Supporting Information

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A Novel Polyketide from the Endophytic Fungus *Aspergillus puniceus*

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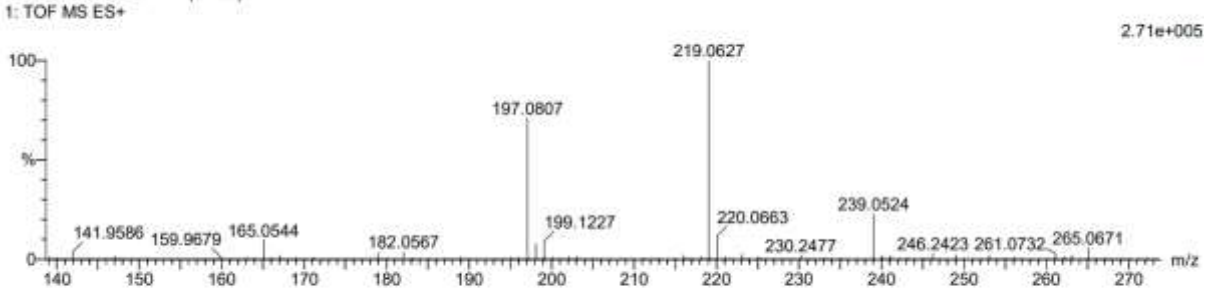
Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
4 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-10 H: 0-13 O: 0-4
20230325-3-G-8-3-7 42 (0.195)
1: TOF MS ES+



Minimum:				-1.5				
Maximum:		5.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
197.0807	197.0814	-0.7	-3.6	4.5	685.2	n/a	n/a	C10 H13 O4

