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December 5-7 | Boston, MA
www.cdd-biologics.com

CDD For Biologics

Optimizing the Development of Biologics Through the Application of Computational Tools

Expert Speakers Including:

Stanley Krystek
Senior Principal Scientist
Bristol Myers-Squibb

Chris Roberts
Professor & Director
University of Delaware

Vanita Sood
Global Head of Drug Structure, Prediction & Design
EMD Serono

Sarah Sirin
Structural Bioinformatician
AbbVie

Bernhardt L. Trout
Professor of Chemical Engineering
MIT

"I'm impressed by how much I learnt by attending the conference. It's a great opportunity to learn the key issues facing the industry and various strategies to address them. It was very rewarding"
Liwei Li, EMD Serono

Program Partner: CHEMICAL COMPUTING GROUP

Lead Partner: SCHRÖDINGER.

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Tel: +1 212 537 5898 Email: info@hansonwade.com
www.cdd-biologics.com Computational Drug Development for Biologics

Welcome to the 2nd Annual Computational Drug Development for Biologics Summit

Harness the Additive Power of In Silico Tools for Biologics

Biologics have increased in prevalence and value in the global marketplace and have continued to become more complex, both by modality and by delivery.

The potential for computational tools to add tangible value to the development of biologics is huge, yet this potential remains largely untapped. CDD for Biologics is dedicated to harnessing the power of in silico tools, to de-risk drug development from early drug discovery through to late preclinical development.

Building upon the framework and success of its inaugural meeting, we will once again gather computational thought leaders in pharma, academia and software providers along with the end-users in computational and structural biology to debate how best to add immediate value to biologics pipelines.

Through sharing novel insights from our industry leading faculty, we will explore how best to add immediate value to biologics pipelines. Discuss: how to improve predictability of target ID and validation, understand protein/protein interactions, enhance rational candidate selection, and optimize developability characteristics.

> The conference offered excellent opportunities for networking. The question and answer sessions were very lively and the panel discussions equally free-flowing with ideas. Everyone I met cared a lot about the field of computational drug development
>
> **Eliud Oloo, Sanofi Pasteur**

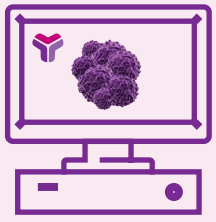
> The conference as a whole expanded my appreciation of the challenges and opportunities in the field
>
> **Enrico Purisima, NRCC**

> Excellent conference and very well organized
>
> **Rafael Depetris, Kadmon LLC**

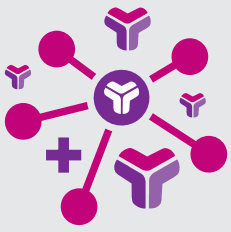
What's New For 2017

1. **A spotlight on the organizational barriers preventing industry wide adoption and implementation**

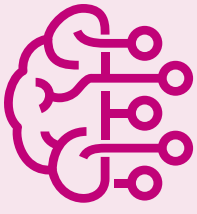
2. **New insights into how computational tools are being utilized to optimize the developability of large molecules**



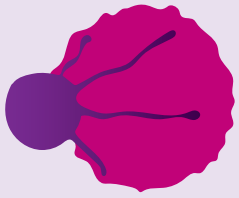
3. **More case studies spanning the applications of in silico methods from discovery, design and PKPD**



4. **Greater understanding for the applications of deep learning and AI in computer aided design of biologics**



5. **Greater focus on the landscape beyond MAb's. Explore how these tools are being utilized to improve the development of bispecific, bacteriotherapy's and mRNA-based therapeutics**



Your Expert Speakers

Jeffrey Way
Senior Staff Scientist, Wyss Institute
Harvard University

Vanita Sood
Global Head of Drug Structure, Prediction & Design
EMD Serono

Stanley Krystek
Senior Principal Scientist
Bristol-Myers Squibb

Satyendra Kumar
Scientist II
EMD Serono

Rafael Depetris
Principal Scientist I
Kadmon Corporation

Sarah Sirin
Structural Bioinformatician
AbbVie

Sandeep Somani
Senior Scientist - High Performance Computing
Janssen

Pratap Singh
Director
Alexion Pharmaceuticals

John Rhoden
Sr Research Scientist
Eli Lilly and Company

Donald Mager
Professor of Pharmaceutical Sciences
University at Buffalo SUNY

Chris Roberts
Professor
University of Delaware

Dheeraj Singh Tomar
Postdoctoral Fellow
Pfizer

Bernhardt L. Trout
Professor of Chemical Engineering
MIT

Tushar Jain
Senior Scientist
Adimab

Feng Dong
Sr. Scientist
Abbvie BioResearch Center

Georg K. Gerber
Assistant Professor, Harvard Medical School, Co-Director
MA Host-Microbiome Center

