

Supporting Information

**Guaiane sesquiterpenoids A–G with cytotoxic activity from the
desert endophytic fungus *Fusarium* sp. HM 166**

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TTCCGTAGGTGAACCTGCGGAGGGATCATTACCGAGTTTACAACCTCCCAAACCCCTGTGAACATACCAATT
GTTGCCTCGGCGGATCAGCCCGCTCCCGGTAAAACGGGACGGCCCGCCAGAGGACCCCTAAACTCTGTTT
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GCTTCCATTGCGTAGTAGTAAAACCCTCGCAACTGGTACGCGGCGCGCCAAGCCGTAAACCCCCAACTT
CTGAATGTTGACCTCGGATCAGGTAGGAATACCCGCTGAACTTAAGCATATCAATAAGCGGAGG

Figure S1. The 16S rRNA sequence of *Fusarium* sp. **HM166**

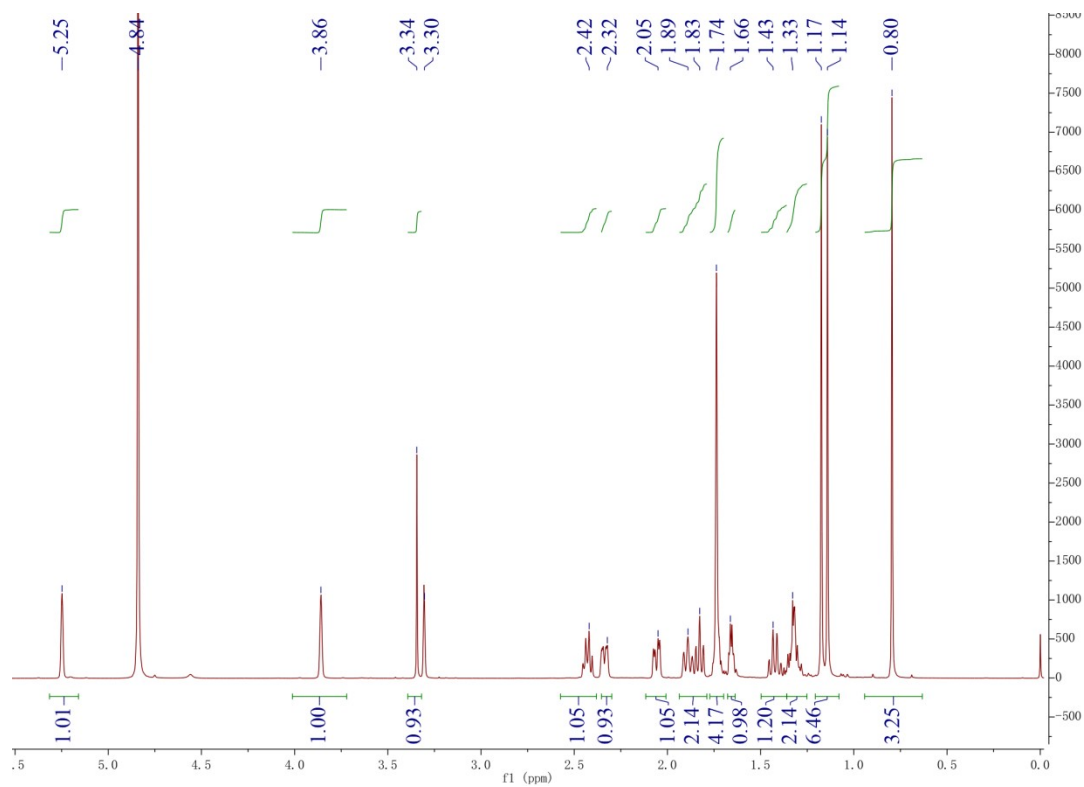


Figure S2-1. The ^1H NMR spectrum of **1**

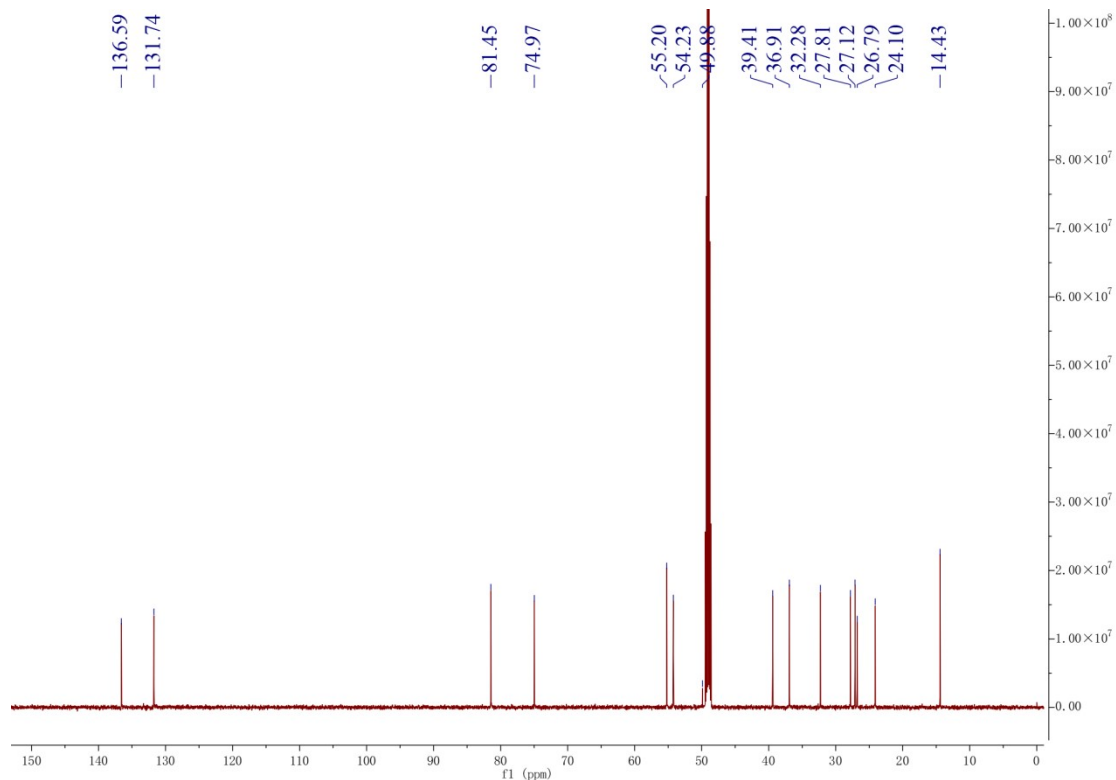


Figure S2-2. The ^{13}C NMR spectrum of **1**

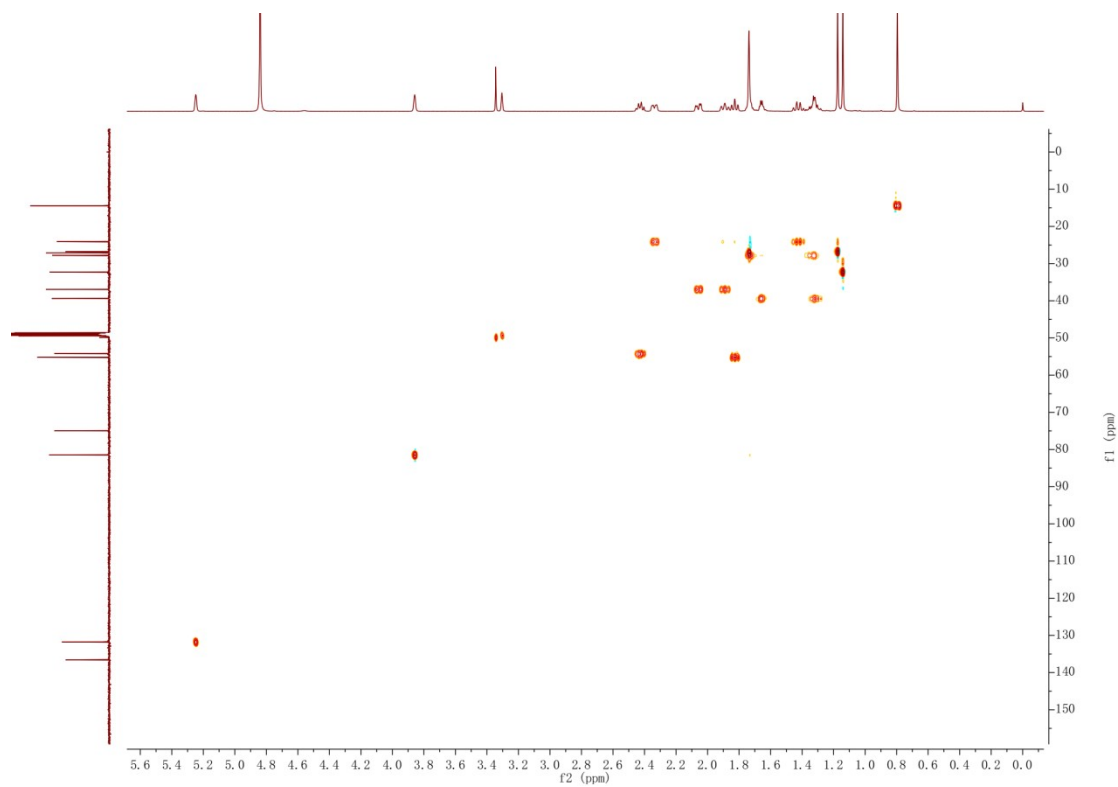


Figure S2-3. The HSQC spectrum of **1**

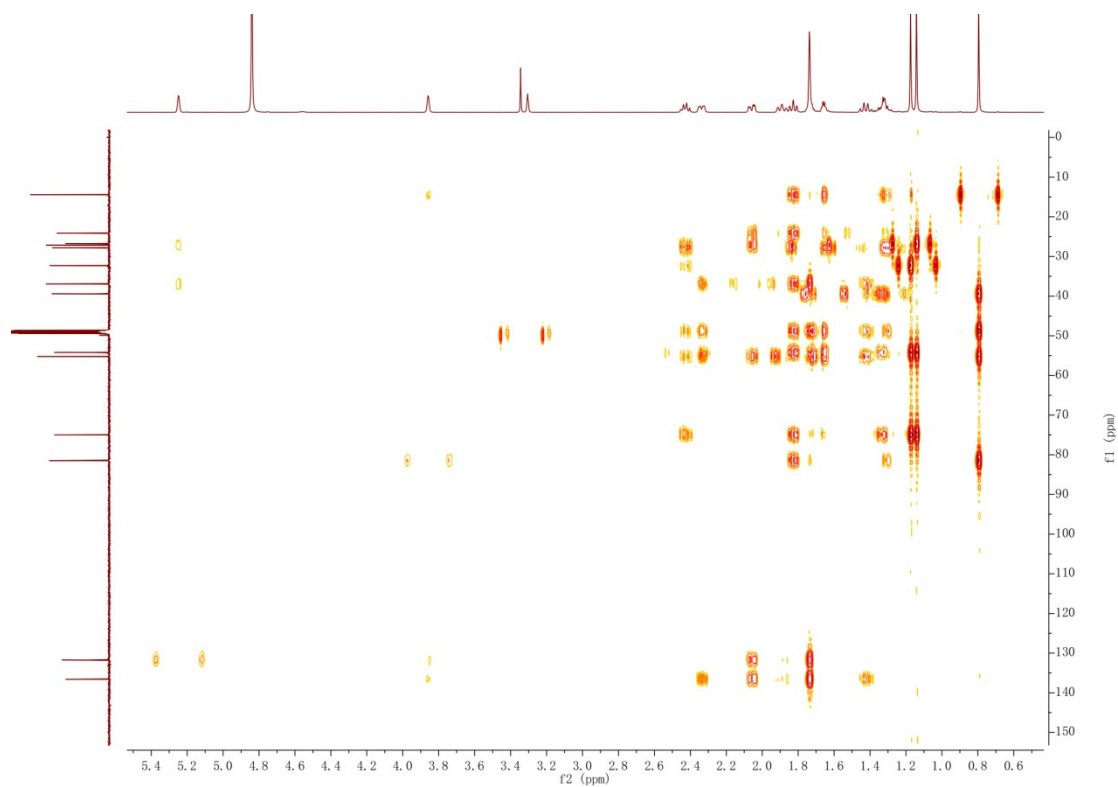


Figure S3-4. The HMBC spectrum of **1**

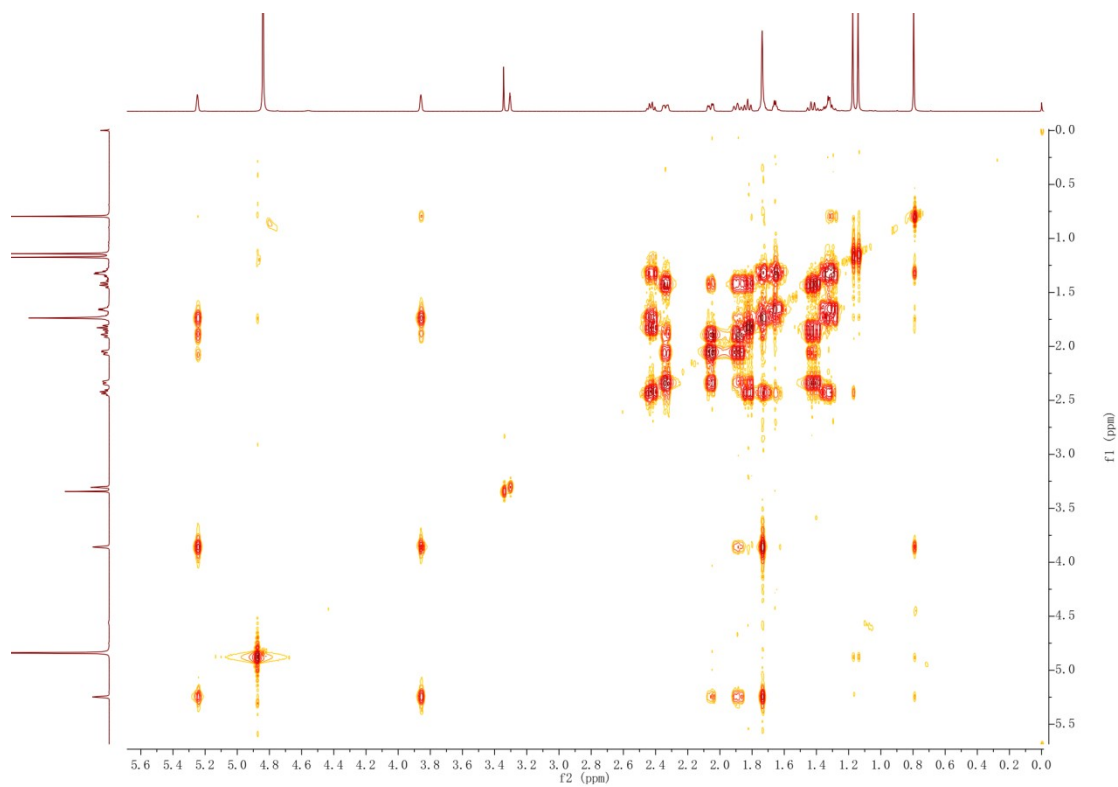


Figure S2-5. The ^1H - ^1H COSY spectrum of **1**

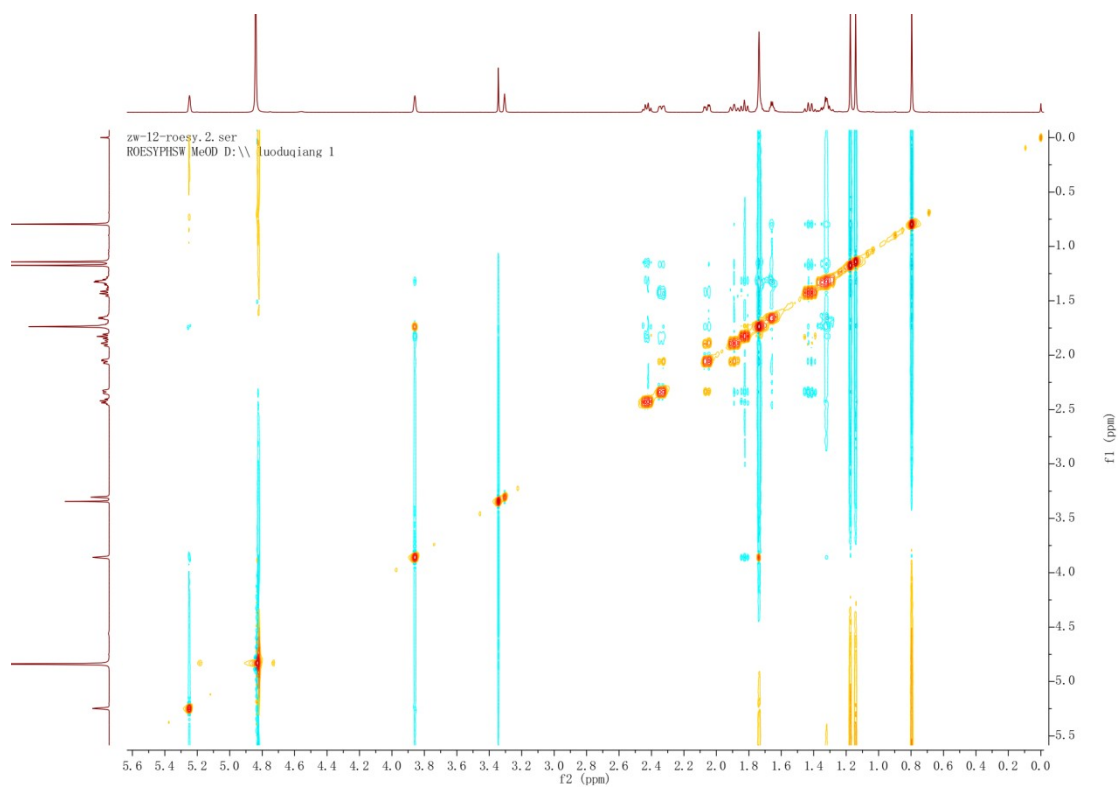


Figure S2-6. The ROESY spectrum of **1**

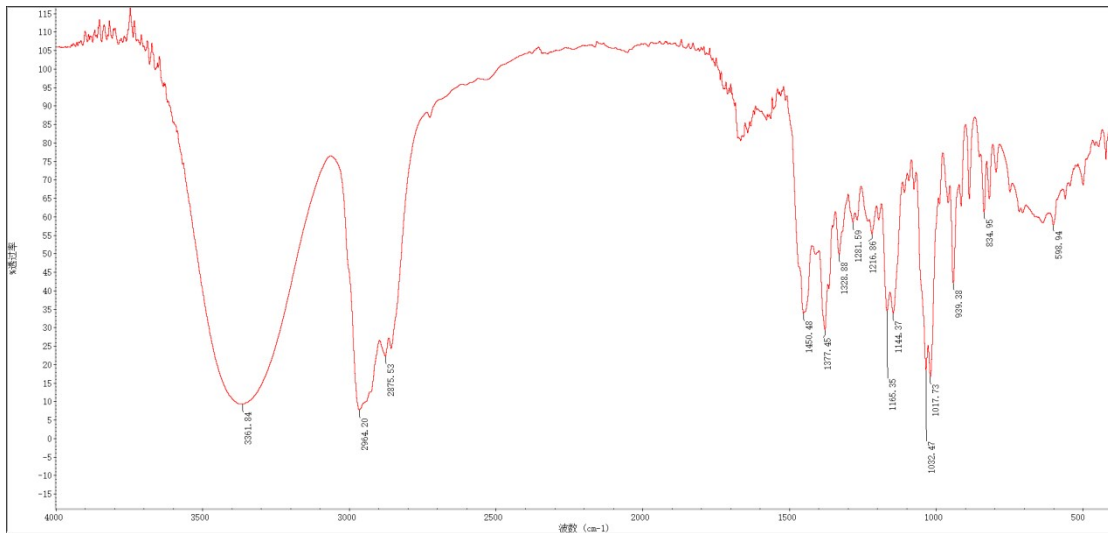
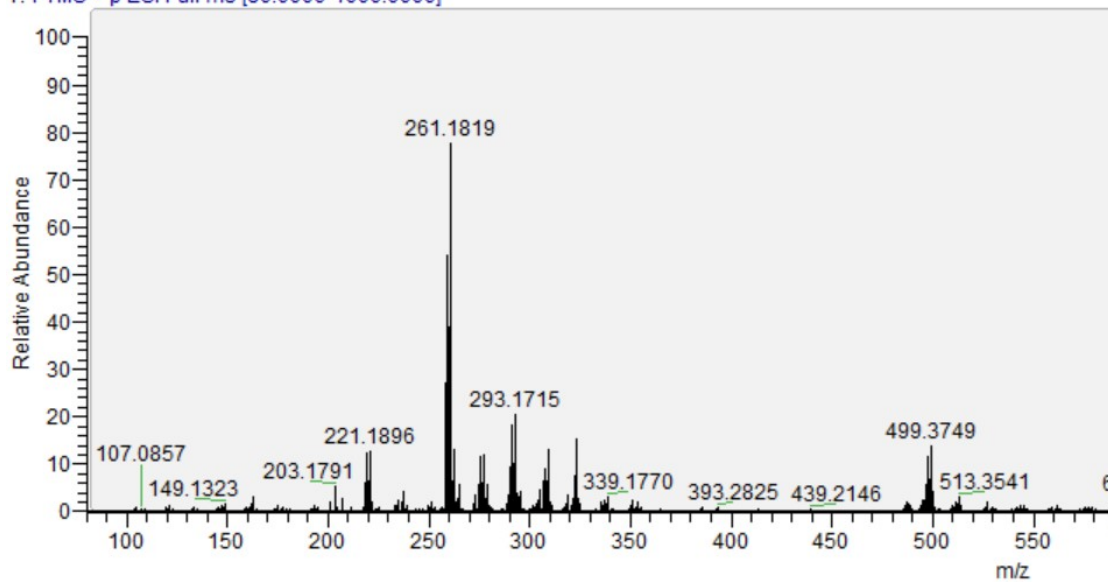


