

## Supporting Information

# **Anti-inflammatory Polyketide Derivatives from the Sponge-Derived Fungus *Pestalotiopsis* sp. SWMU-WZ04-2**

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

Figure S2.  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) spectrum of the new compound **1**

Figure S3.  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ ) spectrum of the new compound **1**

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S36. Computational details for compound **1-4** (ECD)

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Figure S38. Calculated and experimental ECD spectras of **1** using model.

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**Table S2.** Energy analysis for conformers of **2** at B3LYP/6-31G(d) level

**Table S3.** Energy analysis for conformers of **3** at B3LYP/6-31G(d) level

## Qualitative Analysis Report

Data Filename	J-13-POS.d	Sample Name	Sample9
Sample Type	Sample	Position	P1-A9
Instrument Name	Instrument 1	User Name	
Acq Method	default-20200902-pos.m	Acquired Time	7/1/2021 9:47:15 AM
IRM Calibration Status		DA Method	analysis.m
Comment			

Sample Group      Info.

### User Spectra

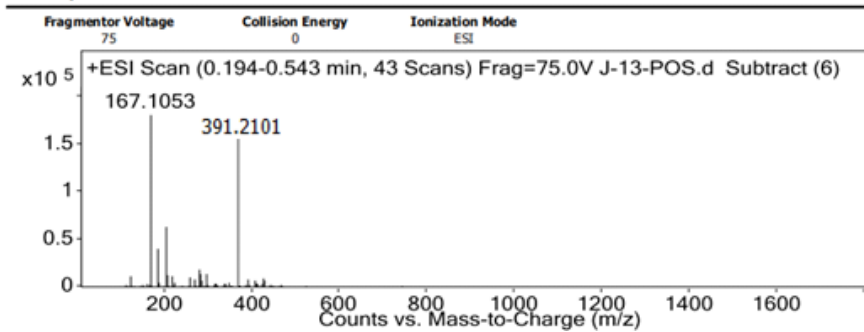


Figure S1. HRESI-MS spectrum of the new compound **1**

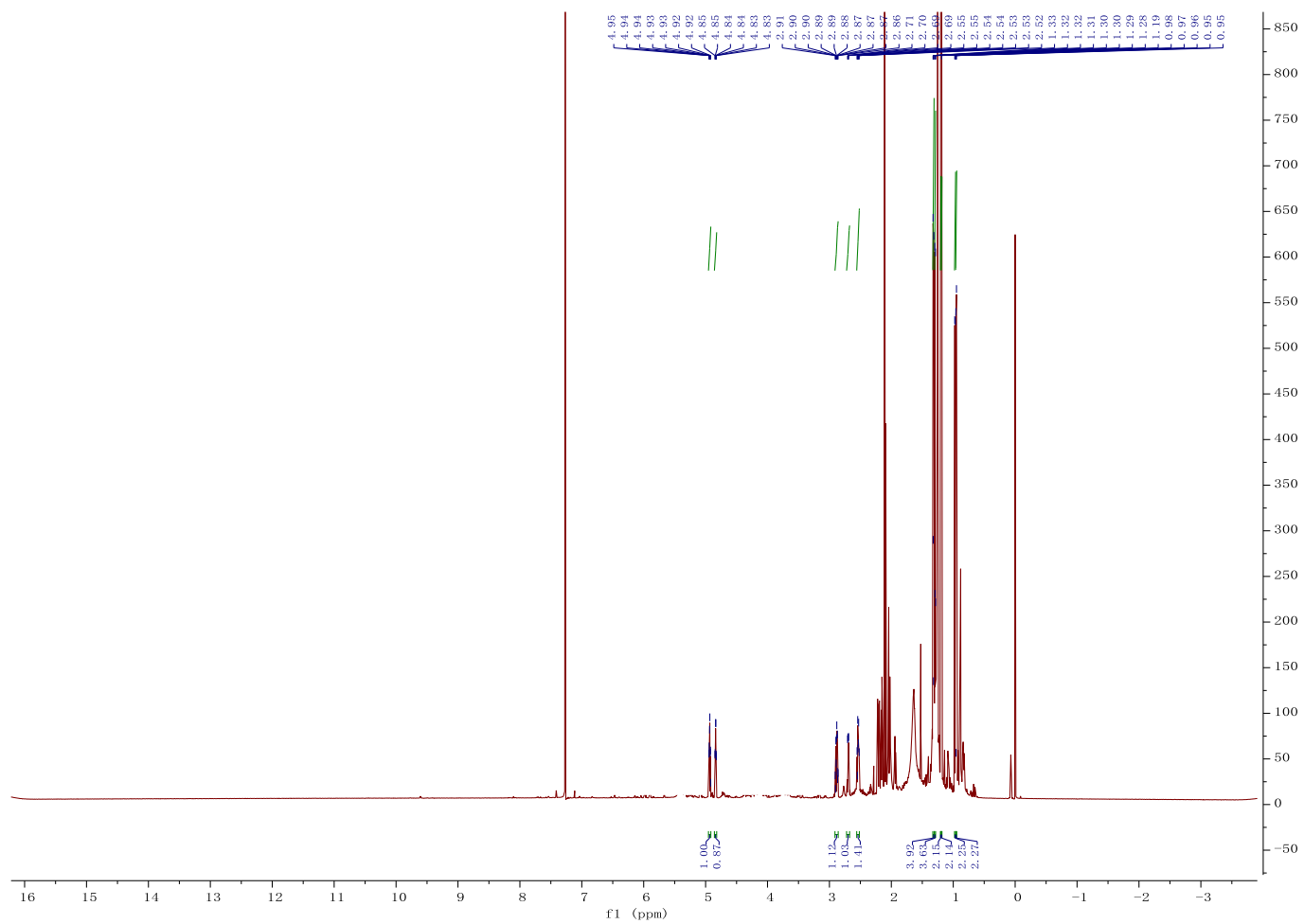


Figure S2.  $^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ ) spectrum of the new compound **1**

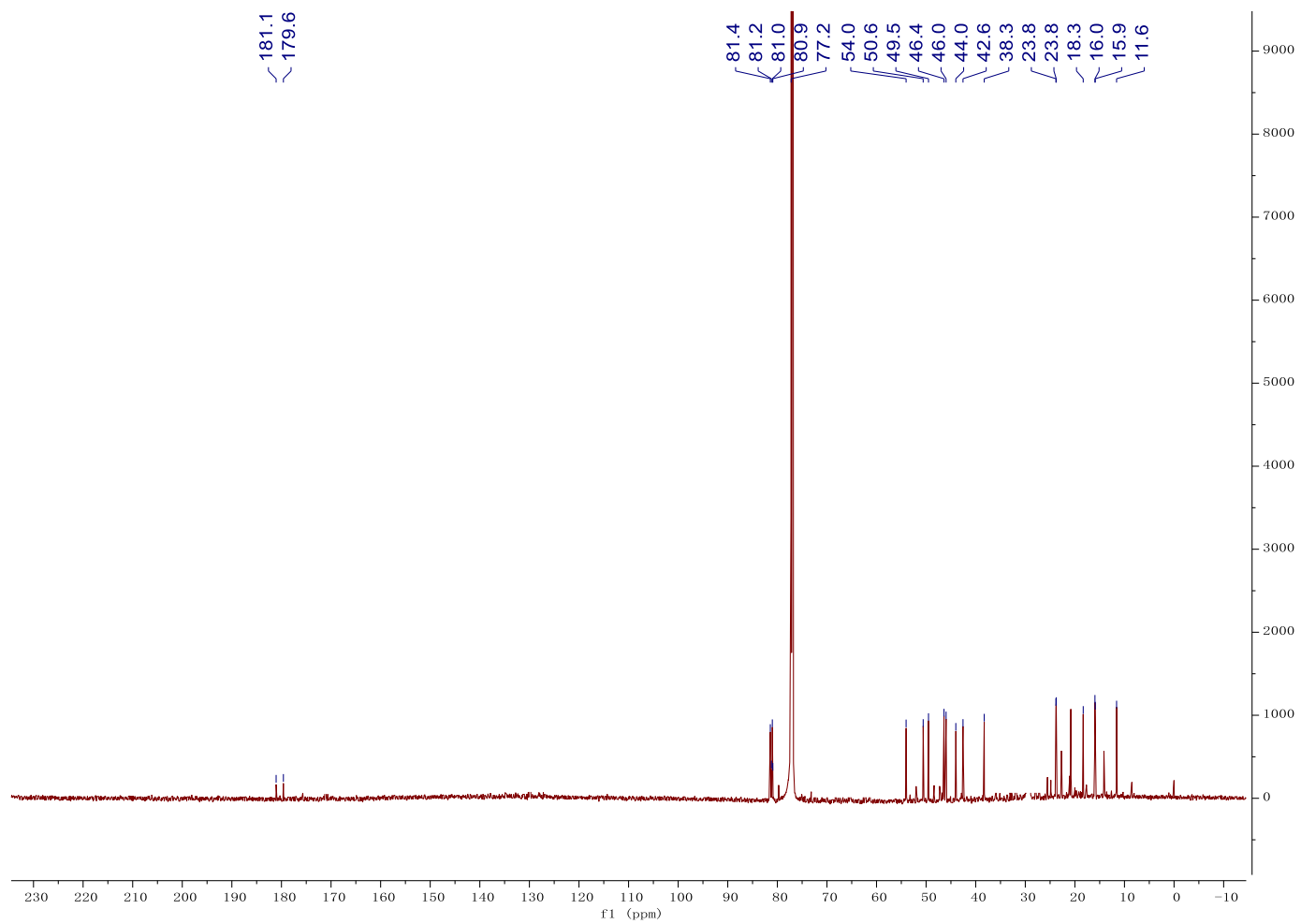


Figure S3. <sup>13</sup>C NMR (150 MHz, CDCl<sub>3</sub>) spectrum of the new compound **1**

