02.2-4 NEW INTERPRETATION OF SECONDARY STRUCTURES IN THE PROTEIN STRUCTURE OF PAPAINT.

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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. (1982) 98, 85). By using computer methods all sterically allowed H-bonds stabilizing secondary structures (helices and B-pleated sheets) in the papain structure have been calculated. Based upon these data a new interpretation of the individual helical regions and B-strands in B-pleated sheets is given. These new results are compared with the results in the original paper (Drenth et al., Adv. Prot. Chem. (1971) 25, 72) and with results given by Levitt and Greer (J. Mol. Biol. (1977) 114, 181). The new values of the fraction of peptides in the papain protein structure: helices 29% (Drenth: 22%), B-structures 22% (Drenth: 16%).

02.2-5 TOPOLOGY: 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 most sophisticated minimization methods 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 organisation 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
(ii) the prediction of the protein secondary structure
(iii) a simulation of the folding process and the prediction of the protein topologies
(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.


02.2-6 EFFECTS OF X-RADIATION OF SINGLE CRYSTALS OF RIBONUCLEASE A. By S.K. Burley, G.A. Petsko and D. Ringe, Chemistry Department, Massachusetts Institute of Technology, Cambridge, Massachusetts, United States of America.

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 10krad were restricted to a few specific sites in the enzyme. All the disulfide 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 disulfide bridges, there was no major conformational change suggestive of general unfolding of the enzyme.