

Supporting Information

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Identification of Diverse Sesquiterpenoids from *Eupatorium adenophorum*

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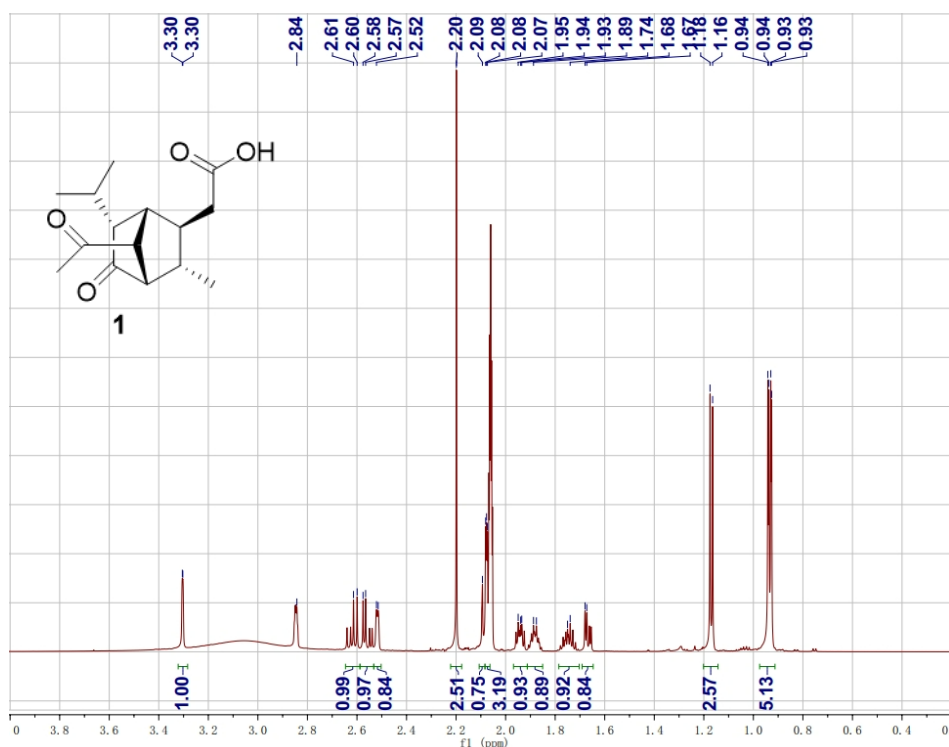


Figure S1: ^1H NMR spectrum of compound 1 in CD_3COCD_3 (600 MHz)

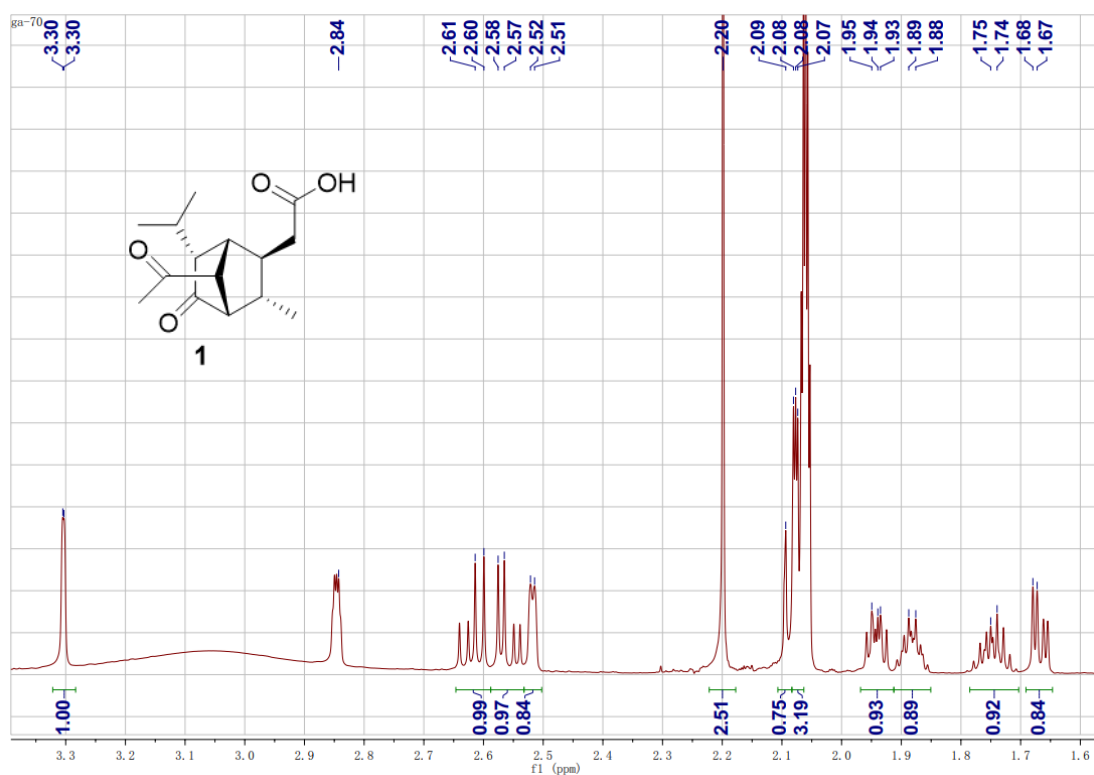


Figure S2: Expanded ^1H -NMR spectrum of compound 1

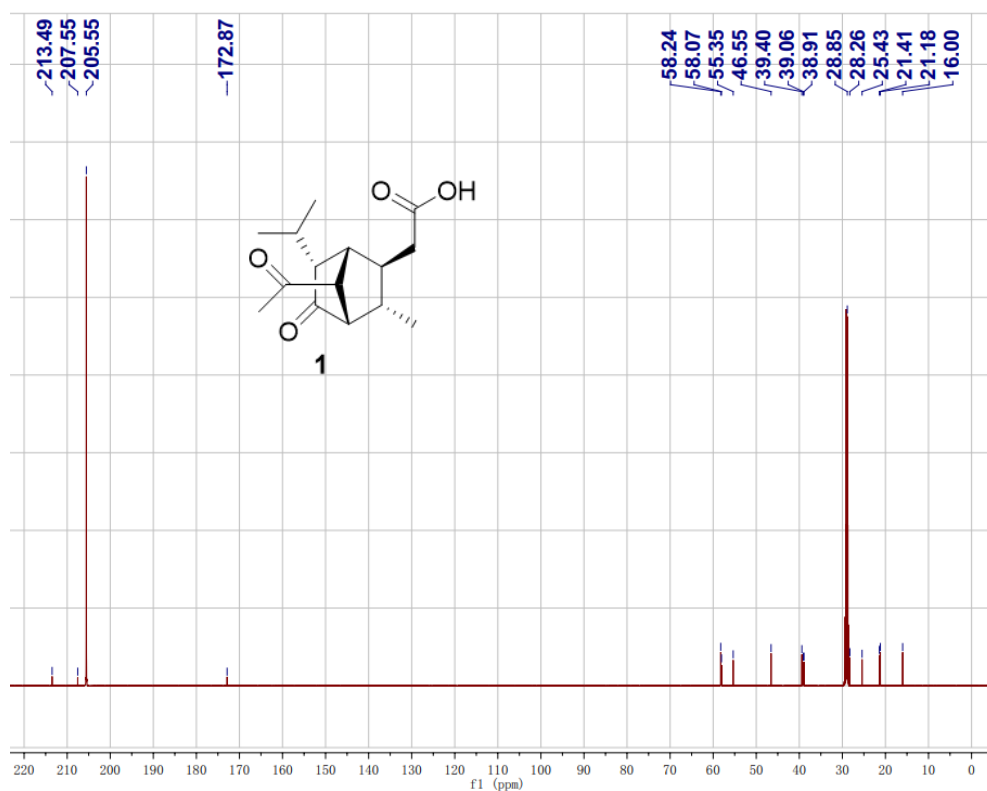


Figure S3: ¹³C NMR spectrum of compound 1 in CD₃COCD₃ (150 MHz)

