A continuous feedback mechanism between the process of data collection and that of data reduction has been developed. It enables modification of these procedures and their adjustment to account for the specific problems of ribosomal crystals. Consequently, the quality of the data has significantly improved: currently the evaluated data sets are of completeness and quality comparable to those obtained from crystalline proteins of average size (RiWeave 5-94).

Special emphasis is put upon the accurate measurement and evaluation of the very low resolution reflections (below 10Å). These reflections are believed to be very important for low resolution phasing by methods other than MIR.


PS-03.10.05 A STUDY OF THE INTERACTION MODES FOR BILE SALTS. By A.R. Compagno, S. Candela de Santos, M. D'Alagni, A. D'Archivio, L. Galantini, E. Giglio, L. Scaramuzza, Dipartimento di Chimica, Università di Roma "La Sapienza", Roma, Italy.

Bile salts, the most important natural detergents, form molecular aggregates in aqueous solutions, which interact in bile and in the small intestines with several important biological compounds as, for example, bilirubin-IXα, cholesterol, phospholipids, glycerides and fatty acids.

There are many indications that the structures of the aggregates in solution are sometimes similar to those found in the crystals and, for this reason, the crystal structure of these compounds is of great interest.

The crystals, difficult to grow, are very seldom single and very often grow like a bunch of thin needles, sometimes unstable in the air. However, we have succeeded in solving a number of crystal structures and we have found that in the crystals the molecules are held together into very stable structural units, sometimes loosely bound to one another, this being a further indication that the aggregate scheme can be similar in the aqueous solutions.

For two bile salts, sodium and rubidium deoxycholate, such similarity has been proved unambiguously. We have found that different bile salts can have very similar aggregation patterns in the crystals and the structures examined so far can be grouped into three basic aggregation schemes.

Generally, the structures are helical (hexagonal, trigonal, twofold) stabilized by hydrogen bond and ion-ion and ion-dipole interactions. Similarities and differences will be discussed. In particular concerning the hydrogen bond network, compared with the other interactions through which the structures are stabilized.

PS-03.10.06 X-RAY ANALYSIS OF YEAST LIPOAMIDE DEHYDROGENASE AT 3.5Å RESOLUTION. By T. Toyoda, O. Masumoto, T. Hatt1 and A. Takanaka, Department of Life Science, Tokyo Institute of Technology, Nagatsuta, Meguro-ku, Yokohama 227, Japan and 1The Analytical and Metabolic Research Laboratory of Shinyo Co. Ltd., Shiniwagawa ku, Tokyo 140, Japan.

The pyruvate dehydrogenase complex is one of the highly organized multi-subunit complexes which catalyse central reactions accurately and efficiently. To elucidate the reaction mechanisms, we are analyzing the crystal structure of lipoyl dehydrogenase which is a component of the complex from yeast. Crystals, newly obtained by a deaerating method, have the same space group as, but are slightly different in the cell parameters from previous ones, the structure of which has already been X-ray analysis at 4.3Å resolution1. Diffraction data were collected up to 2.98Å resolution (max. 3.5Å, 65%) using synchrotron radiation. The crystal structure was solved by molecular replacement with glutathione reductase. Three programs (X-PLOR, MERLOT, MOLREP) gave a significant unique solution with reasonable crystal packing. After several refinements of the poly peptides, the density of the structure was verified using omit maps. The R-factor was further improved by 2% with molecular dynamics. The present R-factor is 10.5% at 3.5Å resolution.

In the electron density map, the main chain could be easily traced, detecting the insertions and deletions of amino acids. Some residual densities are assignable to FAD and sialic chains. The whole molecular model is in construction.