Supporting Information

Heliconols A-C: Antimicrobial Hemiketals from the Freshwater Aquatic Fungus *Helicodendron giganteum* Glen-Bott (Helotiaceae)

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Figure S1. ^1H NMR spectrum of heliconol A (**1**; DMSO- d_6 , 600 MHz)

Figure S2. ^{13}C NMR spectrum of heliconol A (**1**; DMSO- d_6 , 100 MHz)

Figure S3. ^1H NMR spectrum of heliconol B (**2**; DMSO- d_6 , 600 MHz)

Figure S4. ^{13}C NMR spectrum of heliconol B (2; DMSO- d_6 , 100 MHz)

Figure S5. ^1H NMR spectrum of heliconol C (**3**; DMSO- d_6 , 600 MHz)

Figure S6. ^{13}C NMR spectrum of heliconol C (**3**; DMSO- d_6 , 100 MHz)

Figure S7. ^1H NMR spectrum of 4,6-*bis*-(4-bromobenzoyl)-heliconol A (**4**; CDCl_3 , 300 MHz)

Table S1. Crystal Data and Structure Refinement for 4,6-*bis*-(4-bromobenzoyl)-heliconol A (**4**)

Identification code	glo54c
Empirical formula	C ₃₀ H ₃₆ Br ₂ O ₇
Formula weight	668.41
Temperature	190(2) K
Wavelength	0.71069 Å
Crystal system, space group	Triclinic, <i>P</i> 1
Unit cell dimensions	a = 7.6340(8) Å alpha = 90.371(5) deg. b = 11.1342(11) Å beta = 80.428(5) deg. c = 17.5418(17) Å gamma = 87.904(5) deg.
Volume	1469.2(3) Å ³
Z, Calculated density	2, 1.511 Mg/m ³
Absorption coefficient	2.804 mm ⁻¹
F(000)	684
Crystal size	0.17 × 0.13 × 0.03 mm
Theta range for data collection	2.7 to 20.00 deg.
Limiting indices	-7 ≤ h ≤ 7, -10 ≤ k ≤ 10, -16 ≤ l ≤ 16
Reflections collected / unique	15483 / 5107 [<i>R</i> _{int} = 0.093]
Completeness to theta = 20.00	98.2%
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9332 and 0.6472
Refinement method	Full-matrix least-squares on F ²

Data / restraints / parameters	5107 / 80 / 663
Goodness-of-fit on F^2	1.079
Final R indices [$I > 2\sigma(I)$]	$R_1 = 0.0624$, $wR_2 = 0.1272$
R indices (all data)	$R_1 = 0.0840$, $wR_2 = 0.1395$
Absolute structure parameter	0.008(17)
Largest diff. peak and hole	0.471 and -0.535 e. $\text{\AA}^{-3}$

Detailed Account of Disorder in the Crystal of 4,6-*bis*-(4-bromobenzoyl)-heliconol A (4)

Disorder of the C7-nonyl substituent in both molecules and in the C1-C5-C6-C7-O ring of molecule A [ring atoms of the second conformation indicated by a “#” in their atom labels, disorder is 0.542 (9)/0.458 (9)]. The C7A-nonyl substituent is disordered following the ring disorder, the “A” atom label suffix being associated with the first (major) ring conformation and the “C” suffix being associated with the second ring conformation (corresponding to “#” designation in ring atom labels). There is a further complication in that the major conformation splits into a third disorder conformation after C9A. This third disorder conformation is indicated by “E” as an atom label suffix. After C11E the third disorder conformation closely parallels the second conformation (“C” suffix) and was merged for the final cycles of refinement. The C7B-nonyl substituent was also disordered after the C9B atom with the minor disorder conformation indicated with “D” suffix in atom labels. This disorder refined to 0.62 (17)/0.38 (17). Due to high thermal motion and to limit the total number of model parameters, the nonyl C atoms were given isotropic thermal parameters that were restrained to be 10% larger than that of the atom preceding it on the chain [i.e., $U_{\text{iso}}(\text{C10A}) = 1.1 U_{\text{iso}}(\text{C9A})$, etc.]. Additionally, disordered sites were assigned the same thermal parameter [i.e., $U_{\text{iso}}(\text{C12A}) = U_{\text{iso}}(\text{C12C}) = U_{\text{iso}}(\text{C12E})$]. To preserve a physically reasonable model, the C-C distances in the nonyl substituents were restrained to be 1.54 Å and the C-C-C 1,3 distances were restrained to be 2.515 Å (this restrains the angles to be tetrahedral). No further restraints or constraints were imposed on the refinement model.

Figure S8. X-ray Model of 4,6-*bis*-(4-bromobenzoyl)-heliconol A

(4) Showing Intermolecular Interactions in the Crystal

Figure S9. Thermal Ellipsoid Representation of 4,6-*bis*-(4-bromobenzoyl)-heliconol A (**4**) with Atom Label Suffix “B”

Figure S10. X-Ray Model of 4,6-*bis*-(4-bromobenzoyl)-heliconol

A (4) Depicting Disorder with Atom Label Suffixes “A”, “#”, ^a “C”, and “E”

^a The suffix “#” is placed on O1A and the ring oxygen depicting disorder in the ring conformation.

Figure S11. X-Ray Model of 4,6-*bis*-(4-bromobenzoyl)-heliconol

A (4) Depicting Disorder with Atom Label Suffices “B” and “D”