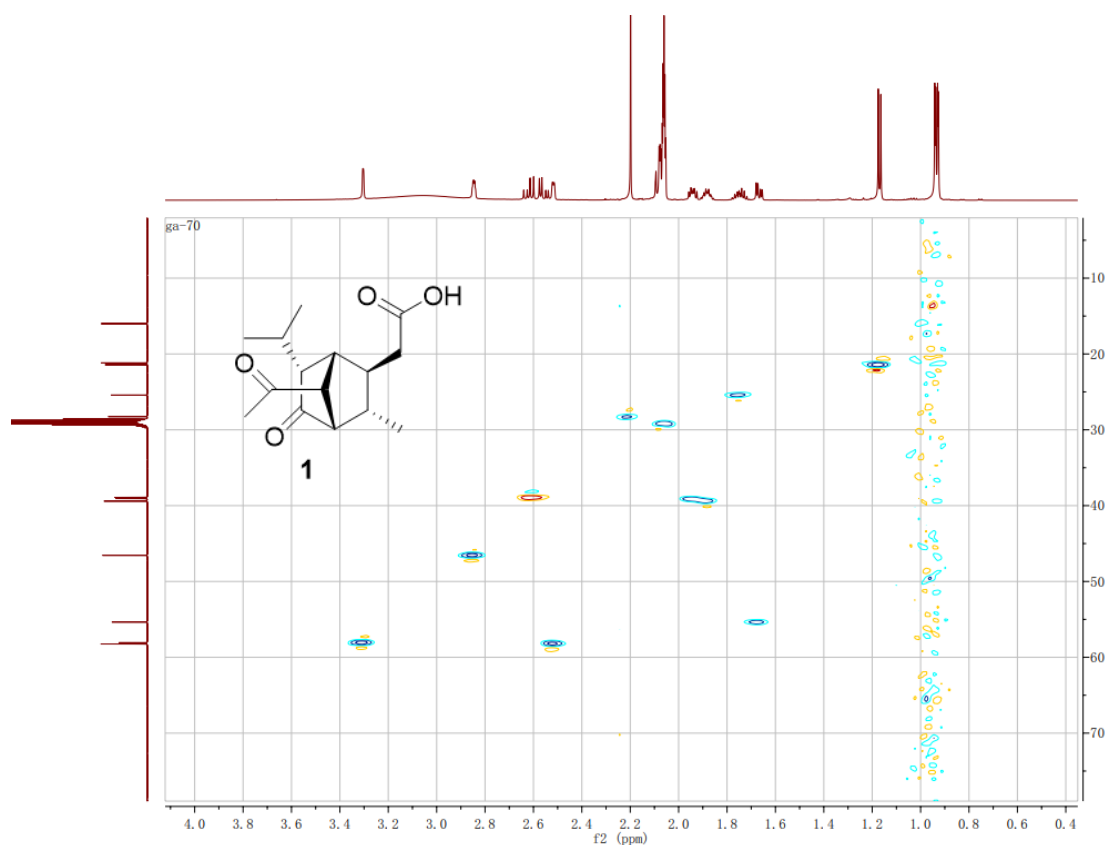


Figure S4: HSQC spectrum of compound 1 in CD₃COCD₃ (600 MHz)

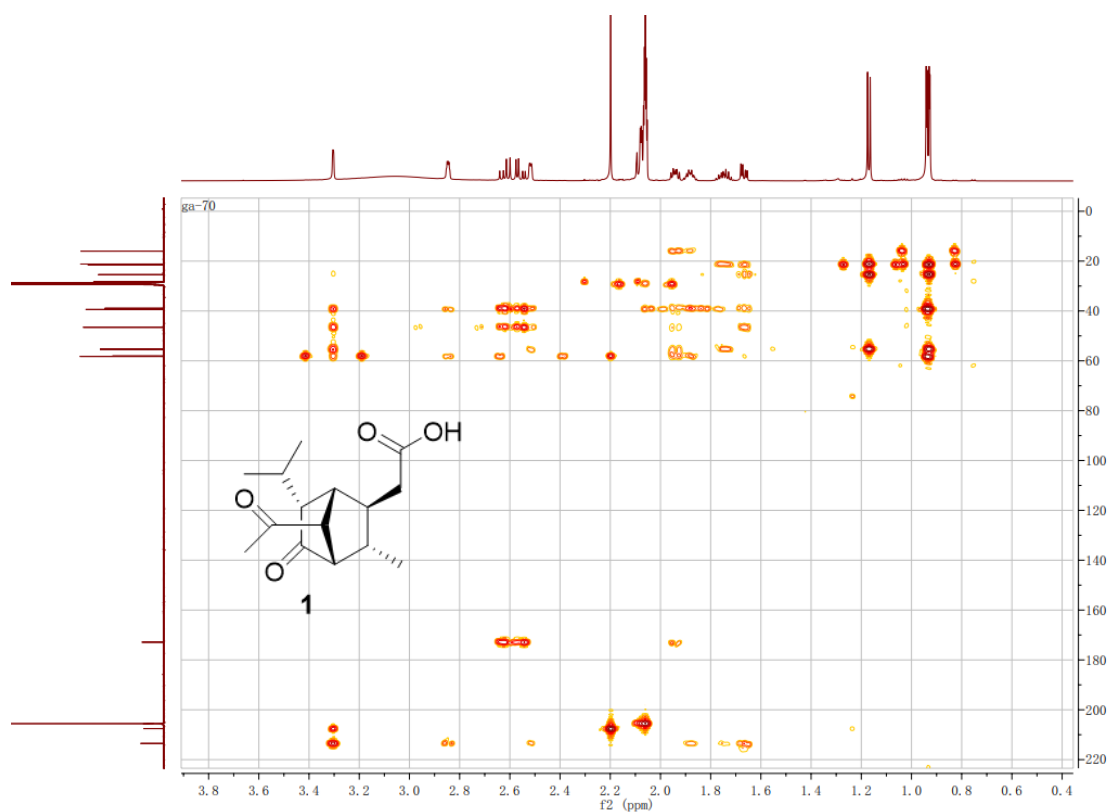


Figure S5: HMBC spectrum of compound **1** in CD_3COCD_3 (600 MHz)

