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Includes Access to
PepTalk
The Protein Science and Production Week

FINAL AGENDA

JANUARY 13-16, 2025 | SAN DIEGO, CA + VIRTUAL

BioLogic SUMMIT 2025

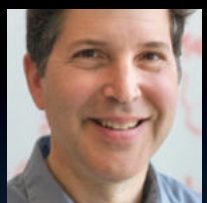
Demystifying AI/ML for Biologic Drug Development

EVENT-AT-A-GLANCE

- Models for *de novo* Design
- Machine Learning in Early Discovery
- Predicting Developability and Optimization Using Machine Learning
- Training Data Generation and Quality

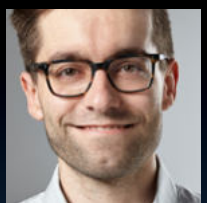
PLENARY KEYNOTES

NOBEL LAUREATE



David A. Baker, PhD
University of Washington

Rebecca Croasdale-Wood, PhD
AstraZeneca



Victor Greiff, PhD
University of Oslo

Marissa Mock, PhD
Amgen Inc.

Vladimir Gligorijević, PhD
Genentech

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BioLogicSummit.com

Training SEMINARS

By Cambridge Healthtech Institute

MONDAY, JANUARY 13, 2025
9am-6pm

All training seminars take place in-person only

TS1A: Introduction to Machine Learning for Biologics Design

Instructors:

Christopher R. Corbeil, PhD, Research Officer, Human Health Therapeutics, National Research Council Canada

Francis Gaudreault, PhD, Associate Research Officer, Human Health Therapeutics, National Research Council Canada

This course offers an introduction to concepts, strategies, and machine learning methods used for biologics design. It includes presentations and demonstrations of the methods used in the field, covering techniques such as triaging sequences, modulating affinity, and designing antibody libraries, along with increasing manufacturability. The course is directed at scientists new to the field and protein engineers wanting an introduction to how machine learning can aid in guiding biologics design.

TS2A: Implementing Artificial Intelligence and Computational Tools in Biopharmaceutical R&D

Instructor:

Ryan Peckner, PhD, Director, Machine Learning, Seismic Therapeutic

Artificial intelligence and other computational techniques have revolutionized biopharma research over the past two decades, leading to the solutions of fundamental problems such as protein folding and the acceleration of numerous aspects of biopharma R&D. This seminar will survey the landscape of AI and computational tools with an emphasis on the steps needed to implement AI-based workflows and programs in biotherapeutic research organizations. We will examine case studies and interactive demonstrations in a range of application areas in which AI has led to acceleration and innovation, including identifying novel drug targets, predicting protein structure, designing small molecules and antibodies, and optimizing biopharmaceutical manufacturing processes.

TS3A: AI-Driven Design of Biologics

Instructors:

Timothy Riley, PhD, Vice President, Discovery, 310 AI

Kathy Y. Wei, PhD, Co-Founder & CSO, 310 AI

Discover how to revolutionize biologics design using cutting-edge AI models for drug discovery and healthcare. In this immersive hands-on seminar, attendees will explore the applications of machine learning tools for protein structure prediction and design. Participants will navigate through practical applications using open-sourced, state-of-the-art tools such as —AlphaFold, ESMFold, ProteinMPNN, RFDiffusion, and others—all within an intuitive Jupyter notebook environment. From understanding the nuances of protein-protein docking (with tools like EquiDock, DiffDock-PP, etc) to harnessing the power of language models (ProGen, IgLM, etc), this seminar will cover a breadth of fields in protein design. Attendees will also delve into the innovative realms of hallucination and diffusion-based models for protein engineering. By the end of the seminar, participants will be equipped with the knowledge and skills to implement these AI-driven tools in their own research and development projects.

Interactive Elements at the BioLogic Summit

In addition to podium presentations, this event will include a significant number of interactive elements, including moderated discussions, and single day training seminars. Interactive forums play an integral role in facilitating networking with potential collaborators and provide an opportunity to be part of a group problem-solving endeavor.

Co-located Event: January 13-16, 2025 | San Diego, CA + Virtual

Hilton Bayfront

24th Annual PepTalk

The Protein Science and Production Week

TUESDAY, JANUARY 14

7:30 am Registration and Morning Coffee

PLENARY KEYNOTE SESSION

8:30 The State of the Art for Antibody Structure Prediction
Victor Greiff, PhD, Associate Professor, Immunology, University of Oslo
Antibody structure prediction is pivotal for understanding antibody function and for enabling *in silico* antibody design. This lecture will outline current key advances as well as unresolved challenges in antibody structure prediction.

9:00 Design of New Protein Functions Using Deep Learning
David A. Baker, PhD, Henrietta & Aubrey David Endowed Professor, Biochemistry, University of Washington
Proteins are biology's workhorses. Our goal is to create new proteins that address current-day problems not faced during evolution. Rather than modify naturally occurring proteins, we design new ones from scratch to optimally solve the problem at hand. Increasingly, we develop and use deep learning methods to generate protein sequence, structure, and function. We then characterize these designed molecules experimentally. In this talk, I will describe several recent projects.

LATEST TOOLS AND APPROACHES FOR DESIGNING PROTEINS USING MODELS

10:00 Chairperson's Opening Remarks
Maria Wendt, PhD, Global Head and Vice President, Digital and Biologics Strategy and Innovation, Sanofi

10:05 KEYNOTE PRESENTATION: Accelerating Biologic Drug Discovery with AI: Advancements and Challenges in *de novo* Antibody Design
Per Greisen, PhD, President, BioMap
The urgent need for novel biologics demands accelerated drug discovery. We leverage AI to expedite therapeutic antibody development, showcasing our progress in *de novo* design of VHH and mAbs targeting specific epitopes. We'll discuss the strengths and limitations of current AI algorithms, challenges in translating designs into functional molecules, and strategies to refine these algorithms for improved *de novo* biologic design success.