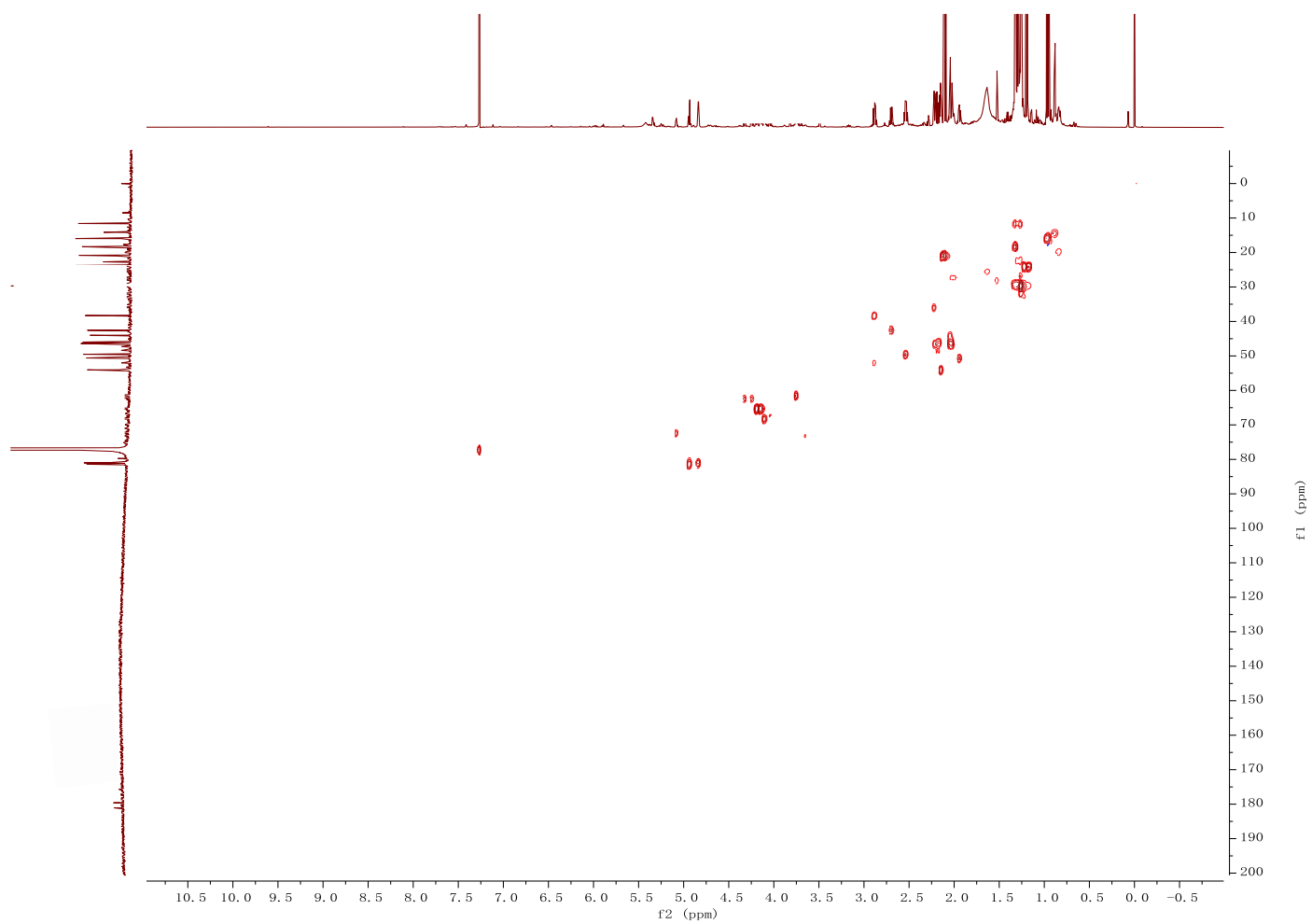


Figure S4. HSQC spectrum of the new compound **1**



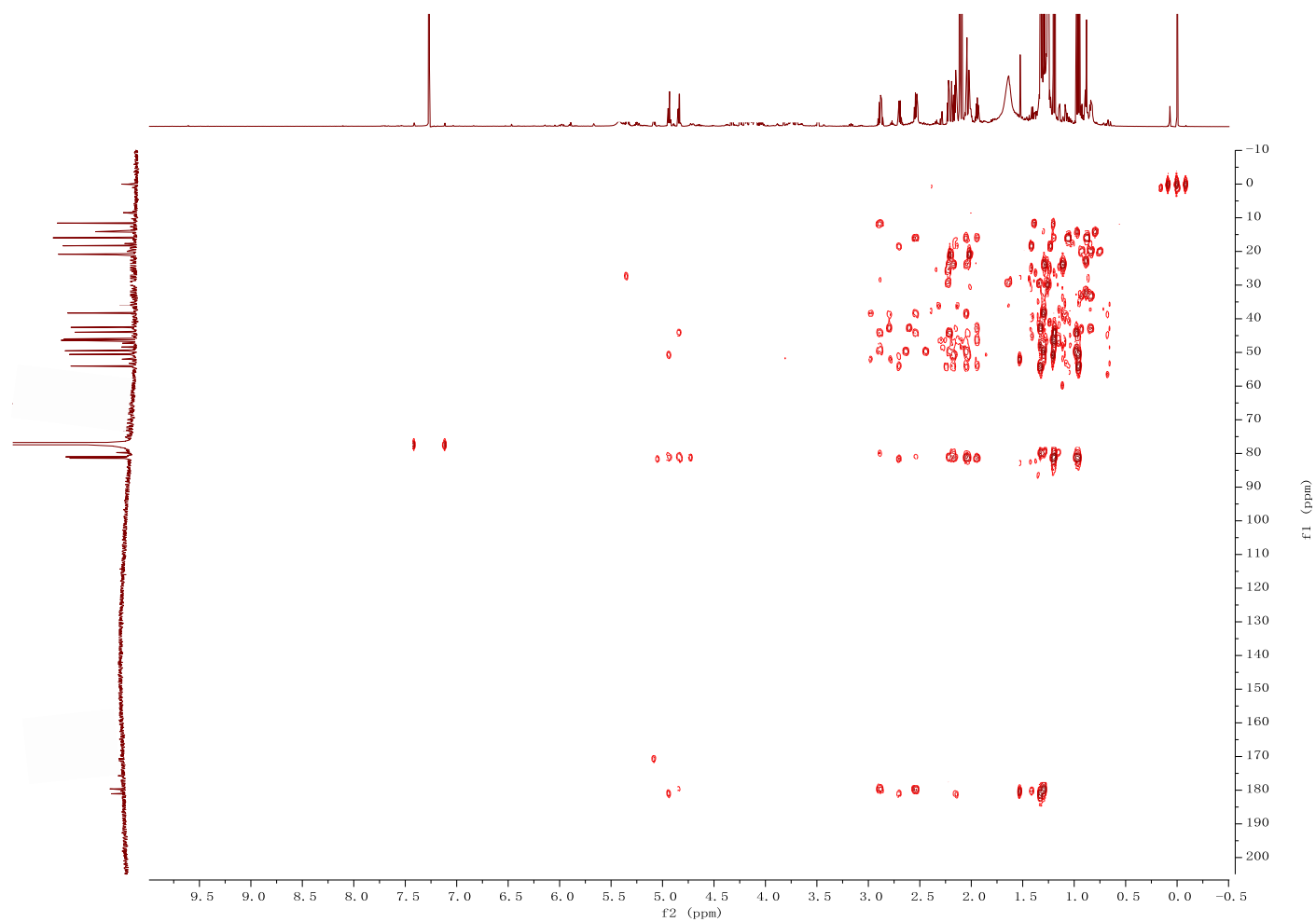


Figure S5. HMBC spectrum of the new compound **1**

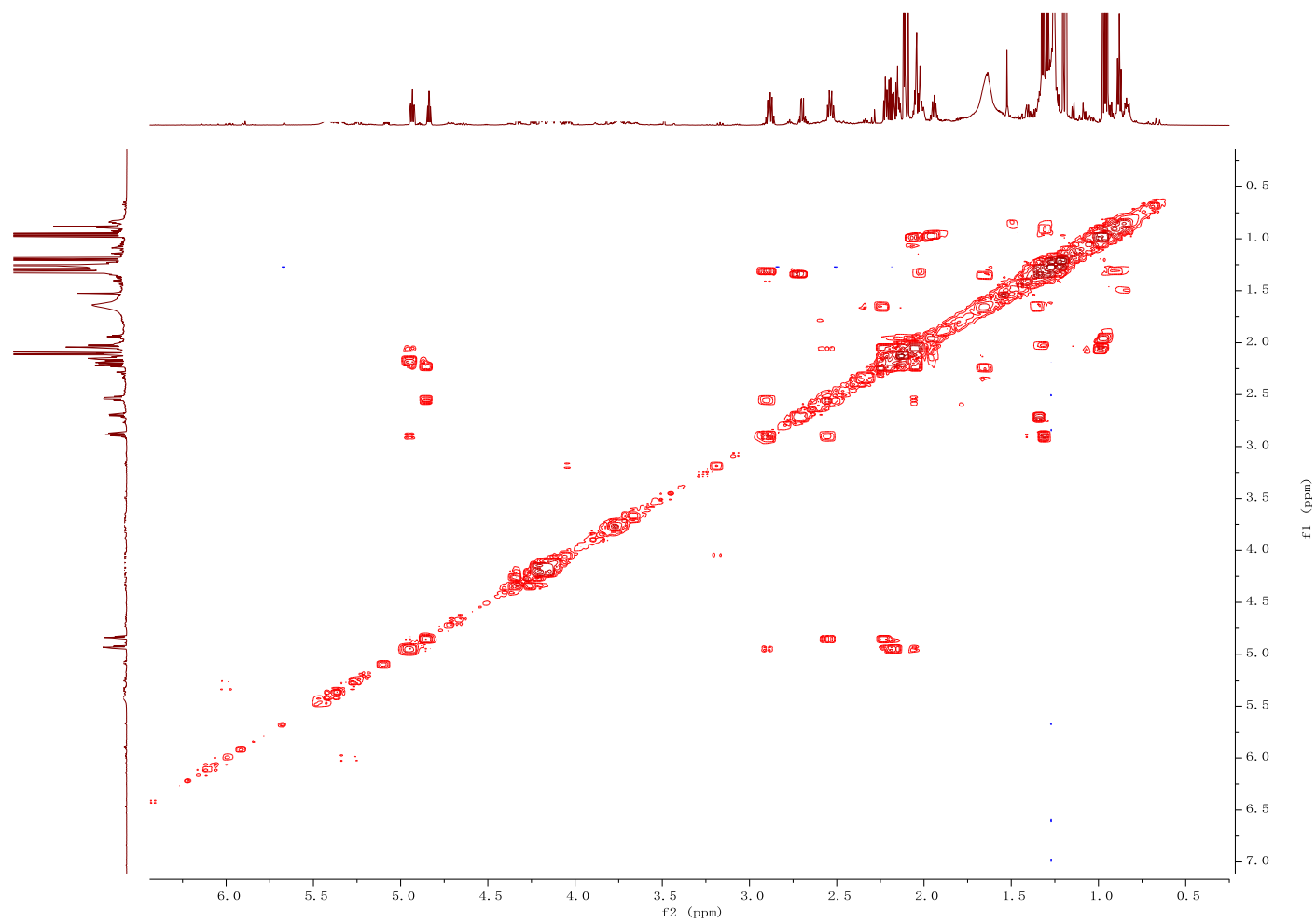


Figure S6. COSY spectrum of the new compound **1**

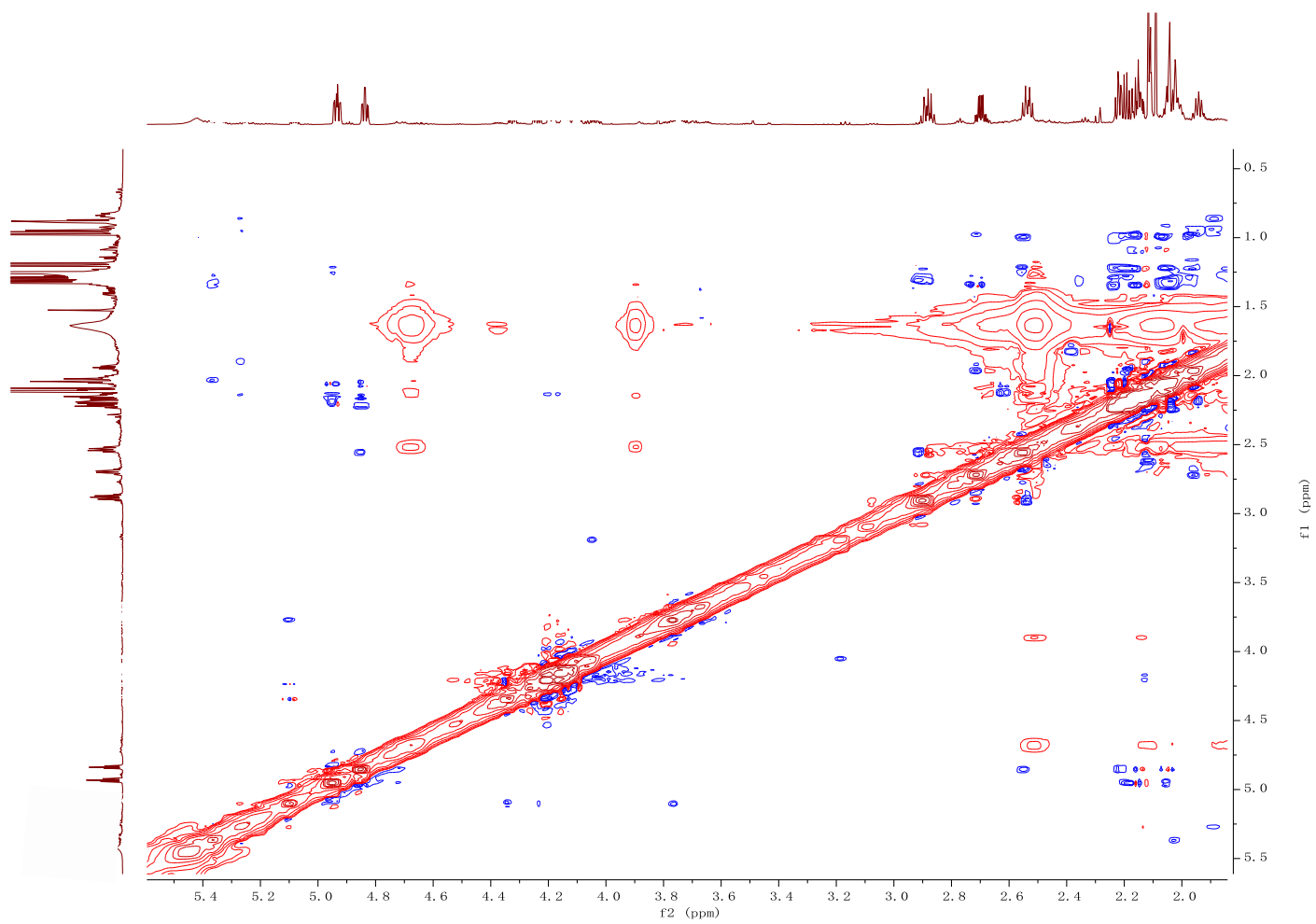


Figure S7. NOESY spectrum of the new compound **1**

## Qualitative Analysis Report

Data Filename	L13-3-NEG.d	Sample Name	Sample11
Sample Type	Sample	Position	P1-B2
Instrument Name	Instrument 1	User Name	
Acq Method	default-20200902-neg.m	Acquired Time	7/1/2021 12:38:29 PM
IRM Calibration Status	Some Ions Missed	DA Method	analysis.m
Comment			

Sample Group      Info.

### User Spectra

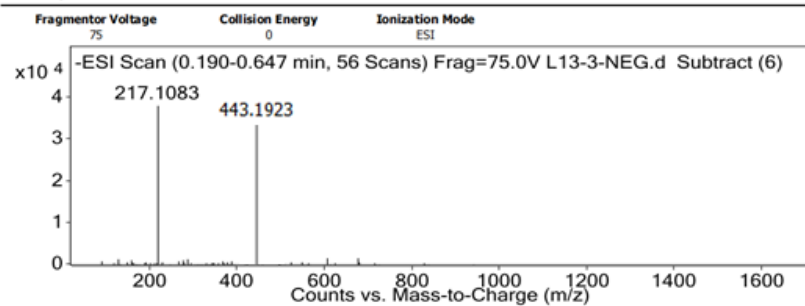


Figure S8. HRESI-MS spectrum of the new compound **2**

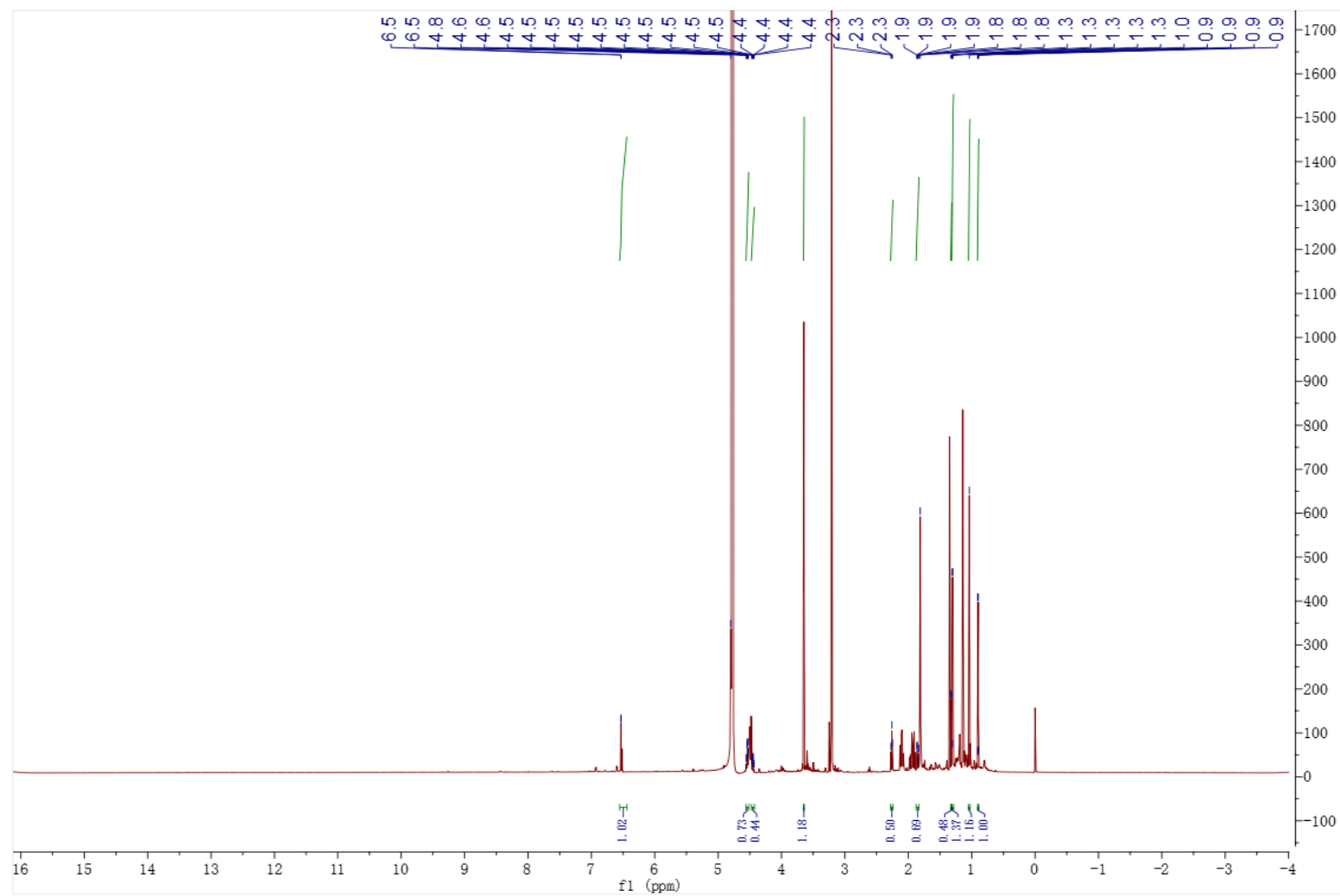


Figure S9.  $^1\text{H}$  NMR (600 MHz,  $\text{CD}_3\text{OD}$ ) spectrum of the new compound **2**

