

Supporting Information

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

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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)

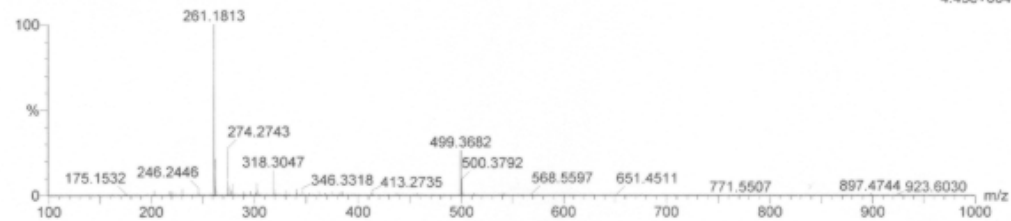
Elements Used:

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

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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)

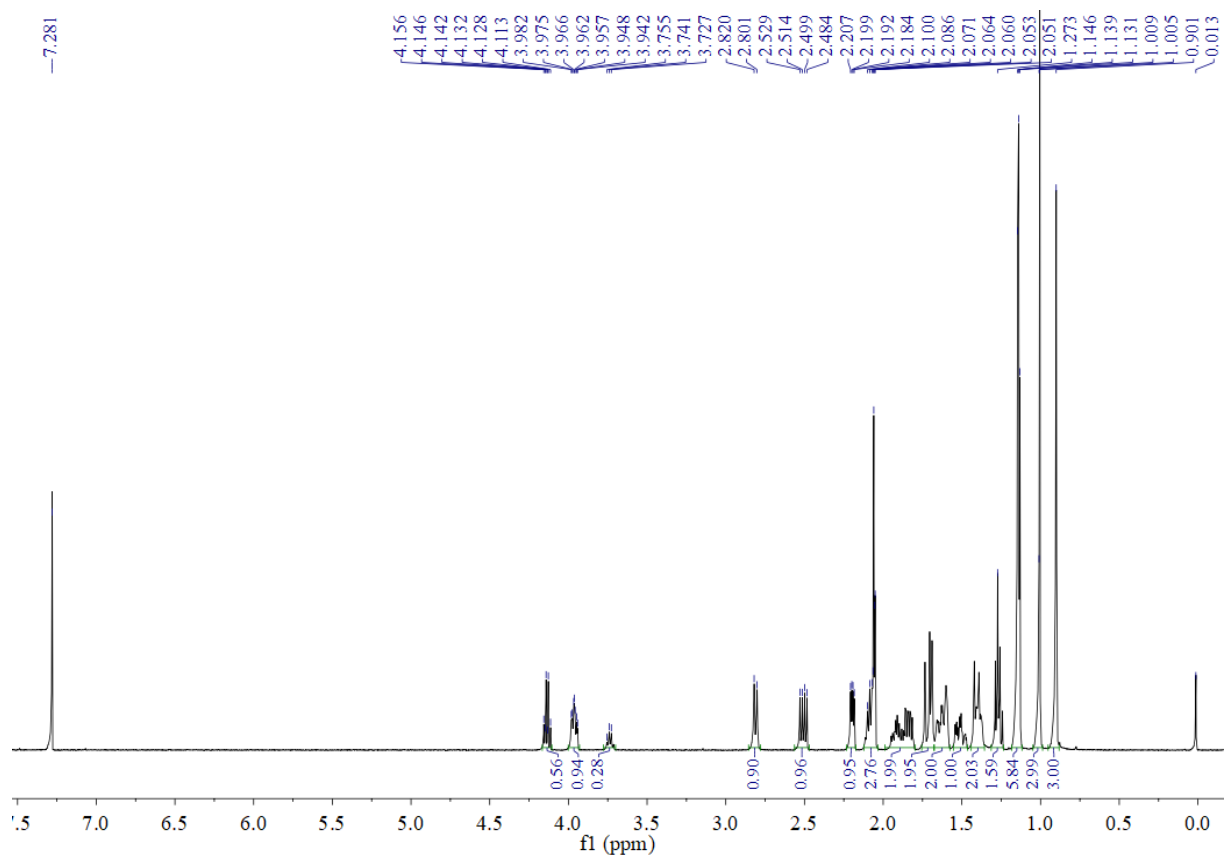


Figure S2: ¹H-NMR (500 MHz, CDCl₃) Spectrum of **1** (isosuberosenol A)

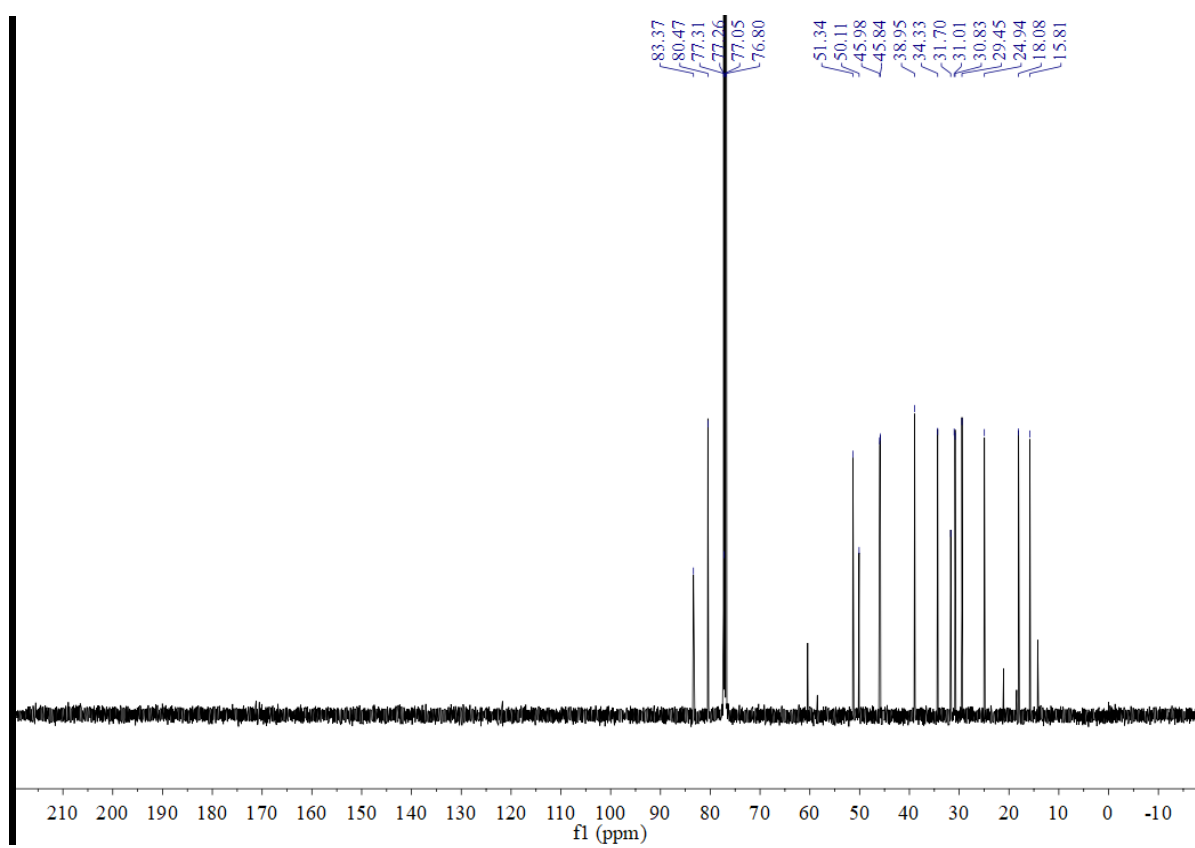


Figure S3: ¹³C-NMR (125 MHz, CDCl₃) Spectrum of **1** (isosuberosenol A)

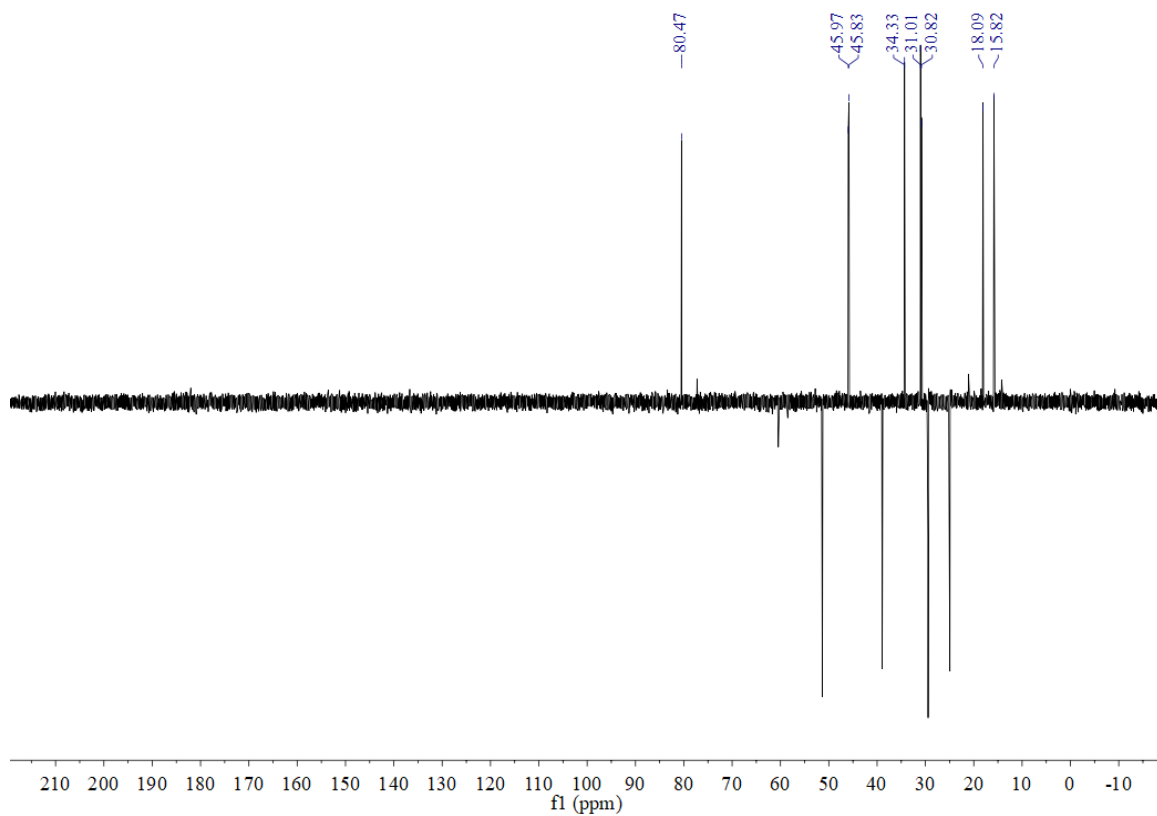


Figure S4: DEPT135 (125 MHz, CDCl₃) Spectrum of **1** (isosuberosenol A)

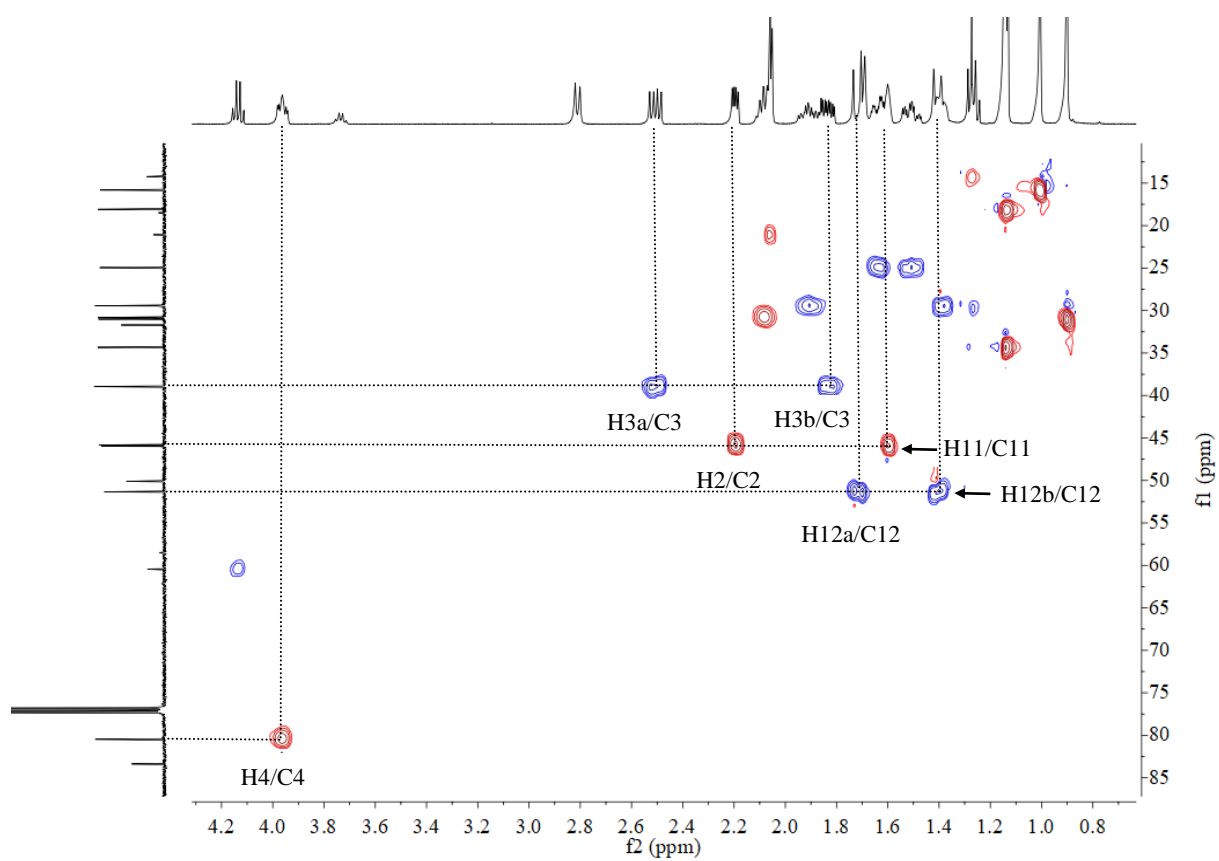


Figure S5: HSQC Spectrum of **1** (isosuberosenol A)

