02.1–31 PROGRESS IN THE REFINEMENT OF APO M_4 LACTATE DEHYDROGENASE FROM DOGFISH (SQUALUS ACANTHIAS). By Celerino Abad-Zapatero, Joel L. Sussman† and Michael G. Rossmann. Department of Biological Sciences, Purdue University, West Lafayette, Indiana, 47907. USA. †Department of Structural Chemistry, Weizmann Institute of Science., Rehovot, Israel.

The chain tracing for the apo M_4 enzyme subunit of lactate dehydrogenase (LDH) was based on a multiple isomorphous replacement (MIR) electron density map to a resolution of 2.8 Å (Adams et al. Nature, 227, 1098-1113, 1970). Minor revisions of the polypeptide tracing were incorporated later and subsequently a model consisting of 329 amino acid residues was built in a Richards optical comparator. A preliminary coordinate list for C atoms has been published (Holbrook et al. In The Enzymes (Boyer, P. D. ed.), 3rd edn. Vol. 11, pp. 191-292,1975) based on a tentative amino acid sequence. This model was revised in a graphics system, using the software developed by Dr. T. A. Jones (Jones, T. A. J. Appl. Crystallogr. 11, 268-272, 1978) and a few amino acid residues were substituted (Eventoff et al. Proc. Nat. Acad. Sci. U.S. 74, 2677-2681, 1977). The map used for this interpretation was a 2.5 Å resolution, MIR map including the strongest reflections (10% of the possible) in the 2.5 to 2.0 resolution shell.

A total of 31 cycles of constrained-restrained least-squares crystallographic refinement (Sussman et al. Acta Cryst. A33, 800-804, 1977) were performed. Three series of refinement iterations were completed, separated by revisions of the model viewed in $(2F_o - F_c)$ maps; the R-factor was 23.5%. A subsequent $(2F_o - F_c)$ map indicated the sites of six sulfate ions and 125 water molecules. Restrained least-squares crystallographic refinement of this model using the Hendrickson-Konnert algorithm and the Purdue University Cyber 205 computer is underway. After 20 cycles of refinement, the R-factor is now 21.3% for 12,183 reflections between 5.0 and 2.5 Å resolution limits.

02.1–32 THE STRUCTURE ANALYSIS OF PROTEIN-S; A CALMODULIN LIKE BACTERIAL DEVELOPMENTAL PROTEIN. By Manju Rajeswaran, G. Jay and R. Sarma, Biochemistry Dept. State Univ. of New York, Stony Brook, N.Y. 11794, U.S.A.

Protein-S is a calcium binding developmental protein produced by the bacterial species, myxococcus xanthus. This bacteria which ordinarily goes through a vegetative cycle, enters a developmental cycle upon starvation and aggregates to form fruiting bodies filled with myxo spores. During this stage Protein-S is produced in large quantities. The protein has been crystallized in an orthorhombic space group $P2_12_12_1$ with cell dimensions a=52.99A; b=60.20A and c=102.16A. Each asymmetric unit consists of two monomers of Protein each having a molecular weight of 23,000. The structure is being determined at a resolution of 2.8A, using a combination of molecular replacement and multiple isomophous replacement. Platinum chloride and mercuric acetate have been used to determine the phase angles.

The amino acid sequence of Protein-S, determined from the sequence of its gene (Inouye,S., Francheschine, T., and Inouye, M. (1983). Proc. Natl. Acad. Sci. U.S.A. Vol. 80. 6829-6833) shows four internally homologous domains. The first and third domains consist of 38 residues and show a homology of 79%; the second and fourth domains consist of 40 residues and show a homology of 65%. There is a sequence of 9 amino acids in the first and third domains that is homologous to the proposed calcium binding sequence of bovine brain calmodulin.

02.1–33 REFINEMENT OF THE CRYSTAL STRUCTURE OF SOYBEAN FERRIC LEGHEMOGLOBIN a NICOTINATE AT 2.4Å RESOLUTION. By W.N. Hunter[1], C.A. Appleby[2], J.M. Guss[1], D.L. Ollis[1] and H.C. Freeman[1],

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The crystal structure was solved at 3.3Å by multiple iosmorphous replacement (Ollis et al., Aust. J. Chem (1983) 36, 451-68). The model obtained from the m.i.r. phases has been improved by a series of real-space (difference maps, computer graphics, FRODO) and reciprocal-space (least-squares refinement, PROLSQ) calculations. Improvement of the model has been accompanied by an extension of the phases from 3.3Å to 2.4Å in three 0.3Å stages.

The asymmetric unit of the crystals comprises two molecules, each with $M_r \sim 17{,}000$. The molecules have been refined independently. The results of the refinement, including a comparison between the two molecules in the asymmetric unit, will be presented.

02.1–34 THE CRYSTAL STRUCTURE OF HPr OF THE PHOSPHOENOLPYRUVATE: SUGAR PHOSPHOTRANSFERASE SYSTEM OF ESCHERICHIA COLI AT 2.5Å RESOLUTION. By O.A.L. El-Kabbani, E.B. Waygood, G.D. Brayer, and L.T.J. Delbaere. Department of Biochemistry, University of Saskatchewan, Saskatoon, Saskatchewan, Canada S7N 0W0.

The phosphenolpyruvate (PEP): Sugar phosphotransferase system (PTS) of E. coli carries out the phosphorylation and concomitant translocation of many hexoses and hexitols across cell membranes. Four proteins are mainly involved in the PTS. These proteins are enzyme I, which is used by all PTS sugars, HPr which is a histidine-containing phosphocarrier protein for non-fructose PTS sugars, factor III which is a sugar-specific phosphocarrier protein and enzyme II which is both the sugar-specific and membrane-bound protein that phosphorylates and translocates the PTS sugars.

HPr from E. coli (MW9017) has been crystallized from 68% saturated Li_2SO_4 at pH 3.7 and 14°C. The **monoclinic** crystals have space group $P2_1$ with a=27.50Å, b=46.10Å, c=25.77Å, β=104° and Z=2. Quantitative diffractometer data to 2.5A resolution were collected for the native and six heavy-atom derivatives. Successful multiple isomorphous replacement phase determination has been carried out for the six derivatives: mercury chloranilate, cis-diamino, dichloro-platinum, gold tetrachloride, sodium mersalyl, uranyl nitrate and a double derivative of sodium mersalyl + cis-diamino, dichloro-platinum. The centric R values for these derivatives are 0.50, 0.36, 0.47, 0.37, 0.41 and 0.34, respectively, and the over-all figure of merit is 0.80. A 2.5Å electron density map has been interpreted in terms of the amino acid sequence of the protein to produce the three dimensional structure of HPr. (Supported by the Medical Research Council of Canada. O.A.L. E.-Kabbani is the recipient of a Saskatchewan Health Research Board Training Fellowship.)