

## Supporting Information

### **New Bioactive Polyketide Metabolites from the Mangrove-Derived Fungus *Penicillium* sp. SCSIO 41411**

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## The physicochemical data of the known compounds 2, 6–13.

**Embeurekol C (2):** Brown oil;  $^1\text{H}$  NMR (500 MHz, DMSO- $d_6$ )  $\delta_{\text{H}}$  6.41 (1H, s, H-6), 5.45 (1H, d,  $J = 2.0$  Hz, H-3), 4.25 (1H, m, H-1'), 3.67 (3H, s, H-10), 0.72 (3H, d,  $J = 6.4$  Hz, H-2');  $^{13}\text{C}$  NMR (125 MHz, DMSO- $d_6$ )  $\delta_{\text{C}}$  168.8 (C, C-1), 157.6 (C, C-5), 154.2 (C, C-7), 140.8 (C, C-9), 134.8 (C, C-4), 104.9 (CH, C-6), 103.2 (C, C-8), 82.5 (CH, C-3), 66.7 (CH, C-1'), 60.4 (4-OCH<sub>3</sub>, C-10), 15.4 (CH<sub>3</sub>, C-2').

**Protocatechuic acid (6):** Brown oil;  $^1\text{H}$  NMR (500 MHz, DMSO- $d_6$ )  $\delta_{\text{H}}$  8.57 (1H, s), 6.56 (1H, d,  $J = 8.5$  Hz, H-2), 6.51 (1H, d,  $J = 2.9$  Hz, H-5), 6.44 (1H, dd,  $J = 8.5, 2.9$  Hz, H-6);  $^{13}\text{C}$  NMR (125 MHz, DMSO- $d_6$ )  $\delta_{\text{C}}$  173.1 (C, C-7), 149.4 (C, C-4), 148.0 (C, C-3), 122.6 (C, C-1), 117.4 (CH, C-6), 115.5 (CH, C-5), 113.9 (CH, C-2).

**5-[(3Z,5E)-3,5-nonadienyl]-1,3-benzenediol (7):** Brown oil;  $^1\text{H}$  NMR (500 MHz, DMSO- $d_6$ )  $\delta_{\text{H}}$  6.03 (2H, d,  $J = 2.1$  Hz, H-4, 6), 6.02 (1H, d,  $J = 2.1$  Hz, H-2), 5.97 (2H, m, H-10, 11), 5.56 (2H, m, H-9, 12), 2.44 (2H, m, H-7), 2.25 (2H, m, H-8, 13), 1.99 (2H, m, H-8, 13), 1.35 (2H, m, H-14), 0.84 (3H, t,  $J = 7.4$  Hz, H-15);  $^{13}\text{C}$  NMR (125 MHz, DMSO- $d_6$ )  $\delta_{\text{C}}$  158.2 (2C, C-1, 3), 143.5 (C, C-5), 132.1 (CH, C-12), 131.4 (CH, C-10), 130.6 (CH, C-9), 130.5 (CH, C-11), 106.3 (2CH, C-4, 6), 100.2 (CH, C-2), 35.3 (CH<sub>2</sub>, C-7), 34.1 (CH<sub>2</sub>, C-13), 33.7 (CH<sub>2</sub>, C-8), 22.1 (CH<sub>2</sub>, C-14), 13.6 (CH<sub>3</sub>, C-15).

**2,4-Dihydroxy-6-(3E,5E)-3,5-nonadien-1-ylbenzoic acid (8):** Red brown solid;  $^1\text{H}$  NMR (500 MHz, DMSO- $d_6$ )  $\delta_{\text{H}}$  6.11 (1H, d,  $J = 2.4$  Hz, H-2), 6.09 (1H, d,  $J = 2.4$  Hz, H-4), 5.98 (2H, m, H-11, 12), 5.56 (2H, m, H-10, 13), 2.86 (2H, t,  $J = 7.8$  Hz, H-8), 2.24 (2H, q,  $J = 7.4$  Hz, H-9), 2.00 (2H, q,  $J = 7.1$  Hz, H-14), 1.34 (2H, m, H-15), 0.85 (3H, t,  $J = 7.3$  Hz, H-16);  $^{13}\text{C}$  NMR (125 MHz, DMSO- $d_6$ )  $\delta_{\text{C}}$  172.7 (C, C-7), 164.3 (C, C-1), 161.1 (C, C-3), 158.2 (C, C-6), 146.3 (C, C-5), 132.0 (CH, C-13), 131.8 (CH, C-10), 130.5 (CH, C-11), 130.4 (CH, C-12), 109.6 (CH, C-2), 100.7 (CH, C-4), 35.3 (CH<sub>2</sub>, C-8), 34.3 (CH<sub>2</sub>, C-9), 34.1 (CH<sub>2</sub>, C-14), 22.1 (CH<sub>2</sub>, C-15), 13.6 (CH<sub>3</sub>, C-16).

**3,5-Dimethoxy-4-(1-methylethyl)[1,1'-biphenyl]-2,4'-diol (9):** Brown oil;  $^1\text{H}$  NMR (500 MHz, DMSO- $d_6$ )  $\delta_{\text{H}}$  7.37 (2H, m, H-8, 12), 6.78 (2H, m, H-9, 11), 6.56 (1H, s, H-6), 3.72 (3H, s, 5-OCH<sub>3</sub>), 3.65 (3H, s, 3-OCH<sub>3</sub>), 3.35 (1H, m, H-17), 1.28 (3H, s, H-18/19), 1.27 (3H, s, H-18/19);  $^{13}\text{C}$  NMR (125 MHz, DMSO- $d_6$ )  $\delta_{\text{C}}$  156.3 (C, C-10), 151.2 (C, C-3), 146.8 (C, C-5), 140.8 (C, C-2), 130.2 (2CH, C-8, 12), 129.2 (C, C-7), 127.4 (C, C-1), 126.5 (C, C-4), 114.8 (2CH, C-9, 11), 108.6 (CH, C-6), 60.9 (CH<sub>3</sub>, 3-OCH<sub>3</sub>), 55.9 (CH<sub>3</sub>, 5-OCH<sub>3</sub>), 25.0 (CH, C-17), 21.3 (2CH<sub>3</sub>, C-18, 19).

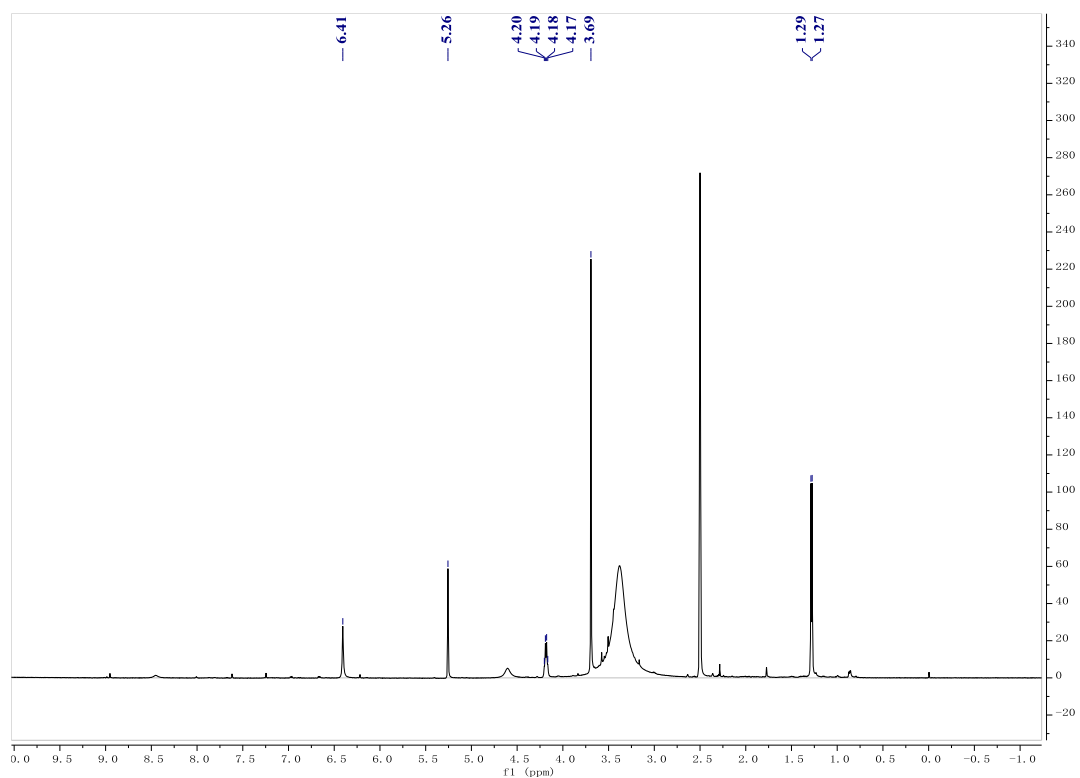
**3-Methyl-6,8-dihydroxyisocoumarin (10):** Orange crystal;  $^1\text{H}$  NMR (700 MHz, DMSO- $d_6$ )  $\delta_{\text{H}}$  6.43 (1H, s, H-4), 6.31 (1H, s, H-5), 6.28 (1H, s, H-7), 2.18 (3H, s, H-9);  $^{13}\text{C}$  NMR (175 MHz, DMSO- $d_6$ )  $\delta_{\text{C}}$  166.3 (C, C-6), 165.7 (C, C-1), 162.9 (C, C-8), 154.4 (C, C-3), 139.9 (C, C-4a), 104.4 (CH, C-4), 102.8 (CH, C-5), 101.7 (CH, C-7), 97.9 (C, C-8a), 19.1 (CH<sub>3</sub>, C-9).

**6,8-dihydroxy-5-methoxy-3-methyl-1H-isochromen-1-one (11):** Orange crystal;  $^1\text{H}$  NMR (500 MHz, DMSO- $d_6$ )  $\delta_{\text{H}}$  10.74 (1H, s), 6.59 (1H, brs, H-7), 6.43 (1H, s, H-4), 3.69 (3H, s, 5-OCH<sub>3</sub>), 2.24 (3H, brs, H-9);  $^{13}\text{C}$  NMR (125 MHz, DMSO- $d_6$ )  $\delta_{\text{C}}$  165.4 (C, C-1), 158.7 (C, C-6), 158.5 (C, C-8), 154.1 (C, C-3), 133.6 (C, C-4a), 131.0 (C, C-5), 102.1 (CH, C-7), 98.7 (C, C-8a), 96.8 (CH,

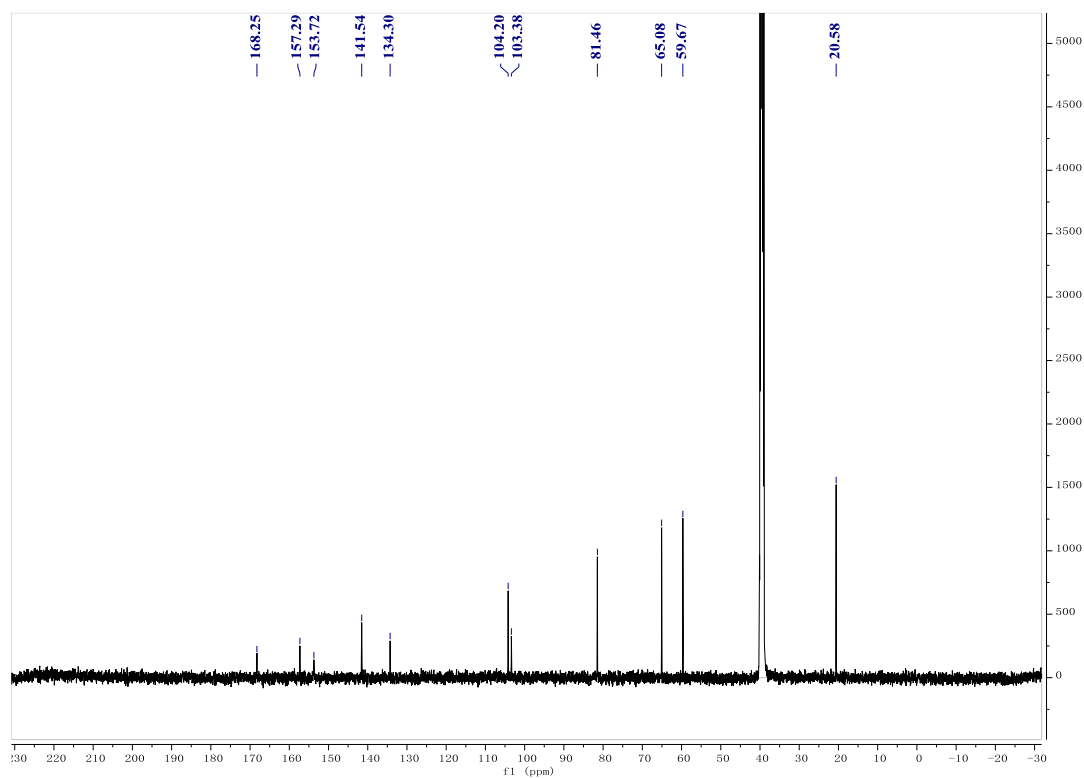
C-4), 60.8 (CH<sub>3</sub>, 5-OCH<sub>3</sub>), 19.1 (CH<sub>3</sub>, C-9).

**Butyrolactone I (12):** Brown oil; <sup>1</sup>H NMR (500 MHz, DMSO-*d*<sub>6</sub>)  $\delta_{\text{H}}$  10.01 (1H, s), 9.21 (1H, s), 7.49 (2H, d,  $J$  = 8.6 Hz, H-2', 6'), 6.87 (2H, d,  $J$  = 8.7 Hz, H-3', 5'), 6.52 (1H, d,  $J$  = 8.2 Hz, H-5''), 6.47 (1H, dd,  $J$  = 8.2, 2.2 Hz, H-6''), 6.36 (1H, d,  $J$  = 2.2 Hz, H-2''), 4.99 (1H, m, H-8''), 3.73 (3H, s, 5-OCH<sub>3</sub>), 3.36 (2H, s, H-6), 2.99 (2H, t,  $J$  = 6.4 Hz, H-7''), 1.61 (3H, s, H-10''/11''), 1.52 (3H, s, H-10''/11''); <sup>13</sup>C NMR (125 MHz, DMSO-*d*<sub>6</sub>)  $\delta_{\text{C}}$  170.0 (C, C-5), 168.1 (C, C-1), 158.0 (C, C-4'), 153.9 (C, C-4''), 138.2 (C, C-2), 131.6 (C, C-9''), 131.0 (CH, C-2''), 128.9 (2CH, C-2', 6'), 128.5 (CH, C-6''), 127.5 (C, C-3''), 126.6 (C, C-3), 123.3 (C, C-1''), 122.4 (CH, C-8''), 121.2 (C, C-1'), 115.9 (2CH, C-3', 5'), 114.2 (CH, C-5''), 84.9 (C, C-4), 53.6 (CH<sub>3</sub>, 5-OCH<sub>3</sub>), 38.2 (CH<sub>2</sub>, C-6), 27.6 (CH<sub>2</sub>, C-7''), 25.6 (CH<sub>3</sub>, C-10''/11''), 17.6 (CH<sub>3</sub>, C-10''/11'').

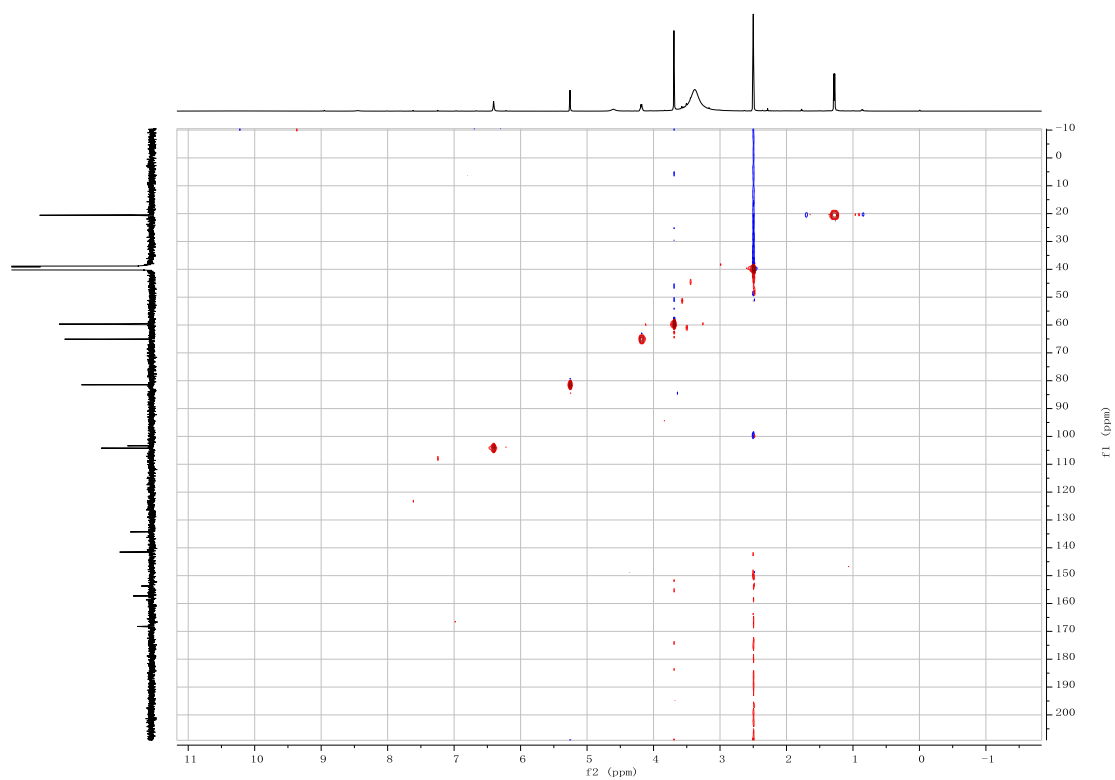
**Polybotrin (13):** Brown oil; <sup>1</sup>H NMR (500 MHz, DMSO-*d*<sub>6</sub>)  $\delta_{\text{H}}$  7.88 (1H, d,  $J$  = 8.1 Hz, H-4'), 5.78 (1H, d,  $J$  = 5.4 Hz, H-2), 5.64 (1H, d,  $J$  = 8.1 Hz, H-5'), 4.02 (1H, t,  $J$  = 5.3 Hz, H-3), 3.96 (1H, t,  $J$  = 4.6 Hz, H-4), 3.84 (1H, q,  $J$  = 3.4 Hz, H-5), 3.62 (1H, dd,  $J$  = 11.9, 3.2 Hz, H-6), 3.54 (1H, dd,  $J$  = 12.0, 3.3 Hz, H-6); <sup>13</sup>C NMR (125 MHz, DMSO-*d*<sub>6</sub>)  $\delta_{\text{C}}$  163.1 (C, C-2'), 150.8 (C, C-3'), 140.7 (CH, C-4'), 101.8 (CH, C-5'), 87.7 (CH, C-2), 84.8 (CH, C-5), 73.5 (CH, C-3), 69.9 (CH, C-4), 60.9 (CH<sub>2</sub>, C-6).