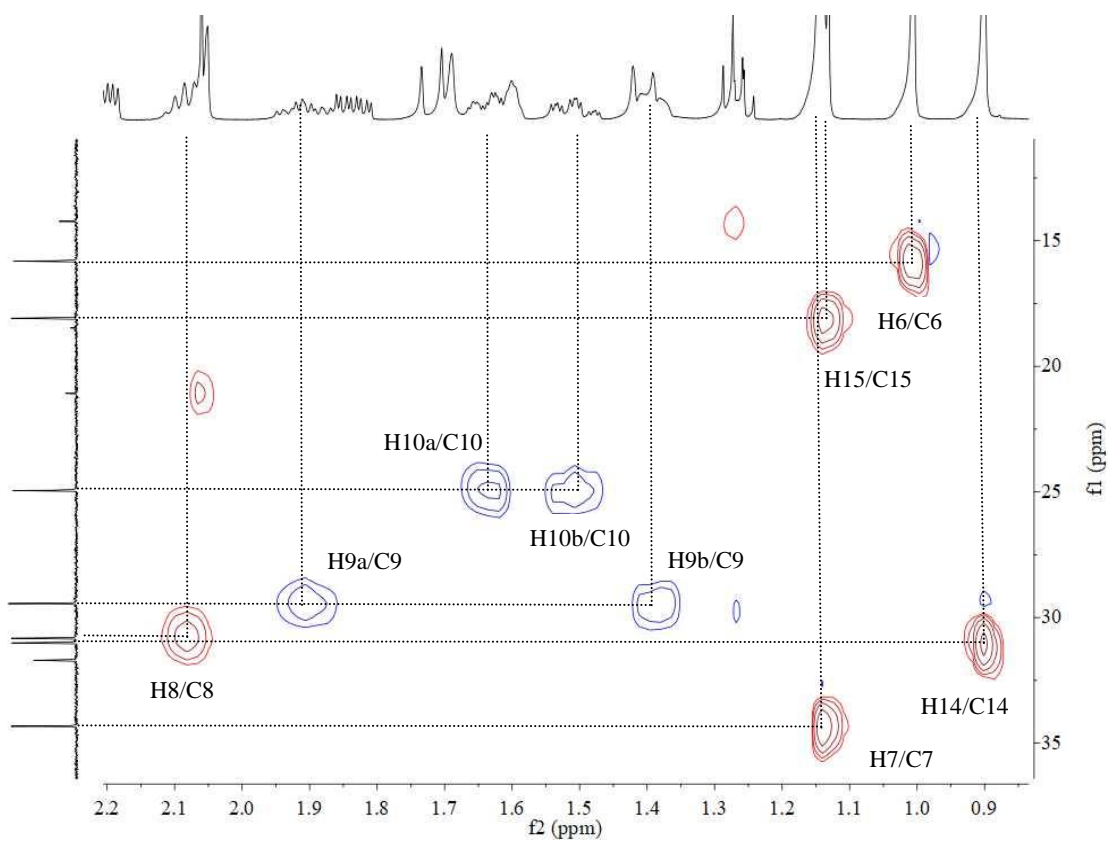


Figure S6: HSQC Spectrum of **1** (isosuberosenol A) (From δ_c 15 ppm to δ_c 35 ppm)

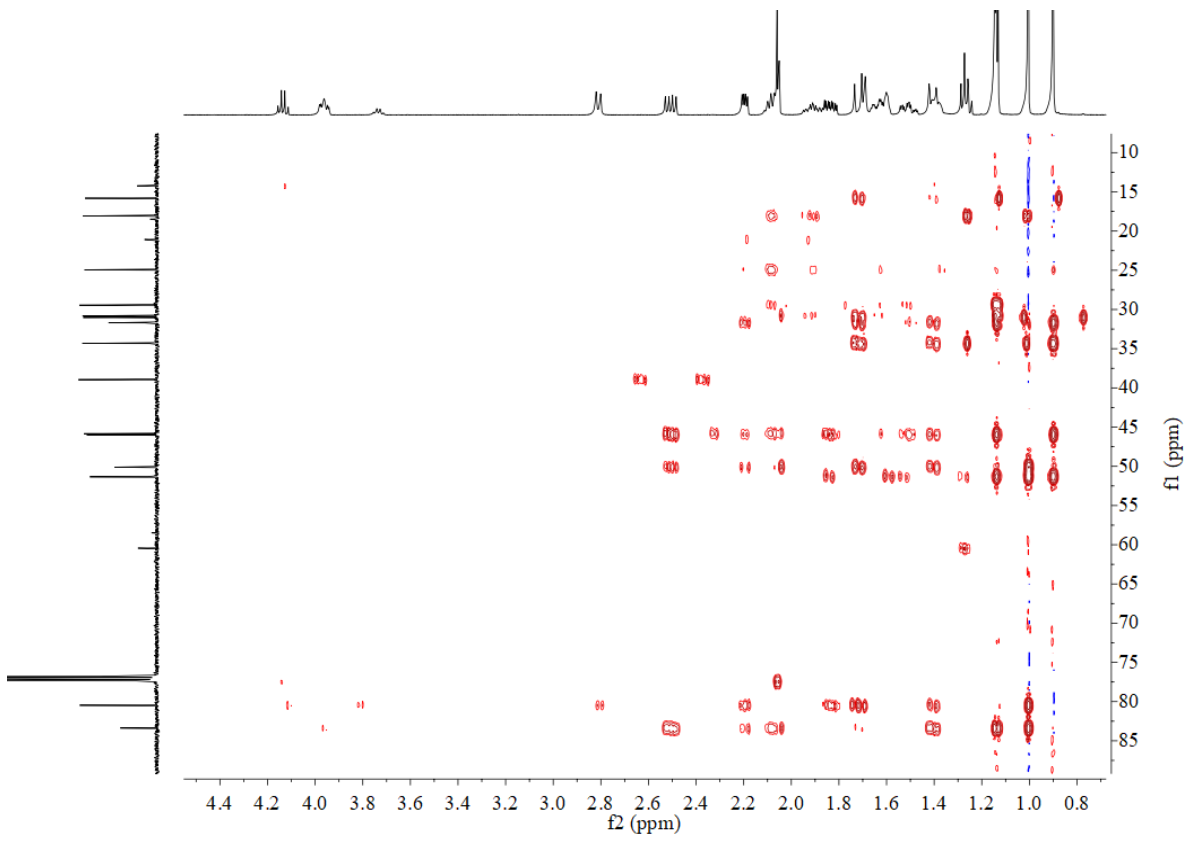


Figure S7: HMBC Spectrum of 1 (isosuberosenol A)

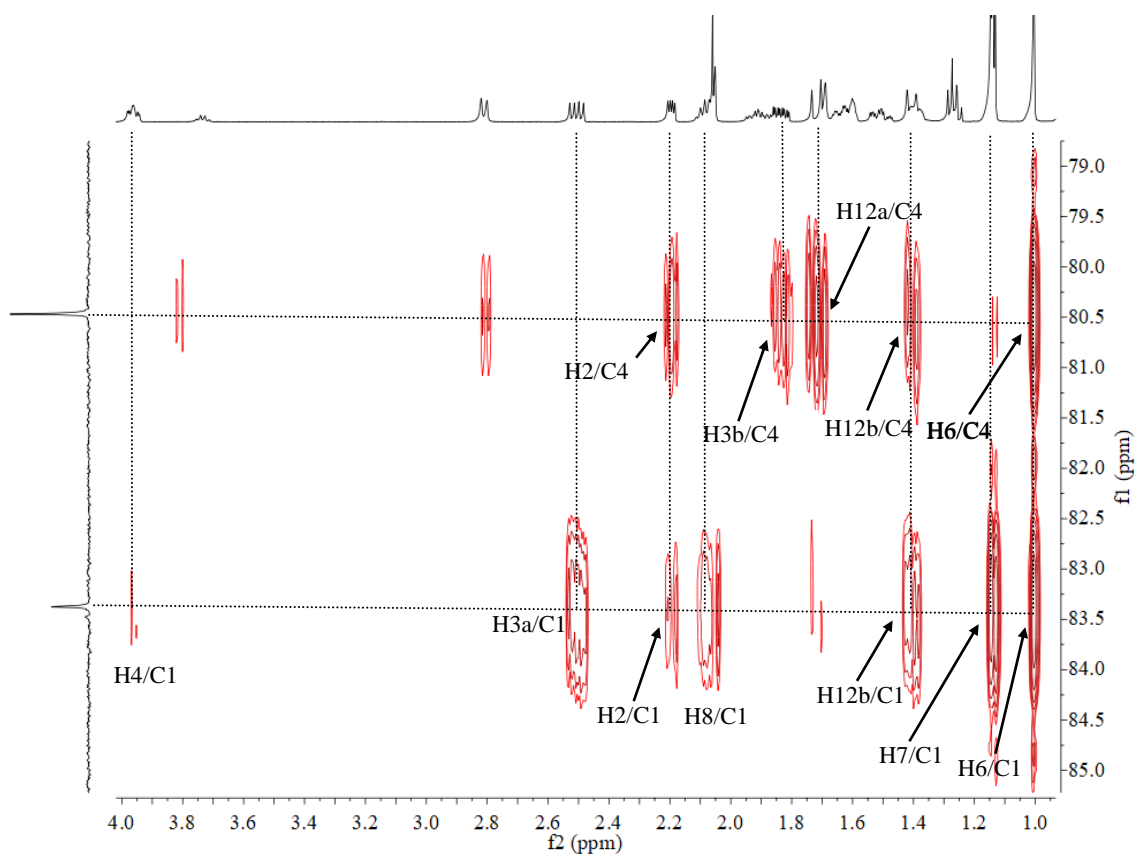


Figure S8: HMBC Spectrum of **1** (isosuberosenol A) (From δ_c 79 ppm to δ_c 85 ppm)

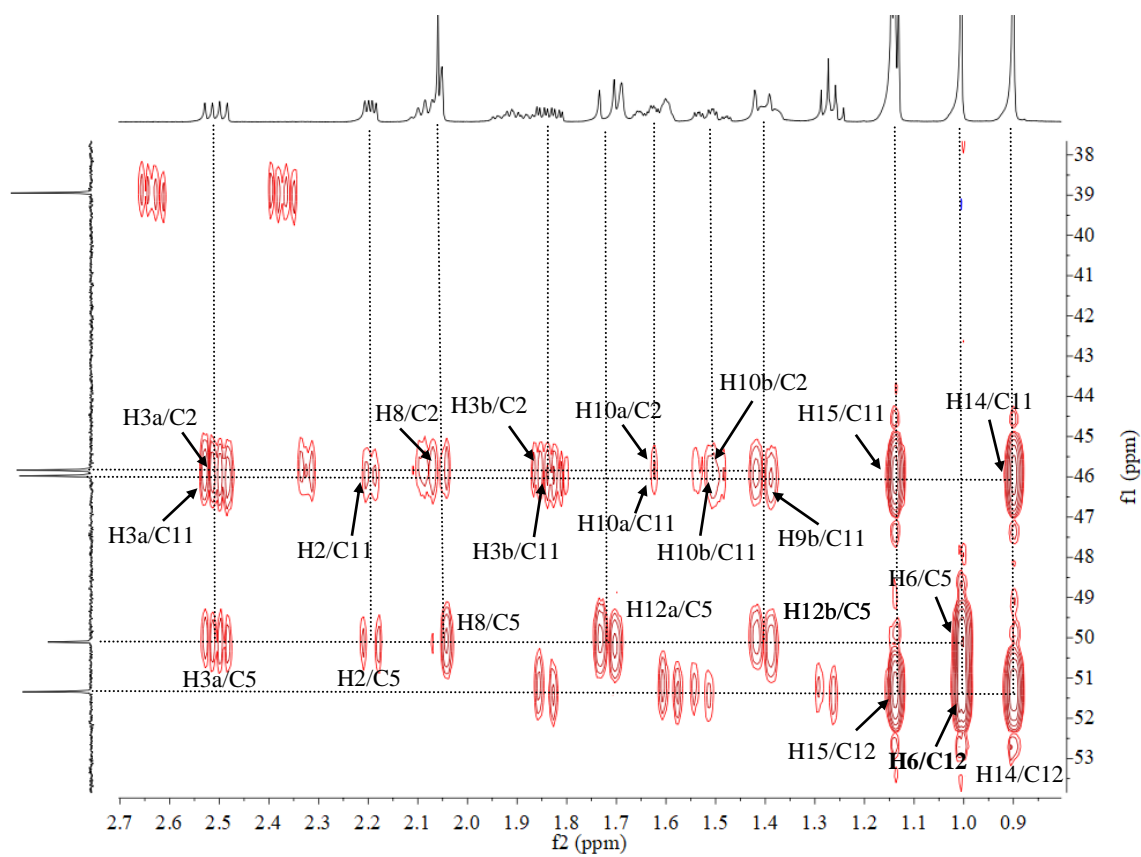


Figure S9: HMBC Spectrum of **1** (isosuberosenol A) (From δ_c 38 ppm to δ_c 53 ppm)

