

**Isolation and Structural Characterization of Specific Bacterial  $\beta$ -Glucuronidase Inhibitors from Noni (*Morinda citrifolia*) Fruits**

Fei Yang, Wenjun Zhu, Shi Sun, Qing Ai, Paba Edirisuriya, and Kequan Zhou\*

Department of Nutrition and Food Science, Wayne State University, Detroit,  
Michigan 48202, United States

Corresponding Author

\*Tel: +1 313-577-3444. Fax: +1 313-577-8616. E-mail: [kzhou@wayne.edu](mailto:kzhou@wayne.edu)

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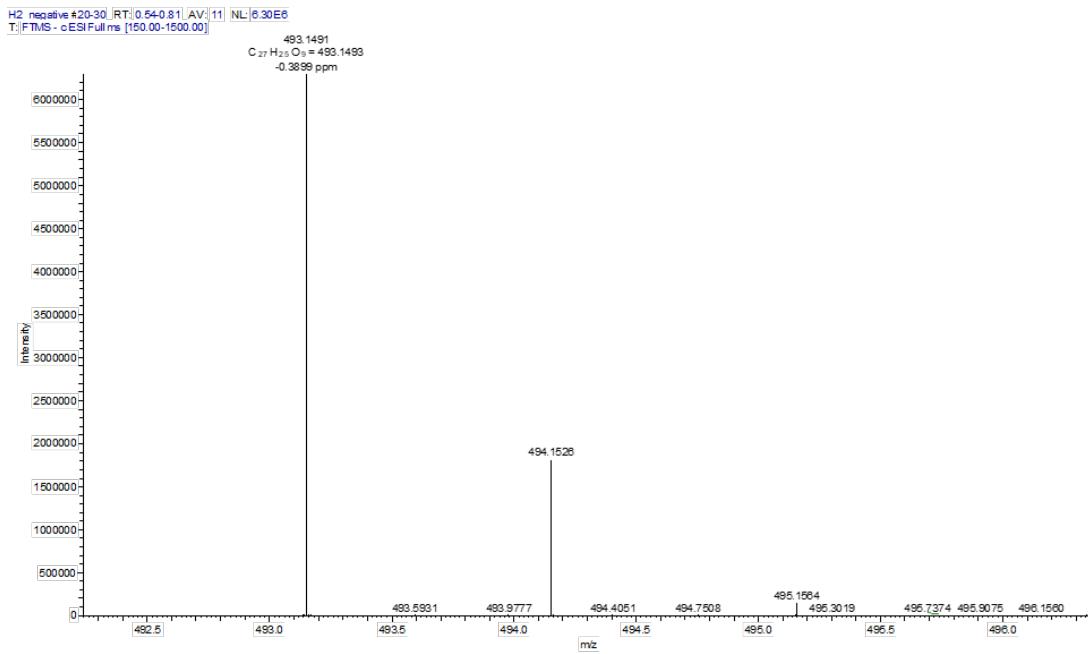


Figure S1. HRESIMS spectrum of (7S,8S,7'R,8'R)-isoamericanol B (**1**)

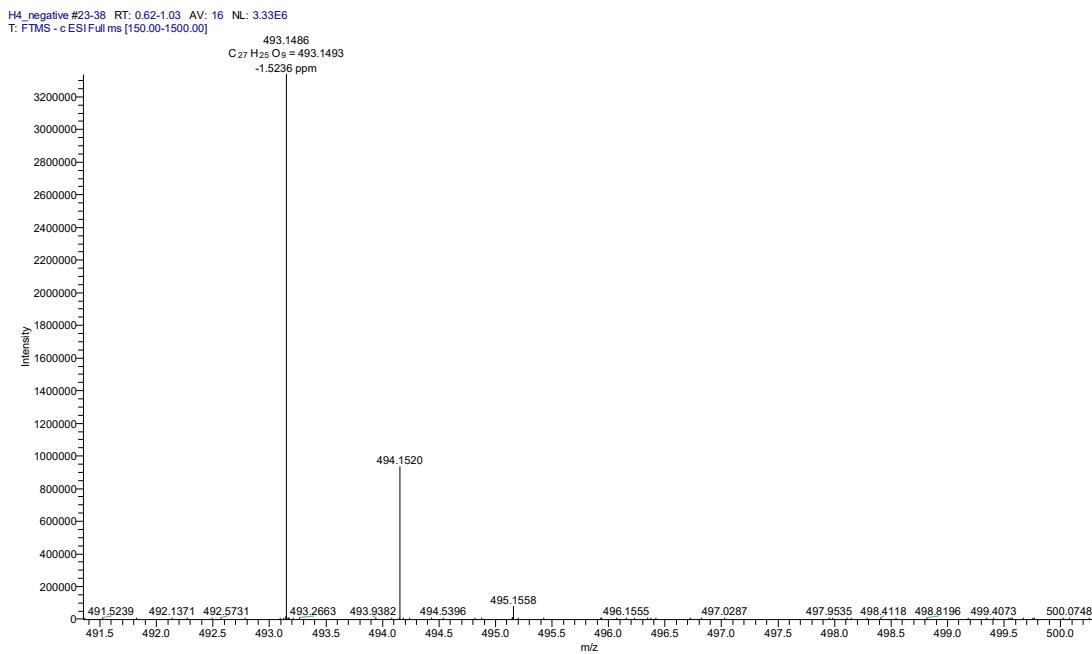


Figure S2. HRESIMS spectrum of americanol B (**2**)

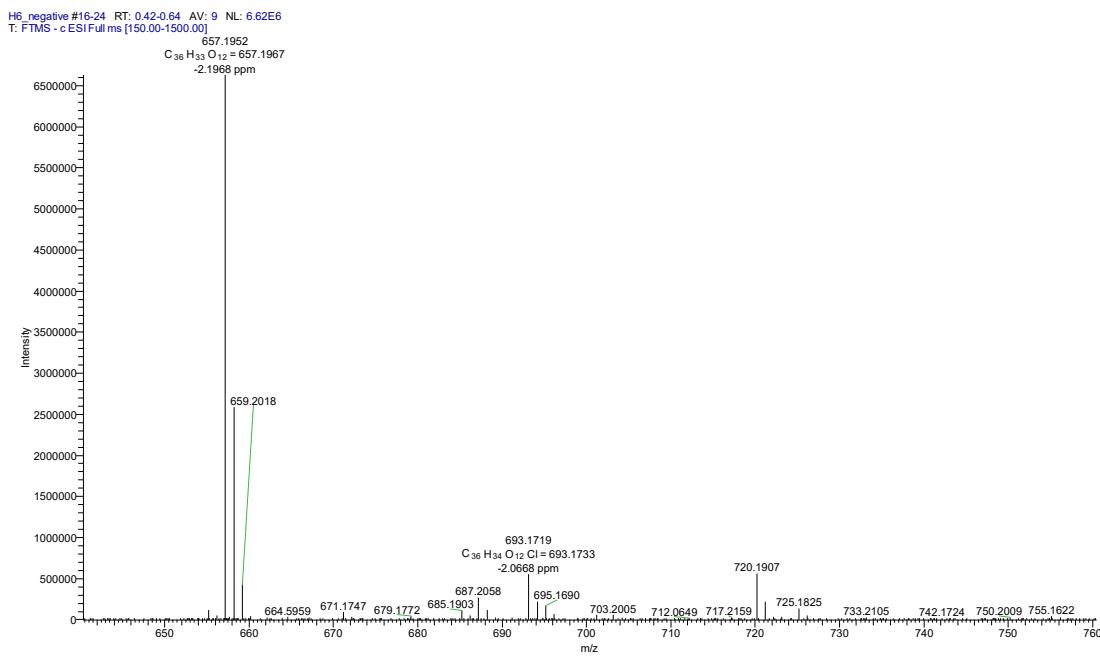


Figure S3. HRESIMS spectrum of moricitin A (**3**)

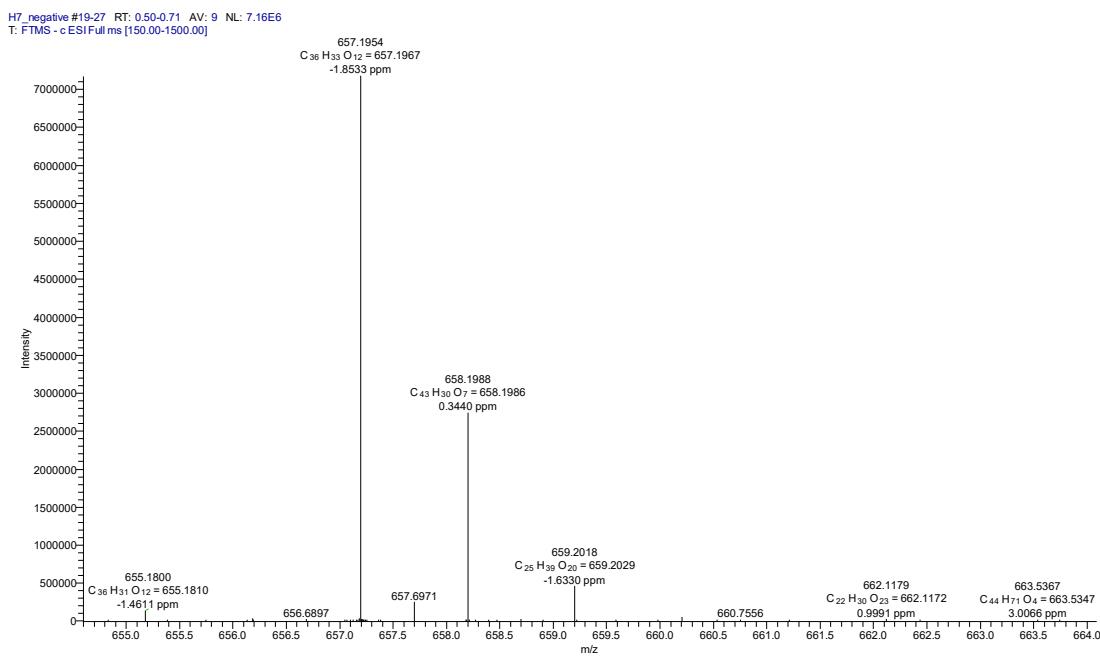


Figure S4. HRESIMS spectrum of moricitin B (**4**)

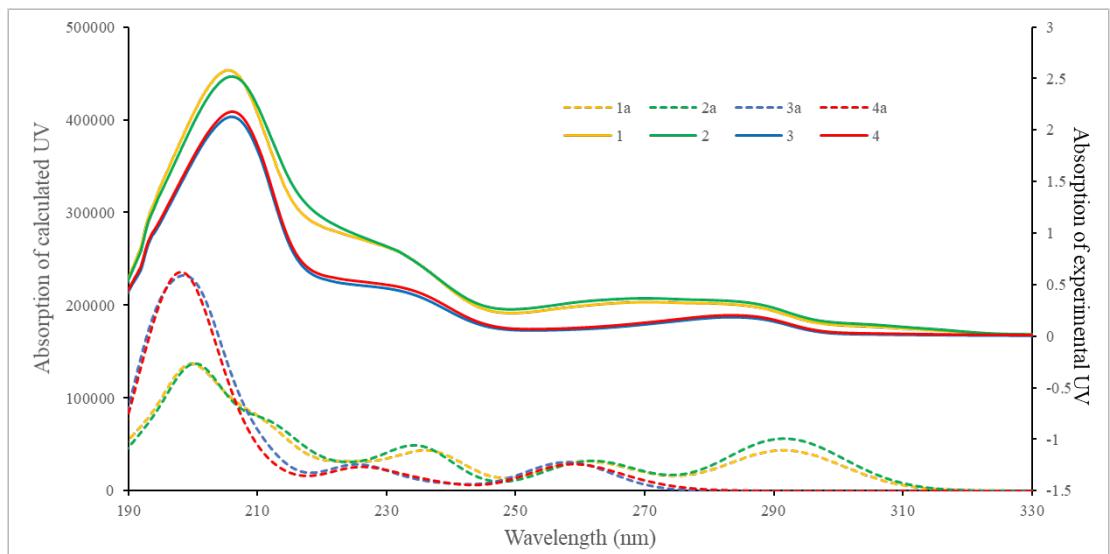
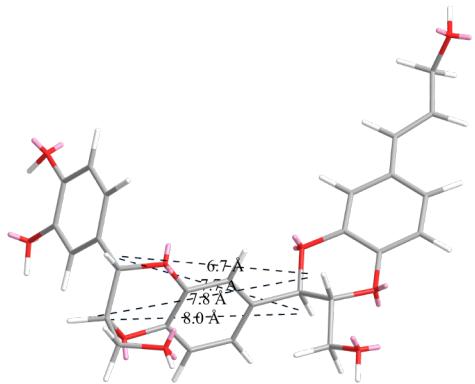
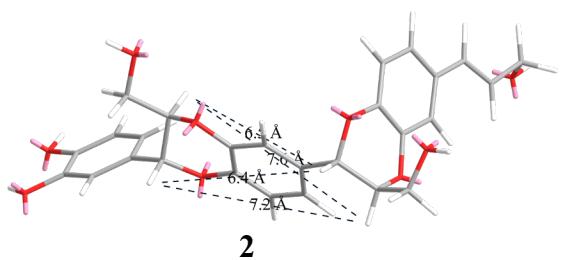


