02.2–4 NEW INTERPRETATION OF SECONDARY STRUCTURES IN THE PROTEIN STRUCTURE OF PAPAIN.

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Based upon new limiting values of the H-bond geometry C=O...H-N deduced from crystal structures of small molecules determined by X-ray crystal structure analyses with high accuracy and based upon calculated H-atomic positions in the crystal structures of proteins a new interpretation and uniform description of secondary structure elements in protein structures was given (Höhne, Kretschmer, studia biophys. (1983) 98, 85). By using computer methods all sterically allowed H-bonds stabilizing secondary structures (helices and ß-pleated sheets) in the papain structure have been calculated. Based upon these data a new interpretation of the individual helical regions and ß-strands in ß-pleated sheets is given. These new results are compared with the results in the original paper (Drenth et al., Adv. Prot. Chem. (1971) 25, 79) and with the results given by Levitt and Greer (J.Mol.Biol. (1977) 114, 181). The new values of the fraction of peptides in the papain structure: helices 29 % (Drenth: 22 %), ß-structures 22 % (Drenth: 16 %).

02.2–6 EFFECTS OF X-IRRADIATION OF SINGLE CRYSTALS OF RIBONUCLEASE A.

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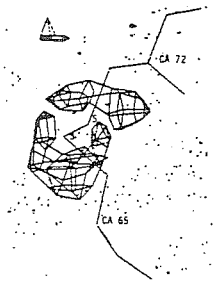
Radiation damage of biomolecules is an important yet poorly understood phenomenon. We have studied X-radiation damage of ribonuclease A by high-resolution X-ray crystallography. Structural changes induced by irradiation with 10Mrad were restricted to a few specific sites in the enzyme. All the disulphide bridges were opened and oxygen atoms appear to have been added to each sulphur atom. The four methionine residues appear to have been changed to methionine sulphones. The aromatic side chains also showed evidence of chemical modification. Despite the scission of the disulphide bridges, there was no major conformational change suggestive of general unfolding of the enzyme.



3-D electron density difference map of radiation damaged and native RNase A ($F_{damaged}-F_{native}$) claculated at 1.5Å. The +ve and -ve differences are shown as lines and points, respectively. The refined structure of native RNase A is shown as a stick figure. The S-S bond between cys65 and cys72. -ve density is visible at the S-S bond. Large, lobate +ve density features surround each sulphur. The positions of the lobes are consistent with the addition of oxygen atoms to the cys sulphurs.

02.2–5 TOPOLO : THE "PREDICTION" OF PROTEIN TERTIARY STRUCTURES.

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All the information required to determine the three-dimensional structure of a protein is carried by its amino acid sequence but to discover the tertiary structure of native proteins it is necessary to describe the folding pathway of the polypeptide chain and the mostsophisticated minimization methods when applied to the current energy function seem unable to simulate such a process. A good way to elucidate protein tertiary structures seems to deal with the residue entity with no information at the atomic level and without any consideration of the specific location of the different residues, using macroscopic energies which may be described from the organization of proteins of known tertiary structures (1).
The program which is described here allow the "prediction" of the tertiary structure of a protein from its amino-acid sequence in a multi step process with :

(i) the definition of protein domains (2)
(ii) the "prediction" of the protein secondary structure
(iii) a simulation of the folding process and the prediction of the protein topologies (1)
(iv) the building of a residual representation (3) of the protein tertiary structures.

The prediction of the tertiary structure of proteins of known X Ray structures will be reported.

(1) BUSETTA,B. & BARRANS,Y.(1982) Biochim.Biophys.Acta 704, 73-83.
(2) BUSETTA,B. & BARRANS,Y. (1984) Biochim.Biophys. Acta (submitted).
(3) BUSETTA,B.(1982),J.Theor.Biol.98, 621-625.

02.2–7 ELECTROSTATIC POTENTIAL ON THE SURFACE OF BIOMOLECULES.

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A simple approach for the understanding of molecular behaviour is to consider the electrostatic potential on the molecular surface (Scrocco and Tomasi, J. Adv. Quantum Chem. (1978) II, 115). For this purpose a program[x)] to generate net charges (Del Ré Method for Sigma Charges, Del Ré, J. Chem. Soc. (1958) 40, 31) and (Pariser and Parr, method for Pi Charges, Pariser and Parr, J. Chem. Phys. (1953) 21, 446 and 767) was developed. The electrostatic potential is computed on the molecular surface in a monopole approximation. The calculation of this potential with an original graphical representation allows elaboration of the scheme of electron transfer from hemoproteins like cytochromes. The role of the dielectric constant is analysed, and we give an image of the electrostatic potential in the crystal of such molecules in order to understand its effect in the crystal formation.

x) The first part of the program generates net charges on all the atoms of polypeptides, hemoproteins and nucleic acids. A new set of atomic parameters is used for sigma charges calculation.

The second part adds protons and counterions on the molecular structures issued from the Protein Data Bank.