Varun Shivashankar
Senior Scientific Computing Engineer
Novartis Institutes for Biomedical Research

Johannes Maier
Principal Scientist
Schrodinger

John Gunn
Senior Research Scientist
Chemical Computing Group

"High praise for gathering such a high-quality group of thought leaders for such a specialized discipline"

Steven Darnell, DNASTAR

PRE-CONFERENCE WORKSHOP

Using Computational Tools To Design & Optimize Novel Biologics

Tuesday, December 5 | 2pm – 5pm

Biologics have emerged as frontline medicines to combat a number of conditions. However, despite some successes, a number of these therapeutic approaches, such as CAR-T's, have taken a very long time to develop. Other approaches, such as the recently withdrawn from market ADC, Mylotarg, have led to unexpected failures. Meanwhile approaches such as antibody-dependent pro-drug therapy (ADEPT) and targeted biologic toxins (e.g. pseudomonas exotoxin) seemed like good ideas, but failed to progress in spite of years of testing.

The goal of this session is to understand quantitative issues around successes and failures of multi-component biological drugs. Here, we will explore the novel quantitative design challenges around such new therapies to answer:

- Why do some of these approaches require so many iterations?
- What went wrong?
- Can you identify if your candidate drug has the same problems as these other problematic therapies?

Workshop Leader

Jeffrey Way, Senior Staff Scientist, Wyss Institute, **Harvard University**

Jeffrey Way, Ph.D. (CEO) is a Senior Staff Scientist at Harvard's Wyss Institute for Biologically Inspired Engineering, where he has led work on targeted fusion proteins and synthetic biology since 2009. Dr. Way is also the founding CEO of General Biologics, Inc.; this Company's goal is to commercialize highly engineered and tissue-targeted fusion proteins. Previously Dr. Way was a Director of Structural Biology and Director of Intellectual Property at a Boston-based unit of Merck KGaA, where he built and led a team that evaluated and conceptualized new engineered proteins based on structural, functional, competitive and IP considerations. He is an inventor on over 10 distinct issued patents on protein engineering and drug development, and an inventor/coauthor on additional patent applications and over 50 scientific publications on drug development, synthetic biology and basic research. While at Merck KGaA he led preclinical R&D for an erythropoietin-based product that entered clinical trials. Dr. Way has served on the DARPA ISAT Synthetic Biology Study Group and as a judge for the iGEM synthetic biology competition. Dr. Way was a professor at Rutgers University and a post-doctoral fellow with Martin Chalfie at Columbia. Dr. Way received his B.A. and Ph.D. from Harvard University.

"I enjoyed this conference and look forward to future conferences around the developing field"

Monica Berrondo, Macromoltek

"Strong program, great speakers and a genuine focus on identifying solutions"

Novartis

Conference Day One | Wednesday, December 6

Breaking Down Barriers to Reduce Organizational Inertia for CDD for Biopharmaceuticals

Vanita Sood
Global Head of Drug Structure, Prediction & Design
EMD Serono

8.00 Atom-Rich, Data-Poor: How Can We Utilize Structural Modeling & Machine Learning Tools Together to Enhance Biologics Development?

- Overview of modeling tools used at EMD Serono
- Exploring practical applications in biologics discovery
- Outlook for the future: what do we need to do now to maximize in silico optimization of our future drugs?

