Supporting Information

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A Novel Monoterpenoid Derivative Isolated from *Chloranthus serratus* Roots with Anti-inflammatory Activity

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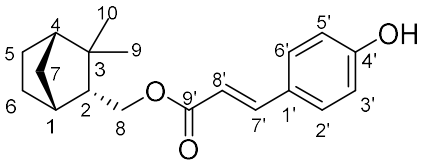

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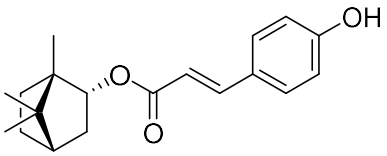
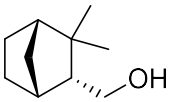


pressafonin-A (**2**)

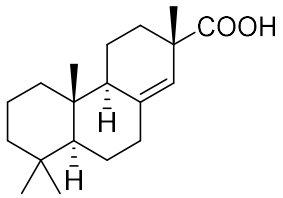


Shionoside A aglycone

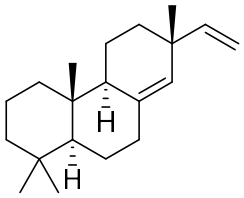
Table S1 : ^{1}H NMR and ^{13}C NMR data of **1**, **2**[1] and Shionoside A aglycone [2]

	Compound **1**[a]		pressafonin-A (**2**)[b]		Shionoside A aglycone [c]	
	δ_H (*J* in Hz)	δ_C	δ_H (*J* in Hz)	δ_C	δ_H (*J* in Hz)	δ_C
1	2.27, br s	40.6		48.9	2.27, br s	39.8
2	1.80, m*	49.0	5.01, ddd (10, 3.5, 2.1)	80.1	1.58, m	52.7
3α		37.2	1.07, m	36.9		36.8
3β			2.42, m			
4	1.79, m*	49.3	1.71, t (4.5)	45.0	1.75, br s	49.2
5*α*	1.31, m*	24.7	1.28, m	28.1	1.31, m	24.5
5*β*	1.62, m		1.78, m		1.36, m	
6*α*	1.31, m*	20.7	1.36, m	27.3	1.28, m	20.3
6*β*	1.39, m		2.04, m		1.58,m	
7a	1.23, br d (9.7)	37.4		47.9	1.20, br d	37.1
7b	1.68, br d (9.7)				1.65, br d	
8*α*	4.20, m	63.8	0.93, s	19.7	3.60, dd (11, 9)	61.2
8*β*					3.65, dd (11, 7)	
9	0.91, s	20.9	0.89, s*	18.9	0.85, s	20.5
10	1.03, s	32.6	0.88, s*	13.5	1.00, s	32.7
1′		127.5		127.2		
2′	7.43, d (8.6)	130.1	7.43, d (12.0)	129.9		
3′	6.85, d (8.6)	116.0	6.88, d (9)	115.9		
4′		157.8		158.4		
5′	6.85, d (8.6)	116.0	6.88, d (9)	115.9		
6′	7.43, d (8.6)	130.1	7.43, d (12.0)	129.9		
7′	7.61, d (16.0)	144.4	7.76, d (15.6)	144.2		
8′	6.28, d (16.0)	116.0	6.33, d (16.0)	116.0		
9′		167.8		168.1		

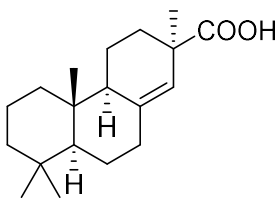
[a] ^{1}H NMR (600 MHz) and ^{13}C NMR (150 MHz) data in $CDCl_3$; [b] ^{1}H NMR (400 MHz) and ^{13}C NMR (100 MHz) data in $CDCl_3$; [c] ^{1}H NMR and ^{13}C NMR data in $CDCl_3$;
* overlapped



(5S,9R,10S,13S)-16-norpimar-8(14)-en-15-oic acid
$[\alpha]_D$ -4.9° (c 0.93, EtOH)



(-)saracopimaradiene
$[\alpha]_D$ -10.29° (c 0.965, $CHCl_3$)



Tagalong C
$[\alpha]_D$ -13 °(c= 0.17, acetone)

Table S2 : ^{1}H NMR and ^{13}C NMR data of **3**, (5*S*,9*R*,10*S*,13*S*)-16-Norpimar-8(14)-en-15-oic acid [3], (-)-Sandaracopimaradiene [4] and Tagalong C [5]

	Compound **3** [a]		(5*S*,9*R*,10*S*,13*S*)-16-Norpimar-8(14)-en-15-oic acid [b]		(-)-Sandaracopimaradiene [a]		Tagalong C [c]	
	δ_H (*J* in Hz)	δ_C	δ_H (*J* in Hz)	δ_C	δ_H (*J* in Hz)	δ_C	δ_H (*J* in Hz)	δ_C
1*α*	1.01, m	39.4	0.94, td (13.4, 4.0)	39.5	0.97, dd (8.0, 3.0)	39.4	1.05*	39.9
1*β*	1.68, m		1.3-1.8, m		1.71, m		1.65, m	
2*α*	1.48, m	18.4	1.3-1.8, m	18.5	1.72, m	18.8	1.48*	19.6
2*β*	1.65, m		1.3-1.8, m		1.62, m		1.39, m	
3*α*	1.18, td (13.2, 3.9)	42.2	1.16, td (13.1, 4.0)	42.3	1.18, br td (13.1, 3.7)	42.2	1.22, m	42.8
3*β*	1.41, br d (13.6)		1.3-1.8, m		1.43, m		1.41, m	
4		33.5		33.5		33.3		33.9
5	1.03, br d (12.7)	54.8	1.01, dd (12.6, 2.4)	54.8	1.02,d (2.0)	54.8	1.11, dd (12.8, 2.8)	55.5
6*α*	1.60, m	22.6	1.3-1.8, m	22.6	1.58, m	22.6	1.64, m	23.3
6*β*	1.29, m		1.27, qd (13.0, 4.5)		1.28, ddd (25.4, 13.0,4.8)		1.33, dd (12.8, 2.8)	
7*α*	2.29, m	36.0	2.27, ddd (14.3, 4.5, 2.0)	36.0	2.25, ddd (25.4, 13.0, 4.8)	36.0	2.06, ddd (14.0, 4.4, 2.0)	36.4
7*β*	2.06, td (13.8, 5.6)		2.03, td (13.7, 5.8)		2.05, td (14.0 6.0)		2.31, m	

8		139.6		139.7		137.3		139.6
9	1.74, m	50.4	1.3-1.8, m	50.5	1.69, m	50.6	1.76, m	51.5
10		38.4		38.5		38.3		39.1
11α	1.46, m	19.1	1.3-1.8, m	19.2	1.42, m	19.0	1.60, m	20.9
11β	1.52, m		1.3-1.8, m		1.52, m		1.48*	
12α	1.77, m	31.6	1.3-1.8, m	31.5	1.48, m	34.6	1.09*	33.9
12β	1.66, m		1.3-1.8, m		1.35, td (12.4, 4.1)		2.16, br d (12.8)	
13		42.9		43.0		37.4		43.2
14	5.54, s	124.1	5.52, br s	124.2	5.21, s	128.5	5.41, br s	126.8
15		183.4		184.5	5.77, dd (17.0, 11.0)	149.1		177.9
16α					4.88, dd (11.0, 1.0)	110.0		
16β					4.90, dd (17.0, 1.0)			
17	1.27, s	24.8	1.25, s	24.8	1.04, s	26.0	1.19, s	28.1
18	0.88, s	33.9	0.86, s	33.9	0.87, s	33.8	0.89, s	34.0
19	0.85, s	22.3	0.82, s	22.3	0.85, s	22.1	0.86, s	22.4
20	0.77, s	15.1	0.75, s	15.1	0.79, s	15.0	0.72, s	14.9

[a] ^{1}H NMR (600 MHz) and ^{13}C NMR (150 MHz) data in $CDCl_3$; [b] ^{1}H NMR (500 MHz) and ^{13}C NMR (125 MHz) data in $CDCl_3$; [c] ^{1}H NMR (400 MHz) and ^{13}C NMR (100 MHz) data in acetone-d_6;
* overlapped

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[5] X. Zhang, W. Li, L. Shen and J. Wu (2018). Four new diterpenes from the mangrove Ceriops tagal and structure revision of four dolabranes with a 4,18-epoxy group, *Fitoterapia*. **124**, 1–7.

Compound **3** ((5*S*,9*R*,10*S*,13*S*)-16-norpimar-8(14)-en-15-oic acid): $[\alpha]_D^{24}$ -8.7° (c 0.10, EtOH); ^{1}H and ^{13}C NMR data, see Table S2.

