

## *Supplementary Material*

### **New pyranone derivatives and sesquiterpenoid isolated from the endophytic fungus *Xylaria* sp. Z184**

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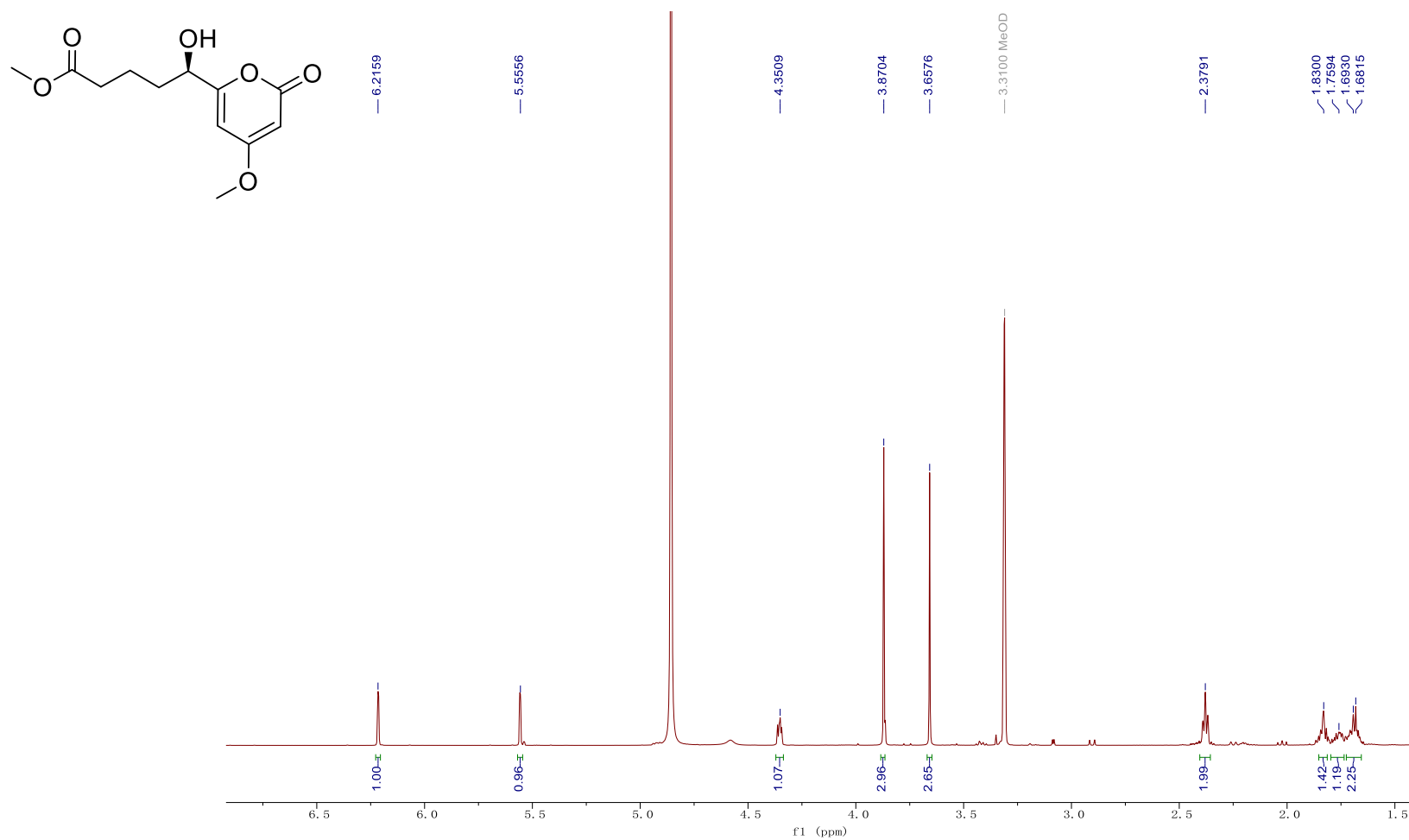
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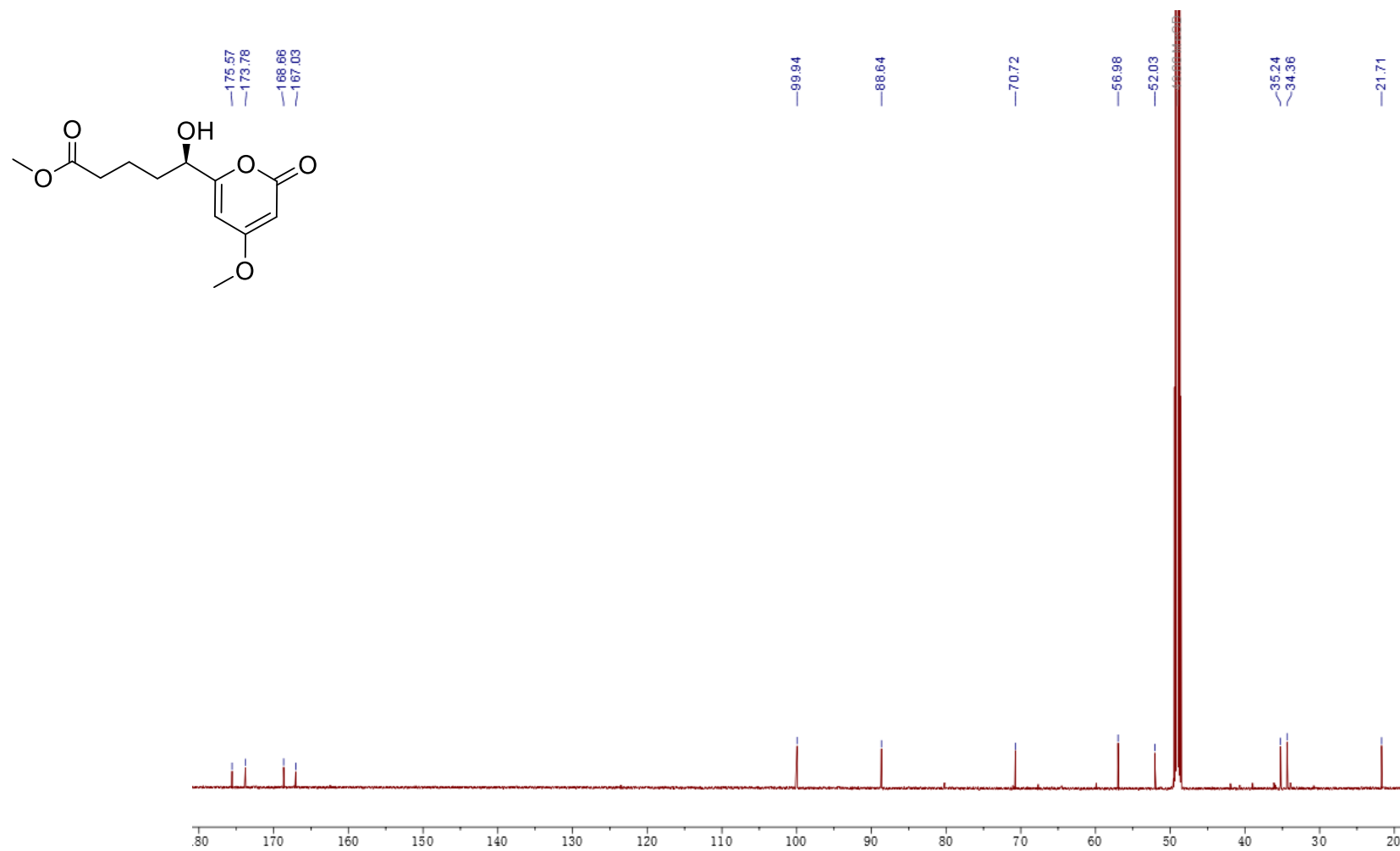
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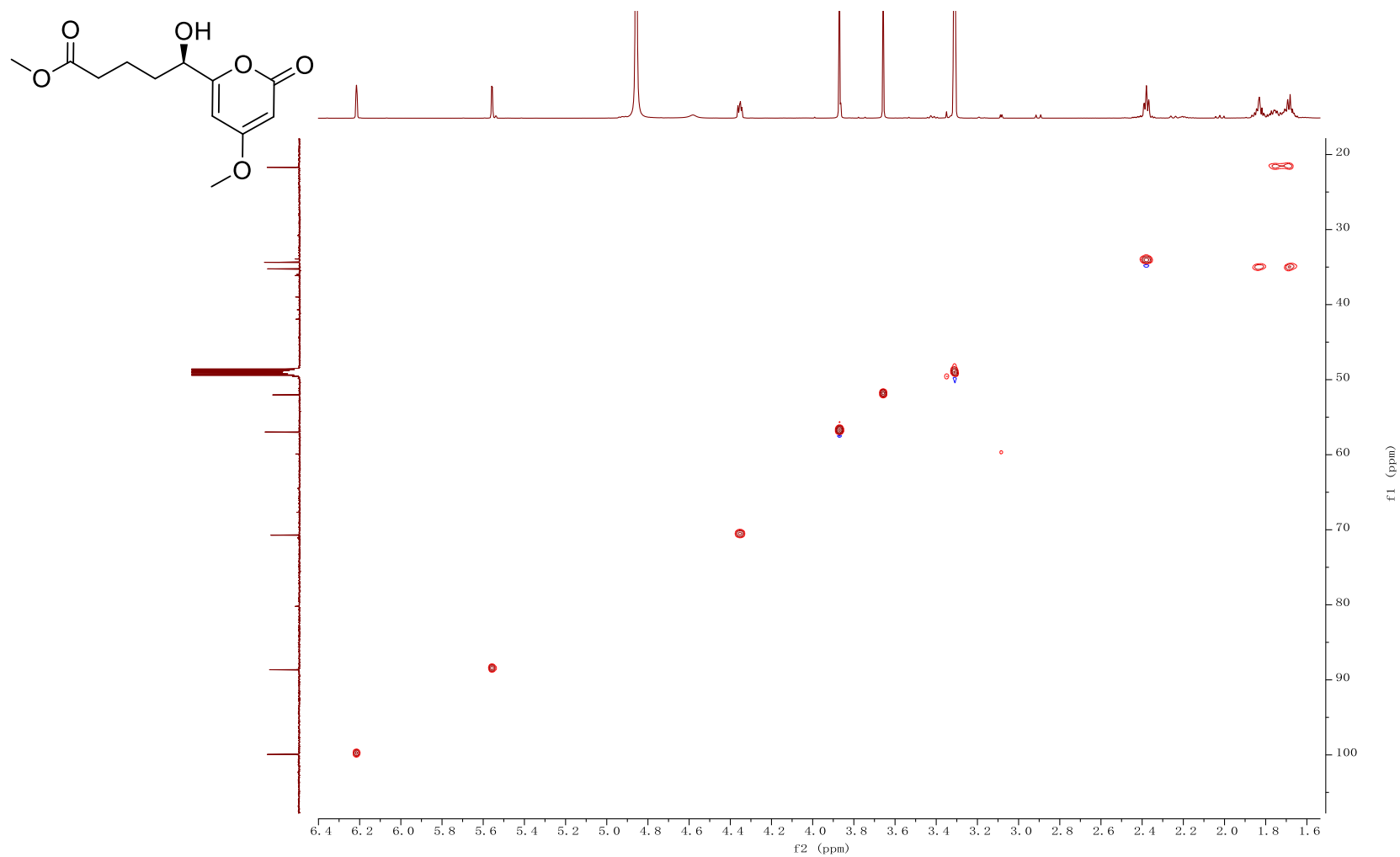
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**Fig. S1** <sup>1</sup>H NMR spectrum of **1** in methanol-*d*<sub>4</sub> (600 MHz).



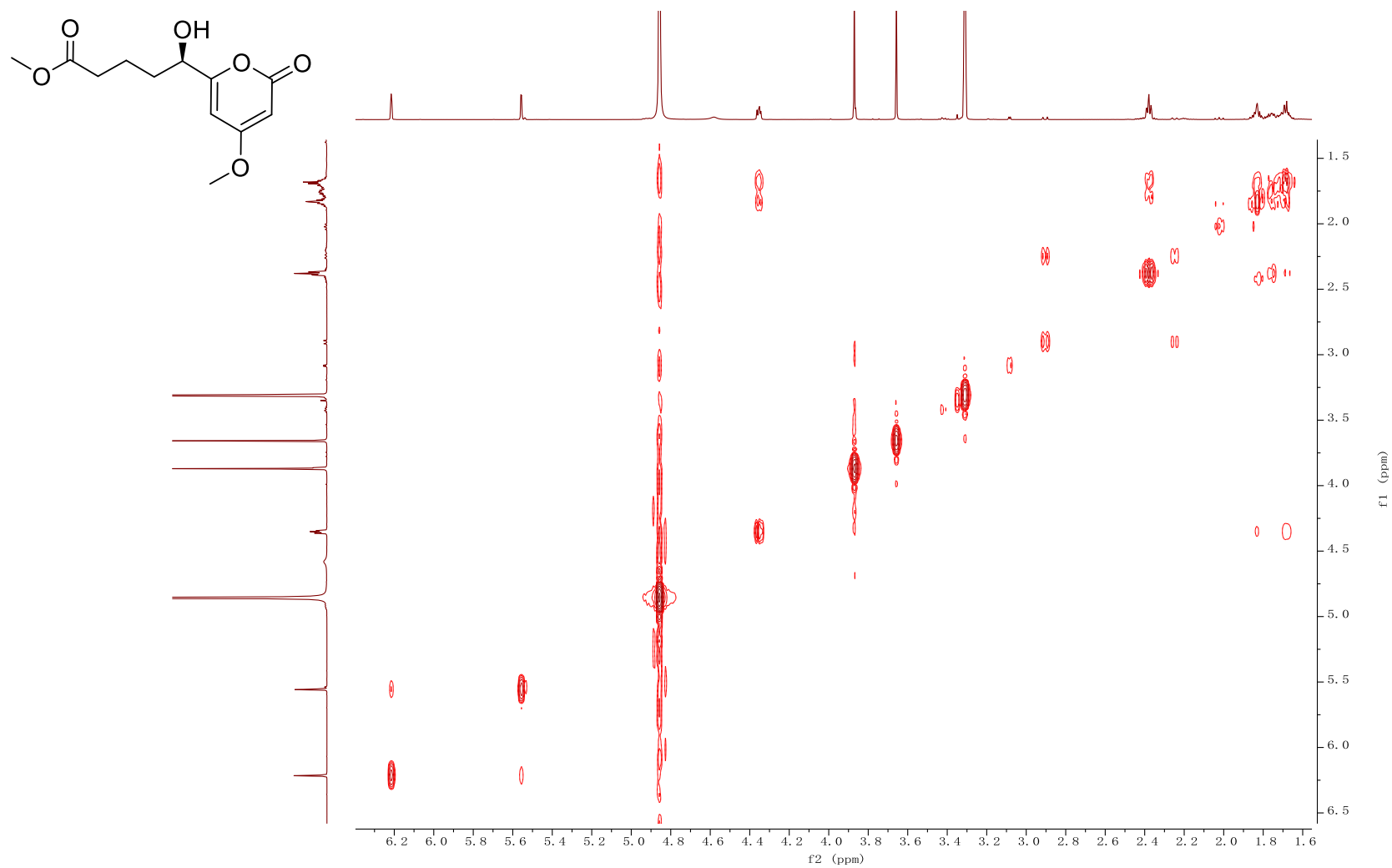
**Fig. S2** <sup>13</sup>C NMR spectrum of **1** in methanol-*d*<sub>4</sub> (150 MHz).



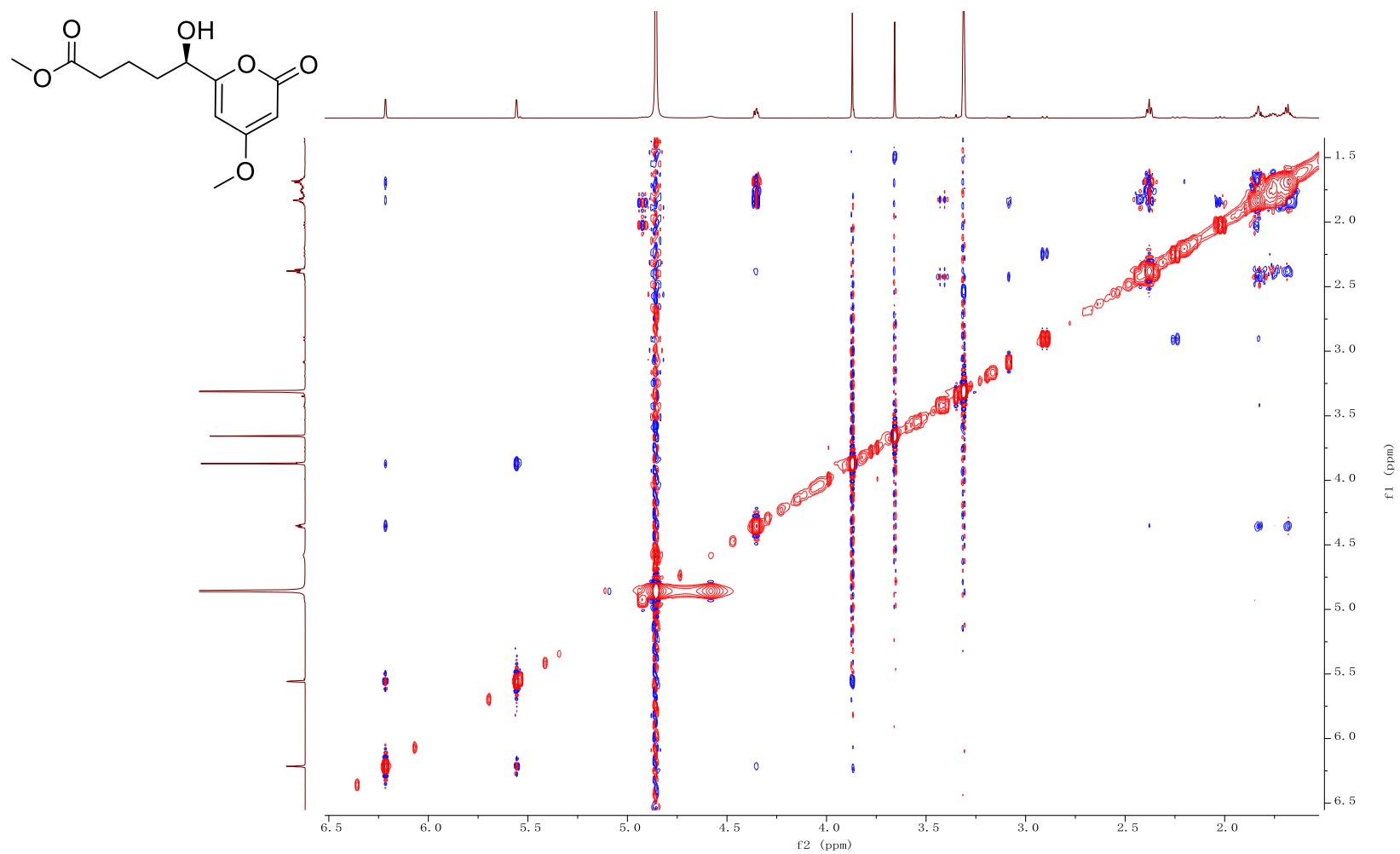
**Fig. S3** HSQC spectrum of **1** in methanol- $d_4$  (600 MHz).







**Fig. S5**  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of **1** in methanol- $d_4$  (600 MHz).



**Fig. S6** ROESY spectrum of **1** in methanol- $d_4$  (600 MHz).

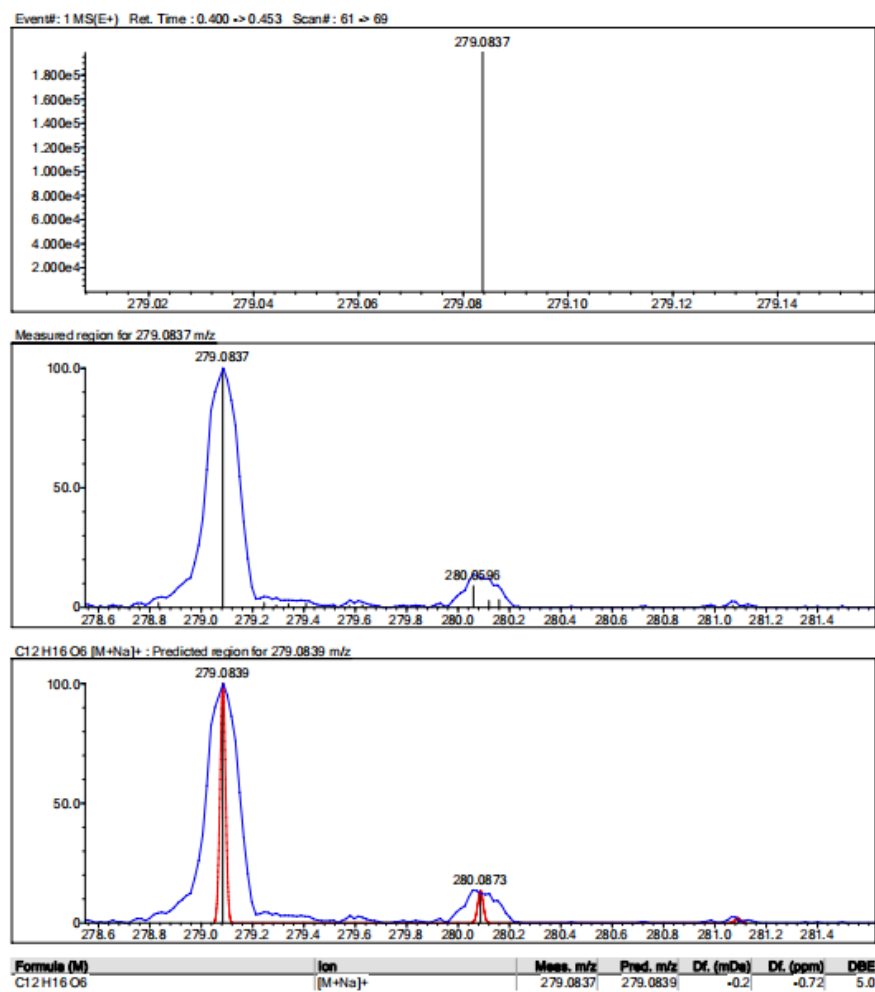
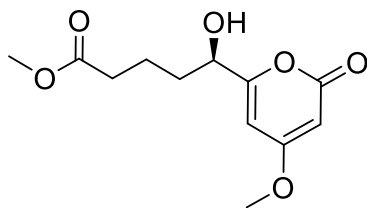
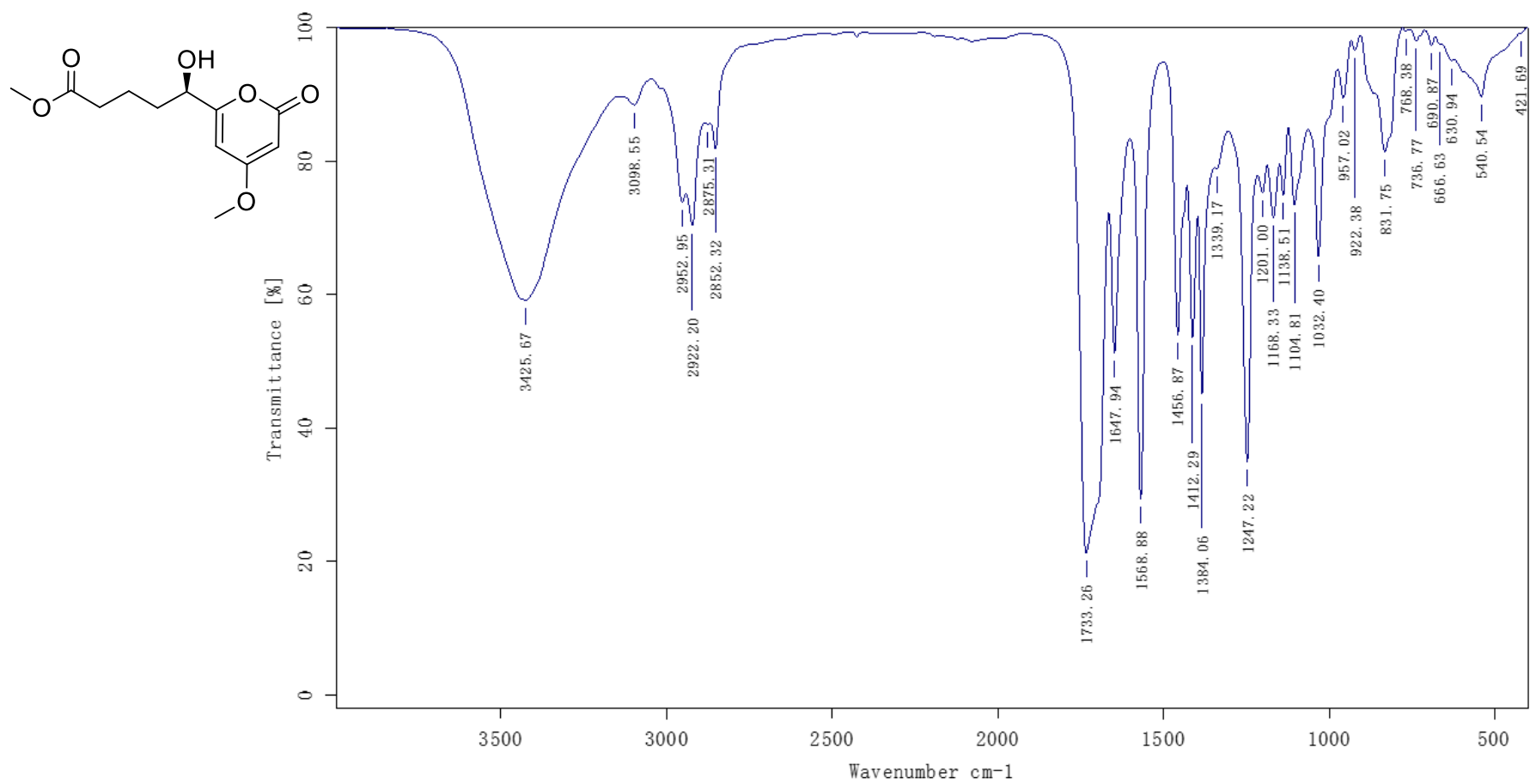
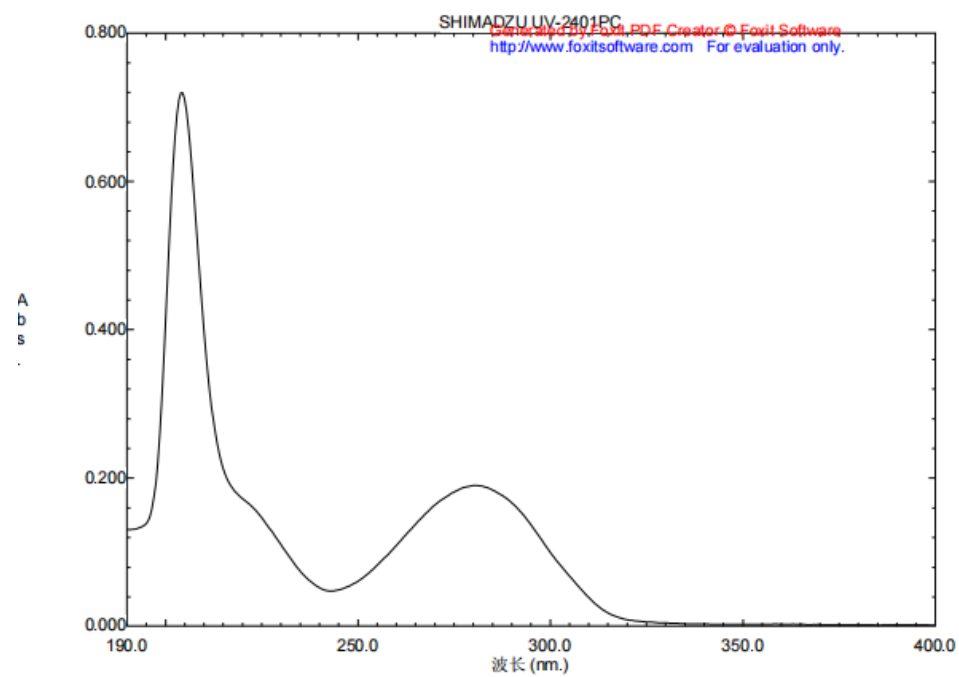
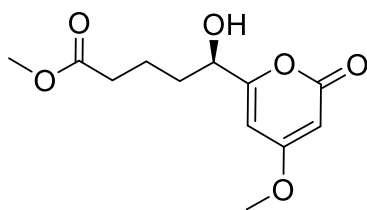


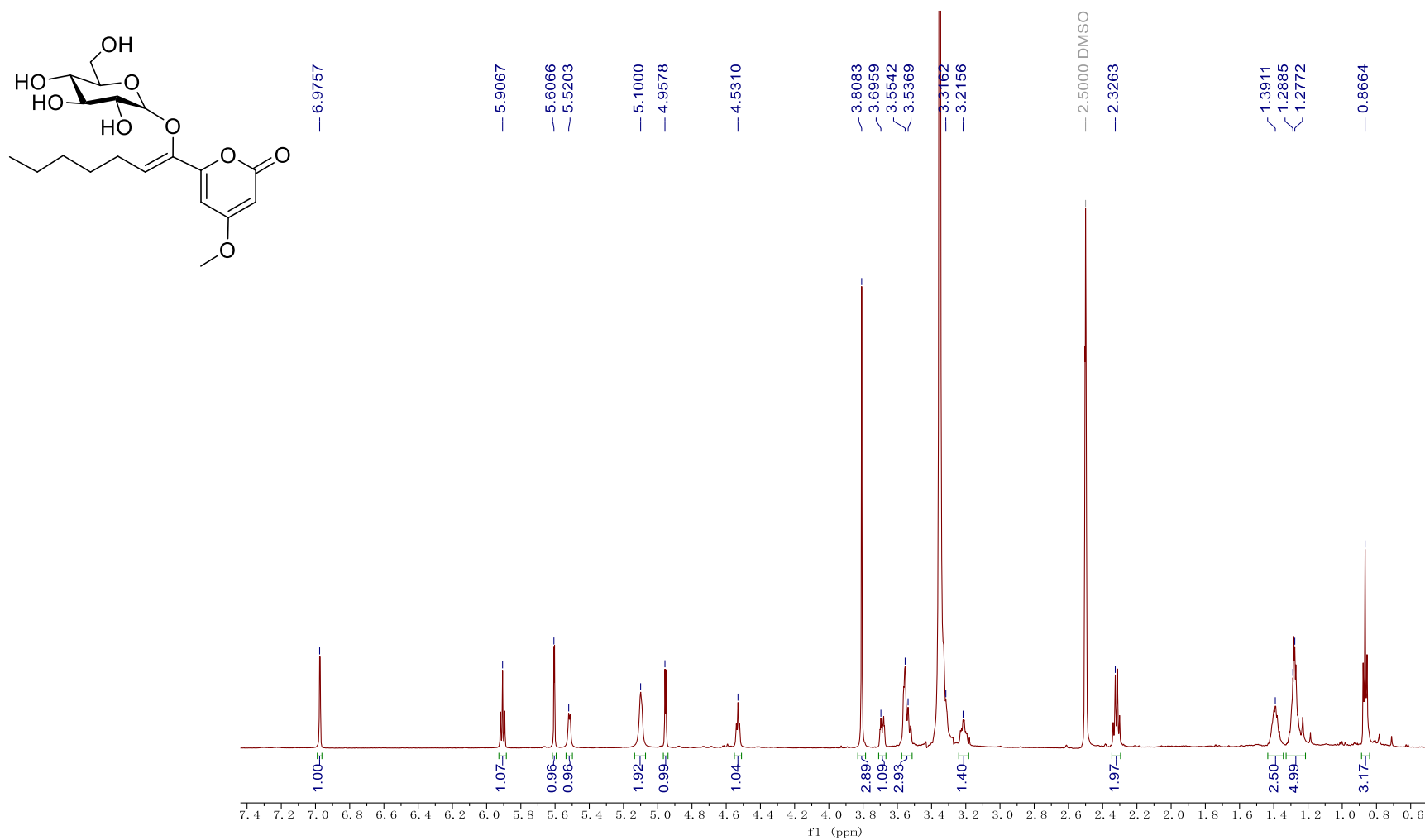
Fig. S7 HRESIMS spectrum of 1.



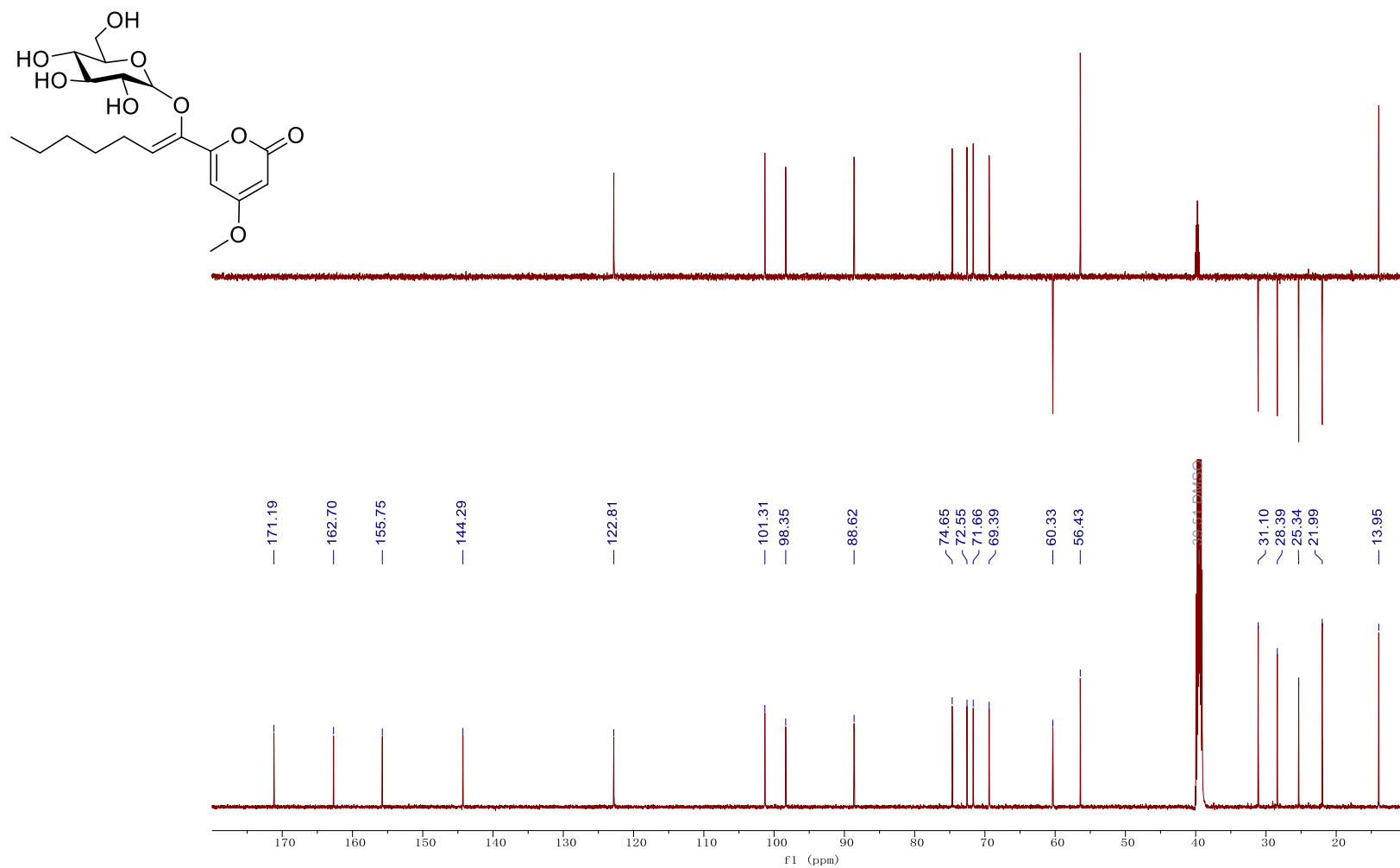
**Fig. S8** IR spectrum of **1**.



