Supporting Information

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New polyketide and chromene derivative isolated from an endophytic *Diaporthe Phaseolorum* associated with *Polygonatum cyrtonema* Hua

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Supplementary data

DNA sequence and images related to *Diaporthe phaseolorum*

GGGGGGCGGGCGGGGAGCGCTTCGGCGCACCCAGAAACCCTTTGTGAACTTATA
CCTATTGTTGCCTCGGCGCAGGCCGGCCTCTTCACTGAGGCCCCCTGGAGACAGG
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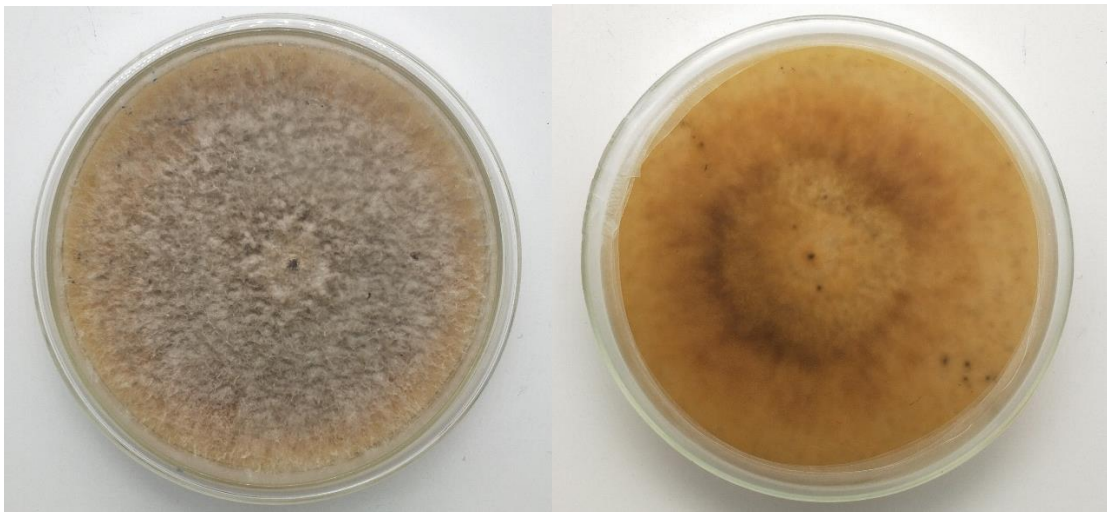


Compound **2** (chermesinone A) : $[\alpha]_D^{20.0}$ = +302.3 (CH_3OH, 0.1) ; ESI-MS *m/z*: 291.1 $[M+H]^+$；分子式：$C_{17}H_{22}O_4$;^1H and ^{13}C NMR see Table 1.

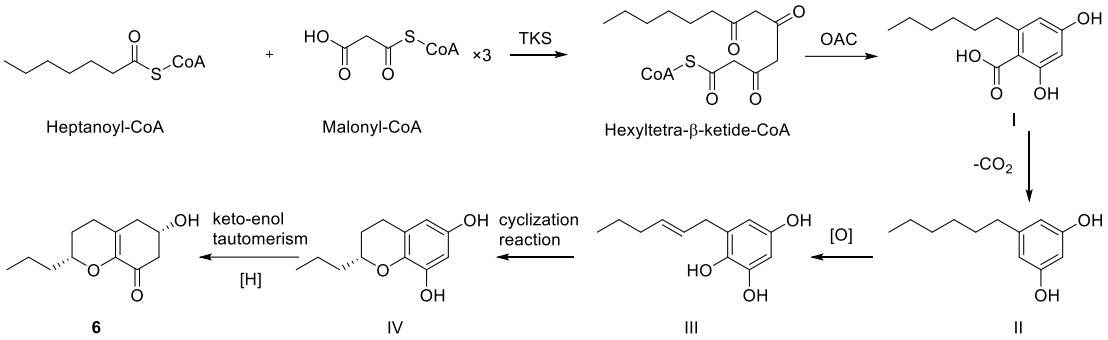
Compound **3** (13*S*-hydroxy-chermesinone A) : $[\alpha]_D^{20.0}$ = +50.3 (CH_3OH, 0.1)；ESI-MS *m/z*: 307.1 $[M+H]^+$; ^1H-NMR (600 MHz, CD_3OD) δ_H: 7.07 (1H, s, H-1), 6.19 (1H, s, H-3), 5.33 (1H, s, H-4), 4.05 (1H, m, H-13), 3.33 (1H, m, H-7), 3.16 (1H, d, *J* = 18.4, H-10), 2.95 (1H, dd, *J* = 18.4, 9.5 Hz, H-10), 2.72 (1H, m, H-12), 2.16 (3H, s, H-15), 1.16 (6H, d, *J* = 6.2 Hz, H-14, H-17), 1.09 (3H, s, H-16); ^{13}C NMR (150 MHz, CD_3OD) δ_C: 147.1 (C-1), 160.8 (C-2), 107.9 (C-3), 105.0 (C-4), 201.3 (C-5), 74.7 (C-6), 41.5 (C-7), 121.3 (C-8), 149.8 (C-9), 39.9 (C-10), 214.0 (C-11), 54.3 (C-12), 69.5 (C-13), 21.0 (C-14), 19.2 (C-15), 21.1 (C-16), 11.5 (C-17).

Compound **4** (13*R*-hydroxy-chermesinone A) : $[\alpha]_D^{20.0}$ = +35.6 (CH_3OH, 0.1) ; ESI-MS *m/z*: 307.1 $[M+H]^+$; ^{1}H-NMR (600 MHz, CD_3OD) δ_H: 7.21 (1H, s, H-1), 6.19 (1H, s, H-3), 5.33 (1H, s, H-4), 3.95 (1H, m, H-13), 3.33 (1H, br d, *J* = 9.7 Hz, H-7), 3.18 (1H, dd, *J* = 18.5, 1.9 Hz, H-10), 2.97 (1H, dd, *J* = 18.5, 9.7 Hz, H-10), 2.61 (1H, m, H-12), 2.15 (3H, s, H-15), 1.21 (3H, d, *J* = 6.2 Hz, H-17), 1.09 (3H, d, *J* = 7.1 Hz, H-14), 1.07 (3H, s, H-16); ^{13}C NMR (150 MHz, CD_3OD) δ_C: 147.4 (C-1), 160.8 (C-2), 107.9 (C-3), 104.9 (C-4), 201.4 (C-5), 74.7 (C-6), 41.1 (C-7), 121.4 (C-8), 149.9 (C-9), 38.5 (C-10), 214.3 (C-11), 56.0 (C-12), 70.7 (C-13), 21.1 (C-14), 19.2 (C-15), 21.4 (C-16), 14.1 (C-17).

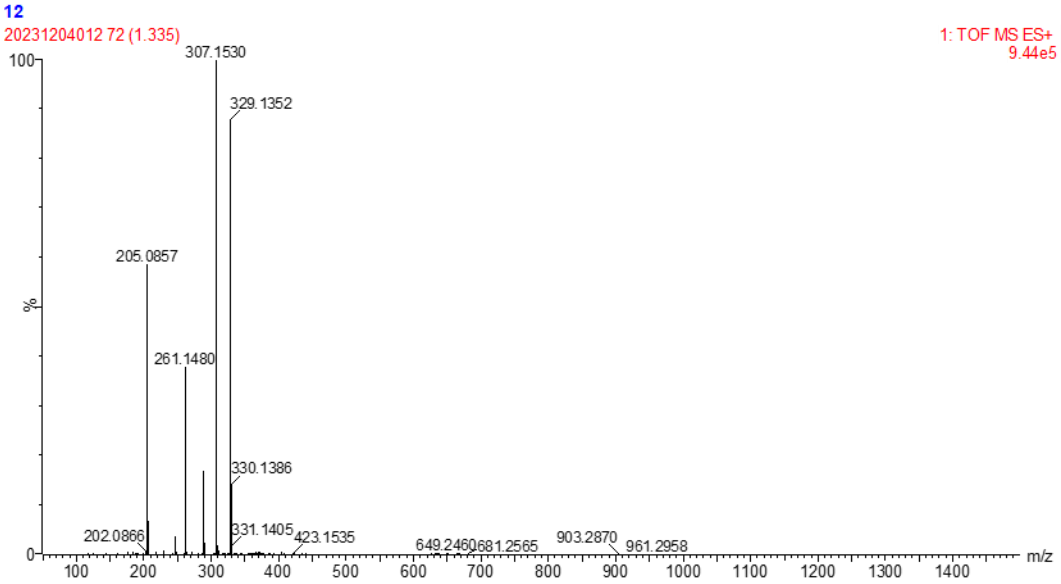
Compound **5** (11-hydrochermesinone B) : $[\alpha]_D^{20.0}$ = +68.6 (CH_3OH, 0.1) ; ESI-MS *m/z*: 319.1 $[M+H]^+$; ^{1}H-NMR (600MHz, $CDCl_3$) δ_H: 7.43 (1H, s, H-1), 6.04 (1H, s, H-3), 5.30 (1H, s, H-4), 3.72 (1H, t, *J* = 7.0 Hz, H-11), 3.50 (1H, dd, *J* = 12.9, 2.0 Hz, H-7), 3.27 (1H, dd, *J* = 12.9, 2.0 Hz, H-10), 2.17 (1H, s, H-15), 1.88 (1H, m, H-12), 1.73 (1H, m, H-13), 1.30 (3H, s, H-16), 1.22 (1H, m, H-13), 0.92-0.90 (6H, m, H-14，H-17); ^{13}C NMR (150 MHz, $CDCl_3$) δ_C: 144.2 (C-1), 158.7 (C-2), 107.2 (C-3), 105.7 (C-4), 173.9 (C-5), 82.6 (C-6), 43.5 (C-7), 117.1 (C-8), 146.3 (C-9), 45.3 (C-10), 73.4 (C-11), 37.7 (C-12), 25.3 (C-13), 10.6 (C-14), 19.7 (C-15), 18.5 (C-16), 16 (C-17), 193.0 (C-18).

Compound **7** (de-*O*-methyldiaporthin) : ESI-MS *m/z*: 237.1 $[M+H]^+$; ^{1}H-NMR (600MHz, CD_3OD) δ_H: 6.35 (1H, s, H-4), 6.29 (2H, m, H-5/7), 4.13 (1H, m, H-2′), 2.57 (2H, m, H-1′), 1.24 (3H, d, *J* = 6.2 Hz, H-3′); ^{13}C-NMR (150 MHz, CD_3OD) δ_C: 167.8 (C-1), 156.2 (C-3), 141.2 (C-4), 99.8 (C-5), 164.8 (C-6), 107.0 (C-7), 167.3 (C-8), 102.6 (C-9), 103.7 (C-10), 66.2 (C-2′), 43.8 (C-1′), 23.3 (C-3′).

