

## Supporting Information

# Neocucurins A and B, two novel rearranged diterpene from marine-derived fungus *Neocucurbitaria unguis- hominis*

Hongxin Liu,<sup>a,b,1</sup> Jihua Hu,<sup>b,1</sup> Yuchan Chen,<sup>b</sup> Shanshan Wei,<sup>c</sup> Haibo Tan,<sup>\*,c</sup> and Weimin Zhang<sup>\*,b</sup>

<sup>a</sup> School of Life and Health Technology, Dongguan University of Technology, Dongguan 523808, People's Republic of China

<sup>b</sup> State Key Laboratory of Applied Microbiology Southern China, Guangdong Provincial Key Laboratory of Microbial Culture Collection and Application, Institute of Microbiology, Guangdong Academy of Sciences, Guangzhou 510070, People's Republic of China

<sup>c</sup> Key Laboratory of South China Agricultural Plant Molecular Analysis and Genetic Improvement, Guangdong Provincial Key Laboratory of Applied Botany, South China Botanical Garden, Chinese Academy of Sciences, Guangzhou 510650, People's Republic of China

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<sup>1</sup>These authors are contributed equally.

\*E-mail: tanhaibo@scbg.ac.cn; wmzhang@gdim.cn

## Contents

<b>S1.</b> X-ray crystallographic data of compounds <b>1</b> and <b>2</b> .....	S4
<b>Figure S1.</b> <sup>1</sup> H NMR spectrum (500 MHz, CD <sub>3</sub> OD) of <b>1</b> .....	S8
<b>Figure S2.</b> <sup>13</sup> C NMR spectrum (125 MHz, CD <sub>3</sub> OD) of <b>1</b> .....	S8
<b>Figure S3.</b> <sup>1</sup> H- <sup>1</sup> H COSY spectrum (500 MHz, CD <sub>3</sub> OD) of <b>1</b> .....	S9
<b>Figure S4.</b> HSQC spectrum of <b>1</b> .....	S9
<b>Figure S5.</b> HMBC spectrum of <b>1</b> .....	S10
<b>Figure S6.</b> NOESY spectrum of <b>1</b> .....	S10
<b>Figure S7.</b> HRESIMS spectrum of <b>1</b> .....	S11
<b>Figure S8.</b> UV spectrum of <b>1</b> .....	S11
<b>Figure S9.</b> CD spectrum of <b>1</b> .....	S12
<b>Figure S10.</b> IR spectrum of <b>1</b> .....	S12
<b>Figure S11.</b> <sup>1</sup> H NMR spectrum (500 MHz, CDCl <sub>3</sub> ) of <b>2</b> .....	S13
<b>Figure S12.</b> <sup>13</sup> C NMR spectrum (125 MHz, CDCl <sub>3</sub> ) of <b>2</b> .....	S13
<b>Figure S13.</b> <sup>1</sup> H- <sup>1</sup> H COSY spectrum (500 MHz, CDCl <sub>3</sub> ) of <b>2</b> .....	S14
<b>Figure S14.</b> HSQC spectrum of <b>2</b> .....	S14
<b>Figure S15.</b> HMBC spectrum of <b>2</b> .....	S15
<b>Figure S16.</b> NOESY spectrum of <b>1</b> .....	S10
<b>Figure S17.</b> HRESIMS spectrum of <b>2</b> .....	S15
<b>Figure S18.</b> UV spectrum of <b>2</b> .....	S16
<b>Figure S19.</b> CD spectrum of <b>2</b> .....	S16
<b>Figure S20.</b> IR spectrum of <b>2</b> .....	S17

## S1. X-ray crystallographic data of compounds 1 and 2

**Table 1 Crystal data and structure refinement for 1.**

Identification code	hujinhua_53p-3-1_collect
Empirical formula	C <sub>60</sub> H <sub>96</sub> O <sub>6</sub>
Formula weight	913.36
Temperature/K	100.00(10)
Crystal system	monoclinic
Space group	P2 <sub>1</sub>
a/Å	9.5634(5)
b/Å	13.0900(7)
c/Å	21.2717(12)
α/°	90
β/°	92.796(5)
γ/°	90
Volume/Å <sup>3</sup>	2659.7(2)
Z	2
ρ <sub>calc</sub> /cm <sup>3</sup>	1.140
μ/mm <sup>-1</sup>	0.547
F(000)	1008.0
Crystal size/mm <sup>3</sup>	0.1 × 0.08 × 0.07
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	7.934 to 133.194
Index ranges	-10 ≤ h ≤ 11, -15 ≤ k ≤ 15, -23 ≤ l ≤ 25
Reflections collected	27177
Independent reflections	9427 [R <sub>int</sub> = 0.0613, R <sub>sigma</sub> = 0.0723]
Data/restraints/parameters	9427/1434/869
Goodness-of-fit on F <sup>2</sup>	1.054
Final R indexes [I ≥ 2σ (I)]	R <sub>1</sub> = 0.0929, wR <sub>2</sub> = 0.2352
Final R indexes [all data]	R <sub>1</sub> = 0.1332, wR <sub>2</sub> = 0.2648
Largest diff. peak/hole / e Å <sup>-3</sup>	0.53/-0.26
Flack parameter	0.4(3)

**Table 1 Crystal data and structure refinement for 2.**

Identification code	53P-3-51
Empirical formula	C <sub>20</sub> H <sub>35</sub> O <sub>3.5</sub>
Formula weight	331.48
Temperature/K	100.00(10)
Crystal system	orthorhombic
Space group	P2 <sub>1</sub> 2 <sub>1</sub> 2
a/Å	18.13060(10)
b/Å	12.68530(10)
c/Å	8.13590(10)
α/°	90
β/°	90
γ/°	90
Volume/Å <sup>3</sup>	1871.19(3)
Z	4
ρ <sub>calc</sub> /cm <sup>3</sup>	1.177
μ/mm <sup>-1</sup>	0.617
F(000)	732.0
Crystal size/mm <sup>3</sup>	0.12 × 0.1 × 0.08
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	8.508 to 148.816
Index ranges	-22 ≤ h ≤ 22, -15 ≤ k ≤ 15, -9 ≤ l ≤ 8
Reflections collected	17894
Independent reflections	3677 [R <sub>int</sub> = 0.0365, R <sub>sigma</sub> = 0.0269]
Data/restraints/parameters	3677/0/227
Goodness-of-fit on F <sup>2</sup>	1.094
Final R indexes [I ≥ 2σ (I)]	R <sub>1</sub> = 0.0316, wR <sub>2</sub> = 0.0816
Final R indexes [all data]	R <sub>1</sub> = 0.0330, wR <sub>2</sub> = 0.0825
Largest diff. peak/hole / e Å <sup>-3</sup>	0.14/-0.15
Flack parameter	-0.06(8)

