Supporting Information

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Identification of Diverse Sesquiterpenoids from *Eupatorium adenophorum*

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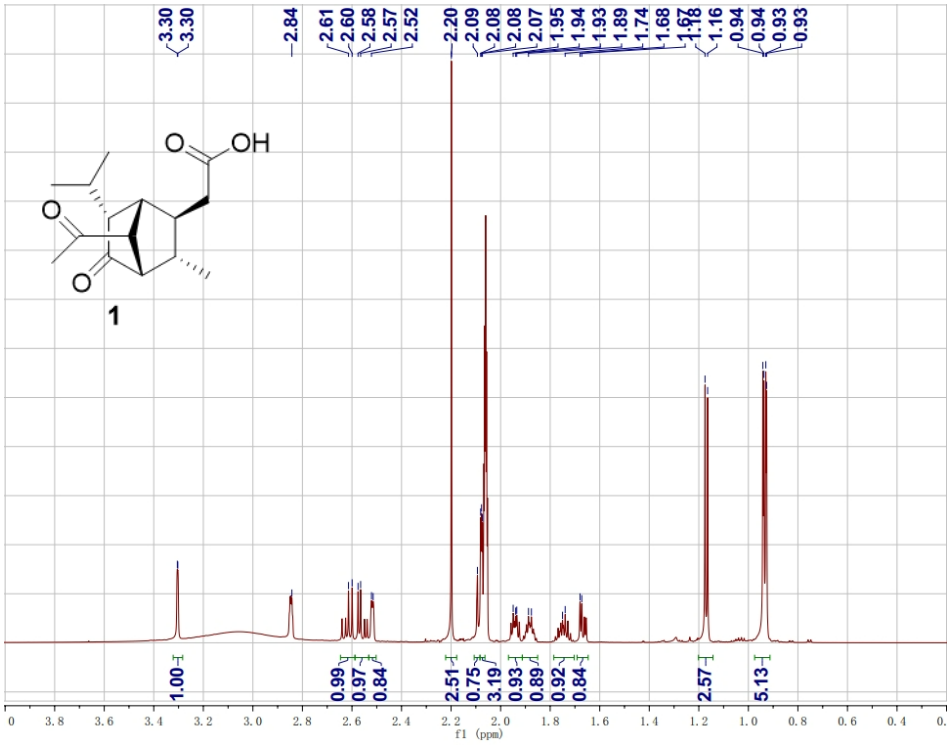

Figure S1: ^{1}H NMR spectrum of compound **1** in CD_3COCD_3 (600 MHz)

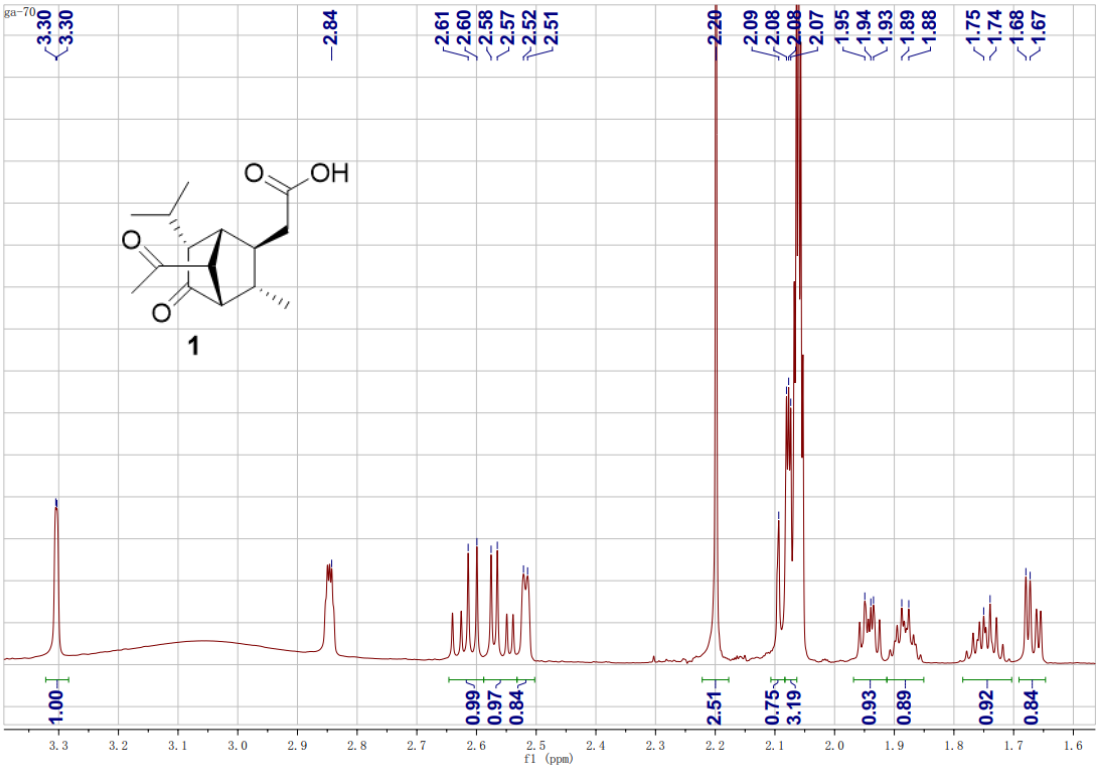

Figure S2: Expanded ^{1}H-NMR spectrum of compound **1**

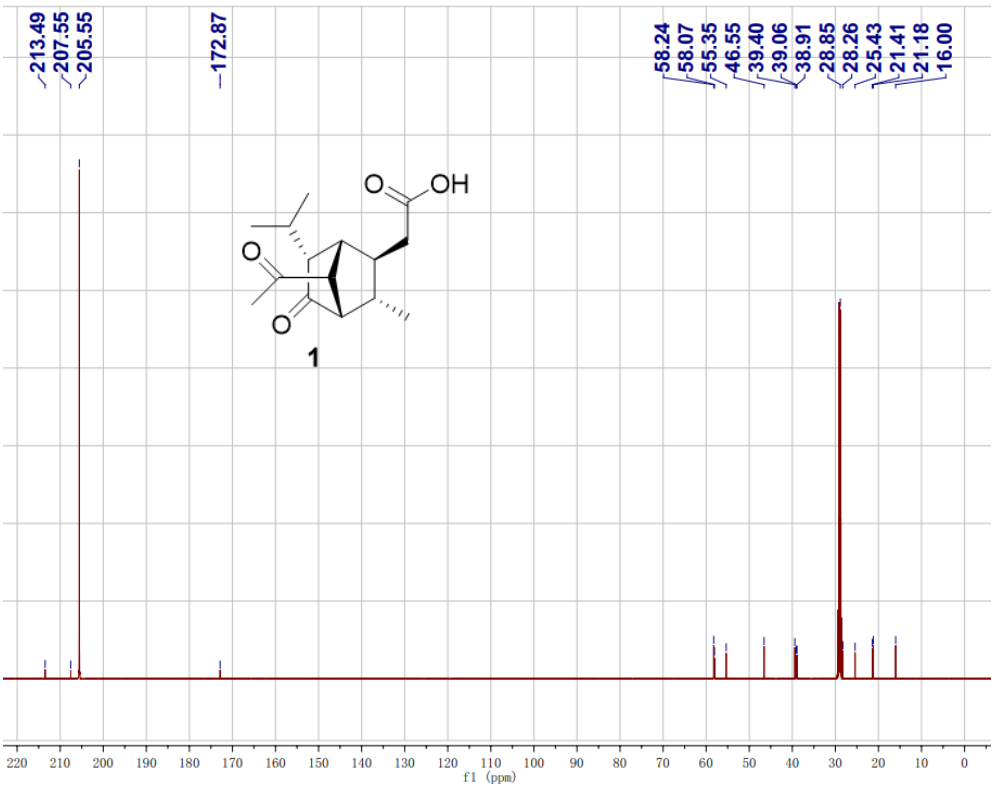

Figure S3: ^{13}C NMR spectrum of compound **1** in CD_3COCD_3 (150 MHz)

