

Supporting Information

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Novel Hopanoic Acid and Depside from the Lichen

Dirinaria applanata

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Table of Contents	Page
1. Supplemental data for structure elucidation of compound 1	3
Table S1. The comparison of NMR data of compound 1 with similar compound 1a	3
2. Supplemental data for structure elucidation of compound 2	4
Figure S1: Some selected key HMBC (a) and NOESY (b) correlations of compound 2.....	4
Table S2. The spectroscopic data of compound 2 (CDCl ₃ , δ in ppm, J in Hz).....	5
3. Supplemental data for structure elucidation of compound 3	6
Figure S2: The two possible structures of compound 3	6
Table S3. ¹ H and ¹³ C-NMR of compound 3 and divaricatic acid 3a in acetone- <i>d</i> ₆ and MeOD- <i>d</i> ₄	7
4. Scanned spectra of all compound	10
Figure S3: (-)HRESI-MS of compound 1 (1β-acetoxy-3β-hydroxy-21α-hopan-29-oic acid)	10
Figure S4: FT-IR of compound 1 (1β-acetoxy-3β-hydroxy-21α-hopan-29-oic acid)	11
Figure S5: Full ¹ H-NMR of compound 1 (1β-acetoxy-3β-hydroxy-21α-hopan-29-oic acid).....	11
Figure S6: Extended ¹ H-NMR of compound 1 (1β-acetoxy-3β-hydroxy-21α-hopan-29-oic acid)..	12
Figure S7: Extended ¹ H-NMR of compound 1 (1β-acetoxy-3β-hydroxy-21α-hopan-29-oic acid)..	12
Figure S8: Full ¹³ C-NMR of compound 1 (1β-acetoxy-3β-hydroxy-21α-hopan-29-oic acid)	13
Figure S9: Extended ¹³ C-NMR of compound 1 (1β-acetoxy-3β-hydroxy-21α-hopan-29-oic acid). 13	
Figure S10: Full DEPT of compound 1 (1β-acetoxy-3β-hydroxy-21α-hopan-29-oic acid)	14
Figure S11: Full COSY of compound 1 (1β-acetoxy-3β-hydroxy-21α-hopan-29-oic acid)	15
Figure S12: Full HSQC of compound 1 (1β-acetoxy-3β-hydroxy-21α-hopan-29-oic acid)	15
Figure S13. Extended HMBC of compound 1 (1β-acetoxy-3β-hydroxy-21α-hopan-29-oic acid) ...	16
Figure S14: Extended HMBC of compound 1 (1β-acetoxy-3β-hydroxy-21α-hopan-29-oic acid)...	16
Figure S15: Extended HMBC of compound 1 (1β-acetoxy-3β-hydroxy-21α-hopan-29-oic acid)...	17
Figure S16: Full NOESY of compound 1 (1β-acetoxy-3β-hydroxy-21α-hopan-29-oic acid).....	17
Figure S17. Extended NOESY of compound 1 (1β-acetoxy-3β-hydroxy-21α-hopan-29-oic acid) .	18

Figure S18: (–)HRESI-MS of compound 2 (21 α -hopane-3 β ,6 β ,22-triol).....	18
Figure S19: FT-IR of compound 2 (21 α -hopane-3 β ,6 β ,22-triol)	19
Figure S20: Full ^1H -NMR of compound 2 (21 α -hopane-3 β ,6 β ,22-triol).....	19
Figure S21: Extended ^1H -NMR of compound 2 (21 α -hopane-3 β ,6 β ,22-triol)	20
Figure S22: Extended ^1H -NMR of compound 2 (21 α -hopane-3 β ,6 β ,22-triol)	20
Figure S23: Full ^{13}C -NMR of compound 2 (21 α -hopane-3 β ,6 β ,22-triol)	21
Figure S24: Extended ^{13}C -NMR of compound 2 (21 α -hopane-3 β ,6 β ,22-triol)	22
Figure S25: Full DEPT of compound 2 (21 α -hopane-3 β ,6 β ,22-triol).....	22
Figure S26: Full HSQC of compound 2 (21 α -hopane-3 β ,6 β ,22-triol).....	23
Figure S27: Extended HSQC of compound 2 (21 α -hopane-3 β ,6 β ,22-triol)	23
Figure S28: Full HMBC of compound 2 (21 α -hopane-3 β ,6 β ,22-triol).....	24
Figure S29: Extended HMBC of compound 2 (21 α -hopane-3 β ,6 β ,22-triol)	24
Figure S30: Extended HMBC of compound 2 (21 α -hopane-3 β ,6 β ,22-triol)	25
Figure S31: Full NOESY of compound 2 (21 α -hopane-3 β ,6 β ,22-triol)	25
Figure S32: Extended NOESY of compound 2 (21 α -hopane-3 β ,6 β ,22-triol).....	26
Figure S33: Extended NOESY of compound 2 (21 α -hopane-3 β ,6 β ,22-triol).....	26
Figure S34: (–)HRESI-MS of compound 3 (2'- <i>O</i> -Methylnordivarinic acid)	27
Figure S35: FT-IR of compound 3 (2'- <i>O</i> -Methylnordivarinic acid).....	27
Figure S36: Full ^1H -NMR of compound 3 (2'- <i>O</i> -Methylnordivarinic acid).....	28
Figure S37: Extended ^1H -NMR of compound 3 (2'- <i>O</i> -Methylnordivarinic acid).....	28
Figure S38: Full ^{13}C -NMR of compound 3 (2'- <i>O</i> -Methylnordivarinic acid).....	29
Figure S39: Full DEPT of compound 3 (2'- <i>O</i> -Methylnordivarinic acid)	29
Figure S40: Full HSQC of compound 3 (2'- <i>O</i> -Methylnordivarinic acid).....	30
Figure S41: Full HMBC of compound 3 (2'- <i>O</i> -Methylnordivarinic acid).....	30
Figure S42: Extended HMBC of compound 3 (2'- <i>O</i> -Methylnordivarinic acid).....	31
Figure S43: Extended HMBC of compound 3 (2'- <i>O</i> -Methylnordivarinic acid).....	31

1. Supplemental data for structure elucidation of compound 1

Table S1. The comparison of NMR data of compound **1** with similar compound **1a**

Position	Compound 1		1β-Acetoxy-21α-hopane-3β,22-diol (1a) [1]	
	¹³ C-NMR (150 MHz)	¹ H-NMR (600 MHz)	¹³ C-NMR (125 MHz)	¹ H-NMR (500 MHz)
1	80.9	4.59 (1H, <i>dd</i> , 11.34 & 4.62 Hz)	80.9	4.59 (1H, <i>dd</i> , J = 11.5 & 5.0 Hz)
2	33.4	1.91 (1H, <i>m</i> , H α) 1.62 (1H, <i>m</i> , H β)	33.4	1.62 (1H, <i>m</i> , H α) 1.91 (1H, <i>m</i> , H β)
3	75.2	3.31 (1H, <i>dd</i> , 12.24 & 4.26 Hz)	75.2	3.30 (1H, <i>dd</i> , J = 12.5 & 4.5 Hz)
4	38.8	-	38.8	-
5	53.0	0.65 (1H, <i>dd</i> , 11.58 & 2.04 Hz)	53.0	0.65 (1H, <i>dd</i> , J = 11.0 & 2.0 Hz)
6	17.9	1.57 (1H, <i>m</i> , H α) 1.49 (1H, <i>m</i> , H β)	17.8	1.58 (<i>m</i> , H α) 1.50 (<i>m</i> , H β)
7	33.1	1.40 (1H, <i>m</i> , H α) 1.21 (1H, <i>m</i> , H β)	33.0	1.42 (<i>m</i> , H α) 1.22 (<i>m</i> , H β)
8	42.2	-	42.2	-
9	50.7	1.45 (1H, <i>m</i>)	50.7	1.45 (<i>m</i>)
10	42.2	-	42.2	-
11	23.0	1.46 (2H, <i>m</i>)	23.0	1.46
12	23.8	1.46 (1H, <i>m</i>) 1.32 (1H, <i>m</i>)	24.0	1.47 (<i>m</i> , H α) 1.34 (<i>m</i> , H β)
13	48.6	1.32 (1H, <i>m</i>)	49.3	1.34 (<i>m</i>)
14	41.9	-	41.9	-
15	33.5	1.16 (1H, <i>m</i> , H α) 1.32 (1H, <i>m</i> , H β)	34.5	1.36 (<i>m</i> , H α) 1.23 (<i>m</i> , H β)
16	19.8	1.28 (1H, <i>m</i> , H α) 1.48 (1H, <i>m</i> , H β)	21.9	1.93 (<i>m</i> , H α) 1.57 (<i>m</i> , H β)
17	53.6	1.25 (1H, <i>m</i>)	53.9	1.44 (<i>m</i>)
18	44.3	-	43.9	-
19	40.9	1.51 (1H, <i>m</i> , H α) 0.90 (1H, <i>m</i> , H β)	41.2	1.50 (<i>m</i> , H α) 0.91 (<i>m</i> , H β)
20	26.6	1.43 (1H, <i>m</i> , H α) 1.87 (1H, <i>m</i> , H β)	26.6	1.75 (<i>m</i> , H α) 1.48 (<i>m</i> , H β)
21	42.0	2.34 (1H, <i>m</i>)	51.1	2.20 (1H, <i>dt</i> , J = 11.0 & 8.5 Hz)
22	42.8	2.36 (1H, <i>m</i>)	73.9	-
23	27.9	0.97 (3H, <i>s</i>)	27.9	0.96 (3H, <i>s</i>)
24	15.0	0.77 (3H, <i>s</i>)	14.9	0.78 (3H, <i>s</i>)
25	12.8	0.98 (3H, <i>s</i>)	12.7	0.99 (3H, <i>s</i>)
26	16.9	0.94 (3H, <i>s</i>)	16.9	0.97 (3H, <i>s</i>)
27	16.6	0.91 (3H, <i>s</i>)	17.0	0.93 (3H, <i>s</i>)
28	15.7	0.70 (3H, <i>s</i>)	16.0	0.74 (3H, <i>s</i>)
29	183.6	-	28.7	1.17 (3H, <i>s</i>)
30	17.6	1.13 (3H, <i>d</i> , 6.48 Hz)	30.9	1.20 (3H, <i>s</i>)
1'	170.5	-	170.5	-
2'	21.9	1.99 (3H, <i>s</i>)	21.8	1.99 (3H, <i>s</i>)

*The highlighted rows showed the main differences between two compounds.

2. Supplemental data for structure elucidation of compound 2

Compound **2** appeared as a white solid. The negative HRESI-MS gave a peak at 459.3840 $[M-H]^-$ (calcd. for $C_{30}H_{51}O_3^-$, 459.3843) which corresponded to chemical formula $C_{30}H_{52}O_3$. The FT-IR showed a hydroxy band at 3414 cm^{-1} . The $^1\text{H-NMR}$ indicated 8 singlet signals of methyl groups at δ_{H} 1.06 (3H, s, H-23), 1.16 (3H, s, H-24), 1.19 (3H, s, H-25), 1.30 (3H, s, H-26), 0.91 (3H, s, H-27), 0.77 (3H, s, H-28), 1.18 (3H, s, H-29), 1.21 (3H, s, H-30). Two peaks at δ_{H} 3.14 (1H, m, H-3) 3.14 (1H, m, H-6) belongs to two oxygen-bearing carbons which were also confirmed by the presence of two signals these at δ_{C} 79.1 (C-3) and 69.0 (C-6) in $^{13}\text{C-NMR}$ and DEPT. Further analyzing carbon spectra proved that there was an oxygenated quaternary carbon at δ_{C} 73.9 (C-22) characterized for a 2-hydroxy-2-propyl fragment. Based on these 1D-NMR characteristics, compound **2** can be reasonably inferred as a regioisomer of a hopanetriol [2].

To reveal the position of three hydroxy groups, HMBC analysis was recorded. The resulted spectra displayed that carbon at δ_{C} 79.1 was C-3 due to the correlation with neighbored protons namely H-1, 2, 5, 23, 24. Additionally, the cross-peaks between carbon at δ_{C} 69.0 and H-5, 7, 23 proved that this oxygenated carbon was C-6. Finally, the obtained data also supported for the presence of 2-hydroxy-2-propyl moiety at C-21 as indicated by the inter-correlations of H-17, 21, 29, 30 to hydroxyl carbon at δ_{C} 73.9 (C-22) [Figure S1a].

More specifically, the relative position of C-1, C-3 and C-21 were readily interpreted by analyzing NOESY spectrum. As shown in [Figure S1b], proton H-3 displayed nuclear overhauser effect with H-1 α , 2 α , 5 α , 23 evidenced that the hydroxy group of C-3 must be *beta*- configuration. By using the same approach, carbon C-6 was similarly assigned for *beta*- configuration due to two important cross-signals from H-6 to H-5, 23. Carbon C-21 was clearly proved to be *alpha*- configuration because of the H-21/H-17 correlated signal. Based on the above evidence, compound **2** was solidly elucidated as 21 α -hopane-3 β ,6 β ,22-triol.

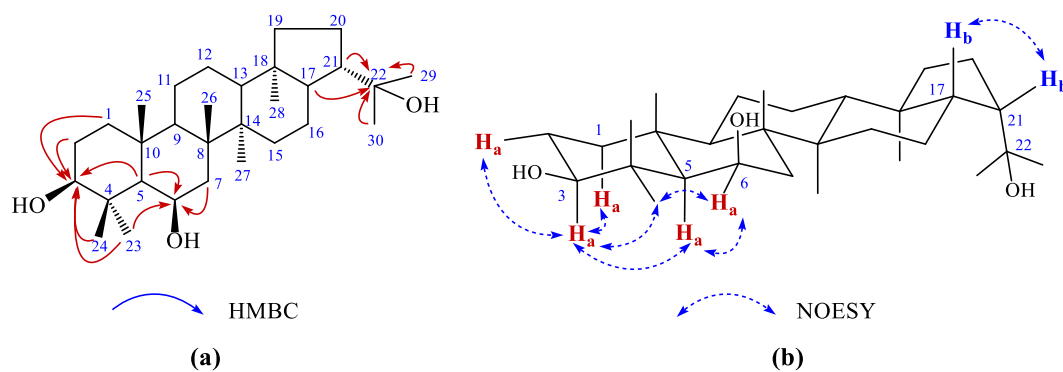


Figure S1: Some selected key HMBC (a) and NOESY (b) correlations of compound **2**

Table S2. The spectroscopic data of compound **2** (CDCl₃, δ in ppm, J in Hz)

No.	¹³ C-NMR (150 MHz)	¹ H-NMR (600 MHz)	HMBC (¹ H → ¹³ C)	NOESY (¹ H → ¹ H)
1	40.8	1.67 (1H, <i>m</i> , H _β)	C-2, 3, 5, 10, 25	H-1 _α , 25
		0.93 (1H, <i>m</i> , H _α)	C-5	H-1 _β , 2 _β , 3, 5, 9
2	27.6	1.64 (1H, <i>m</i> , H _β)	C-1, 3, 4, 10	H-1 _α , 3, 24, 25
		1.57 (1H, <i>m</i> , H _α)		H-3
3	79.1	3.14 (1H, <i>m</i>)	C-23	H-1 _α , 2 _β , 2 _α , 5, 23
4	39.6	-		
5	55.6	0.69 (1H, <i>m</i>)	C-3, 4, 6, 9, 10, 23, 24, 25	H-1 _α , 3, 6, 7 _α , 9, 23, 27
6	69.0	4.55 (1H, <i>s</i>)		H-5, 7 _α , 7 _β , 23, 24
7	41.0	1.72 (1H, <i>m</i> , H _α)	C-5, 6, 8, 14, 26	H-5, 6, 7 _β , 27
		1.47 (1H, <i>m</i> , H _β)	C-5, 6, 9	H-6, 7 _α
8	42.0	-		
9	50.9	1.26 (1H, <i>m</i>)	C-12	H-1 _β , 5, 23
10	36.7	-		
11	24.2	1.45 (2H, <i>m</i>)	C-9, 13	
12	21.1	1.57 (1H, <i>m</i> , H _β)	C-13	
		1.46 (1H, <i>m</i> , H _α)	C-9, 11, 13	H-27
13	48.8	1.47 (1H, <i>m</i>)	C-11, 12, 14	H-26
14	40.7	-		
15	34.5	1.44 (1H, <i>m</i> , H _β)	C-8	H-15 _α , 16 _β
		1.24 (1H, <i>m</i> , H _α)	C-8, 12, 13, 17, 27	H-7 _β , 15 _β , 16 _β , 27
16	21.9	1.94 (1H, <i>m</i> , H _β)	C-8, 15, 17, 18	H-15 _β , 15 _α , 16 _α , 17, 30
		1.58 (1H, <i>m</i> , H _α)		H-16 _β , 27
17	54.0	1.46 (1H, <i>m</i>)	C-16, 18, 22, 28	H-16 _β , 19 _β , 21
18	44.0	-		
19	41.3	1.55 (1H, <i>m</i> , H _α)	C-17, 18, 20, 21, 28	H-19 _β , 28
		0.97 (1H, <i>m</i> , H _β)	C-13, 18, 20, 28	H-17, 19 _α , 20 _β
20	26.6	1.76 (1H, <i>m</i> , H _β)	C-17, 18, 19, 21	H-19 _β , 20 _α , 21
		1.50 (1H, <i>m</i> , H _α)		H-20 _β , 28
21	51.1	2.23 (1H, <i>dt</i> , 10.8 & 9.0 Hz)	C-18, 22	H-17, 20 _β , 29, 30
22	73.9	-		
23	27.6	1.06 (3H, <i>s</i>)	C-3, 4, 5, 6	H-3, 5, 6, 9, 24
24	16.9	1.16 (3H, <i>s</i>)	C-3, 4, 5, 23	H-2 _β , 6, 23, 25
25	17.6	1.19 (3H, <i>s</i>)	C-1, 5, 9, 10, 26	H-1 _β , 2 _β , 24, 26
26	17.3	1.30 (3H, <i>s</i>)	C-7, 8, 9, 14, 25	H-6, 13, 25
27	17.0	0.91 (3H, <i>s</i>)	C-8, 13, 14, 15, 28	H-5, 7 _α , 12 _α , 15 _α , 16 _α , 28
28	16.3	0.77 (3H, <i>s</i>)	C-13, 17, 18, 19, 27	H ¹ -19 _α , 20 _α , 27, 29, 30
29	28.8	1.18 (3H, <i>s</i>)	C-21, 22	H-21, 28
30	30.9	1.21 (3H, <i>s</i>)	C-21, 22	H-16 _β , 21, 28