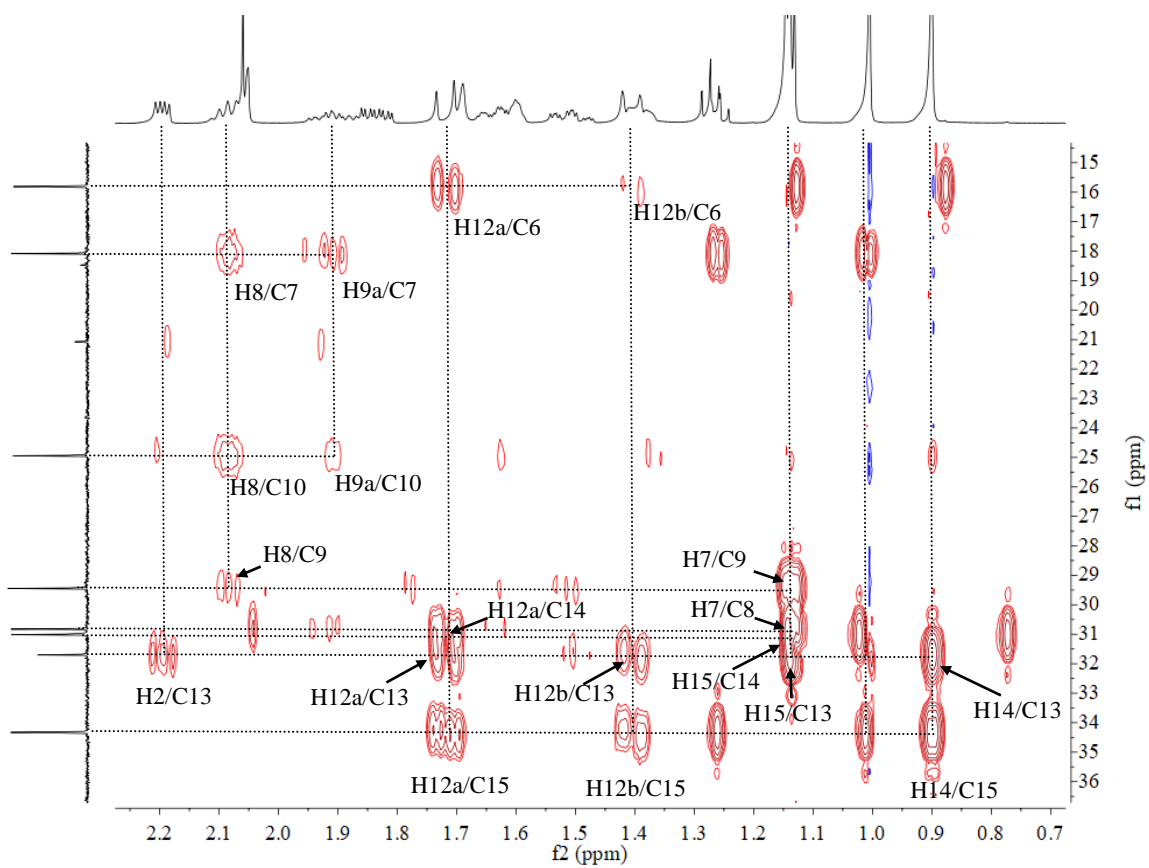


Figure S10: HMBC Spectrum of **1** (isosuberosenol A) (From δ_c 15 ppm to δ_c 36 ppm)

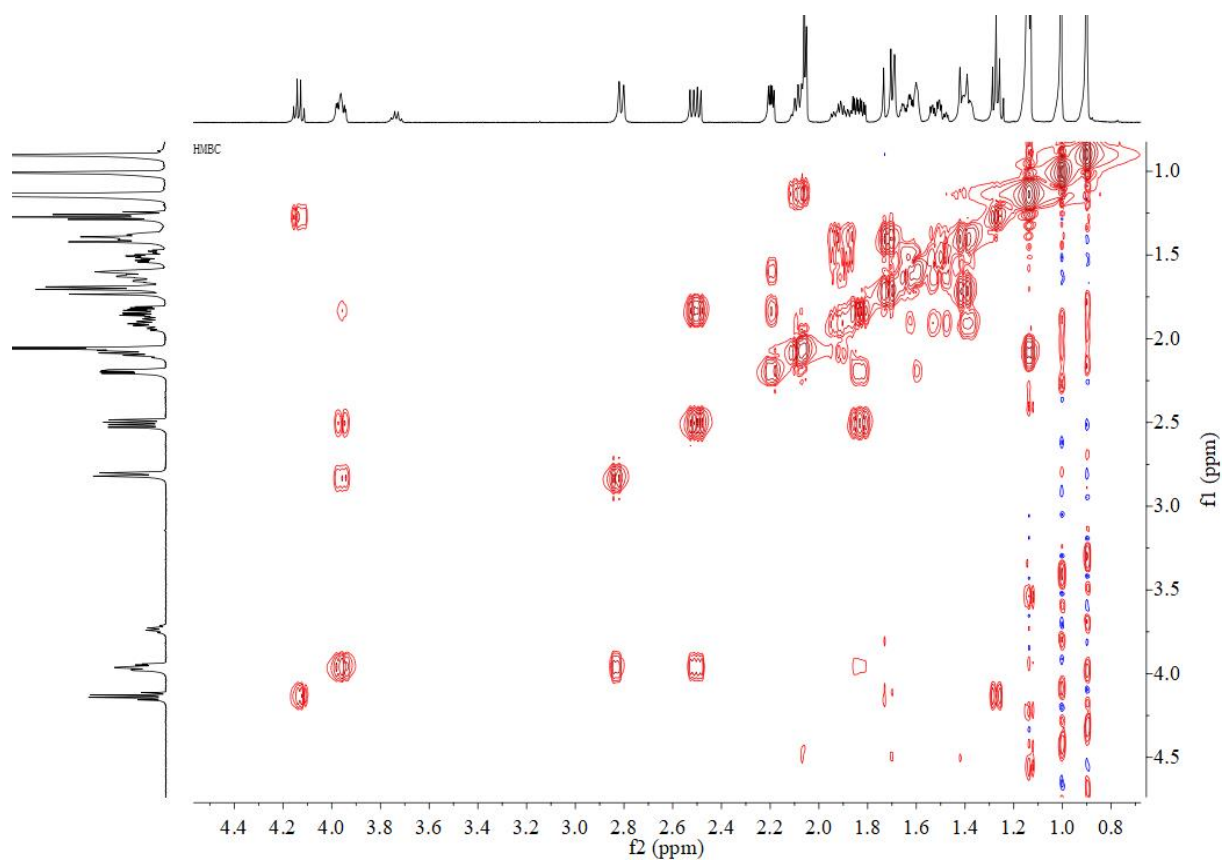


Figure S11: ^1H - ^1H COSY Spectrum of **1** (isosuberosenol A)

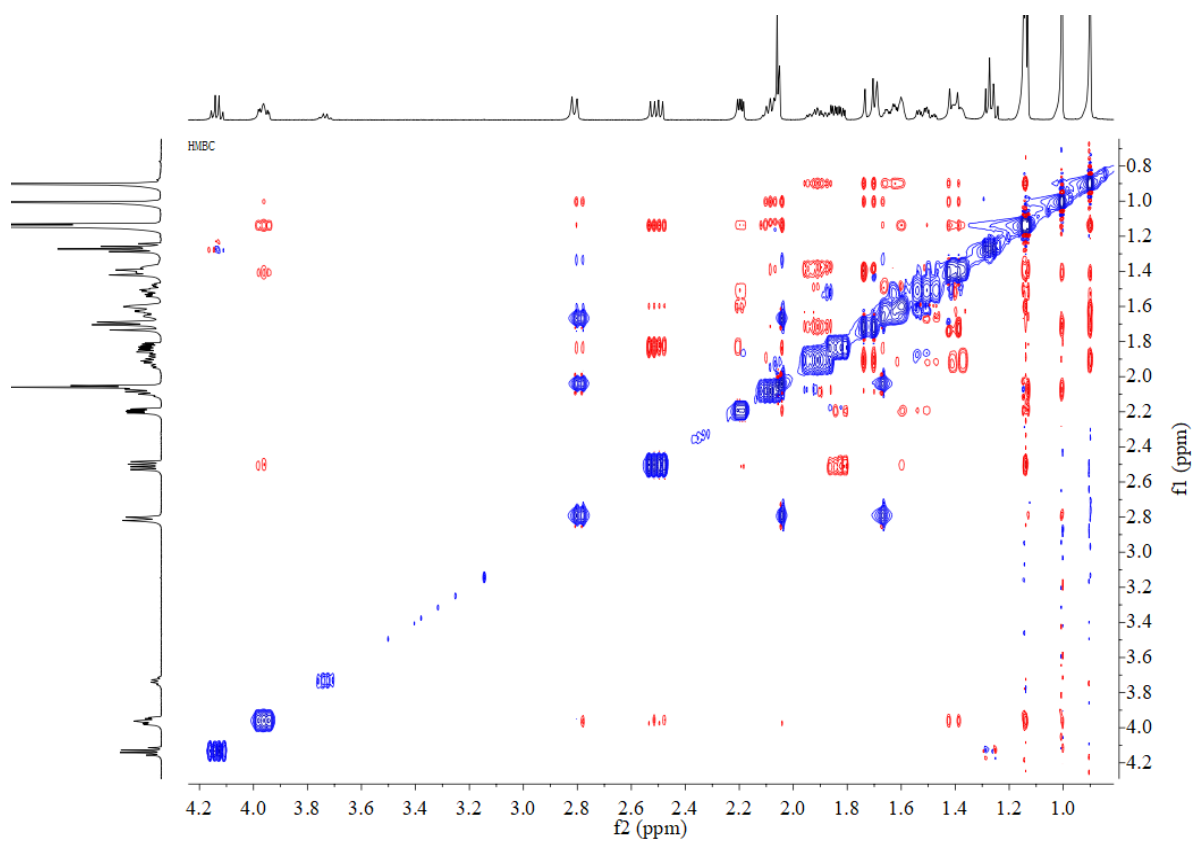


Figure S12: NOESY Spectrum of **1** (isosuberosenol A)

Elemental Composition Report

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)

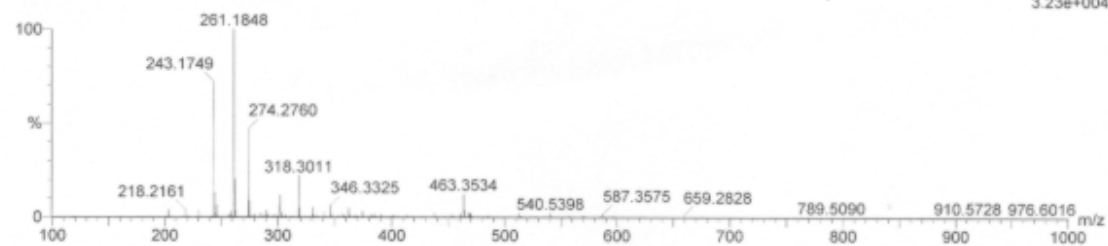
Elements Used:

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)

