

Cytotoxic Polyketides from a Deep-Sea Sediment Derived Fungus *Diaporthe phaseolorum* FS431

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Abstract: Two new chromone-derived polyketides phaseolorins, G and H (**1** and **2**), and one new anthraquinone derivative, phaseolorin I (**3**), together with three known compounds (**4–6**), were isolated from the deep-sea sediment-derived fungus *Diaporthe phaseolorum* FS431. The structures of the new compounds were determined by comprehensive analysis of their spectroscopic data, and the absolute configuration of **1** was established by quantum chemical calculations of electron capture detection (ECD). All the isolated compounds (**1–6**) were tested for their in vitro cytotoxic activities against four human tumor cell lines, of which compound **4** exhibited significant effect against MCF-7, HepG-2, and A549 tumor cell lines with IC₅₀ values of 2.60, 2.55, and 4.64 μ M, respectively.

Keywords: *Diaporthe phaseolorum*; deep-sea derived fungus; polyketides; cytotoxicity

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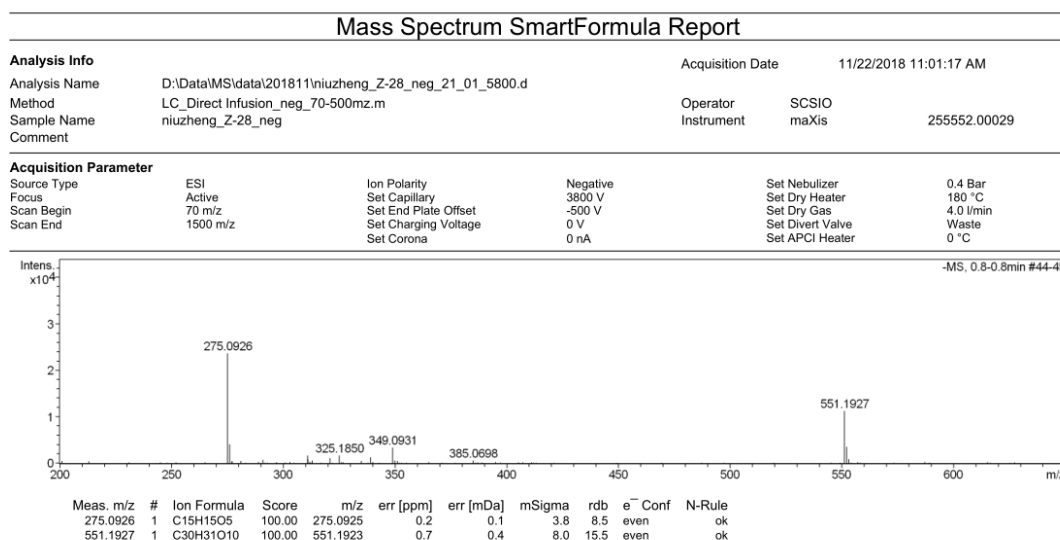


Figure S1. HRESIMS spectrum of Phaseolorin G (1)

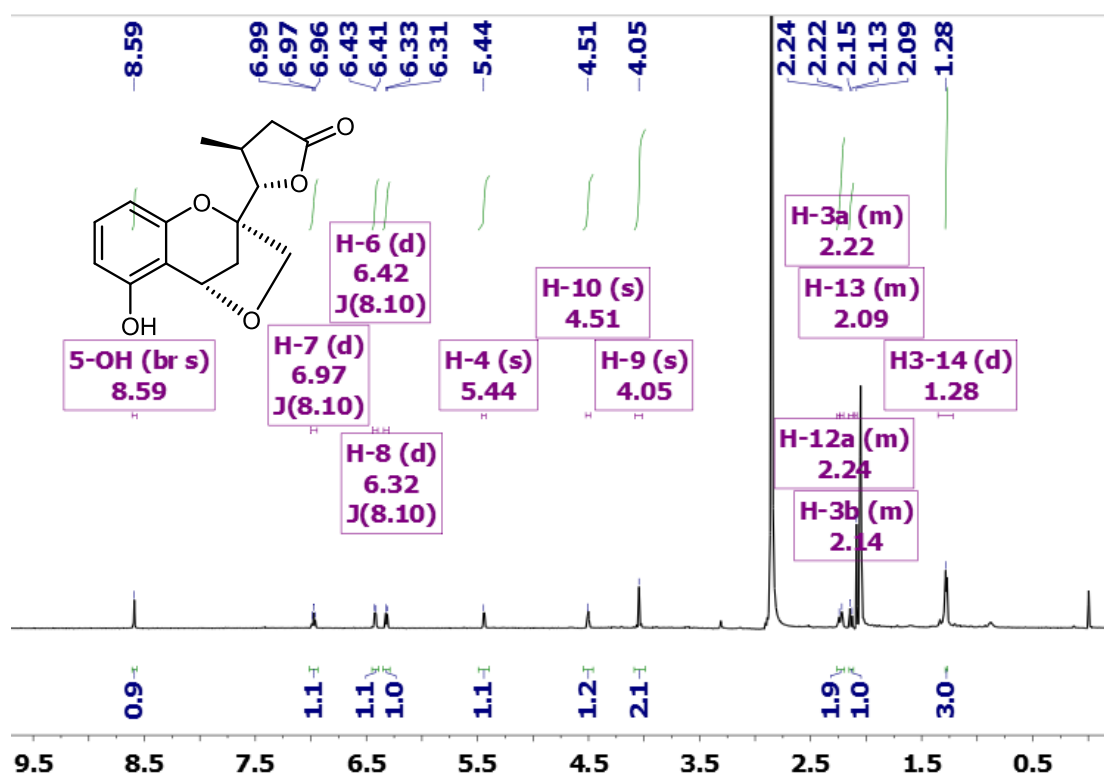


Figure S2. ¹H-NMR spectrum (600 MHz, acetone-*d*₆) of Phaseolorin G (1)

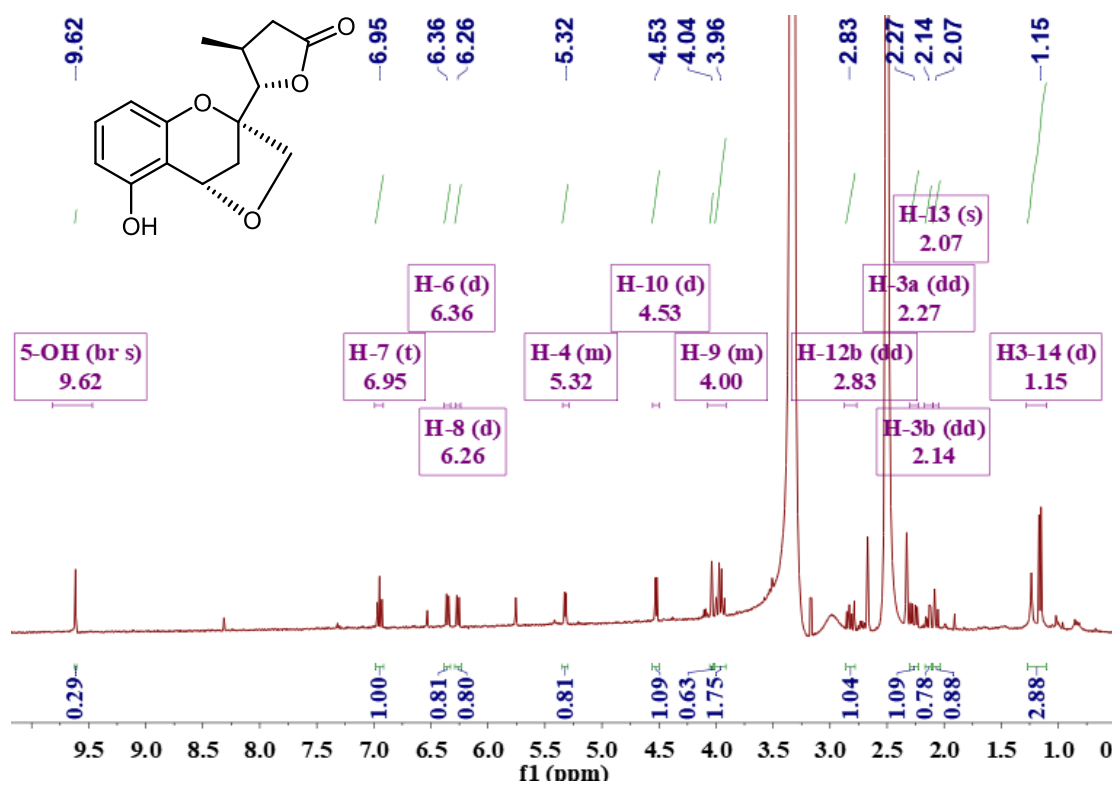


Figure S3. ¹H-NMR spectrum (600 MHz, DMSO-*d*₆) of Phaseolorin G (1)

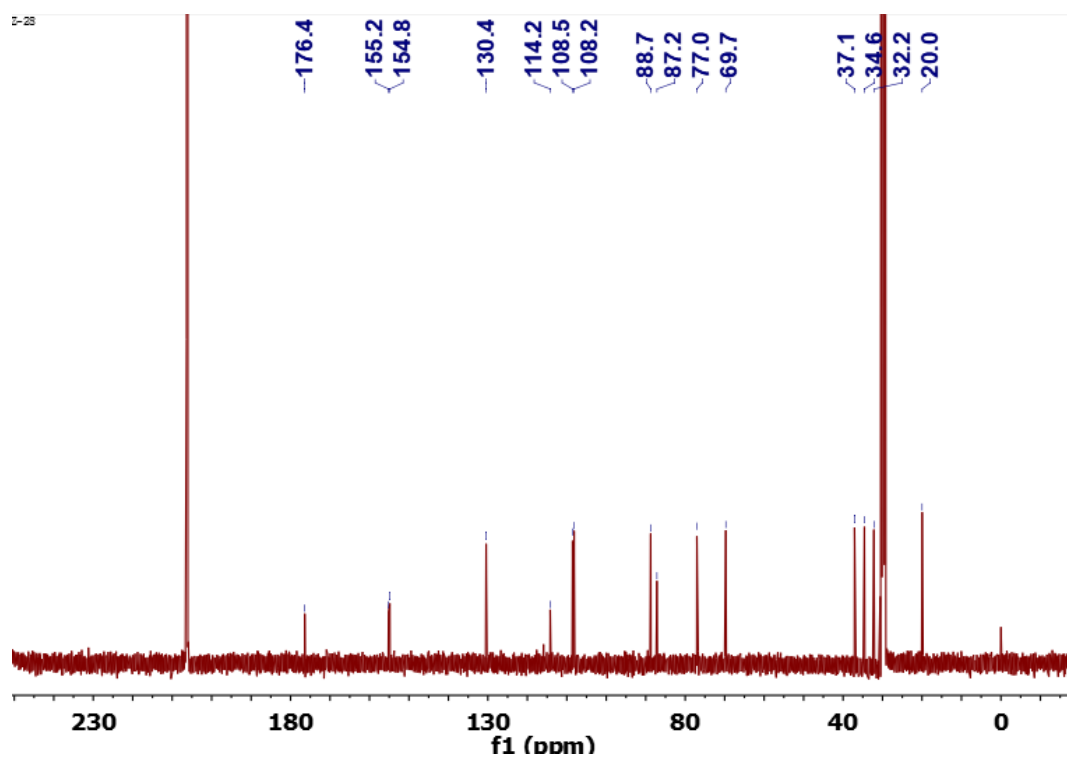


Figure S4. ¹³C-NMR spectrum (150 MHz, acetone-*d*₆) of Phaseolorin G (**1**)

