

Supporting Information

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Eupatorione A, an Unusual Sesquiterpenoid from the Aerial Parts of *Eupatorium adenophorum*

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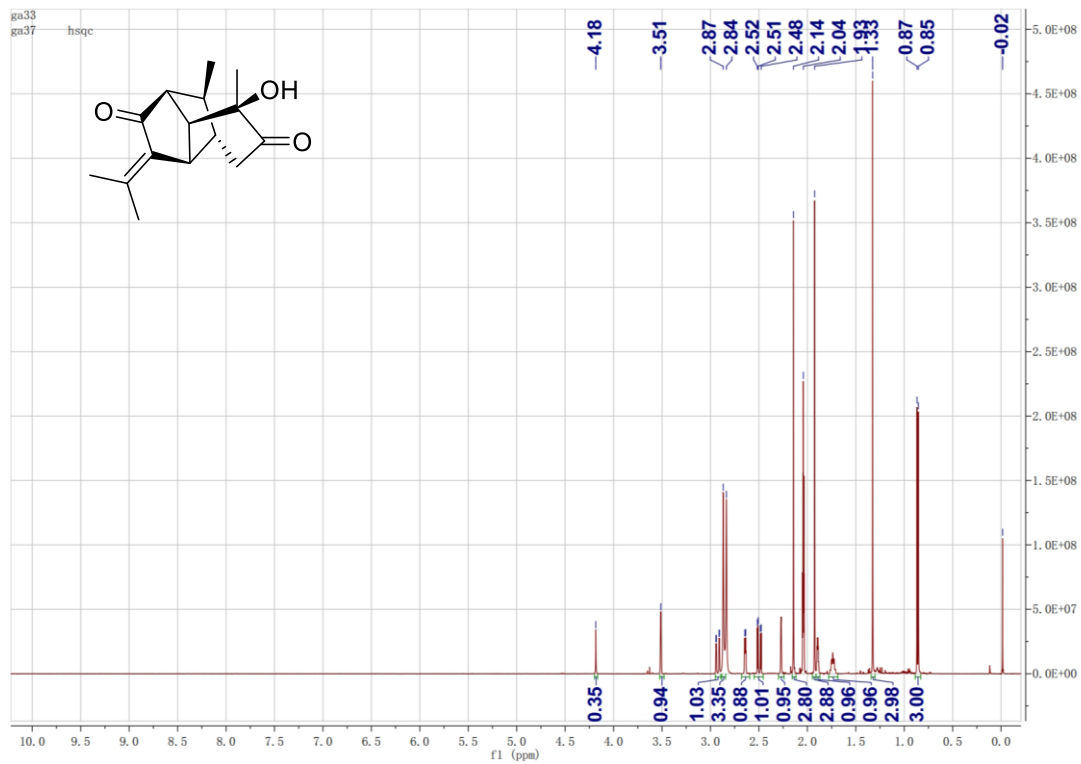


Figure S1 : ^1H NMR spectrum of compound **1** in CD_3COCD_3 (600 MHz)

