

Electronic supplementary information (ESI)

Vulgarisin-type diterpenoids from self-heal (*Prunella vulgaris*) and their neuroprotective effects against ischemia/reperfusion (I/R) via mitochondria-related pathway

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Fig. S75 HRMS spectrum of tentatively identified compound dehydrotrameternic acid (Mw=454)

Table S1 Chemical profile of *P. vulgaris*

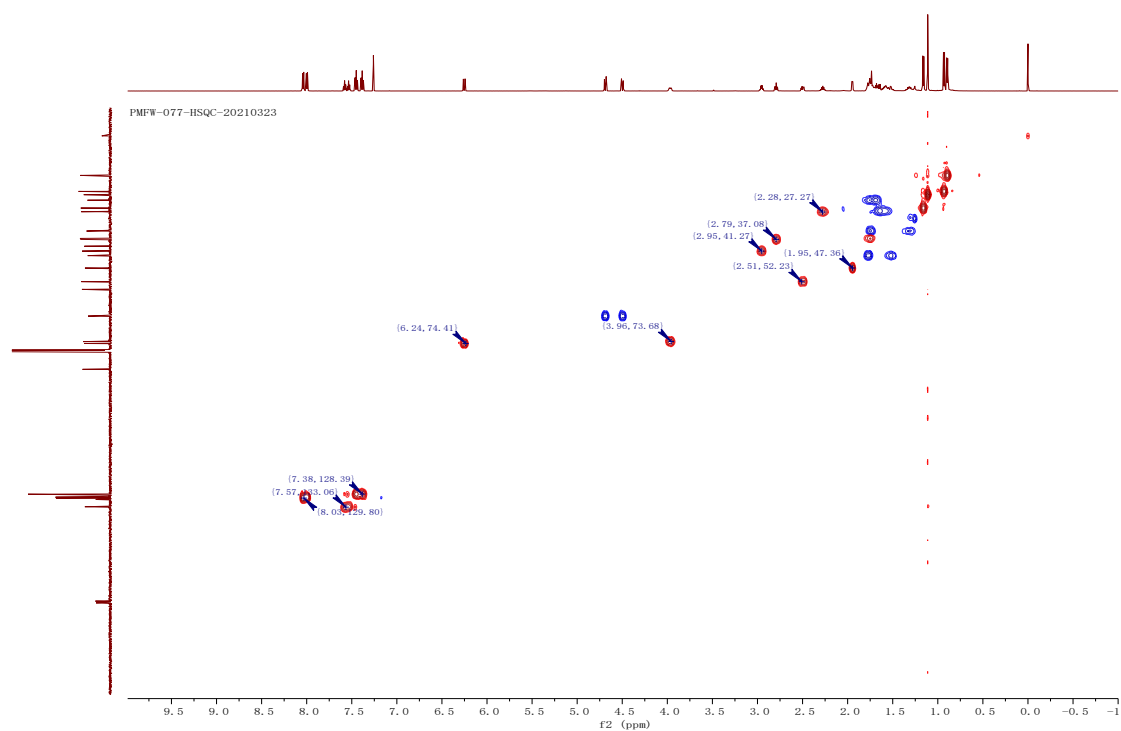


Fig. S3 HSQC spectrum of vulgarisin G (1)

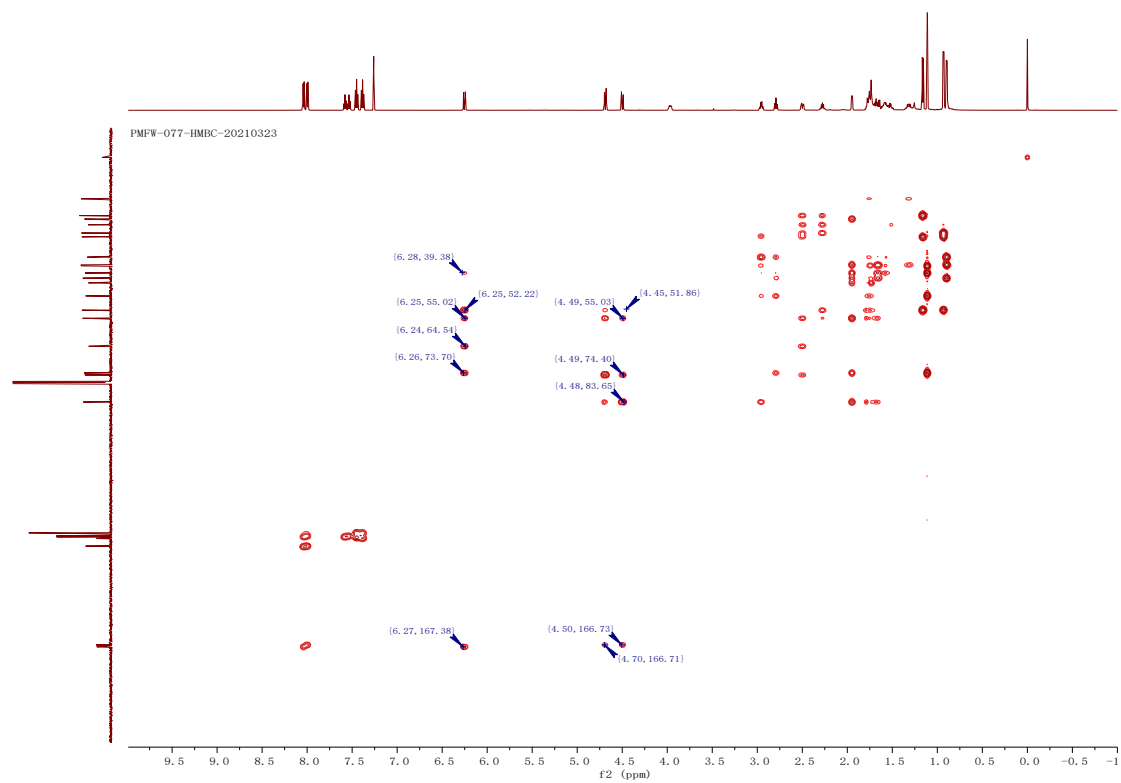


Fig. S4 HMBC spectrum of vulgarisin G (1)

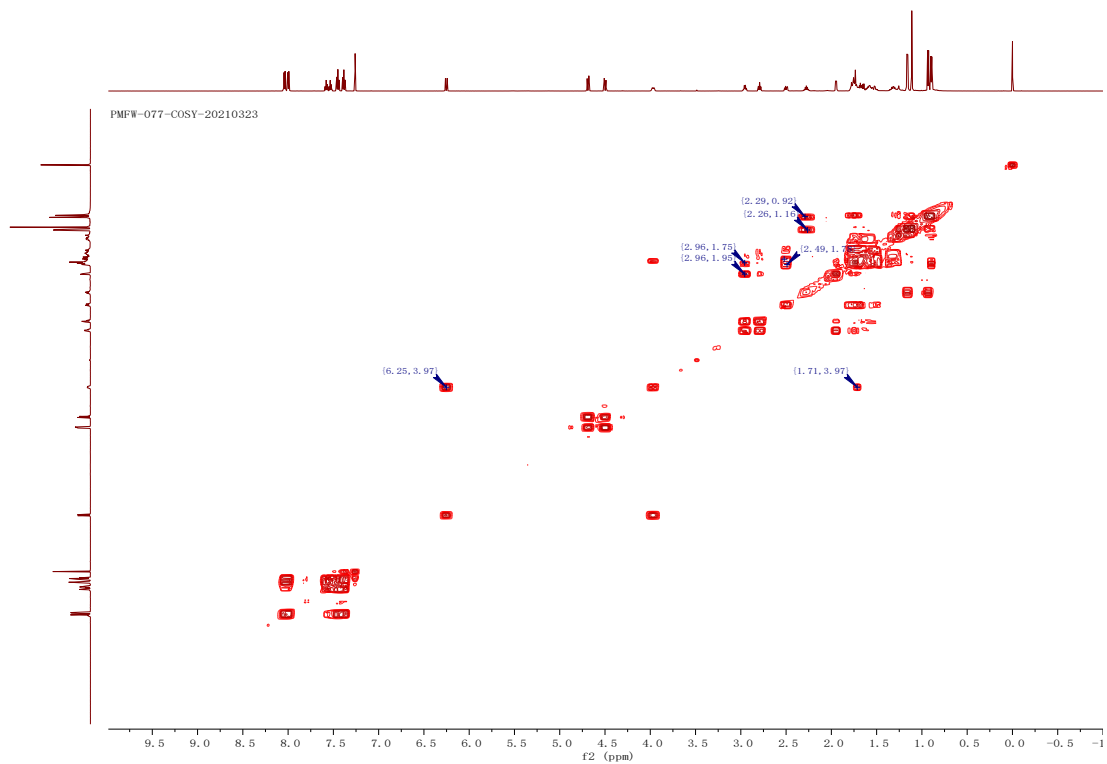


Fig. S5 ^1H - ^1H COSY spectrum of vulgarisin G (**1**)

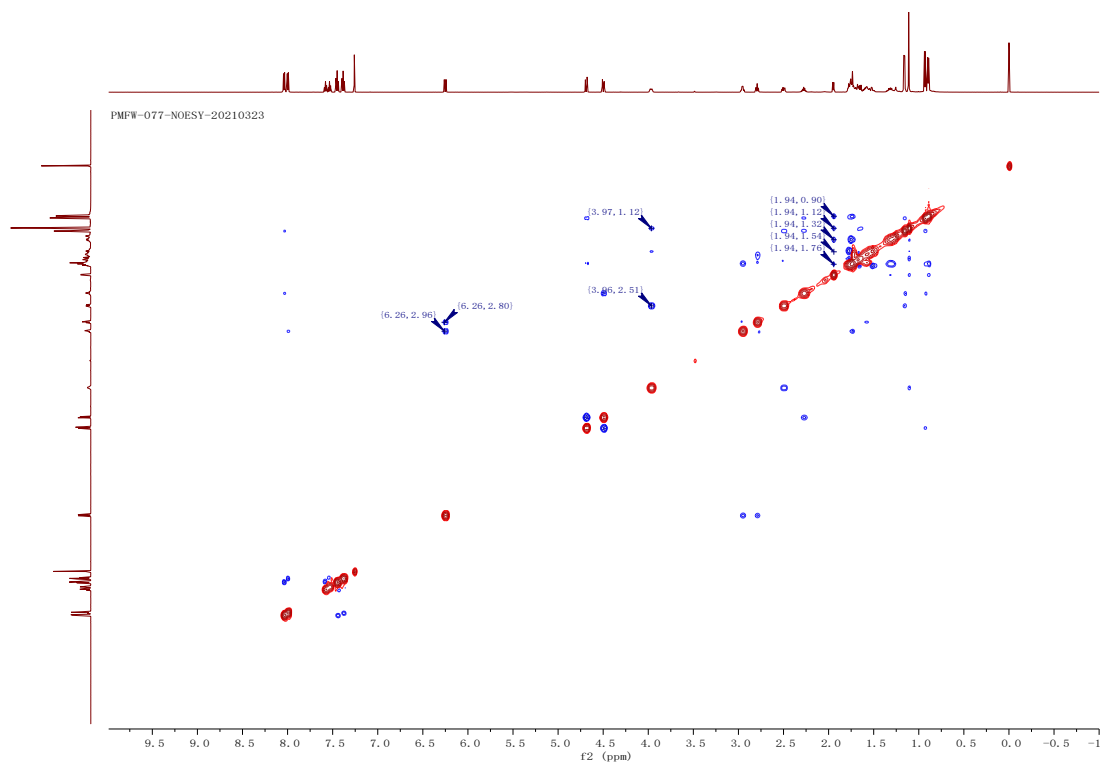


Fig. S6 NOESY spectrum of vulgarisin G (**1**)

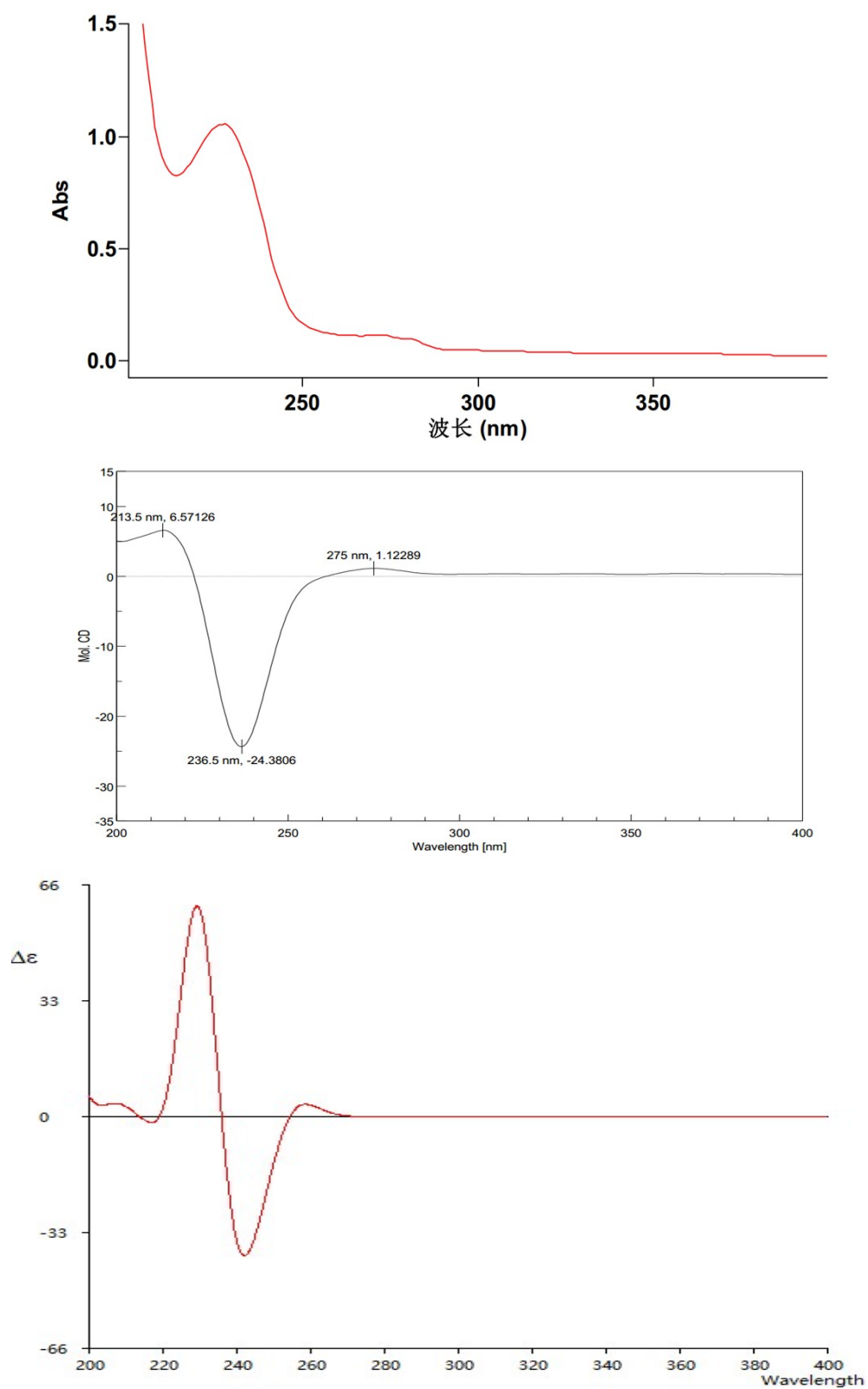
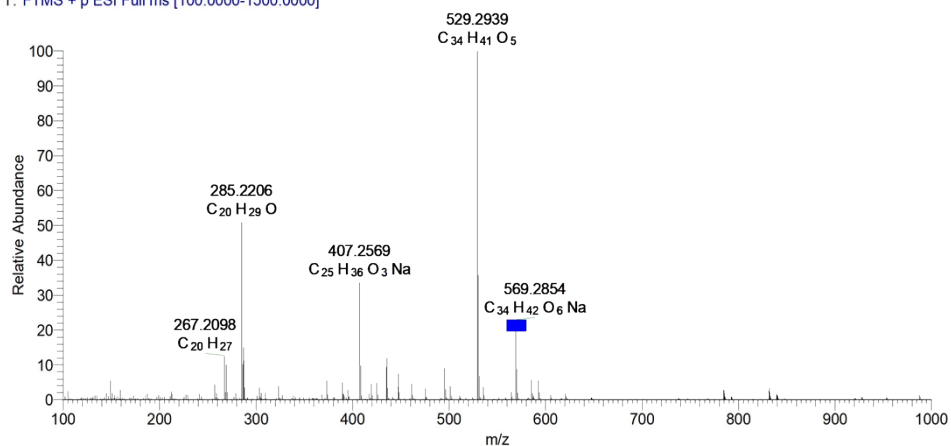


Fig. S7 UV and CD spectra (experimental and calculated) of vulgarisin G (1)

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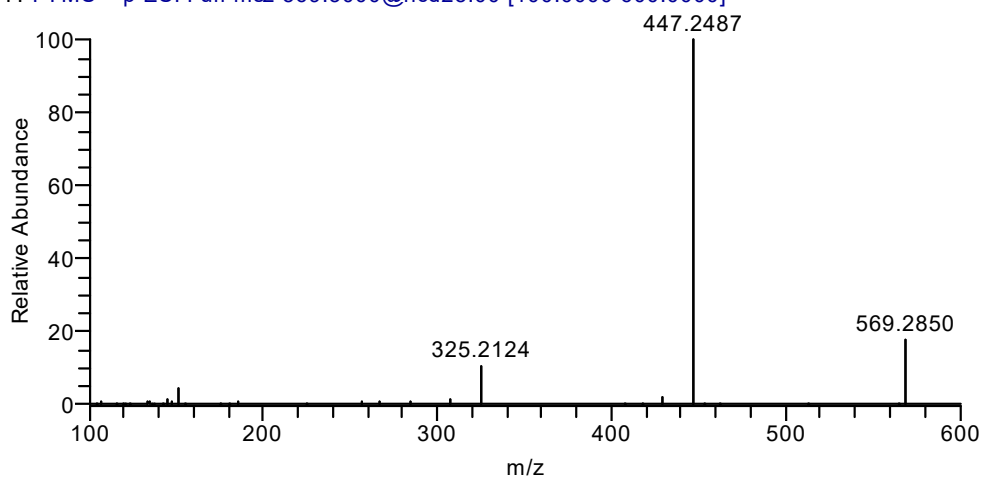


Fig. S8 MS and MS² spectra of vulgarisin G (1)

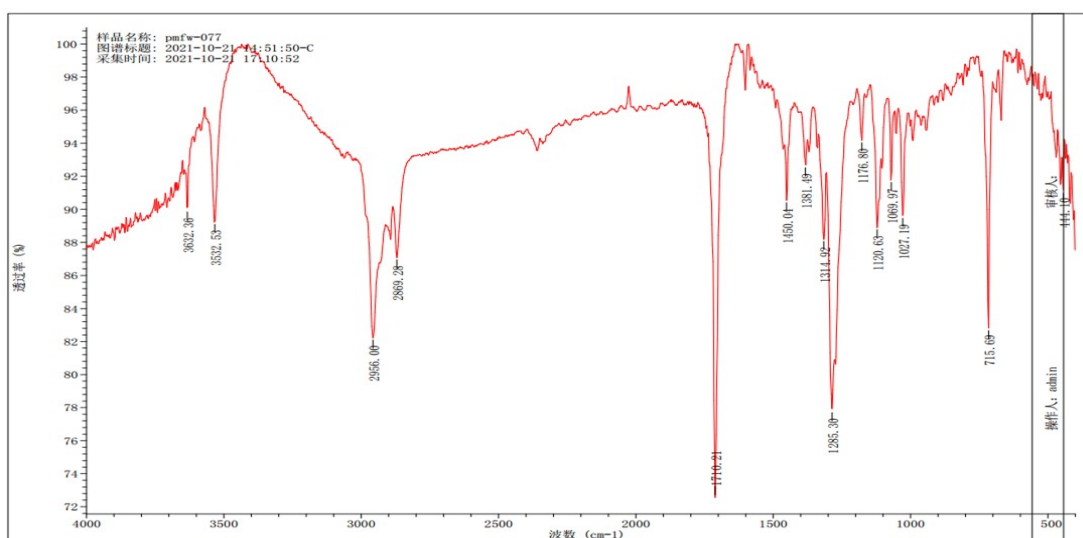


Fig. S9 FT-IR spectrum of vulgarisin G (1)

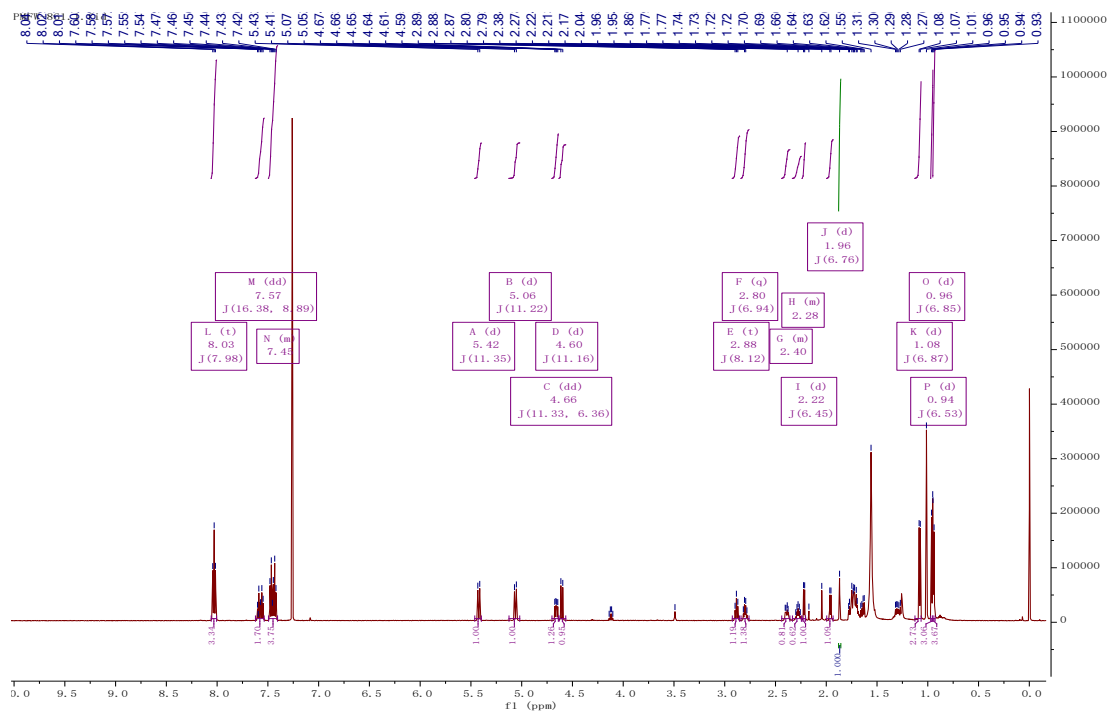


Fig. S10 ^1H NMR spectrum of vulgarisin H (2)