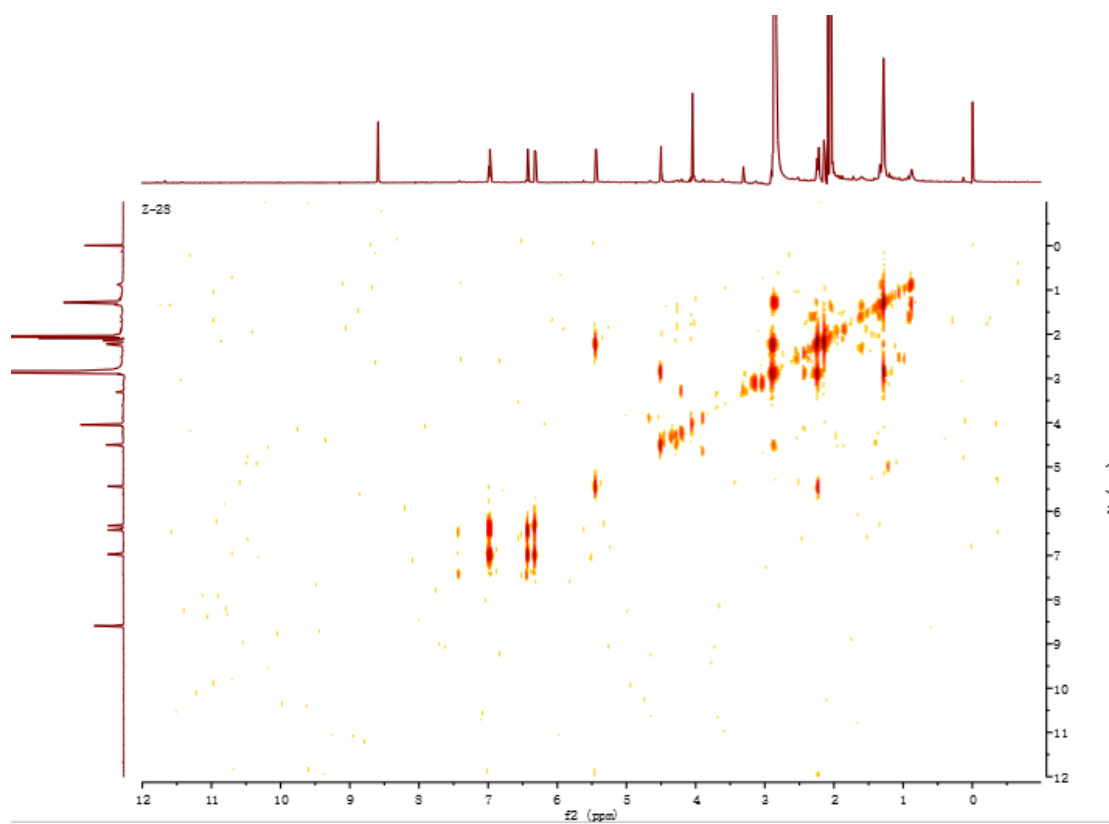


Figure S5. ¹H-¹H COSY spectrum (600 MHz, acetone-*d*₆) of Phaseolorin G (**1**)

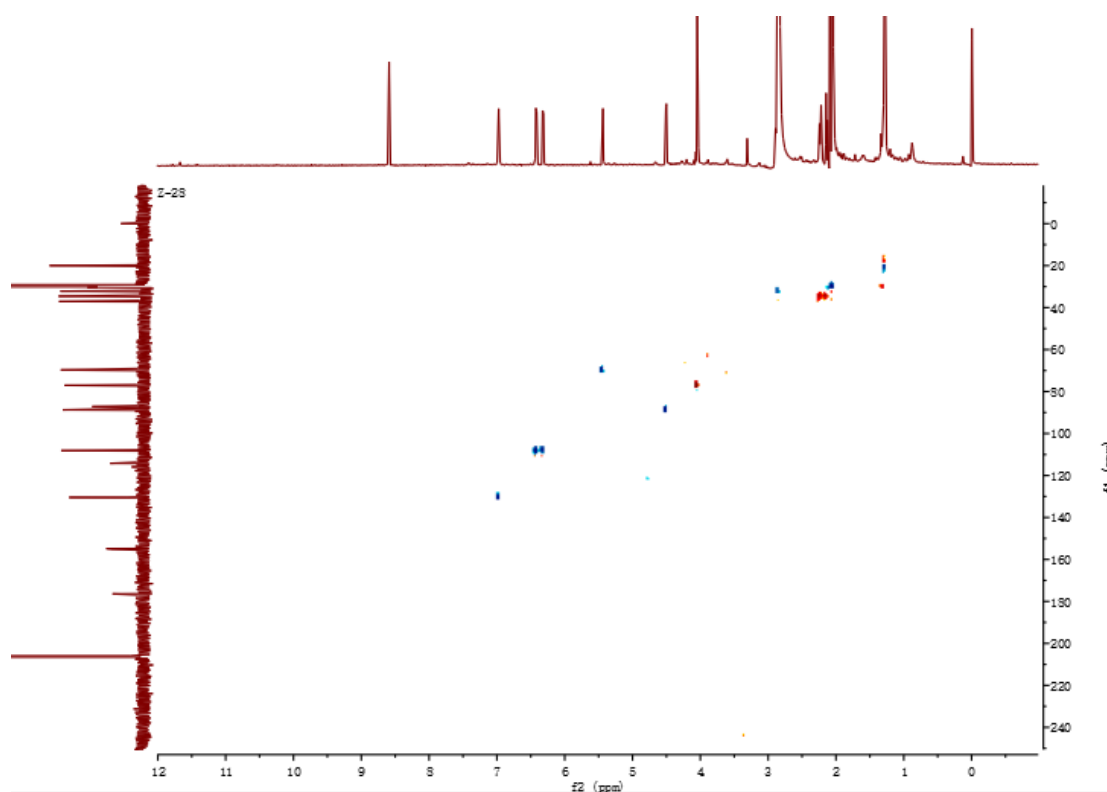


Figure S6. HSQC spectrum of Phaseolorin G (1)

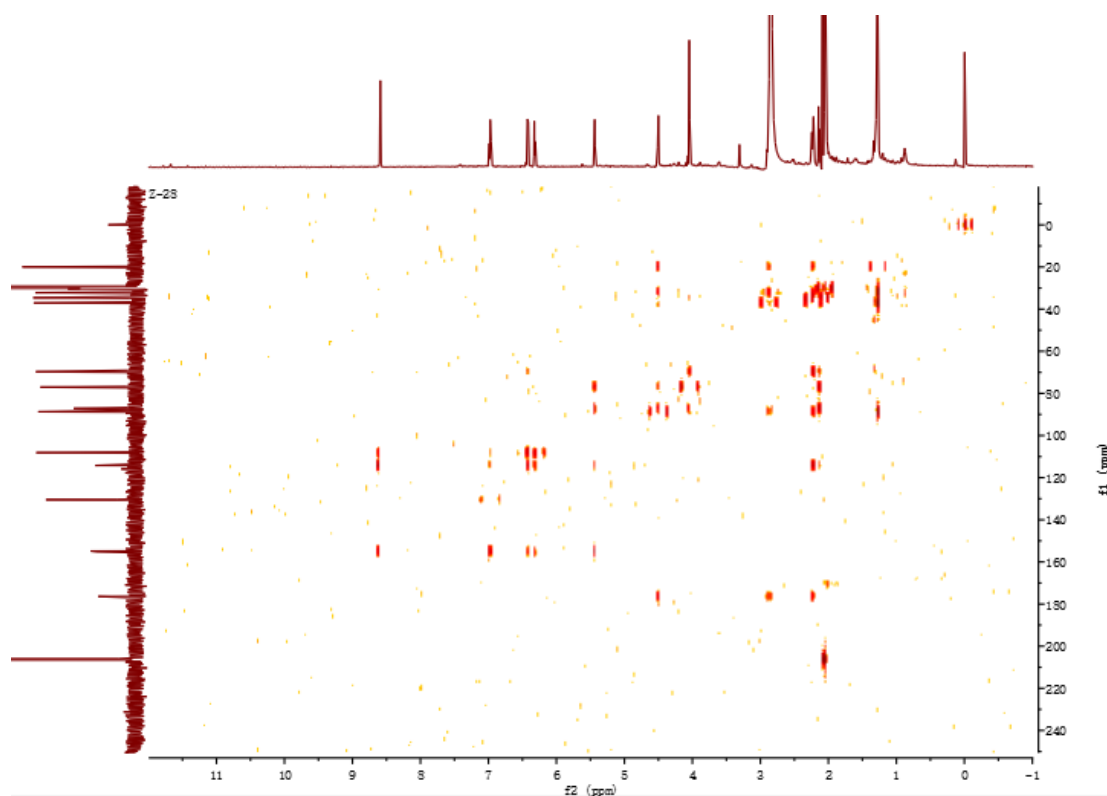


Figure S7. HMBC spectrum of Phaseolorin G (1)

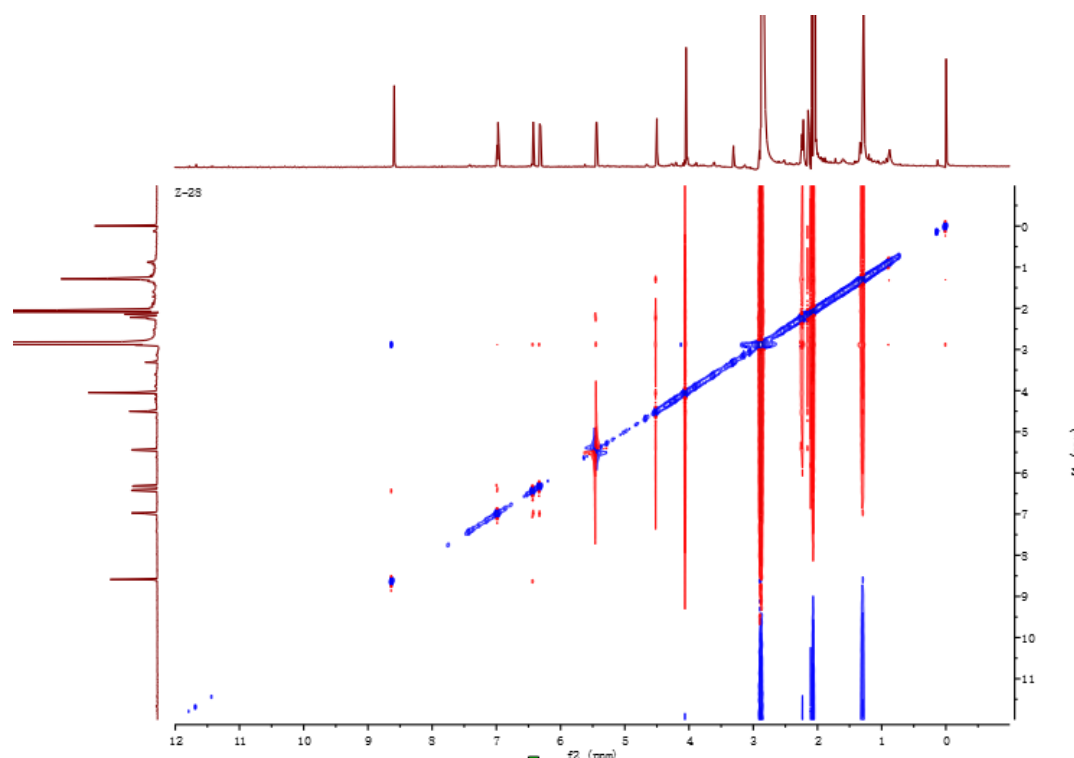


Figure S8. NOESY spectrum (600 MHz, acetone- d_6) of Phaseolorin G (1)