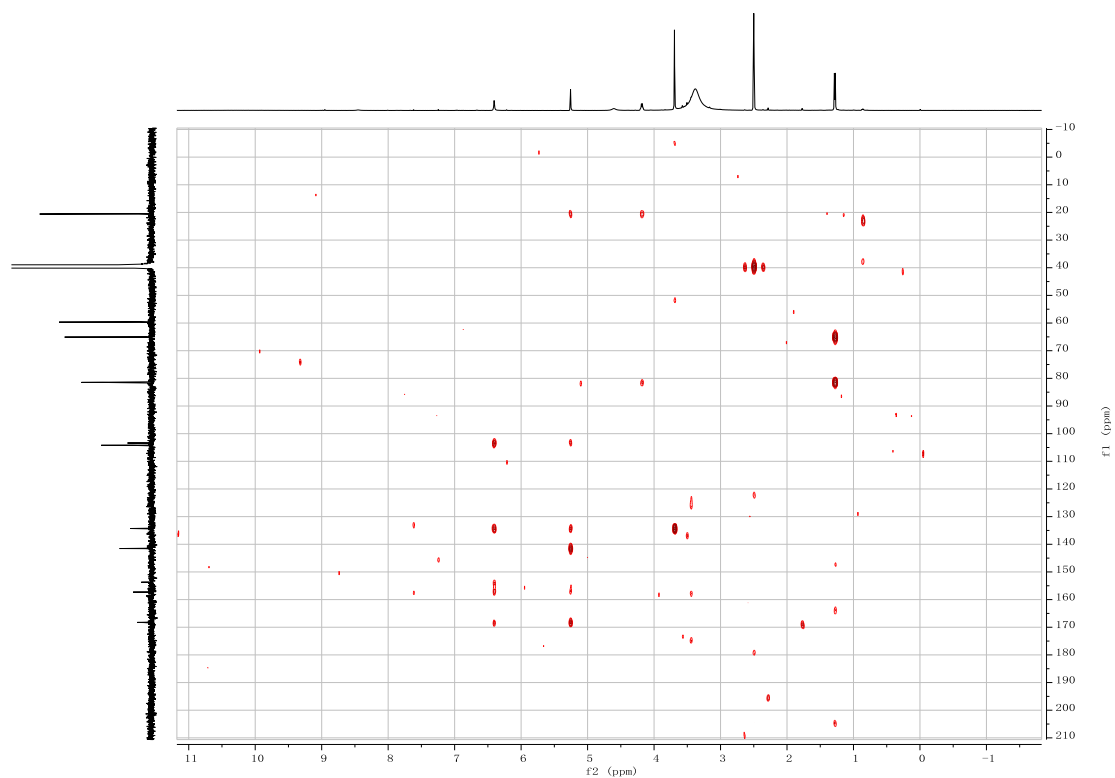
**Figure S1:**  $^1\text{H}$  NMR spectrum of **1** in  $\text{DMSO}-d_6$ .



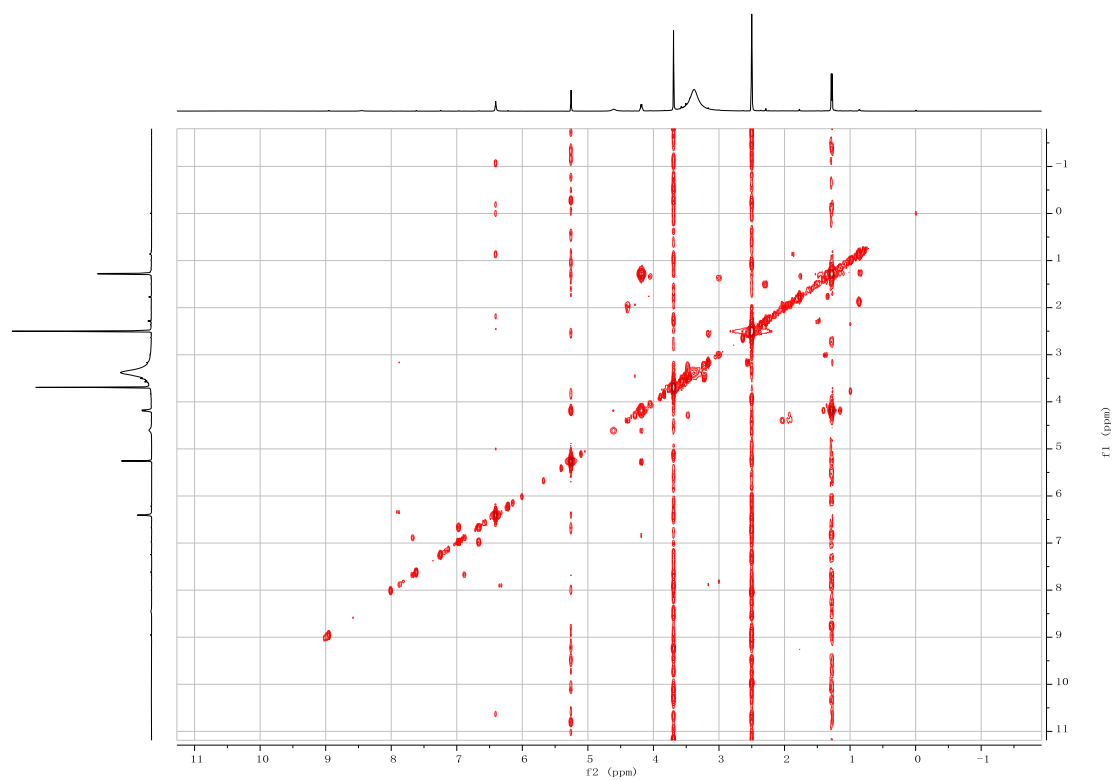
**Figure S2:**  $^{13}\text{C}$  NMR spectrum of **1** in  $\text{DMSO}-d_6$ .



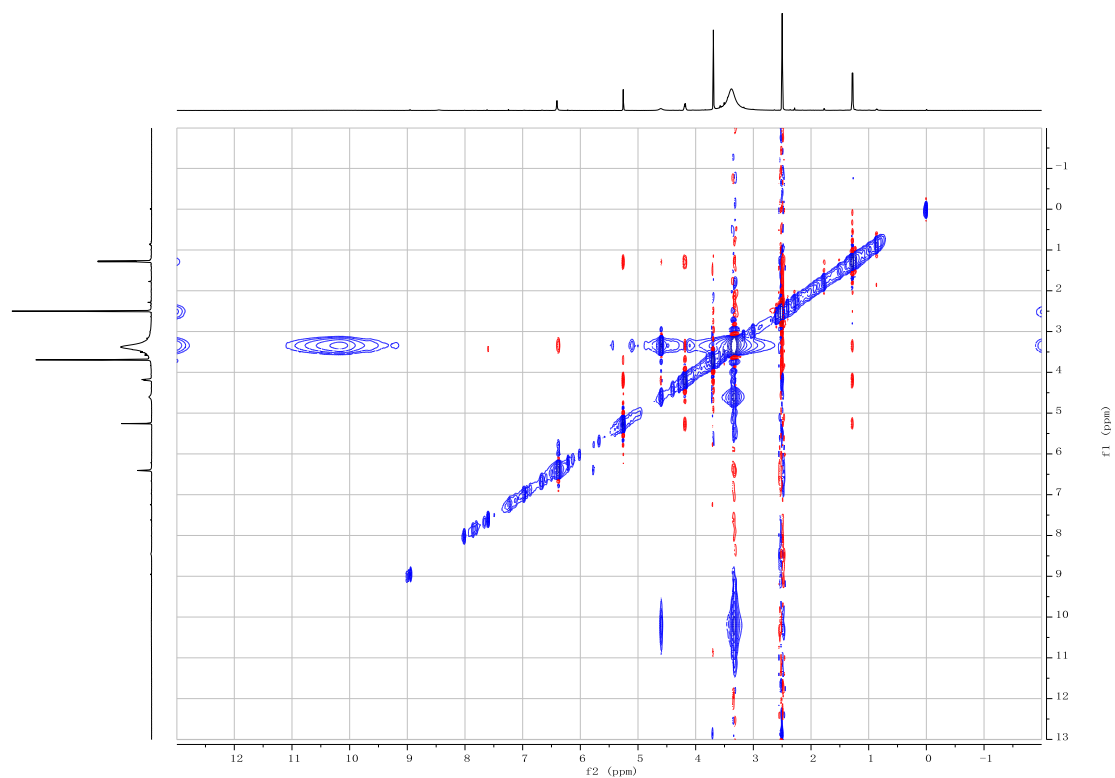
**Figure S3:** HSQC spectrum of **1** in DMSO- $d_6$ .



**Figure S4:** HMBC spectrum of **1** in DMSO- $d_6$ .



**Figure S5:** COSY spectrum of **1** in DMSO- $d_6$ .

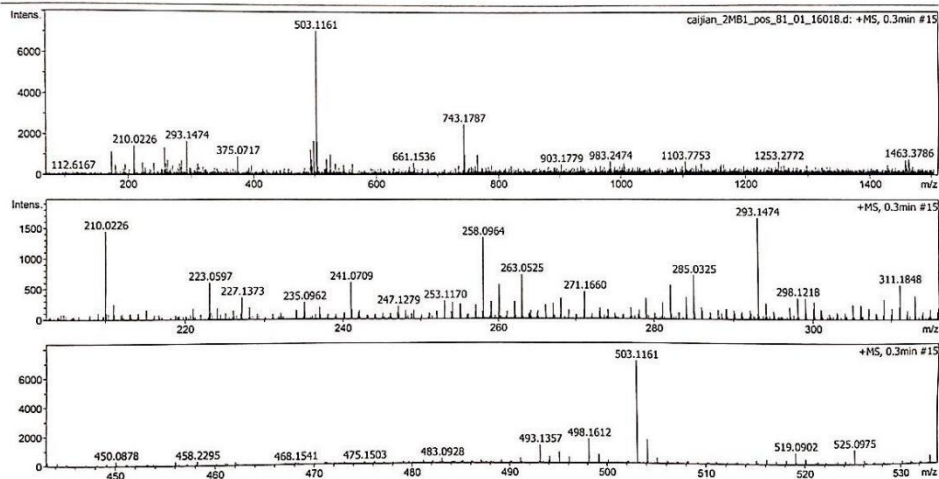


**Figure S6:** NOESY spectrum of **1** in DMSO- $d_6$ .



## Generic Display Report

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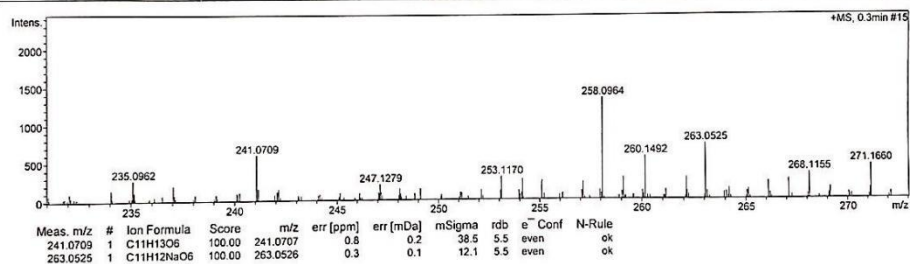


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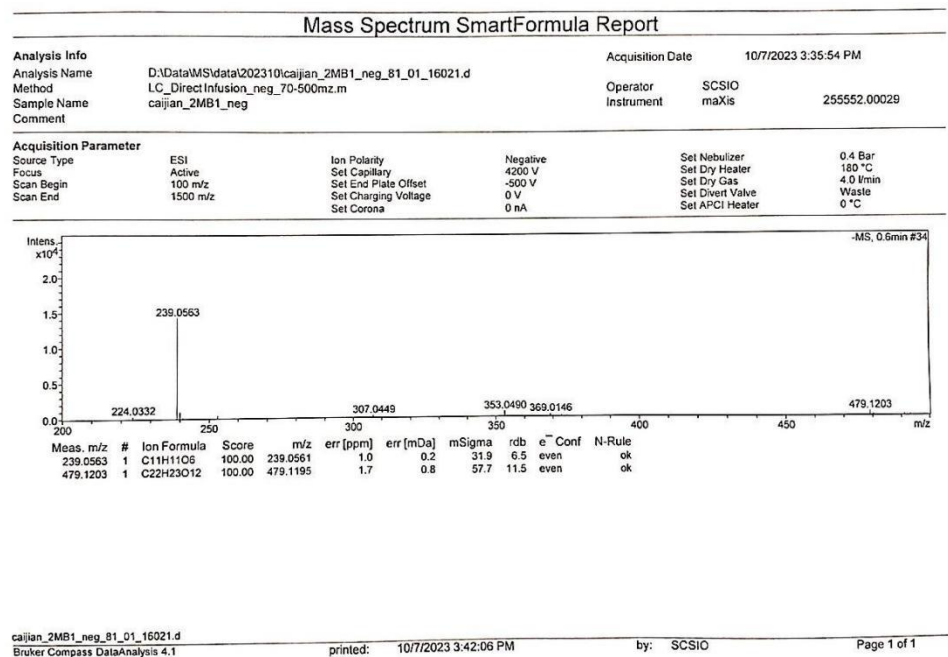
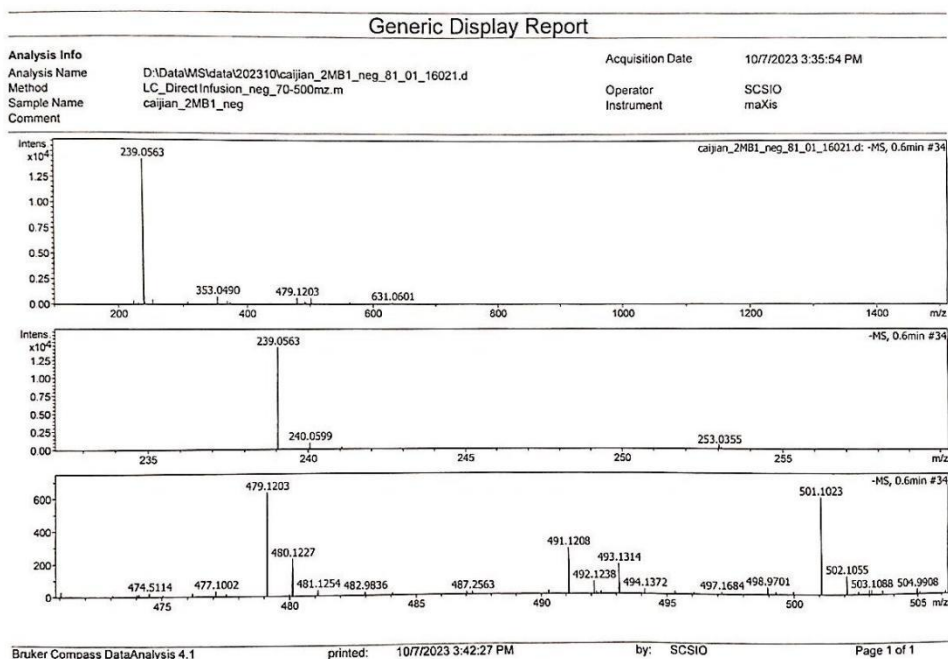
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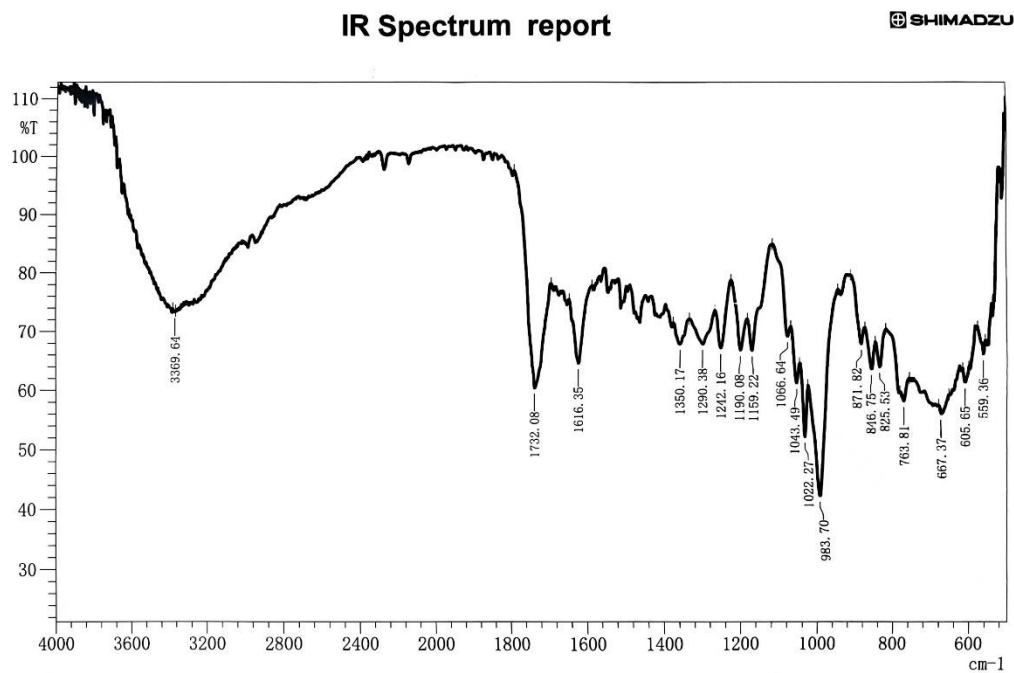
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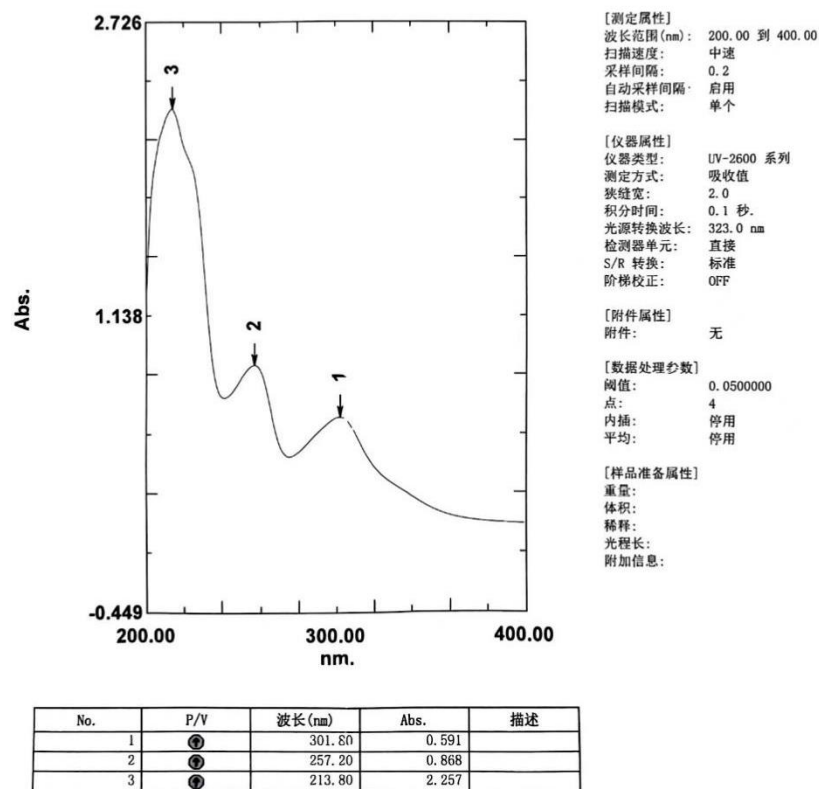
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 Bruker Compass DataAnalysis 4.1



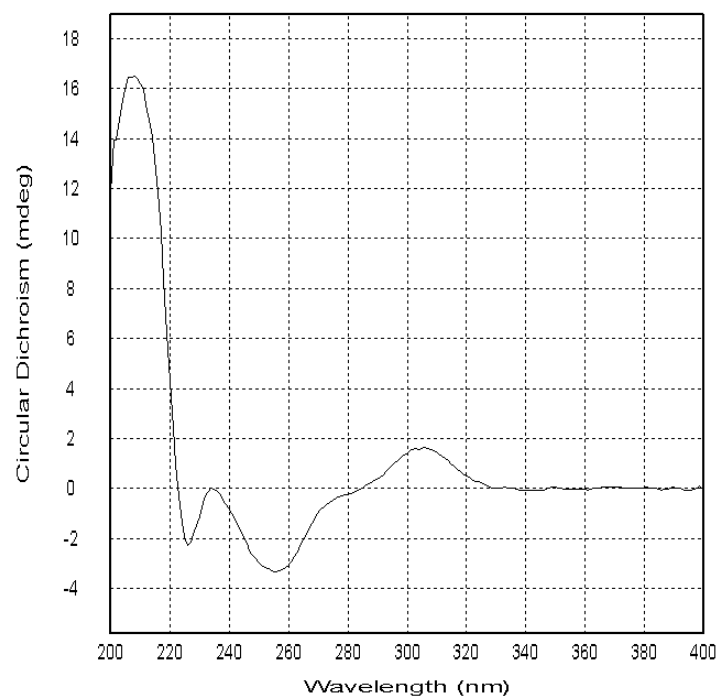
**Figure S7: HRESIMS spectrum of 1.**



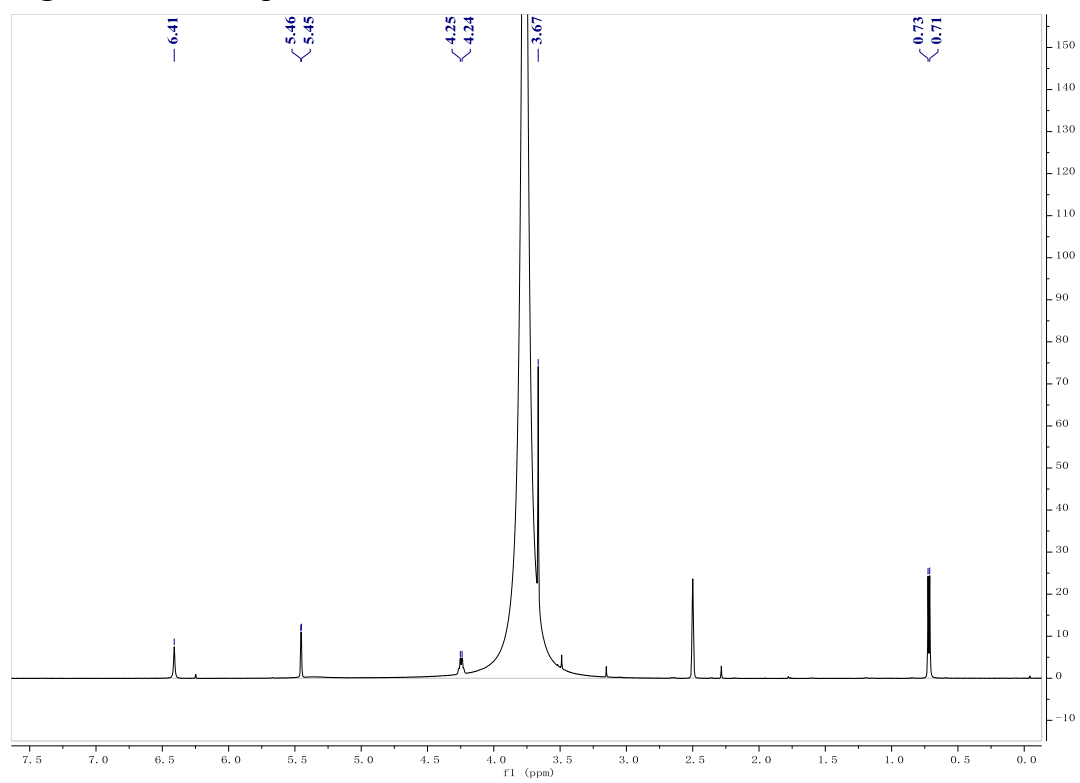
**Figure S8:** IR spectrum of **1**.