Compound **8** (Scytalone) : ESI-MS *m/z*: 192.9 $[M-H]^-$; ^{1}H-NMR (600 MHz, CD_3OD) δ_H: 6.23 (1H, m, H-5), 6.11 (1H, d, *J* = 2.3 Hz, H-7), 4.26 (1H, septet, *J* = 3.8 Hz, H-3), 3.09 (1H, dd, *J* = 16.0, 3.8 Hz, H-4), 2.86 (1H, m, H-4a), 2.84 (1H, m, H-2), 2.62 (1H, dd, *J* = 17.0, 7.7 Hz, H-2a); ^{13}C-NMR (150 MHz, CD_3OD) δ_C: 202.5 (C-1), 47.4 (C-2), 66.9 (C-3), 39.1 (C-4), 146.0 (C-4a), 109.4 (C-5), 166.5 (C-6), 101.6 (C-7), 166.7 (C-8), 111.7 (C-8a)



Scheme S1 Hypothetical biosynthetic pathway of **6**.



m/z	Theo.Mass	Delta(ppm)	Composition	
307.1530	307.1540	-3.256	$C_{17}H_{22}O_5$	M+H

Figure S1: HR-ESI-MS spectrum of **1** (15-hydroxy-chermesinone A)

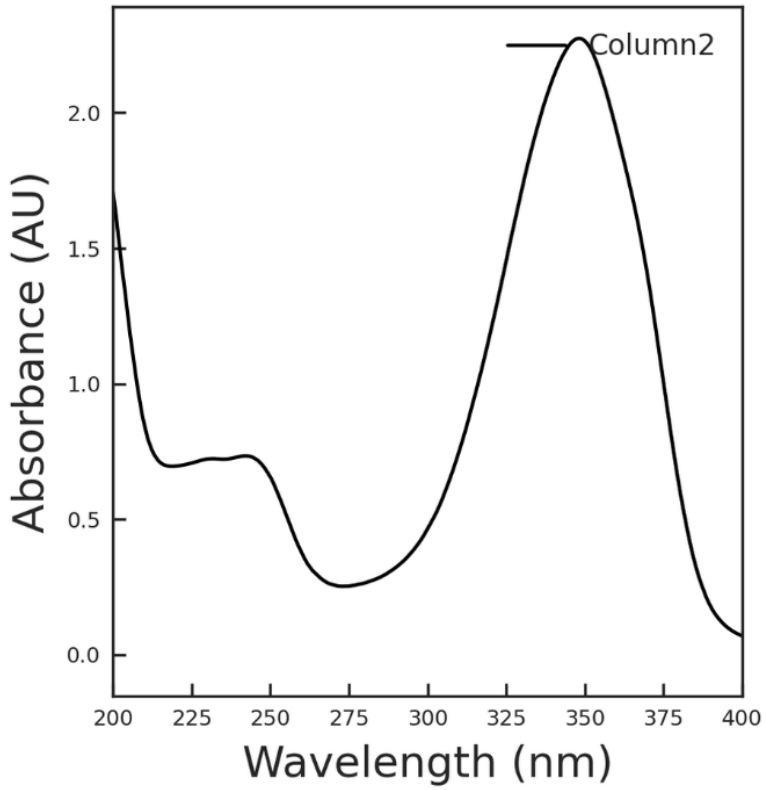


Figure S2: UV spectrum of **1** (15-hydroxy-chermesinone A).

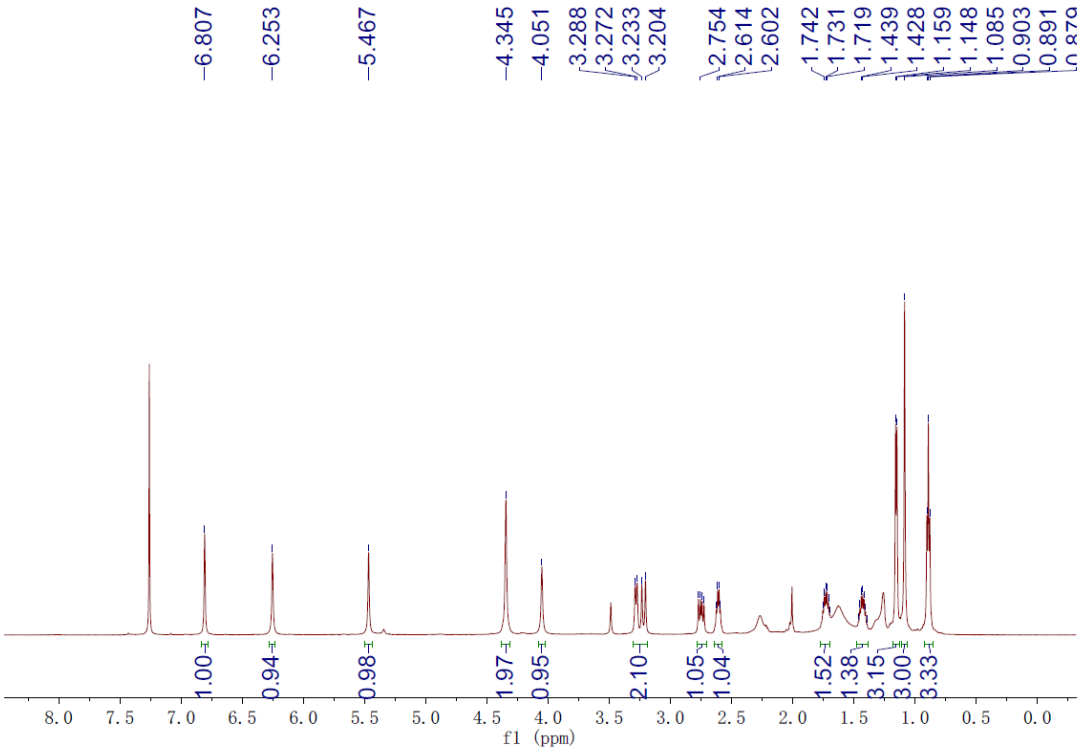


Figure S3: ^{1}H-NMR (600 MHz, $CDCl_3$) spectrum of **1** (15-hydroxy-chermesinone A).

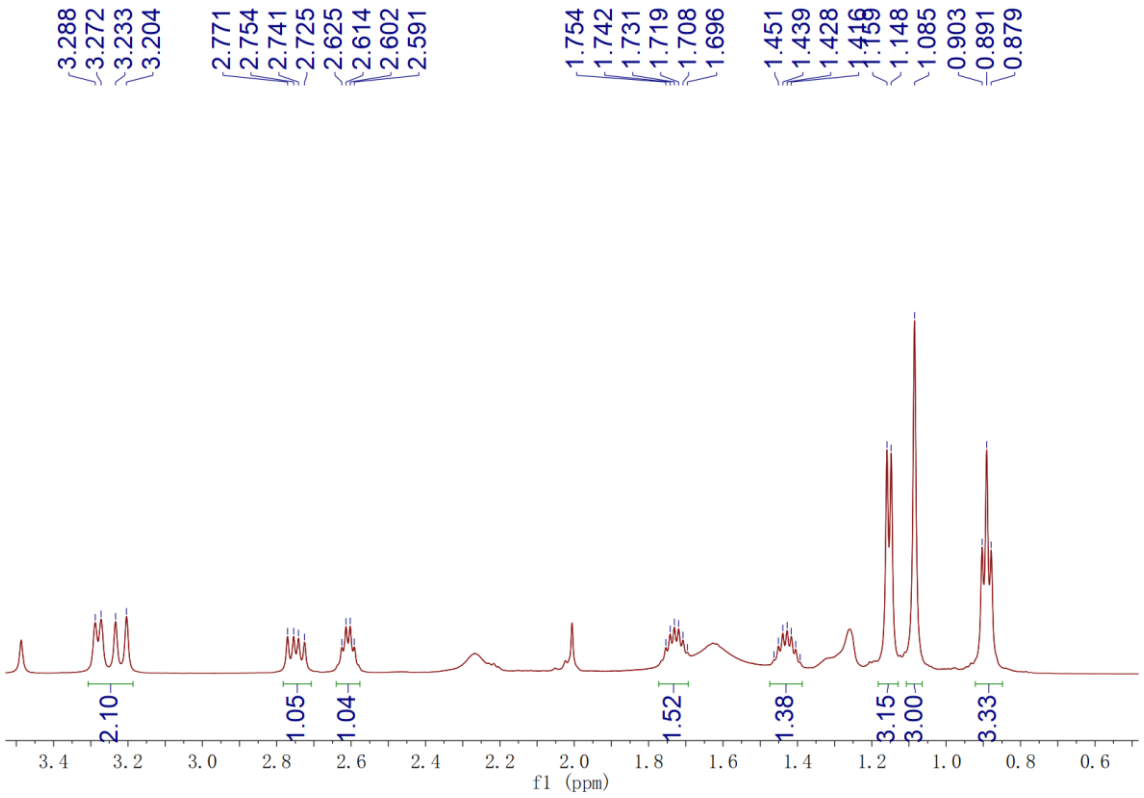


Figure S4: ^{1}H-NMR (600 MHz, $CDCl_3$) spectrum of **1** (15-hydroxy-chermesinone A) (From δ_H 0.5 ppm to δ_H 3.5 ppm).

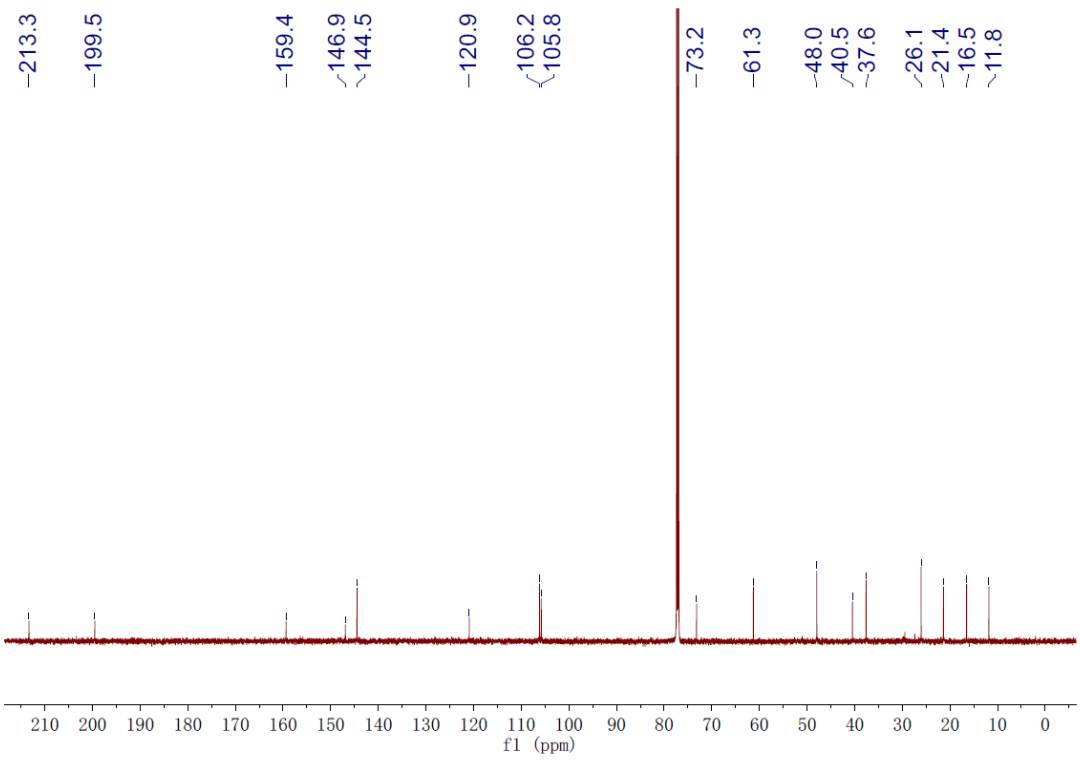


Figure S5: ^{13}C-NMR (150 MHz, $CDCl_3$) spectrum of **1** (15-hydroxy-chermesinone A).