Compound **4** (13-*epi*-torulosol): ^{1}H-NMR (600 MHz, $CDCl_3$) δ_H: 5.90 (1H, dd, *J* = 17.2, 10.8 Hz, H-14), 5.21 (1H, d, *J* = 17.2 Hz, H-15b), 5.06 (1H, d, *J* = 10.8 Hz, H-15a), 4.80 (1H, s, H-17b), 4.48 (1H, s, H-17a), 3.75 (1H, d, *J* = 10.8 Hz, H-19a), 3.38 (1H, d, *J* = 10.8 Hz, H-19b), 2.37 (1H, d, *J* = 12.8 Hz, H-7b), 1.93 (1H, td, *J* = 12.8, 4.6 Hz, H-7a), 1.83-1.80 (3H, m, H-1b, H-6b, H-12b), 1.69 (1H, m, H-3b), 1.54 (1H, m, H-9), 1.50 (2H, m, H-2, H-11b), 1.35-1.29 (4H, m, H-5, H-6a, H-11a, H-12a), 1.27 (3H, s, H-16), 1.07 (2H, m, H-1a, H-3a), 0.97 (3H, s, H-18), 0.64 (3H, s, H-20);^{13}C-NMR (150 MHz, $CDCl_3$) δ_C: 148.4 (C-8), 145.2 (C-14), 111.8 (C-15), 106.8 (C-17), 73.8 (C-13), 65.2 (C-19), 57.4 (C-9), 56.5 (C-5), 41.4 (C-12), 39.9 (C-10), 39. 0 (C-1), 38.8 (C-4), 38.8 (C-7), 35.6 (C-3), 28.2 (C-18), 27.2 (C-16), 24.6 (C-6), 19.1 (C-2), 17.9 (C-11), 15.4 (C-20).

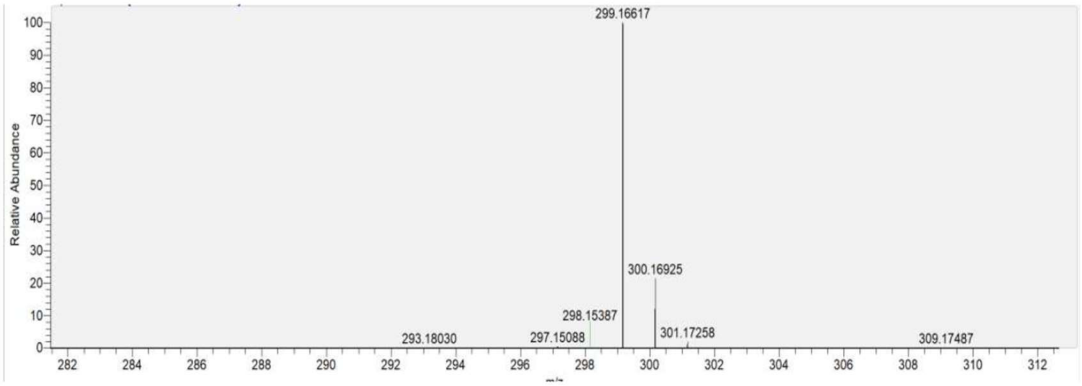
Compound **5** (12*E*-dien-19-ol): ^{1}H-NMR (600 MHz, $CDCl_3$) δ_H: 9.34 (1H, s, H-14), 6.42 (1H, br s, H-12), 4.83 (1H, s, H-17b), 4.39 (1H, s, H-17a), 3.77 (H, d, *J* = 10.8 Hz, H-19b), 3.42 (H, d, *J* = 10.8 Hz, H-19a), 2.47 (2H, m, H-11), 2.39 (1H, m, H-7b), 2.00 (1H, m, H-7a), 1.90 (1H, m, H-9), 1.85 (2H, m, H-1b, H-6b), 1.80 (1H, m, H-3b), 1.75 (3H, s, H-16), 1.56 (1H, m, H-2), 1.34 (1H, m, H-6a), 1.26 (1H, m, H-5), 1.15 (1H, m, H-1a), 1.02 (1H, m, H-3a), 1.00 (3H, s, H-18), 0.73 (3H, s, H-20); ^{13}C-NMR (150 MHz, $CDCl_3$) δ_C:195.4 (C-14), 156.3 (C-12), 147.9 (C-8), 139. 1 (C-13), 108.1 (C-17), 65.2 (C-19), 56.7 (C-5), 56.3 (C-9), 39.6 (C-10), 39.3 (C-1), 39.0 (C-7), 38.0 (C-3), 35.5 (C-4), 27.2 (C-6), 24.6 (C-11), 24.3 (C-18), 19.1 (C-2), 13.0 (C-20), 9.5 (C-16).

Compound **6** (15-nor-14-oxolabda-8(17),12*E*-dien-19-oic acid): ^{1}H-NMR (600 MHz, $CDCl_3$) δ_H:9.34 (1H, s, H-14), 6.43 (1H, br s, H-12), 4.86 (1H, s, H-17b), 4.40 (1H, s, H-17a), 2.55 (1H, m, H-11a), 2.40 (2H, m, H-7), 2.19 (1H, d, *J* = 13.0 Hz, H-3a), 2.00 (2H, m, H-6), 1.87 (2H, m, H-1b, H-9), 1.76 (3H, s, H-16), 1.56 (1H, d, *J* = 13.0 Hz, H-2a), 1.39 (1H, d, *J* = 12.1 Hz, H-5), 1.26 (3H, s, H-18), 1.16 (1H, t, *J* = 12.3 Hz, H-1a), 1.08 (1H, *J* = 12.3 Hz, H-2b), 0.68 (3H, s, H-20); ^{13}C-NMR (150 MHz, $CDCl_3$) δ_C:195.4 (C-14), 183.7 (C-19), 156.3 (C-12), 147.7 (C-

8), 139.1 (C-13), 108.0 (C-17), 56.3 (C-5), 55.9 (C-9), 44.3 (C-4), 40.5 (C-10), 39.5 (C-1), 38.4 (C-7), 38.0 (C-3), 29.0 (C-18), 25.9 (C-6), 24.6 (C-11), 20.0 (C-2), 13.0 (C-20), 9.5 (C-16).

Compound **7** (11*E*-labdadien-19-oic acid): ^{1}H-NMR (600 MHz, $CDCl_3$) δ_H: 6.85 (1H, dd, *J* =15.8, 10.4 Hz, H-11), 6.08 (1H, d, *J* =15.8 Hz, H-12), 4.81 (1H, s, H-17b), 4.43 (1H, s, H-17a), 2.47 (2H, m, H-7), 2.19 (1H, d, *J* = 13.1 Hz, H-3a), 2.02 (2H, m, H-6), 1.92 (1H, m, H-1b), 1. 82 (1H, m, H-9), 1.46 (1H, m, H-2a), 1.35 (1H, d, *J* = 12.4 Hz, H-5), 1.27 (3H, s, H-14), 1.25 (3H, s, H-18), 1.09 (2H, m, H-1a, H-3b), 0.81 (3H, s, H-20); ^{13}C-NMR (150 MHz, $CDCl_3$) δ_C:198.3 (C-19), 182.2 (C-13), 148.1 (C-13), 146.2 (C-17), 133.9 (C-19), 108.9 (C-8), 60.2 (C-5), 55.5 (C-9), 44.2 (C-4), 41.0 (C-10), 40.1 (C-1), 38.1 (C-7), 37.2 (C-3), 29.8 (C-18), 29.0 (C-6), 27.4 (C-11), 25.0 (C-2), 19.7 (C-20), 13.8 (C-16).

Compound **8** (14,15-dinor-13-oxo-8(17)-labden-19-oic acid): ^{1}H-NMR (600 MHz, $CDCl_3$) δ_H: 4.85 (1H, s, H-17a), 4.45 (1H, s, H-17b), 2.59 (1H, m, H-12a), 2.42 (1H, m, H-7b), 2.32 (1H, m, H-12b), 2.22 (2H, m, H-3), 2.11 (3H, s, H-16), 1.97 (1H, m, H-11a), 1.90 (1H, m, H-2b), 1.90-1.82 (4H, m, H-1b, H-6,H-7a, H-12b), 1.58-1.50 (2H, m, H-2a, H-9), 1.32 (1H, H-5), 1.23 (3H, s, H-18), 1.09 (1H, m, H-1a), 0.61 (3H, s, H-20); ^{13}C-NMR (150 MHz, $CDCl_3$) δ_C:209.6 (C-13), 182.2 (C-19), 148.8 (C-8), 106.7 (C-17), 56.3 (C-5), 55.6 (C-9), 44.2 (C-4), 43.0 (C-12), 40.7 (C-10), 39.2 (C-1), 38.8 (C-7), 38.2 (C-3), 30.2 (C-16), 26.2 (C-6), 20.0 (C-18), 19.6 (C-2), 17.8 (C-11), 12.8 (C-20).



