Supporting Information

Withanolide-based steroids from the cultured soft coral *Sinularia brassica*

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Table S1. Crystal data and structure refinement for cu_121107LT_0m.

Identification code	cu_121107lt_0m	
Empirical formula	C28 H38 O4	
Formula weight	438.58	
Temperature	100(2) K	
Wavelength	1.54178 Å	
Crystal system	Orthorhombic	
Space group	P 21 21 21	
Unit cell dimensions	a = 6.1962(2) Å	$\alpha = 90^\circ$.
	b = 12.5597(4) Å	$\beta = 90^\circ$.
	c = 30.5348(11) Å	$\gamma = 90^\circ$.
Volume	2376.29(14) Å ³	
Z	4	
Density (calculated)	1.226 Mg/m ³	
Absorption coefficient	0.633 mm ⁻¹	
F(000)	952	
Crystal size	0.50 x 0.45 x 0.40 mm ³	
Theta range for data collection	2.89 to 66.58°.	
Index ranges	-5<= <i>h</i> <=7, -14<= <i>k</i> <=14, -35<= <i>l</i> <=36	
Reflections collected	17041	
Independent reflections	4139 [R(int) = 0.0239]	
Completeness to theta = 66.58°	99.1 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9493 and 0.8564	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	4139 / 0 / 294	
Goodness-of-fit on F ²	1.048	
Final R indices [I>2sigma(I)]	R1 = 0.0270, wR2 = 0.0685	
R indices (all data)	R1 = 0.0272, wR2 = 0.0687	
Absolute structure parameter	0.12(14)	
Largest diff. peak and hole	0.166 and -0.130 e.Å ⁻³	

Table S2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for cu_121107LT_0m. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	205(2)	11992(1)	1707(1)	26(1)
C(2)	-1013(2)	12807(1)	1833(1)	29(1)
C(3)	-2477(2)	12700(1)	2208(1)	29(1)
C(4)	-2539(2)	11660(1)	2420(1)	28(1)
C(5)	-1350(2)	10831(1)	2290(1)	25(1)
C(6)	-1538(2)	9758(1)	2499(1)	31(1)
C(7)	-1980(2)	8892(1)	2158(1)	29(1)
C(8)	-337(2)	8912(1)	1785(1)	24(1)
C(9)	-289(2)	10032(1)	1573(1)	23(1)
C(10)	258(2)	10918(1)	1919(1)	24(1)
C(11)	1166(2)	10086(1)	1163(1)	28(1)
C(12)	701(2)	9194(1)	834(1)	29(1)
C(13)	767(2)	8097(1)	1050(1)	22(1)
C(14)	-879(2)	8104(1)	1430(1)	23(1)
C(15)	-1151(2)	6920(1)	1540(1)	28(1)
C(16)	-1200(2)	6391(1)	1086(1)	26(1)
C(17)	-178(2)	7199(1)	763(1)	24(1)
C(18)	3055(2)	7858(1)	1212(1)	28(1)
C(19)	2561(2)	10794(1)	2108(1)	29(1)
C(20)	1300(2)	6515(1)	474(1)	24(1)
C(21)	155(2)	6175(1)	54(1)	33(1)
C(22)	1873(2)	5589(1)	781(1)	24(1)
C(23)	2404(2)	4544(1)	563(1)	24(1)
C(24)	3044(2)	3608(1)	857(1)	26(1)
C(25)	4457(2)	2974(1)	536(1)	29(1)
C(26)	5536(2)	3847(1)	278(1)	30(1)
C(27)	6025(3)	2153(1)	715(1)	41(1)
C(28)	4235(2)	3931(1)	1273(1)	32(1)
O(1)	-3576(2)	13458(1)	2336(1)	39(1)
O(2)	24(2)	5422(1)	1054(1)	30(1)
O(3)	4320(2)	4741(1)	294(1)	28(1)
O(4)	7204(2)	3823(1)	76(1)	42(1)

Table S3. Bond lengths [Å] and angles [°] for cu_121107LT_0m.

