

Supporting Information

Rec. Nat. Prod. X:X (202X) XX-XX

Eupbenzofuranside C: A New Benzofuranside with Dual Inhibitory Activities against α -Glucosidase and PTP1B from *Eupatorium chinense* L.

Ting Yan ¹, Ye Deng ,

Yanjie Zeng, Ruixue Jing and Han Shen

Hubei Key Laboratory of Natural Products Research and Development, Key Laboratory of Functional Yeast (China National Light Industry), College of Biological and Pharmaceutical Sciences, China Three Gorges University, Yichang, P. R. China.

Table of Contents	Page
Figure S1: ¹ H NMR spectrum of compound 1	2
Figure S2: ¹ H NMR spectrum of compound 1 (1-4 ppm)	2
Figure S3: ¹ H NMR spectrum of compound 1 (4-8 ppm)	3
Figure S4: ¹³ C NMR spectrum of compound 1	3
Figure S5: DEPT135 spectrum of compound 1	4
Figure S6: HSQC spectrum of compound 1	4
Figure S7: HSQC spectrum of compound 1	5
Figure S8: HSQC spectrum of compound 1	5
Figure S9: ¹ H- ¹ H COSY spectrum of compound 1	6
Figure S10: HMBC spectrum of compound 1	6
Figure S11: HMBC spectrum of compound 1	7
Figure S12: HMBC spectrum of compound 1	7
Figure S13: NOESY spectrum of compound 1	8
Figure S14: Experimental ECD spectrum and the calculated ECD spectrum of 1 in MeOH.	8
Figure S15: HPLC preparation spectrum of compound 1	9
Figure S16: HPLC preparation spectrum of compound 2	9
Figure S17: HPLC preparation spectrum of compound 3	10
Figure S18: HPLC preparation spectrum of compound 4	10
Figure S19: Graphical abstract	11
Figure S20: Scifinder similarity report for compound 1	11
Figure S21: HRESIMS spectrum of compound 1	12
Figure S22: Certificate of language editing	12
Table S1: ¹ H-NMR and ¹³ C-NMR data of compound 1 and the 5-[1'-hydroxyethyl]-2-1'-hydroxyisopropyl]-benzofuran in DMSO- <i>d</i> ₆ . (δ in ppm)	13