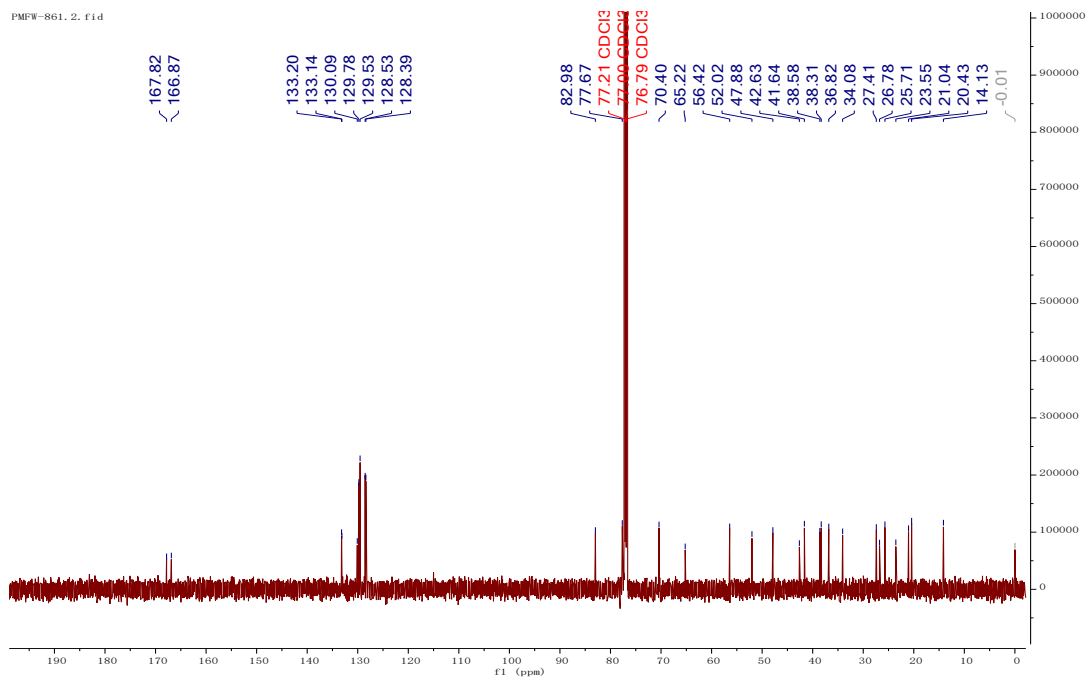


Fig. S11 ^{13}C NMR spectrum of vulgarisin H (2)

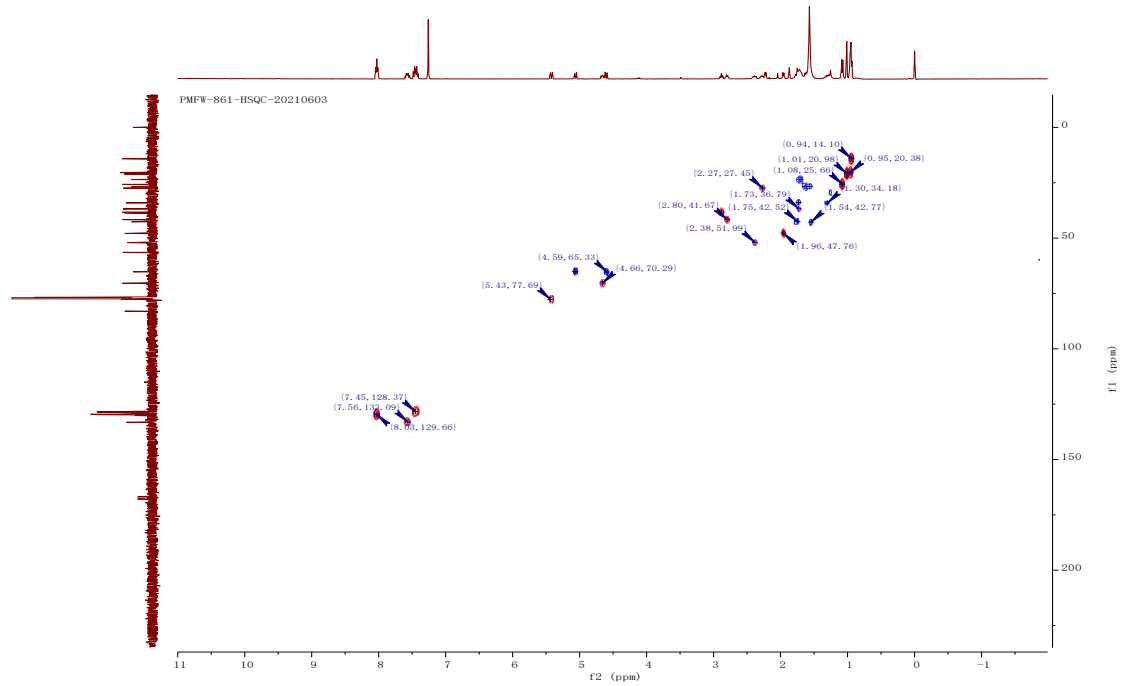


Fig. S12 HSQC spectrum of vulgarisin H (2)

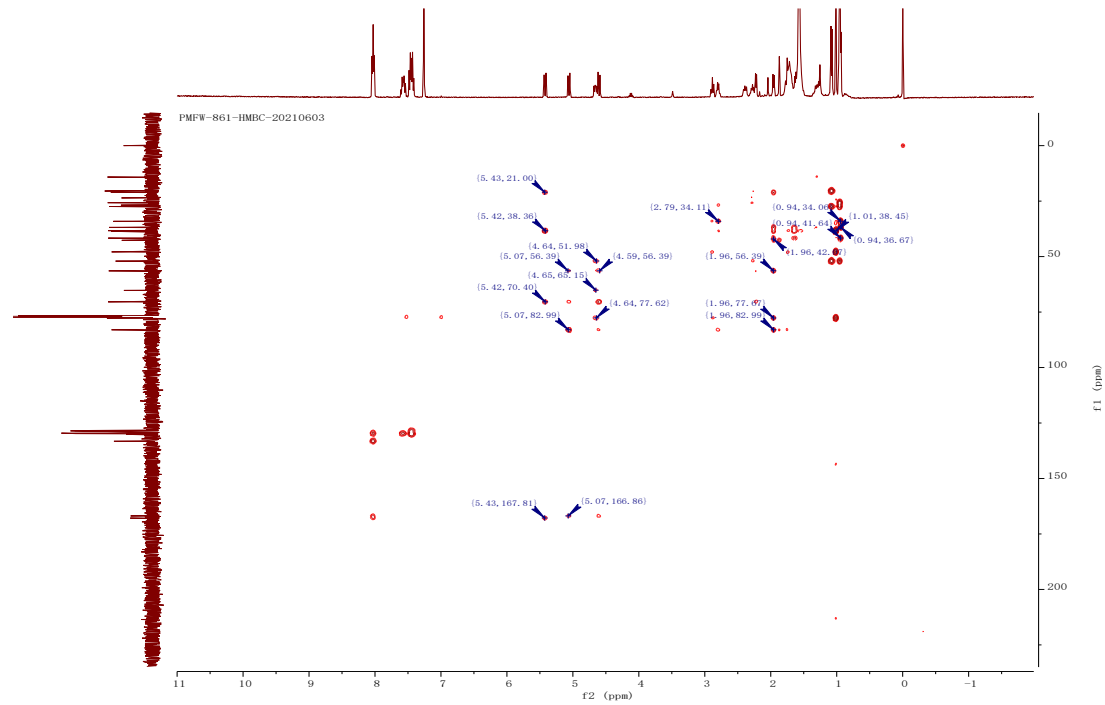


Fig. S13 HMBC spectrum of vulgarisin H (2)

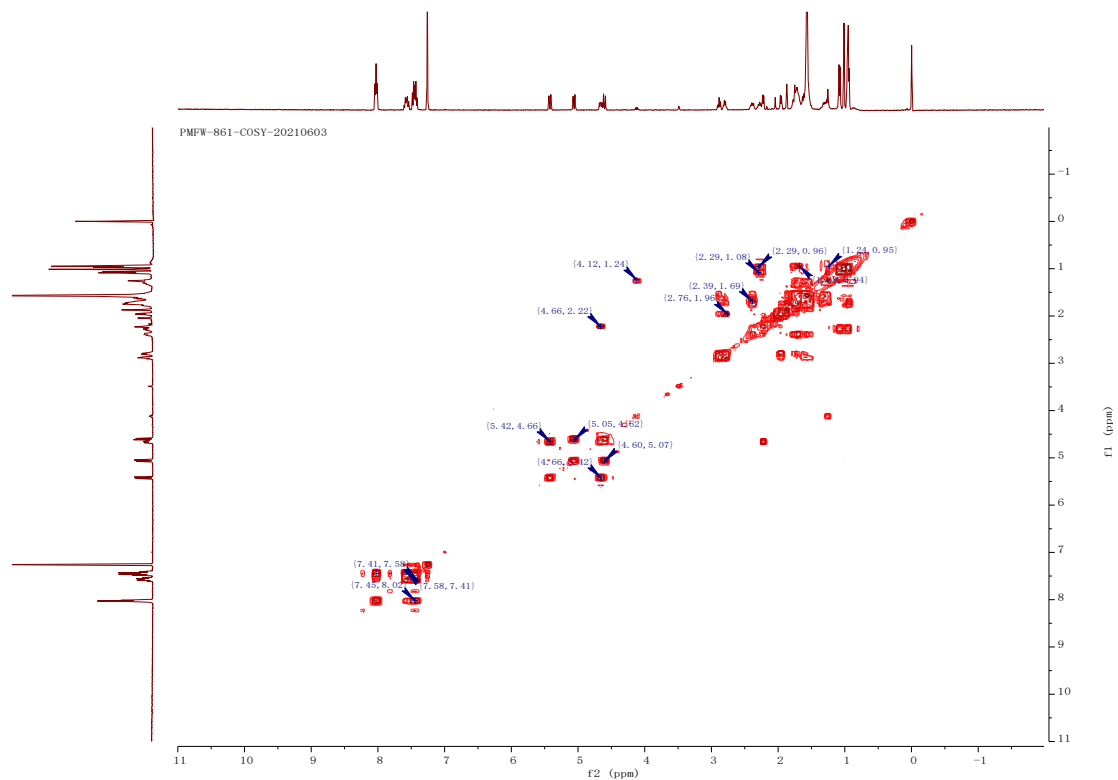


Fig. S14 ^1H - ^1H COSY spectrum of vulgarisin H (2)

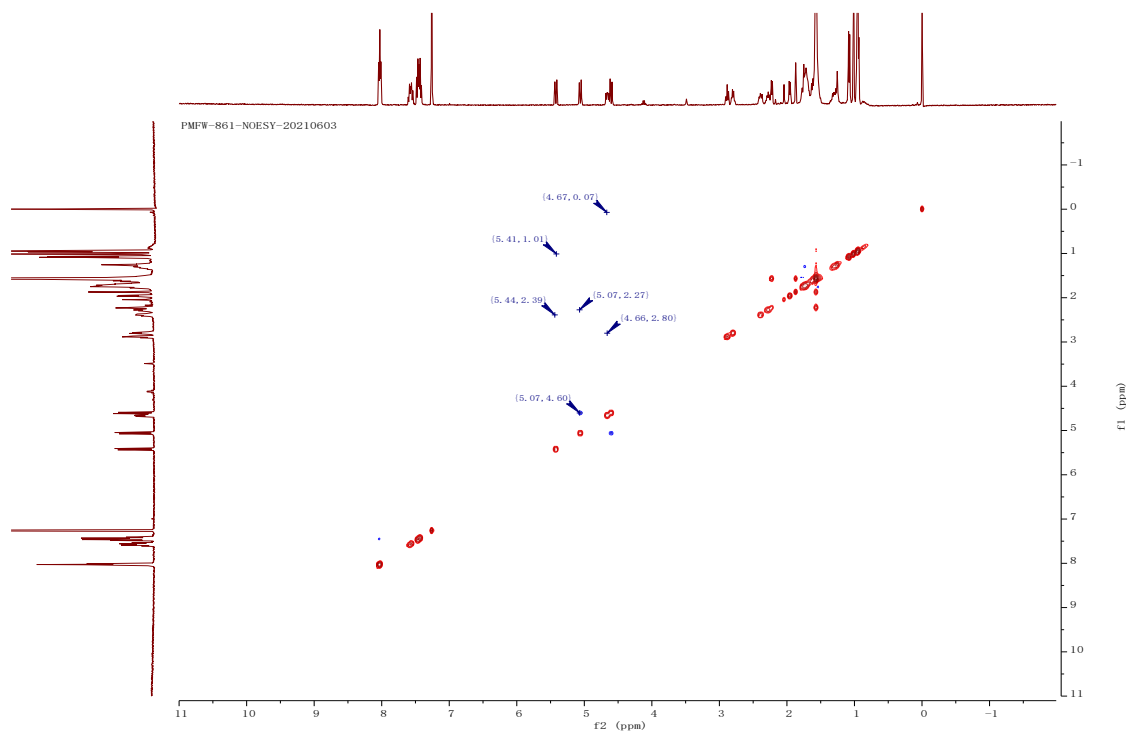


Fig. S15 NOESY spectrum of vulgarisin H (2)

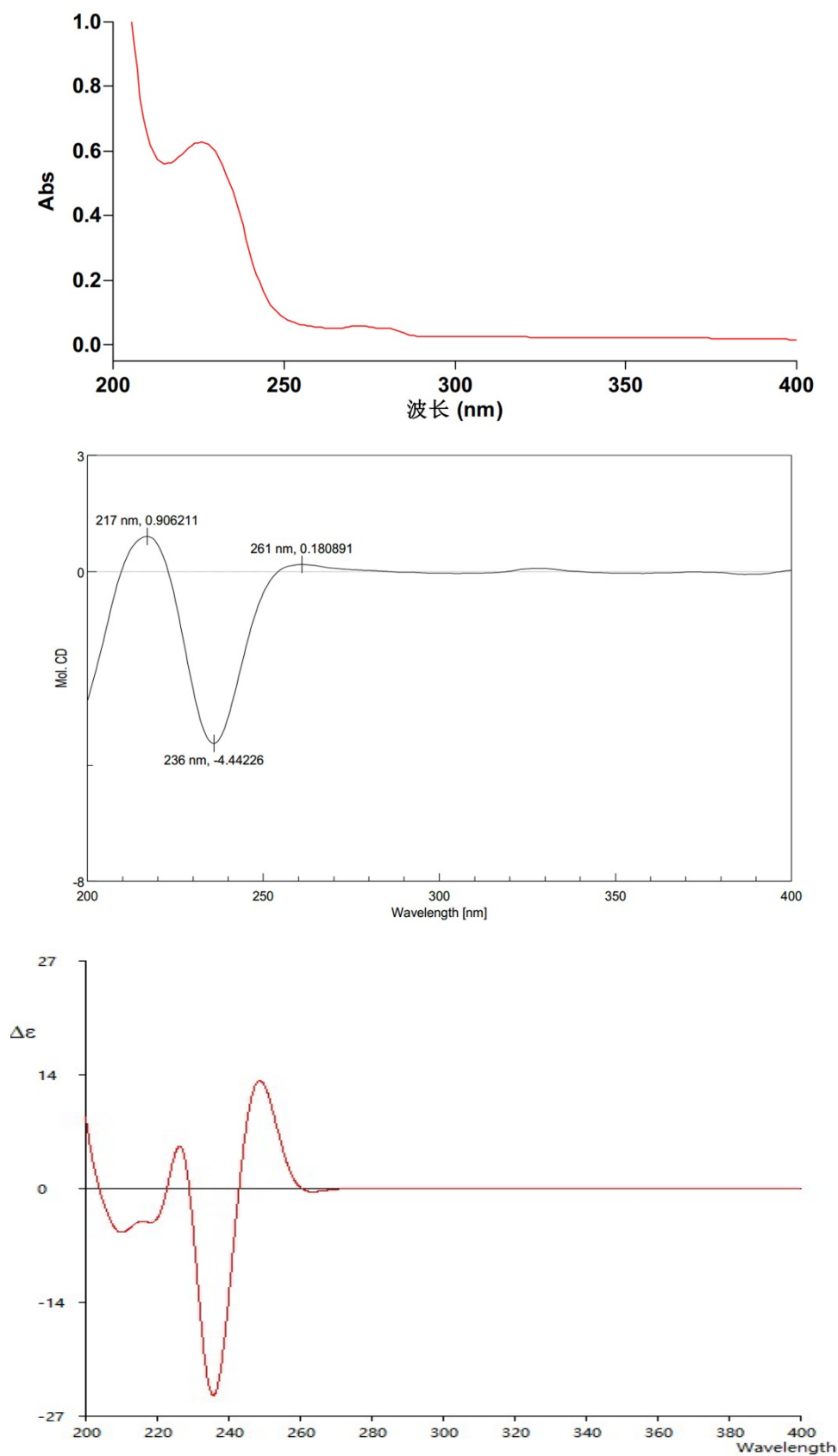
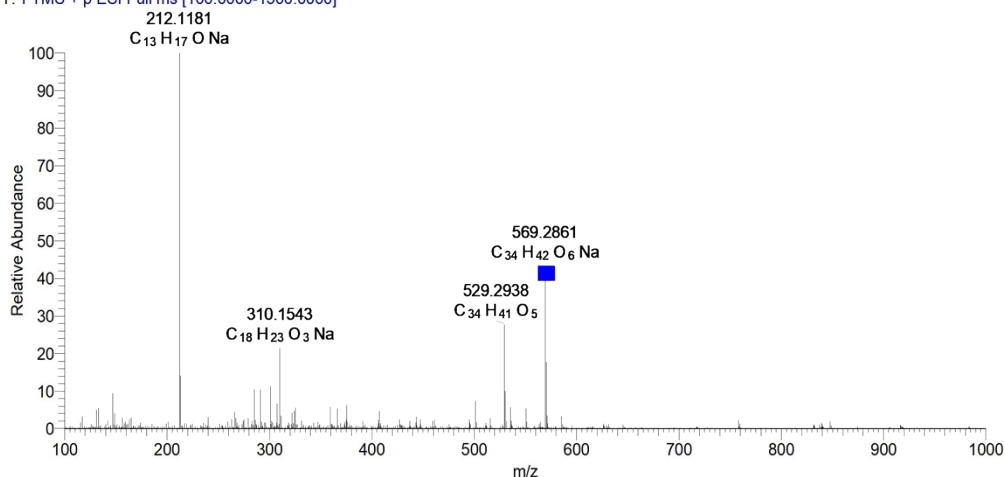


Fig. S16 UV and CD spectra (experimental and calculated) of vulgarisin H (2)

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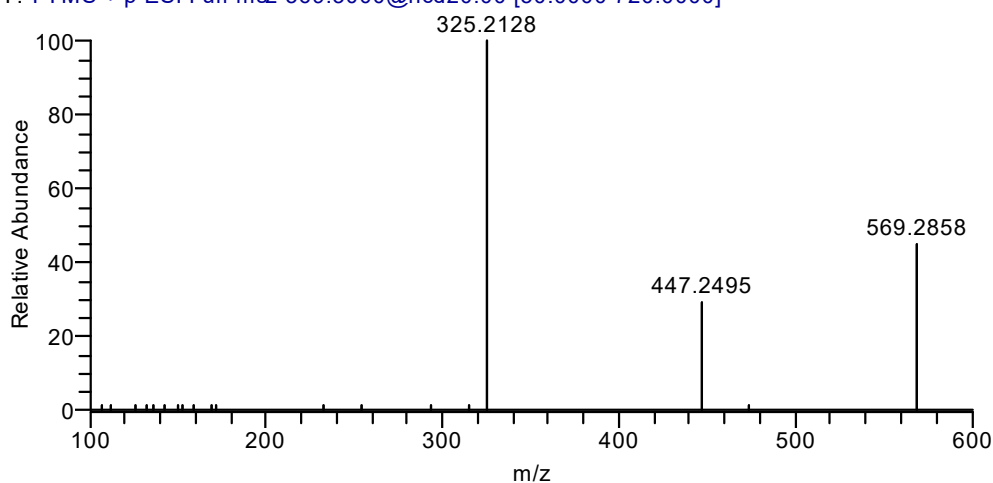


Fig. S17 MS and MS² spectra of vulgarisin H (2)

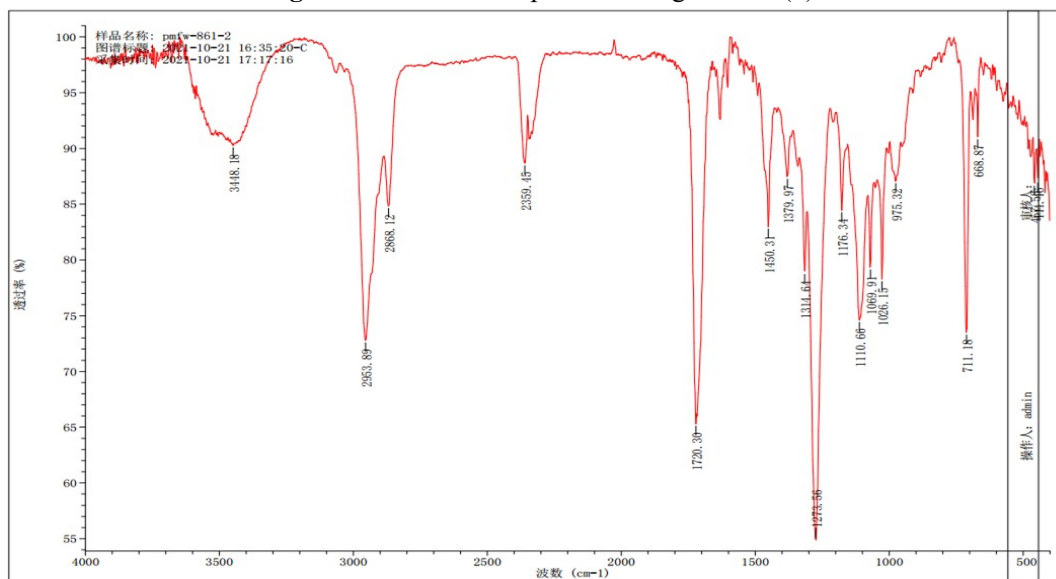


Fig. S18 FT-IR spectrum of vulgarisin H (2)