10:35 Developing and Implementing an Effective IP Strategy for an AI/ML-Driven Biologics Therapeutic Program
Matt Wheeler, Wilson Sonsini Goodrich & Rosati
This talk will focus on understanding IP rights, inventorship, and ownership of AI/ML-based inventions including platform aspects and therapeutic modalities. Deciding between patenting and maintaining trade secret aspects of the platform and modalities will be discussed. It will review life cycle management strategy for a biologics therapeutic program and Freedom to Operate.

11:05 Grand Opening Coffee Break in the Exhibit Hall with Poster Viewing

11:20 Steering Protein Language Models for Functional Protein Design
Jeffrey Ruffolo, PhD, Head of Protein Design, Profluent Bio
Protein language models trained on evolutionarily diverse sequences implicitly model the sequence-function landscape of proteins. These models learn to generate diverse sequences, but must be steered for protein design tasks. We first discuss the generation of diverse CRISPR-Cas effectors for genome editing applications through fine-tuning on curated natural sequences. Next, we present a strategy for steering protein language models through conditioning on structural and functional context.

11:50 *De novo* Designed Proteins Neutralize Lethal Snake Venom Toxins
Susana Vazquez Torres, PhD Student, Protein Design, University of Washington
Here, we use deep learning methods to *de novo* design proteins to bind short- and long-chain α-neurotoxins and cytotoxins from the 3FTx family. With limited experimental screening, we obtain protein designs with remarkable thermal stability, high binding affinity, and near-atomic level agreement with the computational models. The designed proteins effectively neutralize all three 3FTx sub-families *in vitro* and protect mice from a lethal neurotoxin challenge.

12:20 pm Sponsored Presentation *(Opportunity Available)*

12:50 Luncheon Presentation *(Sponsorship Opportunity Available)* **or Enjoy Lunch on Your Own**

1:20 Session Break

1:30 Refreshment Break in the Exhibit Hall with Poster Viewing

NEXT STEPS FOR PREDICTING MOLECULAR DYNAMICS AND FUNCTIONAL EFFECTS OF MUTATIONS

2:00 Chairperson's Remarks
Victor Greiff, PhD, Associate Professor, Immunology, University of Oslo

2:05 Deep Learning Guided Design of Dynamic Proteins
Tanja Kortemme, PhD, Professor, Bioengineering & Therapeutic Sciences, University of California, San Francisco
Methods from artificial intelligence can now "write" proteins *de novo*, without starting from proteins found in nature. I will discuss our recent progress with developing deep learning models for *de novo* protein design, demonstrating that they generalize beyond the training space, and applying them to difficult problems, including atomically accurate design of dynamic proteins. Exciting frontiers lie in constructing synthetic cellular signaling from the ground up using *de novo* proteins.

2:35 Machine Learning Coarse-Grained Potentials of Protein Thermodynamics
Klara Bonneau, PhD Student, Computational Biophysics, Freie Universität Berlin
Coarse-grained (CG) models are an alternative to the expensive all-atom models, but reaching high predictive power has been a longstanding challenge. By combining deep learning methods with a diverse training set of protein simulations, we have developed a CG force field which can be used for molecular dynamics on new sequences not used during model parametrization. This showcases the feasibility of a universal and efficient CG model for proteins.

3:05 Decoding Molecular Mechanisms for Loss of Function Variants
Matteo Cagiada, PhD, Postdoctoral Fellowship Program, Novo Nordisk Foundation, University of Copenhagen
Proteins are essential for cellular function, and missense variants can cause genetic disorders by destabilizing proteins or disrupting key interactions. While prediction of deleterious variants has progressed, understanding of the molecular mechanisms behind these variants remains limited. Thanks to advances in sequence- and structure-based computational predictors, we can now unravel the molecular mechanisms behind loss-of-function and quantify the role of stability in disrupting protein function.

3:35 Refreshment Break in the Exhibit Hall with Poster Viewing

4:15 Interactive Breakout Discussions

How Open Competitions Provide Valuable Benchmarking to Novel Technologies
Andrew R.M. Bradbury, MD, PhD, CSO, Specifica, an IQVIA business
Matthieu Schapira, PhD, Principal Investigator, Structural Genomics Consortium, Professor, Pharmacology & Toxicology, University of Toronto
- Why benchmarking is needed
- Designed competitions, and accidental ones
- Lessons from CACHE
- The AIntibody competition to assess computational methods in antibody discovery

The Use of Tools for Building Gene Editors for Going Beyond Proteins
Jeffrey Ruffolo, PhD, Head of Protein Design, Profluent Bio

AI-Driven Biologics: Accelerating Discovery, Overcoming Challenges
Per Greisen, PhD, President, BioMap
- Motivation: The urgent need for novel biologics is driving the exploration of AI in drug discovery
- Focus: AI's potential in accelerating biologic drug discovery, particularly *de novo* antibody design
- Showcase: Successful AI-driven VHH and mAb designs
- Discussion: AI's strengths in predicting antibody structures, challenges in translating designs into functional molecules, achieving industrial-scale reliability, and closing the gap between computational and experimental results

5:30 **PANEL DISCUSSION: Targeted *de novo* and *in silico* Design of Proteins and Peptides**
Moderator: Monica L. Fernandez-Quintero, PhD, Staff Scientist, General Inorganic & Theoretical Chemistry, Scripps Research Institute
- What can be designed at this point?
- What resources need to be realistically invested to get a hit?
- What are the best tools/workflows out there? How do you decide which one to use?

