

## Supporting Information

*Rec. Nat. Prod.* X:X (2020) XX-XX

### A New Diarylbenzophenone from *Selaginella tamariscina*

Wanling Chen<sup>1#</sup>, Yujie Peng<sup>1#</sup>, Wanxia Huang<sup>1</sup>, Lu Zhou<sup>1</sup>, Xinyu Quan<sup>1</sup>, Qiong Zhao<sup>1</sup>,  
Dan Zhang<sup>1</sup>, Xifeng Sheng<sup>1</sup>, Yixiao Luo<sup>1\*</sup> and Hui Zou<sup>1,2\*</sup>

<sup>1</sup>Key Laboratory of Study and Discovery of Small Targeted Molecules of Hunan Province, School of Medicine, Hunan Normal University, Changsha 410013, R. P. China

<sup>2</sup>Key Laboratory of Epigenetics and Oncology, Research Center for Preclinical Medicine, Southwest Medical University, Luzhou, Sichuan 646000, R. P. China

---

Tables of Contents	page
<b>Figure S1:</b> <sup>1</sup> H NMR spectrum of <b>1</b> in CD <sub>3</sub> OD (400 MHz)	2
<b>Figure S2:</b> enlarged <sup>1</sup> H NMR spectrum of <b>1</b> CD <sub>3</sub> OD (400 MHz)	3
<b>Figure S3:</b> <sup>13</sup> C NMR spectrum of <b>1</b> CD <sub>3</sub> OD (100 MHz)	4
<b>Figure S4:</b> <sup>1</sup> H- <sup>1</sup> H COSY spectrum of <b>1</b>	5
<b>Figure S5:</b> HSQC spectrum of <b>1</b>	6
<b>Figure S6:</b> HMBC spectrum of <b>1</b>	7
<b>Figure S7:</b> HR-ESI-MS spectrum of <b>1</b>	8
<b>Figure S8:</b> Scifinder report for <b>1</b>	9
<b>Figure S9:</b> <sup>1</sup> H NMR spectrum of <b>2</b> in CD <sub>3</sub> OD (400 MHz)	10
<b>Figure S10:</b> <sup>13</sup> C NMR spectrum of <b>2</b> CD <sub>3</sub> OD (100 MHz)	11
<b>Figure S11:</b> <sup>1</sup> H NMR spectrum of <b>3</b> in DMSO- <i>d</i> <sub>6</sub> (400 MHz)	12
<b>Figure S12:</b> <sup>13</sup> C NMR spectrum of <b>3</b> DMSO- <i>d</i> <sub>6</sub> (100 MHz)	13

---

# These authors contributed equally to this work.

\* Corresponding authors: Email: luoyx@hunnu.edu.cn (Yixiao Luo) and zouhui308@163.com (Hui Zou)