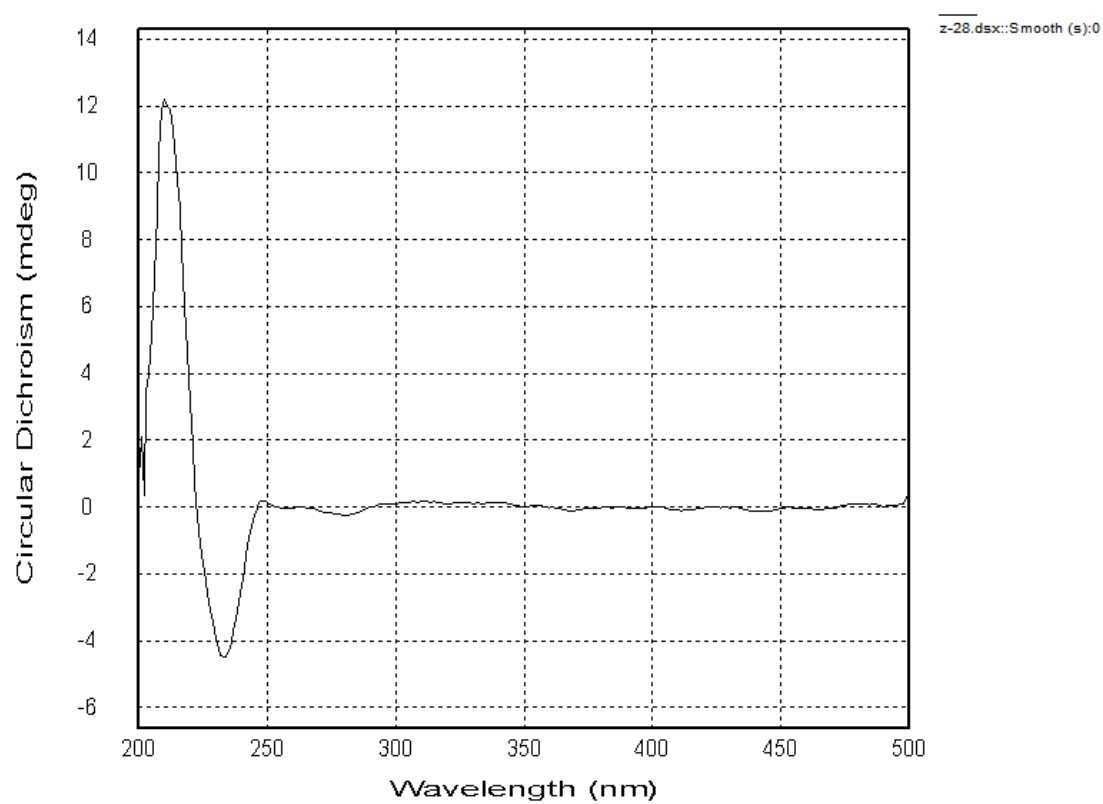


Figure S9. CD spectrum of Phaseolorin G (1)

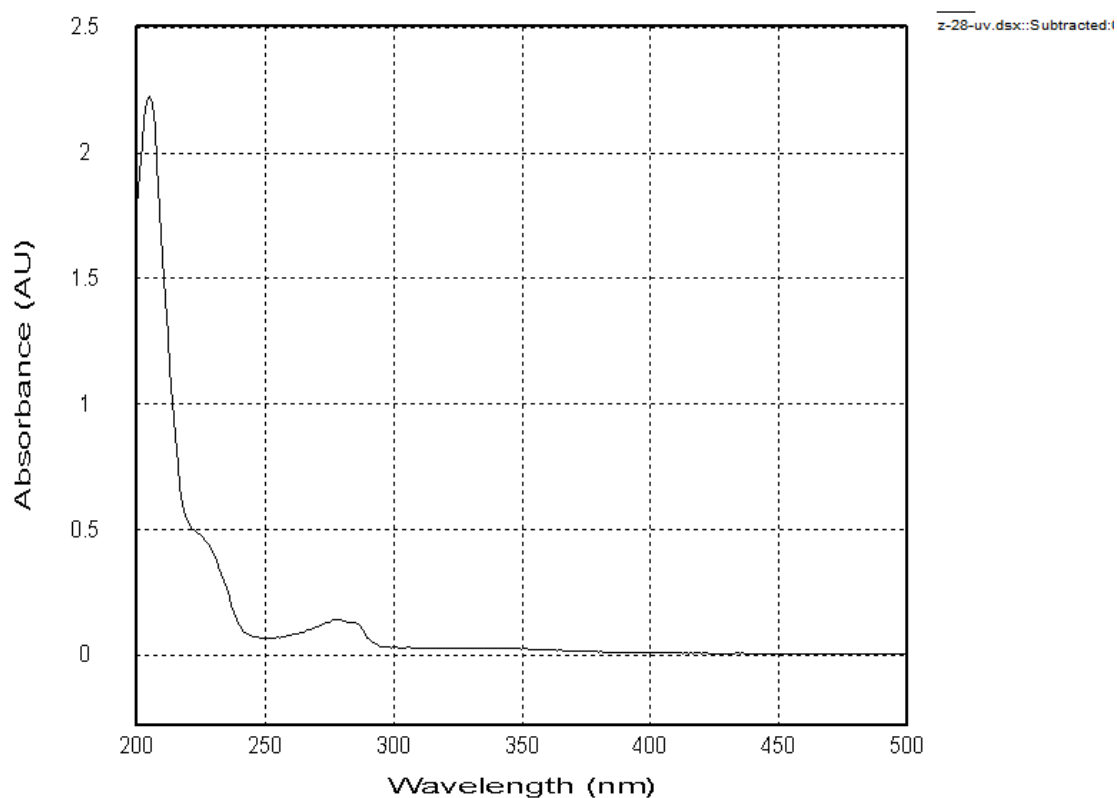


Figure S10. UV spectrum of Phaseolorin G (1)

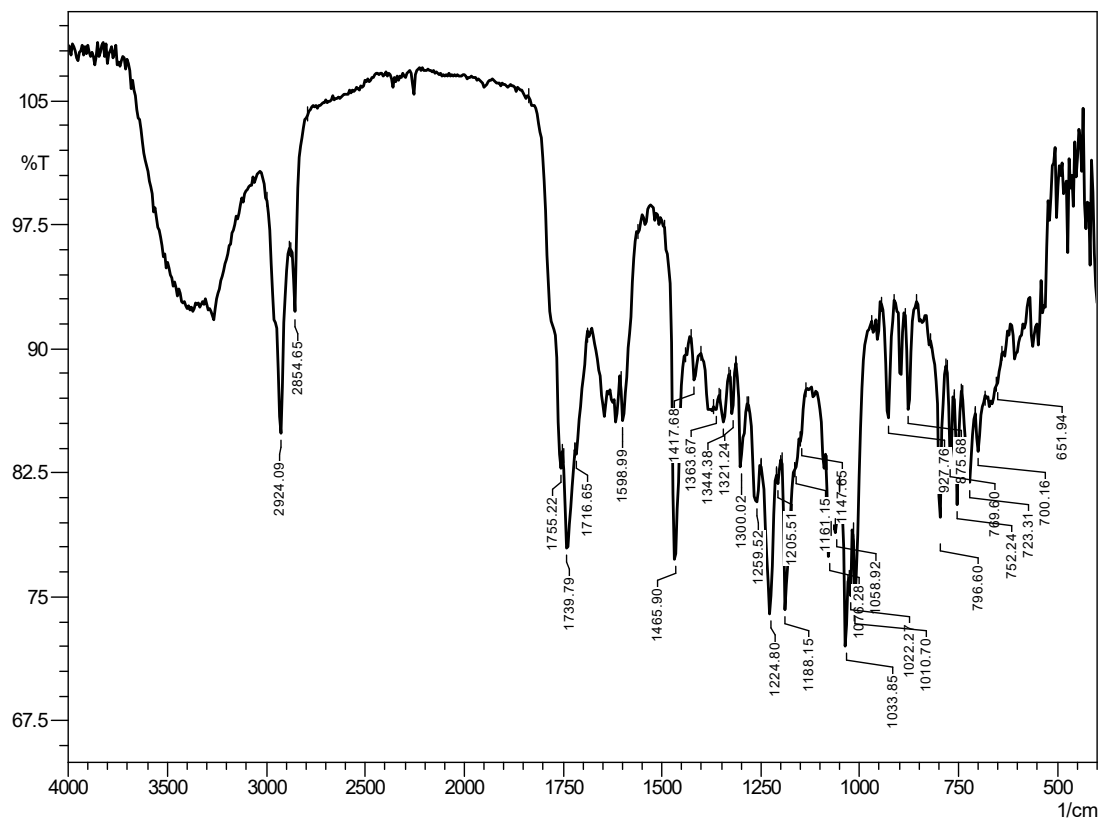


Figure S11. IR spectrum of Phaseolorin G (1)

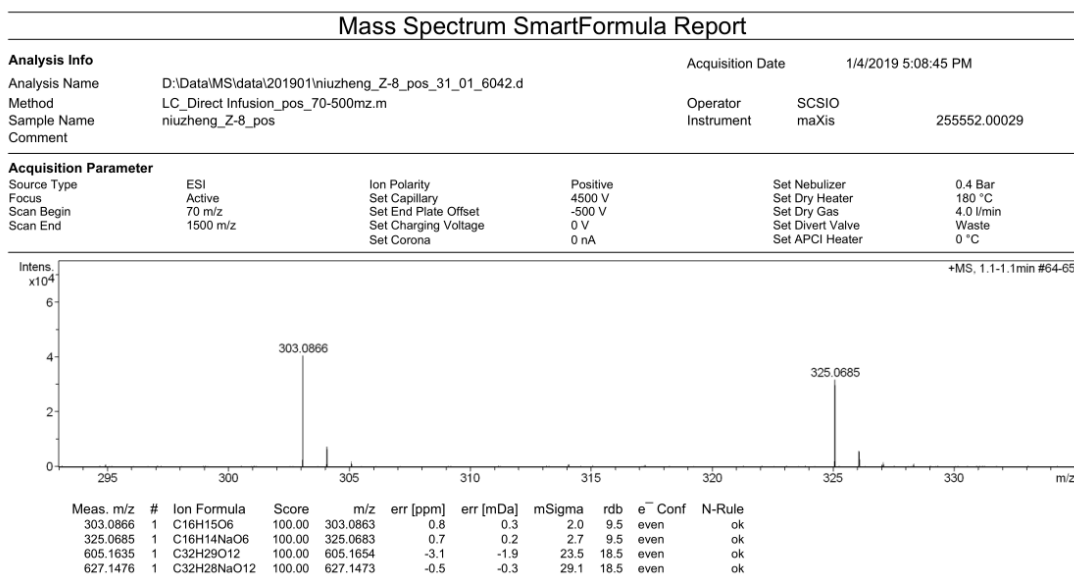


Figure S12. HRESIMS spectrum of Phaseolorin G (1)