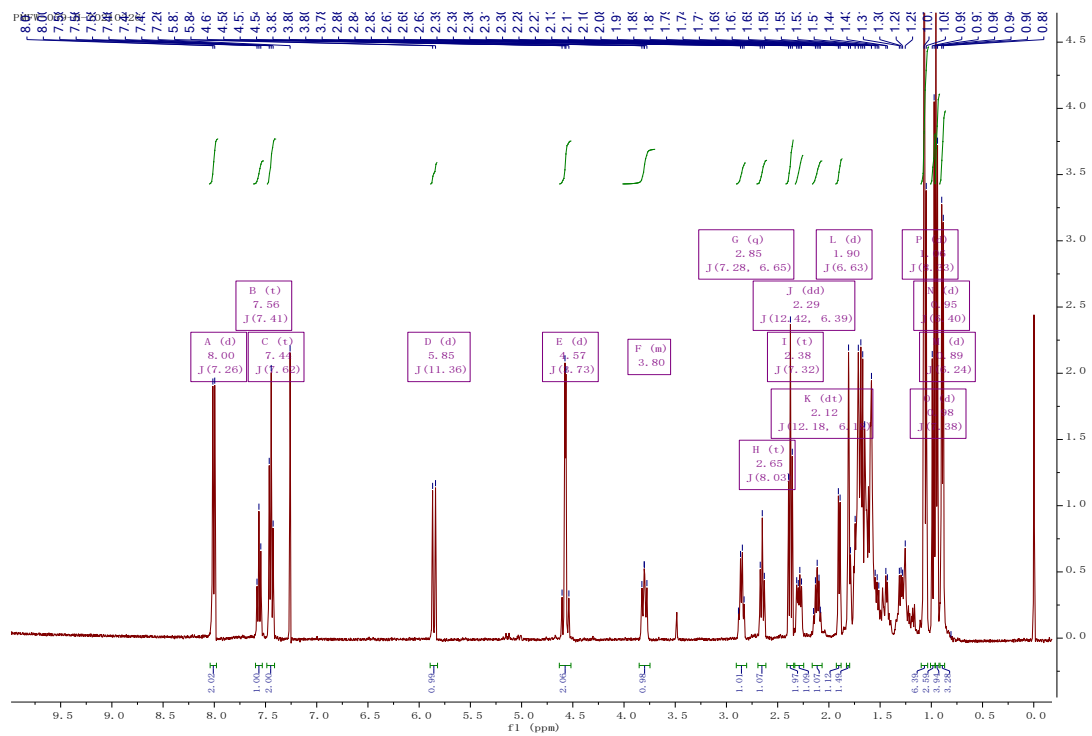


Fig. S19 ¹H NMR spectrum of vulgarisin I (**3**)

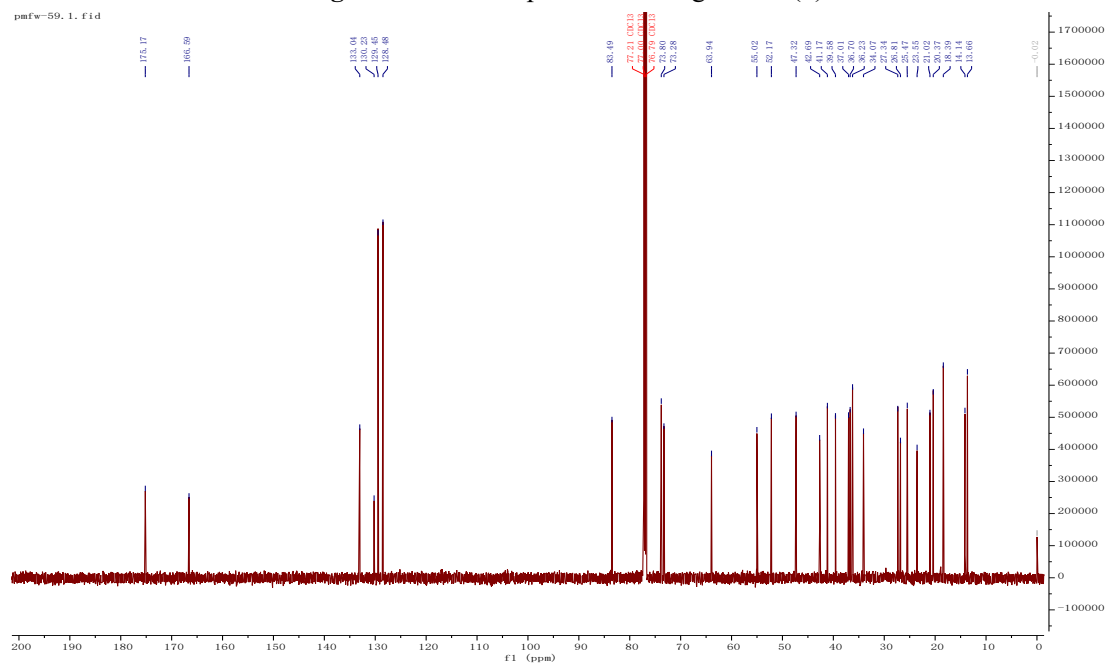


Fig. S20 ¹³C NMR spectrum of vulgarisin I (**3**)

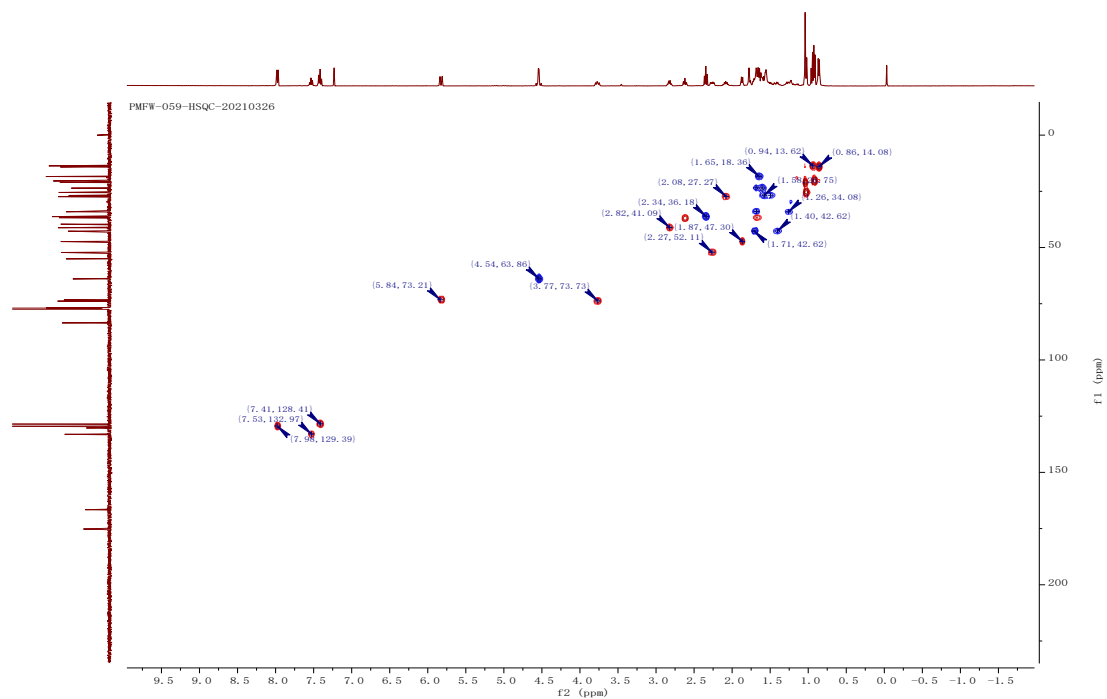


Fig. S21 HSQC spectrum of vulgarisin I (3)

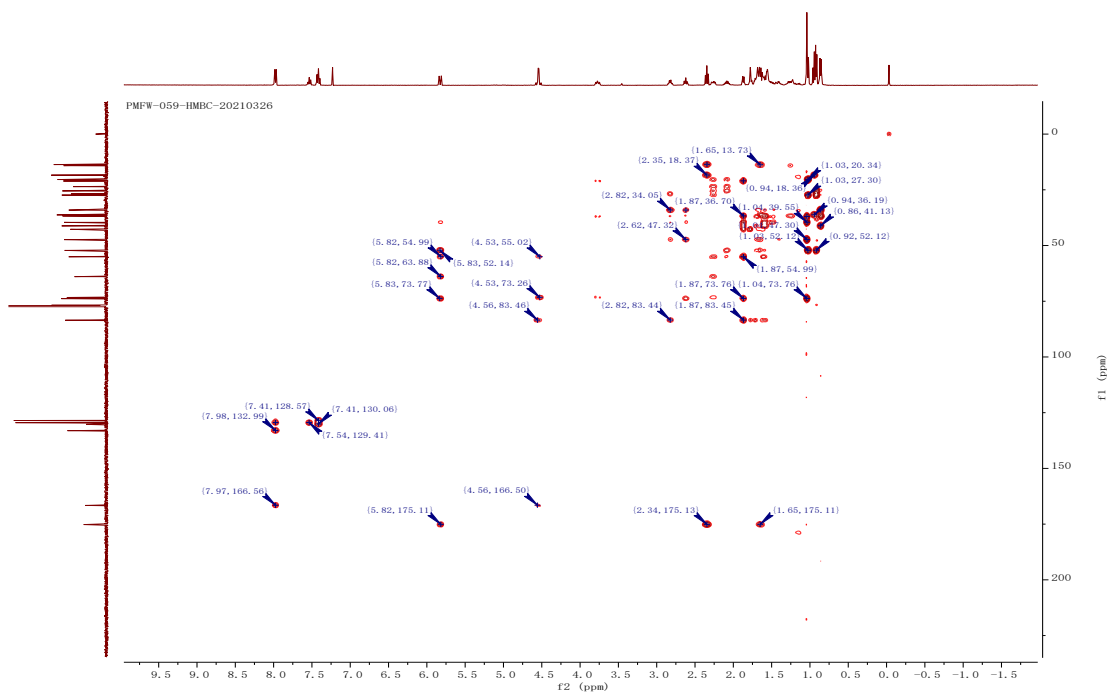


Fig. S22 HMBC spectrum of vulgarisin I (3)

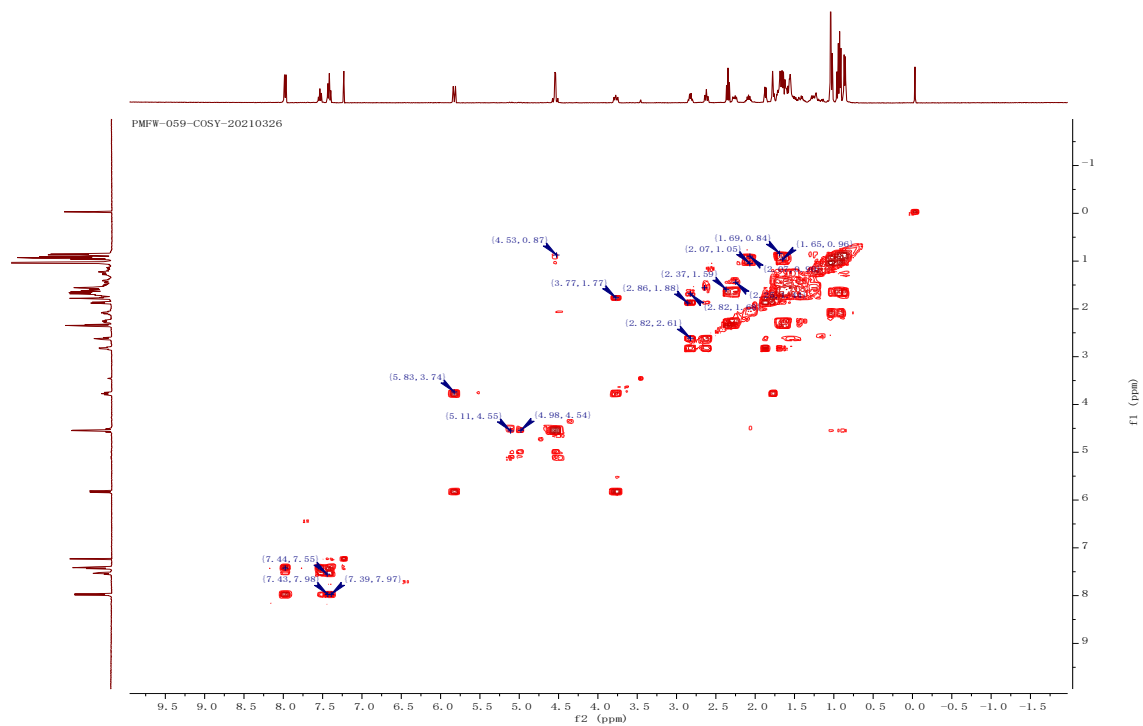


Fig. S23 ^1H - ^1H COSY spectrum of vulgarisin I (3)

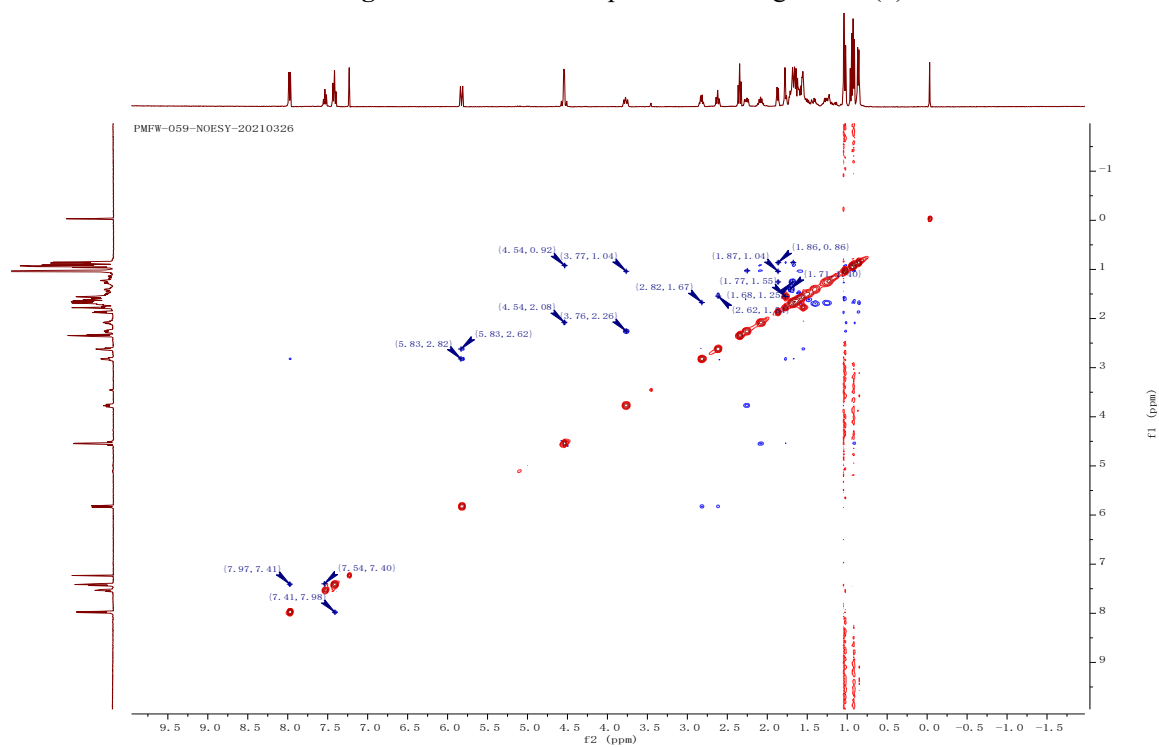


Fig. S24 NOESY spectrum of vulgarisin I (3)

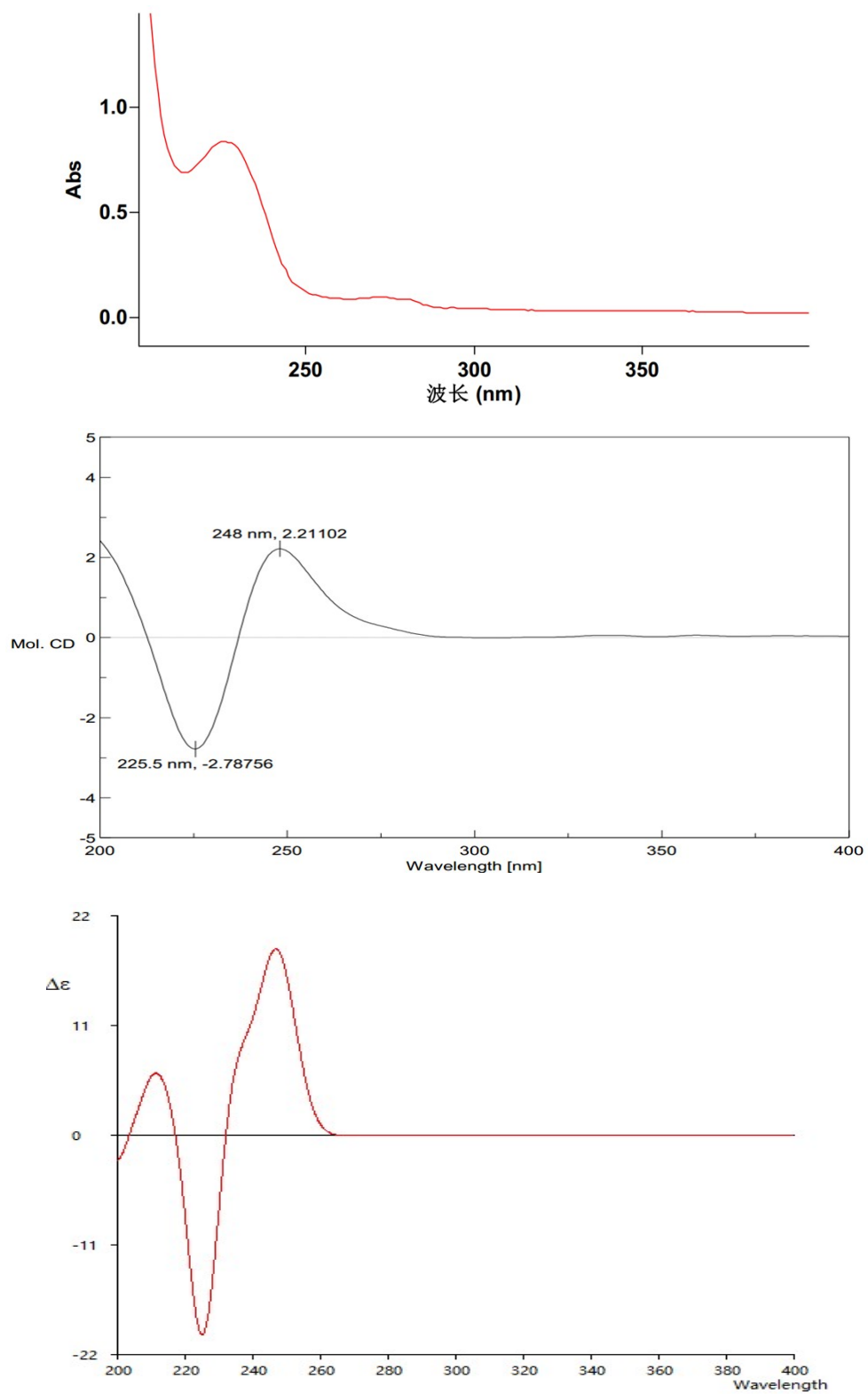


Fig. S25 UV and CD spectra (experimental and calculated) of vulgarisin I (**3**)

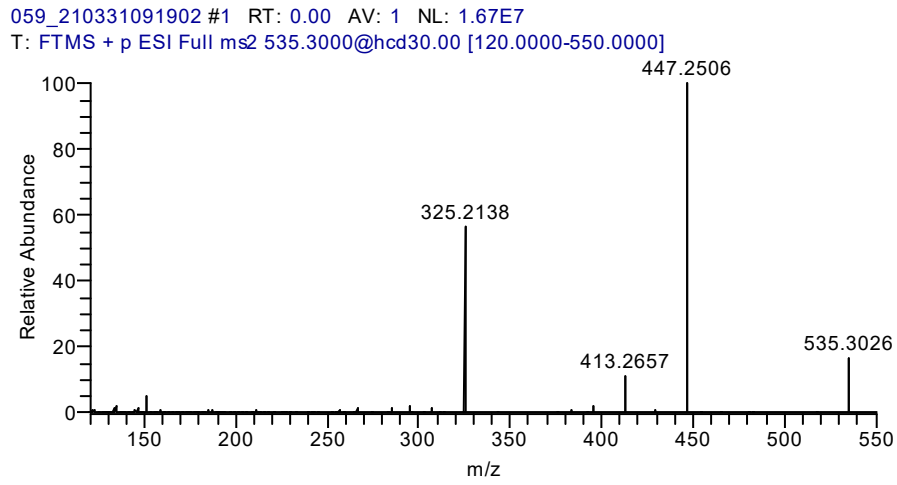
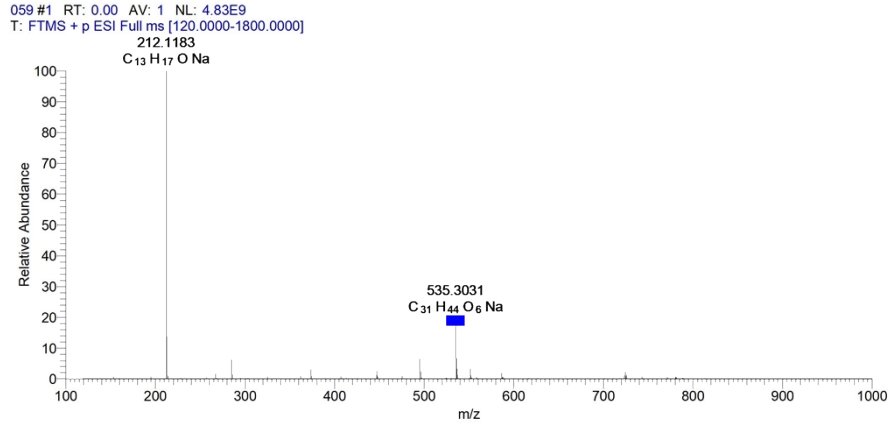


Fig. S26 MS and MS² spectra of vulgarisin I (**3**)

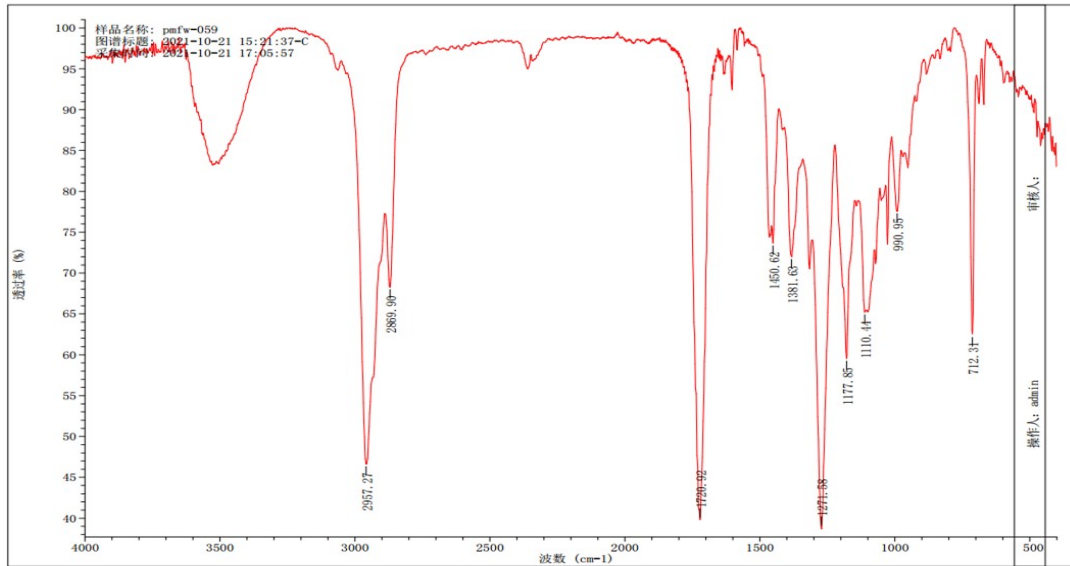


Fig. S27 FT-IR spectrum of vulgarisin I (**3**)