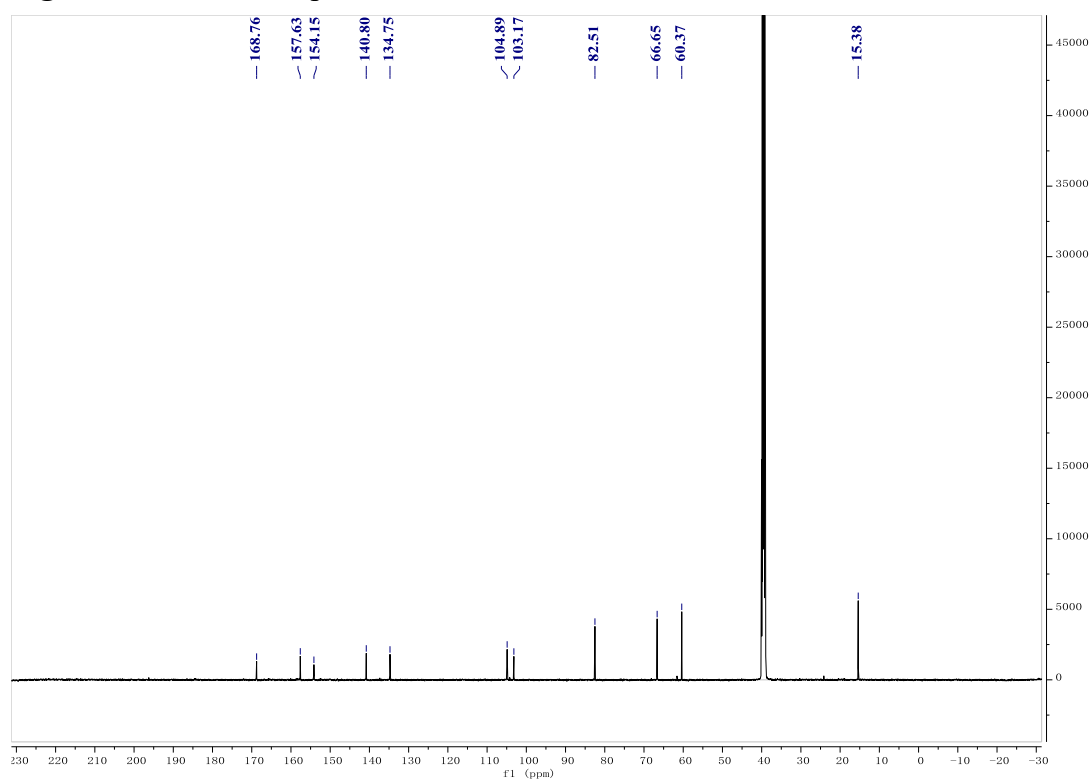
**Figure S9:** UV spectrum of **1** in MeOH.



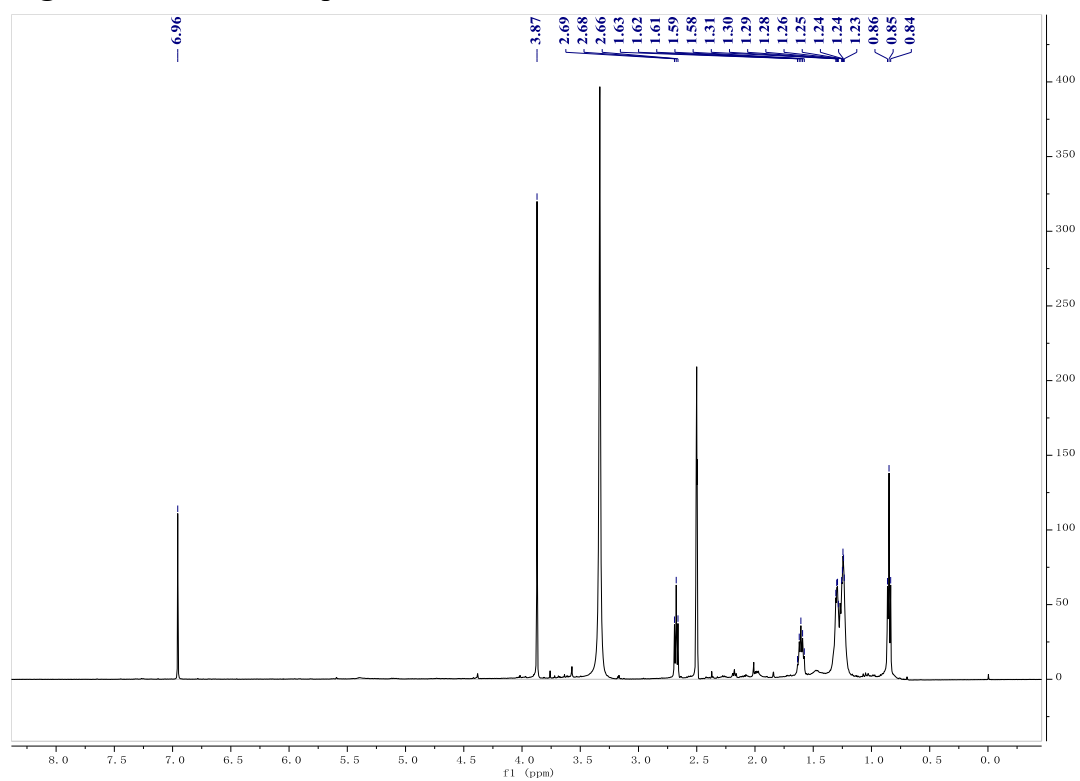
**Figure S10:** ECD spectrum of **1** in MeOH.



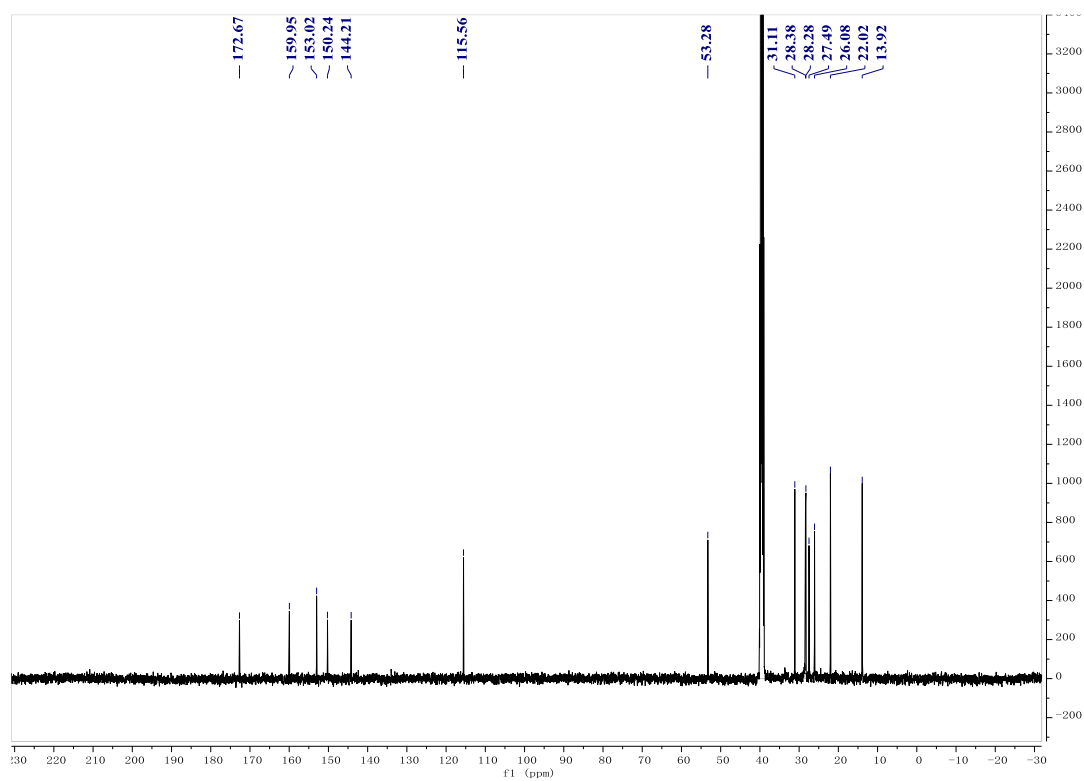
**Figure S11:**  $^1\text{H}$  NMR spectrum of **2** in  $\text{DMSO}-d_6$ .



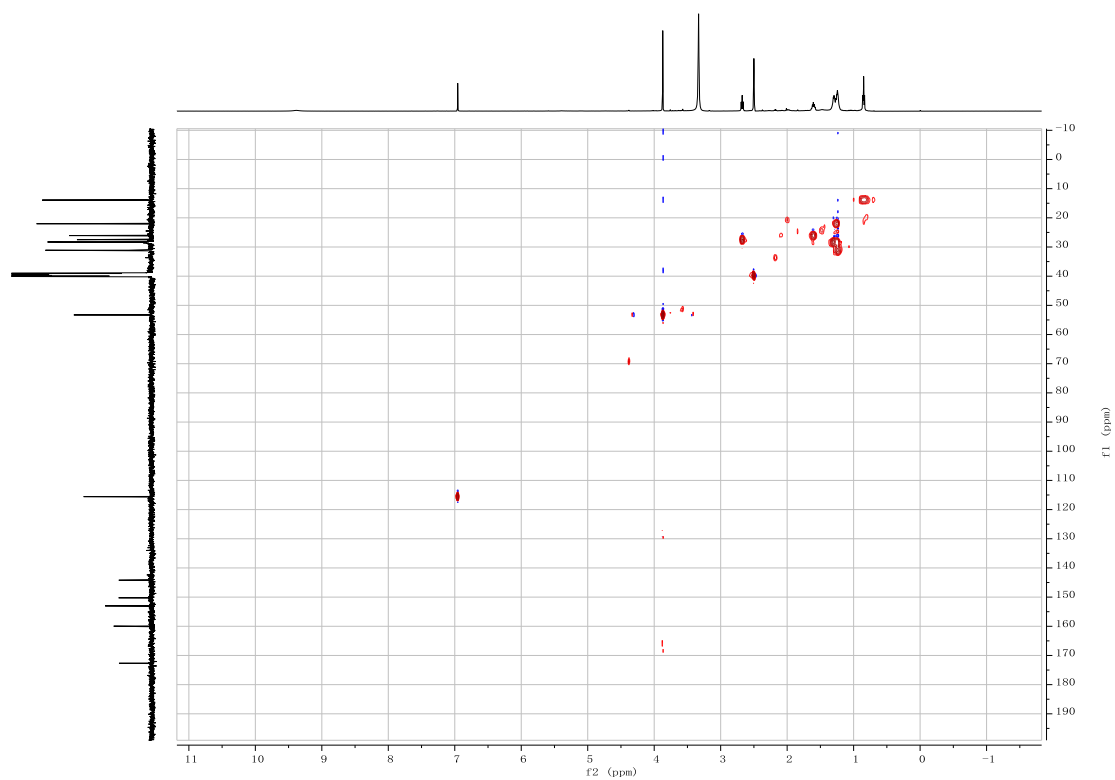
**Figure S12:**  $^{13}\text{C}$  NMR spectrum of **2** in  $\text{DMSO}-d_6$ .



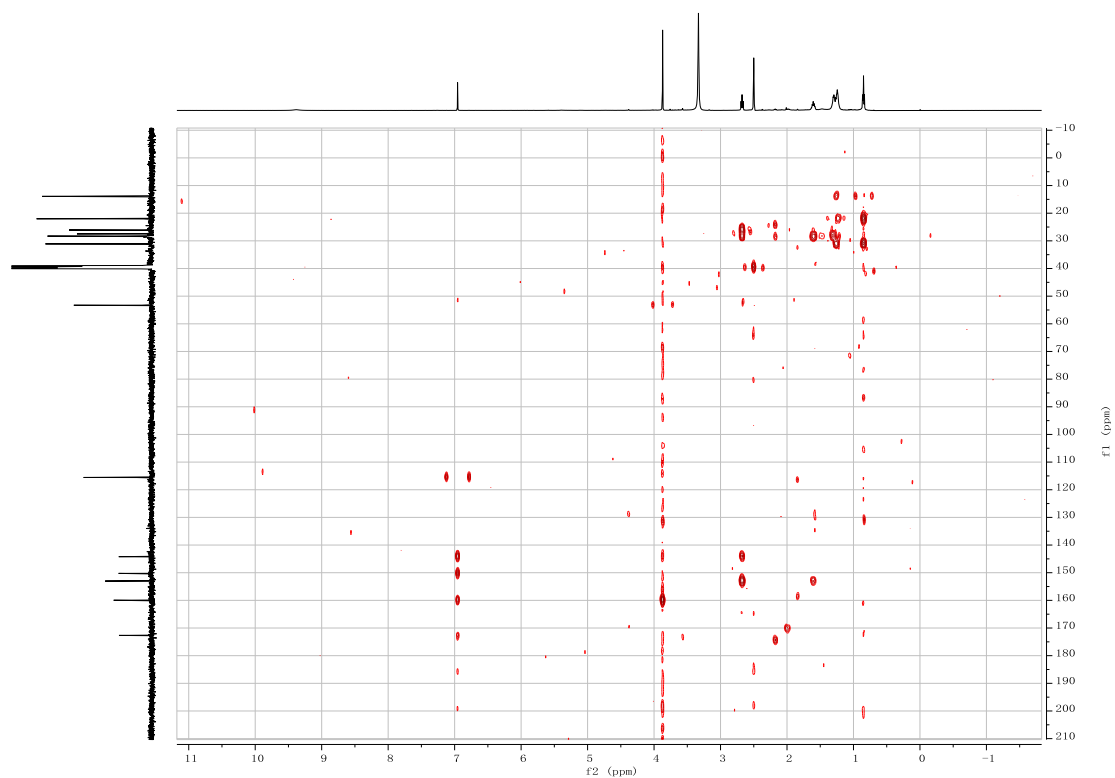
**Figure S13:**  $^1\text{H}$  NMR spectrum of **3** in  $\text{DMSO}-d_6$ .



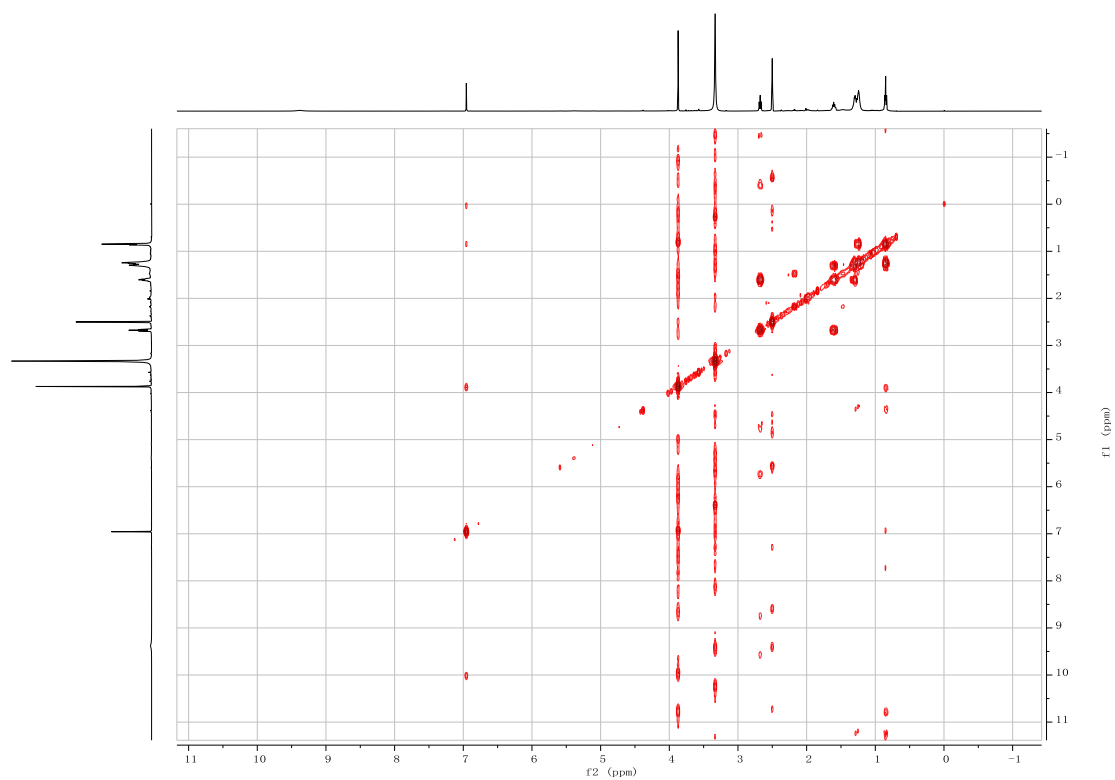
**Figure S14:**  $^{13}\text{C}$  NMR spectrum of **3** in  $\text{DMSO}-d_6$ .



