Speaker Bio

Dr. Jung-Hsin Lin is a Research Fellow at the **Research Center for Applied Sciences (RCAS) & Biomedical Translation Research Center (BioTReC), Academia Sinica (AS), and also jointly appointed Professor at the School of Pharmacy, College of Medicine, National Taiwan University and College of Engineering Sciences, Chang Gung Unviersity,** who has been working in the field of computational drug discovery for nearly 30 years. His lab has been focusing on the development of novel methods for computational drug discovery and structural bioinformatics, based on machine learning, artificial intelligence, statistical mechanics and quantum chemistry, and their innovative applications for exploring new therapeutic candidates and biomolecular targets of natural product molecules and other pharmaceutical agents. As a recent example of such efforts, Dr. Lin's lab published a computational scheme for binding free energy calculations based on first principle of statistical mechanics, which can be applied to general biomolecular interactions, including proteins, peptides and small chemical molecules. Besides, Dr. Lin's lab has committed in improving the accuracy of prediction of molecular docking methods, and also their applicable domains. Examples of novel methods and applications in this area include, MEDock, SLITHER and idTarget, and the last one was the first docking-based proteome-wide target prediction for a given small synthetic chemical molecule or a natural product compound. Deep learning algorithms and other artificial intelligence approaches have also been incorporated in the development of new computational methods for computational drug design. Dr. Lin's lab also contributes to the methodology development for determining the structures of intrinsically disordered proteins (IDPs), with the information from nuclear magnetic resonance (NMR) and small angle X-ray scattering (SAXS). His lab was the first to deposit and publish the structures of an IDP, SERF1a, which would accelerate amyloidogenesis of several neurodegenerative diseases. In the mid of 2024, one small molecule drug from his collaborative team led by Dr. Yijuang Chern for treating neurodegenerative diseases, including Alzheimer's disease, has received the approval as investigating new drugs (INA) from U.S. FDA and Taiwan FDA, respectively. Starting in the February of 2025, this small molecule drug for treating Alzheimer's disease has been in the Phase I first in human (FIH) clinical trial.