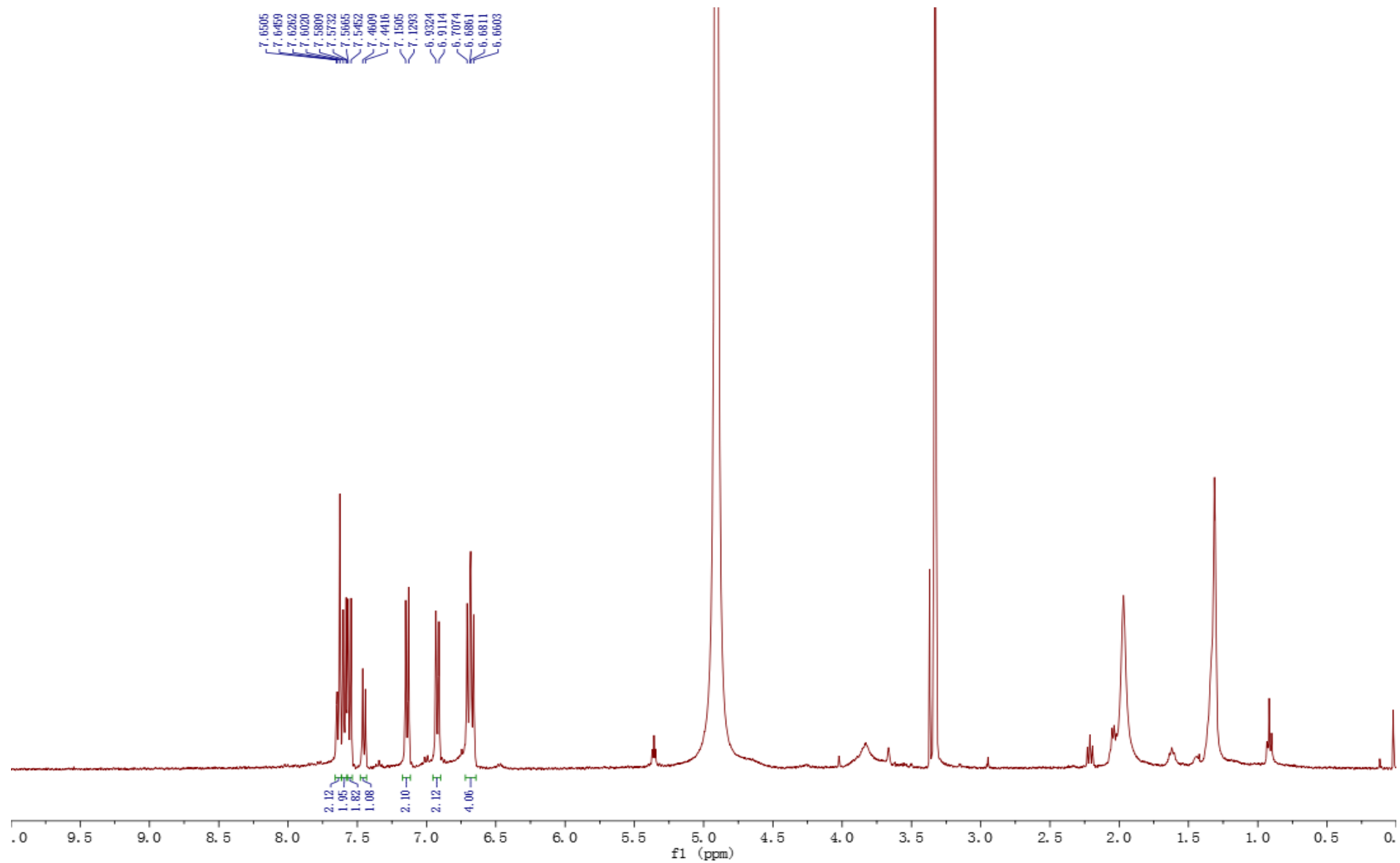
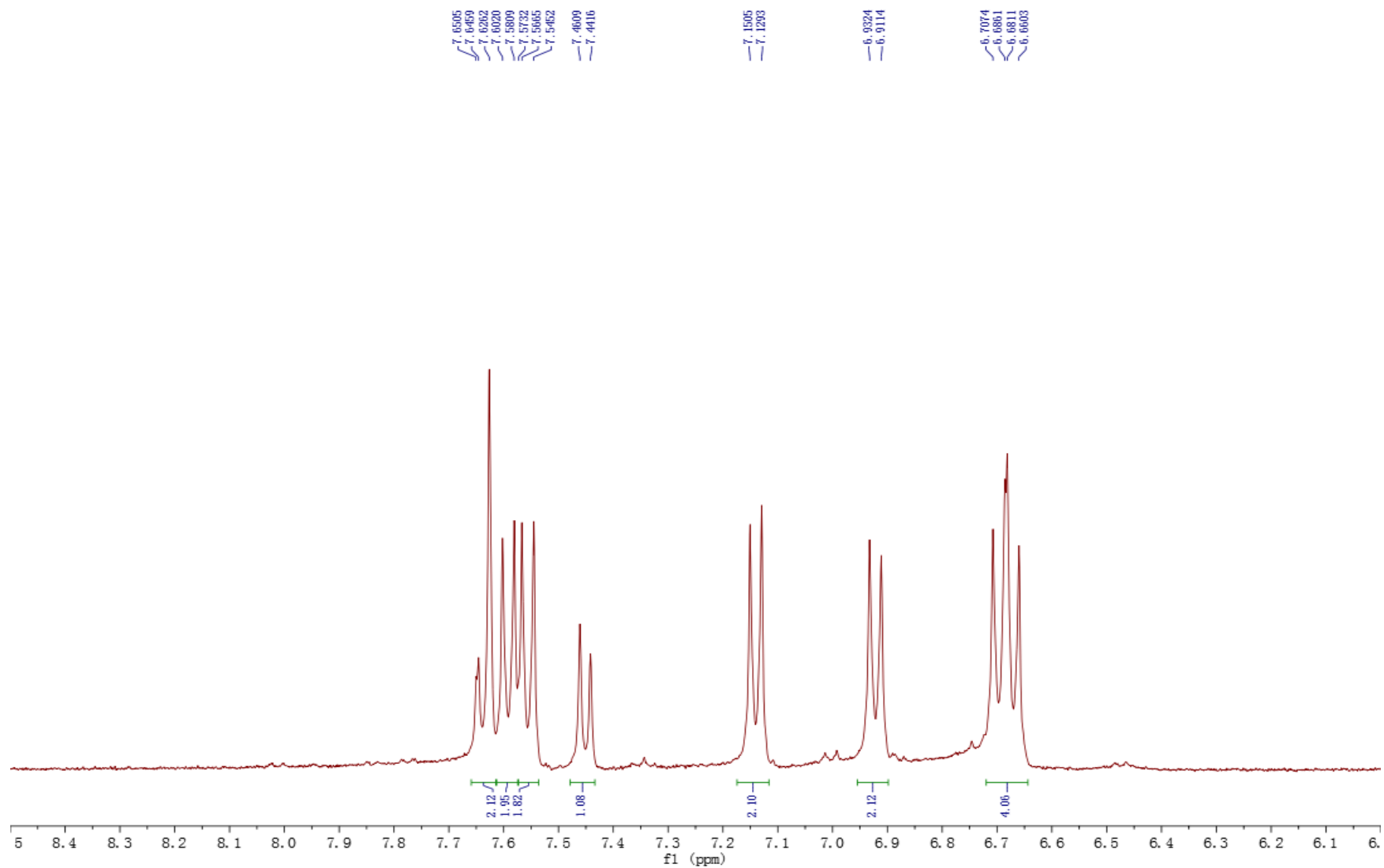
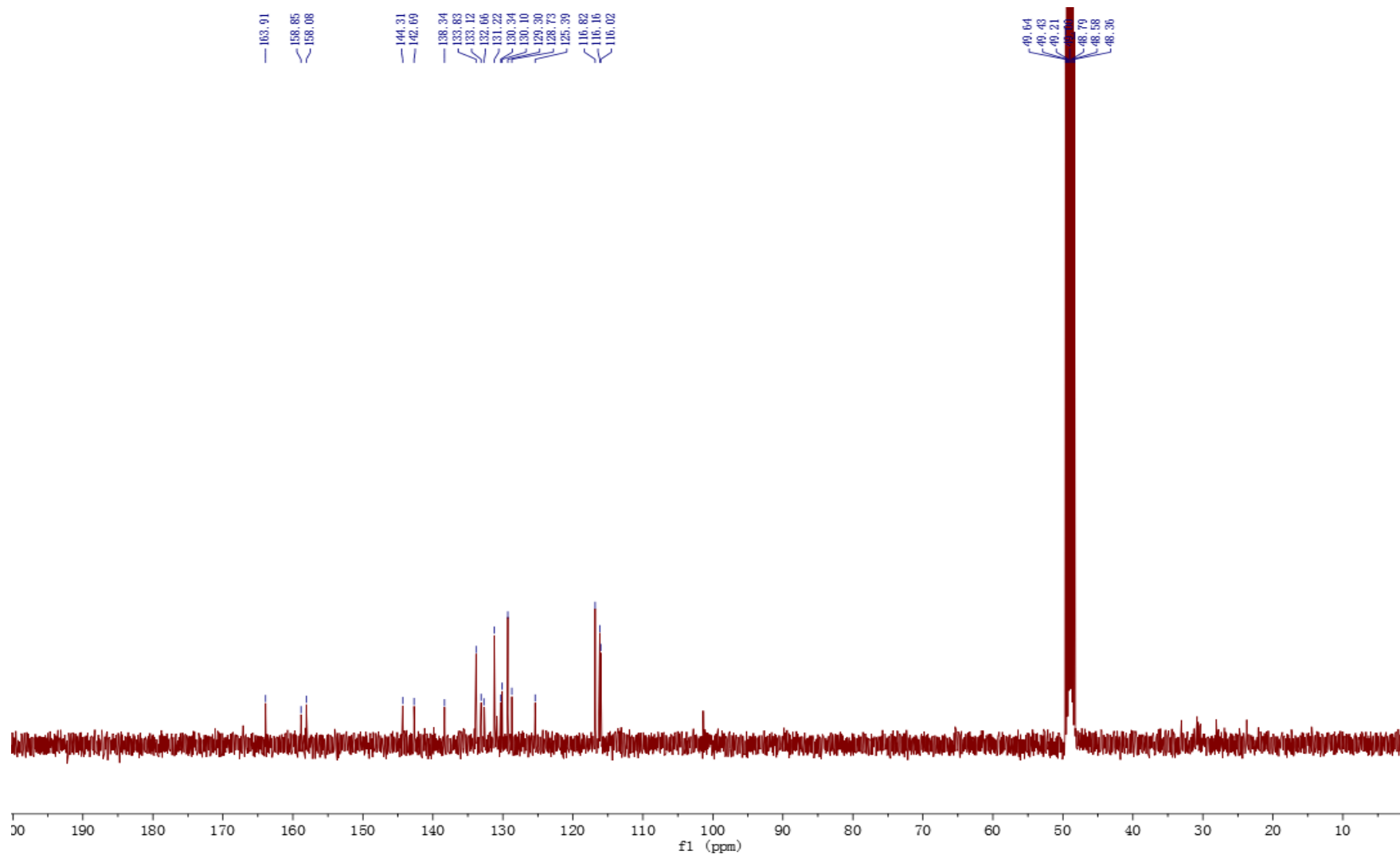