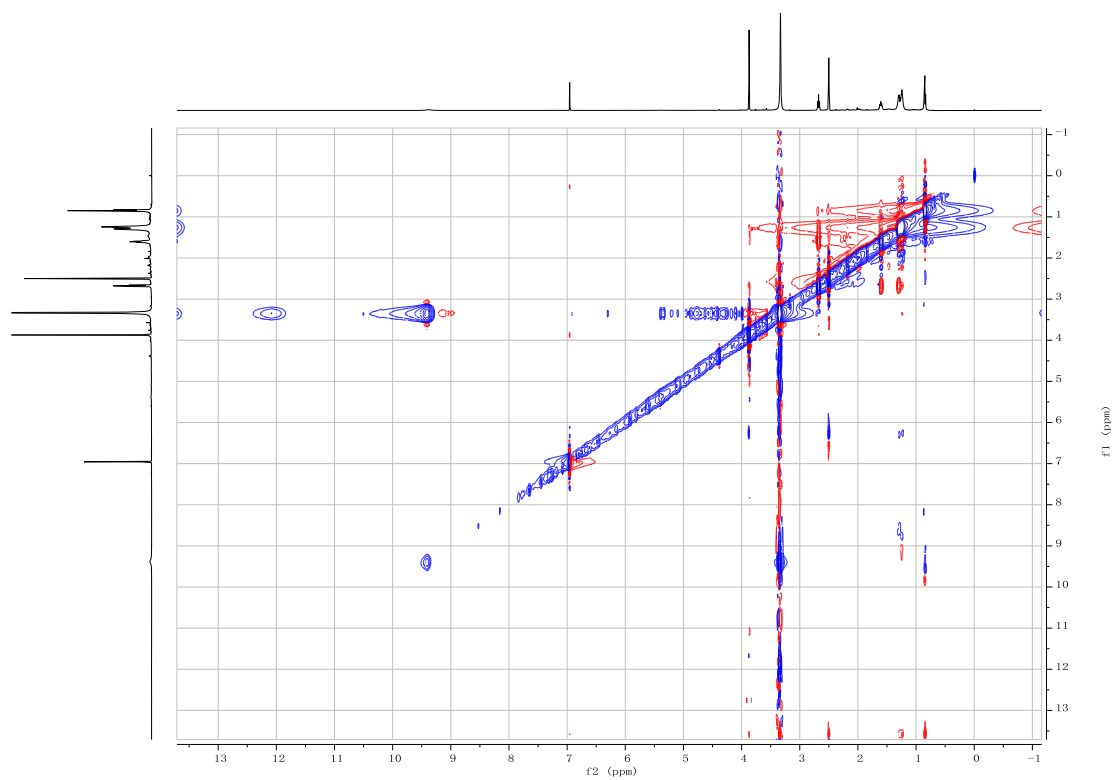
**Figure S15:** HSQC spectrum of **3** in DMSO- $d_6$ .



**Figure S16:** HMBC spectrum of **3** in DMSO- $d_6$ .

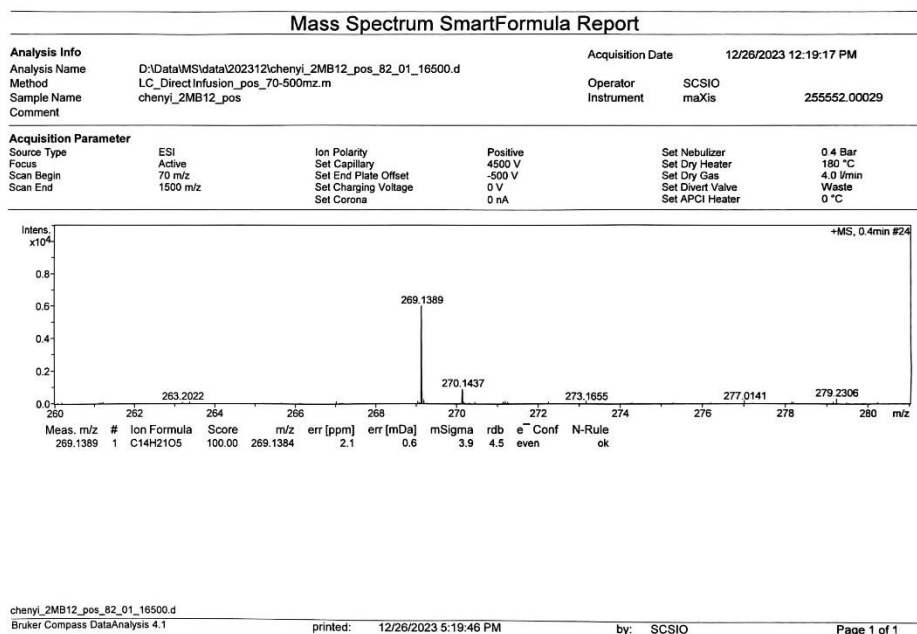


**Figure S17:** COSY spectrum of **3** in DMSO- $d_6$ .

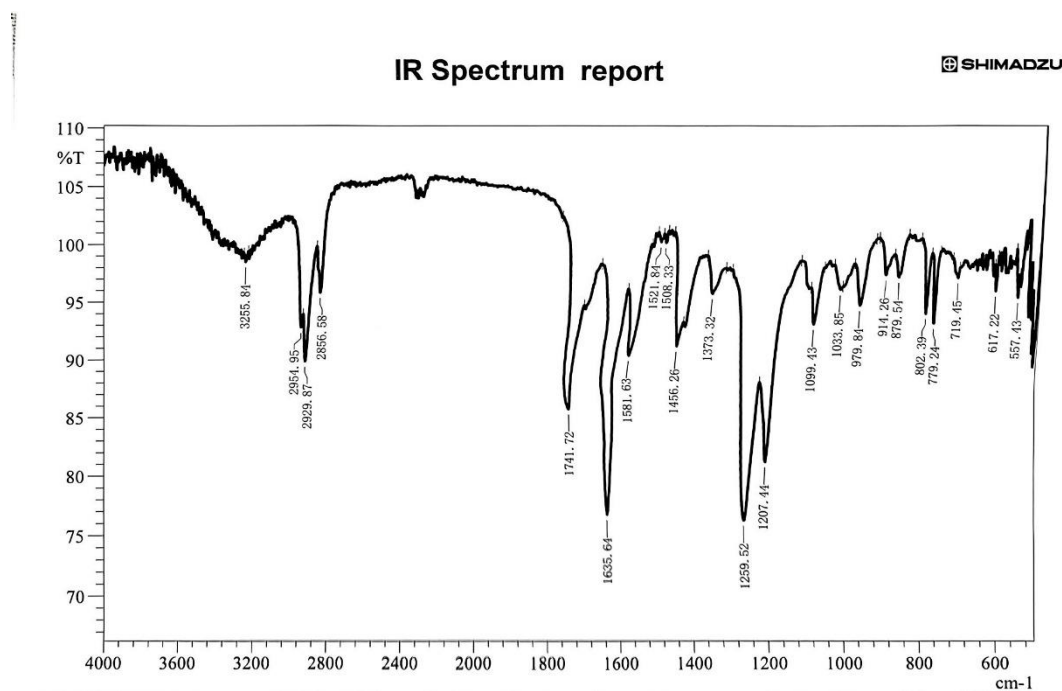


**Figure S18:** NOESY spectrum of **3** in DMSO- $d_6$ .

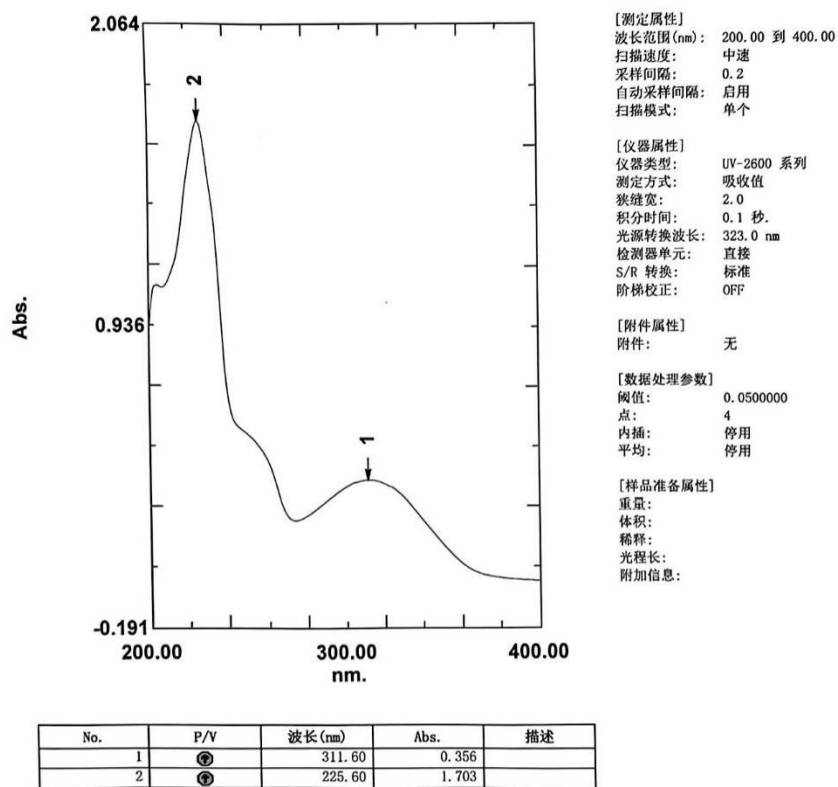




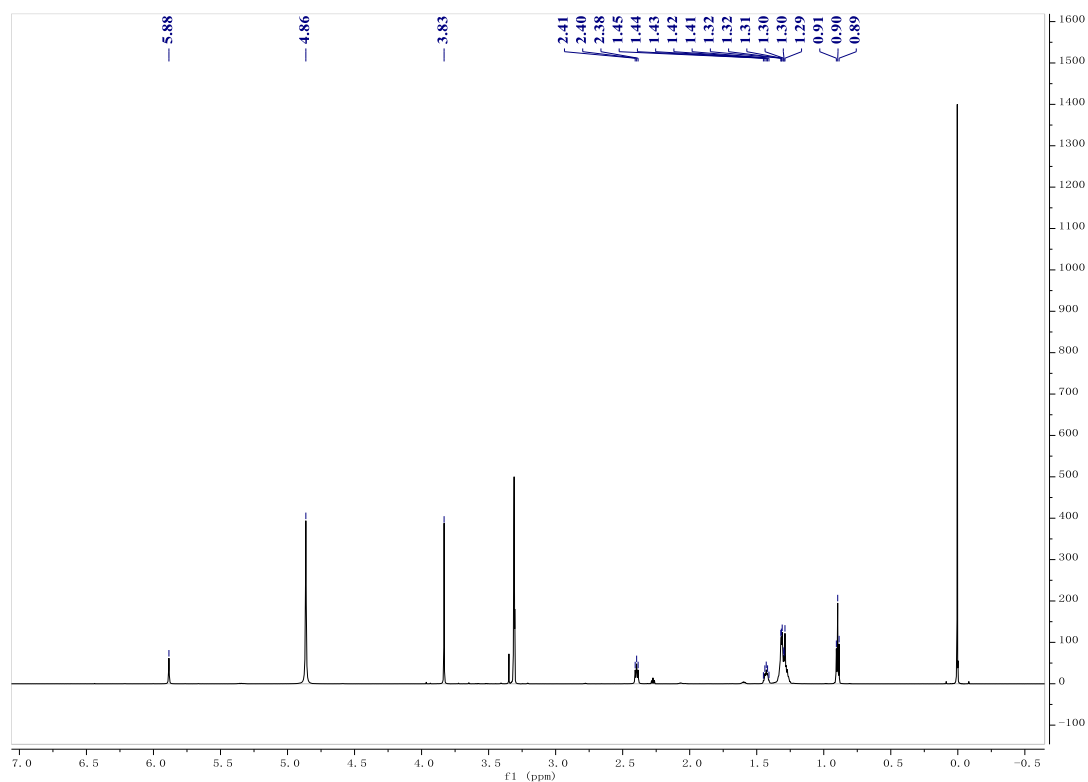
**Figure S19:** HRESIMS spectrum of **3**.



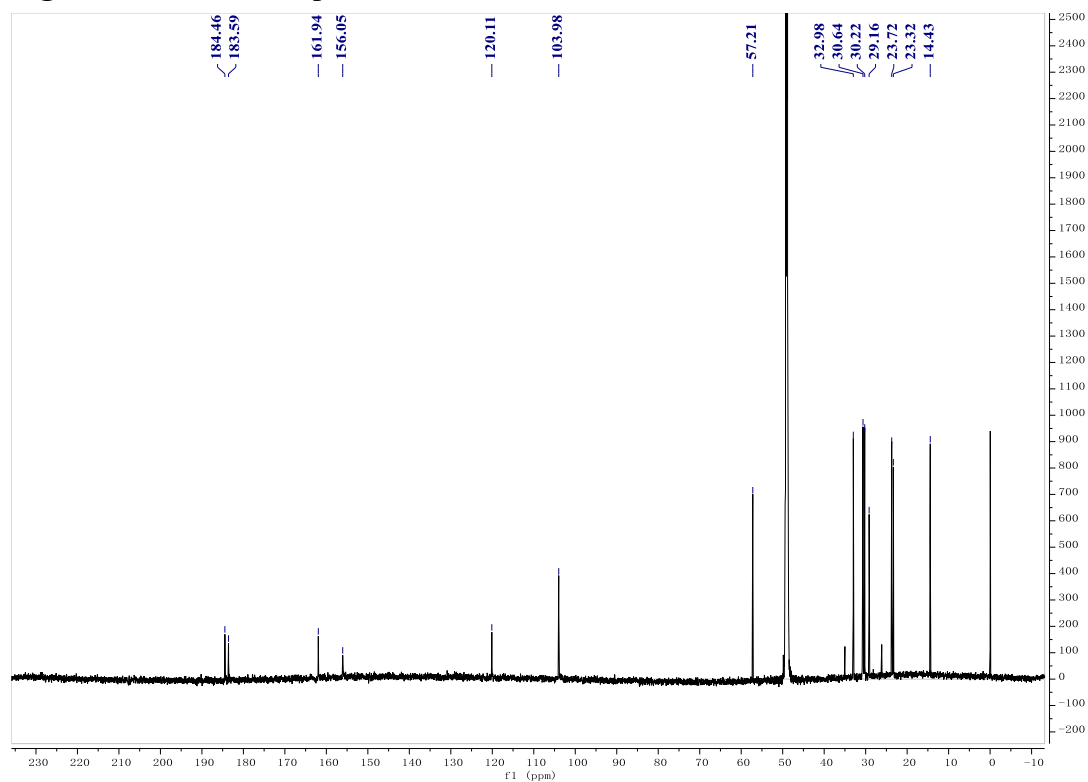
**Figure S20: IR spectrum of 3.**



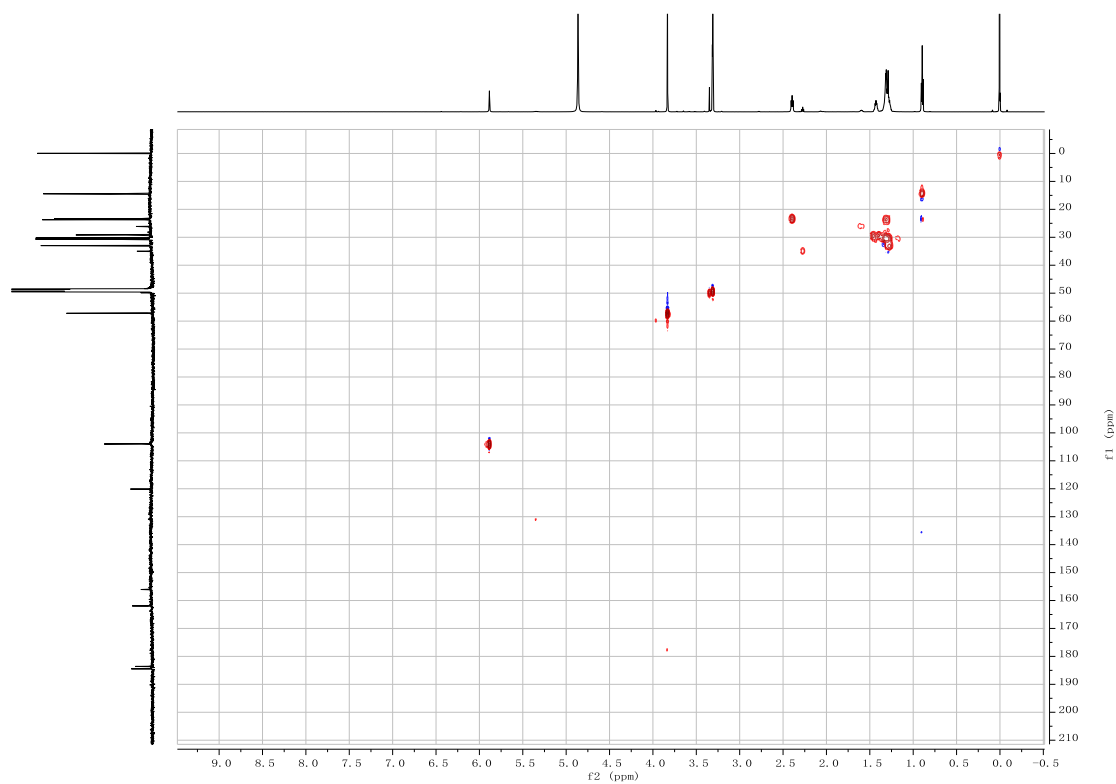
**Figure S21: UV spectrum of 3 in MeOH.**



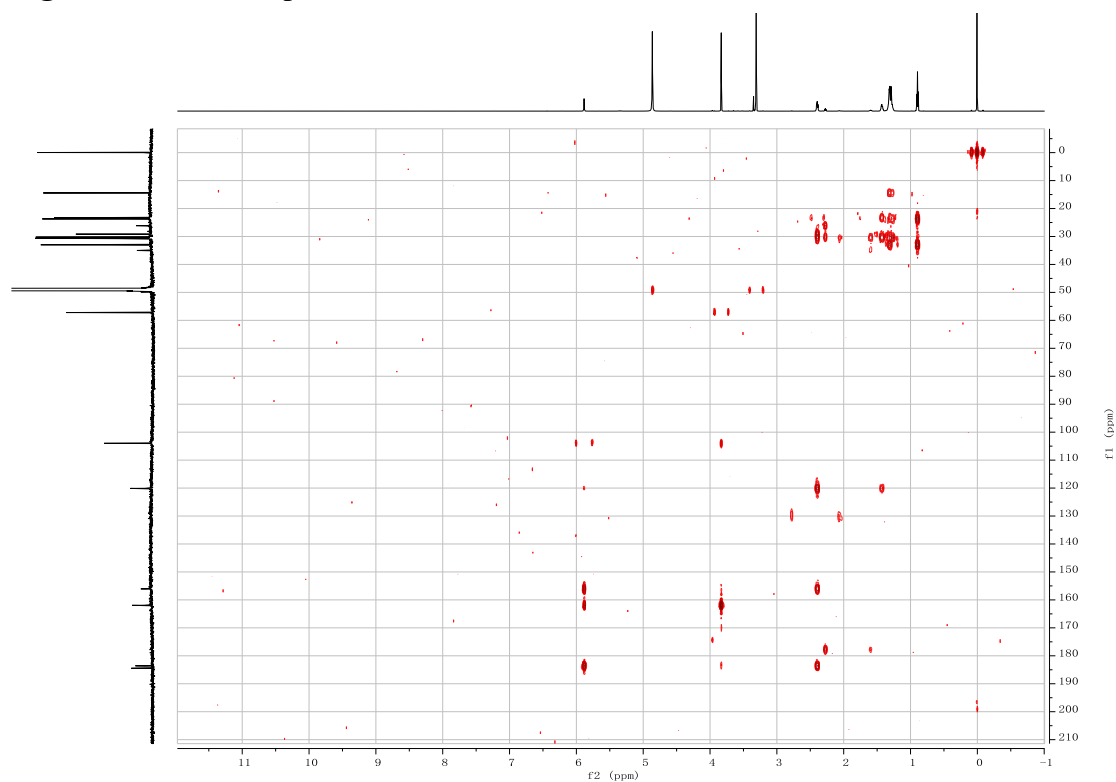
**Figure S22:**  $^1\text{H}$  NMR spectrum of **4** in Methanol- $d_4$ .



