

Supporting Information

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Structurally Diverse Terpenoids from the Resins of *Populus euphratica*

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

Position	1		1'	
	δ_{H}	δ_{C}	δ_{H}	δ_{C}
1 α	2.75 dt (13.4, 3.6)	40.2	2.82 dt (13.6, 3.4)	39.1
1 β	1.01 m		0.97-1.00 m	
2 α	1.70-1.66 m	27.8	1.61-1.65 m	27.2
2 β	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	-	49.1	-	39.0
5 α	0.76 dd (12.0, 2.0)	56.3	0.70 br d (10.4)	55.0
6 α	1.47 dt (11.6, 2.8)	18.6	1.44-1.49 m	17.8
6 β	1.60 q (3.7, 3.0)		1.59-1.65 m	
7 α	1.70-1.66 m	34.3	1.59-1.65 m	33.0
7 β	1.47 dt (11.6, 2.8)		1.35-1.38 m	
8	-	46.4	-	45.5
9 α	2.46-2.41 m	63.2	2.26 s	61.0
10	-	38.6	-	36.3
11	-	202.9	-	199.5
12	5.50 s	128.9	5.72 s	129.1
13	-	174.2	-	165.0
14	-	31.9	-	49.3
15 α	1.37 m	37.4	1.91 d (14.0)	42.8
15 β			3.29 d (14.0)	
16 α	1.23-1.17 m	47.9	-	221.5
16 β	1.72 m	72.4	-	76.5
17	-			
18	2.46-2.41 m	49.5	2.89 dd (14.0, 4.0)	52.4
19 α	2.16 dt (8.4, 2.3)	27.6	1.44-1.49 m	45.8
19 β			1.32-1.33 m	
20	-	44.8	-	30.7
21 α	1.60 q (3.7, 3.0)	27.3	1.59-1.65 m	36.3
21 β	1.29-1.27 m		1.35-1.38 m	
22 α	1.75 dd (9.5, 4.3)	38.2	2.12 dt (12.4, 3.2, 3.2)	30.4
22 β	1.55-1.50 m		1.42-1.46 m	
23	1.79 s	28.7	1.00 s	28.1
24	0.79 s	16.3	0.80 s	15.6
25	1.11 s	16.6	1.12 s	16.0
26	1.13 s	20.3	1.24 s	19.6
27	1.00 s	24.2	1.38 s	24.7
28	1.37 s	23.6	0.97 s	23.5
29	0.93 s	32.8	0.91 s	32.1

The ^1H and ^{13}C NMR data of compound **1** were recorded at 500 MHz, with CD_3OD as solvent; the ^1H and ^{13}C NMR data of the compound **1'** reported in the literature [1] were recorded with a Bruker AM-400, with CDCl_3 as solvent.

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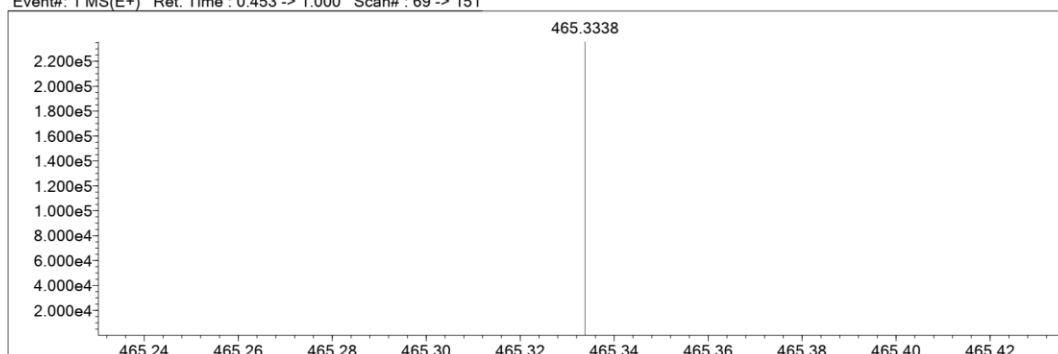
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B	3	0	0	Mg	2	0	0	Cu	2	0	0	Ir	3	0	0	
C	4	5	60	Si	4	0	0	Se	2	0	0					
N	3	0	5	P	3	0	0	Br	1	0	0					
O	2	0	30	S	2	0	0	Pd	2	0	0					

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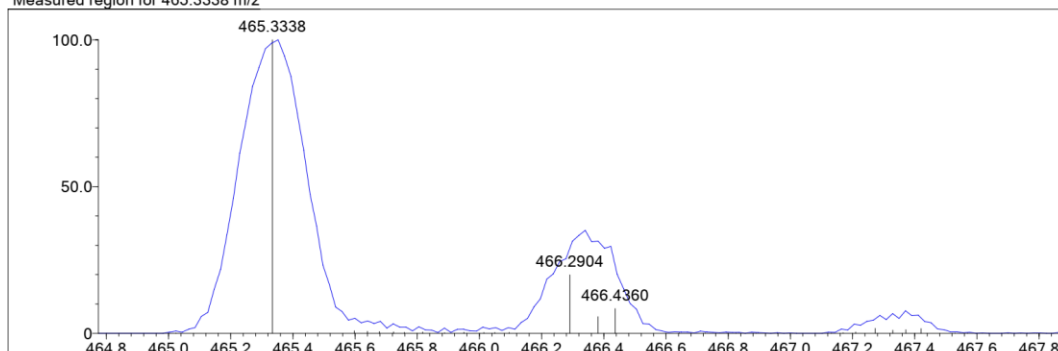
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Electron Ions: both
 Use MSn Info: yes
 Isotope Res: 10000
 Max Results: 30

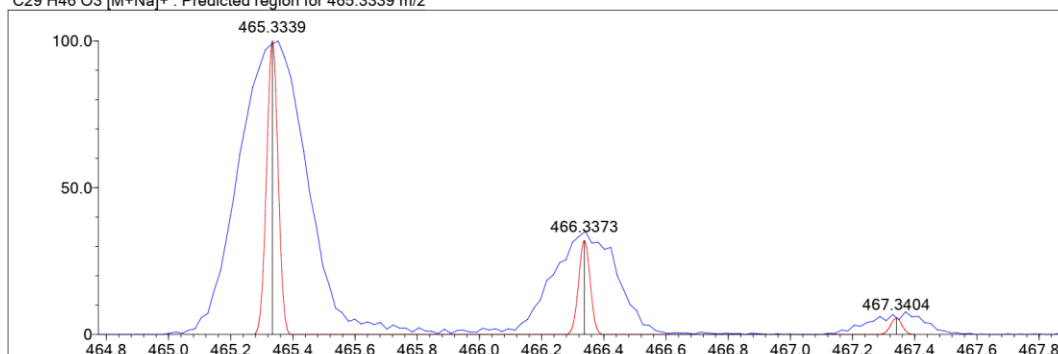
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Measured region for 465.3338 m/z



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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Method File	: 阻尼管一级100-1500.lcm	

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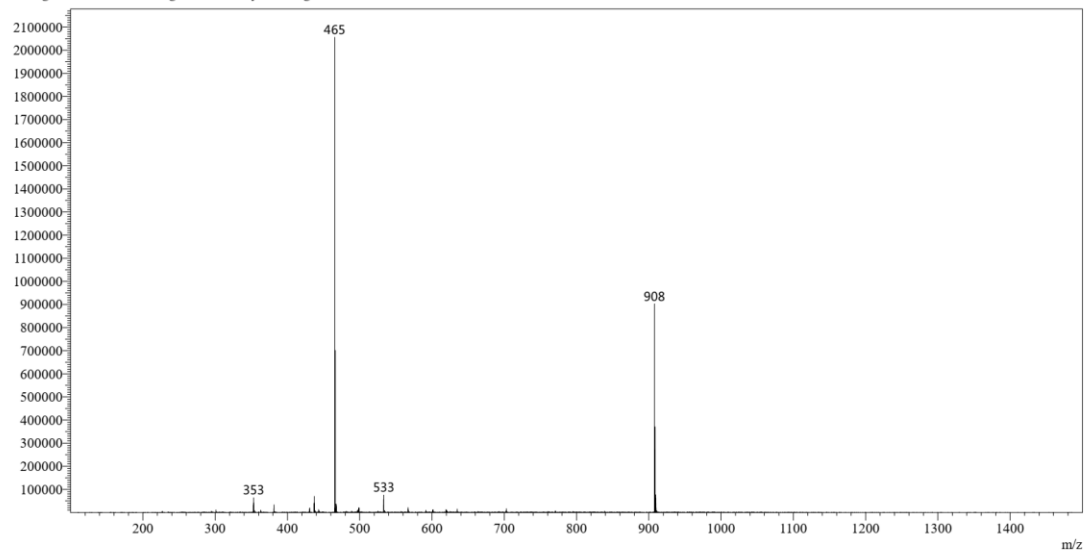