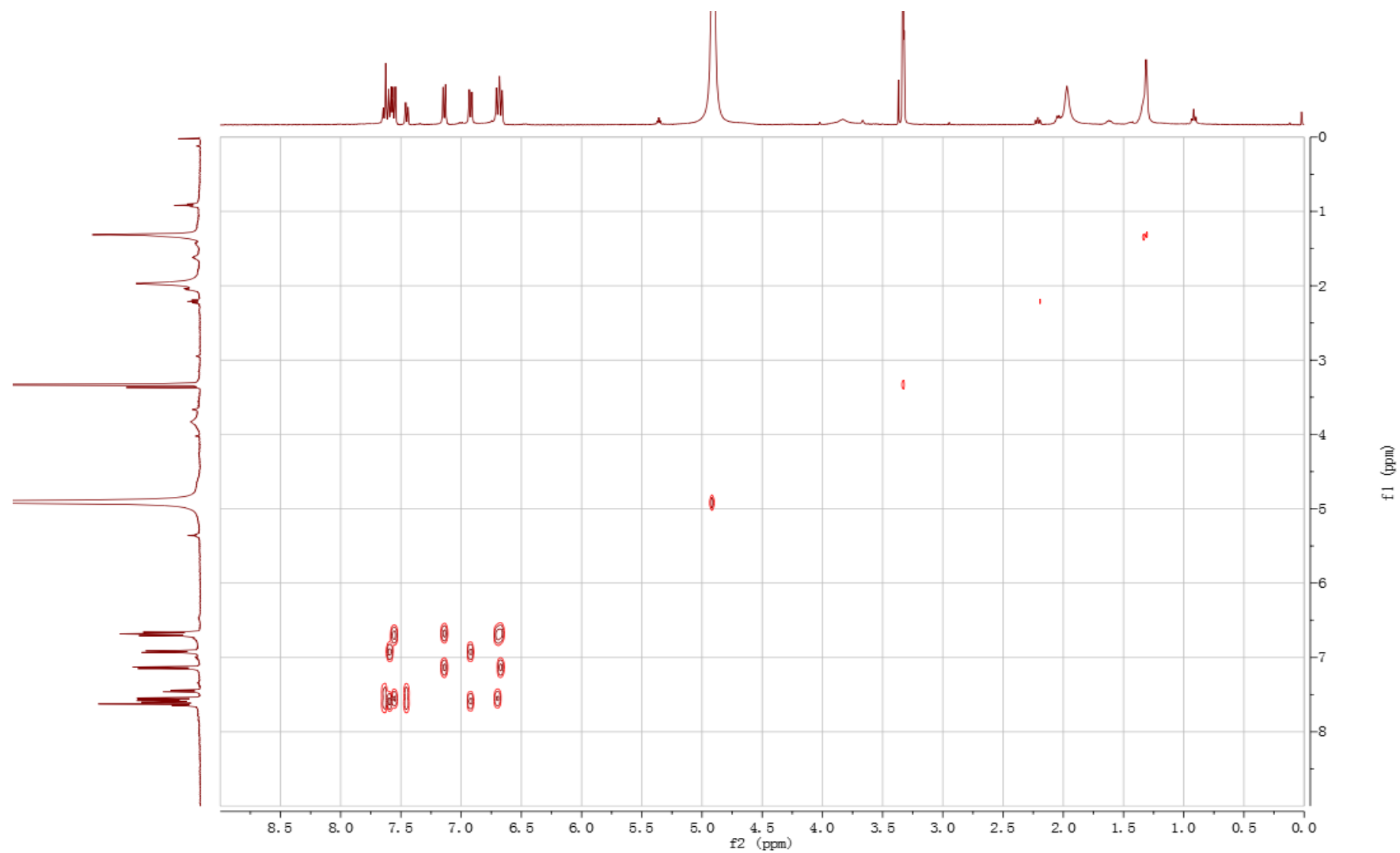
Figure S1:  $^1\text{H}$  NMR spectrum of **1** in  $\text{CD}_3\text{OD}$  (400 MHz)