C(1)-C(2)	1.3292(18)
C(1)-C(10)	1.4969(17)
C(1)-H(1)	0.9500
C(2)-C(3)	1.4671(19)
C(2)-H(2)	0.9500
C(3)-O(1)	1.2341(16)
C(3)-C(4)	1.4569(19)
C(4)-C(5)	1.3356(19)
C(4)-H(4)	0.9500
C(5)-C(6)	1.4960(18)
C(5)-C(10)	1.5133(16)
C(6)-C(7)	1.5289(18)
C(6)-H(6A)	0.9900
C(6)-H(6B)	0.9900
C(7)-C(8)	1.5270(16)
C(7)-H(7A)	0.9900
C(7)-H(7B)	0.9900
C(8)-C(14)	1.5241(16)
C(8)-C(9)	1.5497(16)
C(8)-H(8)	1.0000
C(9)-C(11)	1.5441(16)
C(9)-C(10)	1.5705(16)
C(9)-H(9)	1.0000
C(10)-C(19)	1.5484(17)
C(11)-C(12)	1.5335(16)
C(11)-H(11A)	0.9900
C(11)-H(11B)	0.9900
C(12)-C(13)	1.5284(16)
C(12)-H(12A)	0.9900
C(12)-H(12B)	0.9900
C(13)-C(18)	1.5307(17)
C(13)-C(14)	1.5424(16)
C(13)-C(17)	1.5459(16)
C(14)-C(15)	1.5349(17)
C(14)-H(14)	1.0000
C(15)-C(16)	1.5377(17)
C(15)-H(15A)	0.9900
C(15)-H(15B)	0.9900
C(16)-O(2)	1.4379(15)
C(16)-C(17)	1.5515(16)
C(16)-H(16)	1.0000
C(17)-C(20)	1.5343(17)
C(17)-H(17)	1.0000
C(18)-H(18A)	0.9800
C(18)-H(18B)	0.9800
C(18)-H(18C)	0.9800
C(19)-H(19A)	0.9800
C(19)-H(19B)	0.9800
C(19)-H(19C)	0.9800
C(20)-C(21)	1.5249(16)
C(20)-C(22)	1.5366(16)
C(20)-H(20)	1.0000
C(21)-H(21A)	0.9800
C(21)-H(21B)	0.9800
C(21)-H(21C)	0.9800
C(22)-O(2)	1.4314(14)
C(22)-C(23)	1.5076(17)

C(22)-H(22)	1.0000
C(23)-O(3)	1.4650(15)
C(23)-C(24)	1.5315(16)
C(23)-H(23)	1.0000
C(24)-C(28)	1.5232(17)
C(24)-C(25)	1.5361(18)
C(24)-H(24)	1.0000
C(25)-C(26)	1.5072(18)
C(25)-C(27)	1.5184(19)
C(25)-H(25)	1.0000
C(26)-O(4)	1.2036(17)
C(26)-O(3)	1.3532(16)
C(27)-H(27A)	0.9800
C(27)-H(27B)	0.9800
C(27)-H(27C)	0.9800
C(28)-H(28A)	0.9800
C(28)-H(28B)	0.9800
C(28)-H(28C)	0.9800
C(2)-C(1)-C(10)	125.50(12)
C(2)-C(1)-H(1)	117.2
C(10)-C(1)-H(1)	117.2
C(1)-C(2)-C(3)	120.46(12)
C(1)-C(2)-H(2)	119.8
C(3)-C(2)-H(2)	119.8
O(1)-C(3)-C(4)	122.44(12)
O(1)-C(3)-C(2)	121.13(12)
C(4)-C(3)-C(2)	116.43(11)
C(5)-C(4)-C(3)	123.53(11)
C(5)-C(4)-H(4)	118.2
C(3)-C(4)-H(4)	118.2
C(4)-C(5)-C(6)	122.27(11)
C(4)-C(5)-C(10)	121.95(12)
C(6)-C(5)-C(10)	115.78(10)
C(5)-C(6)-C(7)	111.43(10)
C(5)-C(6)-H(6A)	109.3
C(7)-C(6)-H(6A)	109.3
C(5)-C(6)-H(6B)	109.3
C(7)-C(6)-H(6B)	109.3
H(6A)-C(6)-H(6B)	108.0
C(8)-C(7)-C(6)	112.09(10)
C(8)-C(7)-H(7A)	109.2
C(6)-C(7)-H(7A)	109.2
C(8)-C(7)-H(7B)	109.2
C(6)-C(7)-H(7B)	109.2
H(7A)-C(7)-H(7B)	107.9
C(14)-C(8)-C(7)	111.96(10)
C(14)-C(8)-C(9)	108.05(9)
C(7)-C(8)-C(9)	109.83(10)
C(14)-C(8)-H(8)	109.0
C(7)-C(8)-H(8)	109.0
C(9)-C(8)-H(8)	109.0
C(11)-C(9)-C(8)	112.97(10)
C(11)-C(9)-C(10)	112.84(10)
C(8)-C(9)-C(10)	111.46(9)
C(11)-C(9)-H(9)	106.3
C(8)-C(9)-H(9)	106.3
C(10)-C(9)-H(9)	106.3
C(1)-C(10)-C(5)	112.01(10)

