Supporting Information

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Scoparic acid E: A New Labdane Diterpenoid on Attenuating Palmitate Induced Viability in MIN6 cells from *Scoparia dulcis*

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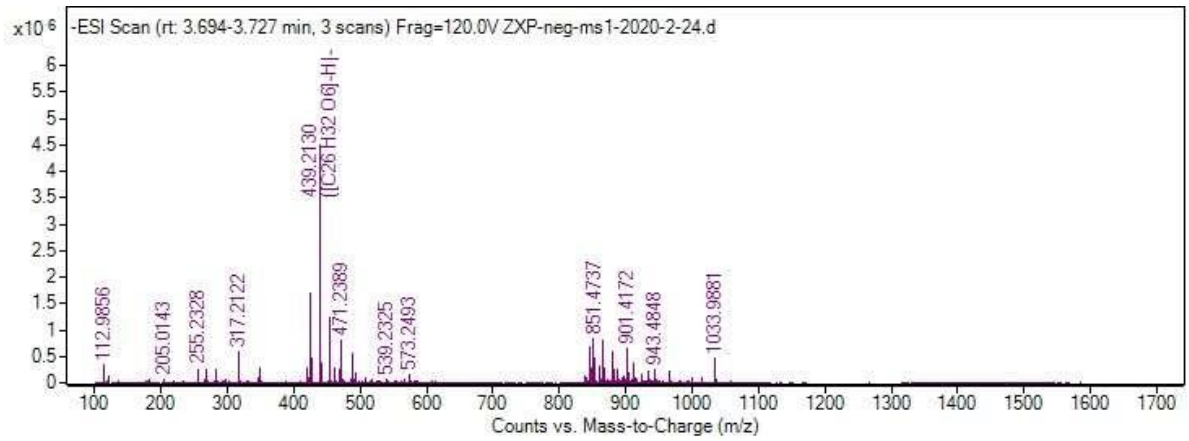


Figure S1: HRESIMS Spectrum of **1** (Scoparic acid E)

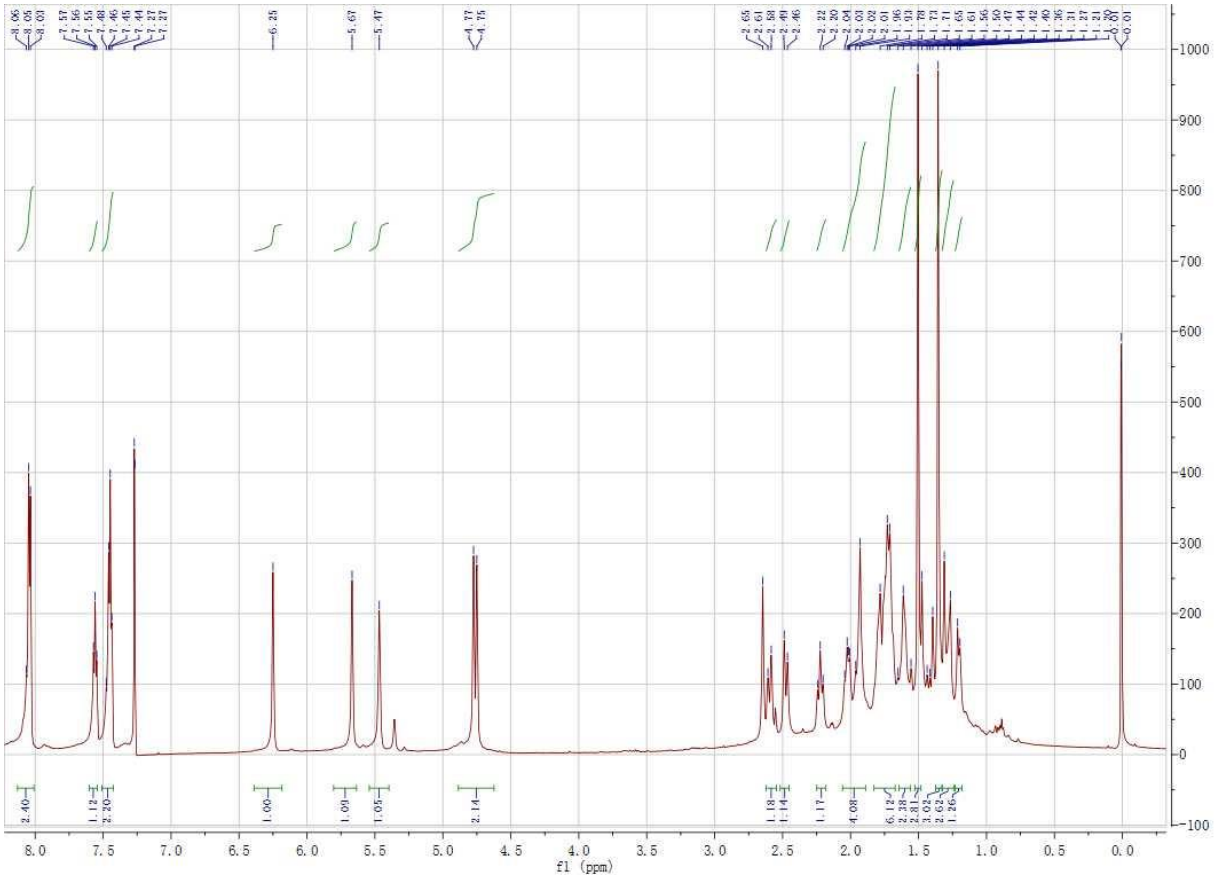


Figure S2: ^{1}H-NMR (600 MHz, $CDCl_3$) Spectrum of **1** (Scoparic acid E)