Figure S1: HR-ESI-MS spectrum of compound **1**

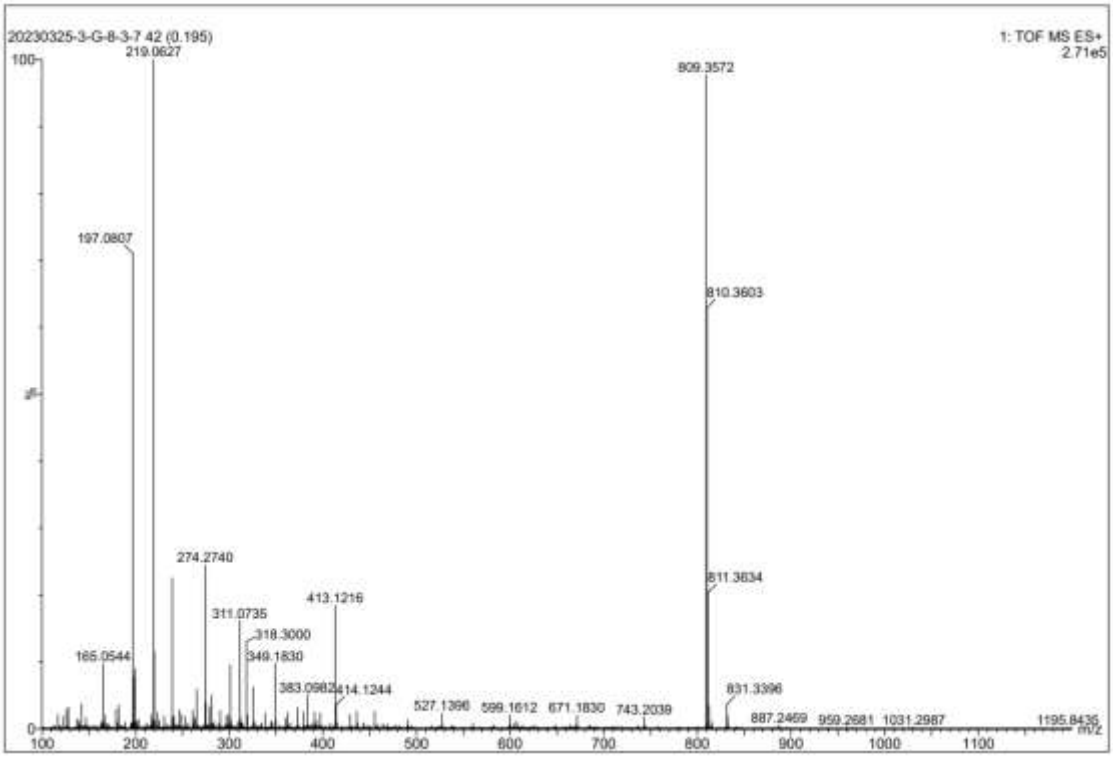


Figure S1-1: Low-resolution spectrum of compound **1**

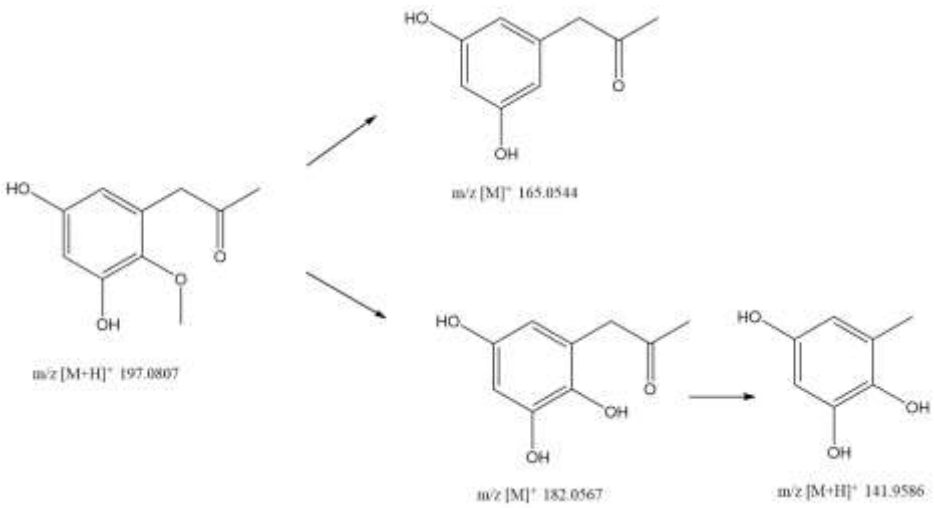


Figure S2: The fragment peak structure of compound **1**

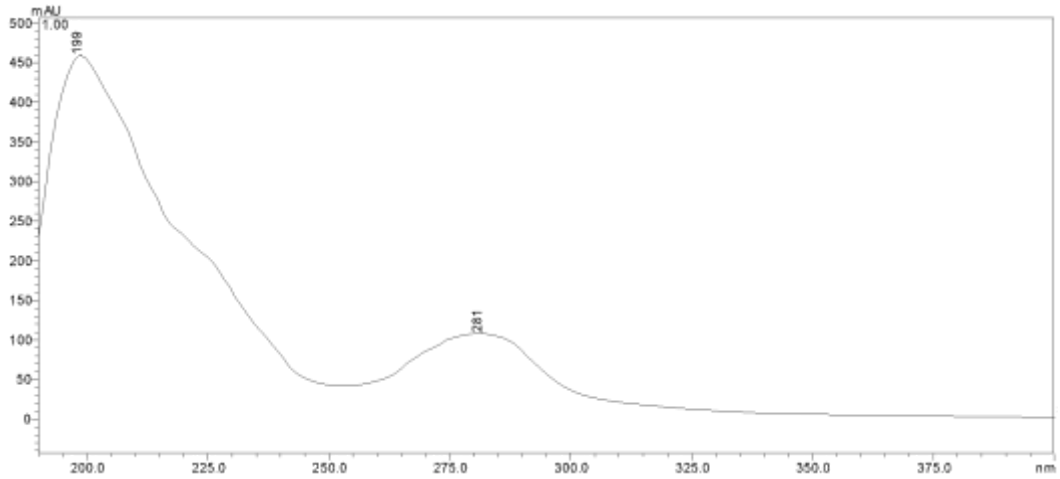


Figure S3: UV spectrum of compound **1**

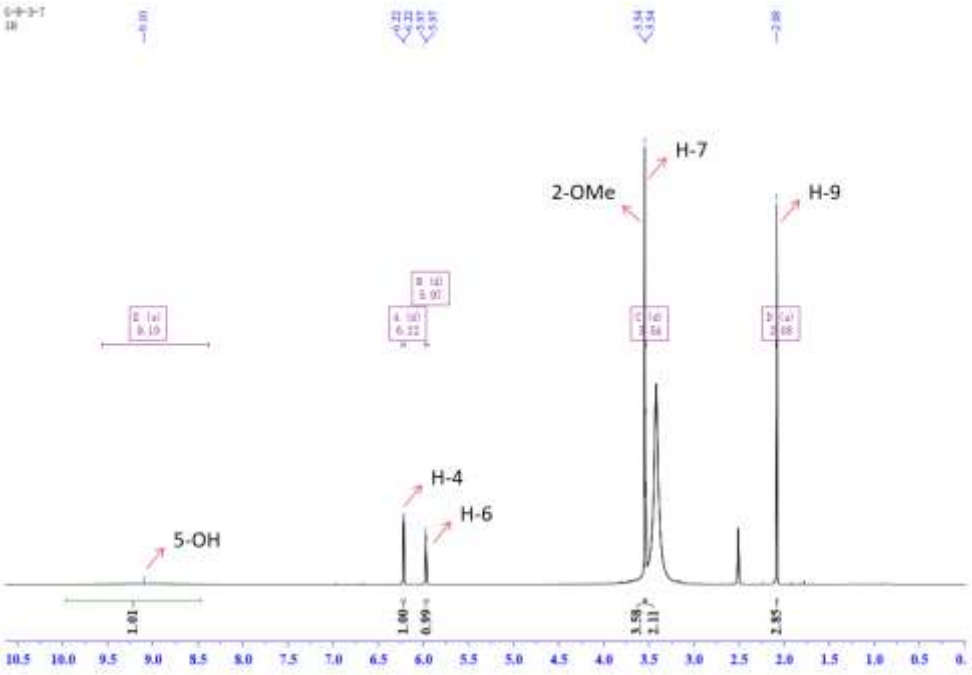


Figure S4: [1]H-NMR spectrum of compound **1**

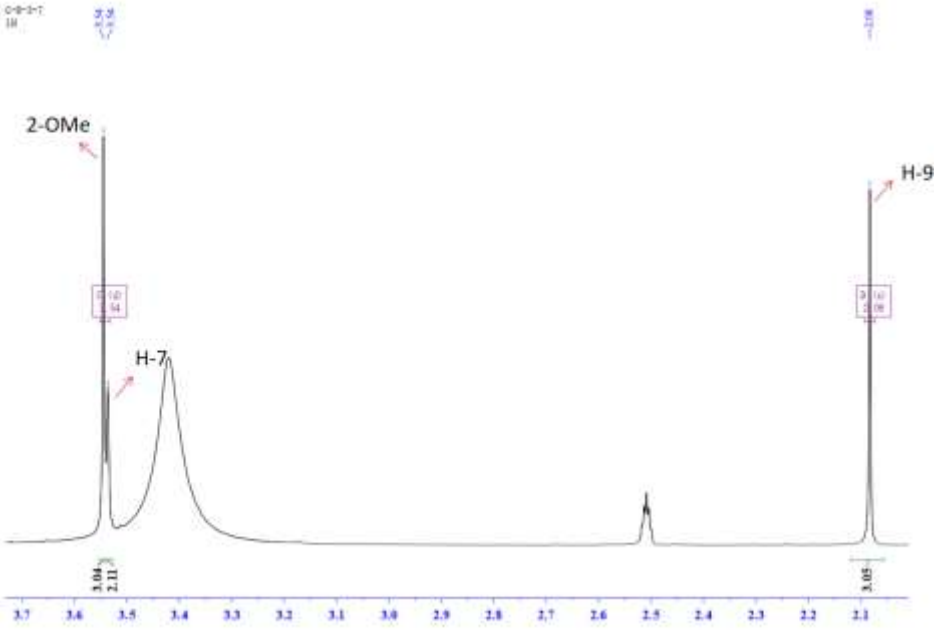


Figure S4-1: [1]H-NMR spectrum of compound **1** (enlarged image)

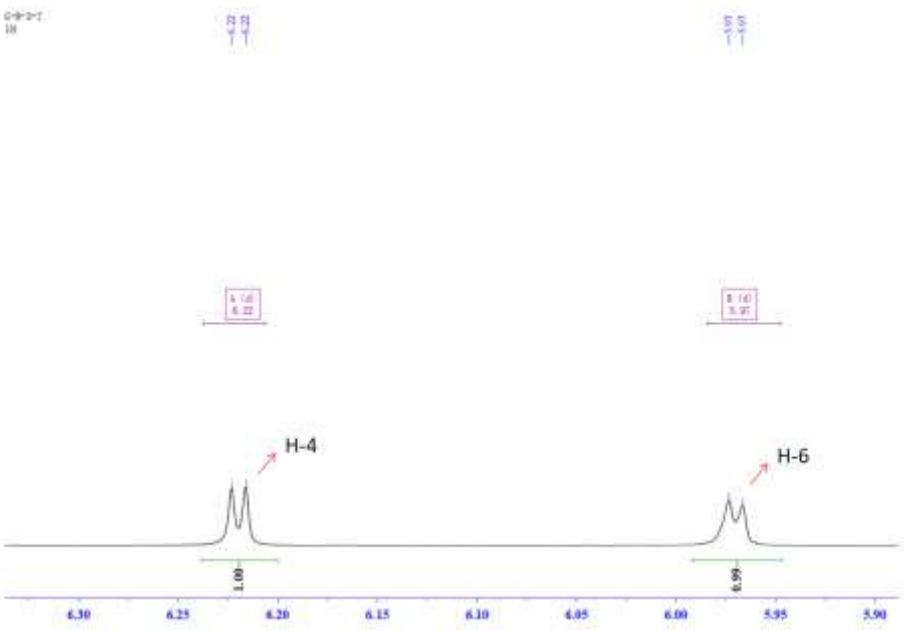


Figure S4-2: ^{1}H-NMR spectrum of compound **1** (enlarged image)

