

8:45A

Welcome - Tim Watson, Gilead Sciences, Chair, IQ Consortium

Introduction – Marguerite Driscoll, Pfizer, IQ SOC Co-Chair

The Selective Deployment of AI in Healthcare

Robert Vandersluis, Vice President, Artificial Intelligence, GSK

Based on Vandersluis, R., & Savulescu, J. (2024). The selective deployment of AI in healthcare. Bioethics, 38, 391-400. <https://doi.org/10.1111/bioe.13281>

(Title to be provided) – **Sharmista Chatterjee, Div. Dir. CDER, US FDA**

A Strategic Roadmap for AI/ML in Biopharma

John Chan, Head of Shinrai Center for AI and Machine Learning, Takeda

Break

PANEL - Morning Speakers

Lunch

Molecular Representation & Their Applications in Drug Discovery

Okko Clevert, Machine Learning Head, Pfizer

Building the Foundation: Data Infrastructure for AI in Pharma

Tim Smith, Head, Data Sciences Community, DSI Takeda

The drug development pipeline generates massive amounts of data from target discovery through the clinic to manufacturing and commercial. All the data along the pipeline creates tremendous opportunities for applying AI/ML to impact the speed and quality of pharma/biotech process. My presentation will detail lessons learned from twenty-two AI/ML projects developed through the MIT-Takeda Program both what worked and what did not. These insights help us to better develop the next generation of AI/ML tools for pharma and biotechnology. Through this process, it became clear that AI means very different things to people across the organization.

The Dawn of AI: Illuminating the Labyrinth of Drug Development

James Lu, Distinguished Scientist, Genentech

Predictive modeling is crucial in drug development, guiding the optimization of safety and efficacy, supporting decision making and ultimately streamlining the path to successful therapeutic interventions. However, this process is fraught with a labyrinth of challenges such as patient variability, nonlinear disease processes, and the presence of confounders.

The exponential growth in data volume, coupled with rapid advancements in machine learning (ML) and generative artificial intelligence (GenAI) algorithms, has opened new horizons. In this presentation, we explore how the synergy between human and machine intelligence can be harnessed at three distinct levels. This integration promises to save time, enhance predictive accuracy, and push the boundaries of current modeling capabilities.

We will demonstrate diverse applications across several therapeutic areas, showcasing how AI can illuminate the path forward and light the way to a brighter future in drug development.

The Ascent of AI: Predicting Drug-Induced Liver Injury

Weida Tong, Director, Division of Bioinformatics & Biostatistics, US FDA

Break

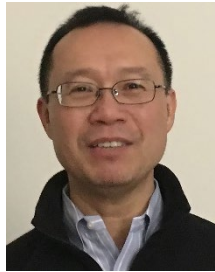
PANEL - Afternoon Speakers

5:00P

Close – Malar Pannirselvam, GSK, IQ SOC Co-Chair

SPEAKERS

John Chan, Ph.D., Head of Shinrai Center for AI and Machine Learning, Takeda



John Chan is a technology executive, trained as a scientist and engineer, with over 25 years of industry experience in computational sciences and informatics. He has led computational teams, built informatics capabilities, and translated ideas into products for global biopharma and biotech start-ups. He is currently the head of the Shinrai Center for AI and Machine Learning at Takeda R&D.

Prior to joining Takeda, John built a neuroscience AI company, Syllable Life Sciences, and as its CEO, led its acquisition by Neumora. Before Syllable, John held several contributor and management roles in computational biology, bioinformatics, and enterprise IT. This includes tenure as a visiting scientist at the Broad Institute, an Executive Director and Head of Informatics and Technology at Novartis, and the Head of computational biology at Millennium Pharmaceuticals, where he led the innovative team that fueled Millennium's drug discovery partnerships. John earned a B.Sc. in population genetics from Marlboro College and a Ph.D. in genetics and molecular biology from the University of Pennsylvania.

James Lu, Ph.D., Distinguished Scientist in AI, Genentech



James Lu is a Distinguished Scientist in AI at Genentech. He received his degrees from MIT, including a S.B. in Mathematics and a Ph.D. in Computational Fluid Dynamics. For the past 19 years, he has been an active researcher in the areas of computational systems biology, in-silico disease modeling, and machine learning in the context of drug discovery & development. James has gained international work experience through computational modeling roles at AstraZeneca in Cambridge (UK) and Roche in Basel (Switzerland). His current research focuses on developing pharmacology-informed machine/deep learning model architectures that integrate longitudinal and high content data across various modalities to enhance predictive analytics capabilities. Additionally, he works on operationalizing ML platforms to support decision making. He has co-authored more than 50 journal and conference publications and is the co-inventor on more than 6 AI/ML patent applications. He has co-chaired sessions at American Conference on Pharmacometrics (ACoP) and the pre-conference of the American Society for Clinical Pharmacology & Therapeutics (ASCPT), as well as delivered seminars and lectures on AI in drug development at UCLA and UCSF. Furthermore, he serves on the editorial board of CPT:Pharmacometrics & Systems Pharmacology.



Robert Vandersluis is VP of Responsible AI at GSK, where he engages with the ethical and public policy implications of using AI systems in drug discovery and clinical applications. As part of these efforts, Robert leads academic collaborations with Stanford University and the University of Adelaide, which undertake independent research aimed at promoting AI-based interventions that are inclusive, empowering, and safe. Robert also undertakes his own research at the Uehiro Centre for Practical Ethics at the University of Oxford. Prior to his work in AI, Robert managed a £20 billion investment portfolio, and he served as a non-executive director for various investment funds with £40 billion of assets under management. Robert was educated at Oxford, Cambridge, Harvard, Michigan, and the LSE – where he explored several different fields, including economics, politics, public policy, philosophy, ethics, and artificial intelligence.

Timothy J. Smith, PhD, is an innovative scientist and technologist in biotech/pharma research with expertise in AI/ML innovation, target and drug discovery, data science, and strategic analytics. He earned his BS in Chemistry from the University of Washington and later his PhD in Toxicology from Cornell University. He currently heads the Data Science Community at Takeda and functionally leads the MIT-Takeda Program featuring twenty-two research projects applying AI/ML to critical problems across the pharma/biotech pipeline. Additionally, he co-created Takeda's ShinrAI Center of Artificial Intelligence and a framework for robust and trustable AI. His passion for bridging science and technology fuels his quest to accelerate biotech/pharma R&D—striving to reduce the time from target to therapy. Before Takeda, Tim developed new information tools to improve cheminformatics, collaboration, data security, and knowledge management at Novartis. Apart from his publications in scientific journals, Timothy is also an author and speaker, known for demystifying AI in his book *How to Profit and Protect Yourself from Artificial Intelligence*.