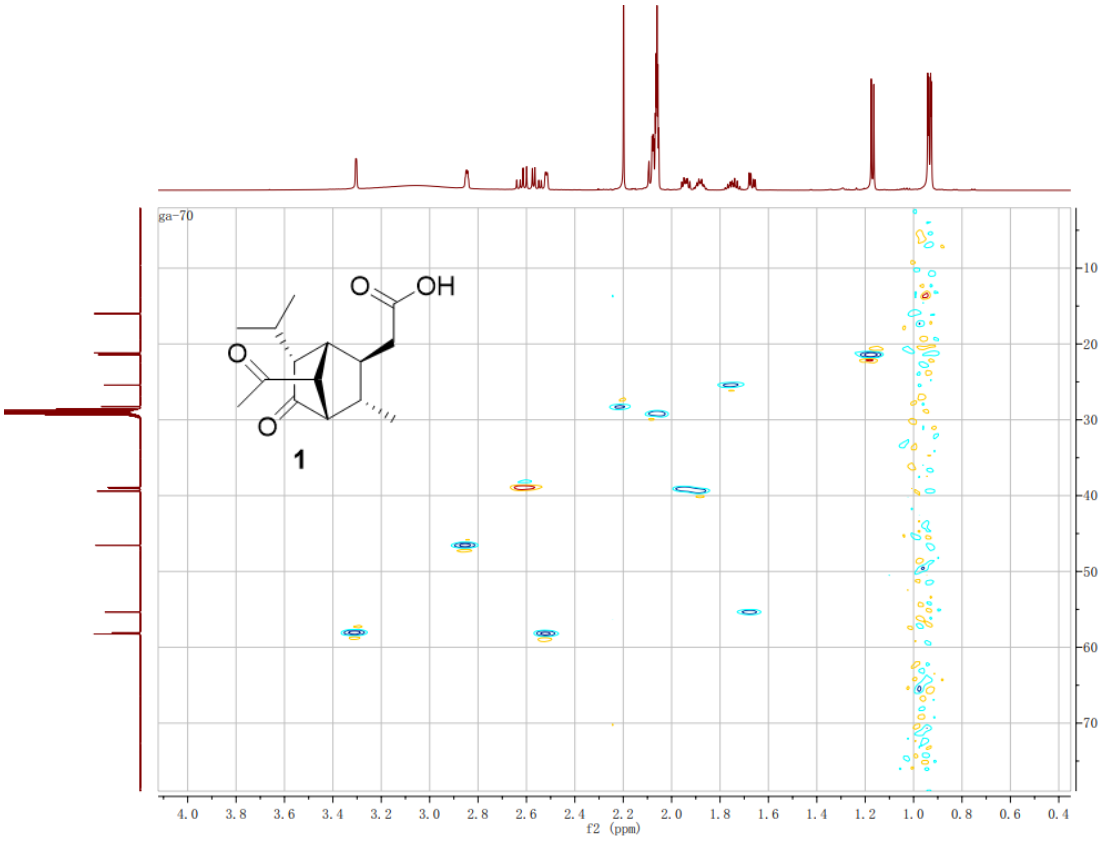

Figure S4: HSQC spectrum of compound **1** in CD_3COCD_3 (600 MHz)

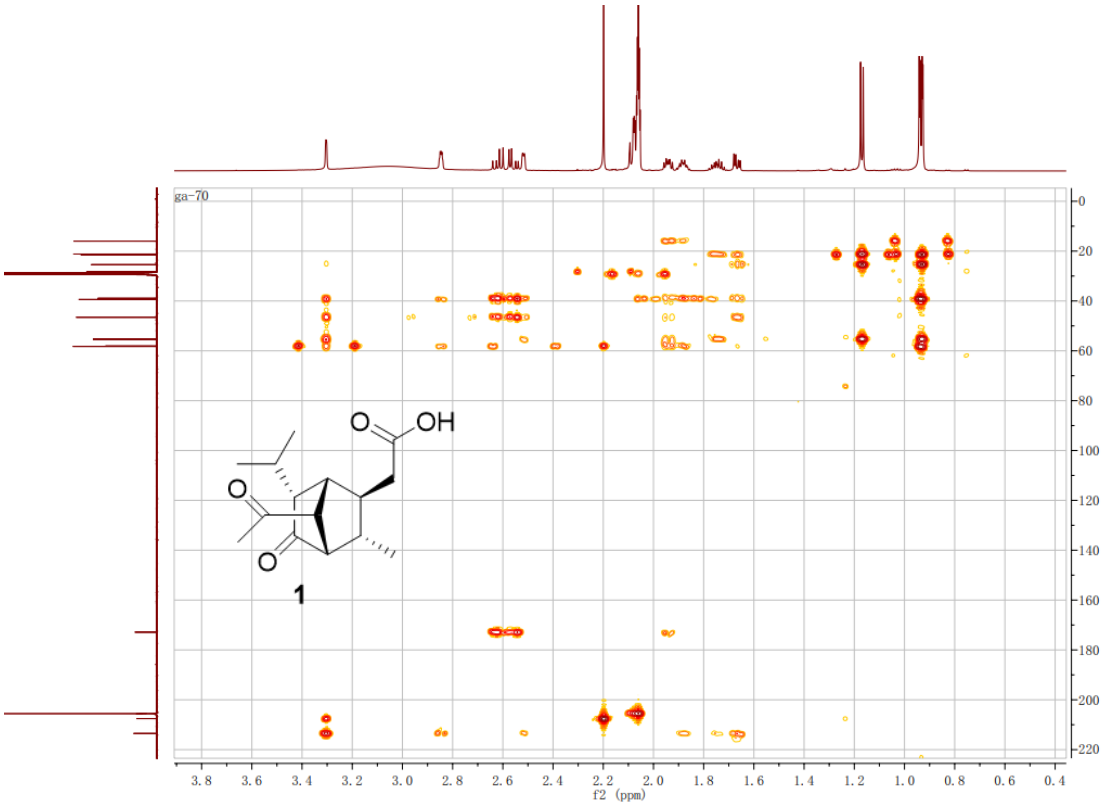

Figure S5: HMBC spectrum of compound **1** in CD_3COCD_3 (600 MHz)