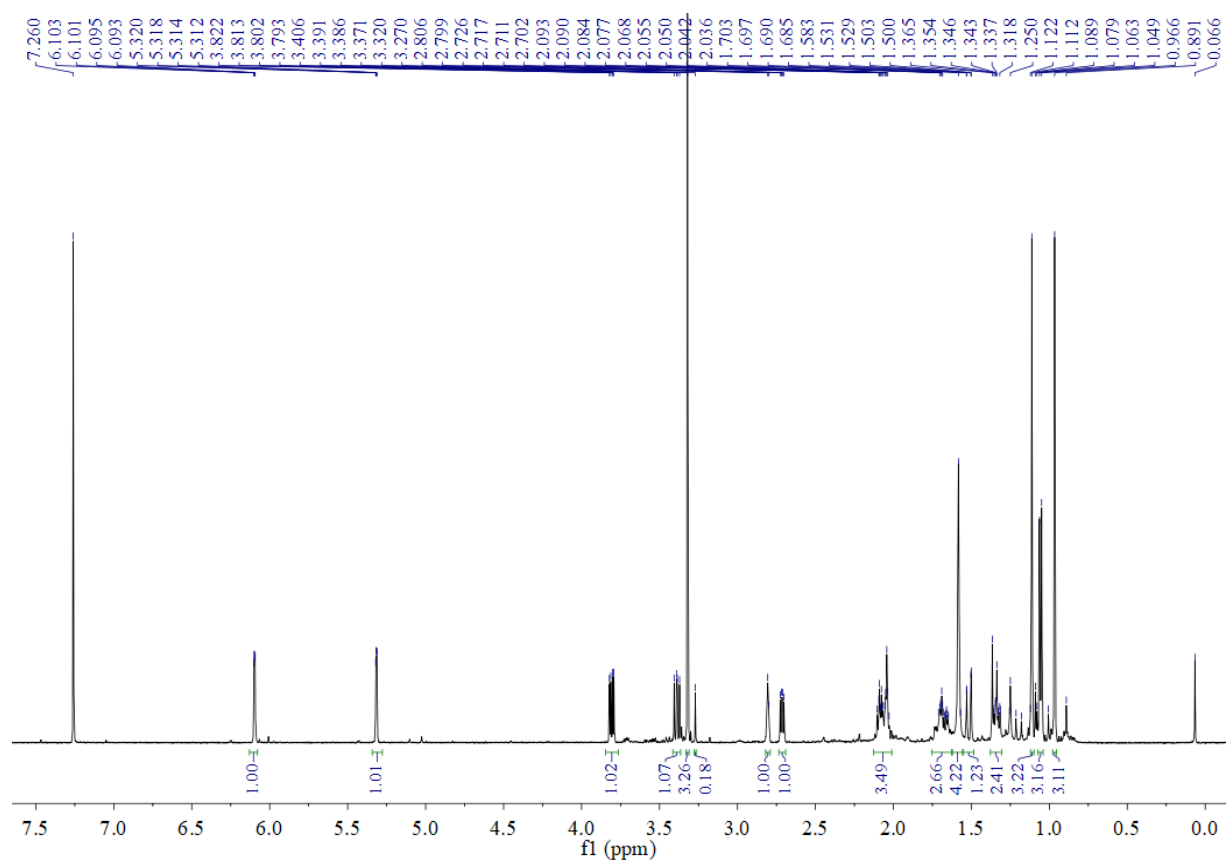


Figure S14: ¹H-NMR (500 MHz, CDCl₃) Spectrum of **2** (suberosain A)

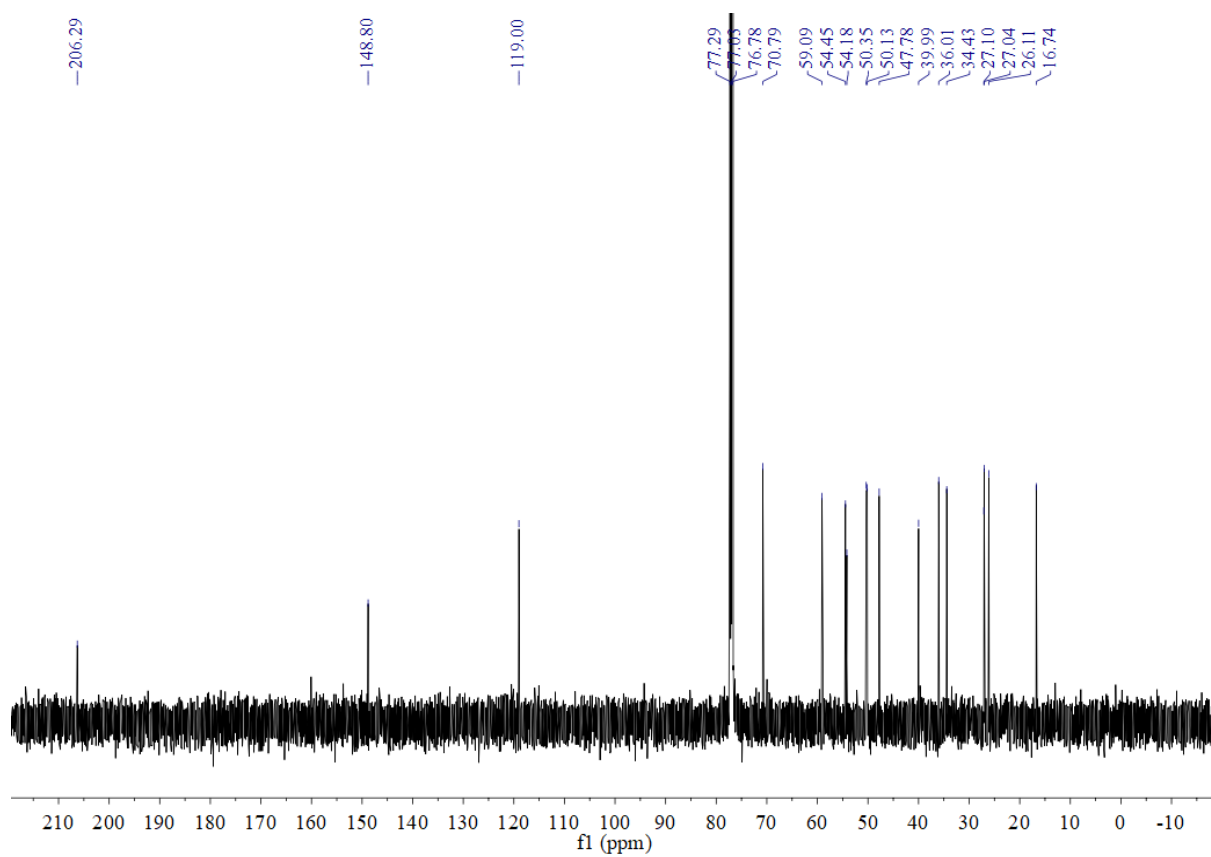


Figure S15: ^{13}C -NMR (125 MHz, CDCl_3) Spectrum of **2** (suberosain A)

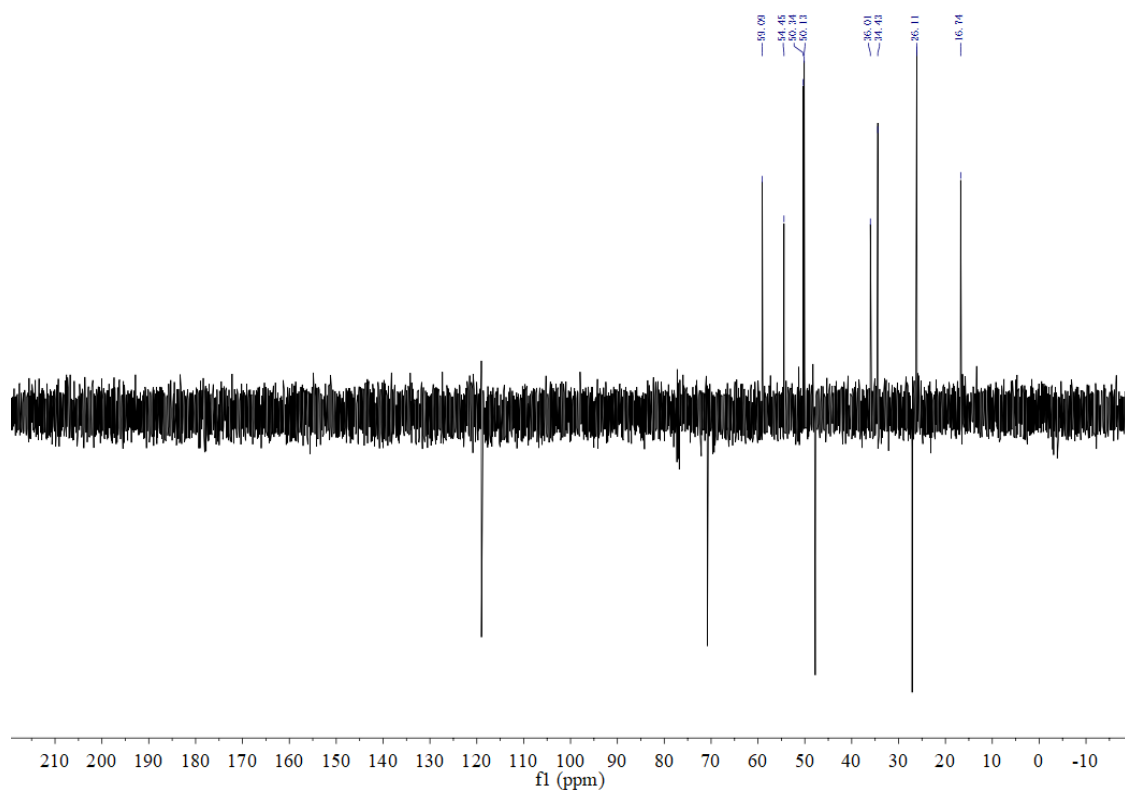


Figure S16: DEPT135 (125 MHz, CDCl₃) Spectrum of **2** (suberosain A)

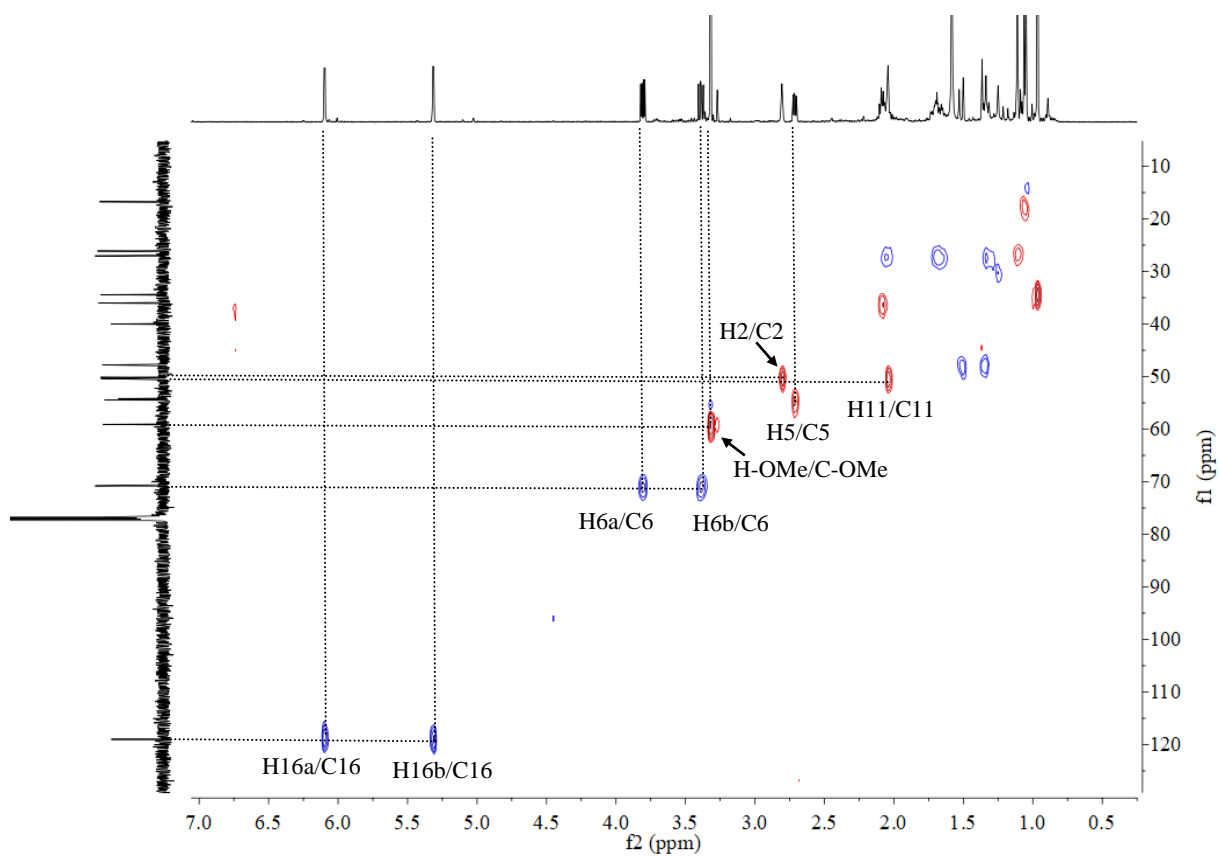


Figure S17: HSQC Spectrum of 2 (suberosain A)

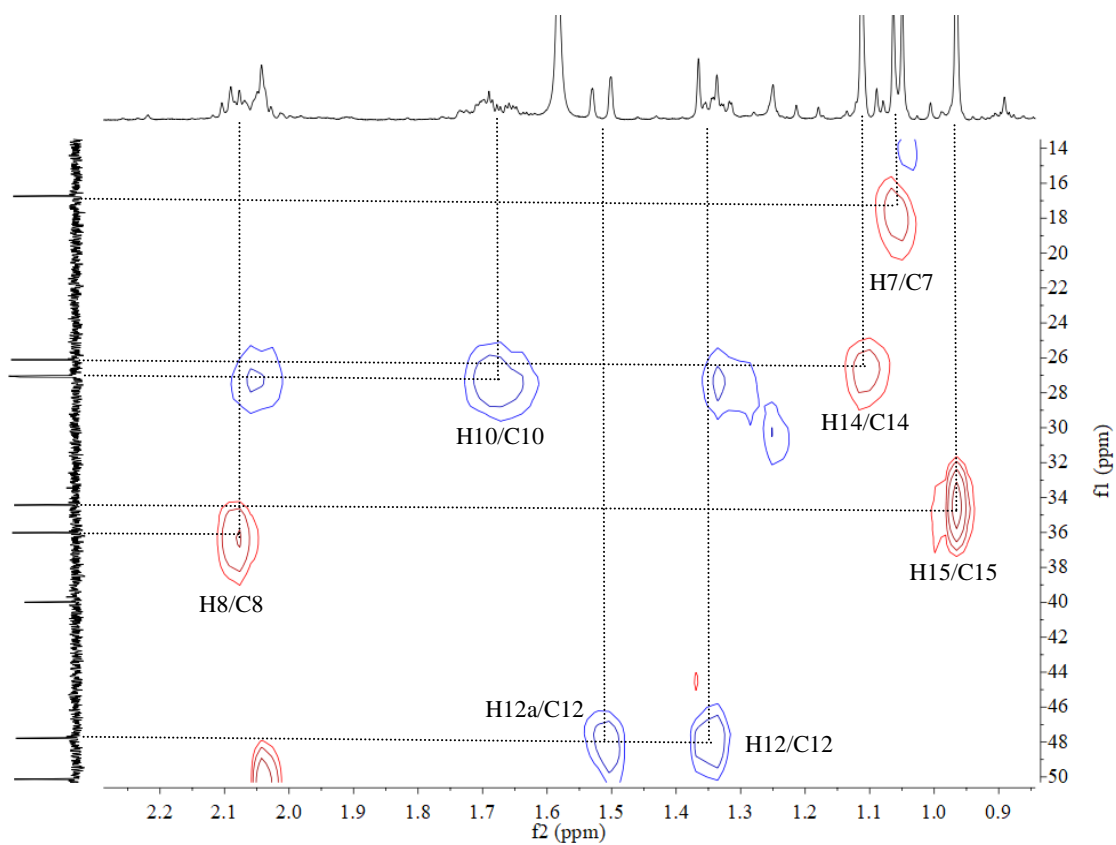


Figure S18: HSQC Spectrum of **2** (suberosain A) (From δ_{C} 14 ppm to 50 ppm)