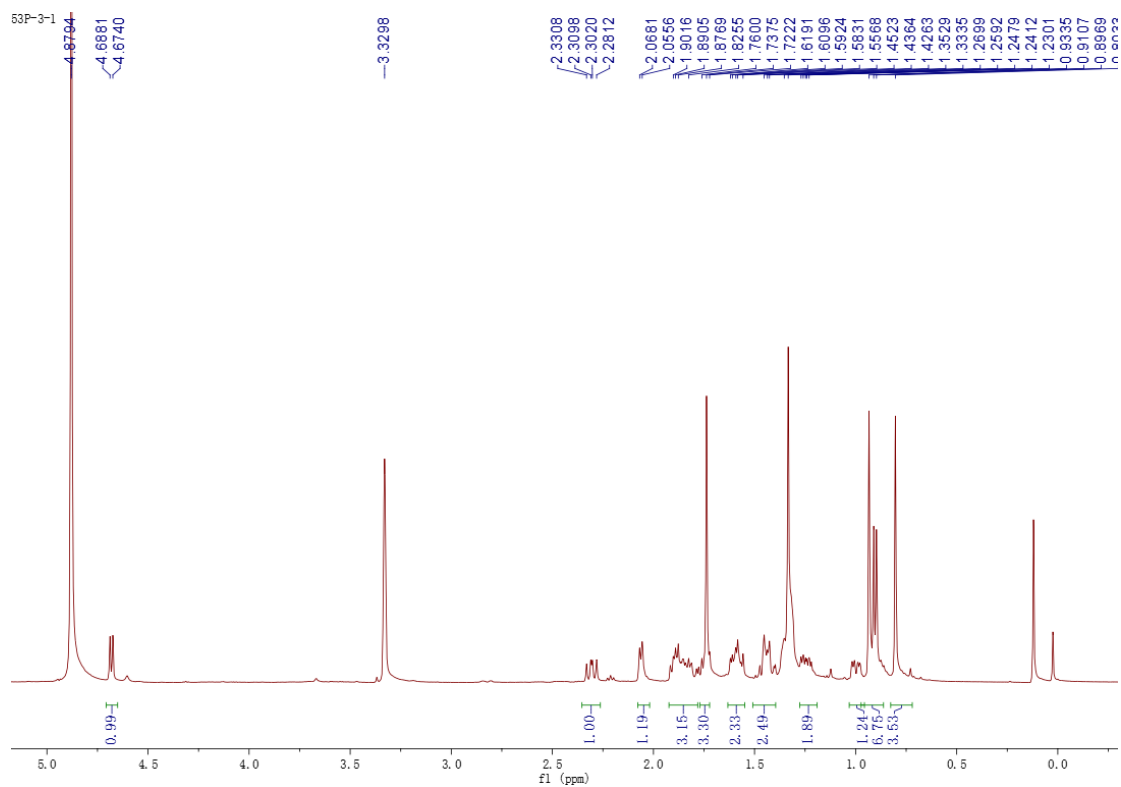


Figure S1.  $^1\text{H}$  NMR spectrum (500 MHz,  $\text{CD}_3\text{COCD}_3$ ) of **1**.

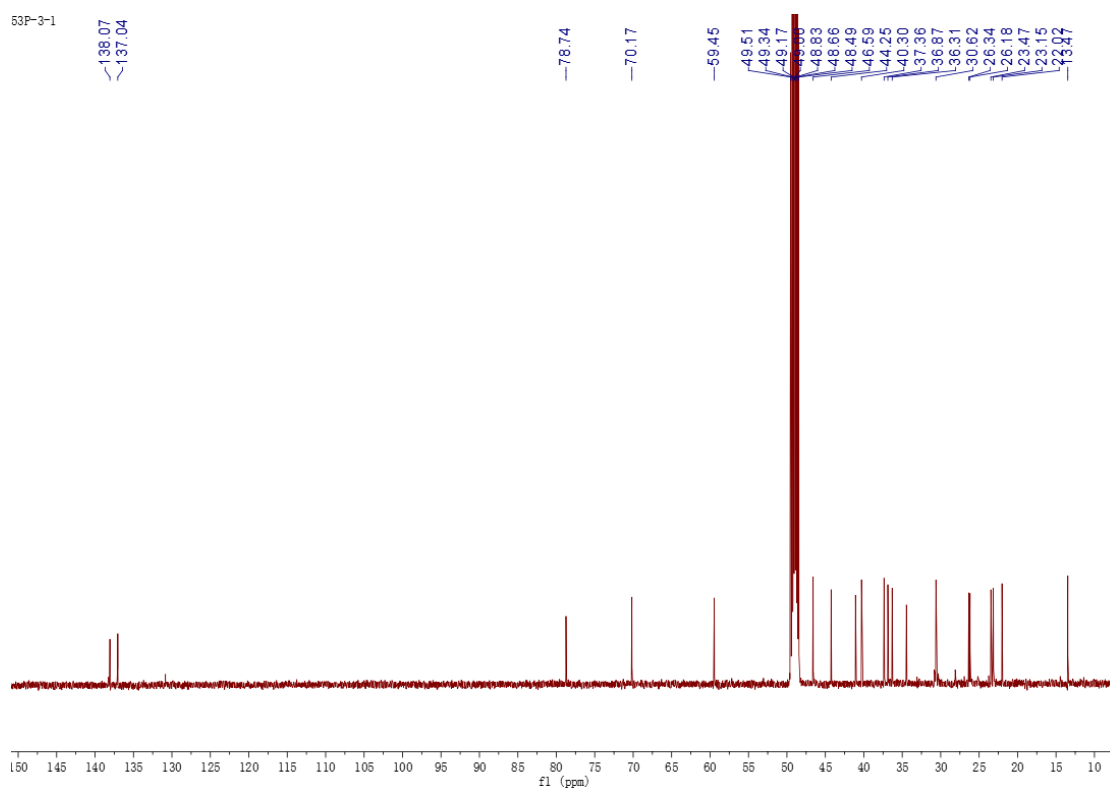
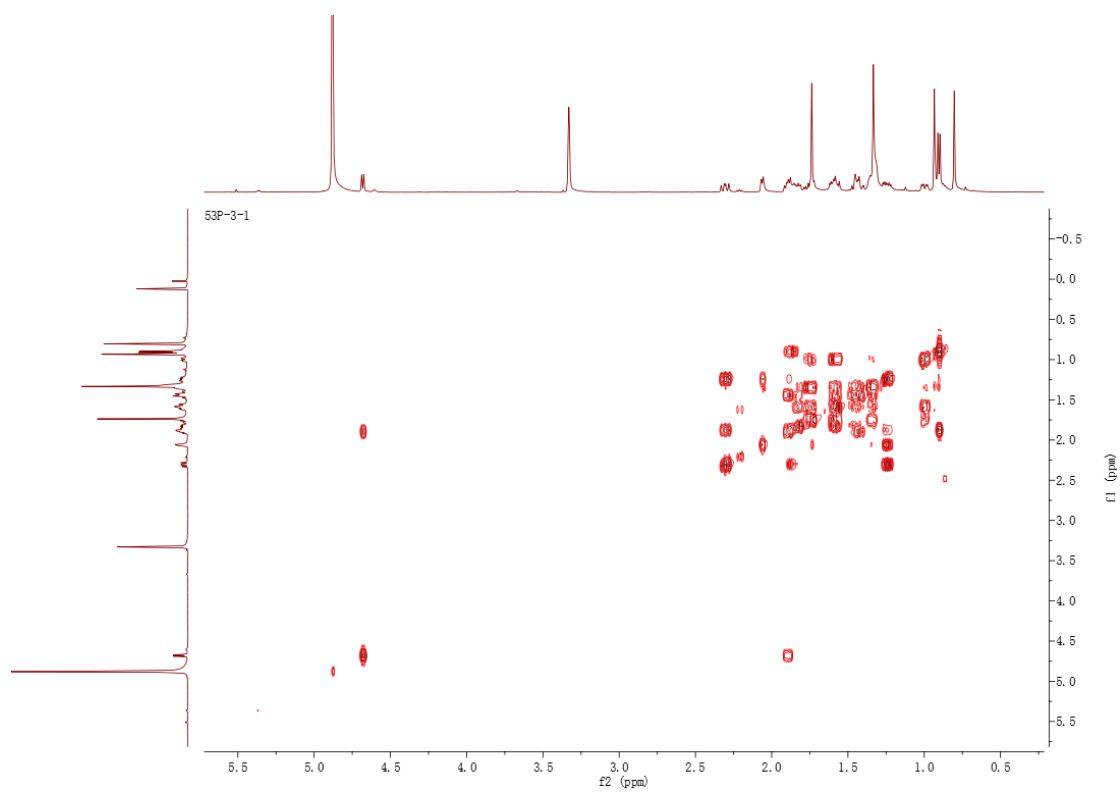
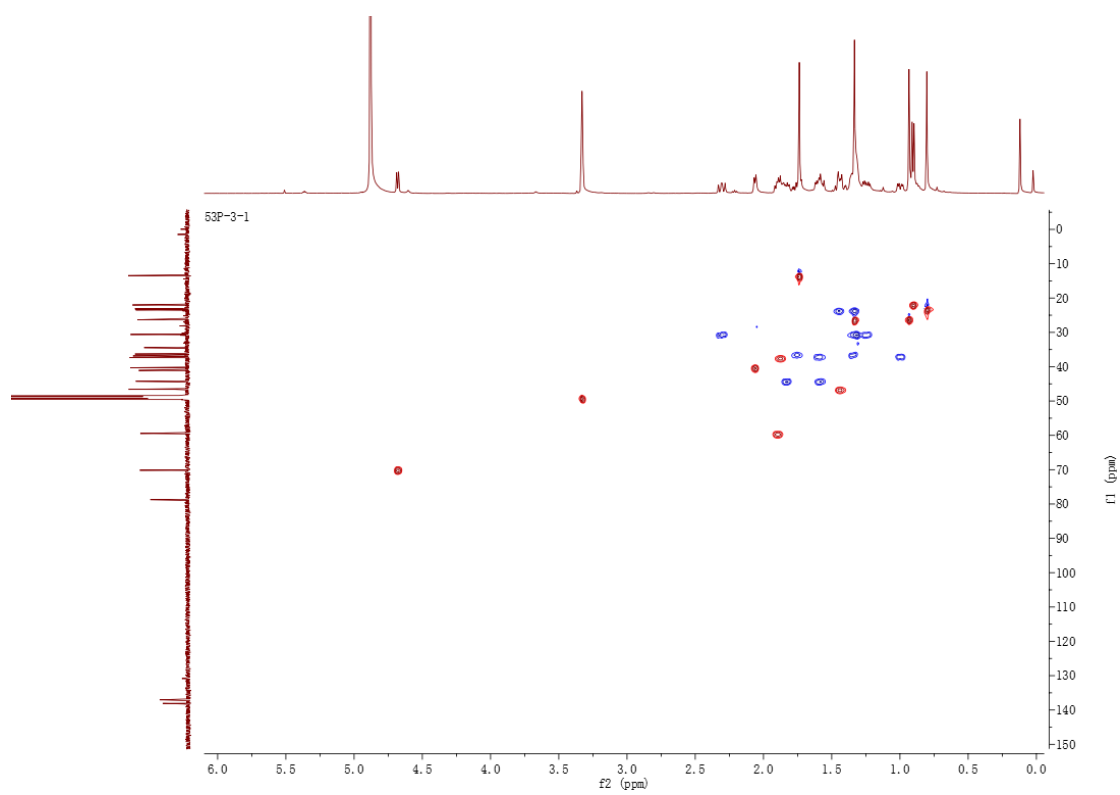