Figure S1-3: ESI-MS spectrum of **1**

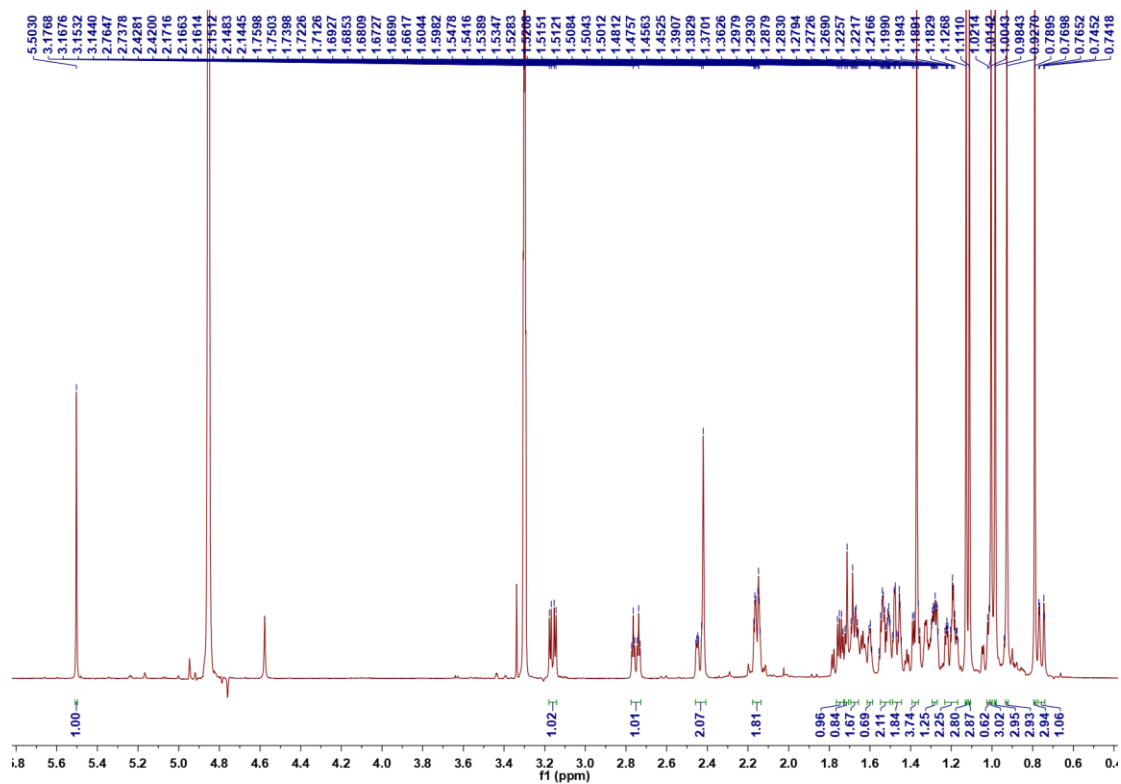


Figure S1-4: $^1\text{H-NMR}$ (500 MHz, CD_3OD) spectrum of **1**

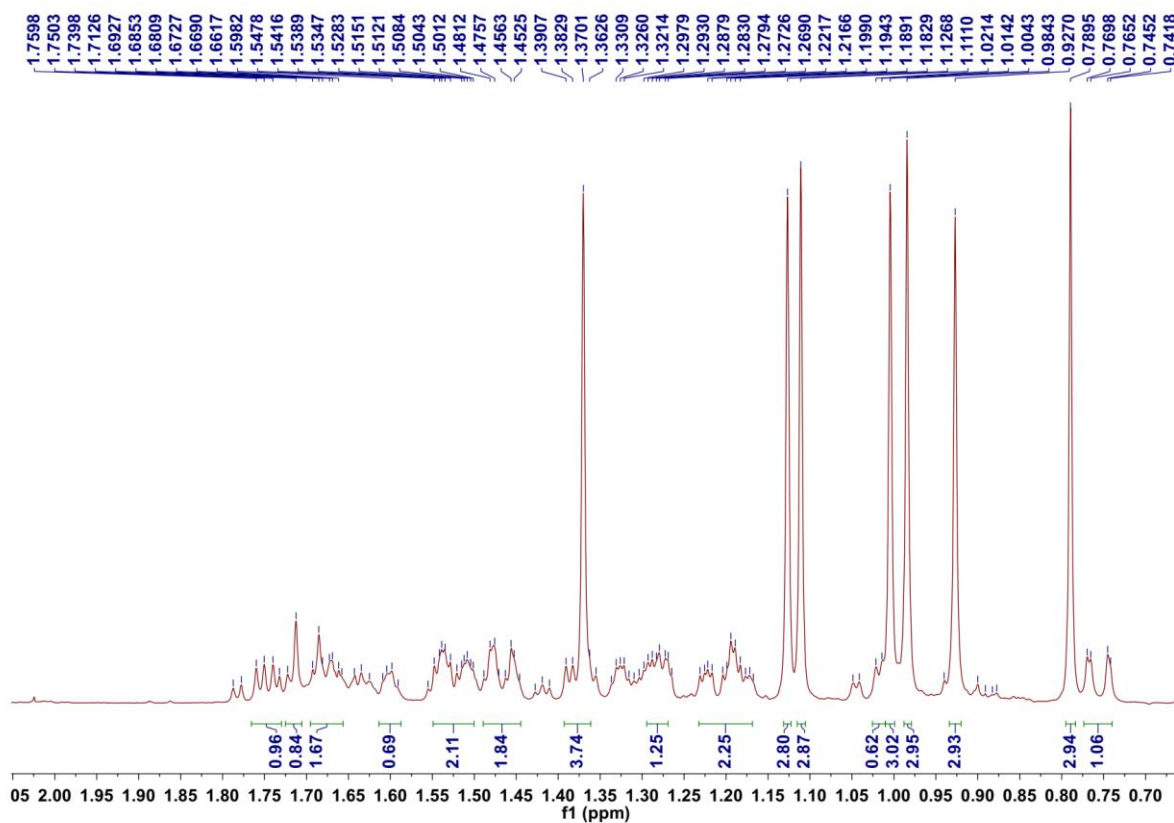


Figure S1-5: ¹H-NMR (500 MHz, CD₃OD) spectrum of **1** (From δ_{H} 0.70 ppm to 2.05 ppm)

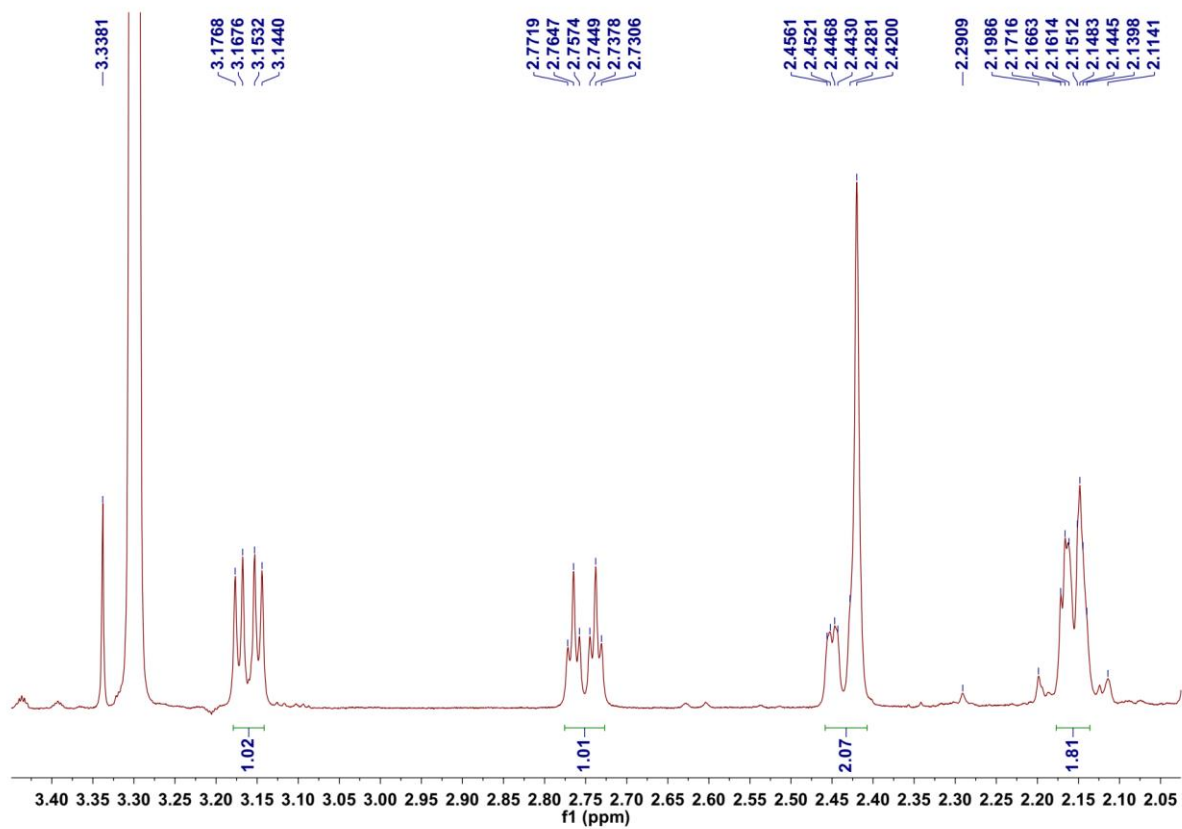


Figure S1-6: $^1\text{H-NMR}$ (500 MHz, CD_3OD) spectrum of **1** (From δ_{H} 2.05 ppm to 3.40 ppm)