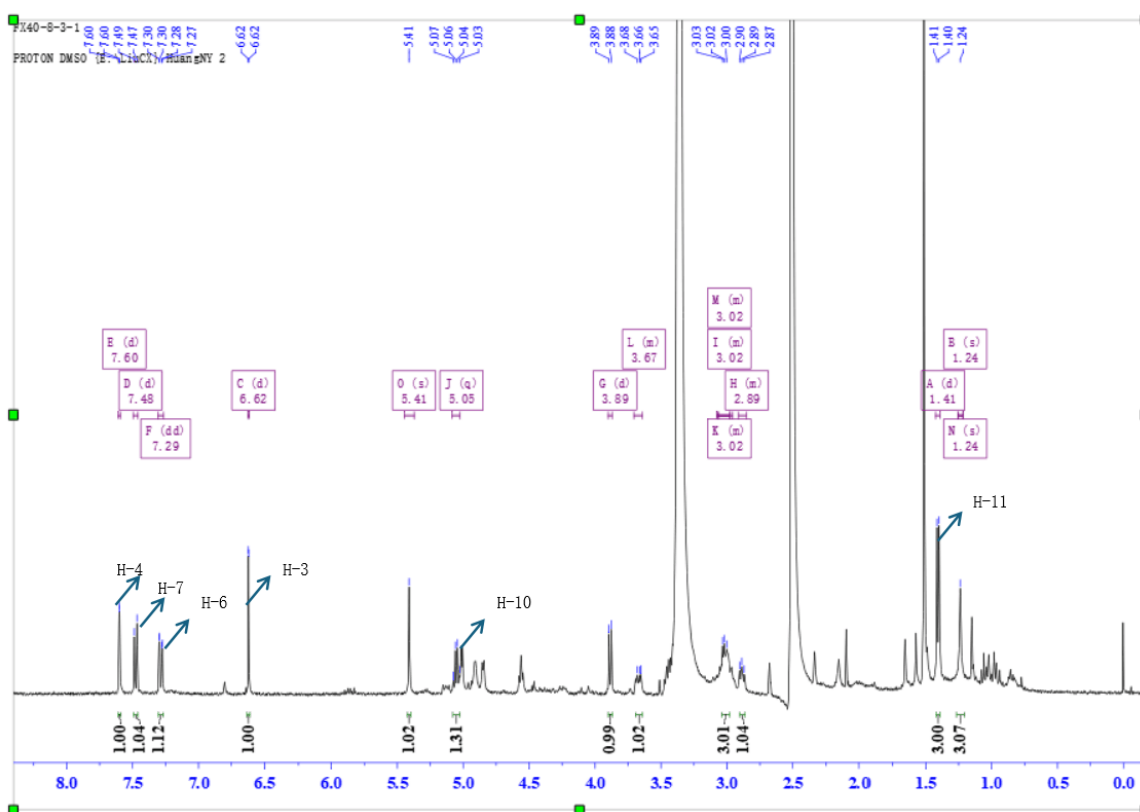


Figure S1: ^1H NMR spectrum of compound 1

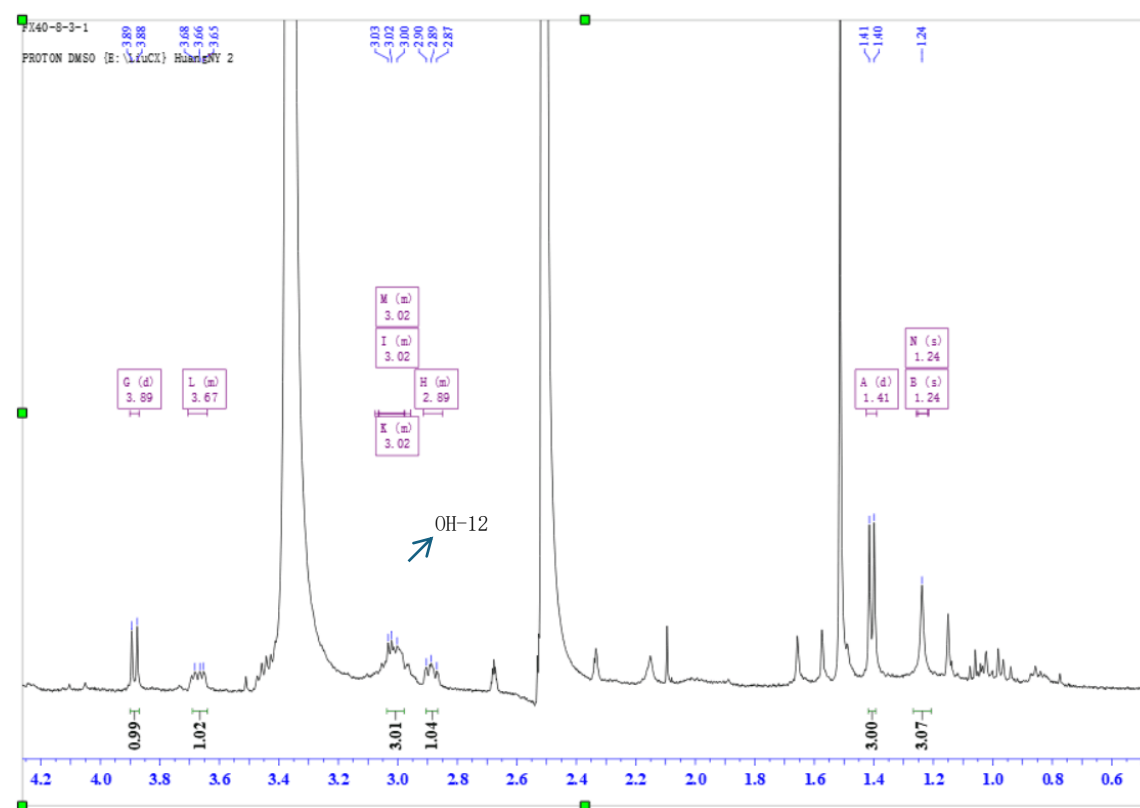


Figure S2: ^1H NMR spectrum of compound 1 (1-4 ppm)

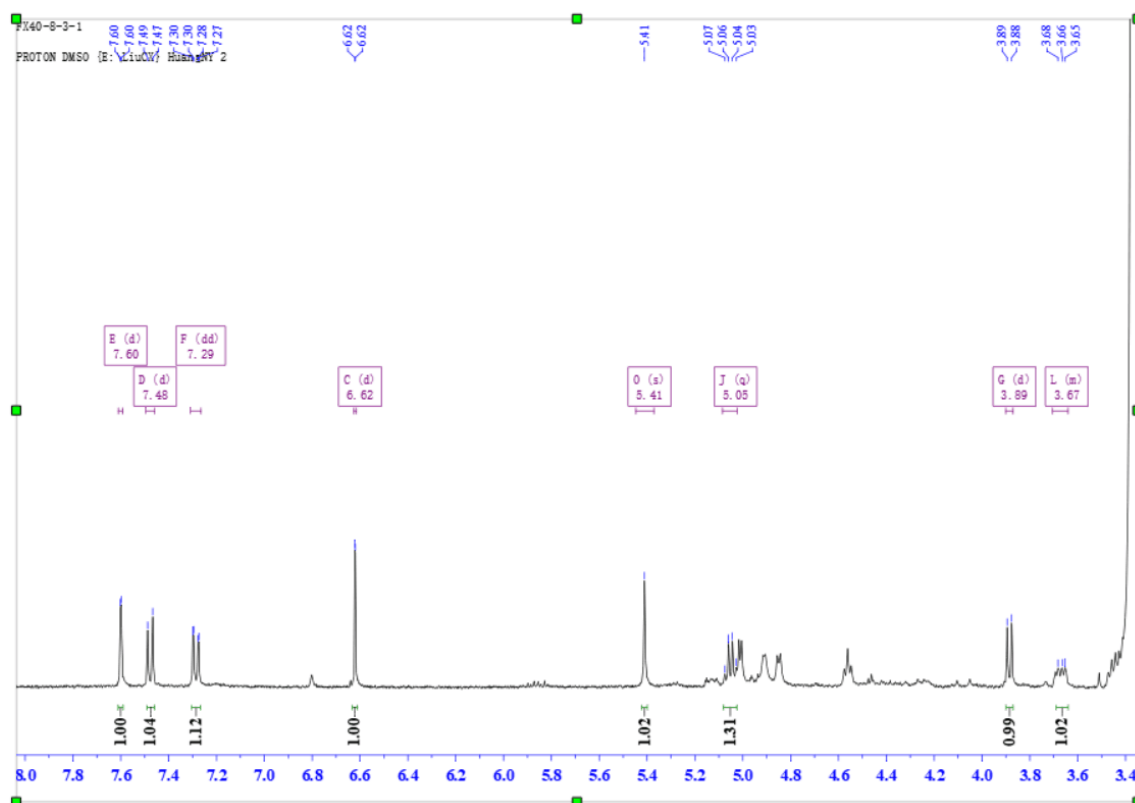


Figure S3: ^1H NMR spectrum of compound 1 (4-8 ppm)

