

Supporting Information

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A New Benzofuran from the Roots of *Eupatorium chinense* L. and Its α -glucosidase and PTP1B Inhibitory Activities

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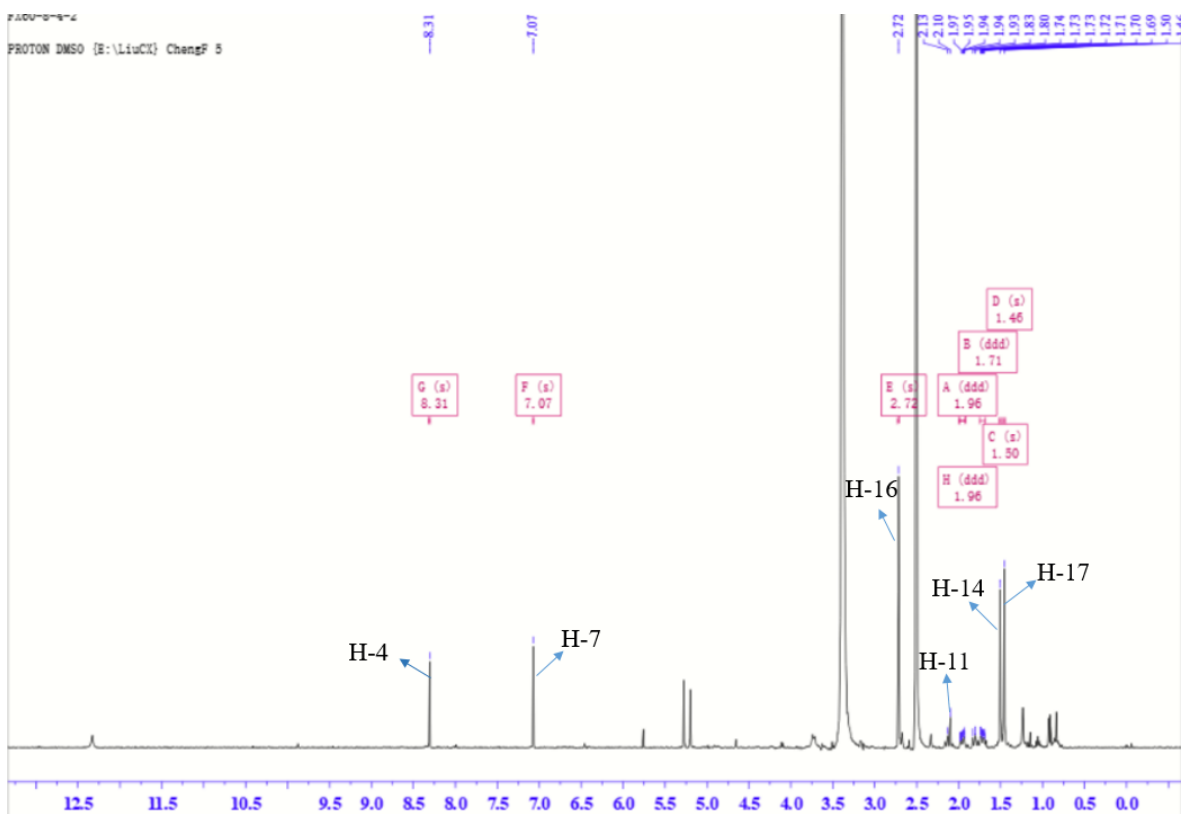


Figure S1: ^1H NMR spectrum of compound **1**

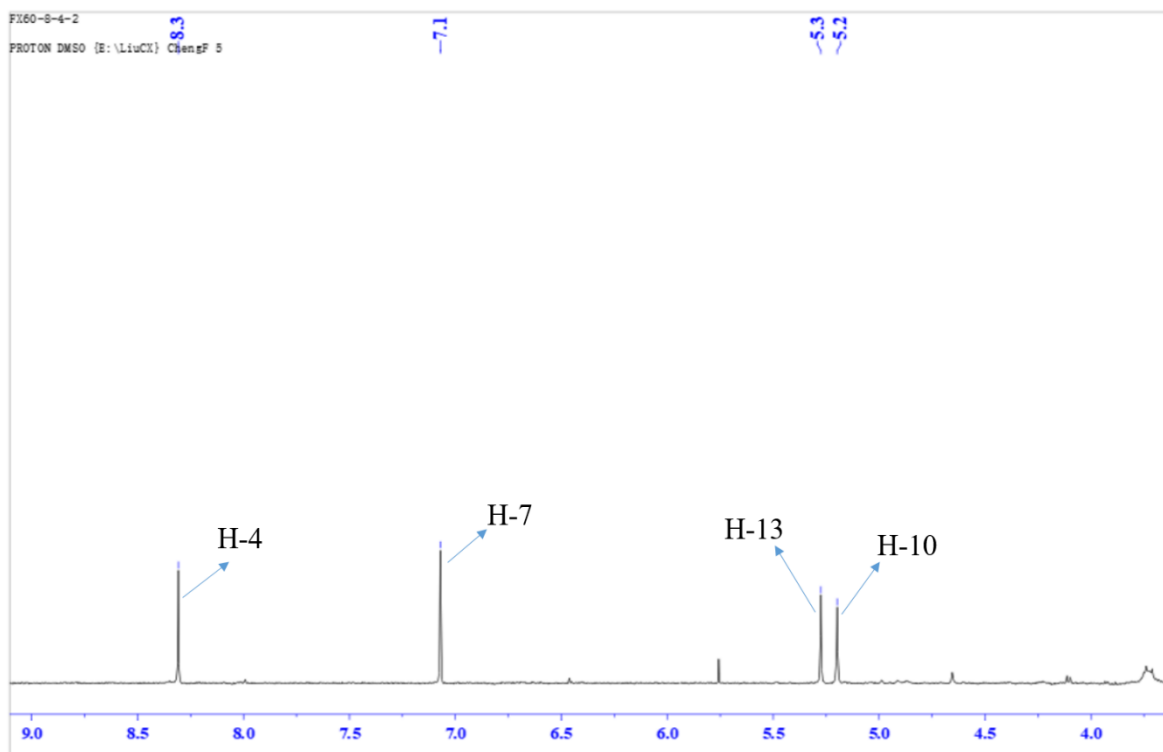


Figure S1-1: ^1H NMR spectrum of compound **1** (enlarged image)