**Fig. S9** UV spectrum of **1**.

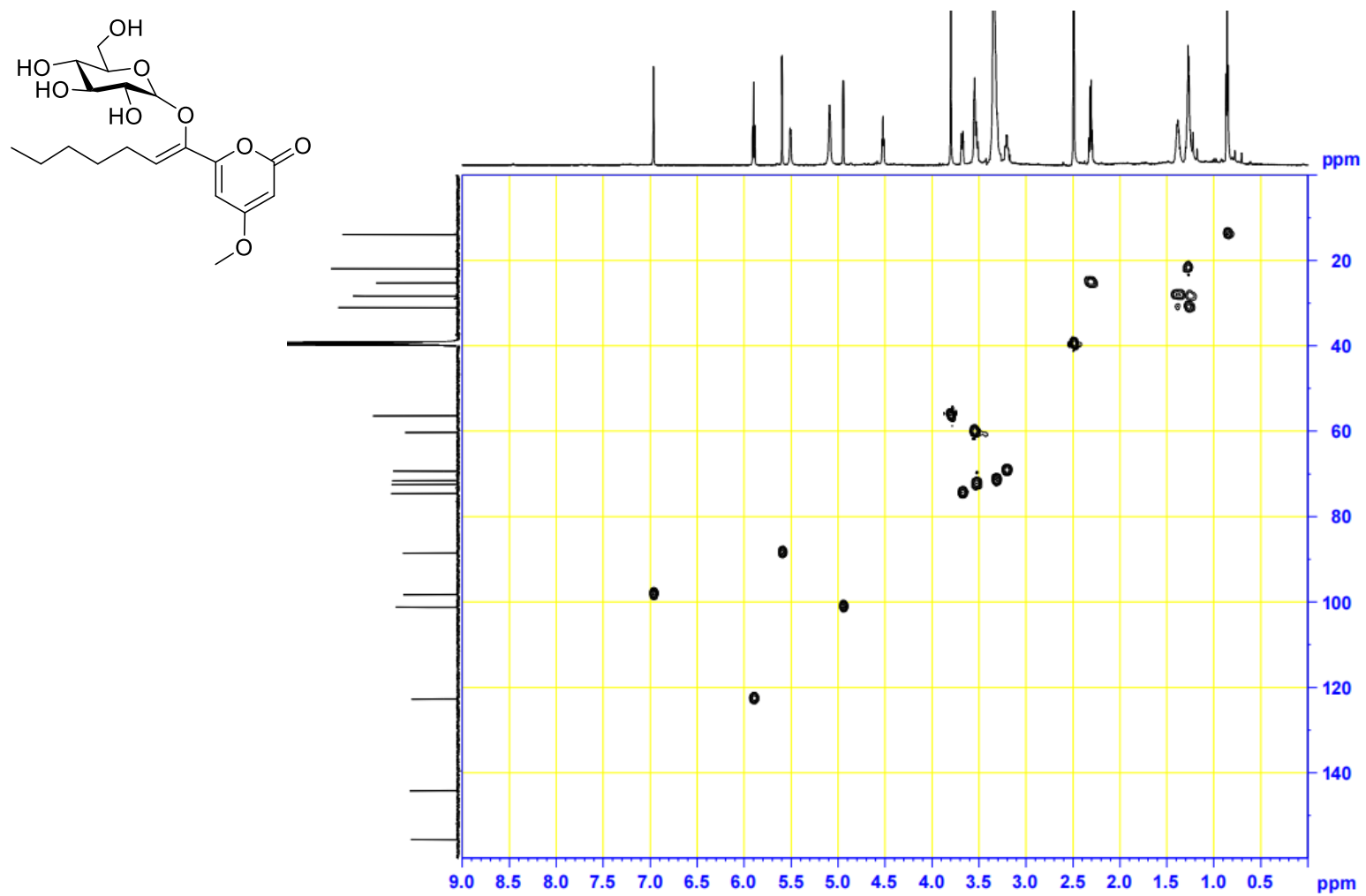


**Fig. S10**  $^1\text{H}$  NMR spectrum of **2** in  $\text{DMSO}-d_6$  (600 MHz).

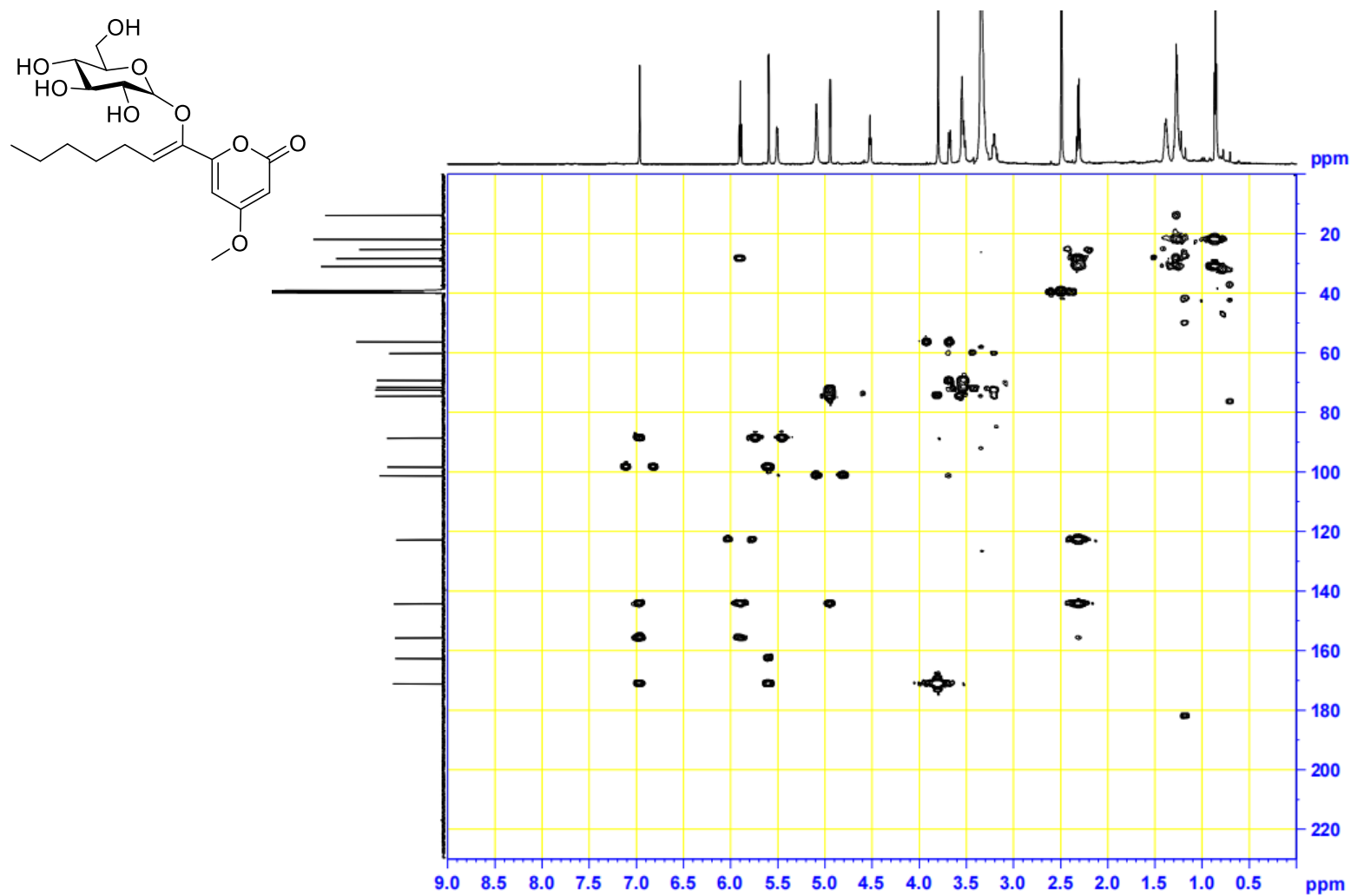


**Fig. S11**  $^{13}\text{C}$  NMR spectrum of **2** in  $\text{DMSO}-d_6$  (150 MHz).

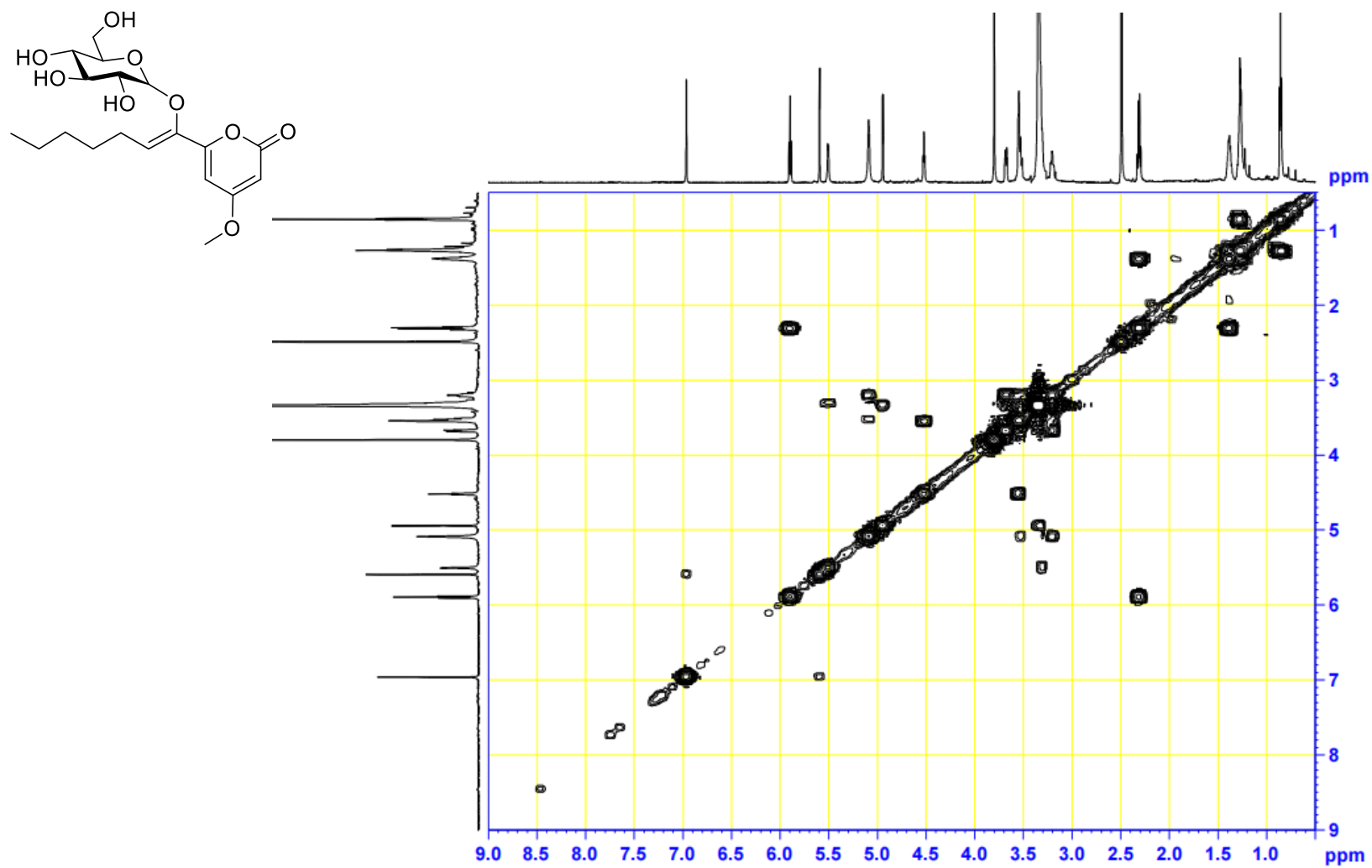




**Fig. S12** HSQC spectrum of **2** in DMSO-*d*<sub>6</sub> (600 MHz).



**Fig. S13** HMBC spectrum of **2** in DMSO-*d*<sub>6</sub> (600 MHz).



**Fig. S14**  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of **2** in  $\text{DMSO}-d_6$  (600 MHz).

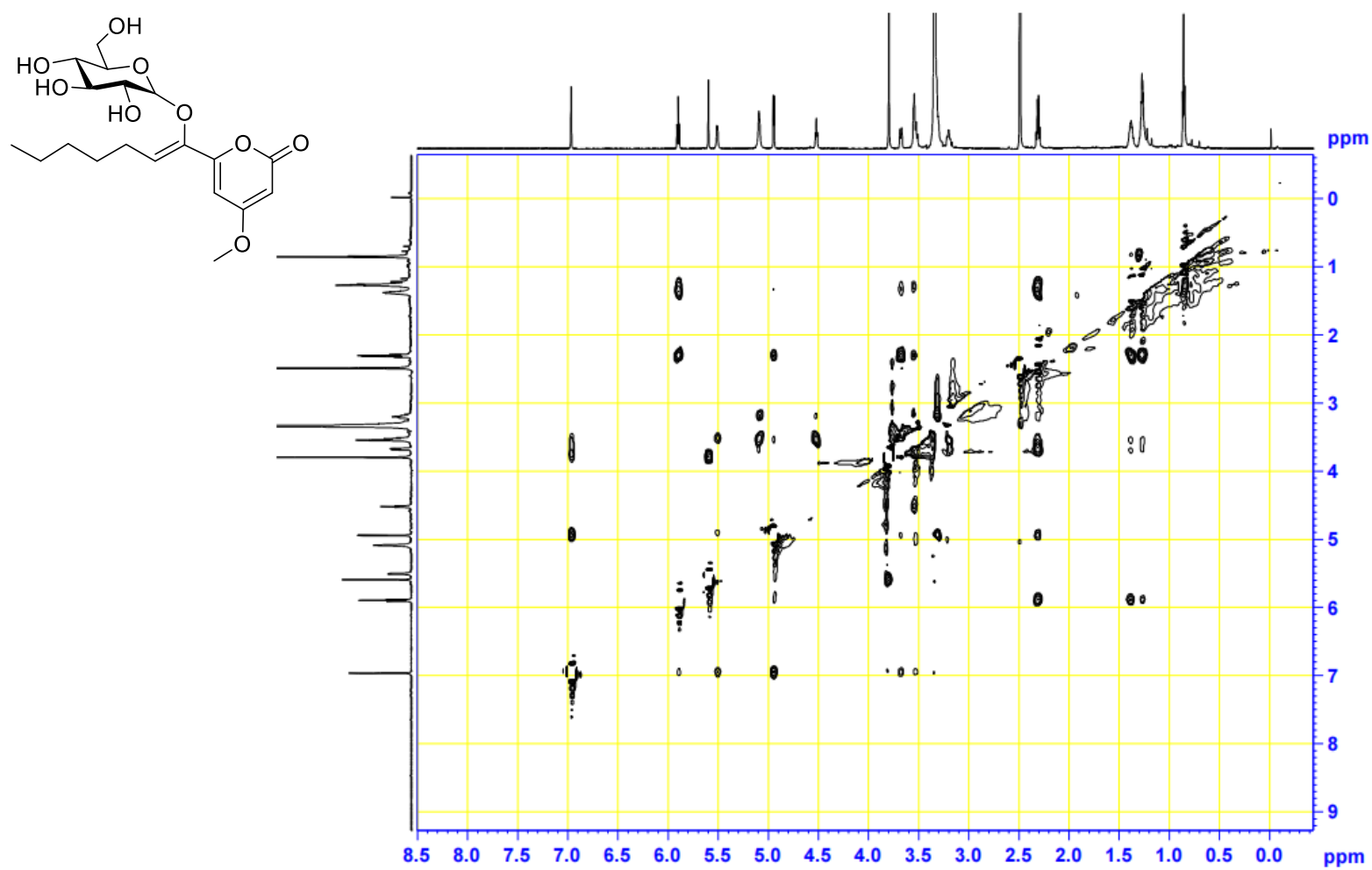
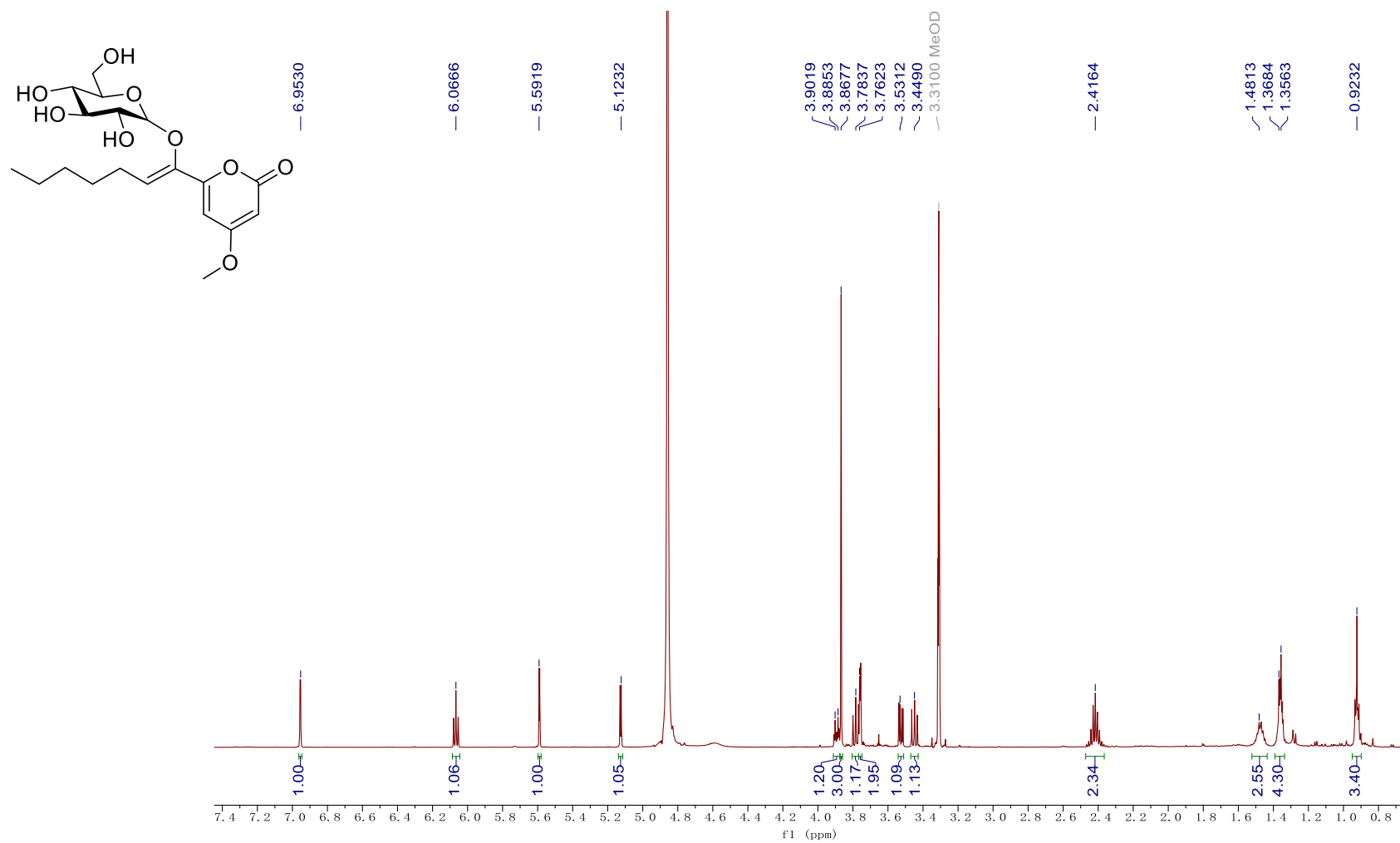
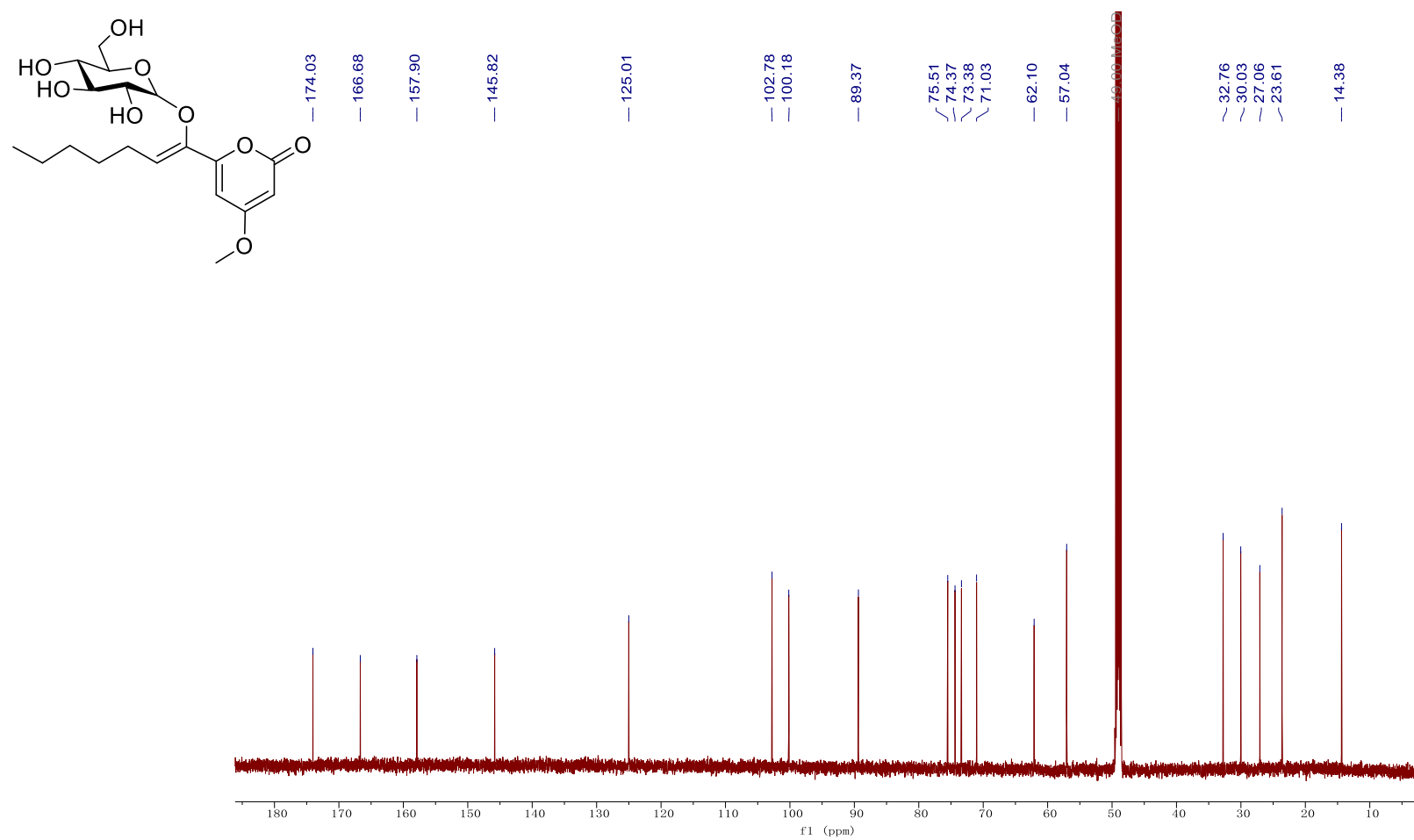


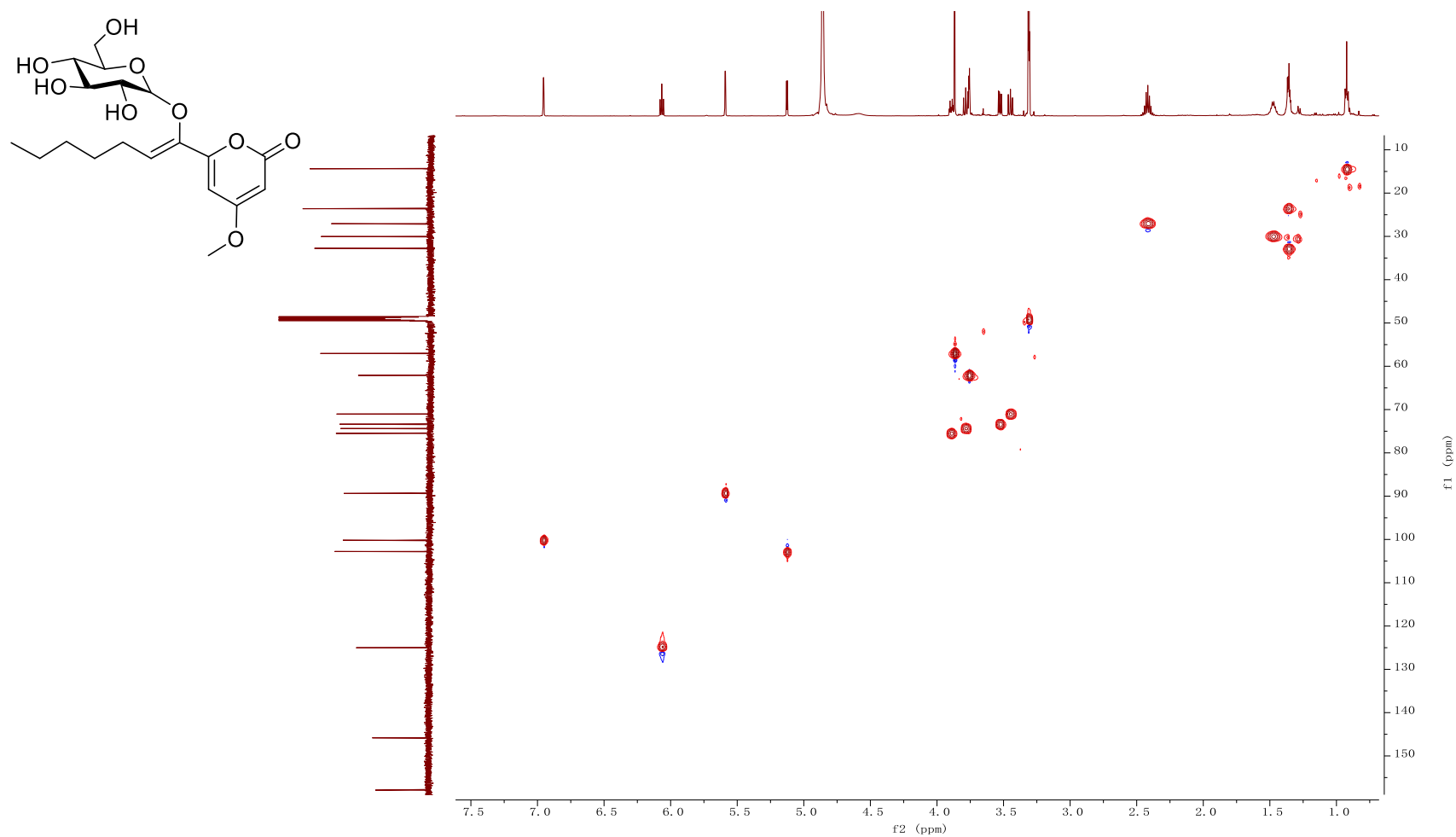
Fig. S15 ROESY spectrum of 2 in DMSO- $d_6$  (600 MHz).



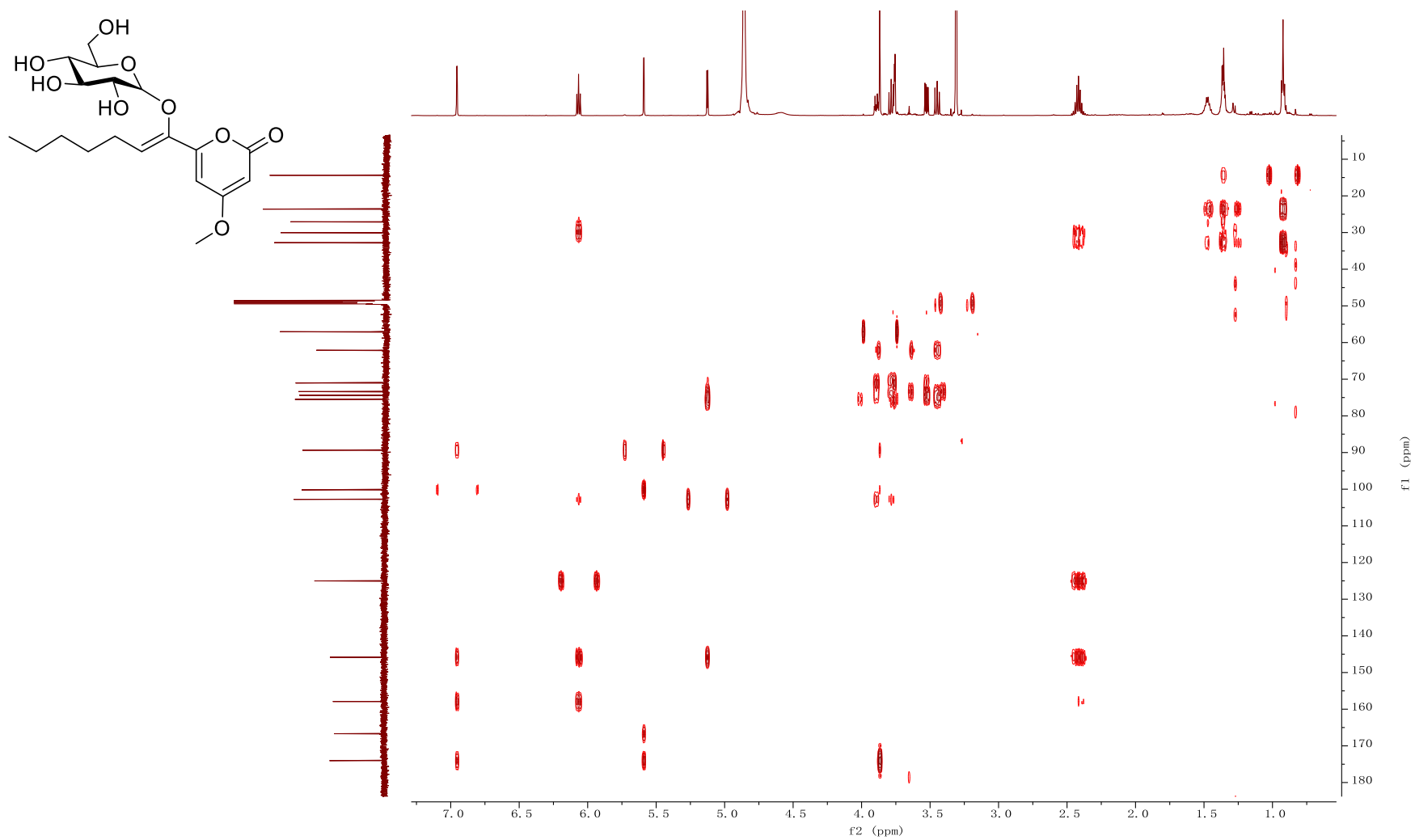
**Fig. S16** <sup>1</sup>H NMR spectrum of **2** in methanol-*d*<sub>4</sub> (600 MHz).



**Fig. S17**  $^{13}\text{C}$  NMR spectrum of **2** in methanol-*d*<sub>4</sub> (150 MHz).

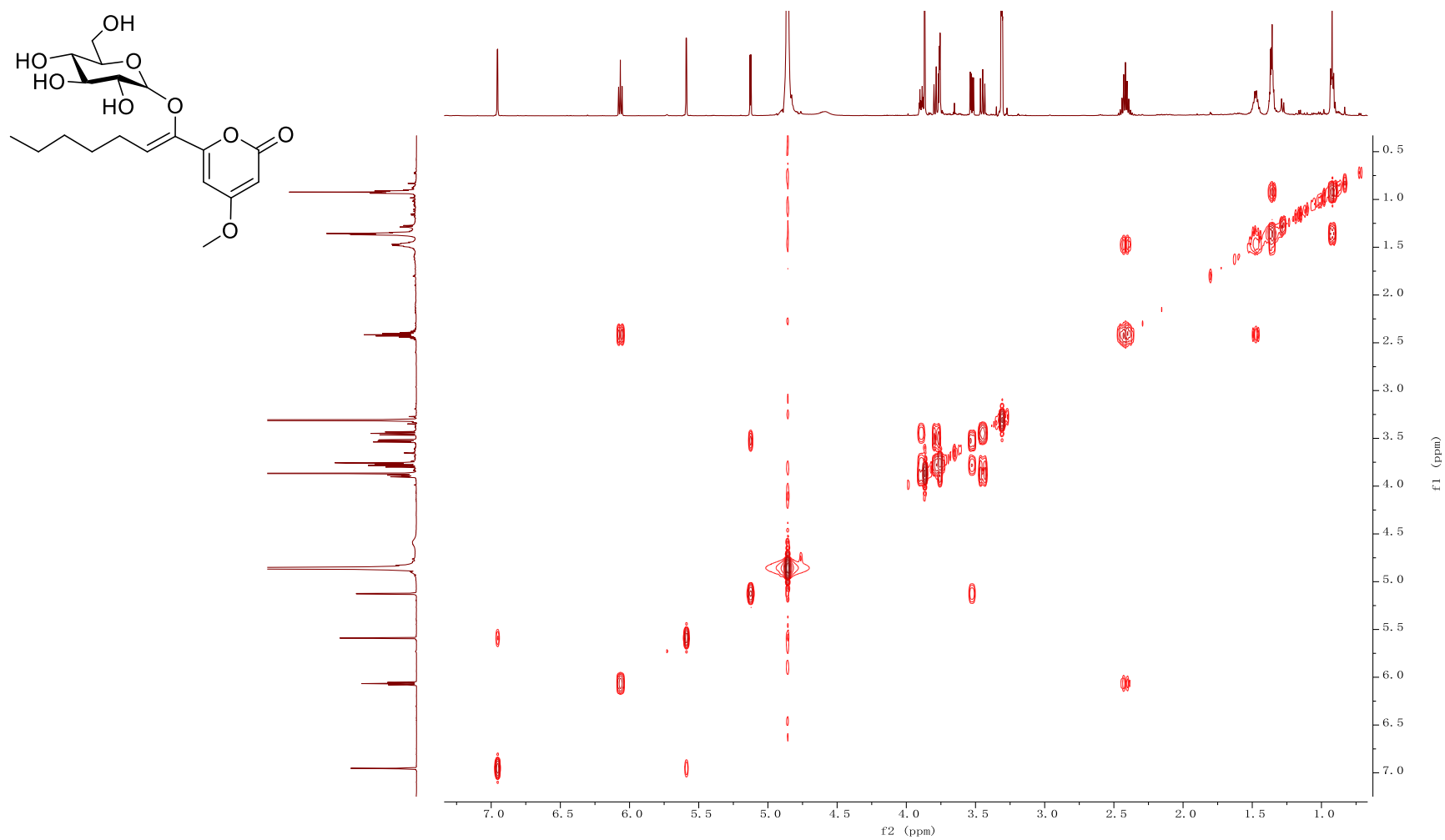


**Fig. S18** HSQC spectrum of **2** in methanol- $d_4$  (600 MHz).

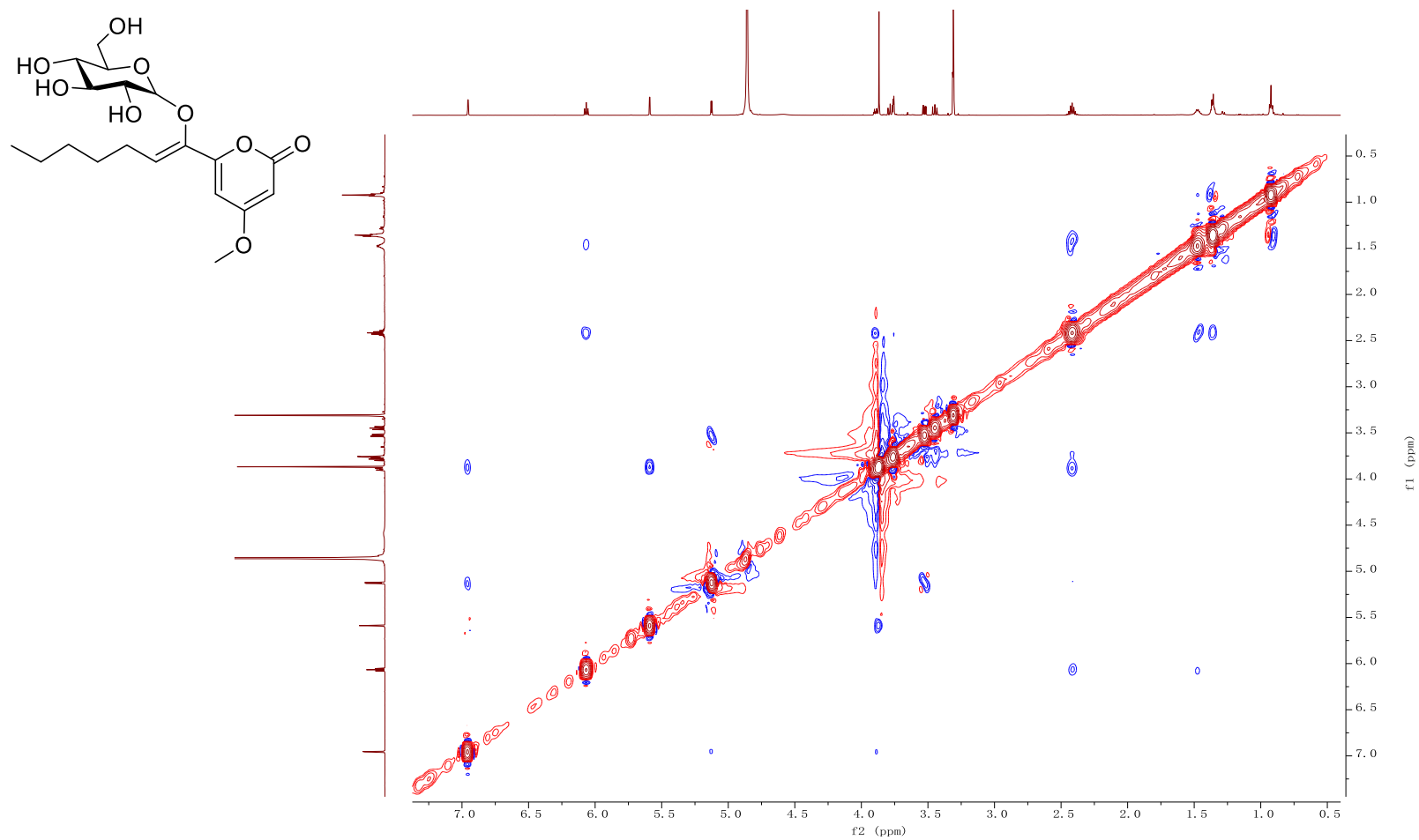


**Fig. S19** HMBC spectrum of **2** in methanol- $d_4$  (600 MHz).

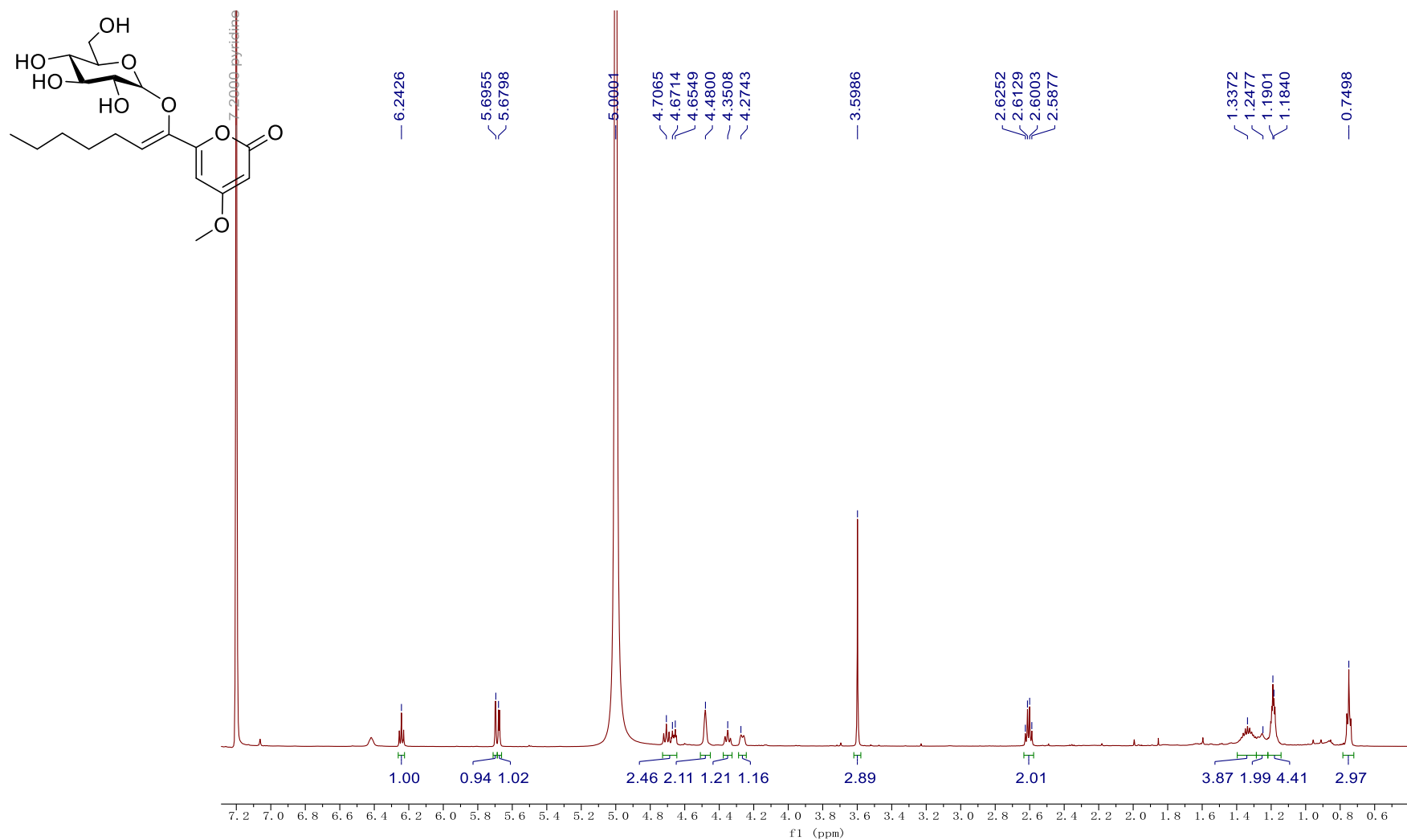




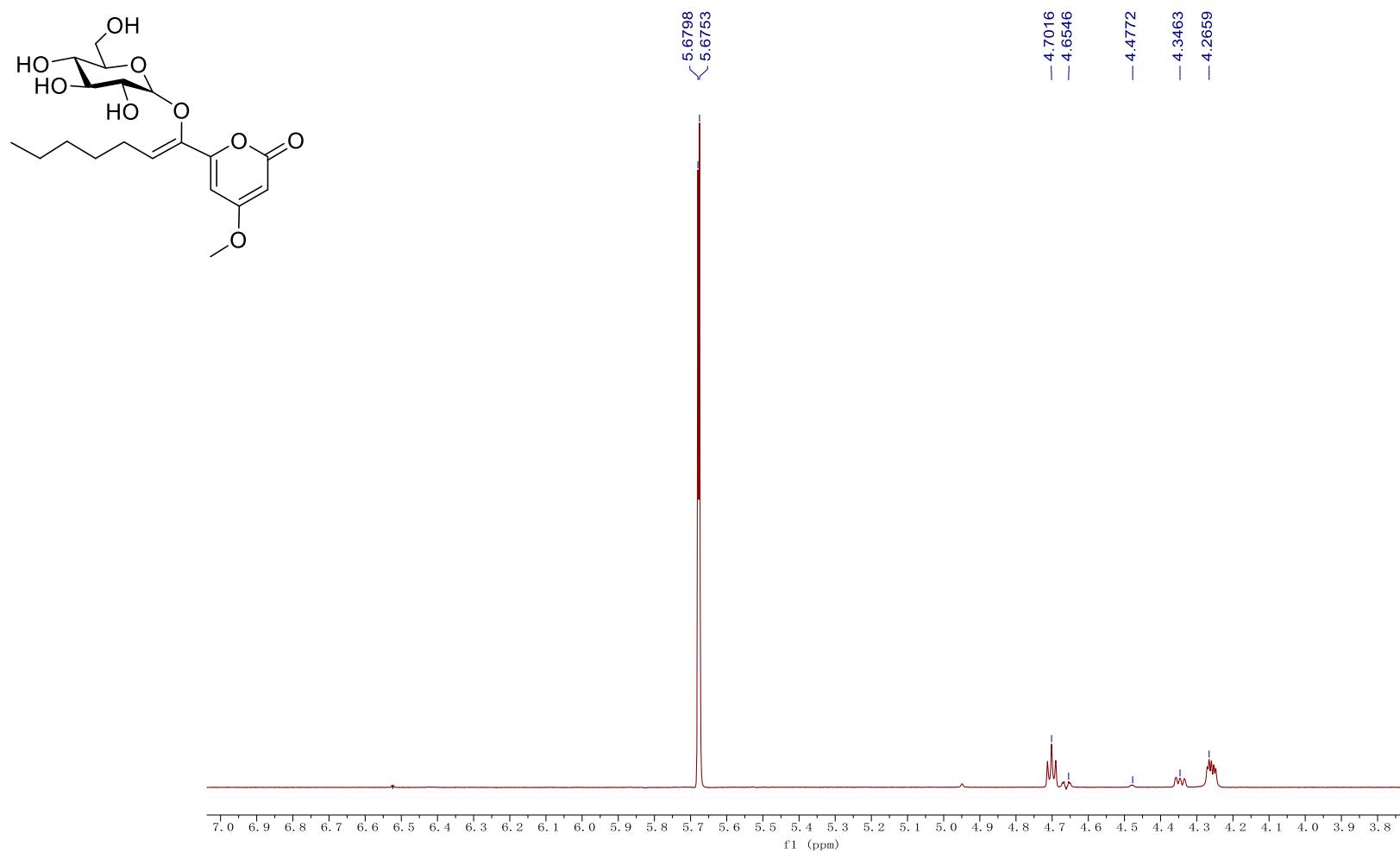
**Fig. S20**  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of **2** in methanol- $d_4$  (600 MHz).



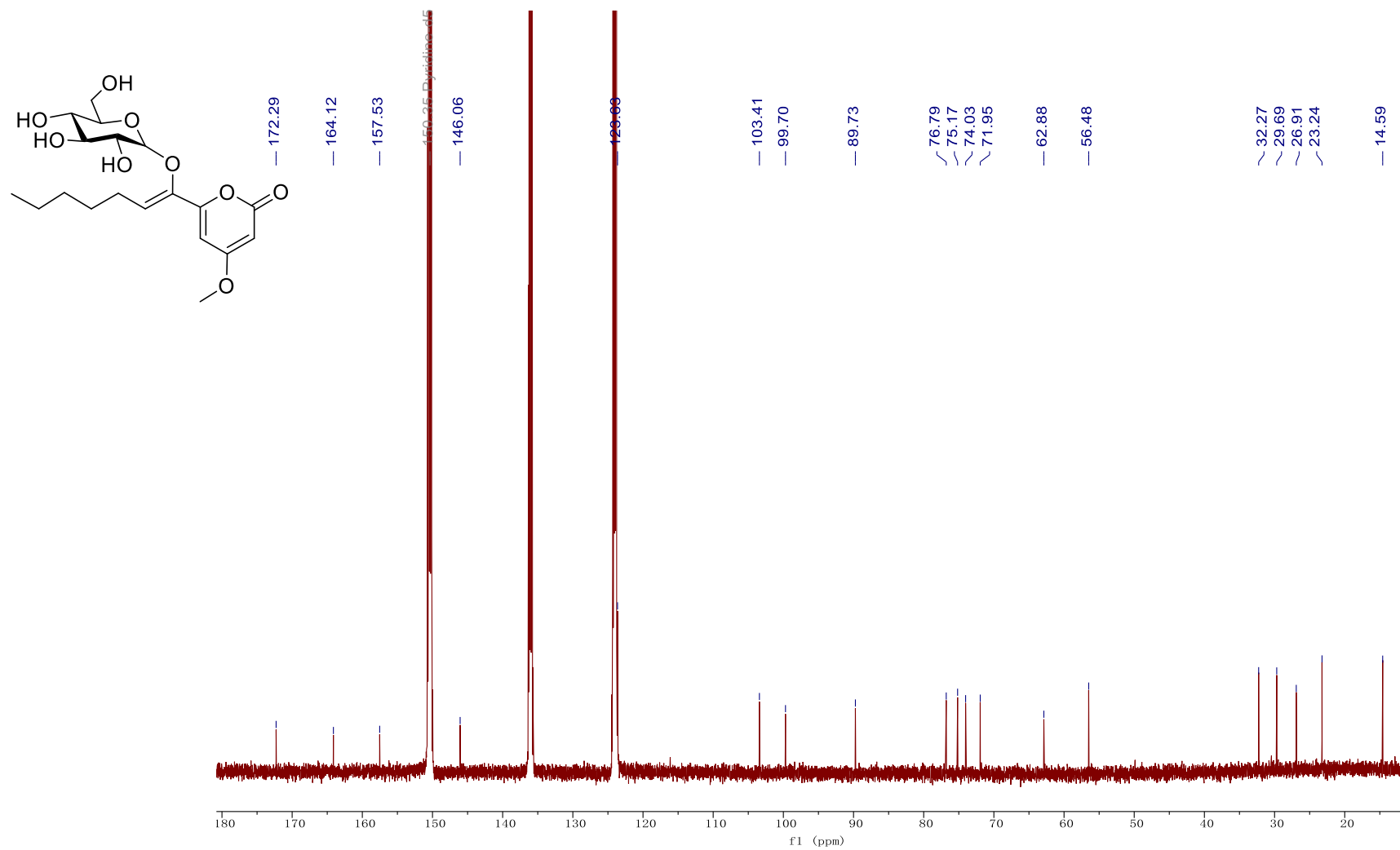
**Fig. S21** ROESY spectrum of **2** in methanol-*d*<sub>4</sub> (600 MHz).



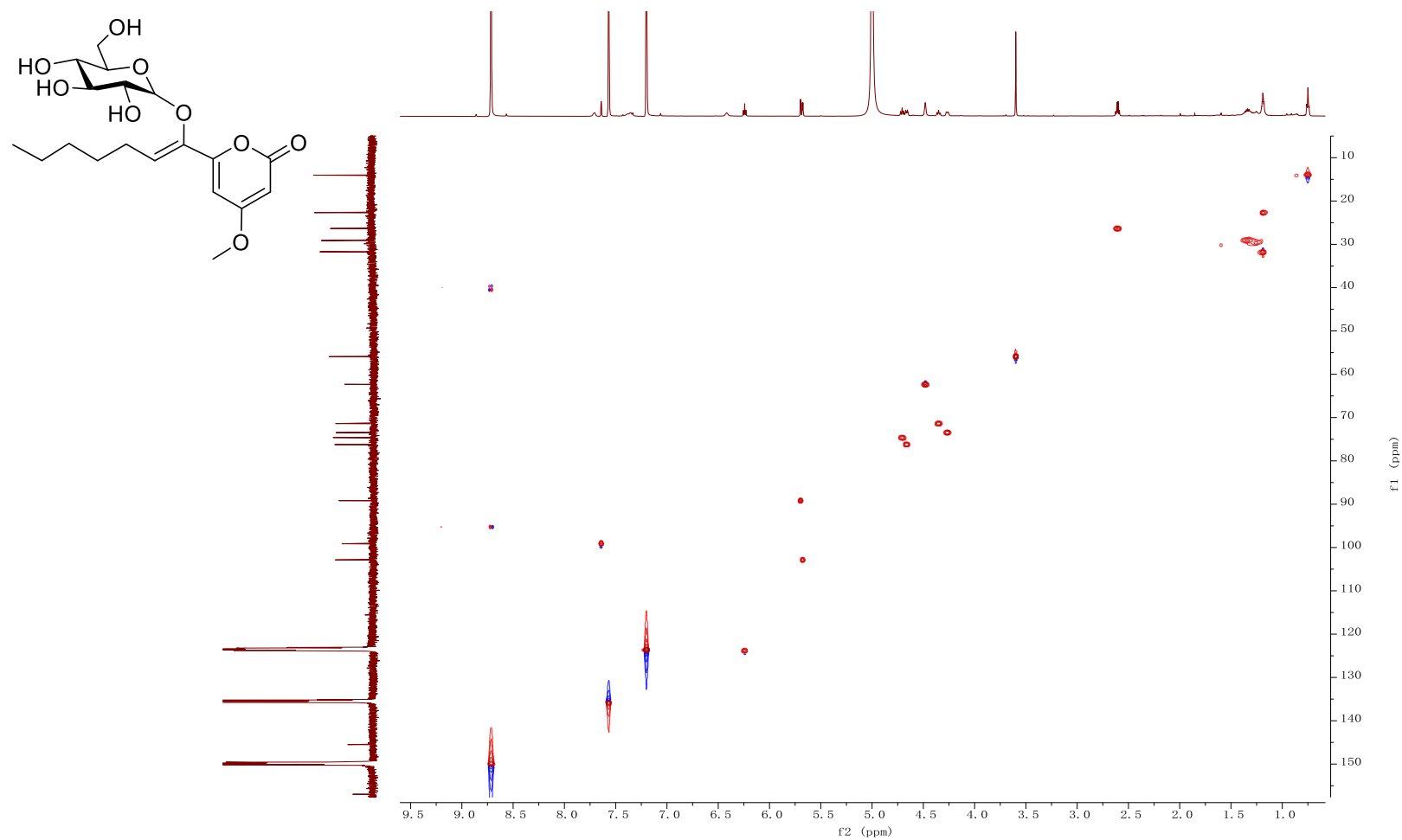
**Fig. S22**  $^1\text{H}$  NMR spectrum of **2** in  $\text{pyridine-}d_5$  (600 MHz).



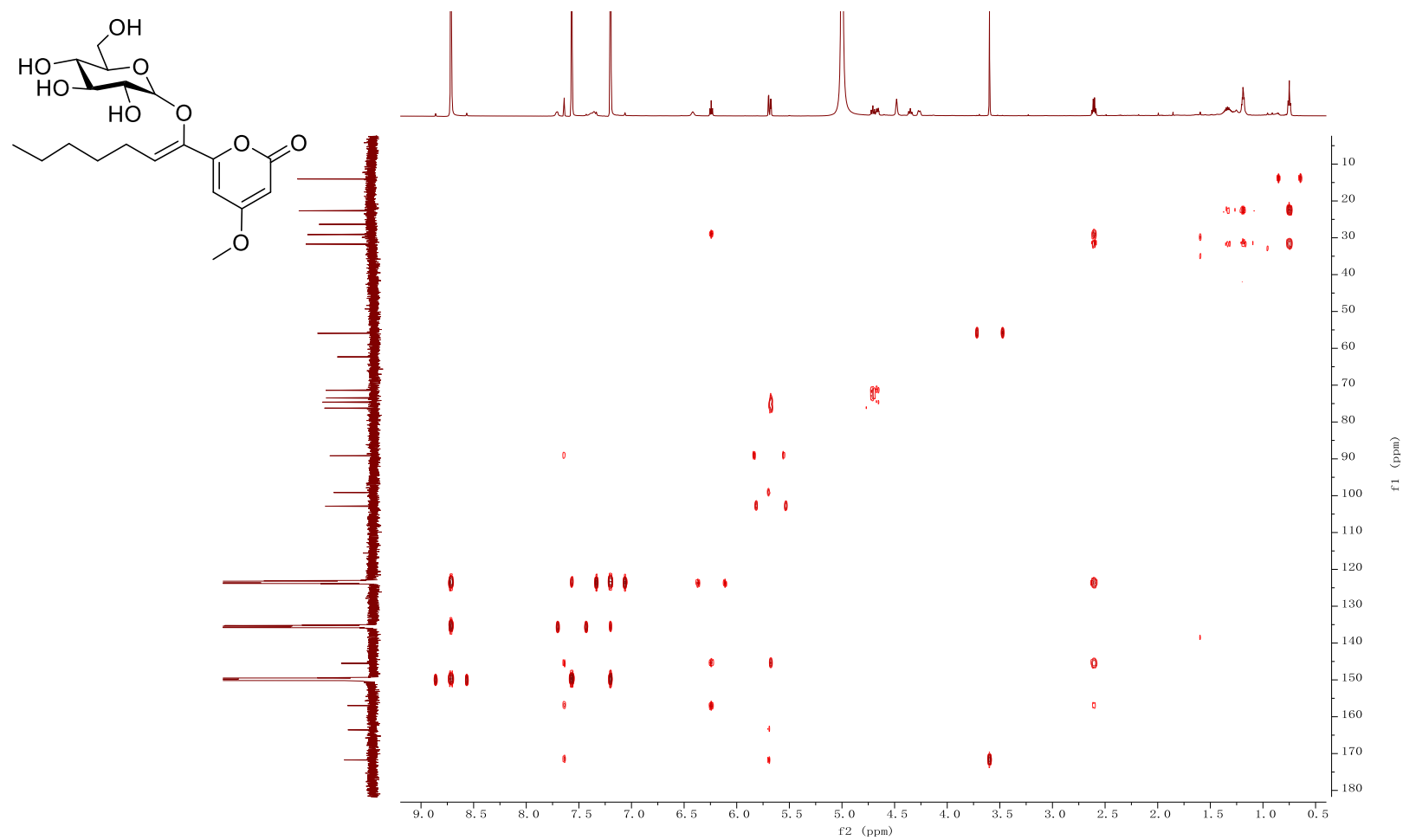
**Fig. S23** 1D-TOCSY spectrum of **2** in pyridine- $d_5$  (800 MHz).



