数学与系统科学研究院

计算数学所学术报告

报告人： **Prof. Huan–xiang Zhou**

(Department of Physics，Florida State University)

报告题目：

Accurate calculation of binding and folding free energies by a scaled generalized Born method

邀请人： **卢本卓副研究员**

报告时间： **2009 年 7 月 27 日(周一)**

下午 2:30—3:30

报告地点： **科技综合楼三层 301**

计算数学所小报告厅

Abstract:

The Poisson–Boltzmann equation is widely used for modeling solvation effects. The computational cost of PB has largely restricted its applications to single–conformation calculations. The generalized Born model provides an approximation at substantially reduced cost. Currently the best GB methods reproduce PB results for electrostatic solvation energies with errors at > 5 to 10 kcal/mol. When two proteins form a complex, the net electrostatic contributions to the binding free energy are typically of the order of 5 to 10 kcal/mol. Similarly, the net contributions of individual residues to protein folding free energy are < 5 kcal/mol. Clearly in these applications the accuracy of current GB methods is insufficient. Here we present a simple scaling scheme that allows our GB method, GBr6 , to reproduce PB results for binding and folding free energies with high

accuracy. From an ensemble of conformations sampled from molecular dynamics simulations, five were judiciously selected for PB calculations. These PB results were used for scaling GBr6 . Tests on protein binding and folding show that effects of point mutations calculated by scaled GBr6 are accurate to within 0.5 kcal/mol or less. This method makes it possible to incorporate conformational sampling in electrostatic modeling without loss of accuracy.

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