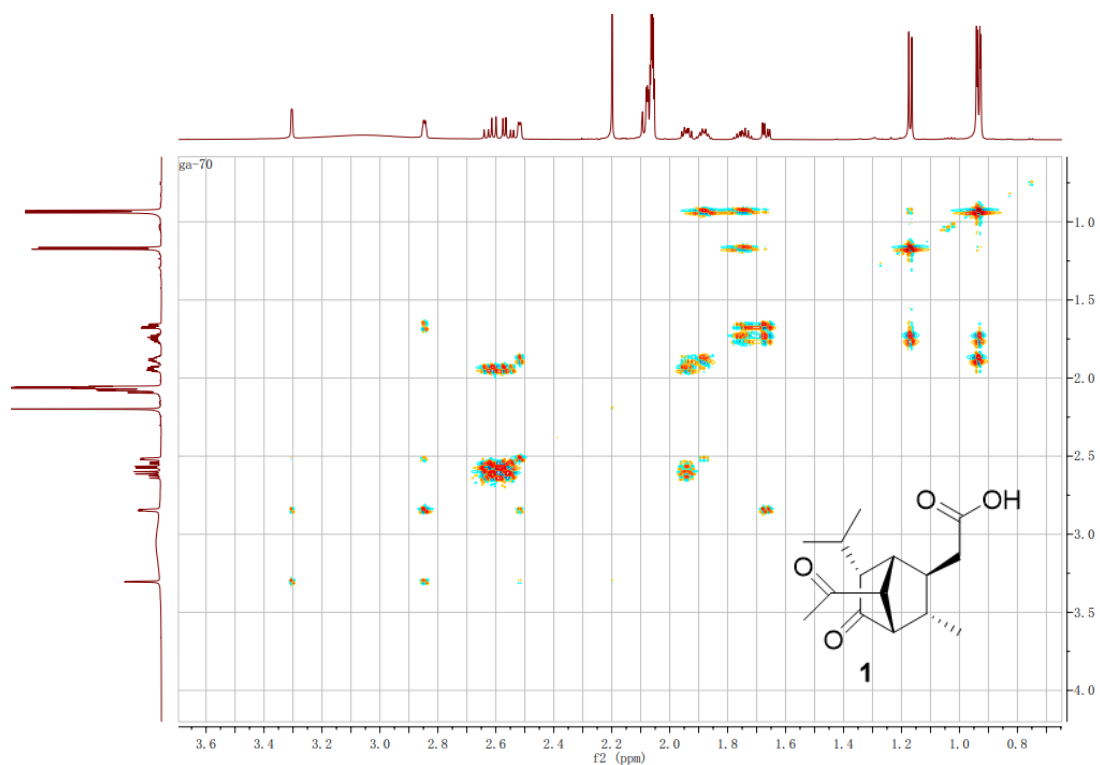


Figure S6: ^1H - ^1H COSY spectrum of compound **1** in CD_3COCD_3 (600 MHz)

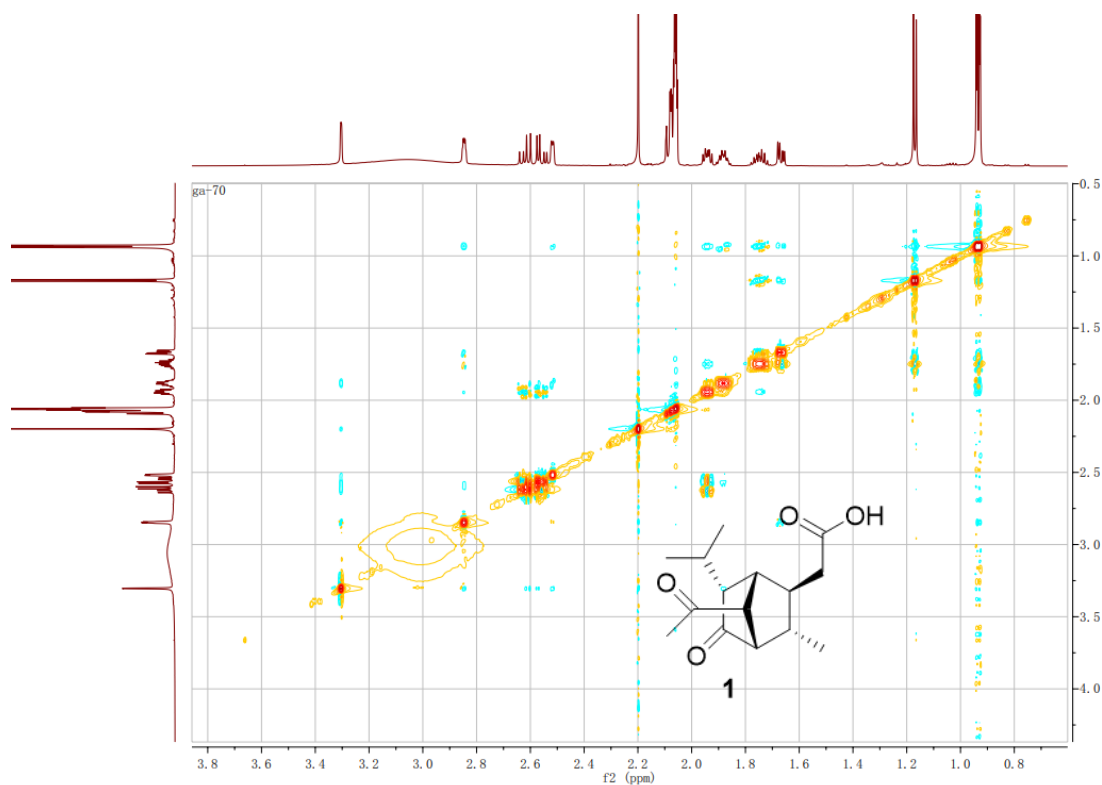
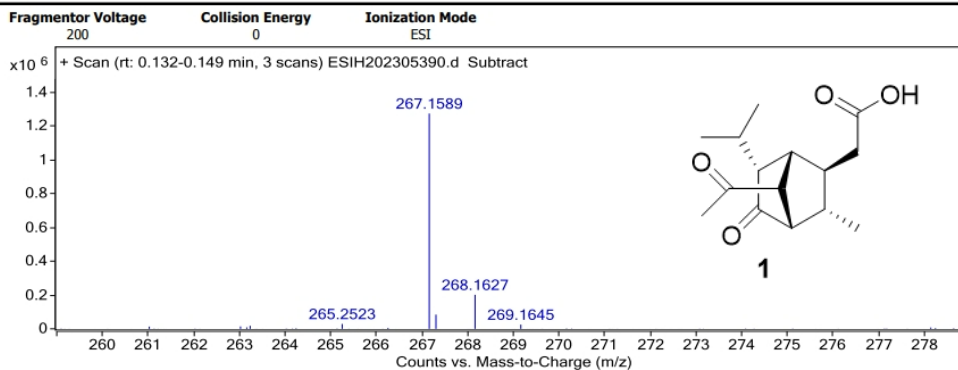


Figure S7: ROESY spectrum of compound **1** in CD₃COCD₃ (600 MHz)

Qualitative Analysis Report

Data Filename	ESI202305390.d	Sample Name	G5-ga-51
Sample ID		Position	P1-A3
Instrument Name	Agilent 6520 Q-TOF	Acq Method	20160322_MS_ESIH_POS_1min.m
Acquired Time	9/13/2023 10:39:57	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
267.1589	267.1591	0.22	0.82	C ₁₅ H ₂₃ O ₄	(M+H) ⁺