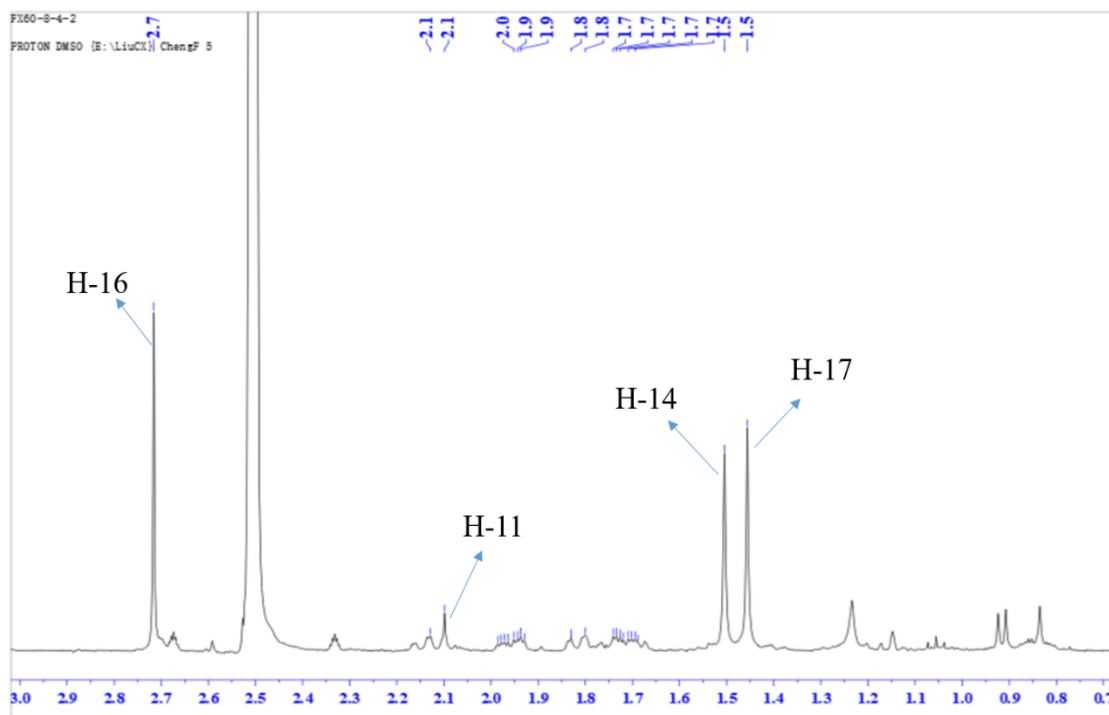


Figure S1-2: ^1H NMR spectrum of compound **1** (enlarged image)