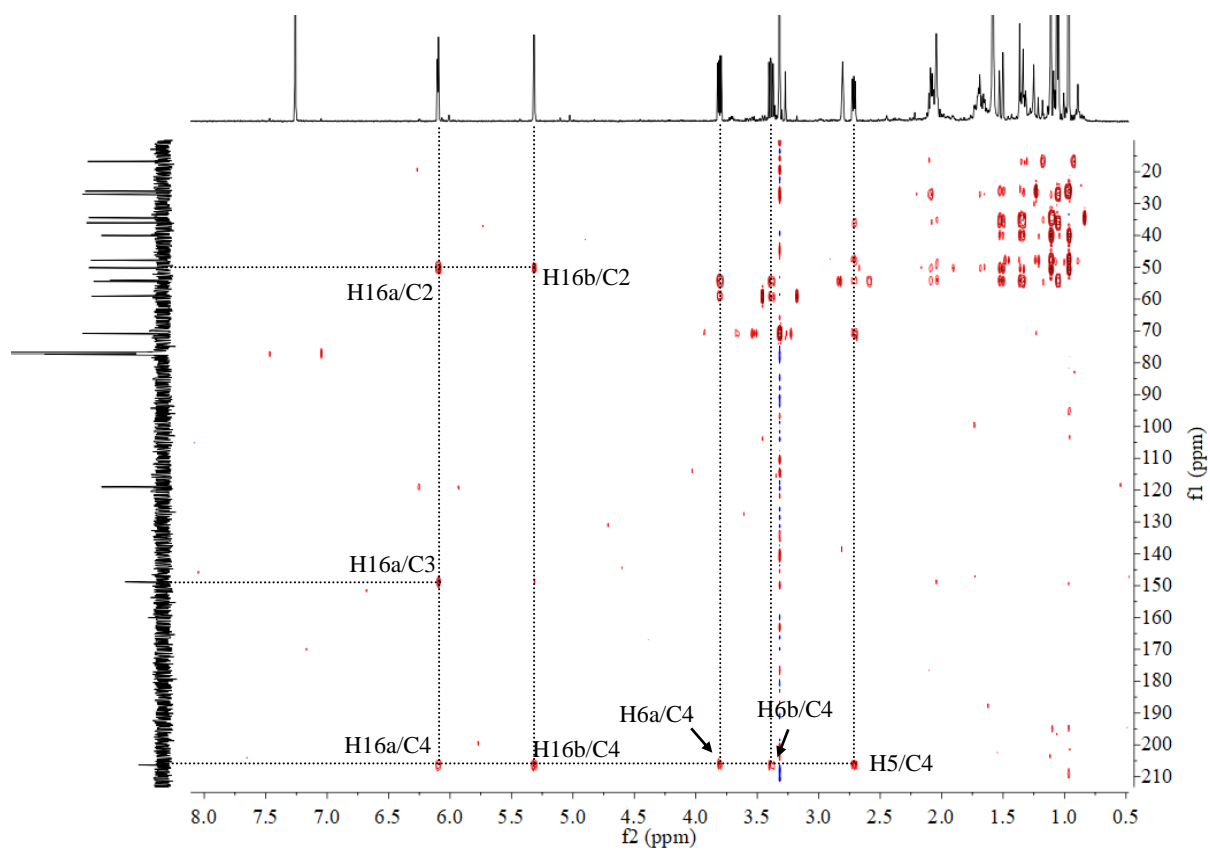


Figure S19: HMBC Spectrum of **2** (suberosain A)

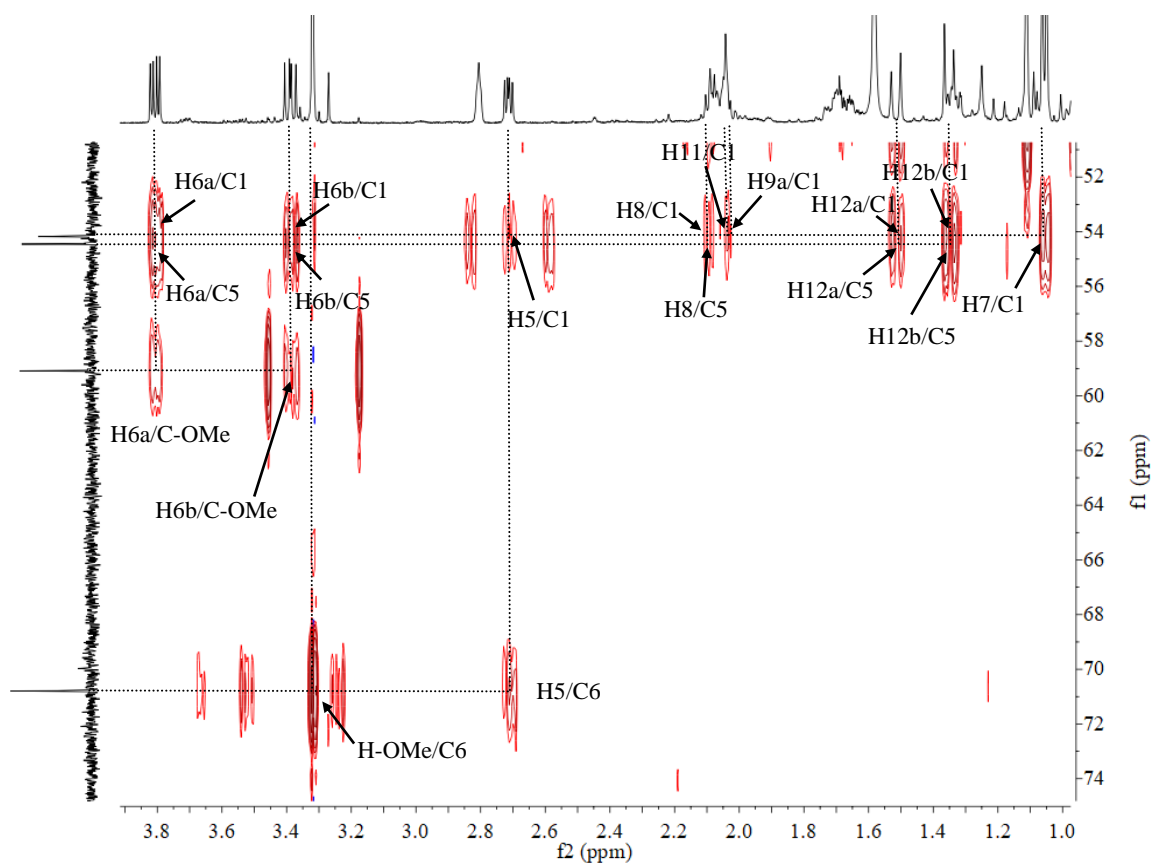


Figure S20: HMBC Spectrum of **2** (suberosain A) (From δ^C 52 ppm to 75 ppm)

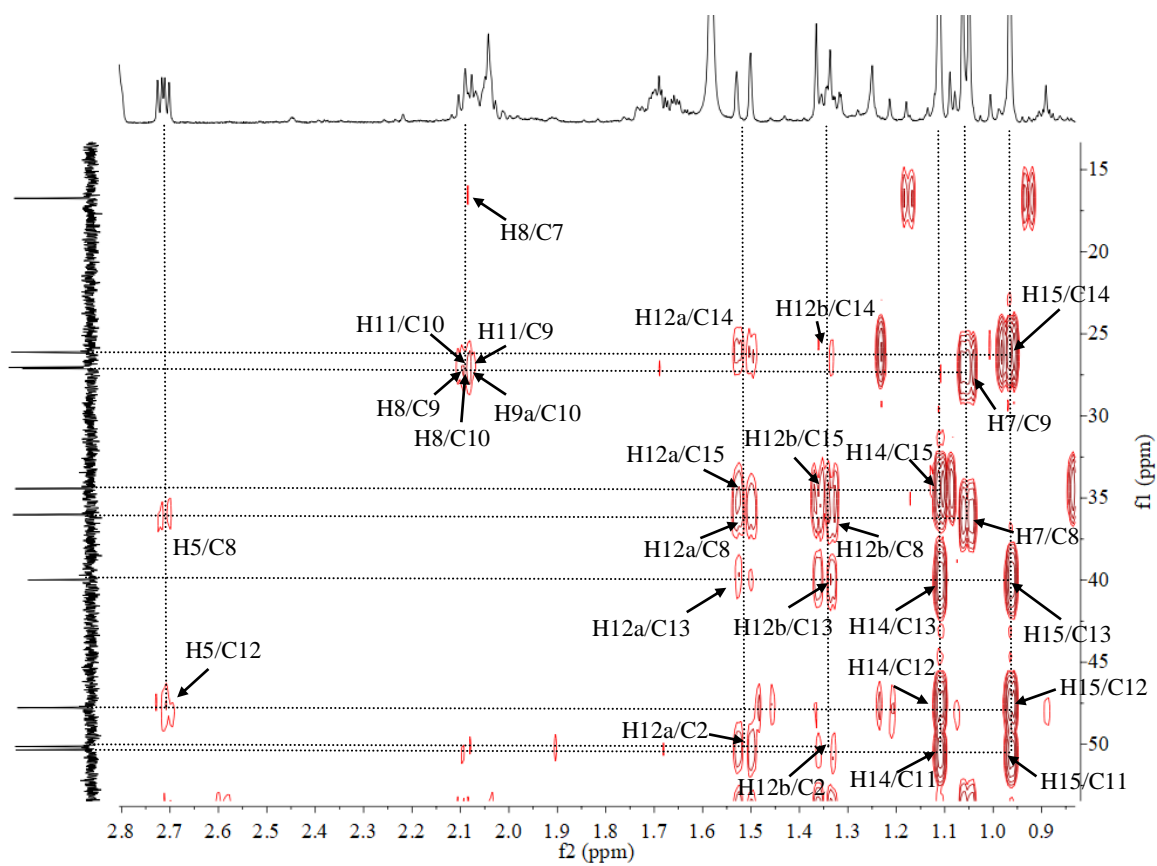


Figure S21: HMBC Spectrum of **2** (suberosain A) (From δ_c 15 ppm to 50 ppm)

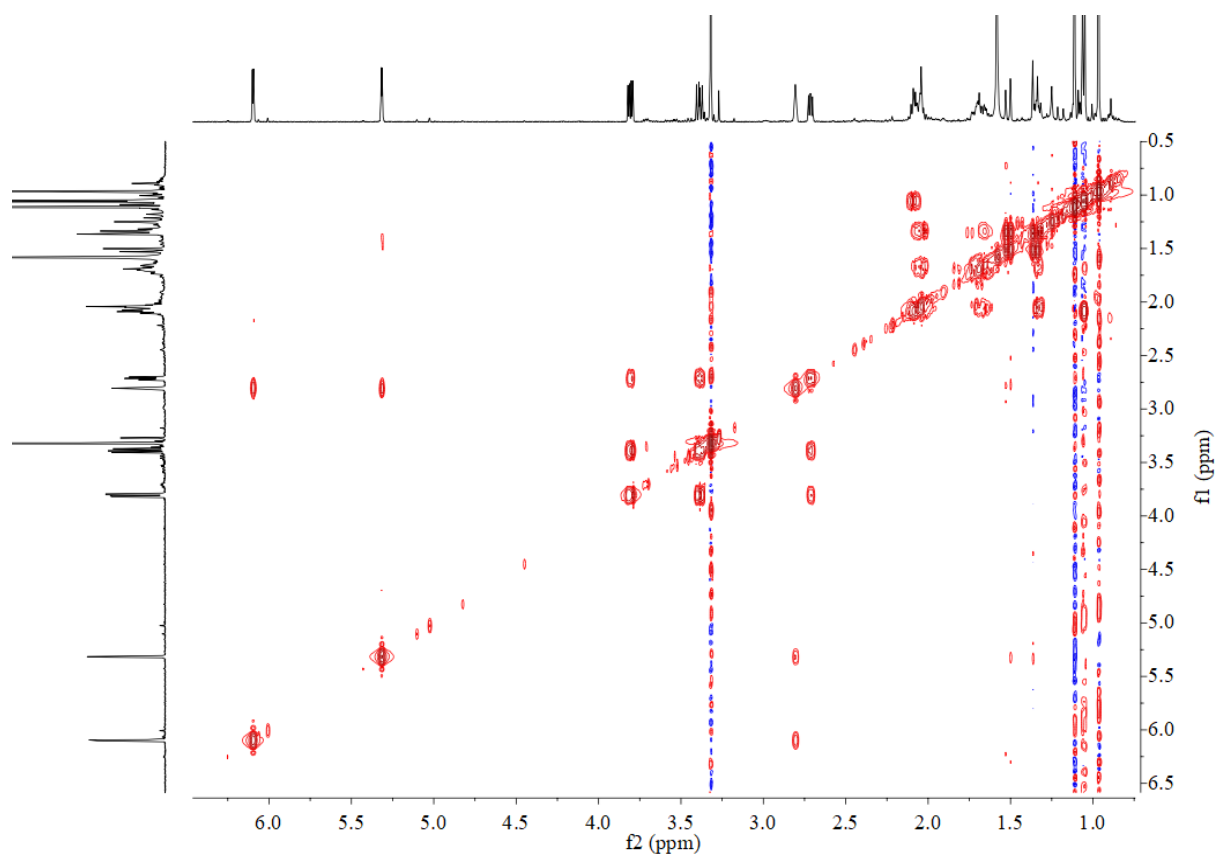


Figure S22: ^1H - ^1H COSY Spectrum of **2** (suberosain A)

