AHeDD 2005-2025 20 Years ANNIVERSARY

Asia Hub for e-Drug Discovery Symposium 2025 (AHeDD2025)

2025 亚洲药物设计大会

Symposium Handbook

会议手册

September 23-25, 2025 @ Hangzhou, CHINA

2025年9月23-25日 中国 · 杭州

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Welcome Message

It is with great pleasure and honor that we extend our warmest welcome to all participants of the Asia Hub for e-Drug Discovery 2025 (AHeDD2025). The symposium is hosted by the School of Pharmacy, Zhejiang University, from September 23 to 25, 2025, in Hangzhou, China.

The AHeDD2025 themed "Application of Artificial Intelligence, Bioinformatics, and Molecular Simulation for Promoting Target Identification and Drug Discovery", aims to serve as a premier platform for researchers, industry experts and students in the field of drug discovery. It provides an opportunity to share cutting-edge advancements in artificial intelligence, bioinformatics and molecular simulation, while also exploring their transformative applications.

The symposium will feature plenary lectures, parallel sessions and poster presentations, bringing together distinguished scholars and industry leaders from the Asia region. We hope all participants enjoy exploring emerging technologies, exchange insights and foster collaborations in the rapidly evolving field of e-drug discovery.

From 2005 to 2025, this year marks the 20th anniversary of AHeDD symposium series, celebrating two decades of continuous success in fostering the exchange of innovative ideas and practical applications. We warmly welcome your participation in this milestone event.

AHeDD2025 Symposium Chairs

Akiyama, Yutaka
Institute of Science Tokyo

No, Kyoung Tai
Yonsei University

Yang, Shengyong
Sichuan University

Zhu, Weiliang
Shanghai Institute of Materia Medica

Zhejiang University (ZJU)

Zhejiang University, established in 1897, has always adhered to the tradition of "Seeking Truth and Pursuing Innovation" as the university motto, with the world development as its responsibility and pursuit for truth as its goal. It is the spirit of ZJU and the common values for all ZJUers to develop a mind as broad as the vast ocean embracing all streams and all rivers, and a soul seeking truth and believing in virtues, to be innovative and

pioneering, and to construct and consolidate our country. The University strives to nurture high-caliber innovators and future leaders with comprehensive development of morality, intelligence, physique, aesthetic beauty, and global competitiveness. Under the cultivation of Zhejiang University, a large number of famous scientists, cultural masters, and elites from all walks of life have emerged, making contributions to the great rejuvenation of the Chinese nation and the promotion of exchanges and mutual learning among human civilizations.

After over 120 years' development, Zhejiang University has become a comprehensive research university with distinctive features and great impact at home and abroad. Of all the 22 disciplines in the list of the Essential Science Indicators (ESI), Zhejiang University has 21 in the world's top 1% and 15 in the top 1‰ (ESI data, November 2024).

School of Pharmacy, ZJU

The Pharmaceutical Sciences of Zhejiang University (CPS-ZJU) has a long history and academic heritage, and stands as one of the earliest modern and higher pharmaceutical education institutions of China. CPS-ZJU aims to become an education epicenter for training next-generation innovators, who are equipped with global vision and interdisciplinary skills for promoting innovation and translation in the field of pharmaceutical science and engineering. Currently, CPS-ZJU consists of two departments and ten research institutes with one Ph.D. Program, one M.S. program and one undergraduate program in pharmaceutical sciences, which complements mutually and functions dynamically under a well-designed teaching and scientific research system. It has edged itself into a nationally acknowledged pharmaceutical college. Its pharmacology and toxicology discipline ranks world's top 1 ‰ by Essential Science Indicators (ESI) and 7th globally by U.S. News in 2025. The discipline of Pharmacy has been listed into the country's Double First-class Initiative in the last national assessment.

Conference Overview

Theme

Application of Artificial Intelligence, Bioinformatics, and Molecular Simulation for Promoting Target Identification and Drug Discovery

Dates

September 23 (Tuesday) - 25 (Thursday), 2025

Location

New Century Grand Hotel Hangzhou
No. 818 Shixin Middle Road, Xiaoshan District, Hangzhou, Zhejiang, China

Host

School of Pharmacy, Zhejiang University

Symposium Topics

Big Data in Biomedicine and Drug Discovery

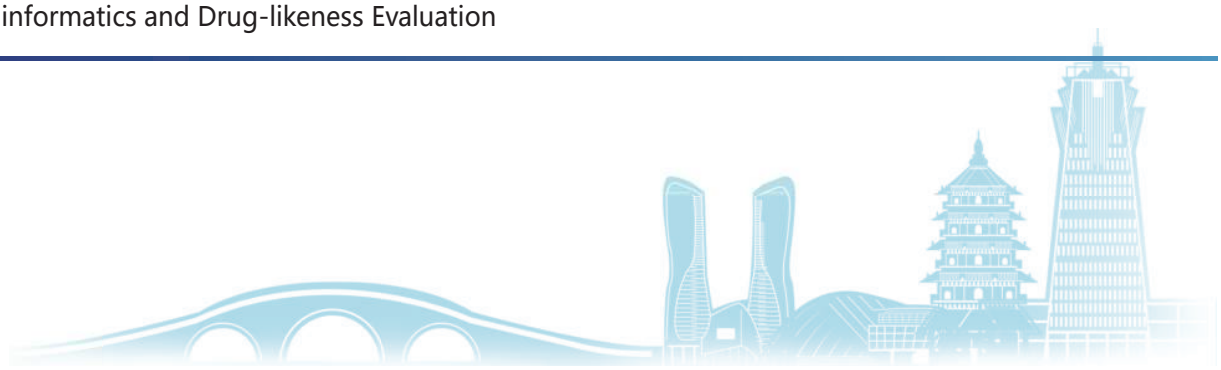
AI-assisted Target Identification

Frontiers in Chemical Biology

AI-driven Small Molecule Design

AI-based Protein Design and Drug Discovery

Cheminformatics and Drug-likeness Evaluation



Conference Overview

Symposium Chairs

Shengyong Yang (Sichuan University)

Weiliang Zhu (Shanghai Institute of Materia Medica)

Kyoung Tai No (Yonsei University)

Yutaka Akiyama (Institute of Science Tokyo)

Symposium Organizing Committee

(Alphabetical by last name)

Tingting Fu	Yichao Ge	Tingjun Hou (Chair)	Chang-Yu Hsieh
Dan Li	Yu Kang	Minjie Mou	Peichen Pan
Chao Shen	Wanxiang Shen	Xiuna Sun	Qingxia Yang
Yintao Zhang	Ying Zhou	Zhan Zhou	Feng Zhu (Secretary)

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Sep 25th Morning New Century Hall B, 4th Floor

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Plenary Speaker

Dr. Luhua Lai
Peking University, Professor

Computational approaches for making undruggable targets druggable

Biography

Dr. Luhua Lai is a full professor in the College of Chemistry and Molecular Engineering, Peking University. She is also a senior principle investigator at the Peking-Tsinghua Center for Life Science and the Center for Quantitative Biology, Peking University. She serves as associated editor for the Journal of Medicinal Chemistry and Quantitative Biology and chairs the Division of Physical Chemistry, the Chinese Chemical Society. Professor Lai's group carries out inter-disciplinary research aiming to design new protein and small molecule drugs for better heath. They develop computational methods and software, and use them to study biomolecules and systems of interest together with experimental approaches. The current research areas of Professor Lai's group include: (I) Structural, systems and artificial intelligence-based drug design and protein design method development and applications. (II) Mechanism of protein allosteric regulation and intrinsically disordered proteins. (III) Cancer metabolism and regulation.

Abstract

Among the disease-related proteins, only a small fraction has been therapeutically targeted. A large part of them remain undruggable. Turning these undruggable or difficult-to-drug targets into druggable ones will enlarge the drug target space and provide novel opportunity for developing treatment plan for complex diseases. Undruggable targets often exhibit unique features, including highly dynamic structures, lacking of well-defined ligand-binding pockets, conserved functional sites, and protein-protein interactions. The speaker's group has been focusing on developing novel computational approaches to target intrinsically disordered proteins, protein allosteric regulation, and protein-protein interaction using both physical and AI-based approaches. Recent advances of methodology development and applications will be presented and discussed.

Plenary Speaker

Dr. Kyoung Tai No
Yonsei University, Professor

From energetics to intelligence:
A journey through the evolution of CAMD

Biography

Dr. Kyoung Tai No received his Ph.D. in Physical Chemistry from KAIST. He began his academic career at SoongSil University, where he founded the Department of Bioinformatics, and later served as Professor of Biotechnology at Yonsei University until retirement. He currently holds the title of Distinguished Professor at Yonsei University. Dr. No has played a pivotal role in advancing computational chemistry and bioinformatics in Asia. In 1997, he established the Bioinformatics & Molecular Design Research Center (BMDRC), serving as Director until 2023, and in 2005 co-founded the Asia Hub for e-Drug Discovery (AHeDD) as a joint initiative among Korea, China, and Japan. Beyond academia, he has founded five biotech ventures and is currently CEO of Baobab AiBIO, a company dedicated to AI-driven protein engineering and Cryo-EM structure. His career bridges academia, industry, and international collaboration in computational life sciences.

Abstract

Computer-Aided Molecular Design (CAMD) has evolved over more than four decades, moving from physics-based energetics to modern AI-driven intelligence. In its early years, CAMD was grounded in the rigorous application of classical mechanics, thermodynamics, statistical mechanics, and quantum mechanics. The field was pioneered by a handful of experts, whose contributions remain foundational today, including Harold A. Scheraga (ECEPP/2), Martin Karplus (CHARMM), Peter Kollman (AMBER), and William Jorgensen (OPLS). Their energy-based methods are still widely used for molecular modeling and simulation. The accumulation of experimental and computational data, combined with advances in computing power, has enabled the rapid rise of AI in CAMD. Over the past five years, breakthroughs in generative AI and GPU acceleration have transformed the field, producing not only predictive models but also creative, generative knowledge. The vast scale of AI-driven outputs now requires AI itself to assist in their interpretation. Looking ahead, quantum computing is poised to extend CAMD even further, with practical applications expected within the next five years. As a researcher who has devoted more than 45 years to CAMD, I view this transformation with both excitement and caution. The convergence of energetics, AI, and quantum computing offers unprecedented opportunities, yet also demands careful reflection to ensure progress remains interpretable, reproducible, and responsibly guided.

Plenary Speaker

Dr. Yutaka Akiyama
Institute of Science Tokyo, Professor

Membrane permeability prediction of cyclic peptides crossing a lipid bilayer based on enhanced sampling molecular dynamics simulations

Biography

Yutaka Akiyama received his Doctor of Engineering degree from Keio University, Japan, in 1990, for his research on neural network theory, in particular the development of Gaussian Machines, a stochastic continuous neural network model and its application to combinatorial optimization. In 1992, he joined Institute for Chemical Research (ICR), Kyoto University, as an Associate Professor and developed the international GenomeNet services. In 2001, he became the founding director of the Computational Biology Research Center (CBRC) at the National Institute of Advanced Industrial Science and Technology (AIST), Japan. Since 2007, he has served as Professor of Computer Science at Tokyo Institute of Technology (now Institute of Science Tokyo). His research focuses on bioinformatics, computational drug discovery, and high-performance computing applications in the life sciences. He is also President of Initiative for Parallel Bioinformatics (IPAB). In 2013, he received the Ministry of Health, Labour and Welfare Award for Contributions to Industry-Academia-Government Collaboration in Japan. He has authored numerous publications and has actively promoted international collaborations in computational biology.

