

## Supporting Information

*Rec. Nat. Prod.* X:X (202X) XX-XX

### Structurally Diverse Terpenoids from the Resins of *Populus euphratica*

Yong-Hui Yang<sup>1</sup>, Yang Yu<sup>1,2</sup>, Shu-Ting Zhang<sup>1</sup>, Bai-Xiang Cai<sup>\*1</sup> and  
Ju-Tao Wang<sup>\*1,2,3</sup>,

<sup>1</sup> School of Pharmacy, Anhui University of Chinese Medicine, Hefei, 230012, PR China

<sup>2</sup> Institute of Medicinal Chemistry, Anhui Academy of Chinese Medicine, Hefei 230012, PR China

<sup>3</sup> Anhui Province Key Laboratory of Research & Development of Chinese Medicine, Hefei, 230012, PR China

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**Table S1-1:**  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectroscopic data for **1** and similar compound **1'** ( $\delta$  in ppm and  $J$  in Hz)

Position	<b>1</b>		<b>1'</b>	
	$\delta_{\text{H}}$	$\delta_{\text{C}}$	$\delta_{\text{H}}$	$\delta_{\text{C}}$
1 $\alpha$	2.75 dt (13.4, 3.6)	40.2	2.82 dt (13.6, 3.4)	39.1
1 $\beta$	1.01 m		0.97-1.00 m	
2 $\alpha$	1.70-1.66 m	27.8	1.61-1.65 m	27.2
2 $\beta$	1.55-1.50 m		1.61-1.65 m	
3	3.16 dd (11.8, 4.6)	79.4	3.22 dd (10.0, 6.0)	78.7
4	-		-	
5 $\alpha$	0.76 dd (12.0, 2.0)	56.3	0.70 br d (10.4)	55.0
6 $\alpha$	1.47 dt (11.6, 2.8)		1.44-1.49 m	
6 $\beta$	1.60 q (3.7, 3.0)	18.6	1.59-1.65 m	17.8
7 $\alpha$	1.70-1.66 m		1.59-1.65 m	
7 $\beta$	1.47 dt (11.6, 2.8)	34.3	1.35-1.38 m	33.0
8	-		-	
9 $\alpha$	2.46-2.41 m	63.2	2.26 s	61.0
10	-		-	
11	-	202.9	-	199.5
12	5.50 s		5.72 s	
13	-	174.2	-	165.0
14	-		-	
15 $\alpha$	1.37 m	37.4	1.91 d (14.0)	42.8
15 $\beta$			3.29 d (14.0)	
16 $\alpha$	1.23-1.17 m	47.9	-	221.5
16 $\beta$	1.72 m		-	
17	-	72.4	-	76.5
18	2.46-2.41 m		2.89 dd (14.0, 4.0)	
19 $\alpha$	2.16 dt (8.4, 2.3)	27.6	1.44-1.49 m	45.8
19 $\beta$			1.32-1.33 m	
20	-	44.8	-	30.7
21 $\alpha$	1.60 q (3.7, 3.0)		1.59-1.65 m	
21 $\beta$	1.29-1.27 m	27.3	1.35-1.38 m	36.3
22 $\alpha$	1.75 dd (9.5, 4.3)		2.12 dt (12.4, 3.2, 3.2)	
22 $\beta$	1.55-1.50 m	38.2	1.42-1.46 m	30.4
23	1.79 s		1.00 s	
24	0.79 s	28.7	0.80 s	28.1
25	1.11 s		1.12 s	
26	1.13 s	20.3	1.24 s	19.6
27	1.00 s		1.38 s	
28	1.37 s	23.6	0.97 s	23.5
29	0.93 s		0.91 s	
		32.8		32.1

The  $^1\text{H}$  and  $^{13}\text{C}$  NMR data of compound **1** were recorded at 500 MHz, with  $\text{CD}_3\text{OD}$  as solvent; the  $^1\text{H}$  and  $^{13}\text{C}$  NMR data of the compound **1'** reported in the literature [1] were recorded with a Bruker AM-400, with  $\text{CDCl}_3$  as solvent.

Data File: E:\DATA\2022\1130\w4133.lcd

Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	5	100	F	1	0	0	Cl	1	0	0	Ag	1	0	0	H
2H	1	0	0	Na	1	0	0	Co	2	0	0	I	3	0	0	Na
B	3	0	0	Mg	2	0	0	Cu	2	0	0	Ir	3	0	0	
C	4	5	60	Si	4	0	0	Se	2	0	0					
N	3	0	5	P	3	0	0	Br	1	0	0					
O	2	0	30	S	2	0	0	Pd	2	0	0					

Error Margin (ppm): 5

HC Ratio: 0.0 - 3.0

Max Isotopes: all

MSn Iso RI (%): 75.00

DBE Range: not fixed

Apply N Rule: no

Isotope RI (%): 1.00

MSn Logic Mode: OR

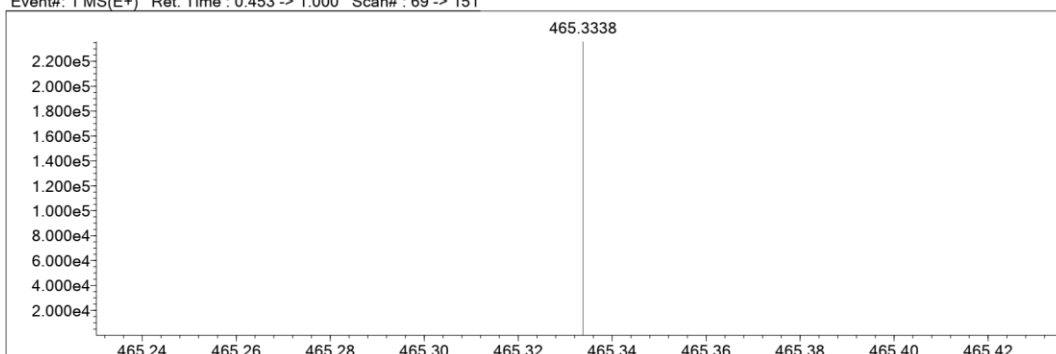
Electron Ions: both

Use MSn Info: yes

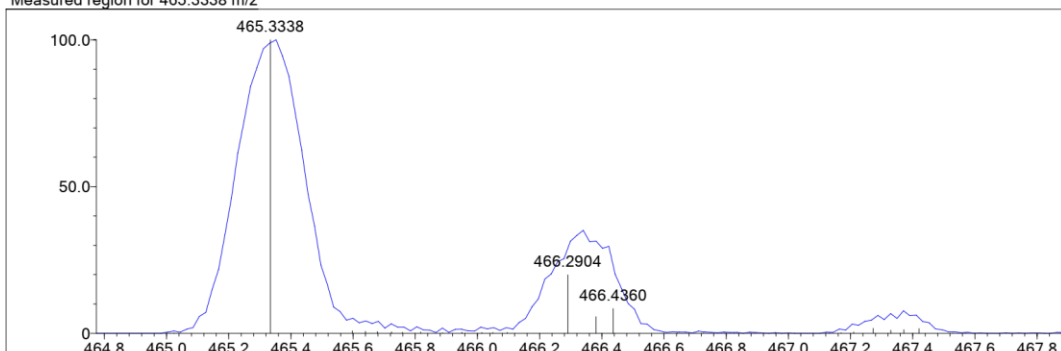
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Max Results: 30

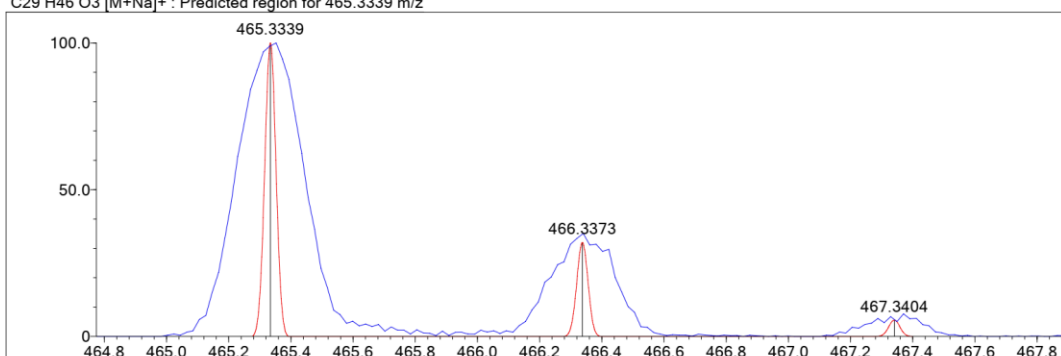
Event#: 1 MS(E+) Ret. Time : 0.453 -&gt; 1.000 Scan#: 69 -&gt; 151



Measured region for 465.3338 m/z



C29 H46 O3 [M+Na]+ : Predicted region for 465.3339 m/z



Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	DBE
C29 H46 O3	[M+Na]+	465.3338	465.3339	-0.1	-0.21	7.0

Figure S1-2: HR-ESI-MS spectrum of 1

==== LCMSsolution Data Report ====

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Date Acquired	: 2022/11/30 12:52:24	
Sample Name	: w4133	
Data File	: w4133.lcd	
Method File	: 阻尼管一级100-1500.lcm	

<Spectrum>

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Spectrum: Averaged 0.427-0.840 (65-127)  
Background: None MS Stage: MS Polarity: Pos Segment1 - Event1 Precursor: ----- Cutoff:

