

SUPPLEMENTARY MATERIAL

Two new compounds from the heartwood of *Dalbergia melanoxylon*

Shuai Lin^a, Rong-hua Liu^a, Guang-qiang Ma^b, Dan-yi Mei^a, Feng Shao^{a*}, Lan-ying Chen^a

a. Key Laboratory of Innovation Drug and Efficient Energy-saving Pharmaceutical Equipment, Jiangxi University of Traditional Chinese Medicine, Nanchang, China

b. College of basic medical, Jiangxi University of Traditional Chinese Medicine, Nanchang, China

Shuai Lin: E-mail: 1070692432@qq.com

Rong-hua Liu: E-mail: rhliu@163.com

Guang-qiang Ma: E-mail: 20101002@jxutcm.edu.cn

Dan-yi Mei: E-mail: 18942351213@163.com

Lan-ying Chen: E-mail: clyxy2513@163.com

*Corresponding author:

Feng Shao: E-mail: shaofeng0729@163.com, Tel. /Fax: +86-791-87118658

Abstract: A new neoflavonoid, named *S*(+)-3'-hydroxy-4',2,4,5-tetramethoxydalbergiquinol (**1**), and a new benzofuran, named (2*S*,3*S*)-5-hydroxy-6-methoxy-3-methyl-2-(4'-hydroxyphenyl)-2,3dihydrobenzofuran (**4**), together with two known neoflavonoids, were isolated from the heartwood of *Dalbergia melanoxylon*. Their structures were elucidated by a combination of spectroscopic methods and comparison with the literature. Compounds **1-4** were evaluated for inhibitory activity against *Staphylococcus aureus* ATCC 25923, *Escherichia coli* ATCC 6538, *Salmonella enteri* CMCC 50041 and *Candida albicans* ATCC 289065 ,which all exhibited inactive or weak activity.

Key words: neoflavonoid; benzofuran; *Dalbergia melanoxylon*; antimicrobial activity

List of Supplemental Material

Figure S1. The HR-ESI-MS spectrum of compound **1**.

Figure S2. The ^1H NMR (600 MHz, CDCl_3) of compound **1**.

Figure S3. The ^{13}C NMR (150 MHz, CDCl_3) of compound **1**.

Figure S4. The HMBC spectrum of compound **1**.

Figure S5. The HSQC spectrum of compound **1**.

Figure S6. The key HMBC correlations of compound **1**.

Figure S7. The UV spectrum of compound **1**.

Figure S8. The IR spectrum of compound **1**.

Figure S9. The HR-ESI-MS spectrum of compound **4**.

Figure S10. The ^1H NMR (600 MHz, CD_3OD) of compound **4**.

Figure S11. The ^{13}C NMR (150 MHz, CD_3OD) of compound **4**.

Figure S12. The HMBC spectrum of compound **4**.

Figure S13. The part of HMBC spectrum of compound **4**.

Figure S14. The HSQC spectrum of compound **4**.

Figure S15. The H-H COSY spectrum of compound **4**.

Figure S16. The NOE spectrum of compound **4**.

Figure S17. The key HMBC correlations of compound **4**.

Figure S18. The UV spectrum of compound **4**.

Figure S19. The IR spectrum of compound **4**.

Figure S20. The CD spectrum of compound **4**.

Figure S21. The ^1H NMR (600 MHz, CDCl_3) of compound **4**.

Figure S22. X-ray ORTEP drawing of compound **4**.

Table S1. Crystal data and structure refinement for compound **4**.

Table S2. The minimum inhibitory concentration (MIC) values of the compounds against bacteria and fungus

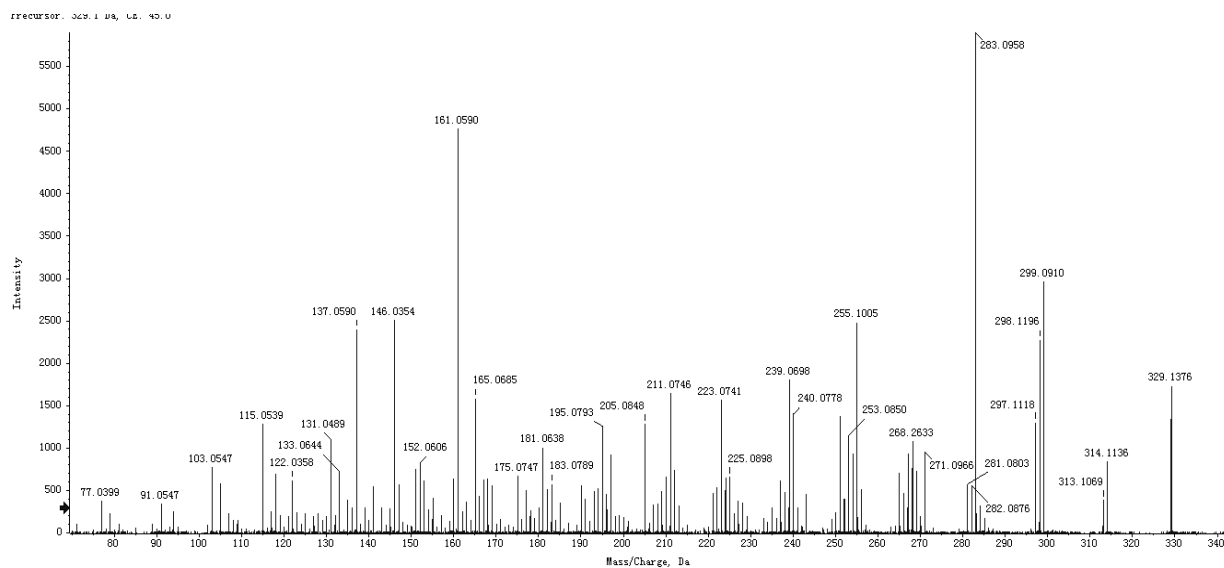


Figure S1. The HR-ESI-MS spectrum of compound 1.

