Computer Program Simulation of Protein Structure I

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Quantum Mechanics is probabilistic, and cannot provide the precise structures of atoms. The Deterministic Theory of Atomic Structure consists of a set of Electrodynamic Equations. Their mathematical solution provides definite stable orbits for electrons to move around the nucleus of atoms and molecules. By this theory, we have calculated the bond length and bond energy of hydrogen bond to accuracy within two decimal places.

Based on the Deterministic Theory of Atomic Structure, we can provide numerical coordinates for each atom in polypeptide chain, the winding of polypeptide chain into alpha helices, and the bending of the alpha helices into tertiary structure. We will provide computer program for these operations. We give few rules for breaking of helix structure.

This computer simulation will give very precise numerical location of each atom of the protein in natural state, and hence a more accurate quantitative description of the protein structure. After translating DNA coding to protein polypeptide sequence, we can use this program to compute its structure. This will provide a theoretical result of protein structure for checking with experimental result. We can also calculate the hydrogen bonding sites and functional sites of proteins. This will help in protein engineering.

References:

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(2) K. U. Lu, Proceeding of International Conference on Mathematics and Engineering Techniques in Medicine and Biological Science, 2000, pp.201, Editor, F. Valafar.

Topic: Protein Engineering.