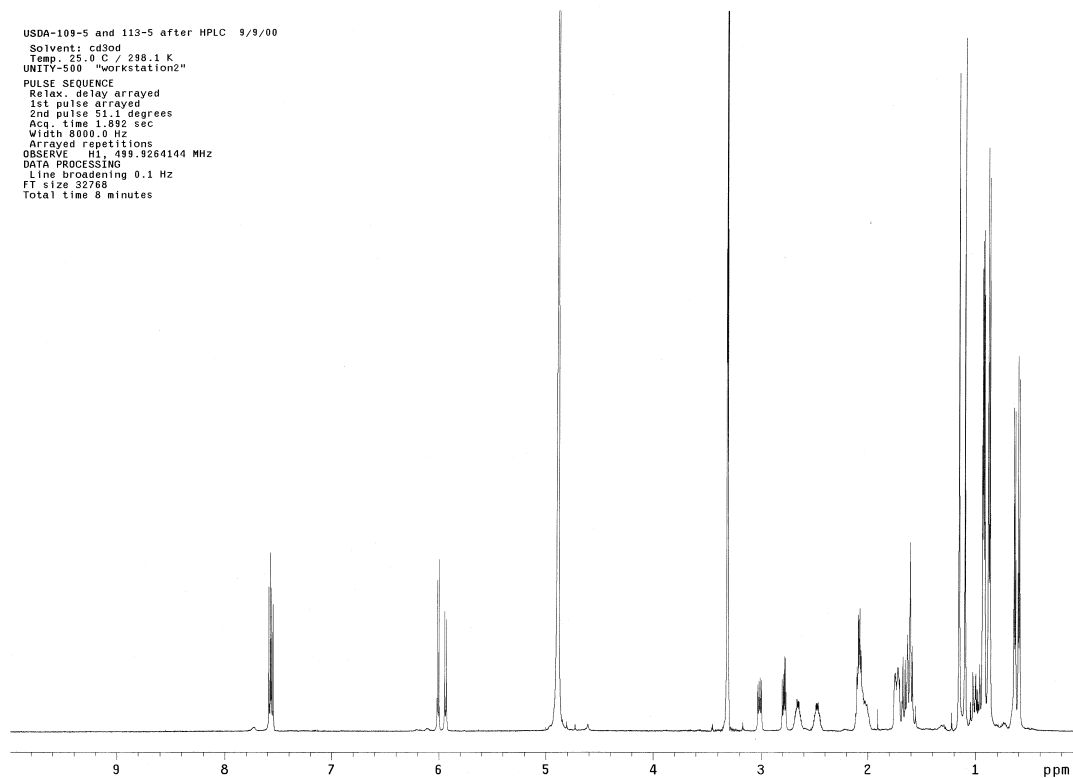


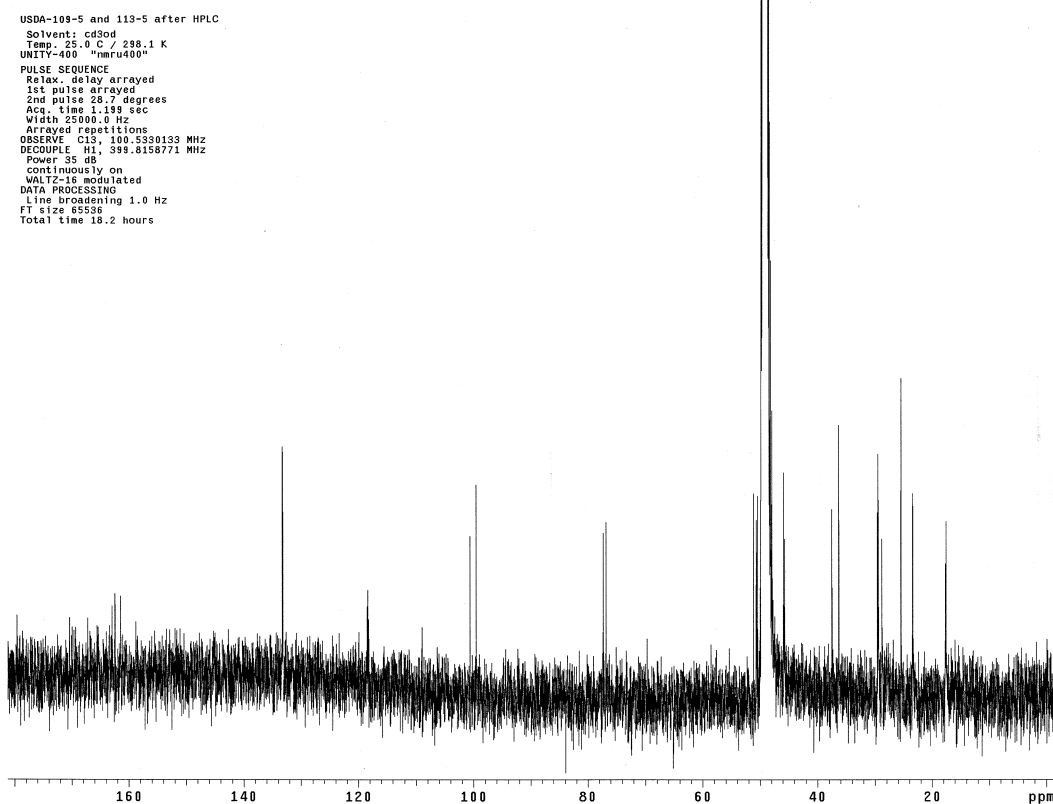
Supplementary Material for

Akanthomycin, a New Antibiotic Pyridone from the Entomopathogenic Fungus *Akanthomyces gracilis*

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Akanthomycin (2) – ^1H NMR

Akanthomycin (2) – ^{13}C NMR

Crystal Data and Structure Refinement for 8-methyl-pyridoxatin (**1a**)

Identification code	8-methyl-pyridoxatin (1a)
Empirical formula	C ₃₂ H ₄₆ N ₂ O ₆
Formula weight	554.71
Temperature	173(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	P2(1)
Unit cell dimensions	a = 13.0949(13) Å $\alpha = 90^\circ$. b = 9.7982(10) Å $\beta = 112.057(2)^\circ$. c = 13.3094(13) Å $\gamma = 90^\circ$.
Volume	1582.7(3) Å ³
Z	2
Density (calculated)	1.164 Mg/m ³
Absorption coefficient	0.080 mm ⁻¹
F(000)	600
Crystal size	0.40 x 0.30 x 0.20 mm ³
Theta range for data collection	1.65 to 28.54°.
Index ranges	-16 ≤ h ≤ 17, -13 ≤ k ≤ 8, -17 ≤ l ≤ 16
Reflections collected	10127
Independent reflections	5318 [R(int) = 0.0225]
Absorption correction	SADABS
Max. and min. transmission	1 and 0.793769
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	5318 / 1 / 545
Goodness-of-fit on F ²	0.894
Final R indices [I > 2σ(I)]	R1 = 0.0343, wR2 = 0.0732
R indices (all data)	R1 = 0.0448, wR2 = 0.0761
Absolute structure parameter	0.04(76)
Largest diff. peak and hole	0.168 and -0.196 e.Å ⁻³

Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 8-methyl-pyridoxatin (**1a**). U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
O(1)	2982(1)	9032(1)	898(1)	31(1)
O(1')	7929(1)	11389(1)	732(1)	26(1)
O(2)	1746(1)	9040(2)	-1181(1)	34(1)
O(2')	6551(1)	11475(2)	-1300(1)	32(1)
O(3)	42(1)	10911(2)	1711(1)	42(1)
O(3')	5204(1)	9139(2)	1692(1)	32(1)
N(1)	1328(1)	9494(2)	-420(1)	28(1)
N(1')	6209(1)	11026(2)	-486(1)	26(1)
C(1)	2024(1)	9539(2)	653(1)	26(1)
C(1')	6981(1)	10884(2)	549(1)	22(1)
C(3)	270(2)	9914(2)	-807(2)	32(1)
C(3')	5142(2)	10653(2)	-797(2)	31(1)
C(4)	-177(2)	10393(2)	-116(2)	34(1)
C(4')	4787(1)	10050(2)	-83(2)	30(1)
C(5)	485(1)	10471(2)	1003(2)	31(1)
C(5')	5544(1)	9796(2)	982(1)	25(1)
C(6)	1595(1)	10105(2)	1393(1)	28(1)
C(6')	6646(1)	10189(2)	1316(1)	22(1)
C(7)	2398(1)	10267(2)	2561(1)	30(1)
C(7')	7530(1)	9932(2)	2431(1)	25(1)
C(8)	1982(2)	9719(3)	3427(2)	47(1)
C(8')	7618(2)	8431(2)	2815(2)	31(1)
C(9)	2923(2)	9802(3)	4540(2)	57(1)
C(9')	8639(2)	8268(2)	3860(2)	36(1)
C(10)	3399(2)	11213(3)	4818(2)	59(1)
C(10')	8701(2)	9268(2)	4753(2)	36(1)
C(11)	3793(2)	11744(3)	3943(2)	44(1)
C(11')	8590(1)	10720(2)	4320(2)	30(1)
C(12)	2900(2)	11737(2)	2786(1)	33(1)
C(12')	7533(1)	10979(2)	3317(1)	25(1)
C(13)	3463(2)	12011(2)	2001(2)	34(1)
C(13')	7612(2)	12397(2)	2912(1)	28(1)
C(14)	3277(2)	12985(3)	1289(2)	58(1)
C(14')	6895(2)	13393(2)	2705(2)	41(1)
C(15)	1558(3)	8260(4)	3167(3)	69(1)
C(15')	7692(2)	7458(2)	1948(2)	44(1)
C(16)	4351(3)	11255(5)	5936(2)	84(1)
C(16')	9765(2)	9108(3)	5746(2)	50(1)
C(17)	2031(2)	12840(3)	2686(2)	44(1)
C(17')	6519(2)	10857(2)	3633(2)	32(1)

Crystal Data and Structure Refinement for 8-methyl-pyridoxatin (**1b**)

Identification code	8-methyl-pyridoxatin (1b)	
Empirical formula	C ₃₄ H ₅₄ N ₂ O ₈	
Formula weight	618.79	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)	
Unit cell dimensions	a = 8.1721(16) Å	α = 90°.
	b = 23.097(4) Å	β = 95.725(17)°.
	c = 9.307(2) Å	γ = 90°.
Volume	1748.0(6) Å ³	
Z	2	
Density (calculated)	1.176 Mg/m ³	
Absorption coefficient	0.083 mm ⁻¹	
F(000)	672	
Crystal size	0.20 x 0.20 x 0.05 mm ³	
Theta range for data collection	2.20 to 23.26°.	
Index ranges	-9 ≤ h ≤ 8, -25 ≤ k ≤ 25, -10 ≤ l ≤ 10	
Reflections collected	12175	
Independent reflections	4988 [R(int) = 0.0311]	
Completeness to theta = 23.26°	99.7 %	
Absorption correction	SADABS	
Max. and min. transmission	0.9959 and 0.866803	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	4988 / 1 / 454	
Goodness-of-fit on F ²	0.981	
Final R indices [I > 2σ(I)]	R1 = 0.0381, wR2 = 0.0896	
R indices (all data)	R1 = 0.0484, wR2 = 0.0953	
Absolute structure parameter	0.9(9)	
Largest diff. peak and hole	0.222 and -0.133 e.Å ⁻³	

Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 8-methyl-pyridoxatin (**1b**). U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
O(1)	-684(2)	11416(1)	1862(2)	45(1)
O(2)	-2661(2)	10522(1)	1295(2)	53(1)
O(3)	-1089(2)	11880(1)	-3127(2)	41(1)
N(2)	-2164(3)	10866(1)	193(2)	38(1)
C(1)	-1193(3)	11341(1)	543(3)	37(1)
C(3)	-2797(3)	10723(1)	-1154(3)	37(1)
C(4)	-2470(3)	11059(1)	-2274(3)	36(1)
C(5)	-1476(3)	11549(1)	-2011(2)	32(1)
C(6)				