SUPPORTING INFORMATION

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Title: "Haouamines A and B: A new class of alkaloids from the ascidian *Aplidium haouarianum*"

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S-2

haouamine A (1)

S-3

haouamine A (1)

peracetyl haouamine B (2a)

peracetyl haouamine B (2a)

Table S1. Crystal data and structure refinement for haouamine A (1).

Empirical formula	$C_{32}H_{27}NO_4 \cdot 2(C_4H_4O)$	
Formula weight	553.63	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1$	
Unit cell dimensions	$a = 9.3195(18)$ Å	$\alpha = 90^\circ$.
	$b = 9.9686(19)$ Å	$\beta = 104.141(3)^\circ$.
	$c = 15.378(3)$ Å	$\gamma = 90^\circ$.
Volume	1385.4(5) Å ³	
Z	2	
Density (calculated)	1.327 Mg/m ³	
Absorption coefficient	0.091 mm ⁻¹	
F(000)	588	
Crystal size	0.36 x 0.24 x 0.15 mm ³	
Theta range for data collection	2.25 to 28.50°.	
Index ranges	$-12 \leq h \leq 12$, $-13 \leq k \leq 13$, $-20 \leq l \leq 19$	
Reflections collected	16842	
Independent reflections	6444 [R _{int} = 0.0428]	
Completeness to theta = 28.50°	94.3 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9867 and 0.9679	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	6444 / 1 / 510	
Goodness-of-fit on F ²	1.019	
Final R indices [$I > 2\sigma(I)$]	R1 = 0.0411, wR2 = 0.0944	
R indices (all data)	R1 = 0.0457, wR2 = 0.0973	
Absolute structure parameter	0.0(7)	
Largest diff. peak and hole	0.253 and -0.225 e.Å ⁻³	

Table S2. Atomic coordinates and equivalent isotropic displacement parameters for haouamine A (1).

#	x	y	z	Ueq
C1	0.54933(19)	-0.07900(18)	0.72419(12)	0.0176(3)
H1A	0.497(2)	-0.1195(19)	0.7646(12)	0.010(4)
H1B	0.551(2)	-0.147(2)	0.6750(14)	0.020(5)
C2	0.70580(19)	-0.04221(18)	-0.04221(18)	0.0159(3)
C3	0.78413(18)	-0.11562(17)	0.85637(11)	0.0161(3)
C4	0.91442(19)	-0.18271(18)	0.85576(12)	0.0173(3)
H4	0.947(2)	-0.1824(19)	0.8036(13)	0.009(4)
C5	0.99147(19)	-0.25427(17)	0.92994(12)	0.0178(4)
O5	1.11299(14)	-0.32583(13)	0.92154(9)	0.0210(3)
H5	1.169(3)	-0.350(3)	0.9779(19)	0.047(8)
C6	0.9418(2)	-0.25695(18)	1.00799(12)	0.0199(4)
H6	0.997(2)	-0.305(2)	1.0609(15)	0.022(5)
C7	C 0.8107(2)	-0.19080(19)	1.00950(12)	0.0193(4)
H7	0.773(2)	-0.193(2)	1.0642(14)	0.020(5)
C8	0.73003(19)	-0.12125(17)	0.93529(12)	0.0171(3)
C9	0.5822(2)	-0.05759(18)	0.92838(11)	0.0176(4)
C10	0.4542(2)	-0.1359(2)	0.91460(13)	0.0225(4)
H10	0.464(2)	-0.223(2)	0.9335(14)	0.021(5)
C11	0.3215(2)	-0.0897(2)	0.86006(13)	0.0240(4)
H11	0.239(3)	-0.149(3)	0.8457(15)	0.032(6)
C12	0.3161(2)	0.03618(19)	0.81967(13)	0.0218(4)
C13	0.4326(2)	0.12501(19)	0.85244(13)	0.0199(4)
H13	0.436(2)	0.216(2)	0.8252(13)	0.011(5)
C14	0.56496(19)	0.07771(18)	0.90604(12)	0.0185(4)
O14	0.68671(14)	0.15925(14)	0.92689(9)	0.0206(3)
H14	0.666(3)	0.233(3)	0.9058(19)	0.044(8)
C15	0.2217(2)	0.0647(2)	0.72692(14)	0.0242(4)
H15A	0.207(2)	0.159(2)	0.7188(13)	0.012(5)
H15B	0.130(3)	0.026(2)	0.7154(14)	0.026(6)
C16	0.3062(2)	0.0097(2)	0.65749(12)	0.0207(4)
H16A	0.286(2)	-0.089(2)	0.6521(13)	0.014(5)
H16B	0.256(2)	0.051(2)	0.5977(14)	0.024(5)
N1	0.46666(15)	0.03929(15)	0.68379(10)	0.0175(3)
C17	0.53023(19)	0.08896(19)	0.61186(12)	0.0176(4)
H17	0.516(2)	0.024(2)	0.5649(14)	0.024(5)
C18	0.4597(2)	0.2232(2)	0.57484(13)	0.0228(4)
H18A	0.356(3)	0.230(3)	0.5873(17)	0.5873(17)