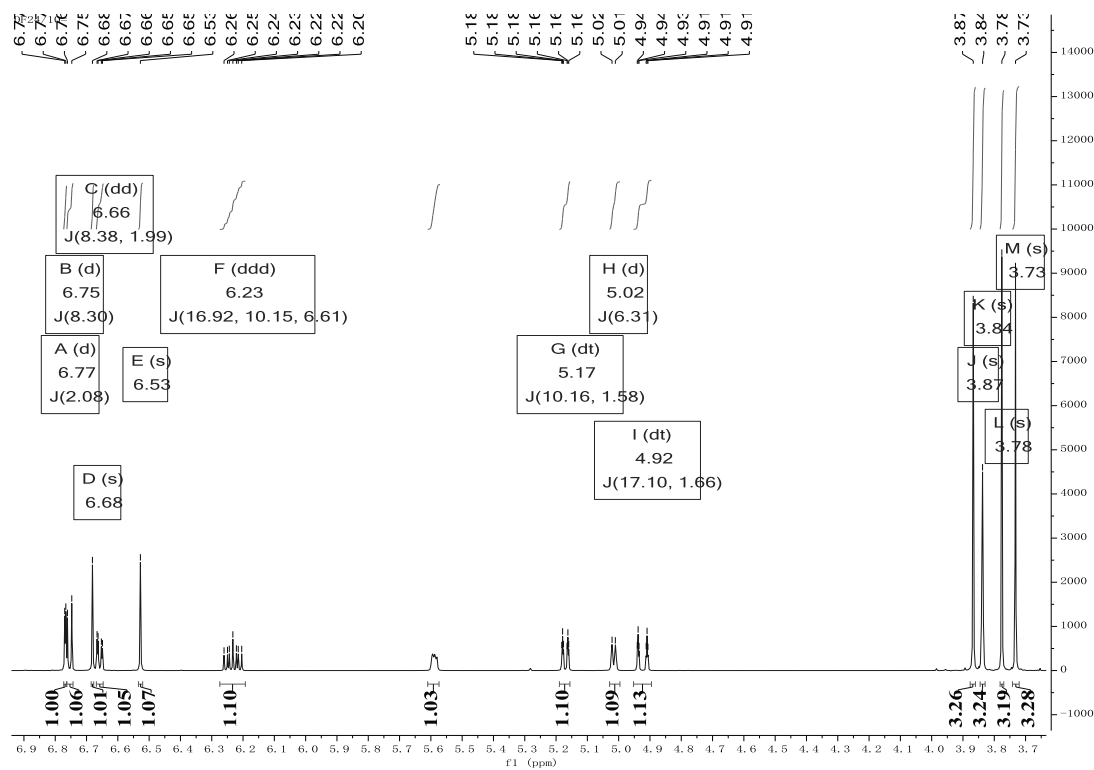


Figure S2. The ¹H NMR (600 MHz, CDCl₃) of compound 1.

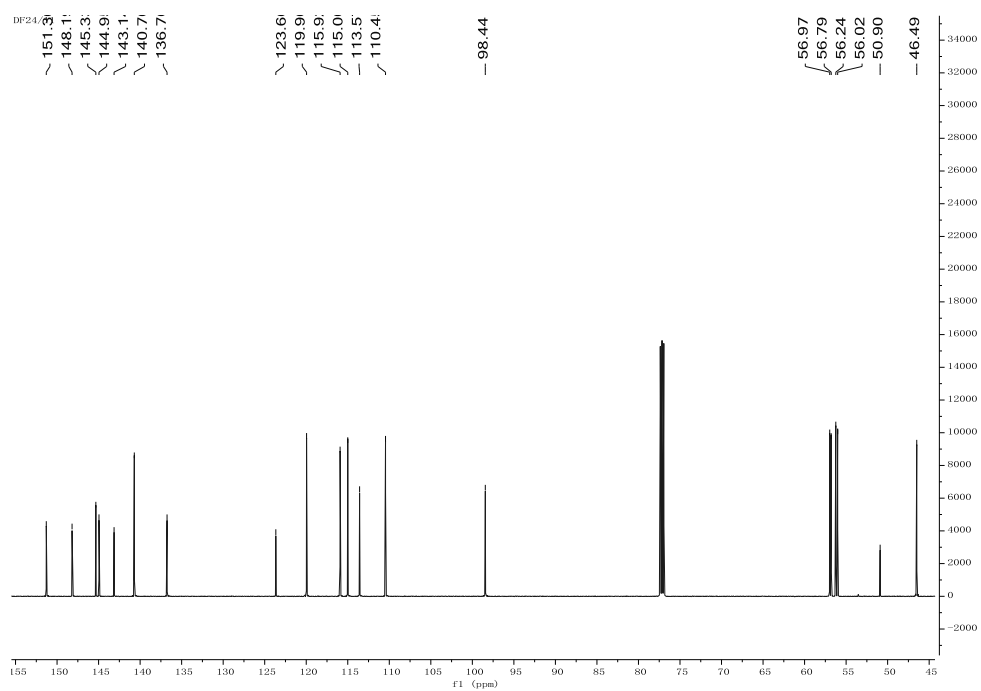


Figure S3. The ¹³C NMR (150 MHz, CDCl₃) of compound **1**.

