**Isolation and Characterization of Kallosin A, A Novel Rearranged
Pseudopterane Diterpenoid from the Caribbean Sea Plume *Pseudopterogorgia*
kallos (Bielschowsky)**

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Supporting Information Available

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1. General Experimental Paragraph
2. Copies of the ^1H and ^{13}C NMR spectra for kallosin A (**1**)
3. Tables of crystal data for **1** (crystal data and structure refinement, atomic coordinates, bond lengths and angles, anisotropic displacement parameters and hydrogen coordinates).

General Experimental Paragraph. ^1H and ^{13}C NMR spectra were measured at 500 and 125 MHz, respectively. The IR spectrum was determined using a diamond cell in an IR microscope, and the UV spectrum was recorded in MeOH solution. Column chromatography was performed in silica gel (35-75 mesh) and TLC analyses were carried out using glass precoated silica gel plates. Molecular modeling was performed using the MacSpartan Pro molecular mechanics program (version 1.0.4, Wavefunction, Inc., 18401 Von Karman Ave., Suite 370, Irvine, CA 92612). All solvents used were of analytical grade. The percentage yields of natural products **1** and **2** are based on the weight of the crude gorgonian extract. The X-ray structure determination was performed on a Bruker SMART 1K CCD diffractometer. Colorless crystals of kallosin A (**1**) were obtained by slow evaporation of its EtOAc/ CHCl_3 /MeOH solution.

S3

S4

kallosin A (1)

CDCl₃

ppm

160

140

120

100

80

60

40

20

Empirical formula	C ₂₀ H ₂₄ O ₅
Formula weight	344.39
Temperature (K)	298(2)
Wavelength (Å)	0.71073
Crystal system	Monoclinic
Space group	C2 (No.5)
Unit cell dimensions	
a (Å)	16.749(4)
b (Å)	6.248(2)
c (Å)	17.816(4)
α (deg)	90
β (deg)	106.363(5)
γ (deg)	90
Volume (Å ³)	1788.8(7)
Z	4
Density (calc.) (Mg m ⁻³)	1.279
Absorption coefficient (mm ⁻¹)	0.091
F(000)	736
Crystal size (mm)	0.14 x 0.07 x 0.05
θ range for data collection (deg)	1.19 to 28.04
Index ranges	-22 ≤ h ≤ 21, -8 ≤ k ≤ 8, -23 ≤ l ≤ 15
Reflections collected	6370
Independent reflections	4154 [R(int) = 0.0311]
Independent reflections [I > 2σ(I)]	2189 [R(int) = 0.0792]
Max. and min. transmission	
Refinement method	Full-matrix least-squares on F ²
Data/restraints/parameters	4154 / 1 / 230
Goodness-of-fit on F ²	1.038
Final R indices [I > 2σ(I)]	R1 = 0.0534, wR2 = 0.1091
R indices (all data)	R1 = 0.1204, wR2 = 0.1339
Largest diff. peak and hole (e Å ⁻³)	0.144 and -0.175

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&!Table 1. Atomic coordinates [$\times 10^4$] and equivalent isotropic displacement parameters [$\text{\AA}^2 \times 10^3$] for ar031. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.&N

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	x	y	z	$U(\text{eq})$
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&J2				
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&E				
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O(1)	-945(1)	11219(4)	7595(2)	62(1)
O(2)	110(2)	4938(4)	8039(2)	67(1)
O(3)	1352(1)	6519(3)	8295(1)	51(1)
O(4)	2412(1)	11734(4)	7501(1)	55(1)
O(5)	1403(2)	13323(4)	6566(2)	73(1)
C(1)	-221(2)	9950(5)	6683(2)	48(1)
C(2)	-495(2)	9442(5)	7413(2)	52(1)
C(3)	217(2)	8854(5)	8163(2)	43(1)
C(4)	1022(2)	10030(5)	8288(2)	44(1)
C(5)	1642(2)	8676(5)	8377(2)	43(1)
C(6)	2560(2)	8844(5)	8462(2)	51(1)
C(7)	2704(2)	9585(5)	7686(2)	52(1)
C(8)	2199(2)	8302(6)	7023(2)	53(1)
C(9)	1599(2)	9459(6)	6571(2)	49(1)
C(10)	835(2)	8738(6)	5968(2)	57(1)
C(11)	170(2)	8067(5)	6351(2)	51(1)
C(12)	-945(2)	10871(6)	6041(2)	62(1)
C(13)	-834(3)	12681(7)	5686(3)	97(2)
C(14)	-1727(2)	9605(8)	5792(2)	86(1)
C(15)	511(2)	6557(6)	8135(2)	48(1)
C(16)	-116(2)	8981(6)	8885(2)	68(1)
C(17)	3061(2)	10083(6)	9176(2)	58(1)
C(18)	3754(3)	9105(8)	9653(2)	91(2)
C(19)	2828(3)	12182(7)	9327(2)	83(1)
C(20)	1751(2)	11700(6)	6833(2)	52(1)