C(1)-C(10)-C(19)	105.82(10)
C(5)-C(10)-C(19)	108.61(9)
C(1)-C(10)-C(9)	110.04(9)
C(5)-C(10)-C(9)	108.13(10)
C(19)-C(10)-C(9)	112.28(10)
C(12)-C(11)-C(9)	112.97(10)
C(12)-C(11)-H(11A)	109.0
C(9)-C(11)-H(11A)	109.0
C(12)-C(11)-H(11B)	109.0
C(9)-C(11)-H(11B)	109.0
H(11A)-C(11)-H(11B)	107.8
C(13)-C(12)-C(11)	111.65(10)
C(13)-C(12)-H(12A)	109.3
C(11)-C(12)-H(12A)	109.3
C(13)-C(12)-H(12B)	109.3
C(11)-C(12)-H(12B)	109.3
H(12A)-C(12)-H(12B)	108.0
C(12)-C(13)-C(18)	109.95(10)
C(12)-C(13)-C(14)	107.60(10)
C(18)-C(13)-C(14)	111.84(9)
C(12)-C(13)-C(17)	113.64(9)
C(18)-C(13)-C(17)	112.99(10)
C(14)-C(13)-C(17)	100.39(9)
C(8)-C(14)-C(15)	120.76(10)
C(8)-C(14)-C(13)	113.15(10)
C(15)-C(14)-C(13)	103.47(9)
C(8)-C(14)-H(14)	106.2
C(15)-C(14)-H(14)	106.2
C(13)-C(14)-H(14)	106.2
C(14)-C(15)-C(16)	102.80(9)
C(14)-C(15)-H(15A)	111.2
C(16)-C(15)-H(15A)	111.2
C(14)-C(15)-H(15B)	111.2
C(16)-C(15)-H(15B)	111.2
H(15A)-C(15)-H(15B)	109.1
O(2)-C(16)-C(15)	114.70(10)
O(2)-C(16)-C(17)	107.11(10)
C(15)-C(16)-C(17)	106.52(9)
O(2)-C(16)-H(16)	109.5
C(15)-C(16)-H(16)	109.5
C(17)-C(16)-H(16)	109.5
C(20)-C(17)-C(13)	120.61(10)
C(20)-C(17)-C(16)	104.14(9)
C(13)-C(17)-C(16)	105.63(9)
C(20)-C(17)-H(17)	108.6
C(13)-C(17)-H(17)	108.6
C(16)-C(17)-H(17)	108.6
C(13)-C(18)-H(18A)	109.5
C(13)-C(18)-H(18B)	109.5
H(18A)-C(18)-H(18B)	109.5
C(13)-C(18)-H(18C)	109.5
H(18A)-C(18)-H(18C)	109.5
H(18B)-C(18)-H(18C)	109.5
C(10)-C(19)-H(19A)	109.5
C(10)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
C(10)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5