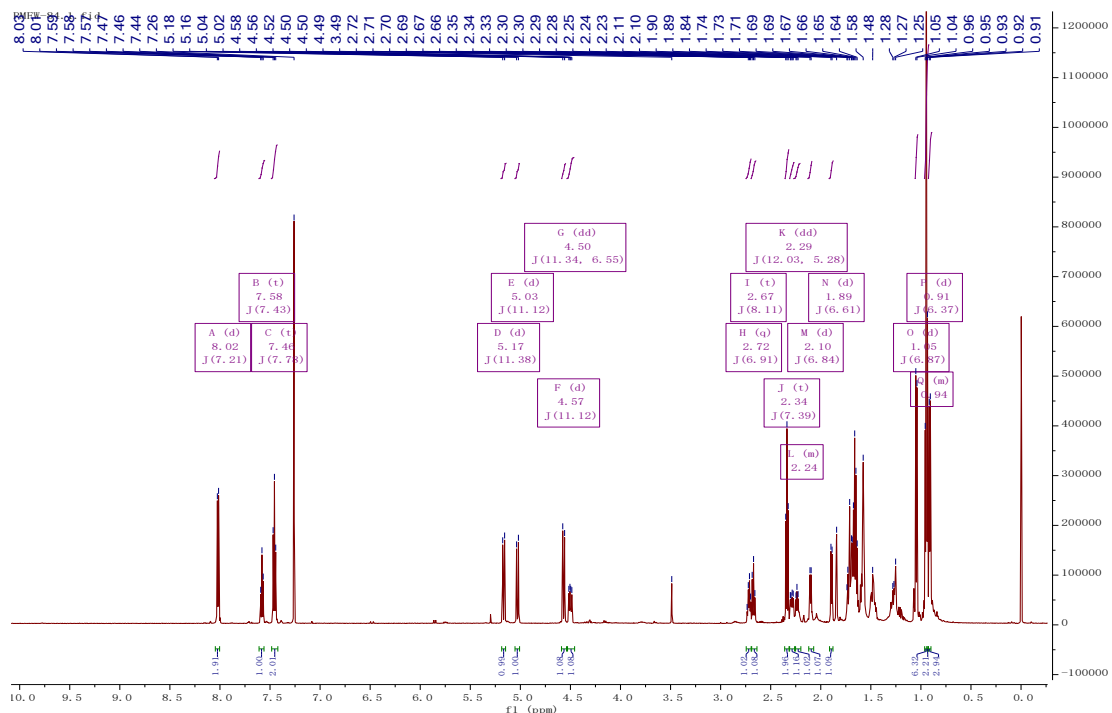


Fig. S28 ¹H NMR spectrum of vulgarisin J (4)

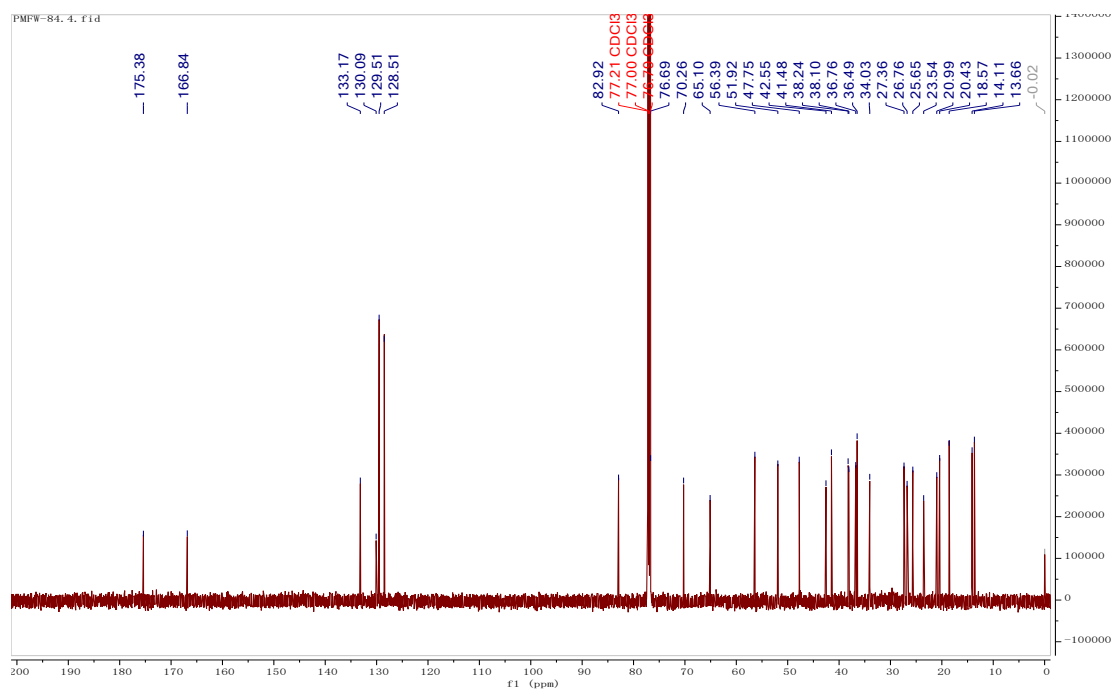


Fig. S29 ¹³C NMR spectrum of vulgarisin J (4)

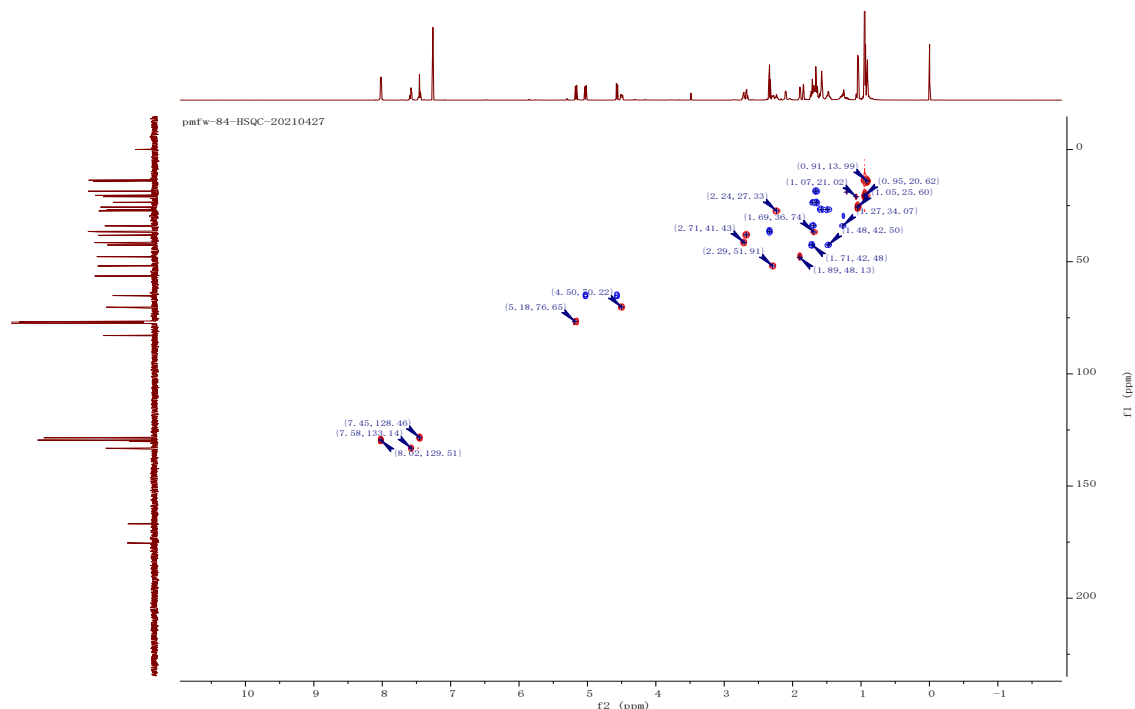


Fig. S30 HSQC spectrum of vulgarisin J (4)

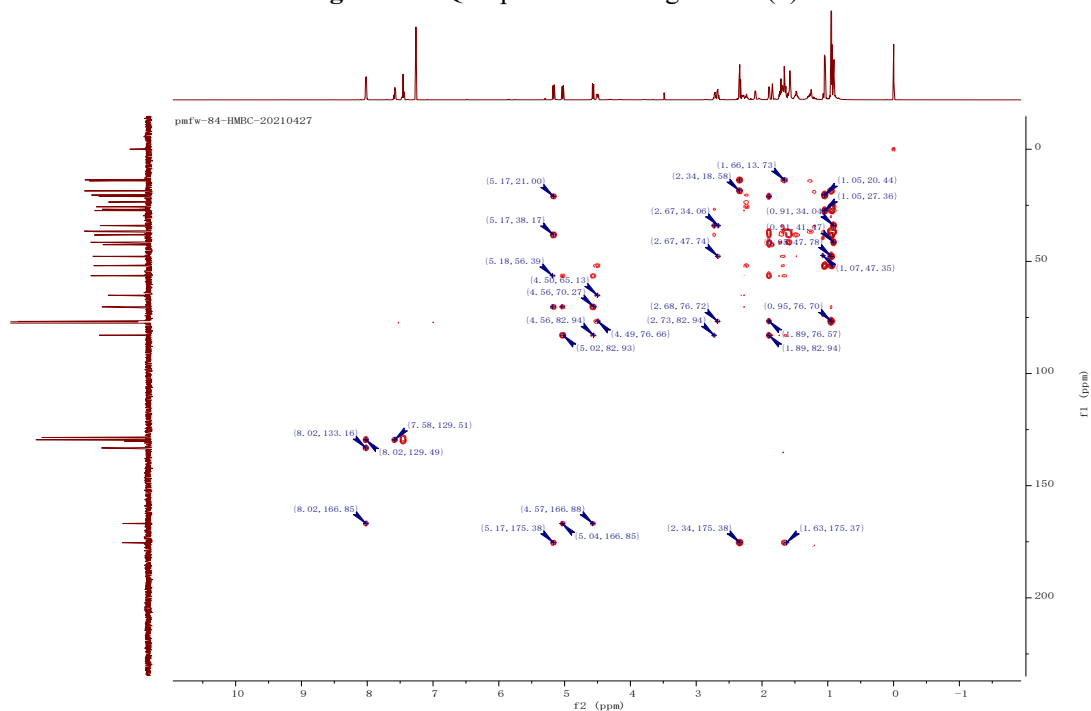


Fig. S31 HMBC spectrum of vulgarisin J (4)

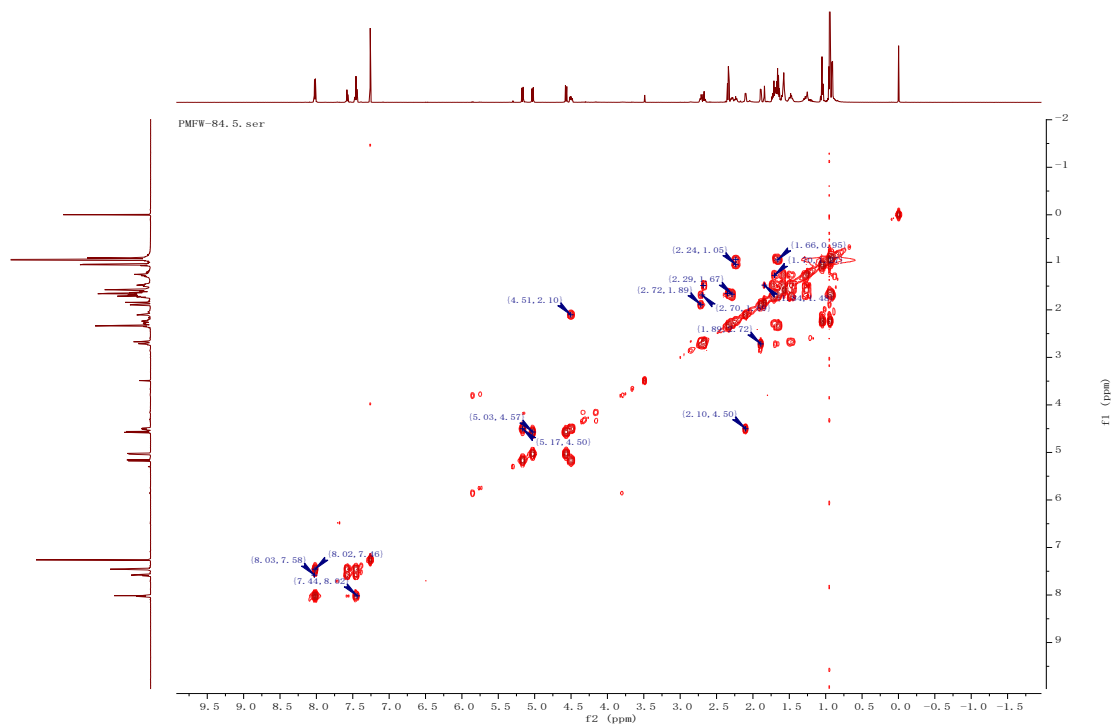


Fig. S32 ^1H - ^1H COSY spectrum of vulgarisin J (4)

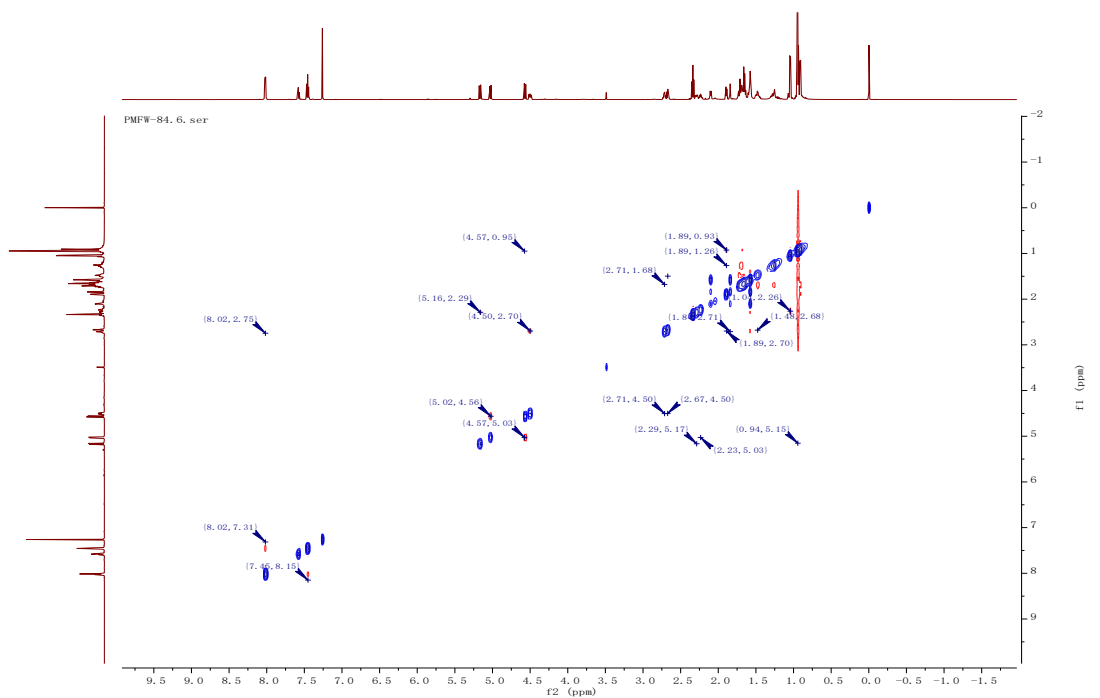


Fig. S33 NOESY spectrum of vulgarisin J (4)

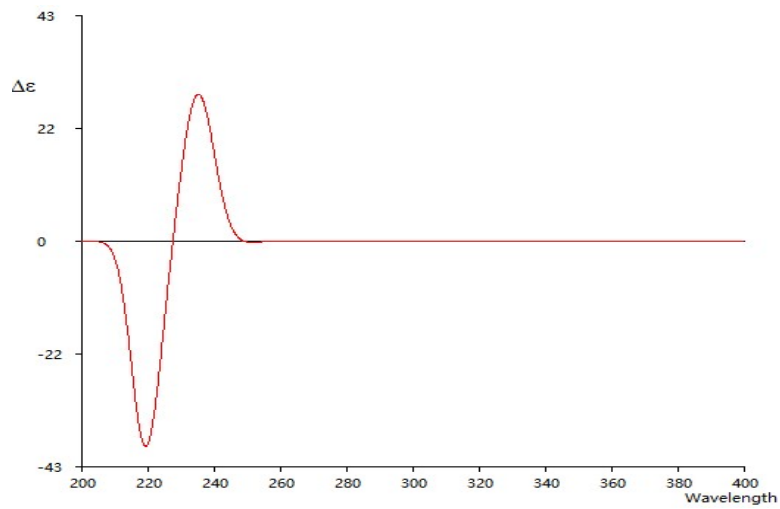
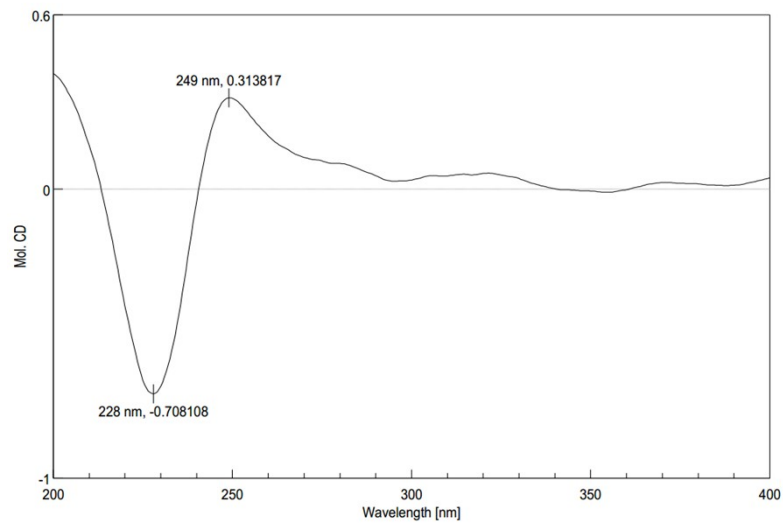
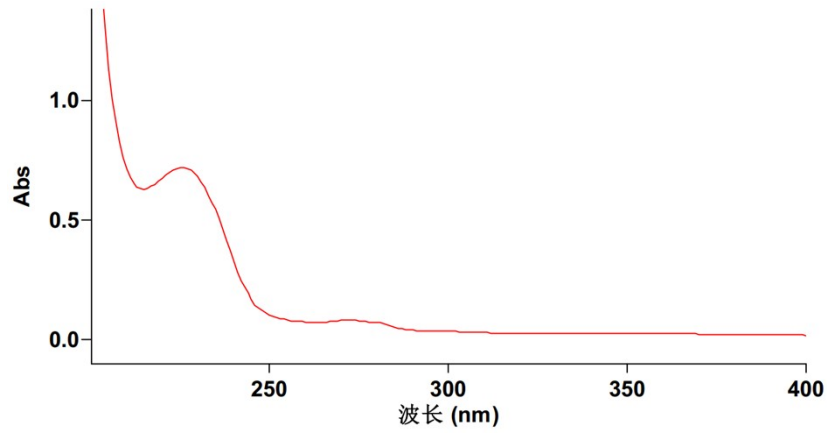
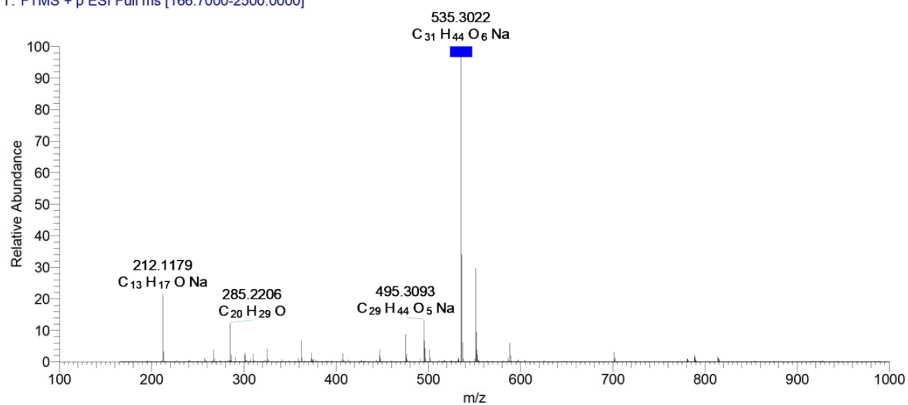


Fig. S34 UV and CD spectra (experimental and calculated) of vulgarisin J (4)

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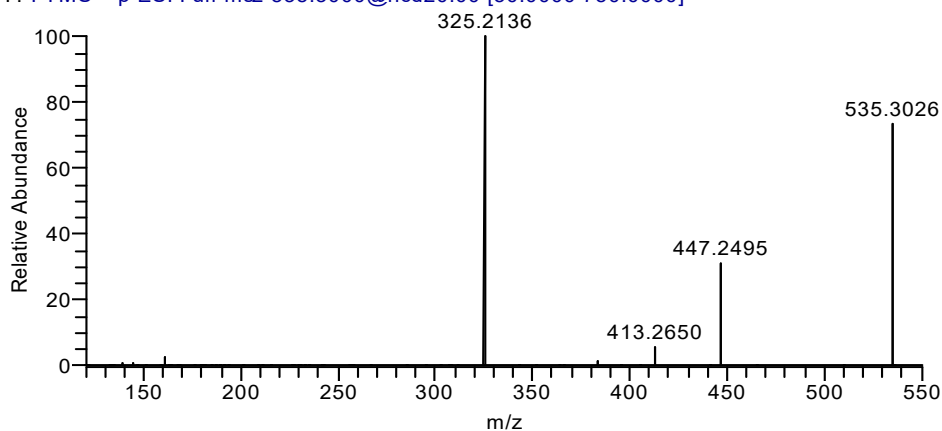


Fig. S35 MS and MS² spectra of vulgarisin J (4)

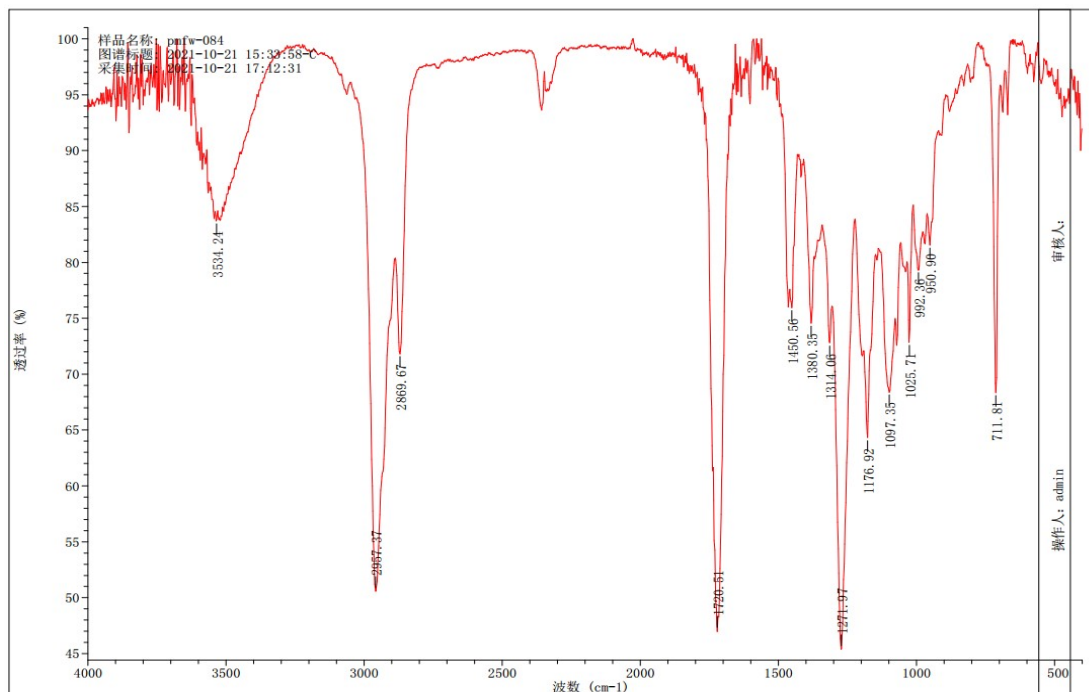


Fig. S36 FT-IR spectrum of vulgarisin J (4)

