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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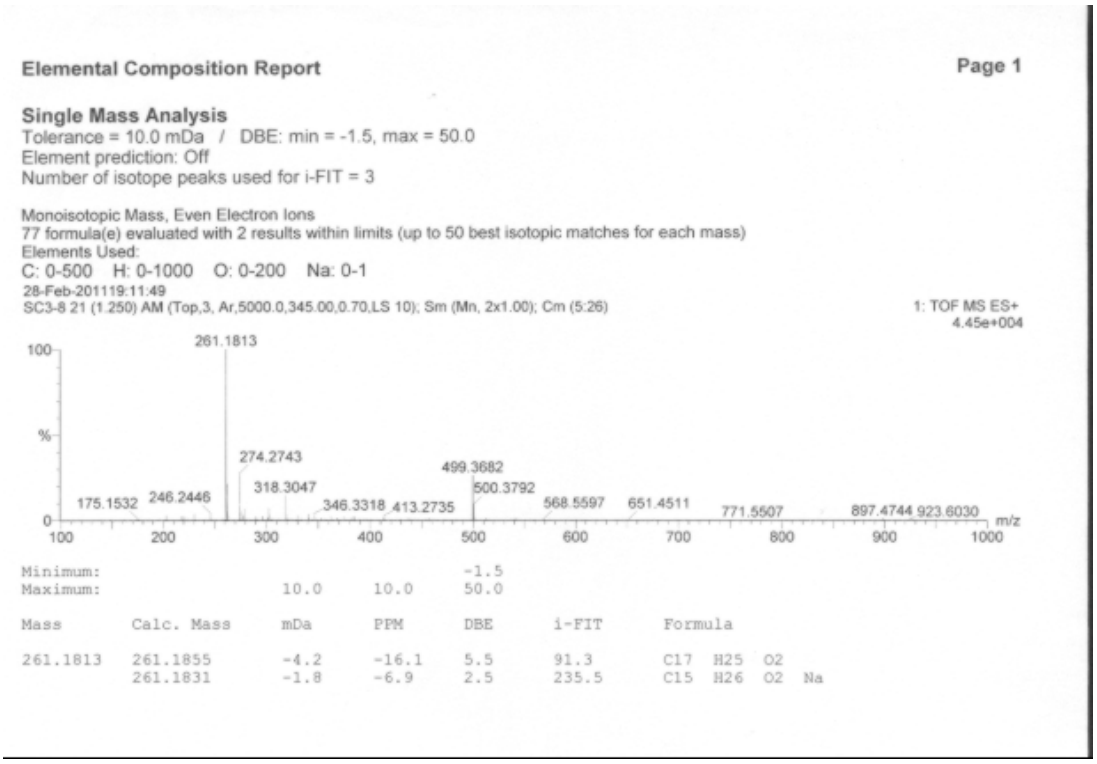


Figure S1: HR-ESI-MS Spectrum of **1** (isosuberosenol A)

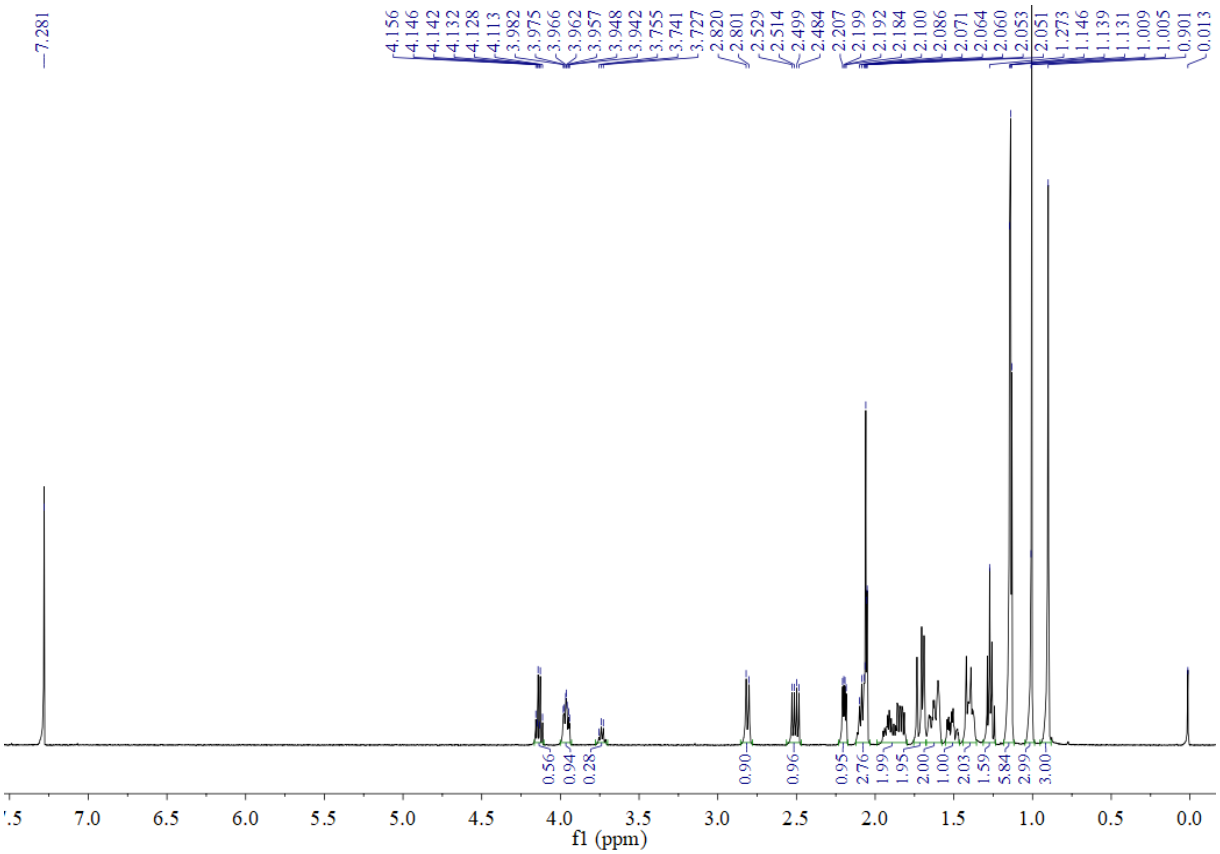


Figure S2: ^{1}H-NMR (500 MHz, $CDCl_3$) Spectrum of **1** (isosuberosenol A)

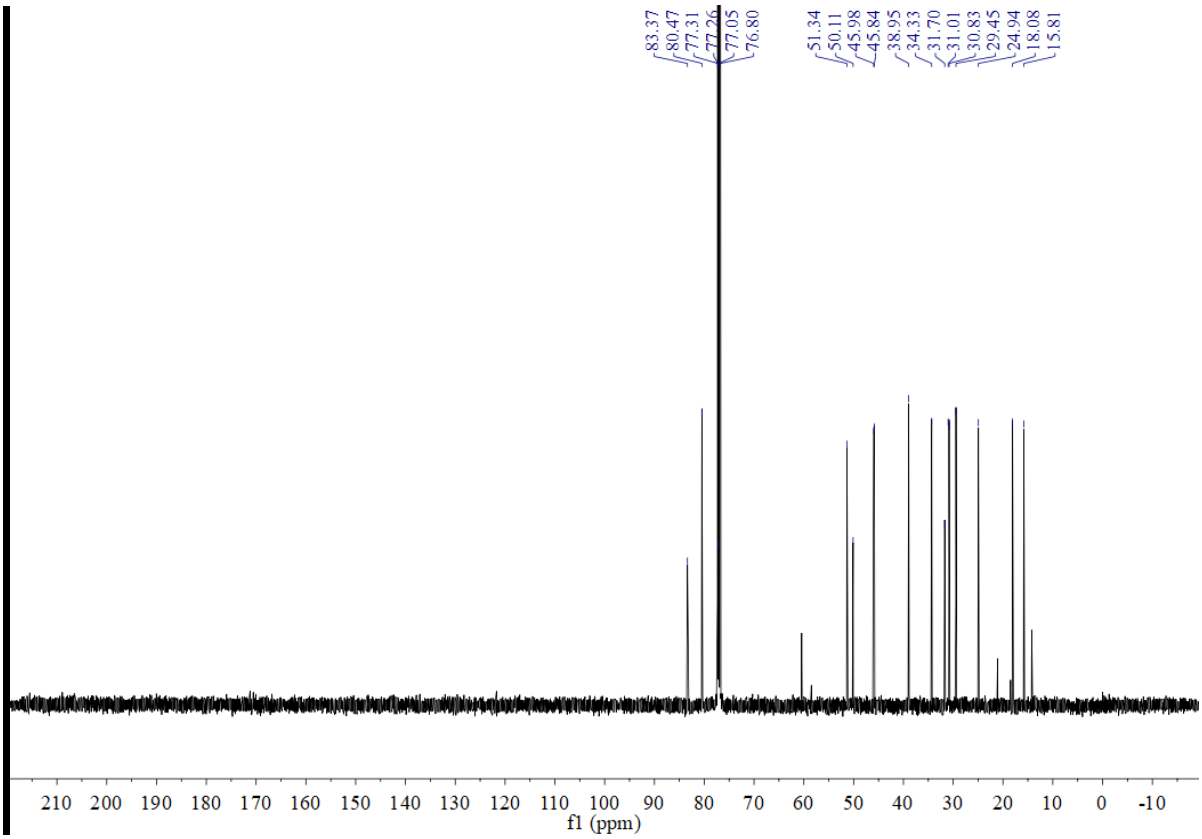


Figure S3: ^{13}C-NMR (125 MHz, $CDCl_3$) Spectrum of **1** (isosuberosenol A)

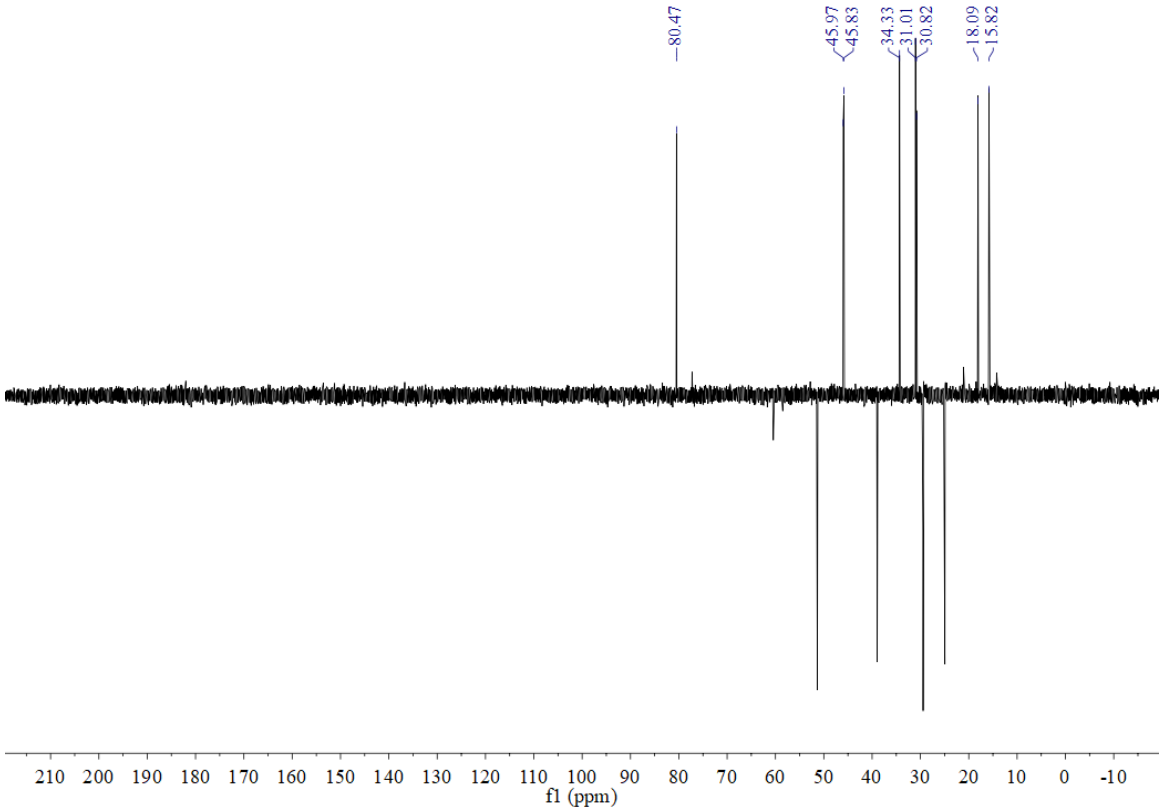


Figure S4: DEPT135 (125 MHz, $CDCl_3$) Spectrum of **1** (isosuberosenol A)

