

# Cytotoxic 20,22-Dihydrodigitoxigenin Glycosides and Other Constituents of *Vallaris glabra* Stem

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## Supporting information

Fig S1  $^1\text{H}$ -NMR spectrum of compound **1** in  $\text{CD}_3\text{OD}$

Fig S2  $J$ modulated  $^{13}\text{C}$ -NMR spectrum of compound **1** in  $\text{CD}_3\text{OD}$

Fig S3 COSY spectrum of compound **1** in  $\text{CD}_3\text{OD}$

Fig S4 HMBC spectrum of compound **1** in  $\text{CD}_3\text{OD}$

Fig S5 1-D TOCSY spectrum of compound **1** in  $\text{CD}_3\text{OD}$

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Fig S10 HMBC spectrum of compound **2** in  $\text{CD}_3\text{OD}$

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Fig S12 1-D TOCSY spectrum of compound **2** in  $\text{CD}_3\text{OD}$

Fig S13  $^1\text{H}$ -NMR spectrum of compound **3** in  $\text{CD}_3\text{OD}$

Fig S14  $J$ modulated  $^{13}\text{C}$ -NMR spectrum of compound **3** in  $\text{CD}_3\text{OD}$

Fig S15  $^1\text{H}$ -NMR spectrum of compound **4** in  $\text{CD}_3\text{OD}$

Fig S16  $J$ modulated  $^{13}\text{C}$ -NMR spectrum of compound **4** in  $\text{CD}_3\text{OD}$

- Fig S17  $^1\text{H}$ -NMR spectrum of compound **5** in  $\text{CD}_3\text{OD}$   
Fig S18  $J$ modulated  $^{13}\text{C}$ -NMR spectrum of compound **5** in  $\text{CD}_3\text{OD}$   
Fig S19  $^1\text{H}$ -NMR spectrum of compound **6** in  $\text{CD}_3\text{OD}$   
Fig S20  $J$ modulated  $^{13}\text{C}$ -NMR spectrum of compound **6** in  $\text{CD}_3\text{OD}$   
Fig S21  $^1\text{H}$ -NMR spectrum of compound **7** in  $\text{CD}_3\text{OD}$   
Fig S22  $J$ modulated  $^{13}\text{C}$ -NMR spectrum of compound **7** in  $\text{CD}_3\text{OD}$   
Fig S23  $^1\text{H}$ -NMR spectrum of compound **8** in  $\text{CD}_3\text{OD}$   
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Fig S25  $^1\text{H}$ -NMR spectrum of compound **9** in  $\text{CD}_3\text{OD}$   
Fig S26  $J$ modulated  $^{13}\text{C}$ -NMR spectrum of compound **9** in  $\text{CD}_3\text{OD}$   
Fig S27  $^1\text{H}$ -NMR spectrum of compound **10** in  $\text{CD}_3\text{OD}$   
Fig S28  $J$ modulated  $^{13}\text{C}$ -NMR spectrum of compound **10** in  $\text{CD}_3\text{OD}$

Fig S1  $^1\text{H}$ -NMR spectrum of compound **1** in  $\text{CD}_3\text{OD}$

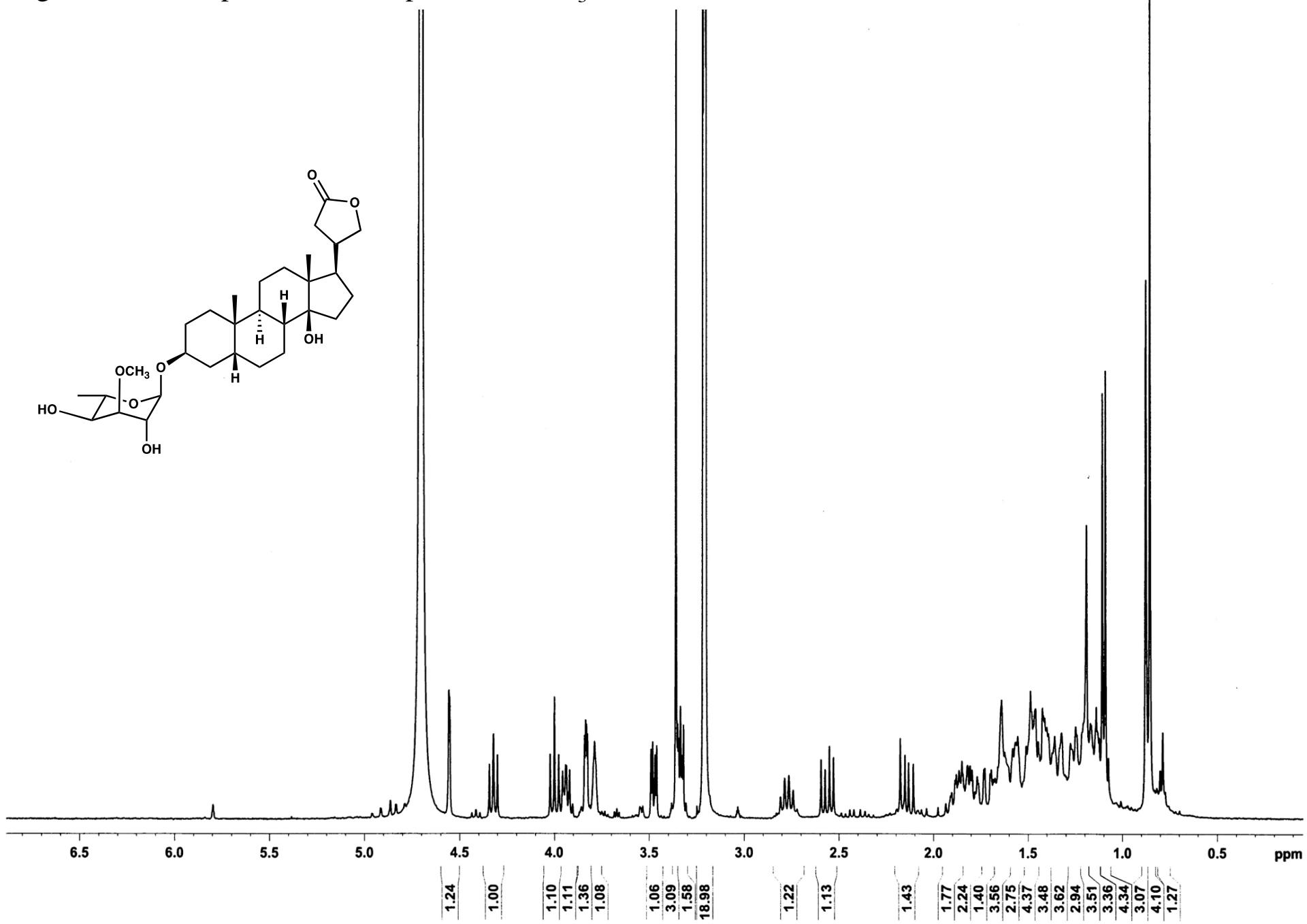
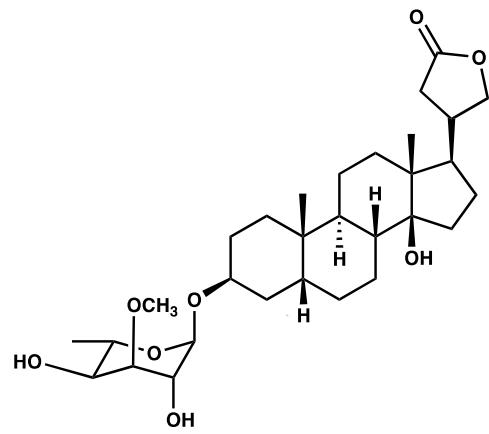


Fig S2 *J*modulated  $^{13}\text{C}$ -NMR spectrum of compound **1** in  $\text{CD}_3\text{OD}$

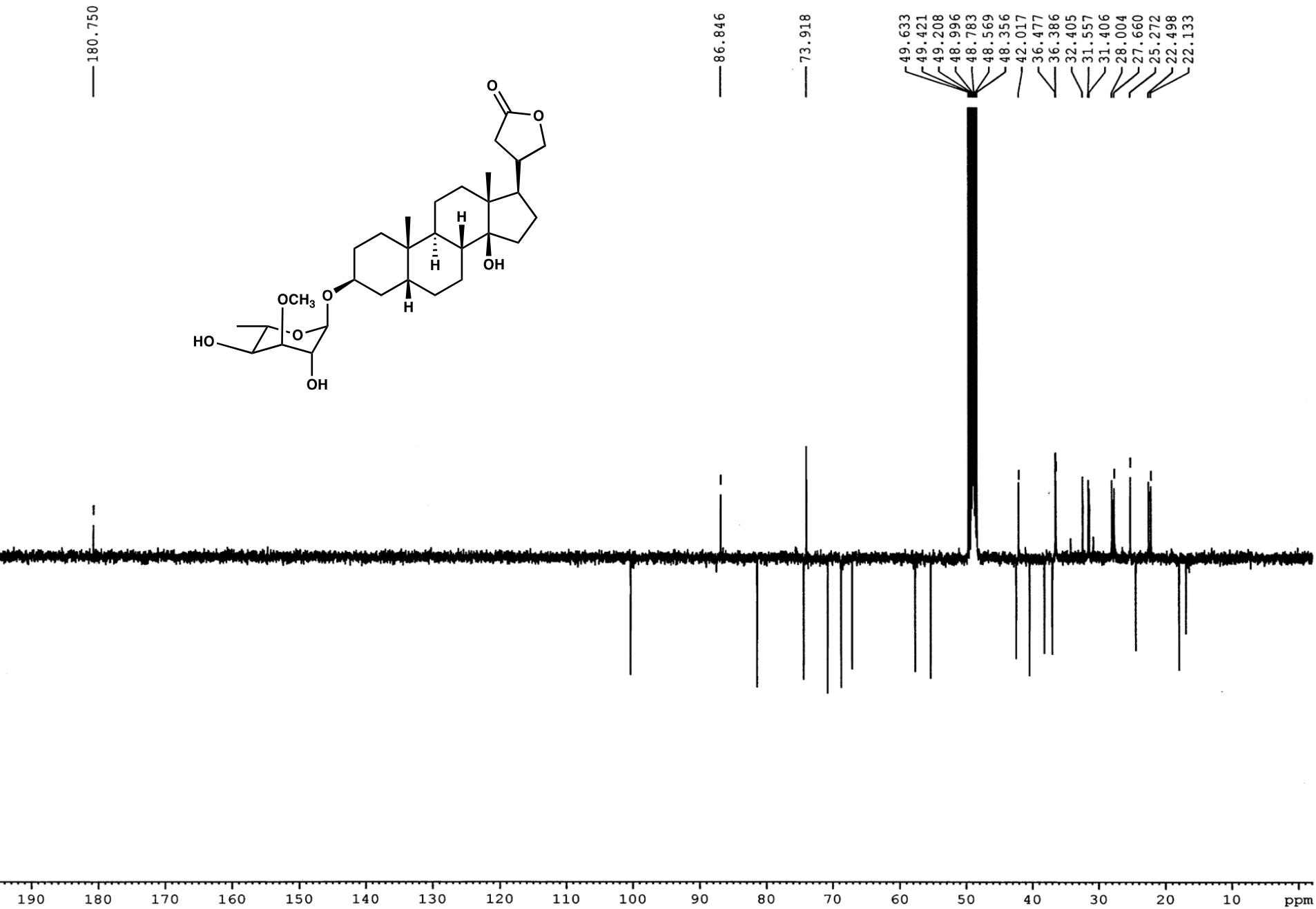


Fig S3 COSY spectrum of compound **1** in  $\text{CD}_3\text{OD}$

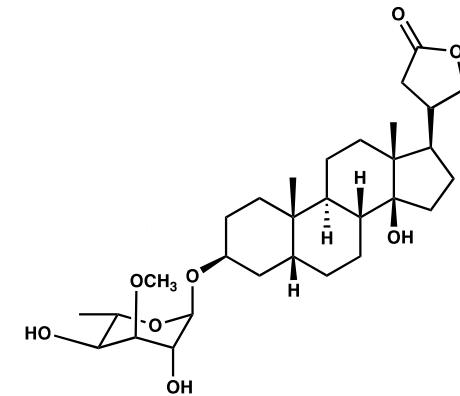
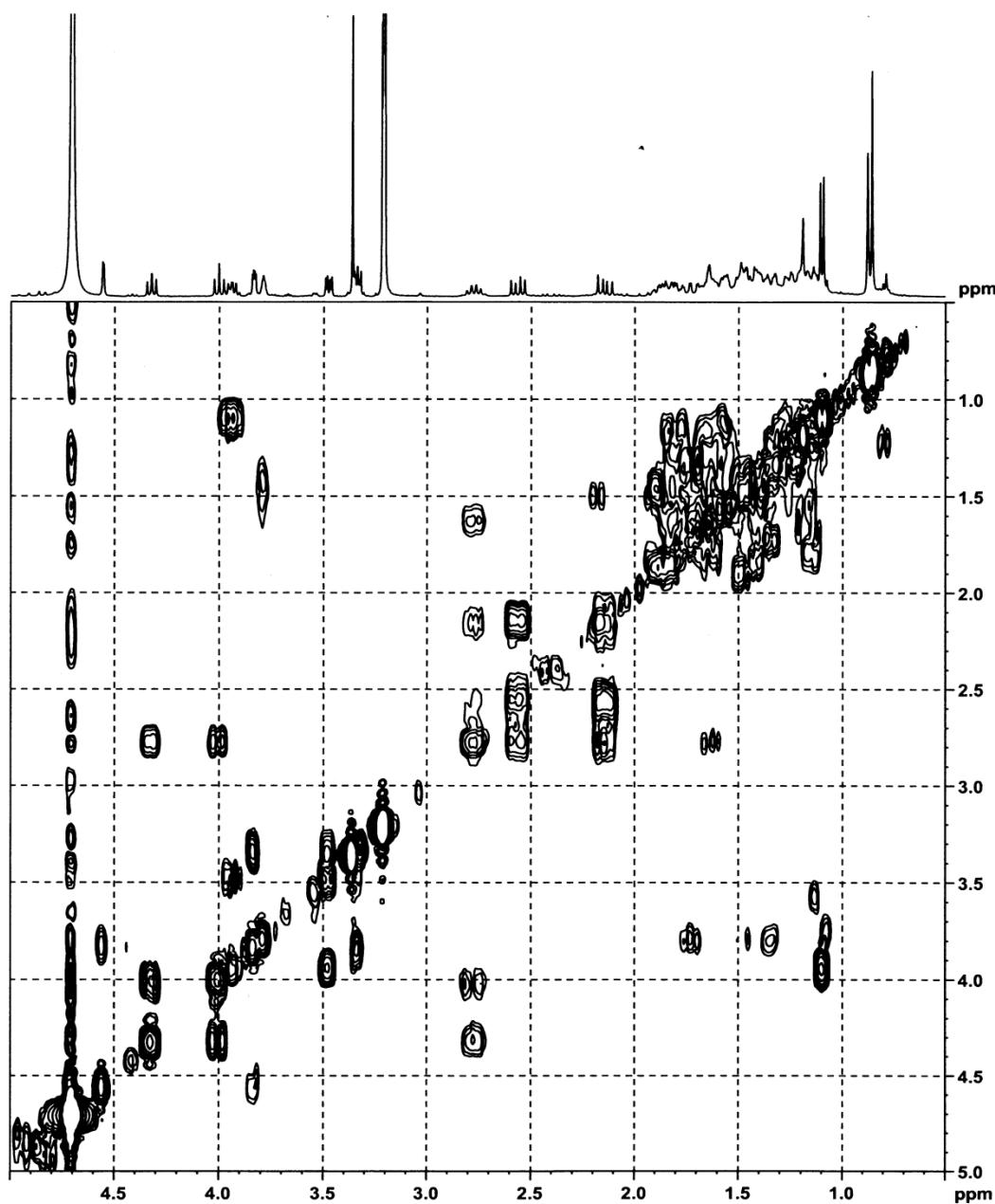