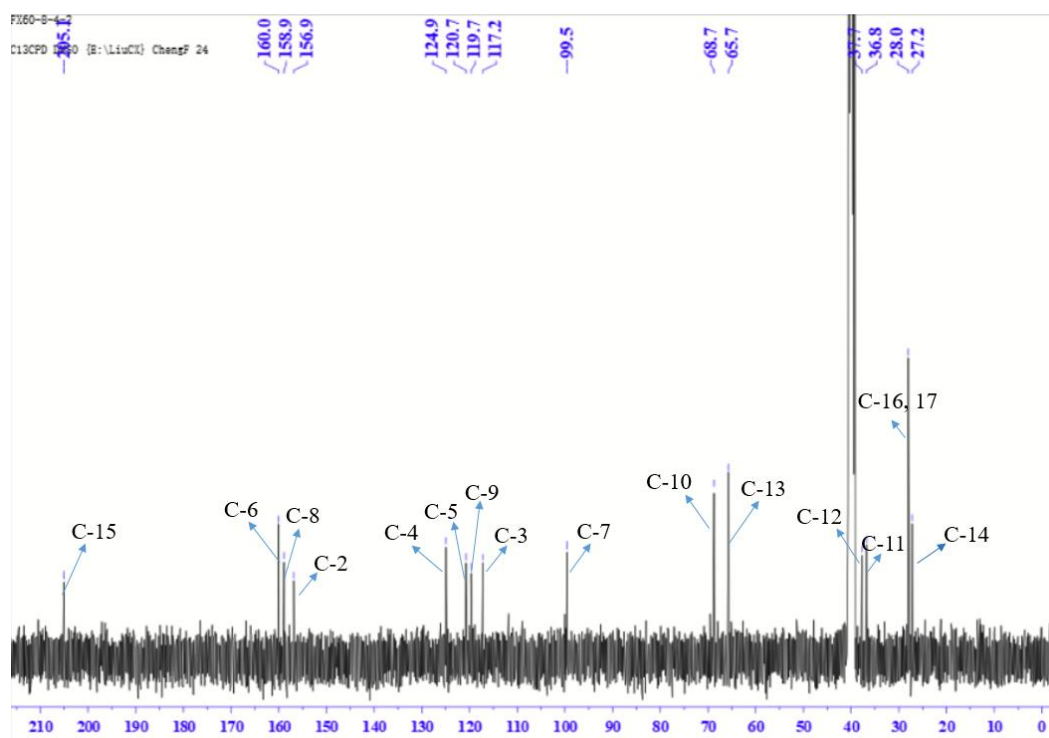


Figure S2: ^{13}C NMR spectrum of compound **1**

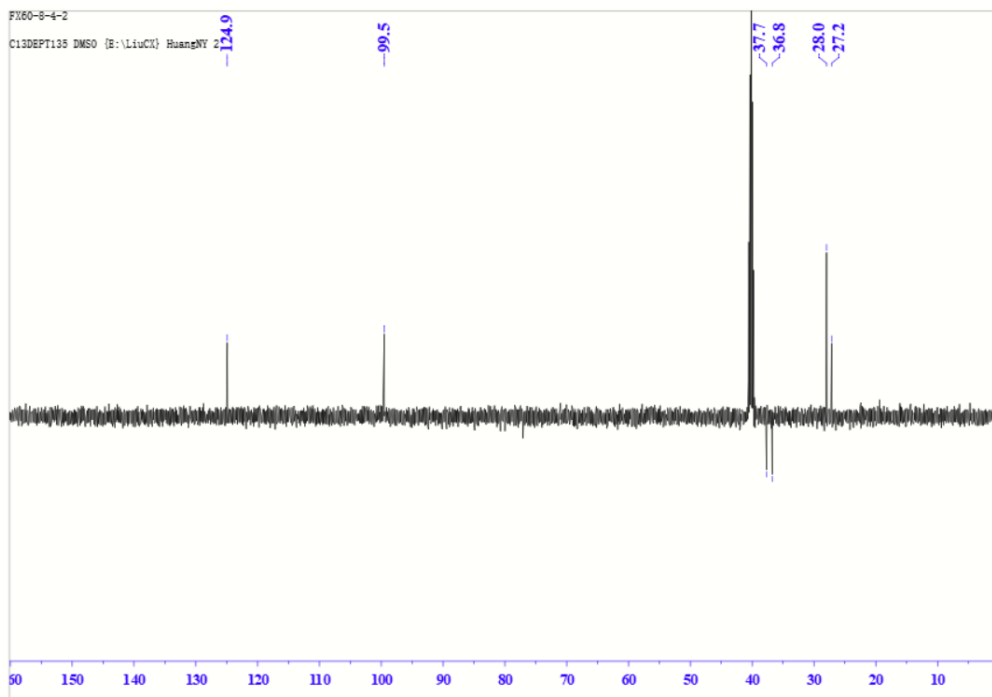


Figure S3: DEPT135 spectrum of compound **1**

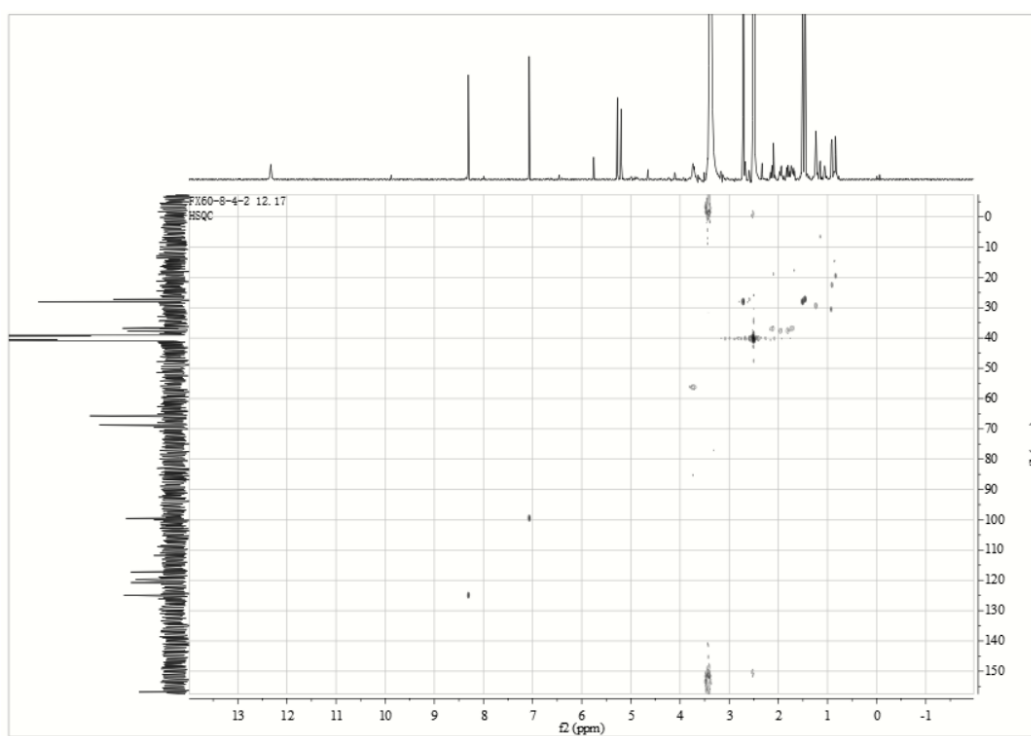


Figure S4: HSQC spectrum of compound **1**

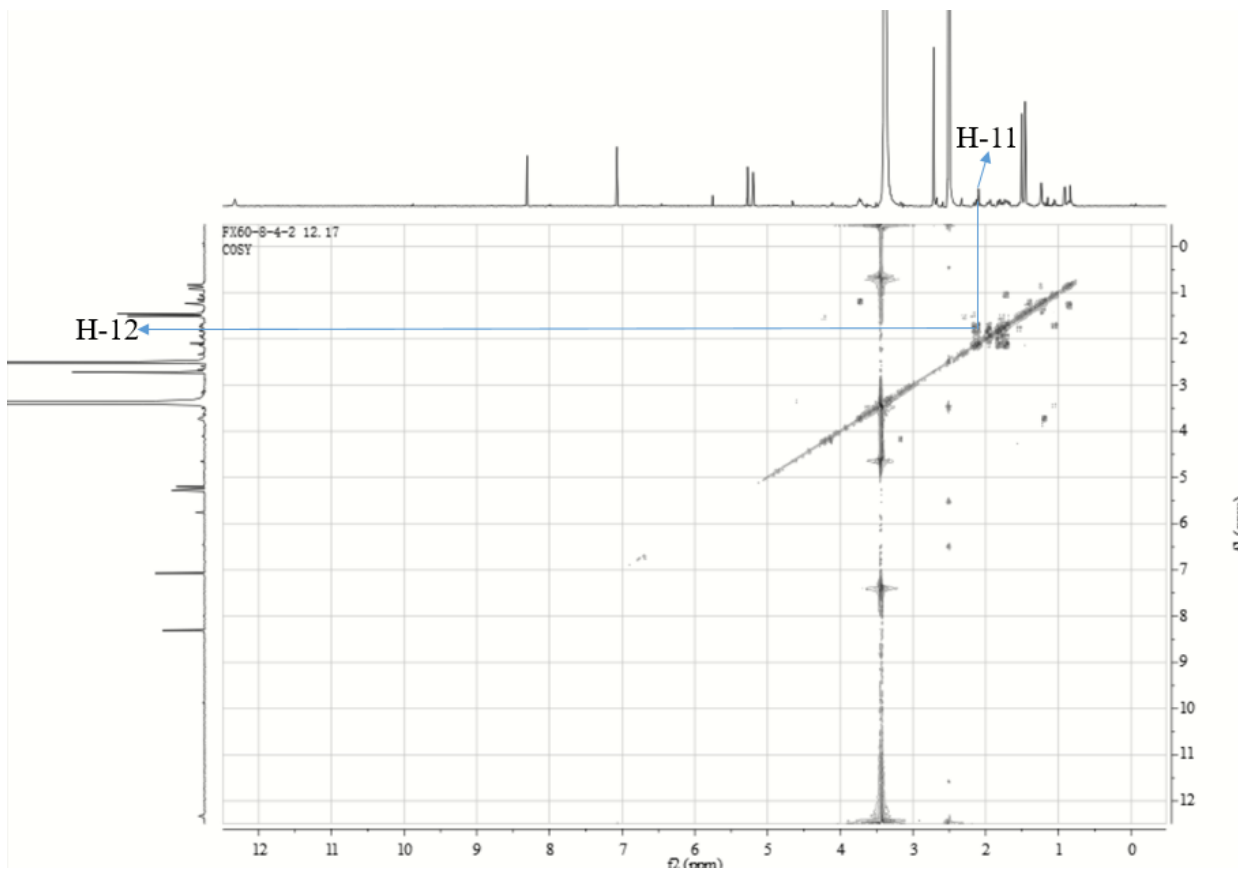


Figure S5: ^1H - ^1H COSY spectrum of compound **1**

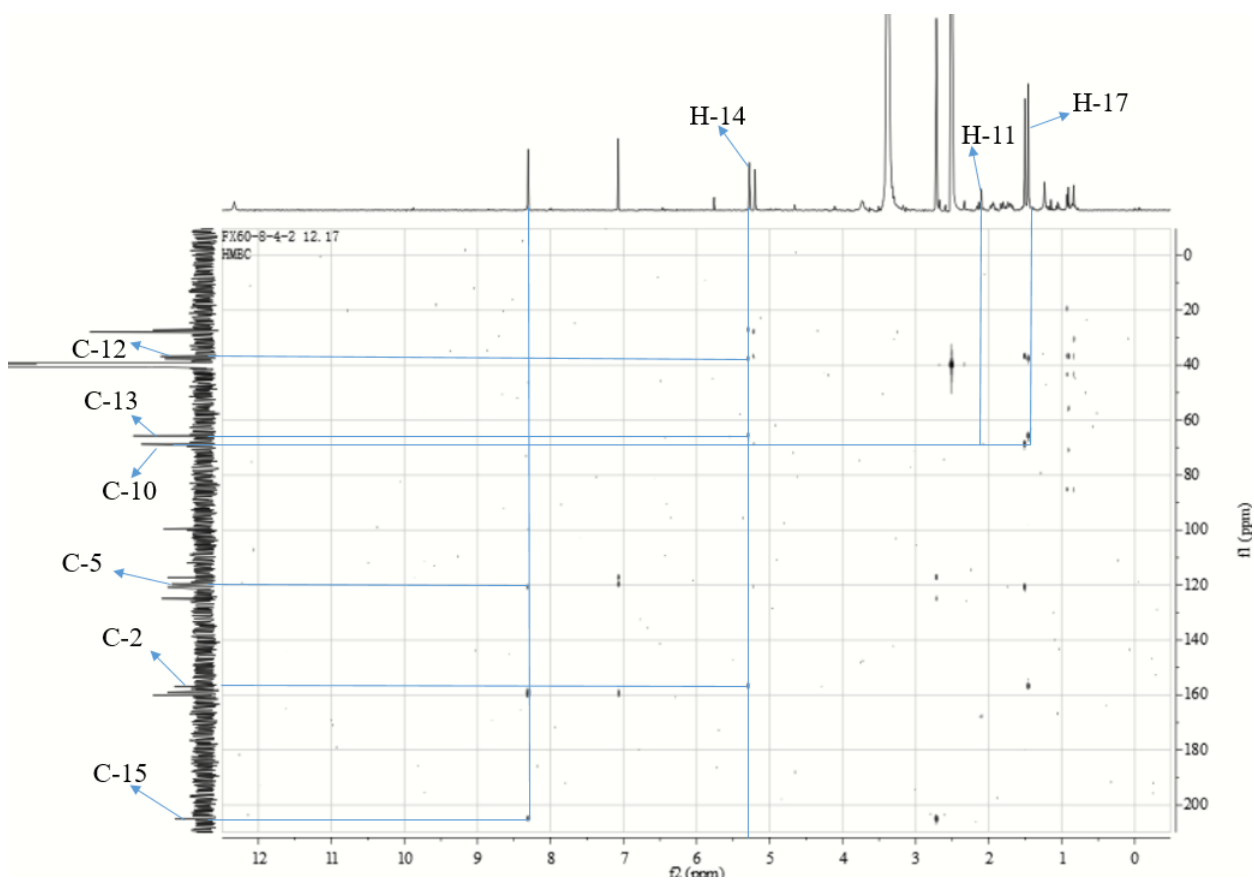


Figure S6: HMBC spectrum of **1** compound

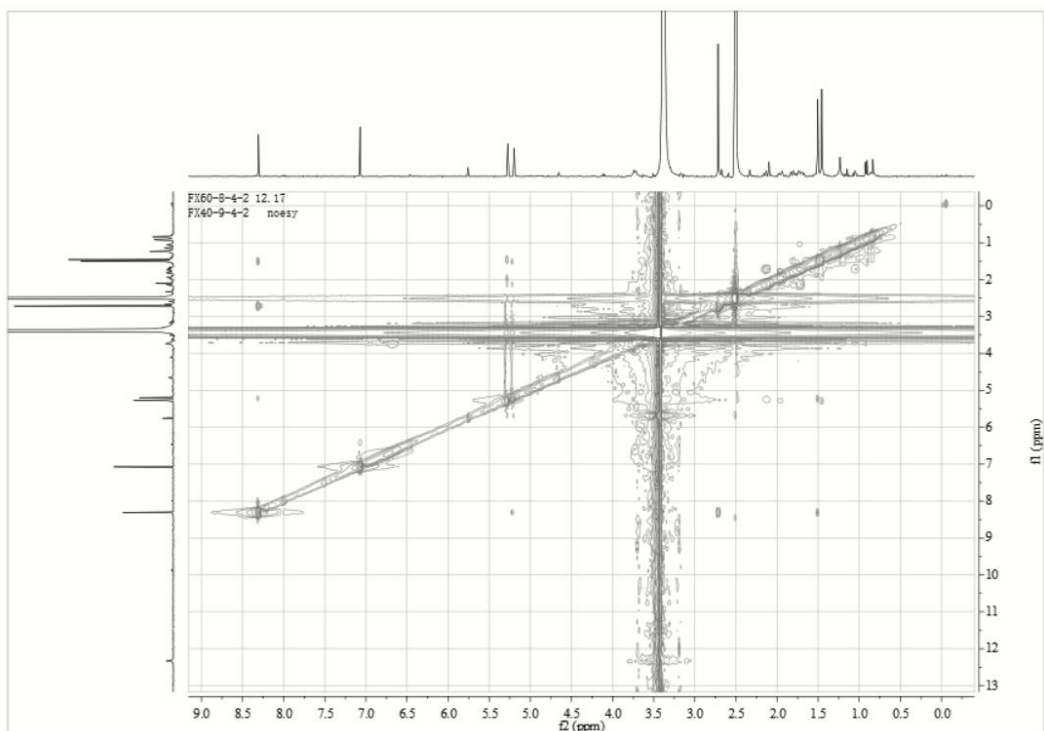


Figure S7: NOESY spectrum of compound 1

