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Drug Discovery & Designing

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Structure and mechanism based drug design, discovery and development

In this talk, I will first give a brief overview of drug discovery and development through state-of-the-art computational design and discuss the general trend of computational drug design and discovery through specific examples of our recent efforts in drug design, discovery and development (from computational design to clinical development). The presentation will show how the state-of-the-art computational modeling and design can effectively be integrated with wet experimental tests (*in vitro* and *in vivo*) for drug discovery and development. Appropriately integrated with wet experimental studies, state-of-the-art computational design is of great value not only for small molecule drug discovery, but also for discovery and development of novel therapeutic proteins engineered from naturally occurring proteins. Integrated computational-experimental drug design and discovery efforts have led to exciting discovery of promising drug candidates, including two Investigational New Drugs (INDs) that are in clinical development; one has received the breakthrough therapy designation by the FDA.

Biography

Chang-Guo Zhan has received his PhD in Physics from Institute for Molecular Science, Japan in 1996 and PhD in Chemistry from University of Notre Dame, USA in 1998 and completed his Post-doctoral training at Department of Medicine, Columbia University in 1999. He currently serves as the Director of Molecular Modeling and Biopharmaceutical Center and Endowed College of Pharmacy Professor in Pharmaceutical Sciences at College of Pharmacy, University of Kentucky. He has received numerous awards, including the Fellow of the American Association of Pharmaceutical Sciences (AAPS), elected in 2010. He has published more than 320 papers in reputed journals and has more than 30 patents.

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