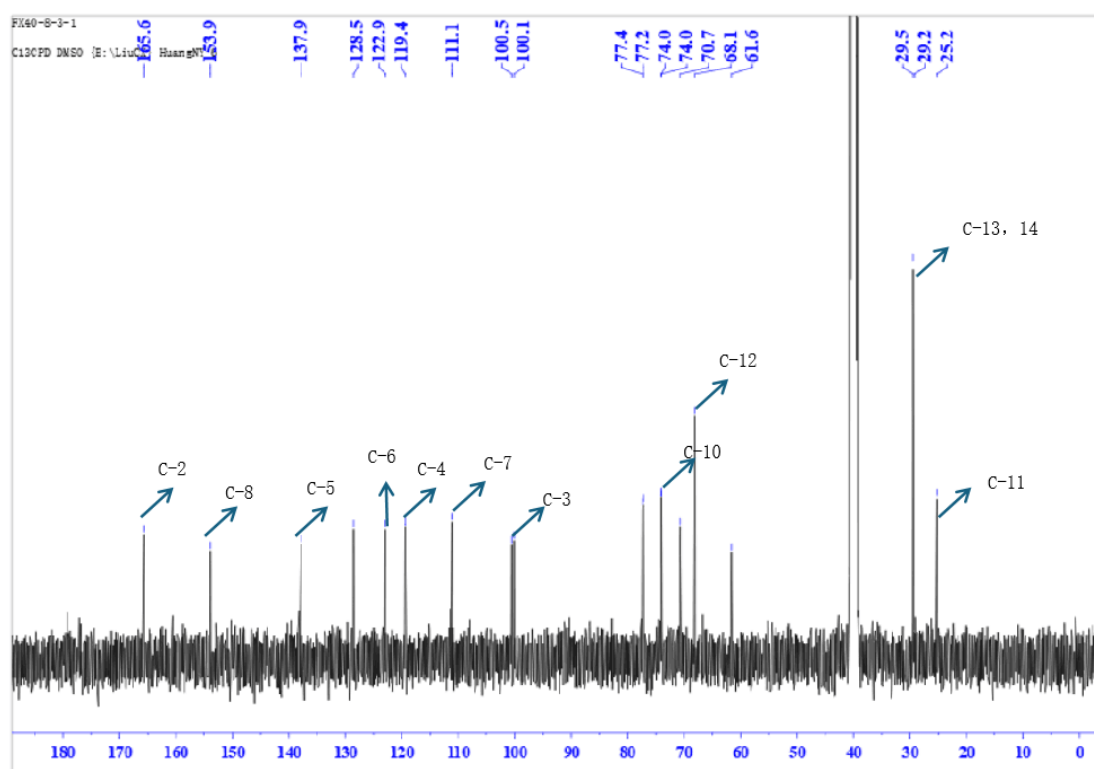


Figure S4: ^{13}C NMR spectrum of compound 1

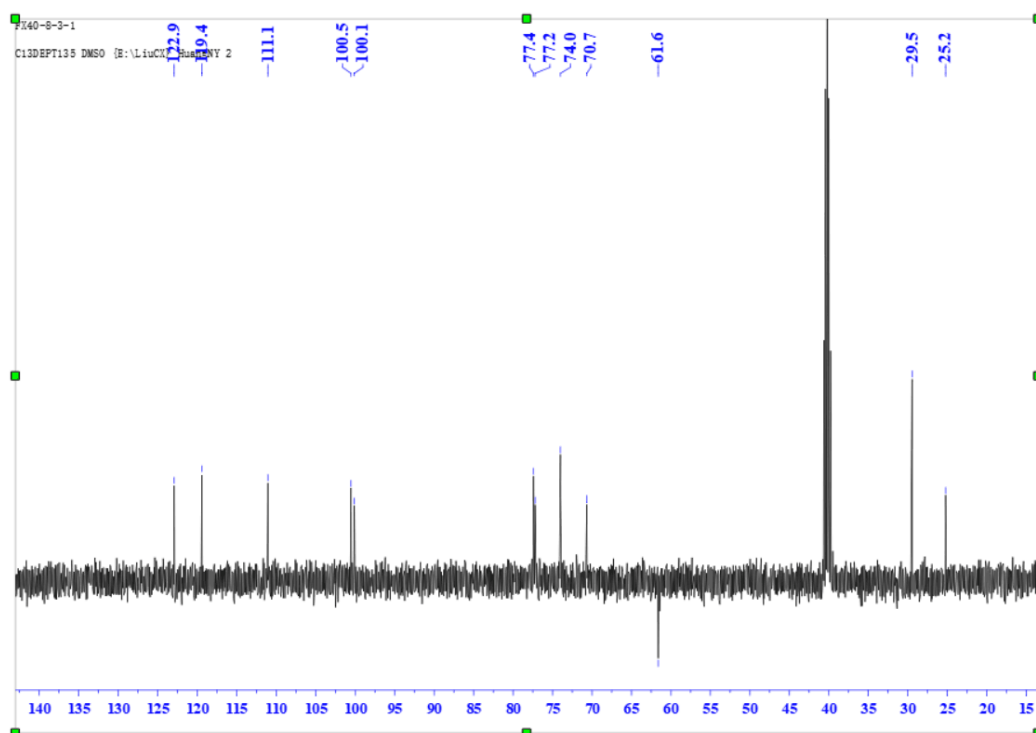


Figure S5: DEPT135 spectrum of compound 1

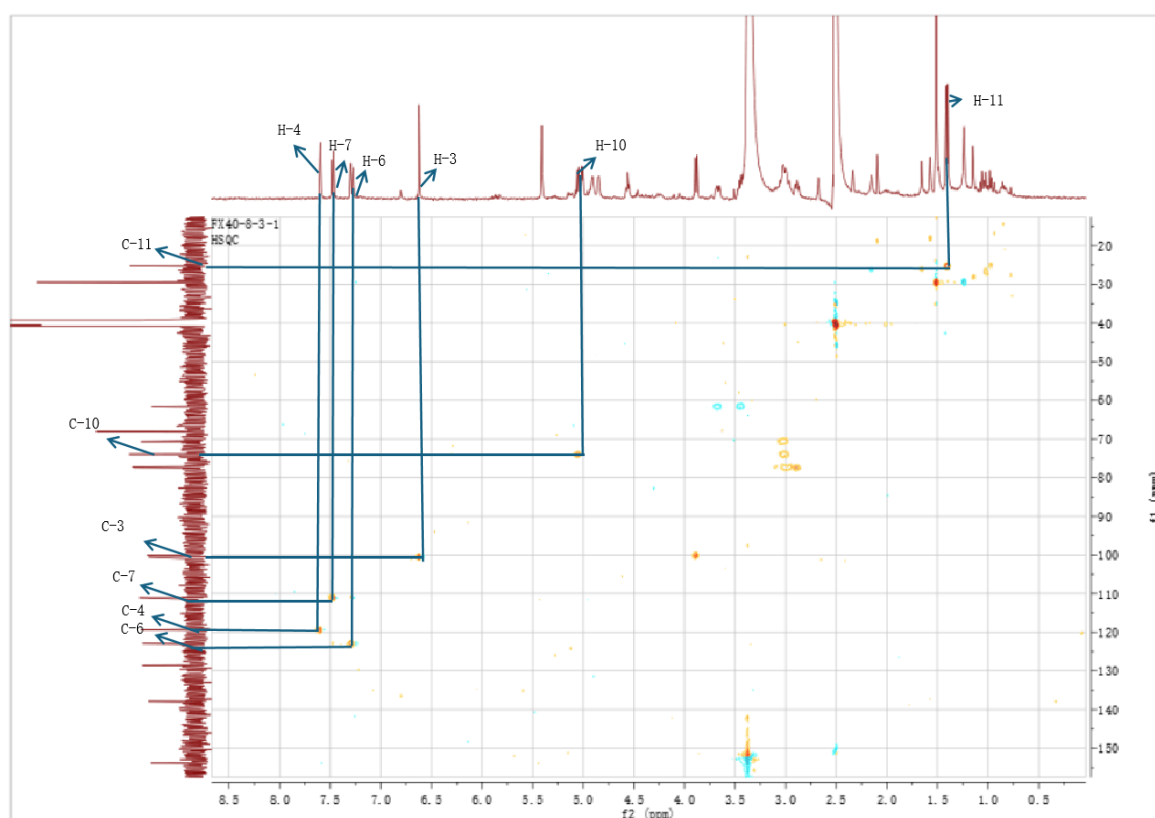


Figure S6: HSQC spectrum of compound 1

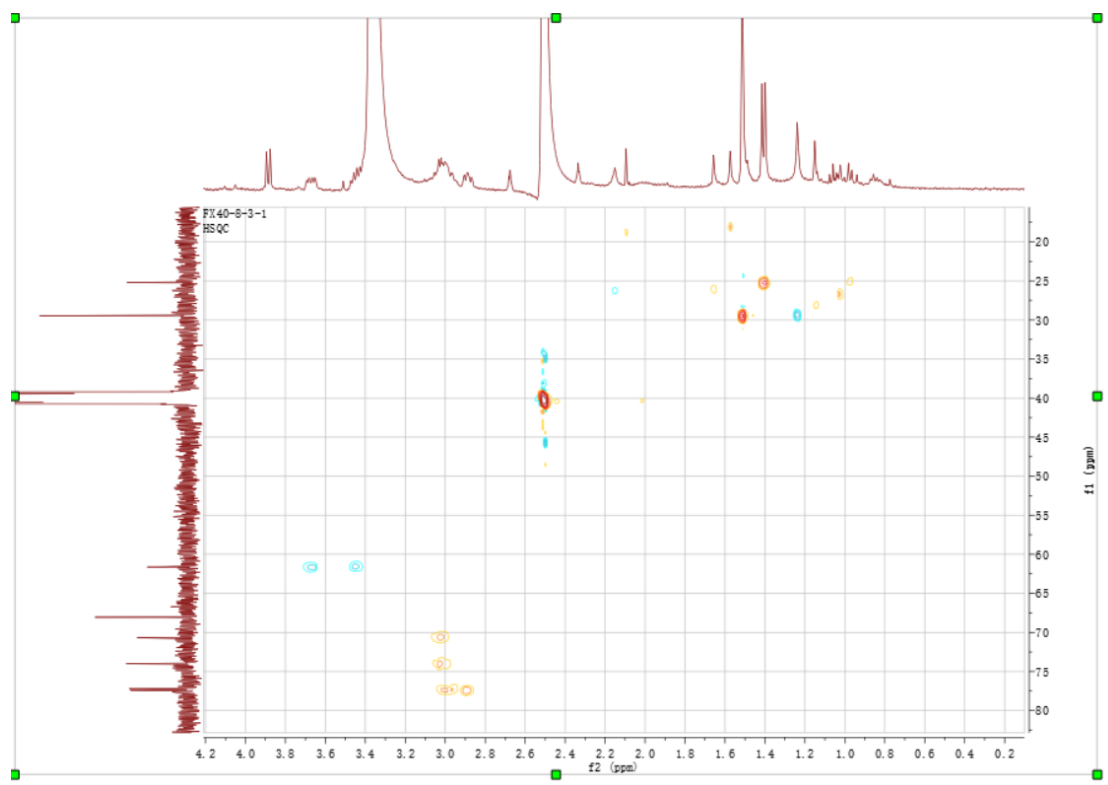