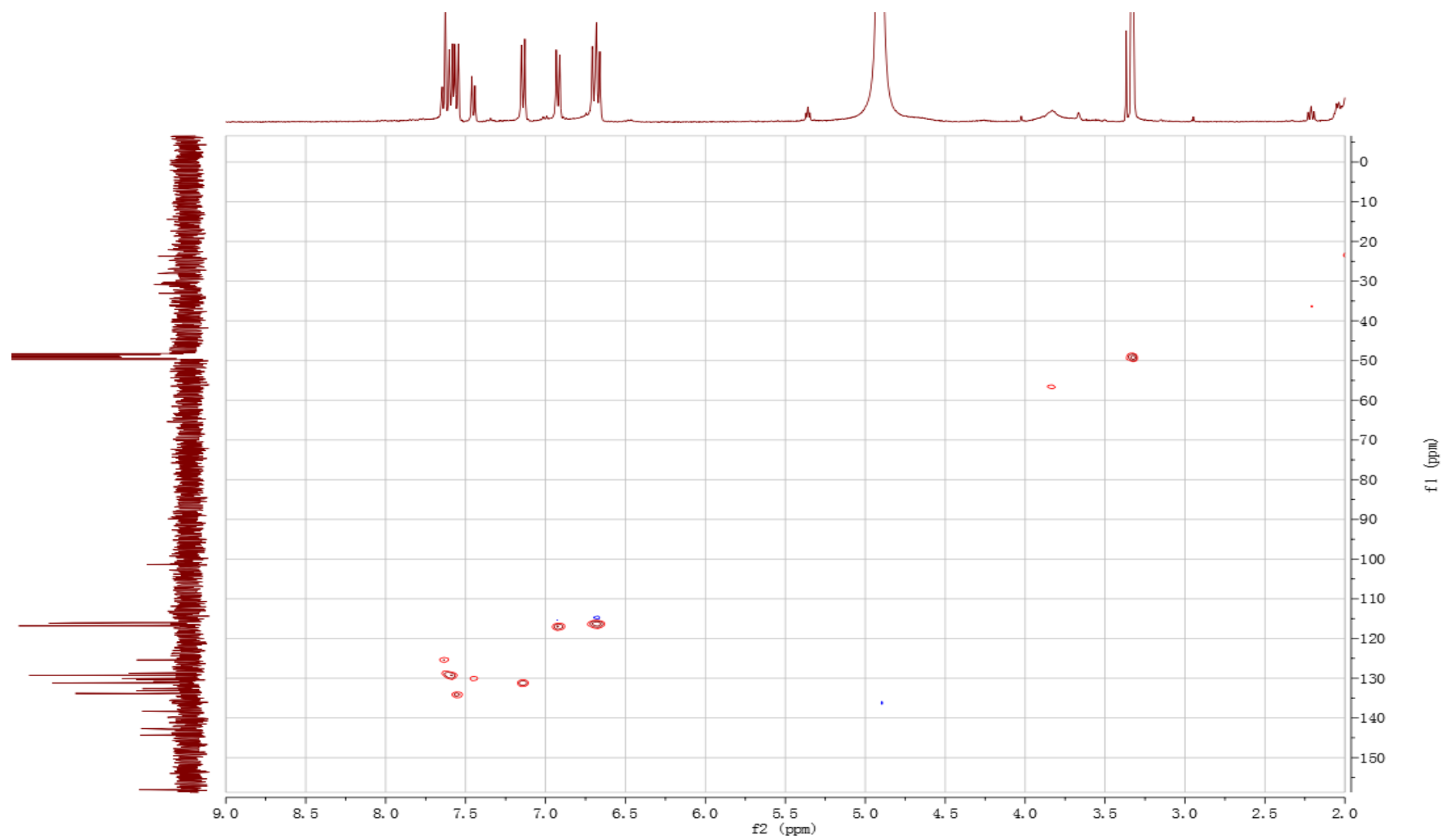
**Figure S2:** enlarged  $^1\text{H}$  NMR spectrum of **1**  $\text{CD}_3\text{OD}$  (400 MHz)