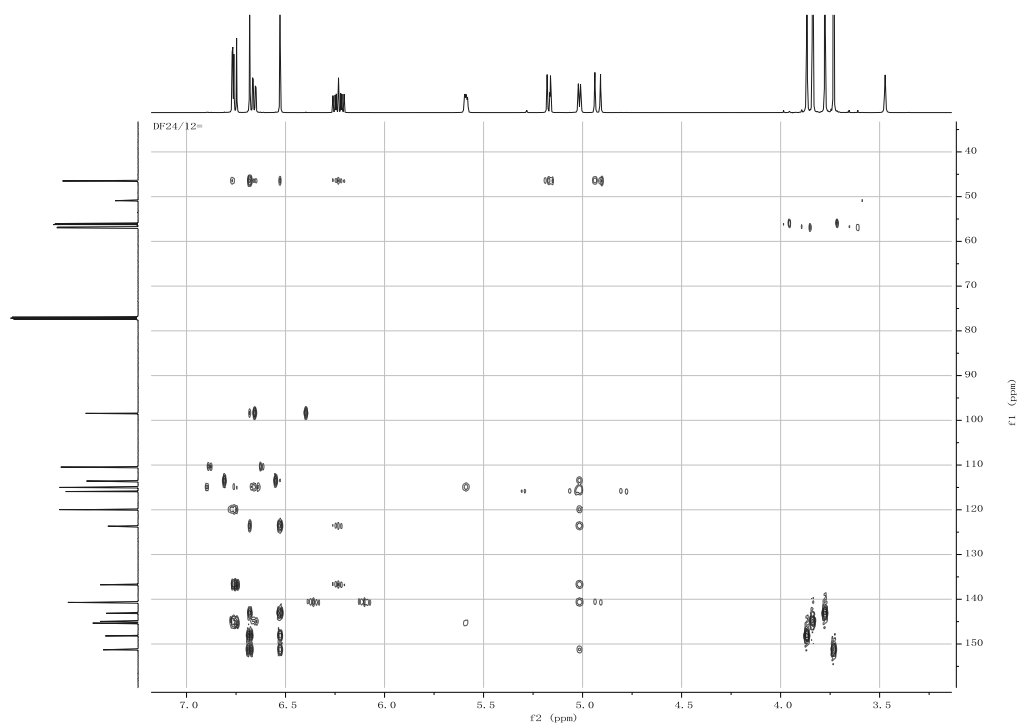


Figure S4. The HMBC spectrum of compound **1**.

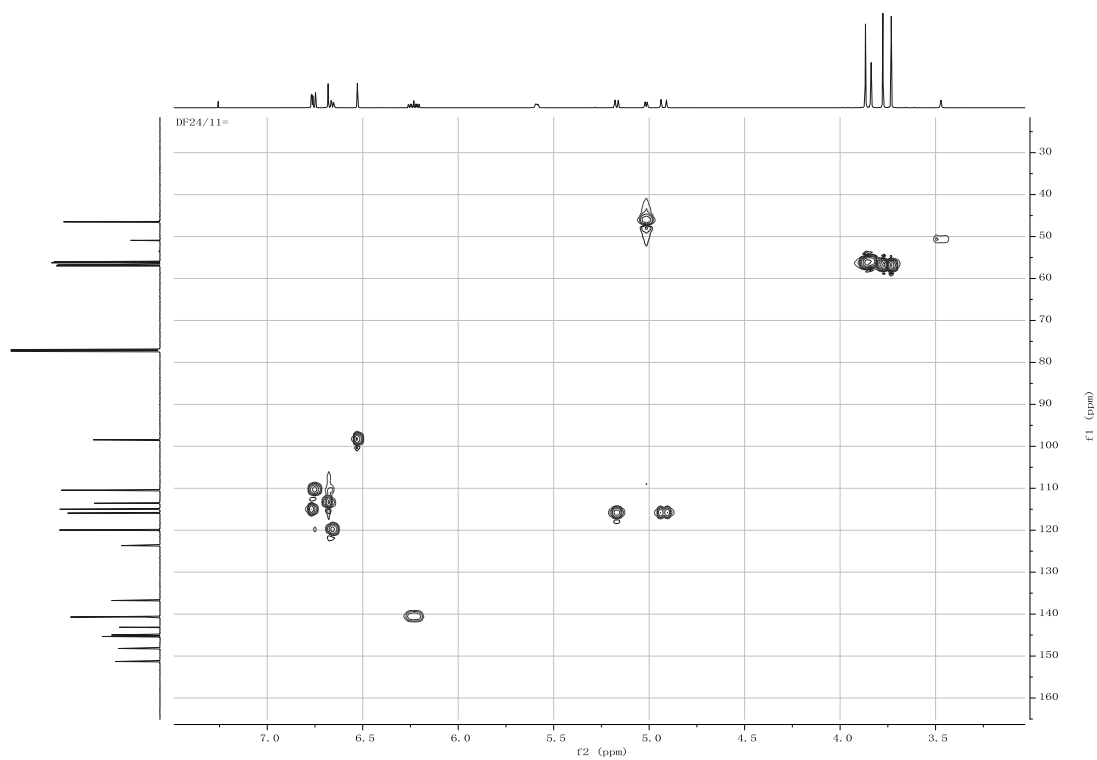


Figure S5. The HSQC spectrum of compound **1**.

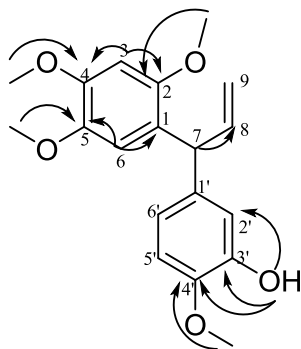


Figure S6. The key HMBC correlations of compound **1**.