Figure S7:HSQC spectrum of compound **1**

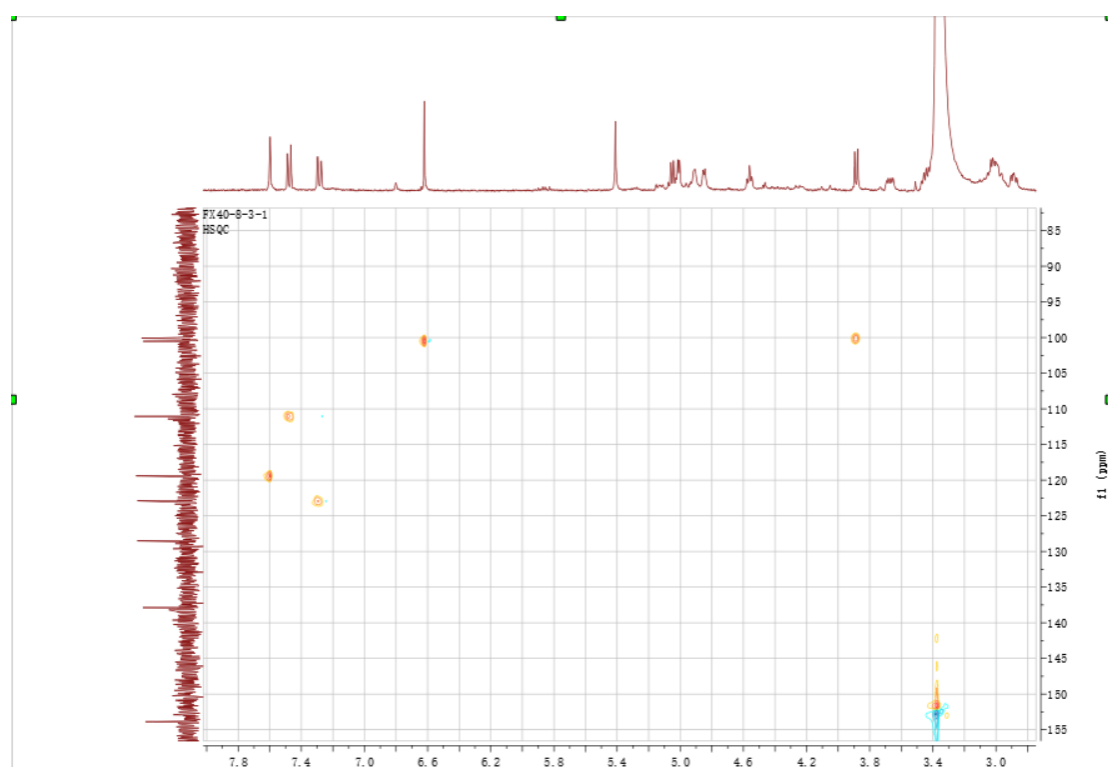


Figure S8: HSQC spectrum of compound **1**

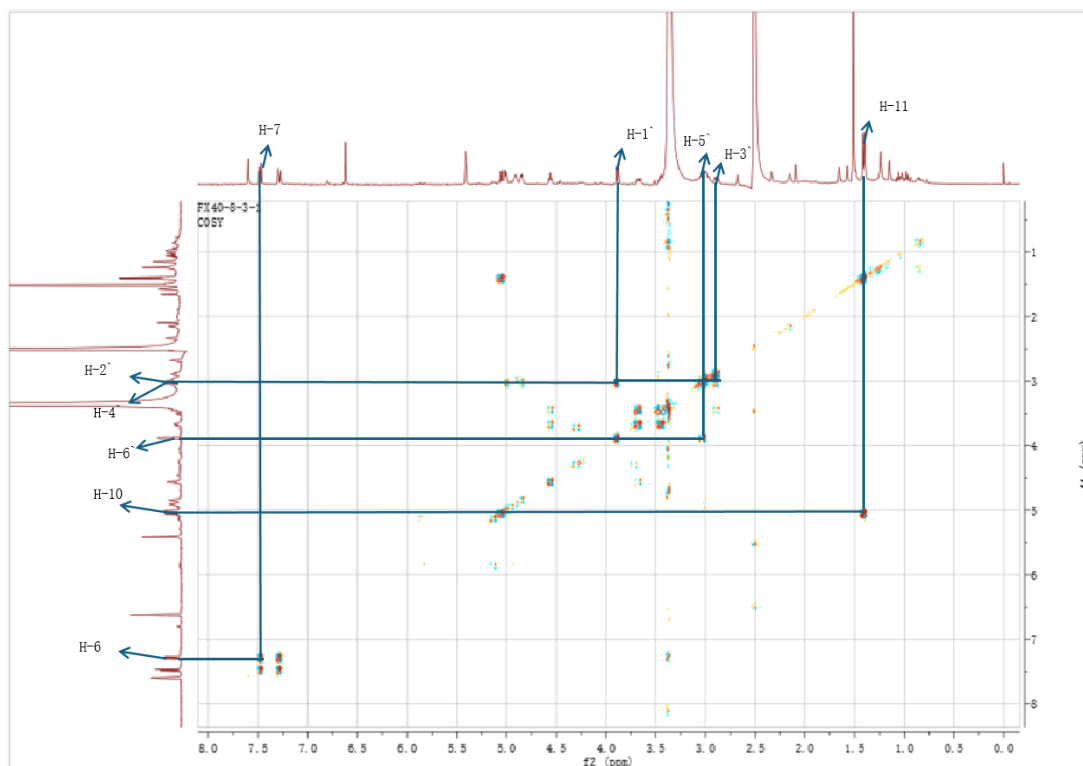


Figure S9: ^1H - ^1H COSY spectrum of compound **1**

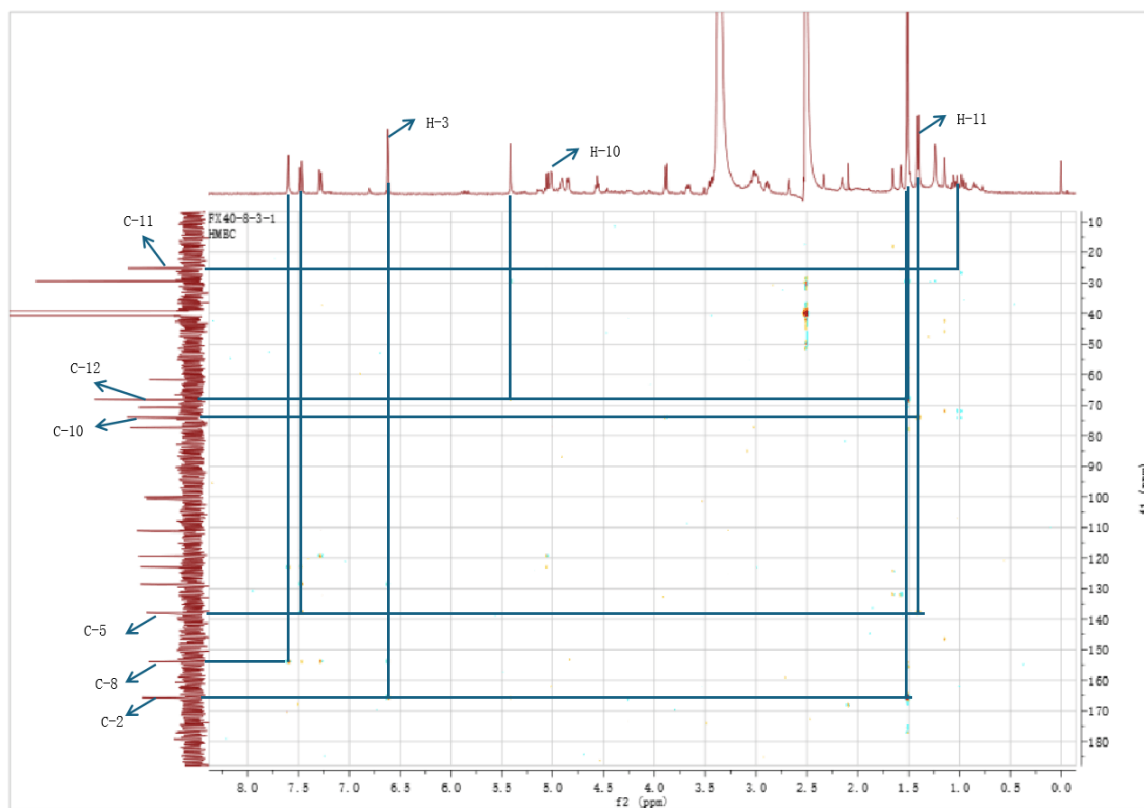


Figure S10: HMBC spectrum of compound **1**

