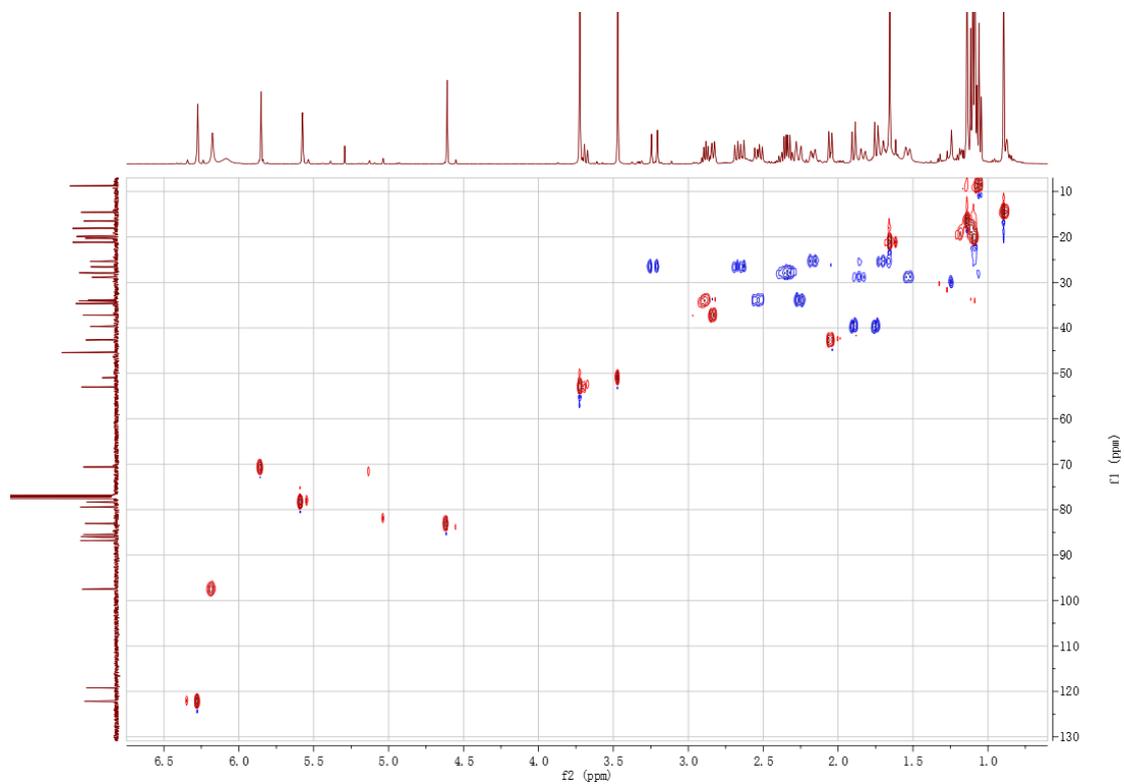


Figure S25.  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of compound **4** in  $\text{CDCl}_3$

