

Oligomeric phenylpropanoids bearing new skeleton and hypoglycemic activity from
Magnolia officinalis var. *biloba*

Kailing Xu, Chuan Li, Chuangjun Li, Jie Ma, Yingda Zang, Fei Ye* and Dongming Zhang*

State Key Laboratory of Bioactive Substance and Function of Natural Medicines, Institute of Materia Medica,
Chinese Academy of Medical Sciences and Peking Union Medical College, Beijing 100050, China

* Corresponding author.

E-mail address: yefei@imm.ac.cn

* Corresponding author.

E-mail address: zhangdm@imm.ac.cn

Supporting Information

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1. X-ray crystallographic analysis of maglignan C (3)

Colorless crystals of compound **3** (CCDC: 2043305) were crystallized in CH₃CN-CH₂Cl₂. Crystal data: C₂₈H₃₄O₂, M = 402.55, monoclinic, space group P2₁ (no. 4), *a* = 10.27250(10) Å, *b* = 9.64240(10) Å, *c* = 23.2486(2) Å, β = 90.2730(10)°, *V* = 2302.78(4) Å³, *Z* = 4, *T* = 100.00(10) K, μ(Cu Kα) = 0.547 mm⁻¹, 52110 reflections measured, and 8309 unique (*R*_{int} = 0.0559, *R*_{sigma} = 0.0310). These parameters were used in all calculations. The final *R*₁ was 0.0419 and *wR*₂ was 0.1063. Flack parameter = -0.05(7). The data can be accessed via www.ccdc.cam.ac.uk

Table S1 Crystal data and structure refinement for compound **3**.

Identification code		moz_4_5a	
Bond precision:	C-C = 0.0039 Å	Wavelength = 1.54178	
Cell:	a=10.2725(1)	b=9.6424(1)	c=23.2486(2)
	alpha=90	beta=90.273(1)	gamma=90
Temperature:	100 K		
	Calculated	Reported	
Volume	2302.78(4)	2302.78(4)	
Space group	P2 ₁	P12 ₁ 1	
Hall group	P2yb	P2yb	
Moiety formula	C ₂₈ H ₃₄ O ₂	C ₂₈ H ₃₄ O ₂	
Sum formula	C ₂₈ H ₃₄ O ₂	C ₂₈ H ₃₄ O ₂	
Mr	402.55	402.55	
Dx (g/cm ⁻³)	1.161	1.161	
<i>Z</i>	4	4	
Mu (mm ⁻¹)	0.547	0.547	
F000	872.0	872.0	
F000'	874.32		
h, k, l max	12, 11, 28	12, 11, 28	
Nref	8432[4489]	8309	
Tmin, Tmax	0.961, 0.978	0.607, 1.000	
Tmin'	0.921		
Correction method= # Reported T Limits: Tmin=0.607 Tmax=1.000			
AbsCorr = MULTI-SCAN			
Data completeness=	1.85/0.99	Theta(max)= 68.243	
R(reflections)=	0.0419(7842)	<i>wR</i> ₂ (reflections)= 0.1063(8309)	
S =	1.057	Npar= 576	

2. Bioassay results

Table S2 α -Glucosidase inhibitory activities of **1–3**.

No.	Inhibition rate (%)	IC ₅₀ (μ M)
Acarbose	75.2 ^a	–
1	86.4 ^b	1.49
(+)- 1	86.0 ^b	1.77
(-)- 1	78.9 ^b	2.16
2	12.8 ^b	–
3	3.7 ^b	–

^a 200 μ M.

^b 10 μ M.

Table S3 PTP1B inhibitory activities of **1–3**.

No.	Inhibition rate (10 μ M, %)	IC ₅₀ (μ M)
CC06240 ^a	99.2	–
1	87.6	0.309
(+)- 1	88.8	0.448
(-)- 1	88.3	0.582
2	55.7	–
3	-1.6	–

^a Positive control substance.

3. NMR, HRESIMS, IR, UV, ECD spectra of maglignans A–C (1–3)

Maglignan A (1)

Fig. S2. ¹H NMR spectrum (500 MHz, DMSO-*d*₆) of maglignan A (1).

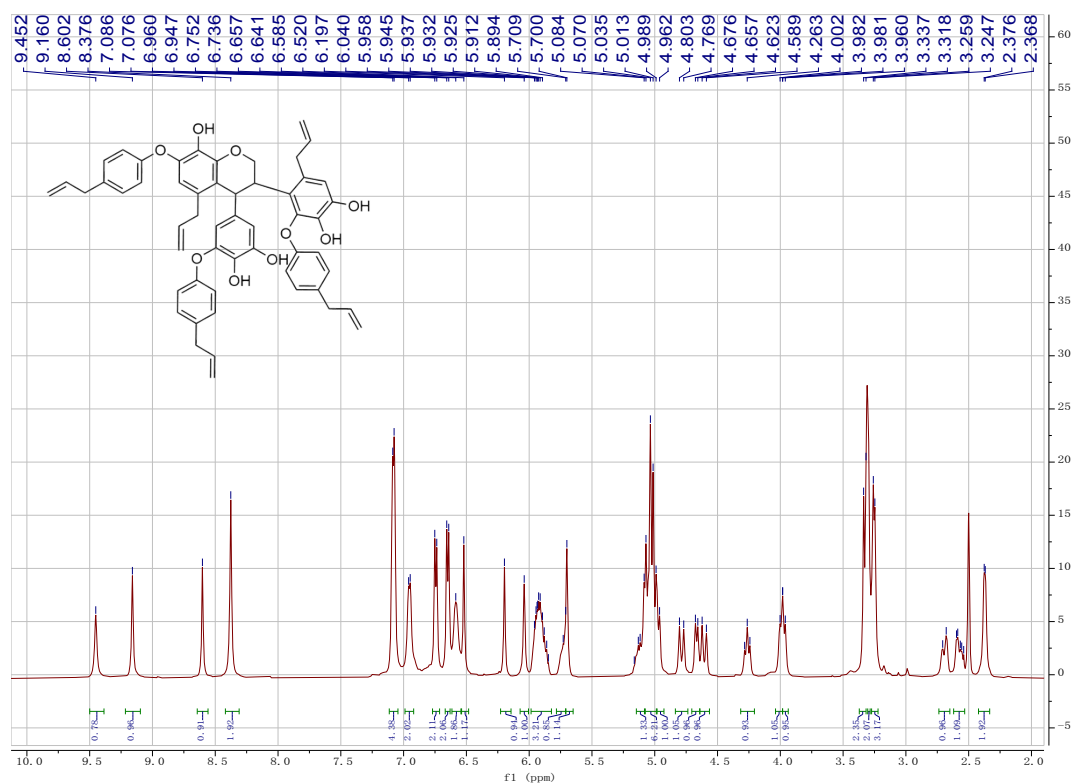


Fig. S3. ¹³C NMR spectrum (100 MHz, DMSO-*d*₆) of maglignan A (1).

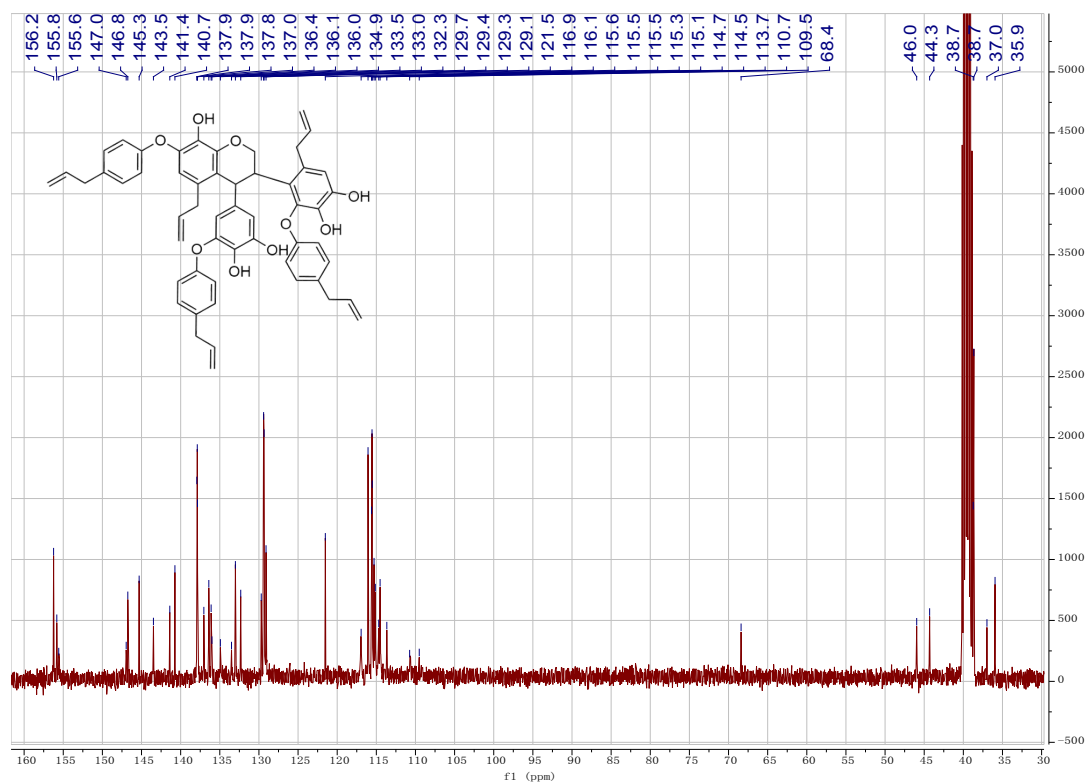


Fig. S4. DEPT spectrum of maglignan A (1).

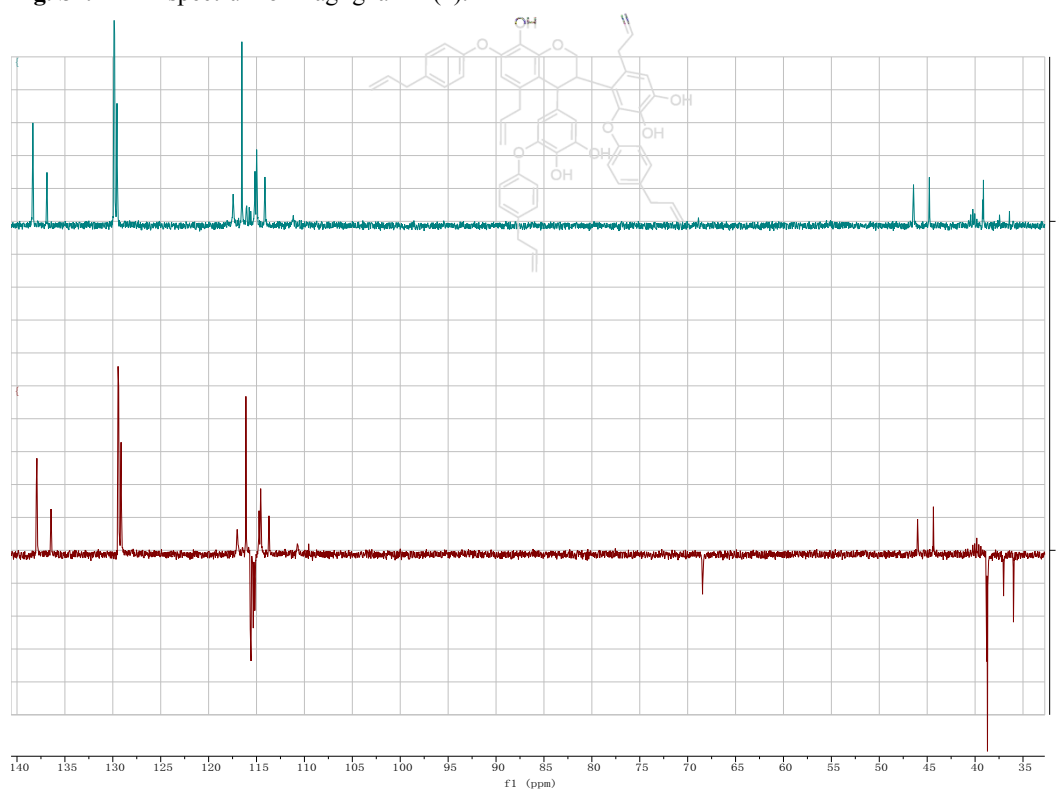


Fig. S5. HSQC spectrum of maglignan A (1).