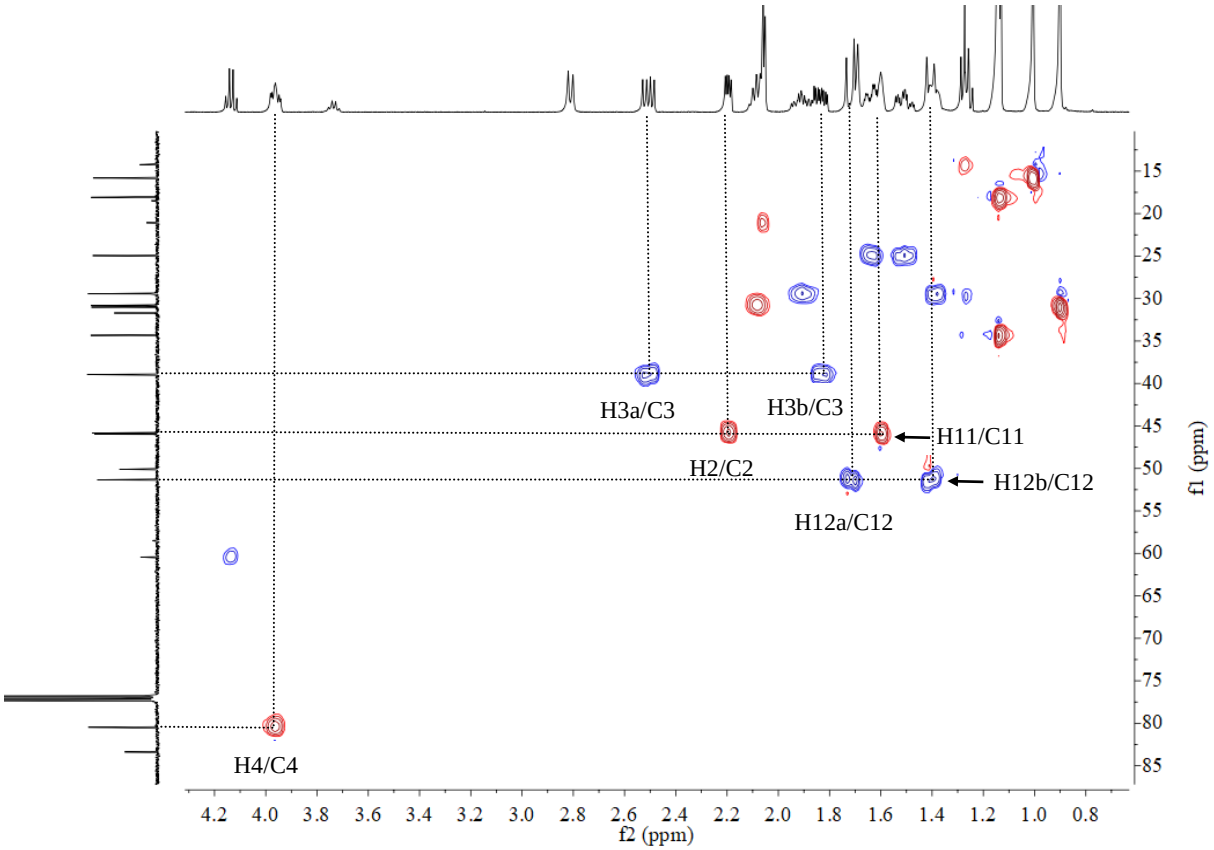


Figure S5: HSQC Spectrum of **1** (isosuberosenol A)

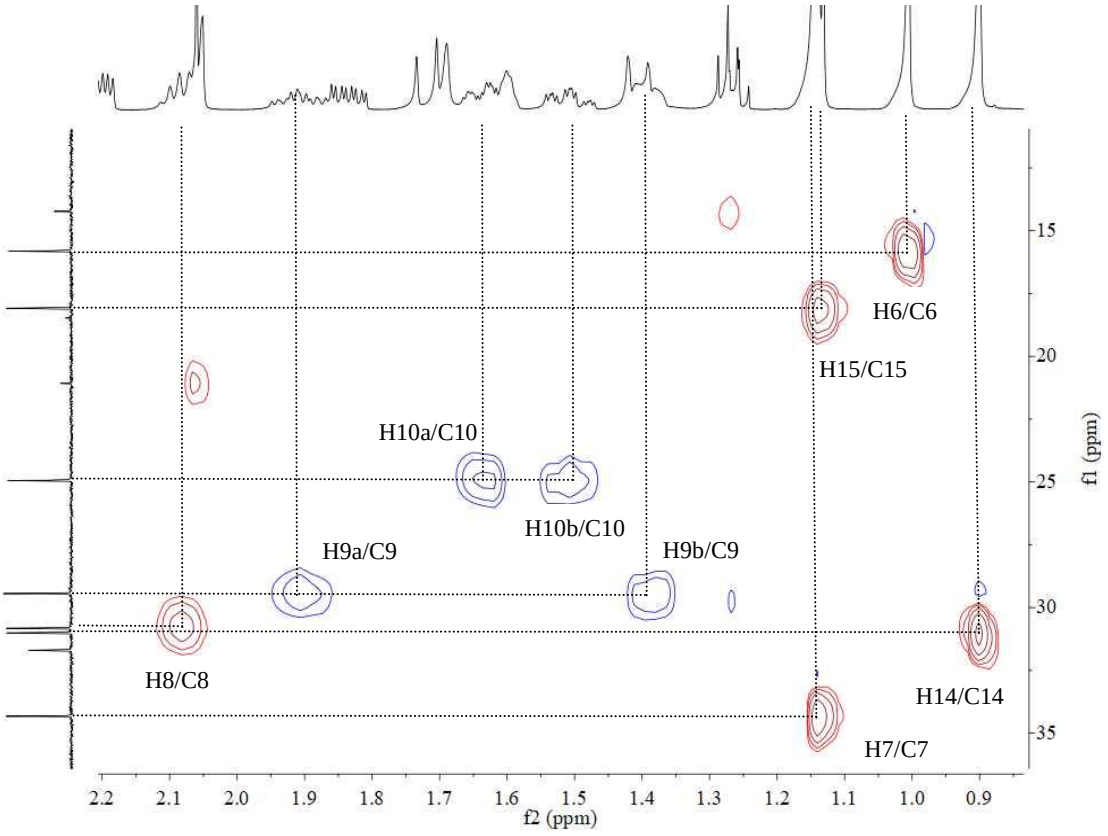


Figure S6: HSQC Spectrum of **1** (isosuberosenol A) (From δ_C15 ppm to δ_C 35 ppm)

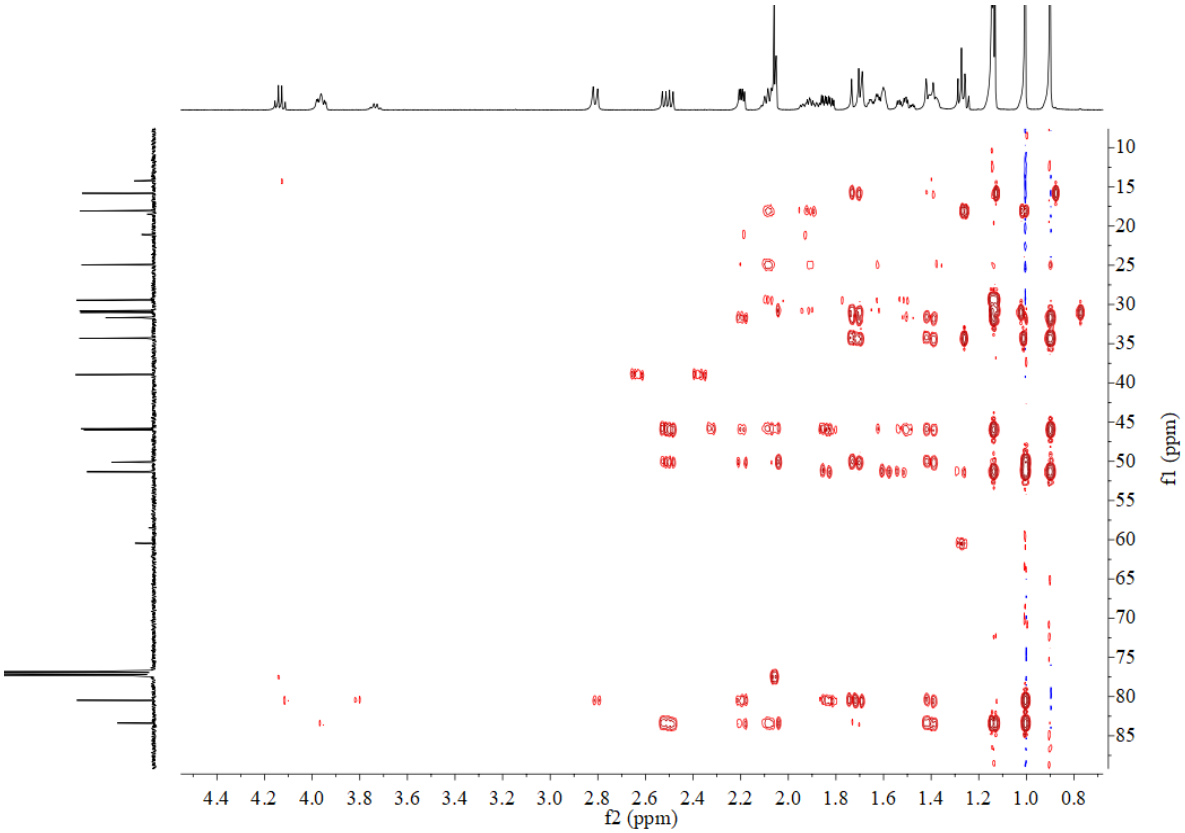


Figure S7: HMBC Spectrum of **1** (isosuberosenol A)

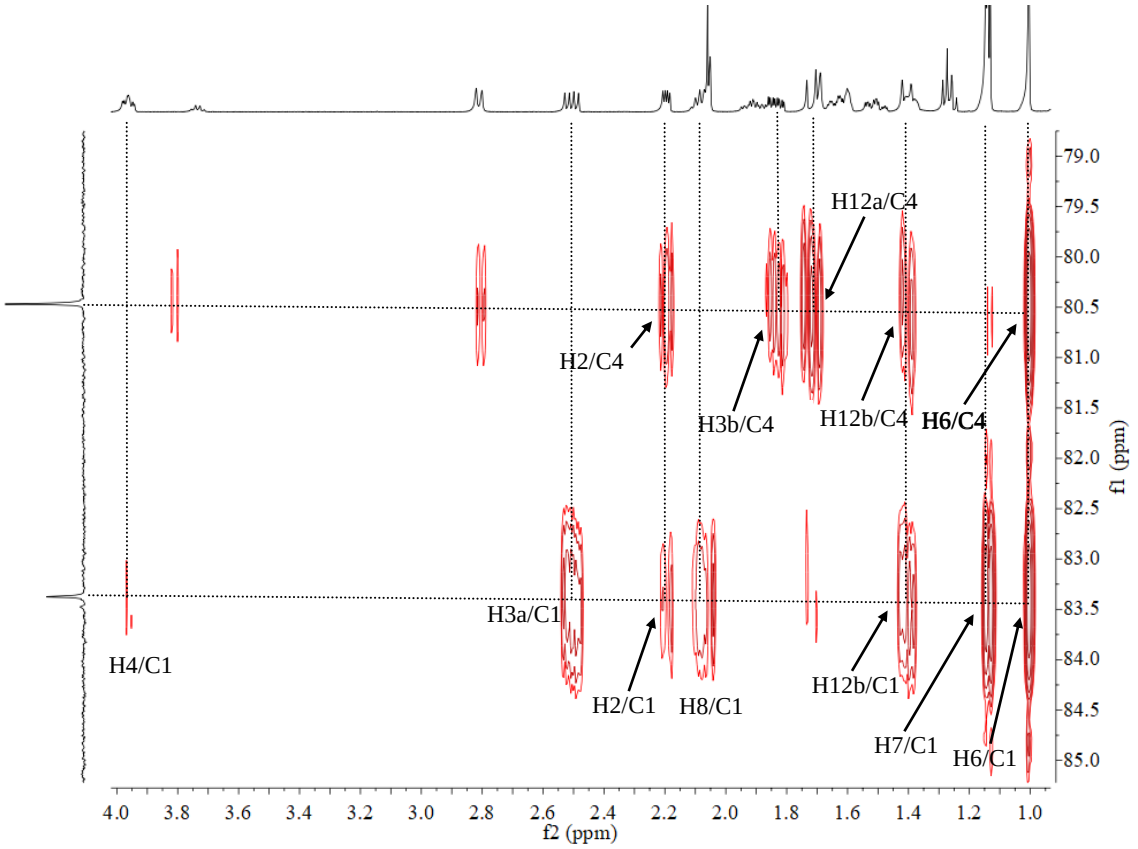


Figure S8: HMBC Spectrum of **1** (isosuberosenol A) (From δ_C 79 ppm to δ_C 85 ppm)

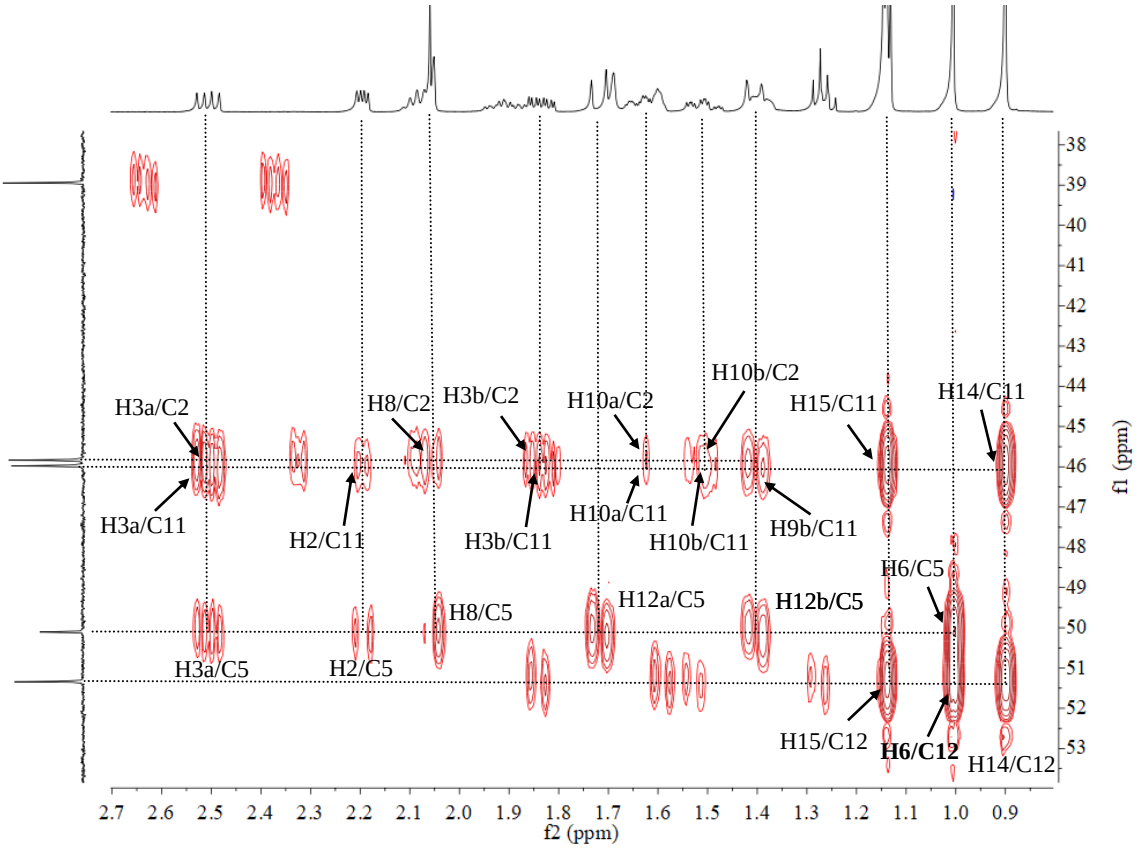


Figure S9: HMBC Spectrum of **1** (isosuberosenol A) (From δ_C 38 ppm to δ_C 53 ppm)