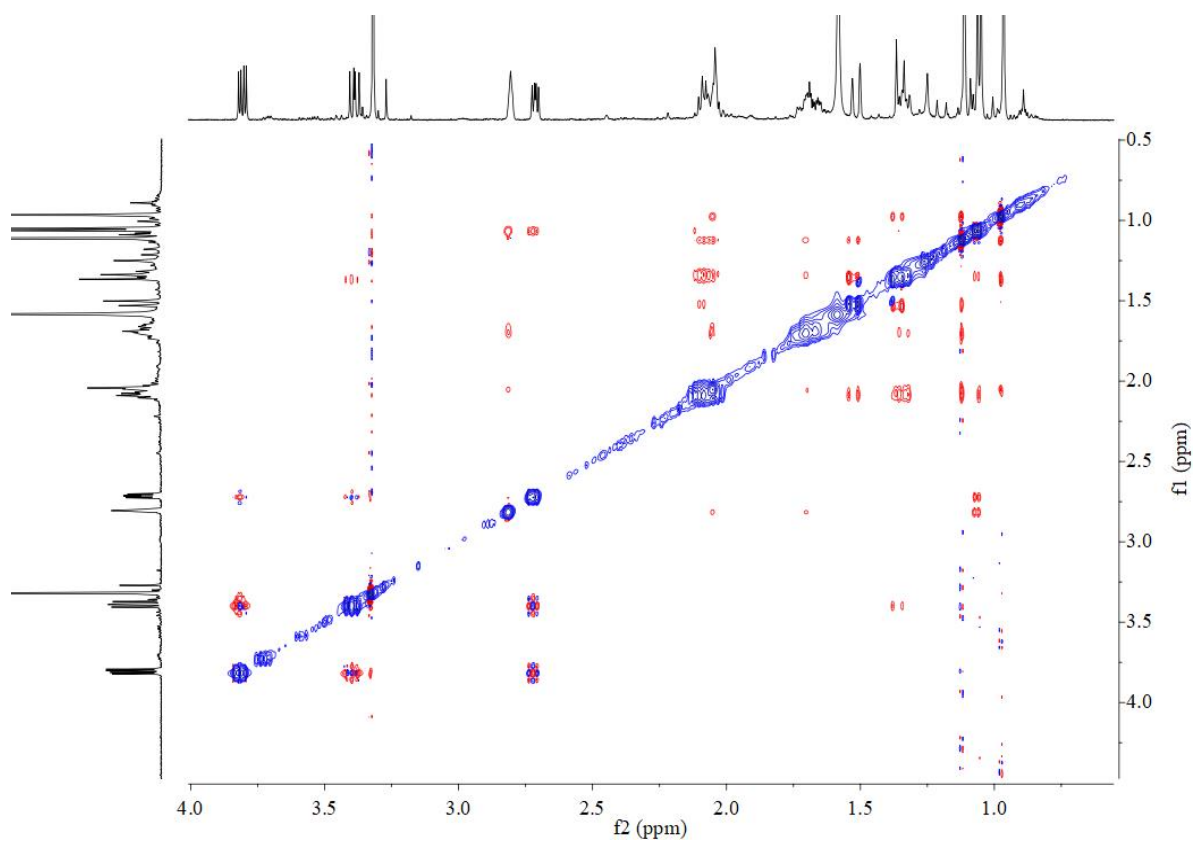


Figure S23: NOESY Spectrum of **2** (suberosain A)

Elemental Composition Report

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)

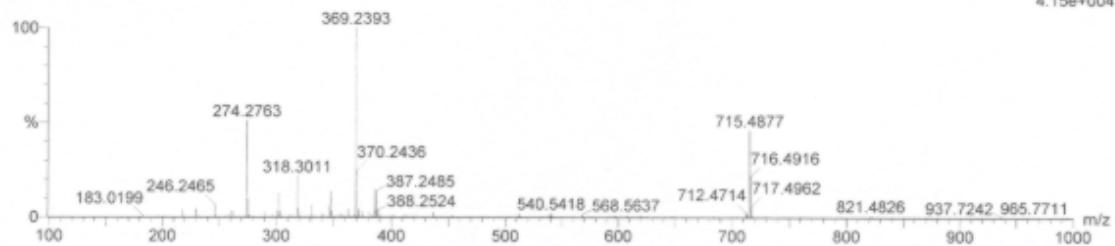
Elements Used:

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: -1.5
Maximum: 5.0 10.0 50.0

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)

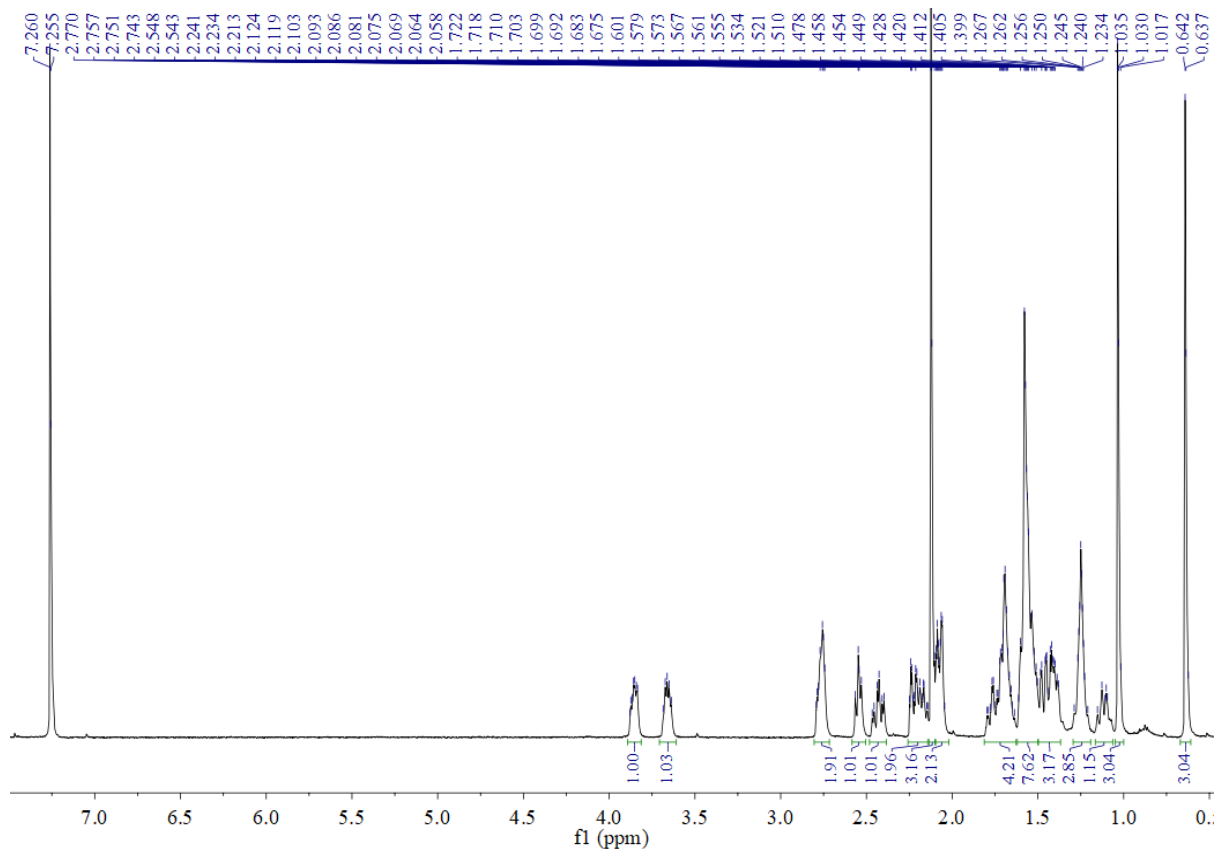


Figure S25: $^1\text{H-NMR}$ (500 MHz, CDCl_3) Spectrum of **3** (4-hydroxymethyl-5 β -pregnan-3, 20-dione)

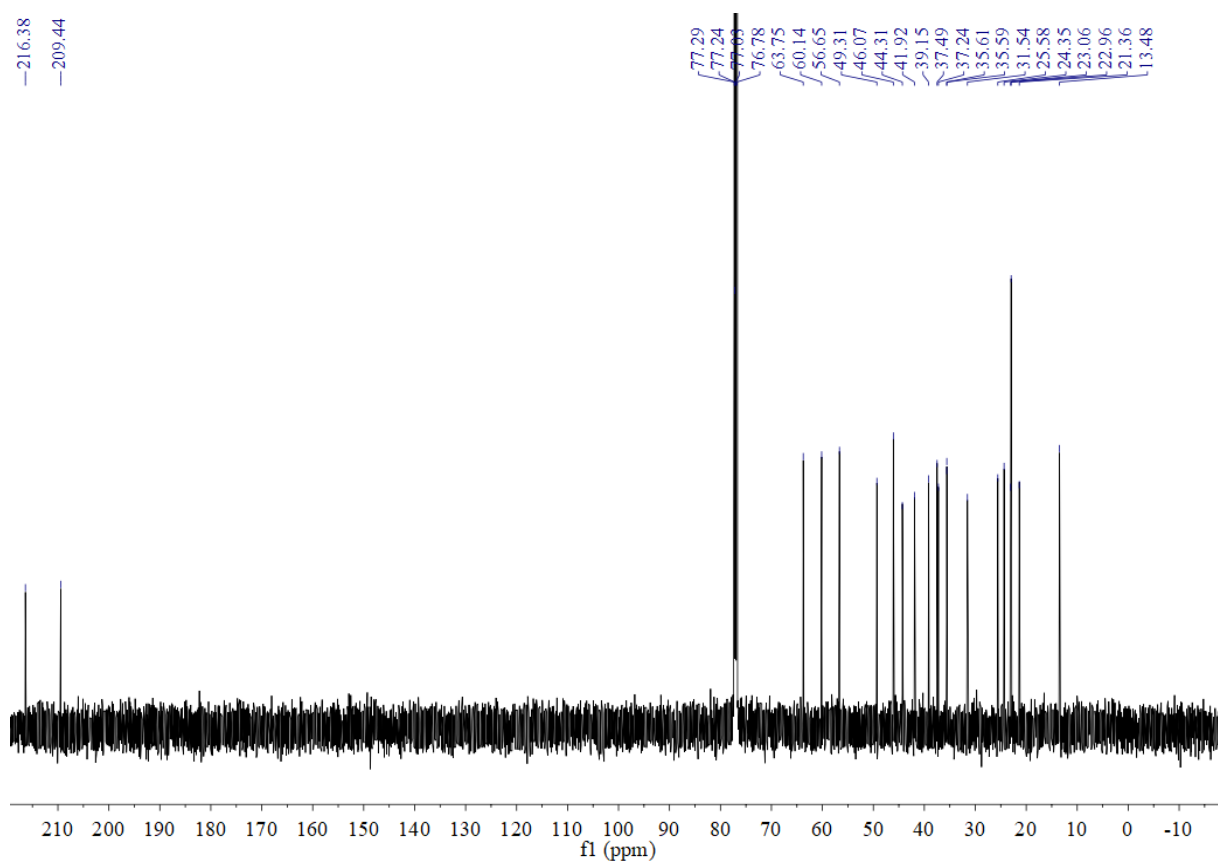


Figure S26: ^{13}C -NMR (125 MHz, CDCl_3) Spectrum of **3** (4-hydroxymethyl-5 β -pregnan-3, 20-dione)

