the determination of the three-dimensional distribution of protein in the unit cell was worked out on the basis of the electron microscope data (projections of the structure). The algorithm is based on using the symmetry of the crystal.

As a result, a spacial model for the distribution of protein in the cell at ~ 15 Å resolution was found. It gives the shape of molecules, their positions and contacts between them. It was established that the catalase molecule has the tetrahedral symmetry; its form can be approximated as a triaxial ellipsoid with dimensions 70, 80 and 95 Å. The subunits of the molecule of 125000 molecular weight stand out clearly.

These results are in agreement with the X-ray structural data. The Fourier synthesis at 20 Å resolution was calculated in which a model of the two-scattering-centers type was used as the first approximation of the molecule. The synthesis distinctly reveals the subunits and is close to an electron microscope model of the structure.


X-ray crystallographic data have been collected from native, D.I.P. inhibited trypsin (P2,2,2) to a resolution of 2.7 Å. Anomalous scattering data are being collected to the same resolution from an isomorphous Tl derivative using chromium X radiation, and a Hg derivative appears suitable for phase analysis as well.

An electron density synthesis should be ready by the time of the Congress using either the single or multiple isomorphous replacement method, anomalous Bijvoet differences, and statistical phase information.

The map will be interpreted in terms of the known amino acid sequence of trypsin, and will be compared with other known structures of proteolytic enzymes.


The pancreatic enzyme ß-cymotrypsin (M.W. 25,000) is one of the end products of activation of cymotrypsinogen A. It is chemically identical with ß-cymotrypsin to which it is believed to be related by a structural modification.

A Fourier synthesis at 2.7 Å resolution has been computed for the enzyme inhibited with tosyl fluoride. The heavy atom derivatives were obtained by inhibiting the enzyme with piperyl fluoride and by iodination.

A preliminary inspection of part of the map indicates that the main features of the map correspond closely to similar features in ß-cymotrypsin. The terminal stretch of ß-helix is clearly visible and the highest peaks of the map correspond to the sulfur atoms of the tosyl group and the disulfide bridges.

Further details of the interpretation of the map will be presented as well as a detailed comparison with ß-cymotrypsin.


The pancreatic trypsin inhibitor (Kunitz, M. and Northrop, J. H., J. Gen. Physiol. 19, 991, 1936) is known to play an important role in regulating the activation of trypsinogen. The amino acid sequence and various chemical properties of this compound have been investigated by Laskowski and co-workers. (Kassel, B. and Laskowski, M. Sr., Acta Biochemica Polonica, 13, 287, 1966). From highly purified samples of the pancreatic trypsin inhibitor, it has been possible to grow single crystals suitable for X-ray diffraction purposes. These crystals are hexagonal with cell dimensions (measured with CuKα radiation, a=1.5418 Å, c=109 Å and b=56 Å.

From comparative volume considerations of other proteins, it appears that the unit cell can accommodate 36 molecules. These considerations, in conjunction with a study of the diffraction pattern, suggest that the space group is P622. This research is continuing. This crystalline form apparently is different from the one obtained by Crick (Crick, F.H.C., Acta Cryst. 6, 221, 1953).