Panelists:
Bryan Briney, PhD, Assistant Professor, Immunology & Microbial Science, Scripps Research Institute
Jeffrey J. Gray, PhD, Professor & Research Mentor & Outreach Advisor, Chemical & Biomolecular Engineering, Johns Hopkins University
Victor Greiff, PhD, Associate Professor, Immunology, University of Oslo

6:30 **Networking Reception in the Exhibit Hall with Poster Viewing**

7:30 **Close of Day**

WEDNESDAY, JANUARY 15

7:45 am **Registration and Morning Coffee**

PLENARY KEYNOTE SESSION

8:00 **Chairperson's Remarks**
Rebecca Croasdale-Wood, PhD, Senior Director, Augmented Biologics Discovery & Design, Biologics Engineering, Oncology, AstraZeneca

8:10 ***De novo* Design of Therapeutic Antibodies**
Vladimir Gligorijević, PhD, Senior Director, AI/ML Prescient Design, Genentech
I will discuss our current efforts in building structure-based diffusion methods for *de novo* design of antibodies, their potential role in overcoming critical design challenges, and accelerating drug discovery programs.

8:40 **Session Break**

LATEST TOOLS AND APPROACHES FOR DESIGNING PROTEINS USING MODELS

8:45 **Chairperson's Remarks**
Maria Wendt, PhD, Global Head and Vice President, Digital and Biologics Strategy and Innovation, Sanofi

8:50 KEYNOTE PRESENTATION: **Discovering Safe, Effective Drugs via Learning and Simulation of 3D Structure**
Ron Dror, PhD, Associate Professor, Computer Science, Artificial Intelligence Lab, Stanford University
Recent years have seen dramatic advances in both experimental determination and computational prediction of macromolecular structures. These structures hold great promise for the discovery of highly effective drugs with minimal side effects, but structure-based design of such drugs remains challenging. I will describe recent progress toward this goal, using both atomic-level molecular simulations and machine learning on three-dimensional structures.

9:20 **AI Tools for Antibody Engineering**
Jeffrey J. Gray, PhD, Professor & Research Mentor & Outreach Advisor, Chemical & Biomolecular Engineering, Johns Hopkins University
AI has become increasingly powerful but can be overhyped. Our lab has used AI methods to develop antibody language models, antibody structure prediction models, protein-protein docking models, and antibody design models. I will share recent results, including testing language models' comprehension of biological antibody maturation processes, benchmarking antibody developability models, and bringing physical energies back into AI predictions. Our results suggest how to use AI tools with appropriate caution.

9:50 **Sponsored Presentation** *(Opportunity Available)*

10:50 **Bagel Booth Crawl with Coffee in the Exhibit Hall with Poster Viewing** *(Sponsorship Opportunity Available)*

PLENARY KEYNOTE SESSION

11:15 **Chairperson's Remarks**
Alissa Hummer, PhD, Postdoctoral Researcher, Biochemistry, Stanford University

11:20 **Benchmarking and Integrating ML/AI Advancements in Biologics Discovery and Optimisation for Pharma**
Rebecca Croasdale-Wood, PhD, Senior Director, Augmented Biologics Discovery & Design, Biologics Engineering, Oncology, AstraZeneca

11:50 **FIRESIDE CHAT WITH PLENARY KEYNOTE**

Moderator: Alissa Hummer, PhD, Postdoctoral Researcher, Biochemistry, Stanford University

Panelists:

Rebecca Croasdale-Wood, PhD, Senior Director, Augmented Biologics Discovery & Design, Biologics Engineering, Oncology, AstraZeneca

12:20 pm **Session Break**

12:30 **Luncheon Presentation** *(Sponsorship Opportunity Available)* **or Enjoy Lunch on Your Own**

1:00 **Close of Models for *de novo* Design Conference**

WEDNESDAY, JANUARY 15

NOVEL PREDICTIVE AND GENERATIVE APPROACHES FOR SOLVING REAL-WORLD ENGINEERING CHALLENGES

1:30 pm Chairperson's Remarks
Kathy Y. Wei, PhD, Co-Founder & CSO, 310 AI

1:35 KEYNOTE PRESENTATION: Antibody Optimization Through Combining Structure-Based Approaches and Deep Learning
Alan Cheng, PhD, Senior Director, Modeling and Informatics, Merck Research Labs
In the discovery of antibody therapeutics, experimental molecular biology and biophysical methods are powerful approaches that can be combined with computational approaches to accelerate identification of better molecules. We share case studies illustrating how the close integration of experimental methods and deep learning can identify new leads and how structure-based and deep learning approaches can be used to optimize molecules for developability properties.

2:05 A Clinically Validated AI-Driven Platform for Designing Smart and Dynamic Antibody Therapeutics
Reshef Shilon, Head of AI, Biolojic Design
Although antibody drugs have great therapeutic benefits, most function primarily as inert antagonists, and don't fulfill the potential of proteins. Biolojic Design's clinically validated AI-driven platform designs dynamic antibodies that are programmed to respond to changes in the environment. In this talk I'll describe Biolojic's AI-platform, which experimentally generates data for AI models—and optimizes, simultaneously, multi-antibody properties—which in turn allows the design of smart and dynamic antibodies.

2:35 Refreshment Break in the Exhibit Hall with Poster Viewing

3:10 Delivering Better Clinical Candidates, Faster: Practical Impacts of Machine Learning on Biologics Preclinical Pipeline
Andrew B. Waight, PhD, Senior Director, Machine Learning, Discovery Biologics & Protein Sciences, Merck Research Labs
AI/ML applications to the field of protein engineering have recently generated immense enthusiasm. In addition to protein folding and *de novo* design, statistical and deep learning technologies are revolutionizing many aspects of the biologics therapeutic discovery. We cover some of the real-world use cases for AI/ML applications—from hit identification to lead optimization stages of discovery biologics—that are facilitating the computational identification of high-quality preclinical candidates and improving efficiency.