Elemental Composition Calculator

Target m/z:	299.16617	**Result type:**	Negative ions	**Species**	$[M-H]^-$
Element:		C(0-30);H(0-60);O(0-15)			
Ion Formula		**Calculated m/z**		**PPM Error**	
C19H23O3		299.16472		4.85	

Figure S1: HR-ESI-MS spectrum of **1** (chloronin A)

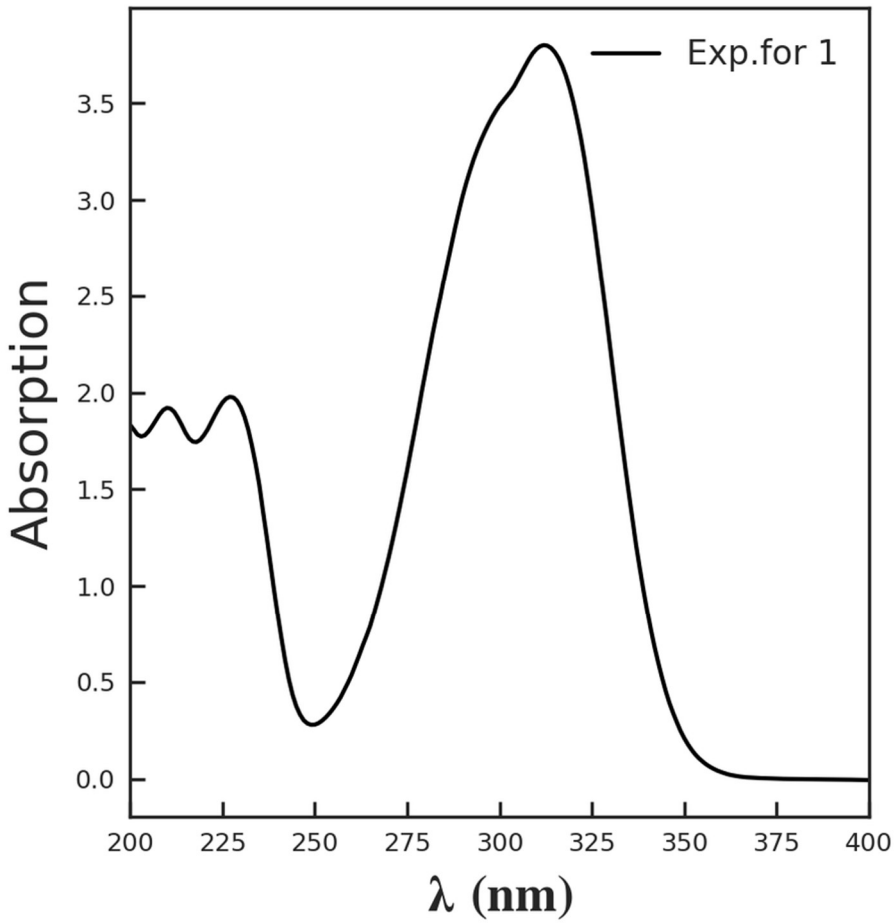


Figure S2: UV spectrum of **1** (chloronin A).

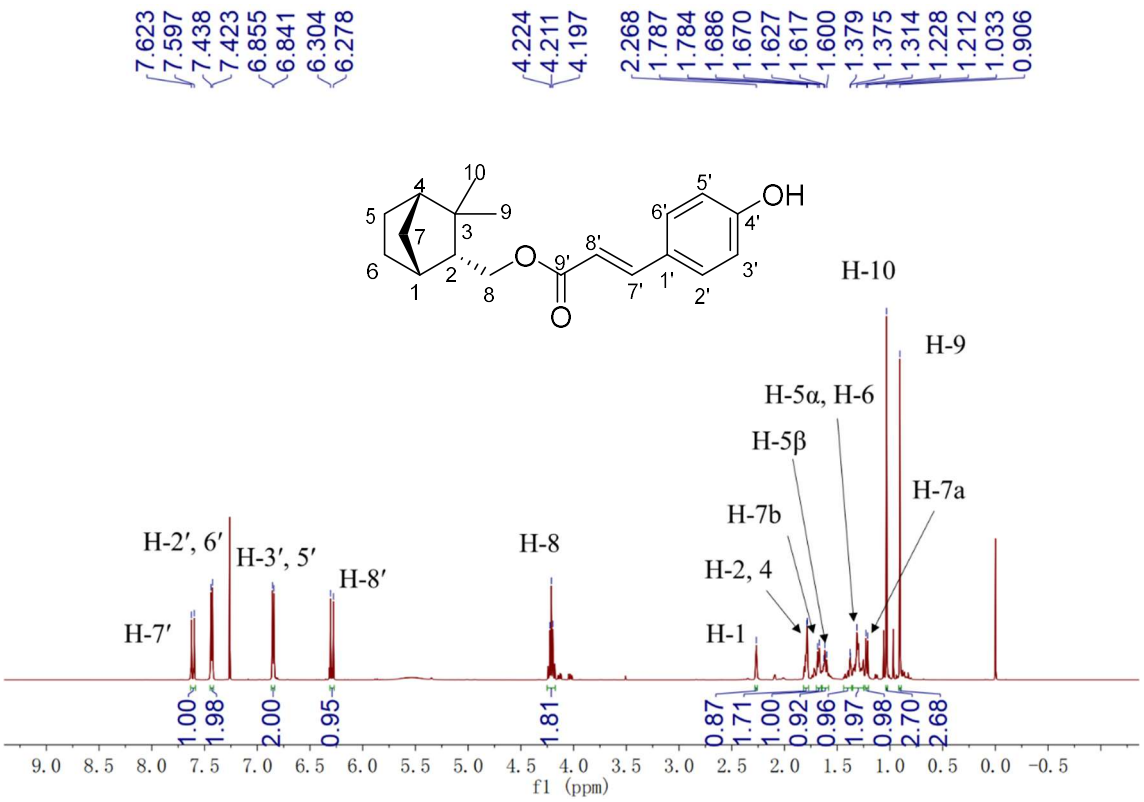


Figure S3: ^{1}H-NMR (600 MHz, $CDCl_3$) spectrum of **1** (chloronin A).

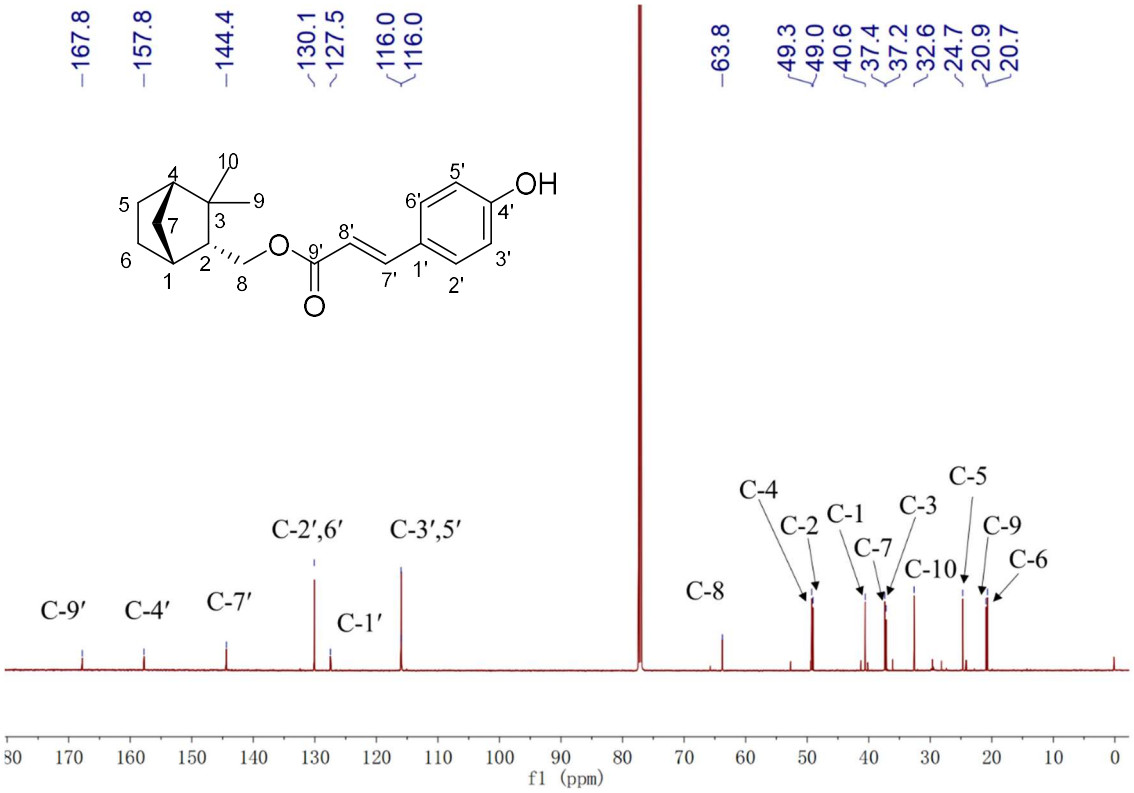


Figure S4: ^{13}C-NMR (150 MHz, $CDCl_3$) spectrum of **1** (chloronin A).

