Book now and save up to $500

December 13-15 2016, **Boston, MA**

Computational Drug Development 2016

Optimizing the development of biologics through the application of computational tools

19 speakers, including:

Brad Sherborne
Director, Computer-Aided Drug Design
Merck

Surjit Dixit
CTO
Zymeworks

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

Stanley Krystek
Senior Principal Scientist
Bristol-Myers Squibb

Chris Bailey-Kellog
Professor
Dartmouth College

Arvind Sivasubramanian
Senior Scientist, Computational Biology
Adimab

Sandeep Kumar
Head, Molecular Modeling, Simulations & Data Analyses Center
Pfizer

Jeffrey Way
Senior Staff Scientist
Wyss Institute, Harvard University

Eliud Oloo
Manager, Structure, Genomics & Bioinformatics
Sanofi Pasteur Biologics

- **Improve the success rate of biologic drug development**
- **Apply computational tools to design libraries and select lead candidates more efficiently**
- **Maximize the physical properties of candidates by applying computational approaches**

"This conference was of outstanding value. First class presentations, great opportunity for networking and perfect logistics!"

MedImmune

www.computationaldrugdevelopment.com

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love what you do

Optimize the development of biologics by harnessing computational power

Biologic drugs represent an increasingly significant proportion of company pipelines. The potential for computational tools to add tangible value to the development of biologics is huge, yet this potential remains largely untapped.

Computational Drug Development 2016 will bridge the gap between the application of computational tools for small molecule and biologic drug development. Join your colleagues to discover how to optimize physical properties, robustly predict protein/protein interactions, enhance library design and candidate selection and seamlessly integrate computational tools into the wet lab workflow.

This conference will enable you to learn directly from computational thought leaders in **pharma/biotech**, **academia** and **software provider organizations**. Add immediate value to your drug development process by engaging with **bioinformaticians**, **computational** and **structural biologists**.

Hear what attendees of our biologics events have to say

"The conference content was precisely what we were looking for, and the networking opportunities allowed us to forge new relationships with almost all the groups we were hoping to."

Zymeworks

"This is an eye-opening conference that has brought together the greatest minds in the subject."

Genentech

10 Reasons to Attend Computational Drug Development 2016

1. Investigate how computational tools can **optimize the manufacturability and physical properties of biotherapeutics**
2. Successfully integrate computational and experimental methods to **improve the success rate of drug development**
3. Use predictive computational tools to **optimize the developability of biologics early in drug discovery**
4. Gain invaluable insights into how **informatics, modeling and simulation** can overcome key challenges encountered in the development of biologics
5. **Benchmark against the leaders in the field** to understand how they have effectively integrated in-house and commercially available computational tools into their biologics development workflow
6. Discuss how the field can **leverage the wealth of computational insights gained in small molecule drug development** to impact the development of biologics successfully
7. Beyond monoclonal antibodies: Understand how computational tools can improve the development of **bispecifics**, **peptides**, **vaccines** and **mRNA-based therapeutics**
8. **Reduce development costs** by designing and selecting lead candidates more efficiently
9. Utilize bioinformatics tools to map out target recognition sites and **enhance structure-based biologic drug design**
10. **Examine real-world case studies** detailing how the use of MD simulations, *in silico* affinity maturation and computational structural modeling have enhanced experimental design

Speakers

Joseph Audie
CEO & CSO
CMDBioscience

Chris Bailey-Kellog
Professor
Dartmouth College

Rafael Depetris
Director, Molecular Oncology
Kadmon Pharmaceuticals

Surjit Dixit
CTO
Zymeworks

Feng Dong
Senior Scientist
Abbvie

Sookhee Ha
Principal Scientist, Modeling & Informatics
Merck

Christine Hajdin
Investigator
Novartis

Philip Kim
Associate Professor
University of Toronto

Stanley Krystek
Senior Principal Scientist
Bristol-Myers Squibb

Sandeep Kumar
Head, Molecular Modeling, Simulations & Data Analyses Center
Pfizer

Michelle Lynn Hall
Senior Scientist, Computational Chemistry
Moderna Therapeutics

Eliud Oloo
Manager, Structure, Genomics & Bioinformatics
Sanofi Pasteur Biologics

Deepangi Pandit
Computational Biologist
Cell Signalling Technology

Enrico Purisima
Team Leader, Molecular Modeling
NRC Canada

Dominic Ryan
Independent Consultant

Brad Sherborne
Director, Computer-Aided Drug Design
Merck

Arvind Sivasubramanian
Senior Scientist, Computational Biology
Adimab

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

Jeffrey Way
Senior Staff Scientist,
Wyss Institute, Harvard University

> "The conference was excellent. A lot of speakers from different occupational backgrounds that shed light on various challenges faced."
> **Vertex**

