

Supporting Information

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A New Aporphine Alkaloids from *Litsea glutinosa* to Attenuate Palmitate Induced Viability in MIN6 Cells

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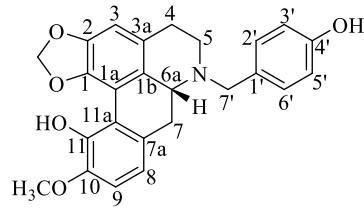
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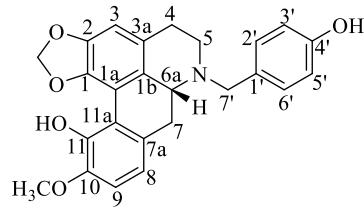
Authors contributed equally to this work.



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Table S1: ^1H (600 MHz) and ^{13}C (150 MHz) NMR data for Litsine E (**1**) in $\text{DMSO}-d_6$

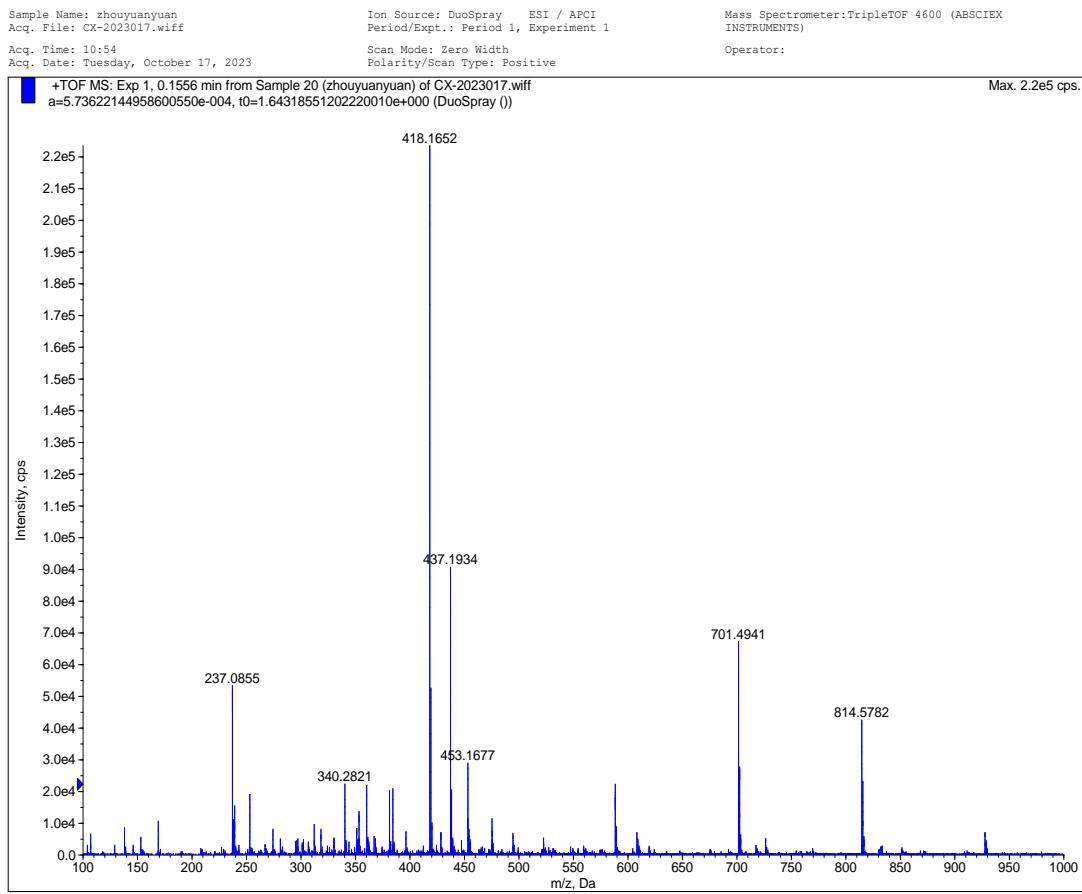
Position	δ_{C} , type	δ_{H} (J in Hz)	COSY	HMBC
1	142.9, C			
1a	114.6, C			
1b	129.0, C			
2	146.5, C			
3	107.3, CH	6.64, s		C- 1, 2, 4, 1b
3a	126.5, C			
4	29.3, CH_2	2.52, br d (15.6) 2.73, m		C- 3a, 5
5	48.5, CH_2	2.20, m 2.91, m		C- 6a, 4, 3a, 7'
6a	60.5, CH	3.01, d (7.3) 2.20, m	H-7	
7	35.2, CH_2	3.22, br d (13.2)		C- 6a, 7a, 11a, 1b
7a	123.6, C			
8	116.2, CH	6.80, d (8.0)	H-9	C- 7a, 11a, 10
9	122.8, CH	6.90, d (8.0)		C- 7a, 11, 10
10	145.7, C			
11	149.7, C			
11a	128.7, C			
10-OMe	60.2, CH_3	3.65, s		C- 10
O-CH₂-O (1,2)	100.5, CH_2	6.04, s 5.90, s		C- 1, 2
1'	129.5, C			
2', 6'	130.4, CH	7.11, d (8.3)	H-3', 5'	C- 1', 4', 3', 5', 7'
3', 5'	115.4, CH	6.72, d (8.2)		C- 1', 4'
4'	156.8, C			
7'	57.9, CH_2	3.23, br d (13.2) 4.11, br d (13.2)		C- 1', 2', 6', 6a, 5



1

Table S2: ^1H (600 MHz) and ^{13}C (150 MHz) NMR data for Litsine E (**1**) in CDCl_3

Position	δ_{C} , type	δ_{H} (J in Hz)
1	142.3, C	
1a	114.0, C	
1b	129.6, C	
2	145.0, C	
3	107.8, CH	6.62, s
3a	126.4, C	
4	29.7, CH_2	2.40, m 3.00, m
5	48.4, CH_2	2.20, m 3.09, m
6a	60.6, CH	2.73, d (13.2)
7	36.0, CH_2	2.20, m 3.21, br d (13.8)
7a	123.4, C	
8	115.3, CH	6.82, d (8.4)
9	122.4, CH	6.92, d (7.8)
10	144.2, C	
11	148.2, C	
11a	128.8, C	
10-OMe	60.3, CH_3	3.62, s
O-CH₂-O (1,2)	100.8, CH_2	6.11, s 5.90, s
1'	129.9, C	
2', 6'	130.6, CH	6.96, d (8.4)
3', 5'	114.2, CH	6.80, d (8.4)
4'	155.8, C	
7'	59.6, CH_2	3.21, br d (13.8) 4.21, br d (13.8)



Analyst Version: 1.7.1

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Figure S1: HR-ESI-MS spectrum of **1** (Litsine E)

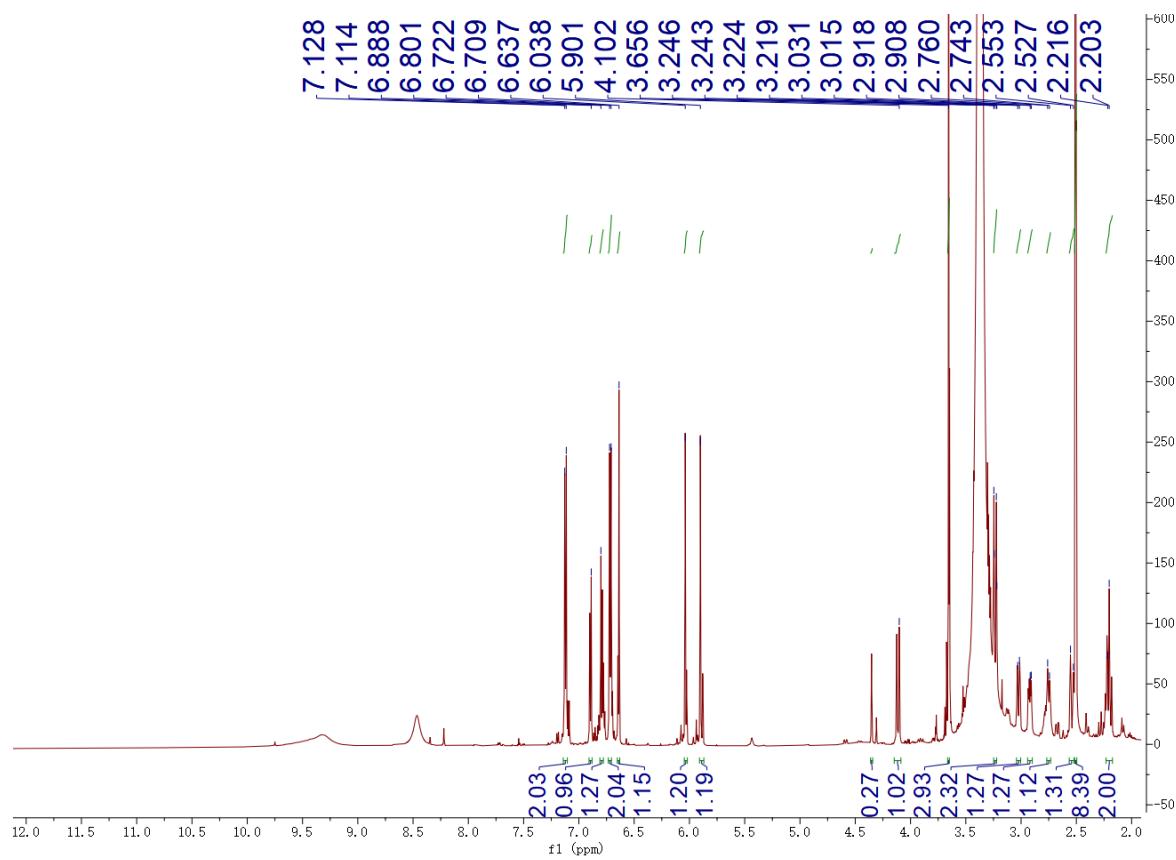


Figure S2: ¹H-NMR (600 MHz, DMSO-*d*₆) spectrum of **1** (Litsine E)

