WEEKLY SEMINAR

Topic: Computational Enzymology: from Mechanistic Study to Inhibitor Design

Speaker: Yingkai Zhang, New York University

Time: 15:30-16:30, 18 March, 2014

Venue: Room153, Geography Building, 3663 Zhongshan Road North, Shanghai

（华东师范大学中山北路校区，地理楼 153 室）

ABSTRACT OF THE TALK

In this talk, I will present our recent progresses in developing and applying state-of-the-art computational methods to provide novel physical-chemical insights into important enzymes, and to facilitate the rational design of their modulators for probing important cellular pathways and for therapeutic use. Our computational approaches center on Born-Oppenheimer ab initio QM/MM molecular dynamics simulation (aiQM/MM-MD) with umbrella sampling, a computational tour-de-force to simulate enzyme reactions. In last few years, we have demonstrated the power of this state-of-the-art computational approach by solving important biochemical problems and making novel insightful suggestions for further experimental studies. One notable example is that we reported the first aiQM/MM study of zinc-dependent histone deacetylases (HDACs), which has been established as one of the most promising targets for the development of anti-tumor drugs. Our work disproved the previous mechanistic hypothesis, and determined a new mechanism which is more consistent with available experimental results. Subsequently, our discovered mechanism has guided the development of a novel class of HDAC inhibitors.

BIOGRAPHY

Yingkai Zhang did his undergraduate study at Nanjing University in China, and obtained his Ph.D. degree from Duke University. After three year's postdoc at UCSD, he moved to NYU in 2003. Currently he is a professor of chemistry at New York University. He was a recipient of the Whitehead Fellowship for Junior Faculty in Biomedical and Biological Sciences, the NYSTAR James D. Watson Young Investigator Award, and the National Science Foundation CAREER Award. His research interests focus on developing and applying state-of-the-art computational methods to provide novel physical-chemical insights into important biological processes, and to facilitate the rational design of their modulators for probing important cellular pathways and for therapeutic use.