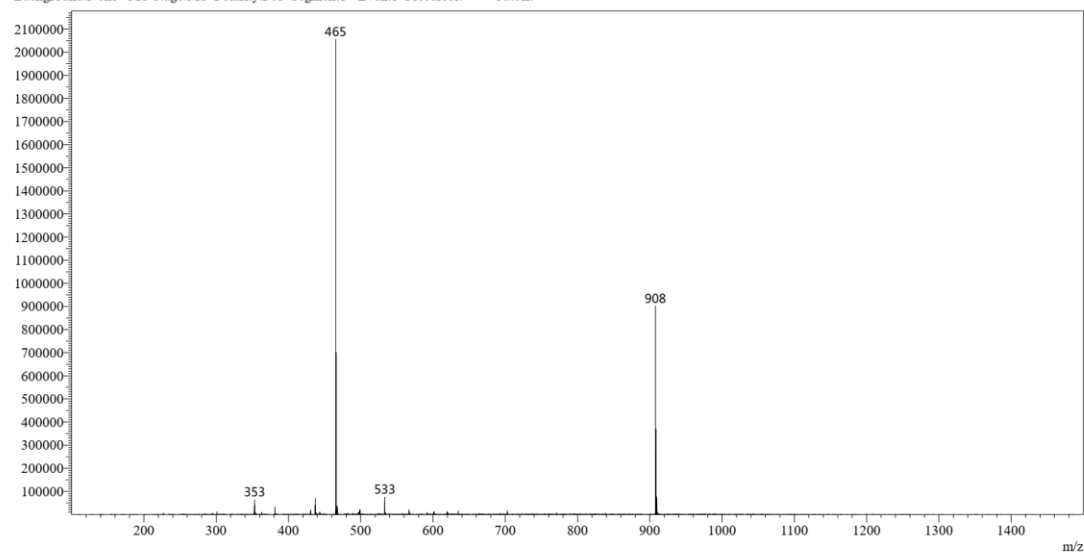
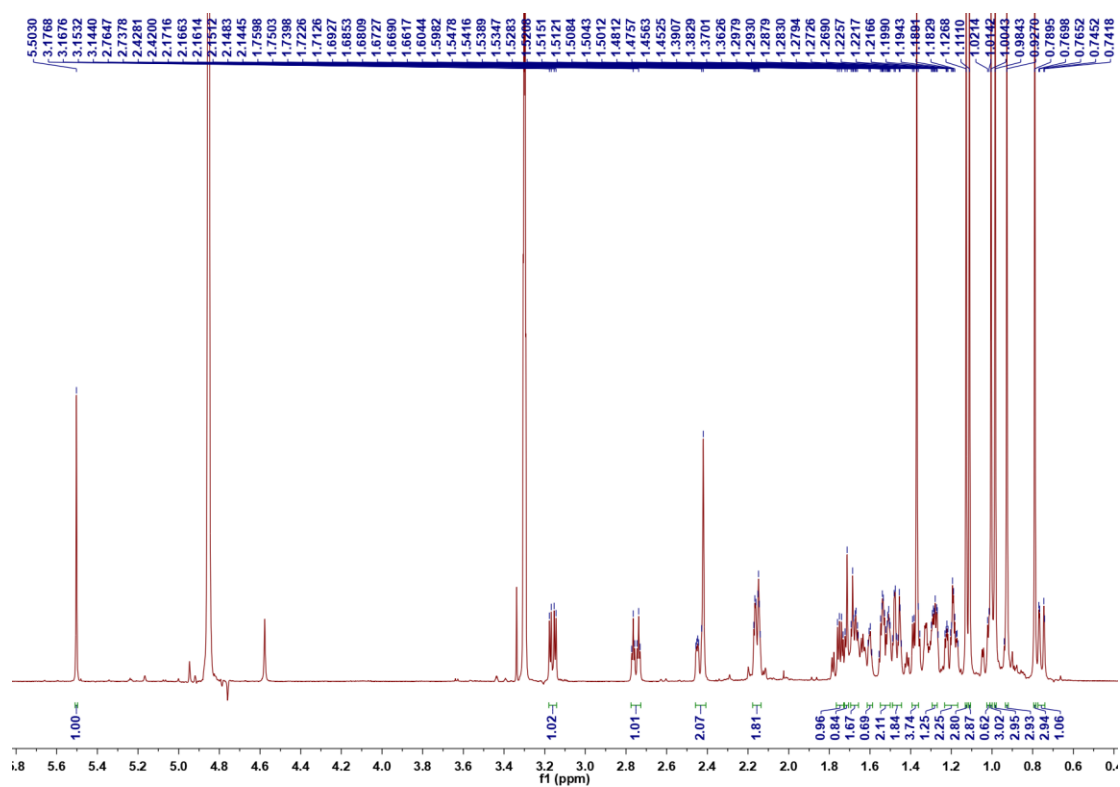
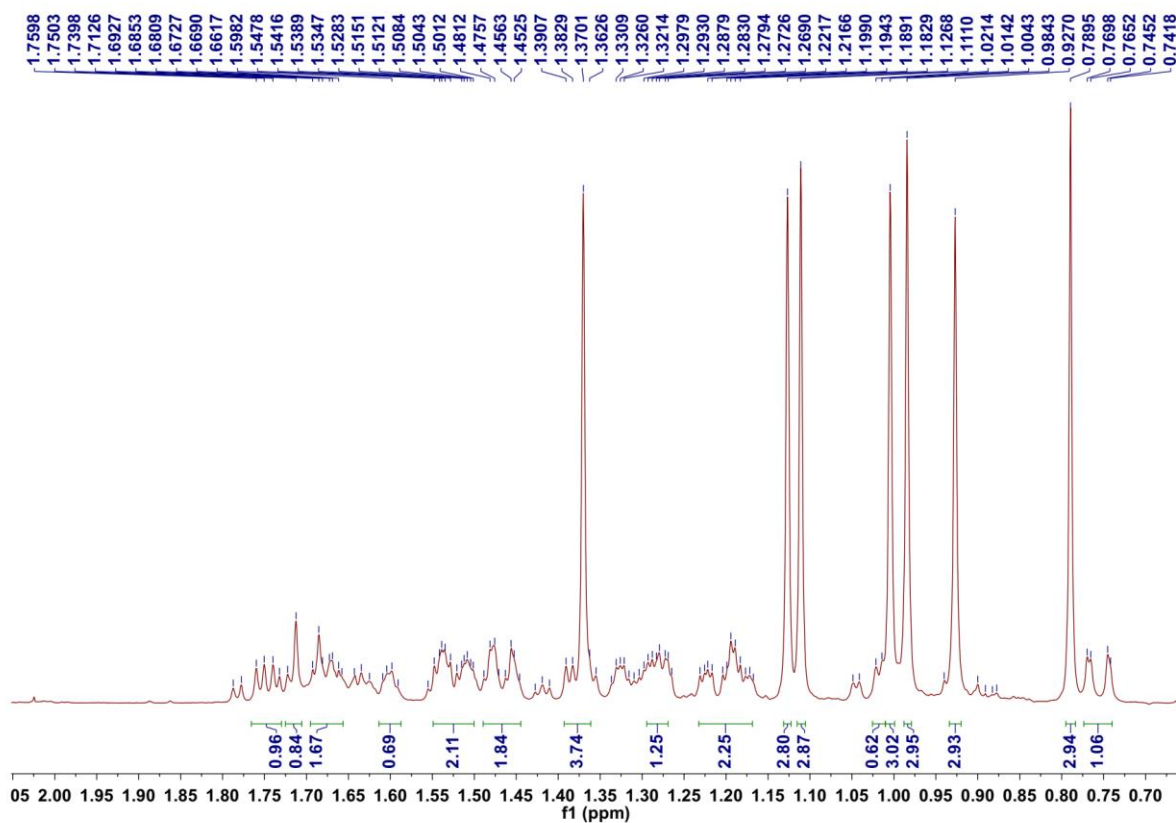