C(21)-C(20)-C(17)	111.19(11)
C(21)-C(20)-C(22)	114.12(10)
C(17)-C(20)-C(22)	102.13(9)
C(21)-C(20)-H(20)	109.7
C(17)-C(20)-H(20)	109.7
C(22)-C(20)-H(20)	109.7
C(20)-C(21)-H(21A)	109.5
C(20)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5
C(20)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
O(2)-C(22)-C(23)	107.70(9)
O(2)-C(22)-C(20)	106.36(10)
C(23)-C(22)-C(20)	116.05(9)
O(2)-C(22)-H(22)	108.8
C(23)-C(22)-H(22)	108.8
C(20)-C(22)-H(22)	108.8
O(3)-C(23)-C(22)	106.15(9)
O(3)-C(23)-C(24)	104.36(10)
C(22)-C(23)-C(24)	117.75(10)
O(3)-C(23)-H(23)	109.4
C(22)-C(23)-H(23)	109.4
C(24)-C(23)-H(23)	109.4
C(28)-C(24)-C(23)	114.17(10)
C(28)-C(24)-C(25)	113.17(11)
C(23)-C(24)-C(25)	99.90(9)
C(28)-C(24)-H(24)	109.7
C(23)-C(24)-H(24)	109.7
C(25)-C(24)-H(24)	109.7
C(26)-C(25)-C(27)	113.45(12)
C(26)-C(25)-C(24)	102.12(10)
C(27)-C(25)-C(24)	119.17(11)
C(26)-C(25)-H(25)	107.1
C(27)-C(25)-H(25)	107.1
C(24)-C(25)-H(25)	107.1
O(4)-C(26)-O(3)	121.17(12)
O(4)-C(26)-C(25)	129.13(12)
O(3)-C(26)-C(25)	109.70(11)
C(25)-C(27)-H(27A)	109.5
C(25)-C(27)-H(27B)	109.5
H(27A)-C(27)-H(27B)	109.5
C(25)-C(27)-H(27C)	109.5
H(27A)-C(27)-H(27C)	109.5
H(27B)-C(27)-H(27C)	109.5
C(24)-C(28)-H(28A)	109.5
C(24)-C(28)-H(28B)	109.5
H(28A)-C(28)-H(28B)	109.5
C(24)-C(28)-H(28C)	109.5
H(28A)-C(28)-H(28C)	109.5
H(28B)-C(28)-H(28C)	109.5
C(22)-O(2)-C(16)	109.76(9)
C(26)-O(3)-C(23)	109.40(9)

Symmetry transformations used to generate equivalent atoms:

Table S4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for cu_121107LT_0m. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2}U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	29(1)	28(1)	22(1)	-2(1)	1(1)	-1(1)
C(2)	33(1)	28(1)	25(1)	-4(1)	-4(1)	0(1)
C(3)	22(1)	36(1)	28(1)	-10(1)	-5(1)	3(1)
C(4)	22(1)	41(1)	22(1)	-8(1)	1(1)	-4(1)
C(5)	20(1)	36(1)	18(1)	-3(1)	-2(1)	-3(1)
C(6)	34(1)	38(1)	21(1)	1(1)	6(1)	-4(1)
C(7)	30(1)	32(1)	24(1)	1(1)	6(1)	-5(1)
C(8)	22(1)	28(1)	21(1)	2(1)	2(1)	-1(1)
C(9)	21(1)	26(1)	20(1)	0(1)	1(1)	0(1)
C(10)	22(1)	28(1)	22(1)	0(1)	2(1)	0(1)
C(11)	36(1)	24(1)	24(1)	1(1)	9(1)	-3(1)
C(12)	39(1)	26(1)	21(1)	1(1)	6(1)	-2(1)
C(13)	22(1)	24(1)	21(1)	0(1)	0(1)	-1(1)
C(14)	19(1)	27(1)	23(1)	2(1)	0(1)	-1(1)
C(15)	28(1)	29(1)	27(1)	2(1)	5(1)	-5(1)
C(16)	21(1)	25(1)	30(1)	1(1)	-1(1)	-2(1)
C(17)	24(1)	25(1)	22(1)	1(1)	-4(1)	0(1)
C(18)	21(1)	31(1)	31(1)	-8(1)	1(1)	-2(1)
C(19)	23(1)	33(1)	30(1)	-3(1)	-2(1)	-1(1)
C(20)	28(1)	24(1)	20(1)	1(1)	0(1)	-1(1)
C(21)	47(1)	28(1)	24(1)	2(1)	-8(1)	5(1)
C(22)	24(1)	27(1)	20(1)	1(1)	1(1)	-2(1)
C(23)	24(1)	27(1)	22(1)	2(1)	0(1)	-3(1)
C(24)	28(1)	25(1)	26(1)	4(1)	-2(1)	-2(1)
C(25)	35(1)	22(1)	30(1)	-2(1)	-4(1)	-1(1)
C(26)	37(1)	25(1)	28(1)	-8(1)	2(1)	0(1)
C(27)	48(1)	32(1)	44(1)	0(1)	-2(1)	10(1)
C(28)	37(1)	32(1)	25(1)	3(1)	-5(1)	4(1)
O(1)	33(1)	41(1)	44(1)	-14(1)	0(1)	10(1)
O(2)	32(1)	26(1)	33(1)	7(1)	10(1)	2(1)
O(3)	34(1)	22(1)	28(1)	0(1)	8(1)	-1(1)
O(4)	44(1)	32(1)	50(1)	-8(1)	17(1)	0(1)

