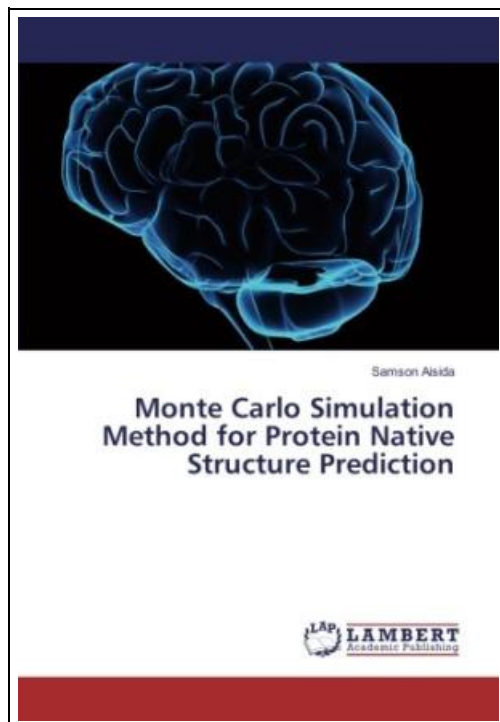


Monte Carlo Simulation Method for Protein Native Structure Prediction



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LAP Lambert Academic Publishing Feb 2017, 2017. Taschenbuch. Condition: Neu. Neuware - Proteins are polymers of Amino Acid which are constructed after translation of genetic code in DNA of organisms and have functionality that depends on their Native Structure. Experimental methods for protein native structure determination are complicated, expensive and time-consuming. Consequently, Computational Methods (CM), including Monte Carlo (MC), aim to circumvent these challenges. However, the MC is complex and inconsistent in native structure Prediction. This study was designed to develop a Move-Biased MC simulation algorithm that may simplify the complexity of existing MC and makes it consistent for native structure prediction. Protein was described as a coarse-grained structure and folding as Self-Avoiding Walks (SAW) on square lattices. Relative Probability Parameters were introduced to determine natural probabilities of protein conformations from SAW and to simulate the desired sequence length from an optimal combination. Thereafter, a graphical algorithm was developed to group the SAW steps into hydrophobic and polar AA units according to the Hydrophobic-Polar (HP) model. 232 pp. Englisch.

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