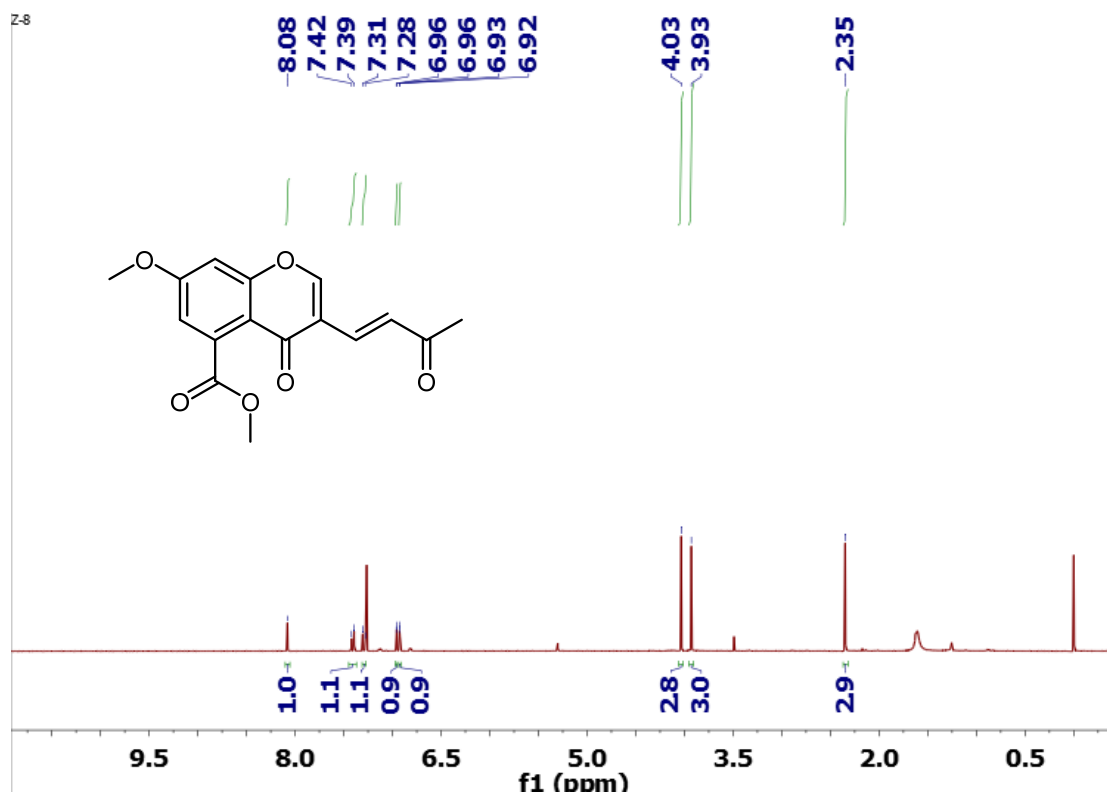


Figure S13. ¹H-NMR spectrum (600 MHz, CHCl₃) of Phaseolorin H (2)

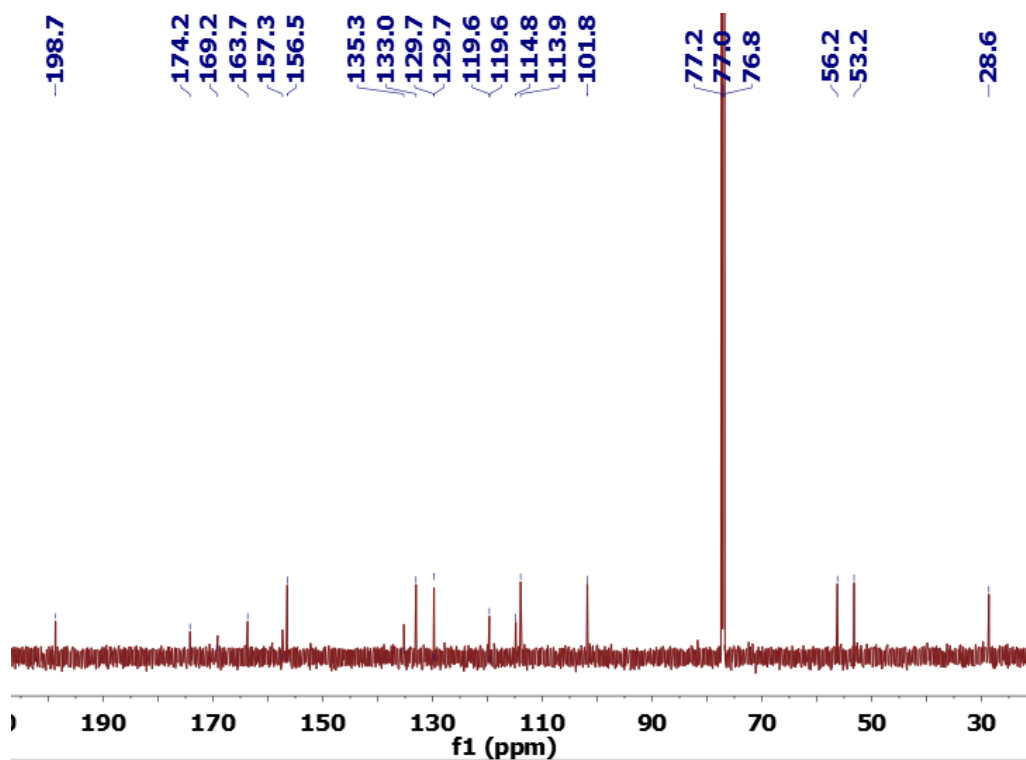


Figure S14. ¹³C-NMR spectrum (150 MHz, CHCl₃) of Phaseolorin H (2)

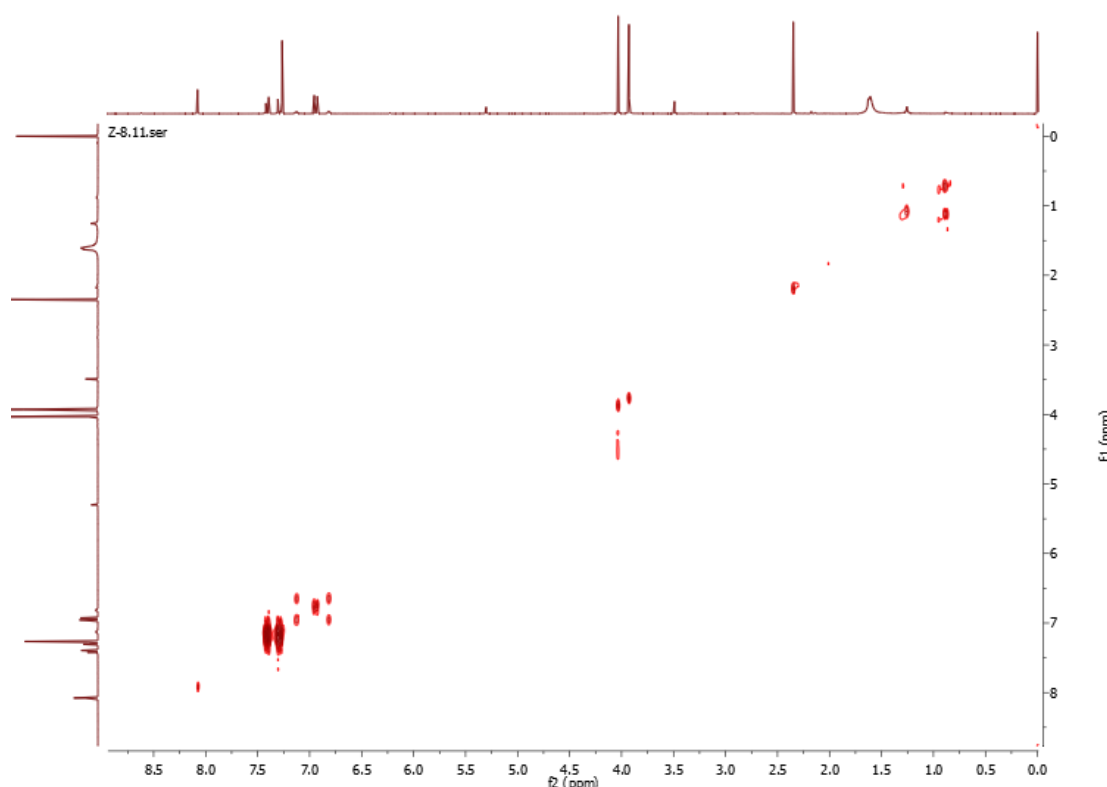


Figure S15. ¹H-¹H COSY spectrum (600 MHz, CHCl₃) of Phaseolorin H (2)

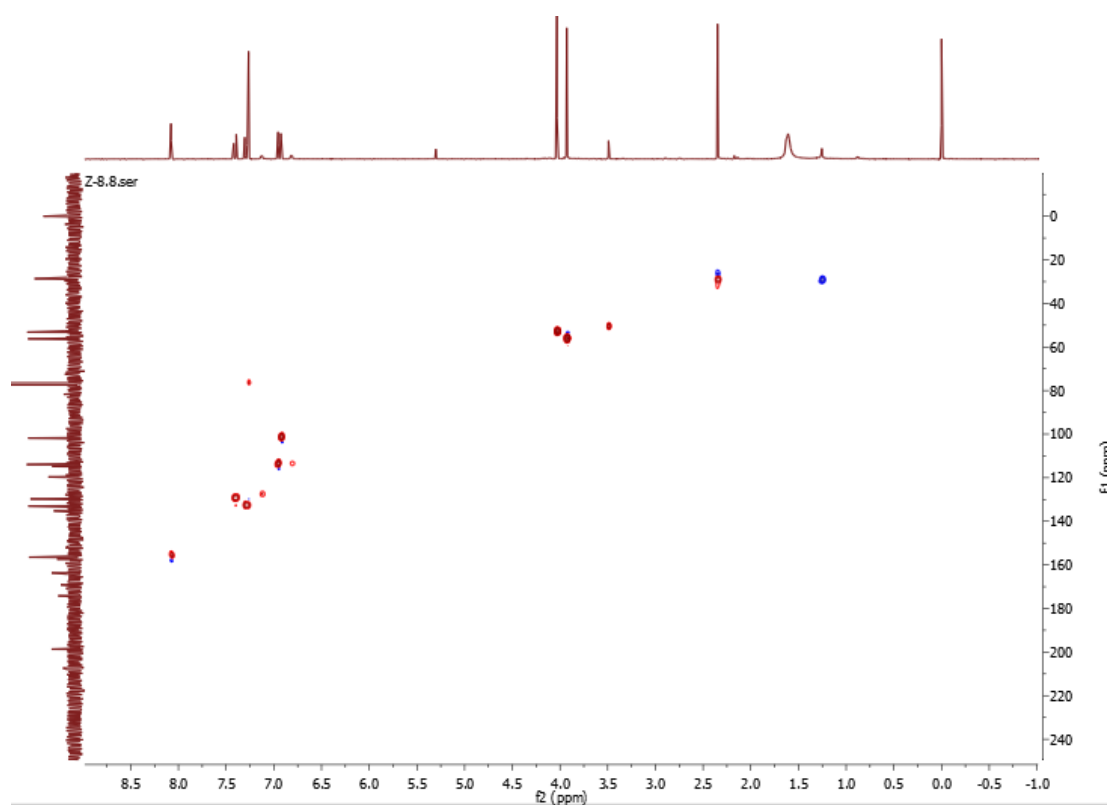


Figure S16. HSQC spectrum of Phaseolorin H (2)