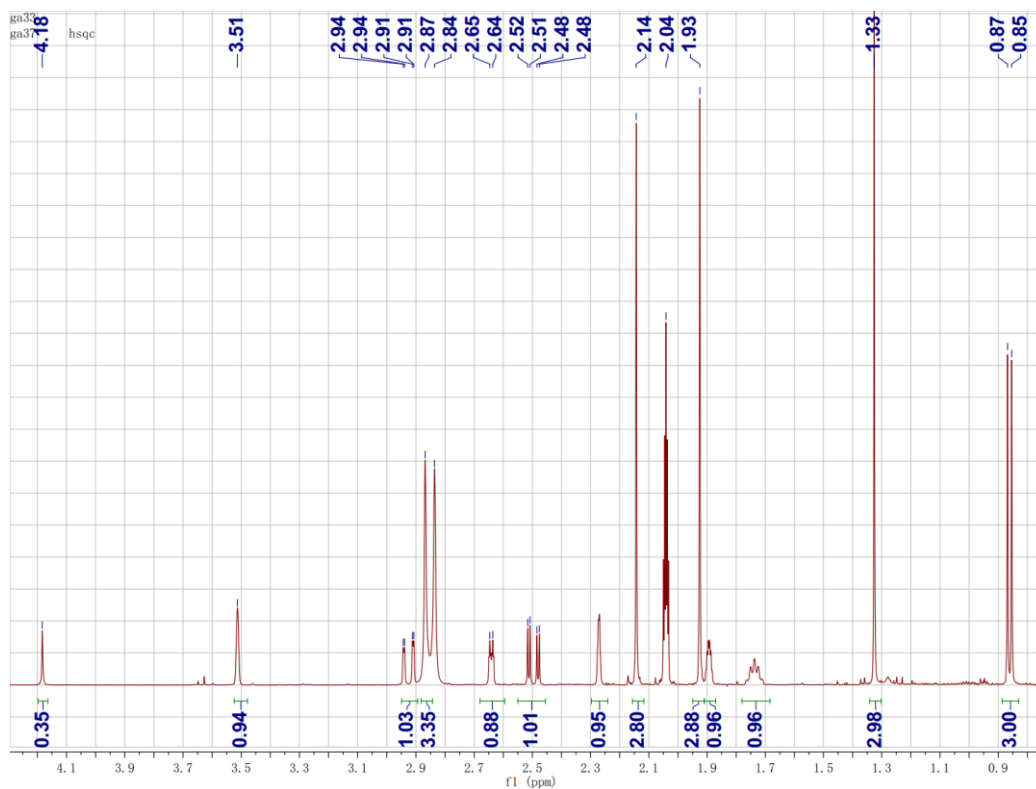


Figure S2 : Enlarge ^1H NMR spectrum of compound **1** in CD_3COCD_3 (600 MHz)

