the center of the peptide molecule. This structure might represent one of the steps involved in the shuttle mechanism of ion transport where the ion is captured at one end of a channel and transported to the other end by the conformational change that allows the ion to be released and recaptured.

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03.1–12 CONFORMATION OF DIASTEREOISOMERIC OCTAPEPTIDES, CYCLO-(D-ALA-GLY-L-PRO-L-PHE)$_2$ AND CYCLO-(D-ALA-GLY-L-PRO-D-PHE)$_2$. K.K. Bhandary and G. Kartha, Biophysics Department, Roswell Park Memorial Institute, Buffalo, New York 14263, USA and K.D. Kopple Department of Chemistry, Illinois Institute of Technology, Chicago, Ilinois, USA 60616.

The diastereomeric cyclic octapeptides, cyclo-(Ala-Gly-L-Pro-Phe)$_2$, were synthesized by Kopple et al.[1] in order to produce cyclic octapeptide backbones of C_2 symmetry. We report here the conformations of two cyclic octapeptides, cyclo-(D-Ala-Gly-L-Pro-L-Phe)$_2$ and cyclo-(D-Ala-Gly-L-Pro-D-Phe)$_2$ as determined by x-ray crystallographic techniques.

The octapeptides contain two β-turns, encompassing L-Pro-Phe residues, connected by straight stretches of D-Ala-Gly residues. As expected, in the cyclo-(D-Ala-Gly-L-Pro-L-Phe)$_2$ there are two type I β-turns while in cyclo-(D-Ala-Gly-L-Pro-D-Phe)$_2$ there are two type II β-turns. The peptide links in both the structures are trans with the non-planarity parameter ω deviating as much as 9°. In the crystalline state both the peptides show an approximate two fold symmetry.

When crystallized from a solution containing sodium thiocyanate the octapeptide cyclo-(D-Ala-Gly-L-Pro-L-Phe)$_2$ shows a change in the backbone conformation. The approximate 2-fold symmetry observed in the absence of sodium thiocyanate is destroyed in the straight stretches of D-Ala-Gly. The major differences in the two stretches occur in the ψ of D-Ala (changes from 179° to 30°) and φ of Gly (changes from 124° to -70°). When compared with the structure of cyclo-(D-Ala-Gly-L-Pro-D-Phe)$_2$, the backbone torsion angles of one straight stretch from the link with D-Phe-D-Ala to the link Gly-L-Pro compares well while the other stretch compares well with the 2-fold symmetric structure of c(D-Ala-Gly-L-Pro-L-Phe)$_2$. All the peptide links are trans with the non-planarity parameter ω between Gly and L-Pro varying by 13°.

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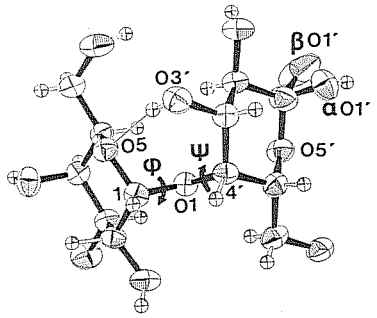
03.1–13 CRYSTAL STRUCTURE OF GALABIOSE: AN INTERNAL PART OF THE FORSSMAN ANTIGEN. By G. Svensson, J. Albertsson, C. Svensson, Inorganic Chemistry 2 and G. Magnusson, Organic Chemistry 2, Chemical Center, University of Lund, P.O.Box 740, S-220 07 Lund, Sweden

The disaccharide unit α-D-galactopyranosyl-(1→4)-β-D-galactopyranose (β-galabiose) is an integral part of several naturally occurring glycolipids present at mammalian cell surfaces. It constitutes for example the terminal portion of blood group P antigens and an internal part of the Forssman antigen. Uropathogenic *E. coli* bacteria use this disaccharide unit as a specific receptor in adhesion to epithelial cells of the human urinary tract (1,2). The present X-ray structure determination of galabiose reveals the conformation about the Galα1 → 4Gal glycosidic linkage (figure below). The crystals (3) are orthorhombic, space group $P2_12_12_1$ with a = 5.826(1), b = 13.904(3) and c = 17.772(4) Å; conventional R = 0.063 for 2758 observed reflections.

Both C-O bonds of the glycosidic linkage are axial with a τ angle (C1-O1-C4') of 117.5°. The ϕ^H and ψ^H torsion angles are H1-C1-O1-C4' = -18.9° and H4'-C4'-O1-C1 = 34.9°; the corresponding ϕ^{O5} and $\psi^{C3'}$ angles are O5-C1-O1-C4' = 98.1(2)° and C3'-C4'-O1-C1 = -81.9(3)°. The virtual torsion angle between the anomeric and aglyconic hydrogen atoms (H1 and H4') is 18.7°. The conformation is stabilized by an O3'···O5 intramolecular hydrogen bond of 2.787(3) Å with the C3'-O3'···O5 and C5-O5···O3' angles 101.6(1) and 120.7(2)° respectively. The geometry of the Galα1 → 4Gal linkage, with an angle 116.5° between the least-squares planes through the six-rings, causes a characteristic folding of the Forssman antigen.



Galabiose

The structure is disordered, containing about equal amounts of α (57 %) and β-galabiose (43 %). Further, the C6-OH groups exist both in *gauche-trans* (≈70 %) and in *trans-gauche* (≈30 %) conformation. The crystal packing is governed by hydrogen bonds engaging all oxygen atoms except the intramolecular acceptor O5 and the glycosidic O1.

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