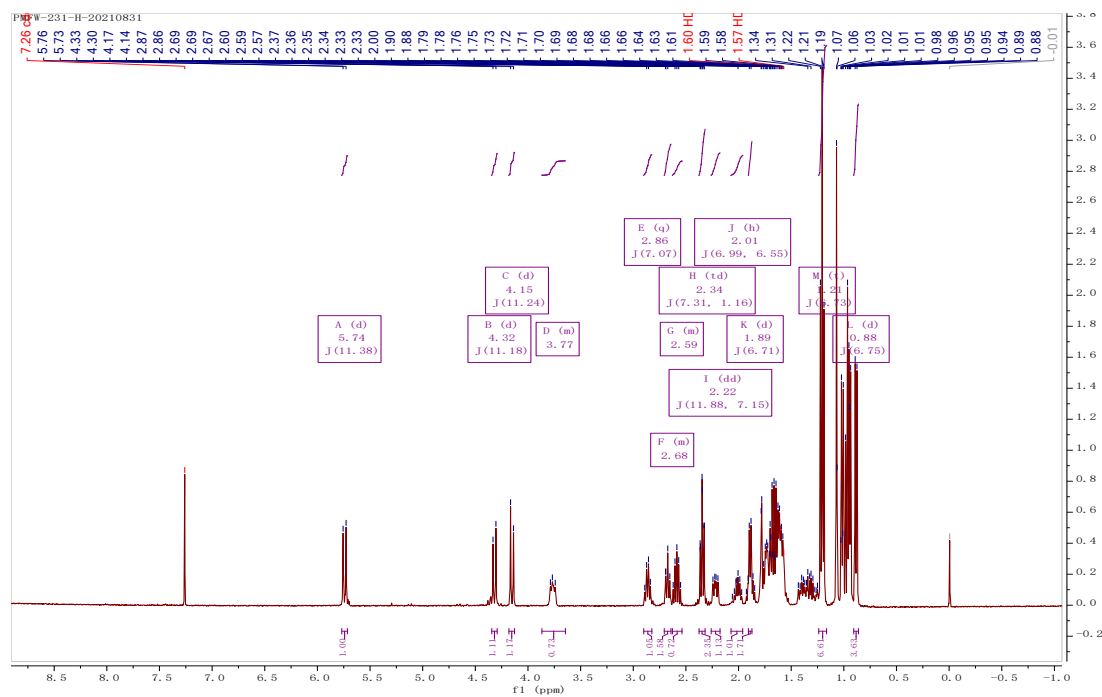


Fig. S37 ¹H NMR spectrum of vulgarisin K (5)

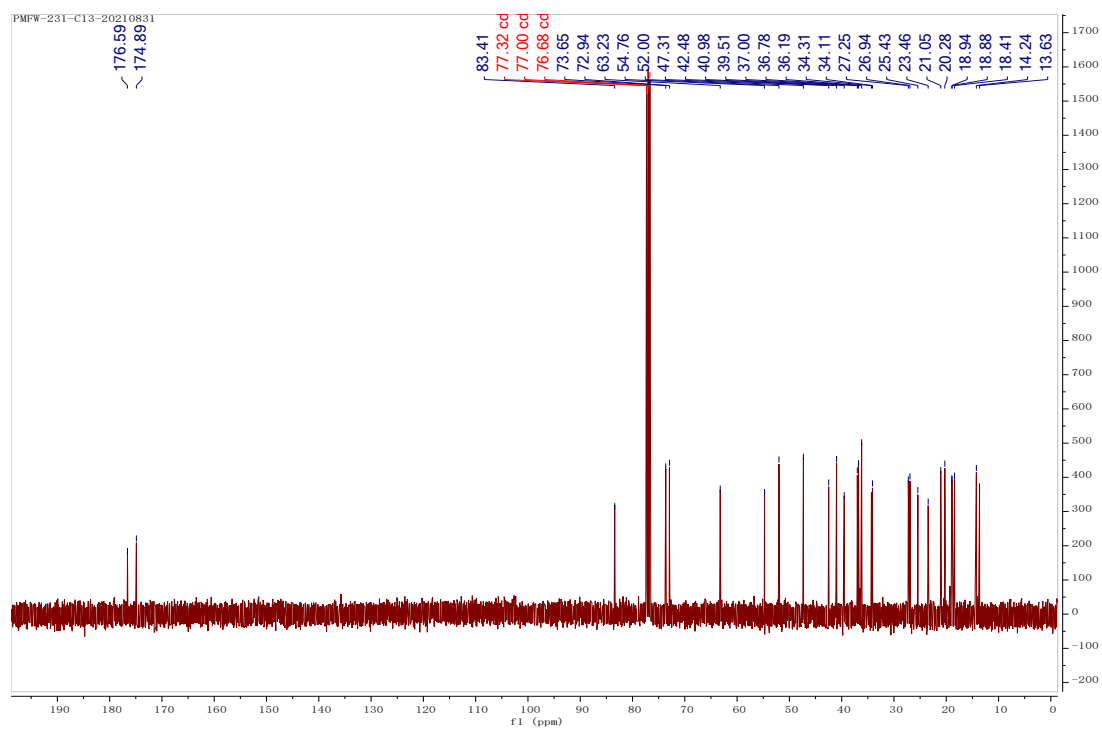


Fig. S38 ¹³C NMR spectrum of vulgarisin K (5)

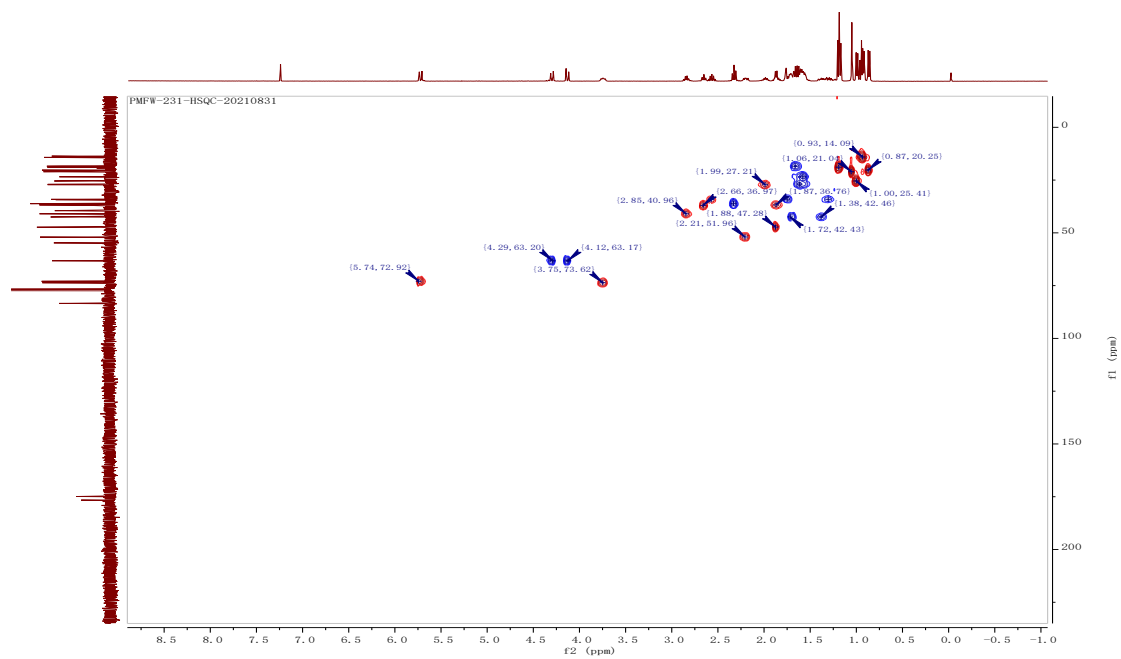


Fig. S39 HSQC spectrum of vulgarisin K (5)

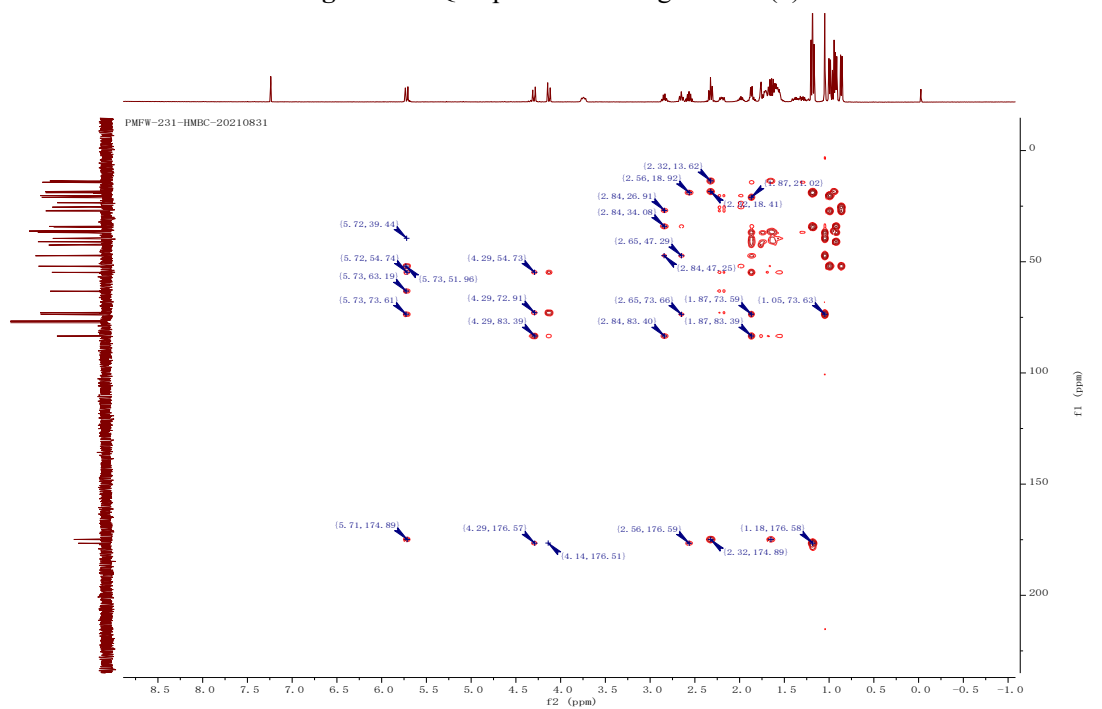


Fig. S40 HMBC spectrum of vulgarisin K (5)

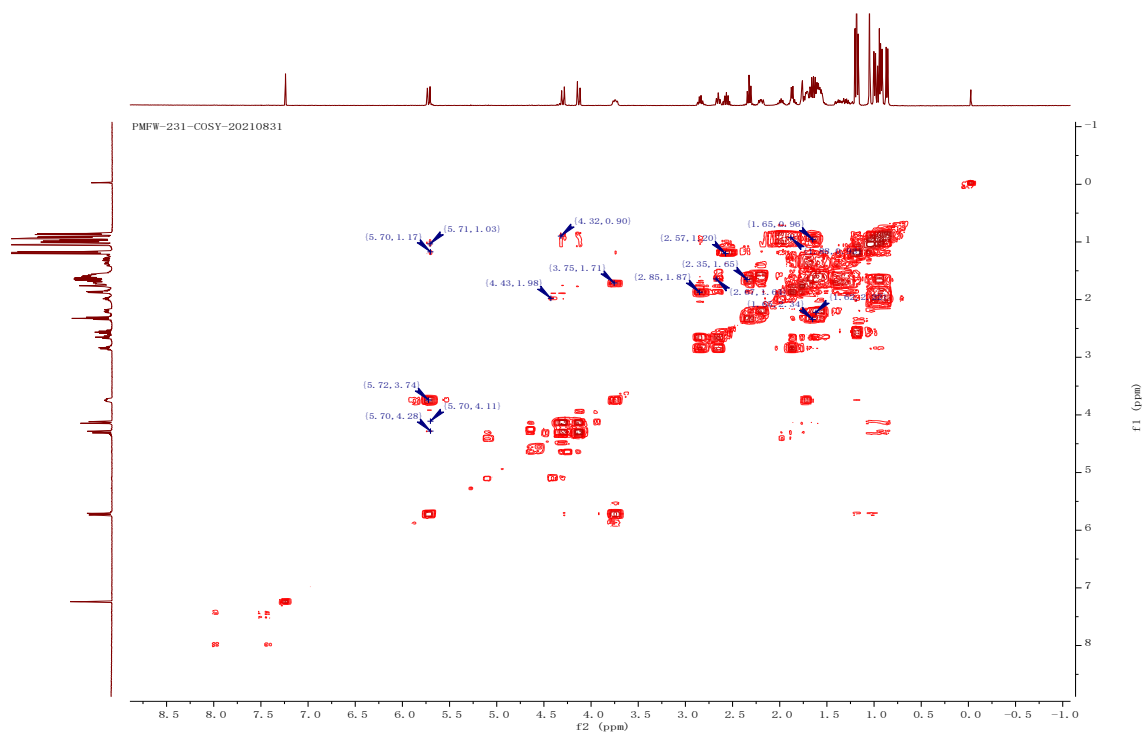


Fig. S41 ^1H - ^1H COSY spectrum of vulgarisin K (5)

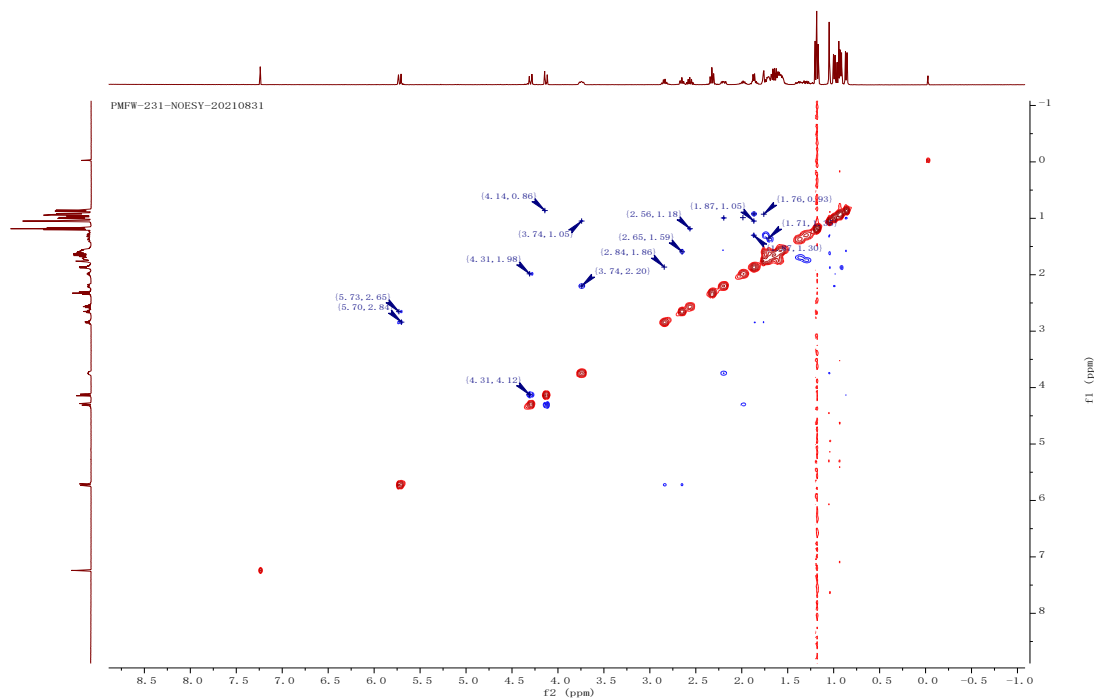


Fig. S42 NOESY spectrum of vulgarisin K (5)

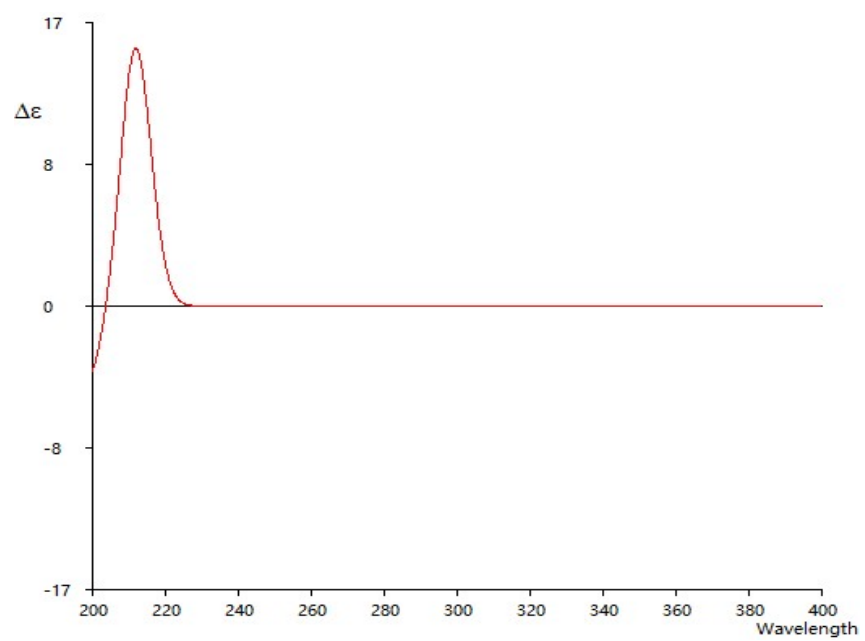
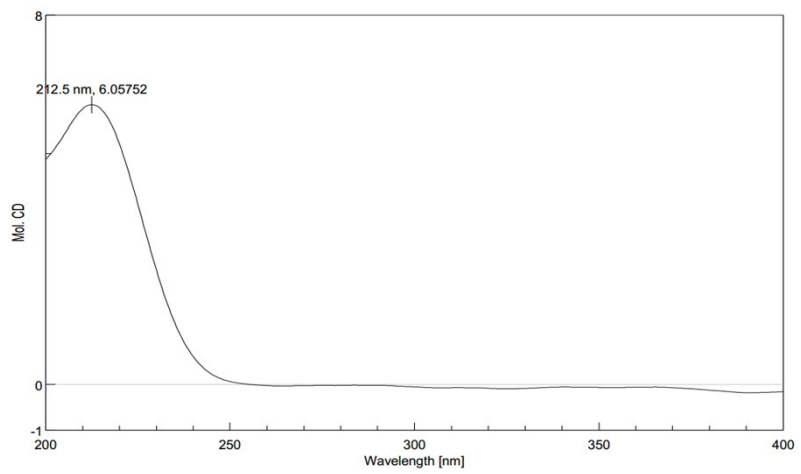
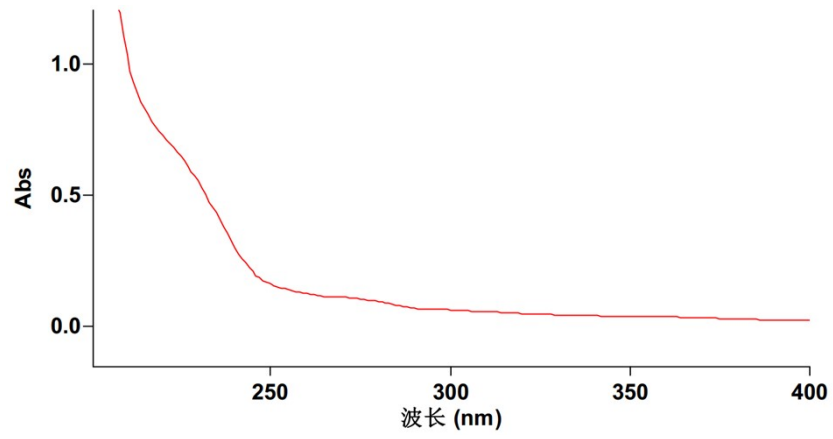
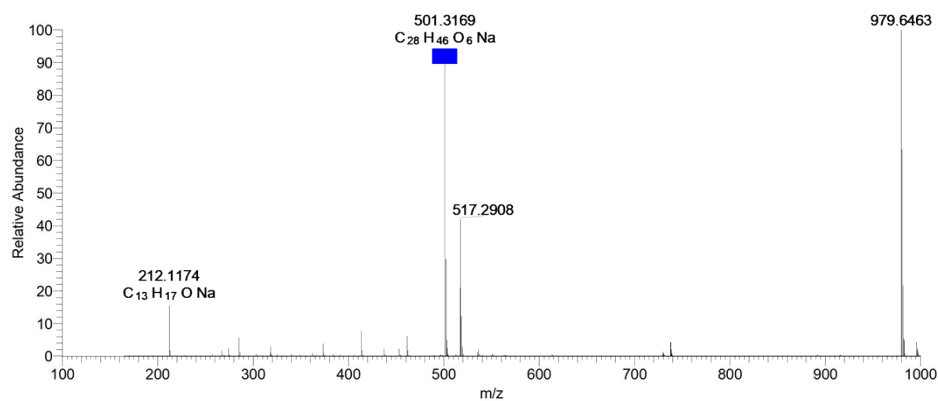


Fig. S43 UV and CD spectra (experimental and calculated) of vulgarisin K (5)

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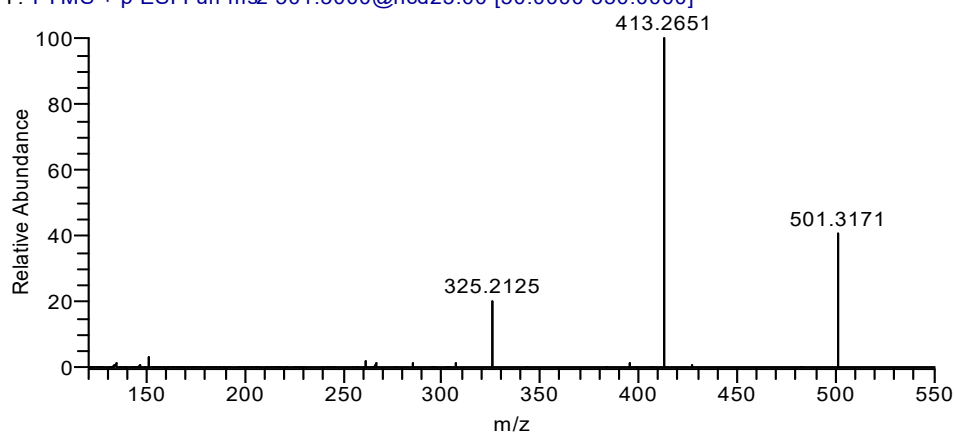


Fig. S44 MS and MS² spectra of vulgarisin K (5)

