

Supporting Information

New triterpenoids from *Lansium domesticum* Corr. cv Kokossan and their cytotoxic activity

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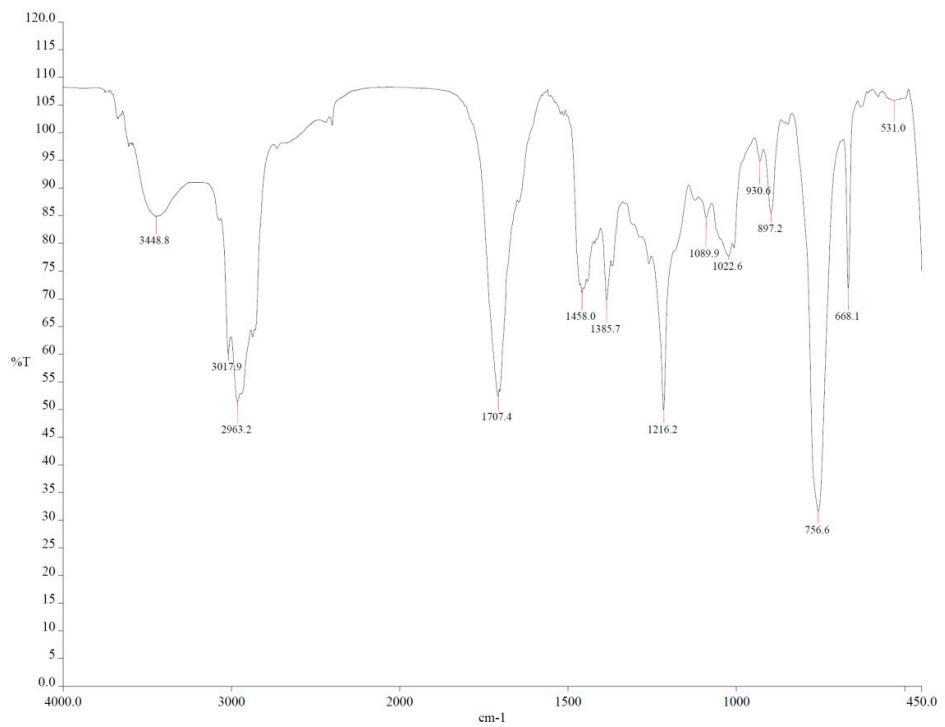


Figure S1 : IR spectrum of **1**

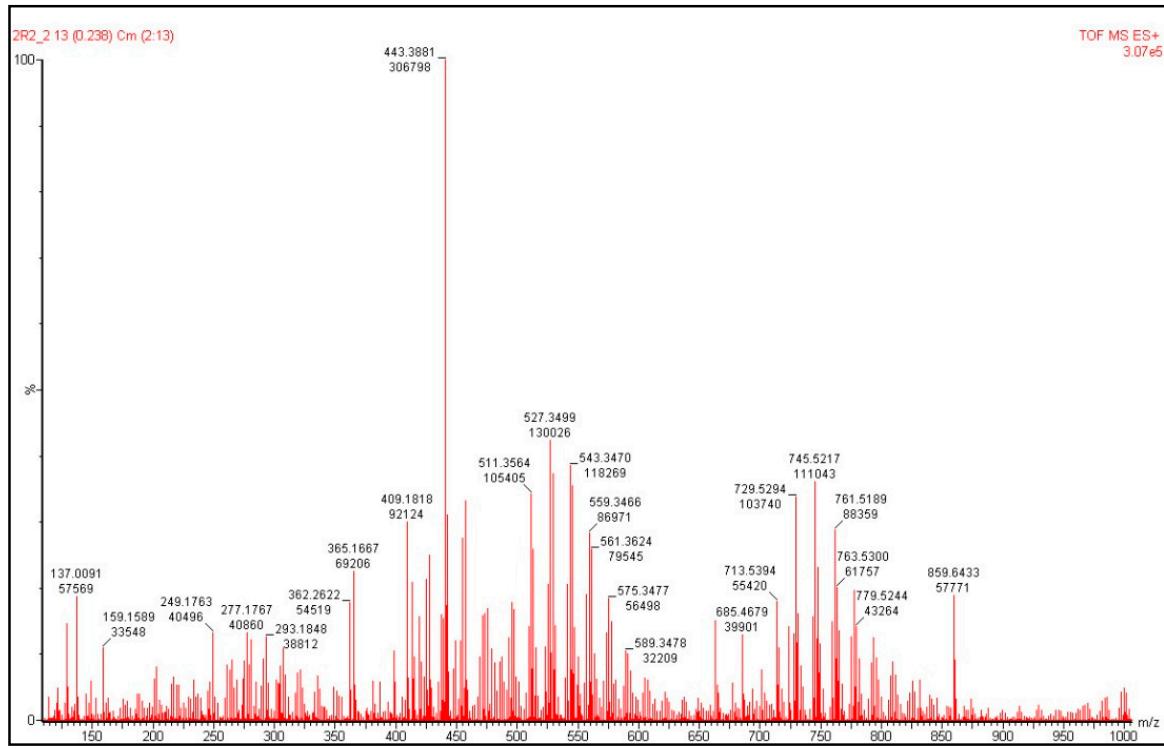


Figure S2: HR-ESI-MS spectrum of 1.

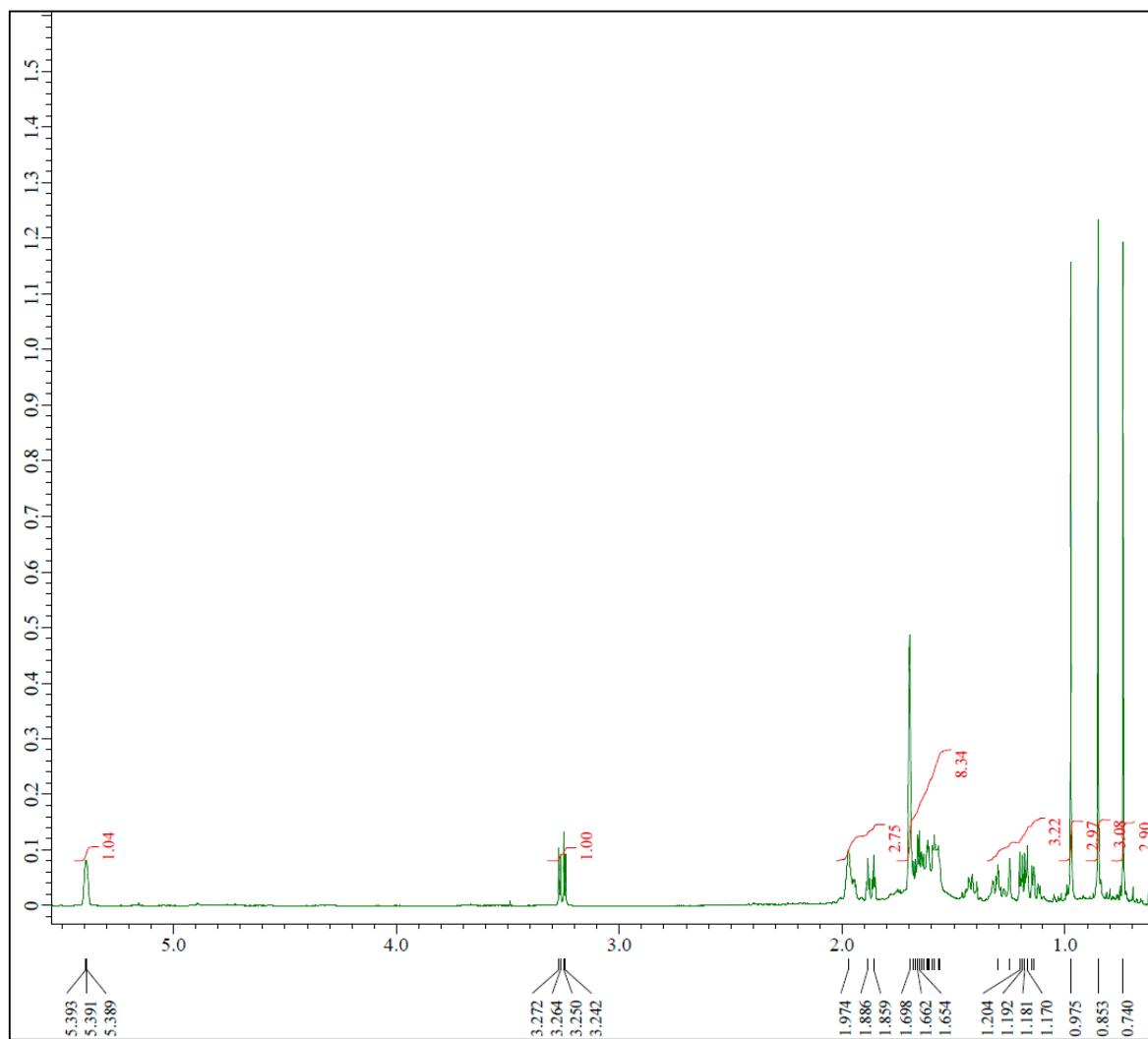


Figure S3: ^1H -NMR (500 MHz, CDCl_3) spectrum of **1**.

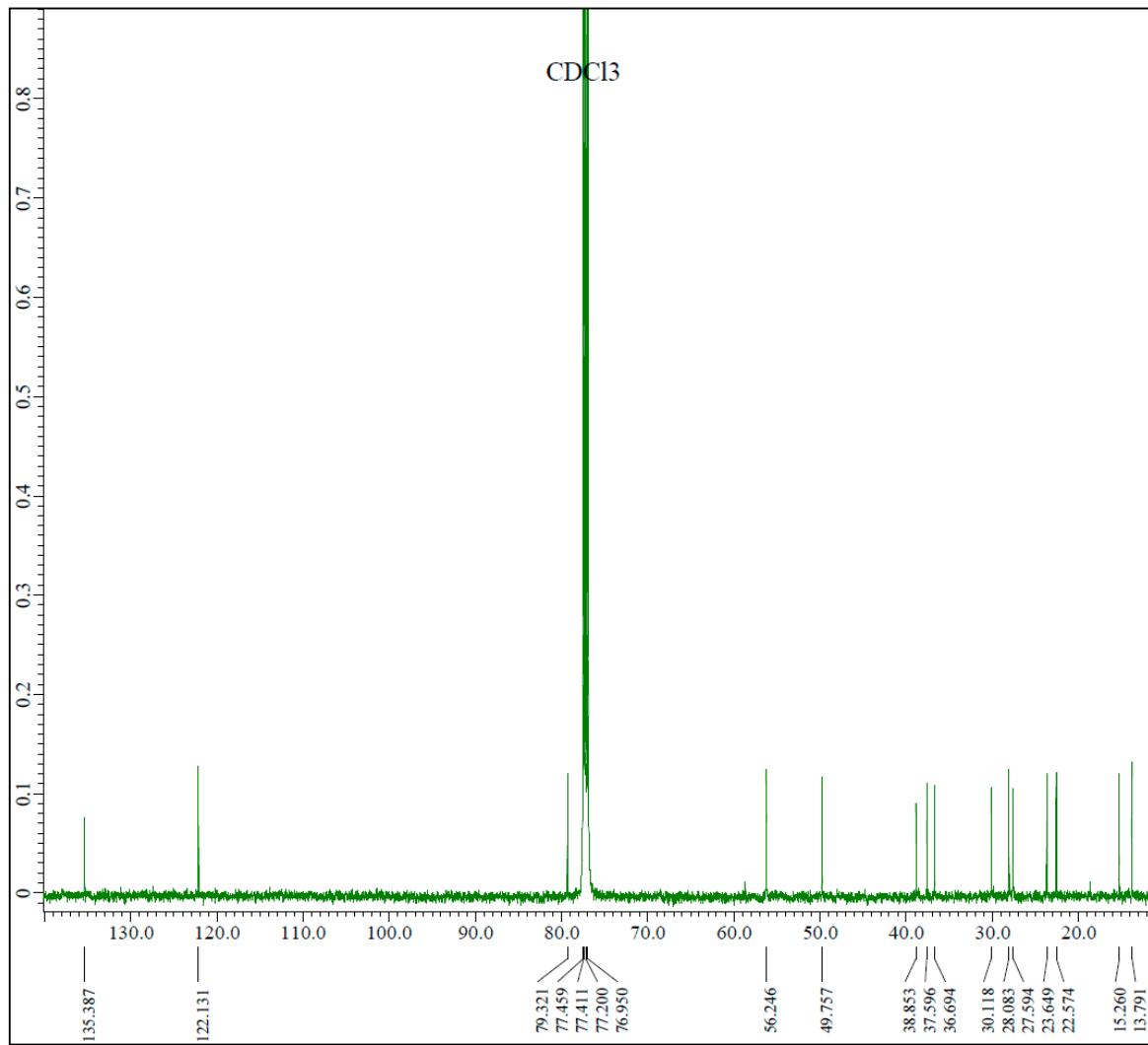


Figure S4: ^{13}C -NMR (125 MHz, CDCl_3) spectrum of **1**.

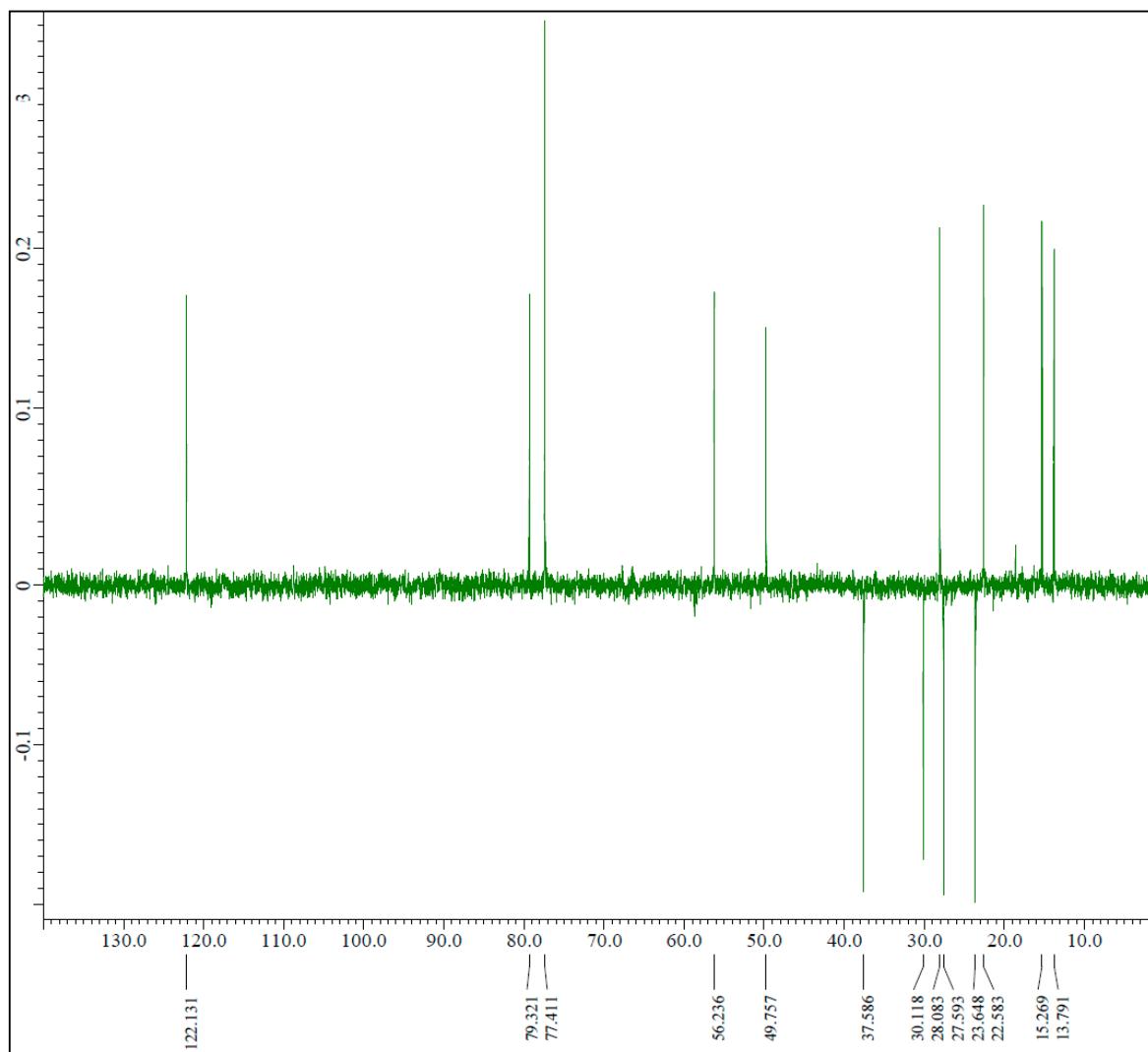


Figure S5: DEPT135 (125 MHz, CDCl_3) spectrum of **1**.