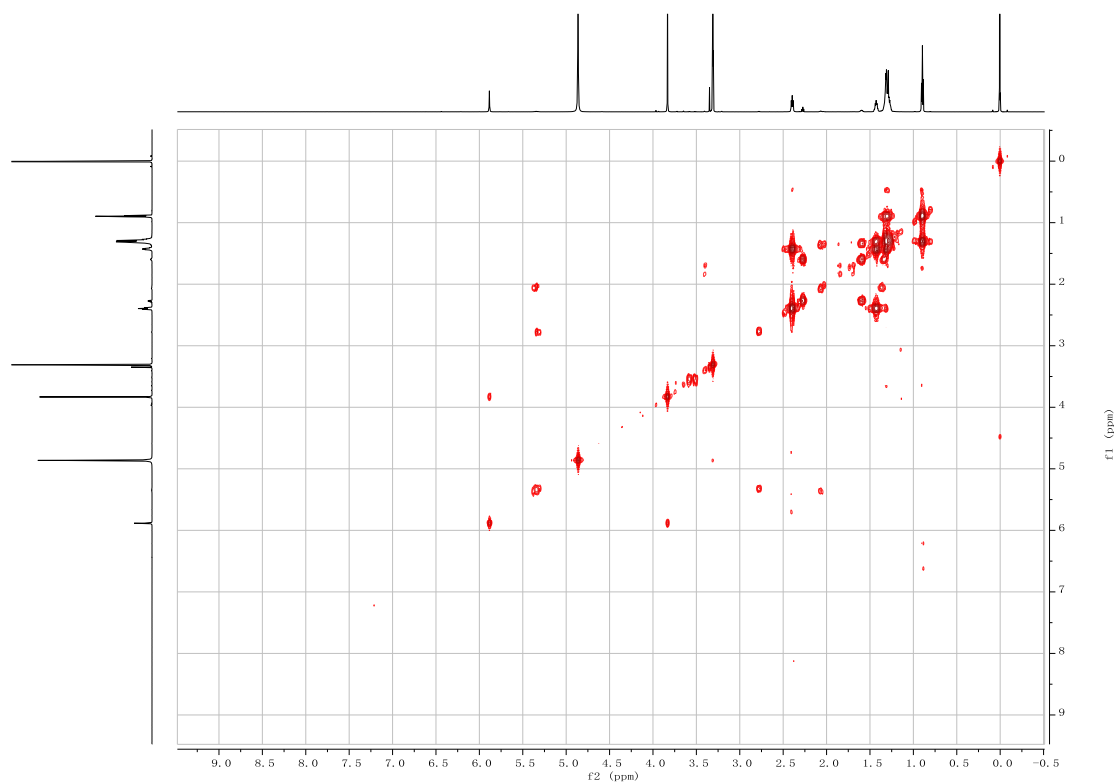
**Figure S23:**  $^{13}\text{C}$  NMR spectrum of **4** in Methanol- $d_4$ .



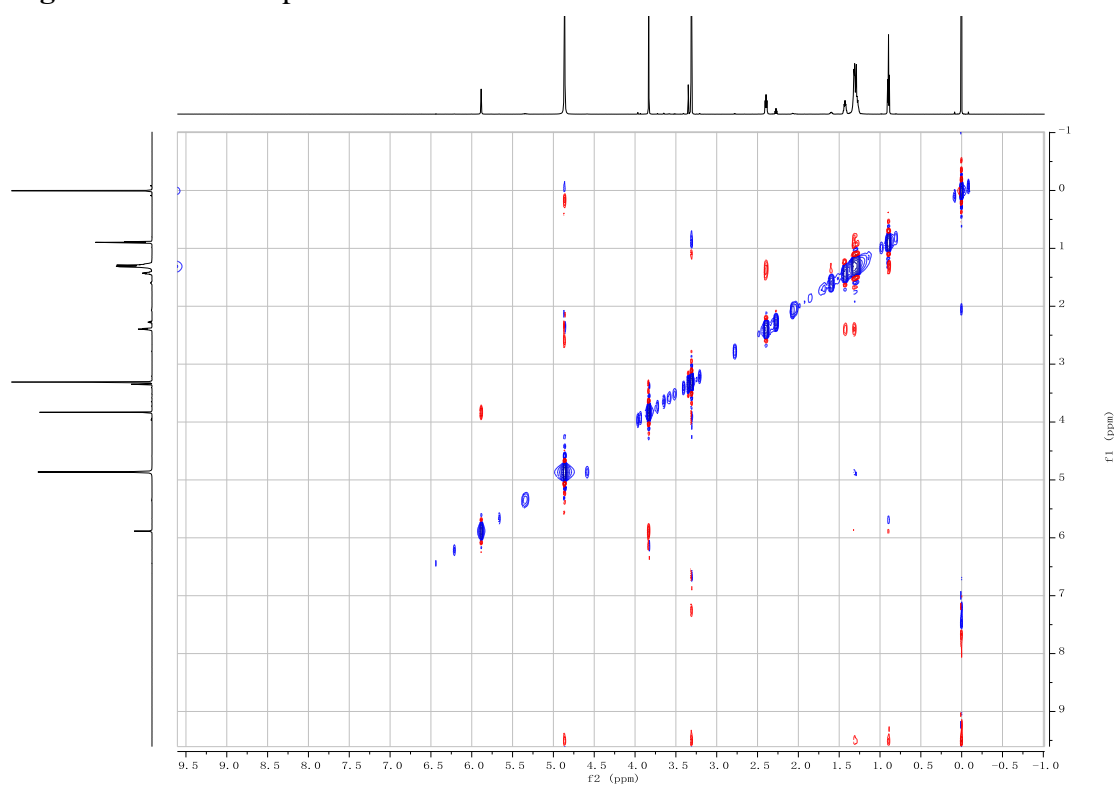
**Figure S24:** HSQC spectrum of **4** in Methanol-*d*<sub>4</sub>.



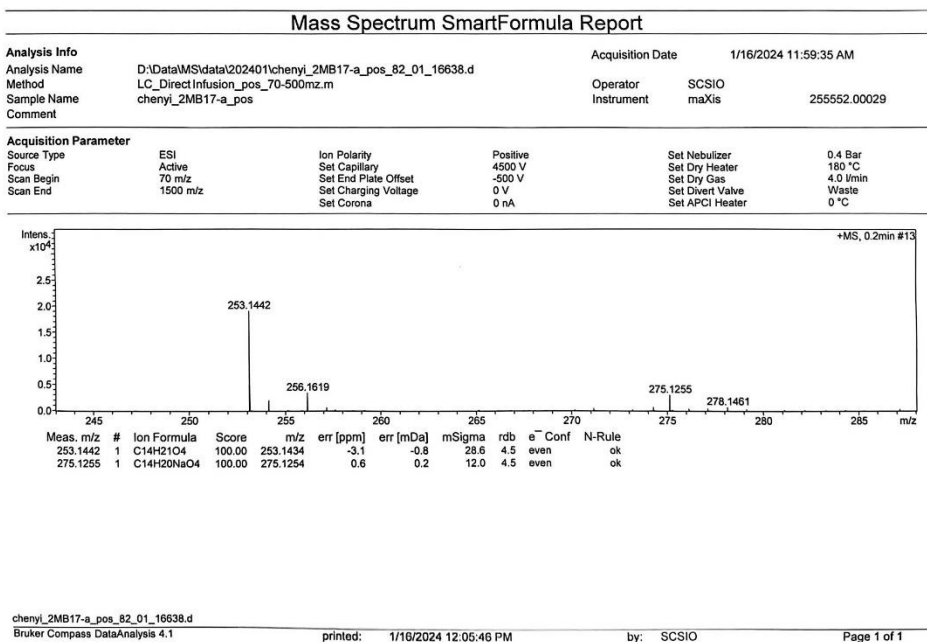
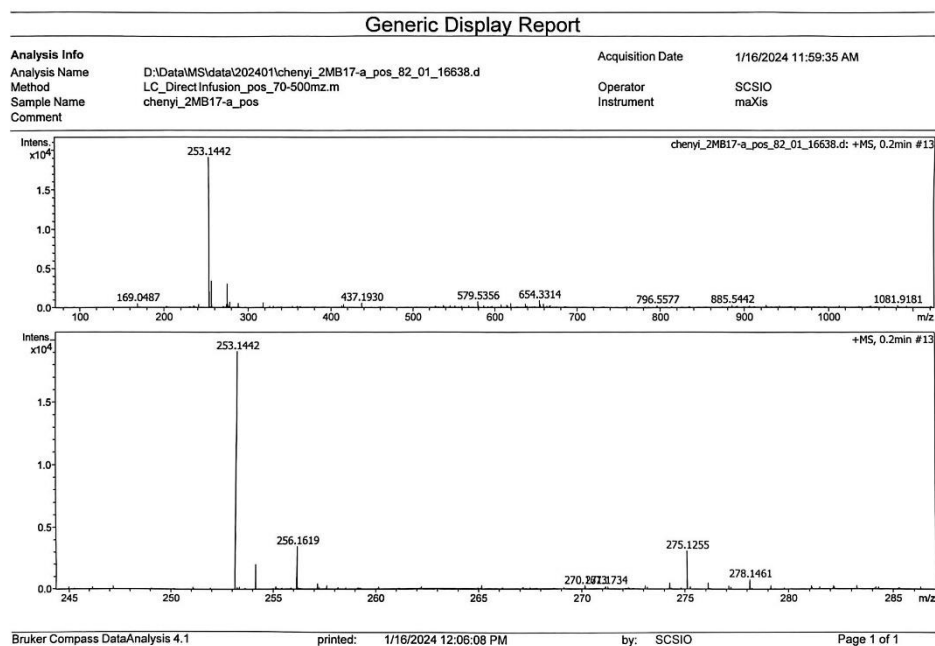
**Figure S25:** HMBC spectrum of **4** in Methanol-*d*<sub>4</sub>.



**Figure S26:** COSY spectrum of **4** in Methanol- $d_4$ .



**Figure S27:** NOESY spectrum of **4** in Methanol- $d_4$ .



**Figure S28:** HRESIMS spectrum of 4.

# IR Spectrum report

SHIMADZU

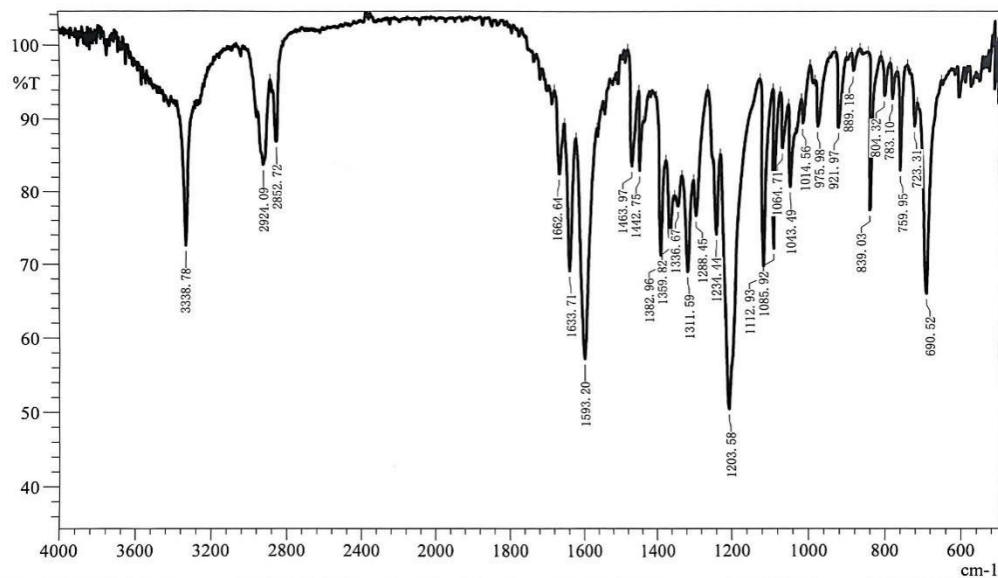
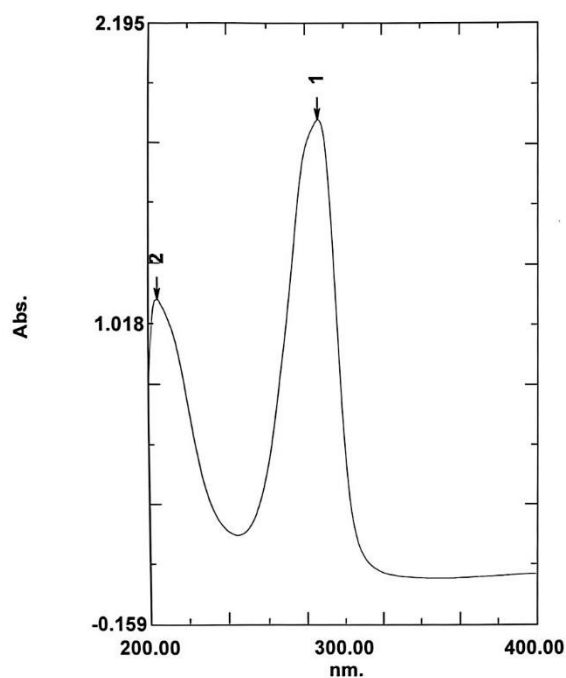


Figure S29: IR spectrum of 4.



[测定属性]  
 波长范围 (nm): 200.00 到 400.00  
 扫描速度: 中速  
 采样间隔: 0.2  
 自动采样间隔: 启用  
 扫描模式: 单个

[仪器属性]  
 仪器类型: UV-2600 系列  
 测定方式: 吸收值  
 狭缝宽: 2.0  
 积分时间: 0.1 秒  
 光源转换波长: 323.0 nm  
 检测器单元: 直接  
 S/R 转换: 标准  
 阶梯校正: OFF

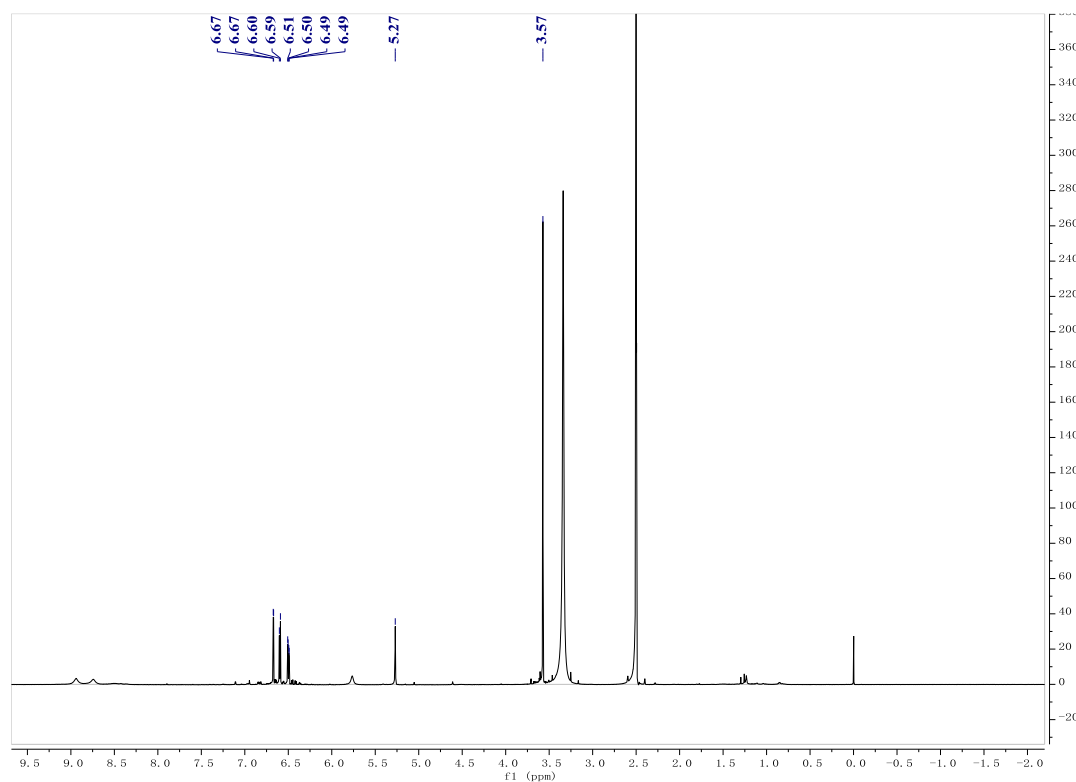
[附件属性]  
 附件: 无

[数据处理参数]  
 阈值: 0.0500000  
 点: 4  
 内插: 停用  
 平均: 停用

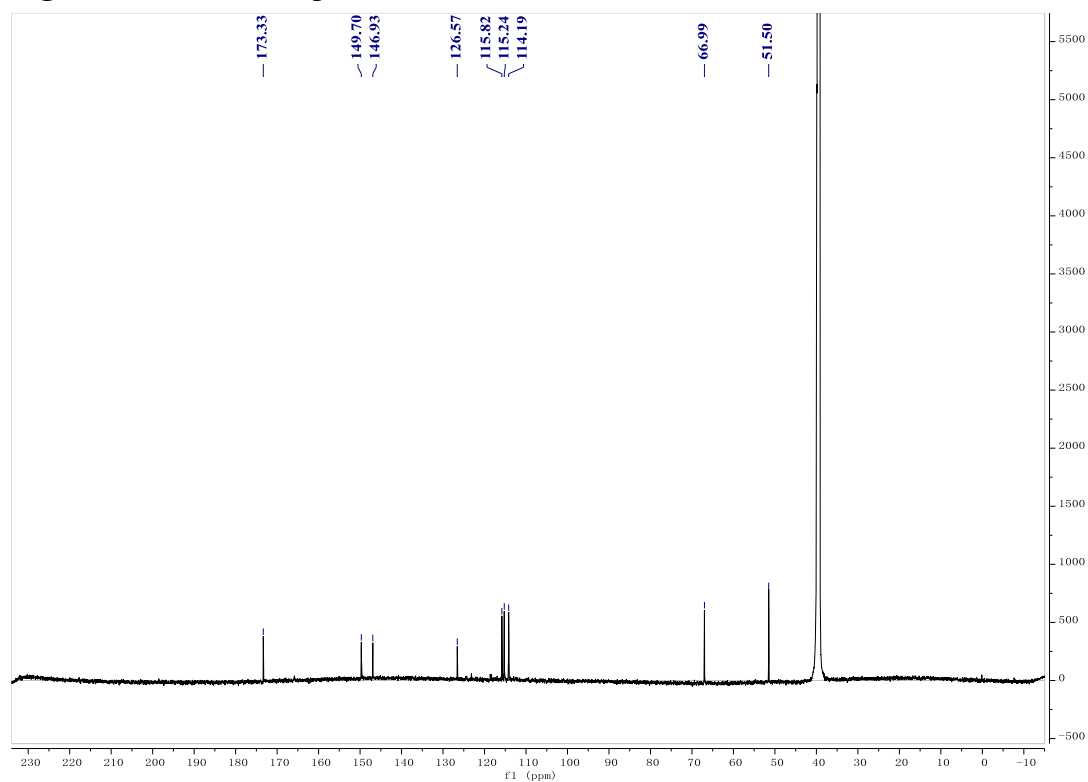
[样品准备属性]  
 重量:  
 体积:  
 稀释:  
 光程长:  
 附加信息:

No.	P/V	波长 (nm)	Abs.	描述
1	②	286.80	1.818	
2	①	204.60	1.114	

Figure S30: UV spectrum of 4 in MeOH.