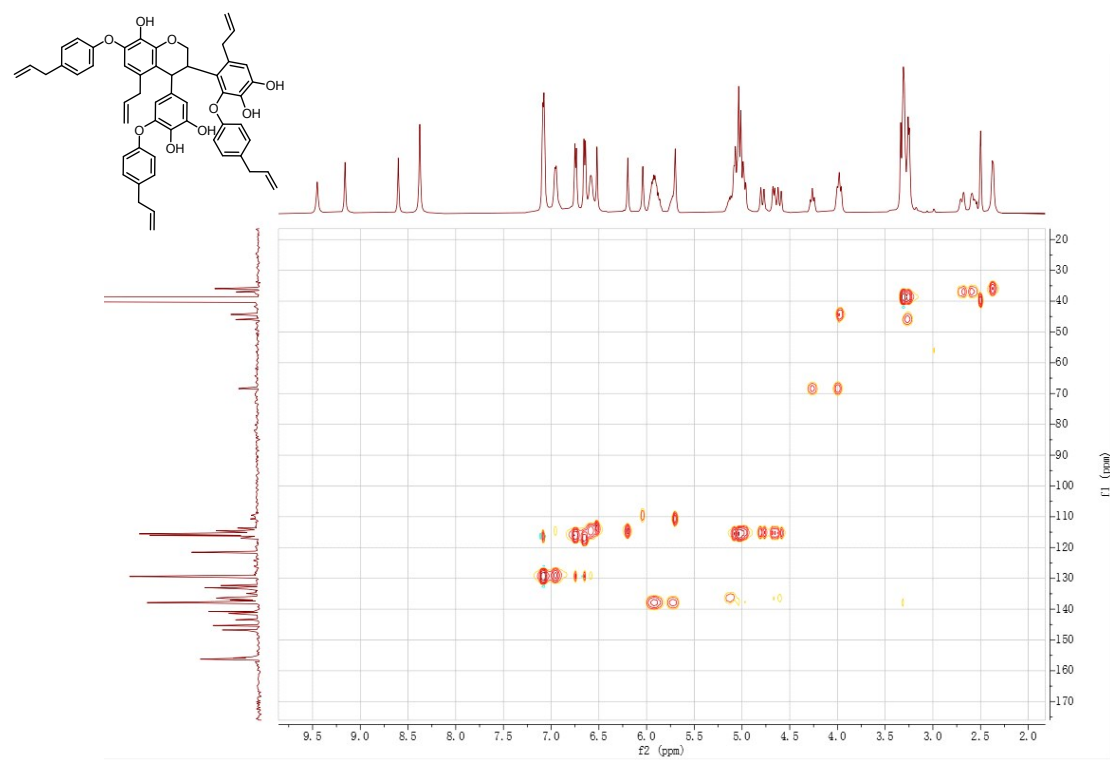


Fig. S6. HMBC spectra (400 MHz and 600 MHz) of maglignan A (1).

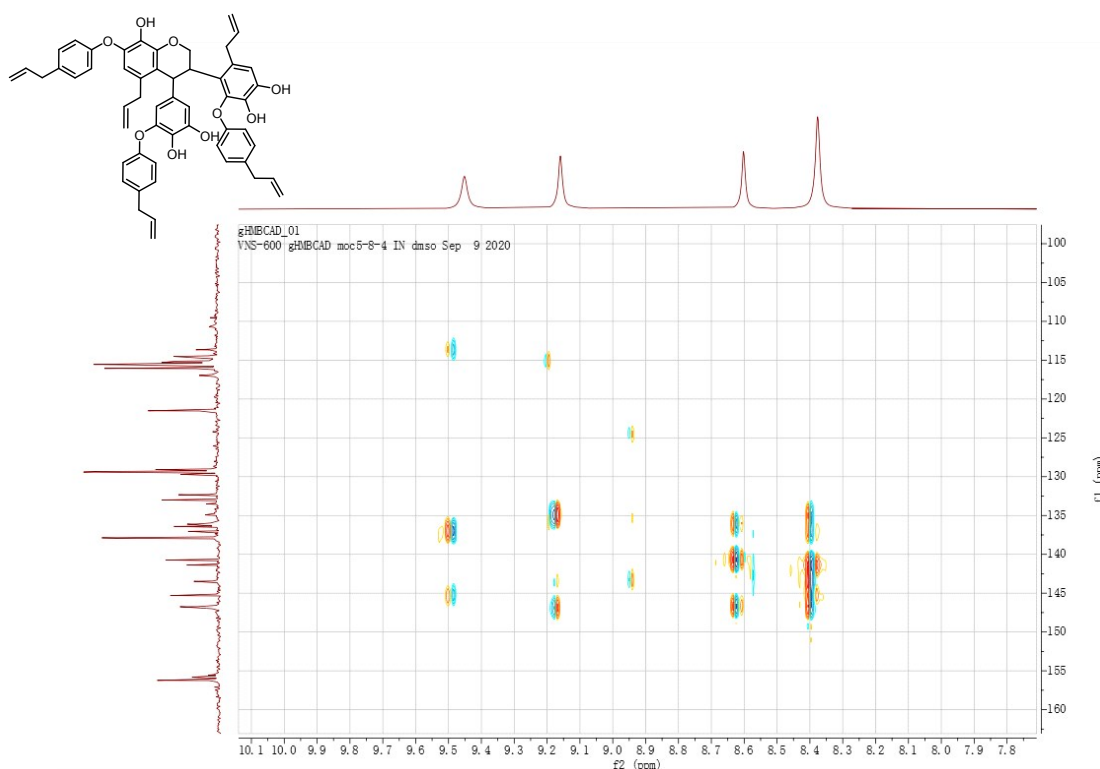
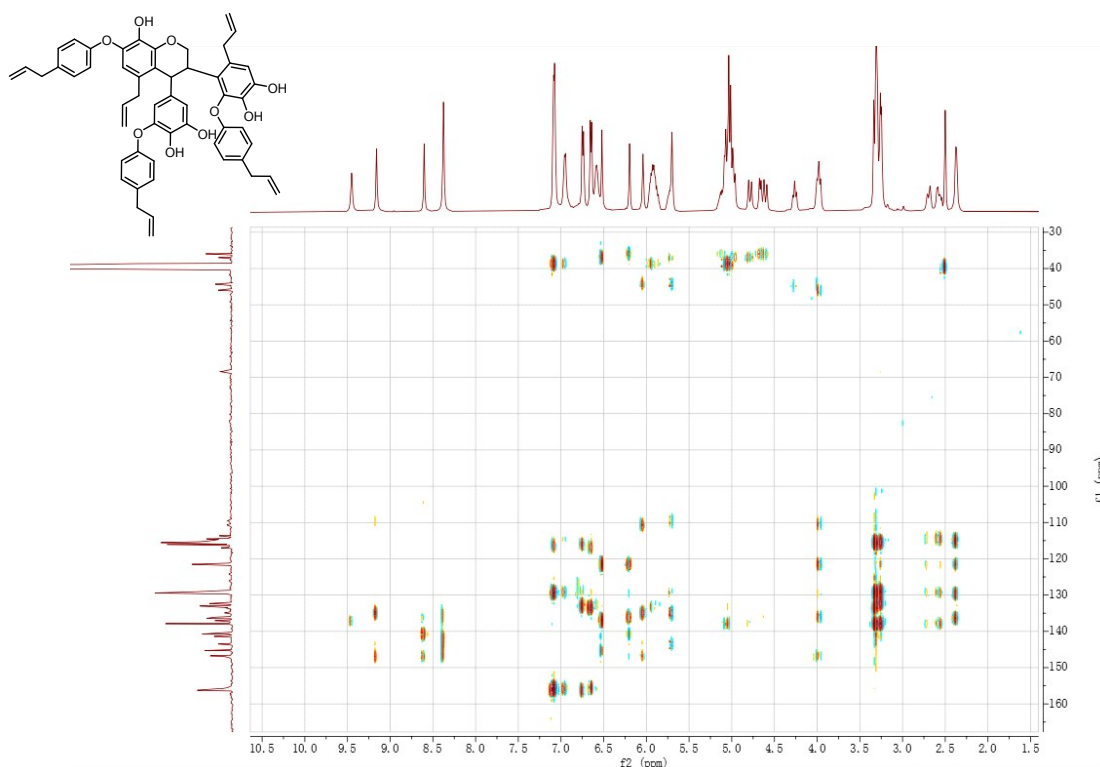


Fig. S7. ^1H - ^1H COSY spectrum of maglignan A (**1**).

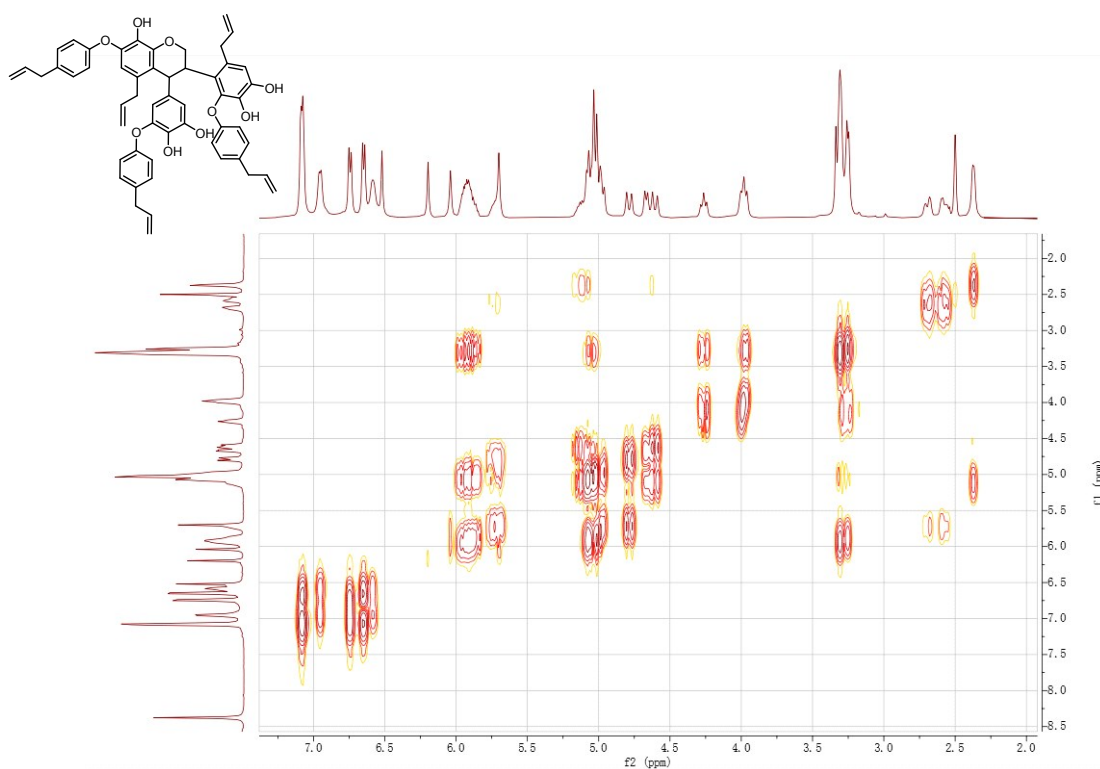
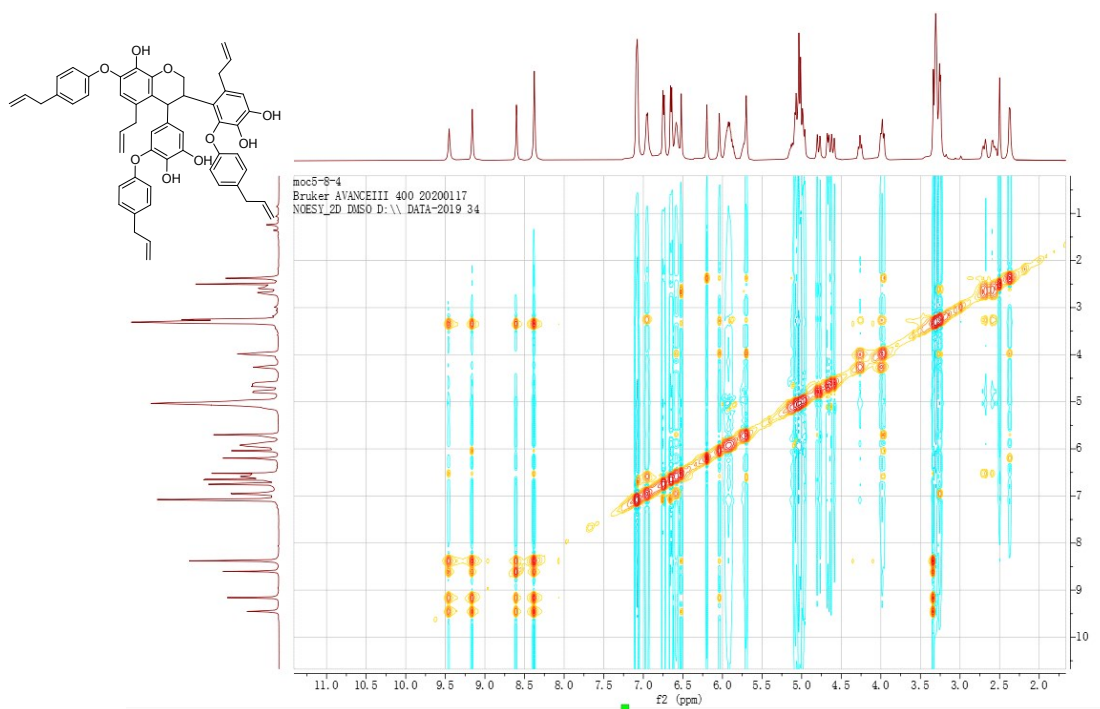


Fig. S8. NOESY spectrum of maglignan A (**1**).