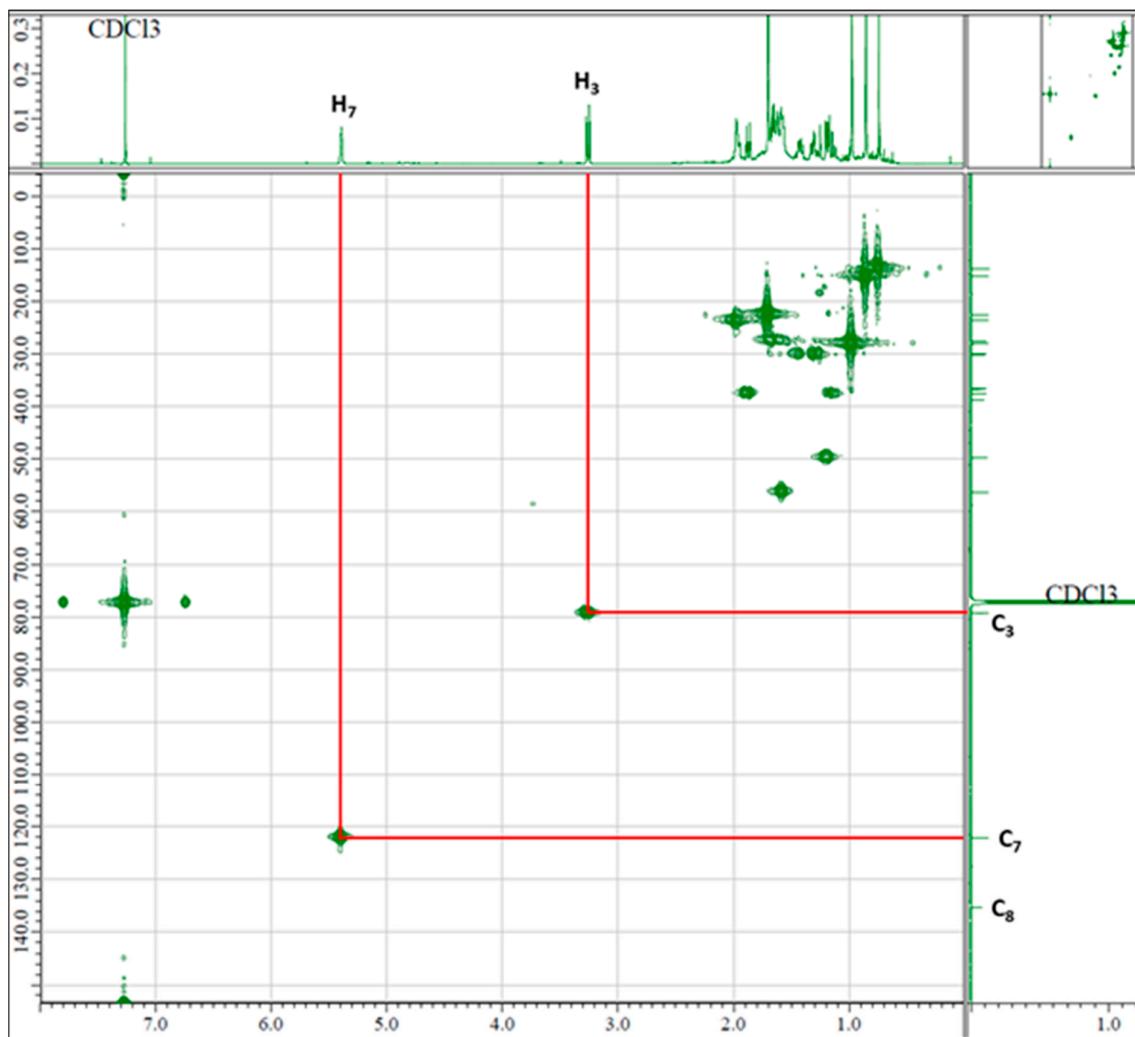


Figure S6: HMQC spectrum of **1**.

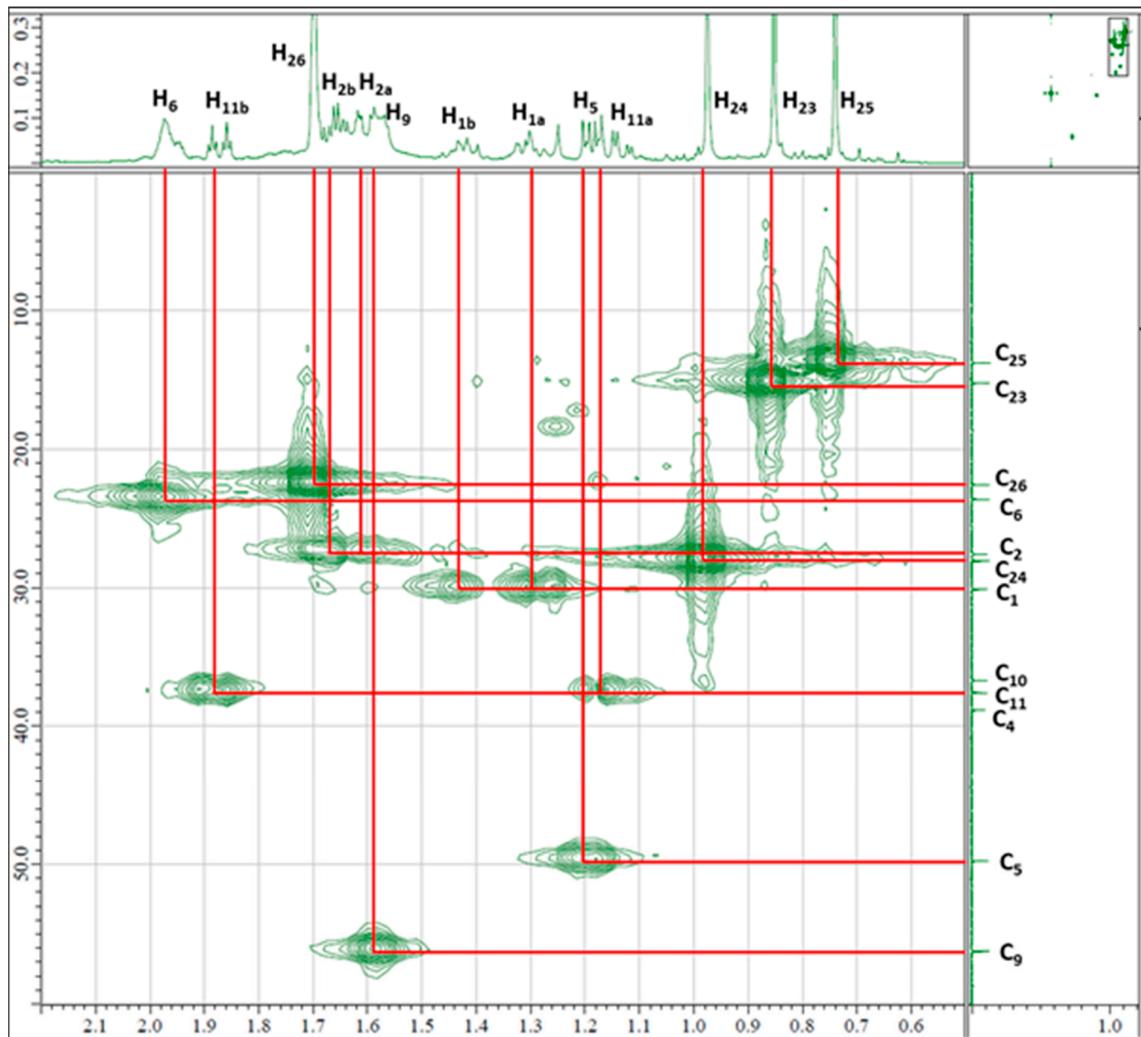


Figure S7: HMQC spectrum of **1** (From $\delta_{\text{C}} 10$ ppm to $\delta_{\text{C}} 60$ ppm).



Figure S8: HMBC spectrum of **1**.



Figure S9: HMBC spectrum of **1** (From δ_{C} 10 ppm to δ_{C} 60 ppm).

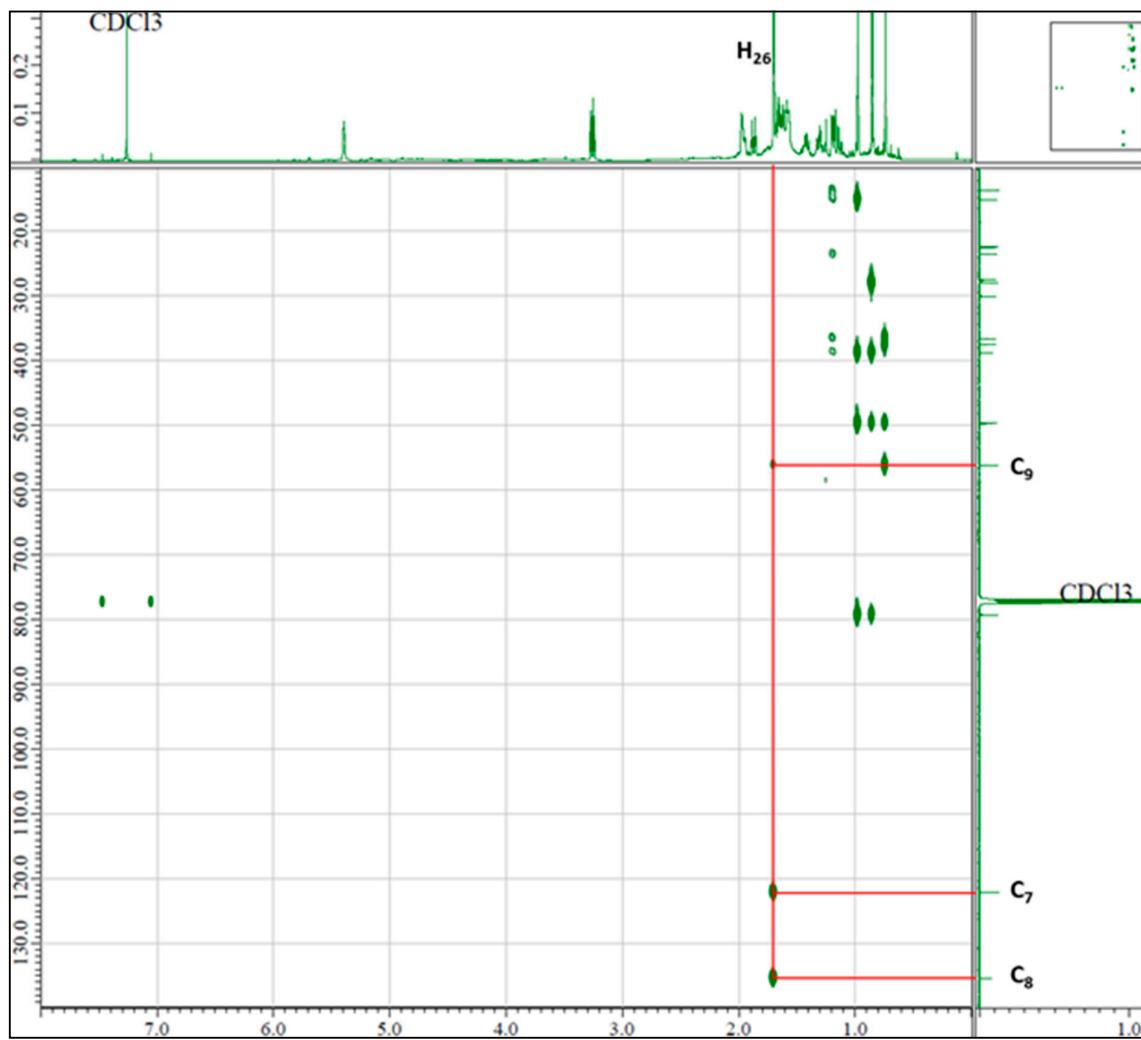


Figure S10: HMBC spectrum of **1** (From δ_{C} 10 ppm to δ_{C} 140 ppm).

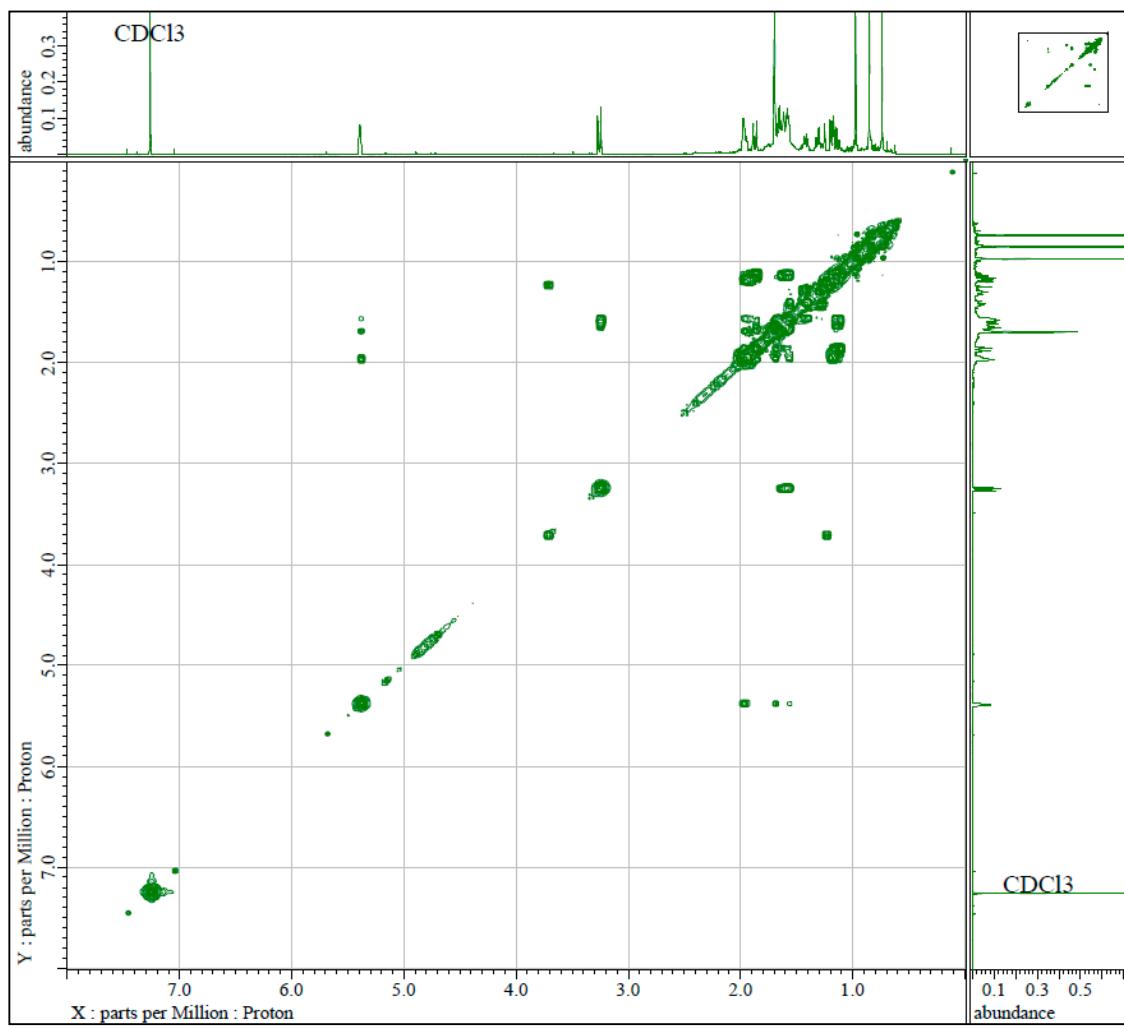


Figure S11: ^1H - ^1H COSY spectrum of 1.

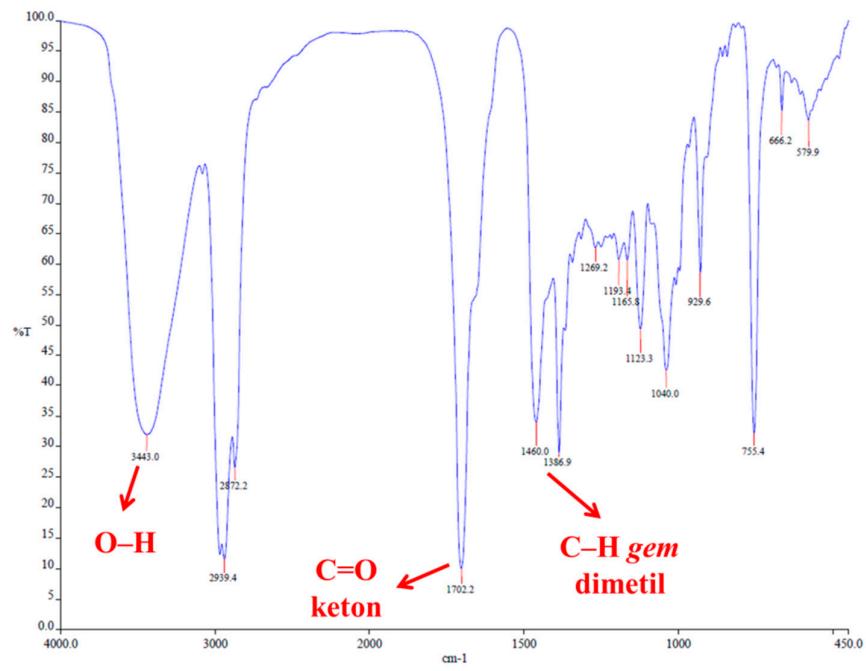


Figure 12. IR spectrum of 2

Single Mass Analysis

Tolerance = 10.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

114 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

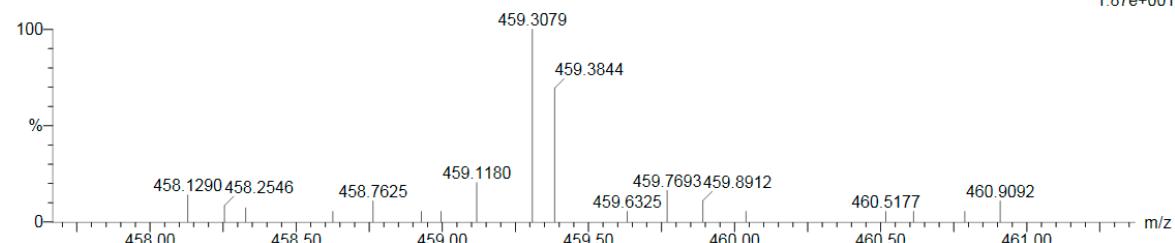
Elements Used:

C: 0-500 H: 0-1000 O: 0-200

ZUL 03- 18 (0.323) Cm (18)

TOF MS ES-

1.87e+001



Minimum:

-1.5

Maximum:

10.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
459.3844	459.3838	0.6	1.3	5.5	27.4	0.0	C30 H51 O3

Figure S13: HR-ESI-MS spectrum of 2.