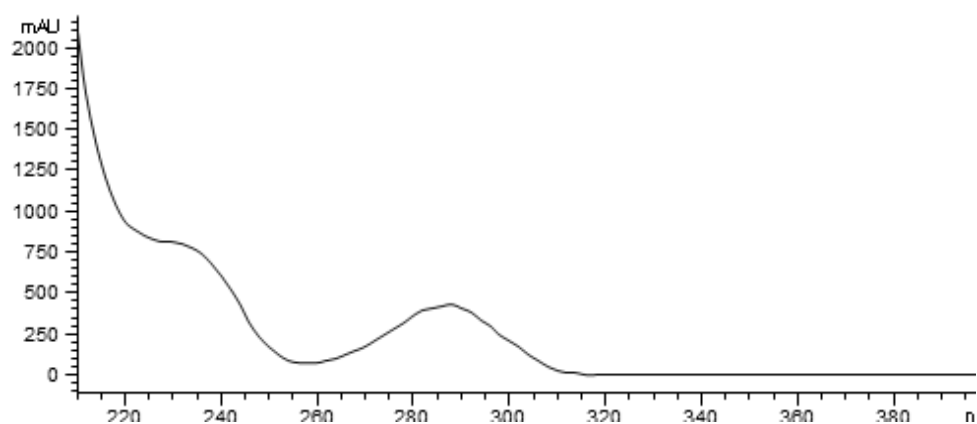


Figure S7. The UV spectrum of compound **1**.

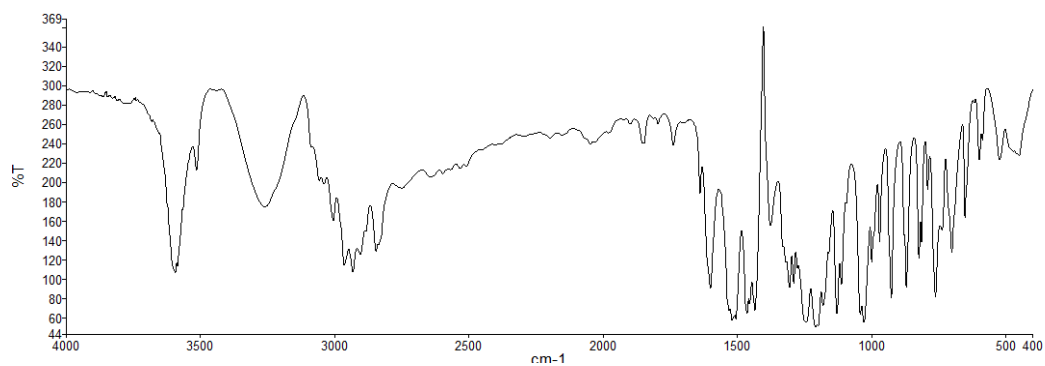


Figure S8. The IR spectrum of compound **1**.

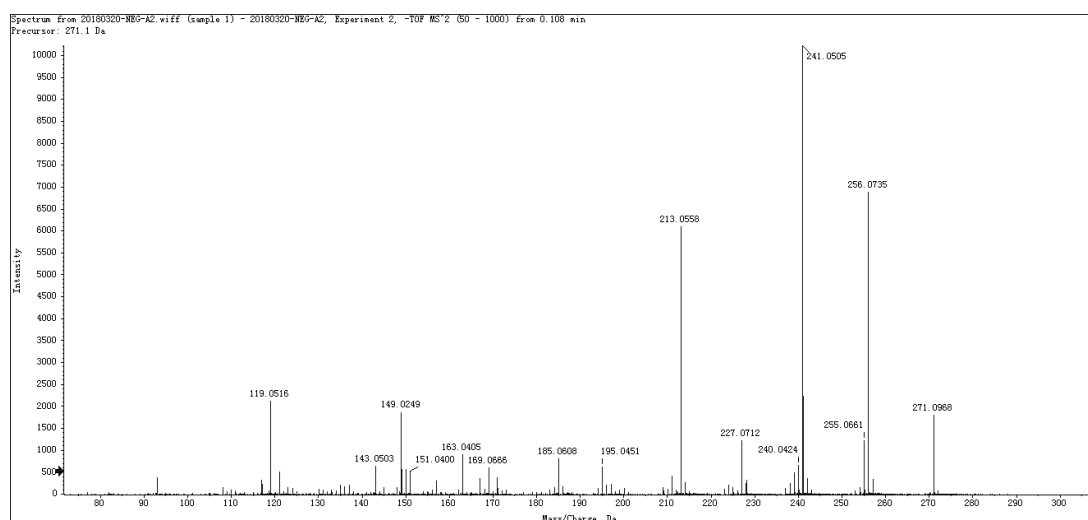


Figure S9. The HR-ESI-MS spectrum of compound **4**.