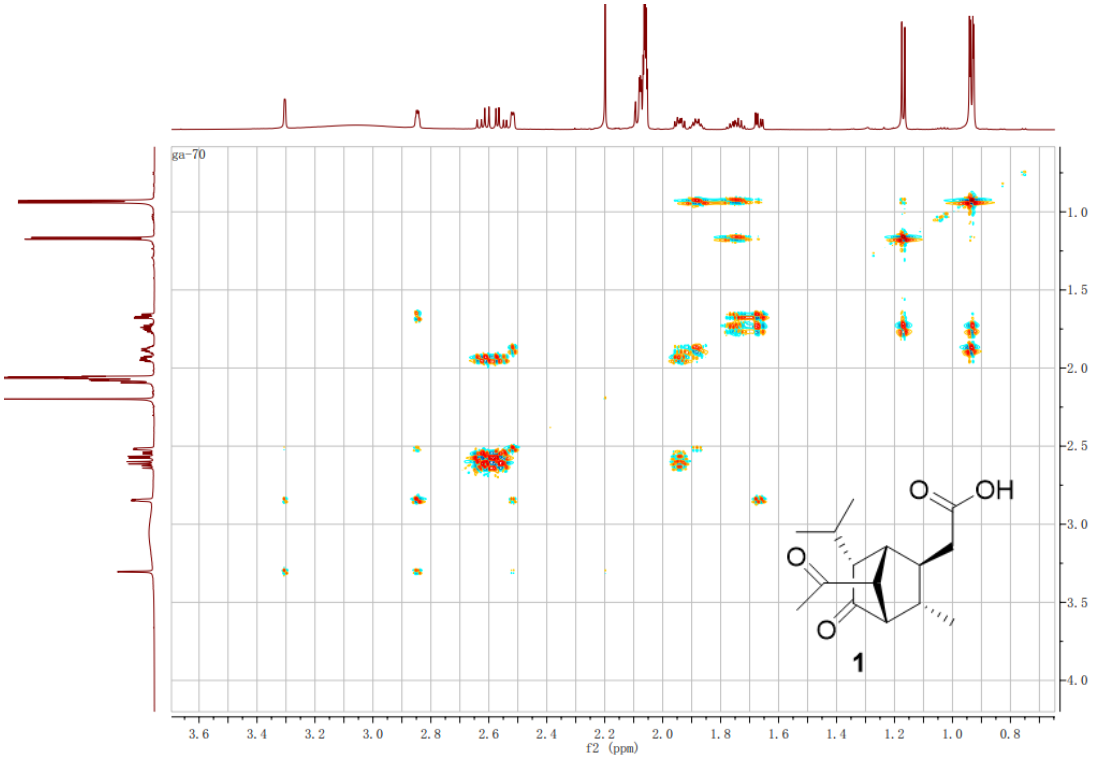

Figure S6: ^1H- ^1H COSY spectrum of compound **1** in CD_3COCD_3 (600 MHz)

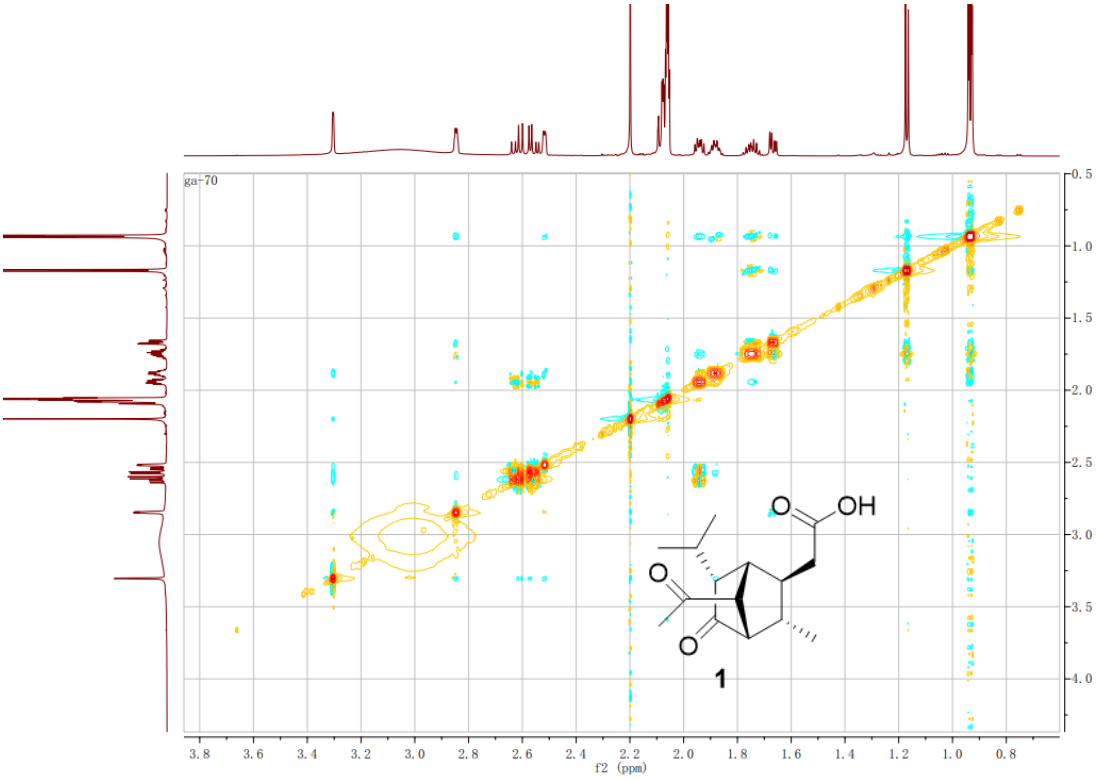

Figure S7: ROESY spectrum of compound **1** in CD_3COCD_3 (600 MHz)

Qualitative Analysis Report

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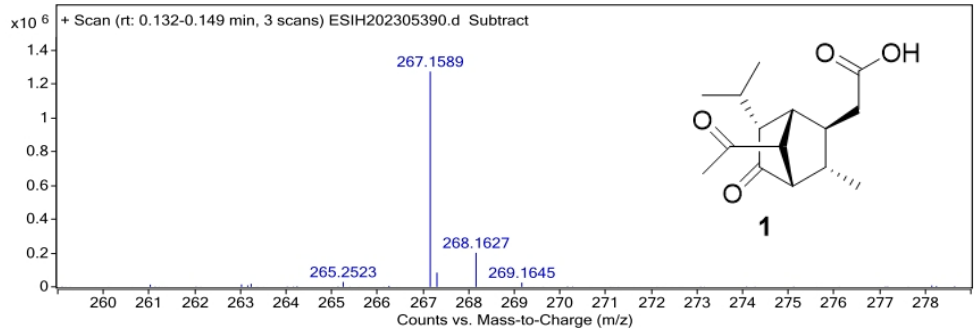
Sample ID		**Position**	P1-A3
Instrument Name	Agilent 6520 Q-TOF	**Acq Method**	20160322_MS_ESIH_POS_1min.m
Acquired Time	9/13/2023 10:39:57	**IRM Calibration Status**	Success
DA Method	small molecular data analysis method.m	**Comment**	ESIH by fangsu

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
200	0	ESI



Formula Calculator Results

m/z	Calc m/z	Diff (mDa)	Diff (ppm)	Ion Formula	Ion
267.1589	267.1591	0.22	0.82	C15 H23 O4	(M+H)+