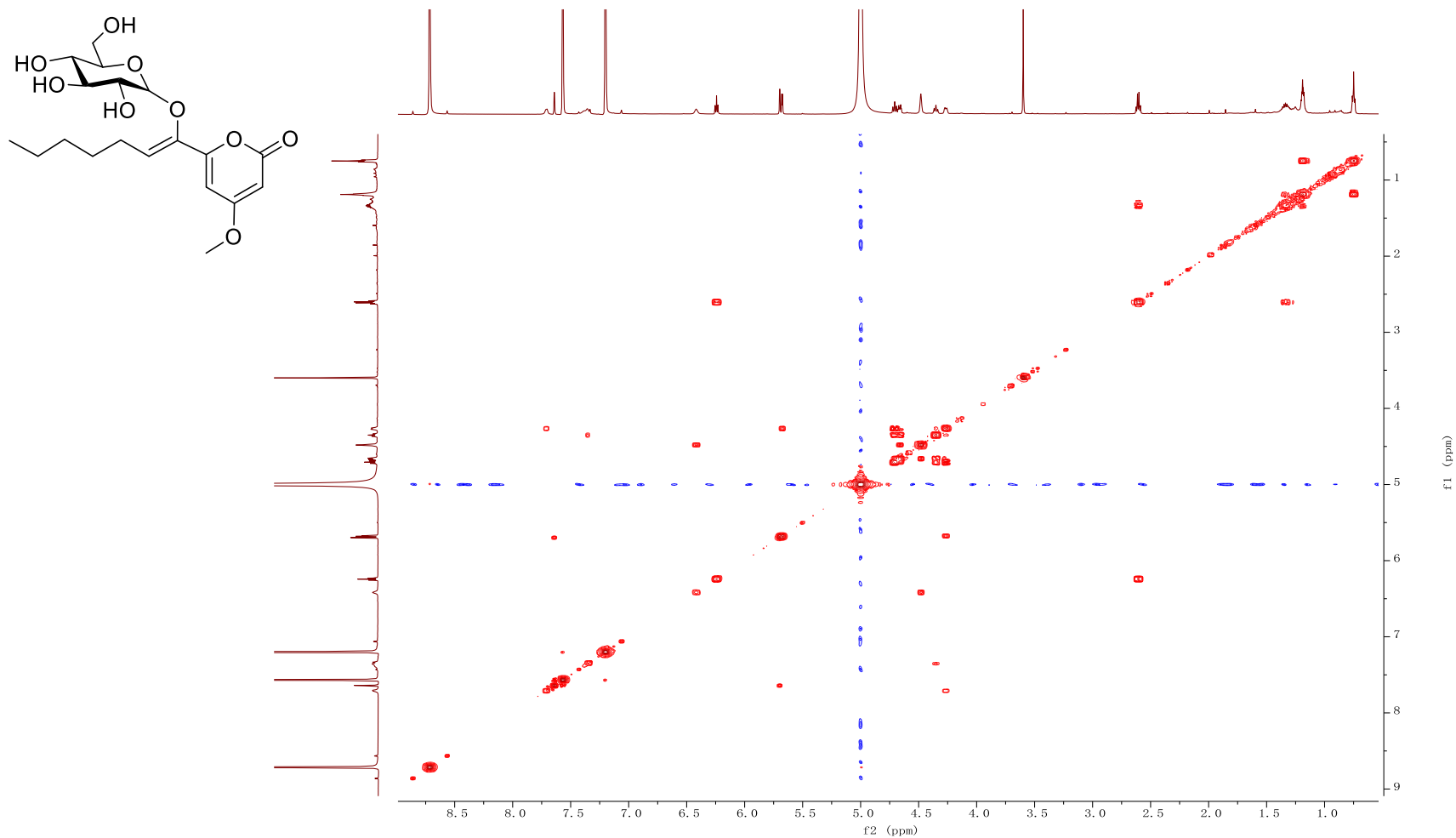
**Fig. S24**  $^{13}\text{C}$  NMR spectrum of **2** in pyridine- $d_5$  (150 MHz).



**Fig. S25** HSQC spectrum of **2** in pyridine- $d_5$  (600 MHz).



**Fig. S26** HMBC spectrum of **2** in pyridine-*d*<sub>5</sub> (600 MHz).



**Fig. S27**  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of **2** in  $\text{pyridine-}d_5$  (600 MHz).



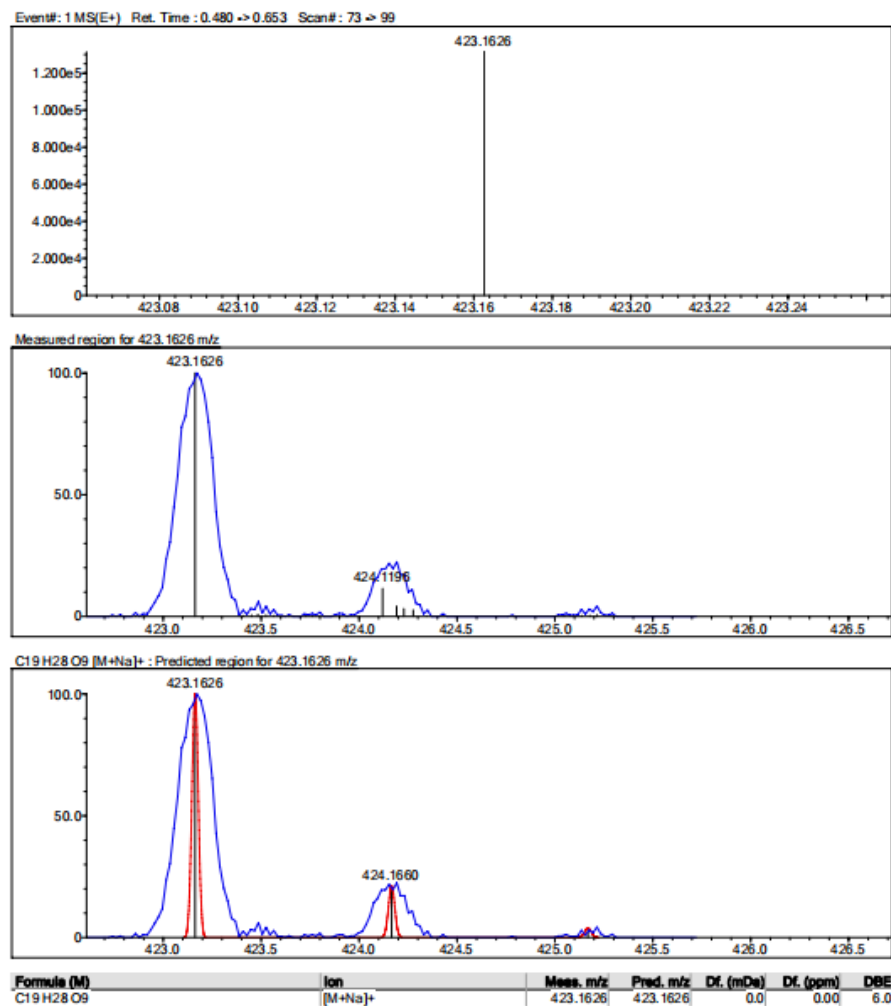
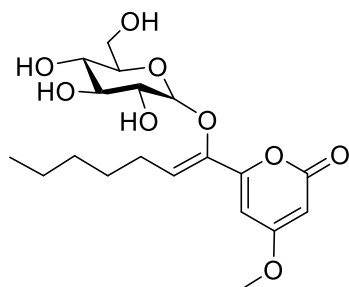


Fig. S28 HRESIMS spectrum of 2.

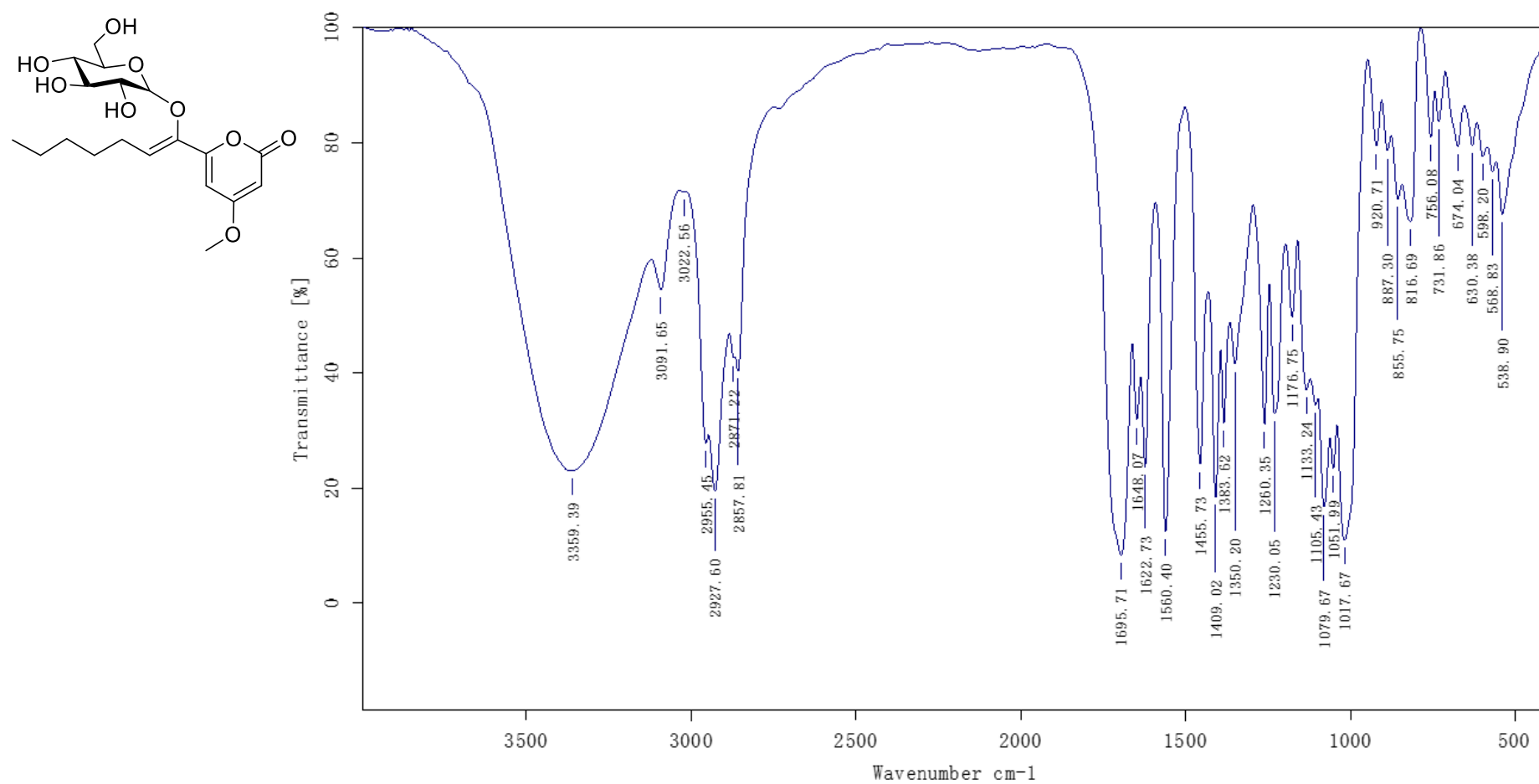
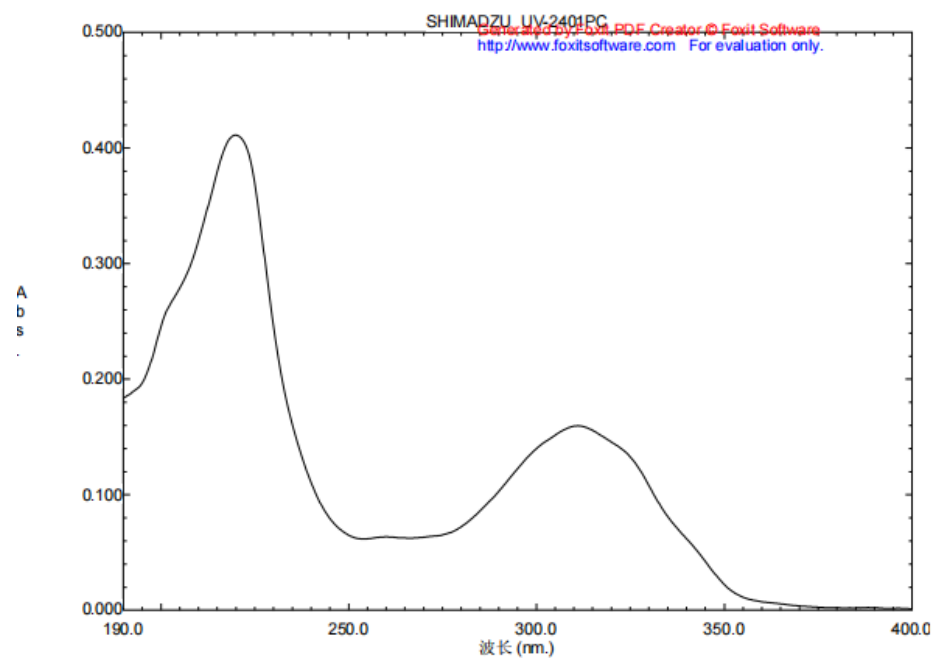
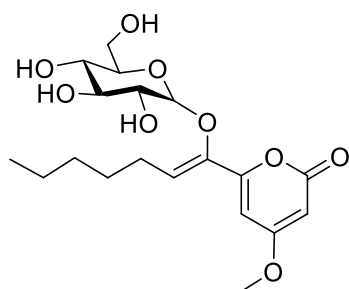
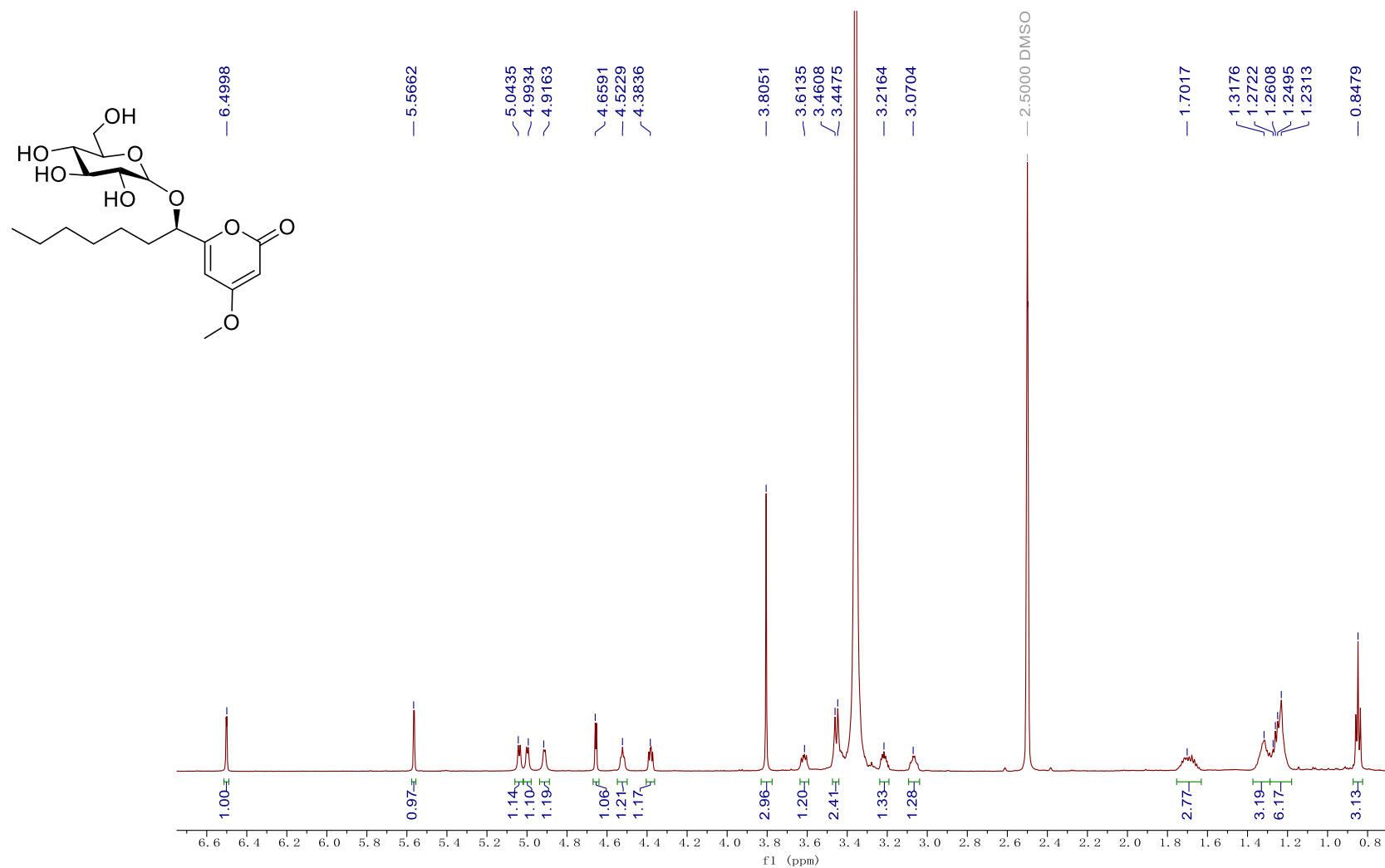


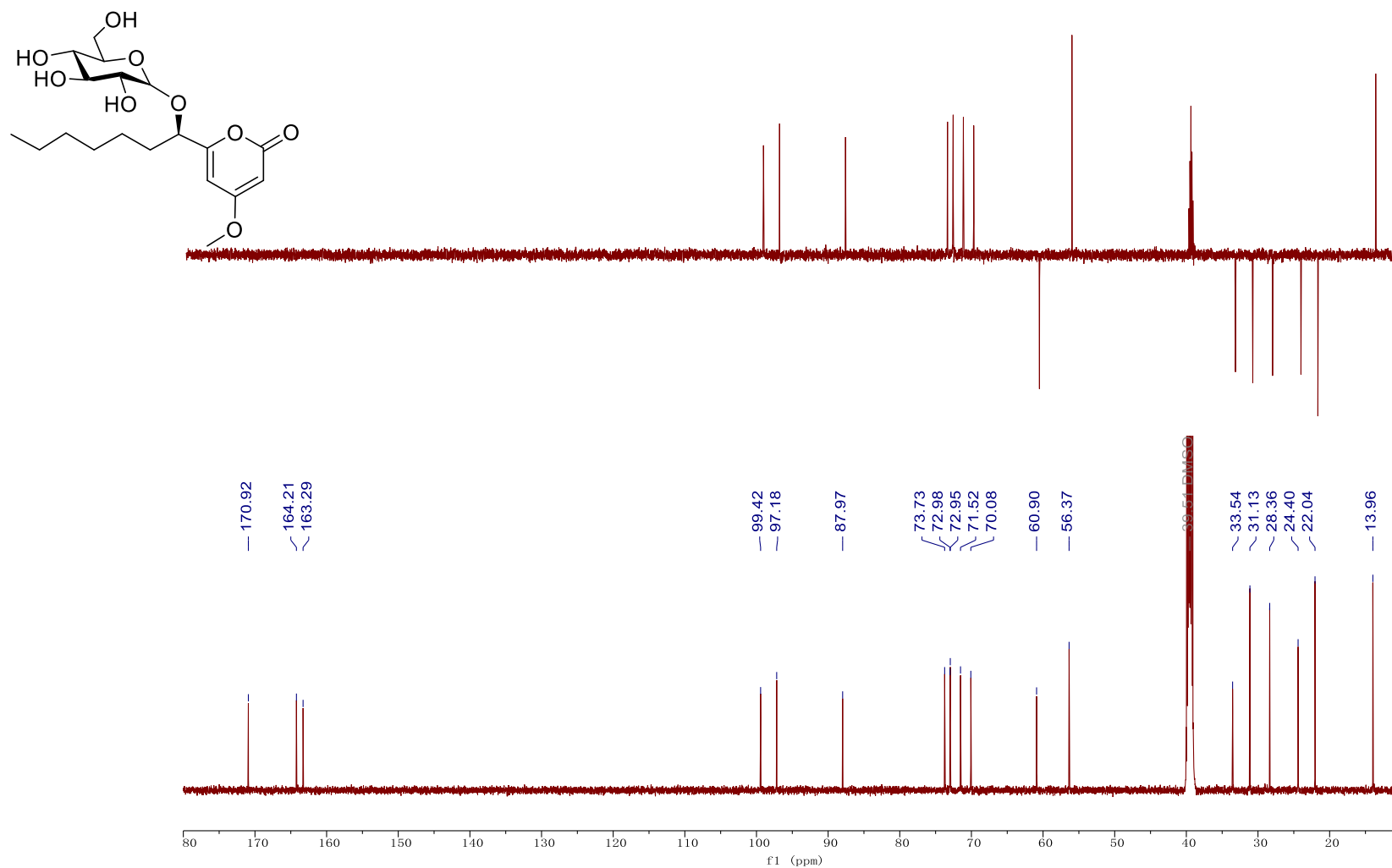
Fig. S29 IR spectrum of 2.



**Fig. S30** UV spectrum of **2**.



**Fig. S31** <sup>1</sup>H NMR spectrum of **3** in DMSO-*d*<sub>6</sub> (600 MHz).



**Fig. S32** <sup>13</sup>C NMR spectrum of **3** in DMSO-*d*<sub>6</sub> (600 MHz).

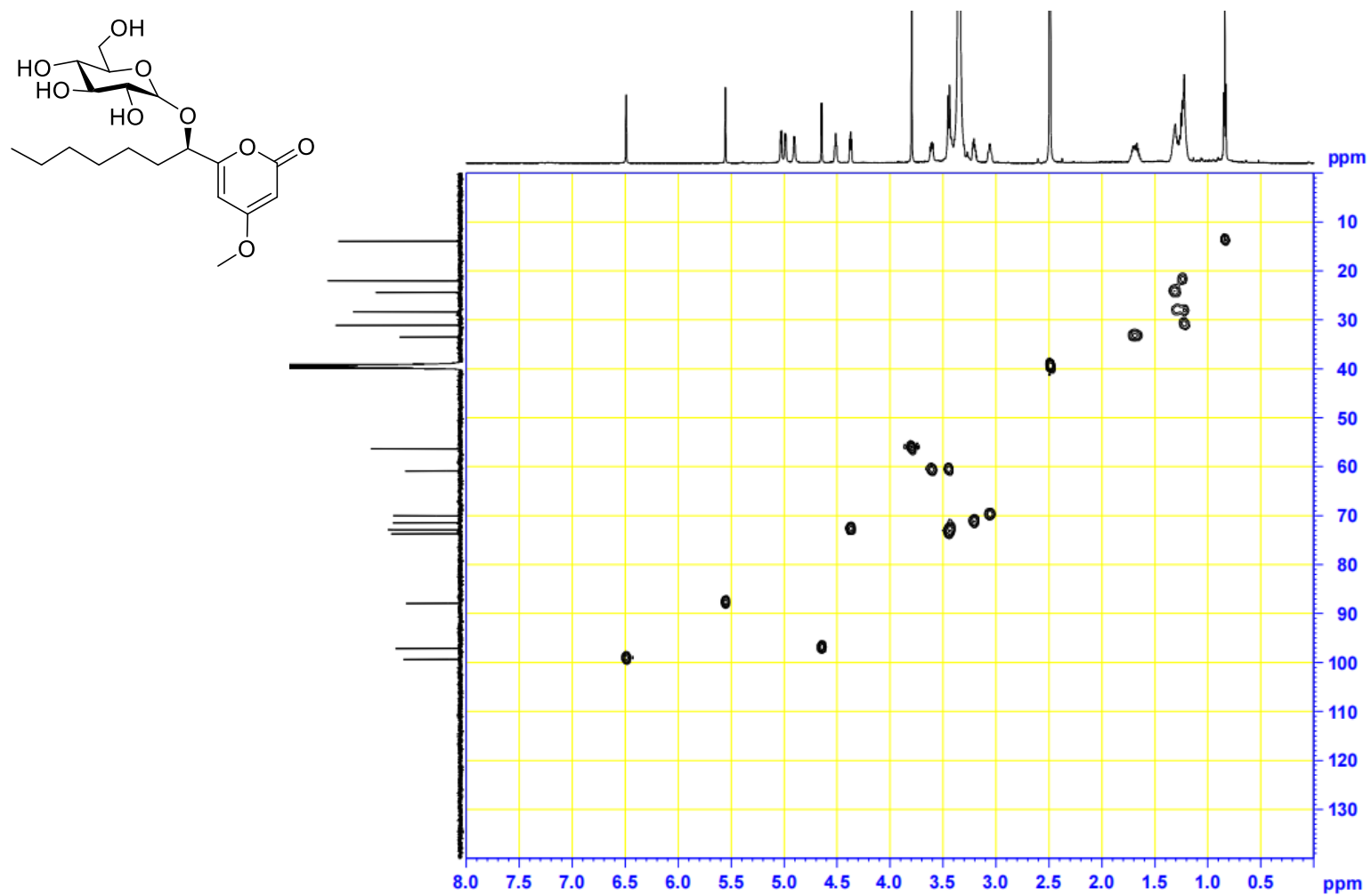


Fig. S33 HSQC spectrum of **3** in  $\text{DMSO}-d_6$  (600 MHz).

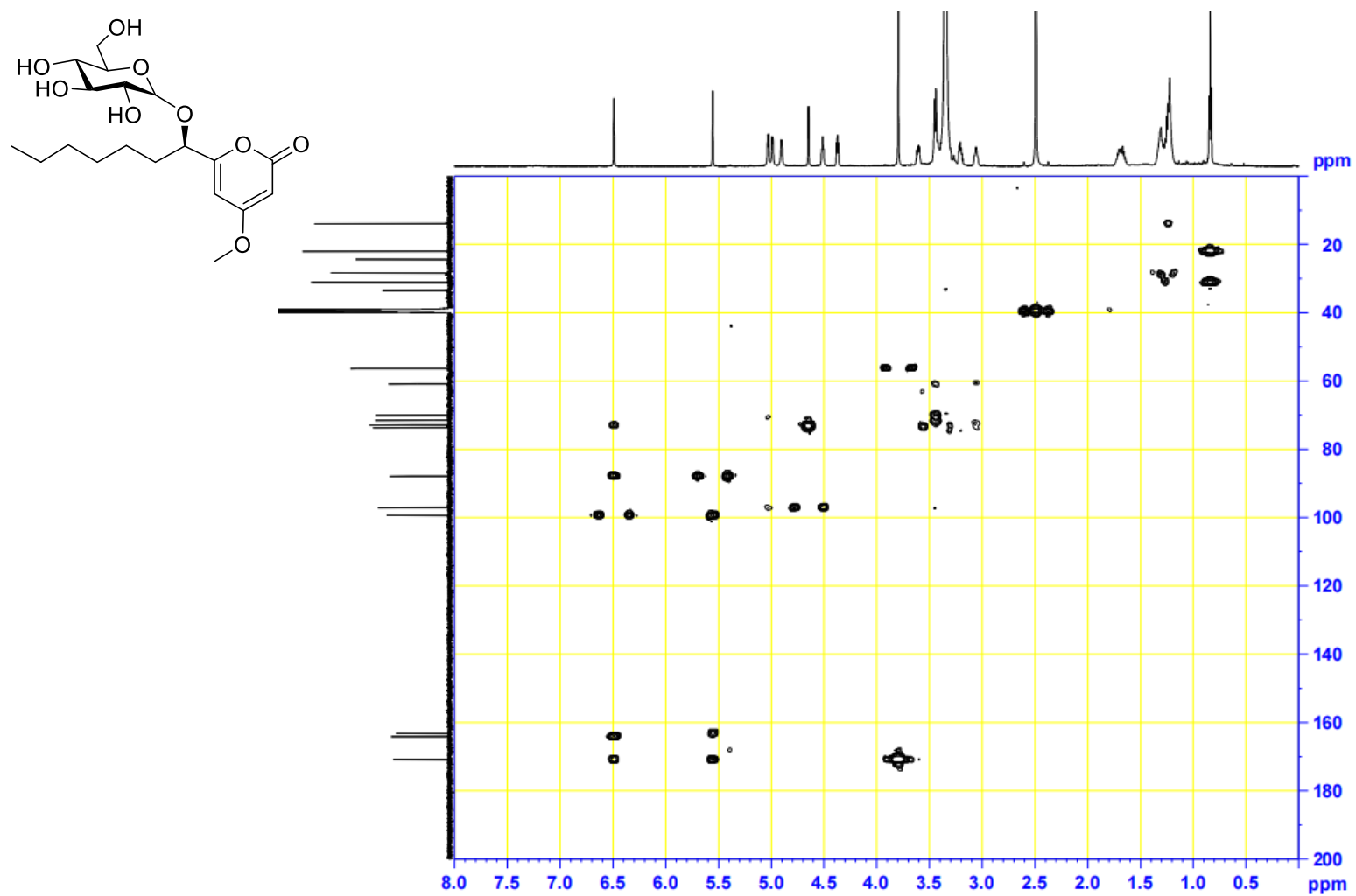


Fig. S34 HMBC spectrum of **3** in DMSO- $d_6$  (600 MHz).

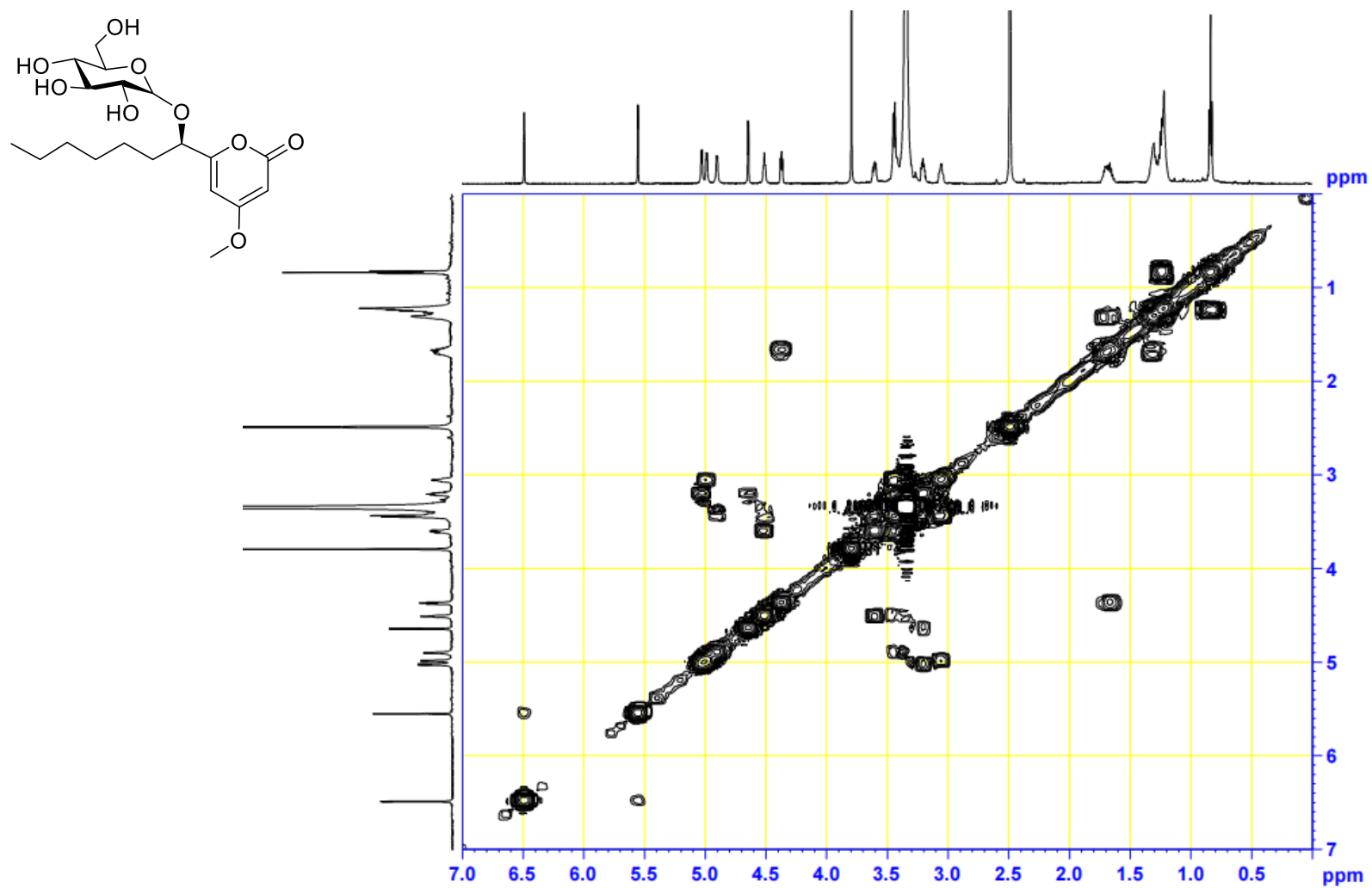
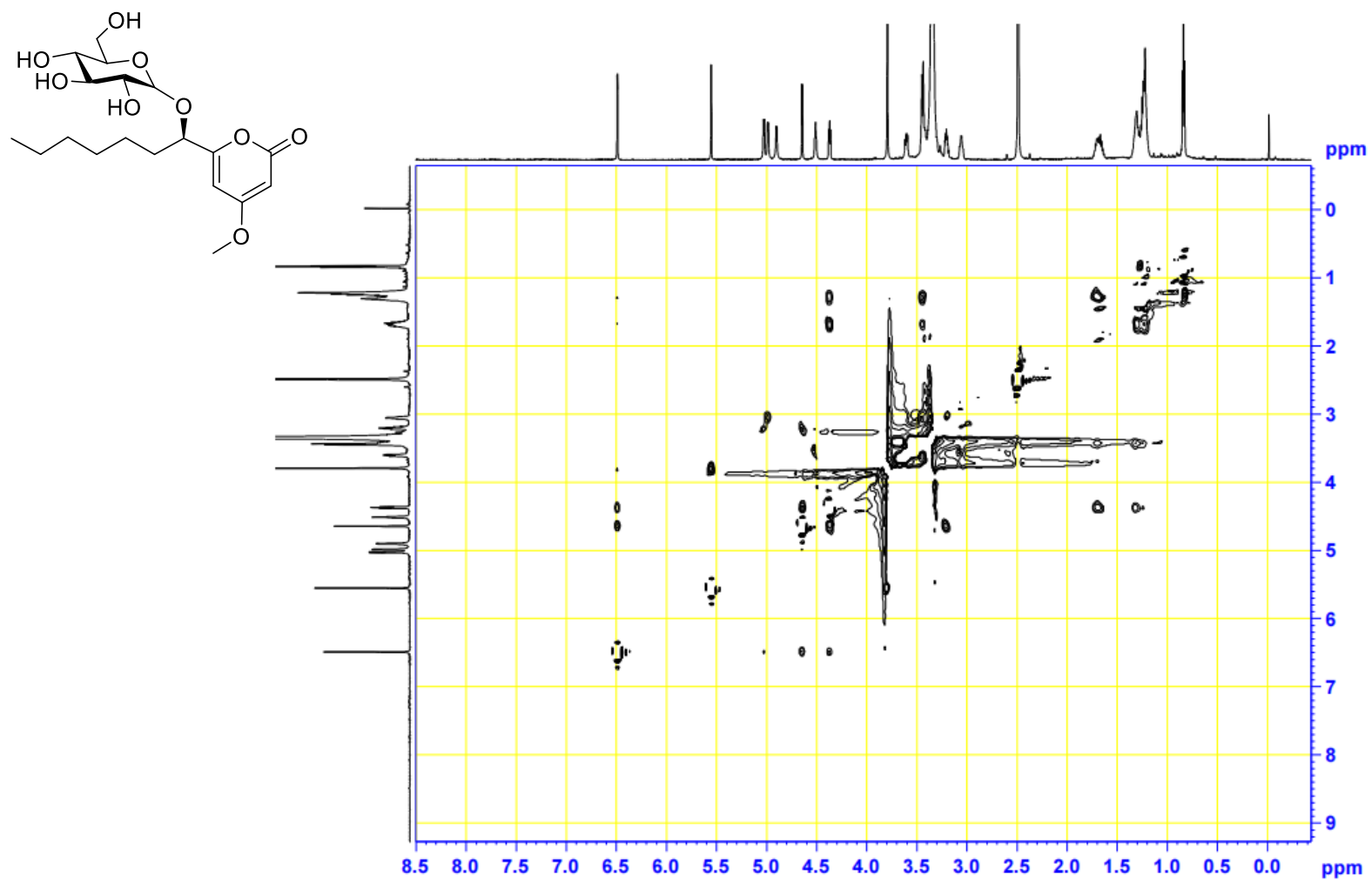
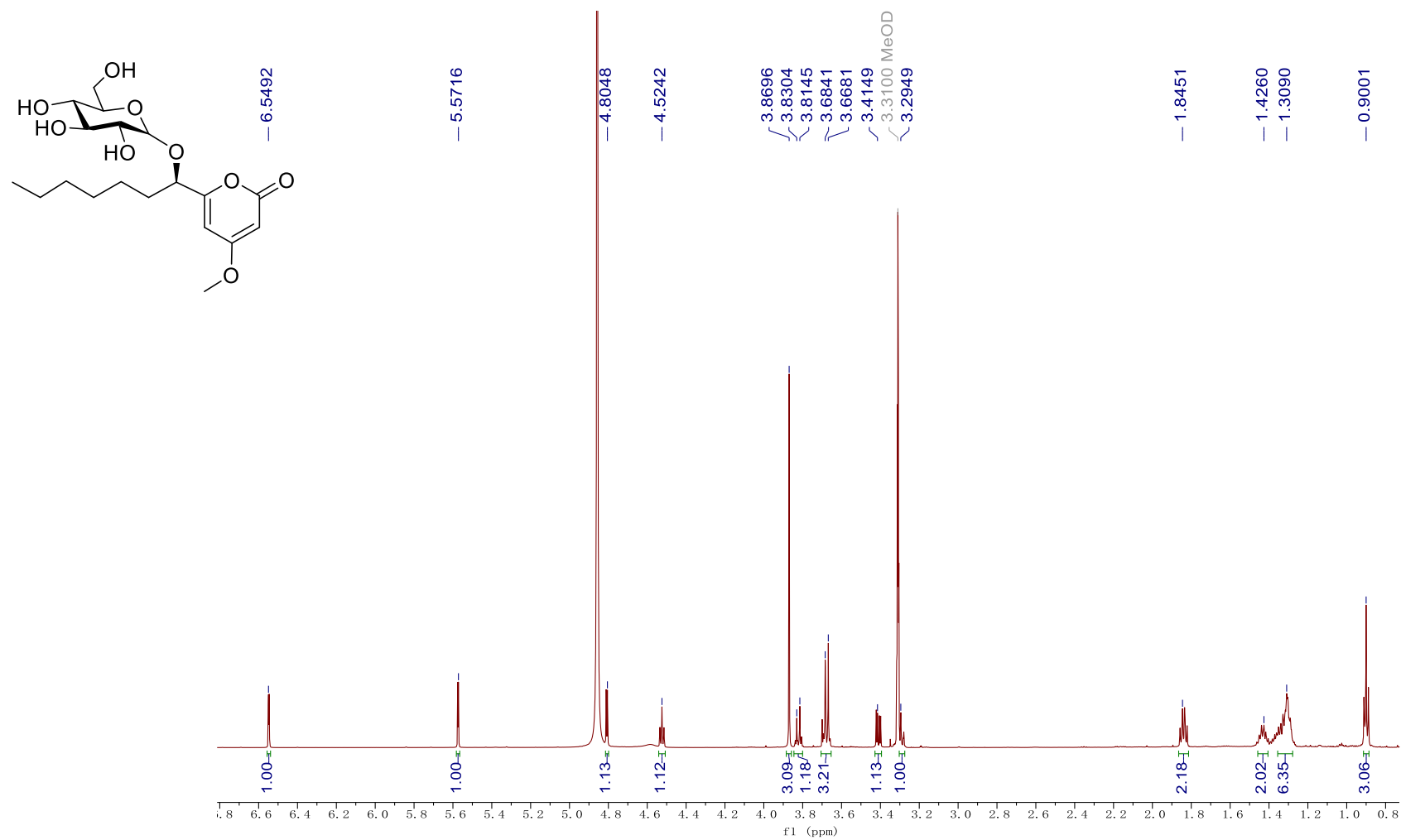


Fig. S35  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of **3** in  $\text{DMSO}-d_6$  (600 MHz).

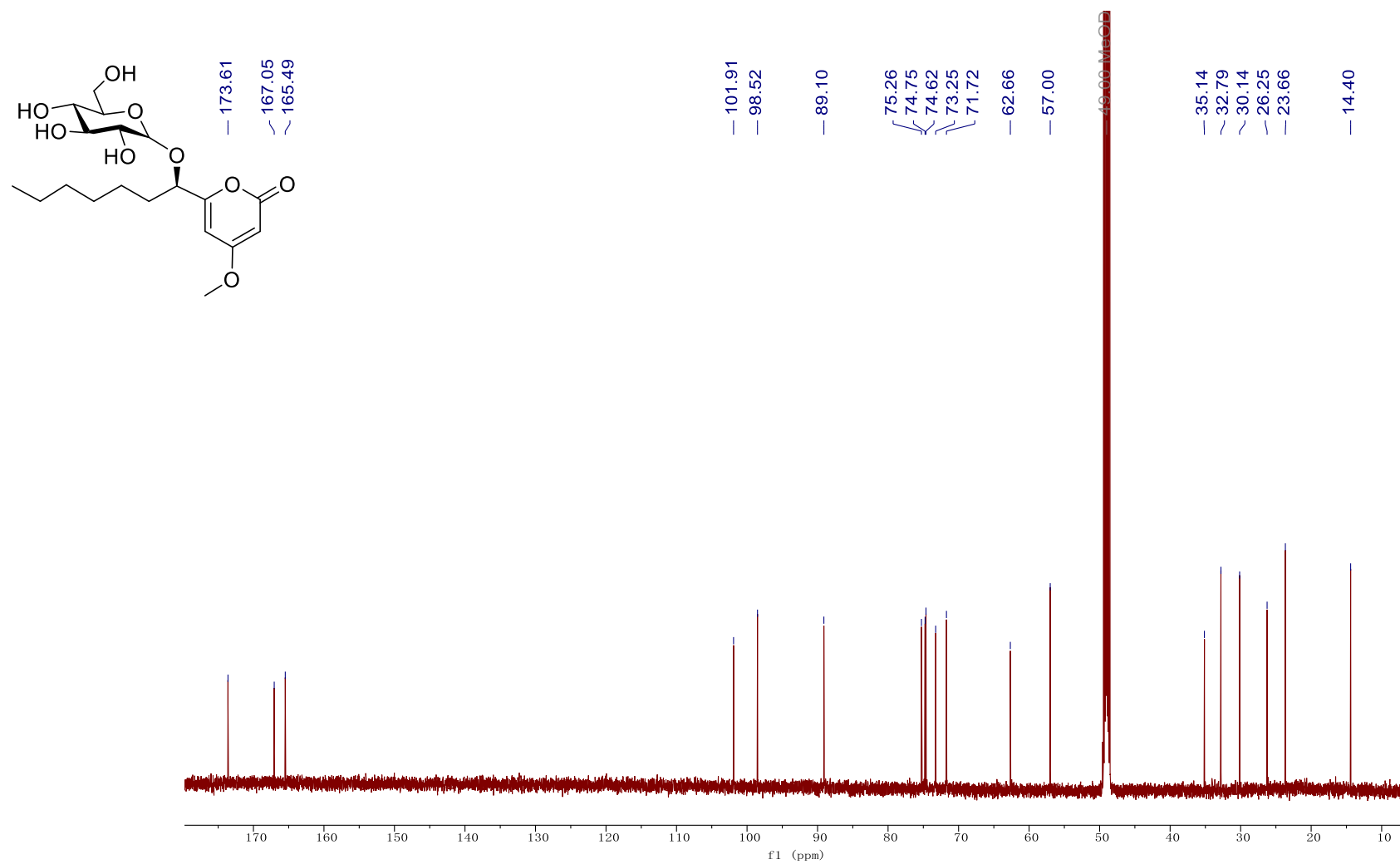




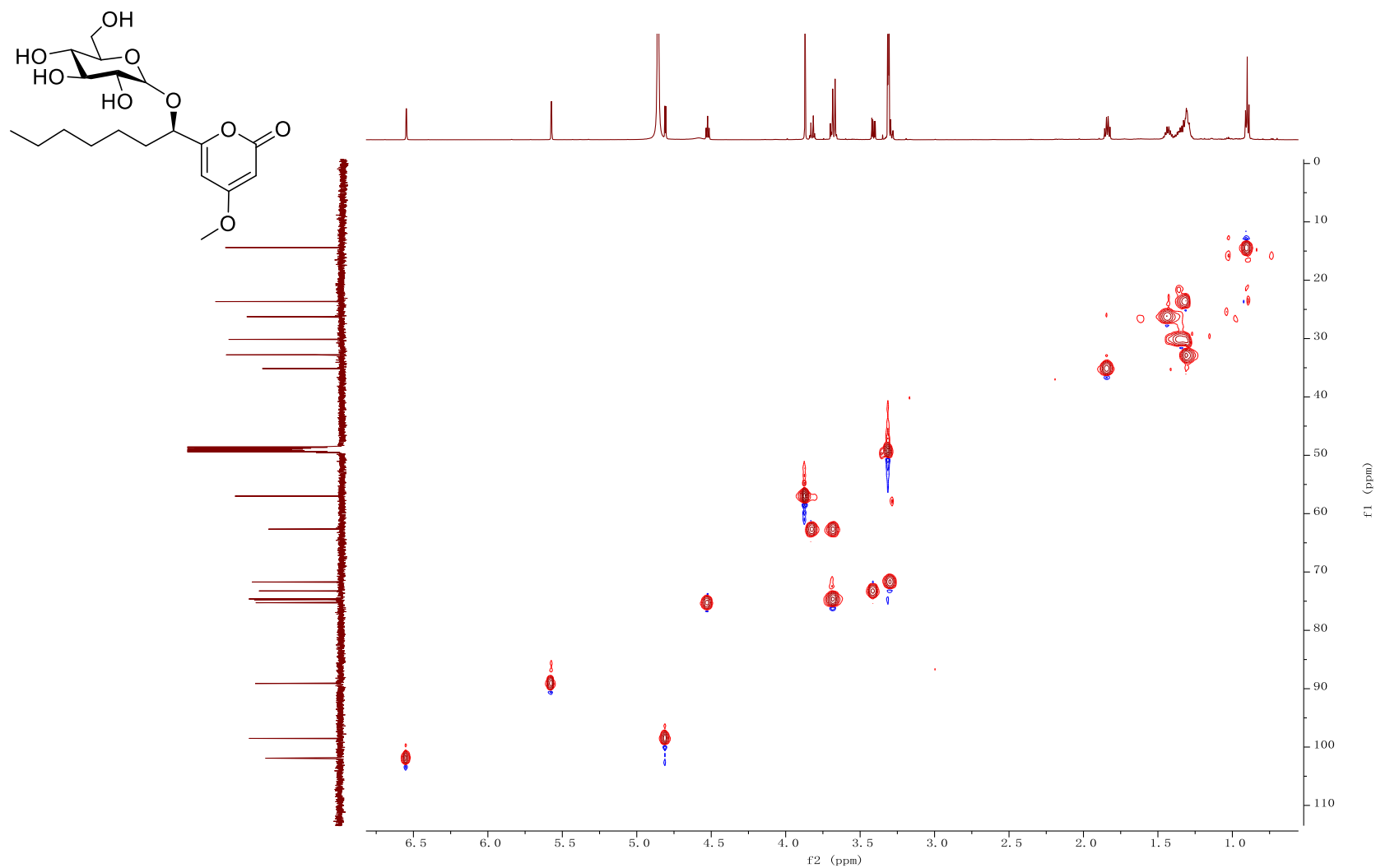
**Fig. S36** ROESY spectrum of **3** in DMSO-*d*<sub>6</sub> (600 MHz).