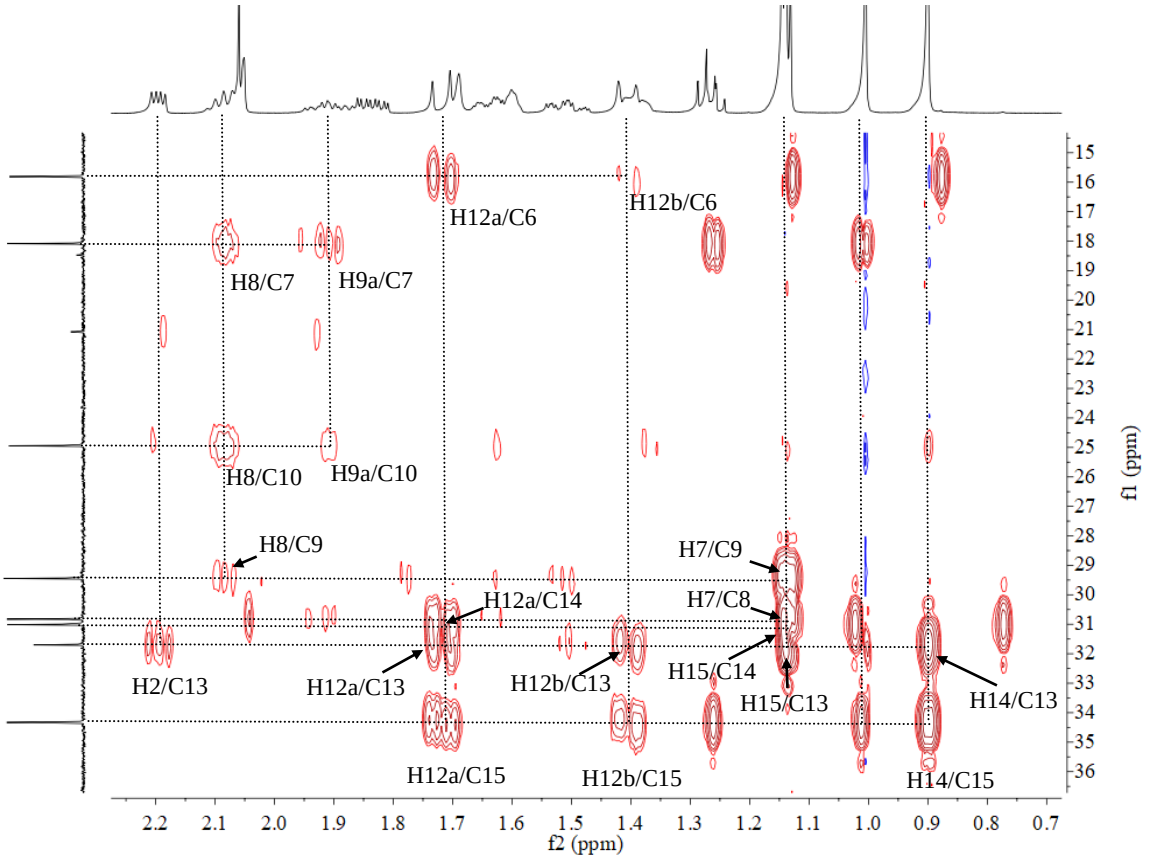


Figure S10: HMBC Spectrum of **1** (isosuberosenol A) (From δ_C 15 ppm to δ_C 36 ppm)

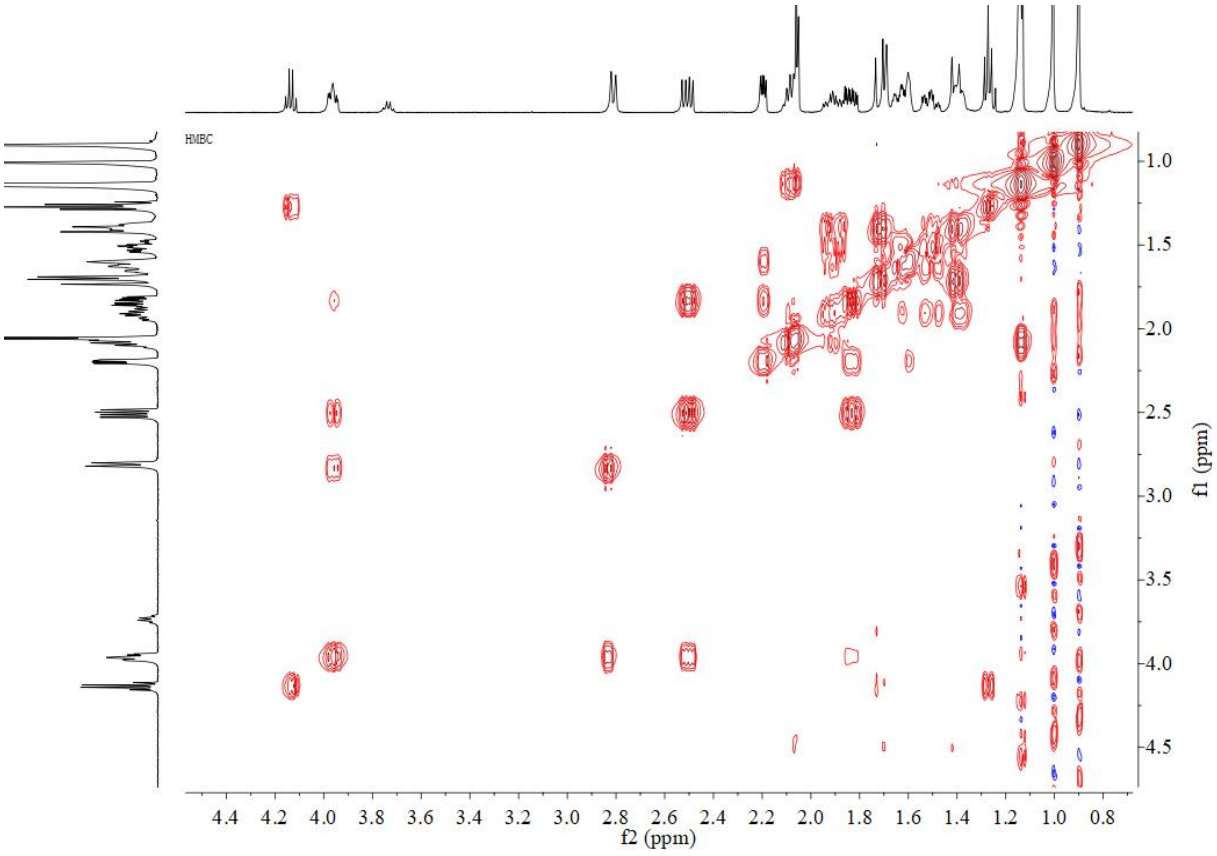


Figure S11: ^{1}H-^{1}H COSY Spectrum of **1** (isosuberosenol A)

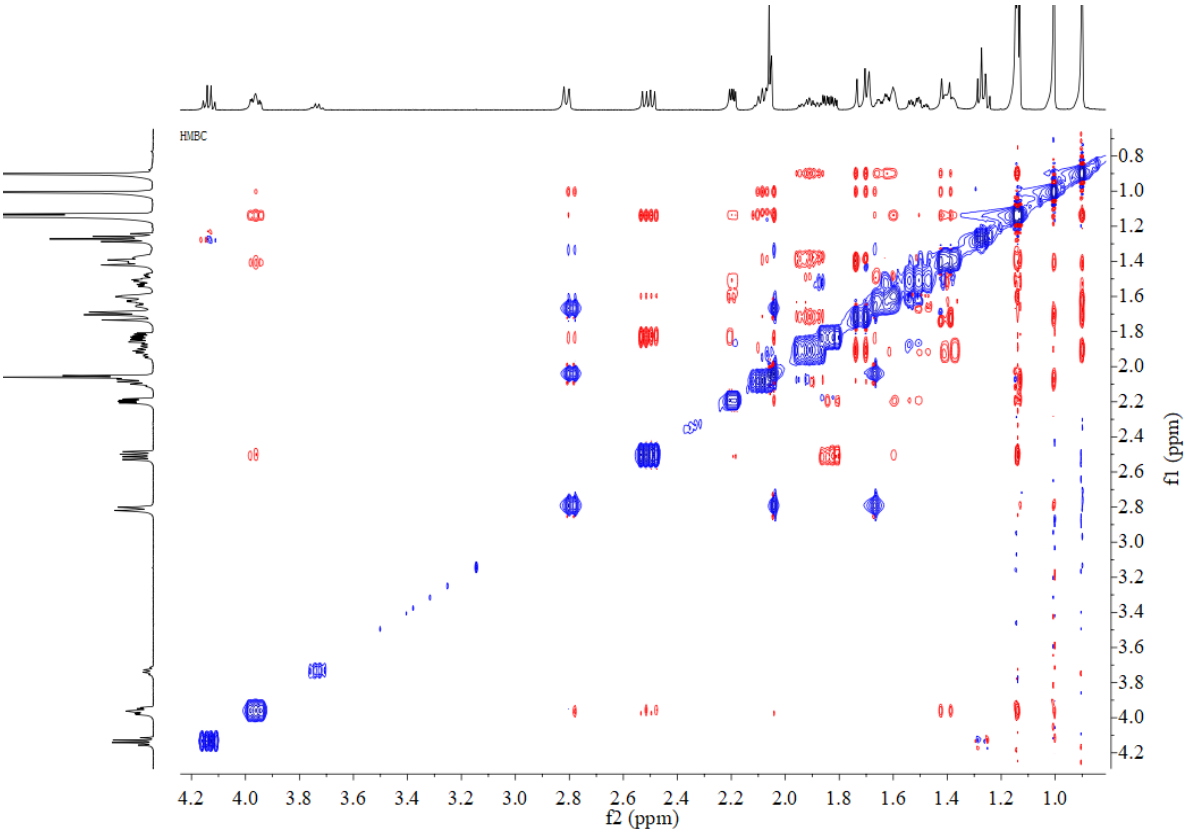
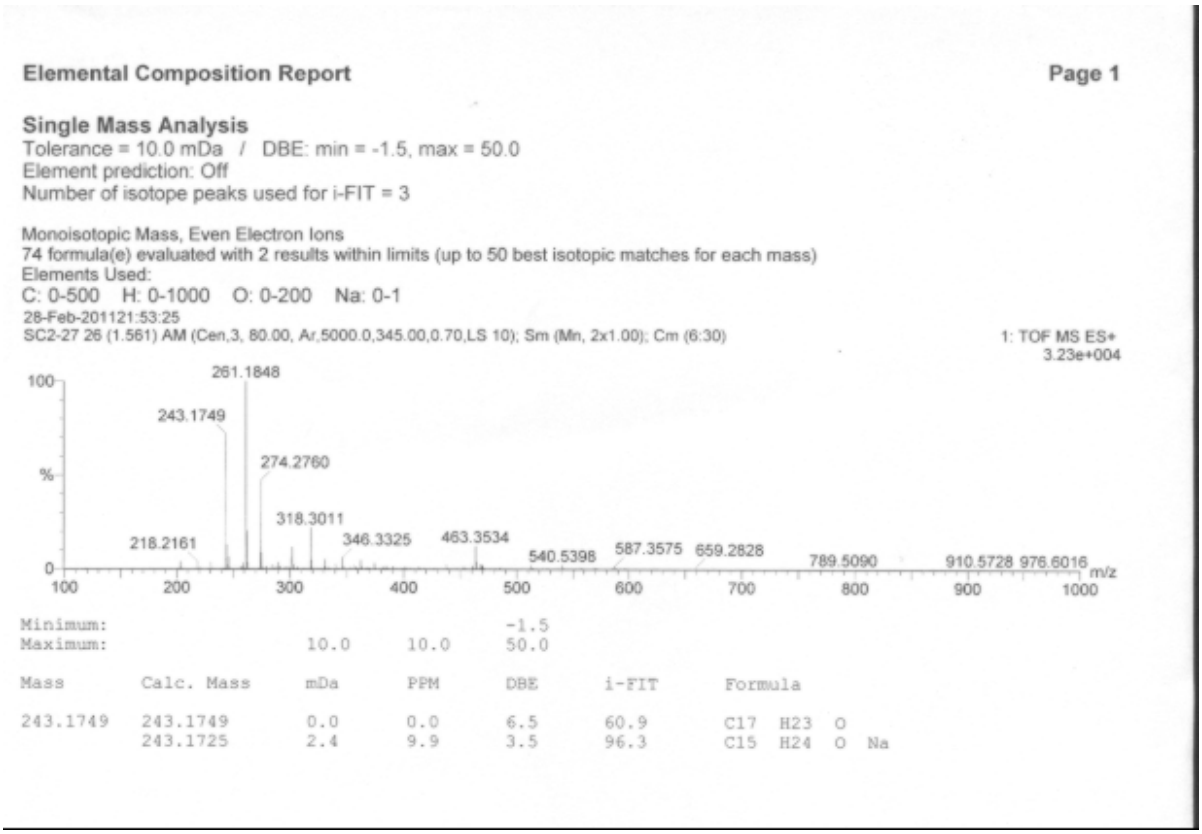


Figure S12: NOESY Spectrum of **1** (isosuberosenol A)



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-201121:53:25
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)

