

JANUARY 19 - 22, 2026 | SAN DIEGO, CA + VIRTUAL

2nd Annual



BioLogic SUMMIT 2026

EVENT-AT-A-GLANCE

Data Strategies and the Future of AI Models



- Optimizing Training Data Pipelines
- Active Learning Integration
- Overcoming Data Scarcity
- Emerging Model Architectures
- Practical Deployment in R&D

ML/AI for Biologics Developability, Optimization, and *de novo* Design



- Lab-in-the-Loop Approaches
- Generative & Multi-Modal AI Models
- Structure-Based & Physics-Informed Design
- Developability & Optimization Predictions
- AI-Driven Predictive Preclinical Models

SAVE \$200!
Register by January 16

2026 KEYNOTE PRESENTATIONS



**New Frontier of
Biotherapeutic Discovery:
Where Machine Learning
Meets Molecular Design**

Stephanie Truhlar, PhD
Eli Lilly & Company



**Incorporating *in silico*
Tools into Antibody
Discovery: Challenges
and Opportunities**

Andrew Nixon, PhD
Boehringer Ingelheim
Pharmaceuticals



**AI for Antibody Design -
Going Beyond the Static**

Charlotte Deane, PhD
University of Oxford



**Designing the Next
Generation of Biologics**

Peyton Greenside, PhD
BigHat Biosciences



**Redesigning Antibody
CDRs to Improve
Developability Properties
Using Machine Learning**

Peter Tessier, PhD
University of Michigan

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Training SEMINARS

By Cambridge Healthtech Institute

MONDAY, JANUARY 19, 2026 | 8:30 am - 5:00 pm

All training seminars take place in-person only

TS7A: 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 optimization, 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.

TS8A: Introduction to Antibody Engineering for ML/AI Scientists

Instructors:

Andrew R.M. Bradbury, MD, PhD, CSO, Specifica, an IQVIA business

James D. Marks, MD, PhD, Professor and Vice-Chairman, Department of Anesthesia and Perioperative Care, UCSF

In this training seminar, designed for ML/AI students wishing to learn more about antibodies, students will learn about antibody basics, including the antibody therapeutic market, structure, genetics, and the generation of diversity, as well as the generation of potential therapeutic antibodies. This latter part will include antibody humanization, affinity and specificity maturation, display technologies, creation of naïve libraries, and antibody characterization. The seminar will be fully interactive with students providing ample opportunities to discuss technology with instructors.



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 19-22, 2026 | San Diego, CA + Virtual
Hilton Bayfront

25th Annual
PepTalk

The Protein Science and Production Week



2nd Annual

Data Strategies and the Future of AI Models

Empowering Machine Learning with Smarter Data and Next-Generation Tools

TUESDAY, JANUARY 20

7:30 am Registration and Morning Coffee

8:30 Organizer's Welcome Remarks

TRAINING DATA ACQUISITION AND GENERATION

8:35 Chairperson's Remarks

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

8:40 Benchmarking Design Tools and Data Strategies for Active Learning and Multi-Objective Optimization of Antibody and Non-Antibody Biologics

Jung-Eun (June) Shin, PhD, Senior Machine Learning Scientist, Seismic Therapeutic

We develop and apply machine learning models to simultaneously optimize multiple drug-like properties of biologics, including antibodies and enzymes. We present generative models that harness both the design of functional proteins and the prediction of drug-like properties to engineer therapeutically developable proteins. We produce and experimentally characterize these designs for fitness, function, and developability, exploring the synergy of these methods in a generalized multi-objective optimization pipeline for biologics.

9:10 Machine Learning Models for Nanobody Developability Trained on a Custom Multi-Readout Dataset

Roberto Spreafico, PhD, Vice President, Head, Discovery Data Science, Genmab
Biophysical characterization of biologics is resource-intensive and requires extensive wet-lab experimentation. To scale such efforts to millions of candidate molecules, protein language models offer a promising approach for predicting experimental outcomes computationally. However, the performance of current ML models is constrained by the limited availability of large, high-quality training datasets. Here, we introduce a purpose-designed, information-rich dataset, tailored to train ML models for predicting nanobody developability with improved accuracy.



9:40 FEATURED PRESENTATION: Active Learning for Improving Out-of-Distribution Lab-in-the-Loop Experimental Design

Victor Greiff, PhD, Associate Professor, University of Oslo; Director, Computational Immunology, IMPRINT

We present advances in understanding and improving biological sequence-based machine learning. First, we introduce an attribution method for generative models trained on positive-only data, enabling interpretability without requiring negatives. Second, we show that training data composition critically impacts generalization and rule learning across distributions. Together, these works underscore the importance of biologically grounded interpretability and deliberate dataset design in unlocking robust and explainable models for AI-powered antibody design.

10:10 Structure-Based Calculations for Predicting Properties and Profiling Antibody Therapeutics

Alain Ajamian, Director of Business Development, Chemical Computing Group



We present a method for modeling antibodies and performing pH-dependent conformational sampling, which can enhance property calculations. Structure-based descriptors are evaluated for their predictive performance on HIC and viscosity data. From this, we devised four rules for therapeutic antibody profiling which address developability issues arising from hydrophobicity and charged-based solution behavior, and the ability to enrich for those that are approved by the FDA. Antibody modeling and docking accuracy is assessed and compared to recent ML tools.

10:25 Applying *in silico* Tools for Protein Design: A Practical Review

Deniz Kavi, CEO & Co Founder, Tamarind Bio

This talk will present benchmarks, empirical results and best practices in applying the leading literature of molecular design tools for protein engineering applications. We will evaluate state-of-the-art computational tools for *de novo* design, optimizations, and scoring of biologics, along with processes to create pipelines ready to be applied to discovery problems at scale. We will also discuss shortcomings and ongoing challenges and limitations of applying AI and physics-based tooling to practical discovery problems.

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

11:20 High-Throughput Data Generation and Active Learning for Developing Multispecific Antibodies

Winston Haynes, PhD, Vice President, Computational Sciences and Engineering, LabGenius Therapeutics

Due to their highly engineered formats and complex effector mechanisms, multispecific antibodies (including T-cell engagers [TCEs]) require context-specific training datasets to power ML models. We provide insights into our highly integrated and automated experimental and computational infrastructure that enables our cycle-based, multi-objective optimisation of multispecifics. We highlight our success deploying this infrastructure to develop a pipeline of highly potent and selective TCEs.

11:50 Accelerating Biologic Design with *in silico* Active Learning for Multi-Objective Optimization

Jiangyan Feng, PhD, Senior Advisor, Biotechnology Discovery Research, Eli Lilly and Company

Dr. Jiangyan Feng earned her Ph.D. in Computational Biology from the University of Illinois at Urbana-Champaign, where she specialized in molecular dynamics simulations to investigate protein conformational dynamics and applied bioinformatics for machine learning model development. She currently works at Eli Lilly, where her research focuses on antibody engineering and the application of *in silico* methods to accelerate biologics discovery and optimization.

