

Supplementary data

New Unsaturated Lactones and a Meroterpenoid from *Ganoderma lucidum*

Qi-Hang Xin^{1*}, Qi Luo^{2*}, Ze-Hong Wu¹, Jiao-Jiao Zhang¹, Li-Zhong Liu¹, and Yong-Xian Cheng¹

^a School of Basic Medicine, School of Pharmaceutical Sciences, Shenzhen University Health Science Center, Shenzhen 518060, China

^b State Key Laboratory of Phytochemistry and Plant Resources in West China, Kunming Institute of Botany, Chinese Academy of Sciences, Kunming 650201, China

¹These authors contributed equally to this paper.

yxcheng@szu.edu.cn; liulz@szu.edu.cn

Contents

1. Optical value calculations of compound **1**

2. Supplementary Figures

Figure S2. HRESIMS spectrum of **1**

Figure S3. ^1H NMR spectrum of **1** in methanol- d_4

Figure S4. ^{13}C NMR and DEPT spectra of **1** in methanol- d_4

Figure S5. ^1H - ^1H COSY spectrum of **1** in methanol- d_4

Figure S6. HSQC spectrum of **1** in methanol- d_4

Figure S7. HMBC spectrum of **1** in methanol- d_4

Figure S8. HRESIMS of **2**

Figure S9. ^1H NMR spectrum of **2** in methanol- d_4

Figure S10. ^{13}C NMR spectrum of **2** in methanol- d_4

Figure S11. ^1H - ^1H COSY spectrum of **2** in methanol- d_4

Figure S12. HSQC spectrum of **2** in methanol- d_4

Figure S13. HMBC spectrum of **2** in methanol- d_4

Figure S14. HRESIMS of **3**

Figure S15. ^1H NMR spectrum of **3** in methanol- d_4

Figure S16. ^{13}C NMR spectrum of **3** in methanol- d_4

Figure S17. ^1H - ^1H COSY spectrum of **3** in methanol- d_4

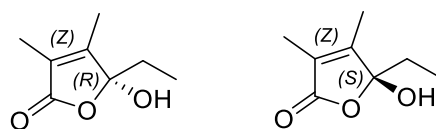
Figure S18. HSQC spectrum of **3** in methanol- d_4

Figure S19. HMBC spectrum of **3** in methanol- d_4

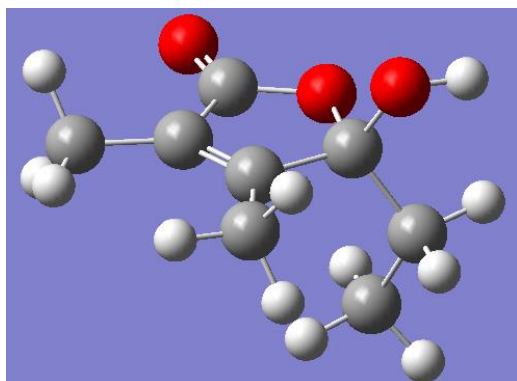
Figure S20. ROESY spectrum of **3** in methanol- d_4

Figure S21. CD spectrum of **3** in methanol

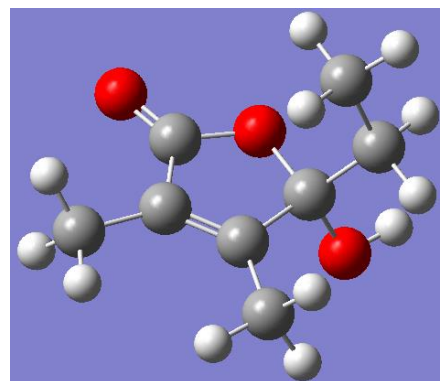
1. Optical value calculations of leucocontextum C



Model compounds



4R



4S

Figure S1. Optimized geometries of predominant conformers for model compounds at the B3LYP/6-311G (d, p) level in MeOH.

Table S1. Important thermodynamic parameters (a.u.) at B3LYP/6-311G (d, p) level in MeOH.

conformer	E+ZPE	G	[Alpha] (5893.0 Å)
4R	−537.735128	−537.772566	−54.0
4S	−537.735128	−537.772566	+54.0

E+ZPE, G: total energy with zero point energy (ZPE) and Gibbs free energy at 298.15 K.