**Figure S3:**  $^{13}\text{C}$  NMR spectrum of **1**  $\text{CD}_3\text{OD}$  (100 MHz)



**Figure S4:**  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of **1**



**Figure S5:** HSQC spectrum of compound 1

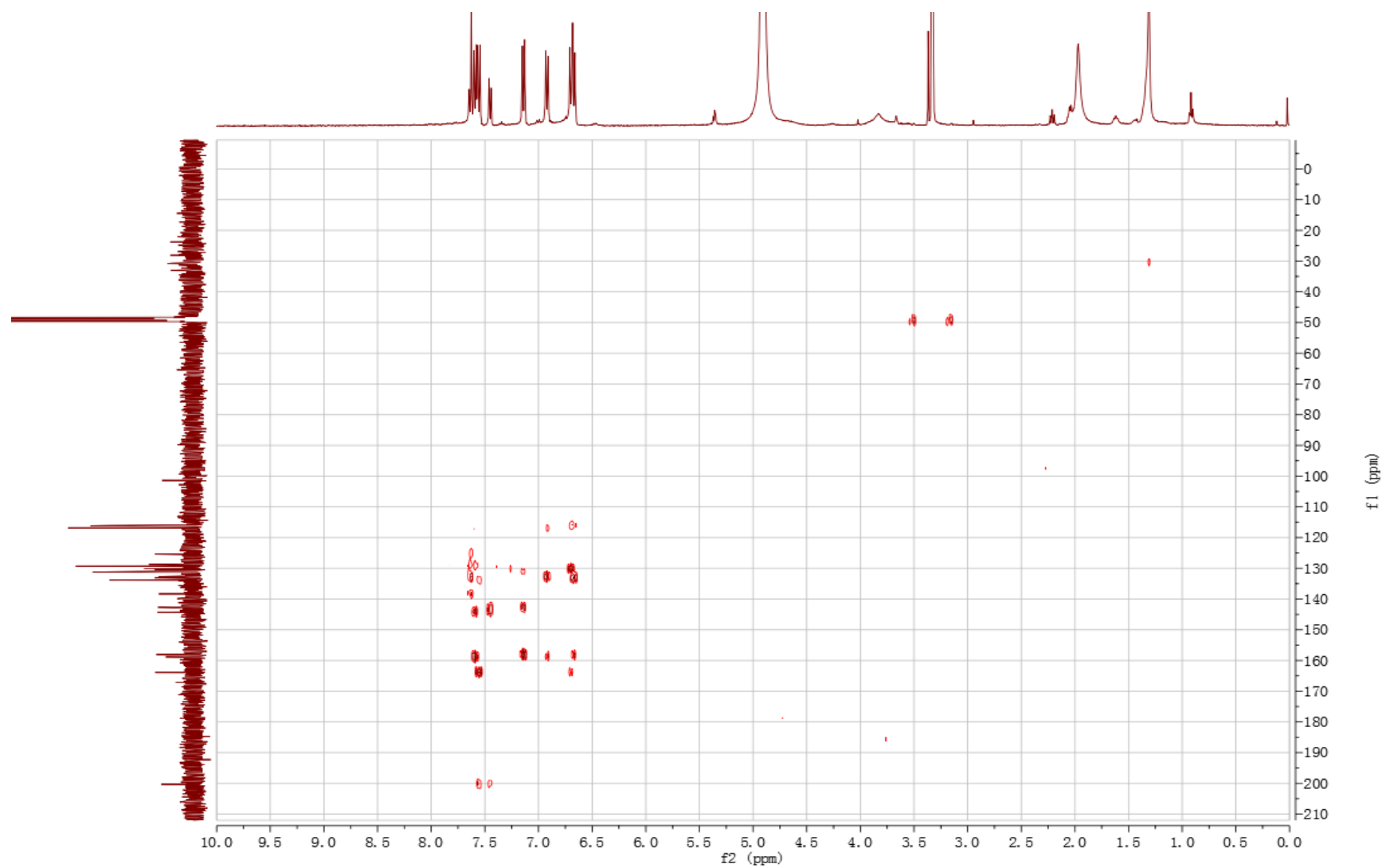
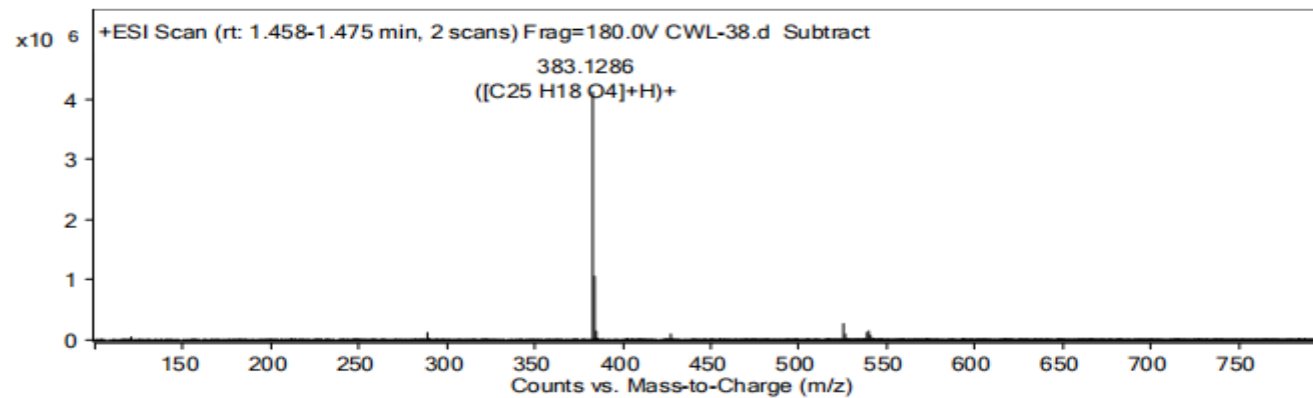


Figure S6: HMBC spectrum of **1**

Fragmentor Voltage      Collision Energy      Ionization Mode  
180                              0                              ESI