Figure S5. Experimental (solid lines) and calculated (dashed lines) UV spectra of compounds **1-4** and their model structures



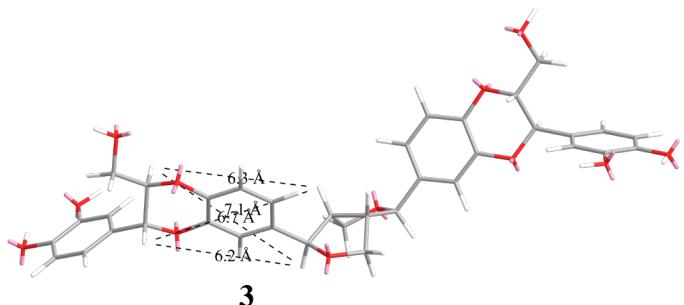
**1**

proton	distance
H-7 to H-7'	7.7 Å
H-7 to H-8'	6.7 Å
H-8 to H-7'	8.0 Å
H-8 to H-8'	7.8 Å



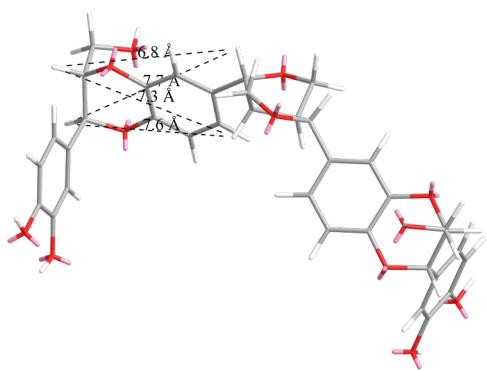
**2**

proton	distance
H-7 to H-7'	6.4 Å
H-7 to H-8'	7.2 Å
H-8 to H-7'	6.5 Å
H-8 to H-8'	7.6 Å



**3**

proton	distance
H-7 to H-7"	6.2 Å
H-7 to H-8"	6.7 Å
H-8 to H-7"	7.1 Å
H-8 to H-8"	6.3 Å



**4**

proton	distance
H-7 to H-7"	7.7 Å
H-7 to H-8"	6.8 Å
H-8 to H-7"	7.6 Å
H-8 to H-8"	7.3 Å

Figure S6. Distances between protons of steric centers for compounds **1-4** (energy minimized by MM2 force field)

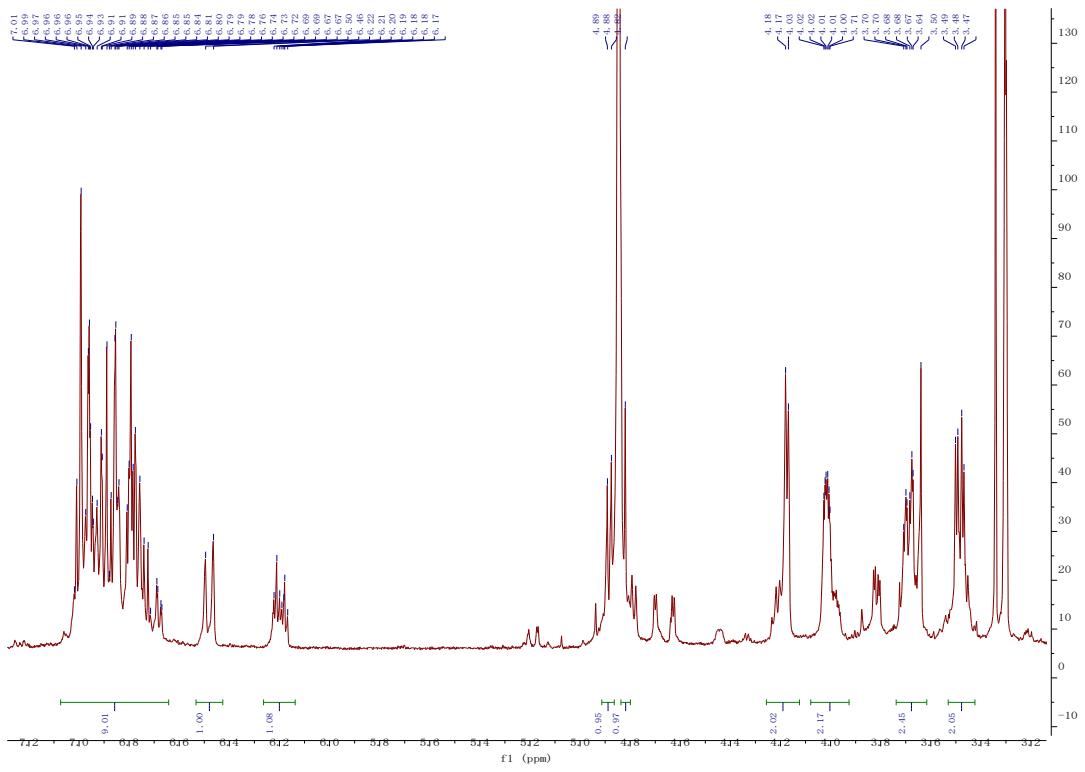


Figure S7.  $^1\text{H}$  NMR (500 MHz,  $\text{CD}_3\text{OD}$ ) spectrum of (7*S*,8*S*,7'*R*,8'*R*)-isoamericanol B (**1**)

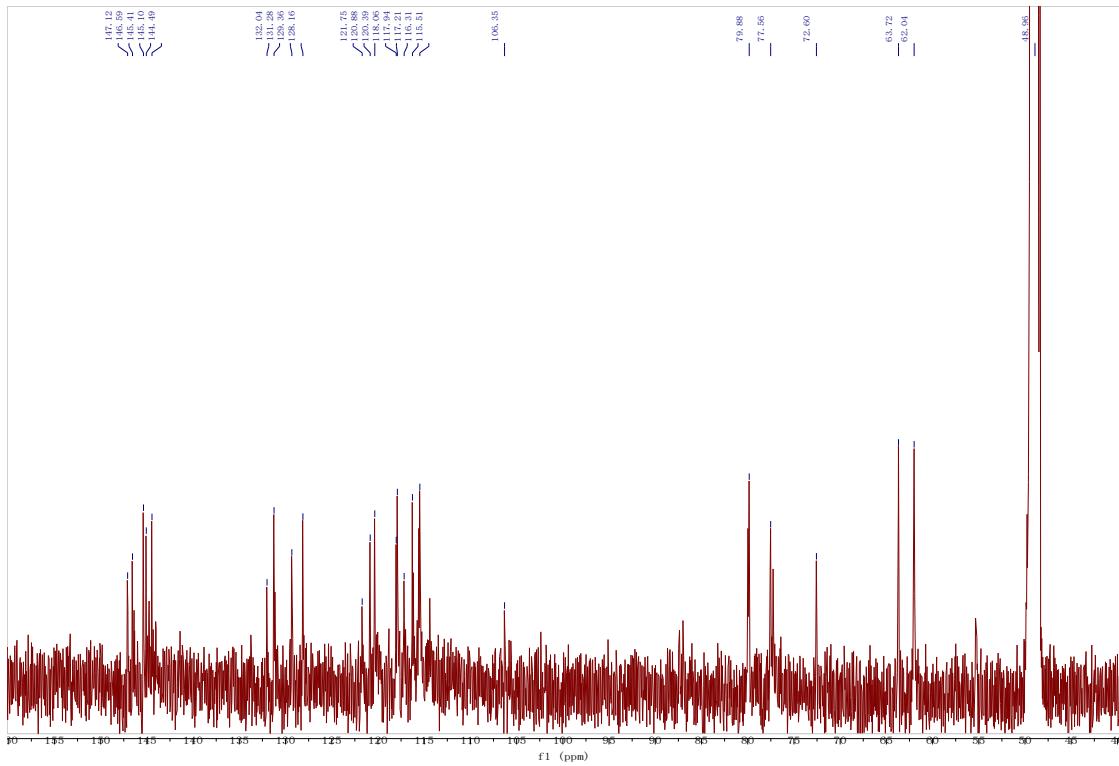


Figure S8.  $^{13}\text{C}$  NMR (125 MHz,  $\text{CD}_3\text{OD}$ ) spectrum of (7*S*,8*S*,7'*R*,8'*R*)-isoamericanol B (**1**)

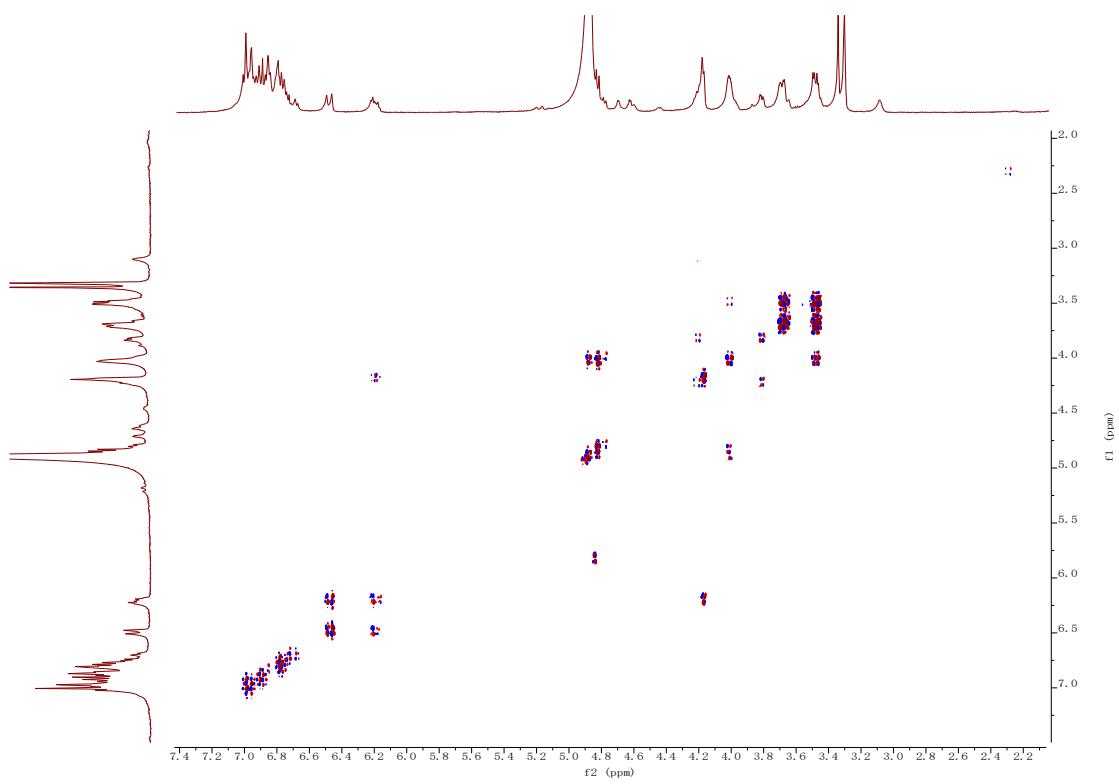


Figure S9. COSY ( $\text{CD}_3\text{OD}$ ) spectrum of ( $7\text{S},8\text{S},7'\text{R},8'\text{R}$ )-isoamericanol B (**1**)