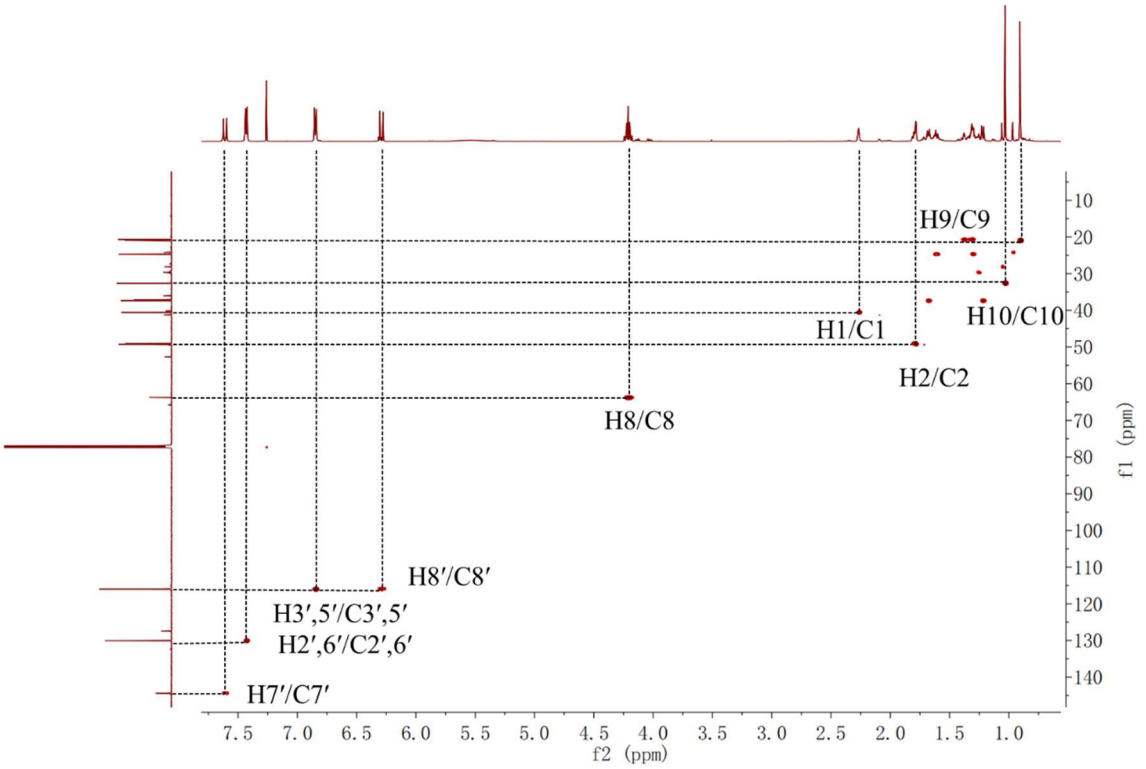


Figure S5: HSQC spectrum of **1** (chloronin A).

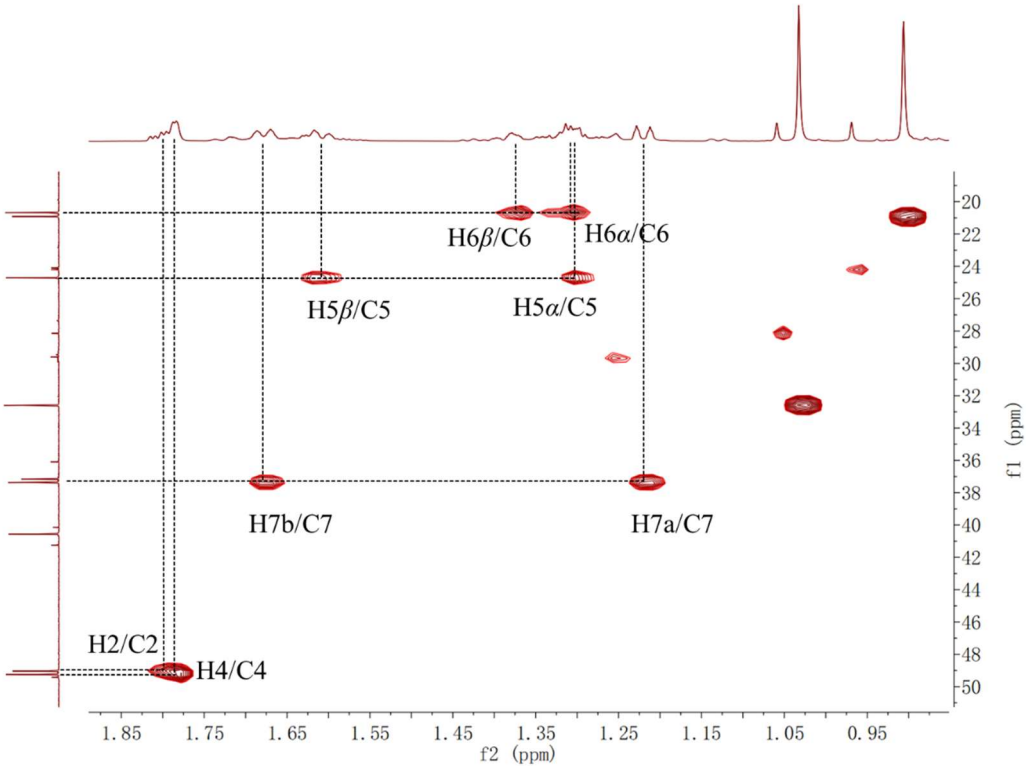


Figure S6: HSQC spectrum of **1** (chloronin A) (From δ_C 20 ppm to δ_C 50 ppm).

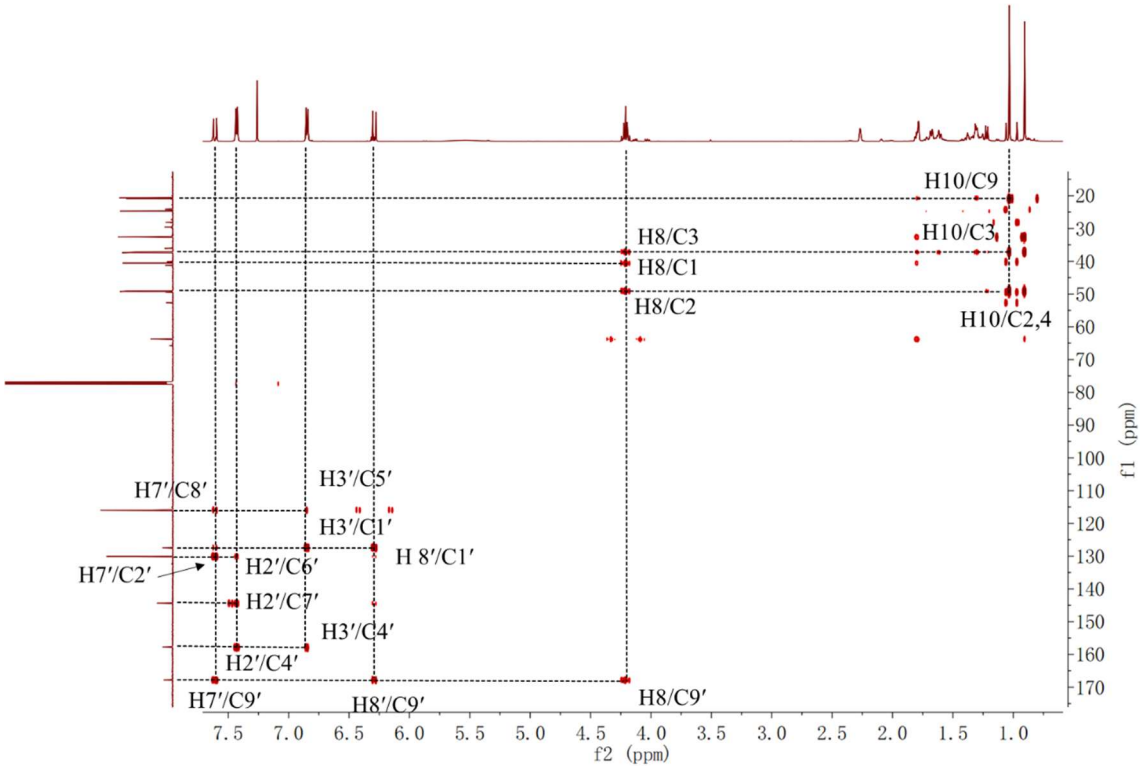


Figure S7: HMBC spectrum of **1** (chloronin A).