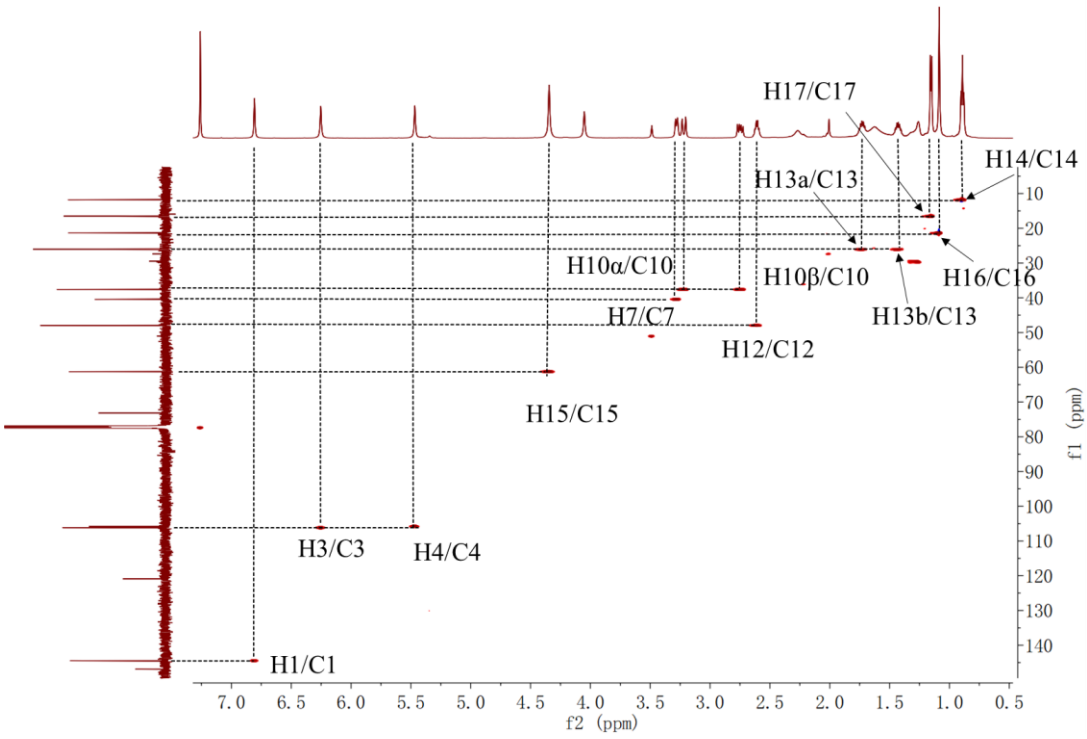


Figure S6: HSQC spectrum of **1** (15-hydroxy-chermesinone A).

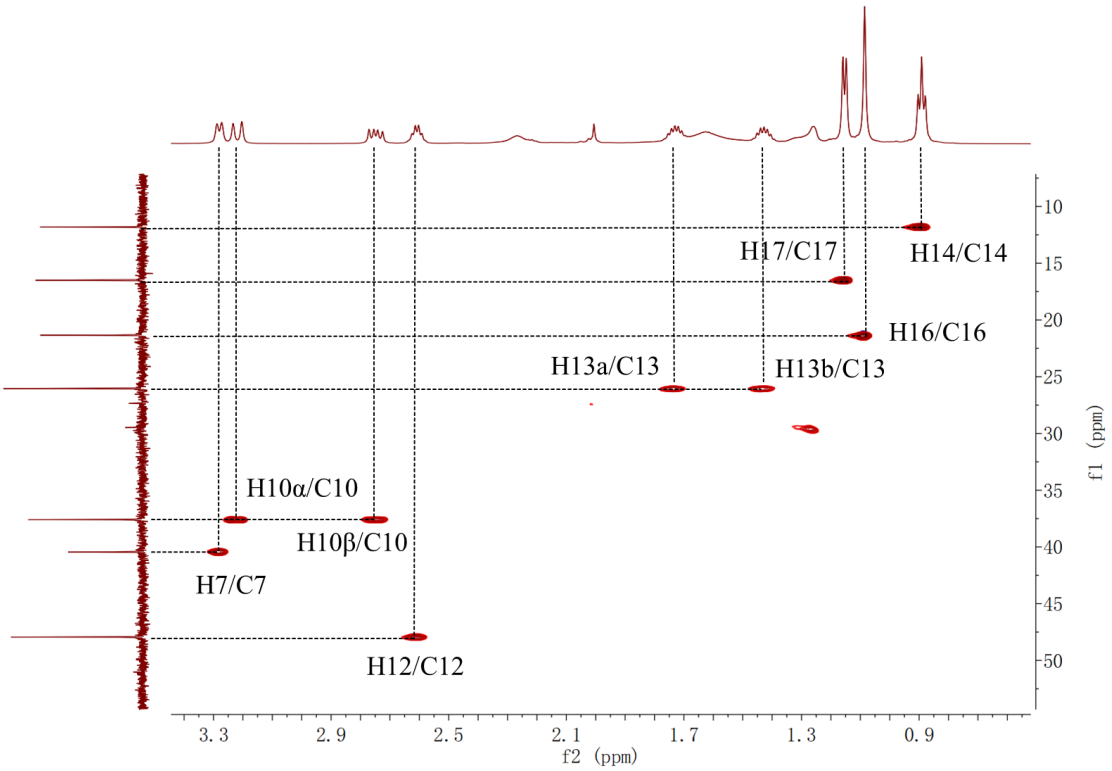


Figure S7: HSQC spectrum of **1** (15-hydroxy-chermesinone A) (From δ_H 0.5 ppm to δ_H 3.5 ppm).

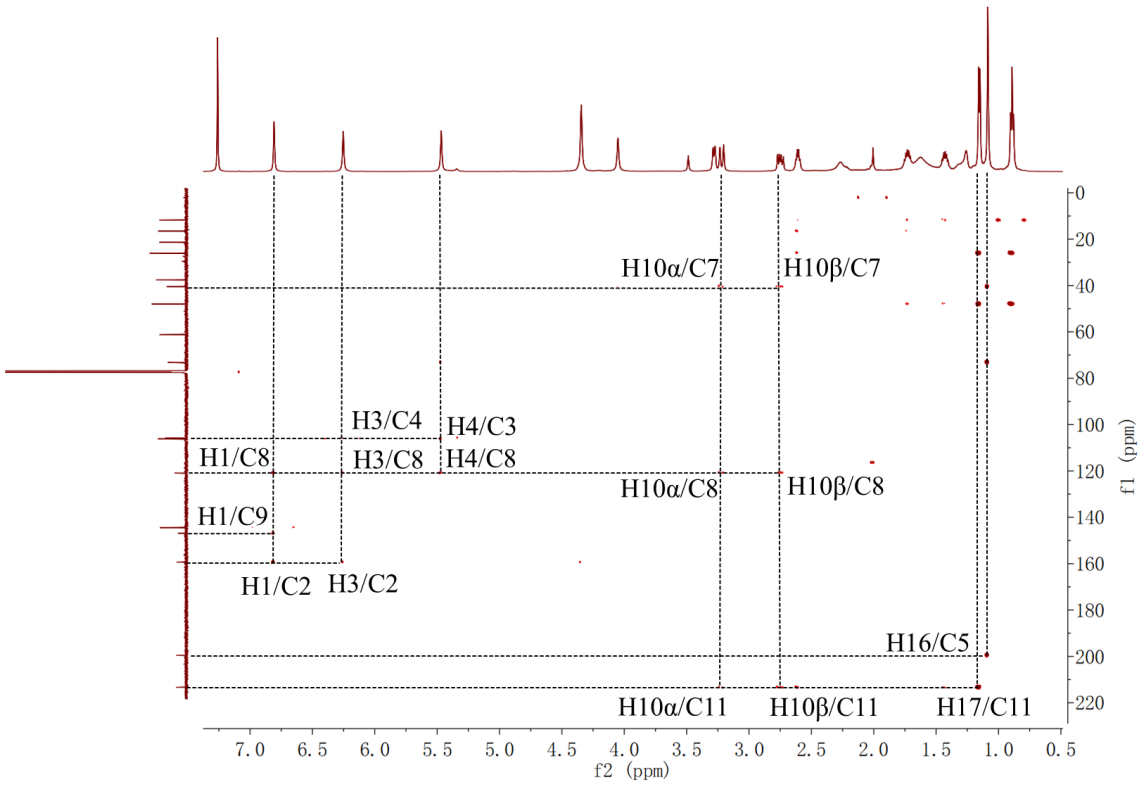


Figure S8: HMBC spectrum of **1** (15-hydroxy-chermesinone A).

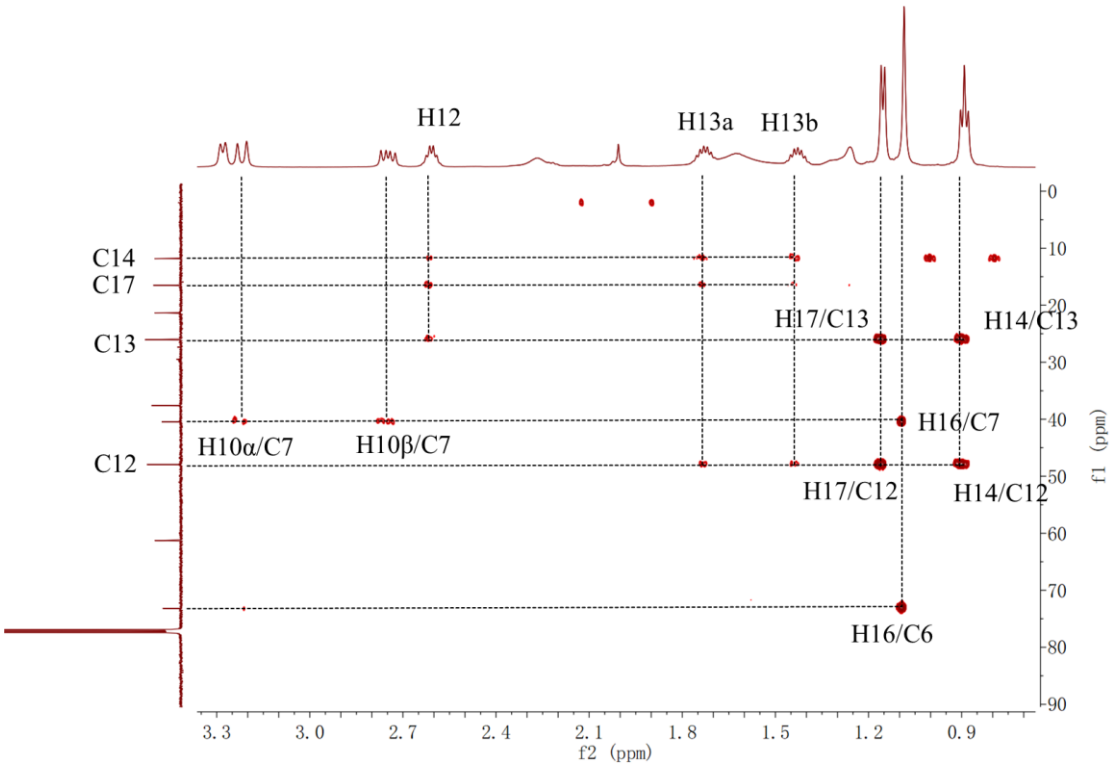


Figure S9: HMBC spectrum of **1** (15-hydroxy-chermesinone A) (From δ_H 0.5 ppm to δ_H 3.5 ppm).