Table S5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^{-3}$) for cu_121107LT_0m.

	x	y	z	U(eq)
H(1)	1120	12100	1461	32
H(2)	-936	13463	1679	34
H(4)	-3475	11568	2663	34
H(6A)	-2725	9768	2716	37
H(6B)	-182	9590	2656	37
H(7A)	-1938	8187	2302	35
H(7B)	-3446	8994	2036	35
H(8)	1125	8747	1906	28
H(9)	-1792	10179	1470	27
H(11A)	953	10782	1017	34
H(11B)	2695	10041	1255	34
H(12A)	-741	9307	702	35
H(12B)	1783	9220	595	35
H(14)	-2282	8339	1299	28
H(15A)	-2512	6791	1702	33
H(15B)	76	6655	1717	33
H(16)	-2730	6251	1000	31
H(17)	-1349	7504	575	28
H(18A)	4017	7768	960	41
H(18B)	3044	7203	1386	41
H(18C)	3569	8450	1393	41
H(19A)	3622	10866	1872	43
H(19B)	2707	10090	2244	43
H(19C)	2814	11346	2329	43
H(20)	2635	6924	399	29
H(21A)	-1183	5800	129	49
H(21B)	1097	5701	-114	49
H(21C)	-186	6806	-121	49
H(22)	3118	5806	970	28
H(23)	1176	4327	370	29
H(24)	1733	3184	935	32
H(25)	3461	2593	332	35
H(27A)	6786	1811	471	61
H(27B)	5229	1615	882	61
H(27C)	7073	2505	907	61
H(28A)	5537	4332	1195	47
H(28B)	4641	3292	1437	47
H(28C)	3292	4377	1454	47

Table S6. Crystal data and structure of sinubrasolide A (**1**)

Empirical formula	C ₂₈ H ₃₈ O ₄
Formula weight	438.58
Temperature	100(2) K
Wavelength	1.54178 Å
Crystal system	Orthorhombic
Space group	<i>P</i> 2 ₁ 2 ₁ 2 ₁ (#19)
Unit cell dimension	<i>a</i> = 6.1962(2) Å α = 90°. <i>b</i> = 12.5597(4) Å β = 90°. <i>c</i> = 30.5348(11) Å γ = 90°.
Volume	2376.29(14) Å ³
<i>Z</i>	4
Density (calculated)	1.226 Mg/m ³
Absorption coefficient	0.633 mm ⁻¹
<i>F</i> (000)	952
Crystal size	0.50 x 0.45 x 0.40 mm ³
Theta range for data collection	2.89 to 66.58°.
Reflections collected/ unique	17041
Completeness to theta = 66.58°	99.1 %
Refinement method	Full-matrix least-squares on <i>F</i> ²
Data / restraints / parameters	4139 / 0 / 294
Goodness-of-fit on <i>F</i> ²	1.048
Final <i>R</i> indices [<i>I</i> > 2σ(<i>I</i>)]	<i>R</i> ₁ = 0.0270, <i>wR</i> ₂ = 0.0685
<i>R</i> indices (all data)	<i>R</i> ₁ = 0.0272, <i>wR</i> ₂ = 0.0687
Largest diff. peak and hole	0.166 and -0.130 e.Å ⁻³