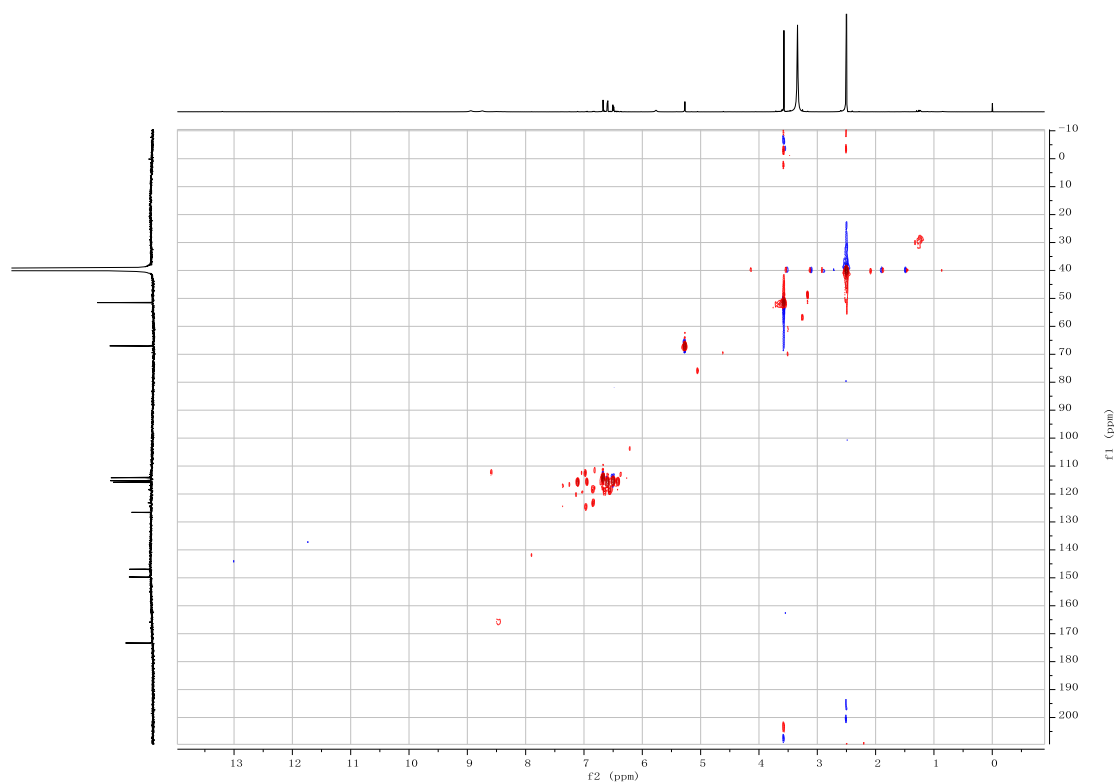


**Figure S31:** <sup>1</sup>H NMR spectrum of **5** in DMSO-*d*<sub>6</sub>.

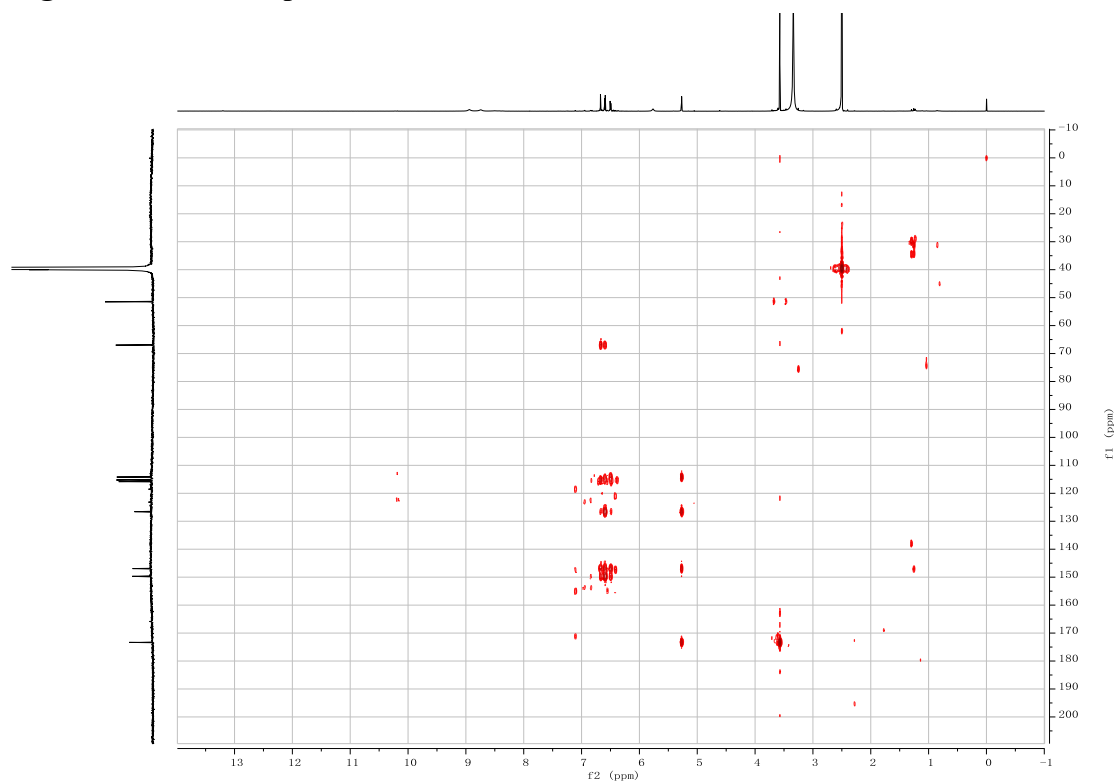


**Figure S32:** <sup>13</sup>C NMR spectrum of **5** in DMSO-*d*<sub>6</sub>.

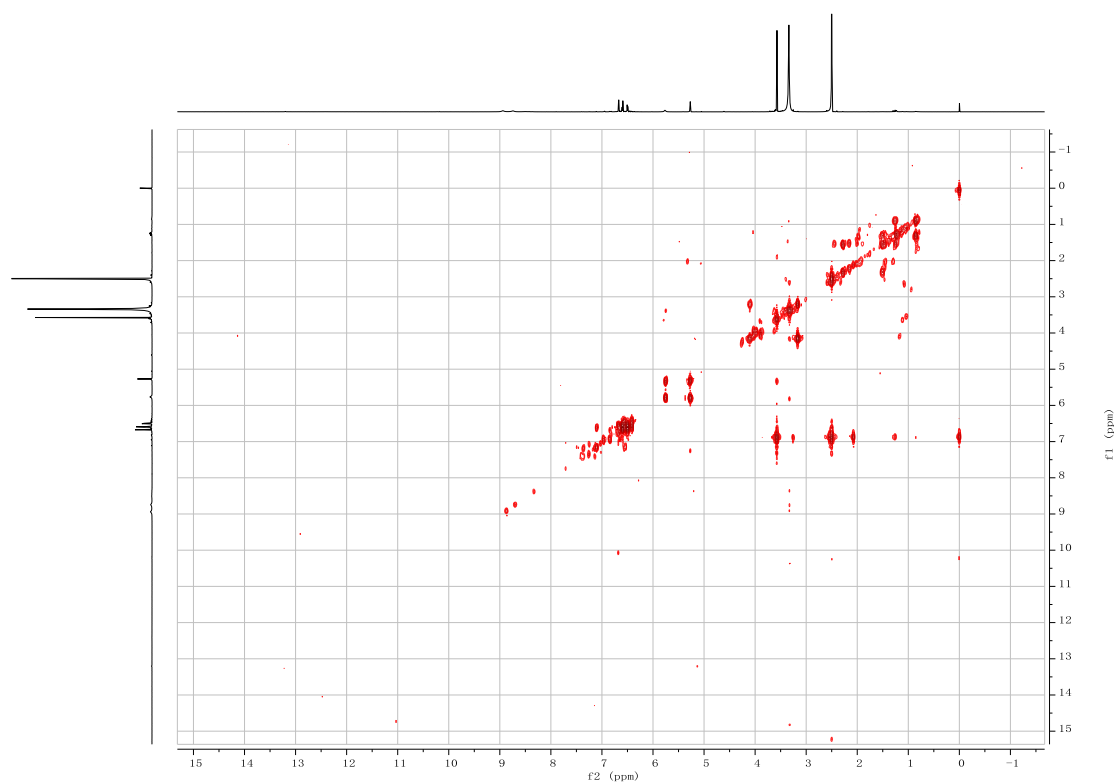




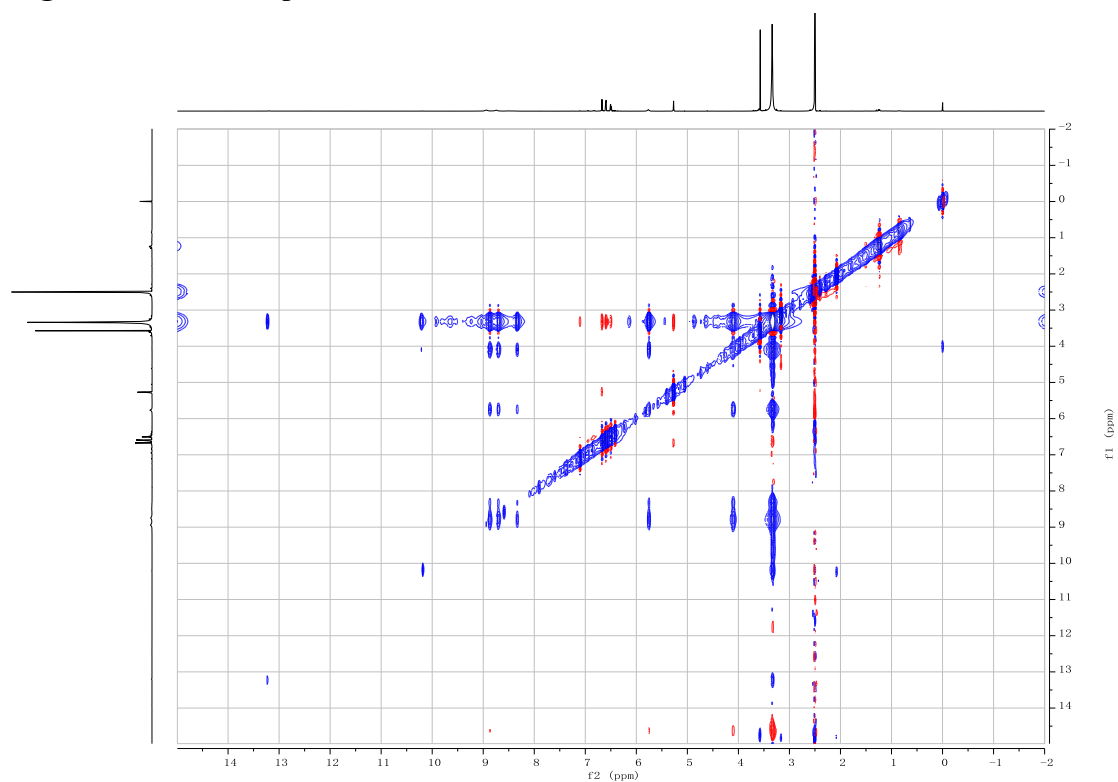
**Figure S33:** HSQC spectrum of **5** in  $\text{DMSO}-d_6$ .



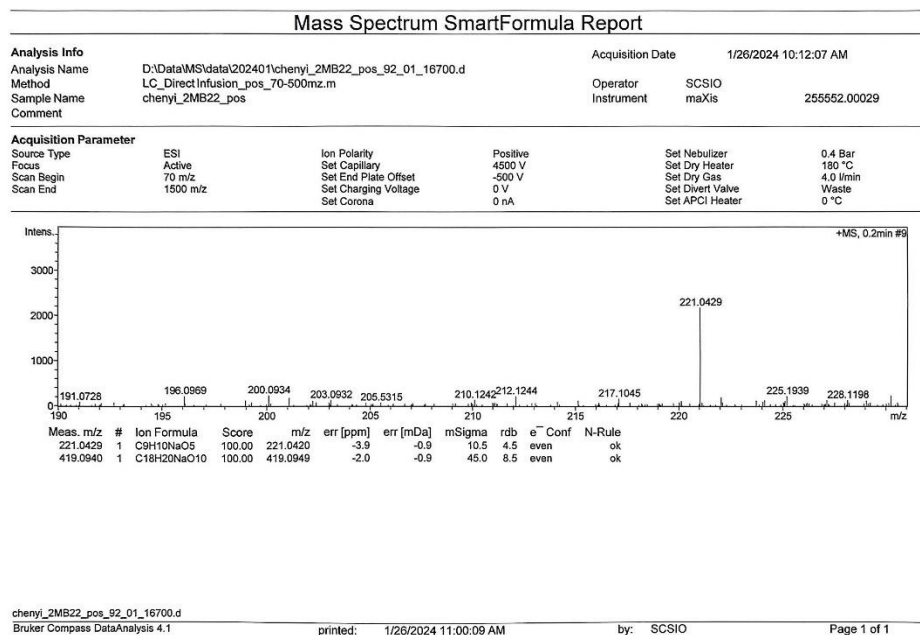
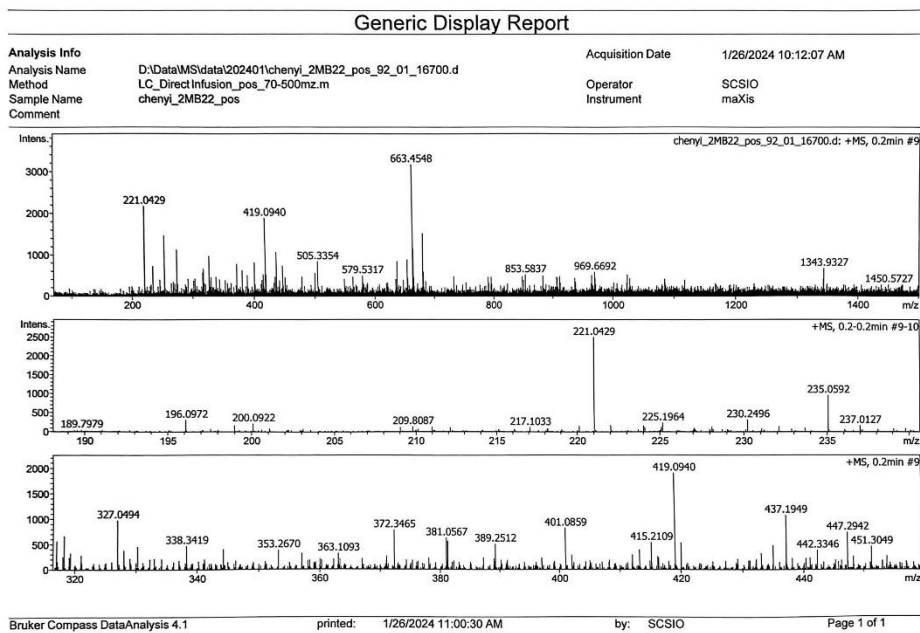
**Figure S34:** HMBC spectrum of **5** in  $\text{DMSO}-d_6$ .



**Figure S35:** COSY spectrum of **5** in DMSO- $d_6$ .



**Figure S36:** NOESY spectrum of **5** in DMSO- $d_6$ .



**Figure S37: HRESIMS spectrum of 5.**

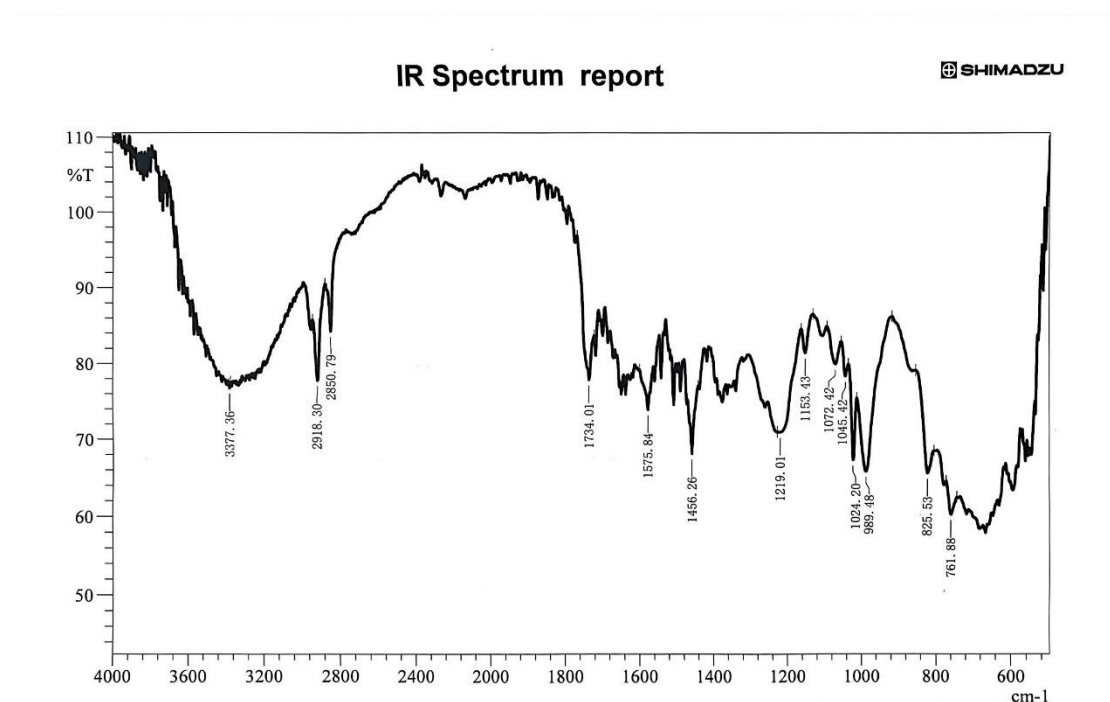
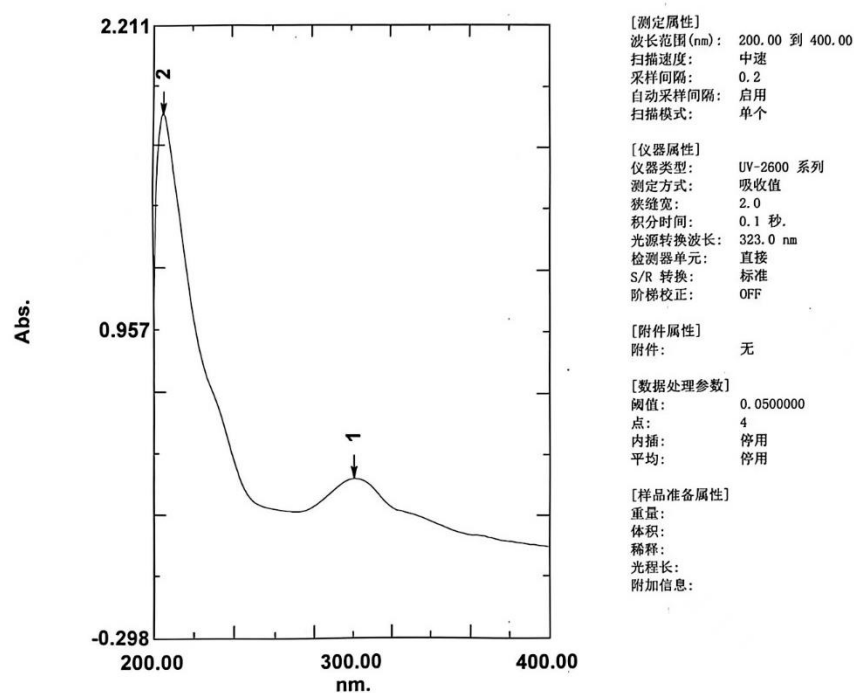
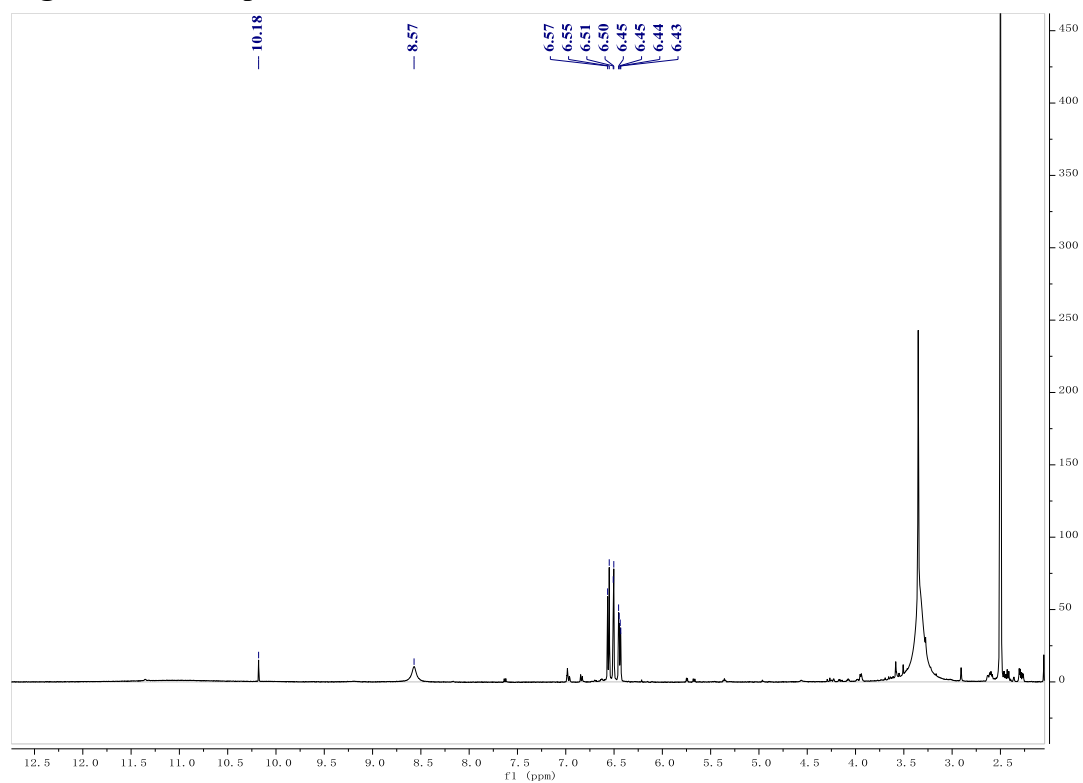


Figure S38: IR spectrum of **5**.