Abstract

Cyclic peptides are promising drug candidates but often suffer from poor membrane permeability, which limits their therapeutic potential. In this talk, I will present an enhanced sampling molecular dynamics protocol that predicts and explains the permeability of large cyclic peptides (≥ 10 residues) across lipid bilayers. The approach is based on a combined REST/REUS strategy, enabling efficient sampling of peptide conformations along the entire permeation coordinate. This large-scale protocol requires extensive GPU resources, reflecting the computational challenges of realistic peptide-membrane simulations. Using cholesterol-containing membrane models, the method achieved high agreement with experimental data ($R > 0.8$) for a diverse set of peptides. These results highlight the critical role of membrane composition in peptide permeation. They also demonstrate the value of advanced sampling strategies in connecting molecular simulations with drug design. Ultimately, the protocol provides a practical framework for understanding and designing cell-permeable cyclic peptide drugs.

Plenary Speaker

Dr. Shengyong Yang
Sichuan University, Professor

Computing-assisted drug discovery targeting GPCRs

Biography

Shengyong Yang, Dr., Professor of the State Key Laboratory of Biotherapy (SKLB), West China Hospital, Sichuan University (Sichuan, China). He earned his PhD from Sichuan University in 1999 and subsequently pursued postdoctoral research at the Hong Kong University of Science and Technology from 1999 to 2001. From 2002 to 2005, Dr. Yang worked as a research scientist in Prof. Tom Ziegler's group at the University of Calgary in Alberta, Canada. At the end of 2005, he joined SKLB at West China Hospital, Sichuan University. His research encompasses the methodology of computer-aided drug discovery (CADD) and the research and development (R&D) of small-molecule targeted drugs. To date, Dr. Yang has published over 200 papers in international journals such as Science, Nature Medicine, Nature Microbiology, Nature Machine Intelligence, Nature Chemical Biology, PNAS, among others. Ten drug candidates developed under his leadership have been transferred to pharmaceutical companies, with five progressing to clinical trials. Dr. Yang has been honored as a Cheung Kong Scholar by the Ministry of Education (MOE) and received the National Science Fund for Distinguished Young Scholars in 2013. He is also recognized as a New Cornerstone Investigator.

Abstract

Currently, structure-based drug design strategies primarily rely on the static structures of target proteins; however, the structures of target proteins are actually in a state of dynamic change. For instance, G protein-coupled receptors (GPCRs) are a class of membrane proteins that participate in regulating cellular signal transduction through conformational changes. In this study, we took cannabinoid receptors CB1 and CB2 as entry points to investigate the dynamic regulatory mechanisms of target proteins and explore innovative drug discovery. Firstly, we employed enhanced sampling molecular dynamics simulations to construct a complete free energy landscape for the allosteric modulation of cannabinoid receptor CB1 activation. We discovered that transmembrane helix 2 (TM2) plays an exceptionally critical role in its signal transduction, overturning the traditional view that TM6 is key to GPCR activation. The allosteric modulator CB-05, discovered based on this mechanism, exhibits significant analgesic effects without addictive side effects, achieving the transformation of cannabis from a "toxic" substance to a "medicinal" one. Furthermore, we proposed, for the first time, a novel entropy-driven subtype selectivity mechanism for cannabinoid receptor CB2 ligands. Through precise design, we identified a novel, highly active, and selective CB2 agonist, YL035. This compound demonstrates remarkable efficacy in pain models and is devoid of the side effects associated with CB1 orthosteric ligands.

Plenary Speaker

Dr. Gyoonhee Han
Yonsei University, Professor

Structure based optimization of TEAD1 inhibitors for anti-cancer chemotherapy

Biography

Professor Gyoonhee Han is a distinguished professor at Yonsei University (YU). He graduated from Seoul National University College of Pharmacy with a B.S. and M.S. and earned his Ph.D. in organic chemistry from the Pennsylvania State University. Before joining YU, he was a research scientist at Bayer Healthcare AG and KRIBB. Since joining YU, he has served YU as an associate dean at UIC and a dean at the College of Pharmacy. His major is chemical biology and medicinal chemistry, and he is working toward discovering novel medicines for incurable diseases using computers and AI tools.

Abstract

The Hippo signaling pathway plays a pivotal role in controlling cell proliferation, maintaining tissue equilibrium, and determining organ size. Aberrations in this pathway have been closely linked to various diseases, particularly cancer, due to their impact on downstream effectors like Yes-associated protein (YAP) and transcriptional coactivator with PDZ-binding motif (TAZ) which interact with transcriptional enhanced associate domain (TEAD) proteins. In this study, we identified a TEAD1-selective inhibitor through structure-based drug discovery (SBDD) by utilizing our previously developed pan-TEAD inhibitor. Computational docking and energy calculations facilitated the design of a compound that exhibits TEAD1 selectivity.

Plenary Speaker

Dr. Yasuteru Shigeta
University of Tsukuba, Professor

Integrated computational chemistry methods for protein function analysis and drug discovery

Biography

Prof. Yasuteru Shigeta is a Theoretical Chemist working at University of Tsukuba as a full professor since 2014. He has published more than 370 scientific papers and received the PCCP award of Royal Society of Chemistry (UK) in 2007, Young-chemists award of the Chemical Society of Japan in 2009, the Young-scientists award of Ministry of Education, Culture, Sports, Science, and Technology (MEXT) Japan in 2010, the Young-scientists award of Japan Society for Molecular Science in 2012, and the QSCP Promising Scientist Prize of CMOA in 2017.

Abstract

Integrated computational chemistry methods are crucial for deciphering protein function and accelerating drug discovery since phenomena and targets are quite complicated. This presentation will highlight recent advancements and applications from our group, focusing on understanding complex biological processes at an atomistic level. We employ enhanced molecular dynamics simulations, including Parallel Cascade Selection Molecular Dynamics (PaCS-MD), to efficiently explore protein conformational changes and rare events, which are critical for understanding ligand-binding processes and protein-ligand interactions. Our work incorporates QM/MM approaches to investigate detailed reaction mechanisms and other biological systems. Furthermore, we apply these integrated computational strategies to rational drug design, covering aspects such as virtual screening, elucidation of ligand binding modes, and prediction of membrane permeability for various therapeutic targets, including viral proteins (e.g., SARS-CoV-2, HIV-1, Dengue, Zika). These efforts aim to provide atomistic insights that inform and accelerate the development of novel therapeutic agents.

Invited Speaker

Dr. Weiliang Zhu
Shanghai Institute of Materia Medica, Professor

Halogen bonding and its application in drug design

Biography

Weiliang Zhu obtained his PhD in 1998 from Shanghai Institute of Materia Medica (SIMM), Chinese Academy of Sciences. He is currently working in SIMM as a professor and principal investigator in the research areas of CADD/AIDD, Medicinal Chemistry and Phytochemistry. He has published 300+ papers and submitted 80+ patent applications.

Abstract

Halogen bonding refers to the noncovalent interactions between halogen atoms and Lewis bases. In the past 17 years, we focused on halogen bonding with the aim to understanding the nature of the interaction between organohalogens and proteins and its application in drug design. We observed that the interactions featured with charge transfer from lone pair electrons of the acceptor atom to the antibonding orbital of the carbon-halogen bond, we found that the interaction could be used to optimize both bioactivity of druggability of lead compound, we also found that halogen bonding between organofluorine and protein could be induced by hydrogen bond, we tried with success to run lead optimization via designing halogen bond.

Invited Speaker

Dr. Taisuke Boku

University of Tsukuba, Professor

Advanced GPU computing technologies for MD simulations and next generation's Japanese flagship supercomputing project

Biography

Taisuke Boku graduated the Department of Electrical Engineering, Faculty of Science and Technology, Keio University and received PhD degree in 1990. He has been researching HPC system architecture, system software, and performance tuning and evaluation on various scientific applications. From 2019 to 2024, he was the Director for Center for Computational Sciences, University of Tsukuba, a co-designing center with both application researchers and HPC system researchers. He played the central roles for development of original supercomputers in the center including CP-PACS (ranked as number one in TOP500 in 1996), FIRST, PACS-CS, HA-PACS, Cygnus and Pegasus systems, the representative supercomputers in Japan. He was the President of HPCI (High Performance Computing Infrastructure) Consortium in Japan in 2020-2022, and currently the Vice President in 2024-2026. He received ACM Gordon Bell Prize in 2011. He has been one of the Program Directors of the Feasibility Study of the Next Generation Supercomputer in Japan (“Post-Fugaku”) under MEXT (2023-2025).

Abstract

In this talk, two topics for advanced accelerated supercomputing for various computational sciences. At first, the GPU performance improvement technology to efficiently utilize the GPU core resources by MPS (Multi-Process Service) in advanced NVIDIA GPUs for Replica-Exchange MD Simulations by AMBER is introduced toward 2x performance improvement on membrane permeation process of a drug candidate peptide. MPS is an advanced feature of recent NVIDIA GPUs such as A100 and H100 to dynamical core sharing by multiple processes running on a single GPU-node. In the AMBER simulation, parallel processes under MPI are not perfectly synchronized and the parallelism of GPU cores vary on different code sections. We investigated the best way to apply MPS in such a simulation and improved the GPU core utilization rate with approximately double of the original case to run multiple cases quite efficiently. In addition, I will introduce the plan of Japan's next generation of National Flagship Supercomputer (NFS), tentatively named "post-Fugaku" or "Fugaku-Next" of which goal of productive run in 2030. The system will introduce the accelerators such as advanced GPUs as the first challenge to apply in the NFS of Japan. The talk also covers the new support program for advanced GPU code shift in nation-wide scale.

Invited Speaker

Dr. Yun Tang
East China University of Science and Technology, Professor

Network-based methods applied in drug discovery for complex diseases

Biography

Dr. Yun Tang is a professor and director of Shanghai Key Laboratory of New Drug Design, School of Pharmacy, East China University of Science and Technology. Dr. Tang got his PhD degree from Shanghai Institute of Materia Medica, Chinese Academy of Sciences in 1996. After that, he had worked overseas for eight years, including Sweden, USA and Canada. He came back China in May 2004 as a professor at School of Pharmacy, Fudan University. Since September 2004 he has been working in School of Pharmacy, East China University of Science and Technology. His research interests include computer-aided drug design (CADD), computational toxicology, network pharmacology, and computational biology. Up to now, Prof. Tang has published more than 300 papers in peer-review journals, and holds 25 software copyrights and 7 patents.

Abstract

Drug discovery is a costly and time-consuming process, so new technologies, such as artificial intelligence (AI), have been developed to reduce the cost and shorten the procedure. For complex diseases, such as Alzheimer's disease, the situation is more complicated. As the development of systems biology and network pharmacology, network-based methods have emerged as powerful tools in drug discovery of complex diseases. Here, Dr. Yun Tang would first introduce the background and concept of network-based methods. Then, the applications of network-based methods were described across various areas of drug discovery, such as target prediction, virtual screening, and elucidation of molecular mechanisms. In addition, some useful web servers were provided for researchers to use network-based methods in specific applications. Finally, he would discuss several challenges of network-based methods and the directions for future development.