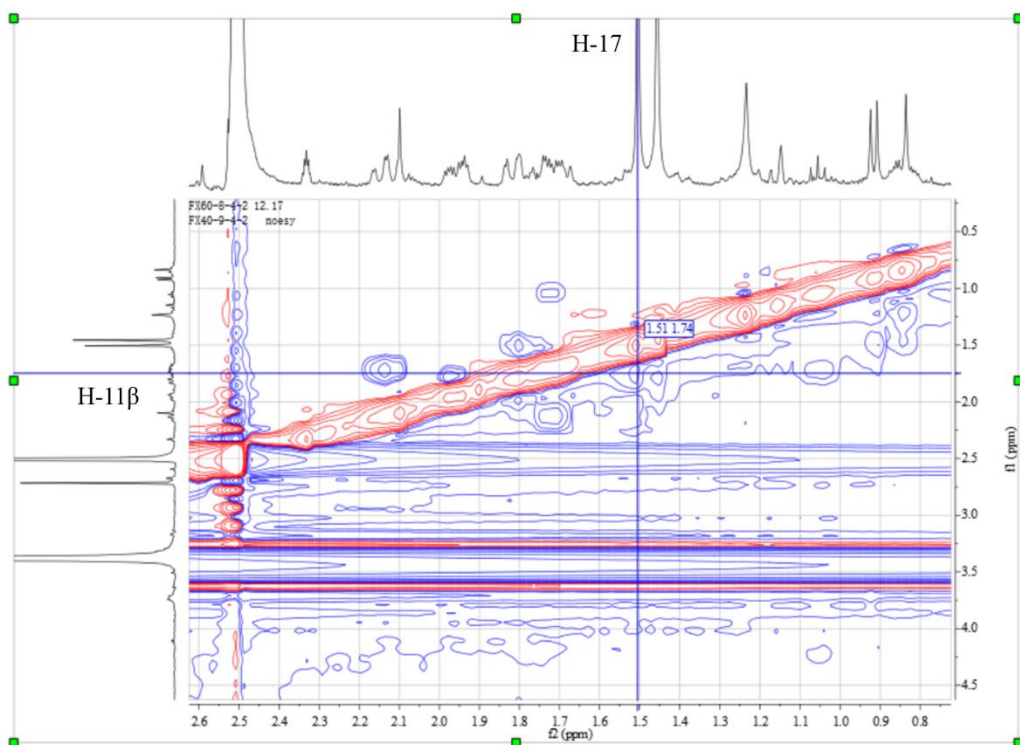


Figure S7-1: NOESY expanded spectrum of compound 1

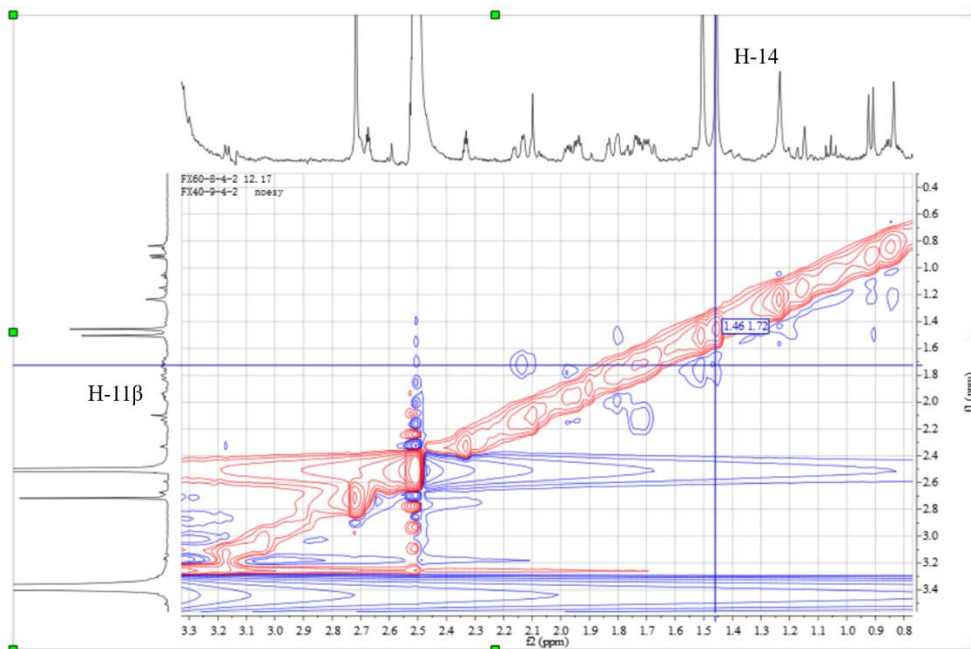


Figure S7-2: NOESY expanded spectrum of compound 1

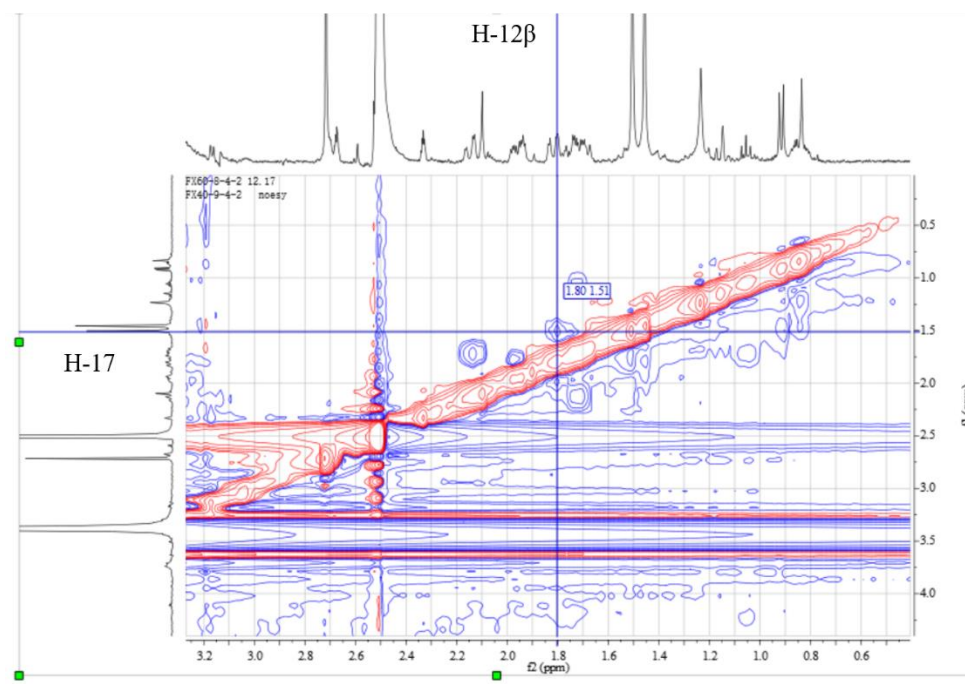


Figure S7-3: NOESY expanded spectrum of compound 1

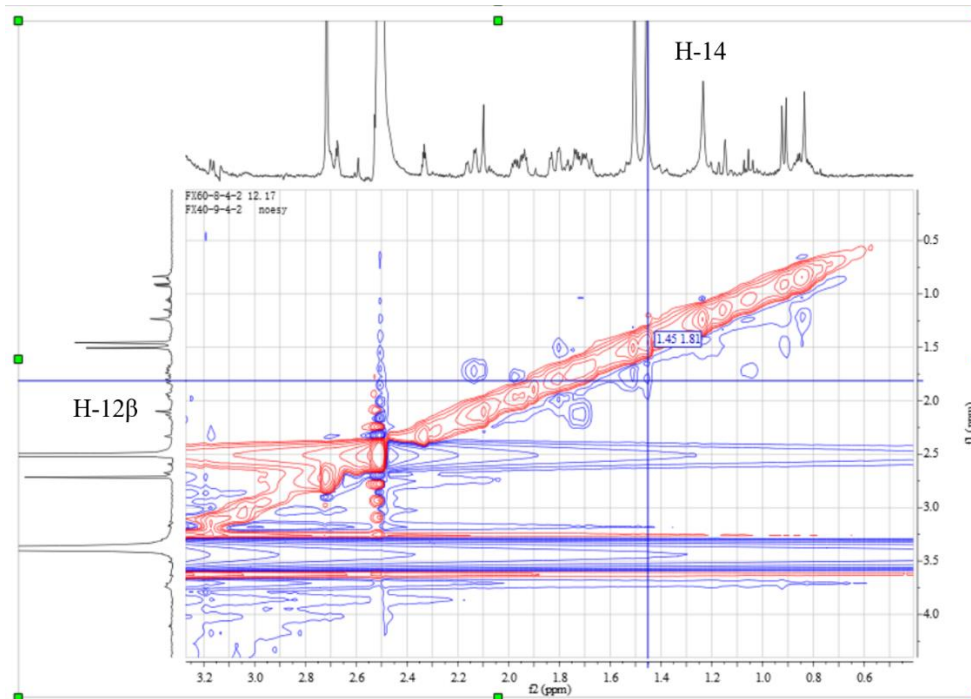


Figure S7-4: NOESY expanded spectrum of compound 1

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
 Element prediction: Off
 Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

809 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