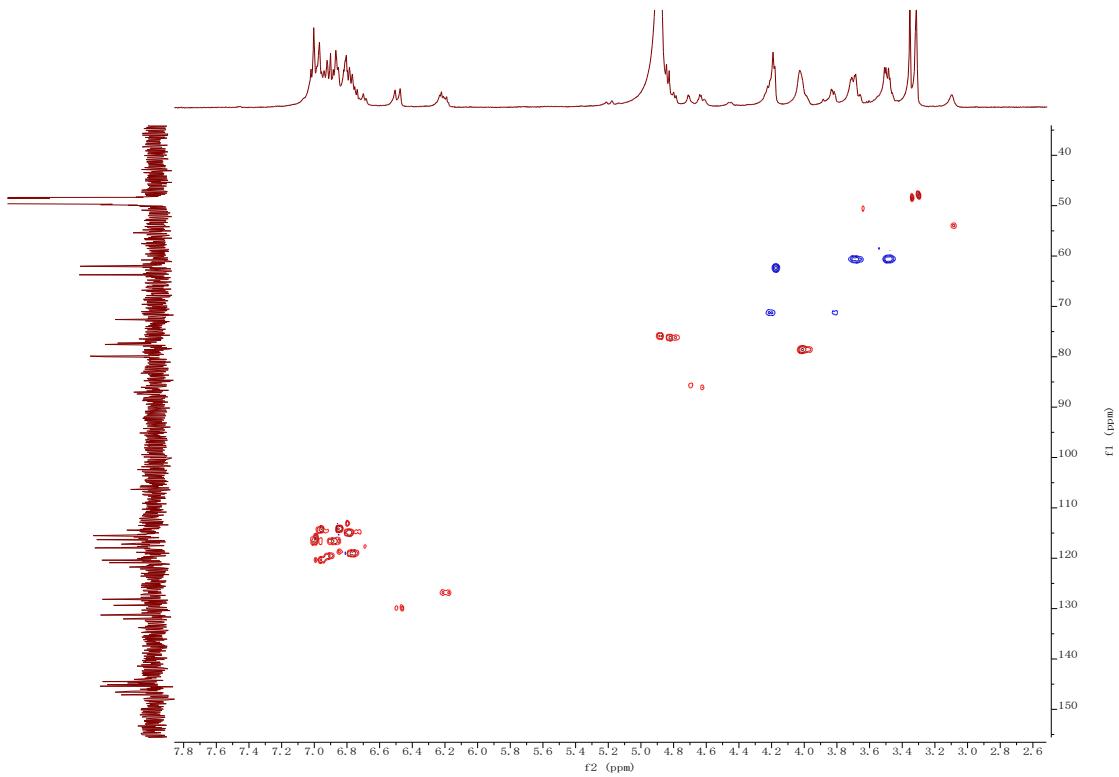


Figure S10. HSQC ( $\text{CD}_3\text{OD}$ ) spectrum of ( $7\text{S},8\text{S},7'\text{R},8'\text{R}$ )-isoamericanol B (**1**)

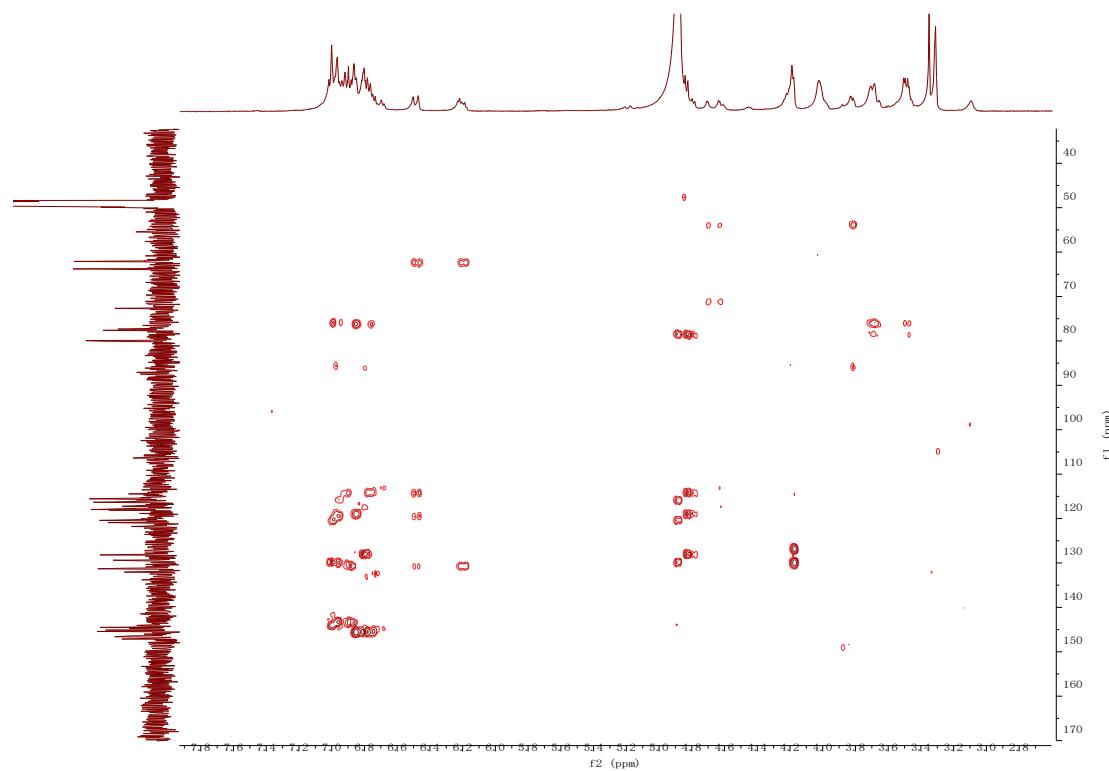


Figure S6. HMBC ( $\text{CD}_3\text{OD}$ ) spectrum of (7*S*,8*S*,7'*R*,8'*R*)-isoamericanol B (**1**)

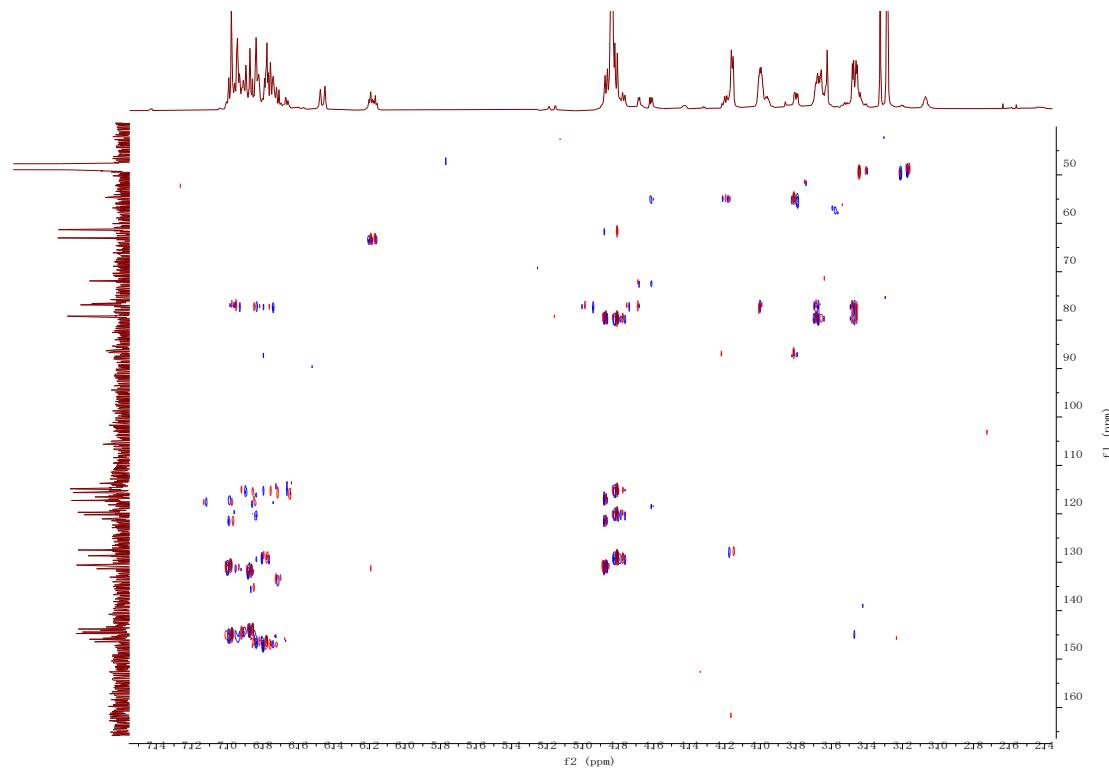


Figure S7. HMBC (600 MHz,  $\text{CD}_3\text{OD}$ , coupling constant = 3 Hz) spectrum of (7*S*,8*S*,7'*R*,8'*R*)-isoamericanol B (**1**)

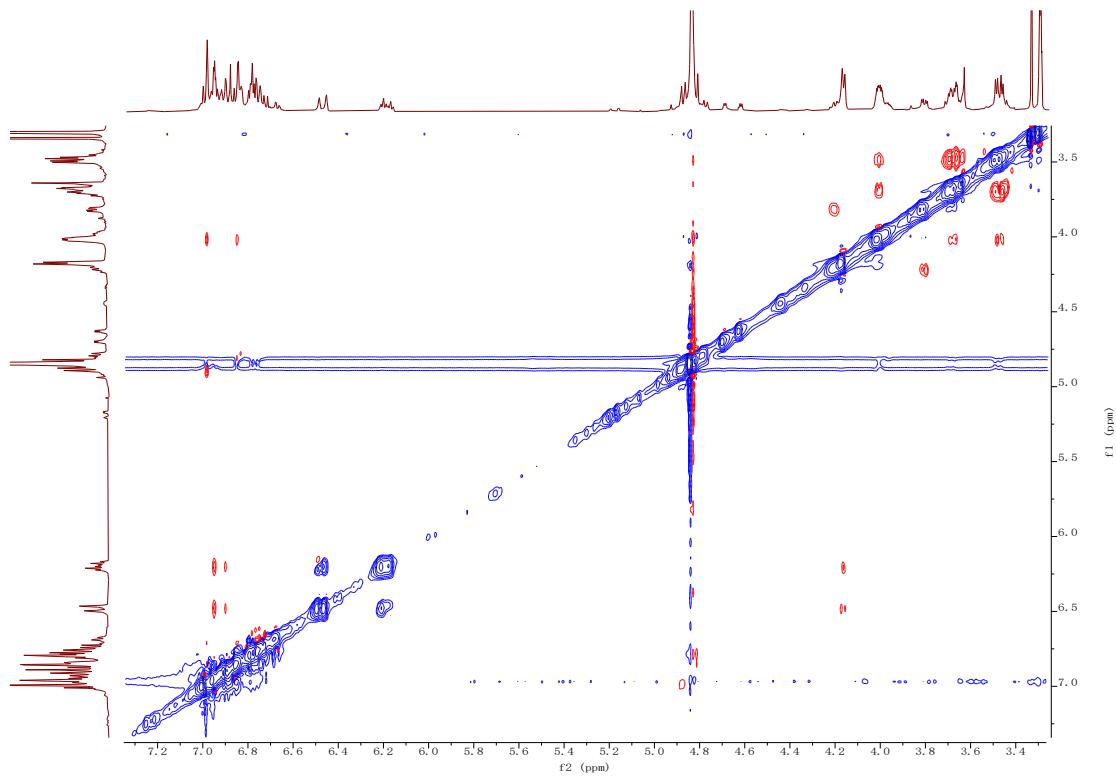


Figure S8. ROESY ( $\text{CD}_3\text{OD}$ ) spectrum of (*7S,8S,7'R,8'R*)-isoamericanol B (**1**)