Invited Speaker

Dr. Woo Youn Kim
Korea Advanced Institute of Science and Technology, Professor

Generative modelling for drug discovery

Biography

Dr. Woo Youn Kim is focused on developing state-of-the-art, domain-specific deep learning models to accelerate new drug discovery. Since the mid-2010s, he has pioneered the development of generative AI for molecular design. His recent research involves leveraging domain-specific data as well as knowledge from Large Language Models (LLMs). Under the belief that "chemistry changes the world, and digital technology changes chemistry," he founded the startup HITS in 2020. He majored in chemistry and physics at POSTECH, where he also earned a Ph.D. in computational chemistry in 2009. Following his doctorate, he was a postdoctoral researcher in theoretical physics at the Max Planck Institute in Germany. From 2011, he is serving as an assistant/associate/full professor in the Department of Chemistry at KAIST.

Abstract

Generative AI is a powerful tool for molecular design, yet its real-world application in drug discovery is hindered by challenges in achieving synthetic feasibility, novelty, and diversity. This presentation provides an overview of state-of-the-art models including graph-based methods, generative flow networks, and diffusion models designed to address these issues. We highlight strategies that improve synthesizability by incorporating chemical reaction templates, ensuring generated compounds are both drug-like and accessible. Furthermore, advanced sampling and adaptive learning techniques enable the exploration of diverse molecular structures, including those with novel building blocks, while optimizing for key properties like binding affinity. Through case studies, we demonstrate how these generative approaches effectively balance novelty, diversity, and synthetic feasibility, paving the way for more practical and innovative solutions in drug discovery.

Invited Speaker

Dr. Yuzong Chen
Ningbo University, Professor

Applications of manifold transformation in drug discovery

Biography

Professor Yuzong Chen is focused on AI-driven drug design, cheminformatics, bioinformatics and natural products research. He pioneered the application of artificial intelligence to drug design and bioinformatics as early as 2002, invented the reverse docking approach for target discovery, and founded the widely used Therapeutic Target Database (TTD). His research has revealed the synergistic mechanisms of Western medicines and herbal remedies through network-based approaches and uncovered clustering patterns of drug-producing species. Over the past two decades, Professor Chen has published more than 240 articles in leading journals, including Nature Biotechnology, Nature Reviews Drug Discovery, Pharmacological Reviews, Trends in Pharmacological Sciences and PNAS.

Abstract

Manifold Transformation enables the ordering of unstructured data and leverages the powerful learning capacity of convolutional neural networks (CNNs) to enhance the analysis and predictive performance of biomedical data. It demonstrates particular strengths in drug-related molecular, omics and spectroscopic deep learning tasks, especially under conditions of data complexity and limited sample size. This presentation will highlight the applications and potential of Manifold Transformation in drug property prediction, treatment outcome prediction based on clinical omics, Raman spectroscopy-based identification of drug-resistant bacteria and quality control of traditional Chinese medicine.

Invited Speaker

Dr. Huaiyu Yang

East China Normal University, Professor

New activation and inhibition strategies of voltage-gated potassium channels

Biography

Huaiyu Yang, Professor of the School of Life Sciences and the School of Pharmacy at East China Normal University. His group primarily focuses on drug design studies targeting ion channels. He conducts small-molecule modulation and functional study of ion channels with a new strategy of targeting ion channel dynamics. Leveraging the rich dynamic behaviors of ion channels, novel regulatory strategies have been uncovered, including dynamic sites identified within the pore region and its adjacent areas, as well as new regulatory mechanisms such as "small molecule squeezes the gate to close." A series of active small molecules have been discovered for ion channels related to neurological diseases, including the first selective agonists or inhibitors for channels such as TASK-3, TREK-1 and Hv1. These selective small molecules were used for pharmacological function analysis, revealing that these channels are potential targets for analgesia or antidepressant effects.

Abstract

The classic paradigm of drug development involves identifying molecules that enhance or weaken the physiological functions of proteins, with the corresponding molecular mechanism being the binding of these molecules to the protein's inherent structure or dynamic conformations. We continue to develop new theories for regulating ion channels, discovering that small molecules can be used to create novel functional states of ion channels-rather than merely enhancing or weakening their inherent functions. Voltage-gated ion channels (VGICs), such as KCNQ2, control the passive yet selective ion flow across the plasma membranes. Dysfunction of VGICs, resulting from genetic mutations or post-translational modifications, can lead to diseases such as epilepsy, cardiac arrhythmias and myotonia. We firstly revealed that small molecules can induce the pore region of the KCNQ2 channel to adopt a conformation more open than its physiological open state, thereby generating novel conductance properties in the ion channel. Recently, we also reported a new breakthrough in creating inhibition states of ion channels using small molecules. Specifically, we discovered small molecules capable of inducing an inactivated state in the non-inactivating potassium channel KCNQ2, revealing a novel inhibitory mechanism where small molecules induce gate closure in the activated state. This presentation will introduce these advancements.

Invited Speaker

Dr. Xiangxiang Zeng
Hunan University, Professor

Molecular world models for drug discovery

Biography

Recipient of the National Science Fund for Distinguished Young Scholars and Hunan Provincial Science Fund for Distinguished Young Scholars. Awarded the Wu Wenjun Award for Outstanding Young Artificial Intelligence, the Amazon Machine Learning Research Award, and the CCF Science and Technology Award. Selected as one of the 2022 "China Intelligent Computing Technology Innovation Figures" (MIT Technology Review). From 2020 to 2024, consecutively listed in Clarivate's "Global Highly Cited Researchers" and Elsevier's "China Highly Cited Scholars" lists. His achievements were included in the World Artificial Intelligence Conference's "Yunfan Award" list. In recent years, he has published over 100 papers as first author or corresponding author in journals and conferences such as Nature sub-journals (e.g Nature Machine Intelligence, Nature Computational Science, Nature Communications, Cell sub-journals, ICML, NeurIPS, ICLR, AAAI, and IJCAI. Won the Best Paper Award at the ICIC2024 International Conference, the China 2021 Annual Best Paper Award from Cell Publishing House, and the 2020 Best Paper Award from IMCS Society. The DrugAI WeChat public account he founded was selected as one of China's "Top10 Academic Media Accounts".

Abstract

Drug discovery is characterized by high costs, prolonged timelines, and low success rates. The implementation of intelligent drug discovery methodologies has the potential to significantly reduce research and development expenses and enhance the probability of successful outcomes. However, the current field of intelligent drug discovery faces challenges, including insufficient interpretability, limited generalizability, and a lack of domain-specific expertise. Human knowledge and multi-modal self-supervised pre-training large models such as vision and language are possible ways to solve this problem. This report will introduce the Hunan University DrugAI research team's exploration in molecular world models which includes knowledge graph, molecular vision pre-training model, multi-modal language pre-training model, etc., as well as applications such as drug repositioning, drug combination, molecular property prediction, antimicrobial peptide discovery, and molecule generation. Finally, we put forward our thoughts and prospects on the large multi-modal model for drug research and development.

Invited Speaker

Dr. Masahito Ohue
Institute of Science Tokyo, Associate Professor

Applications of AlphaFold protein structure prediction: from protein-protein interaction prediction to multimodality drug discovery

Biography

Masahito Ohue received his Ph.D. in Computer Science from Tokyo Institute of Technology (Tokyo Tech) in 2014. He then served as a JSPS Postdoctoral Fellow (PD), before becoming Assistant Professor at Tokyo Tech in 2015. In 2020, he launched his own laboratory as a tenure-track Assistant Professor, and since 2024 he has been Associate Professor at the School of Computing, Institute of Science Tokyo (formerly Tokyo Tech). His research focuses on the fusion of bioinformatics and supercomputing, especially the development of protein-protein/ligand/peptide/antibody interaction prediction methods. He has been a JST FOREST researcher since 2022 and has received numerous honors, including the JSPS Ikushi Prize (2014), the MEXT Young Scientist Award (2019), and the Special Award for Science Tokyo Advanced Researchers [STAR] (2025).

Abstract

The emergence of AlphaFold has dramatically changed the landscape of structural bioinformatics by enabling rapid prediction of protein 3D structures with remarkable accuracy. These predictions open the door to diverse applications, including ligand docking, protein-protein interaction analysis, and drug discovery. With the release of AlphaFold3, which can model heterocomplexes with small molecules and nucleic acids, its potential impact on multimodality drug discovery has become even more evident. However, a critical question remains: can AlphaFold-predicted structures be directly relied upon for molecular design in practice? Our studies have sought to address this challenge by developing strategies to enhance the usability of AlphaFold models. For instance, we introduced SpatialPPI, a framework for predicting novel protein-protein interactions, and established approaches to optimize AlphaFold parameters for generating structures suitable for virtual screening. We further explored rational criteria for selecting ligands in AlphaFold3-based complex modeling, and demonstrated that the reliability of AlphaFold structures as starting points for ligand design can approach that of typical experimental PDB structures. In addition, we have extended these concepts toward antibody design, highlighting the potential of AI-driven models for therapeutic development. Collectively, these approaches underscore that, with careful adaptation, AlphaFold can serve as a powerful engine for practical and accurate drug discovery.

Invited Speaker

Dr. Takashi Ishida
Institute of Science Tokyo, Professor

Retrosynthesis prediction for efficient drug discovery

Biography

Takashi Ishida received his Ph.D. in Agriculture from the University of Tokyo in 2006. He subsequently worked as a Researcher at the University of Tokyo before joining Tokyo Institute of Technology in 2009 as a Specially Appointed Assistant Professor under the Global COE Program. He was promoted to Associate Professor in 2014 and, since 2024, has been serving as a Professor at Institute of Science Tokyo (formerly Tokyo Tech). From 2017 to 2019, he also held the position of Science and Technology Policy Fellow at the Cabinet Office of Japan, where he contributed to national strategies in science and innovation policy. His primary research field is bioinformatics, with a focus on protein structure prediction. He has developed machine learning-based computational methods for modeling complex biomolecules, including intrinsically disordered proteins. More recently, his work has expanded to drug discovery applications, particularly the prediction of protein-ligand interactions.

Abstract

Modern drug discovery faces significant challenges in designing novel therapeutic compounds with optimal pharmacological properties. Computational molecular design has emerged as a powerful strategy to explore vast chemical space and identify promising drug candidates. However, these advances are limited without ensuring efficient synthetic accessibility. Retrosynthetic prediction addresses this critical gap by enabling automated route planning for computationally designed molecules. Traditional retrosynthetic analysis has relied heavily on expert intuition, often creating bottlenecks in the drug development process. In contrast, machine learning-based retrosynthetic prediction models now provide unprecedented capabilities to rapidly assess synthetic feasibility, propose diverse pathways, and guide medicinal chemists toward synthetically accessible molecular designs. We have been developing several novel retrosynthetic prediction methods, including an approach that leverages molecular substructure fingerprints. In parallel, we are constructing a large-scale database to accelerate research in chemical synthesis. This resource integrates more than 3.2 million reactions from USPTO, ORD, and CRD, providing standardized access to synthesis data for retrosynthetic prediction, route planning, and benchmarking. In this talk, I will present an overview of both our prediction methods and the database.

Invited Speaker

Dr. Feng Zhu
Zhejiang University, Professor

Artificial intelligence-based target identification and novel ligand design

Biography

Dr. Zhu is a distinguished tenured professor of Zhejiang University. He employs bioinformatic approaches and OMIC technologies to discover the druggability and biological characteristics of therapeutic targets, develop novel methods for new drug target discovery, and investigate the interaction mechanism between drug and target. He serves as the Associate Editor of J. Chem. Inf. Model., the Vice-President of Zhejiang Bioinformatics Society, and the Secretary-General of the Computer Chemistry Committee of Chinese Chemical Society. His research has been ranked as the "China's Top-100 Most Influential International Papers" released by the ISTIC of the Chinese Ministry of Science and Technology, and included into the "2022 Top-10 Advances in Chinese Bioinformatics". He has published over 200 papers in such journals as Nature Biotechnol, Nature Protoc, Nature Mach Intell, Nature Rev Drug Discov, Genome Biol, PNAS.