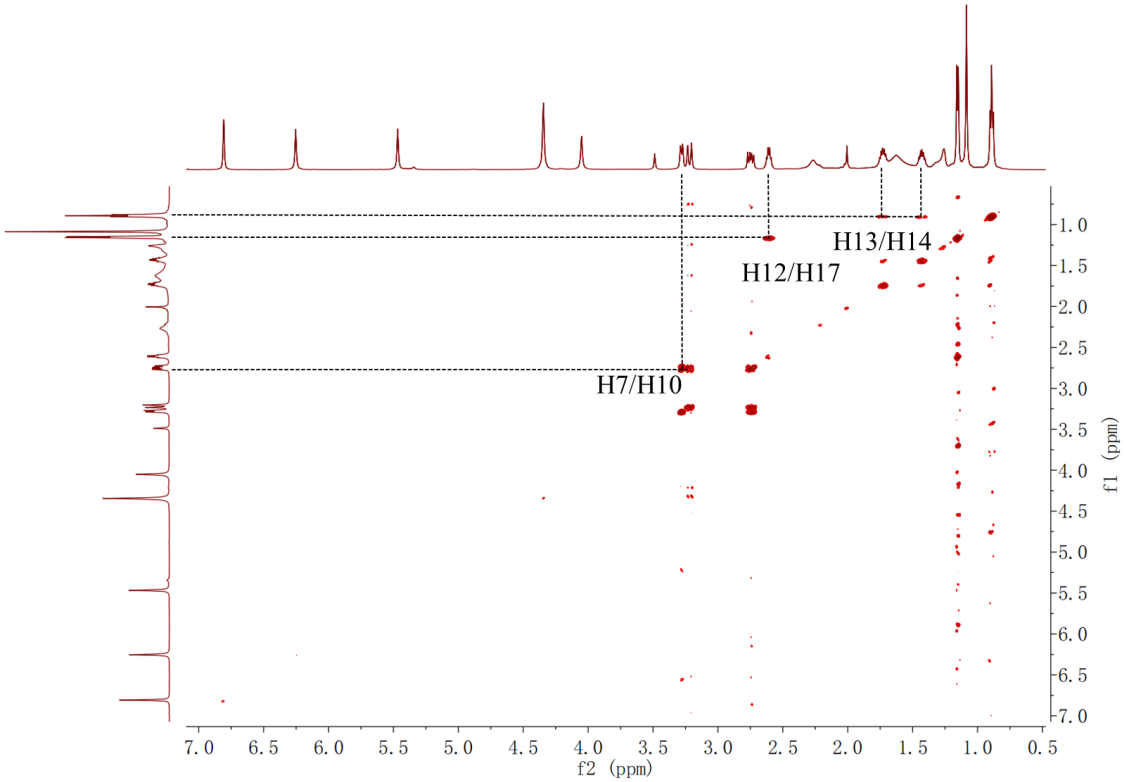


Figure S10: ^{1}H-^{1}H COSY spectrum of **1** (15-hydroxy-chermesinone A).

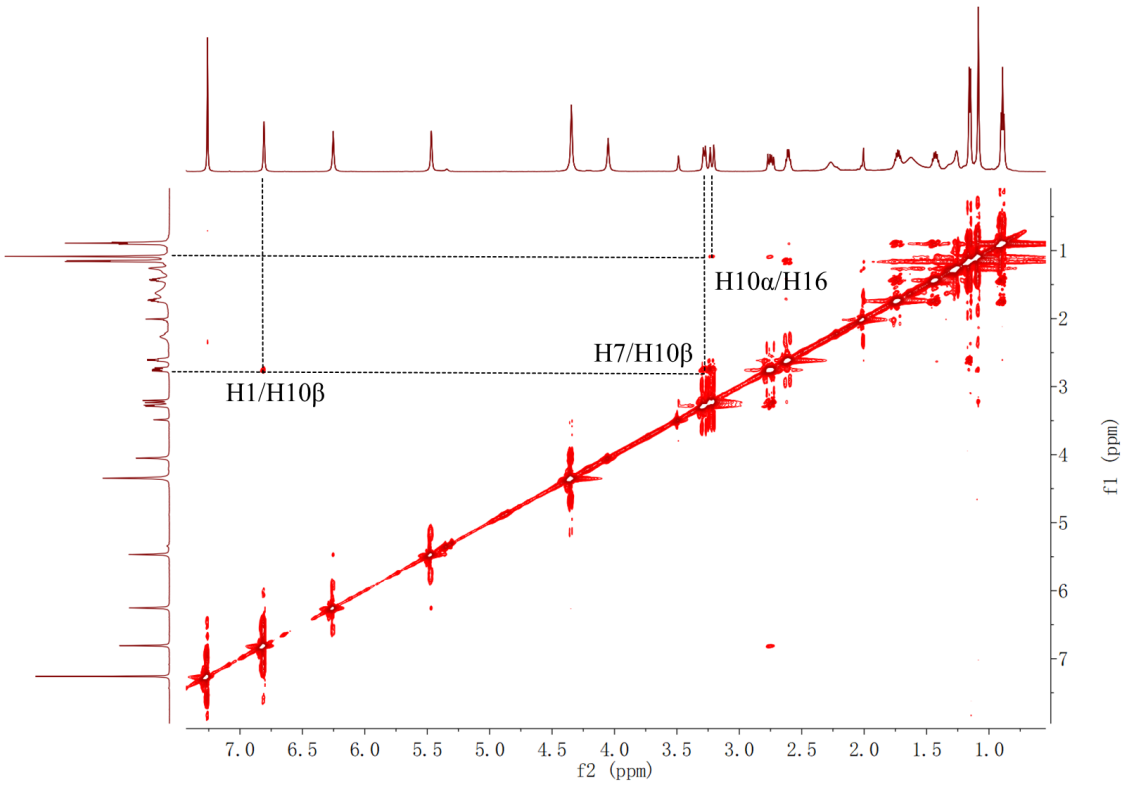
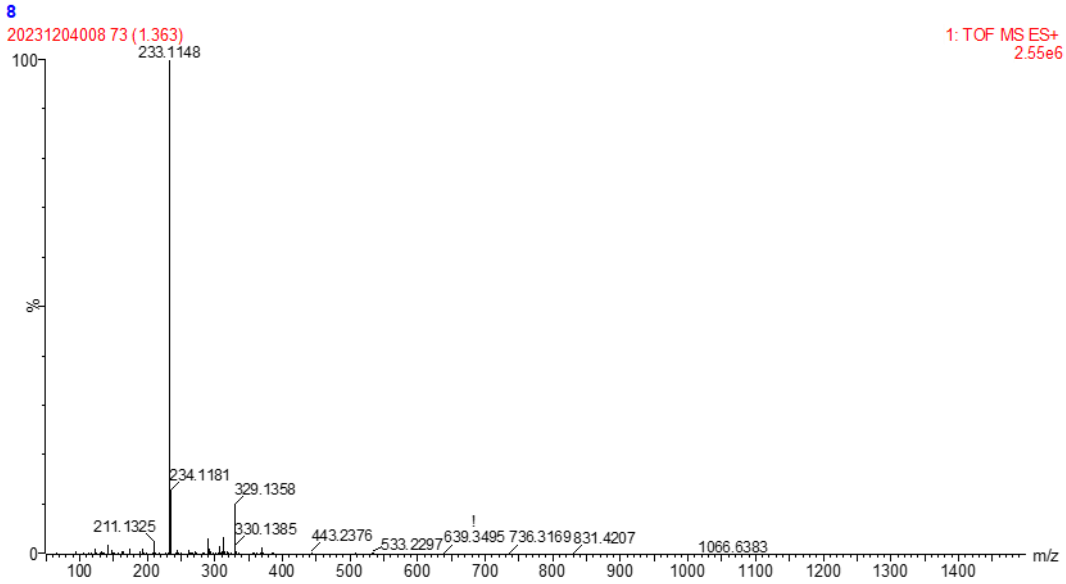


Figure S11: ROESY spectrum of **1** (15-hydroxy-chermesinone A).



m/z	Theo.Mass	Delta(ppm)	Composition	
233.1148	233.1148	0.03	$C_{12}H_{18}O_3$	M+Na

Figure S12: HR-ESI-MS spectrum of **6** (6*S*-hydroxy-2*R*-phomochromene)

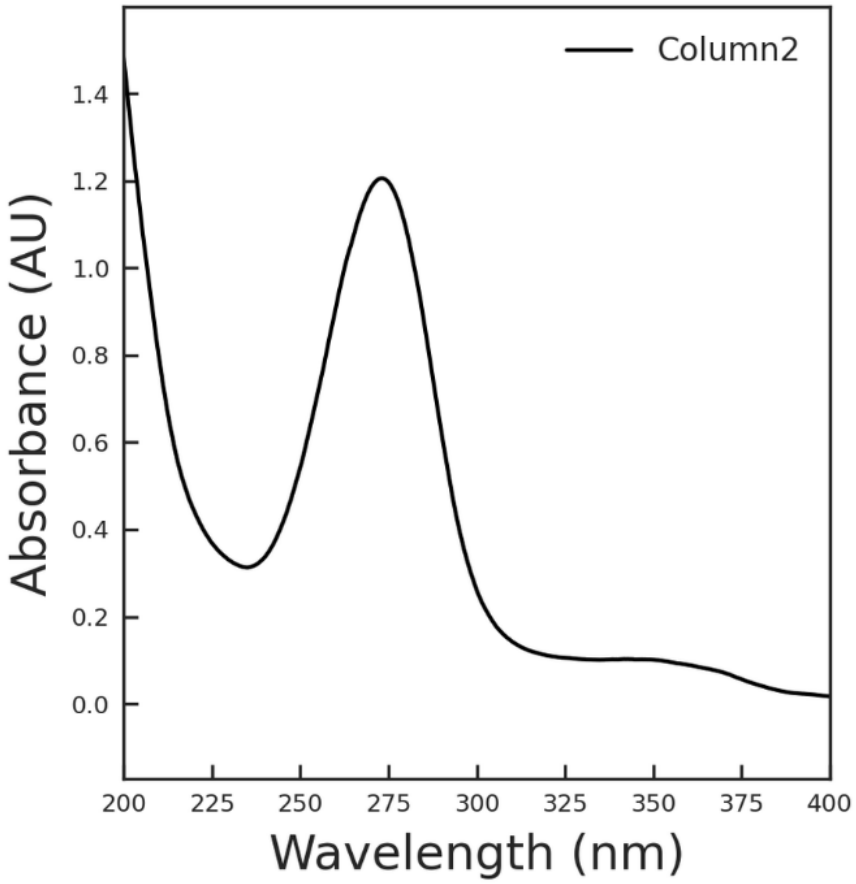


Figure S13: UV spectrum of **6** (6*S*-hydroxy-2*R*-phomochromene).