3. Supplemental data for structure elucidation of compound 3

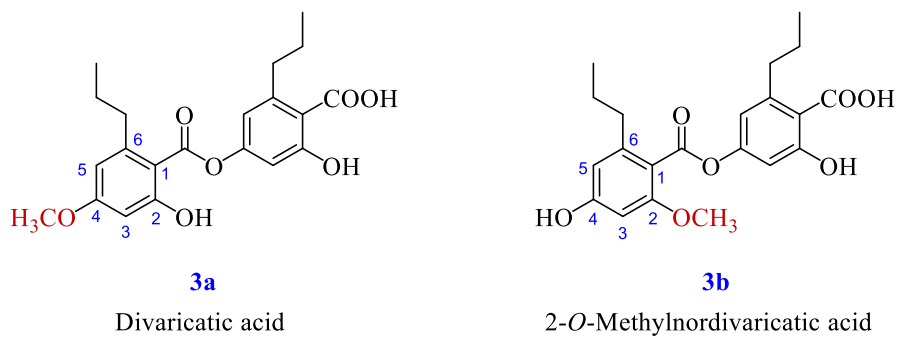


Figure S2: The two possible structures of compound 3

Table S3. ^1H and ^{13}C -NMR of compound **3** and divaricatic acid **3a** in acetone- d_6 and MeOD- d_4

Position	Acetone- d_6				MeOD- d_4			
	Compound 3		Divaricatic acid 3a [3]		Compound 3		Divaricatic acid 3a [4]	
	^{13}C -NMR (125 MHz)	^1H -NMR (500 MHz)	^{13}C -NMR (150 MHz)	^1H -NMR (600 MHz)	^{13}C -NMR (125 MHz)	^1H -NMR (500 MHz)	^{13}C -NMR (100 MHz)	^1H -NMR (400 MHz)
1	105.7		105.4		107.3		105.5	
2	166.1		166.4		165.6		163.9	
3	99.8	6.39 (1H, <i>d</i> , 2.5 Hz)	99.9	6.41 (1H, <i>d</i> , 2.5 Hz)	100.1	6.40 (1H, <i>d</i> , 2.5 Hz)	98.54	6.30 (1H, <i>s</i>)
4	165.3		165.6		165.4		163.7	
5	111.3	6.45 (1H, <i>d</i> , 2.5 Hz)	111.6	6.46 (1H, <i>d</i> , 2.5 Hz)	111.2	6.42 (1H, <i>d</i> , 2.5 Hz)	109.4	6.08 (1H, <i>s</i>)
6	148.4		148.6*		148.4		146.8	
7	170.2		169.2		170.5		171.5	
8	39.3	2.95 (2H, overlap)	39.3*	2.93-3.00 (2H, <i>m</i>)	39.5	2.93 (2H, <i>t</i> , 7.5 Hz)	38.0	2.79 (2H, <i>t</i> , 7.6 Hz)
9	25.9	1.70 (2H, <i>m</i>)	25.7*	1.61-1.77 (2H, <i>m</i>)	26.4	1.65-1.73 (2H, <i>m</i>)	24.7	1.57 (2H, <i>m</i>)
10	14.4	0.95 (3H, <i>t</i> , 7.0Hz)	14.4*	0.93-1.00 (3H, <i>m</i>)	14.5	0.99 (3H, <i>t</i> , 7.5 Hz)	13.3	0.94 (3H, <i>t</i> , 7.2 Hz)
1'	116.2		112.2		116.9		110.1	
2'	165.3		165.2		164.5		157.9	
3'	114.5	6.57 (1H, <i>d</i> , 2.5Hz)	109.3	6.79 (1H, <i>d</i> , 2.3 Hz)	115.2	6.54 (1H, <i>d</i> , 2.0 Hz)	99.8	6.08 (1H, <i>d</i> , 2,4 Hz)
4'	152.8		155.0		153.4		159.3	
5'	108.2	6.50 (1H, <i>d</i> , 2.5Hz)	116.6	6.77 (1H, <i>d</i> , 2.3 Hz)	108.3	6.49 (1H, <i>d</i> , 2.5 Hz)	108.8	6.08 (1H, <i>d</i> , 2,4 Hz)
6'	149.3		149.1*		149.5		148.0	
7'	176.7		173.3		#		175.12	
8'	38.0	3.12 (2H, <i>t</i> , 7.5 Hz)	38.7*	2.93-3.00 (2H, <i>m</i>)	38.4	3.14 (2H, <i>t</i> , 7.5 Hz)	37.31	3.00 (2H, <i>t</i> , 7.6 Hz)
9'	25.5	1.63 (2H, <i>sextet</i> , 7.5 Hz)	25.9*	1.61-1.77 (2H, <i>m</i>)	26.1	1.65-1.73 (2H, <i>m</i>)	24.7	1.57 (2H, <i>m</i>)
10'	14.4	0.90 (3H, <i>t</i> , 7.0Hz)	14.5*	0.93-1.00 (3H, <i>m</i>)	14.6	0.98 (3H, <i>t</i> , 6.5 Hz)	13.1	0.93 (3H, <i>t</i> , 7.2 Hz)
2-OH	-	11.17 (1H, <i>s</i>)	-					
2'-OCH₃	55.9	3.86 (3H, <i>s</i>)	-	-	55.9	3.84 (3H, <i>s</i>)	-	-
4-OCH₃	-	-	55.9	3.86 (3H, <i>s</i>)			54.4	3.78 (3H, <i>s</i>)
-COOH		14.22 (1H, <i>brs</i>)						

* These signals were interchangeable # This signals was not observed in ^{13}C -NMR

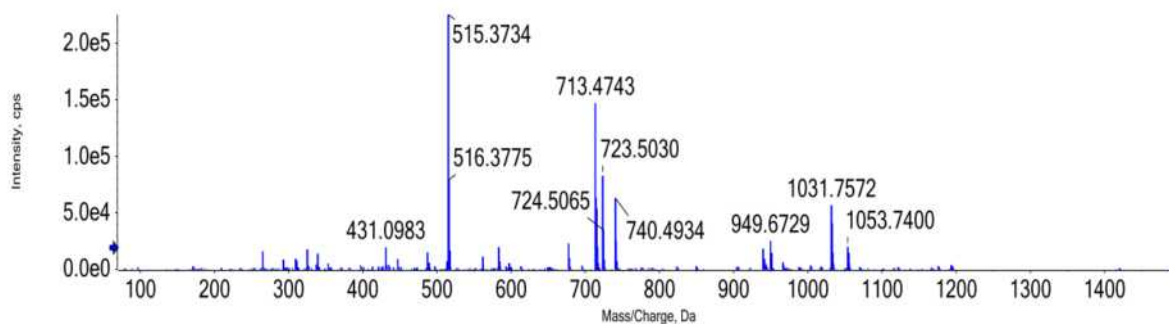
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4. Scanned spectra of all compounds

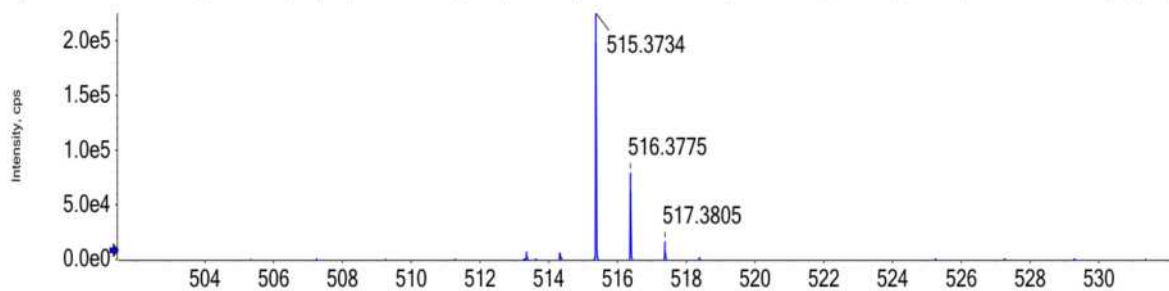
Full mass spectrum

Spectrum from DA.EA04+ESI_TUÂN.wiff2 (sample 3) - DA.EA04+ESI_TUÂN, -TOF MS (70 - 150...om 0.185 min, noise filtered (noise multiplier = 1.5), Gaussian smoothed (0.5 points))



Expanded spectrum

Spectrum from DA.EA04+ESI_TUÂN.wiff2 (sample 3) - DA.EA04+ESI_TUÂN, -TOF MS (70 - 150...om 0.185 min, noise filtered (noise multiplier = 1.5), Gaussian smoothed (0.5 points))



Formula (M)	Ion formula	m/z	Calcd m/z	Diff (ppm)
$C_{32}H_{52}O_5$	$C_{32}H_{51}O_5^-$	515.3734	515.3736	0.39 ppm

Figure S3: (-)HRESI-MS of compound **1** (1β -acetoxy- 3β -hydroxy- 21α -hopan-29-oic acid)

Compound 1

ThermoFisher
SCIENTIFIC
FT-IR Nicolet 6700, Thermo

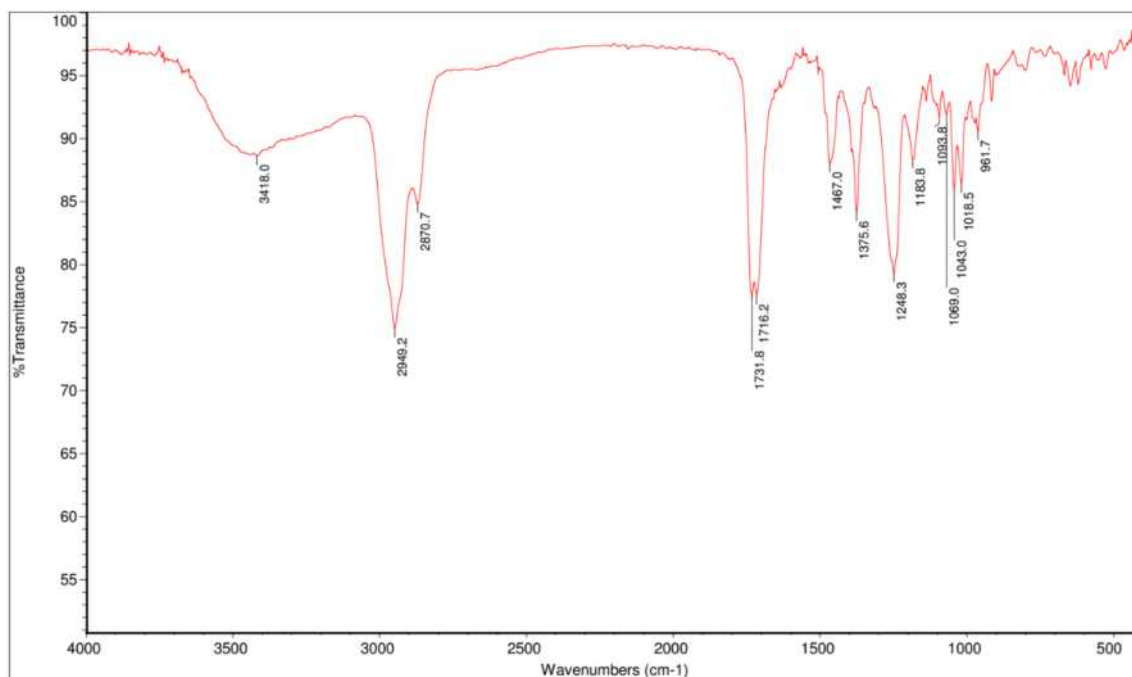


Figure S4: FT-IR of compound 1 (1β -acetoxy- 3β -hydroxy- 21α -hopan-29-oic acid)

Compound 1 (¹H, CDCl₃, 600MHz)

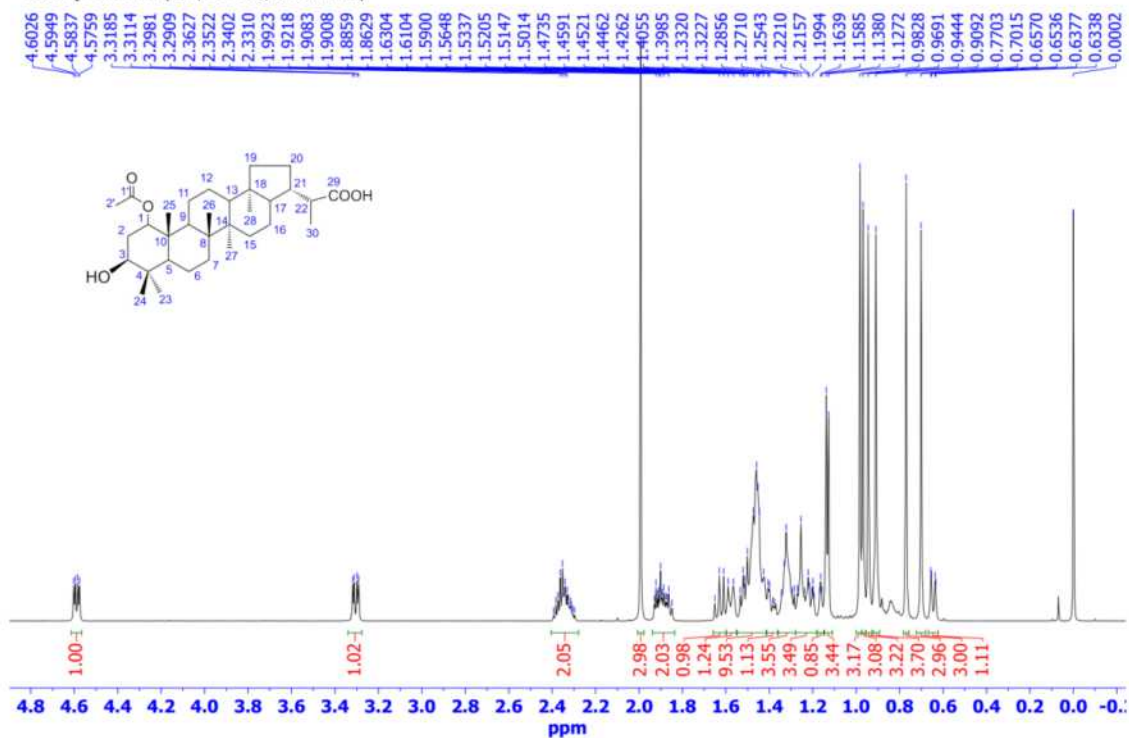


Figure S5: Full ¹H-NMR of compound 1 (1β -acetoxy- 3β -hydroxy- 21α -hopan-29-oic acid)

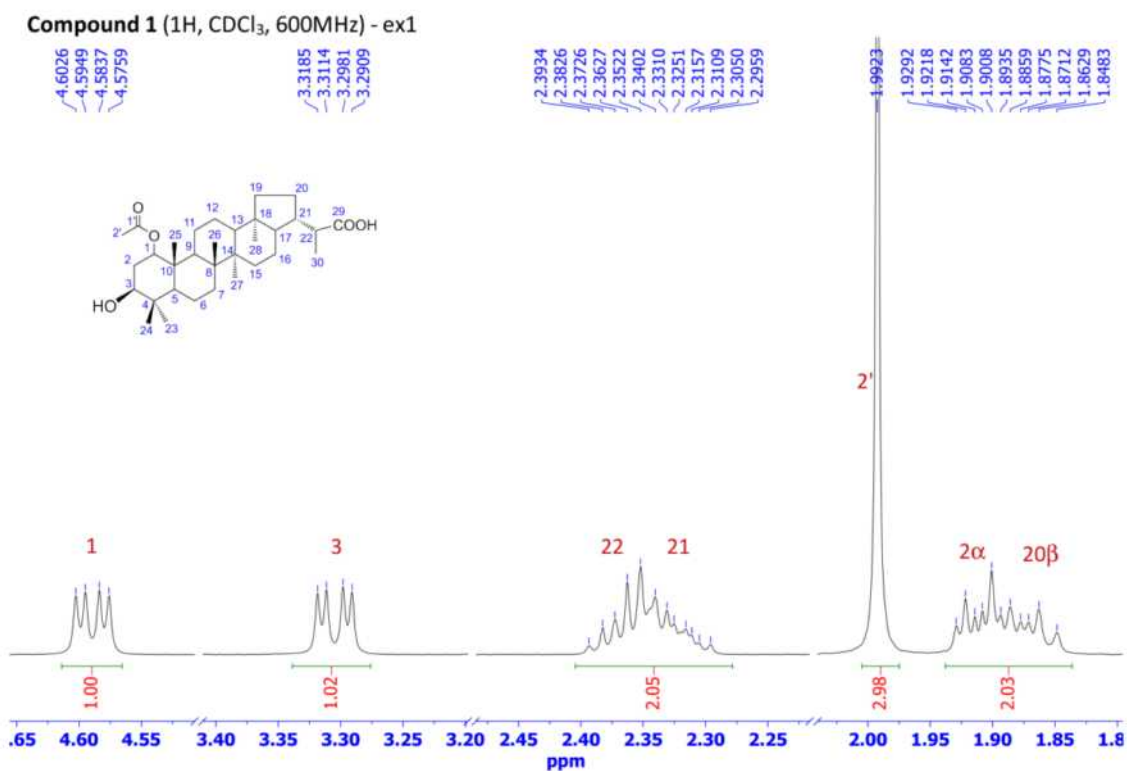


Figure S6: Extended ¹H-NMR of compound 1 (1 β -acetoxy-3 β -hydroxy-21 α -hopan-29-oic acid)