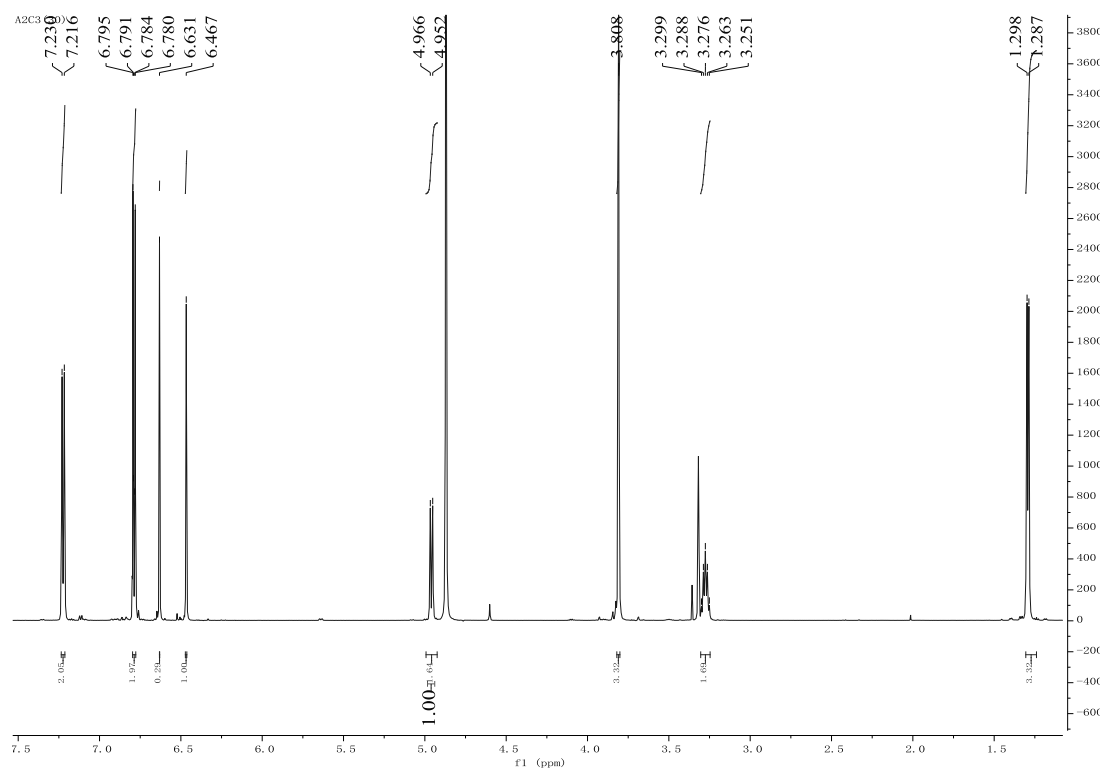


Figure S10. The ^1H NMR (600 MHz, CD_3OD) spectrum of compound **4**.

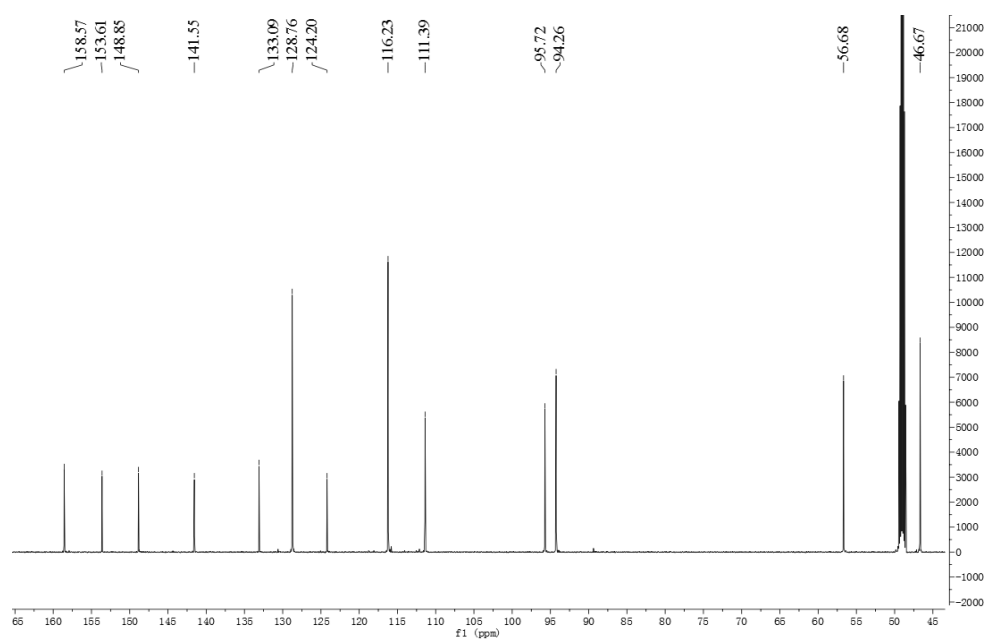


Figure S11. The ¹³C NMR (150 MHz, CD₃OD) spectrum of compound **4**.

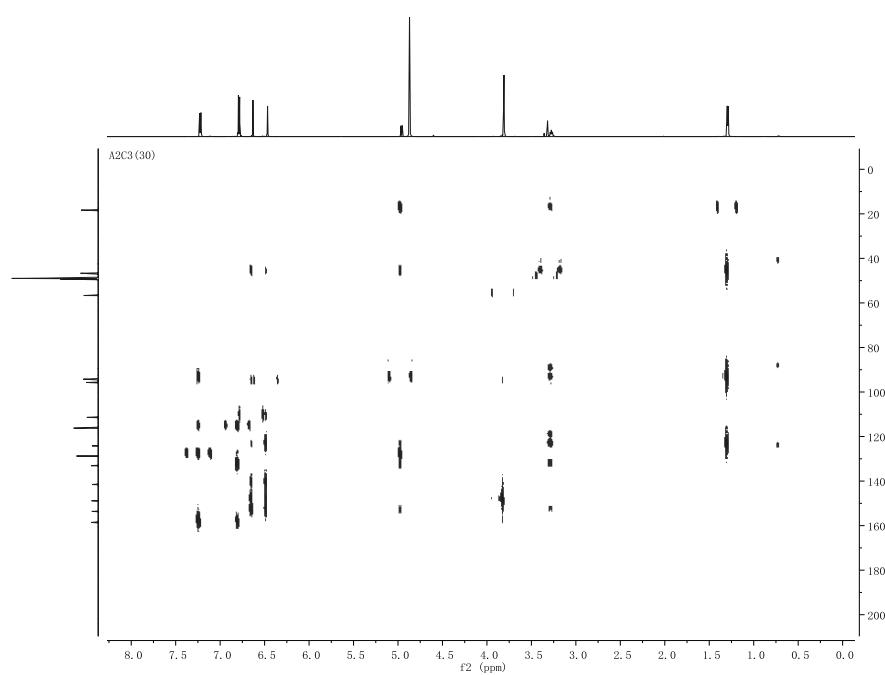


Figure S12. The HMBC spectrum of compound **4**.

