AI IN PHARMA DISCOVERY

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

9:00 AM Chair's Opening Remarks

Pavan Choksi, Partner**,** **Arkitekt Ventures**

9:10 AM 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**

9:35 AM 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 and ADME optimization

Marcel Hop, Vice President, **Genentech**

10:00 AM 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?
- What examples of internal solutions & success stories have you seen?

Tommaso Mansi, VP of AI/ML & Digital Health, **The Janssen Pharmaceutical Companies of Johnson & Johnson**
Lihua Yu, Chief Data Officer, **FogPharma**
Bino John, Global Team Leader, Director, **AstraZeneca**
Shane Lewin, Vice President of AI/ML**, GSK**
Kathy Gibson, VP Innovation and Strategic Alliances, **CAS**

CAS
A division of the
American Chemical Society

10:45 AM Morning Break

11:15 AM Presentation: Leveraging Physics-Based Approaches, De Novo Design and Machine Learning to Accelerate Small Molecule Discovery

Sathesh Bhat, Executive Director, Drug Discovery Group, **Schrödinger**

Schrödinger

11:40 AM Presentation: Leveraging AI/ML to explain epigenetic regulation and design mRNA therapeutics as programmable epigenetic medicines

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

12:05 AM 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
- How do we let the machine do the exploration and make decisions, even when it doesn't align with the chemist

Jiye Shi, AVP, Head of Computational Design and Automation Platforms, **Eli Lilly & Company**

Patrick Riley, SVP, AI, **Relay Therapeutics**
Chris Wasden, CTO, **Twill**

12:50 PM Lunch

2:00 PM 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**

2:25 PM Presentation: Drug Development to Counter Nerve Agent and Pesticide Poisoning

Organophosphorus chemical nerve agents and pesticides present significant threats to civilian and military populations. Organophosphorus compounds include the nefarious G and V chemical nerve agents from around World War II, but more commonly, civilians are exposed to less toxic organophosphorus pesticides, while resulting in the same negative toxicological effects and thousands of deaths on an annual basis. After decades of research, no new therapeutics have been approved since the late 1900s. Upon phosphylation of the catalytic serine residue, known as inhibition, there is an accumulation of acetylcholine in the brain synapses and neuromuscular junctions, leading to a cholinergic crisis and eventually death. Oxime nucleophiles can reactivate select organophosphorus-inhibited acetylcholinesterase. Yet, the fields of reactivation of acetylcholinesterase and butyrylcholinesterase encounter additional challenges as broad-spectrum reactivation of either inhibited enzyme is difficult. Additional problems include the ability to cross the blood brain barrier and to provide therapy in the central nervous system. Yet another complication arises in a competitive reaction, known as aging, whereby the organophosphorus-inhibited cholinesterase is converted to an inactive form, that until very recently, had been impossible to reverse to an active, functional form. Our research team is focused on developing medical countermeasures against the use of organophosphorus agents, for the warfighter and for civilians. We have worked on a number of different approaches for post-exposure medical countermeasures. Specifically, we will discuss how large computational data and chemical informatics have guided the drug development process, along with experimental in vitro and in vivo studies, and with a goal of saving lives from organophosphorus intoxication.

Dr. Christopher M. Hadad, Professor of Chemistry and Biochemistry, **Ohio State University**

2:50 PM 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**

3:15 PM Case study: The Application of AI in Digital Medicine

Fahimeh Mamashli, Associate Director, **Pfizer**

3:40 PM Afternoon Break

4:10 PM Presentation: Discovery of Interpretable Clinical Features From Time Series Data Using AI

Brian Tracey, Director Statistics, **Takeda**
Marco Vilela, Principal Data Scientist, **Takeda**

4:35 PM Presentation: A Path to Faster Drug Interaction Calculations

In this interactive session, discover the next steps in accelerating drug discovery through the best classical computing has to offer—with quantum-computing readiness as a fast follow. Attendees will learn about:

- Flexing the latest in computational power, specifically GPUs, to accelerate drug candidate and target discovery.
- How to deploy highly accurate binding energy calculations for small molecule discovery, for systems up to 1,500 atoms at a rate far faster than modern CPU methods.
- How QC Ware's method performs on the gold-standard dimer interaction database.

Andrew Simmonett, Quantum Chemist**, QC Ware**
Yianni Gamvros, SVP, Business Development, **QC Ware**

5:05 PM 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**
Yinghao Ma, Assistant Director, **American Chemical Society (ACS)**

5:50 PM Chair's Closing Remarks

Drinks Reception Hosted by ACS Publications

A 1.5 hour drinks reception hosted by ACS Publications

End of AI in Pharma Summit 2022