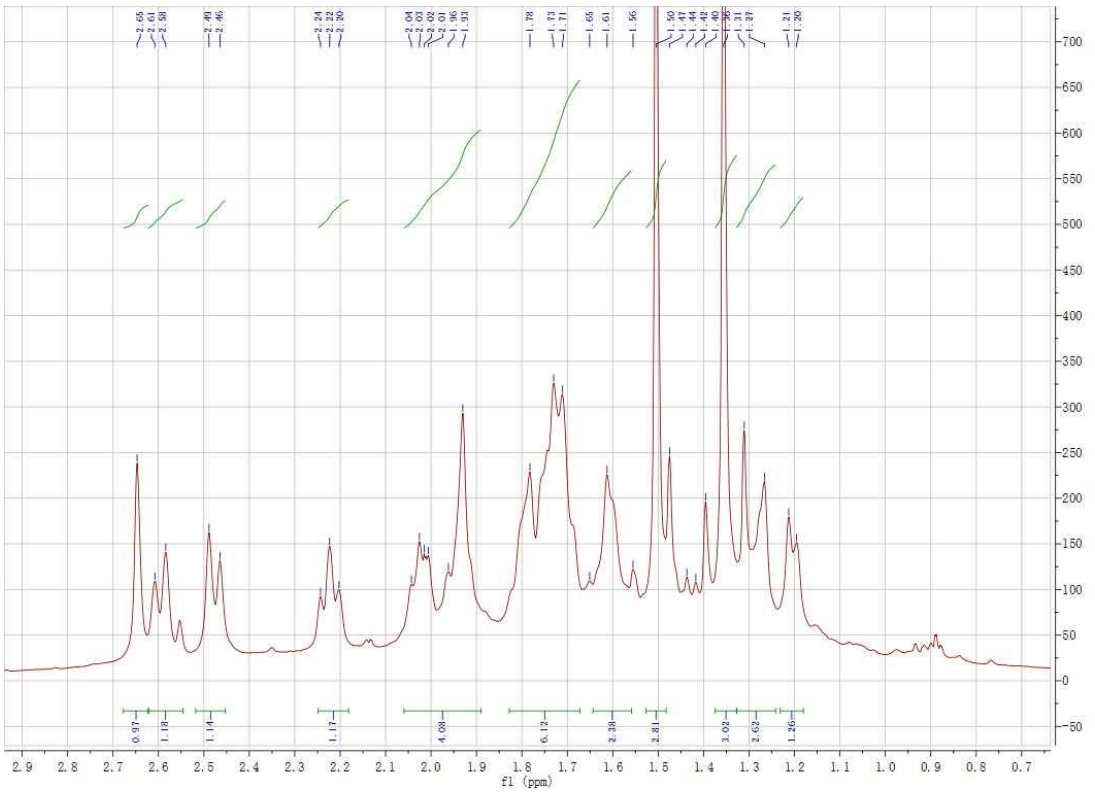


Figure S3: Enlarged ^{1}H-NMR (600 MHz, $CDCl_3$) Spectrum of **1** (Scoparic acid E)

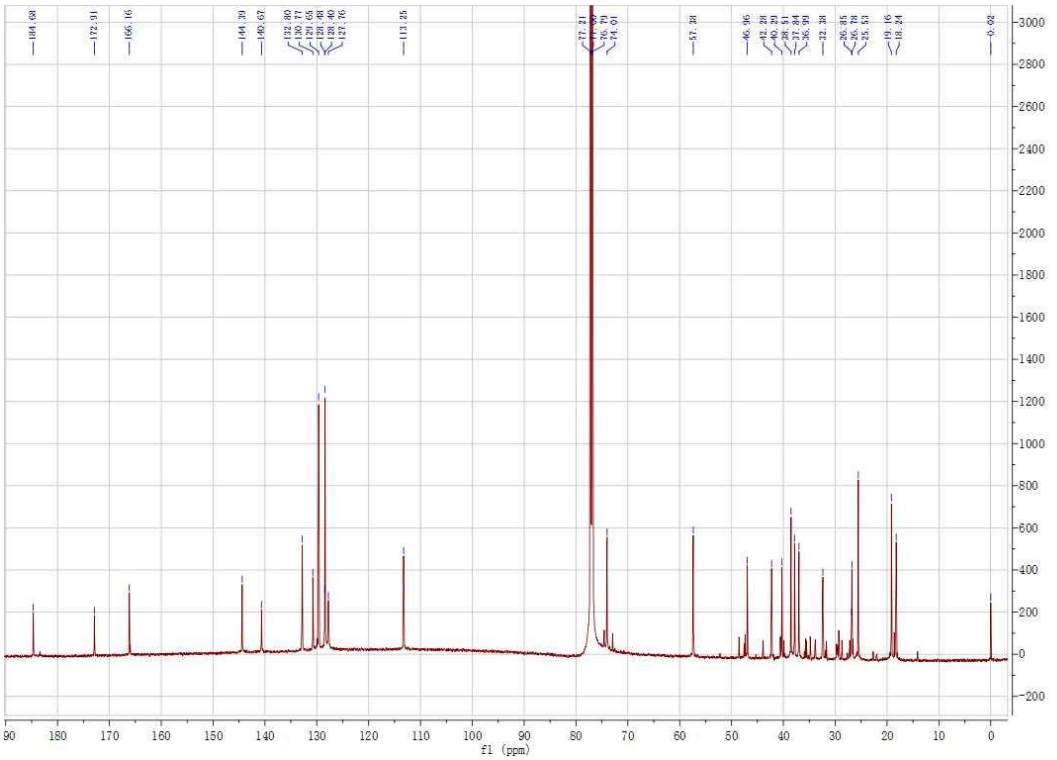


Figure S4: ^{13}C-NMR (150 MHz, $CDCl_3$) spectrum of **1** (Scoparic acid E)