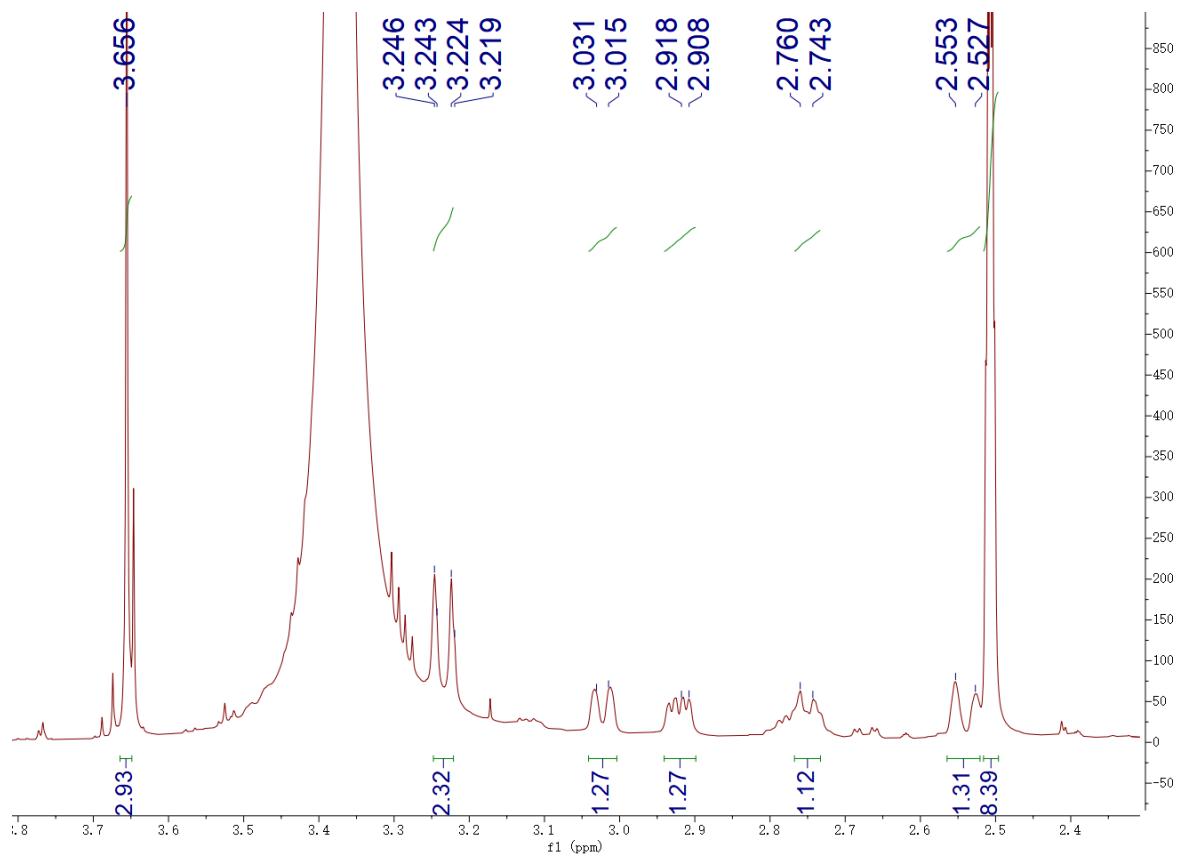


Figure S3: ^1H -NMR (600 MHz, $\text{DMSO}-d_6$) spectrum of **1** (Litsine E)

(From δH 2.5 ppm to δH 3.8 ppm)

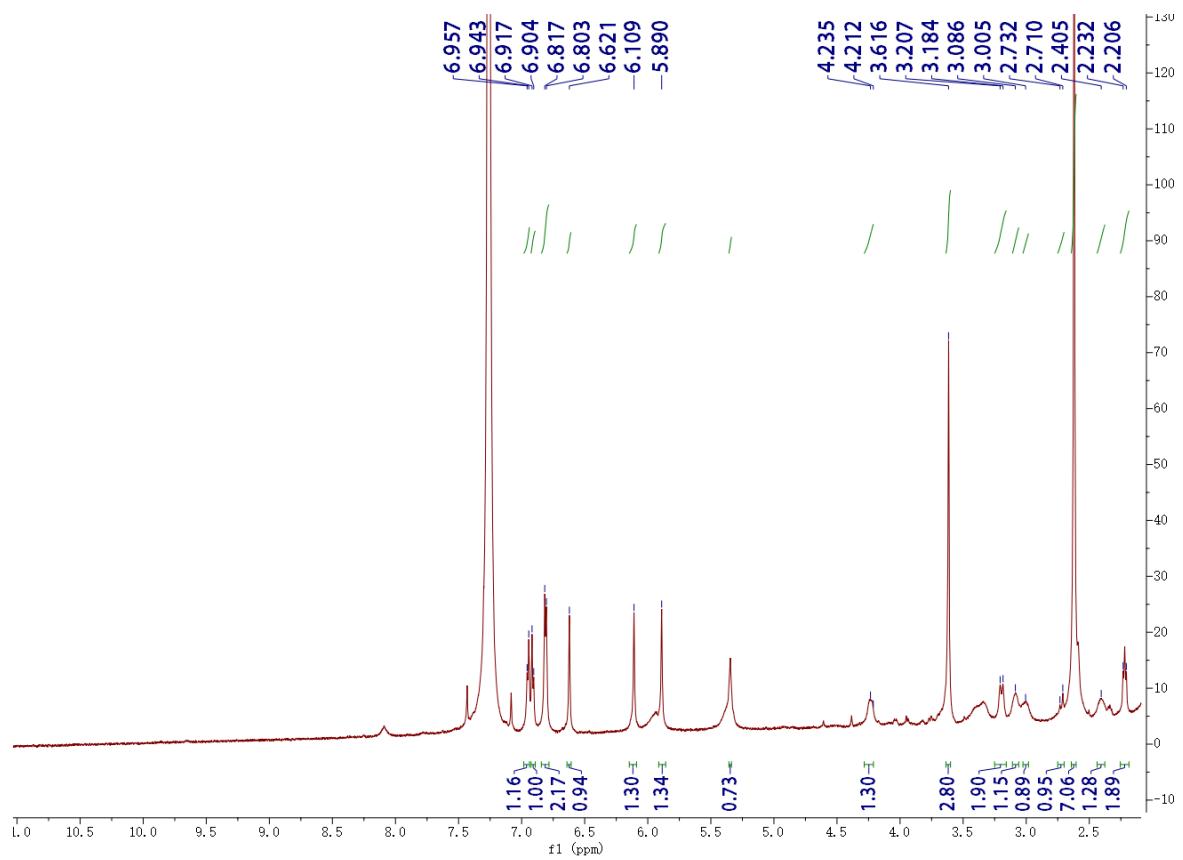


Figure S4: ¹H-NMR (600 MHz, CDCl₃) spectrum of **1** (Litsine E)