Abstract

Therapeutic target discovery is the starting point for developing targeted drugs, as well as the key to conducting new drug design, screening, and optimization. Related studies have become a cutting-edge hotspot in clinical drug development. Although global investment in target discovery has increased over the past two decades, the number of innovative therapeutic targets with new drug approval remains limited. Some academically recognized issues have seriously restricted the discovery of new targets. These problems have a severe impact on the subsequent R&D chain of novel drugs and are key scientific issues that urgently need to be addressed in the field of drug design. This report will introduce the latest work completed by Prof. Zhu's team in the field of artificial intelligence-assisted target discovery.

Invited Speaker

Dr. Ji Cao
Zhejiang University, Professor

Identification of anti-tumor drug targets using targeted protein degradation strategies

Biography

Prof Ji Cao is a Professor at the College of Pharmaceutical Sciences, Zhejiang University. He is renowned for his research in anti-tumor drug target discovery and innovative drug development, with special expertise in tumor pharmacology, protein degradation, and the application of artificial intelligence in pharmaceuticals. Prof. Cao has published widely in high-impact journals such as Cell Metabolism, Nature Communications, and PNAS, and has been recognized with numerous awards for his scientific contributions. He actively contributes to the advancement of cancer therapeutics and translational medicine through academic leadership and international collaboration.

Abstract

Recent advances in Targeted Protein Degradation (TPD) have revolutionized the identification and validation of novel anti-tumor drug targets. In this talk, I will present our integrative approach combining TPD strategies with phenotype screening to systematically uncover and validate key oncogenic targets such as CDK12 and BUB1B. I will introduce the synthesis and rapid evaluation of Proteolysis Targeting Chimeras (PROTACs), highlighting the development and application of the streamlined pre-Tca system for high-throughput assessment of degrader efficacy and selectivity. A novel strategy, Catalytic Proximal Protein Oligomerization (CaPPO), will also be discussed. By inducing WDR5 protein oligomerization, CaPPO effectively blocks its oncogenic functions, offering an alternative avenue for modulating challenging drug targets. Finally, I will explore the expanding role of artificial intelligence in the field of targeted protein degradation. Specifically, I will outline how AI-driven methods accelerate the design, prediction, and optimization of degraders, thereby enhancing our capability to identify and develop next-generation therapeutics for cancer treatment.

Invited Speaker

Dr. Yoonji Lee
Chung-Ang University, Associate Professor

Graph-based prediction of liver metabolic fate integrating stability and site of metabolism

Biography

Yoonji Lee is an Associate Professor at the College of Pharmacy, Chung-Ang University, South Korea. Her research focuses on the intersection of cheminformatics, structural bioinformatics, and in silico drug discovery. She received her Ph.D. in molecular modeling and drug design from Ewha Womans University in 2013. From 2017 to 2020, she worked as an Assistant Instructor and later as an Instructor in the Department of Biophysics at UT Southwestern Medical Center, TX, USA, and joined Chung-Ang University in 2020. Throughout her career, she has focused on improving the efficiency of hit identification and lead optimization through computational methods that elucidate ligand-receptor interactions. She also applies structural bioinformatics to model and annotate protein structures, offering insights into structure-function relationships critical for drug discovery. Recently, her work has expanded to include AI-driven predictive modeling to support early-stage drug discovery.

Abstract

Hepatic metabolism critically influences a drug's half-life, bioavailability, toxicity, and risk of drug-drug interactions. These outcomes are largely determined by a drug's overall metabolic stability and the specific sites of metabolism (SoMs). To address both aspects, we designed graph neural network (GNN) approaches trained on newly curated datasets of metabolic stability and cytochrome P450 sites of metabolism. For stability prediction, we represented molecular structures as graphs and applied contrastive learning-based pretraining to capture structural diversity, while incorporating cross-species variation between human and mouse liver microsomes, which yielded the greatest improvement in predictive performance. For SoM prediction, we constructed a multi-level GNN integrating atom-, bond-, and molecule-level representations, trained on experimentally confirmed cytochrome P450 SoM data aggregated from public databases and literature. In both models, attention analysis highlighted chemically relevant substructures that contributed to predictions, providing interpretable insights. Taken together, these approaches offer complementary perspectives on drug metabolism and support more accurate and efficient structure optimization during drug discovery.

Invited Speaker

Dr. Ky-Youb Nam
Pharos iBio Co., Ltd., CTO

AI drug discovery platform and its application: CHEMIVERSE™

Biography

Ky-Youb Nam, Ph.D. brings deep experience building AI/ML-driven computational chemistry for drug discovery. He is currently co-founder, president and Chief Technology Officer at Pharos iBio Co., Ltd. and is responsible for oncology drug developing PHI-101 of FLT3 inhibitor and PHI-501 of pan-RAF inhibitor from investigational new drug (IND) applications to Phase I clinical trials. Previously, he served as team leader for drug discovery at Bioinformatics and Molecular Design Research Institute. He also currently serves as a member of Executive Committee Directors at Korean Chemical Society. He studied computational biophysics at University of Maryland Biotech Institute in USA. He received his Ph.D. degree from Soongsil University Graduate School and a B.Sc. in Chemistry from Soongsil University.

Abstract

Involvement of artificial intelligence (AI) in the drug discovery and development from transforming the bio big data to healthcare can be imagined given that it can aid rational drug design and assist in decision making. Pharos iBio Co., Ltd. is a leading biotech company developing a portfolio of oncologic therapies for acute myeloid leukemia (Phase 1), colorectal cancer and multiple melanoma (Phase 1), and ovarian cancer (Phase 1). Pharos is also advancing its pipeline and discovery activities using AI Based platform technology of CHEMIVERSE™ . The CHEMIVERSE™ AI platform is unique and multifunctional, accurately identifying hit compounds based on 3D target protein structure and quantum mechanical energy calculations, assessing predicting ADME/Tox. and analyzing drug-target-disease network. in silico virtual screening from virtual chemical spaces along with structure and ligand-based approaches helps to select appropriate molecules for starting points for a medicinal chemistry project, employing 3D target protein structure-based drug discovery (SBDD). To increase the success rate of innovative drug discovery and development, we are utilizing 1) AI platforms, 2) orphan and intractable diseases, 3) biomarkers, and 4) open innovation strategies. PHI-101 is going on the completion of a global Phase 1 clinical trial for patients with FLT3-mutated acute myeloid leukemia, and PHI-501 is entering in Phase 1 clinical development for solid tumors with BRAF, KRAS, and NRAS mutations. As a new Discovery project, we are conducting lead identification research by applying a 3D protein structure-based AI model.

Invited Speaker

Dr. Zhijian Xu
Shanghai Institute of Materia Medica, Professor

Identification of USP2 dynamic pocket as a novel anticancer target

Biography

Dr. Zhijian Xu (b. 1985) earned his Ph.D. from Shanghai Institute of Materia Medica, Chinese Academy of Sciences (SIMM) in 2012 and is currently a full professor at the SIMM. Specializing in molecular simulation and drug design, he develops innovative computational methods and applies them to drug discovery. With over 150 publications, including 4 papers cited > 200 times, he has filed 50+ patents and holds 6 software copyrights.

Abstract

The natural product gambogic acid (GA) inhibits the deubiquitinating activity of ubiquitin-specific protease 2 (USP2) by forming a covalent bond with its Cys284 residue, leading to KRAS degradation and thereby suppressing the proliferation of multiple myeloma cells. In crystal structures, Cys284 is embedded within the protein's interior. Through molecular dynamics (umbrella sampling), we identified a conformational state where Cys284 becomes exposed, revealing a newly formed pocket. Virtual screening combined with activity assays targeting this pocket identified the non-covalent inhibitor ICU30, which significantly inhibits multiple myeloma cell growth. Our study demonstrates that the novel pocket in USP2 represents a promising therapeutic target. Inhibiting USP2 to induce KRAS degradation may offer a novel therapeutic strategy for cancers harboring KRAS mutations.

Invited Speaker

Dr. Chang-Yu Hsieh
Zhejiang University, Professor

BioScore: A universal scoring function

Biography

Dr. Chang-Yu (Kim) Hsieh is a Professor at the College of Pharmaceutical Sciences, Zhejiang University. Before joining Zhejiang University, he led the Theory Division at Tencent Quantum Lab in Shenzhen, focusing on AI and quantum simulation for drug and material discovery. Prior to that, he was a postdoctoral researcher in the Department of Chemistry at MIT. His primary research interests lie in developing advanced computing algorithms, including AI and quantum computing, to simulate and model material and molecular properties.

Abstract

Recent deep learning algorithms, such as the AlphaFold series, have achieved high-precision protein structure prediction. However, a core challenge in drug discovery remains: designing effective scoring functions for complex conformation evaluation. Existing scoring functions are often limited to protein-small molecule interactions, lack flexibility for other biological complexes and are typically task-specific. We introduce BioScore, a universal scoring function for biological complexes, which makes three key highlights. First, it uses an all-atom coarse-grained representation to model 3D biological complexes as a unified, non-hierarchical geometric set graph. Second, it employs a universal E(3)-equivariant Transformer within a dual-tower model to balance four capabilities: scoring, ranking, docking, and affinity prediction. Third, a novel hybrid density network output strategy allows a single model to effectively score a variety of complexes. BioScore demonstrates strong performance on protein-small molecule and protein-protein benchmarks, significantly outperforming traditional tools and existing deep learning methods, especially for protein-protein interactions.

Invited Speaker

Dr. Lianyi Han
Jiangsu Hengrui Pharmaceuticals Co., Ltd., Professor/AIDD Team Leader

AI-powered drug discovery: From target identification & validation to molecular design & optimization

Biography

Dr. Han brings over 18 years of extensive research and development experience spanning both academia and industry. Prior to joining Hengrui, he served as a Senior Scientist at the National Center for Biotechnology Information (NCBI), National Institutes of Health (NIH) in the United States. Dr. Han subsequently held key roles as chief scientist and principal investigator at Tencent's U.S.-based AI healthcare laboratory, and also served as a professor and doctoral advisor at Fudan University. His research expertise covers AI-driven drug discovery (AIDD) and AI-enabled digital therapeutics (AIDT). He has led and participated in multiple international projects in areas including protein function prediction, target drugability assessment, PubChem 3D, NCBI SPARCLE, NCBI BioSystems, AI-powered high-throughput virtual screening, as well as AI-assisted drug development and digital diagnosis and treatment solutions for dermatological and neurodegenerative diseases.

Abstract

Current clinical drug development faces numerous challenges, including extended timelines, high costs, and significant risks. It often relies on existing biological hypotheses, with validation processes being both time-consuming and expensive. Meanwhile, the diversity of clinical data and the complexity of information-spanning multiple platforms and multi-omics datasets-further complicate data integration. With the rapid advancement of AI technology, the paradigm of drug development is shifting. This presentation will highlight the achievements and ongoing challenges of AI in two key areas: target discovery and molecular design. In target discovery, AI applications include target identification based on multi-omics data, imaging-based biomarker recognition, construction of knowledge graphs and biological networks, real-world data mining, and virtual cell exploration. In molecular design, AI contributes through molecular design and optimization, prediction of ADMET properties, computer-assisted synthesis planning, and AI-facilitated drug repurposing.