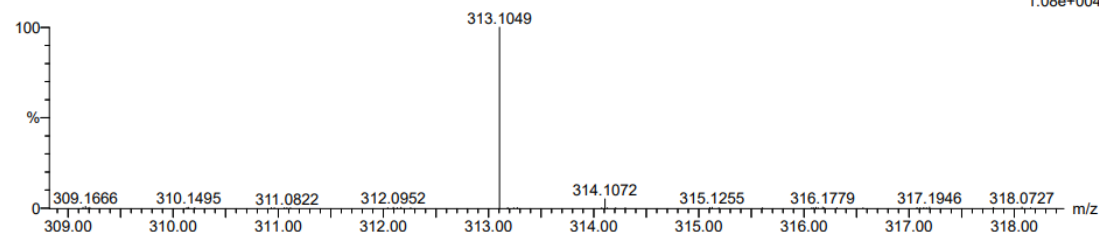
Elements Used:

C: 16-16 H: 18-18 N: 0-100 O: 0-100 Na: 0-4

11

240316-6-539-5-FX40-8-4-2 11 (0.076)

1: TOF MS ES+
1.08e+004



Minimum: -1.5
 Maximum: 5.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
313.1049	313.1052	-0.3	-1.0	7.5	83.5	n/a	n/a	C16 H18 O5 Na

Figure S8: HRESIMS spectrum of compound 1 (positive ion mode)

Structure Match

As Drawn (0)

Substructure (0)

Similarity (4,540)

Chemscape Analysis

Visually explore structure similarity with a powerful new tool. Learn more about Chemscape.

Create Chemscape Analysis

Filter Behavior

Filter by Exclude

Search Within Results

Similarity

85-89 (2)

75-79 (26)

70-74 (91)

65-69 (445)

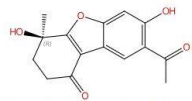
Filtering: Similarity: 85-89 X Number of Components: 1 X Clear All Filters

2 Results

Sort: Relevance View: Partial

1 88 ...

1441640-84-1



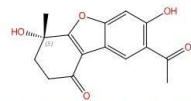
Absolute stereochemistry shown, Rotation (+)

$C_{15}H_{14}O_5$
(4*R*)-8-Acetyl-3,4-dihydro-4,7-dihydroxy-4-methyl-1(2*H*)-dibenzofuranone

2 References 0 Reactions 0 Suppliers

2 88 ...

