

Supporting Information

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Two Novel Sesquiterpenes and A New Pregnane Derivative from the South China Sea Gorgonian *Subergorgia suberosa*

Xian-Qiang Chen ^{1,2}, Nannan Xing³, Bin Yang ², Xuefeng Zhou ², Chenghai
Gao ¹ and Yonghong Liu ^{1,2*}

¹ Institute of Marine Drugs, Guangxi University of Chinese Medicine, Nanning, Guangxi 530200,
P. R. China

² Key Laboratory of Marine Bio-resources Sustainable Utilization; Guangdong Key Laboratory
of Marine Materia Medica; Research Center for Marine Microbes, South China Sea Institute of
Oceanology, Chinese Academy of Sciences, Guangzhou, Guangdong 510301, P. R. China

³ Guangxi Key Laboratory of Chinese Medicine Foundation Research, Guangxi Scientific
Experimental Center of Traditional Chinese Medicine, Guangxi University of Chinese Medicine,
Nanning, Guangxi 530200, P. R. China

Table of Contents	Page
Figure S1: HR-ESI-MS Spectrum of 1 (isosuberosenol A)	3
Figure S2: ¹ H-NMR (500 MHz, CDCl ₃) Spectrum of 1 (isosuberosenol A)	4
Figure S3: ¹³ C-NMR (125 MHz, CDCl ₃) Spectrum of 1 (isosuberosenol A)	5
Figure S4: DEPT135 (125 MHz, CDCl ₃) Spectrum of 1 (isosuberosenol A)	6
Figure S5: HSQC Spectrum of 1 (isosuberosenol A)	7
Figure S6: HSQC Spectrum of 1 (isosuberosenol A) (From δ_C 15 ppm to δ_C 35 ppm)	8
Figure S7: HMBC Spectrum of 1 (isosuberosenol A)	9
Figure S8: HMBC Spectrum of 1 (isosuberosenol A) (From δ_C 79 ppm to δ_C 85 ppm)	10
Figure S9: HMBC Spectrum of 1 (isosuberosenol A) (From δ_C 38 ppm to δ_C 53 ppm)	11
Figure S10: HMBC Spectrum of 1 (isosuberosenol A) (From δ_C 15 ppm to δ_C 36 ppm)	12
Figure S11: ¹ H- ¹ H COSY Spectrum of 1 (isosuberosenol A)	13
Figure S12: NOESY Spectrum of 1 (isosuberosenol A)	14
Figure S13: HR-ESI-MS Spectrum of 2 (suberosain A)	15
Figure S14: ¹ H-NMR (500 MHz, CDCl ₃) Spectrum of 2 (suberosain A)	16
Figure S15: ¹³ C-NMR (125 MHz, CDCl ₃) Spectrum of 2 (suberosain A)	17
Figure S16: DEPT135 (125 MHz, CDCl ₃) Spectrum of 2 (suberosain A)	18
Figure S17: HSQC Spectrum of 2 (suberosain A)	19
Figure S18: HSQC Spectrum of 2 (suberosain A) (From δ_C 14 ppm to 50 ppm)	20
Figure S19: HMBC Spectrum of 2 (suberosain A)	21
Figure S20: HMBC Spectrum of 2 (suberosain A) (From δ_C 52 ppm to 75 ppm)	22
Figure S21: HMBC Spectrum of 2 (suberosain A) (From δ_C 15 ppm to 50 ppm)	23
Figure S22: ¹ H- ¹ H COSY Spectrum of 2 (suberosain A)	24
Figure S23: NOESY Spectrum of 2 (suberosain A)	25
Figure S24: HR-ESI-MS Spectrum of 3 (4-hydroxymethyl-5 β -pregnan-3, 20-dione)	26
Figure S25: ¹ H-NMR (500 MHz, CDCl ₃) Spectrum of 3 (4-hydroxymethyl-5 β -pregnan-3, 20-dione)	27

Figure S26: ^{13}C -NMR (125 MHz, CDCl_3) Spectrum of 3 (4-hydroxymethyl-5 β -pregnan-3, 20-dione)	28
Figure S27: DEPT135 (125 MHz, CDCl_3) Spectrum of 3 (4-hydroxymethyl-5 β -pregnan-3, 20-dione)	29
Figure S28: HSQC Spectrum of 3 (4-hydroxymethyl-5 β -pregnan-3, 20-dione)	30
Figure S29: HSQC Spectrum of 3 (4-hydroxymethyl-5 β -pregnan-3, 20-dione) (From δ_{C} 12 to 42)	31
Figure S30: HMBC Spectrum of 3 (4-hydroxymethyl-5 β -pregnan-3, 20-dione)	32
Figure S31: HMBC Spectrum of 3 (4-hydroxymethyl-5 β -pregnan-3, 20-dione) (From δ_{C} 42 to 70)	33
Figure S32: HMBC Spectrum of 3 (4-hydroxymethyl-5 β -pregnan-3, 20-dione) (From δ_{C} 12 to 40)	34
Figure S33: ^1H - ^1H COSY Spectrum of 3 (4-hydroxymethyl-5 β -pregnan-3, 20-dione)	35
Figure S34: NOESY Spectrum of 3 (4-hydroxymethyl-5 β -pregnan-3, 20-dione)	36

Elemental Composition Report

Page 1

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

77 formula(e) evaluated with 2 results within limits (up to 50 best isotopic matches for each mass)

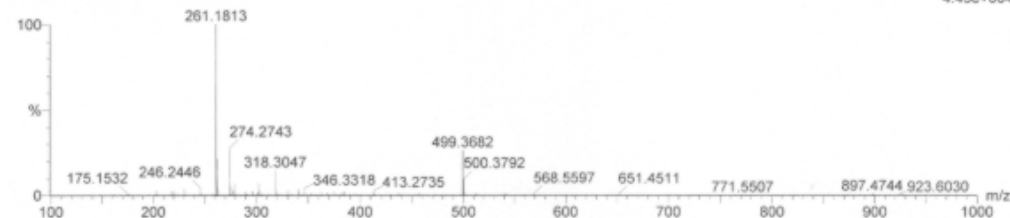
Elements Used:

C: 0-500 H: 0-1000 O: 0-200 Na: 0-1

28-Feb-2011 11:11:49

SC3-8 21 (1.250) AM (Top, 3, Ar, 5000.0, 345.00, 0.70, LS 10); Sm (Mn, 2x1.00); Cm (5.26)

1: TOF MS ES+
4.45e+004



Minimum: -1.5
Maximum: 10.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
261.1813	261.1855	-4.2	-16.1	5.5	91.3	C17 H25 O2
	261.1831	-1.8	-6.9	2.5	235.5	C15 H26 O2 Na

Figure S1: HR-ESI-MS Spectrum of 1 (isosuberosenol A)

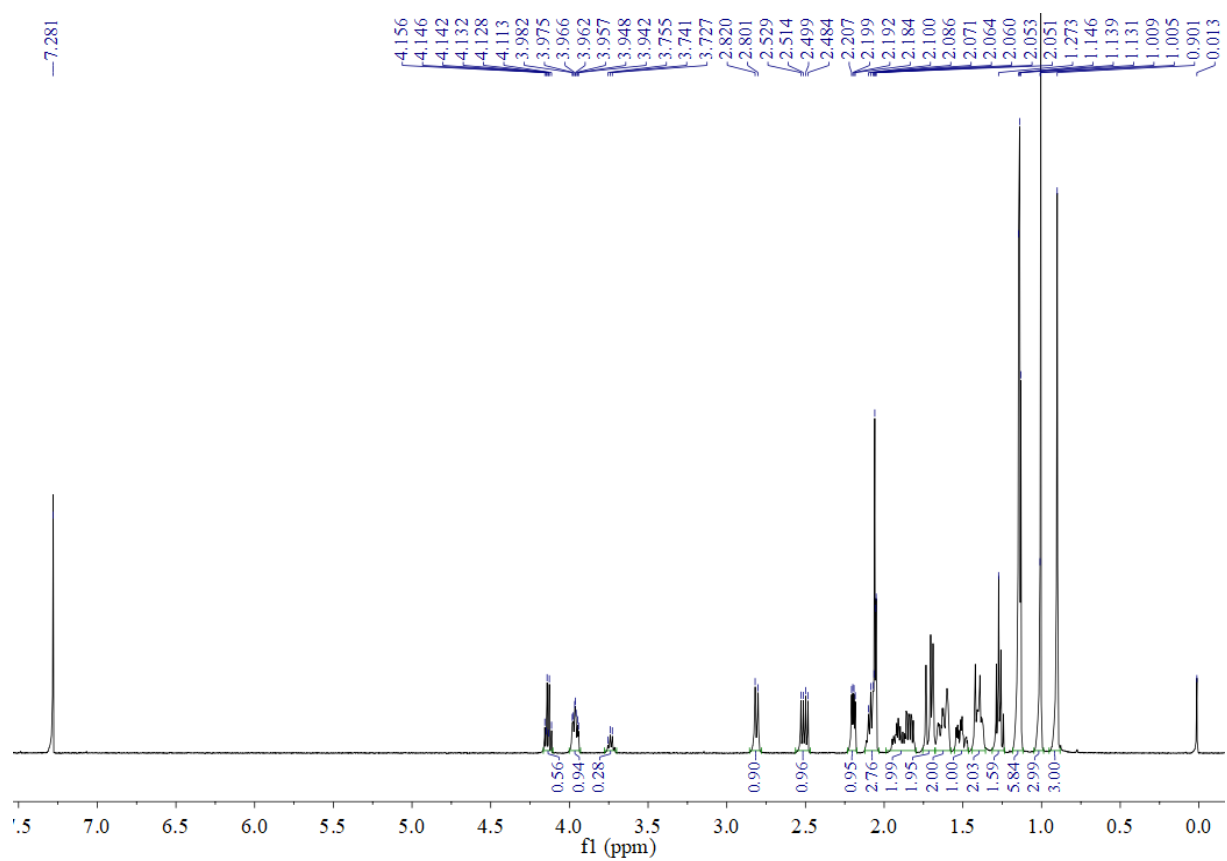


Figure S2: ^1H -NMR (500 MHz, CDCl_3) Spectrum of **1** (isosuberosenol A)

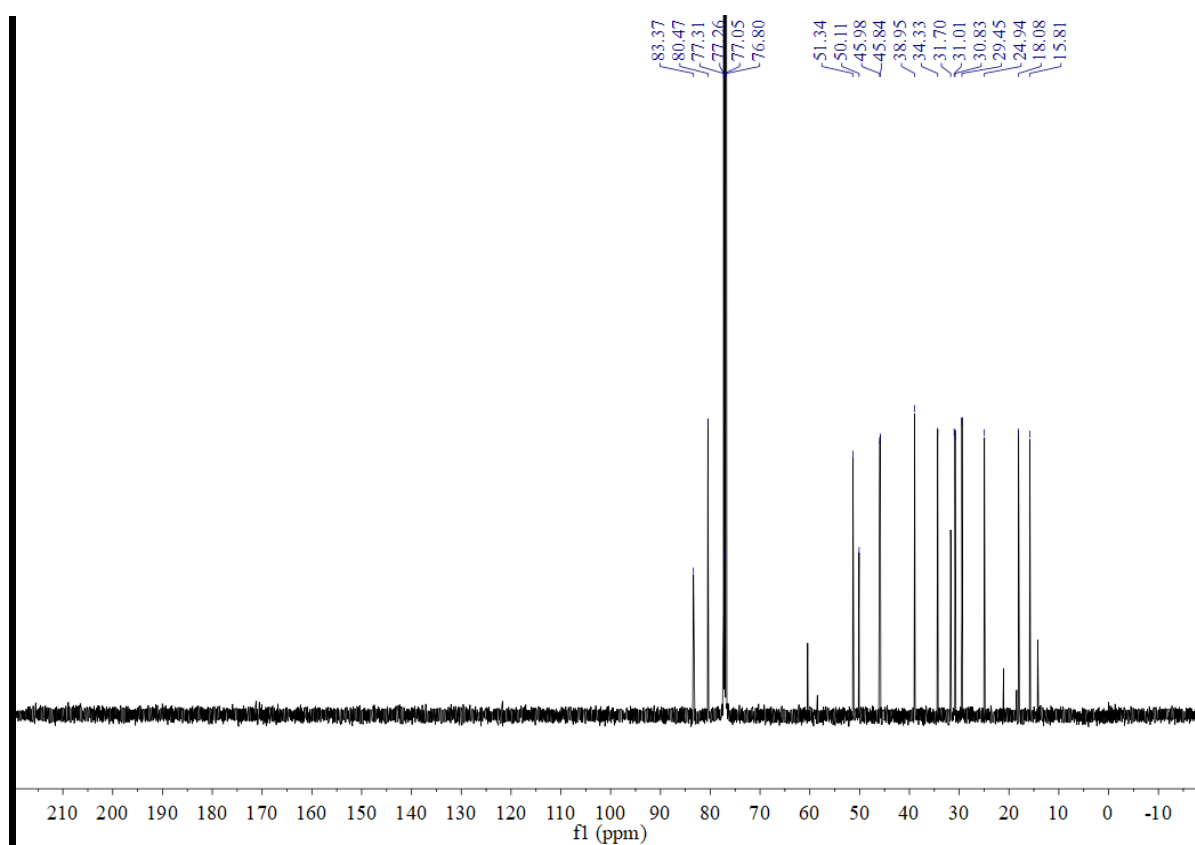


Figure S3: ¹³C-NMR (125 MHz, CDCl₃) Spectrum of **1** (isosuberosenol A)

