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Supporting information for article:

The crystal structure of the lipoaminopeptaibol helioferin, an antibiotic peptide from *Mycogone rosea*

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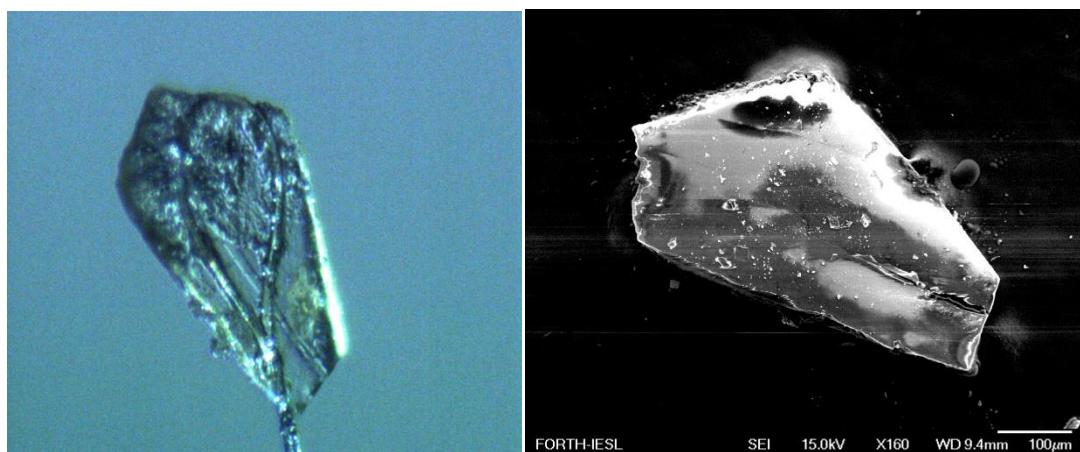


Figure S1 Crystal used for X-ray analysis and energy-dispersive X-ray spectroscopy in almost the same orientation. Left: after x-ray data collection on the mounting loop with traces of grease used for fishing and fixing, right in the EDS - facility (Jeol Scanning microscope 7000F) of IESL-FORTH, Heraklion.

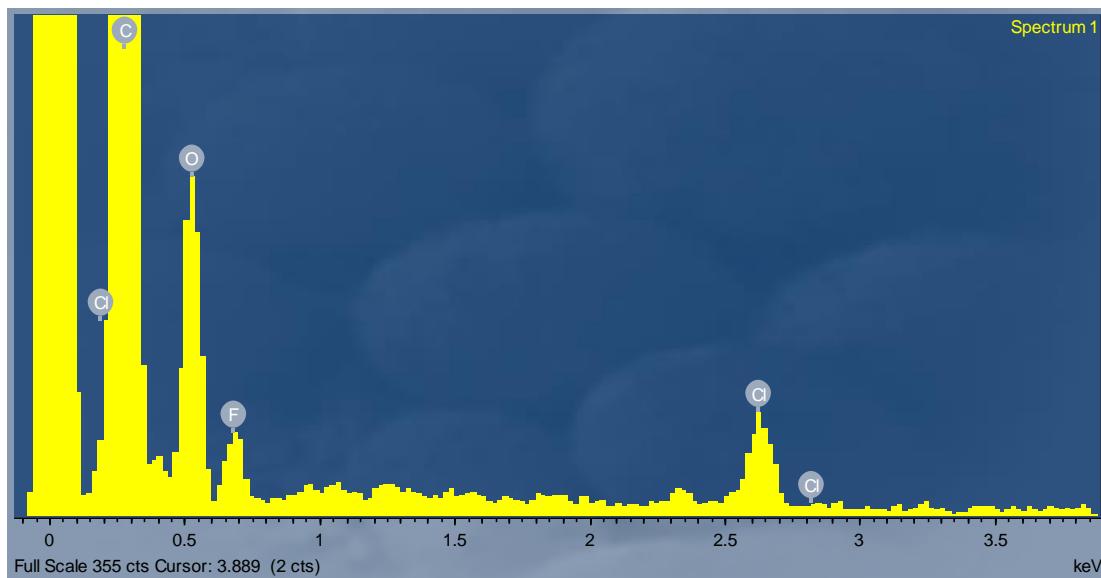


Figure S2 Energy-dispersive X-ray emission spectrum (EDS) of the above helioferin crystal, identifying the anions fluoride ($K\alpha$, 0.68) and chloride ($K\alpha$, 2.6 and $K\beta$, 2.8 keV).

Table S1 Torsion angles of helioferin (°)

	φ	ψ	ω	χ^1	χ^2	χ^3/χ^3	χ^4	θ^4	χ^5	χ^6	χ^7
Pro 1	-67(1)	-33(1)	-178.8(9)	25(1)	-38(1)	35(1)	-20(1)	-4(1)			
Ahmod 2	-73(1)	-41(1)	174.1(9)	-52(1)	-52(1)/ -176(1)	-57(1)	-58(2)/ -177(1)		-69(2)	-37(2)/ 149(1)	175(2)
Ala 3	-62(1)	-40(1)	-179.9(9)								
Aib4	-53(1)	-50(1)	-175.7(8)								
Ile 5	-63(1)	-46(1)	-177.7(9)	² 169.9(8) / ¹ -67(1)	171(1)						
Ile 6	-63(1)	-49(1)	179.6(9)	² 174(2) /145(5)/178(4) ¹ 64(2)/ -85(6) /-65(5)	-48(3)/57(8)/ 164(6)						
Aib 7	-57(1)	-49(2)	-174.2(11)								
Aib 8	-56(1)	-40(1)	178(1)*								
Apae 9	-113(3)*	57(4)/57(4)*	-173(5)/- 178(4)*	152(5)/-159(6)	61(8)/100(6)						