Figure S2.  $^{13}\text{C}$  NMR spectrum (125 MHz,  $\text{CD}_3\text{COCD}_3$ ) of **1**.



**Figure S3.**  $^1\text{H}$ - $^1\text{H}$  COSY spectrum (500 MHz,  $\text{CD}_3\text{COCD}_3$ ) of **1**.



**Figure S4.** HSQC spectrum of **1**.

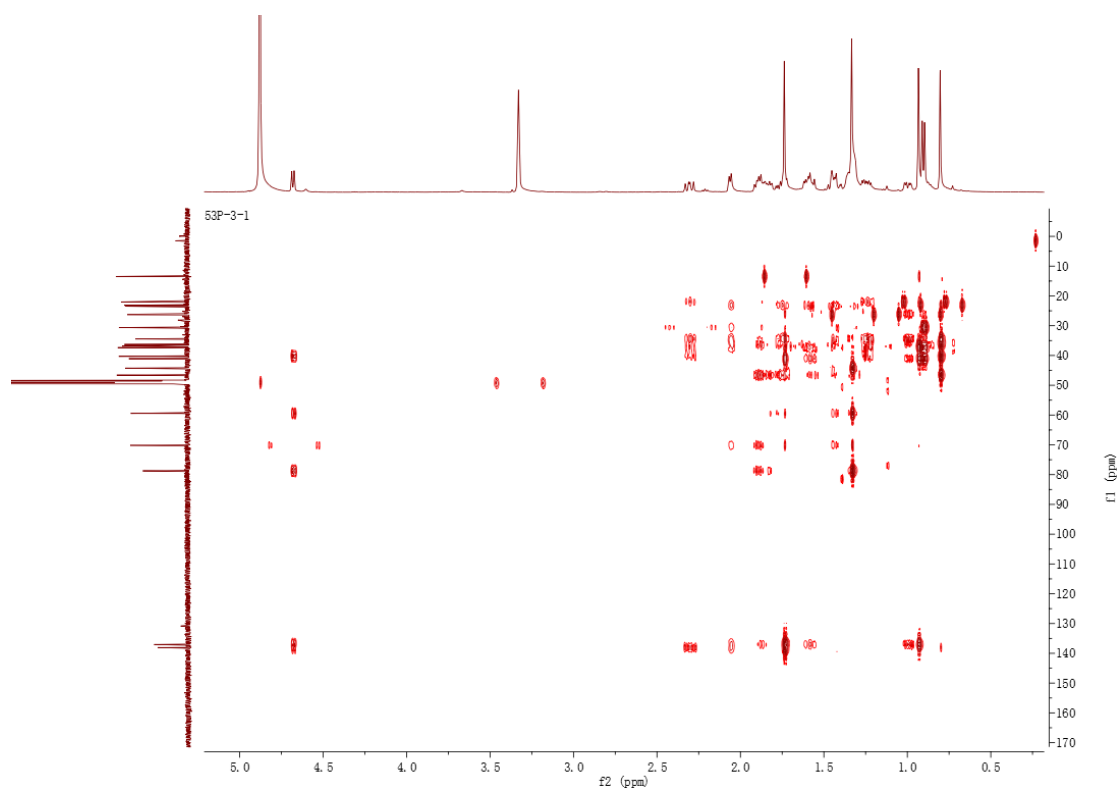


Figure S5. HMBC spectrum of 1.