**Peak List**

m/z	z	Abund	Formula	Ion
383.1286	1	4118602	C <sub>25</sub> H <sub>18</sub> O <sub>4</sub>	(M+H) <sup>+</sup>
384.132	1	1050968.63	C <sub>25</sub> H <sub>18</sub> O <sub>4</sub>	(M+H) <sup>+</sup>

**Formula Calculator Element Limits**

Element	Min	Max
C	3	60
H	0	120
O	0	30

Figure S7: HR-ESI-MS spectrum of 1



**SUBSTANCES**

Analyze Refine

Analyze by:  
*No substances available*

Chemical Structure similarity

**SUBSTANCES**

Select All Deselect All

0 of 7 Similarity Candidates Selected

	Substances
<input type="checkbox"/> ≥ 99 (most similar)	0
<input type="checkbox"/> 95-98	0
<input type="checkbox"/> 90-94	14
<input type="checkbox"/> 85-89	85
<input type="checkbox"/> 80-84	396
<input type="checkbox"/> 75-79	1647
<input type="checkbox"/> 70-74	5294
<input type="checkbox"/> 65-69	16157
<input type="checkbox"/> 0-64 (least similar)	44952

Get Substances

**Figure S8:** Scifinder report for 1

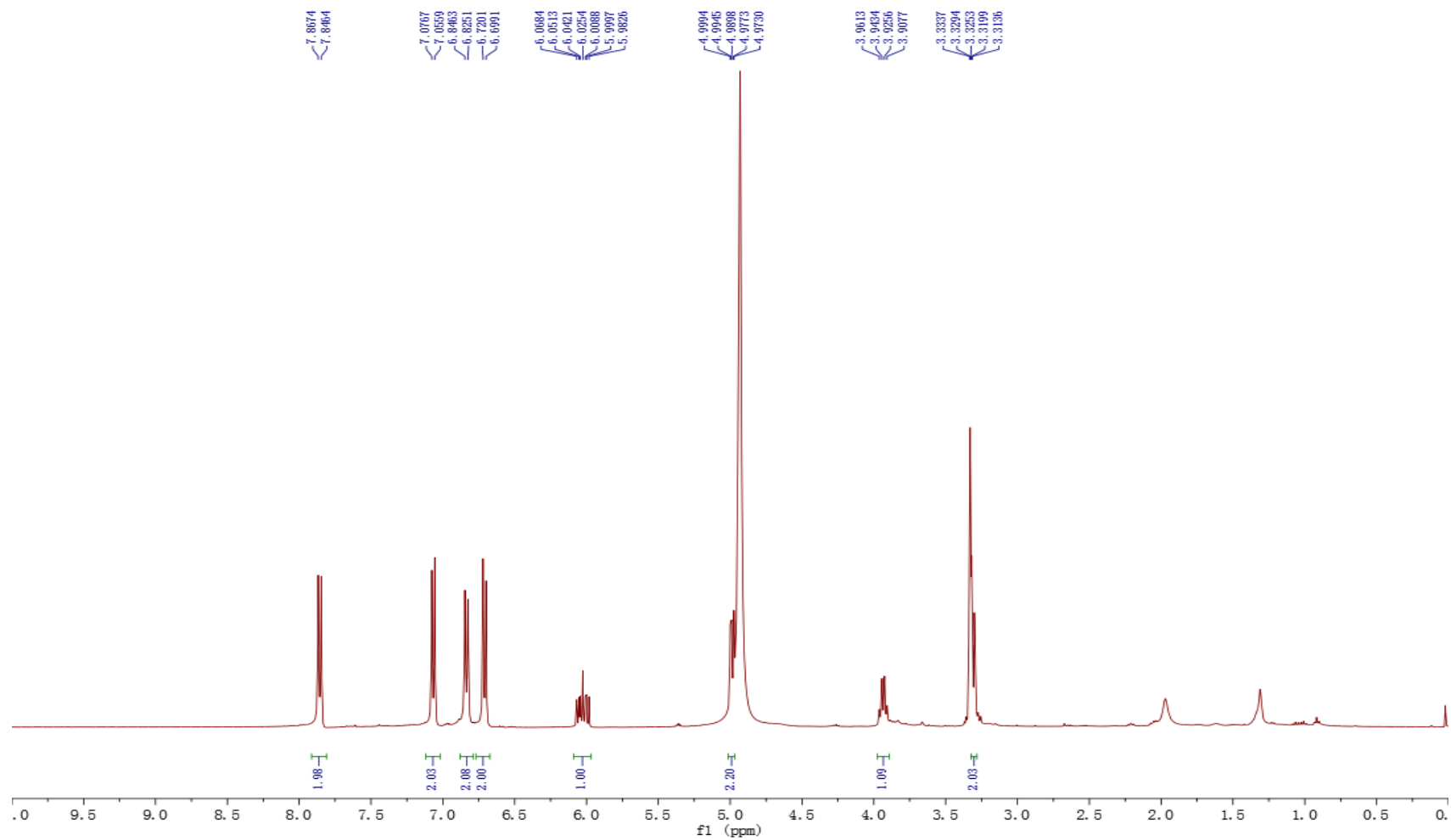
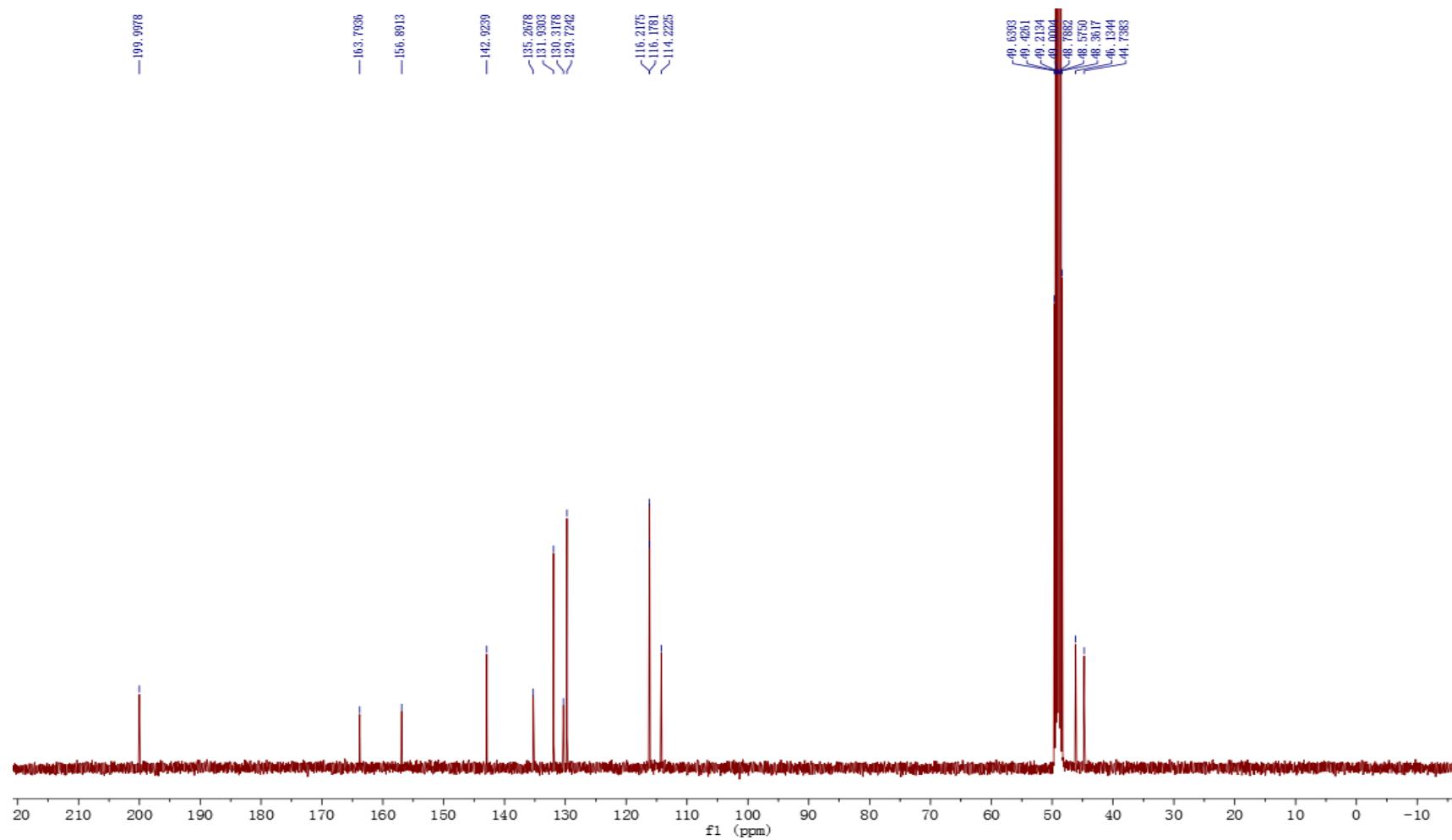
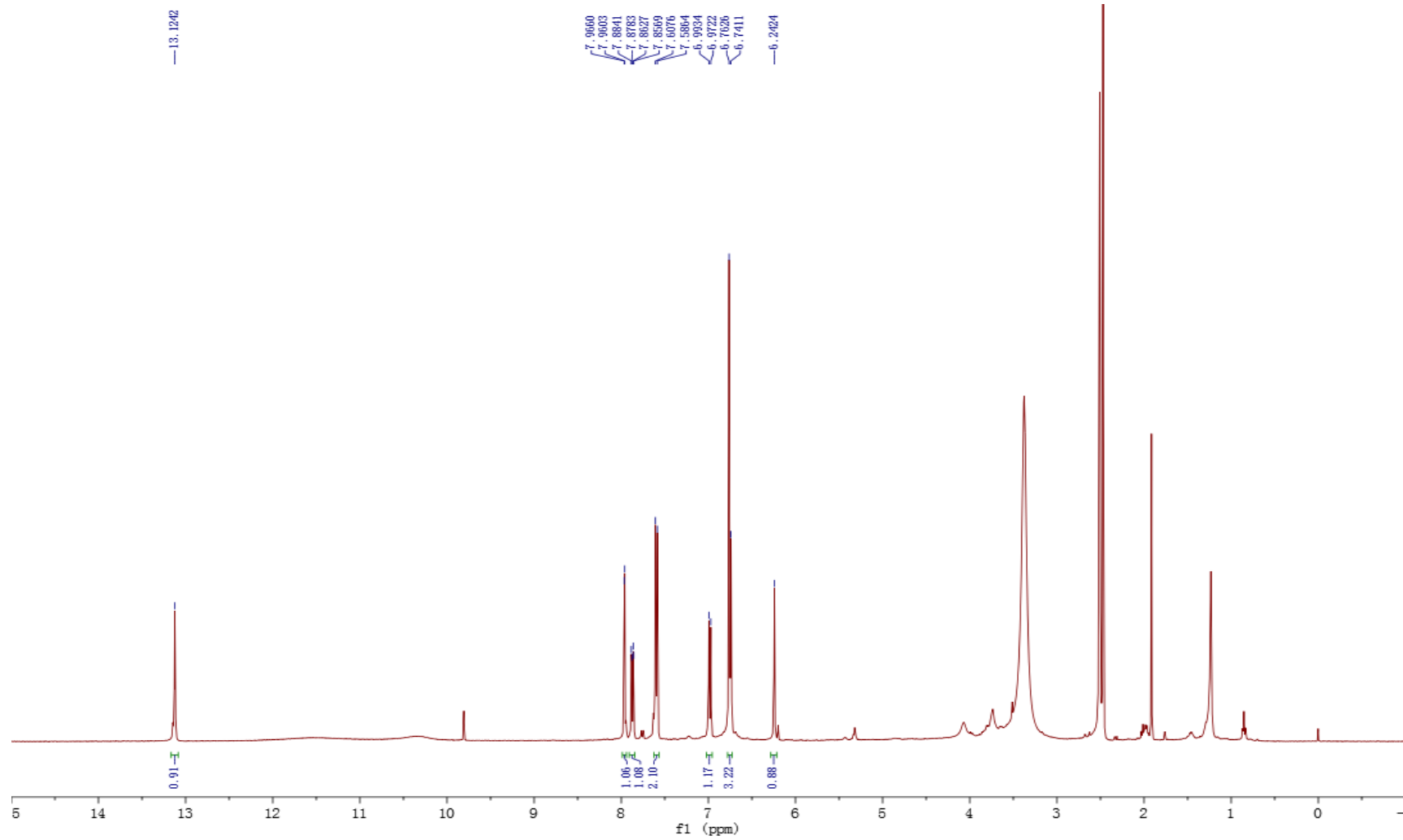