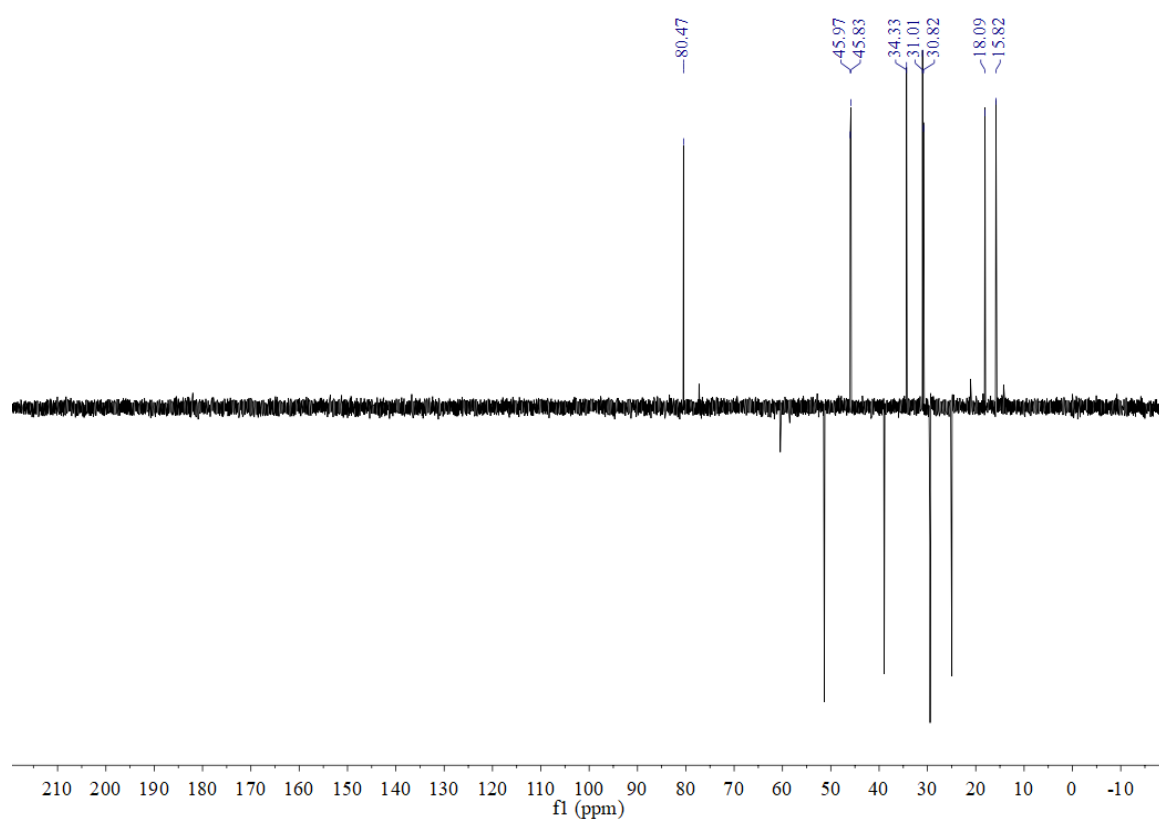


Figure S4: DEPT135 (125 MHz, CDCl_3) Spectrum of **1** (isosuberosenol A)

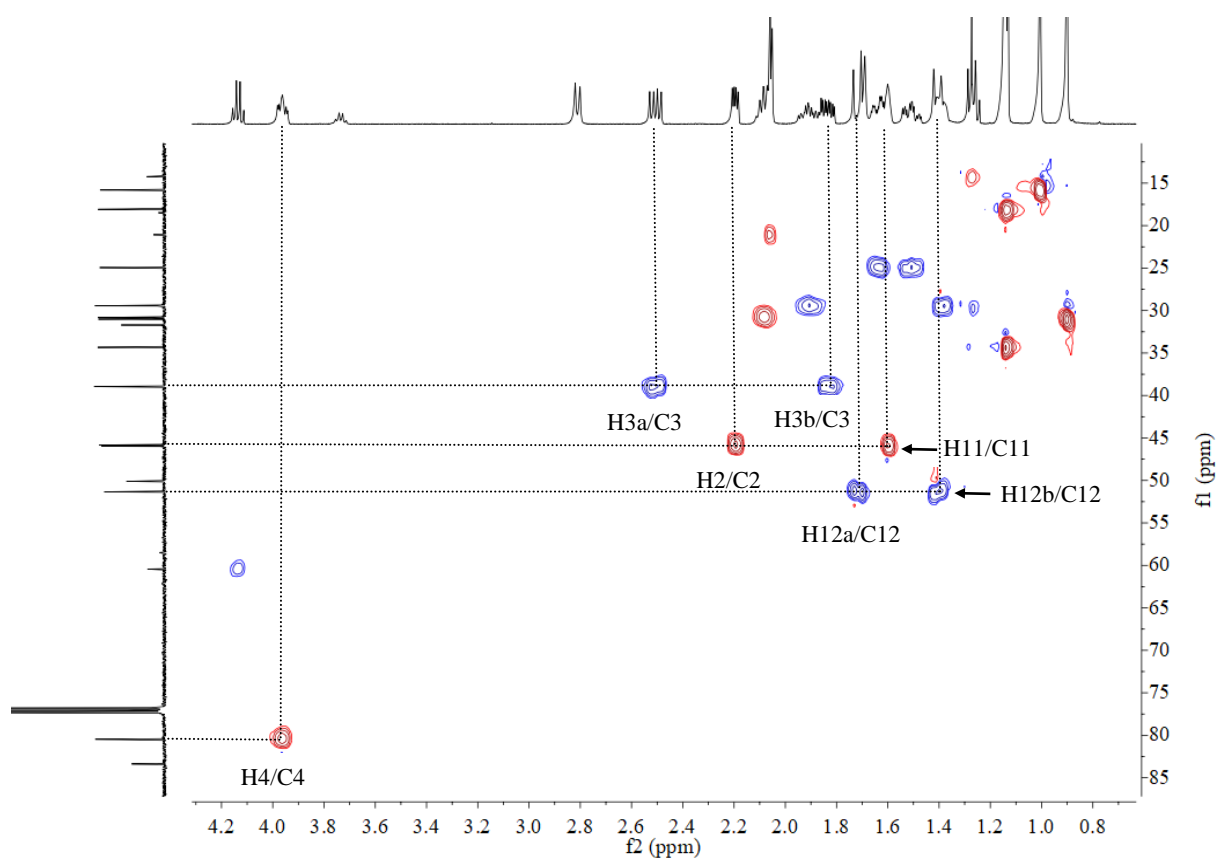


Figure S5: HSQC Spectrum of **1** (isosuberosenol A)

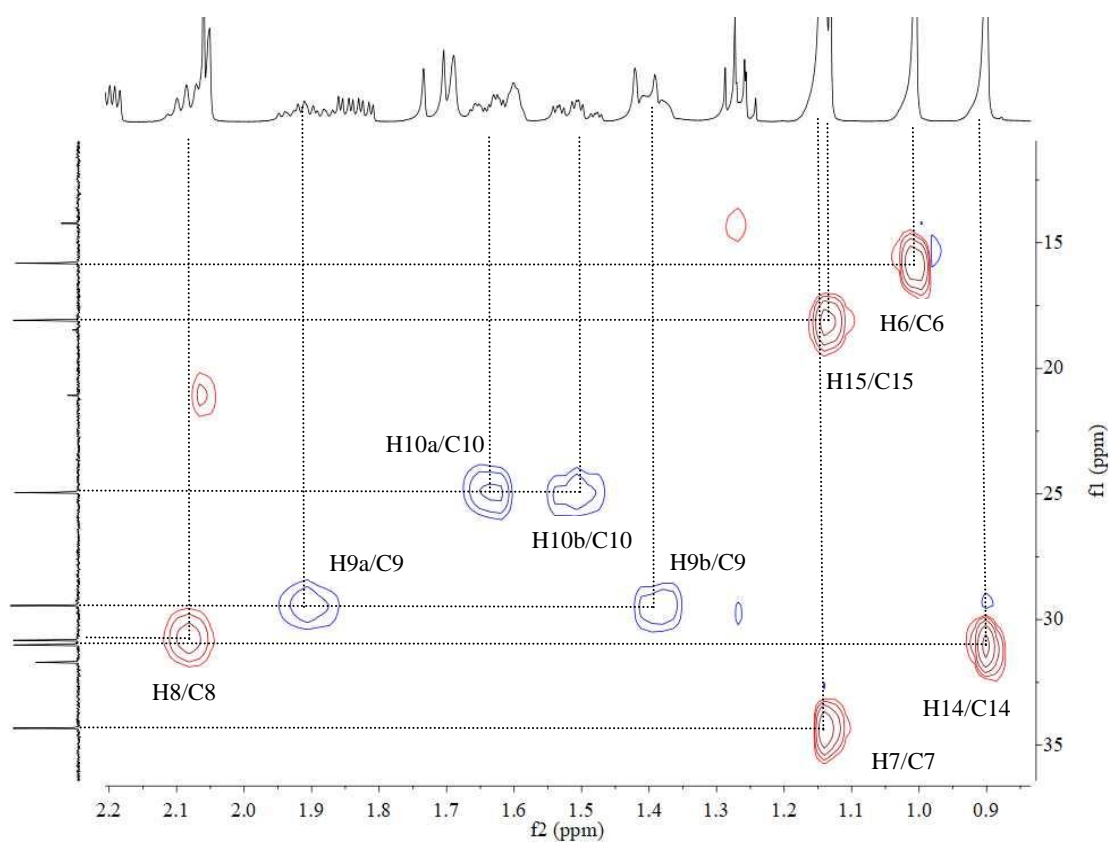


Figure S6: HSQC Spectrum of **1** (isosuberosenol A) (From $\delta_{\text{C}}15$ ppm to $\delta_{\text{C}}35$ ppm)

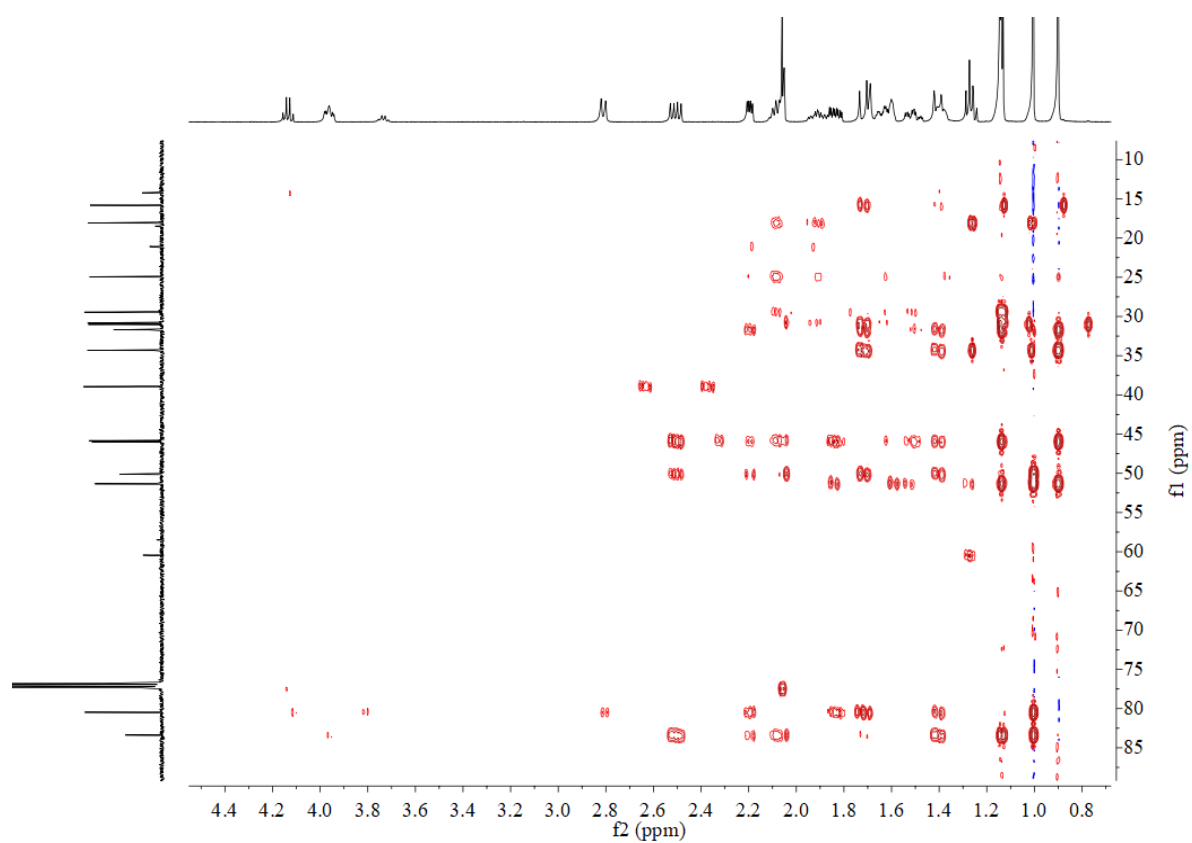


Figure S7: HMBC Spectrum of **1** (isosuberosenol A)