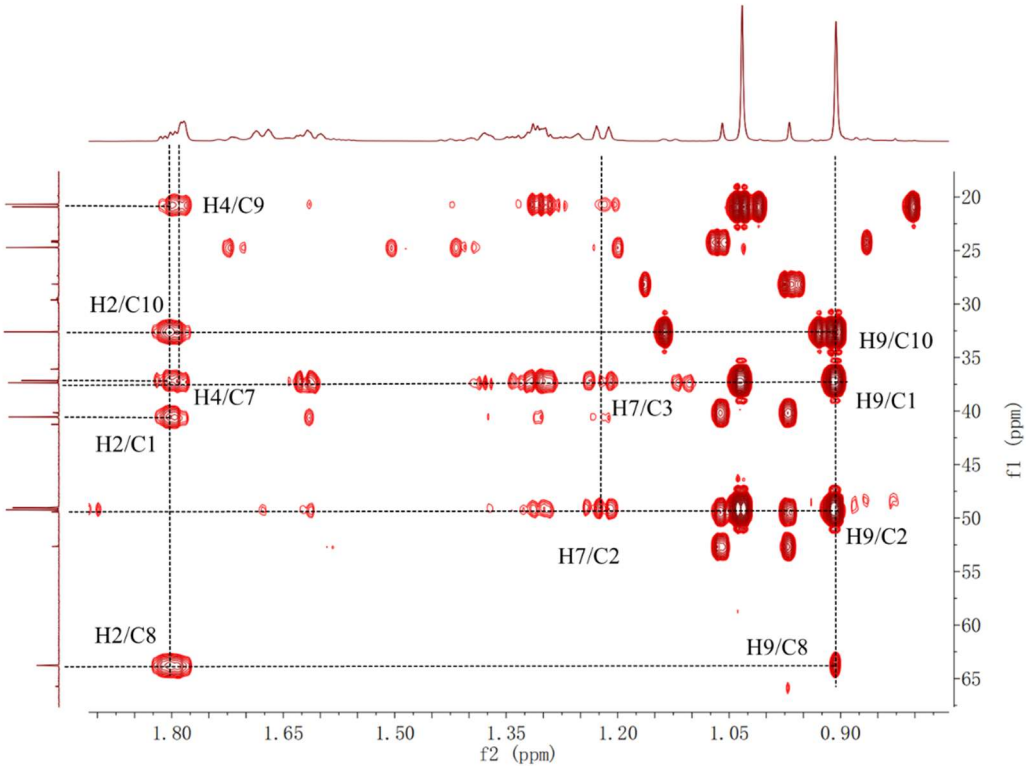


Figure S8: HMBC spectrum of **1** (chloronin A) (From δ_C20 ppm to δ_C 65 ppm).

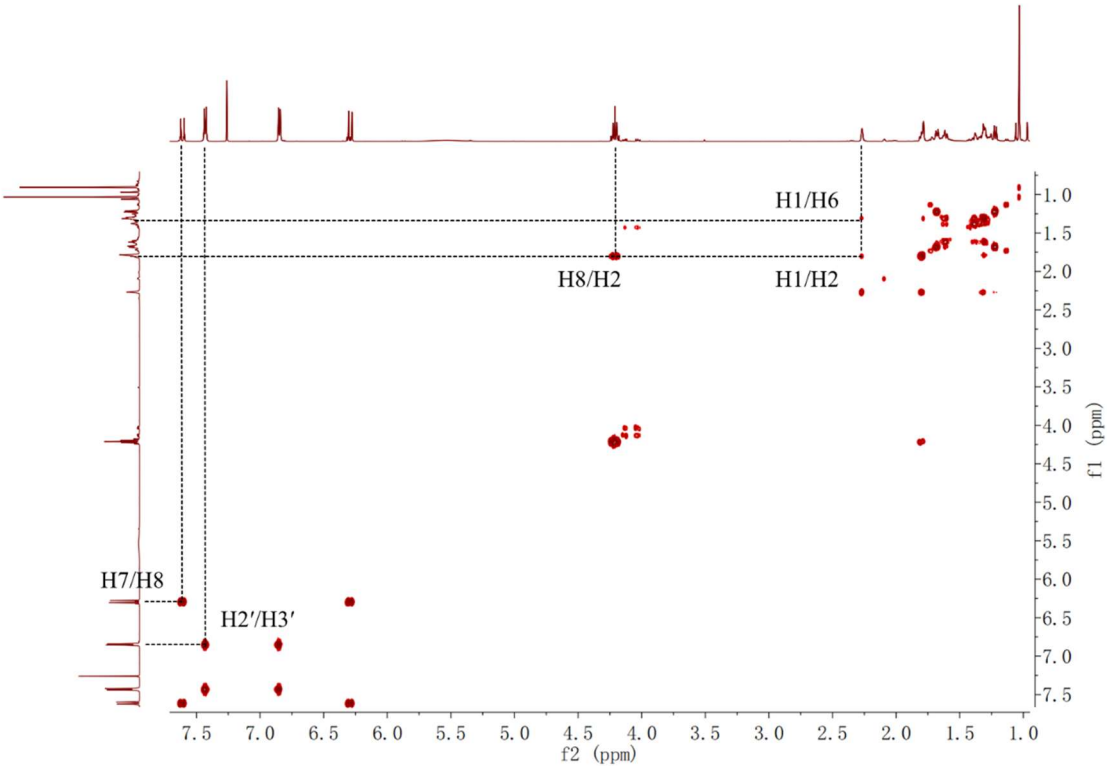


Figure S9: ^{1}H-^{1}H COSY spectrum of **1** (chloronin A).

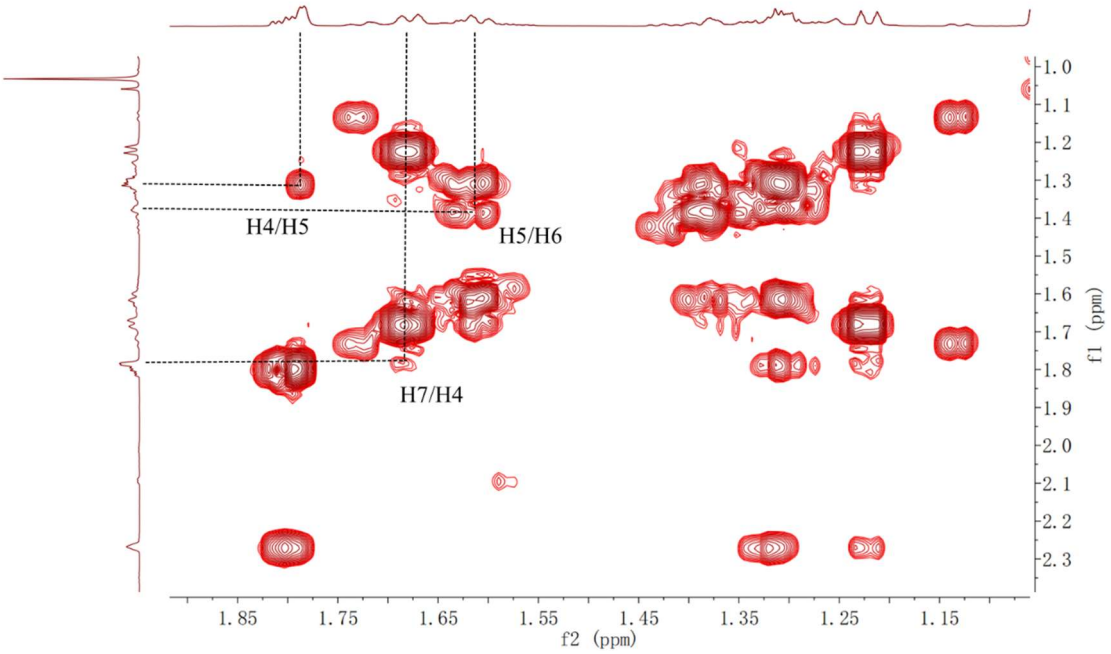


Figure S10: ^{1}H-^{1}H COSY spectrum of **1** (chloronin A) (From δ_H 1.0 ppm to δ_H 2.5 ppm).