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

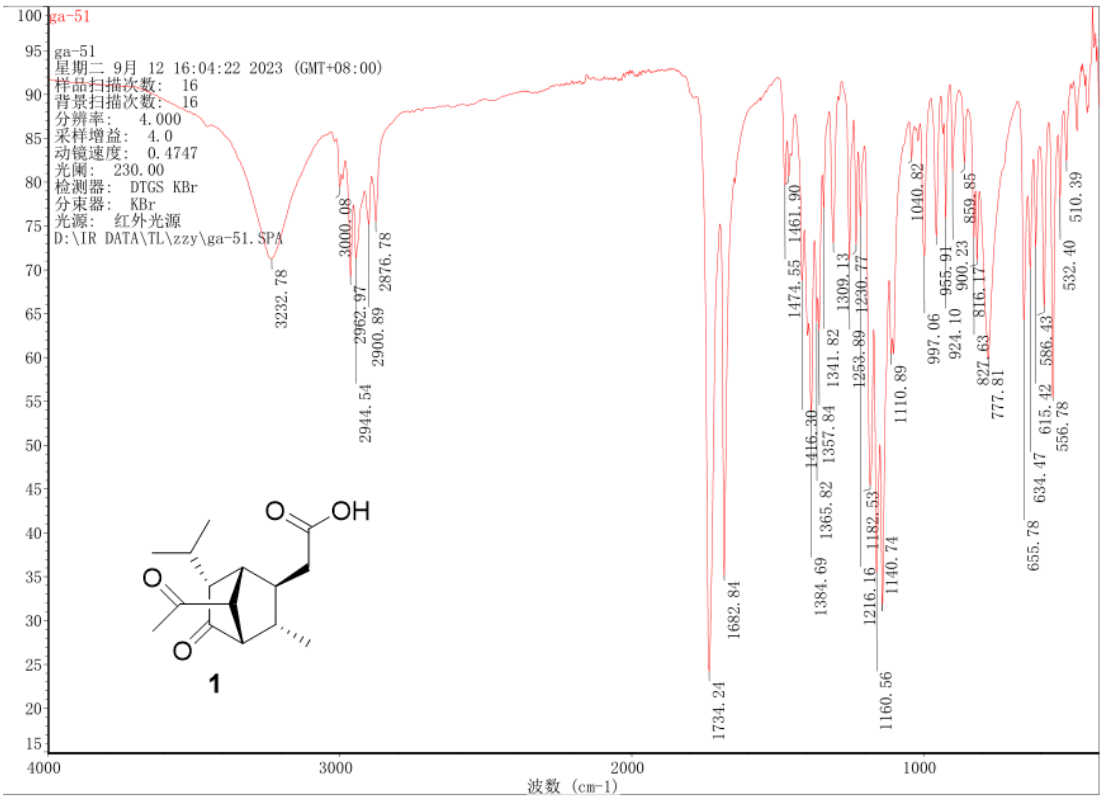

Figure S9: IR spectrum of compound **1**

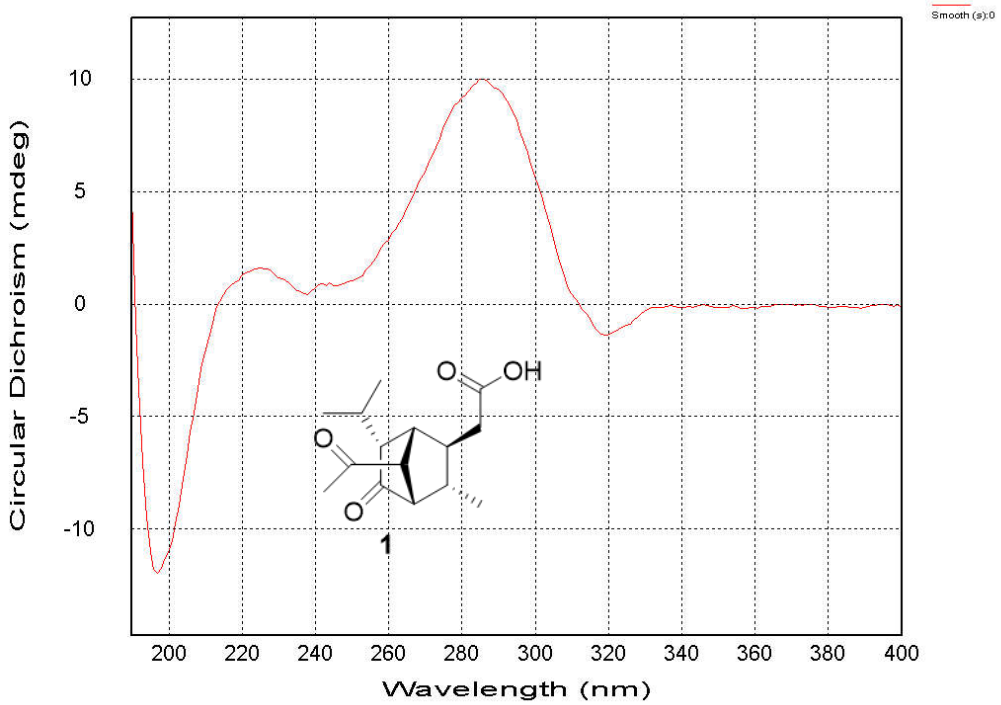

Figure S10: Experimental CD spectrum of **1**

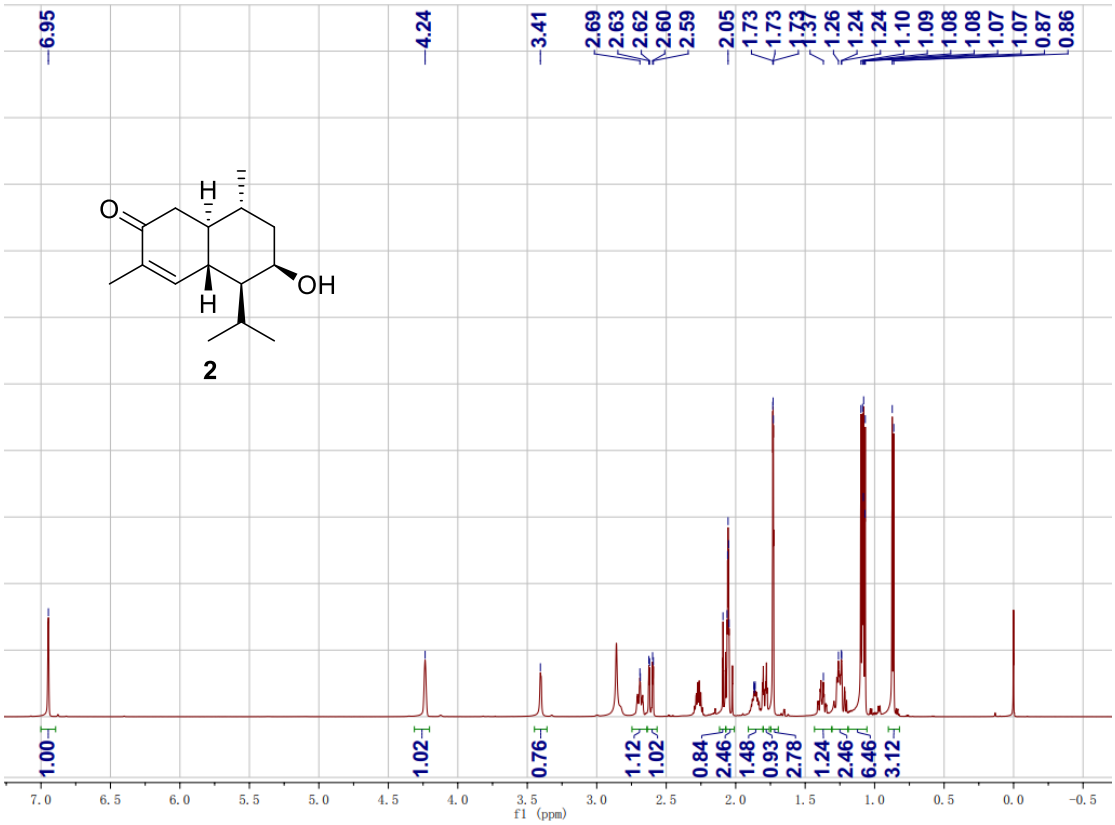

Figure S11: ^{1}H NMR spectrum of compound **2** in CD_3COCD_3 (600 MHz)