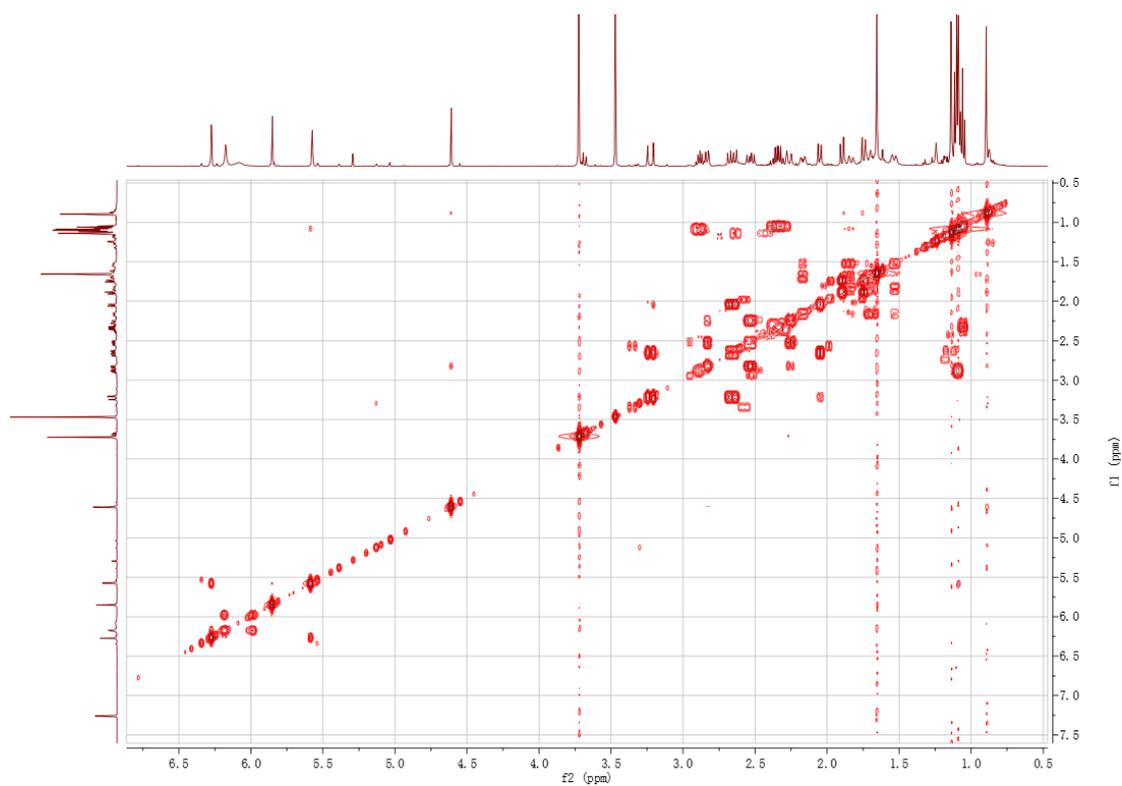


Figure S26. HMBC spectrum of compound **4** in  $\text{CDCl}_3$

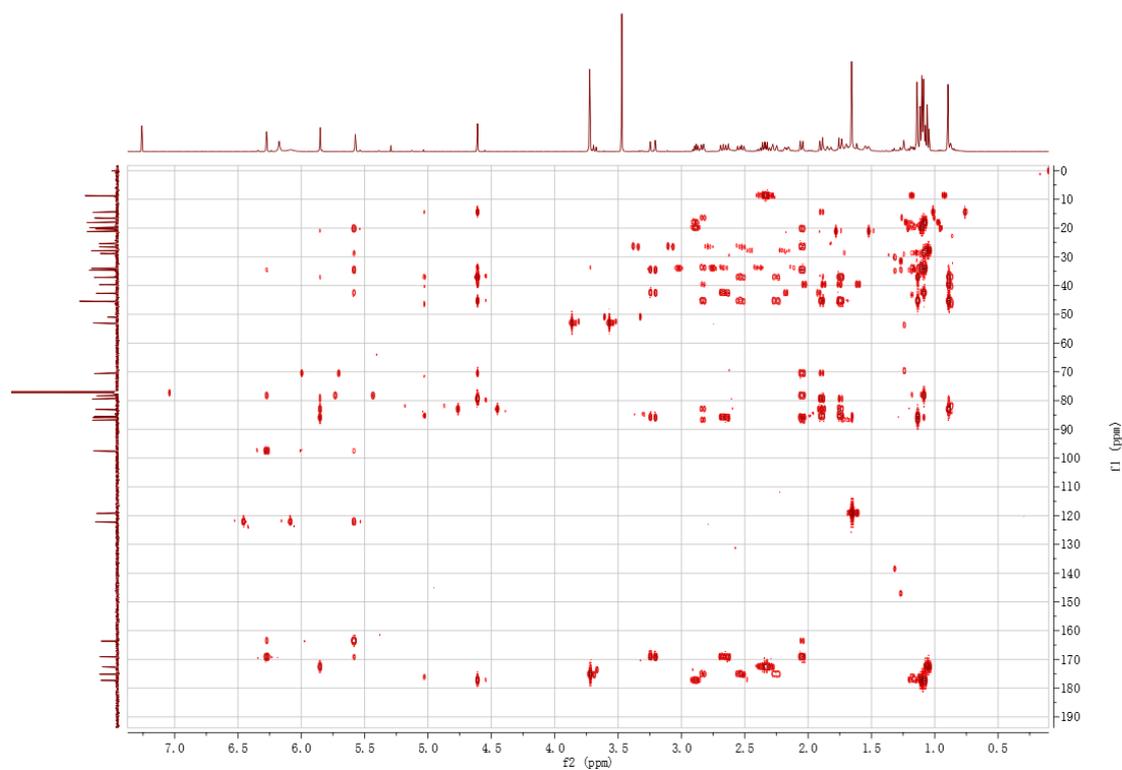