Fig S4 HMBC spectrum of compound **1** in  $\text{CD}_3\text{OD}$

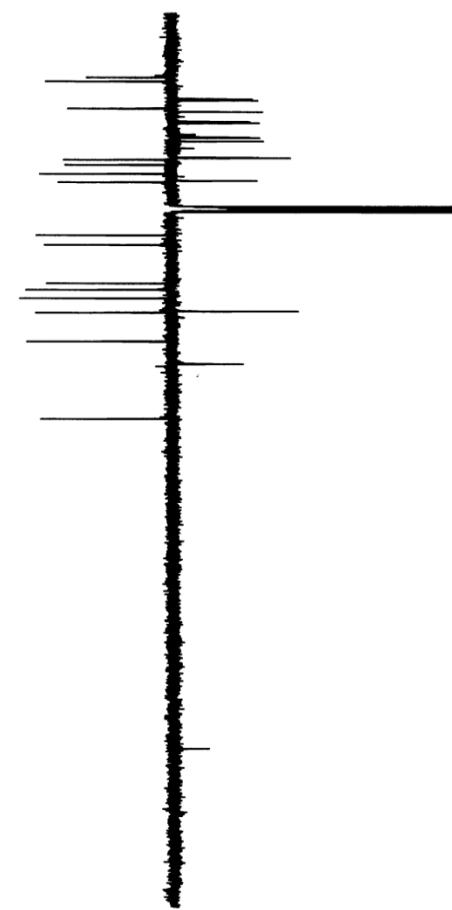
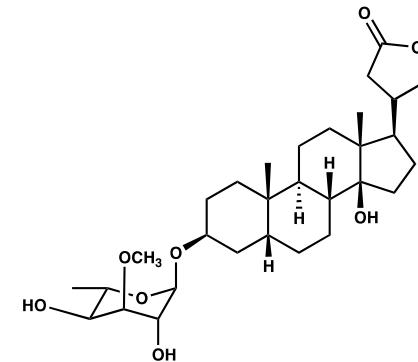
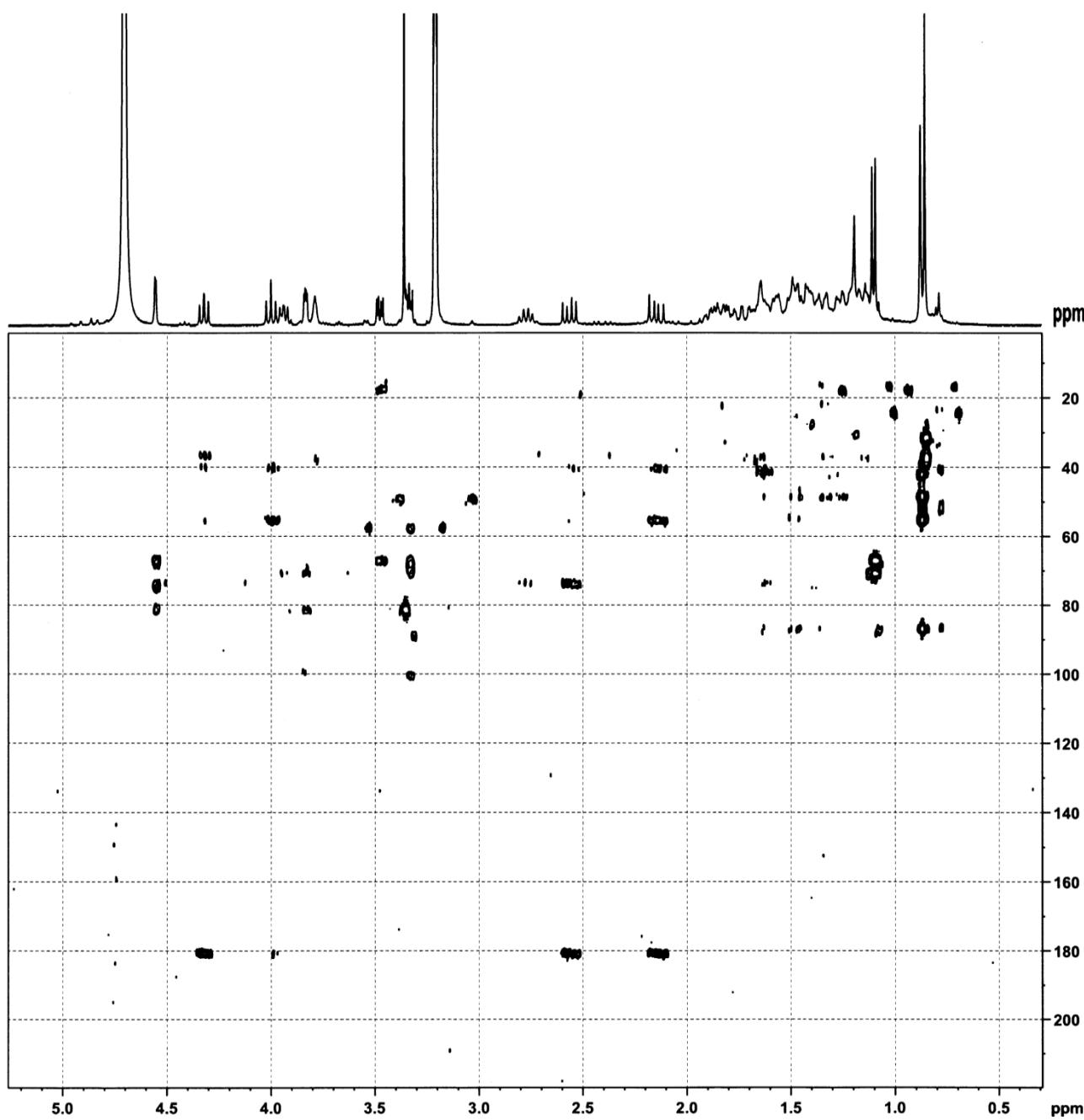