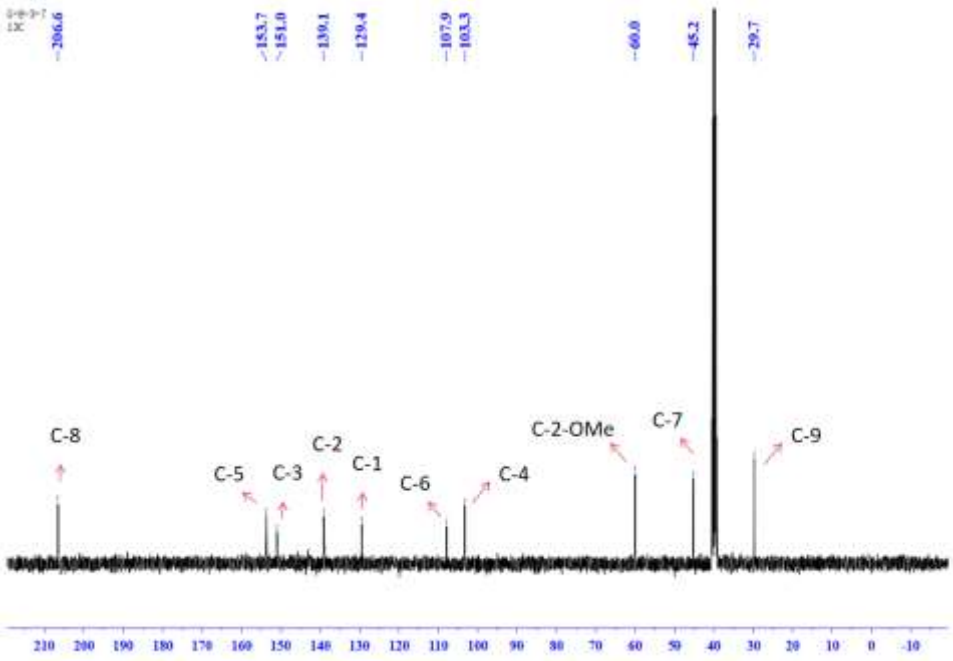


Figure S5: ^{13}C-NMR spectrum of compound **1**

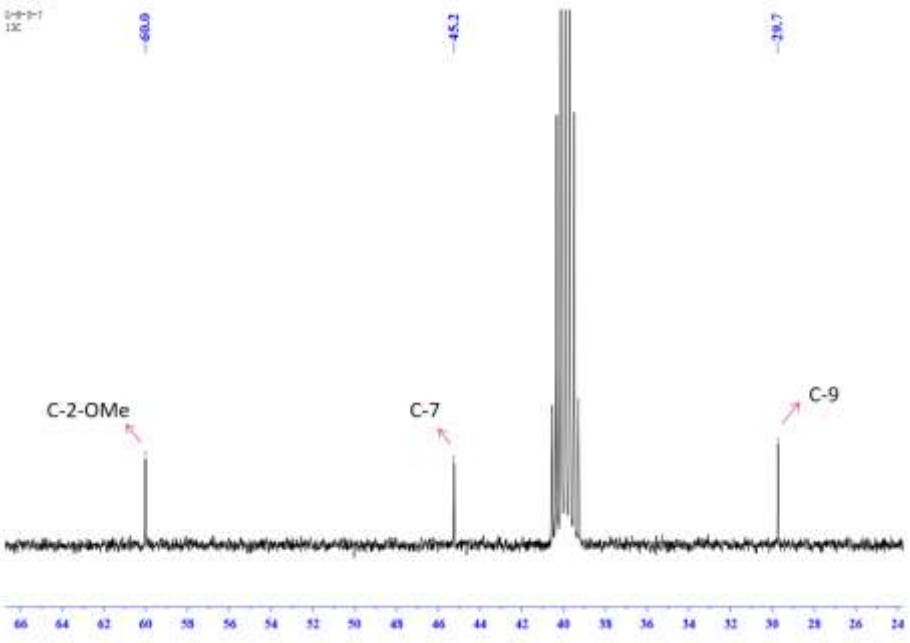


Figure S5-1: ^{13}C-NMR spectrum of compound **1** (enlarged image)

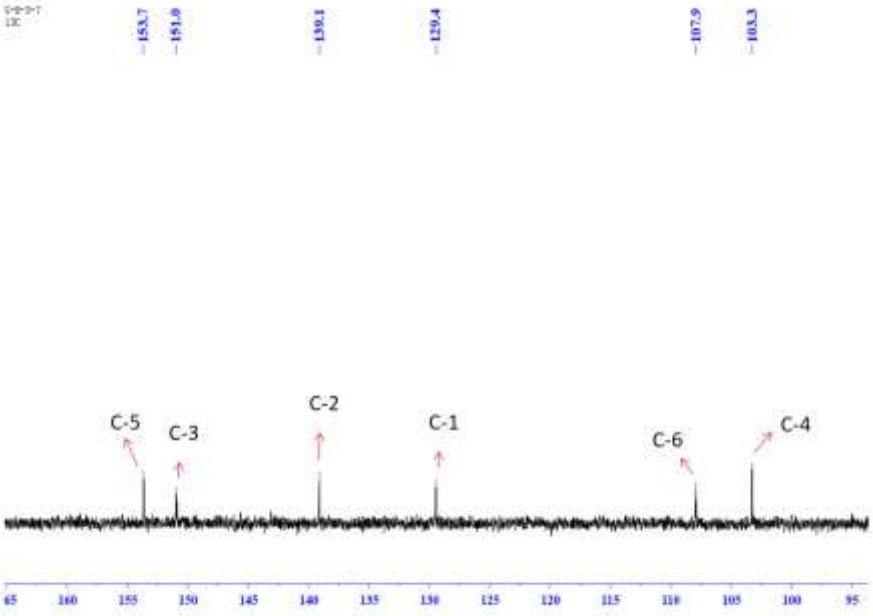


Figure S5-2: ^{13}C-NMR spectrum of compound **1** (enlarged image)

