COMPUTATIONAL CHEMISTRY
BI-WEEKLY SEMINAR SERIES

TOPIC: Computational Prediction of RNA Tertiary Structures

SPEAKER: Prof. Yi Xiao, Huazhong University of Science and Technology

TIME: March 16, 2016, Wednesday, 1:30-2:30PM

VENUE: Room 264, Geography Building, Zhongbei Campus

ABSTRACT OF THE TALK

RNA molecules are involved in various biological processes, such as catalytic and regulatory ones. To perform these functions, they need to form special tertiary structures. At present, the number of RNA tertiary structures solved experimentally are very limited and so computational methods have been proposed to predict RNA tertiary structures, such as, FARNA/FARFAR, MC- Fold/MC-Sym, iFoldRNA, V-fold model. Here I give a brief review of the definition, problems, difficulties and current status of RNA tertiary structure prediction. Furthermore, I shall introduce our method of RNA tertiary structure prediction called 3dRNA, which is based on RNA sequence and secondary structure and has a performance with a mean RMSD 3.24 Å and INF 0.91 for a test set of 32 RNAs with lengths from 12 to 101 nt and with a speed of only a few seconds for predicting a model of a RNA less than 100nt.

BIOGRAPHY

Dr. Xiao received his Master's Degree in Theoretical Biology from Institute of Biophysics of Chinese Academy of Science and his Ph.D. in Theoretical Physics from Shanghai Jiao Tong University. His research interests are in developing computational methods to build three dimensional structures of nucleic acids and their complexes with proteins and applying molecular dynamics simulation method to study the dynamics and folding of nucleic acids and proteins in order to understand the physical principle of structure organization and relationship between structure, dynamics and function of biological molecules.