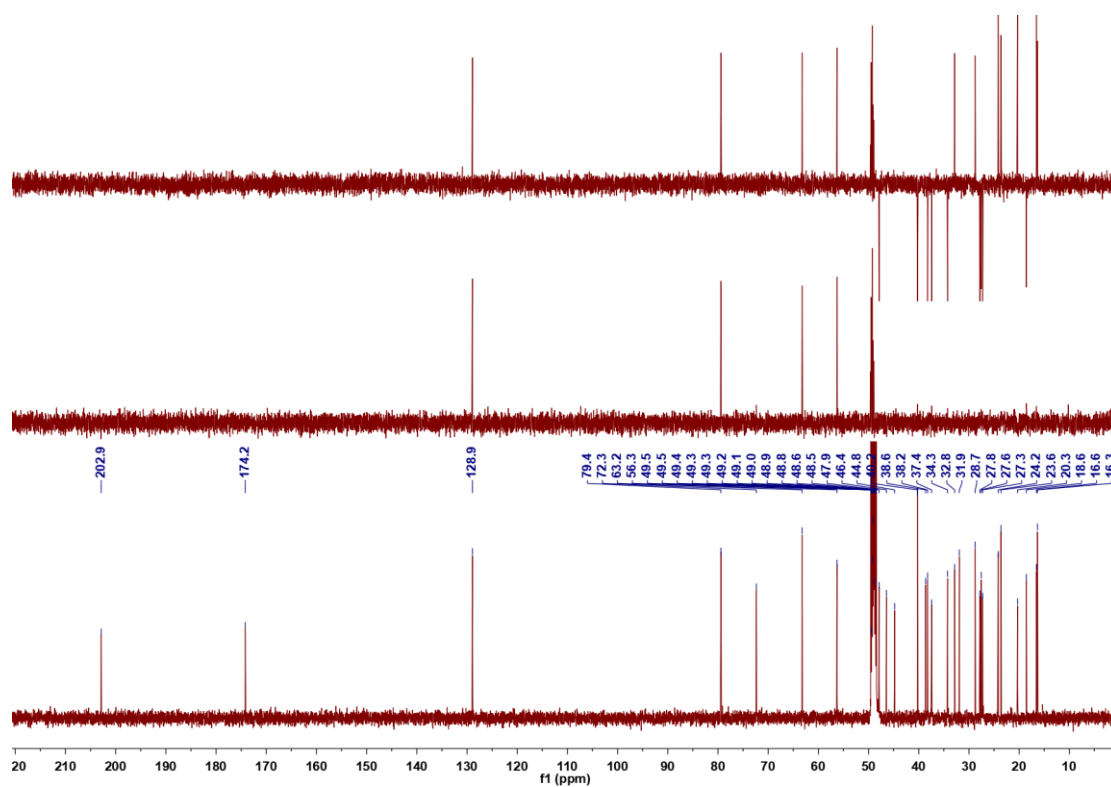


Figure S1-7: ^{13}C -NMR and DEPT (125 MHz, CD_3OD) spectrum of **1**

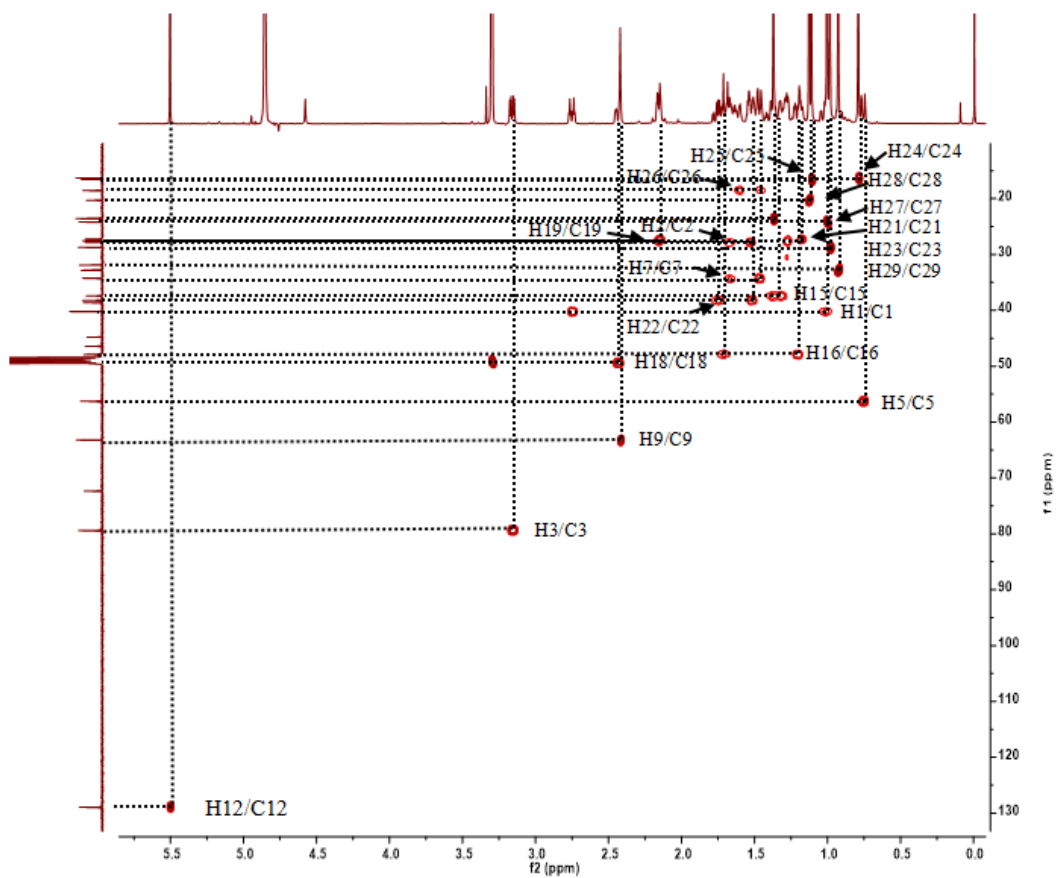


Figure S1-8: HSQC spectrum of 1

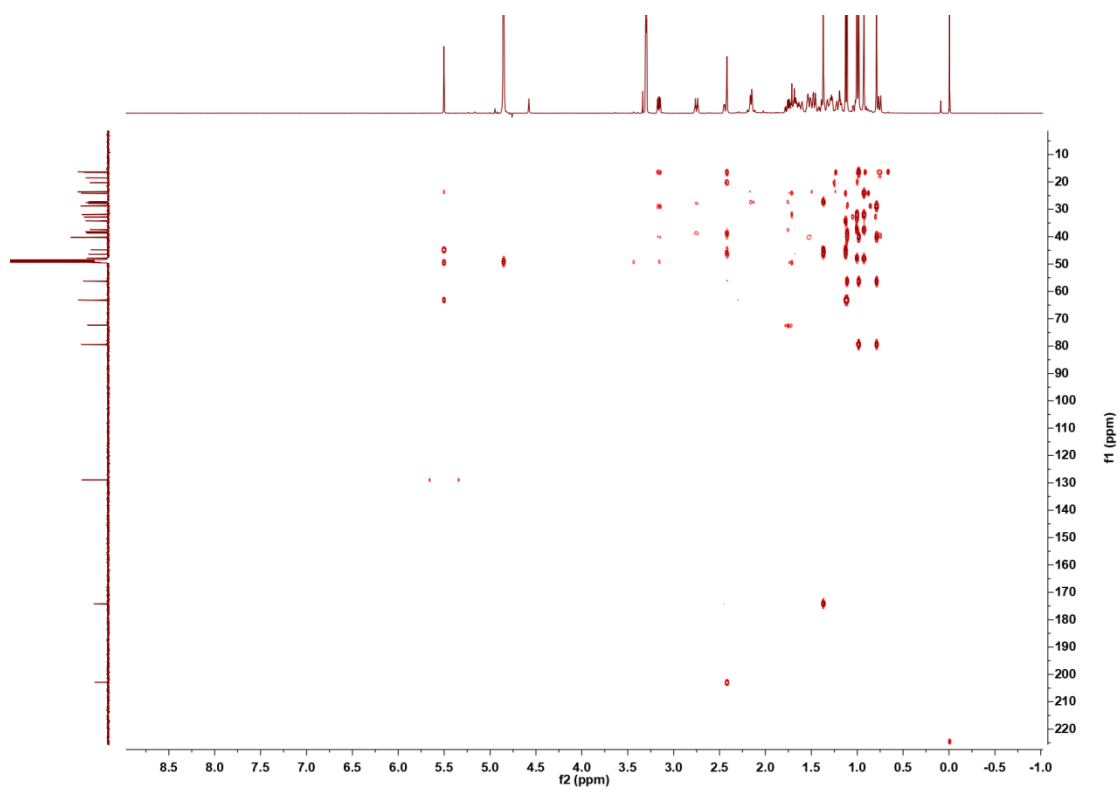


Figure S1-9: HMBC spectrum of **1**

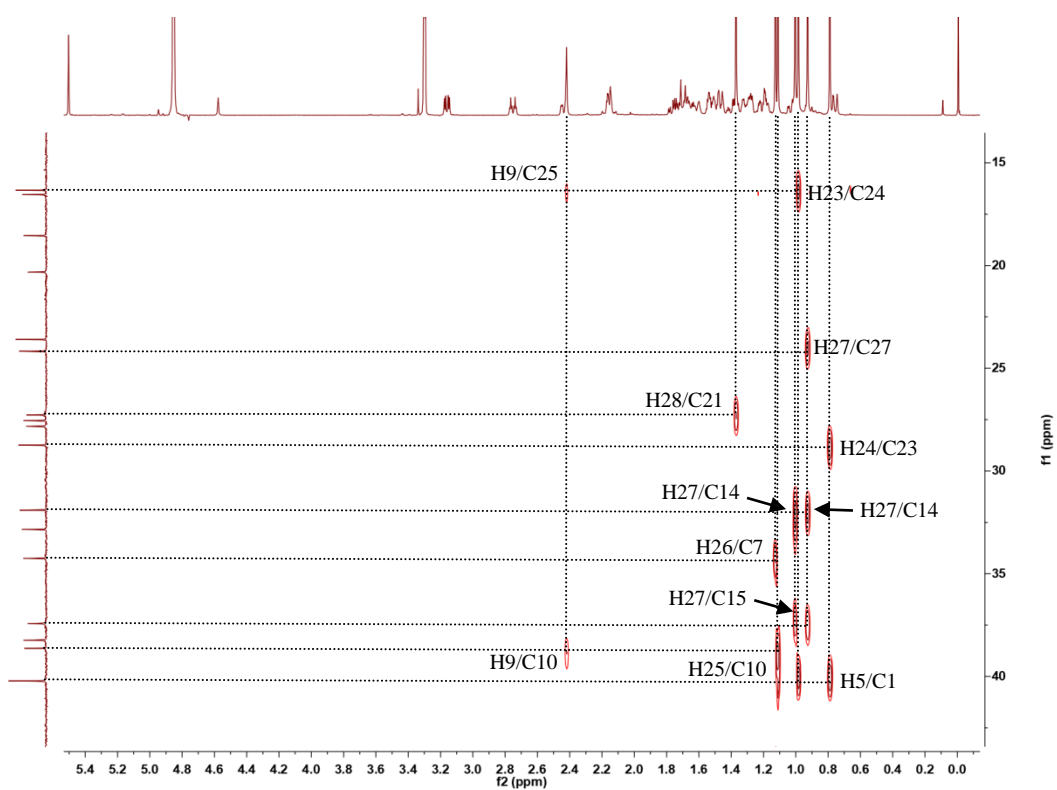


Figure S1-10: HMBC spectrum of **1** (From δ_c 15 ppm to δ_c 45ppm)