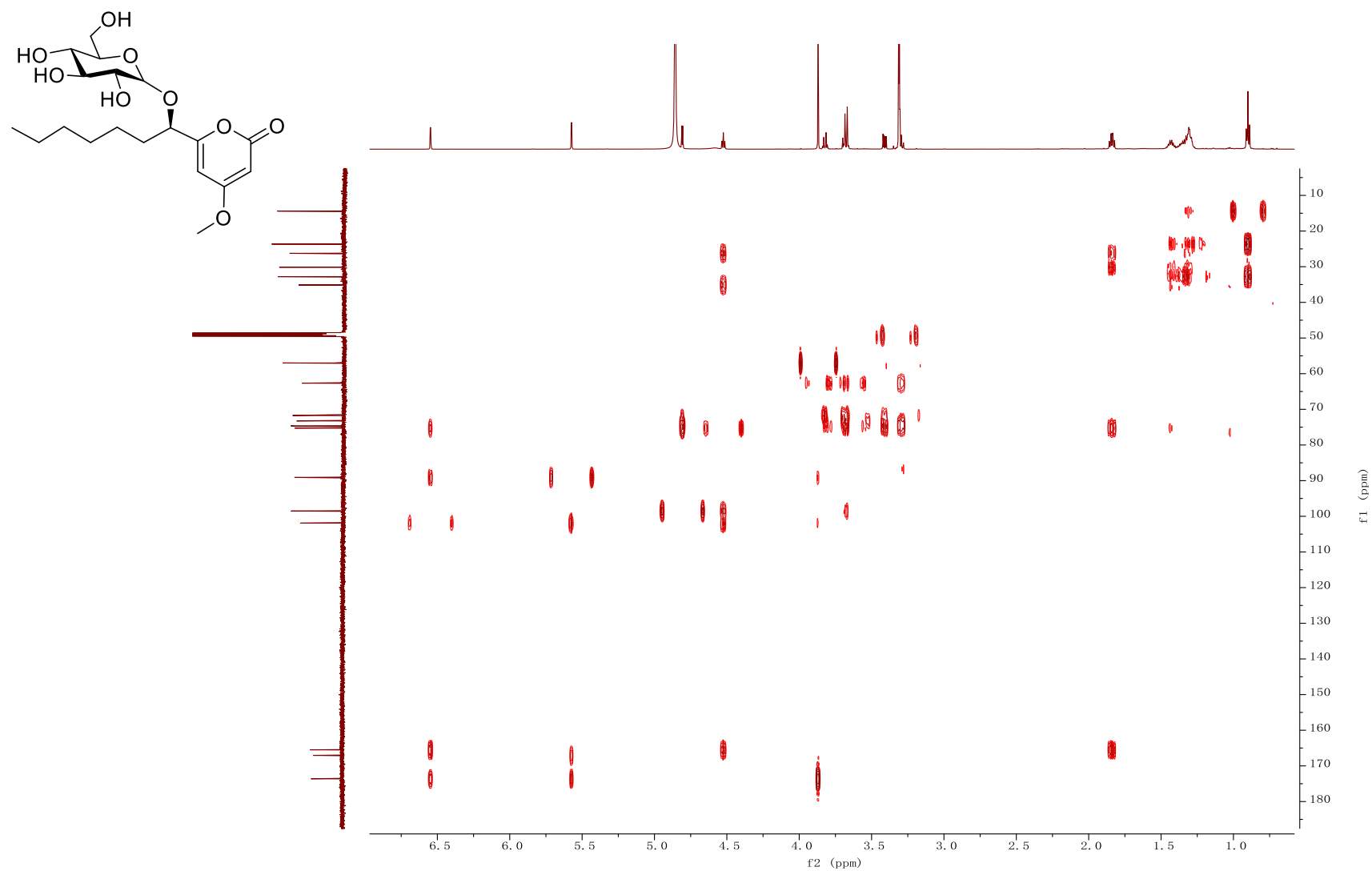
**Fig. S37**  $^1\text{H}$  NMR Spectrum of **3** in methanol- $d_4$  (600 MHz)



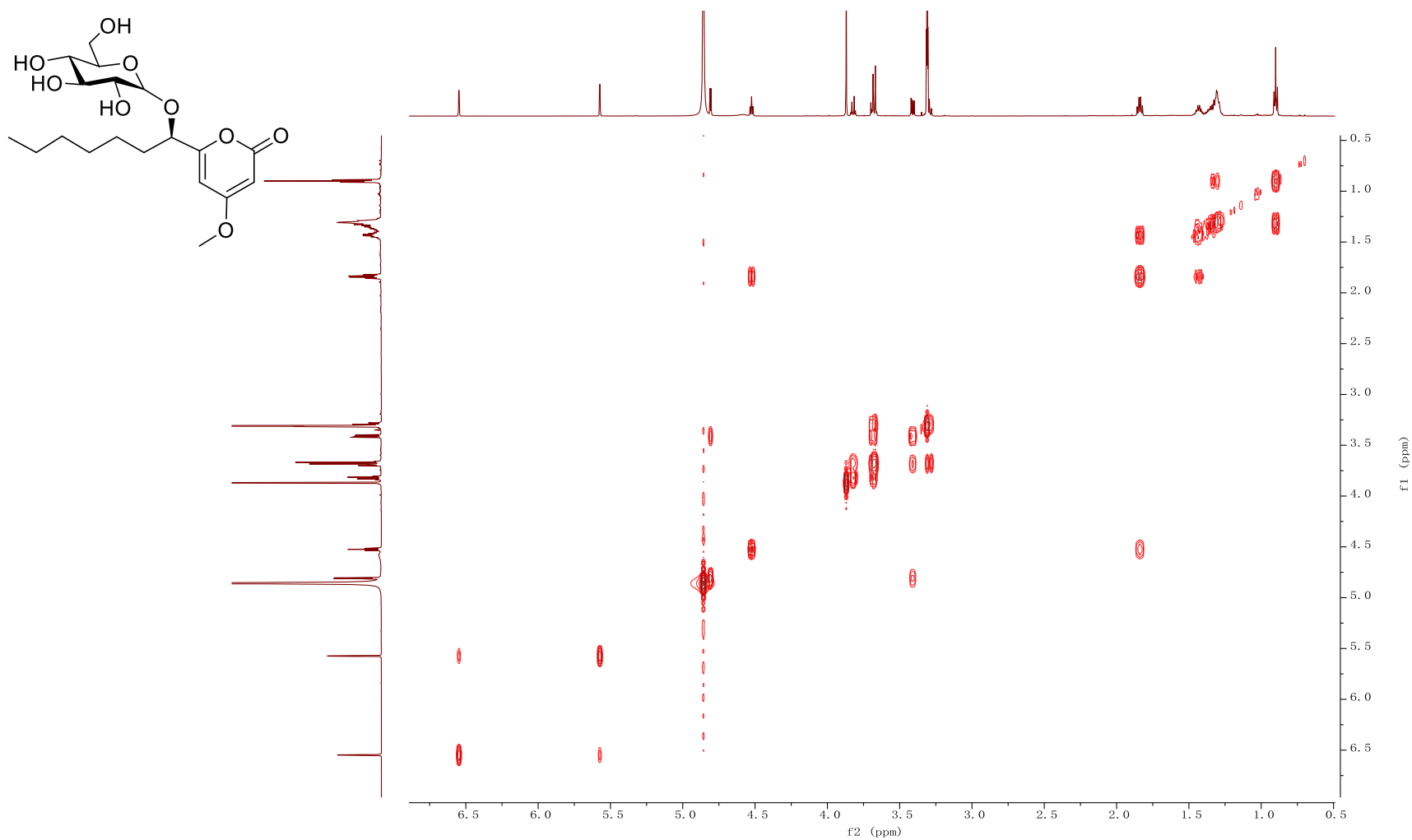
**Fig. S38**  $^{13}\text{C}$  NMR spectrum of **3** in methanol- $d_4$  (600 MHz).



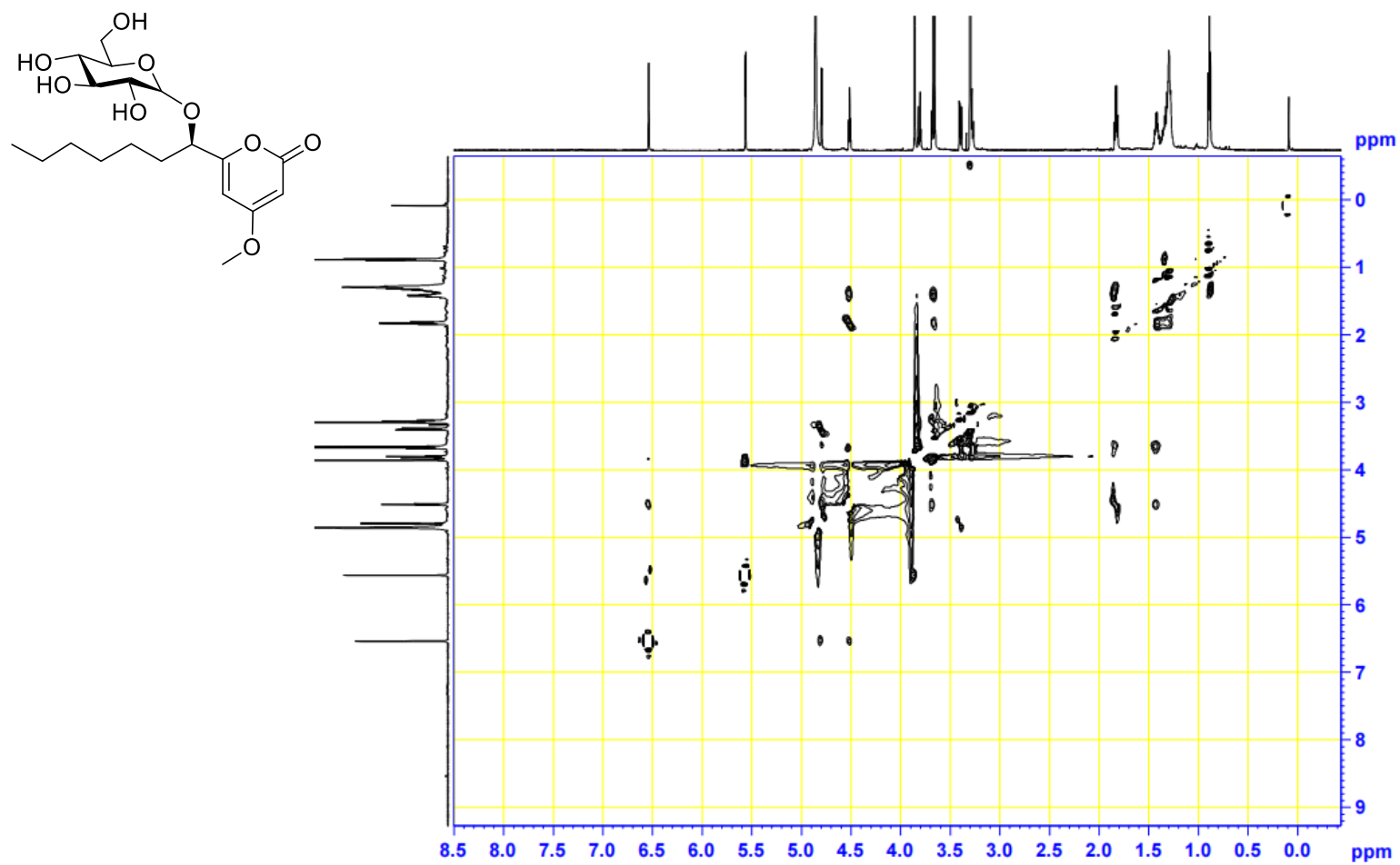
**Fig. S39** HSQC spectrum of **3** in methanol-*d*<sub>4</sub> (600 MHz).



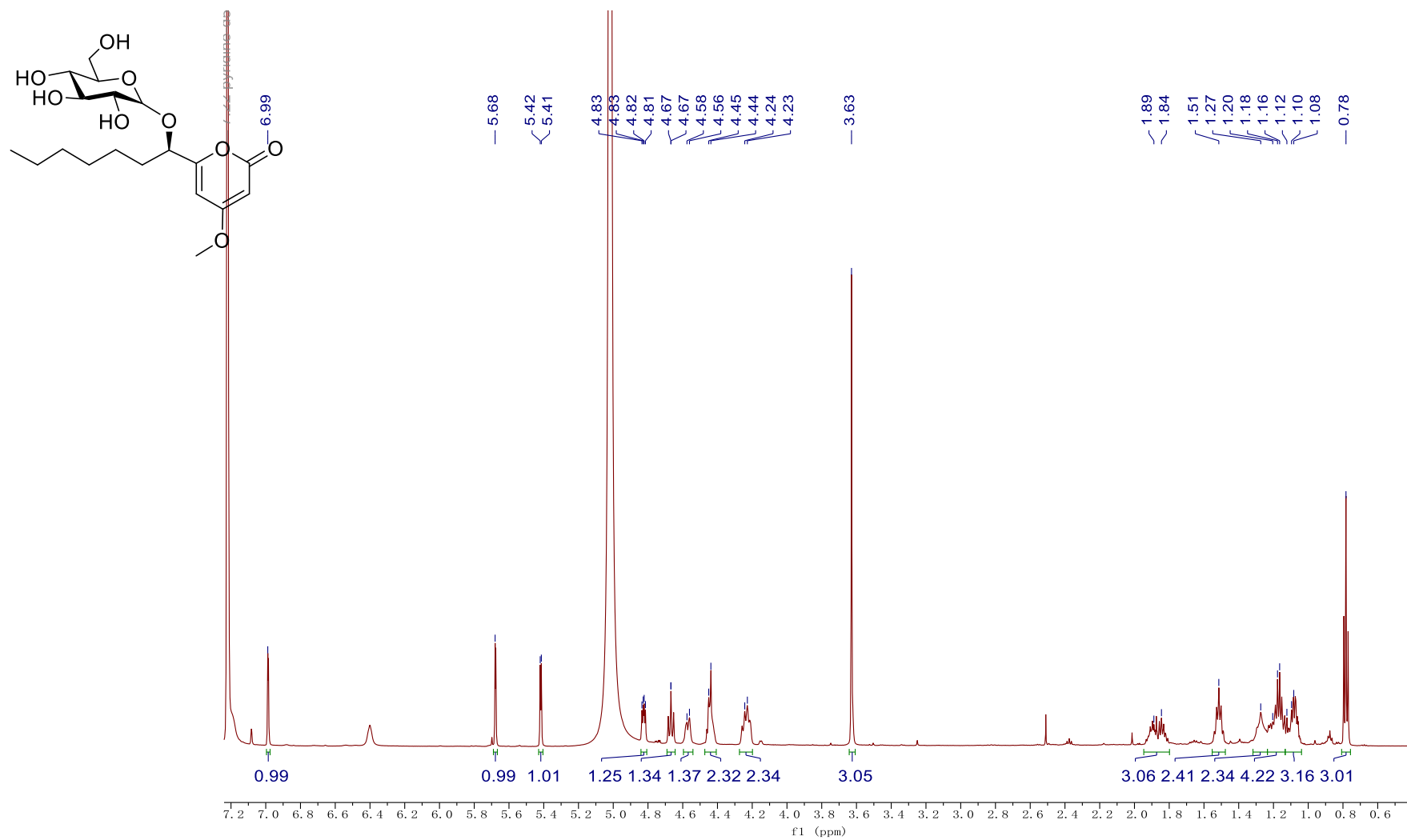
**Fig. S40** HMBC spectrum of **3** in methanol- $d_4$  (600 MHz).



**Fig. S41**  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of **3** in methanol- $d_4$  (600 MHz).

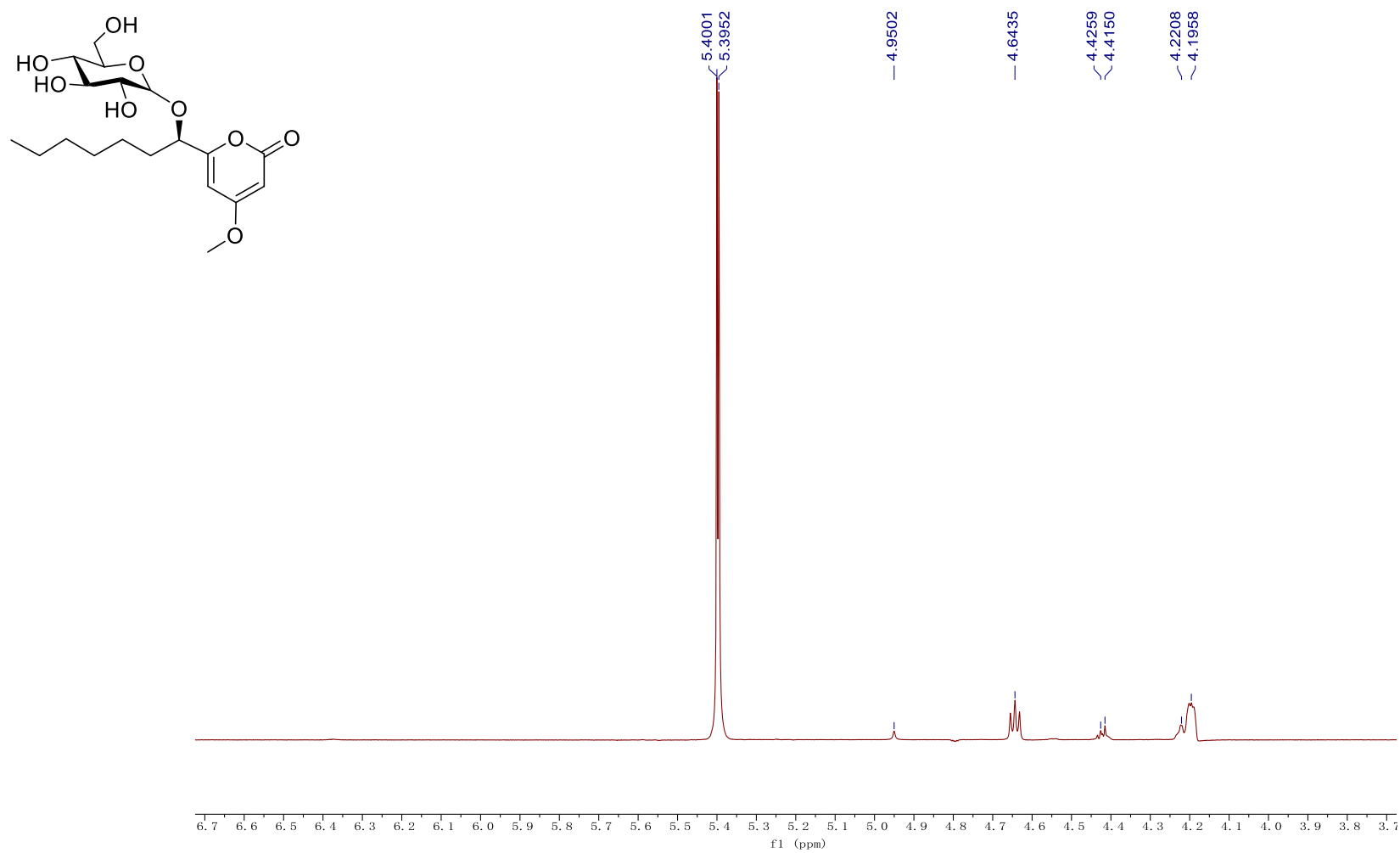


**Fig. S42** ROESY spectrum of **3** in methanol-*d*<sub>4</sub> (600 MHz).

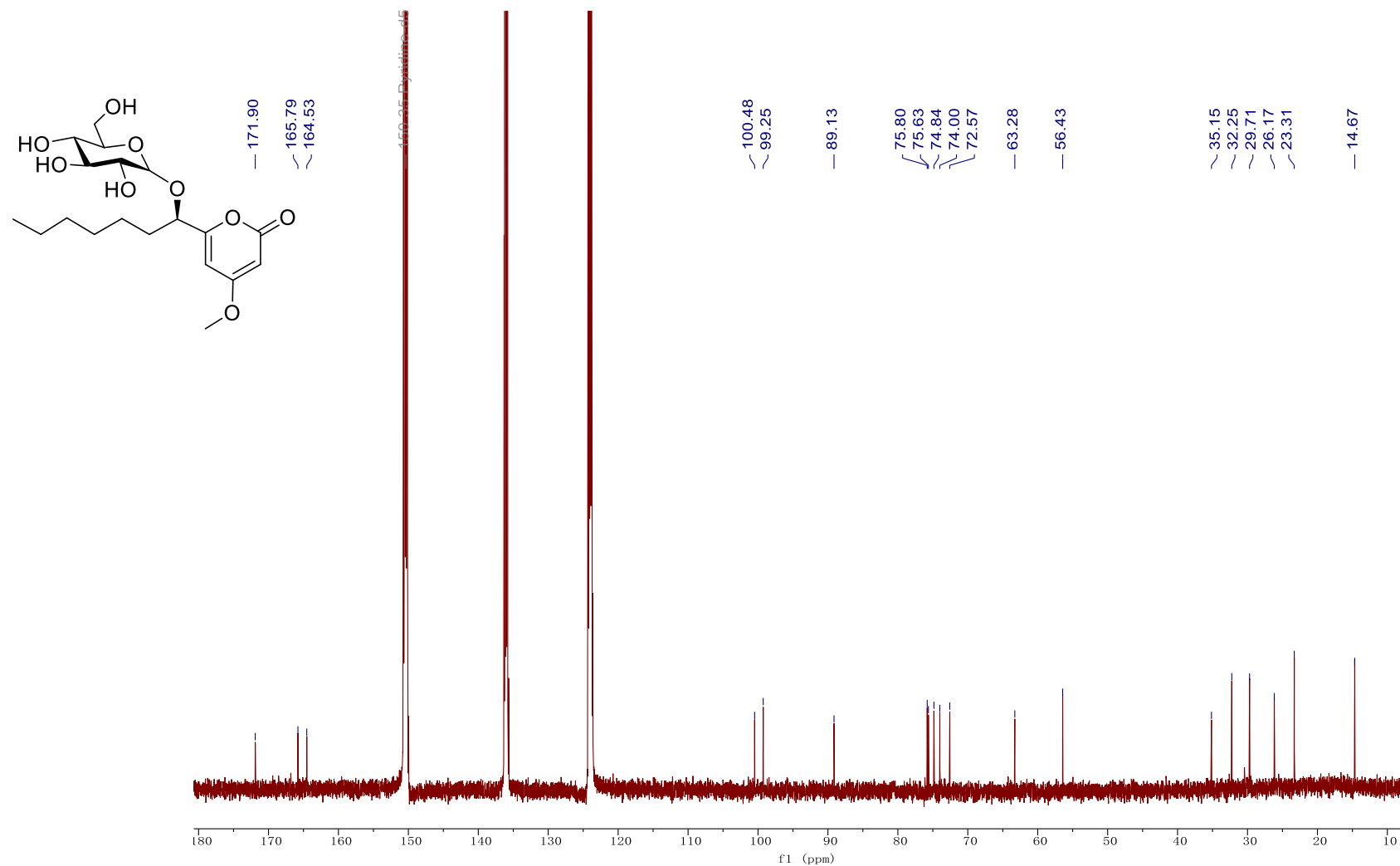


**Fig. S43**  $^1\text{H}$  NMR spectrum of **3** in  $\text{pyridine-}d_5$  (600 MHz).

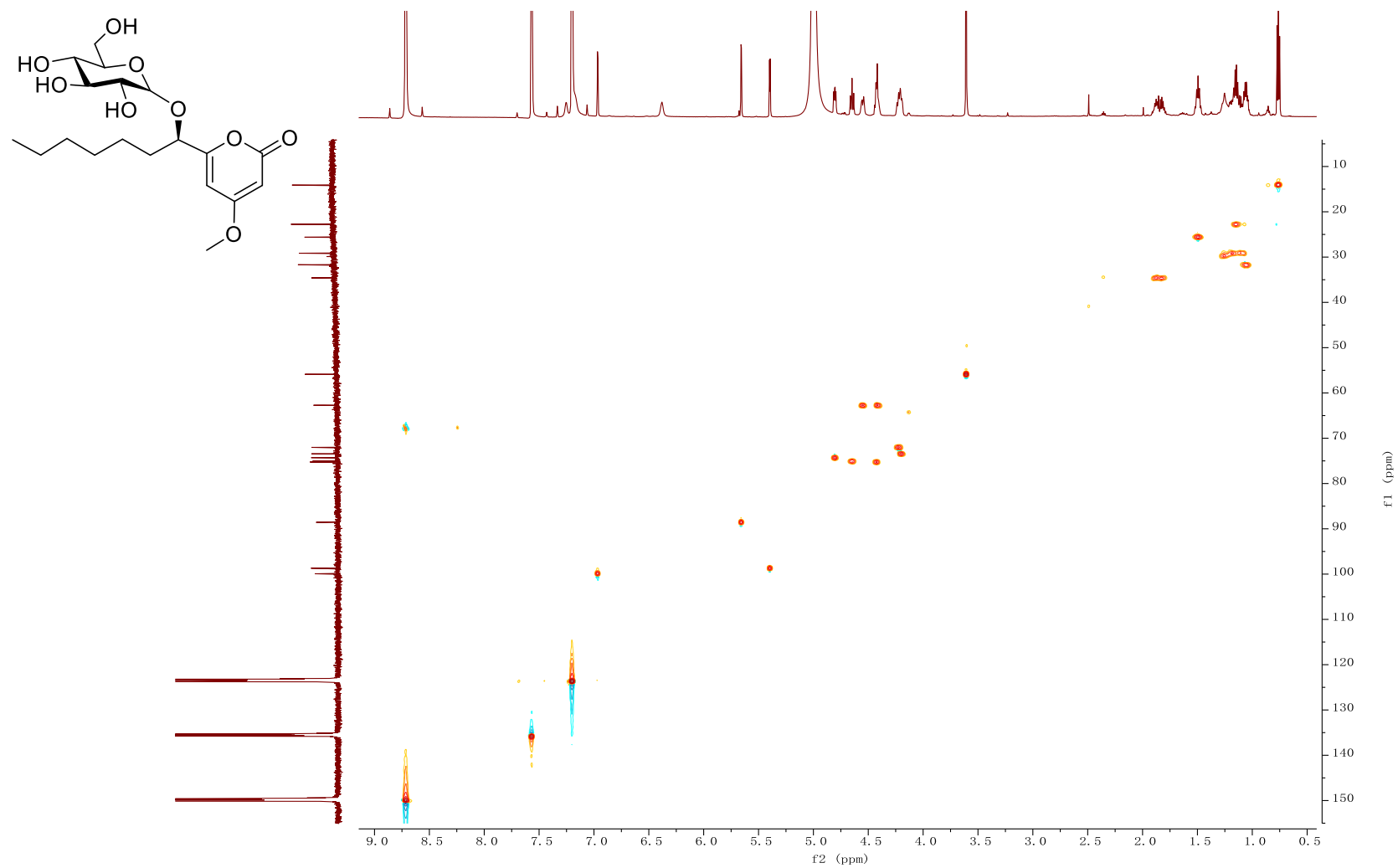




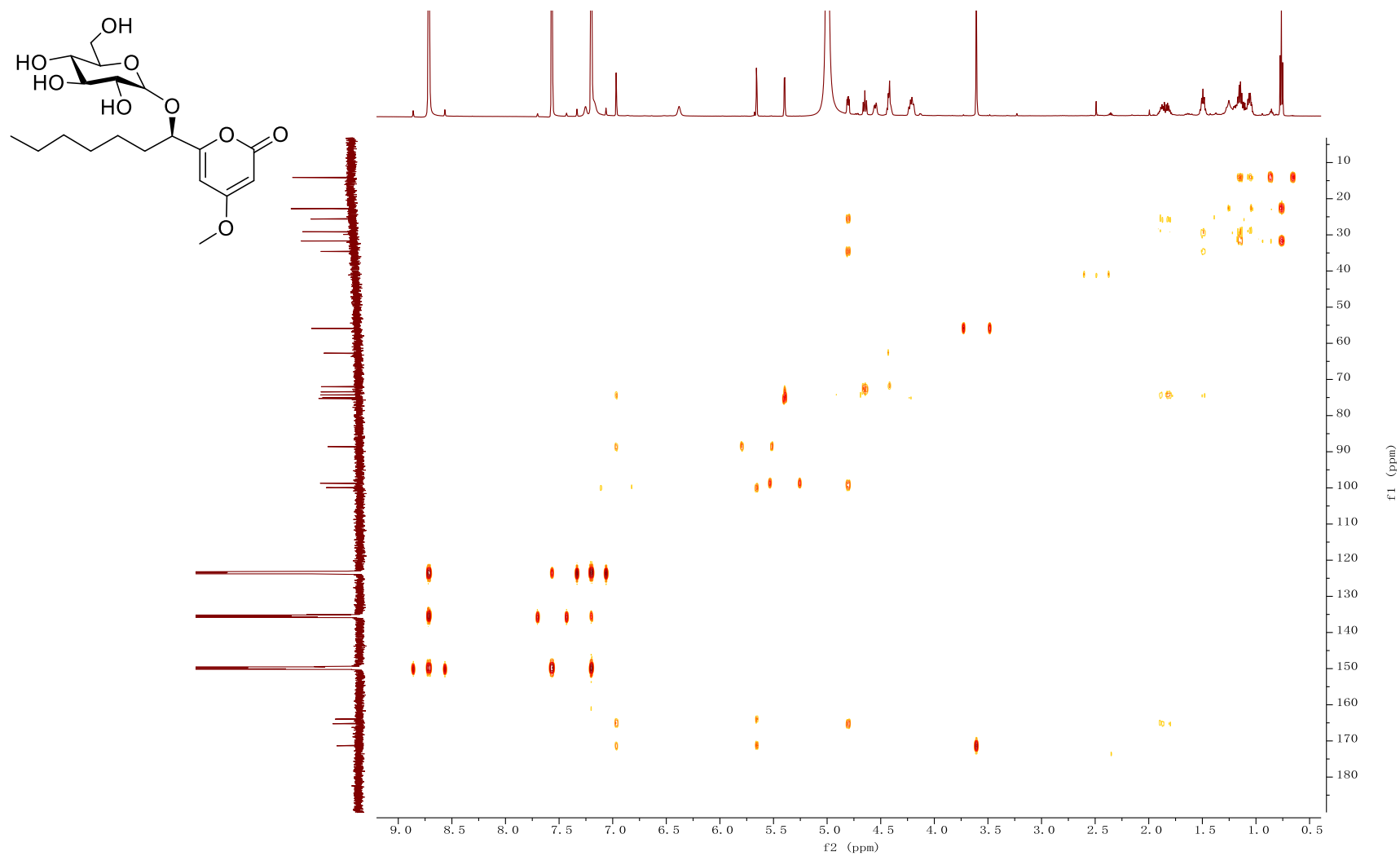
**Fig. S44** 1D-TOCSY spectrum of **3** in pyridine- $d_5$  (800 MHz).



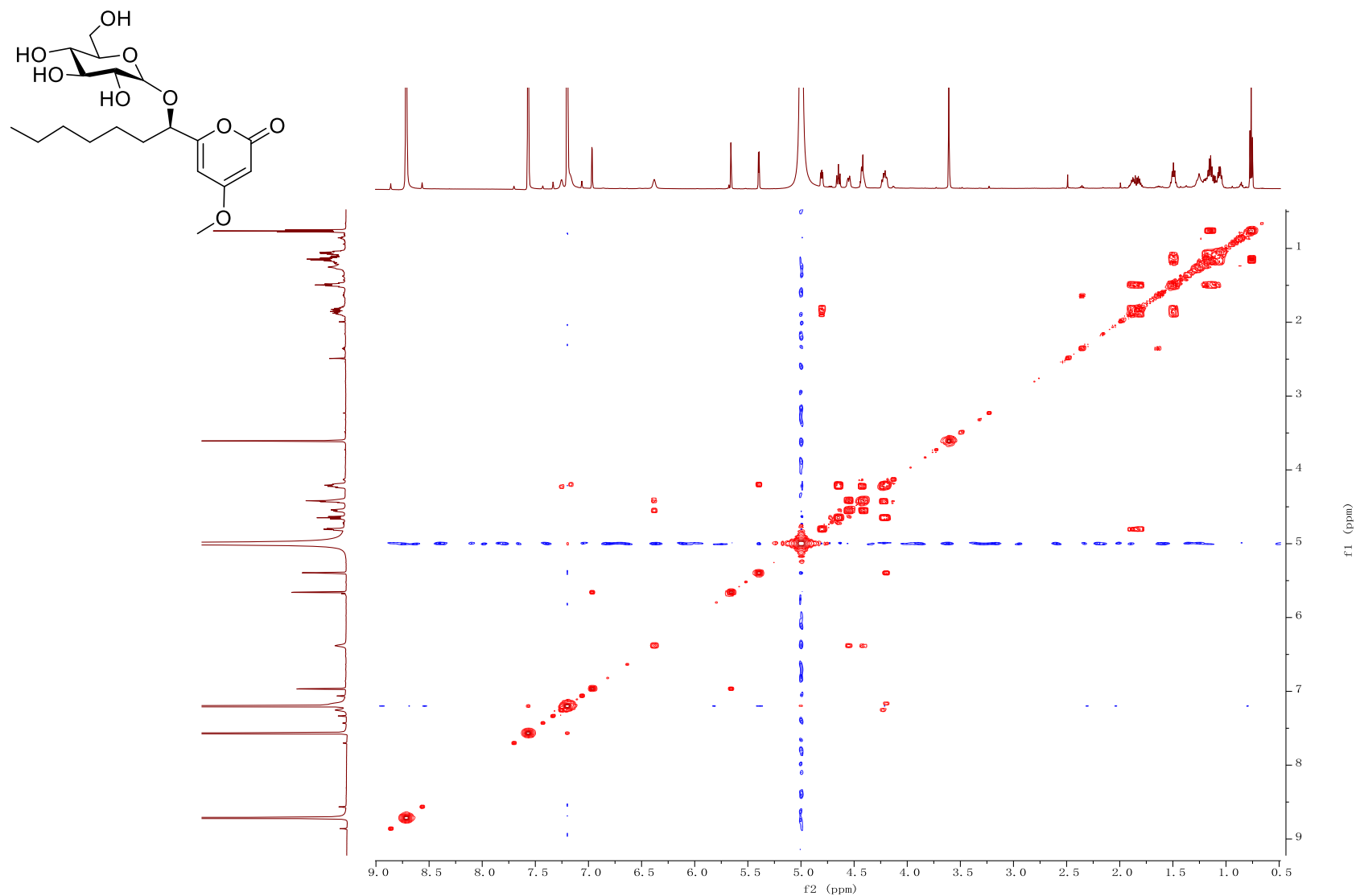
**Fig. S45**  $^{13}\text{C}$  NMR spectrum of **3** in pyridine- $d_5$  (150 MHz).



**Fig. S46** HSQC spectrum of **3** in pyridine- $d_5$  (600 MHz).



**Fig. S47** HMBC spectrum of **3** in pyridine-*d*<sub>5</sub> (600 MHz).



**Fig. S48**  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of **2** in  $\text{pyridine-}d_5$  (600 MHz).

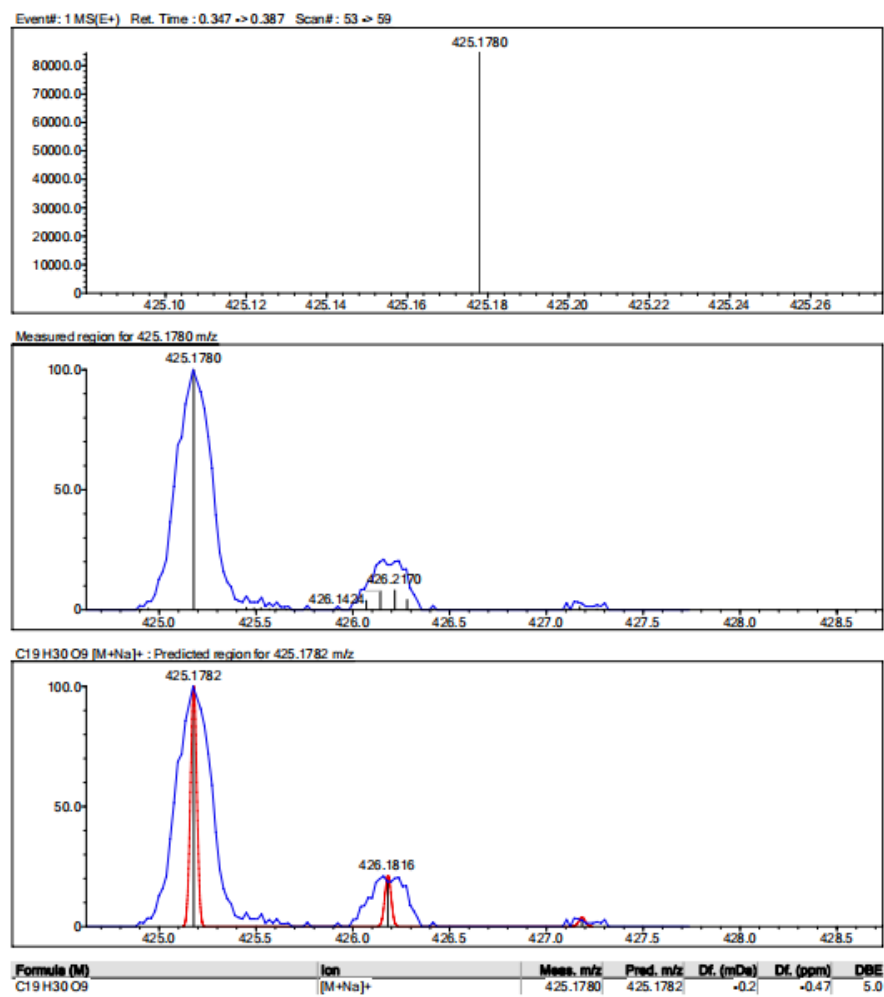
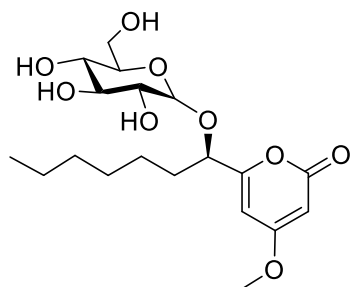
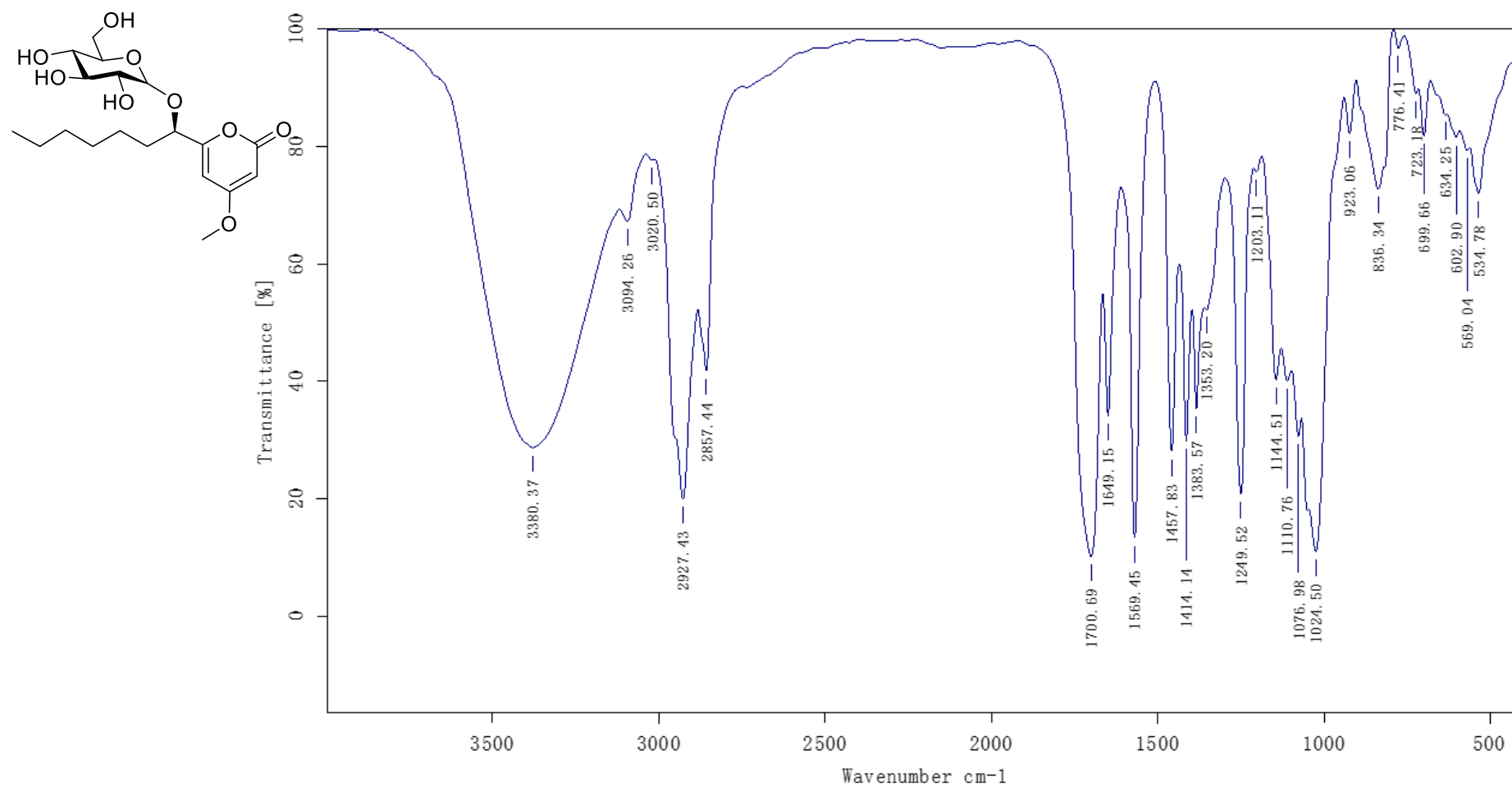
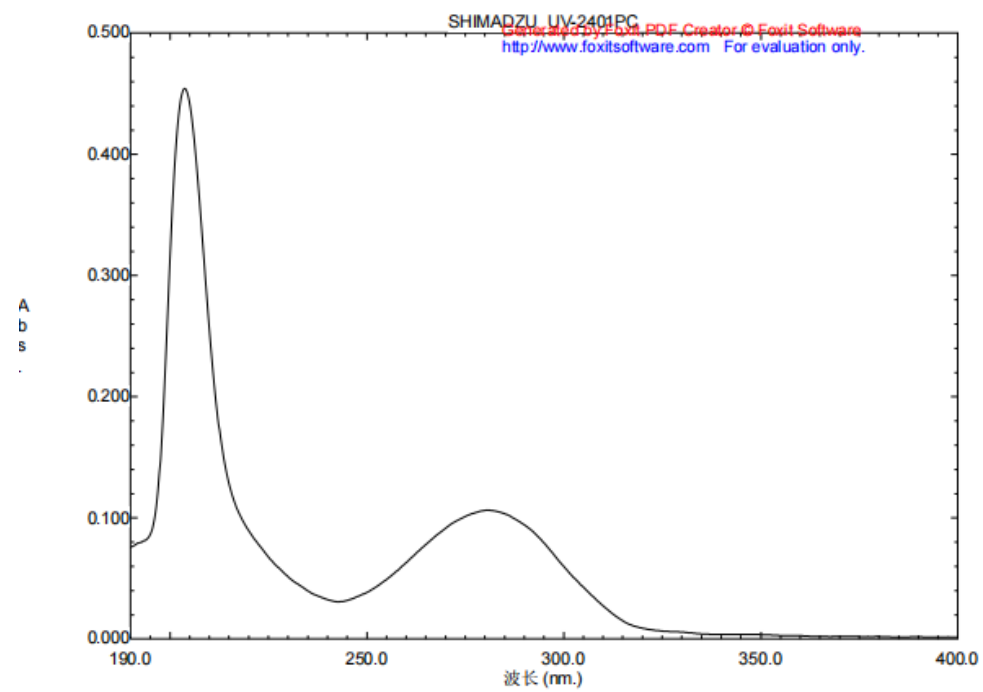
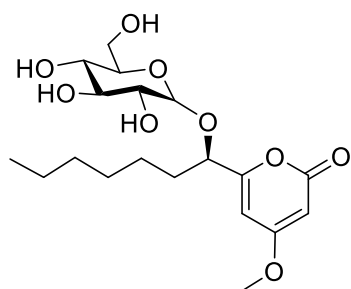


Fig. S49 HRESIMS spectrum of 3.