² Ile torsion angle N-CA-CB-CG2; ¹ Ile torsion angle N-CA-CB-CG1. The three values belong to conformation A, B and C;

* defined consecutively as follows CA-C-N-C1; C-N-C1-C2; N-C1-C2-N2; C1-C2-N2_C3; C2-N2-C3-C4; N2-C3-C4-O

Table S2 Hydrogen bond parameters of helioferin (\AA , $^\circ$)

Don-Acc*	N-H	N--O	H---O	N-H--O	H--O-C
N_4---O_0	0.8(1)	2.95(1)	2.2(1)	165(12)	157(3)
N_5---O_1	0.9(1)	3.37(1)	2.5(1)	153(9)	140(2)
N_6---O_2	0.7(1)	3.24(1)	2.5(1)	175(12)	155(3)
N_7---O_3	0.88	2.89(1)	2.0	178	164
N_8---O_4	0.8(1)	3.04(1)	2.2(1)	165(11)	150(3)
N_9---O_5	0.94(1)	3.16(1)	2.3(1)	164(11)	148(3)
N2_9a---O_6		3.12(8)			
N2_9a---O_7		2.79(7)			
N2_9b---O_6		3.07(9)			
N2_9b---O_7		2.98(6)			
intermolecular					
to -x+2,y,-z+2	O-H	O--O\$	O--H\$	O-H--O\$	
O9A---O9B	0.842	3.04(6)	2.81	74	
O9B---O9A	0.840	3.04(6)	3.16	97	

*Don: H-bond donor, Acc: H-bond acceptor; \$ symmetry related; if no estimated standard deviations are listed, the hydrogen is in riding position (H_7 on N_7, H_9 on O_9) or missing (N2_9).

Table S3 Geometric parameters of the potential interactions in the F⁻ and Cl⁻ sites

Blue denotes van der Waals and electrostatic interaction; distances and angles are either measured in Coot or calculated by Shelxl with estimated standard deviation.

Distances (Å)	Distances to F ⁻		Distances to Cl ⁻	Symmetry operation
N1-F van der Waals	3.57(1)	N1-CL	3.58(1)	x-1/2,y+1/2,z
N2-F Hydrogen bond	3.39(1)	N2-CL	3.13(1)	x-1/2,y+1/2,z
OE2-F Hydrogen bond	2.96(1)	OE2-CL	3.35(1)	x-1/2,y+1/2,z
N3_F Hydrogen bond	4.03(1)	N3-CL	3.33(1)	x-1/2,y+1/2,z
N2a_9-F electrostatic	3.52(8)	N2_9-CL	4.16	x,y,z
N2b_9-F electrostatic	3.56	N2_9-CL	4.18(7)	x,y,z
O_9a-F weak hydrogen bond	3.49(5)	O_9a-CL	3.64	x,y,z
O_9b-F weak hydrogen bond	3.45(3)	O_9b-CL	2.98(3)	-x+2,y,-z+2
Angles (°)				
N_1-F-N_2	47.3(2)	N_1-CL-N_2	48.8(2)	
N_1-F-OE_2	131.0(4)	N_1-CL-OE_2	118.5(4)	
N_1-F-N_3	71.6(2)	N_1-CL-N_3	80.4(3)	
N_1-F-N2a_9	112.4(8)	N_1-CL-N2a_9	99.	
N_1-F-N2b_9	118.	N_1-CL-N2b_9	104.	
N_1-F-Oa_9 3.50	125(1)	N_1-CL-Oa_9 3.64	120	
N_1-F-Ob_9 3.45	123	N_1-CL-Ob_9 2.98	140	-x+2,y,-z+2
N_2-F-OE_2	98.9(3)	N_2-Cl-OE_2	96.4(3)	
N_2-F-N_3	43.3(2)	N_2-CLN_3	51.3(3)	
N_2-F-N2a_9	150.3(6)	N_2-CL-N2a_9	132	
N_2-F-N2b_9	152.6(6)	N_2-CL-N2b_9	135	
N_2-F-Oa_9 3.50	156.4(9)	N_2-CL-Oa_9 3.64	169	
N_2-F-Ob_9 3.45	110.2(3)	N_2-CL-Ob_9 2.98	133	-x+2,y,-z+2
OE_2-F-N_3	110.0(3)	OE_2-CL-N_3	119.2(3)	
OE_2-F-N2a_9	79.5(8)	OE_2-CL-N2a_9	66	
OE_2-F-N2b_9	76	OE_2-CL-N2b_9	64	
OE_2-F-Oa_9 3.50	99(1)	OE_2-CL-Oa_9 3.64	90	
OE_2-F-Ob_9 3.45	99	OE_2-CL-Ob_9 2.98	101	-x+2,y,-z+2
N_3-F_N2a_9 3.52	164.1(6)	N_3-F_N2a_9	174.0(5)	
N_3-F_N2b_9 3.56	162	N_3-F_N2b_9	173	
N_3-F-Oa_9 3.50	115.5(7)	N_3-CL-Oa_9	132.1(5)	

N_3-F-Ob_9 3.45	67	N_3-CL-Ob_9	82	-x+2,y,-z+2
N2a_9-F-Ob_9	99	N2a_9-CL-Ob_9	94	-x+2,y,-z+2
N2b_9-F-Oa_9	78	N2b_9-CL-Oa_9	74	-x+2,y,-z+2
Oa_9-F-Ob_9	52	Oa_9-CL-Ob_9SR	53	-x+2,y,-z+2
Ob_9-F-Oa_9	38	Ob_9-CL-Oa_9	37	-x+2,y,-z+2