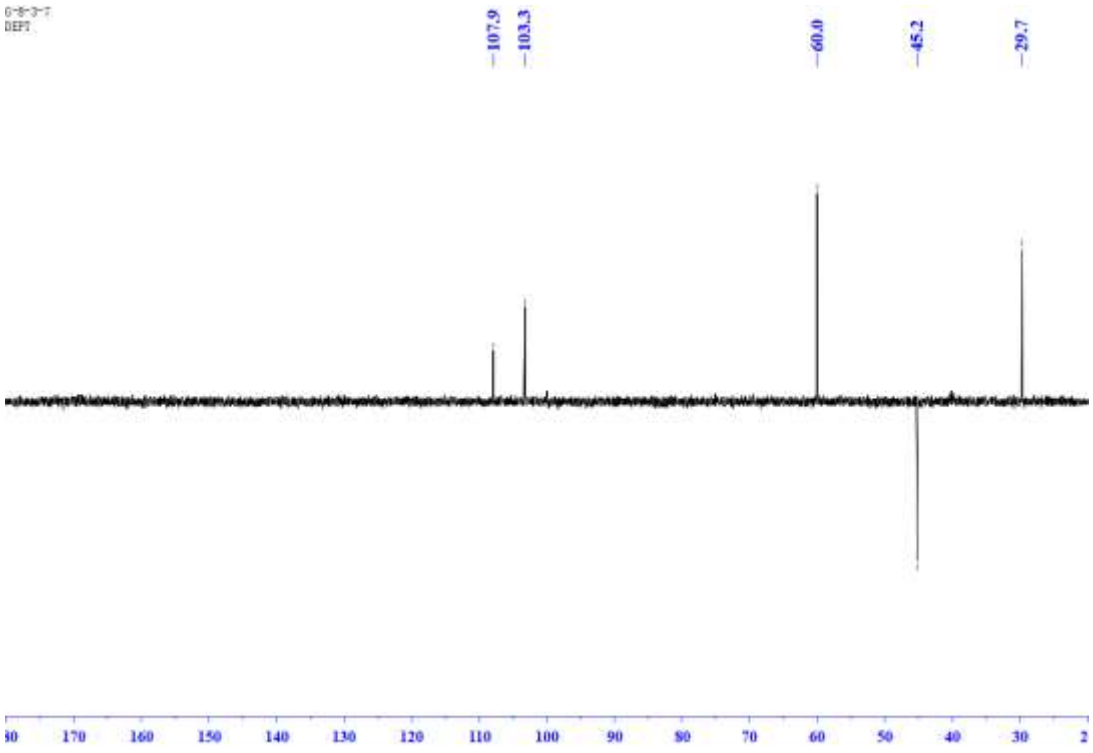


Figure S6: DEPT135 spectrum of compound **1**

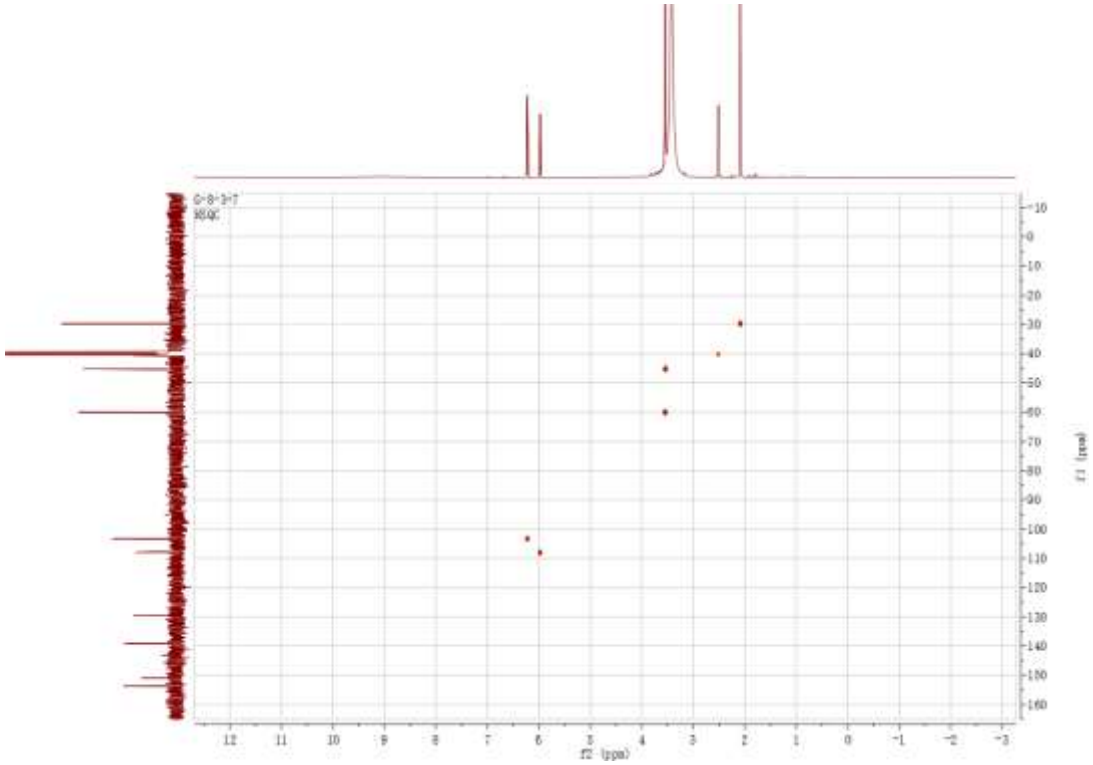


Figure S7: HSQC spectrum of compound **1**

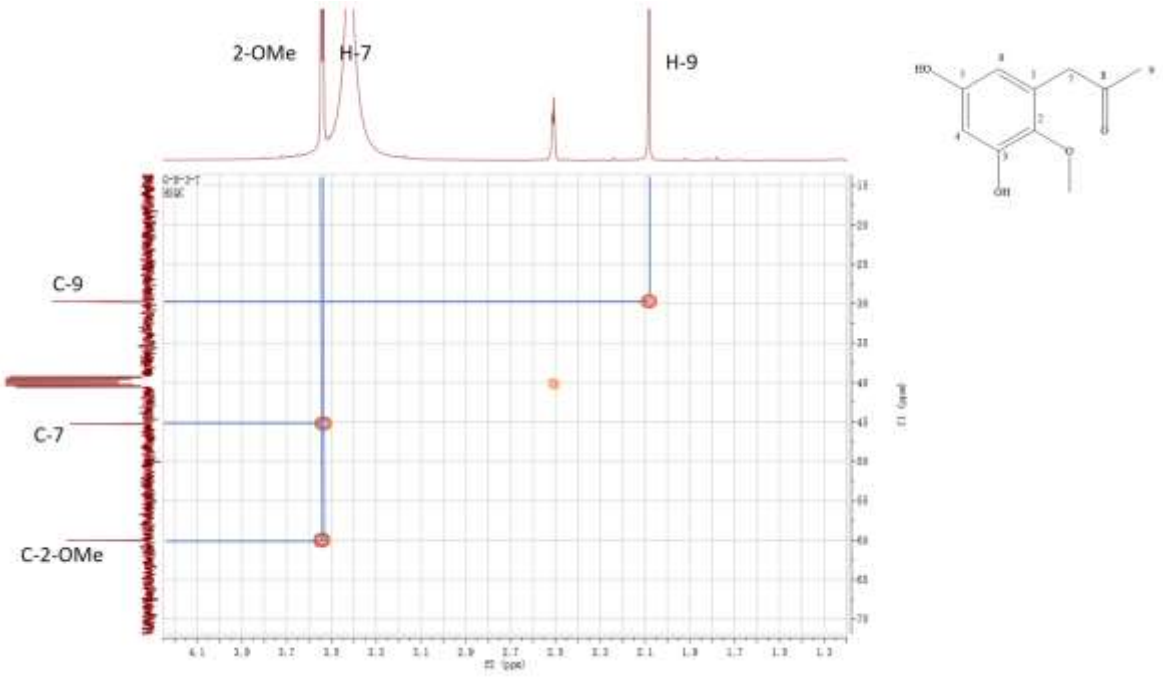


Figure S7-1: HSQC spectrum of compound **1** (enlarged image)

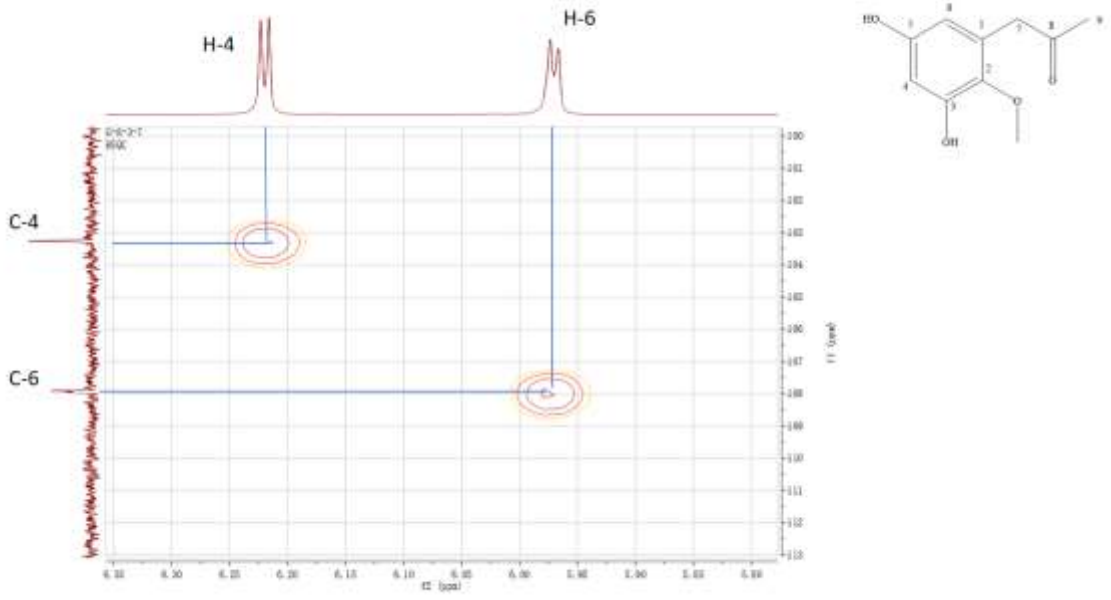


Figure S7-2: HSQC spectrum of compound **1** (enlarged image)