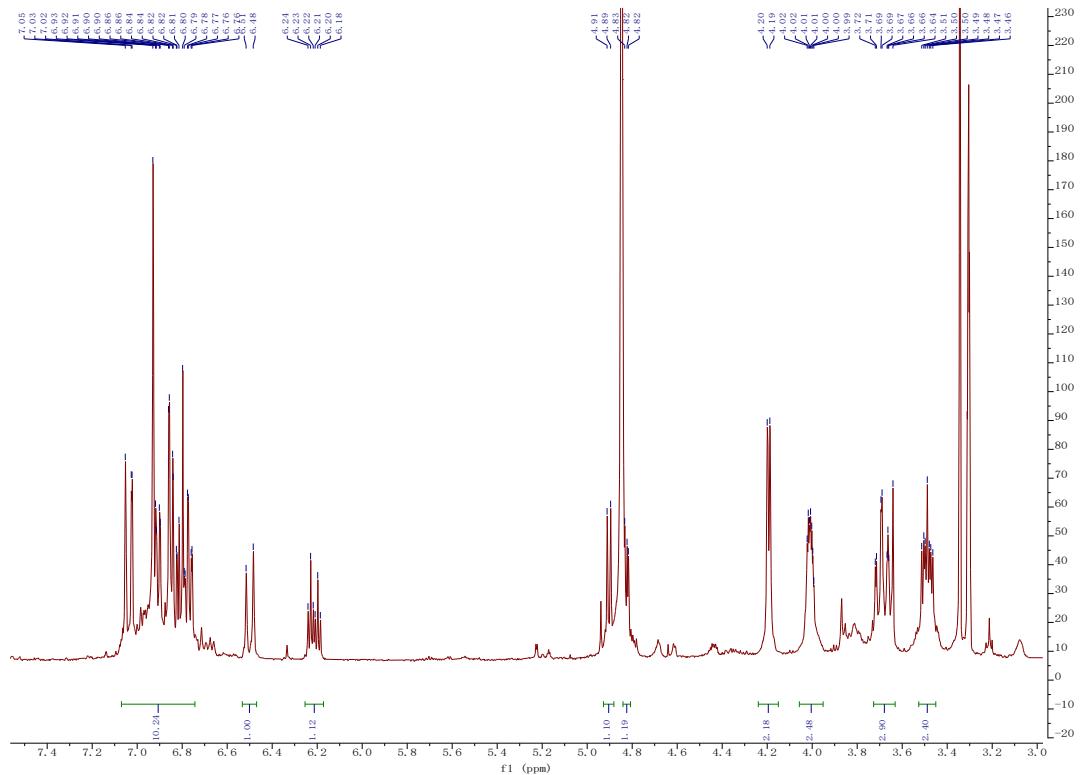


Figure S9. <sup>1</sup>H NMR (500 MHz,  $\text{CD}_3\text{OD}$ ) spectrum of americanol B (**2**)

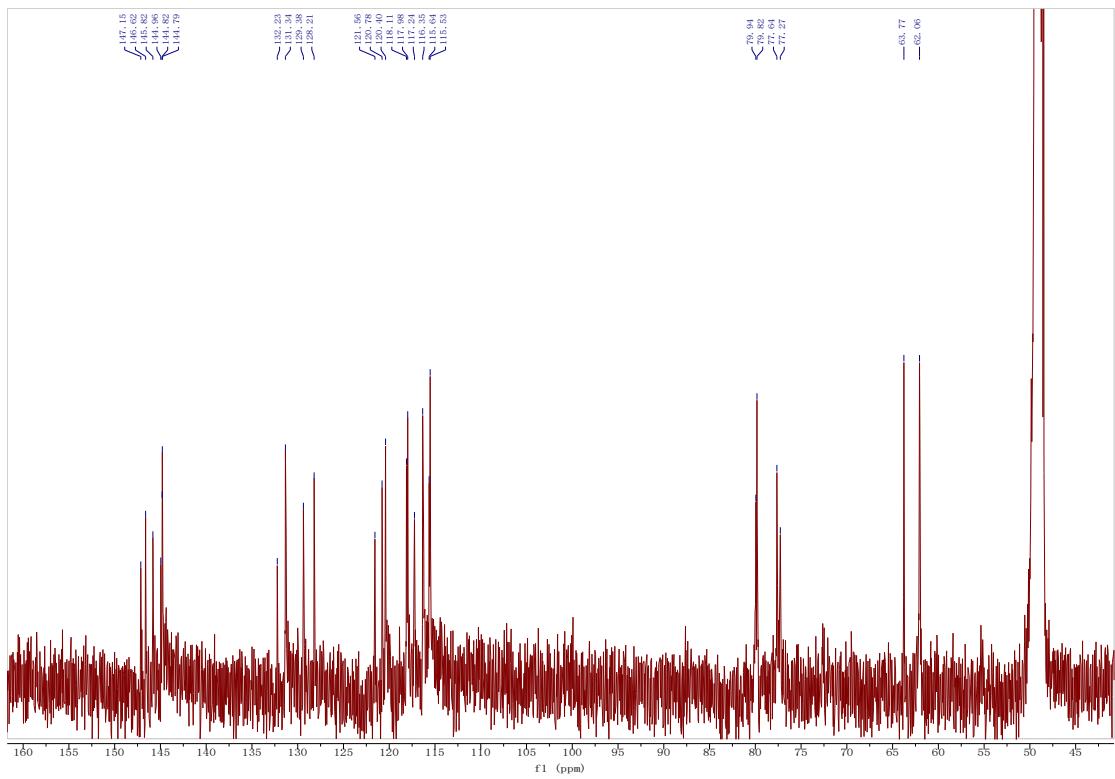


Figure S10.  $^{13}\text{C}$  NMR (125 MHz,  $\text{CD}_3\text{OD}$ ) spectrum of americanol B (2)

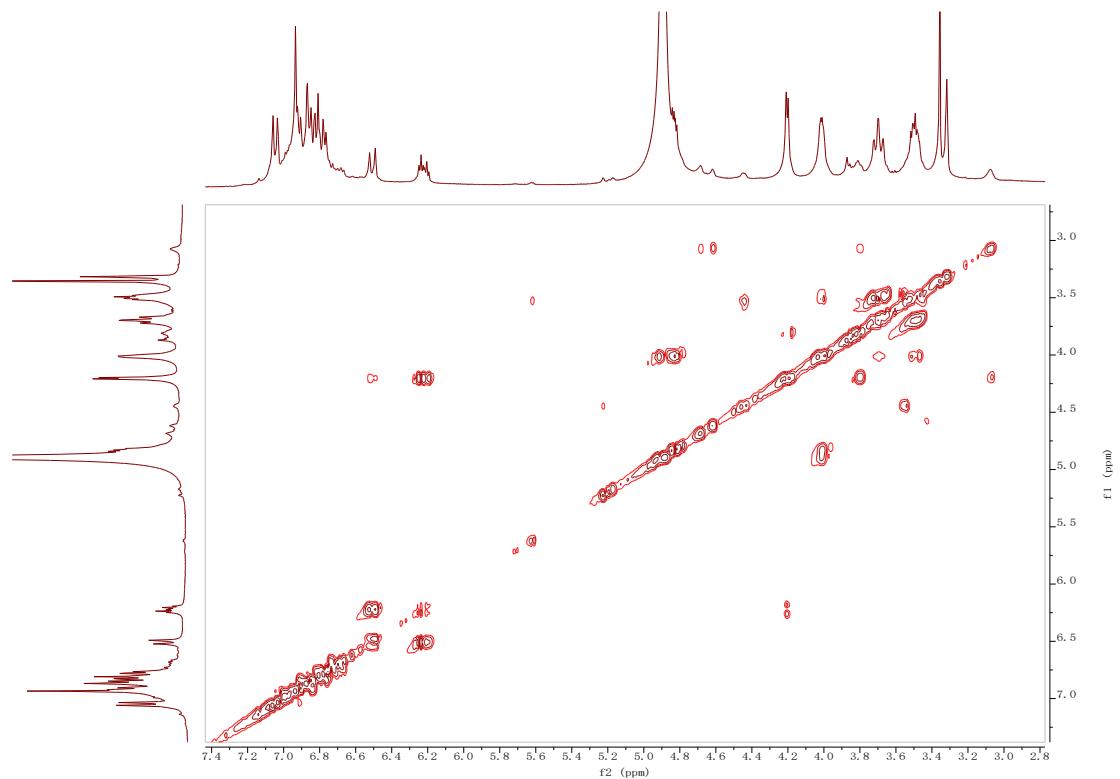


Figure S11. COSY ( $\text{CD}_3\text{OD}$ ) spectrum of americanol B (2)

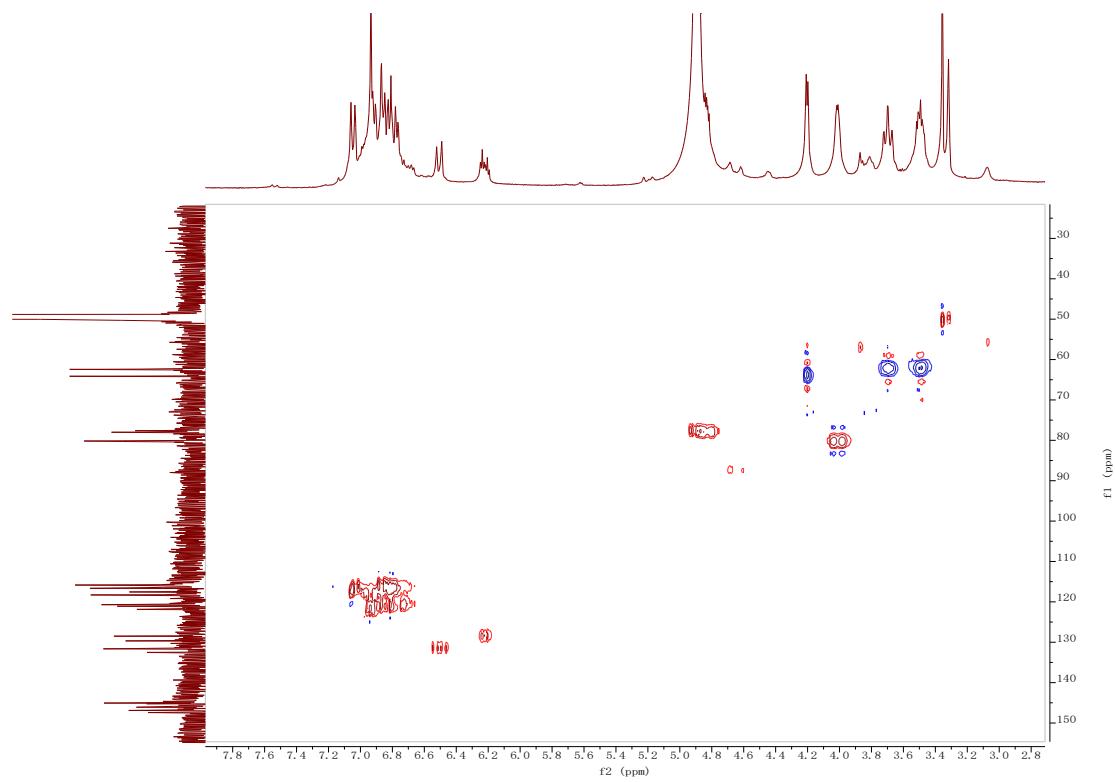


Figure S12. HSQC ( $\text{CD}_3\text{OD}$ ) spectrum of americananol B (2)