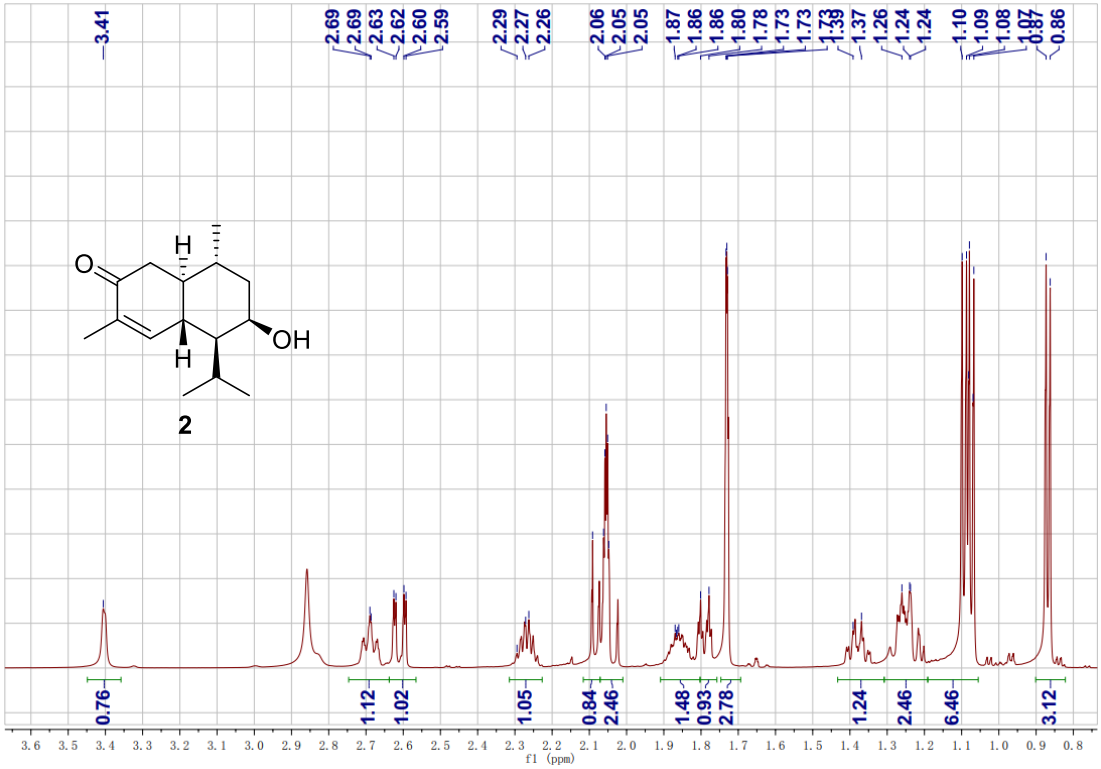

Figure S12: Expanded 1H-NMR spectrum of compound **2**.

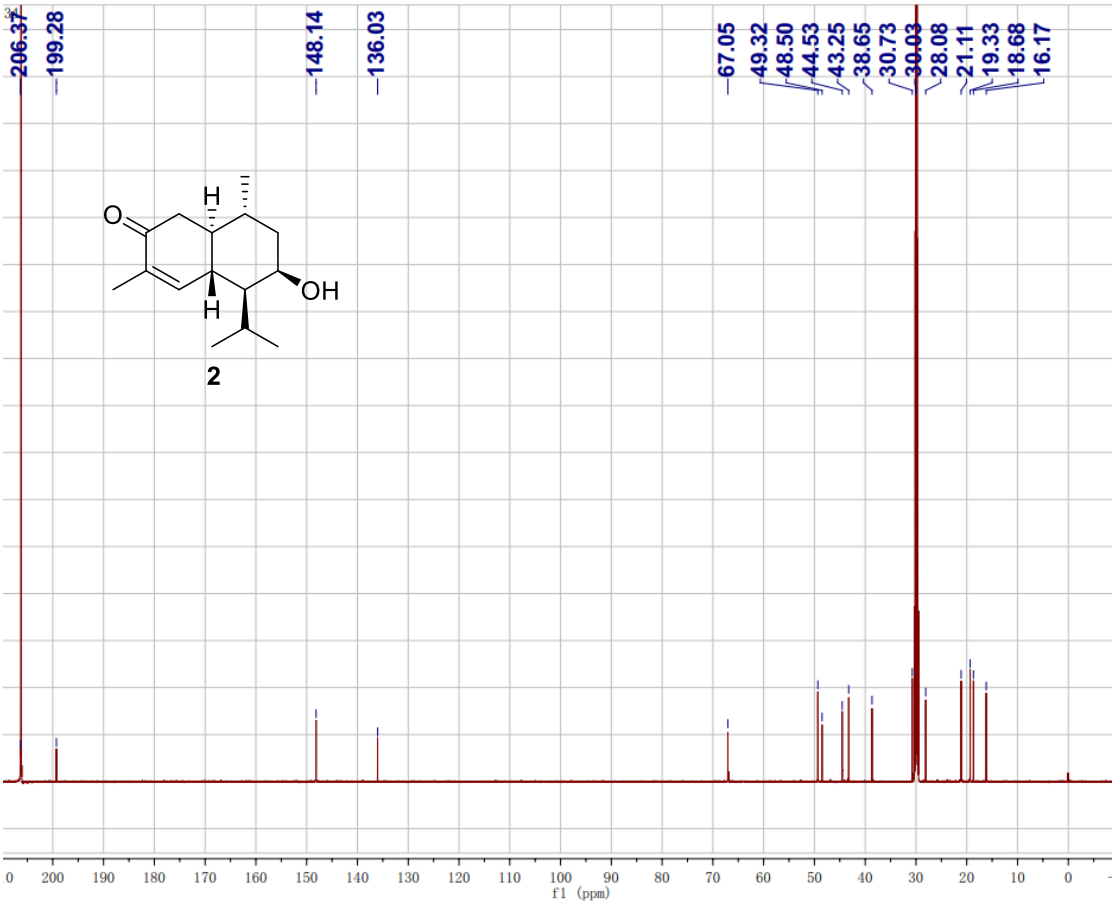

Figure S13: ^{13}C NMR spectrum of compound **2** in CD_3COCD_3 (150 MHz)