Conference Day One | Wednesday December 14

7.30 **Registration, Coffee & Networking**

Sandeep Kumar
Head, Molecular Modeling, Simulations & Data Analyses Center
Pfizer

8.20 **Chair's Opening Remarks**

Brad Sherborne
Director, Computer-Aided Drug Design
Merck

8.30 **Keynote: More Than Pretty Pictures And Numbers: Opportunities And Lessons From Computational Drug Discovery**

- Transferrable lessons from computational drug discovery: Molecular modelers and data scientists
- Examples of the breadth of impact and versatility of computational approaches
- The science, technology and tool lifecycle as a guide to gaining and maturing impact

Computational Tools To Enhance Biologic Candidate Selection

Stanley Krystek
Senior Principal Scientist
Bristol-Myers Squibb

9.00 **Incorporating Risk Assessment For Protein Therapeutics In Early Discovery Research**

- Discuss the role of discovery research moving beyond optimization of biological activity utilizing antigen design and epitope steering
- Identifying structural or sequence-based elements that may compromise the stability and developability of a given biopharmaceutical using predictive computational tools
- Insights into the role of protein engineering used to generate drug candidates or candidate libraries with improved pharmaceutical properties

Philip Kim
Associate Professor
University of Toronto

9.30 **Integrated Computational And Experimental Methods For Inhibitor Engineering**

- Discover how tight integration of computational and design and screening proves advantageous in many respects
- New approaches in sampling methods take optimal advantage
- Enabling of screening methods that can screen previously untargetable proteins

10.00 **Speed Networking & Morning Refreshments**

Feng Dong
Senior Scientist
Abbvie

11.30 **Fully Automated Structure-Based Antibody Humanization Design**

- Understanding the relationship among antibody sequence, structure and function
- Learn about a fully automated antibody design program including sequence analysis, structure modeling, and structure-based design
- Discussing the impact of the computational design in biologics drug discovery

Interactive group discussion

12.00 **Mastermind: Cross-Industry Perspectives On The Successful Integration Of Computational Tools In The Drug Development Process**

- How can computational tools enhance experimental design?
- Enhancing the communication between bioinformaticians and structural and computational biologists
- Discussing strategies to increase the awareness of computational capabilities within organizations
- Developing clear, testable hypotheses against which computational models can be tested

This session facilitates in-depth discussions between participants in an informal environment. Collaborate with your peers to discuss the most pressing issues in the field and leave with clear, actionable insights to enhance the integration of computational tools at your organization.

12.45 **Lunch & Networking**

Applying Key Computational Approaches To Macromolecular Drug Development

Rafael Depetris
Director, Molecular Oncology
Kadmon Pharmaceuticals

2.15 Structural Analysis Of Fabs By Modeling And X-Ray Crystallography: Two Ends That Meet

- Investigate the structures of two Fabs obtained by modeling and X-Ray crystallography
- Compare the data obtained by either modeling or X-Ray
- Discuss examples of how the structural analysis may lead to the improvement in the affinity of a large molecule therapeutic for its target

Arvind Sivasubramanian
Senior Scientist, Computational Biology
Adimab

2.45 Computational Modeling Of Antibodies And Antibody: Antigen Interactions

- Energy- and knowledge-based modeling of antibody 3D structures
- Structure-based design of antibody libraries
- Computational characterization of antibody: antigen complexes

3.15 Afternoon Refreshments & Networking

Optimizing Drug Discovery Through Bioinformatics And Structural Tools

Christine Hajdin
Investigator
Novartis

3.45 An Informatics Approach To Describing Protein/Protein And RNA/Protein Interfaces

- Methods for docking macro-molecules to predict interfaces
- Advantages of clustering by interface fingerprints
- Predicting homologous interfaces and identifying likely off targets

Eliud Oloo
Manager, Structure, Genomics & Bioinformatics
Sanofi Pasteur Biologics

4.15 Computational Approaches To Designing Novel Vaccine Antigens Targeted At Diverse And Rapidly Mutating Pathogens

- Outline the challenges of designing vaccines against constantly changing targets
- Insights into the application of bioinformatics tools to map out the diversity of the genetic and antigenic landscapes of key antigens
- Investigate practical examples of structure-based antigen design guided by the integration of empirical data with computational modeling and simulation

Michelle Lynn Hall
Senior Scientist, Computational Chemistry
Moderna Therapeutics

4.45 *In Silico* Design Of mRNAs As Novel Therapeutics, From Bioinformatics To Quantum Mechanics