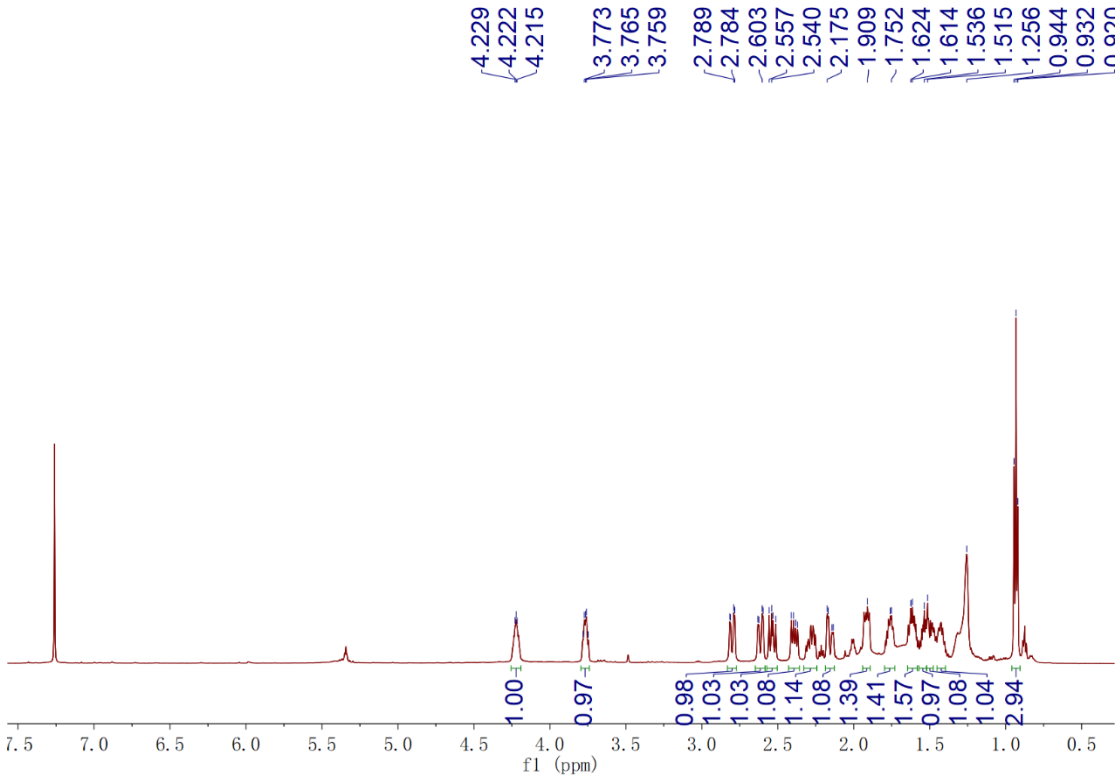


Figure S14: ^{1}H-NMR (600 MHz, $CDCl_3$) spectrum of **6** (6*S*-hydroxy-2*R*-phomochromene).

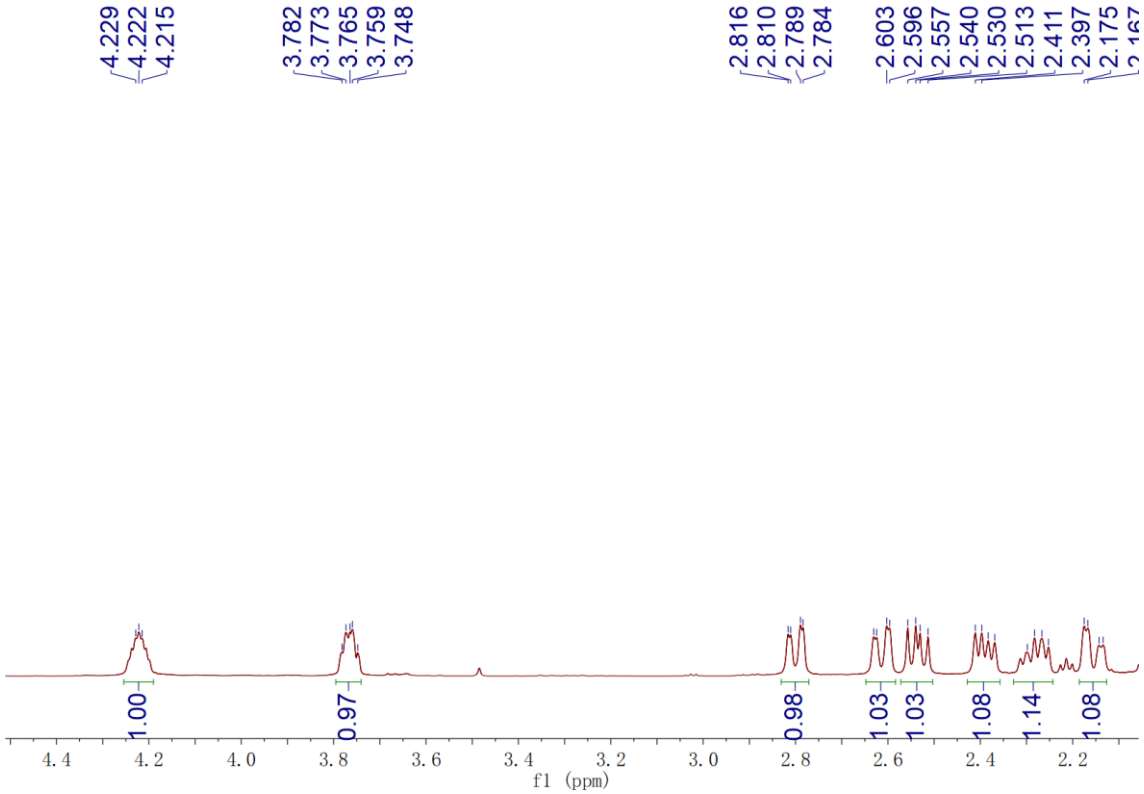


Figure S15: ^{1}H-NMR (600 MHz, $CDCl_3$) spectrum of **6** (6*S*-hydroxy-2*R*-phomochromene) (From δ_H 2.0 ppm to δ_H 4.5 ppm).

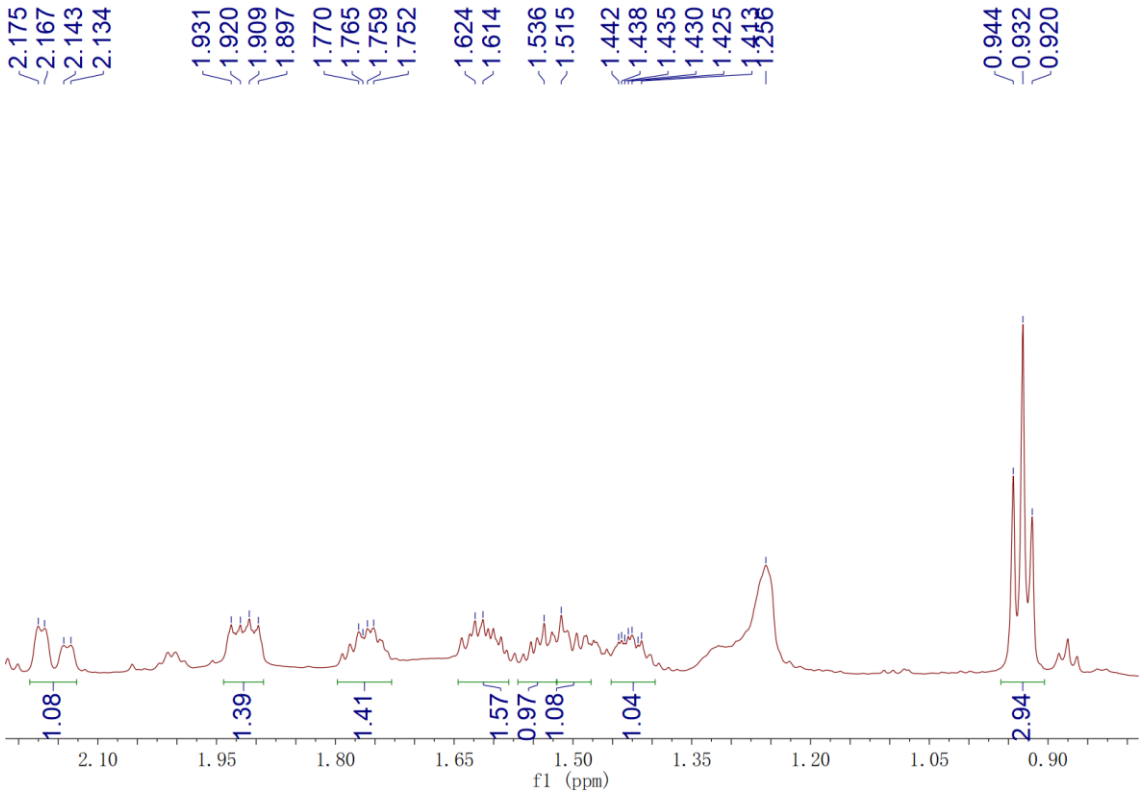


Figure S16: ^{1}H-NMR (600 MHz, $CDCl_3$) spectrum of **6** (6*S*-hydroxy-2*R*-phomochromene) (From δ_H 0.8 ppm to δ_H 2.2 ppm).