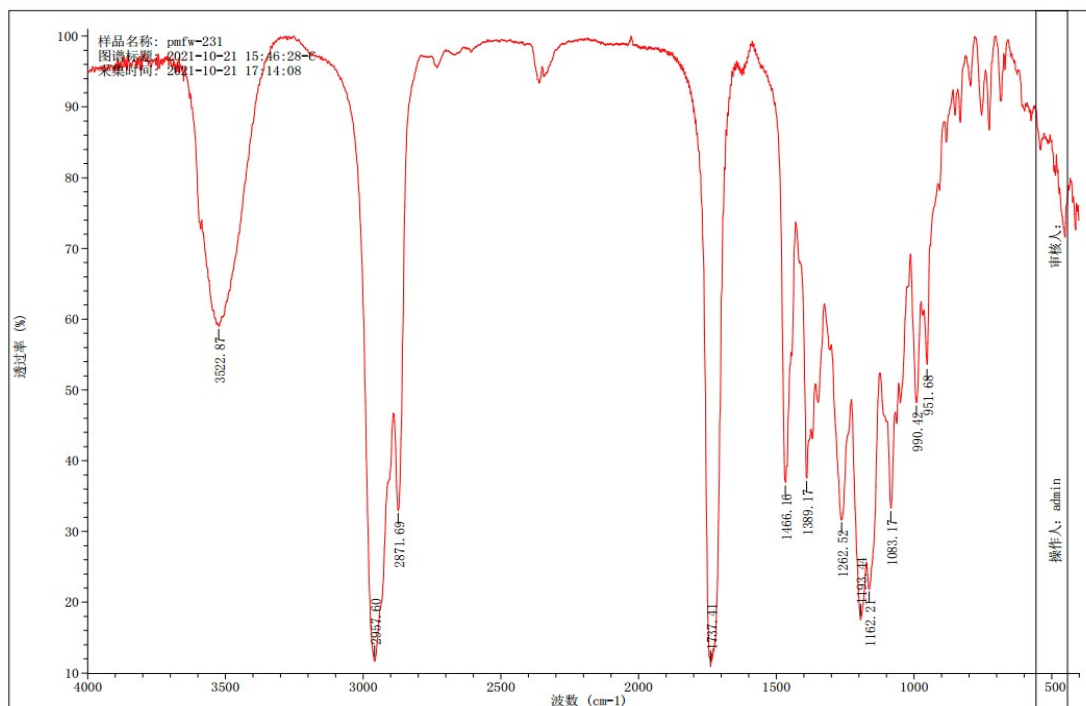


Fig. S45 FT-IR spectrum of vulgarisin K (5)

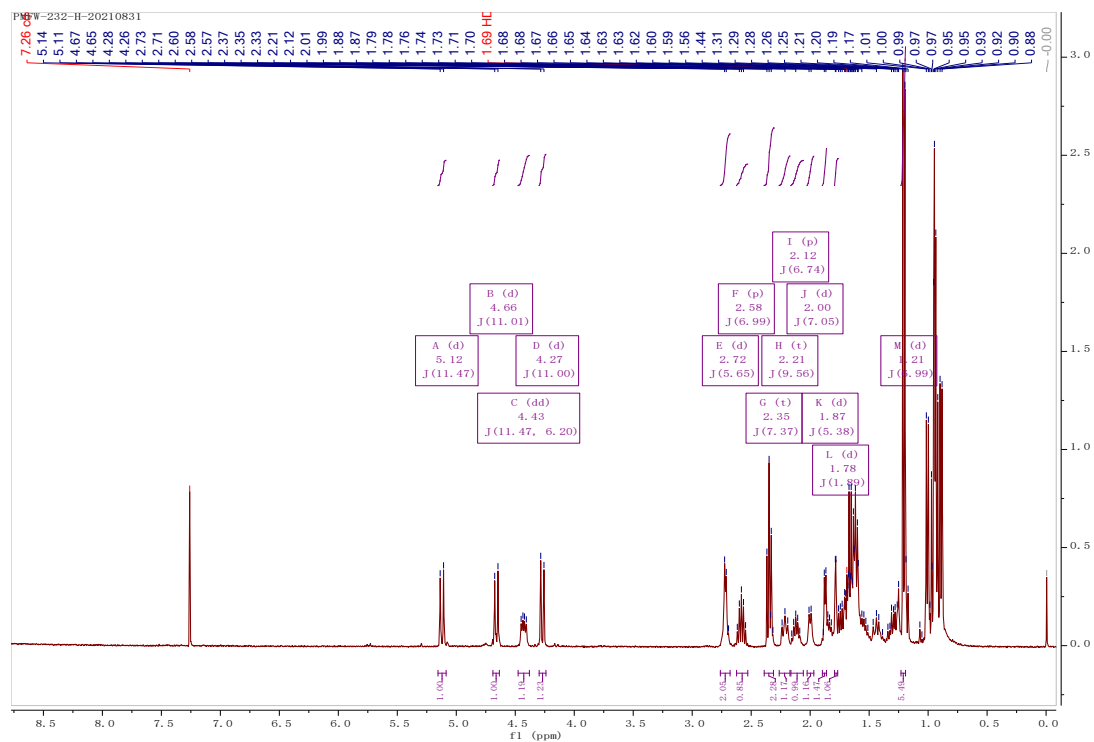


Fig. S46 ^1H NMR spectrum of vulgarisin L (6)

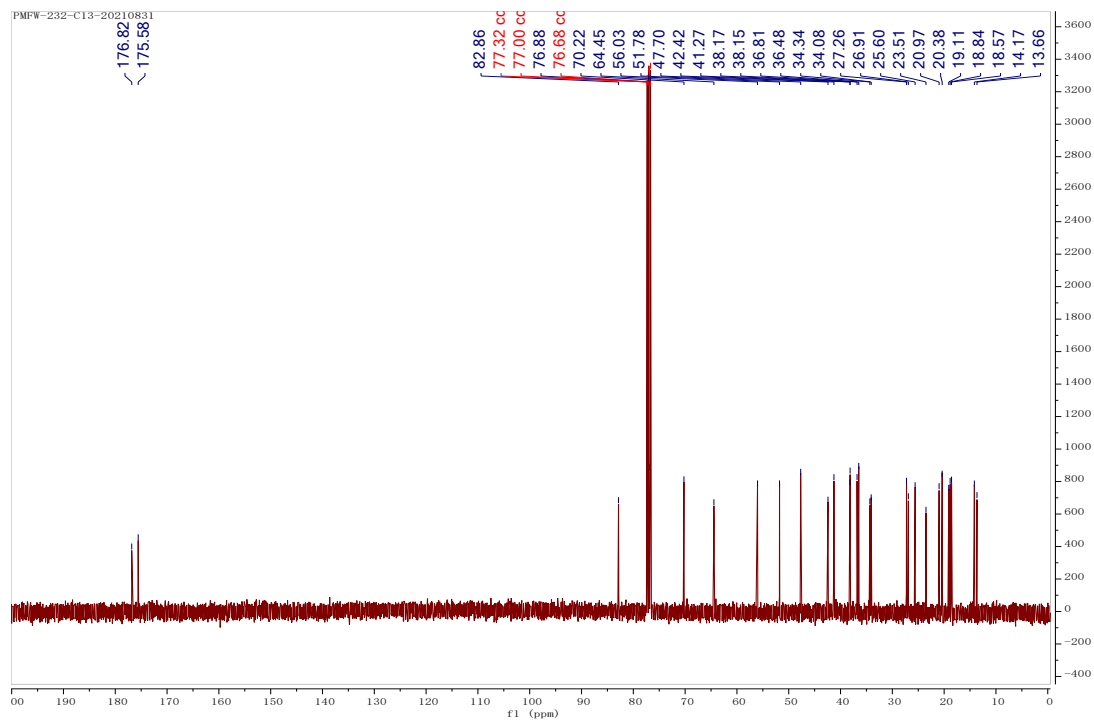


Fig. S47 ^{13}C NMR spectrum of vulgarisin L (6)

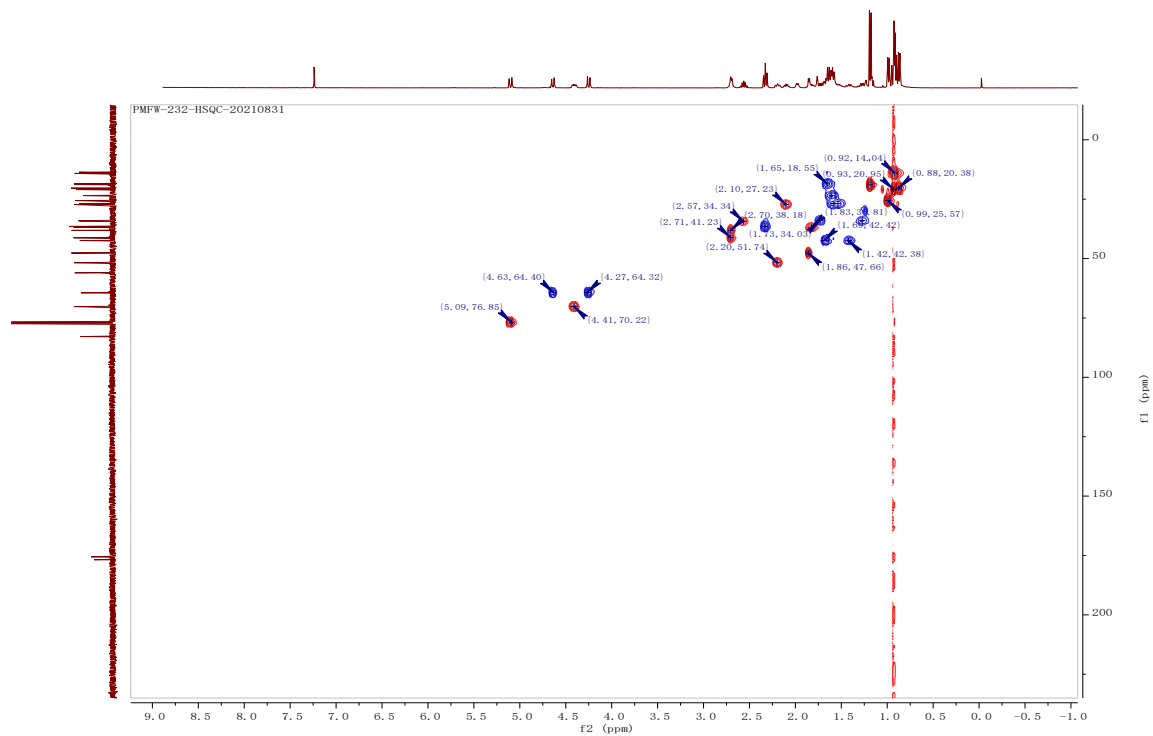


Fig. S48 HSQC spectrum of vulgarisin L (6)

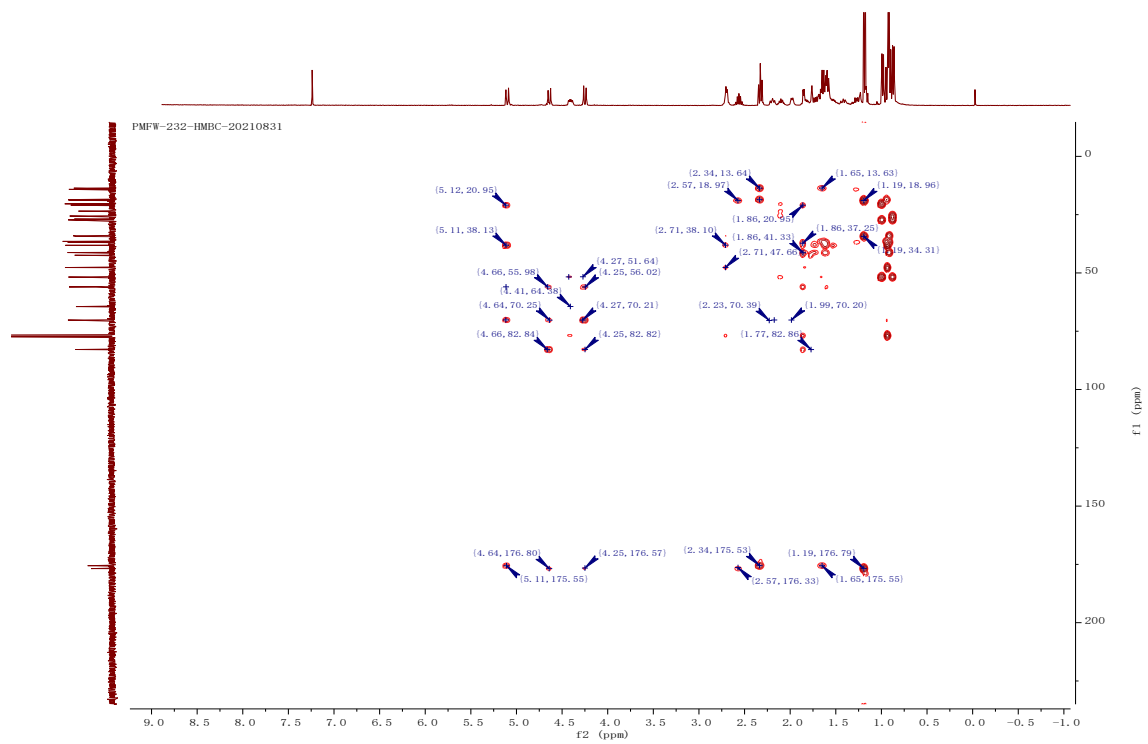


Fig. S49 HMBC spectrum of vulgarisin L (6)

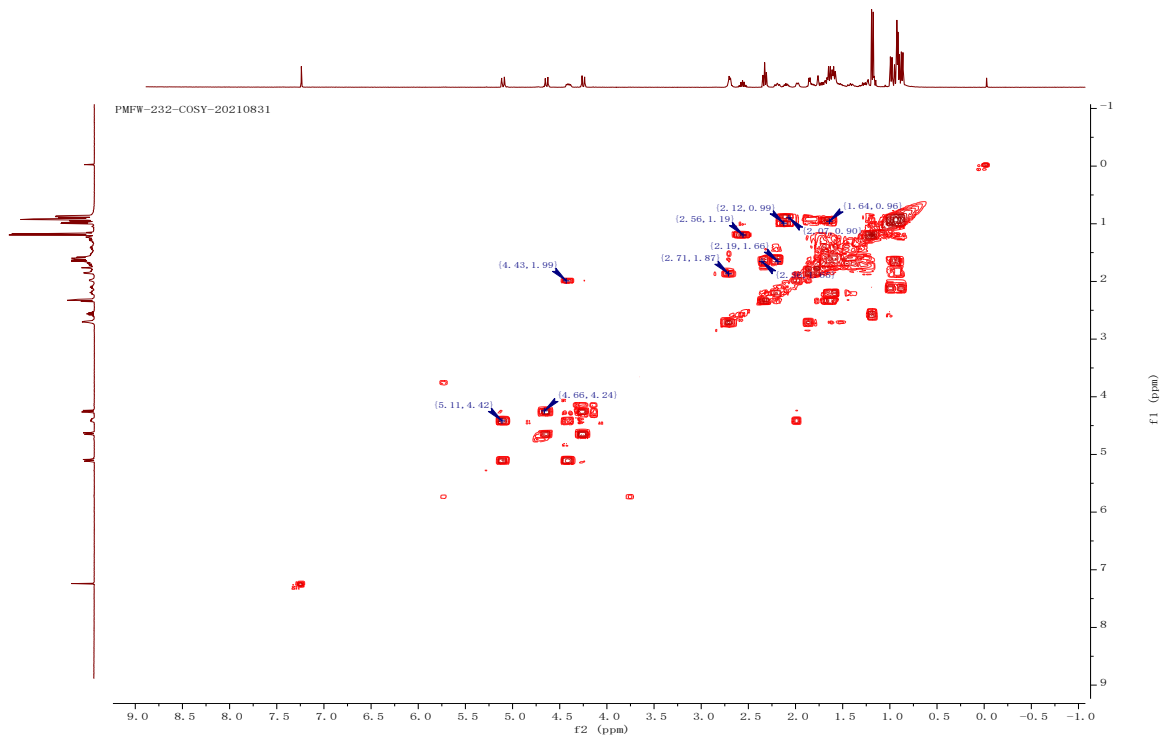


Fig. S50 ^1H - ^1H COSY spectrum of vulgarisin L (6)

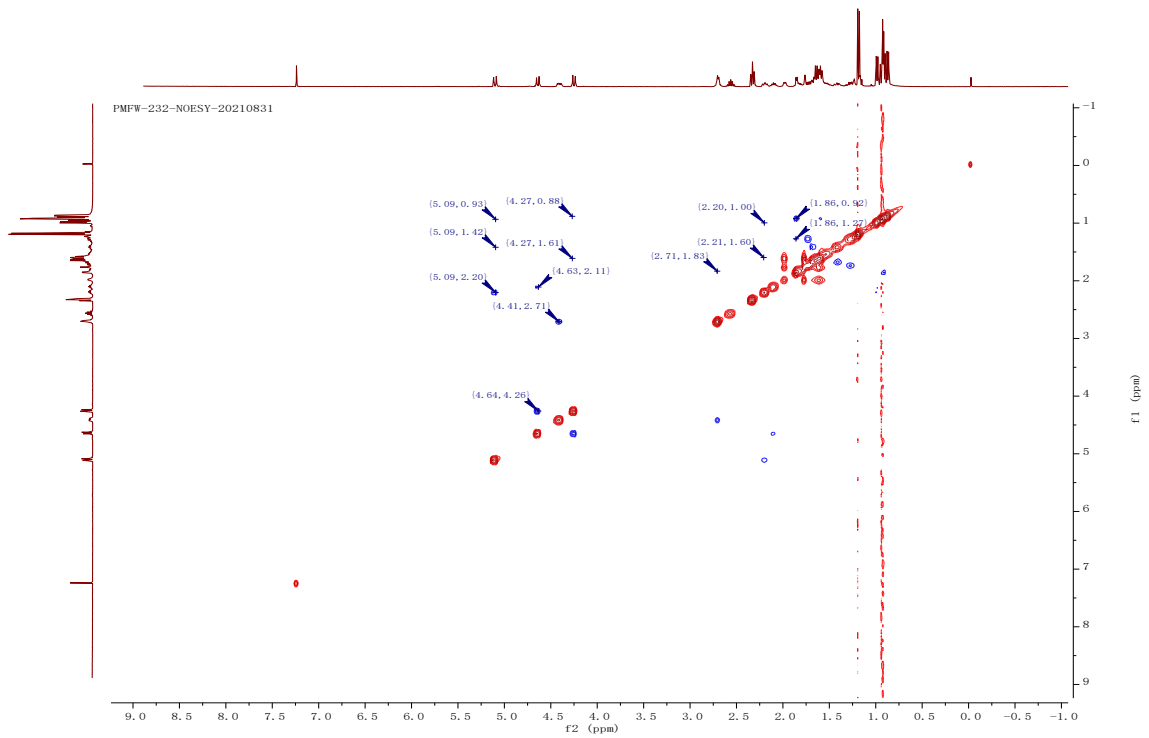


Fig. S51 NOESY spectrum of vulgarisin L (6)

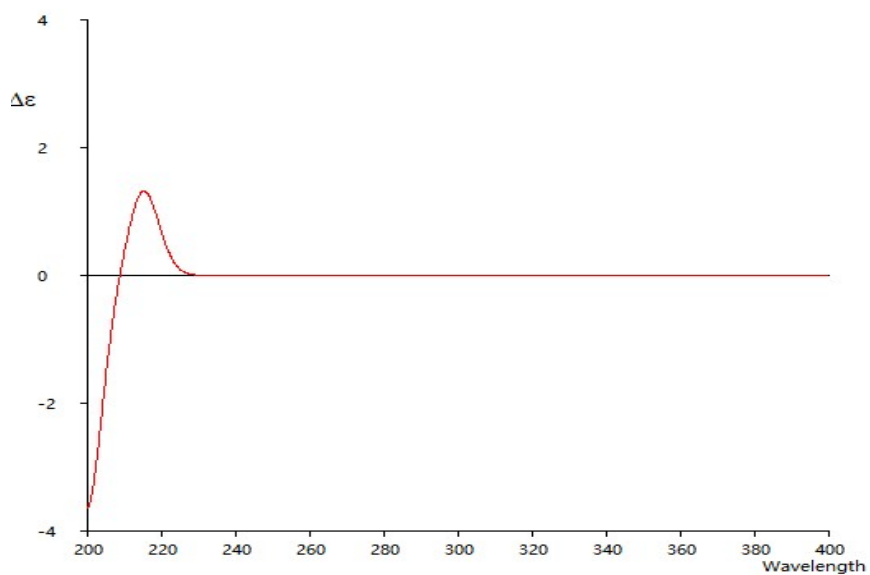
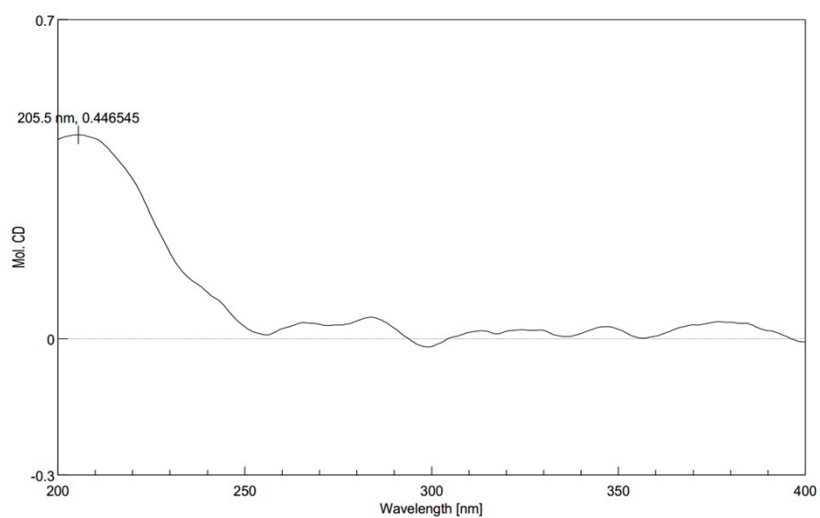
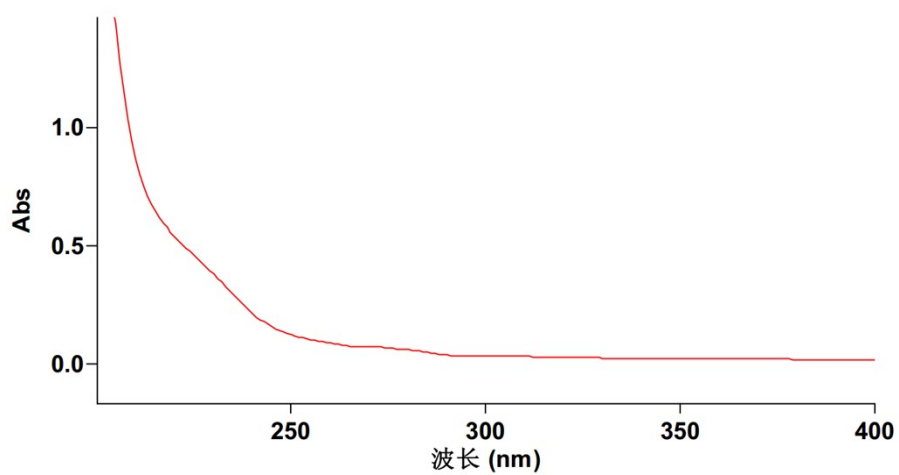