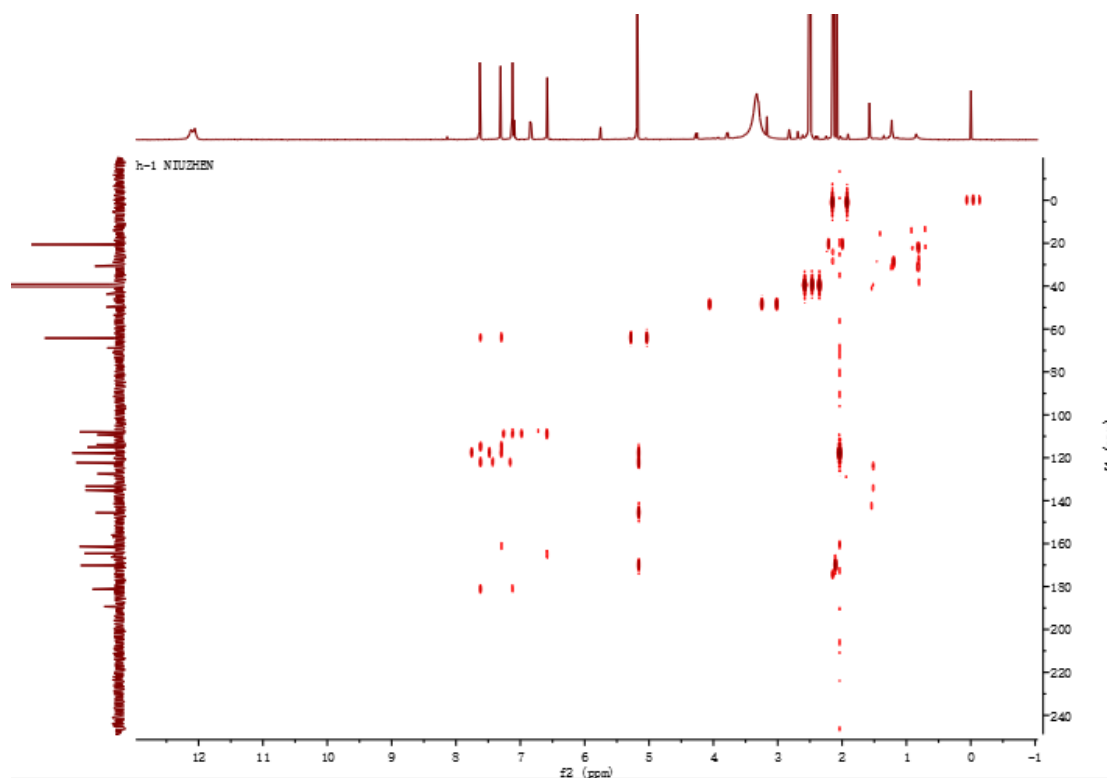


Figure S17. HMBC spectrum of Phaseolorin H (2)

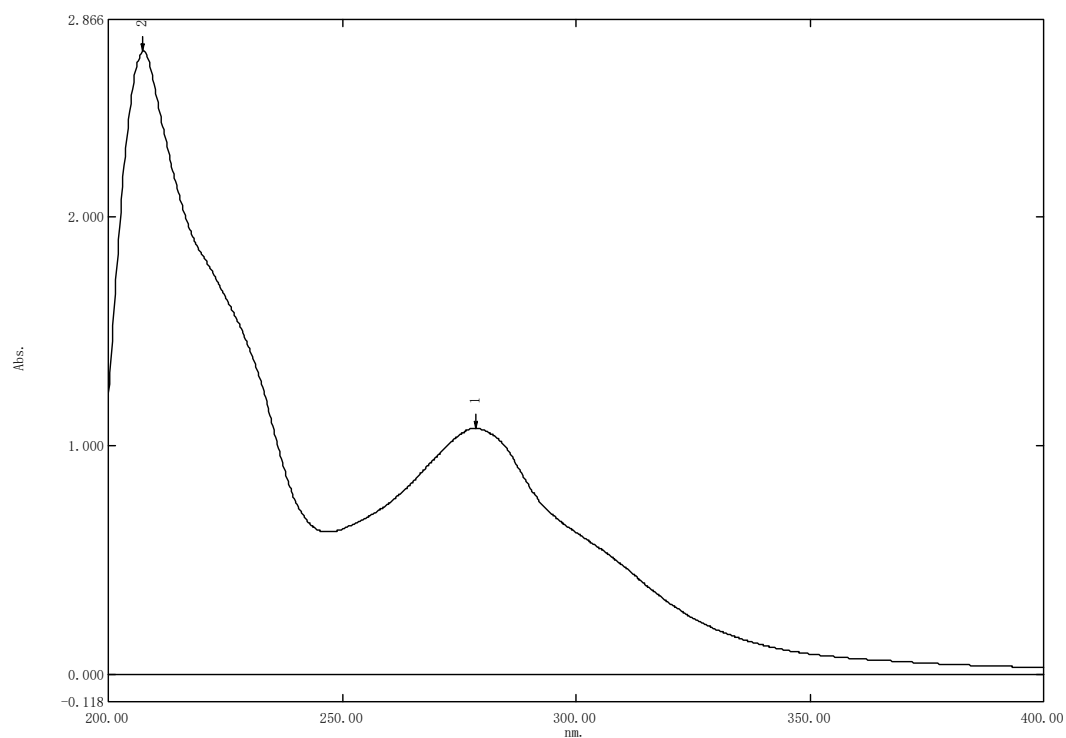


Figure S18. UV spectrum of Phaseolorin H (2)

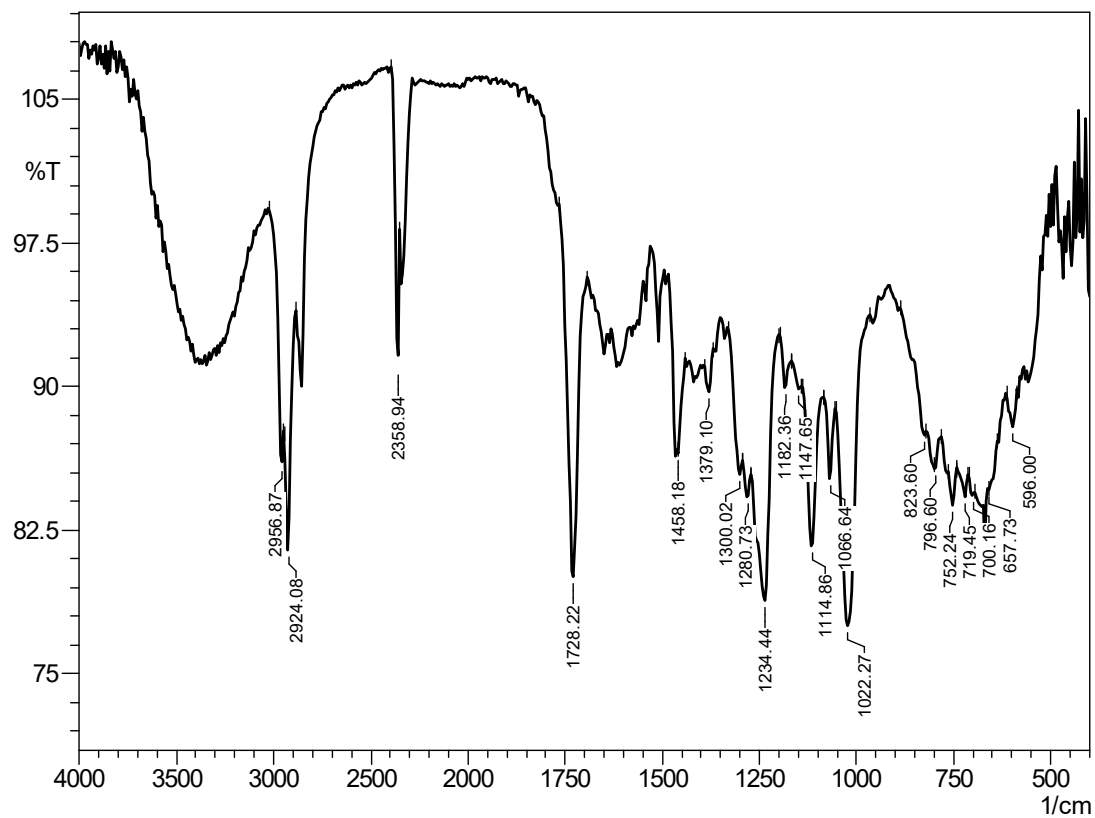


Figure S19. IR spectrum of Phaseolorin H (2)

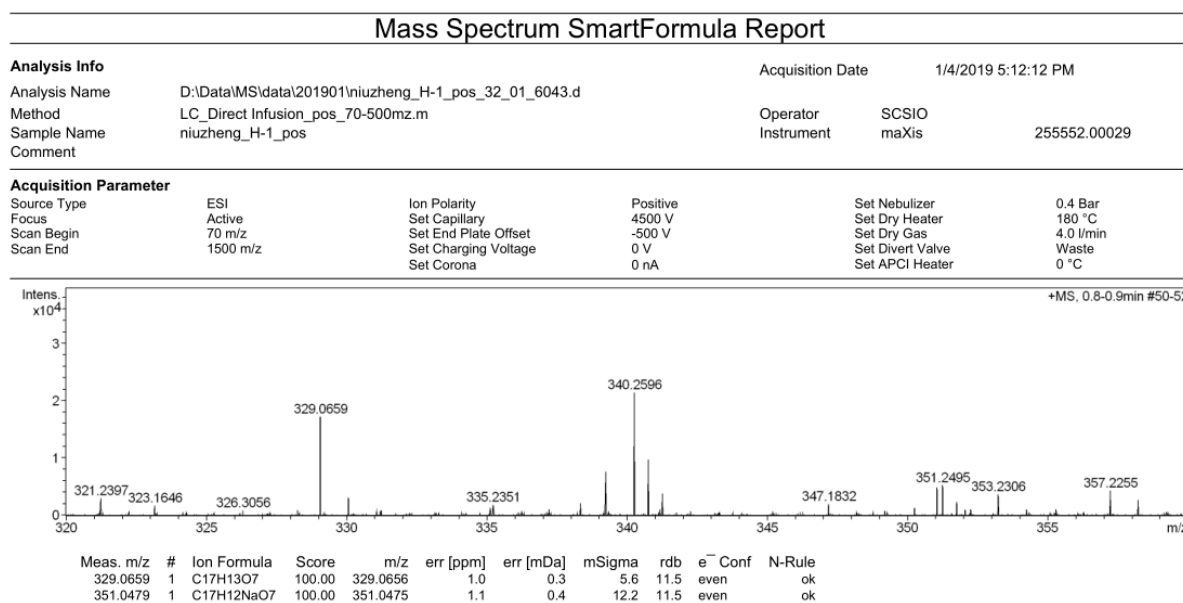


Figure S20. HRESIMS spectrum of Phaseolorin I (3)

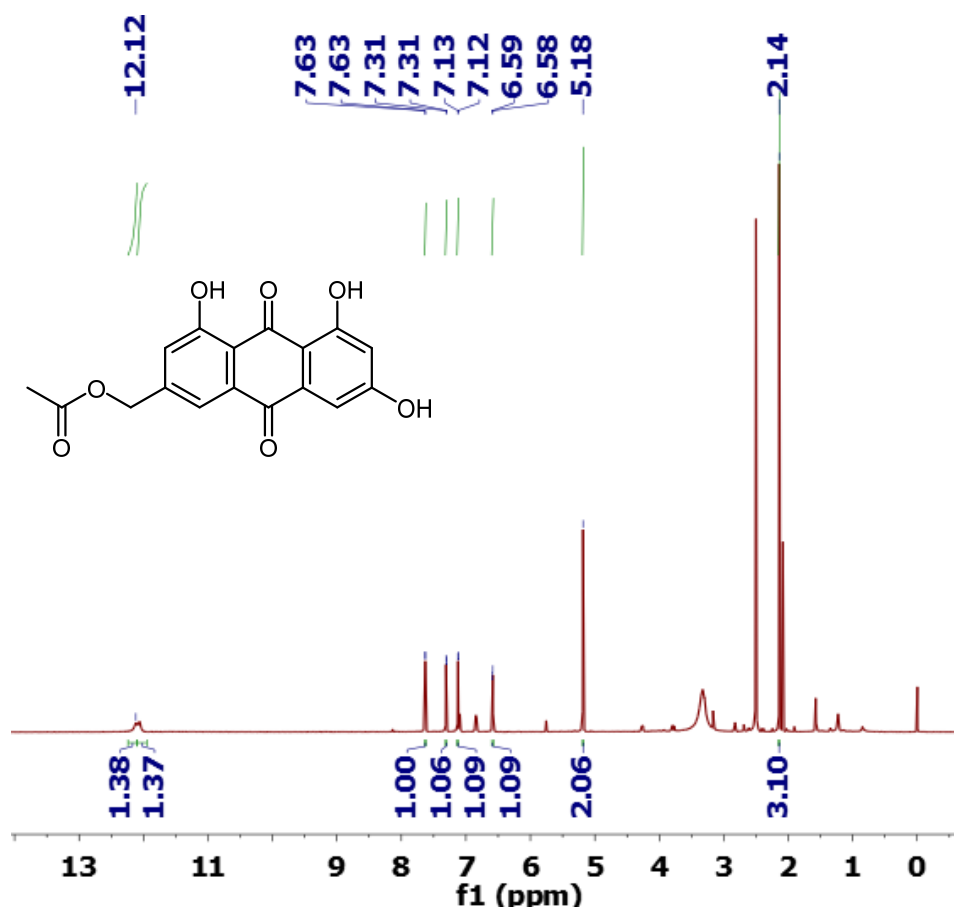


Figure S21. ¹H-NMR spectrum (600 MHz, DMSO-*d*₆) of Phaseolorin I (3)