Fig S5 1-D TOCSY spectrum of compound **1** in CD<sub>3</sub>OD

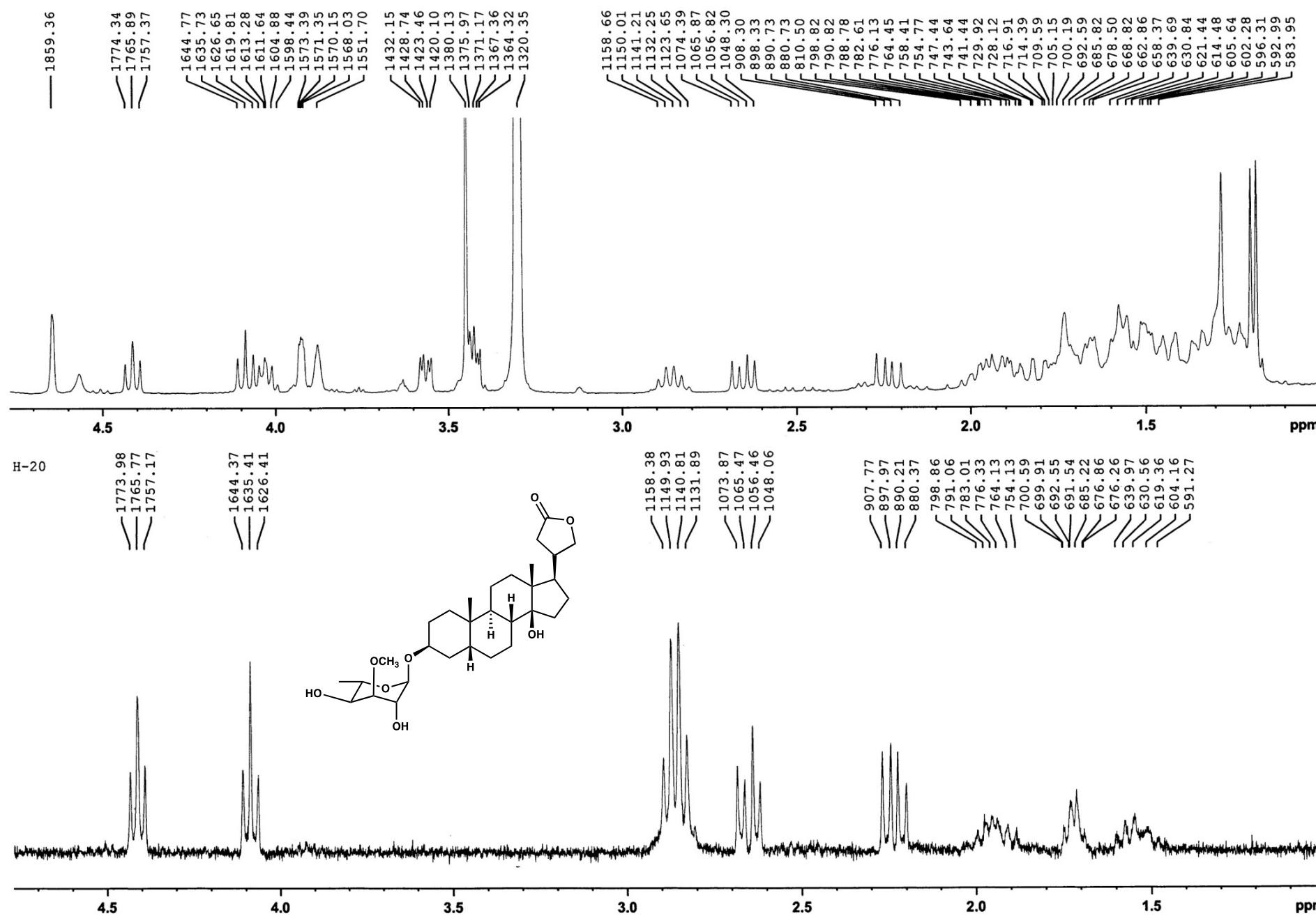


Fig S6 NOESY spectrum of compound **1** in  $\text{CD}_3\text{OD}$

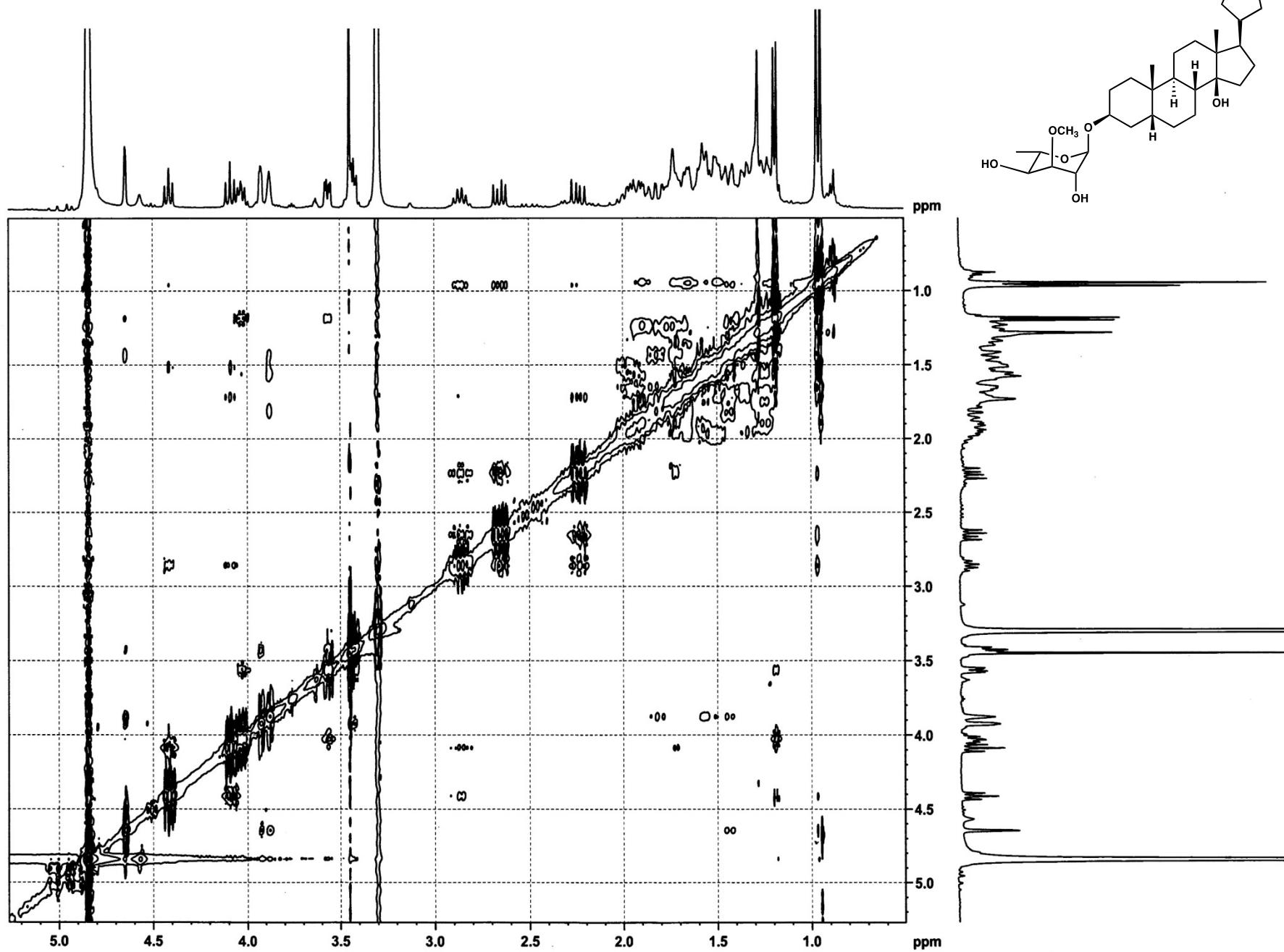


Fig S7  $^1\text{H}$ -NMR spectrum of compound **2** in  $\text{CD}_3\text{OD}$

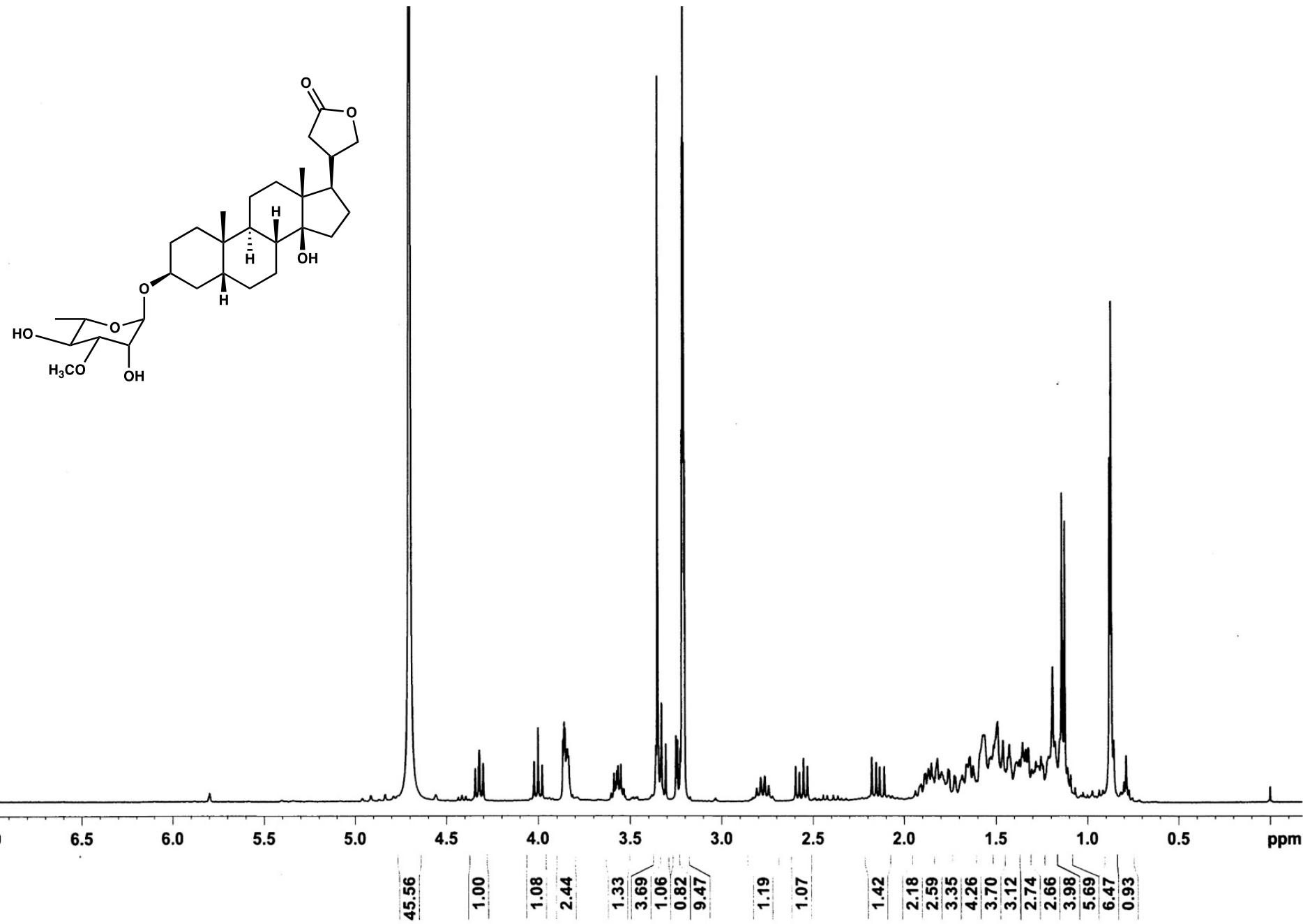
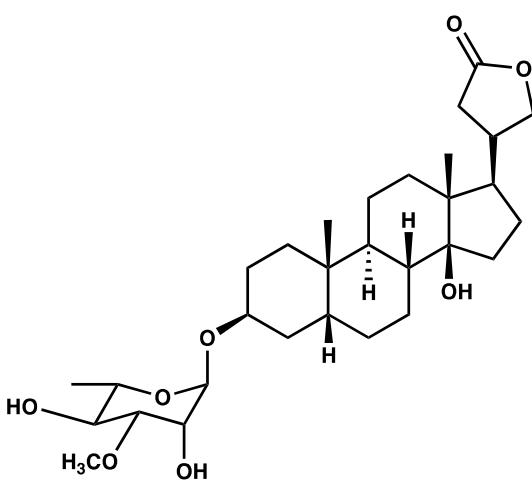


Fig S8 *J*modulated  $^{13}\text{C}$ -NMR spectrum of compound **2** in  $\text{CD}_3\text{OD}$

— 180.693



— 86.786

— 73.906

49.638  
49.426  
49.213  
48.999  
48.786  
48.574  
48.361  
42.011  
36.477  
36.397  
32.440  
31.658  
30.888  
27.930  
27.473  
25.270  
22.449  
22.130