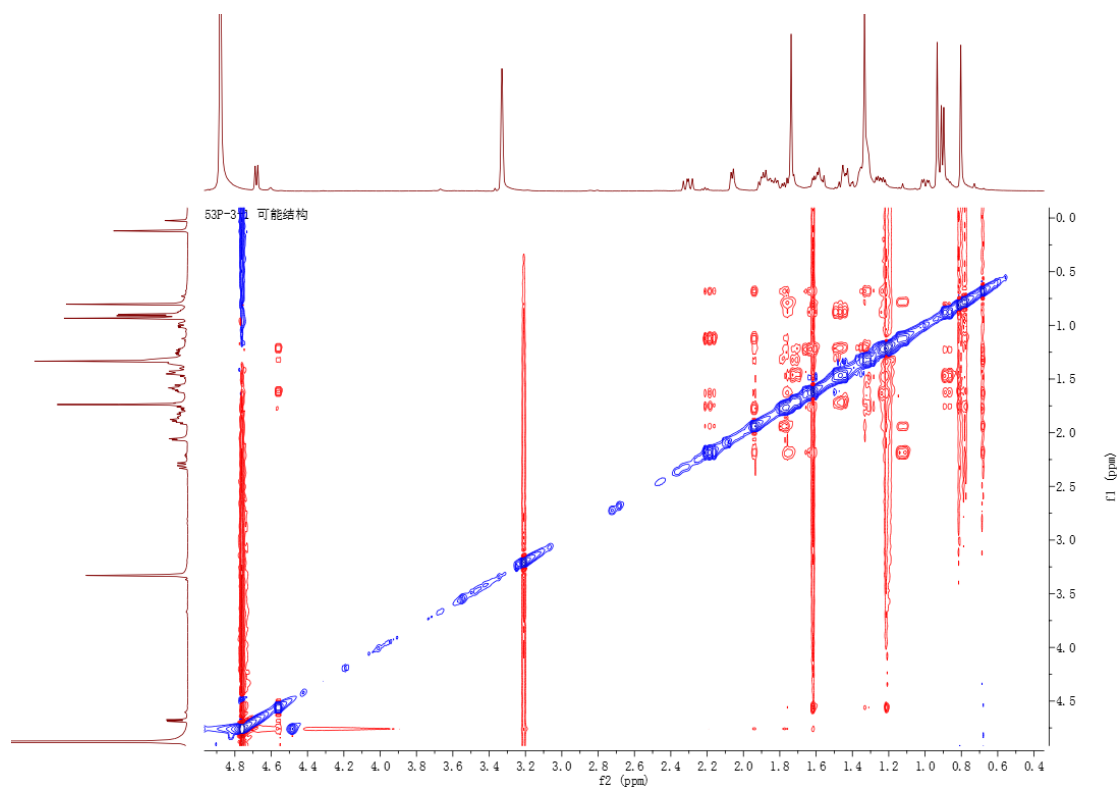
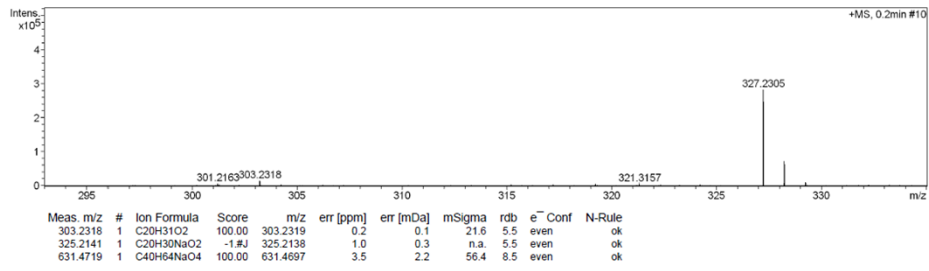


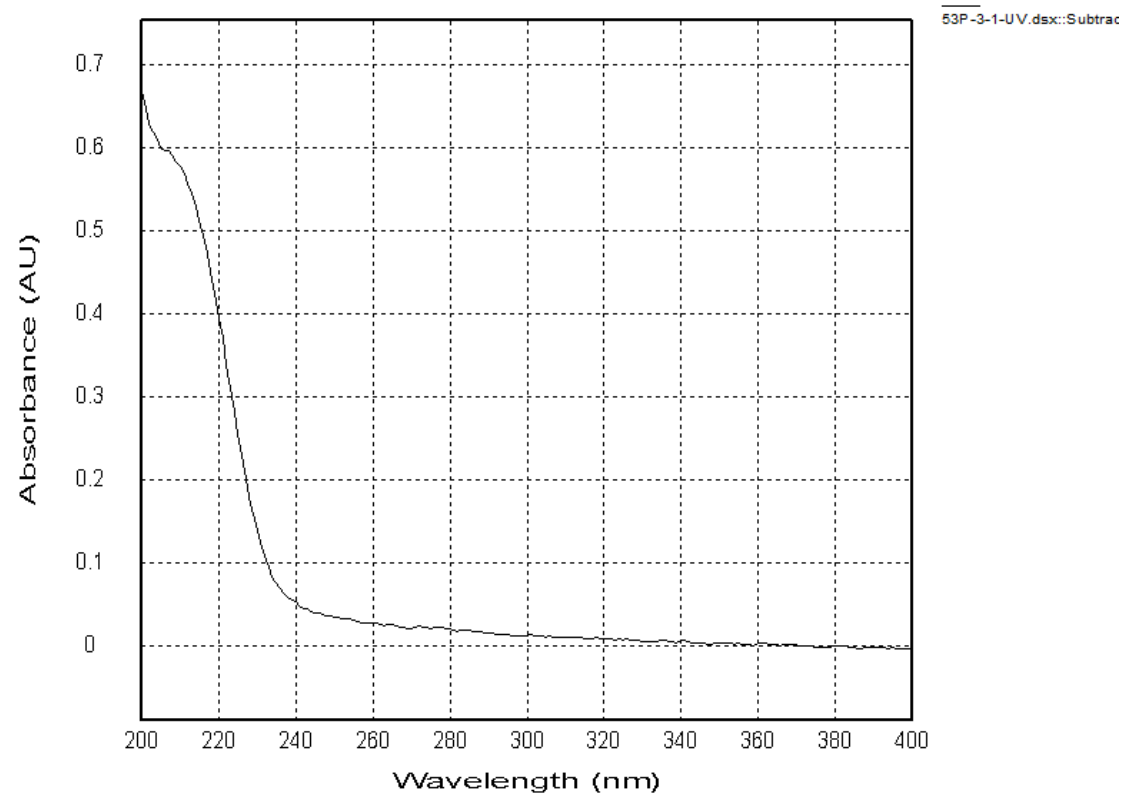
Figure S6. NOESY spectrum of 1.

### Mass Spectrum SmartFormula Report

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Sample Name	hujinhua_53P-3-1_pos			255552.00029	
Comment					
Acquisition Parameter					
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Scan Begin	70 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Charging Voltage	0 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