Figure S2-7. The IR spectrum of **1**

T: FTMS + p ESI Full ms [80.0000-1000.0000]



$C_{15}H_{26}O_2Na^+$ Calculated 261.1825 Found 261.1819

Figure S3-8. The HRESIMS spectrum of **1**

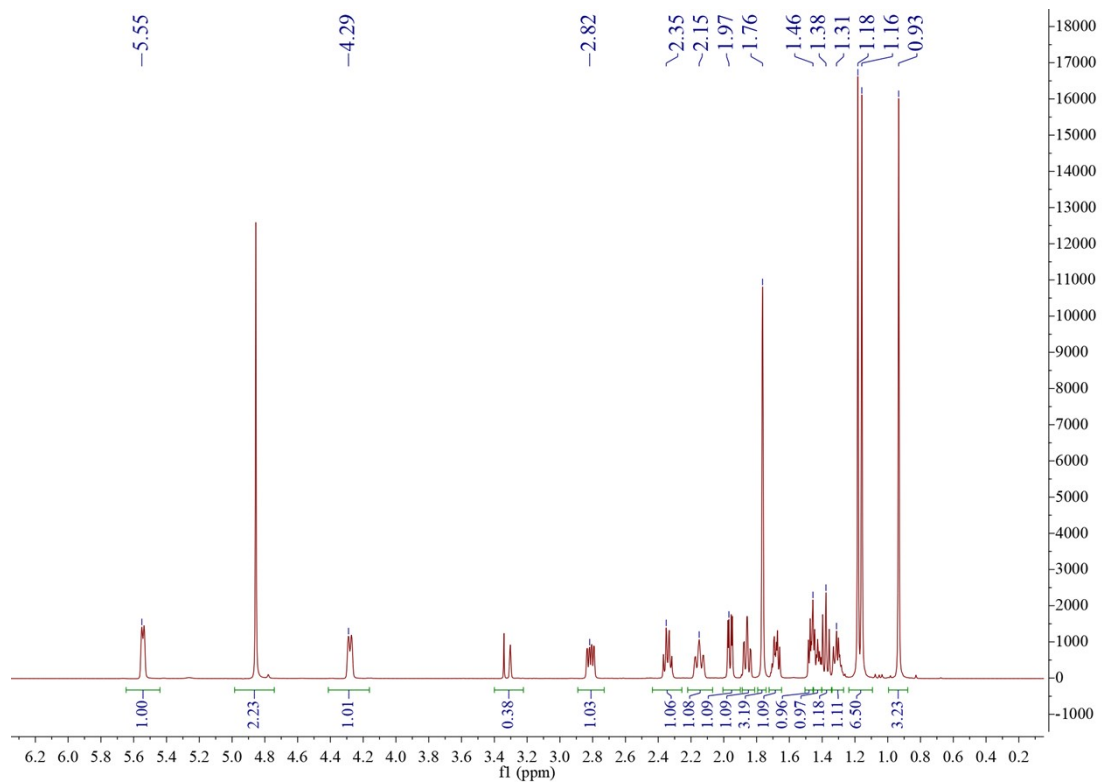


Figure S3-1. The ^1H NMR spectrum of **2**

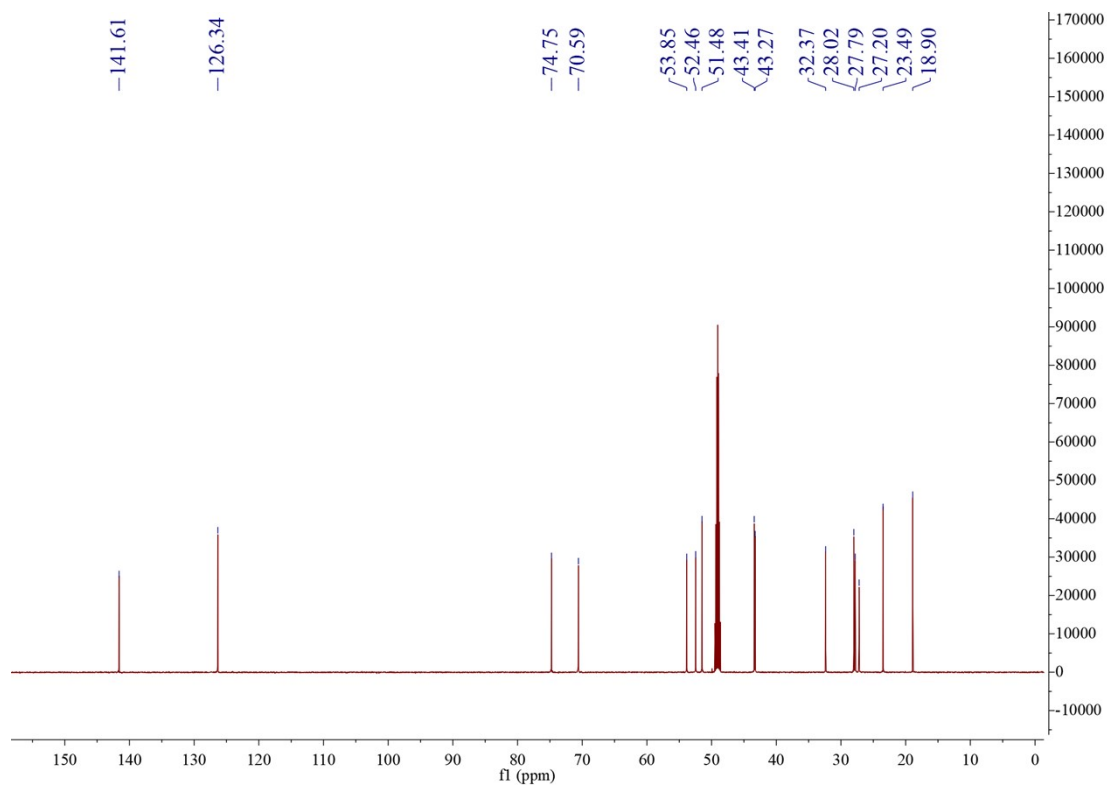


Figure S3-2. The ^{13}C NMR spectrum of **2**

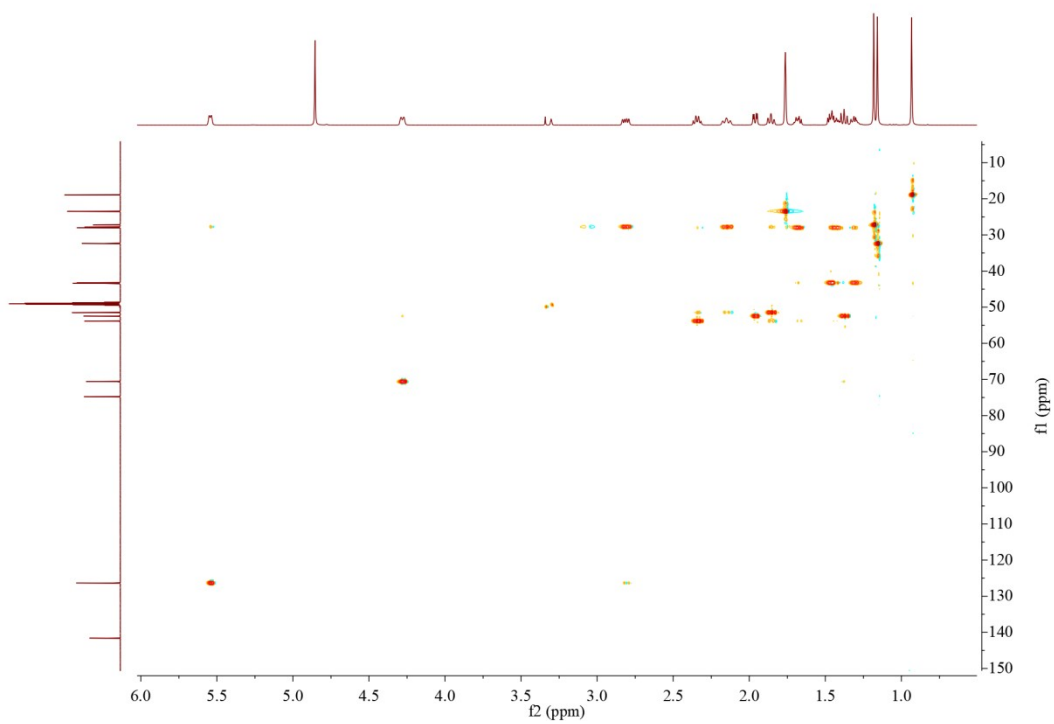


Figure S3-3. The HSQC spectrum of **2**

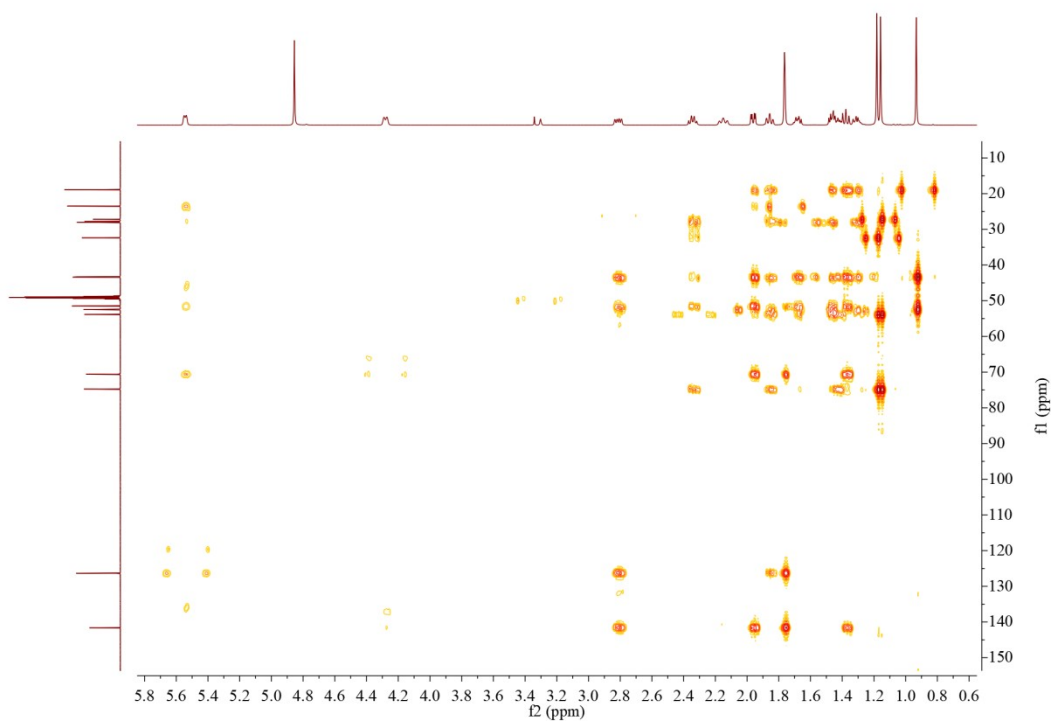


Figure S3-4. The HMBC spectrum of **2**

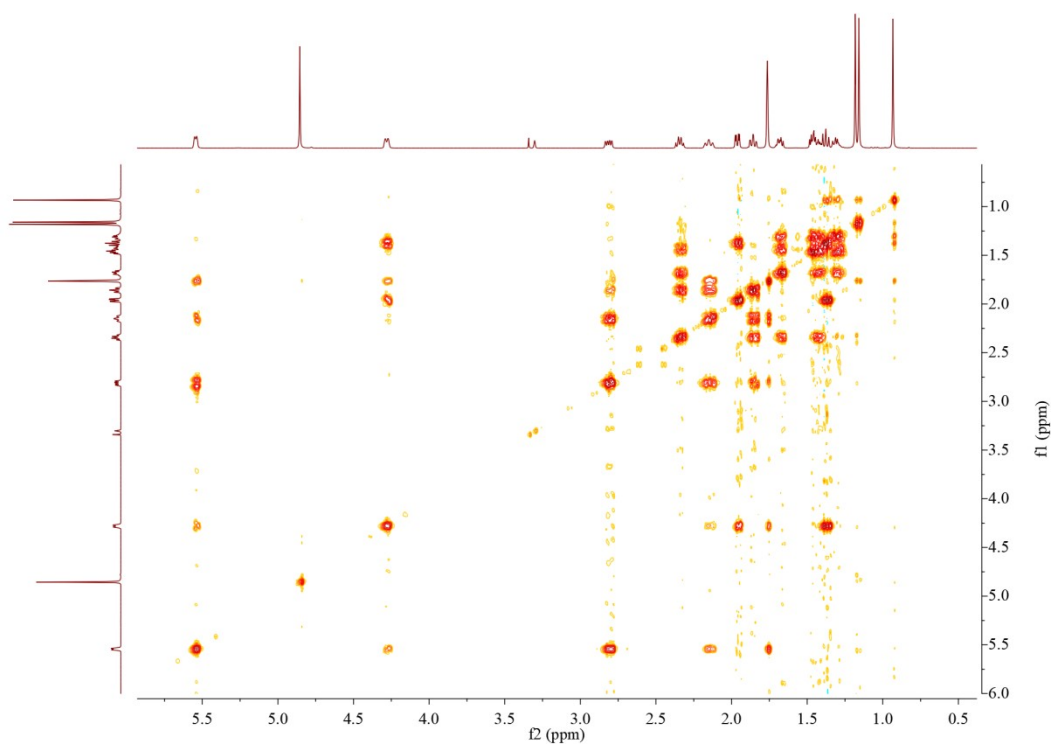


Figure S3-5. The ^1H - ^1H COSY spectrum of **2**

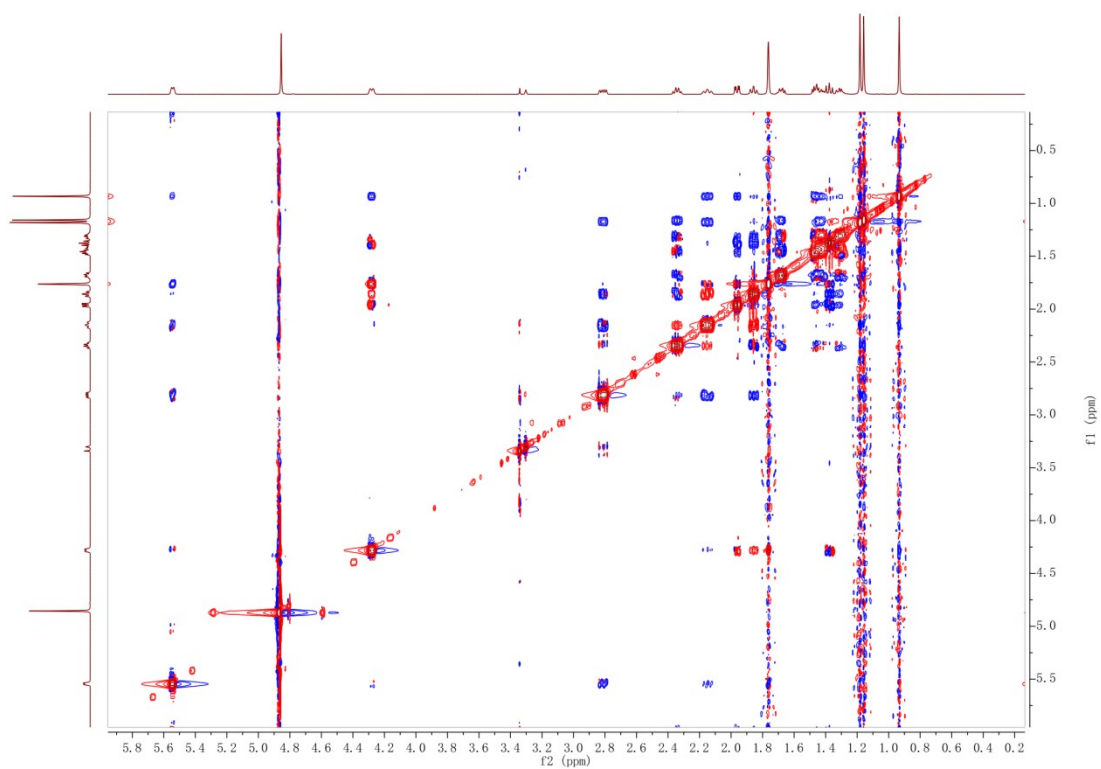


Figure S3-6. The ROESY spectrum of **2**

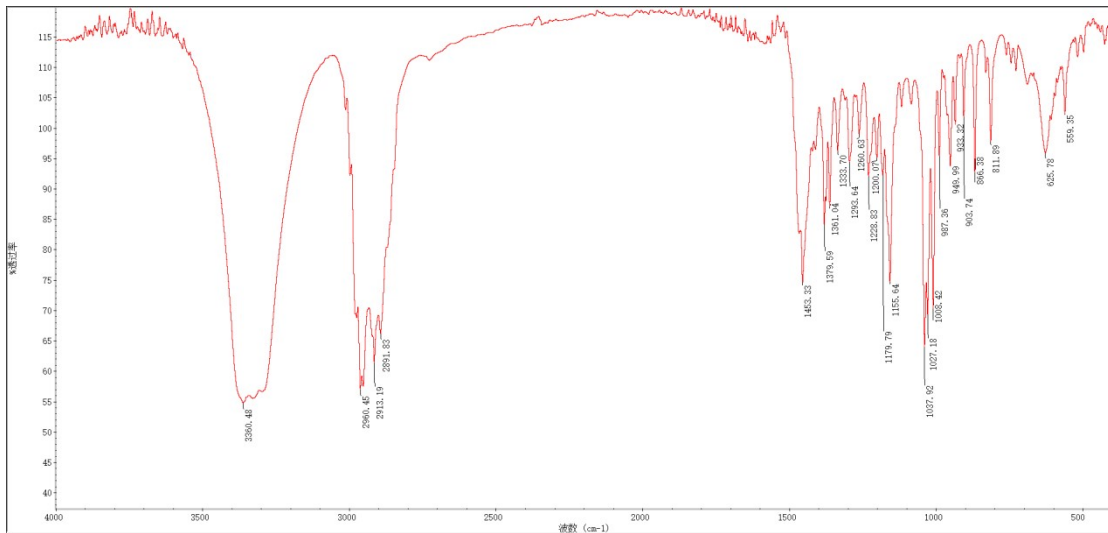
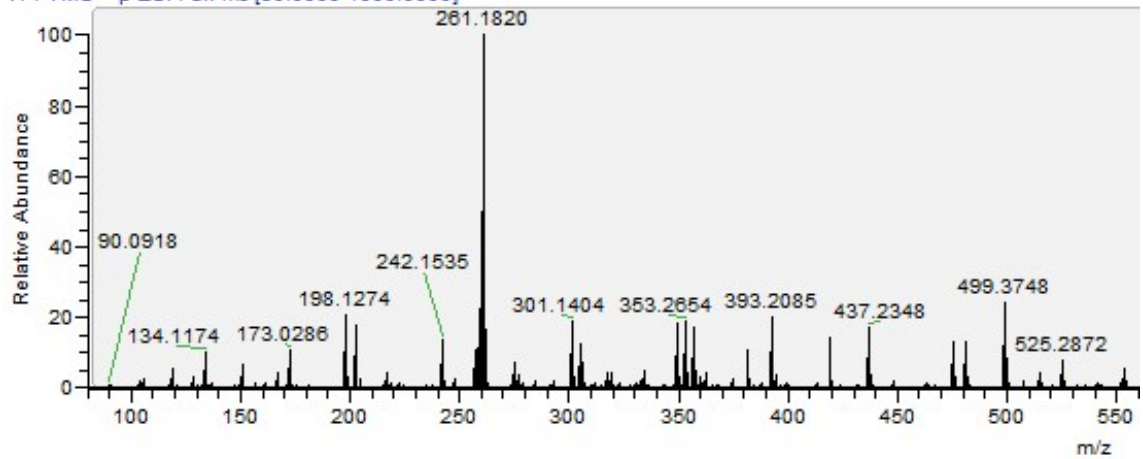