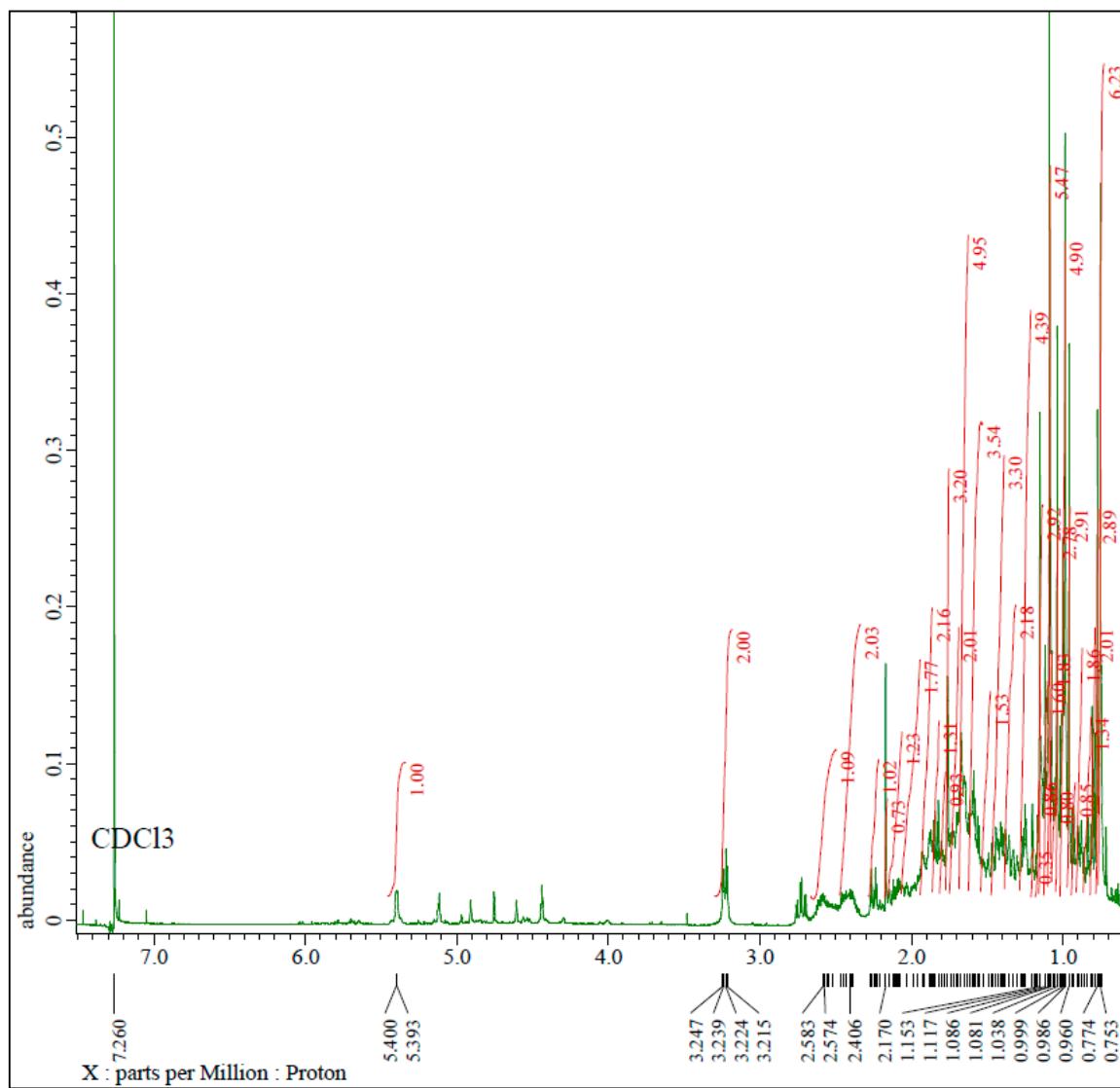


Figure S14: ¹H-NMR (500 MHz, CDCl₃) spectrum of **2**.

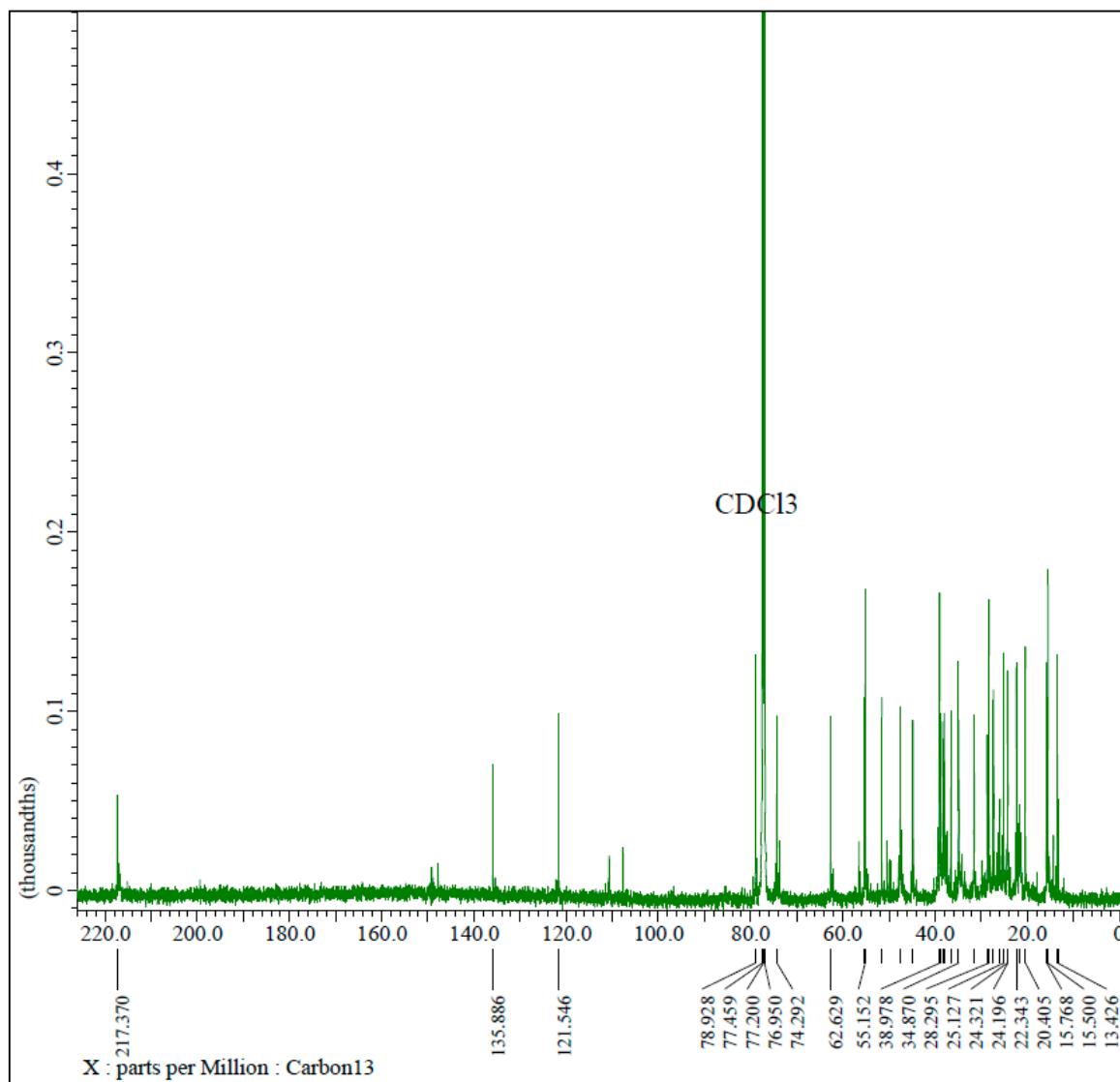


Figure S15: ^{13}C -NMR (125 MHz, CDCl₃) spectrum of **2**.

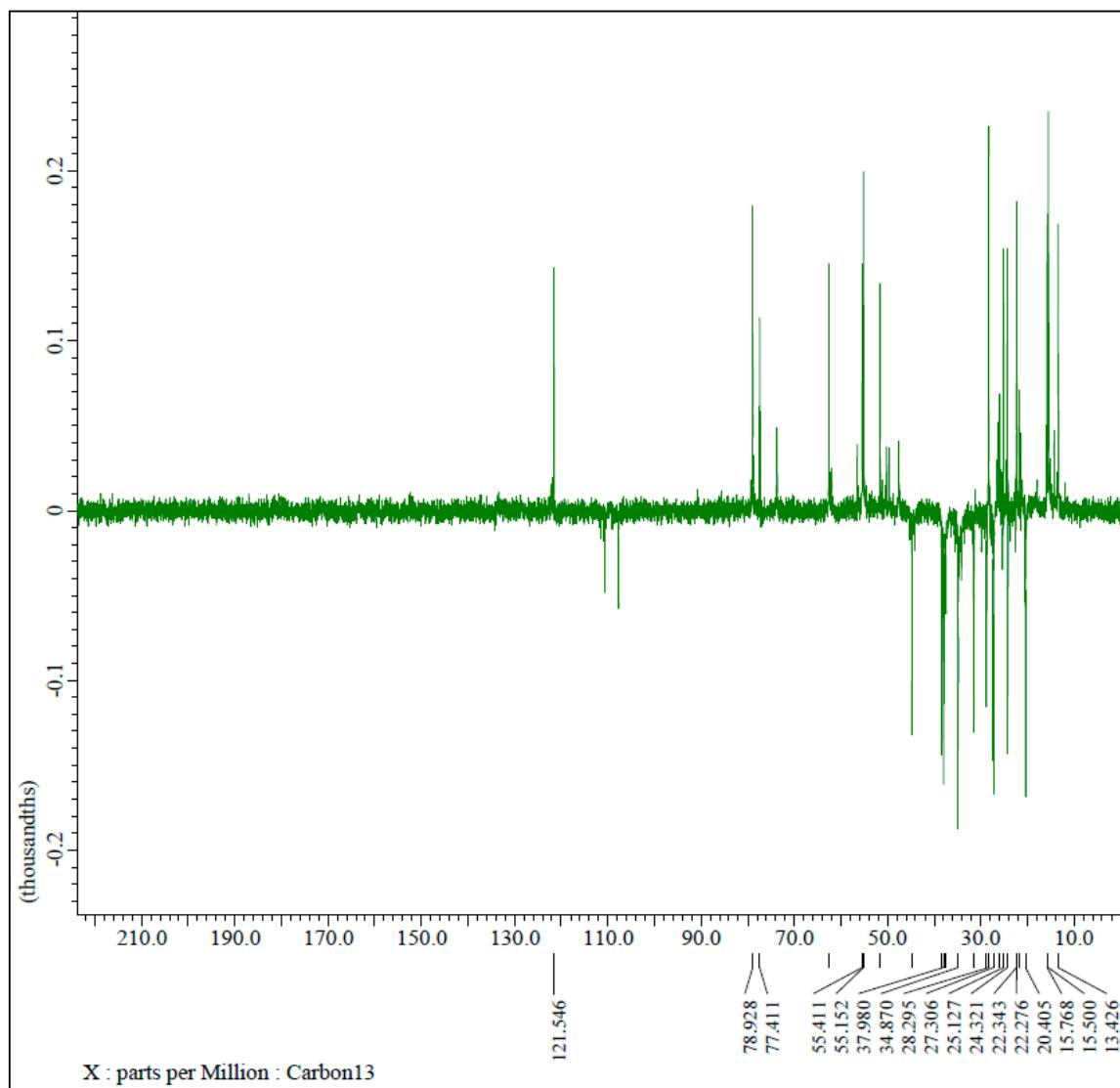


Figure S16: DEPT135 (125 MHz, CDCl₃) spectrum of **2**.

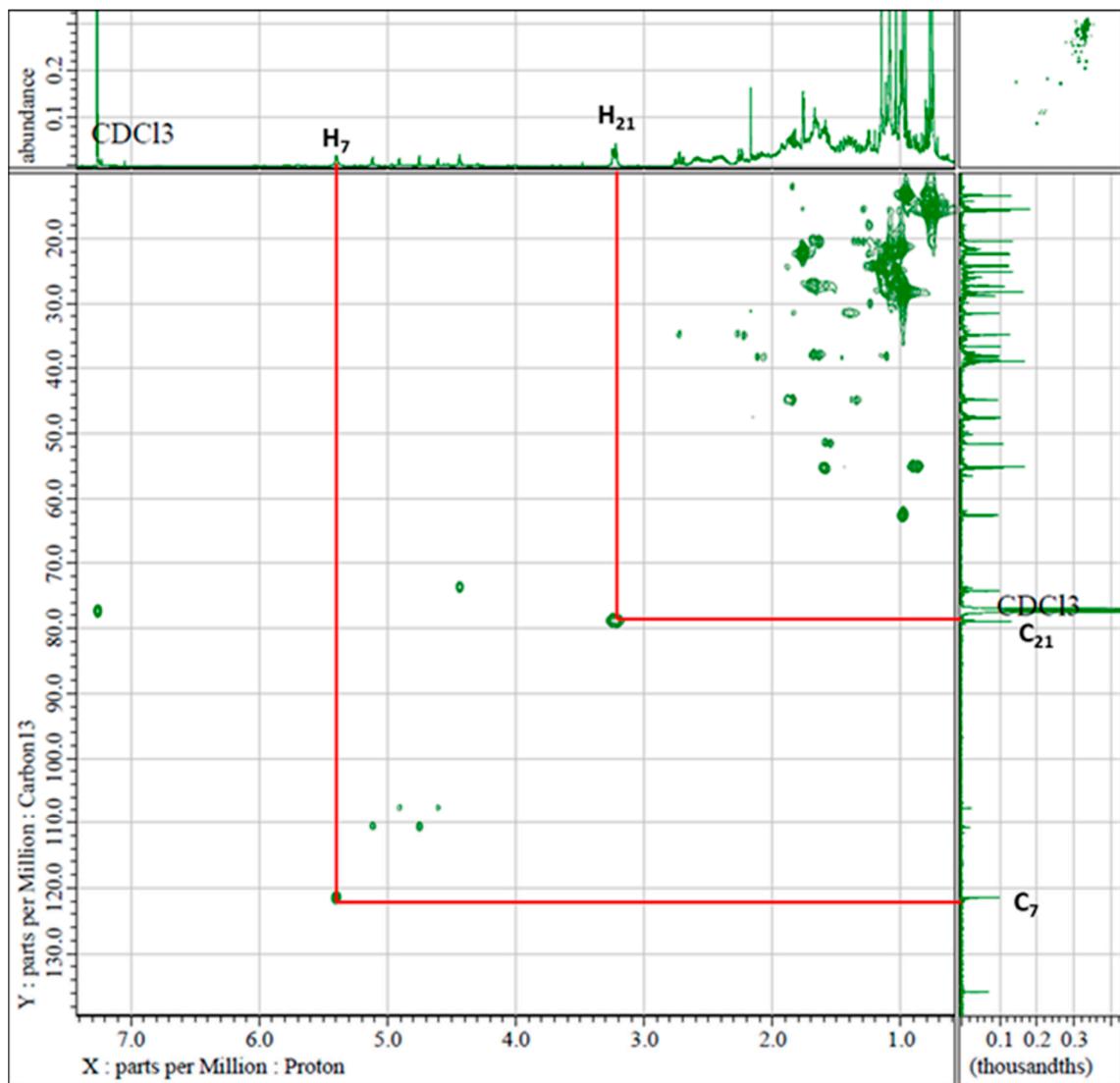


Figure S17: HMQC spectrum of 2.

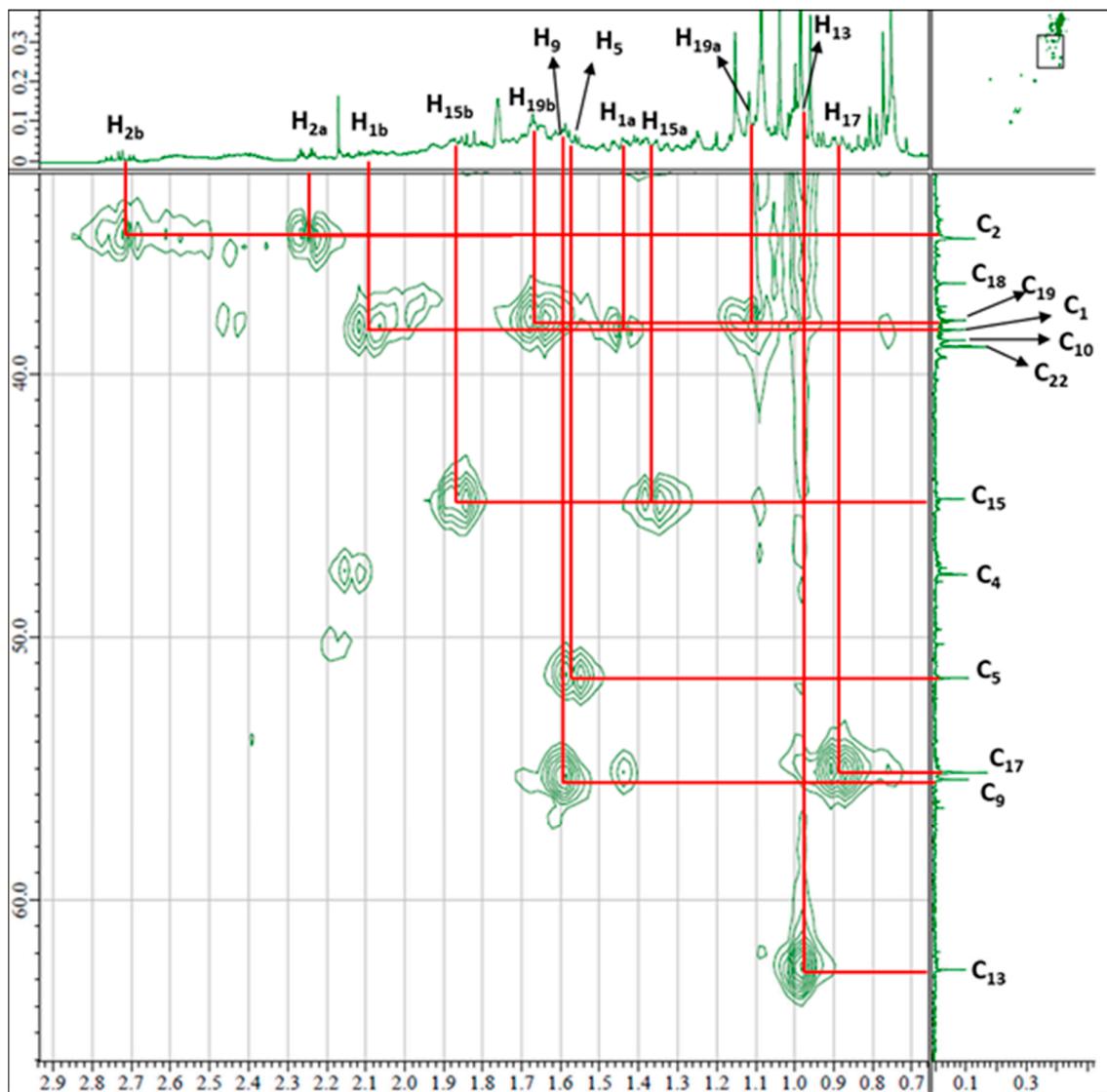


Figure S18: HMQC spectrum of **2** (From δ_{C} 30 ppm to 70 ppm).