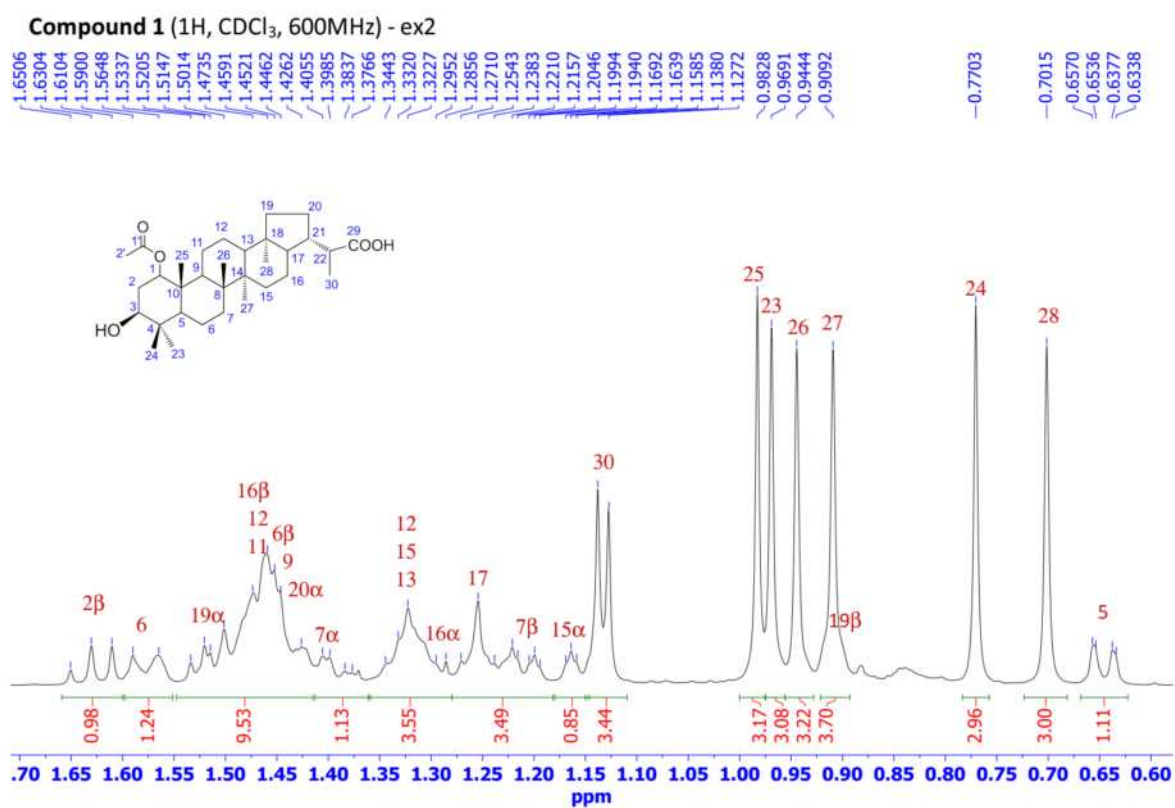


Figure S7: Extended ¹H-NMR of compound 1 (1 β -acetoxy-3 β -hydroxy-21 α -hopan-29-oic acid)

Compound 1 (13C, CDCl₃, 150MHz)

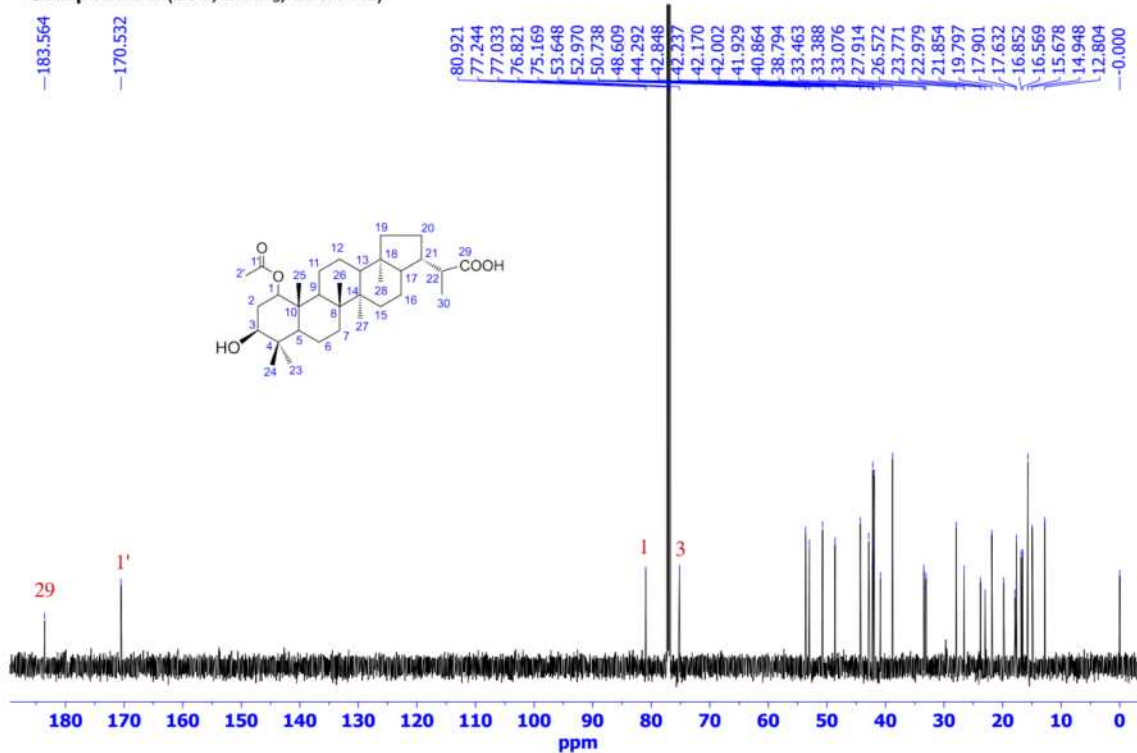


Figure S8: Full ¹³C-NMR of compound 1 (1β-acetoxy-3β-hydroxy-21α-hopan-29-oic acid)

Compound 1 (13C, CDCl₃, 150MHz) - ex

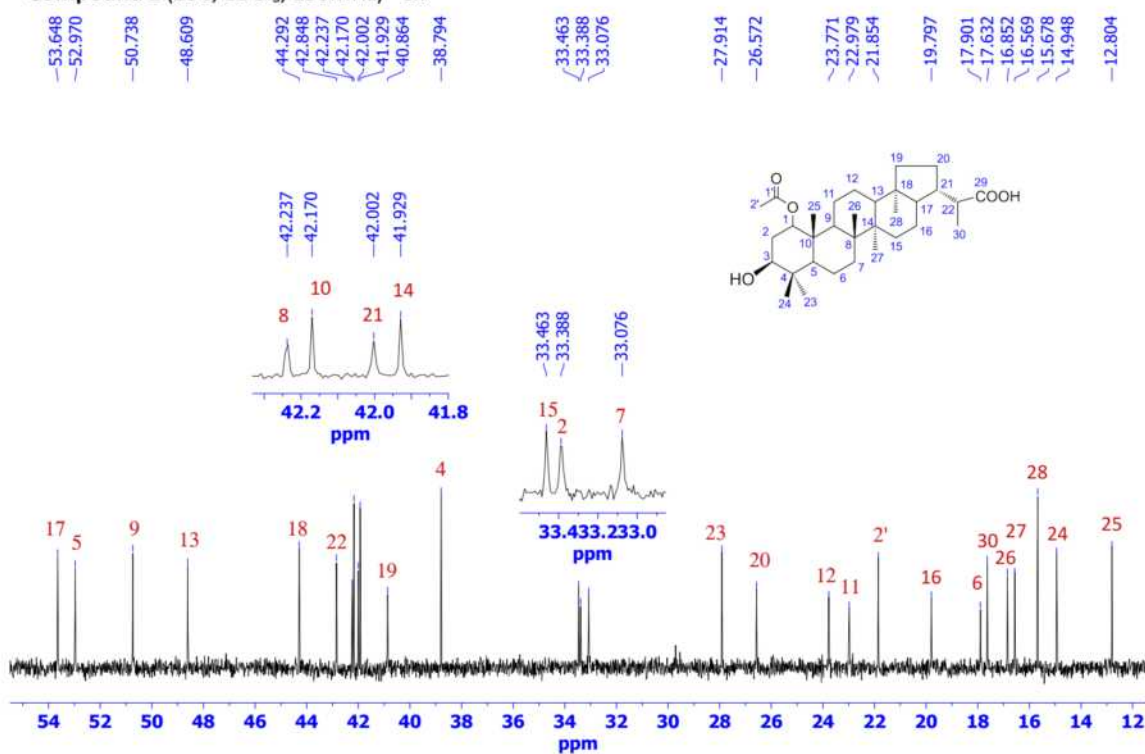


Figure S9: Extended ¹³C-NMR of compound 1 (1β-acetoxy-3β-hydroxy-21α-hopan-29-oic acid)

Compound 1 (DEPT, CDCl₃)

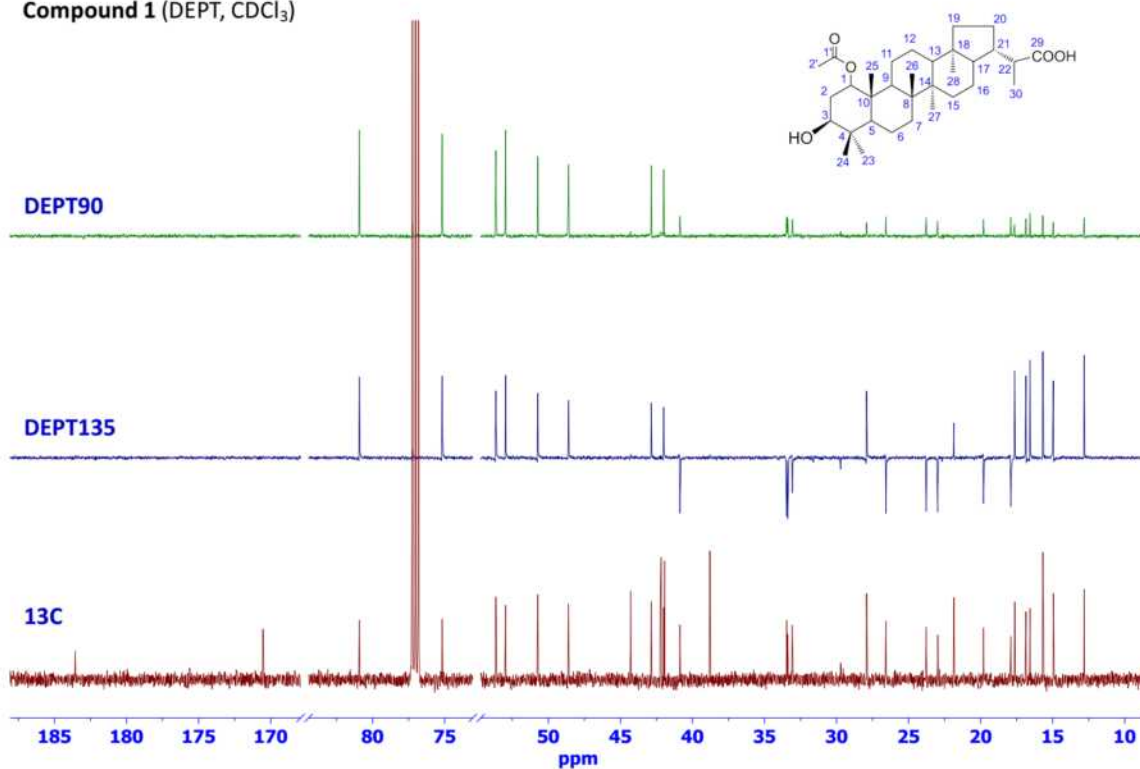


Figure S10: Full DEPT of compound 1 (1 β -acetoxy-3 β -hydroxy-21 α -hopan-29-oic acid)

Compound 1 (COSY, CDCl₃)

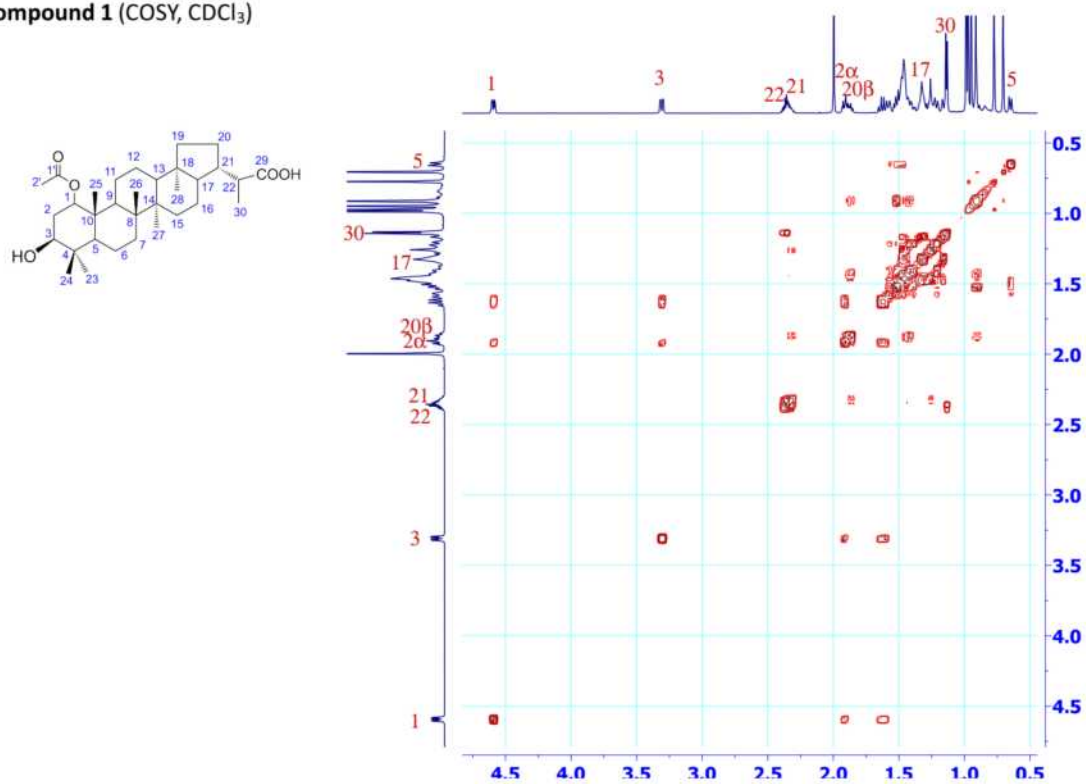


Figure S11: Full COSY of compound **1** (1 β -acetoxy-3 β -hydroxy-21 α -hopan-29-oic acid)

Compound 1 (HSQC, CDCl₃)

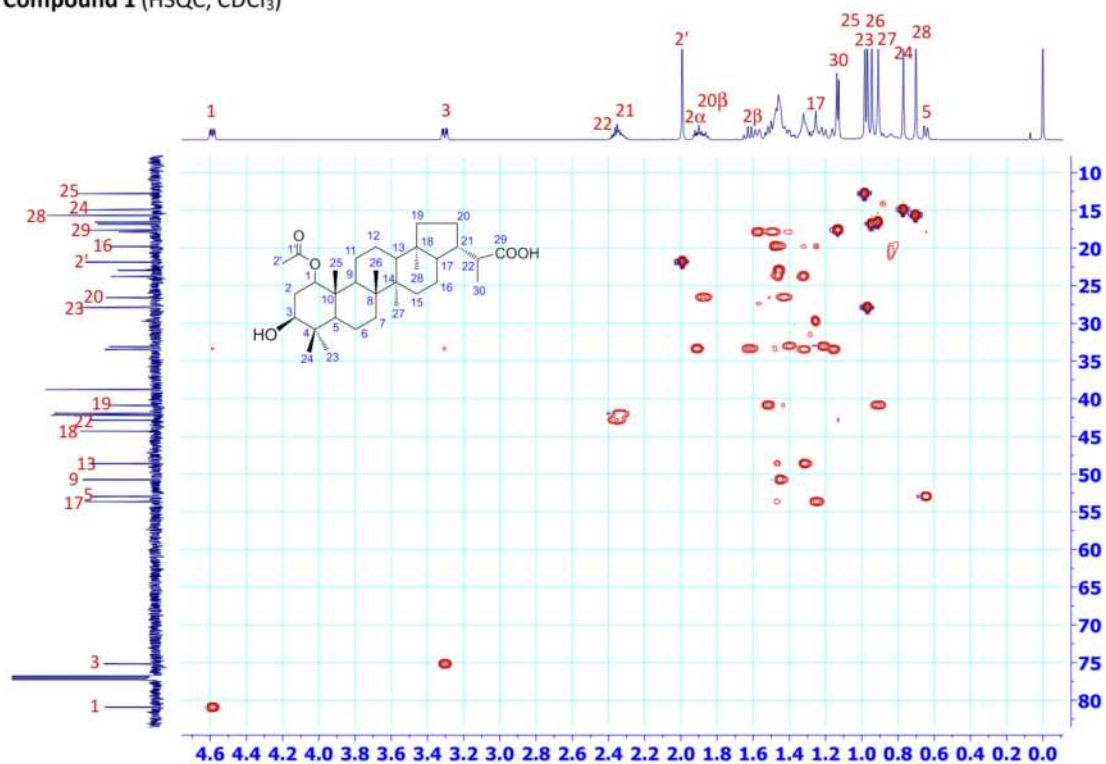


Figure S12: Full HSQC of compound **1** (1 β -acetoxy-3 β -hydroxy-21 α -hopan-29-oic acid)