Figure S3-7. The IR spectrum of **2**

20191231_21 #11 RT: 0.10 AV: 1 NL: 2.74E8
 T: FTMS + p ESI Full ms [80.0000-1000.0000]



$C_{15}H_{26}O_2Na^+$ Calculated 261.1825 Found 261.1820

Figure S3-8. The HRESIMS spectrum of **2**

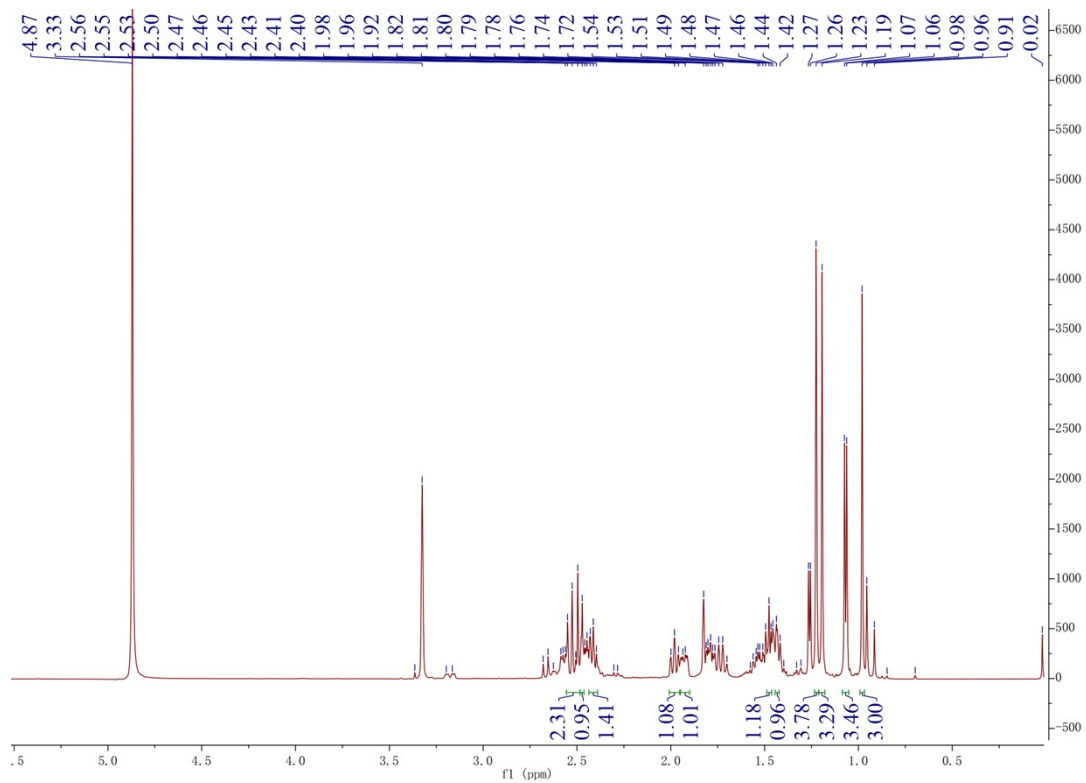


Figure S4-1. The ^1H NMR spectrum of **3**

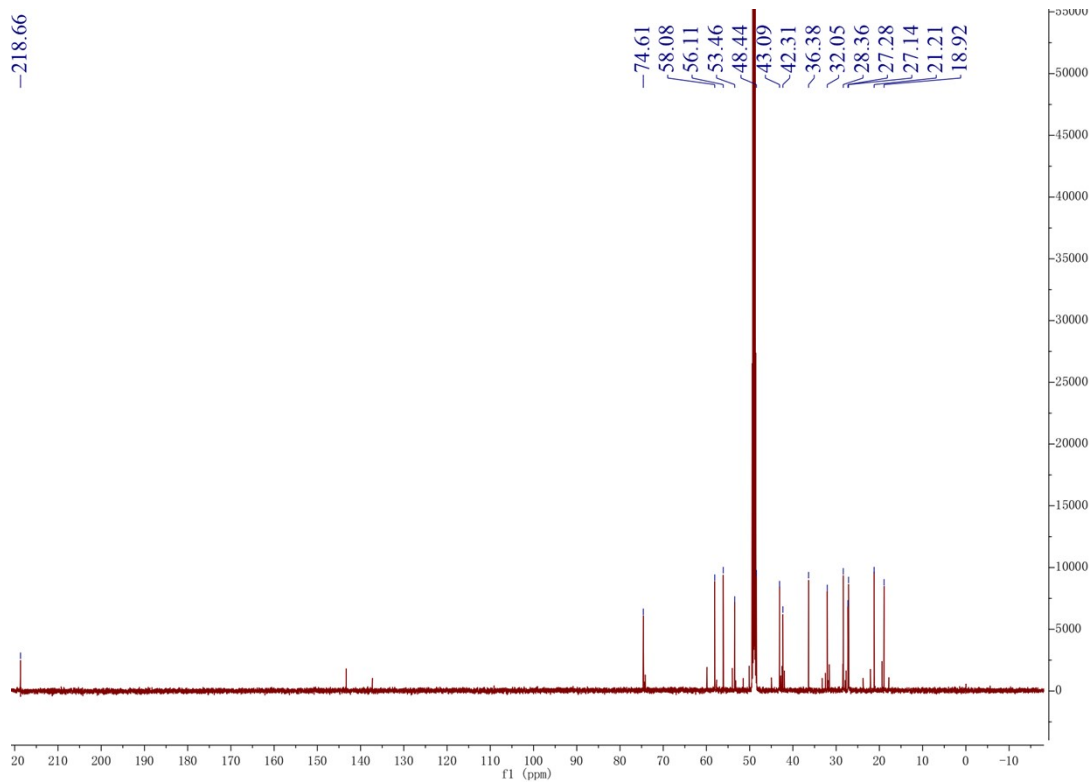


Figure S4-2. The ^{13}C NMR spectrum of **3**

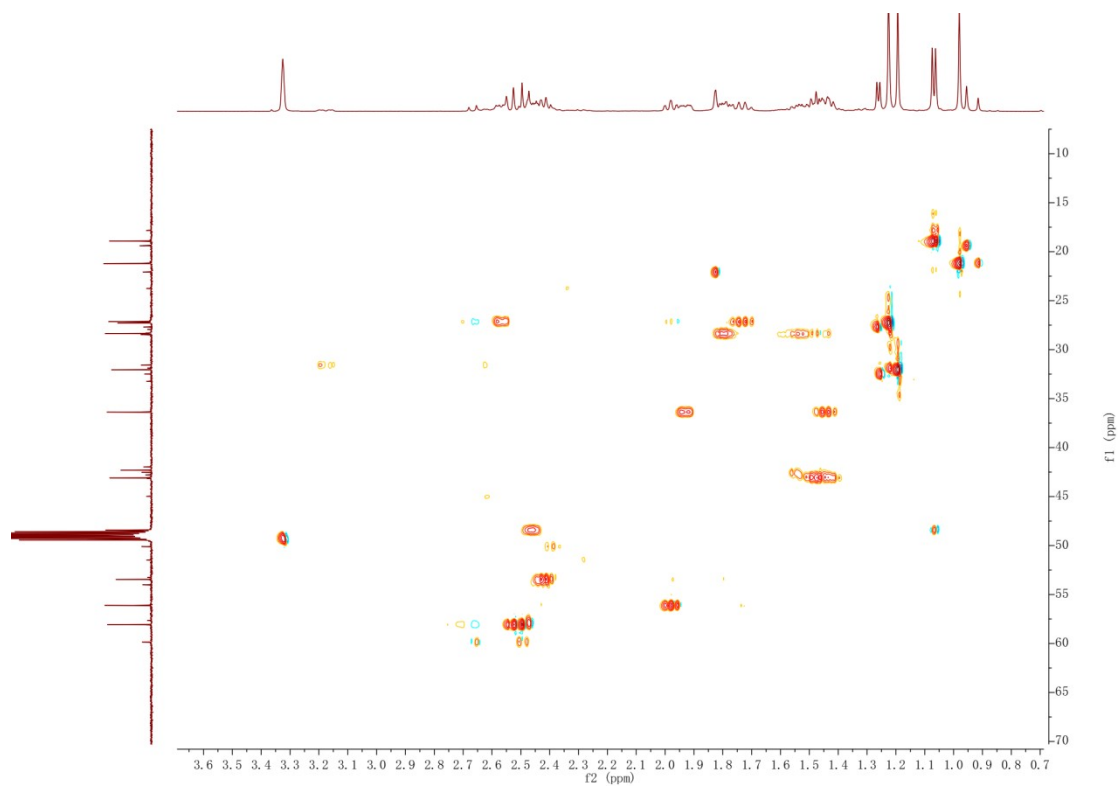


Figure S4-3. The HSQC spectrum of **3**

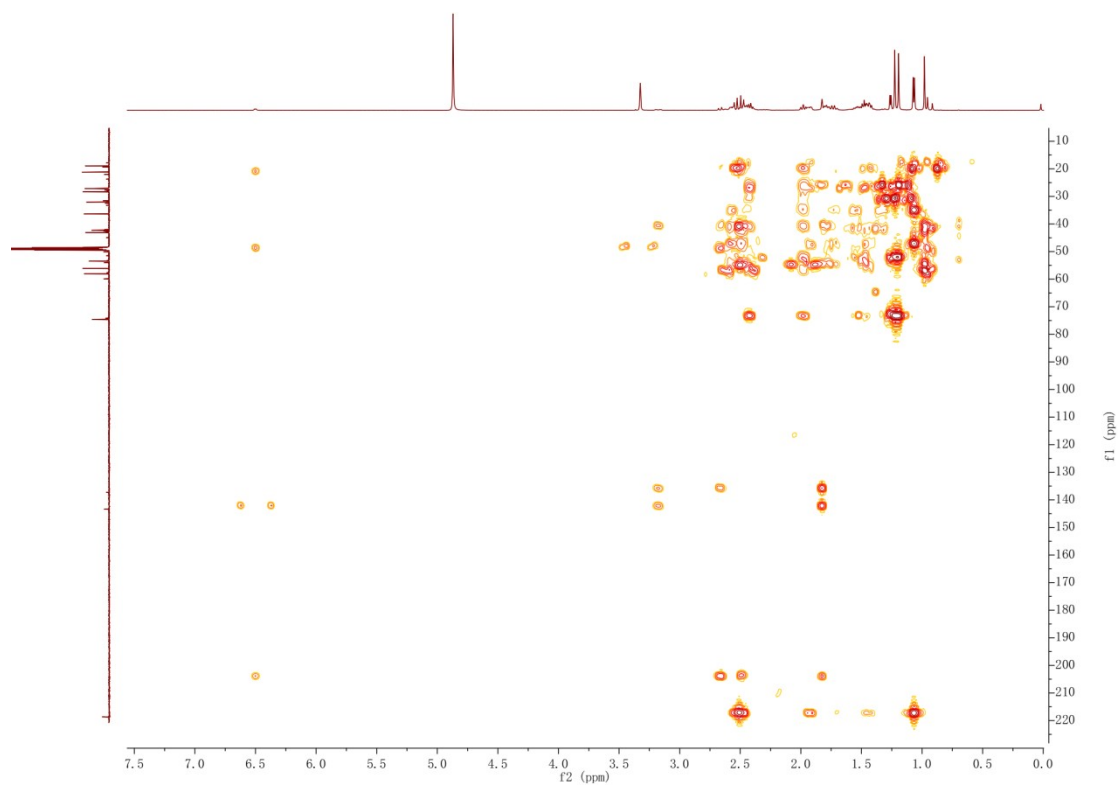


Figure S4-4. The HMBC spectrum of **3**

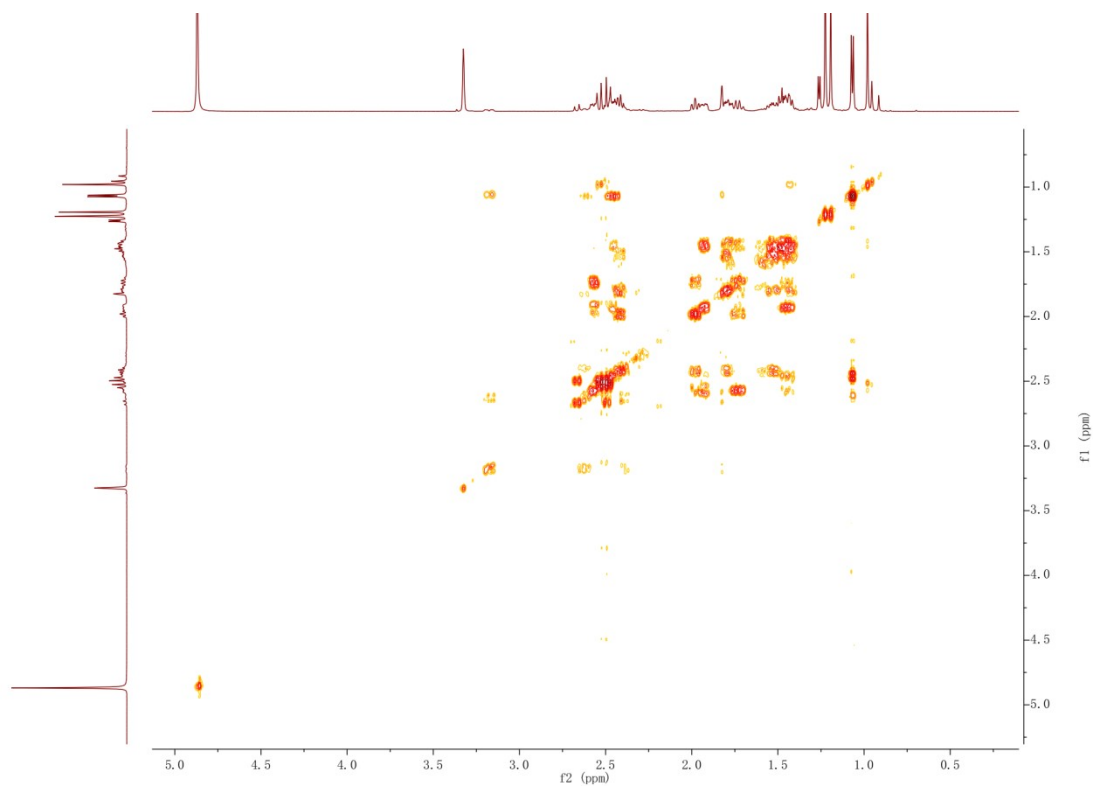


Figure S4-5. The ^1H - ^1H COSY spectrum of **3**

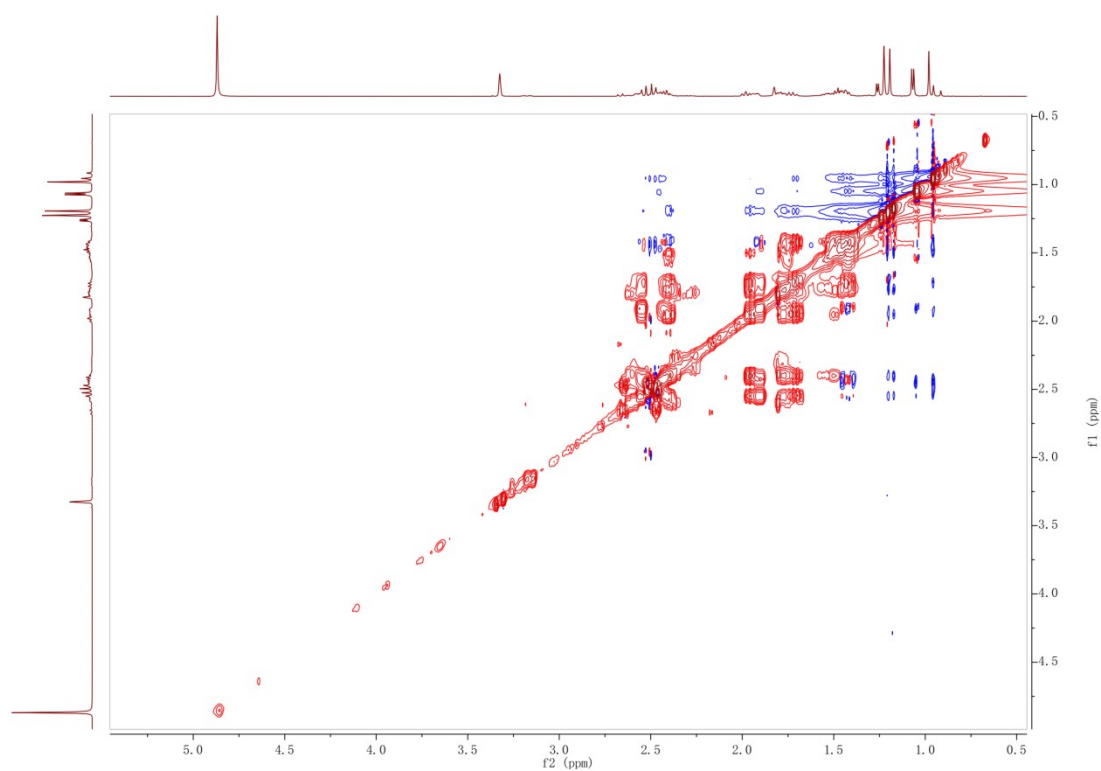


Figure S4-6. The ROESY spectrum of **3**

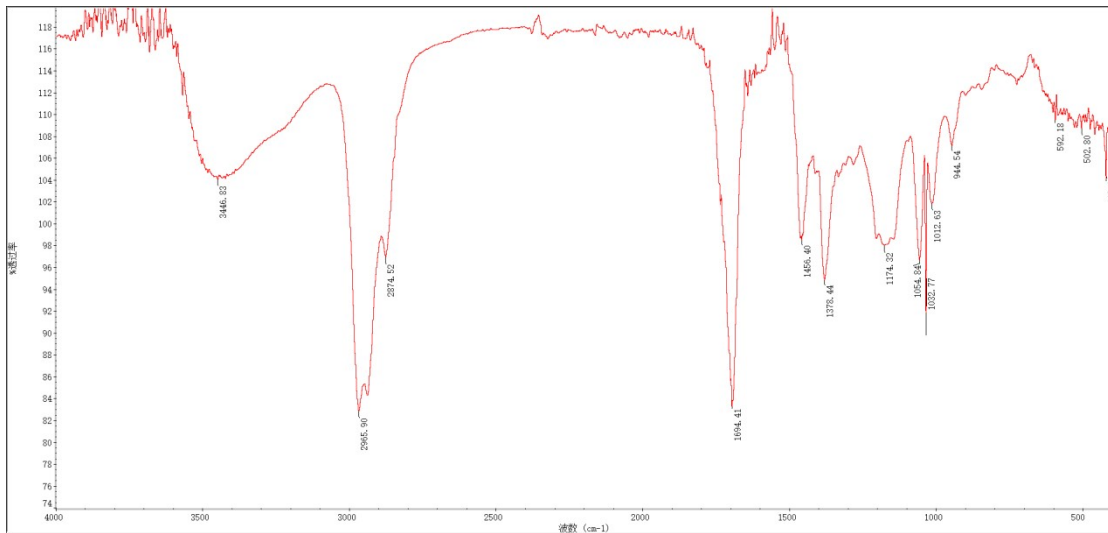
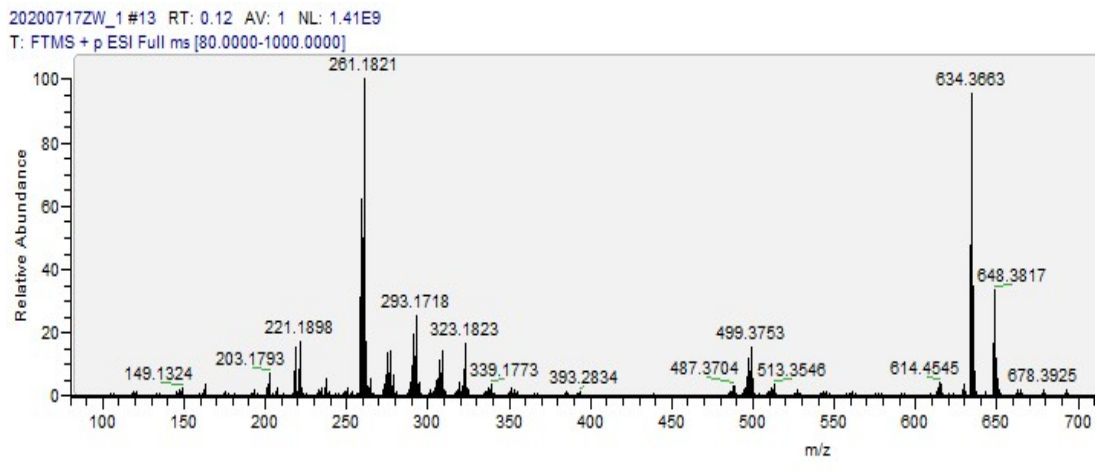