Figure S27. ROESY spectrum of compound 4 in CDCl<sub>3</sub>

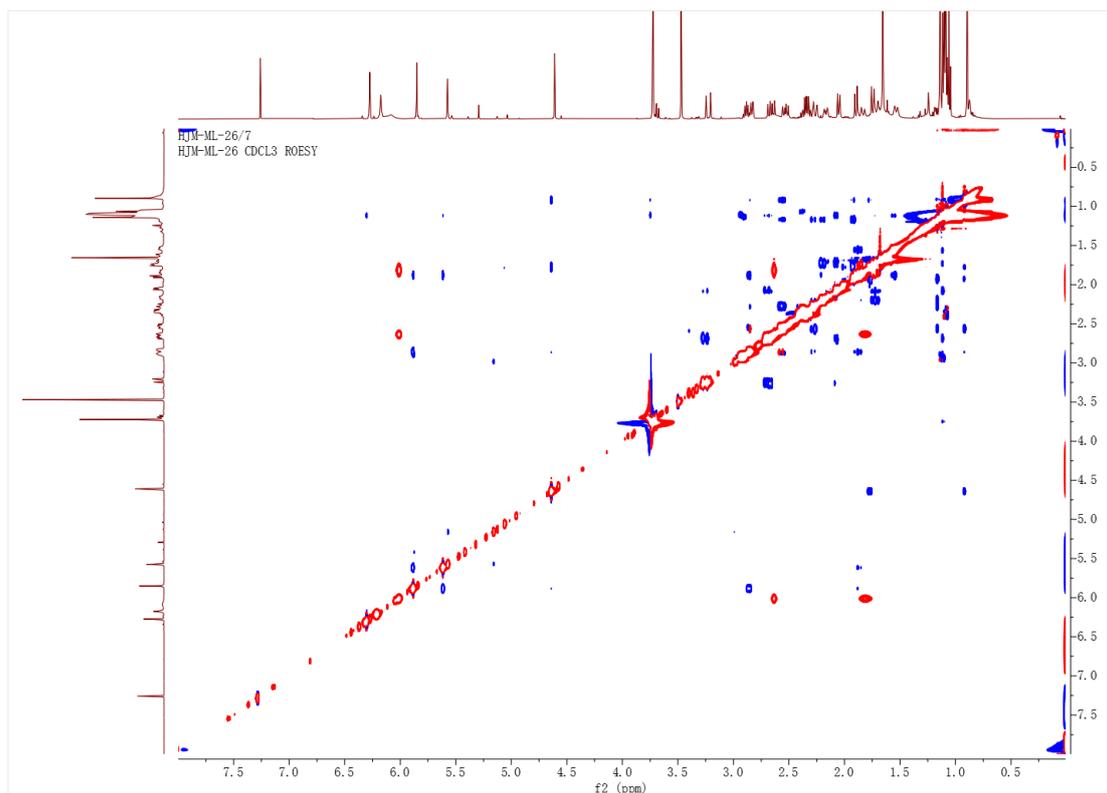
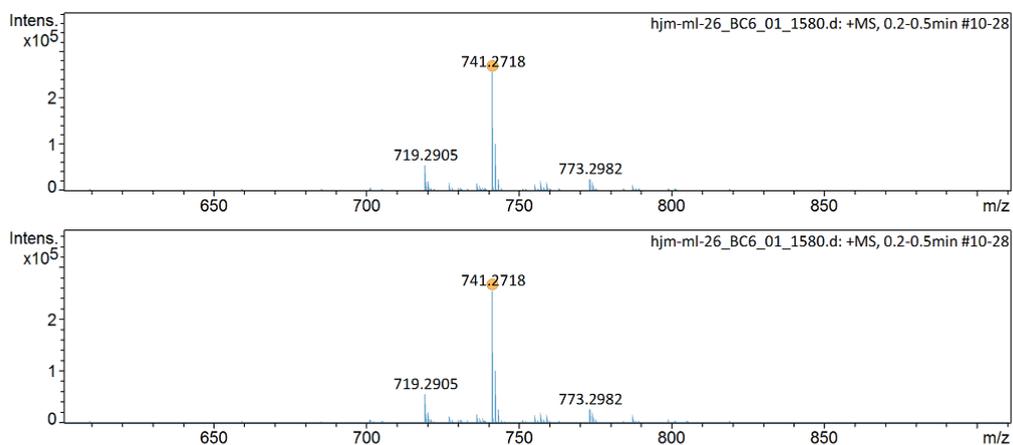