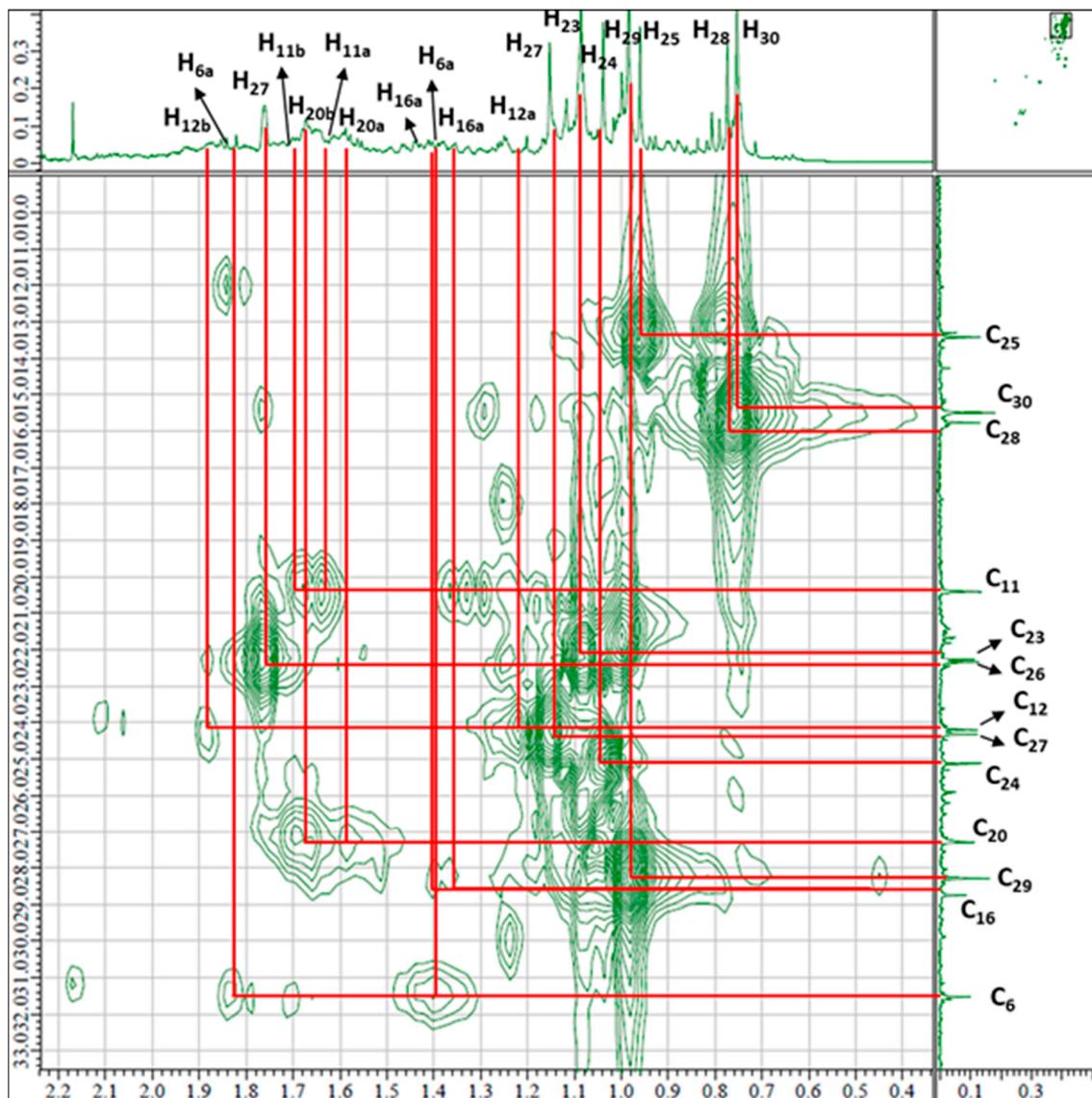


Figure S19: HMQC spectrum of **2** (From δ_{C} 13 ppm to 32 ppm).

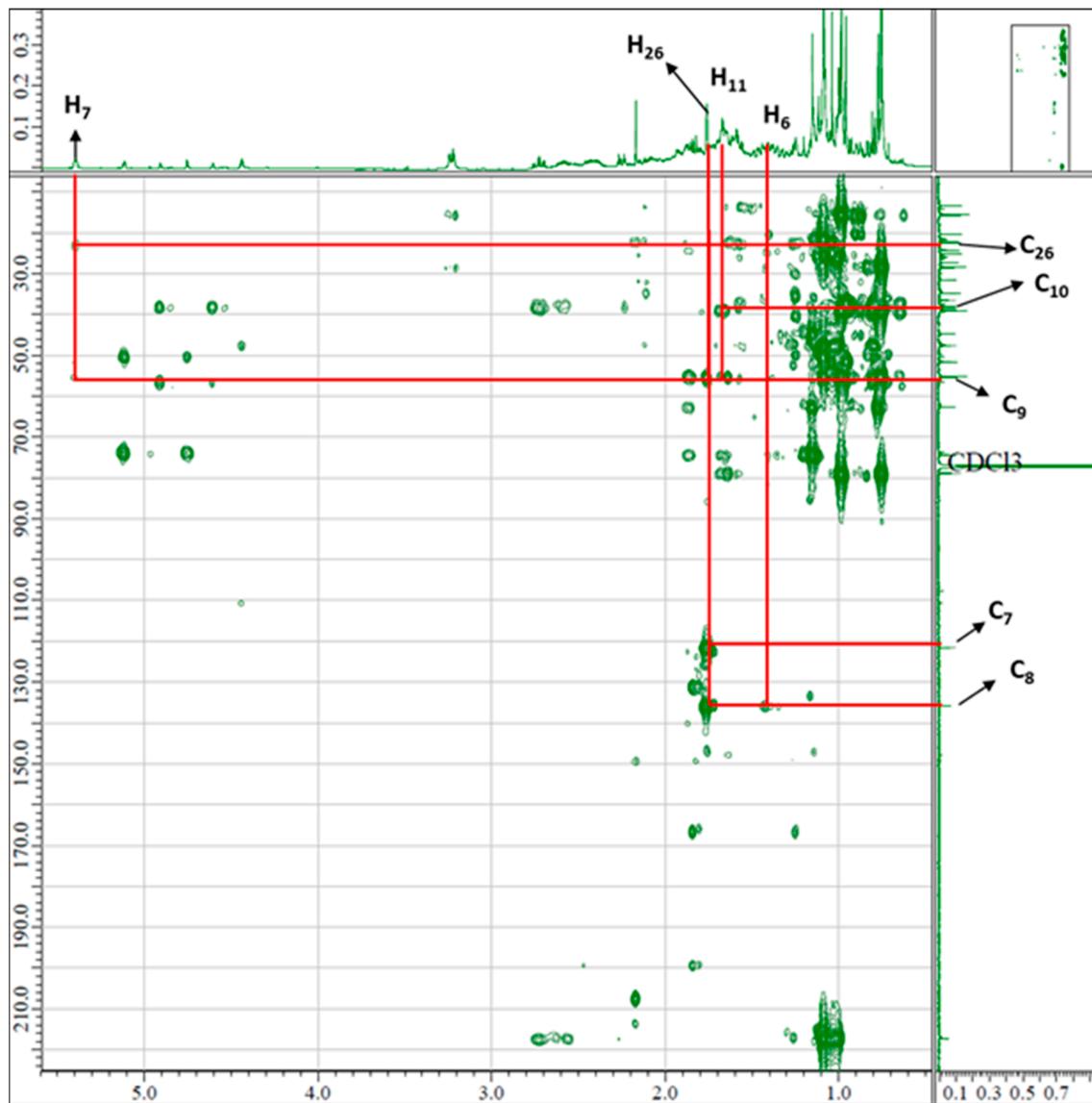


Figure S20: HMBC spectrum of 2.

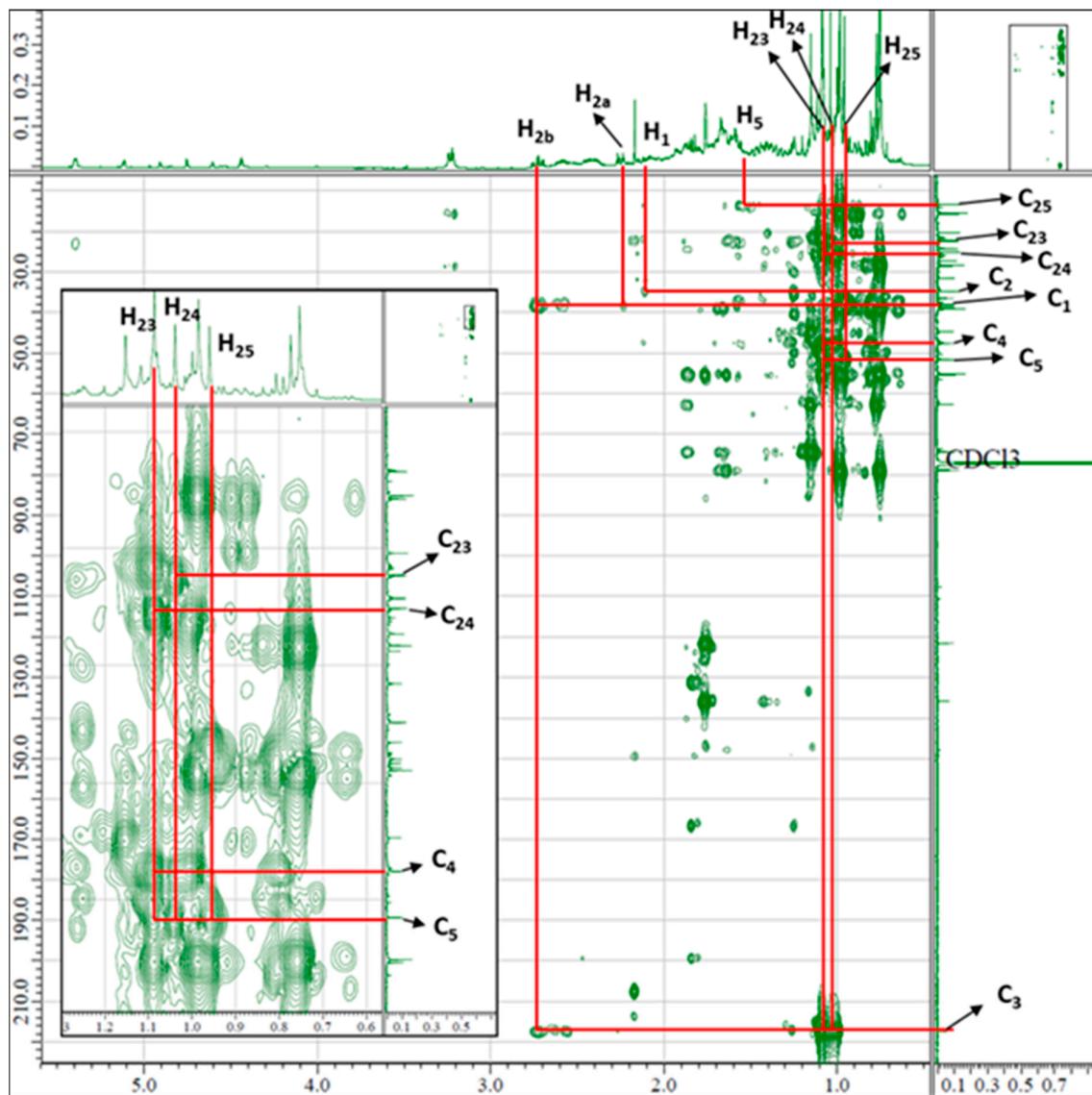


Figure S21: HMBC spectrum of **2** (expansion).

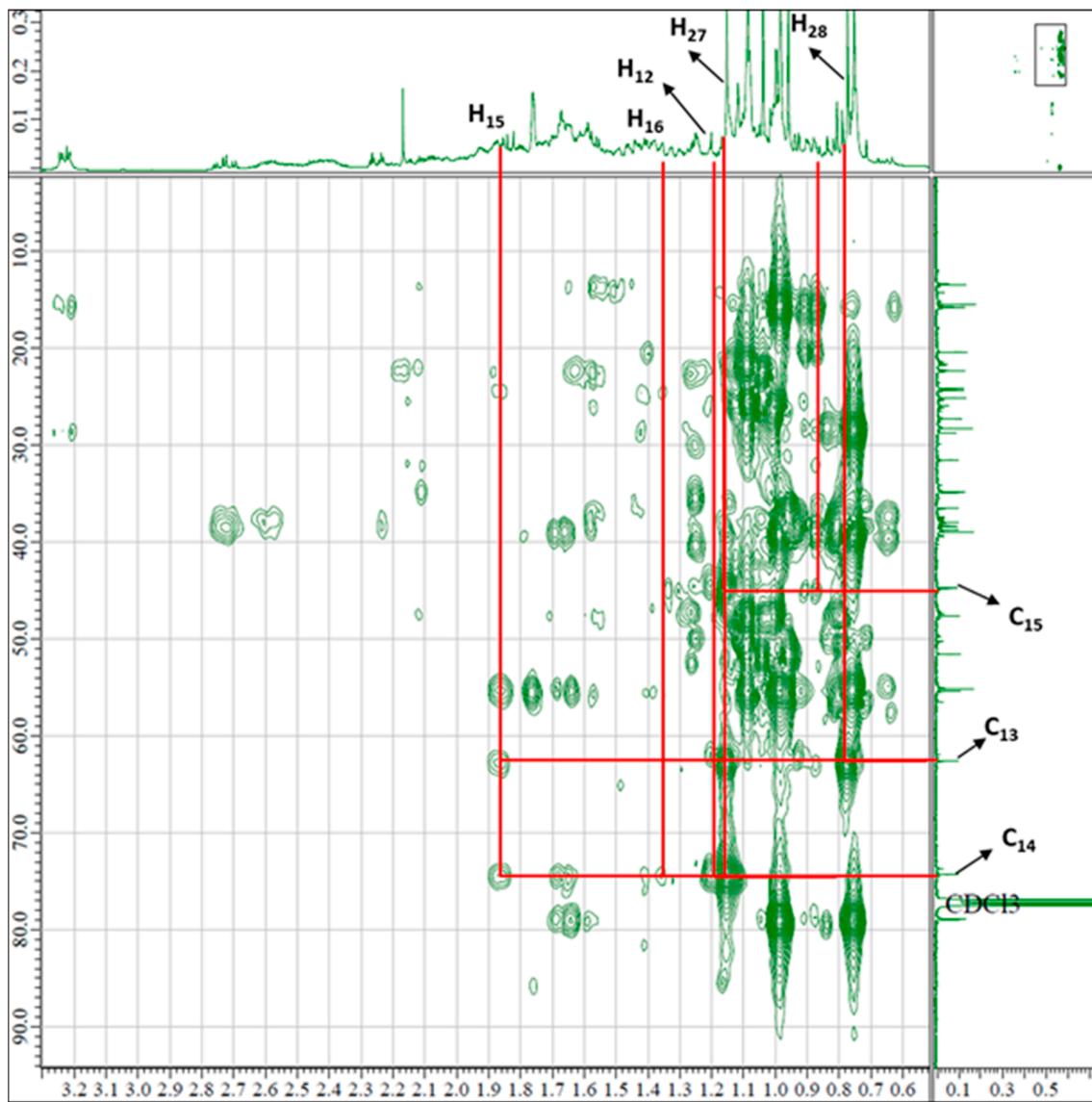


Figure S22: HMBC spectrum of **2** (From δ_{C} 40 ppm to 80 ppm).

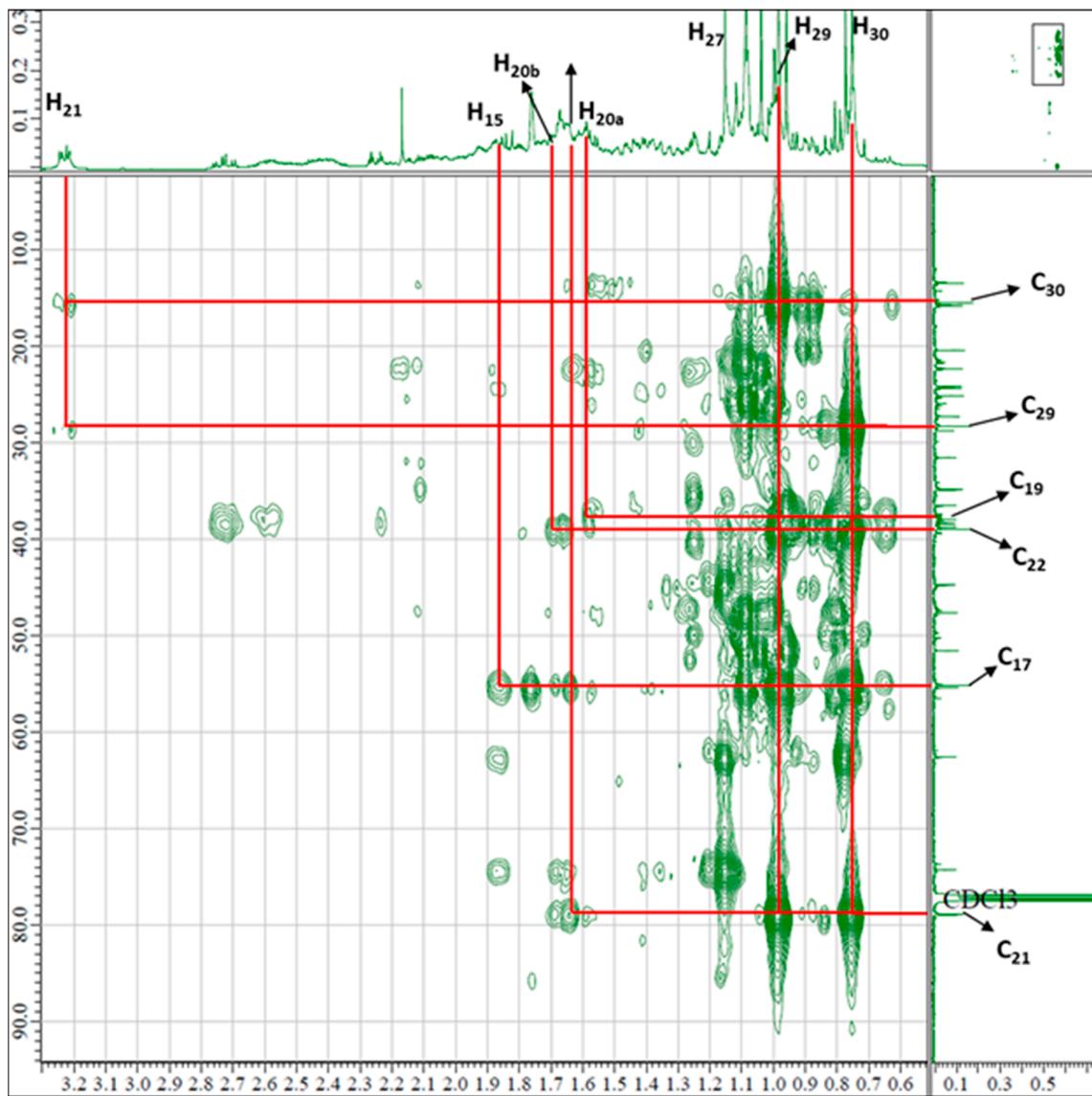


Figure S23: HMBC spectrum of **2** (From δ_{C} 10 ppm to 80 ppm).

