
PLENARY PRESENTATIONS

**DRUG DISCOVERY AND REPOSITIONING STUDIES ASSISTED BY
ARTIFICIAL INTELLIGENCE**

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Computer-aided and artificial intelligence-aided drug design (CADD and AIDD) have long confronted a fundamental challenge: accurate prediction of the binding between dynamically evolving proteins and small-molecule ligands, not to mention the induced-fit interactions that occur throughout the binding process. This talk will introduce our efforts in developing innovative computational strategies to address this core challenge, as well as their practical applications in novel drug discovery and drug repurposing. The key points of this talk are summarized as follows:

- (1) Development of enhanced molecular dynamics (MD) sampling methods (e.g., vsREMD), which substantially improve the efficiency of MD simulations for capturing protein conformational changes;
- (2) Development of D3Pockets, which is a novel computational approach for quantitatively characterizing the dynamic properties of ligand-binding pockets based on MD simulation trajectories;
- (3) Development of D3CARP, a multifunctional computational platform for protein target prediction and drug virtual screening;
- (4) Identification and optimization of first-in-class lead compounds for novel therapeutic targets, alongside the drug repurposing.