Compound 1 (HMBC) - ex1

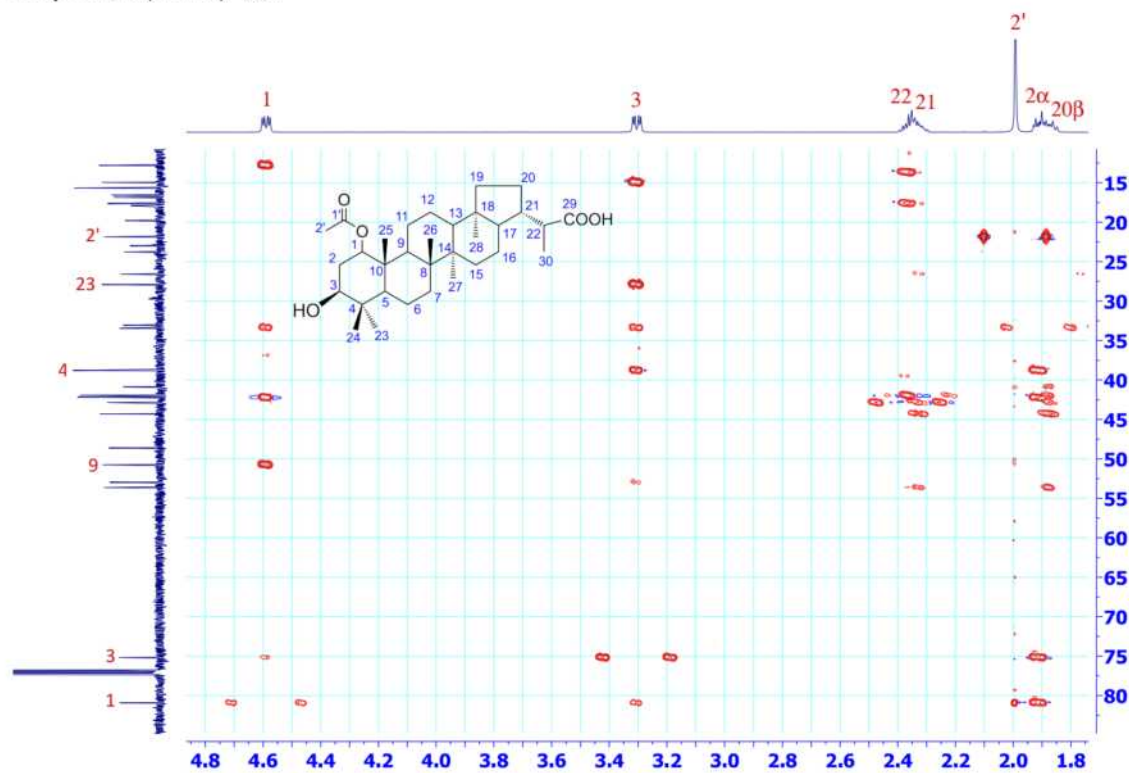


Figure S13: Extended HMBC of compound **1** (*1 β -acetoxy-3 β -hydroxy-21 α -hopan-29-oic acid*)

Compound 1 (HMBC) - ex2

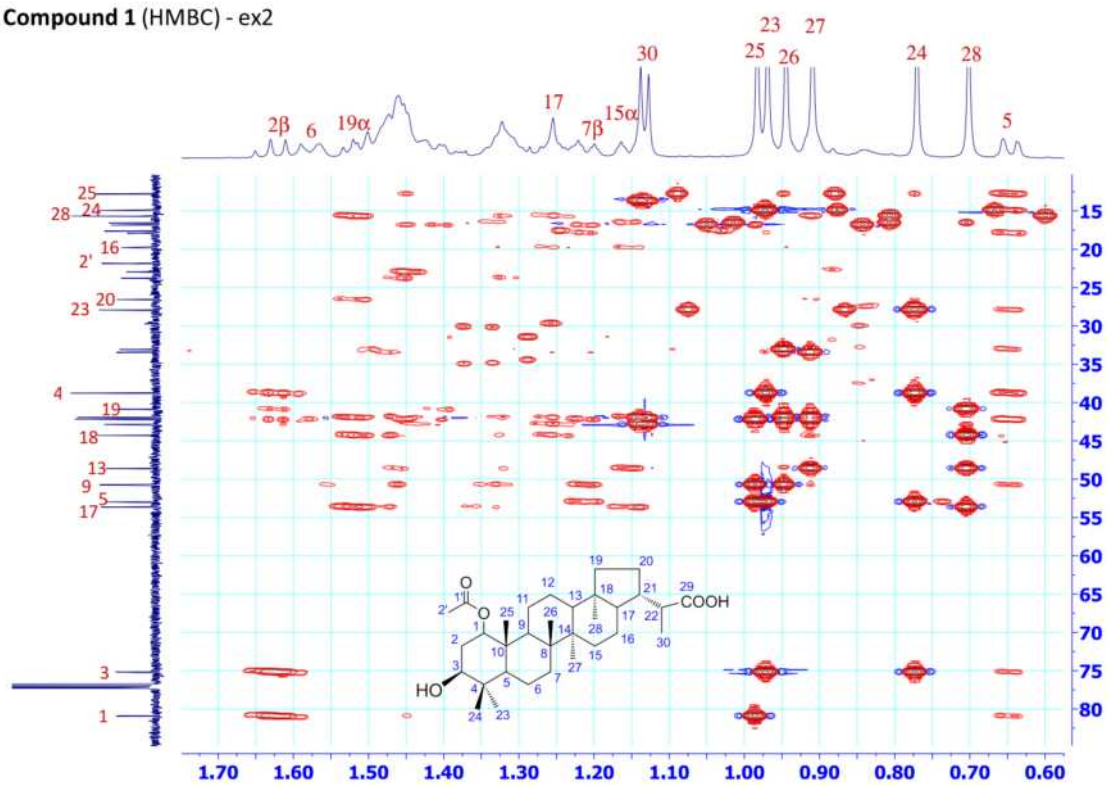


Figure S14: Extended HMBC of compound **1** (*1 β -acetoxy-3 β -hydroxy-21 α -hopan-29-oic acid*)

Compound 1 (HMBC) - ex3

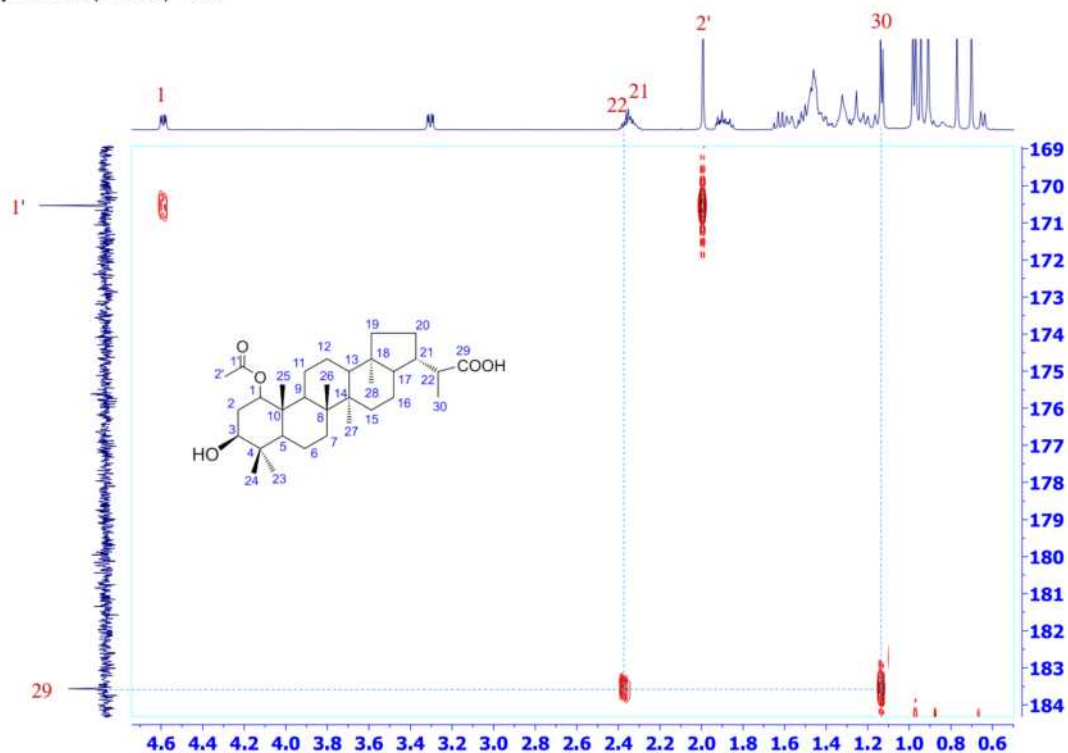


Figure S15: Extended HMBC of compound 1 (1 β -acetoxy-3 β -hydroxy-21 α -hopan-29-oic acid)

Compound 1 (NOESY, CDCl₃)

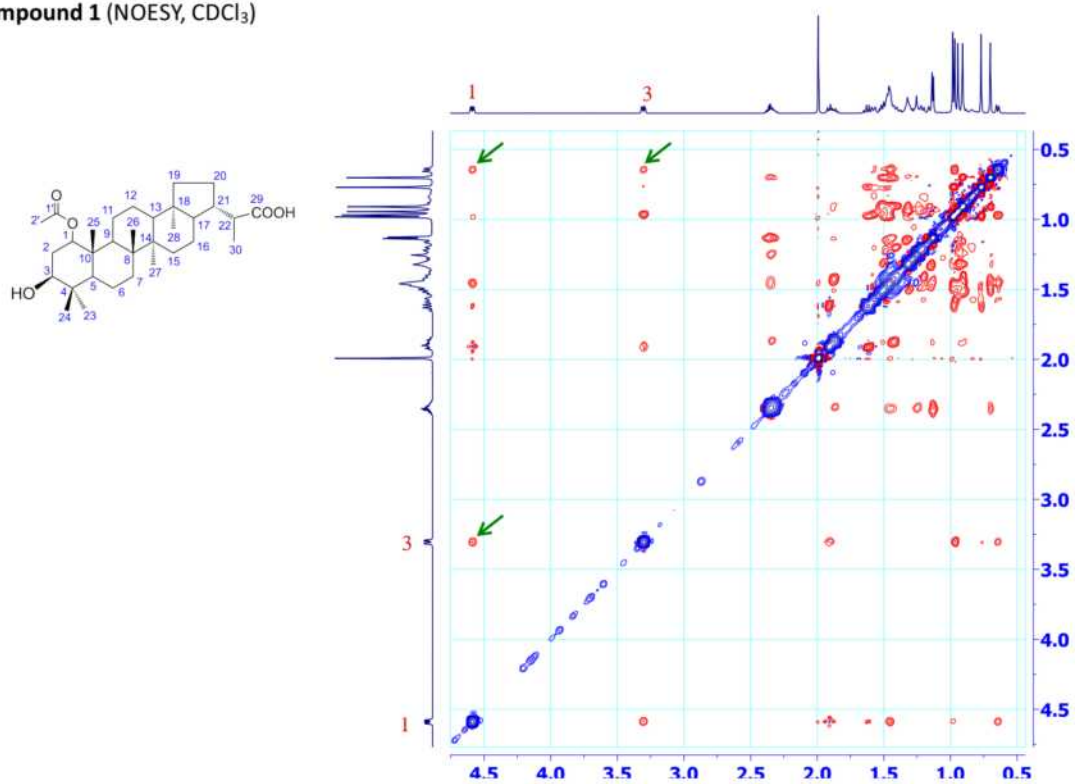


Figure S16: Full NOESY of compound 1 (1 β -acetoxy-3 β -hydroxy-21 α -hopan-29-oic acid)

Compound 1 (NOESY, CDCl₃) - ex

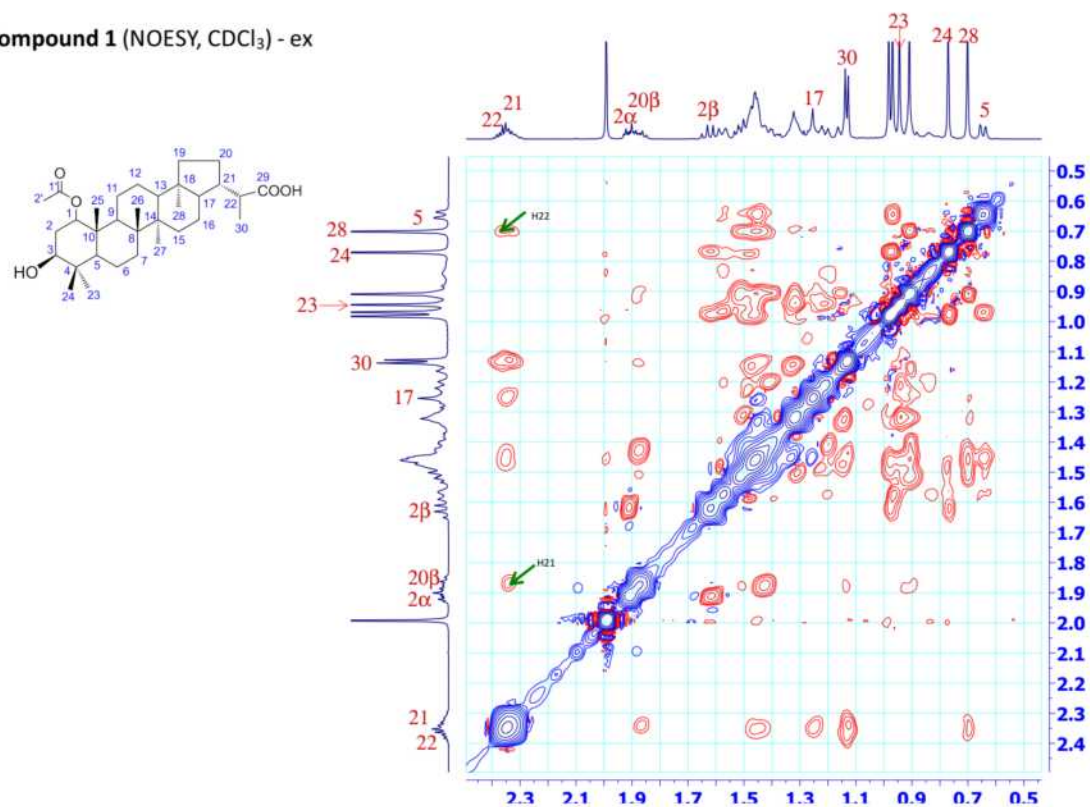
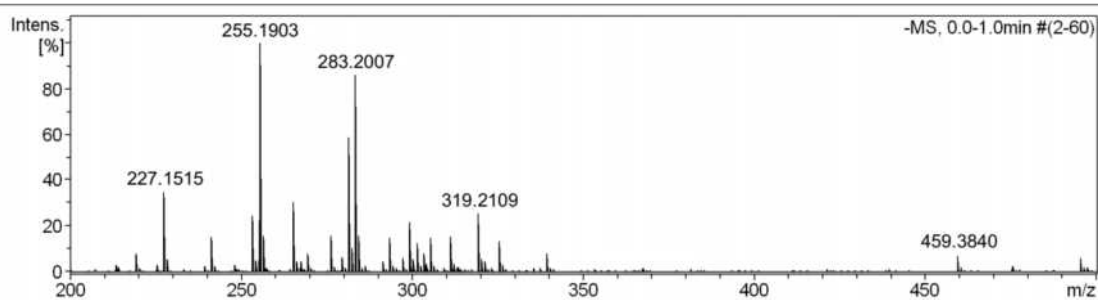


Figure S17: Extended NOESY of compound 1 (1β-acetoxy-3β-hydroxy-21α-hopan-29-oic acid)

Acquisition Parameter

Source Type	ESI	Ion Polarity	Negative	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	200 m/z	Set End Plate Offset	-500 V	Set Dry Gas	5.0 l/min
Scan End	1000 m/z			Set Divert Valve	Source



Formula (M)	Ion formula	<i>m/z</i>	Calcd <i>m/z</i>	Diff (ppm)
C ₃₀ H ₅₂ O ₃	C ₃₀ H ₅₁ O ₃	459.3840	459.3843	0.65

Figure S18: (-)HRESI-MS of compound 2 (21α-hopane-3β,6β,22-triol)

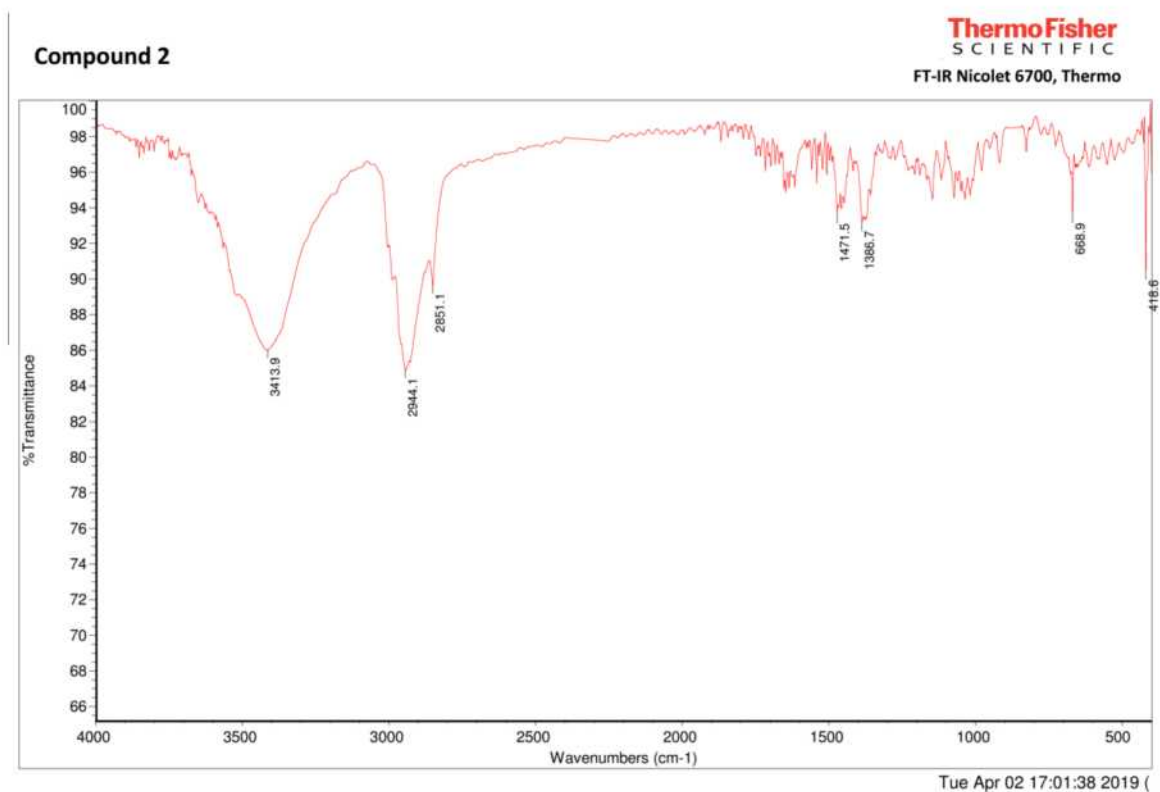


Figure S19: FT-IR of compound 2 (21 α -hopane-3 β ,6 β ,22-triol)