--- End Of Report ---

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

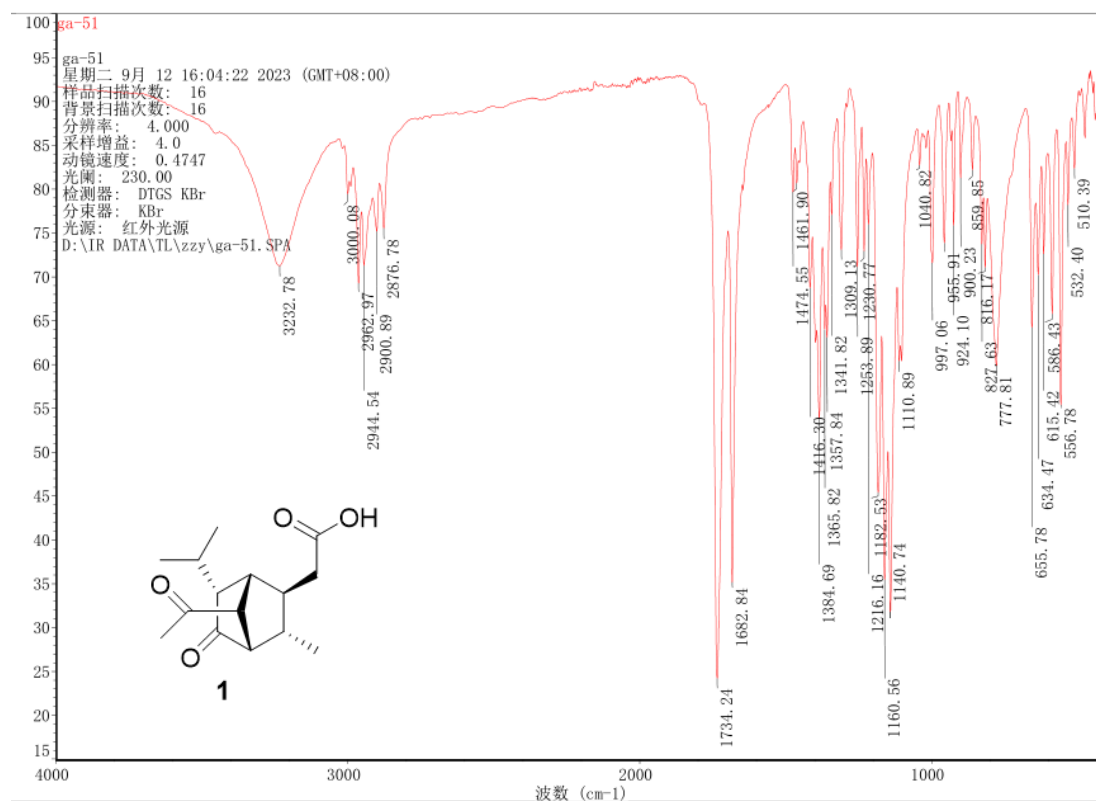


Figure S9: IR spectrum of compound **1**

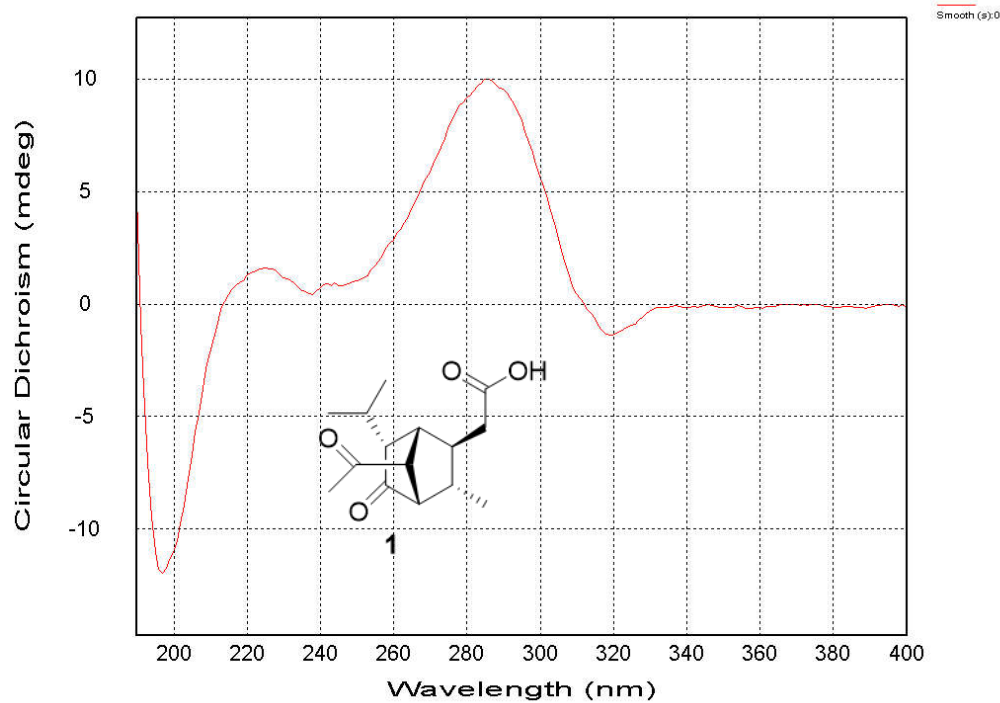


Figure S10: Experimental CD spectrum of **1**

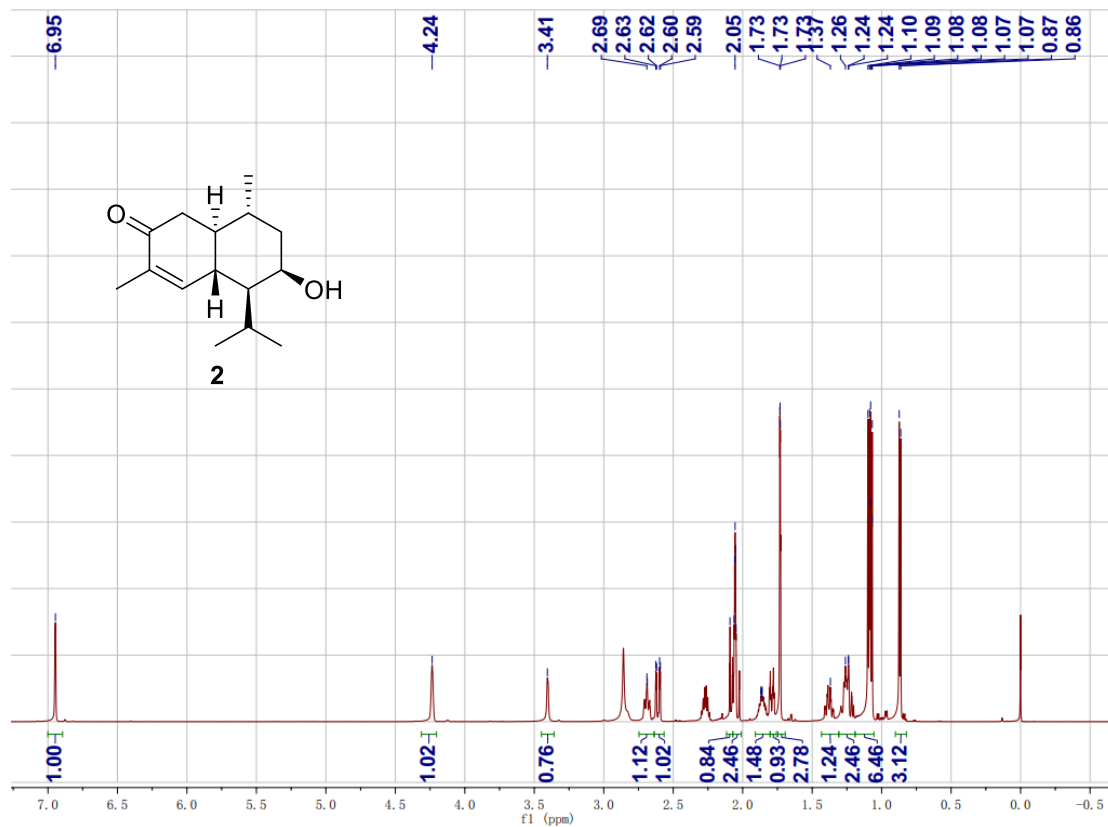


Figure S11: ¹H NMR spectrum of compound 2 in CD₃COCD₃ (600 MHz)