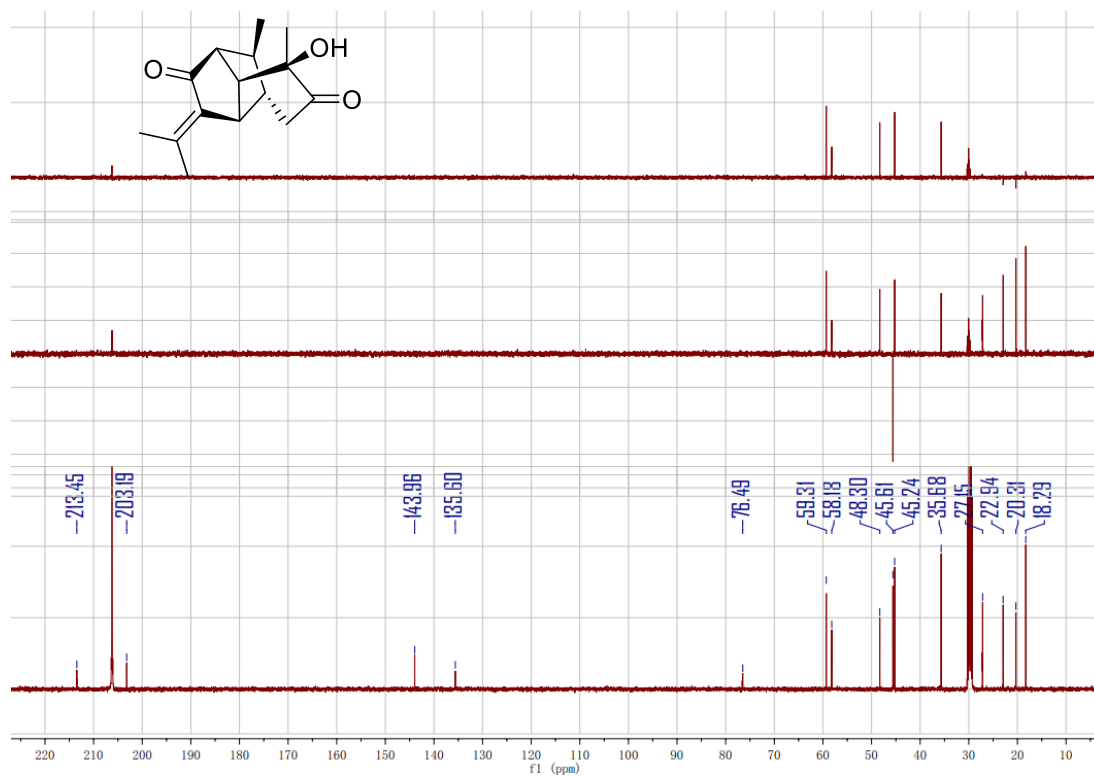


Figure S3 : ^{13}C NMR spectrum of compound **1** in CD_3COCD_3 (150 MHz)

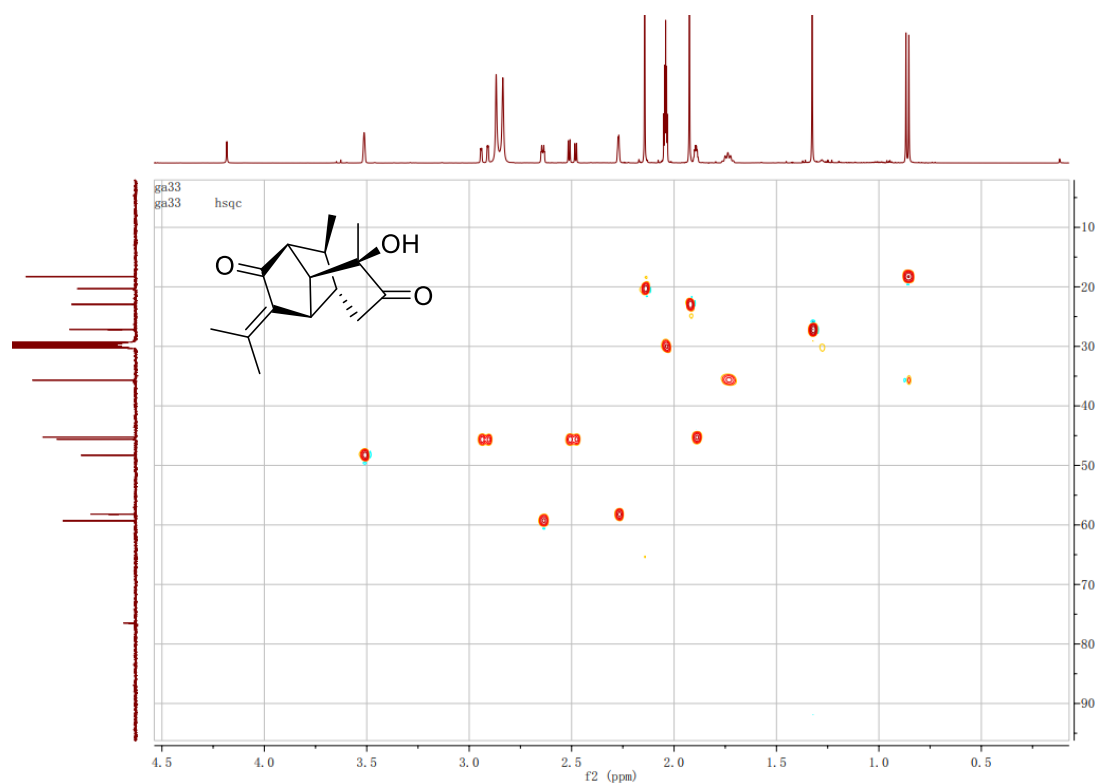


Figure S4 : HSQC spectrum of compound **1** in CD₃COCD₃ (600 MHz)