Figure S28. HRESI-MS spectrum of compound 4



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e <sup>-</sup> Conf	N-Rule	Adduct
741.2718	1	C <sub>36</sub> H <sub>46</sub> NaO <sub>15</sub>	741.2729	1.5	5.0	1	100.00	14.0	even	ok	M+Na

Figure S29. <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) spectrum of compound 5

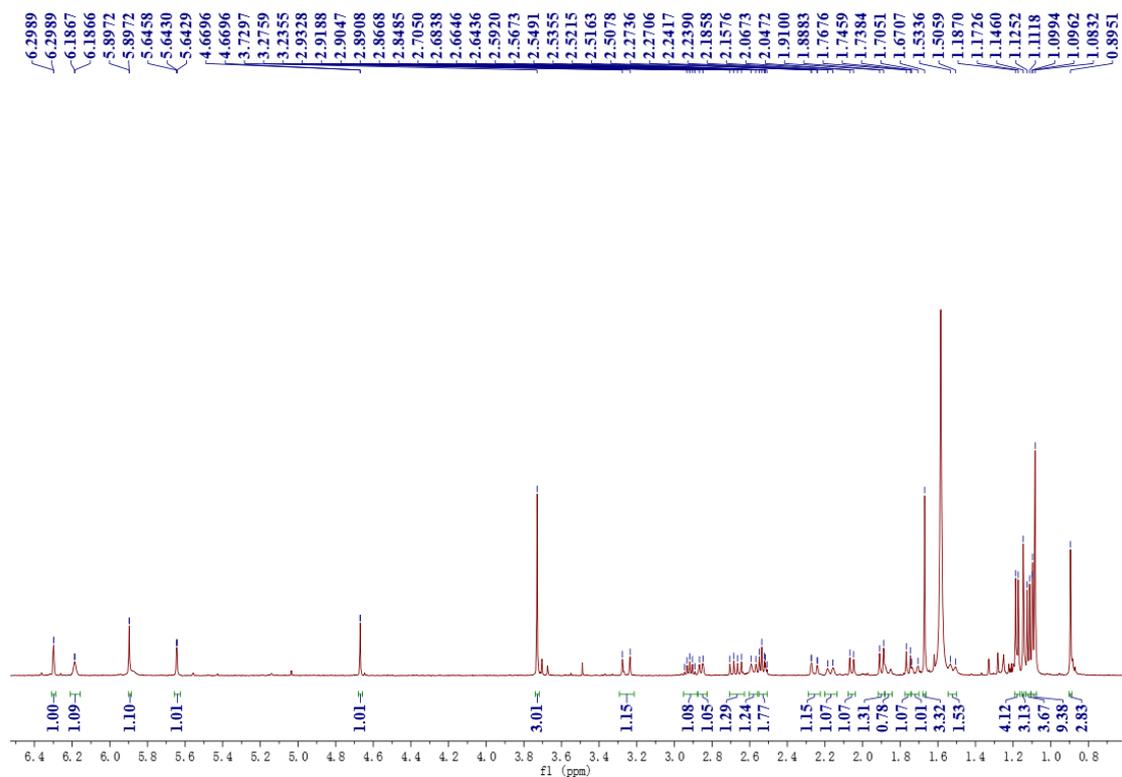


Figure S30. <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) spectrum of compound 5

