AI in Pharma 2023: Drug Design Agenda
8th in the Series **Thursday, April 6th | West Coast**

Chair's Opening Remarks & Setting the Scene

Name, Title, **Company**

Keynote Presentation: Where We've Been, and Where We Are Currently in Utilizing AI in the Drug Design Process

- Compare the past and present applications of AI in Drug Design,
- Recap on how the use of AI in Drug Design has matured in the last 10 years,
- Identify the most pivotal moments in the industry to date
- Discuss the main advantages of using AI in accelerating drug discovery.

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Keynote Panel: Addressing the Primary Bottlenecks in AI for Drug Design

The application of AI in drug design is far from straightforward, however let's address the elephant in the room - one of the main bottlenecks here continues to be data. In this panel, we delve into the main challenges the industry faces as we continue to integrate AI methods into the drug design process…

- Where are the main bottlenecks in leveraging AI in the drug design process?
- Which are continuous issues, and which can we overcome?
- Are we adequately addressing the "data issue" as an industry and what other measures can be taken to improve this?
- How are different stakeholders in the space addressing the key bottlenecks in drug design?
- Can cross-industry collaboration across stakeholders overcome key challenges in the space?

Jiye Shi, AVP Head of Computational Design and Automation Platforms, **Eli Lilly & Company**
Andrew Radin, CEO and Co-founder, **Aria Pharmaceuticals**
Name, Title, **Company,**
Name, Title, **Company,**
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Morning Refreshments
Establishing Industry Data Standards

Breakout Sessions: Coming Together to Establish Prospective Industry Data Standards

The need for universal data standards is essential in ensuring that we get the best output from our algorithms. These intimate breakout sessions allow for small groups of attendees alongside thought leaders from key stakeholder groups, to come together and propose 5 data standards that they believe would be beneficial as universal industry standards.

- How is the lack of clear data standards hindering innovation in drug design?
- In what ways is this acting as a barrier to partnerships?
- What are 5 of the most significant data standards that would benefit drug design?

Recap: Reviewing Proposed Data Standards - Peer to Peer Learning

The chair and key data science industry leaders share some of their most beneficial standards, with a link to a full list perhaps on screen/website?

- How can we get the ball rolling to implement these standards?
- Who should be leading and implementing these changes?
- Why is the industry still lacking a medium to share data?

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Lunch

Drug Design in Practice

Case Study: Alternative to AlphaFold

Vanita Sood, SVP Head of Research, **Oracle Biotherapeutics**

Case Study: Computational Chemistry and Drug Design Across Oncology, Inflammation and CNS

Martin Wythes, Head of Oncology Medicinal Chemistry Design, **Pfizer**

Case Study:

Afternoon Break

Case Study: Addressing the Issue of Low Interpretability and Reproducibility in AI

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Presentation: The Astrazeneca iLab: The Automated Lab of the Future

- An overview of the work currently being done at The iLab Astrazeneca,
- Examine how the Astrazeneca iLab is automating the design-make-test-analyze (DMTA) cycle of drug discovery and how this is optimizing drug design,
- A mini case study of a small/large molecule drug designed in iLab and currently in clinical trials.

Alexander Marziale, Director of Discovery Sciences**, The Astrazeneca iLab**

Panel and Open Q/A: What Does the Future Hold for AI in Drug Design and The Lab of the Future?

- What is the 'lab of the future' concept?
- Are closed-loop systems the key to enable automated computer-aided drug design?
- Where do the main difficulties lie in using closed-loop discovery platforms?
- How can we facilitate the cultural acceptance of automated labs in the industry?
- How will this accelerate drug discovery in the future and how can we expect to see a development across the industry in 5 years?

Alexander Marziale, Director of Discovery Sciences**, The Astrazeneca iLab,**
Connor Coley (MIT), Nathan Collins (SRI), Alan Aspuru-Guzik (Toronto)

Chair's Closing Remarks

End of AI in Pharma 2023 Day 2