01.3–2 CRYSTALLIZATION AND STRUCTURE DETERMINATION OF POTATO PHOSPHORYLASE. By H.J. Hecht, K. Jahnke and M. Buehner, Forschergruppe Roentgenstrukturanalyse, Universitaet Wuerzburg, D-8700 Wuerzburg, Fed. Rep. of Germany.

The non-allosteric dimeric enzyme phosphorylase from potato (mol. weight 2 x 108.000) crystallizes is space group P 3_121, a=129.0 Å, c=119.5 Å. Crystals diffract to at least 2.8 Å resolution. Details of the structure determination by Molecular Replacement using rabbit muscle phosphorylase a (Fletterick et al.) as a model and first results will be given.

Fletterick, R.J., Goldsmith, E., and Sprang, S.R., personal communication of co-ordinates.

01.3–3 DETERMINATION OF THE CRYSTAL STRUCTURE OF THE PROTEIN ANTIBIOTIC MACROMOMYCIN USING MOLECULAR REPLACEMENT METHODS. Patrick Van Roey and Paula M. D. Fitzgerald, Medical Foundation of Buffalo, Inc., Buffalo, New York 14203, U.S.A.

Auromomycin (AUR), a potent antitumor antibiotic isolated from Streptomyces macromomyceticus, inhibits DNA synthesis by causing single-strand breaks in DNA. AUR is composed of a 12,000 MW apoprotein, macromomycin (MCR), and a 600 MW non-protein chromophore. The chromophore, which is the active component, is very unstable in isolated form. The protein, which is inactive, protects the chromophore from degradation by reducing agents and must interact with the cell membrane for release of the chromophore into the cell.

The apoprotein MCR has been crystallized from 10 mM $CaCl_2$, 25 mM Tris at pH 8.0 with MPD as the precipitating agent. These crystals have the symmetry of space group $P2_1$, cell dimensions a=36.20Å, b=35.82Å, c=37.95Å, β=99.76° and they diffract to at least 1.7Å resolution. The structure of MCR has been determined by molecular replacement methods. The structure of the related and partially homologous protein antibiotic actinoxanthin (AXN) was used as the model. Ignoring five additional residues in the MCR sequence, the two sequences show about 45% homology. The proteins are predominantly hydrophobic with two disulfide bridges that are in nearly identical positions in the sequences. The model consisted of the main chain and β-carbon atoms of the 2.5Å AXN structure (Pletnev et al., Biopolymers, 21, 287 (1982)). Application of the Crowther rotation function and the Crowther-Blow translation function, using the data between 10 and 5Å resolution, resulted in a unique solution. The highest incorrect features in the maps corresponded to 78.3% of the height of the correct orientation and 90.1% of the correct position. R-value minimization reduced the residual from 0.589 to 0.516 while changing the rotational and translational parameters by less than 3° and 1.5Å respectively.

Examination of the electron density maps of MCR at 3Å prior to refinement shows the overall structure to be very similar to that of AXN. The structure consists of two domains: a larger one that contains seven anti-parallel β-strands and a smaller one that is much less ordered. Both disulfide bridges are located in the small domain. Differences between the conformations of MCR and AXN appear to be largest in two loops which correspond to the sites of the largest sequence differences. The turn from residue 21 to residue 30 is different, probably because of the addition of two residues in positions 28 and 30. The loop from residue 35 to residue 46, which contains one of the disulfide bridges, appears to be twisted differently.

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01.3–4 THE STRUCTURE OF *PANULIRUS INTERRUPTUS* HEMOCYANIN AT 3.2 Å RESOLUTION. By A. Volbeda, W.P.J. Gaykema and W.G.J. Hol, Laboratory of Chemical Physics, Nijenborgh 16, Groningen, The Netherlands.

Hemocyanins are the large, copper-containing oxygen transport proteins of numerous invertebrate. The hexameric hemocyanin of *Panulirus interruptus* has a molecular weight of 450.000 but is nevertheless one of the smallest hemocyanins known. Its three-dimensional structure has been determined at 3.2 Å resolution by the use of multiple isomorphous replacement and molecular averaging techniques. Phases between 4.0 and 3.2 Å were obtained without heavy atom derivative information. Each subunit consists of three domains; the first two largely helical, the third having an anti-parallel β-barrel as core from which long loops extend.

The binuclear copper site is situated in the centre of the second domain. Each copper ion is liganded by three histidine side chains. All six ligands are helical residues. The distance between the copper ions is about 3.8 Å. Sequence information is rapidly becoming available and details of the copper environment will be presented.

The β-barrel of the third domain is surprisingly similar to those in Cu,Zn superoxide dismutase and in the immunoglobulins. A comparison of the aligned sequences and superimposed conformations will be described.

During the last year several hemocyanin sequences have become available. Preliminary alignments show that the three domain structure observed for Panulirus hemocyanin is common to all arthropodan hemocyanins, but that a major deletion in the first domain has to be postulated. Progress on these evolutionary aspects of hemocyanin will also be reported upon.