3:40 Enhancing AI Capabilities through Smart Data Collection and Evolutionary Intelligence in Antibody Development
M. Frank Erasmus, PhD, Head, Bioinformatics, Specifica, an IQVIA business
Exploring the bilateral importance of leveraging strategic data collection and intelligent experimental design to enhance AI capabilities in antibody development. Discussing the utilization of evolutionary intelligence to refine and optimize affinity maturation strategies, leading to the discovery of antibodies with superior binding properties and therapeutic potential.

4:10 Presentation to be Announced

ATUM

4:40 Generative and Predictive Machine Learning for Iterative Multi-Objective Therapeutic Antibody Optimization
Hunter Elliott, PhD, Senior Director, Machine Learning, BigHat Biosciences
The path from discovered binder to developable modern antibody therapeutics represents a complex protein engineering challenge. At BigHat, we frame this as a multi-objective Bayesian optimization problem, with machine learning models in-the-loop with a high-throughput wet lab on a weekly build-test-train cycle. We present several case studies of novel predictive and generative ML methods deployed on this platform to solve real-world antibody therapeutic engineering challenges.

Interactive Breakout Discussion: Applying AI to Improve Manufacturability and Developability of Multispecific Biologics
Mahiuddin Ahmed, PhD, President and CSO, VITRUVIAE
Jeffrey J. Gray, PhD, Professor & Research Mentor & Outreach Advisor, Chemical & Biomolecular Engineering, Johns Hopkins University
- Improving humanization and predicting immunogenicity
- Reducing off-target binding
- Predicting aggregation, viscosity, and excipient formulation
- Combining targets for improved efficacy

6:00 Meet-Up

THURSDAY, JANUARY 16

7:45 am Registration and Morning Coffee

PLENARY KEYNOTE SESSION

8:15 Chairperson's Remarks
M. Frank Erasmus, PhD, Head, Bioinformatics, Specifica, an IQVIA business

8:20 Transforming Therapeutic Protein Engineering
Marissa Mock, PhD, Senior Research Director, Amgen Inc.
Generative biology is an emerging discipline that integrates artificial intelligence (AI) and machine learning (ML) with advanced life science technologies. The application of generative biology to protein engineering is accelerating the discovery and design of complex proteins with therapeutic potential—and, maximizing the benefits of these novel technologies will require seamless integration of both wet- and dry-laboratory technologies.

8:50 Session Break

INTEGRATING AI/ML FOR ENHANCED ANTIBODY SELECTION AND DEVELOPABILITY

8:55 Chairperson's Remarks
M. Frank Erasmus, PhD, Head, Bioinformatics, Specifica, an IQVIA business

9:00 Generative AI-Guided Design of Vaccine Immunogens
Reda Rawi, PhD, Staff Scientist and Co-Head, Structural Bioinformatics Core, NIH NIAID
Structure-based vaccine design campaigns that aim to stabilize full-length proteins will not succeed when the virus is evading immune response by sequence diversity. In this work, we capitalized on the recent major advanced that have been achieved in protein design using generative AI tools. We *in silico* designed *de novo* proteins that scaffold sequence-conserved epitope regions of the antigens of interest.

9:30 ML Optimization of Candidate Antibody Yields Highly Diverse Sub-Nanomolar Affinity Libraries
Lin Li, PhD, Senior Staff Member, Lincoln Laboratory, Massachusetts Institute of Technology
The design and discovery of early-stage antibody therapeutics is time- and cost-intensive. I will present an end-to-end machine learning-driven single-chain variable fragments (scFv) design framework that uniquely combines large language models, Bayesian optimization, and high-throughput experimentation. The method enables rapid and cost-effective design of

thousands of scFvs across all complementary determining regions. The designed antibodies exhibit strong binding affinities, at high levels of diversity, to a given antigen.

10:00 Presentation to be Announced

10:15 AI-Driven paratope mapping (KisoSeek™): A new paradigm for antibody discovery

Morteza Babaie, Senior AI Scientist, Kisoji Biotechnology Inc

The KisoSeek™ platform leverages AI-driven paratope mapping to accelerate therapeutic antibody discovery. Integrating autoencoders, structural/sequence data and large language models to visualize antibody repertoires in multidimensional maps, enabling functional clustering. Built on KisoMouse(R) HCAb immunization libraries, this approach improves the exploration of diversity through various sampling strategies, including probability-based and targeted selections. KisoSeek™ supports VHH and VH-VL antibodies, driving efficient and versatile candidate selection for therapeutic development.

10:30 Coffee Break in the Exhibit Hall with Poster Viewing

11:00 Efficient Evolution of Antibodies from General Protein Language Models

Varun Shanker, MD-PhD Student, Biophysics, Stanford University

This talk will cover how large language models of protein sequences and structures can learn evolutionary rules that help guide the artificial evolution of human antibodies. We will cover how algorithms known as protein language models can guide the affinity maturation of antibodies against diverse antigens using sequence information alone. Next, we will cover how multimodal language models can further improve the ability to guide antibody evolution completely unsupervised.

11:30 Interactive Breakout Discussions

AI/ML-Driven Design of Conditionally Active Molecules

Hunter Elliott, PhD, Senior Director, Machine Learning, BigHat Biosciences

- What is the therapeutic potential of conditional activity and how do we best balance this against increased complexity and risk?
- Which challenges are unique to ML-driven design of conditional molecules?
- How does the optimal ML toolkit vary between conditional and unconditional design?
- How can we best overcome challenges in data acquisition and availability?
- What are the currently tractable forms of conditional activity and what can we envision for the future?

