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Using Folding Pathways to Predict Protein Structure[1]

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Since the demonstration that the amino acid sequence of a protein encodes its structure, the prediction of structure from sequence remains an outstanding problem that impacts numerous scientific disciplines. By iteratively fixing secondary structure assignments of residues during Monte Carlo simulations of folding, a coarse grained model without homology information or explicit side chains outperforms current homology-based secondary structure prediction methods. The computationally rapid algorithm also generates tertiary structures with backbone conformations of comparable accuracy to existing all-atom methods for many small proteins, particularly for low homology sequences. Given appropriate search strategies and scoring functions, reduced representations can accurately predict secondary structure as well as three-dimensional structures, thereby increasing the size of proteins approachable by *ab initio* methods and the accuracy of template-based methods, in particular for sequences with low homology. In addition, we will discuss recent advances in understanding non-linear electrostatic contributions to transfer free energies in continuum electrostatic models.

[1]Work done in collaboration with Joe DeBartolo, Andres Colubri, Abhishek Jha, James Fitzgerald, and Tobin Sosnick.