Figure S4-7. The IR spectrum of **3**



$C_{15}H_{26}O_2Na^+$ Calculated 261.1825 Found 261.1821

Figure S4-8. The HRESIMS spectrum of **3**

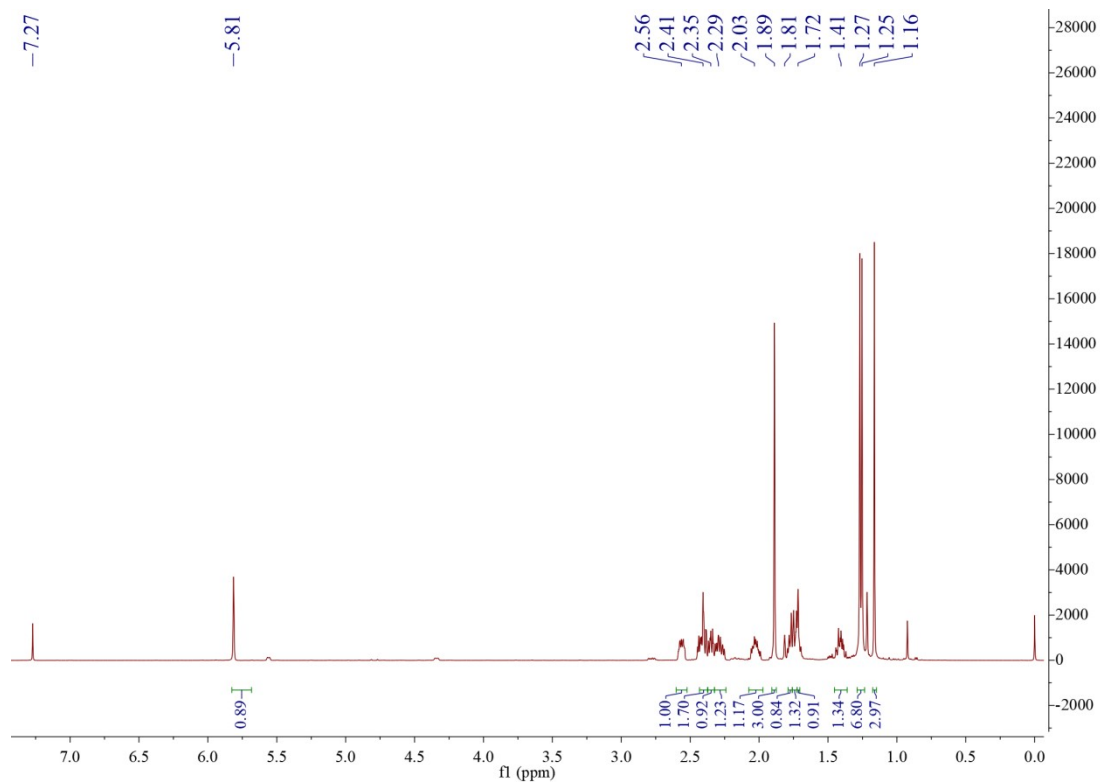


Figure S5-1. The ^1H NMR spectrum of **4**

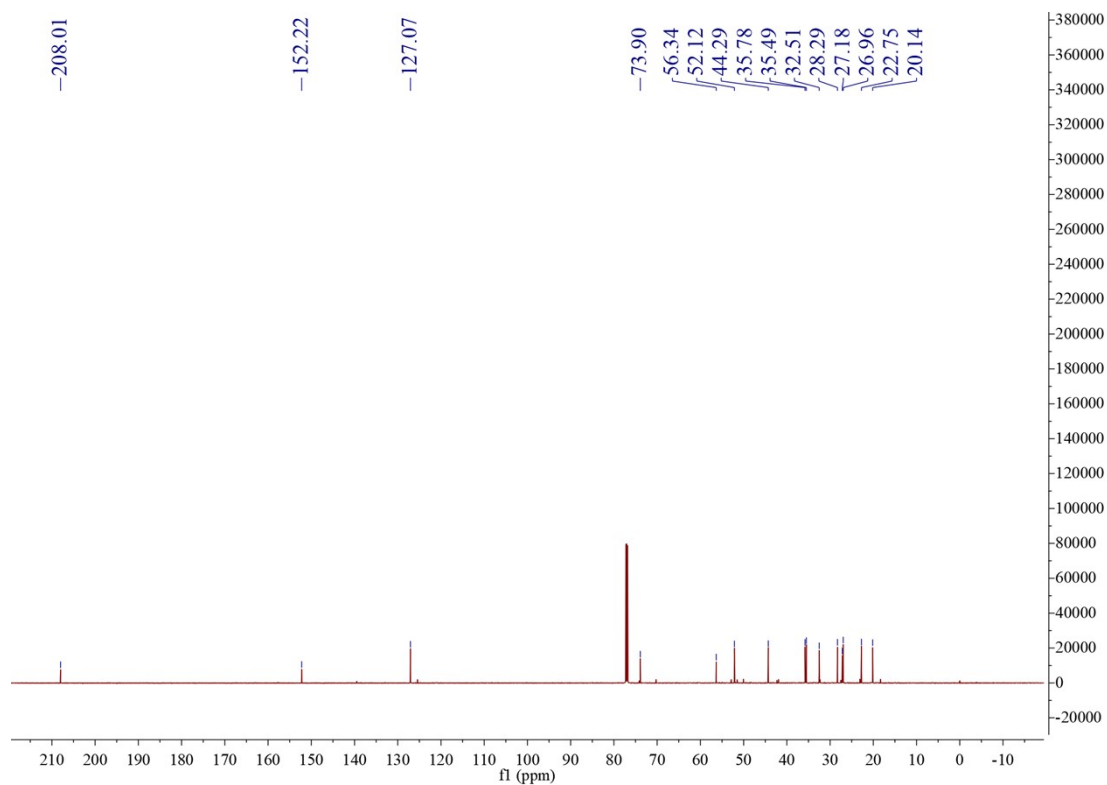


Figure S5-2. The ^{13}C NMR spectrum of **4**

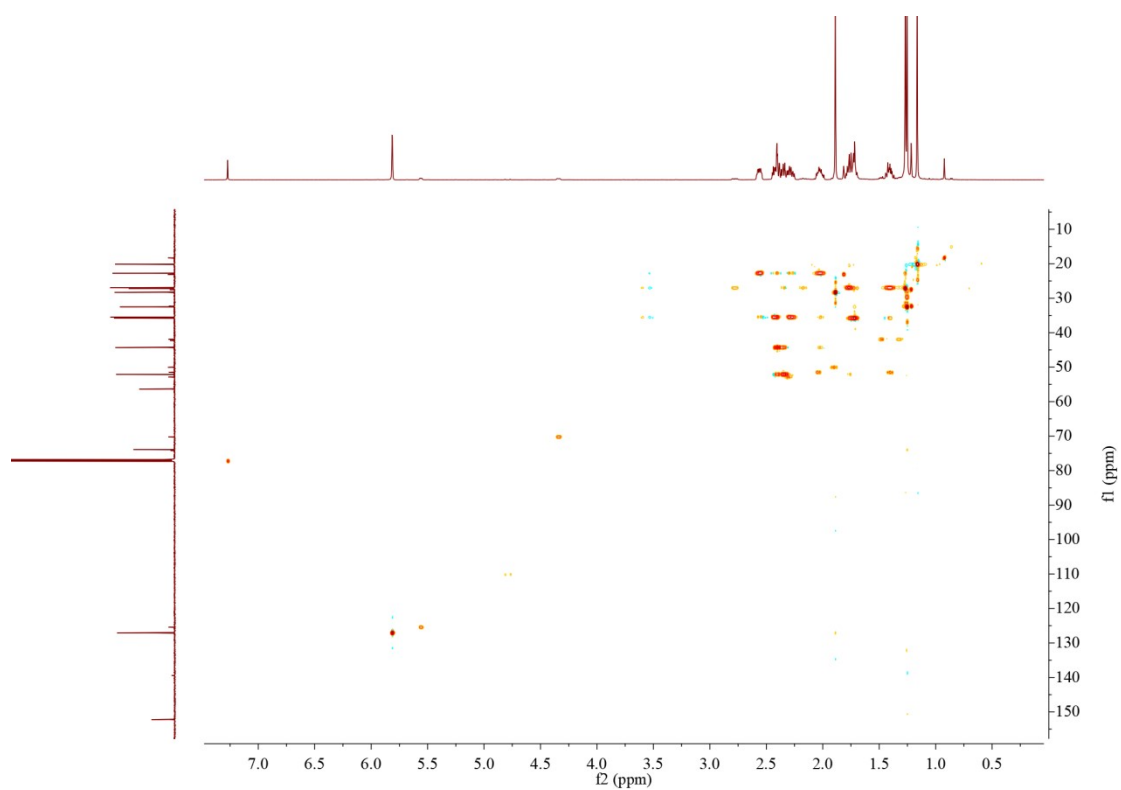


Figure S5-3. The HSQC spectrum of **4**

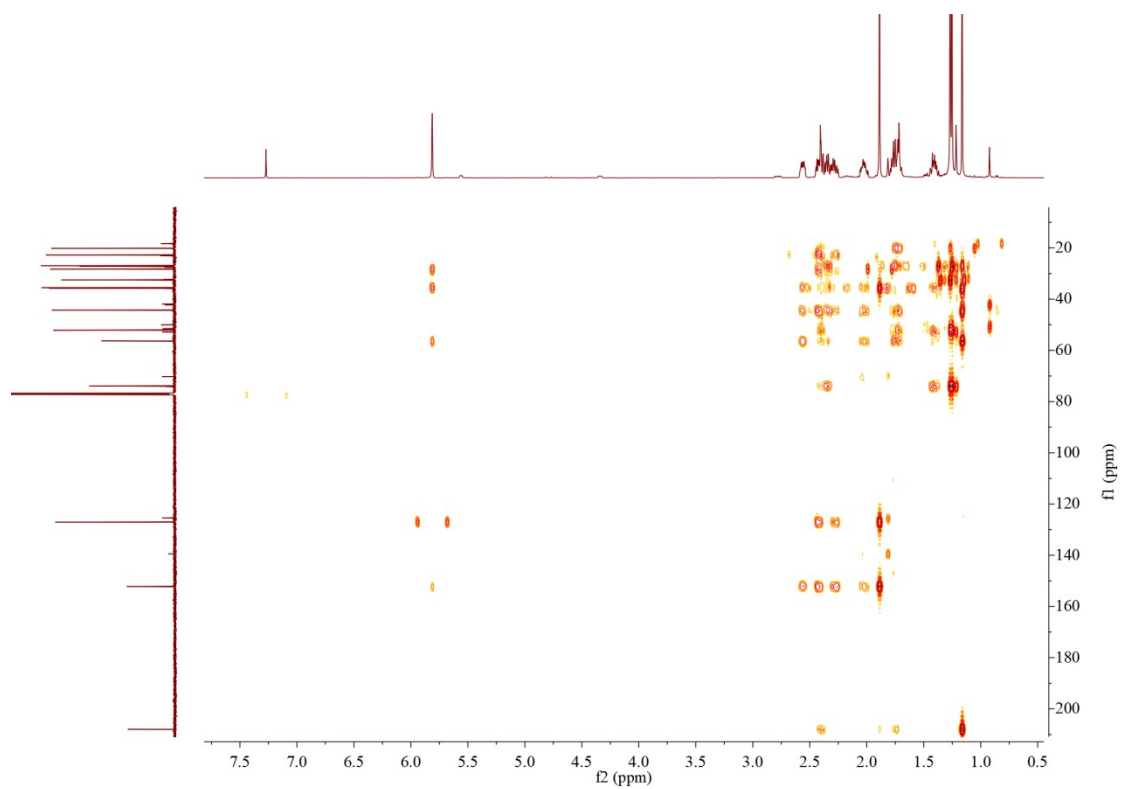


Figure S5-4. The HMBC spectrum of **4**

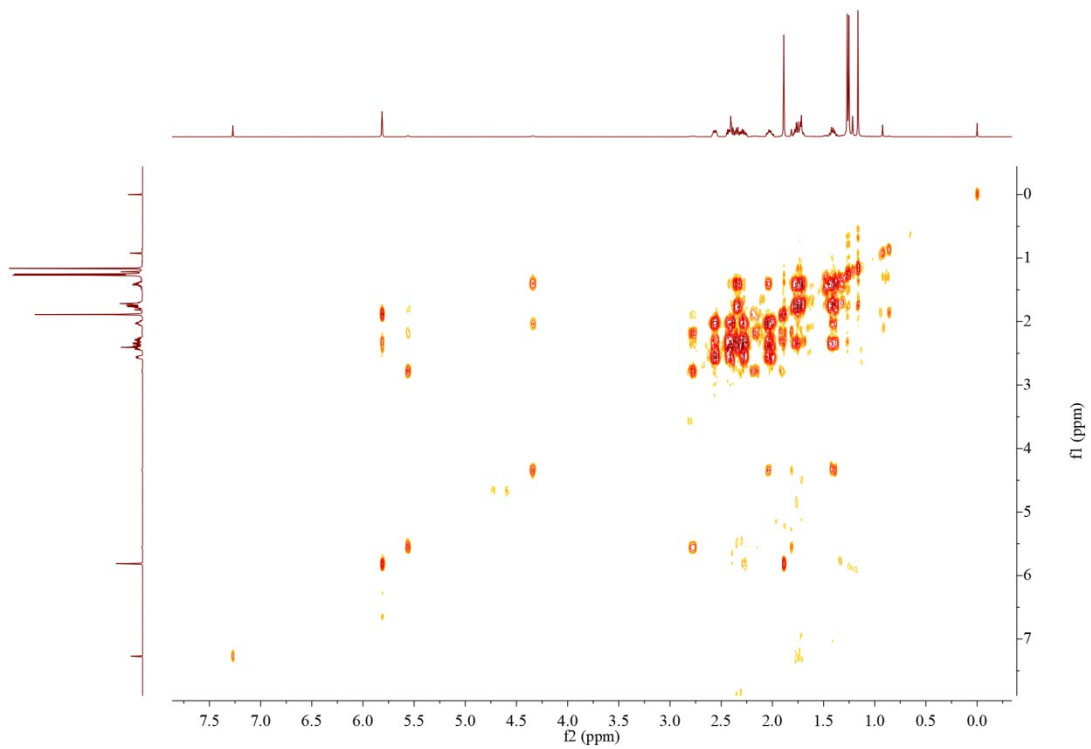


Figure S5-5. The ^1H - ^1H COSY spectrum of **4**

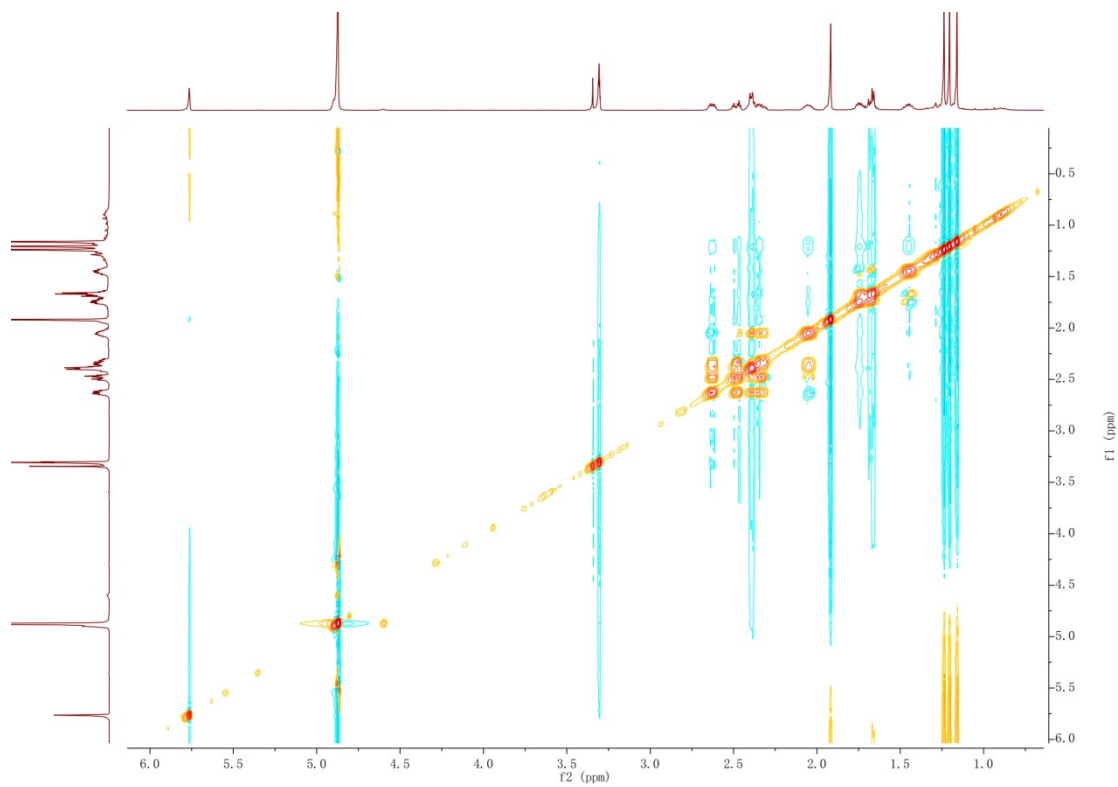


Figure S5-6. The ROESY spectrum of **4**

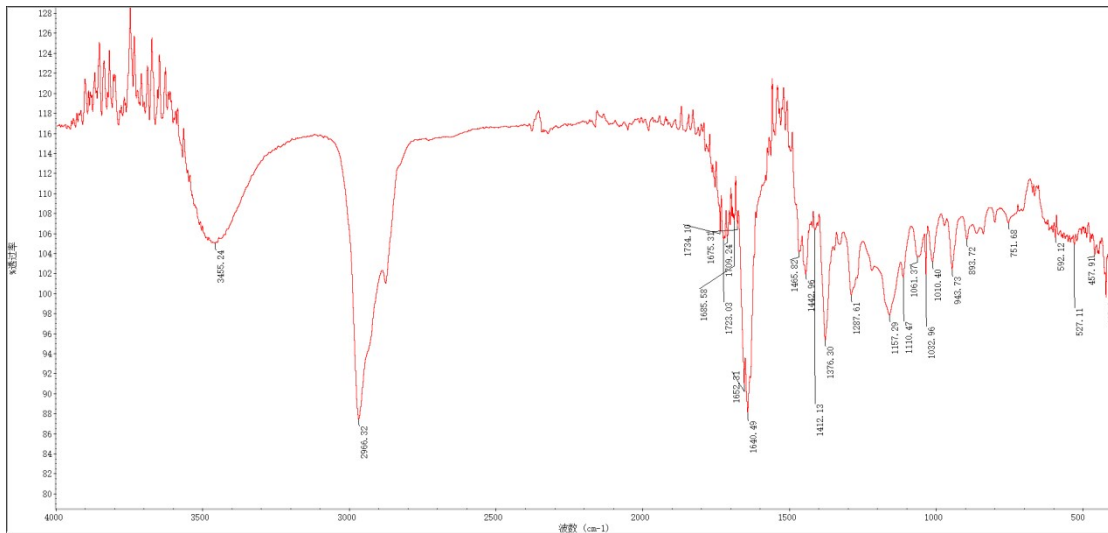
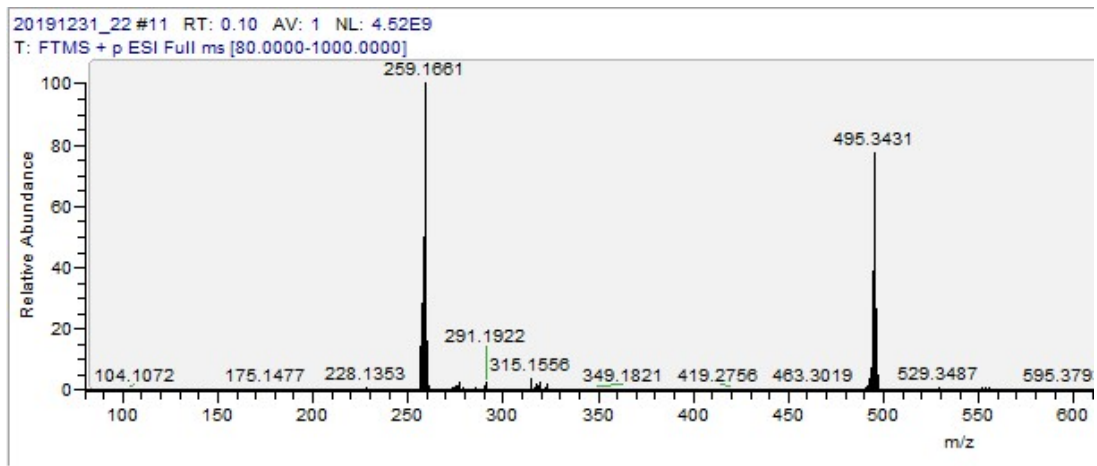