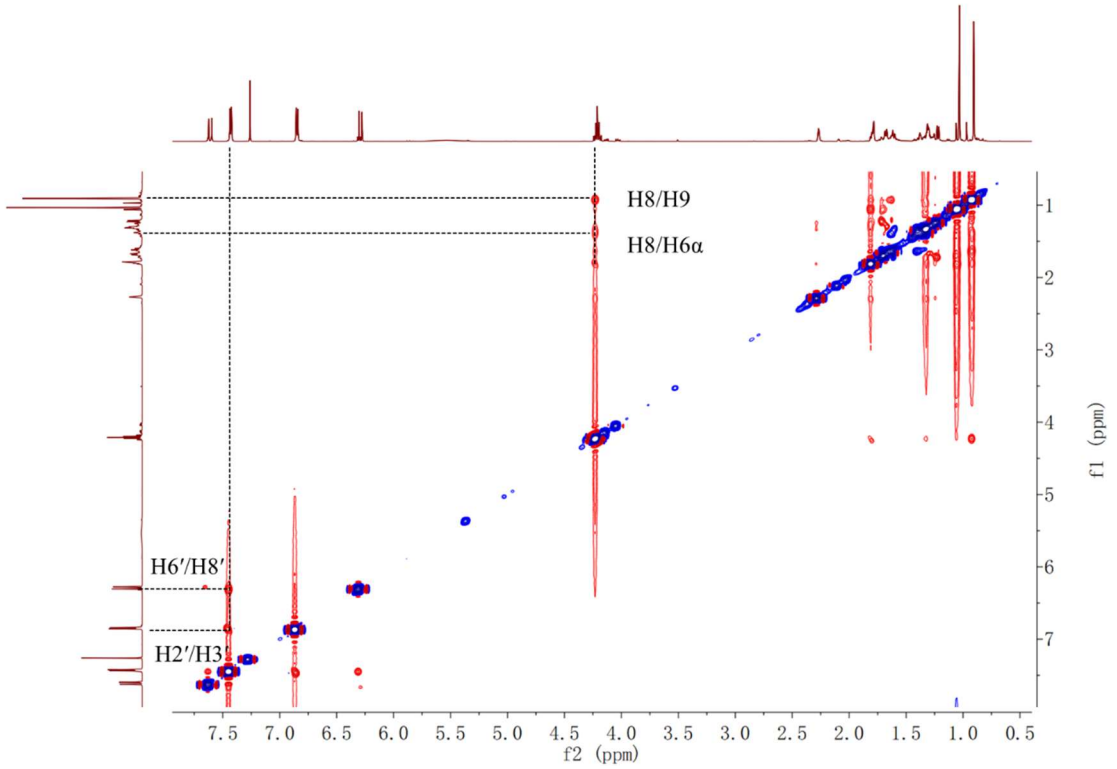


Figure S11: ROESY spectrum of **1** (chloronin A).

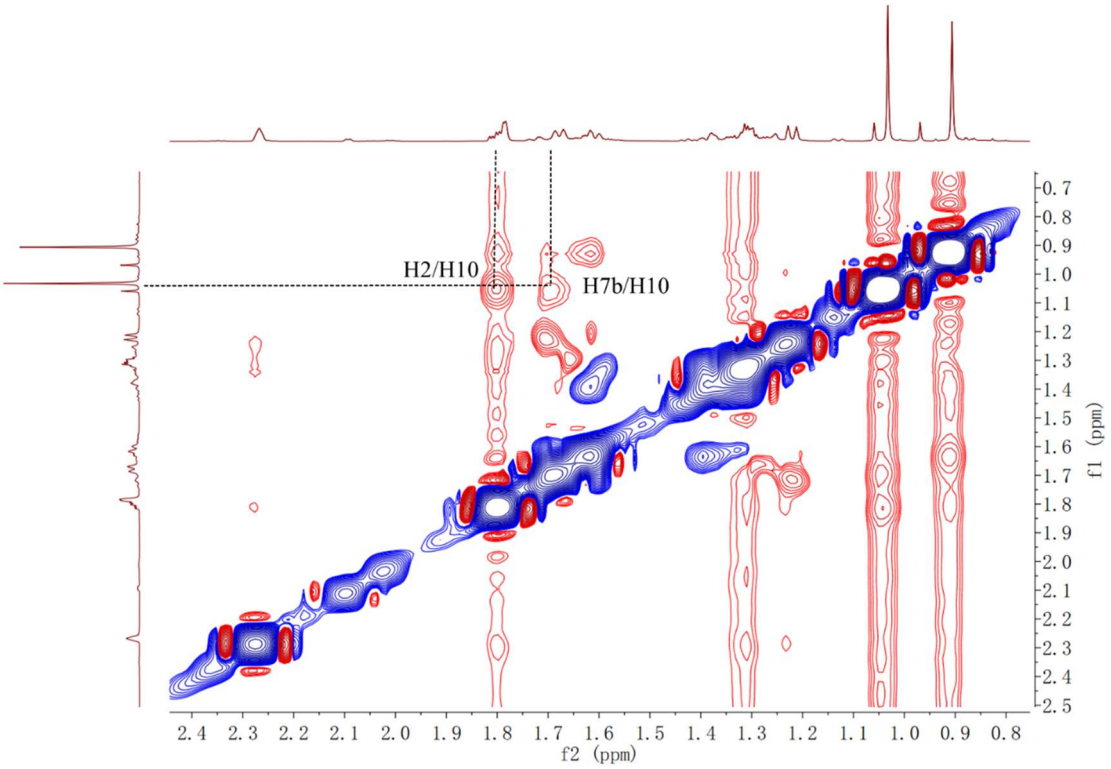


Figure S12 ROESY**:** spectrum of **1** (chloronin A) (From δ_H 0.5ppm to δ_H 2.5 ppm).

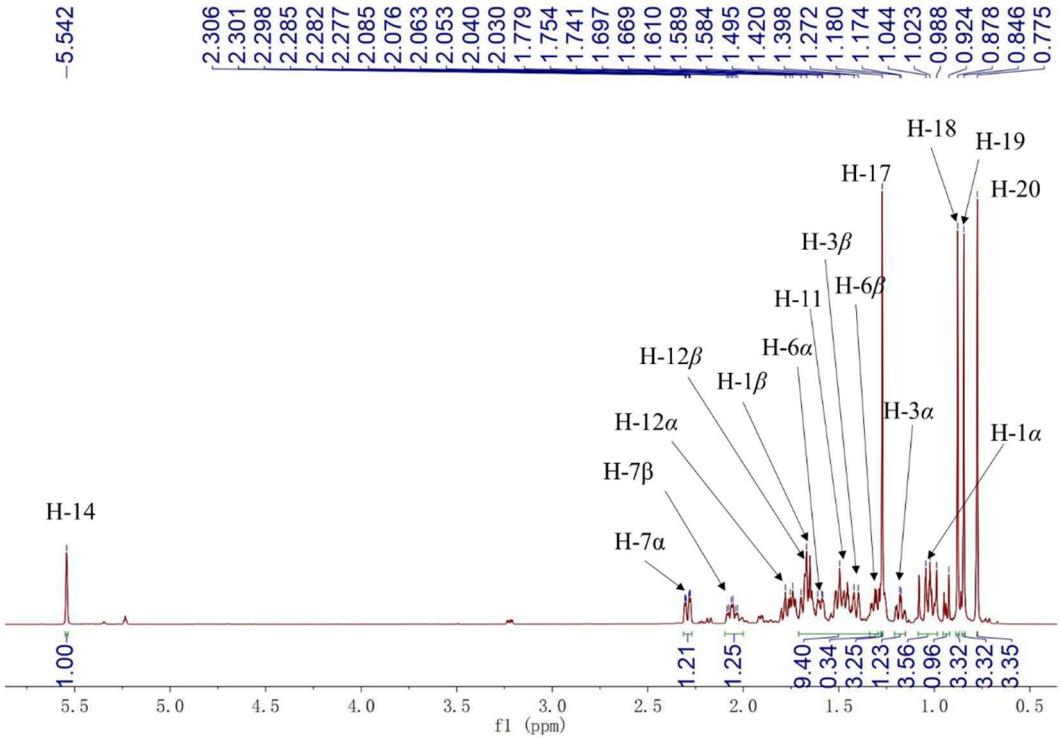


Figure S13: ^{1}H-NMR (600 MHz, $CDCl_3$) spectrum of **3** [5*S*,9*R*,10*S*,13*S*)-16-Norpimar-8(14)-en-15-oic acid].