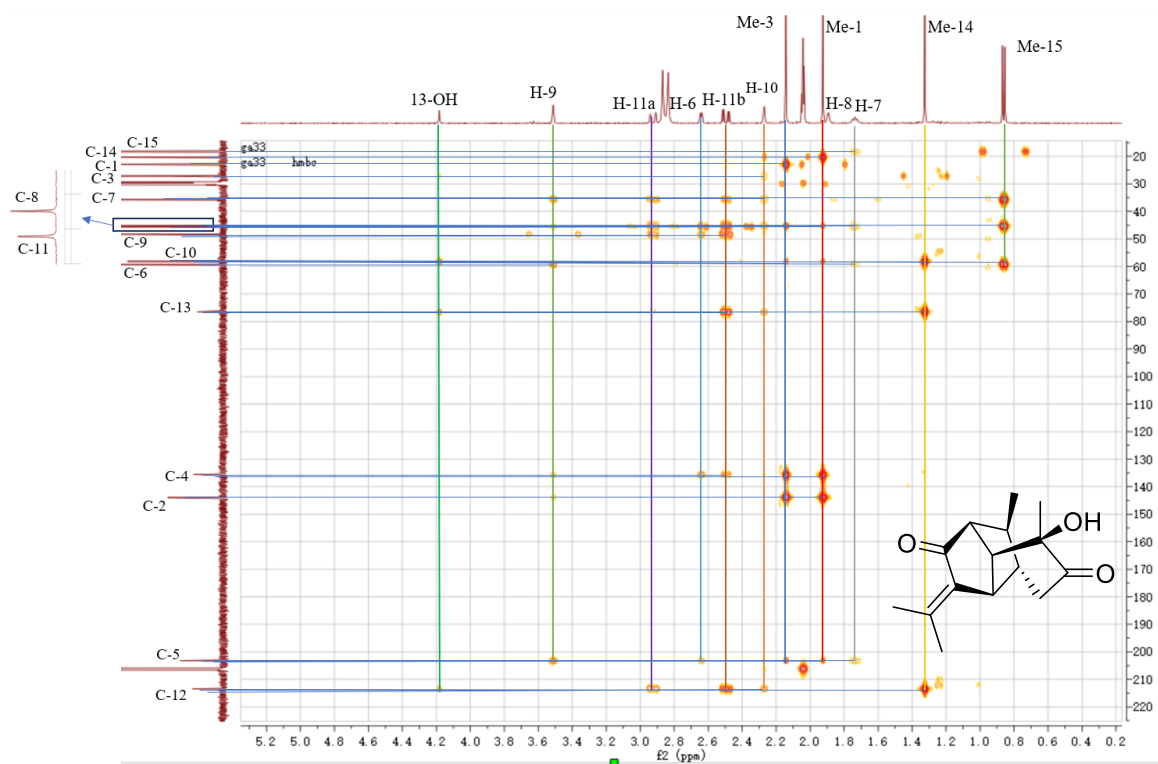


Figure S5 : HMBC spectrum of compound **1** in CD₃COCD₃ (600 MHz)