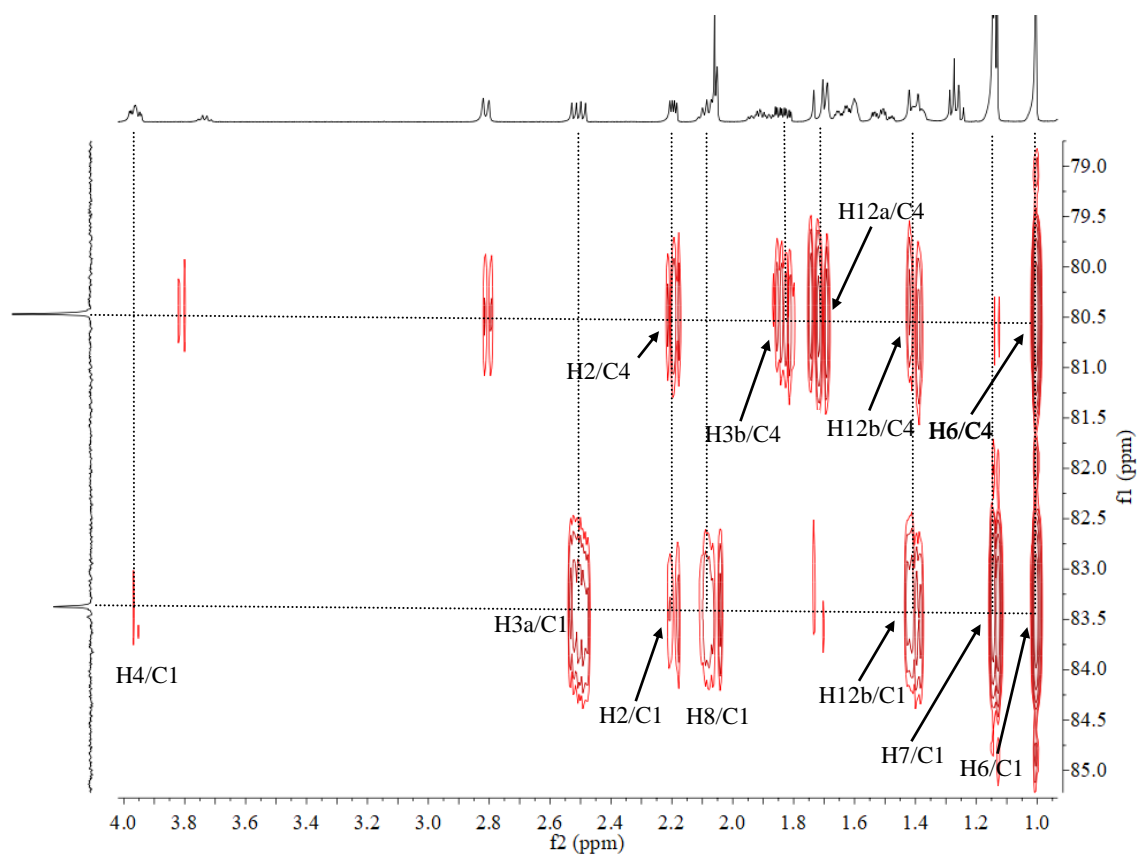


Figure S8: HMBC Spectrum of **1** (isosuberosenol A) (From δ_c 79 ppm to δ_c 85 ppm)

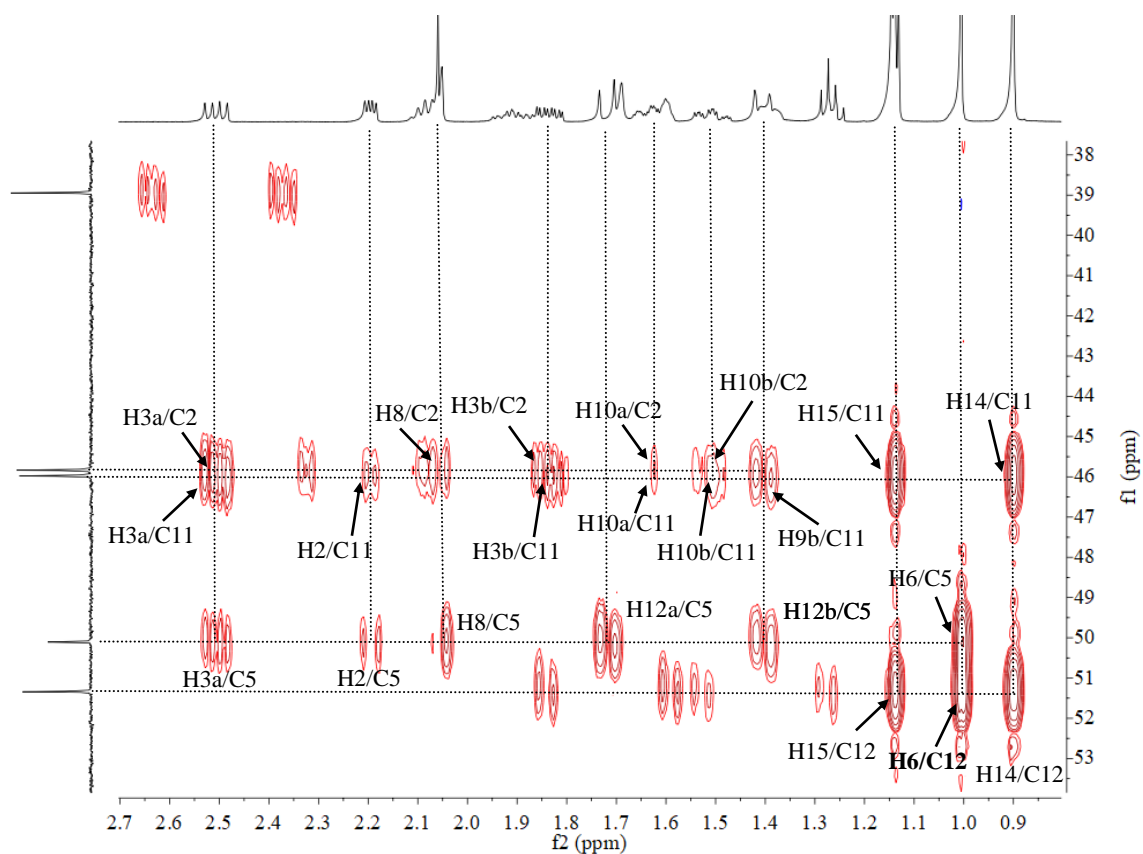


Figure S9: HMBC Spectrum of **1** (isosuberosenol A) (From δ_c 38 ppm to δ_c 53 ppm)

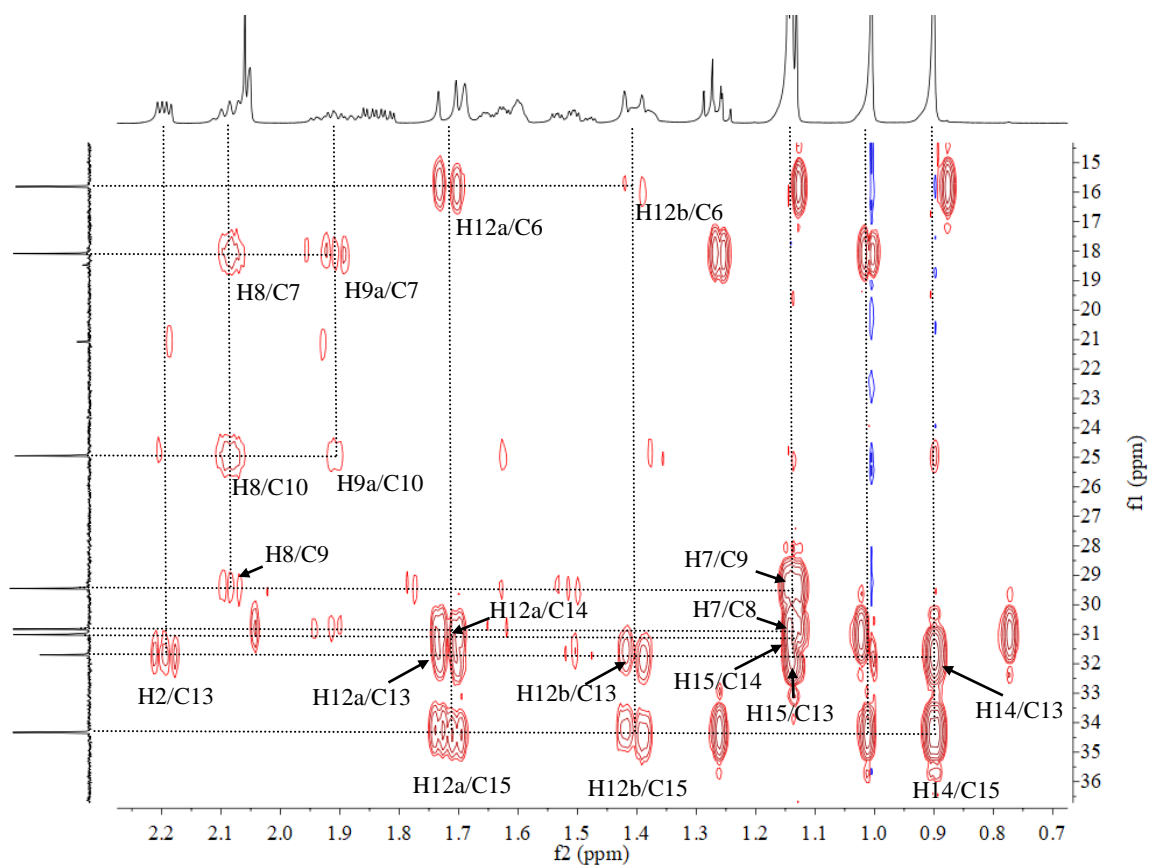


Figure S10: HMBC Spectrum of **1** (isosuberosenol A) (From δ_{C} 15 ppm to δ_{C} 36 ppm)

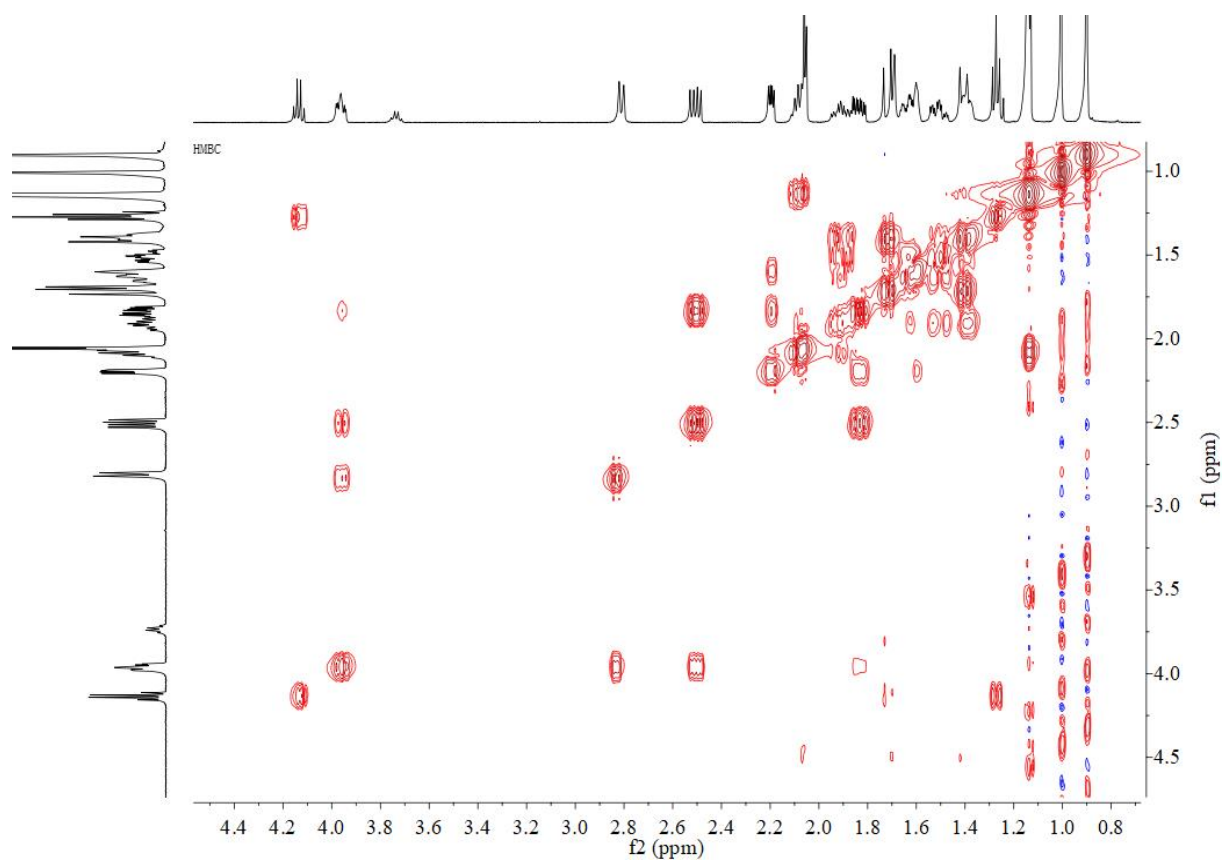


Figure S11: ^1H - ^1H COSY Spectrum of **1** (isosuberosenol A)