Invited Speaker

Dr. Zhenming Liu
Peking University, Professor

Pharmaceutical intelligence revolution: Artificial intelligence reshapes the new paradigm of biomedical research

Biography

Dr. Liu Zhenming is a Principal Investigator and Professor of Pharmacology at Peking University School of Pharmacy. His research focuses on innovative drug discovery technologies and the development of AI algorithms and models for drug research. Dr. Liu has led and participated in 21 national research projects, including the National Natural Science Foundation of China, the 863 Program, and the National Science and Technology Major Projects. Over the past five years, he has published more than 70 research papers as the first or corresponding author in journals such as Nat. Mach. Intell., Signal Transduct. Target. Ther., and J. Hematol. Oncol. He has also edited and co-edited five textbooks and monographs and holds 12 Chinese invention patents. Dr. Liu serves as a member of the Computational Chemistry Committee of the Chinese Chemical Society, a standing committee member of the Health Data and Digital Medicine Branch of the China International Medical Exchange and Promotion Association, and as an Associate Editor for the European Journal of Medicinal Chemistry and European Journal of Medicinal Chemistry Reports.

Abstract

This report systematically elaborates on the paradigm shift in AI-driven drug discovery and development, focusing on five core scenarios: target discovery, molecular generation, intelligent TCM modernization, biologics acceleration, and virtual clinical trials. Leveraging Peking University's "Pharmaceutical Intelligence Super Brain" infrastructure, breakthrough achievements include the identification of 3 novel targets, development of 12 specialized models, and generation of 15 preclinical candidates, alongside the deployment of a drug knowledge engine and an integrated AIDD platform. The report proposes leveraging Asia's clinical resources (30% of global share) and the "Digital Pharmacy Silk Road" alliance to collaboratively address challenges in data fusion, regulatory frameworks, and ethical governance, thereby advancing from incremental innovation to paradigm revolution and ultimately redefining the future of AI-powered drug R&D.

Invited Speaker

Dr. Inhee Choi

Institut Pasteur Korea, Team Leader

Tackling ADMET with a combined AI and collective intelligence approach

Biography

She has extensive expertise in computer-aided drug design with a background in pharmacy. In 2006, she earned her Ph.D. in computer-aided drug design from the College of Pharmacy at Ewha Womans University in Korea. She then completed her postdoctoral training at BMDRC in Korea and at the National Institutes of Health (NIH) in Maryland, USA, in 2010. That same year, she joined Institut Pasteur Korea (IPK) upon returning to Korea. Actively engaged in computer-aided drug discovery research, she has successfully predicted the binding modes of anti-tubercular agents such as Pretomanid and Telacebec. Since 2020, she has been leading the AI Drug Discovery (ADD) group at IPK, which focuses on early-stage discovery of novel treatments for infectious diseases by integrating medicinal chemistry-driven synthesis with cutting-edge AI technologies to accelerate effective drug development.

Abstract

ADMET-absorption, distribution, metabolism, elimination, and toxicity-represents a critical factor in determining the success of new drug candidates. Early and reliable assessment of ADMET properties helps identify compounds with favorable profiles while eliminating those likely to fail due to safety or pharmacokinetic issues. In recent years, computer-based approaches have been increasingly applied to predict ADMET, offering faster and more cost-effective alternatives to traditional experimental testing. Despite these advances, accurate prediction remains challenging due to the complexity of human biology and limitations in existing models. The rapid growth of artificial intelligence (AI) provides new opportunities to address these challenges. This presentation will examine current limitations in in silico ADMET prediction, highlight emerging AI-based strategies, and discuss how these innovations can enhance efficiency and reduce attrition in early drug development. By integrating AI with traditional methods, the field is moving toward a more reliable and streamlined process, accelerating the discovery of safe and effective treatments.

Invited Speaker

Dr. Keisuke Yanagisawa
Institute of Science Tokyo, Assistant Professor

FraSCO-VS: Fragment-based drug virtual screening by combinatorial optimization with quantum annealer

Biography

Keisuke Yanagisawa received his Ph.D. in Computer Science from Tokyo Institute of Technology (Tokyo Tech) in 2019. He then served as a JSPS Postdoctoral Fellow at the University of Tokyo before becoming an Assistant Professor at Tokyo Tech in 2020. His research focuses on computer-aided drug discovery (CADD), particularly on developing computational methods for compound virtual screening of target proteins. He has introduced novel approaches such as REstretto, an efficient fragment-based protein-ligand docking tool, and AAp-MSMD, a mixed-solvent molecular dynamics (MSMD) method for protein-peptide interactions. In addition to his research activities, he is committed to education in data science and artificial intelligence, contributing to institute-wide DS&AI programs at Science Tokyo. His current research interests include the application of quantum annealing methods to CADD, especially fragment-based virtual screening.

Abstract

Protein–ligand docking plays a significant role in structure-based drug discovery. This methodology aims to estimate the binding mode and binding free energy between the drug-targeted protein and candidate small molecules, utilizing protein tertiary structure information. In this study, we formulated fragment-based protein-ligand flexible docking as a quadratic unconstrained binary optimization (QUBO) problem, focusing on fragments (rigid chemical substructures of compounds). The Hamiltonian incorporated four essential factors for fragment-based docking: (1) interaction energy between the target protein and each fragment, (2) steric clashes between fragments, (3) covalent bonds between fragments, and (4) the constraint that each fragment of the compound is selected for a single placement. A proof-of-concept implementation using SQBM+, a simulated quantum annealer, demonstrated that a redocking experiment with aldose reductase protein-ligand complex successfully reproduced a near-native bound pose (RMSD = 1.26 Å), and these results have been published (Yanagisawa et al., Entropy, 2024). Furthermore, we now aim to extend the QUBO formulation and quantum annealing with SQBM+ to virtual screening of large compound libraries, and we will report on the efficiency of this approach.

Invited Speaker

Dr. Fang Bai
Shanghai Tech University,
Assistant Professor

From structure to phenotype: AI-powered strategies for lead compound discovery

Biography

Dr. Fang Bai is a tenured associate professor in the School of Life Science and Technology at Shanghai Tech University & The Shanghai Institute for Advanced Immunochemical Studies. She received her Ph.D. in Biomedical Engineering from Dalian University of Technology in 2014 and completed postdoctoral training at the Center for Theoretical Biological Physics at Rice University. Before joining Shanghai Tech University in October 2019, she served briefly as an assistant professor at the University of Texas Health Science Center at Houston. Dr. Bai's research centers on advancing computational methods for drug design, including the application of artificial intelligence algorithms. Her recent work emphasizes developing new approaches to design drugs against undruggable targets, such as protein-protein interactions, with a focus on designing degraders like molecular glues and PROTACs. She has published more than 80 papers and licensed out 1 candidate anti-cancer drug.

Abstract

Identifying lead compounds that can be translated into effective therapeutics remains a central challenge in drug discovery. Traditional approaches are often hindered by limited chemical space coverage, incomplete structural information, and the difficulty of connecting molecular activity to cellular or organismal phenotypes. Recent advances in artificial intelligence offer new opportunities to address these challenges by integrating diverse scales of information-from molecular structures to cellular responses. This talk will present a newly developed AI-based lead identification framework that spans multiple methodological layers: ligand-based prediction models, protein structure-constrained discovery strategies, and phenotype-driven compound prioritization at the cellular level. Together, these approaches highlight a scalable paradigm for accelerating drug discovery and bridging the gap between chemical design and biological outcome.

Invited Speaker

Dr. Fei Ye
Zhejiang Sci-Tech University,
Professor

Drug design based on dynamic regulation

Biography

Fei Ye, Ph.D., Professor and Doctoral Supervisor, is Associate Dean of the School of Life Sciences and Medicine, Zhejiang Sci-Tech University, and Youth Committee Member of the Intelligent Pharmaceutics Division, Chinese Pharmaceutical Association. She obtained her B.S. from Zhejiang University (2008) and Ph.D. from the Shanghai Institute of Materia Medica, CAS (2013), followed by visiting research at Arizona State University and UCSF. Her research integrates computational biology, molecular drug design, and experimental validation for mechanism-driven drug discovery. She has led multiple national/provincial projects, published 60+ SCI papers (30+ as first/corresponding author, in Nature, Nat Commun., Angew. Chem. Int. Ed., JACS, J. Med. Chem.), and holds 10+ patents (7 granted, 2 translated). Honors include the CAS President's Award and Zhejiang provincial talent programs.

Abstract

The discovery and optimization of lead compounds for disease-related targets are central to drug development, yet current design strategies face major challenges, including limited efficiency, low target selectivity, and poor translational success. A critical reason lies in the reliance of traditional drug design on static structural information, overlooking the intrinsic dynamics and conformational diversity of proteins under physiological conditions. To address this, our work systematically advances drug discovery from three perspectives. First, we investigate the dynamic behavior of target proteins to uncover the link between conformational changes and functional regulation, thereby identifying novel druggable sites. Second, we characterize the binding pathways and conformational transitions of small molecules during target recognition, elucidating underlying mechanisms to guide rational lead optimization. Third, building on these insights, we establish a dynamic regulation-based drug design strategy that integrates computational simulations with experimental validation. This approach has been successfully applied to multiple therapeutic targets, markedly enhancing the efficiency and selectivity of small-molecule modulator discovery. Taken together, these studies provide mechanistic insights into target-ligand interactions and demonstrate a generalizable framework for mechanism-driven drug discovery.

Invited Speaker

Dr. Yuta Kikuchi
Institute of Science Tokyo,
Assistant Professor

Comprehensive analysis of biosynthetic gene clusters in bacteria and discovery of *Tumebacillus* as a potential producer of natural products

Biography

Yuta Kikuchi received his Ph.D. in Life Science from Kitasato University in 2024. In the same year, he was appointed Assistant Professor in Infection Control Science at Kitasato University. Prior to that, he conducted research on microbial drug discovery at the Ōmura Satoshi Memorial Institute, Kitasato University. Since 2025, he has been a Specially Appointed Assistant Professor at the School of Computing, Institute of Science Tokyo. His research focuses on natural product drug discovery, with a particular emphasis on the discovery and application of novel natural products. For this purpose, he applies chemo- and bioinformatics methods in combination with experimental natural product chemistry.

Abstract

Bacteria are valuable sources of natural products (NPs) with potent bioactivities, that are very important for drug discovery. However, limited bacterial genera, such as Streptomyces, have been extensively studied, while the potential of many others remains underexplored. Recent advances in genome analysis, including next-generation sequencing and biosynthetic gene cluster (BGC) prediction, suggest that overlooked genera may harbor numerous BGCs and represent promising NP producers. In this study, we aimed to detect neglected bacterial genera with high biosynthetic potential. A total of 21,052 complete bacterial genomes were analyzed using the antiSMASH pipeline to detect BGCs associated with polyketide, non-ribosomal peptide, and terpene biosynthesis. The average number of BGCs was calculated for each genus. This analysis revealed that the genus *Tumebacillus* possesses, on average, 13 BGCs, comparable to those of known prolific NP producers. Next, we cultured *Tumebacillus permanentifrigoris* JCM 14557T and isolated four compounds. Among them, tumebacin and tumepyrazine were identified as novel metabolites, while 4-(2-nitroethyl)phenol and Le-pyrrolopyrazine B were known compounds. These findings indicate that *Tumebacillus* is a new source of natural products and highlight the value of genome-guided approaches for expanding chemical diversity in drug discovery.