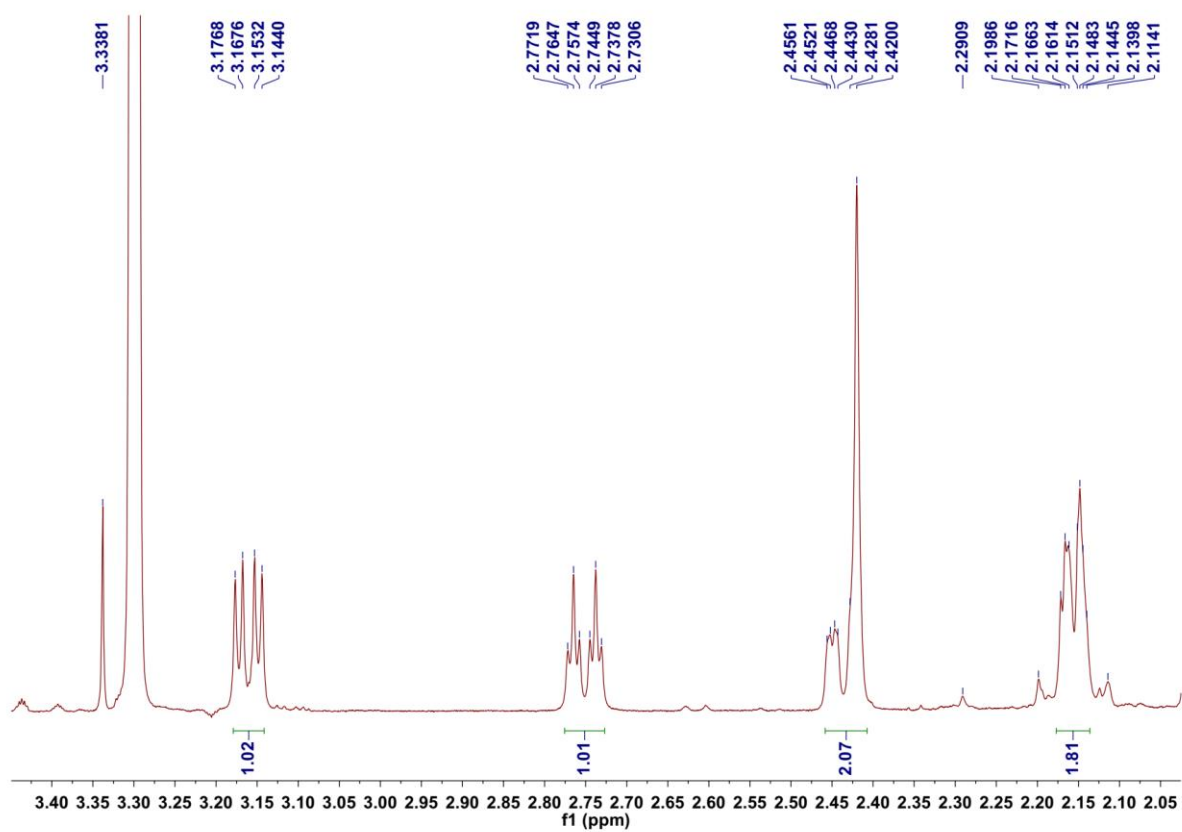
Figure S1-3: ESI-MS spectrum of **1**



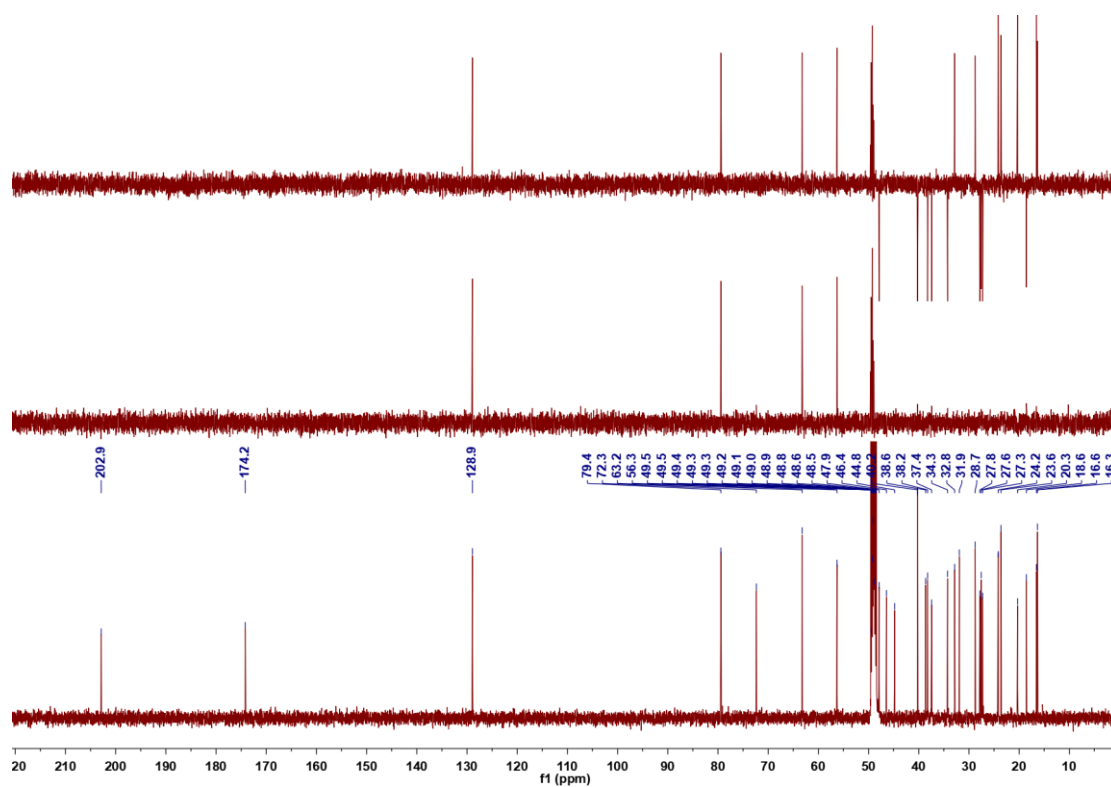
**Figure S1-4:** <sup>1</sup>H-NMR (500 MHz, CD<sub>3</sub>OD) spectrum of **1**



**Figure S1-5:**  $^1\text{H}$ -NMR (500 MHz,  $\text{CD}_3\text{OD}$ ) spectrum of **1** (From  $\delta_{\text{H}}$  0.70 ppm to 2.05 ppm)

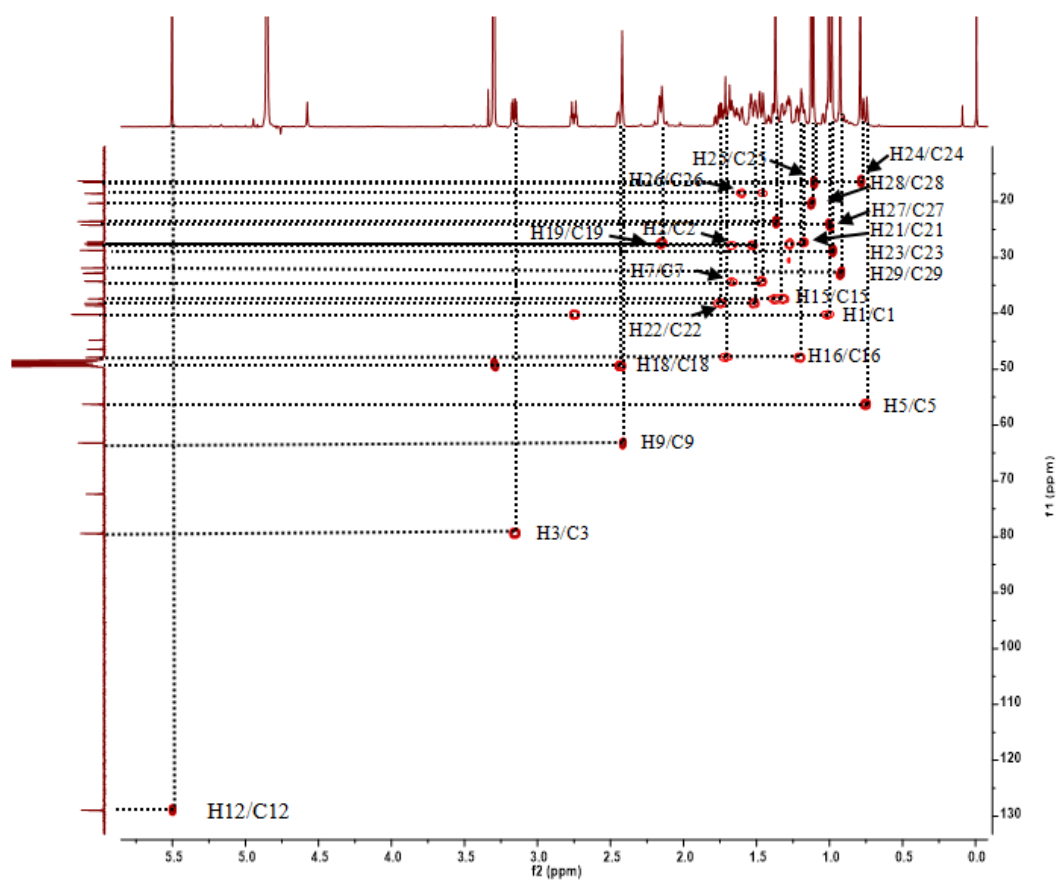


**Figure S1-6:**  $^1\text{H}$ -NMR (500 MHz,  $\text{CD}_3\text{OD}$ ) spectrum of **1** (From  $\delta_{\text{H}}$  2.05 ppm to 3.40 ppm)