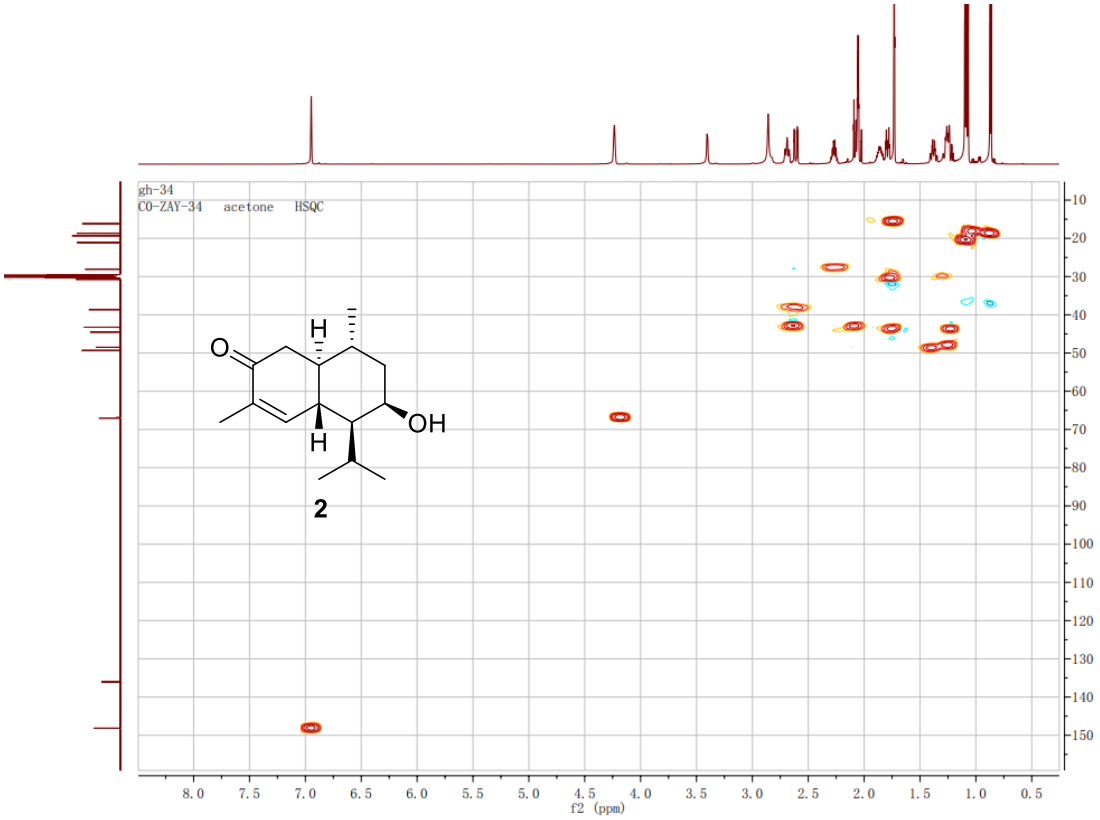

Figure S14: HSQC spectrum of compound **2** in CD_3COCD_3 (600 MHz)

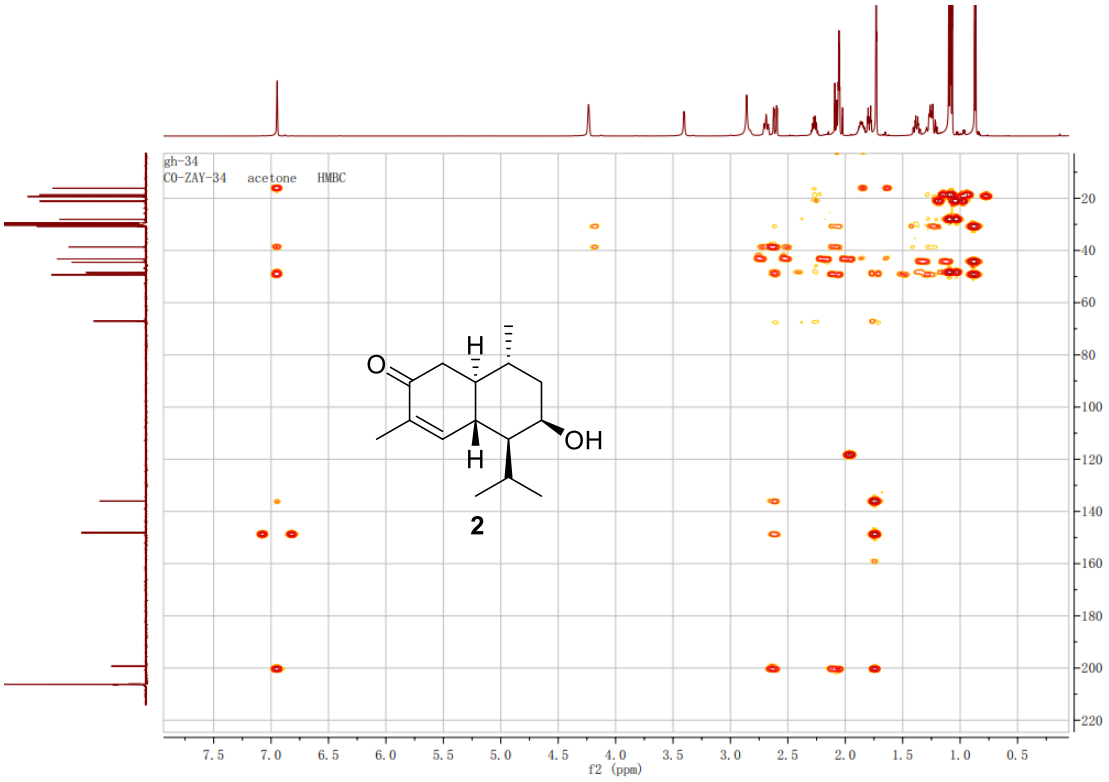

Figure S15: HMBC spectrum of compound **2** in CD_3COCD_3 (600 MHz)

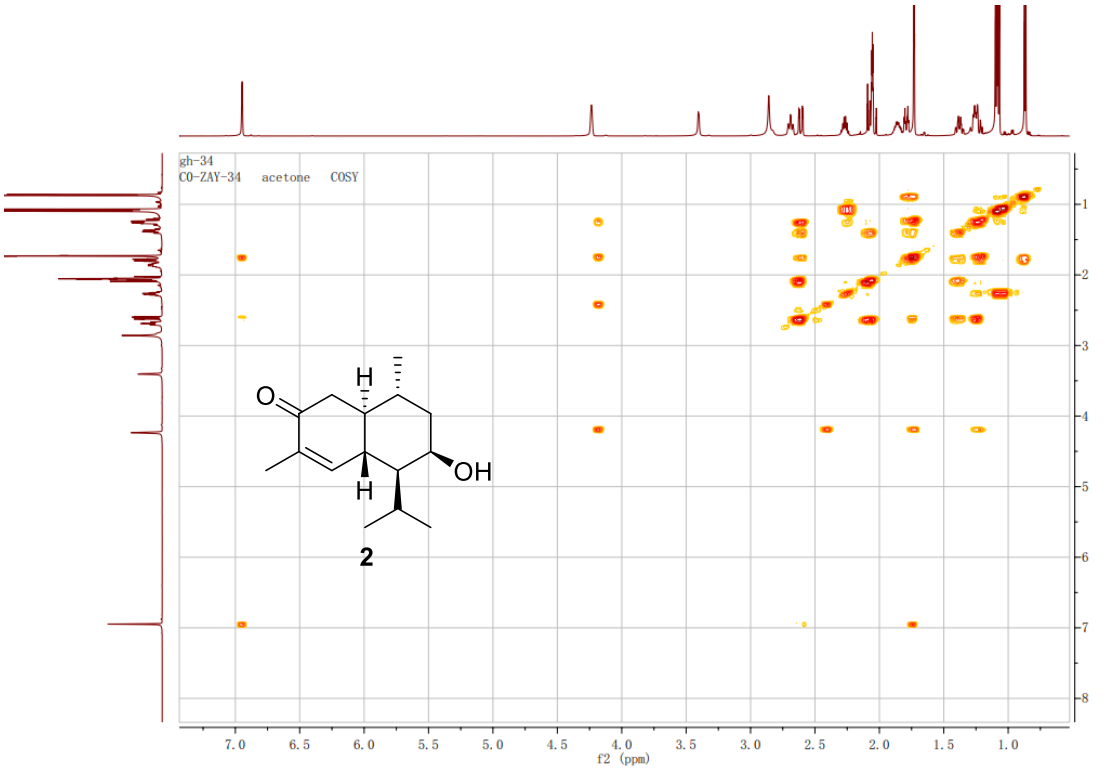

Figure S16: ^1H- ^1H COSY spectrum of compound **2** in CD_3COCD_3 (600 MHz)