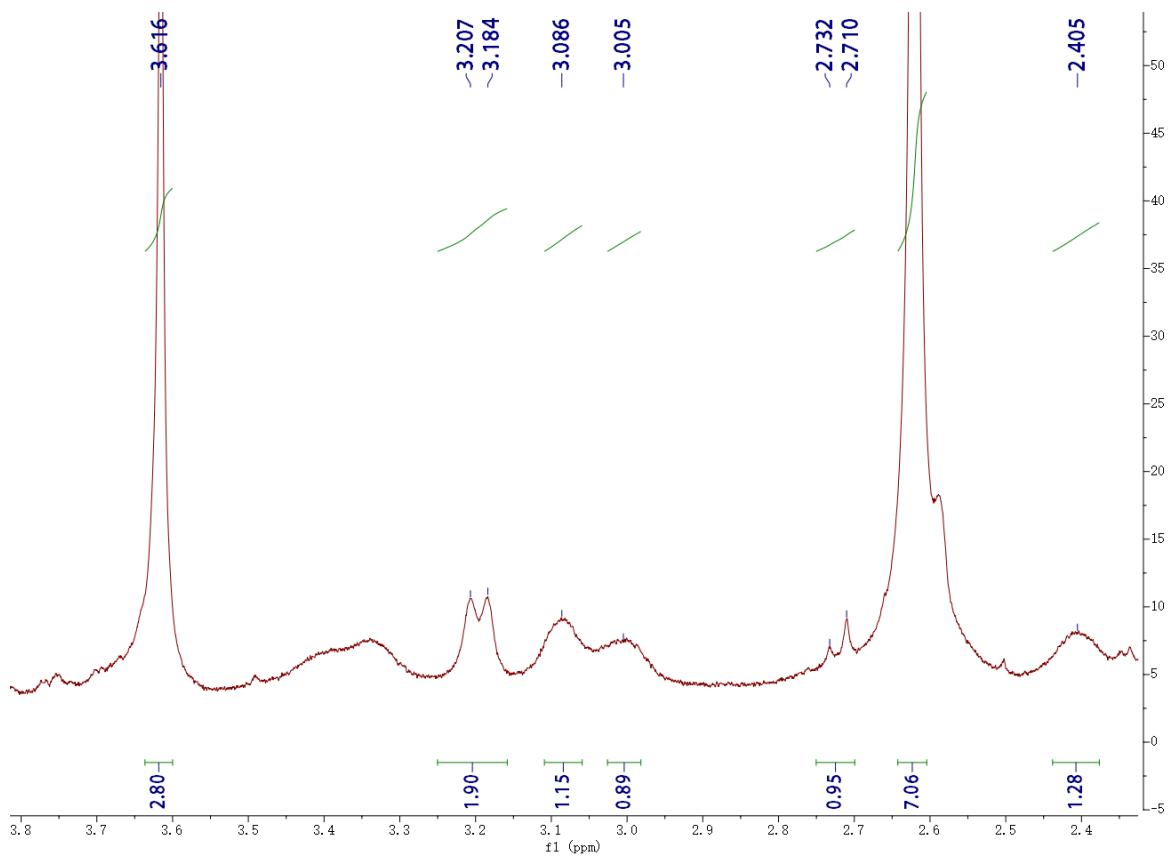


Figure S5: ^1H -NMR (600 MHz, CDCl_3) spectrum of **1** (Litsine E) (From δH 2.5 ppm to δH 3.8 ppm)

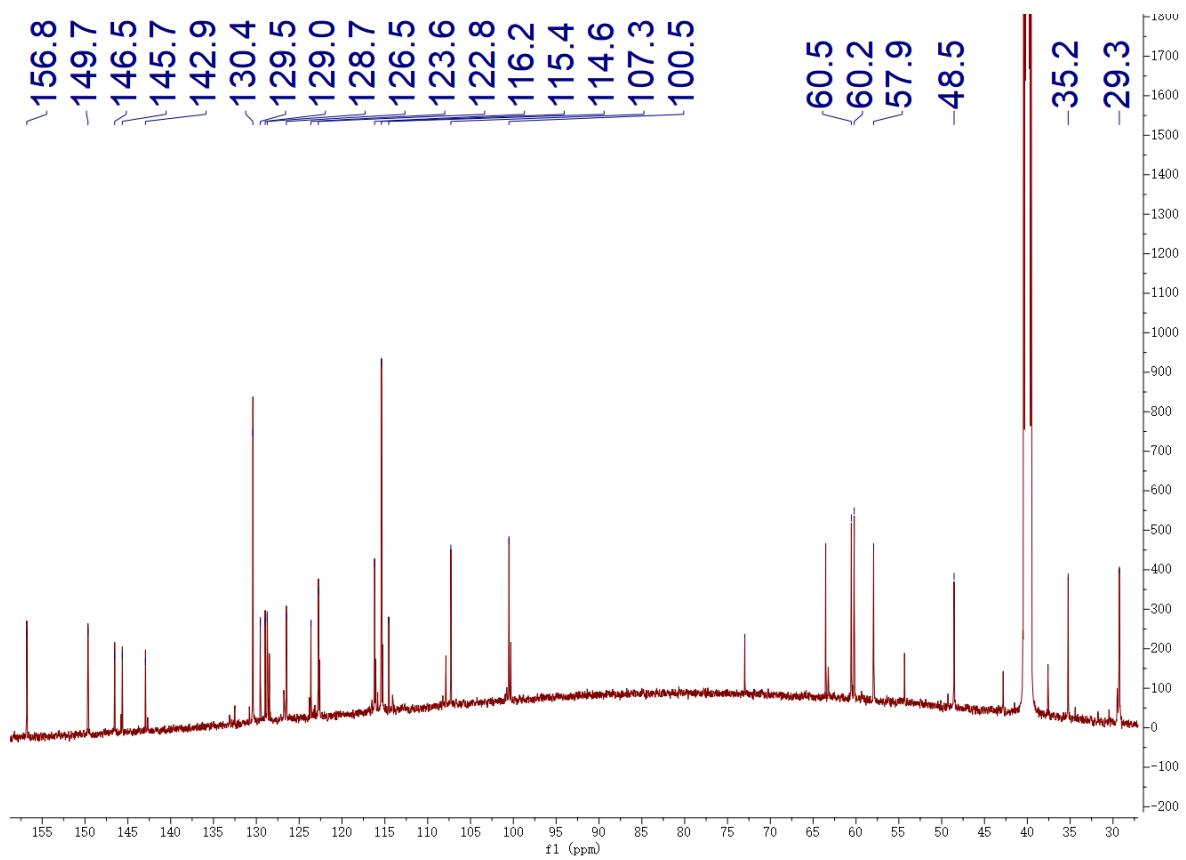


Figure S6: ^{13}C -NMR (150 MHz, $\text{DMSO}-d_6$) spectrum of **1** (Litsine E)

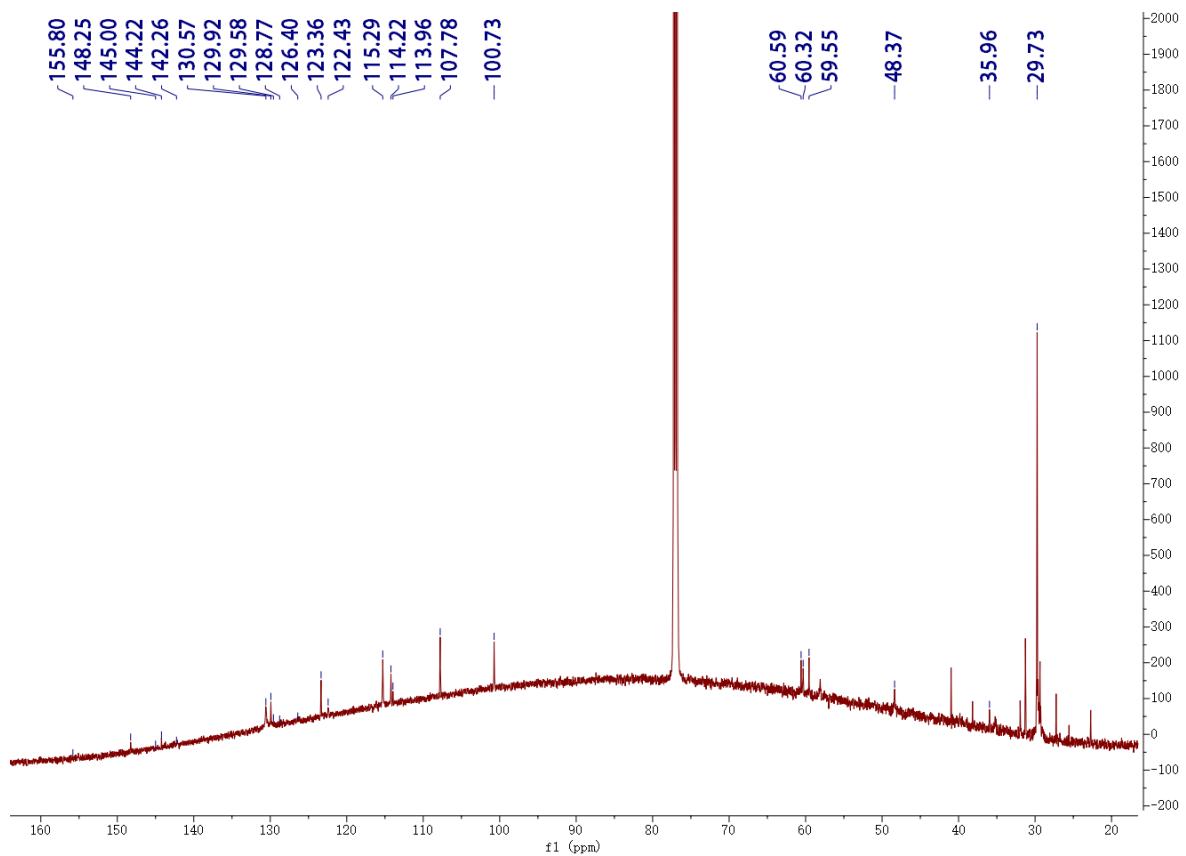


Figure S7: ^{13}C -NMR (150 MHz, CDCl_3) spectrum of **1** (Litsine E)