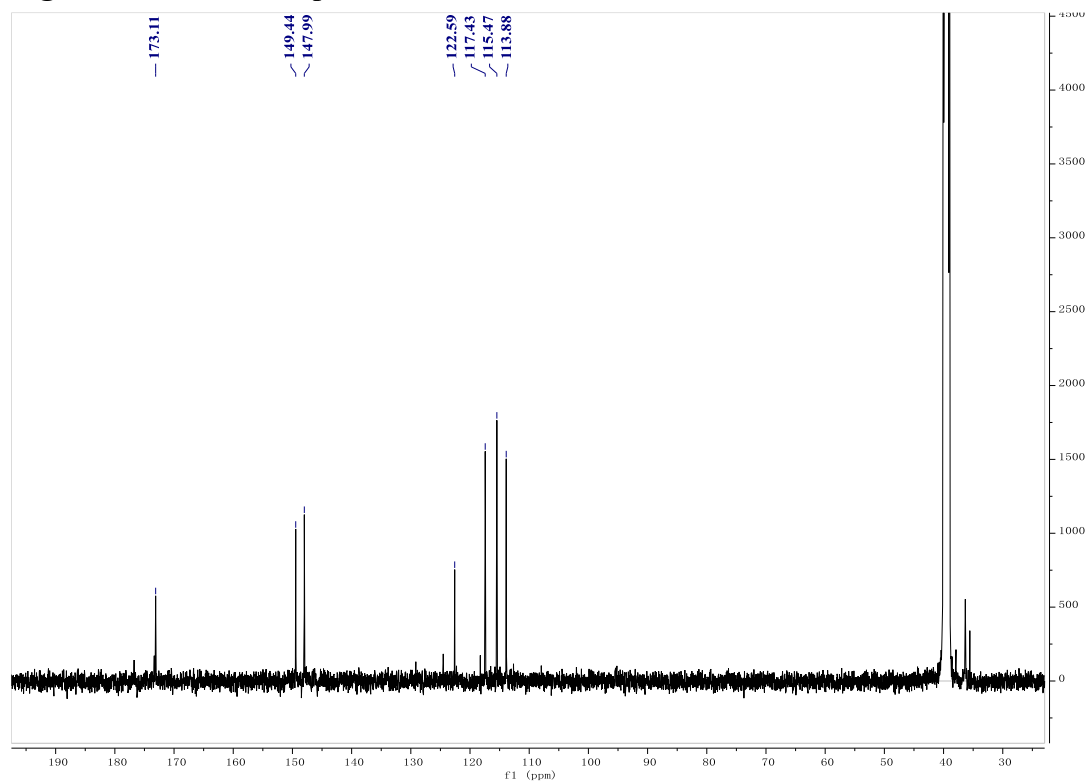


No.	P/V	波长(nm)	Abs.	描述
1	●	300.60	0.355	
2	●	205.00	1.841	

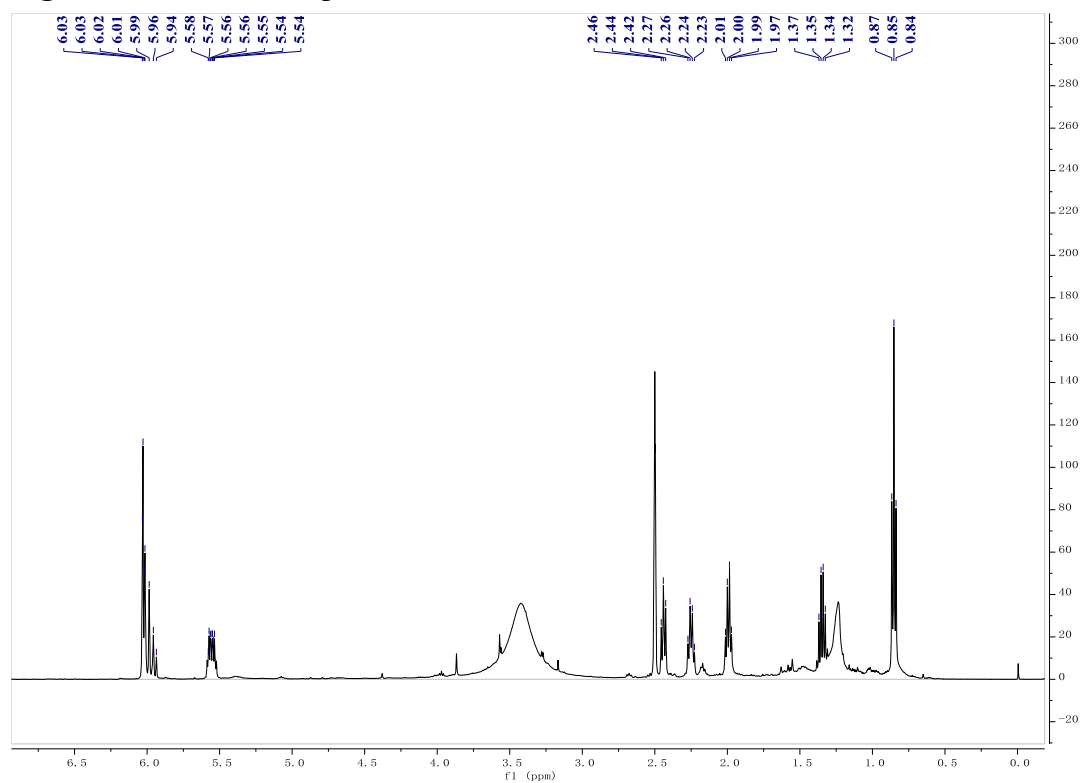
**Figure S39:** UV spectrum of **5** in MeOH.



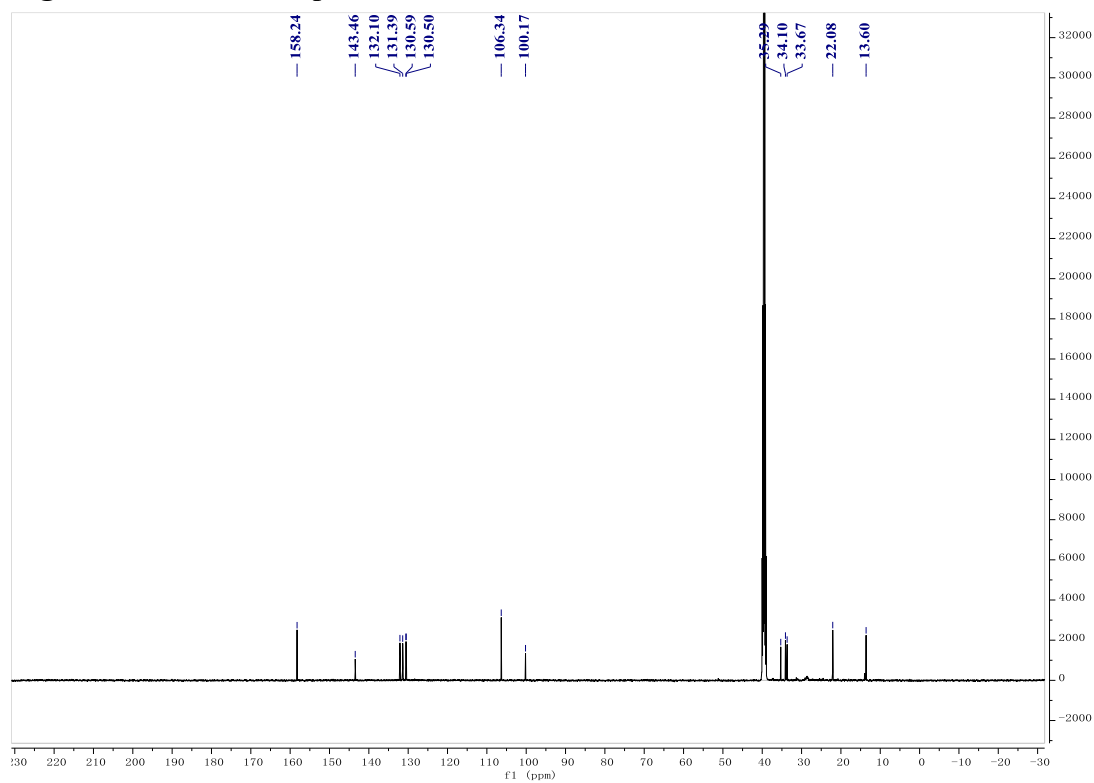
**Figure S40:**  $^1\text{H}$  NMR spectrum of **6** in  $\text{DMSO-}d_6$ .



**Figure S41:**  $^{13}\text{C}$  NMR spectrum of **6** in  $\text{DMSO-}d_6$ .



**Figure S42:**  $^1\text{H}$  NMR spectrum of **7** in  $\text{DMSO-}d_6$ .



13C NMR spectrum of compound 1. The x-axis represents the chemical shift in ppm, ranging from -30 to 230. The y-axis represents the intensity, ranging from -1000 to 11000. The spectrum shows several peaks, with the most intense peak at 34.10 ppm. Other labeled peaks include 172.73, 164.26, 161.11, 158.22, 146.33, 131.98, 131.76, 130.53, 130.37, 109.58, 100.70, 35.44, 34.23, 22.09, and 13.59 ppm.

Figure S45:  $^{13}\text{C}$  NMR spectrum of **8** in  $\text{DMSO}-d_6$ .

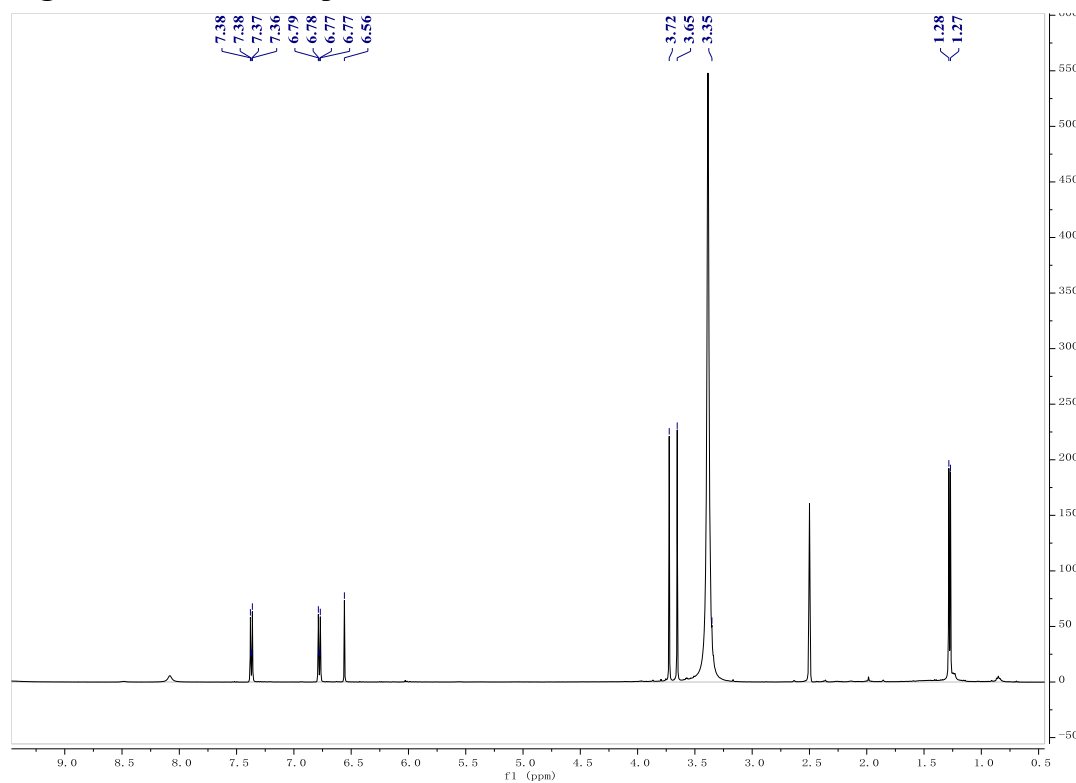
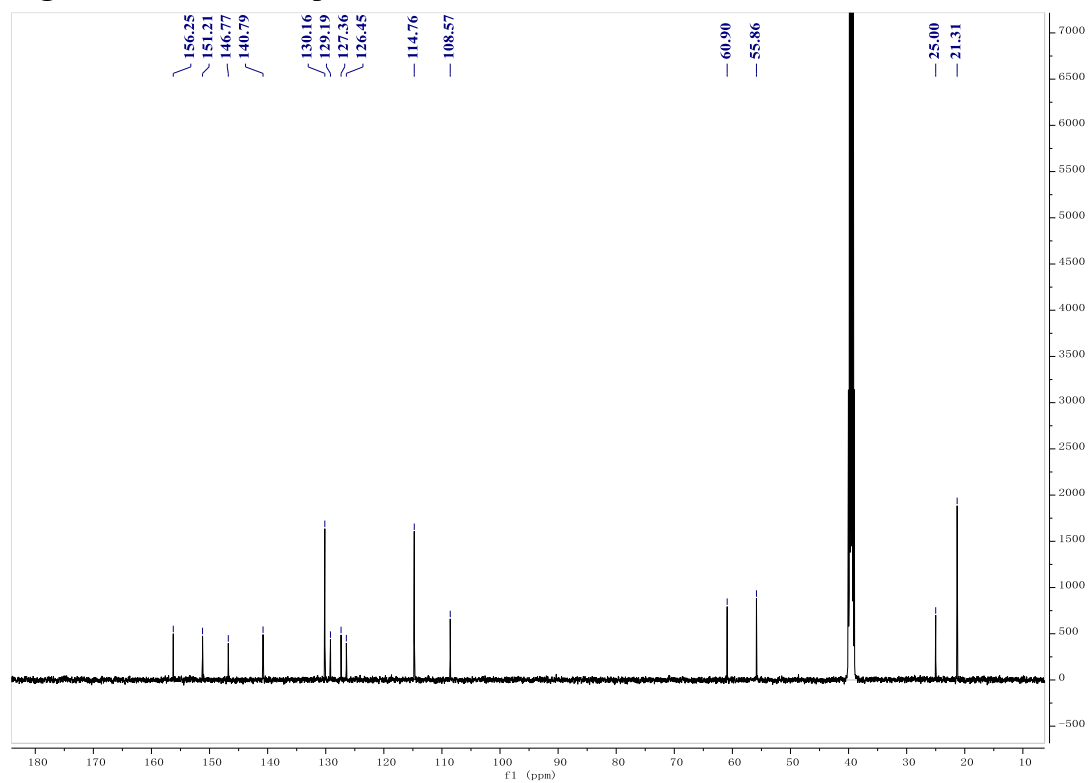
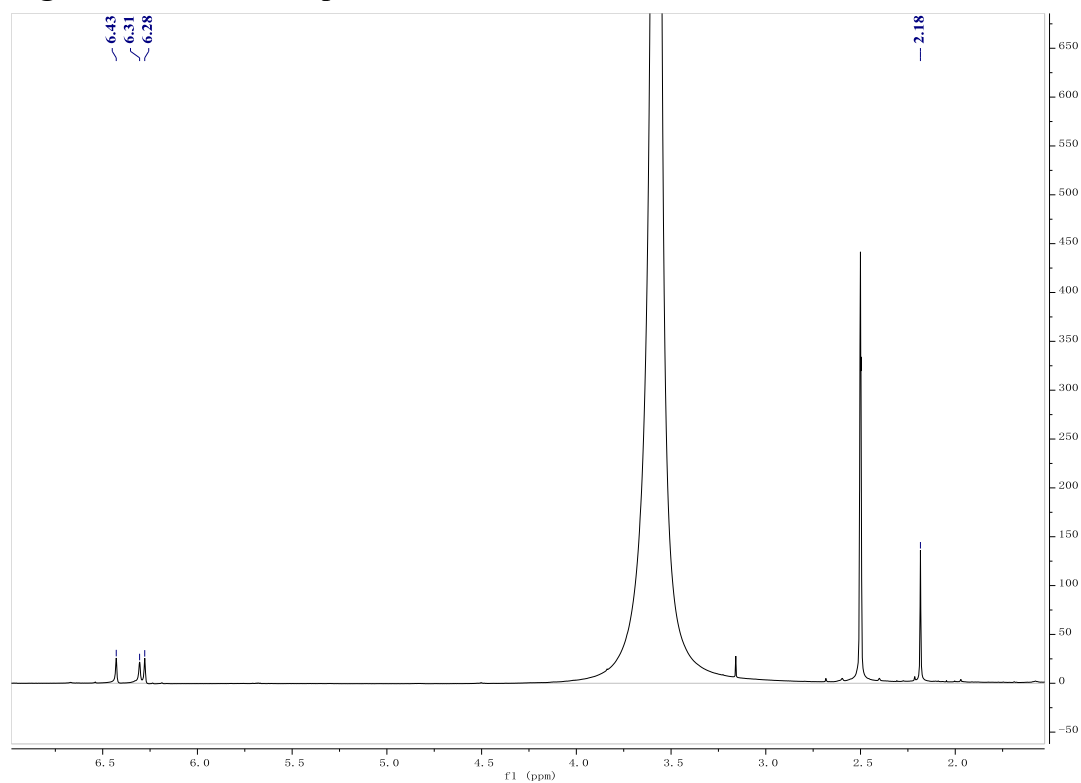


Figure S46:  $^1\text{H}$  NMR spectrum of **9** in  $\text{DMSO}-d_6$ .

