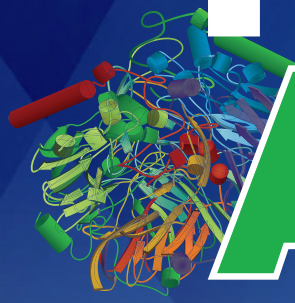
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THE PROTEIN SCIENCE AND PRODUCTION WEEK

THIRD ANNUAL

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PEGS AI SUMMIT



JANUARY 18 - 21, 2027

NEW VENUE

OMNI LA COSTA RESORT & SPA
CARLSBAD, CA
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Reinventing Biologic Drug Development with AI-Guided Design

EVENT-AT-A-GLANCE

JANUARY 19 - 20

- Driving *de novo* Design of Biologics
- AI-Powered Drug and Target Discovery

JANUARY 20 - 21

- Predicting Developability and Optimization Using AI
- Computational Models for Advancing Biologics

2027 PLENARY AND KEYNOTE SPEAKERS



Vanessa Braunstein
Eli Lilly and Company



Kristine Deibler, PhD
Novo AS



Jeffrey J. Gray, PhD
Johns Hopkins University



Gevorg Grigoryan, PhD
Generate Biomedicines



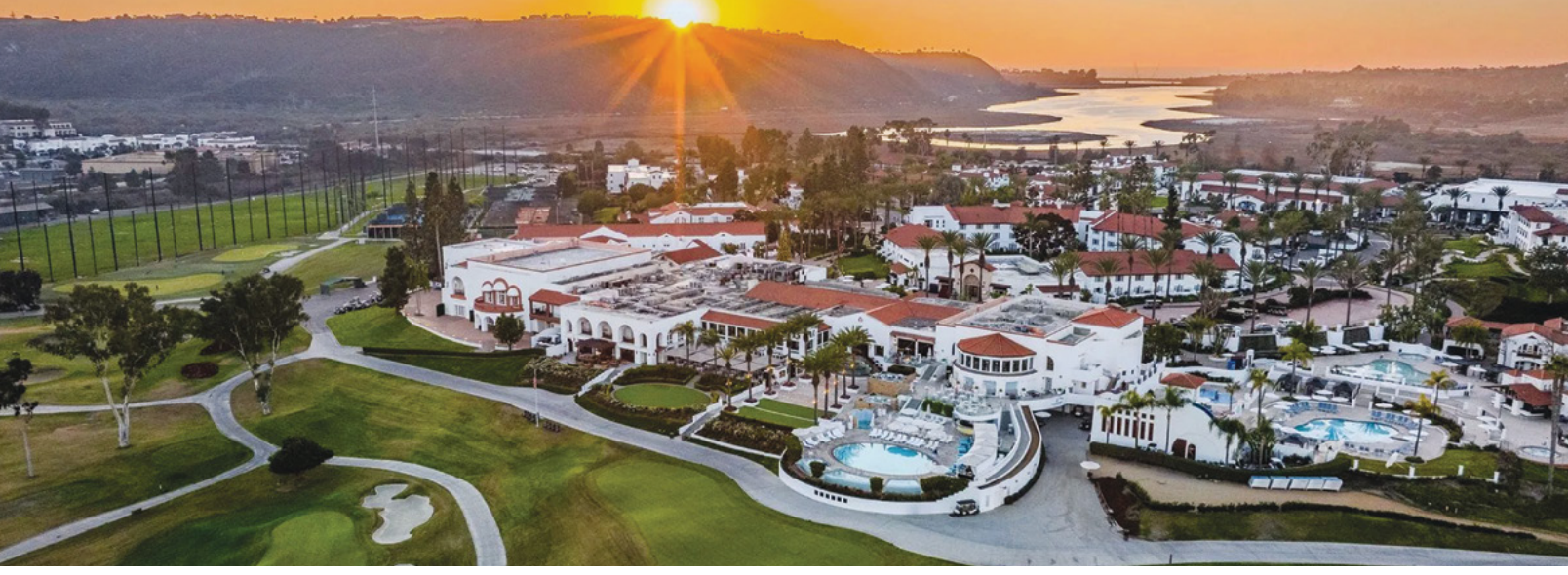
Sergey Ovchinnikov, PhD
Massachusetts Institute of Technology



Samuel Stanton, PhD
Anthropic
Coefficient Bio



Andrew Watkins, PhD
Genentech



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Training SEMINARS
By Cambridge Healthtech Institute

MONDAY, JANUARY 18, 2027 | 8:30 am - 5:00 pm

All training seminars take place in-person only

TS6A: AI-Driven Design of Biologics: A Hands-On Guide to Using State-of-the-Art ML Protein Models

Instructor:

David P. Nannemann, PhD, Vice President, Rosetta Commons Foundation

Since 2021, artificial intelligence models have revolutionized AI-driven biologics development, enabling breakthroughs in structure prediction, sequence design, and protein engineering. This course equips researchers and professionals with the expertise to leverage cutting-edge tools for structure prediction (AlphaFold, ImmuneBuilder), protein engineering with protein language models (ESM, AntiBERTy) and structure-based design (ProteinMPNN and RFDiffusion). Through a blend of lectures and hands-on exercises, participants will learn best practices for tool selection, method optimisation, and design selection. By exploring real-world applications and emerging techniques, such as BindCraft and RFAntibody, attendees will gain a practical understanding of performance capabilities, limitations, and effective workflows.

To ensure a cohesive and focused learning environment, moving between conference sessions and the training seminars is not allowed.

TS7A: Immunogenicity of de novo and Generatively Designed Biologics

Instructors:

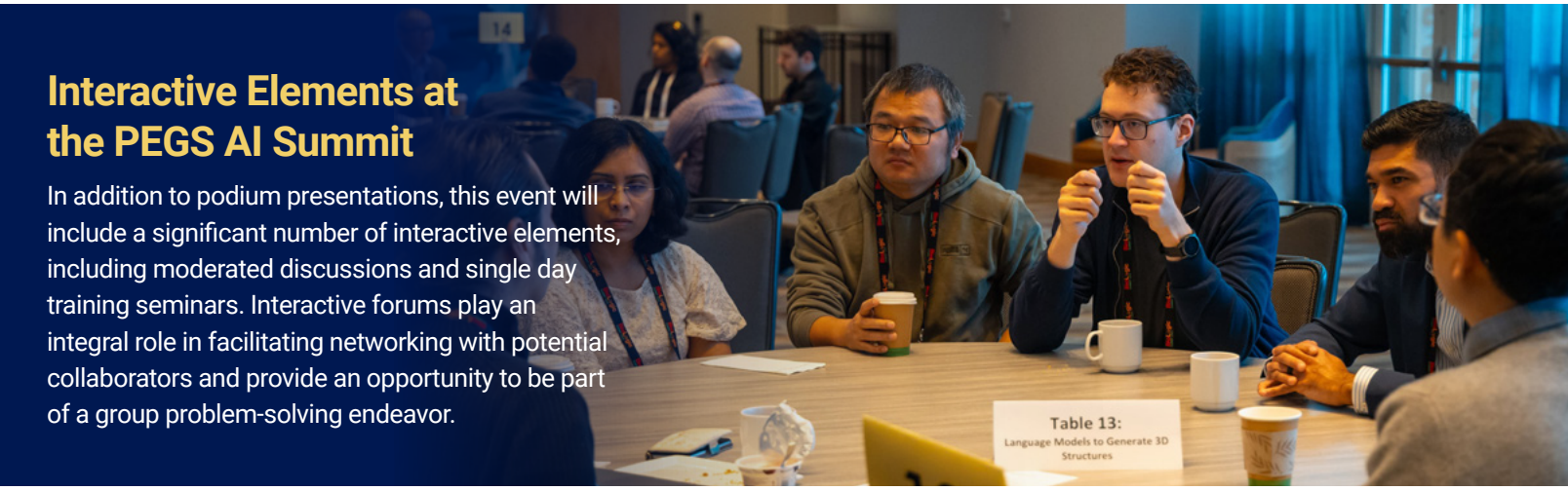
Timothy Hickling, PhD, Consultant, Quasor Ltd; CSO, Open Immune

Daniel Leventhal, PhD, Principal Consultant, Tactyl

This full day training seminar will explore the immunogenicity challenges associated with *de novo* and generatively designed biologics, with particular emphasis on how novel sequences, structures, and formats may create risks that differ from conventional proteins. The course will review key immunogenicity principles, including innate and adaptive immune responses, MHC II presentation, T cell activation, antibody formation, structural novelty, aggregation, and product related factors. Participants will examine current approaches for predicting and reducing immunogenicity, including *in silico* tools, AI and machine learning models, deimmunization strategies, and integration of immunogenicity assessment into generative design and candidate selection. The seminar will also consider appropriate preclinical validation strategies, including HLA binding and cellular assays, and how testing approaches may need to adapt to novel scaffolds and mechanisms. Examples and regulatory considerations will illustrate how computational, experimental, developability, product quality, and clinical evidence can be combined to support informed development decisions and translation.

Interactive Elements at the PEGS AI 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.



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26th Annual

PepTalk

The Protein Science and Production Week

January 18-21, 2027 | Carlsbad, CA, North County San Diego, CA + Virtual

Omni La Costa Resort & Spa

De novo Design of Biologics

Creating Antibodies, Complex Formats, Peptides, and Mini Proteins *in silico*

TUESDAY, JANUARY 19

7:30 am Registration and Morning Coffee

ROADMAP FOR PROTEIN DESIGN: Designing with Purpose and Function

8:30 Organizer's Remarks

Christina Lingham, Fellow & Executive Director, Conferences, Cambridge Healthtech Institute

8:35 Chairperson's Remarks

Monica L. Fernandez-Quintero, PhD, Associate Professor, Department of Microbiology and Immunology, Novo Nordisk Foundation Initiative for Vaccines and Immunity (NIVI)



8:40 FEATURED PRESENTATION: Beyond the Frontier: Unlocking Real-World Portfolio Impact with AI for Molecule Drug Discovery

Franziska Seeger, PhD, Senior Director, AI for Drug Discovery, Genentech Inc.

Generative AI promises breakthroughs, yet highest impact often comes from pragmatic approaches: functional modeling, format prediction, and systematic workflows. Drawing on antibody engineering, complex formats, and *de novo* efforts, we explore methods delivering measurable portfolio impact. Where do frontier methods excel versus simpler approaches? How do we bridge computation and validation? Core insight: impact requires not just better algorithms, but integration of data, models, and portfolio strategy.

9:10 Predicting Heavy-Light Chain Compatibility for Antibody Engineering and Design

Franca Fraternali, PhD, Head & Professor, Bioinformatics & Computational Biology, University College London

Antibody diversity is traditionally viewed as arising from combinatorial heavy-light chain pairing, yet the extent to which this process is truly random remains unclear. I will present ImmunoMatch, a language-model–based framework that learns the sequence determinants of heavy-light chain compatibility. By uncovering the molecular grammar of antibody assembly, ImmunoMatch provides a quantitative compatibility score with applications in antibody discovery, repertoire analysis, and the design of next-generation of antibody therapeutics.

9:40 Lessons from *de novo* Design of Antibodies: Benchmarks, Inflection Points, and Common Failure Modes

Roberto Spreafico, PhD, Senior Director, Biologics AI Innovation, AstraZeneca

De novo antibody design is maturing, yet uneven. I'll share lessons from multiple campaigns—hit rates, epitope-to-epitope variability, and methodological biases—anchored by the critical need for standardized benchmarks. We'll examine metrics: which truly predict success and which mislead. I'll highlight inflection points for success rate and emphasize needs beyond binding—robust expression and minimized aggregation—to translate computational promise into developable therapeutics.

10:10 Sponsored Presentation *(Opportunity Available)*

10:40 Grand Opening Coffee Break in the Exhibit Hall with Poster Viewing

11:20 *De novo* Design of a Peptide Modulator to Reverse Sodium Channel Dysfunction Linked to Cardiac Arrhythmia and Epilepsy

Ryan Mahling, PhD, Postdoctoral Fellow, Department of Physiology and Cellular Biophysics, Columbia University

Gain-of-function defects in sodium channel (Na_v) function underlie numerous diseases ranging from cardiac arrhythmia to epilepsy. Despite intense effort, engineering synthetic modulators that precisely tune Na_v function remains challenging. Through computational protein design we have engineered a *de novo* peptide modulator, ELIXIR, that targets these disease-linked deficits in Na_v function. Our findings highlight the potential utility of *de novo* protein design for the rational development of ion channel modulators.

11:50 Efficient Generation of Epitope-Targeted *de novo* Antibodies with Germinal

Xiaojing J. Gao, PhD, Assistant Professor, Chemical Engineering, Stanford University

When we engineer proteins for human applications, it is common to simultaneously optimize for multiple objectives. Such tasks are cumbersome or even impossible with conventional experimental approaches. I will share two ML/AI-enabled examples, one to create antibody-like binders, and the other to remove potentially immunogenic peptides from biologics.

12:20 pm Transition to Lunch

12:25 Luncheon Presentation *(Sponsorship Opportunity Available)* **or Enjoy Lunch on Your Own**

12:55 Refreshment Break in the Exhibit Hall with Poster Viewing

LEARNING FROM NATURE: AI-Driven Mining of Immune Repertoires

1:25 Chairperson's Remarks

Victor Greiff, PhD, Professor, University of Oslo; CTO, IMPRINT

1:30 A Community Challenge to Benchmark Machine Learning Methods for Adaptive Immune Profiling

Victor Greiff, PhD, Professor, University of Oslo; CTO, IMPRINT

We organized the first community challenge to benchmark ML approaches on two central repertoire-analysis tasks: predicting immune state from labelled repertoires (a diagnostic use case) and recovering immune-state-associated receptors (a therapeutic discovery use case), using approximately 75,000 experimentally generated and biologically realistic simulated T-cell receptor repertoires.