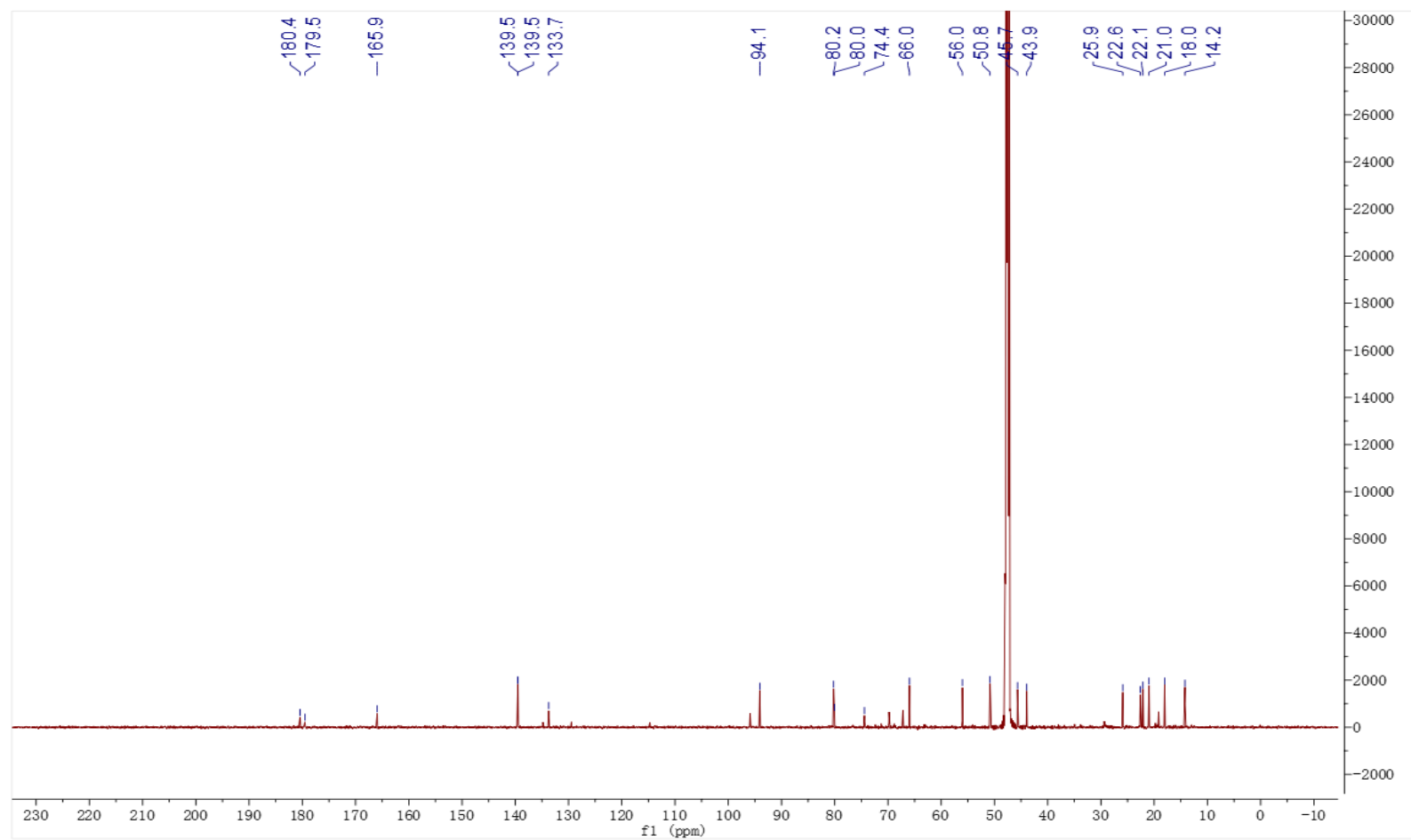


Figure S10. <sup>13</sup>C NMR (150 MHz, CD<sub>3</sub>OD) spectrum of the new compound **2**

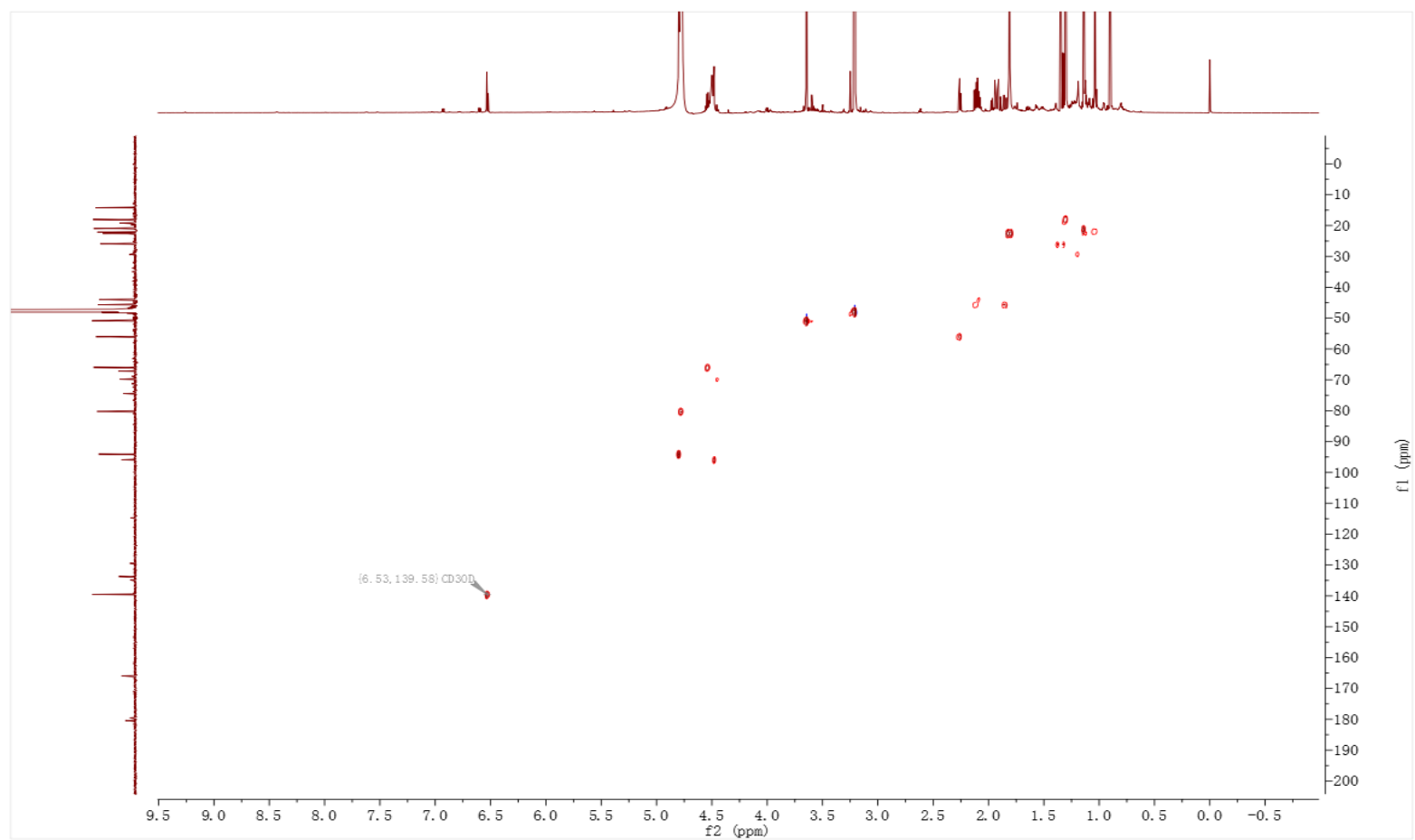


Figure S11. HSQC spectrum of the new compound **2**

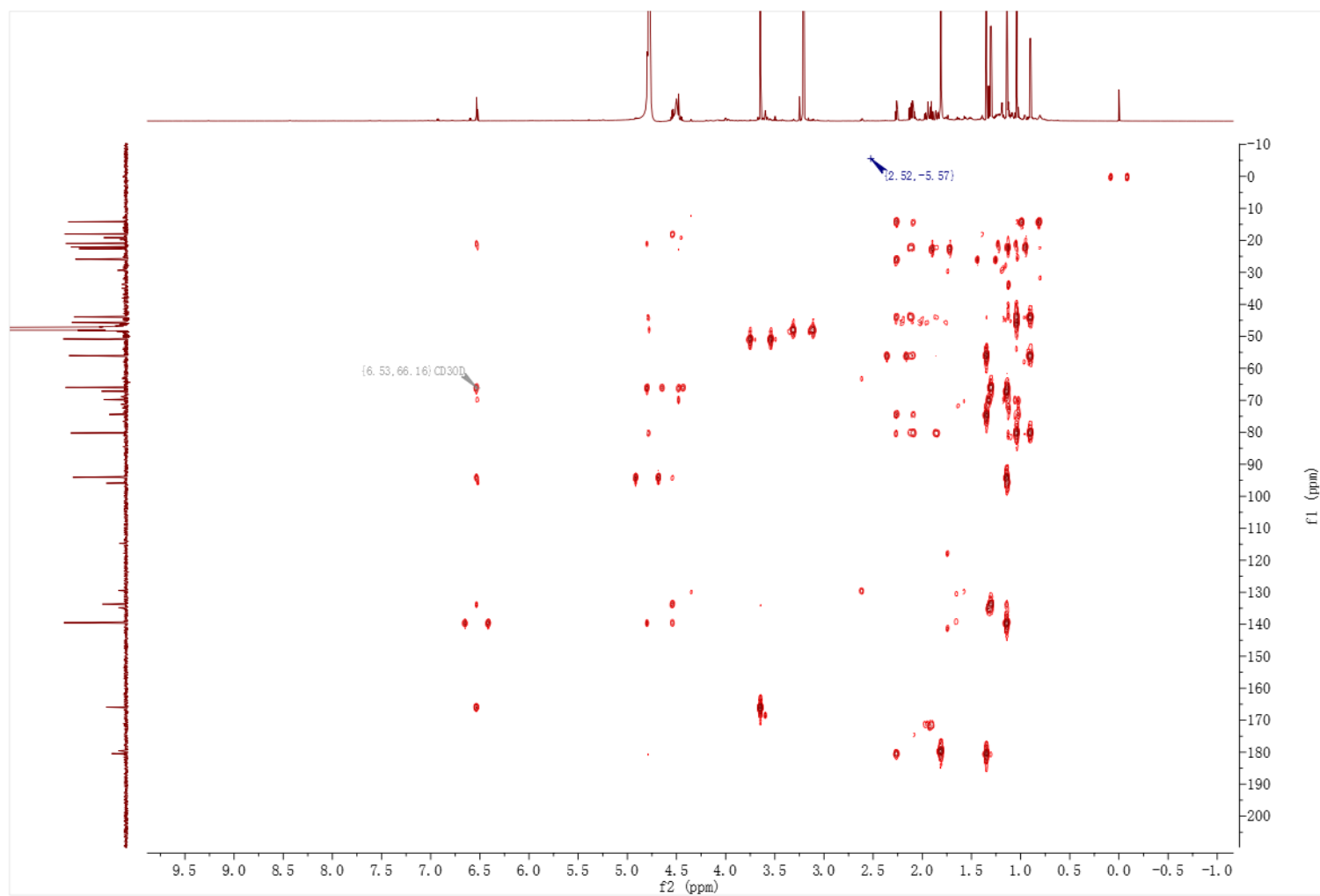


Figure S12. HMBC spectrum of the new compound **2**



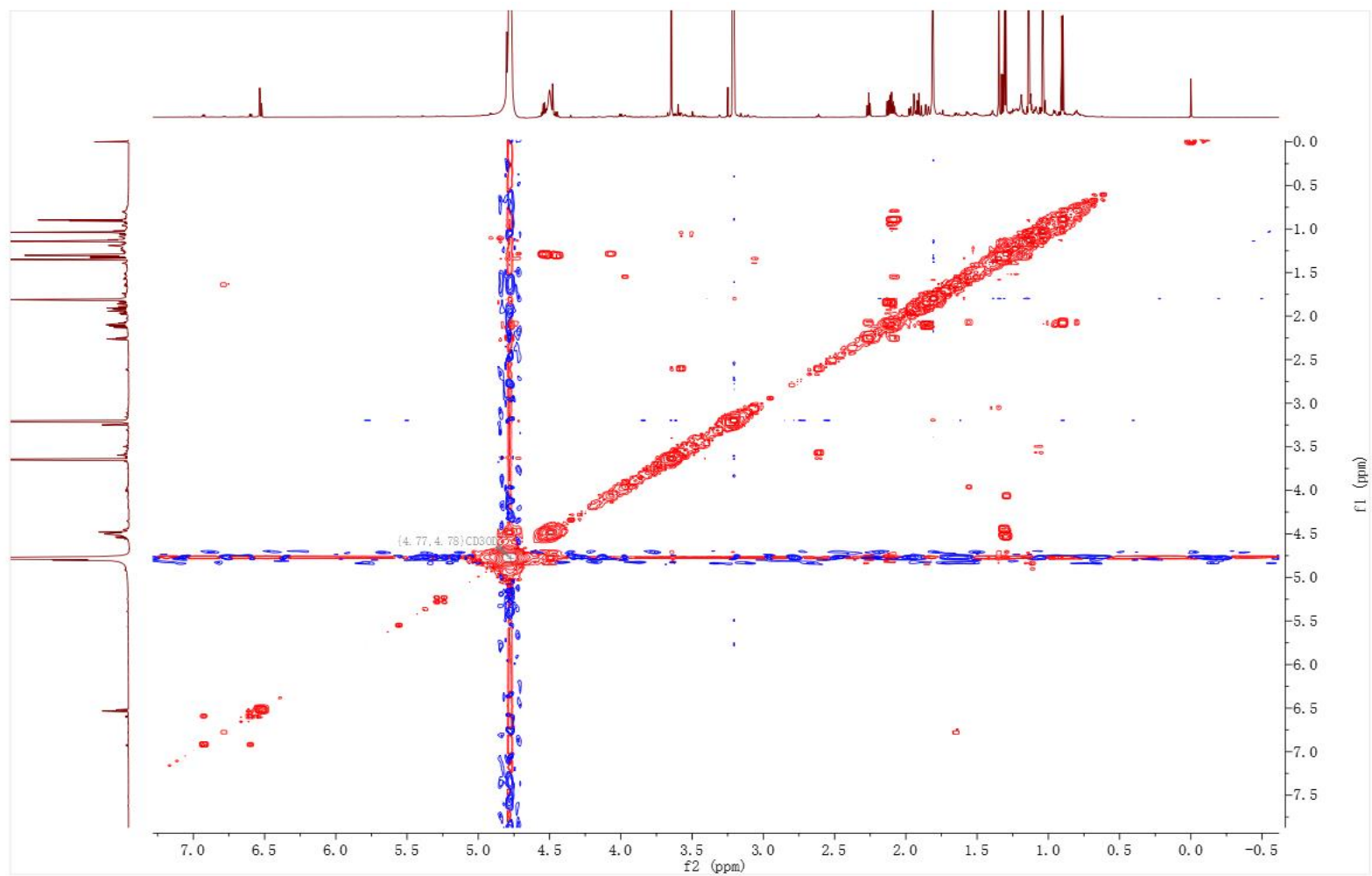


Figure S13. COSY spectrum of the new compound **2**

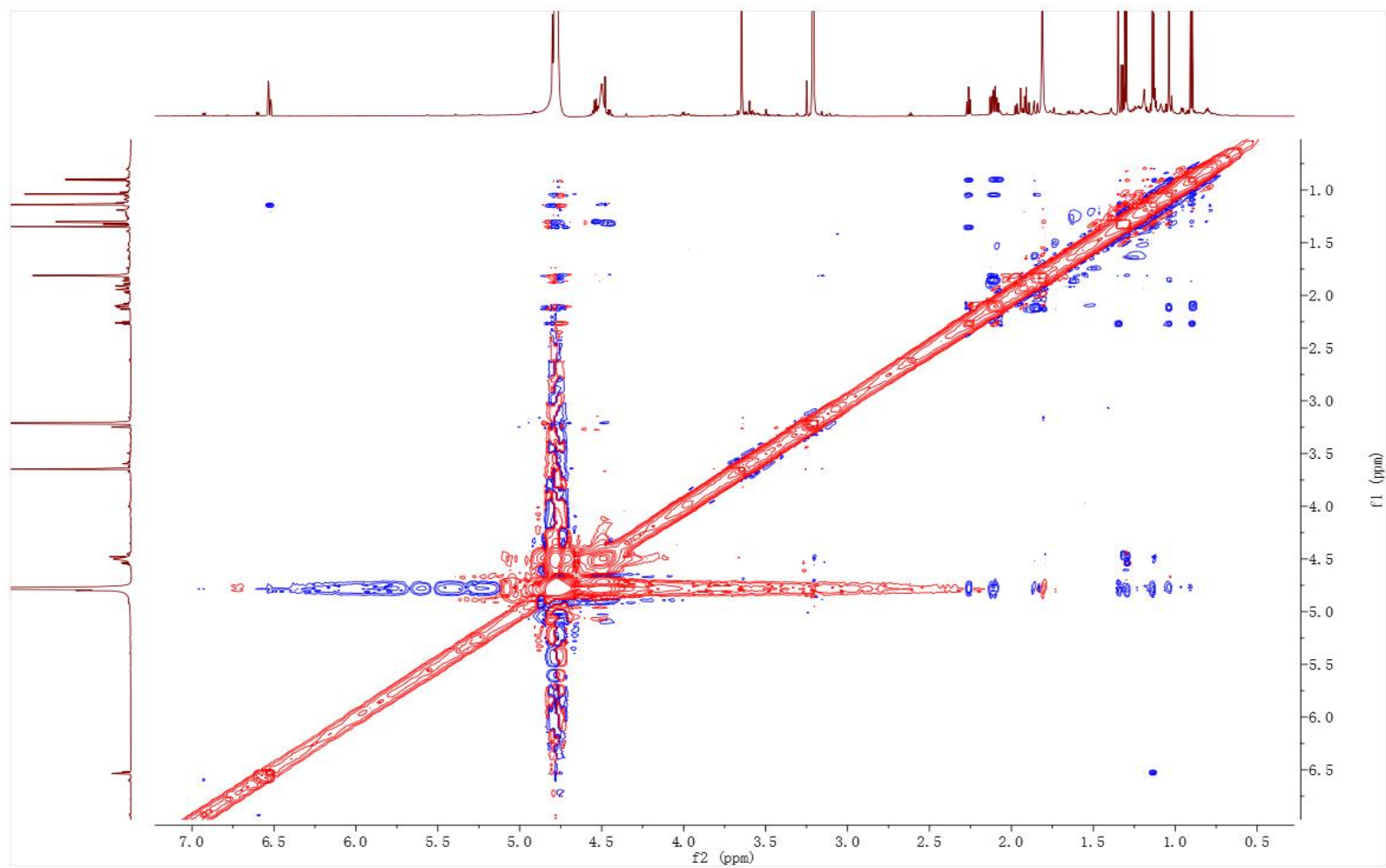


Figure S14. NOESY spectrum of the new compound **2**

## Qualitative Analysis Report

Data Filename	J-12-POS.d	Sample Name	Sample10
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Instrument Name	Instrument 1	User Name	
Acq Method	default-20200902-pos.m	Acquired Time	7/1/2021 9:49:07 AM
IRM Calibration Status		DA Method	analysis.m
Comment			

Sample Group      Info.