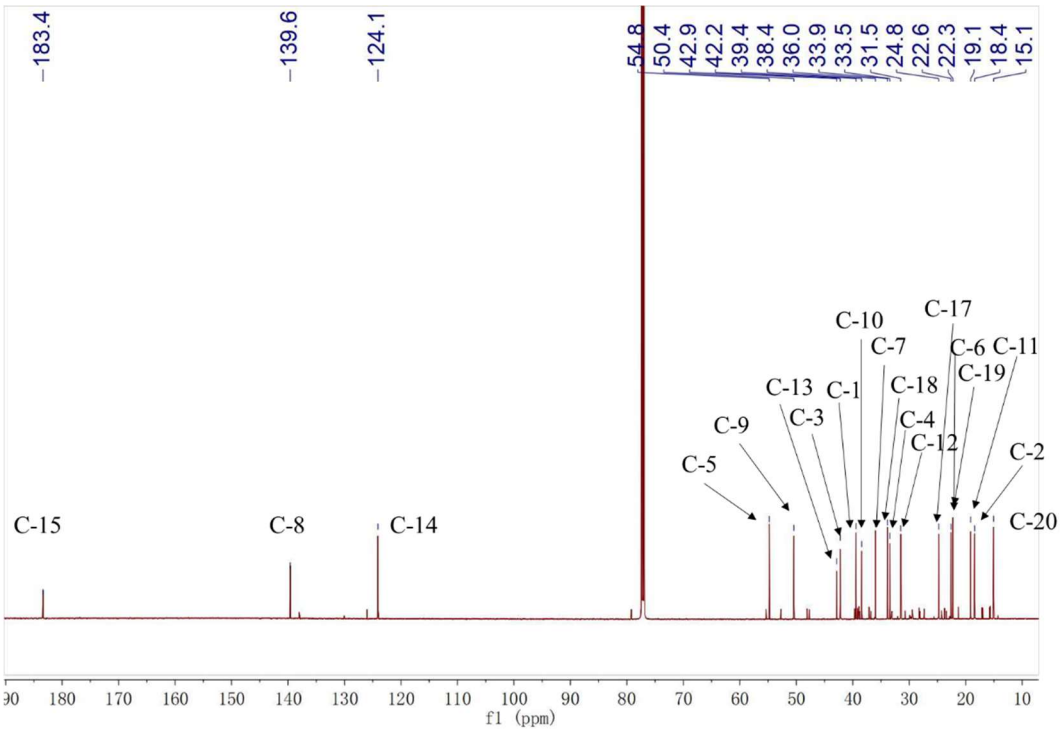


Figure S14: ^{13}C-NMR (150 MHz, $CDCl_3$) spectrum of **3** [5*S*,9*R*,10*S*,13*S*)-16-Norpimar-8(14)-en-15-oic acid].

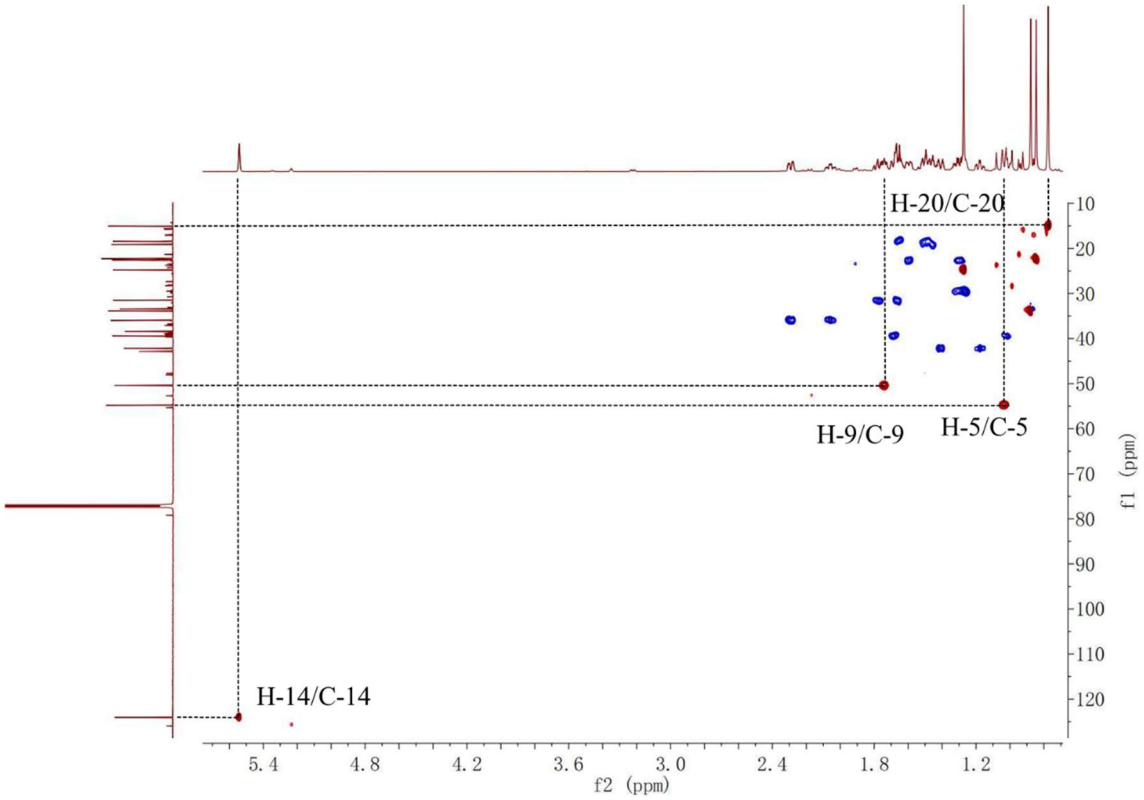


Figure S15: HSQC spectrum of **3** [5*S*,9*R*,10*S*,13*S*)-16-Norpimar-8(14)-en-15-oic acid].

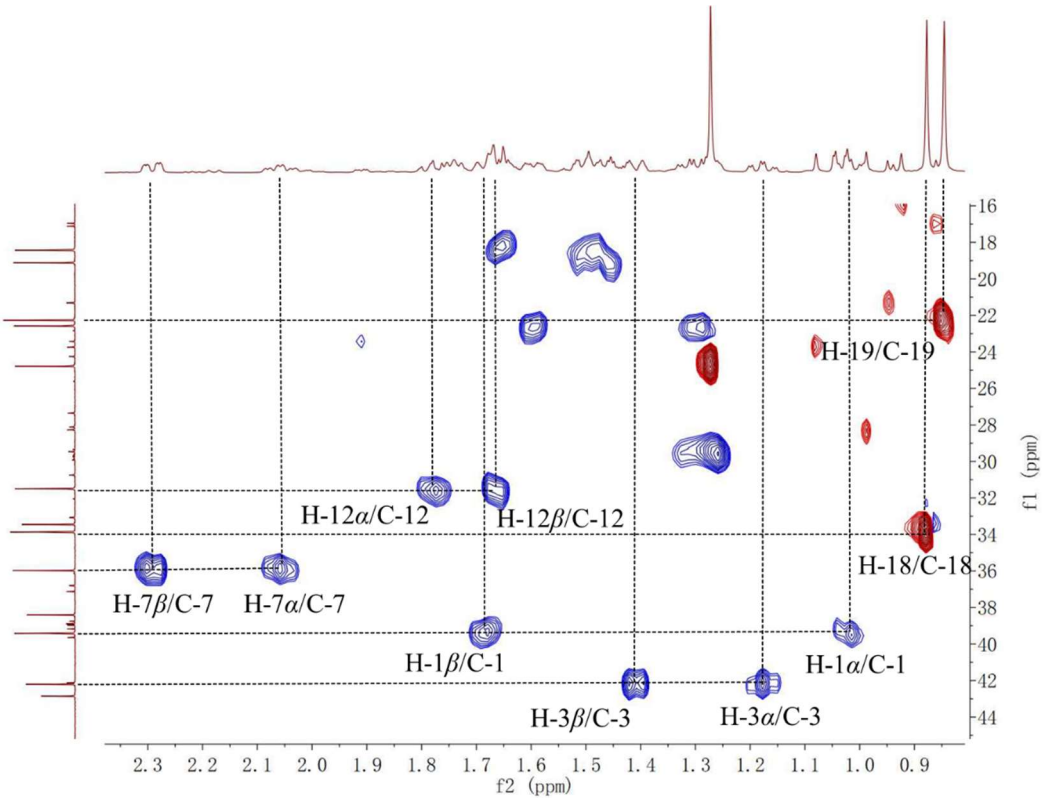


Figure S16: HSQC spectrum of **3** [5*S*,9*R*,10*S*,13*S*)-16-Norpimar-8(14)-en-15-oic acid] (From δ_C 15ppm to δ_C 45 ppm).

