

Predicting protein structure using inter-residue distances

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Knowledge of a protein's structure is important in understanding its function. The usual experimental structure determination methods can be costly and time-consuming. We present an idea for a fast and inexpensive protein structure prediction method that combines modeling with less expensive experimental data. Our method involves three steps: (1) building a decoy set, (2) measuring inter-residue distances in a target protein, and (3) comparing the measured distances with those calculated in each decoy. We postulate that structures with a small number of similar inter-residue distances will also have similar three-dimensional structure. We further hypothesize that the minimum number of distances needed to determine structure is much less than the total number of inter-residue distances in the protein. We will also present our refined scoring procedure which uses threading and molecular dynamics.