### User Spectra

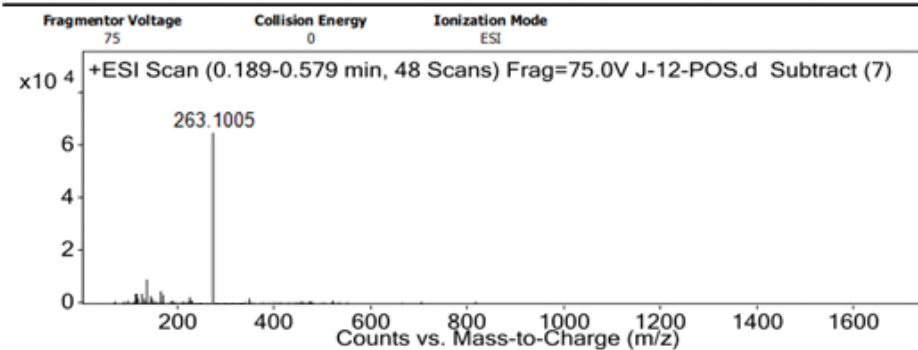


Figure S15. HRESI-MS spectrum of the new compound **3**

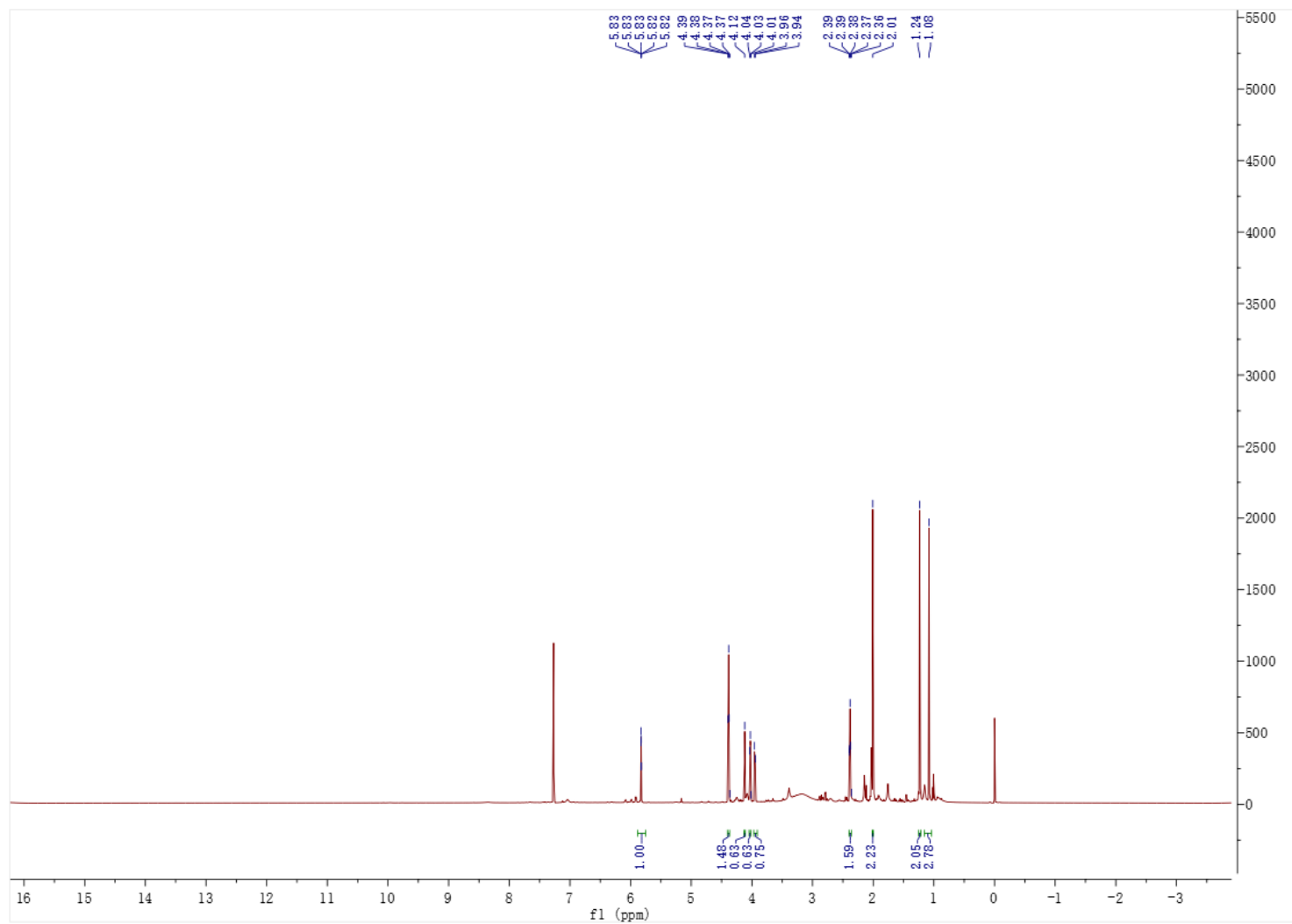


Figure S16.  $^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ ) spectrum of the new compound **3**

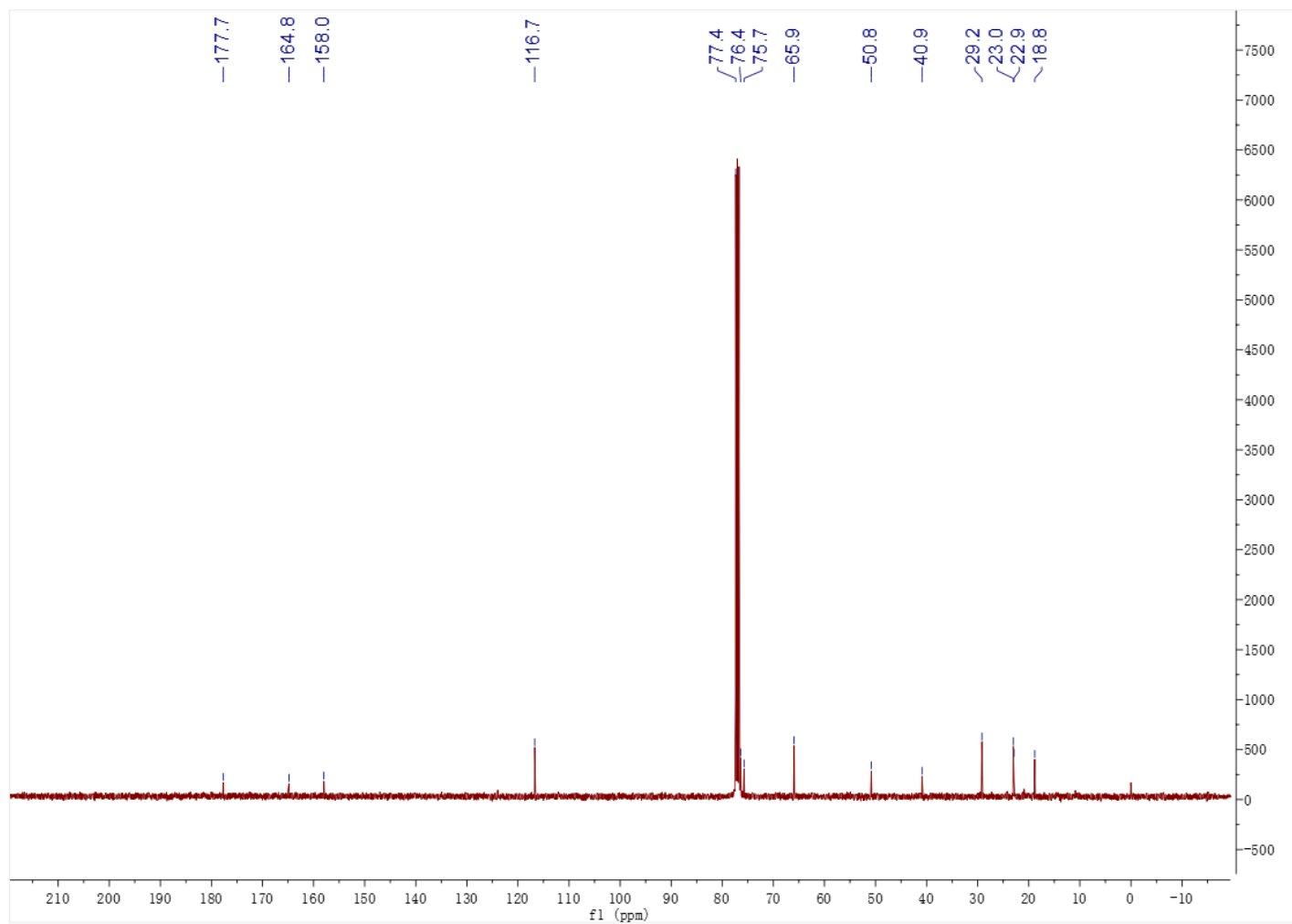


Figure S17. <sup>13</sup>C NMR (150 MHz, CDCl<sub>3</sub>) spectrum of the new compound **3**