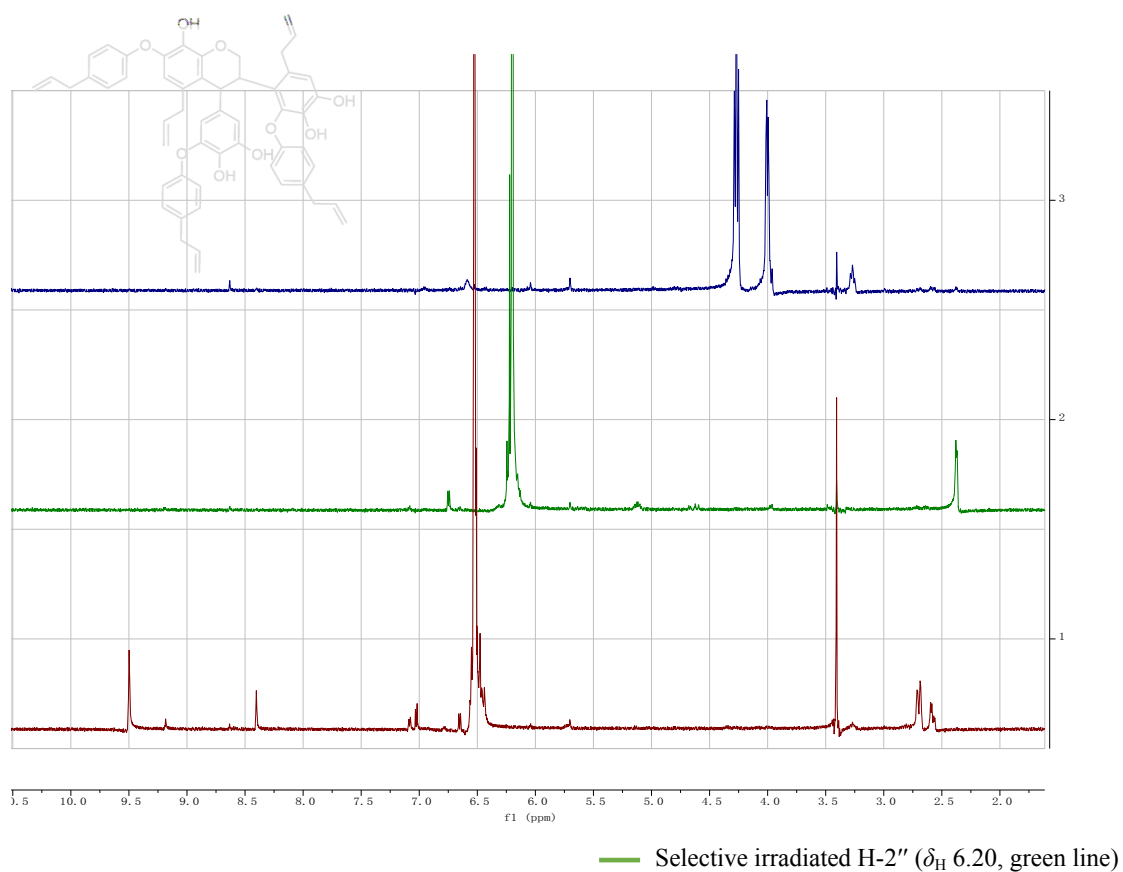


Fig. S9. IR spectrum of maglignan A (1).

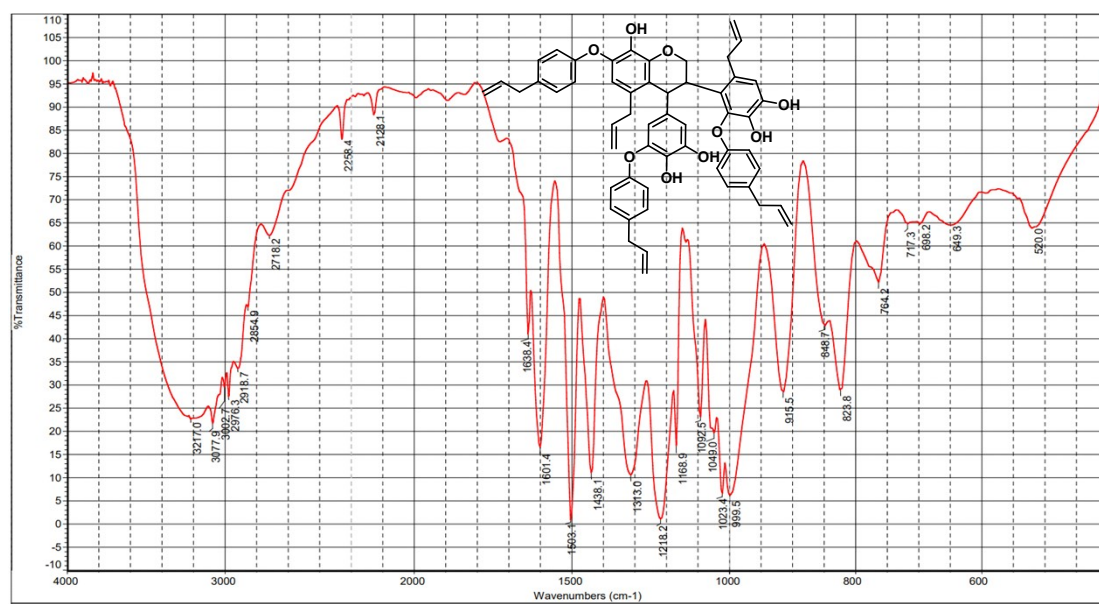


Fig. S10. UV spectrum of maglignan A (1).

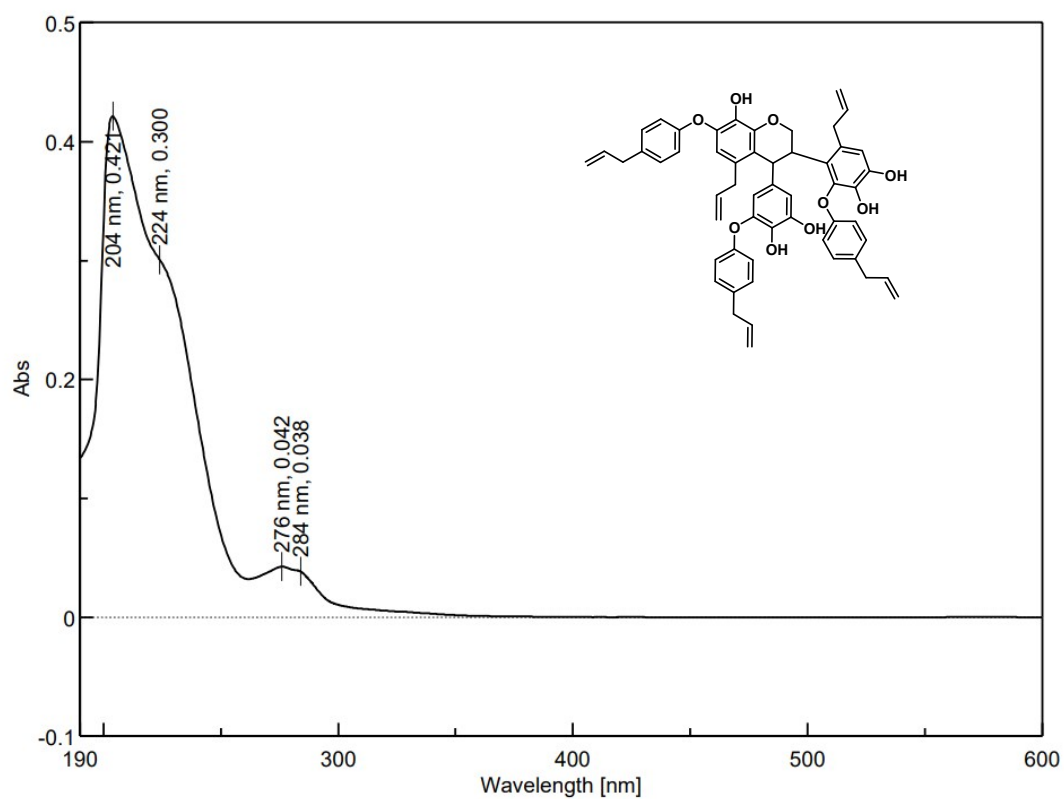


Fig. S11 HPLC separation chromatogram of (+)/(-)-1 on the chiral AD-H column.

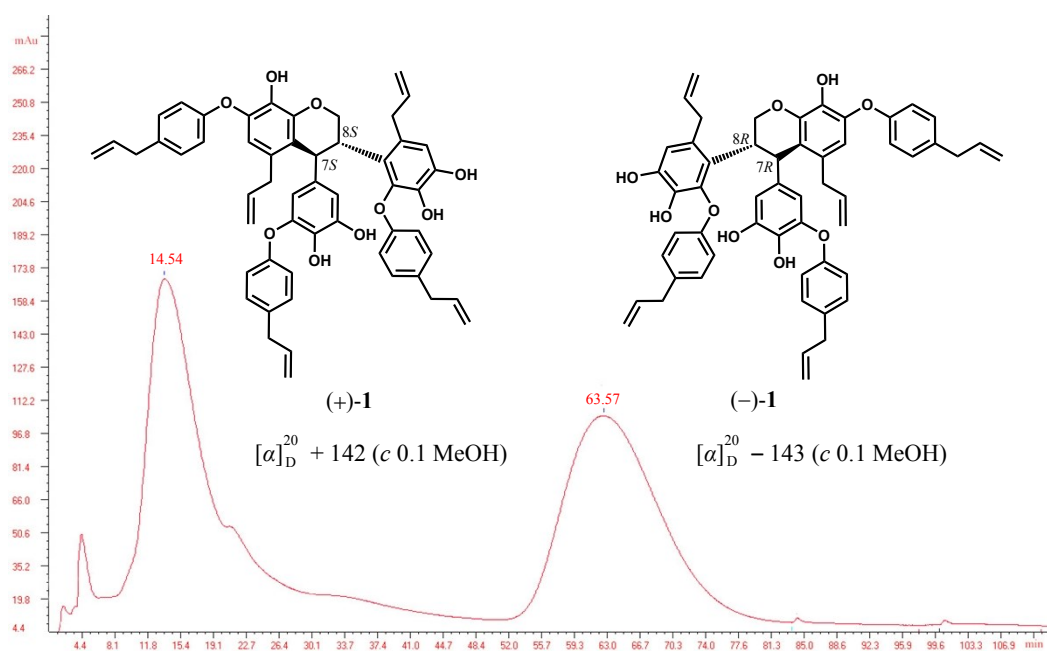


Fig. S12. ECD spectrum of maglignan A (**1**).