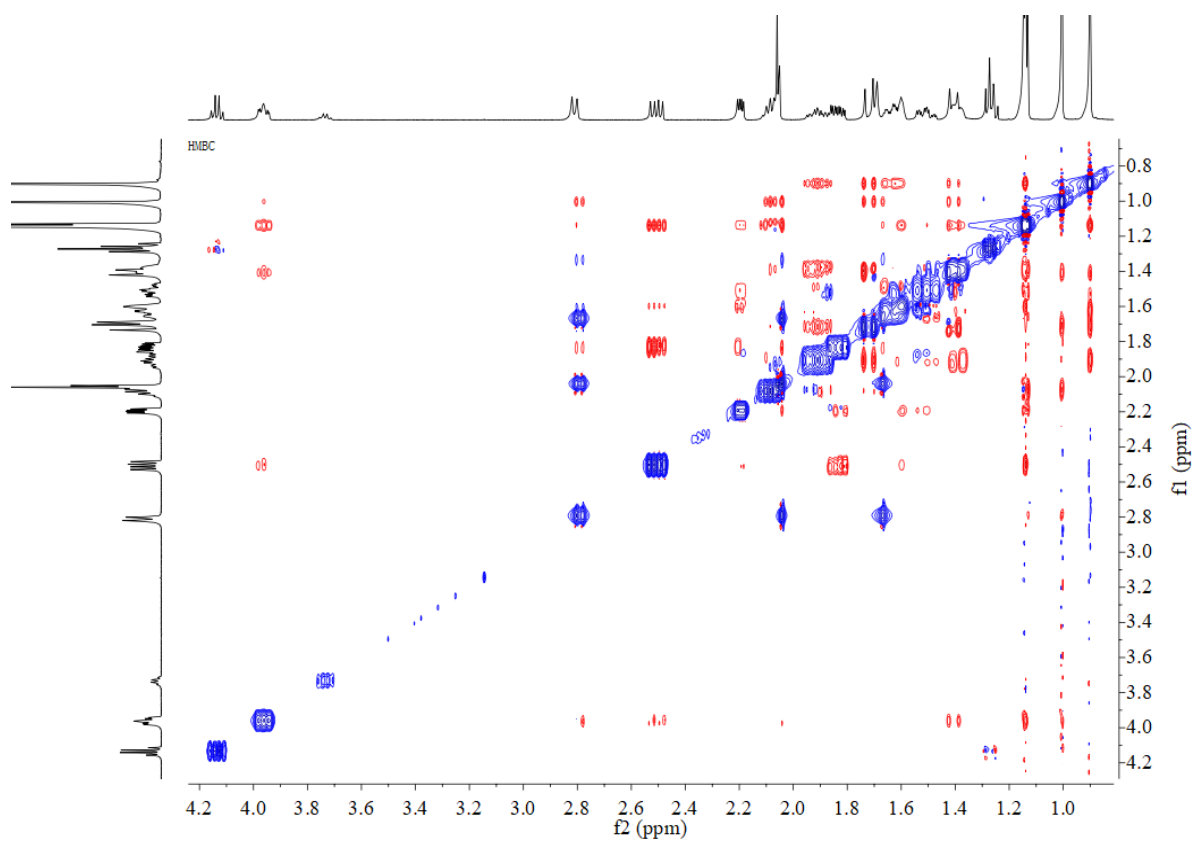


Figure S12: NOESY Spectrum of **1** (isosuberosenol A)

Elemental Composition Report

Page 1

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

74 formula(e) evaluated with 2 results within limits (up to 50 best isotopic matches for each mass)

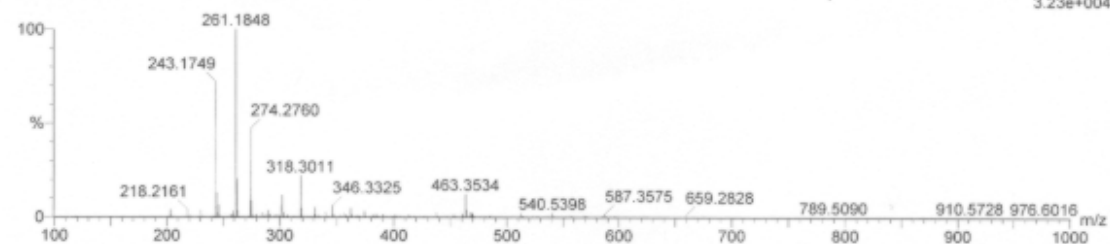
Elements Used:

C: 0-500 H: 0-1000 O: 0-200 Na: 0-1

28-Feb-2011 21:53:25

SC2-27 26 (1.561) AM (Cen,3, 80.00, Ar,5000.0,345.00,0.70,LS 10); Sm (Mn, 2x1.00); Cm (6:30)

1: TOF MS ES+
3.23e+004



Minimum: -1.5
Maximum: 10.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
243.1749	243.1749	0.0	0.0	6.5	60.9	C17 H23 O
	243.1725	2.4	9.9	3.5	96.3	C15 H24 O Na

Figure S13: HR-ESI-MS Spectrum of **2** (suberosain A)

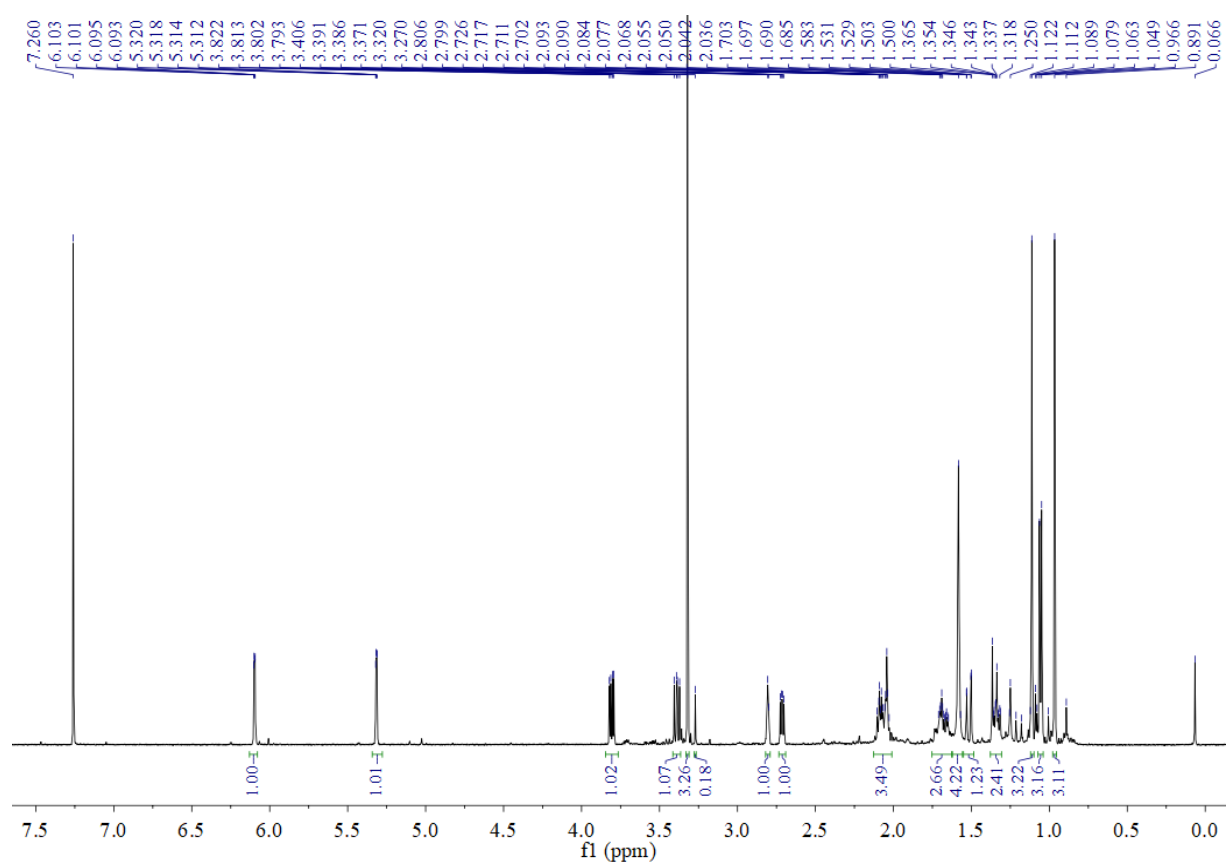


Figure S14: ^1H -NMR (500 MHz, CDCl_3) Spectrum of **2** (suberosain A)

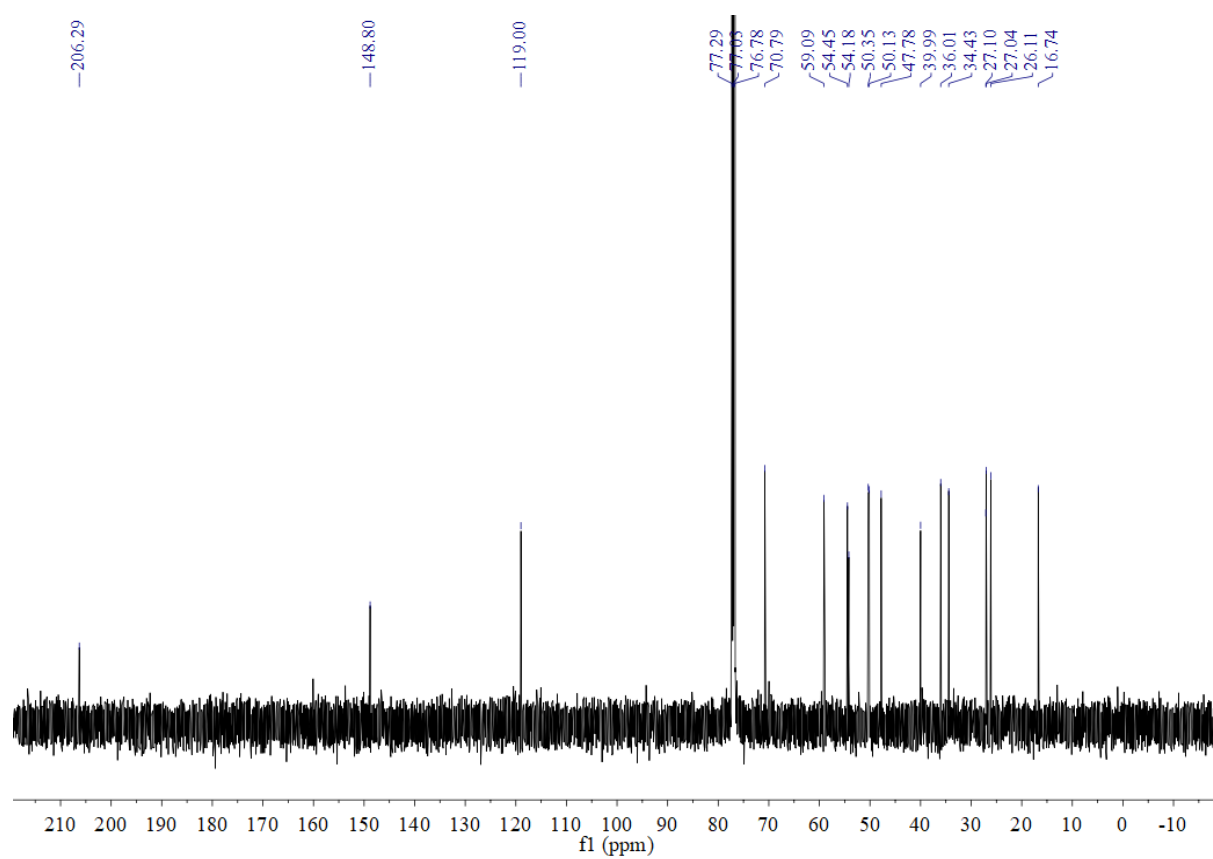


Figure S15: ¹³C-NMR (125 MHz, CDCl₃) Spectrum of **2** (suberosain A)

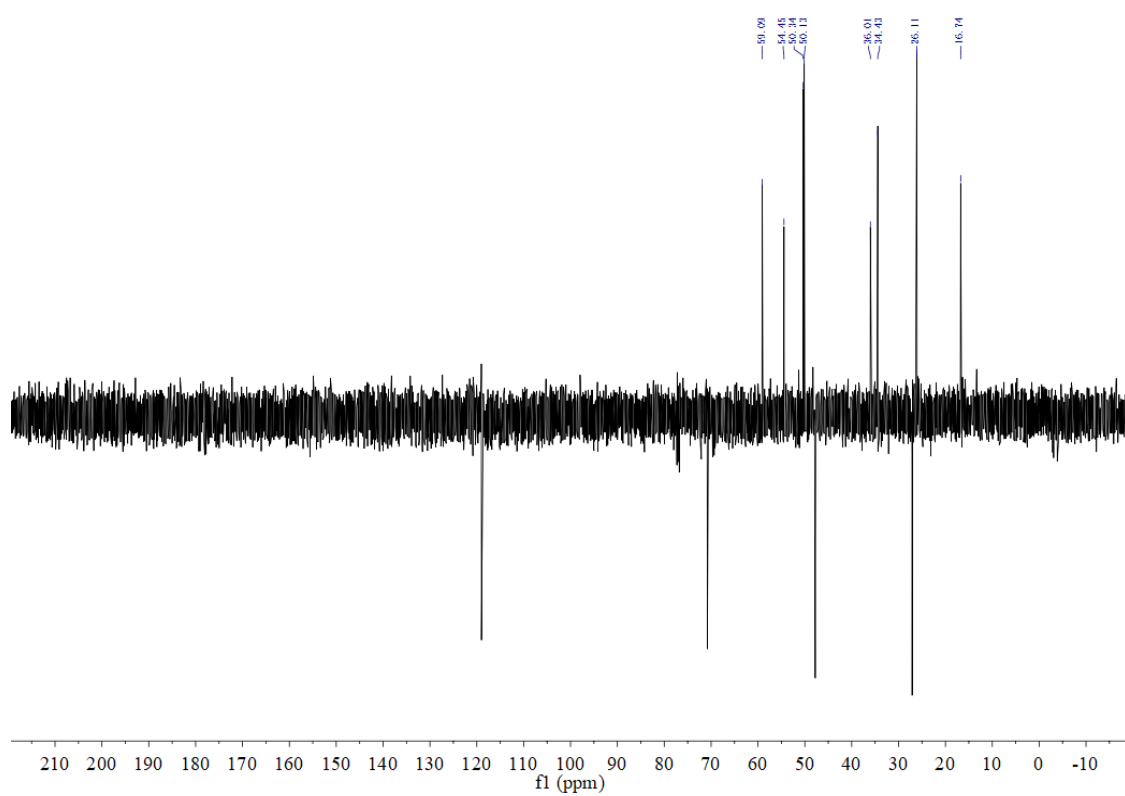


Figure S16: DEPT135 (125 MHz, CDCl₃) Spectrum of **2** (suberosain A)