**Figure S7. HRESIMS spectrum of 1.**



**Figure S8. UV spectrum of 1.**



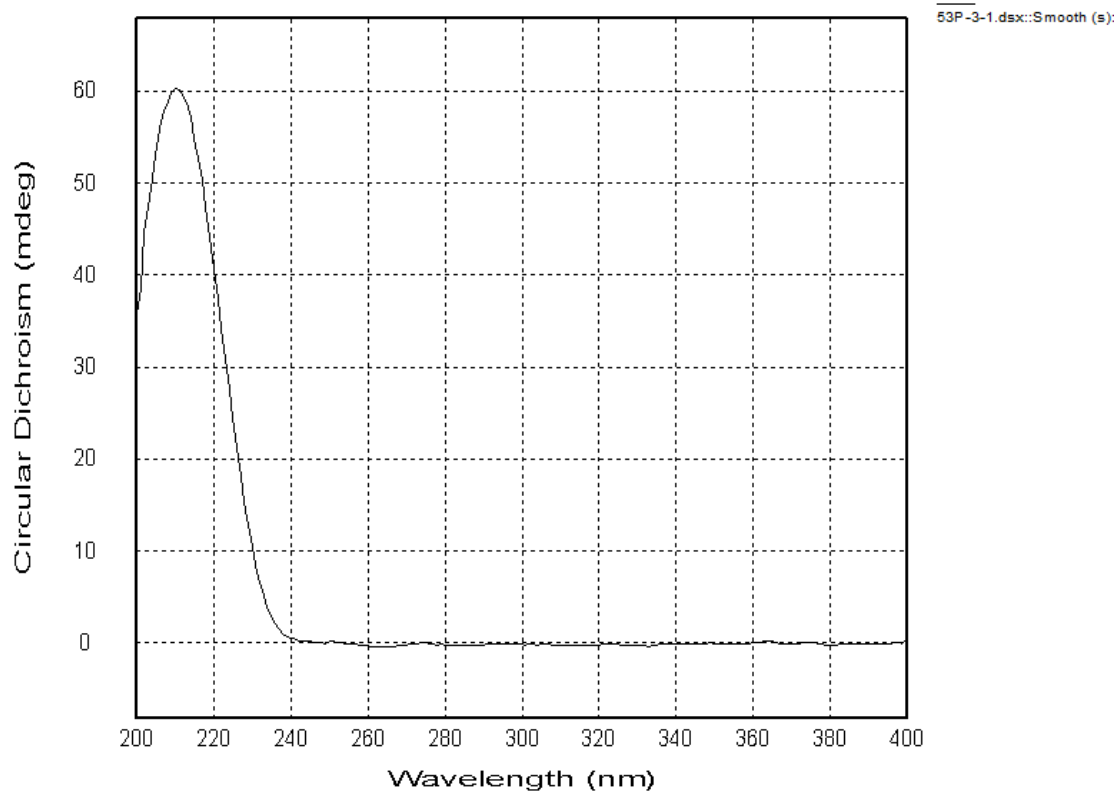


Figure S9. CD spectrum of 1.

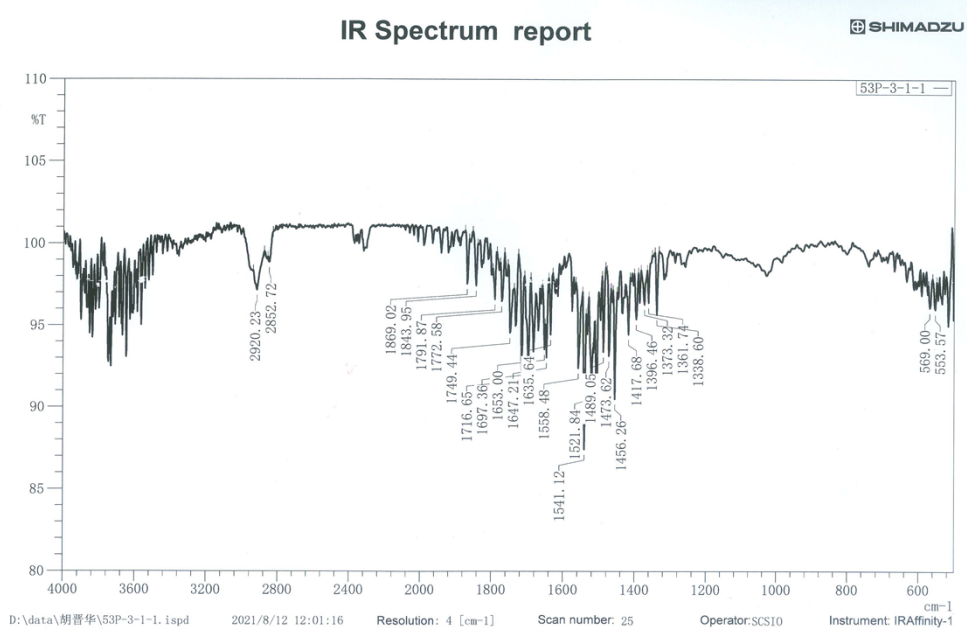


Figure S10. IR spectrum of 1.

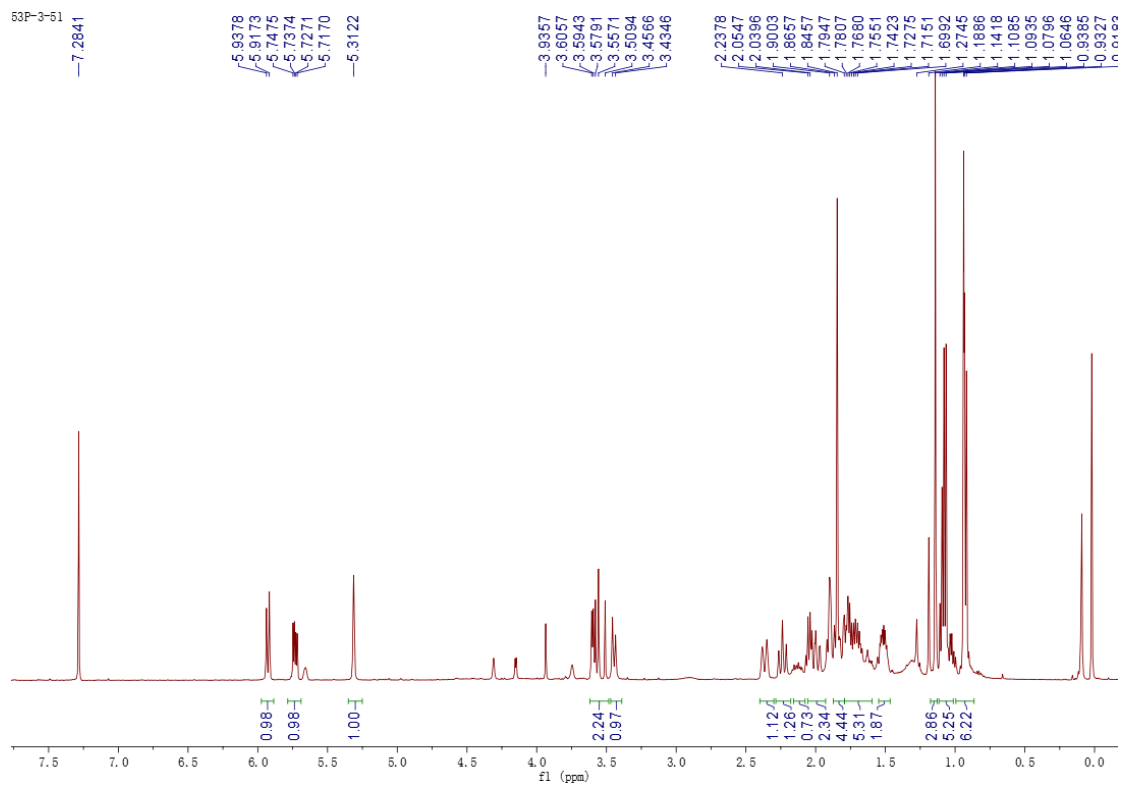


Figure S11.  $^1\text{H}$  NMR spectrum (500 MHz,  $\text{CDCl}_3$ ) of **2**.