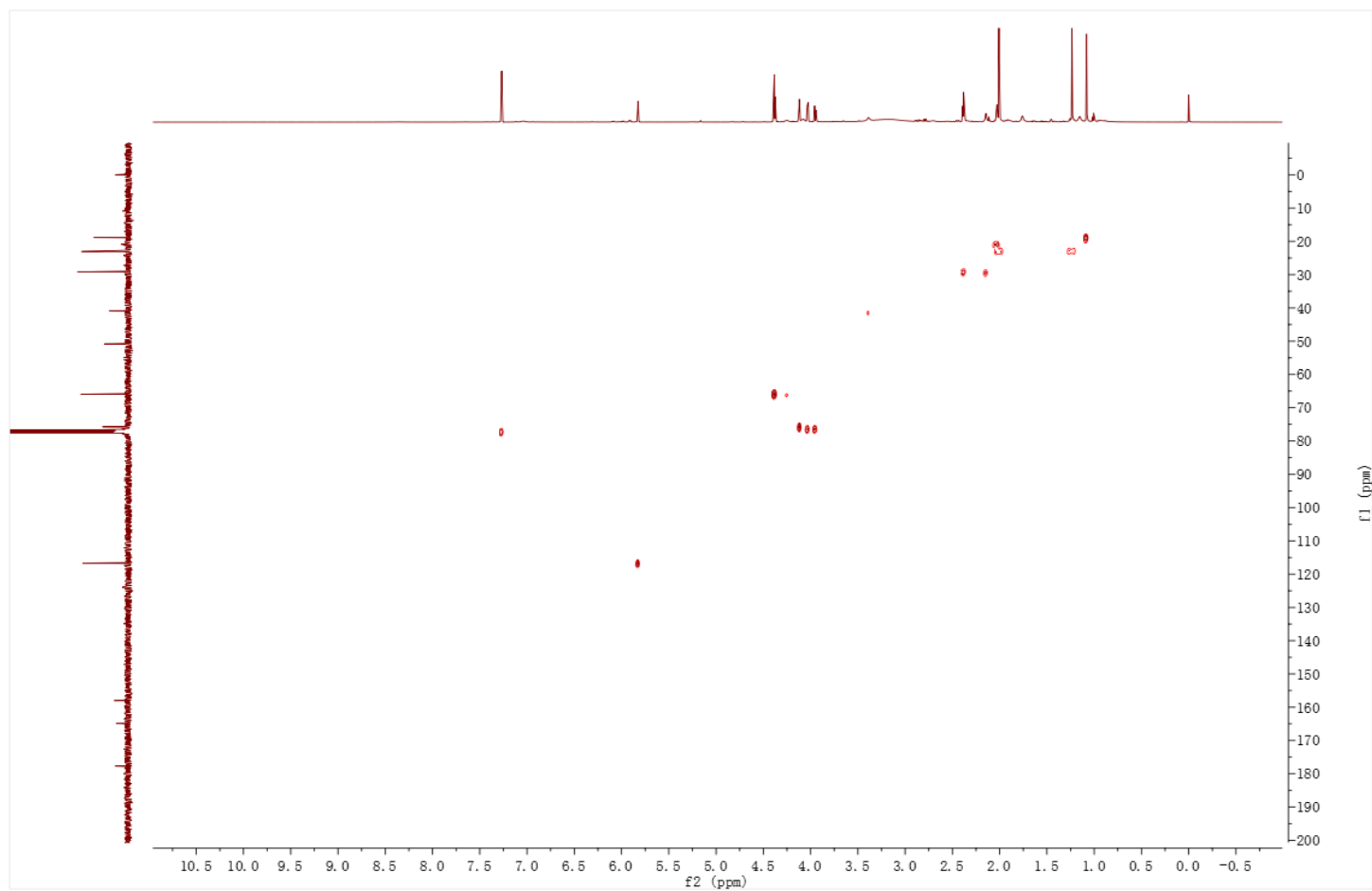


Figure S18. HSQC spectrum of the new compound **3**

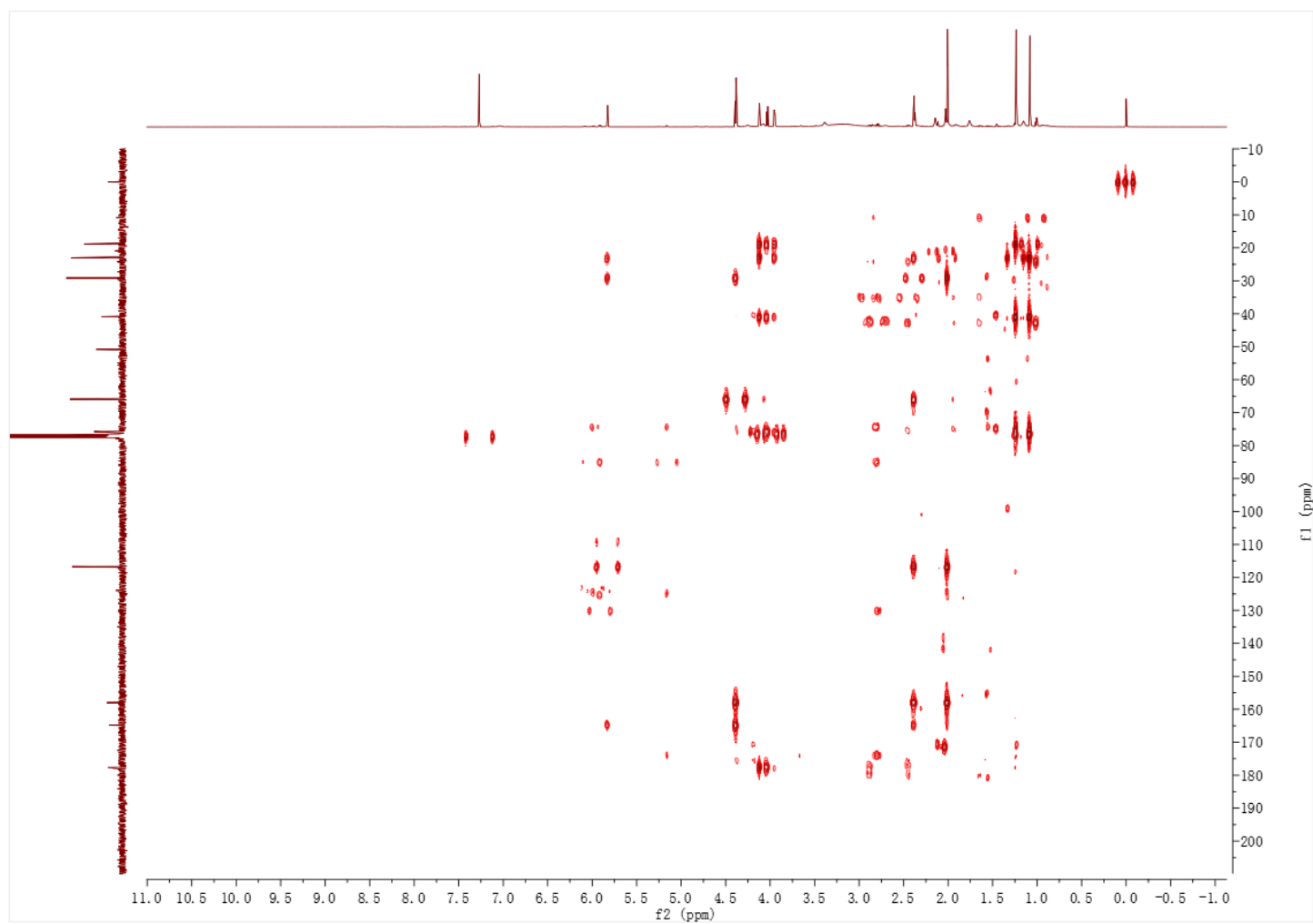


Figure S19. HMBC spectrum of the new compound **3**

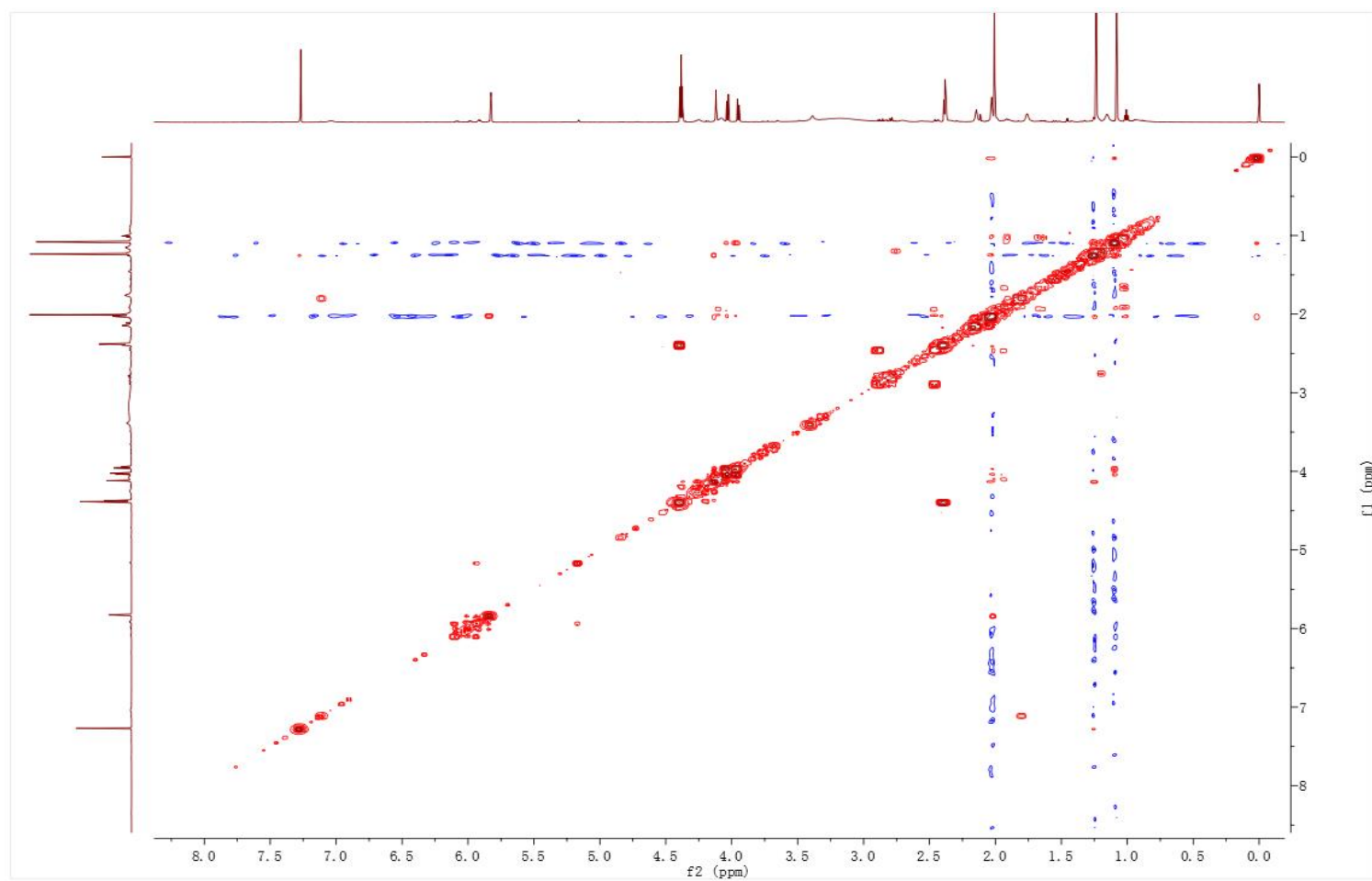


Figure S20. COSY spectrum of the new compound **3**



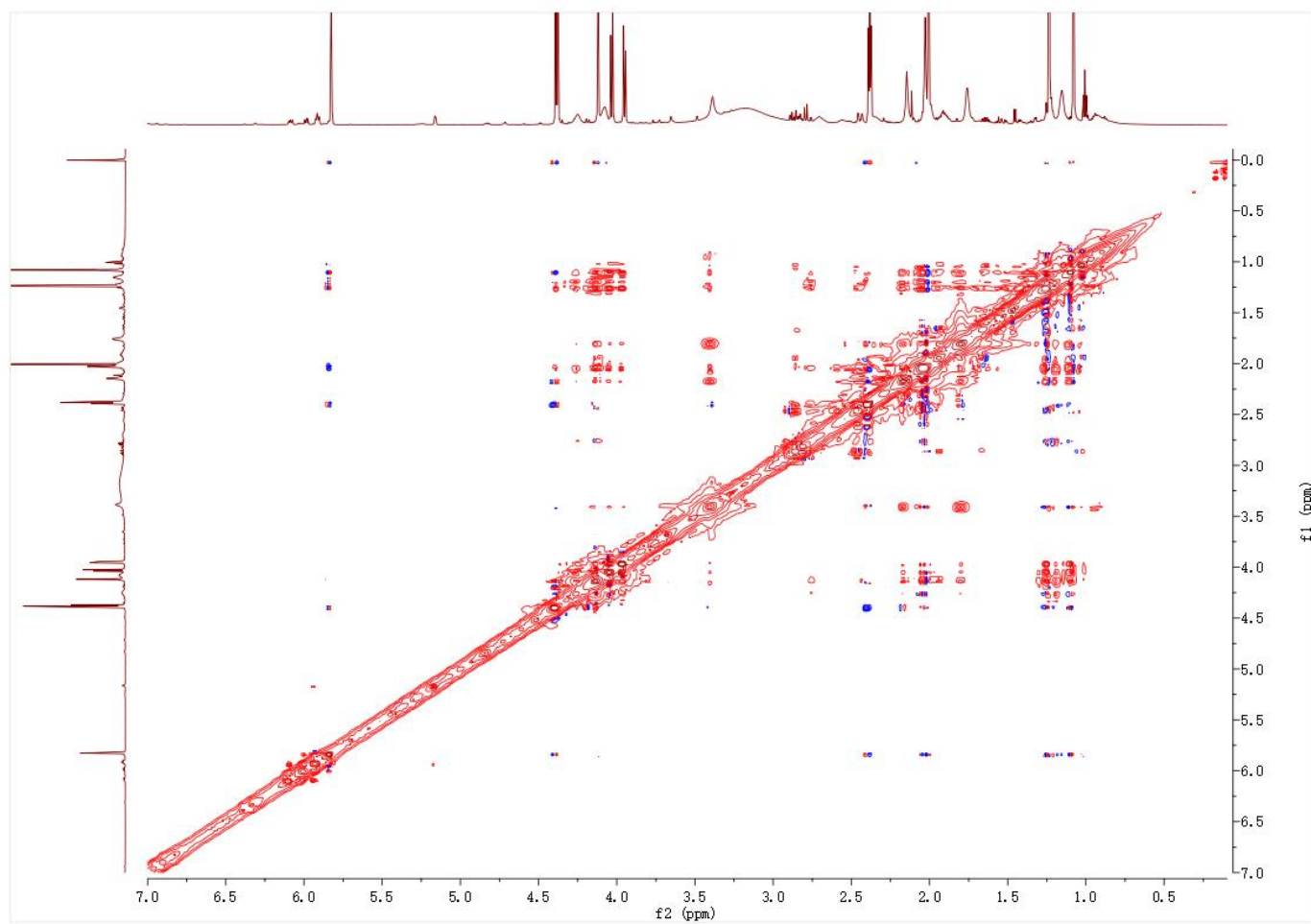


Figure S21. NOESY spectrum of the new compound **3**

## Qualitative Analysis Report

Data Filename	NEU-105-POS.d Sample	Sample Name	Sample13
Sample Type	Instrument 1	Position	P1-B3
Instrument Name	default-20200902-pos.	User Name	
Acq Method		Acquired Time	7/1/2021 13:38:20
IRM Calibration Status		DA Method	analysis.m
Comment			

### User Spectra

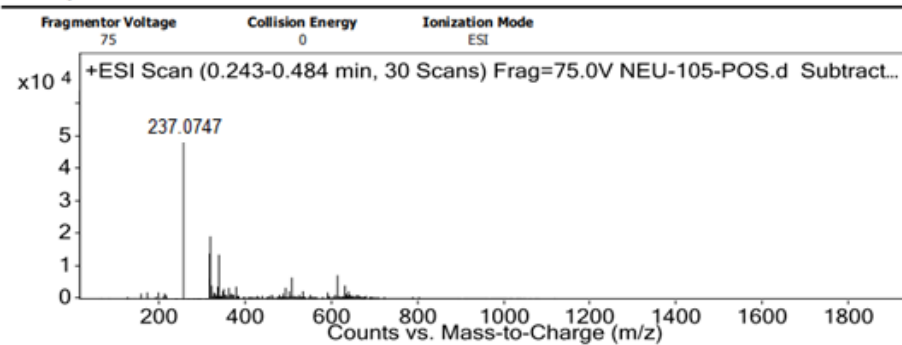


Figure S22. HRESI-MS spectrum of the new compound **4**

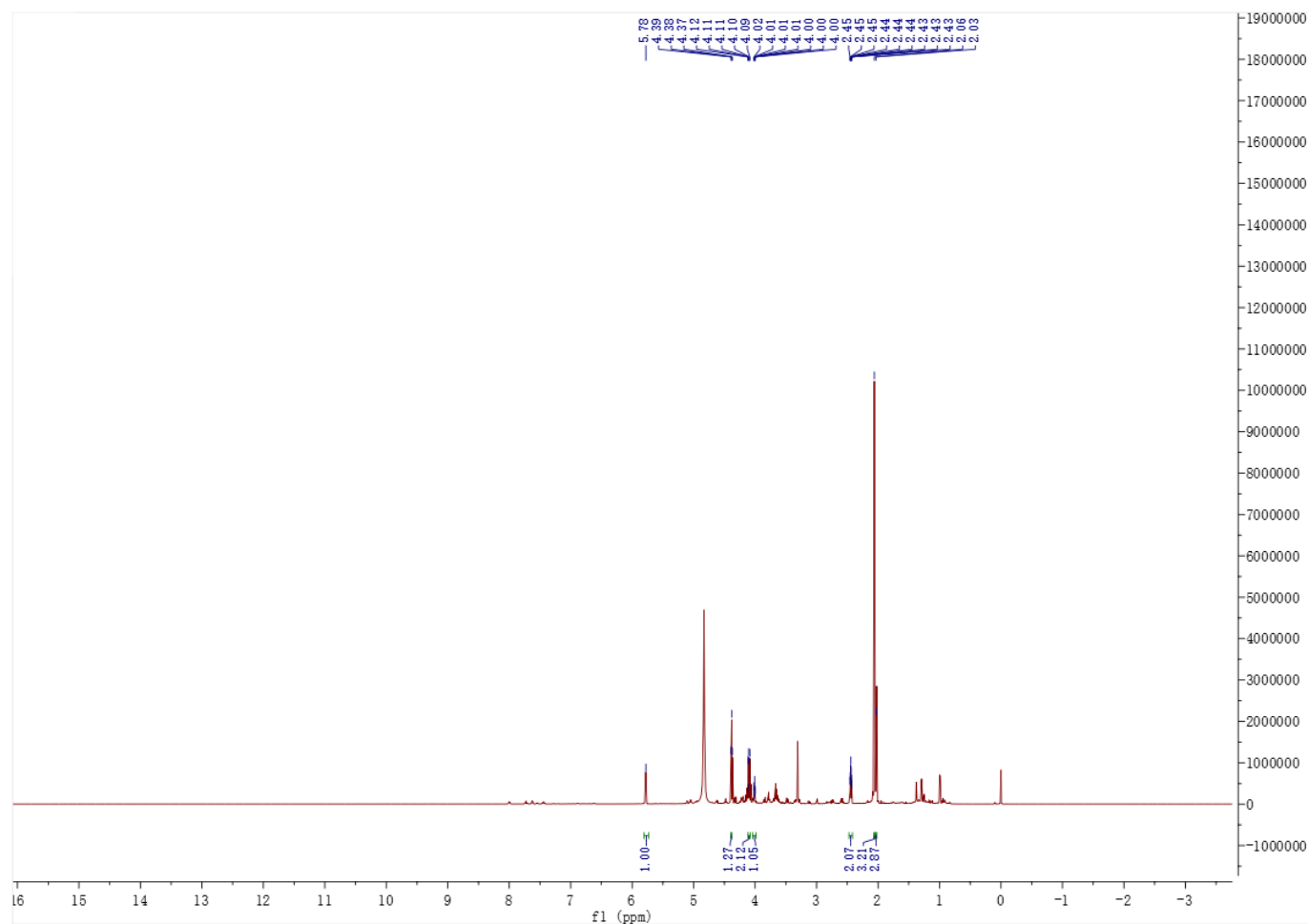


Figure S23.  $^1\text{H}$  NMR (600 MHz,  $\text{CD}_3\text{OD}$ ) spectrum of the new compound **4**