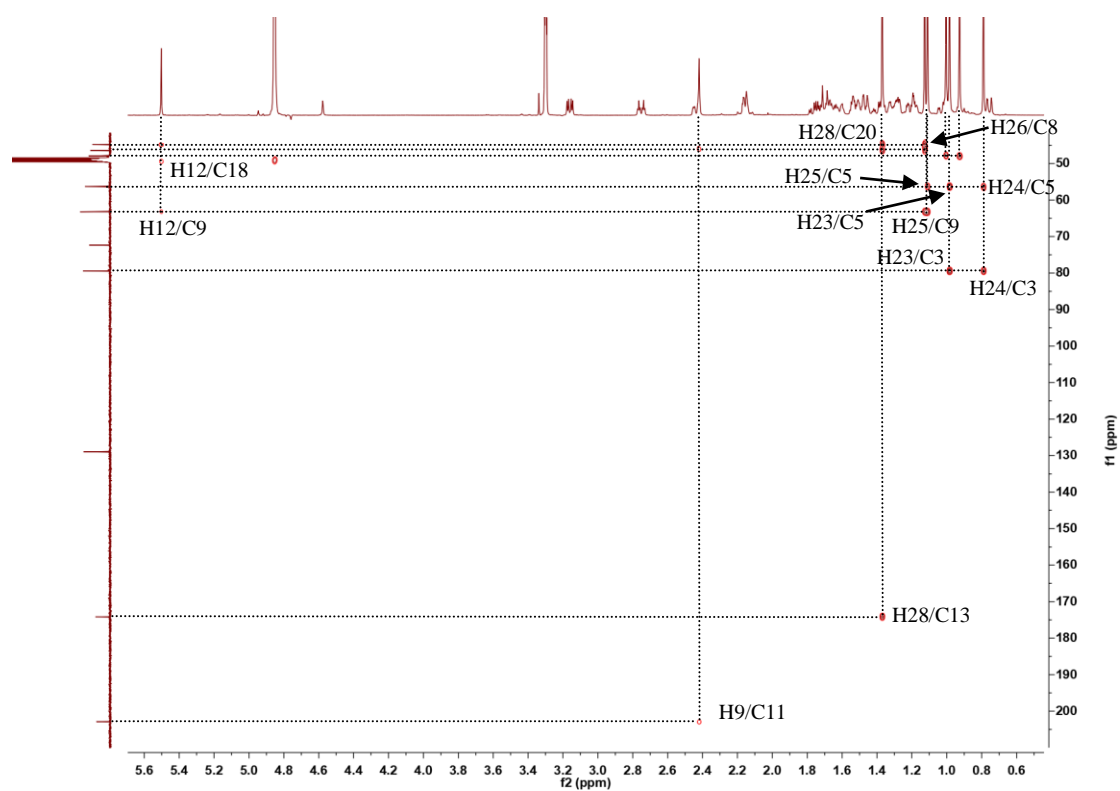


Figure S1-11: HMBC spectrum of **1** (From δ_C 45 ppm to δ_C 210 ppm)

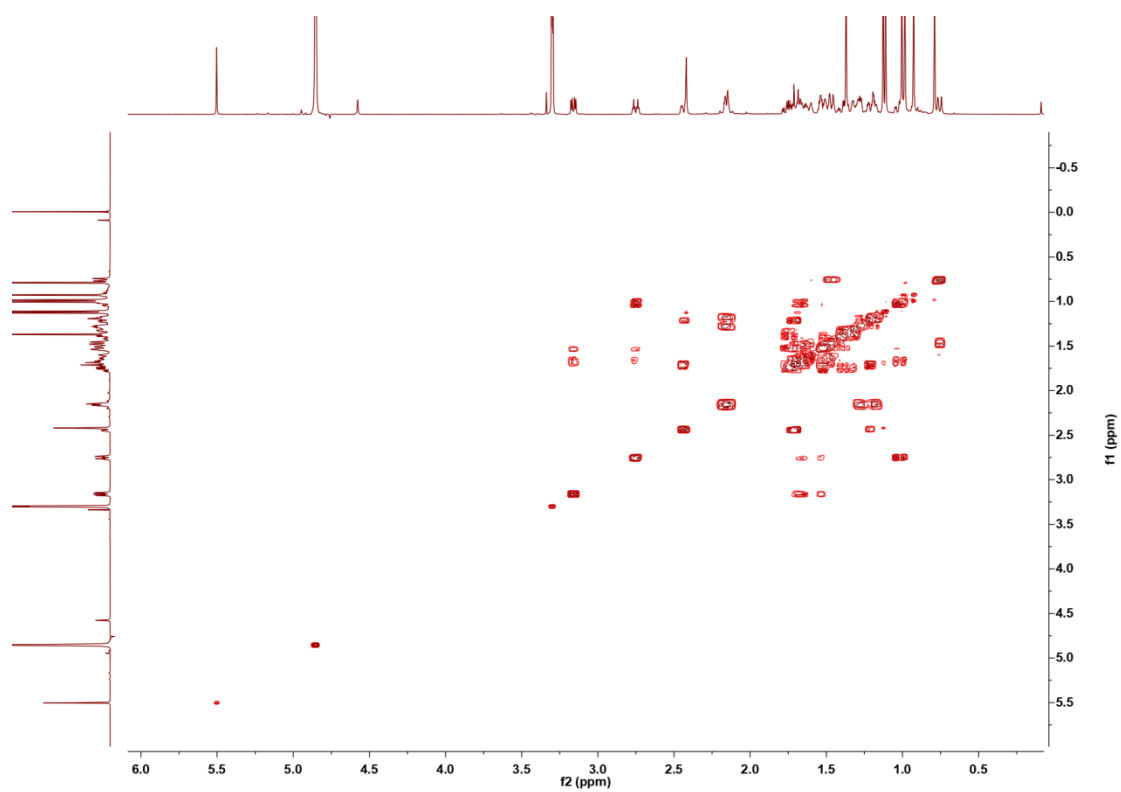


Figure S1-12: ^1H - ^1H COSY spectrum of **1**

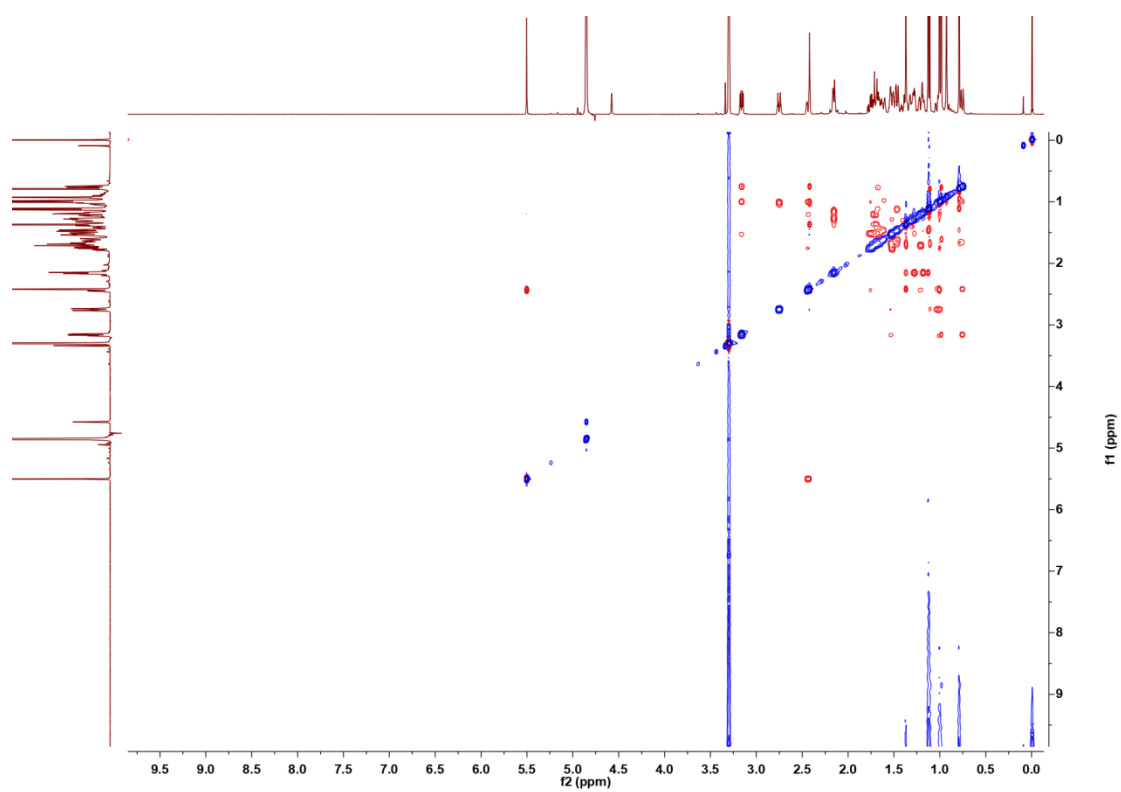


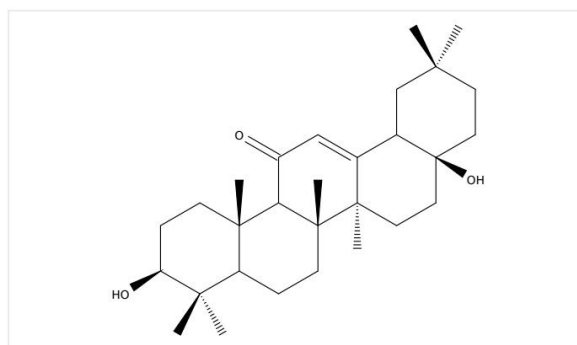
Figure S1-13: ROESY spectrum of 1

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	View Results

 Substances (0)[View in SciFinder®](#)