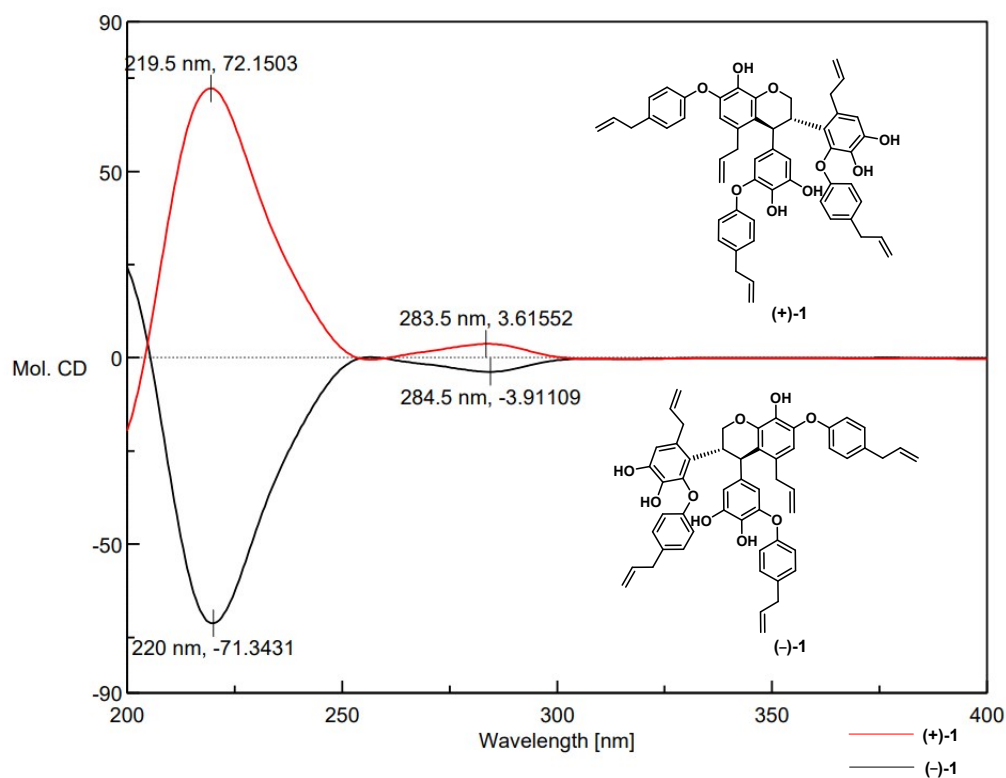
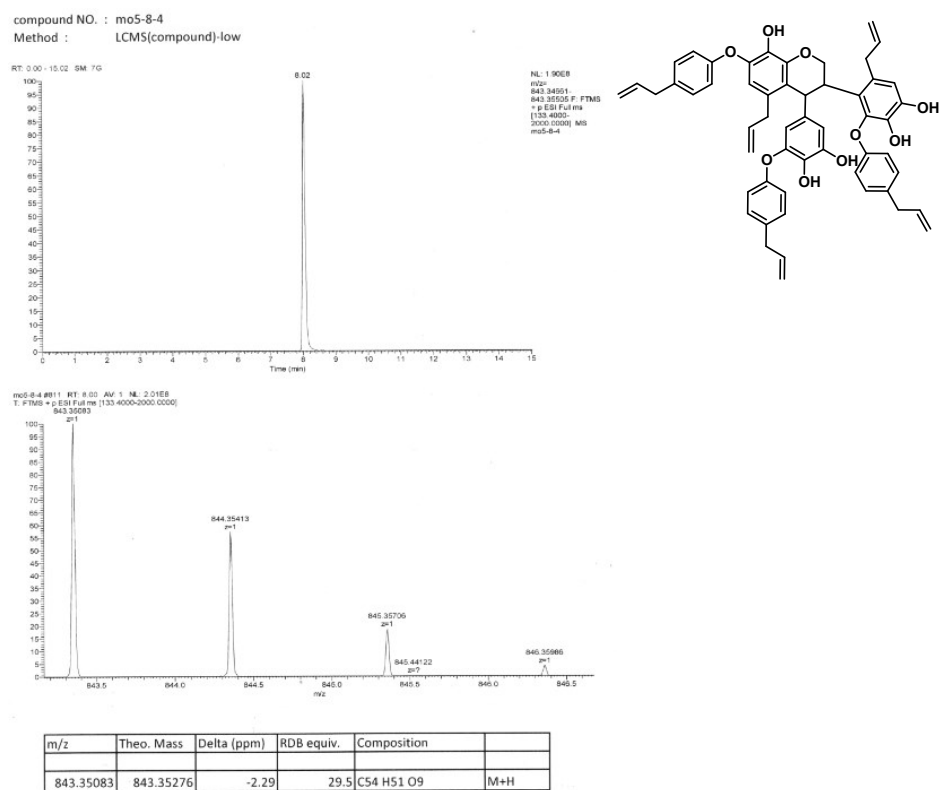


Fig. S13. HRESIMS spectrum of maglignan A (**1**).



Maglignan B (2)

Fig. S14. ¹H NMR spectrum (600 MHz, DMSO-*d*₆) of maglignan B (2).

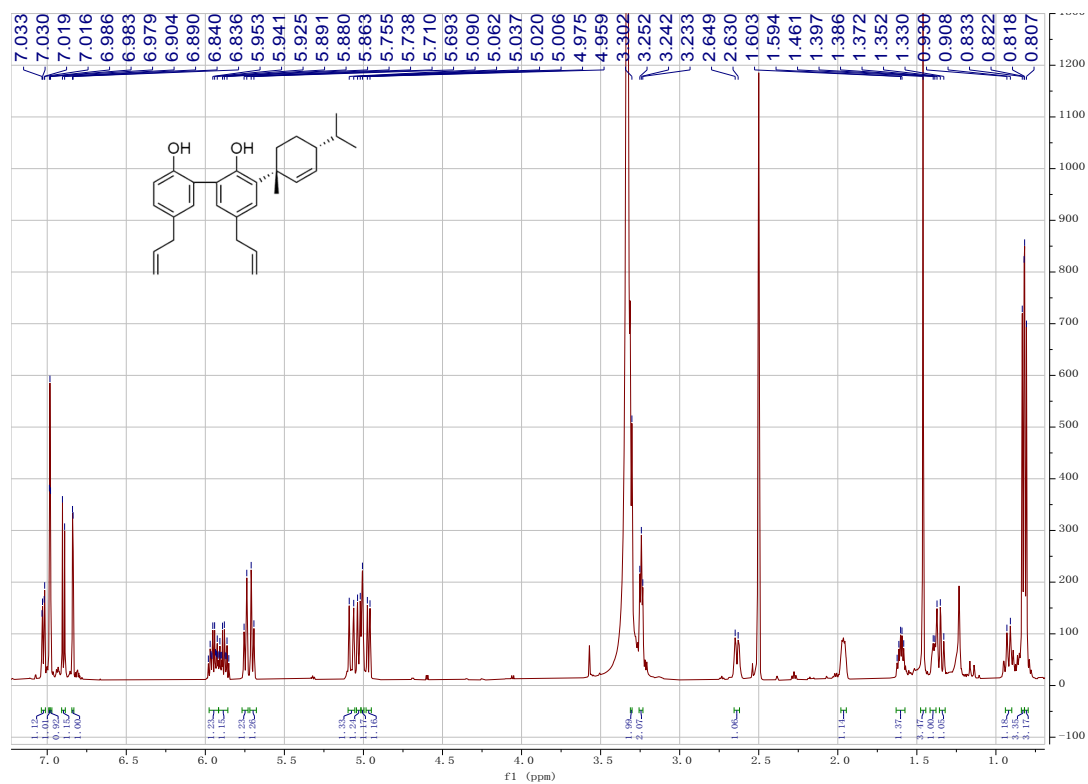


Fig. S15. ¹³C NMR spectrum (100 MHz, DMSO-*d*₆) of maglignan B (2).

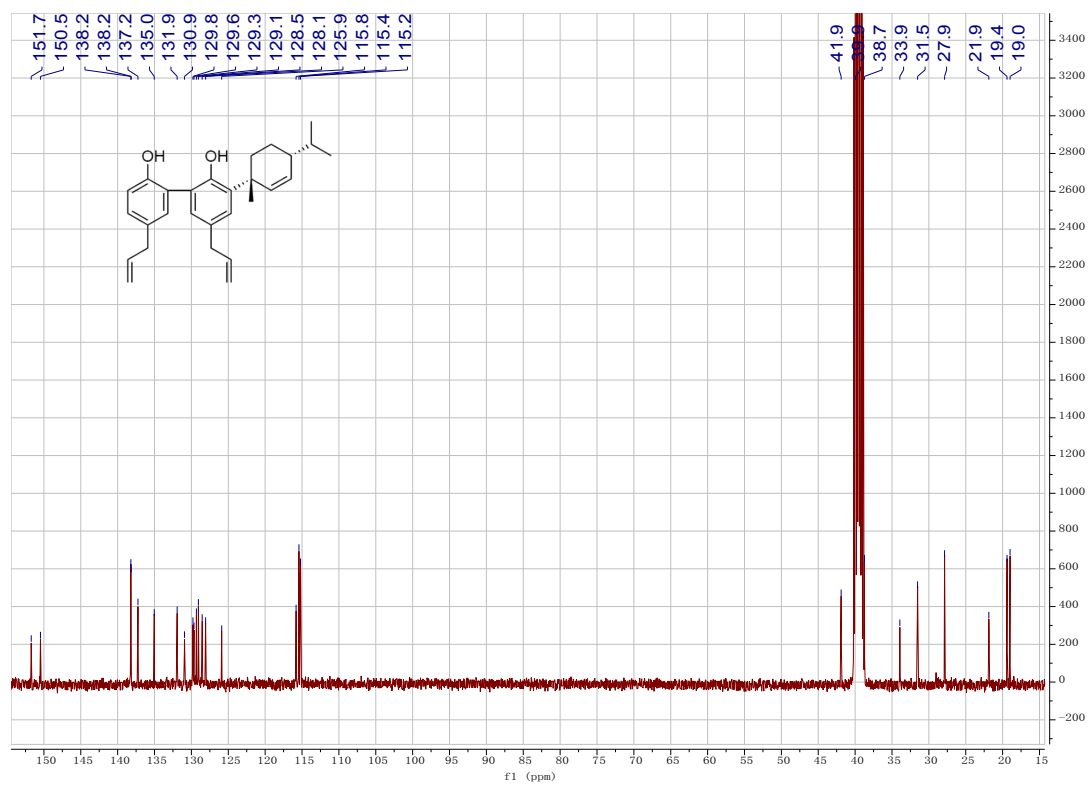


Fig. S16. DEPT spectrum of maglignan B (2).

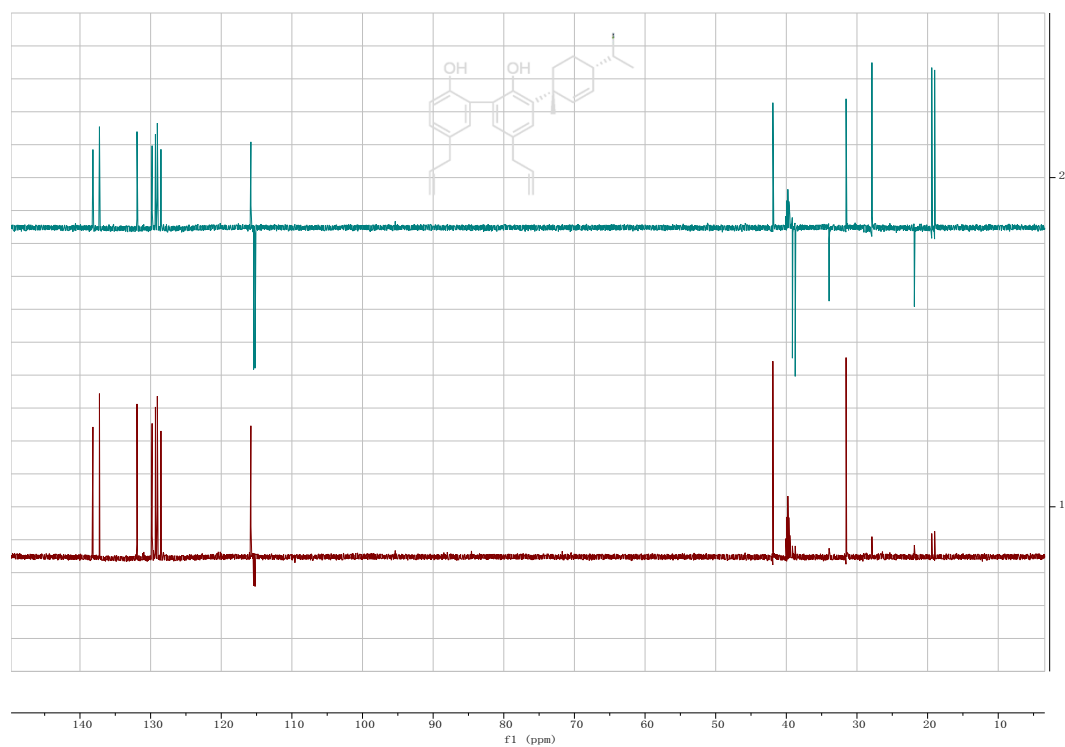


Fig. S17. HSQC spectrum of maglignan B (2).