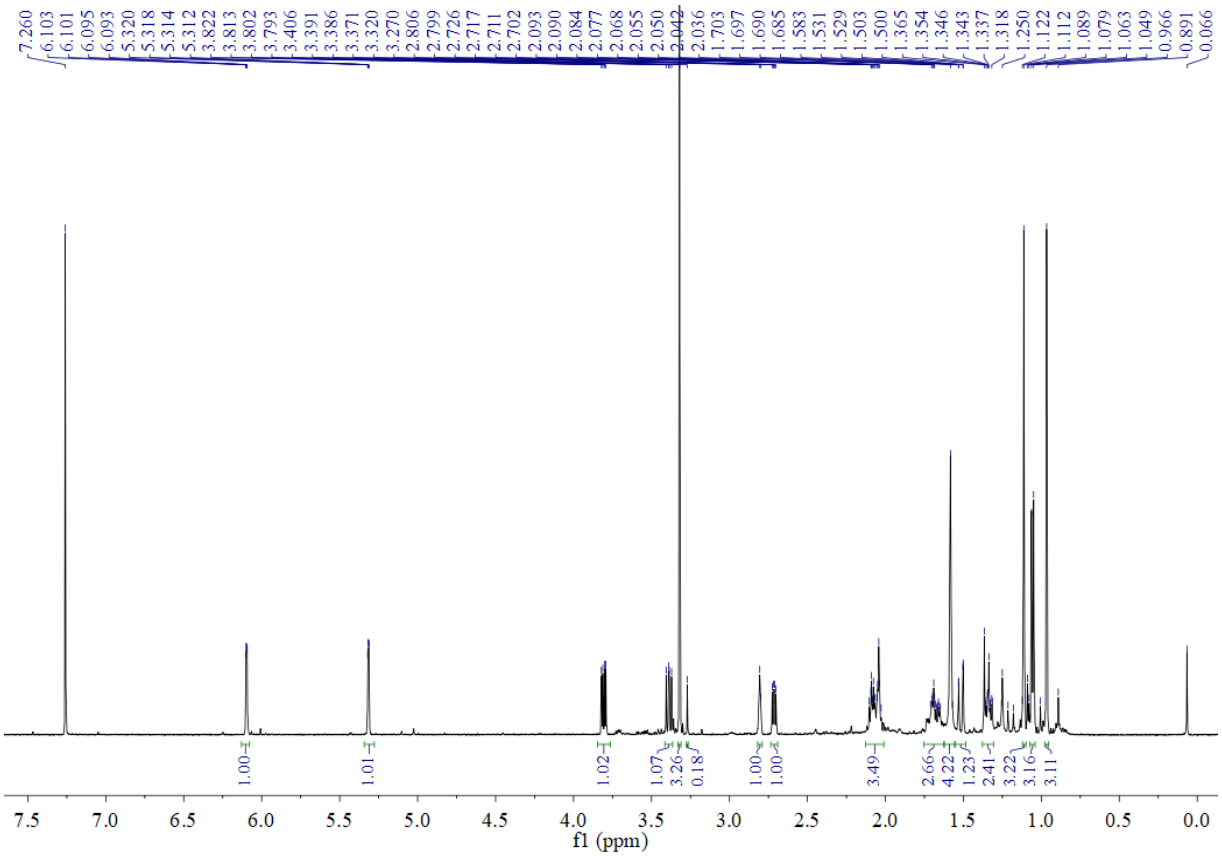


Figure S14: ^{1}H-NMR (500 MHz, $CDCl_3$) Spectrum of **2** (suberosain A)

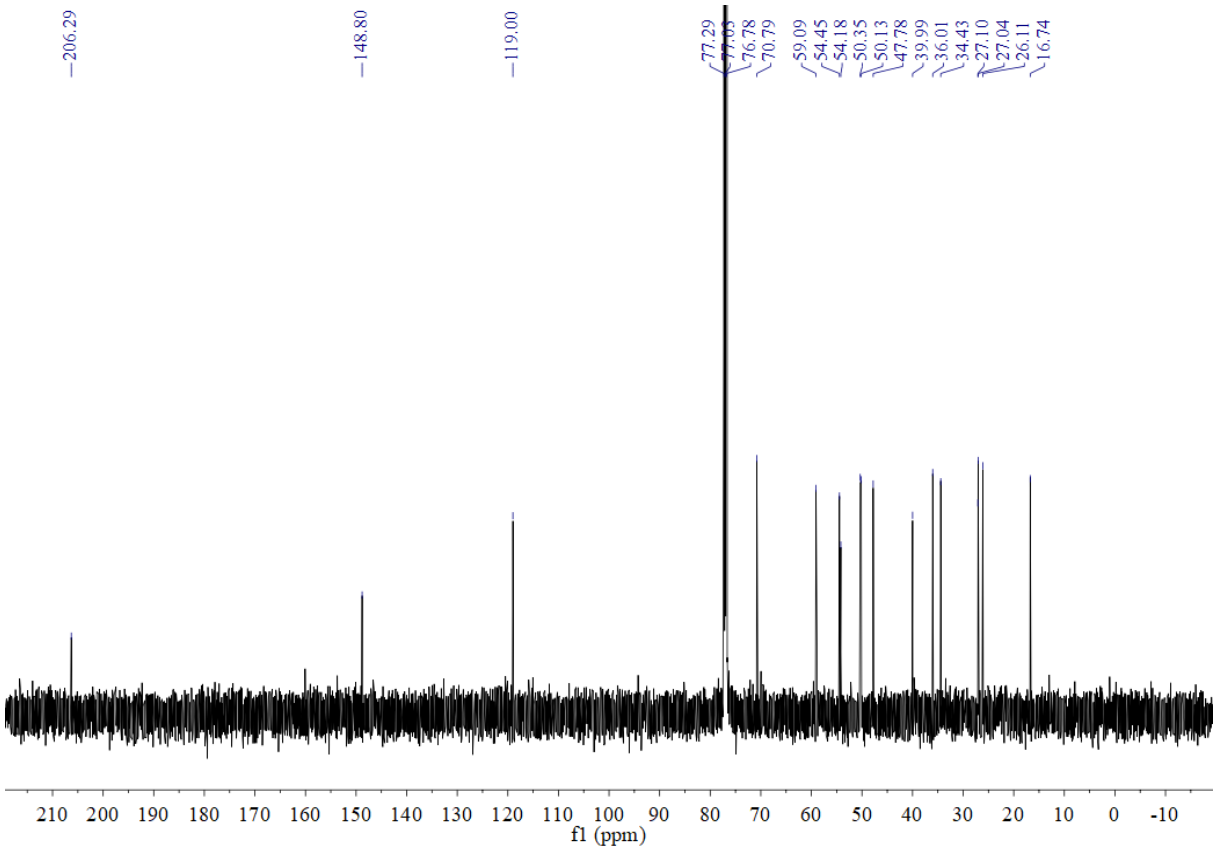


Figure S15: ^{13}C-NMR (125 MHz, $CDCl_3$) Spectrum of **2** (suberosain A)

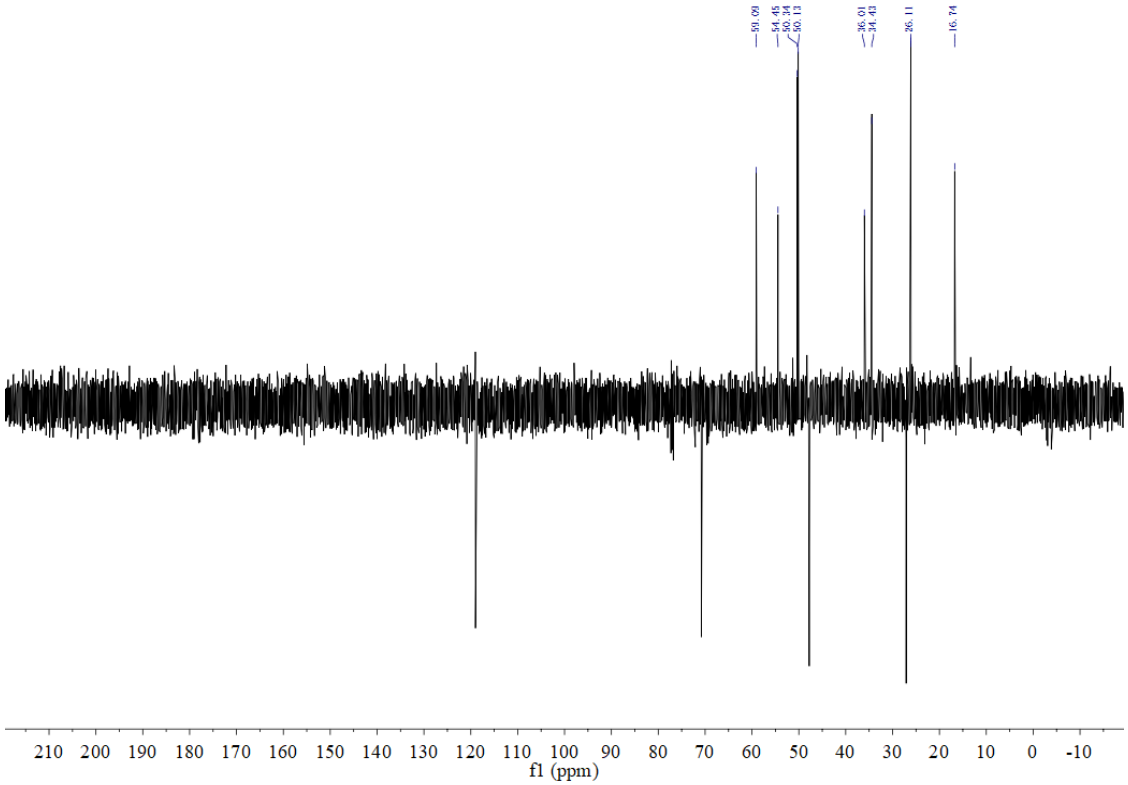


Figure S16: DEPT135 (125 MHz, $CDCl_3$) Spectrum of **2** (suberosain A)

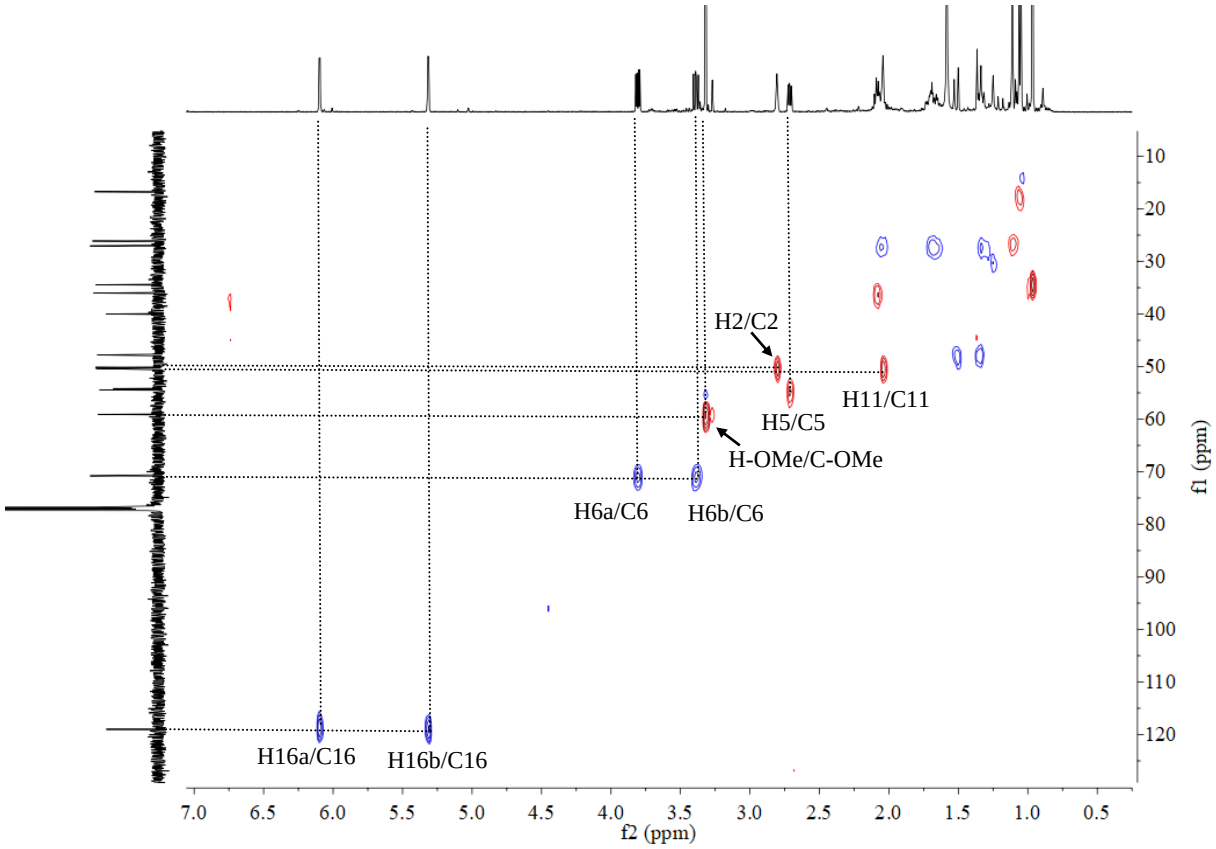


Figure S17: HSQC Spectrum of **2** (suberosain A)

