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A Novel Empirical Potential Function and A Monte Carlo Sampling Technique

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In protein folding study, two major issues are effective potential function and powerful sampling technique. In this meeting, recent results in both directions will be presented. In terms of potential function, we have developed an orientation-dependent statistical all-atom potential derived from side-chain packing. Test of the new potential on decoy set recognition indicates that it outperforms all the known statistical potential functions in the literature. Applications of this potential in substantially improving side-chain modeling will also be discussed. In terms of sampling technique, I will discuss some new results of a novel Monte Carlo sampling technique that performs simulation via direct computation of partition functions. The results will be compared with those of the well-known Wang-Landau sampling scheme. Application of this new MC method in studying protein folding will also be discussed.