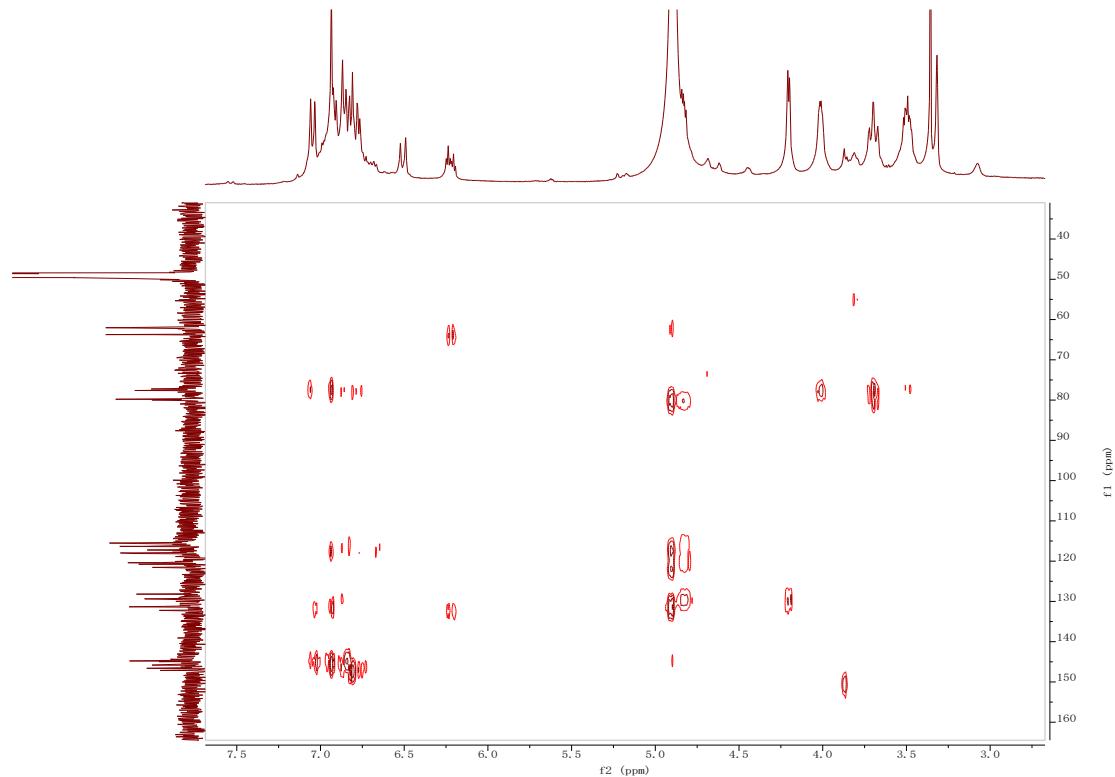


Figure S13. HMBC ( $\text{CD}_3\text{OD}$ ) spectrum of americananol B (2)

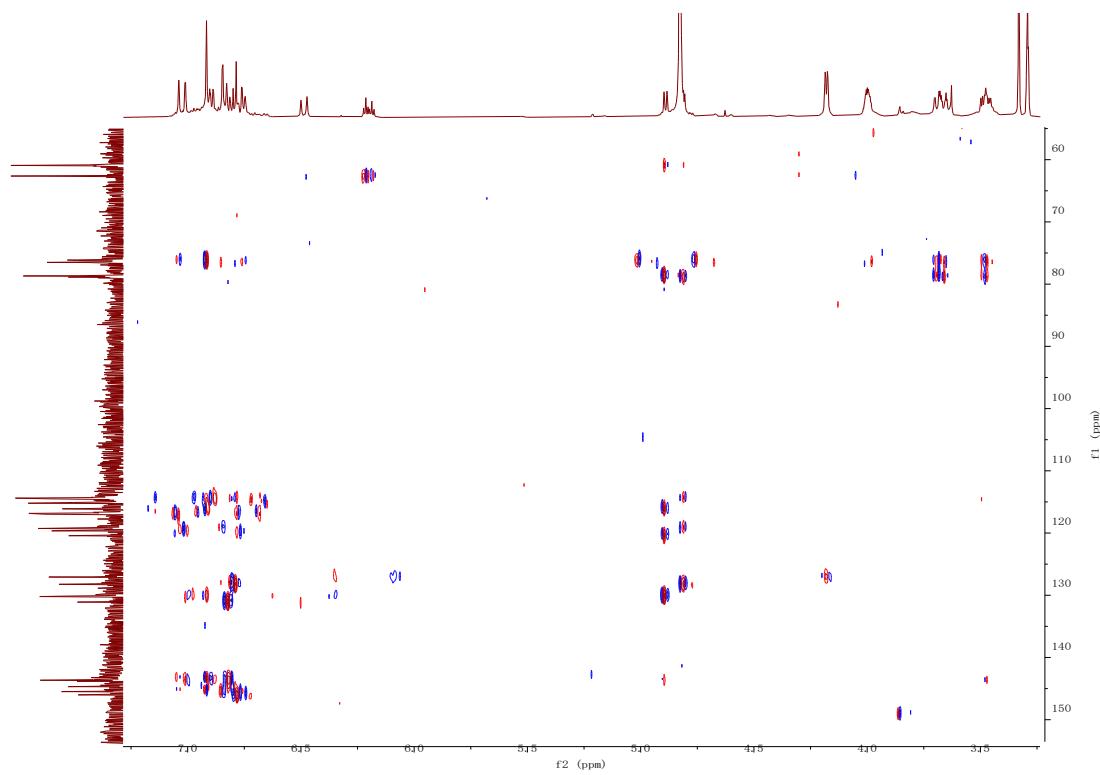


Figure S14. HMBC (600 MHz, CD<sub>3</sub>OD, coupling constant = 3 Hz) spectrum of americananol B (**2**)

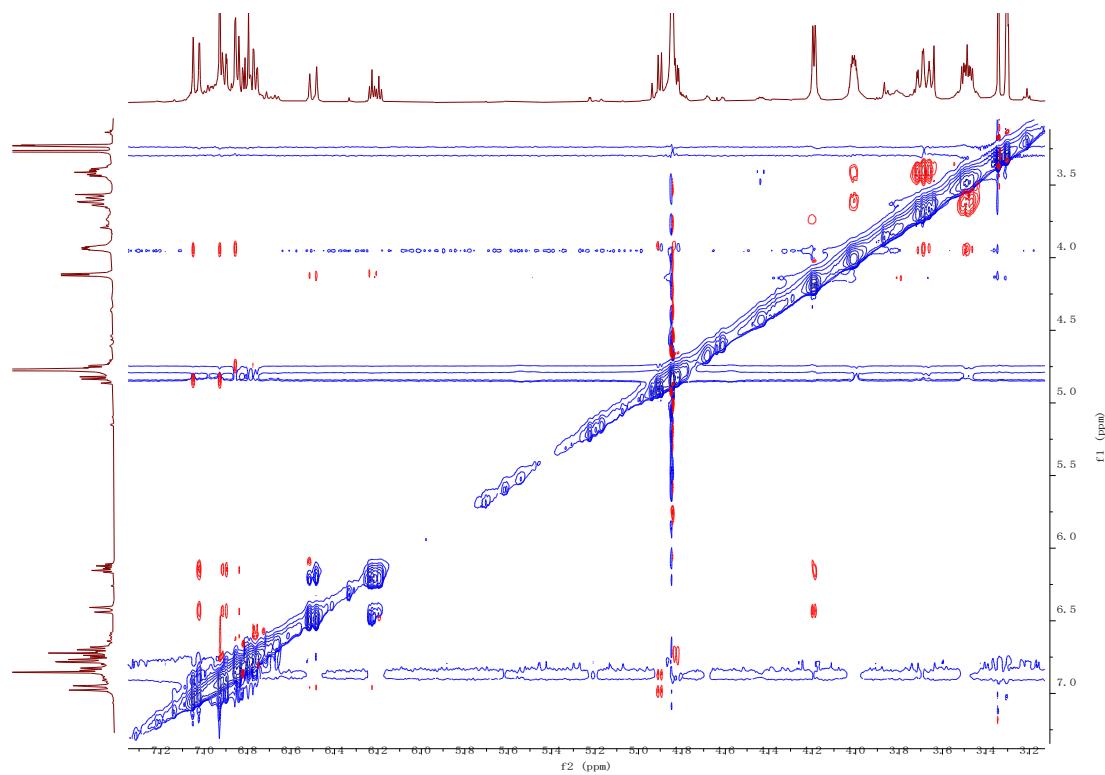


Figure S20. ROESY (CD<sub>3</sub>OD) spectrum of americananol B (**2**)

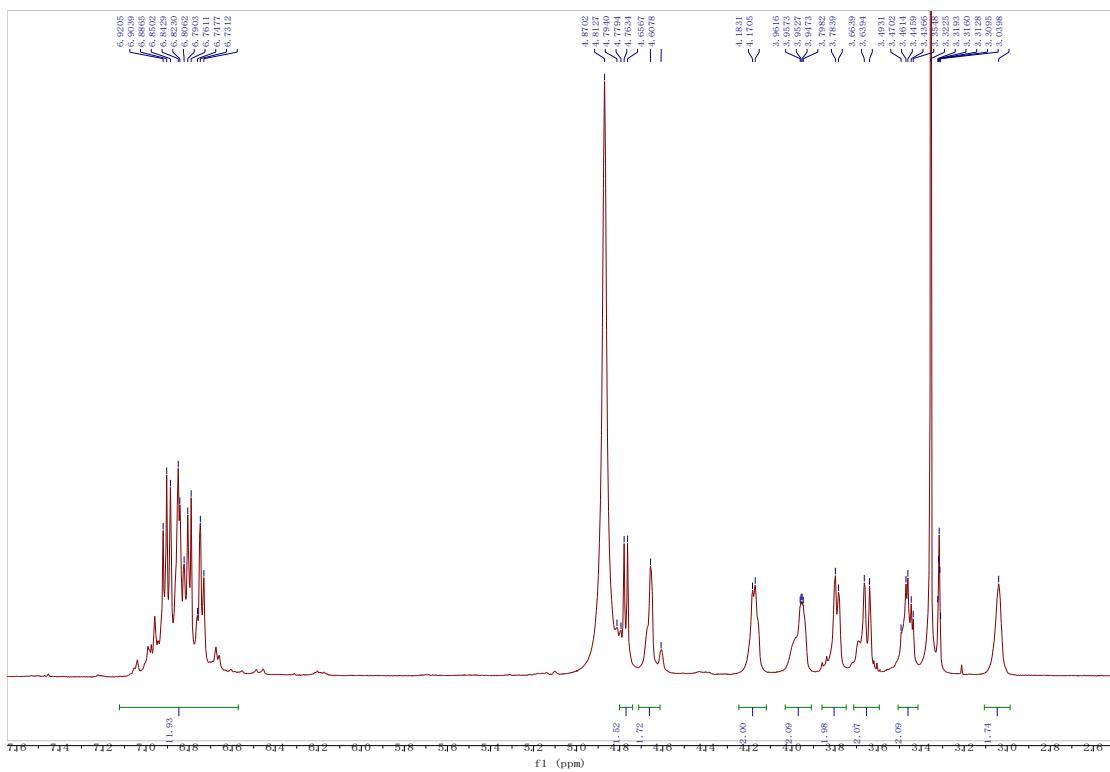


Figure S21.  $^1\text{H}$  NMR (500 MHz,  $\text{CD}_3\text{OD}$ ) spectrum of moricitin A (**3**)