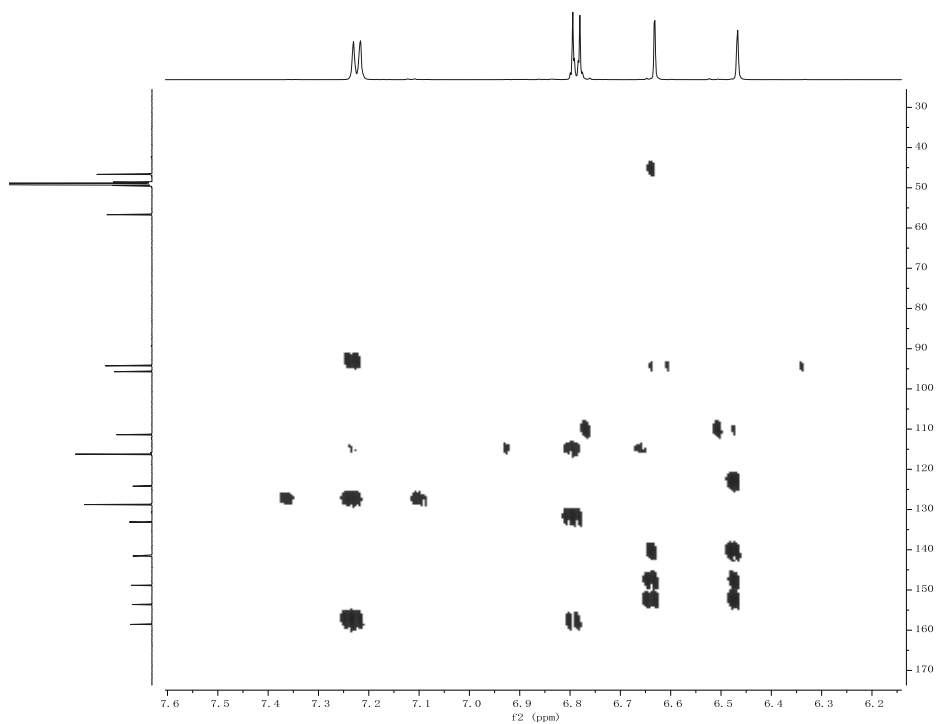


Figure S13. The part of HMBC spectrum of compound **4**.

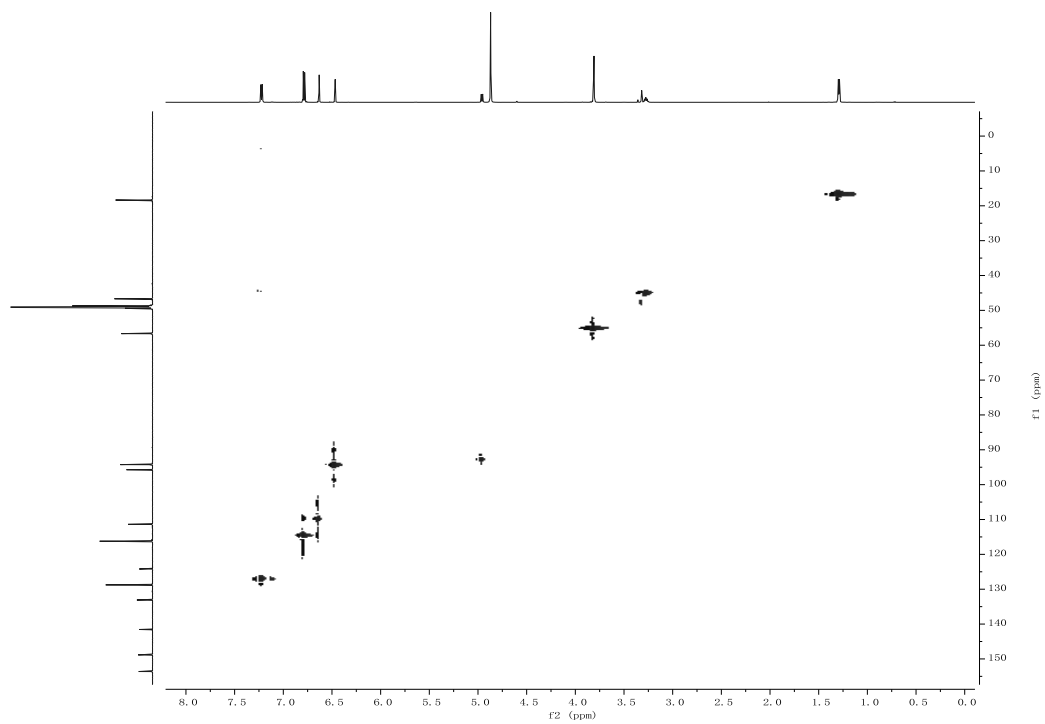


Figure S14. The HSQC spectrum of compound **4**.