Vanita Sood
EMD Serono

Sarah Sirin
AbbVie

Stanley Krystek
Bristol-Myers Squibb

8.30 Panel Discussion and Open Q&A: Why CDD & Why Now?

- Developing cross-industry collaborations that encourage data and open library development
- Defining a strategic framework for the changing landscape of biotherapeutic development
- Business process engineering: exploring ways to enhance cross departmental collaboration and communication

9.15 Speed Networking & Morning Refreshments

Johannes Maier
Principal Scientist
Schrodinger

10.15 A Computational Tool Set for the Detection of Liabilities in Bio-Therapeutics

- Identification of aggregation hotspots that is based on the calculation of hydrophobic and electrostatic surface patches on the interaction surface of 3D structures
- Scoring function for aggregation propensity factoring in the intensity, size and relative orientation of the respective surface patches
- Using this approach we can demonstrate how aggregation prone regions can be identified and rationally explained using the Protein Surface Analyzer tool
- The concept of the surface patches has also been employed to develop a series of descriptors that are used in combination with other protein-specific descriptors to derive QSAR-based prediction models for aggregation, solubility and viscosity

Antigen Engineering for Feature Selection of Candidate Therapeutics

Stanley Krystek
Senior Principal Scientist
Bristol-Myers Squibb

10.45 "Garbage In, Garbage Out": Liability Models for Antigen Design

- Highlighting approaches used for antigen design
- Epitope steering leads to diverse antibody repertoire
- Modeling epitope/paratope contact residues

Satyendra Kumar
Scientist II
EMD Serono

11.15 Computational Prediction of Antigen Driven Secondary Immune Repertoire for Novel Antibody Discovery

- Exploring the use of error and biases free NGS library preparation to capture original B cell diversity
- Demonstrating feature selection/engineering relevant to antibody discovery
- Highlighting the uses of machine learning in antibody discovery from total B cell repertoire
- Showcasing a comparison of in silico predicted hits with conventional methods (yeast display library) for affinity

Rafael Depetris
Principal Scientist I
Kadmon Corporation

11.45 Analysis of Antibody - Antigen Interactions by Directed In-Silico Modeling & Generation of Interface Fingerprints

- Demonstrating modeling of an antibody-antigen interface and its validation
- Describing the different inputs that improve modeling accuracy
- Showcasing cutting-edge tools to generate fingerprints of protein surfaces and their impact on the classification of binding sites
- Revealing the utility of antibody-antigen interface fingerprint to predict the binding energy through a vector regression model

12.15 Lunch & Networking

In Silico Approaches for Macromolecular Discovery

Sarah Sirin
Structural Bioinformatician
AbbVie

1.15 Computational Antibody Design: Computational Tools for Accelerating Antibody Design & Discovery

- The need for high-affinity and high-specificity antibodies in research and medicine
- Modeling fundamental physical-chemical principles that regulate activity
- Highlighting the utility and performance of computational tools in antibody engineering

John Gunn
Senior Research Scientist
Chemical Computing Group

1.45 Prediction of Protein-Protein Binding Sites & Epitope Mapping

- Protein surface patch analysis and characterization with patch-type interaction fingerprints
- Conformational ensemble methodology for computational prediction of protein binding motifs
- Direct incorporation of experimental HDX data in identifying and scoring interactions

Sandeep Somani
Senior Scientist - High Performance Computing
Janssen

2.15 High-Throughput In Silico Assessment of Antibody Developability

- Exploring case studies of experimental validation of developability prediction models
- Questioning whether useful predictions can be made based on antibody homology models
- Highlighting approaches for incorporating structural flexibility in prediction models
- Considerations for incorporating predictive models in antibody discovery programs

2.45 Afternoon Refreshments & Networking

Accelerating Biologics Discovery & Development Using Mechanistic PK/PD Modeling

Pratap Singh
Director
Alexion Pharmaceuticals

3.45 Optimal Affinity of Monoclonal Antibodies: Guiding Principles Derived from the Mechanistic Modeling Analyses

- Highlighting general principles or rules of thumb to determine the optimal affinity range for monoclonal antibodies against three of the most common types of targets:
- Soluble membrane-bound targets that internalize, targets that exist in both membrane-bound and shed soluble forms
- Demonstrating that, similar to the Lipinski's rule of 5 for small molecule drugs, these general principles are developed to provide actionable guidance for project teams considering biotherapeutic drug development

John Rhoden
Sr Research Scientist
Eli Lilly and Company

4.15 Design Criteria for Bispecific Antibodies: Learnings from Mathematical Modeling

- Showcasing in silico and experimental data for the enhanced potency of bispecific antibodies relative to the combination of parental mab
- Highlighting the utility of mathematical models for bispecific antibody interactions with their cellular receptor targets in designing antibodies with optimal affinity, valency, and structure
- Detailing the preclinical effort to support predictions and engineer a novel bispecific to minimize clearance while maintaining target cell binding
- Providing insight into non-intuitive mechanisms and features of bispecifics, such as the role of the relative antigen density of the target receptors

Donald Mager
Professor of Pharmaceutical Sciences
University at Buffalo SUNY

4.45 Quantitative Predictions of Target Mediated Drug Disposition of Monoclonal Antibodies from Preclinical to Clinic

- The basic tenets and expectations of target-mediated drug disposition (TMDD)
- Contrast simple compartmental and physiologically-based models of TMDD properties
- Highlight examples in which mechanistic TMDD models are used to translate preclinical pharmacokinetics to humans and guide antibody drug development

5.15 Close of Day One

SCHRÖDINGER.