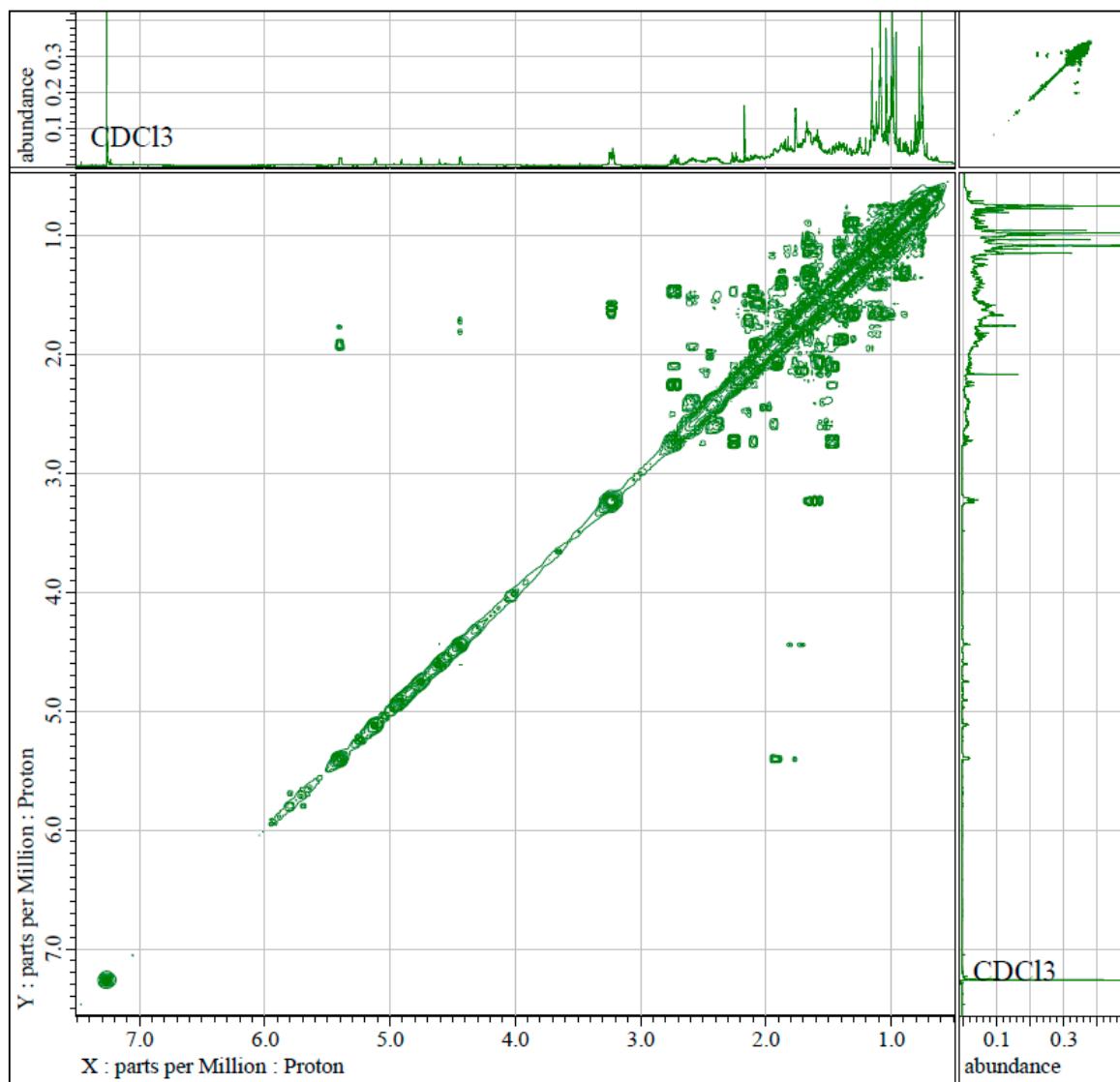


Figure S24: ^1H - ^1H COSY spectrum of **2**.

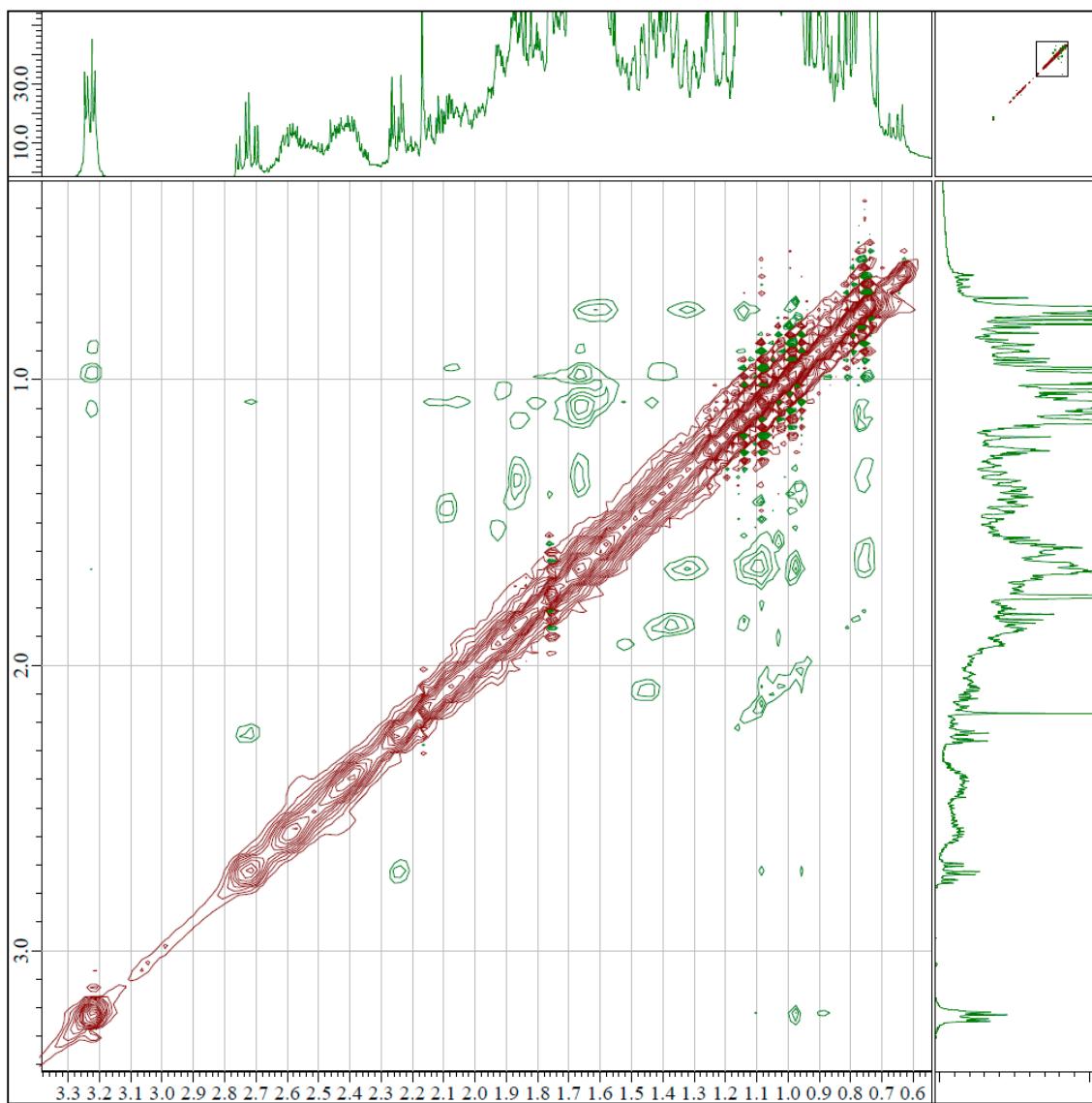


Figure S25: NOESY spectrum of **2**.

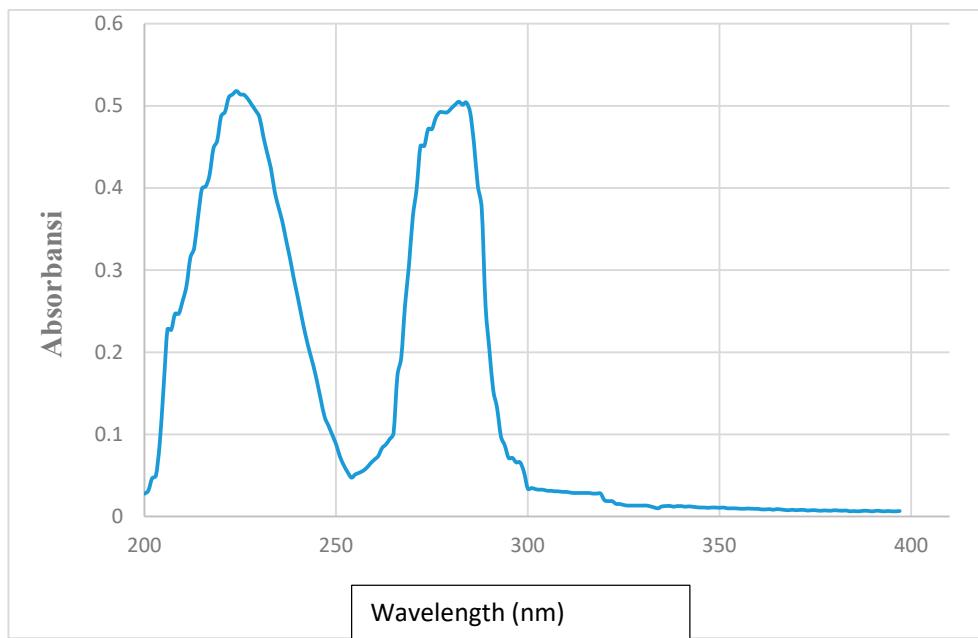


Figure 26. UV spectrum of **3**

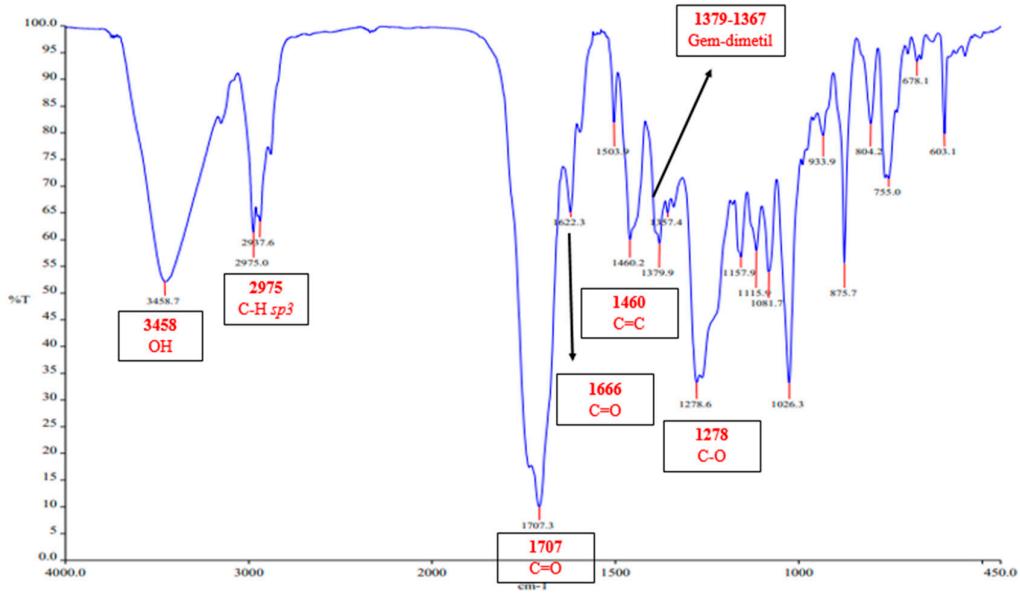


Figure 27. IR spectrum of **3**

Single Mass Analysis

Tolerance = 10.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

127 formula(e) evaluated with 4 results within limits (up to 50 closest results for each mass)

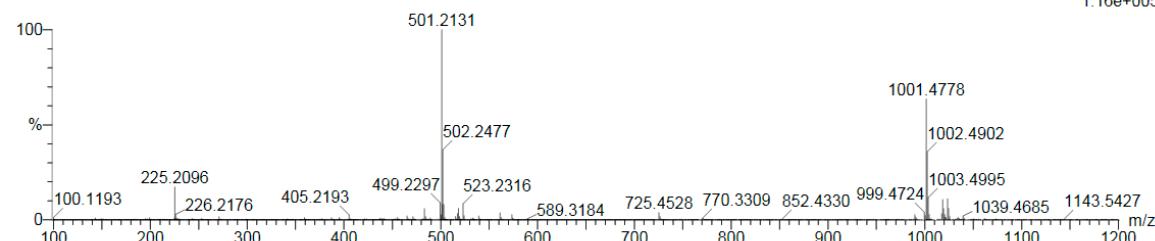
Elements Used:

C: 0-500 H: 0-1000 O: 0-200

ISOLAT SARAH 1 31 (0.544) Cm (31:32)

TOF MS ES+

1.16e+005



Minimum: -1.5
Maximum: 10.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
501.2131	501.2125	0.6	1.2	11.5	119.1	5.6	C27 H33 O9
	501.2183	-5.2	-10.4	2.5	122.4	8.9	C20 H37 O14
	501.2066	6.5	13.0	20.5	113.5	0.0	C34 H29 O4
	501.2218	-8.7	-17.4	24.5	118.6	5.1	C38 H29 O

Figure S28: HR-ESI-MS spectrum of 3.

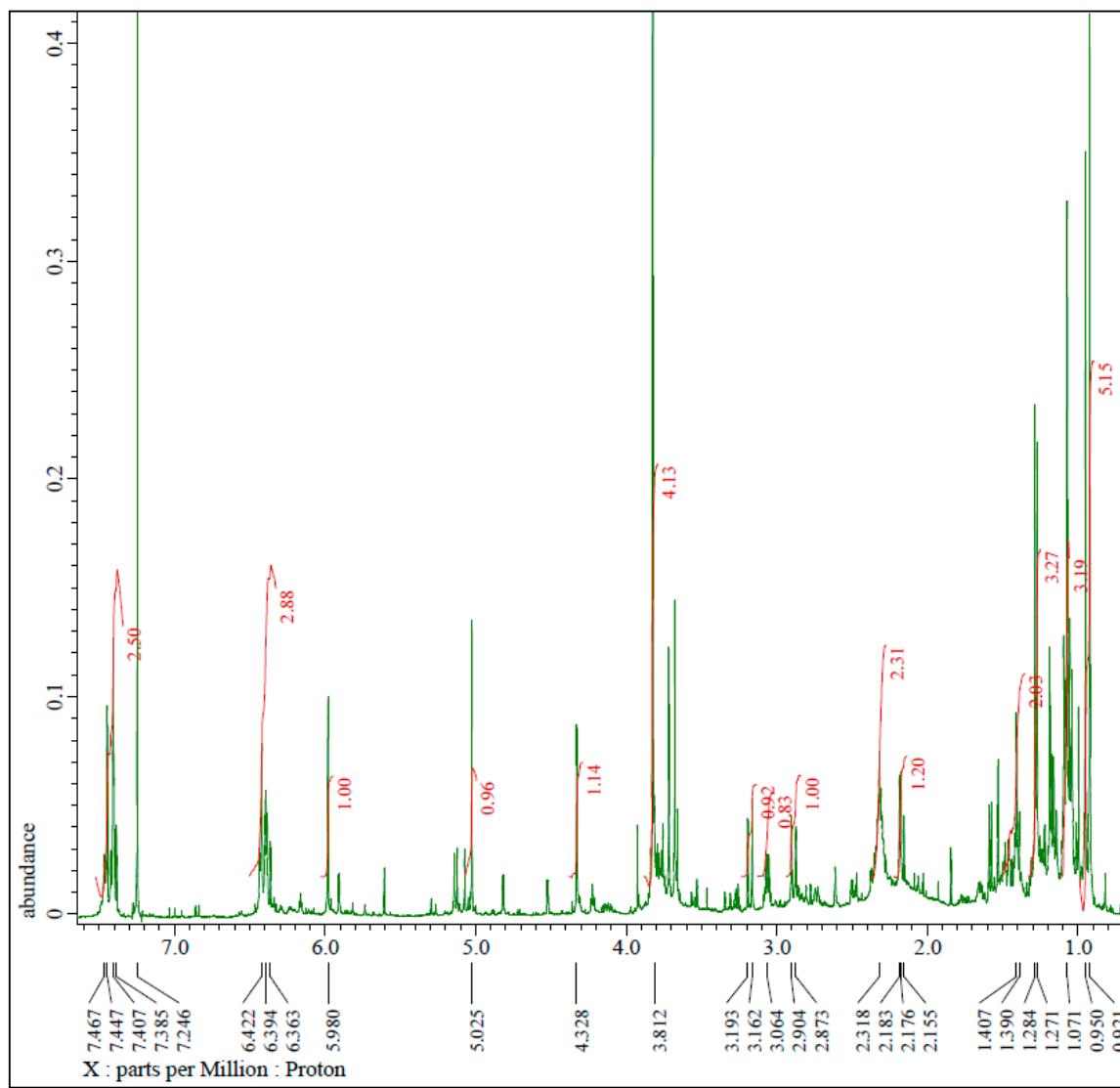


Figure S29: ^1H -NMR (500 MHz, CDCl_3) spectrum of **3**.