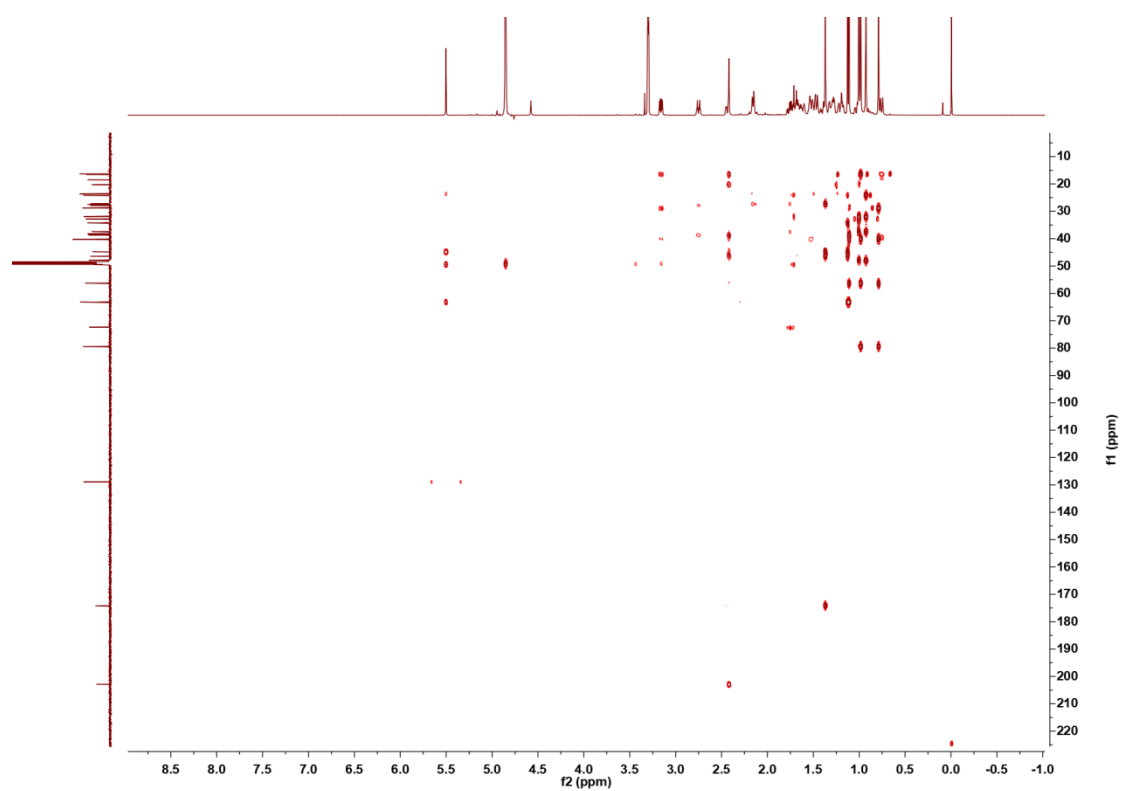


**Figure S1-7:**  $^{13}\text{C}$ -NMR and DEPT (125 MHz,  $\text{CD}_3\text{OD}$ ) spectrum of **1**

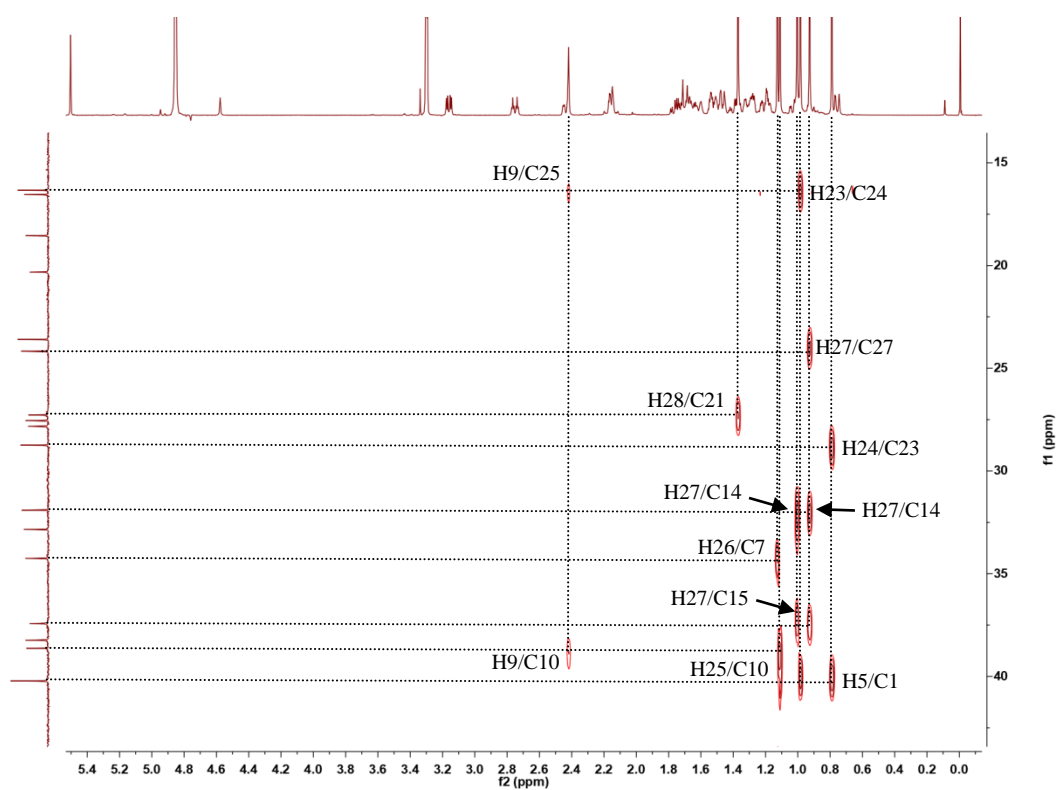




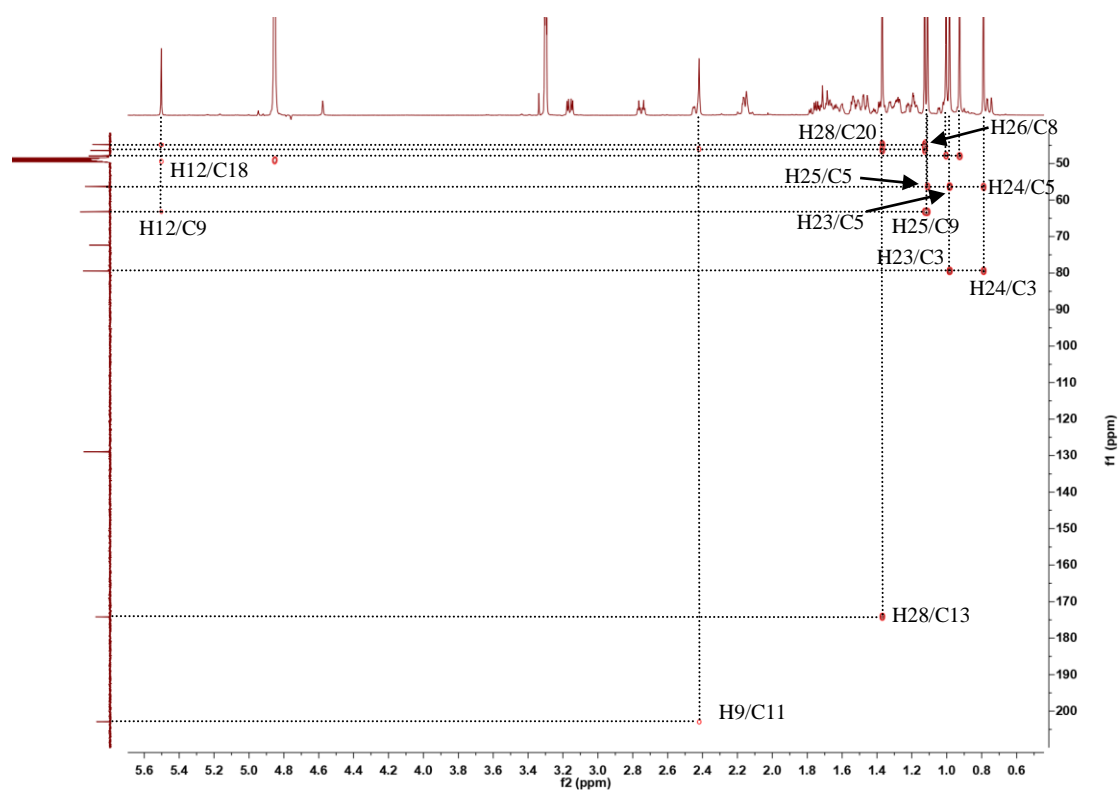
**Figure S1-8:** HSQC spectrum of **1**



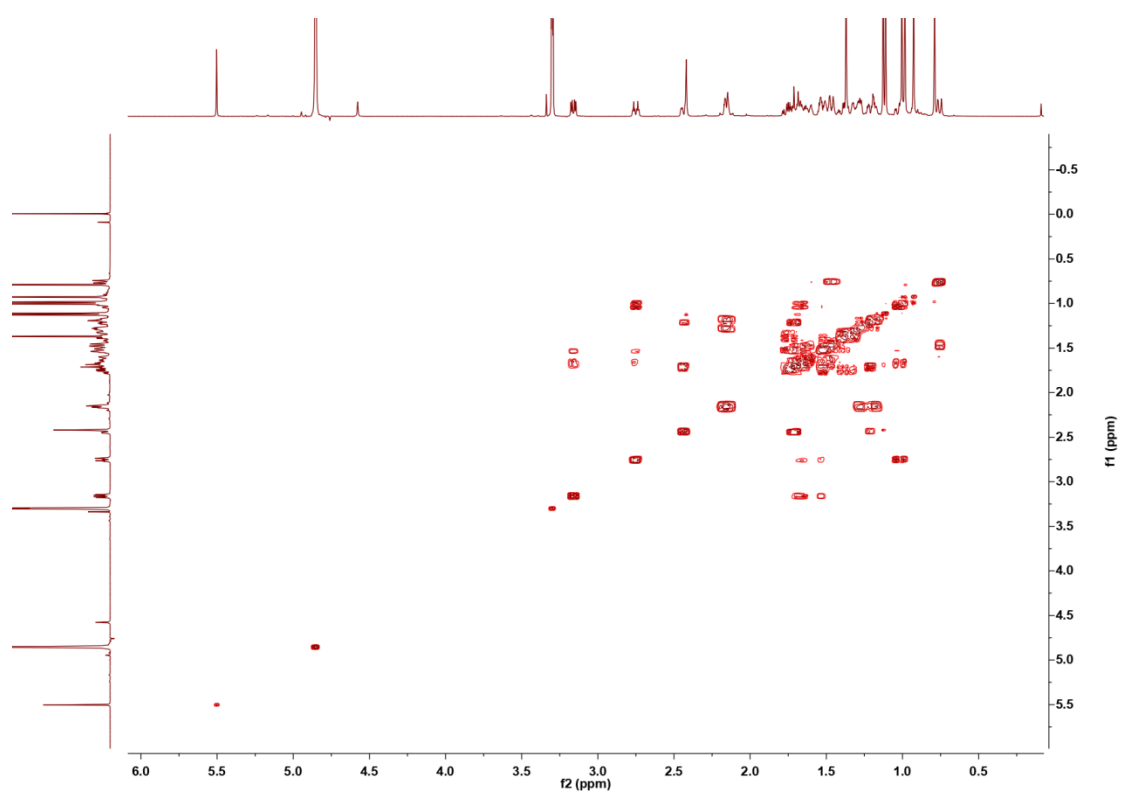
**Figure S1-9:** HMBC spectrum of **1**



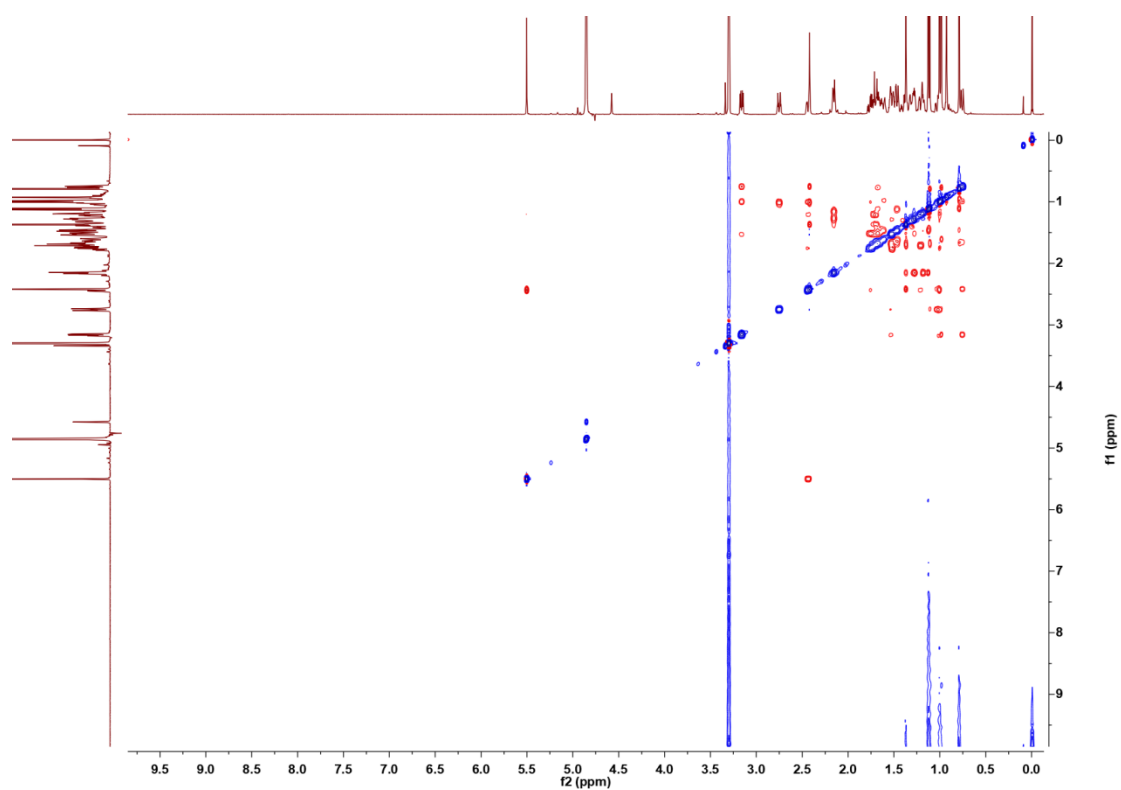
**Figure S1-10:** HMBC spectrum of **1** (From  $\delta_c$  15 ppm to  $\delta_c$  45ppm)



**Figure S1-11:** HMBC spectrum of **1** (From  $\delta_C$  45 ppm to  $\delta_C$  210 ppm)



**Figure S1-12:**  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of **1**



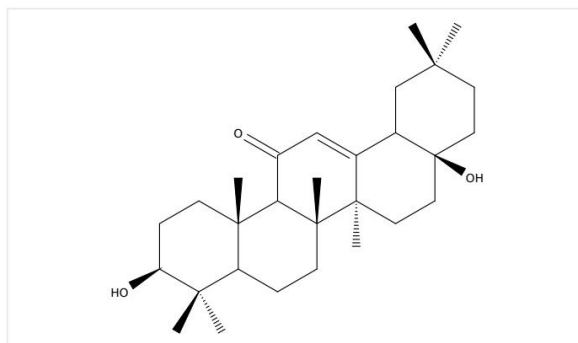
**Figure S1-13:** ROESY spectrum of **1**

## Initiating Search

June 1, 2023, 10:47AM


 Substances:

Filtered By:



Structure Match: As Drawn

## Search Tasks

Task	Search Type	View
Exported: Returned Substance Results + Filters (0)	 Substances	<a href="#">View Results</a>

 Substances (0)[View in SciFinder<sup>®</sup>](#)

We couldn't find any results. Please update your search query and try again.