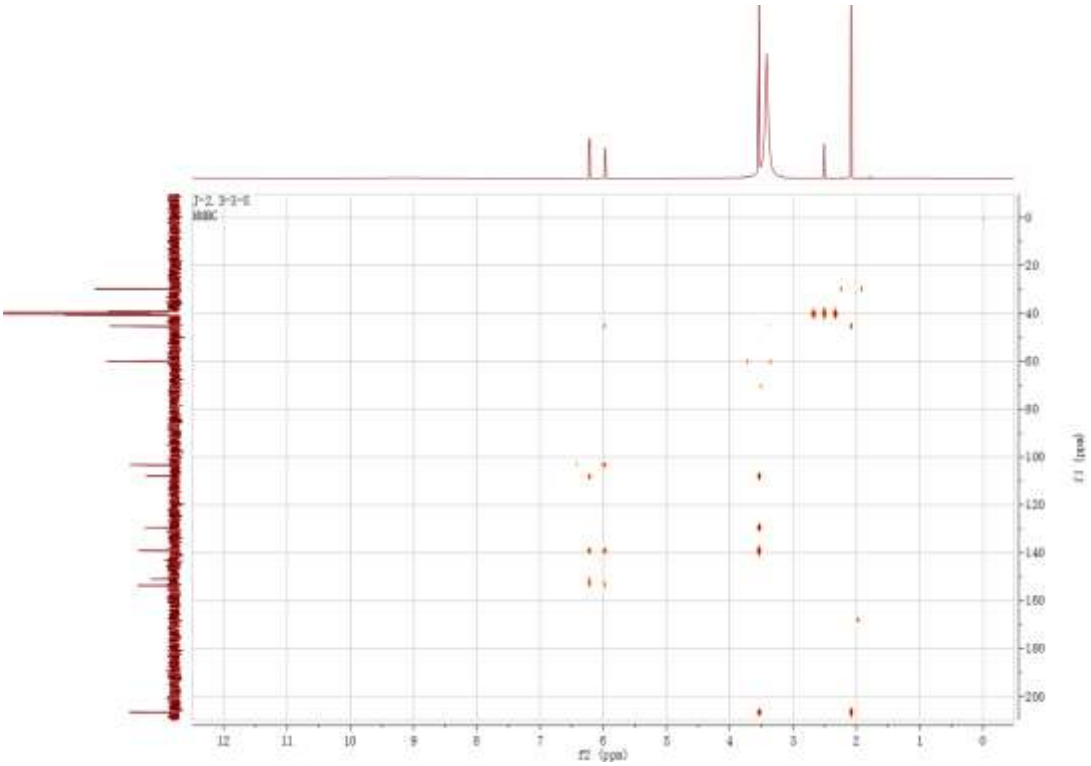


Figure S8: HMBC spectrum of compound **1**

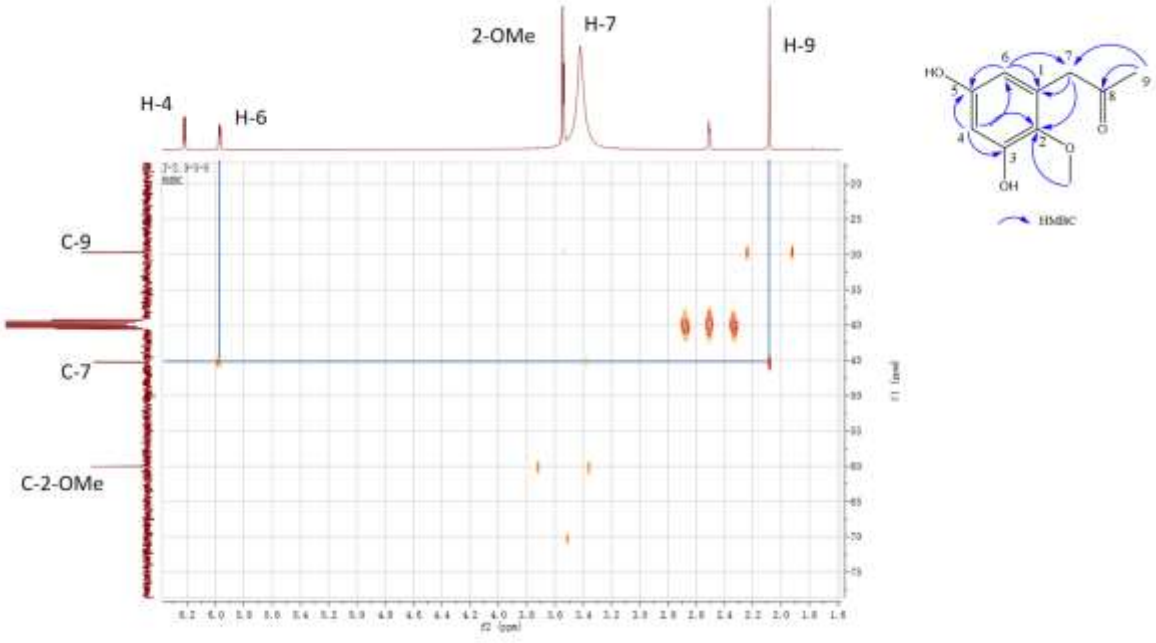


Figure S8-1: HMBCspectrum of compound **1** (enlarged image)

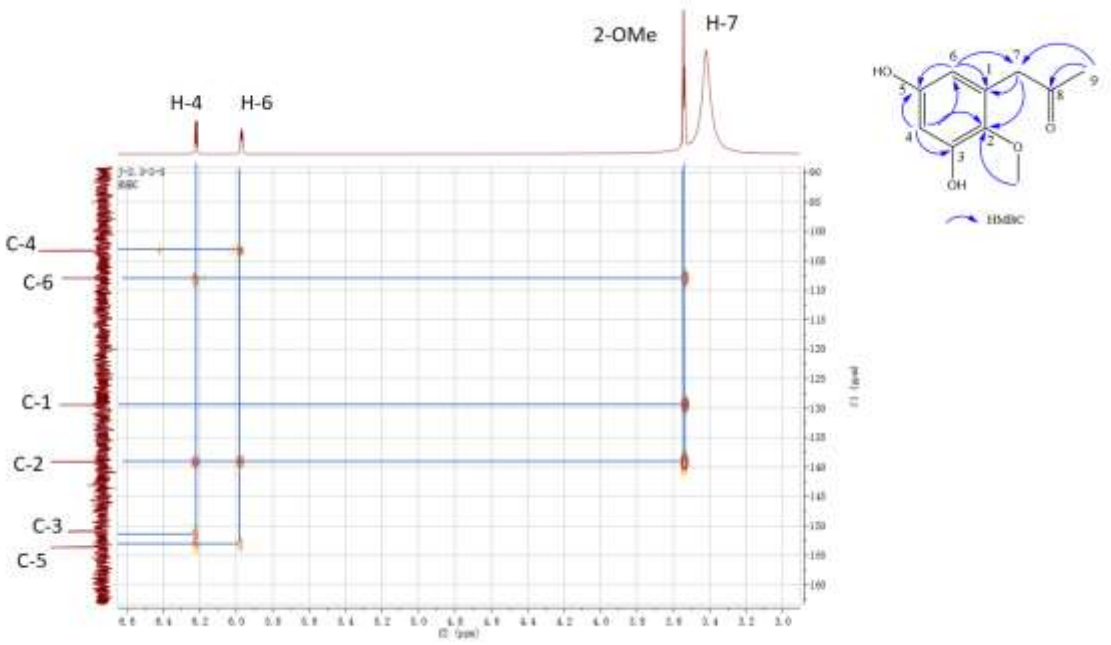


Figure S8-2: HMBC spectrum of compound **1** (enlarged image)

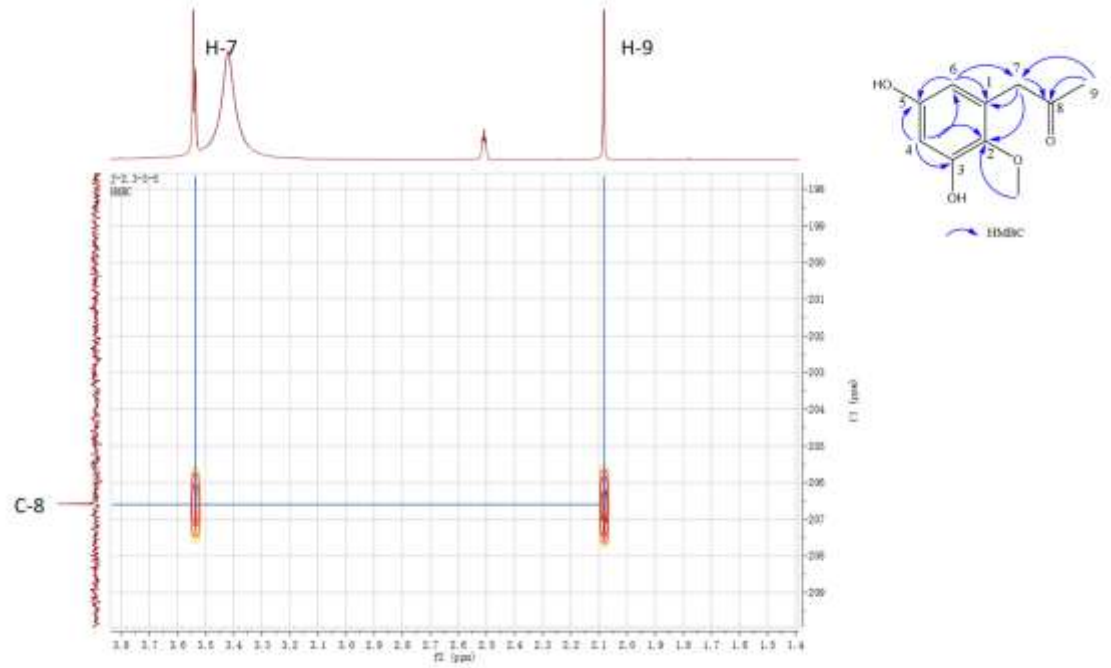


Figure S8-3: HMBC spectrum of compound **1** (enlarged image)

