962-92-1400 **Harold A Scheraga*** (has5@cornell.edu). *Global Optimization of Potential Energy in the Protein Folding Problem.*

The structures biological molecules, correspond to particular arrangements of their constituent atoms, and one structure can be converted to another by rotations about the bonds that connect each pair of atoms in the molecule. Allowing for rotation about all bonds in a molecule will generate an astronomical number of structures of a given molecule. Nature prefers that particular arrangement of the atoms within a given molecule for which the free energy (taken here as potential energy) is the lowest. To compute the lowest energy arrangement for a protein, one is faced with a global optimization problem in a very high dimensional space. Algorithms for minimization are available but, in general, they lead only to the local minimum closest to the starting point. Because of the great importance of the protein folding problem, we need algorithms that will lead to the global-minimum structure. This talk will describe the global optimization algorithms that we have developed to try to solve the protein folding problem. Illustrative examples will be cited in order to demonstrate the capabilities and limitations of these algorithms, and point out the need for further developments to improve the efficiencies of global optimization procedures in spaces of high dimensions. (Received October 03, 2000)