Substances with (0) results

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Internal use only. Redistribution is subject to the terms of your SciFinder<sup>®</sup> License Agreement and CAS information Use Policies.

**Figure S1-14: Scifinder search report of 1**

**Table S2-1:**  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectroscopic data for **2** and similar compound **2'**  
( $\delta$  in ppm and  $J$  in Hz)

Position	<b>2</b>		<b>2'</b>	
	$\delta_{\text{H}}$	$\delta_{\text{C}}$	$\delta_{\text{H}}$	$\delta_{\text{C}}$
1	2.98 d (16)	56.9	1.99 dd (8.7, 18.1)	54.8
2 $\alpha$	2.16 dd (13.3, 5.3)	26.8	1.46 ddd (4.9, 10.6, 22.6)	25.6
2 $\beta$	1.93-1.86 m		1.52-1.58 m	
3 $\alpha$	2.56-2.49 m	34.6	1.63-1.65 m	30.6
3 $\beta$	2.32 dd (16.5, 6.6)		1.12-1.19 m	
4	-	145.5	1.89-1.99 m	38.6
5	-	142.8	1.79-1.82 m	46.1
6 $\alpha$	4.33 - 4.26 m	69.1	0.82 dd (12.7, 23.1)	21.3
6 $\beta$			1.65 br. d (10.0)	
7	1.54 - 1.44 m	52.8	1.73-1.76 m	43.0
8 $\alpha$	0.80d (6.8)	21.4	1.05-1.08 m	23.9
8 $\beta$	1.54 - 1.44 m		1.74-1.77 m	
9 $\alpha$	1.81dd (13.4, 6.5)	47.3	1.73-1.54 m	33.8
9 $\beta$	1.54 - 1.44 m		1.30-1.33 m	
10	-	77	-	72.4
11 $\alpha$	4.22 d (16.0)	59.3	-	74.5
11 $\beta$	4.33-4.26 m			
12	2.10 ddt (11.4, 7.0, 4.3)	28.9	3.21 s	67.8
13	0.80 d (7.0)	16.1	0.87 s	19.4
14	0.96 d (7.0)	21.7	0.89 d (7.0)	30.9
15	1.06 s	21.7	1.01 s	16.3

The  $^1\text{H}$  and  $^{13}\text{C}$  NMR data of compound **2** were recorded at 500 MHz, with  $\text{CD}_3\text{OD}$  as solvent; the  $^1\text{H}$  and  $^{13}\text{C}$  NMR data of the compound **2'** reported in the literature [2] were recorded with a Bruker DRX-600, with  $\text{DMSO}-d_6$  as solvent.



Data File: E:\DATA\2022\1130\w484.lcd

Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
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2H	1	0	0	Na	1	0	0	Co	2	0	0	I	3	0	0	Na
B	3	0	0	Mg	2	0	0	Cu	2	0	0	Ir	3	0	0	
C	4	5	60	Si	4	0	0	Se	2	0	0					
N	3	0	5	P	3	0	0	Br	1	0	0					
O	2	0	30	S	2	0	0	Pd	2	0	0					

Error Margin (ppm): 5

HC Ratio: 0.0 - 3.0

Max Isotopes: all

MSn Iso RI (%): 75.00

DBE Range: not fixed

Apply N Rule: no

Isotope RI (%): 1.00

MSn Logic Mode: OR

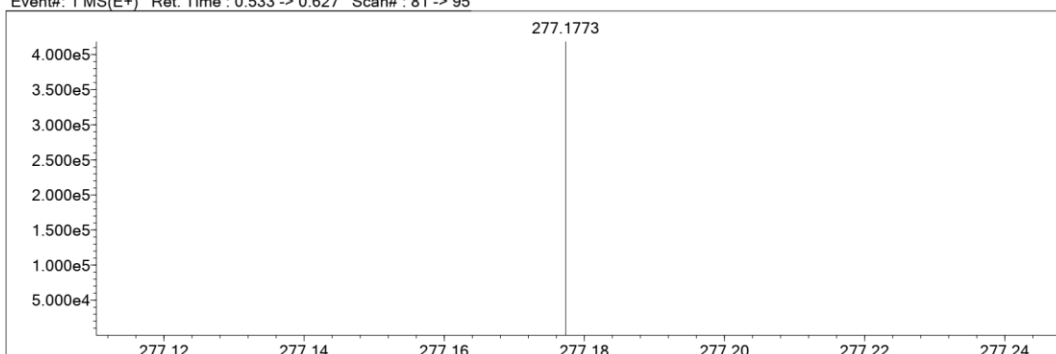
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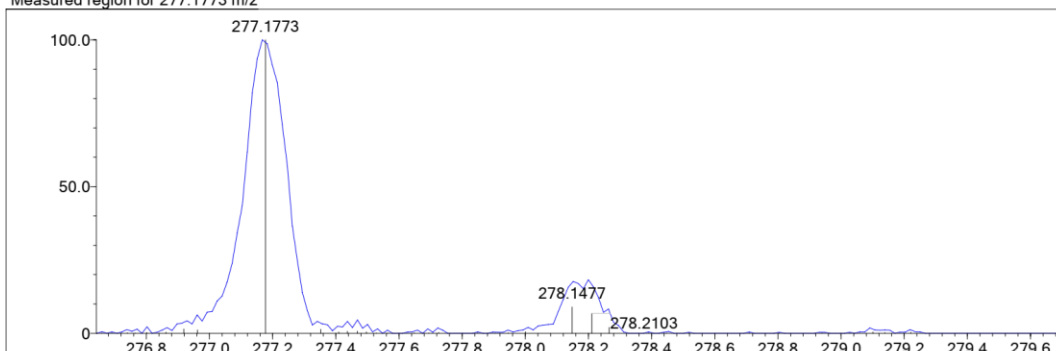
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Max Results: 30

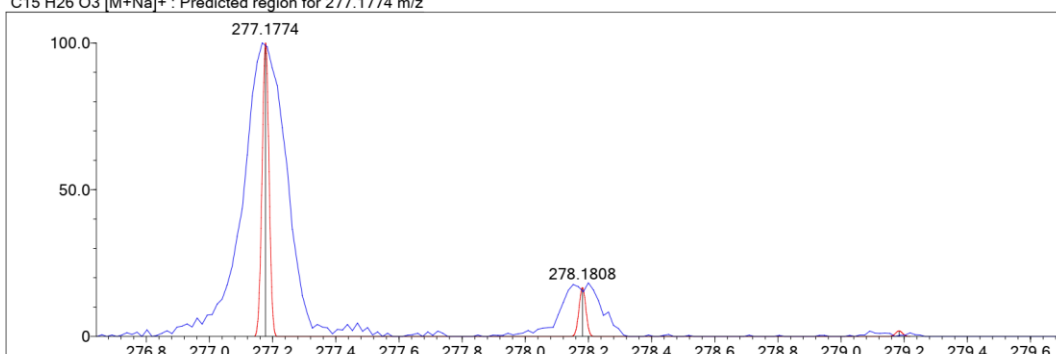
Event#: 1 MS(E+) Ret. Time : 0.533 -&gt; 0.627 Scan#: 81 -&gt; 95



Measured region for 277.1773 m/z



C15 H26 O3 [M+Na]+ : Predicted region for 277.1774 m/z



Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	DBE
C15 H26 O3	[M+Na]+	277.1773	277.1774	-0.1	-0.36	3.0

Figure S2-2: HR-ESI-MS spectrum of **2**

==== LCMSsolution Data Report ====

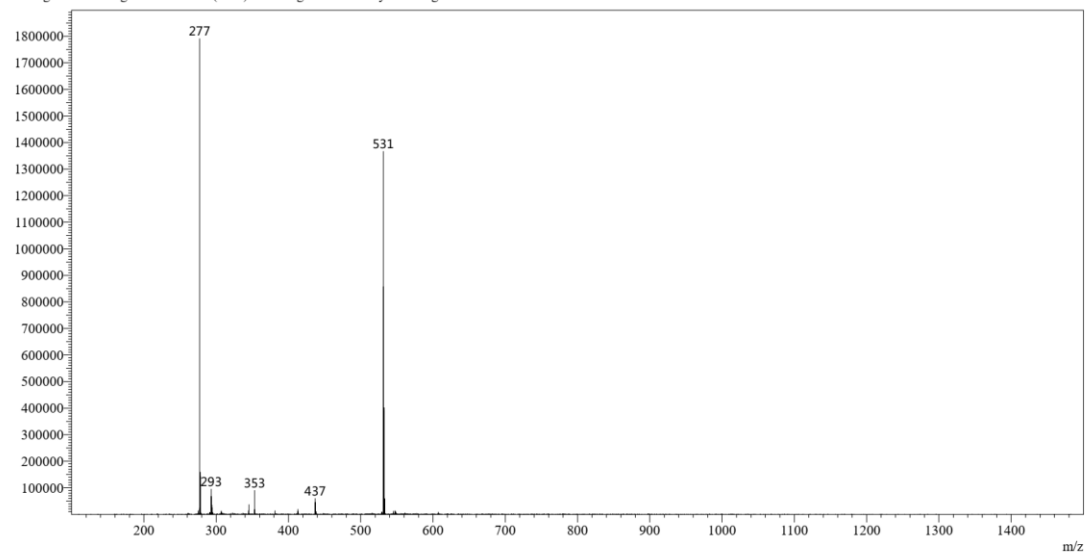
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Method File	: 阻尼管一级100-1500.lcm	