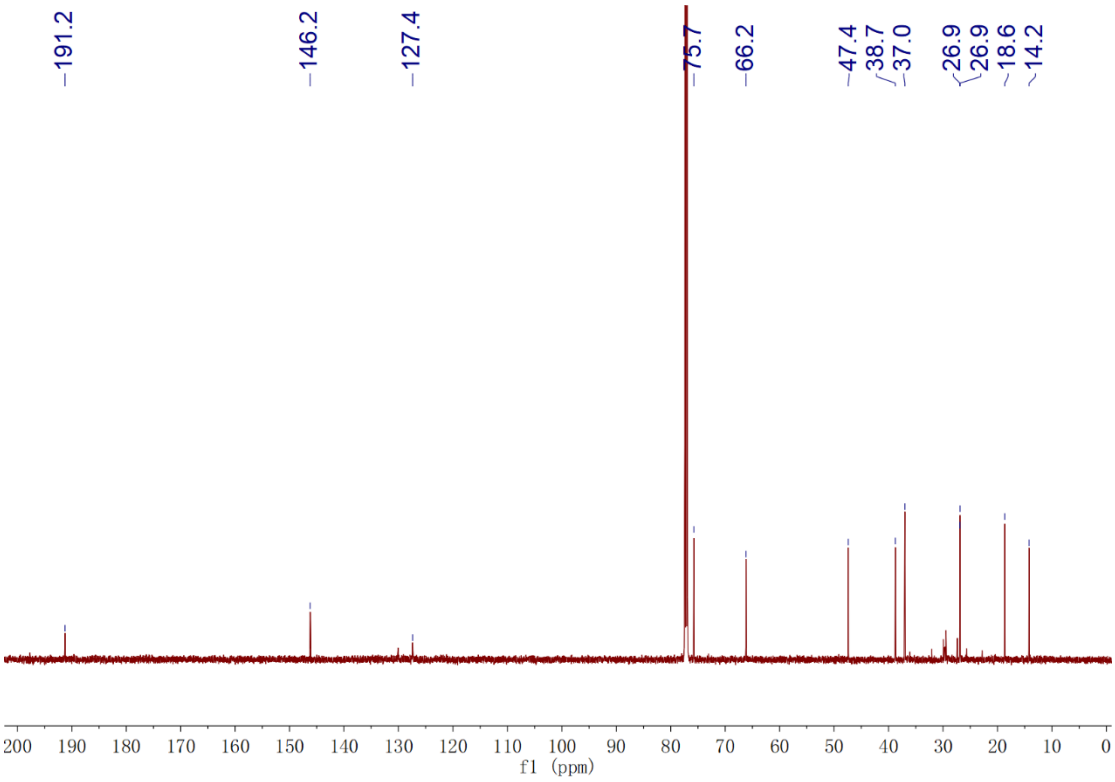


Figure S17: ^{13}C-NMR (150 MHz, $CDCl_3$) spectrum of **6** (6*S*-hydroxy-2*R*-phomochromene).

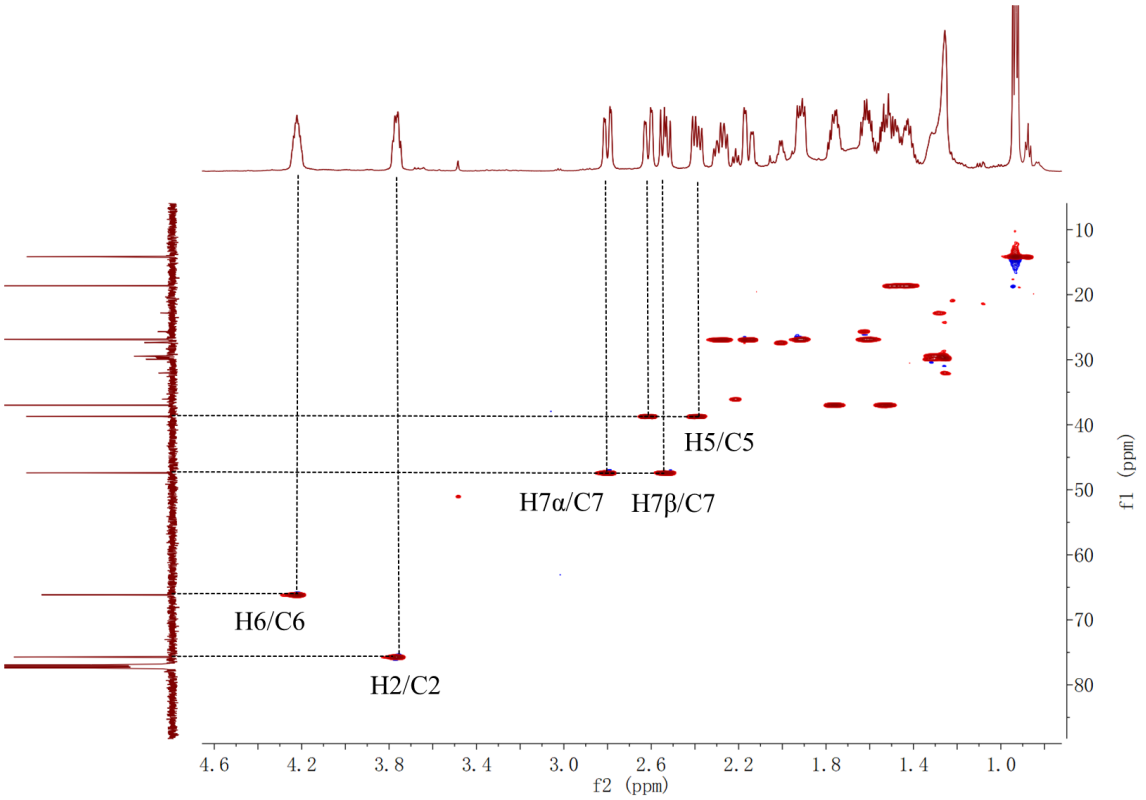


Figure S18: HSQC spectrum of **6** (6*S*-hydroxy-2*R*-phomochromene).

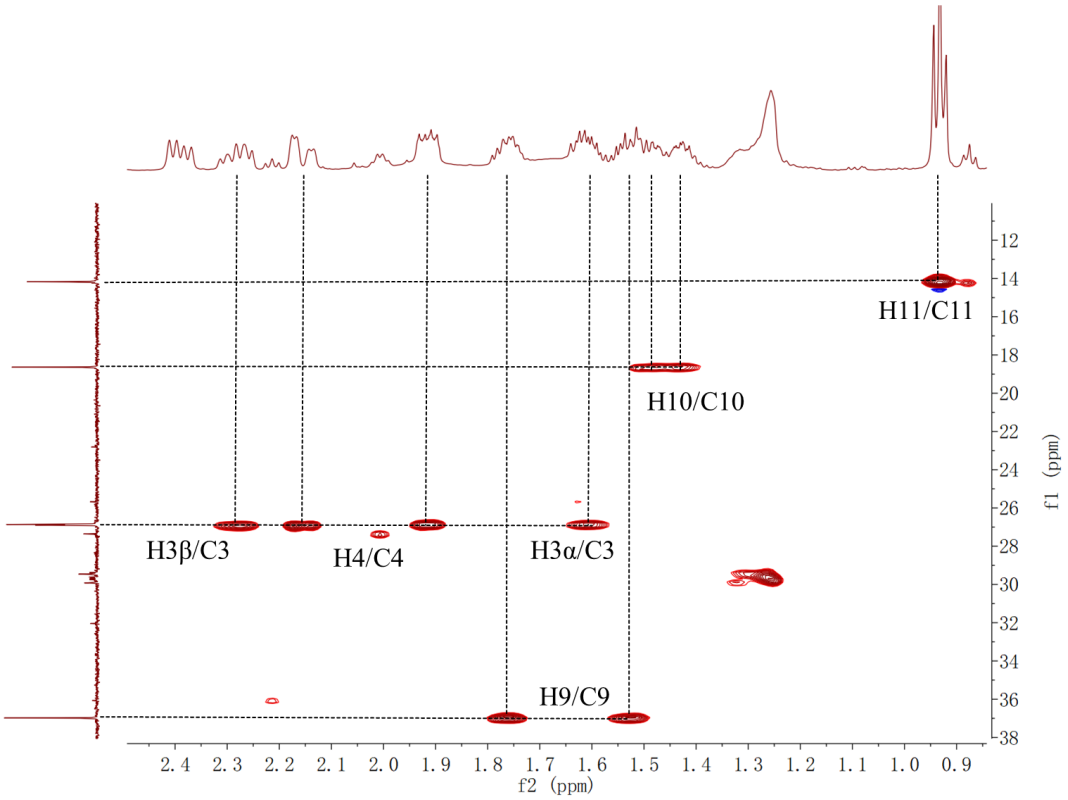


Figure S19: HSQC spectrum of **6** (6*S*-hydroxy-2*R*-phomochromene) (From δ_H 0.8 ppm to δ_H 2.5 ppm).

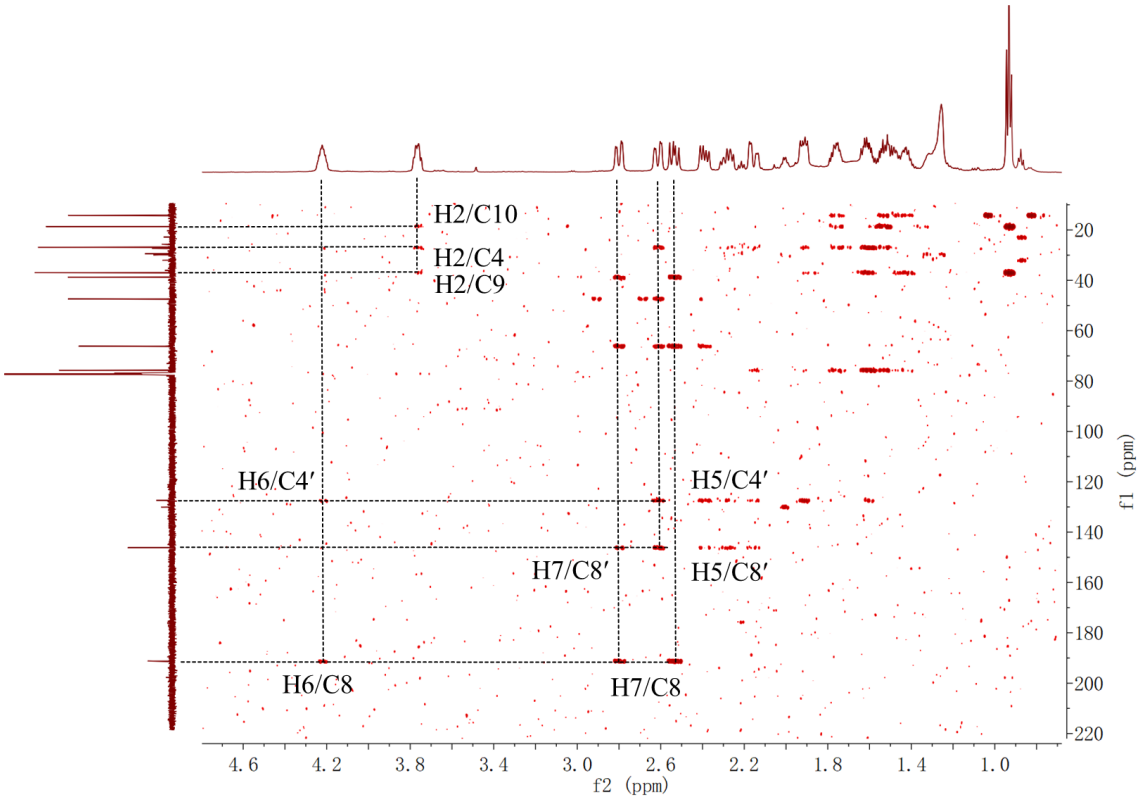


Figure S20: HMBC spectrum of **6** (6*S*-hydroxy-2*R*-phomochromene).