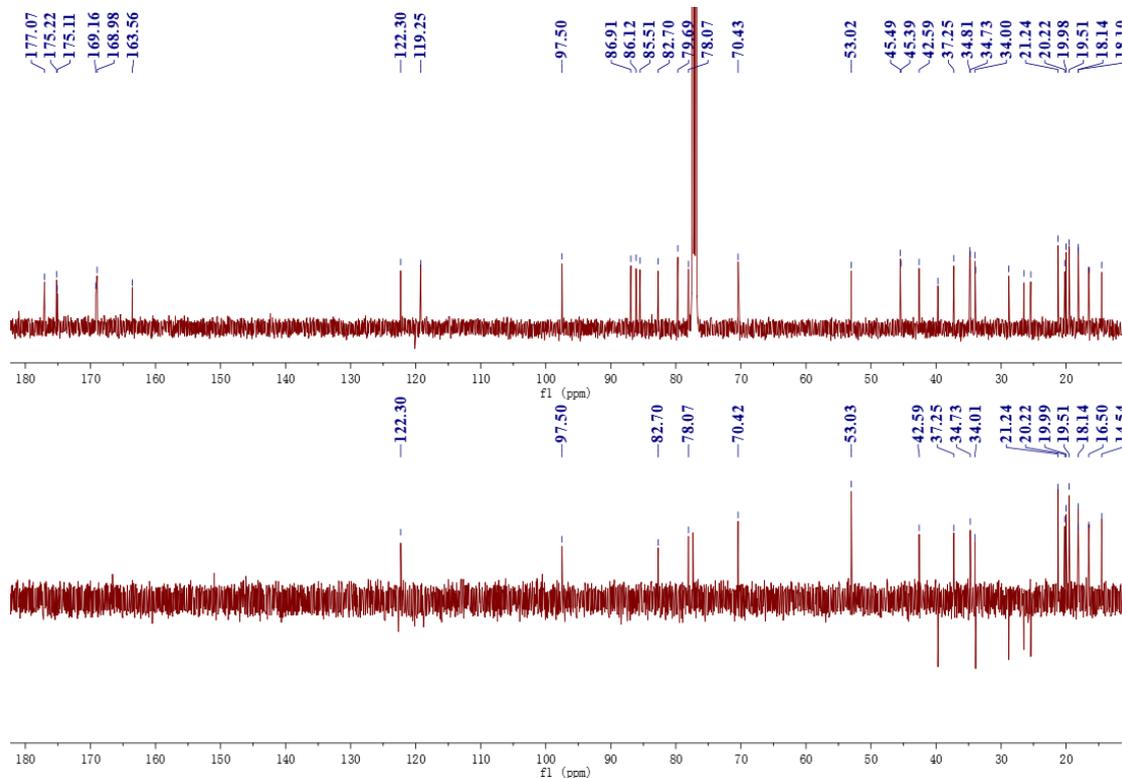


Figure S31. HSQC spectrum of compound 5 in CDCl<sub>3</sub>

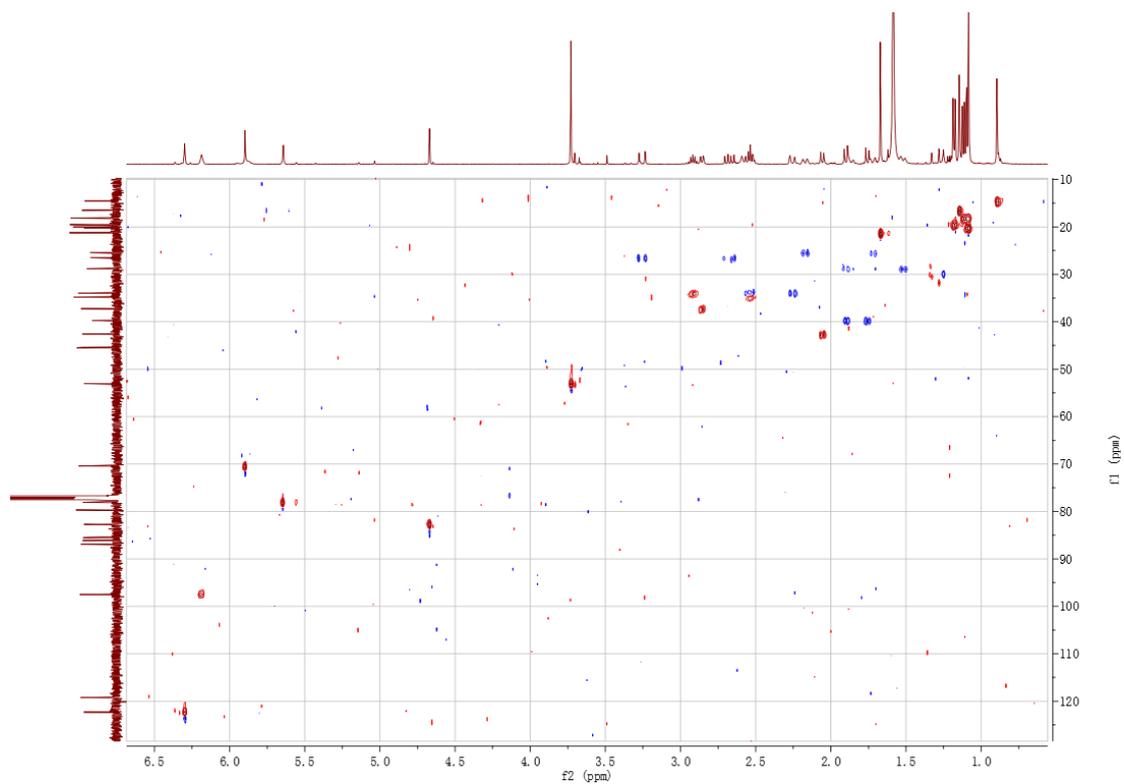


Figure S32. <sup>1</sup>H-<sup>1</sup>H COSY spectrum of compound 5 in CDCl<sub>3</sub>