Practical Impacts of Machine Learning on Biologics Preclinical Pipeline

Andrew B. Waight, PhD, Senior Director, Machine Learning, Discovery Biologics & Protein Sciences, Merck Research Labs

12:30 pm Session Break

12:40 Luncheon Presentation to be Announced

1:10 Ice Cream & Cookie Break in the Exhibit Hall with Last Chance for Poster Viewing

INTEGRATING AI/ML FOR ENHANCED ANTIBODY SELECTION AND DEVELOPABILITY

2:00 Chairperson's Remarks

M. Frank Erasmus, PhD, Head, Bioinformatics, Specifica, an IQVIA business

2:05 Towards Enhancement of Antibody Thermostability and Affinity by Computational Design in the Absence of Antigen

Gilad Kaplan, PhD, Director, Biologics Engineering, AstraZeneca

DeepAb, a deep learning model for predicting antibody Fv structure directly from sequence, was used in conjunction with experimental deep mutational scanning (DMS) enrichment data to design 200 potentially optimized variants of an anti-hen egg lysozyme (HEL) antibody. We discuss the improvement rate of the designed clones for affinity, thermostability, and developability—and what the results would have been without using experimental DMS data to guide the design process.

2:35 Towards Optimal Clone Selection: Enhancing Antibody Discovery with AI/ML Approaches

Adrian Carr, PhD, Associate Director, Data Science, AI Innovation—Antibodies, Large Molecules Research (LMR), Sanofi

Optimal clone selection strikes a balance between selecting desirable antibody properties and diversity, aiming to maximize the range of targeted epitopes while minimizing redundancy. At Sanofi, we are exploring *in silico* screening, leveraging AI/ML methods to enhance success rates and accelerate the transition from discovery to lead. In parallel, generative AI can be used to augment natural and experimental repertoires, eliminating undesirable traits while preserving desirable characteristics.

3:05 PANEL DISCUSSION: AI DRIVEN OPTIMIZATION OF ANTIBODY PROPERTIES

Moderator: M. Frank Erasmus, PhD, Head, Bioinformatics, Specifica, an IQVIA business

- Where has there been the most benefit to cost or time savings?
- Are we noticing developability tools showing improvements in preclinical studies?
- Are we noticing reduction in immunogenicity or timeline?
- Where does *in silico* modeling allow us to remove experimental efforts and use computational modeling to replace?
- Have we seen benefits to the implementation of Federated Learning?
- Are we seeing benefits to optimization and developability?

Panelists:

Hunter Elliott, PhD, Senior Director, Machine Learning, BigHat Biosciences

Yue Liu, PhD

Andrew B. Waight, PhD, Senior Director, Machine Learning, Discovery Biologics & Protein Sciences, Merck Research Labs

4:05 Close of BioLogic Summit

Machine Learning in Early Discovery

Exploiting the Power of ML in Early-Stage Biotherapeutic R&D

JANUARY 14 - 15, 2025

TUESDAY, JANUARY 14

7:30 am Registration and Morning Coffee

PLENARY KEYNOTE SESSION

8:30 The State of the Art for Antibody Structure Prediction

Victor Greiff, PhD, Associate Professor, Immunology, University of Oslo

Antibody structure prediction is pivotal for understanding antibody function and for enabling *in silico* antibody design. This lecture will outline current key advances as well as unresolved challenges in antibody structure prediction.

9:00 Design of New Protein Functions Using Deep Learning

David A. Baker, PhD, Henrietta & Aubrey David Endowed Professor, Biochemistry, University of Washington

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MACHINE LEARNING FOR TARGET IDENTIFICATION

10:00 Chairperson's Remarks

Brian Pierce, PhD, Associate Professor, Cell Biology & Molecular Genetics, Institute for Bioscience and Biotechnology Research, University of Maryland

10:05 KEYNOTE PRESENTATION: *De novo* Antibody Design with RFantibody

Nathaniel Bennett, PhD, Co-Founder, Xaira Therapeutics

Despite the central role that antibodies play in modern medicine, there is currently no way to rationally design novel antibodies to bind a specific epitope on a target. I will discuss the development and experimental validation of RFantibody, a deep-learning pipeline capable of designing *de novo* antibodies that bind to user-specified epitopes.

10:35 Drug Target Prediction through Deep Learning Functional Representation of Gene Signatures

Hao Chen, PhD, Assistant Professor, University of Illinois Chicago

The L1000 program systematically generated 1.3 million gene expression signatures in human cell lines with diverse genomic and pharmacological perturbations. Similar L1000 gene signatures offer an unbiased data-driven mechanism to identify compound-target pairs. Current methods rely on matching gene identities when comparing gene signatures. We developed FRoGS, an approach that represents gene signatures projected onto their biological functions, instead of their identities, which results in more effective compound-target predictions.

11:05 Grand Opening Coffee Break in the Exhibit Hall with Poster Viewing

11:20 Multi-Dimensional Functional Interrogation and Network Modeling of Tissue Tregs Reveals Novel Therapeutics for Autoimmunity and Inflammation

Christopher Yohn, PhD, Executive Director, Computational Biology, TRexBio

Our discovery biology platform provides a deep understanding of the regulatory circuits underlying human tissue Treg behavior. A suite of disease-relevant phenotypic assays facilitates multi-dimensional functional interrogation of key genes in human Tregs. These complex *in silico* tools combined with translational *in vitro* assays identify novel regulatory nodes and form the foundation of our growing pipeline of a new class of tissue Treg-focused therapeutics for immune-mediated diseases.

11:50 Spatial Proteomics and Virtual Cell Models

Emma Lundberg, PhD, Associate Professor, Bioengineering and Pathology, Stanford University

This research integrates bioimaging, proteomics, and AI to study human cell biology to explore protein distribution in time and space, investigating how localization variations affect cell functions and disease. Our goal is to create a spatiotemporal proteome model of a human cell. Using ML, we interpret spatial data from image collections and combine it with other datatypes to build whole-proteome multi-scale cell models, with potential to enhance drug discovery processes.