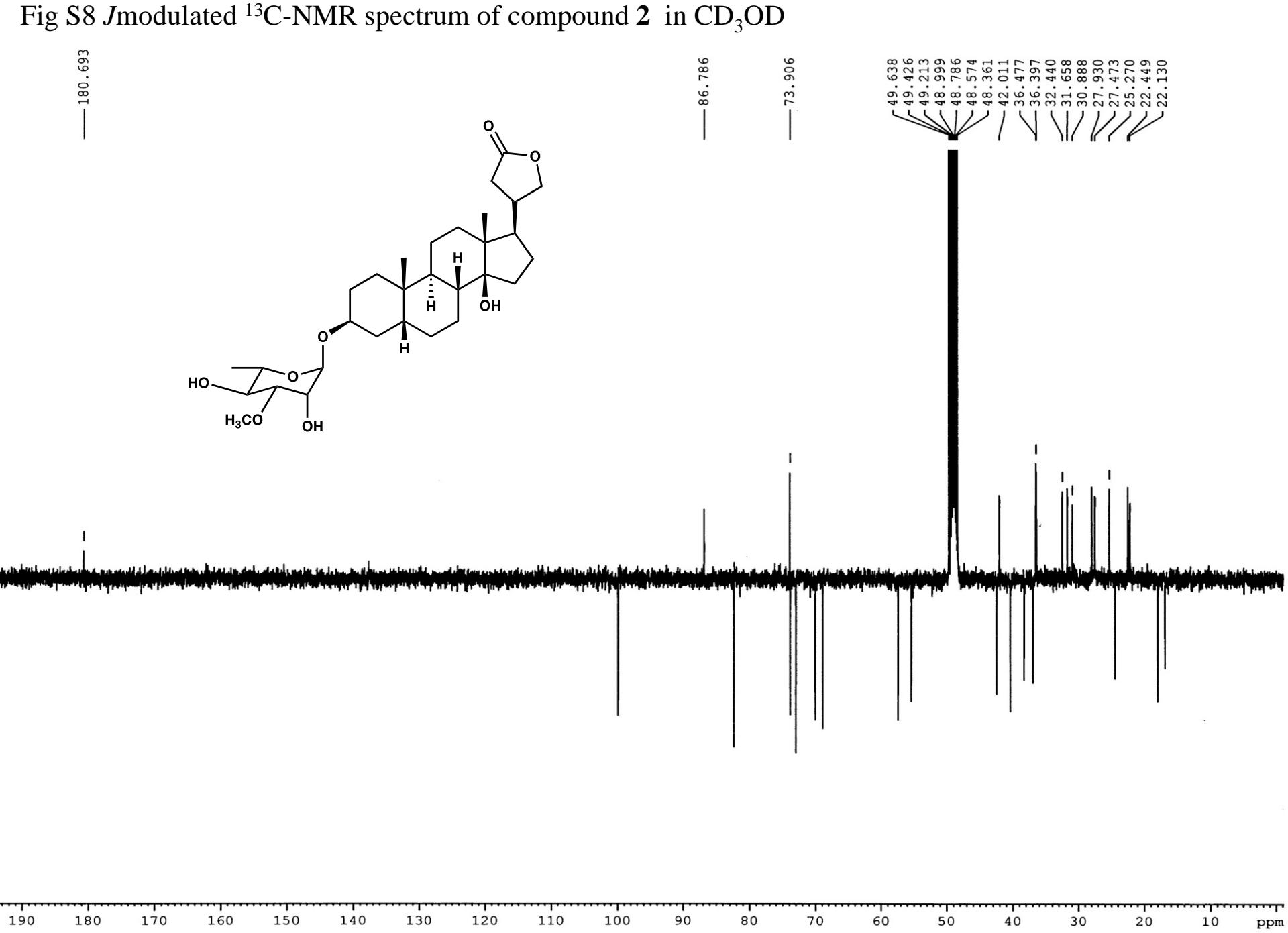


Fig S9 COSY spectrum of compound **2** in  $\text{CD}_3\text{OD}$

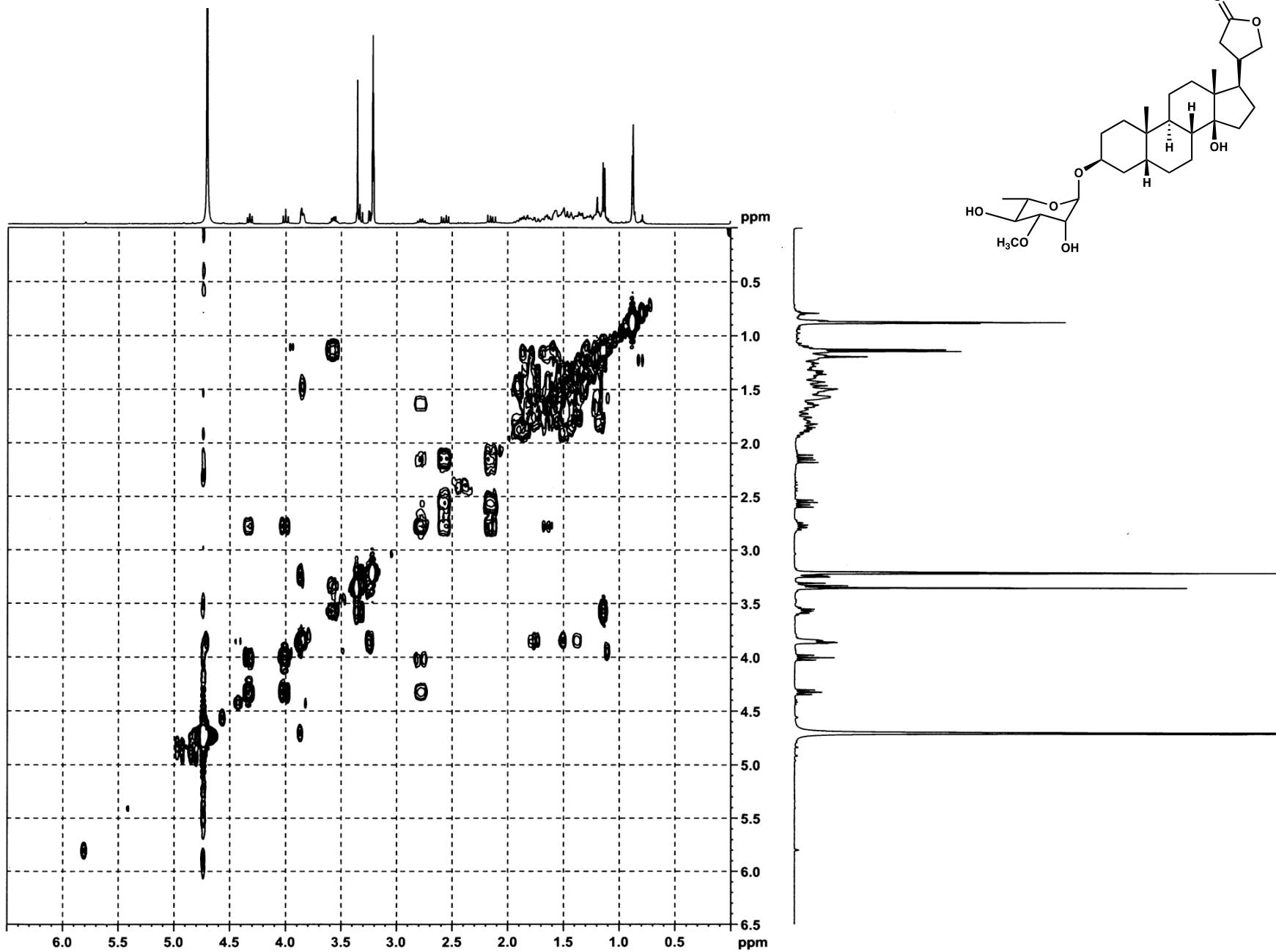


Fig S10 HMBC spectrum of compound 2 in CD<sub>3</sub>OD

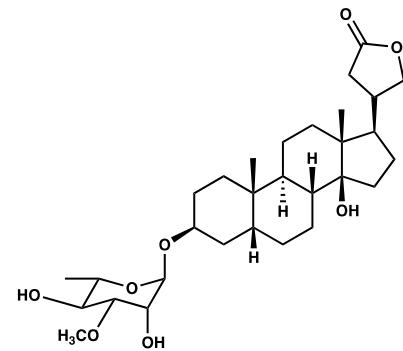
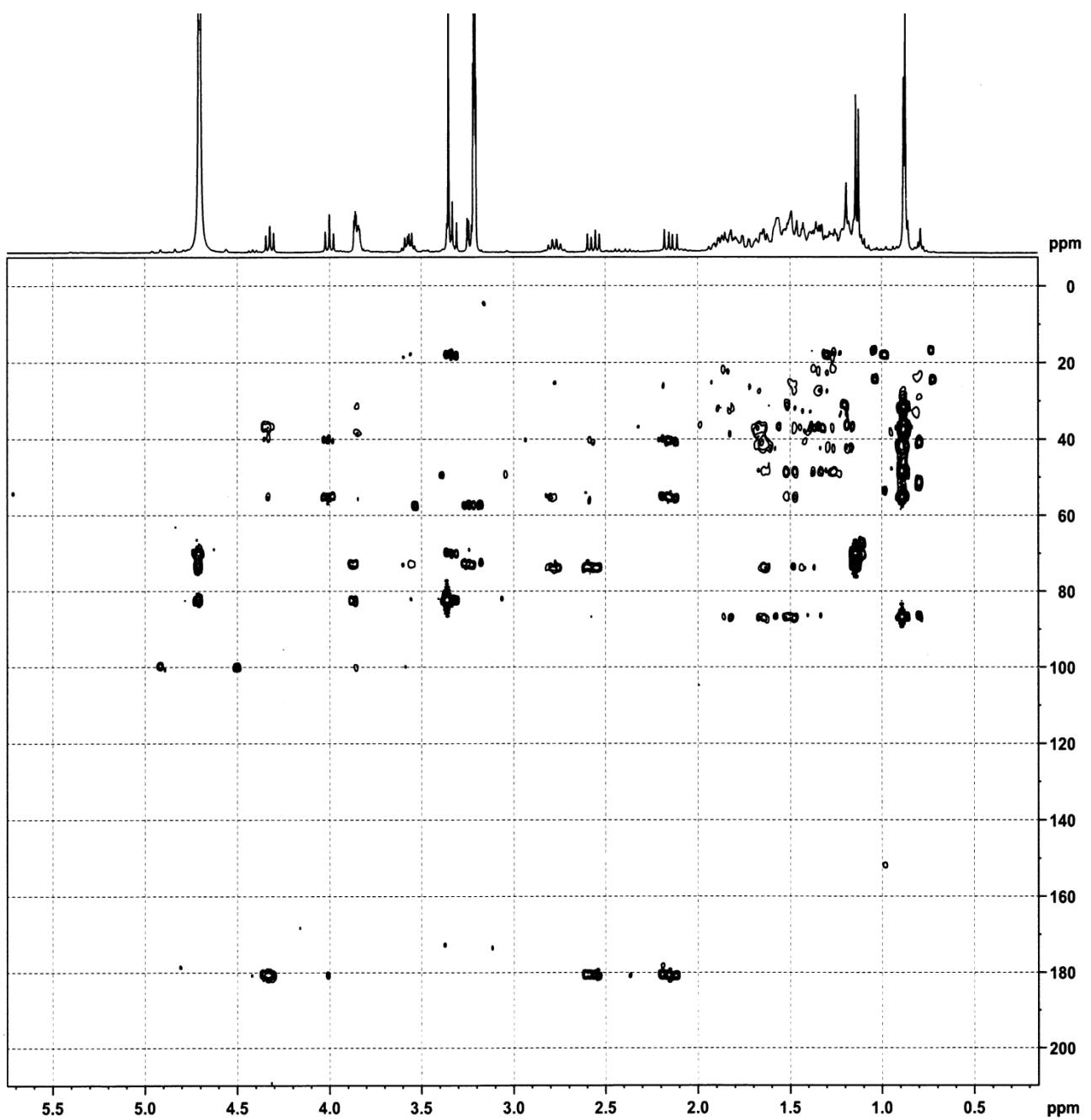


Fig S11 1-D TOCSY spectrum of compound **2** in CD<sub>3</sub>OD

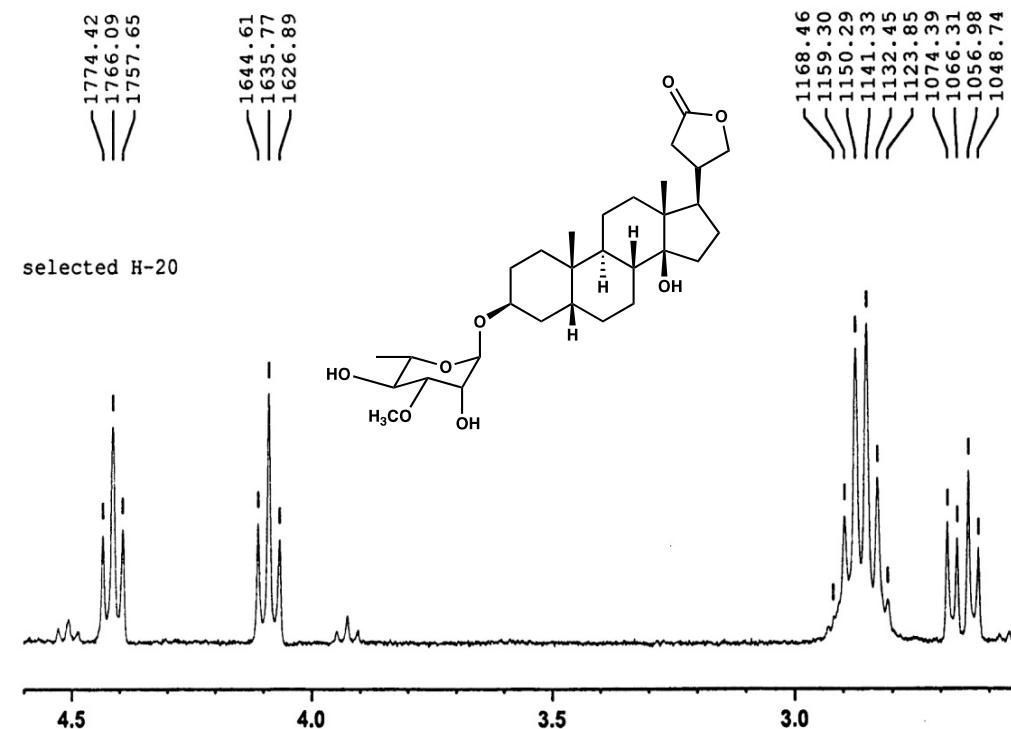
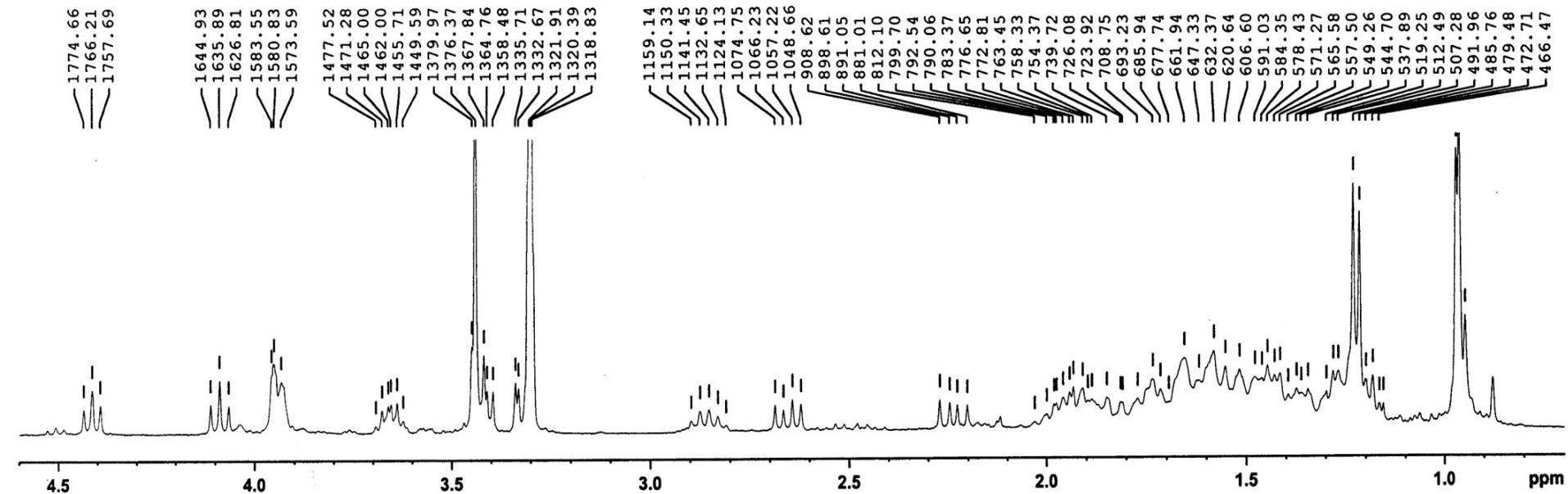