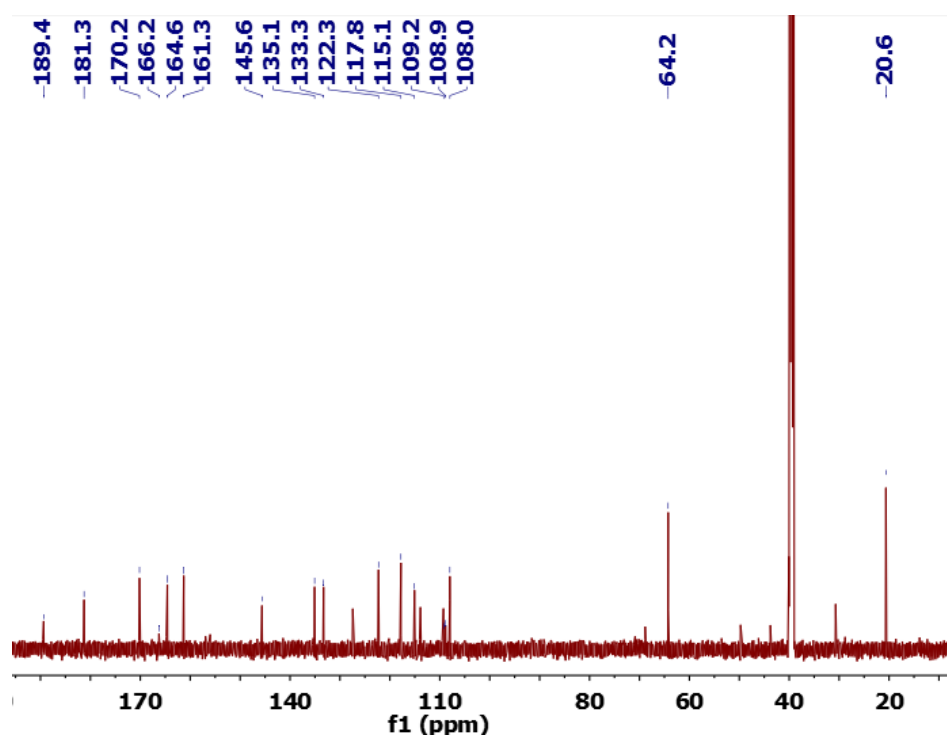


Figure S22. ^{13}C -NMR spectrum (150 MHz, $\text{DMSO}-d_6$) of Phaseolorin I (3)

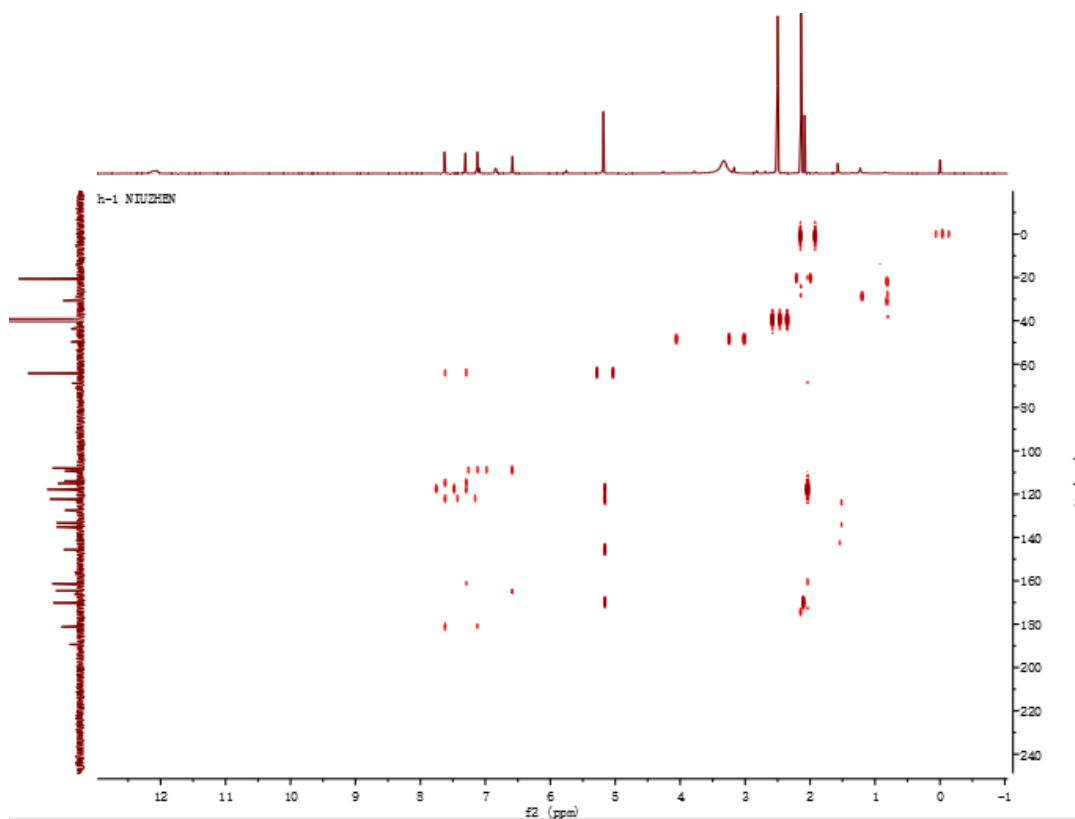


Figure S23. HMBC spectrum of Phaseolorin I (3)

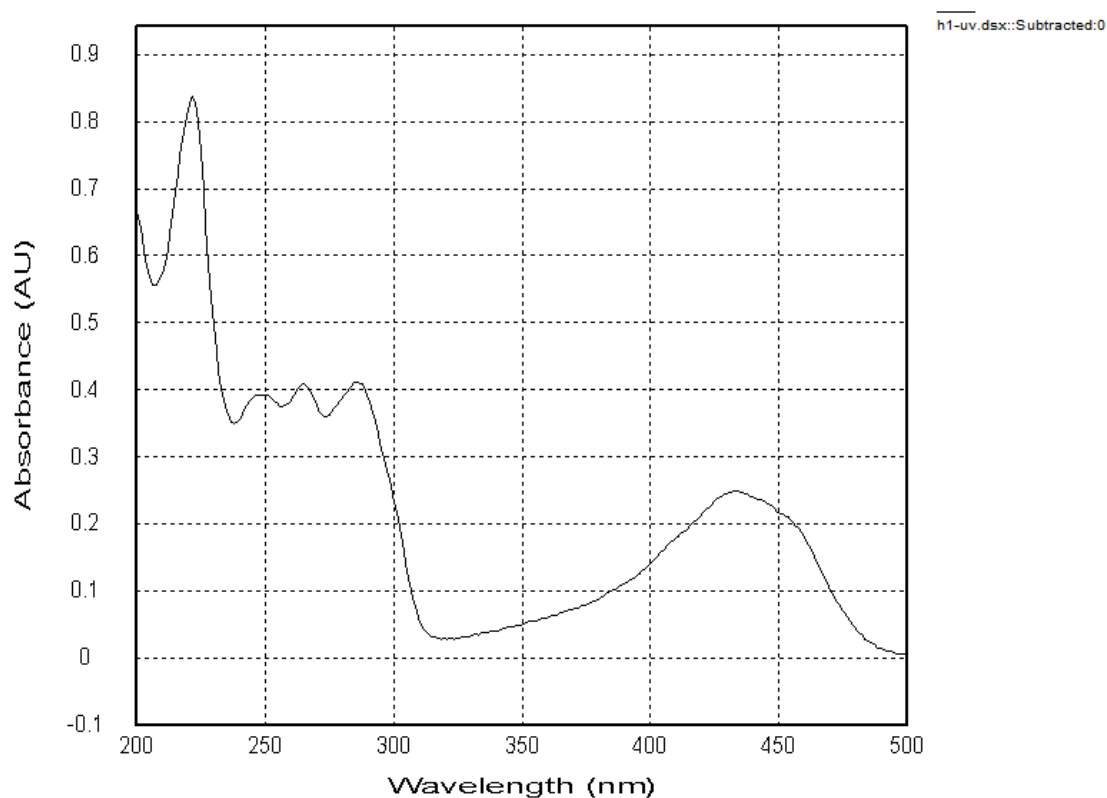


Figure S24. UV spectrum of Phaseolorin I (3)

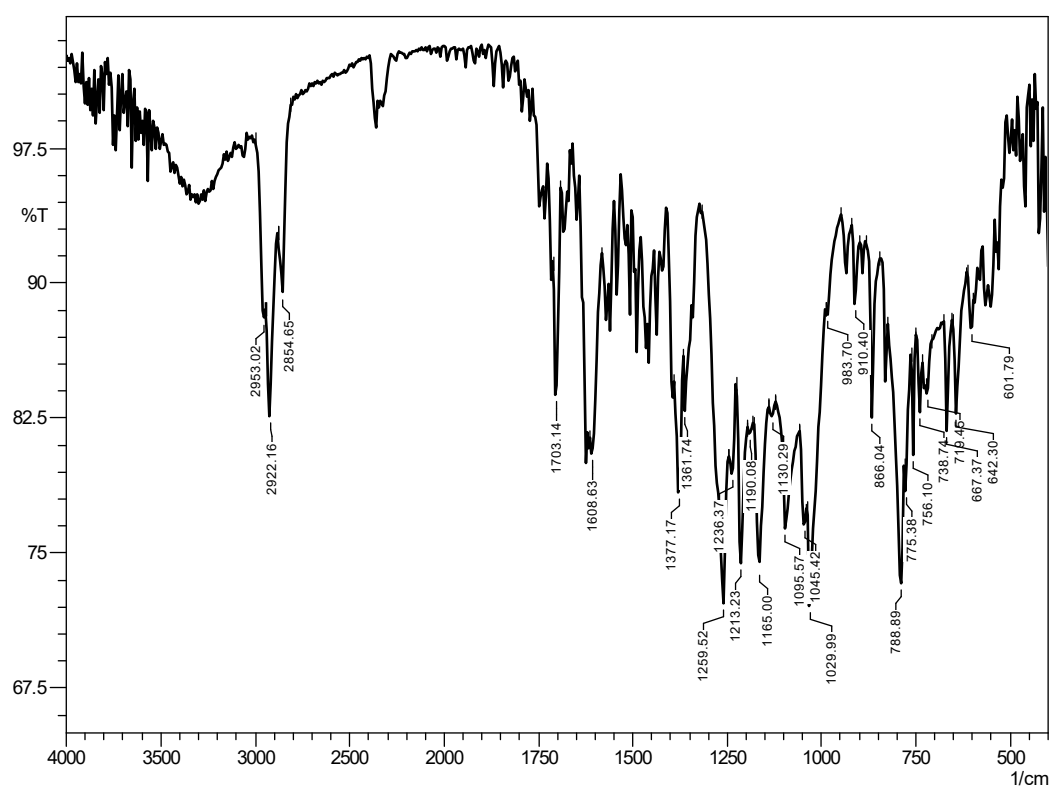


Figure S25. IR spectrum of Phaseolorin I (3)