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

Substances with (0) results

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Figure S1-14: Scifinder search report of 1

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

Position	2		2'	
	δ_{H}	δ_{C}	δ_{H}	δ_{C}
1	2.98 d (16)	56.9	1.99 dd (8.7, 18.1)	54.8
2 α	2.16 dd (13.3, 5.3)	26.8	1.46 ddd (4.9, 10.6, 22.6)	25.6
2 β	1.93-1.86 m		1.52-1.58 m	
3 α	2.56-2.49 m	34.6	1.63-1.65 m	30.6
3 β	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 α	4.33 - 4.26 m	69.1	0.82 dd (12.7, 23.1)	21.3
6 β			1.65 br. d (10.0)	
7	1.54 - 1.44 m	52.8	1.73-1.76 m	43.0
8 α	0.80d (6.8)	21.4	1.05-1.08 m	23.9
8 β	1.54 - 1.44 m		1.74-1.77 m	
9 α	1.81dd (13.4, 6.5)	47.3	1.73-1.54 m	33.8
9 β	1.54 - 1.44 m		1.30-1.33 m	
10	-	77	-	72.4
11 α	4.22 d (16.0)	59.3	-	74.5
11 β	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 ^1H and ^{13}C NMR data of compound **2** were recorded at 500 MHz, with CD_3OD as solvent; the ^1H and ^{13}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.

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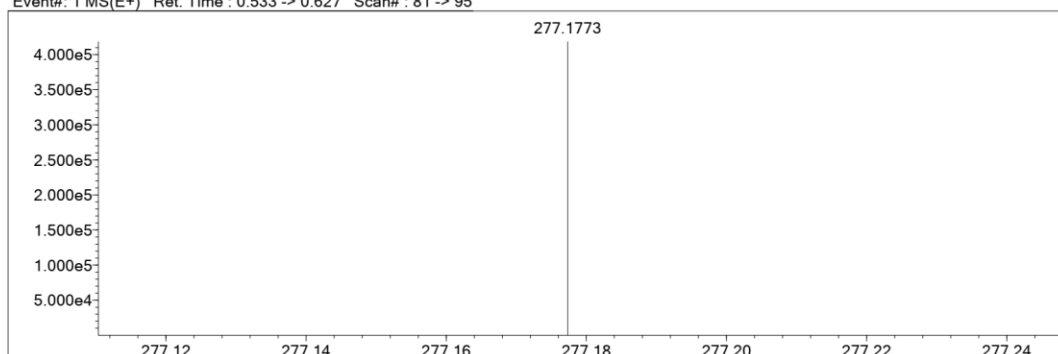
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B	3	0	0	Mg	2	0	0	Cu	2	0	0	Ir	3	0	0	
C	4	5	60	Si	4	0	0	Se	2	0	0					
N	3	0	5	P	3	0	0	Br	1	0	0					
O	2	0	30	S	2	0	0	Pd	2	0	0					

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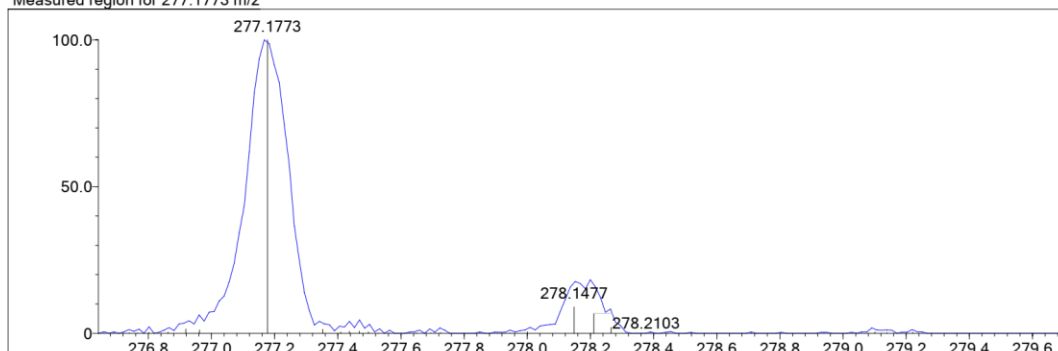
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Electron Ions: both
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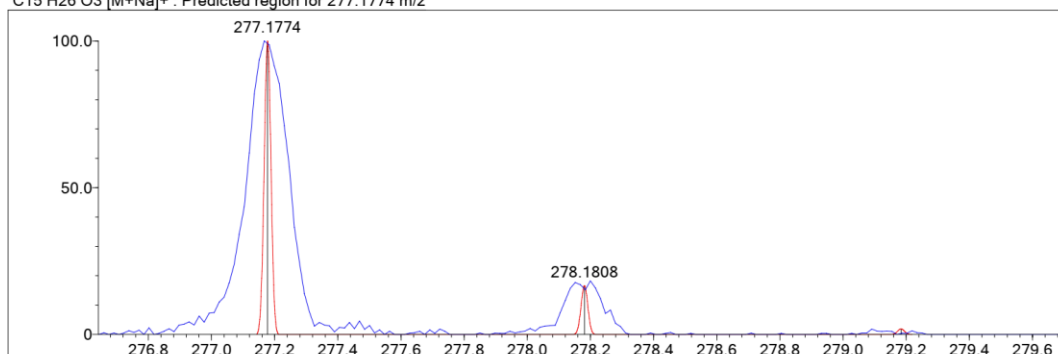
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Measured region for 277.1773 m/z



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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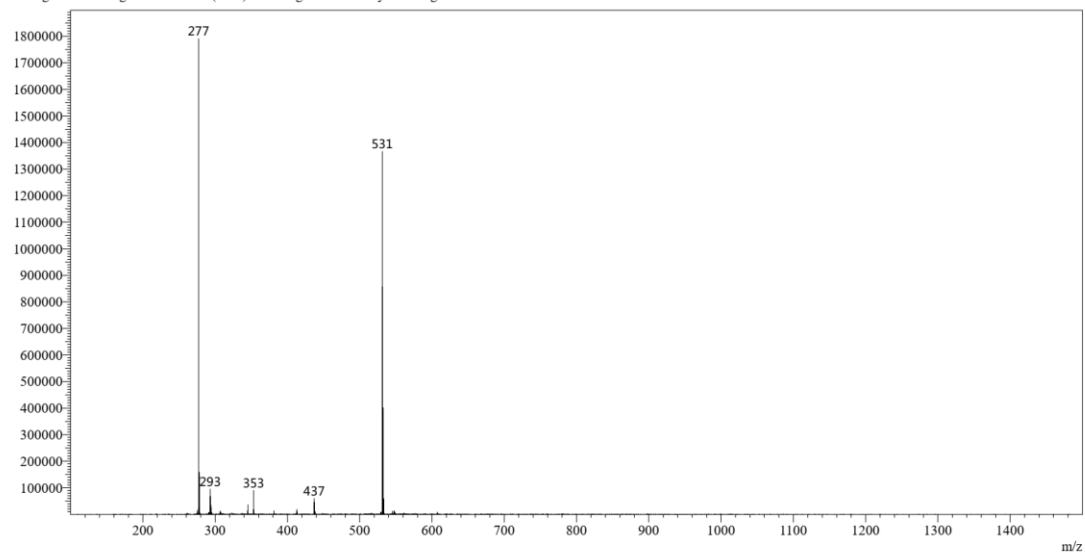