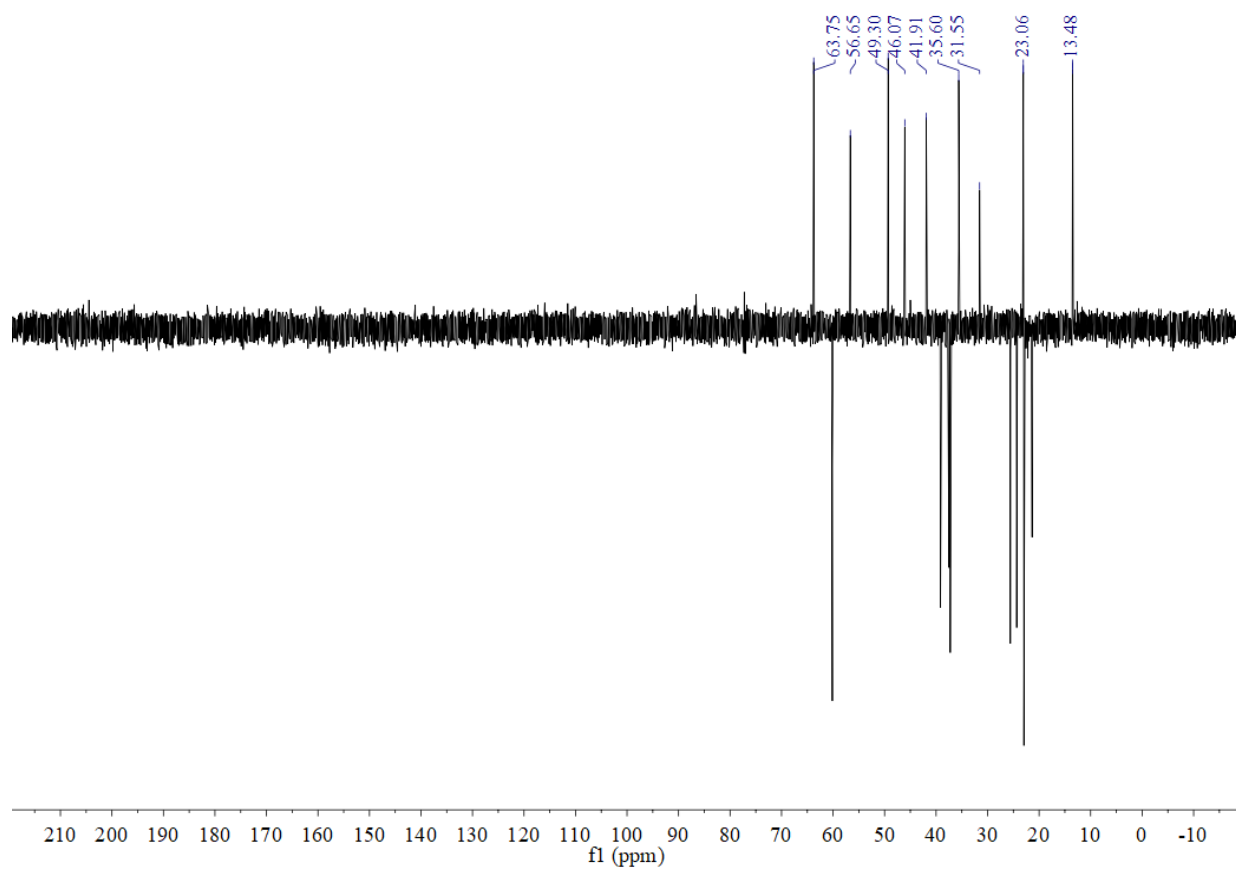


Figure S27: DEPT135 (125 MHz, CDCl₃) Spectrum of **3** (4-hydroxymethyl-5 β -pregnan-3, 20-dione)

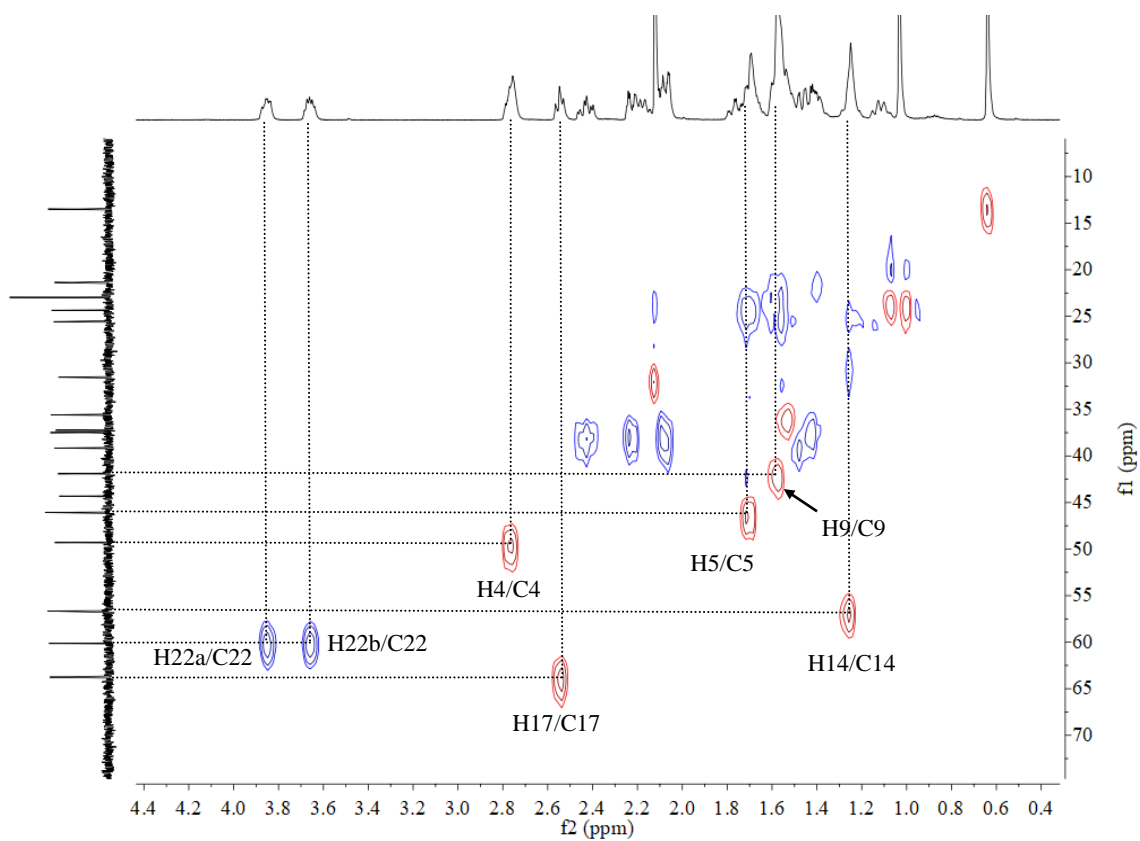


Figure S28: HSQC Spectrum of **3** (4-hydroxymethyl-5 β -pregnan-3, 20-dione)

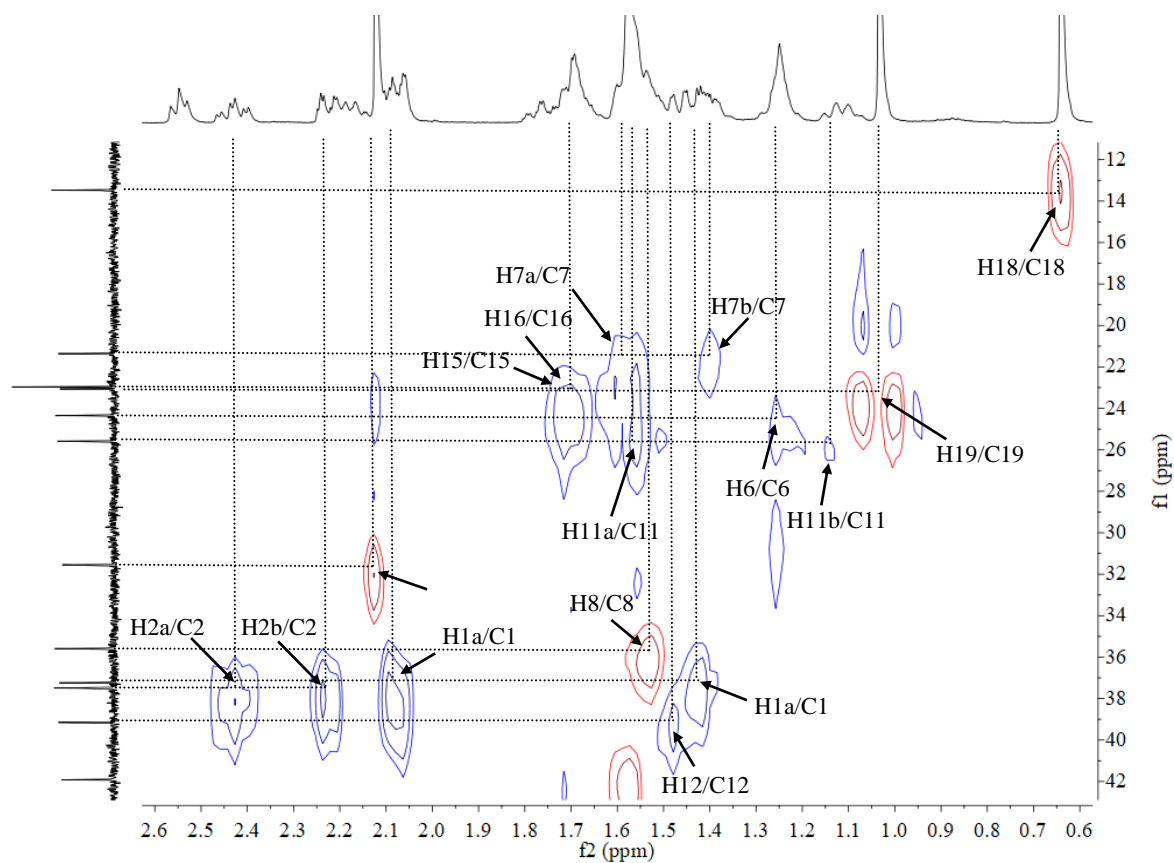


Figure S29: HSQC Spectrum of **3** (4-hydroxymethyl-5 β -pregnan-3, 20-dione) (From δ_c 12 to 42)

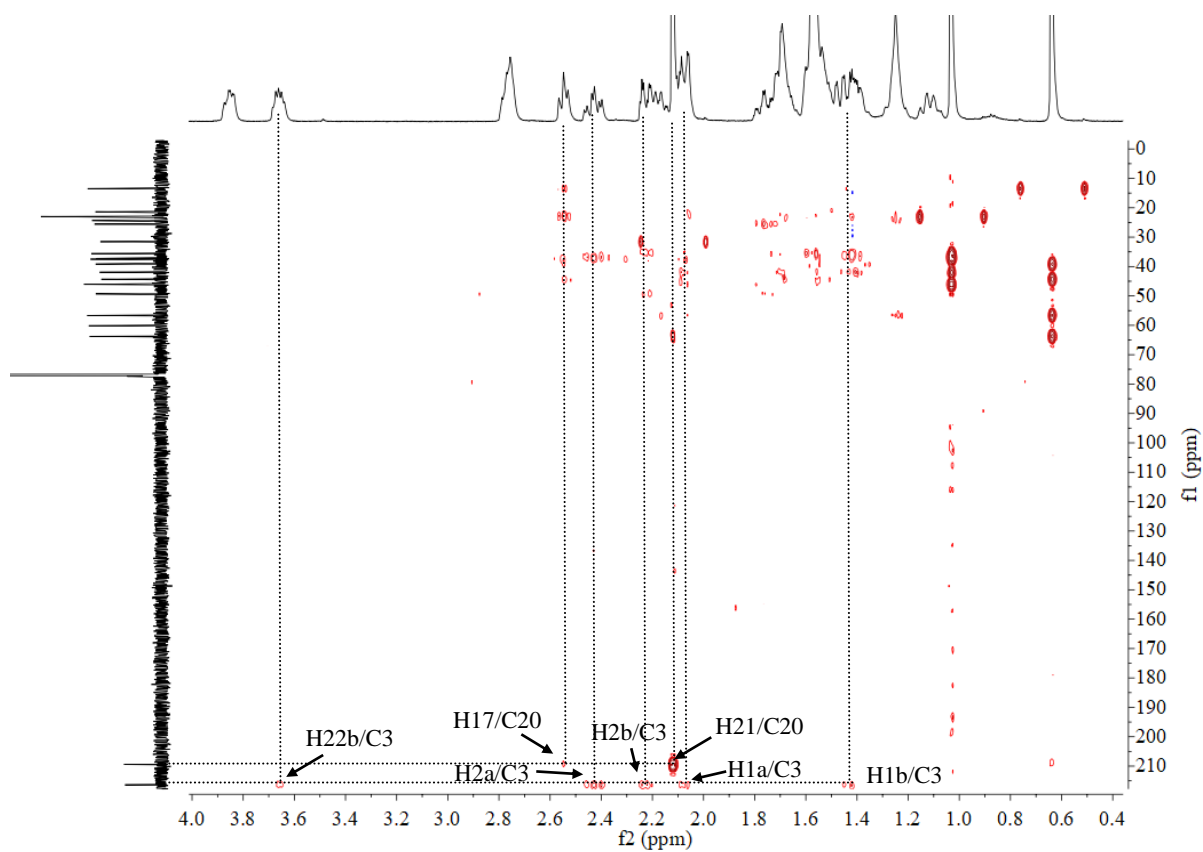


Figure S30: HMBC Spectrum of **3** (4-hydroxymethyl-5 β -pregnan-3, 20-dione)