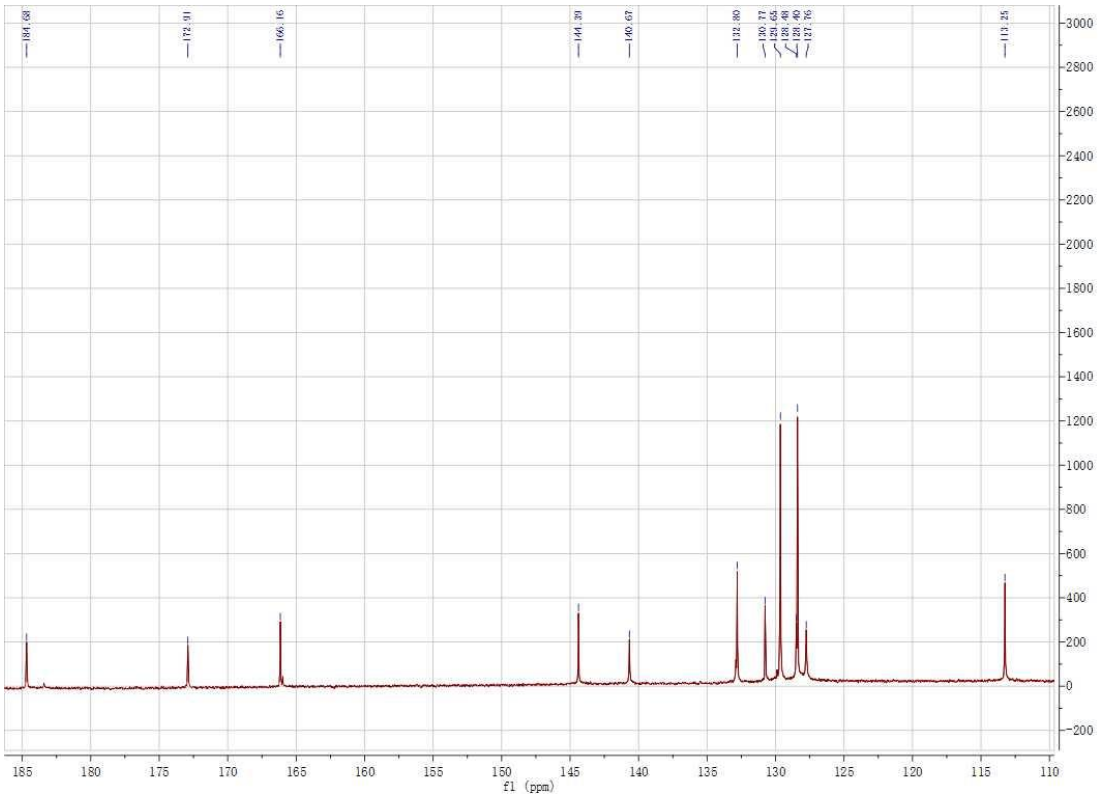


Figure S5: Enlarged ^{13}C-NMR (150 MHz, $CDCl_3$) spectrum of **1** (Scoparic acid E)