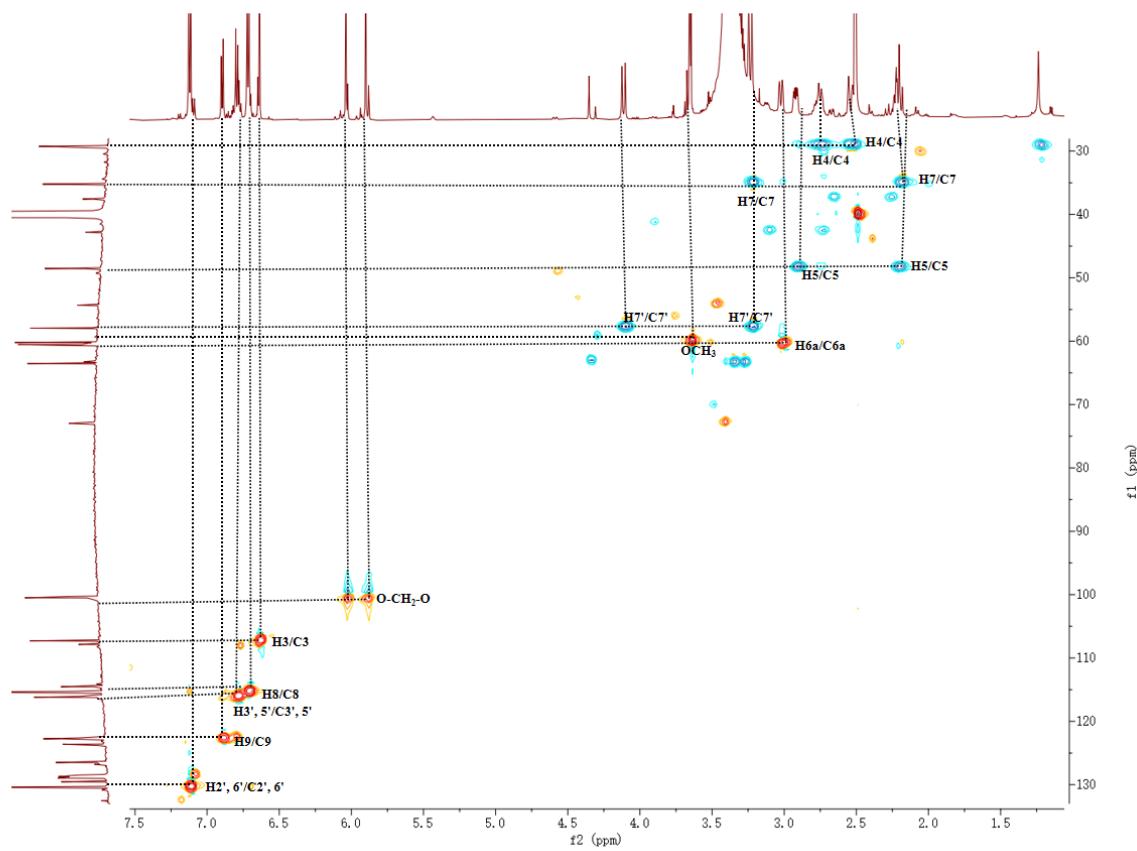


Figure S8: HSQC spectrum of **1** (Litsine E)

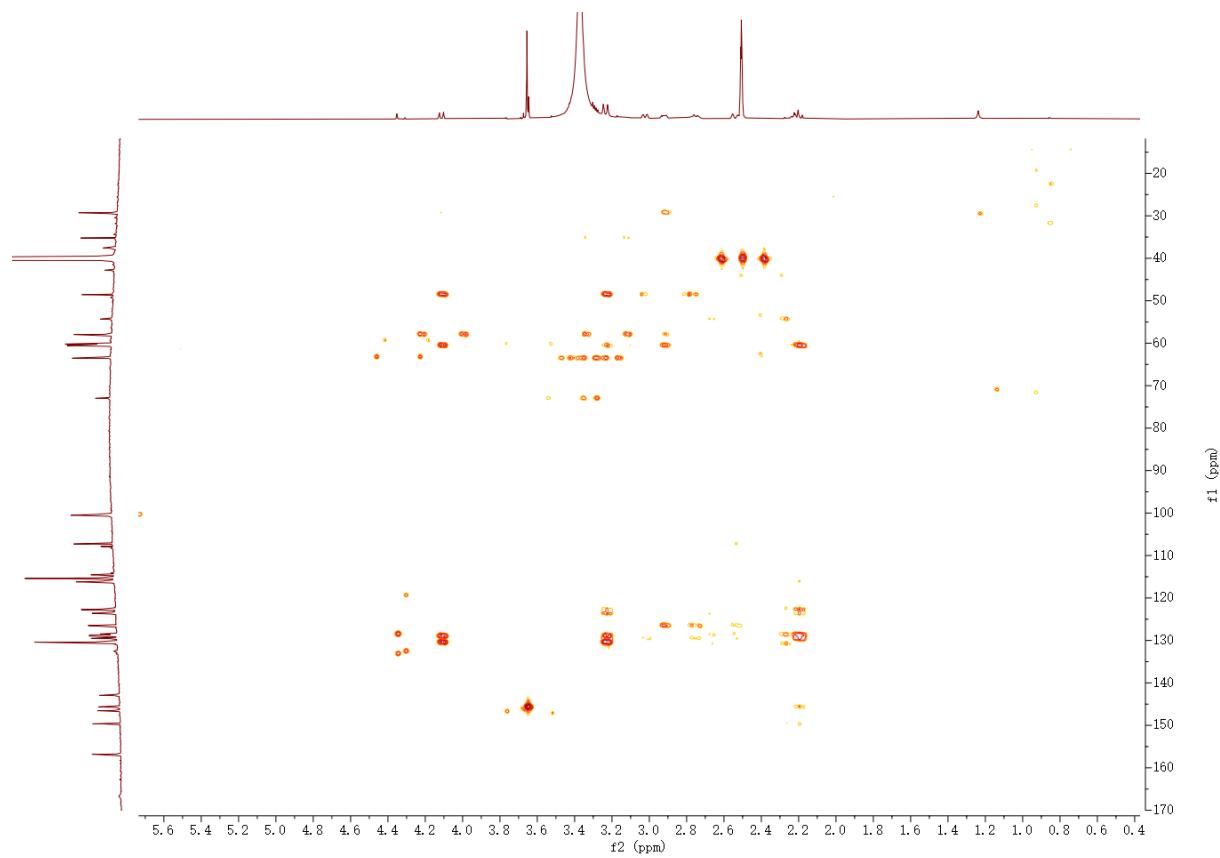


Figure S9: HMBC spectrum of **1** (Litsine E)

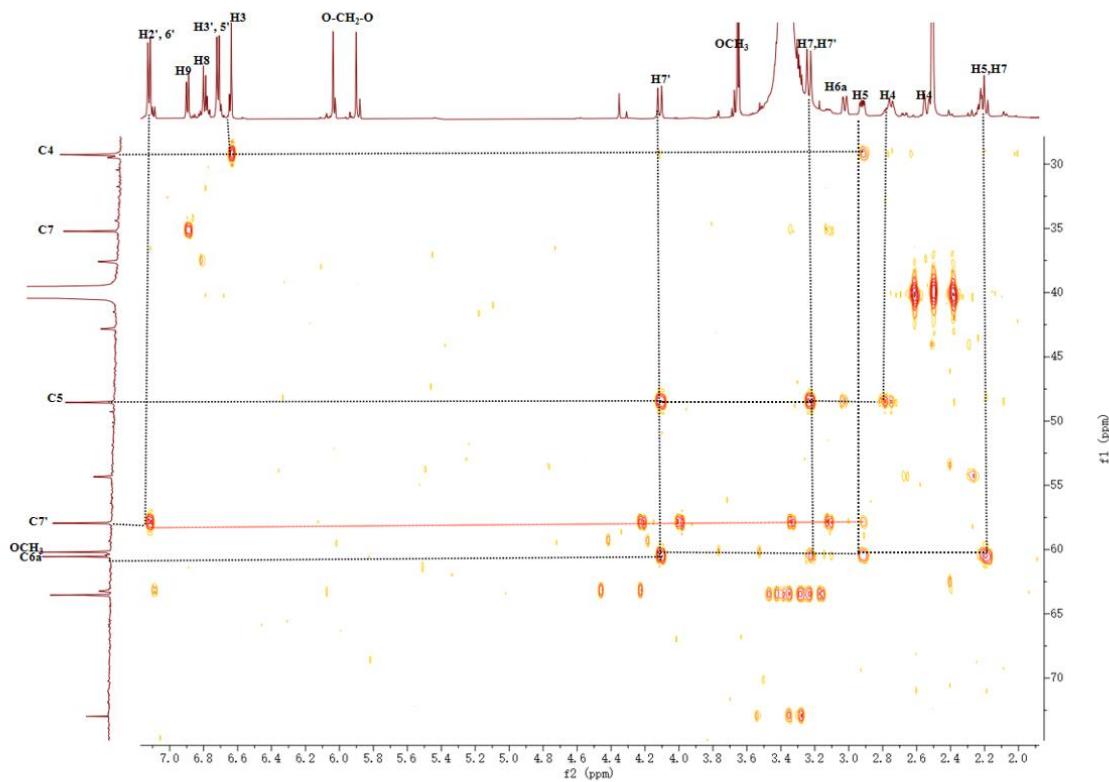


Figure S10: HMBC spectrum of **1** (Litsine E) (Frm δ_{C} 25 ppm to δ_{C} 70 ppm)