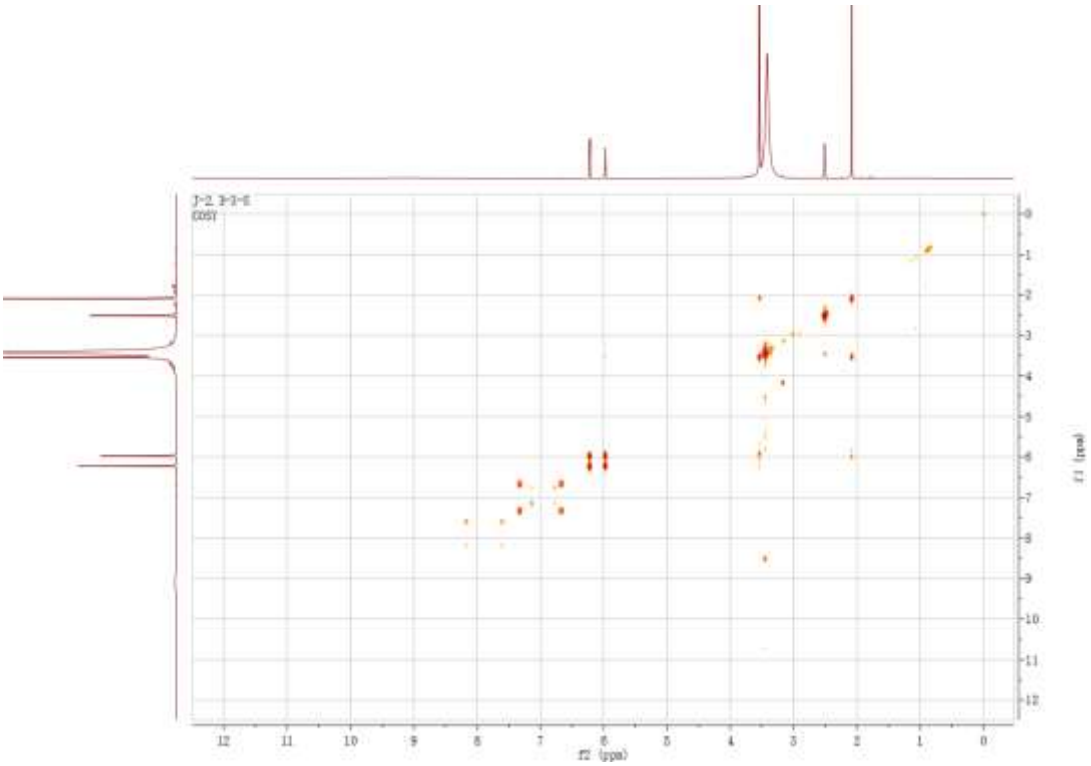


Figure S9: ^{1}H-^{1}H COSY spectrum of compound **1**

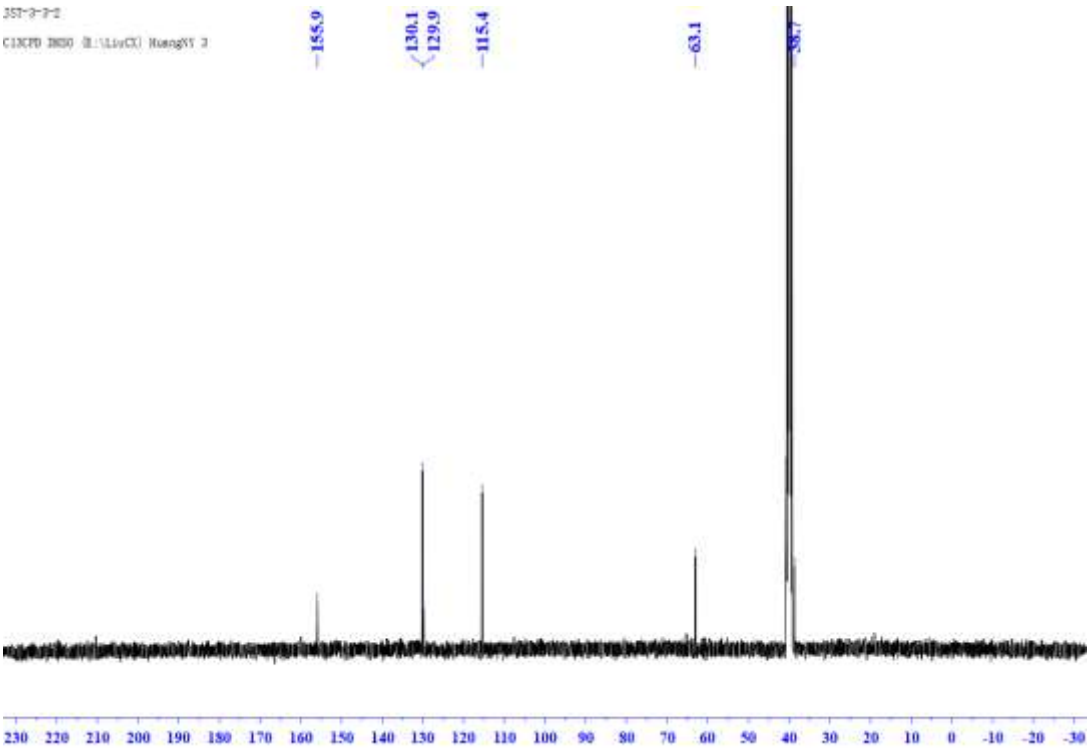


Figure S10: ^{13}C-NMR spectrum of compound **2**

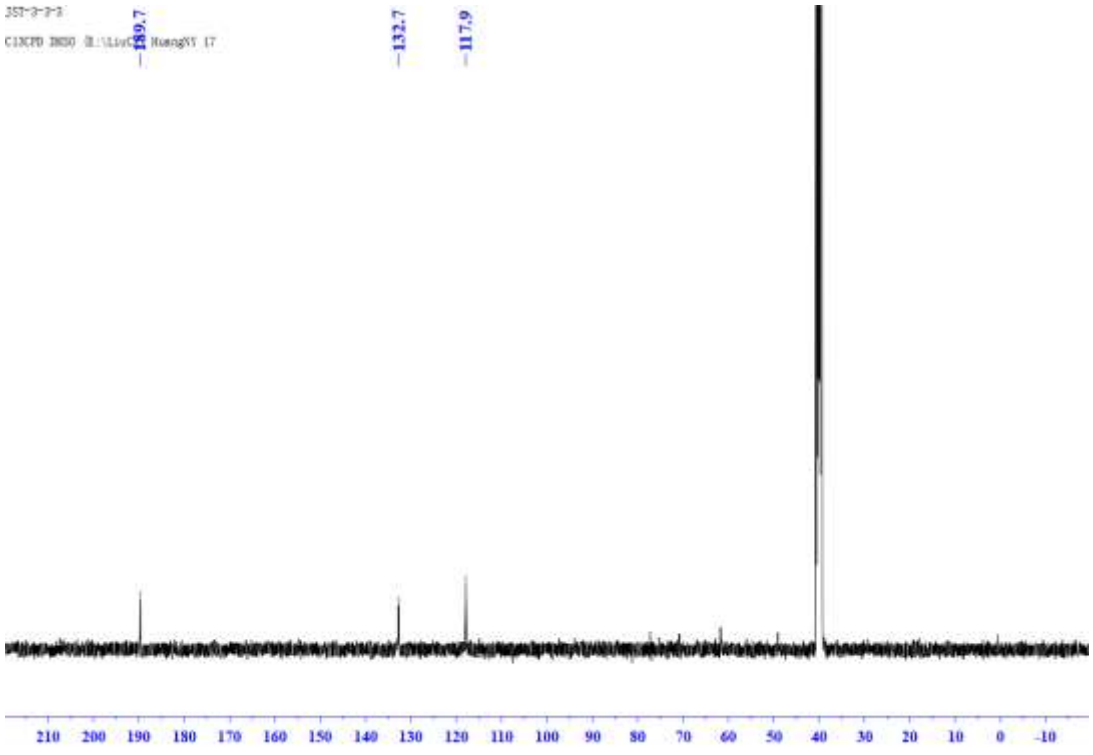


Figure S11: ^{13}C-NMR spectrum of compound **3**

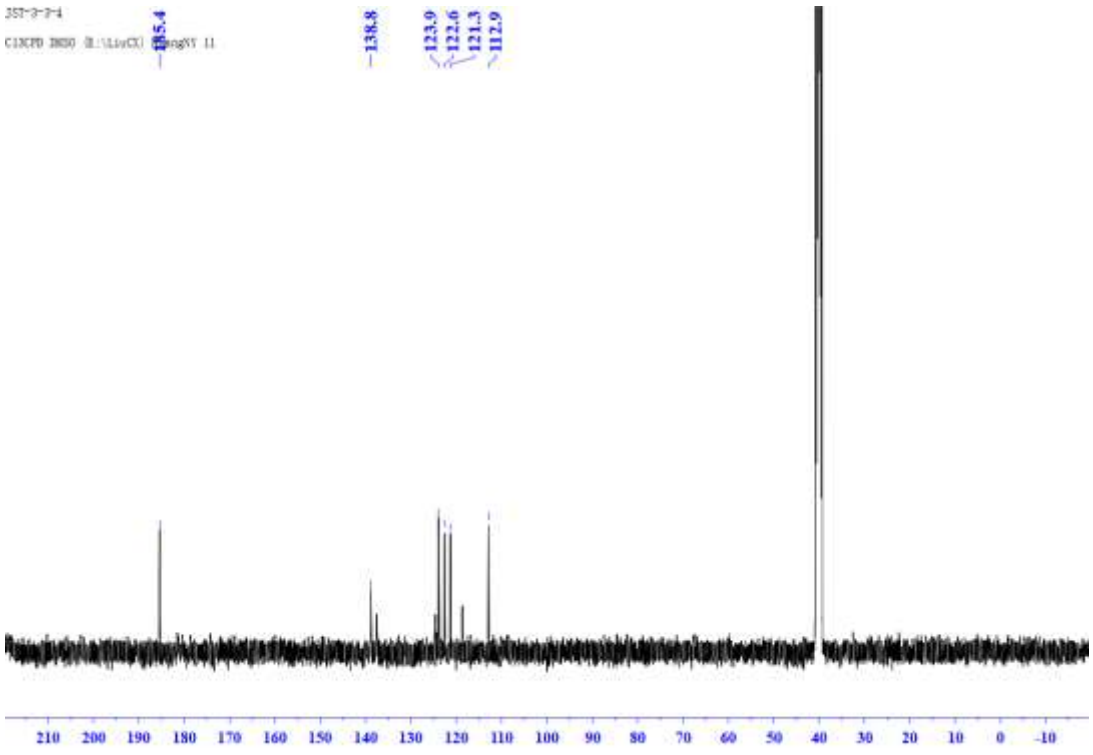


Figure S12: ^{13}C-NMR spectrum of compound **4**

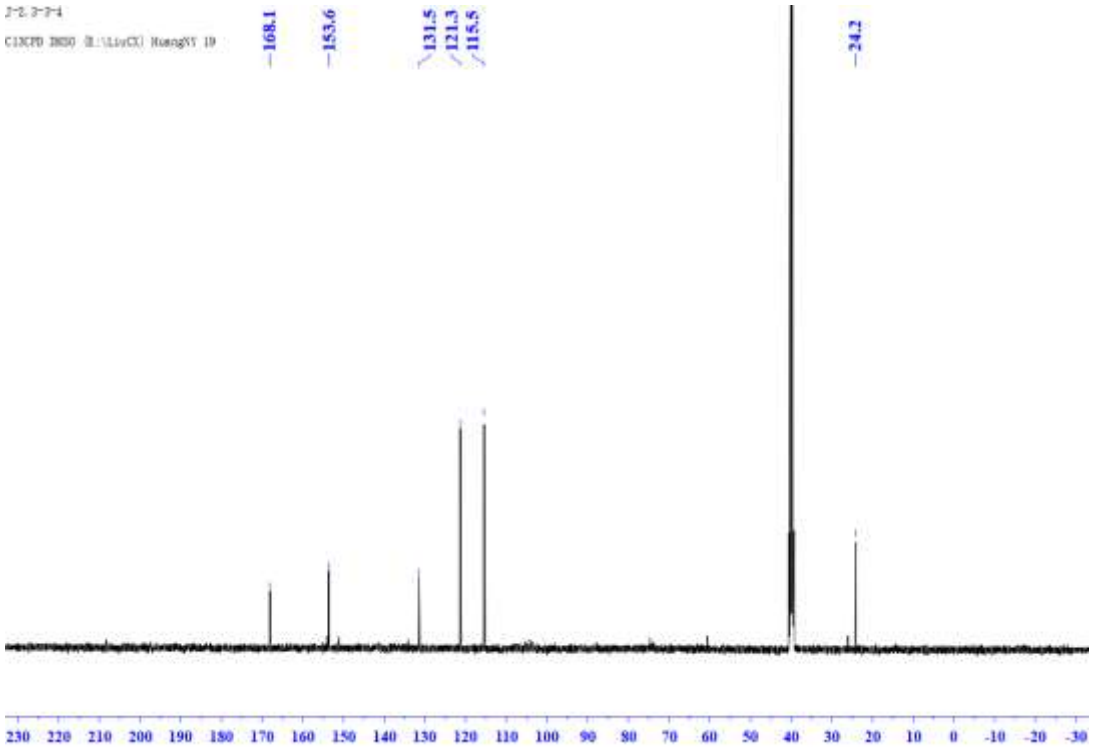


Figure S13: ^{13}C-NMR spectrum of compound **5**