2:00 Revised Adaptive Immune Receptor Data in the Immune Epitope Database

Lonneke Scheffer, PhD, Postdoctoral Researcher, Computational Immunology, La Jolla Institute for Immunology

The Immune Epitope Database (IEDB) curates experimentally defined immune epitopes and their associated T and B cell receptors, currently comprising ~185,000 TCRs and ~5,000 antibodies with validated specificity. We applied a standardization and validation pipeline to the full receptor dataset, correcting nomenclature and sequence delimitation inconsistencies. The resulting harmonized dataset is ready to use for bioinformatics applications, including immune repertoire annotation and machine learning-based receptor specificity prediction.

2:30 Repertoire-Scale Antibody Structural Prediction Informs Therapeutic Design

Yi Shi, PhD, Associate Professor, Protein Engineering, Icahn School of Medicine, Mount Sinai

AF3-TurboAb enables repertoire-scale antibody–antigen structural decoding by removing preprocessing bottlenecks and supporting rapid, near-experimental complex modeling on a single GPU. Applied to immunization-derived antibody repertoires, it substantially expands the current antibody structural landscape, revealing unmapped epitopes, affinity hotspots, and convergent binding solutions. These insights guide durable multiepitope neutralizer design, cancer checkpoint binder discovery, real-time binder triage, and multivalent engineering for challenging biomedical applications.

3:00 Sponsored Presentation *(Opportunity Available)*

3:30 Refreshment Break in the Exhibit Hall with Poster Viewing

De novo Design of Biologics

Creating Antibodies, Complex Formats, Peptides, and Mini Proteins *in silico*

PLENARY KEYNOTE SESSION

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Christina Lingham, Fellow & Executive Director, Conferences, Cambridge Healthtech Institute

4:20 Chairperson's Remarks
Kristine Deibler, PhD, Director, Molecular Artificial Intelligence, Novo AS

4:25 FIRESIDE CHAT: AI's Real Impact on Biologic Drug Discovery: The Honest Scorecard






Moderator: Kristine Deibler, PhD, Director, Molecular Artificial Intelligence, Novo AS
AI promises faster discovery, better molecules, and smarter decisions, but how much measurable progress has actually been made? This candid discussion will separate genuine advances from inflated expectations and explore where AI is beginning to transform drug discovery.
Panelists:
Vanessa Braunstein, Senior Director, TuneLab AI Drug Discovery Platform, Eli Lilly and Company
Gevorg Grigoryan, PhD, Co-Founder & CTO, Generate Biomedicines
Andrew Watkins, PhD, Senior Director, Structure and Simulation, AI for Drug Discovery, Prescient Design, Genentech

5:25 Networking Reception in the Exhibit Hall with Poster Viewing

WOMEN IN AI MEET-UP IN THE EXHIBIT HALL

Women in AI Meet-Up
Kristine Deibler, PhD, Director, Molecular Artificial Intelligence, Novo AS
Franziska Seeger, PhD, Senior Director, AI for Drug Discovery, Genentech Inc.

6:25 Close of Day

WEDNESDAY, JANUARY 20

8:00 am Registration and Morning Coffee

DE NOVO DESIGN OF BIOLOGICS

8:30 Chairperson's Remarks
Franziska Seeger, PhD, Senior Director, AI for Drug Discovery, Genentech Inc.

8:35 The Next Era of Drug Discovery: *De novo* Design of Biologics
Anna Vangone, PhD, Director of AI/ML Large Molecule for Drug Discovery, Computational Science Center of Excellence, Roche/Genentech
The paradigm of biologics discovery is fundamentally shifting from discovering what exists in nature to designing what is required in the clinic. This presentation explores how generative AI enables the *de novo* creation of novel therapeutic proteins with tailored functionalities, discussing the current breakthroughs and future landscape of this revolution.

9:05 *De novo* Design of Miniproteins Targeting GPCRs
Green Ahn, PhD, Assistant Professor, Chemistry, University of Washington
We designed *de novo* proteins that engage endogenous internalizing receptors for cell-type-specific degradation and delivery of protein-based nanocages. To further enhance the precision of designed proteins, we sought to program selective responsiveness to native environmental cues. Together, these efforts establish a foundation for employing molecular engineering and ML-driven protein design to create precision molecules that reprogram cellular processes.

9:35 PANEL DISCUSSION: Quality Metrics and Standards in the *de novo* Design Space
Moderator: Franziska Seeger, PhD, Senior Director, AI for Drug Discovery, Genentech Inc.
- Preprints or tech reports, claiming performance of *de novo* models, different data sets, different levels of validation.
- CryoEM complex structures- gold standard of *de novo* design.
- No clear standard of what goes into training data, are you mimicking known info?
- Are you having truly *de novo* sequences?

Panelists:
Green Ahn, PhD, Assistant Professor, Chemistry, University of Washington
Anna Vangone, PhD, Director of AI/ML Large Molecule for Drug Discovery, Computational Science Center of Excellence, Roche/Genentech

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De novo Design of Biologics

Creating Antibodies, Complex Formats, Peptides, and Mini Proteins *in silico*

10:05 Presentation to be Announced

A-ALPHA BIO

10:35 Coffee Break in the Exhibit Hall with Poster Viewing

SPEED NETWORKING IN THE EXHIBIT HALL

Speed Networking
Kevin Brawley, Project Manager, Production Operations & Communications, Cambridge Innovation Institute

KEYNOTE SESSION

11:00 Chairperson's Remarks
Monica L. Fernandez-Quintero, PhD, Associate Professor, Department of Microbiology and Immunology, Novo Nordisk Foundation Initiative for Vaccines and Immunity (NIVI)



11:05 Applying Frontier Models and LLMs to Biologic Discovery and Design
Samuel Stanton, PhD, Member, Technical Staff, Anthropic; Co-Founder, Coefficient Bio
Machine learning models have evolved from specialized prediction tools to general purpose assistants for the entire research lifecycle. LLMs have encyclopedic recall of documented public knowledge and competently execute well-defined mechanical workflows involving specialized tools. Frontier human-AI collaboration has shifted to distilling tacit knowledge, uncovering errors in theories and data, and improving observatory instrumentation. The result is not the complete automation of science, but a more ambitious vision of its future.