12:20 pm Transition to Lunch

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

1:00 Refreshment Break in the Exhibit Hall with Poster Viewing

KEYNOTE PRESENTATION



1:30 Designing the Next Generation of Biologics with Enhanced Functionality Using Machine Learning and a Rapid Iteration Wet Lab

Peyton Greenside, PhD, Co-Founder & CSO, BigHat Biosciences

BigHat Biosciences is transforming antibody discovery

by combining machine learning and synthetic biology in rapid design-build-test cycles that generate thousands of candidates each week. Our platform goes beyond improving biophysics to engineer antibodies with enhanced functionality such as conditional binding and logic-based control (OR, AND, NOT) for greater safety and efficacy.



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Empowering Machine Learning with Smarter Data and Next-Generation Tools

KEYNOTE PANEL DISCUSSION

2:00 Building Multi-Scale and Multi-Modal Models

Moderator: Winston Haynes, PhD, Vice President, Computational Sciences and Engineering, LabGenius Therapeutics

This panel will explore the design, training, and application of multi-scale and multi-modal computational models in therapeutic antibody and protein engineering. Industry and academic experts will discuss both technical challenges and practical use cases, offering insight into how multi-modal and multi-scale approaches are shaping the future of biologic drug discovery.

Panelists:

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

Peyton Greenside, PhD, Co-Founder & CSO, BigHat Biosciences

Jeremy Wohlwend, PhD, CTO, Boltz

2:55 Session Break

3:05 PAIA's high-throughput developability assay platform: a versatile and robust technology for the generation of high-quality training data for different antibody formats.

PAIA[®]

Sebastian Giehring, PAIA Biotech GmbH

In this talk we present our assay technology capable of characterizing hundreds to thousands of antibodies and proteins for different biophysical parameters, such as hydrophobicity and non-specific binding.

The assay technology is microplate-based and only needs minute amounts of protein, making it an ideal tool for the fast and efficient screening of large discovery campaigns.

We will be showing data for different antibody formats and building blocks for bispecifics and multispecific antibodies, illustrating the versatility of the approach.

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

PLENARY KEYNOTE SESSION: TRENDS AND INNOVATION DRIVING THE FUTURE OF BIOTHERAPEUTICS

4:30 Welcome Remarks

Mimi Langley, Executive Director, Life Sciences, Cambridge Healthtech Institute



4:35 Chairperson's Remarks

Deborah Moore-Lai, PhD, Vice President, Protein Sciences, ProFound Therapeutics



4:40 From Targets to Biologics: AI Powering the Next Leap in Discovery at Takeda

Yves Fomekong Nanfack, PhD, Head of AI/ML Research, Takeda

Takeda's AI/ML strategy is redefining the path from targets to biologics, using advanced models to identify and validate novel targets, decode complex biology, and design the next generation of high-quality therapeutic molecules. By integrating agentic, generative, and large language model-driven approaches, AI is powering the next leap in discovery at Takeda.



4:50 Agentic AI for Biologics: Scalable Infrastructure for GxP-Compliant, Insight-Driven Testing

Lieza M. Danan, PhD, Co-Founder & CEO, LiVeritas Biosciences

As biotherapeutics become more complex, automation of traditional testing labs falls short of delivering the insights needed for regulatory success. This talk introduces a GxP-native, full-stack AI platform designed to orchestrate and optimize mass spectrometry-based testing workflows across CMC, bioanalysis, and regulatory reporting. Rooted in regenerative system design, this infrastructure enables scalable, adaptive, and compliant operations, empowering biopharma teams to accelerate product development with confidence, clarity, and scientific precision.



5:00 Technological Trends Shaping the Landscape of Biopharmaceuticals

Aline de Almeida Oliveira, PhD, Competitive Intelligence Office (AICOM), Bio-Manguinhos/Fiocruz, Brazil

Currently, the biopharmaceutical industry is undergoing rapid technological advancements that are revolutionizing the development and production of biopharmaceuticals. Consequently, new therapeutic categories are gaining prominence, such as antibody-drug conjugates, bispecific antibodies, advanced therapies, among others. This rapid evolution requires constant vigilance to identify breakthroughs and guide strategic decision-making in this dynamic field. The aim of this strategic foresight analysis is to discuss technological trends for the future of biopharmaceuticals.

5:10 PLENARY FIRESIDE CHAT



Moderator: Deborah Moore-Lai, PhD, Vice President, Protein Sciences, ProFound Therapeutics

Kicking off with three focused 10-minute presentations, the Fireside Chat transitions into an engaging 30-minute fireside discussion. Panelists will delve into cutting-edge topics, including the role of AI/ML in biologics discovery, advancements in next-generation analytics and tools, entrepreneurial trends and investment landscapes, and emerging therapeutic modalities. In tribute to Dr. King's legacy, this session will also highlight the importance of fostering diversity, equity, and inclusion within the biotech innovation ecosystem.

Panelists:

Lieza M. Danan, PhD, Co-Founder & CEO, LiVeritas Biosciences

Aline de Almeida Oliveira, PhD, Competitive Intelligence Office (AICOM), Bio-Manguinhos/Fiocruz, Brazil

Yves Fomekong Nanfack, PhD, Head of AI/ML Research, Takeda

5:40 Networking Reception in the Exhibit Hall with Poster Viewing

YOUNG SCIENTIST MEET-UP

Meet the Moderator at the Plaza in the Exhibit Hall

Maria Calderon Vaca, PhD Student, Chemical Environmental & Materials Engineering, University of Miami

6:40 Close of Day

WEDNESDAY, JANUARY 21

7:15 am Registration Open

7:30 Interactive Breakout Discussions with Continental Breakfast

Engage in in-depth discussions with industry experts and your peers about the progress, trends, and challenges you face in implementing ML/AI in your work! Interactive discussion groups play an integral role in networking with potential collaborators, provide an opportunity to share examples from your work, and allow you to be part of a group problem-solving endeavor. Please visit the Interactive Breakouts page on the conference website for a complete listing of topics and descriptions.



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TABLE 10: Bridging the Gap between AI-Driven Biologics Design to Novel Molecules Entering Clinical Trials

Joost Schymkowitz, PhD, Professor & Group Leader, Switch Lab, VIB-KU Leuven

TABLE 11: Comparing and Contrasting Machine Learning-Based Design of Antibody and Non-Antibody Biologics

Jung-Eun (June) Shin, PhD, Senior Machine Learning Scientist, Seismic Therapeutic

TABLE 12: Overcoming the Data Bottleneck in AI-Driven Antibody Engineering

Roberto Spreafico, PhD, Vice President, Head, Discovery Data Science, Genmab

STRATEGIES TO OVERCOME DATA LIMITATIONS

8:15 Chairperson's Remarks

Jung-Eun (June) Shin, PhD, Senior Machine Learning Scientist, Seismic Therapeutic

8:20 *In vitro*-Validated Synthetic Structures for Structural Foundation Models and Applications in *de novo* Design

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

There is a severe lack of protein-protein interaction (PPI) structural data, especially for antibody-antigen systems. We present an approach to create thousands of putative PPI structures, wherein we computationally design many *de novo* PPI structures and subsequently validate them *in vitro* with AlphaSeq. We show that the validated putative structures form a dataset on which we can train downstream machine learning models to yield improved model performance.

