# 数学与系统科学研究院

# 计算数学所学术报告

报告人：　　兰花 博士

（ 北京生命科学研究所 ）

报告题目：

**Developing and applying a novel grid-based QM scoring method in vHTS**

邀请人：　　戴小英 副研究员

报告时间：**2015** 年 **12** 月 **24** 日（周四）

上午 **10:00~11:00**

报告地点：　数学院南楼七层

**702** 会议室

# Abstract:

**With the significant advances in computer power, structure-based virtual high-throughput screening (vHTS) has been increasingly used to identify promising hits from a large chemical database of millions of compounds by rapidly estimating ligand-receptor interactions with a scoring function. This would significantly reduce the cost and time of discovering novel lead compounds. However, its application in drug discovery has been unsatisfactory partially due to the use of deficient atomic potential energy functions in the classical force field (FF). While for the highly accurate scoring functions based on quantum mechanics (QM), the calculations are prohibitively expensive to be applied to vHTS. We aim to develop a novel grid-based QM scoring method which is highly accurate yet efficient in order to improve docking accuracy. By generating a database of pre-computed potential energy surface (PES) using a QM method for any pair of protein-ligand fragments in the full phase space, any protein complex can be decomposed into fragments and reassembled onto 3D grids and the protein-ligand interaction energy can be estimated by a robust interpolation method. Our method has shown higher accuracy than classical force field for gas phase non-bonded interactions, and with the use of pre-computed energy data, high throughput efficiency is guaranteed. By calculating the gas phase protein-ligand interactions with our method, a novel scoring function for estimating ligand binding affinity has been developed. This scoring function will potentially assist in the innovative structure-based drug discovery, especially for "tough" drug targets which are challenging for conventional scoring functions.**


欢迎大家参加！