Figure S5-7. The IR spectrum of **4**



$C_{15}H_{24}O_2Na^+$ Calculated 259.1669 Found 259.1661

Figure S5-8. The HRESIMS spectrum of **4**

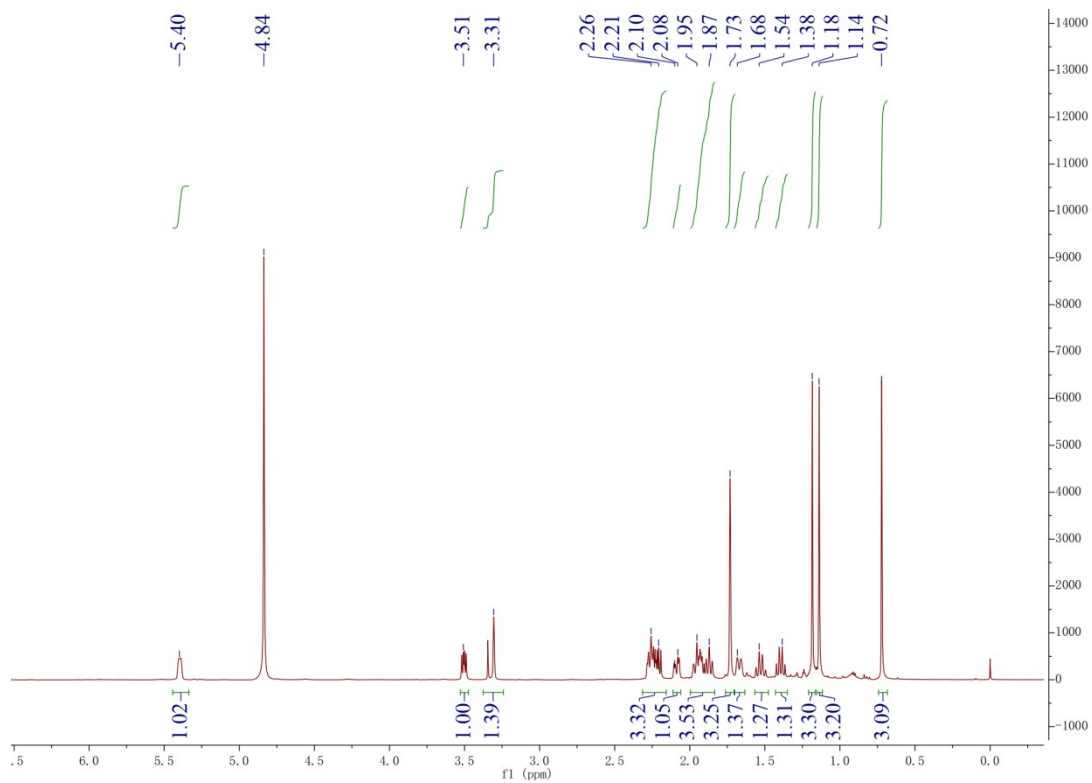


Figure S6-1. The ^1H NMR spectrum of **5**

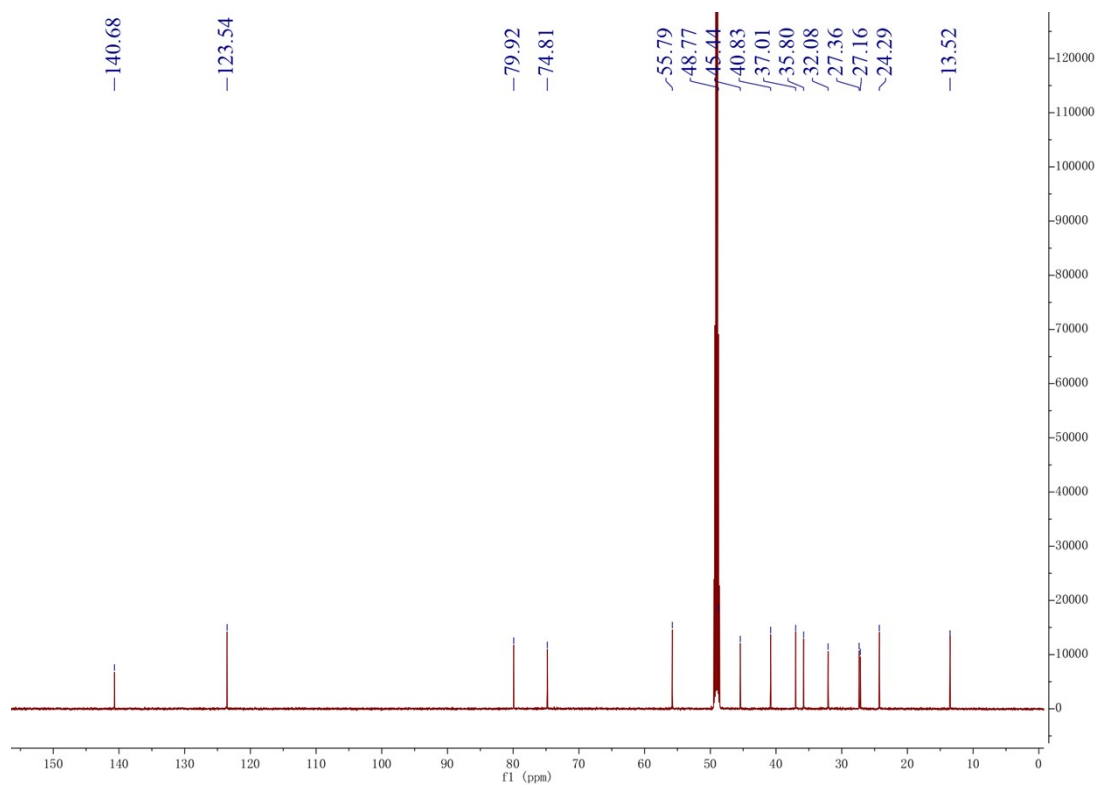


Figure S6-2. The ^{13}C NMR spectrum of **5**

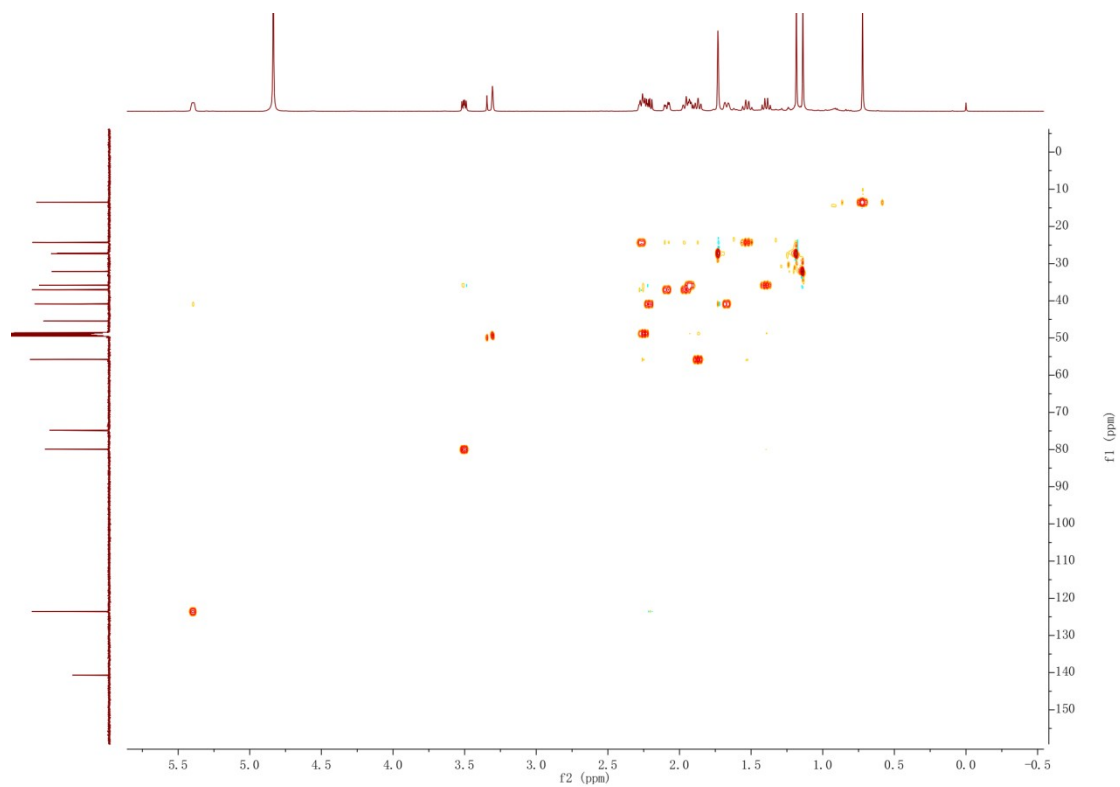


Figure S6-3. The HSQC spectrum of **5**

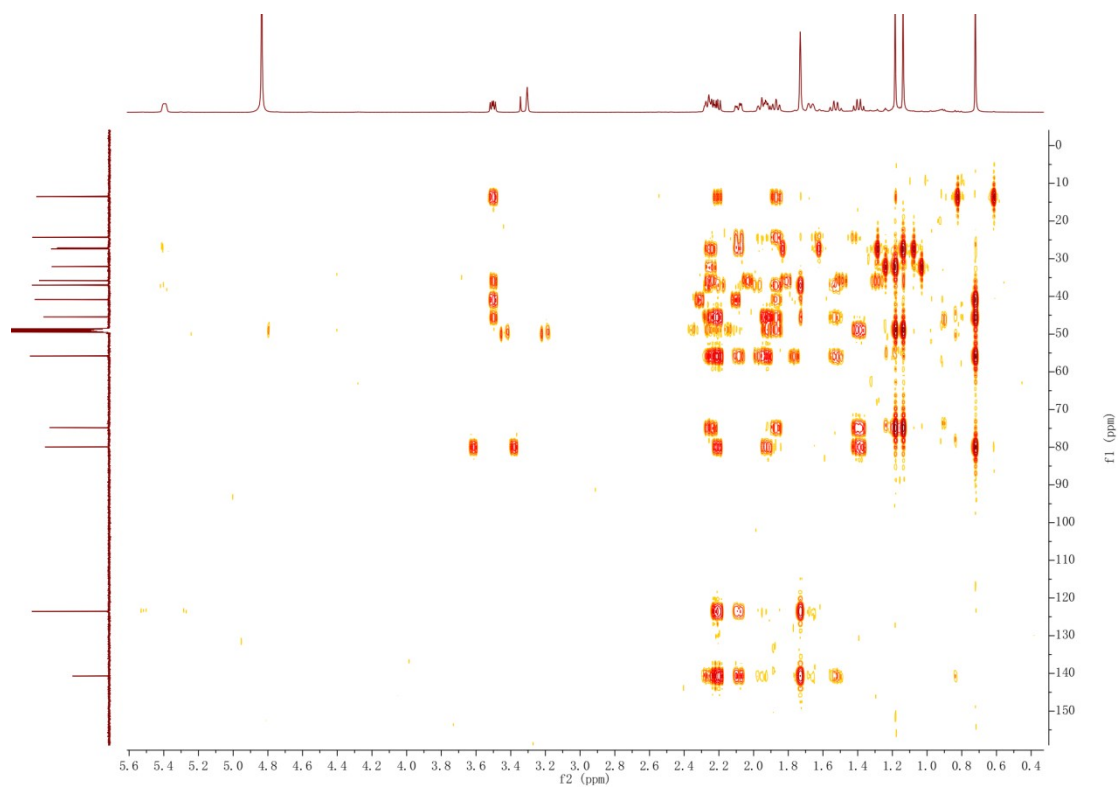


Figure S6-4. The HMBC spectrum of **5**

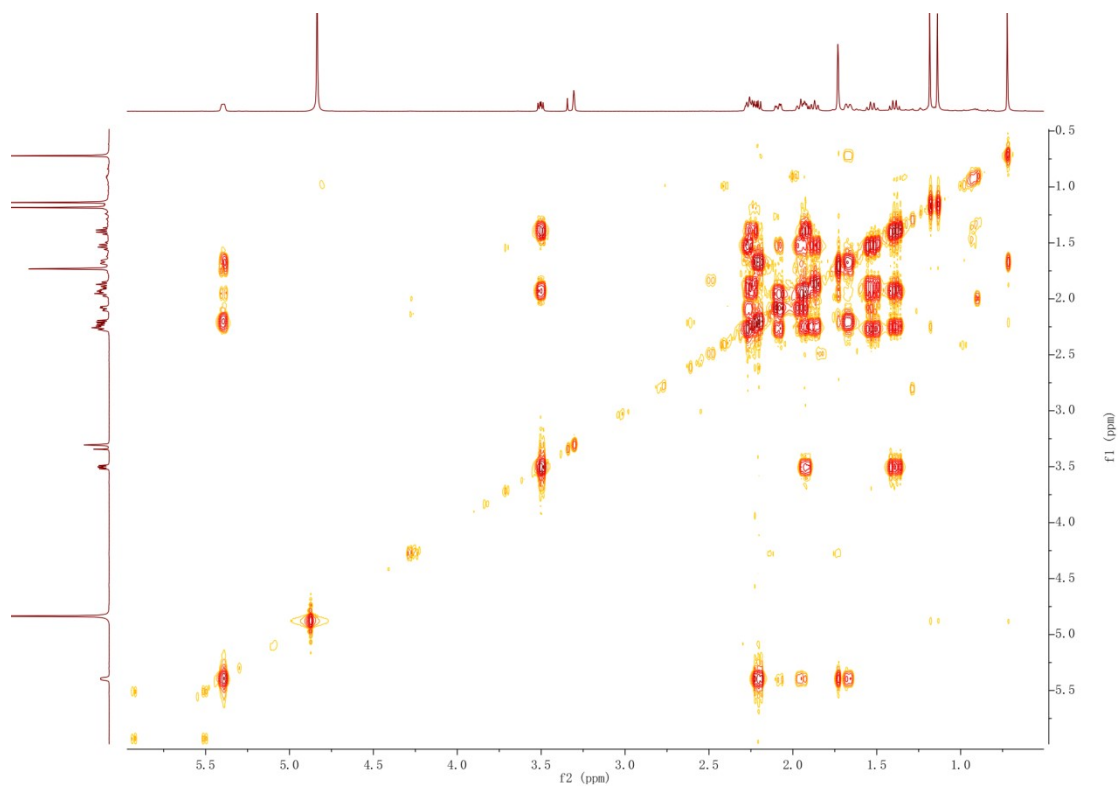


Figure S6-5. The ^1H - ^1H COSY spectrum of **5**

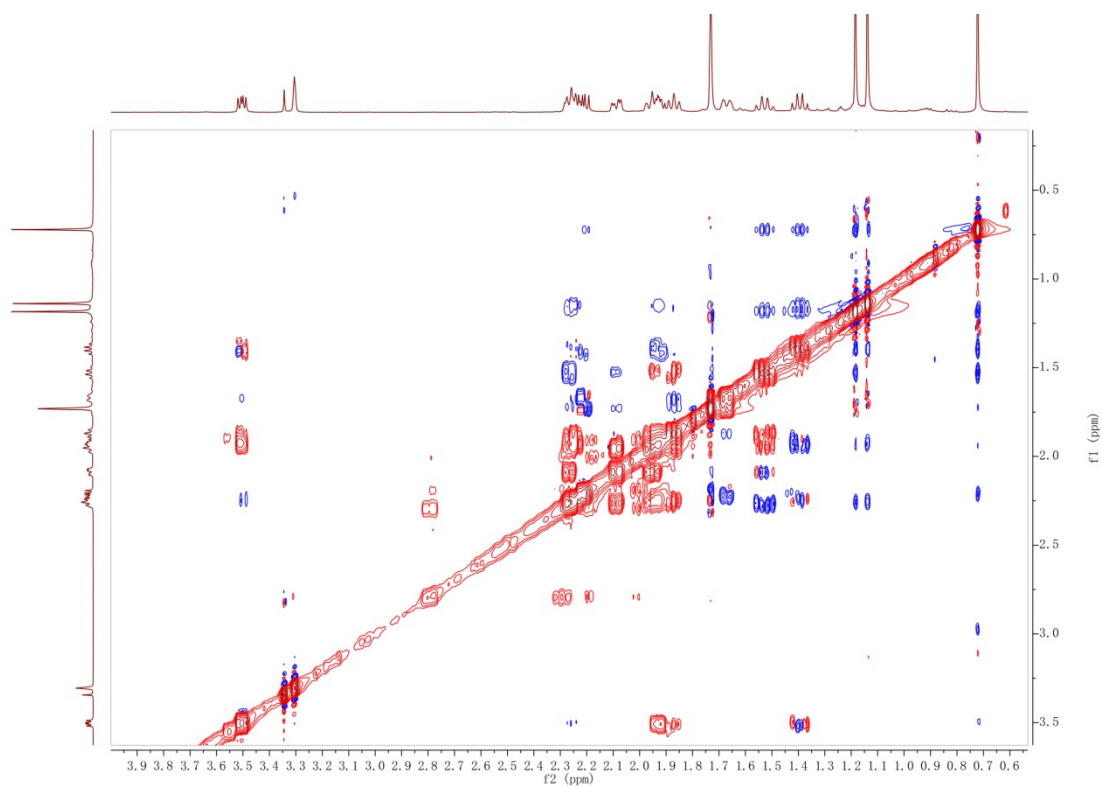


Figure S6-6. The ROESY spectrum of **5**

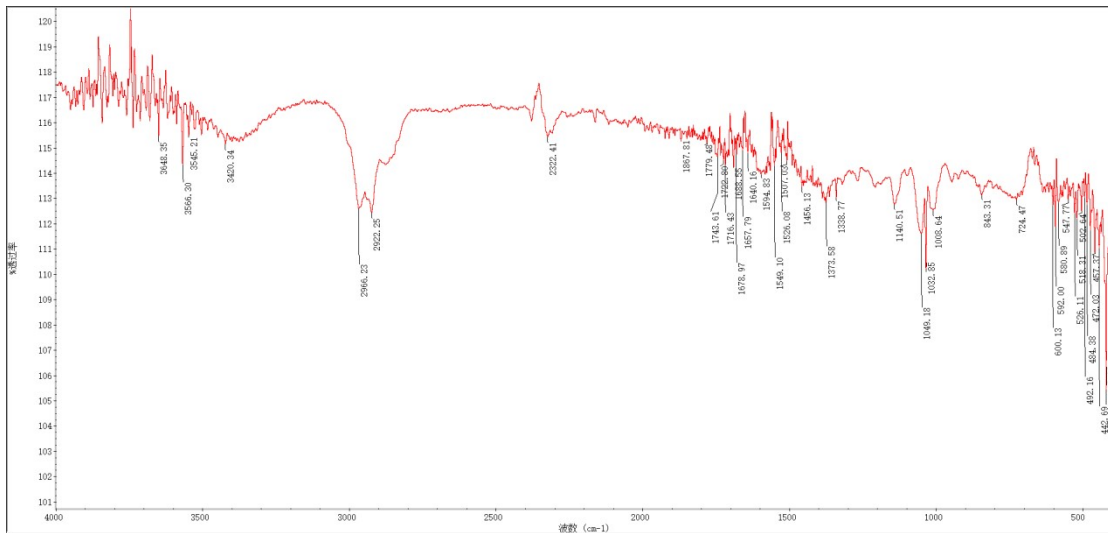
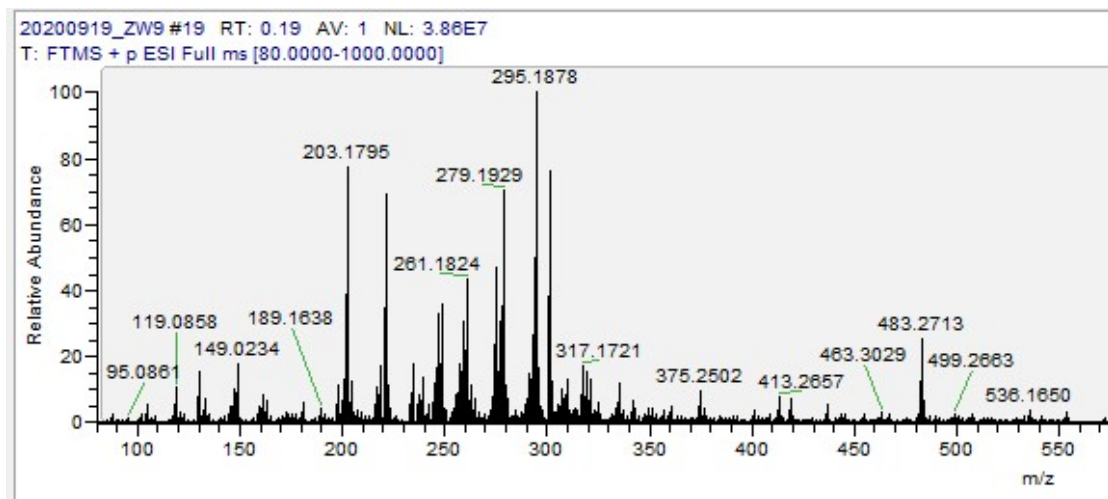