8:50 AI Structural Biology Network: Improving Protein Co-Folding Predictions by Leveraging Data from Multiple Pharma Companies

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

The AI Structural Biology Network brings together pharmaceutical companies and cutting-edge federated learning technology to leverage the collective data of multiple parties to improve AI-driven drug discovery. In this session, we will show results on how we improved OpenFold3—an open-source reproduction of AlphaFold3—with the proprietary structural data of the participating pharma companies.

9:20 OpenBind: Unlocking AI-Driven Drug Discovery with the World's Largest Protein-Drug Interaction Dataset

Warren Thompson, PhD, Senior Computational Scientist, Diamond Light Source

The OpenBind consortium represents a transformative opportunity to address the critical data bottleneck for evolving co-folding models. This talk will highlight the progress made for routine collection of structural-affinity pairs at a scale never attempted in the public domain. This challenge requires coordinating diverse scientific work packages: from AI-assisted compound design, automated synthesis, to high-throughput structural and affinity measurements, and finally data dissemination and blind challenges.

9:50 Talk Title to be Announced

Jonathan Fauerbach, Head of R&D, R&D, LenioBio GmbH



10:20 Coffee Break in the Exhibit Hall with Poster Viewing

KEYNOTE SESSION

11:00 Chairperson's Remarks

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



11:05 Incorporating *in silico* Tools into Antibody Discovery: Challenges and Opportunities

Andrew Nixon, PhD, Senior Vice President, Global Head Biotherapeutics Discovery, Boehringer Ingelheim Pharmaceuticals Inc.

Antibody discovery is being transformed by the integration of *in silico* tools, from machine learning models to structure-based design. This presentation will explore how computational methods are being incorporated into discovery pipelines at scale, highlighting key opportunities for accelerating candidate selection and improving developability. It will also address ongoing challenges—including data quality, model interpretability, and cross-disciplinary integration—that must be overcome to realize the full potential of AI-driven antibody discovery.



11:35 AI for Antibody Design - Going Beyond the Static

Charlotte M. Deane, PhD, Professor, Structural Bioinformatics, Statistics, University of Oxford; Executive Chair, Engineering and Physical Sciences Research Council (EPSRC)

We can now computationally predict a single, static protein structure with high accuracy. However, we are not yet able to reliably predict structural flexibility. This ability to adapt their shape can be fundamental to their functional properties. A major factor limiting such predictions is the scarcity of suitable training data. I will show novel tools and databases that help to overcome this.



12:05 pm Redesigning Antibody CDRs to Improve Developability Properties Using Machine Learning

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

Antibody complementarity-determining regions (CDRs) form complex 3D surfaces that mediate high-affinity interactions with their target antigens. Some of the same sites in CDRs that mediate specific antibody binding also mediate undesirable developability properties. Here, we report methods for redesigning antibody CDRs—including those at sites in or near the paratope—to improve developability while maintaining high affinity and specificity.

12:35 Transition to Lunch

12:40 LUNCHEON PRESENTATION: Ginkgo Datapoints Antibody Developability Competition Outcomes: Limited Model Performance and a Call for Data Standardization



Josh Moller, Senior Biological Engineer, AI, Ginkgo Datapoints

Antibody clinical viability depends critically on developability attributes, yet predictive model development is hampered by limited, heterogeneous data and poor generalization. To address this gap, we established the 2025 Ginkgo Datapoints Developability Competition, creating a new, blinded benchmark for developability modeling. We will share key observations of the competition, including model overfitting and limited out-of-distribution generalization. Future advances in modeling require larger, standardized datasets and more rigorous evaluation frameworks to translate predictive models into reliable design tools.

1:10 Session Break

1:45 Refreshment Break in the Exhibit Hall with Poster Viewing

AGENTIC AND MULTI-MODAL MODELS

2:15 Chairperson's Remarks

Elahe Vedadi, PhD, Research Scientist, Google/DeepMind

2:20 NextGenPLM: A Novel Structure-Infused Foundational Protein Language Model for Antibody/NANOBODY VHH Discovery and Optimization

Abhinav Gupta, PhD, Principal Machine Learning Scientist, AI Innovation, Large Molecule Research, Sanofi

Sequence-only PLMs lack spatial context and miss critical folding, interface, and environment-dependent cues, while structure-prediction and docking methods are too slow and underperform on antibody and VHH complexes.



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NextGenPLM bridges this gap with a modular, scalable design that fuses pretrained PLMs with multimodal inputs—from raw sequences and functional assays to high-resolution structures—via spectral contact-map embeddings. Using results from internal campaigns, we will demonstrate its potential for rapid, data-driven biologics discovery.

2:50 AI Co-Scientist Use Cases in Discovery, Engineering, and Development of Therapeutic Proteins

Elahe Vedadi, PhD, Research Scientist, Google/DeepMind

Accelerating scientific discovery requires novel computational approaches. AI co-scientist, a multi-agent system, helps uncover new knowledge and formulate novel research hypotheses. Using a “generate, debate, and evolve” approach with scaled test-time compute, it augments the scientific discovery process. For example, in therapeutic protein development, it identified novel epigenetic targets for liver fibrosis and proposed drug repurposing candidates for AML, both validated *in vitro*, demonstrating its potential to advance complex research.

3:20 PANEL DISCUSSION: An Honest Conversation about What It Takes to Make ML Work in Biotherapeutics

Moderator: Nicola Bonzanni, PhD, CEO, ENPICOM

We'll explore what it really takes to make machine learning useful in biologics discovery and engineering. From bridging lab and data science workflows, to dealing with scattered data and real-world model limitations, we'll talk about what works, what doesn't, and why. Expect a grounded look at the everyday decisions behind successful ML implementation: practical insights on preparing data, aligning teams, and deploying models where they matter most—in scientists' hands.

Panelists:

Abhinav Gupta, PhD, Principal Machine Learning Scientist, AI Innovation, Large Molecule Research, Sanofi

Melody Shahsavarian, PhD, Director, Data Strategy & Digital Transformation, Biotherapeutics Discovery Research, Eli Lilly & Company
Roberto Spreafico, PhD, Vice President, Head, Discovery Data Science, Genmab

Michail Vlysidis, PhD, Principal Engineer, AbbVie

Daniel Yoo, Scientific Associate Director, Large Molecule Discovery & Research Data Science, Amgen, Inc.

4:20 Refreshment Break in the Exhibit Hall with Poster Viewing

4:50 Interactive Breakout Discussions

Engage in in-depth discussions with industry experts and your peers about the progress, trends, and challenges you face in implementing ML/AI in your work! Interactive discussion groups play an integral role in networking with potential collaborators, provide an opportunity to share examples from your work, and allow you to be part of a group problem-solving endeavor. Please visit the Interactive Breakouts page on the conference website for a complete listing of topics and descriptions.

