MIT Industrial Liaison Program Faculty Knowledgebase Report

AI-Driven Drug Discovery

October 12, 2023 11:00 am - 1:00 pm

11:00 AM	Welcome & Introduction Sheryl Greenberg Program Director, MIT Industrial Liaison Program

Sheryl Greenberg
Program Director
MIT Industrial Liaison Program

Sheryl Greenberg initiates and promotes the interactions and development of relationships between academic and industrial entities to facilitate the transfer of new ideas and technologies between MIT and companies, and has created numerous successful partnerships. By understanding the business, technology, and commercial problems within a company, and understanding the technologies and expertise of MIT researchers, Greenberg identifies appropriate resources and expertise to foster new technology applications and collaborative opportunities.

Prior to MIT, Greenberg created and directed the Office of Technology Transfer at Brandeis University. In the process of managing intellectual property protection, marketing, and licensing, she has promoted the successful commercialization of technologies as diverse as new chemicals and manufacturing, biotechnology, food compositions, software, and medical devices. She facilitated the founding and funding of new companies, as well as creating a profitable technology transfer program. She also facilitated the patenting, marketing, and licensing of Massachusetts General Hospital technologies. In addition to her cellular, biochemical, and genetic research experience in academic and corporate environments, she has also created intellectual property for medical uses. Greenberg has been an independent intellectual property and business development consultant, is a U.S. Patent Agent, and has previously served the Juvenile Diabetes Research Foundation as Co-Chair of the Islet Research Program Advisory Committee and grant reviewer. She currently also mentors startup companies and facilitates partnering them with large life science and healthcare companies.

11:05 AM

Building the Infinite Loop for Machine Learning-Guided Discovery, Delivery, and Rapid Manufacturing of Potential Medicines

Bradley L. Pentelute
Professor, MIT Department of Chemistry

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Brad Pentelute, Professor in the Department of Chemistry, modifies naturally occurring proteins to enhance their therapeutic properties for human medicine, focusing on the use of cysteine arylation to generate abiotic macromolecular proteins, the precision delivery of biomolecules into cells, and the development of fast flow platforms to rapidly produce polypeptides.

Pentelute earned a B.S. in chemistry and a BA in psychology at the University of Southern California, followed by a Ph.D. in organic chemistry at the University of Chicago. After a postdoc fellowship at Harvard Medical School, Pentelute joined the MIT faculty in 2011. His awards and honors include an Alfred P. Sloan Research Fellowship, a Novartis Early Career Award, and an Amgen Young Investigator Award.

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We're facing a challenge in the world of chemistry: our lack of data is slowing down how we can use clever computer programs, known as machine learning, to create powerful new medicines. In this piece, I'll walk you through what we're doing to solve this problem by creating data highways from millions of small molecules, peptides and small proteins. We are now able to use machine learning to discover and create new functional molecules quickly. Sometimes, these computer-designed molecules are even better than what we can make ourselves! Our next step is to create an infinite loop where we automatically design, build, and test potential new medicines.

11:35 AM

Drug Design and Medicine in the Age of AI

Marinka Zitnik
Assistant Professor, Department of Biomedical Informatics
Harvard Medical School

We are laying the foundations for AI to enhance understanding of medicine and drug design, eventually enabling AI to learn and innovate on its own. Large language models and generative AI are profoundly transforming the deep learning paradigm. Instead of training task-specific models for every task across stages of drug development and therapeutic modalities, we can now adapt a single pretrained large foundation model to many tasks through fine-tuning and few-shot prompting. Central to our approach is the integration of molecular structure, biological knowledge, and patient data into AI models. We are advancing self-supervised learning, which leverages vast unlabeled datasets, and geometric deep learning, which leverages the inherent geometry of biochemical data. This is complemented by generative AI that helps design and optimize useful and novel biomolecules. We fuse modalities from genetic code, single-cell atlases, and molecular structures to clinical treatments via multimodal knowledge graph networks and large pretrained language models. Our research disentangles this complexity, creating avenues to develop new kinds of therapies to give the right patient the right treatment at the right time and have medicinal effects that are consistent from person to person and with results in the laboratory.

12:05 PM

AI for Genomic Medicine: Deciphering and Reversing Human Disease Circuitry at Single-Cell Resolution

Manolis Kellis
Member, Broad Institute of MIT and Harvard
Professor, MIT Computer Science and Artificial Intelligence Lab

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Manolis Kellis is a professor of computer science at MIT, a member of the Broad Institute of MIT and Harvard, a principal investigator of the Computer Science and Artificial Intelligence Lab at MIT, and head of the MIT Computational Biology Group (compbio.mit.edu). His research includes disease circuitry, genetics, genomics, epigenomics, coding genes, non-coding RNAs, regulatory genomics, and comparative genomics, applied to Alzheimer's Disease, Obesity, Schizophrenia, Cardiac Disorders, Cancer, and Immune Disorders, and multiple other disorders. He has helped lead several large-scale genomics projects, including the Roadmap Epigenomics project, the ENCODE project, the Genotype Tissue-Expression (GTEx) project, and comparative genomics projects in mammals, flies, and yeasts. He received the US Presidential Early Career Award in Science and Engineering (PECASE) by US President Barack Obama, the Mendel Medal for Outstanding Achievements in Science, the NIH Director's Transformative Research Award, the Boston Patent Law Association award, the NSF CAREER award, the Alfred P. Sloan Fellowship, the Technology Review TR35 recognition, the AIT Niki Award, and the Sprowls award for the best Ph.D. thesis in computer science at MIT. He has authored over 280 journal publications cited more than 148,000 times. He has obtained more than 20 multi-year grants from the NIH, and his trainees hold faculty positions at Stanford, Harvard, CMU, McGill, Johns Hopkins, UCLA, and other top universities. He lived in Greece and France before moving to the US, and he studied and conducted research at MIT, the Xerox Palo Alto Research Center, and the Cold Spring Harbor Lab. For more info, see: compbio.mit.edu

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We seek to understand the mechanistic basis of human disease, develop new therapeutics that reverse disease circuitry, and enable personalized medicine using AI and machine learning to integrate genetics and genomics, single-cell epigenomics and transcriptomics, and high-throughput experiments.

Our work spans six areas:
(1) Understanding genomes, their programming language, their circuitry, epigenomics, dynamics, and single-cell multi-omics.
(2) Disease mechanism, genetic variation, patient subtyping, personalized medicine, electronic health records.
(3) Application to neuroscience, Alzheimer's, schizophrenia, cardiovascular disease, obesity, cancer, and evolution.
(4) Therapeutic design, drug repurposing, high-throughput experiments, drug screening, genome circuitry manipulation, and disease reversal.
(5) Statistical genetics, causal inference, geometric deep learning, joint embeddings, contrastive learning, computational chemistry, and therapeutic design.
(6) Embedding space idea representations, visualization, and navigation for learning, discovery, invention, and collaboration.

12:35 PM

Panel Discussion
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1:00 PM	Adjournment