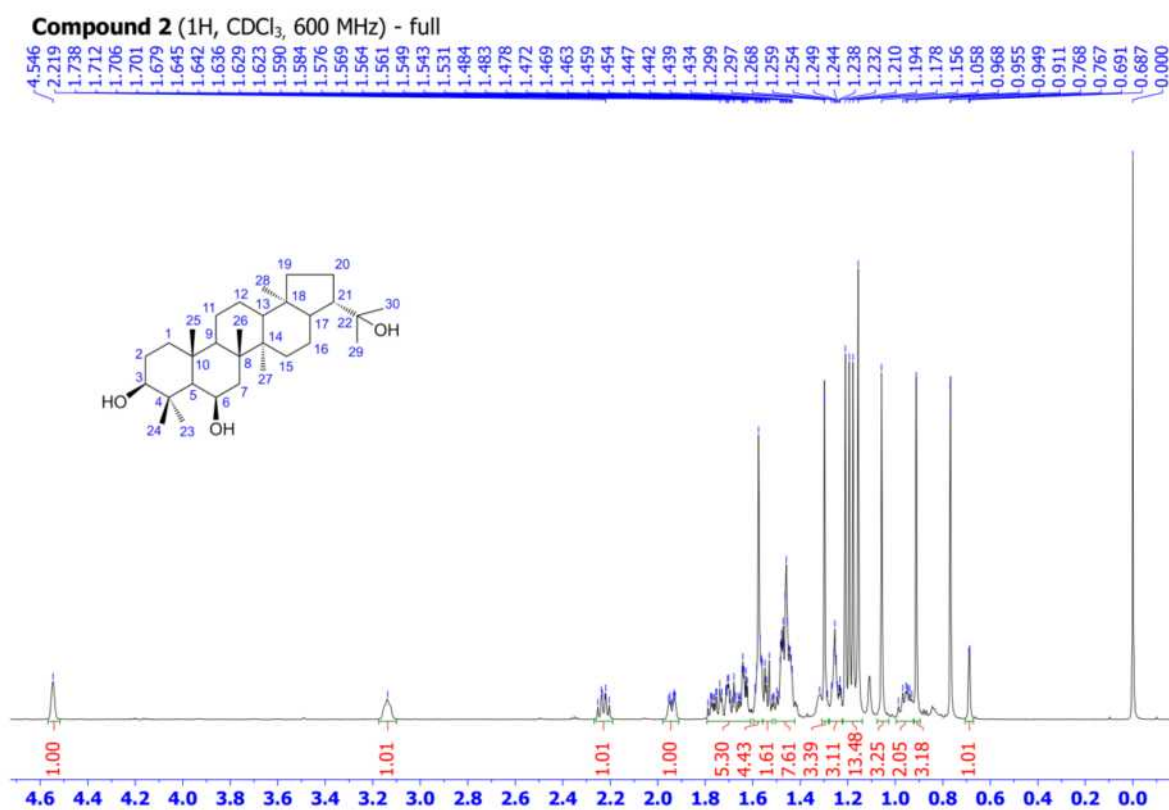


Figure S20: Full ¹H-NMR of compound 2 (21 α -hopane-3 β ,6 β ,22-triol)

Compound 2 (1H, CDCl₃, 600 MHz) - ex1

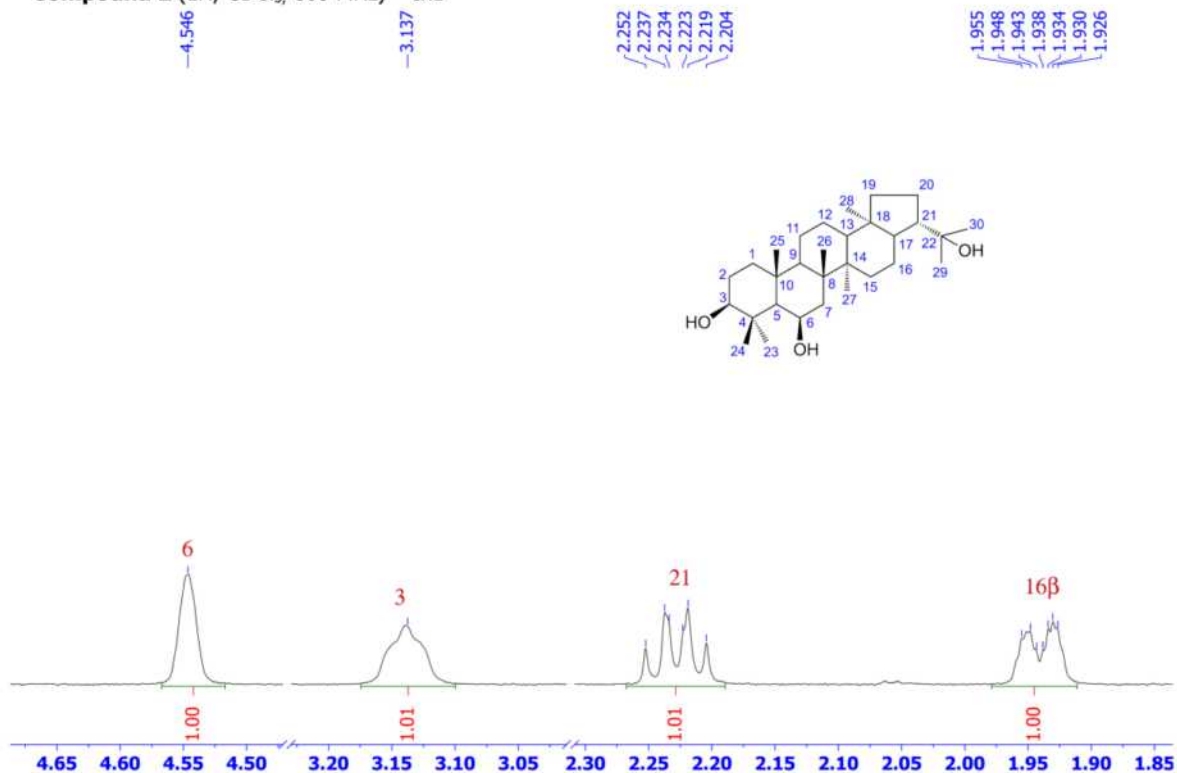


Figure S21: Extended ¹H-NMR of compound 2 (21α-hopane-3β,6β,22-triol)

Compound 2 (1H, CDCl₃, 600 MHz) - ex2

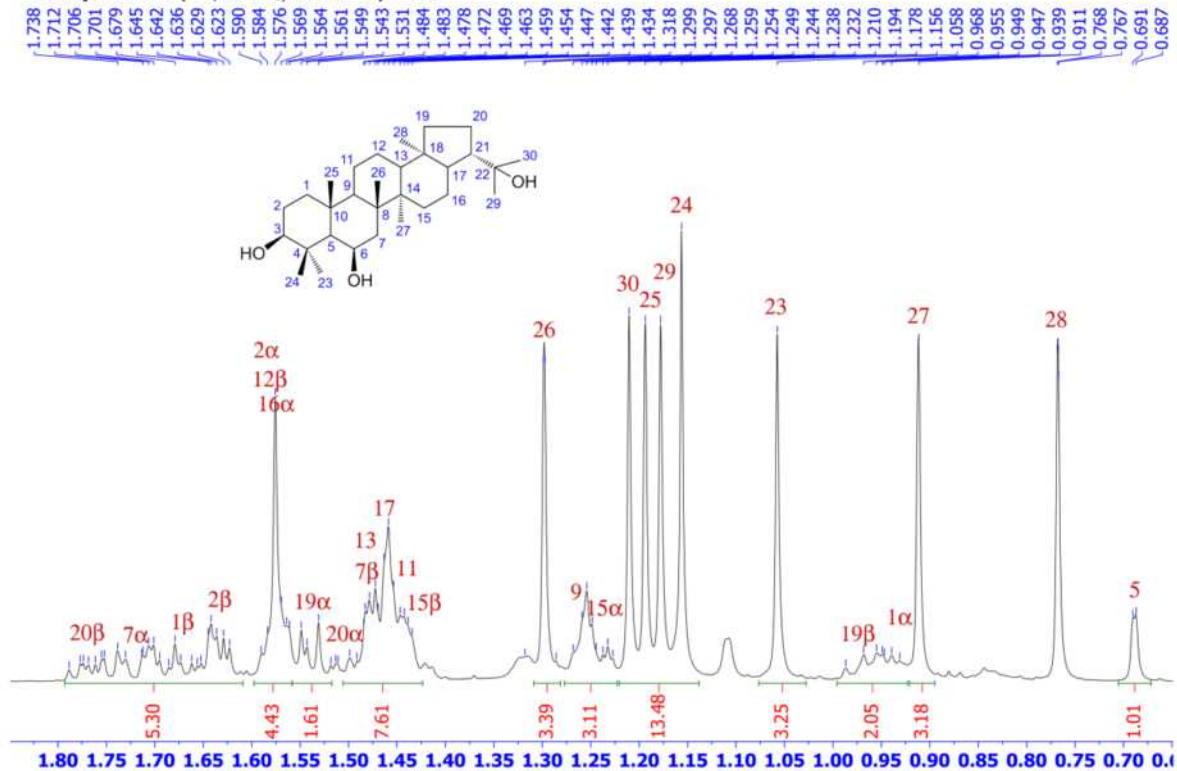


Figure S22: Extended ¹H-NMR of compound 2 (21α-hopane-3β,6β,22-triol)

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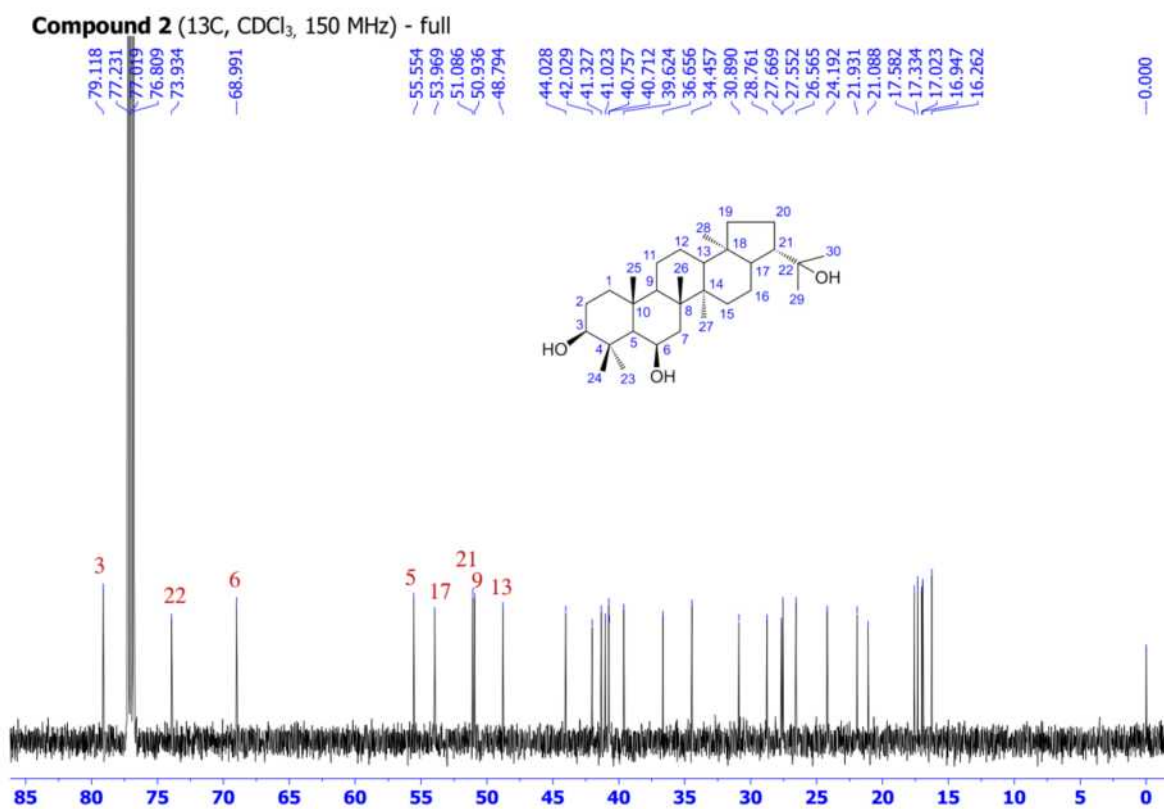


Figure S23: Full ^{13}C -NMR of compound 2 (21 α -hopane-3 β , 6 β , 22-triol)

Compound 2 (13C, CDCl₃, 150 MHz) - ex

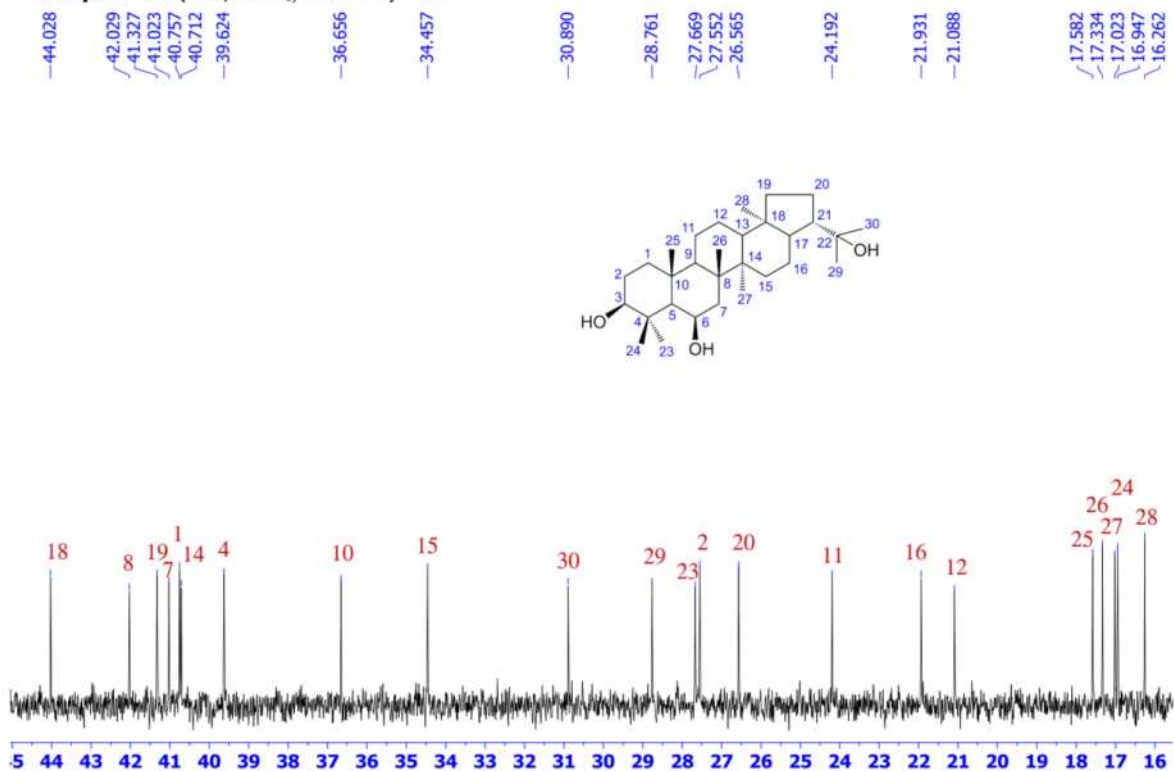


Figure S24: Extended ¹³C-NMR of compound 2 (21 α -hopane-3 β ,6 β ,22-triol)

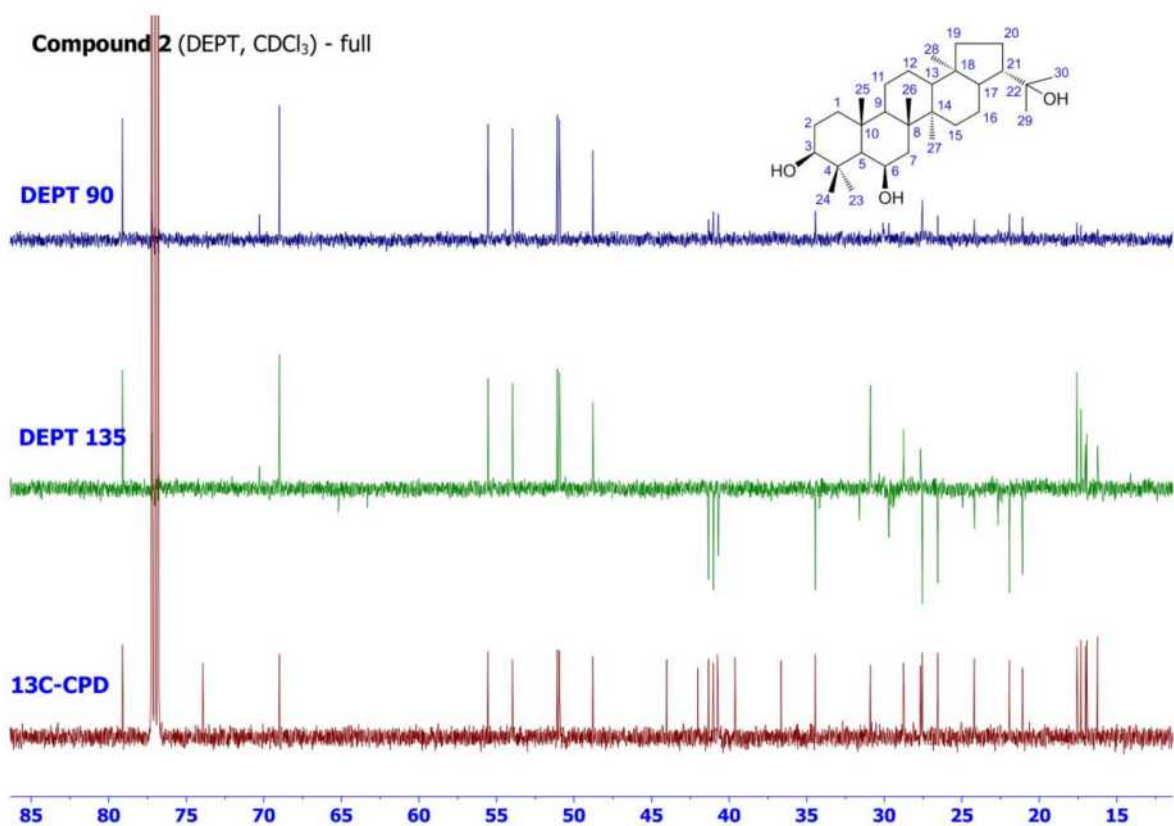


Figure S25: Full DEPT of compound 2 (21 α -hopane-3 β ,6 β ,22-triol)