Figure S6-7. The IR spectrum of **5**



$C_{15}H_{26}O_2Na^+$ Calculated 261.1825 Found 261.1824

Figure S6-8. The HRESIMS spectrum of **5**

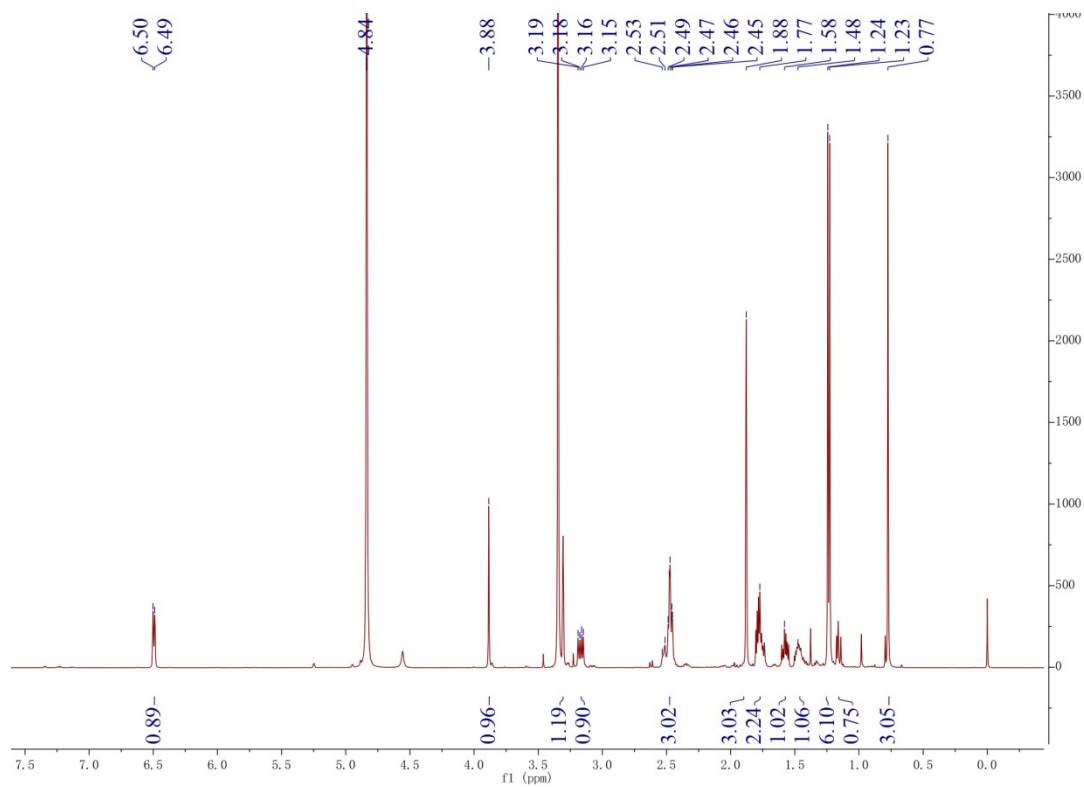


Figure S7-1. The ^1H NMR spectrum of **6**

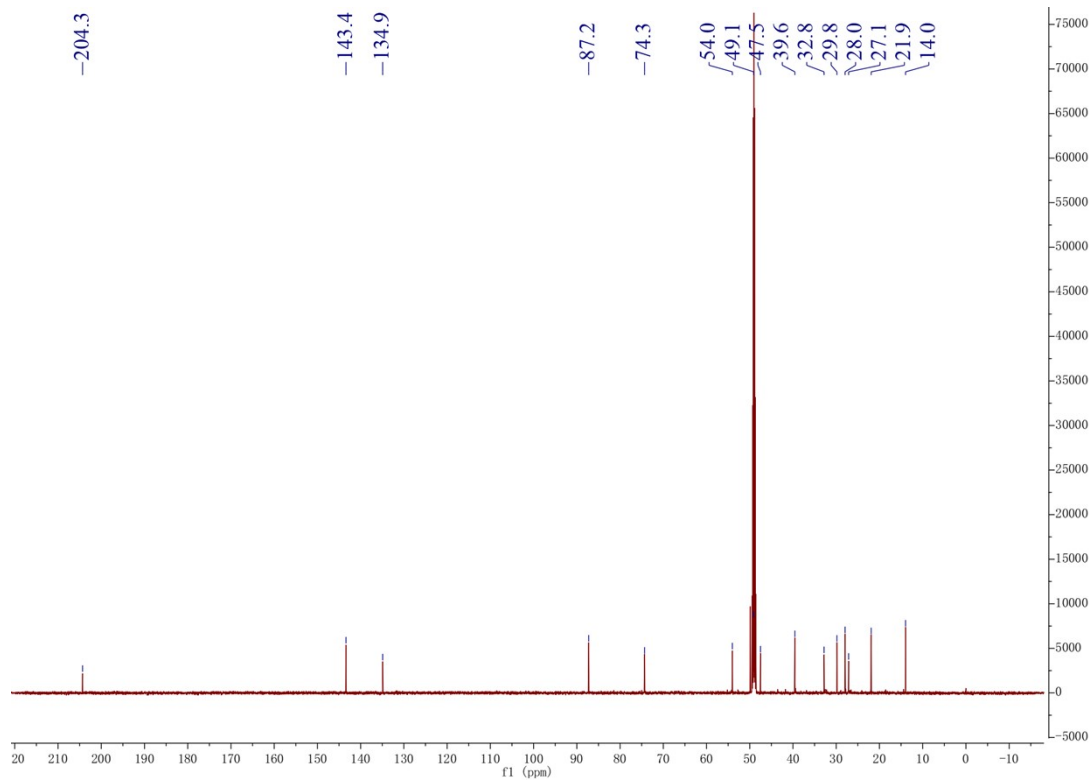


Figure S7-2. The ^{13}C NMR spectrum of **6**

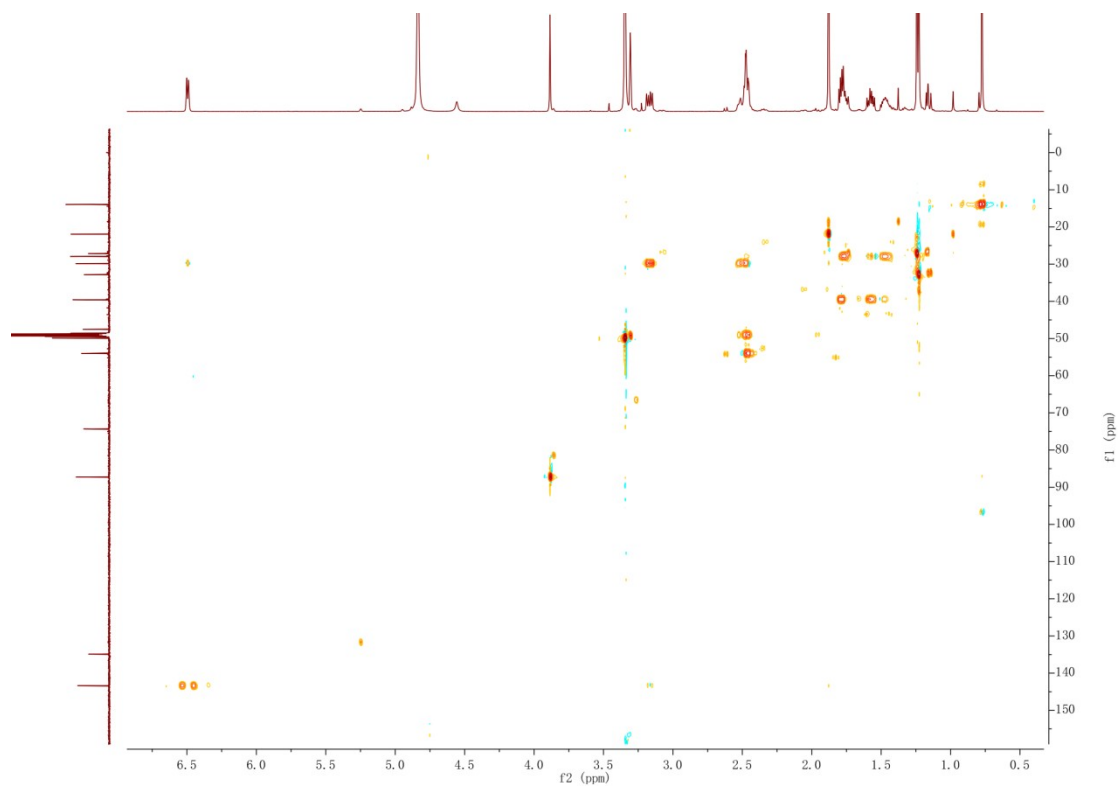


Figure S7-3. The HSQC spectrum of **6**

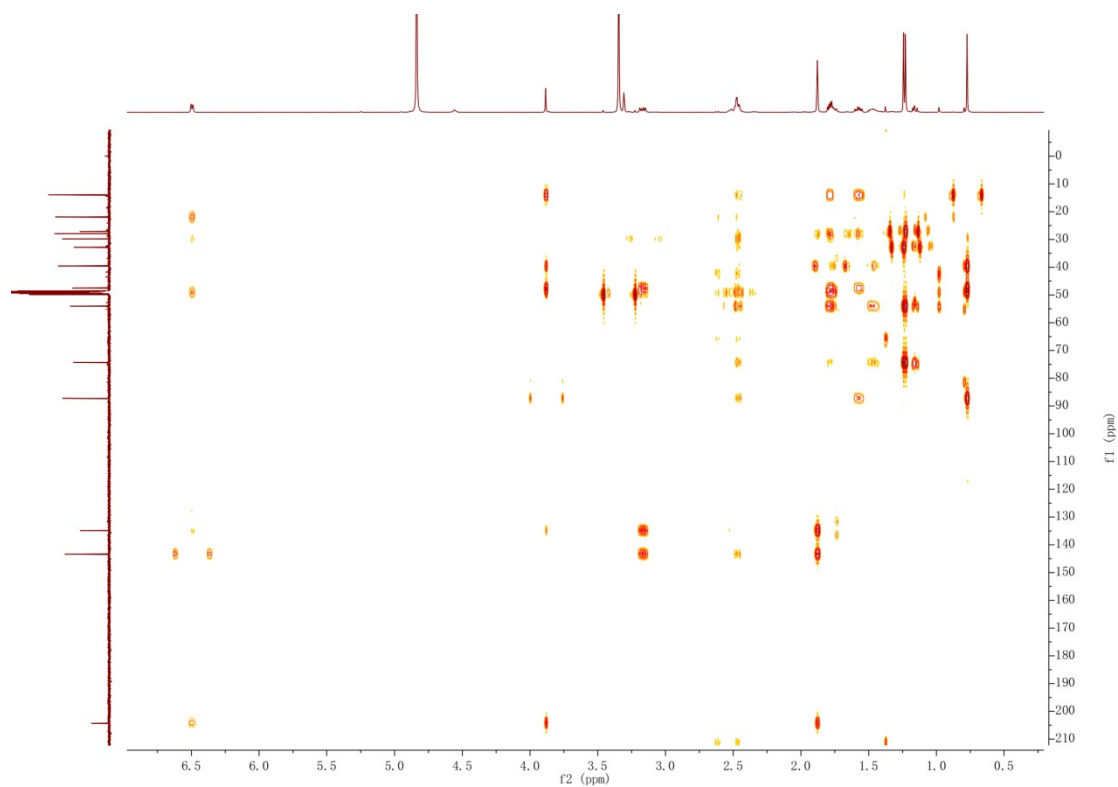


Figure S7-4. The HMBC spectrum of **6**

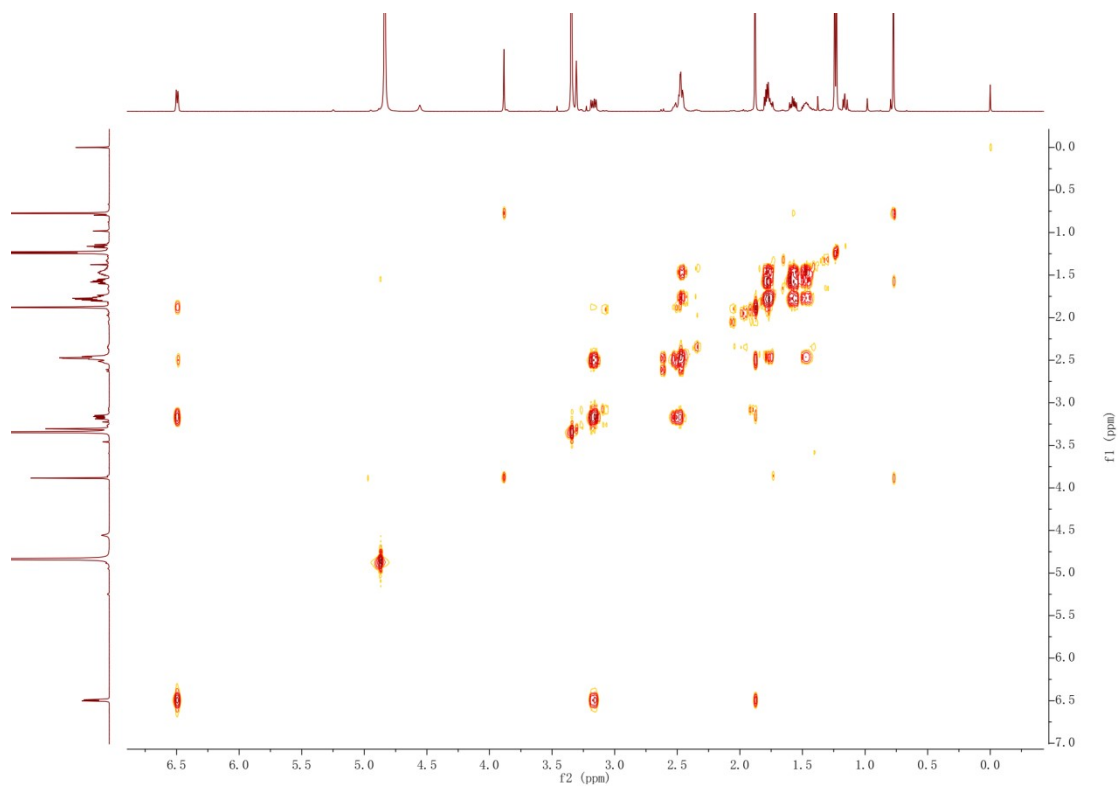


Figure S7-5. The ^1H - ^1H COSY spectrum of **6**

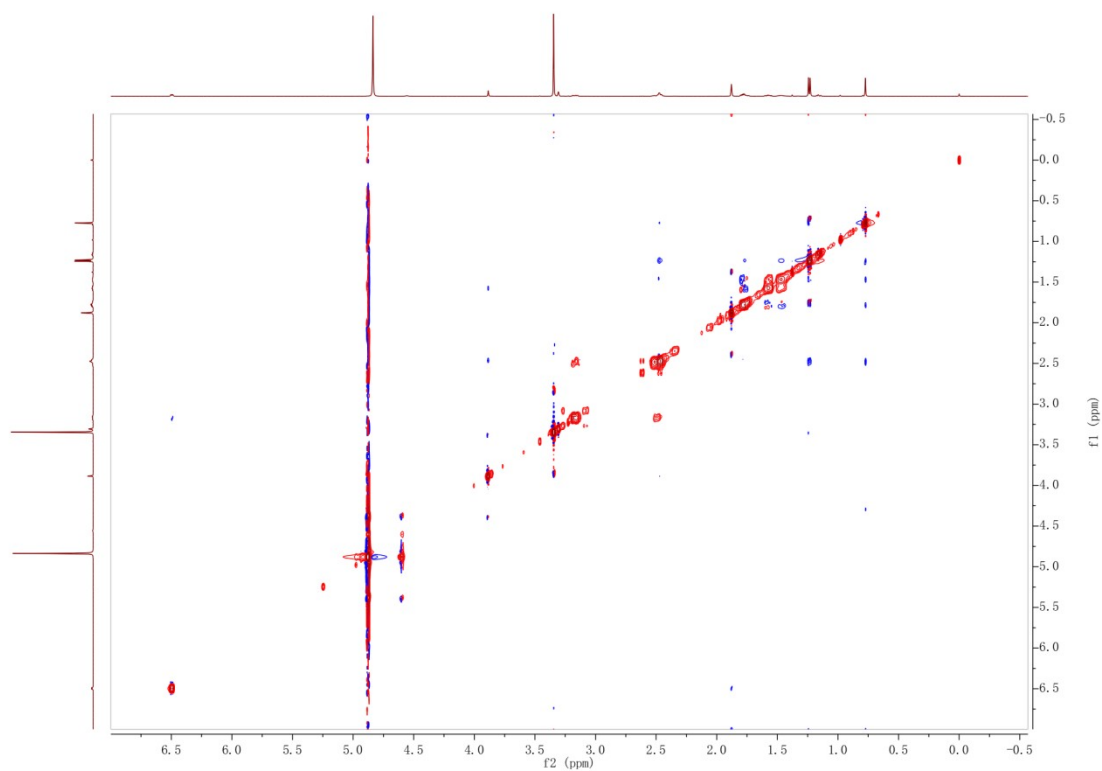


Figure S7-6. The ROESY spectrum of **6**

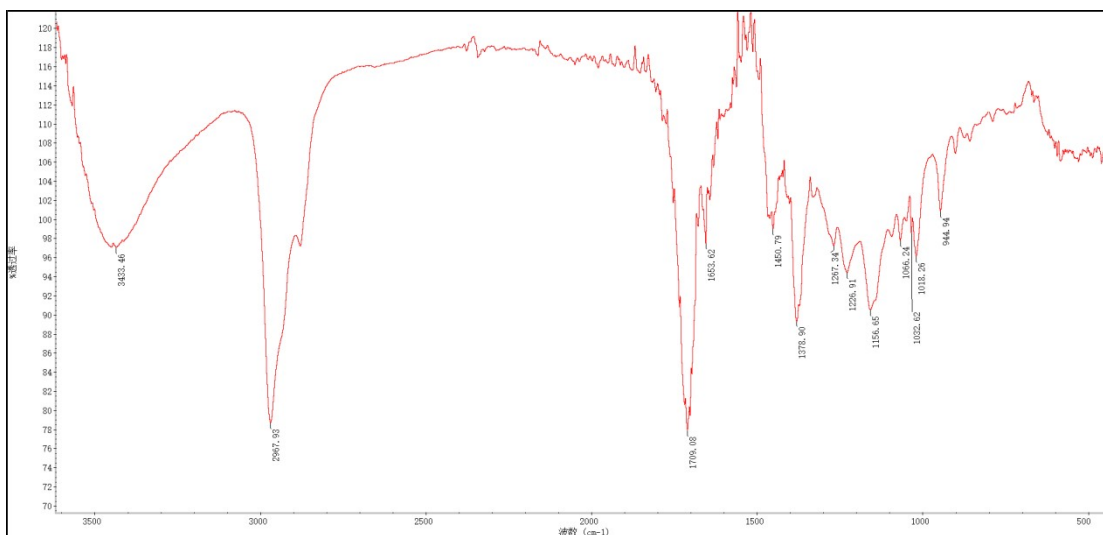
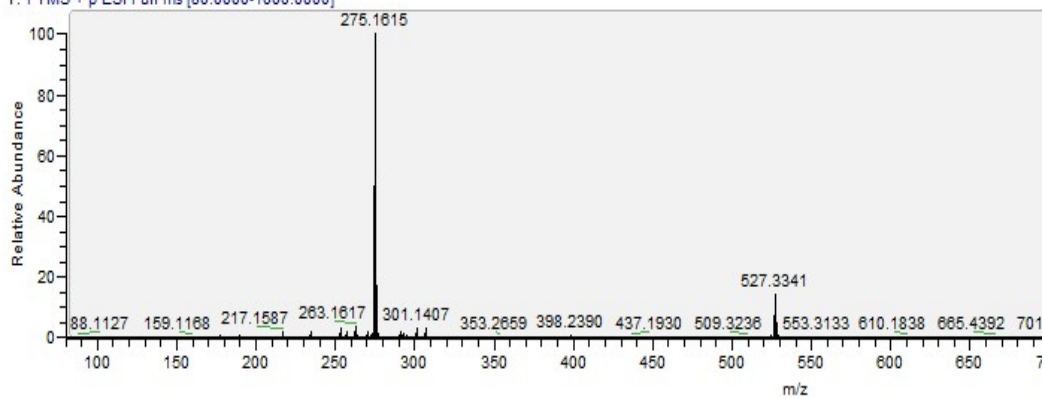


Figure S7-7. The IR spectrum of **6**

20200905_ZW_11 #13 RT: 0.12 AV: 1 NL: 1.16E9
 T: FTMS + p ESI Full ms [80.0000-1000.0000]



