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ENERGY MINIMIZATION AND CONFORMATION ANALYSIS OF MOLECULES USING CONJUGATE GRADIENT METHOD

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ABSTRACT

Function optimization is a calculation that pervades much of numerical analysis. In the context of macromolecules, the function to be optimized (minimized) is an energy. The goal of energy minimization is simply to find the local energy minimum. The energy at this local minimum may be much higher than the energy of the global minimum. Physically, energy minimization corresponds to an instantaneous freezing of the system; a static structure in which no atom feels a net force corresponds to a temperature of 0 K. The potential energy calculated by summing the energies of various interactions is a numerical value for a single conformation. Energy minimization is usually performed by gradient optimization: atoms are moved so as to reduce the net forces on them. The minimized structure has small forces on each atom and therefore serves as an excellent starting point for molecular dynamics simulations.

KEYWORDS: Conjugate Gradient, Energy Minimization, Conformation Analysis, Molecules