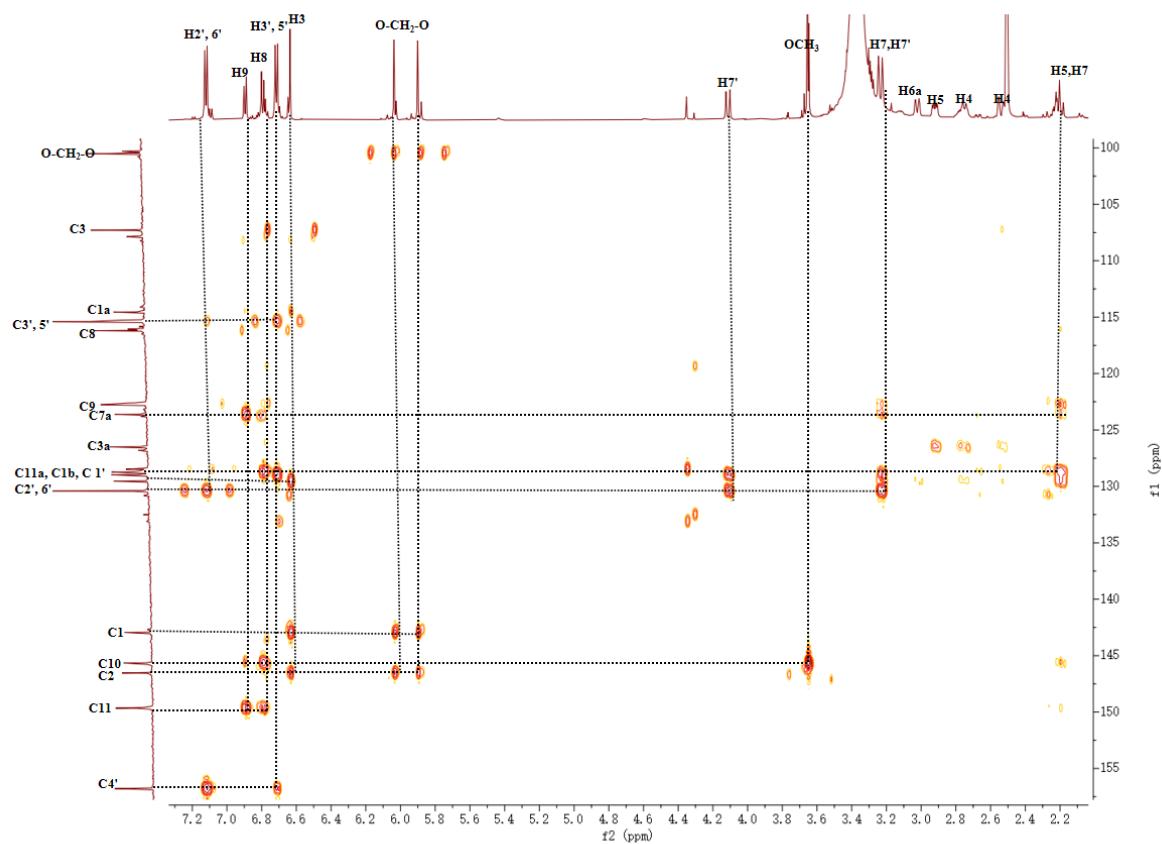


Figure S11: HMBC spectrum of **1** (Litsine E) (From δ_C 100 ppm to δ_C 160 ppm)

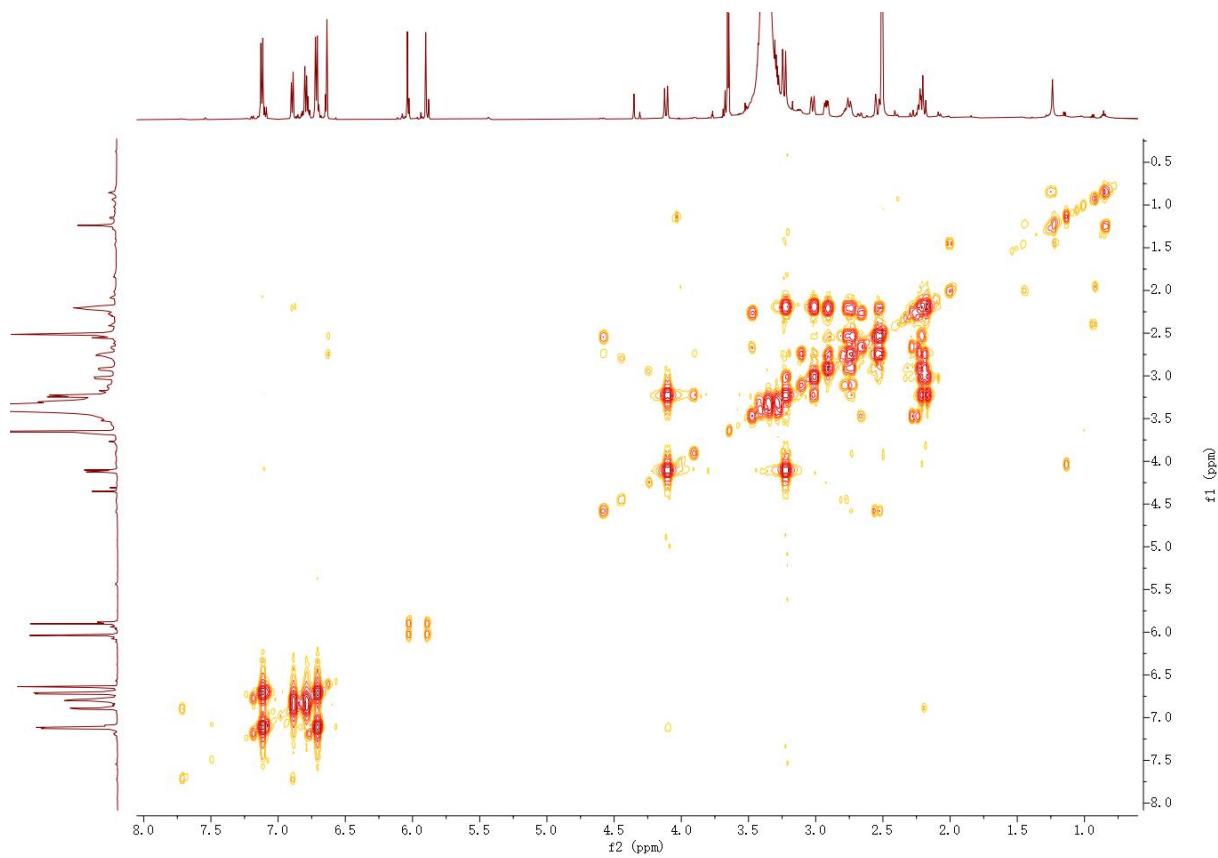


Figure S12: ^1H - ^1H COSY spectrum of **1** (Litsine E)