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&!Table 2. Bond lengths [$\text{\AA}$] and angles [$^\circ$] for ar031.&H

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O(1)-C(2)	1.429(4)
O(2)-C(15)	1.199(4)
O(3)-C(15)	1.356(4)
O(3)-C(5)	1.426(4)
O(4)-C(20)	1.379(4)
O(4)-C(7)	1.435(4)

O(5)-C(20)	1.199(4)
C(1)-C(12)	1.526(5)
C(1)-C(2)	1.529(5)
C(1)-C(11)	1.543(4)
C(2)-C(3)	1.563(5)
C(3)-C(4)	1.496(4)
C(3)-C(15)	1.523(5)
C(3)-C(16)	1.543(4)
C(4)-C(5)	1.314(4)
C(5)-C(6)	1.506(4)
C(6)-C(17)	1.523(5)
C(6)-C(7)	1.541(5)
C(7)-C(8)	1.481(5)
C(8)-C(9)	1.314(5)
C(9)-C(20)	1.475(5)
C(9)-C(10)	1.489(5)
C(10)-C(11)	1.521(5)
C(12)-C(13)	1.334(6)
C(12)-C(14)	1.486(6)
C(17)-C(18)	1.373(5)
C(17)-C(19)	1.416(5)

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C(15)-O(3)-C(5)	108.0(3)
C(20)-O(4)-C(7)	108.8(3)
C(12)-C(1)-C(2)	110.6(3)
C(12)-C(1)-C(11)	109.4(3)
C(2)-C(1)-C(11)	115.4(3)
O(1)-C(2)-C(1)	109.6(3)
O(1)-C(2)-C(3)	108.2(3)
C(1)-C(2)-C(3)	115.9(2)
C(4)-C(3)-C(15)	100.4(3)
C(4)-C(3)-C(16)	111.9(3)
C(15)-C(3)-C(16)	105.8(3)
C(4)-C(3)-C(2)	116.8(3)
C(15)-C(3)-C(2)	111.7(3)
C(16)-C(3)-C(2)	109.4(3)
C(5)-C(4)-C(3)	110.5(3)
C(4)-C(5)-O(3)	111.2(3)
C(4)-C(5)-C(6)	135.8(3)
O(3)-C(5)-C(6)	112.6(3)
C(5)-C(6)-C(17)	115.2(3)
C(5)-C(6)-C(7)	110.2(3)
C(17)-C(6)-C(7)	114.1(3)
O(4)-C(7)-C(8)	104.0(3)
O(4)-C(7)-C(6)	111.0(2)
C(8)-C(7)-C(6)	110.7(3)
C(9)-C(8)-C(7)	111.0(3)
C(8)-C(9)-C(20)	107.1(3)
C(8)-C(9)-C(10)	129.0(3)
C(20)-C(9)-C(10)	123.5(3)
C(9)-C(10)-C(11)	110.4(3)
C(10)-C(11)-C(1)	114.0(3)
C(13)-C(12)-C(14)	122.6(4)
C(13)-C(12)-C(1)	119.2(4)
C(14)-C(12)-C(1)	118.0(4)
O(2)-C(15)-O(3)	121.5(3)

O(2)-C(15)-C(3) 128.7(3)
 O(3)-C(15)-C(3) 109.6(3)
 C(18)-C(17)-C(19) 121.7(4)
 C(18)-C(17)-C(6) 117.4(3)
 C(19)-C(17)-C(6) 120.9(3)
 O(5)-C(20)-O(4) 120.8(4)
 O(5)-C(20)-C(9) 130.9(4)
 O(4)-C(20)-C(9) 108.3(3)