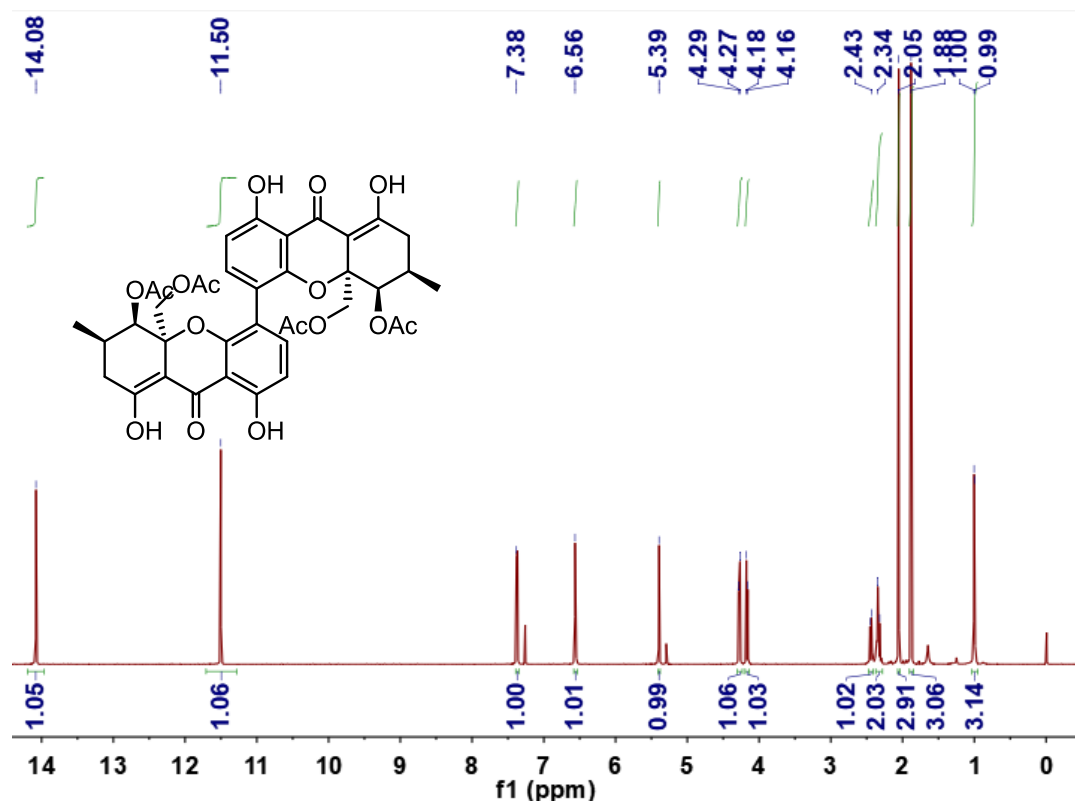


Figure S26. ^1H -NMR spectrum (600 MHz, CHCl_3) of Phomoxanthone A (4)

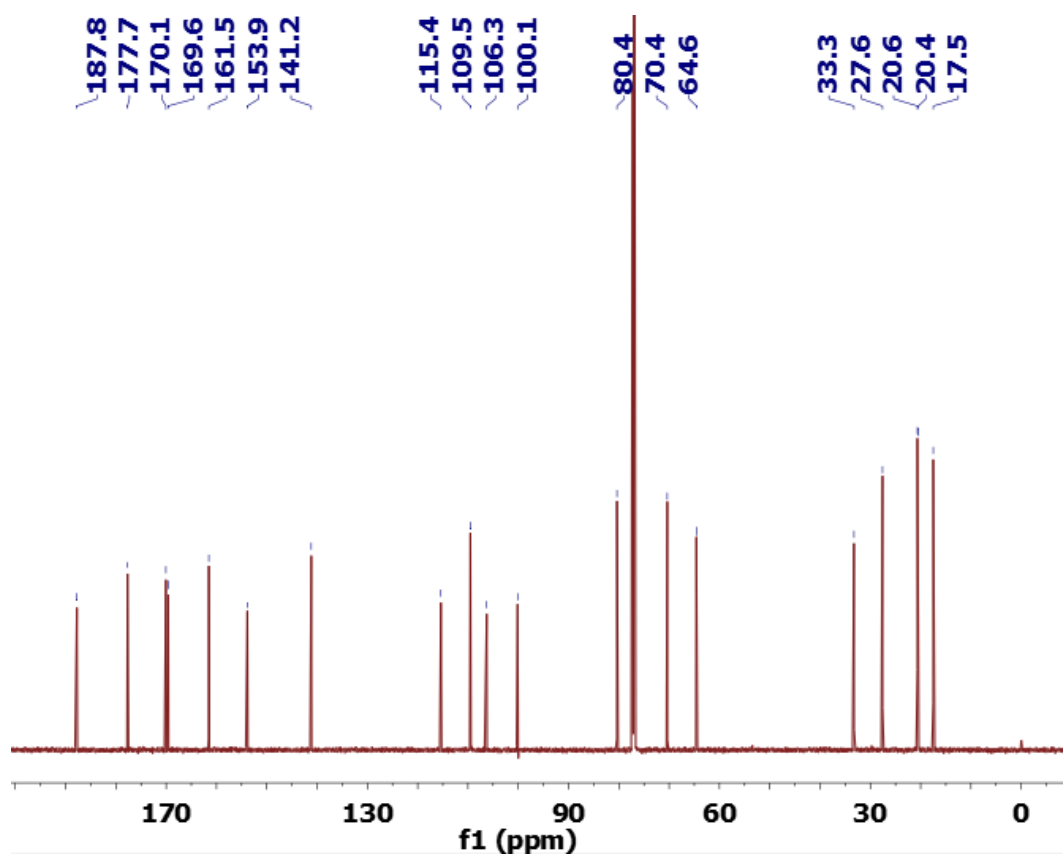


Figure S27. ^{13}C -NMR spectrum (150 MHz, CHCl_3) of Phomoxanthone A (4)

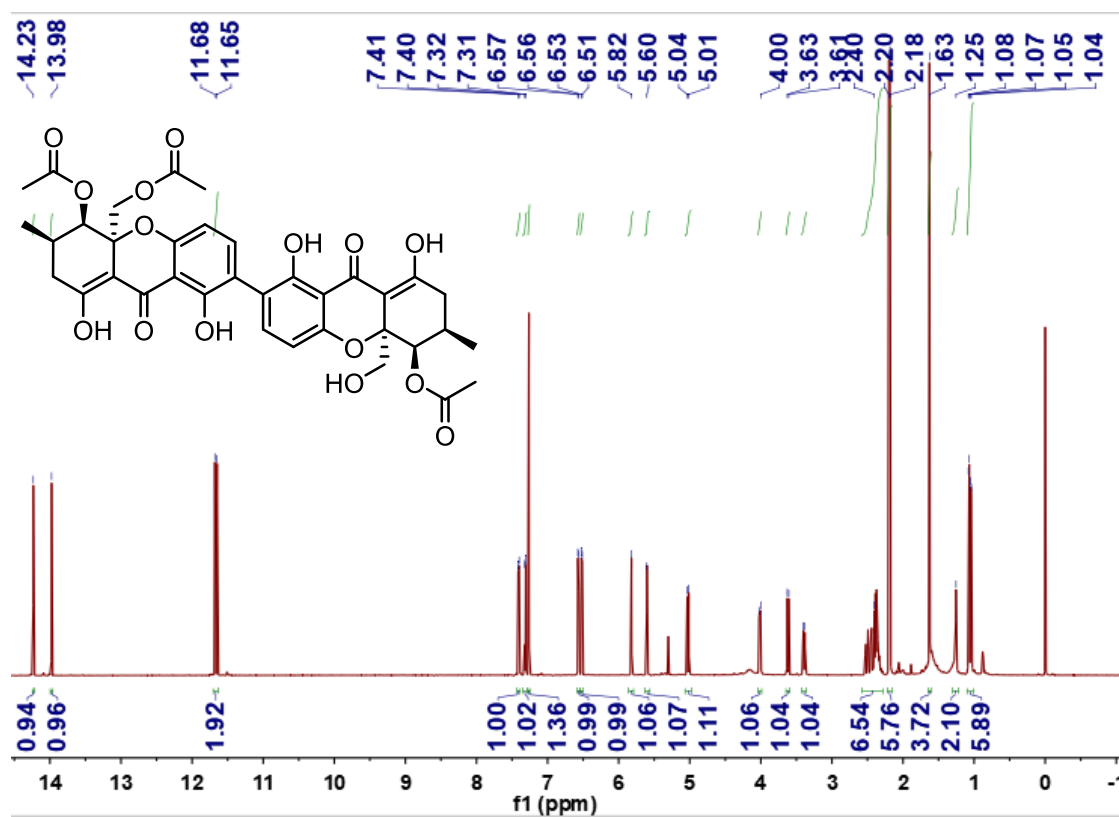


Figure S28. ^1H -NMR spectrum (600 MHz, CHCl_3) of Dicerandrol B (5)

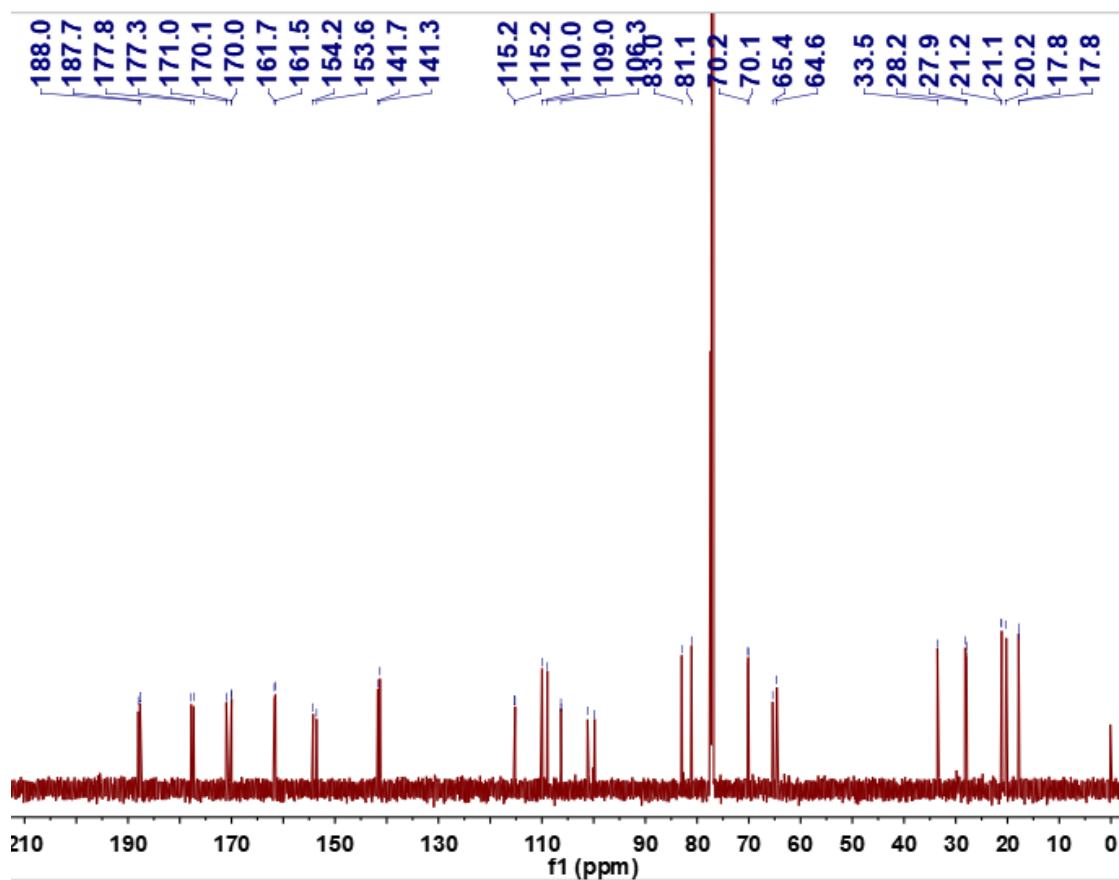


Figure S29. ^{13}C -NMR spectrum (150 MHz, CHCl_3) of Dicerandrol B (5)

