02.1-11 THE THREE-DIMENSIONAL STRUCTURE OF NEURAMINIDASE OF SUBTYPE N9. A.T. Baker, J.N. Varghese, W.G. Laver(1), G.M. Air(2), R.G.Webster(3) and P.M. Colman, *CSIRO Division of Protein Chemistry, (1) John Curtin School of Medical Research, ANU, (2) Department of Microbiology, University of Alabama and (3) Dept. of Virology and Molecular Biology, St. Jude Children's Research Hospital, Memphis.*

Different subtypes of neuraminidase from influenza viruses are characterised by the absence of serological cross-reactivity and amino acid sequence homology of approximately 50%. The three dimensional structure of the neuraminidase antigen of subtype N9 from an avian influenza virus has been determined by X-ray crystallography (space group I432, a=185.1A) and shown to be folded similarly to neuraminidase of subtype N2 isolated from a human influenza virus. N9 neuraminidase in the form of rosettes of intact molecules has the additional activity of haemagglutination at 4C. Studies using monoclonal antibodies have suggested that the haemagglutination site is removed from the neuraminidase active site. Small differences in the way in which the subunits are organised around the molecular four-fold axis are observed. Insertions and deletions with respect to N2 NA occur in four regions, only one of which is located within the major antigenic determinants around the enzyme active site.

02.1-12 STRUCTURAL STUDIES OF D-XYLOSE ISOMERASE FROM S. RUBIGINOSUS AT 2.5Å RESOLUTION. H. L. Carrell. The Institute for Cancer Research, The Fox Chase Cancer Center, Philadelphia, Pa. 19111 USA

The enzyme D-xylose isomerase catalyzes the conversion of D-xylose to xylulose and D-glucose to fructose and is known to require divalent metal ions (Mn^{2+},Co^{2+},Mg^{2+}) for activity. The enzyme from Streptomyces Rubiginosus has a molecular weight of 172,840 and consists of 4 subunits of MW 43,210 each containing 388 amino acid residues. The enzyme crystallizes in space group I222 with Z=2 with cell dimensions are a=93.88, b=99.64, c=102.90 Å. The x-ray diffraction data has been measured by automated diffractometry to a resolution of 2.5Å.

The study reveals that each subunit consists of two domains, the larger of which is made up of alternating β-sheet and α-helix in the now familiar $(\beta\alpha)_8$ folding pattern. The details of the refinement of the structure, the secondary and tertiary structure, and substrate and inhibitor binding will be presented. In addition, the role of the metal ions will be discussed.

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02.1-13 STRUCTURAL SIMILARITY BETWEEN PEANUT LECTIN AND CONCANAVALIN A. By S.C. Mande, S. Raghunathan, M. Islam Khan, A. Surolia and M. Vijayan, Molecular Biophysics Unit, Indian Institute of Science, Bangalore 560012, India.

We had earlier shown, using rotation function studies and chemical crosslinking experiments, that the tetrameric peanut lectin is a dimer of dimers (J.Biol.Chem., 1985, 260, 13576). It was reported that legume lectins, including Concanavalin A, pea lectin, favin and peanut lectin, are related to one another by circularly permuted homology. The available partial sequence of peanut lectin has been compared with those of the other three proteins. To the extent sequence information is available, peanut lectin exhibits 40% or more sequence identity with them. The metal binding sites are almost entirely conserved whereas considerable variability exists in the carbohydrate binding region. Glycines with D conformation in Concanavalin A are retained in peanut lectin. Thus sequence comparison indicates the probability of considerable 3-D structural homology between Concanavalin A and peanut lectin whose structure we seek to determine. The cross-rotation function, at 4.5 Å resolution, between peanut lectin and Concanavalin A tetramer contains one large non-origin peak consistent with the self rotation function of peanut lectin, suggesting structural similarity between the two proteins. In order to achieve a more precise definition of this similarity, cross rotation function studies using Concanavalin A dimer and monomer as search molecules are in progress.

02.1-14 CRYSTALLOGRAPHIC ANALYSIS OF GRIFFONIA SIMPLICIFOLIA LECTIN IV AND ITS COMPLEX WITH A SYNTHETIC LEWIS b BLOOD GROUP DETERMINANT. M. Vandonselaar, L.T.J. Delbaere, J.W. Quail, U. Spohr, and R.U. Lemieux, Departments of Biochemistry and Chemistry, University of Saskatchewan and Department of Chemistry, University of Alberta, Canada.

Lectin IV, isolated from the seeds of Griffonia simplicifolia, is a 58,000 molecular weight glycoprotein dimer which binds to the Lewis b human blood group determinant (αLFuc(1→2)βDGal(1→3)[αLFuc(1→4)]βDGlcNAc). The nature of this binding has been probed chemically by synthesizing a number of modified tetrasaccharides related to the Lewis b determinant and by comparing their binding properties (Spohr, Hindsgaul, and Lemieux, Can.J.Chem., 1985, 63, 2644-2652). Further information on the recognition and binding will be obtained from the three-dimensional structure of the lectin and its complex with the Lewis b tetrasaccharide.

Crystals of the lectin and also of the complex were obtained from 38-40% saturated ammonium sulfate, 0.1M PIPES buffer, pH 6.2. The crystals are tetragonal, space group $P4_22_12$ with unit cell dimensions a = 79.4Å, c = 89.1Å. Heavy-atom derivatives of the native lectin were prepared with dichloro(ethylenediamine)platinum, uranyl nitrate and lead acetate. Heavy-atom derivatives of the complex were also obtained by cocrystallizing an iodinated derivative of the Lewis b tetrasaccharide with the lectin, and by soaking both the complex and the iodinated complex with dichloro(ethylenediamine)platinum. Intensity data were collected from crystals of the native lectin, crystals of the complex of tetrasaccharide-lectin and also derivatized crystals. Analysis of these data is now in progress.
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