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# PROTEIN FOLDING

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A Brownian dynamics approach is applied to the simulation of the protein folding of the three proteins: Bovine Pancreatic Trypsin Inhibitor, Carp parvalbumin, and the variable part of Immunoglobin. Expeditious choice of simulation time-steps in terms of fixed maximum amino residue displacement per time-step permits simulation of real time folding of up to $10^{-5}$ seconds.

The dynamical elements of the simulation are $\alpha$-helices situated along the protein primary sequence. The helices are predicted on grounds of hydrophobic shielding, structural stability, and rules provided by (published) statistical analysis of known protein structures.

Explicitly included in the simulation are: the viscosity of the solvent (water), helix dipole/dipole interactions; amino residue-residue van der Waals and hydrophobic/hydrophilic interactions; and connectivity of helical dynamical elements.

Results indicate that Brownian dynamics provides a satisfactory alternative to energy minimisation and molecular dynamics for simulation of protein molecule behaviour. In addition the simulation results provide strong support for acceptance of the importance of hydrophobic and helix dipole interactions in the co-operative drive toward a unique stable folded structure of a protein molecule for realistic folding times. Within the

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limitations of the dynamical elements chosen for the simulation, predicted native protein structure is in agreement with known X-ray diffraction results. This also applies to the case where the proteins are not highly helical.

Possible extensions of this approach to the more general case where dynamical elements of the simulation are not necessarily helical and which may deform are discussed.

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