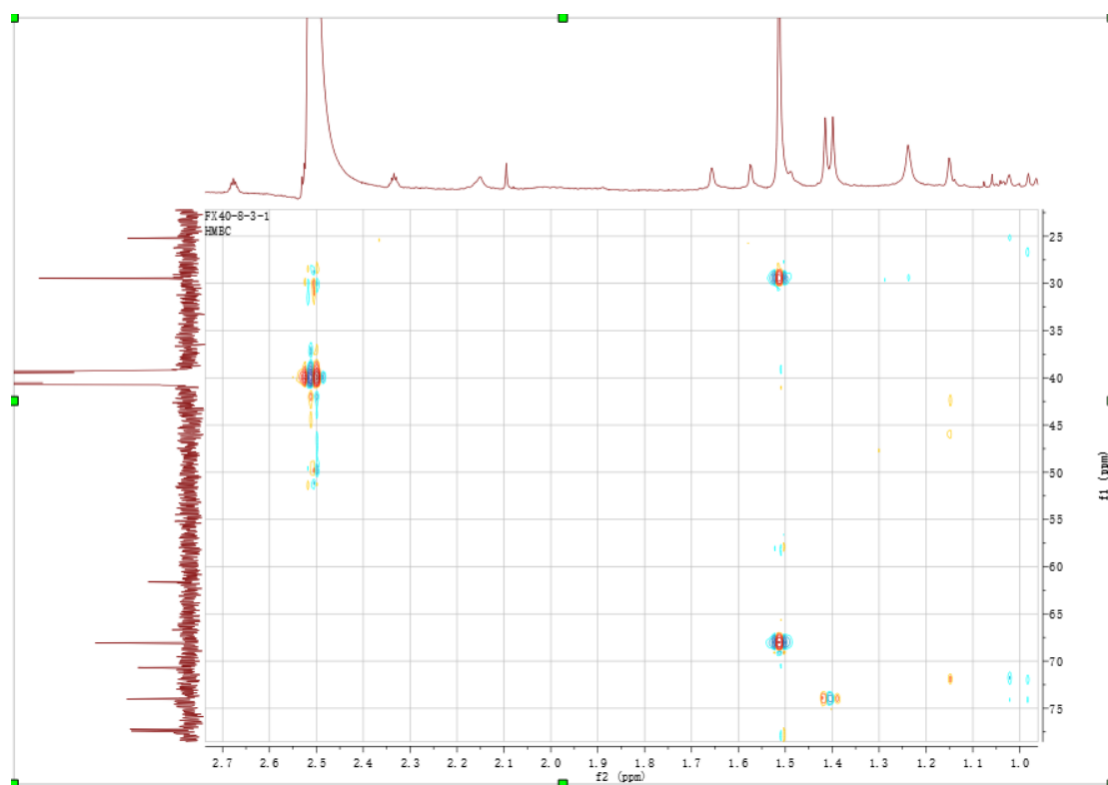


Figure S11: HMBC spectrum of compound **1**

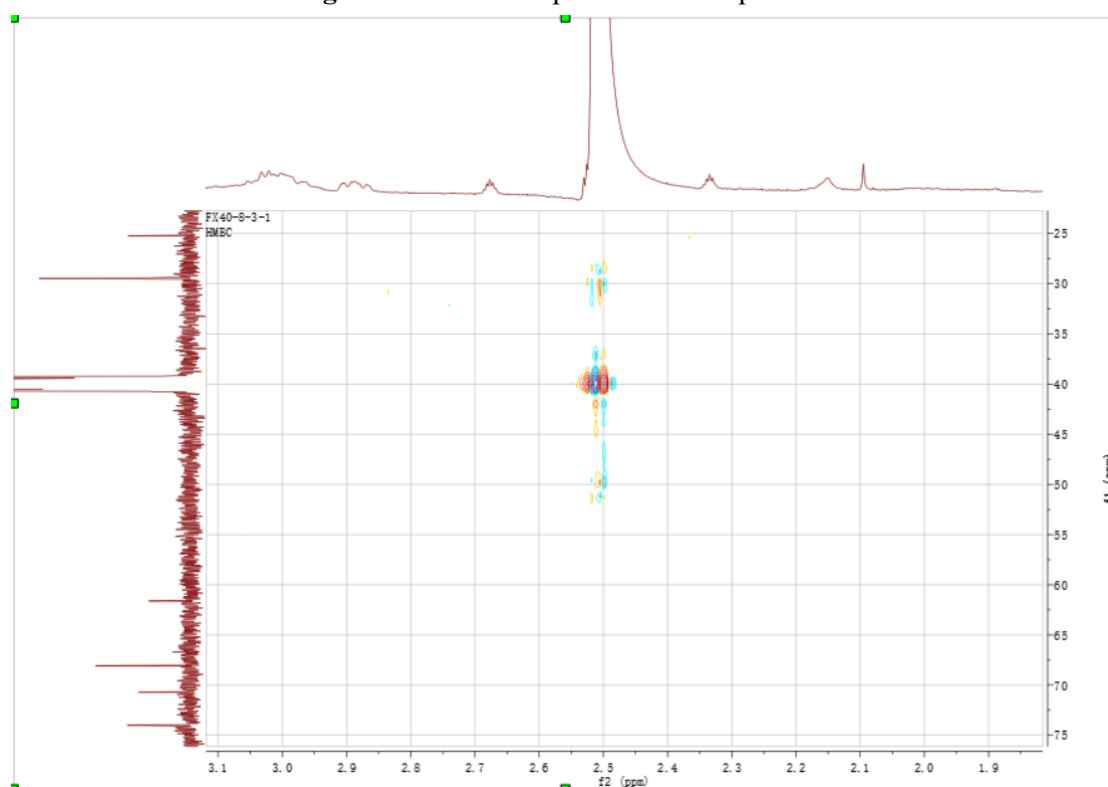


Figure S12: HMBC spectrum of compound **1**

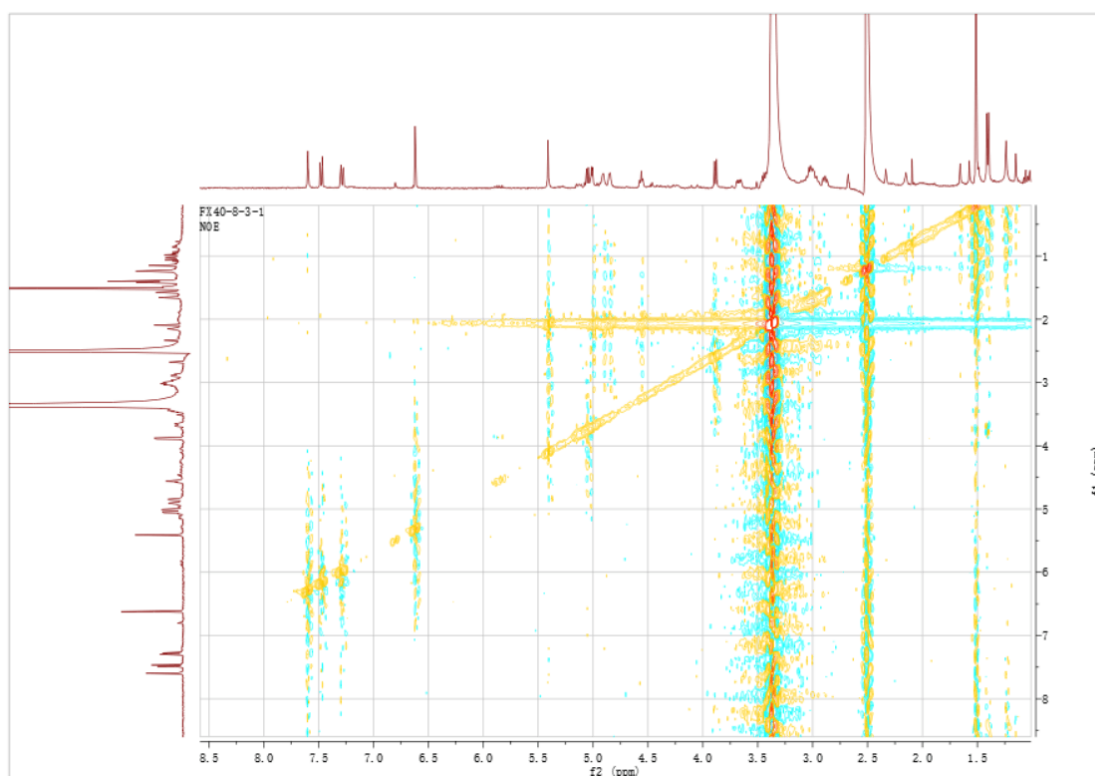


Figure S13: NOESY spectrum of compound **1**

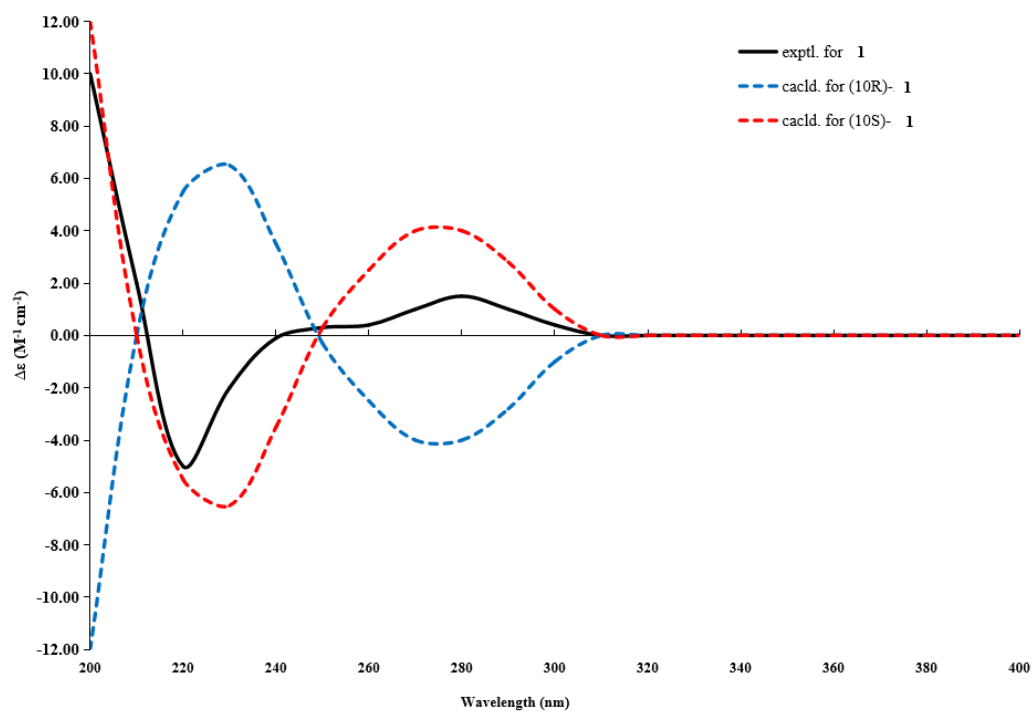