11:35 When Proteins Become Code: Generative AI for Programmable Medicines
Gevorg Grigoryan, PhD, Co-Founder & CTO, Generate Biomedicines
Proteins are biology's actuators, and generative AI is making them programmable. This talk explores why protein structure is learnable, how models can translate biological intent into novel molecules, and why models alone are insufficient. Programmable medicines require coupling generation with hypothesis-driven experimentation at scale and integrating drug development into a continuous learning system. Drawing on Generate Biomedicines' experience, I will show how this approach is reaching the clinic.



12:05 pm Using AI for Protein Structure Modeling and Design
Sergey Ovchinnikov, PhD, Helen and Irwin Sizer Career Development Professor, Department of Biology, Massachusetts Institute of Technology (MIT)
In this talk, I'll describe the latest advancements in predicting protein structure and contacts using MSA pairformer and ProteinEBM. I'll show evidence that the first model can go beyond a single static structure, while the latter model can generalize outside of evolutionary space for variant effect prediction and design.

12:35 PANEL DISCUSSION: Q&A with Keynotes







Moderator: Monica L. Fernandez-Quintero, PhD, Associate Professor, Department of Microbiology and Immunology, Novo Nordisk Foundation Initiative for Vaccines and Immunity (NIVI)
Panelists:
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Samuel Stanton, PhD, Member, Technical Staff, Anthropic; Co-Founder, Coefficient Bio
Masatoshi Uehara, PhD, Member, Technical Staff, OpenAI

1:05 Transition to Lunch

1:10 Luncheon Presentation *(Sponsorship Opportunity Available)* **or Enjoy Lunch on Your Own**

1:40 Refreshment Break in the Exhibit Hall with Poster Viewing

2:00 Close of *De novo* Design of Biologics Conference



AI-Powered Drug and Target Discovery

Turning AI, Data, and Biology into Faster Discovery Decisions

TUESDAY, JANUARY 19

7:30 am Registration and Morning Coffee

TRANSFORMING BIOLOGICS DISCOVERY IN THE ERA OF AI

8:30 Organizer's Remarks

Daniel Barry, Senior Conference Director, Cambridge Healthtech Institute

8:35 Chairperson's Remarks

Qing Chai, PhD, Assistant Vice President, Computational Science, Biotechnology Discovery Research, Eli Lilly and Company

8:40 Using Antibody Language Models to Reverse-Translate Disease Resilience into Novel Drugs and Drug Targets

Jake D. Galson, PhD, Vice President, Technology, Alchemab Therapeutics

Traditional antibody discovery starts with a hypothesised target and hopes it matters in patients. Alchemab inverts this: we start with disease-resilient individuals, and then train language models on their antibody repertoires to find the protective antibodies and deconvolute the targets they recognise. This AI-led process surfaces novel targets and therapeutics in one step and is now validated by a clinical candidate for ALS advancing through Phase 1.

9:10 Closing the Loop: Building the Infrastructure, Models, and Automated Labs for AI-First Biologics

Simon Chell, PhD, Vice President, Biologics Engineering, AstraZeneca

What does it take to embed AI in large molecule drug discovery at scale? We explore the infrastructure required, from fit-for-purpose data foundations and prospective validation of ML models to automated laboratories that complete the design, make, test cycle in days rather than months. We also examine the practical challenges of scaling data and AI capabilities globally, including compute infrastructure, organizational complexity and deploying the right digital tools.



9:40 FEATURED PRESENTATION: Transforming Biologics Discovery in the Era of AI

Athena Hadjixenofontos, PhD, Director, Data Science & Head of AI/ML, Biotherapeutics and Genetic Medicines, Discovery Research, AbbVie

Combining the capabilities of a leading antibody-discovery organization with cutting-edge machine learning unlocks transformative opportunities in biotherapeutics discovery. At AbbVie, we are embedding predictive models directly into scientific workflows, enabling programs to progress faster through stage gates, while also making better medicines by exploring previously inaccessible sequence space and targets. We will share the principles that guide the building of this powerful discovery engine, and the successes that follow.

10:10 Presentation to be Announced

Dalton™

10:40 Grand Opening Coffee Break in the Exhibit Hall with Poster Viewing

IDENTIFYING AND UNLOCKING CHALLENGING TARGETS

11:20 Leveraging Single-Cell Sequencing to Identify Highly Precise Single and Combination T Cell Engager Targets

Alexander J. Martinko, PhD, Senior Director, Antibody Engineering & Design, Cartography Biosciences Inc.

T cell engagers (TCEs) hold promise for solid tumors, but progress is limited by the scarcity of targets that combine potency with safety. Cartography's ATLAS and SUMMIT platforms integrate single-cell RNA sequencing and AI-powered therapeutic design to identify highly precise single and paired targets and build TCEs that exploit those target opportunities. Using this approach, we advanced CBI-1214 into the clinic and are extending it to multispecific, AND-gated TCEs.

11:50 Unlocking Challenging Targets: Drug Discovery via Immune Repertoire Analysis

Yulei Zhang, PhD, Senior Advisor, Eli Lilly and Company

Antibody discovery against difficult targets is bottlenecked by the throughput of conventional binding-based screens. Exhaustively testing candidate clones is impractical. We developed an antigen-agnostic approach that prioritizes antibodies directly from repertoire sequencing data, without requiring a preliminary binding assay. Across multiple discovery campaigns the method enriched for hits over baseline selection, and enabled discovery against membrane proteins. These results demonstrate that NGS-driven clone prioritization can be applied to antibody discovery.

12:20 pm Transition to Lunch

12:25 Luncheon Presentation to be Announced

TWIST BIOSCIENCE

12:55 Refreshment Break in the Exhibit Hall with Poster Viewing

1:25 Chairperson's Remarks

Björn L. Frendeus, PhD, CSO, BioInvent International AB

1:30 Computationally Solubilized Antigens for Functional Antibody Discovery against Membrane-Obligate Targets

Arvind Sivasubramanian, PhD, Director, Computational Biology & Platform Technologies, Adimab LLC

Membrane-Obligate Targets (MOTs) require the cell membrane for native protein folding and expression, creating challenges for the discovery and optimization of functional antibody-based therapeutics. Recent advances in the computational design of membrane protein analogs have opened up new approaches in this space. Herein, we discuss discovery and optimization of functional antagonist and agonist antibodies against membrane-obligate targets using computationally solubilized antigens.

2:00 AI-Designed Radiopharmaceuticals: Going After Difficult Targets

Jake Kraft, PhD, Co-Founder & CEO, Lila Biologics, Inc.

Radioligand therapy (RLT) targets radionuclides to cancer cells to induce DNA damage and cell death. Lila Bio uses AI to design best-in-class *de novo* minibinder-based RLTs for hard-to-drug targets inaccessible to small molecules or peptides. Its lead program targets avß6 integrin, and a collaboration with Eli Lilly on undisclosed solid tumor targets highlights the strength of its AI-driven design platform to create RLTs with compelling profiles for challenging targets.