12:20 pm Presentation to be Announced

aureka

12:50 Luncheon Presentation *(Sponsorship Opportunity Available)* **or Enjoy Lunch on Your Own**

1:20 Session Break

1:30 Refreshment Break in the Exhibit Hall with Poster Viewing

MODELING FOR EARLY-STAGE DISCOVERY AND ENGINEERING

2:00 Chairperson's Remarks

Christopher Yohn, PhD, Executive Director, Computational Biology, TRexBio

2:05 Novel Machine Learning Approach for Activity and Affinity Prediction

Di Wu, PhD, Director, Biotechnology Discovery Research, Eli Lilly and Company

This presentation introduces a novel ML approach for predicting molecular activity and binding affinity in early discovery. Our model analyzes chemical structures and their interactions with biological targets using advanced algorithms. Incorporating diverse datasets and new feature extraction techniques improves accuracy in predicting compound behavior. This enhances lead identification and optimization, potentially accelerating drug discovery and reducing costs. We'll discuss implementation strategies, preliminary results, and future applications of this approach.

2:35 Applications of Protein Language Models and Generative AI for Antibody Discovery

Matthew Massett, PhD, Senior ML Scientist, Sanofi

Monoclonal antibodies are important biotherapeutics, but developing them is expensive and difficult since they must be specific and able to be produced at commercial-scale. We present a transformer-based antibody language model, trained on large amounts of antibody data. This model can be used to inform and de-risk early antibody discovery by increasing the quantity of viable antibodies.

3:05 Sponsored Presentation *(Opportunity Available)*

3:35 Refreshment Break in the Exhibit Hall with Poster Viewing

4:15 Interactive Breakout Discussions

The Transition of Experimentalists into a Computational Paradigm in Pharmaceutical R&D

Qing Chai, PhD, Research Advisor, Biotechnology Discovery Research, Eli Lilly and Company

- Addressing skills gaps
- Benchmarking progress compared with traditional structures
- Best practices for collaboration between experimentalists and data scientists
- Examples of successful transitions
- Implementing models/tools and workflows based on AI/ML approaches

5:30 RESP AI Model Accelerates Identification of Tight-Binding Antibodies
Wei Wang, PhD, Professor, Chemistry and Biochemistry, University of California San Diego
We present RESP2, an enhanced version of our RESP pipeline, designed for the discovery of antibodies against diverse antigens with simultaneously optimized developability properties. We used the RBD of the COVID-19 spike protein as a case study, and discover a highly human antibody with broad binding to different variants, which demonstrated the power of this pipeline for antibody discovery against a challenging target.

6:00 Assessing AlphaFold for Modeling Antibody and T Cell Receptor Recognition: Insights and Optimization Strategies
Brian Pierce, PhD, Associate Professor, Cell Biology & Molecular Genetics, Institute for Bioscience and Biotechnology Research, University of Maryland
Accurate modeling of immune recognition remains a major challenge in computational biology. To provide insights into the performance of deep learning for modeling immune recognition, we performed detailed benchmarking of multiple AlphaFold2 and AlphaFold3 approaches for modeling antibody and T cell receptor complexes. This revealed approaches with higher performance, overall limitations in success, as well the utility of confidence scores in the selection of accurate models.

6:30 Networking Reception in the Exhibit Hall with Poster Viewing

7:30 Close of Day

WEDNESDAY, JANUARY 15

7:45 am Registration and Morning Coffee

PLENARY KEYNOTE SESSION

8:00 Chairperson's Remarks
Rebecca Croasdale-Wood, PhD, Senior Director, Augmented Biologics Discovery & Design, Biologics Engineering, Oncology, AstraZeneca

8:10 *De novo* Design of Therapeutic Antibodies
Vladimir Gligorijević, PhD, Senior Director, AI/ML Prescient Design, Genentech
I will discuss our current efforts in building structure-based diffusion methods for *de novo* design of antibodies, their potential role in overcoming critical design challenges, and accelerating drug discovery programs.

8:40 Session Break

NOVEL APPLICATIONS OF ML IN BIOPHARMACEUTICAL R&D

8:45 Chairperson's Remarks
Wing Ki Wong, PhD, Senior Scientist, Pharmaceutical Research and Development, Large Molecule Research, Roche Diagnostics GmbH

8:50 Data- and Model-Guided Antibody and TCR Optimization
Arvind Sivasubramanian, PhD, Director, Computational Biology & Platform Technologies, Adimab LLC
We have developed an NGS-guided workflow for multi-dimensional optimization of biologics such as antibodies and TCRs. The workflow involves the rational design of targeted CDR combinatorial diversity guided by Deep Mutational Scanning, followed by yeast library selections. We will present antibody and TCR optimization case studies demonstrating substantial gain in affinity that is competitive with standard approaches, good developability, and minimal variant mutational load.

9:20 Repertoire Expansion for Antibody Discovery and Optimization Using Machine Learning Approaches
Wing Ki Wong, PhD, Senior Scientist, Pharmaceutical Research and Development, Large Molecule Research, Roche Diagnostics GmbH
In antibody discovery, repertoire sequencing unfolds a broad antigen-specific sequence space and informs of the potential mutational space. Integrating this information and advances in experimental techniques with different machine learning approaches, we are now able to efficiently explore and extend the sequence space to identify alternative binders and improve existing binders.

9:50 Using Machine Learning and Molecular Mimicry of Complex Biologies to Design New GLP-1 Agonists
Marcin Paduch, PhD, Vice President, Head of Platform Biology, Metaphore Biotechnologies
Targeting GPCRs with agonists is a significant challenge in biologics design. Our approach employs molecular mimicry to optimize both developability and functional outcomes, including biased agonism. Leveraging machine learning algorithms backed by extensive empirical data acquisition and protein engineering, we thoroughly explore the pharmacophore space within live cells. This enables us to create designer molecules that address complex biological processes, ultimately leading to the development of novel GLP1R modulators.

