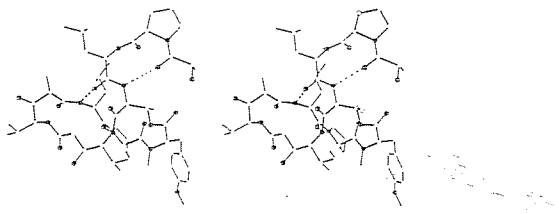
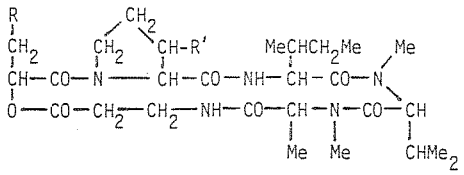
7699 reflections, $2\theta_{max}$ = 150° at 138K. Structure was determined by direct methods (G.M. Sheldrick, "SHELXS-86") and refined by block-diagonal least-squares to a final R = 0.046 for 7074 observed reflections.



03.2-9 THE CRYSTAL STRUCTURE OF DESTRUXIN B. By J. L. Rios Steiner and C. L. Barnes, Department of Chemistry, University of Puerto Rico, Rio Piedras, P.R., U.S.A. 00931.

The destruxins are a family of cyclohexadepsipeptides produced by the entomapathogenic fungus Metarrihzium anisopliae (Pais, M., et al, Phytochemistry, 1981, 20, 715-723). The molecular structure of Destruxin B, a member of this family, is shown below. The backbone conformation of Destruxin B is very similar to that of Roseotoxin B. a related mycotoxin isolated from cultures of Tricothecium roseum (Springer, J. P., et al, J. Am. Chem. Soc., 1984, 106, 2388-2392).



Destruxin B R = $CHMe_2$ R′ = H

Roseotoxin B R = $CH=CH_2$ R′ = Me

Intensity data were collected on an Enraf-Nonius Cad4 diffractometer at room temperature using CuK_α radiation to $2\theta_{max}$=150°. The structure was solved using Direct Methods and refined to a final unweighted R of 5.1% for 3718 observed reflections ($I>3\sigma(I)$).

03.2-10 THE CONFORMATION OF THIOAMIDE CONTAINING PEPTIDES. By Troels la Cour, Department of Chemistry, Aarhus University, Denmark.

Endothiopeptides are oligopeptides in which one or more oxyacyl moities in peptide groups are replaced with thioacyl moities. The paper will describe results from structural studies of small thiopeptide containing peptides. It is shown that the geometry of the peptide backbone is unaffected by this replacement and that the conformations of (ϕ, ψ) around C_α carbon atoms in proteins are also stereochemically favourable for thiopeptides.

The use of thiopeptide analogs of naturally occurring peptides could be of benefice in the study of for example structure/function relationship in enzymic catalysis. Another application of this type of peptide modification is in the field of medicinal chemistry, since the digestion pattern of thiopeptides is different from that of normal dietary proteins.

03.2-11 PREFERRED CONFORMATIONAL STATES OF GLYCINE - CONTAINING PEPTIDES. By E. Subramanian, Department of Crystallography and Biophysics, University of Madras, Madras 600025 and V. Ganesh, Department of Physics, Indian Institute of Technology, Madras 600036, India.

The crystal structures of several tripeptides with defined sequences have been analysed to investigate the influence of immediate neighbours on the conformational states of a given residue. In view of the numerous possible tripeptides (20x20x20 = 8000), the analysis has been restricted to the subsets of tripeptide sequences such as x-gly-gly and gly-gly-x in order to determine the conformational preferences of the middle glycine residue. Presently, crystal structure studies are available for pro-gly-gly (V. Lalitha, E. Subramanian and R. Parthasarathy, Int. J. Peptide Protein Res., 1986, 27, 223), val-gly-gly (V. Lalitha, R. Murali and E. Subramanian, Int. J. Peptide Protein Res., 1986, 27, 472), ala-gly-gly (E. Subramanian, and V. Lalitha, Biopolymers, 1983, 22, 833), leu-gly-gly (K.N. Goswami, V.S. Yadava and V.M. Padmanabhan, Acta Cryst., 1977, B33, 1280), trp-gly-gly (E. Subramanian, unpublished), tyr-gly-gly (W.M. Carson and M.L. Hackert, Acta Cryst., 1978, B34, 1275), leu-gly-gly-gly (T. Srikrishnan and R. Parthasarathy, unpublished), gly-gly-val (V. Lalitha, E. Subramanian and J. Bordner, Int. J. Peptide Protein Res., 1984, 24, 437), gly-gly-ile (V. Lalitha, E. Subramanian and J. Bordner, Int. J. Peptide Protein Res., 1984, 24, 123), gly-gly-phe (R. Murali and E. Subramanian, Int. J. Peptide Protein Res., 1987, in press) and gly-gly-gly (V. Lalitha and E. Subramanian, Cryst. Str. Commun., 1982, 11, 561). We find that the middle glycine adopts a 'D-residue' type of conformation when preceded or followed by a residue with aromatic side-chain or a side-chain with branching at C^γ atom. Empirical energy calculations also confirm this observation.