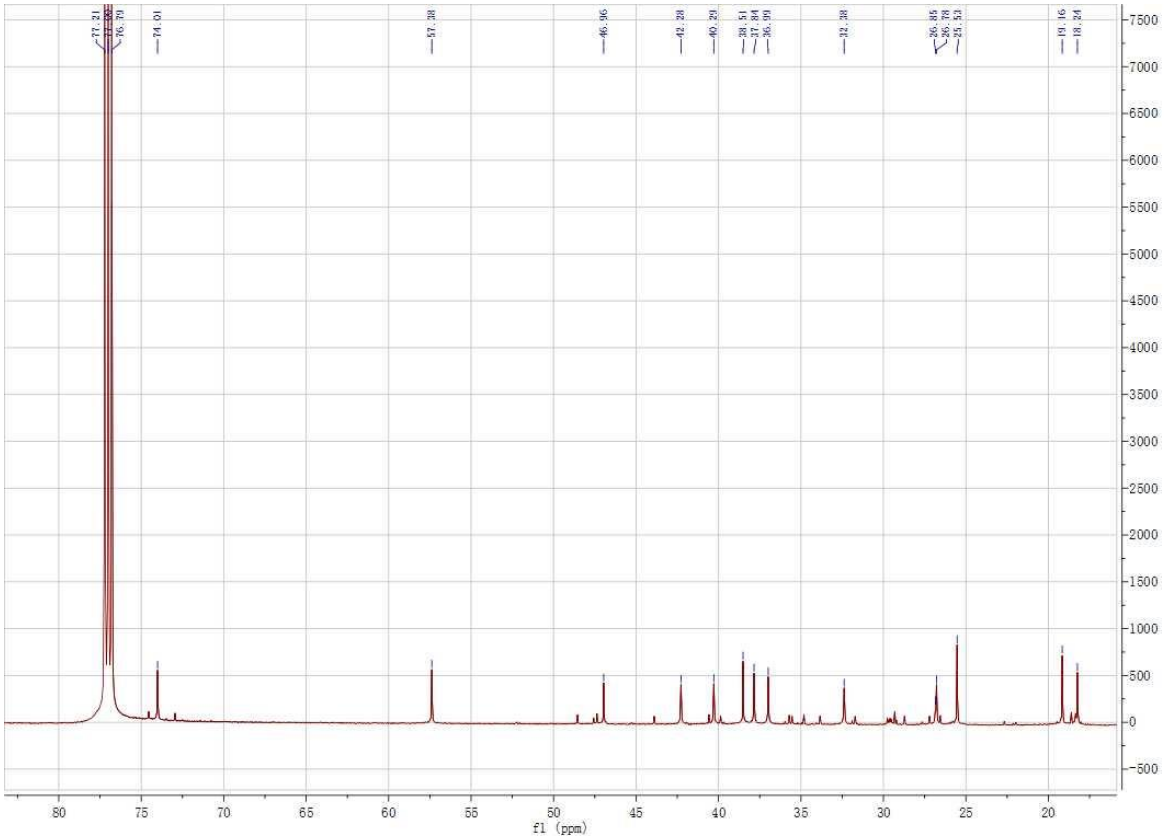


Figure S6: Enlarged ^{13}C-NMR (150 MHz, $CDCl_3$) spectrum of **1** (Scoparic acid E)

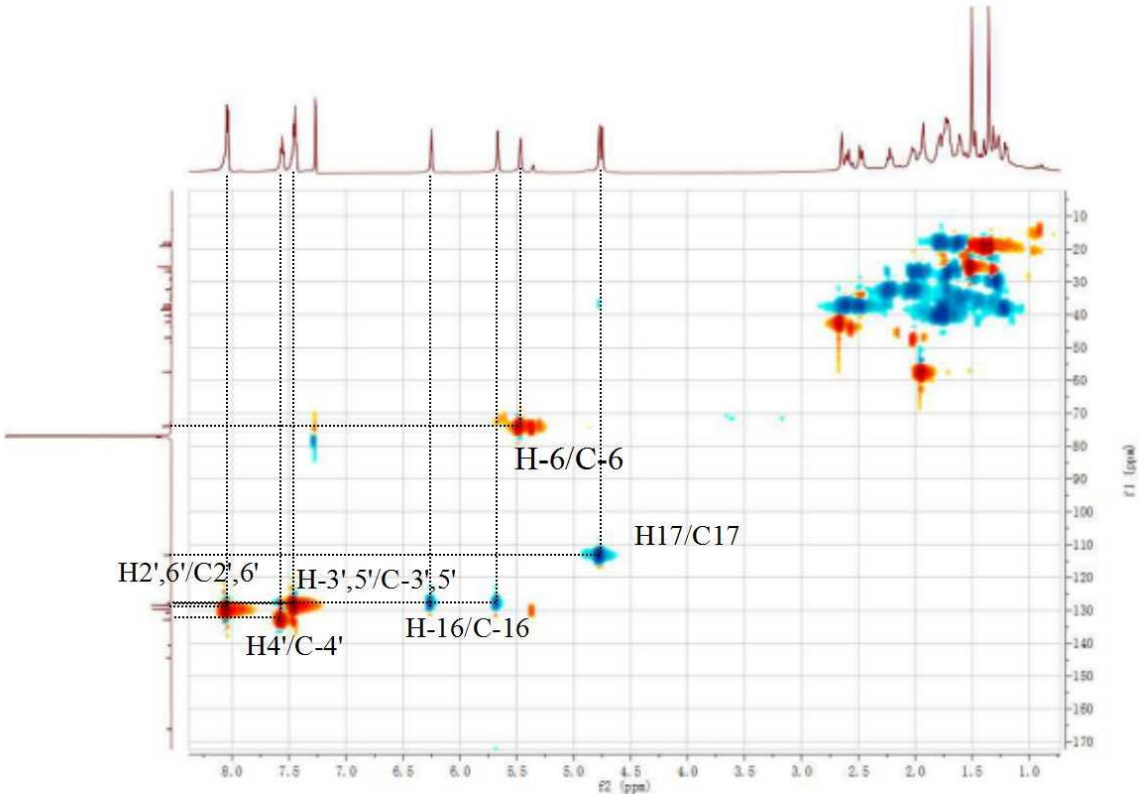


Figure S7: HSQC spectrum of **1** (Scoparic acid E)