TABLE 1: Accelerating Antibody Engineering with AI-Driven Active Learning: Optimizing DMTA Cycles

Jiangyan Feng, PhD, Senior Advisor, Biotechnology Discovery Research, Eli Lilly and Company

TABLE 2: Best Practices for Using Agentic and Multi-Agent Systems in R&D

Elahe Vedadi, PhD, Research Scientist, Google/DeepMind

5:40 Close of Day

THURSDAY, JANUARY 22

8:00 am Registration Open

PLENARY KEYNOTE SESSION

8:25 Welcome Remarks

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

8:30 Plenary Keynote Introduction

Andrew Nixon, PhD, Senior Vice President, Global Head Biotherapeutics Discovery, Boehringer Ingelheim Pharmaceuticals Inc.

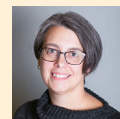


8:35 New Frontier of Biotherapeutic Discovery:

Where Machine Learning Meets Molecular Design

Stephanie Truhlar, PhD, Vice President, Biotechnology Discovery Research, Eli Lilly and Company

9:00 PLENARY FIRESIDE CHAT: End-to-End *in silico*-Designed Biologics



Moderator: *Andrew Nixon, PhD, Senior Vice President, Global Head Biotherapeutics Discovery, Boehringer Ingelheim Pharmaceuticals Inc.*

- How is the path to drug development different with ML/AI?
- How far off is *de novo* design for biologics? For antibodies?
- How is ML/AI used for target selection?
- How do you accelerate DMTA cycles?
- Data standardization—how to incorporate historical data?
- Federated learning—how do you ensure you have enough data to build a model?
- Promoting change management

Panelists:

Charlotte M. Deane, PhD, Professor, Structural Bioinformatics, Statistics, University of Oxford; Executive Chair, Engineering and Physical Sciences Research Council (EPSRC)

Garegin Papoian, PhD, Co-Founder & CSO, DeepOrigin

Stephanie Truhlar, PhD, Vice President, Biotechnology Discovery Research, Eli Lilly and Company

9:30 Coffee Break in the Exhibit Hall with Poster Viewing

WOMEN IN SCIENCE MEET-UP

Meet the Moderators at the Plaza in the Exhibit Hall

Michelle R. Gaylord, MS, Former Principal Scientist, Protein Expression & Advanced Automation, Velia Therapeutics

Deborah Moore-Lai, PhD, Vice President, Protein Sciences, ProFound Therapeutics

PHYSICS-BASED MODELS

10:20 Chairperson's Remarks

Frank Teets, PhD, Head, Computational Science, AI Proteins

10:25 Scalable Emulation of Protein Equilibrium Ensembles with Generative Deep Learning

Frank Noé, PhD, Partner Research Manager, Microsoft; Professor, Machine Learning for the Sciences, Free University Berlin

Predicting protein structure changes at scale remains challenging. BioEmu is a deep learning system that generates thousands of independent protein structures per hour on a single GPU. Trained on MD simulations, static structures, and stability data, it captures diverse motions and predicts free



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energies within 1 kcal/mol accuracy. BioEmu offers mechanistic insights by modeling structural ensembles and thermodynamics, enabling scalable protein function prediction and design.

10:55 Integrating Physics in Deep Learning Algorithms: A Force Field as a PyTorch Module

Joost Schymkowitz, PhD, Professor & Group Leader, Switch Lab, VIB-KU Leuven

We present a dual-framework approach for therapeutic antibody design that combines EvolveX, a structure-based CDR design pipeline using FoldX, with MadraX, a PyTorch-integrated differentiable force field. This physics-informed strategy enables data-efficient, interpretable protein engineering. EvolveX achieved >1000-fold affinity gains with structural and functional validation, while MadraX bridges deep learning and biophysics by allowing gradient flow through energy functions, enhancing design in data-scarce contexts.

11:25 Learning Millisecond Protein Dynamics from What Is Missing in NMR Spectra

Gina El Nesr, Graduate Researcher, Biophysics, Stanford University

Many proteins' biological functions rely on micro- to millisecond dynamics, but large-scale data to study these motions is minimal. By curating >100 NMR relaxation datasets, we noticed that an observable hides in plain sight in >10,000 proteins in the BMRB. We trained Dyna-1 on this observable and found that it also predicts μ s–ms motion directly measured in NMR relaxation experiments. Dynamics linked to biological function are particularly well-predicted.

11:55 Attend Parallel Presentation or Enjoy Lunch on Your Own

1:00 pm Ice Cream & Cookie Break in the Exhibit Hall with Last Chance for Poster Viewing

PHYSICS-BASED MODELS (CONT.)

1:40 Chairperson's Remarks

Michail Vlysidis, PhD, Principal Engineer, AbbVie

1:45 Modeling Antibody Conformational Ensembles with Physics-Based Simulations and Deep Learning

Fabian Spoendlin, Researcher, Oxford Protein Informatics Group, University of Oxford

Antibodies exhibit structural flexibility often central to their function. Here, we introduce two approaches to model conformational ensembles of antibodies at scale. First, we developed a high-throughput MD workflow that reproduces ensemble metrics observed in all-atom simulations and experimental datasets. Using this pipeline, we simulated over 150,000 antibodies to investigate flexibility profiles. Second, we trained a deep learning model on MD data and demonstrate its ability to predict key conformations.

NEXT-GENERATION MODELS AND CAPABILITIES

2:15 Zero-Shot Antibody Design in a 24-Well Plate with Chai Discovery

Matthew McPartlon, PhD, Co-Founder, Chai Discovery

Despite advances in AI-driven protein design, fully *de novo* antibody discovery without extensive screening has remained elusive. We present Chai-2, a multimodal generative framework that reliably produces antibodies, nanobodies, and miniproteins zero-shot from target structures. Evaluated on 52 novel targets, Chai-2 achieves a ~16% binding hit rate—over 100-fold improvement—identifying binders for ~50% of targets in a single experimental round and producing structurally novel, picomolar-affinity minibinders within two weeks.

2:45 Functional and Epitope Specific Monoclonal Antibody Discovery Directly from Immune Sera Using Cryo-EM

James Ferguson, Postdoctoral Associate, Integrative Structural & Computational Biology, Scripps Research Institute

Traditional antibody discovery is labor-intensive and poorly scalable. We developed a streamlined approach combining structural analysis and bioinformatics to determine heavy and light chain sequences from cryo-EM maps of serum-derived polyclonal antibodies bound to antigens. Using ModelAngelo for automated structure-building, our pipeline reduces analysis time from weeks to under one day while improving precision. Validation with HIV vaccine and influenza studies demonstrates enhanced antibody discovery for vaccine development and therapeutics.

3:15 Protein Language Models Instead of Structure-Based Models for Biologics Predictions

Michail Vlysidis, PhD, Principal Engineer, AbbVie

Protein language models (PLMs) offer a fast and cost-effective alternative to traditional structure-based descriptors, which are computationally expensive and time-consuming. By generating encodings directly from sequence data, PLMs bypass the need for resolved protein structures. This talk explores whether PLMs can match the accuracy of traditional methods while providing a more efficient solution. We discuss comparative analyses that evaluate PLMs' precision and highlight their potential to accelerate drug discovery.