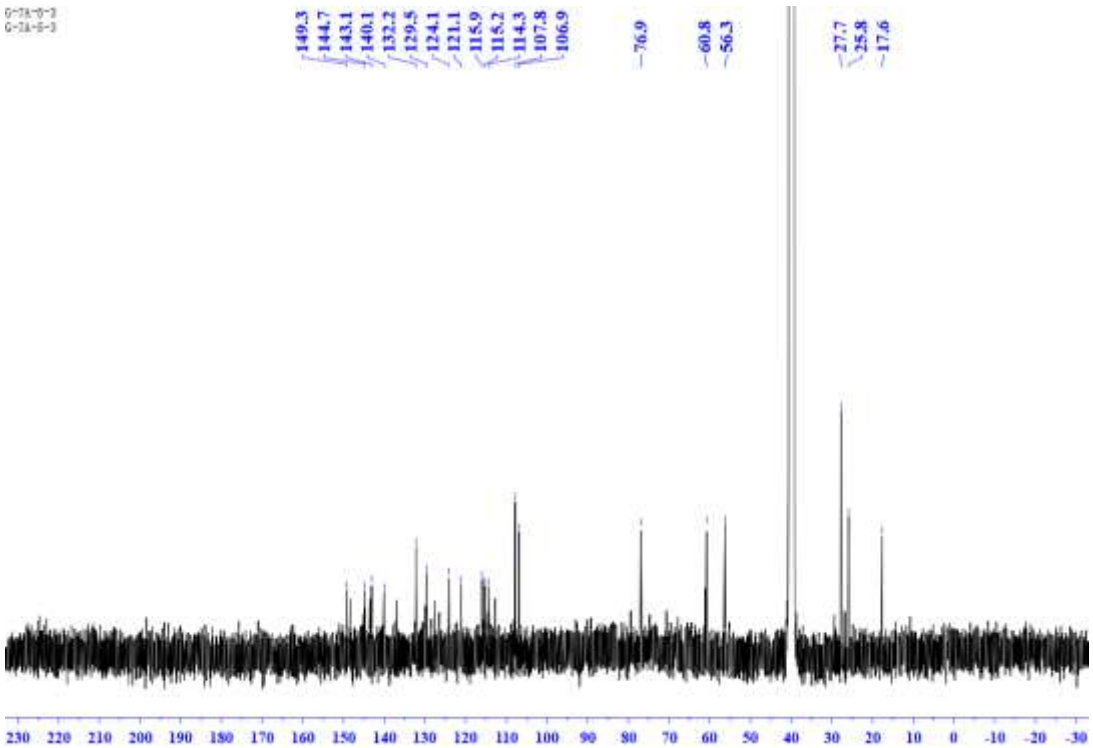


Figure S14: ^{13}C-NMR spectrum of compound **6**

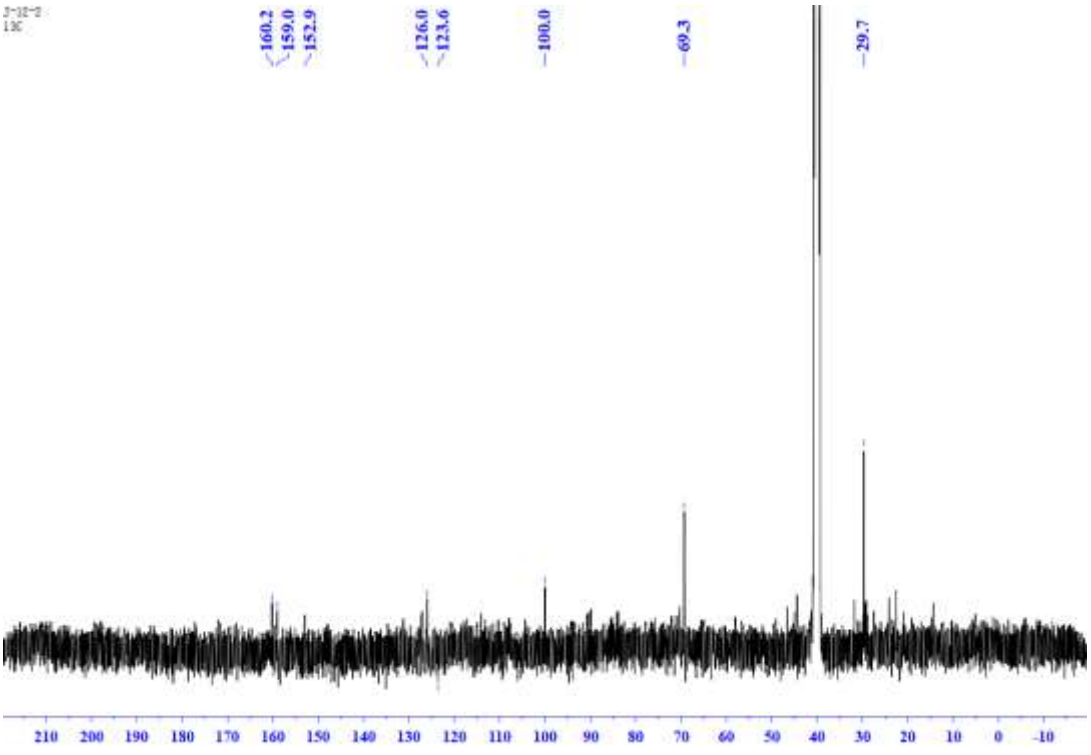


Figure S15: ^{13}C-NMR spectrum of compound **7**

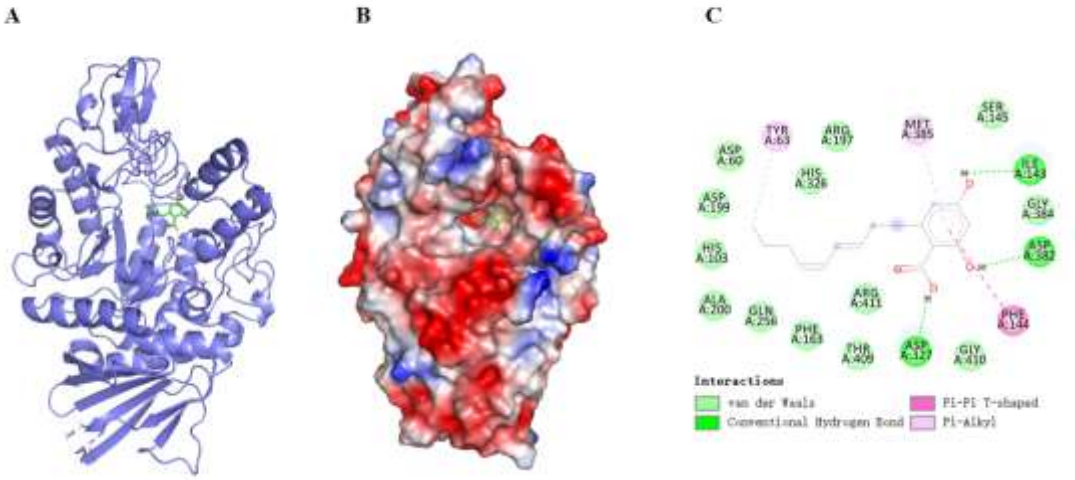


Figure S16. The binding mode of α-glucosidase protein with compound **6**

(**A**: 3D binding mode of compound **6** with α-glucosidase, **B**: 2D binding mode of compound **6** with α-glucosidase, **C**: Amino acid residue binding interactions of compound **6** with α-glucosidase)