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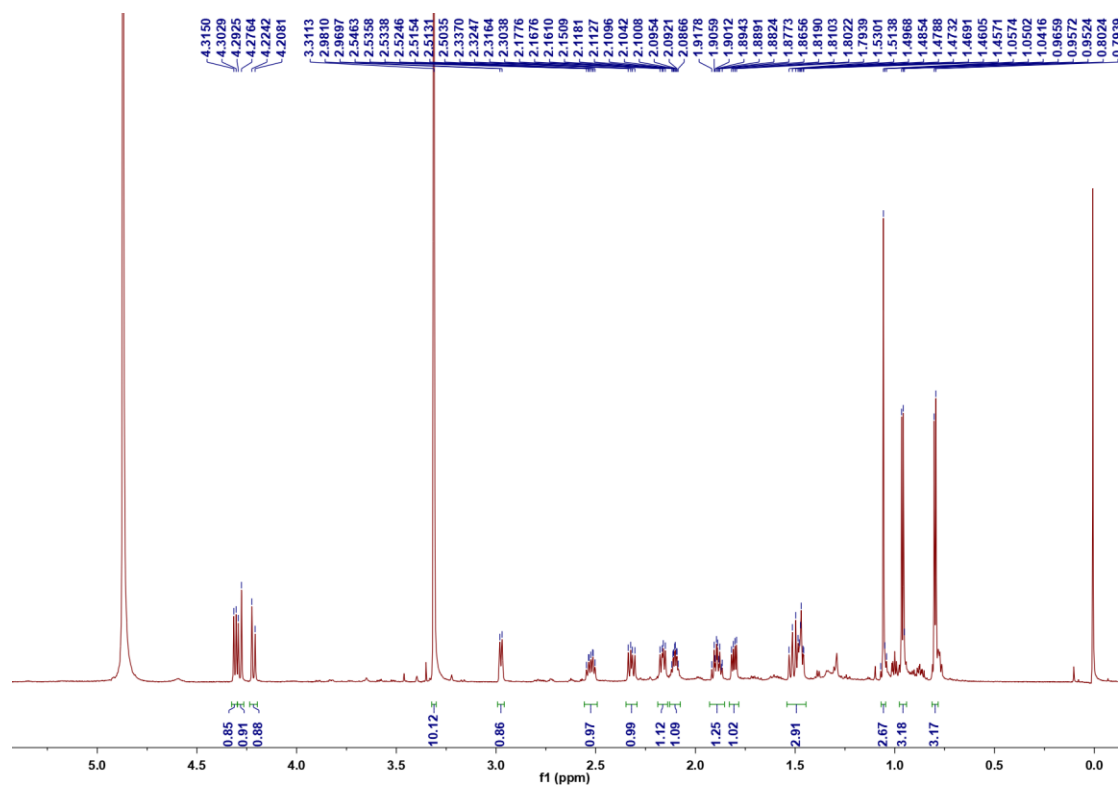
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Spectrum: Averaged 0.440-0.733(67-111)

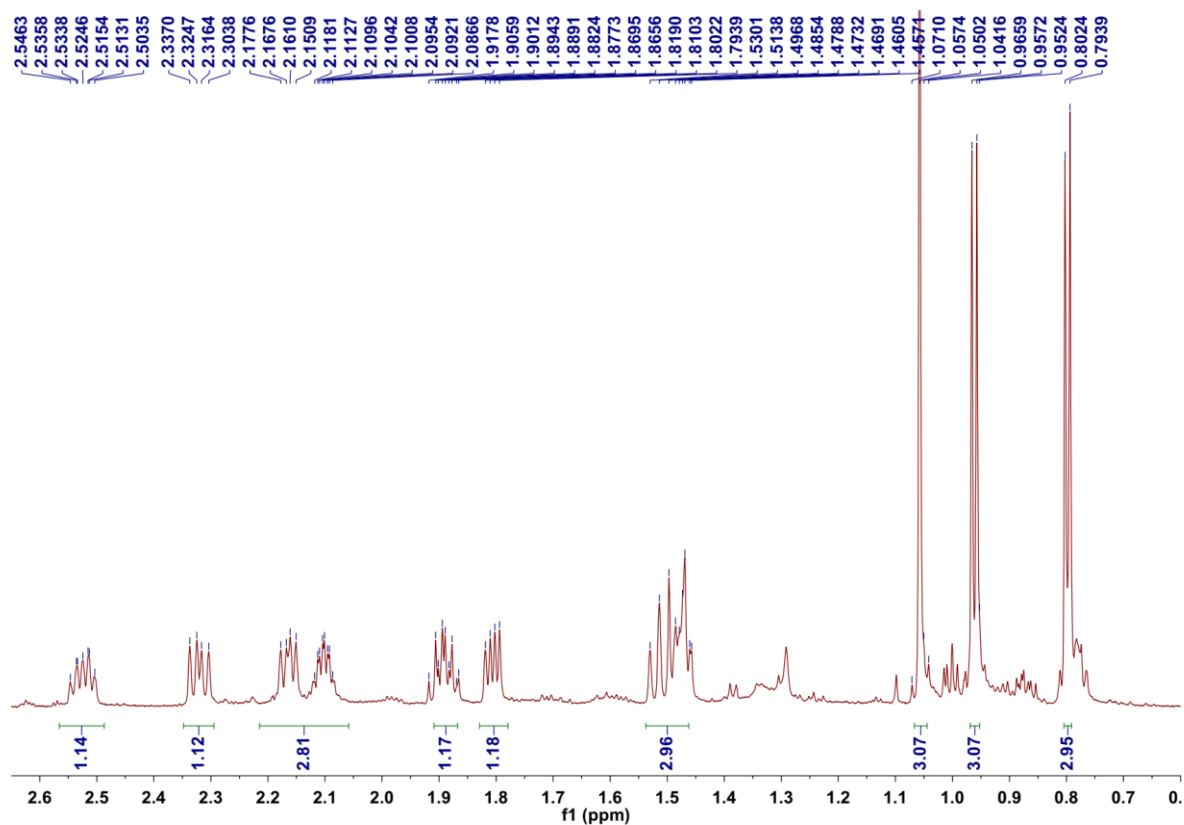
Background: Averaged 0.000-0.449(1-69) MS Stage: MS Polarity: Pos Segment1 - Event1 Precursor: ----- Cutoff:



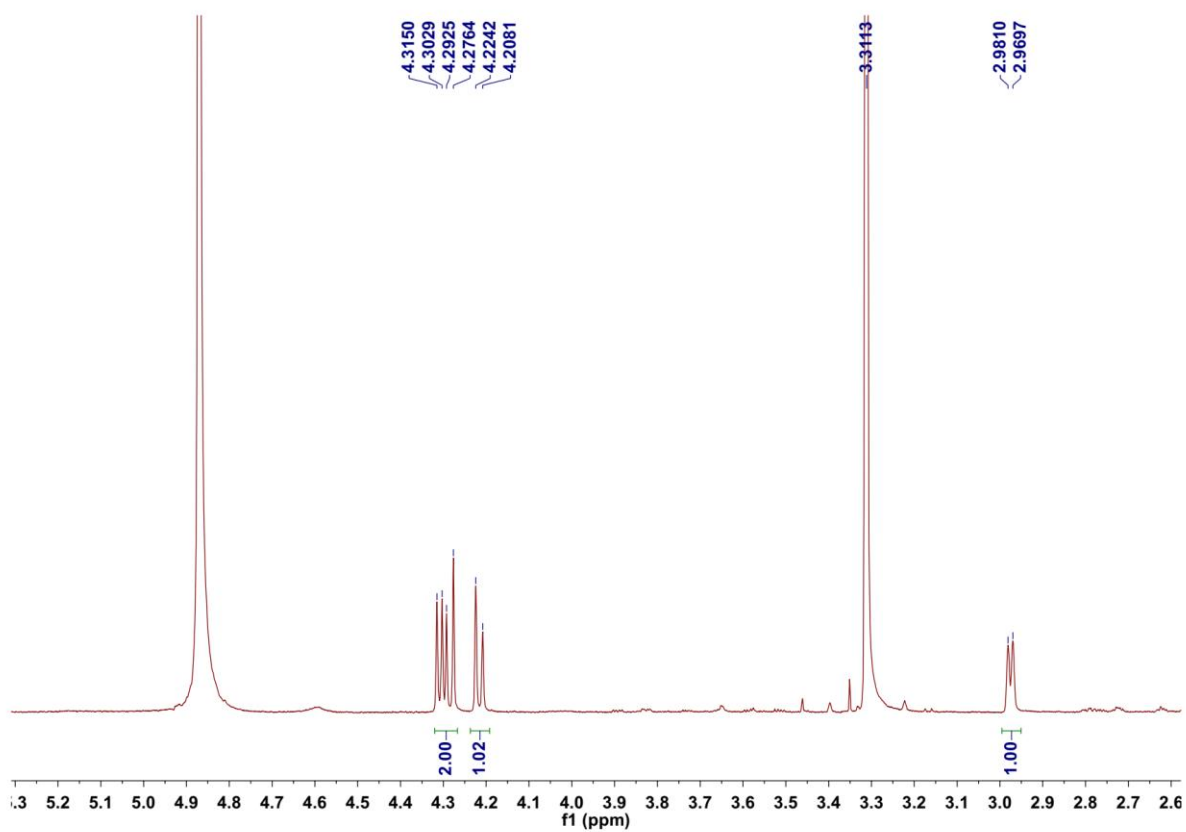
**Figure S2-3:** ESI-MS spectrum of **2**



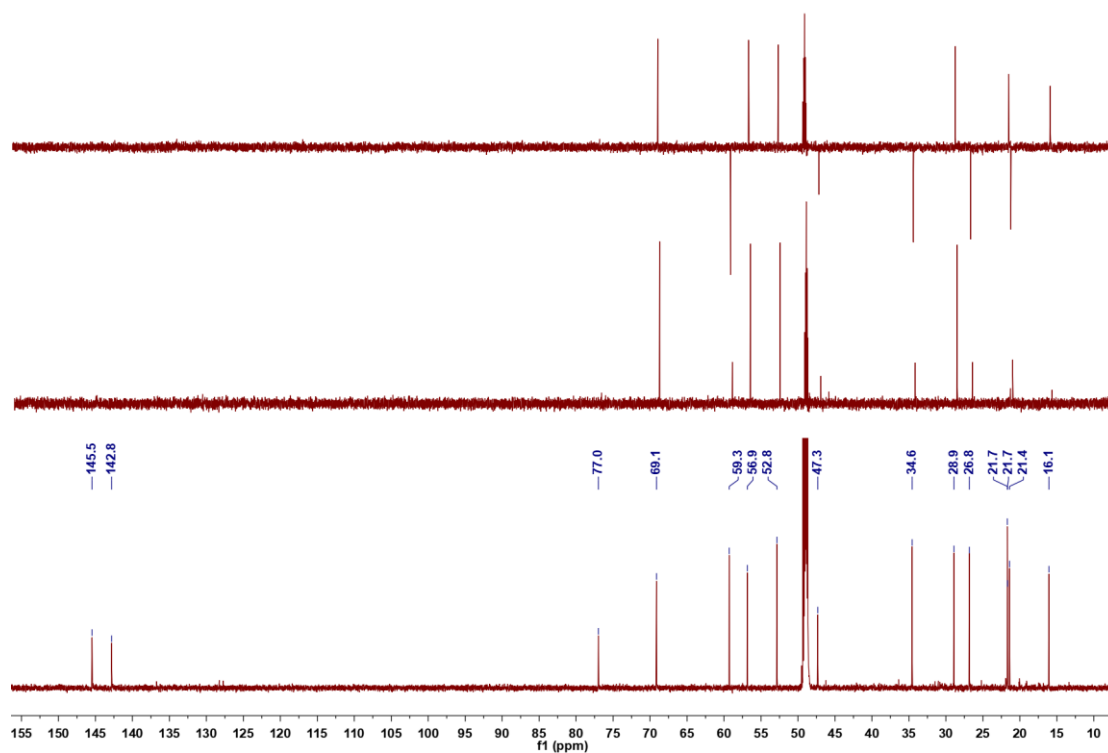
**Figure S2-4:**  $^1\text{H}$ -NMR (500 MHz,  $\text{CD}_3\text{OD}$ ) spectrum of **2**