#	x	y	z	Ueq
H18B	0.445(3)	0.231(2)	0.5087(17)	0.032(6)
C19	0.5669(2)	0.32961(19)	0.61939(11)	0.0198(4)
C20	0.5415(2)	0.4665(2)	0.62126(13)	0.0241(4)
H20	0.442(2)	0.499(2)	0.5980(14)	0.021(5)
C21	0.6584(2)	0.5490(2)	0.66179(13)	0.0258(4)
H21	0.643(2)	0.646(2)	0.6648(14)	0.021(5)
C22	0.7976(2)	0.4958(2)	0.69915(13)	0.0234(4)
H22	0.879(3)	0.559(3)	0.7263(15)	0.032(6)
C23	0.8225(2)	0.35778(18)	0.69763(11)	0.0181(4)
O23	1.018(3)	0.370(3)	0.7527(18)	0.044(7)
H23	0.95840(14)	0.30388(13)	0.73414(9)	0.0209(3)
C24	0.7051(2)	0.27324(18)	0.65812(11)	0.0172(3)
C25	0.77211(19)	0.05374(18)	0.73705(11)	0.0165(3)
H25	0.870(2)	0.080(2)	0.7639(13)	0.016(5)
C26	0.70273(19)	0.12108(17)	0.64866(11)	0.0160(4)
C27	0.78145(19)	0.07298(19)	0.57650(11)	
C28	0.8314(2)	-0.0586(2)	0.57877(13)	0.0219(4)
H28	0.810(2)	-0.115(2)	0.6221(17)	0.031(6)
C29	0.8925(2)	-0.1081(2)	0.51148(13)	0.0260(4)
H29	0.9296(19)	-0.2012(19)	0.5063(11)	0.003(4)
C30	0.9023(2)	-0.0272(2)	0.44000(13)	0.0244(4)
H30	0.955(2)	-0.059(2)	0.3993(15)	0.025(6)
C31	0.8511(2)	0.1040(2)	0.43659(12)	0.0224(4)
O31	0.877(3)	0.128(3)	0.3229(18)	0.046(8)
H31	0.85517(17)	0.18695(15)	0.36642(10)	0.0307(3)
C32	0.7919(2)	0.1548(2)	0.50548(12)	0.0203(4)
H32	0.760(2)	0.2476(19)	0.5066(12)	0.005(4)

Table S3. Bond lengths [Å] for haouamine A (1).

#	length	#	lengths	#	lengths
C1-N1	1.462(2)	C5-C6	1.388(3)	C11-C12	1.396(3)
C1-C2	1.513(2)	O5-H5	0.93(3)	C11-H11	0.96(2)
C1-H1A	0.967(19)	C6-C7	1.393(3)	C12-C13	1.396(3)
C1-H1B	1.02(2)	C6-H6	0.97(2)	C12-C15	1.509(3)
C2-C25	1.329(3)	C7-C8	1.389(3)	C13-C14	1.388(3)
C2-C3	1.503(2)	C7-H7	0.99(2)	C13-H13	1.00(2)
C3-C4	1.388(2)	C8-C9	1.497(2)	C14-O14	1.369(2)
C3-C8	1.424(2)	C9-C14	1.391(3)	O14-H14	0.80(3)
C4-C5	1.388(2)	C9-C10	1.398(3)	C15-C16	1.572(3)
C4-H4	0.922(19)	C10-C11	1.392(3)	C15-H15A	0.95(2)
C5-O5	1.371(2)	C10-H10	0.91(2)	C15-H15B	0.92(2)
C16-N1	1.481(2)	C20-H20	0.97(2)	C27-C32	1.385(3)
C16-H16A	1.00(2)	C21-C22	1.389(3)	C27-C28	1.389(3)
C16-H16B	1.01(2)	C21-H21	0.98(2)	C28-C29	1.388(3)
N1-C17	1.463(2)	C22-C23	1.396(3)	C28-H28	0.93(3)
C17-C18	1.538(3)	C22-H22	1.00(2)	C29-C30	1.384(3)
C17-C26	1.601(2)	C23-O23	1.364(2)	C29-H29	1.000(18)
C17-H17	0.96(2)	C23-C24	1.397(3)	C30-C31	1.388(3)
C18-C19	1.503(3)	O23-H23	0.86(3)	C30-H30	0.94(2)
C18-H18A	1.03(3)	C24-C26	1.523(3)	C31-O31	1.367(2)
C18-H18B	1.00(3)	C25-C26	1.512(2)	C31-C32	1.404(2)
C19-C20	1.387(3)	C25-H25	0.94(2)	O31-H31	0.95(3)
C19-C24	1.398(2)	C26-C27	1.548(2)	C32-H32	0.974(19)
C20-C21	1.385(3)				

Table S4. Bond angles [deg] for haouamine A (1).