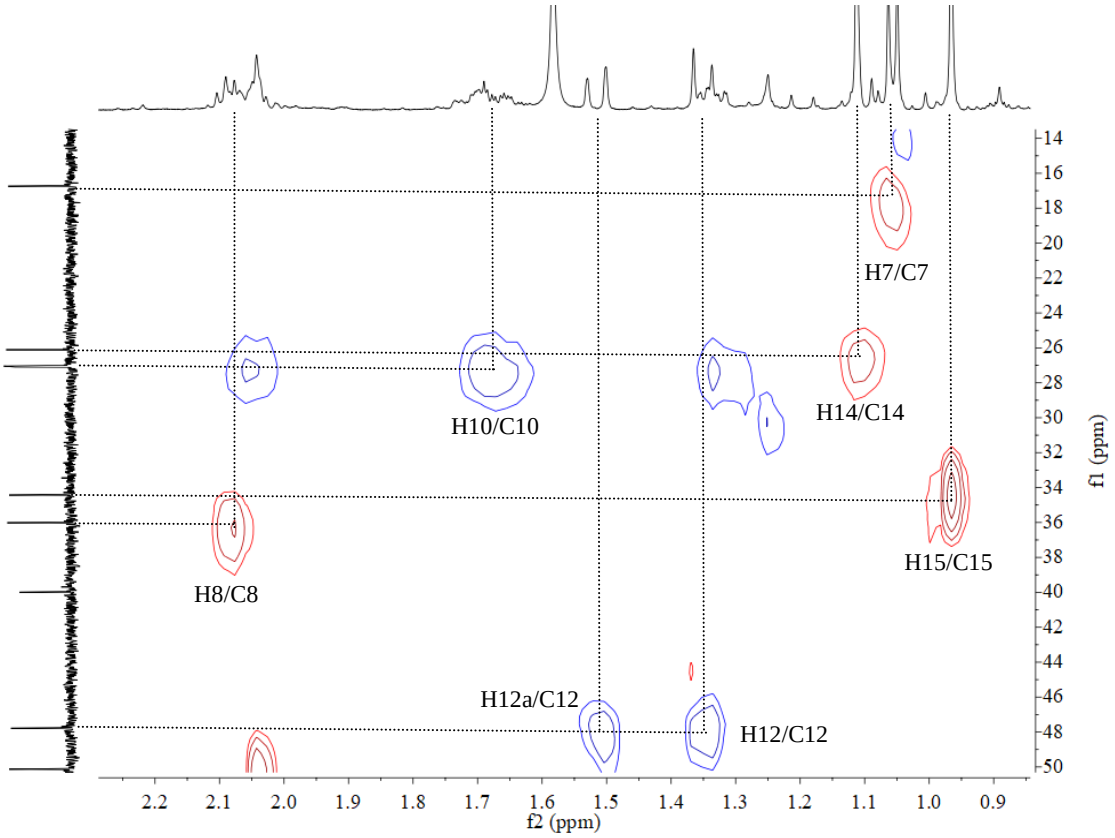


Figure S18: HSQC Spectrum of **2** (suberosain A) (From δ_C 14 ppm to 50 ppm)

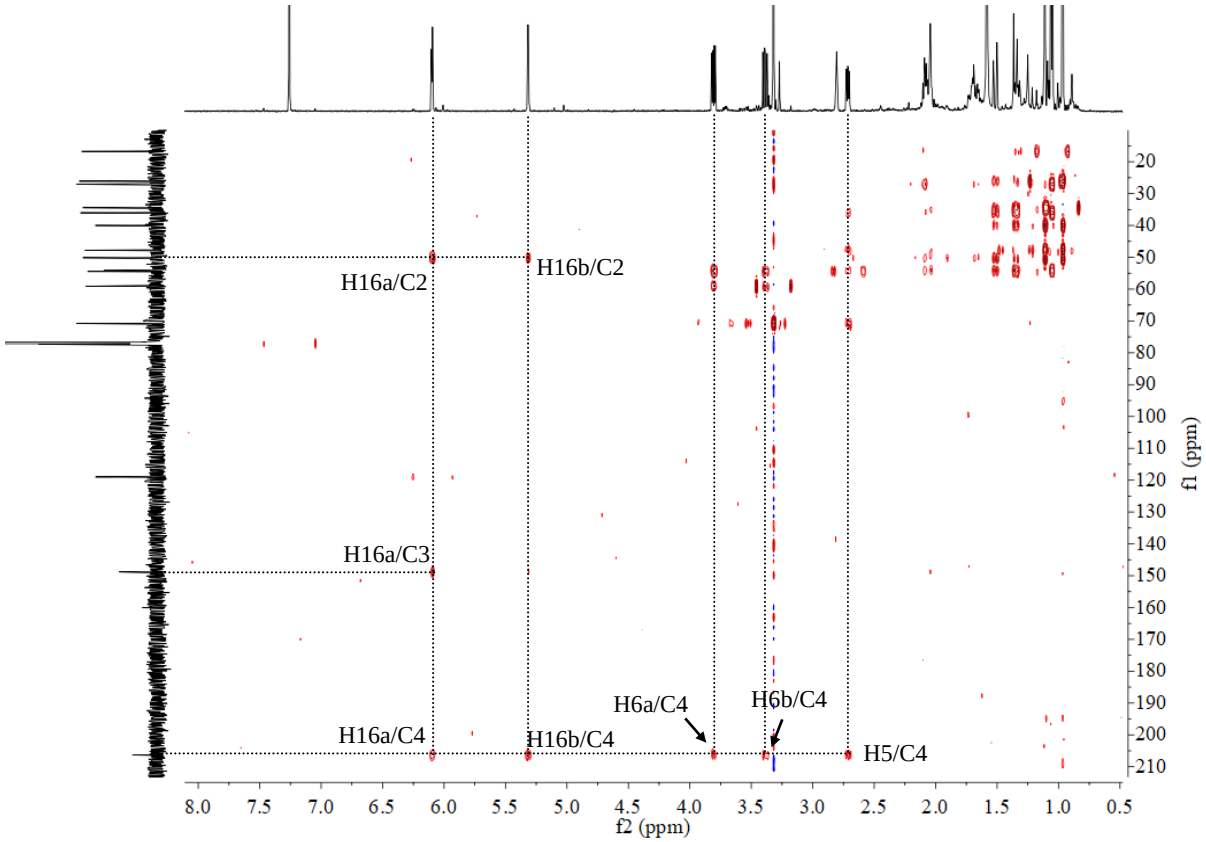


Figure S19: HMBC Spectrum of **2** (suberosain A)

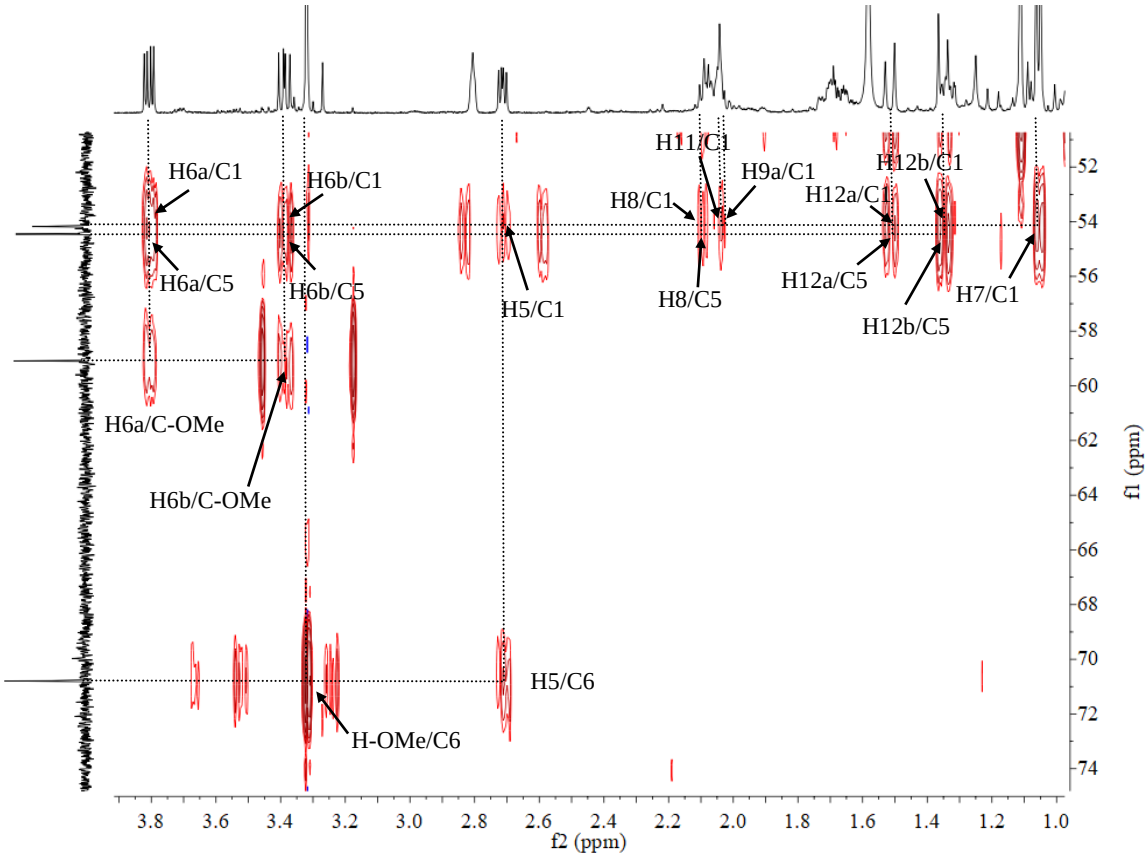


Figure S20: HMBC Spectrum of **2** (suberosain A) (From δ_C 52 ppm to 75 ppm)

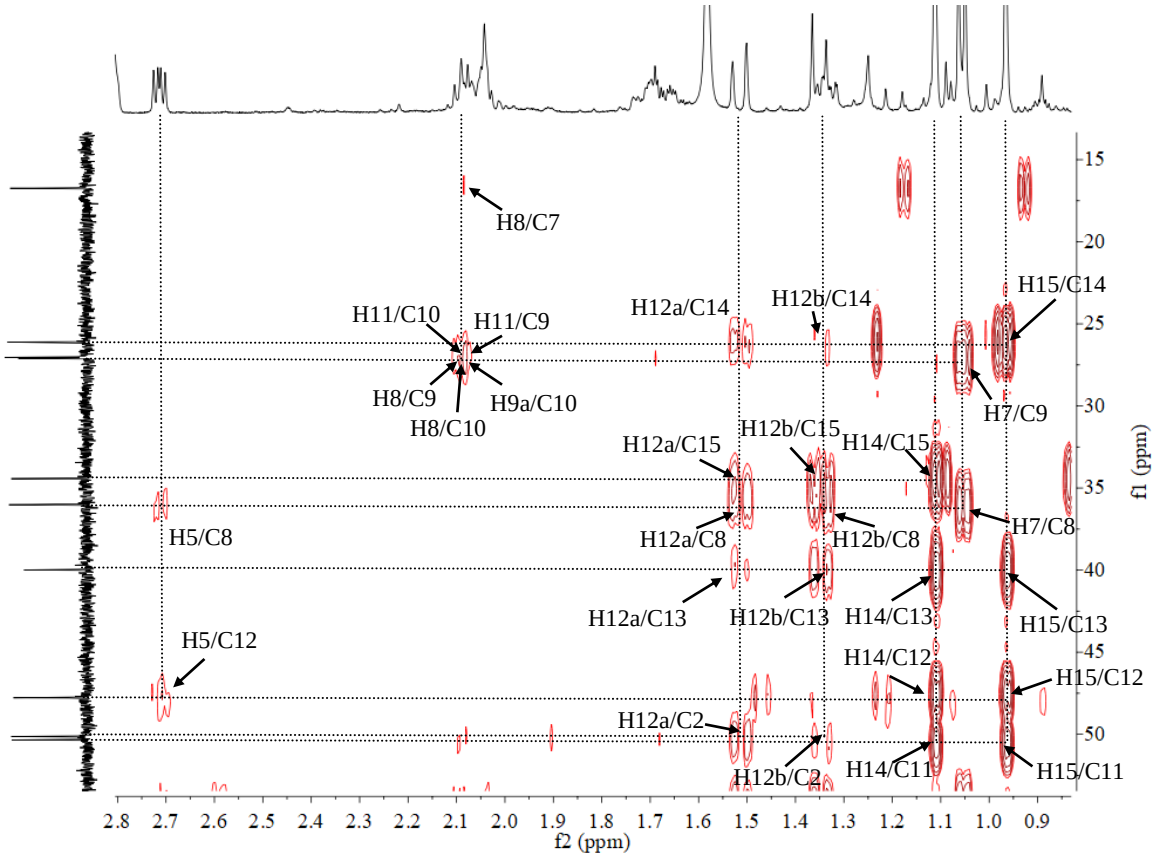


Figure S21: HMBC Spectrum of **2** (suberosain A) (From δ_C 15 ppm to 50 ppm)

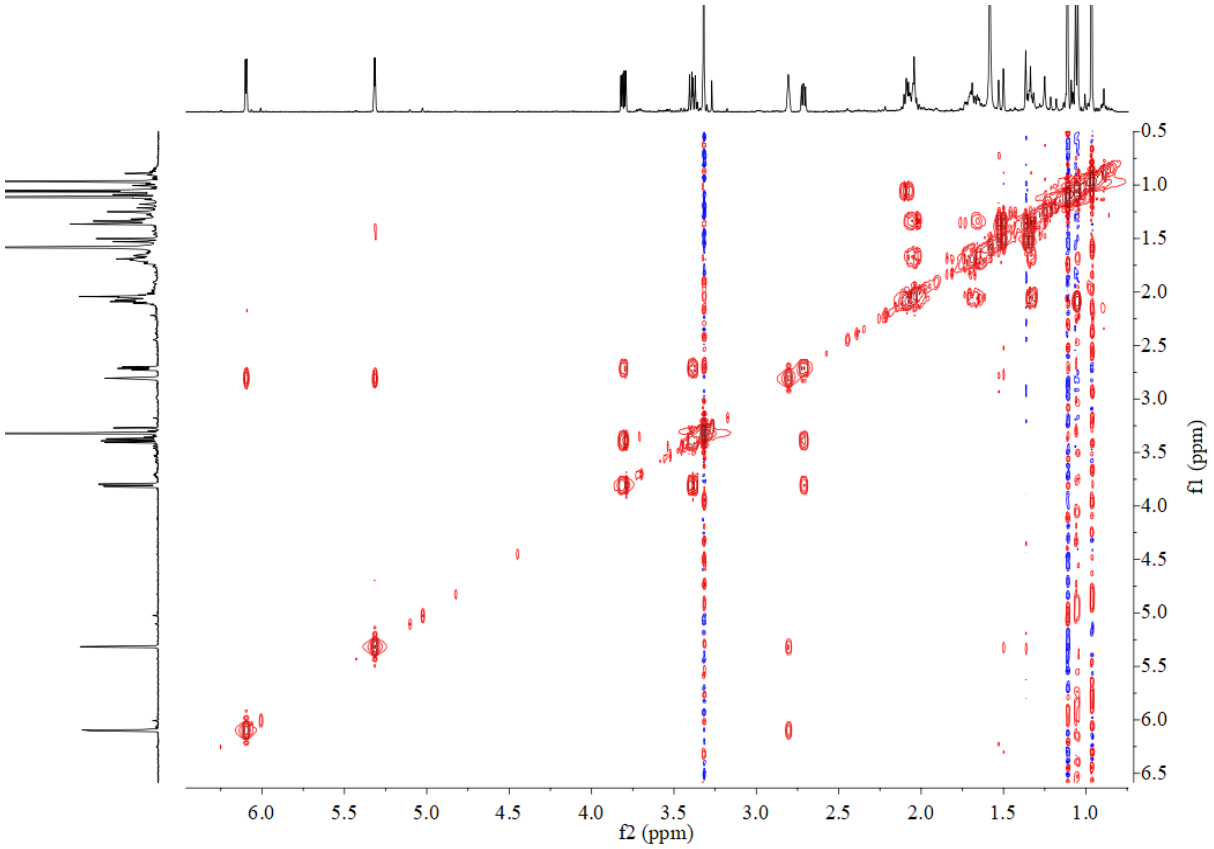


Figure S22: ^{1}H-^{1}H COSY Spectrum of **2** (suberosain A)