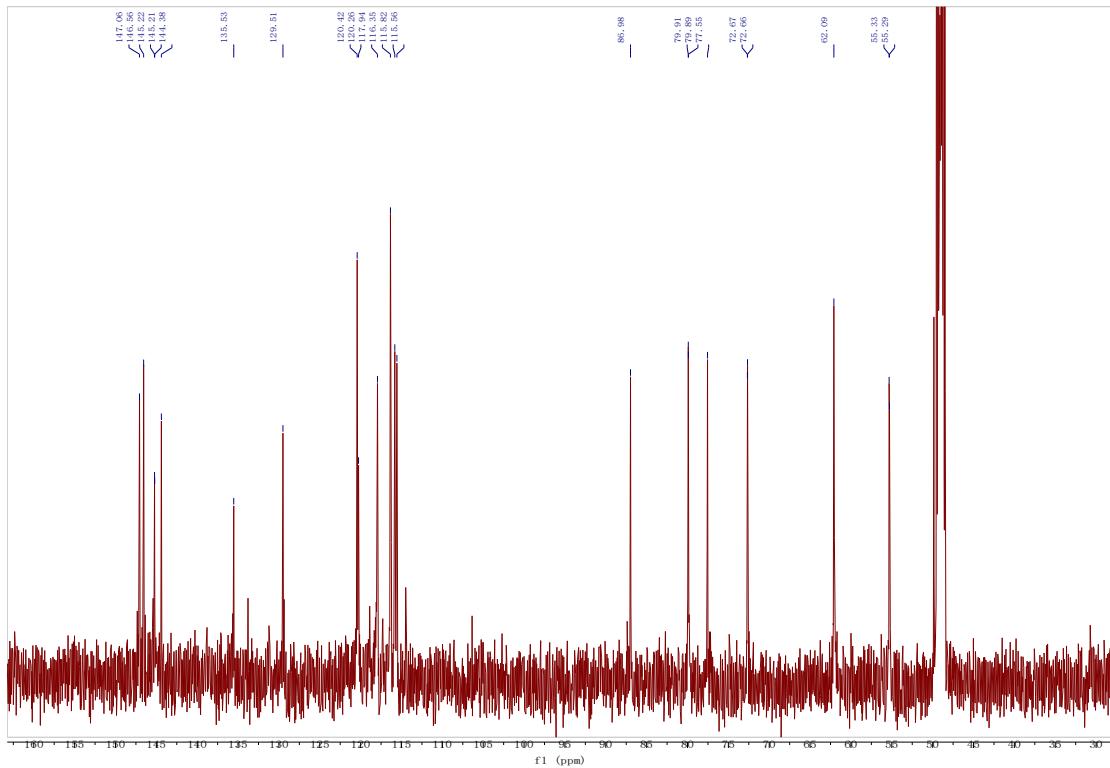


Figure S22.  $^{13}\text{C}$  NMR (125 MHz,  $\text{CD}_3\text{OD}$ ) spectrum of moricitin A (**3**)

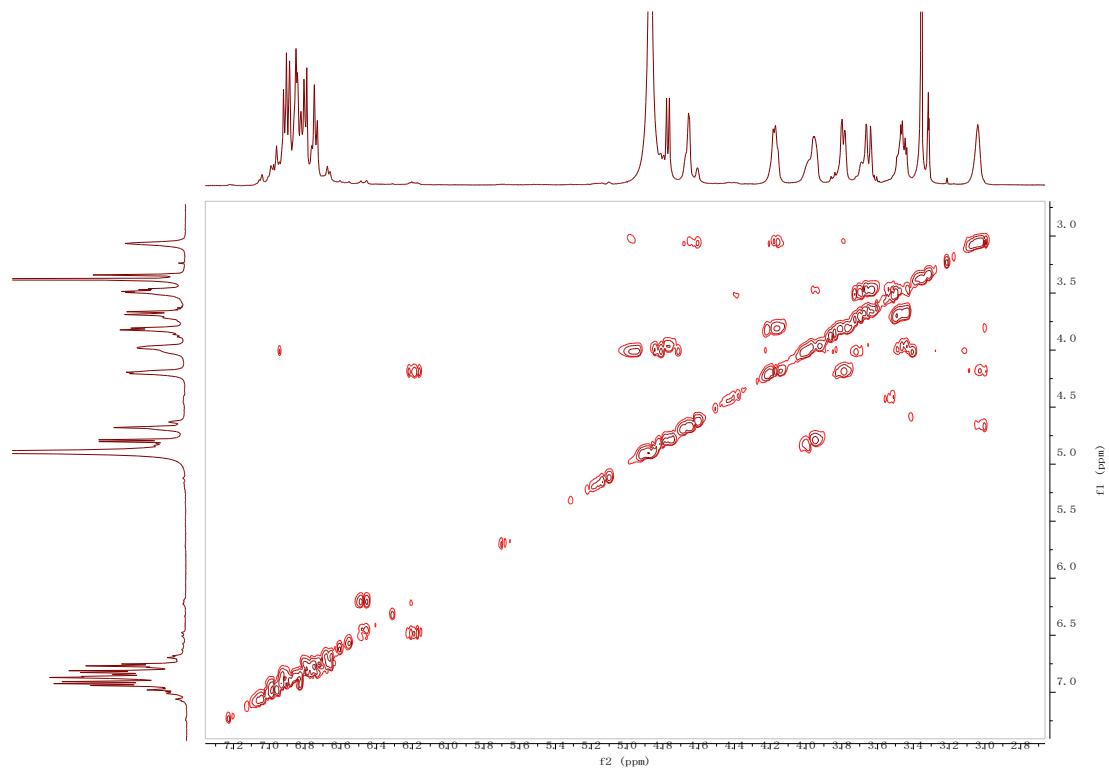


Figure S15. COSY (CD<sub>3</sub>OD) spectrum of moricitin A (**3**)

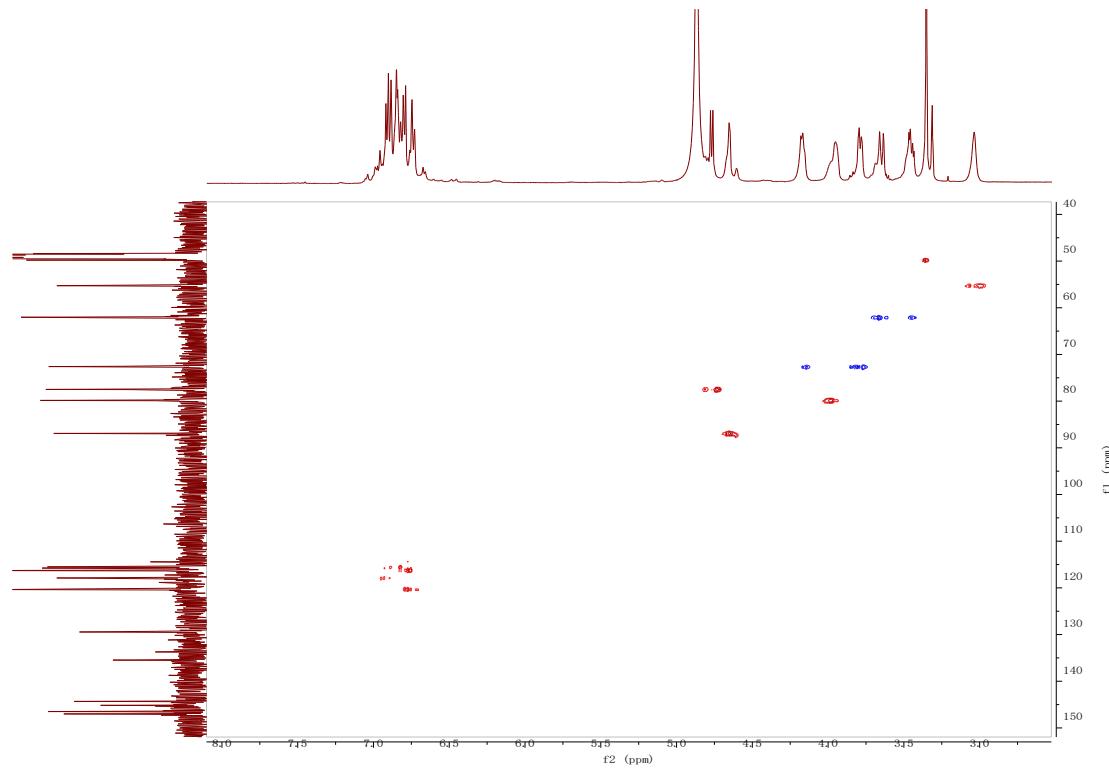


Figure S16. HSQC (CD<sub>3</sub>OD) spectrum of moricitin A (**3**)

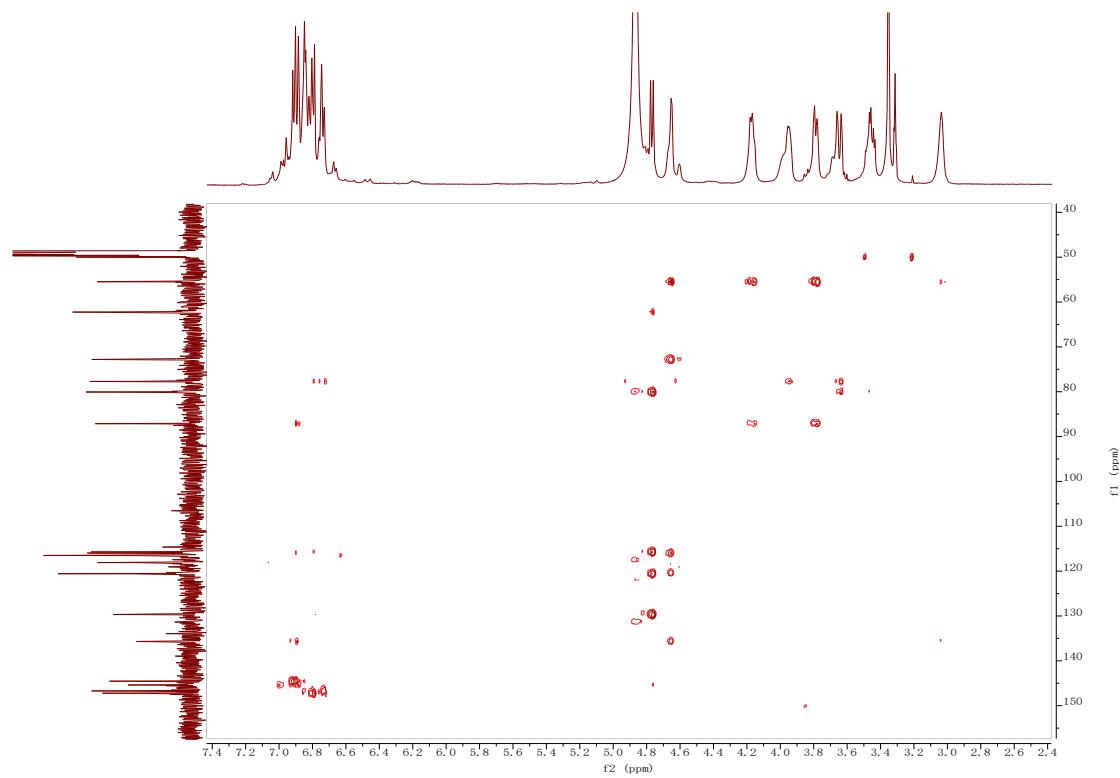


Figure S17. HMBC (CD<sub>3</sub>OD) spectrum of moricitin A (**3**)

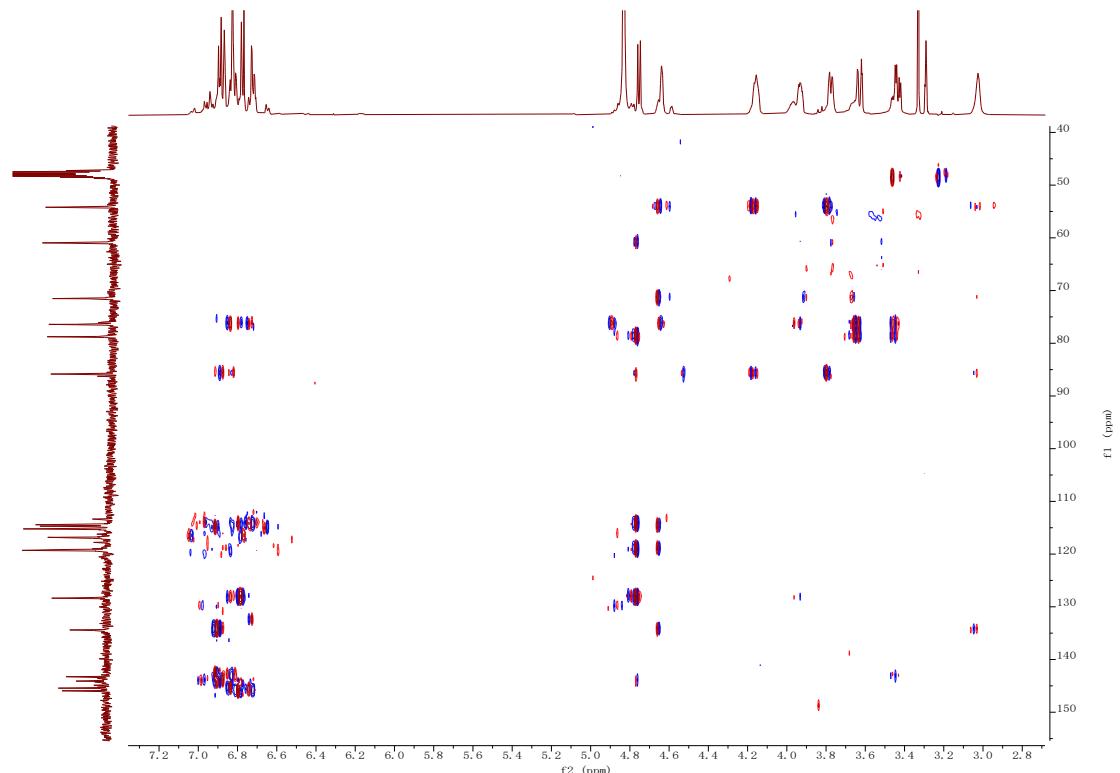


Figure S18. HMBC (600 MHz, CD<sub>3</sub>OD, coupling constant = 3 Hz) spectrum of moricitin A (**3**)