Fig S12 1-D TOCSY spectrum of compound **2** in CD<sub>3</sub>OD

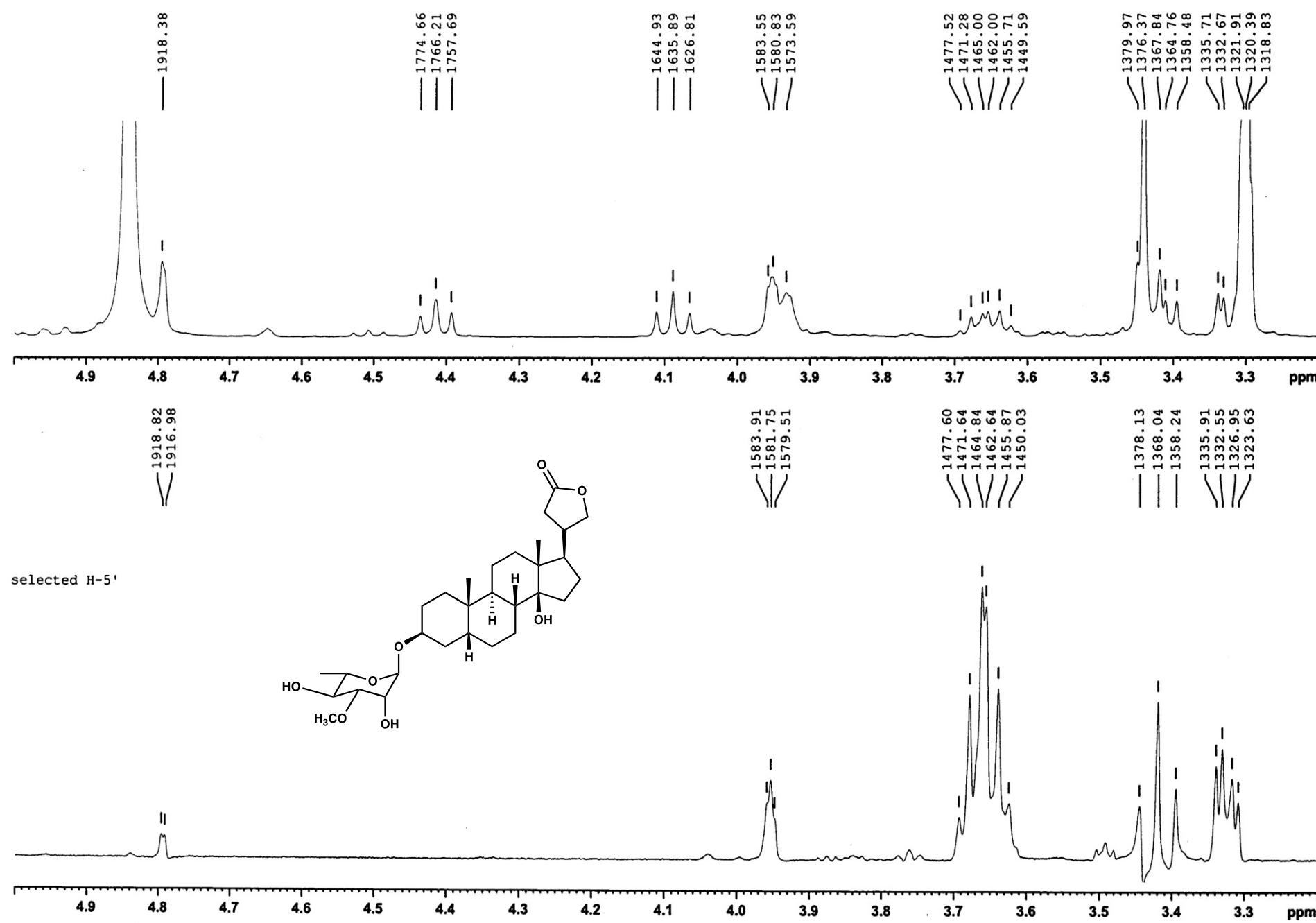


Fig S13  $^1\text{H}$ -NMR spectrum of compound **3** in  $\text{CD}_3\text{OD}$

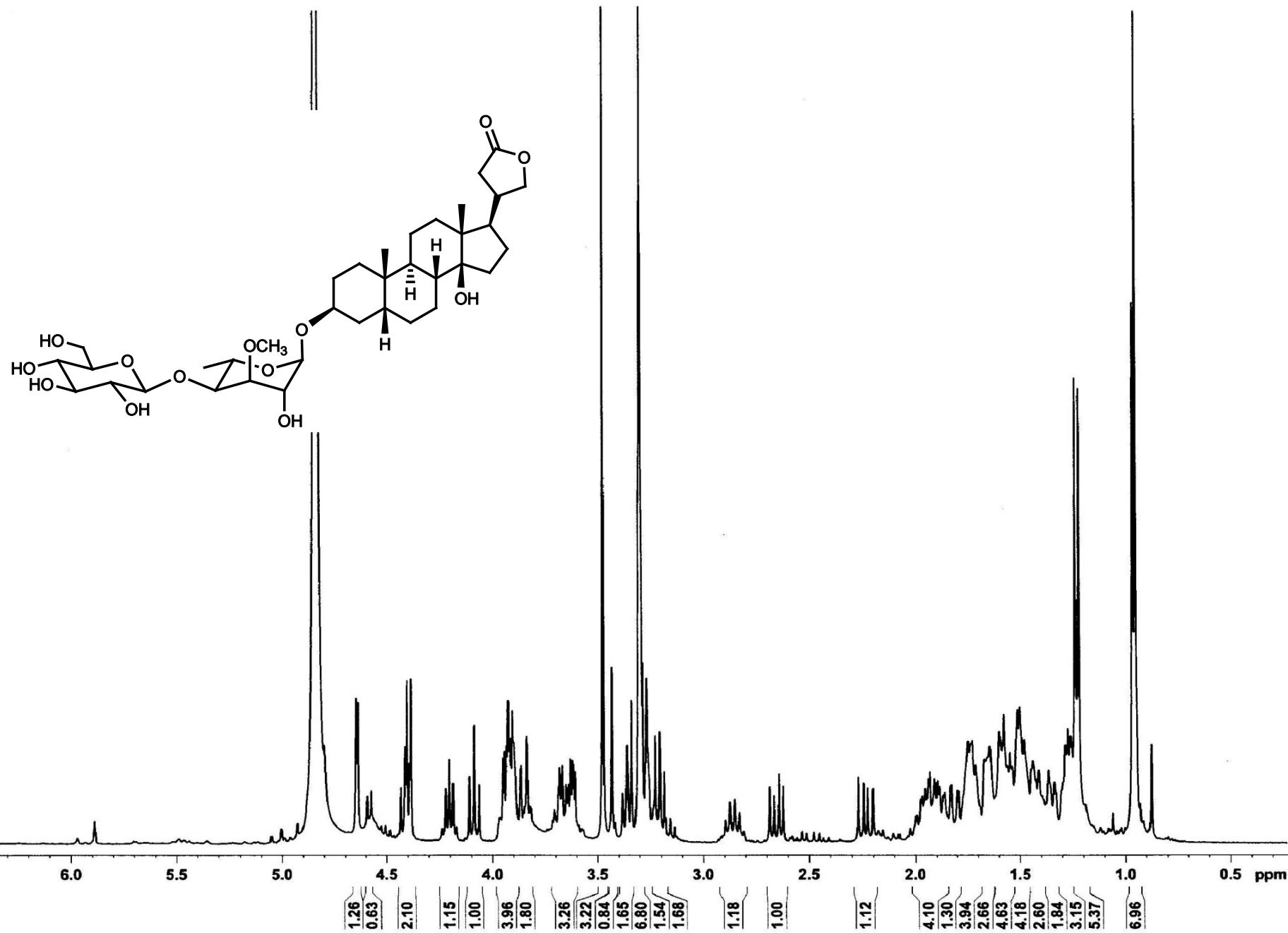


Fig S14 *J*modulated  $^{13}\text{C}$ -NMR spectrum of compound **3** in  $\text{CD}_3\text{OD}$

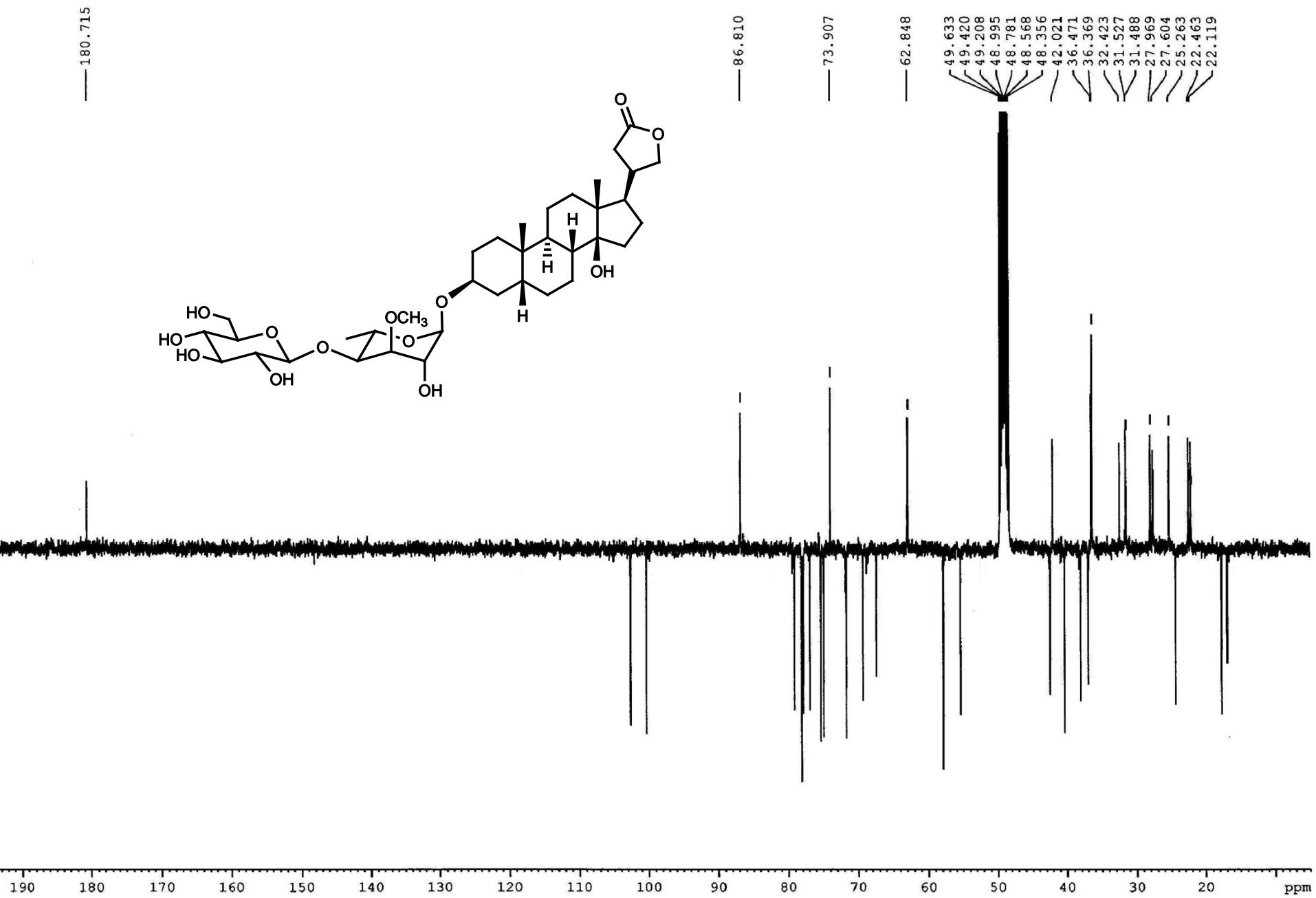


Fig S15  $^1\text{H}$ -NMR spectrum of compound **4** in  $\text{CD}_3\text{OD}$

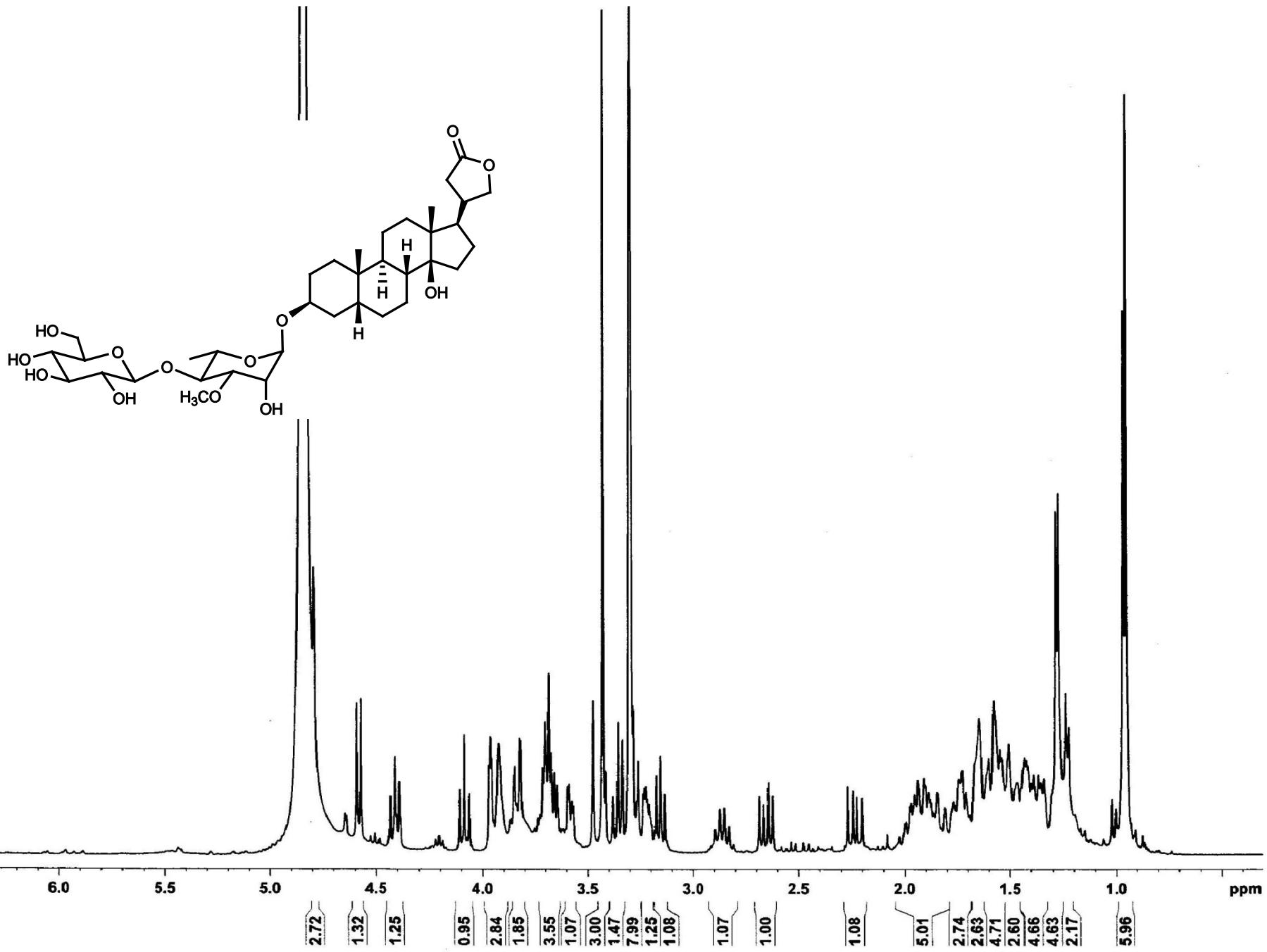


Fig S16 *J*modulated  $^{13}\text{C}$ -NMR spectrum of compound **4** in  $\text{CD}_3\text{OD}$

