AI IN PHARMA DISCOVERY

Wednesday 4th October 2023

9:00 AM Chair's Opening Remarks and Setting the Scene

Pradeep Bandaru, Director of Data Strategy and Knowledge Management, **Generate Biomedicines**

9:15 AM Keynote Presentation- The AI and ML Revolution: The Implementation of AI into R&D

- Explore how Moderna is preparing for the era of quantum computing
- Deep-dive into how Moderna utilise new technologies to produce a diverse pipeline of phase 1-3 drug candidates
- Discuss the AI-based methods that can be used to identify quality druggable target candidates

Wade Davis, VP of Computational Sciences, **Moderna**

9:40 AM Panel Discussion with Open Q&A - Evolution Vs Revolution: How Should the Culture around AI be Managed?

A huge wave of excitement surrounding the implementation of AI within drug discovery has been building but resistance to this change should not be underestimated. Transparency around hesitancies and the true challenges of AI implementation is essential in order for the continued progression of AI and ML implementation.

- How mature is AI within drug development and how is it being used to alleviate some of the traditional bottlenecks in R&D?
- How can decision makers be upskilled on both the uses and limitations of AI and ML applications to avoid 'black box' mistrust?
- How can explainable and reproducible computational workflows be built in order to build trust in the quality of computational models?
- Why is a culture of effective collaboration across multiple disciplines needed for the cohesive implementation of AI?
- Should AI implementation in R&D be described as undergoing evolutionary or revolutionary growth and how should hype be differentiated from actual achievement?

Aaron Mackey, VP, Head of AI and ML, **Sonata Therapeutics**
Han Chang, Senior Director, Head of Late Stage Oncology, Translational Bioinformatics, **Bristol Myers Squibb**
Neil Dhawan, CEO, CSO and Co-Founder, **Totus Medicines**
Hannah Gordon, VP of Product, **Enveda Biosciences**
Moderator**: Niki Santo**, President, **Harvard Club of Silicon Valley**

10:25 AM Morning Refreshments and Networking

11:05 AM Presentation- Bio-AI: Combining Machine Learning with Patient-on-a-chip Platform for Better Drug Toxicity Prediction

- Quris Hybrid BIO-AI Approach Achieve State-of-the-art Performance in Drug Drug-Induced Liver Injury Prediction
- Quris Platform Enables Non-Invasive Assessment of Viability in 3D Cultures
- AI-Staining: Generative AI Uncovers Pathological Mechanisms of Toxicity

Shahar Harel, VP of AI, **Quris**

11:30 AM Presentation- Equivariant Generative Models for Conditional Drug Design

- Explore symmetry in deep learning and equivariant models
- Deep-dive into feature generation for 3D point clouds
- Discuss conditional generation of novel small molecules

Bradley Parry, Chief Technology Officer, **AI Therapeutics**

11:55 AM Presentation- Determining Structure with Generative Deep Learning Models

- Uncover how Enveda Biosciences use generative deep learning models to predict chemical properties and structure directly from MS2 spectra
- Explore how the early-stage drug discovery process has been redesigned via the use of ML and llm type models
- Discuss the future potential of using these models to aid natural product discovery at industrial scale

Hannah Gordon, VP of Product, **Enveda Biosciences**

12:20 PM Presentation- Utilising AI and ML as Predictive Models

- Learn how AI and ML has accelerated A-Alpha Bio's ability to make better and earlier predictions
- Explore how quantitative AlphaSeq data can be used to train highly predictive machine learning models for therapeutically critical properties
- Discuss how computational screens for expression, stability, solubility and other properties are used to enrich developmental designs

Ryan Emerson, VP of Data Science, **A-Alpha Bio**

12:45 PM Panel Discussion with Open Q&A - How is it Best to Invest Time, Money and Resources into AI?