Figure S2-3: ESI-MS spectrum of 2

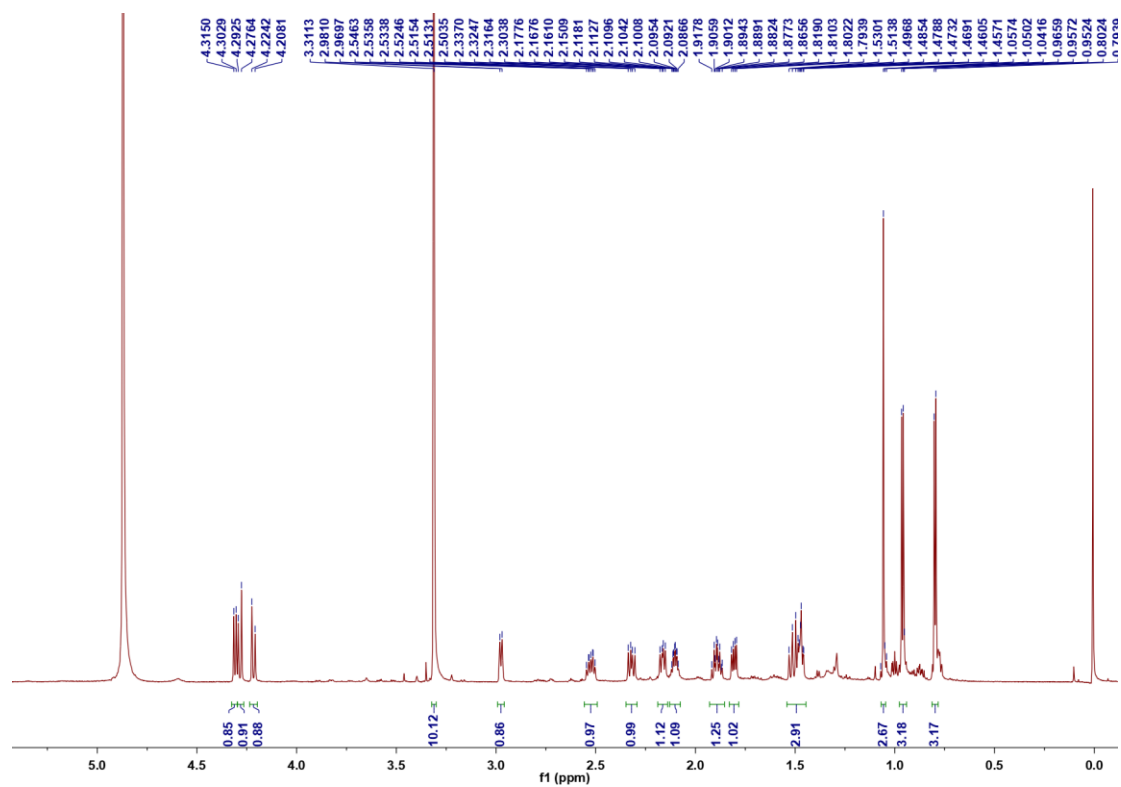


Figure S2-4: $^1\text{H-NMR}$ (500 MHz, CD_3OD) spectrum of **2**

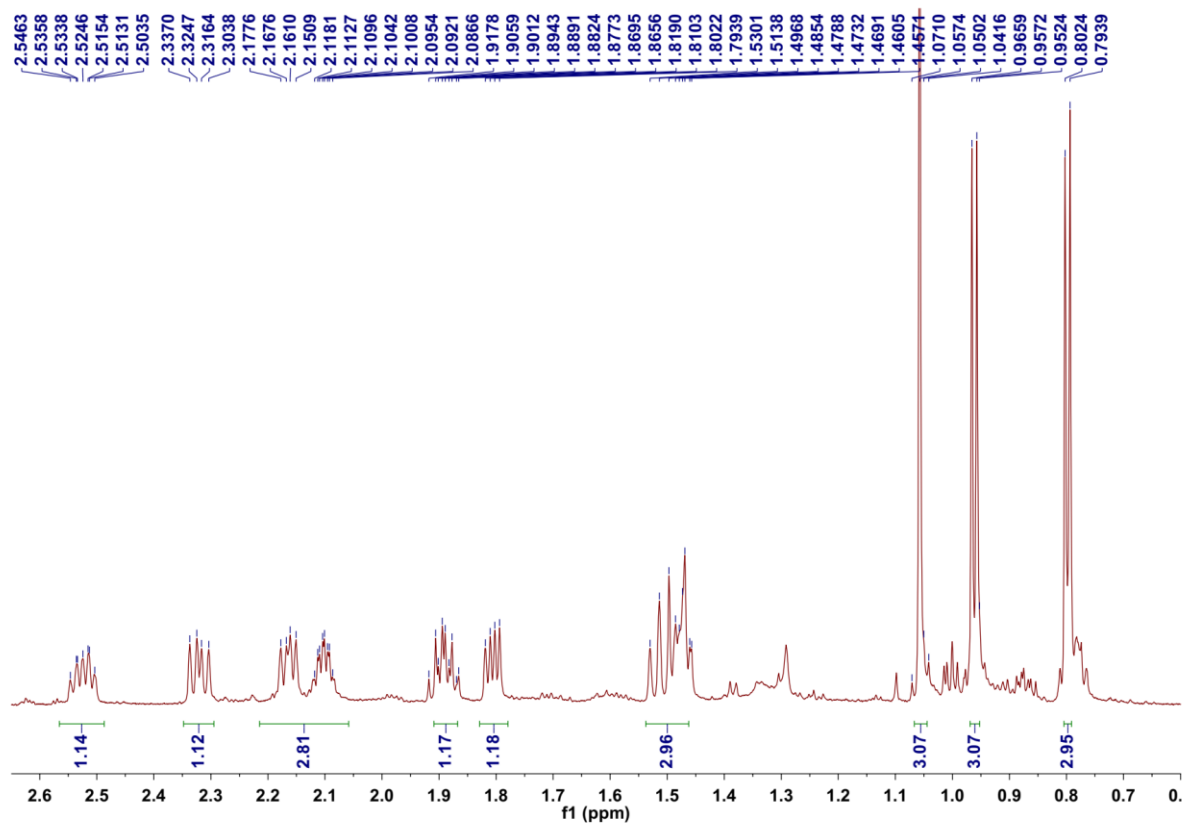


Figure S2-5: $^1\text{H-NMR}$ (500 MHz, CD_3OD) spectrum of **2** (From δ_{H} 0.70 ppm to δ_{H} 2.60 ppm)

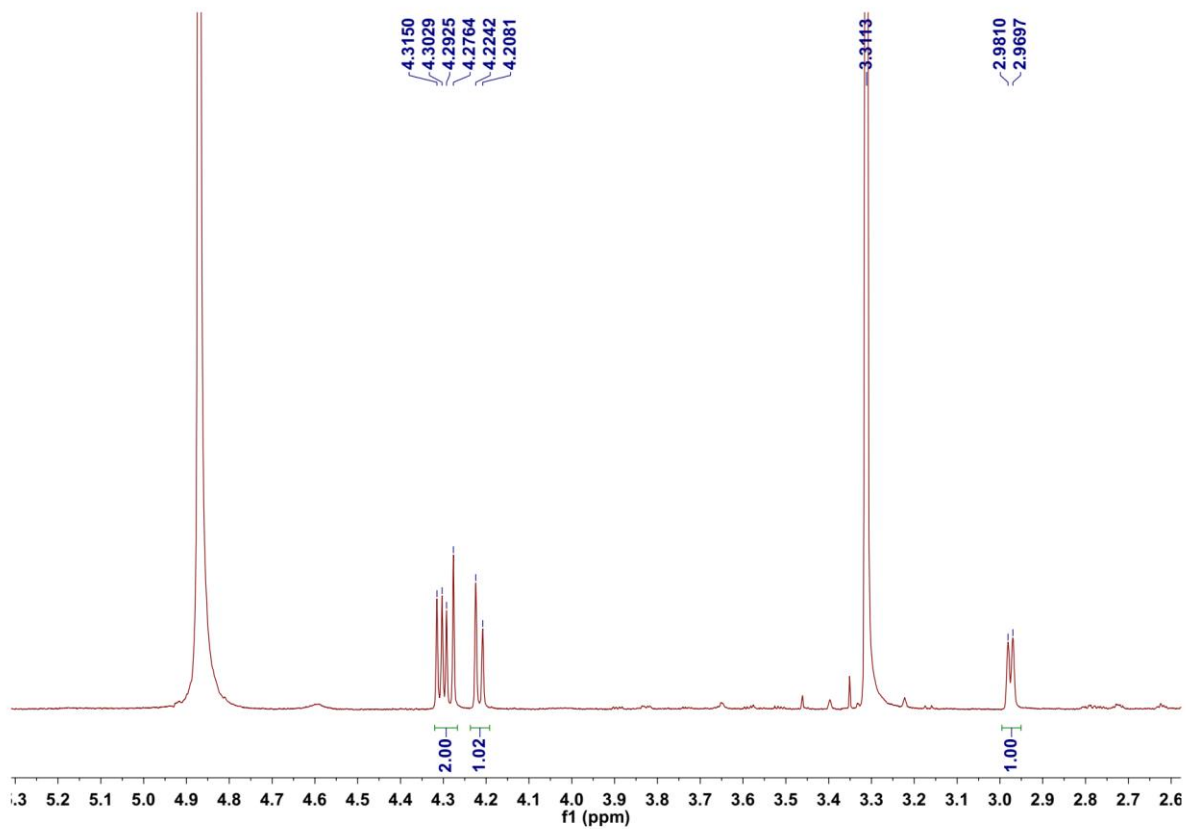


Figure S2-6: ¹H-NMR (500 MHz, CD₃OD) spectrum of **2** (From δ_{H} 2.80 ppm to δ_{H} 5.10 ppm)

