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Drug discovery and development via structure and mechanism based rational design

In this talk, I will first briefly discuss the general strategies and integrated computational-experimental approaches used to understand the detailed molecular mechanisms of increasingly complex biological systems (such as those related to cancers, HIV virus, neurodegenerative diseases, inflammation, cardiovascular diseases, and drug addiction) and perform mechanism-based design, discovery, and development of novel drugs. I will also discuss the general trend of rational drug design and discovery through specific examples of our integrated efforts from understanding molecular mechanism to clinical development. The presentation will show how powerful understanding the detailed molecular mechanism and mechanism-based computational design are in the current drug design, discovery, and development. The integrated computational-experimental approaches are of great value not only for small-molecule drug discovery, but also for discovery and development of novel therapeutic proteins. Integrated computational-experimental drug design and discovery efforts have led to exciting discovery of promising drug candidates, including our designed novel drugs in Phase II clinical trials; one has received the *Breakthrough Therapy Designation* by the FDA.

Biography

Chang-Guo Zhan is an Endowed Professor of Pharmaceutical Sciences and Director of Molecular Modeling and Biopharmaceutical Center in the College of Pharmacy, University of Kentucky. He also serves as Director of Chemoinformatics and Drug Design Core of the Center for Pharmaceutical Research and Innovation at the University of Kentucky. With a research activity ranging from basic sciences to practical applications, Dr. Zhan has published more than 340 scientific papers in peer-reviewed journals, and has been more than 37 patents or patent applications. Dr. Zhan has developed new computational algorithms used to understand detailed structures, properties, and mechanisms of potential drug molecules interacting with their targets in solution. He has further developed novel, reliable and efficient computational design approaches, including the *virtual screening of transition states*, in structure-and-mechanism-based computational drug design and discovery. Using the *virtual screening of transition states* approach which he pioneered, Dr. Zhan has demonstrated its value by making a breakthrough in design and discovery of highly efficient therapeutic enzymes as novel, promising therapeutic candidates. Two of the therapeutic candidates are currently in Phase II clinical trials in humans. He has been very successful in securing nationally competitive research funding, including more than $20M from the NIH and NSF as PI. At the University of Kentucky, Dr. Zhan was named as *University Research Professor* by the President and Board of Trusty in 2016, and won *Kirwan Prize* (the top research award at the University of Kentucky) in 2017. He is a winner of 2005 *Emerging Computational Technology Prize*, American Chemical Society (ACS) Division of Computers in Chemistry, and is the current recipient of the *NIDA Translational Avant-Garde Award* from the NIH. Dr. Zhan was elected *AAPS Fellow* in 2010, and won 2016 *AAPS Research Achievement Award in Drug Discovery and Development Interface.*

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