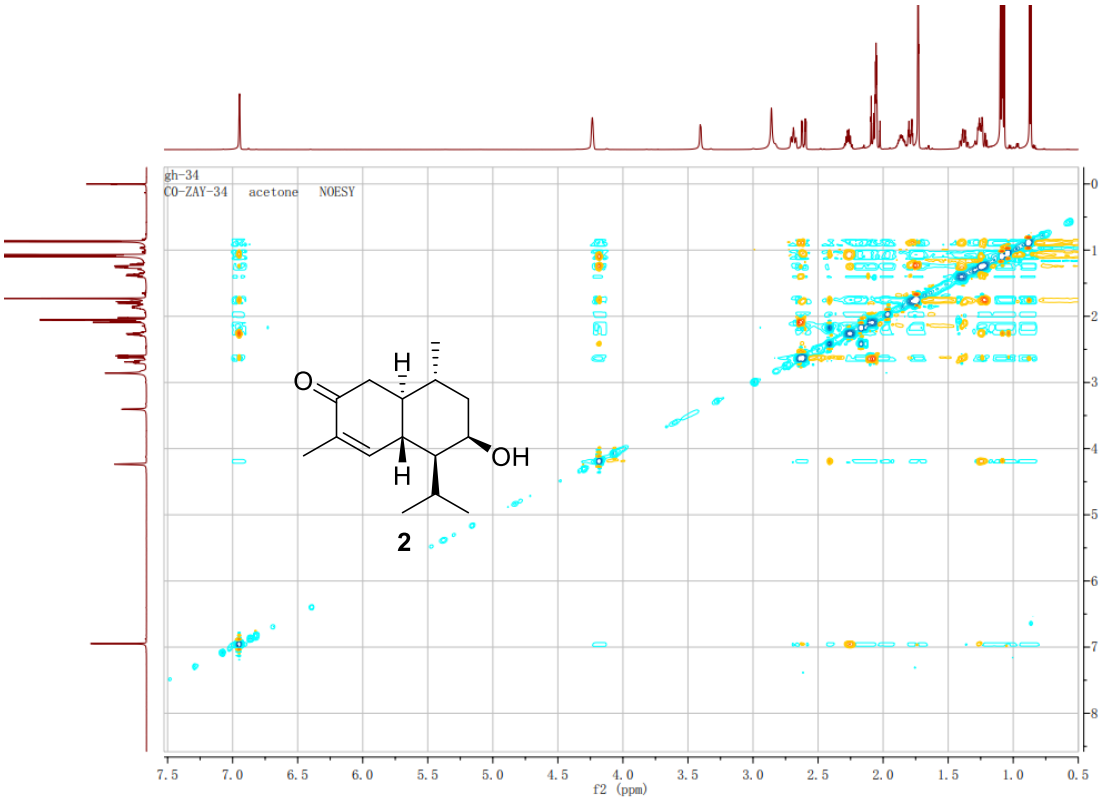

Figure S17: ROESY spectrum of compound **2** in CD_3COCD_3 (600 MHz)

Qualitative Analysis Report

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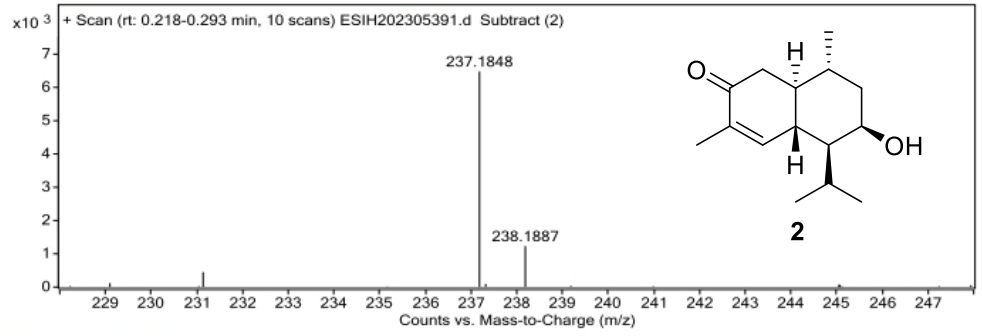
Sample ID		**Position**	P1-A4
Instrument Name	Agilent 6520 Q-TOF	**Acq Method**	20160322_MS_ESIH_POS_1min.m
Acquired Time	9/13/2023 10:41:28	**IRM Calibration Status**	Success
DA Method	small molecular data analysis method.m	**Comment**	ESIH by fangsu