2. Supplementary Figures

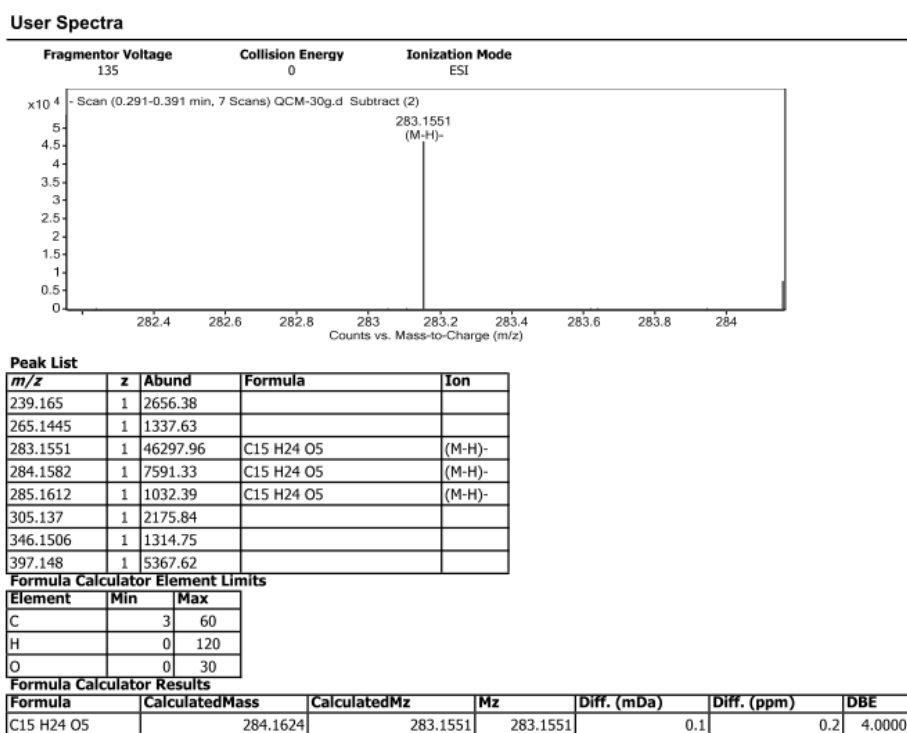


Figure S2. HRESIMS of **1**

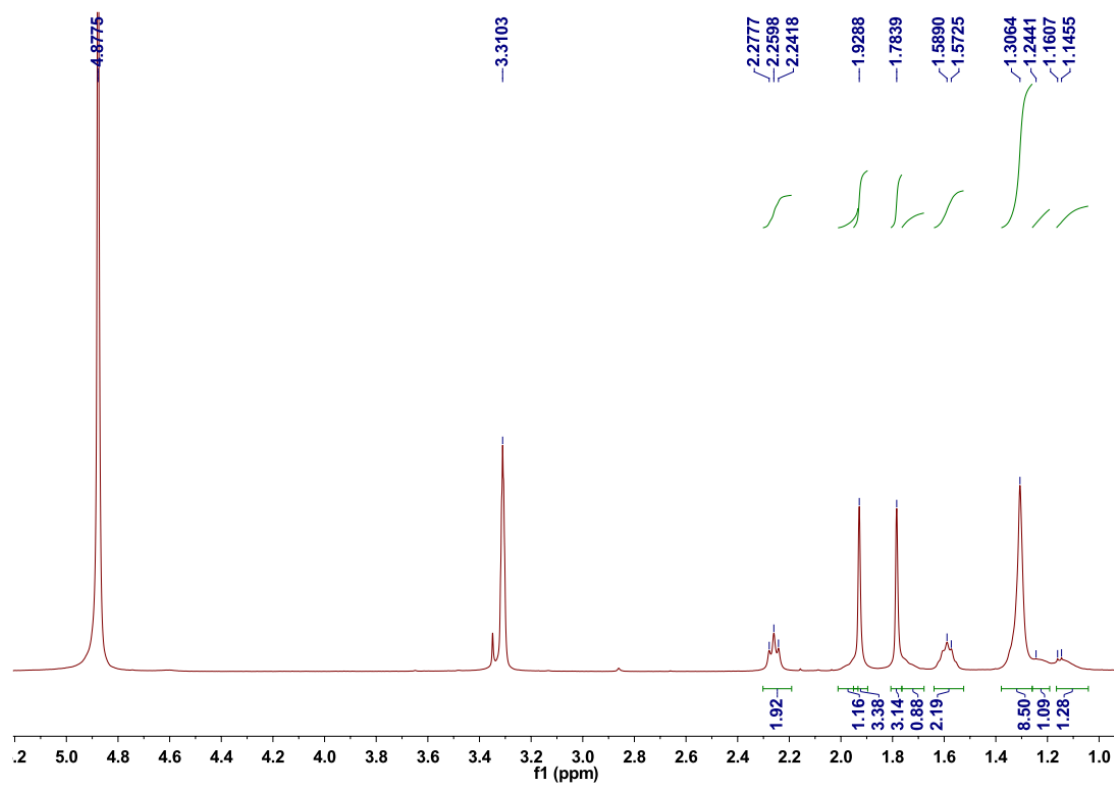


Figure S3. ¹H NMR spectrum of **1** in methanol-*d*₄

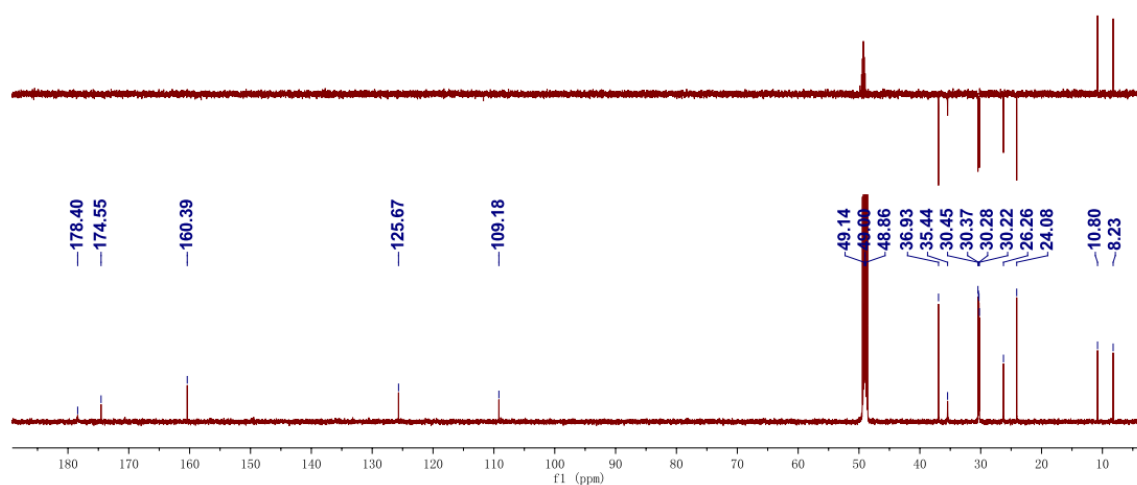


Figure S4. ^{13}C NMR and DEPT spectra of **1** in methanol- d_4