5.20 Drinks Reception – Kindly sponsored by Schrodinger

Relax with after a hard day's learning with your peers and take this great opportunity to network over drinks and canapes

Conference Day Two | Thursday, December 7

In Silico Modeling for Antibody Engineering & Risk Mitigation

Chris Roberts
Professor
University of Delaware

8.30 Balancing Coarse-Grained & Molecular Models to Predict Low & High Concentration Protein-Protein Interactions

- Assessing different levels of coarse-grained molecular models to predict attractive vs. repulsive protein-protein interactions at low and high protein concentrations
- Balancing the level of structural resolution with the computational burden for predictions of protein-protein interactions
- Methods to identify key domain-domain interactions or amino acid pairings that cause strong attractions that promote protein aggregation

Dheeraj Singh Tomar
Postdoctoral Fellow
Pfizer

9.00 Predictive Tools for Developability Assessment of Antibody Molecules

- Introducing biopharmaceutical informatics, an approach to predict antibody solution properties using standardized experiments, molecular modeling, and machine learning
- Describing all the experiments performed and discuss how experimental properties are related to each other
- Presenting equations to predict protein-protein interactions from molecular modeling and machine learning

9.30 Morning Refreshments & Networking

10.30 Roundtable Discussions Followed by Moderator Feedback & Audience Debate

This 2 hour session offers the opportunity to catch up on the latest advancements within the field and learn from your fellow colleagues in this interactive and informal format. A valuable chance for attendees to unite around hot topics and debate best practice. No more sitting quietly, this is a dedicated opportunity for you to voice your experiences and identify unique solutions.

1. Informing computational models through insights from bioinformatics

2. Balancing Model Complexity Against Function

3. Formulation design for biologics in the age of lab automation and biological performance screening

4. Predicting biophysical characterisation to enhance candidate selection and lead optimisation

12.30 Lunch & Networking

Advanced Molecular Assessment Tools for Antibody Design

Bernhardt L. Trout
Professor of Chemical Engineering
MIT

1.30 Enabling Developability via Molecular Modeling

- Reviewing key molecular assessment developability tools, their scope, and validation
- Exploring cutting-edge approaches for formulation analysis and design
- Highlighting strategies for implementation of developability

Tushar Jain
Senior Scientist
Adimab

2.00 Machine Learning for Predicting Developability from Sequence

- Discussing experimental data to validate and motivate in silico model development
- Applying algorithm to predict experimental data
- Utilizing HTP methods to design and prioritize antibody libraries

2.30 Afternoon Refreshments & Networking

Applying MAb Learnings to the Developability of Other Biologic Modalities

Feng Dong
Sr. Scientist
AbbVie BioResearch Center

3.00 Predicting Biophysical & Drug-Like Properties of Bi/Multispecific Molecules

- Using rationale-design to enable manipulation of agonist function
- DVD-IG: overcoming issues in combining two or more variabile domains
- Highlighting the necessity of stability and interface engineering

Georg K. Gerber
Assistant Professor, Harvard Medical School, Co-Director
MA Host-Microbiome Center

3.30 Computational Modeling of Precision Bacteriotherapies

- Showcasing what precision bacteriotherapies are and articulating the challenges in designing and predicting the effects of such therapies
- Providing a conceptual understanding of dynamic systems based modeling for bacteriotherapy applications
- Develop a conceptual understanding of approaches for inferring dynamical systems model parameters from in vivo microbiome data

Varun Shivashankar
Senior Scientific Computing Engineer
Novartis Institutes for Biomedical Research

4.00 Identifying Global Trends Across the RNA Binding Protein (RBP) Interactome Using Deep Learning

- Integrating RNA structure and genome sequence knowledge of cognate binding elements with our eCLIP data to have a better understand of binding dynamics
- Leveraging this learning model in predicting RBP binding site on a genomic scale and porting this to cell lines without eCLIP data
- Expanding scope of model to predict other interaction fingerprints

4.30 Close of Conference

"I'm impressed by how much I learnt by attending the conference. It's a great opportunity to learn the key issues facing the industry and various strategies to address them. It was very rewarding"

Liwei Li, EMD Serono

PARTNER WITH US

WHY PARTNER?