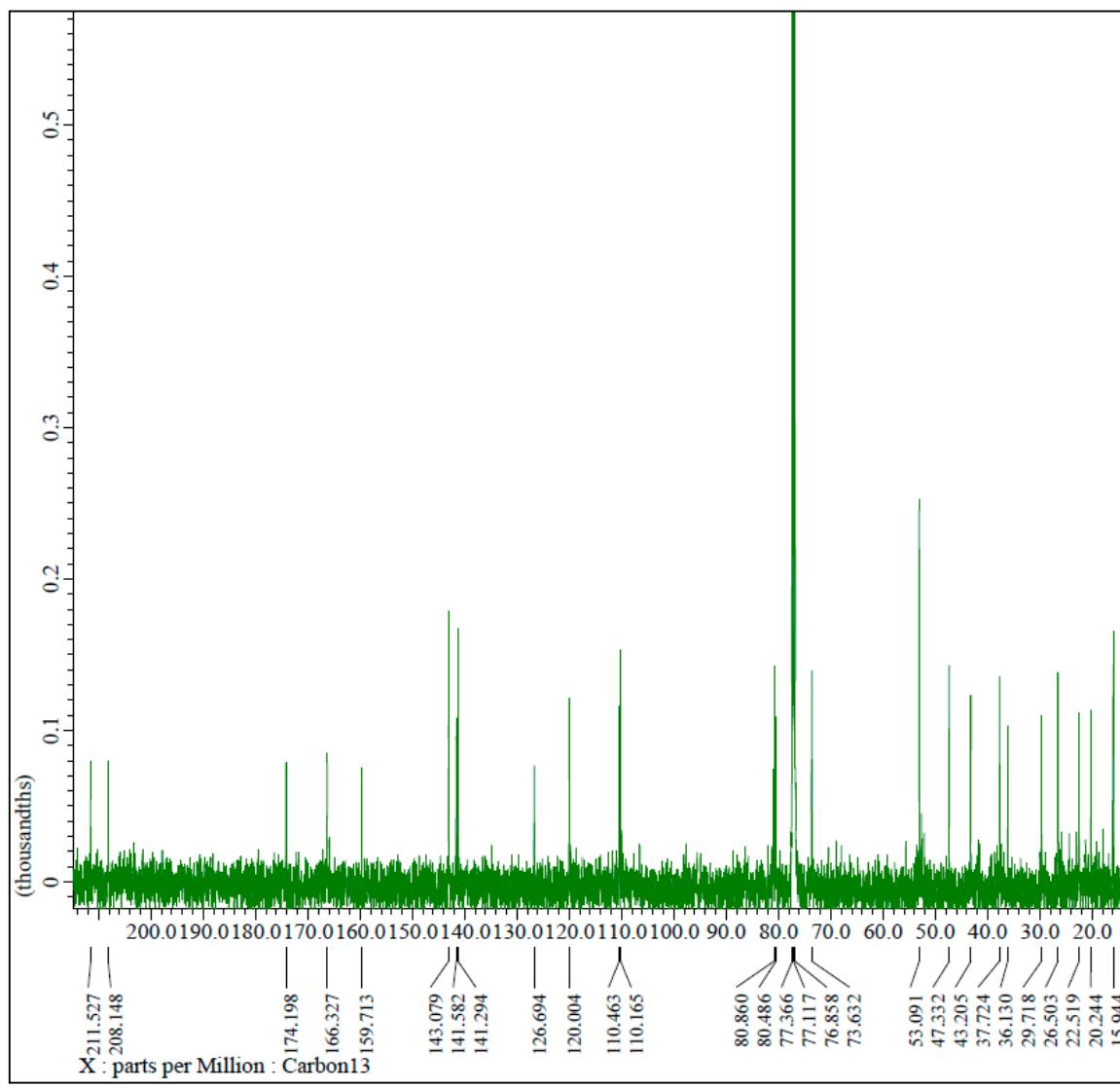


Figure S30: ^{13}C -NMR (125 MHz, CDCl_3) spectrum of **3**.

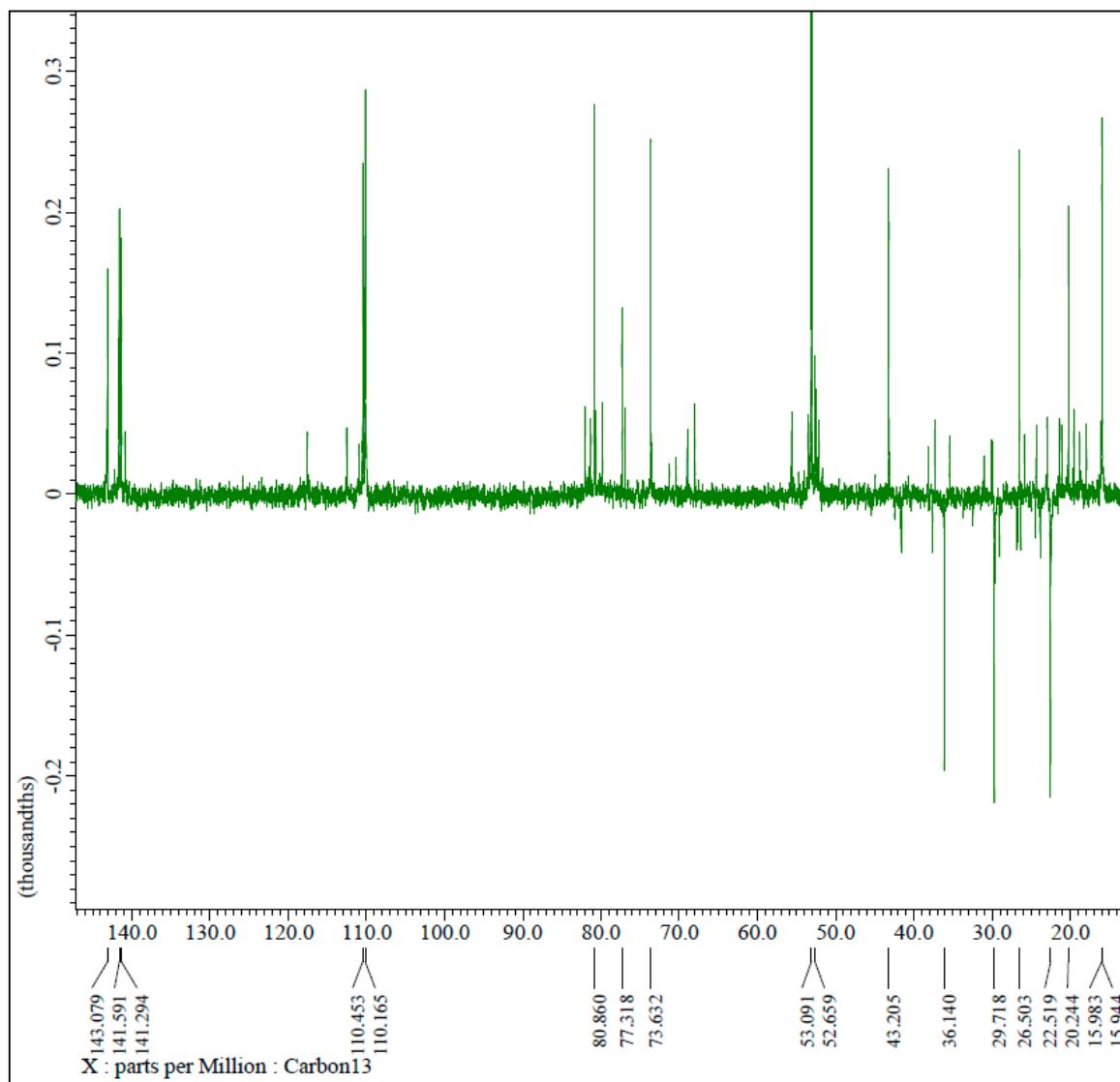


Figure S31: DEPT135 (125 MHz, CDCl_3) spectrum of **3**.

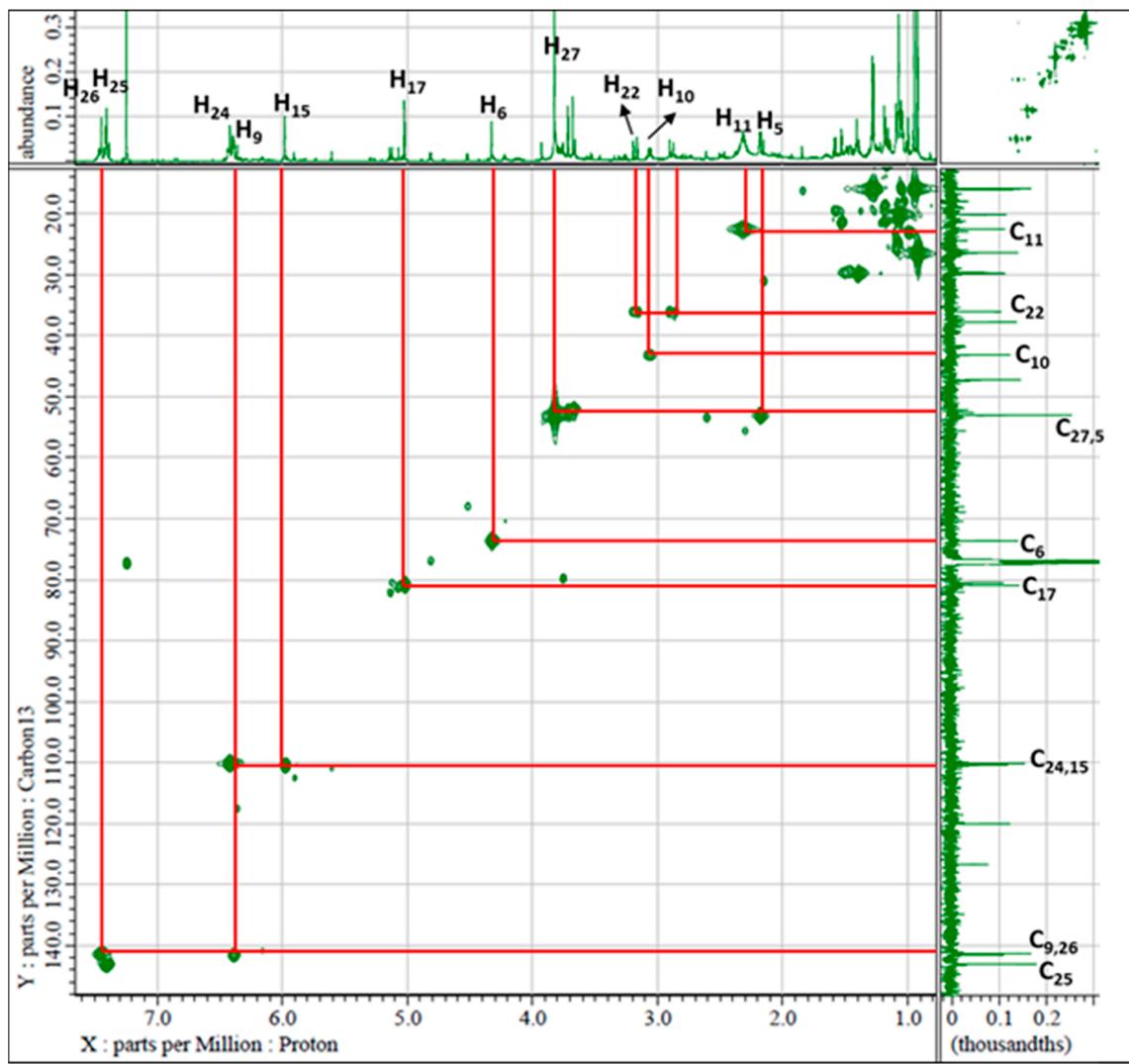


Figure S32: HMQC spectrum of **3**.

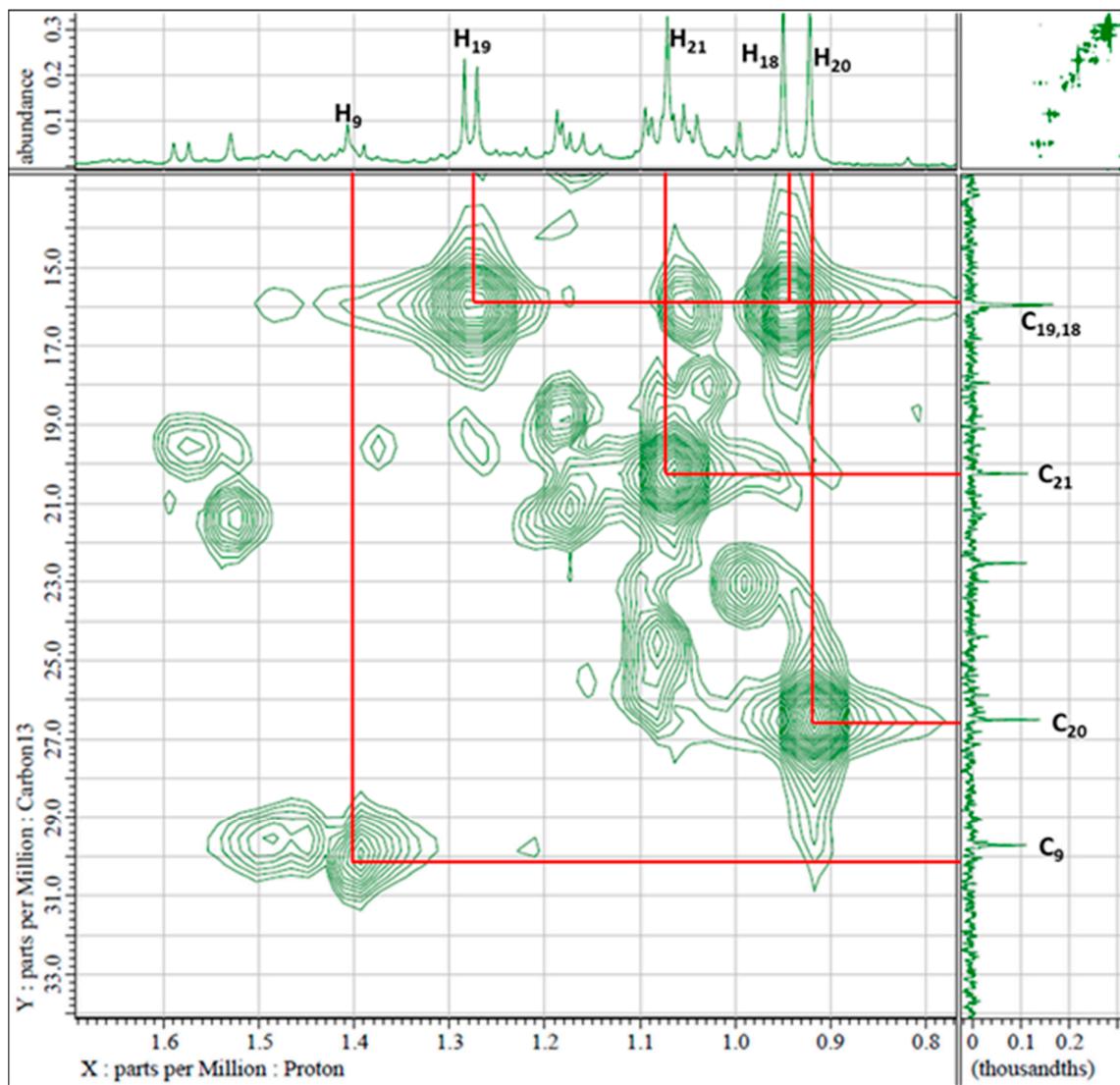


Figure S33: HMQC spectrum of **3** (From δ_{C} 15 ppm to 31 ppm).

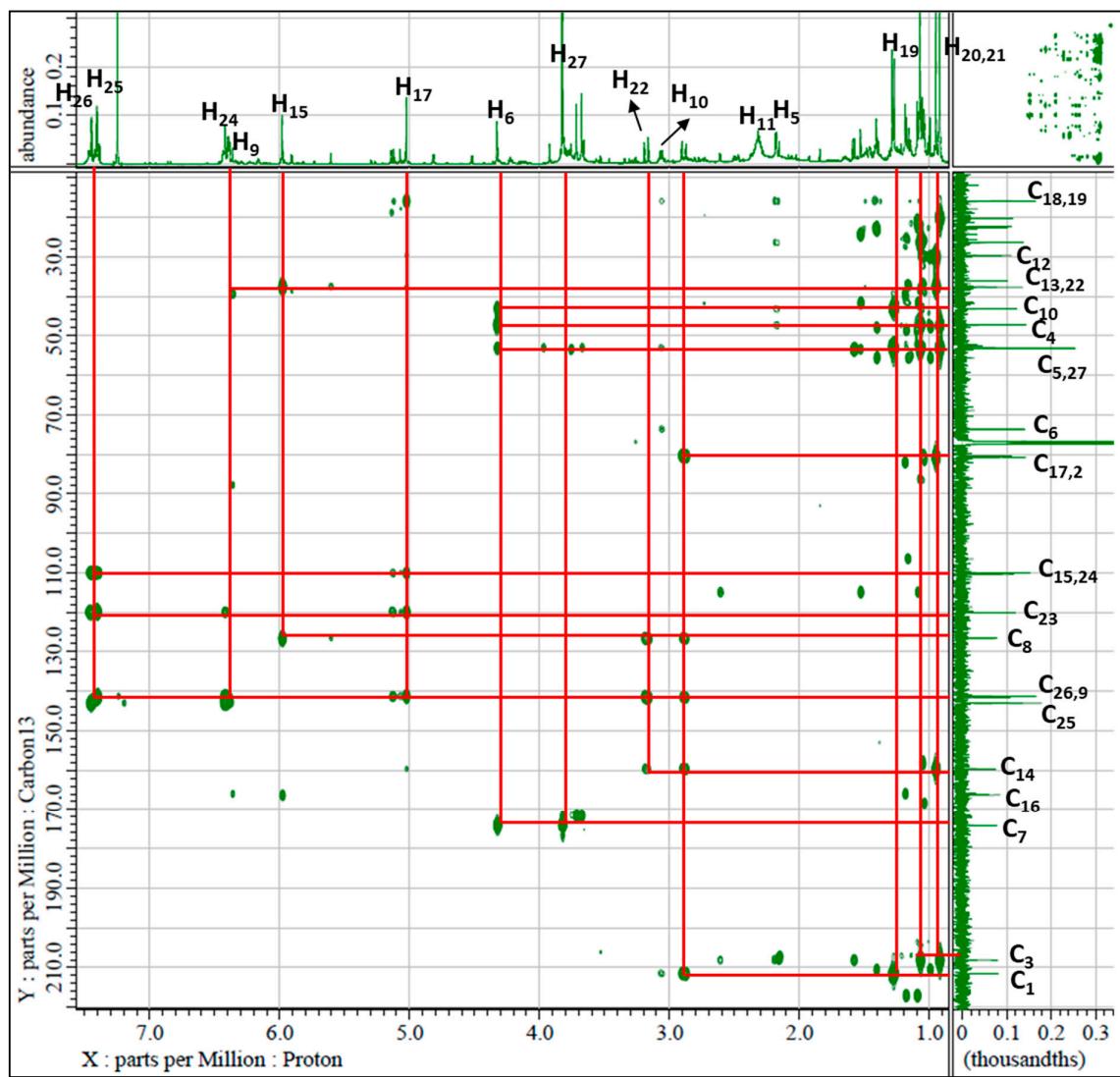


Figure S34: HMBC spectrum of 3.