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
200	0	ESI



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 ---

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

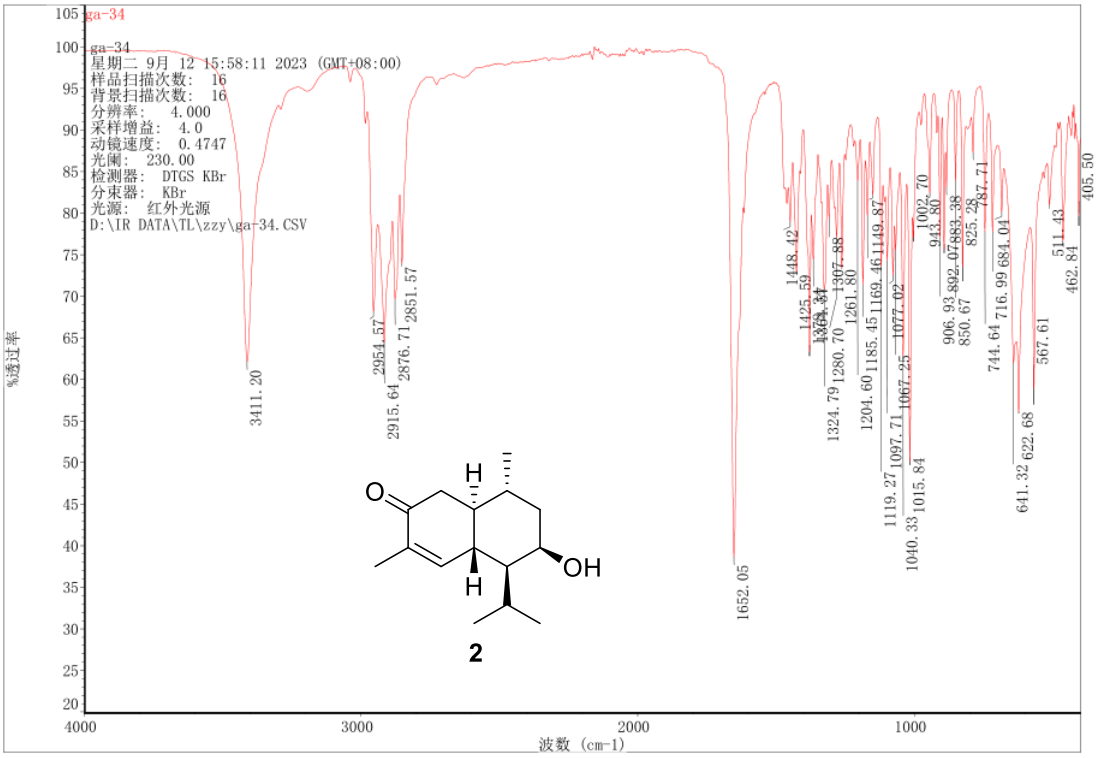

Figure S19: IR spectrum of compound **2**

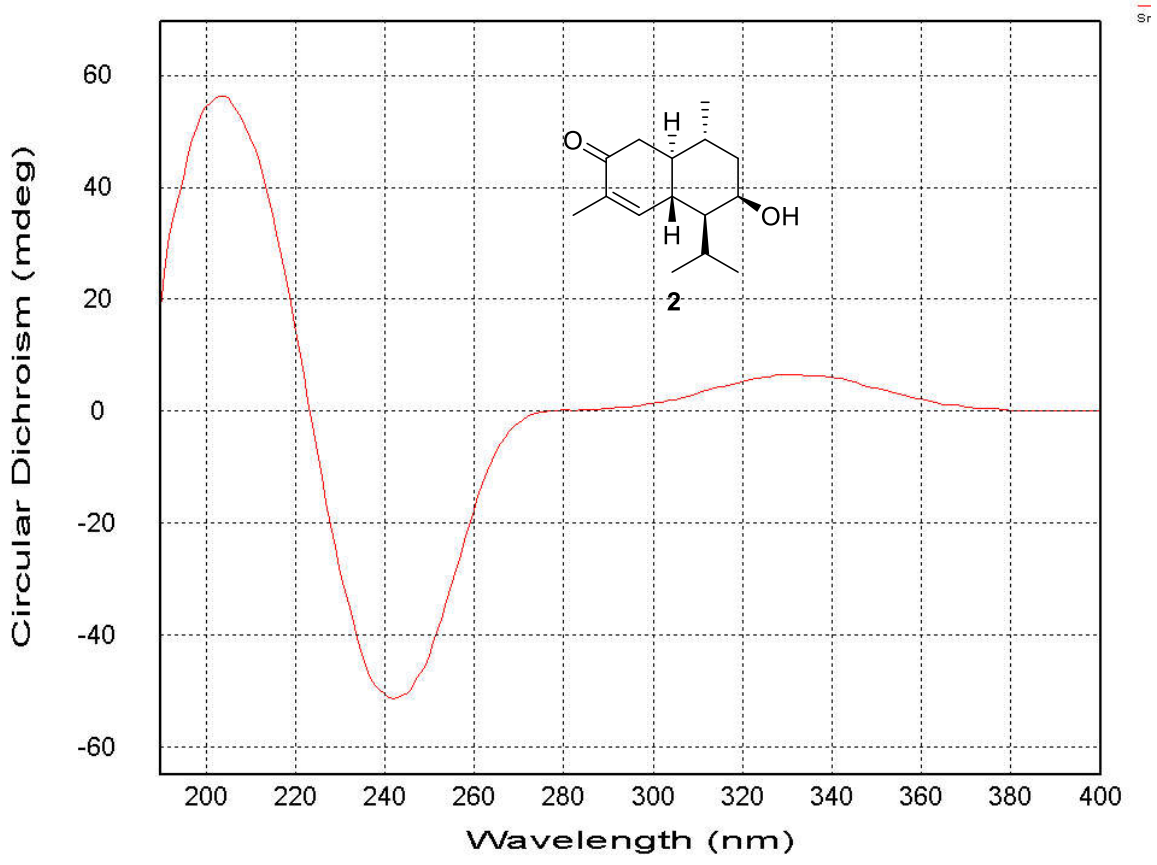

Figure S20: Experimental CD spectrum of **2**

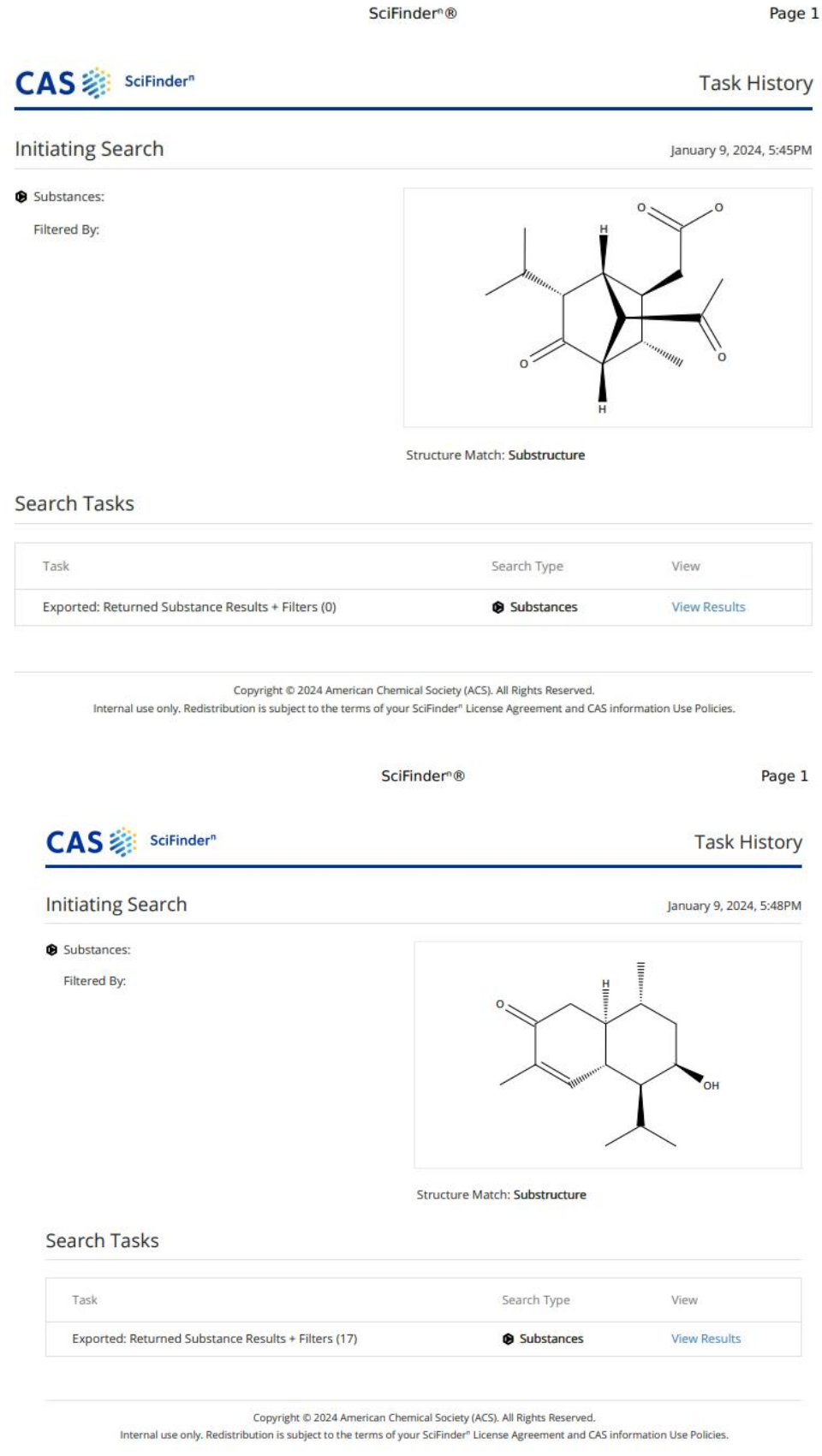

Figure S21. Scifinder search report of the new compounds **1** and **2**

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, 6	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 $(CD_3)_2CO$ as solvent.