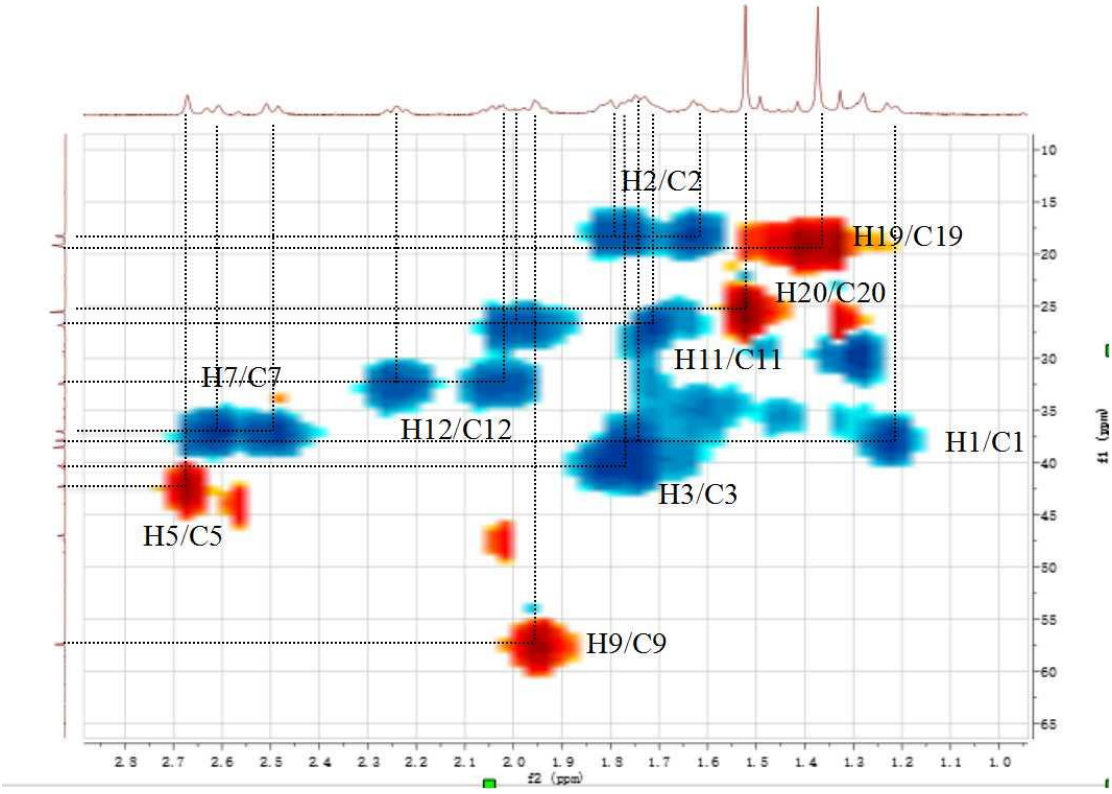


Figure S8: Enlarged HSQC spectrum of **1** (Scoparic acid E)

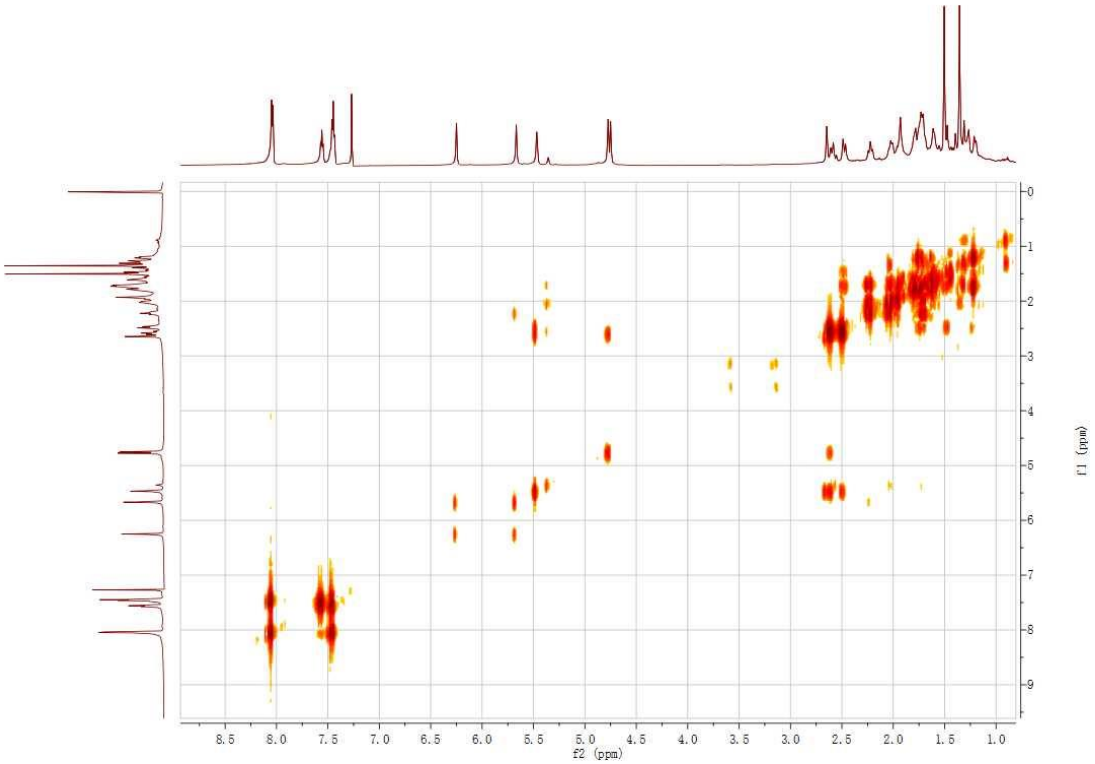


Figure S9: ^{1}H-^{1}H COSY spectrum of **1** (Scoparic acid E)