10:20 Sponsored Presentation *(Opportunity Available)*

10:50 Bagel Booth Crawl with Coffee in the Exhibit Hall with Poster Viewing *(Sponsorship Opportunity Available)*

PLENARY KEYNOTE SESSION

11:15 Chairperson's Remarks
Alissa Hummer, PhD, Postdoctoral Researcher, Biochemistry, Stanford University

11:20 Benchmarking and Integrating ML/AI Advancements in Biologics Discovery and Optimisation for Pharma
Rebecca Croasdale-Wood, PhD, Senior Director, Augmented Biologics Discovery & Design, Biologics Engineering, Oncology, AstraZeneca

11:50 FIRESIDE CHAT WITH PLENARY KEYNOTE

Moderator: Alissa Hummer, PhD, Postdoctoral Researcher, Biochemistry, Stanford University

Panelists:

Rebecca Croasdale-Wood, PhD, Senior Director, Augmented Biologics Discovery & Design, Biologics Engineering, Oncology, AstraZeneca

12:20 pm Session Break

12:30 Luncheon Presentation *(Sponsorship Opportunity Available)* **or Enjoy Lunch on Your Own**

1:00 Close of Machine Learning in Early Discovery Conference

Training Data Generation and Quality

Ensuring Quality Predictions via Attention to Data Quality

JANUARY 15 - 16, 2025

WEDNESDAY, JANUARY 15

BENCHMARKING, BIAS, AND CONTROLS

1:30 pm Chairperson's Remarks
Arvind Sivasubramanian, PhD, Director, Computational Biology & Platform Technologies, Adimab LLC

1:35 Protein Language Models Are Biased by Unequal Sequence Sampling across the Tree of Life
Frances Ding, PhD, Machine Learning Scientist, Prescient Design, Genentech
Protein language models (PLMs), like all machine learning models, learn biases from data. In this talk I will show that PLMs unintentionally learn a strong species bias. Specifically, PLM likelihoods of protein sequences from certain species (e.g., human, *E. coli*) are systematically higher, independent of the protein in question. I trace this bias's origins and demonstrate how it can be detrimental for some protein design applications, such as enhancing thermostability.

2:05 Improving Antibody Language Models with Native Pairing
Bryan Briney, PhD, Assistant Professor, Immunology & Microbial Science, Scripps Research Institute
We developed Baseline Antibody Language Models (BALM) using Jaffe's dataset of 1.6 million natively paired human antibody sequences. Training with paired sequences (BALM-paired) outperformed unpaired training, demonstrating learning of cross-chain immunological features. ESM-2, a protein language model, showed similar improvements when fine-tuned with paired data. This approach addresses limitations in current antibody models, enhancing our understanding of antibody structure-function relationships. We discuss implications for antibody engineering and therapeutic development.

2:35 Refreshment Break in the Exhibit Hall with Poster Viewing

3:10 AI Benchmarking Competition Based on High-Throughput Automation and Cloud Lab Experimentation
Peter Kelly, Director, Open Datasets Initiative, Align to Innovate
Align to Innovate, a non-profit research organization, is on a mission to shepherd biology into a data-first discipline through reproducible, scalable, and sharable experimentation. We run a suite of programs that work in conjunction to develop automated wet-lab experimental methods accessible to the community, collect large-scale public protein engineering datasets, and benchmark predictive and generative protein design algorithms. All our work is community-driven, collaborative, and operates under open science principals.

3:40 KEYNOTE PRESENTATION: Generation of High-Quality Aggregation Propensity Datasets for Machine Learning by Deep Mutational Scanning and an *in vivo* Assay
David J. Brockwell, PhD, Professor, School of Molecular and Cellular Biology, University of Leeds
A key requisite of any machine learning campaign is the availability of large volumes of high-quality training data that reports on the property to be predicted. Here we show that a tripartite beta-lactamase assay previously used by our group as a directed evolution screen can be reconfigured into a deep mutational screening format, providing datasets that can subsequently be used to train predictive models for different biophysical properties.

4:10 Sponsored Presentation *(Opportunity Available)*

HIGH-THROUGHPUT EXPERIMENTATION

4:40 FEATURED PRESENTATION: High-Throughput Data Generation and Experimental Validation
Gabriel J. Rocklin, PhD, Assistant Professor, Pharmacology, Northwestern University
All proteins continuously fluctuate between different conformational states according to the energies of these states and the barriers between them. Even rare, high-energy states can have large impacts on protein function, aggregation, immunogenicity, and more. These high-energy states are challenging to observe and have never been examined at scale. Using a new high-throughput approach, we quantified protein energy landscapes for 5,000 domains and applied these data to guide protein engineering.

5:10 High-Throughput Screens to Validate Model Performance
Amir P. Shanehsazzadeh, Artificial Intelligence Scientist, Absci Corp.
Several *in silico* metrics have been proposed as a means of assessing antibody design strategies. While these metrics have been utilized to evaluate and benchmark models, there has been little *in vitro* validation to determine the validity of such metrics. We showcase experiments designed to assess whether or not ranking antibodies by these metrics increases binding rates or binding affinities.

5:40 Close of Day

THURSDAY, JANUARY 16

7:45 am Registration and Morning Coffee

PLENARY KEYNOTE SESSION

8:15 Chairperson's Remarks
M. Frank Erasmus, PhD, Head, Bioinformatics, Specifica, an IQVIA business

8:20 Transforming Therapeutic Protein Engineering
Marissa Mock, PhD, Senior Research Director, Amgen Inc.
Generative biology is an emerging discipline that integrates artificial intelligence (AI) and machine learning (ML) with advanced life science technologies. The application of generative biology to protein engineering is accelerating the discovery and design of complex proteins with therapeutic potential—and, maximizing the benefits of these novel technologies will require seamless integration of both wet- and dry-laboratory technologies.