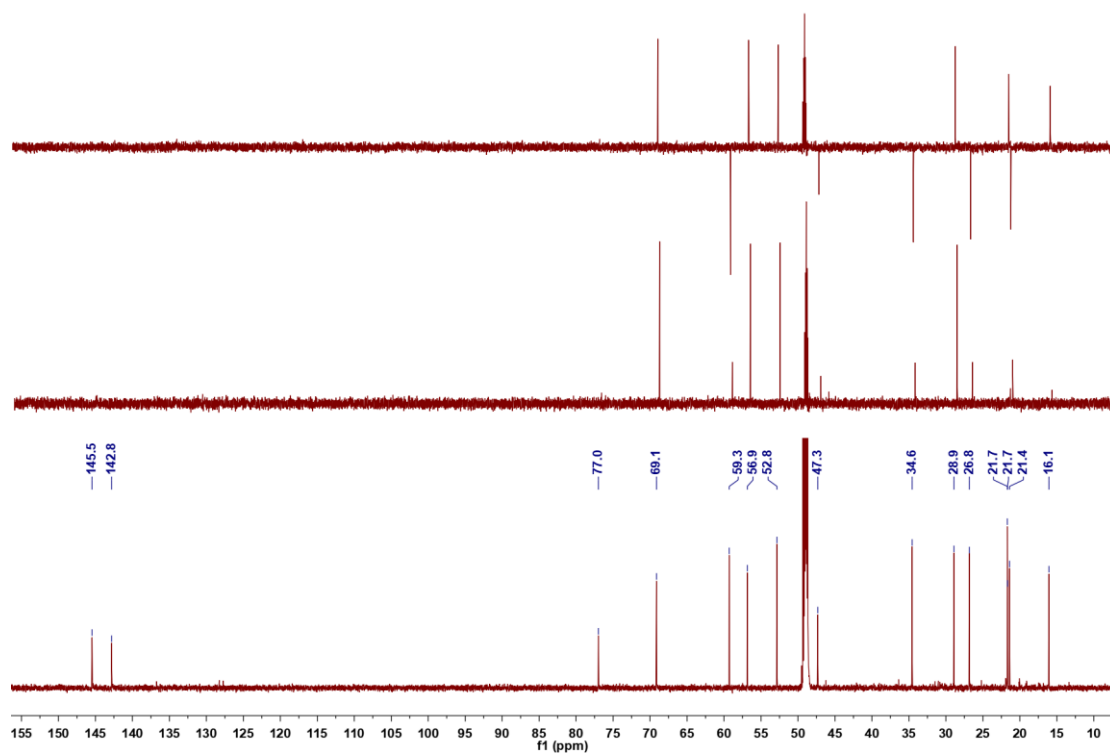


Figure S2-7: ^{13}C -NMR and DEPT (125 MHz, CD_3OD) spectrum of **2**

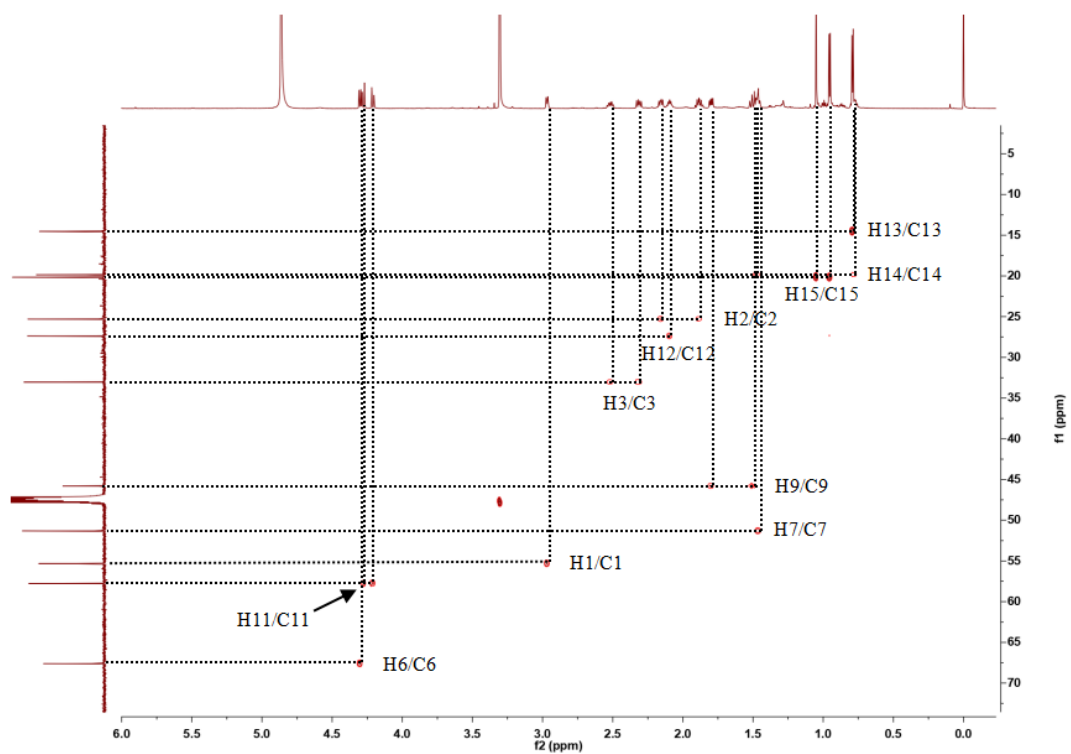


Figure S2-8: HSQC spectrum of **2**

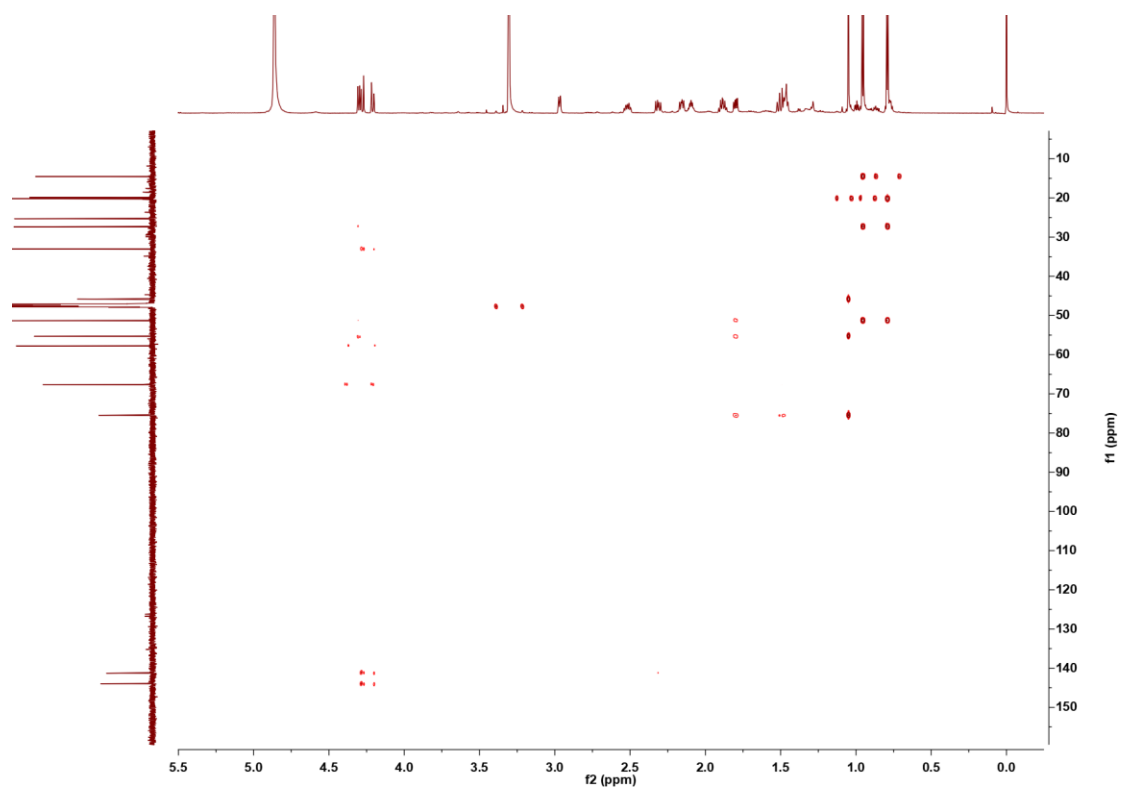


Figure S2-9: HMBC spectrum of **2**

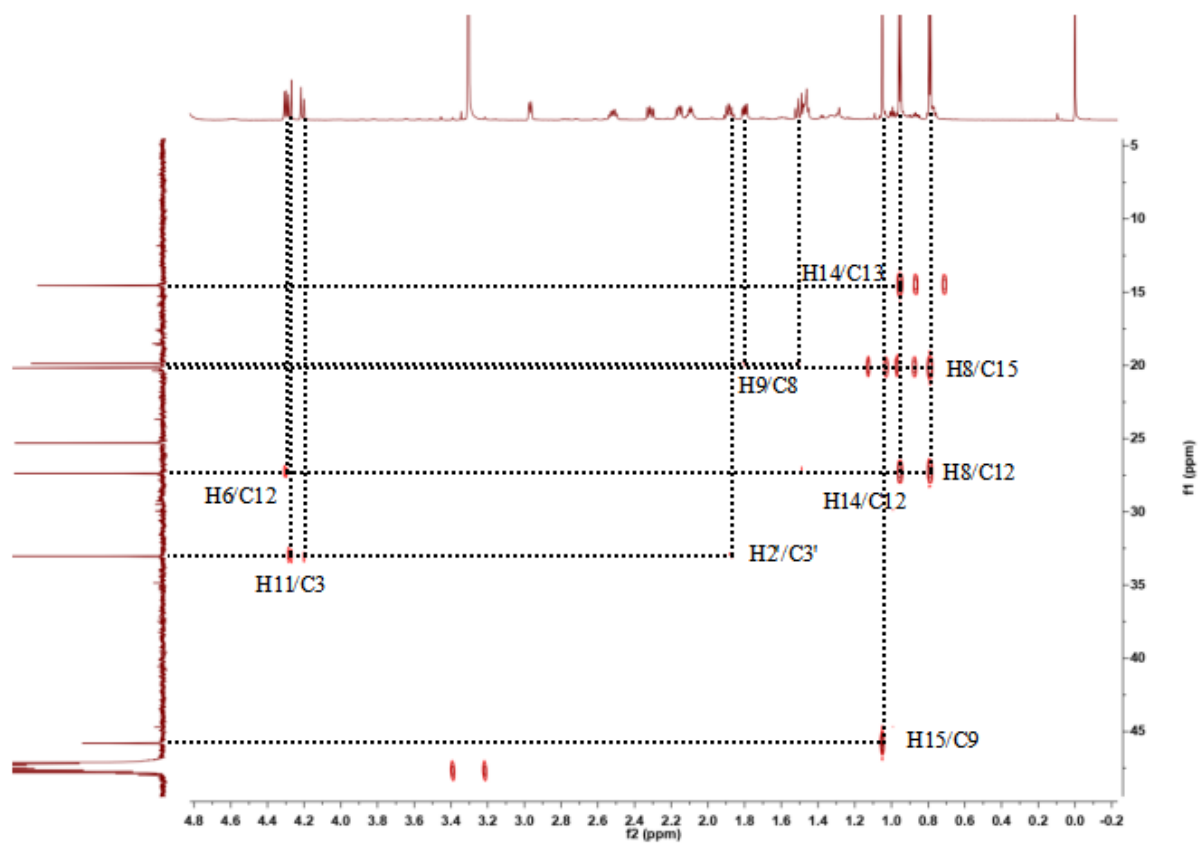


Figure S2-10: HMBC spectrum of **2** (From δ_c 5 ppm to δ_c 50 ppm)