Figure S14: Experimental ECD spectrum of compound **1**

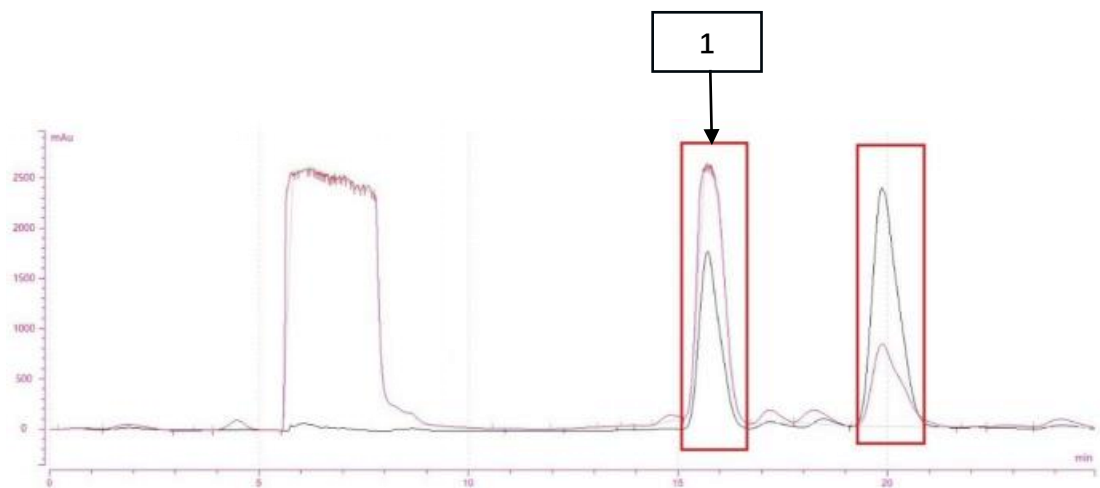


Figure S15. HPLC preparation spectrum of compound **1**
(28.9 mg, ACN: H₂O=30:70, v/v, 2 mL/min, 16 min)

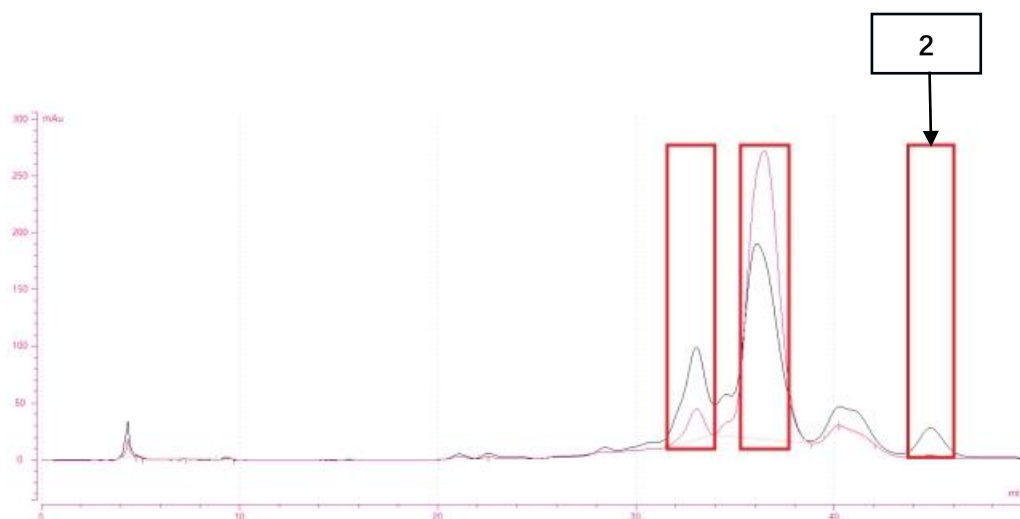


Figure S16: HPLC preparation spectrum of compound **2**