Projections indicate that the effective use of AI and ML has the potential to save over $70 billion USD throughout the drug discovery process by 2028. Collectively, the industry is trying to turbocharge the rate of AI and ML application but both biotechnology and pharmaceutical companies alike need to assess when the optimum moment is to invest time and resources into AI based technology.

- How does current investment and adoption of AI within your industry compare with five years ago?
- What are the macroeconomic factors that have the biggest influence on industry investment?
- What major challenges need to be overcome to boost investment in AI R&D applications?
- How can you measure the impact of AI compared with classical R&D success?
- Looking to the future, how can the implementation of AI and ML within the R&D industry be boosted, even in instances of restricted budgets?

Nishtha Jain, Head of Innovation and Digital Technology, **Takeda**
Kyle Kaniecki, VP of Life Sciences and Healthcare, **New York City Economic Development Corporation**
Artem Trotsyuk, Venture Partner, **LongeVC**
Wade Davis, VP of Computational Sciences, **Moderna**
Moderator: **Pavan Choksi**, Partner, **Arkitekt**

1:30 PM Lunch

3:00 PM Presentation - Utilising AI to Improve Infectious Disease Diagnostics and Monitor Emerging Pathogens

- Uncover the promising benefits of machine learning and genomic data to identify emerging pathogens and antimicrobial resistance
- Discuss how machine learning can be deployed to drive innovative research within microbial and drug resistance identification
- Learn how AI can act as an assistant to build a global platform for pandemic preparedness using genomic, epidemiological and climate change data

Dorottya Nagy-Szakal, Research Assistant Professor, **SUNY Downstate Health Sciences University**

3:25 PM Presentation - Leveraging advanced knowledge management to uncover hidden value in R&D proprietary information

Many organizations capture and store key research findings but struggle to access and apply this valuable information to future efforts. CAS, a specialist in scientific information solutions, designs custom solutions that enable organizations to search scientific concepts across projects, make connections between internal and external data, and reveal deeper insights to guide decision-making. To improve the value of your proprietary data, CAS leverages the specialized technologies and scientific expertise used to manage the largest human-curated collection of scientific insights in the world.

Pillhum Son, Solution Consultant, **CAS Custom Services**

3:50 PM Afternoon Refreshments and Networking

4:35 PM Presentation - A Data-Driven Quantitative Approach to Target Identification: Accelerating the Next Generation of Immuno-Oncology Drug Candidates

- Learn about Novasenta's platform enabled pipeline of next-gen I/O therapies
- Discuss challenges with regards to discovery of novel targets and how Novasenta leverages KnowledgeGraphs and NLP to address these challenges
- Explore how Novasenta leverages its AI-driven platforms to prioritize targets & manage human bias for target selection

Mani Mohindru, Chief Executive Officer, **Novasenta**

5:00 PM Panel Discussion with Open Q&A- Industry 4.0: How Data Analytics and AI is Fueled By Both Hopes and Fears

AI and ML can now extract information that previously remained hidden within data sets and Natural Language Processing can help identify previously overlooked patterns and relationships. However, data still prevails as the main barrier to fully utilising the power of AI within R&D.

- How has the application of data analytics and AI within R&D changed in the last five years and what lessons have been learnt?
- How are stakeholders adapting to these changes and what main barriers still remain?
- What is the value proposition for enhancing the use of data analytics and AI within R&D?
- What techniques can be used to increase cross-collaboration and the sharing of data

optimize the use of data analytics and AI in R&D?
- What do you see as the future for AI and data analytics?

Shruthi Bharadwaj, Global Lead, Digital & Analytics, R&D Global Operations, **Sanofi**
Xiong Liu, Director Data Science and AI, **Novartis**
Mehdi Sarmady, VP, Head of Genomic and Data Sciences, **Spark Therapeutics**
Hall Gregg, Chief Portfolio Officer, **Pistoia Alliance**
Moderator: **Ami Lakdawala**, Head of AI Product, **GSK**

5:45 PM Chair's Closing Remarks