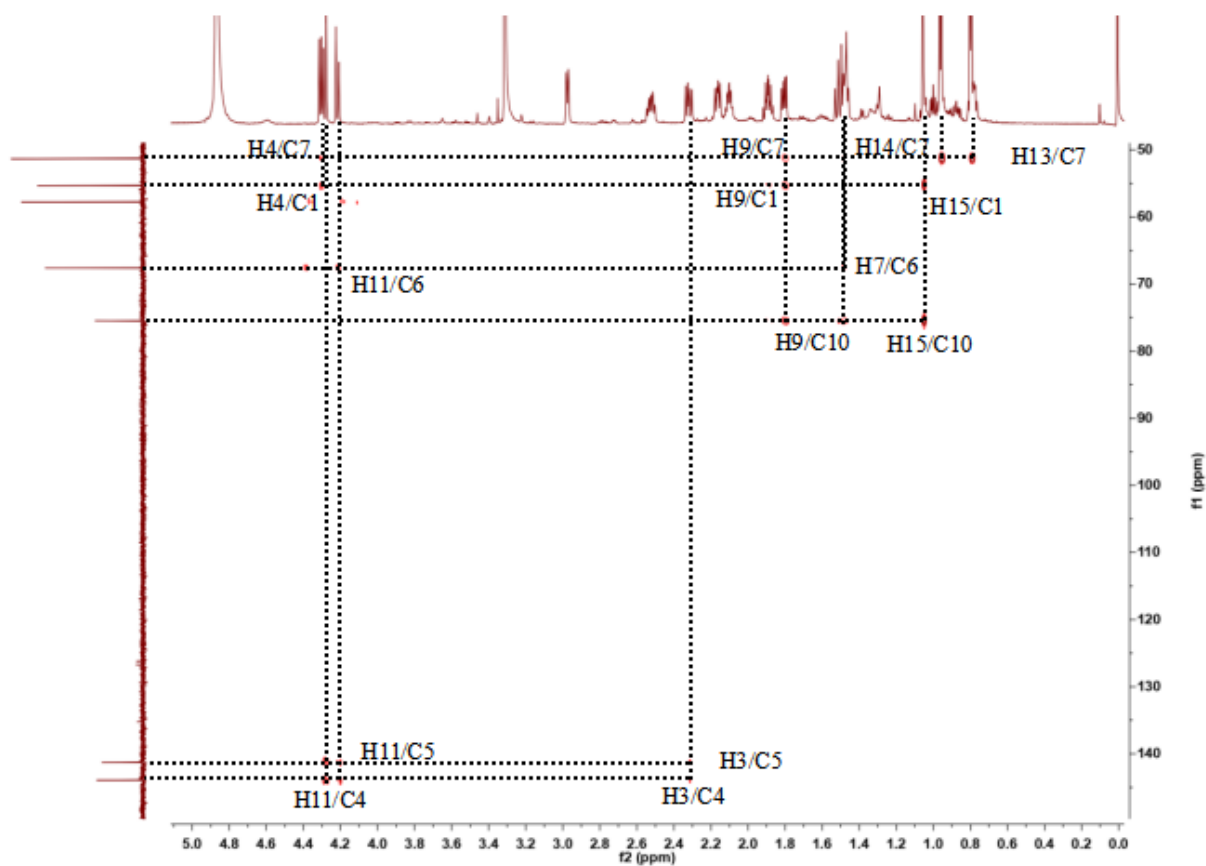


Figure S2-11: HMBC spectrum of **2** (From δ_c 50 ppm to δ_c 150 ppm)

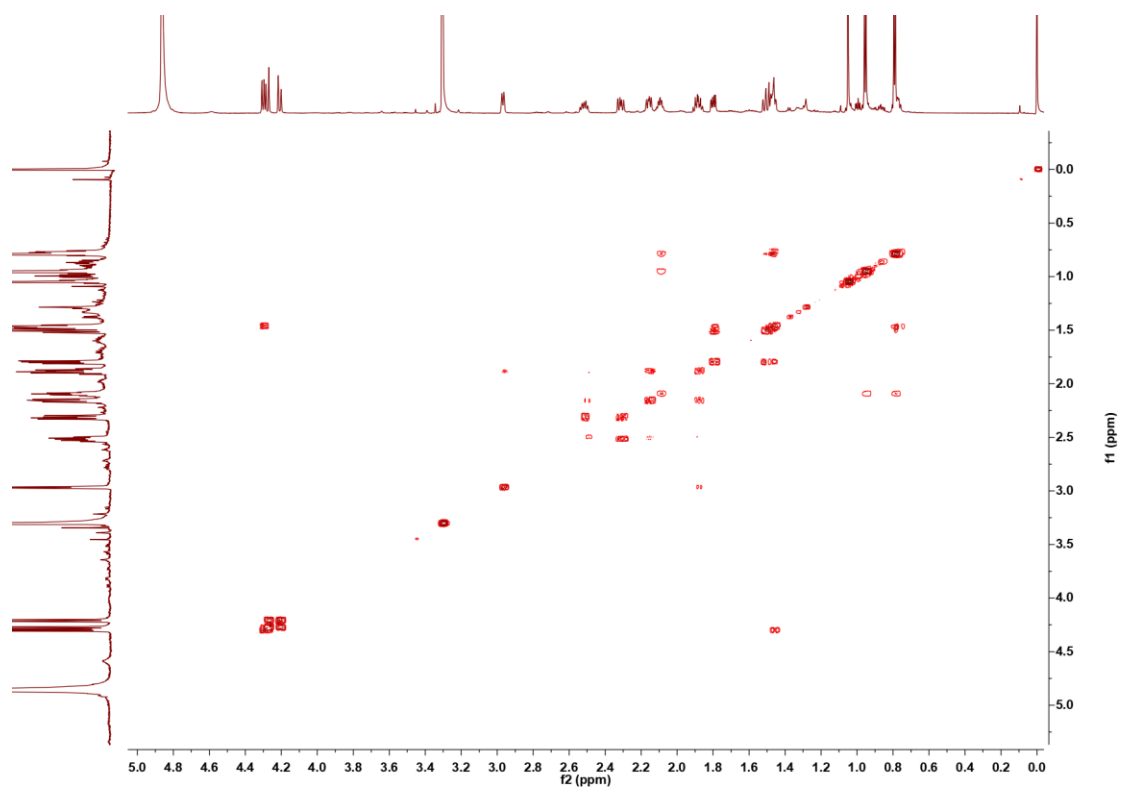


Figure S2-12: ^1H - ^1H COSY spectrum of **2**

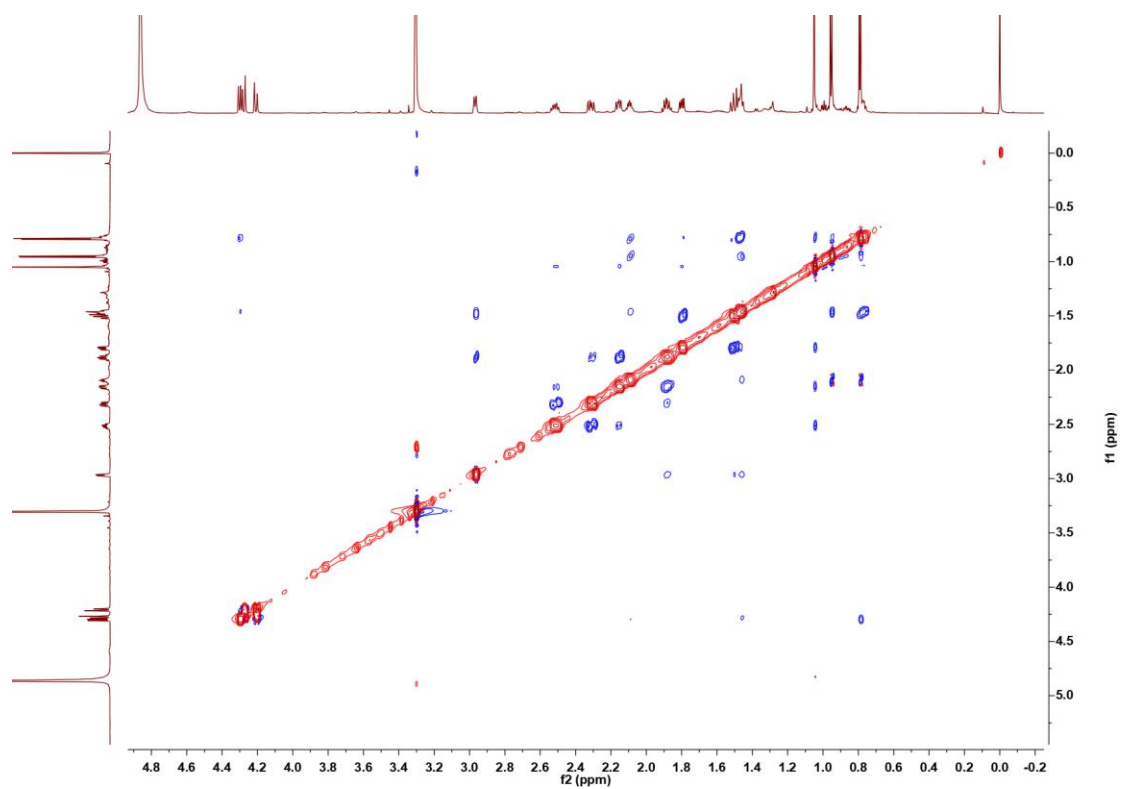


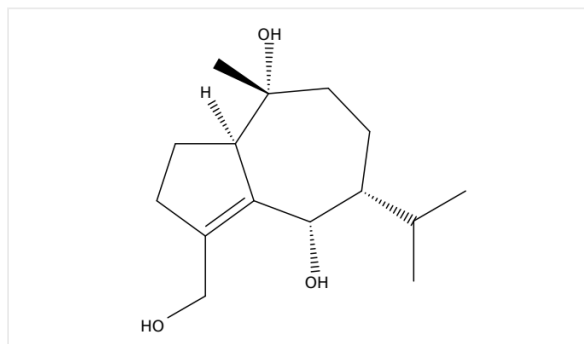
Figure S2-13: ROESY spectrum of **2**

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	View Results

Substances (0)

[View in SciFinder[®]](#)

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