3:45 Model for Predicting Protein Expression for Miniproteins

Frank Teets, PhD, Head, Computational Science, AI Proteins

We present a lightweight, fully sequence-based convolutional neural network for predicting miniprotein expression. Trained on curated in-house data labeled for production fidelity, the model operates as a binary classifier and generalizes across topologies with >90% accuracy. Now integrated into all drug discovery pipelines, it enables efficient downsampling of designed proteins, reduces synthesis waste, and exemplifies the value of automated design-build-test loops in AI-driven protein design.

4:15 Close of BioLogic Summit



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ML/AI for Biologics Developability, Optimization, and *de novo* Design

Unfolding Applications and Real-World Examples

TUESDAY, JANUARY 20

7:30 am Registration and Morning Coffee

8:30 Organizer's Welcome Remarks

APPLICATIONS OF LAB-IN-THE-LOOP FOR ANTIBODY AND PROTEIN DESIGN

8:35 Chairperson's Remarks

Victor Greiff, PhD, Associate Professor, University of Oslo; Director, Computational Immunology, IMPRINT

8:40 Good Targets, Bad Targets: Lessons from Testing Binders for over 50 Different Protein Targets

Julian Englert, MS, Co-Founder and CEO, Adaptiv Biosystems

We're running a high-throughput wet lab for protein designers. To date, we've synthesized and tested over 10,000 different proteins and performed binding assays against more than 50 different targets. In this talk, we'll share insights on what makes some targets more difficult than others, how target properties influence protein design strategies, and what types of experimental data are most useful for improving machine learning models in this domain.

9:10 Lab-in-the-Loop Therapeutic Antibody Design with Deep Learning

Ji Won Park, PhD, Principal ML Scientist, Prescient Design, Genentech

Therapeutic antibody design is a complex multi-property optimization problem that traditionally relies on expensive searches through sequence space. Here, we introduce "lab-in-the-loop"—a new approach to antibody design that orchestrates generative machine learning models, multi-task property predictors, active learning ranking and selection, and *in vitro* experimentation in a semi-autonomous, iterative optimization loop. In this talk, we will discuss considerations for scaling model-driven design across complex modalities and targets.

9:40 How to Think about Designing Smart Antibodies in the Age of GenAI: Integrating Biology, Technology, and Experience

Annie Kwon, PhD, Principal Scientist, Amgen Inc

Amgen is applying an integrated approach to therapeutic antibody engineering, combining modern computational protein design, predictive and generative AI, and high-throughput experimentation. Rational protein design approaches allow us to make precise, platform-wide optimizations in therapeutic developability and productivity, while purpose-built ML models enable rapid generation and selection of therapeutic candidates with favorable developability indicators.

10:10 Structure-Based Calculations for Predicting Properties and Profiling Antibody Therapeutics

Alain Ajamian, Director of Business Development, Chemical Computing Group

We present a method for modeling antibodies and performing pH-dependent conformational sampling, which can enhance property calculations. Structure-based descriptors are evaluated for their predictive performance on HIC and viscosity data. From this, we devised four rules for therapeutic antibody profiling which address developability issues arising from hydrophobicity and charged-based solution behavior, and the ability to enrich for those that are approved by the FDA. Antibody modeling and docking accuracy is assessed and compared to recent ML tools.



10:25 Applying *in silico* Tools for Protein Design: A Practical Review

Deniz Kavi, CEO & Co Founder, Tamarind Bio

This talk will present benchmarks, empirical results and best practices in applying the leading literature of molecular design tools for protein engineering applications. We will evaluate state-of-the-art computational tools for *de novo* design, optimizations, and scoring of biologics, along with processes to create pipelines ready to be applied to discovery problems at scale. We will also discuss shortcomings and ongoing challenges and limitations of applying AI and physics-based tooling to practical discovery problems.

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

ML/AI FOR BIOLOGICS ENGINEERING & OPTIMIZATION: FROM *IN SILICO* DEVELOPMENT TO REAL-WORLD DEPLOYMENT

11:19 Chairperson's Remarks

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

11:20 Assessing Generative Model Coverage of Protein Structures with SHAPES

Possu Huang, PhD, Assistant Professor, Bioengineering, Stanford University

Protein structural generative models have been applied to a wide range of design tasks. As part of our efforts toward designing functional proteins involving structural dynamics, we developed an all-atom model, Protpardelle, that leverages a language model-based architecture to generate 3D structures. The SHAPES metric reveals biases in state-of-the-art generative models according to their design decisions.

11:50 Toward Biologics by Design: Computational Design and Optimization of VHH Therapeutics

Norbert Furtmann, PhD, Head of AI Innovation, Large Molecules Research, Sanofi

This talk will present an overview of Sanofi's state-of-the-art computational pipeline for *de novo* design of VHH therapeutics. The integration of the computational workflow with customized wet-lab processes for efficient molecule discovery and optimization will be discussed. A use case demonstrating the application of the pipeline for the computational design of VHH building blocks against therapeutic targets will be shared.

12:20 pm Transition to Lunch

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

1:00 Refreshment Break in the Exhibit Hall with Poster Viewing

KEYNOTE PRESENTATION



1:30 Designing the Next Generation of Biologics with Enhanced Functionality Using Machine Learning and a Rapid Iteration Wet Lab

Peyton Greenside, PhD, Co-Founder & CSO, BigHat Biosciences

BigHat Biosciences is transforming antibody discovery by combining machine learning and synthetic biology in rapid design-build-test cycles that generate thousands of candidates each week. Our platform goes beyond improving biophysics to engineer antibodies with enhanced functionality such as conditional binding and logic-based control (OR, AND, NOT) for greater safety and efficacy.



2nd Annual

ML/AI for Biologics Developability, Optimization, and *de novo* Design

Unfolding Applications and Real-World Examples

KEYNOTE PANEL DISCUSSION

2:00 Building Multi-Scale and Multi-Modal Models

Moderator: Winston Haynes, PhD, Vice President, Computational Sciences and Engineering, LabGenius Therapeutics

This panel will explore the design, training, and application of multi-scale and multi-modal computational models in therapeutic antibody and protein engineering. Industry and academic experts will discuss both technical challenges and practical use cases, offering insight into how multi-modal and multi-scale approaches are shaping the future of biologic drug discovery.

Panelists:

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

Peyton Greenside, PhD, Co-Founder & CSO, BigHat Biosciences

Jeremy Wohlwend, PhD, CTO, Boltz

2:55 Session Break

3:05 PAIA's high-throughput developability assay platform: a versatile and robust technology for the generation of high-quality training data for different antibody formats.

Sebastian Giehring, PAIA Biotech GmbH

In this talk we present our assay technology capable of characterizing hundreds to thousands of antibodies and proteins for different biophysical parameters, such as hydrophobicity and non-specific binding.

The assay technology is microplate-based and only needs minute amounts of protein, making it an ideal tool for the fast and efficient screening of large discovery campaigns. We will be showing data for different antibody formats and building blocks for bispecifics and multispecific antibodies, illustrating the versatility of the approach.