2:30 Accelerate Early-Stage Drug Discovery with a First-of-Its-Kind Collaborative Platform

Vanessa Braunstein, Senior Director, TuneLab AI Drug Discovery Platform, Eli Lilly and Company

Hao Zheng, Senior Director, AI/ML Product Lead, Eli Lilly

Lilly TuneLab is a first-of-its-kind collaborative AI/ML drug discovery platform created by Eli Lilly and Company to accelerate biotech innovation by enabling participating companies to access models trained on decades of Lilly's proprietary research data, representing research on hundreds of thousands of unique molecules. Learn how member companies are using the models in their workflows and contributing data via privacy-preserving federated learning to make the models more generalizable.

3:00 Presentation to be Announced

GINKGO DATAPOINTS

3:30 Refreshment Break in the Exhibit Hall with Poster Viewing

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Women in AI Meet-Up
Kristine Deibler, PhD, Director, Molecular Artificial Intelligence, Novo AS
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6:25 Close of Day

WEDNESDAY, JANUARY 20

8:00 am Registration and Morning Coffee

AGENTIC AI AND CO-SCIENTISTS

8:30 Chairperson's Remarks
Arvind Sivasubramanian, PhD, Director, Computational Biology & Platform Technologies, Adimab LLC

8:35 Robin: A Multi-Agent System for Automating Scientific Discovery
Samuel Rodriques, CEO, FutureHouse
Robin is a multi-agent AI system that automates both hypothesis generation and data analysis in experimental biology, combining literature-search and data-analysis agents to iteratively propose, test, and refine hypotheses. Applied to dry age-related macular degeneration, it identified ripasudil and KL001 as candidates that boost retinal pigment epithelium phagocytosis, then designed a follow-up RNA-seq study revealing ABCA1, a lipid-efflux gene, as a potential new target—demonstrating autonomous, lab-in-the-loop scientific discovery.

9:05 Advancing Drug Discovery, Science, and Medicine with Collaborative AI Agents
Vivek Natarajan, AI Researcher, Google Deepmind Inc
Co-Scientist is a Gemini-based multi-agent AI system designed for structured scientific reasoning, generating novel, testable research hypotheses from a given objective and existing evidence. Agents iteratively propose, critique, and refine ideas through a tournament-style evolution process, with quality improving as test-time compute scales. Validated across drug repurposing, target discovery, and antimicrobial resistance, Co-Scientist identified new repurposing candidates and synergistic combination therapies for acute myeloid leukaemia, confirmed via *in vitro* experiments.

9:35 Biomni: A General-Purpose Biomedical AI Agent
Kexin Huang, PhD, Co-Founder & CEO, Phylo Inc.
Biomedical research is slowed by fragmented workflows. We introduce Biomni, a general-purpose AI agent that autonomously executes research tasks. Its action-discovery agent mines tools, databases, and protocols from thousands of publications across 25 domains, integrating LLM reasoning, retrieval-augmented planning, and code execution to compose workflows. Benchmarks show generalization across gene prioritization, drug repurposing, rare-disease diagnosis, microbiome analysis, and molecular cloning, with studies in multi-modal data, protein design, and lab automation.

10:05 PANEL DISCUSSION: Talk Title to be Announced ENPICOM
Moderator: Speaker to be Announced, ENPICOM

10:35 Coffee Break in the Exhibit Hall with Poster Viewing

SPEED NETWORKING IN THE EXHIBIT HALL

Speed Networking
Kevin Brawley, Project Manager, Production Operations & Communications, Cambridge Innovation Institute

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1:40 Refreshment Break in the Exhibit Hall with Poster Viewing

2:00 Close of AI-Powered Drug and Target Discovery Conference





Predicting Developability and Optimization Using AI

At the Inflection Point for Biologics

WEDNESDAY, JANUARY 20

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Sergey Ovchinnikov, PhD, Helen and Irwin Sizer Career Development Professor, Department of Biology, Massachusetts Institute of Technology (MIT)
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12:35 PANEL DISCUSSION: Q&A with Keynotes







Moderator: Monica L. Fernandez-Quintero, PhD, Associate Professor, Department of Microbiology and Immunology, Novo Nordisk Foundation Initiative for Vaccines and Immunity (NIVI)
Panelists:
Gevorg Grigoryan, PhD, Co-Founder & CTO, Generate Biomedicines
Sergey Ovchinnikov, PhD, Helen and Irwin Sizer Career Development Professor, Department of Biology, Massachusetts Institute of Technology (MIT)
Samuel Stanton, PhD, Member, Technical Staff, Anthropic; Co-Founder, Coefficient Bio
Masatoshi Uehara, PhD, Member, Technical Staff, OpenAI

1:00 Registration Open

1:40 Refreshment Break in the Exhibit Hall with Poster Viewing

FROM PREDICTION TO AUTONOMOUS OPTIMIZATION: AI Systems that Design, Test, Improve Antibodies

2:25 Chairperson's Remarks
M. Frank Erasmus, PhD, Head, Bioinformatics, Specifica, an IQVIA business

2:30 Prediction of Antibody Non-Specificity Using Protein Language Models
Laila Sakhnini, PhD, Principal Scientist, Biophysics & Injectable Formulation, Novo AS
Nonspecific binding remains a major developability liability for therapeutic antibodies, with potential consequences for pharmacokinetics and safety. Reliable sequence-based prediction could support earlier decision-making, but remains challenging. Here, we present machine learning models based on protein language model embeddings and biophysical descriptors to predict antibody non-specificity. The models identify the VH domain, heavy-chain CDRs, and isoelectric point as key determinants, achieving up to 71% accuracy.

3:00 Protein Language Models for Antibody Developability, Prediction, and Optimization
Ye Wang, PhD, Principal Scientist, Machine Learning, Biogen
Protein language models provide a powerful framework for learning sequence–property relationships in antibodies, but their industrial reliability is underexplored. We evaluate state-of-the-art PLMs on internal data from numerous therapeutic programs across three developability assays (PSR, HIC, AC-SINS). Domain-adaptive fine-tuning consistently outperforms pretrained representations, and pretrained sequence likelihoods offer useful unsupervised risk signals. Together, these results show PLMs provide robust, complementary signals for early-stage antibody developability assessment and candidate selection.

3:30 Where AI Truly Optimizes Affinity Maturation, Benchmarked against a Proven *in vitro* Process
Hetu Kamichetty, PhD, CTO, Xaira Therapeutics
AI-driven antibody optimization is often developed in isolation, without experimental benchmarks, so apparent gains obscure real ones. With access to affinity maturation benchmarks for head-to-head evaluation, we investigate where AI can truly optimize existing experimental protocols, across novel target epitopes and distinct antibody backbones and paratopes. Automated curation builds training-ready datasets that continually fine-tune optimization models; variants are measured experimentally, so gains are confirmed and utilized for follow-up iterations.