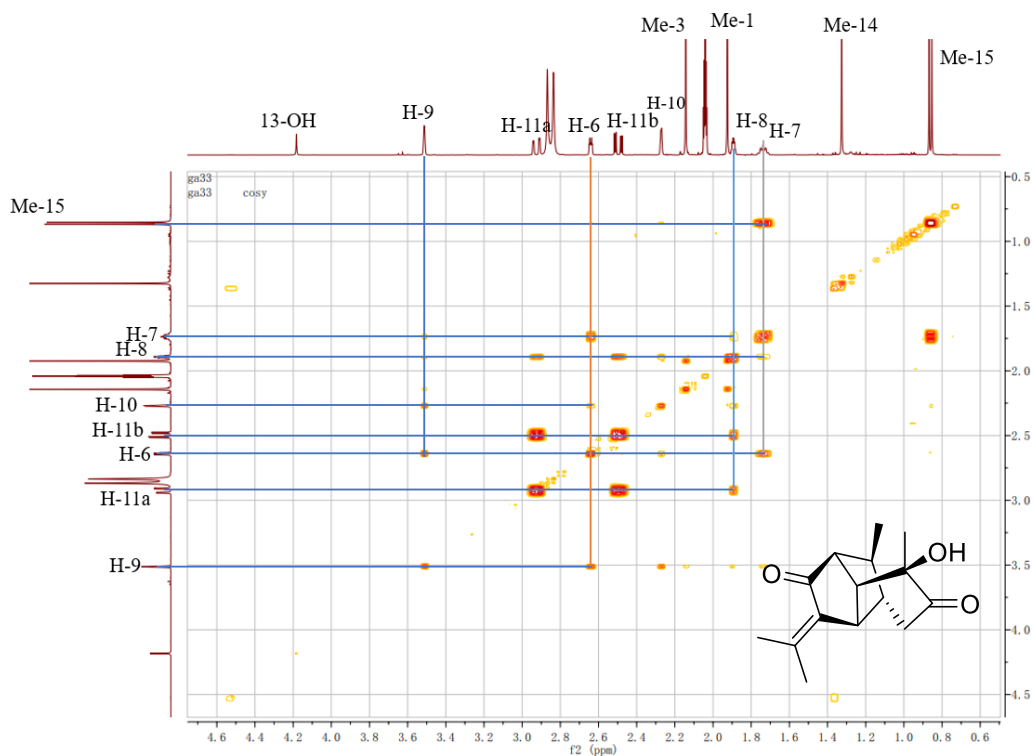


Figure S6 : ^1H - ^1H COSY spectrum of compound **1** in CD_3COCD_3 (600 MHz)

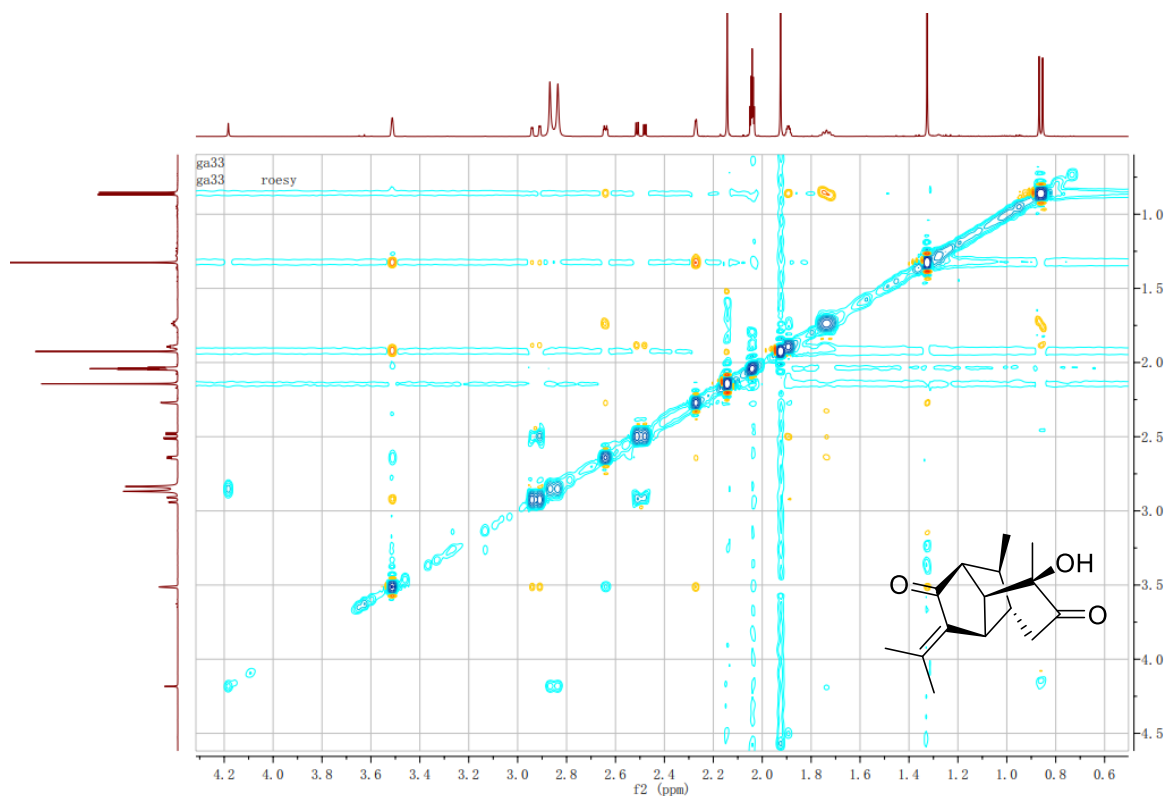


Figure S7 : ROESY spectrum of compound **1** in CD_3COCD_3 (600 MHz)