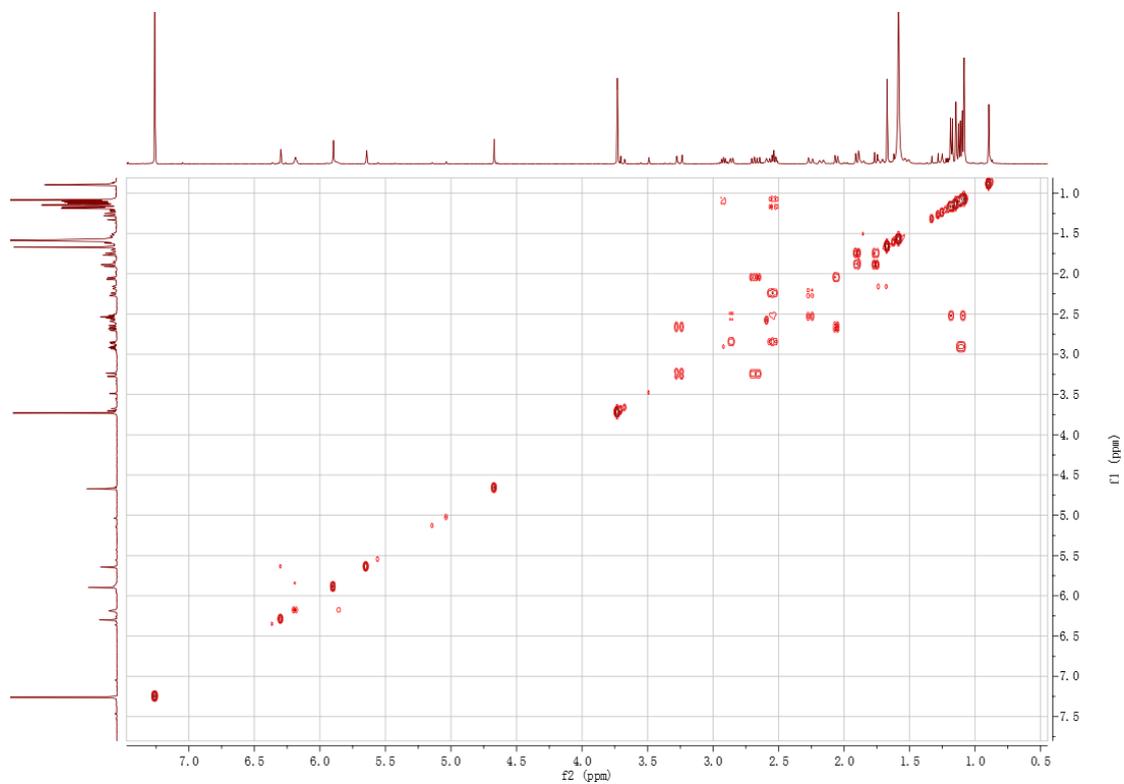


Figure S33. HMBC spectrum of compound **5** in CDCl<sub>3</sub>

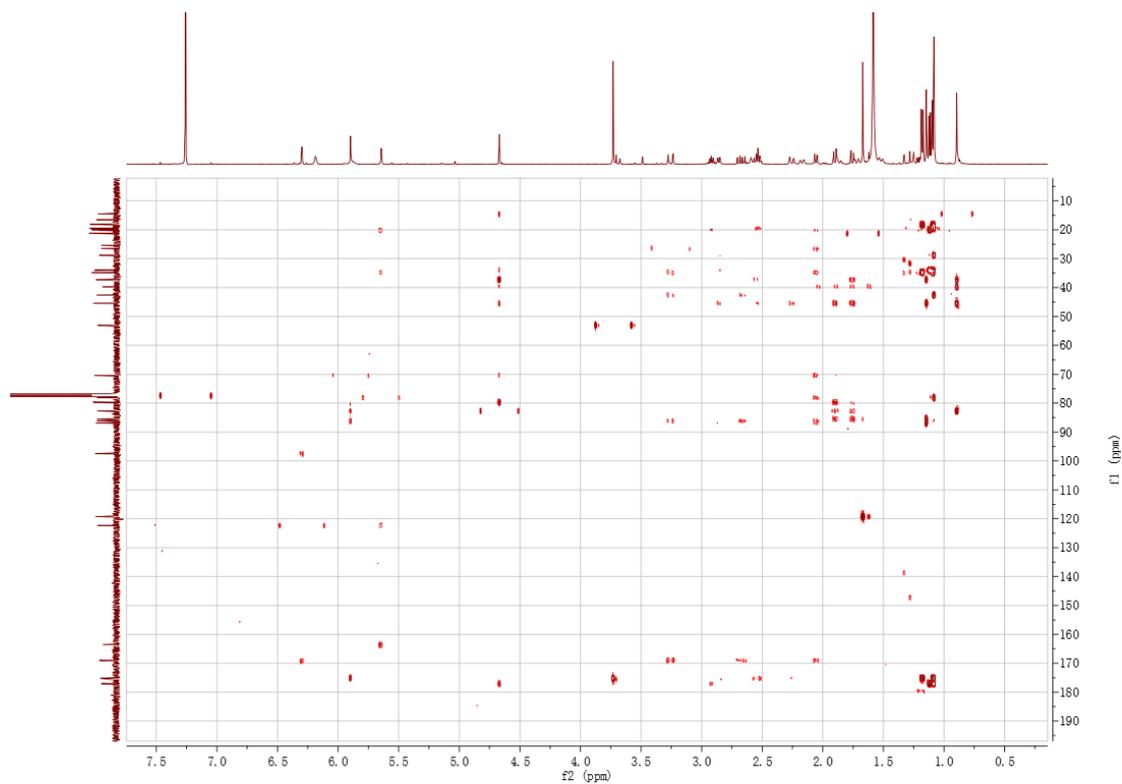


Figure S34. ROESY spectrum