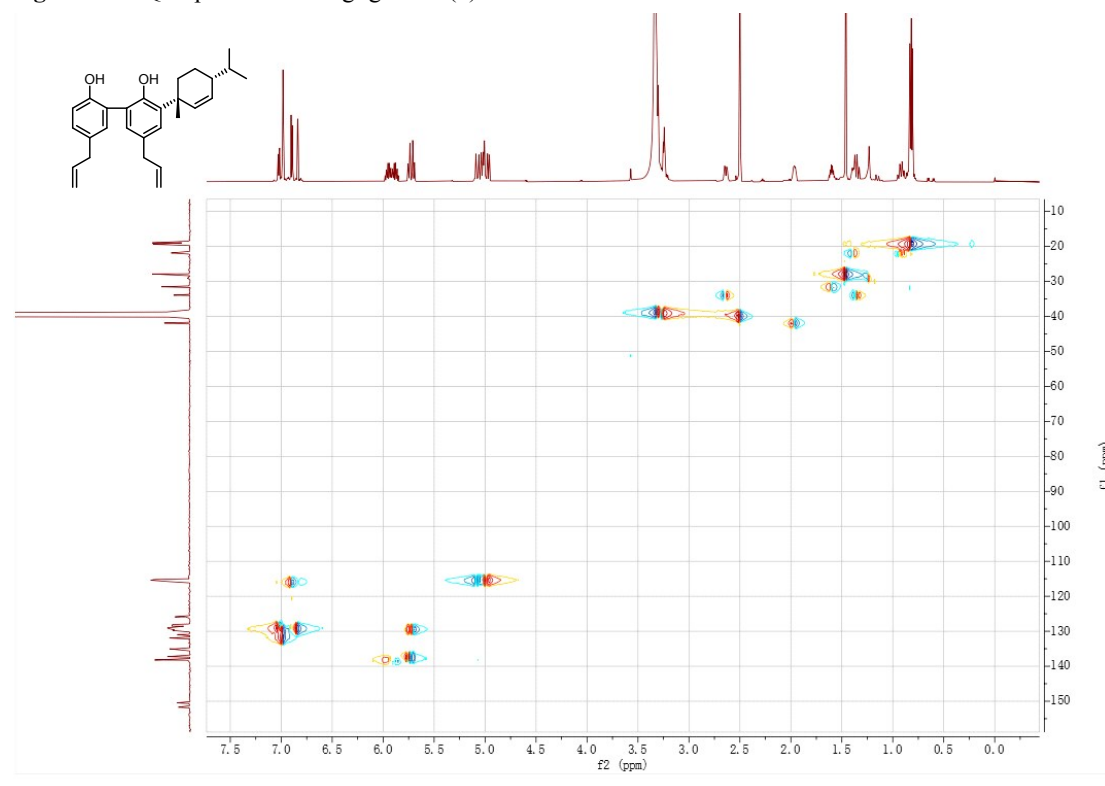


Fig. S18. HMBC spectrum of maglignan B (2).

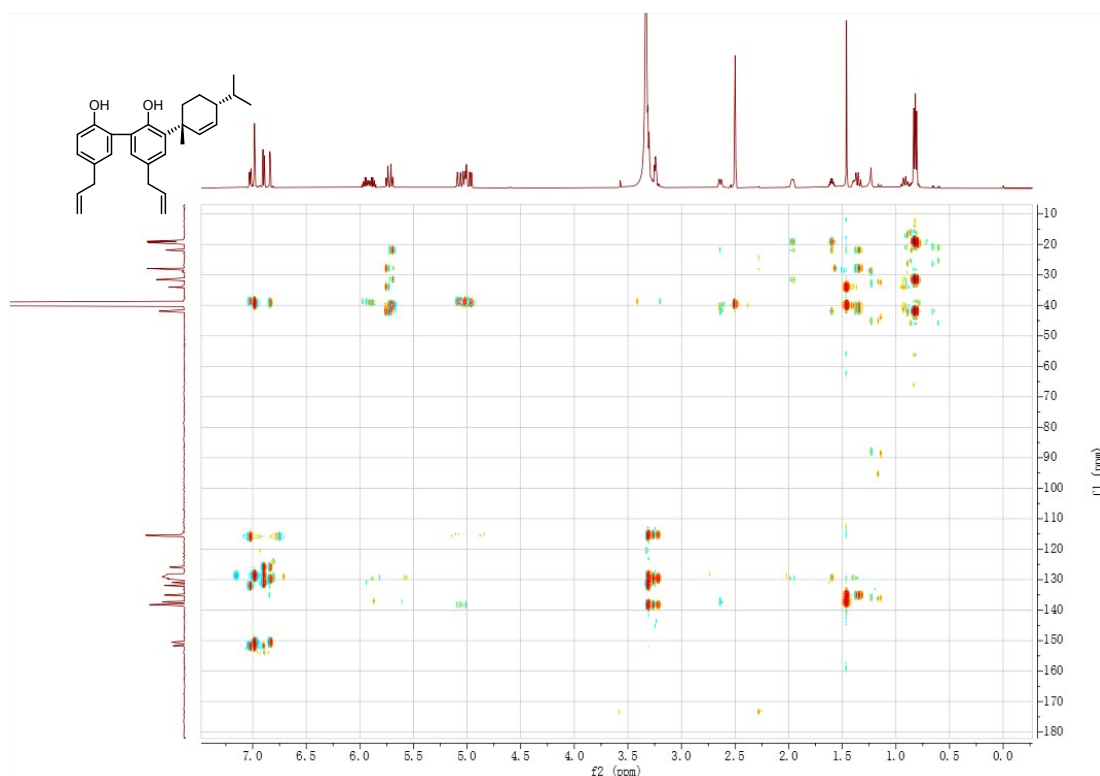


Fig. S19. ¹H-¹H COSY spectrum of maglignan B (2).

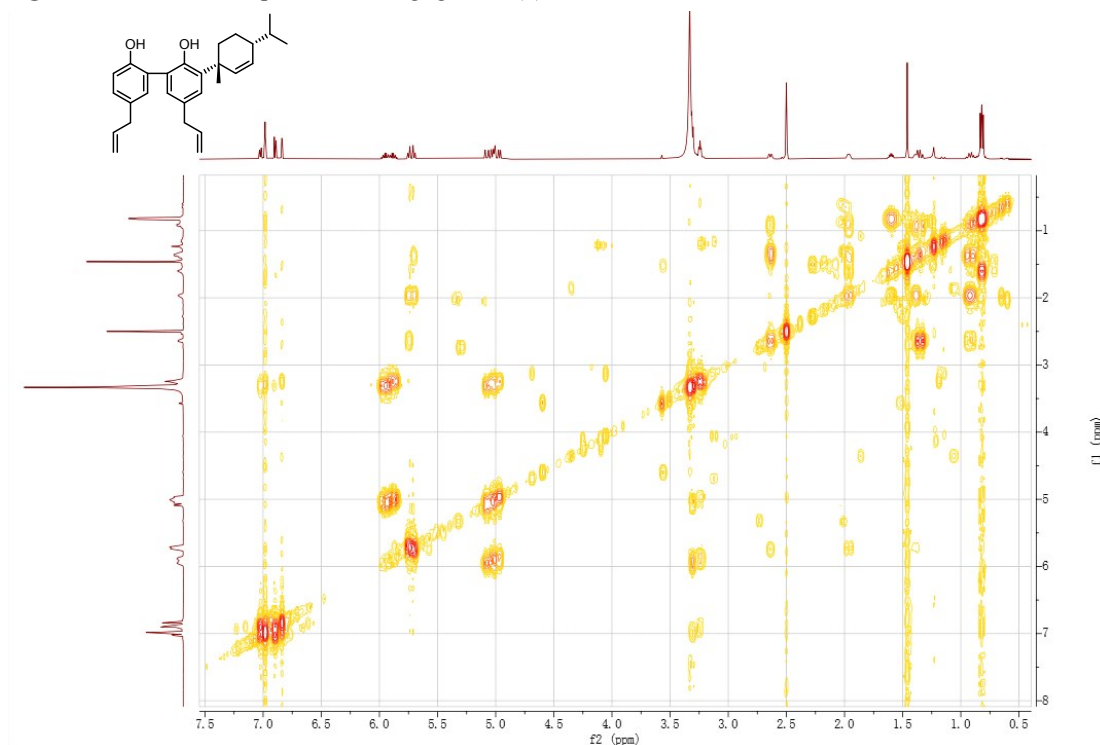


Fig. S20. NOESY spectrum of maglignan B (2).

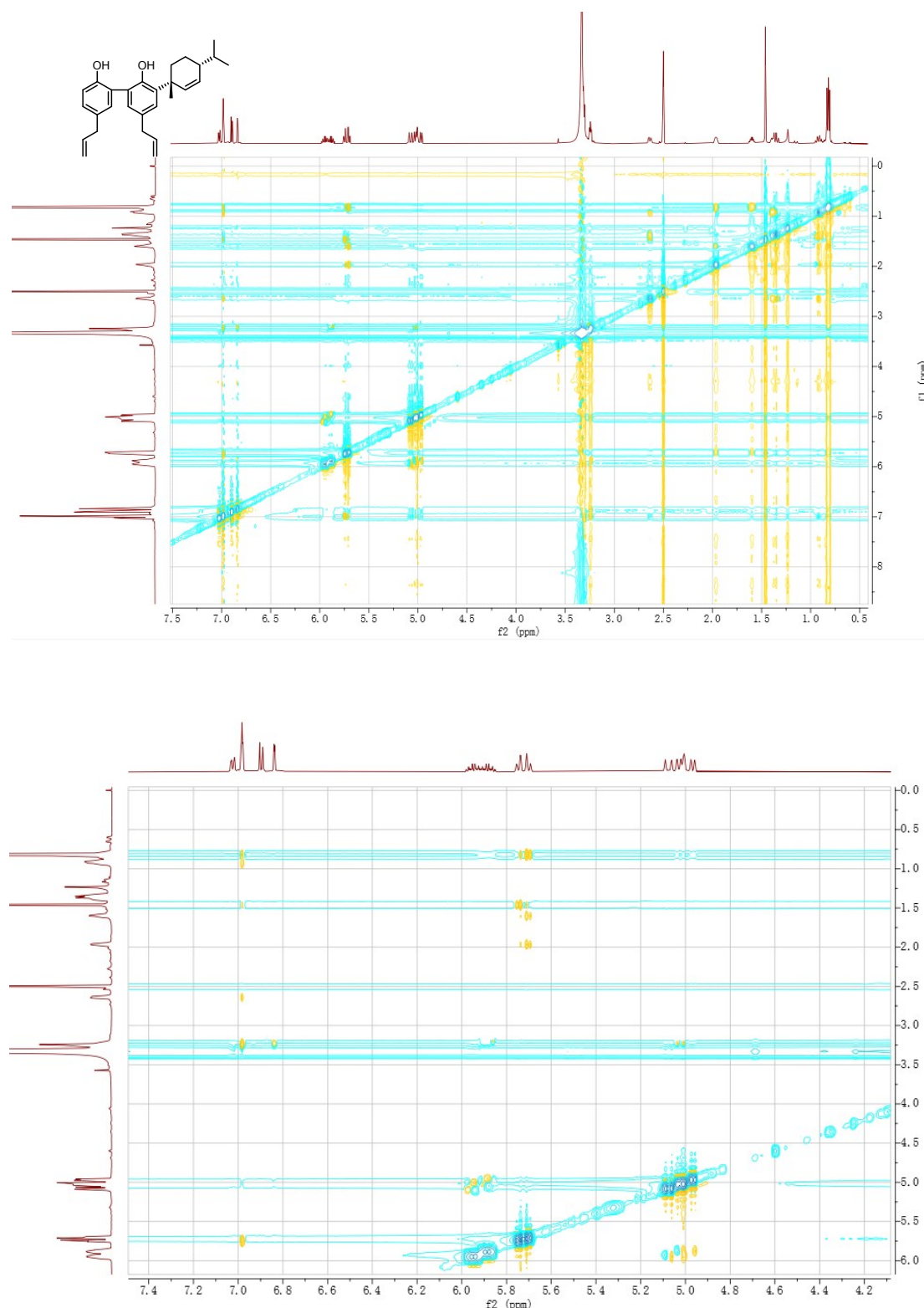


Fig. S21. IR spectrum of maglignan B (2).

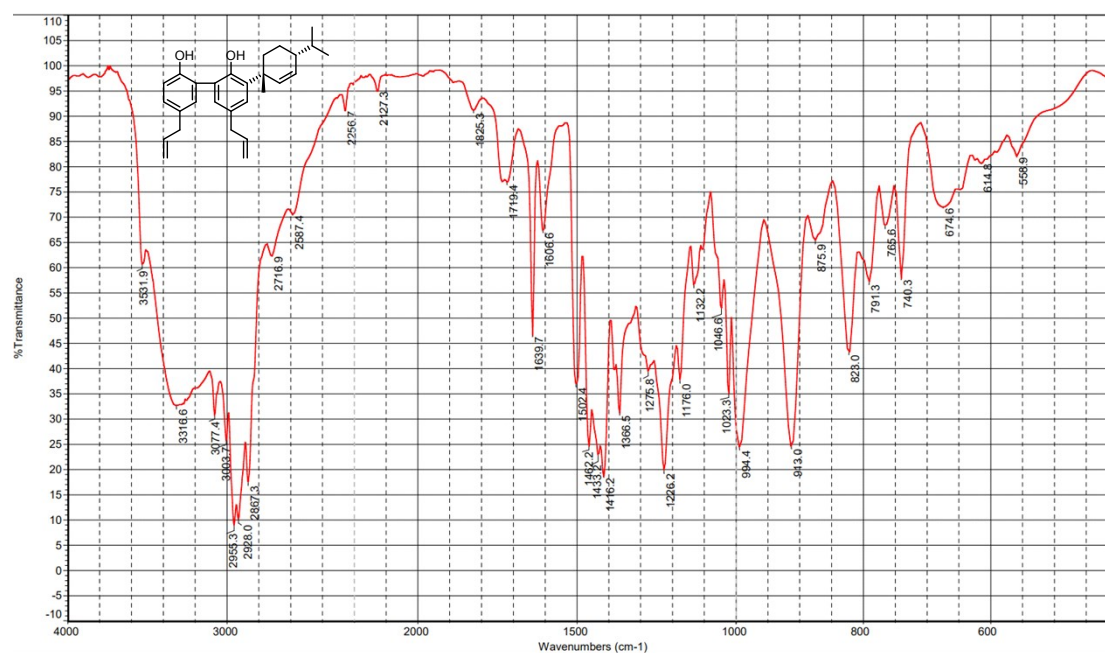


Fig. S22. UV spectrum of maglignan B (2).