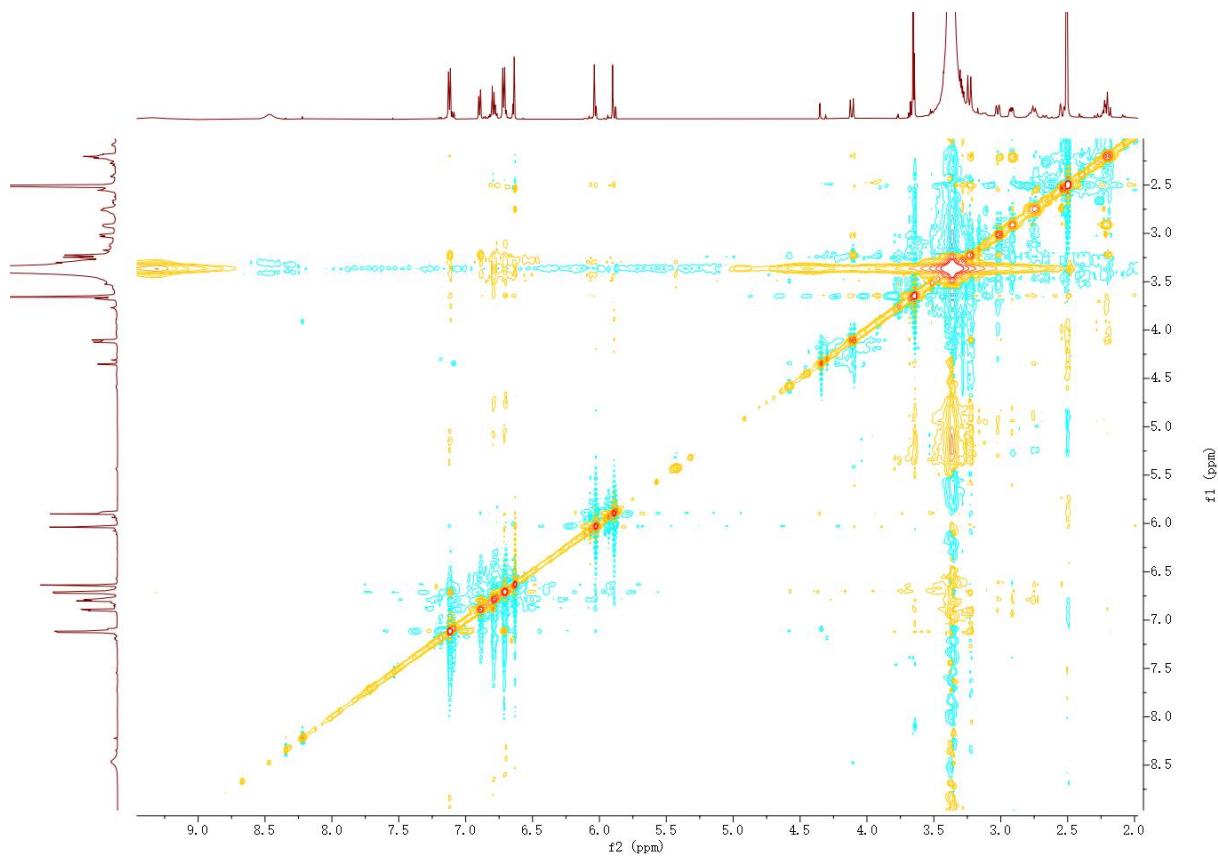


Figure S13: NOESY spectrum of **1** (Litsine E)

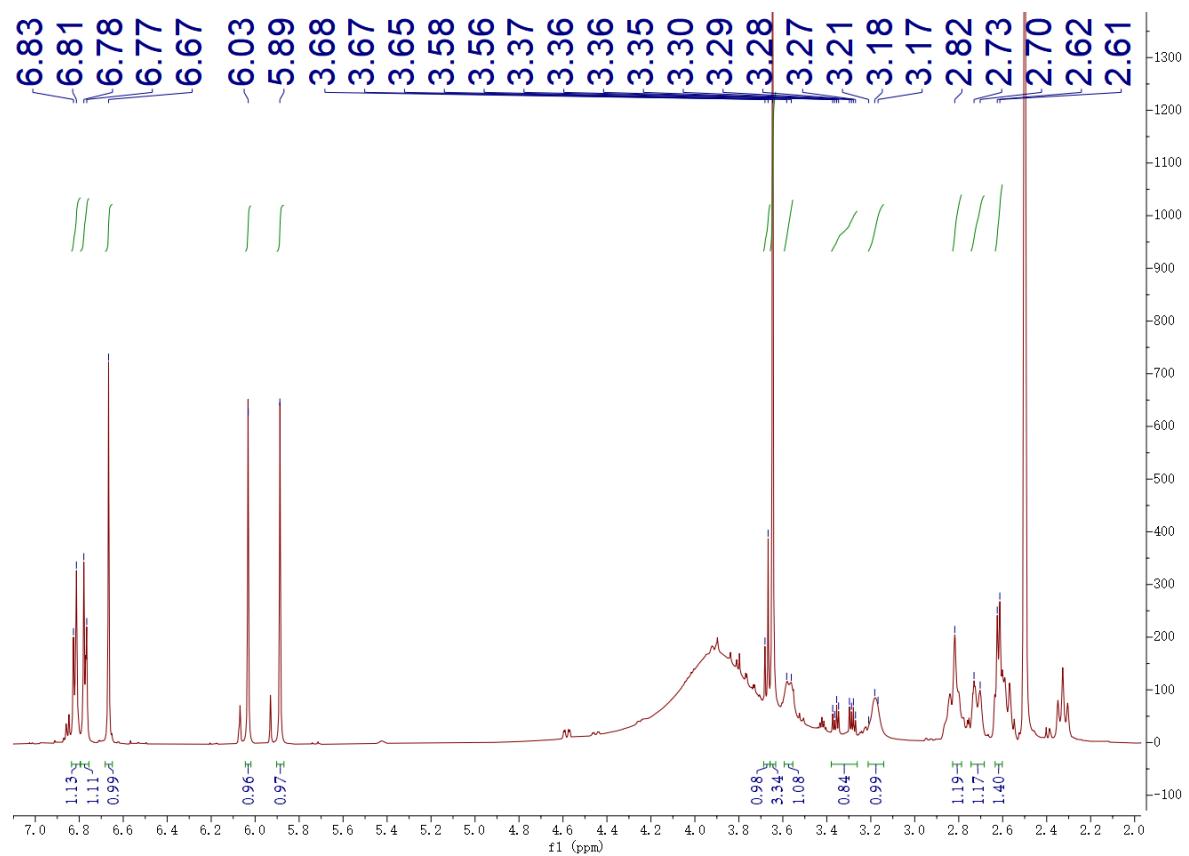


Figure S14: ^1H -NMR (600 MHz, $\text{DMSO}-d_6$) spectrum of **2** (Boldine)

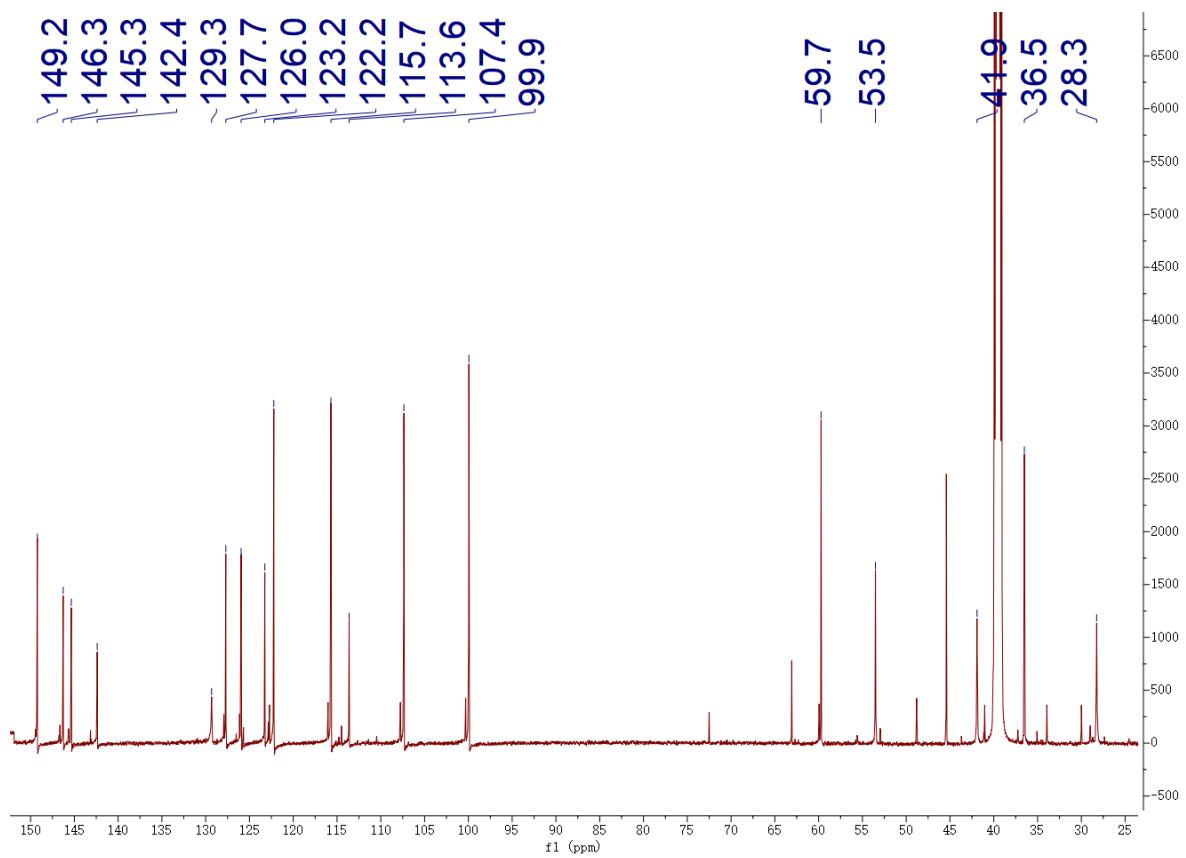


Figure S15: ¹³C-NMR (150 MHz, DMSO-*d*₆) spectrum of **2** (Boldine)