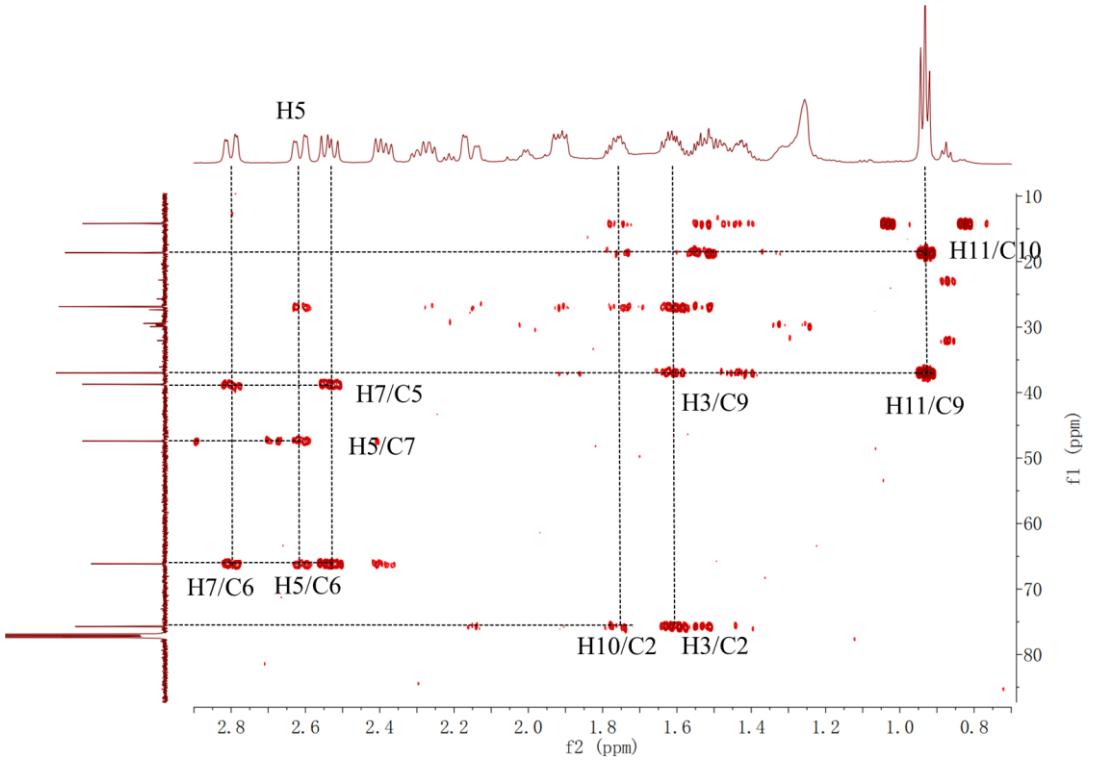


Figure S21: HMBC spectrum of **6** (6*S*-hydroxy-2*R*-phomochromene) (From δ_H 0.8 ppm to δ_H 3.0 ppm).

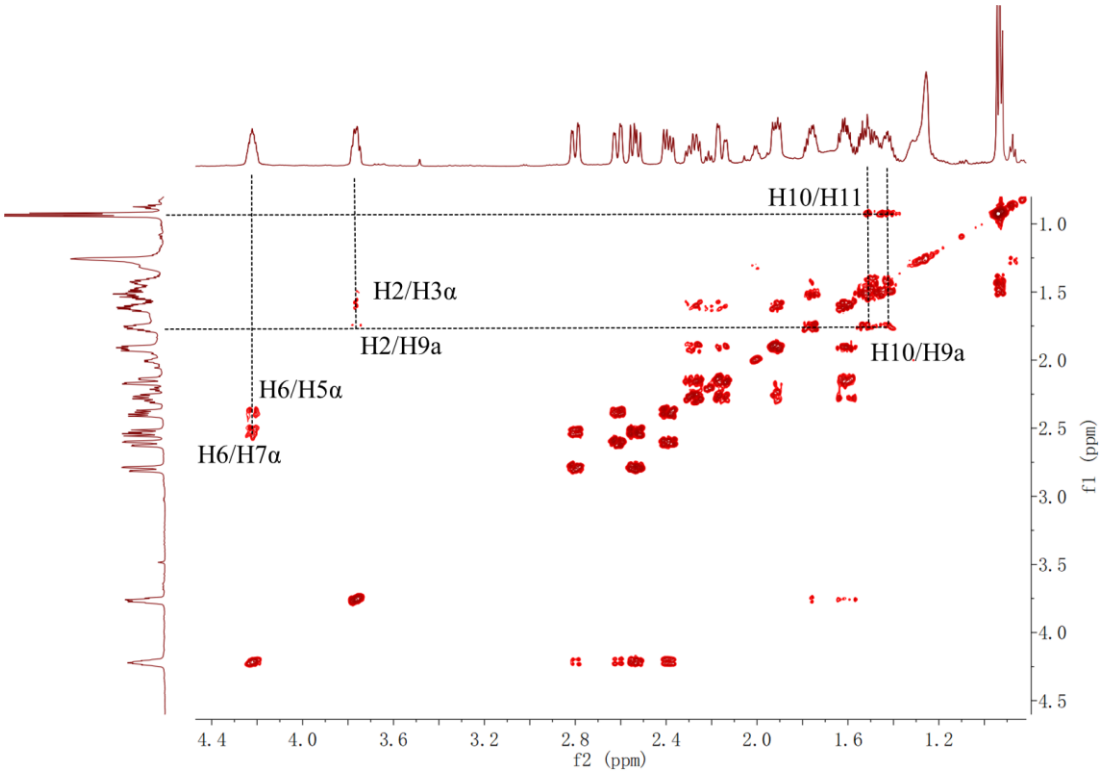


Figure S22: ^{1}H-^{1}H COSY spectrum of **6** (6*S*-hydroxy-2*R*-phomochromene).

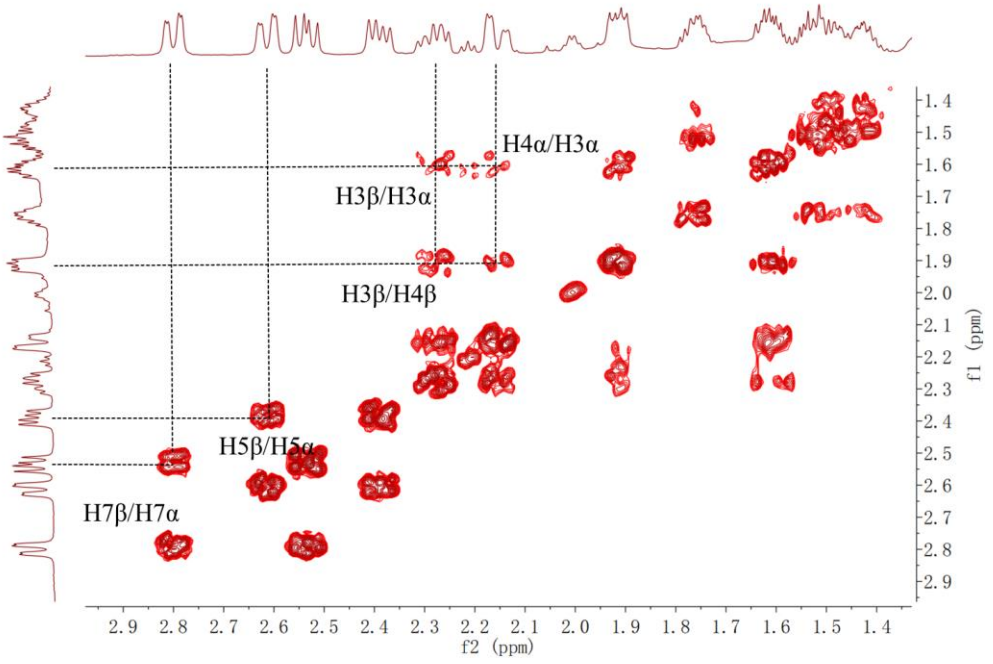


Figure S23: ^{1}H-^{1}H COSY spectrum of **6** (6*S*-hydroxy-2*R*-phomochromene) (From δ_H 1.2 ppm to δ_H 3.0 ppm).

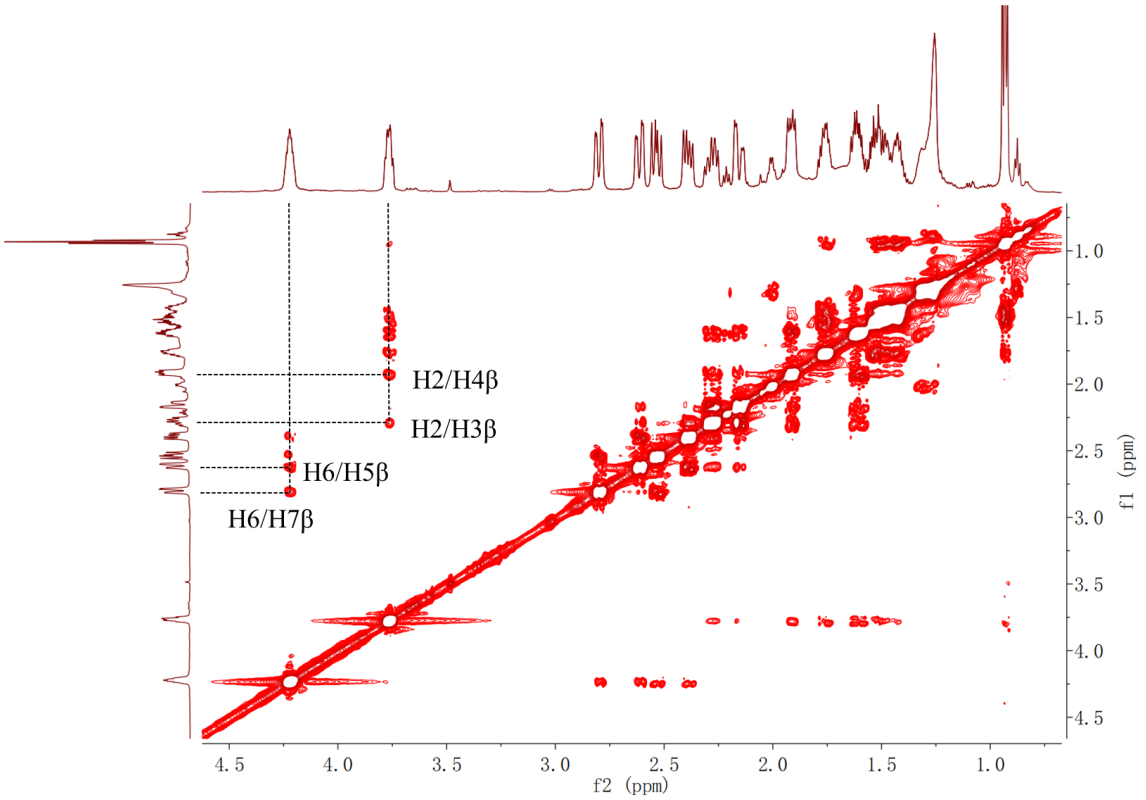


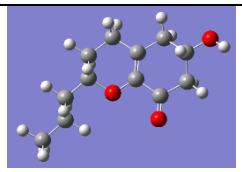
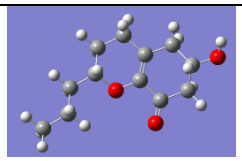
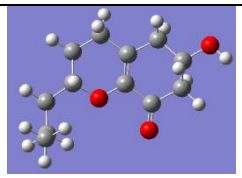
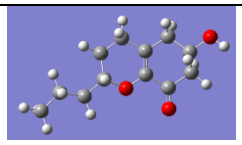
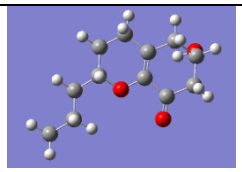
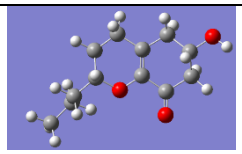
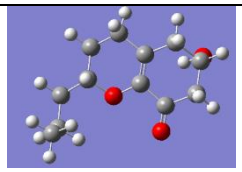
Figure S24: ROESY spectrum of **6** (6*S*-hydroxy-2*R*-phomochromene).