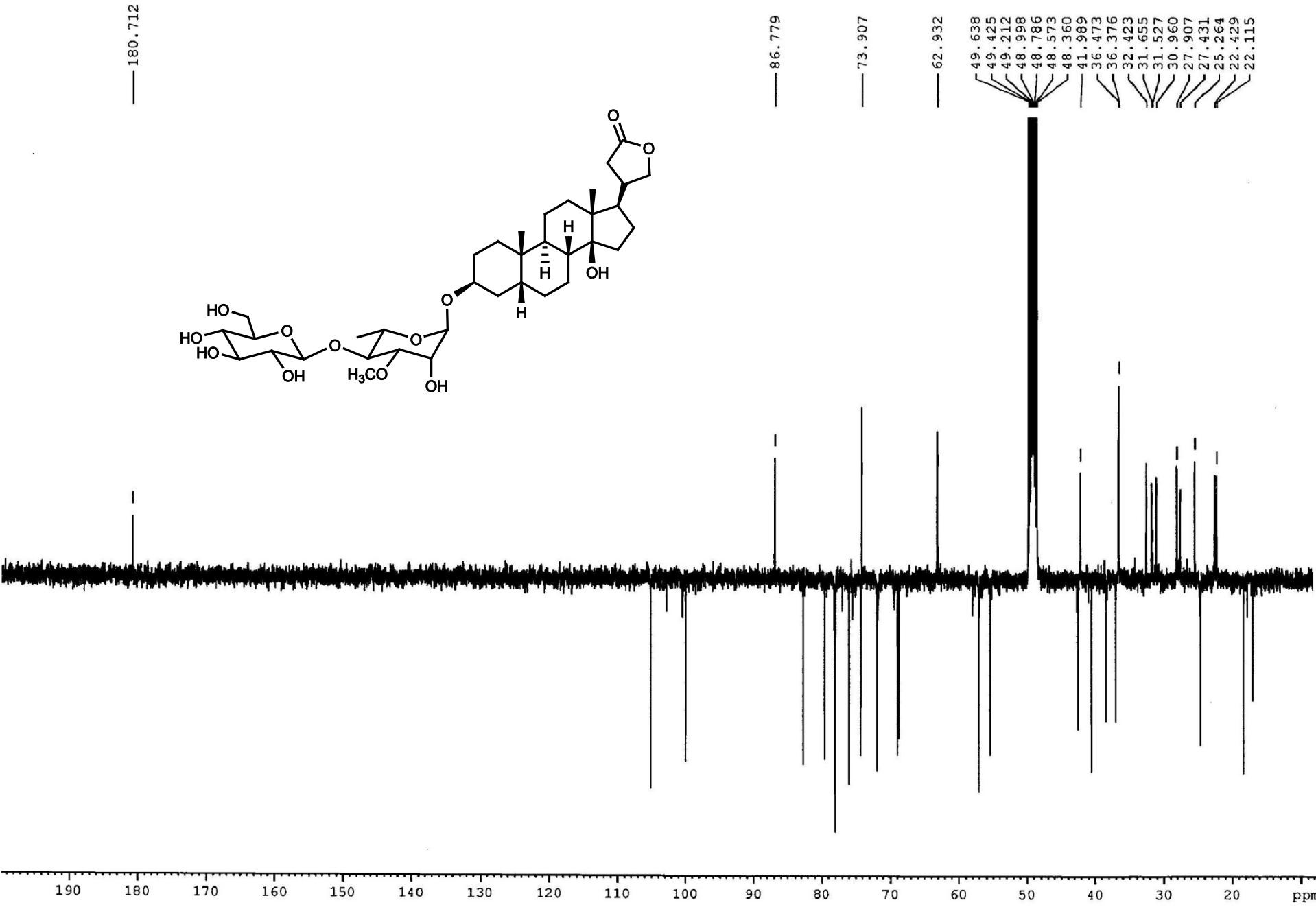


Fig S17  $^1\text{H}$ -NMR spectrum of compound 5 in  $\text{CD}_3\text{OD}$

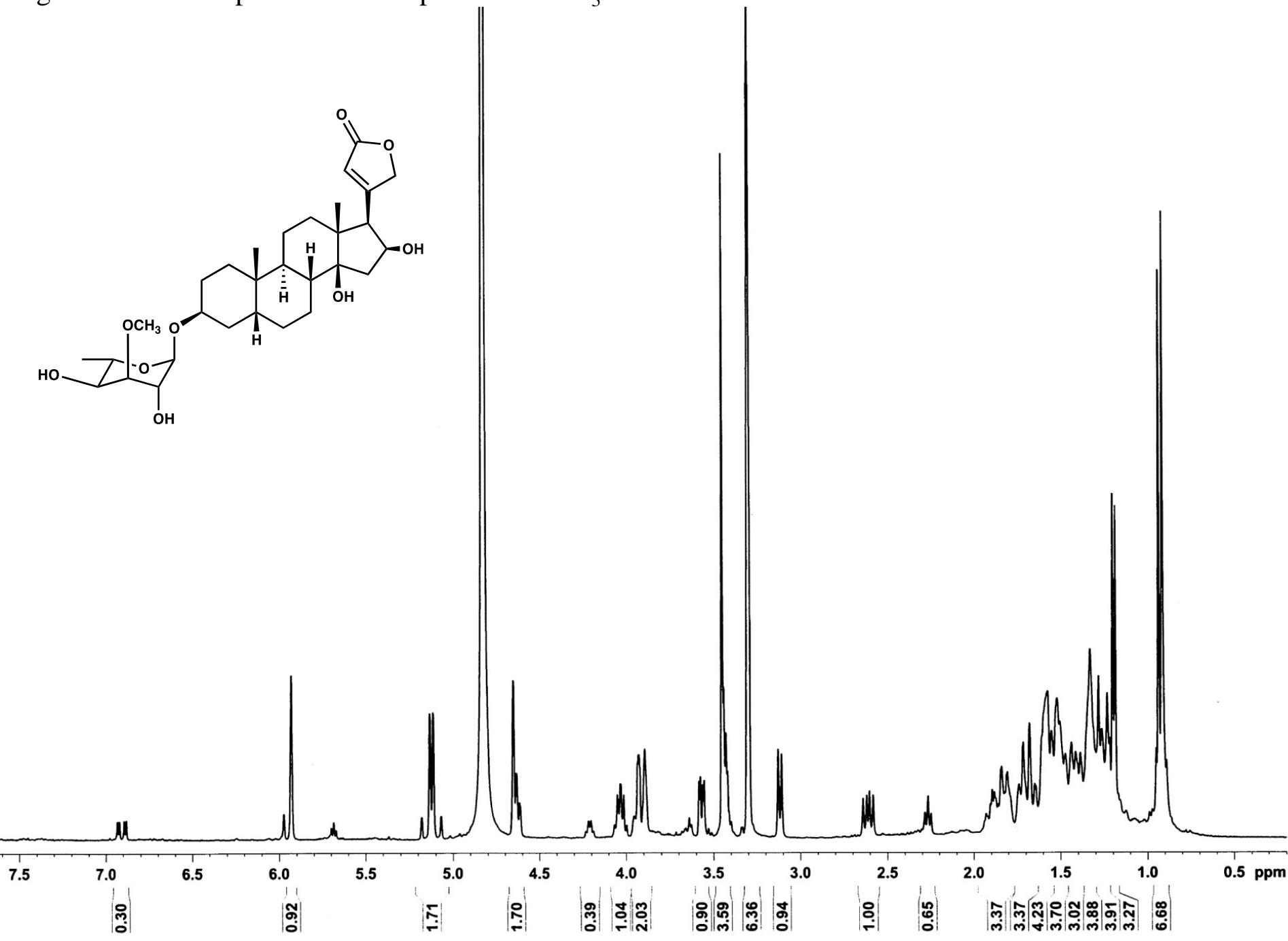


Fig S18 Jmodulated  $^{13}\text{C}$ -NMR spectrum of compound 5 in  $\text{CD}_3\text{OD}$

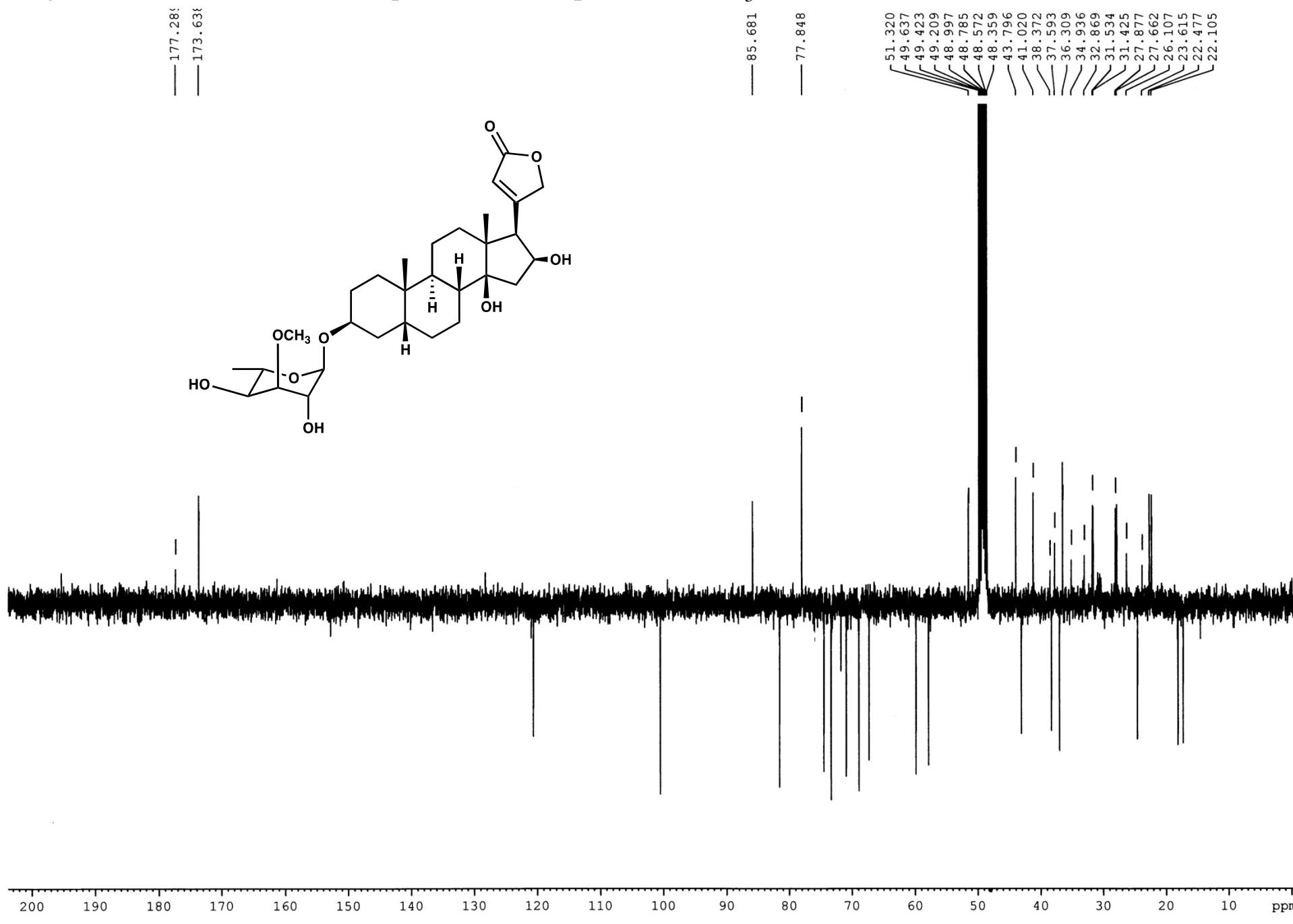


Fig S19  $^1\text{H}$ -NMR spectrum of compound **6** in  $\text{CD}_3\text{OD}$

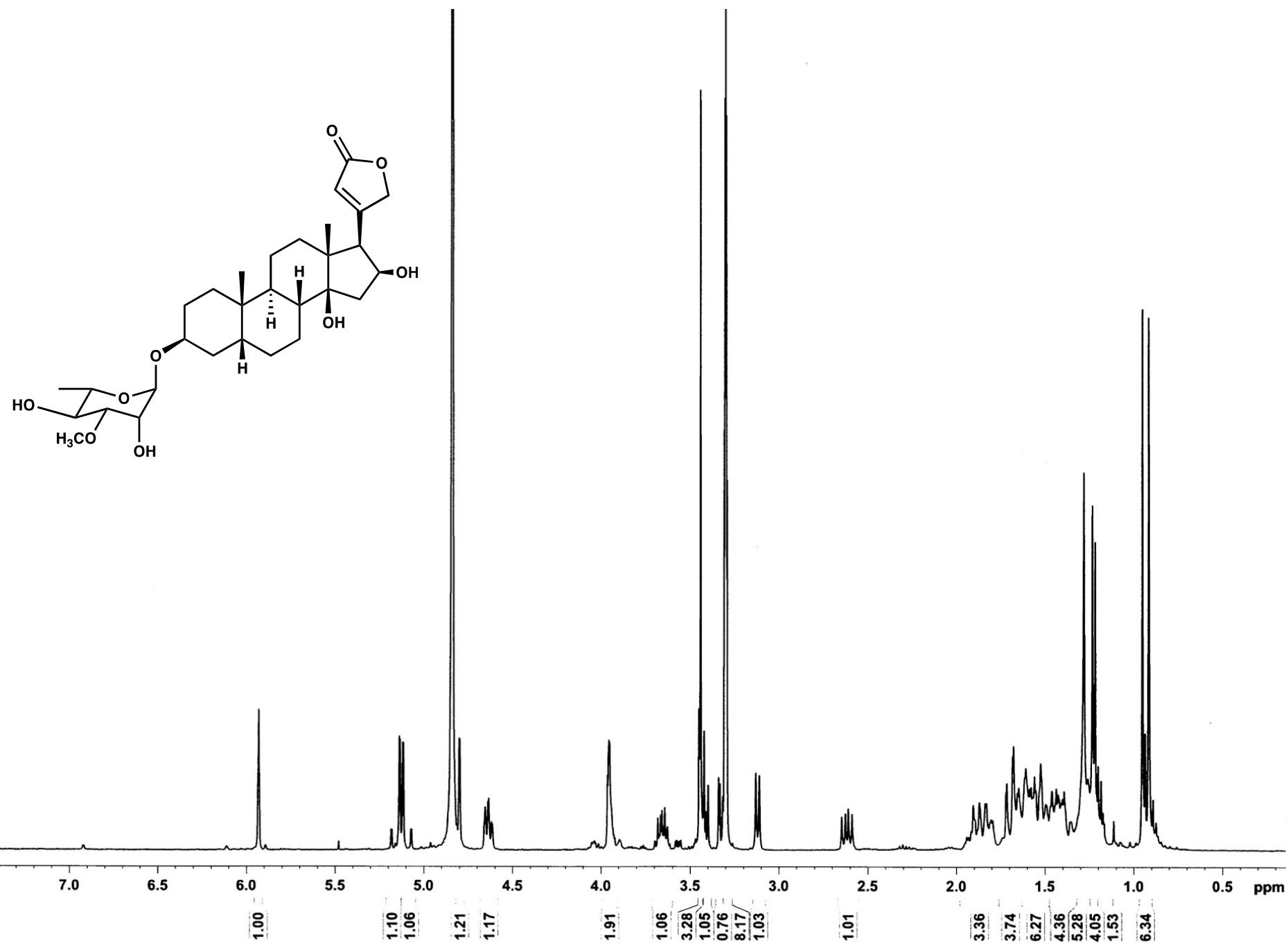


Fig S20 Jmodulated  $^{13}\text{C}$ -NMR spectrum of compound **6** in  $\text{CD}_3\text{OD}$