Fig. S52 UV and CD spectra (experimental and calculated) of vulgarisin L (6)

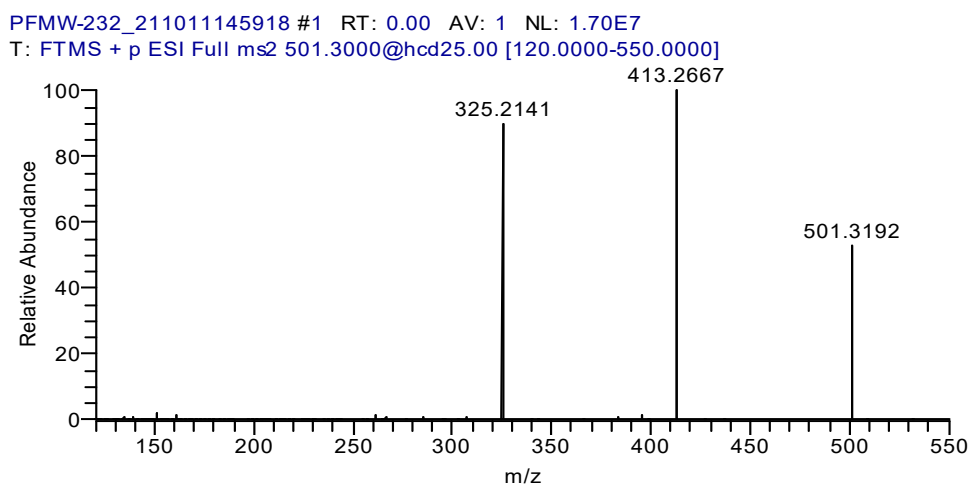
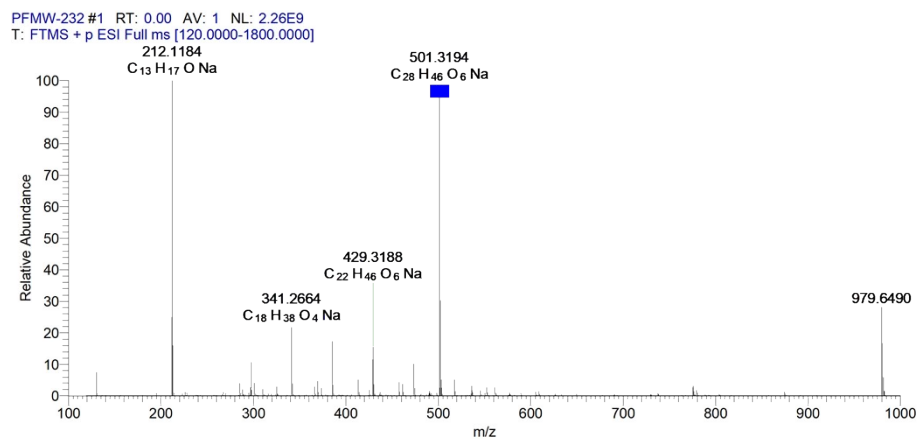


Fig. S53 MS and MS² spectra of vulgarisin L (6)

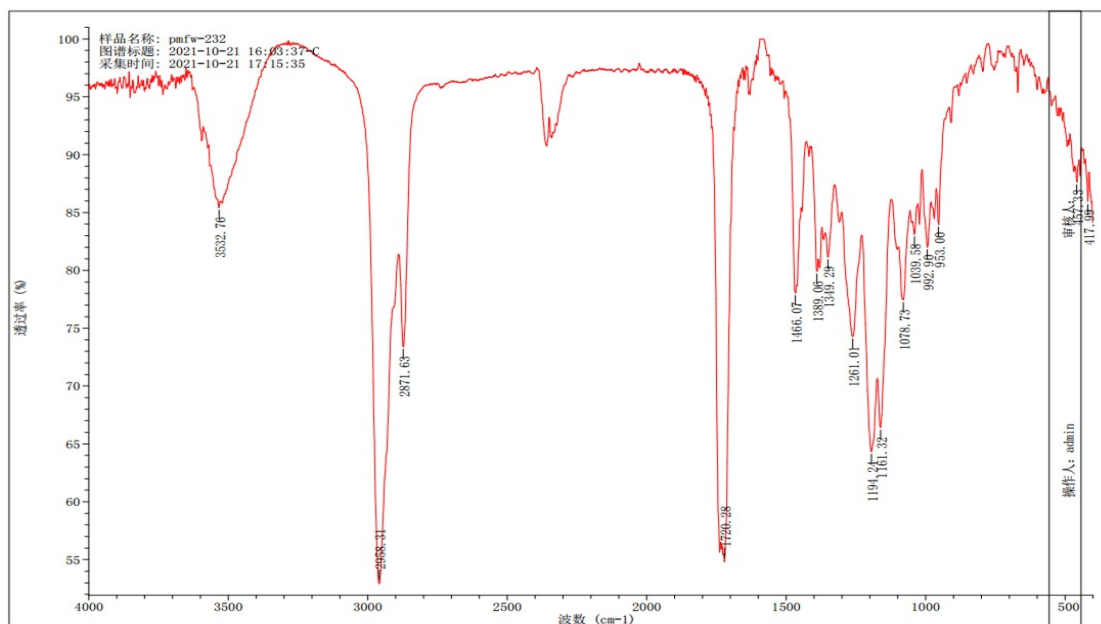


Fig. S54 FT-IR spectrum of vulgarisin L (6)

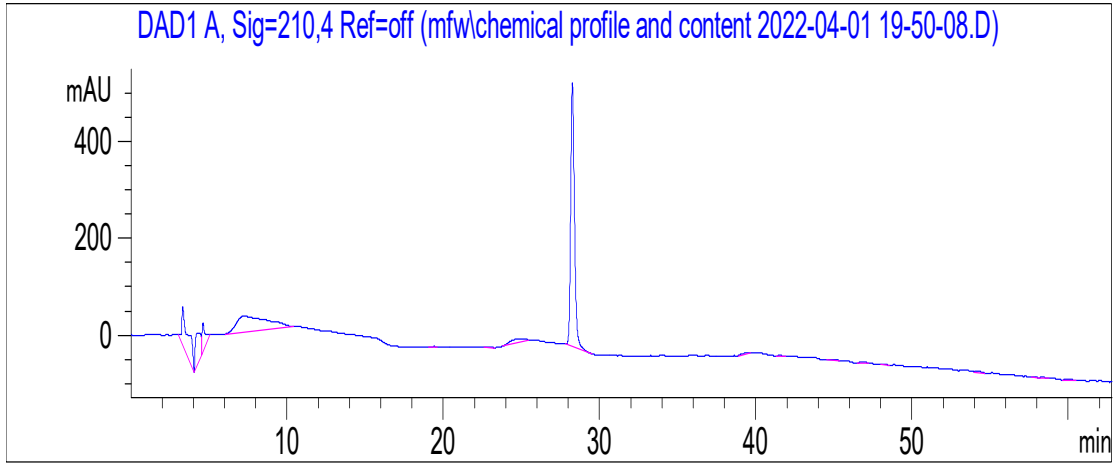


Fig. S55 HPLC chromatogram of reference standard caffeic acid

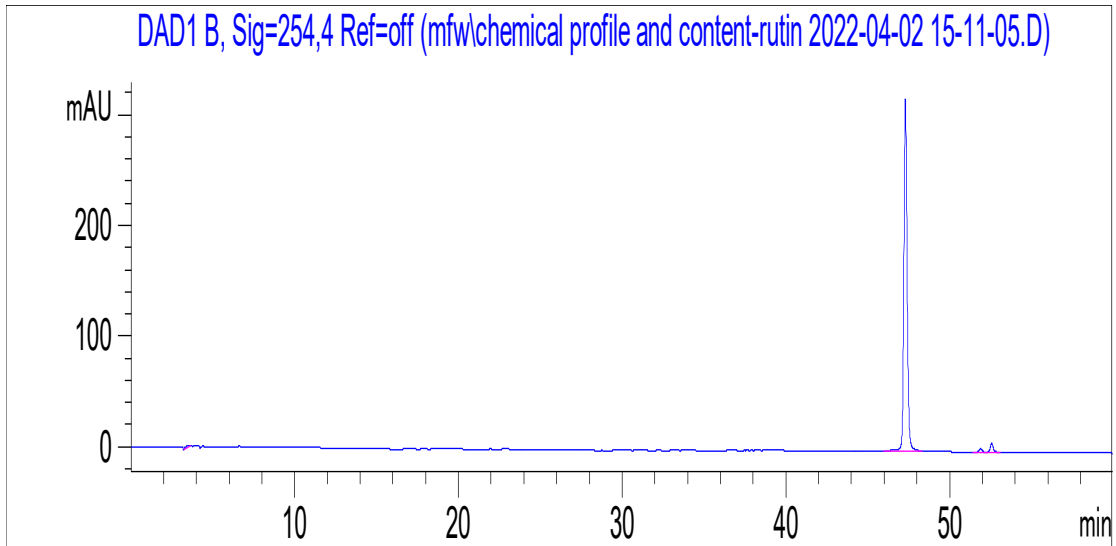


Fig. S56 HPLC chromatogram of reference standard rutin

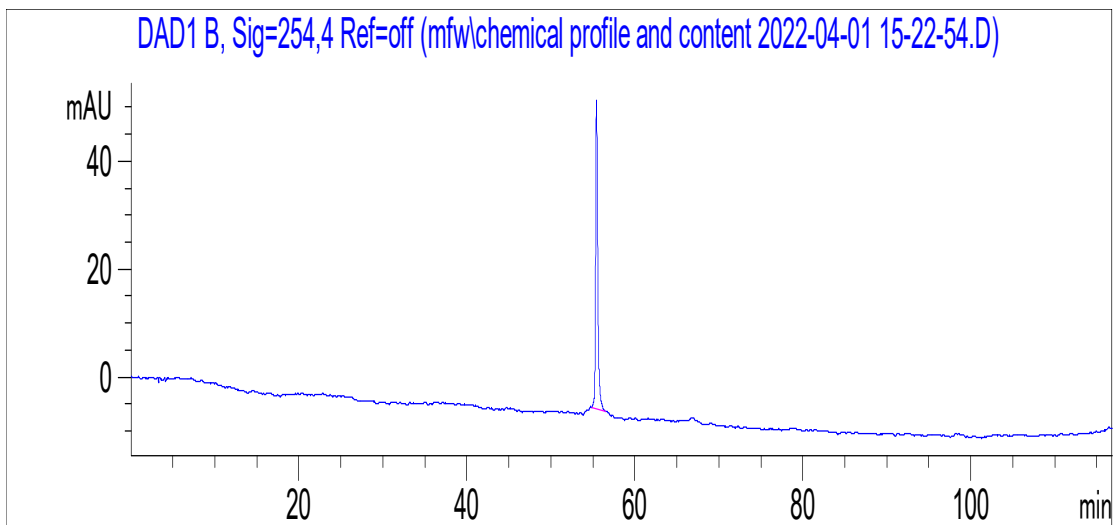


Fig. S57 HPLC chromatogram of reference standard rosmarinic acid

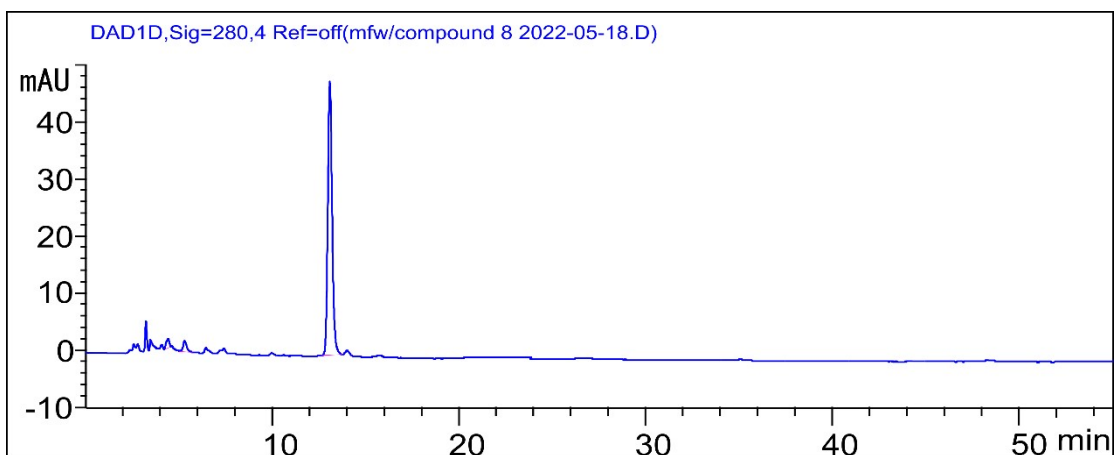


Fig. S58 HPLC chromatogram of isolated reference compound vulgarism F (8)

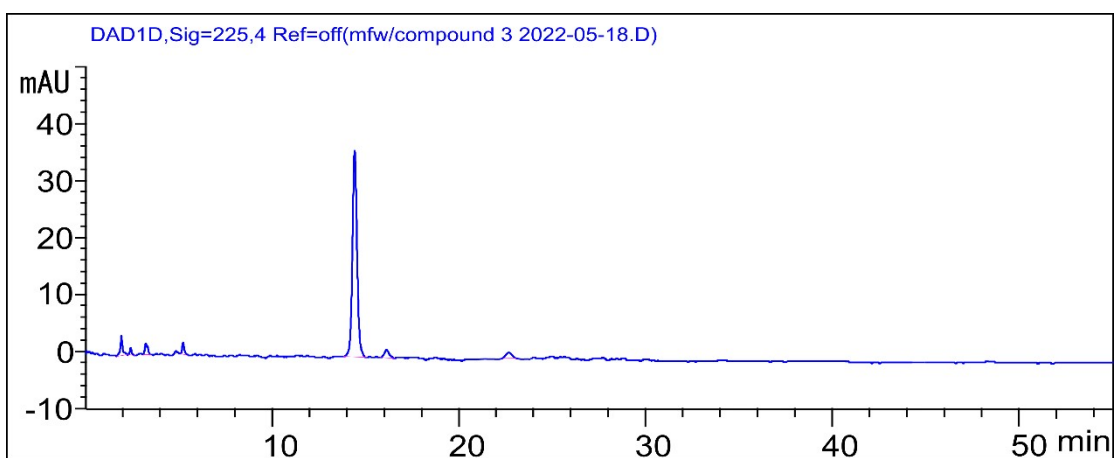


Fig. S59 HPLC chromatogram of isolated reference compound vulgarism I (3)

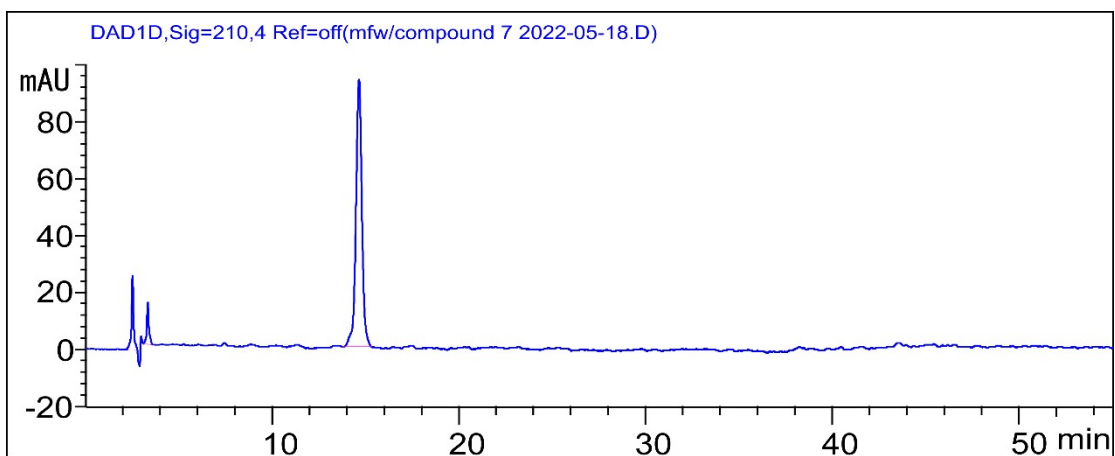


Fig. S60 HPLC chromatogram of isolated reference compound vulgarism E (7)

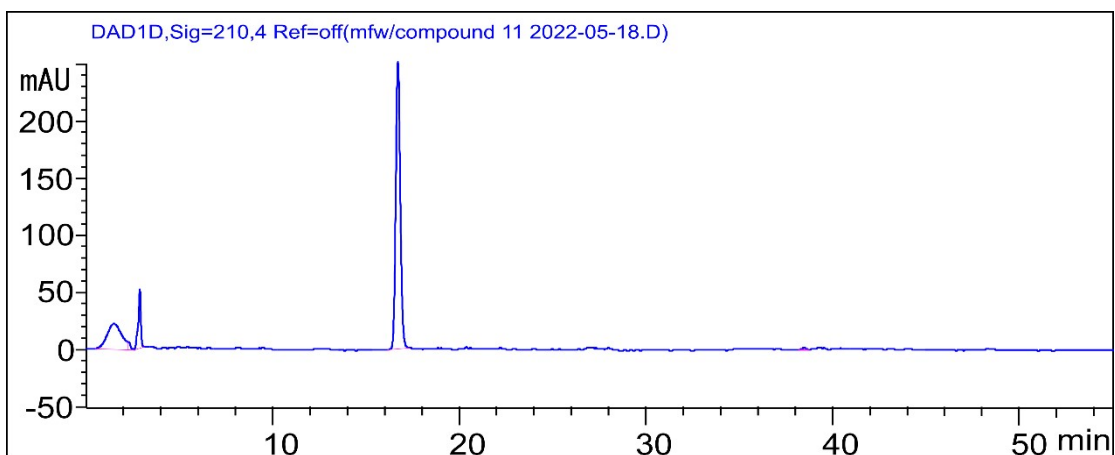


Fig. S61 HPLC chromatogram of isolated reference compound vulgarism C (11)

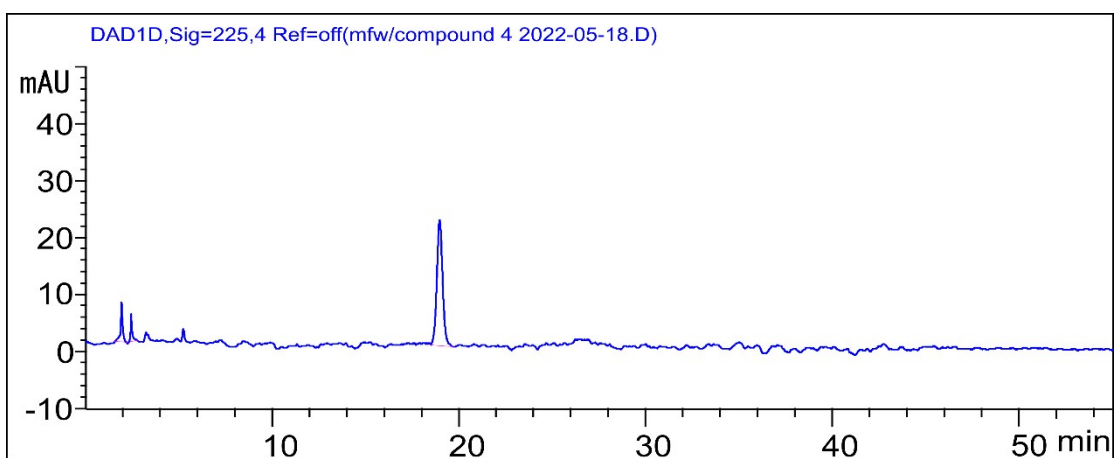


Fig. S62 HPLC chromatogram of isolated reference compound vulgarism J (4)

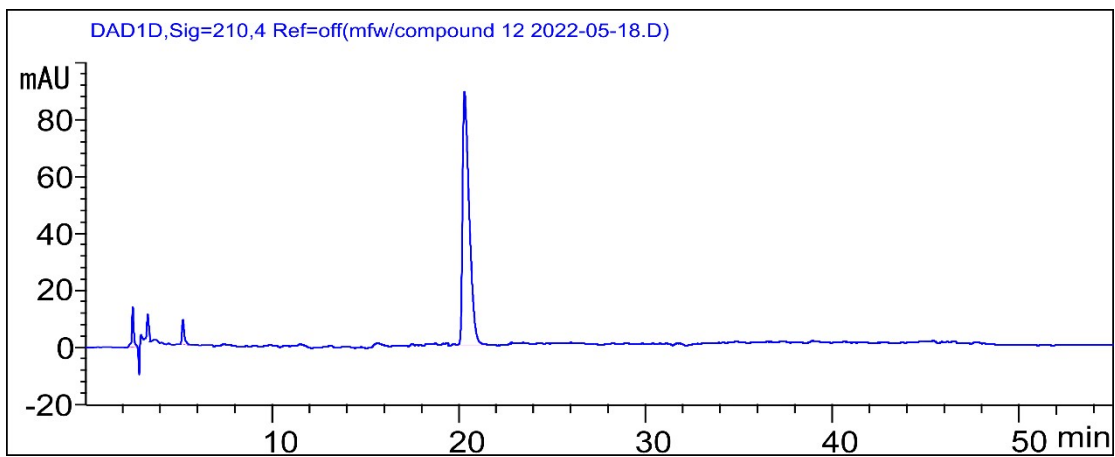


Fig. S63 HPLC chromatogram of isolated reference compound vulgarism B (12)

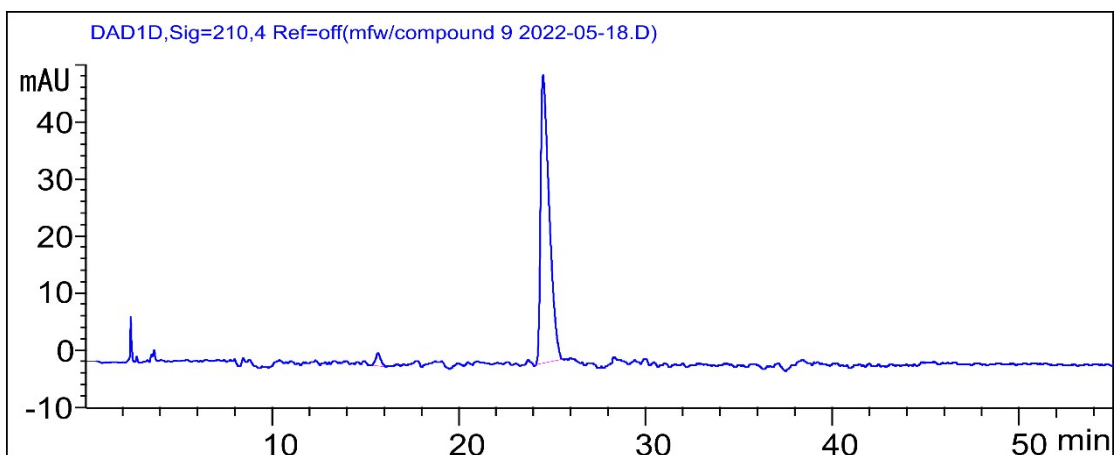


Fig. S64 HPLC chromatogram of isolated reference compound vulgarism D (9)