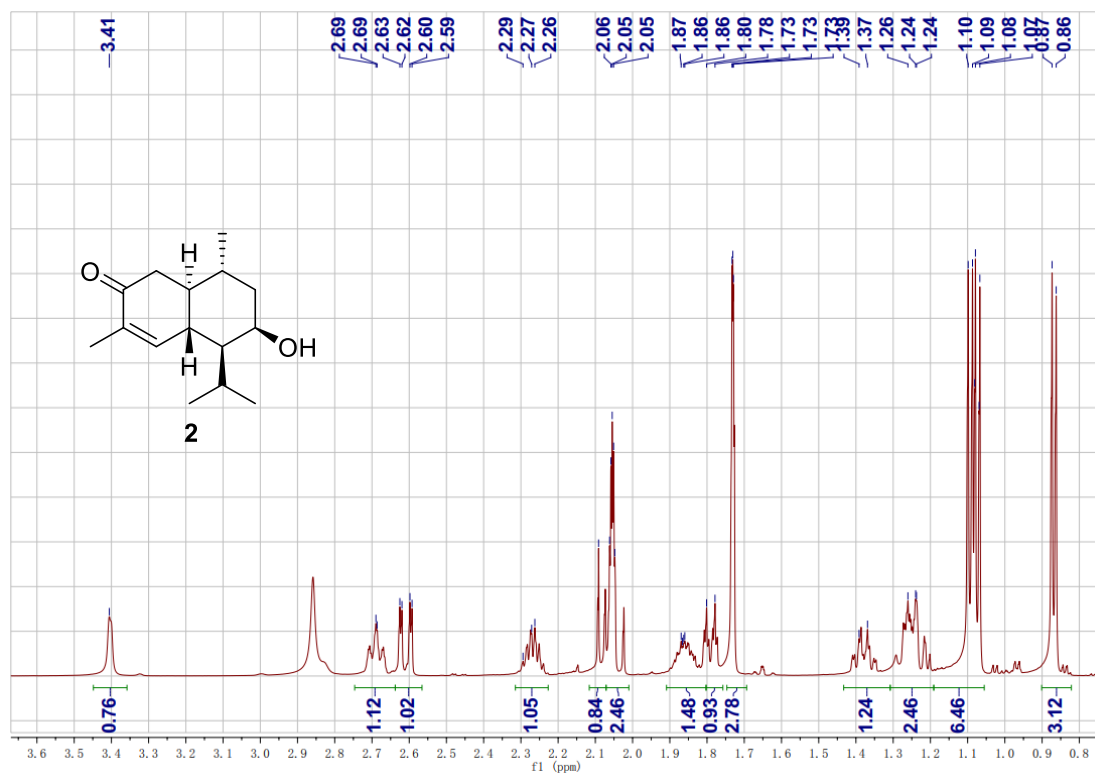


Figure S12: Expanded ¹H-NMR spectrum of compound 2.

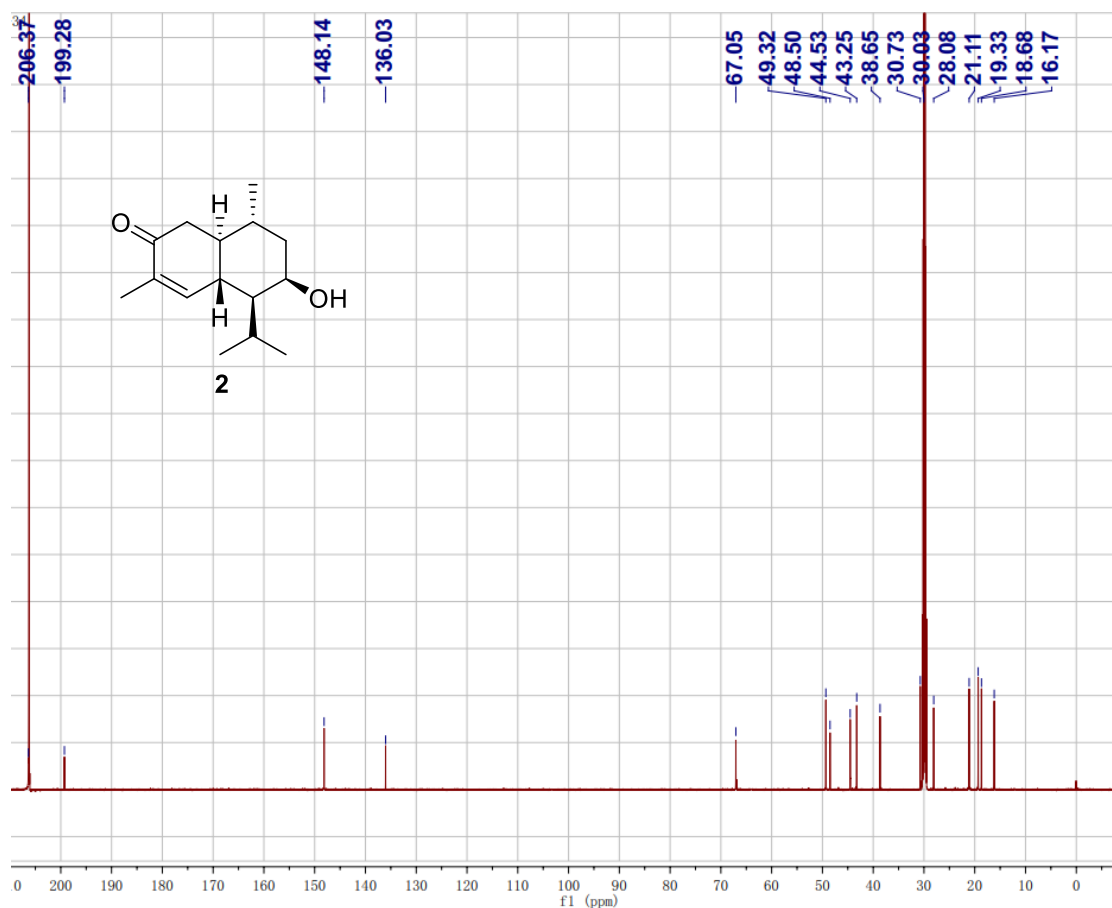


Figure S13: ¹³C NMR spectrum of compound 2 in CD₃COCD₃ (150 MHz)

