武汉物数所理论交叉学术交流系列报告

(第一六〇期)

Fragment Based Drug Design and Virtual Screening

Dr. Zeng Jun
Royal Melbourne Institute of Technology,
SRD Biosciences Co. Ltd.

2017年02月25日(周六)
下午15:00–16:00
综合楼4楼会议室

Abstract：The success of Fragment based drug design (FBDD) and structure–based drug design in general depends crucially on the accuracy of the algorithms used in the underlying docking and evaluation methods. Available software packages almost exclusively use molecular mechanics approximations based on Newtonian mechanics to describe target and ligand molecules. While reliable force fields are available for proteins and DNA molecules, a force field representation, and often even the 3D coordinates, of a given small organic molecules that is accurate and consistent with the protein force field used is in most cases still a hit–and–miss. In particular hydrogen bond interactions between ligands and protein and interactions involving metal ions are often misrepresented.

We have implemented a computational FBDD approach ("MFMD") based on molecular dynamics simulations combined with quantum mechanical optimization, in order to avoid artifacts from empirical force fields and to take more accurately into account electron–electron interactions between fragments and protein side chains. Examples for FBDD using MFMD for the inhibitor design for kinases and malaria aminopeptidases will be presented. More importantly, the feasibility of advanced quantum mechanical based virtual screening of chemical library for the first time is demonstrated.

报告人简介：曾军，澳大利亚墨尔本皇家理工学院副教授、SRD生物科技有限公司CEO。1995年毕业于悉尼大学，获得博士学位。1996年-1998年在法国遗传、分子和细胞生物所（IGBMC）任马丁学者。1998年-2000年在澳大利亚Ludwig癌症研究所任马丁学者。2001年-2008年任澳大利亚Cytopia有限公司首席科学家。2009年-2012年人Qubist分子设计有限公司任首席科学官。2012年-2016年任澳大利亚计算生物纳米有限公司董事及联合创始人。2010年创办SRD生物科学有限公司。2015年起在澳大利亚墨尔本皇家理工学院任兼职副教授。曾军博士于2007年任四川大学客座教授，已在主流学术期刊发表论文四十余篇。

主办单位:武汉物数所理论与交叉研究部