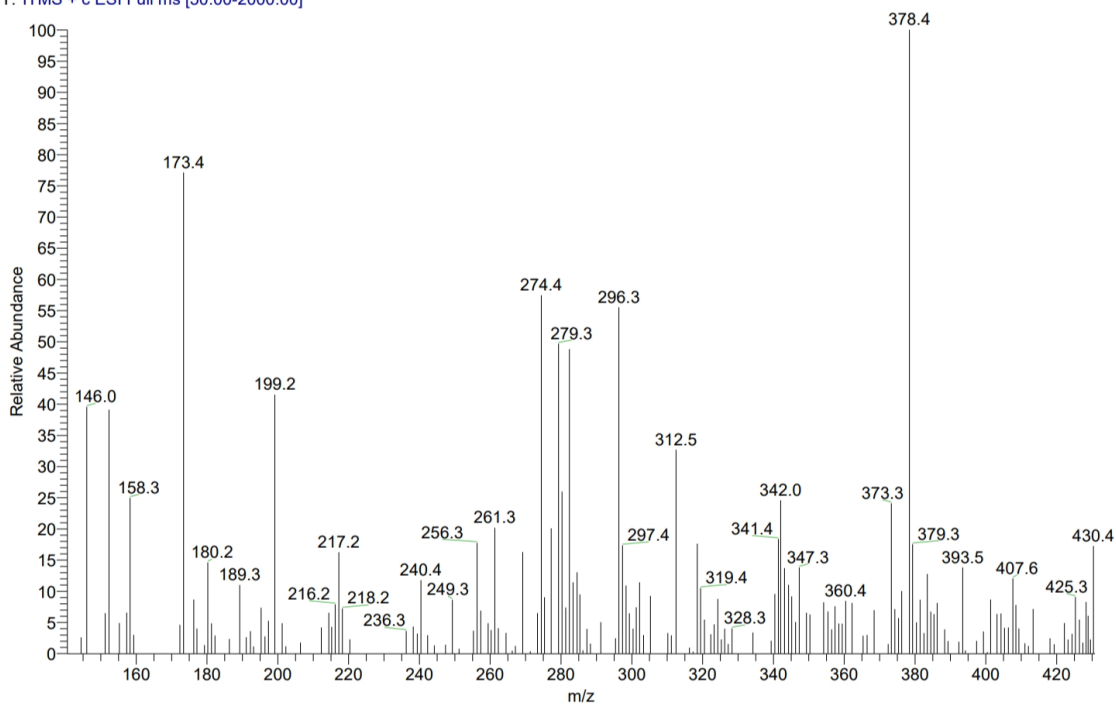
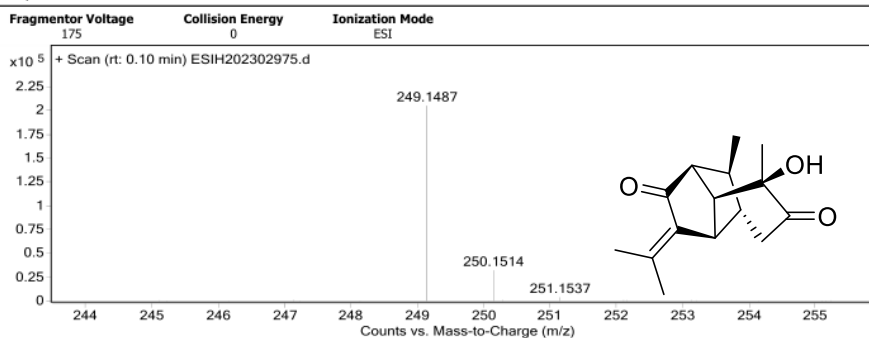