mPW1PW91		PCM		6-311+G(d,p)	
		DP4+	100.00%	0.00%	-
Nuclei	sp2?	Experimenta	Isomer 1	Isomer 2	Isomer 3
C		26.8	31.4228	31.11305817	
C		75.6	76.7124	75.67487804	
C	x	146.2	152.4430	150.1194989	
C	x	127.4	136.6751	133.8238835	
C		26.9	31.9700	31.67145338	
C	x	191.2	195.2526	192.2165152	
C		47.4	51.9140	50.69526406	
C		66.7	70.4512	69.92867461	
C		38.7	41.8196	41.05762392	
C		37	41.7733	41.20115298	
C		18.6	23.6253	23.16823993	
C		14.2	16.9141	16.65487921	
H		2.28	1.8894549	1.65707457	
H		1.62	1.656935944	1.878358874	
H		3.76	3.716494497	3.671751859	
H		1.91	2.236615146	2.31669757	
H		2.15	2.544069569	2.576986422	
H		2.8	2.774322538	2.667835426	
H		2.54	2.666612856	2.637804392	
H		4.22	4.242415619	4.236013529	
H		2.39	2.586083016	2.541400969	
H		2.61	2.823371424	2.754250434	
H		1.42	1.609631822	1.611366776	
H		1.5	1.702954881	1.711477542	
H		1.77	1.896313051	1.952481984	
H		1.54	1.613092098	1.605850604	
H		0.93	1.147036156	1.144571056	

Figure S25: DP4+ analyses of calculated and experimental NMR chemical shifts of **6.**（**Isomer 1**：2*R**, 6*S**-**6**，**Isomer 2**：2*S**, 6*S**-**6**）

Table S1.

Energy analyses of conformers (2*R*, 6*S*)-**6**a-n

NO.	3D comformers	Free energy		
		E (Hartree)	ΔE (Kcal/mol)	Boltzmann distribution
6a		-693.0267112	0	24.90%
6b		-693.0264688	0.152114885	19.26%
6c		-693.0260685	0.403323161	12.60%
6d		-693.0259377	0.485372315	10.97%
6e		-693.0258197	0.559430847	9.68%
6f		-693.0252806	0.897723362	5.47%
6g		-693.0249399	1.111491671	3.81%

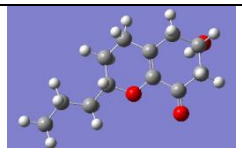
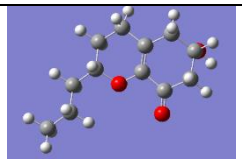
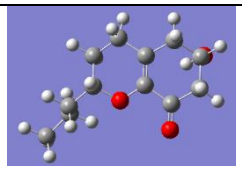
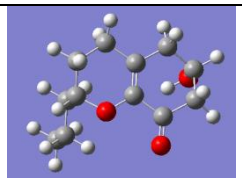
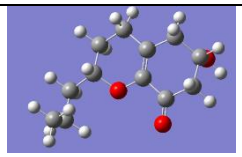
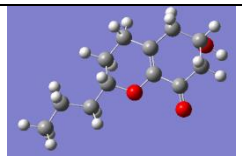
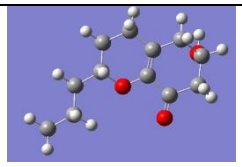
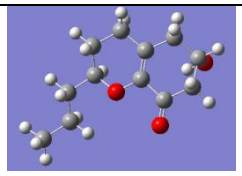
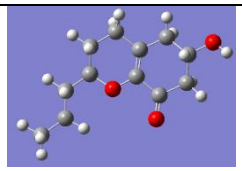
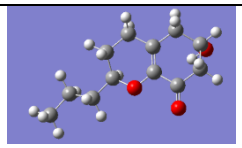
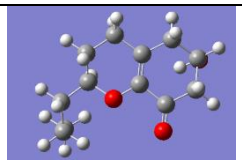
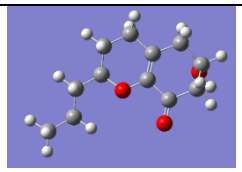
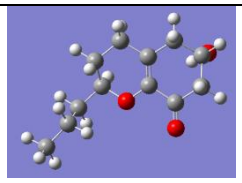
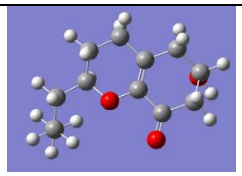
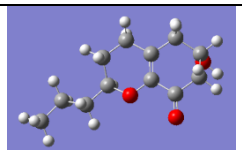
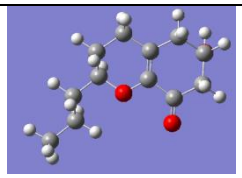
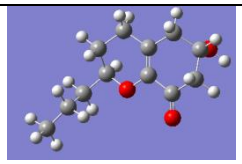
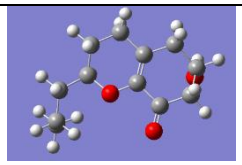
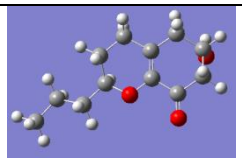
6h		-693.0248576	1.163176584	3.49%
6i		-693.0245479	1.35745716	2.52%
6j		-693.0242303	1.556754623	1.80%
6k		-693.0239752	1.716873936	1.37%
6l		-693.0238289	1.808639974	1.17%
6m		-693.0236934	1.893705536	1.02%
6n		-693.023678	1.90333457	1.00%

Table S2.

Energy analyses of conformers (2*S*, 6*S*)-**6** a-l

NO.	3D comformers	Free energy		
		E (Hartree)	ΔE (Kcal/mol)	Boltzmann distribution
6a		-693.0264147	0	26.12%
6b		-693.0258161	0.375649651	13.85%
6c		-693.0256418	0.485002716	11.51%
6d		-693.0256044	0.508464426	11.07%
6e		-693.0254389	0.612313662	9.29%
6f		-693.0251618	0.786213569	6.92%
6g		-693.0248965	0.9526989	5.23%

6h		-693.0246773	1.090217437	4.14%
6i		-693.0245312	1.181904411	3.55%
6j		-693.0242955	1.329804358	2.76%
6k		-693.0238987	1.578795038	1.82%
6l		-693.0236853	1.712698531	1.45%

NMR Computational details

The initial conformational analysis of the compound **6** was executed by employing Monte Carlo searching algorithm via the MMFF94 molecular mechanics force field[1], with the aid of the SPARTAN'16 program package, leading to afford a panel of relatively favored conformations in an energy range of 3 kcal/mol above the global minimum. The force field minimum energy conformers thus obtained were subsequently optimized by applying the density functional theory (DFT) with the B3LYP/6-31G(d) level in vacuum, implemented in the Gaussian 09 software package [2]. Harmonic vibrational frequencies were also performed to confirm no imaginary frequencies of the finally optimized conformers. Gauge-Independent Atomic Orbital (GIAO) calculations of NMR chemical shifts were accomplished by DFT at the mPW1PW91/6-311+g (d, p) level in Chloroform with the PCM solvent model in Gaussian 09 software. NMR chemical shifts of TMS were calculated in the same level and used as the references. Regression analysis of calculated versus experimental NMR chemical shifts of **6**

was carried out. Linear correlation coefficients (R^2) and Root-mean-square deviation (RMSD) were calculated for the evaluation of the results.

After Boltzmann weighing of the predicted chemical shift of each isomers, the DP4+ parameters were calculated using the excel file provided by Ariel M. Sarotti. [3]

ECD Computational details

The initial conformational analysis of the compound **6** was executed by employing Monte Carlo searching algorithm via the MMFF94 molecular mechanics force field [1], with the aid of the SPARTAN'16 program package, leading to afford a panel of relatively favored conformations in an energy range of 3 kcal/mol above the global minimum. The force field minimum energy conformers thus obtained were subsequently optimized by applying the density functional theory (DFT) with the B3LYP/6-31G(d) level in vacuum, implemented in the Gaussian 09 software package [2]. Harmonic vibrational frequencies were also performed to confirm no imaginary frequencies of the finally optimized conformers. These predominant conformers were subjected to theoretical calculation of ECD by utilizing Time-dependent density functional theory (TDDFT) calculations at the B3LYP/6-311g (2d, p) level in MeOH using the Polarizable Continuum Model (PCM) solvent model. The energies, oscillator strengths, and rotational strengths of each conformers were carried out with Gaussian 09 software package. The oretical calculations of ECD spectra for each conformer were then approximated by the Gaussian distribution. The final ECD spectrum of the individual conformers was summed up on the basis of Boltzmann-weighed population contribution by the SpecDisv1.64.[3]

Measurement of NO production

NO production was quantified by measuring the accumulation of nitrite in the cell culture supernatant with Griese reagent [4]. Briefly, RAW 264.7 cells (6×10^6 cells/mL) were seeded in 96-well plates and pretreatment with compounds for 1 h before LPS (1μg/mL) stimulation. The isolated culture supernatant was mixed with Griese reagent (Beyotime Biotechnology, China). $NaNO_2$ was used to generate a standard curve, and the absorbance of the mixture was measured at 540 nm. In the experiment, monomethylarginine monoacetate (L-NMMA) was used as a positive control.

References

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3. Bruhn T, Schaumloffel A, Hemberger Y, Bringmann G. *Chirality*, 2013, **25**: 243-244.
4. S. S. Wei, J. Chi, M. M. Zhou, R. J. Li, Y. R. Li, J. Luo and L. Y. Kong. *Ind Crop Prod*. 2019, **137**, 367–376

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