$C_{15}H_{26}O_2Na^+$ Calculated 275.1615 Found 275.1615

Figure S7-8. The HRESIMS spectrum of **6**

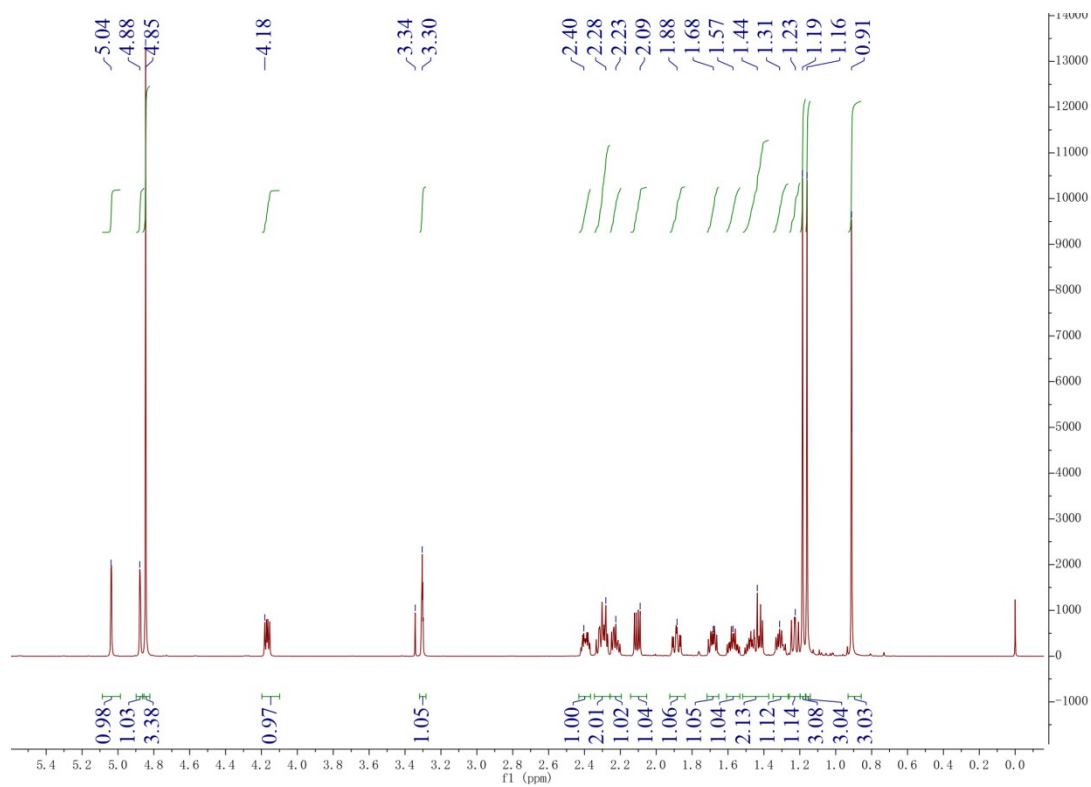


Figure S8-1. The ^1H NMR spectrum of **7**

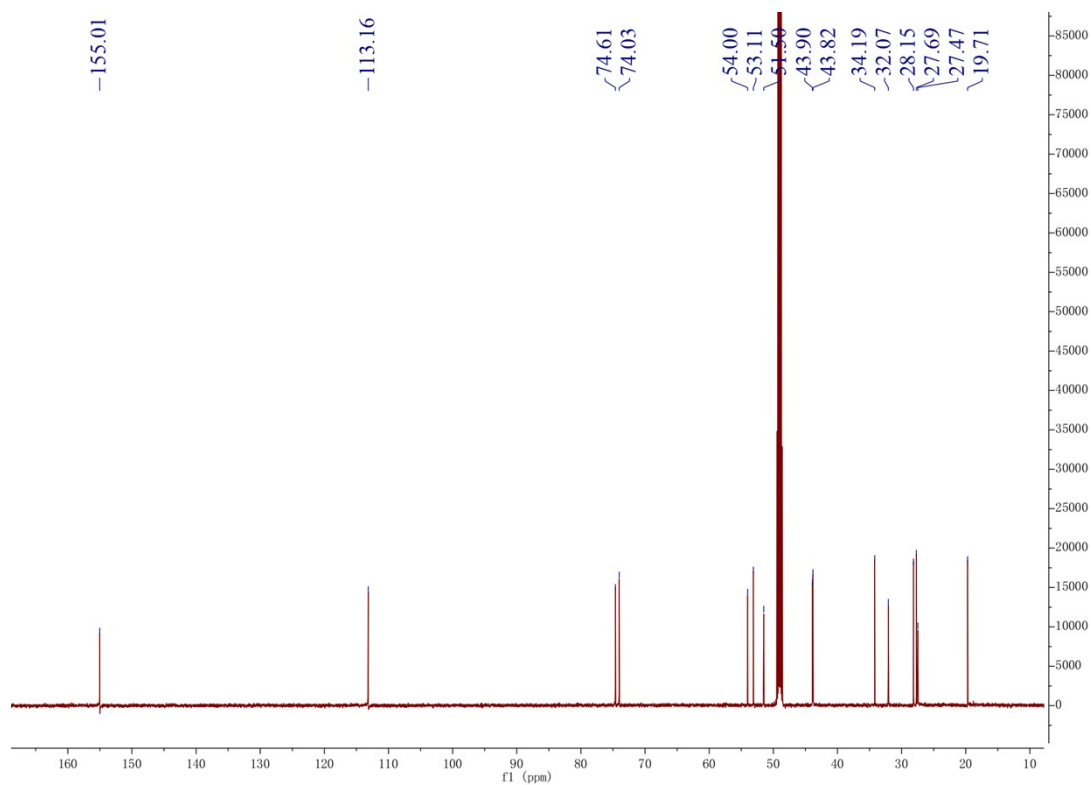


Figure S8-2. The ^{13}C NMR spectrum of **7**

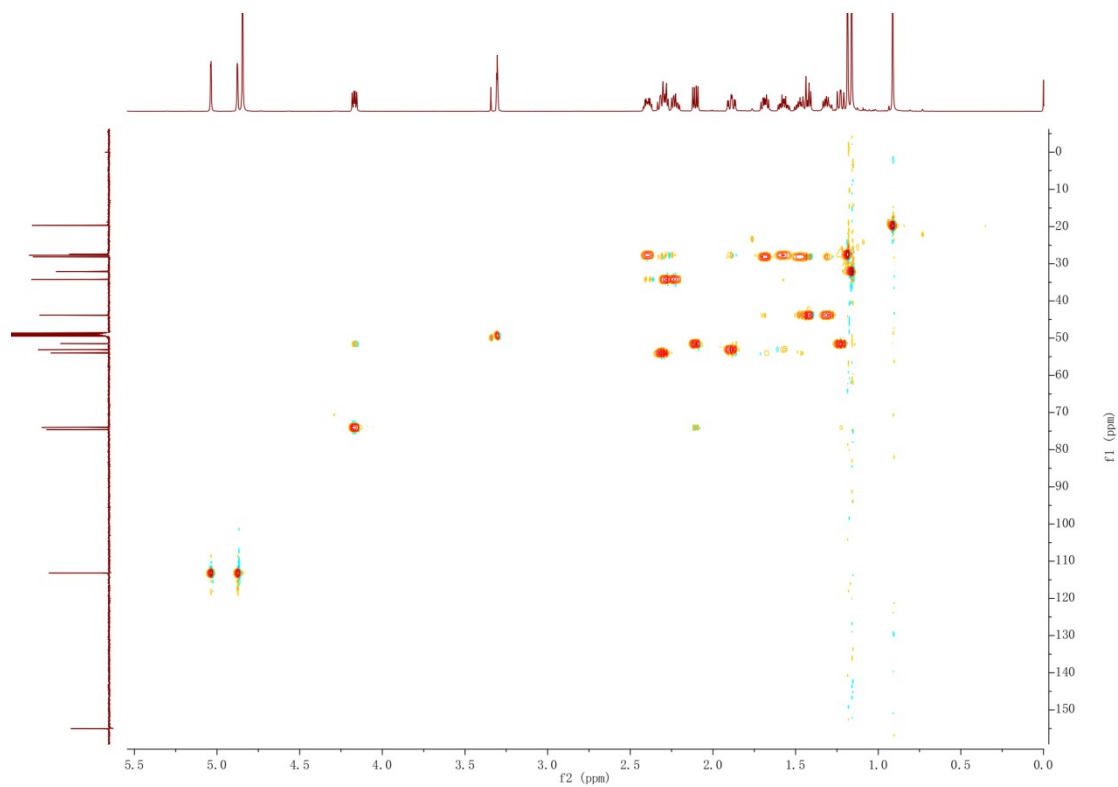


Figure S8-3. The HSQC spectrum of **7**

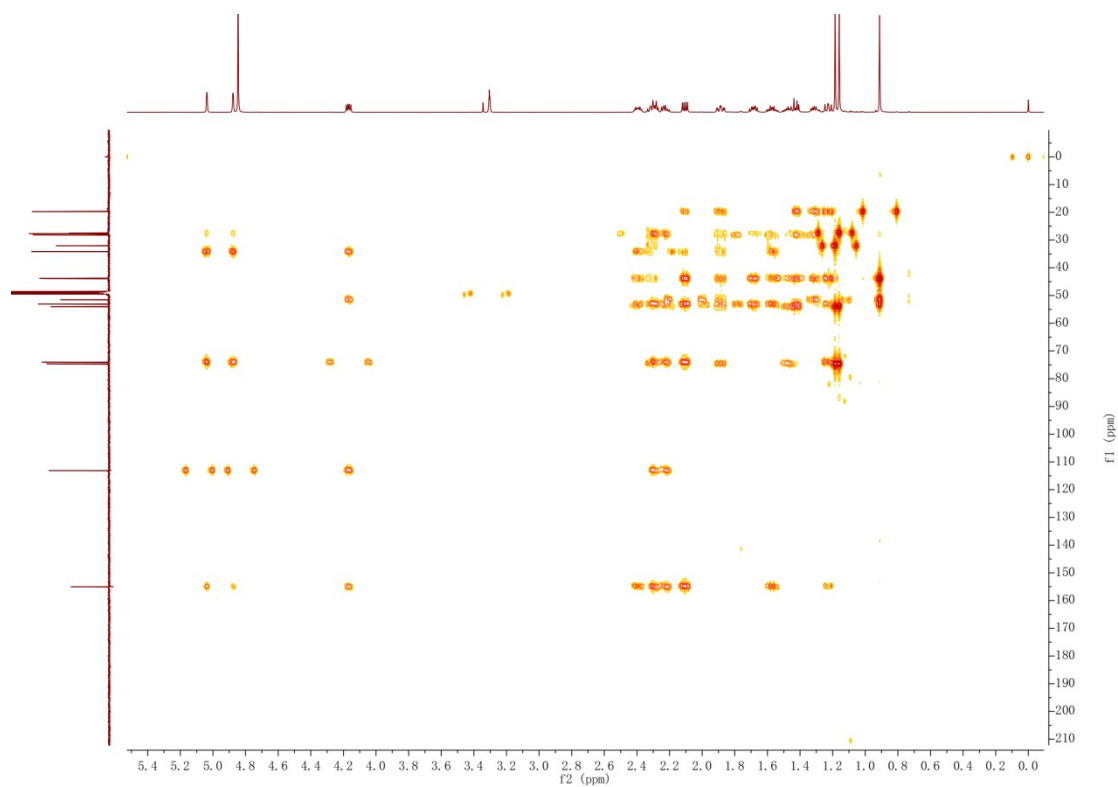


Figure S8-4. The HMBC spectrum of **7**

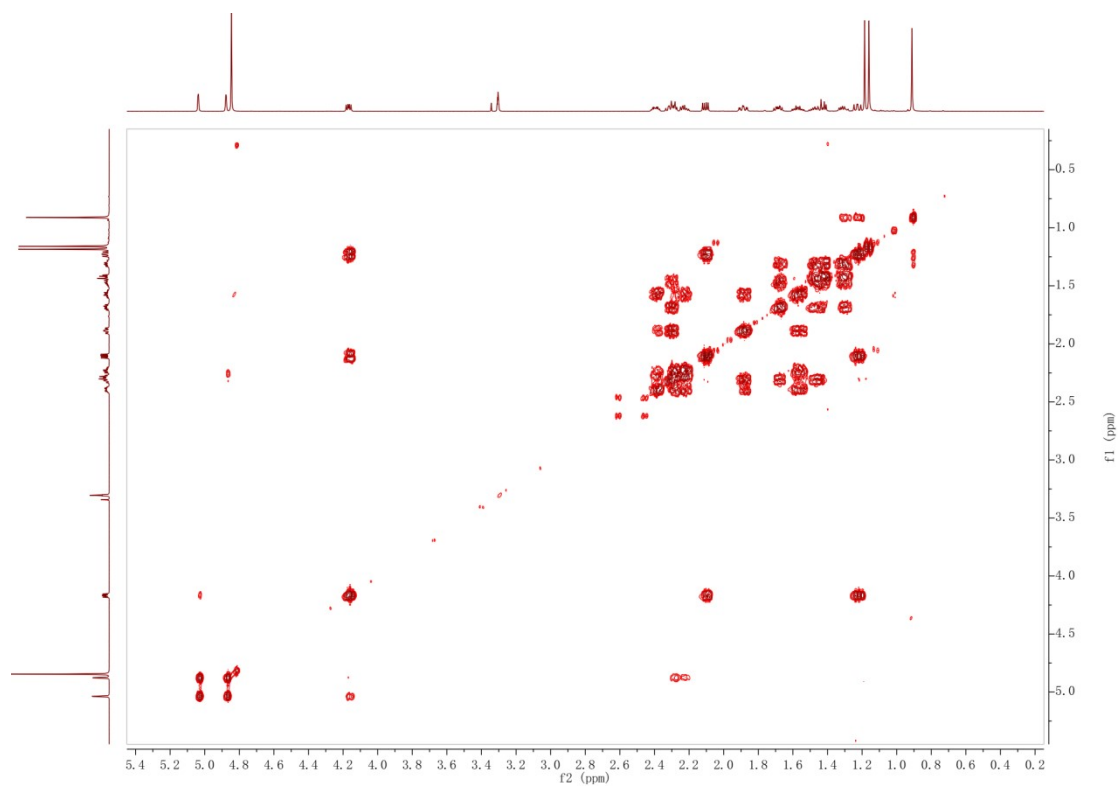


Figure S8-5. The ^1H - ^1H COSY spectrum of **7**

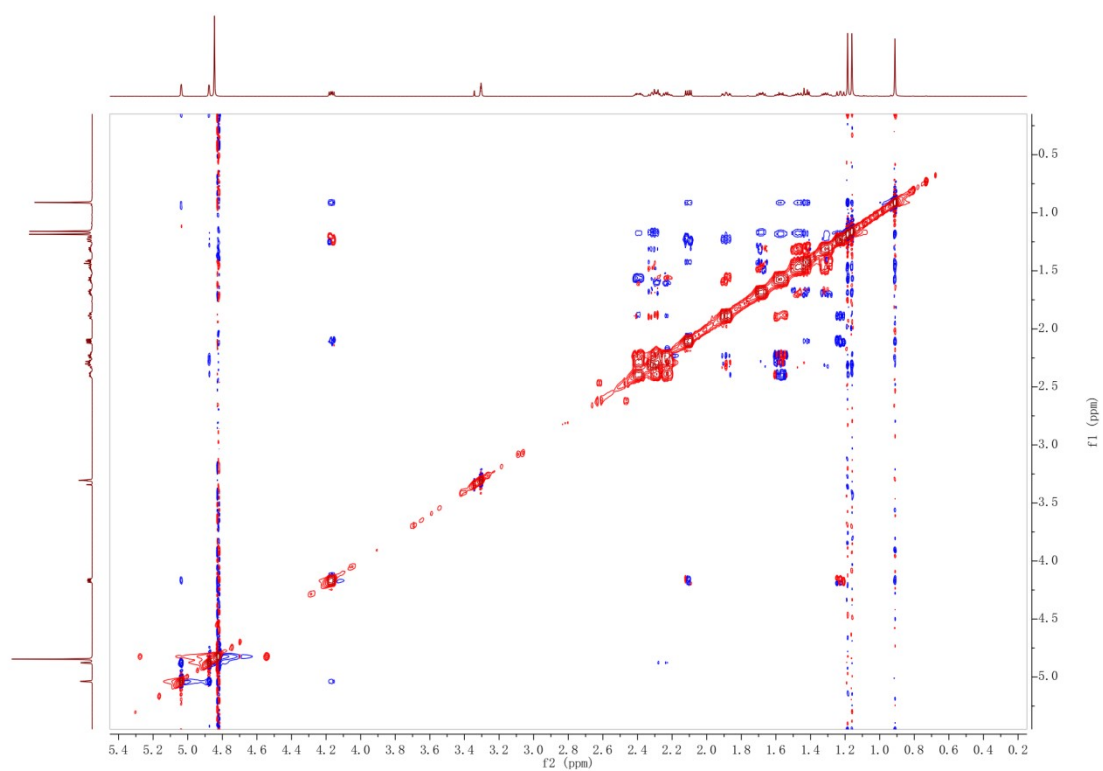


Figure S8-6. The ROESY spectrum of **7**

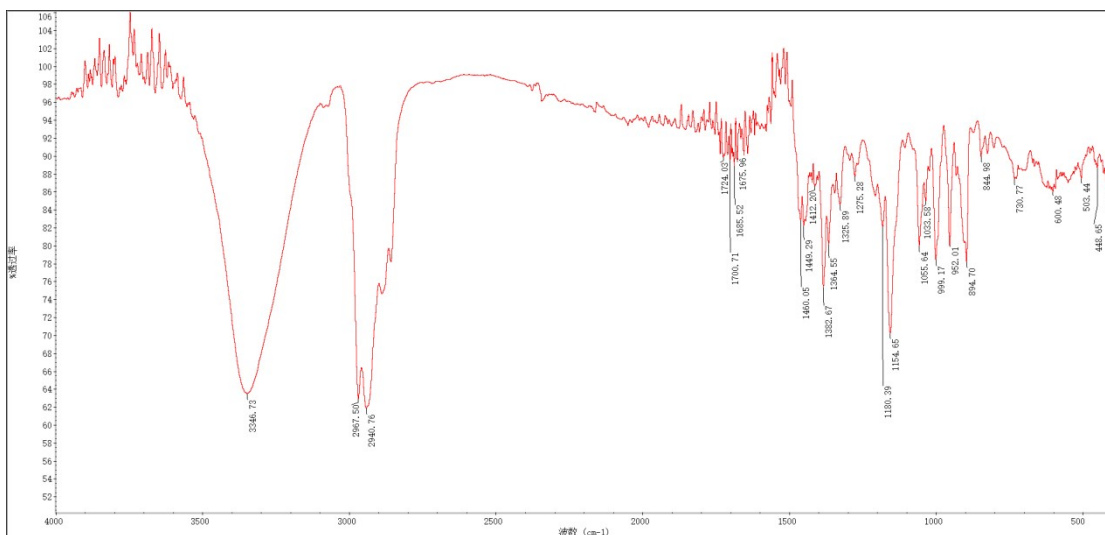
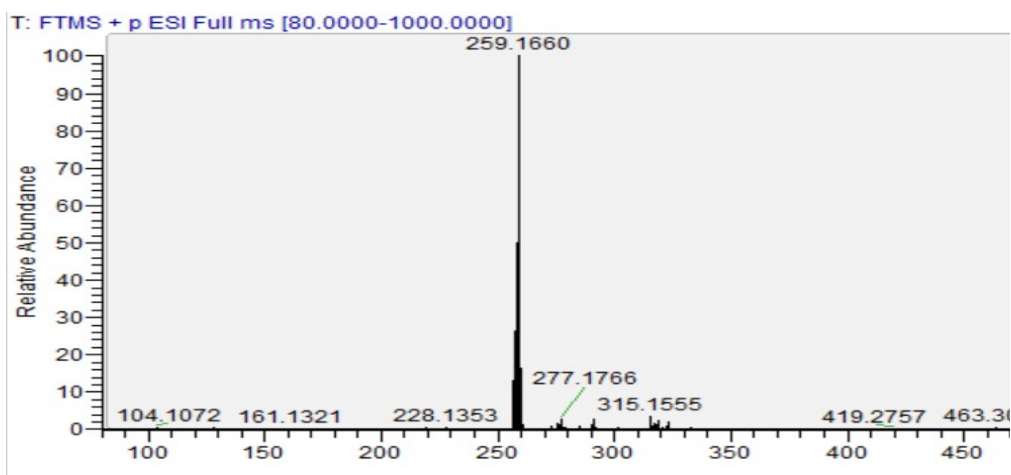


Figure S8-7. The IR spectrum of **7**



$C_{15}H_{26}O_2Na^+$ Calculated 259.1661 Found 259.1660

Figure S8-8. The HRESIMS spectrum of **7**

Compounds	IC ₅₀ (μM) ^a				