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

PLENARY KEYNOTE SESSION: TRENDS AND INNOVATION DRIVING THE FUTURE OF BIOTHERAPEUTICS

4:30 Welcome Remarks

Mimi Langley, Executive Director, Life Sciences, Cambridge Healthtech Institute



4:35 Chairperson's Remarks

Deborah Moore-Lai, PhD, Vice President, Protein Sciences, ProFound Therapeutics



4:40 From Targets to Biologics: AI Powering the Next Leap in Discovery at Takeda

Yves Fomekong Nanfack, PhD, Head of AI/ML Research, Takeda

Takeda's AI/ML strategy is redefining the path from targets to biologics, using advanced models to identify and validate novel targets, decode complex biology, and design the next generation of high-quality therapeutic molecules. By integrating agentic, generative, and large language model-driven approaches, AI is powering the next leap in discovery at Takeda.



4:50 Agentic AI for Biologics: Scalable Infrastructure for GxP-Compliant, Insight-Driven Testing

Lieza M. Danan, PhD, Co-Founder & CEO, LiVeritas Biosciences

As biotherapeutics become more complex, automation of traditional testing labs falls short of delivering the insights needed for regulatory success. This talk introduces a GxP-native, full-stack AI platform

designed to orchestrate and optimize mass spectrometry-based testing workflows across CMC, bioanalysis, and regulatory reporting. Rooted in regenerative system design, this infrastructure enables scalable, adaptive, and compliant operations, empowering biopharma teams to accelerate product development with confidence, clarity, and scientific precision.



5:00 Technological Trends Shaping the Landscape of Biopharmaceuticals

Aline de Almeida Oliveira, PhD, Competitive Intelligence Office (AICOM), Bio-Manguinhos/Fiocruz, Brazil

Currently, the biopharmaceutical industry is undergoing rapid technological advancements that are revolutionizing the development and production of biopharmaceuticals. Consequently, new therapeutic categories are gaining prominence, such as antibody-drug conjugates, bispecific antibodies, advanced therapies, among others. This rapid evolution requires constant vigilance to identify breakthroughs and guide strategic decision-making in this dynamic field. The aim of this strategic foresight analysis is to discuss technological trends for the future of biopharmaceuticals.

5:10 PLENARY FIRESIDE CHAT



Moderator: Deborah Moore-Lai, PhD, Vice President, Protein Sciences, ProFound Therapeutics

Kicking off with three focused 10-minute presentations, the Fireside Chat transitions into an engaging 30-minute fireside discussion. Panelists will delve into cutting-edge topics, including the role of AI/ML in biologics discovery, advancements in next-generation analytics and tools, entrepreneurial trends and investment landscapes, and emerging therapeutic modalities. In tribute to Dr. King's legacy, this session will also highlight the importance of fostering diversity, equity, and inclusion within the biotech innovation ecosystem.

Panelists:

Lieza M. Danan, PhD, Co-Founder & CEO, LiVeritas Biosciences

Aline de Almeida Oliveira, PhD, Competitive Intelligence Office (AICOM), Bio-Manguinhos/Fiocruz, Brazil

Yves Fomekong Nanfack, PhD, Head of AI/ML Research, Takeda

5:40 Networking Reception in the Exhibit Hall with Poster Viewing

YOUNG SCIENTIST MEET-UP

Meet the Moderator at the Plaza in the Exhibit Hall

Maria Calderon Vaca, PhD Student, Chemical Environmental & Materials Engineering, University of Miami

6:40 Close of Day

WEDNESDAY, JANUARY 21

7:15 am Registration Open

7:30 Interactive Breakout Discussions with Continental Breakfast

Engage in in-depth discussions with industry experts and your peers about the progress, trends, and challenges you face in implementing ML/AI in your work! Interactive discussion groups play an integral role in networking with potential collaborators, provide an opportunity to share examples from your work, and allow you to be part of a group problem-solving endeavor. Please visit the Interactive Breakouts page on the conference website for a complete listing of topics and descriptions.

TABLE 13: Language Models to Generate 3D Structures

Possu Huang, PhD, Assistant Professor, Bioengineering, Stanford University



2nd Annual

ML/AI for Biologics Developability, Optimization, and *de novo* Design

Unfolding Applications and Real-World Examples

This discussion group will convene for a discussion of applying language model architecture to protein structural features.

TABLE 14: Leveraging Large Language Models, Deep Learning, and Graph-Based Architectures to Accelerate Biological Design

Omar Abudayyeh, PhD, McGovern Fellow/Principal Investigator, Massachusetts Institute of Technology

Jonathan S. Gootenberg, PhD, McGovern Fellow/Principal Investigator, McGovern Institute, Massachusetts Institute of Technology

- Developing programmable tools across biological scales
- Creating EVOLVEpro, a few-shot active learning framework optimizing protein function using language models and targeted experimentation
- Developing virtual cell models predicting responses to genetic/chemical perturbations
- Applying these to map aging mechanisms through single-cell perturbation atlases, identifying factors restoring youthful cell states
- Demonstrating how machine learning can model biological complexity and accelerate therapeutic development

AI-DRIVEN PROTEIN DESIGN WITH EXPERIMENTAL VALIDATION

8:15 Chairperson's Remarks

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

8:20 Smarter, Not Bigger: Domain-Adapted Multi-Modal ML/AI for Better Antibody Design

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

Much recent work on multimodal ML/AI for protein design has focused primarily on building larger models. We take an alternative approach, with experiments designed for better multi-modal models—and vice versa. We show that joint modeling allows intelligent integration of alternating rounds of ML-guided display selections and active-learning driven multi-objective optimization of antibodies produced in high throughput via cell-free synthesis, yielding highly developable binders unattainable via either modality alone.

8:50 AI Technologies for Programming Biology and Health

Omar Abudayyeh, PhD, McGovern Fellow/Principal Investigator, Massachusetts Institute of Technology

Jonathan S. Gootenberg, PhD, McGovern Fellow/Principal Investigator, McGovern Institute, Massachusetts Institute of Technology

We leverage large language models, deep learning, and graph-based architectures to build hierarchical AI systems spanning protein engineering to virtual human models. Our bottom-up approach integrates multiomics and multi-modal data across molecular-to-clinical scales, creating predictive frameworks for disease mechanisms, aging, and personalized health interventions. These platforms accelerate biological design and therapeutic discovery while enabling modeling and optimization of human health trajectories.

9:20 Soluble Scaffolding of GPCR Binding Sites with Structure- and ML/AI-Based Methods

Jingzhou Wang, PhD, Associate Principal Scientist, Merck & Co.

ML/AI-designed epitope scaffolds show promise for ligand discovery in challenging targets, with recent efforts emphasizing the maintenance of binding sites during design. We discuss two studies where we demonstrate the successful creation of scaffolds with significant ligand binding without requiring an empirically determined protein structure and successfully produced the proteins rapidly and at low cost in *E. coli* while maintaining disulfide bonds.