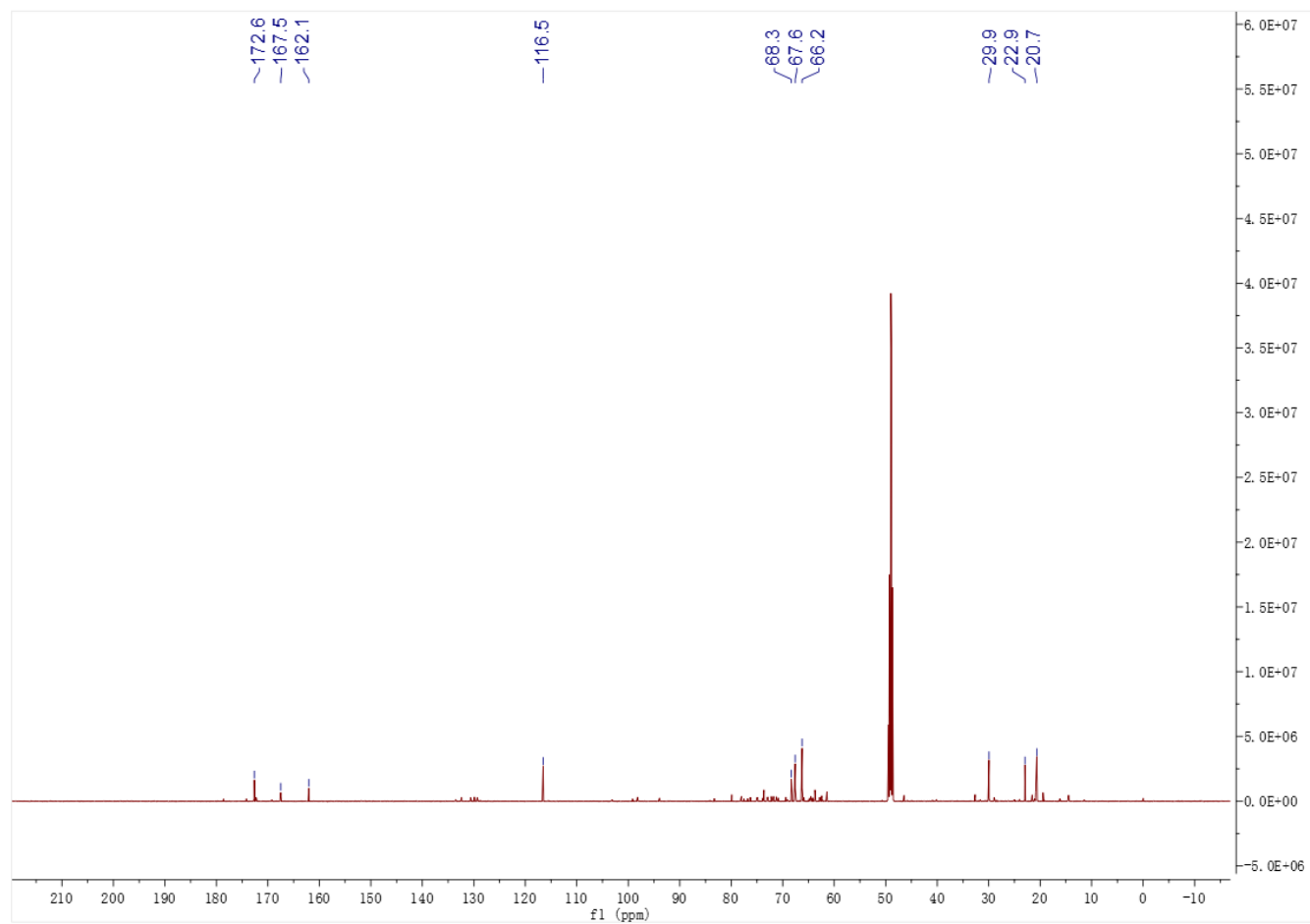


Figure S24.  $^{13}\text{C}$  NMR (150 MHz,  $\text{CD}_3\text{OD}$ ) spectrum of the new compound **4**