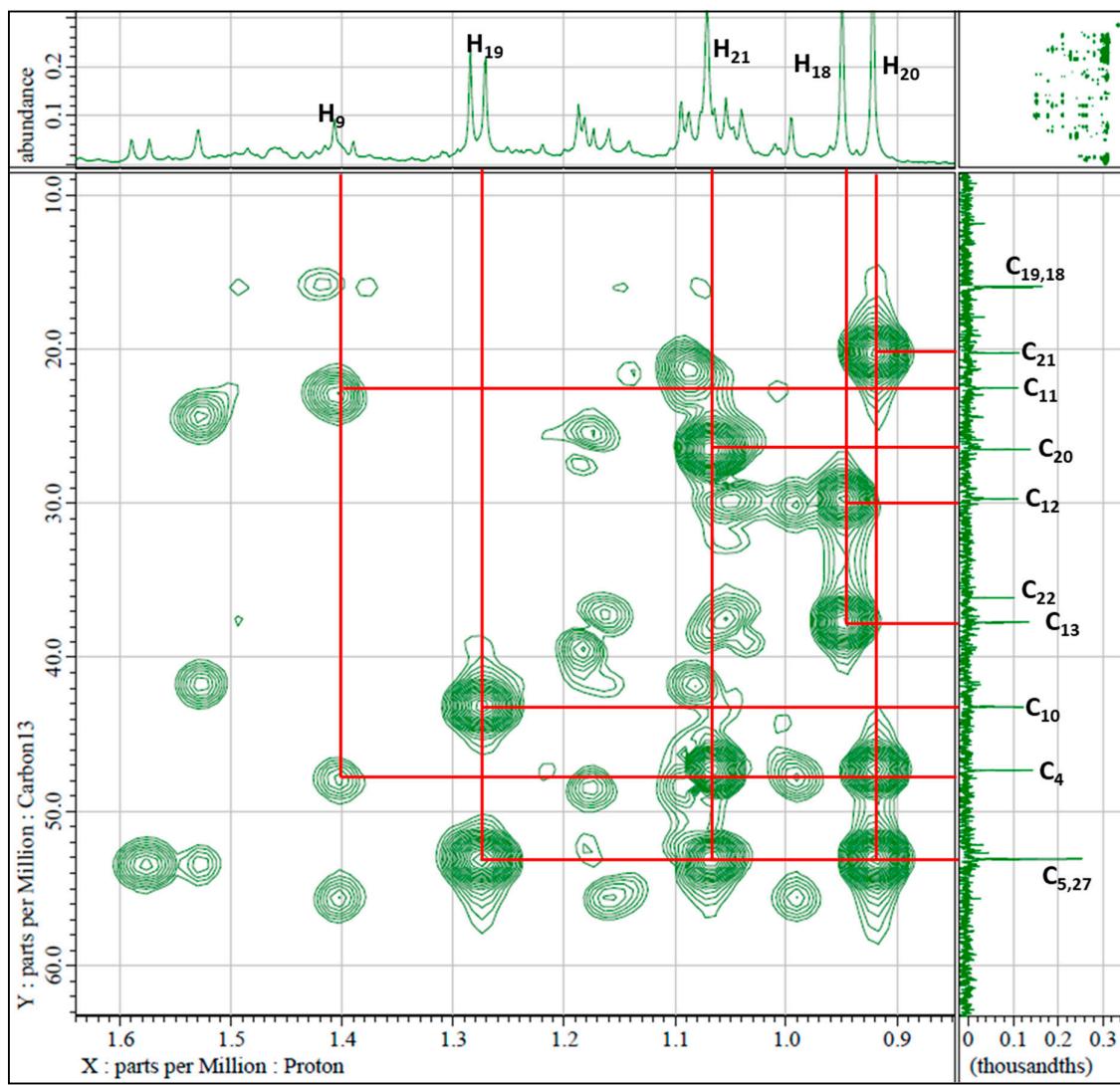


Figure S35: HMBC spectrum of **3** (From δ_C 10 ppm to 60 ppm).

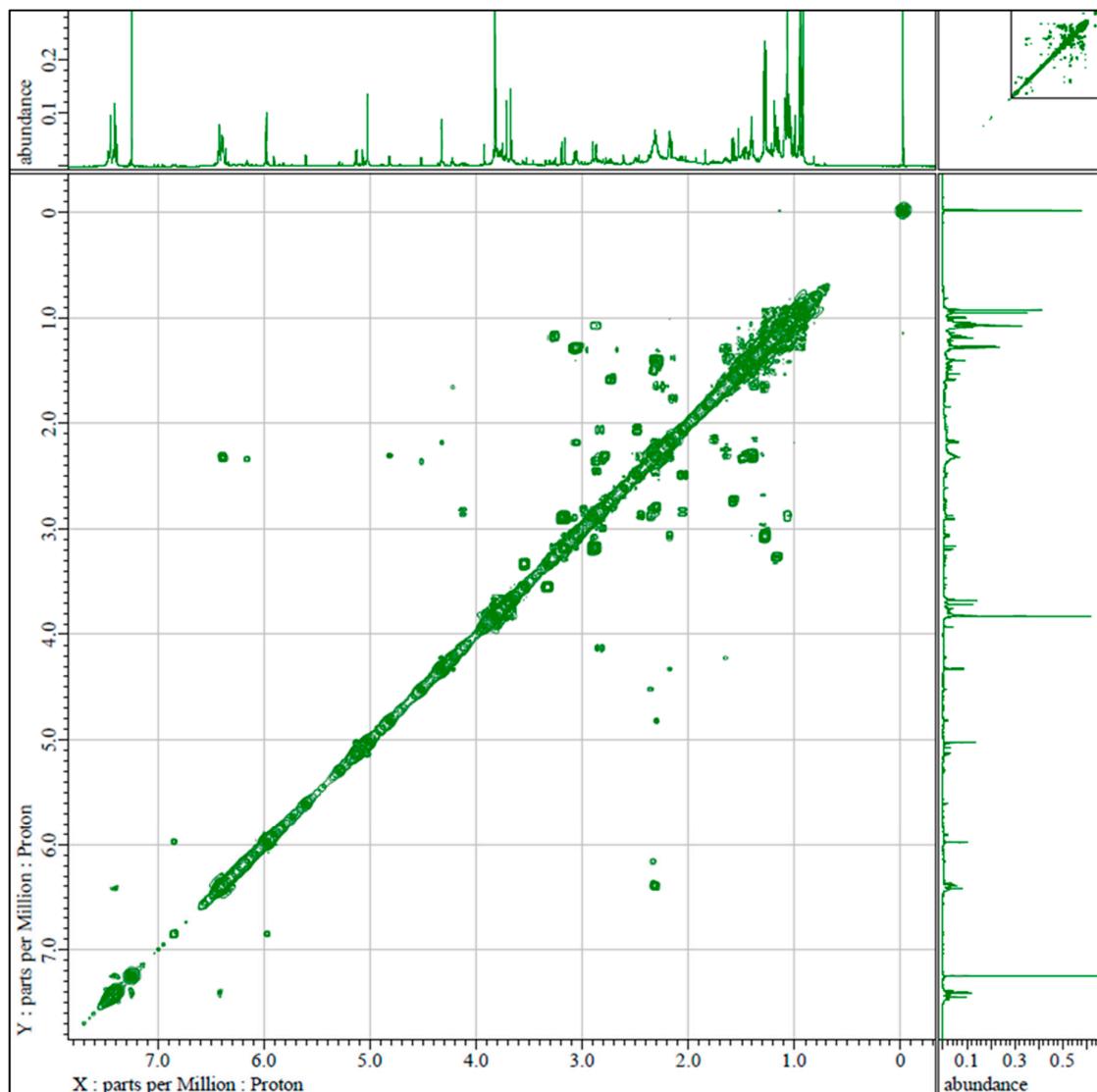


Figure S36: ^1H - ^1H COSY spectrum of 3.

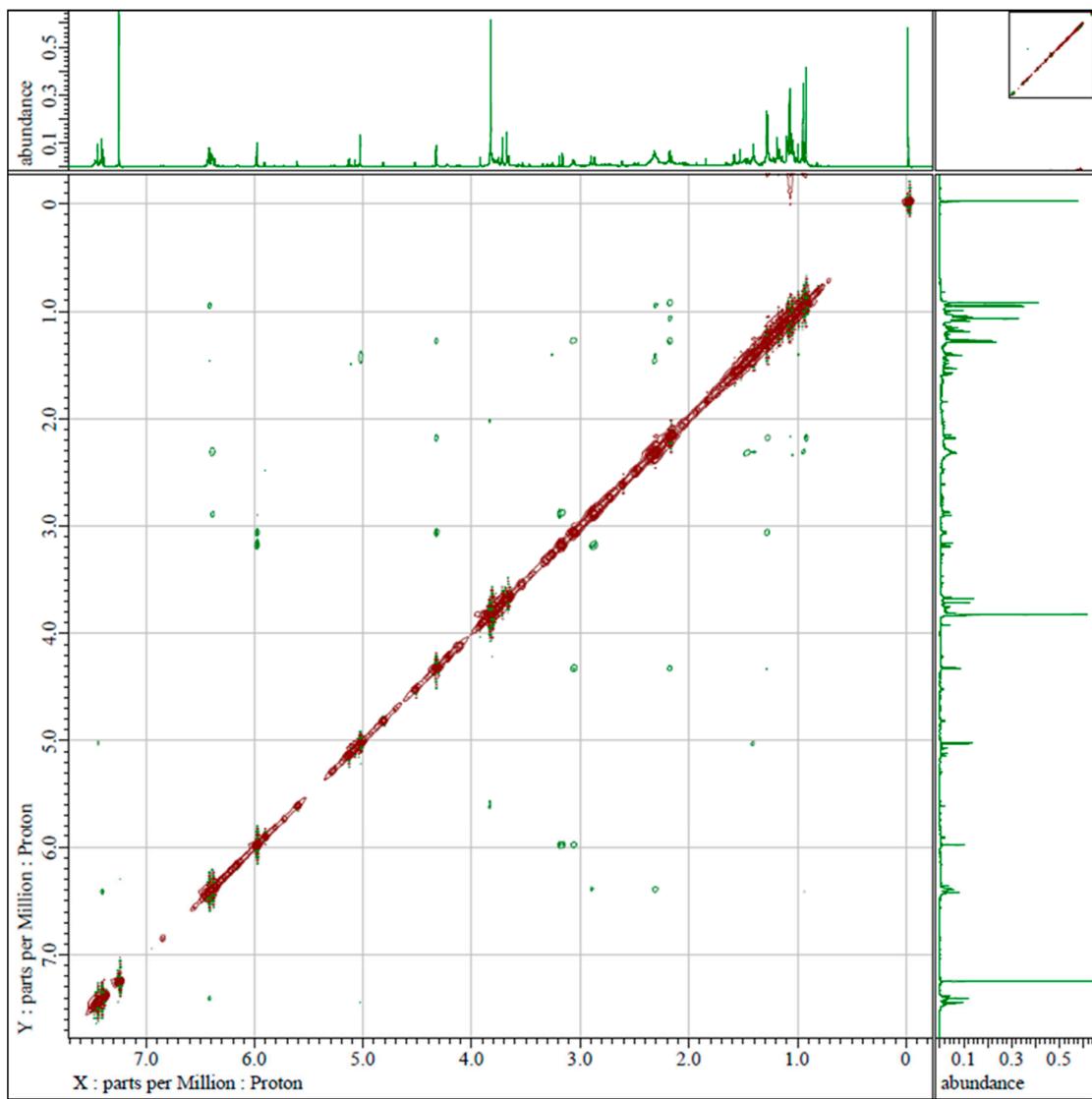


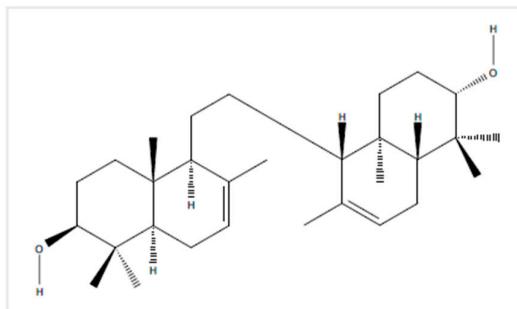
Figure S37: NOESY spectrum of 3.

Initiating Search

October 11, 2022, 10:55AM

 Substances:

Filtered By:



Structure Match: As Drawn

Search Tasks

Task	Search Type	View
Exported: Returned Substance Results + Filters	<input type="checkbox"/> 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 S38: Scifinder reports of compounds 1.



⊖ Substances (8)

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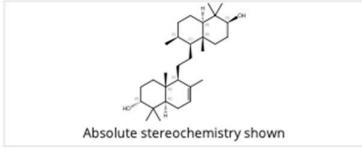
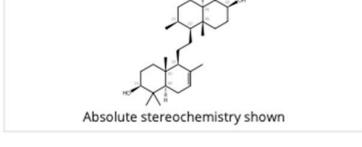
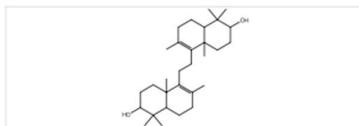
1	Similarity Score: 98
90686-40-1  <p>Absolute stereochemistry shown</p>	Key Physical Properties Molecular Weight 444.73 Boiling Point (Predicted) 522.2±50.0 °C Press: 760 Torr Density (Predicted) 0.962±0.06 g/cm ³ Temp: 20 °C; Press: 760 Torr pKa (Predicted) 15.18±0.70 Most Acidic Temp: 25 °C
C₃₀H₅₂O₂ 2-Naphthalenol, decahydro-1,1,4a,6-tetramethyl-5-[2-[(1S,4aR,6R,8aR)-1,4,4a,5,6,7,8,8a-octahydro-6-hydroxy-2,5,5,8a-tetramethyl-1-naphthalenyl]ethyl]-, (2R,4aR,5S,6S,8aR)-	
 6 References  0 Reactions  0 Suppliers	
2	Similarity Score: 98
90686-41-2  <p>Absolute stereochemistry shown</p>	Key Physical Properties Molecular Weight 444.73 Boiling Point (Predicted) 522.2±50.0 °C Press: 760 Torr Density (Predicted) 0.962±0.06 g/cm ³ Temp: 20 °C; Press: 760 Torr pKa (Predicted) 15.18±0.70 Most Acidic Temp: 25 °C
C₃₀H₅₂O₂ 2-Naphthalenol, decahydro-1,1,4a,6-tetramethyl-5-[2-[(1S,4aR,6S,8aR)-1,4,4a,5,6,7,8,8a-octahydro-6-hydroxy-2,5,5,8a-tetramethyl-1-naphthalenyl]ethyl]-, (2S,4aR,5S,6S,8aR)-	
 3 References  0 Reactions  0 Suppliers	

Figure S39: Scifinder reports with similarity score 98 to compounds **1**.

3 Similarity Score: 95

6049-24-7



C₃₀H₅₀O₂
(2S,2'S,4aS,4'aS,8aR,8'aR)-5,5'-(1,2-Ethanediyl)
bis[1,2,3,4,4a,7,8,8a-octahydro-1,1,4a,6-tetramethyl-2-naphthalenol]

Key Physical Properties	Value	Condition
Molecular Weight	442.72	-
Boiling Point (Predicted)	527.4±50.0 °C	Press: 760 Torr
Density (Predicted)	0.985±0.06 g/cm ³	Temp: 20 °C; Press: 760 Torr
pKa (Predicted)	14.86±0.70	Most Acidic Temp: 25 °C

[Experimental Properties](#) | [Spectra](#)

 8 References

 4 Reactions

 1 Supplier

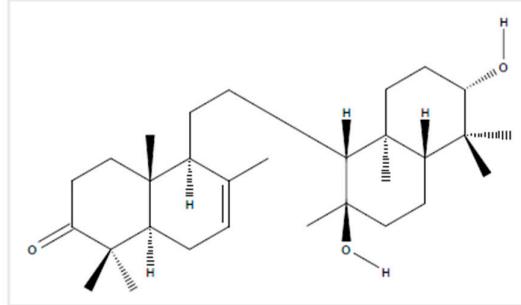
Figure S40: Scifinder reports with similarity score 95 to compounds **1**

Initiating Search

October 11, 2022, 10:57AM

 Substances:

Filtered By:



Structure Match: As Drawn

Search Tasks

Task	Search Type	View
Exported: Returned Substance Results + Filters	<input type="checkbox"/> Substances	View Results

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Substances with (0) results

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Figure S41: Scifinder reports of compounds 2.