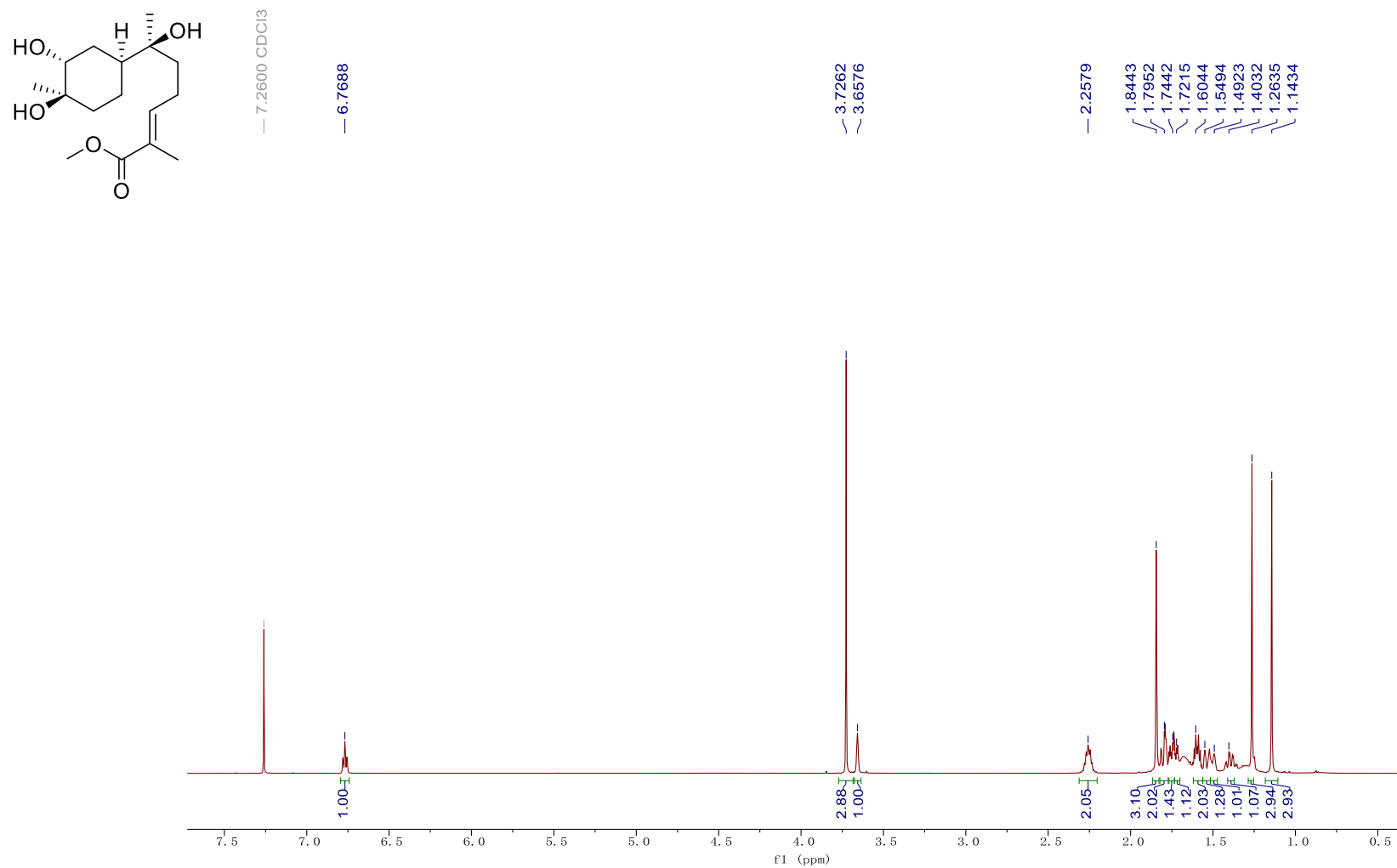


**Fig. S50** IR spectrum of **3**.

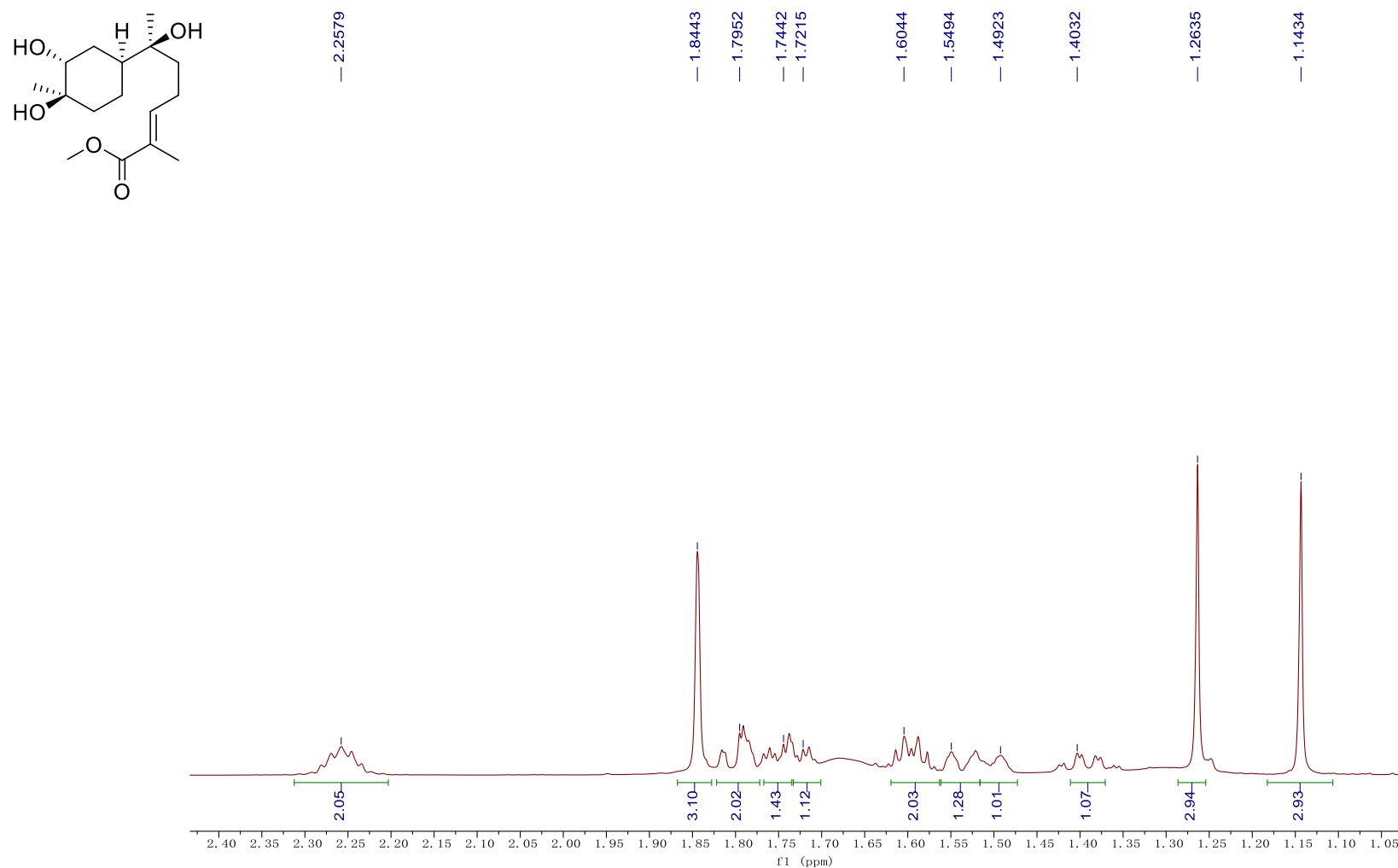


**Fig. S51** UV spectrum of **3**.

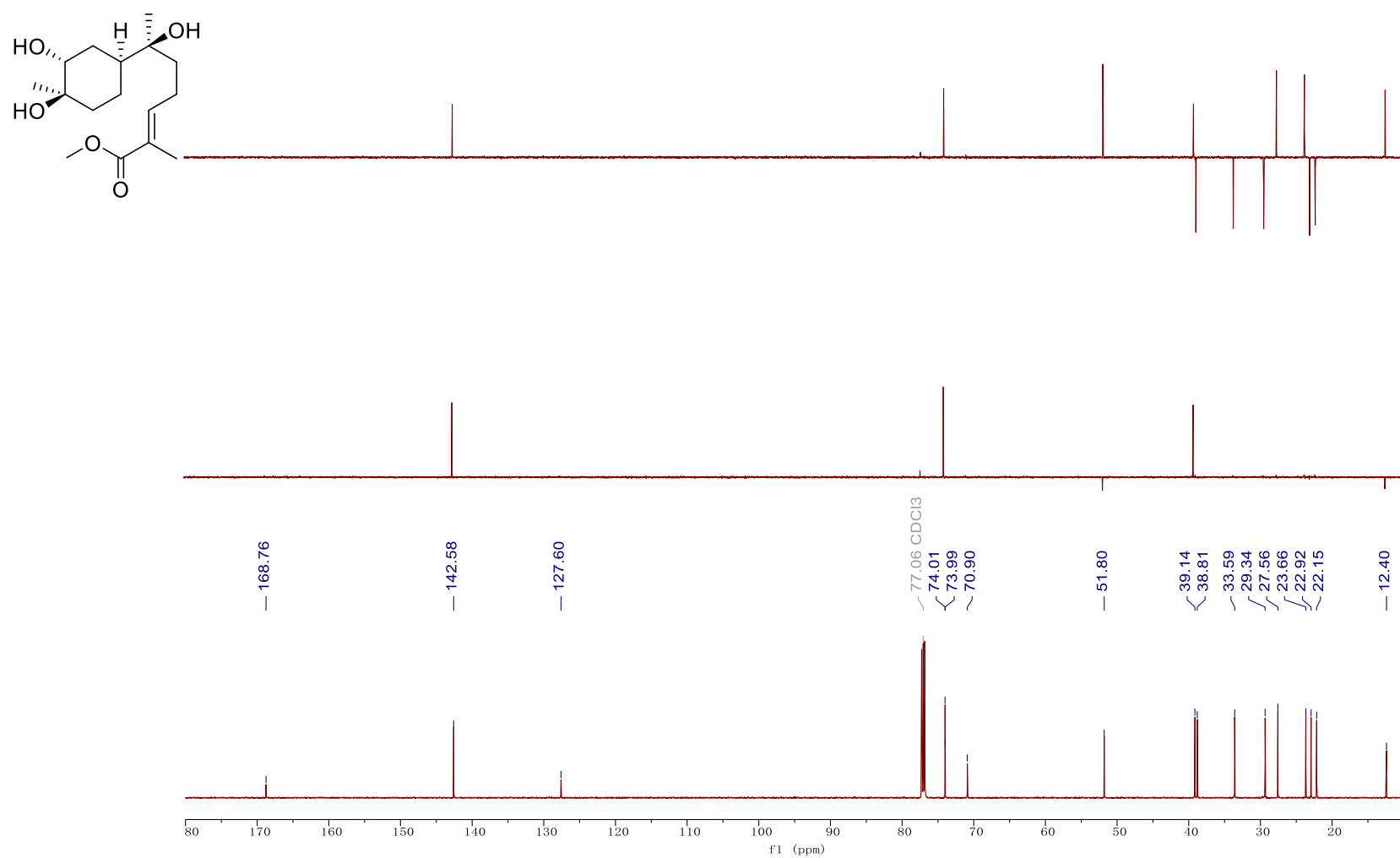




**Fig. S52** <sup>1</sup>H NMR Spectrum of **4** in chloroform-*d* (600 MHz).



**Fig. S53** <sup>1</sup>H NMR Spectrum of **4** in chloroform-*d* (600 MHz) (expanded).



**Fig. S54** <sup>13</sup>C NMR Spectrum of **4** in chloroform-*d* (150 MHz).

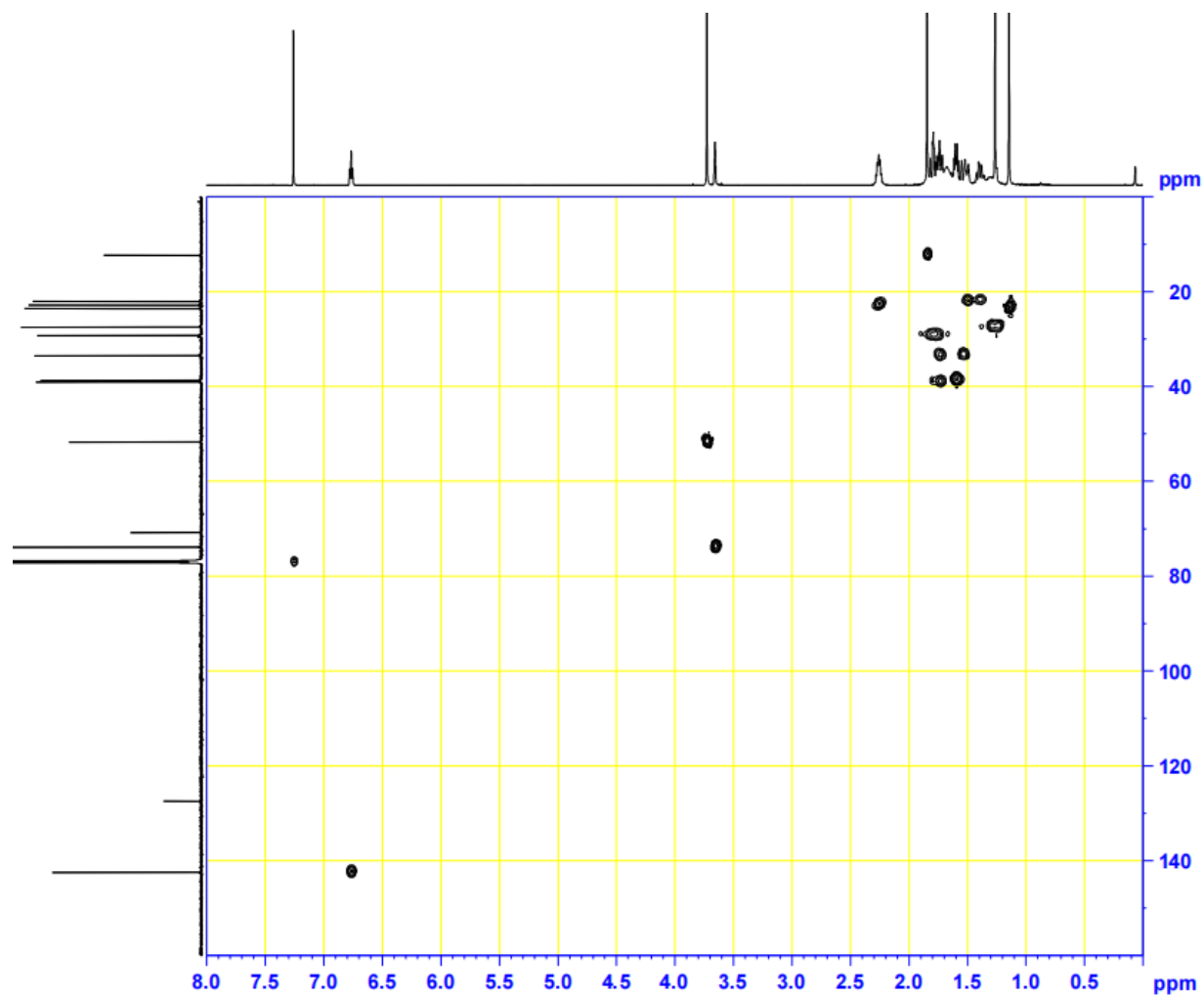
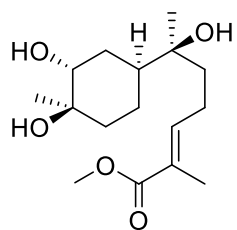


Fig. S55 HSQC Spectrum of **4** in chloroform-*d* (600 MHz).

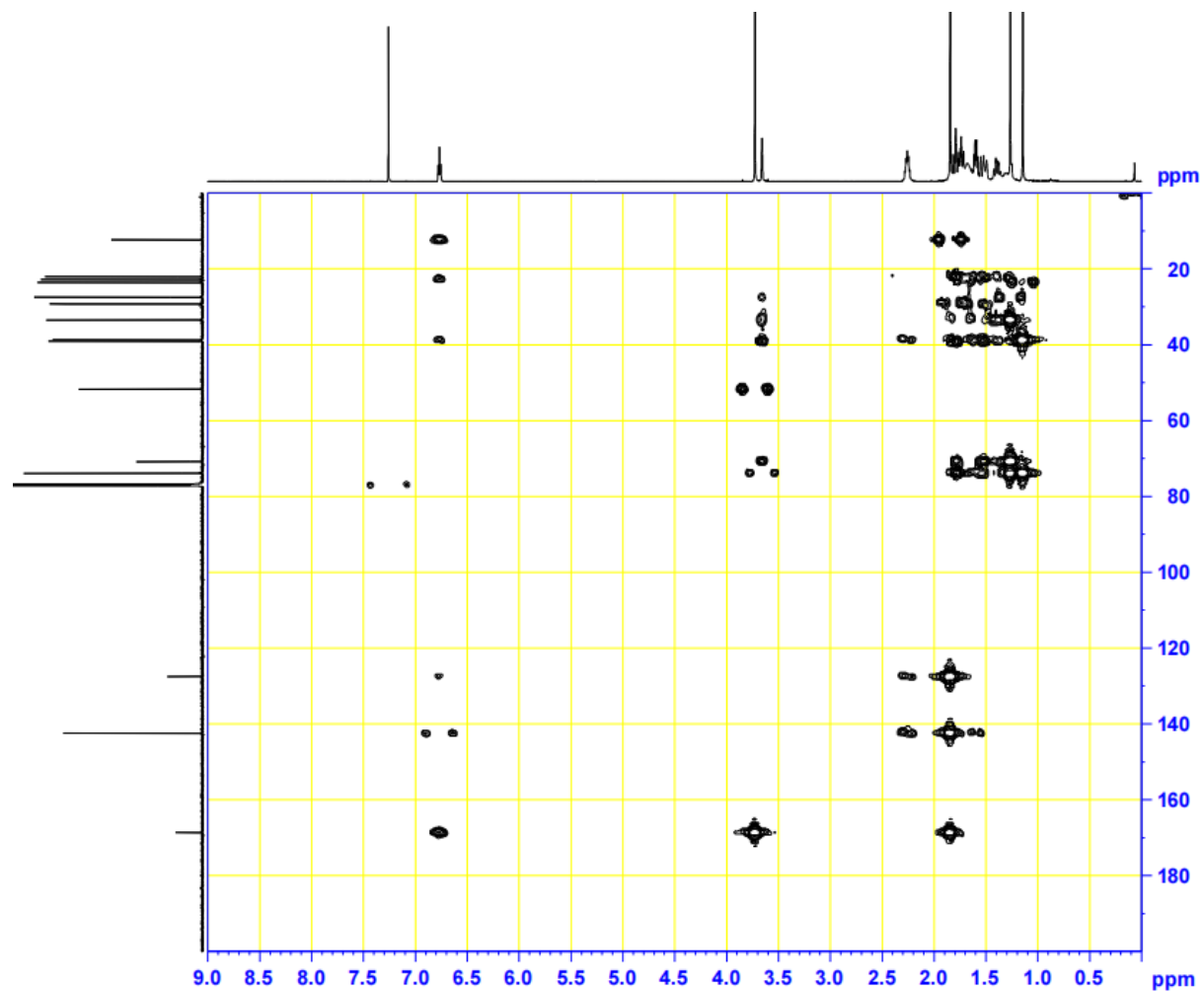
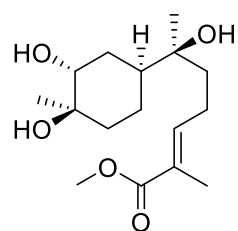
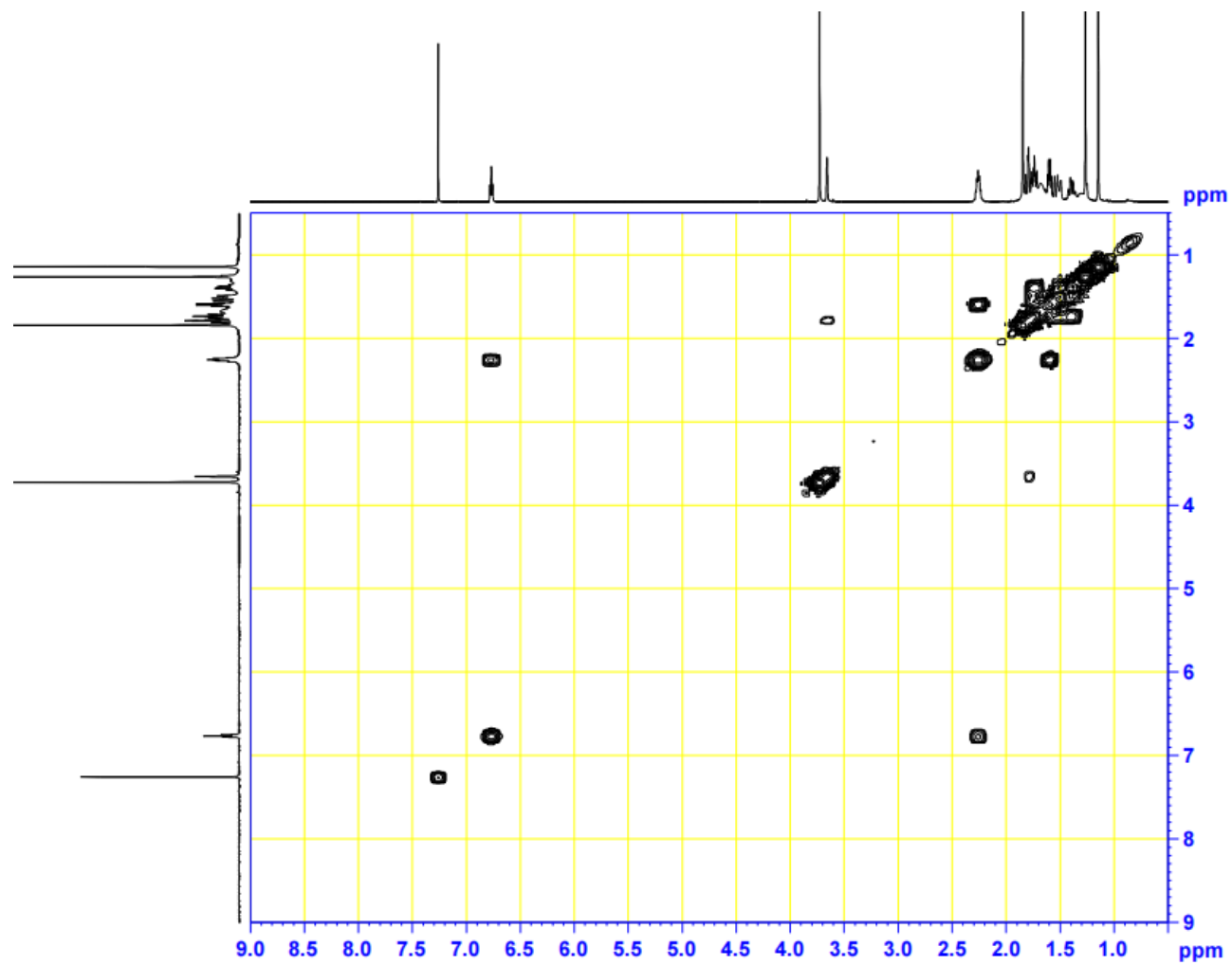
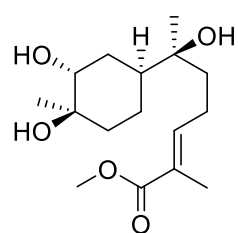


Fig. S56 HMBC Spectrum of **4** in chloroform-*d* (600 MHz).



**Fig. S57**  $^1\text{H}$ - $^1\text{H}$  COSY Spectrum of **4** in chloroform-*d* (600 MHz).

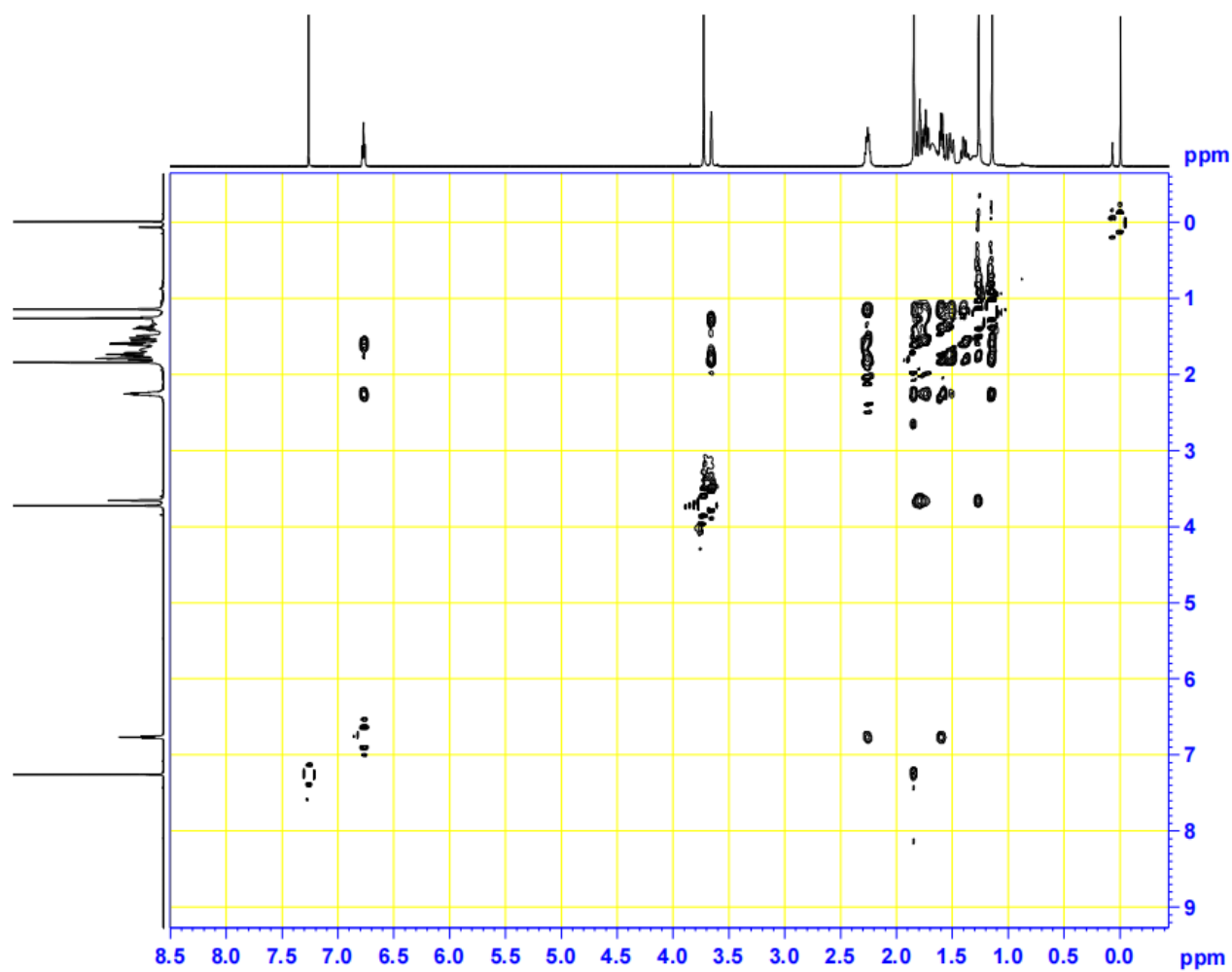
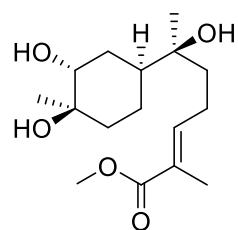


Fig. S58 ROESY Spectrum of **4** in chloroform-*d* (600 MHz).

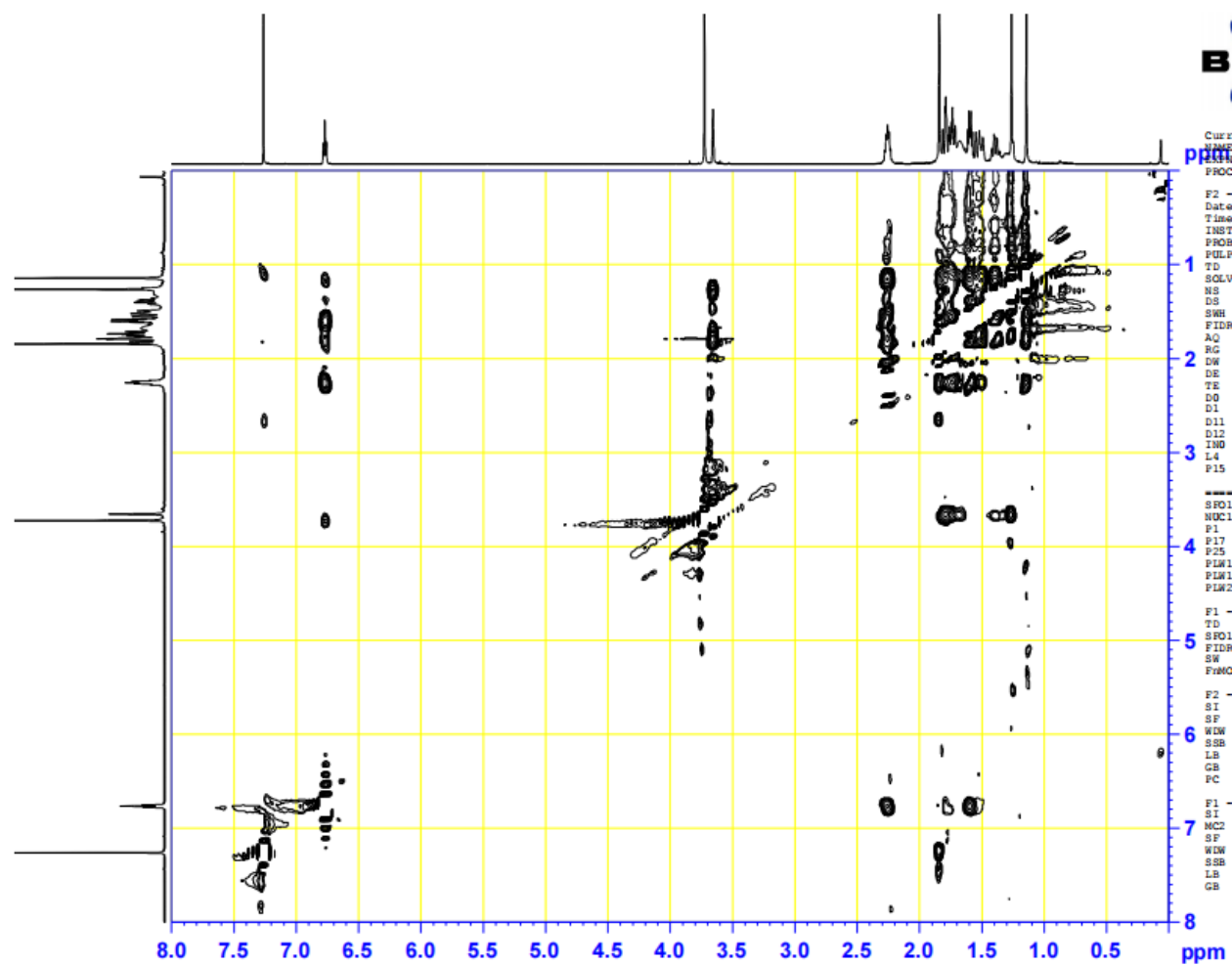
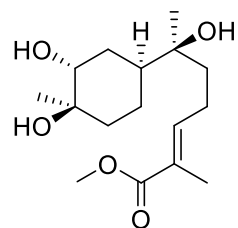


Fig. S59 ROESY Spectrum of **4** in chloroform-*d* (600 MHz) (expanded).



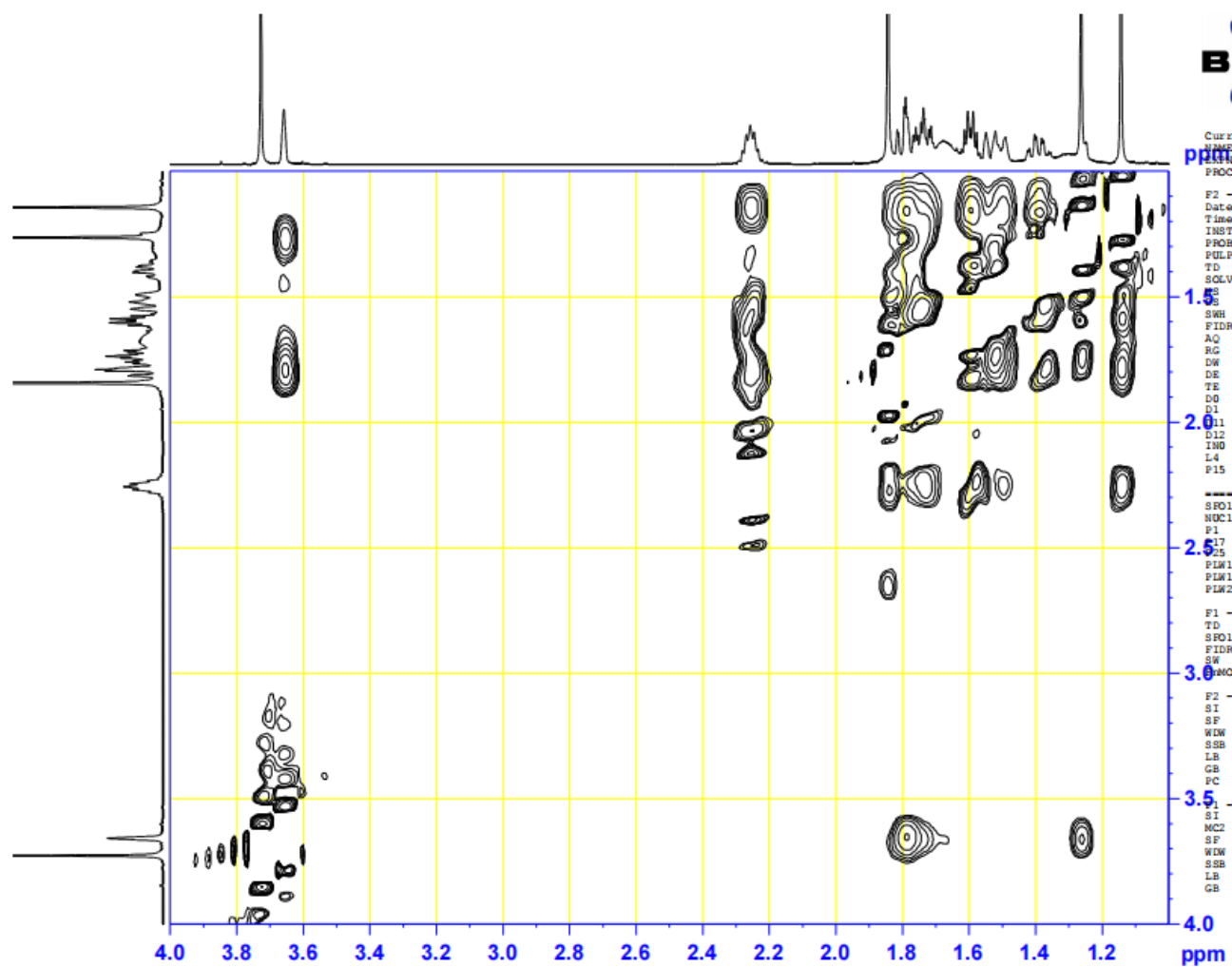
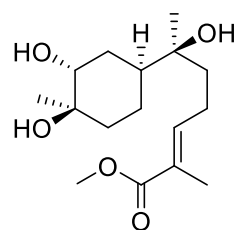
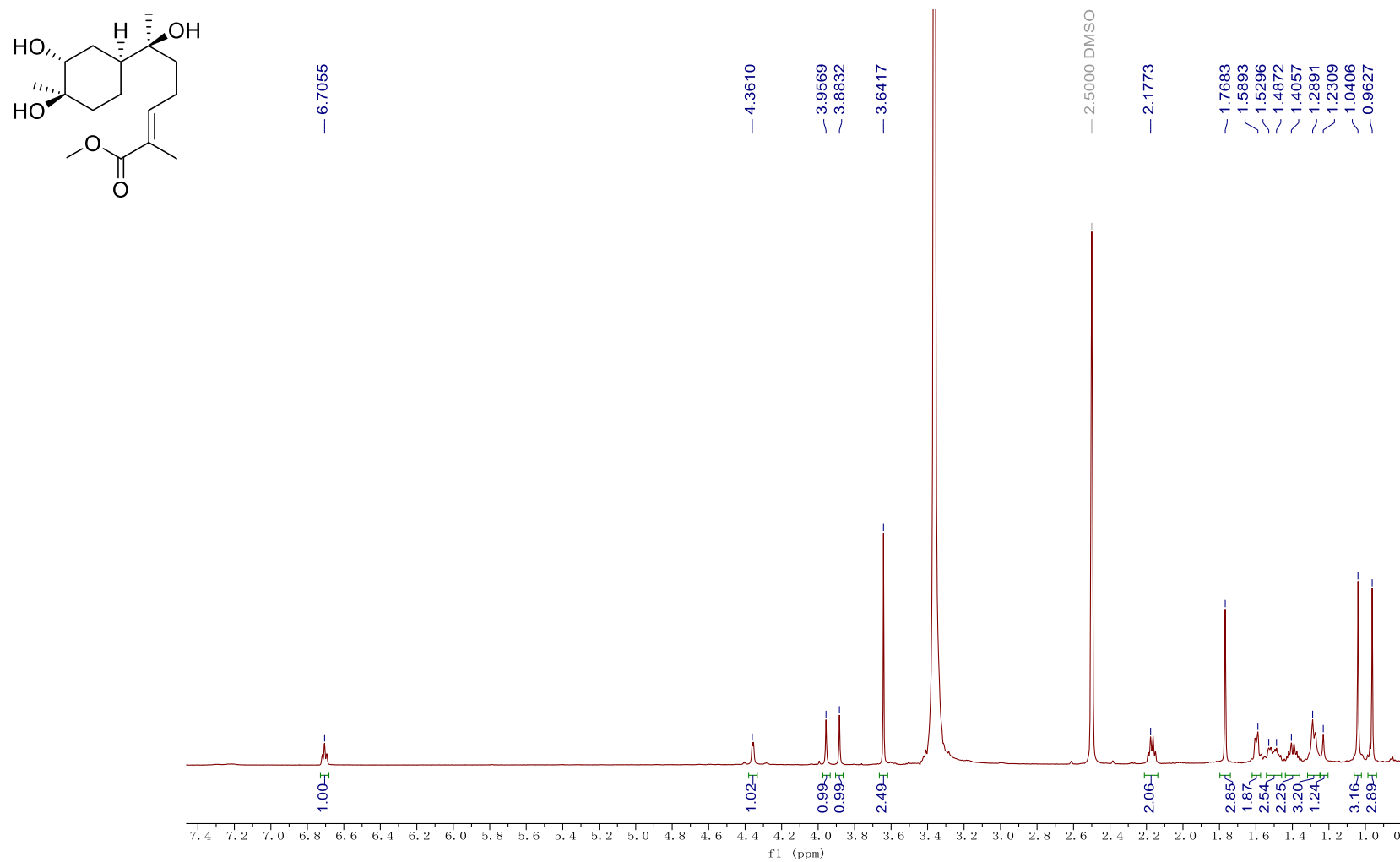
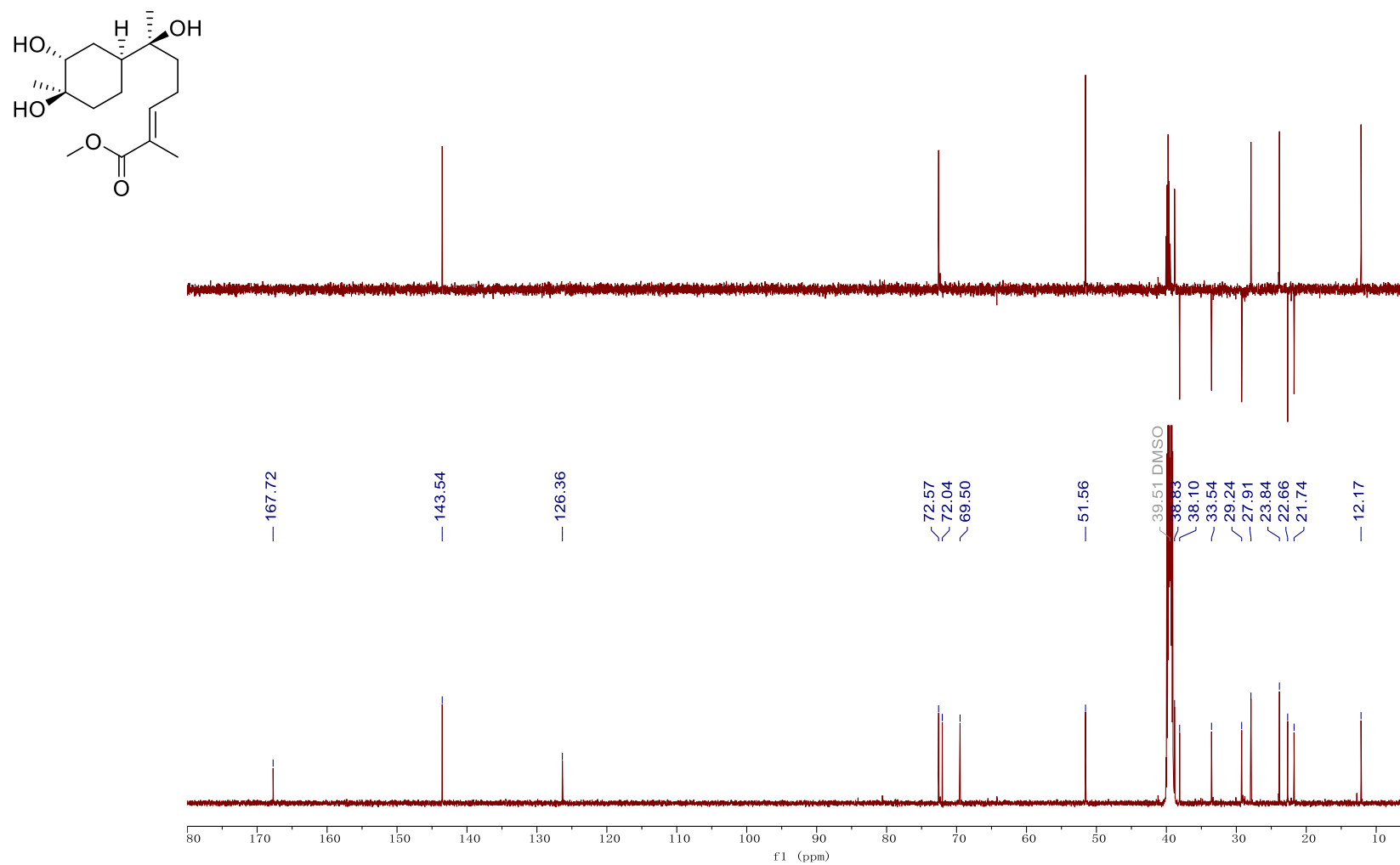


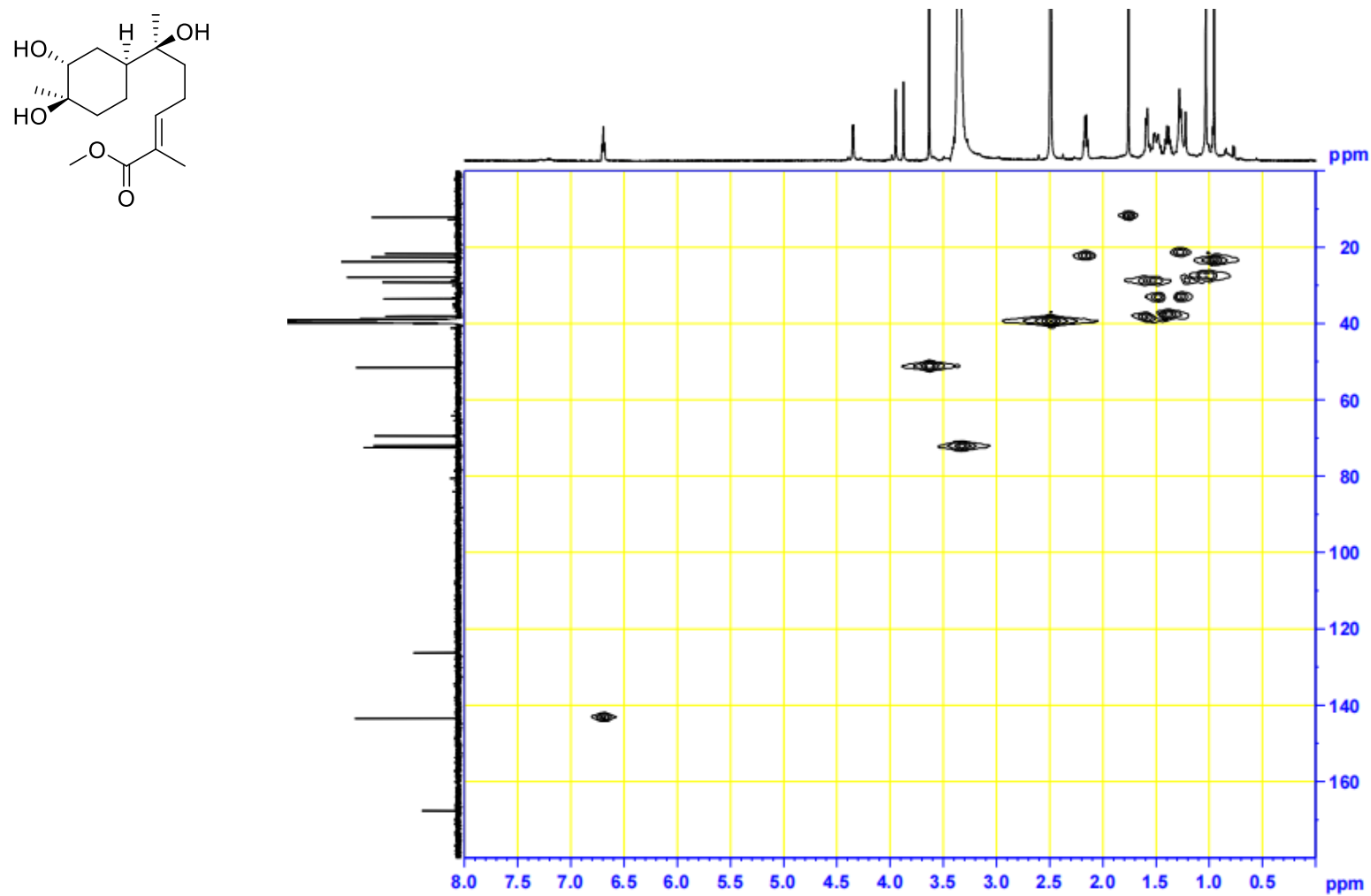
Fig. S60 ROESY Spectrum of **4** in chloroform-*d* (600 MHz) (expanded).