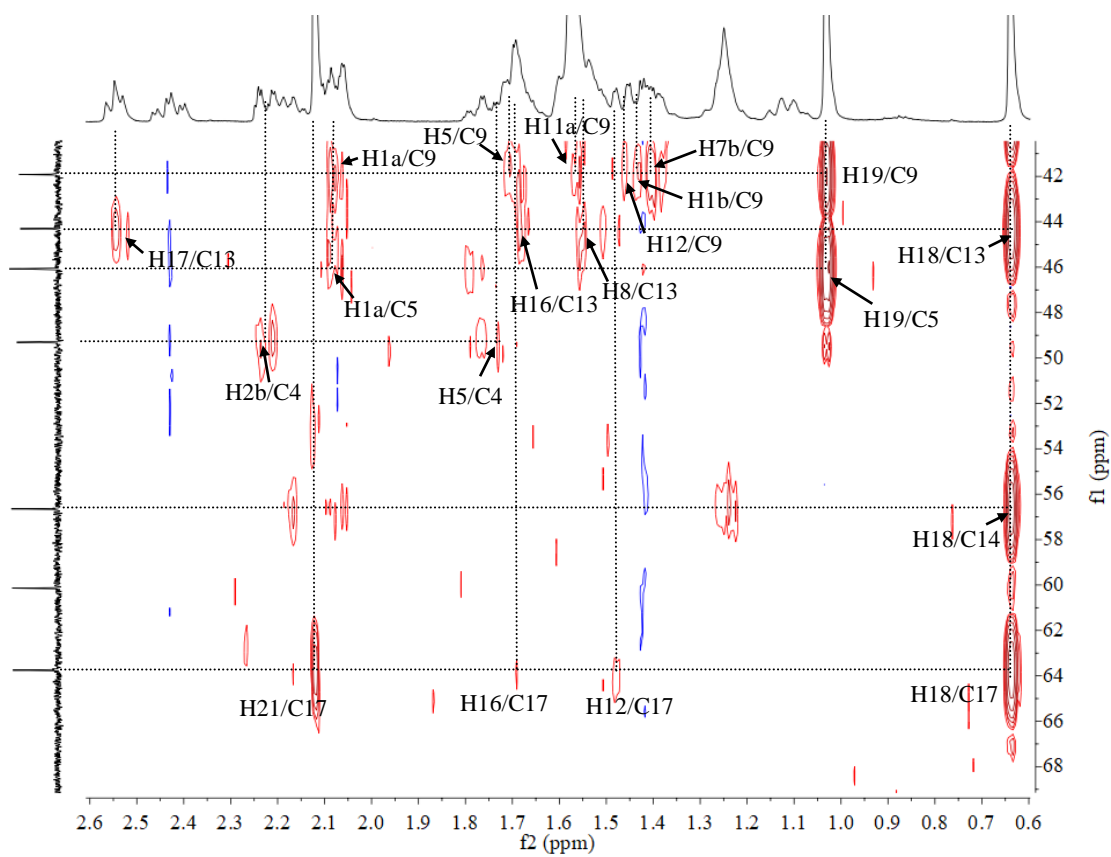


Figure S31: HMBC Spectrum of **3** (4-hydroxymethyl-5 β -pregnan-3, 20-dione) (From δ_c 42 to 70)

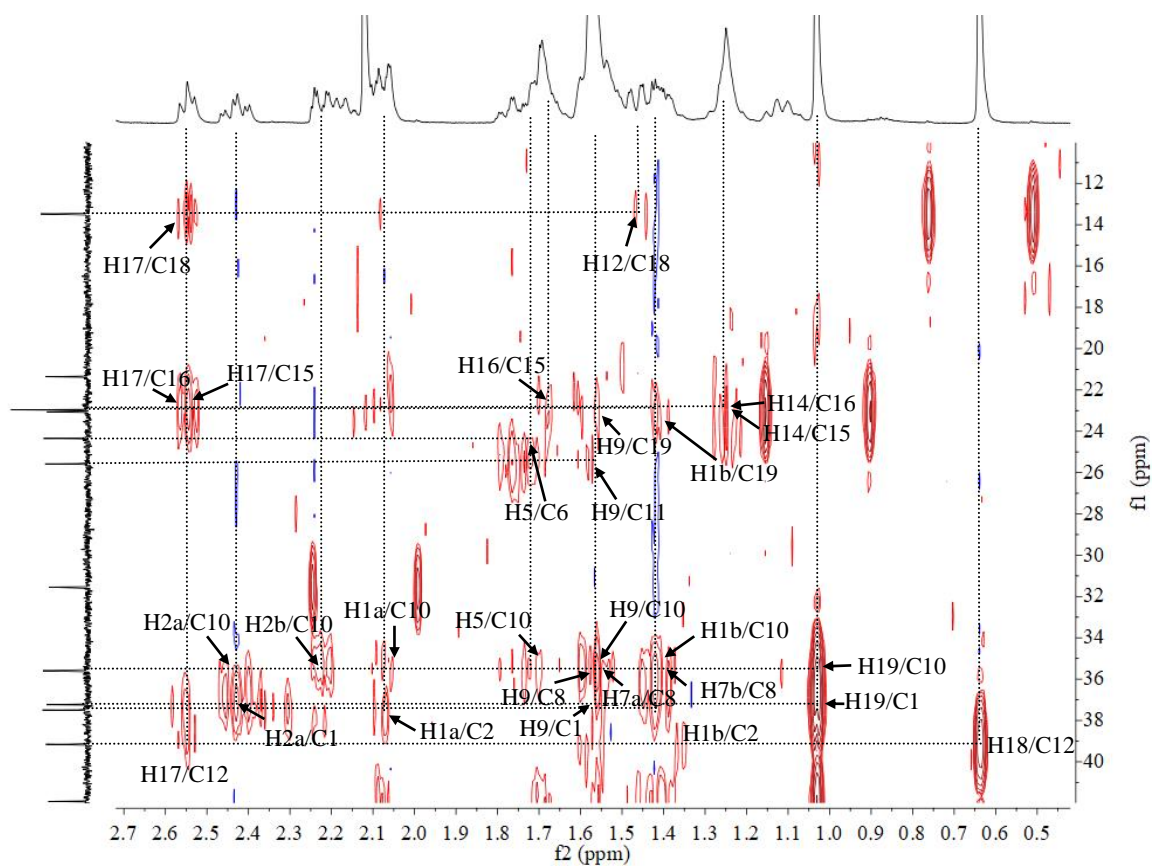


Figure S32: HMBC Spectrum of 3 (4-hydroxymethyl-5 β -pregnan-3, 20-dione) (From δ_C 12 to 40)

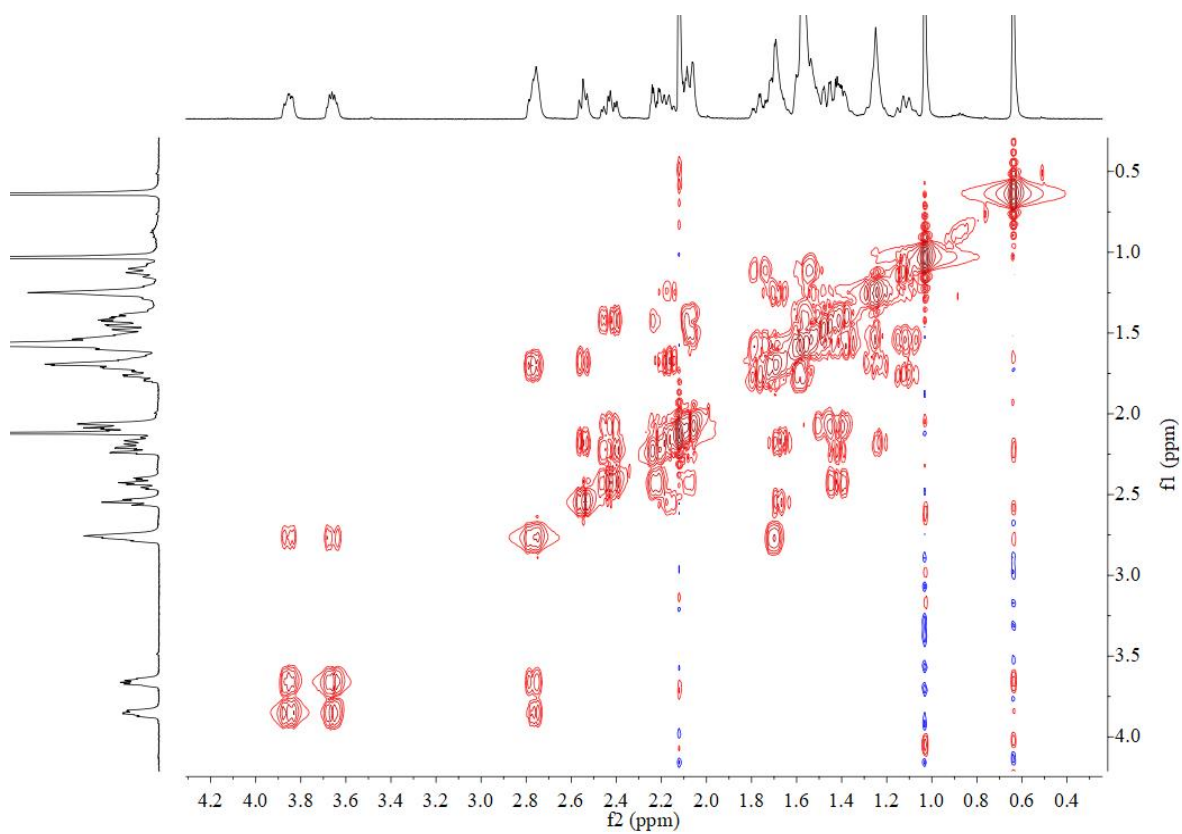


Figure S33: ^1H - ^1H COSY Spectrum of **3** (4-hydroxymethyl-5 β -pregnan-3, 20-dione)

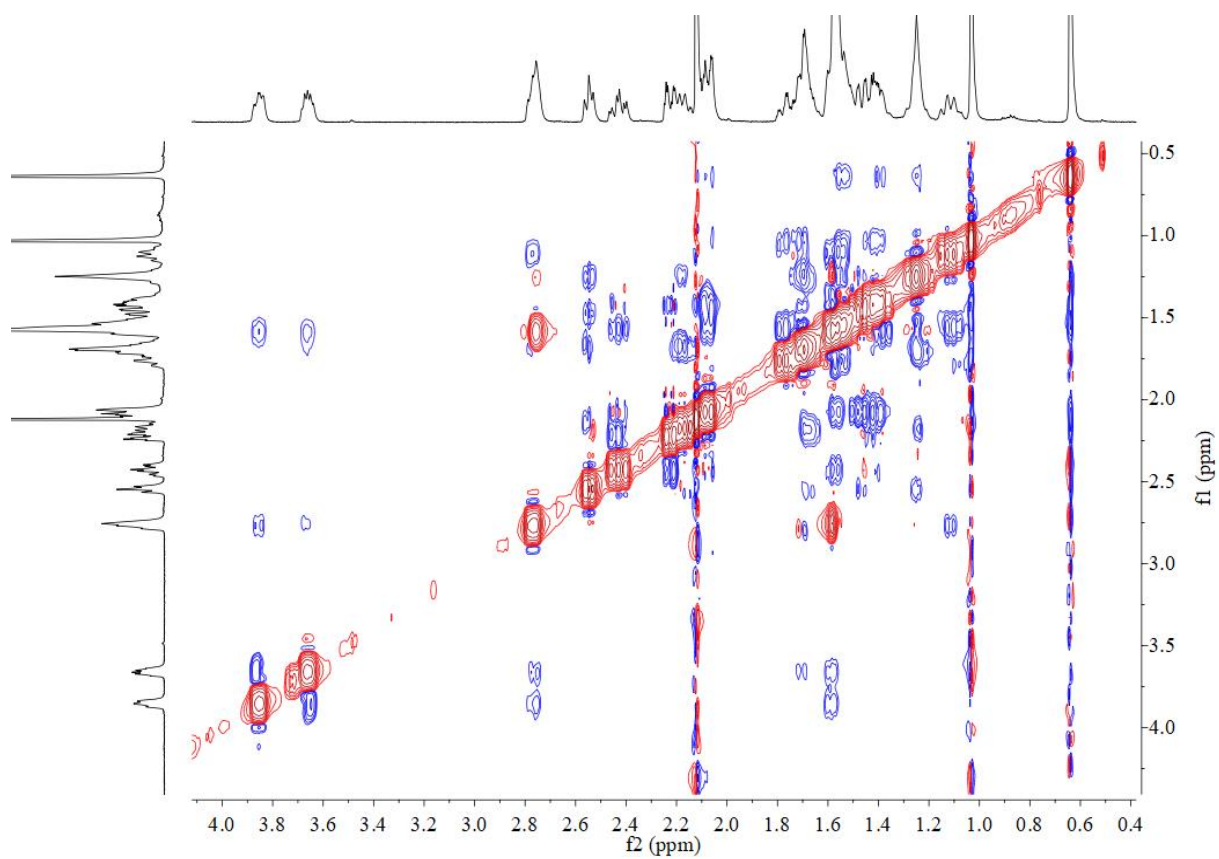


Figure S34: NOESY Spectrum of **3** (4-hydroxymethyl-5 β -pregnan-3, 20-dione)