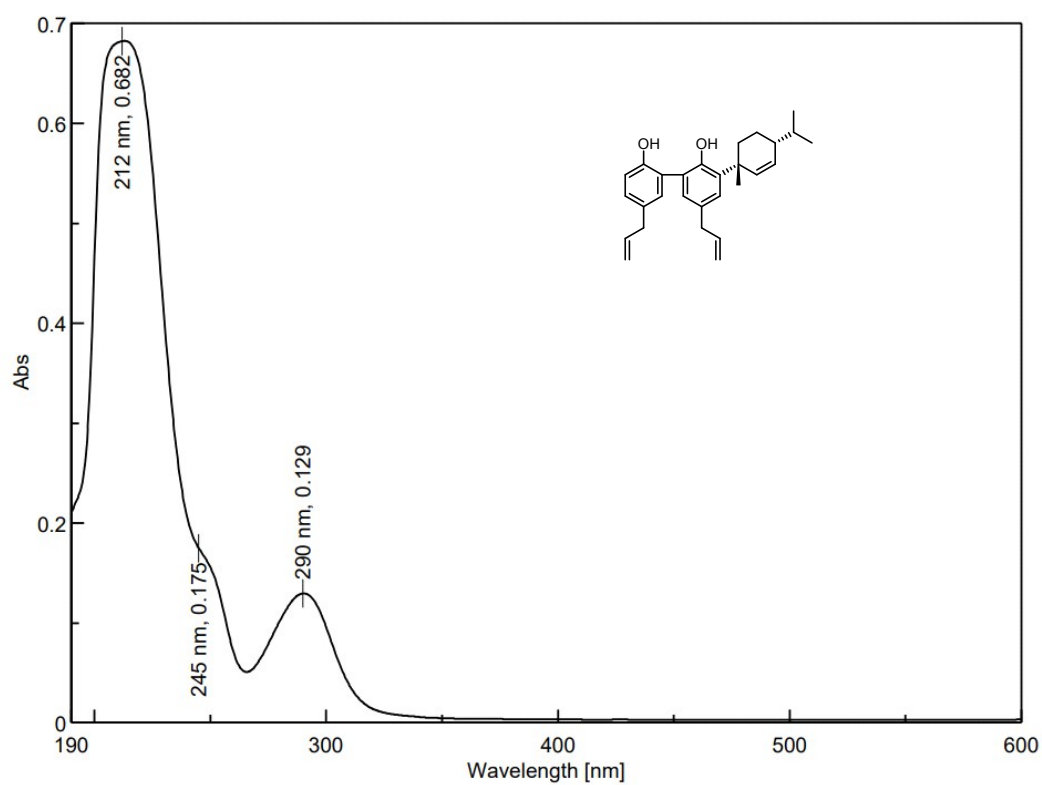


Fig. S23. ECD spectrum of maglignan B (2).

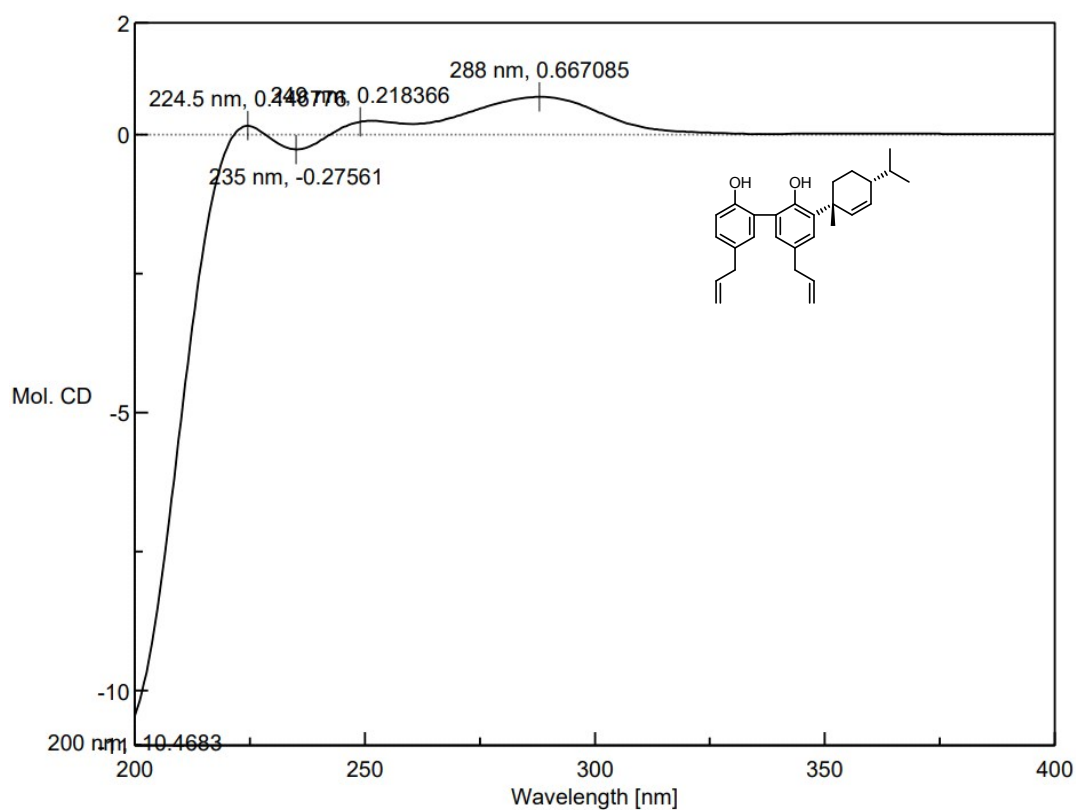
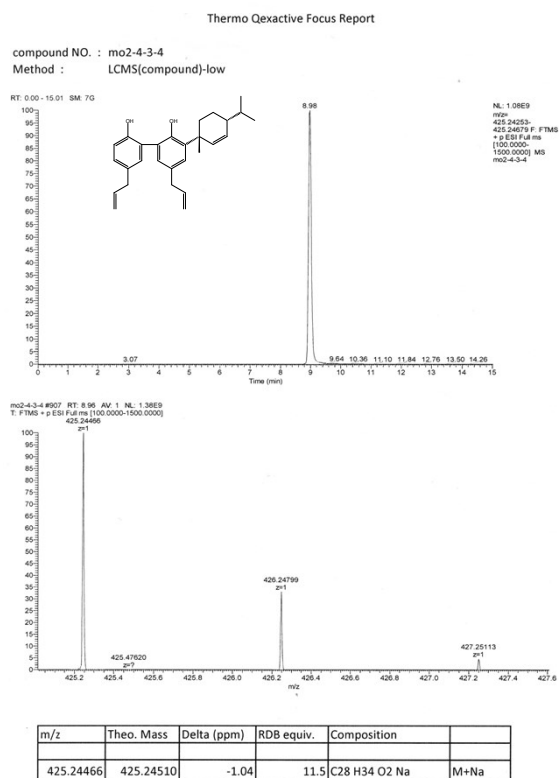


Fig. S24. HRESIMS spectrum of maglignan B (2).



Maglignan C (3)

Fig. S25. ¹H NMR spectrum (400 MHz, DMSO-*d*₆) of maglignan C (3).

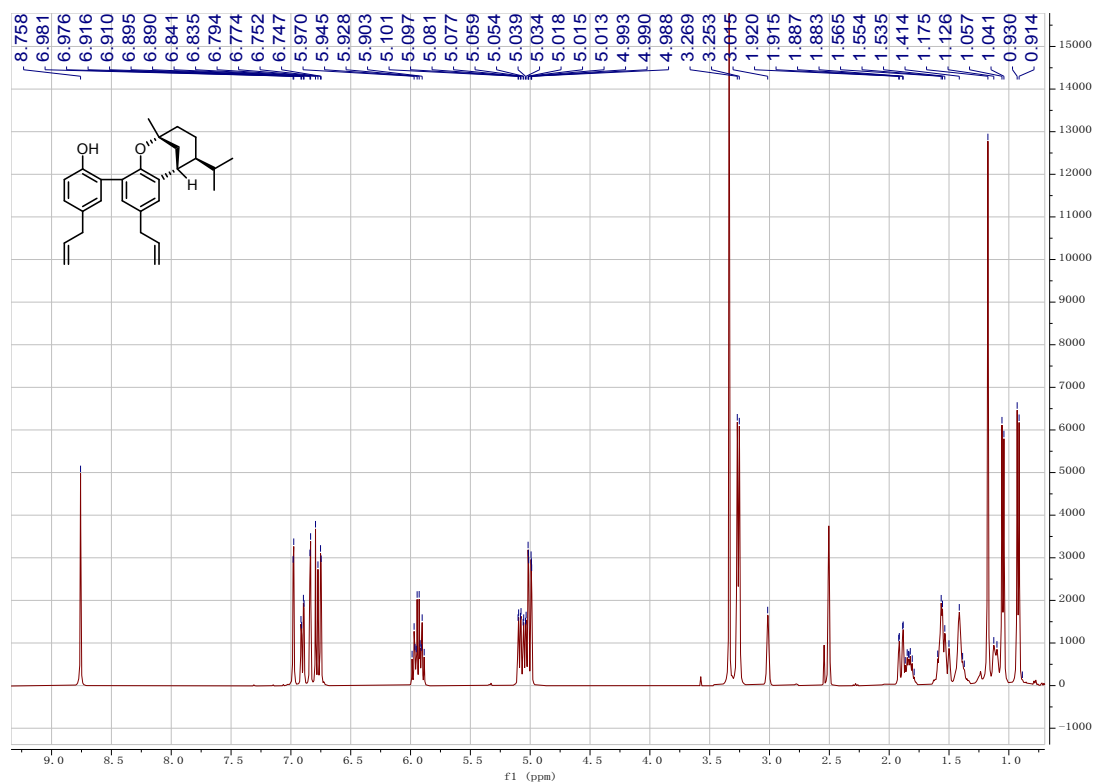


Fig. S26. ¹³C NMR spectrum (100 MHz, DMSO-*d*₆) of maglignan C (3).

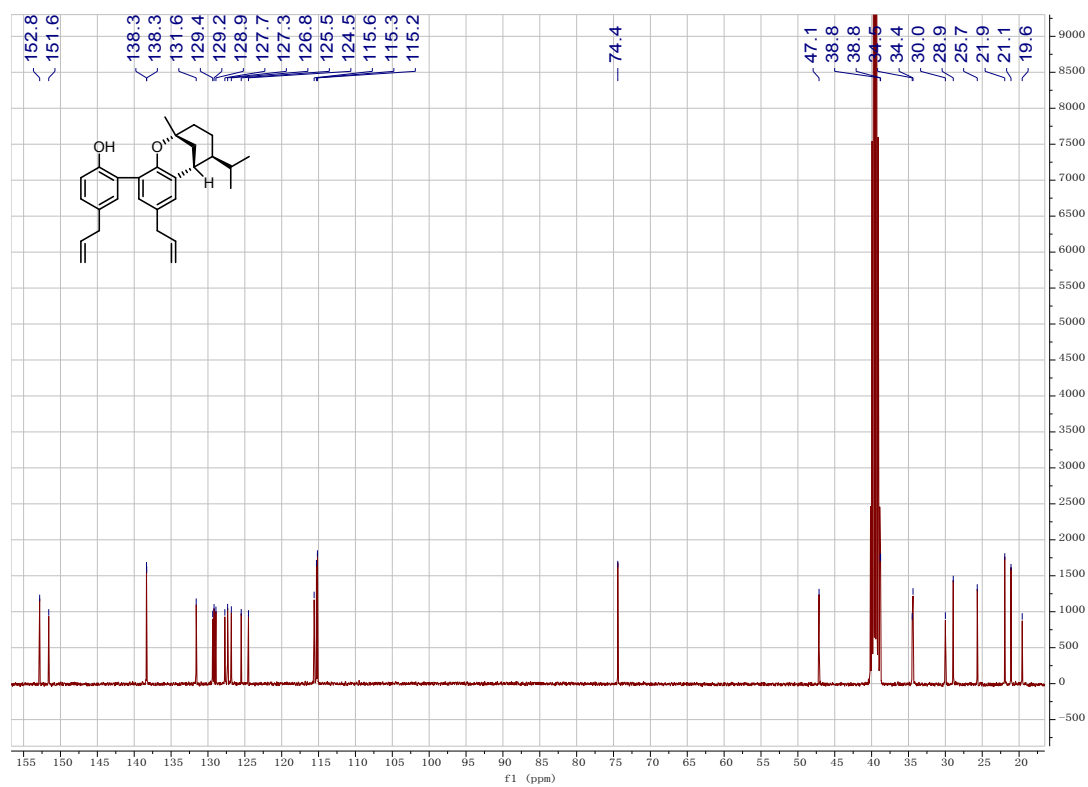


Fig. S27. DEPT spectrum of maglignan C (3).

