02.1-54 LOW-RESOLUTION STRUCTURE OF PISUM SATIVUM AGGLUTININ. E. J. Meehan, Jr., Chemistry Department, University of Alabama in Huntsville, Huntsville, AL 35807. H. Einspahr, F. L. Suddath and C. E. Bugg, Biochemistry Department, University of Alabama in Birmingham, Birmingham, AL 35205

The amino acid sequences of the mitogenic lectins from the green pea, Pisum sativum Agglutinin (PsA) and the jack bean, concanavalin A (Con A) appear to be circularly permuted. This affords a unique opportunity for examining the interdependent influences of primary, secondary, and tertiary structure. PsA has been isolated by affinity chromatography and its physical and biological properties characterized. Very large single crystals of PsA have been grown from polyethylene glycol solutions. The crystals are orthorhombic space group $P2_12_12_1$ and diffract to 1.8 Å resolution. The unit-cell parameters are a = 50.85(5), b = 61.23(5), and c = 137.3(2) Å. The density of the PsA crystals is 1.196 g cm^{-3} and there is one complete PsA molecule, a dimer (49,000 daltons), per asymmetric unit. The crystalline volume/mass ratio is 2.20 $Å^3$/dalton. Six-angstrom data from native crystals and from a uranyl derivative have been collected with a Picker FACS-1 diffractometer. The coordinates of the uranium atom were obtained from a three-dimensional Patterson map and refined by least-squares techniques to an R index of .45. A three-dimensional Fourier synthesis was calculated with phases obtained from the single isomorphous derivative together with its anomalous component. The low-resolution structure of PsA is strikingly similar to that of Con A. Three-angstrom native data collection is in progress.

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02.1-55 STRUCTURAL PREDICTION OF SUGAR-BINDING PROTEINS FUNCTIONAL IN CHEMOTAXIS AND TRANSPORT. P. Argos, W. C. Mahoney and M. A. Hermodson. Department of Biological Sciences, Purdue University, West Lafayette, Indiana 47907, U.S.A.

Comparisons of the D-galactose- and D-ribose-binding protein amino acid sequences and secondary structure predictions with the known primary and three-dimensional structure of L-arabinose-binding protein suggest that the three proteins have similar molecular structures. These studies also indicate an evolutionary relationship among the proteins. One region of striking homology between the galactose- and ribose-binding proteins suggests that this may be the protein-protein contact site for interaction with the membrane-bound chemotaxis receptor. The ligands and the geometry of the galactose binding site are also predicted.

02.1-56 THYROID HORMONE INTERACTIONS WITH PREALBUMIN. By Stuart Oatley, Jane Burridge, Patricia de la Paz and Colin Blake, Laboratory of Molecular Biophysics, University of Oxford, South Parks Road, Oxford OX1 3PS, England.

Prealbumin is a tetrameric serum protein, MW 55,000, which has a dual role in the transport both of the thyroid hormones and of vitamin A. Its native structure has been determined by X-ray analysis at 1.8Å resolution and refined by difference Fourier and restrained least-squares methods to R = 0.19 for all terms with d <10Å. The interactions of L-thyroxine (T_4), 3,5,3'-triiodo-L-thyronine (T_3) and 3,5-diiodo,3',5'-diisopropyl-L-thyronine have been examined at similar high resolution while a variety of other biologically active hormone analogues have been studied at medium (2.7Å) resolution. The thyroid hormone binding site is located deep within a channel which runs for 50Å completely through the centre of the protein molecule. This site is seen to provide favourable environments for each of the characteristic substituents of the hormone but the precise mode and position of binding of each analogue appears to be critically dependent on the nature of the substituents of the thyronine nucleus.

02.1-57 THREE-DIMENSIONAL STRUCTURE OF ACTINOXANTHIN AT 2.5 Å RESOLUTION. By V.Z. Pletnev, A.P. Kuzin and S. D. Trakhanov, Shemyakin Institute of Bioorganic Chemistry, Academy of Sciences of the USSR, Moscow, USSR.

The protein actinoxanthin (M.W. 10300, 107 amino acid residues) isolated from the culture fluid of Actinomyces globisporus is characterized by the ability to inhibit the growth of some Gram-positive bacterial strains and to retard the development of tumor tissues. The three-dimensional structure of actinoxanthin at 2.5 Å resolution has been determined by X-ray multiple isomorphous replacement method. The heavy atom binding sites in isomorphous derivatives were located by X-ray direct methods. A distinctive feature of the actinoxanthin structure is the absence of α-helices and the presence of enhanced content of antiparallel β-structure (~55%). The molecule has two domains differing in size (70 and 30%) and separated by a well-defined cavity. The larger unit has regular β-supersecondary structure containing the N- and C-terminals. It has the form of a slightly flattened cylinder with a two-layer arrangement of seven antiparallel β-strands. The inner part of β-cylindrical barrel is tightly packed with hydrophobic side chains oriented towards the axis. Hydrophilic side chains are arranged mainly on the external surface. The characteristic cavity found in the actinoxanthin structure undoubtedly has a direct relation to its biological activity. It is the probable binding site for the chromophore in the active complex.