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Compound 2 (HSQC, CDCl₃) - full

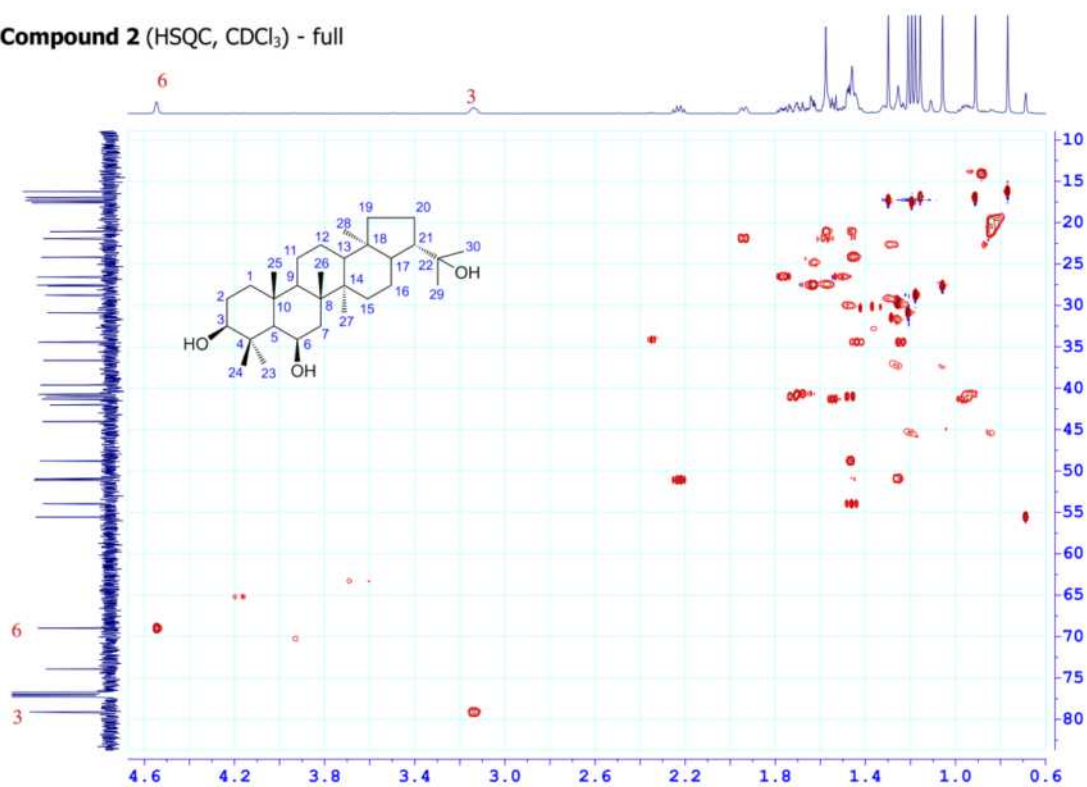


Figure S26: Full HSQC of compound 2 (21 α -hopane-3 β ,6 β ,22-triol)

Compound 2 (HSQC, CDCl₃) - full

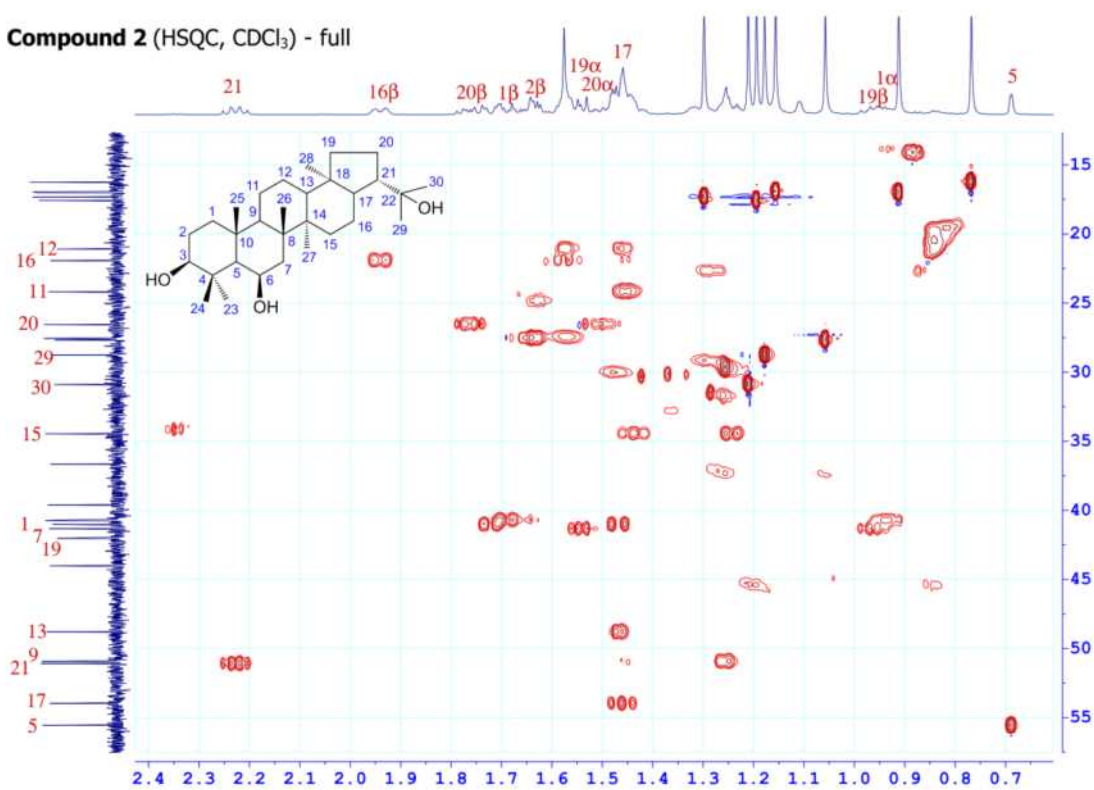


Figure S27: Extended HSQC of compound 2 (21 α -hopane-3 β ,6 β ,22-triol)

Compound 2 (HMBC, CDCl₃) - full

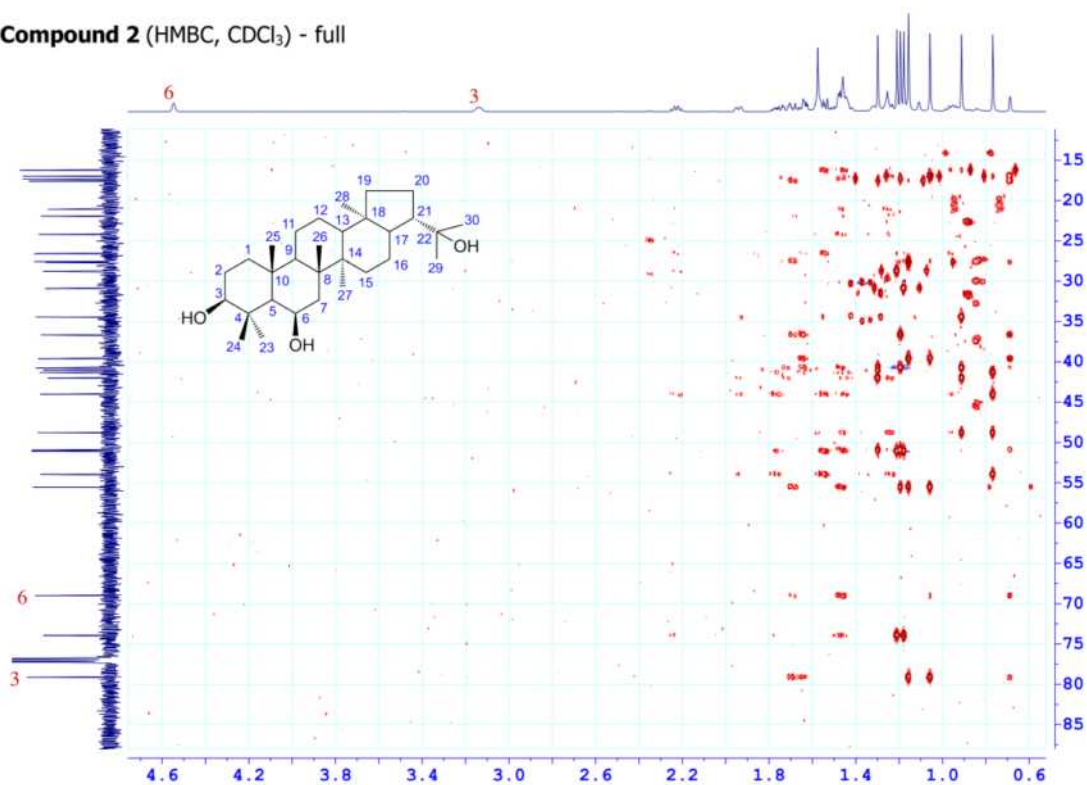


Figure S28: Full HMBC of compound **2** (*21* α -hopane-*3* β ,*6* β ,*22*-triol)

Compound 2 (HMBC, CDCl₃) - ex1

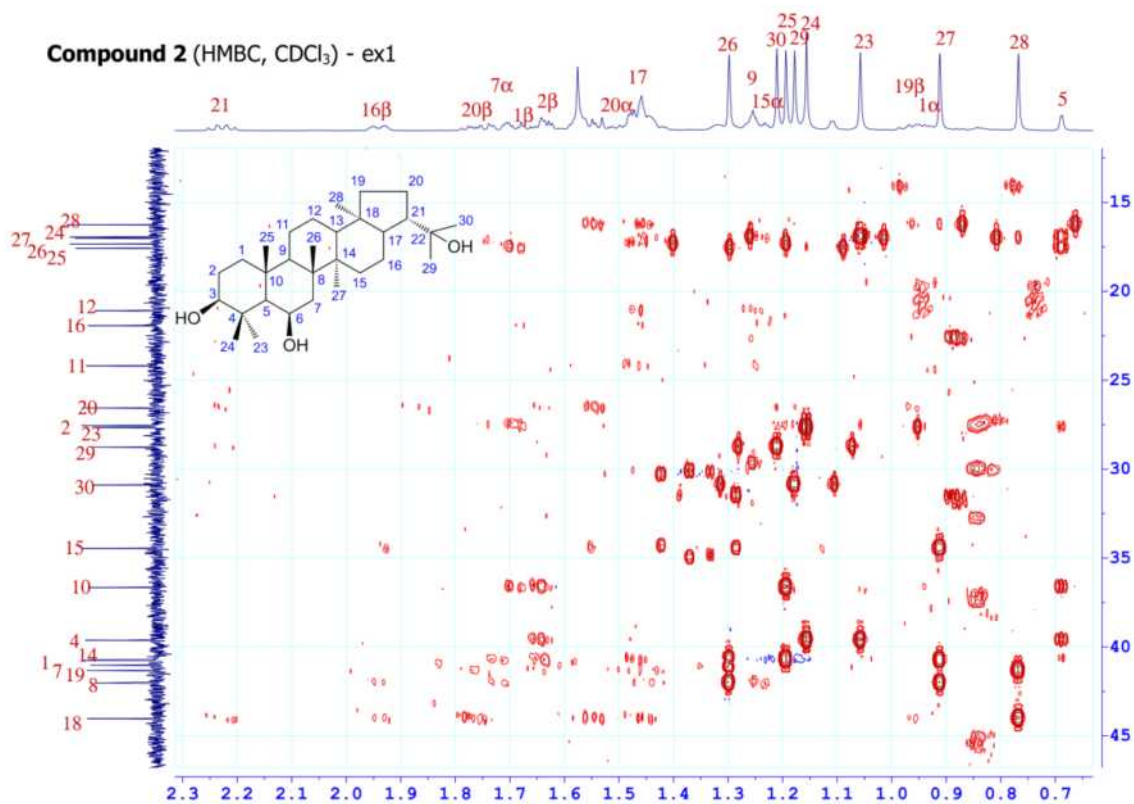


Figure S29: Extended HMBC of compound **2** (*21* α -hopane-*3* β ,*6* β ,*22*-triol)

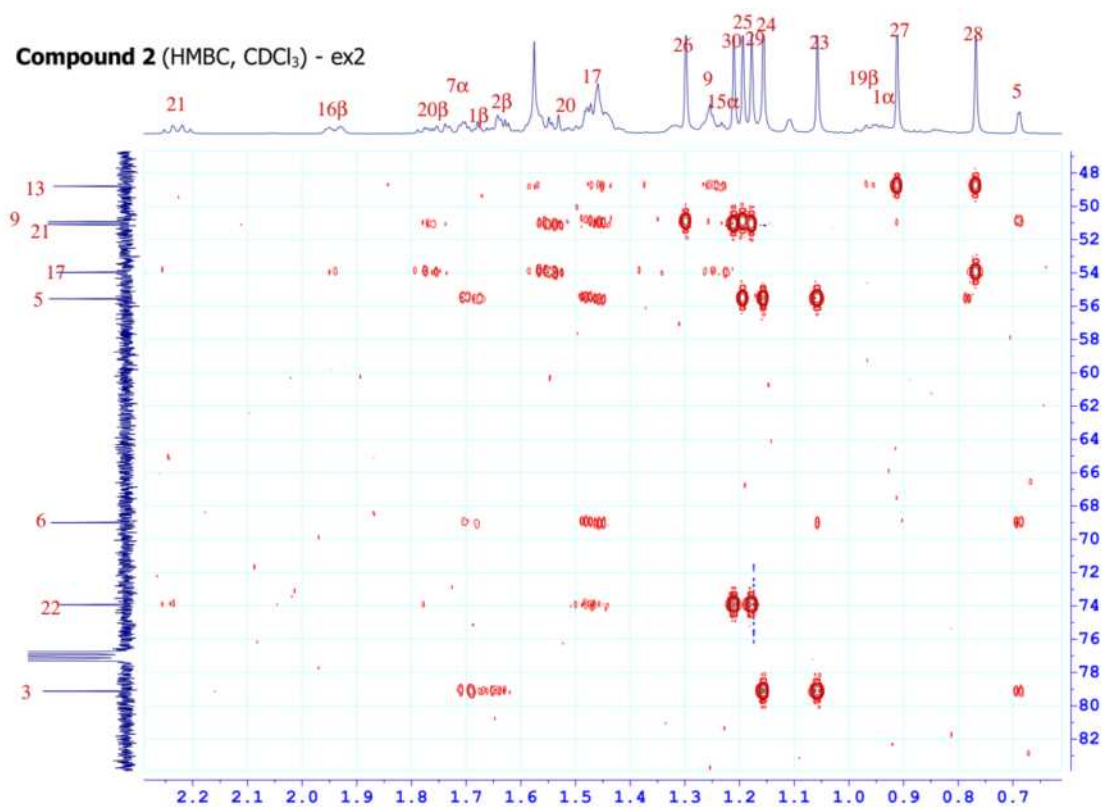


Figure S30: Extended HMBC of compound **2** (21 α -hopane-3 β ,6 β ,22-triol)

Compound 2 (NOESY, CDCl₃) - full

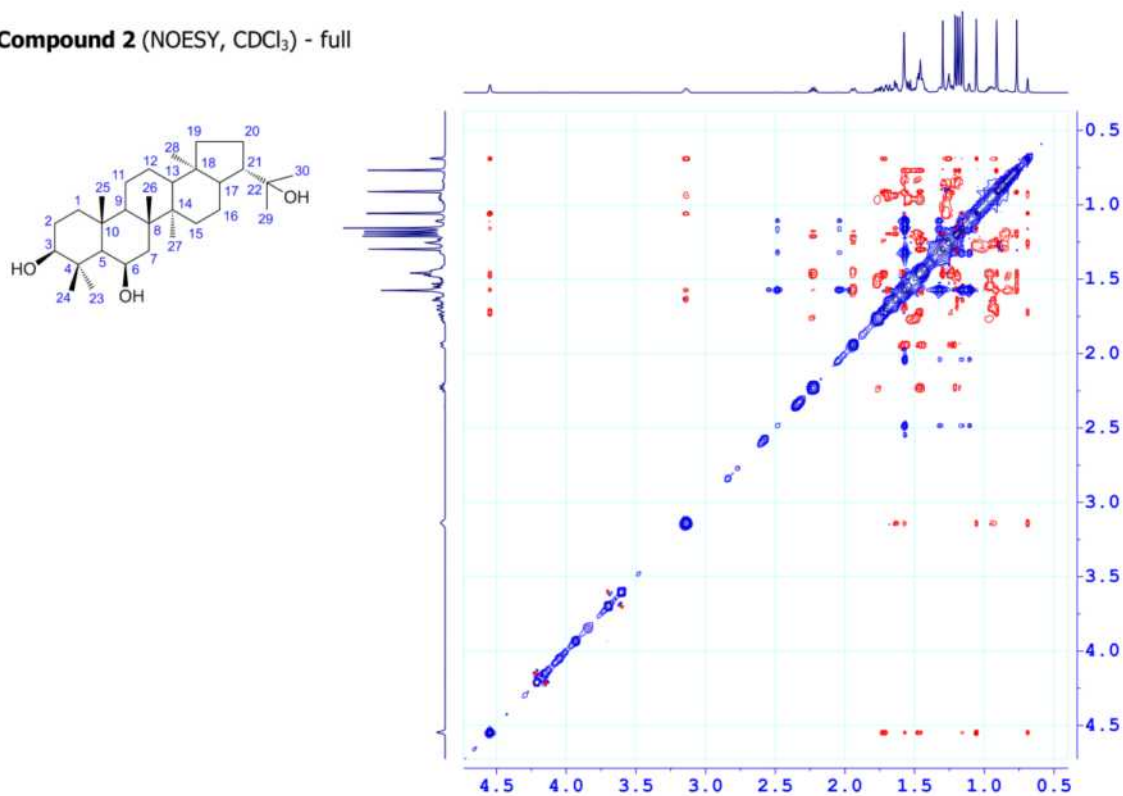


Figure S31: Full NOESY of compound **2** (21 α -hopane-3 β ,6 β ,22-triol)