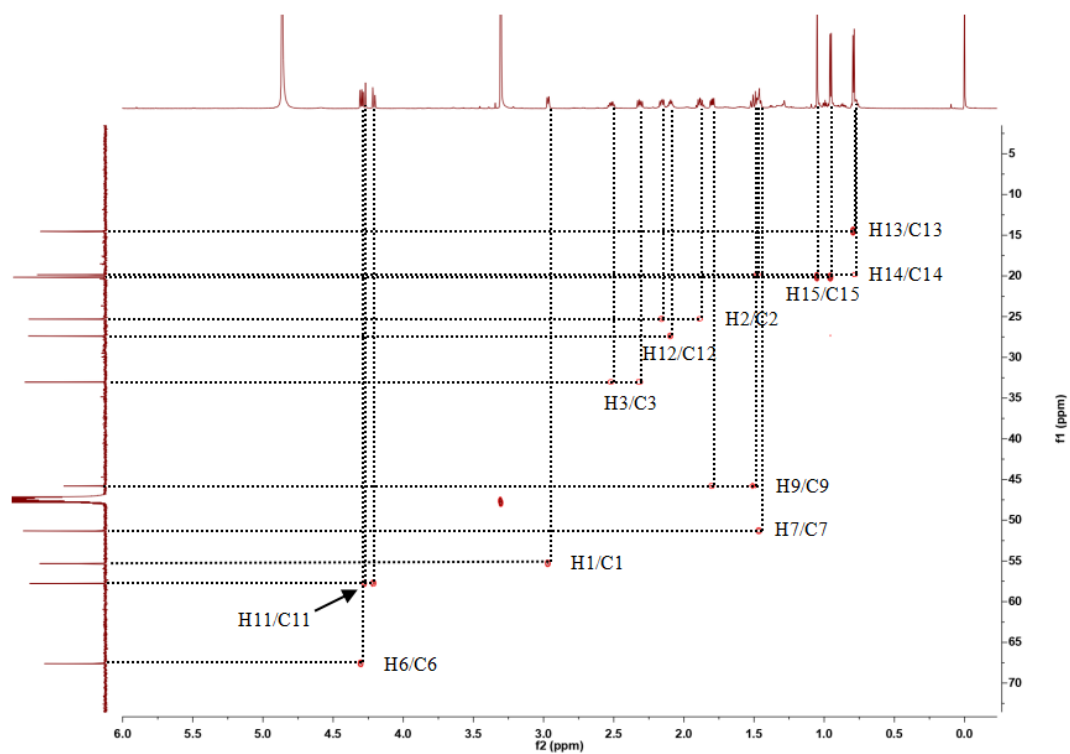
**Figure S2-5:**  $^1\text{H}$ -NMR (500 MHz,  $\text{CD}_3\text{OD}$ ) spectrum of **2** (From  $\delta_{\text{H}}$  0.70 ppm to  $\delta_{\text{H}}$  2.60 ppm)



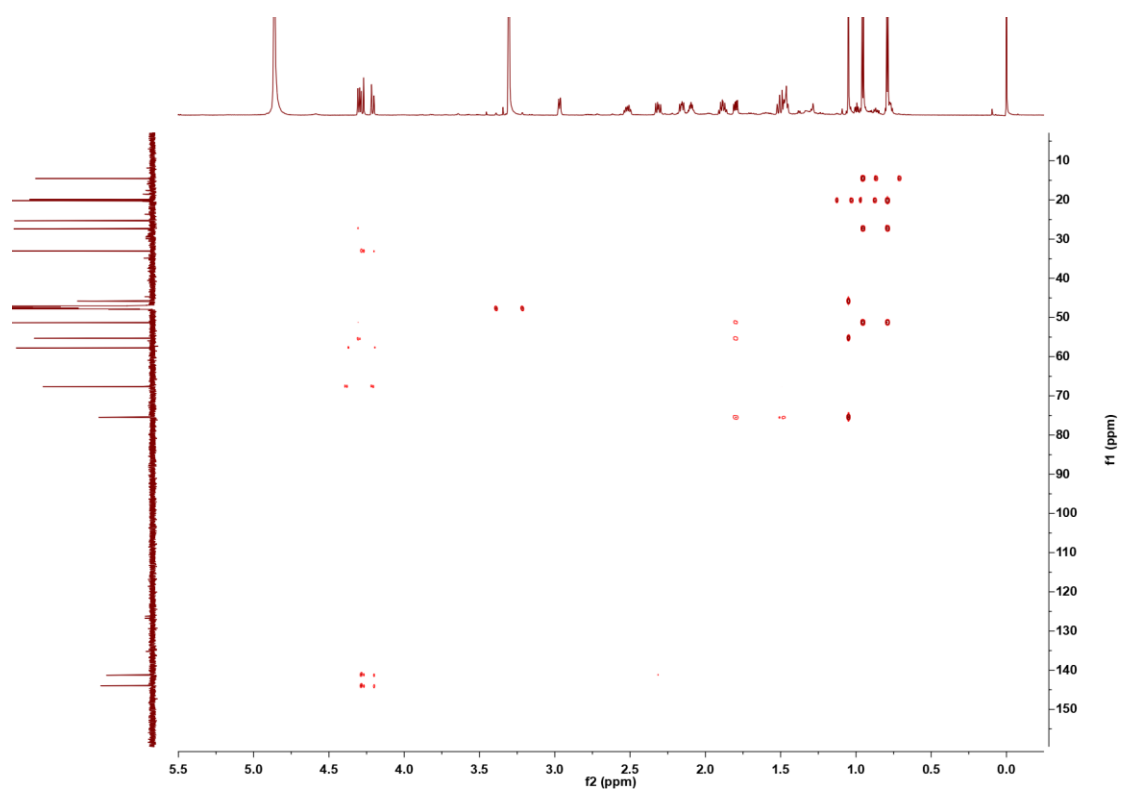
**Figure S2-6:**  $^1\text{H}$ -NMR (500 MHz,  $\text{CD}_3\text{OD}$ ) spectrum of **2** (From  $\delta_{\text{H}}$  2.80 ppm to  $\delta_{\text{H}}$  5.10 ppm)