(16.8 mg, ACN: H₂O=47:53, v/v, 2 mL/min, 45 min)

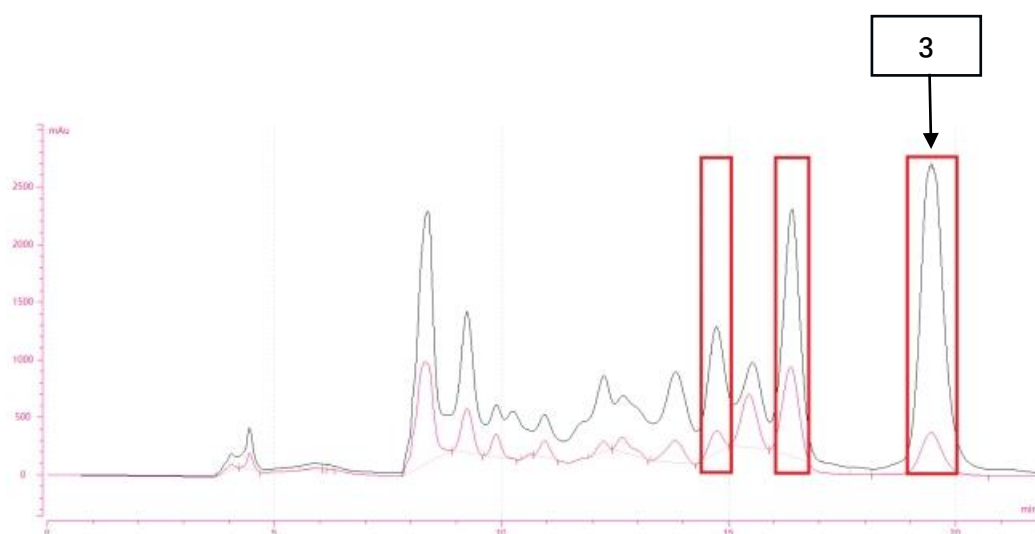


Figure S17: HPLC preparation spectrum of compound **3**
(4.3 mg, ACN: H₂O=37:63, v/v, 2 mL/min, 19 min)

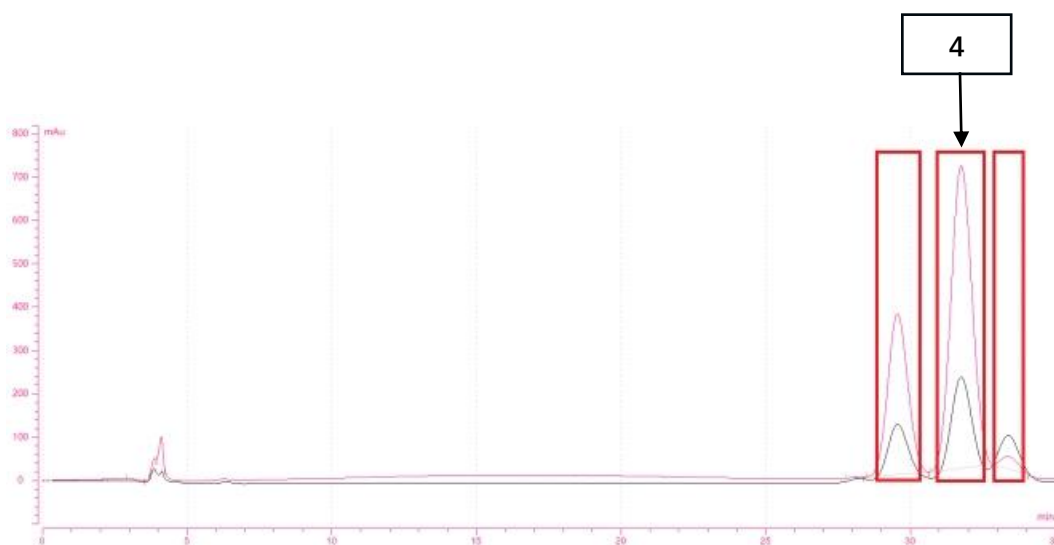
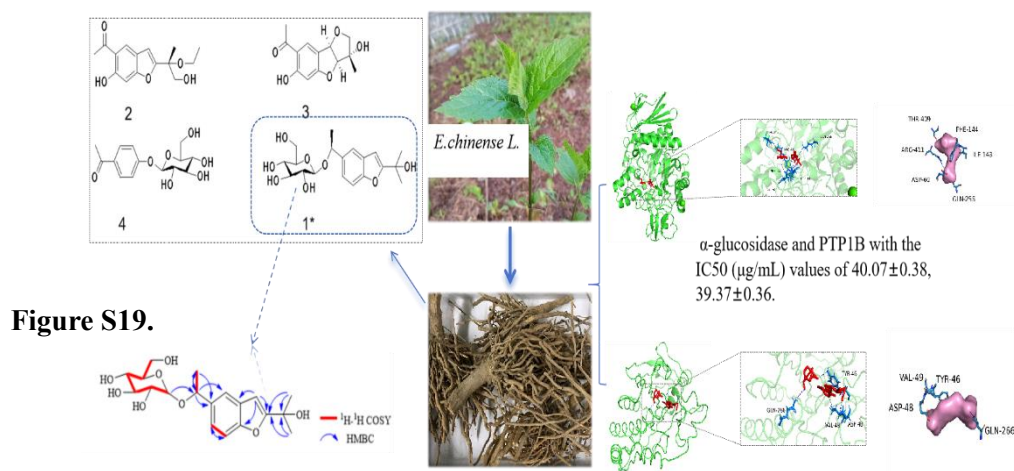