4:00 Presentation to be Announced

4:15 3dpredict: Scalable High Quality Developability Predictions
Speaker to be Announced, Chemical Computing Group
Predicting potential liabilities, aggregation, viscosity etc. is of importance in monoclonal antibody development. Computational property prediction methods are routinely used in the selection and optimization of candidate antibodies. High quality property prediction involves prediction of ensembles of 3D structures at specified pH to reduce sensitivity to single conformational states. We present 3dpredict/Ab which calculates ensemble-based predictions of antibody developability descriptors and putative liabilities. 3dpredict/Ab allows for out-of-the-box SaaS automation and integration of such complex simulations of hundreds or thousands of sequences.

4:30 Refreshment Break in the Exhibit Hall with Poster Viewing

WOMEN IN SCIENCE MEET-UP IN THE EXHIBIT HALL

Women in Science Meet-Up
Deborah Moore-Lai, PhD, Vice President, Protein Sciences, ProFound Therapeutics

Predicting Developability and Optimization Using AI

At the Inflection Point for Biologics

5:10 Developability by Design: Integrating *in silico* and Experimental Data for Antibody Engineering

Lasse Møller Blaabjerg, PhD, Data Scientist, Discovery Data Science, Genmab

Developability plays a key role in modern antibody engineering but is costly and time-consuming to characterize in the lab. In this talk, we present a method for constructing datasets that are designed for training new machine learning models to predict features of antibody developability.

Interactive Breakout Discussions

5:40 Interactive Breakout Discussions

Interactive Breakout Discussions are informal, moderated discussions, allowing participants to exchange ideas and experiences and develop future collaborations around a focused topic. Each discussion will be led by a facilitator who keeps the discussion on track and the group engaged. To get the most out of this format, please come prepared to share examples from your work, be a part of a collective, problem-solving session, and participate in active idea sharing. Please visit the Interactive Breakout Discussions page on the conference website for a complete listing of topics and descriptions.

TABLE: What Constitutes True *de novo* Design vs. Optimization and Best Ways to Test/Characterize?

Monica L. Fernandez-Quintero, PhD, Associate Professor, Department of Microbiology and Immunology, Novo Nordisk Foundation Initiative for Vaccines and Immunity (NIVI)

- Overview of current tools
- Defining true *de novo* vs. optimization
- Best tests and metrics of design success
- Open challenges

TABLE: *De novo* Design: Commercial vs. Open-Source Options

Roberto Spreafico, PhD, Senior Director, Biologics AI Innovation, AstraZeneca

- Performance of commercial vs. open solutions: today and tomorrow
- Business motivations for picking commercial vs open solutions: beyond predictive performance
- In 5 years: towards a database of designed antibodies available off the shelf?
- Will *in silico* design replace or augment traditional wet-lab discovery? What is next?

6:40 Close of Day

THURSDAY, JANUARY 21

8:00 am Registration and Morning Coffee

DEVELOPABILITY OF COMPLEX FORMATS: Data, Methods, and Applications

8:35 Chairperson's Remarks

Norbert Furtmann, PhD, Head, Biologics AI & Design, Computational and AI Strategy, Sanofi

8:40 Conquering Huge Design Spaces: AI-Driven Developability for Next-Generation Biotherapeutics

Norbert Furtmann, PhD, Head, Biologics AI & Design, Computational and AI Strategy, Sanofi

Achieving developable multispecific antibody and NANOBODY therapeutics requires moving beyond retrospective assessment toward proactive, design-integrated prediction. We describe machine learning models for developability properties embedded into our multispecific design workflows. We discuss large-scale experimental campaigns underpinning these models, sharing insights on data strategy and model building. Project case studies illustrate how computational predictions translate into real design decisions, and we address the critical gaps that currently limit the field.

9:10 From VHHs to IgGs: Predicting and Engineering Antibody Developability

Peter M. Tessier, PhD, Albert M. Mattocks Professor, Pharmaceutical Sciences & Chemical Engineering, University of Michigan

Antibody developability reflects multiple coupled properties that are difficult to optimize simultaneously. We combine machine learning, antibody repertoire information, and experimental measurements to predict and engineer developability across VHH and IgG formats. Examples include identifying sequence and surface features that drive VHH aggregation, predicting IgG self-association and high-concentration behavior, and using conservative CDR germlining to improve biophysical properties while preserving affinity and function.

9:40 AI/ML-Enabled Developability Prediction for Antibody Therapeutics and Multi-Specifics

Olga Obrezanova, PhD, AI Principal Scientist, Biologics Engineering, Oncology R&D, AstraZeneca

We will present an overview of AI-enabled approaches for predicting developability for biologics including multi-specifics. The talk will touch on data foundations, modeling strategies, and workflow integration across biologics discovery, with selected examples showing how *in silico* methods can support design, chain pairing, lead optimization, and candidate selection while balancing efficacy, developability, and potential immunogenicity considerations.

10:10 PANEL DISCUSSION: Talk Title to be Announced

10:10 Sponsored Presentation *(Opportunity Available)*

10:40 Coffee Break in the Exhibit Hall with Poster Viewing

11:20 Generative Design for Multispecific Antibodies: From Monospecific Success to the Next Frontier

Surge Biswas, PhD, Founder & CEO, Nabla Bio, Inc.

Generative protein design now reliably produces *de novo* monospecific antibodies. This talk presents examples of zero-shot design and optimization of multispecific antibodies using generative models, and discusses what it will take to bring this same level of reliability to multispecific formats.

ADVANCING PHYSICS-BASED APPROACHES TO DEVELOPABILITY

11:50 Chairperson's Remarks

Andrew Buchanan, PhD, FRSC, Head of Discovery, Stealth Mode Biotech



11:51 KEYNOTE PRESENTATION: AI vs Physics for Protein Engineering

Jeffrey J. Gray, PhD, Professor, Chemical & Biomolecular Engineering, Johns Hopkins University; Director, Rosetta Commons

I will discuss the differences and complementarities of AI and physics approaches, sharing recent work extracting an energy function from AI methods, efforts toward data valuation and interpretability. We envision a future where AI methods can be combined with physics for powerful and interpretable biomolecular engineering.