Figure S8 : MS spectrum of compound 1

Qualitative Analysis Report

Data Filename	ESIH202302975.d	Sample Name	A8-A8-Ga-3-3
Sample ID		Position	P1-A1
Instrument Name	Agilent 6520 Q-TOF	Acq Method	20160322_MS_ESIH_POS_1min.m
Acquired Time	5/5/2023 13:20:26	IRM Calibration Status	Success
DA Method	small molecular data analysis method.m	Comment	ESIH by fangsu

User Spectra



Formula Calculator Results

m/z	Calc m/z	Diff (mDa)	Diff (ppm)	Ion Formula	Ion
249.1487	249.1485	-0.16	-0.63	C15 H21 O3	(M+H) ⁺

--- End Of Report ---

Figure S9 : HRESIMS spectrum of compound 1

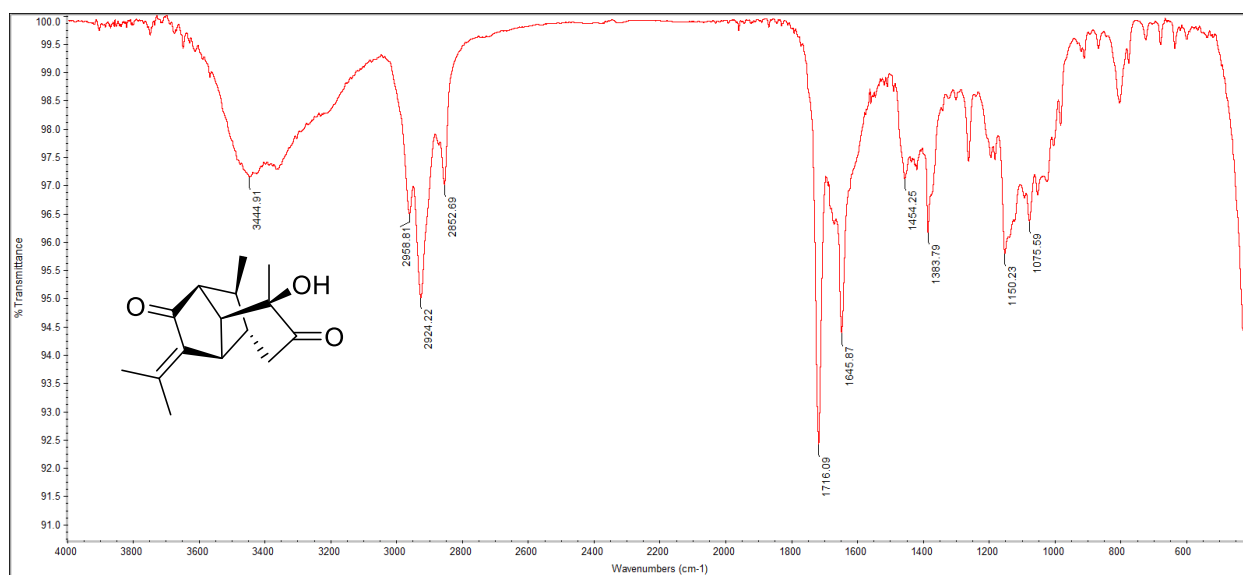
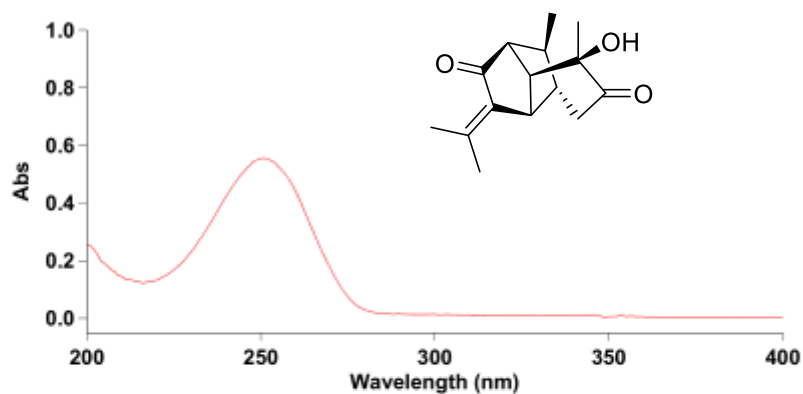