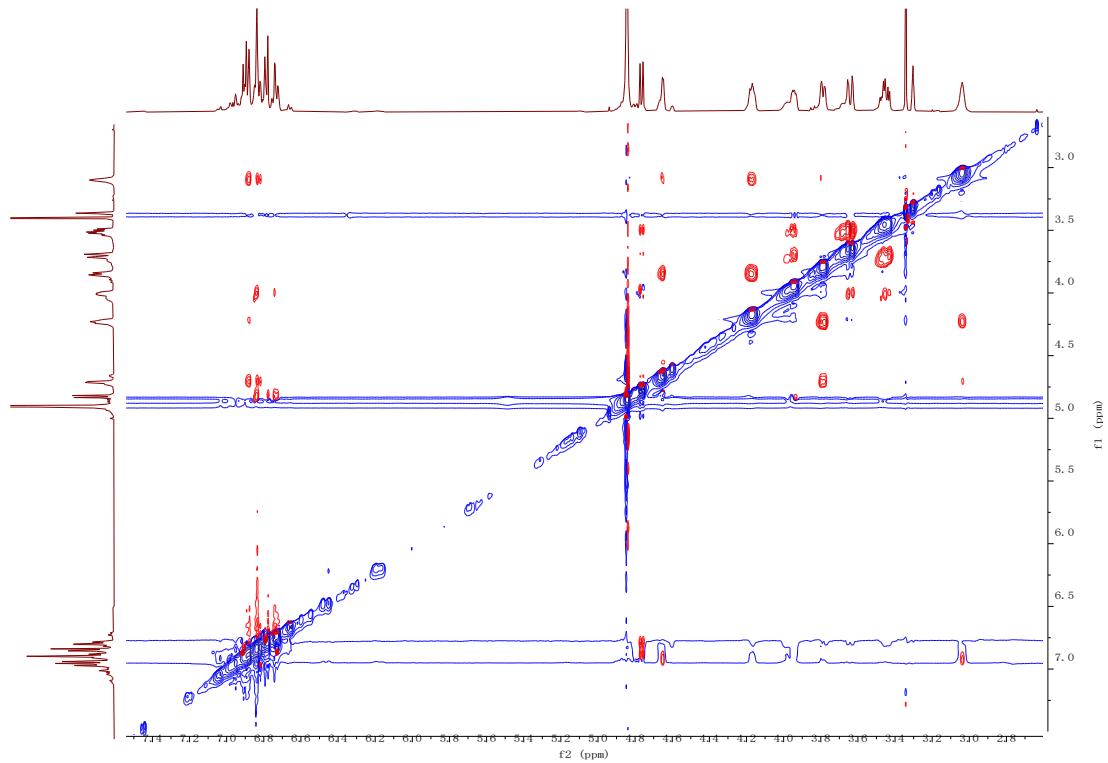


Figure S19. ROESY (CD3OD) spectrum of moricitrin A (**3**)

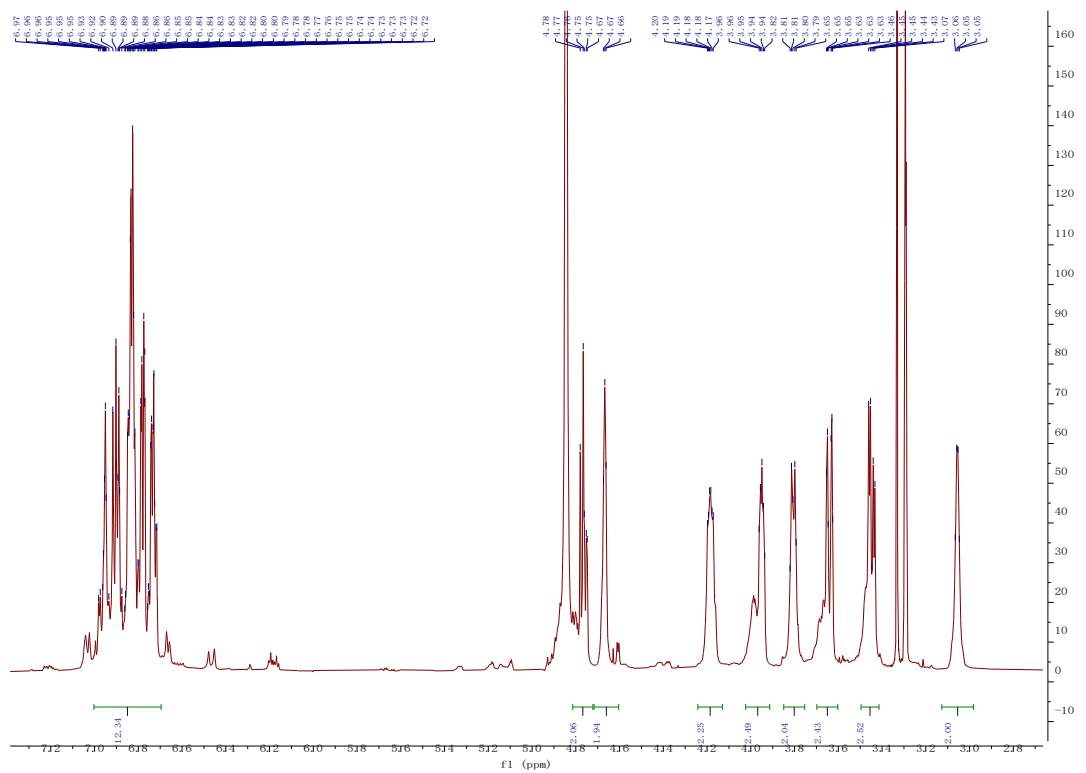


Figure S20.  $^1\text{H}$  NMR (500 MHz,  $\text{CD}_3\text{OD}$ ) spectrum of moricitrin B (**4**)

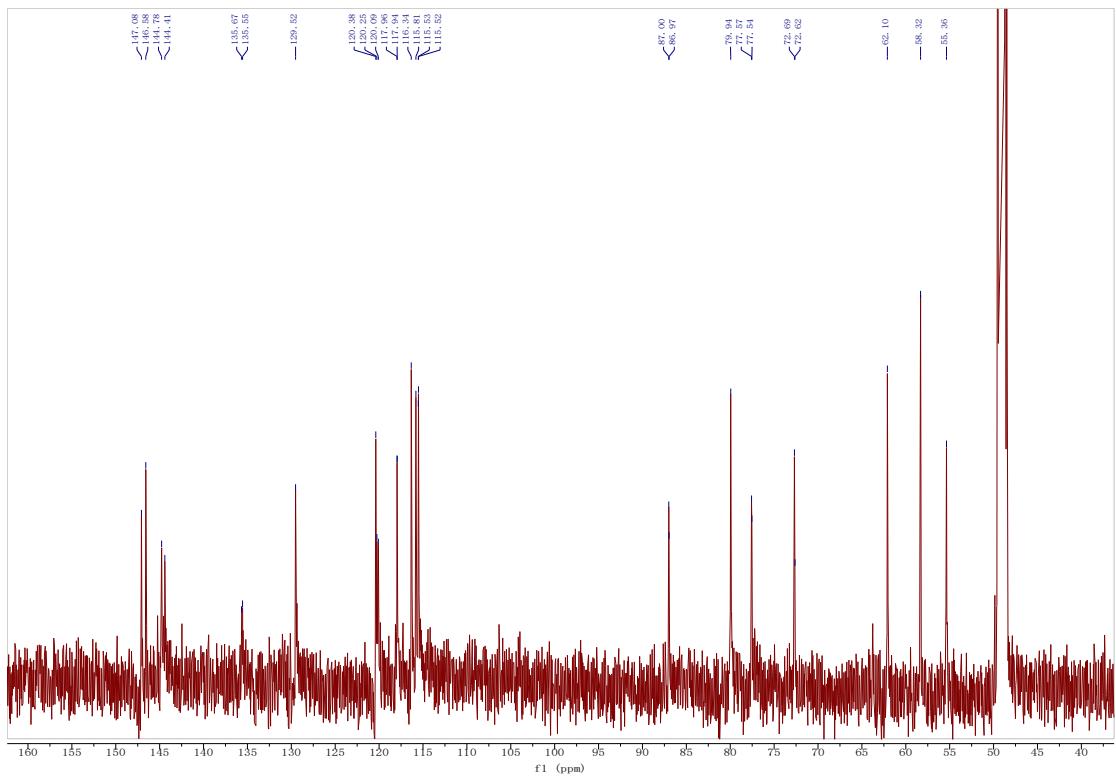


Figure S21.  $^{13}\text{C}$  NMR (125 MHz,  $\text{CD}_3\text{OD}$ ) spectrum of moricitrin B (**4**)

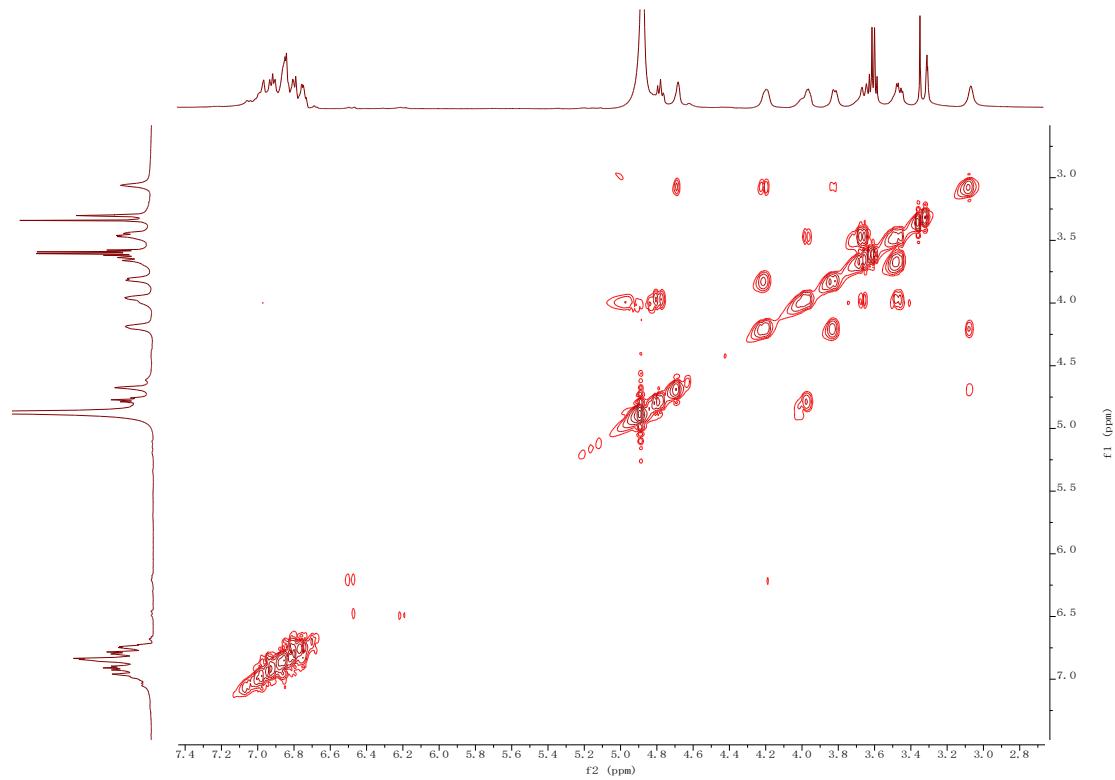


Figure S30. COSY ( $\text{CD}_3\text{OD}$ ) spectrum of moricitrin B (4)

