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STRUCTURE AND MECHANISM-BASED DESIGN OF NANOPARTICLES AS THERAPEUTIC CANDIDATES

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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 including nanoparticles. 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, therapeutically promising nanoparticles. 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. His lab has successfully designed and discovered several promising therapeutic candidates, including two in Phase II clinical trials; one has received the Breakthrough Therapy Designation by the FDA. 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. He was elected AAPS Fellow in 2010 and won 2016 AAPS Research Achievement Award in Drug Discovery and Development Interface. He is also a UK Chapter Inductee of the National Academy of Inventors (NAI).

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