**Fig. S61** <sup>1</sup>H NMR Spectrum of **4** in DMSO-*d*<sub>6</sub> (600 MHz).



**Fig. S62**  $^{13}\text{C}$  NMR Spectrum of **4** in  $\text{DMSO-}d_6$  (150 MHz).



**Fig. S63** HSQC Spectrum of **4** in DMSO-*d*<sub>6</sub> (600 MHz).

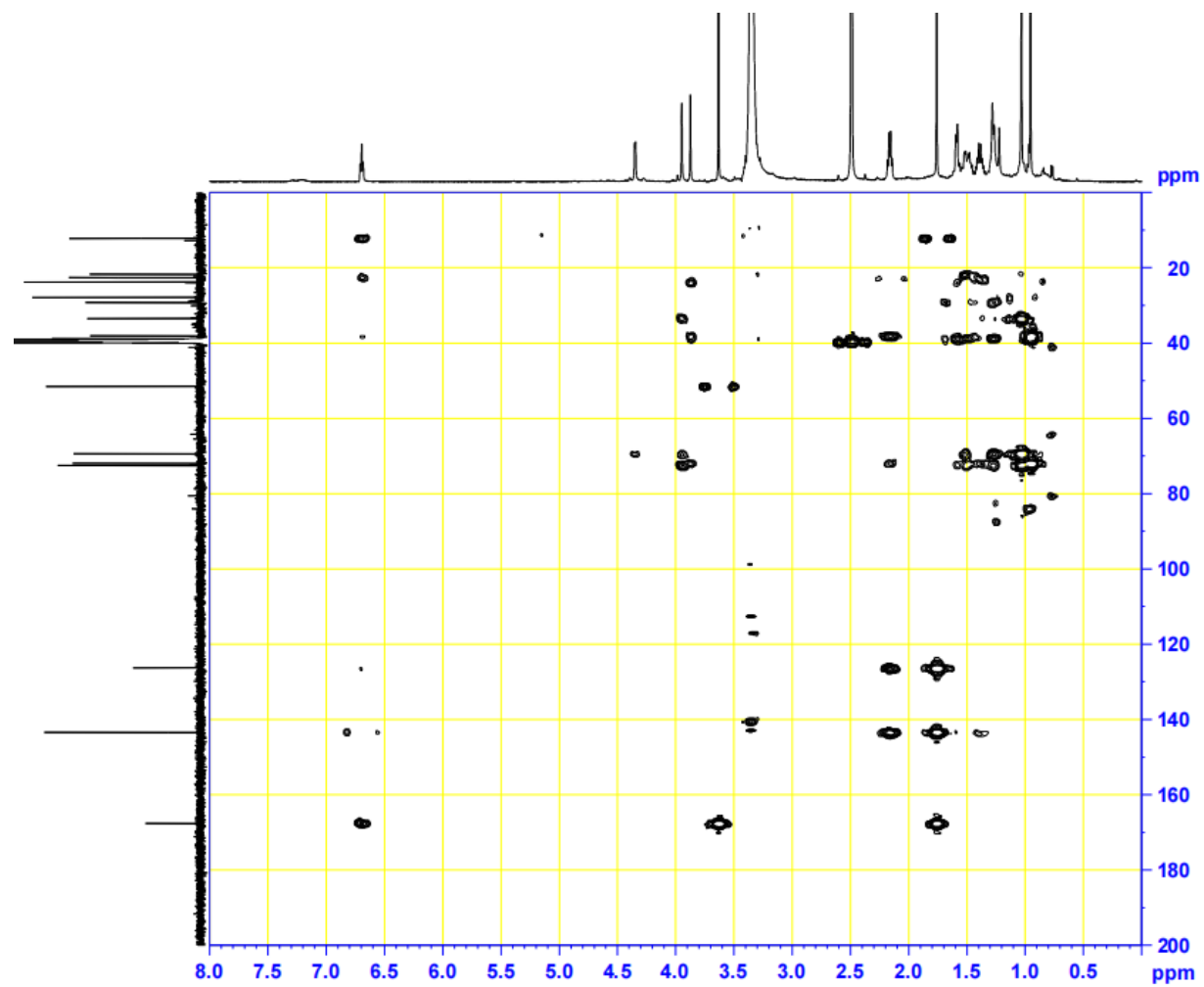
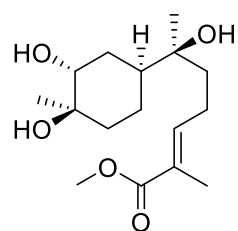
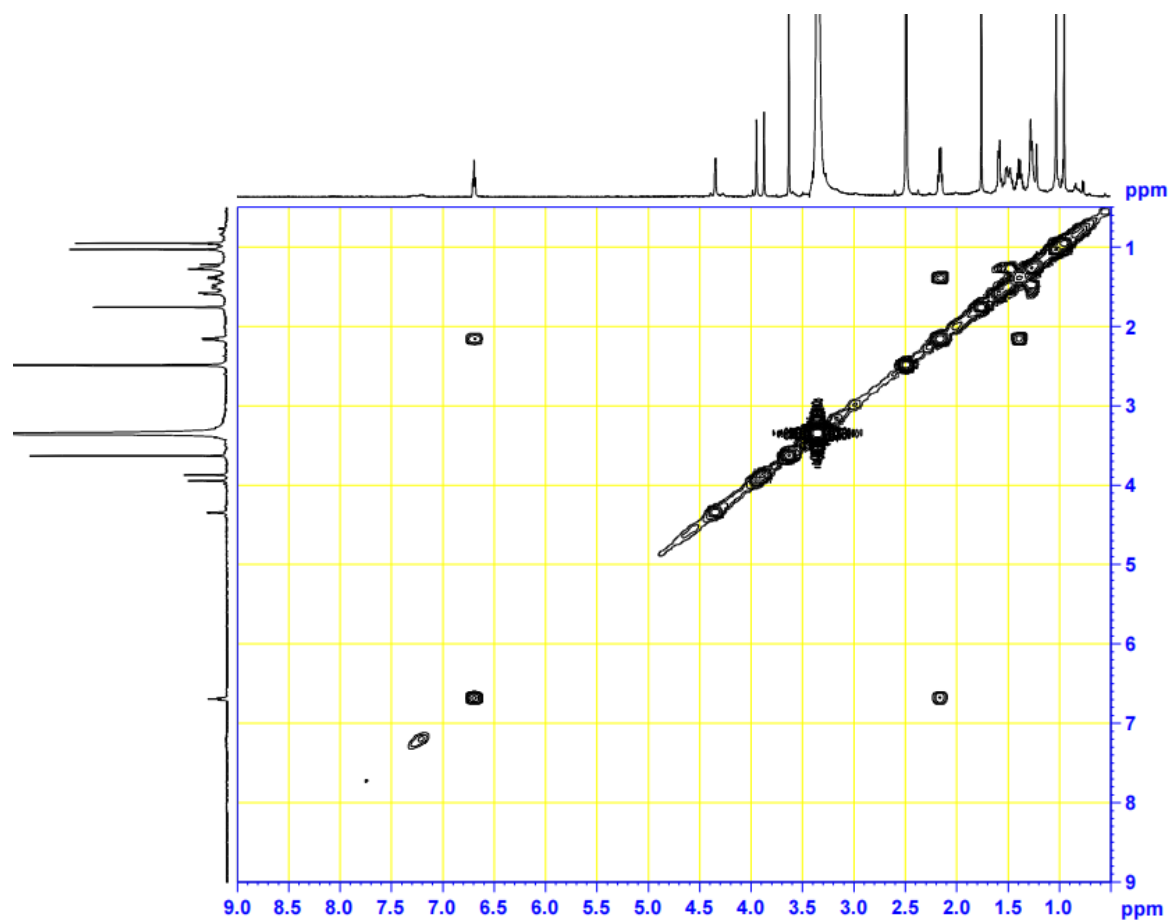
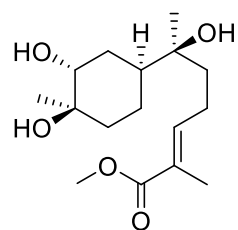
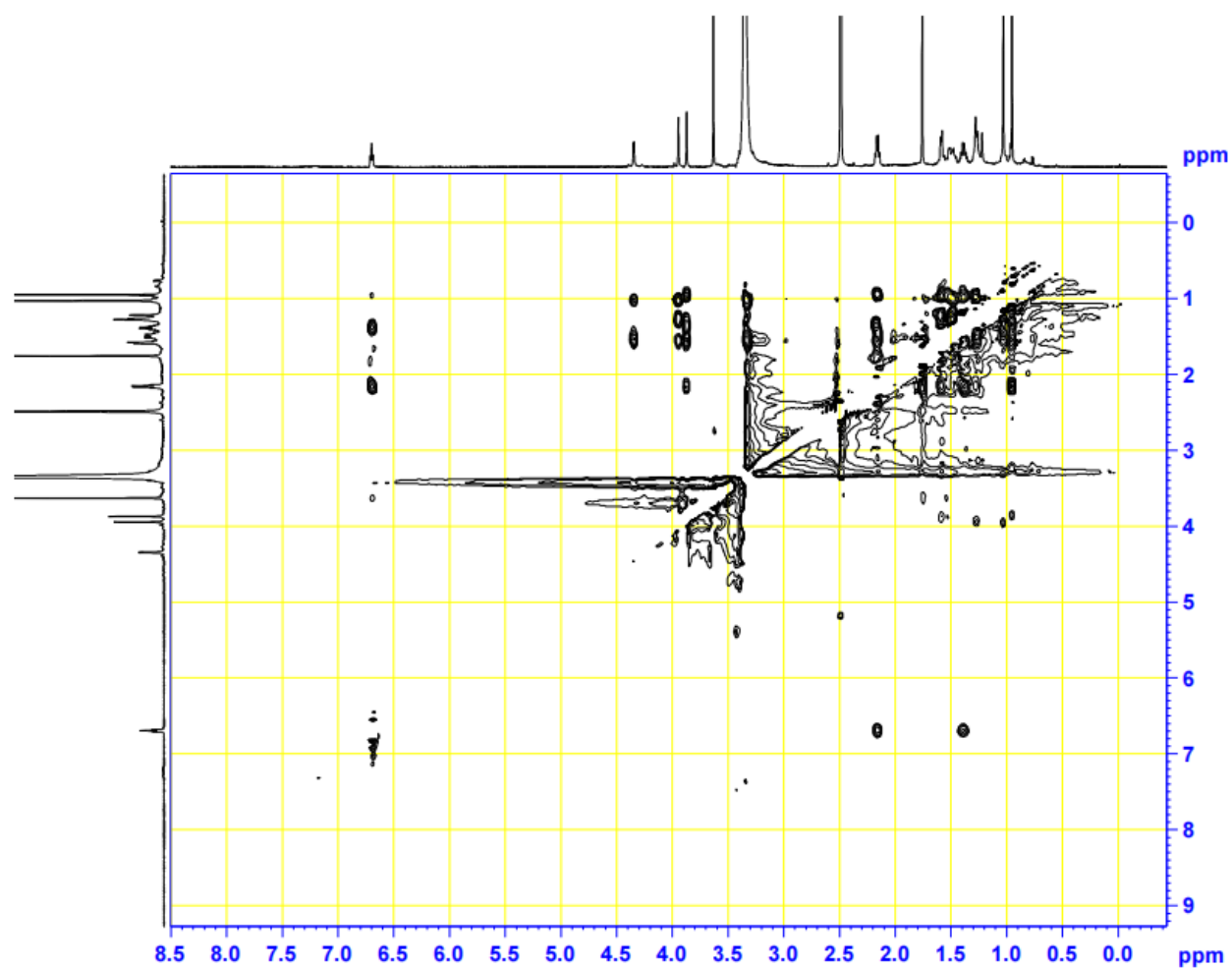
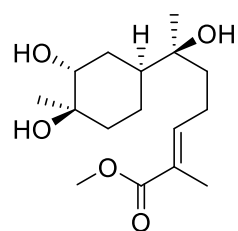


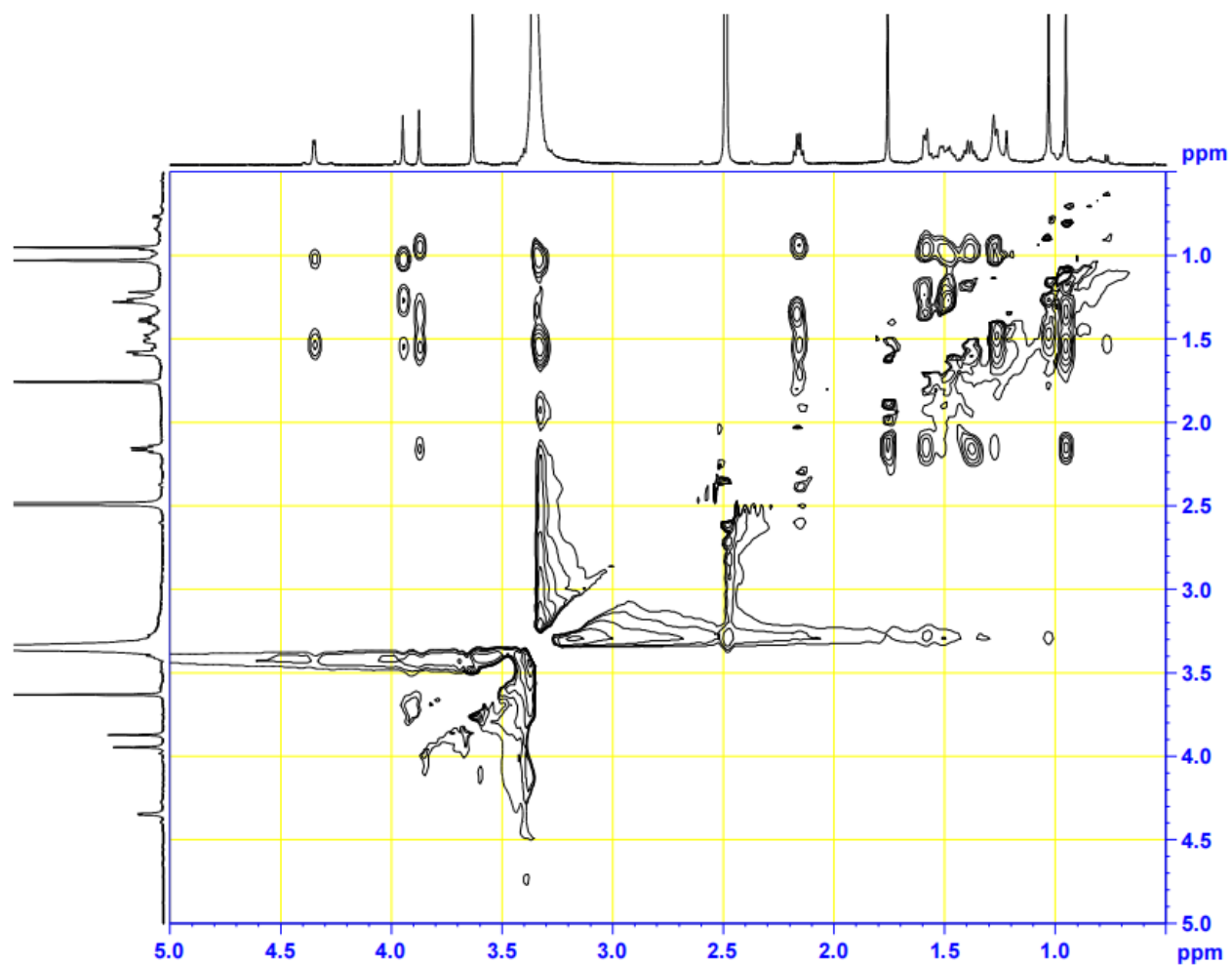
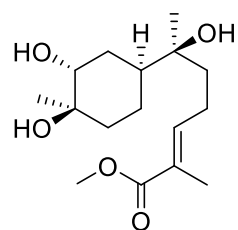
Fig. S64 HMBC Spectrum of **4** in DMSO- $d_6$  (600 MHz)



**Fig. S65**  $^1\text{H}$ - $^1\text{H}$  COSY Spectrum of **4** in  $\text{DMSO}-d_6$  (600 MHz).



**Fig. S66** ROESY Spectrum of **4** in DMSO- $d_6$  (600 MHz).



**Fig. S67** ROESY Spectrum of **4** in DMSO-*d*<sub>6</sub> (600 MHz) (expanded).



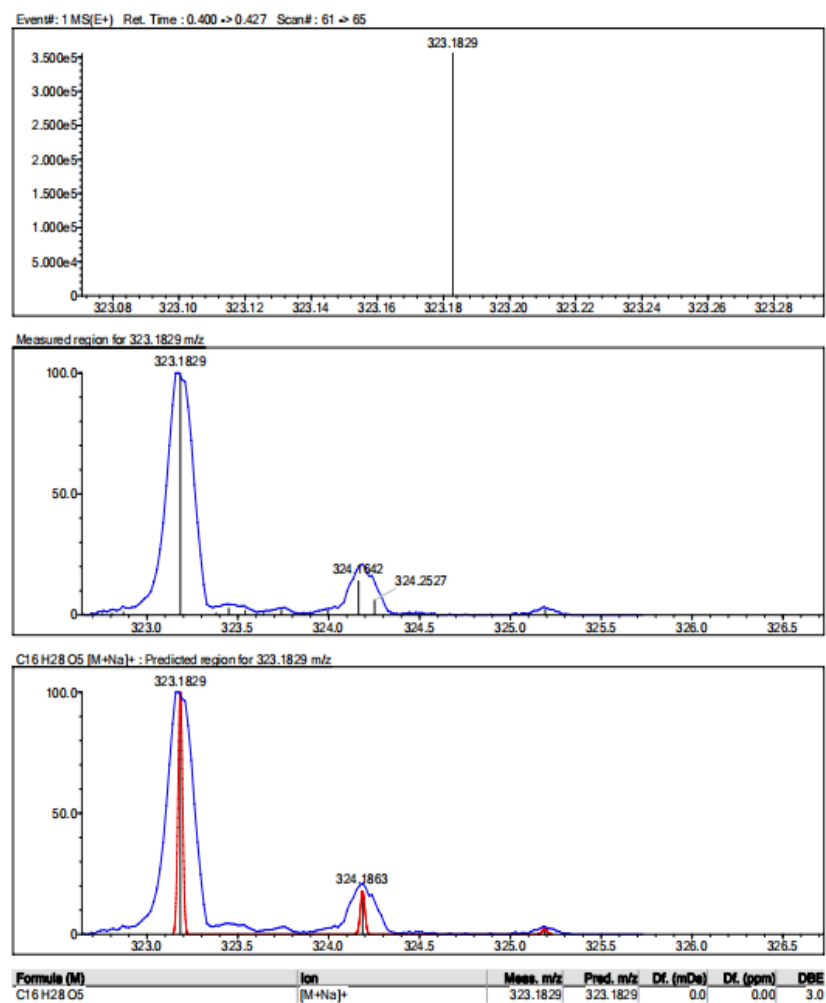
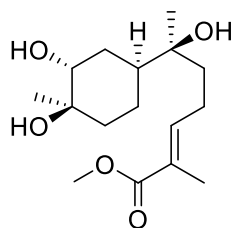


Fig. S68 HRESIMS Spectrum of 4.

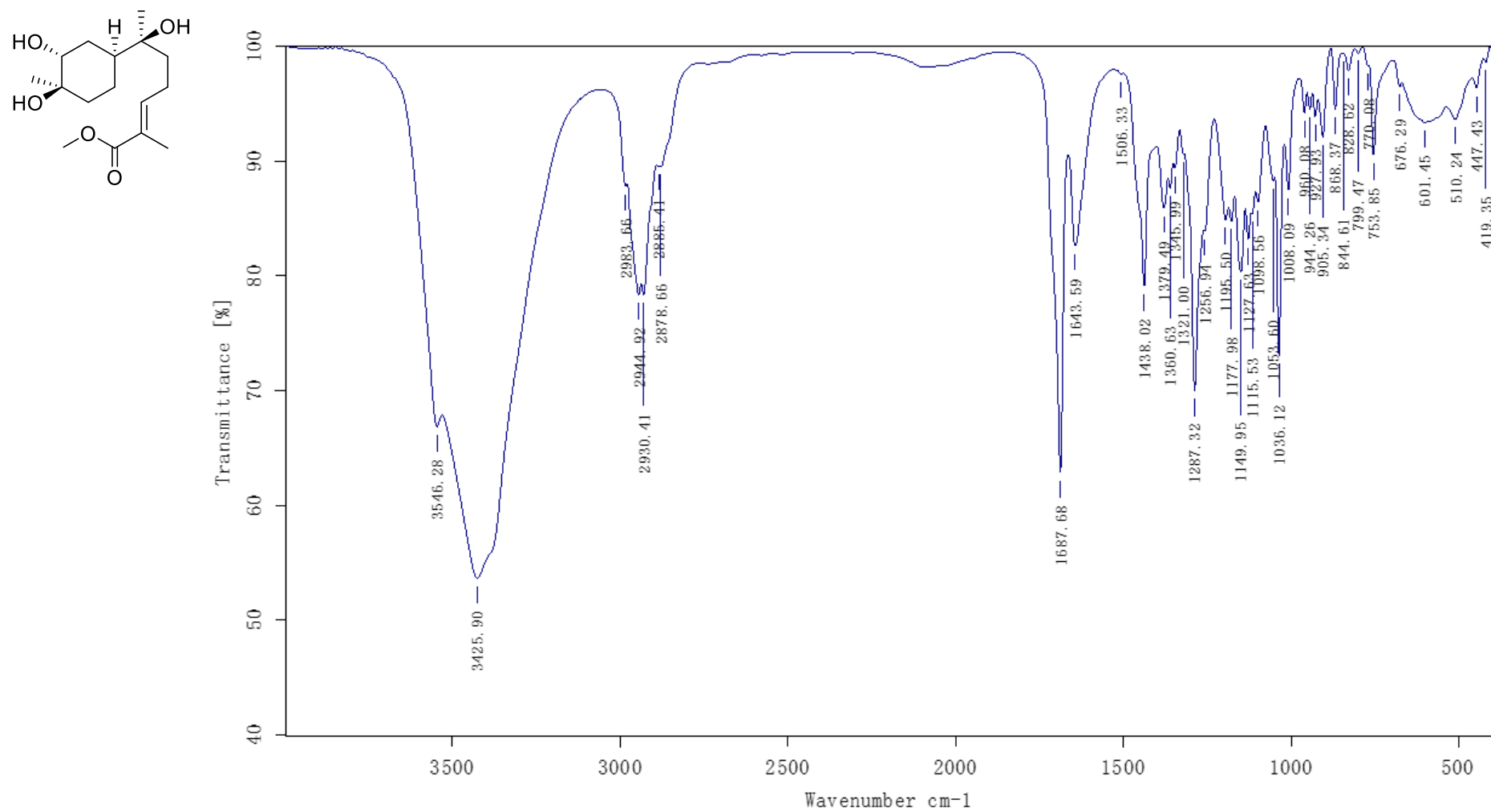
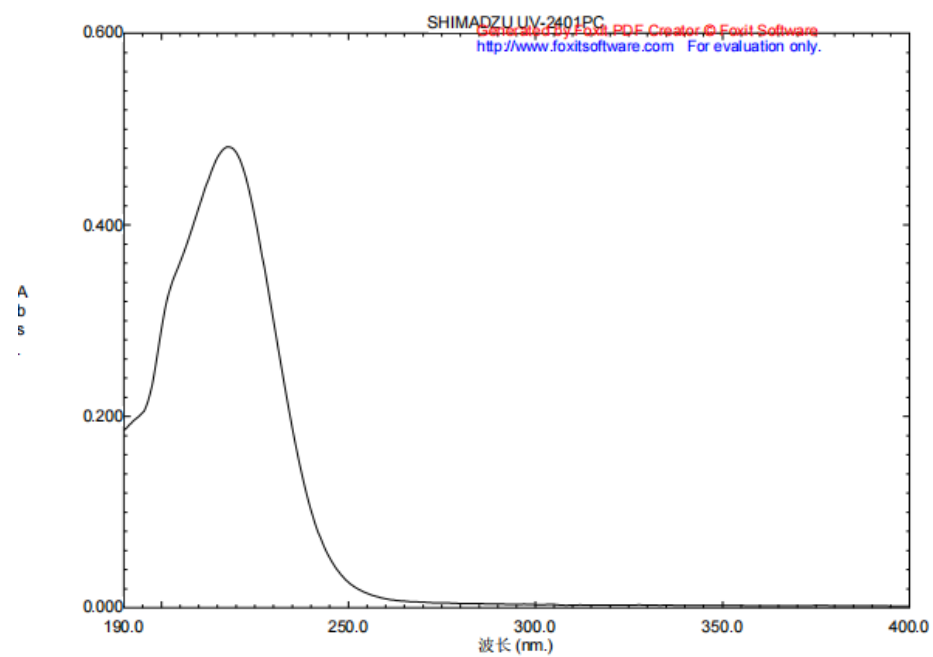
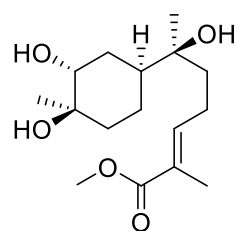
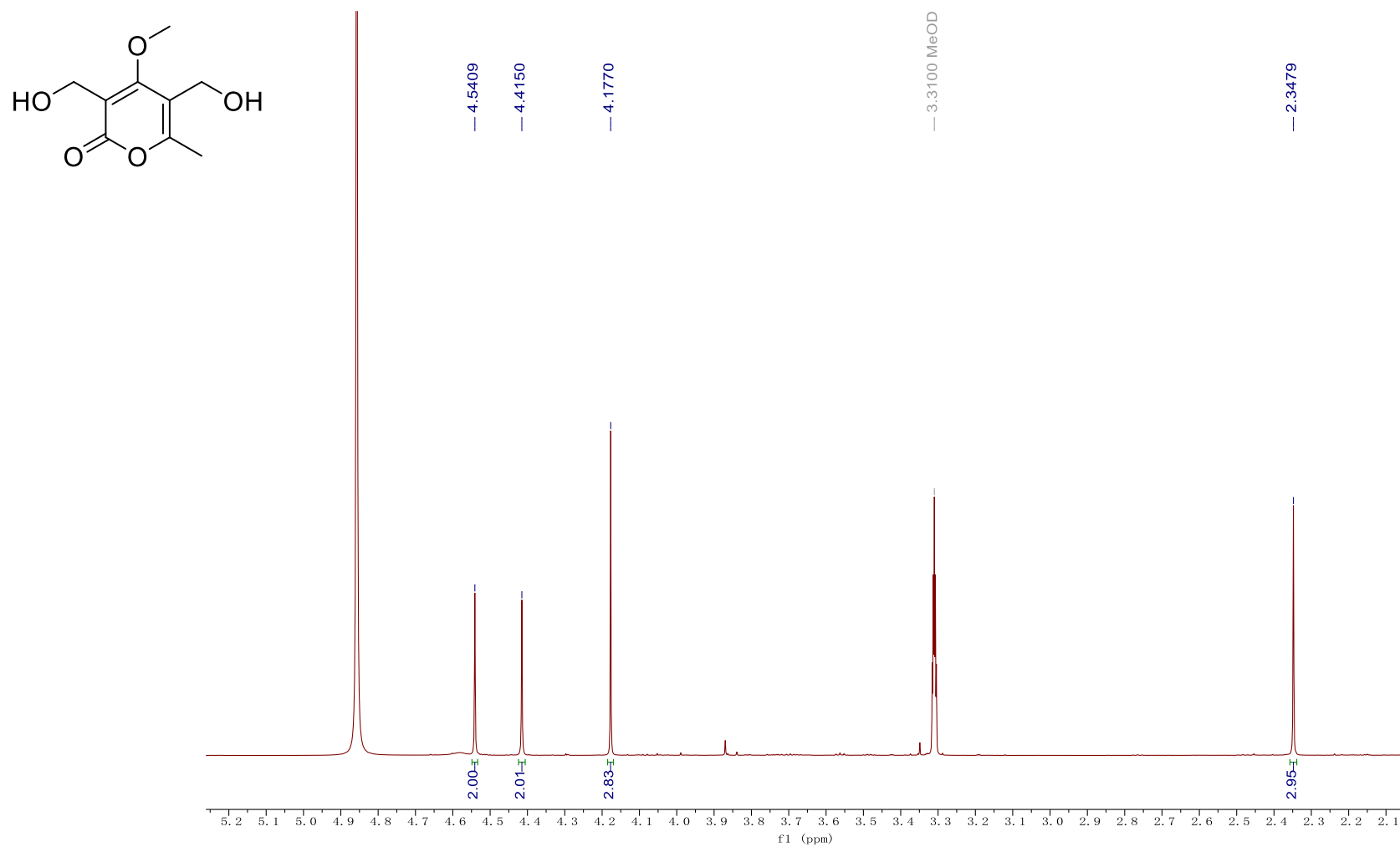


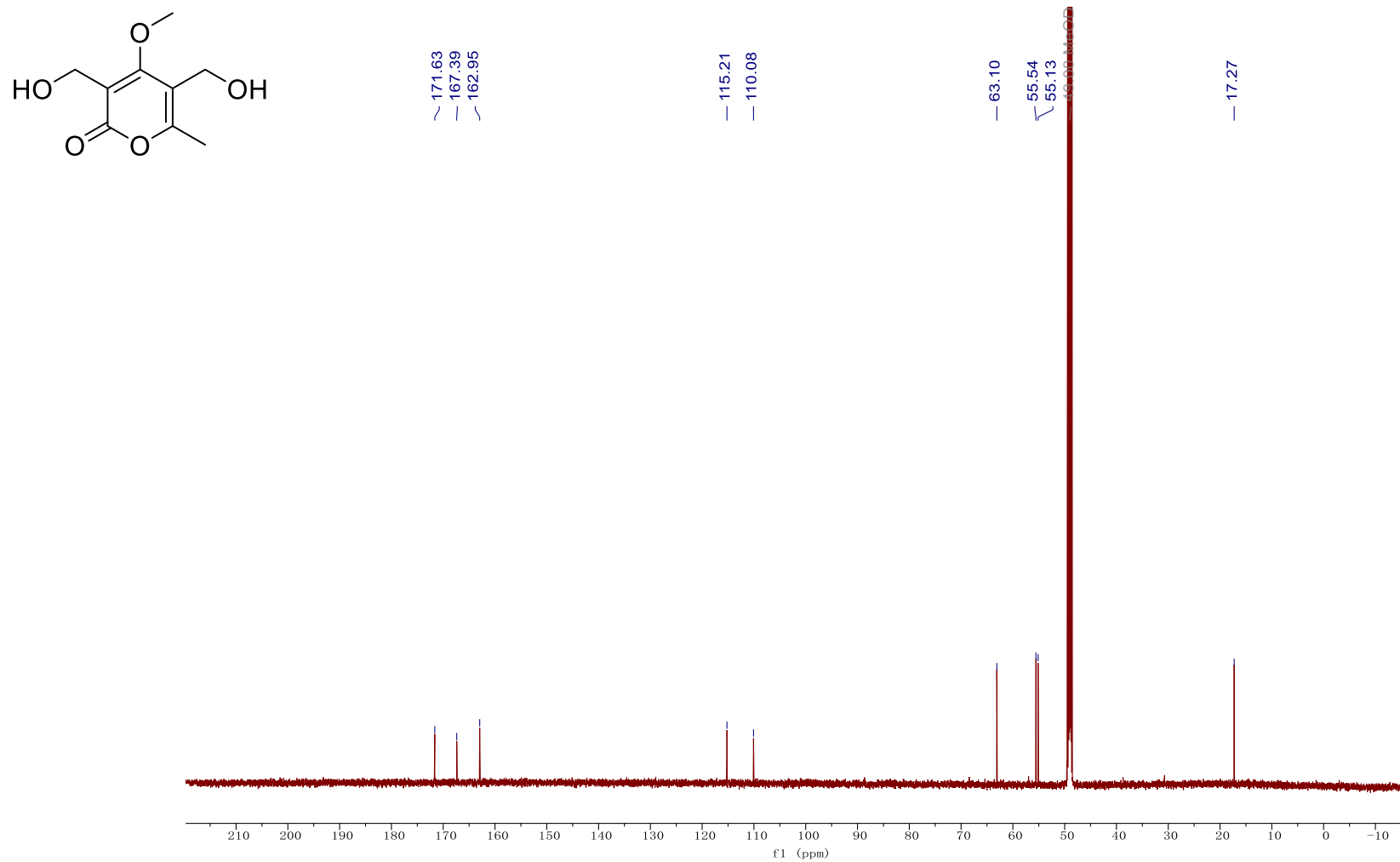
Fig. S69 IR Spectrum of 4.



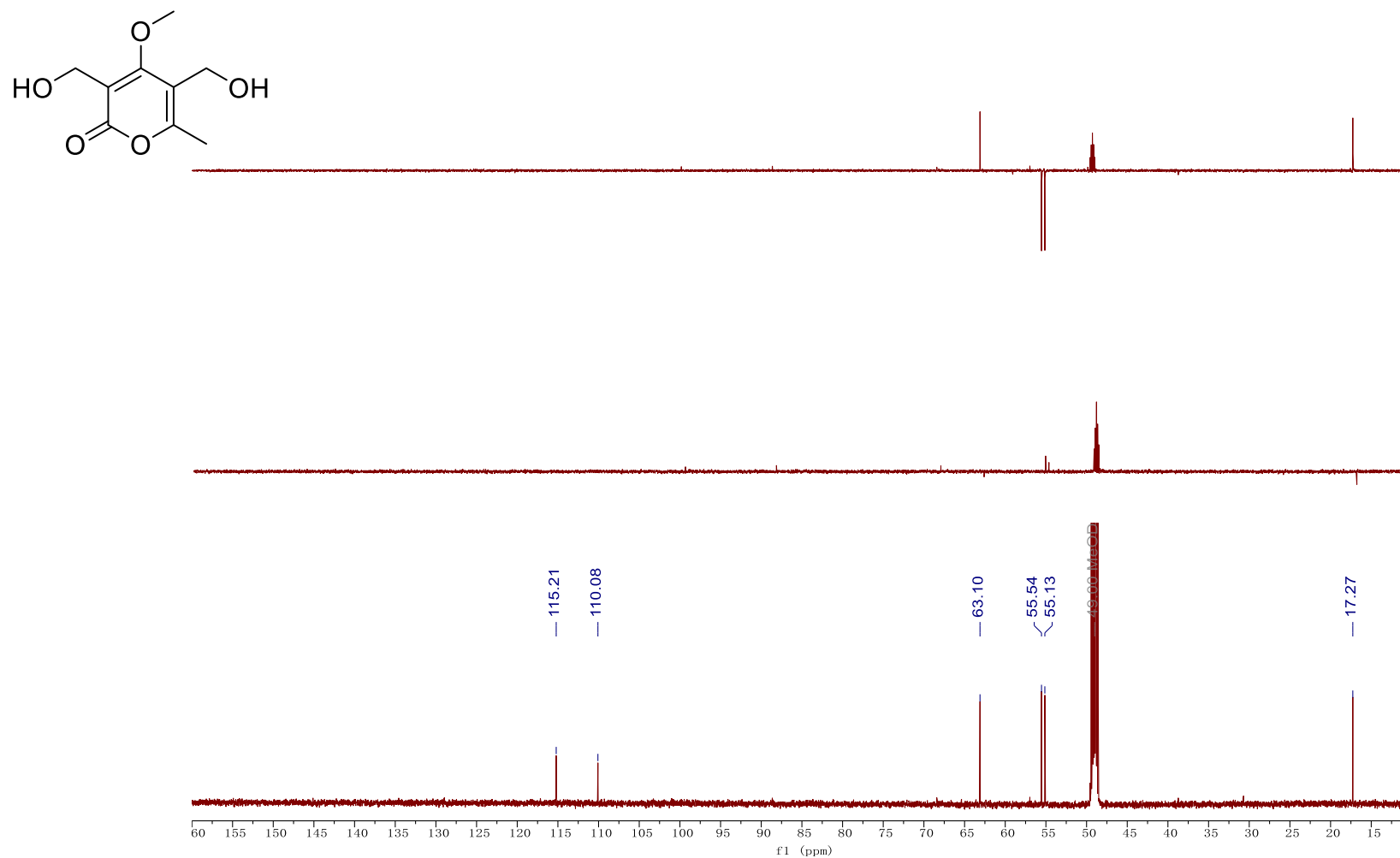
**Fig. S70** UV Spectrum of **4**.



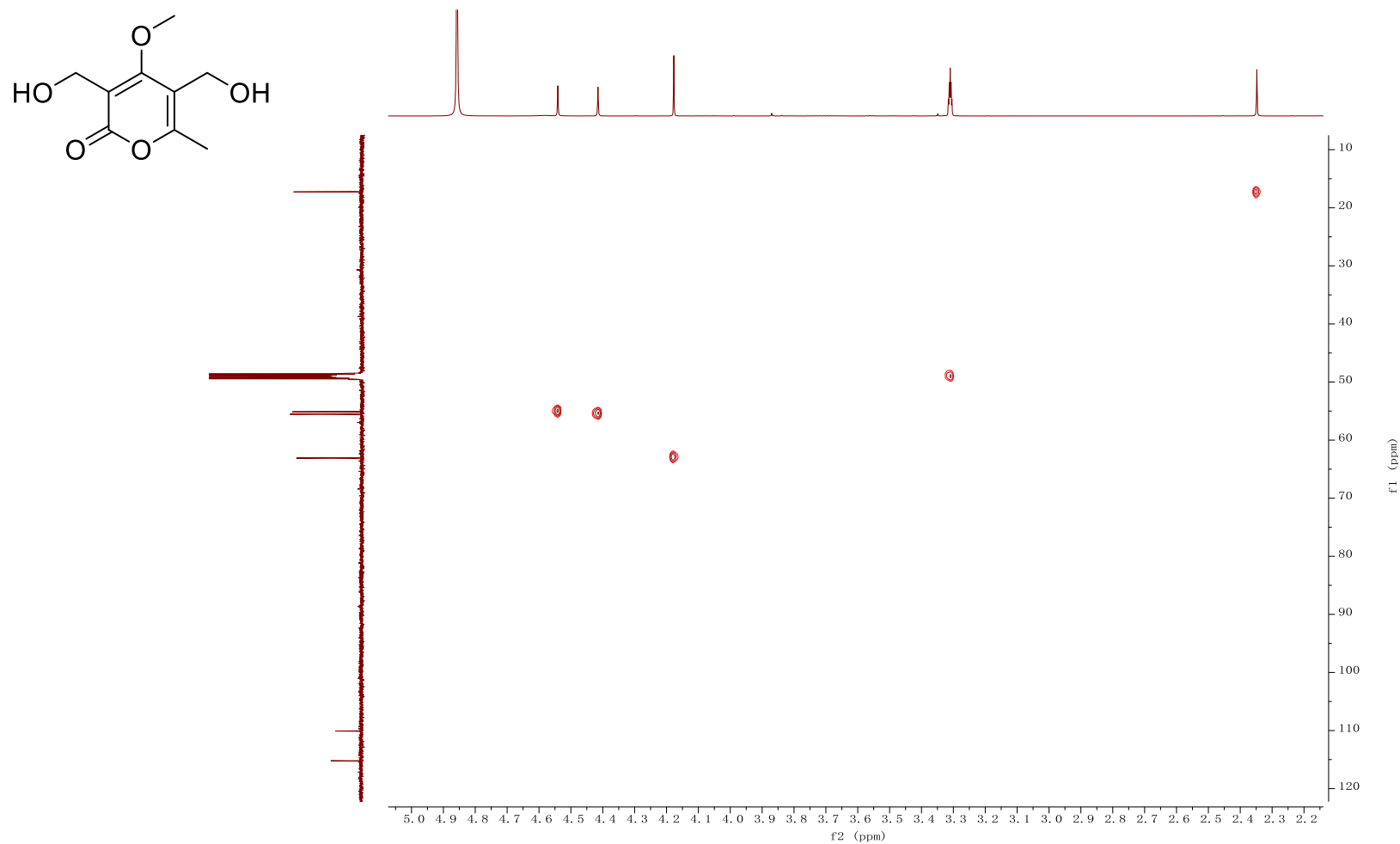
**Fig. S71**  $^1\text{H}$  NMR Spectrum of **5** in methanol- $d_4$  (600 MHz).



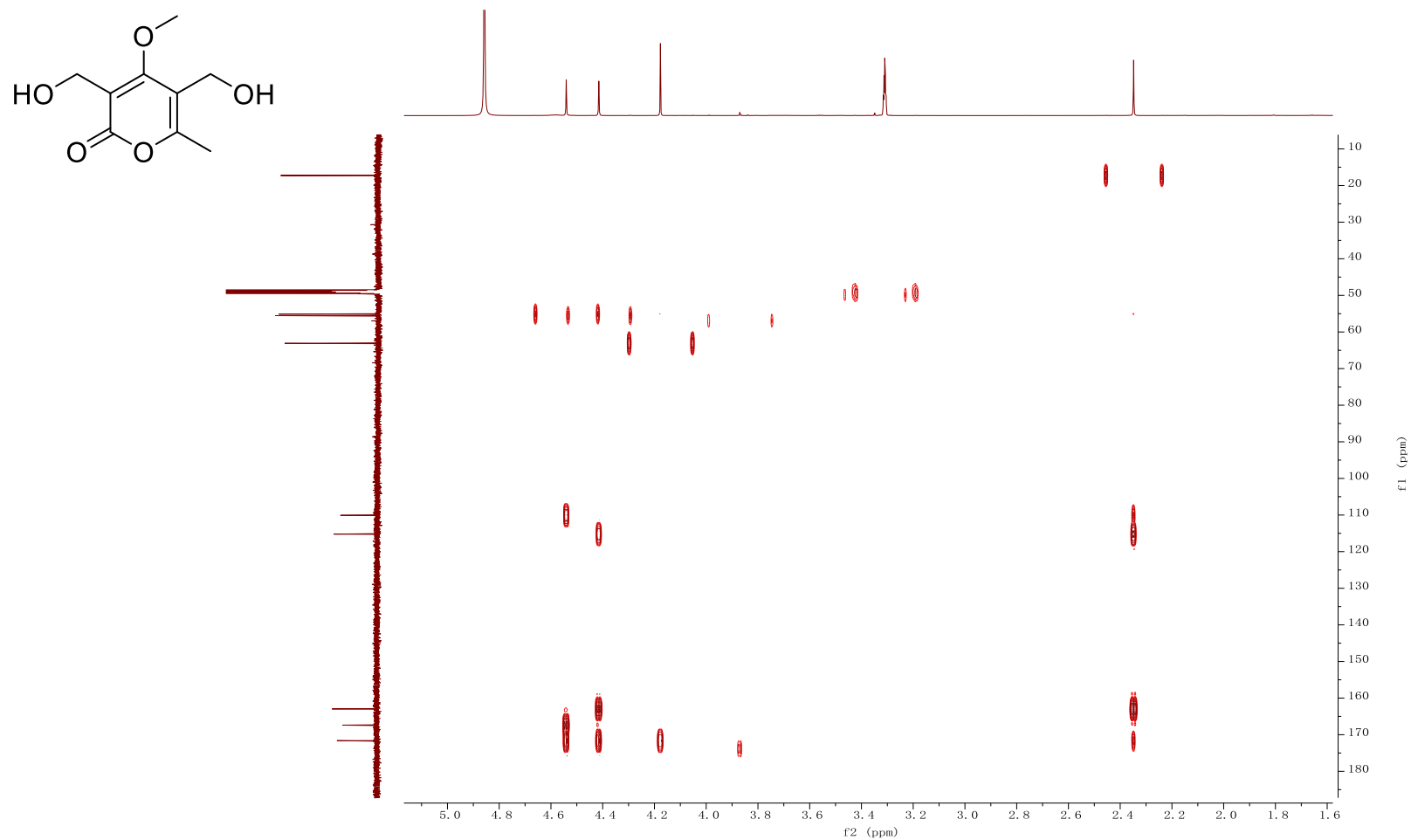
**Fig. S72**  $^{13}\text{C}$  NMR Spectrum of **5** in methanol- $d_4$  (150 MHz).