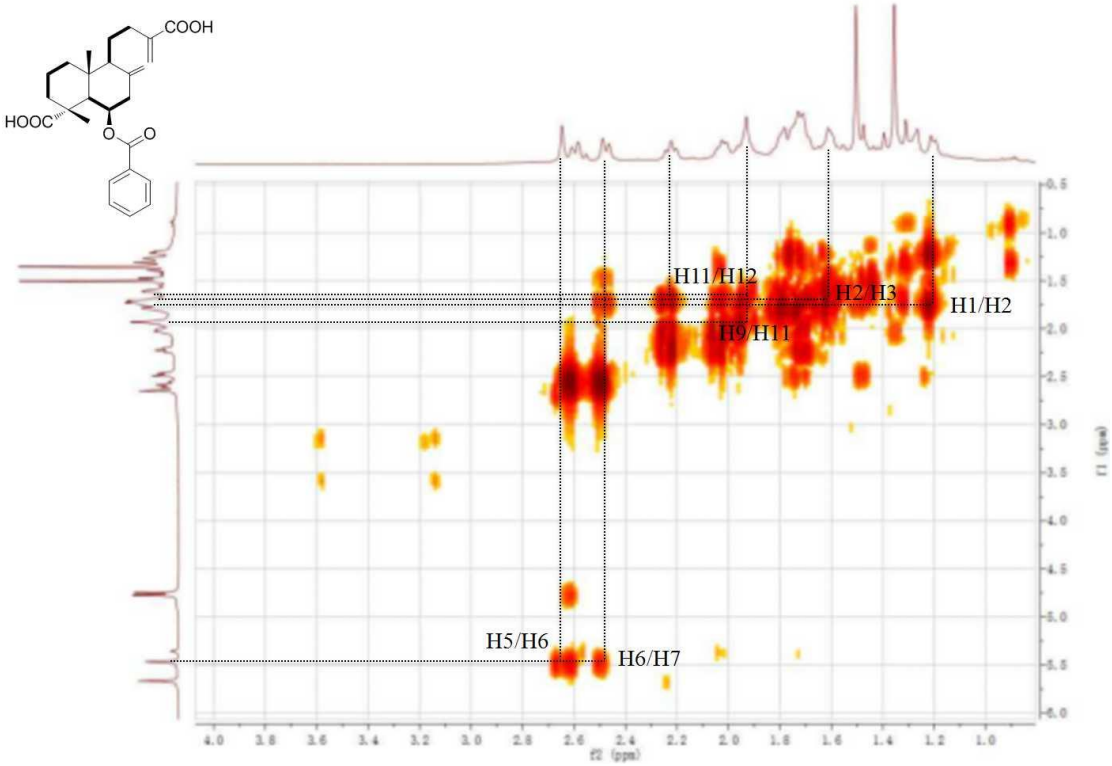


Figure S10: Enlarged ^{1}H-^{1}H COSY spectrum of **1** (Scoparic acid E)

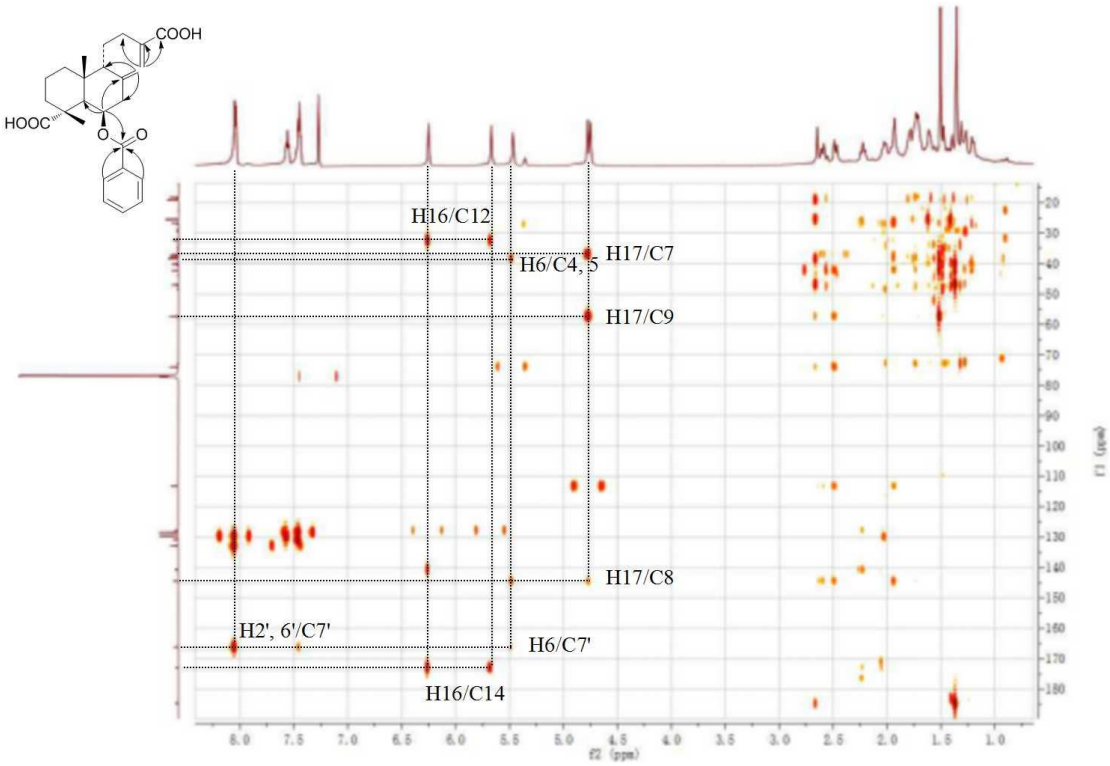


Figure S11: HMBC spectrum of **1** (Scoparic acid E)

