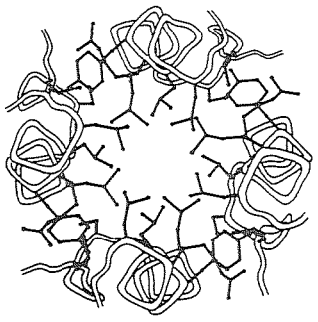
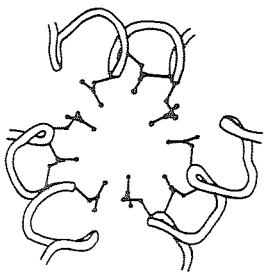
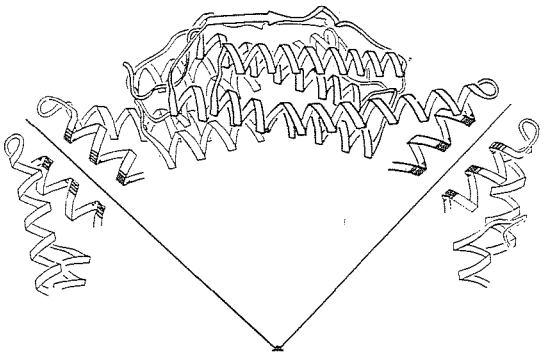


12 Leucines from 4 helices around the 4-fold axis make a hydrophobic channel.



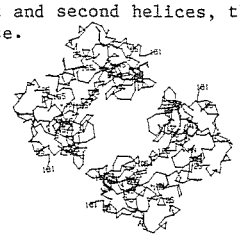
The 3-fold channel is very hydrophilic. Each subunit donates a SER,ASP and GLU.



Ribbon diagram of the apoferritin dimer and parts of two other subunits. The hydrophobic face of the short helix facing the 4-fold channel is shaded.

02.1–44 MANGANESE AND IRON SUPEROXIDE DISMUTASES ARE STRUCTURAL HOMOLOGS. W. Stallings, K.A. Pattridge, and M.L. Ludwig, Biophysics Research Division and Department of Biological Chemistry, University of Michigan, Ann Arbor, MI 48109.

The crystal structure of a tetrameric manganese superoxide dismutase from a thermophilic bacterium, Thermus thermophilus HB8, has been determined at 4.4 Å resolution by local averaging of electron density maps calculated by isomorphous replacement. The enzyme crystallizes from ammonium sulfate at pH 5.7 and pH 7.0 in space group $P4_12_12$ with a = 146.6 and c = 55.6Å. The spatial arrangement of the principal secondary structural features of iron superoxide dismutase is repeated in manganese dismutase, as demonstrated by superposition of the polypeptide chains of Fe and Mn dismutases. Density peaks corresponding to bound Mn^{+3} occur at locations equivalent to the Fe positions in iron dismutase, indicating one metal binding site per chain, or four sites per tetramer. The Mn dismutase tetramers have molecular 222 symmetry with one of the twofold axes coincident with a crystallographic diad. The tetramer is approximately rectangular in shape and appears to be constructed with only two unique interfaces. One set of interchain contacts closely resembles the dimer interface of Fe dismutase, but the other interface utilizes a polypeptide segment, inserted between the first and second helices, that has no equivalent in Fe dismutase.



02.1–45 THE STRUCTURE ANALYSIS OF DIPHTHERIA TOXIN by B. McKeever and R. Sarma, Biochemistry Department, State Univ. of New York, Stony Brook, N.Y. 11794, U.S.A.

The Diphteria Toxin, produced by Corynebacterium diphtheriae is responsible for the observed lesions associated with that desease. The Protein is a single polypeptide chain of molecular weight 60,000. It is made of two domains, the C terminal domain recognizes and binds to receptors on susceptible cell surface and internalizes the N terminal domain, which upon entering the cytoplasm catalyzes the hydrolysis of NAD^+ and the ADP ribosylation of a unique diphthamide residue on the eukarvotic elongation Factor-2, resulting in the termination of Protein synthesis.

The purified Protein can be isolated into sixteen fractions with different identifiable properties; monomer-dimer; nucleotide bound or free and so on. The bound dimer fraction yields diffraction quality crystals belong to the space group $P3_112$ or its enantiomorph with unit cell dimensions a=b=97.9A; c=100.3A. The diffraction data is being collected using oscillation photographs and the structure is being determined using multiple isomorphous replacement method. The results of the electron density map will be presented.

02.1–46 AN X-RAY DIFFRACTION STUDY OF A PEPTIDE HORMONE DEAMINO-OXYTOCIN. By T. L. Blundell, S. Cooper, J-Y. Li, J. E. Pitts, I. J. Tickle, A. C. Treharne and S. P. Wood, Laboratory of Molecular Biology, Department of Crystallography, Birkbeck College, University of London, London WC1E 7HX, UK; V. J. Hruby, Department of Chemistry, University of Arizona, Tucson, Arizona 85721, USA; and H. R. Wyssbrod, Department of Physiology and Biophysics, Mount Sinai Medical Centre, New York 10029, USA.

Oxytocin, a nanopeptide hormone composed of a twenty-membered ring and acyclic tail, has hormonal activities eliciting smooth muscle contraction in mammary glands and uteri. The highly potent 6-sulphur deamino oxytocin has been crystallised in the dry form with space group C_2 and cell dimensions a = 27.08, b = 9.06, c = 22.98Å, β = 102.1° and data collected to 1.20Å resolution (after Low; Science 151 1552 (1966)). The 6-seleno deamino oxytocin analogue crystallised isomorphously with cell dimensions a = 27.01, b = 9.14, c = 22.98Å, β = 102.2° and data have been collected to 1.92Å resolution. The phases were calculated using anomalous and isomorphous differences and the models refined with restraints using SHELX and RESTRAIN (Moss, Morffew, Haneef, Stanford and Borkakoti). There are type II β-turns between residues 2 to 5 of the rings and type I β-turns involving residues 6 to 9. There is conformational disorder at the disulphide bridge. The crystal structure will be compared to conformations from NMR and other spectroscopic studies in water and DMSO and in terms of binding to neurophysin and receptors.