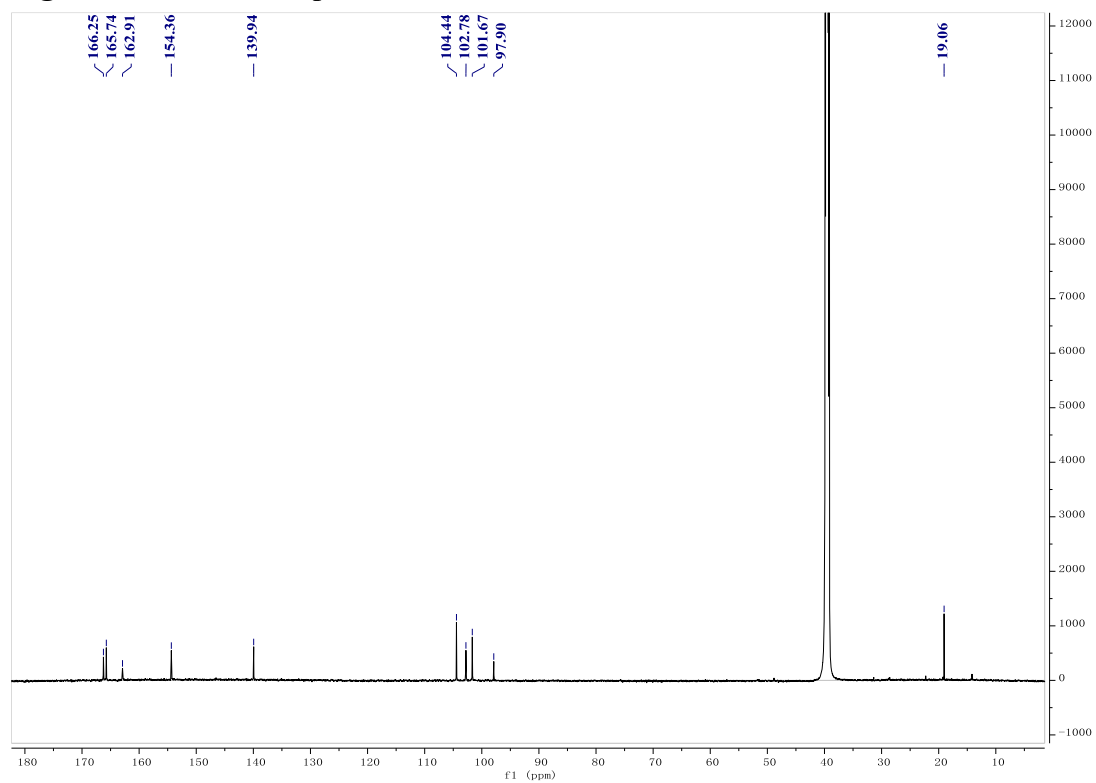




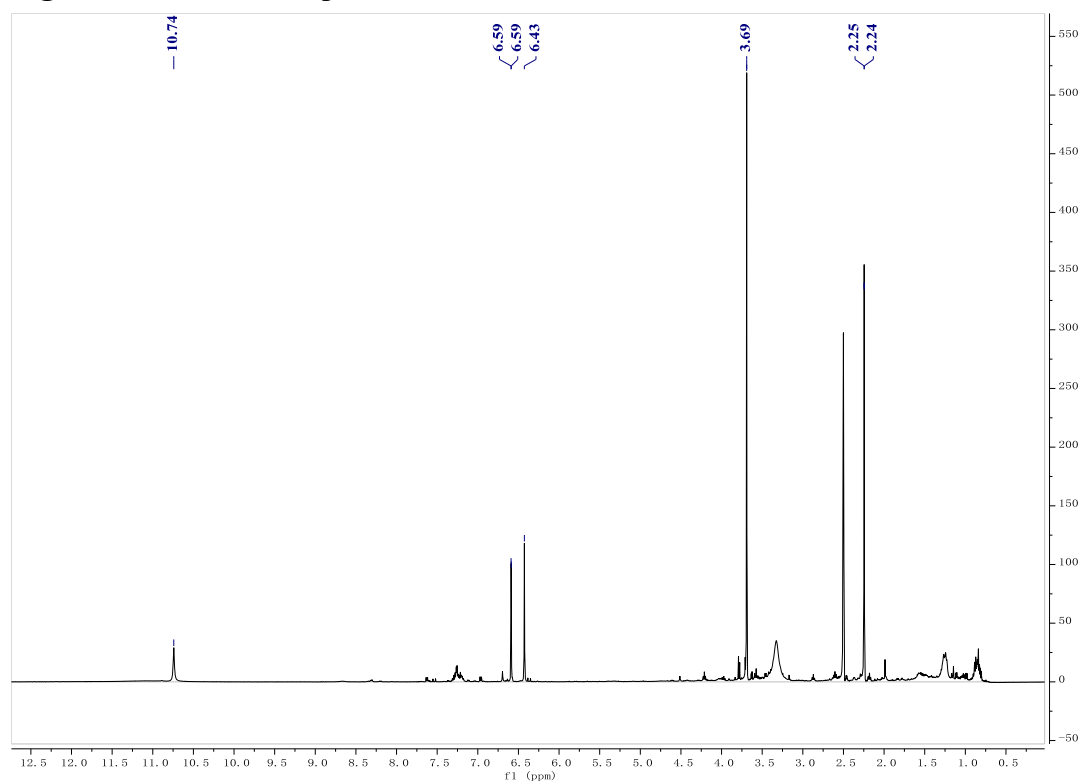
**Figure S47:**  $^{13}\text{C}$  NMR spectrum of **9** in  $\text{DMSO-}d_6$ .



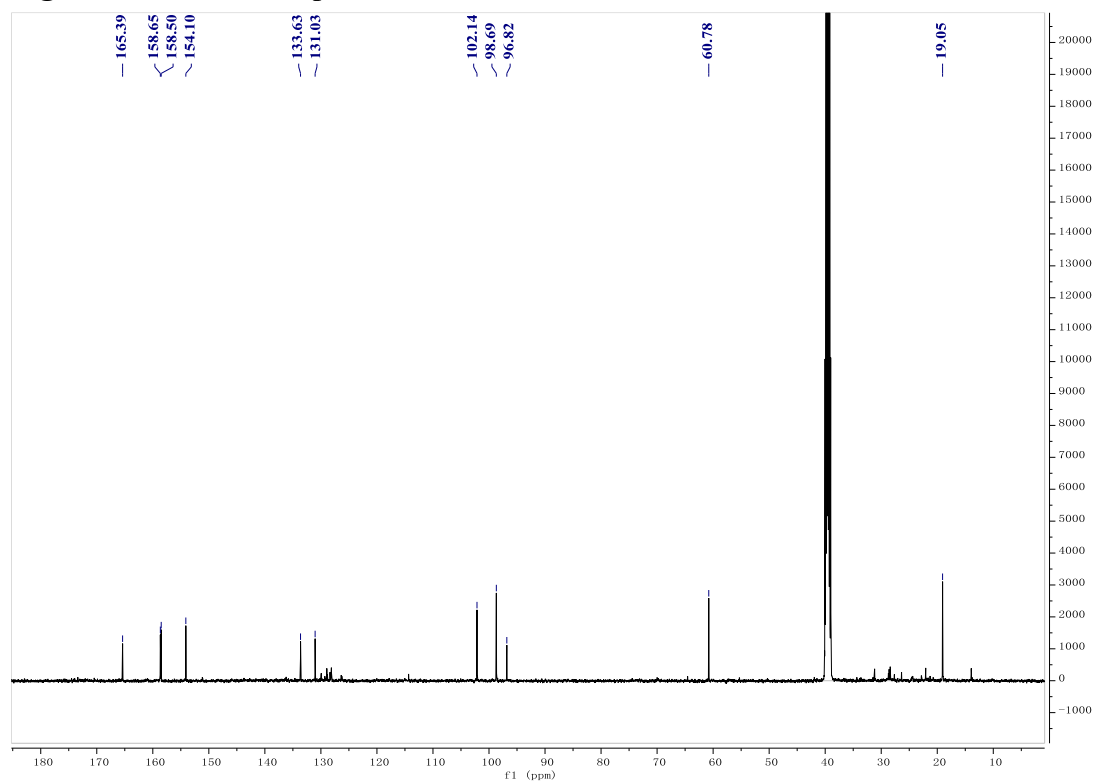
**Figure S48:**  $^1\text{H}$  NMR spectrum of **10** in  $\text{DMSO-}d_6$ .



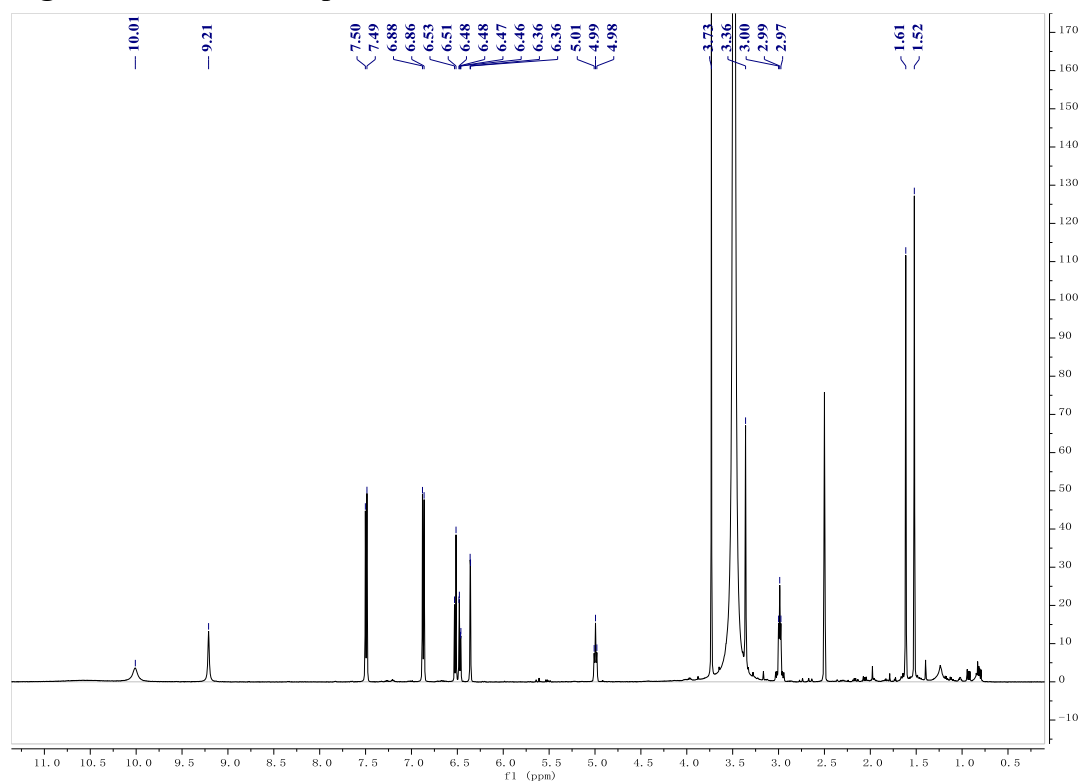
**Figure S49:**  $^{13}\text{C}$  NMR spectrum of **10** in  $\text{DMSO-}d_6$ .



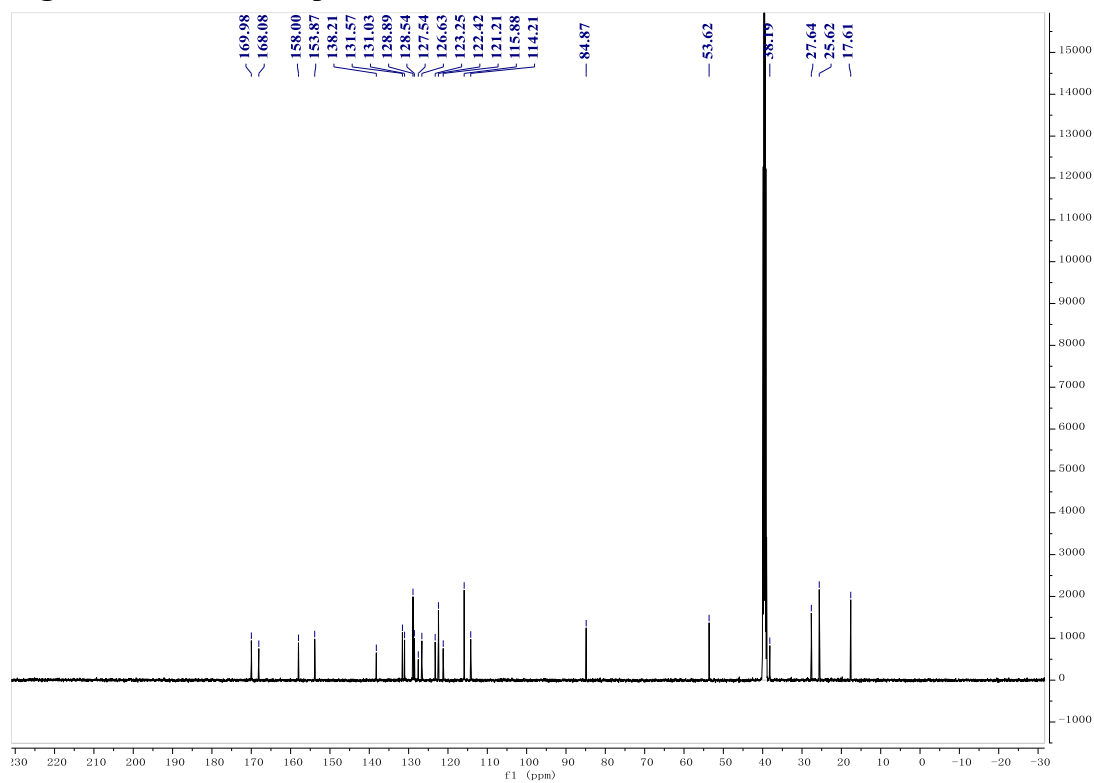
**Figure S50:**  $^1\text{H}$  NMR spectrum of **11** in  $\text{DMSO-}d_6$ .



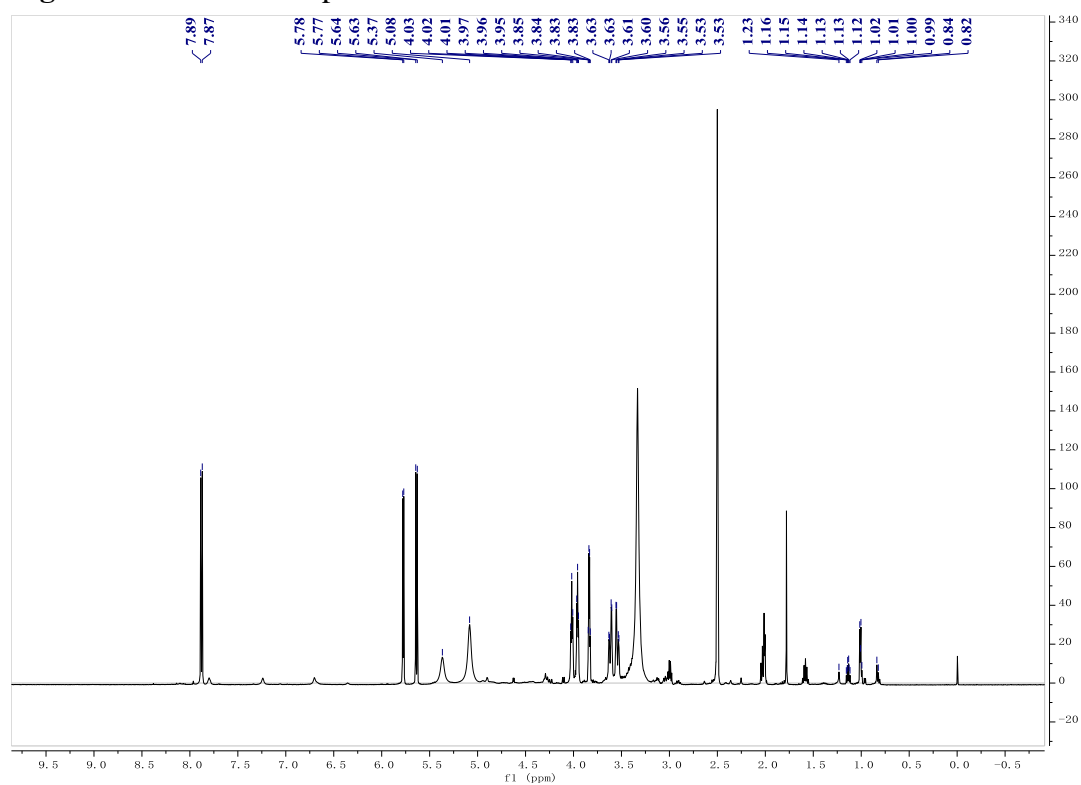
**Figure S51:**  $^{13}\text{C}$  NMR spectrum of **11** in  $\text{DMSO}-d_6$ .



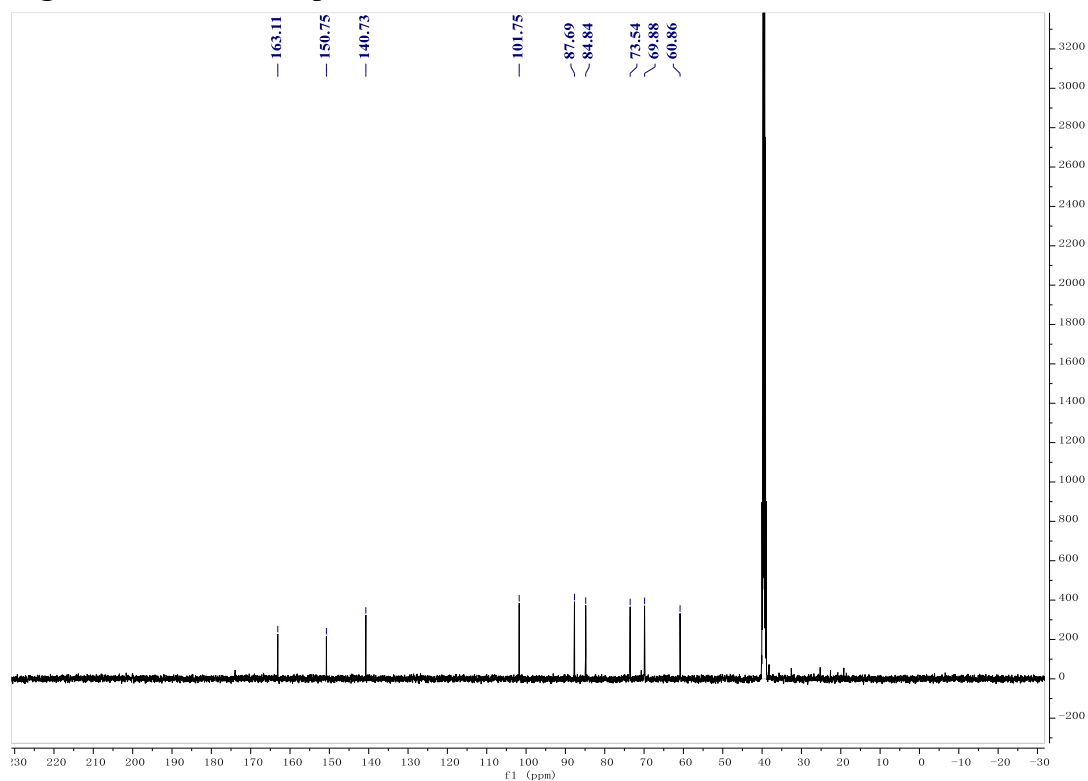
**Figure S52:**  $^1\text{H}$  NMR spectrum of **12** in  $\text{DMSO}-d_6$ .



**Figure S53:**  $^{13}\text{C}$  NMR spectrum of **12** in  $\text{DMSO-}d_6$ .



**Figure S54:**  $^1\text{H}$  NMR spectrum of **13** in  $\text{DMSO-}d_6$ .



**Figure S55:**  $^{13}\text{C}$  NMR spectrum of **13** in  $\text{DMSO-}d_6$ .

**ITS sequence of the strain *Penicillium* sp. SCSIO 41411**

TGATATGCTTAAGTTCAGCGGGTATCCCTACCTGATCCGAGGTCAACCTGAGAAAGATT  
GAGGGGGGTCGCCGGCGGGCGCCGGCCGGGCCTACAGAGCGGGTGACGAAGCCCCAT  
ACGCTCGAGGACCGGACGCGGTGCCGCCGCTGCCTTTCGGGCCCCGCCCCCGGTAGC  
CGGGGGGCGGGGCCCAACACACAAGCCGTGCTTGAGGGCAGCAATGACGCTCGGAC  
AGGCATGCCCCCGGAATACCAGGGGGCGCAATGTGCGTTCAAAGACTCGATGATTCA  
CTGAATTCTGCAATTCACATTACTTATCGCATTTCGCTGCGTTCTTCATCGATGCCGGAA  
CCAAGAGATCCGTTGTTGAAAGTTTTAACTGATTAGCTAATCGCTCAGACTGCATTCT  
TCAGACAGCGTTCAATGGTGTCTTCGGCGGGCGCGGGCCCGGGGGCGGATGCCCCC  
GGCGGCCGGAACGGCGGGCCCGCCGAAGCAACAAGGTACGATAAACACGGGTGGGA  
GGTTGGACCCAGAGGGCCCTCACTCGGAATGATCCTTCCGCA