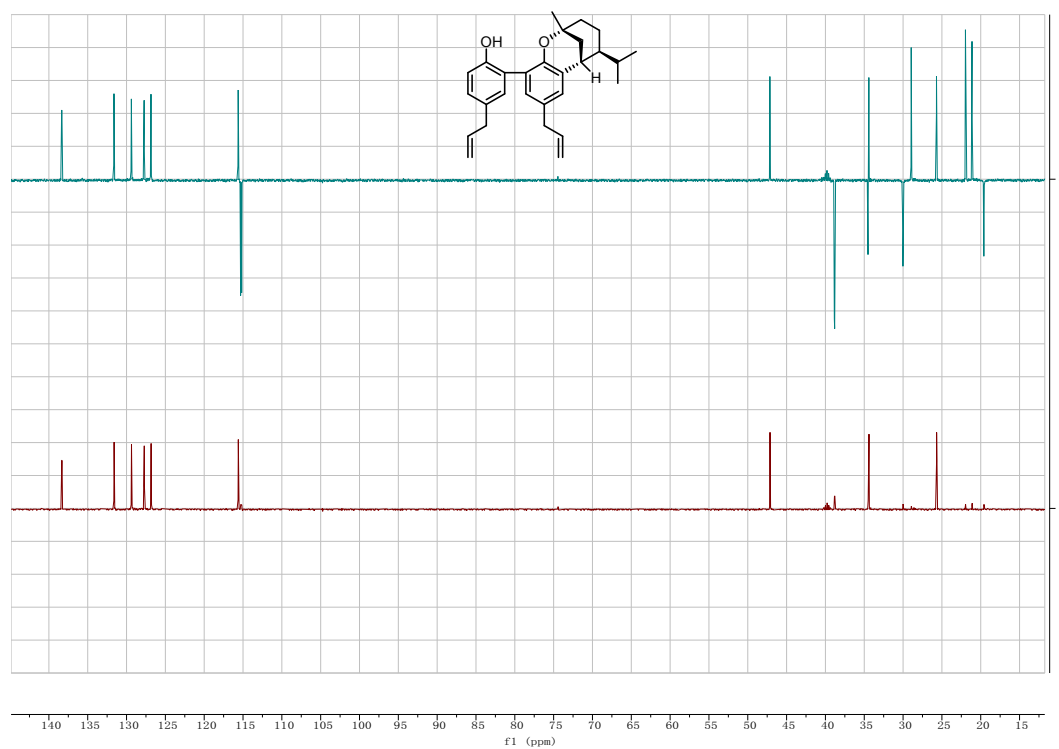


Fig. S28. HSQC spectrum of maglignan C (3).

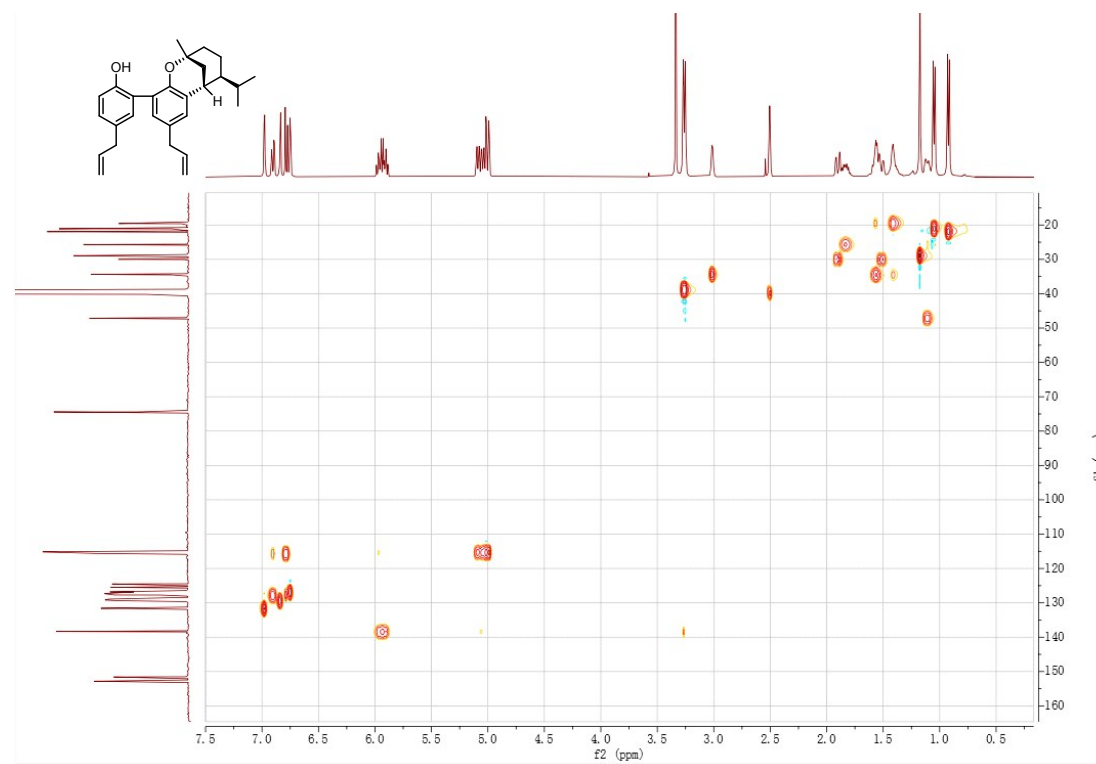


Fig. S29. HMBC spectrum of maglignan C (3).

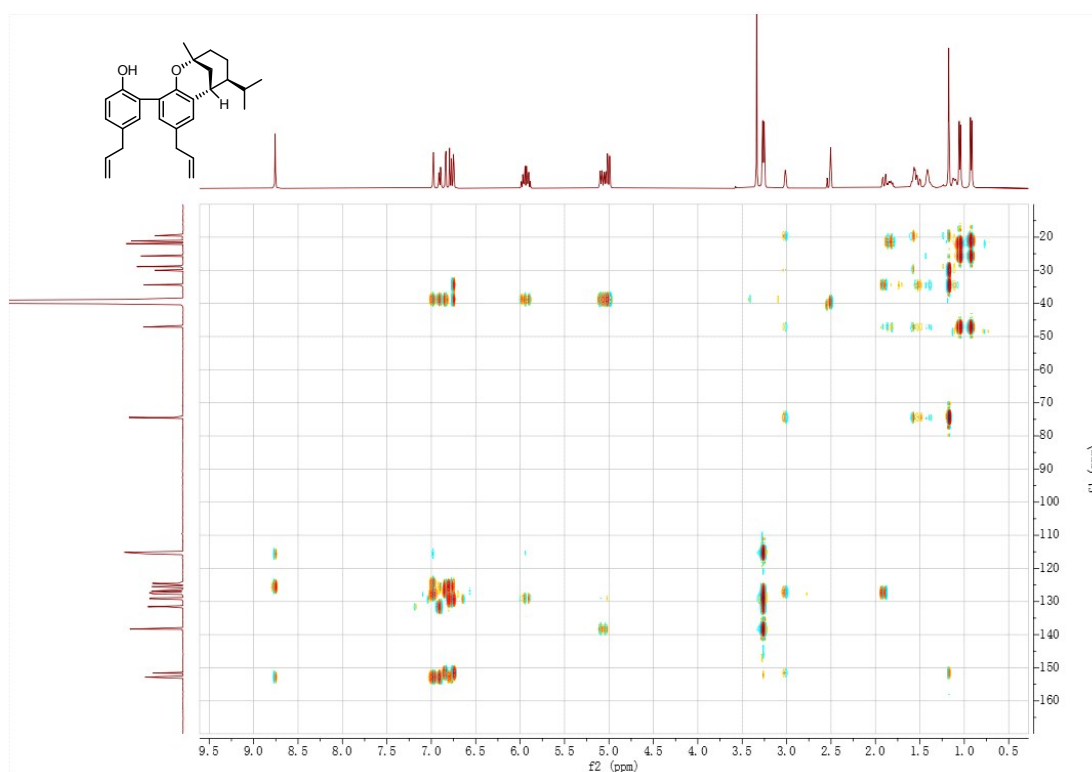


Fig. S30. ^1H - ^1H COSY spectrum of maglignan C (3).

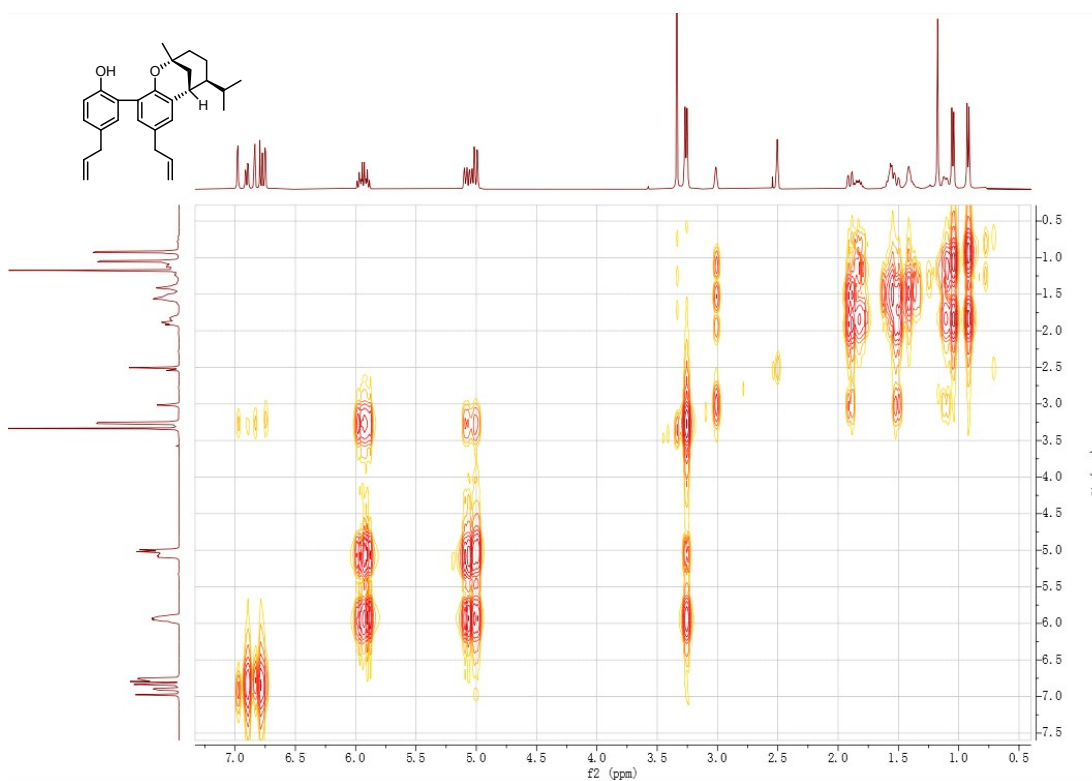


Fig. S31. NOESY spectrum of maglignan C (3).