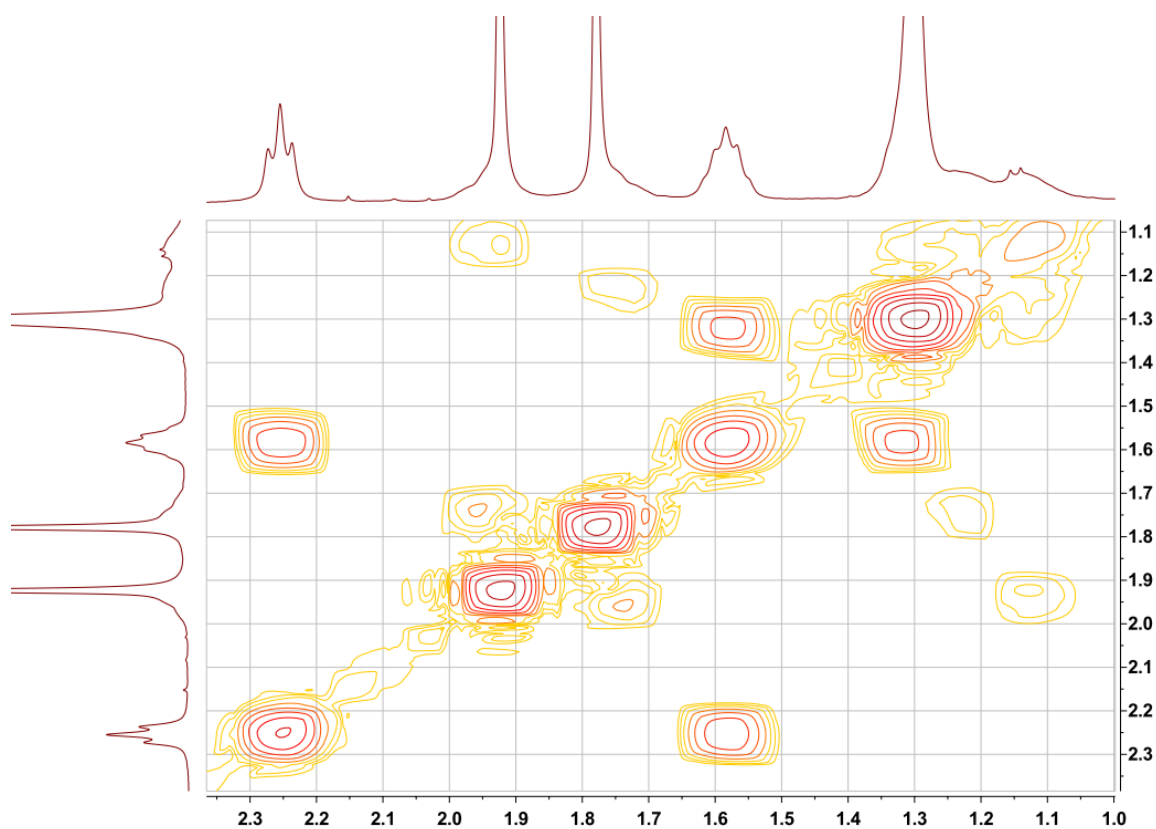


Figure S5. ^1H - ^1H COSY spectrum of **1** in methanol- d_4

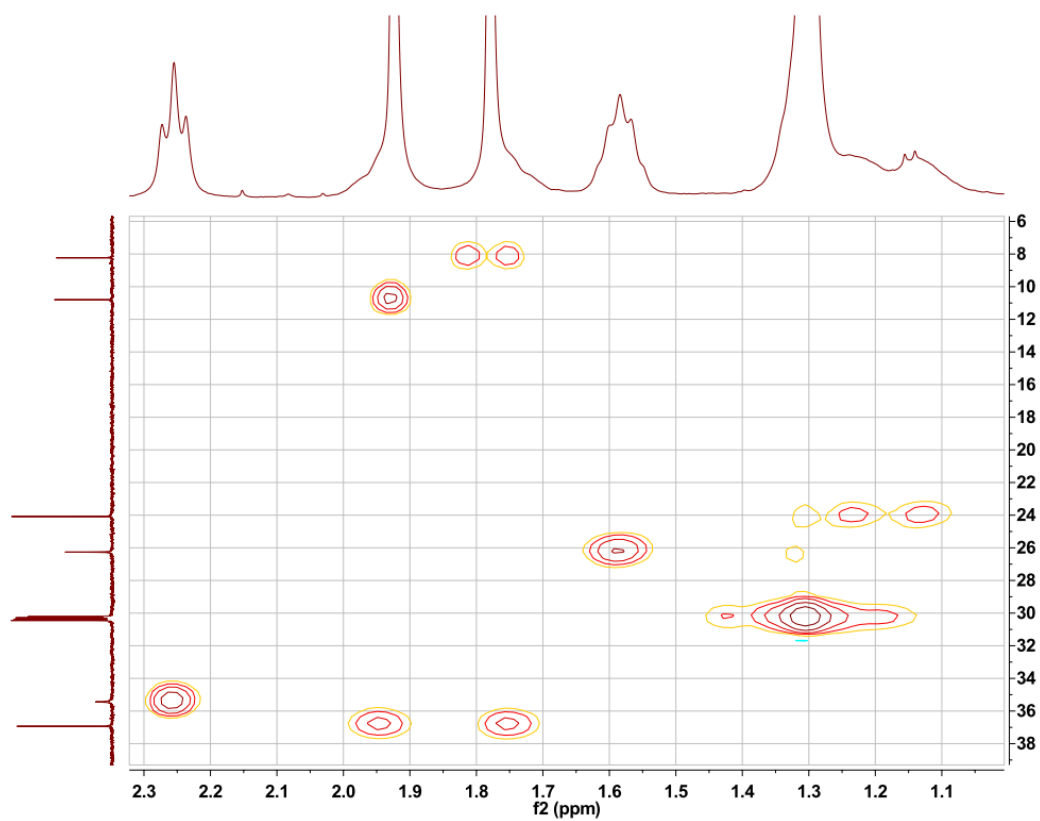


Figure S6. HSQC spectrum of **1** in methanol-*d*₄

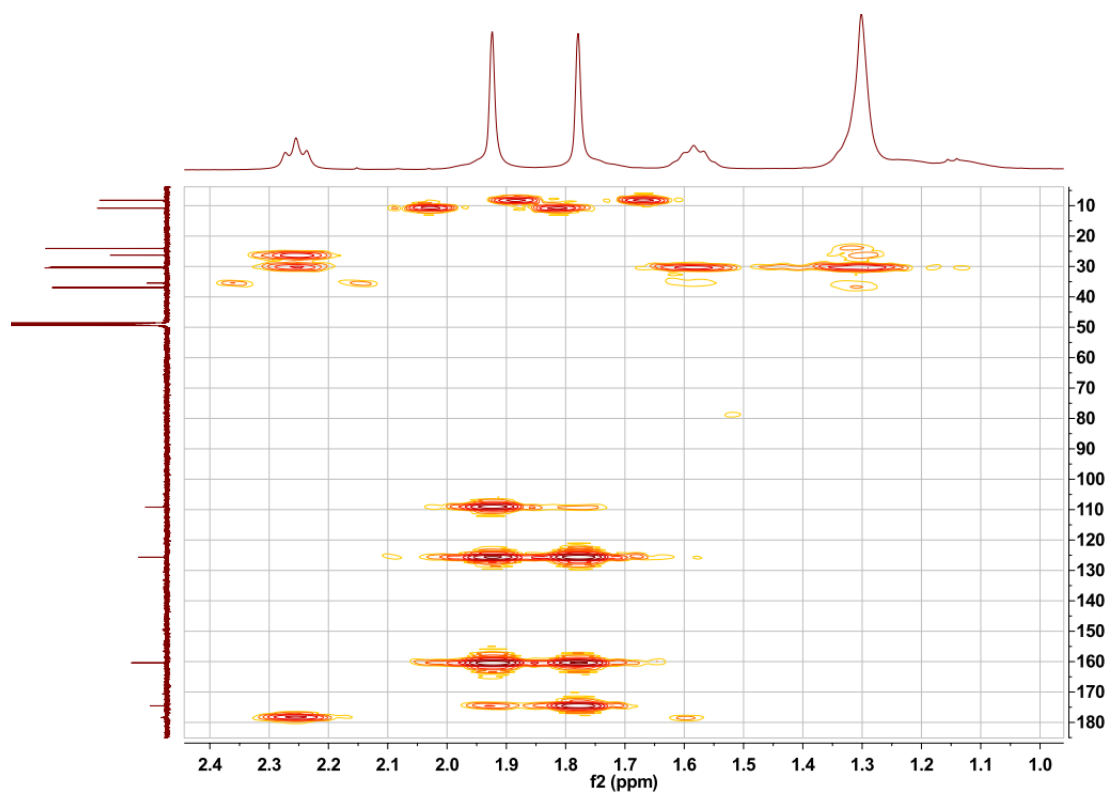


Figure S7. HMBC spectrum of **1** in methanol-*d*₄