9:50 Talk Title to be Announced

Jonathan Fauerbach, Head of R&D, R&D, LenioBio GmbH



10:20 Coffee Break in the Exhibit Hall with Poster Viewing

KEYNOTE SESSION

11:00 Chairperson's Remarks

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



11:05 Incorporating *in silico* Tools into Antibody Discovery: Challenges and Opportunities

Andrew Nixon, PhD, Senior Vice President, Global Head Biotherapeutics Discovery, Boehringer Ingelheim Pharmaceuticals Inc.

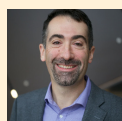
Antibody discovery is being transformed by the integration of *in silico* tools, from machine learning models to structure-based design. This presentation will explore how computational methods are being incorporated into discovery pipelines at scale, highlighting key opportunities for accelerating candidate selection and improving developability. It will also address ongoing challenges—including data quality, model interpretability, and cross-disciplinary integration—that must be overcome to realize the full potential of AI-driven antibody discovery.



11:35 AI for Antibody Design - Going Beyond the Static

Charlotte M. Deane, PhD, Professor, Structural Bioinformatics, Statistics, University of Oxford; Executive Chair, Engineering and Physical Sciences Research Council (EPSRC)

We can now computationally predict a single, static protein structure with high accuracy. However, we are not yet able to reliably predict structural flexibility. This ability to adapt their shape can be fundamental to their functional properties. A major factor limiting such predictions is the scarcity of suitable training data. I will show novel tools and databases that help to overcome this.



12:05 pm Redesigning Antibody CDRs to Improve Developability Properties Using Machine Learning

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

Antibody complementarity-determining regions (CDRs) form complex 3D surfaces that mediate high-affinity interactions with their target antigens. Some of the same sites in CDRs that mediate specific antibody binding also mediate undesirable developability properties. Here, we report methods for redesigning antibody CDRs—including those at sites in or near the paratope—to improve developability while maintaining high affinity and specificity.

12:35 Transition to Lunch

12:40 LUNCHEON PRESENTATION: Ginkgo Datapoints Antibody Developability Competition Outcomes: Limited Model Performance and a Call for Data Standardization



Josh Moller, Senior Biological Engineer, AI, Ginkgo Datapoints

Antibody clinical viability depends critically on developability attributes, yet predictive model development is hampered by limited, heterogeneous data and poor generalization. To address this gap, we established the 2025 Ginkgo Datapoints Developability Competition, creating a new, blinded benchmark for developability modeling. We will share key observations of the competition, including model overfitting and limited out-of-distribution generalization. Future advances in modeling require larger, standardized datasets and more rigorous evaluation frameworks to translate predictive models into reliable design tools.

1:10 Session Break

1:45 Refreshment Break in the Exhibit Hall with Poster Viewing



2nd Annual

ML/AI for Biologics Developability, Optimization, and *de novo* Design

Unfolding Applications and Real-World Examples

USE OF STRUCTURE-PREDICTION METHODS TO UNCOVER BIOLOGY AND MECHANISMS

2:15 Chairperson's Remarks

Maria Wendt, PhD, Global Head (Vice President) of Digital and Biologics Strategy and Innovation, Large Molecule Research, Novel Modalities, Synthetic Biology and AI, Sanofi

2:20 Biomolecular Modeling with Boltz

Jeremy Wohlwend, PhD, CTO, Boltz

Accurately modeling biomolecular interactions is a central challenge in modern biology. While recent advances have substantially improved our ability to predict biomolecular complex structures, these models still fall short in predicting binding affinity and generating accurate *de novo* designs. Here, we present the Boltz model series, open-source models for structure, binding affinity, and design that provide a robust and extensible foundation for both academic and industrial research.

2:50 AI-Assisted Protein Design to Rapidly Convert Antibody Sequences to Intrabodies Targeting Diverse Peptides and Histone Modifications

Tim Stasevich, PhD, Associate Professor; Dean and Ping Ping Tsao Professor of Biochemistry; CSU Monfort Professor Boettcher Investigator, Biochemistry & Molecular Biology, Colorado State University

An AI-guided pipeline will be discussed that integrates AlphaFold2, ProteinMPNN, and live-cell screening to convert conventional antibody sequences into functional intrabodies for use inside living cells. Our approach optimizes antibody frameworks while preserving epitope-binding regions, rescuing 18 previously nonfunctional sequences—including a panel for imaging histone modifications. This method offers a scalable, cost-effective route to intrabody development and opens new doors for live-cell imaging and functional studies.

3:20 Sponsored Presentation (Opportunity Available)

3:50 Sponsored Presentation (Opportunity Available)

4:20 Refreshment Break in the Exhibit Hall with Poster Viewing

4:50 Interactive Breakout Discussions

Engage in in-depth discussions with industry experts and your peers about the progress, trends, and challenges you face in implementing ML/AI in your work! Interactive discussion groups play an integral role in networking with potential collaborators, provide an opportunity to share examples from your work, and allow you to be part of a group problem-solving endeavor. Please visit the Interactive Breakouts page on the conference website for a complete listing of topics and descriptions.

TABLE 3: Large-Scale Antibody Discovery Benchmarking Challenge #2

Andrew R.M. Bradbury, MD, PhD, CSO, Specifica, an IQVIA business

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

- Review launch of the next phase of the Antibody Competition Series, during which participants will have four months, using any method (*in vivo* immunization, *in vitro* techniques, or ML/AI) to generate human antibodies against targets to be revealed at the challenge's start
- Evaluate target affinity, developability (minimum score), and submission time
- Summarize goals of the challenge

TABLE 4: Structure-Guided Antibody and Immunogen Design

Monica L. Fernandez-Quintero, PhD, Staff Scientist, Integrative Structural and Computational Biology Department, Scripps Research Institute

- Structural biology to map epitope footprints—how important is it still to define epitopes/paratopes experimentally for precise targeting—is AI already there?
- Structure prediction and computational design—machine learning or physics-based?
- Antibody challenges—structure prediction, dynamics, design, diversity, glycan shields, breadth
- When will we have an AI designed therapeutic/vaccine?

5:40 Close of Day

THURSDAY, JANUARY 22

8:00 am Registration Open

PLENARY KEYNOTE SESSION

8:25 Welcome Remarks

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

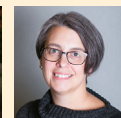
8:30 Plenary Keynote Introduction

Andrew Nixon, PhD, Senior Vice President, Global Head Biotherapeutics Discovery, Boehringer Ingelheim Pharmaceuticals Inc.



8:35 New Frontier of Biotherapeutic Discovery: Where Machine Learning Meets Molecular Design
Stephanie Truhlar, PhD, Vice President, Biotechnology Discovery Research, Eli Lilly and Company

9:00 PLENARY FIRESIDE CHAT: End-to-End *in silico*-Designed Biologics



Moderator: Andrew Nixon, PhD, Senior Vice President, Global Head Biotherapeutics Discovery, Boehringer Ingelheim Pharmaceuticals Inc.

