AI FOR DRUG DISCOVERY
OPEN INNOVATION FORUM

Wednesday, October 30, 2024 8:00 am – 6:30 pm

Boston University, Center for Computing & Data Sciences 665 Commonwealth Ave, Room 1750 (17th Floor)

8:30 am – 8:35 am

Welcome

Gloria Waters, Provost and Chief Academic Officer at Boston University

8:35 am – 8:50 am

State Remarks

Yvonne Hao, Secretary of Economic Development
Kirk Taylor MD, President and CEO of the Massachusetts Life Sciences Center

8:50 am – 9:00 am

Introduction

Yannis Paschalidis PhD, Director, Hariri Institute for Computing
Jianying Hu PhD, IBM Fellow, Director, HCLS Research and Global Science Leader, AI for Health

Keynote Speakers

9:00 am – 9:25 am

Joseph Loscalzo MD, PhD, Samuel A. Levine Professor of Medicine, Hersey Distinguished Professor of the Theory and Practice of Medicine, Harvard Medical School, Physician-in-Chief Emeritus, Brigham and Women's Hospital: "*Challenges in Contemporary Drug Discovery*"

9:25 am – 9:50 am

Jeremy Jenkins PhD, US Head Discovery Sciences, Novartis: "*Generative AI Applications in Early Drug Discovery*"

9:50 am – 10:05 am

Coffee Break

10:05 am – 10:30 am

Mona Singh PhD, Wang Family Professor in Computer Science, Princeton University: *"Protein Language Models: Their Power, Limitations and Future Directions"*

10:30 am – 10:55 am

Sean Mooney PhD, Director, Center for Information Technology, NIH: "*AI@NIH: Drug Discovery, Clinical Healthcare, and Multimodal AI*"

10:55 am – 12:00 pm

Panel Discussion

"Drug discovery bottlenecks and how AI can help"

Moderator: **Diane Joseph-McCarthy** PhD, Executive Director, Bioengineering Technology & Entrepreneurship Center; Professor of the Practice (BME, Chemistry)

Etai Jacob Senior Director, Head of Data Science and AI, Early Oncology, AstraZeneca PLC
Ashwini Ghogare Head of AI and Automation in Drug Discovery, MilliporeSigma
Juli Klemm Program Director, Center for Strategic Scientific Initiatives, National Cancer Institute (NCI)
Rob Moccia Senior Director, Machine Learning Research Lead, Pfizer
Pat Walters Chief Data Officer, Relay Therapeutics

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12:00 pm – 12:45 pm Networking Lunch

12:45 pm – 1:45 pm Panel Discussion

"New generative AI approaches for drug discovery and need for open innovation"

Moderator: **Michal Rosen-Zvi** Director, AI for Drug Discovery, IBM Research

Kaitlin McCardle Senior Editor, Nature Computational Science
Vlad Ivanov Director, Group Lead, AI/ML Quantitative Data Sciences, Pfizer
Feixiong Cheng PhD, Inaugural Director, Cleveland Clinic Genome Center
Jim Collins Termeer Professor of Medical Engineering & Science, Professor, Department of Biological Engineering, Massachusetts Institute of Technology; Wyss Institute, Harvard University; Broad Institute of MIT and Harvard

1:45 pm – 2:00 pm Coffee Break

2:00 pm – 3:00 pm Breakout sessions

"Prioritization of Open Innovation Tasks"

The "Breakout Session" of the program will be 2:00pm - 3:00pm, see below for each breakout session's assigned room location. The "readout" portion of the program will resume, 3:00pm - 3:45pm, on the 17th floor. Please allow transition time.

*Benchmarks—**Location: CDS 548 (5th Floor)***

*Multi-Modal Fusion—**Location: CDS 1101 (11th Floor)***

*Model Architecture—**Location: CDS 701 (7th Floor)***

*Challenges/Competitions—**Location: CDS 1238 (12th Floor)***

3:00 pm – 3:45 pm Workstream Readout & Next Steps**—Location: CDS 1750 (17th Floor)**

3:45 pm – 4:00 pm Coffee Break

4:00 pm – 5:00 pm Hands-On Session—**Location: CDS 1101 (11th Floor)**

"Open-source software tools to support AI model building"

Please register for a NERC account prior to the session, instructions at registration table

5:00 pm – 5:15 pm Closing Remarks

Yannis Paschalidis PhD, Director, Hariri Institute for Computing
Jianying Hu PhD, IBM Fellow, Director, HCLS Research and Global Science Leader, AI for Health

5:15 pm – 6:30 pm Networking Reception

Boston University Wifi

The BU Guest network allows visitors to access the Internet through BU's wireless network. Please note that personal wireless access points are prohibited on the BU network because they interfere with network traffic. To access BU Guest (unencrypted): Connect to the network called "BU Guest (unencrypted)" from your list of available networks.

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