- mRNA therapeutics as an alternative to traditional, biologics-based therapeutics
- Molecular modeling approaches to design novel, synthetic mRNA therapeutics using both proprietary, in-house and commercially-available tools
- Rational, structure-based design to facilitate optimal drug product efficacy

Sandeep Kumar
Head, Molecular Modeling, Simulations & Data Analyses Center **Pfizer**

5.15 Chair's Closing Remarks

Conference Day Two | Thursday December 15

Sandeep Kumar
Head, Molecular Modeling, Simulations & Data Analyses Center **Pfizer**

8.50 **Chair's Opening Remarks**

Sandeep Kumar
Head, Molecular Modeling, Simulations & Data Analyses Center **Pfizer**

9.00 **Keynote: Biopharmaceutical Informatics – A Strategic Vision for Improved Translation of Biologic Drug Discoveries into Medicines**

- Understand the concept of biopharmaceutical informatics and its applications to drug discovery and development
- Enable Materials-free developability assessments via computational tools of informatics and molecular biophysics
- Discover new computational applications to make the biologic drug discovery and development process more efficient

Improving The Developability Of Biologics Using Computation: Focus On Manufacturability

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

9.30 **Combining Informatics, Molecular Modeling And Empirical Approaches For Improved Manufacturability Of Biologics**

- Gain insights into an in-house developed antibody informatics tools and algorithms for use in hit discovery and hit optimization
- Investigate the use of molecular modeling and protein design to streamline antibody optimization and epitope mapping
- The power of combining *in silico* approaches with high throughput *in vitro* and rapid analytical methods

10.00 **Morning Refreshments & Networking**

Surjit Dixit
CTO
Zymeworks

11.00 **Structure Guided Approaches To Multifunctional Therapeutic Protein Design**

- Discuss the elements of computational tools with applications in protein engineering
- Discuss protein engineering as an iterative process of understanding structure-function relationships
- Learn about the development of the Azymetric bispecific antibody platform and its utility

Chris Bailey-Kellog
Professor
Dartmouth College

11.30 **Enhancing Therapeutic Efficacy Through The Computationally-Driven Depletion Of T Cell Epitopes**

- Novel computational methods to optimize biotherapeutics simultaneously for immunogenicity and function
- Examine methods to integrate protein sequence and structure analysis with epitope prediction, and design individual variants or combinatorial libraries
- Examine a case study in which the depletion of T cell epitopes in application to the potent anti-staphylococcal enzyme lysostaphin resulted in a reduced antibody response and consequently enhanced efficacy in an immune competent disease model

Brad Sherborne
Director, Computer-Aided Drug Development
Merck

Stanley Krystek
Senior Principal Scientist
Bristol-Myers Squibb

Deepangi Pandit
Computational Biologist
Cell Signalling Technology

12.00 **Panel Discussion: What Properties Do We Need To Model?**

- Examining the properties that we are currently able to model using computational tools
- Which models are effective? How do we calculate and interpret success?
- How can these models be improved in the future and which properties should modeling tools be applied to?

Hear a variety of perspectives from some of the leading experts in computational drug development. This focused discussion provides the chance to engage with the panellists over any issues that have arisen during the course of the conference program and have your most burning questions answered.

12.45 **Lunch & Networking**

Improving The Developability Of Biologics Using Computation: Focus On Physical Properties

Enrico Purisima
Team Leader, Molecular Modeling
NRC Canada

1.45 **ADAPT (Assisted Design of Antibody and Protein Therapeutics)**

- Assessment of consensus scoring functions for antibody-antigen binding affinity ranking
- Investigate a robust platform for affinity maturation that interleaves *in silico* virtual mutations with experimental validation
- Case studies validating and applying the ADAPT platform

Joseph Audie
CEO & CSO
CMDBioscience

2.15 **Data-Driven And Physics-Based Computer-Enabled Peptide Drug Design With CMDInventus**

- Development and validation of CMDInventus
- Case study one: Using CMDInventus to design peptide modulators of challenging protein-protein interactions
- Case study two: Using CMDInventus to optimize peptide proteolytic stability

2.45 **Afternoon Refreshments & Networking**

Sookhee Ha
Senior Research Fellow **Merck**

3.15 **Optimizing The Permeability Of Peptides**

- Examining physicochemical parameters that are related to permeability
- Discussing library design and selection of peptide using physicochemical parameters
- Analyzing permeability vs target affinity

Jeffrey Way
Senior Staff Scientist
Wyss Institute, Harvard University

3.45 **Quantitative And Spatial Optimization Of Therapeutic Fusion Proteins**

- Constructing a therapeutic fusion protein requires optimizing elements that have evolved in a different context
- Coarse-grained molecular dynamics allow modeling of artificial protein behavior
- Targeted erythropoietin as an optimized, tissue-targeted therapeutic with reduced side effects

Sandeep Kumar
Head, Molecular Modeling, Simulations & Data Analyses Center **Pfizer**

4.15 **Chair's Closing Remarks**

"I was delighted to see how openly technical issues and unsolved scientific problems were discussed."