Invited Speaker

Dr. Juyong Lee
Seoul National University,
Associate Professor

Enhanced drug candidate discovery using artificial intelligence and physical energy calculations

Biography

Dr. Juyong Lee is an Associate Professor at the College of Pharmacy at Seoul National University. He received his Ph.D., M.S., and B.S. degrees in Chemistry from Seoul National University. His research career includes a position as a Research Fellow at the Laboratory of Computational Biology, NHLBI/NIH, where he was a Lenfant Biomedical Fellow, and an Assistant Professor at Kangwon National University. Dr. Lee's research focuses on developing and applying computational tools for drug discovery and biological system analysis, with an emphasis on AI-driven protein-ligand interaction prediction, molecular modeling, and cheminformatics. He also serves as the Chief Technical Officer at Arontier Co., an AI-assisted drug discovery company.

Abstract

The integration of artificial intelligence (AI) and molecular dynamics (MD) simulations is rapidly transforming the drug discovery process. Recent advancements demonstrate that state-of-the-art computational techniques are accelerating the discovery of drug candidates across various modalities, including small molecules, peptides, and antibodies. This presentation will explore recent progress in AI models applied to drug screening and candidate generation, with several case studies illustrating their practical applications. First, I will present our findings on the discovery of novel inhibitor candidates for autotaxin using AK-Score, an AI-based scoring function designed to predict protein-ligand interactions. Next, I will discuss the identification of new E3 ligase ligands for targeted protein degrader, PROTAC discovery, leveraging a combination of molecular docking, molecular dynamics simulations, and free energy calculations. Finally, our work on designing novel nanobody sequences using a protein generative model combined with empirical binding free energy calculations will be presented and discuss the status of protein generative models in drug discovery. In all three cases, the success rate for identifying novel candidates was significantly higher compared to traditional high-throughput screening approaches, underscoring the practical advantages of AI-driven strategies in modern drug discovery.

Invited Speaker

Dr. Nam-Chul Cho
Korea Research Institute of Chemical and Technology, Team Leader

Recent trends and future directions of the Korea Chemical Bank (KCB)

Biography

Nam-Chul Cho, Ph.D. serves as Director at the Korea Research Institute of Chemical Technology (KRICT), where he leads the Korea Chemical Bank and Drug Information Platform Center. His research focuses on cheminformatics, computational chemistry, and computer-aided drug discovery, with expertise in GPCR targets and molecular modeling.

Abstract

Since its start in 2000, the Korea Chemical Bank (KCB) has grown from a simple storage facility into a key center for drug discovery in Korea. It holds a massive, quality-controlled collection of over 750,000 chemical compounds and related data. This presentation will highlight the KCB's major developments and future plans. A central part of its success is the korea.chembank.org online platform, which gives all researchers easy-to-use tools for finding and testing new drug candidates. We will show how the KCB is making a real impact, with more companies using its services and successful collaborations, like the recent partnership with Daewoong Pharmaceutical. This partnership marks a major step towards open innovation in Korea. Looking ahead, the KCB is also building a national DNA-Encoded Library (DEL) Core Bank, a new technology to make the first step of drug discovery much faster. By combining its large chemical library, powerful online tools, and key partnerships, the KCB is speeding up drug development and boosting Korea's position in the global pharmaceutical field.

Invited Speaker

Dr. Xiaogen Zhou
Zhejiang University of Technology, Professor

An automated platform for multi-domain protein structure and function prediction

Biography

Dr. Xiaogen Zhou is a Professor and Ph.D. supervisor at Zhejiang University of Technology, and a recipient of the National High-Level Young Talents Program. His main research area is structural bioinformatics. He has published more than 20 first-author papers in journals such as PNAS, Nature Computational Science, and Nature Protocols. He has co-developed several multi-domain protein structure modeling and function prediction servers, including DEMO, DEMO-EM, and I-TASSER-MTD. His related achievements have been recognized with the Second Prize of Natural Science Award of the Chinese Association of Automation, the First Prize of Natural Science Award of the Zhejiang Bioinformatics Society, and the Excellent Doctoral Dissertation Award of Zhejiang Province.

Abstract

Most proteins in cells are composed of multiple folding units (or domains) to perform complex functions in a cooperative manner. We developed I-TASSER-MTD to model the structures and functions of multi-domain proteins through a progressive protocol that combines sequence-based domain parsing, single-domain structure folding, inter-domain structure assembly and structure-based function annotation in a fully automated pipeline. Advanced deep-learning models have been incorporated into each of the steps to enhance both the domain modeling and inter-domain assembly accuracy. The protocol allows for the incorporation of experimental cross-linking data and cryo-electron microscopy density maps to guide the multi-domain structure assembly simulations. I-TASSER-MTD is built on I-TASSER but substantially extends its ability and accuracy in modeling large multi-domain protein structures and provides meaningful functional insights for the targets at both the domain- and full-chain levels from the amino acid sequence alone.

Invited Speaker

Dr. Feng Ni
Ningbo University, Professor

Enabling high-throughput, in-cell ligand discovery through automated chemoproteomics for AI-guided optimization

Biography

Feng Ni, received his B.S. and Ph.D. from Xiamen University. He completed postdoctoral training in medicinal chemistry and chemical biology at the University of Southern California (USC), where he later served as a senior scientist leading chemical-probe design and target-identification programs. In 2017, he joined Ningbo University as a Professor. Dr. Ni's research centers on the discovery and development of next-generation chemical probes and chemoproteomics technologies to enable target deconvolution and ligand discovery directly in live cells. He is also the founder of LeadArt Biotechnologies Inc., a chemoproteomics platform company that builds and applies comprehensive probe libraries together with automation- and AI-enabled live-cell protein-profiling workflows to accelerate high-throughput ligand screening and mechanism-of-action studies.

Abstract

Small molecule ligand discovery remains a key bottleneck in early drug development. Thousands of disease-relevant proteins still lack ligands or chemical tools, and many high-value targets are considered difficult-to-drug due to complex binding mechanisms or cellular environments. Traditional in vitro screening approaches often require purified proteins and lack physiological context-leading to hits that fail to translate in cell-based or in vivo models.

To address these limitations, we have developed a next-generation ligand discovery platform that integrates automated chemoproteomics, live-cell screening, and AI-guided optimization. This end-to-end system enables high-throughput, physiologically relevant ligand discovery directly in live cells, accelerating the development of novel therapeutics and chemical probes for previously intractable targets.

Invited Speaker

Dr. Kowit Hengphasatporn
University of Tsukuba,
Assistant Professor

Ligand-binding parallel cascade selection molecular dynamics simulation for drug discovery

Biography

Dr. Kowit Hengphasatporn is an Assistant Professor at the Center for Computational Sciences, University of Tsukuba, Japan. He specializes in computational biology, with research interests in molecular modeling, drug discovery, and enzyme catalysis using various computational techniques, particularly the Fragment Molecular Orbital (FMO) method and molecular dynamics (MD) simulations. His primary focus is the development of drug screening platforms. Dr. Hengphasatporn earned his Ph.D. in Bioinformatics from Chulalongkorn University, Thailand, in 2019 under the supervision of Prof. Thanyada Rungrotmongkol, following a B.S. in Zoology from Chiang Mai University (2011) and an M.Ed. in Biology from Srinakharinwirot University (2015). He joined Prof. Yasuteru Shigeta's group at the University of Tsukuba as a postdoctoral researcher before being appointed Assistant Professor in 2022. He has published 30 peer-reviewed articles and has received multiple presentation awards at national and international conferences.

Abstract

Ligand-binding Parallel Cascade Selection Molecular Dynamics (LB-PaCS-MD) in combination with Fragment Molecular Orbital (FMO) analysis offers a computational framework that may be considered as a form of in silico crystallization. LB-PaCS-MD enables efficient sampling of ligand-binding pathways without predefined reaction coordinates, capturing native-like binding poses, intermediate states, and conformational adjustments of both ligand and protein. These simulated structures can serve as computational analogues to experimentally determined complexes, providing realistic models for subsequent high-accuracy quantum mechanical evaluation. FMO analysis further decomposes the interaction energies between ligand and protein residues, helping to identify key stabilizing contacts and inform rational optimization. This integrated approach has the potential to complement experimental crystallography by generating and characterizing plausible binding conformations entirely in silico, thereby supporting structure-based drug design.

Invited Speaker

Dr. Haiyan Jin
Bioinformatics and Molecular Design Research Center, Team Leader

Discovery of TEAD lipid pocket inhibitors using FMO and MM-GBSA

Biography

Haiyan Jin is a Researcher at the Bioinformatics and Molecular Design Research Center (BMDRC), where she leads the AI-driven Drug Design Team. Her research focuses on computational small-molecule design, integrating artificial intelligence with physics-based approaches. She earned her Bachelor's degree in Clinical Medicine from Fujian Medical University, followed by a Master's degree in Neurology from Yanbian University in China. She later received her Doctoral degree in Integrative Biotechnology from Yonsei University in Korea.

Abstract

The Hippo pathway controls organ size and homeostasis and is linked to numerous diseases, including cancer. The transcriptional enhanced associate domain (TEAD) family of transcription factors acts as a receptor for downstream effectors, namely yes-associated protein (YAP) and transcriptional co-activator with PDZ-binding motif (TAZ), which binds to various transcription factors and is essential for stimulated gene transcription. YAP/TAZ-TEAD facilitates the upregulation of multiple genes involved in evolutionary cell proliferation and survival. TEAD1-4 overexpression has been observed in different cancers in various tissues, making TEAD an attractive target for drug development. The central drug-accessible pocket of TEAD is crucial because it undergoes a post-translational modification called auto-palmitoylation. Crystal structures of the C-terminal TEAD complex with small molecules are available in the Protein Data Bank, aiding structure-based drug design. In this study, we utilized the FMO method, MD simulations, shape-based screening, and MM-GBSA calculations for virtual screening, and we identified a novel non-covalent inhibitor-BC-001 with IC50 = 3.7 μM in a reporter assay. Subsequently, we optimized several analogs of BC-001 and found that the optimized compound BC-011 exhibited an IC50 of 72.43 nM. These findings can be used to design effective TEAD modulators with anticancer therapeutic implications.

Invited Speaker

Dr. Peichen Pan
Zhejiang University, Assistant Professor

AI-driven screening and design of CLIP1-LTK fusion protein inhibitors

Biography

Dr. Peichen Pan got his PhD in Medicine from Zhejiang University and then did his postdoctoral training at Harvard Medical School. Currently, he is an assistant professor at Zhejiang University. With long-term dedication to the development of innovative algorithms for molecular simulation and AI-assisted drug design, as well as their applications in drug discovery, he has pioneered a series of advanced computational tools, including AI-based molecular docking, molecular generation, scoring functions, and covalent binding site prediction. He has published over 80 papers in authoritative journals, including Nature Mach Intell, Nature Comput Sci, Sci Adv, JACS, ACS Cent Sci, and J Med Chem. The papers have been cited more than 3,300 times, with an H-index of 30.

Abstract

In recent years, AI has made significant strides in the field of drug discovery, demonstrating strong potential in areas such as virtual screening, molecular generation, and binding affinity prediction. However, whether AI-predicted compounds can exhibit the expected activity in experimental validation remains a core challenge in AI-driven drug design. In 2021, the journal Nature first reported the discovery of the CLIP1-LTK fusion gene, confirming that the CLIP1-LTK fusion protein is a novel oncogenic driver and a key target for the development of targeted therapies for non-small cell lung cancer. Nevertheless, there is currently a lack of targeted drugs specifically designed for the CLIP1-LTK fusion protein. This study developed multiple AI-based drug design algorithms, including generative AI models for *de novo* drug design and optimization, as well as AI-powered protein-ligand docking and scoring methods. It also explored and established a virtual screening strategy based on AlphaFold-predicted structures. Addressing real-world drug design scenarios, the research conducted a comprehensive workflow from virtual screening to rational design, combined with molecular, cellular, and animal efficacy models. As a result, several CLIP1-LTK inhibitors with promising drug potential were successfully identified.