Compound 2 (NOESY, CDCl₃) - ex1

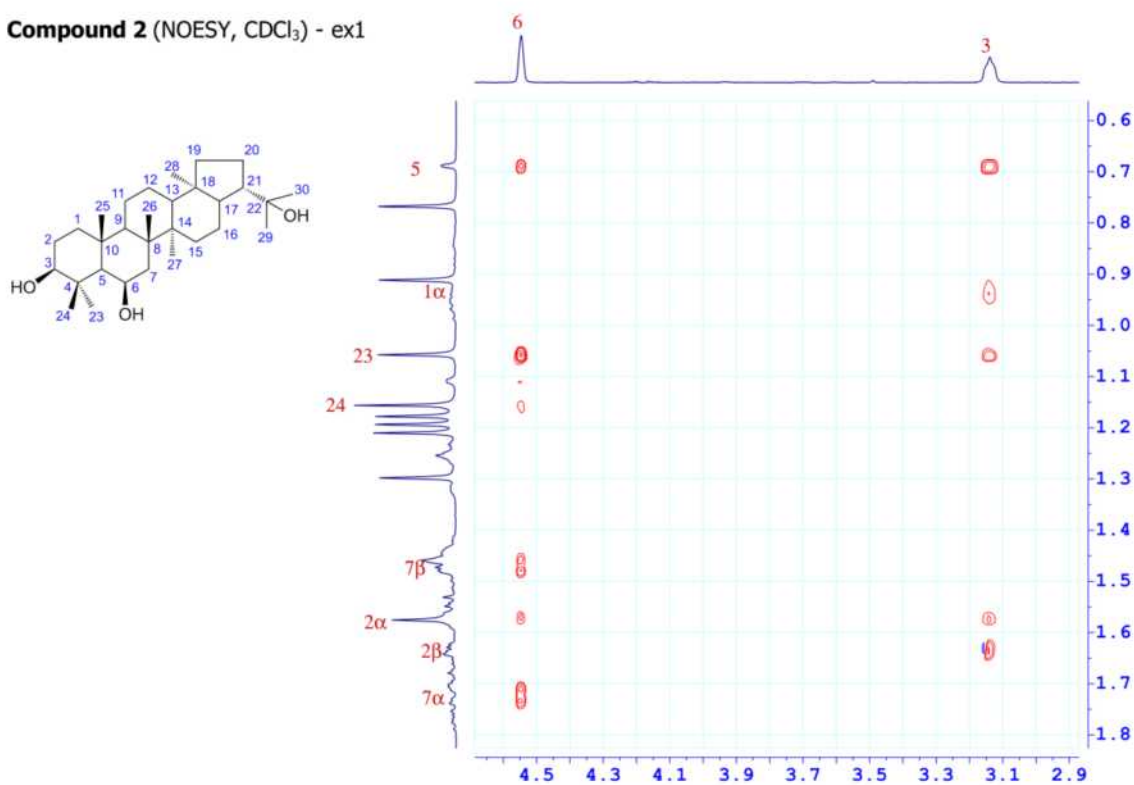


Figure S32: Extended NOESY of compound **2** (21 α -hopane-3 β ,6 β ,22-triol)

Compound 2 (NOESY, CDCl₃) - ex2

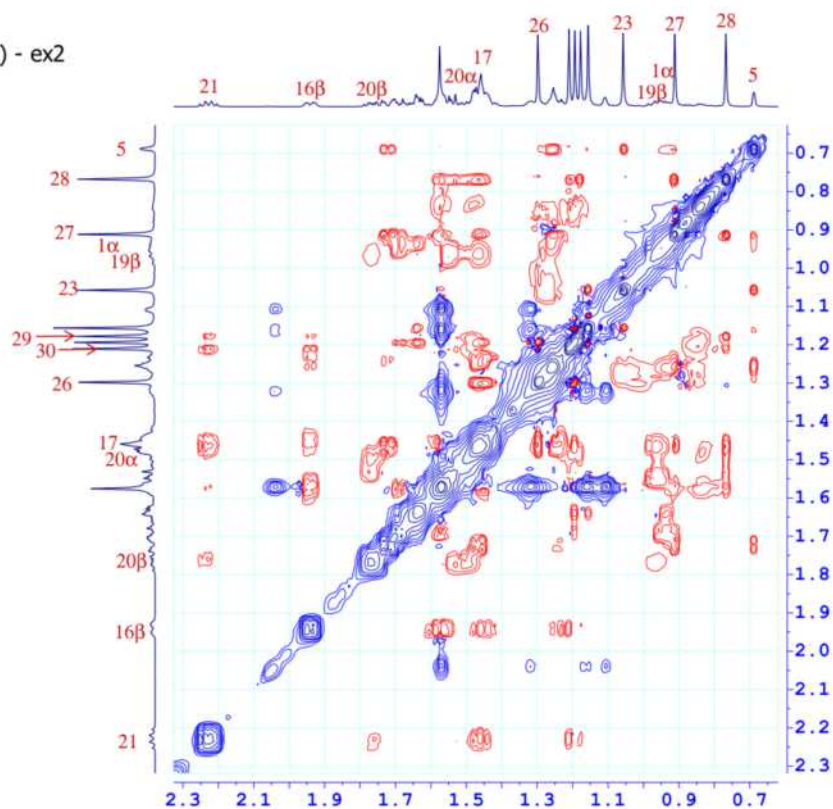
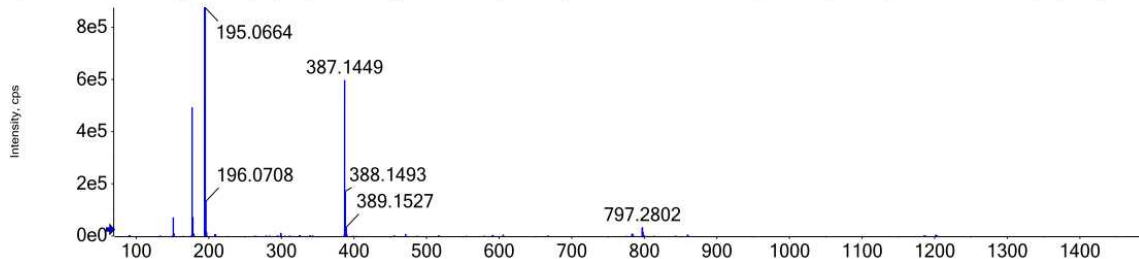


Figure S33: Extended NOESY of compound **2** (21 α -hopane-3 β ,6 β ,22-triol)

Full mass spectrum

Spectrum from DA-Me03_(-)ESI.wiff2 (sample 1) - DA-Me03_(-)ESI, -TOF MS (70 - 1500) from 0.171 min, noise filtered (noise multiplier = 1.5), Gaussian smoothed (0.5 points)



Formula (M)	Ion formula	<i>m/z</i>	Calcd <i>m/z</i>	Diff (ppm)
C ₂₁ H ₂₄ O ₇	C ₂₁ H ₂₃ O ₇ ⁻	387.1449	387.1449	0

Figure S34. (-)HRESI-MS of compound **3** (2'-*O*-Methylnordivarcic acid)

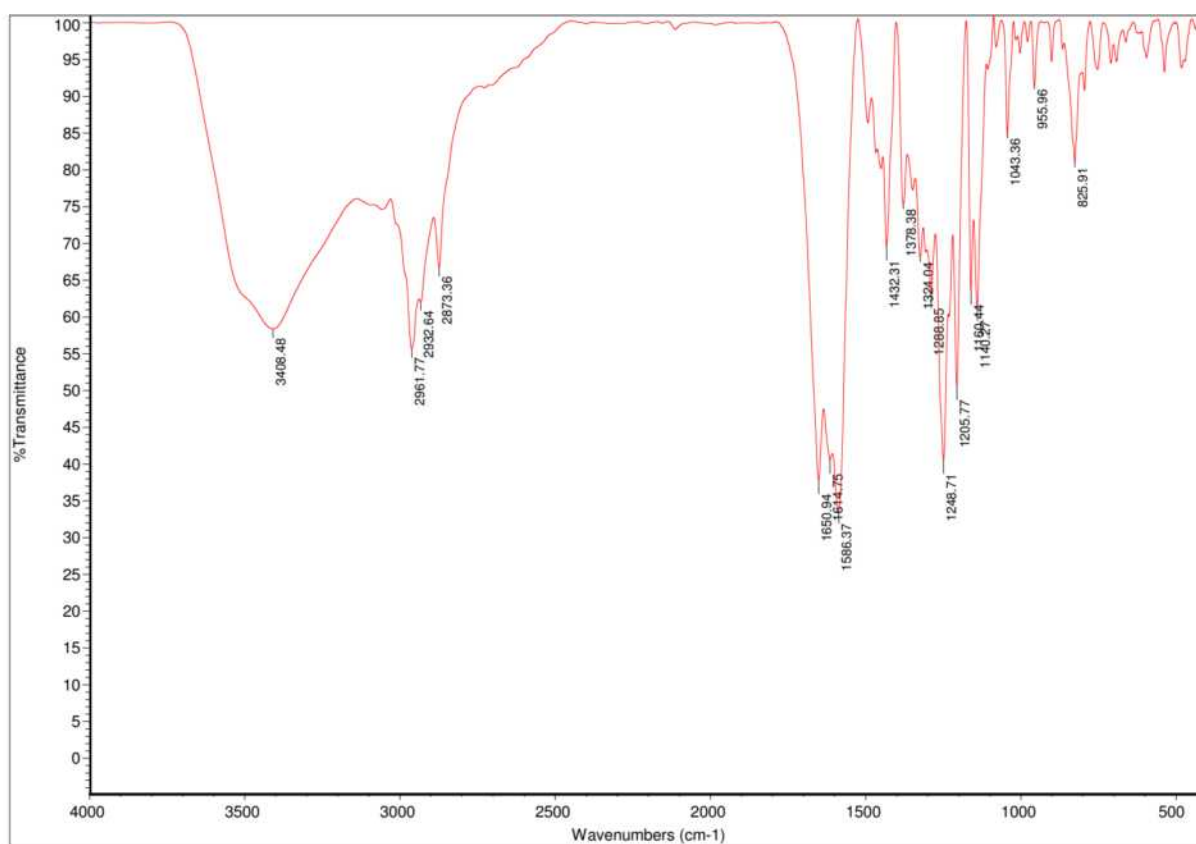


Figure S35: FT-IR of compound **3** (2'-*O*-Methylnordivarcic acid)

Compound 3 (1H, acetone-d6) - full

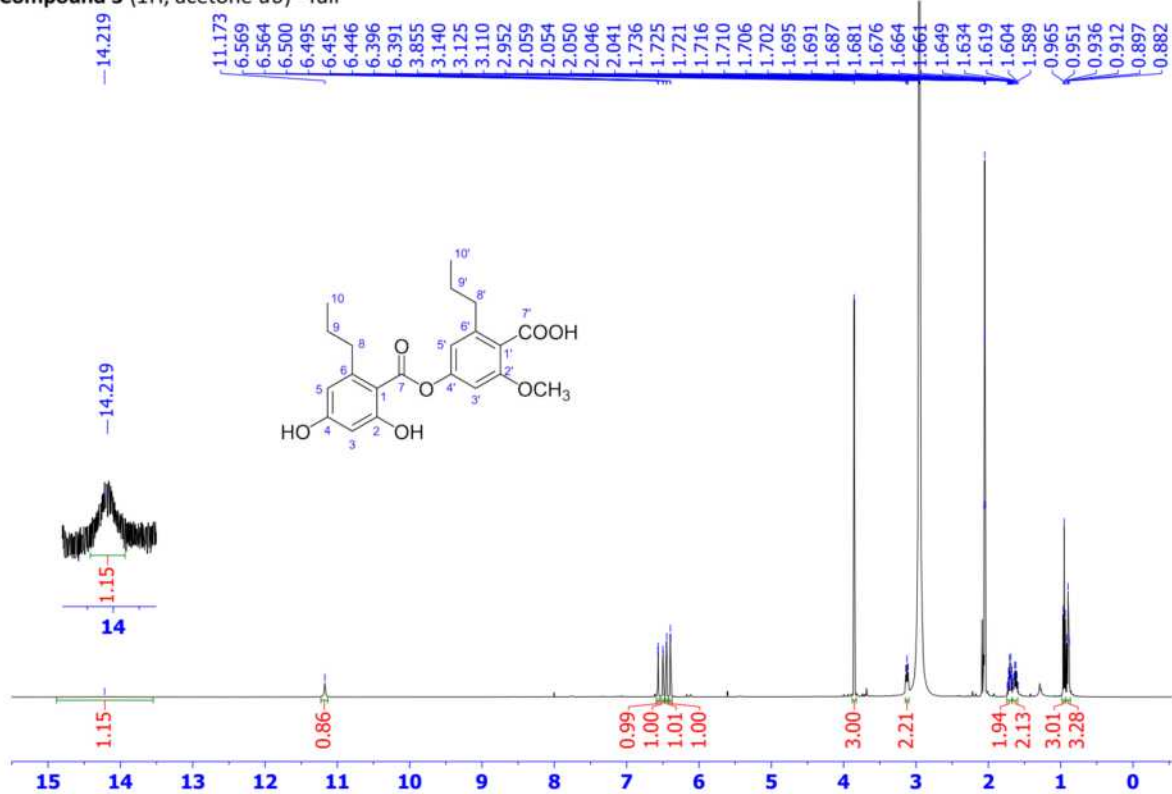


Figure S36: Full ¹H-NMR of compound 3 (2'-O-Methylnordivarcic acid)

Compound 3 (1H, acetone-d6) - ex1

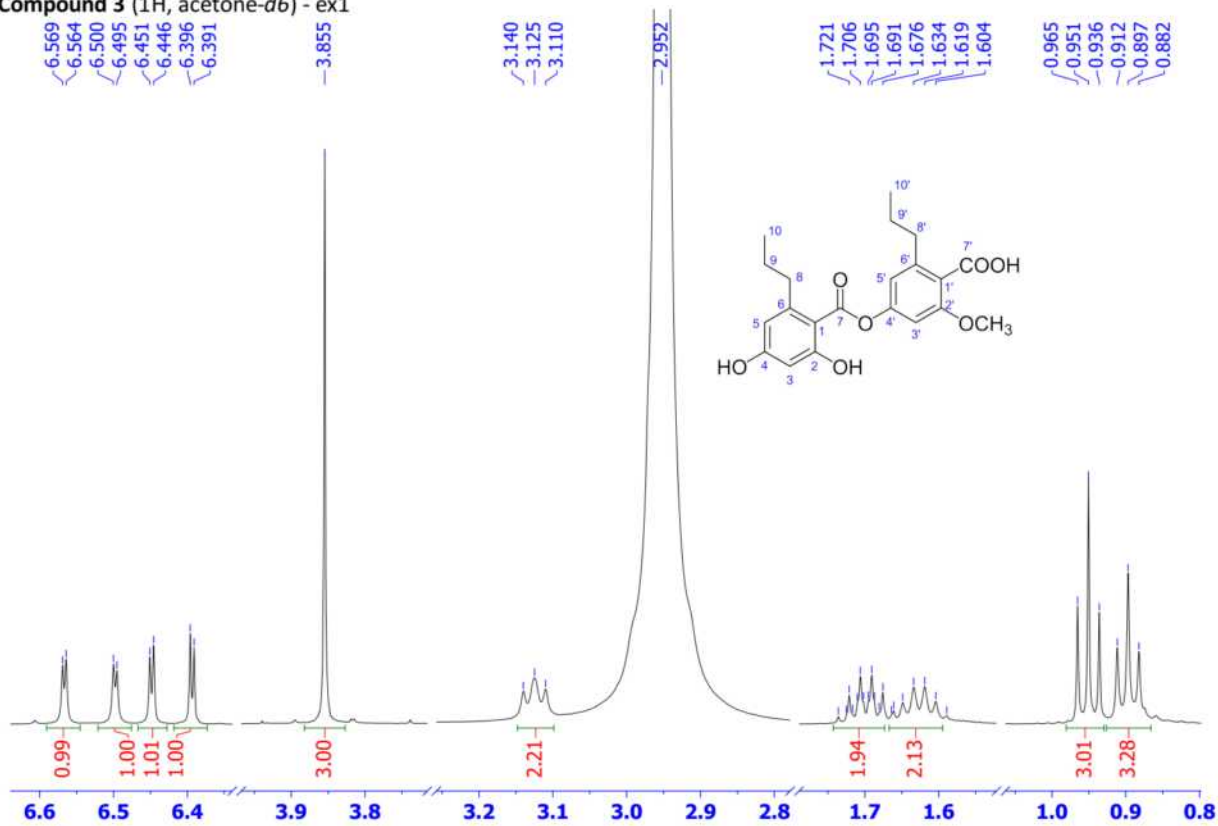


Figure S37: Extended ¹H-NMR of compound 3 (2'-O-Methylnordivarcic acid)