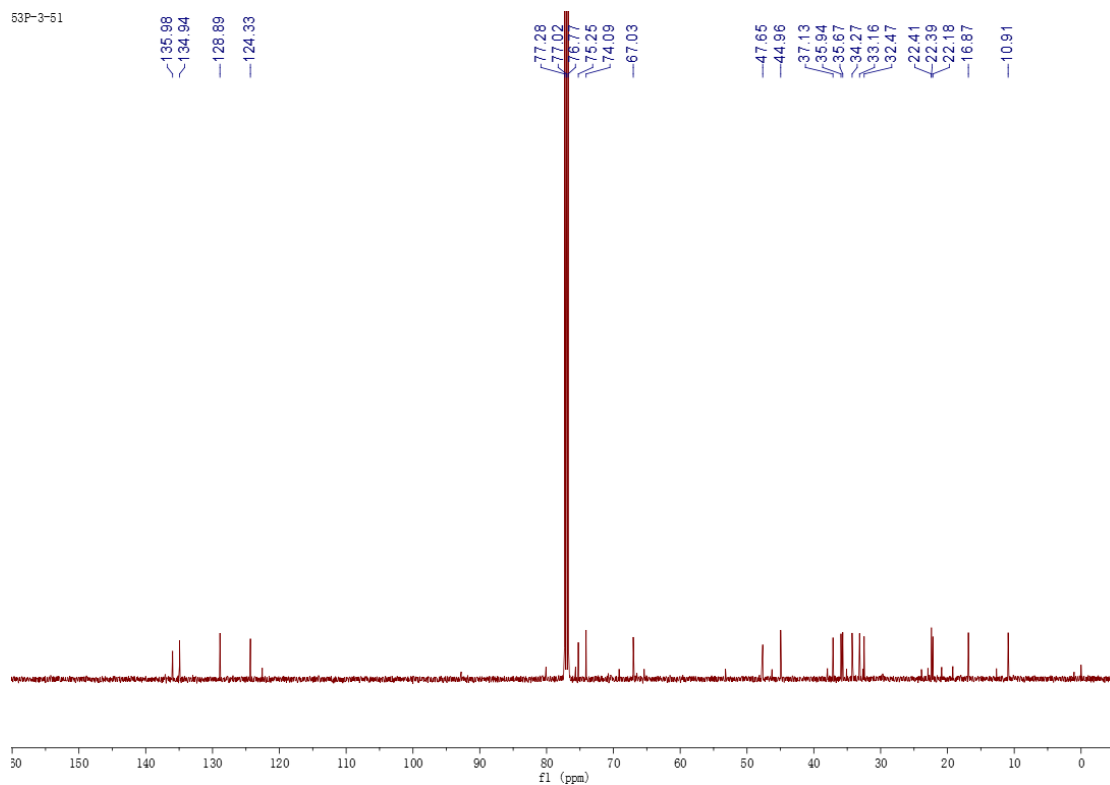
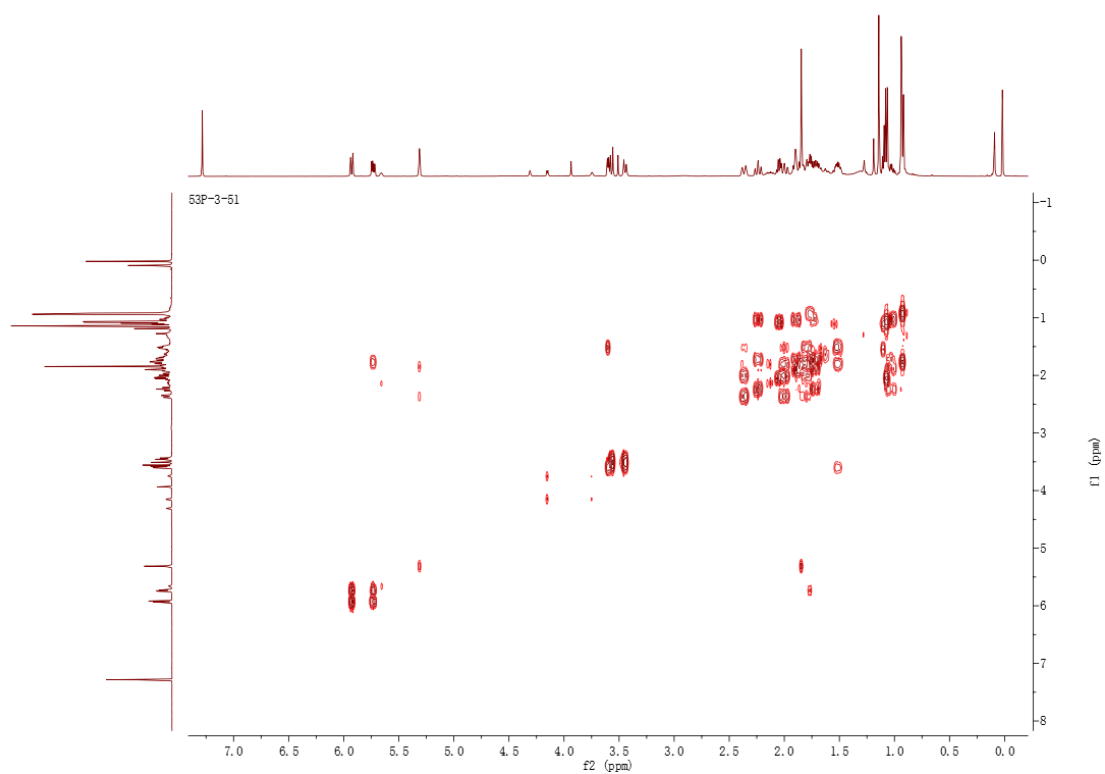
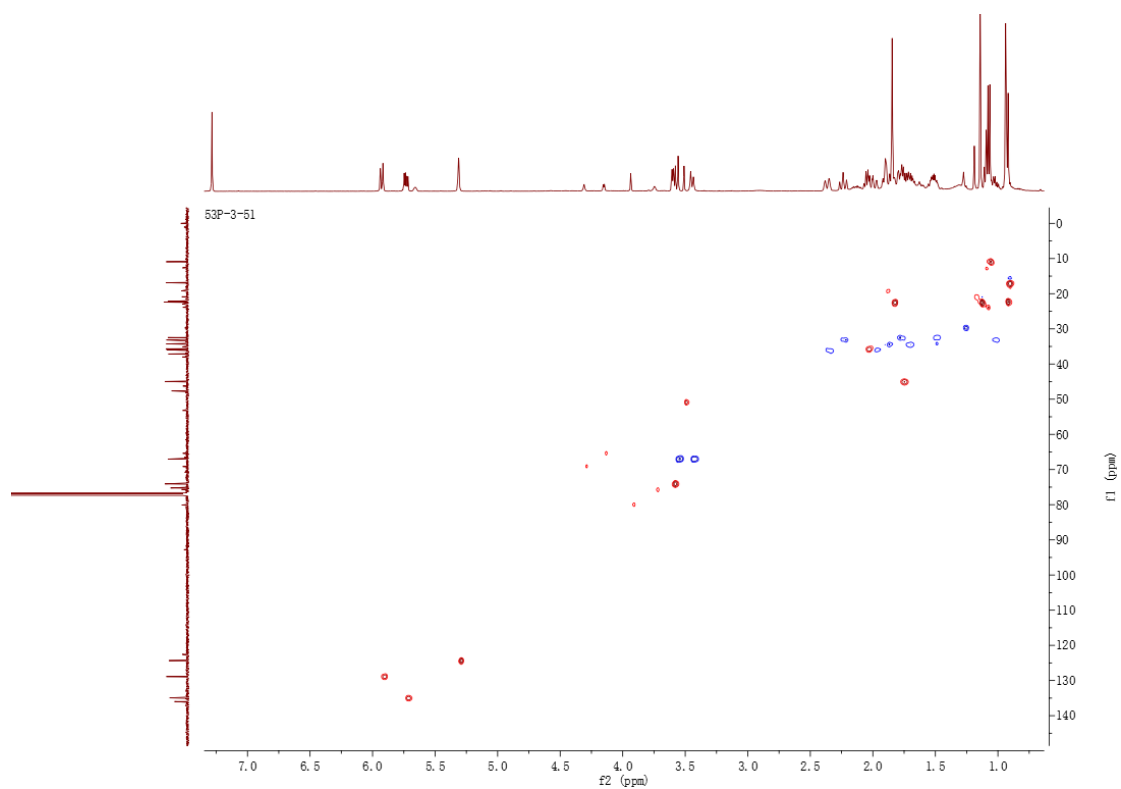


Figure S12.  $^{13}\text{C}$  NMR spectrum (125 MHz,  $\text{CDCl}_3$ ) of **2**.