User Spectra

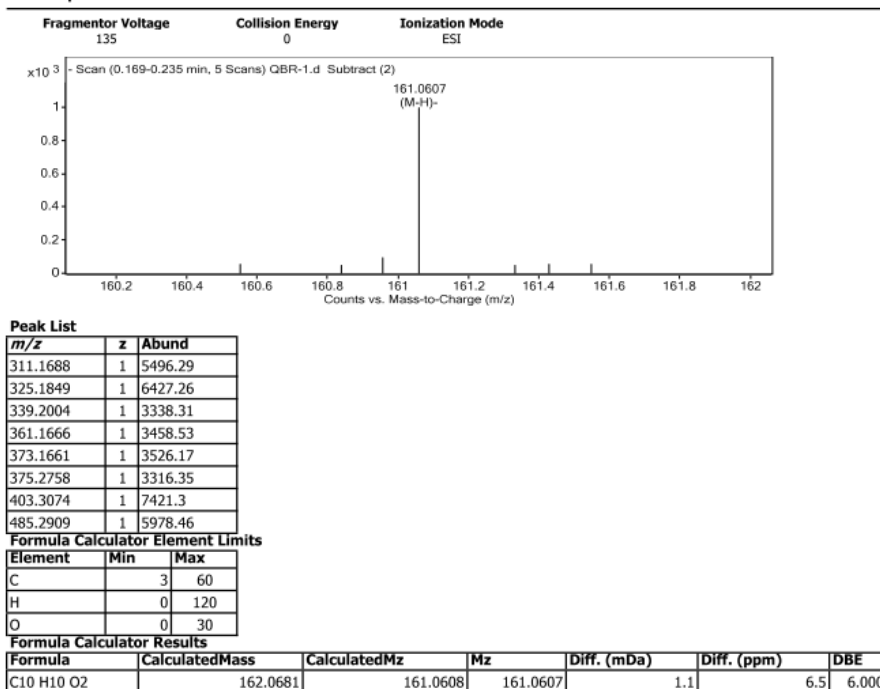


Figure S8. HRESIMS of **2**

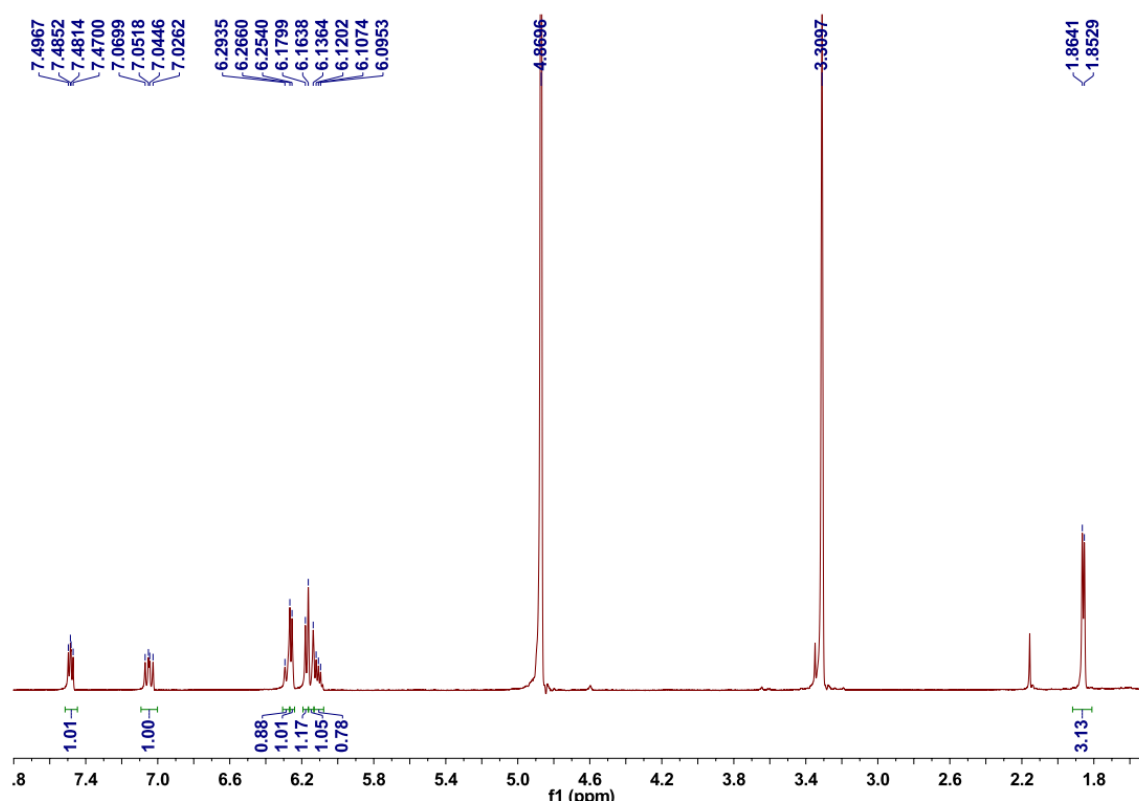


Figure S9. ¹H NMR spectrum of **2** in methanol-*d*₄

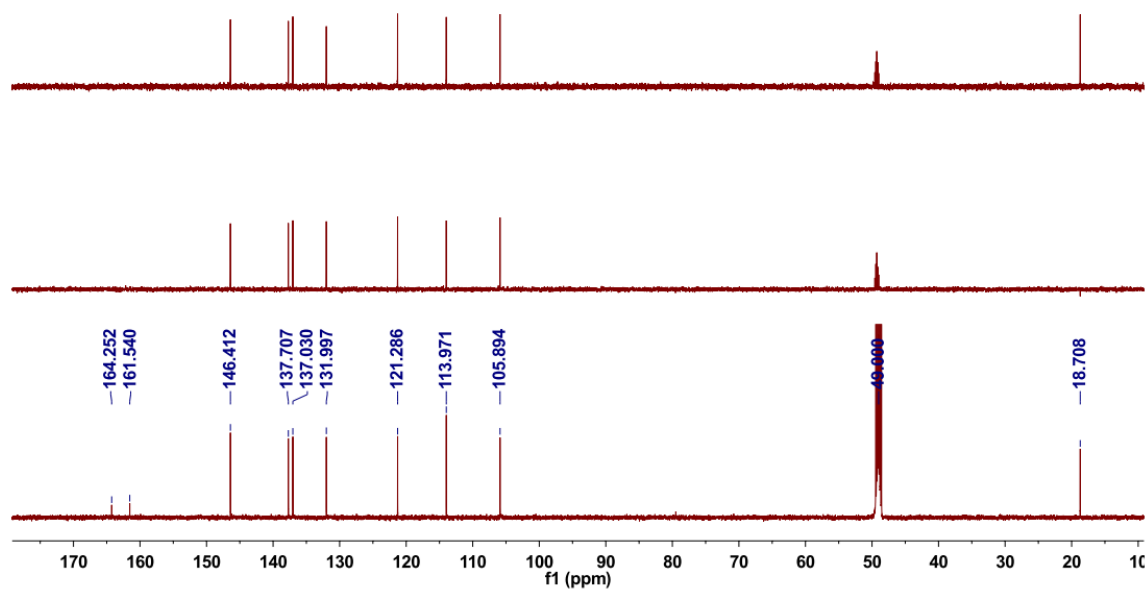


Figure S10. ^{13}C NMR spectrum of **2** in methanol- d_4