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Compound 3 (13C, acetone-d6) - ex1

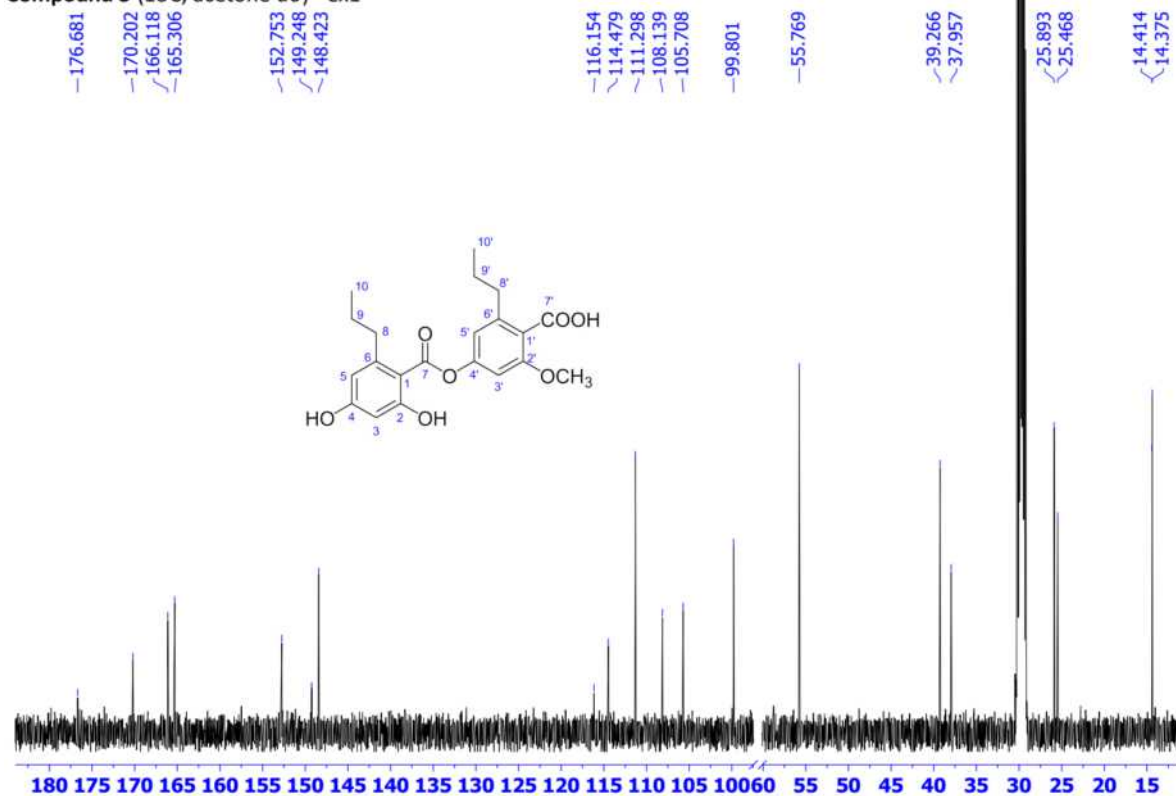


Figure S38: Full ^{13}C -NMR of compound 3 (2'-O-Methylnordivarinic acid)

Compound 3 (DEPT, acetone-d6) - full

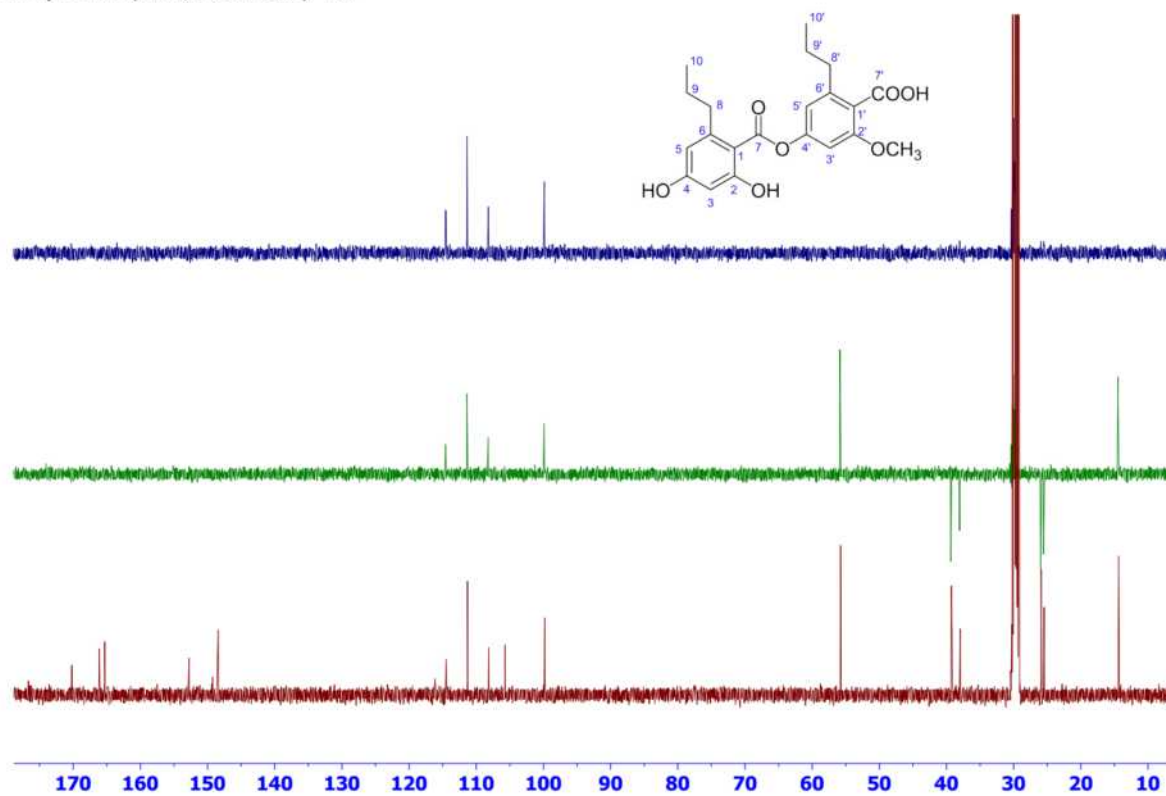


Figure S39: Full DEPT of compound 3 (2'-O-Methylnordivarinic acid)

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Compound 3 (HSQC, acetone-*d*6) - full

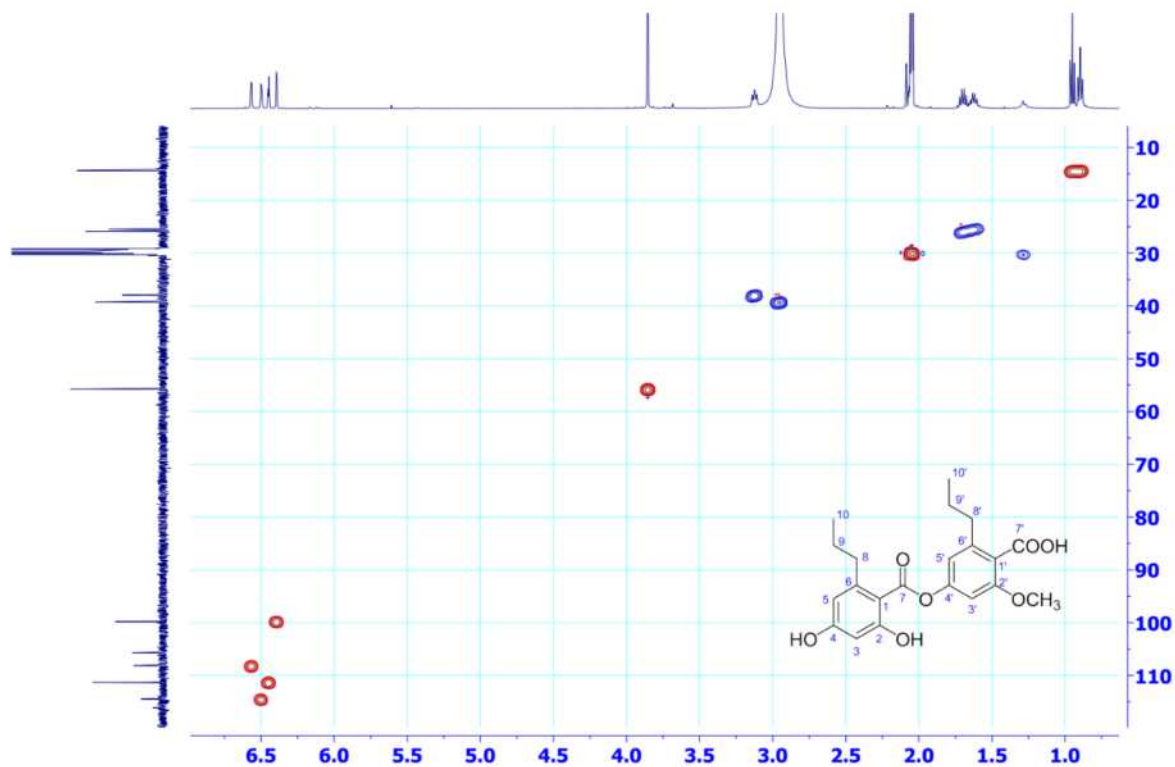


Figure S40: Full HSQC of compound 3 (2'-O-Methylnordivarinic acid)

Compound 3 (HMBC, acetone-*d*6) - full

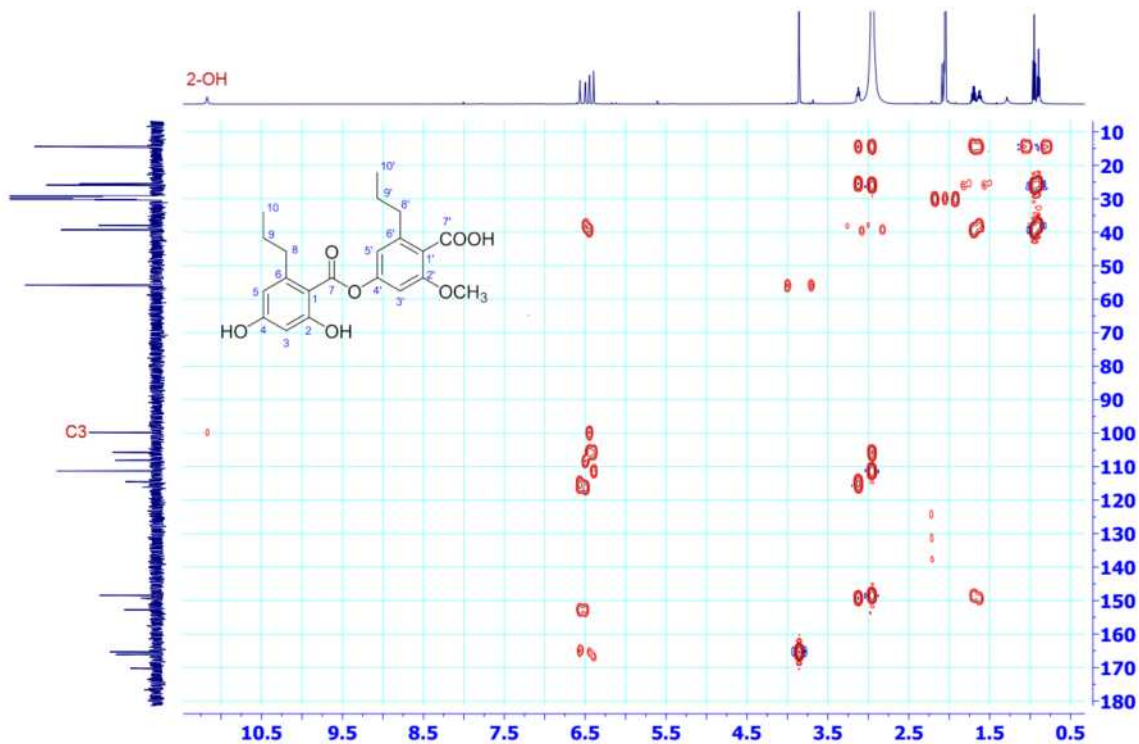


Figure S41: Full HMBC of compound 3 (2'-O-Methylnordivarinic acid)

Compound 3 (HMBC, acetone-*d*6) - ex1

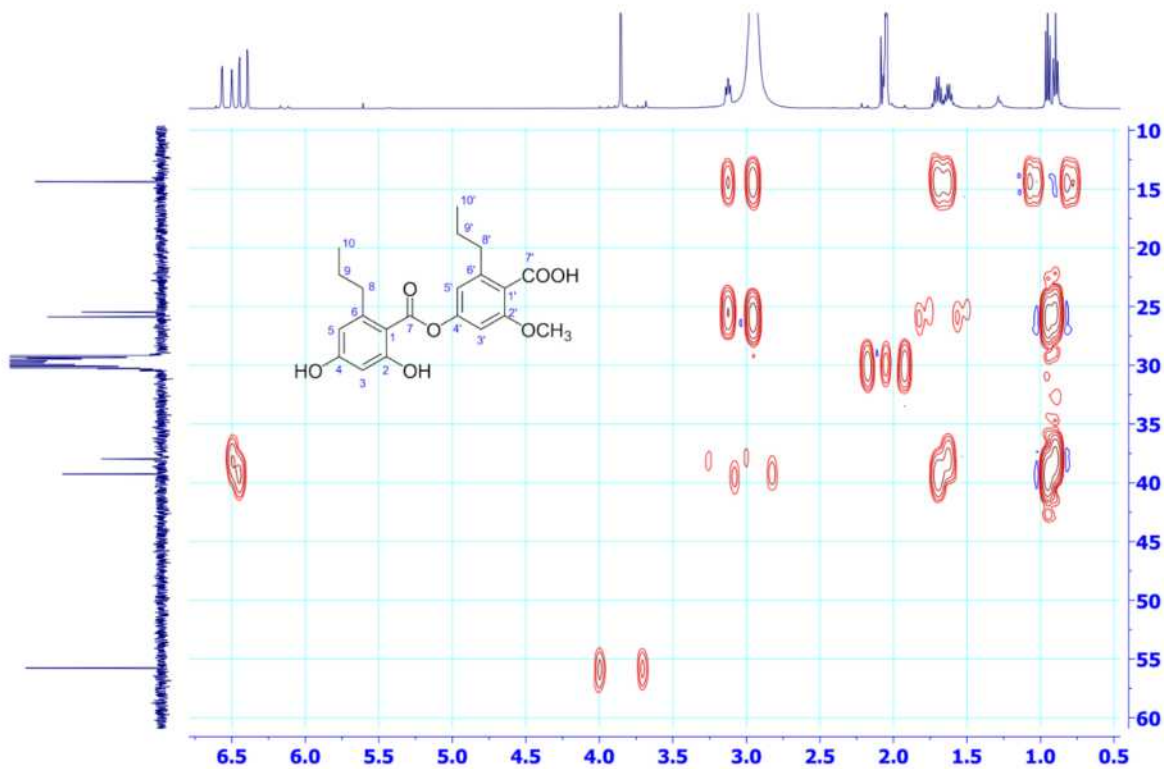


Figure S42: Extended HMBC of compound 3 (2'-O-Methylnordivarinic acid)

Compound 3 (HMBC, acetone-*d*6) - ex2

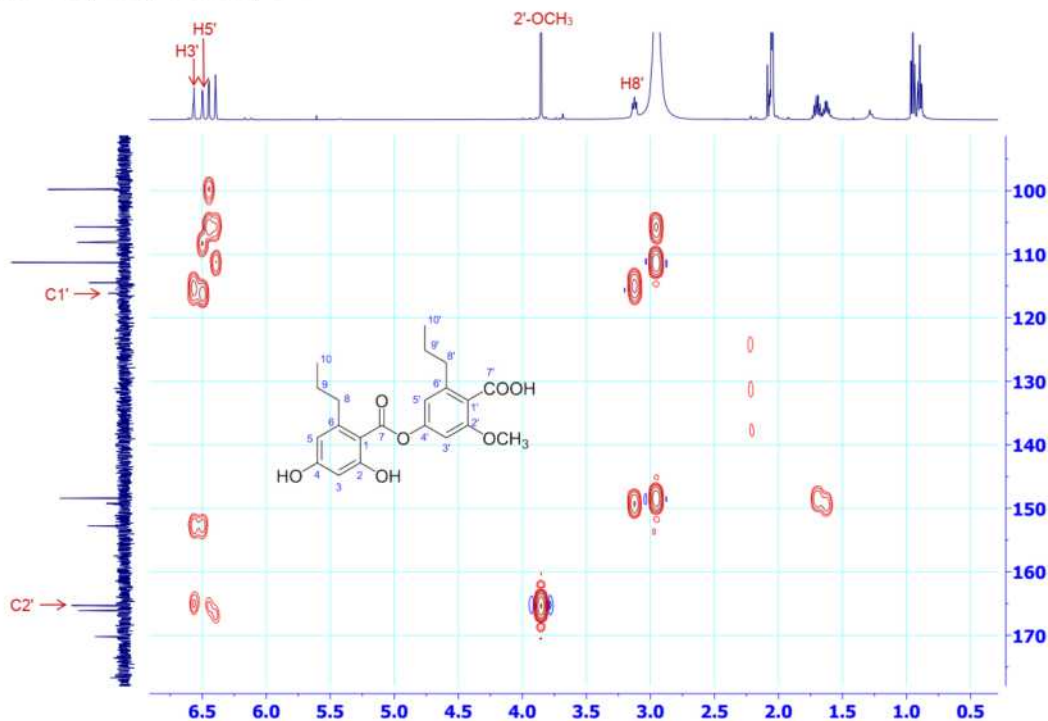


Figure S43: Extended HMBC of compound 3 (2'-O-Methylnordivarinic acid)