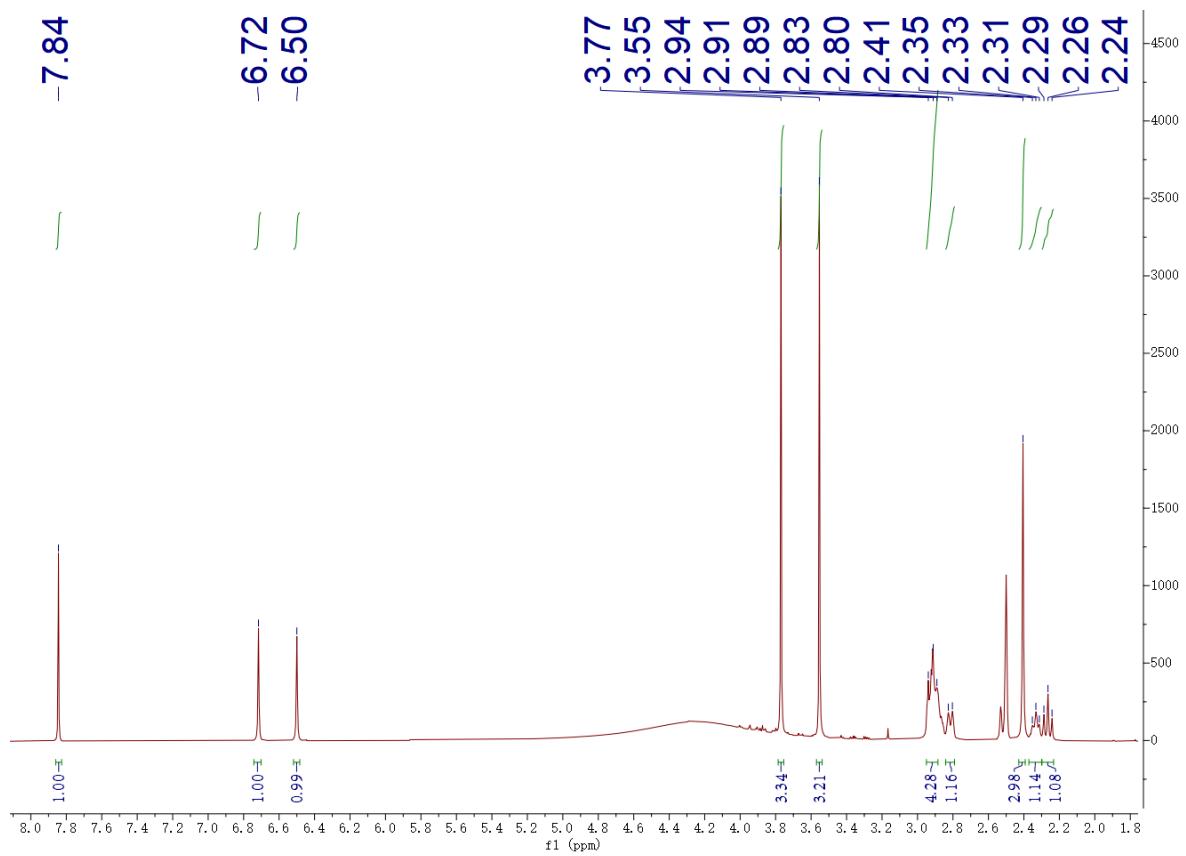


Figure S16: ¹H-NMR (600 MHz, DMSO-*d*₆) spectrum of **3** (Isoboldine)

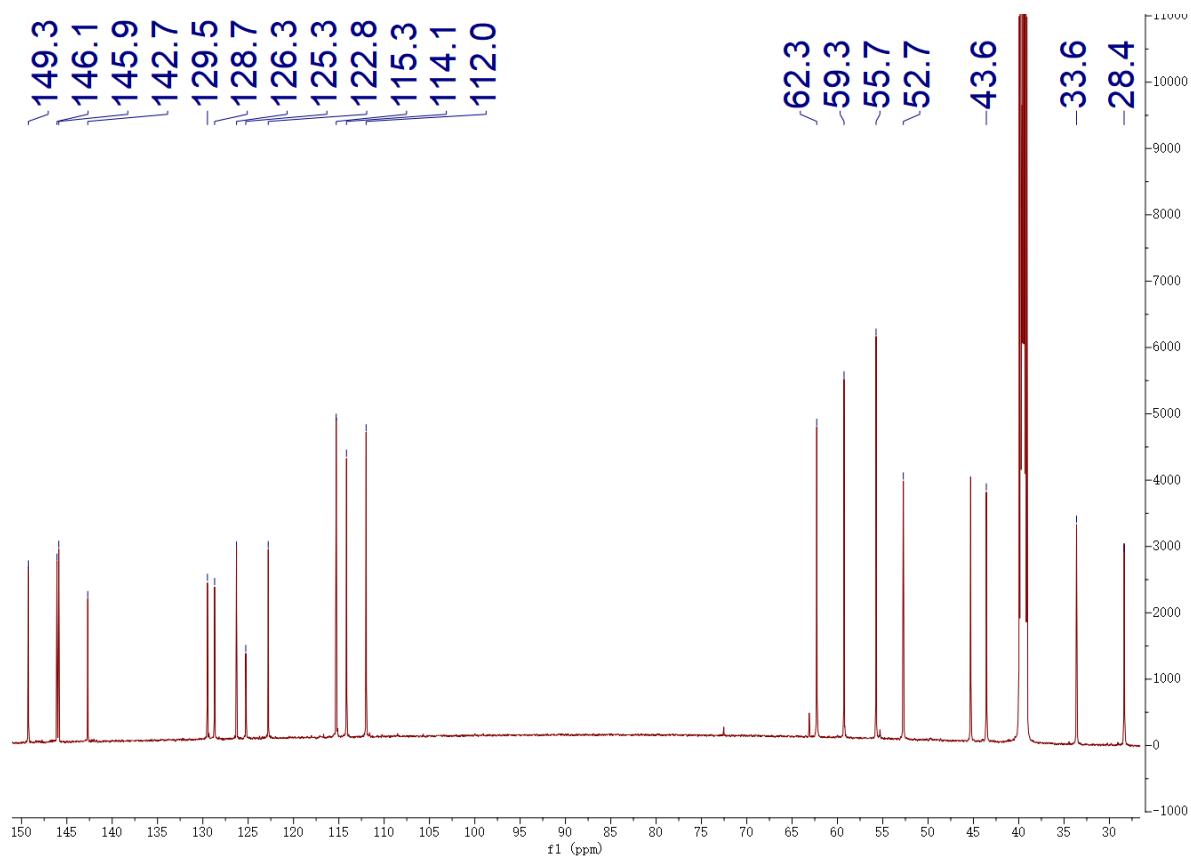


Figure S17: ^{13}C -NMR (150 MHz, $\text{DMSO}-d_6$) spectrum of **3** (Isoboldine)

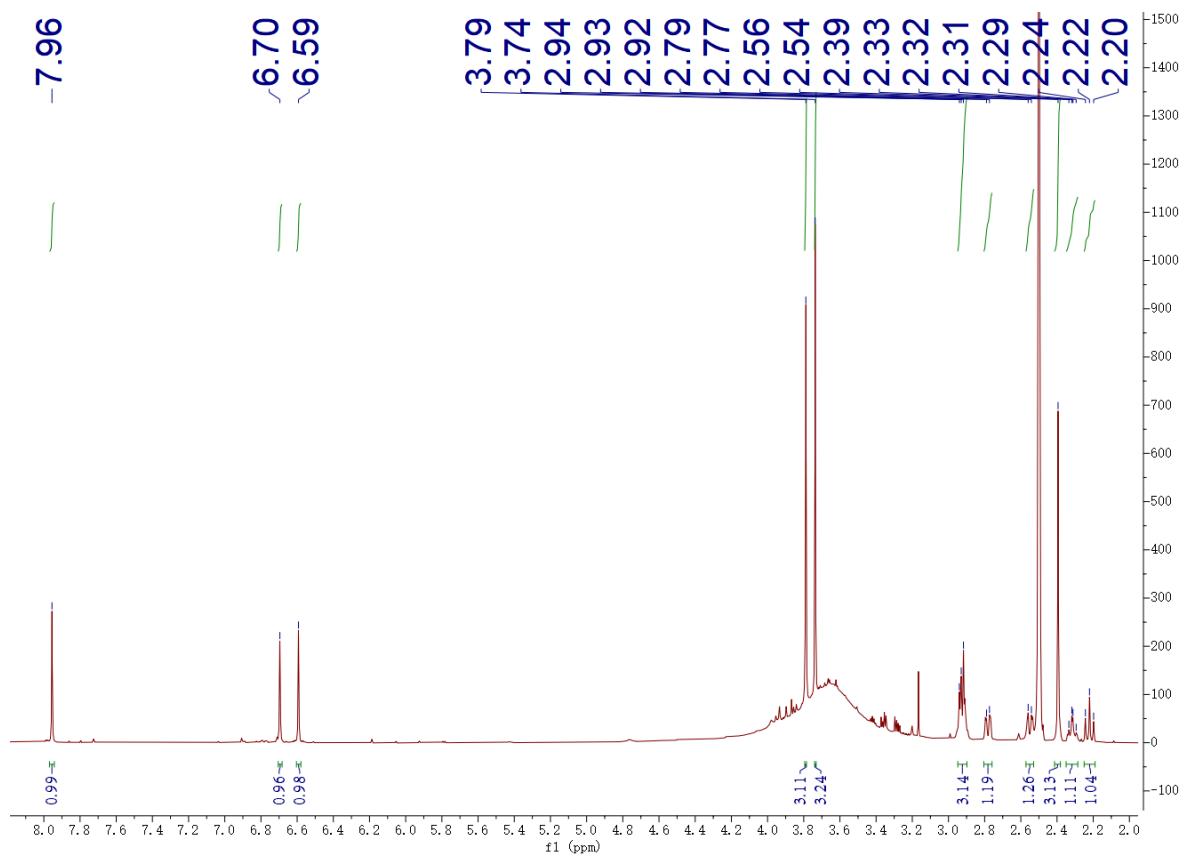


Figure S18: ^1H -NMR (600 MHz, $\text{DMSO}-d_6$) spectrum of **4** (Launobine)