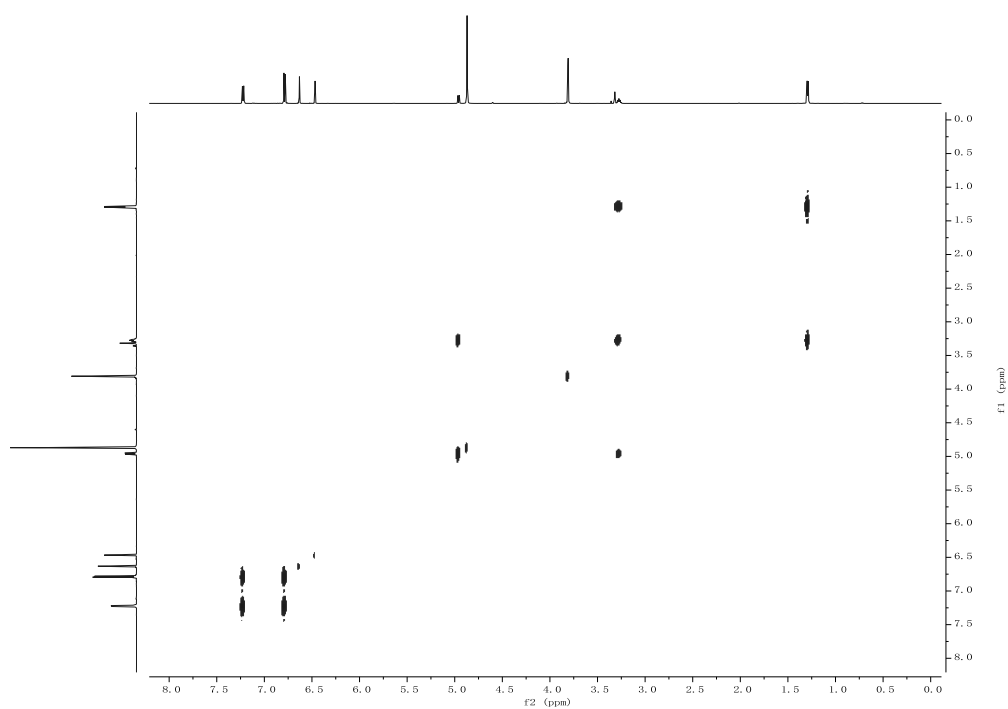


Figure S15. The H-H COSY spectrum of compound **4**.

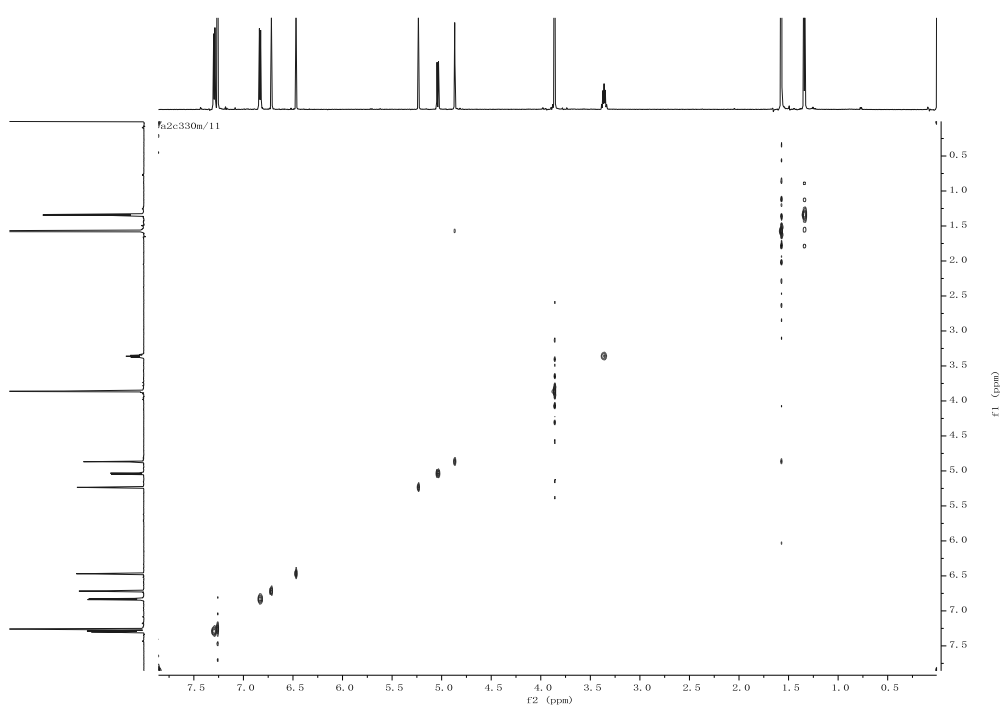


Figure S16. The NOE spectrum of compound **4**.

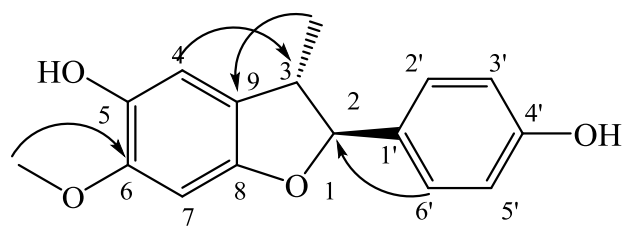


Figure S17. The key HMBC correlations of compound **4**.