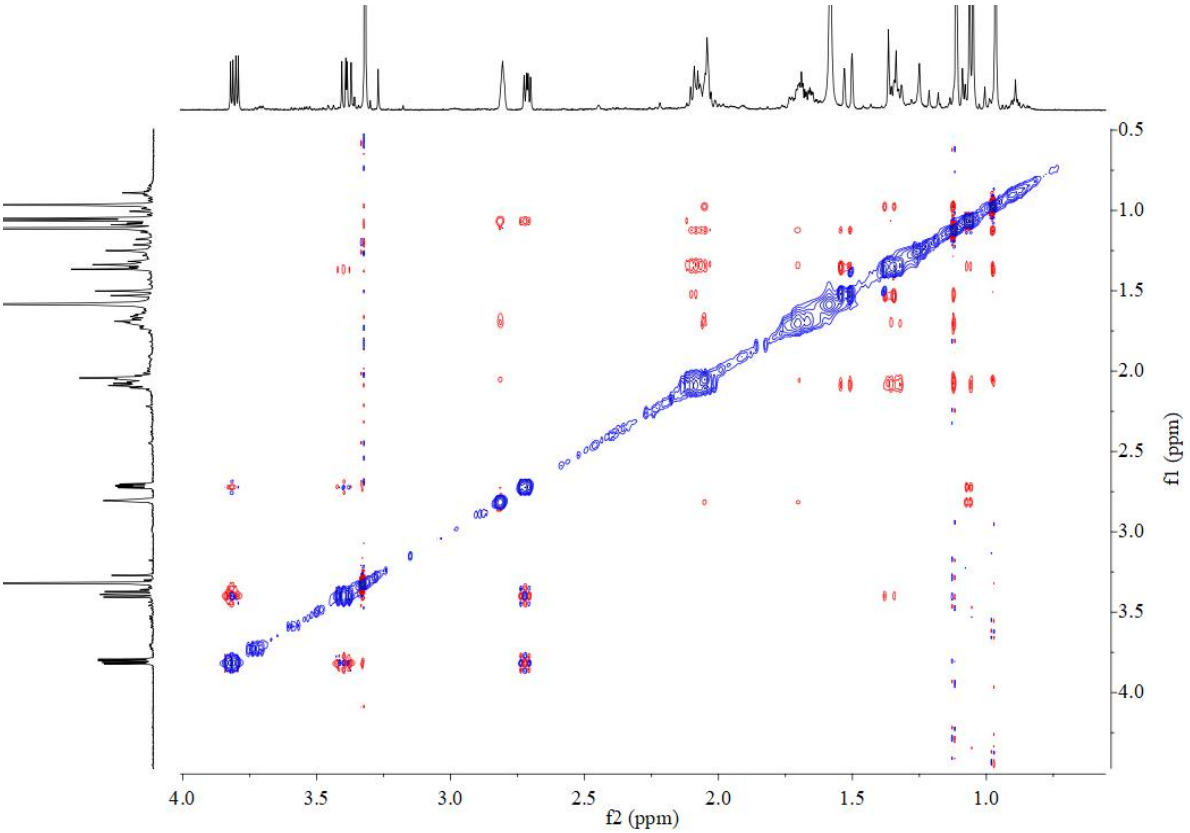


Figure S23: NOESY Spectrum of **2** (suberosain A)

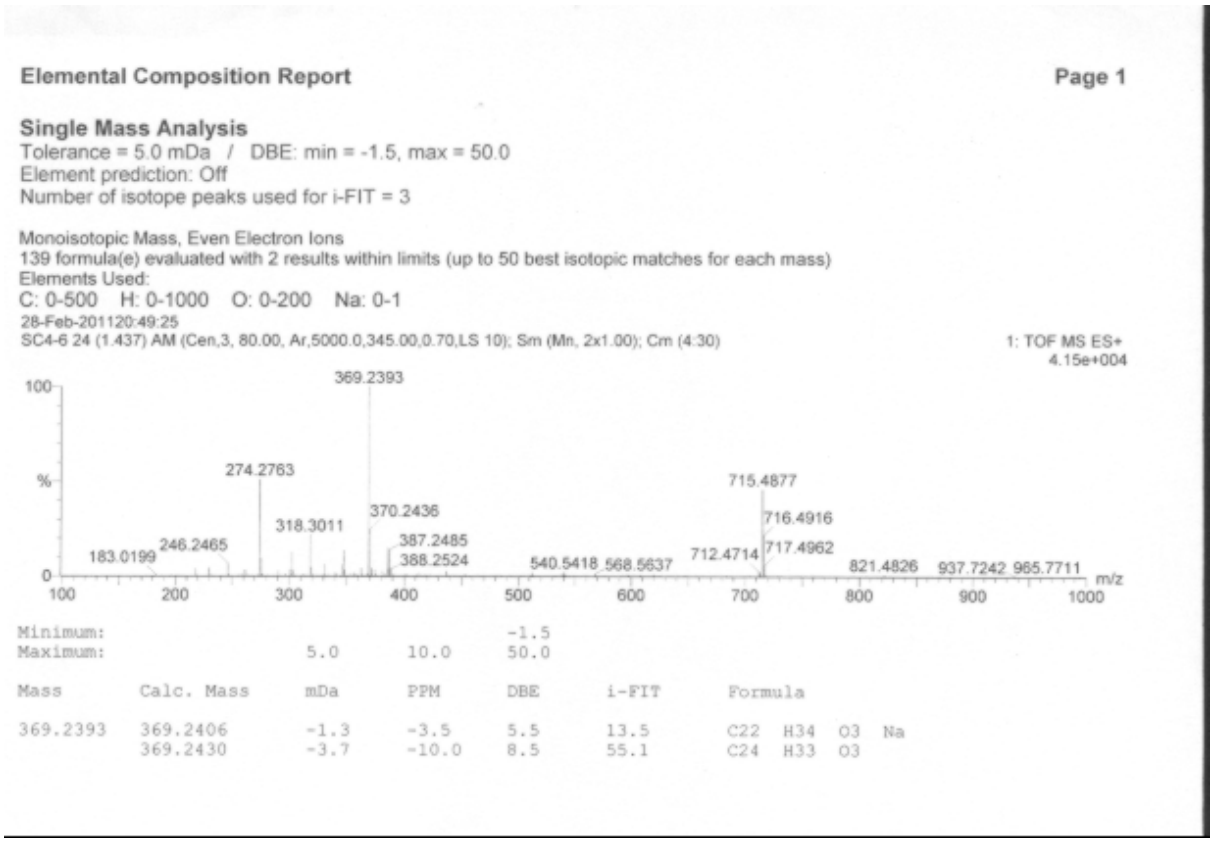


Figure S24: HR-ESI-MS Spectrum of **3** (4-hydroxymethyl-5β-pregnan-3, 20-dione)

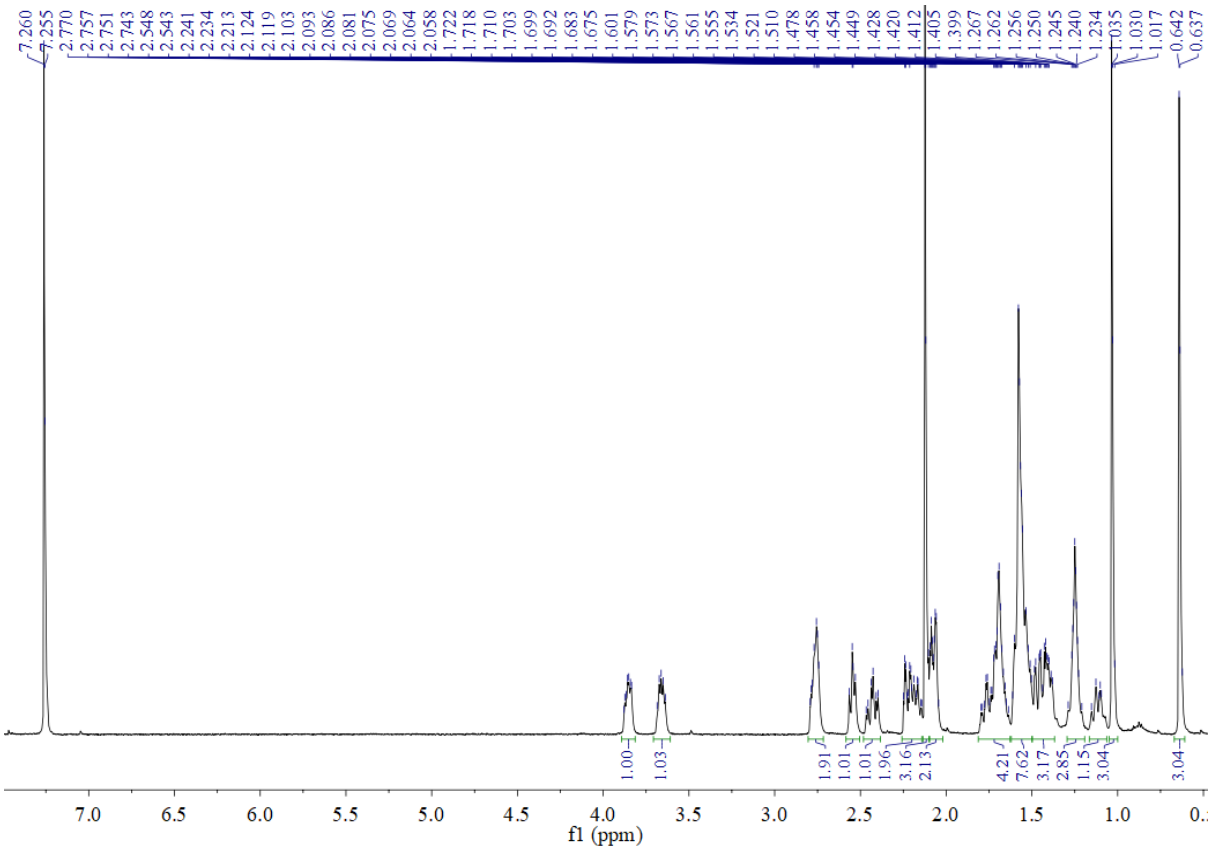


Figure S25: ^{1}H-NMR (500 MHz, $CDCl_3$) Spectrum of **3** (4-hydroxymethyl-5*β*-pregnan-3, 20-dione)

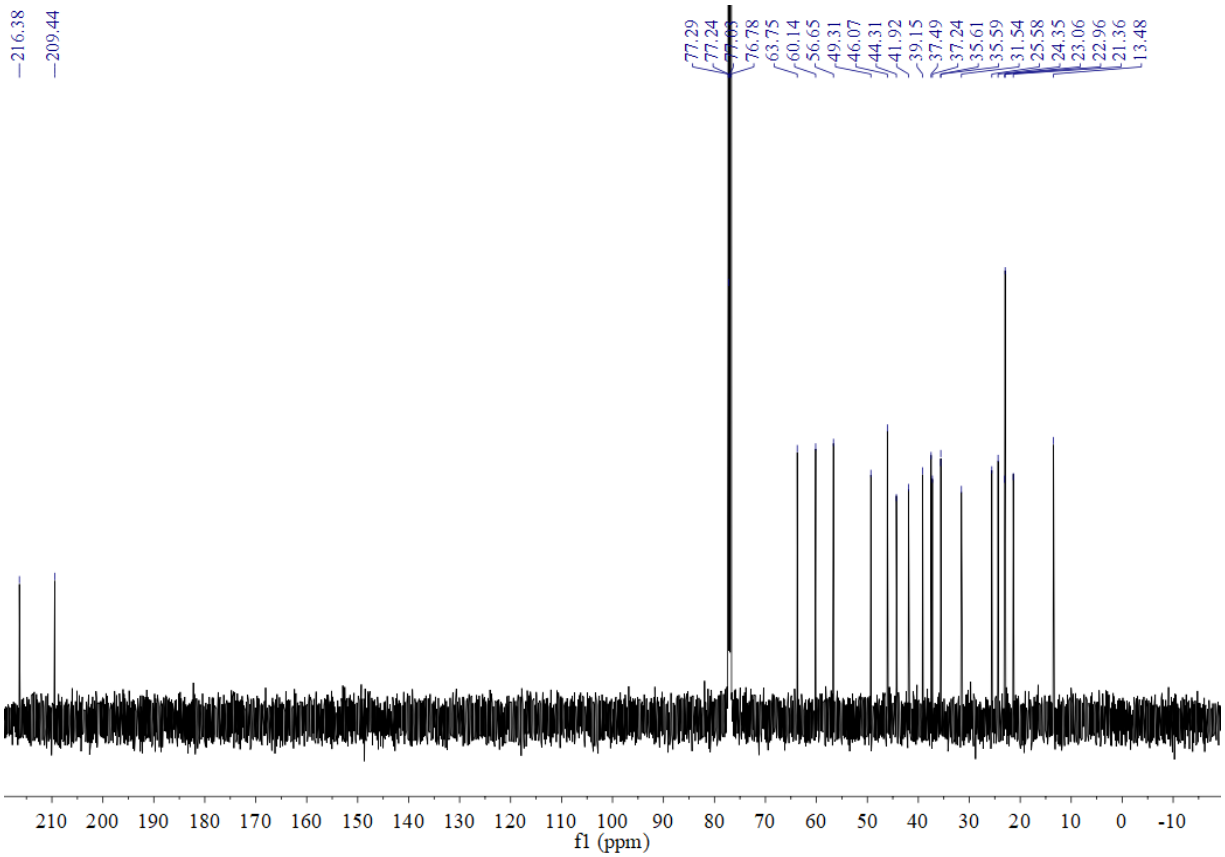


Figure S26: ^{13}C-NMR (125 MHz, $CDCl_3$) Spectrum of **3** (4-hydroxymethyl-5*β*-pregnan-3, 20-dione)