Figure S18: HPLC preparation spectrum of compound **4**
(4.8 mg, ACN: H₂O=25:75, v/v, 2 mL/min, 32 min)



Graphical abstract

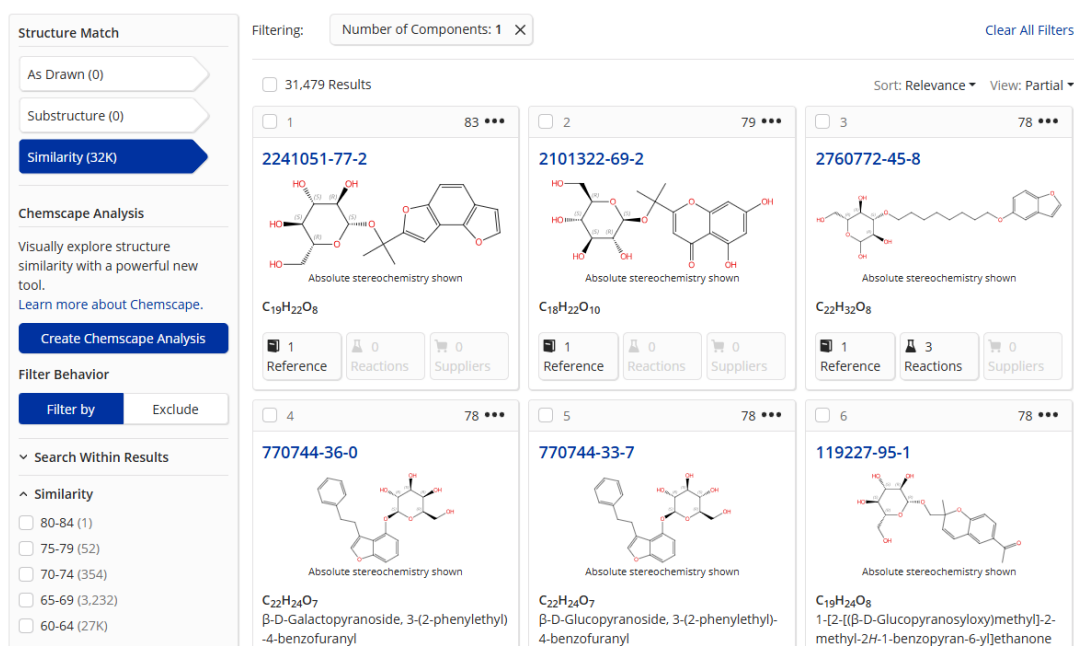


Figure S20: Scifinder similarity report for compound 1

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 = 5

Monoisotopic Mass, Even Electron Ions

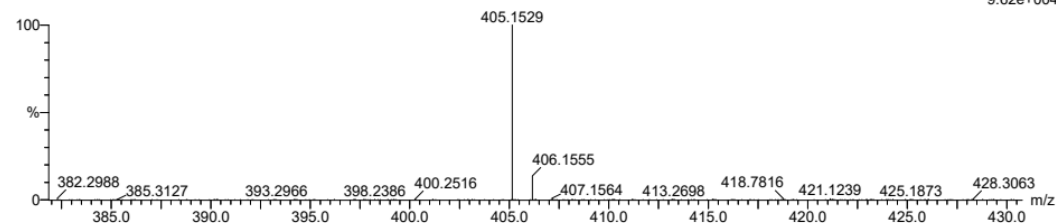
1890 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 19-19 H: 26-26 N: 0-100 O: 0-100 Na: 0-7

11

240316-6-539-5-FX40-8-3-1 14 (0.087)

1: TOF MS ES+
9.62e+004

Minimum: -1.5
Maximum: 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
405.1529	405.1525	0.4	1.0	6.5	197.8	n/a	n/a	C ₁₉ H ₂₆ O ₈ Na

Figure S21: HRESIMS spectrum of compound 1



Figure S22: Certificate of language editing

Table S1: ^1H -NMR and ^{13}C -NMR data of compound **1** and the 5-[1'-hydroxyethyl]-2-1'-hydroxyisopropyl]-benzofuran in DMSO- d_6 . (δ in ppm)

Position	compound 1		5-[1'-hydroxyethyl]-2-1'-hydroxyisopropyl]-benzofuran	
	δ_{C}	$\delta_{\text{H}}J(\text{Hz})$	δ_{C}	$\delta_{\text{H}}J(\text{Hz})$
2	164.8	-	165.4	-
3	100.1	6.62 (d, 0.8)	100.6	6.56 (d, 1)
4	119.4	7.60 (d, 1.5)	117.8	7.54 (d, 2)
5	137.9	-	128.4	-
6	122.9	7.29 (dd, 8.6, 1.5)	121.8	7.29 (dd, 8.5, 2)
7	111.0	7.48 (d, 8.6)	110.7	7.42 (d, 8.5)
8	154.9	-	153.4	4.99(q, 6.5)
9	128.2	-	128.4	1.54(d, 6.5)
10	74.1	5.05 (q, 6.5)	68.7	-
11	25.2	1.41 (d, 6.5)	26.9	1.68(s)
12	68.1	-	68.1	-
13	29.4	1.51 (s)	29.5	-
14	29.4	1.51 (s)	29.5	-
Glc-1'	100.5	3.89 (d, 7.5)	-	-
Glc-2'	77.4	2.87(m)	-	-
Glc-3'	77.2	2.97(m)	-	-
Glc4'	74.1	2.89(m)	-	-
Glc-5'	70.8	3.02(m)	-	-
Glc-6'	61.7	3.67(m),3.44(m)	-	-
12-OH		5.41(s)		