If your business strategy is to target biotherapeutic developers, CDD for Biologics is a critical step in advancing your success.

Building on the successful framework of its inaugural meeting, CDD for Biologics offers you the ideal platform to both assess the needs of drug developers and to demonstrate your expertise in this emerging and impactful area.

Meet the decision-makers from pharma and biotech who are committed to speeding up the development of their biotherapeutic pipeline. Showcase your company's expertise and become a partner of choice. Generate new business leads, and source opportunities for partnerships. Act now to stay ahead of the curve and maximize the wealth of opportunity on offer.

To find out more, email sponsor@hansonwade.com

> "I very much enjoyed this computationally-focused symposium on biologics. Lots of opportunities to connect with people in the field"
>
> **Ye Che, Pfizer**

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Schrödinger is a science and technology leader in developing chemical simulation software aimed at transforming drug discovery research. The company's products are used by nearly all the top pharmaceutical companies worldwide. Schrödinger also engages in drug discovery collaborations utilizing its best-in-class software solutions for modeling small molecules and protein therapeutics.

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CCG (Chemical Computing Group) is a leading supplier of software solutions for life sciences. With a proven track record in scientific innovation, CCG continues to provide state-of-the-art applications in drug discovery to pharmaceutical, biotechnology and academic researchers. CCG's software platform is the Molecular Operating Environment (MOE) which is used by computational chemists, medicinal chemists and biologists in the major pharmaceutical and biotechnology companies throughout the world.

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3 EASY WAYS TO BOOK

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1. Gain invaluable insights to improve the developability and manufacturability of your biologics pipeline
2. Understand how the industry leaders have applied computational tools to benchmark against their progress
3. Leave with clear actionable insights to enhance the integration of computational tools at your organization

SECURE YOUR PLACE

INDUSTRY PRICING	Register & Pay By October 6	Standard Rate
Conference + 1 Workshop	$2998 **(save $400)**	$3198 **(save $200)**
Conference Only	$2499 **(save $200)**	$2699
Workshop Only	$699	

ACADEMIC/ SMALL BIOTECH PRICING	Register & Pay By October 6	Standard Rate
Conference + 1 Workshop	$1798 **(save $400)**	$1998 **(save $200)**
Conference Only	$1499 **(save $200)**	$1699
Workshop Only	$399	

***T&Cs Apply: Small biotech rate is subject to organizer approval. Please visit the event website for more details.**

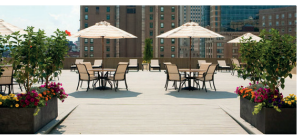
Team Discounts*

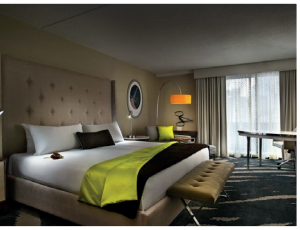
- **10% discount – 3 delegates**
- **15% discount – 4 delegates**
- **20% discount – 5+ delegates**

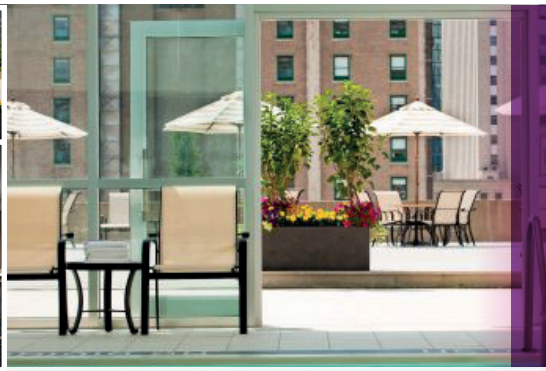
Please note that discounts are only valid when three or more delegates from one company book and pay at the same time.

"Super networking opportunity - I'm sure this has kicked off a couple of long term collaborations"

Bradley Sherborne, Merck & Co.







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