Invited Speaker

Dr. Hocheol Lim
Bioinformatics and Molecular Design Research Center, Team Leader

Scoring-Assisted Generative Exploration (SAGE) for *de novo* molecular design

Biography

Hocheol Lim is a Senior Researcher at the Bioinformatics and Molecular Design Research Center (BMDRC), where he leads the AI-driven Protein Design Team. His research focuses on computational molecular design, integrating machine learning and quantum chemistry approaches.

Abstract

De novo design of molecules with desired properties by searching the vast chemical and sequence space remains a significant challenge in biotechnology and materials science. While deep generative models offer a promising solution, achieving simultaneous optimization of multiple, often competing, objectives is non-trivial. Here, we introduce Scoring-Assisted Generative Exploration (SAGE), a novel computational framework developed to generate molecules with desired multi-property profiles. SAGE integrates generative models with a suite of quantitative scoring functions, enabling an iterative and guided exploration of the chemical and sequence space to identify novel candidates that satisfy complex design criteria. The effective versatility of the SAGE framework is demonstrated across three distinct domains. In drug discovery, SAGE successfully generated novel dual-target inhibitors by concurrently optimizing for binding affinity, synthetic accessibility, aqueous solubility, and a profile of 12 ADME/T properties. In materials science, the framework was applied to design functional materials for carbon capture, yielding novel ionic liquids with high CO2 solubility and amine solvents with high CO2 absorption capacity by optimizing key physicochemical properties. Finally, in protein design, SAGE generated new proteins exhibiting enhanced enzymatic activity and solubility, highlighting its potential for generalized, data-driven design across diverse optimization landscapes. Collectively, these applications validate SAGE as a powerful and adaptable strategy for multi-objective optimization in *de novo* molecular design. Consequently, SAGE is poised to significantly accelerate discovery cycles and expand the frontiers of biotechnology and materials science.

Invited Speaker

Dr. Sangwon Lee
Bioinformatics and Molecular Design Research Center, Team Leader

FLORAGENESIS : Advancing natural product development and application deep learning-based interpretation of LC-MS/MS spectra

Biography

Dr. Sangwon Lee is a distinguished Team Leader at the Bioinformatics and Molecular Design Research Center (BMDRC), where he has directed multiple research programs since 2016. He excels in leading collaborative projects that merge computational technology with scientific inquiry, focusing on natural products and advanced data analysis. Dr. Lee earned his Ph.D. in Biotechnology from Yonsei University. His doctoral research culminated in the creation of BMDMS-NP, a comprehensive ESI-MS/MS spectral database designed to streamline the identification of natural compounds. This foundational work demonstrates his expertise in designing and improving complex lab protocols and scientific databases. His primary research interests lie at the intersection of chemoinformatics, computational biology for pharmacology, and mass spectrometry-based metabolomics. Dr. Lee is dedicated to developing novel, computer-based solutions that solve critical scientific problems, thereby accelerating advancements in drug discovery and analytical chemistry. His work continues to contribute significantly to the field.

Abstract

Natural product research using LC-MS/MS-based metabolomics is often hindered by the "identification bottleneck," where a vast majority of detected metabolites remain unidentified. To address this challenge, we developed FloraGenesis, an integrated, AI-powered platform that streamlines the entire research workflow from analysis to functional prediction. FloraGenesis is built upon BMDMS-NP, our large-scale MS/MS spectral database. The platform employs a dual AI approach. First, it uses deep learning to directly infer structural similarity from MS/MS spectra, overcoming experimental inconsistencies across different instruments and improving the accuracy of compound identification. Second, in a novel framework, it transforms raw LC-MS/MS data into 2D spectral images. This allows deep learning models to classify biological activity directly from these images, bypassing the need for exhaustive metabolite identification. As a proof of concept, this image-based approach was applied to predict the antioxidant activity of Glycine soja accessions, achieving 84.9% accuracy and outperforming traditional methods. Collectively, FloraGenesis provides a powerful, end-to-end solution for metabolite profiling, identification, and functional prediction, significantly accelerating drug discovery and the development of functional materials.

Invited Speaker

Dr. Haiwei Shen
Hangzhou Institute of Advanced Study, UCAS, Assistant Professor

Deep-learning based discovery of MTX-ENPP1 targeting for drug development

Biography

Dr. Shen completed his postdoctoral training at the Hangzhou Institute for Advanced Study (HIAS) under the supervision of Academician Hualiang Jiang. His research focuses on pharmaceutical science and technology, specializing in structural modification of bioactive compounds and process development for drugs and intermediates. Dr. Shen has made significant contributions to the field, with 10 publications in leading journals including Green Chem., J. Org. Chem., Green Synth. Catal., Org. Chem. Front., and holds 7 granted invention patents.

Abstract

ENPP1 is an extracellular phosphodiesterase that negatively regulates the cGAS-STING pathway by hydrolyzing cGAMP. Through a deep learning-based drug target prediction model (SSGCN), we identified and experimentally validated methotrexate (MTX) as a novel inhibitor of ENPP1. This finding reveals an immunomodulatory mechanism of MTX beyond its classic antifolate function: in addition to inhibiting nucleotide synthesis through DHFR suppression, MTX attenuates ENPP1-mediated hydrolysis of cGAMP and production of adenosine, thereby potentiating STING signaling and reversing immunosuppression in the tumor microenvironment. We further discovered that MTX exhibits a "dual-action" mode in antitumor immunity-it not only selectively induces cGAMP accumulation within tumor cells but also inhibits its extracellular hydrolysis by ENPP1. This synergistic mechanism underpins the ability of low-dose MTX to significantly enhance the efficacy of both immunotherapy and radiotherapy in animal models and early clinical observations. Leveraging these insights, we are now designing dual ENPP1/DHFR inhibitors by integrating computational druggability predictions with experimental validation to develop promising drug candidates that demonstrate both synergistic antitumor efficacy and favorable druggability.

Invited Speaker

Dr. Min Hyung Cho
Bioinformatics and Molecular Design Research Center, Team Leader

From data to discovery: Applying AI and big data for scalable innovation in natural product research

Biography

Dr. Min-Hyung Cho is a senior researcher and team leader specializing in big data analytics and AI-driven model development in the biological sciences. Currently leading the AI systems biology Team at the Bioinformatics and Molecular Design Research Center (BMDRC), he integrates large-scale biological datasets with advanced computational methods to generate viable and impactful research outcomes. With a Ph.D. in Biology from Johns Hopkins University, Dr. Cho has developed expertise in systems biology, bioinformatics, and AI platform construction for natural product discovery and functional material development. His work spans from high-throughput algorithm design for biological data processing to specialized AI platforms enabling innovation in biotechnology, food science, and medicine. Distinguished as an early-career researcher making innovative progresses, he continues to bridge computational power with biological insight to advance sustainable solutions.

Abstract

Natural products remain an invaluable source for drug discovery and preventive healthcare, offering diverse chemical scaffolds with therapeutic potential. Yet, their systematic use is limited by fragmented data, outdated annotations, and underutilization of computational tools. Advances in artificial intelligence (AI) and big data analytics now enable large-scale integration of biological and clinical datasets, but natural product research has lagged due to scarce digitized resources, heterogeneous formats, and obsolete terminologies. Fully exploiting these technologies requires standardization of unstructured data and semantic reorganization. We present strategies for preparing and structuring natural product data to ensure compatibility with AI-driven analysis. Our framework systematically integrates heterogeneous biological information-including molecular structures, bioactivity profiles, and species-level annotations-into a machine-readable network. Using graph-based analytics and optimized learning algorithms, we developed predictive models capable of inferring compound bioactivities, identifying targets, and generating mechanistic hypotheses. Additionally, integration with LC-MS/MS-based metabolomic profiling has facilitated the identification of novel natural product sources, yielding several promising candidates for further development. We propose that coupling curated big data with knowledge-based AI can accelerate lead identification and hypothesis generation in natural product science. Combined with high-throughput experimental validation, this approach establishes a scalable platform for next-generation discovery.

Poster Session

P01 Dynamic clinical trial success rates for drugs in the 21st century

Hangwei Xu (Zhejiang University)

P02 Enhancing molecular property prediction through task-oriented transfer learning: Integrating universal structural insights and domain-specific knowledge

Yanjing Duan (Hong Kong Baptist University)

P03 DeepUMQA-X: Comprehensive and insightful estimation of model accuracy for protein single-chain and complex

Dong Liu (Zhejiang University of Technology)

P04 Learning metabolic dynamics from partial observations by bidirectional time-series state transfer network

Shaohua Xu (Zhejiang University)

P05 Identification of cancer mini-drivers by deciphering selective landscape in the cancer genome

Xunuo Zhu (Zhejiang University)

P06 CYP-MAP: Enhancing site of metabolism prediction with multi-level GNNs

Jisan Kim (Chung-Ang University)

P07 CovPotDB: A covalent potency database

Haojia Tang (Fudan University)

P08 Protocol for membrane permeability prediction of cyclic peptides by combining molecular dynamics simulations and machine learning

Yutaka Akiyama (Institute of Science Tokyo)

P09 druglikeFilter 1.0: An AI powered filter for collectively measuring the drug-likeness of compounds

Yuntao Qian (Zhejiang University)

P10 **An automatic iterative refinement protocol for restraint parameters in REUS molecular dynamics**

Masahiro Shimizu (Institute of Science Tokyo)

P11 **HCGT-PL: A heterogeneous contrastive graph transformer unifying protein - ligand affinity prediction and structure-based virtual screening**

Yunjiang Zhang (Beijing University of Technology)

P12 **DEMO-EMol: Modeling protein-nucleic acid complex structures from cryo-EM maps by coupling chain assembly with map segmentation**

Ziying Zhang (Zhejiang University of Technology)

P13 **ComplexDnet: A network-based strategy to discover critical targets and screen active compounds for complex diseases**

Fei Pan (East China University of Science and Technology)

P14 **Solute carrier data center**

Yuhan Wang (Chongqing University)

P15 **pepADMET: The first novel computational platform for systematic ADMET evaluation of peptides**

Qianhui Liu (Central South University)

P16 **Prediction of octanol-water partition coefficients for cyclic peptides via molecular dynamics simulations**

Takuya Fujie (Institute of Science Tokyo)

P17 **M-DeepAssembly: Enhanced DeepAssembly based on multi-objective multi-domain protein conformation sampling**

Xinyue Cui (Zhejiang University of Technology)

P18 **DIVERGE v4: A platform for large-scale analysis of functional divergence across multi-gene families**

Yichang Chen (Zhejiang University)

P38 **EMPPNet: Enhancing molecular property prediction via cross-modal information flow and hierarchical attention**

Shiping Li (Shandong Normal University)

P39 **MPMA: The medicinal plant microbiome atlas**

Runze Yang (Ningbo University)

P40 **MetaboGNN: Prediction of liver metabolic stability using graph neural networks and cross-species data**

Ri Han (Chung-Ang University)

P41 **FMO and ML-guided design of potent darunavir analogs targeting HIV-1 protease**