Substances (12)

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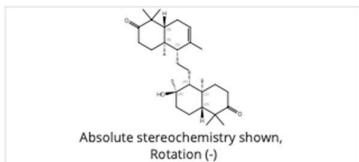
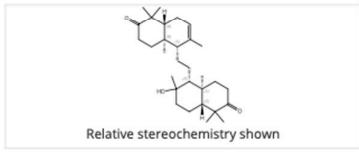
1	Similarity Score: 99
1246091-10-0	
 Absolute stereochemistry shown, Rotation (-)	Key Physical Properties Value Condition
	Molecular Weight 456.70 -
	Boiling Point (Predicted) 544.9±50.0 °C Press: 760 Torr
	Density (Predicted) 1.000±0.06 g/cm ³ Temp: 20 °C; Press: 760 Torr
	pKa (Predicted) 15.12±0.70 Most Acidic Temp: 25 °C
	Experimental Properties Spectra
C₃₀H₄₈O₃ (4a <i>S</i> ,5 <i>R</i> ,6 <i>R</i> ,8a <i>R</i>)-Octahydro-6-hydroxy-1,1,4a,6-tetramethyl-5-[2-[(1 <i>S</i> ,4 <i>a</i> <i>R</i> ,8a <i>R</i>)-1,4,4a,5,6,7,8,8a-octahydro-2,5,5,8a-tetramethyl-6-oxo-1-naphthalenyl]ethyl]-2(1 <i>H</i>)-naphthalenone	
 2 References	 0 Reactions
 0 Suppliers	
2	Similarity Score: 99
2649754-72-1	
 Relative stereochemistry shown	Key Physical Properties Value Condition
	Molecular Weight 456.70 -
	Boiling Point (Predicted) 544.9±50.0 °C Press: 760 Torr
	Density (Predicted) 1.000±0.06 g/cm ³ Temp: 20 °C; Press: 760 Torr
	pKa (Predicted) 15.12±0.70 Most Acidic Temp: 25 °C
C₃₀H₄₈O₃	
 0 References	 0 Reactions
 1 Supplier	

Figure S42: Scifinder reports with similarity score 99 to compounds **2**

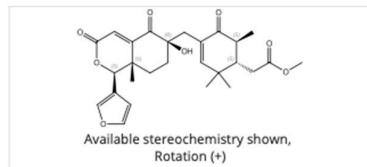


Substances (21)

[View in SciFinder[®]](#)

1

Similarity Score: 95

1613602-59-7

Key Physical Properties	Value	Condition
Molecular Weight	484.54	-
Boiling Point (Predicted)	625.5±55.0 °C	Press: 760 Torr
Density (Predicted)	1.28±0.1 g/cm ³	Temp: 20 °C; Press: 760 Torr
pKa (Predicted)	11.86±0.60	Most Acidic Temp: 25 °C

C₂₇H₃₂O₈

rel(+)-Methyl (1*S*,6*S*)-4-[[[(1*R*,6*S*,8*a**R*)-1-(3-furanyl)-3,5,6,7,8,8*a*-hexahydro-6-hydroxy-8*a*-methyl-3,5-dioxo-1*H*-2-benzopyran-6-yl]methyl]-2,2,6-trimethyl-5-oxo-3-cyclohexene-1-acetate

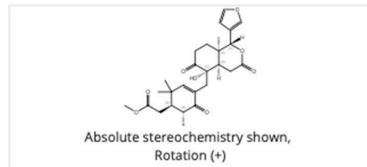
 1
Reference

 0
Reactions

 0
Suppliers

2

Similarity Score: 95

1621959-55-4

Key Physical Properties	Value	Condition
Molecular Weight	486.56	-
Boiling Point (Predicted)	648.2±55.0 °C	Press: 760 Torr
Density (Predicted)	1.206±0.06 g/cm ³	Temp: 20 °C; Press: 760 Torr
pKa (Predicted)	11.58±0.60	Most Acidic Temp: 25 °C

C₂₇H₃₄O₈

Methyl (1*R*,6*R*)-4-[[[(1*R*,4*a**R*,5*S*,8*a**R*)-1-(3-furanyl)octahydro-5-hydroxy-8*a*-methyl-3,6-dioxo-1*H*-2-benzopyran-5-yl]methyl]-2,2,6-trimethyl-5-oxo-3-cyclohexene-1-acetate

 1
Reference

 0
Reactions

 0
Suppliers

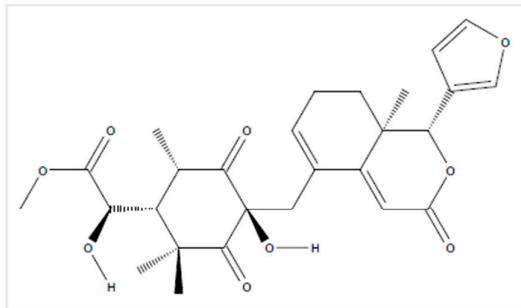
Figure S43: Scifinder reports with similarity score 95 to compounds 2

Initiating Search

October 11, 2022, 10:58AM

 Substances:

Filtered By:



Structure Match: As Drawn

Search Tasks

Task	Search Type	View
Exported: Returned Substance Results + Filters	<input type="checkbox"/> 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 S44 Scifinder reports of compounds **3**.

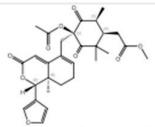
3	Similarity Score: 95		
2580943-28-6			
 Absolute stereochemistry shown	Key Physical Properties	Value	
	Molecular Weight	526.58	
	Boiling Point (Predicted)	661.5±55.0 °C	
	Density (Predicted)	1.26±0.1 g/cm ³	
		Press: 760 Torr Temp: 20 °C; Press: 760 Torr	
C₂₉H₃₄O₉			
Cyclohexaneacetic acid, 4-(acetoxy)-4-[[[(1 <i>R</i> , 8 <i>aR</i>)-1-(3-furanyl)-3,7,8 <i>a</i> -tetrahydro-8 <i>a</i> - methyl-3-oxo-1 <i>H</i> -2-benzopyran-5-yl]methyl]- 2,2,6-trimethyl-3,5-dioxo-, methyl ester, (1 <i>R</i> , 4 <i>S</i> ,6 <i>S</i>)-	 1 Reference	 0 Reactions	 0 Suppliers

Figure S45: Scifinder reports with similarity score 95 to compounds 3

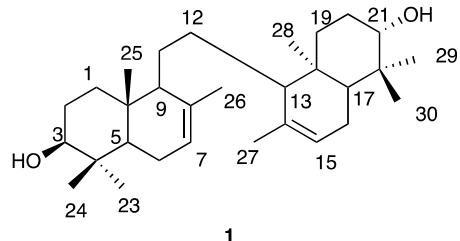


Table S1: NMR data comparison of compound **1** with 3-hydroxy-8,14-secogammacer-7,14-dien-21-one [21].

No.	1		3-hydroxy-8,14-secogammacer-7,14-dien-21-one [21]	
	¹³ C NMR δ _c	¹ H NMR δ _H (Integral, mult, J=Hz)	¹³ C NMR δ _c	¹ H NMR δ _H (Integral, mult, J=Hz)
1	30.1	1.25, 1.45 (each 1H, m)	37.5	1.14, 1.86 (each 1H, m)
2	27.6	1.62, 1.66 (each 1H, m)	27.4	1.65 (2H, m)
3	79.3	3.26 (1H, dd, 11.0, 4.0)	79.1	3.29 (1H, m)
4	38.9	-	38.7	-
5	49.8	1.20 (1H, m)	51.5	1.62 (1H, m)
6	23.7	1.97 (2H, m)	29.8	1.35, 1.50 (each 1H, m)
7	122.1	5.39 (1H, brs)	121.7	5.40 (1H, m)
8	135.4	-	135.4	-
9	56.3	1.59 (1H, m)	55.3	1.66 (1H, m)
10	36.7	-	36.5	-
11	37.6	1.17, 1.88 (each 1H, m)	24.1	1.99, 2.10 (each 1H, m)
12	37.6	1.17, 1.88 (each 1H, m)	23.5	1.98, 2.10 (each 1H, m)
13	56.3	1.59 (1H, m)	56.0	1.59 (1H, m)
14	135.4	-	134.9	-
15	122.1	5.39 (1H, brs)	122.3	5.40 (1H, m)
16	23.7	1.97 (2H, m)	29.9	1.35, 1.50 (each 1H, m)
17	49.8	1.20 (1H, m)	49.6	1.20 (1H, m)
18	36.7	-	36.5	-
19	30.1	1.25, 1.45 (each 1H, m)	38.4	1.51, 2.15 (each 1H, m)
20	27.6	1.62, 1.66 (each 1H, m)	34.7	2.29, 2.77 (each 1H, m)
21	79.3	3.26 (1H, dd, 11.0, 4.0)	217.0	-
22	38.9	-	47.5	-
23	15.3	0.85 (3H, s)	15.1	0.87 (3H, s)
24	28.1	0.98 (3H, s)	27.9	1.00 (3H, s)
25	13.8	0.74 (3H, s)	13.3	0.99 (3H, s)
26	22.6	1.70 (3H, s)	22.3	1.75 (3H, s)
27	22.6	1.70 (3H, s)	22.4	1.72 (3H, s)
28	13.8	0.74 (3H, s)	13.6	0.76 (3H, s)
29	15.3	0.85 (3H, s)	22.1	1.12 (3H, s)
30	28.1	0.98 (3H, s)	25.0	1.08 (3H, s)

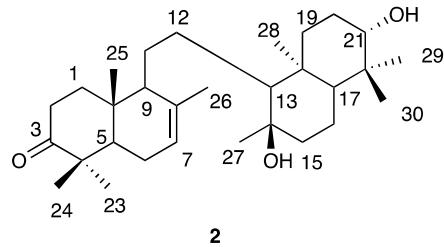


Table S2: NMR data comparison of compound **2** with kokosanolide B [14].

No.	2		kokosanolide B [14]	
	¹³ C NMR δ _c	¹ H NMR δ _H (Integral, mult, <i>J</i> =Hz)	¹³ C NMR δ _c	¹ H NMR δ _H (Integral, mult, <i>J</i> =Hz)
1	38.3	1.44, 2.10 (each 1H, m)	38.5	1.91, 2.08 (each 1H, m)
2	34.9	2.26, 2.72 (each 1H, m)	34.8	2.23, 2.41 (each 1H, m)
3	217.4	-	216.9	-
4	47.6	-	47.6	-
5	51.6	1.57 (1H, m)	51.6	1.57 (1H, m)
6	28.8	1.40, 1.84 (each 1H, m)	28.9	1.12, 2.56 (each 1H, m)
7	121.6	5.40 (1H, brs)	121.7	5.41 (1H, m)
8	135.9	-	135.3	-
9	55.4	1.59 (1H, m)	55.5	1.59 (1H, m)
10	38.7	-	36.6	-
11	20.4	1.32, 1.66 (each 1H, m)	21.5	1.61, 2.41 (each 1H, m)
12	24.2	1.22, 1.88 (each 1H, m)	21.5	1.62, 1.76 (each 1H, m)
13	62.6	0.99 (1H, m)	61.8	1.12 (1H, m)
14	74.3	-	74.0	-
15	44.8	1.36, 1.86 (each 1H, m)	44.2	1.46, 2.23 (each 1H, m)
16	31.5	1.36, 1.40 (each 1H, m)	31.4	1.51, 1.84 (each 1H, m)
17	55.2	0.88 (1H, m)	55.2	1.42 (1H, m)
18	36.6	-	36.6	-
19	38.0	1.10, 1.65 (each 1H, m)	38.4	1.78, 2.10 (each 1H, m)
20	27.3	1.59, 1.68 (each 1H, m)	34.1	2.26, 2.73 (each 1H, m)
21	78.9	3.23 (1H, dd, 11.5; 4.0)	217.1	-
22	39.0	-	47.6	-
23	22.3	1.09 (3H, s)	22.3	1.08 (3H, s)
24	25.1	1.04 (3H, s)	25.1	1.04 (3H, s)
25	13.4	0.96 (3H, s)	13.4	0.96 (3H, s)
26	22.3	1.76 (3H, s)	22.3	1.77 (3H, s)
27	24.3	1.15 (3H, s)	24.2	1.21 (3H, s)
28	15.8	0.77 (3H, s)	15.1	0.93 (3H, s)
29	28.3	0.99 (3H, s)	21.4	1.02 (3H, s)
30	15.5	0.75 (3H, s)	26.5	1.09 (3H, s)

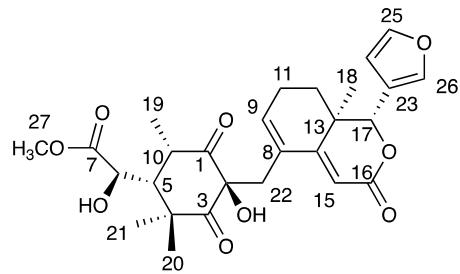


Table S3: NMR data comparison of compound **3** with kokosanolide A [14].

No.	3		kokosanolide A [14]	
	¹³ C NMR δc	¹ H NMR δ _H (Integral, mult, J=Hz)	¹³ C NMR δc	¹ H NMR δ _H (Integral, mult, J=Hz)
1	211.5	-	108.4	-
2	80.4	-	76.1	-
3	208.1	-	208.6	-
4	47.3	-	48.4	-
5	53.0	2.18 (1H, dd, 1.5, 1.0)	56.4	2.27 (1H, dd, 4.0, 7.0)
6	73.8	4.32 (1H, d, 1.0)	77.4	4.81 (1H, d, 4.0)
7	174.1	-	172.4	-
8	126.7	-	34.6	2.64 (1H, dd, 5.3, 6.5)
9	141.5	6.39 (1H, t, 1.0)	69.5	4.39 (1H, m)
10	43.2	3.06 (1H, m)	37.3	3.33 (1H, q, 8.0)
11	22.5	2.30 (2H, m)	25.3	1.79, 1.91 (each 1H, m)
12	29.7	1.39 (2H, m)	27.8	1.26, 1.74 (each 1H, m)
13	37.7	-	39.6	-
14	159.7	-	168.6	-
15	110.4	5.97 (1H, m)	116.7	6.28 (1H, s)
16	166.3	-	165.4	-
17	80.8	5.02 (1H, s)	81.5	5.17 (1H, s)
18	15.9	0.95 (3H, s)	18.2	1.07 (3H, s)
19	16.0	1.27 (3H, d, 6.4)	12.2	1.13 (3H, d, 8)
20	26.5	0.91 (3H, s)	23.7	0.98 (3H, s)
21	20.2	1.07 (3H, s)	30.1	1.37 (3H, s)
22	36.1	2.86, 3.19 (each 1H, s)	25.4	2.46 (1H, dd, 7.5, 5.3) 2.77 (1H, dd, 7.4, 4.7)
23	120.0	-	120.5	-
24	110.2	6.41 (1H, d, 2.0)	110.8	6.43 (1H, d, 4.4)
25	143.1	7.40 (1H, d, 2.0)	143.5	7.40 (1H, d, 4.4)
26	141.1	7.44 (1H, s)	141.9	7.47 (1H, s)
27	53.0	3.80 (3H, s)	52.6	3.67 (3H, s)

Table S4: Results of cytotoxic activity of **1** against MCF-7 cell line.

Concentration of sample ($\mu\text{g/mL}$)	% Inhibition		
	1	2	3
500	99.2414	98.4165	100.1733
100	98.7816	99.7180	99.1832
10	16.7126	27.2668	1.1634
1	16.7126	25.5315	13.7871

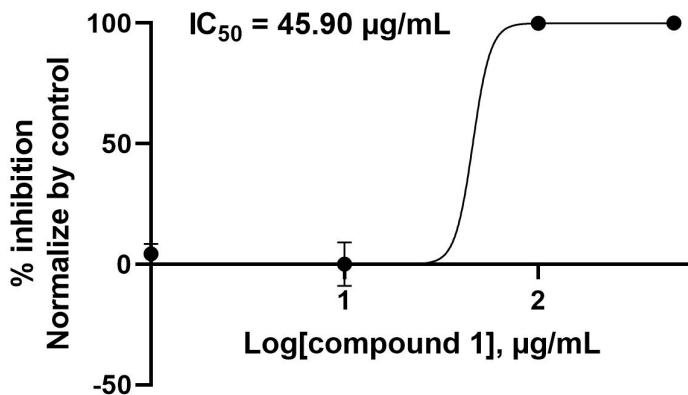


Table S5: Results of cytotoxic activity of **2** against MCF-7 cell line.

Concentration of sample ($\mu\text{g/mL}$)	% Inhibition		
	1	2	3
500	99.1453	101.9066	99.9343
100	13.9382	9.2045	20.6443
50	9.2045	10.5851	10.3879
10	11.1769	6.2459	13.1492
1	1.9066	0.8547	7.4293

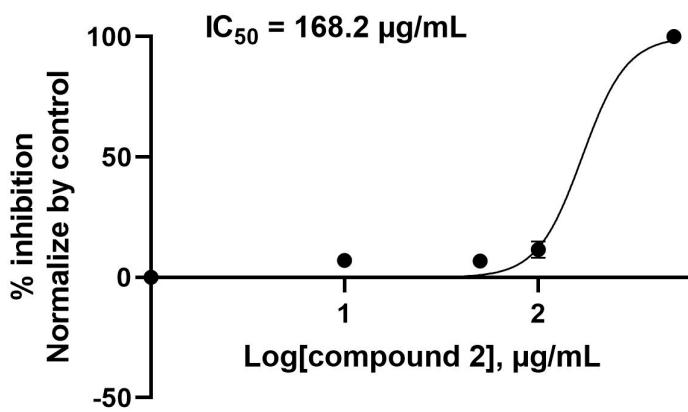
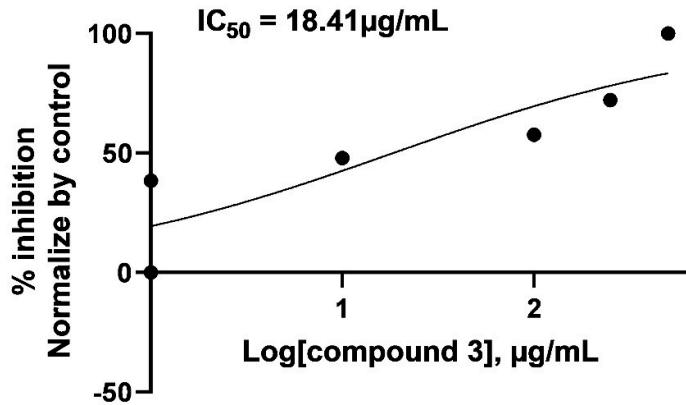


Table S6: Results of cytotoxic activity of **3** against MCF-7 cell line.

Concentration of sample	% inhibition

(μ g/mL)	1	2	3
500	99.06617	99.22625	99.62647
250	75.21345	70.97118	68.89007
100	60.24546	55.68303	55.84312
10	45.91782	44.39701	52.48132
1	36.23266	40.47492	37.75347



References

- [14] Mayanti, T.; Tjokronegoro, R.; Supratman, U.; Mukhtar, M.R.; Awang, K.; Hadi, A.H.A. Antifeedant triterpenoids from the seeds and bark of *Lansium domesticum* Corr. cv *kokossan* (Meliaceae), *Molecules*. **2011**, *16*, 2785-2795.
- [21] Zulfikar; Putri, N.K; Fajriah, S.; Yusuf, M.; Maharani, R.; Al Anshori, J.; Supratman U.; Mayanti, T. 3-hydroxy-8,14-secogammacera-7,14-dien-21-one: A new onoceranoid triterpenes from *Lansium domesticum* Corr. cv *kokossan*, *Molbank* **2020**, *4*, M1157.