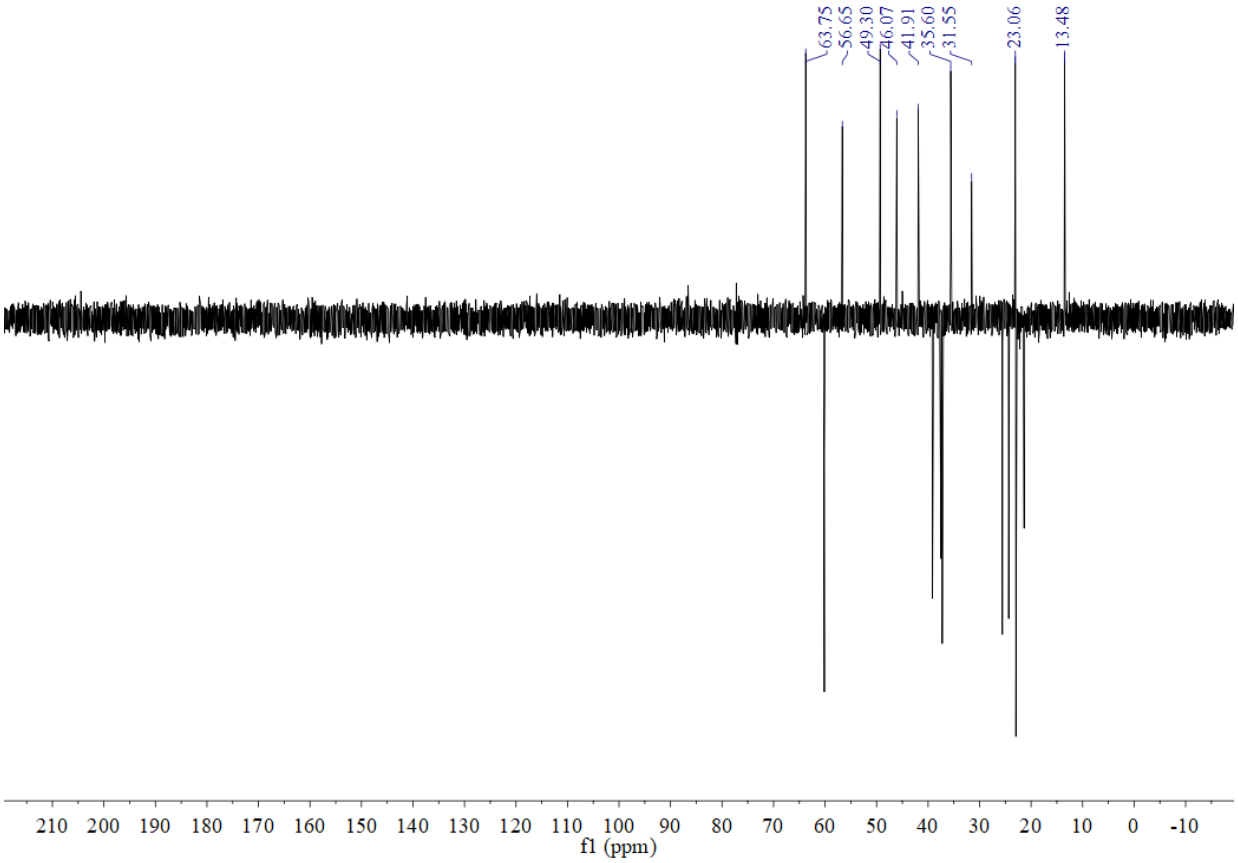


Figure S27: DEPT135 (125 MHz, $CDCl_3$) Spectrum of **3** (4-hydroxymethyl-5*β*-pregnan-3, 20-dione)

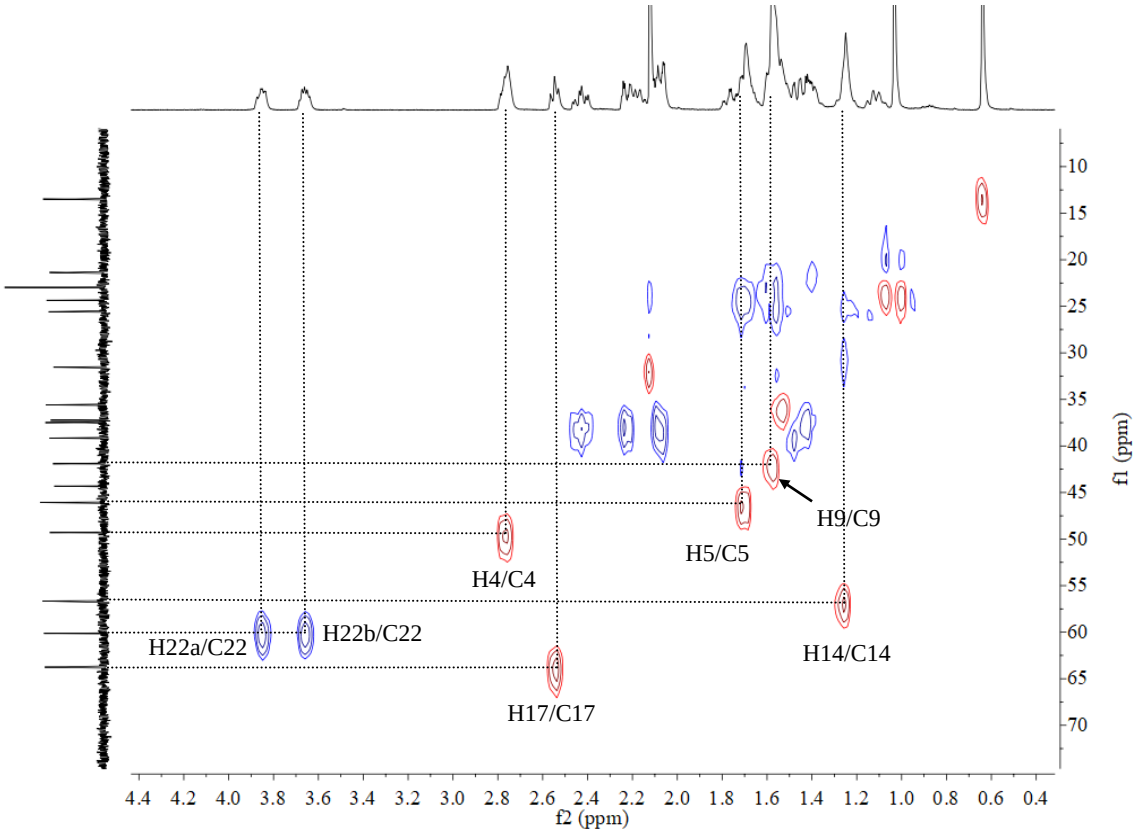


Figure S28: HSQC Spectrum of **3** (4-hydroxymethyl-5*β*-pregnan-3, 20-dione)

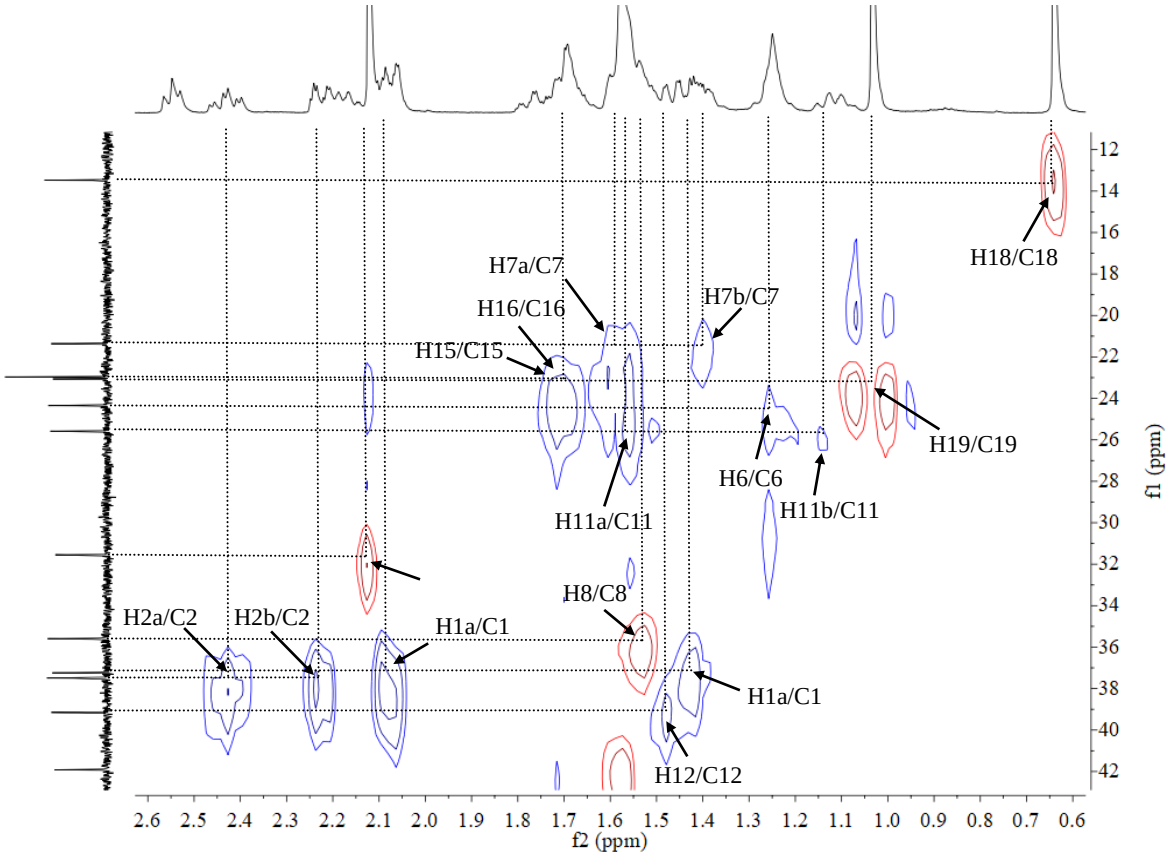


Figure S29: HSQC Spectrum of **3** (4-hydroxymethyl-5β-pregnan-3, 20-dione) (From δ_C 12 to 42)

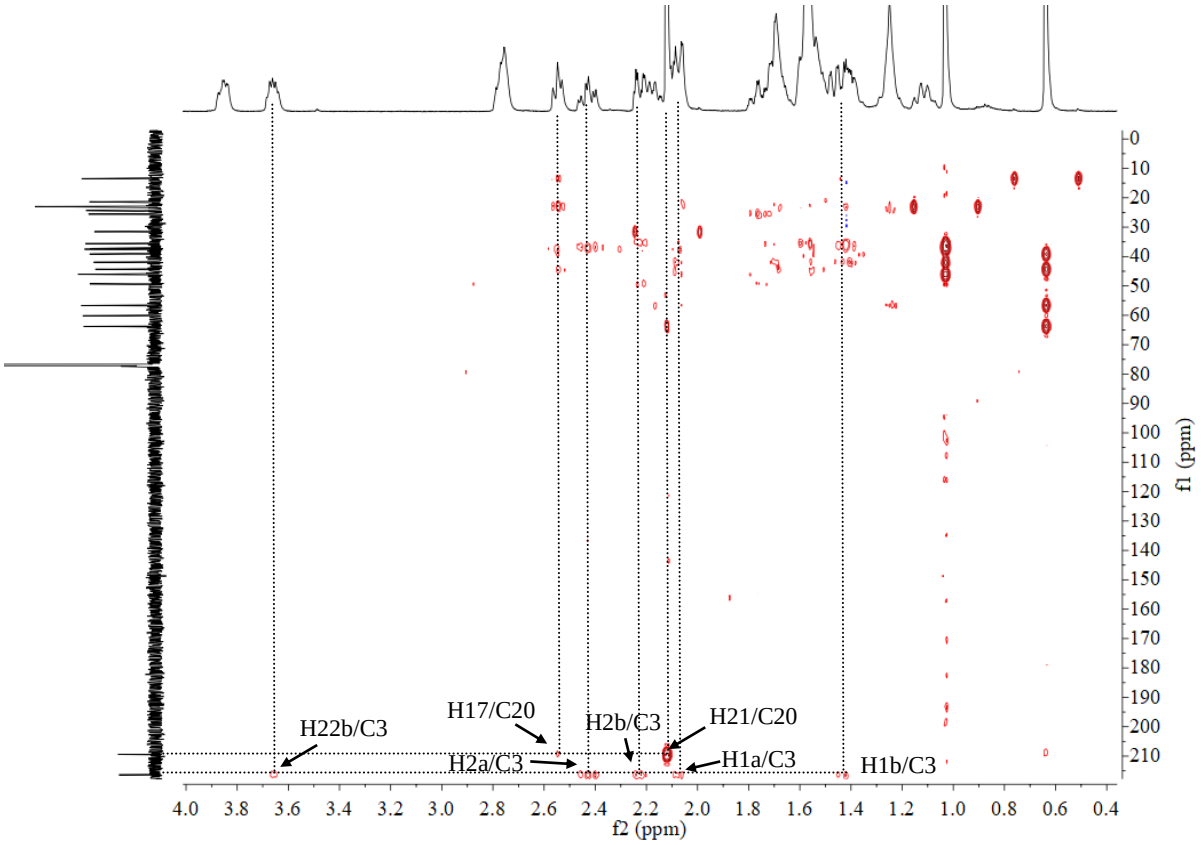


Figure S30: HMBC Spectrum of **3** (4-hydroxymethyl-5*β*-pregnan-3, 20-dione)