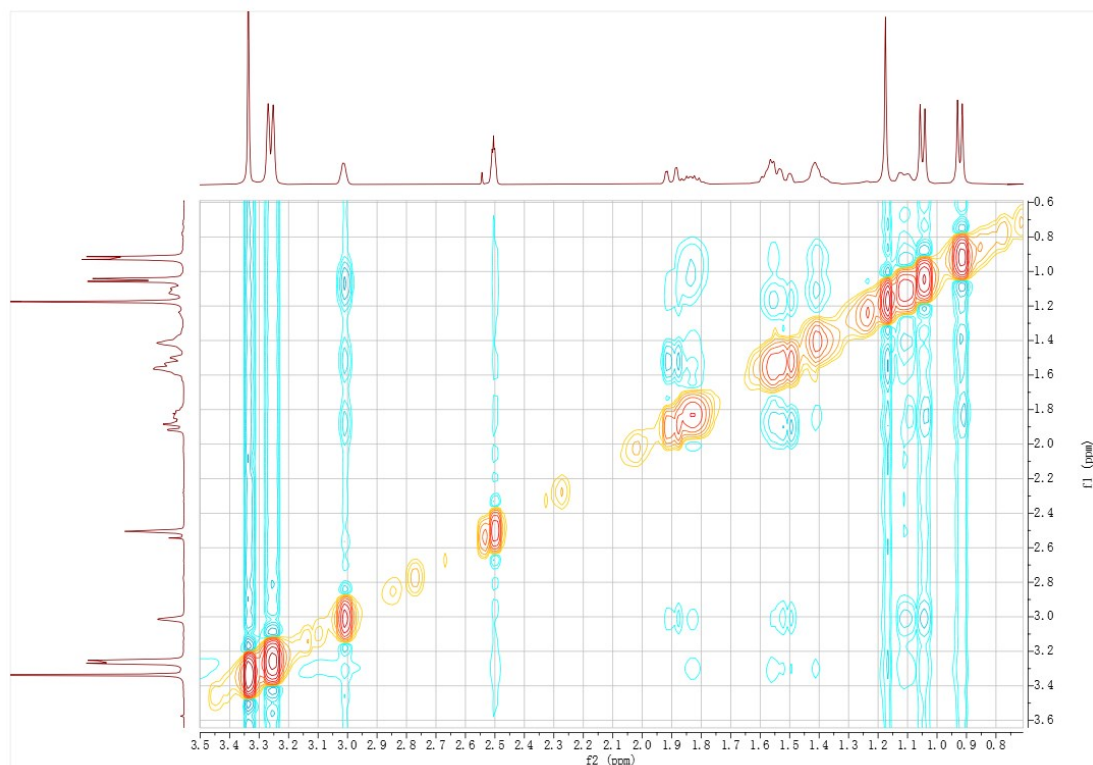
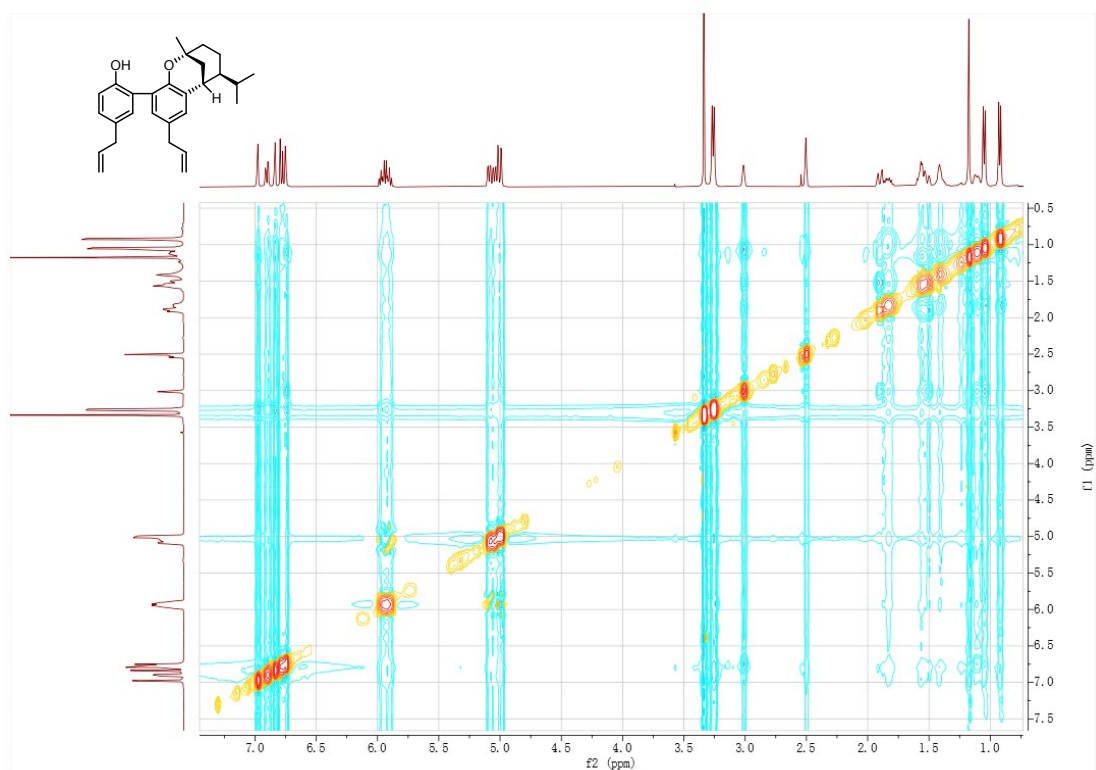


Fig. S32. IR spectrum of maglignan C (3).

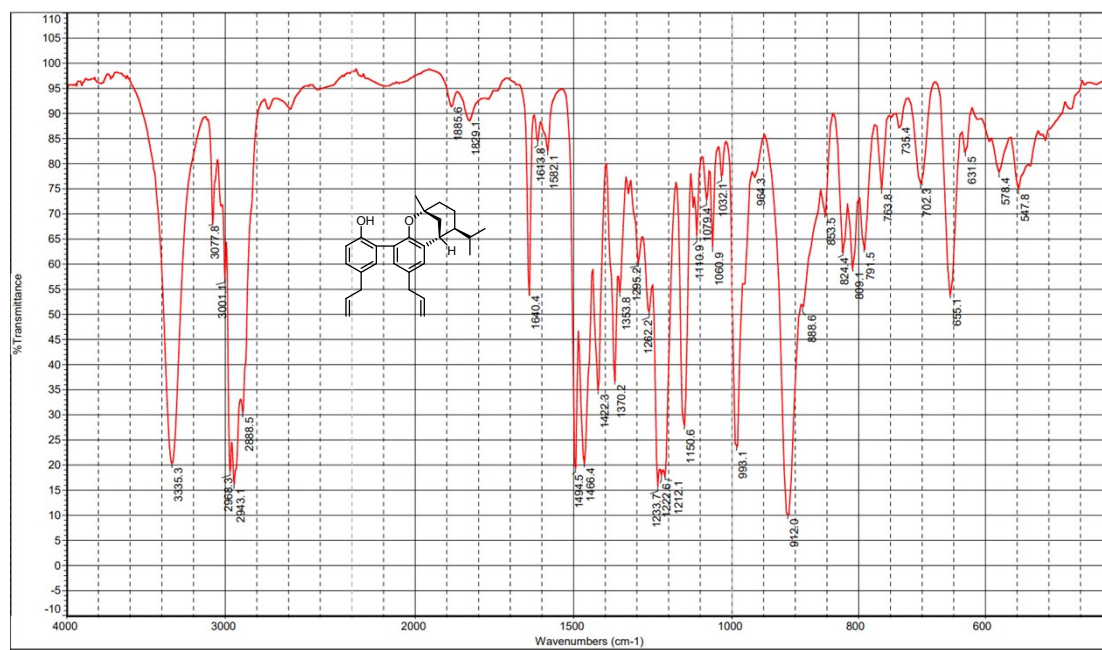


Fig. S33. UV spectrum of maglignan C (3).

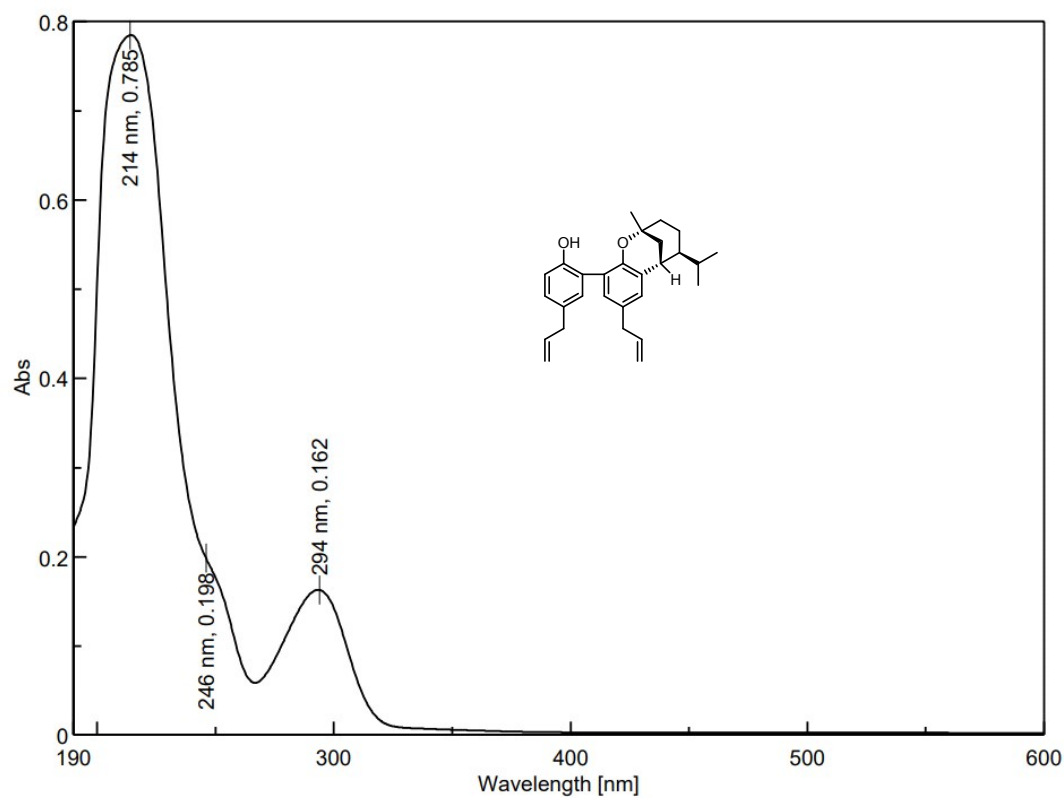


Fig. S34. CD spectrum of maglignan C (3).

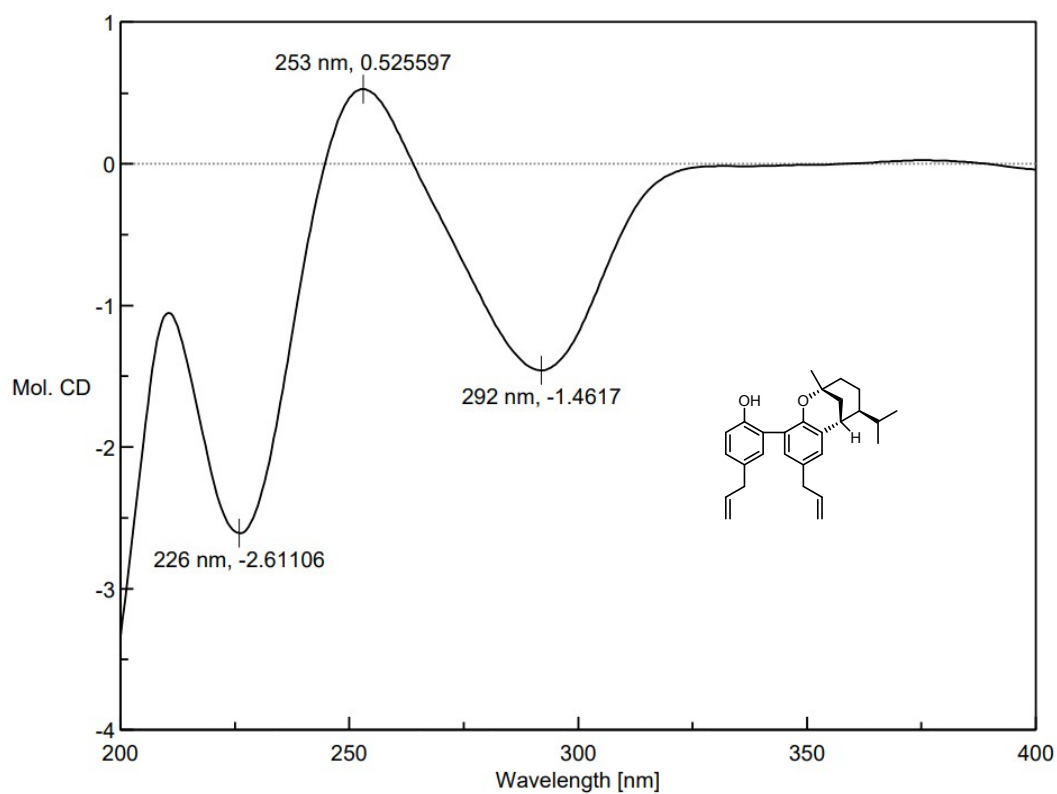


Fig. S35. HRESIMS spectrum of maglignan C (3).