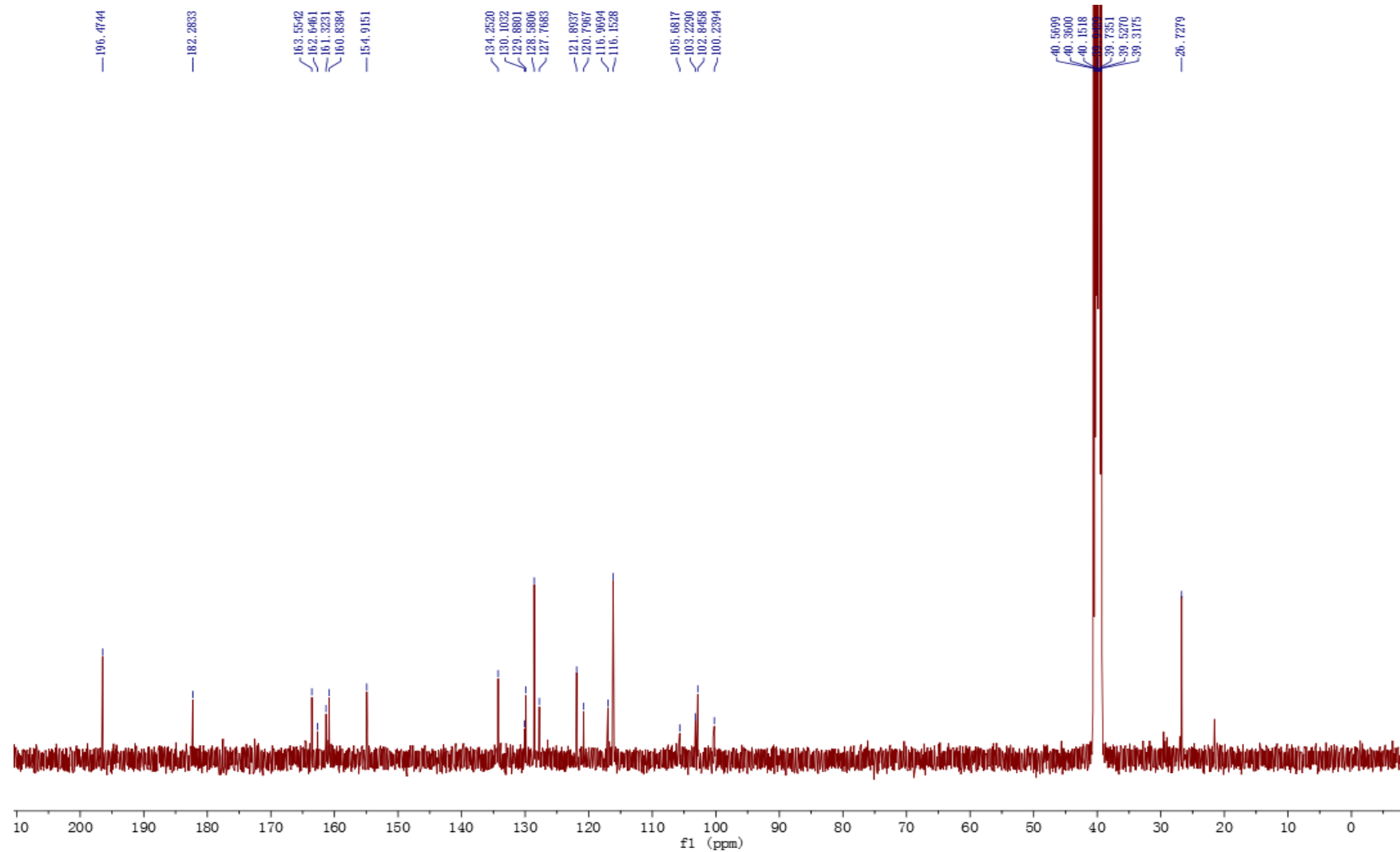
Figure S9:  $^1\text{H}$  NMR spectrum of **2** in  $\text{CD}_3\text{OD}$  (400 MHz)



**Figure S10:**  $^{13}\text{C}$  NMR spectrum of **2**  $\text{CD}_3\text{OD}$  (100 MHz)



**Figure S11:**  $^1\text{H}$  NMR spectrum of **3** in  $\text{DMSO-}d_6$  (400 MHz)



**Figure S12:**  $^{13}\text{C}$  NMR spectrum of **3**  $\text{DMSO-}d_6$  (100 MHz)