1441640-83-0



Absolute stereochemistry shown, Rotation (-)

$C_{15}H_{14}O_5$
(4*S*)-8-Acetyl-3,4-dihydro-4,7-dihydroxy-4-methyl-1(2*H*)-dibenzofuranone

1 Reference 0 Reactions 0 Suppliers

Figure S9: Scifinder similarity report for compound 1

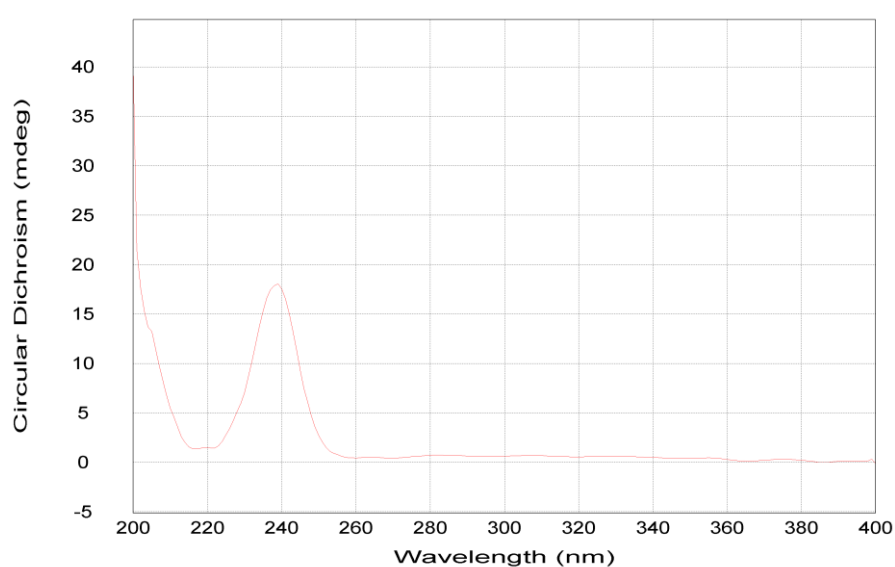


Figure S10: Experimental ECD spectrum of compound 1

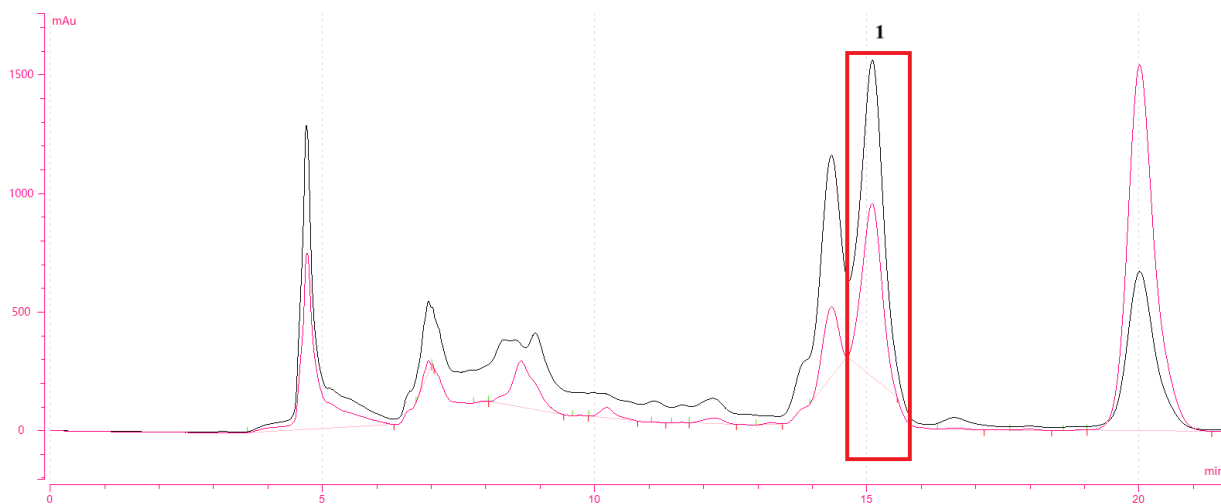


Figure S11: HPLC preparation spectrum of compound 1

(5.9 mg, ACN:H₂O=60:40, v/v, 2 mL/min, 15 min)

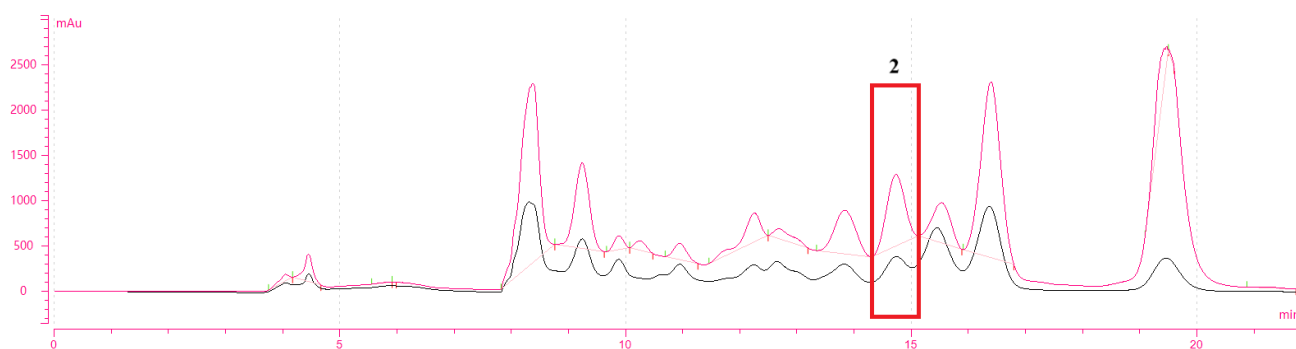


Figure S12: HPLC preparation spectrum of compound 2

(8.9 mg, ACN:H₂O=37:63, v/v, 2 mL/min, 14 min).

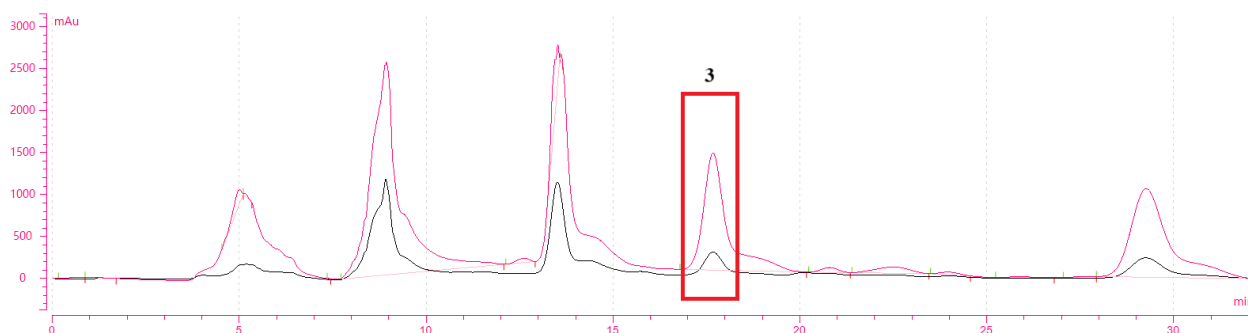


Figure S13: HPLC preparation spectrum of compound 3

(22.8 mg, ACN:H₂O=45:55, v/v, 2 mL/min, 18 min)