**Figure S2-7:**  $^{13}\text{C}$ -NMR and DEPT (125 MHz,  $\text{CD}_3\text{OD}$ ) spectrum of **2**

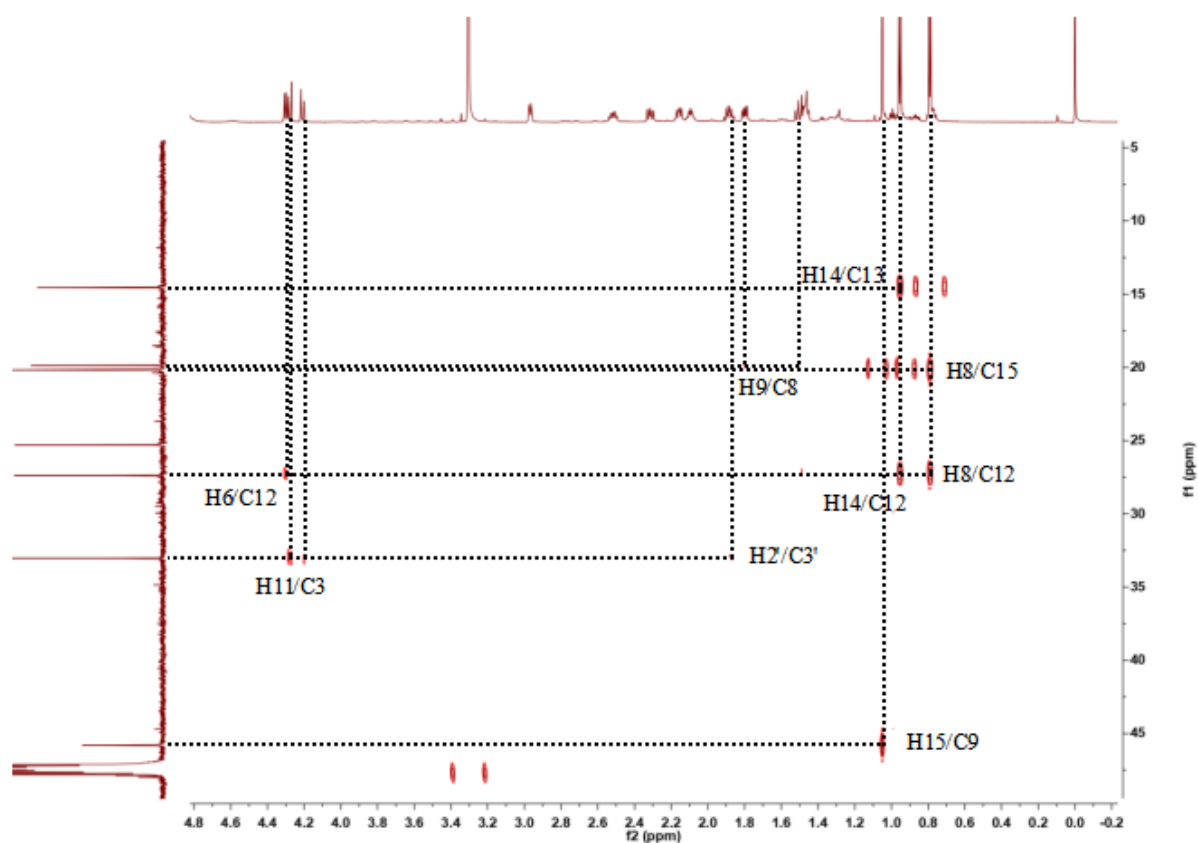


**Figure S2-8:** HSQC spectrum of **2**

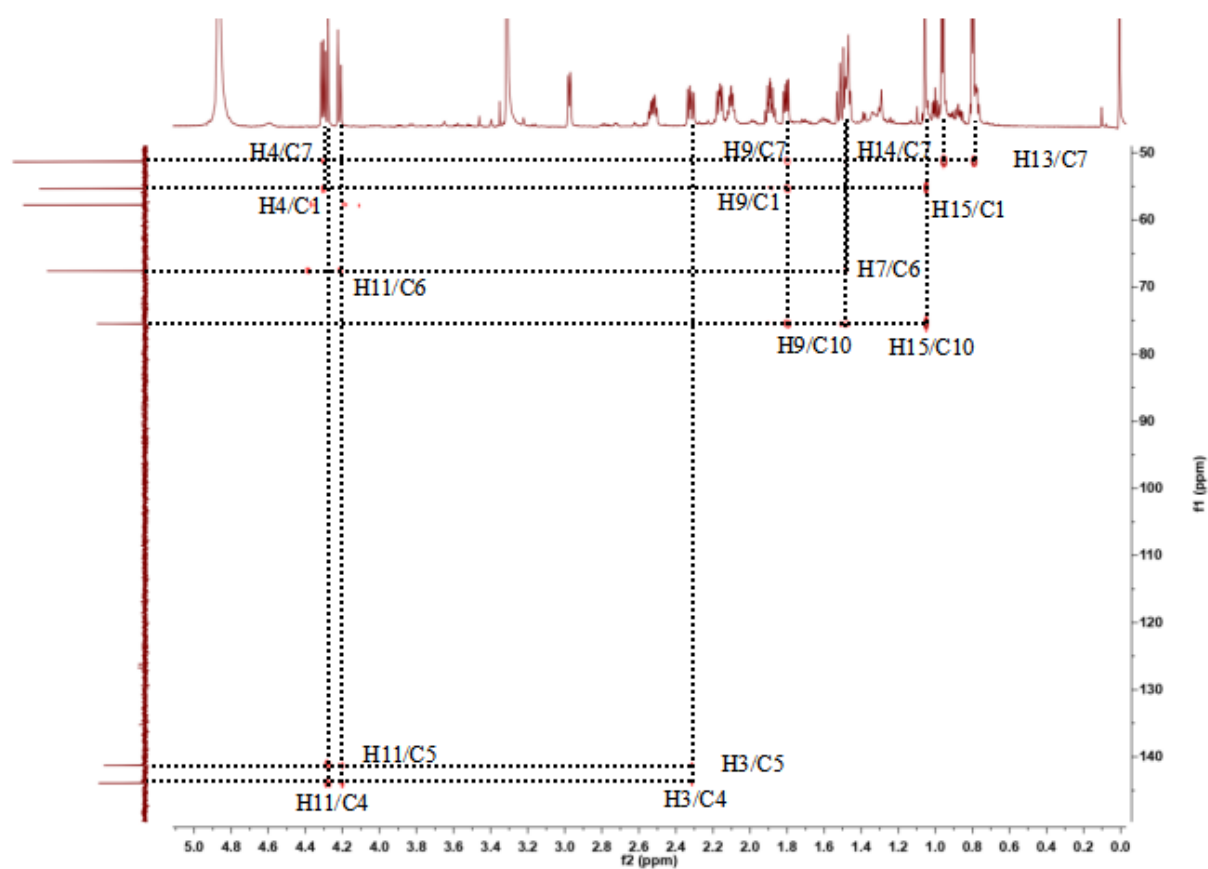


**Figure S2-9:** HMBC spectrum of **2**

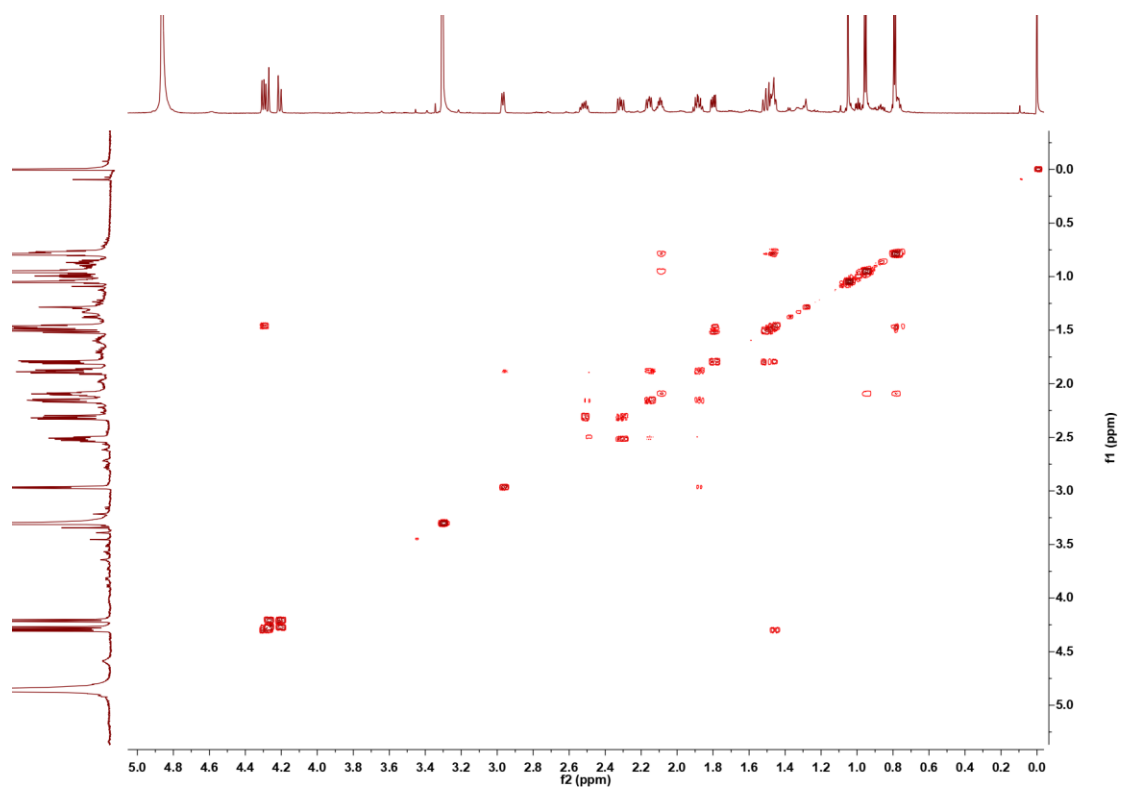




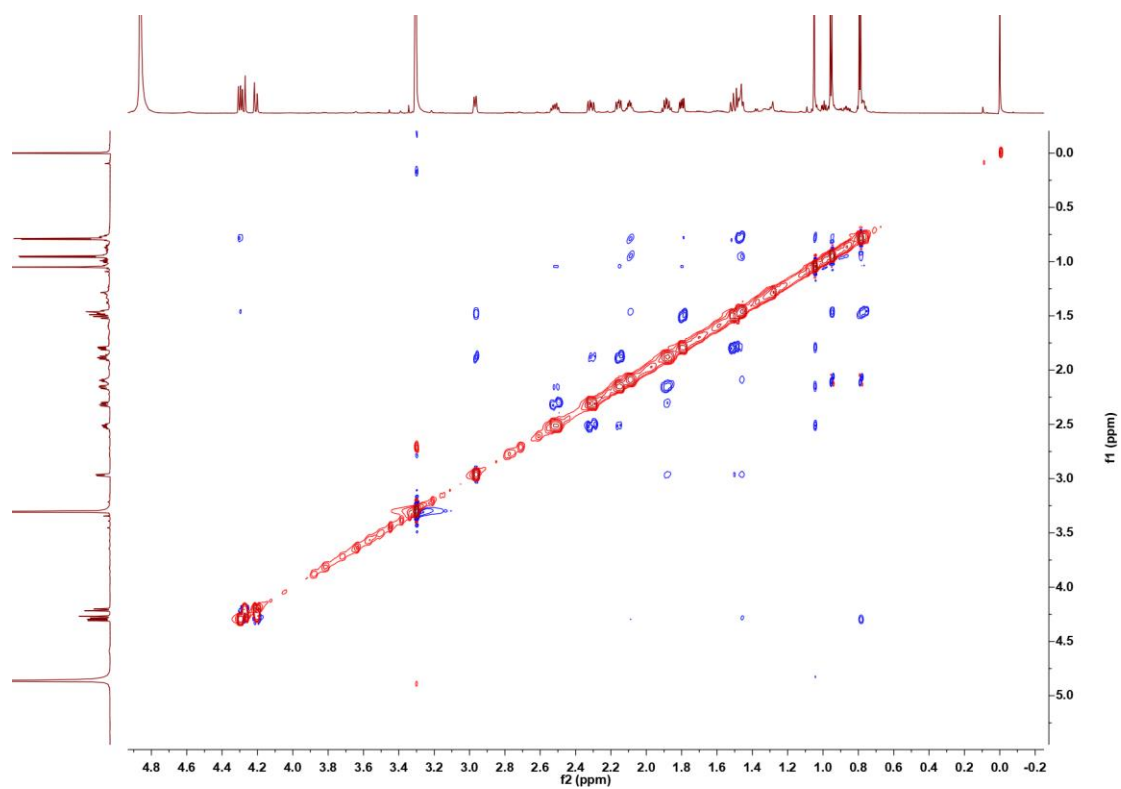
**Figure S2-10:** HMBC spectrum of **2** (From  $\delta_{\text{C}}$  5 ppm to  $\delta_{\text{C}}$  50 ppm)



**Figure S2-11:** HMBC spectrum of **2** (From  $\delta_{\text{C}}$  50 ppm to  $\delta_{\text{C}}$  150 ppm)



**Figure S2-12:**  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of **2**



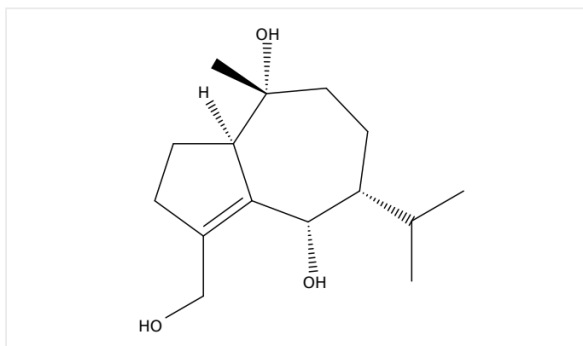
**Figure S2-13: ROESY spectrum of 2**

## Initiating Search

June 1, 2023, 10:55AM

Substances:

Filtered By:



Structure Match: As Drawn

## Search Tasks

Task	Search Type	View
Exported: Returned Substance Results + Filters (0)	Substances	<a href="#">View Results</a>

## Substances (0)

[View in SciFinder<sup>n</sup>](#)

We couldn't find any results. Please update your search query and try again.

Substances with (0) results

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**Figure S2-14:** Scifinder search report of 2