of compound **5** in CDCl<sub>3</sub>

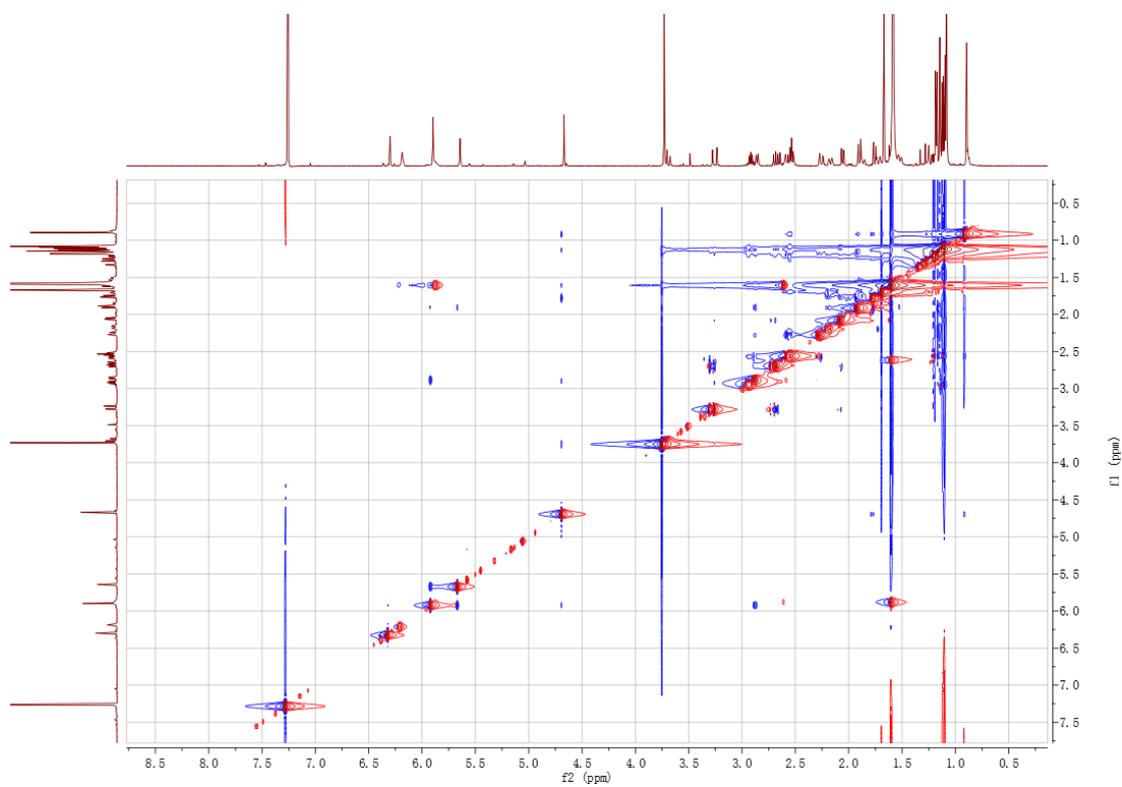
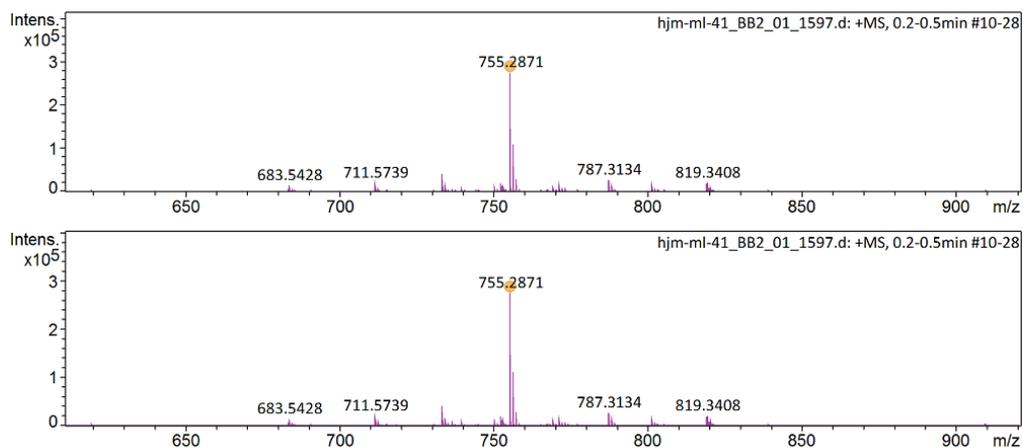


Figure S35. HRESIMS spectrum of compound 5



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e <sup>-</sup> Conf	N-Rule	Adduct
755.2871	1	C <sub>37</sub> H <sub>48</sub> NaO <sub>15</sub>	755.2885	2.0	7.3	1	100.00	14.0	even	ok	M+Na