12:20 pm Transition to Lunch

12:25 Luncheon Presentation to be Announced

UNCHAINED LABS

12:55 Ice Cream & Cookie Break in the Exhibit Hall with Last Chance for Poster Viewing

ADVANCING PHYSICS-BASED APPROACHES TO DEVELOPABILITY

1:40 Antibody Multi-objective Optimisation via Physics-based Empirical Approaches and Diffusion-Based Inverse Folding

Pietro Sormanni, PhD, Associate Professor & Royal Society University Research Fellow, Chemical Engineering, Imperial College London

Predicting Developability and Optimization Using AI

At the Inflection Point for Biologics

2:10 PANEL DISCUSSION: Advancing Physics-Based Approaches to Developability

Moderator: Andrew Buchanan, PhD, FRSC, Head of Discovery, Stealth Mode Biotech

- Where physics-based models add value
- What tools are being used day-to-day
- Cases where physics-based prediction has matched (or missed) wet-lab reality

Panelists:

Dan Cannon, PhD, Head of Biologics Modelling, Schrödinger

Pietro Sormanni, PhD, Associate Professor & Royal Society University Research Fellow, Chemical Engineering, Imperial College London

Roberto Spreafico, PhD, Senior Director, Biologics AI Innovation, AstraZeneca

NEW METHODS TO OLD PROBLEMS: New Approaches in ML

2:40 Chairperson's Remarks

Hunter Elliott, PhD, Vice President, AI/ML, BigHat Biosciences

2:41 Designing Deliverable Drugs: AI/ML for Gene Therapy and Small-Molecule Discovery

Rohit Singh, PhD, Research Scientist, Computer Science & AI Lab, Massachusetts Institute of Technology

Foundation models trained across protein and molecular data are reshaping how we design therapeutics, not merely predicting properties but optimizing them. I'll show how protein language models power two AI/ML efforts: Raygun, which miniaturizes and redesigns natural proteins to improve developability, and PRECISE, a structure-based platform for drug-target screening and engagement. Together they show how learned representations enable more efficient and effective gene therapy and lead discovery.

3:10 Automating Therapeutic Epitope Selection with Agentic AI Workflows

Cody Krivacic, PhD, Principal Scientist, Machine Learning & Computational Protein Design, GSK

Expert-driven epitope selection for *in silico* protein design is a major bottleneck in DMTA cycles. We introduce Epitope Mapper, a hybrid agentic pipeline that automates this step using focused agents with biological tools. It synthesizes literature, performs biophysical calculations, and proposes ranked epitopes that are consistent with human expertise. The system's suggestions can be steered by user-provided context, enabling large-scale protein design and accelerating fully automated end-to-end therapeutic discovery.

3:40 Close of Conference





Computational Models for Advancing Biologics

Turning Complex Data into Smarter Biotherapeutic Designs

WEDNESDAY, JANUARY 20

KEYNOTE SESSION

11:00 am Chairperson's Remarks
Monica L. Fernandez-Quintero, PhD, Associate Professor, Department of Microbiology and Immunology, Novo Nordisk Foundation Initiative for Vaccines and Immunity (NIVI)



11:05 Applying Frontier Models and LLMs to Biologic Discovery and Design
Samuel Stanton, PhD, Member, Technical Staff, Anthropic; Co-Founder, Coefficient Bio
Machine learning models have evolved from specialized prediction tools to general purpose assistants for the entire research lifecycle. LLMs have encyclopedic recall of documented public knowledge and competently execute well-defined mechanical workflows involving specialized tools. Frontier human-AI collaboration has shifted to distilling tacit knowledge, uncovering errors in theories and data, and improving observatory instrumentation. The result is not the complete automation of science, but a more ambitious vision of its future.



11:35 When Proteins Become Code: Generative AI for Programmable Medicines
Gevorg Grigoryan, PhD, Co-Founder & CTO, Generate Biomedicines
Proteins are biology's actuators, and generative AI is making them programmable. This talk explores why protein structure is learnable, how models can translate biological intent into novel molecules, and why models alone are insufficient. Programmable medicines require coupling generation with hypothesis-driven experimentation at scale and integrating drug development into a continuous learning system. Drawing on Generate Biomedicines' experience, I will show how this approach is reaching the clinic.



12:05 pm Using AI for Protein Structure Modeling and Design
Sergey Ovchinnikov, PhD, Helen and Irwin Sizer Career Development Professor, Department of Biology, Massachusetts Institute of Technology (MIT)
In this talk, I'll describe the latest advancements in predicting protein structure and contacts using MSA pairformer and ProteinEBM. I'll show evidence that the first model can go beyond a single static structure, while the latter model can generalize outside of evolutionary space for variant effect prediction and design.

12:35 PANEL DISCUSSION: Q&A with Keynotes







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Samuel Stanton, PhD, Member, Technical Staff, Anthropic; Co-Founder, Coefficient Bio
Masatoshi Uehara, PhD, Member, Technical Staff, OpenAI

1:00 Registration Open

1:40 Refreshment Break in the Exhibit Hall with Poster Viewing

LATEST ADVANCES IN LARGE LANGUAGE MODELS

2:25 Chairperson's Remarks
Michail Vlysidis, PhD, Principal Engineer, AbbVie



2:30 FEATURED PRESENTATION: AI Models to Enhance Scientific Discovery
Quanquan Gu, PhD, Associate Professor, Computer Science, University of California Los Angeles
Recent breakthroughs in LLMs have transformed AI through scaling. Biology is the next frontier. This talk explores scaling biomolecular foundation models for AI-driven drug discovery, integrating sequence, structure, function, and experimental data to enable next-generation therapeutic discovery.

3:00 ESMFold2: Language Modeling Materializes a World Model of Protein Biology
Tom Hayes, Principal Researcher, Biohub, Co-Founder, EvolutionaryScale
Language models trained on evolutionary sequences develop representations that organize protein biology, from atomic structure to function. ESMFold2 translates these representations into accurate atomic-resolution predictions of biomolecular structures and interactions and, coupled with computational search, yields experimentally validated, nanomolar-affinity miniprotein and antibody binders. Together, these results show how language models can serve as world models of protein biology, enabling virtual experiments at scale to accelerate biologic discovery and therapeutic design.

3:30 How Active Learning Can Help Identify the Right Sequences for Optimal Model Performance
Michail Vlysidis, PhD, Principal Engineer, AbbVie
Active learning offers an efficient strategy for improving predictive model performance in biologics design by prioritizing the most informative sequences for training. This talk will discuss how active learning can identify sequences expected to maximize model gain through uncertainty, diversity, and information-based criteria. Key practical considerations for implementing active learning in computational biologics applications will also be addressed, including how this approach can accelerate model refinement and reduce experimental burden.

4:00 Presentation to be Announced

4:15 Sponsored Presentation *(Opportunity Available)*

4:30 Refreshment Break in the Exhibit Hall with Poster Viewing

WOMEN IN SCIENCE MEET-UP IN THE EXHIBIT HALL

Women in Science Meet-Up
Deborah Moore-Lai, PhD, Vice President, Protein Sciences, ProFound Therapeutics

5:10 Closed-Loop Integration of Immune Repertoires and Generative Models for Discovery of Lead-Quality Antibodies against Challenging Targets
Zhao Huang, PhD, Principal Research Scientist II, Protein Therapeutics, Gilead Sciences Inc
Computational design and immune-derived antibody discovery are often conducted independently with limited information exchange. Here, we first generated large-scale B-cell sequences and functional data following immunization. Sequence function data were used to train and tune structure-based and protein language models. Our approach efficiently generated antibodies with improved epitope diversity, function, and developability.