Kowit Hengphasatporn (University of Tsukuba)

P42 **Structure-based discovery of a new LpxH-targeted chemotype with activity against *Klebsiella pneumoniae***

Gao Zhang (Chinese Academy of Medical Sciences)

P43 **SpatialPPIv2: Enhancing protein - protein interaction prediction through graph neural networks with protein language models**

Masahito Ohue (Institute of Science Tokyo)

P44 **CalVSP: A program for analyzing the molecular surface areas, volumes, and polar surface areas**

Yuzhu Li (Shanghai Jiao Tong University)

P45 **RNA-ligand interaction scoring via data perturbation and augmentation modeling**

Hongli Ma (Harbin Institute of Technology)

P46 **ALLM-Ab: Active learning-driven antibody optimization using fine-tuned protein language models**

Kairi Furui (Institute of Science Tokyo)

P56 4-Hydroxy-2,5-dihydrothiazole derivatives as a new class of small-molecule antibiotics for MRSA: AI-integrated design, chemical synthesis and biological evaluation

Rui Teng (Chinese Academy of Medical Sciences)

P57 POFF database: A flavor-centric information source for data-driven modernization food-medicine homology product and dietary intervention

Lyuhan Zhu (Ningbo University)

P58 PaCS-Q: Parallel cascade selection QM/MM molecular dynamics method for enzymatic reaction analysis

Liang Duan (University of Tsukuba)

P59 Navigating the data processing for cytometry-based single-cell proteomics

Huaicheng Sun (Zhejiang University)

P60 Multiscale simulations reveal conformational inactivation of PITRM1 and enable modulation in alzheimer's disease

Zhonglan Shi (Yichun University)

P61 Artificial avidity optimization of T-cell receptors through integrating deep learning model and mammalian cell surface display

Chaoqun Pan (Zhejiang University)

Important

Poster Display: From 12:00, September 24 to 18:00, September 24

Expert Review Time: From 13:30, September 24 to 16:30, September 24

Poster Dismantling: 18:30, September 24

General Information

Transportation Information

Hangzhou Xiaoshan International Airport

Plan 1: The distance is about 22 kilometers from the hotel. A taxi ride takes approximately 30 minutes and costs around 45 RMB.

Plan 2: Take Metro Line 7 from Xiaoshan International Airport Station and transfer to Metro Line 2 at Jianshe 3rd Road Station. Alight at Renmin Square Station (Exit D) and walk 350 meters to the hotel. The total travel time is approximately 60 minutes.

Hangzhou East Railway Station

Plan 1: The distance is about 16 kilometers from the hotel. A taxi ride takes approximately 35 minutes and costs around 35 RMB.

Plan 2: Take Metro Line 4 from Hangzhou East Railway Station and transfer to Metro Line 2 at Qianjiang Road Station. Alight at Renmin Square Station (Exit D) and walk 350 meters to the hotel. The total travel time is approximately 40 minutes.

Hangzhou Railway Station

Plan 1: The distance is about 15 kilometers from the hotel. A taxi ride takes approximately 30 minutes and costs around 25 RMB.

Plan 2: Take Metro Line 5 from Hangzhou Railway Station and get off at Renmin Square Station (Exit D). Walk 350 meters to the hotel. The total travel time is approximately 40 minutes.

Hangzhou West Railway Station

Plan 1: The distance is about 40 kilometers from the hotel. A taxi ride takes approximately 60 minutes and costs around 80 RMB.

Plan 2: Take Metro Line 19 from Hangzhou West Railway Station and transfer to Metro Line 2 at Shentangqiao Station. Alight at Renmin Square Station (Exit D) and walk 350 meters to the hotel. The total travel time is approximately 80 minutes.

Hangzhou South Railway Station

Plan 1: The distance is about 5 kilometers from the hotel. A taxi ride takes approximately 15 minutes and costs around 15 RMB.

Plan 2: Take Metro Line 5 from Hangzhou South Railway Station at Renmin Square Station (Exit D) and walk 350 meters to the hotel. The total travel time is approximately 20 minutes.

Meal Information

Venue

Mediterranean Cafe (3F), Grand New Century Hotel

Schedule

Date	Time	Meal	Notes
Sept 24	06:30 – 10:00	Breakfast	For in-house guests only
	12:00 – 13:20	Lunch	Buffet, By meal voucher only
	18:10 – 20:00	Dinner	Buffet, By meal voucher only
Sept 25	06:30 – 10:00	Breakfast	For in-house guests only
	12:10 – 14:00	Lunch	Buffet, By meal voucher only

Important

Please present your meal voucher at the restaurant entrance.

Please arrange your time accordingly. Meals will be served strictly during the times indicated.

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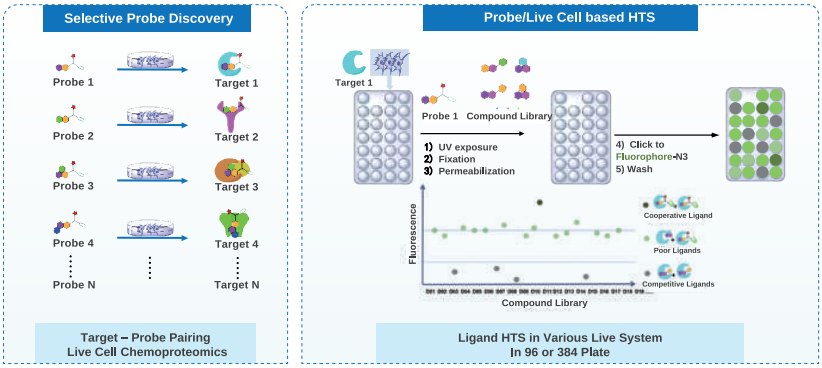

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An advanced method designed to measure interactions between ligands and their target proteins using specially engineered probes. This assay enables high-throughput screening (HTS) of chemical ligands derived from foods, dietary supplements, or pharmaceuticals across diverse protein targets.

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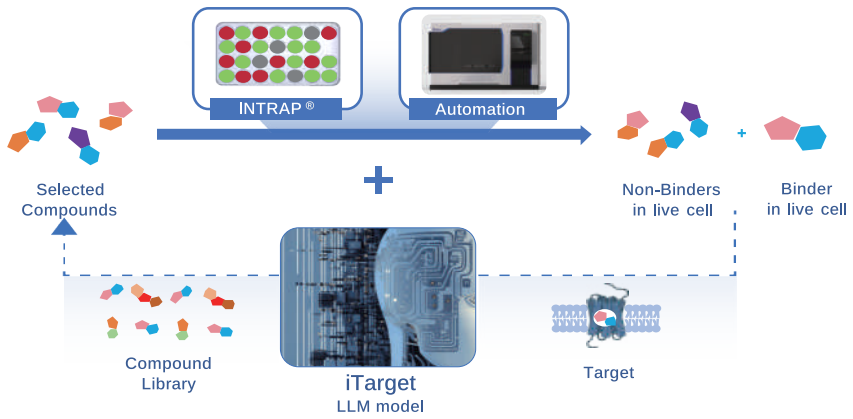
AI : Predicts potentially active compounds from large-scale libraries, narrowing the scope of experimental screening.
Automated Platform : Performs large-scale experimental operations rapidly and accurately, reducing human error and improving data accuracy and reliability.



- Customized Probe Development
- High-Throughput Ligand Screening
- Personalized Drug Discovery
- Automated Sample Preparation

PCT/CN2024/085651 Drug and Bioactive Substance Live-Cell Screening Technology

ABOUT US

Ningbo LeadArt Biotechnologies Co., Ltd., a National High-Tech Enterprise, was founded in 2017. The company completed its angel round in 2018 and pre-A round in 2022, raising nearly RMB 60 million in investments from renowned venture capital institutions in China and the United States. LeadArt has been recognized with multiple honors and received tens of millions of RMB in funding, including the Ningbo Municipal High-Level Overseas Innovation and Entrepreneurship Team (3315 Program), Cixi Shanglin Talent Plan, and Ningbo Major Sci-Tech Innovation 2025 Special Project.

As one of China's first and among the world's earliest biotechnology companies based on chemoproteomics technology, LeadArt is also the first globally to successfully automate chemoproteomics-based drug discovery platforms. The company possesses world-leading chemical biology technologies that enable rapid early-stage drug screening directly in human live cells using proteomic "target fishing probes." With a mission to lead the digital transformation of drug discovery, LeadArt has established a world-class automated and data-driven innovative drug discovery platform. It is committed to building the largest and highest-quality live-cell human target/ligand binding database, aiming to identify ligands and active compounds for every disease-relevant protein target.

Looking forward to collaboration opportunities!
For more information, Please contact: info@leadartech.com

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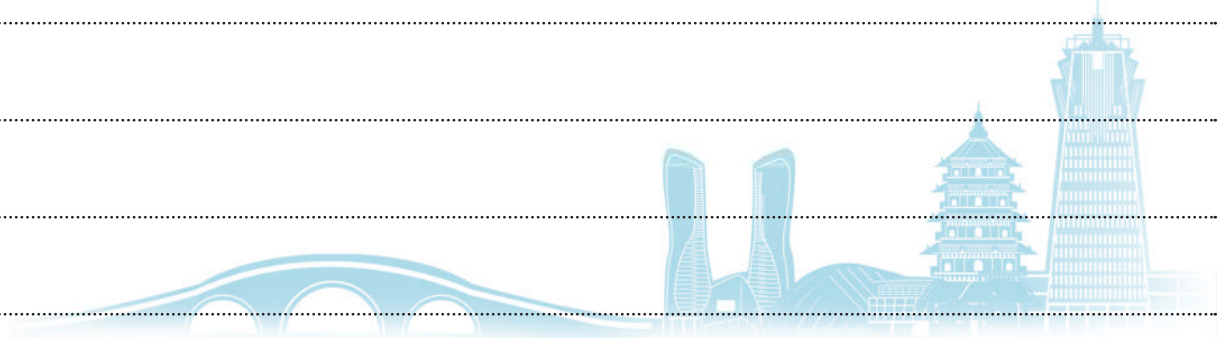

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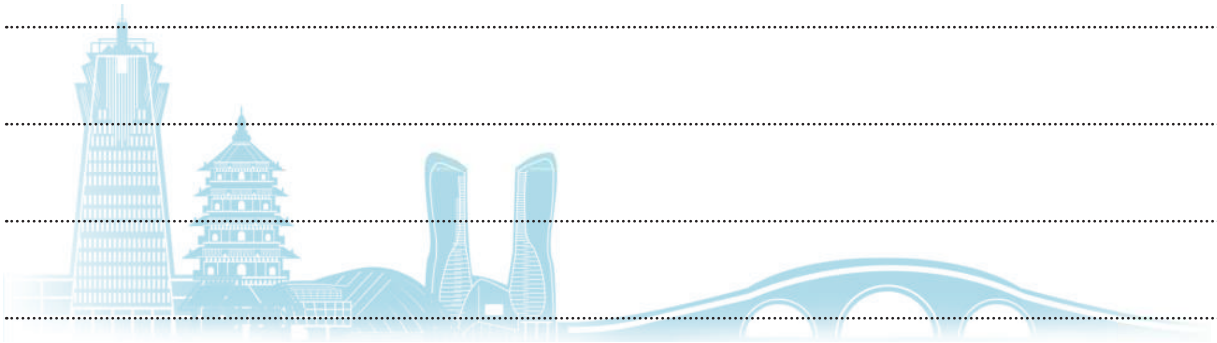

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