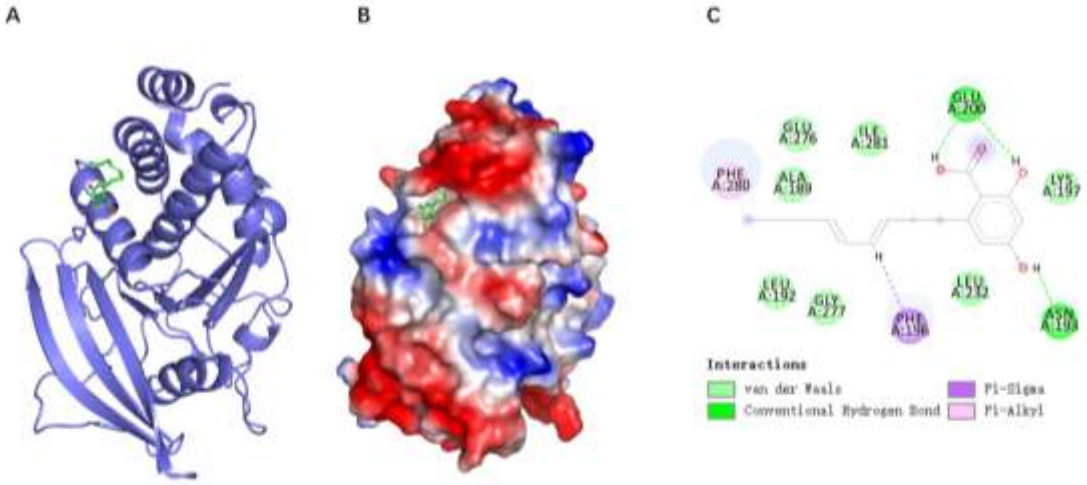


Figure S17. The binding mode of PTP1B with compound **6**

(**A**: 3D binding mode of compound **6** with PTP1B, **B**: 2D binding mode of compound **6** with PTP1B, **C**: Amino acid residue binding interactions of compound **6** with PTP1B).

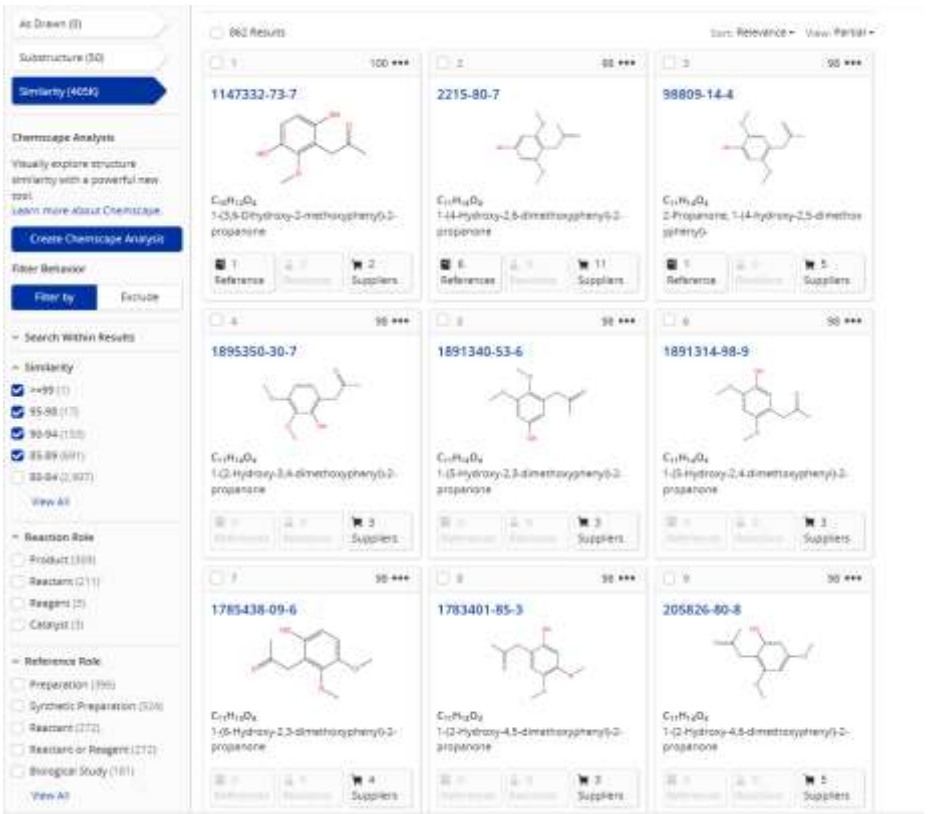


Figure S18: Scifinder report for compound **1**

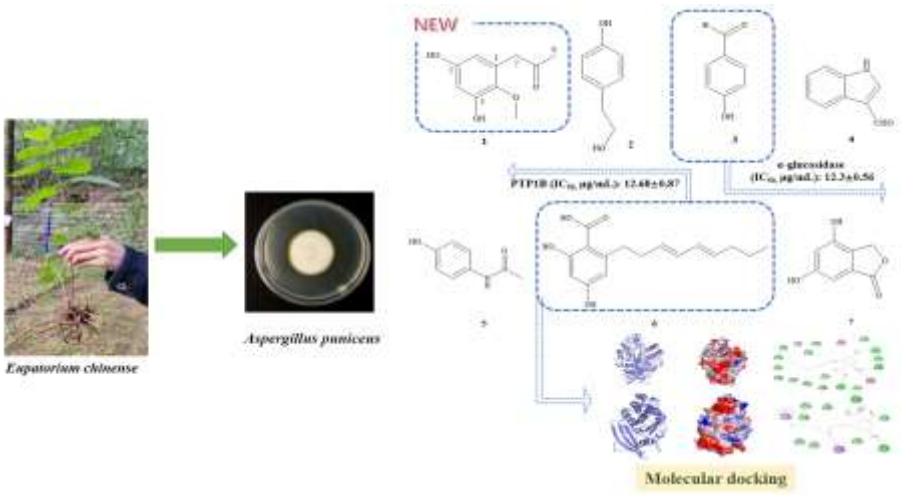


Figure S19: Graphical abstract