## **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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Elementa	I Compositio	n Report									Page 1
Single Ma Tolerance Element pr Number of	ass Analysis = 10.0 mDa / ediction: Off isotope peaks	DBE: min = used for i-FIT	-1.5, max =	50.0							
Monoisotopi 77 formula(e Elements U: C: 0-500 28-Feb-2011: SC3-8 21 (1.3	c Mass, Even Eli e) evaluated with sed: H: 0-1000 O: 19:11:49 (50) AM (Top,3, Ar	ectron lons 2 results withi 0-200 Na: 5000.0,345.00,	in limits (up t 0-1 0.70,LS 10); S	o 50 best isoti im (Mn, 2x1.00)	opic matche	es for each i	nass)			1:	TOF MS ES+
100	261.1	813									4.45e+004
%-	532 246.2446	274.2743 318.3047 34	6.3318_413.2	499.3682 500.3792 735	568.5597	651.4511	771 4	507		897 4744 9	23 6030
100	200	300	400	500	600	700		800		900	1000
Minimum: Maximum:		10.0	10.0	-1.5 50.0							
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Form	ula				
261.1813	261.1855 261.1831	-4.2 -1.8	-16.1 -6.9	5.5 2.5	91.3 235.5	C17 C15	H25 H26	02 02	Na		

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



Figure S2: <sup>1</sup>H-NMR (500 MHz, CDCl<sub>3</sub>) Spectrum of **1** (isosuberosenol A)



Figure S3: <sup>13</sup>C-NMR (125 MHz, CDCl<sub>3</sub>) Spectrum of 1 (isosuberosenol A)



Figure S4: DEPT135 (125 MHz, CDCl<sub>3</sub>) Spectrum of 1 (isosuberosenol A)



Figure S5: HSQC Spectrum of 1 (isosuberosenol A)



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



Figure S7: HMBC Spectrum of 1 (isosuberosenol A)



Figure S8: HMBC Spectrum of 1 (isosuberosenol A) (From  $\delta_C$  79 ppm to  $\delta_C$  85 ppm )



Figure S9: HMBC Spectrum of 1 (isosuberosenol A) (From  $\delta_C$  38 ppm to  $\delta_C$  53 ppm )



Figure S10: HMBC Spectrum of 1 (isosuberosenol A) (From  $\delta_C$  15 ppm to  $\delta_C$  36 ppm )



**Figure S11:** <sup>1</sup>H-<sup>1</sup>H COSY Spectrum of **1** (isosuberosenol A)



Figure S12: NOESY Spectrum of 1 (isosuberosenol A)

Elementa	I Compositio	n Report							Page 1
Single Ma Tolerance Element pr Number of	ass Analysis = 10.0 mDa / rediction: Off isotope peaks u	DBE: min = - used for i-FIT	-1.5, max = = 3	50.0					
Monoisotop 74 formula( Elements U C: 0-500 28-Feb-2011 SC2-27 26 (1	ic Mass, Even Ele e) evaluated with sed: H: 0-1000 O: 21:53:25 .561) AM (Cen.3, 8	ectron lons 2 results within 0-200 Na: 0.00, Ar,5000.0,	n limits (up to 0-1 345.00,0.70,L	50 best isot S 10); Sm (Mn,	opic matches , 2x1.00); Cm	6:30)	355)	1:1	OF MS ES+
100	261.18	348							3.238+004
	243.1749								
%-		274.2760							
	218.2161	318.3011 346.	3325 463.	540.539	587.3575	659.2828	789.5090	910.5728 9	976.6016
100	200	300	400	500	600	700	800	900	1000
Minimum: Maximum:		10.0	10.0	-1.5 50.0					
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formul	a		
243.1749	243.1749 243.1725	0.0 2.4	0.0 9.9	6.5 3.5	60.9 96.3	C17 H C15 H	123 O 124 O Na		

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



Figure S14: <sup>1</sup>H-NMR (500 MHz, CDCl<sub>3</sub>) Spectrum of 2 (suberosain A)



Figure S15: <sup>13</sup>C-NMR (125 MHz, CDCl<sub>3</sub>) Spectrum of 2 (suberosain A)



Figure S16: DEPT135 (125 MHz, CDCl<sub>3</sub>) Spectrum of 2 (suberosain A)



Figure S17: HSQC Spectrum of 2 (suberosain A)



Figure S18: HSQC Spectrum of 2 (suberosain A) (From  $\delta_{\rm C}$  14 ppm to 50 ppm)



Figure S19: HMBC Spectrum of 2 (suberosain A)



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



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



Figure S22: <sup>1</sup>H-<sup>1</sup>H COSY Spectrum of 2 (suberosain A)



Figure S23: NOESY Spectrum of 2 (suberosain A)

Elemen	tal Composition	n Report								Page 1
Single I Tolerand Element Number	Mass Analysis ce = 5.0 mDa / D prediction: Off of isotope peaks u	BE: min = -	-1.5, max = 50 T = 3	0.0						
Monoisote 139 forme Elements C: 0-500 28-Feb-20 SC4-6 24	opic Mass, Even Ele ula(e) evaluated with Used: H: 0-1000 O: ( 1120:49:25 (1.437) AM (Cen,3, 80.	ctron lons 2 results wit 0-200 Na: 00, Ar,5000.0,	thin limits (up to : 0-1 ,345.00,0.70,LS	o 50 best is 10); Sm (Mn,	otopic match	es for eac	h mass	)	1: 1	FOF MS ES+
100		369.	2393							4.15e+004
%	274.2	2763				715.4	1877			
1	83.0199 246.2465	318.3011	370.2436 387.2485 388.2524	540.54	418_568.5637	712.4714	716.491	6 2 821.4826	937.7242.96	5.7711
100	200	300	400	500	600	700		800	900	1000
linimum Maximum	:	5.0	10.0	-1.5 50.0						
lass	Calc. Mass	mDa	PPM	DBE	i-FIT	For	nula			
69.239	3 369.2406 369.2430	-1.3 -3.7	-3.5 -10.0	5.5	13.5 55.1	C22 C24	H34 H33	03 Na 03		

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



**Figure S25:** <sup>1</sup>H-NMR (500 MHz, CDCl<sub>3</sub>) Spectrum of **3** (4-hydroxymethyl-5β-pregnan-3, 20-dione)



**Figure S26:** <sup>13</sup>C-NMR (125 MHz, CDCl<sub>3</sub>) Spectrum of **3** (4-hydroxymethyl-5β-pregnan-3, 20-dione)



**Figure S27:** DEPT135 (125 MHz, CDCl<sub>3</sub>) Spectrum of **3** (4-hydroxymethyl-5β-pregnan-3, 20-dione)



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



**Figure S31:** HMBC Spectrum of **3** (4-hydroxymethyl-5 $\beta$ -pregnan-3, 20-dione) (From  $\delta_{C}$  42 to 70)



**Figure S32:** HMBC Spectrum of **3** (4-hydroxymethyl-5 $\beta$ -pregnan-3, 20-dione) (From  $\delta_{\rm C}$  12 to 40)



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



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