**Figure S13.**  $^1\text{H}$ - $^1\text{H}$  COSY spectrum (500 MHz,  $\text{CDCl}_3$ ) of **2**.



**Figure S14.** HSQC spectrum of **2**.

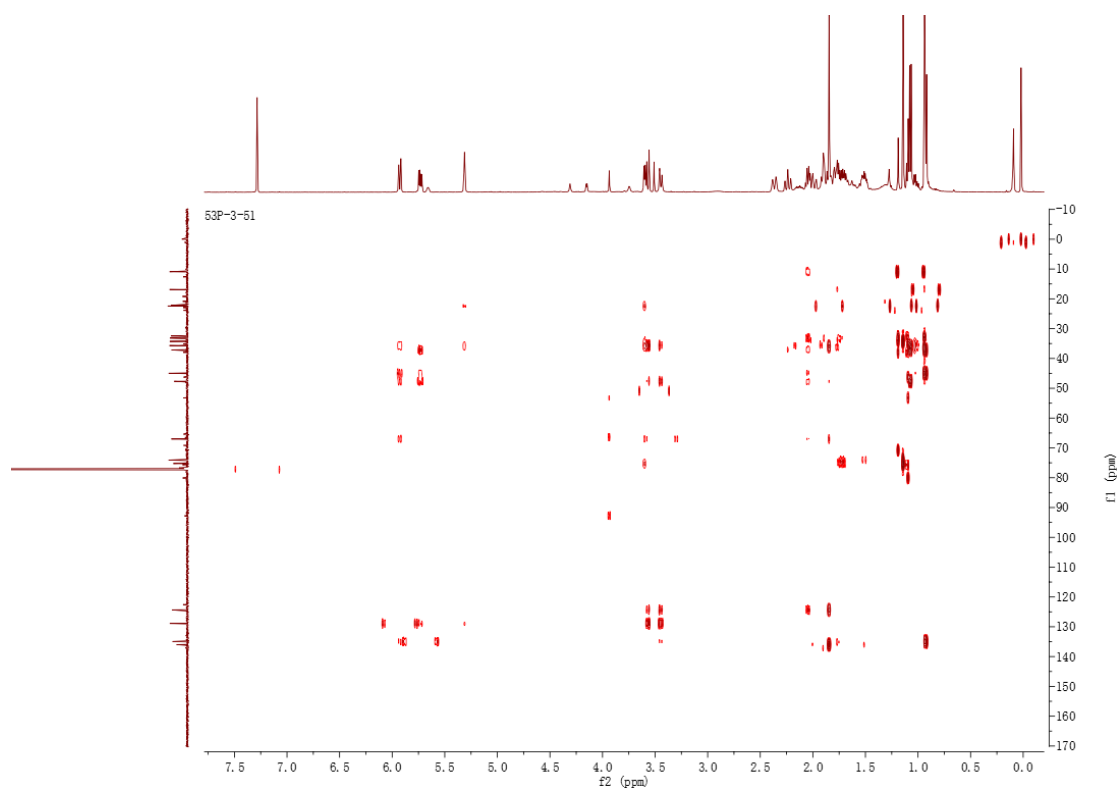


Figure S15. HMBC spectrum of **2**.

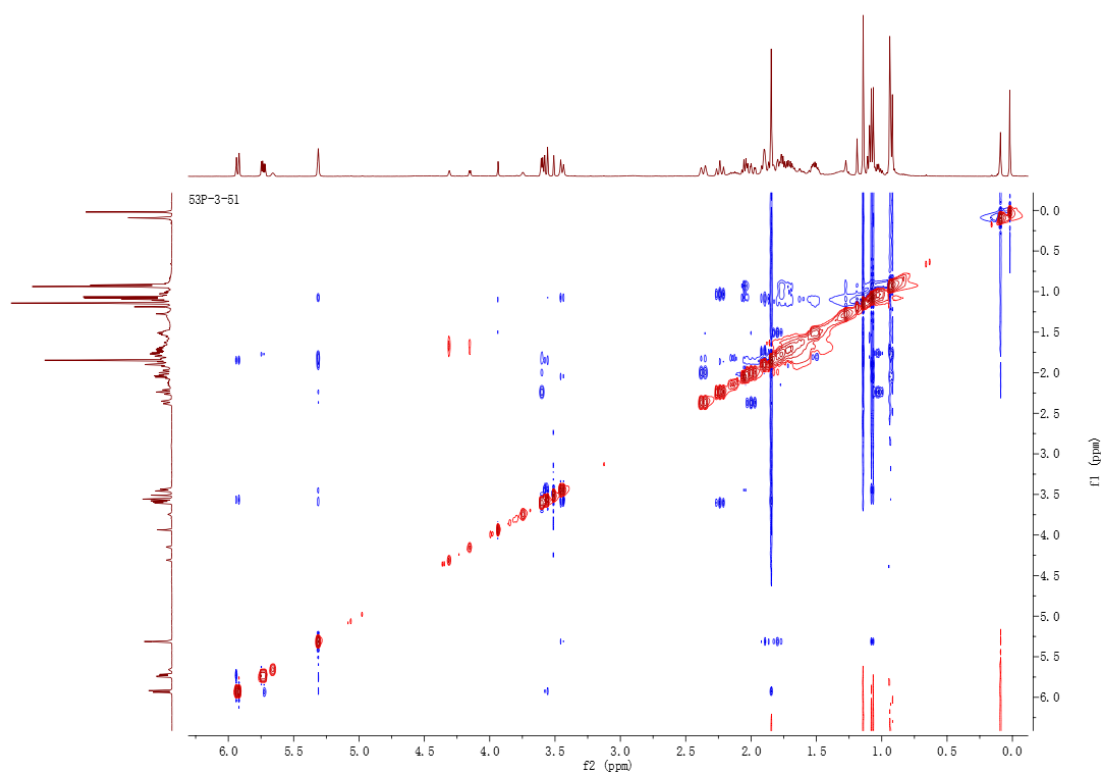


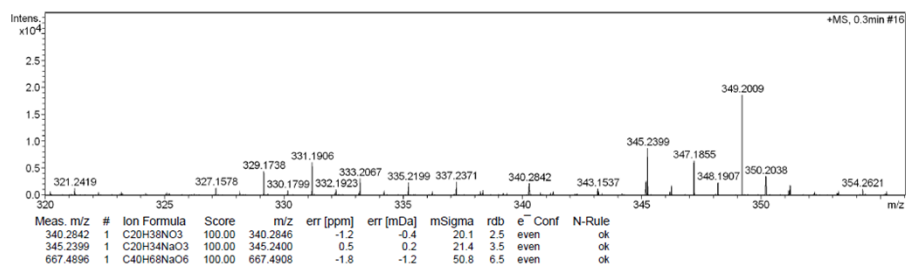
Figure S16. NOESY spectrum of **2**.