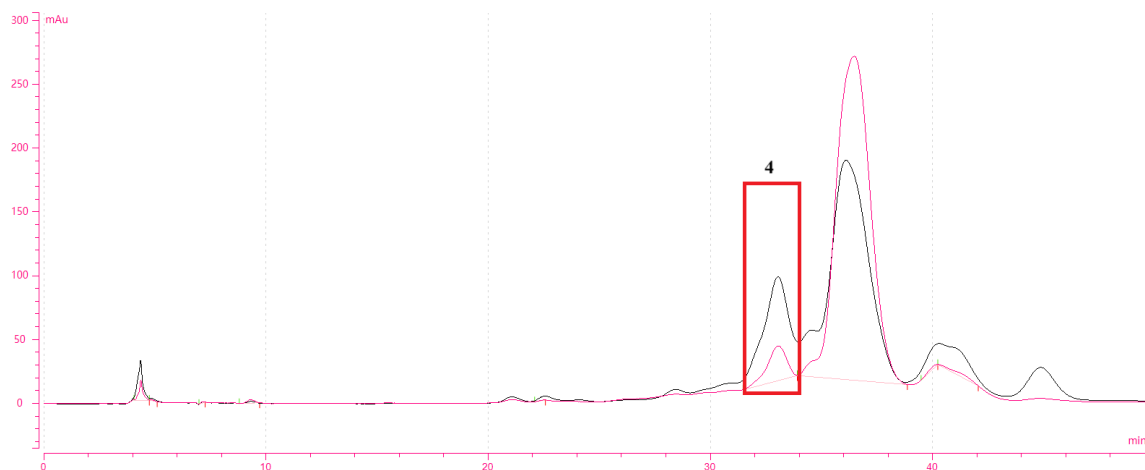


Figure S14: HPLC preparation spectrum of compound **4**

(21.8 mg, ACN:H₂O=47:53, v/v, 2 mL/min, 33 min)

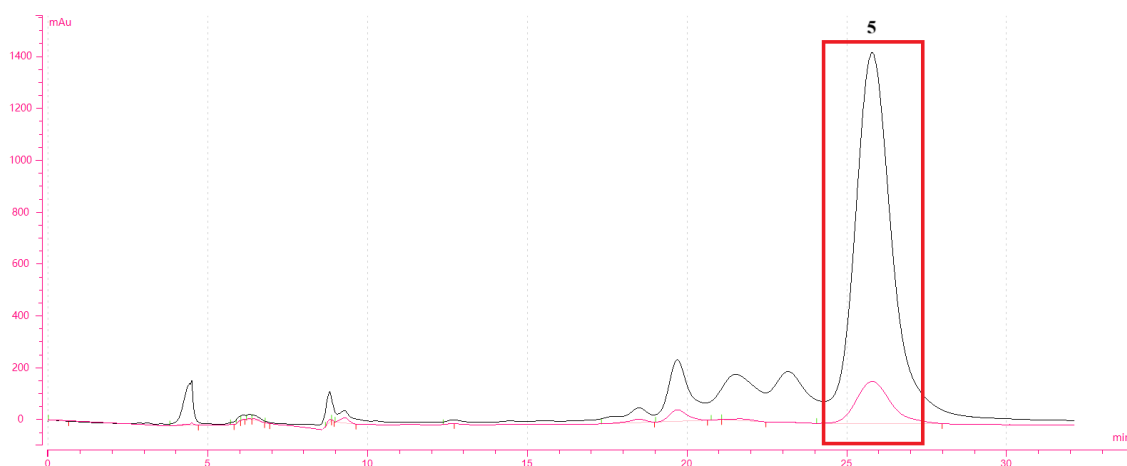


Figure S15: HPLC preparation spectrum of compound **5**

(8.8 mg, ACN:H₂O=35:65, v/v, 2 mL/min, 25 min)

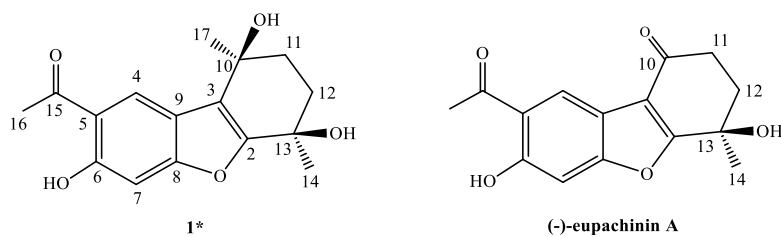


Table S1: ^1H (400 MHz) and ^{13}C NMR (100 MHz) data of compound **1** and the analogue (-)- eupachinin A in DMSO- d_6 . (δ in ppm)

Position	compound 1		(-)- eupachinin A	
	δ_{C}	$\delta_{\text{H}}J$ (Hz)	δ_{C}	$\delta_{\text{H}}J$ (Hz)
2	156.86	-	171.0	-
3	117.22	-	115.8	-
4	124.92	8.31 (s)	125.2	8.43 (s)
5	120.73	-	118.2	-
6	160.04	-	162.0	-
7	99.52	7.07 (s)	100.4	7.05 (s)
8	158.92	-	159.0	-
9	119.66	-	115.1	-
10	68.74	-	194.1	-
11	36.77	2.13 (m), 1.73 (m)	35.7	2.36 (m)
12	37.71	1.95 (ddd, 13.8, 5.8, 3.0), 1.81 (m)	38.2	2.63 (ddd, 17.0, 6.6, 5.0), 2.92 (ddd, 17.0, 9.0, 5.0)
13	65.69	-	67.4	-
14	27.18	1.45 (s)	25.8	1.78 (s)
15	205.05	-	204.6	-
16	27.99	2.72 (s)	27.2	2.74 (s)
17	27.99	1.50 (s)	-	-
6-OH	-	12.33 (s)	-	-
10-OH	-	5.20 (s)	-	-
13-OH	-	5.28 (s)	-	-