Interactive Breakout Discussions

5:40 Interactive Breakout Discussions
Interactive Breakout Discussions are informal, moderated discussions, allowing participants to exchange ideas and experiences and develop future collaborations around a focused topic. Each discussion will be led by a facilitator who keeps the discussion on track and the group engaged. To get the most out of this format, please come prepared to share examples from your work, be a part of a collective,

Computational Models for Advancing Biologics

Turning Complex Data into Smarter Biotherapeutic Designs

problem-solving session, and participate in active idea sharing. Please visit the Interactive Breakout Discussions page on the conference website for a complete listing of topics and descriptions.

TABLE: Matching AI/ML Strategy to Target Knowledge: From Function-First Discovery to AI/ML-Enhanced Mechanistic Drug Characterization and Development

Björn L. Frendeus, PhD, CSO, BioInvent International AB

TABLE: TABLE: Post Training and Reinforcement Learning for Large Foundation Models

Frédéric Dreyer, PhD, Principal ML Scientist, Prescient Design, Genentech

6:10 **Close of Day**

THURSDAY, JANUARY 21

8:00 am **Registration and Morning Coffee**

MODELS FOR IMPROVING *DE NOVO* DESIGNS

8:35 **Chairperson's Remarks**

Philip H. Bradley, PhD, Professor, Public Health Sciences Division, Program Head, Herbold Computational Biology Program, Fred Hutch Cancer Center

8:40 **The Synthetic Epitope Atlas: High-Throughput Design and Validation of *de novo* Antibody-Antigen Complexes**

Adrian Lange, PhD, Director, Machine Learning Research, A-Alpha Bio

De novo antibody design models lack sufficient training data to reliably generalize. We demonstrate scalable generation of structural training data for machine learning-driven antibody design by linking *in silico* designs of antibody-antigen complexes to high-throughput experimental binding validation.

9:10 **Rethinking Design Objectives in the Path from Computational Biologics to the Clinic**

Jorge Roel-Touris, PhD, Head, Biologics Design, Digital Biologics Platform, Large Molecules Research, Sanofi

De novo design promises intentional creation of functional therapeutics, yet translation into the clinic remains uncertain. Binding, though necessary, is an insufficient design objective. We discuss that function should instead guide the design process and be operationalized through an integrated design-build-test-learn paradigm. This way, experimental characterization actively informs and refines computational design—effectively transforming experimental readouts into active sources of learning instead of means of validation.

9:40 **Designing Programmable Biologics with Generative Sequence Models**

Pranam Chatterjee, PhD, Assistant Professor, Bioengineering, University of Pennsylvania

The Chatterjee Lab at the University of Pennsylvania develops generative AI models for functional biologic design. We create language models that *de novo* generate molecules targeting undruggable disease proteins and diffusion- and flow-based models that optimize binding, specificity, and drug-like properties. These frameworks now extend to peptide-drug conjugates, isoform, motif, and conformationally selective binders, and molecules capable of directing cellular state transitions, enabling new approaches to therapeutic discovery and engineering.

10:10 **Sponsored Presentation** *(Opportunity Available)*

10:40 **Coffee Break in the Exhibit Hall with Poster Viewing**

CO-FOLDING, PREDICTIVE MODELS

11:20 **Co-Folding: Accurate Structure Prediction of Large Molecules**

Frédéric Dreyer, PhD, Principal ML Scientist, Prescient Design, Genentech

11:50 **Distilling Energetic Scores into an Antibody Binding Prediction Model**

Bowen Dai, PhD, Advisor, Computational Biology, Eli Lilly and Company

Accurate prediction of antibody-antigen binding remains constrained by the cost and throughput of physics-based energy calculations. We present a distillation framework that transfers knowledge from computationally expensive energetic scoring functions into a lightweight, generalizable binding prediction model. By training on energetic labels derived from structural scoring, our approach achieves strong predictive performance while dramatically reducing inference cost, enabling scalable, high-throughput antibody screening for real-world discovery pipelines.

12:20 pm **Transition to Lunch**

12:25 **Luncheon Presentation** *(Sponsorship Opportunity Available)* **or Enjoy Lunch on Your Own**

12:55 **Ice Cream & Cookie Break in the Exhibit Hall with Last Chance for Poster Viewing**

1:35 **Chairperson's Remarks**

Robin Roehm, PhD, CEO & Co-Founder, Apheris

1:40 **Prediction and Design of T Cell Receptor Specificity with Structural Models**

Philip H. Bradley, PhD, Professor, Public Health Sciences Division, Program Head, Herbold Computational Biology Program, Fred Hutch Cancer Center

The specificity of alpha/beta T cell receptors (TCRs) for peptide epitopes underpins adaptive immunity. The ability to predict and design TCR-epitope recognition could open new therapeutic and diagnostic avenues with transformative potential. In this talk, I will describe work toward this goal, leveraging 3D structural modeling and deep neural networks to predict TCR-epitope pairing and to design TCRs and TCR-mimic antibodies.

2:10 **Leveraging AI and Data to Boost Efficiency in Biologics Discovery**

Yuan Lin, Director Digital Biologics Products, Pfizer Inc.

Biologics R&D is generating increasingly complex data across sequences, structures, assays, developability, and workflows. This talk highlights how integrated biologics data platforms, combined with AI/ML, can improve discovery by connecting fragmented data, enabling predictive antibody design and optimization, supporting earlier developability assessment, and accelerating more confident candidate selection.

FEDERATED DATASETS TO IMPROVE DRUG DISCOVERY

2:40 **Trustworthy *in silico* Antibody Binding: Building Predictive Models on the World's Largest Federated Pharma Data Network**

Leonardo V. Castorina, PhD, Senior ML Engineer, Apheris

Robin Roehm, PhD, CEO & Co-Founder, Apheris

Predicting whether and where an antibody binds its antigen still depends on experimental measurement. We show how federated learning across pharma partners' proprietary antibody-antigen data trains co-folding models, a binder-confidence head, and an affinity-ranking capability tied to physically measured binding. We report how this was done operationally—from data harmonization to federated training across partner environments—and aim to share first results.

3:10 **Federated Learning for Biologics: Updates and Learnings from the FAiTE Consortium**

Ittai Dayan, MD, Partner, FAiTE Consortium (Federated AI Therapeutic Engineering); Co-Founder & CEO, Rhino Federated Computing

Five major pharmaceutical companies are collaborating via federated computing to train models on antibody developability, a class of biologics properties hard to characterize, due to relatively low-throughput wet-lab assays. Federation provides access to collective data that no single company has, with better economics and speed than generation of such data. We will share early results and lessons from the consortium, highlighting the potential impact of advancing prediction in this space.

3:40 **Close of Conference**

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