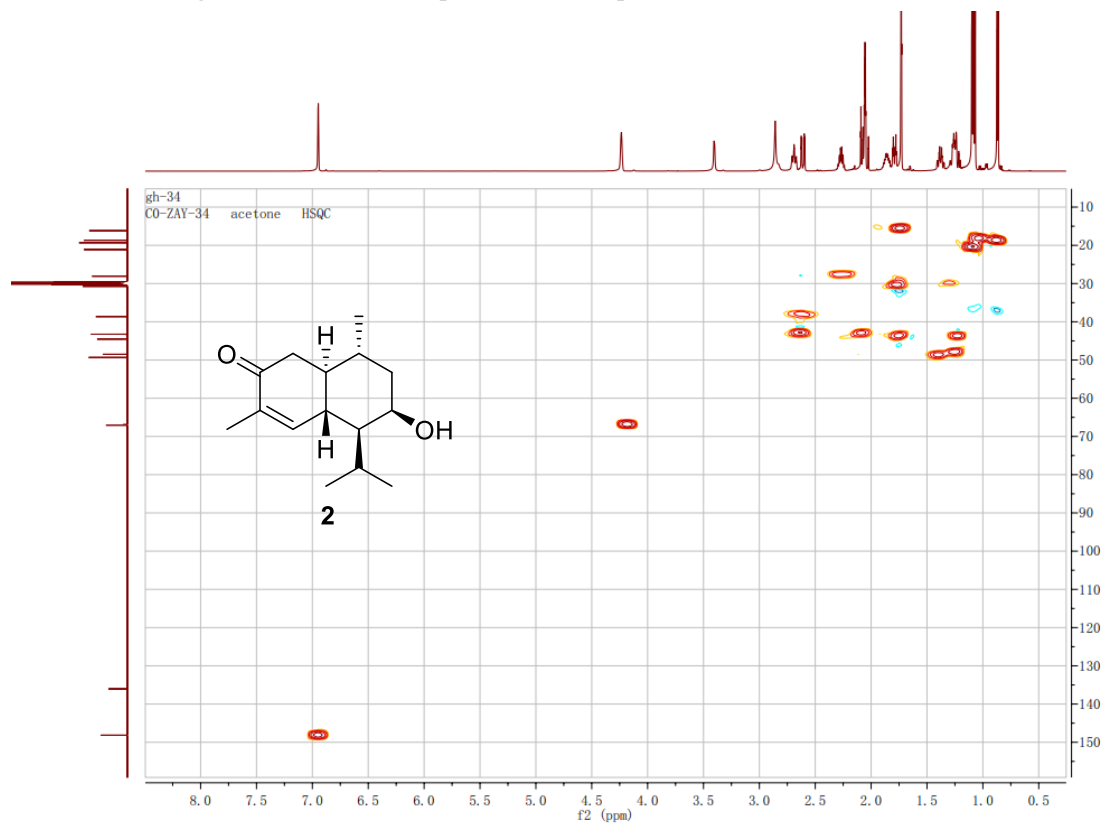


Figure S14: HSQC spectrum of compound **2** in CD₃COCD₃ (600 MHz)

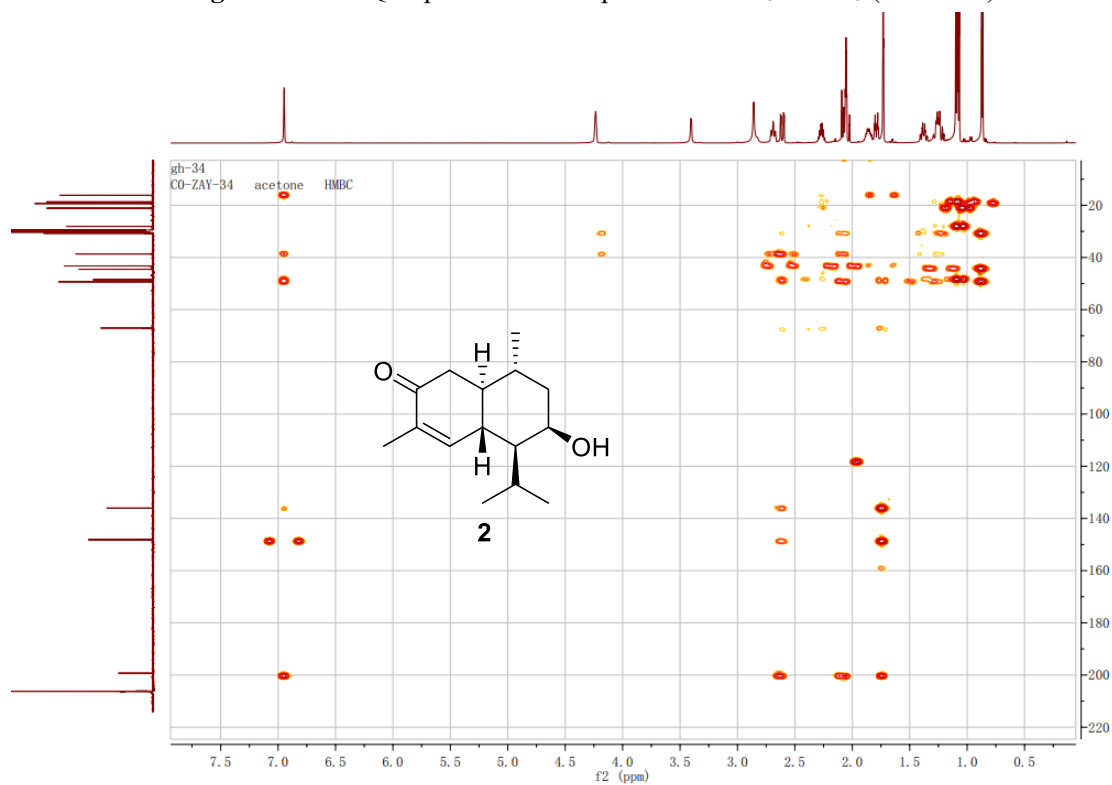


Figure S15: HMBC spectrum of compound **2** in CD₃COCD₃ (600 MHz)