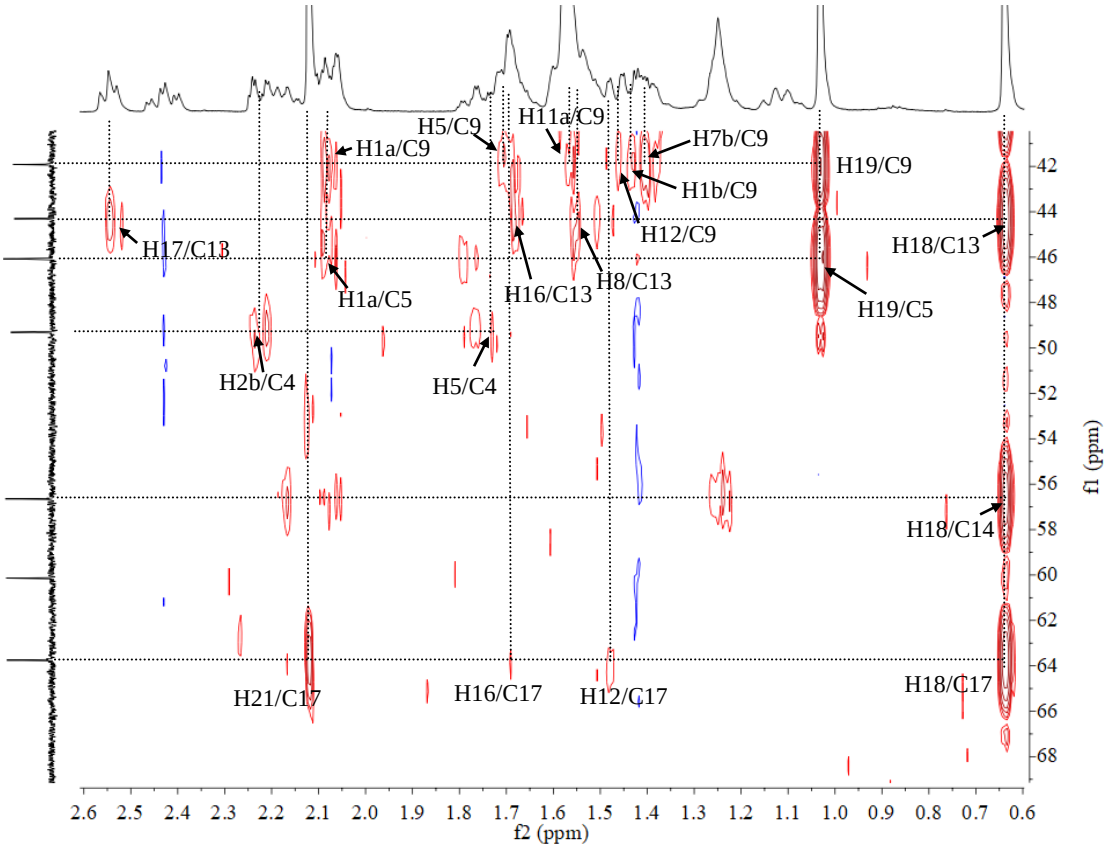


Figure S31: HMBC Spectrum of **3** (4-hydroxymethyl-5β-pregnan-3, 20-dione) (From δ_C 42 to 70)

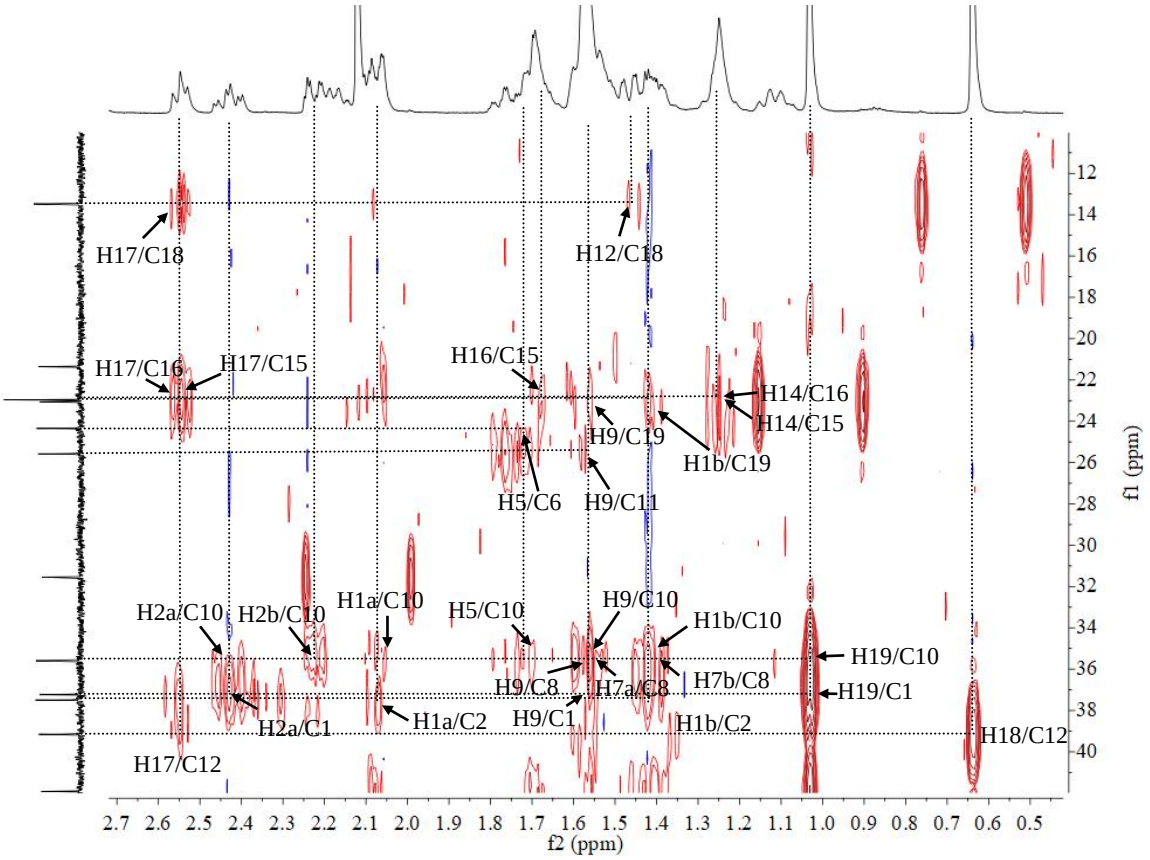


Figure S32: HMBC Spectrum of **3** (4-hydroxymethyl-5β-pregnan-3, 20-dione) (From δ_C 12 to 40)

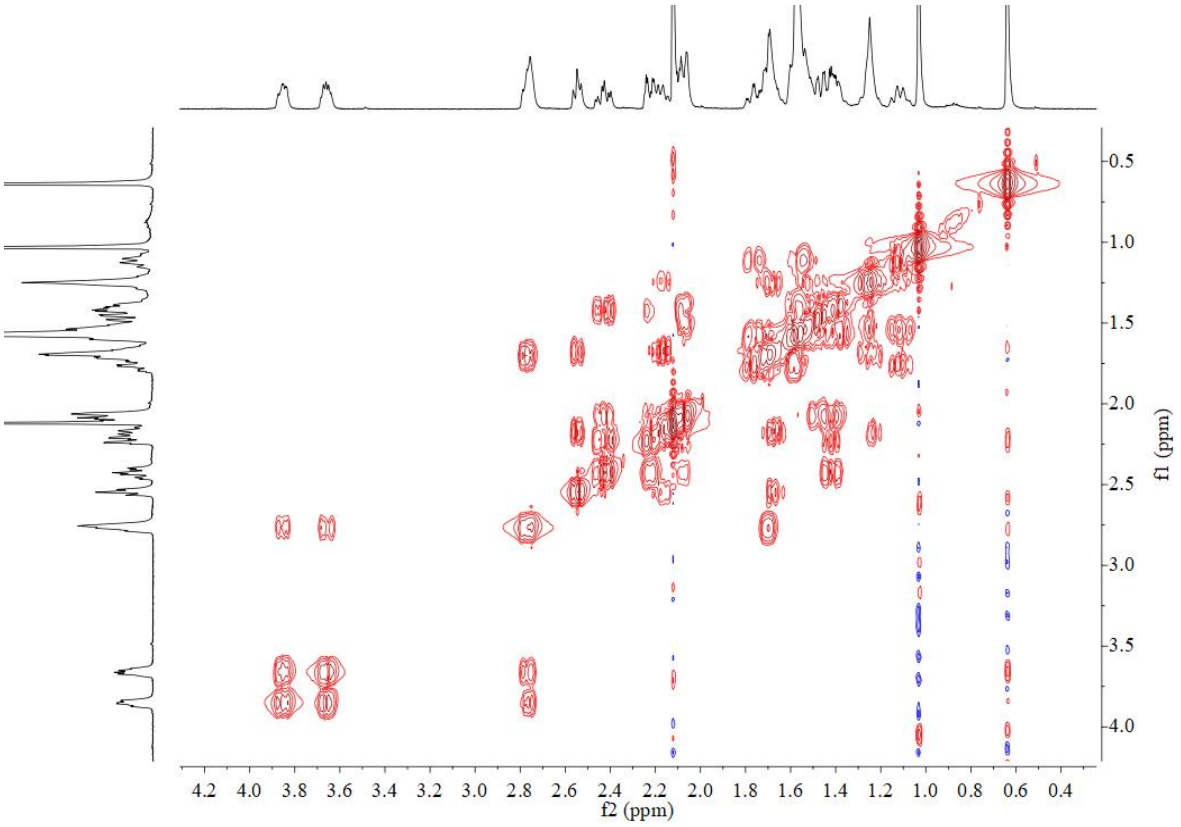


Figure S33: ^{1}H-^{1}H COSY Spectrum of **3** (4-hydroxymethyl-5*β*-pregnan-3, 20-dione)

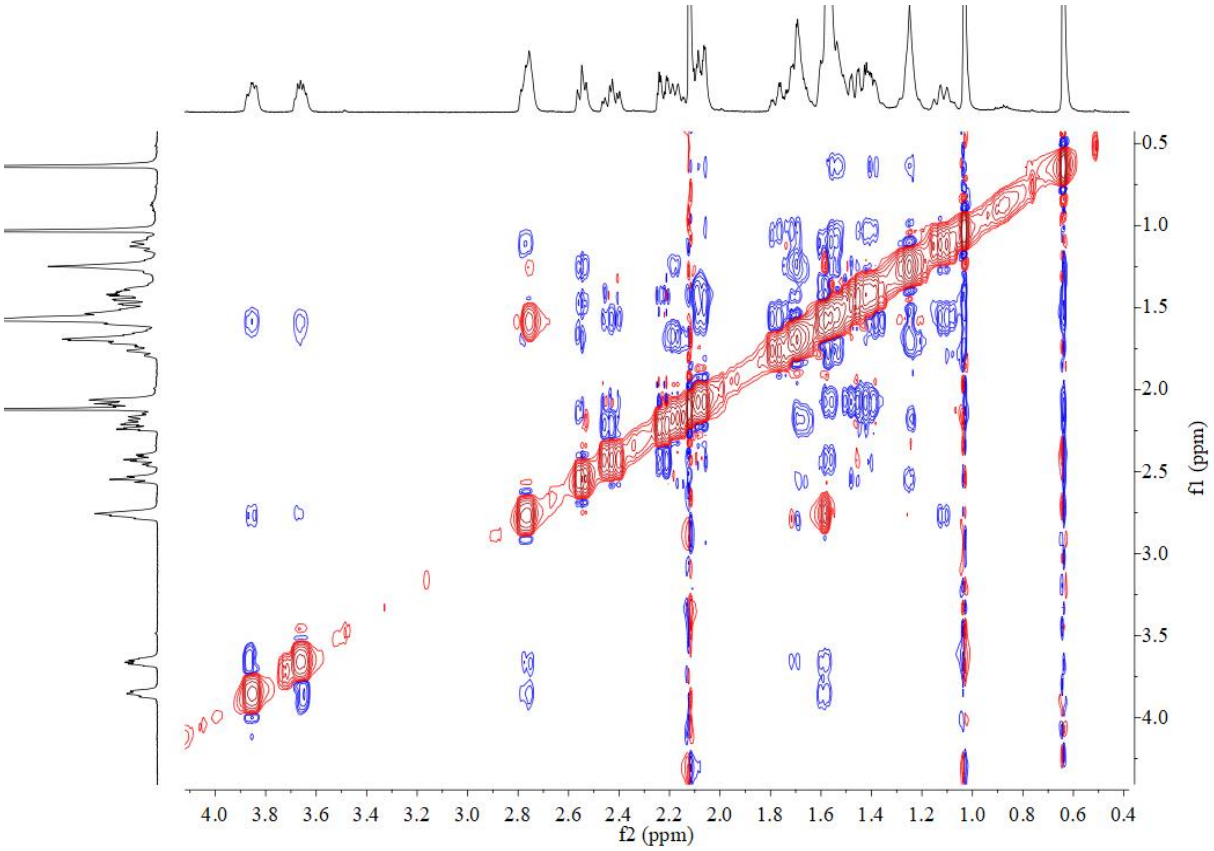


Figure S34: NOESY Spectrum of **3** (4-hydroxymethyl-5β-pregnan-3, 20-dione)