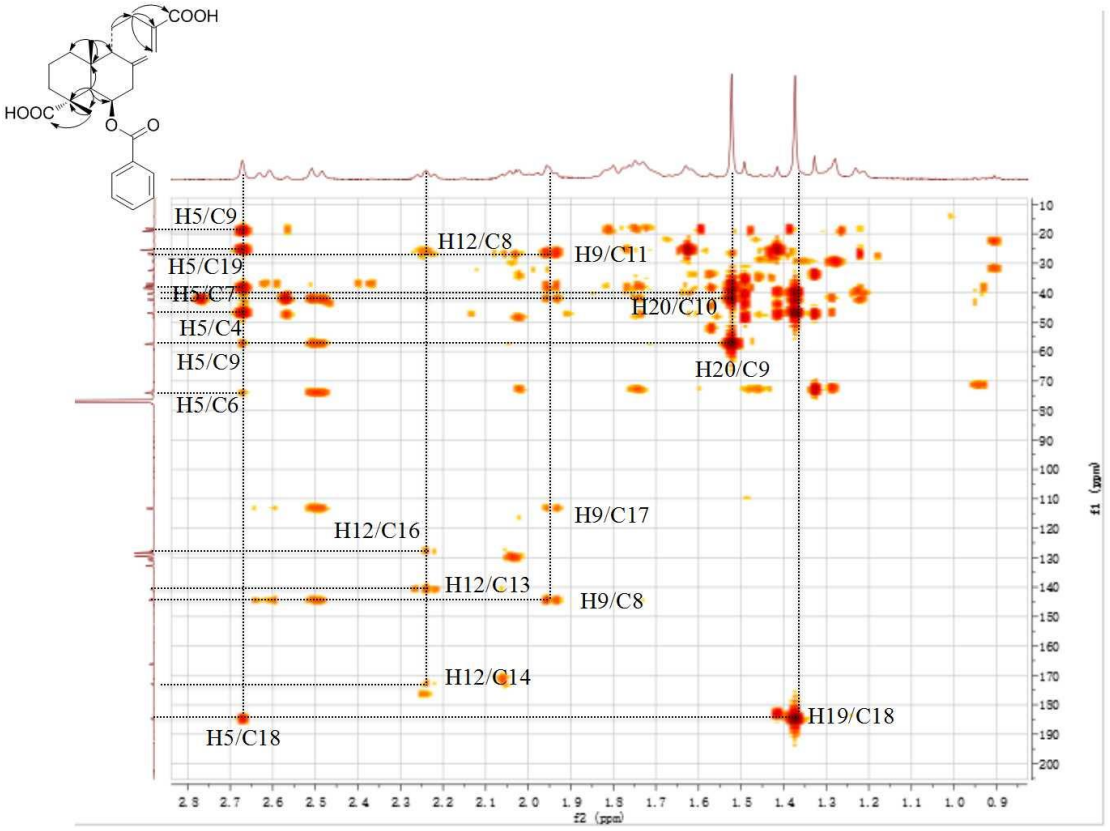


Figure S12: Enlarged HMBC spectrum of **1** (Scoparic acid E)

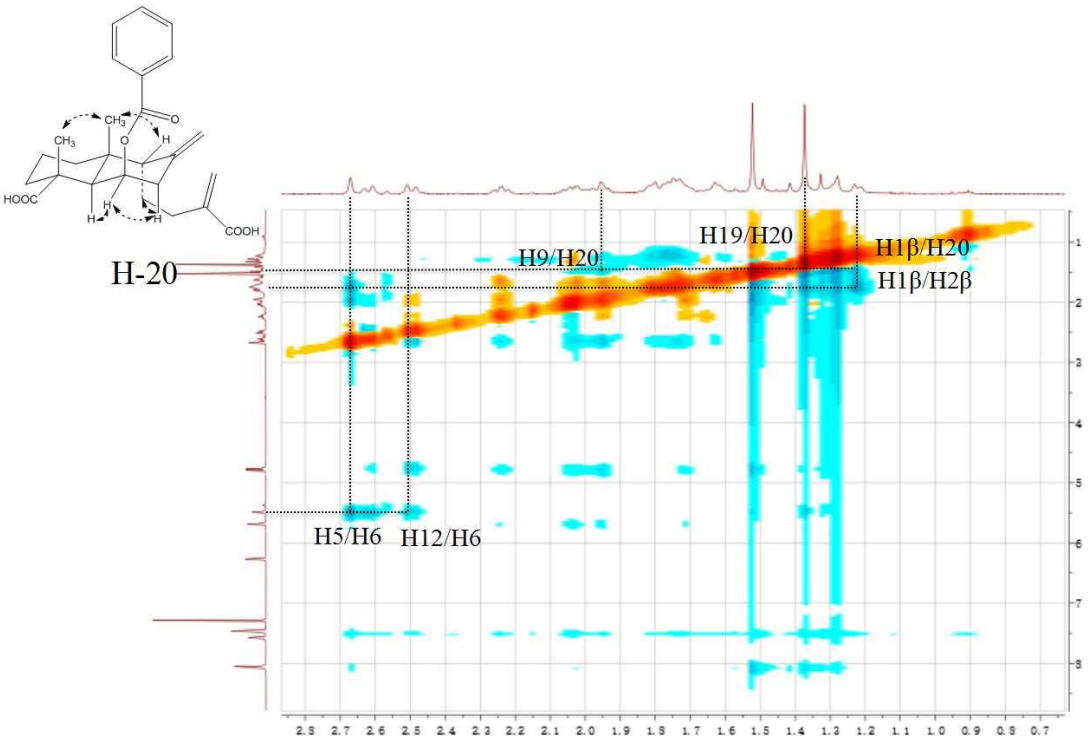


Figure S13: ROESY Spectrum of **1** (Scoparic acid E)