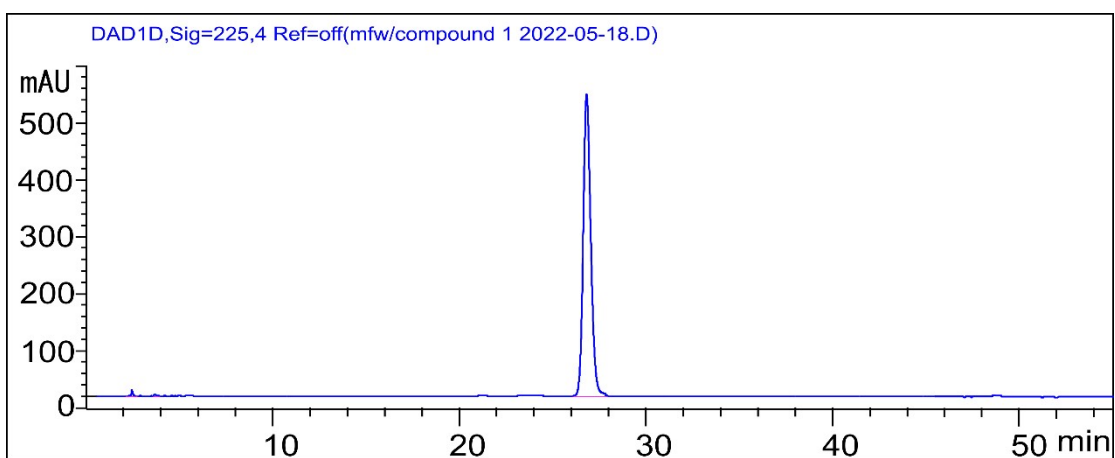


Fig. S65 HPLC chromatogram of isolated reference compound vulgarism G (1)

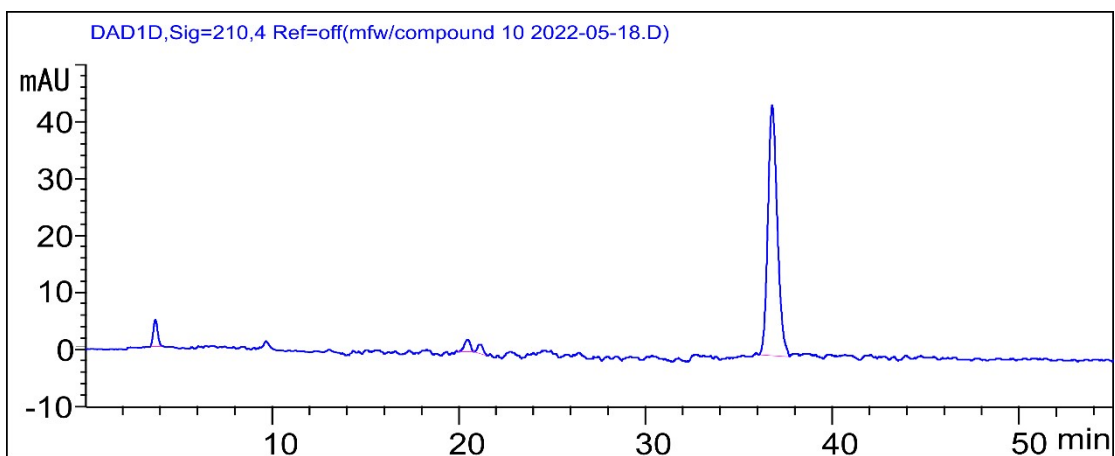


Fig. S66 HPLC chromatogram of isolated reference compound vulgarism A (10)

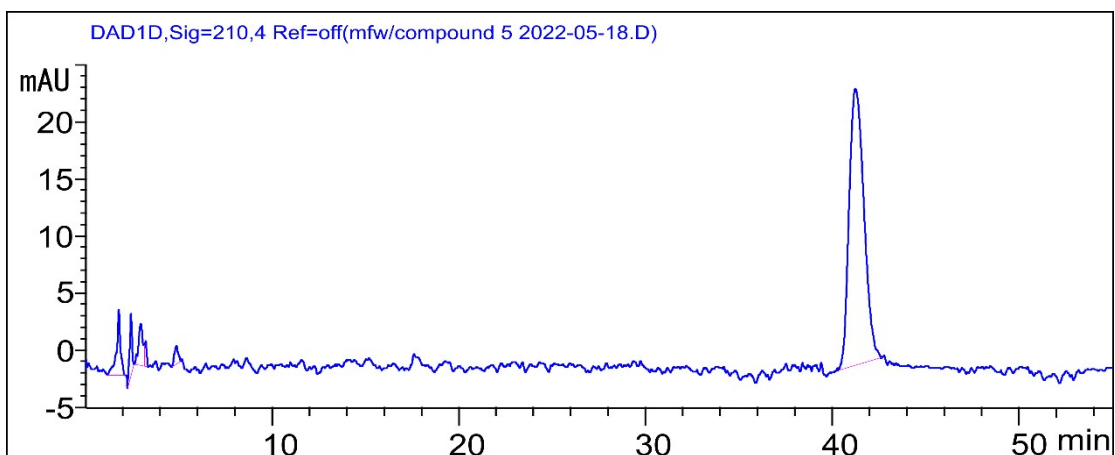


Fig. S67 HPLC chromatogram of isolated reference compound vulgarism K (5)

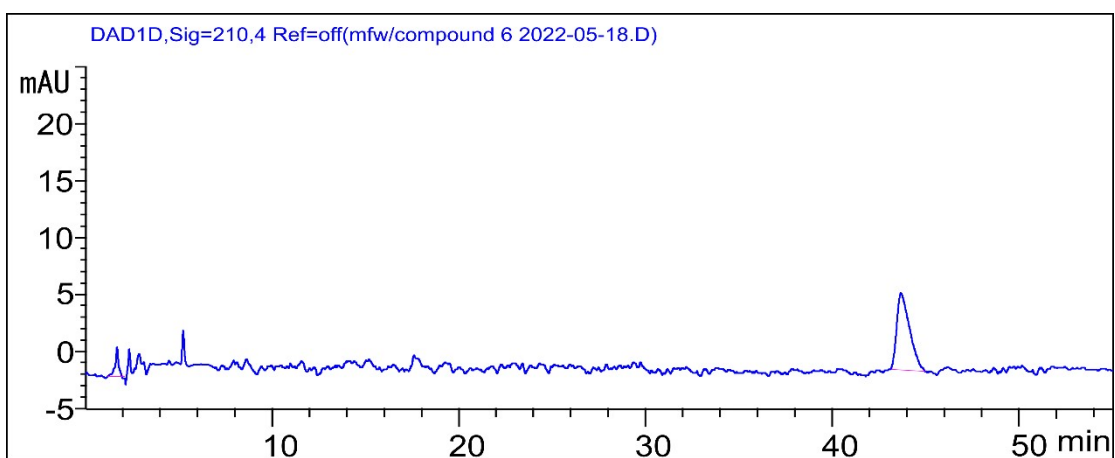


Fig. S68 HPLC chromatogram of isolated reference compound vulgarism L (6)

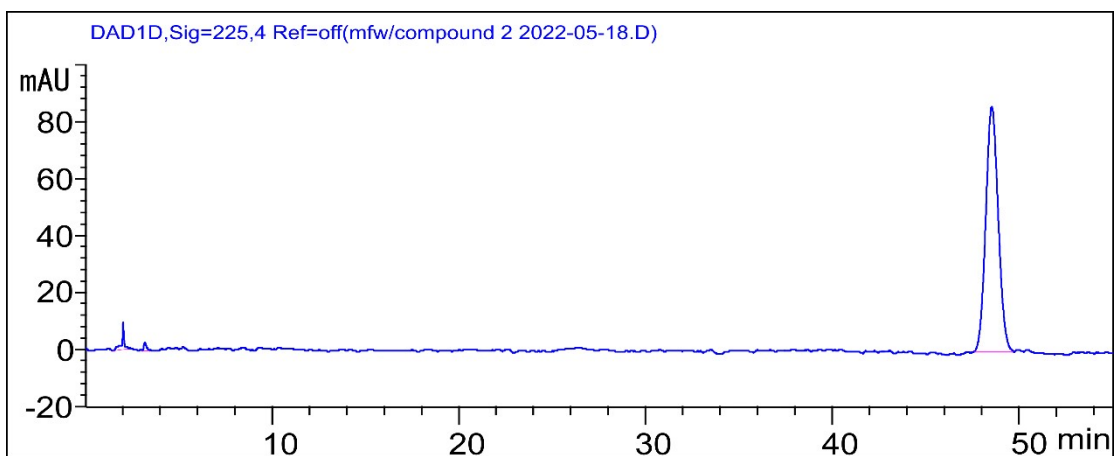


Fig. S69 HPLC chromatogram of isolated reference compound vulgarism H (2)

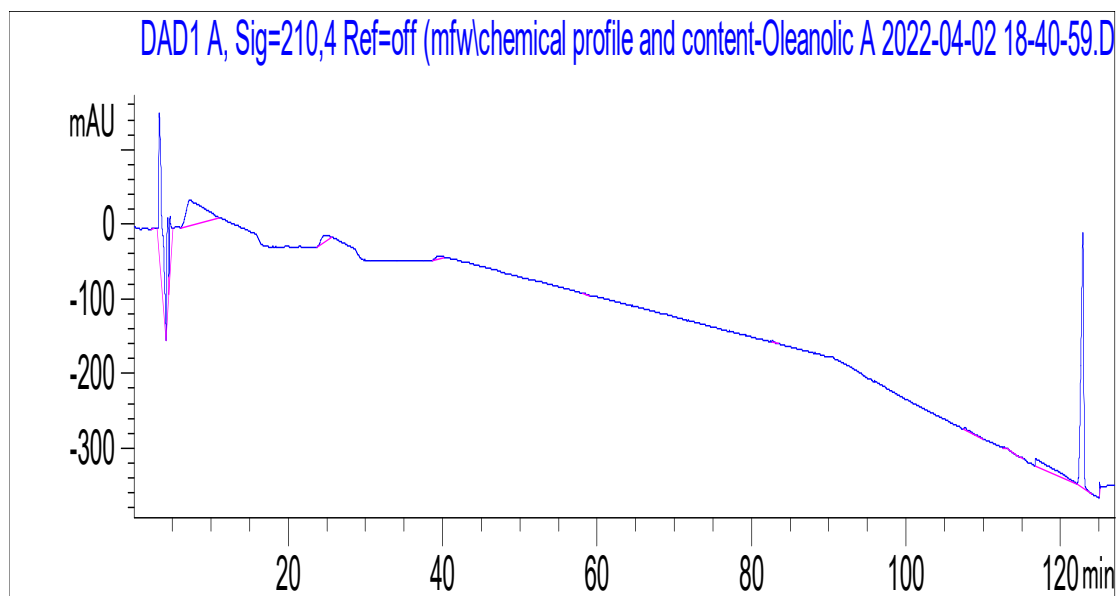


Fig. S70 HPLC chromatogram of reference standard ursolic acid

xkc-0301 #3390 RT: 18.35 AV: 1 NL: 4.84E8
T: FTMS - p ESI Full ms [100.0000-1200.0000]

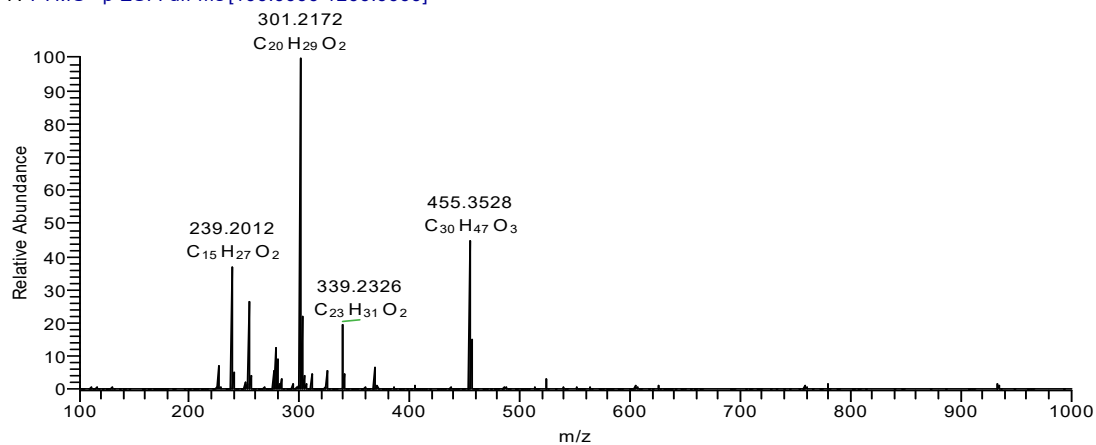


Fig. S71 HRMS spectrum of tentatively identified compound oleanolic acid (Mw=456)

xkc-0301 #3362 RT: 18.20 AV: 1 NL: 3.37E9
T: FTMS - p ESI Full ms [100.0000-1200.0000]

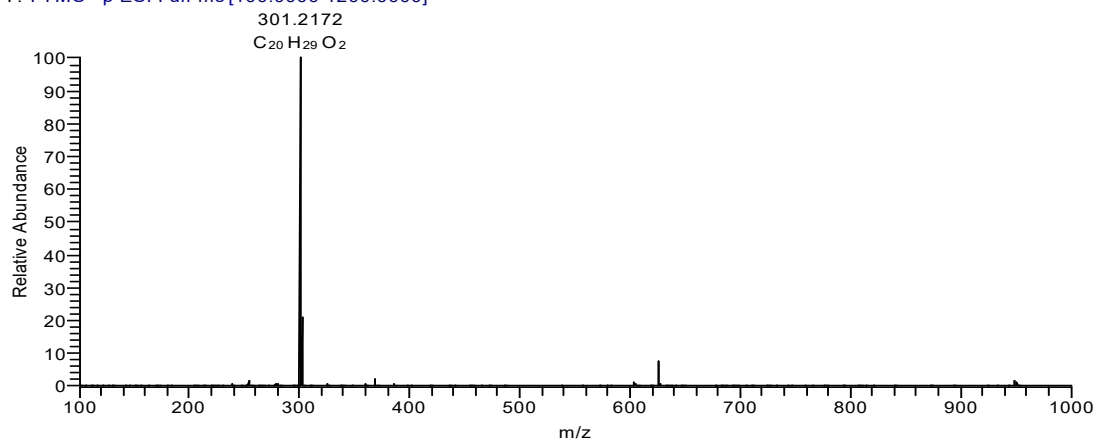


Fig. S72 HRMS spectrum of tentatively identified compound abietic acid (Mw=302)

xkc-0301 #3528 RT: 19.09 AV: 1 NL: 1.10E8
T: FTMS + p ESI Full ms [100.0000-1200.0000]

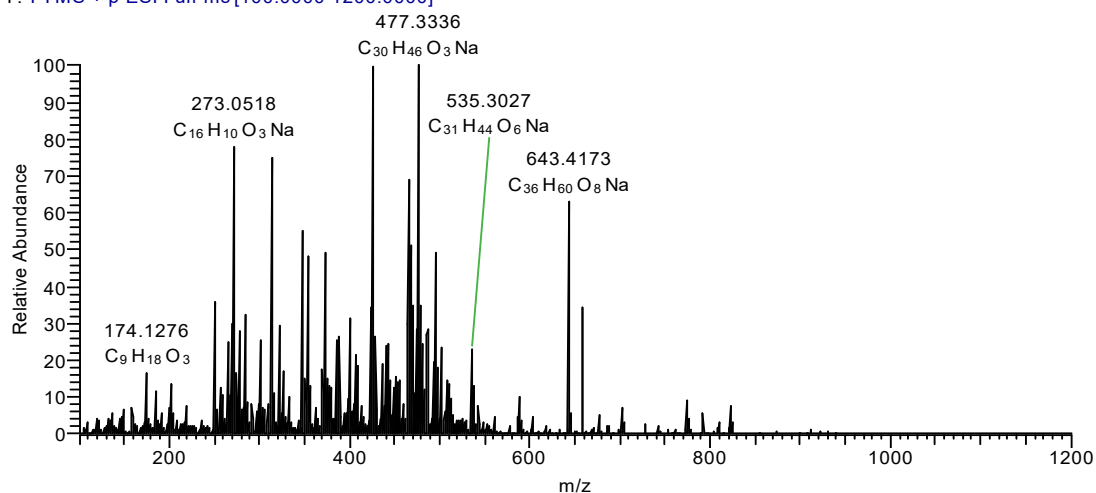


Fig. S73 HRMS spectrum of tentatively identified compound ursonic acid (Mw=454)

xkc-0301 #3414 RT: 18.48 AV: 1 NL: 3.51E7
T: FTMS - p ESI Full ms [100.0000-1200.0000]

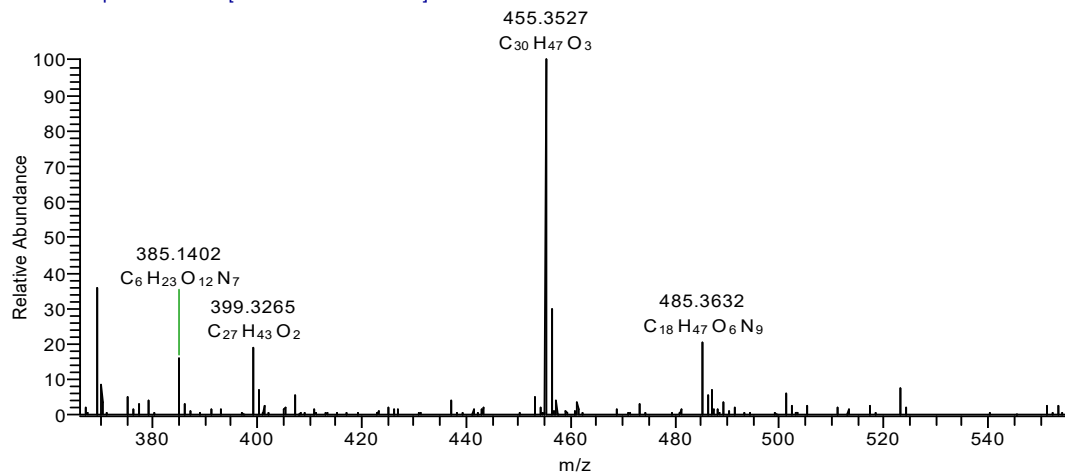


Fig. S74 HRMS spectrum of tentatively identified compound betulinic acid (Mw=456)

xkc-0301 #3558 RT: 19.25 AV: 1 NL: 6.49E8
T: FTMS - p ESI Full ms [100.0000-1200.0000]

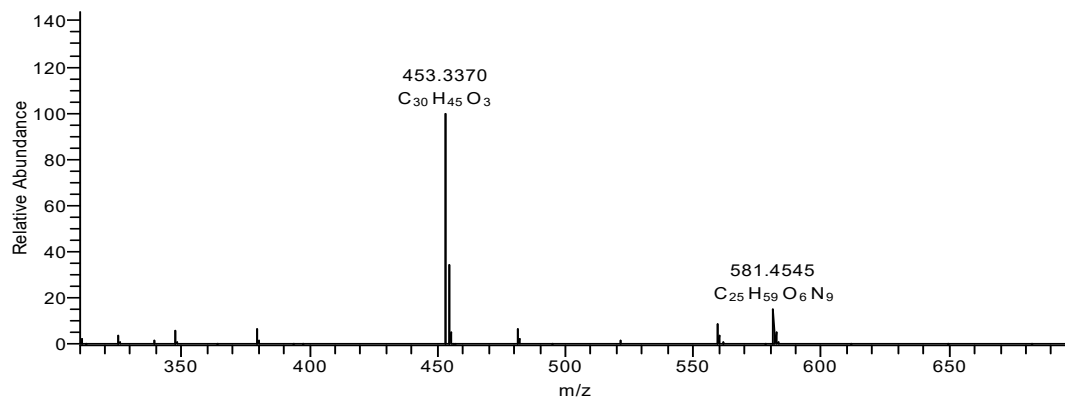


Fig. S75 HRMS spectrum of tentatively identified compound dehydrotrameternolic acid
(Mw=454)

No.	Compounds	Identification method	Elementary composition	Reference
1	Caffeic acid	reference standard	C ₉ H ₈ O ₄	Fig. S55
2	Rutin	reference standard	C ₂₇ H ₃₀ O ₁₆	Fig. S56
3	Rosmarinic acid	reference standard	C ₁₈ H ₁₆ O ₈	Fig. S57
4	Vulgarisin F (8)	isolated compound	C ₃₃ H ₄₆ O ₆	Fig. S58
5	Vulgarisin I (3)	isolated compound	C ₃₁ H ₄₄ O ₆	Fig. S59
6	Vulgarisin E (7)	isolated compound	C ₃₁ H ₄₄ O ₆	Fig. S60
7	Vulgarisin C (11)	isolated compound	C ₃₁ H ₄₄ O ₆	Fig. S61
8	Vulgarisin J (4)	isolated compound	C ₃₁ H ₄₄ O ₆	Fig. S62
9	Vulgarisin B (12)	isolated compound	C ₃₁ H ₄₄ O ₆	Fig. S63
10	Vulgarisin D (9)	isolated compound	C ₂₈ H ₄₆ O ₆	Fig. S64
11	Vulgarisin G (1)	isolated compound	C ₃₄ H ₄₂ O ₆	Fig. S65
12	Vulgarisin A (10)	isolated compound	C ₂₈ H ₄₆ O ₆	Fig. S66
13	Vulgarisin K (5)	isolated compound	C ₂₈ H ₄₆ O ₆	Fig. S67
14	Vulgarisin L (6)	isolated compound	C ₂₈ H ₄₆ O ₆	Fig. S68
15	Vulgarisin H (2)	isolated compound	C ₃₄ H ₄₂ O ₆	Fig. S69
16	Ursolic acid	reference standard	C ₃₀ H ₄₈ O ₃	Fig. S70
17	Oleanolic acid	HRMS	C ₃₀ H ₄₈ O ₃	Fig. S71
18	Abietic acid	HRMS	C ₂₀ H ₃₀ O ₂	Fig. S72
19	Ursonic acid	HRMS	C ₃₀ H ₄₆ O ₃	Fig. S73
20	Betulinic acid,	HRMS	C ₃₀ H ₄₈ O ₃	Fig. S74
21	Dehydrotrameternolic acid	HRMS	C ₃₀ H ₄₆ O ₃	Fig. S75
22	Baicalin	HRMS	C ₂₁ H ₁₈ O ₁₁	-
23	Cafestol	HRMS	C ₂₀ H ₂₈ O ₃	-
24	Salviaflaside	literature	C ₂₄ H ₂₆ O ₁₃	1
25	Sterol glucosides	literature	-	2,3
26	Coumarins	literature	-	4
27	Flavones	literature	-	5

Table S1 Chemical profile of *P. vulgaris*

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3. H. Kojima, N. Sato, A. Hatano and H. Ogura, Sterol glucosides from *Prunella vulgaris*, *Phytochemistry*, 1990, **29**, 2351-2355.
4. S. I. Dmitruk, Coumarins of *Prunella vulgaris*, *Chemistry of Natural Compounds*, 1986, **22**, 480.
5. I. S. Dmitruk, S. E. Dmitruk, T. P. Berezovskaya and T. P. Prishchep, Flavones of *Prunella vulgaris*, *Chemistry of Natural Compounds*, 1987, **23**, 374-375.

Reference