**Fig. S73** The DEPT Spectrum of **5** in methanol-*d*<sub>4</sub> (150 MHz).

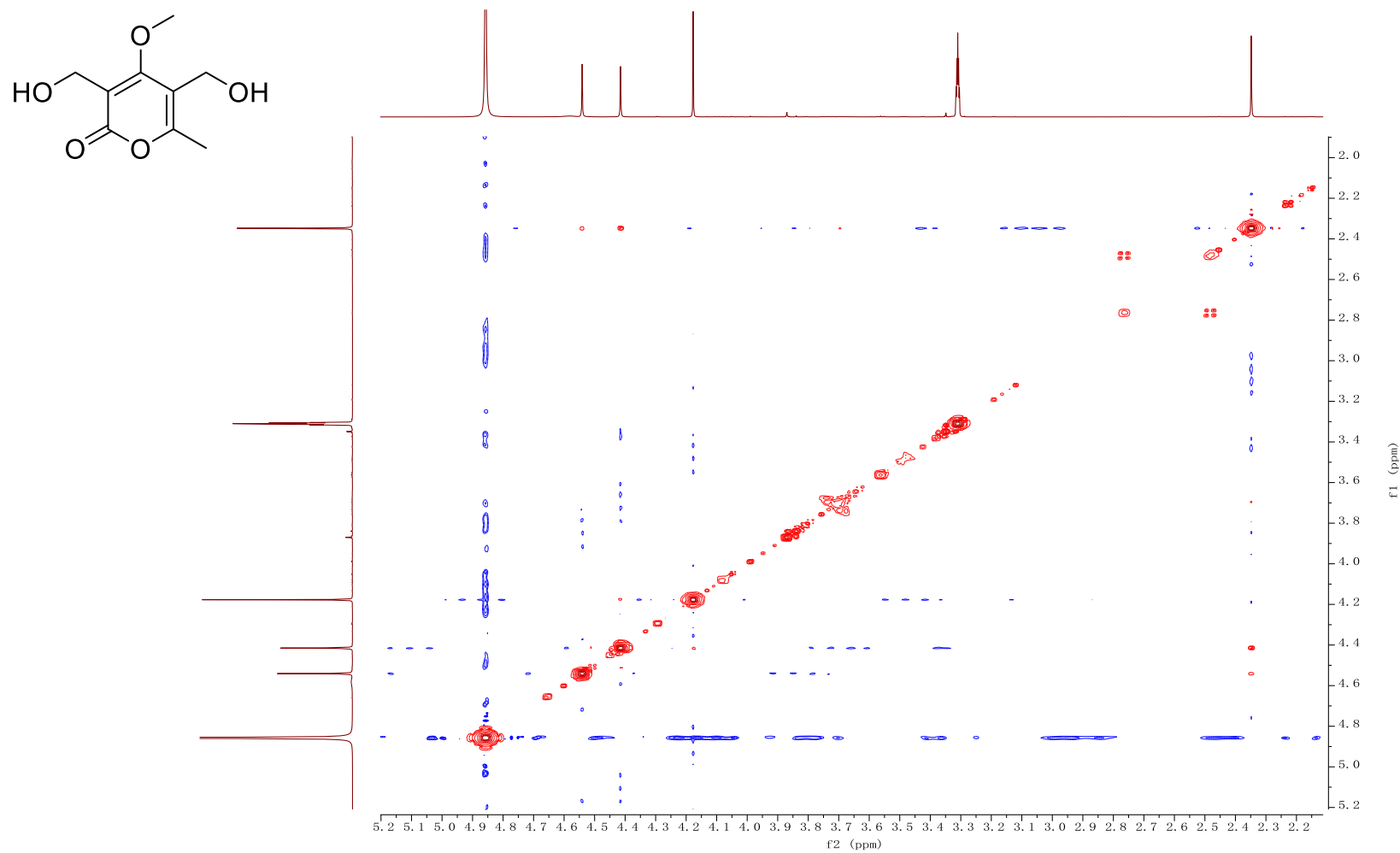


**Fig. S74** HSQC Spectrum of **5** in methanol-*d*<sub>4</sub> (600 MHz).



**Fig. S75** HMBC Spectrum of **5** in methanol-*d*<sub>4</sub> (600 MHz).





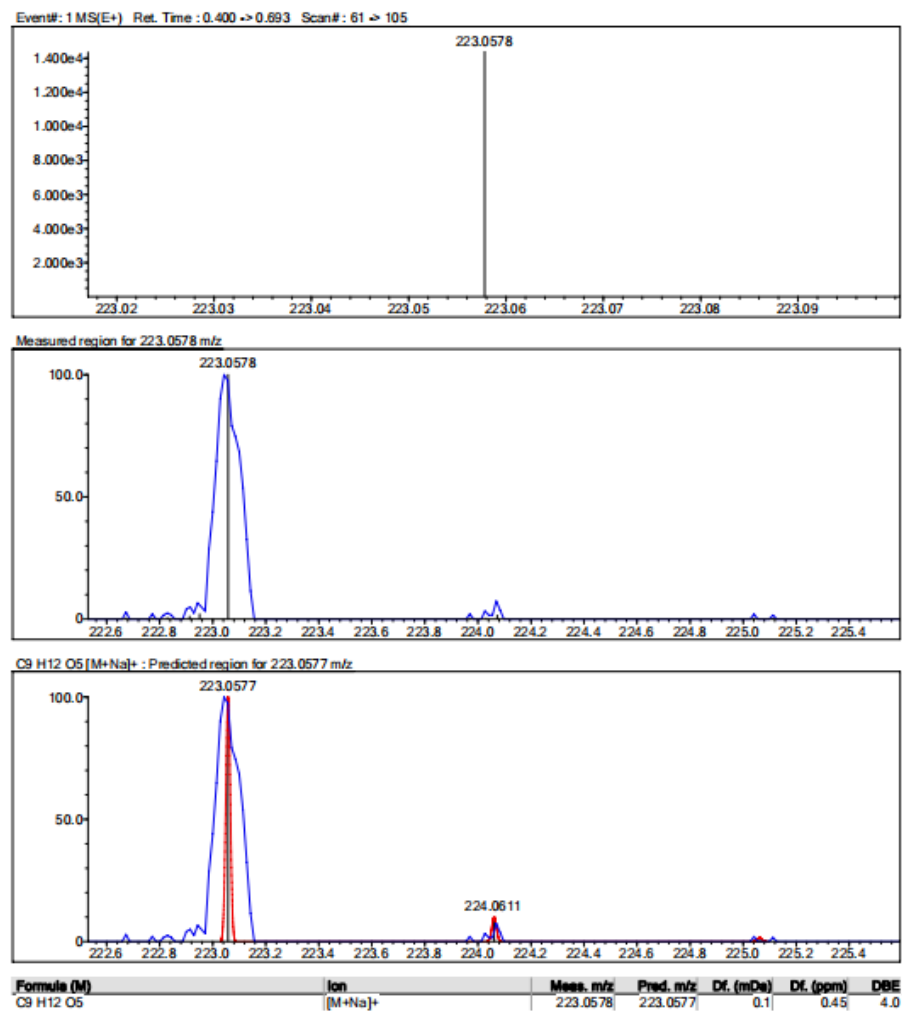
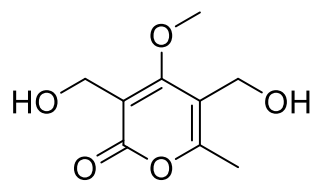
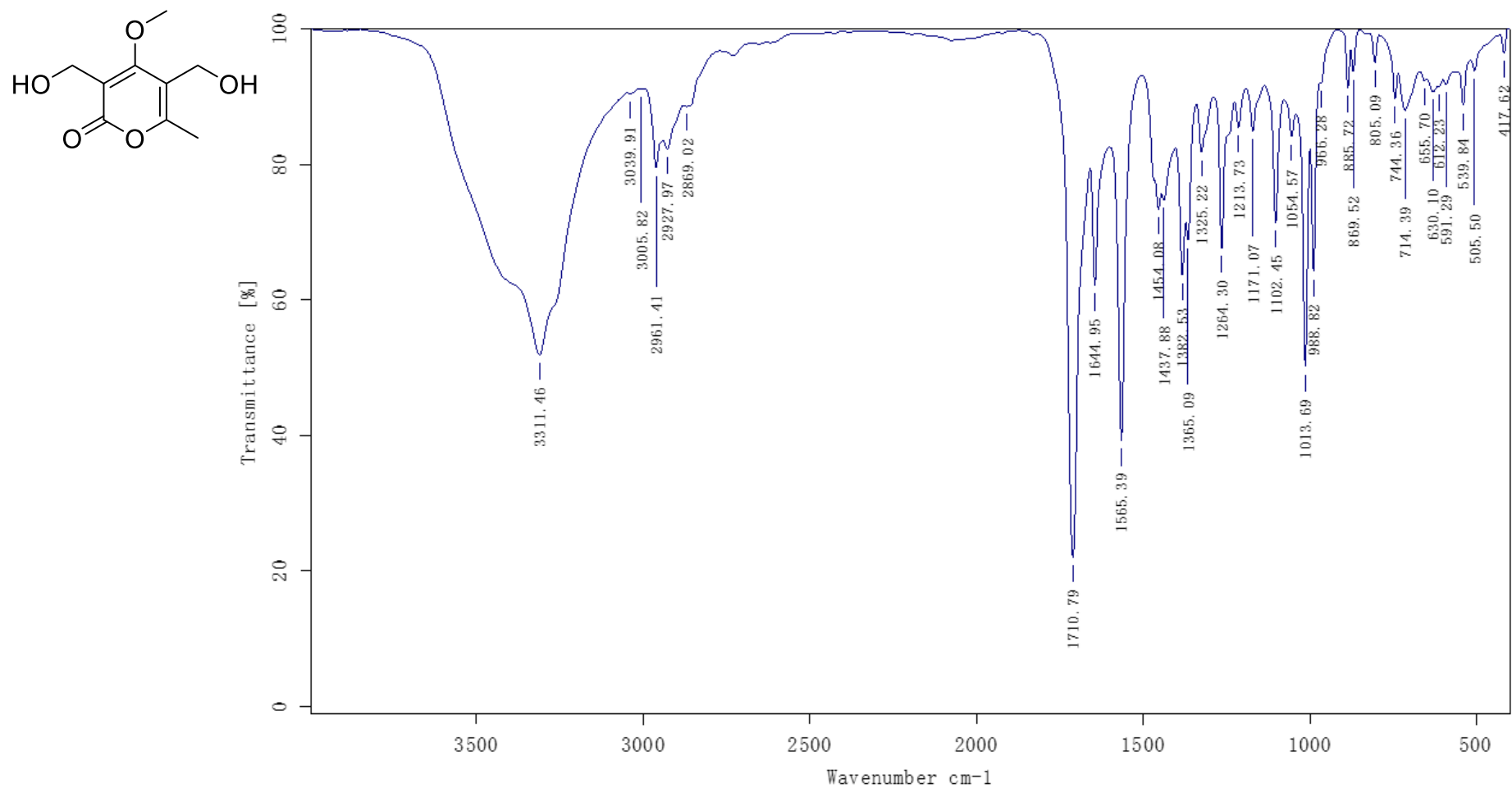
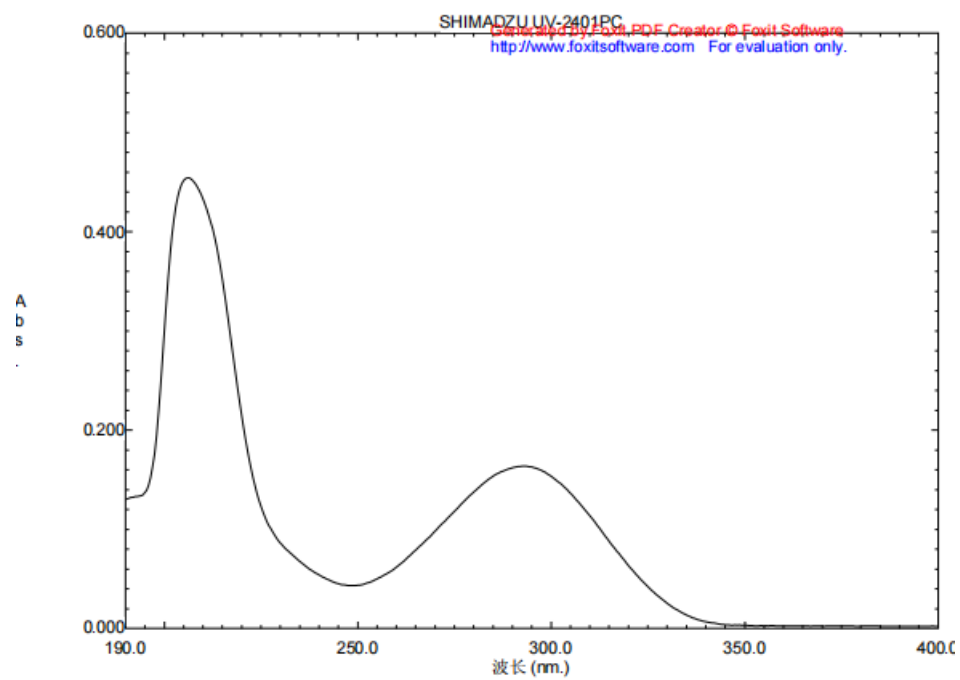
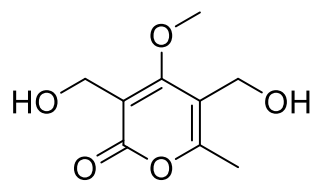


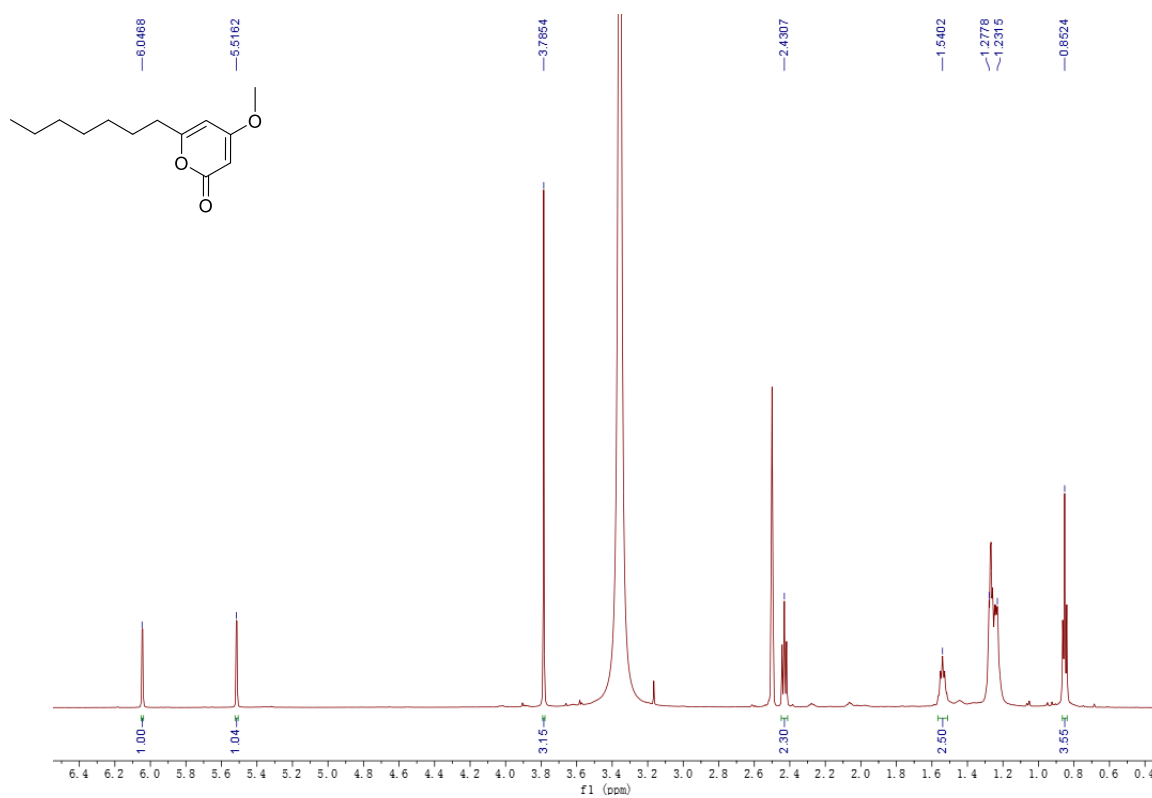
Fig. S77 HRESIMS Spectrum of 5.



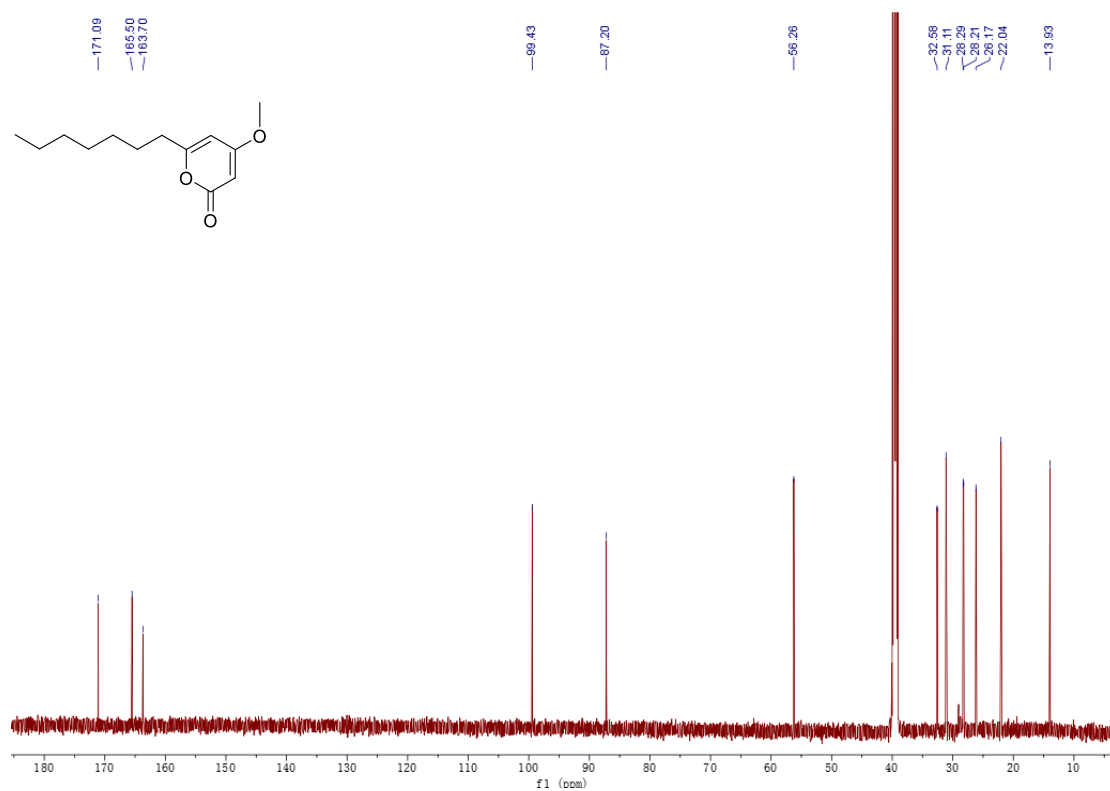
**Fig. S78** IR Spectrum of **5**.



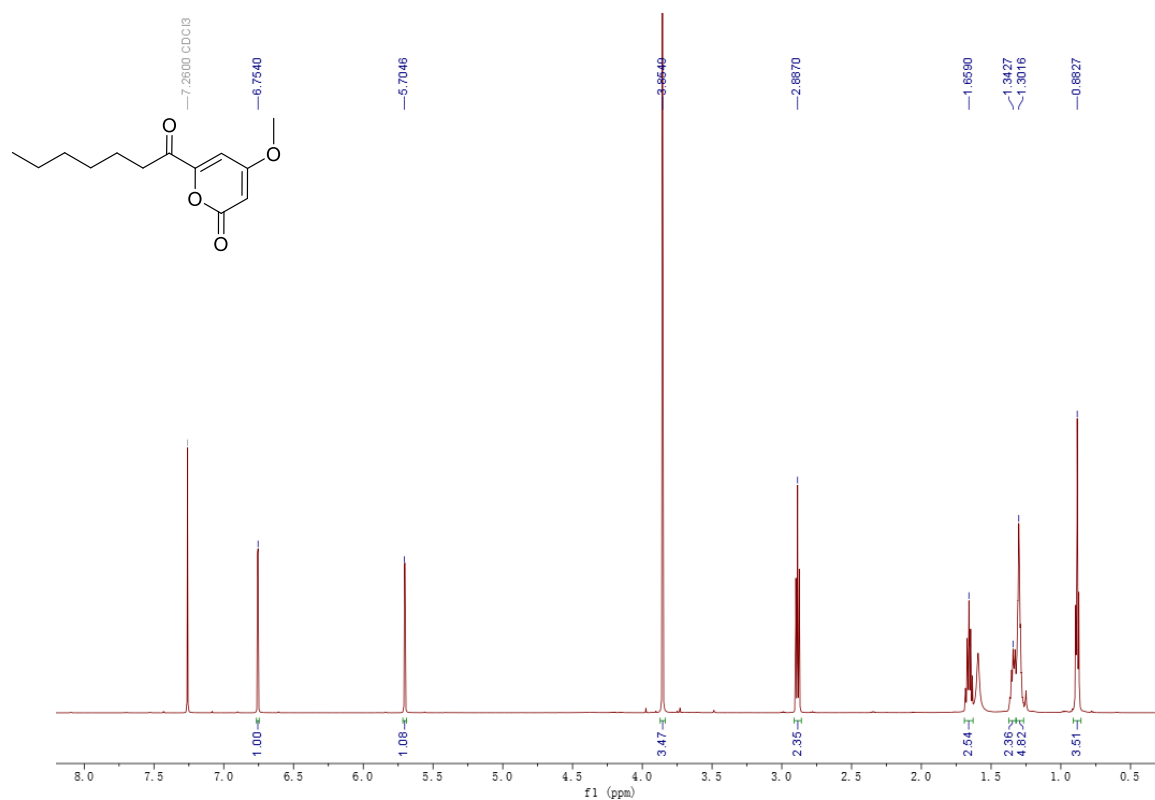
**Fig. S79** UV Spectrum of **5**.



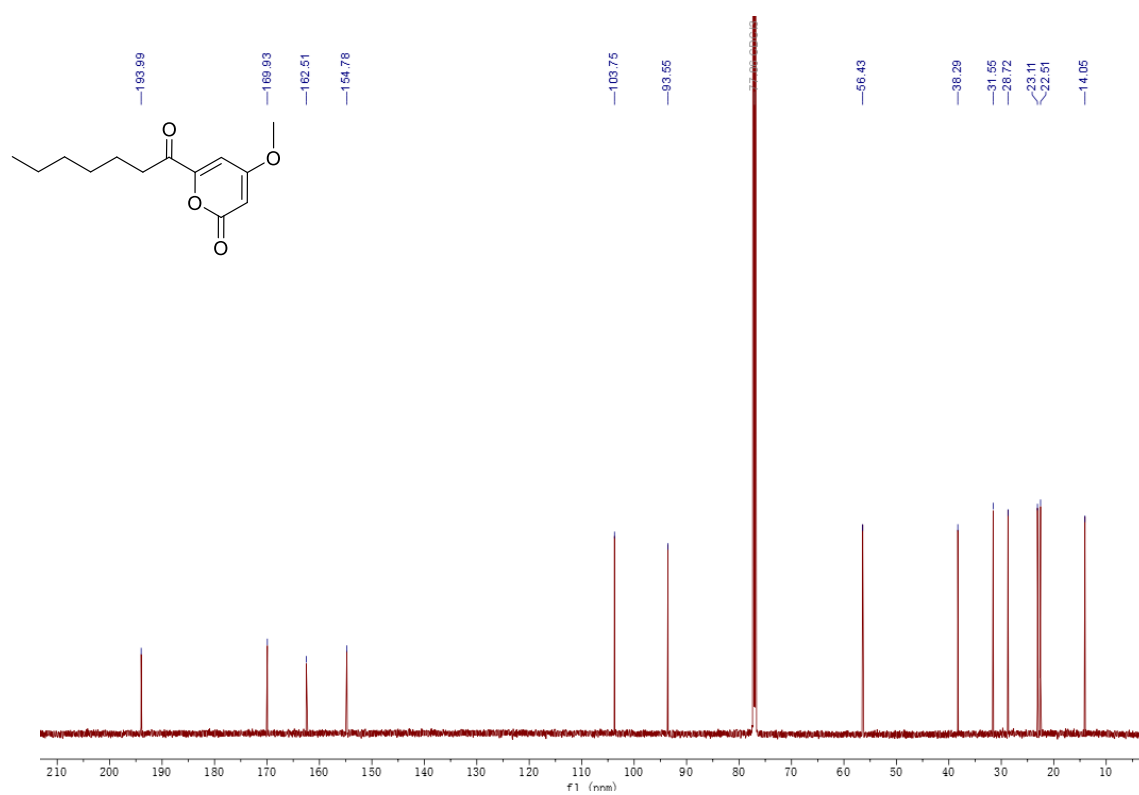
**Fig. S80** <sup>1</sup>H NMR spectrum of **6** in DMSO-*d*<sub>6</sub> (600 MHz).



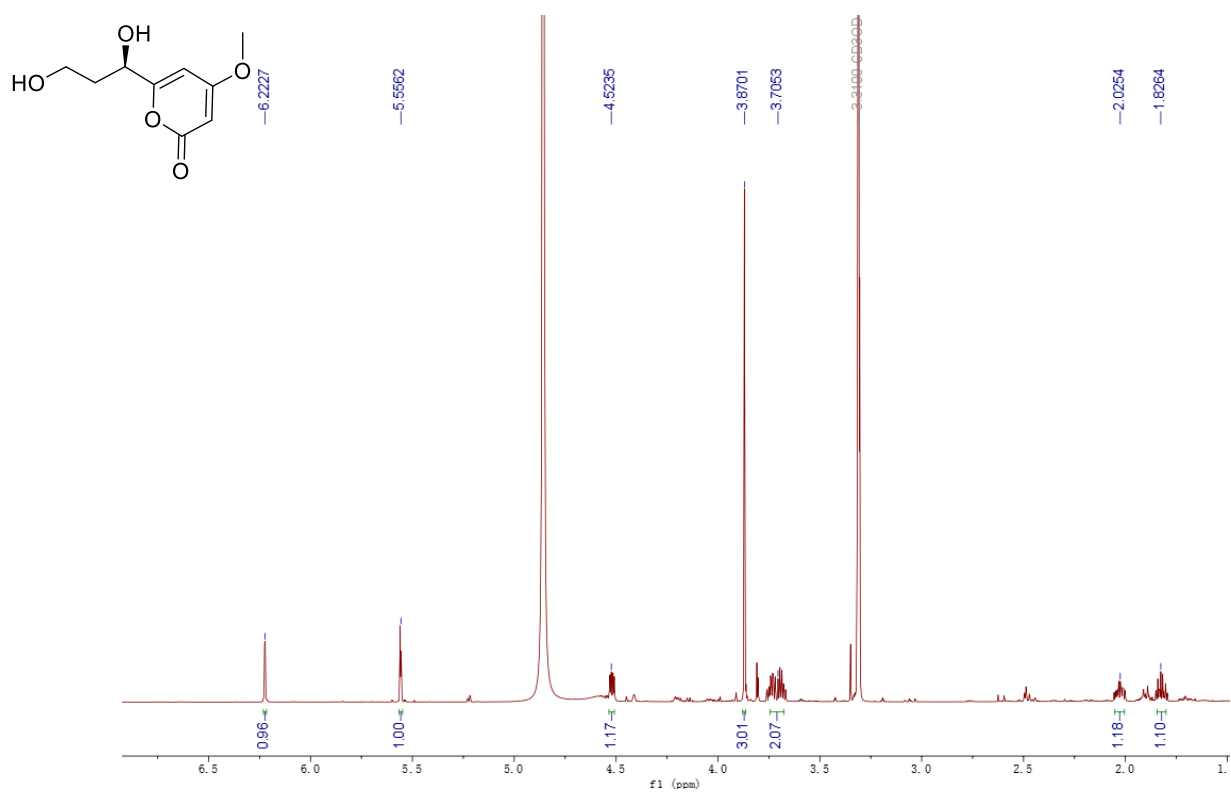
**Fig. S81** <sup>13</sup>C NMR spectrum of **6** in DMSO-*d*<sub>6</sub> (150 MHz).



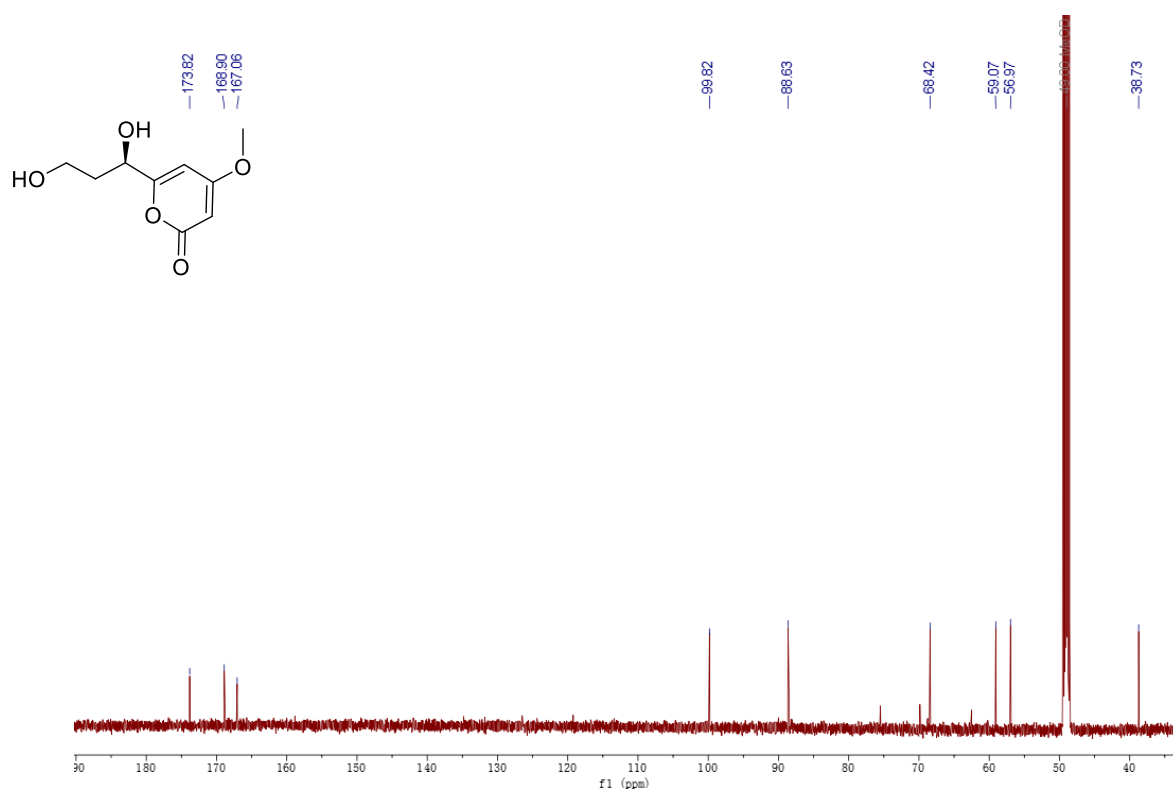
**Fig. S82** <sup>1</sup>H NMR spectrum of **7** in chloroform-*d* (600 MHz).



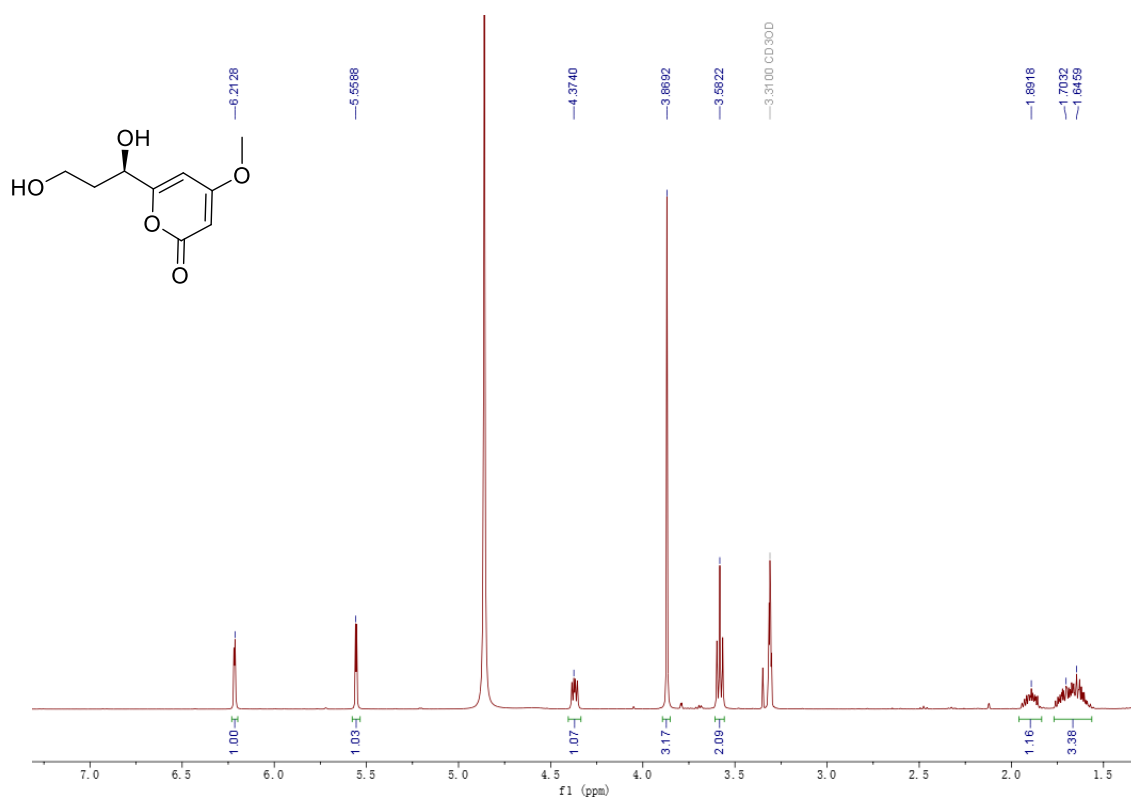
**Fig. S83** <sup>13</sup>C NMR spectrum of **7** in chloroform-*d* (150 MHz).



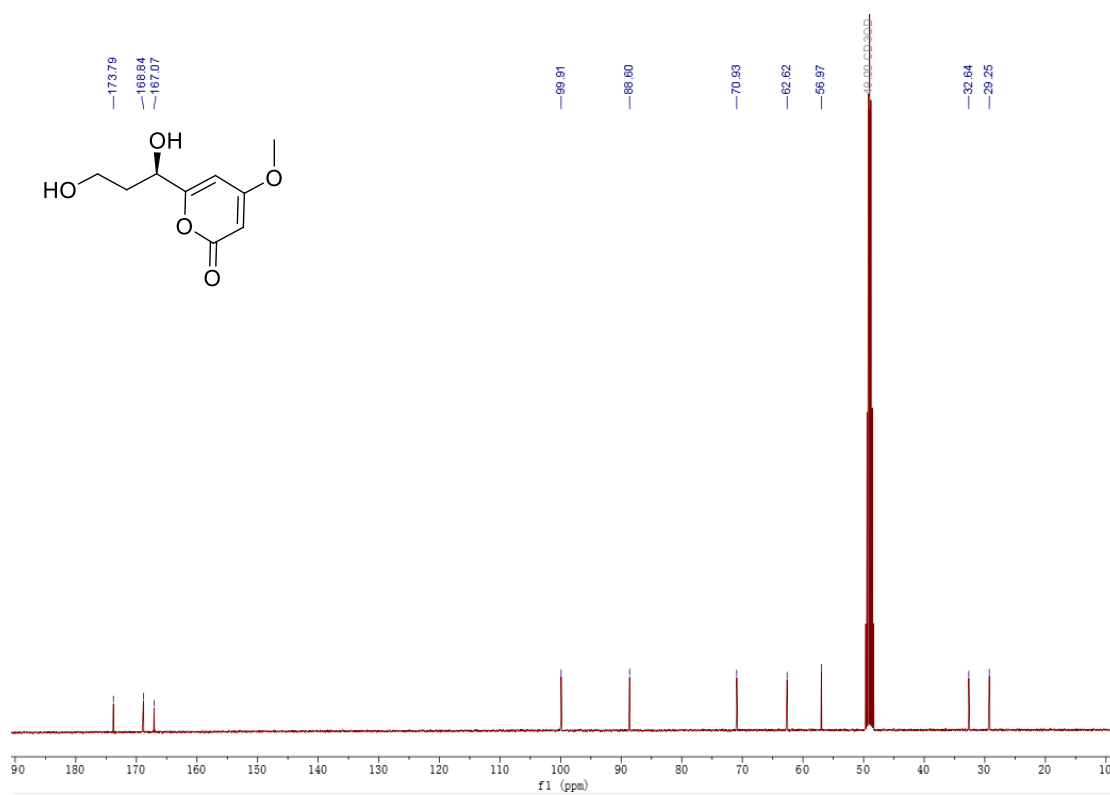
**Fig. S84** <sup>1</sup>H NMR spectrum of **8** in methanol-*d*<sub>4</sub> (600 MHz).



**Fig. S85** <sup>13</sup>C NMR spectrum of **8** in methanol-*d*<sub>4</sub> (150 MHz).

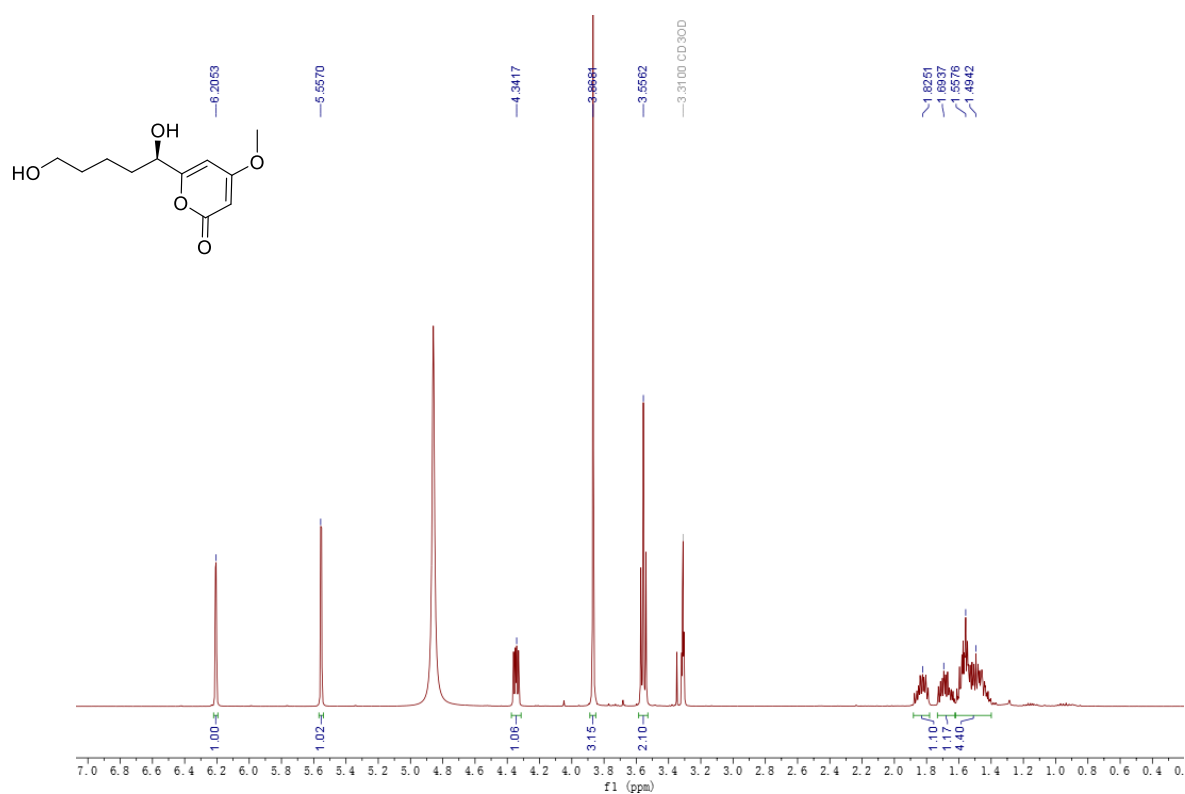


**Fig. S86** <sup>1</sup>H NMR spectrum of **9** in methanol-*d*<sub>4</sub> (600 MHz).

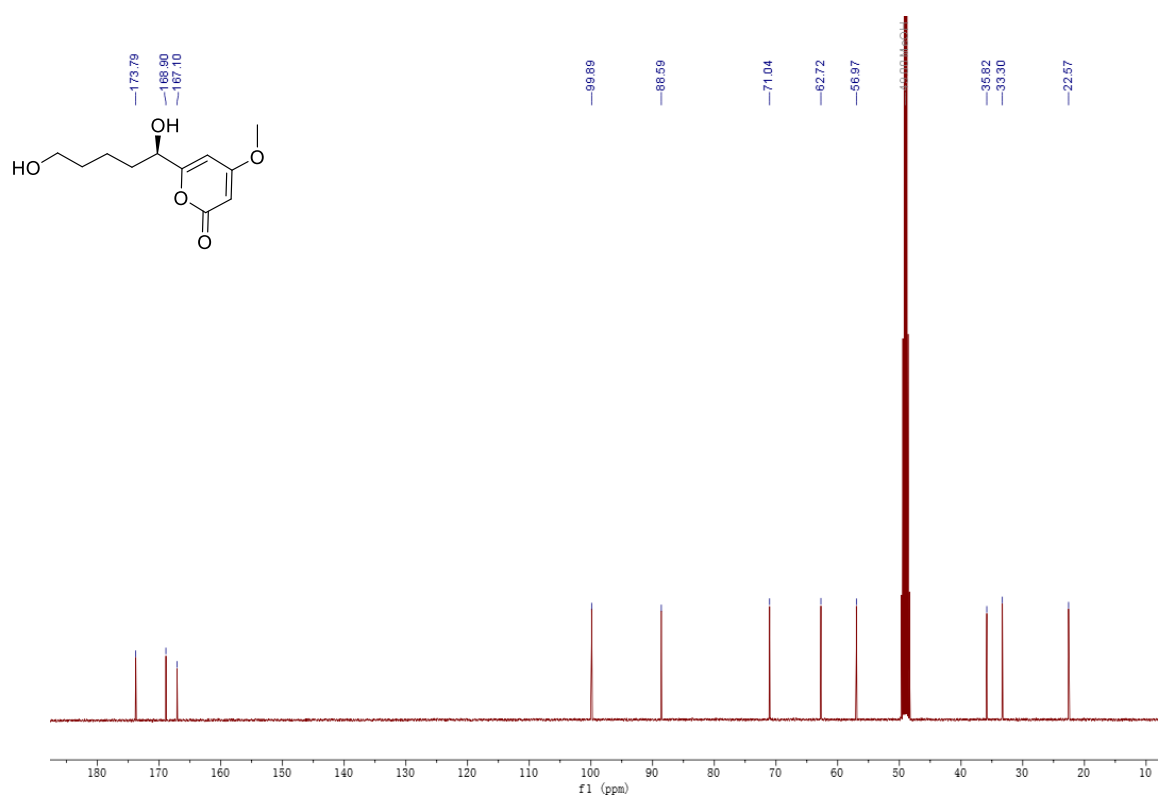


**Fig. S87** <sup>13</sup>C NMR spectrum of **9** in methanol-*d*<sub>4</sub> (150 MHz).

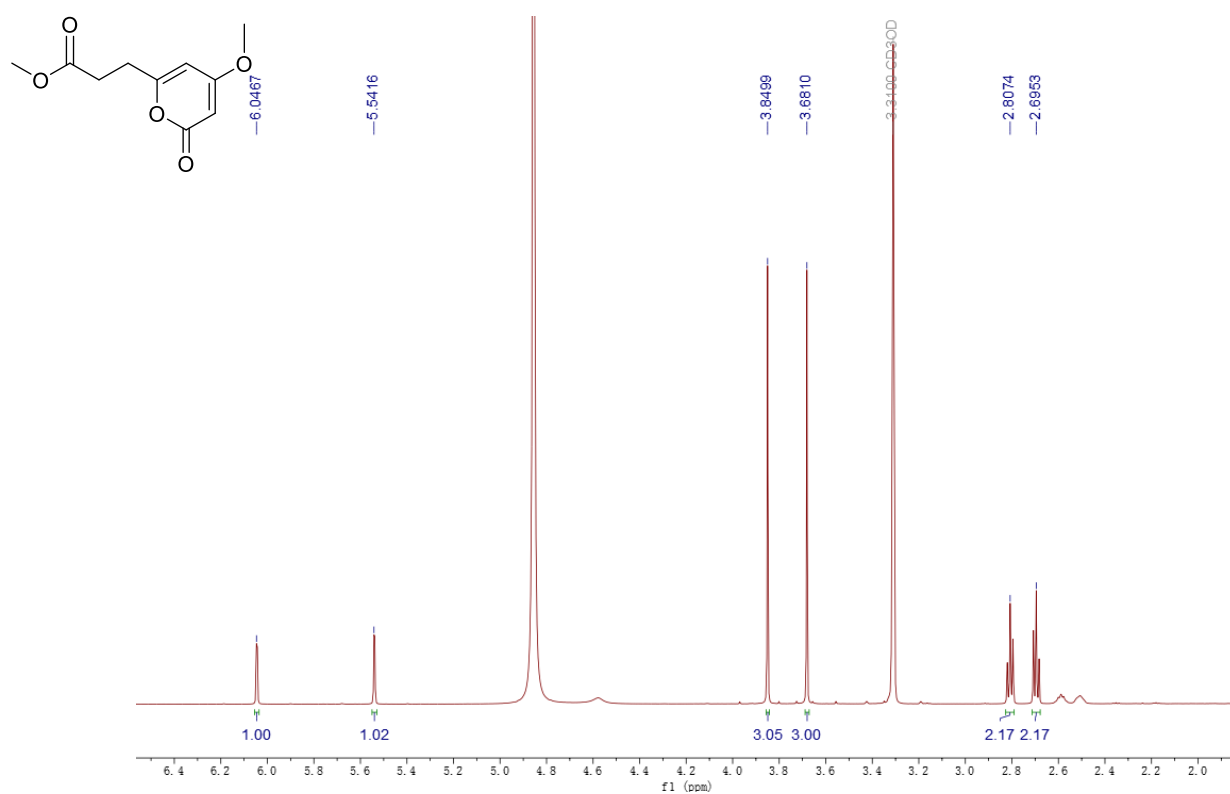




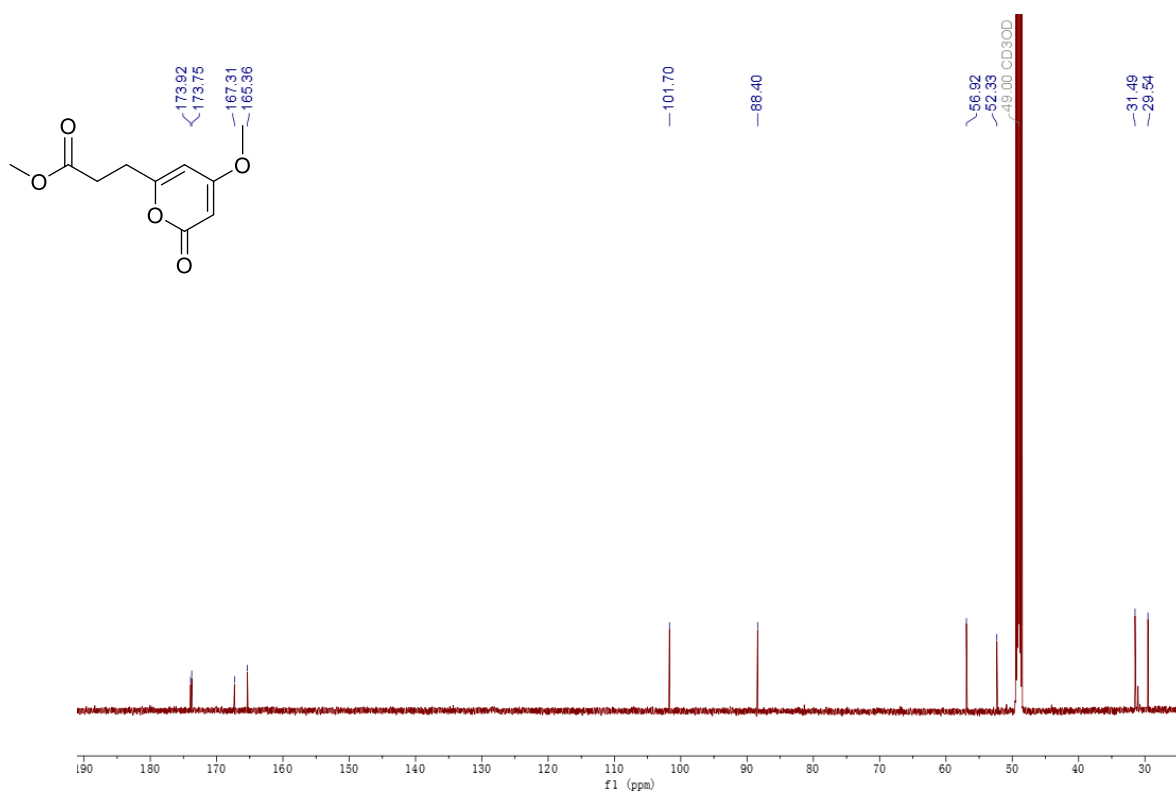
**Fig. S88** <sup>1</sup>H NMR spectrum of **10** in methanol-*d*<sub>4</sub> (400 MHz).