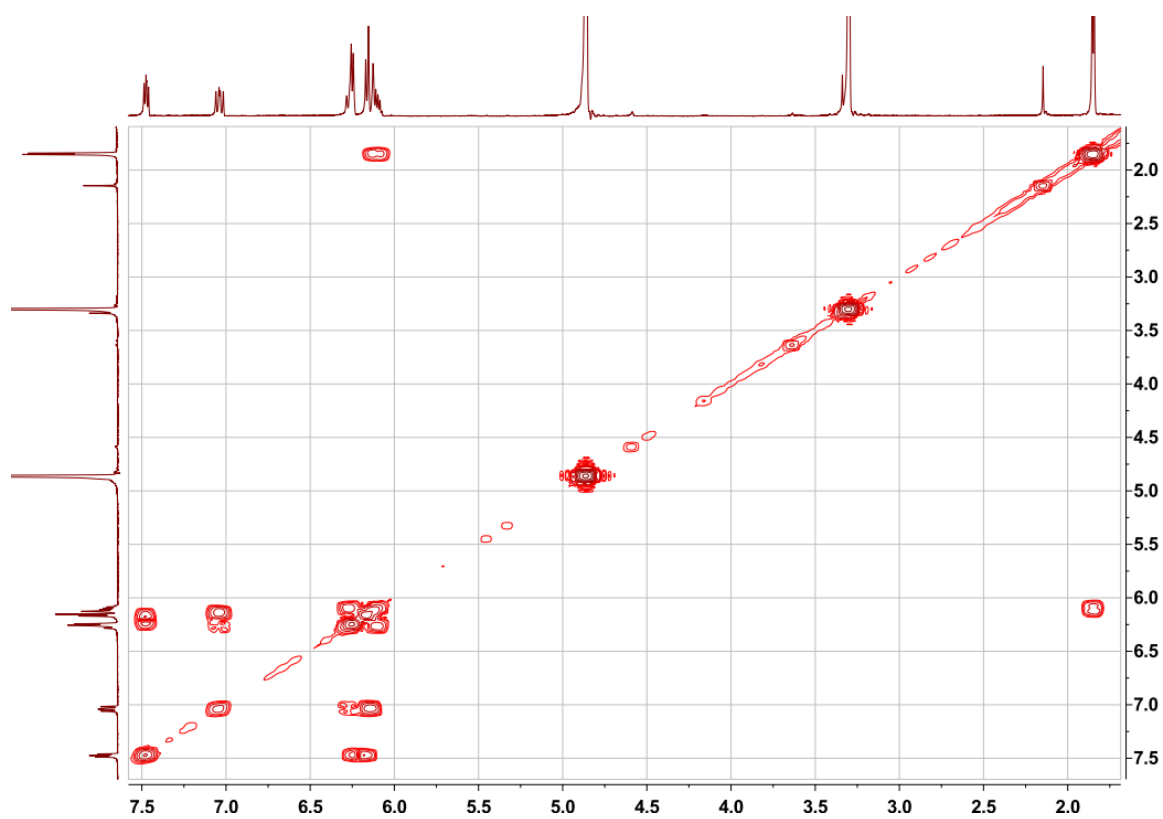


Figure S11. ^1H - ^1H COSY spectrum of **2** in methanol- d_4

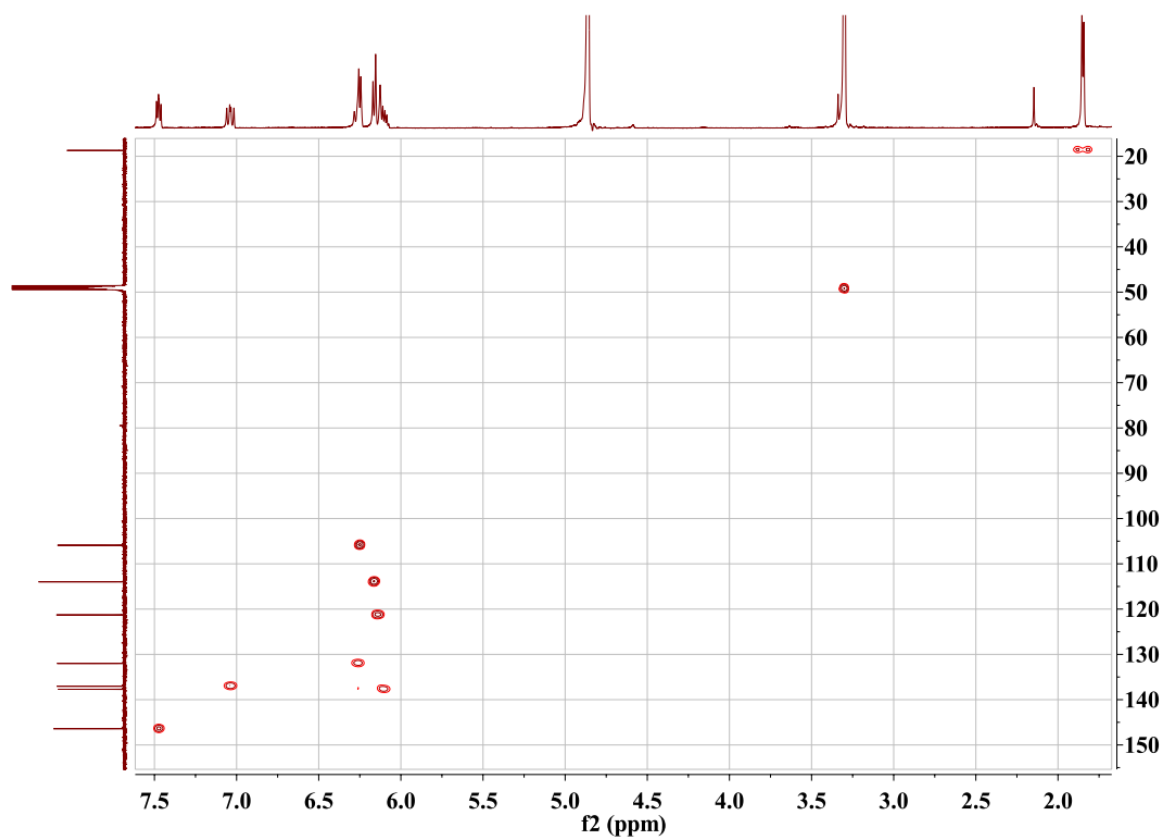


Figure S12. HSQC spectrum of **2** in methanol-*d*₄

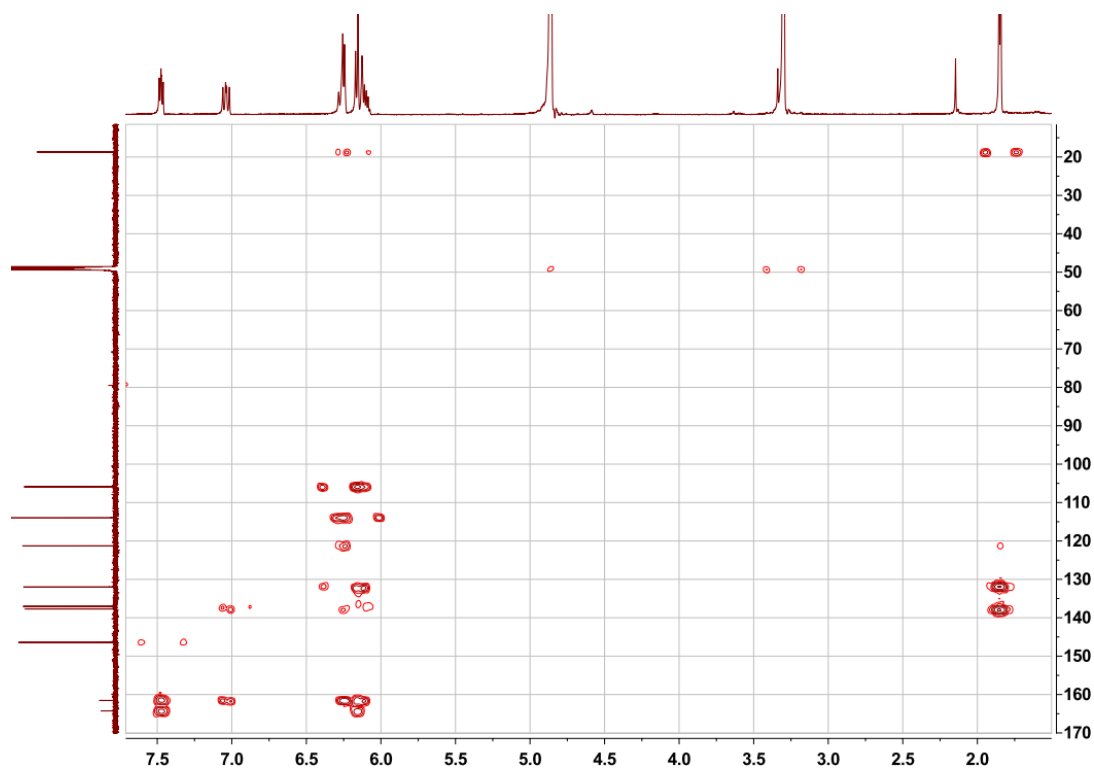
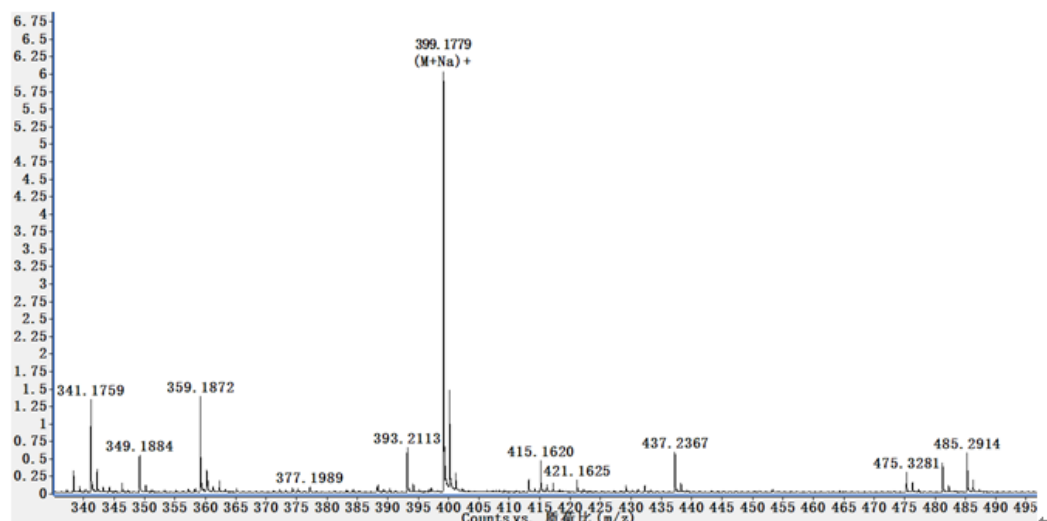


Figure S13. HMBC spectrum of **2** in methanol-*d*₄

Generic Display Report			
Analysis Info			Acquisition data:27/01/2019
Analysis name:dylz-38			
Method	esi_pos_50-1000_with calibration for 1min.m		operator: WHS
Sample Name:	Instrument: Agilent 6210 ESI/TOF MS		
Comment			