#	angle	#	angle	#	angle
N1-C1-C2	111.05(15)	C6-C7-H7	119.8(12)	C12-C15-H15A	110.0(12)
N1-C1-H1A	108.3(11)	C7-C8-C3	119.10(16)	C16-C15-H15A	109.5(12)
C2-C1-H1A	111.1(11)	C7-C8-C9	125.04(16)	C12-C15-H15B	113.8(14)
N1-C1-H1B	108.7(12)	C3-C8-C9	115.72(15)	C16-C15-H15B	108.5(14)
C2-C1-H1B	110.0(12)	C14-C9-C10	117.44(17)	H151-C15-H15B	107.3(18)
H1A-C1-H1B	107.6(16)	C14-C9-C8	118.53(16)	N1-C16-C15	112.64(15)
C25-C2-C3	121.77(16)	C10-C9-C8	120.71(16)	N1-C16-H16A	111.8(11)
C25-C2-C1	117.31(16)	C11-C10-C9	120.40(18)	C15-C16-H16A	106.6(11)
C3-C2-C1	120.88(15)	C11-C10-H10	120.8(14)	N1-C16-H16B	112.3(12)
C4-C3-C8	118.62(16)	C9-C10-H10	117.8(13)	C15-C16-H16B	106.1(12)
C4-C3-C2	118.16(15)	C10-C11-C12	119.73(18)	H161-C16-H16B	106.9(17)
C8-C3-C2	123.22(15)	C10-C11-H11	118.9(14)	C1-N1-C17	109.00(13)
C3-C4-C5	121.32(16)	C12-C11-H11	121.1(14)	C1-N1-C16	110.34(14)
C3-C4-H4	118.3(12)	C11-C12-C13	117.99(17)	C17-N1-C16	115.45(14)
C5-C4-H4	120.3(12)	C11-C12-C15	122.65(18)	N1-C17-C18	111.04(14)
O5-C5-C4	117.61(16)	C13-C12-C15	116.37(17)	N1-C17-C26	110.96(13)
O5-C5-C6	121.95(16)	C14-C13-C12	119.92(17)	C18-C17-C26	104.98(14)
C4-C5-C6	120.37(17)	C14-C13-H13	116.2(11)	N1-C17-H17	109.5(13)
C5-O5-H5	109.6(16)	C12-C13-H13	121.5(11)	C18-C17-H17	110.2(13)
C5-C6-C7	118.97(16)	O14-C14-C13	120.19(17)	C26-C17-H17	110.1(13)
C5-C6-H6	121.0(13)	O14-C14-C9	118.59(16)	C19-C18-C17	105.60(15)
C7-C6-H6	120.0(13)	C13-C14-C9	120.56(17)	C19-C18-H18A	114.7(15)
C8-C7-C6	121.57(17)	C14-O14-H14	110(2)	C17-C18-H18A	108.9(14)
C8-C7-H7	118.6(12)	C12-C15-C16	107.65(15)	C19-C18-H18B	108.3(14)
C17-C18-H18B	112.9(14)	C23-O23-H23	106.7(18)	C29-C28-C27	120.85(18)
H181-C18-H18B	106.6(19)	C23-C24-C19	119.00(16)	C29-C28-H28	121.1(15)
C20-C19-C24	122.05(18)	C23-C24-C26	129.35(16)	C27-C28-H28	117.5(15)
C20-C19-C18	127.35(17)	C19-C24-C26	111.65(16)	C30-C29-C28	120.21(19)
C24-C19-C18	110.56(16)	C2-C25-C26	123.51(16)	C30-C29-H29	112.8(10)
C21-C20-C19	118.30(18)	C2-C25-H25	121.2(12)	C28-C29-H29	127.0(10)
C21-C20-H20	123.3(13)	C26-C25-H25	115.2(13)	C29-C30-C31	119.36(18)
C19-C20-H20	118.3(13)	C25-C26-C24	111.29(14)	C29-C30-H30	118.4(14)
C20-C21-C22	120.78(18)	C25-C26-C27	109.47(14)	C31-C30-H30	121.8(14)
C20-C21-H21	120.1(12)	C24-C26-C27	112.23(14)	O31-C31-C30	121.61(17)
C22-C21-H21	119.1(13)	C25-C26-C17	113.63(14)	O31-C31-C32	117.96(18)
C21-C22-C23	120.76(19)	C24-C26-C17	102.89(14)	C30-C31-C32	120.43(18)
C21-C22-H22	118.3(14)	C27-C26-C17	107.18(13)	C31-O31-H31	103.6(16)
C23-C22-H22	120.9(14)	C32-C27-C28	119.23(17)	C27-C32-C31	119.91(18)
O23-C23-C22	121.51(17)	C32-C27-C26	121.28(16)	C27-C32-H32	117.7(11)
O23-C23-C24	119.41(16)	C28-C27-C26	119.26(16)	C31-C32-H32	122.4(11)
C22-C23-C24	119.09(17)				

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ORTEP drawing of haouamine A (1)