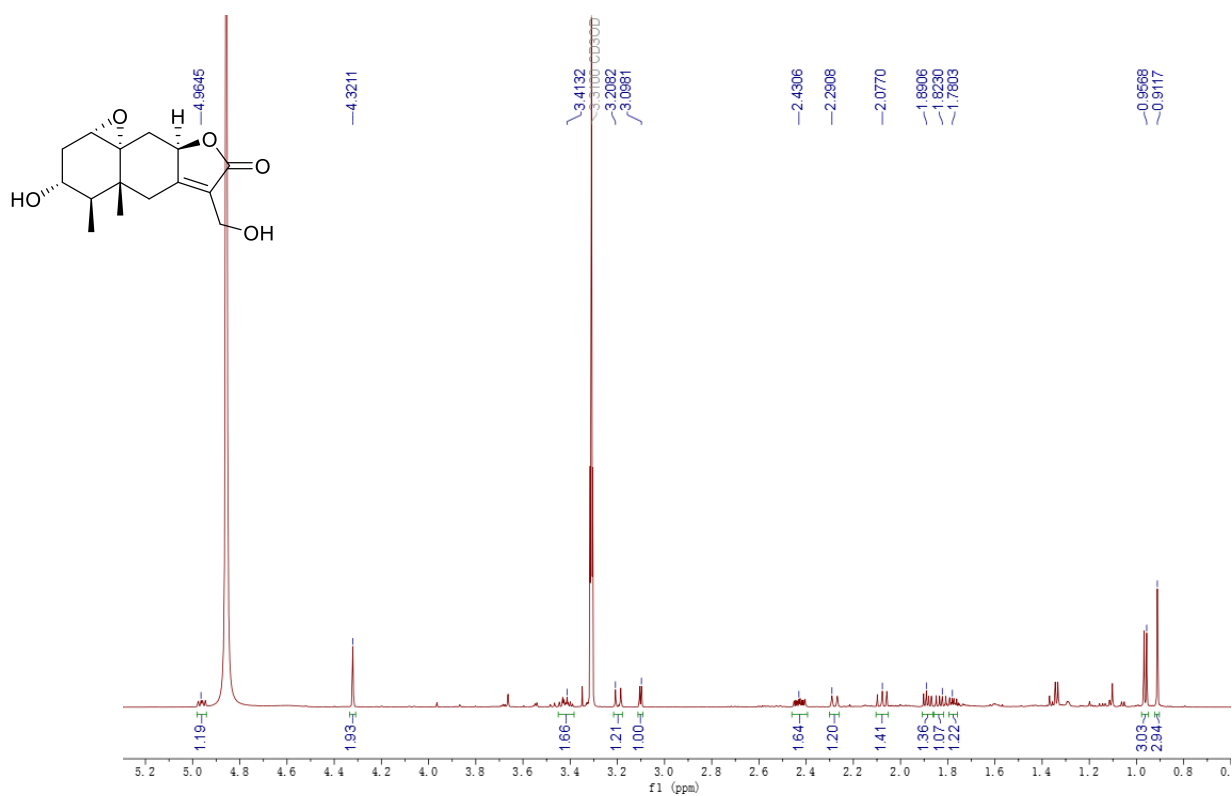
**Fig. S89** <sup>13</sup>C NMR spectrum of **10** in methanol-*d*<sub>4</sub> (100 MHz).



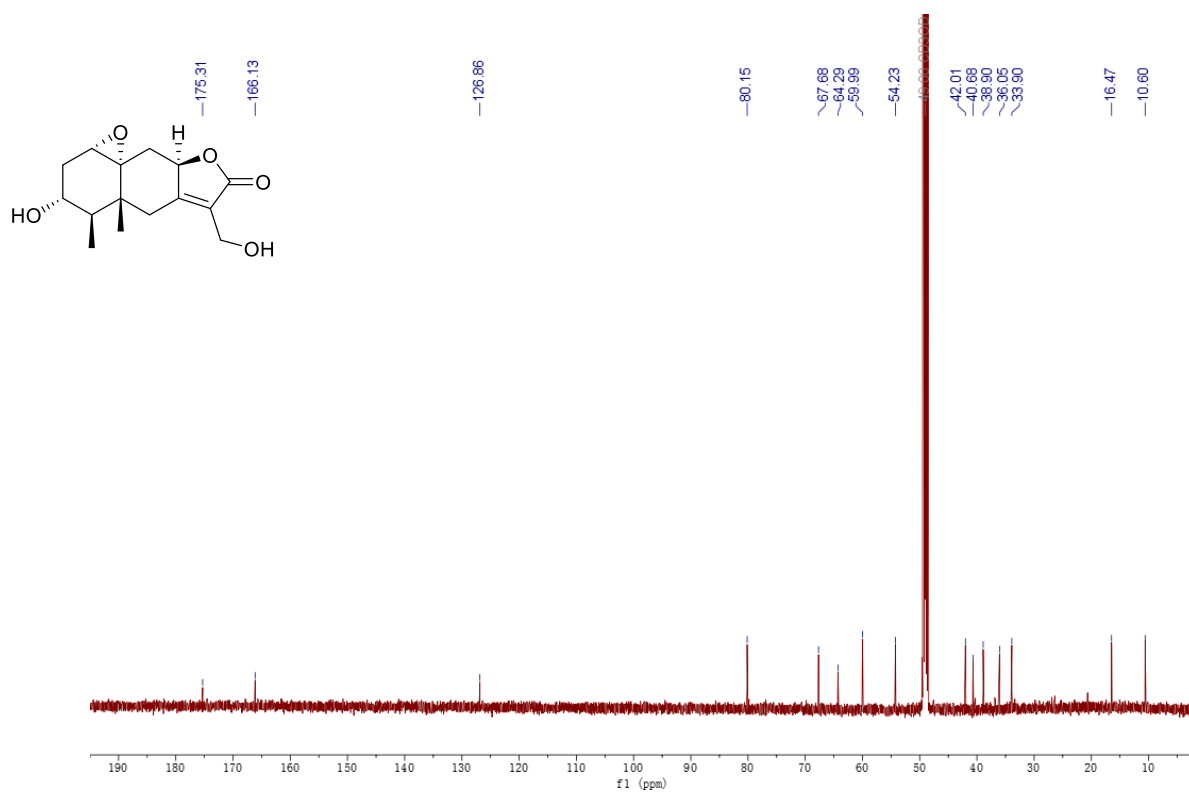
**Fig. S90** <sup>1</sup>H NMR spectrum of **11** in methanol-*d*<sub>4</sub> (600 MHz).



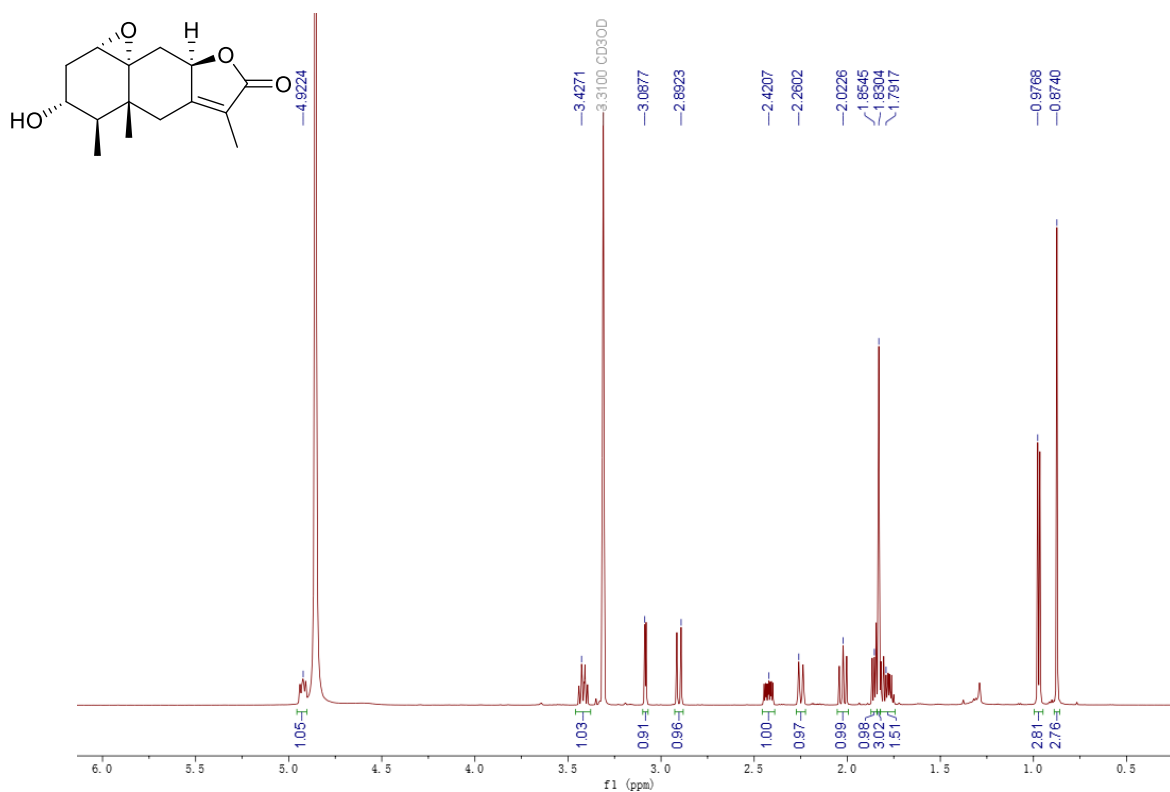
**Fig. S91** <sup>13</sup>C NMR spectrum of **11** in methanol-*d*<sub>4</sub> (150 MHz).



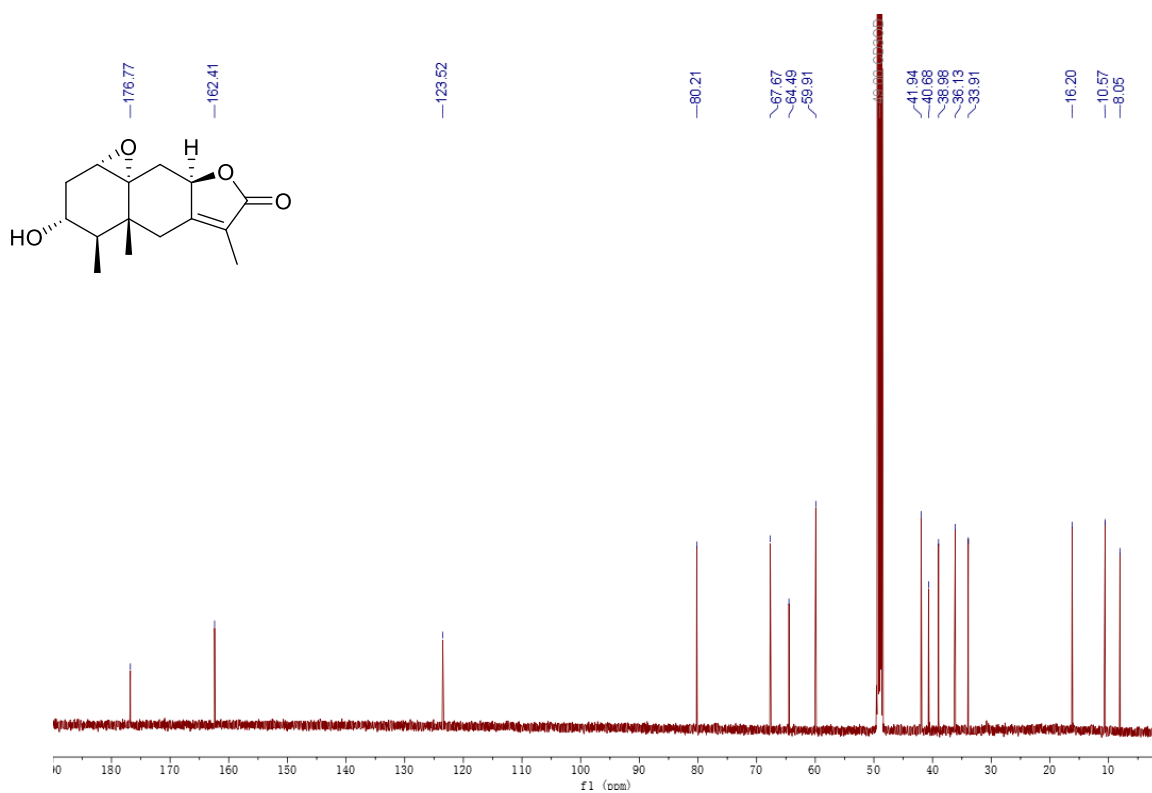
**Fig. S92**  $^1\text{H}$  NMR spectrum of **12** in methanol- $d_4$  (600 MHz).



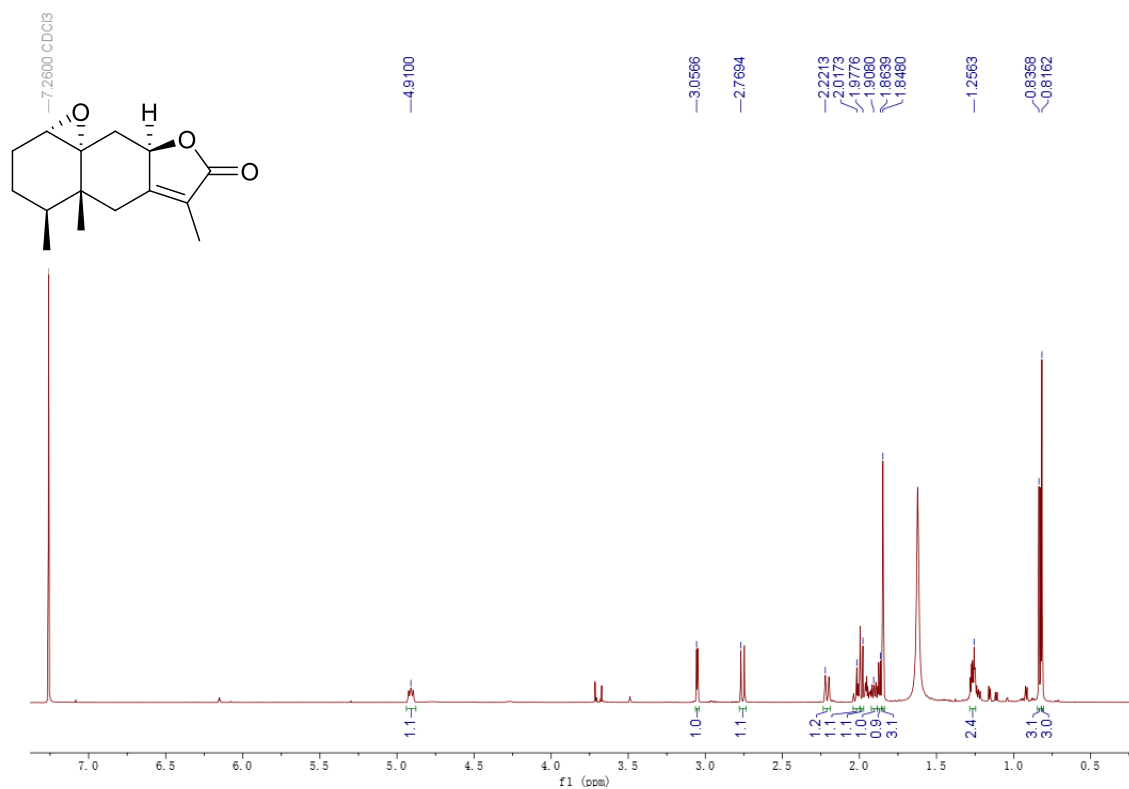
**Fig. S93**  $^{13}\text{C}$  NMR spectrum of **12** in methanol- $d_4$  (150 MHz).



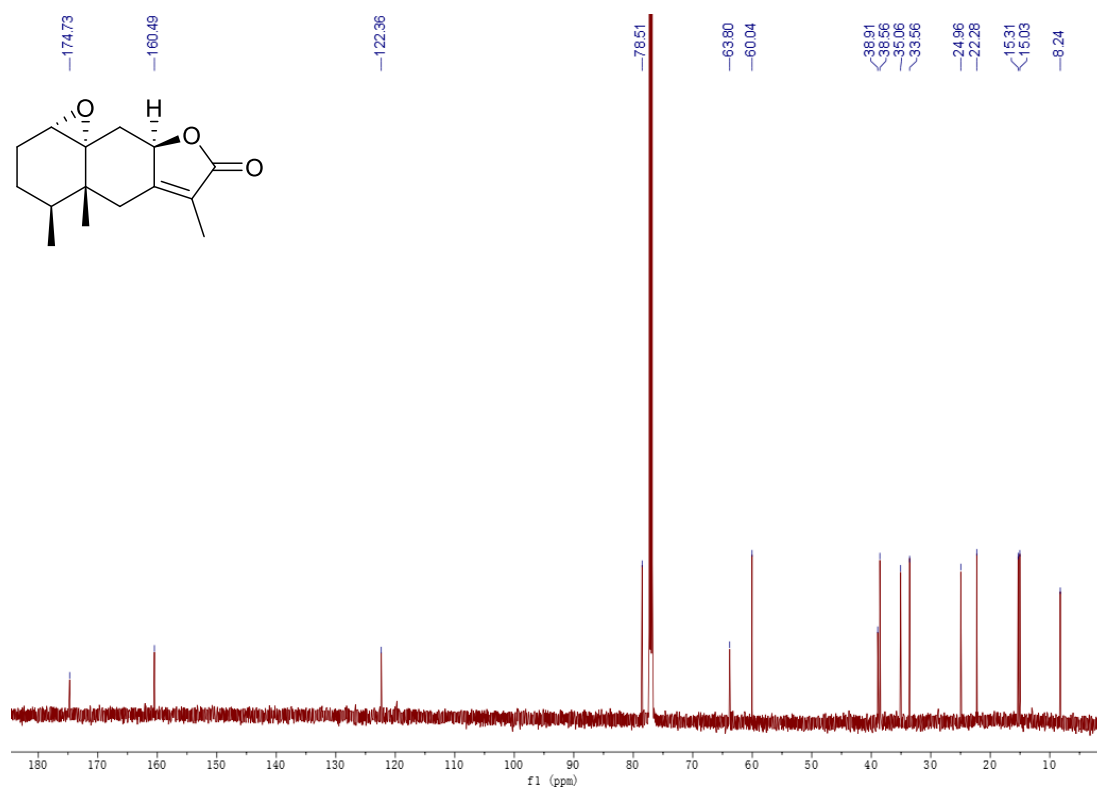
**Fig. S94** <sup>1</sup>H NMR spectrum of **13** in methanol-*d*<sub>4</sub> (600 MHz).



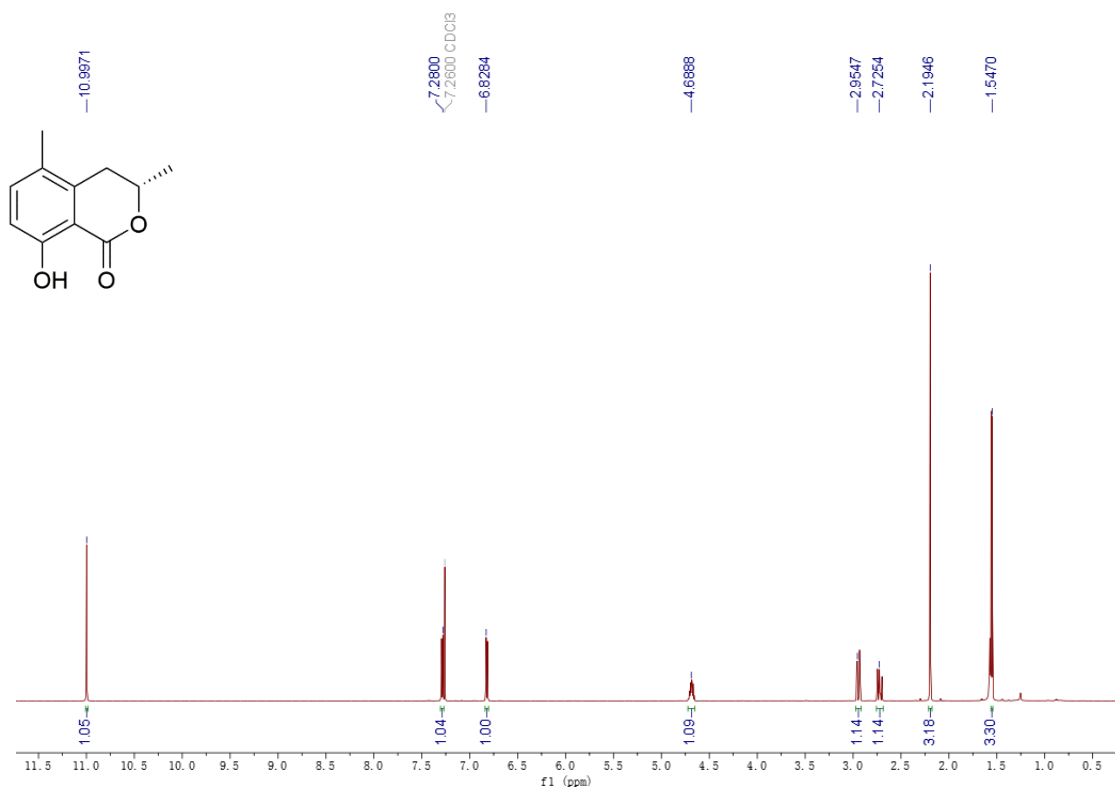
**Fig. S95** <sup>13</sup>C NMR spectrum of **13** in methanol-*d*<sub>4</sub> (150 MHz).



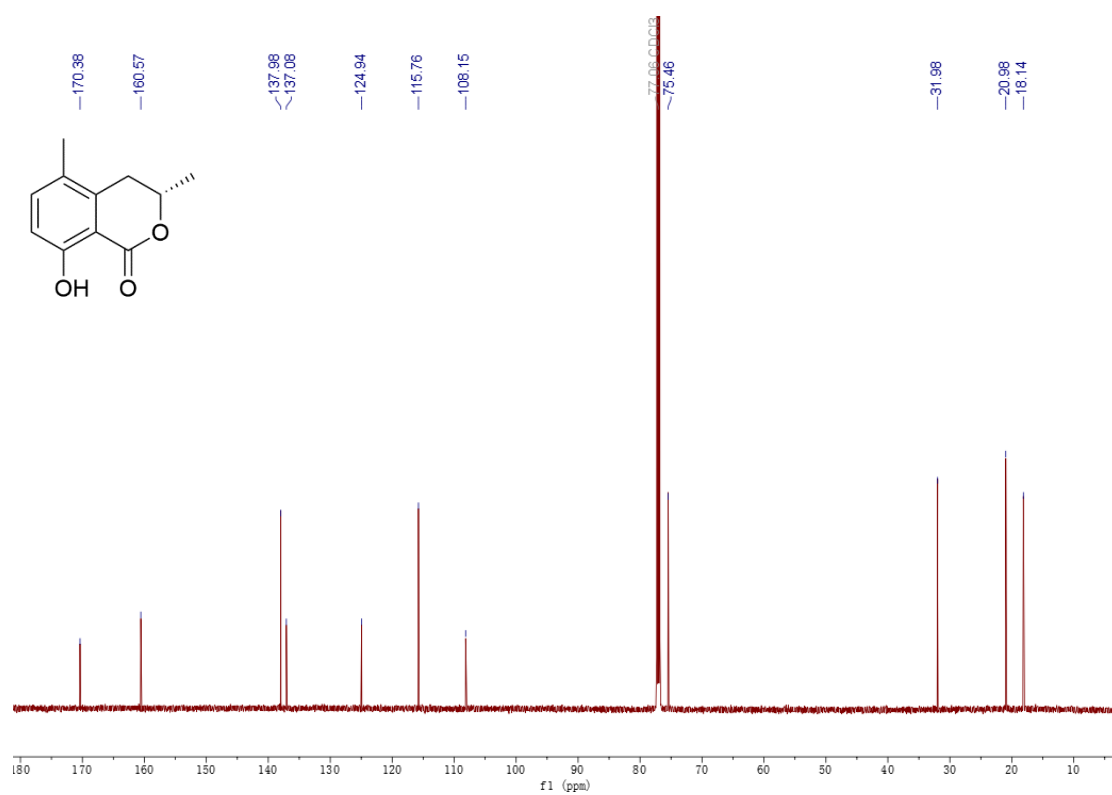
**Fig. S96** <sup>1</sup>H NMR spectrum of **14** in chloroform-*d* (600 MHz).



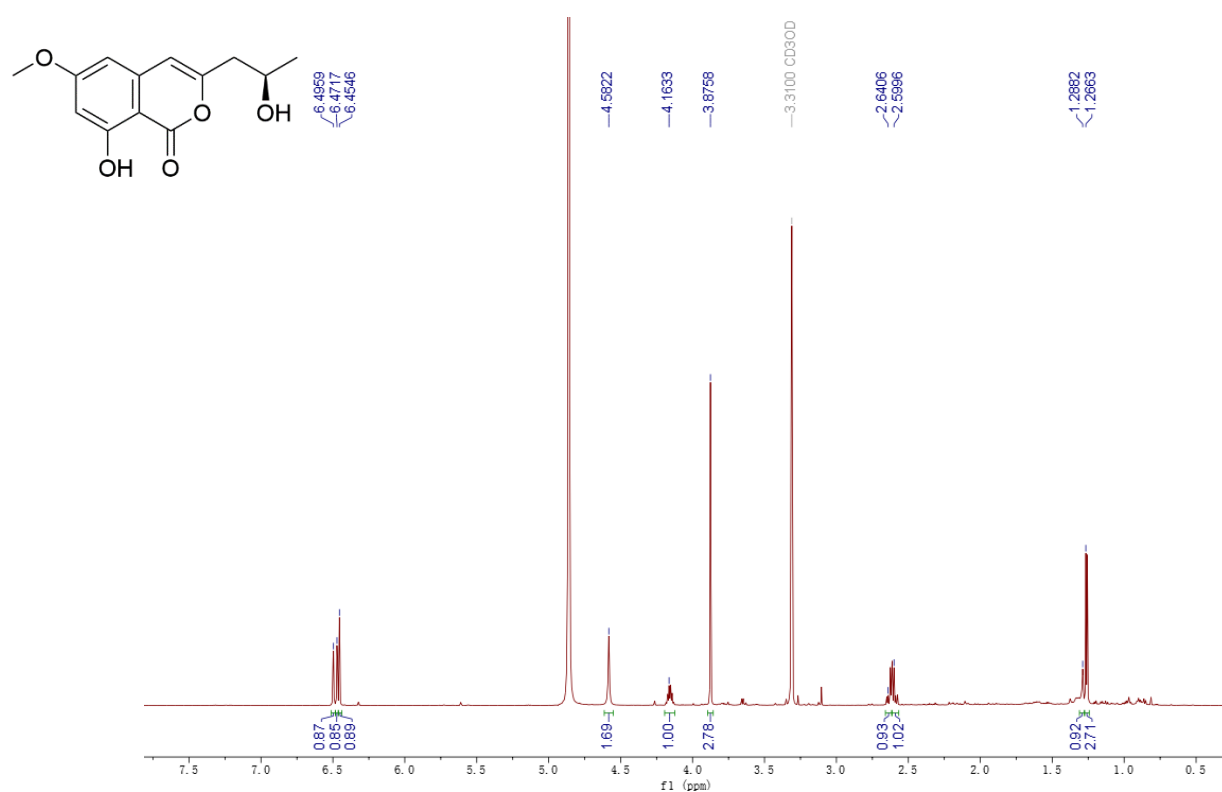
**Fig. S97** <sup>13</sup>C NMR spectrum of **14** in chloroform-*d* (150 MHz).



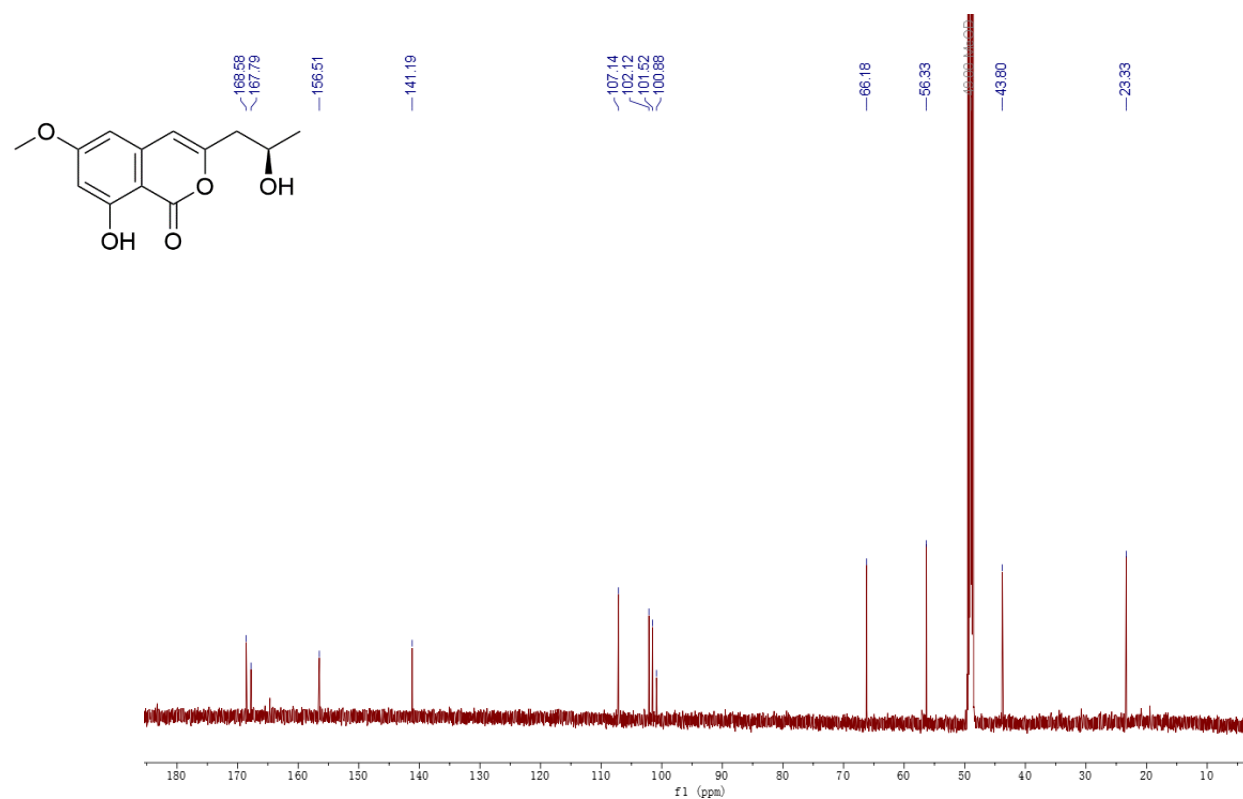
**Fig. S98** <sup>1</sup>H NMR spectrum of **15** in chloroform-*d* (600 MHz).



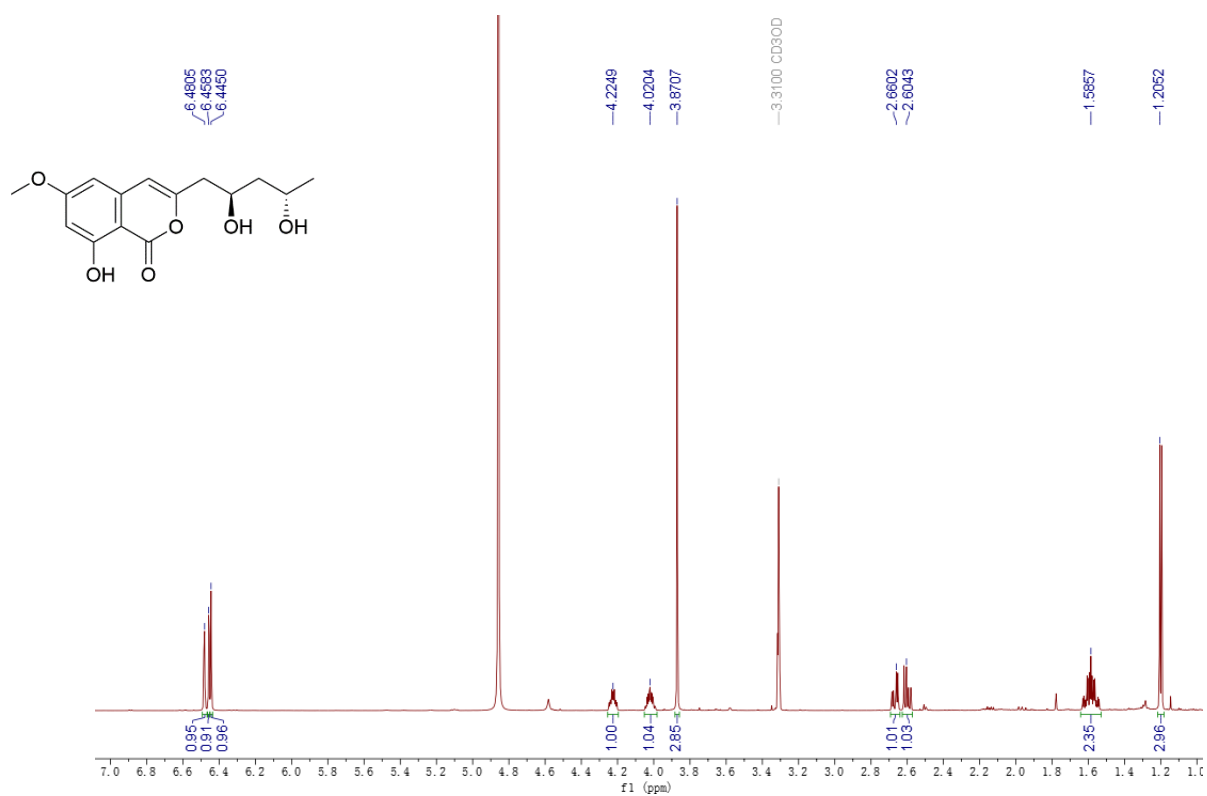
**Fig. S99** <sup>13</sup>C NMR spectrum of **15** in chloroform-*d* (150 MHz).



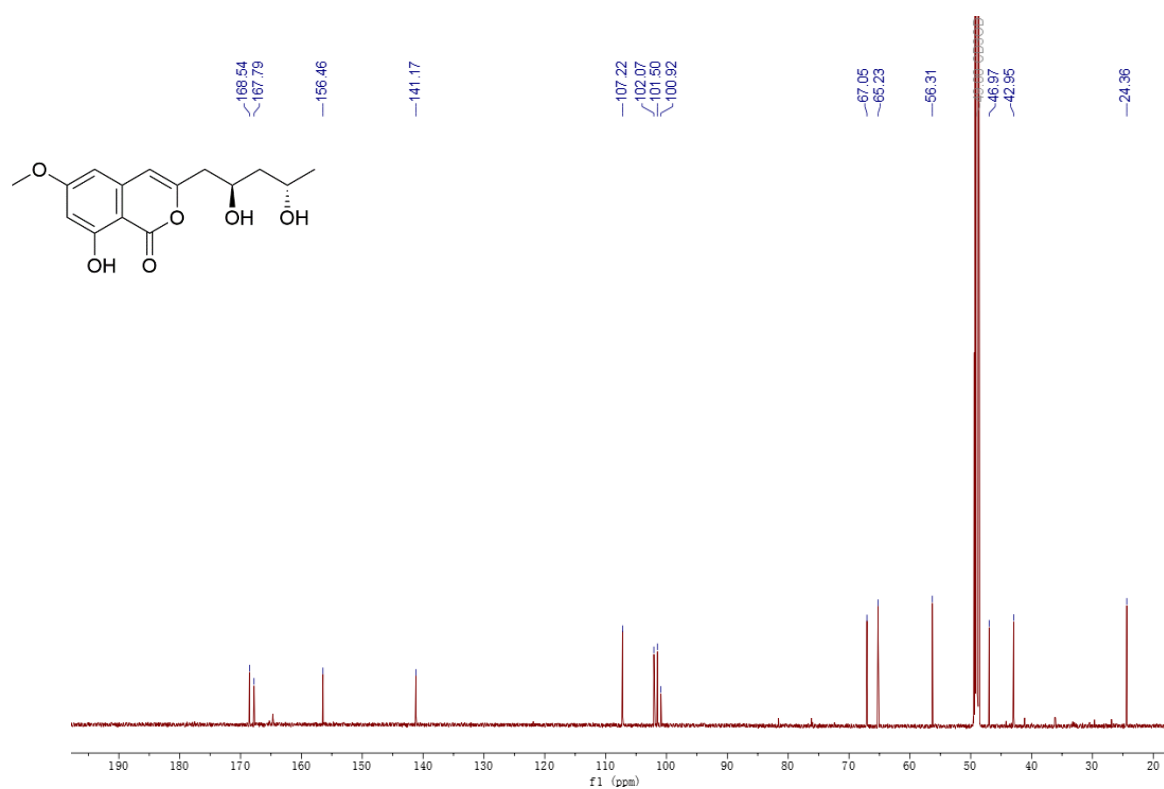
**Fig. S100** <sup>1</sup>H NMR spectrum of **16** in methanol-*d*<sub>4</sub> (600 MHz).



**Fig. S101** <sup>13</sup>C NMR spectrum of **16** in methanol-*d*<sub>4</sub> (150 MHz).

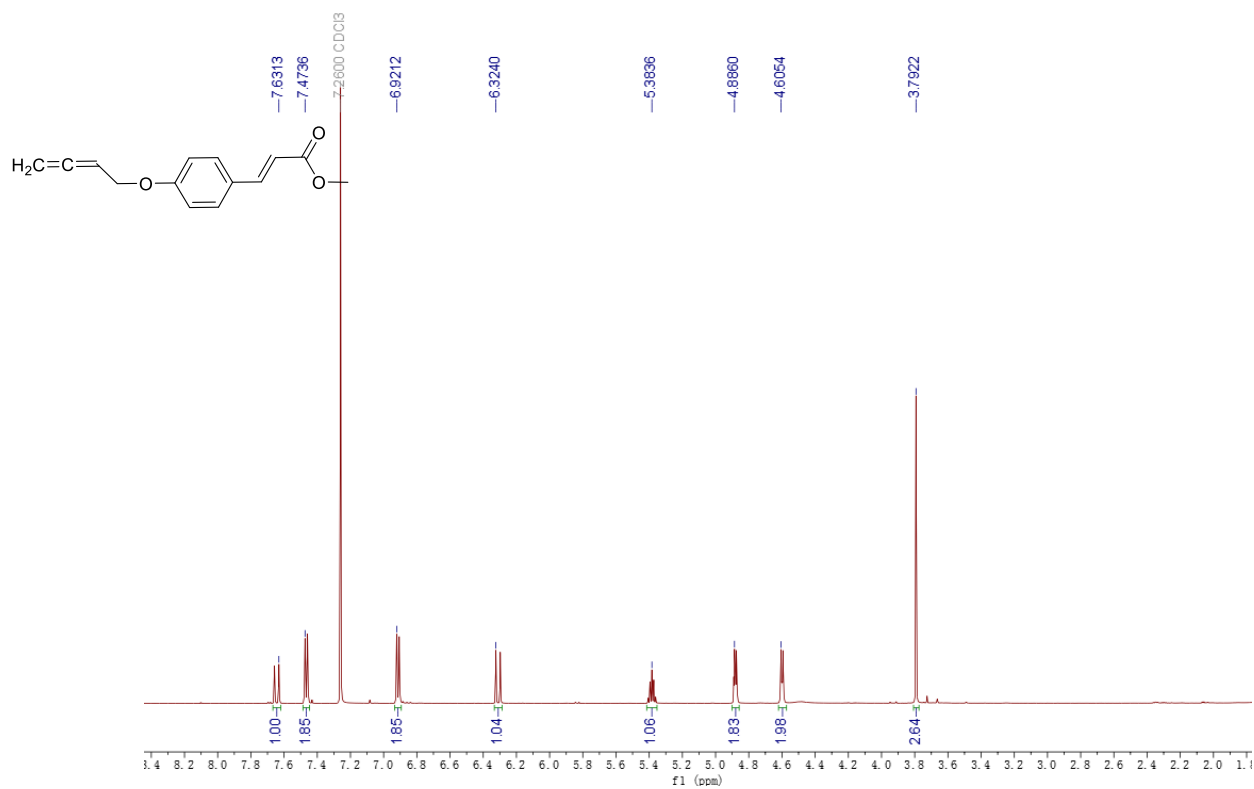


**Fig. S102** <sup>1</sup>H NMR spectrum of **17** in methanol-*d*<sub>4</sub> (600 MHz).

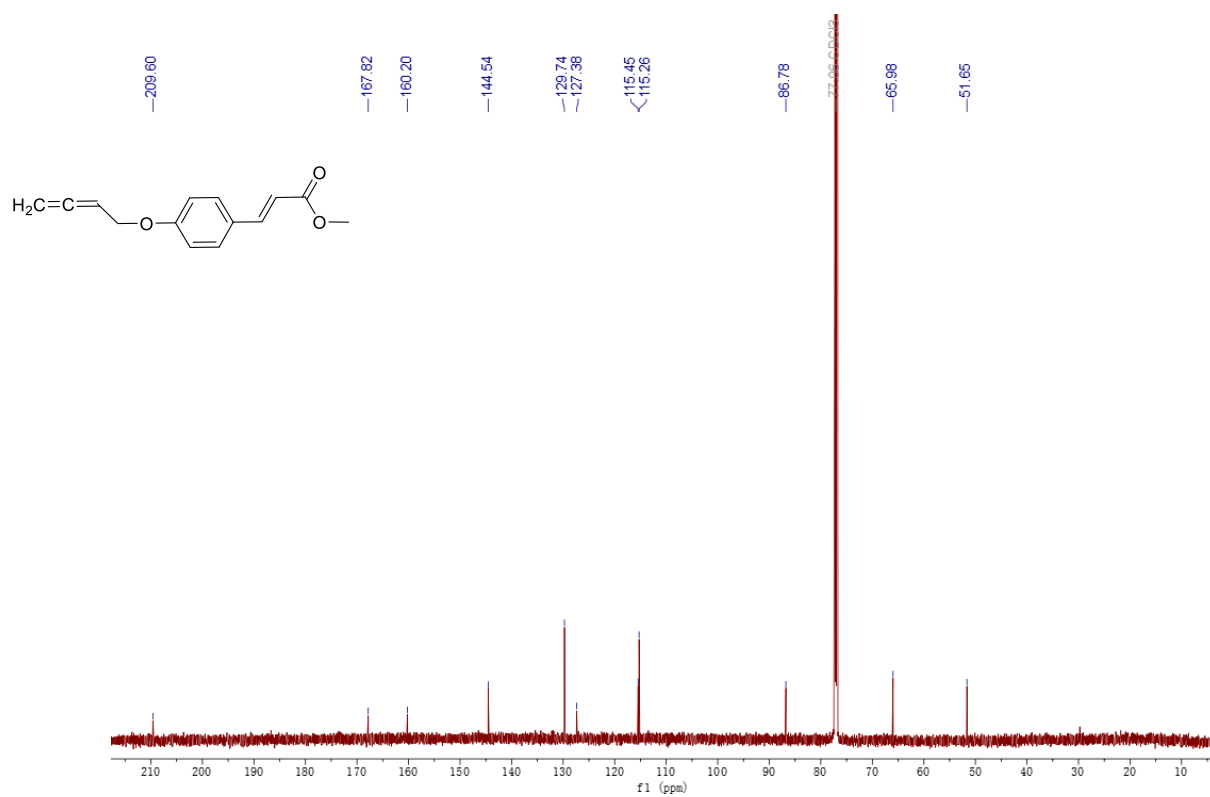


**Fig. S103** <sup>13</sup>C NMR spectrum of **17** in methanol-*d*<sub>4</sub> (150 MHz).





**Fig. S104** <sup>1</sup>H NMR spectrum of **18** in chloroform-*d* (600 MHz).



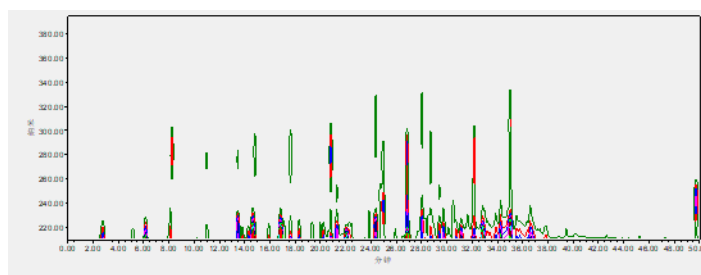
**Fig. S105** <sup>13</sup>C NMR spectrum of **18** in chloroform-*d* (150 MHz).

HPLC system: Waters, Waters e2695 pump, Waters 2996 detector.

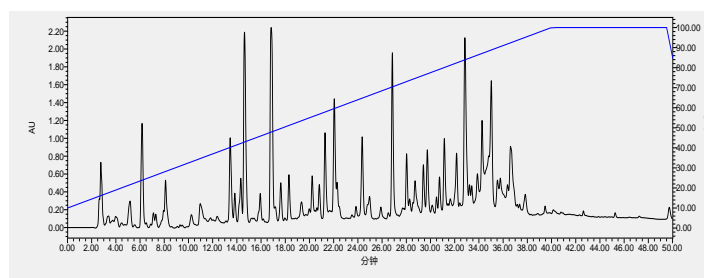
-Column: XB-C18, 5  $\mu\text{m}$ , 4.6  $\times$  250 mm.

-Solvent system.

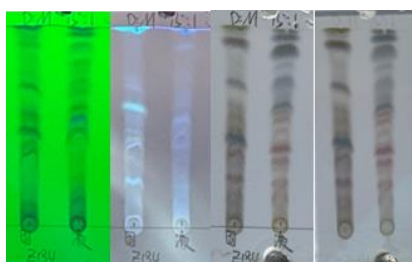
Time (min), Flow rate (1 mL/min)	MeOH (%)	Water (%)
-	10	90
40	100	0
50	100	0



(a) HPLC analysis



Wavelength at 215 nm.



(b) TLC analysis (dichloromethane: methanol = 15:1) of crude extract.

**Fig. S106** The TLC and HPLC profiles of the crude extract of *Xylaria* sp. Z184.