- How is the path to drug development different with ML/AI?
- How far off is *de novo* design for biologics? For antibodies?
- How is ML/AI used for target selection?
- How do you accelerate DMTA cycles?
- Data standardization—how to incorporate historical data?
- Federated learning—how do you ensure you have enough data to build a model?
- Promoting change management

Panelists:

Charlotte M. Deane, PhD, Professor, Structural Bioinformatics, Statistics, University of Oxford; Executive Chair, Engineering and Physical Sciences Research Council (EPSRC)

Garegin Papoian, PhD, Co-Founder & CSO, DeepOrigin

Stephanie Truhlar, PhD, Vice President, Biotechnology Discovery Research, Eli Lilly and Company

9:30 Coffee Break in the Exhibit Hall with Poster Viewing

WOMEN IN SCIENCE MEET-UP

Meet the Moderators at the Plaza in the Exhibit Hall

Michelle R. Gaylord, MS, Former Principal Scientist, Protein Expression & Advanced Automation, Velia Therapeutics

Deborah Moore-Lai, PhD, Vice President, Protein Sciences, ProFound Therapeutics

PROTEIN DESIGN AND ML-BASED STRUCTURE PREDICTIONS

10:20 Chairperson's Remarks

Monica L. Fernandez-Quintero, PhD, Staff Scientist, Integrative Structural and Computational Biology Department, Scripps Research Institute



2nd Annual

ML/AI for Biologics Developability, Optimization, and *de novo* Design

Unfolding Applications and Real-World Examples

10:25 Targeted Protein Design and Down-Selections for Diagnostics and Therapeutics

Johannes Loeffler, PhD, Postdoctoral Researcher, Ward Lab, Scripps Research Institute

De novo protein design traditionally overlooks conformational dynamics and desolvation—factors critical for protein function. We introduce a computational workflow that integrates these properties at the earliest design stages. By analyzing molecular dynamics and calculating desolvation energies, our approach more effectively identifies viable candidates than static methods. This strategy boosts the predictive power of design tools, significantly improving the success rate for developing stable and functional proteins.

10:55 Next-Generation Rationally Designed Vaccines for Broad Influenza Immunity

Kylie Konrath, PhD, Postdoctoral Fellow, Department of Integrative Structural and Computational Biology, Scripps Research Institute

Influenza vaccines tend to induce strain-specific antibodies against the hemagglutinin (HA) protein that protect against a narrow range of strains, thus requiring updated annual vaccines for ongoing protection. Rare, broadly reactive antibodies that recognize a diverse range of influenza HAs have been isolated from humans. We explore these broadly reactive antibodies as templates for designing universal vaccines for influenza.

11:25 *De novo* Antibody & VHH Library Design Using Diffusion, GNN, and Language Models

Leigh J. Manley, PhD, Scientist, Machine Learning, Seismic Therapeutic

Generating a library of antibody designs that is epitope-specific and highly developable is extremely challenging. There have been few, if any, studies rigorously combining and comparing design approaches to identify an optimal toolbox. To systematically address this problem, we compared exhaustive combinations of classical and deep learning-based methods according to their relative success rates in yeast display binding measurements. This allowed us to identify optimal workflows for similar design efforts.

AI-DRIVEN PROTEIN DESIGN WITH EXPERIMENTAL VALIDATION (CONT.)

11:55 LICHEN: Light-Chain Immunoglobulin Sequence Generation Conditioned on the Heavy Chain and Experimental Needs

Henriette Capel, PhD Student, University of Oxford

In developing therapeutic antibodies, the heavy chain is often prioritized while appropriate pairing of the light sequence is important for functionality. We introduce LICHEN, a heavy-chain-conditioned light sequence generation tool that enables collaborative design by leveraging computational capabilities alongside experimental expertise. LICHEN generates valid and diverse light sequences which are a fit for the heavy sequence, as demonstrated with high expression yields and retained affinity *in vitro*.

12:25 pm Transition to Lunch

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

1:00 Ice Cream & Cookie Break in the Exhibit Hall with Last Chance for Poster Viewing

AI FOR DESIGNING DEVELOPABLE MULTISPECIFIC ANTIBODIES

1:40 Chairperson's Remarks

Amy Wang, PhD, Structural & Computational Biologist, Prescient Design, Genentech

1:45 Predictive Modeling for Bi- and Trispecific Antibodies

Frédéric Dreyer, PhD, Senior ML Scientist, Prescient Design

Computational models are now widely used to predict critical antibody properties such as binding affinity, immunogenicity, and developability. While most AI-driven methods have been tailored for conventional monoclonal antibodies, the therapeutic landscape is increasingly dominated by complex multispecific formats. This talk will address this gap by focusing on property modeling for bi- and trispecific antibodies.

2:15 Developability and Molecular Assessment of Multispecifics

Hubert Kettenberger, PhD, Head, Computational Protein Engineering, Roche

The growing interest in bi- and multispecific therapeutic proteins stems from their unique modes of action. While significant progress has been made in predicting developability for standard antibodies, these complex formats present ongoing research challenges, highlighting the need for improved tools. This presentation will discuss various *in silico* approaches (and their associated remaining challenges) aimed at predicting the critical features required for designing developable multispecific drug candidates.

2:45 Multibodies: Multispecific Antibodies with High Affinity and Specificity and Good Developability Profile Designed Using AI

Reshef Shilon, Director of AI, Biologic Design

Design of multispecific biologics typically involves connecting different subunits that bind different targets. These non-natural asymmetric formats present major developability challenges, including poor expression, suboptimal stability, high immunogenicity, charge asymmetry, and manufacturing difficulties. Here, we show AI usage for designing multibodies: natural, symmetric IgG antibodies that are multispecific and highly developable. We present numerous examples of multibodies with experimental data suggesting that multibodies can solve many challenges of therapeutic multispecifics.

3:15 Expanding *in silico* Developability Assessment from Conventional Antibodies to Multi-Specifics

Jenna Caldwell, PhD, Associate Principal Scientist, Early Stage Formulation Sciences & Biopharmaceutical Development, AstraZeneca

AstraZeneca's InSiDe (*In Silico* Developability) platform provides cross-pipeline insights into antibody developability risk via machine learning models for non-specific binding, self-association, chemical liabilities, etc. As interest in multi-specific therapeutics grows, so does the need for *in silico* developability predictions for these complex formats, posing additional challenges relative to conventional antibodies. Here, we identify gaps where computational approaches used for conventional antibodies are insufficient and discuss approaches to overcome these hurdles.

3:45 PANEL DISCUSSION: Toward Improved Multispecific Antibody Design

Moderator: Frédéric Dreyer, PhD, Senior ML Scientist, Prescient Design

- Can AI improve and streamline production of complex format antibodies?
- Which predictive methods will benefit the most from collecting bespoke data, and what data should be prioritized?
- Can structure inform better modeling capabilities?
- How can we achieve a standardization of data across formats and assays?

Panelists:

Victor Greiff, PhD, Associate Professor, University of Oslo; Director, Computational Immunology, IMPRINT

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

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

Stephanie Truhlar, PhD, Vice President, Biotechnology Discovery Research, Eli Lilly and Company

4:15 Close of BioLogic Summit

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