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# COMPUTATIONAL CHEMISTRY BI-WEEKLY SEMINAR SERIES

**TOPIC:** Development of a High-Quality Benchmark for Scoring Function Evaluation

**SPEAKER:** Renxiao Wang, Shanghai Institute of Organic Chemistry, Chinese Academy of Sciences

**TIME:** 14:00-15:00, 15 October 2014

**VENUE:** Room 152, Geography Building, 3663 Zhongshan Road North, Shanghai (中山北路校区, 地理楼 152 室)

## ABSTRACT OF THE TALK

Scoring functions are widely applied in combination with molecular docking methods to predict ligand binding poses and ligand binding affinities or to identify active compounds through virtual screening. An objective benchmark for assessing the performance of current scoring functions is expected to provide practical guidance for the users to make smart choices among available methods. It can also elucidate the common weakness in current methods for future improvements. This lecture describes our continuous efforts on the development of the PDBbind database and the so-called comparative assessment of scoring functions (CASF) benchmark based on it. The key idea of CASF is to compare the general performance of scoring functions on a diverse set of protein–ligand complexes. In order to avoid testing scoring functions in the context of molecular docking, the scoring process is separated from the docking (or sampling) process by using ensembles of ligand binding poses that are generated in prior. Our latest study, i.e., CASF-2013, evaluated 20 popular scoring functions on a set of 195 protein-ligand complexes selected out of the PDBbind database (version 2013).

## BIOGRAPHY

Prof. Renxiao Wang received both B.S. (1994) and Ph.D. (1999) in physical chemistry from Peking University. He did his postdoctoral training at the University of California Los Angeles and Georgetown University (1999-2001). He then worked for University of Michigan Medical School as a research investigator (2001-2005). In 2005, he joined the faculty of Shanghai Institute of Organic Chemistry as a “One-Hundred Talents” professor. Prof. Wang’s current research interests focus on understanding how small organic molecules regulate their biological targets through molecular modeling approaches. Prof. Wang has published over 90 scientific papers in peer-reviewed journals with a H-index of 30. In 2012, he received the Corwin Hansch Award from the International Cheminformatics & QSAR Society for his outstanding contributions to this field.