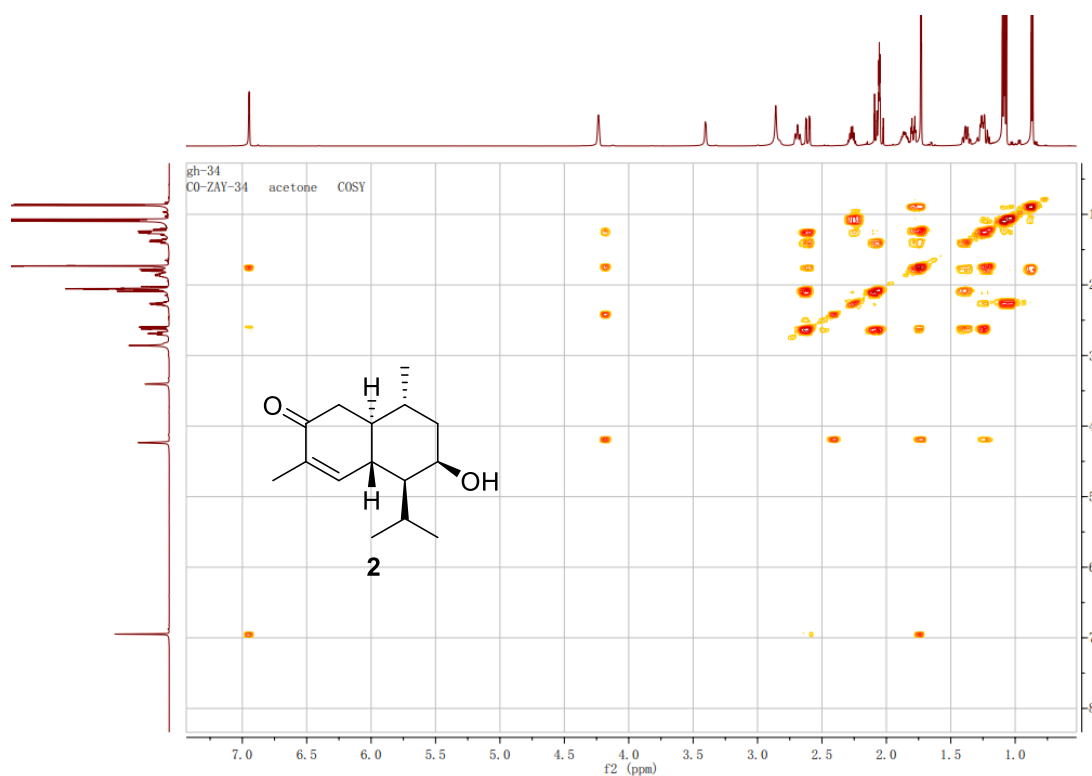


Figure S16: ¹H-¹H COSY spectrum of compound **2** in CD₃COCD₃ (600 MHz)

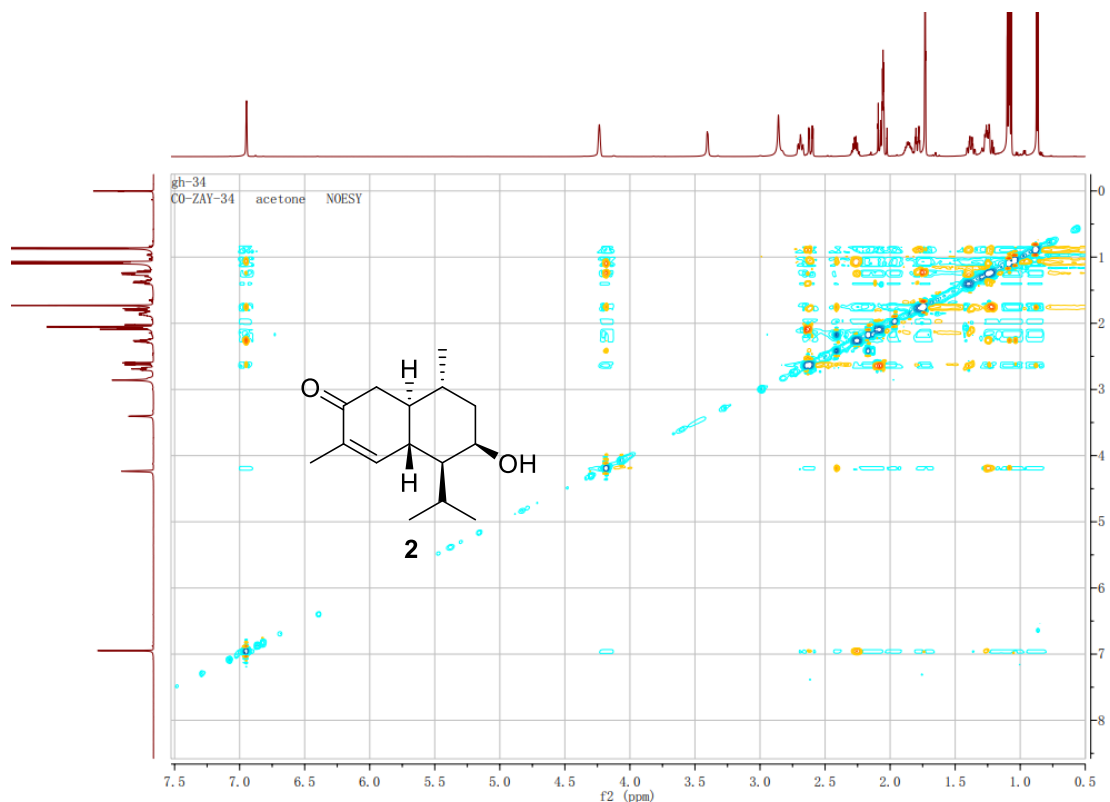
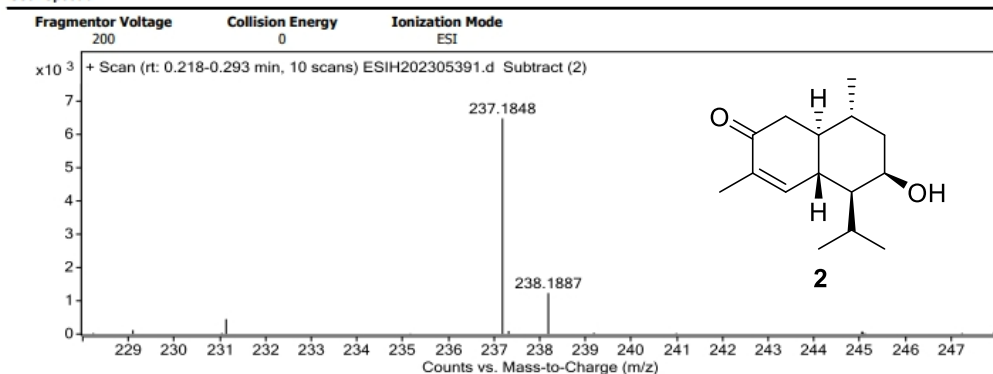


Figure S17: ROESY spectrum of compound **2** in CD₃COCD₃ (600 MHz)

Qualitative Analysis Report

Data Filename	ESIH202305391.d	Sample Name	G5-ga-34
Sample ID		Position	P1-A4
Instrument Name	Agilent 6520 Q-TOF	Acq Method	20160322_MS_ESIH_POS_1min.m
Acquired Time	9/13/2023 10:41:28	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
237.1848	237.1849	0.12	0.51	C15 H25 O2	(M+H) ⁺