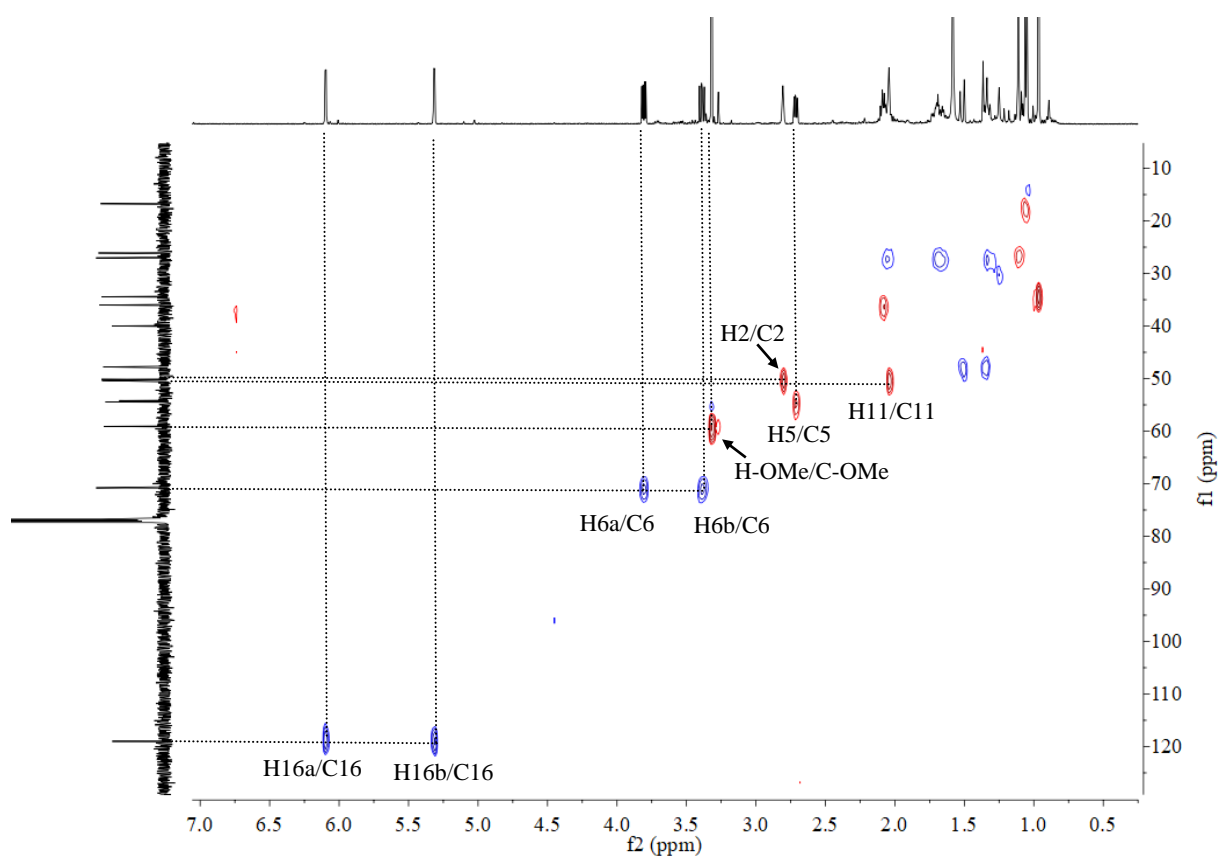


Figure S17: HSQC Spectrum of **2** (suberosain A)

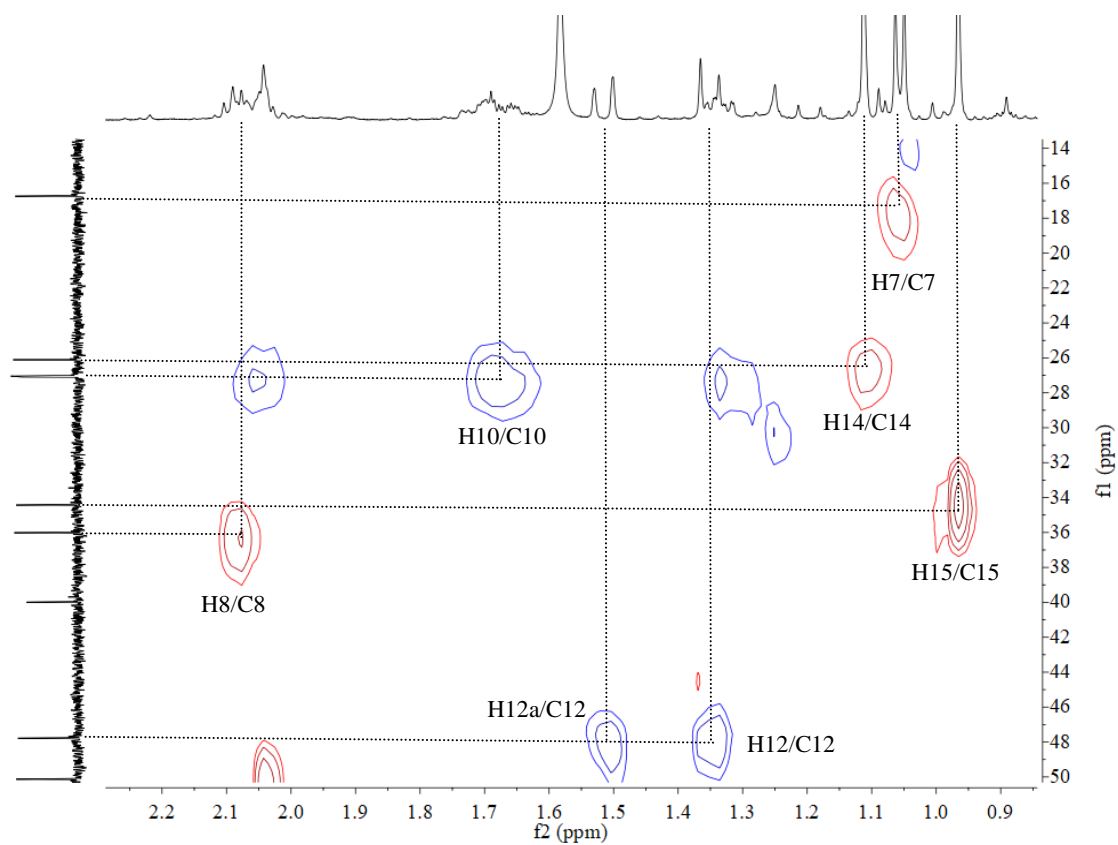


Figure S18: HSQC Spectrum of **2** (suberosain A) (From δ_{C} 14 ppm to 50 ppm)

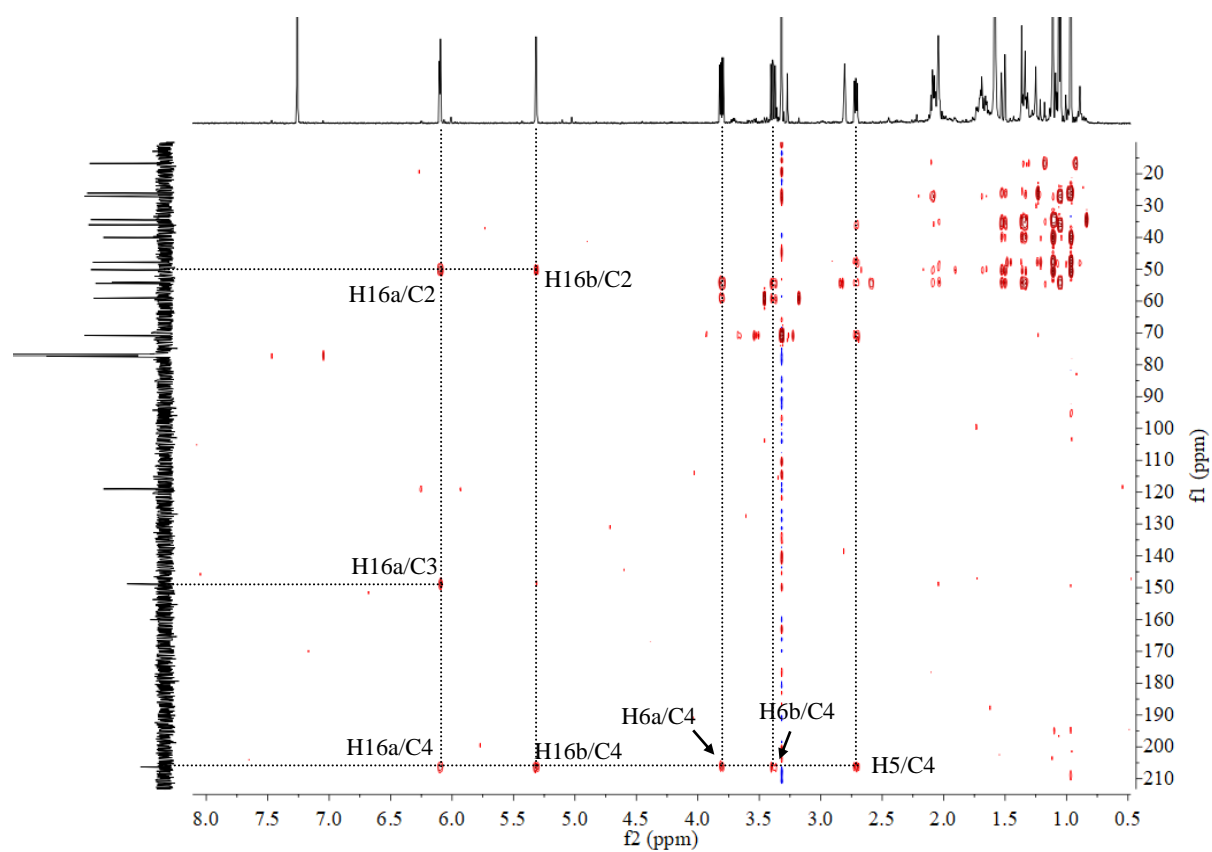


Figure S19: HMBC Spectrum of **2** (suberosain A)

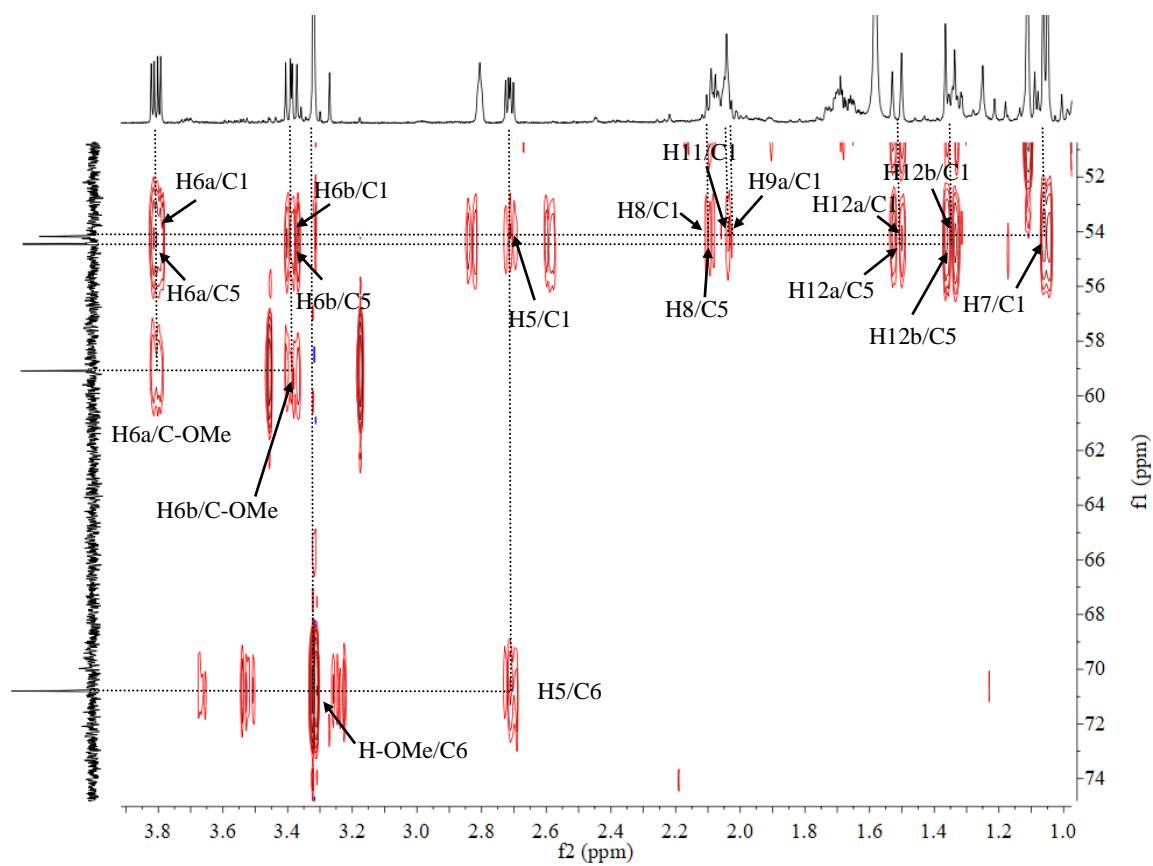


Figure S20: HMBC Spectrum of 2 (suberosain A) (From δ_c 52 ppm to 75 ppm)