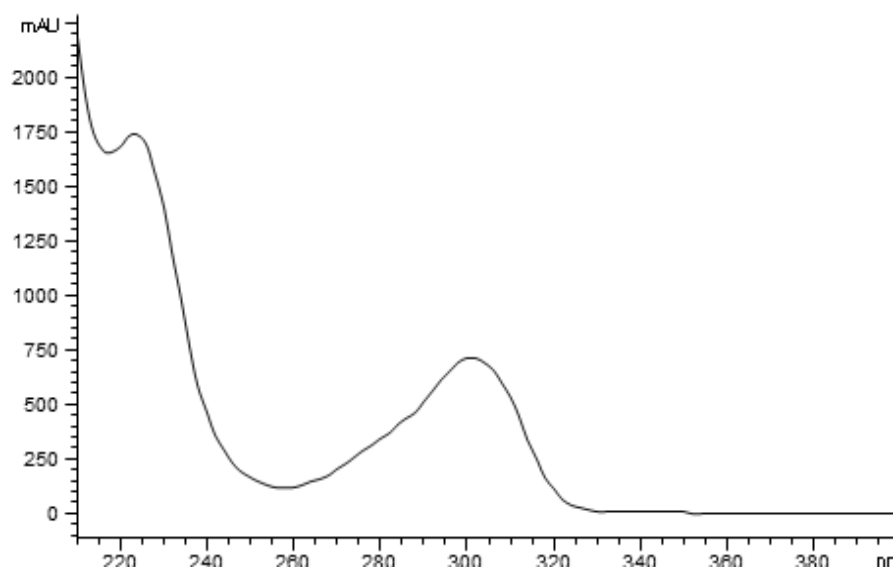


Figure S18. The UV spectrum of compound **4**.

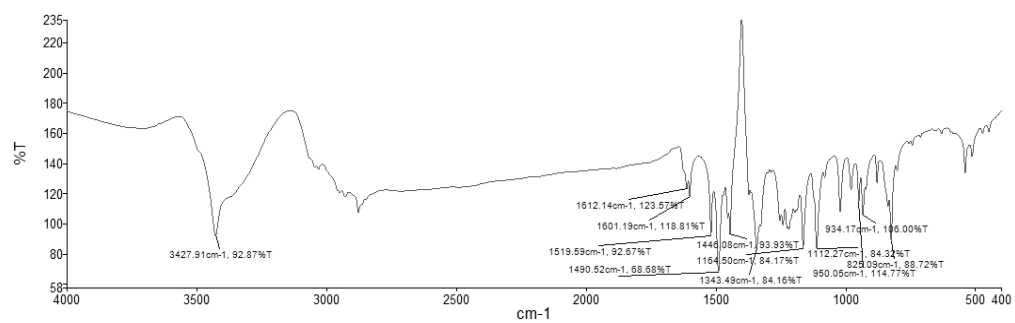


Figure S19. The IR spectrum of compound **4**.

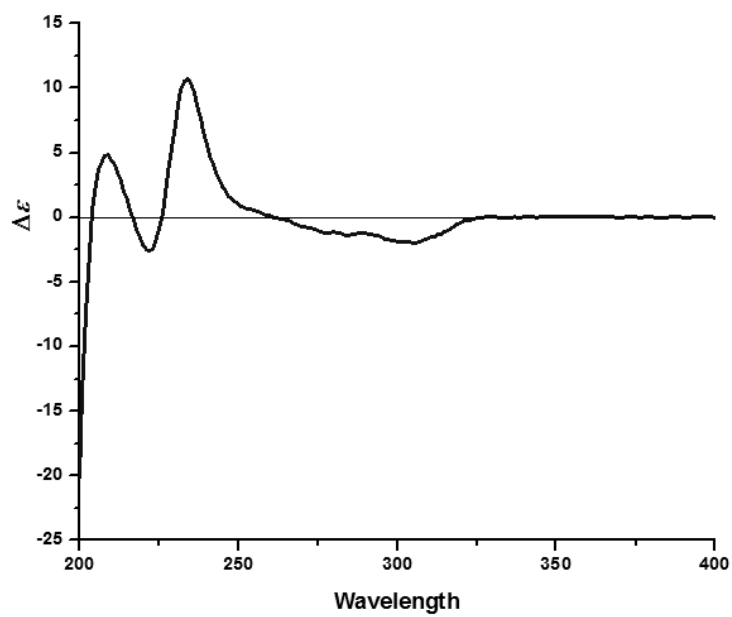


Figure S20. The CD spectrum of compound **4**.

Table S1. Crystal data and structure refinement for compound **4**.

Empirical formula	C ₁₆ H ₁₆ O ₄
Formula weight	272.29
Temperature	100.00 (10)
Wavelength	1.54184 Å
Crystal system, space group	monoclinic, I2
Unit cell dimensions	a = 16.4490 (3) Å, alpha = 90 deg. b = 5.27330 (10) Å, beta = 95.084 (2) deg. c = 15.2232 (3) Å, gamma = 90 deg.
Volume/	1315.27 (4) Å ³
Z, Calculated density	4, 1.375 Mg/m ³
Absorption coefficient mu	0.810 mm ⁻¹
F(000)	576.0
Crystal size	0.13 × 0.12 × 0.11 mm
2Θ range for data collection	7.584 to 147.014 deg.
Limiting indices	-19<=h<=20, -5<=k<=6, -18<=l<=18
Reflections collected / unique	5028/2373 [R(int) = 0.0289]
Max. and min. transmission	1.00000 and 0.69005
Data / restraints / parameters	2373/1/186
Goodness-of-fit on F ²	1.117
Final R indices [I>2sigma(I)]	R ₁ = 0.0343, wR ₂ = 0.0943
R indices (all data)	R ₁ = 0.0350, wR ₂ = 0.0955
Largest diff. peak and hole	0.24 and -0.19 e.Å ⁻³
Flack parameter	0.22 (11)

Table S2. The minimum inhibitory concentration (MIC) values of the compounds against bacteria and fungus

Compound	MIC (mg/ml)			
	<i>S. aureus</i>	<i>E. coli</i>	<i>S. enteri</i>	<i>C. albicans</i>
1	25.0±0.0	0.4±0.1	6.3±0.1	1.6±0.1
2	0.8±0.2	1.6±0.4	1.6±0.1	0.8±0.1
3	3.1±0.1	6.3±0.1	3.1±0.1	3.1±0.1
4	50.0±0.0	25.0±0.0	50.0±0.0	50.0±0.0