Formula	Cal. Mass (Na+)	Mass(Na+)	Err(ppm)
C ₂₁ H ₂₈ O ₆	399.1778	399.1779	-0.24

Figure S14. HRESIMS of **3**

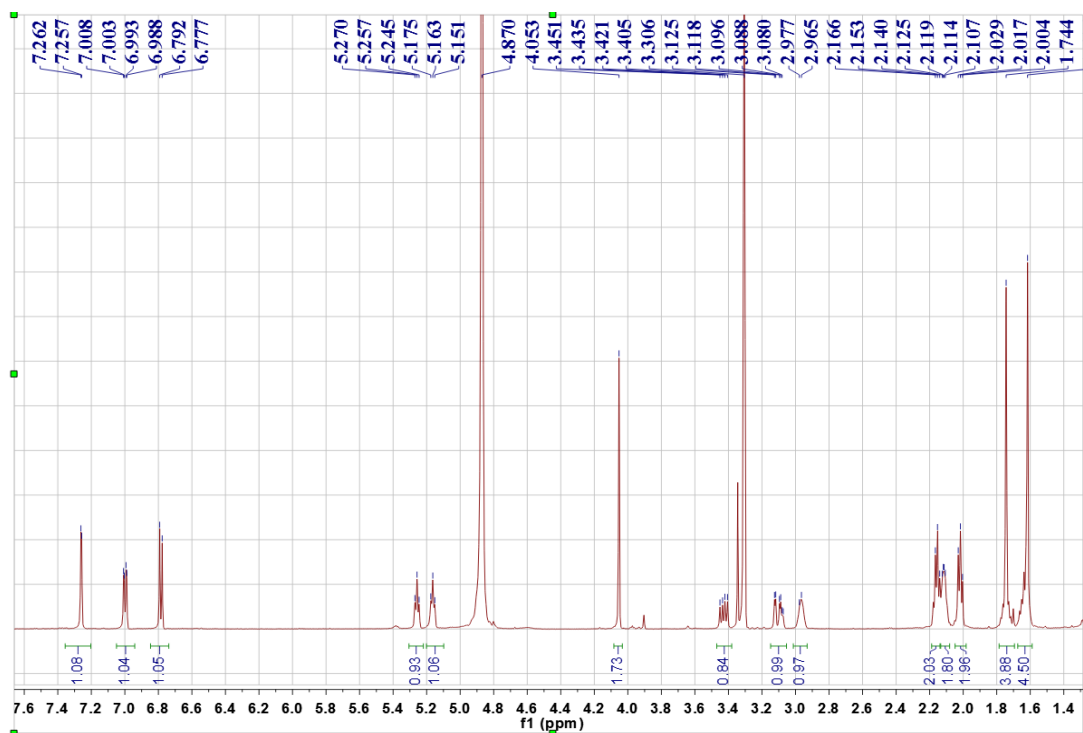


Figure S15. ¹H NMR spectrum of **3** in methanol-*d*₄

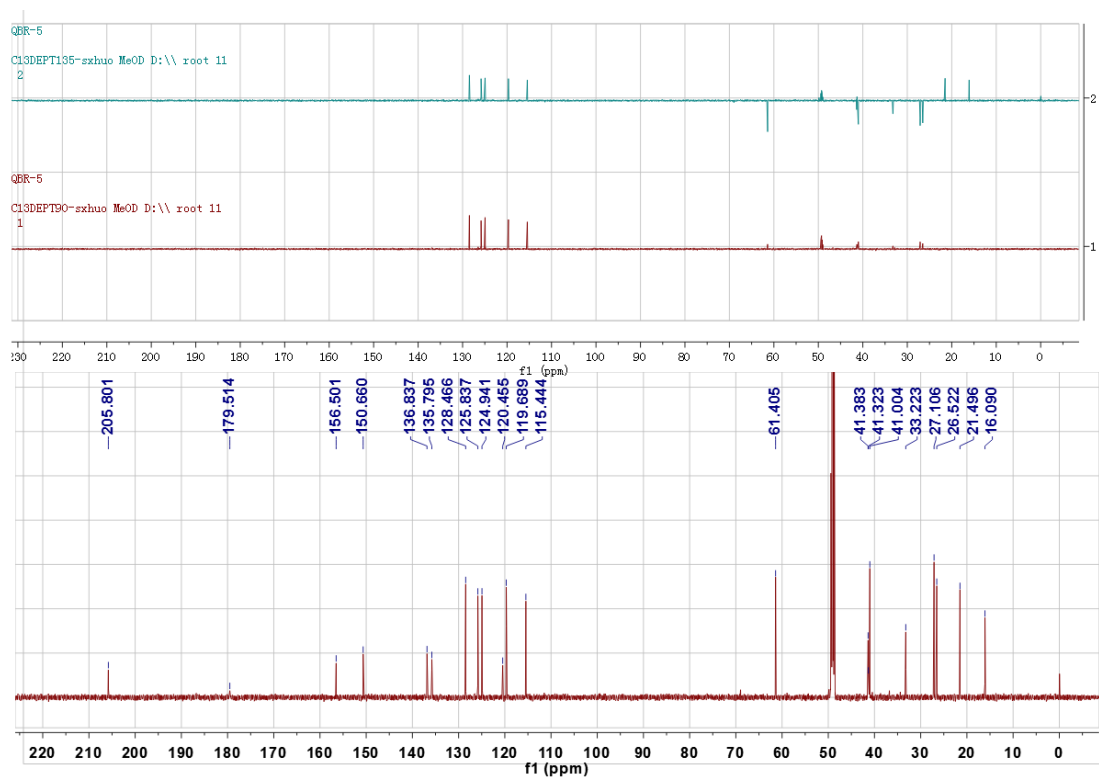


Figure S16. ^{13}C NMR spectrum of **3** in methanol- d_4

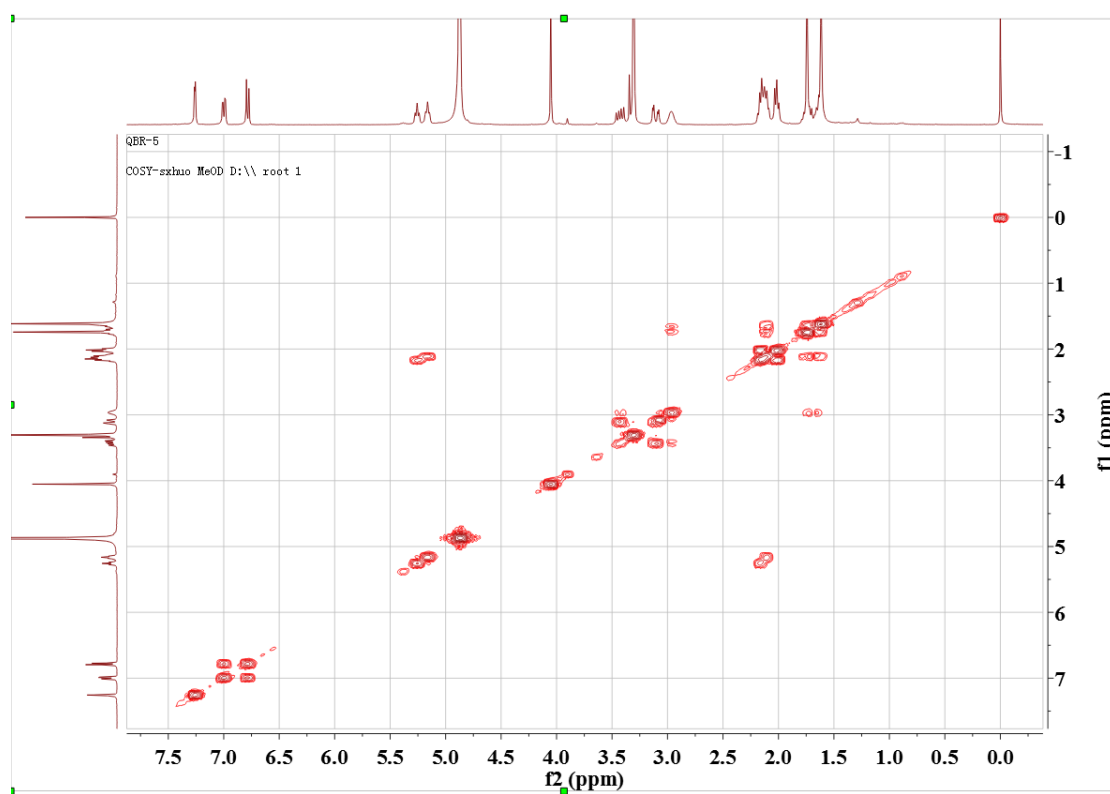


Figure S17. ^1H - ^1H COSY spectrum of **3** in methanol- d_4