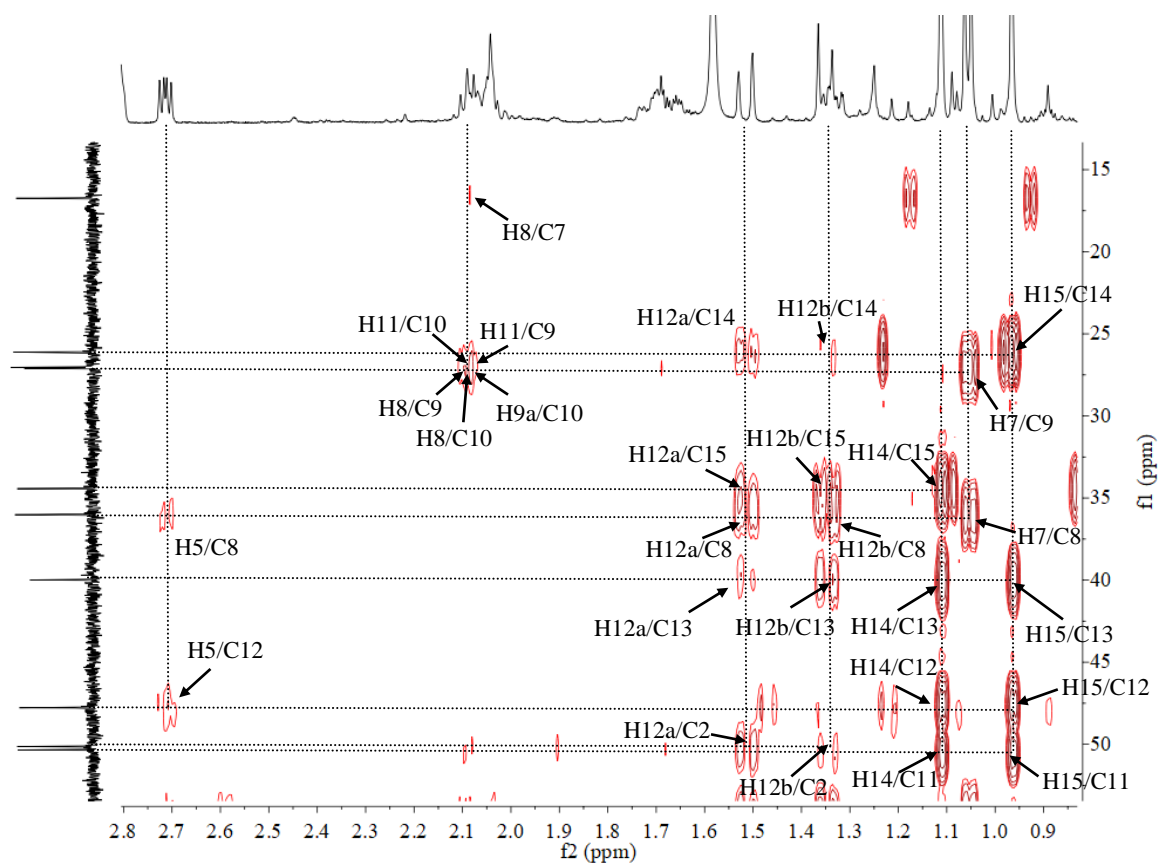


Figure S21: HMBC Spectrum of **2** (suberosain A) (From δ_c 15 ppm to 50 ppm)



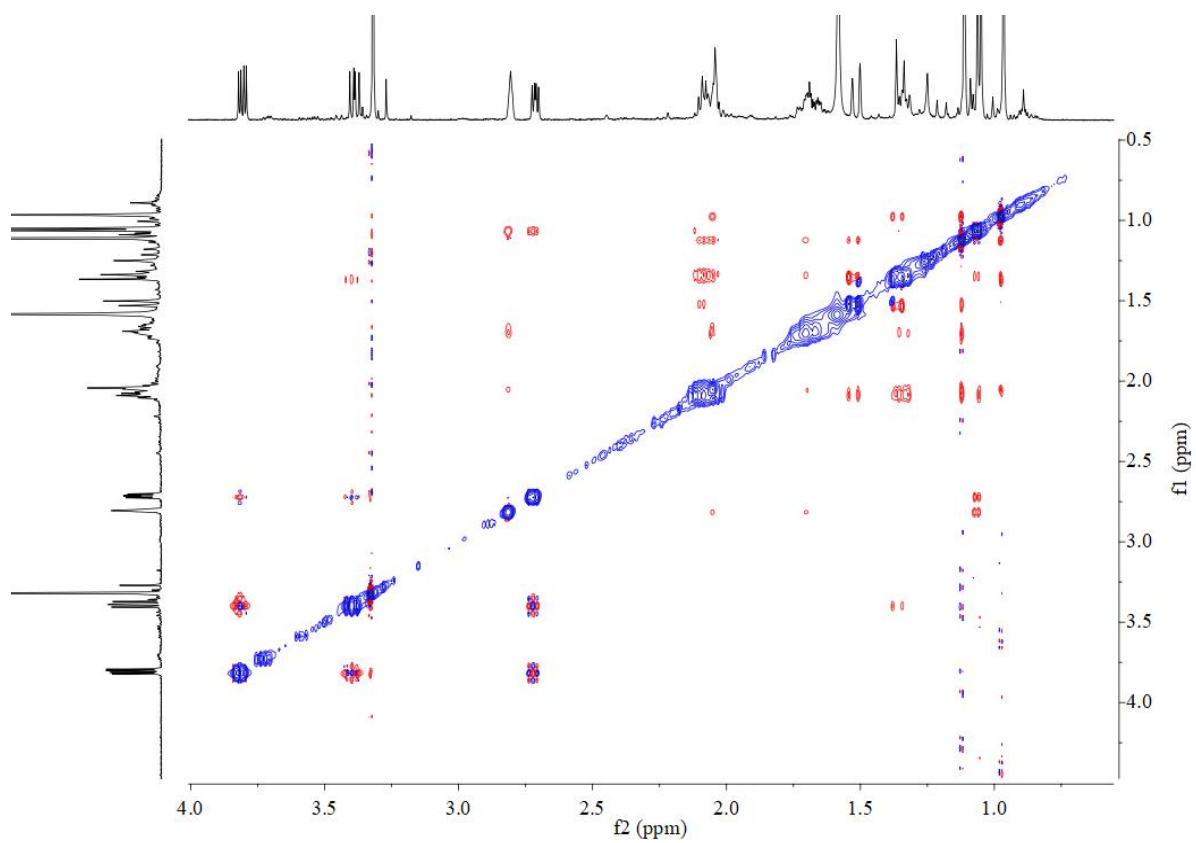


Figure S23: NOESY Spectrum of **2** (suberosain A)

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 5.0 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

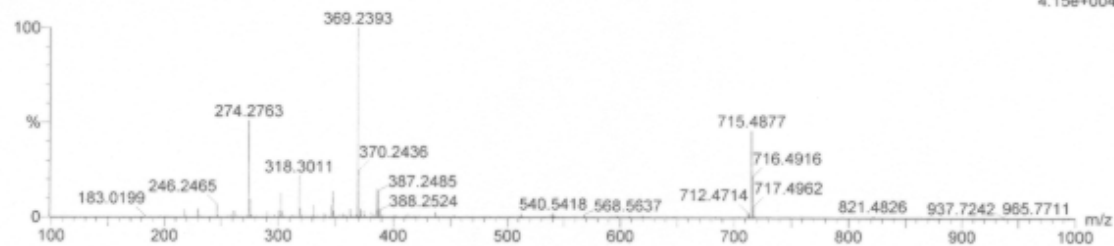
139 formula(e) evaluated with 2 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

C: 0-500 H: 0-1000 O: 0-200 Na: 0-1

28-Feb-2011 20:49:25

SC4-6 24 (1.437) AM (Cen,3, 80.00, Ar,5000.0,345.00,0.70,LS 10); Sm (Mn, 2x1.00); Cm (4.30)

1: TOF MS ES+
4.15e+004

Minimum:

Maximum:

Mass

Calc. Mass

mDa

PPM

DBE

i-FIT

Formula

369.2393

369.2406

-1.3

-3.5

5.5

13.5

C22 H34 O3 Na

369.2430

-3.7

-10.0

8.5

55.1

C24 H33 O3

Figure S24: HR-ESI-MS Spectrum of **3** (4-hydroxymethyl-5 β -pregnan-3, 20-dione)

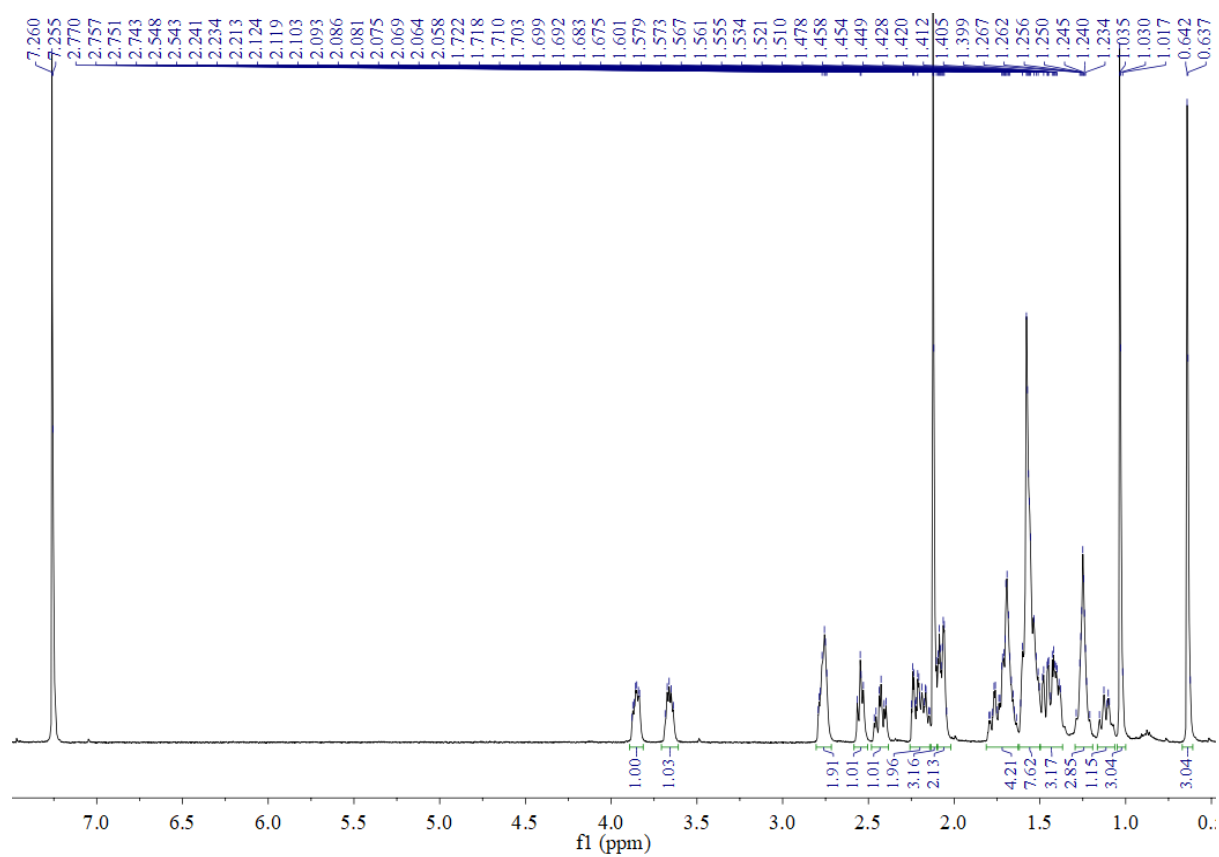


Figure S25: ¹H-NMR (500 MHz, CDCl₃) Spectrum of **3** (4-hydroxymethyl-5β-pregnan-3, 20-dione)

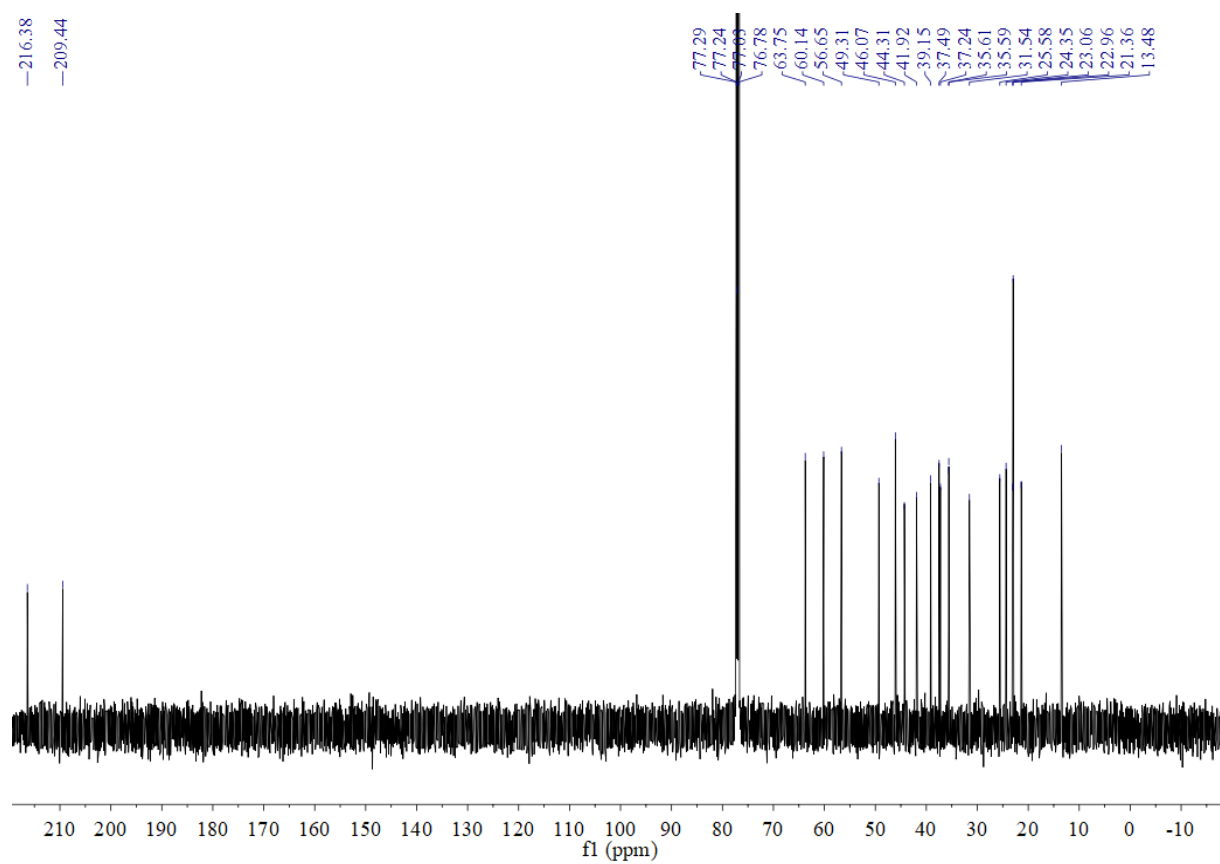


Figure S26: ^{13}C -NMR (125 MHz, CDCl_3) Spectrum of **3** (4-hydroxymethyl-5 β -pregnan-3, 20-dione)

