THE CRYSTAL STRUCTURES OF ACTH 4-10 AND ACTH 4-10

The backbone structure of ACTH 4-10 could be determined by visual inspection of the Patterson synthesis and extension of the fragment found by the program DIDDIF. This structure has been presented at earlier conferences (Admiraal, Verweij and Vos, Abstracts Sixth European Crystallographic Meeting, Barcelona, Spain, 5/25).

The linear polypeptide ACTH 4-7 (Met-Glu-His-Leu), molecular formula C_{14}H_{13}N_{4}O_{7} S_{3} H_{2}O crystallizes in the monoclinic space group C2 with a^2 = 23.333(6), b = 5.674(11) Å, c = 24.783(5) Å, B = 115.03(2)°, Z = 4, d(calc) = 1.33 g.cm^{-3}. The structure determination proved to be difficult. Both MOLTN and symbolic addition by the program SHELX (H. Schenk et al., Amsterdam, The Netherlands) failed to give a solution. Reliable peaks corresponding with S----S distances were not found in sharpened Patterson syntheses. Patterson search for a dispeptide fragment (C---C---C---C---C---C---C---C) for various values of the torsion angles Θ = C-N-C-C and Ψ = N-C-C-C gave by far the best fit for Θ = -90 and Ψ = -33°. With this fragment as starting point the structure was solved by DIDDIF. Anisotropic refinement gave R = 5.8%.

The structure of the molecule is shown in the figure. At C (His) the conformation of the peptide backbone is extended (β = -172, γ = 171°) and at the other C atoms there are helix type bands. The Nat and the side chains show disorder. Difference Fourier revealed peaks for all Nat atoms, indicating that the NH2 and the His group are protonated. The CO2 groups of Ser is hydrogen bonded to NH2 via a water molecule. No further solvent molecules were discovered in the difference maps.

Successive molecules in the crystal are linked by hydrogen bonds along b and c. At Oxy (Oxy) successive layers of molecules interact via hydrogen bonds and at (lys) by hydrophobic forces. The conformation of the molecule will be compared with that of other tetrapeptides and the hydrogen bonds in the crystal will be described in more detail.

THE CRYSTAL AND MOLECULAR STRUCTURE OF THE SIDEROPHORE PERICUS PSEUDOBACTIN. By M. B. Hossain, C. L. Barnes, D. van der Helm, M. Teintze and J. Leong. Chemistry Departments University of California, Morehead, UK, 79203, USA and University of California, San Diego, La Jolla, CA, 92039, USA.

Previously it was shown 1,2 that pseudobactin, the siderophore of a specific plant growth-promoting Pseudomonas strain, is able to mimic the plant growth enhancement of its producer.

Perricus pseudobactin (C_{16}H_{30}O_{22}Fe), crystallizes in space group I2, a = 29.006(23), b = 14.511(13), c = 28.791(21), β = 96.05(5), with 2 molecules and 26 water molecules in the asymmetric unit. All 1296 unique data (8999 with I > 2σ(I)) with 20 ≤ 50° using MoKα, were taken at -135°C. Final R-factor is 0.06.

The structure consists of a linear hexapeptide, L-Lys-D-threo-S-OH-Asp-L-Ala-D-allo-Thr-L-Ala-D-Ala-L-Val, in which the orimine is cyclized, and the 


The membrane exciting peptide antibiotics alamethicin, suzukacillin and trichotoxin include N-terminal helices, according to their 13C-NMR and CO-spectra. All data have been interpreted in terms of α-helices, but some authors have argued that these peptides, containing the unusual amino acid 2-methylalanine (=Aib), may show 3₁₀-helical N-termini, because short peptides with Aib-residues crystallize with incipient 3₁₀-helix conformations.

We have synthesized and crystallized the following model of the alamethicin N-terminus: Boc-L-Ala-Aib-L-Ala-Aib-L-Ala-L-Glu(0Bu1)-L-Ala-Ala-L-Ala-D-Val and Boc-L-Ala-Aib-L-Ala-Aib-L-Ala-L-Glu. 1

1 crystallizes in P2₁, Z = 2 and 6 dichloroethane solvent molecules. The solution of the phase problem by direct methods proved to be very difficult (90 nonhydrogen atoms), but was recently achieved by a novel random-phases + E-Fourier recycling procedure. The current R-value in isotropic refinement is 0.128 for 4272 observations with F > 3σ(F).

Nine of the eleven amino acids are part of a α-helix, only the last two C-terminal amino acids form a β-turn.