Figure S10: IR spectrum of compound 1



Scan Analysis Report

Report Time : Sun 07 May 09:44:14 AM 2023
Method:
Batch: D:\gyw\jy\ga-3-3.DSW
Software version: 4.20(470)
Operator:

Sample Name: ga-3-3

Collection Time 5/7/2023 9:44:16 AM

Peak Table
Peak Style Peaks
Peak Threshold 0.0100
Range 400.00nm to 200.00nm

Wavelength (nm)	Abs
251.00	0.554

Figure S11 : UV spectrum of compound 1

Initiating Search

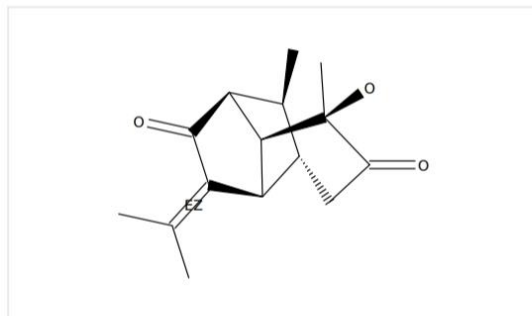
August 9, 2023, 9:40PM

Substances:

Filtered By:

Similarity: 90-94

Number of Components: 1



Structure Match: Similarity

Search Tasks

Task	Search Type	View
Exported: Returned Substance Results + Filters (2)	Substances	View Results

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Structure Match

As Drawn (0)

Substructure (0)

Similarity (36K)

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

Filtering: Similarity: 90-94 X Number of Components: 1 X

2 Selected 2 Results

1 91

2129128-77-2

Absolute stereochemistry shown

C₁₅H₂₀O₂
3,7-Methano-1*H*-indene-2,5(3*H*,4*H*)-dione, tetrahydro-4,8-dimethyl-1-(1-methylethyl...

1 Reference 0 Reactions 0 Suppliers

2 91

1616703-98-0

C₁₅H₂₀O₂
Hexahydro-7,8-dimethyl-3-(1-methylethylidene)-1,4-methano-1*H*-indene-2,6-dione

1 Reference 0 Reactions 0 Suppliers

Figure S12 : The Scifinder similarity report for 1

Table S1 : Crystal data for 1

Identification code	cu_2023603_0m
Empirical formula	C ₁₅ H ₂₀ O ₃
Formula weight	248.31
Temperature/K	100
Crystal system	monoclinic
Space group	P2 ₁
a/Å	7.0436(5)
b/Å	7.0873(5)
c/Å	13.7049(10)
α/°	90
β/°	96.271(4)
γ/°	90
Volume/Å ³	680.06(8)
Z	2
ρ _{calc} /cm ³	1.213
μ/mm ⁻¹	0.669
F(000)	268.0
Crystal size/mm ³	0.11 × 0.03 × 0.01
Radiation	CuKα (λ = 1.54178)
2θ range for data collection/°	6.488 to 148.928
Index ranges	-7 ≤ h ≤ 8, -8 ≤ k ≤ 8, -16 ≤ l ≤ 17
Reflections collected	12254
Independent reflections	2765 [R _{int} = 0.1181, R _{sigma} = 0.1109]
Data/restraints/parameters	2765/1/168
Goodness-of-fit on F ²	1.086
Final R indexes [I ≥ 2σ (I)]	R ₁ = 0.0831, wR ₂ = 0.2137
Final R indexes [all data]	R ₁ = 0.0874, wR ₂ = 0.2189
Largest diff. peak/hole / e Å ⁻³	0.56/-0.34
Flack parameter	-0.3(2)