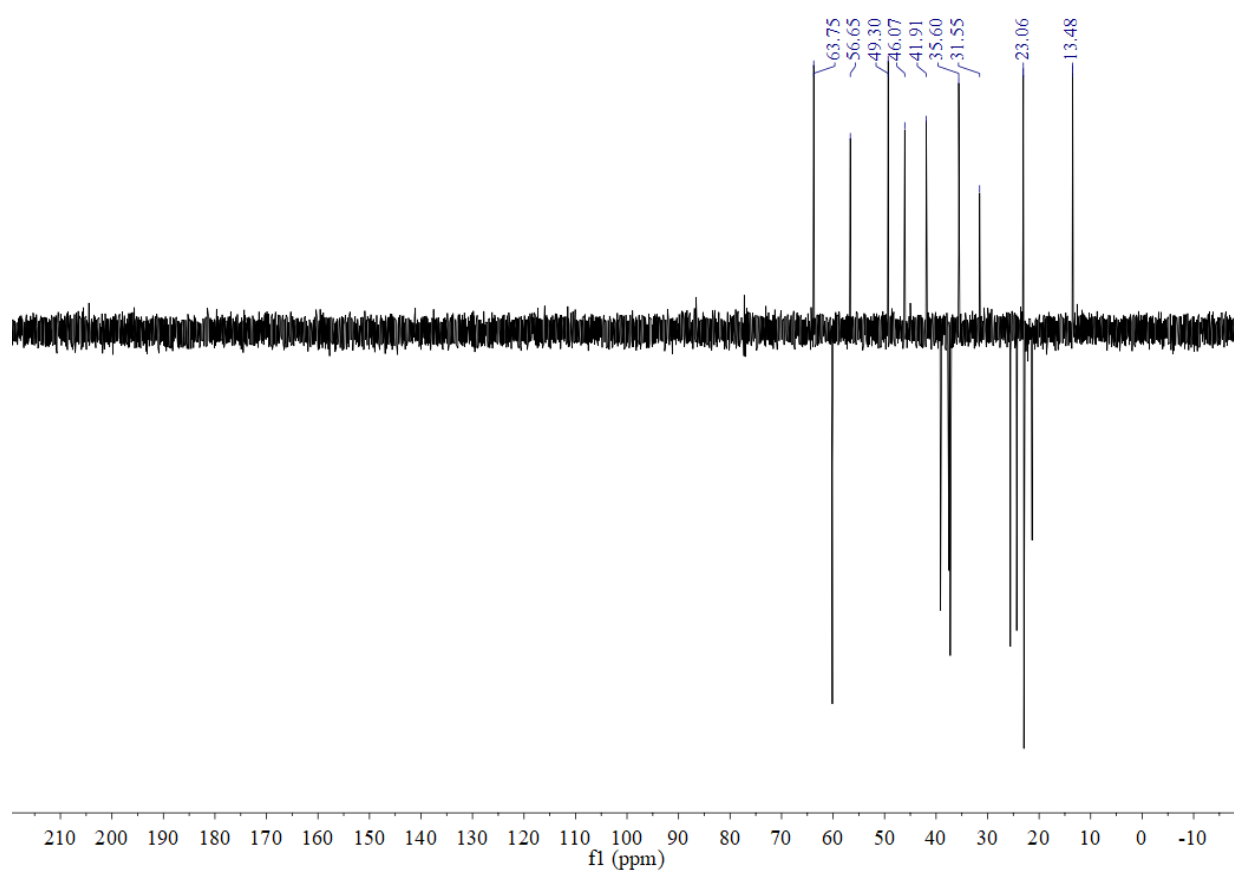


Figure S27: DEPT135 (125 MHz, CDCl₃) Spectrum of **3** (4-hydroxymethyl-5 β -pregnan-3, 20-dione)

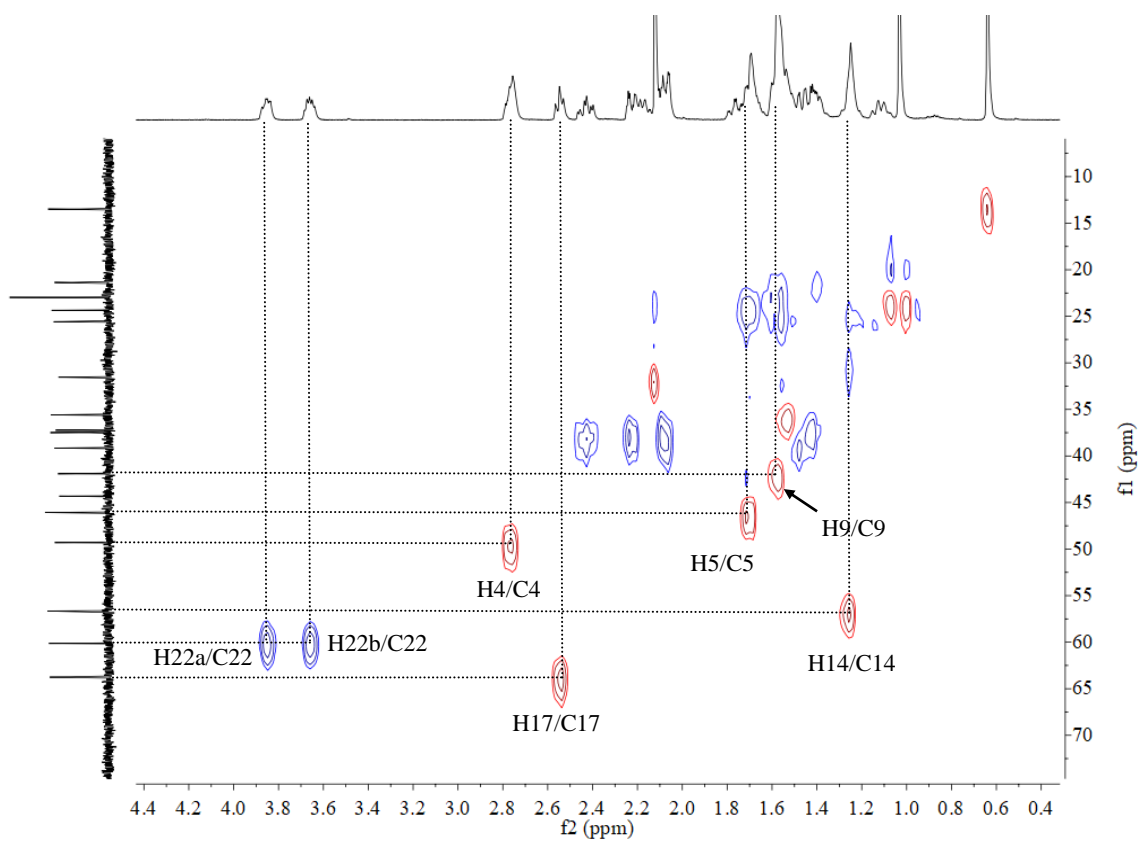


Figure S28: HSQC Spectrum of **3** (4-hydroxymethyl-5 β -pregnan-3, 20-dione)

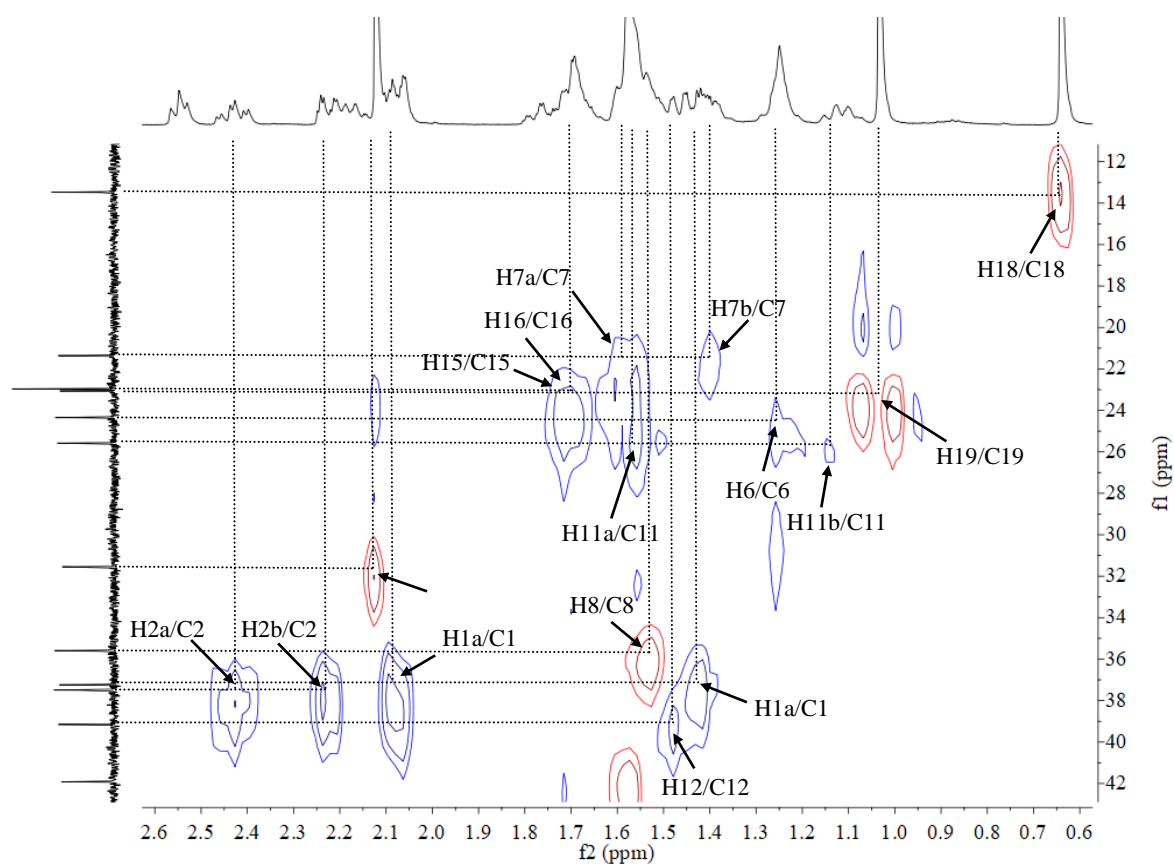


Figure S29: HSQC Spectrum of **3** (4-hydroxymethyl-5 β -pregnan-3, 20-dione) (From δ_C 12 to 42)

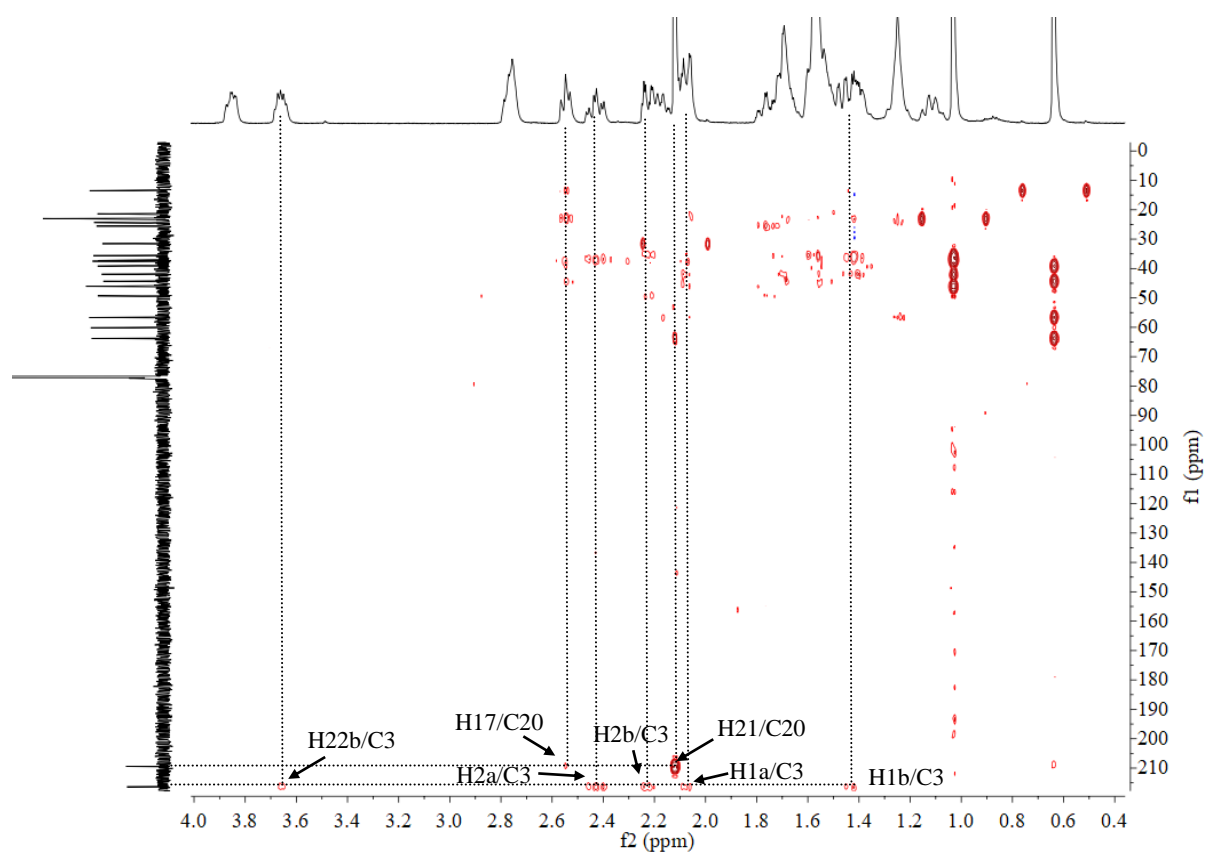


Figure S30: HMBC Spectrum of **3** (4-hydroxymethyl-5 β -pregnan-3, 20-dione)