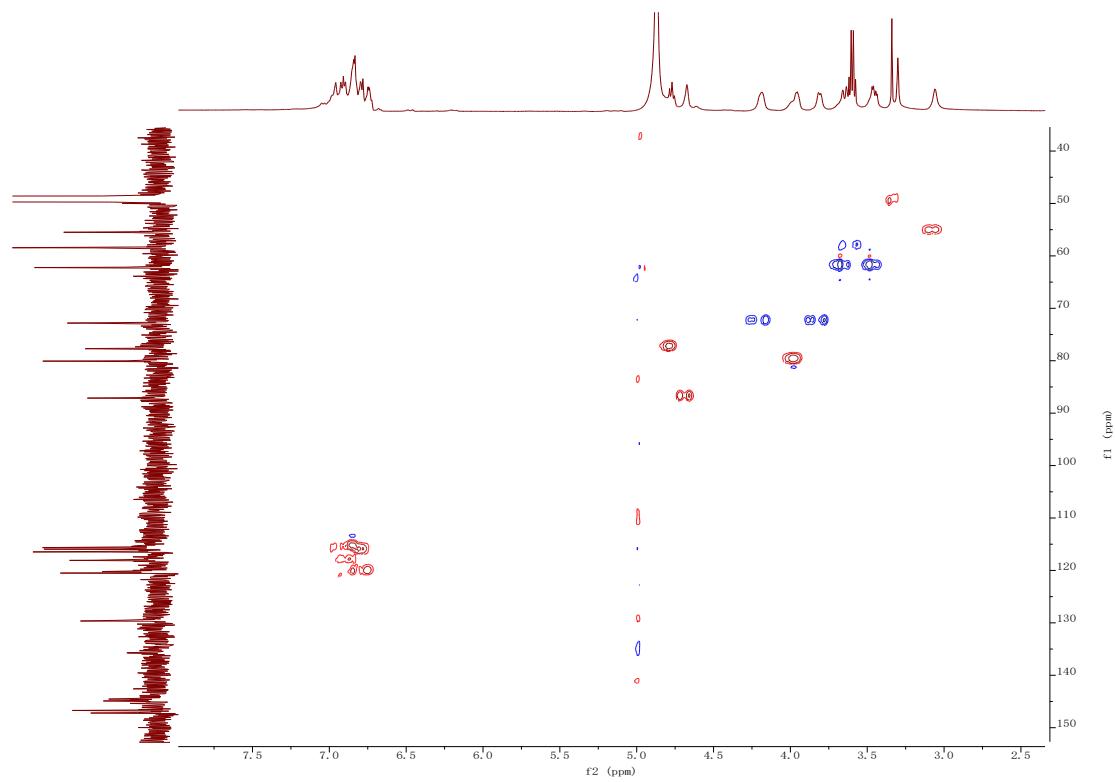


Figure S31. HSQC (CD<sub>3</sub>OD) spectrum of moricitin B (**4**)

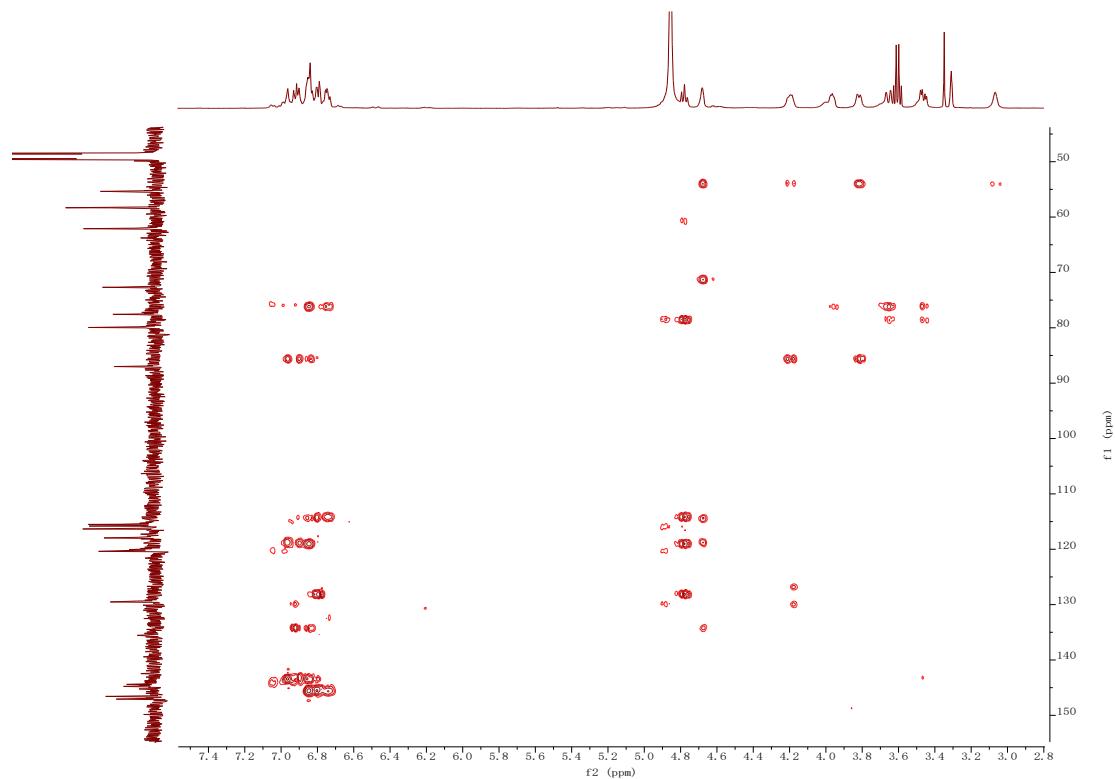


Figure S32. HMBC (CD<sub>3</sub>OD) spectrum of moricitin B (**4**)

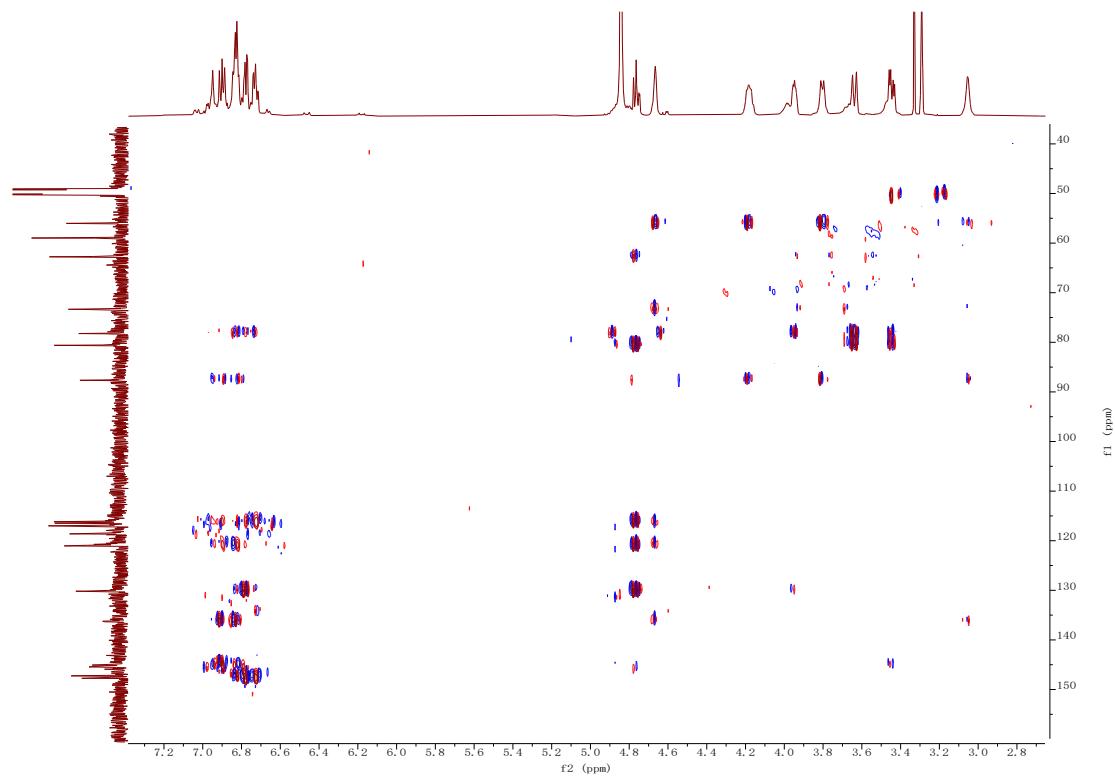


Figure S33. HMBC (600 MHz,  $\text{CD}_3\text{OD}$ , coupling constant = 3 Hz) spectrum of moricitin B (**4**)

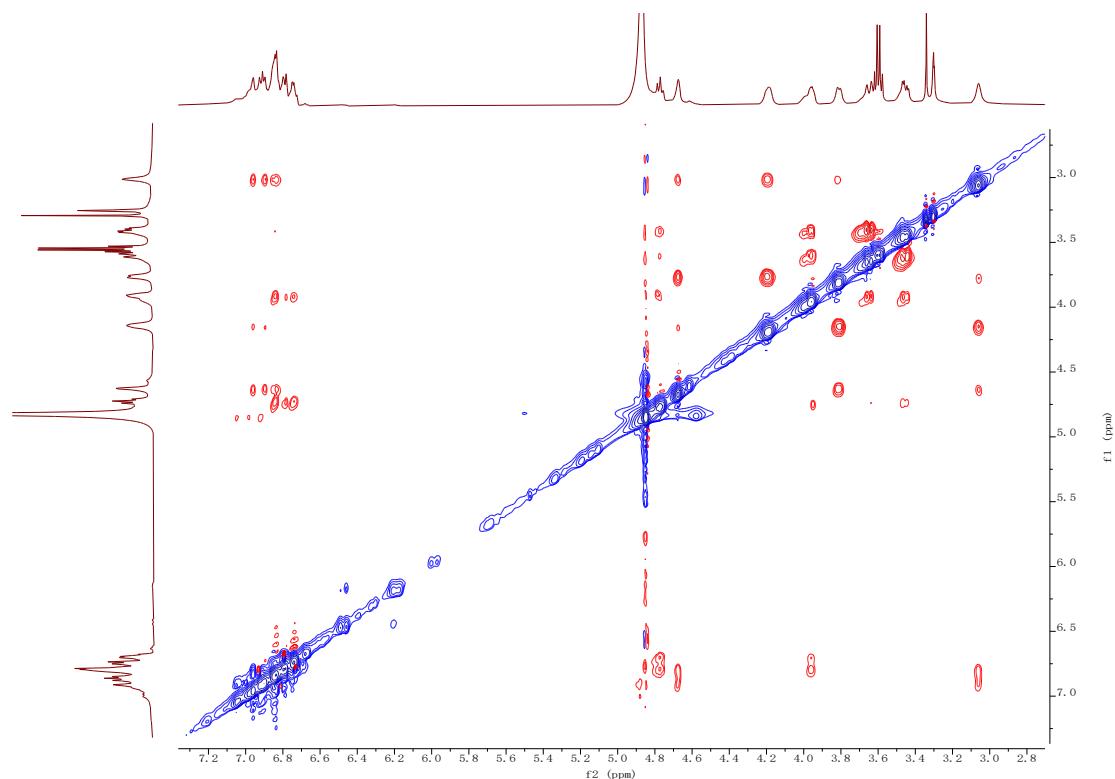


Figure S34. ROESY ( $\text{CD}_3\text{OD}$ ) spectrum of moricitin B (**4**)