Mahidol University
Institute of
Molecular Biosciences

AI-DRIVEN DRUG DISCOVERY

THE FUTURE OF MEDICINE

MINI-SYMPOSIUM

2 Nov 2023

Prince Mahidol Hall Conference Center, Mahidol University, Salaya Campus

8:30 a.m. : Registration

9:15 a.m. : Welcome Ceremony

9:30 a.m. : Professor Sir Tom Blundell *(Keynote Speaker)*

University of Cambridge, UK
Topic: "Revolutionary developments in the design of new medicines: from computational statistical & X-ray experimental methods of 1960s to AI/ML and cryoEM approaches in the 2020s"

10:30 a.m. : Coffee Break

11:00 a.m. : Professor Ruben Abagyan

University of California San Diego, USA
Topic: "New docking/AI platform to screen billions of compounds for a specific target-property profile" Live talk via zoom

12:00 p.m. : Lunch

1:00 p.m. : Asst. Prof. Duangrudee Tanramluk

Mahidol University, Thailand
Topic: "Solving biomolecular design puzzles with data-driven drug discovery platforms: MANORAA and SIMFONEE"

1:45 p.m. : Jiye Shi, Ph.D.

Eli Lilly and Company, USA
Topic: "Generative AI: a co-pilot for drug discovery"

2:30 p.m. : Afternoon Break

3:00 p.m. : Arun Prasad Pandurangan, Ph.D.

University of Cambridge, UK
Topic: "Protein mutant stability prediction: analyses of drug resistance mutations in infectious diseases"

3:45 p.m. : Q&A Session and Closing Remarks

WORKSHOP

3 Nov 2023 or 1 Dec 2023

(Please choose a date at your convenience)

Computer Laboratory, Institute of Molecular Biosciences

Jiraporn Panmanee, Ph.D.
Ittipat Meewan, Ph.D.
Asst. Prof. Duangrudee Tanramluk, Ph.D.

8:30 a.m. : Registration

9:00 a.m. : Practical Workshop #1
"Theory and practice: Structural bioinformatics and drug discovery platforms"
Asst. Prof. Duangrudee Tanramluk, Ph.D.

12:00 p.m. : Lunch

1:00 p.m. : Practical Workshop #2
"Hands-on Workshop: Practical Insights into Molecular Docking for Drug Discovery"
Ittipat Meewan, Ph.D. & Jiraporn Panmanee, Ph.D.

2:30 p.m. : Afternoon Break

2:45 p.m. : Practical Workshop #2 (continued)
"Hands-on Workshop: Practical Insights into Molecular Docking for Drug Discovery"
Ittipat Meewan, Ph.D. & Jiraporn Panmanee, Ph.D.

4:00 p.m. : Closing Ceremony and Certificate Presentation

	MU students & staff	Government sector	Private sector
Mini-Symposium	Free of charge	THB 1,500	THB 3,000
Workshop	Free of charge	THB 4,000	THB 10,000
Mini Symposium + Workshop	Free of charge	THB 5,000	THB 12,000

For more information, please contact
- Miss Kaewklao Banjong 080-981-4948 / kaewklao.ban@mahidol.edu
- Miss Chanikarn Boonchuay 099-245-1698

Scan to Register

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LIST OF SPEAKERS

Prof. Sir Tom Blundell, University of Cambridge, UK (Keynote Speaker)

Professor Sir Tom Blundell is a world class expert in structural biology and drug discovery, currently at the Biomedical Campus of University of Cambridge. He has produced software for homology modelling, for example Modeller cited 13,000 times, and now also leading generative AI/ML and cryoEM packages. As pioneer of fragmentbased drug discovery, co-founding Astex, now with 2 oncology drugs on the market. He founded the UK research council BBSRC and was earlier scientific advisor of the conservative PM Margaret Thatcher.

Prof. Ruben Abagyan
University of California San Diego, USA

Prof. Ruben Abagyan is Professor of at Skaggs School of Pharmacy and Pharmaceutical Sciences at the University of California San Diego. Dr. Abagyan and his group work in specialized in developing and utilizing techniques for structure-based discovery, molecular modeling, and optimization of potential drug candidates, identifying targets, large scale bioinformatics and bioinformatics. The applications include viral, cancer, neurodegeneration, parasitic, and endocrine diseases.

Asst. Prof. Duangrudee Tanramluk
Mahidol University, Thailand

Dr. Duangrudee Tanramluk is an Assistant Professor in Structural Bioinformatics at Mahidol University in Thailand. She lead the development of a revolutionary AI systems for Drug Discovery: MANORAA & SIMFONEE packages. Her data-driven drug discovery platform enables in-depth and big picture analysis of small molecule drug discovery via programmable URL. Her field of expertise is on building software to decipher protein specificity and promiscuity. Her webservice foster sustainability in drug design education and bring new hope for precision medicine.

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LIST OF SPEAKERS

Jiye Shi, Ph.D.
Eli Lilly and Company, USA

Dr. Jiye Shi is the Associate Vice President, Global Head of Computational Design and Automation Platforms at Eli Lilly and Company. He is the world-class expert in AIinspired biologics and small molecule drug discovery. His computional talents lead to the discovery of Romosozumab and Bimekizumab. He has developed novel structurebased AI/ML antibody design algorithms which led to the design of antibodies targeting a specific epitope and the design of dual-specific antibodies. He has established strong partnerships with academic and industrial partners, led to talents recruited by AI and biotech companies (e.g. DeepMind, BenevolentAI, Exscientia).

Dr. Arun Prasad Pandurangan, Ph.D.
University of Cambridge, UK

Dr Arun Prasad Pandurangan is a senior researcher at the Heart & Lung Research Institute, University of Cambridge. He is an expert in structural bioinformatics, genomics and modelling cryo-EM maps with specific interest in understanding the impacts of genetic mutations in disease and drug resistance. He is Associate Editors of BMC Bioinformatics, Computational and Structural Biotechnology Journal, etc.

Jiraporn Panmanee, Ph.D.
Mahidol University, Thailand

Jiraporn Panmanee is currently a Lecturer at the Institute of Molecular Biosciences, Mahidol University. She possess a Ph.D. in Biological Sciences with research focuses on in silico structure-based drug design, neurotoxicity assessment of pesticides, structural biology, and neurobiology of neurodegenerative diseases. Her academic pursuit has focused on unraveling complexities in these domains to contribute to advancements in healthcare and environmental science.

Ittipat Meewan, Ph.D.
Mahidol University, Thailand

Ittipat Meewan is Lecturer at the Institutes of Molecular Biosciences, Mahidol University. His current research focuses on computational-aided development of small molecules and peptide antivirals, targeting viruses such as SARS-CoV-2, HBV, HCV, ZIKV, DENV, and HPV. The primary techniques include molecular docking, molecular dynamics, and machine learning are employed for virtual screening of large libraries against target proteins and identify potential drug candidates which are then validated experimentally.