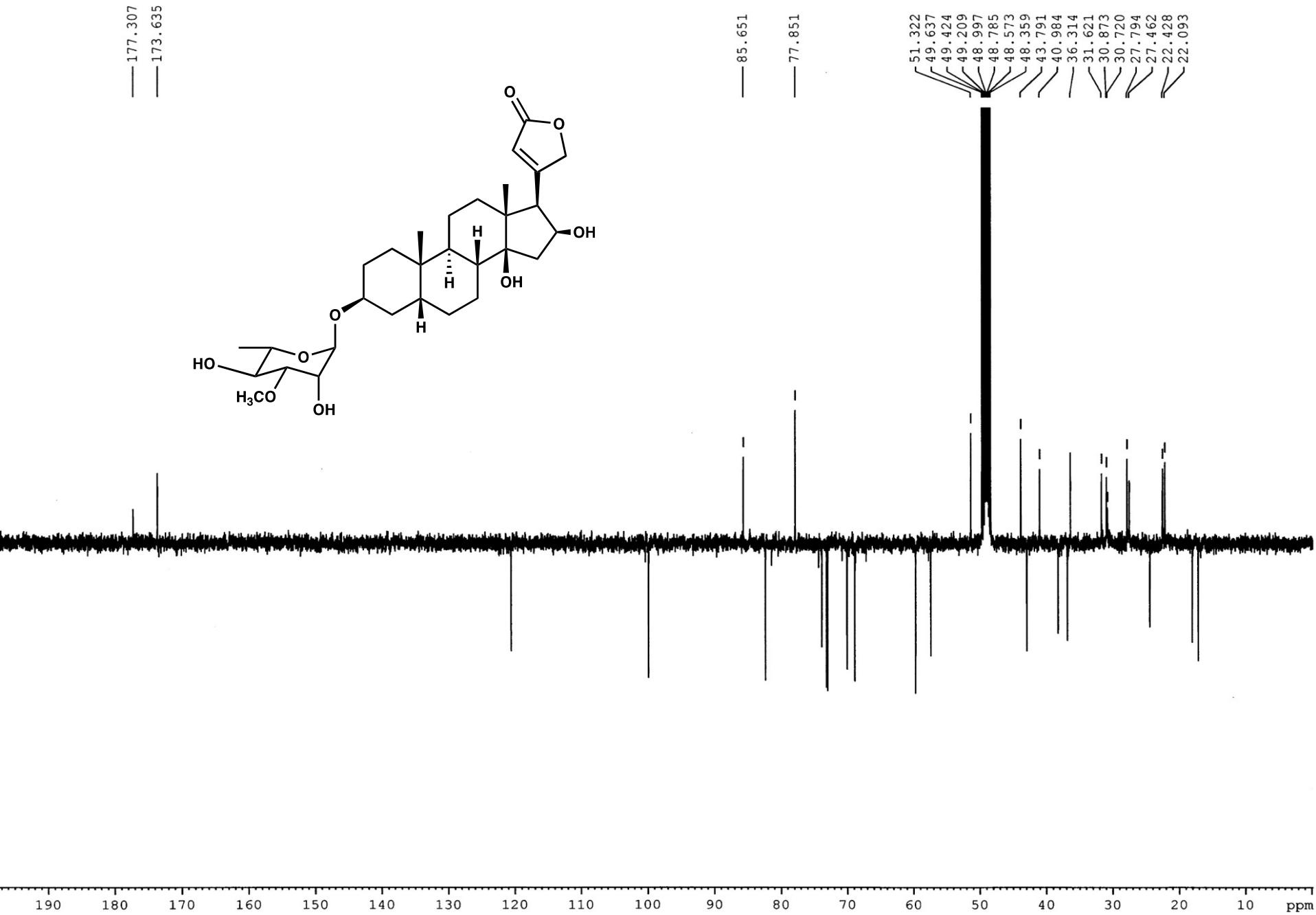


Fig S21  $^1\text{H}$ -NMR spectrum of compound 7 in  $\text{CD}_3\text{OD}$

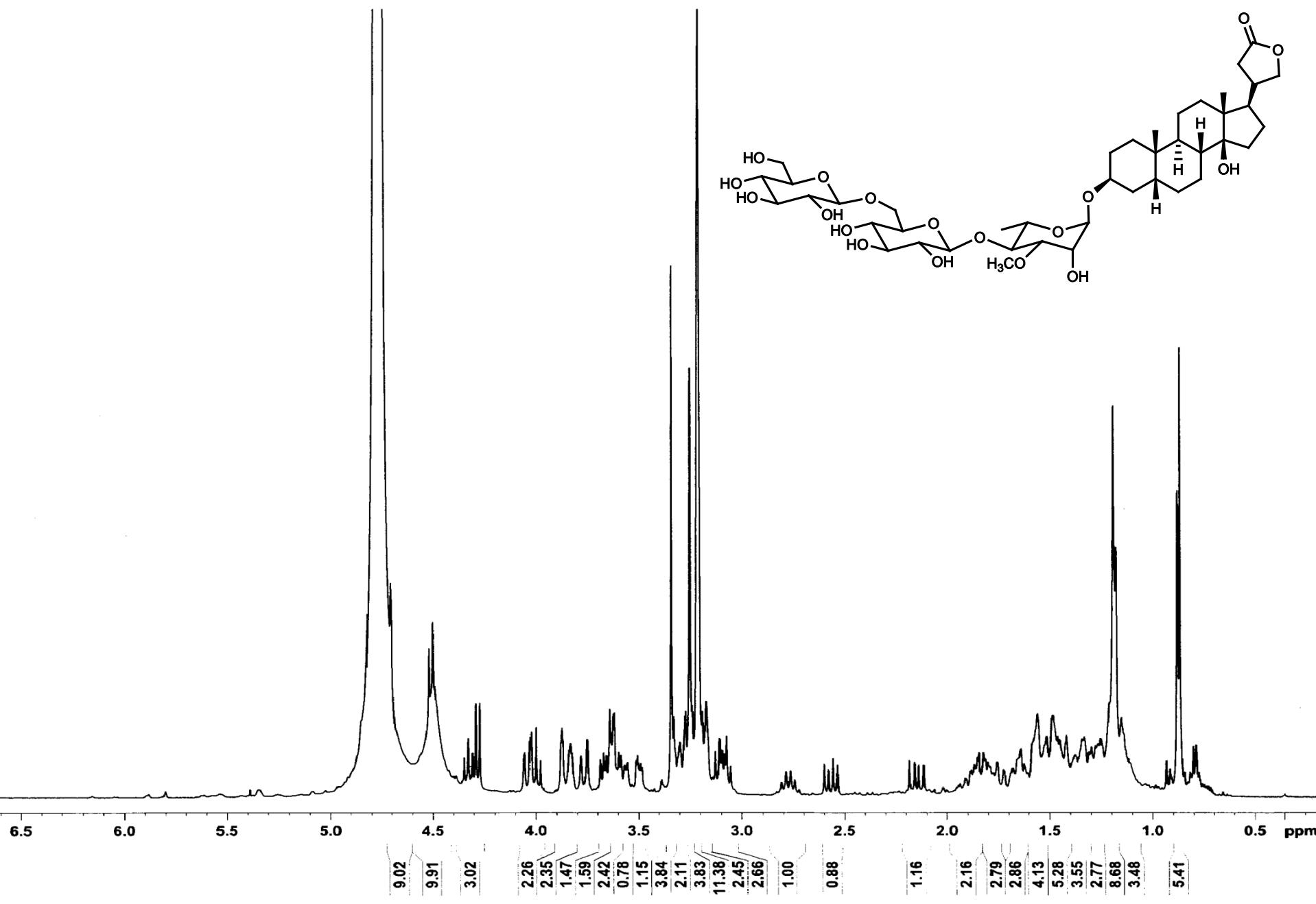


Fig S 22 *J*modulated  $^{13}\text{C}$ -NMR spectrum of compound 7 in  $\text{CD}_3\text{OD}$

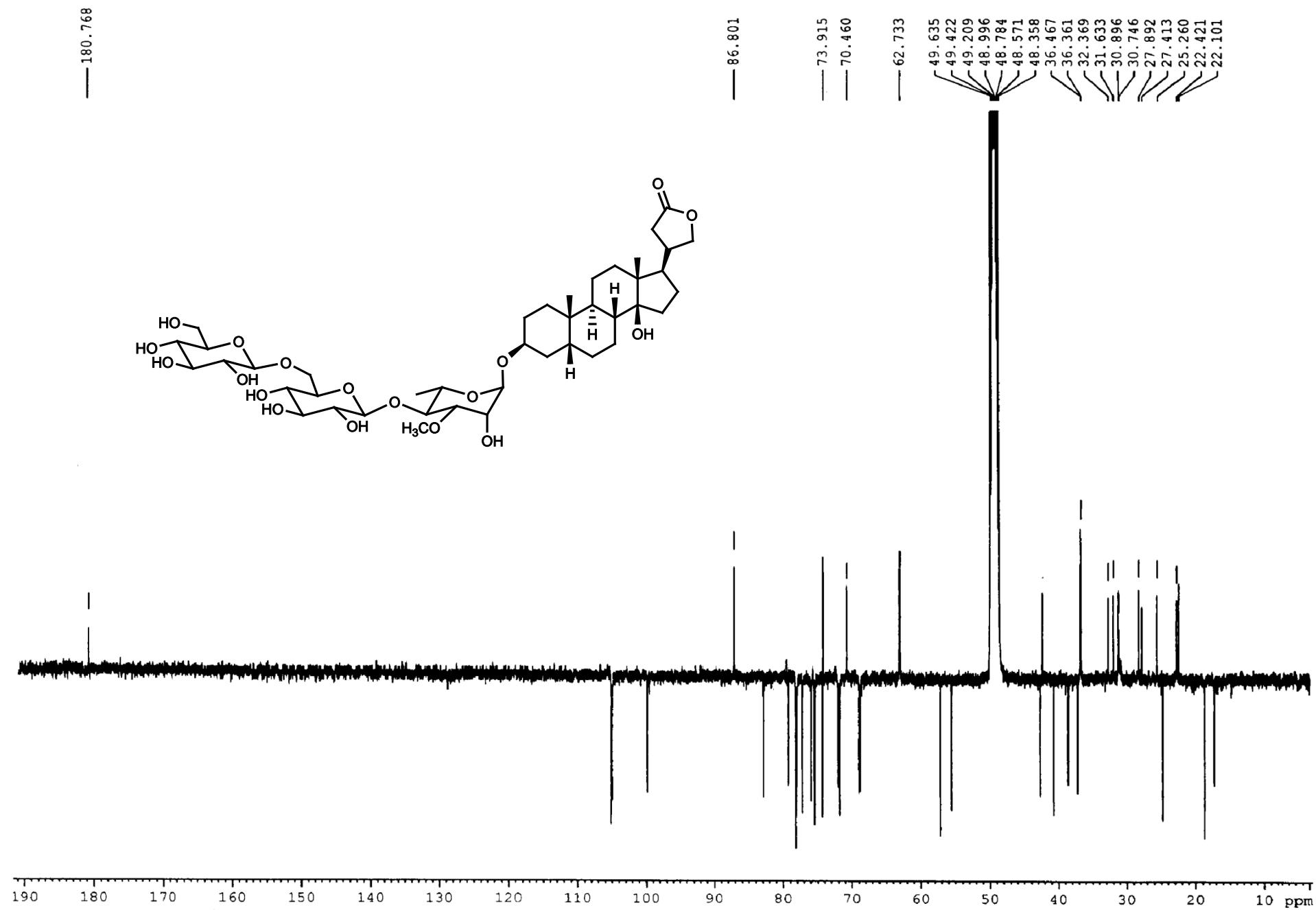


Fig S 23  $^1\text{H}$ -NMR spectrum of compound **8** in  $\text{CD}_3\text{OD}$

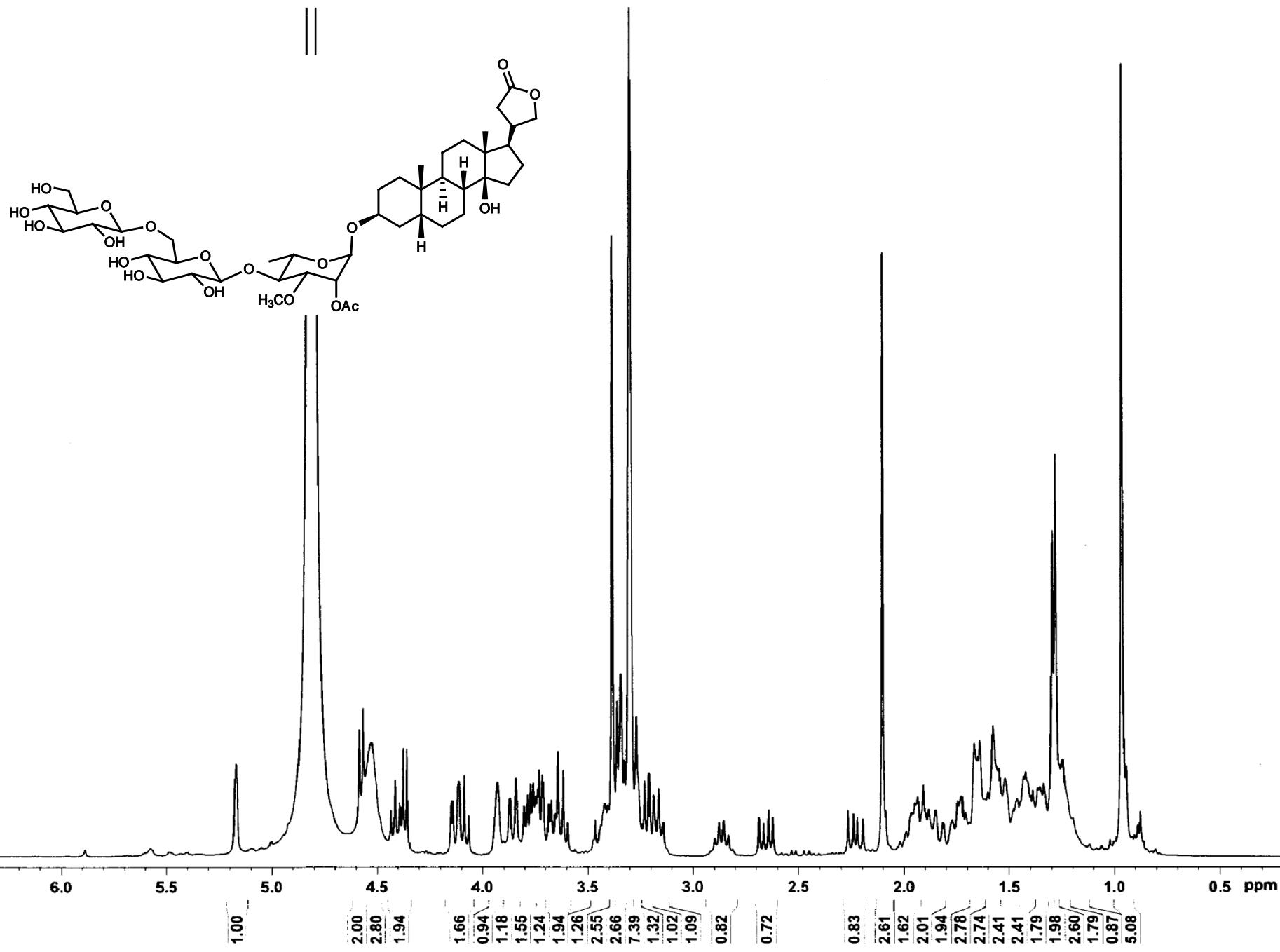


Fig S24 *J*modulated <sup>13</sup>C-NMR spectrum of compound **8** in CD<sub>3</sub>OD