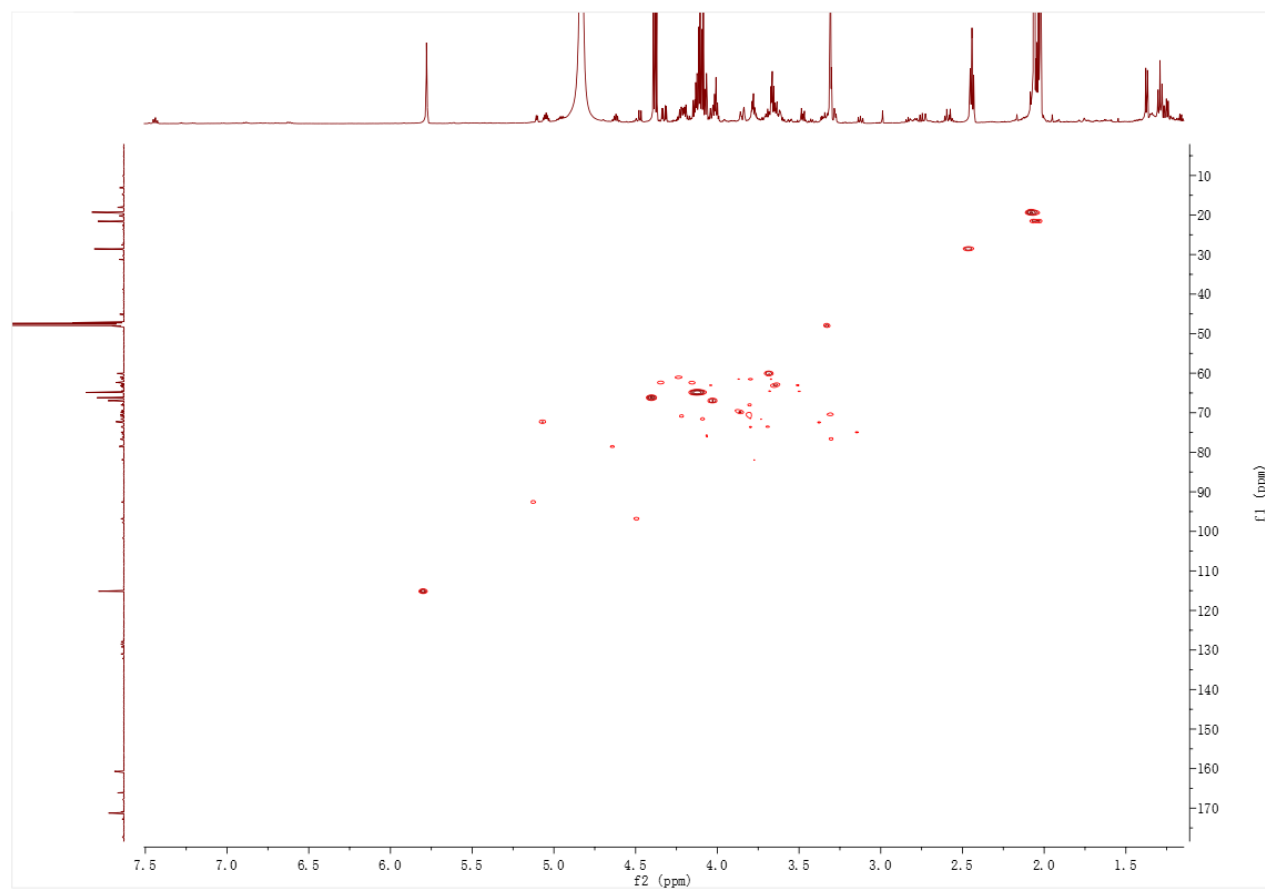


Figure S25. HSQC spectrum of the new compound **4**

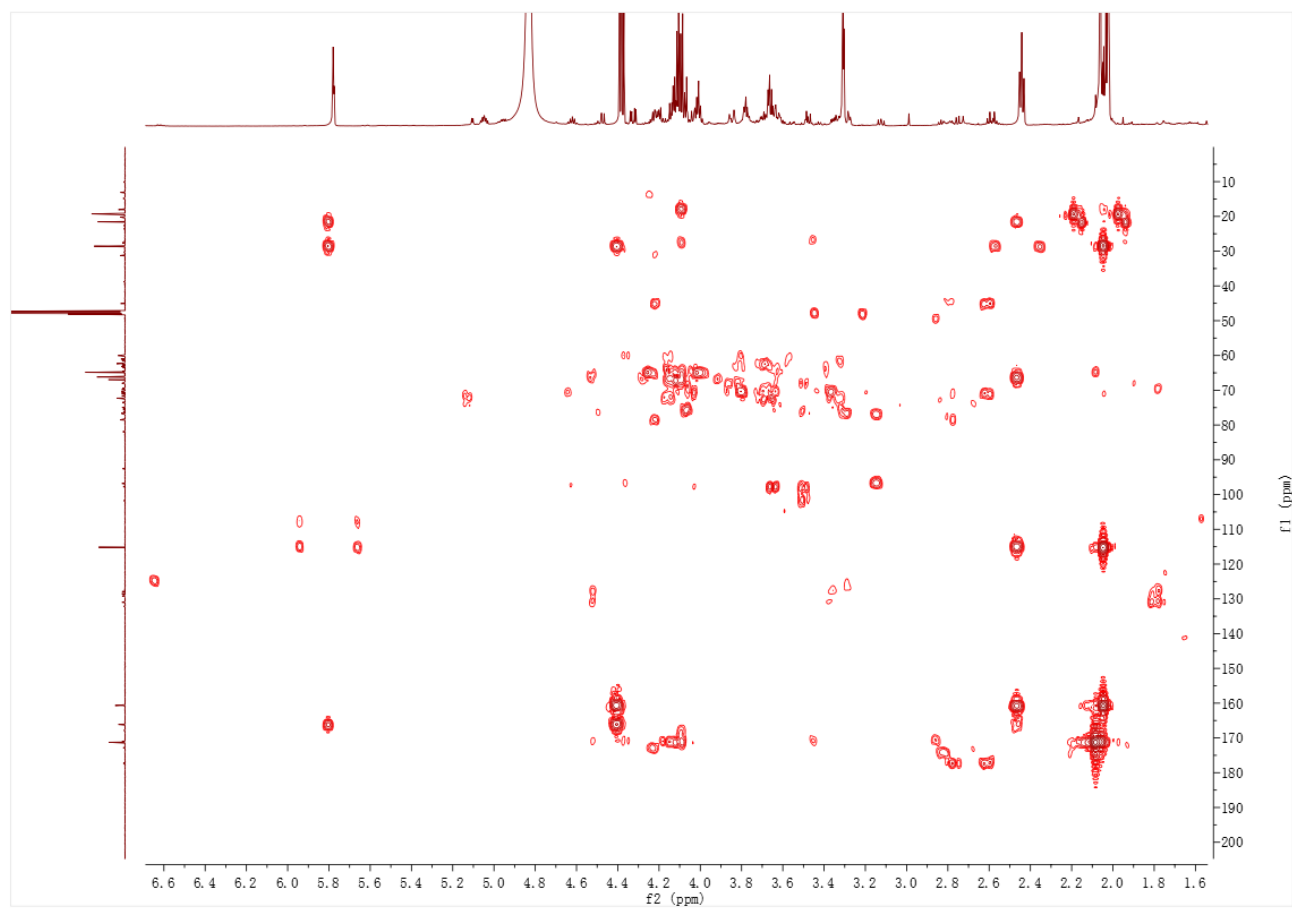


Figure S26. HMBC spectrum of the new compound **4**

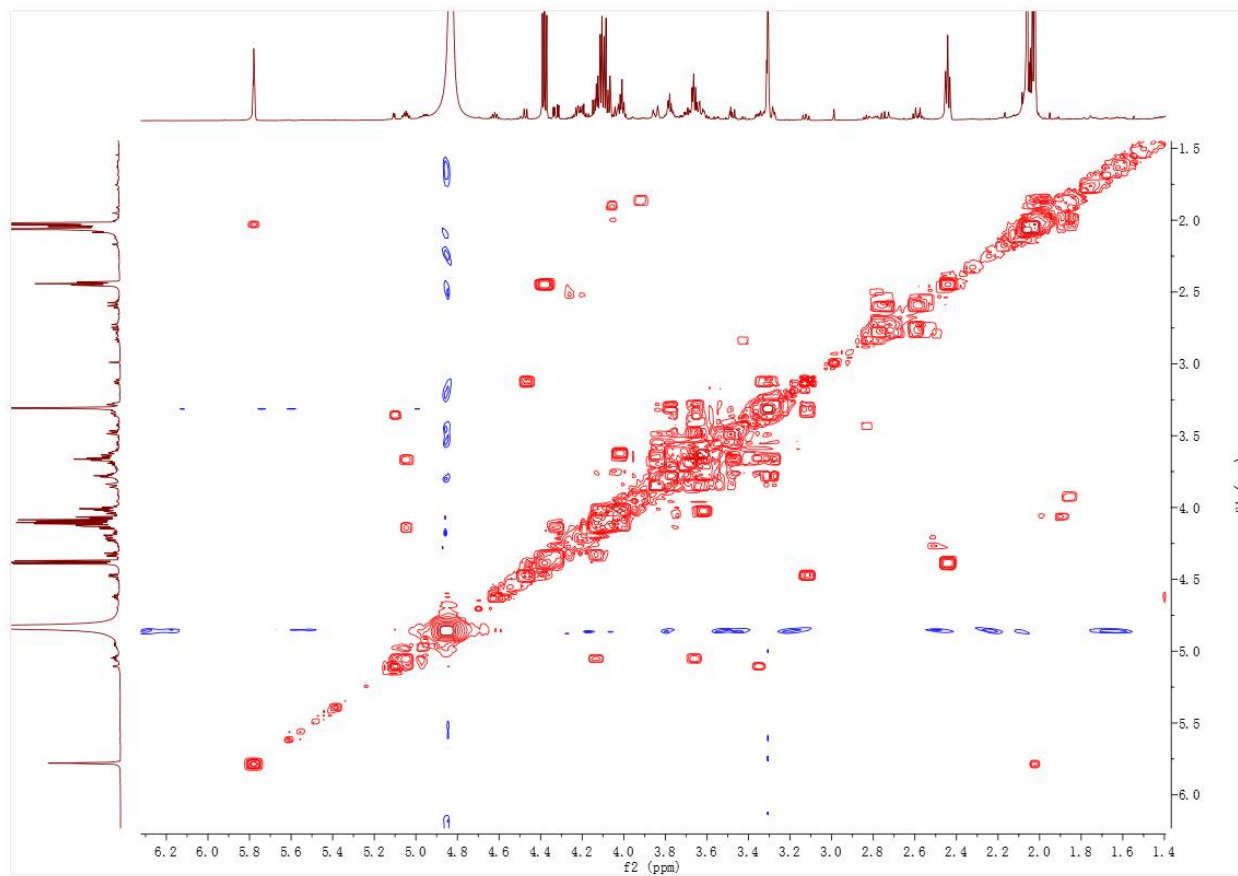


Figure S27. COSY spectrum of the new compound **4**

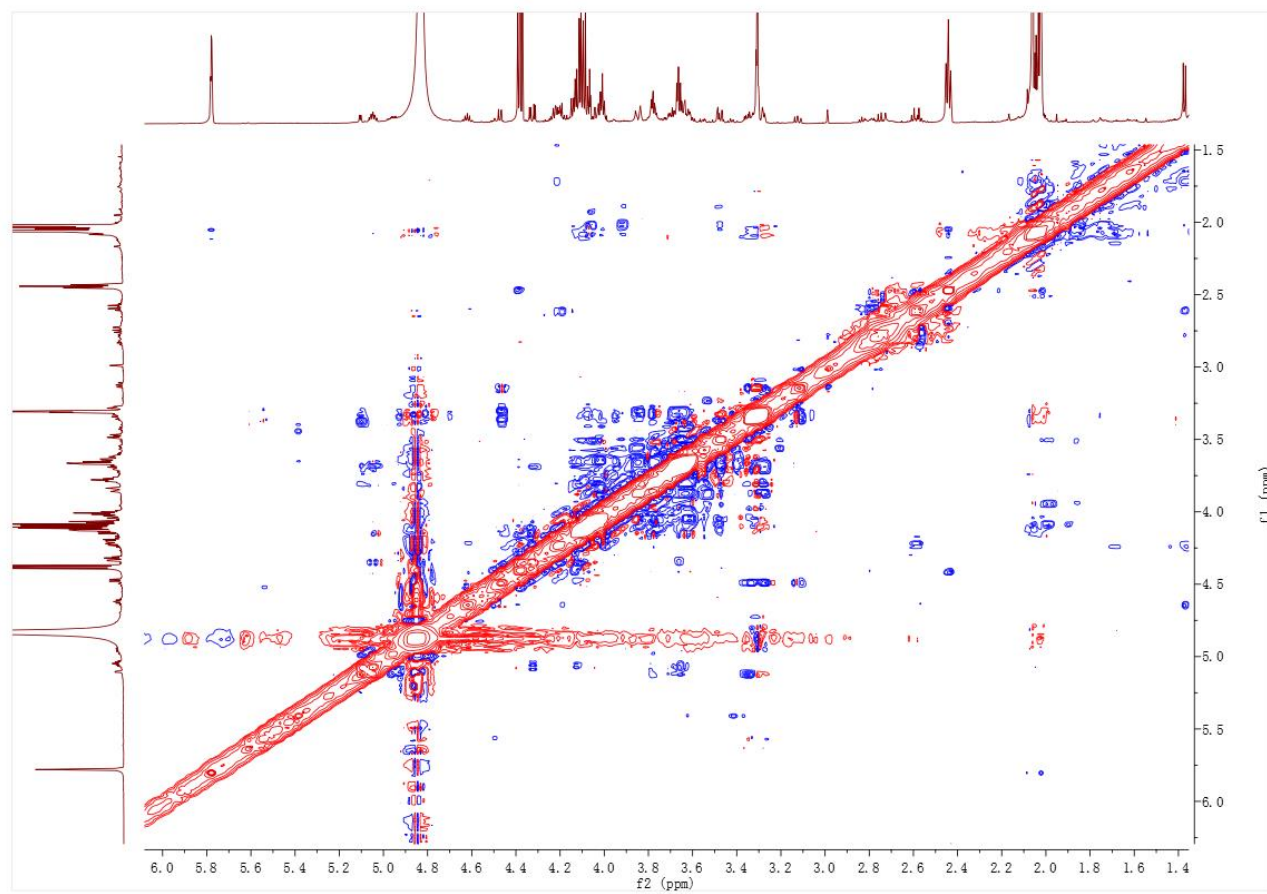


Figure S28. NOESY spectrum of the new compound **4**



## Qualitative Analysis Report

Data Filename	OMP451-NEG.d	Sample Name	Sample13
Sample Type	Sample	Position	P1-B4
Instrument Name	Instrument 1	User Name	
Acq Method	default-20200902-neg.m	Acquired Time	7/1/2021 12:42:16 PM
IRM Calibration Status	Some Ions Missed	DA Method	analysis.m
Comment			

Sample Group      Info.

### User Spectra

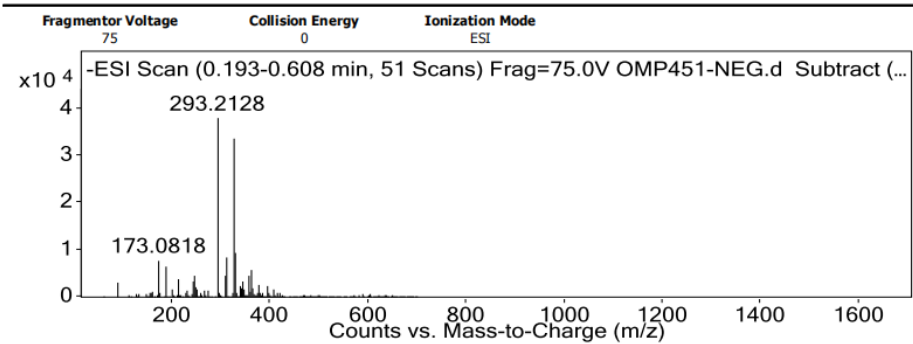


Figure S29. HRESI-MS spectrum of the new compound **5**

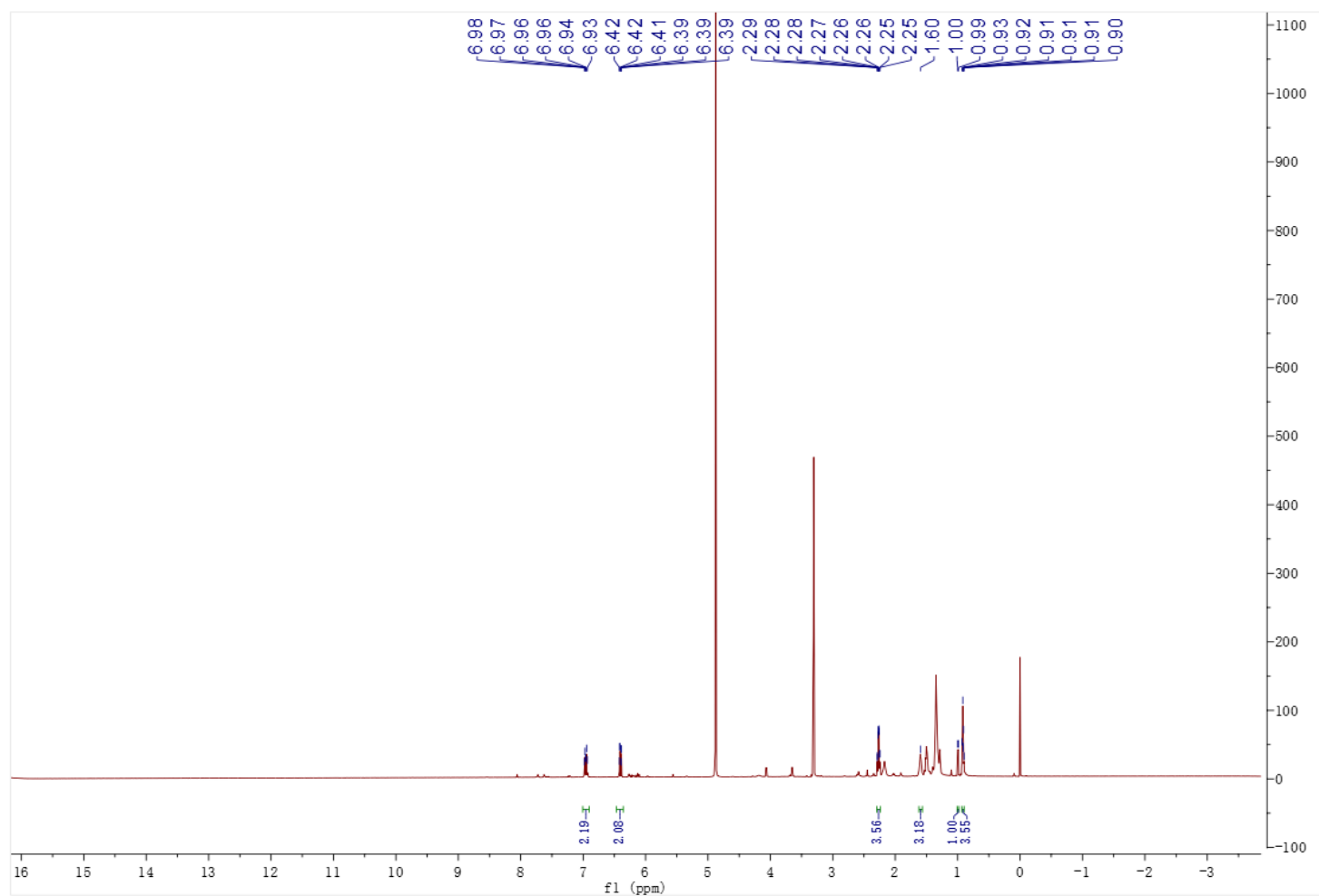


Figure S30. <sup>1</sup>H NMR (600 MHz, CD<sub>3</sub>OD) spectrum of the new compound **5**

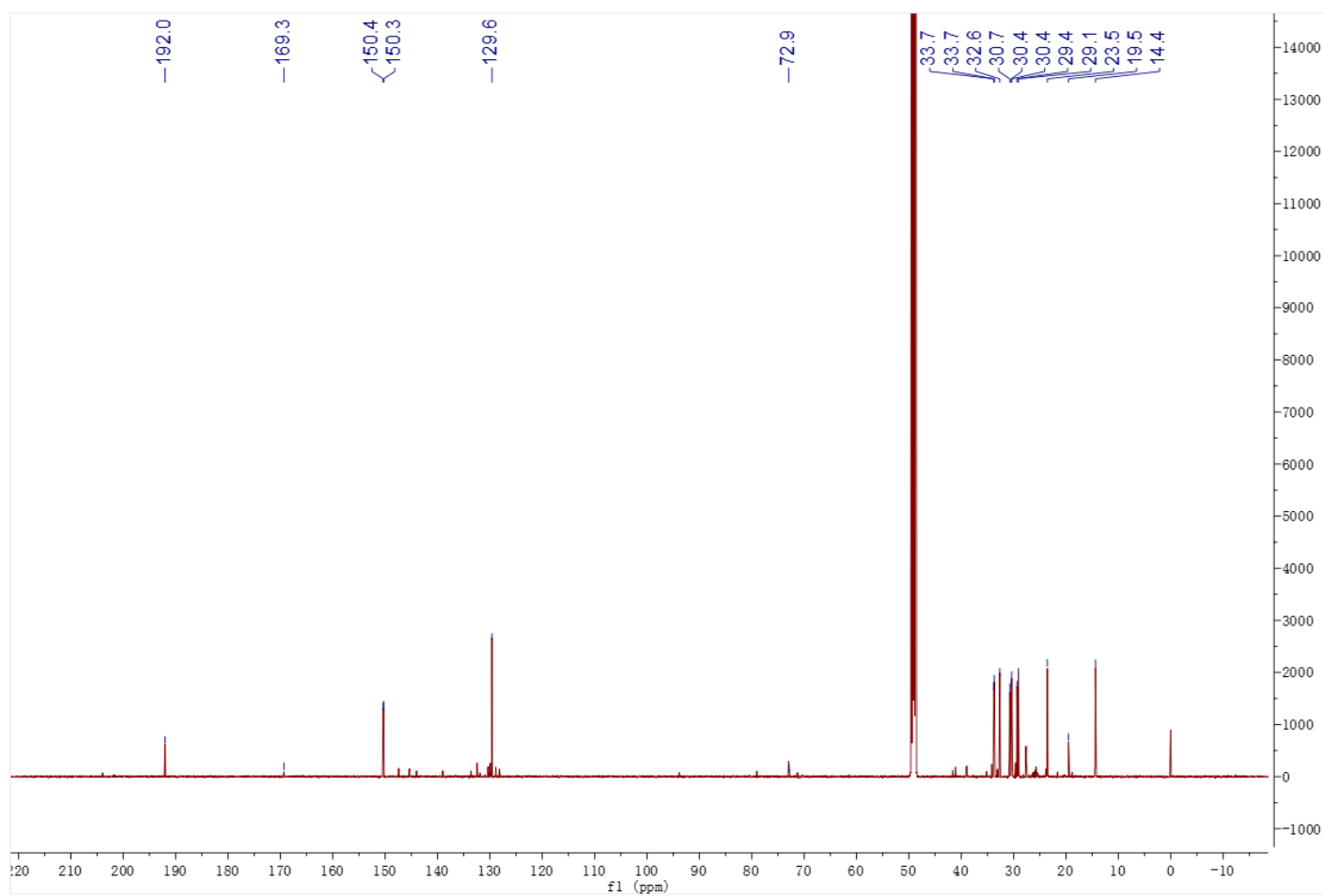


Figure S31. <sup>13</sup>C NMR (150 MHz, CD<sub>3</sub>OD) spectrum of the new compound **5**