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Comment			255552.00029

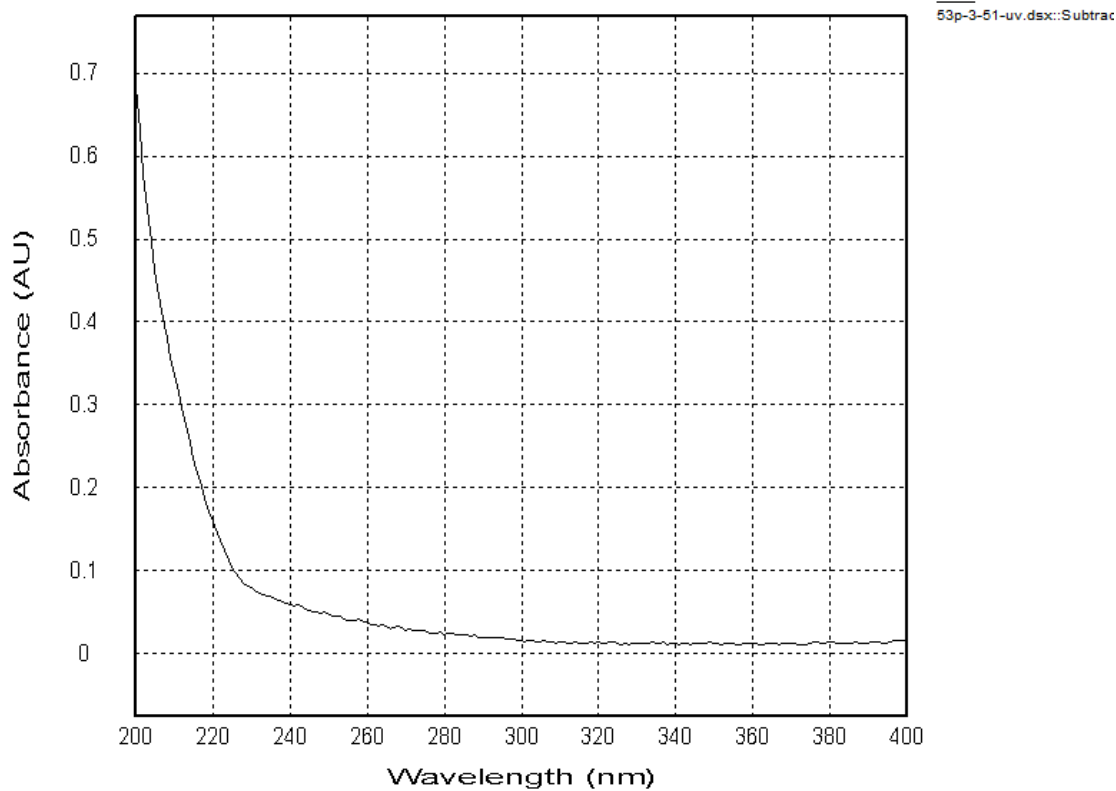
  

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Scan End	1500 m/z	Set Charging Voltage	0 V	Set Divert Valve	Waste	
		Set Corona	0 nA	Set APCI Heater	0 °C	



hujinhua\_53P-3-51\_pos\_34\_01\_14721.d  
 Bruker Compass DataAnalysis 4.1 printed: 3/23/2023 10:35:21 AM by: SCSIO Page 1 of 1

**Figure S17.** HRESIMS spectrum of **2**.



**Figure S18.** UV spectrum of **2**.

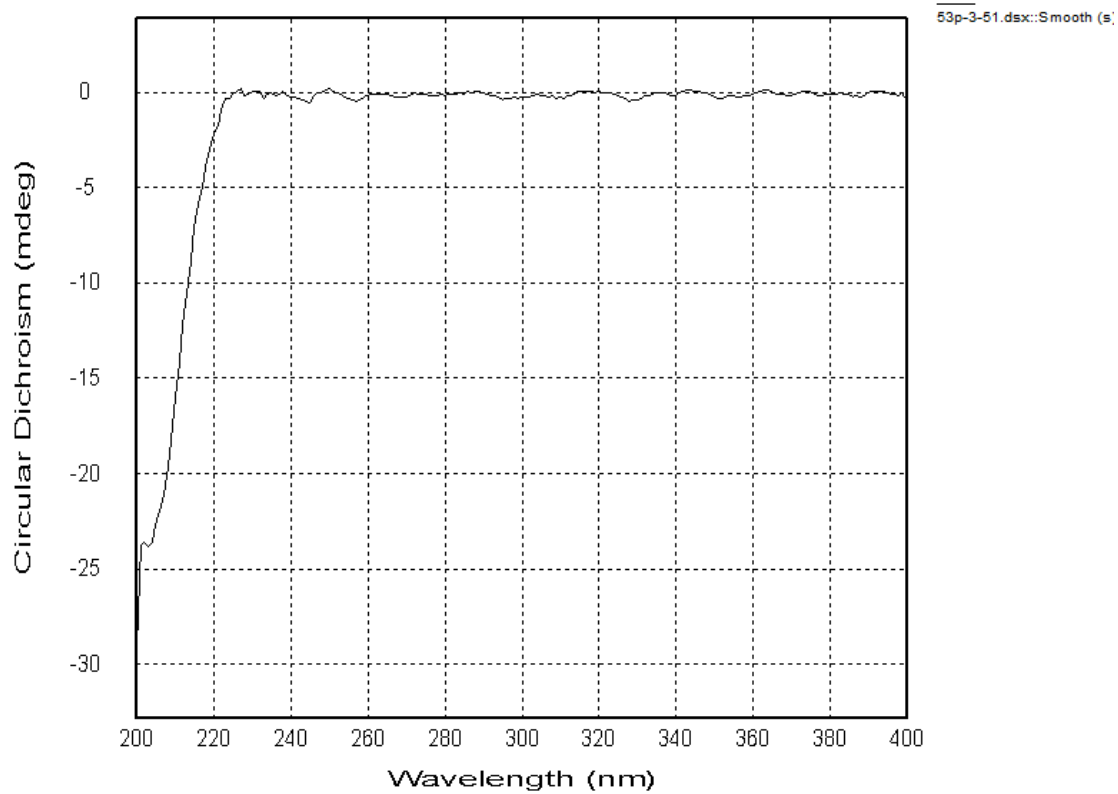


Figure S19. CD spectrum of 13.

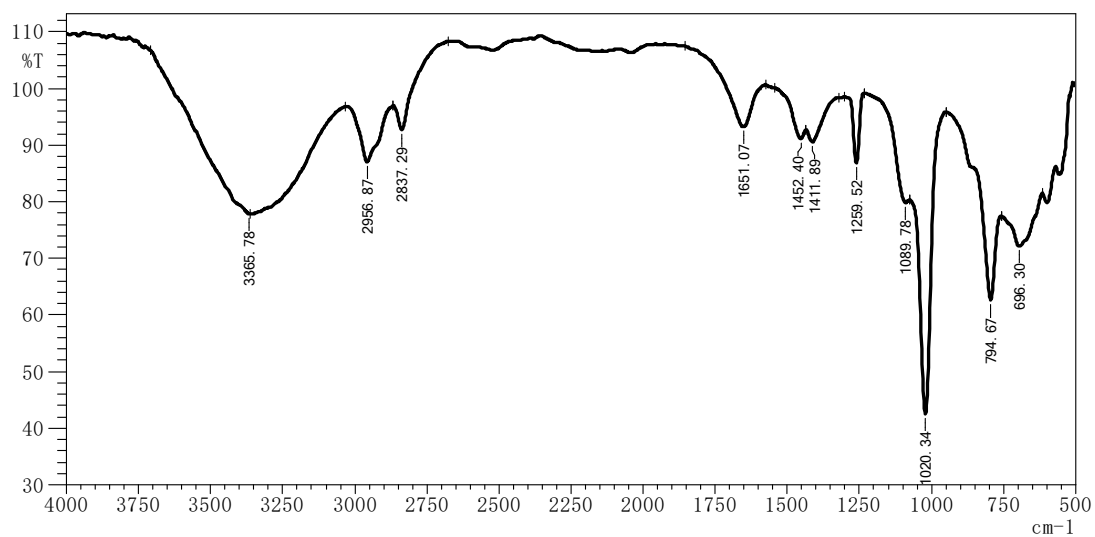


Figure S20. IR spectrum of 2.