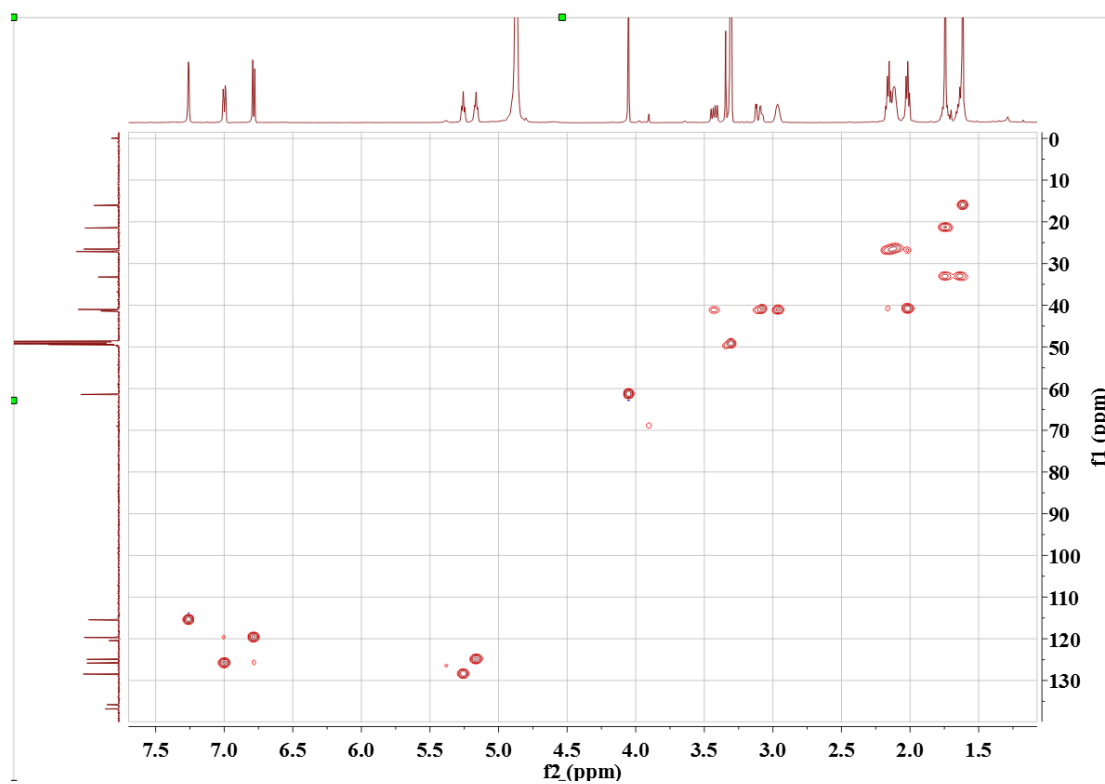


Figure S18. HSQC spectrum of **3** in methanol-*d*₄

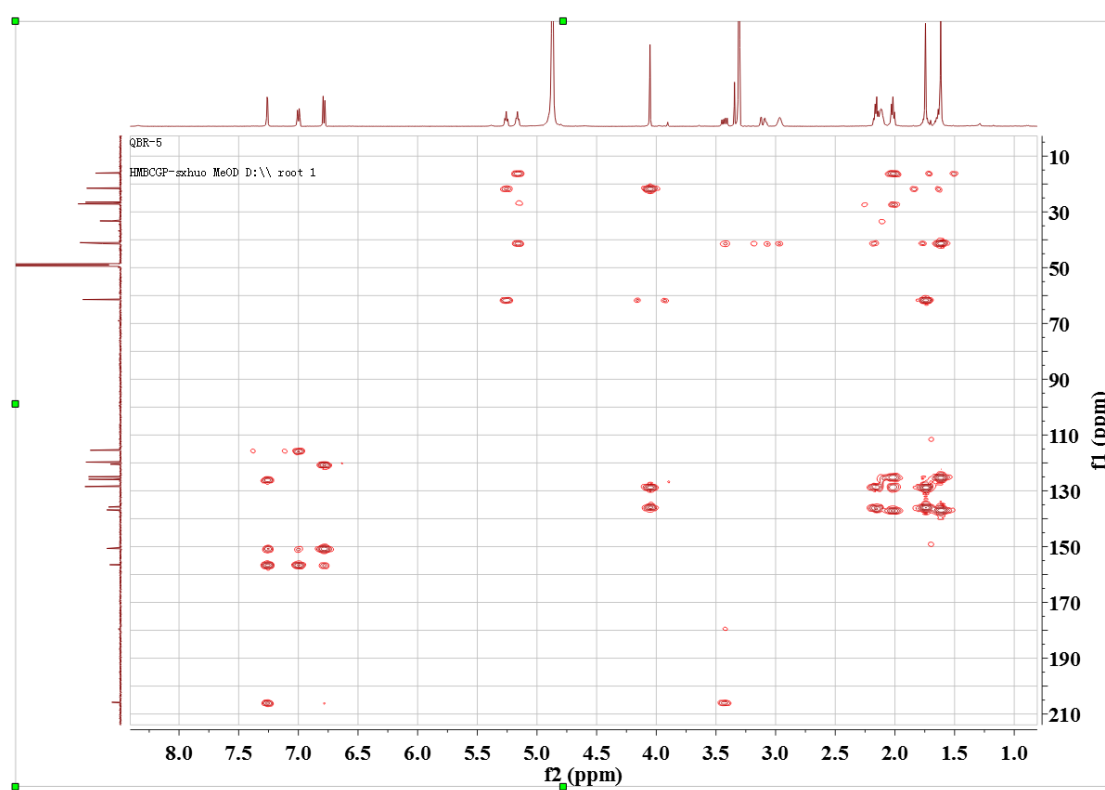


Figure S19. HMBC spectrum of **3** in methanol-*d*₄

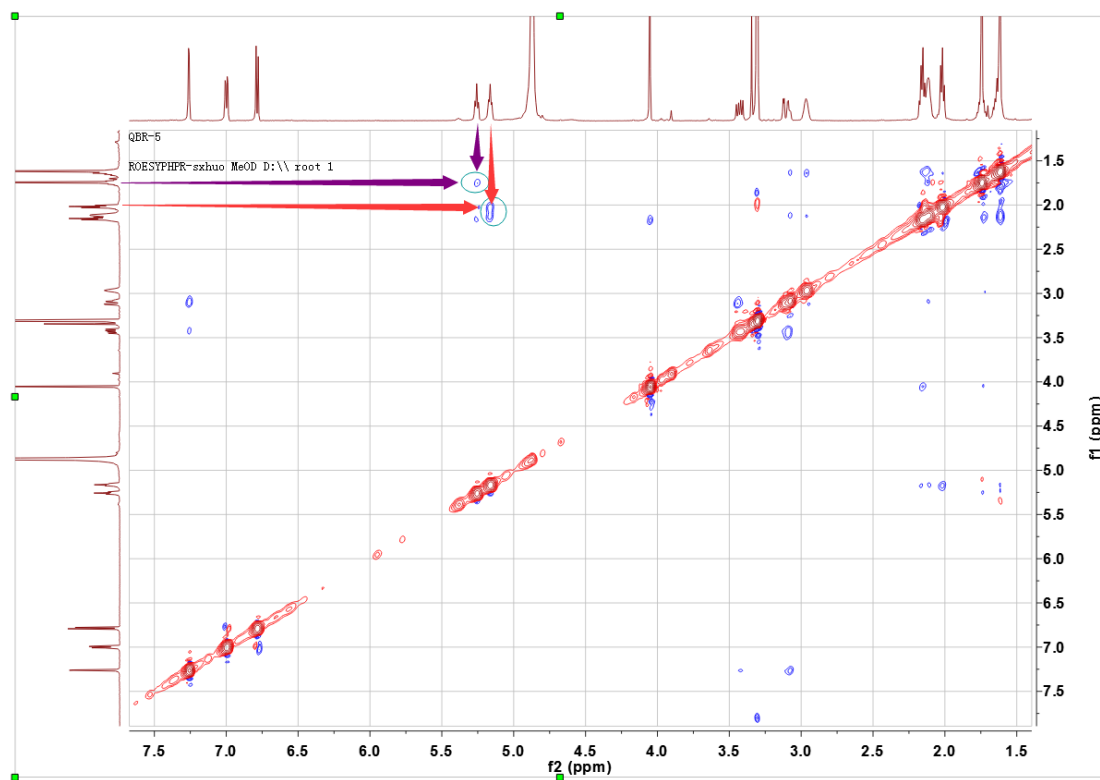


Figure S20. ROESY spectrum of **3** in methanol-*d*₄

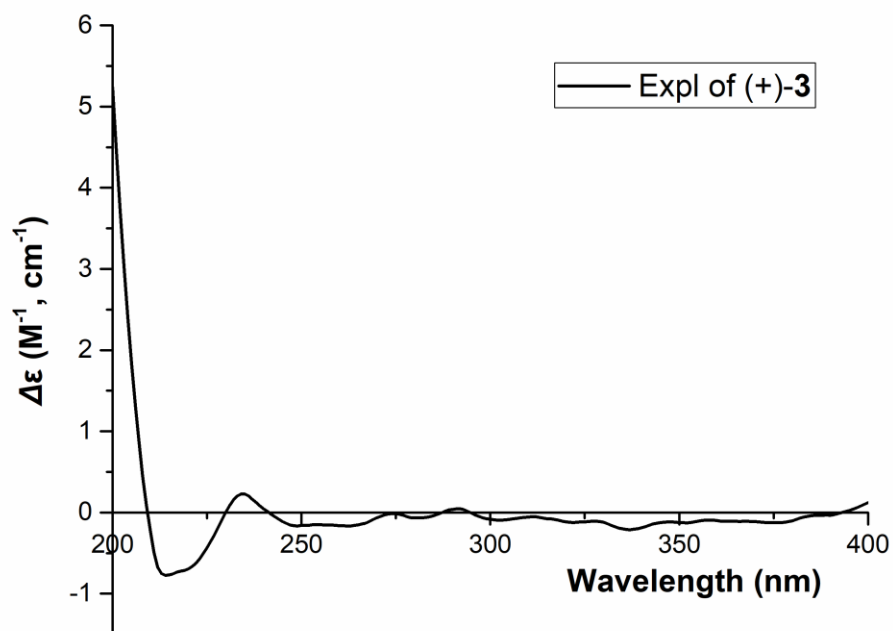


Figure S21. CD spectrum of **3** in methanol