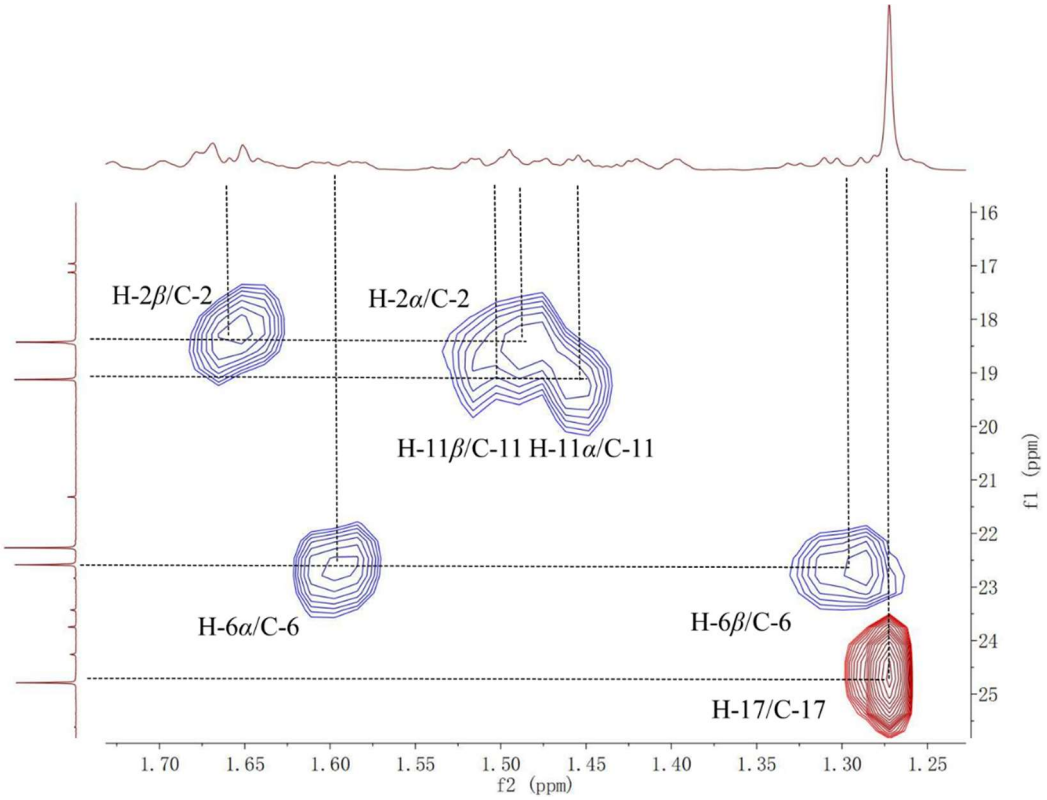
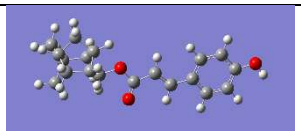
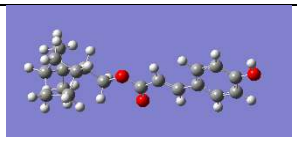
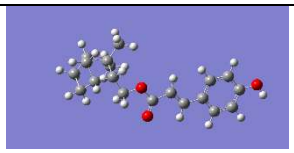


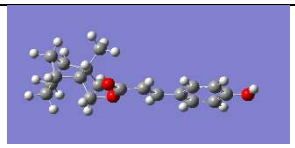
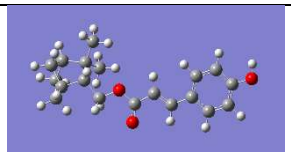
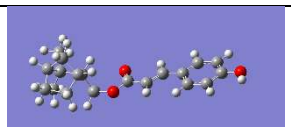
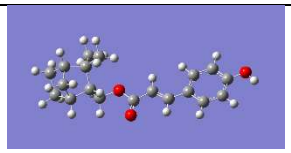
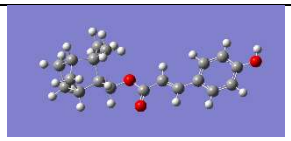
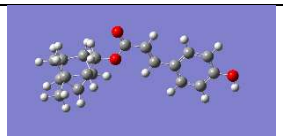
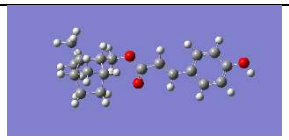
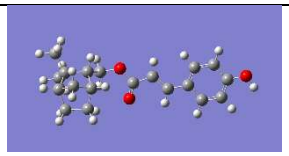
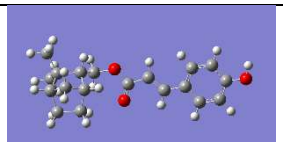
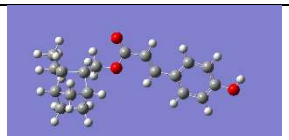
Figure S17: HSQC spectrum of **3** [5*S*,9*R*,10*S*,13*S*)-16-Norpimar-8(14)-en-15-oic acid] (From δ_C 15 ppm to δ_C 30 ppm).

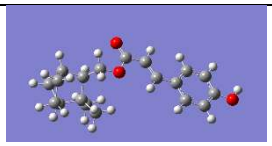
ECD Computational details

The initial conformational analysis of the compound **1** 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. Theoretical 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]

Table S3: Energy analyses of conformers (1*R*,2*R*,4*S*)-**1**a-n

NO.	3D comformers	Free energy		
		E (Hartree)	ΔE (Kcal/mol)	Boltzmann distribution
1a		-963.0981042	0	16.50%
1b		-963.0978256	0.174822336	12.30%
1c		-963.097506	0.375372295	8.78%

1d		-963.0972417	0.541221337	6.63%
1e		-963.0972643	0.52703977	6.80%
1f		-963.0970954	0.633025026	5.68%
1g		-963.0969455	0.727087726	4.85%
1h		-963.0967714	0.836335998	4.03%
1i		-963.0965739	0.960267841	3.27%
1j		-963.0979645	0.087662169	14.28%
1k		-963.0965504	0.975014161	3.20%
1l		-963.097625	0.300699438	9.97%
1m		-963.0958415	1.419851038	1.51%

1n		-963.0961576	1.22149734	2.10%

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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2. Frisch MJ, Trucks GW, Schlegel H B, Scuseria GE, Robb MA, Cheeseman JR, Scalmani G, Barone V, Mennucci B, Petersson GA, Nakatsuji H, Caricato M, Li X, Hratchian H P, Izmaylov AF, Bloino J, Zheng G, Sonnenberg JL, Hada M, Ehara M, Toyota K, Fukuda R, Hasegawa J, Ishida M, Nakajima T, Honda Y, Kitao O, Nakai H, Vreven T, Montgomery Jr JA, Peralta JE, Ogliaro F, Bearpark M, Heyd JJ, Brothers E, Kudin KN, Staroverov VN, Kobayashi R, Normand J, Raghavachari K, Rendell A, Burant JC, Iyengar SS, Tomasi J, Cossi M, Rega N, Millam JM, Klene M, Knox JE, Cross J B, Bakken V, Adamo C, Jaramillo J, Gomperts R, Stratmann RE, Yazyev O, Austin AJ, Cammi R, Pomelli C, Ochterski JW, Martin RL, Morokuma K, Zakrzewski VG, Voth GA, Salvador P, Dannenberg JJ, Dapprich S, Daniels AD, Farkas Ö, Foresman JB, Ortiz JV, Cioslowski J, Fox DJ, Gaussian 09, Rev. C 01; Gaussian, Inc., Wallingford CT, 2009.
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

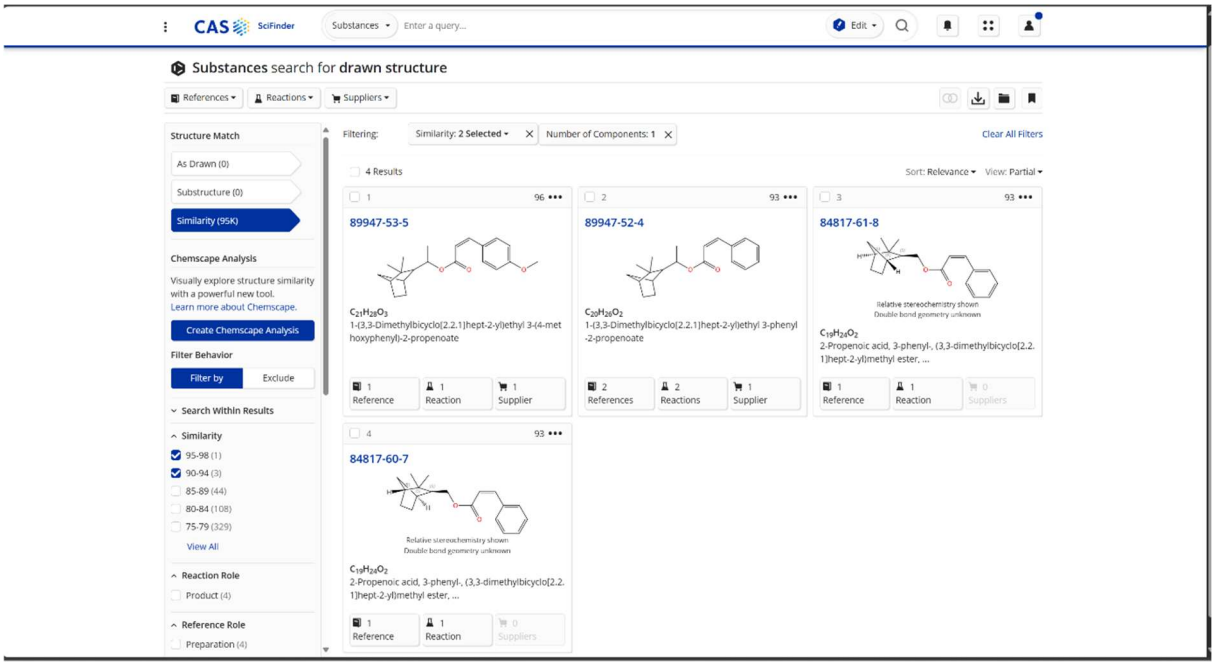

Figure S18: New compounds search report of SciFinder