AI IN PHARMA DISCOVERY

6th Annual
Wednesday, October 12th | Boston, MA

Chair's Opening Remarks

Keynote Presentation: An Overview of the Challenges, Opportunities and Breakthroughs for the use of AI in Drug Discovery

Tommaso Mansi, VP of AI/ML & Digital Health, **The Janssen Pharmaceutical Companies of Johnson & Johnson**

Keynote Panel Discussion: How can we Overcome Data Limitations?

Data continues to be a main barrier in fully harnessing the power of AI to improve drug discovery in the pharmaceutical industry. This panel will discuss how we can overcome these challenges to accelerate the use of AI in the drug discovery process.

- What are the main data challenges facing the adoption of AI in the drug discovery process?
- How can we navigate the issue of data sparsity and working in a low data regime?
- How can we integrate varying data sets when quality and collection of data is so disparate?
- How can we overcome the challenge of data which has not been curated or collected for AI and ML technologies?
- Is collaboration and breaking data silos key in overcoming data limitations?

Shane (John) L, Vice President of AI/ML, **GSK**
Lihua Yu, Chief Data Officer, **FogPharma**
Bino John, Global Team Leader, Director, **AstraZeneca**

Morning Break

Presentation: Using Predictive Tools to Guide and Inform Preclinical Experiments

- Discussing how data scientists can collaborate with medicinal chemists to guide drug discovery experiments
- Exploring how AI can accelerate the drug discovery and preclinical efforts

- Integrating predictive tools into the drug discovery workflow

Charles O'Donnell, Vice President, Head of Computational Genomics and Data Sciences, **Omega Therapeutics**

Panel: How do we Address the Cultural Problems Within the Drug Discovery Industry to Shift to a Data-driven Culture?

- Exploring how we can shift to a new way of doing things which not everyone within the pharmaceutical industry is fully on board with
- Addressing the issue of not having enough skilled and trained professionals
- Discussing how data scientists can work with medicinal scientists to improve the models and generated data

Jiye Shi, AVP, Head of Computational Design and Automation Platforms, **Eli Lilly & Company**
Patrick Riley, SVP, AI, **Relay Therapeutics**
Jeremy Jenkins, US Head Chemical Biology & Therapeutics, **Novartis Institutes for BioMedical Research**

Lunch

Case Study: Using AI in Small Molecule Design

- A deep dive into how AI can augment medicinal chemists in designing small molecule drug
- Discussing how AI tools can be used for triaging the number of molecules down
- Exploring the successes and challenges of using AI in small molecule drug design

Marcel Hop, Vice President, **Genentech**

Case study: Leveraging AI for Drug Discovery

- How Aria's AI platform reveals novel biology and their strategic advantage
- Discussing how this platform has been used to produce pre-clinical data for developing drugs against Lupus
- Exploring snapshots of other pipeline programs, with preclinical data

Aaron Daugherty, Vice President, Discovery, **Aria Pharmaceuticals**

Case Study: Harnessing NLP in the Drug Discovery Process

- Leveraging knowledge graphs to drive and guide the decision making in the drug discovery process
- Discussing how we can harness AI tools to turn disease landscapes into targets

Peter Henstock, AI & ML Technical Lead, **Pfizer**

Afternoon Break

Presentation: The Limitations of Computational Power, Storage and Processing

- Discussing the challenge of storing tremendous amounts of data
- Exploring the enormous computational power required to enable analysis of huge datasets

Panel Discussion: How Do We Assess the Hype and Distinguish the Hype from True Promise?

There is a lot of hype surrounding the use of AI in drug discovery. We need to create realistic expectations when applying AI to answer challenges in the drug development process to prevent the hype cycle, which in turn hinders investment. AI is going to play a huge role in transforming drug discovery, however there is an appreciation that AI will only be part of the solution.

- Is the hype around using AI and Ml tools for drug discovery deserved?
- How can we identify the areas where AI technologies can make an impact now and use these to set realistic expectations?
- How can we apply AI to answer the more complex problems facing the drug discovery industry?
- What problems can AI tools accurately answer?
- Discussing the importance of planning and building explainable and reproducible computational models that allow users to trust the quality of the resulting models and avoiding 'Black Box' models

Moderated by: **Bulent Kiziltan**, Head, AI Innovation Lab, Data Science & AI, **Novartis**
Guillermo Del Angel, Head of Bioinformatics and Data Science**, Alexion**
Bevan Emma Huang, Head, Pharmaceutical Data Sciences for Cross-Sector Initiatives, **Johnson & Johnson**
Lee Herman, Director of Computational Chemistry, **Sunovion Pharmaceuticals**

Chair's Closing Remarks

End of AI in Pharma Summit 2022