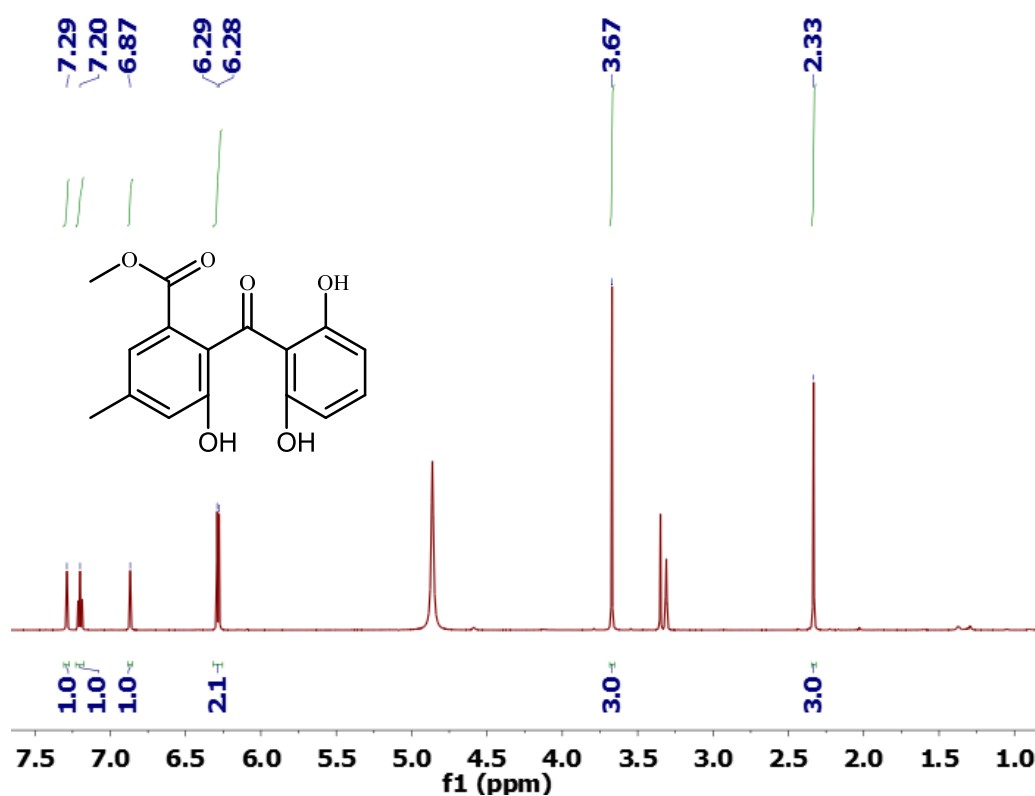


Figure S30. ¹H-NMR spectrum (600 MHz, CD₃OD) of 2,2',6'-trihydroxy-4-methyl-6-methoxy-acyl-diphenylmethanone (6)

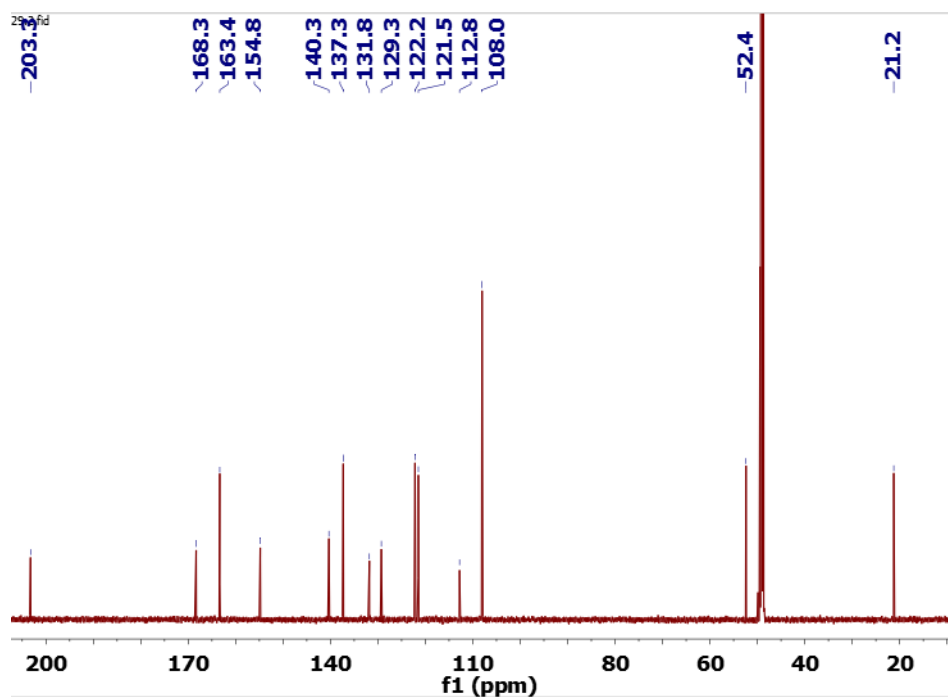


Figure S31. ¹³C-NMR spectrum (150 MHz, CD₃OD) of 2,2',6'-trihydroxy-4-methyl-6-methoxy-acyl-diphenylmethanone (6)

Table S1. Energy analysis for the Conformers of **1a** (**1**).

Compounds	CONFORMATION	E (Hartree)	E (Kcal/mol)	rel.E (Kcal/mol)	Boltzmann Dist (%)
1a	1a-1	-957.4240435	-600786.3638	0	76.40%
	1a-2	-957.42160243	-600784.832	1.531751521	5.75%
	1a-3	-957.42259761	-600785.4565	0.90727695	16.51%
	1a-4	-957.42023030	-600783.971	2.392771468	1.34%

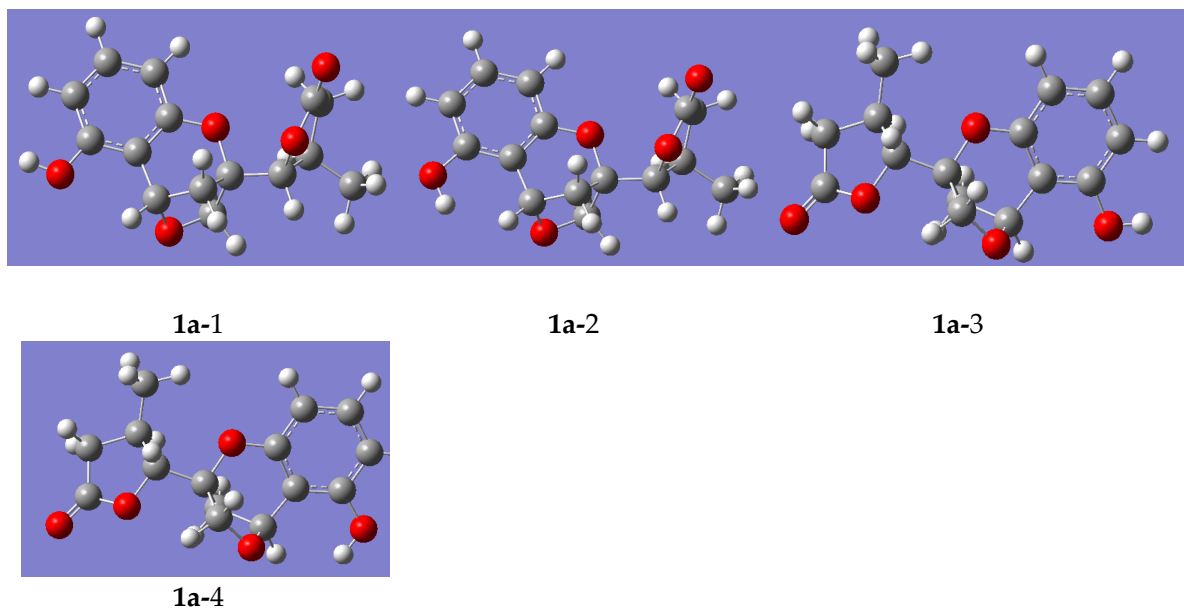


Figure S32. B3LYP/6-31G(d,p) optimized low-energy conformers of **1a** (**1**)

Table S2. Energy analysis for the Conformers of **1b** (**1**).

Compounds	Conformation	E (Hartree)	E (Kcal/mol)	rel.E (Kcal/mol)	Boltzmann Dist (%)
1b	1b-1	-957.4240957	-600786.3966	0	76.65%
	1b-2	-957.42169738	-600784.8916	1.50497911	6.03%
	1b-3	-957.42261675	-600785.4685	0.928069259	15.99%
	1b-4	-957.42027066	-600783.9964	2.400248793	1.33%

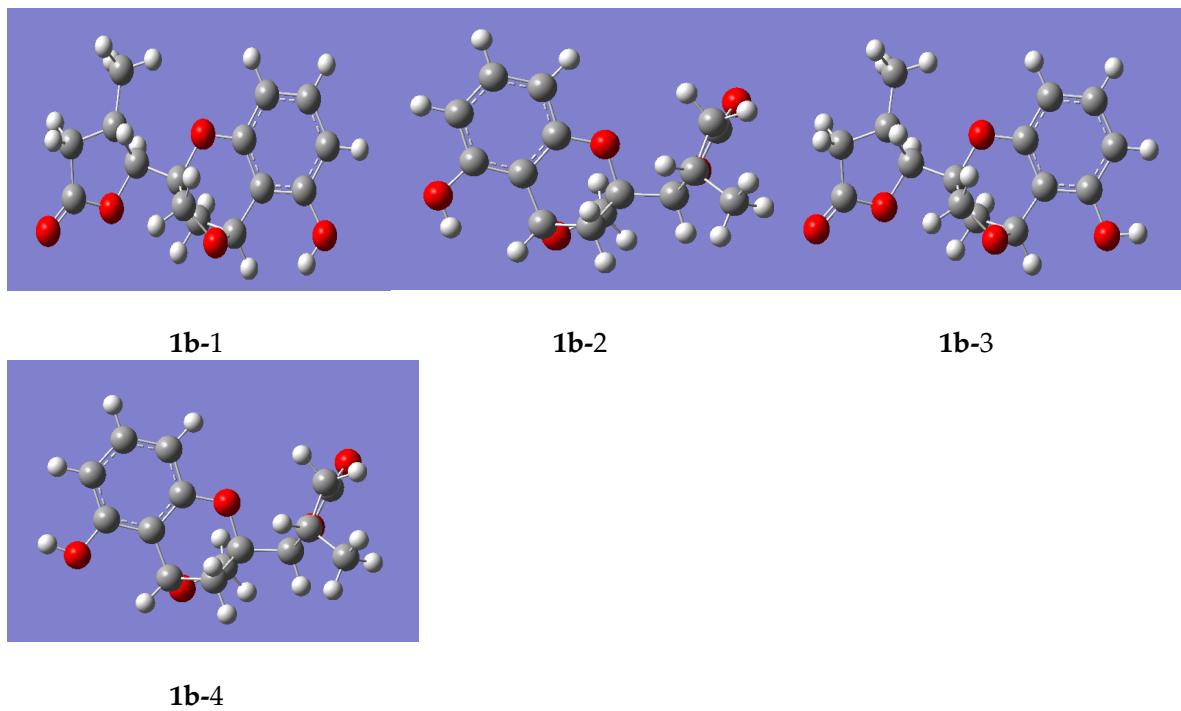


Figure S33. B3LYP/6-31G(d,p) optimized low-energy conformers of **1b** (**1**)