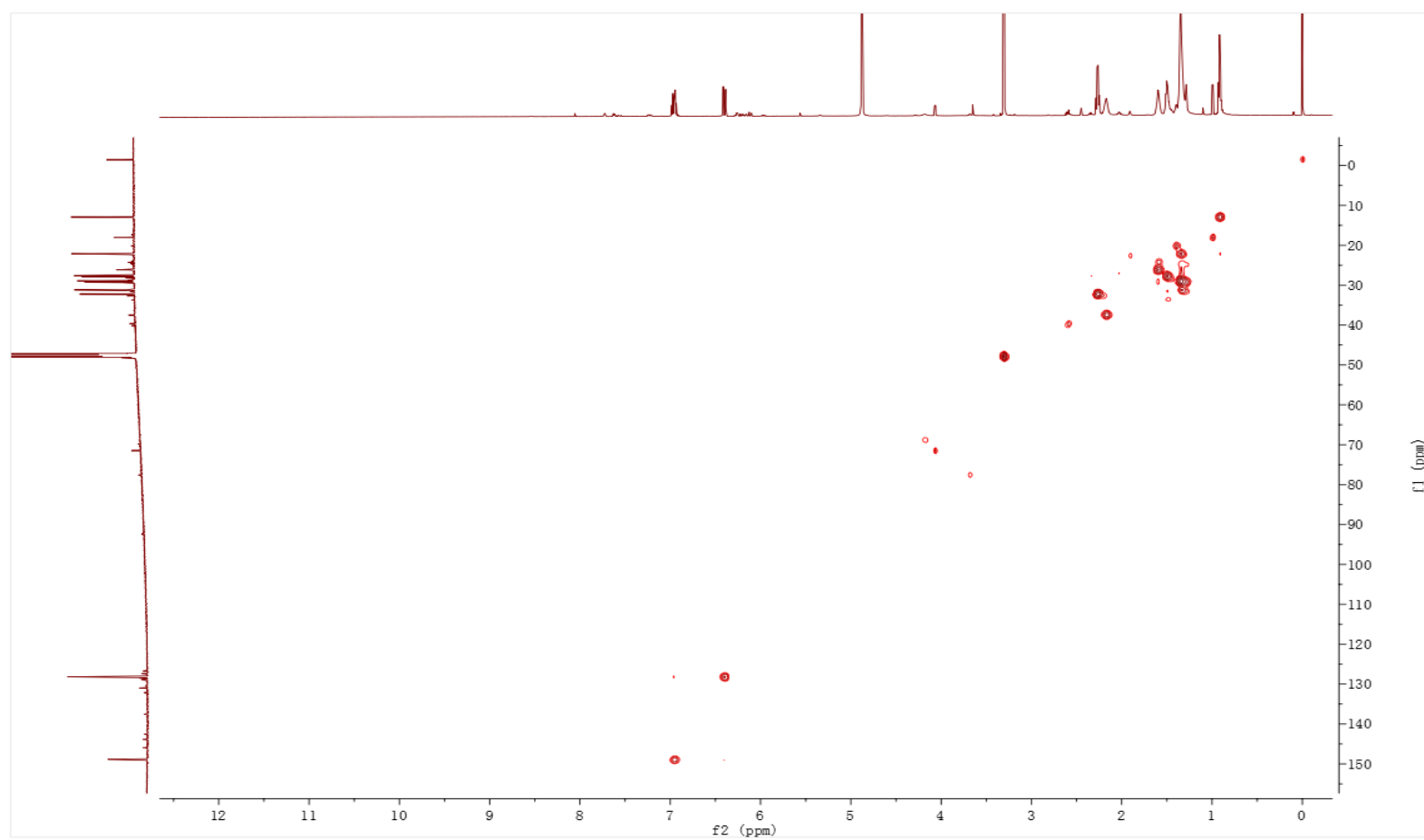


Figure S32. HSQC spectrum of the new compound **5**

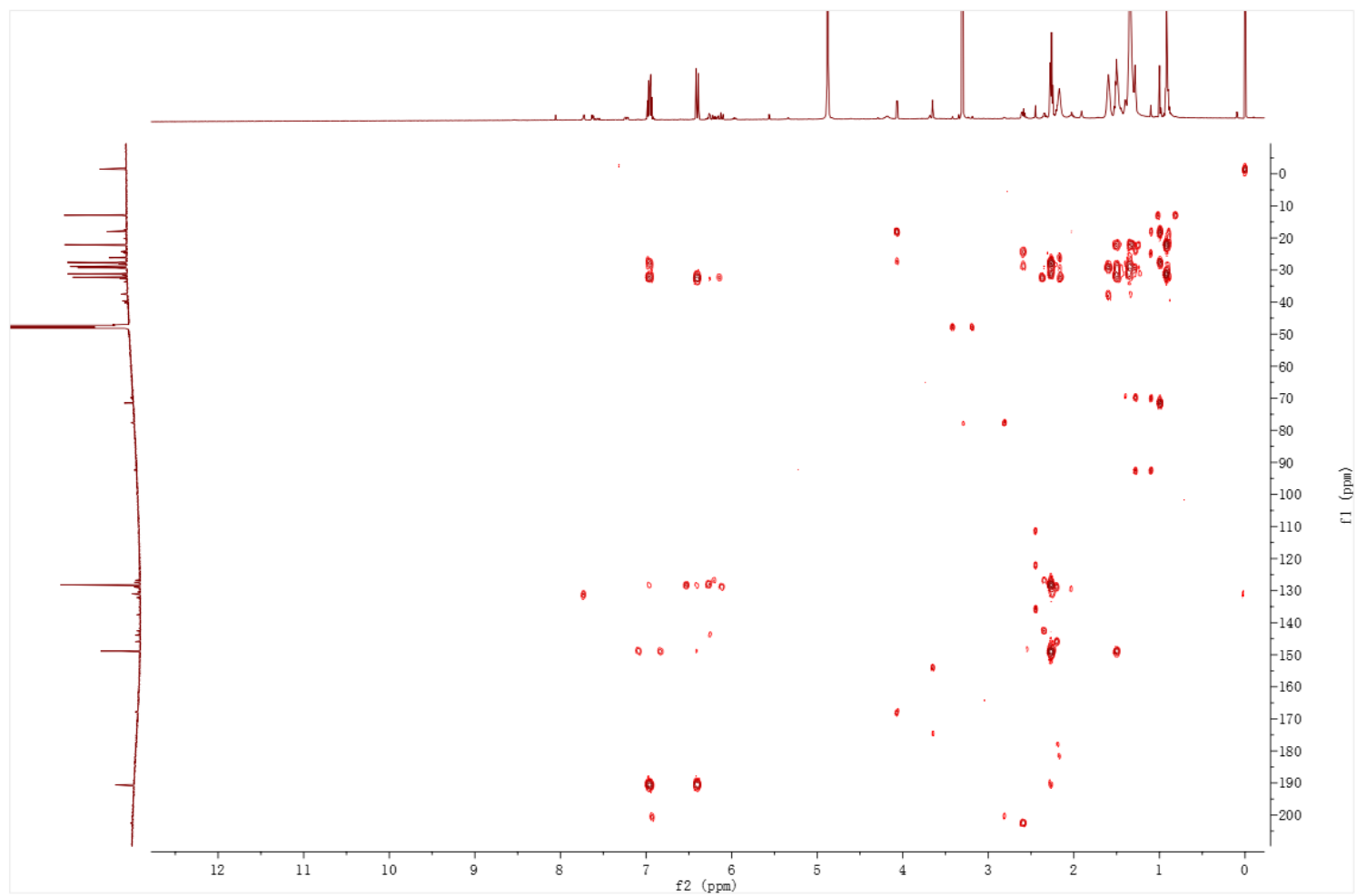


Figure S33. HMBC spectrum of the new compound **5**

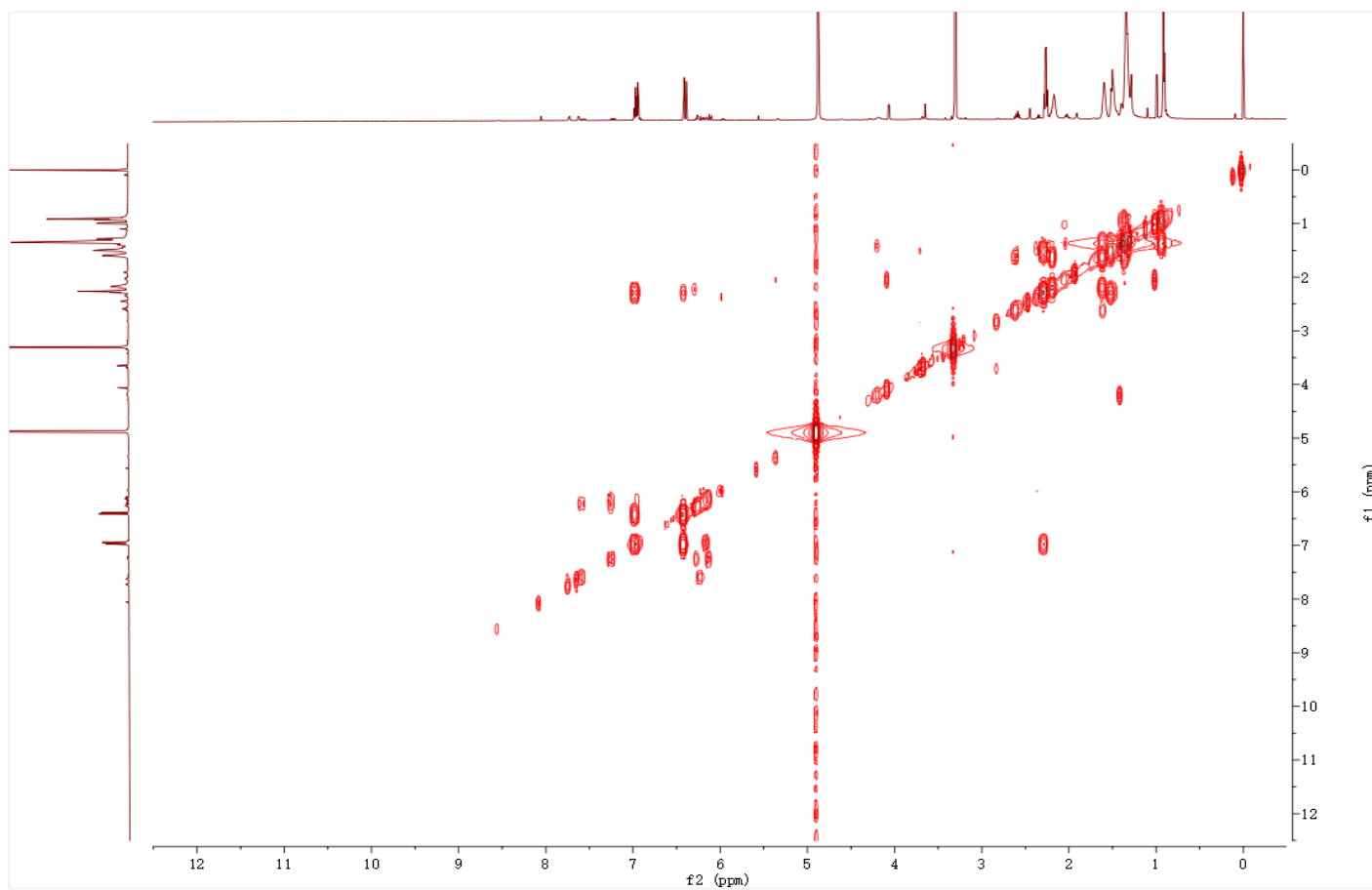


Figure S34. COSY spectrum of the new compound **5**

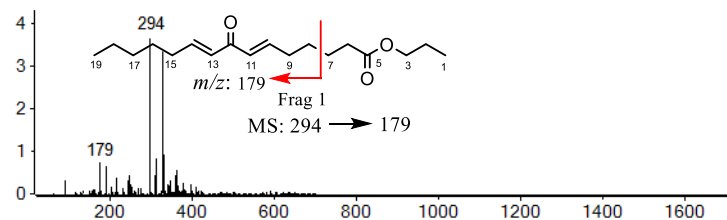
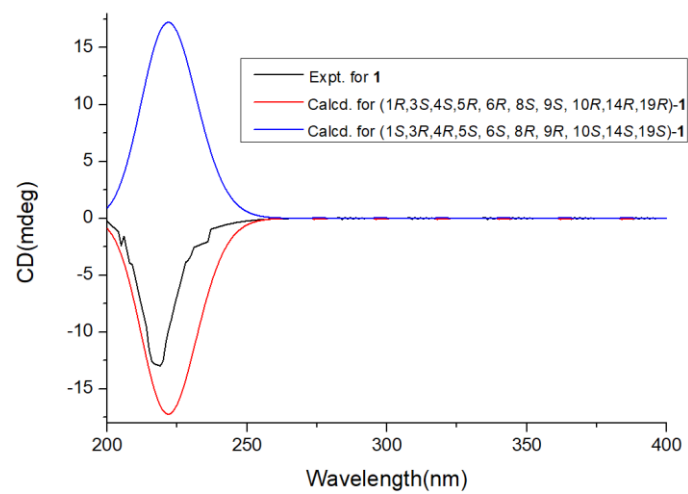


Figure S35. ESI-MS spectrum of compound **5**.

### S36. Computational details for compound 1-4 (ECD)

The calculations of new compounds **1-4** were performed by using the density functional theory (DFT) as carried out in the Gaussian 09. Conformation search were performed with MMFF94S force fields using MacroModel software. All these conformers were further optimized by the density functional theory method at the B3LYP/6-31G(d) level (Boltzmann distribution over 5%, the relative energy within 6 kcal/mol). The ECD were calculated using density functional theory (TDDFT) at B3LYP/6-31+G(d) level. The ECD spectra of different conformers were generated using the program SpecDis by applying a Gaussian band shape with a 0.30 eV width, according to the Boltzmann-calculated contribution after UV correction.



**Figure S37.** Comparison of the calculated ECD spectra for **1** with the experimental spectrum of **1**

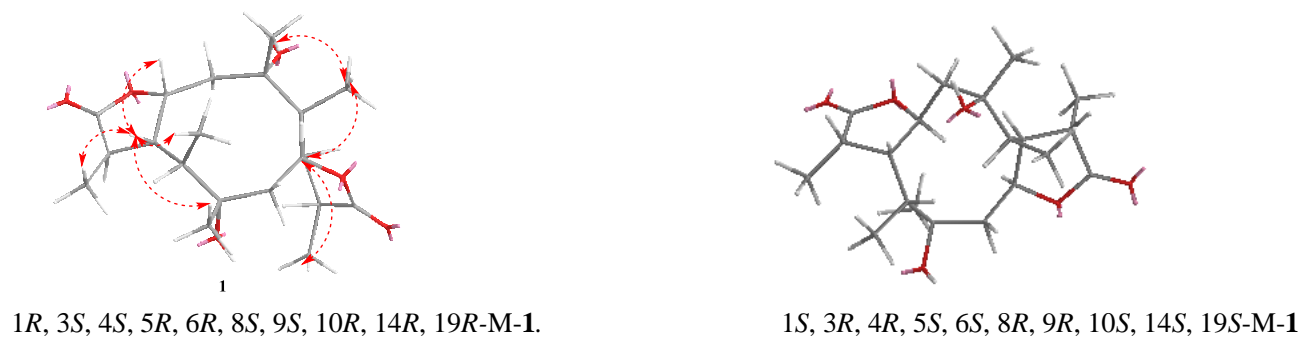


Figure S38. calculated and experimental ECD spectras of **1** using model.

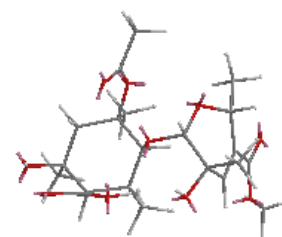
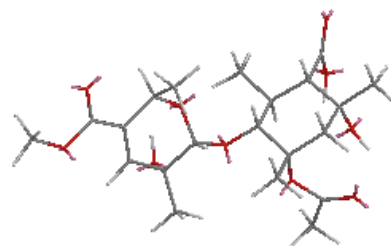
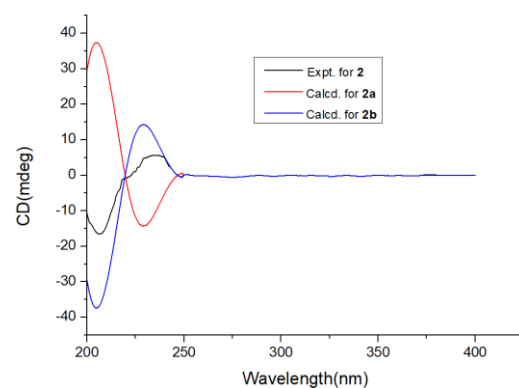


**Table S1.** Energy analysis for conformers of **1** at B3LYP/6-31G(d) level

Conformer	Energy (hartree)	Ratio (%)
1	-864.14735	1.71
2	-864.14747	1.27
4	-864.14833	2.85
6	-864.14831	3.09
10	-864.13144	89.09
12	-864.14767	1.41
16	-864.11758	1.43
20	-864.11825	3.98
36	-864.11793	2.29
40	-864.11826	3.27
66	-864.12736	1.26
70	-864.12871	4.24
84	-864.12812	2.81
89	-864.12738	1.29
93	-864.12614	1.38

96	-864.12813	3.26
98	-864.12946	4.31

**Table S2.** Energy analysis for conformers of **2** at B3LYP/6-31G(d) level



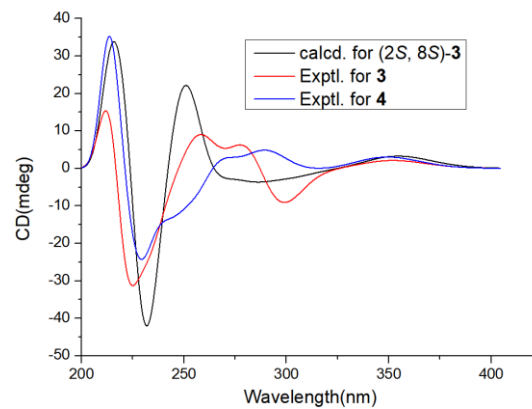
Compound 2

	Model-1	model-2
Conformer	Energy (hartree)	Ratio (%)
2	-734.6934336	7.45
3	-734.6952926	2.64
4	-734.6939118	64.45
5	-734.6945719	9.36
8	-734.6941533	6.23
9	-734.6958112	4.16

10	-734.6955858	3.25
12	-734.6957623	4.65
13	-734.6944719	8.01
14	-734.6951045	6.34
15	-734.6941238	2.18
16	-734.6941029	6.01
21	-734.6956123	3.93
22	-734.6952278	3.48
25	-734.6956833	3.61
27	-734.6952934	3.08
29	-734.6959934	4.31
30	-734.6958118	5.18

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**Table S3.** Energy analysis for conformers of **3** at B3LYP/6-31G(d) level



conformer	Energy (hartree)	Ratio(%)
1	-794.6644631	68.52
2	-794.6626493	28.32
4	-794.6620634	2.30
5	-794.6620483	1.57