--- End Of Report ---

Figure S18: HRESIMS spectrum of compound **2**

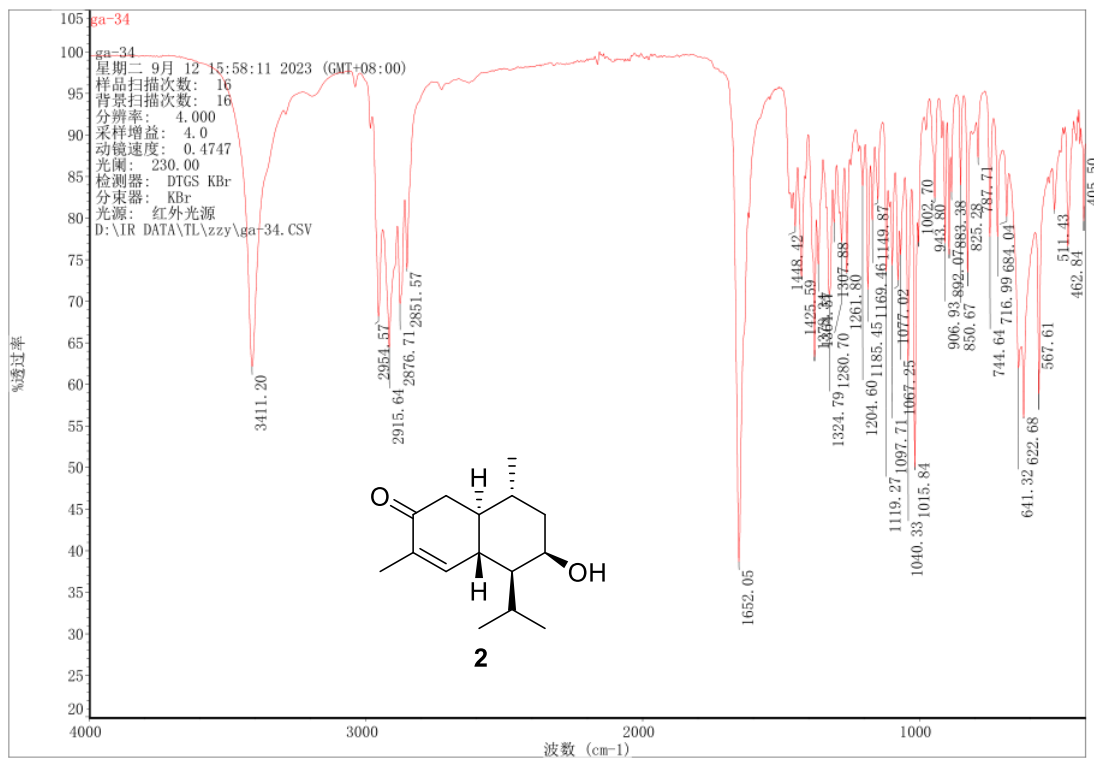


Figure S19: IR spectrum of compound **2**

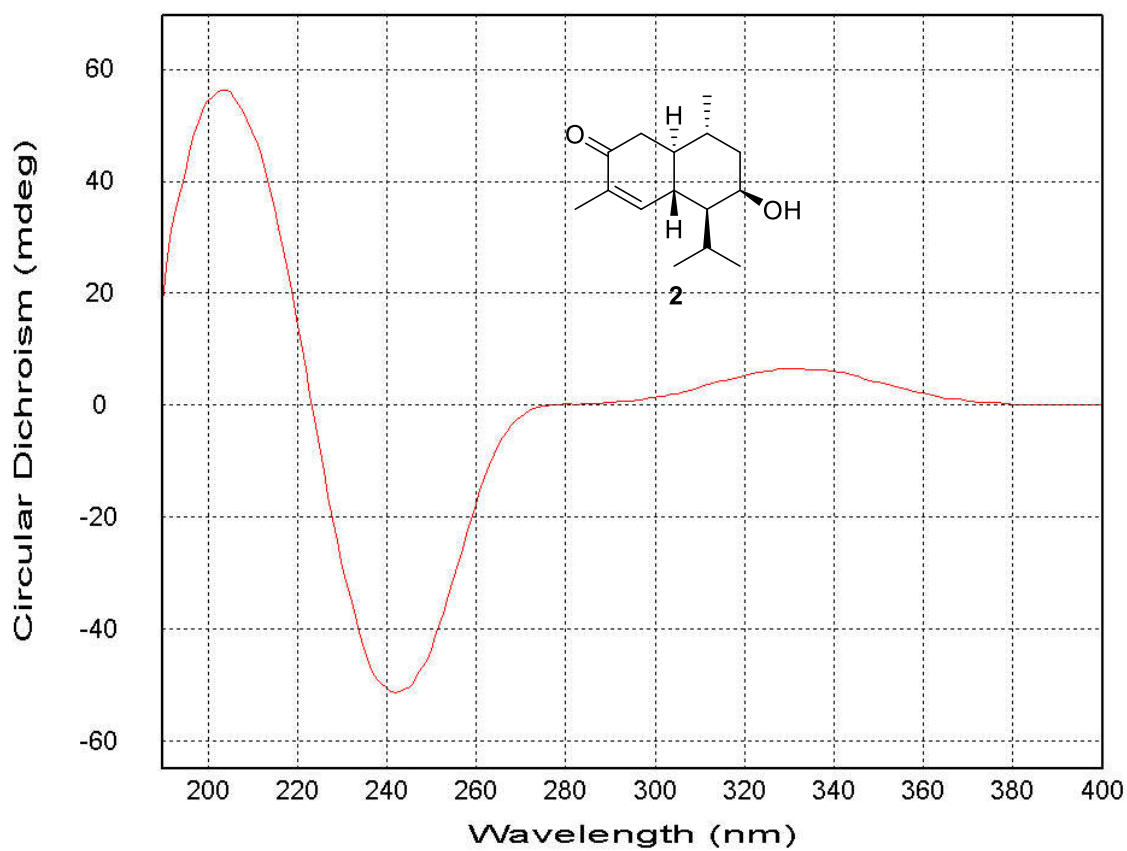


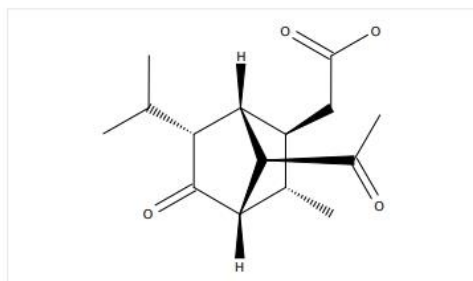
Figure S20: Experimental CD spectrum of **2**

Initiating Search

January 9, 2024, 5:45PM

Substances:

Filtered By:

Structure Match: **Substructure**

Search Tasks

Task	Search Type	View
Exported: Returned Substance Results + Filters (0)	Substances	View Results

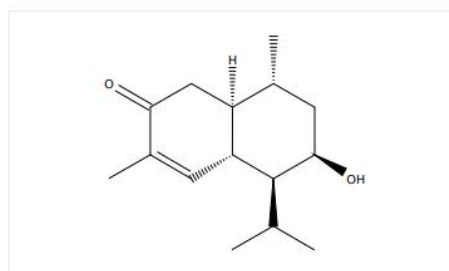
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Initiating Search

January 9, 2024, 5:48PM

Substances:

Filtered By:

Structure Match: **Substructure**

Search Tasks

Task	Search Type	View
Exported: Returned Substance Results + Filters (17)	Substances	View Results

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Figure S21. Scifinder search report of the new compounds **1** and **2**



1r

Table S1: The comparison ^{13}C NMR data of the new compounds **1-2** and the most similar compounds.

No.	1^a	Eupatorid A^a	2^a	3^a
	δ_{C} , type	δ_{C} , type	δ_{C} , type	δ_{C} , type
1	58.2, d	59.6, d	43.1, t	43.0, t
2	213.4, s	202.3, s	199.2, s	198.7, s
3	55.1, d	134.7, s	136.0, s	131.9, s
4	39.0, d	49.7, d	148.1, d	147.8, d
5	45.5, d	47.5, d	38.6, d	38.1, d
6	39.4, d	39.2, d	48.4, t	46.5, d
7	58.0, d	59.2, d	67.0, d	66.4, d
8	16.0, q	17.5, q	44.4, t	43.8, t
9	25.4, d	143.1, s	30.6, d	25.5, d
10	21.4, q	20.0, q	49.3, d	52.4, d
11	21.1, q	22.9, q	16.1, q	15.8, q
12	207.5, s	207.2, s	28.1, d	23.5, d
13	28.9, q	28.9, q	21.0, q	21.0, q
14	38.9, t	39.3, t	18.5, q	19.1, q
15	172.8, s	173.4, s	19.3, q	20.6, q

a): The ^{13}C NMR data of all compounds were recorded at 150 MHz, with $(\text{CD}_3)_2\text{CO}$ as solvent.