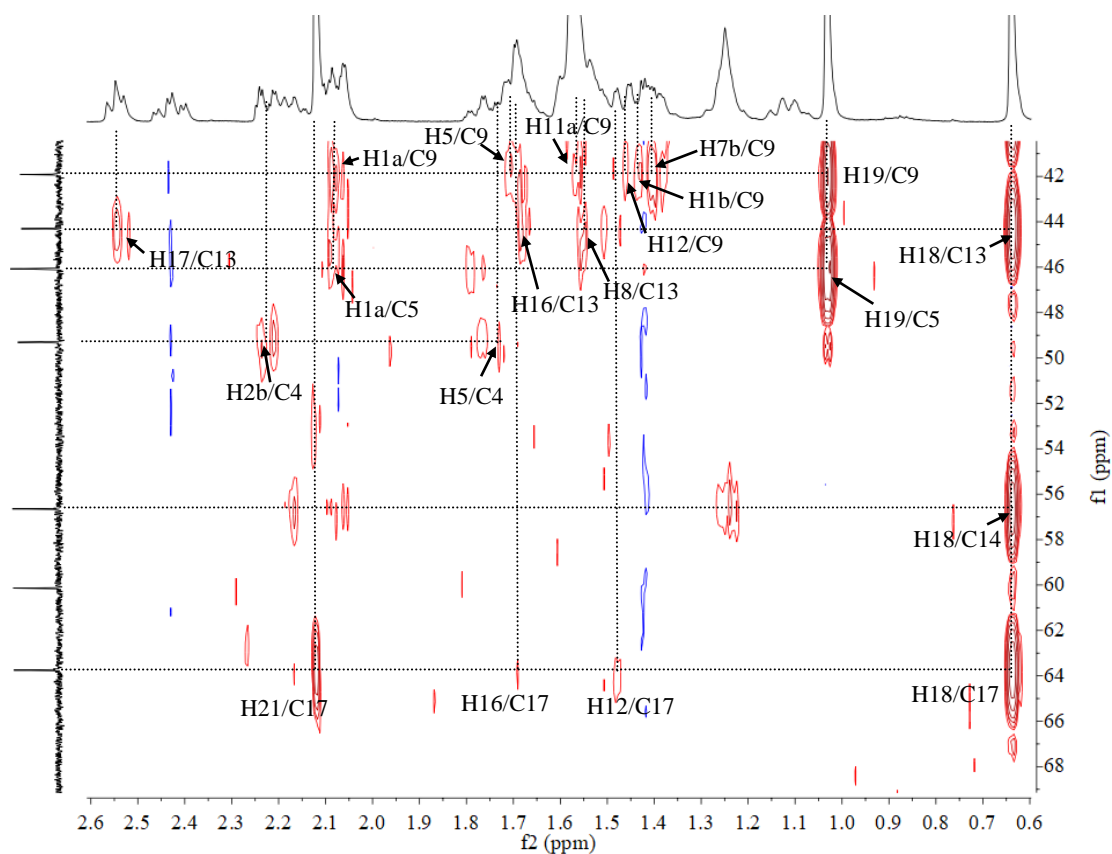


Figure S31: HMBC Spectrum of **3** (4-hydroxymethyl-5 β -pregnan-3, 20-dione) (From δ_c 42 to 70)

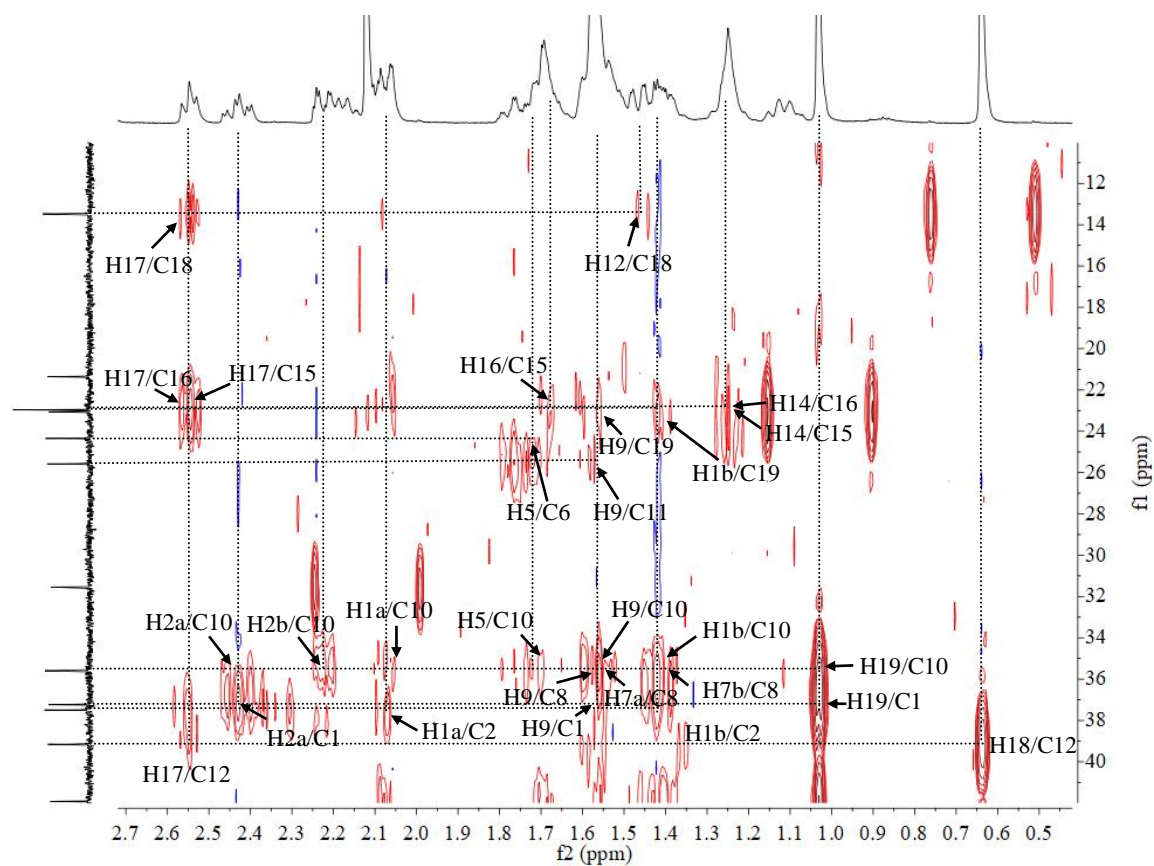


Figure S32: HMBC Spectrum of **3** (4-hydroxymethyl-5 β -pregnan-3, 20-dione) (From δ_C 12 to 40)

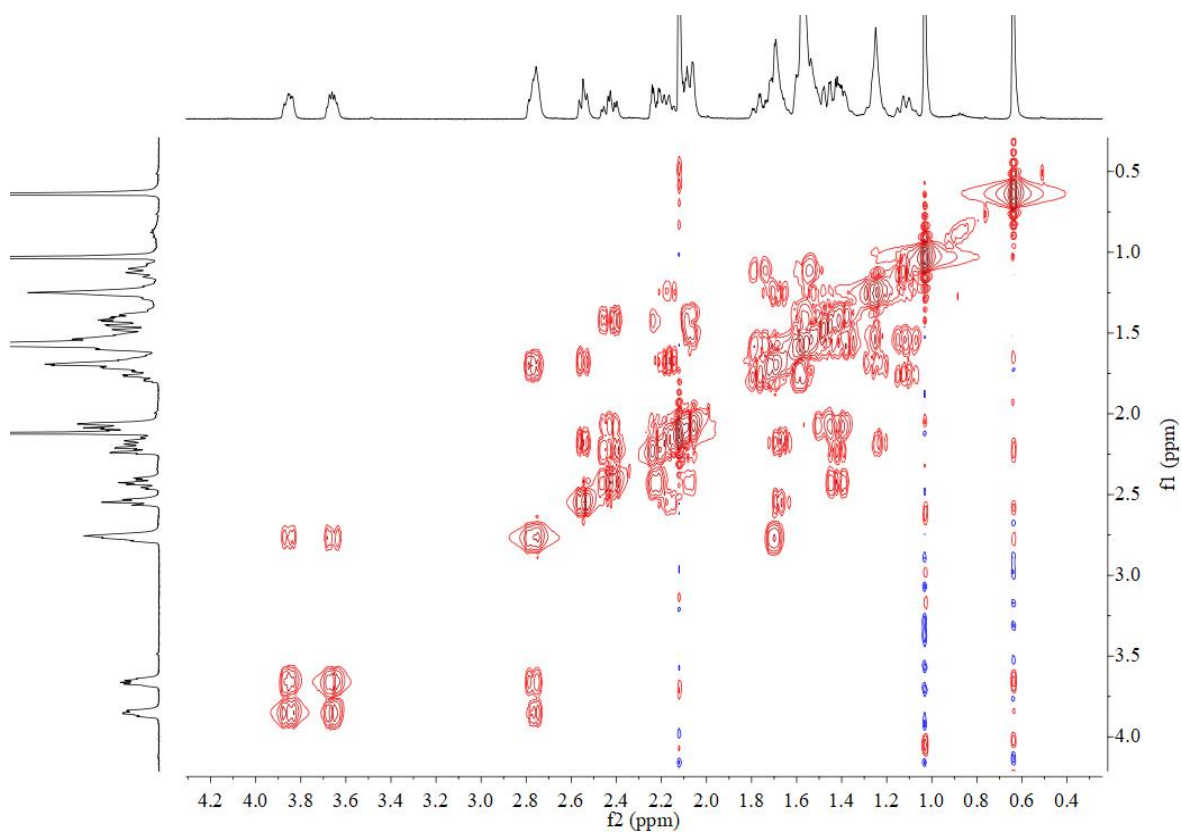


Figure S33: ^1H - ^1H COSY Spectrum of **3** (4-hydroxymethyl-5 β -pregnan-3, 20-dione)

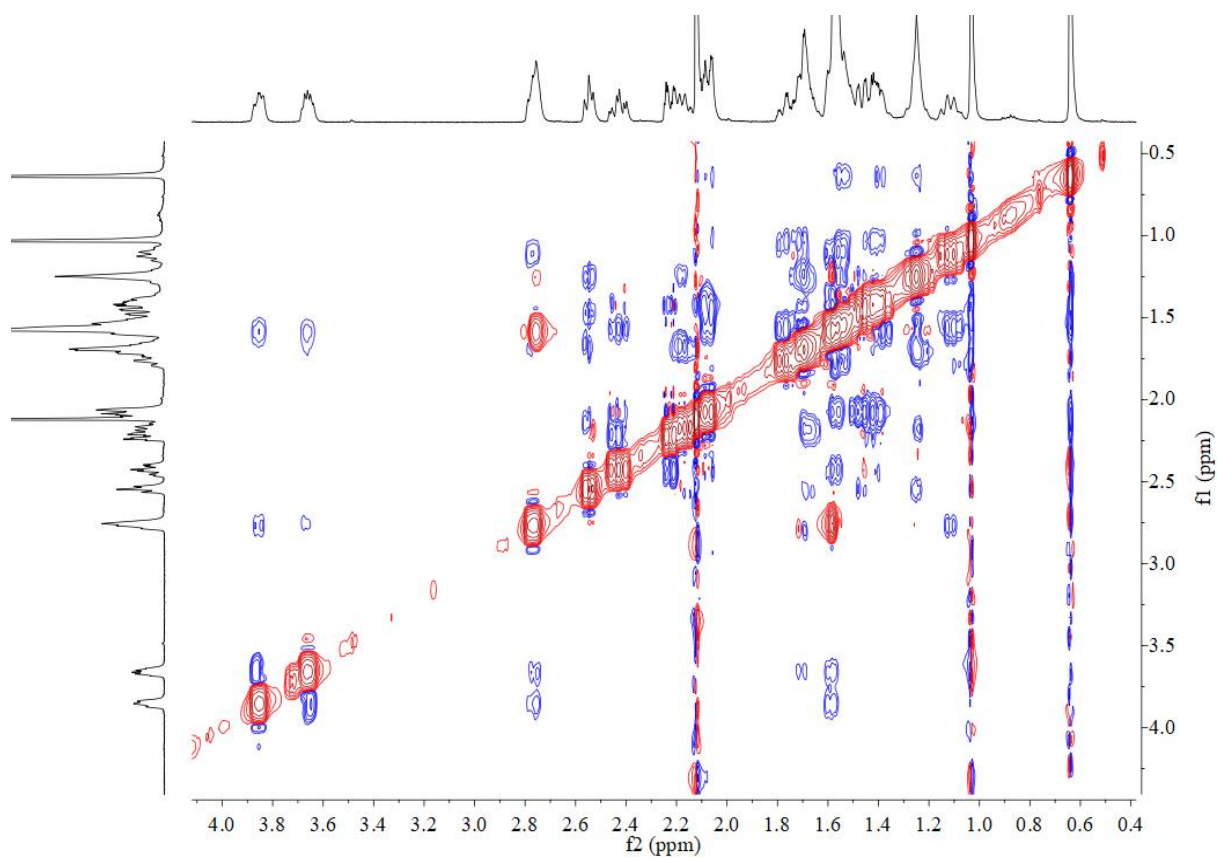


Figure S34: NOESY Spectrum of **3** (4-hydroxymethyl-5 β -pregnan-3, 20-dione)