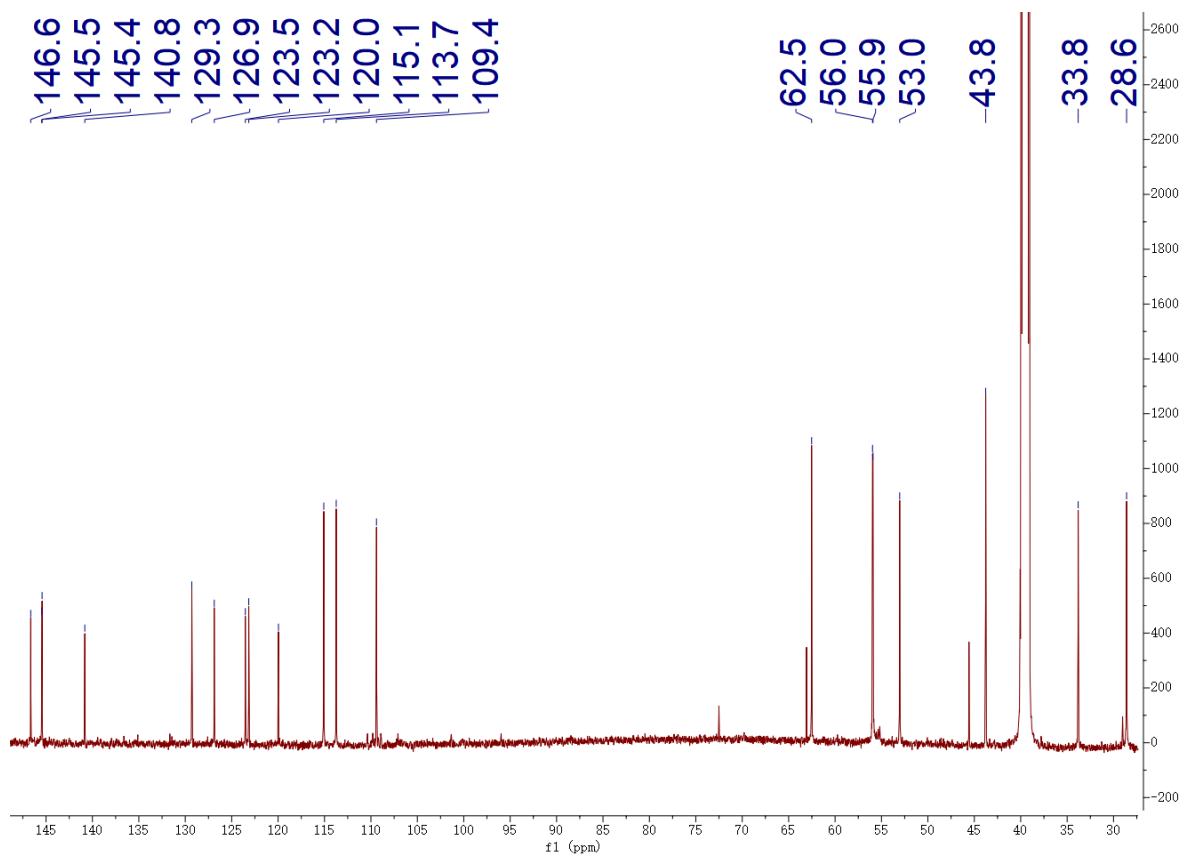


Figure S19: ¹³C-NMR (150 MHz, DMSO-*d*₆) spectrum of **4** (Launobine)

Drawn Structure All Search | CAS x +

https://scifinder-n.cas.org/search/all/652e18c7dbfa1d2ae175af3

All Enter a query... Edit ...

Return to Home Show only Substances (110,780) Reactions (0) References (0) Suppliers (0)

All Search Type Results for drawn structure

Top two results by relevance from each search type.

Substances (110,780)

1 2968499-97-8 92
2 2968499-96-7 92

Absolute stereochemistry shown. Rotation (-)

C₂₅H₂₃NO₃

1 Reference 0 Reactions 0 Suppliers

Absolute stereochemistry shown. Rotation (-)

C₂₅H₂₃NO₃

1 Reference 0 Reactions 0 Suppliers

View All Substances

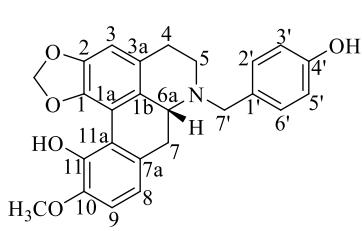
Reactions (0)

We couldn't find any results. Please update your search

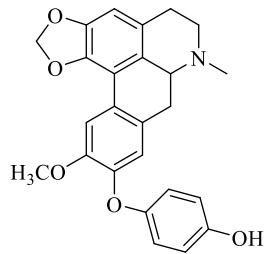
Feedback

The screenshot shows the SciFinder search results for the drawn structure of Litsine E. The search bar at the top contains the query 'Drawn Structure All Search'. The results are categorized under 'All Search Type Results for drawn structure' with a note that 'Top two results by relevance from each search type.' are shown. The first result is 'Substances (110,780)' with two entries: 2968499-97-8 and 2968499-96-7. Both entries show a chemical structure with absolute stereochemistry indicated by rotation arrows, a chemical formula C₂₅H₂₃NO₃, and links for Reference, Reactions, and Suppliers. The second result is 'Reactions (0)', which displays a message stating 'We couldn't find any results. Please update your search'. On the right side of the interface, there is a vertical sidebar with various icons for account management, notifications, and search history.

Figure S20: Scifinder search report of **1** (Litsine E)



1



Corybungine G (the most similar compound)

Table S3: ^1H (600 MHz) and ^{13}C (150 MHz) NMR data for Litsine E (**1**) in $\text{DMSO}-d_6$ and ^1H (600 MHz) and ^{13}C (150 MHz) NMR data for Corybungine G (the most similar compound) in methanol- d_4

Position	δ_{C} , type Litsine E (1)	δ_{C} , type (Corybungine G)	δ_{H} (<i>J</i> in Hz) Litsine E (1)	δ_{H} (<i>J</i> in Hz) (Corybungine G)
1	142.9, C	144.2		
1a	114.6, C	117.4		
1b	129.0, C	123.8		
2	146.5, C	149.5		
3	107.3, CH	108.1	6.64, s	6.65, s
3a	126.5, C	126.4		
4	29.3, CH_2	28.0	2.52, m 2.73, m	2.87, m 3.21, m
5	48.5, CH_2	54.1	2.20, m 2.91, m	3.46, dd (11.6, 5.4) 3.09, td (12.0, 3.2)
6a	60.5, CH	63.5	3.01, d (7.3)	3.84, m
7	35.2, CH_2	32.8	2.20, m 3.22, m	2.67, t (14.0) 3.20, m
7a	123.6, C	126.4		
8	116.2, CH	119.6	6.80, d (8.0)	6.79, s
9	122.8, CH	148.1	6.90, d (8.0)	
10	145.7, C	151.1		
11	149.7, C	113.2		7.82, s
11a	128.7, C	126.9		
10-OMe	60.2, CH_3	56.7	3.65, s	3.86, s
O-CH₂-O (1,2)	100.5, CH_2	102.7	6.04, s 5.90, s	6.15, d (1.2) 6.01, d (1.2)
1'	129.5, C	151.2		
2', 6'	130.4, CH	120.7	7.11, d (8.3)	6.83, m
3', 5'	115.4, CH	117.1	6.72, d (8.2)	6.76, m
4'	156.8, C	154.7		
7'	57.9, CH_2		3.23, m 4.11, br d (13.5)	3.23, m 4.11, br d (13.5)
N-CH₃		42.3		2.85, s

The Research method of Cell Viability Assay: The MIN6 cell line was cultured under optimal conditions until reaching the medium logarithmic growth stage. At this stage, cells were harvested and seeded at a density of 10,000 cells per well. Subsequently, 100 μ L of the cell suspension was transferred to a 96-well plate and incubated for 24 hours to allow for cell attachment and growth. On day 2, cells were treated with 300 μ M palmitic acid (PA) along with varying concentrations of the isolated compound for an additional 24 hours. On day 3, the prepared CCK-8 solution (100 μ L per well) was added to the cells. After incubation at 37°C with 5% CO₂ for 1 hour, the optical density (OD) was measured at 450 nm using an enzyme label, and cell viability was subsequently calculated.