	Huh-7	MCF-7	A549	MDA-MB-231	IDH1 ^{R132h} mutant
1	>100	>100	>100	>100	>53.3
2	>100	43.38±7.22	>100	>100	>53.3
3	>100	>100	>100	>100	>53.3
4	>100	>100	>100	>100	22.27 ± 0.24
5	>100	>100	>100	>100	>53.3
6	>100	>100	>100	>100	>53.3
7	>100	>100	>100	>100	>53.3
8	>100	>100	>100	>100	>53.3
9	>100	>100	>100	>100	>53.3
10	47.03±2.48	38.33±2.04	70.48±4.40	49.06±1.81	13.99 ± 0.37
DDP	7.55±2.94	1.27±0.18	3.72±0.66	2.84±0.47	
Ivosidenb					0.051

^aValues are expressed as the mean ± SD.

Table 1. Cytotoxicity of compounds **1–10** against four tumor cell lines and the IDH1^{R132h} mutant

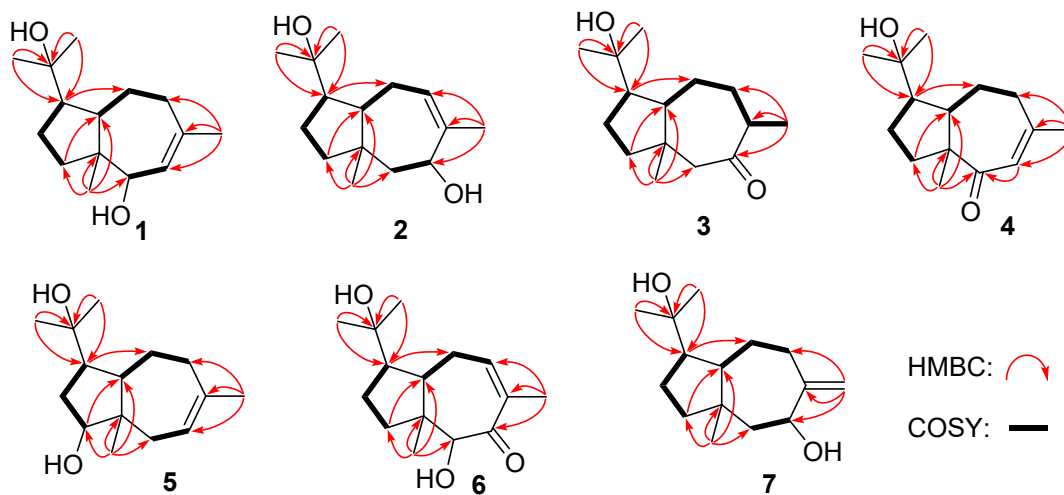


Figure S9. Key ^1H - ^1H and HMBC correlations of 1-7

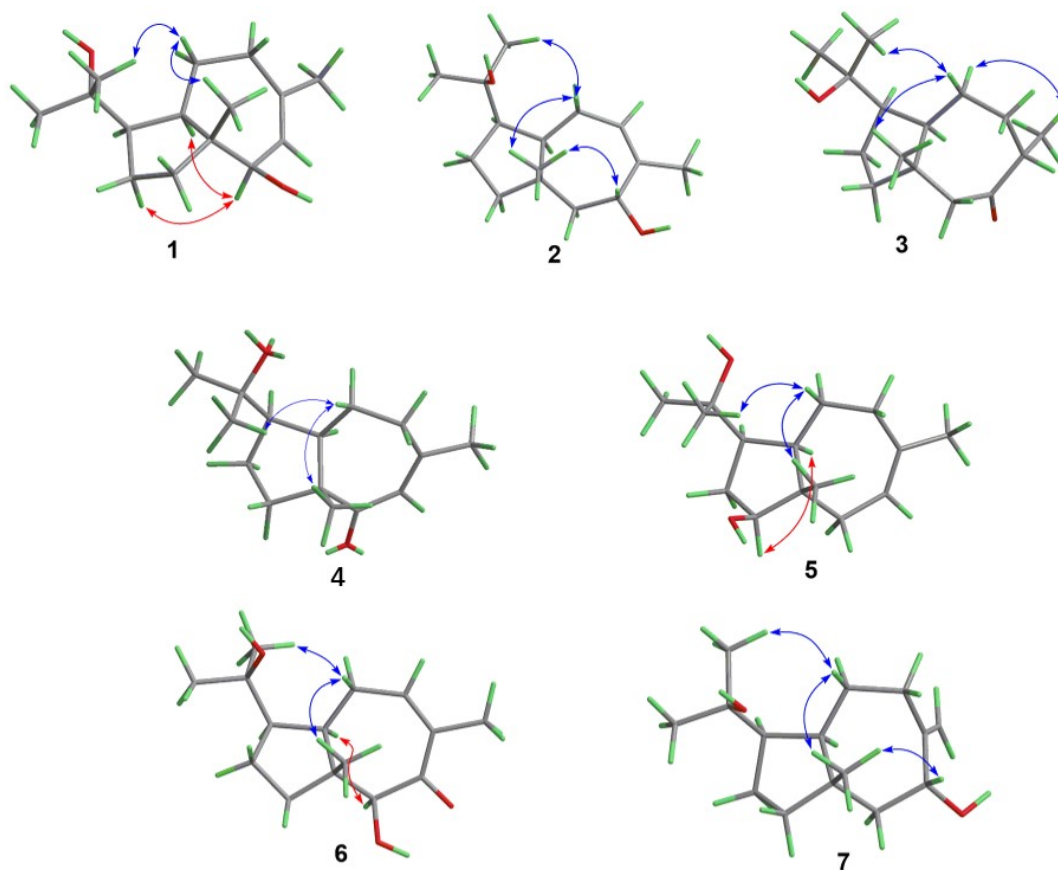


Figure S10. Key ROESY correlations of 1-7

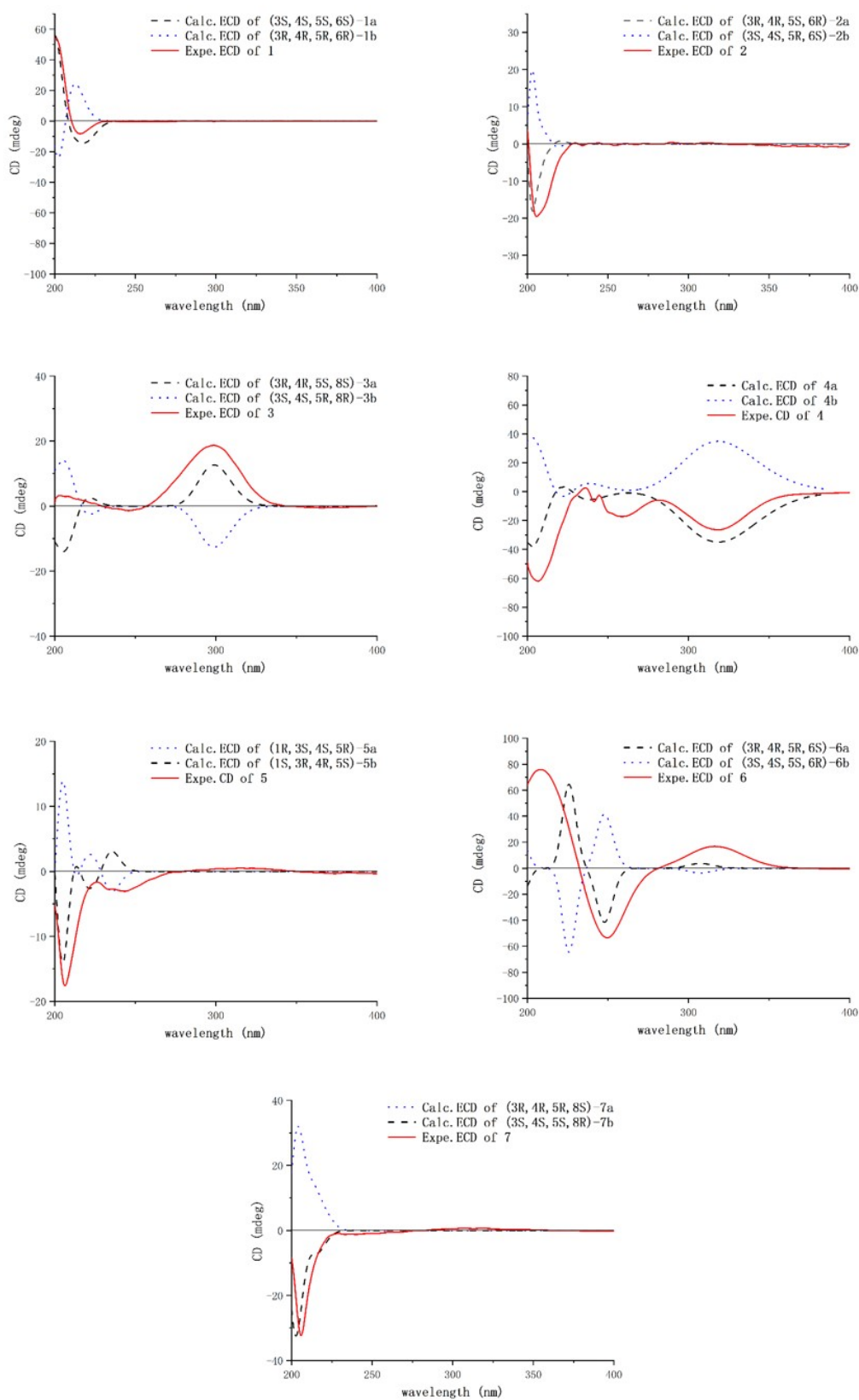


Figure S11. Calculated and experimental electronic circular dichroism (ECD) spectra of 1-7