Select All Deselect All

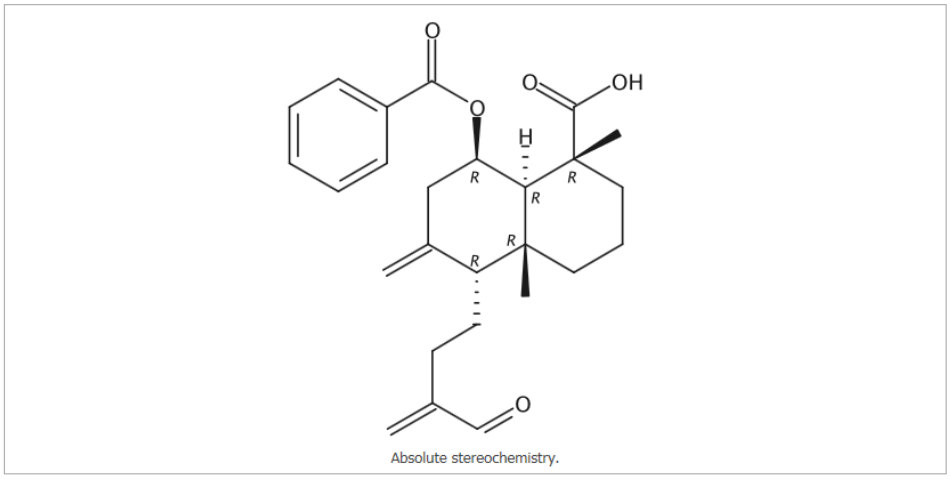
0 of 8 Similarity Candidates Selected	Substances
≥ 99 (most similar)	0
95-98	1
90-94	4
85-89	8
80-84	6
75-79	162
70-74	1778
65-69	10823
0-64 (least similar)	52711

Get Substances

Figure S14: Scifinder Search Report for **1** (Scoparic acid E)

Score: 95

1. **116425-28-6**



Absolute stereochemistry.

$C_{26}H_{32}O_5$

1-Naphthalenecarboxylic acid, 8-(benzoyloxy)-5-(3-formyl-3-buten-1-yl)decahydro-1,4a-dimethyl-6-methylene-, (1*R*,4a*R*,5*R*,8*R*,8a*R*)-

▸ **Key Physical Properties**

Figure S15: Scifinder Search Report for 95% Similar Compound **1** (Scoparic acid E)

Table S1: NMR Data of Scoparic acid E and Scoparic acid C (δ in ppm, J values in Hz)

No.	Scoparic acid E[a]		Scoparic acid C	
	δ_C	δ_H	δ_C	δ_H
1	37.8	1.74, m 1.20, m	38.16	
2	18.2	1.78, m 1.61, m	18.79	
3	40.0	1.72, m	40.21	
4	47.0		48.18	
5	42.3	2.65, brs	44.08	2.42, brs
6	74.0	5.47, brs	74.10	4.71, brs
7	37.0	2.60, brd, (13.2) 2.48, brd, (13.2)	37.61	1.97, m
8	144.4		144.40	
9	57.4	1.93, brs	57.71	
10	38.6		38.55	
11	26.8	2.10, m 2.22, t, (13.2)	24.28	
12	32.4	2.00, m 2.15, m	26.70	
13	140.7		150.39	
14	172.9		194.82	
15				
16	127.6	5.67, s 6.26, s	134.23	5.91, s 6.26, s
17	113.7	4.76, m	113.14	4.65, brs
18	184.7		185.30	
19	19.2	1.36, s	19.73	1.07, s
20	25.6	1.50, s	25.53	1.36,s
1'	129.6		130.73	
2', 6'	130.7	8.04, d, (8.4)	129.88	7.95, d, (7.3)
3', 5'	128.4	7.46, t, (8.4)	128.32	7.30, t, (7.3)
4'	132.8	7.56, t, (8.4)	132.89	7.46, t, (7.3)
7'	166.2		167.35	

[a] Measured at 600 MHz for ^{1}H NMR and 150 MHz for ^{13}C NMR in $CDCl_3$.

S1: Detail of Bioactivity Test-Cell Viability Assay

Cell Lines and Cell Culture

The MIN6 cells were cultured in DRPMI 1640 Medium equilibrated with 5% CO_2 and 95% air at 37°C. The medium was supplemented with 10% fetal calf serum, 100 U/ml penicillin sulfate and 50 μg/ml gentamycin. All experiments were performed when cells reached 80%-90% confluence.

Cell Viability Assay

Cell viability was assessed by the MTT assay. Briefly, MIN6 cells were seeded in 96 well plates at 1×10^4 cells/well. Cells were incubated with 300 μM palmitate for 24 h. MTT solution was added to the cells at a final concentration of 0.5 mg/ml. After incubating for 4 h at 37 °C, with 5% CO_2, the solution was removed, and 150 μL DMSO was added. The precipitate in each well was dissolved for 10min and the optical density (OD) was determined at 570 nm using a microplate reader. The viability of the new compound treated cells was performed as above. The cell viability was calculated according to the following formula.

$$\text{Cell viability（%）} = \frac{\text{PA (OD)- Normal (OD)}}{\text{Compound (OD)-Normal (OD)}} \times 100\%$$