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 &J0
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 &J3
 &H Symmetry transformations used to generate equivalent atoms:&N
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&! Table 3. Anisotropic displacement parameters [$\text{\AA}^2 \times 10^3$]
 for ar031. The anisotropic displacement factor exponent takes the form:
 $-2\text{\AA}^2 \text{Gp} [(\text{h}\text{\AA}^2) \text{U}_{11} + \dots + 2\text{h}\text{\AA} \text{b}\text{\AA} \text{U}_{12}]$
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	U11	U22	U33	U23	U13	U12
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O(1)	47(2)	50(2)	94(2)	-6(2)	27(1)	11(1)
O(2)	64(2)	37(1)	102(2)	3(1)	24(2)	-9(1)
O(3)	45(1)	31(1)	76(2)	0(1)	16(1)	1(1)
O(4)	52(2)	43(1)	73(2)	-4(1)	24(1)	-5(1)
O(5)	81(2)	43(2)	92(2)	13(1)	19(2)	-2(2)
C(1)	47(2)	37(2)	57(2)	-6(2)	10(2)	3(2)
C(2)	37(2)	40(2)	79(3)	-7(2)	17(2)	1(2)
C(3)	41(2)	37(2)	55(2)	-3(2)	19(2)	3(2)
C(4)	43(2)	31(2)	55(2)	-5(2)	12(2)	-2(2)
C(5)	41(2)	33(2)	51(2)	1(2)	9(2)	-1(2)
C(6)	39(2)	40(2)	67(2)	-3(2)	7(2)	9(2)
C(7)	42(2)	48(2)	72(2)	-4(2)	26(2)	6(2)
C(8)	50(2)	50(2)	64(2)	-13(2)	23(2)	3(2)
C(9)	50(2)	51(2)	52(2)	-5(2)	21(2)	2(2)
C(10)	69(3)	50(2)	53(2)	-6(2)	17(2)	7(2)
C(11)	59(2)	39(2)	54(2)	-8(2)	14(2)	2(2)
C(12)	59(3)	57(3)	62(2)	-10(2)	3(2)	15(2)
C(13)	111(4)	59(3)	97(4)	8(3)	-10(3)	17(3)
C(14)	56(3)	99(4)	86(3)	-20(3)	-5(2)	10(3)
C(15)	51(2)	36(2)	61(2)	2(2)	21(2)	0(2)
C(16)	71(3)	72(3)	69(3)	-2(2)	35(2)	3(2)
C(17)	40(2)	59(2)	69(3)	-5(2)	9(2)	-4(2)
C(18)	81(3)	81(3)	86(3)	-15(3)	-18(3)	16(3)
C(19)	66(3)	79(3)	94(3)	-36(3)	8(2)	1(2)
C(20)	52(2)	52(2)	59(2)	0(2)	26(2)	-5(2)

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&!Table 4. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for ar031.&H
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&C

	x	y	z	U(eq)
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&E				
&C				
H(1)	-733	12338	7506	94
H(1A)	203	11072	6829	58
H(2)	-877	8222	7289	62
H(4)	1076	11512	8302	52
H(6)	2771	7373	8540	61
H(7)	3296	9482	7714	63
H(8)	2293	6867	6938	64
H(10A)	970	7540	5679	69
H(10B)	626	9893	5601	69
H(11A)	413	7075	6772	61
H(11B)	-267	7314	5968	61
H(13A)	-1255	13197	5266	116
H(13B)	-335	13428	5860	116
H(14A)	-2089	10222	5326	129
H(14B)	-1998	9619	6200	129
H(14C)	-1599	8156	5688	129
H(16A)	286	8380	9330	101
H(16B)	-627	8192	8786	101
H(16C)	-215	10450	8990	101
H(18A)	4083	9823	10087	109
H(18B)	3893	7724	9541	109
H(19A)	2765	13051	8870	124
H(19B)	3251	12785	9756	124
H(19C)	2311	12134	9459	124

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&!Table 5. Torsion angles [$^\circ$] for ar031.&H
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