8:50 Session Break

DATASET TRAINING FOR SPECIFIC MODELS AND EXPERIMENTS

8:55 Chairperson's Remarks
Bismark Amofah, PhD, Senior Scientist, Biologics Engineering, AstraZeneca

9:00 Training Data Requirements for Antibody-Antigen Binding Affinity Prediction under Multiple Circumstances
Alissa Hummer, PhD, Postdoctoral Researcher, Biochemistry, Stanford University
Antibodies are an important class of medicines, whose efficacy is driven by specific target binding. Given the therapeutic relevance, there have been multiple attempts to predict antibody-antigen binding affinity computationally. I will discuss our findings on how training data influences the success and selection of machine learning strategies to tackle this challenge, ranging from antigen-specific to generalizable and zero-shot affinity prediction.

9:30 Enhanced Prediction of Protein-Protein Interface Structure via Augmentation with *in vitro* Affinity Data

David Noble, Data Scientist II, A Alpha Bio Inc.

The structural complex of a PPI can yield important mechanistic insights that support drug discovery efforts. Predictive models such as AlphaFold multimer remain poor quality for difficult but clinically significant systems. Here we present AFInjection, a framework for generating and incorporating *in vitro* experimental data simulating coevolution to AlphaFold to significantly improve complex prediction. We demonstrate the utility of this method on antibody-antigen systems and weak PPIs with disordered regions.

10:00 Sponsored Presentation *(Opportunity Available)*

10:30 Coffee Break in the Exhibit Hall with Poster Viewing

11:00 HT Developability Analysis to Support Model Training

Bismark Amofah, PhD, Senior Scientist, Biologics Engineering, AstraZeneca

Classic developability assays are low-medium throughput and require complex reagent generation. The large, normalized datasets required for ML tool building require adapting or replacing these assays with ones amenable to high throughput automation. We describe our process and results for validating replacement HT developability assays and a HT developability package compatible with very early HT screening.

11:30 Interactive Breakout Discussions

Internal Data Generation and Curation

Kevin Metcalf, PhD, Associate Principal Scientist, Merck & Co., Inc.

- Amplification strategies
- Avoiding bias
- Closed-loop experimentation
- Controls and validation
- Dealing with skewed data
- Historical data

Machine Learning in Biologic Drug Discovery: Leveraging External Data Sources

David Noble, Data Scientist II, A Alpha Bio Inc.

- Quality: Diversity, leakage, reproducibility, quality vs. quantity
- Collaborative data generation: Industry-academia partnerships, data sharing consortia
- Federated learning: Technical challenges, open-source foundation models
- Intellectual property: Data ownership, balancing openness with commercial interests
- Open-source data: Curation quality, integrating diverse sources with proprietary data

12:30 pm Session Break

12:40 Luncheon Presentation *(Sponsorship Opportunity Available)* **or Enjoy Lunch on Your Own**

1:10 Ice Cream & Cookie Break in the Exhibit Hall with Last Chance for Poster Viewing

DATASET GENERATION AND CURATION

2:00 Chairperson's Remarks

Geraldene Munsamy, PhD, Senior Scientist, Deep Learning, Basecamp Research Ltd.

2:05 Improving AlphaFold2 Performance with a Global Metagenomic & Biological Data Supply Chain

Geraldene Munsamy, PhD, Senior Scientist, Deep Learning, Basecamp Research Ltd.

Scaling laws estimate over a trillion species exist, yet less than 0.00001% have been studied. Powered by a global metagenomic data supply chain, BaseFold offers improved protein structure prediction with increased accuracy, achieving up to 80% reductions in RMSD values. Leading to more reliable predictions, better docking results, and advancements in therapeutic development, all while incentivizing biodiversity protection.

2:35 Curation Strategies for R&D Pipeline Data

Kevin Metcalf, PhD, Associate Principal Scientist, Merck & Co., Inc.

Model-based prediction of biologics developability properties will increase speed to clinic. Previous pipeline program data is a valuable data source for training models but requires data curation, contextualization, annotation, and quality control for this new use. I will describe how we incorporated historical data using data quality control protocols to create reusable data products for machine learning prediction of key attributes, including hydrophobicity and polyspecificity of monoclonal antibodies.

3:05 ML Models for Nanobody Developability trained on a Purpose-Built Multi-Readout Dataset

Samuel Demharter, PhD, Senior Data Scientist, Discovery Data Science and Protein Science & Technologies, Genmab

The biophysical characterisation of biologics requires significant wet-lab resources. To enable large-scale predictions of millions of molecules, protein-language models have become an attractive proposition to accurately predict lab readouts. However, current machine-learning models are limited in accuracy largely due to lack of high-quality and high-volume training data. In this talk, we present the generation of a maximally informative dataset for the purpose of training machine-learning models for nanobody developability predictions.

3:35 A Machine Learning-Driven Approach for Multi-Parametric Optimization of T Cell Engagers

Winston Haynes, PhD, Head, Data Science & Machine Learning, LabGenius Ltd.

T cell engagers (TCEs) promise breakthroughs in the treatment of solid tumors, but their progression in the clinic is limited by on-target, off-tumor toxicity. In this talk, I describe how our platform integrates active learning, automation, and high-throughput functional assays to efficiently identify highly selective and potent TCEs. I highlight our utilization of the design-build-test-learn ecosystem to generate high-quality data that powers our machine learning models and therapeutic assets.

4:05 Close of BioLogic Summit

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