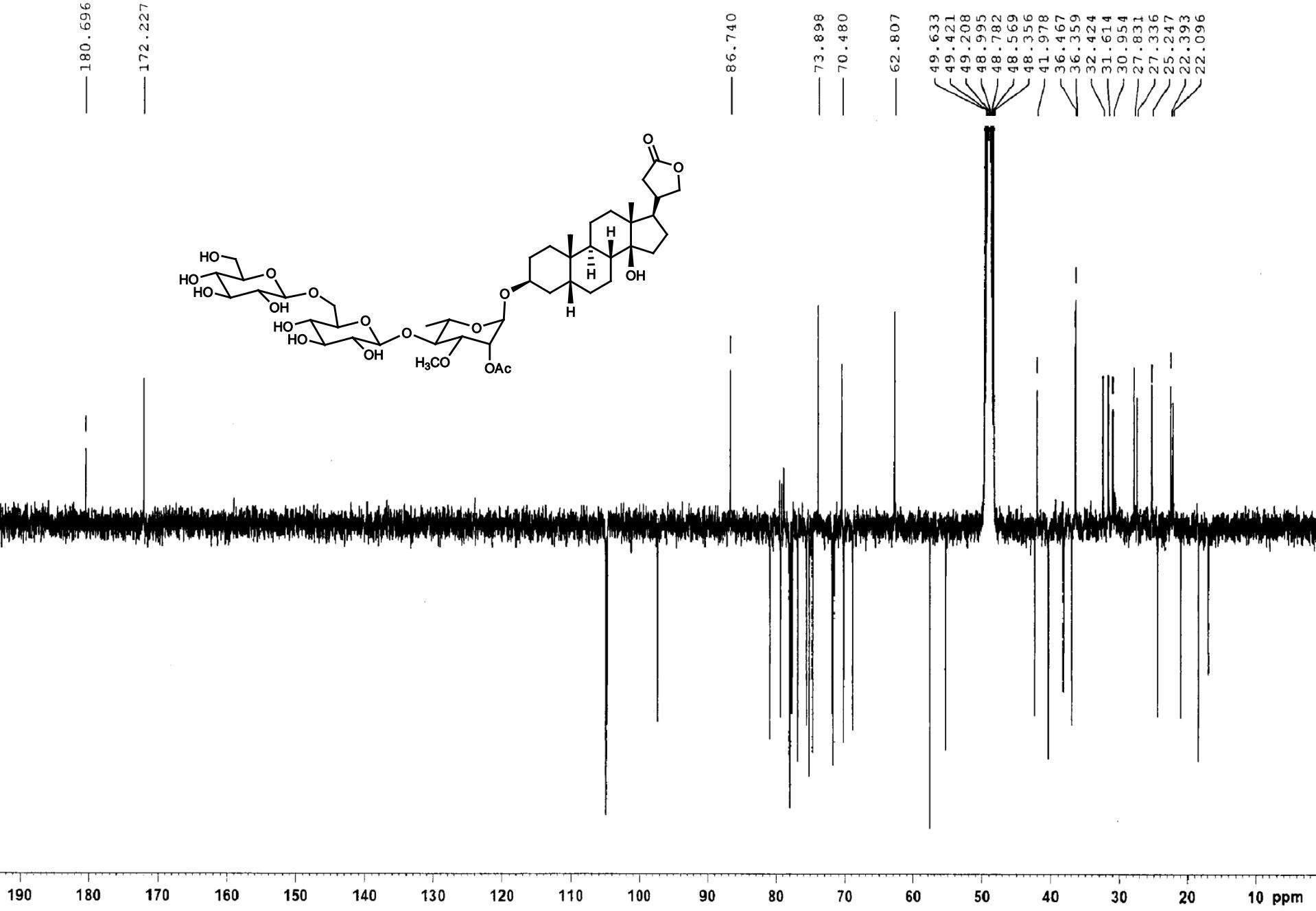


Fig S25  $^1\text{H}$ -NMR spectrum of compound **9** in  $\text{CD}_3\text{OD}$

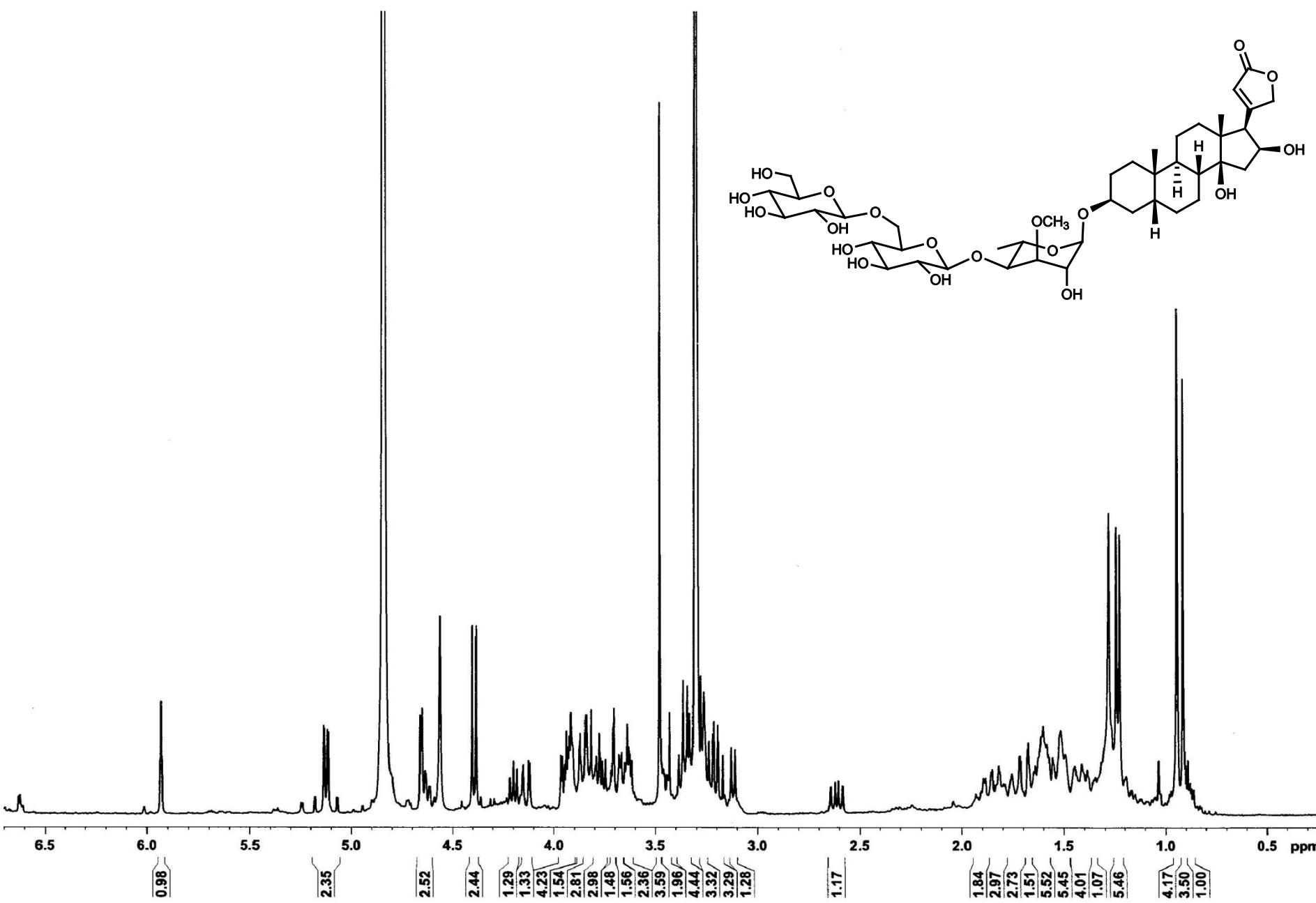


Fig S26 *J*modulated  $^{13}\text{C}$ -NMR spectrum of compound **9** in  $\text{CD}_3\text{OD}$

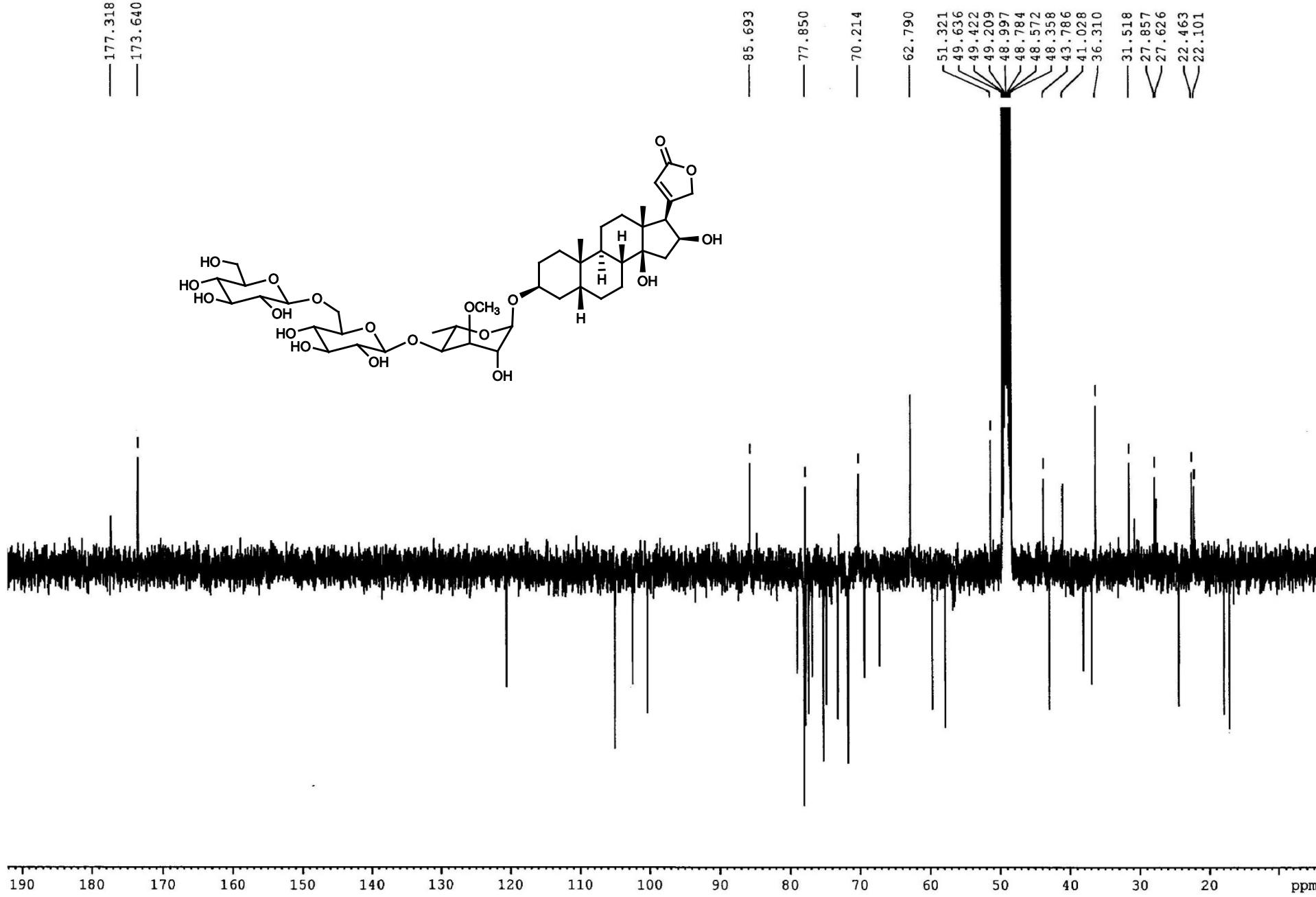


Fig S27  $^1\text{H}$ -NMR spectrum of compound **10** in  $\text{CD}_3\text{OD}$

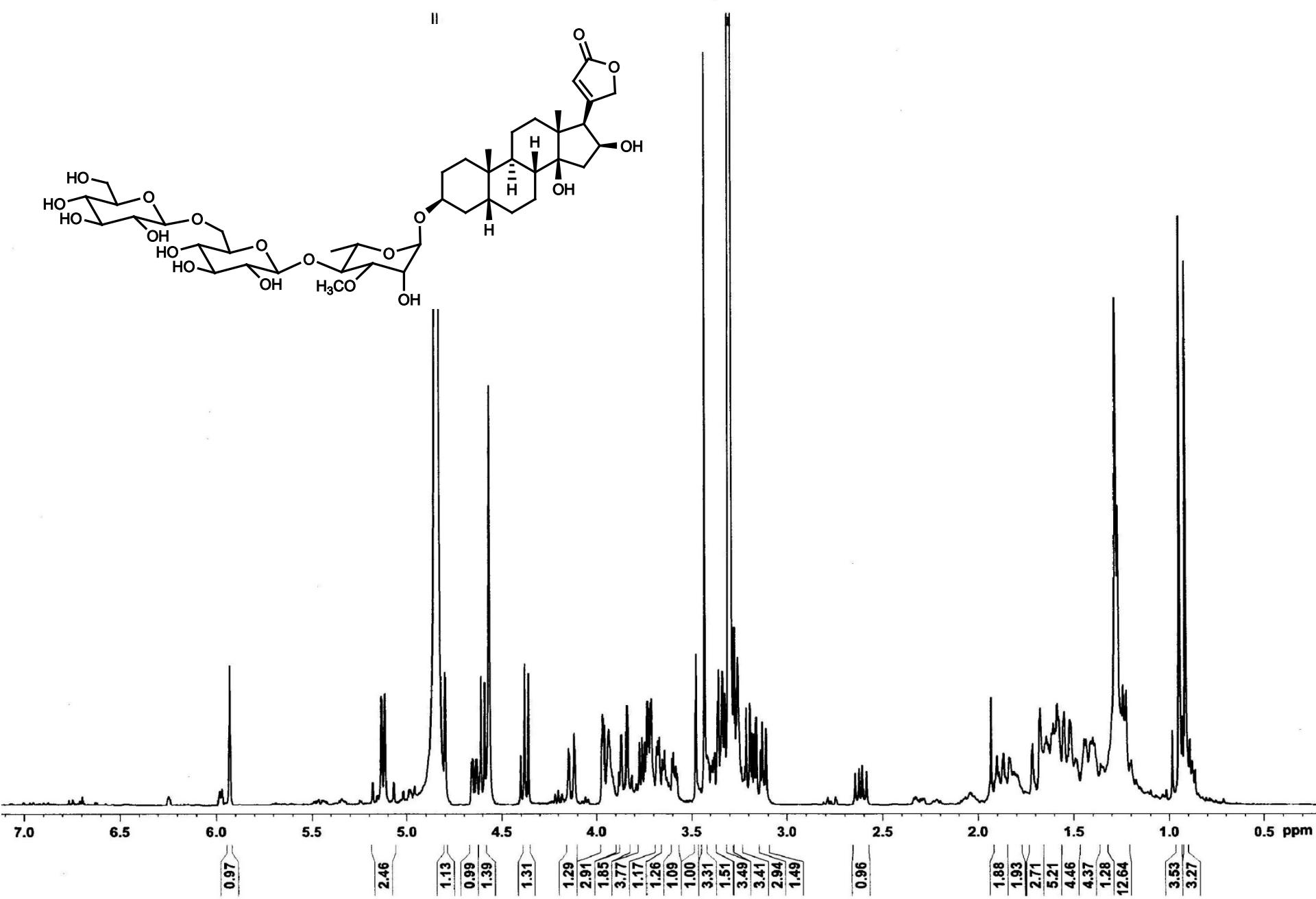


Fig S28 *J*modulated  $^{13}\text{C}$ -NMR spectrum of compound **10** in  $\text{CD}_3\text{OD}$