Agenus

Workshop A

Utilizing Bioinformatics In The Discovery Of Biotherapeutics

Tuesday December 13, 2016 | Time: 9:00am-12:00pm

Biologicals are one of the fastest growing pharmaceuticals. Good science decisions depend on digesting a growing scale of complexity in information. It is important to differentiate data collection and data warehousing from decision making that shapes experimental design.

This workshop will focus on how information feeds experiment.

Examining real-life case studies and examples, this interactive session will discuss how biologics need to satisfy the following key goals:

- Target action (potency, selectivity...)
- Pharmaceutical properties (viscosity, solubility...)
- Drug properties (antigenicity, PK...)
- Safety (surprising biology...)
- Intellectual property protection

Antibody production libraries have been improved. They increase the odds of obtaining well behaved products. Even so, the feedback loop of experiment, selection and properties represents a significant information challenge.

The needed properties benefit from a structural understanding. Crystal structures are now more easily obtained, sources of sequence data are rapidly growing and excellent tools for structural modeling are available. These are increasingly important sources of information but are also increasing in complexity.

This workshop will examine how these factors can enhance experimental design. We will discuss the problems in a pre-competitive setting, share experiences and highlight emerging challenges and solutions.

Workshop leader

Dominic Ryan, Independent Consultant

Dominic Ryan is a drug discovery executive who moves between chemistry and biology, identifying the right question and applying the right and emerging tools to solve tomorrow's problems. Over 26 years in drug discovery, he has built, led and managed high throughput screening, protein crystallography, SPR, compound management, NMR spectroscopy, bioinformatics, cheminformatics, molecular modeling and high throughput purification.

Workshop B

Using Computational Tools To Design And Optimize Novel Biologics

Tuesday December 13, 2016 | Time: 1:00pm-4:00pm

The potential space of multi-component engineered therapeutic proteins is large and has scarcely been explored. In contrast to small molecules, there is no paradigm for design and optimization of such proteins. Attend this workshop for the chance to discuss the landscape of novel biotherapeutics, with a focus on fusion proteins.

Engage directly with computational drug developers and protein engineers to learn how to implement the computational tools that can aid in the design and development of novel protein-based therapeutics. Create novel therapeutics that go beyond monoclonal antibodies and naturally occurring proteins.

Join your colleagues to discuss:

- How to define product profiles that can be achieved by rational design
- How to design useful starting molecules
- How to develop computational tools that can enhance the development of biologic therapeutics
- Factors that contribute to immunogenicity
- Engineering cell and tissue targeting to minimize side effects
- Optimizing pharmacokinetics

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.

Partnership Opportunities

Why partner with us?

The increased prevalence of biologic drugs in pipelines means that drug developers are actively looking to partner with solution providers who can enhance the development of these drug candidates.

Uniting key opinion leaders and influencers from the computational field, Computational Drug Development 2016 is the ideal platform both to assess the needs of drug developer organizations and to demonstrate expertise in this emerging area.

Align your solution with the areas of need that drug developers are experiencing. Our focused delegate audience are looking to partner with:

- **Software Providers** with the ability to demonstrate real-world situations in which their suite of computational tools have enhanced the development of biologics
- **Data Management Companies** with the capacity to gain meaningful insights and extract clear signals from the large and complex data sets
- **Contract Research Organizations** with the expertise and experience to handle the complex outsourced computational requirements of biologic development

To find out more, email sponsor@hansonwade.com

Expect to meet the following job titles:

- Structural biologists
- Bioinformaticians
- Computational chemists
- Biophysicists
- Molecular biologists
- Heads of *in silico* drug design

Companies who have attended our biologics events

abbvie, Adimab, AMGEN, Bayer HealthCare, Bristol-Myers Squibb, Boehringer Ingelheim, Celgene, Eisai, ImmunoGen, Inc., Lilly, EMD Serono, Genentech, GSK, janssen, Kadmon, Lonza, MedImmune, MERCK, moderna, NOVARTIS, novo nordisk, MacroGenics, Pfizer, Roche, Sanofi Pasteur, Shire, REGENERON, SeattleGenetics, zymeworks, Takeda

> "Very useful – combined the delivery of cutting edge research with an opportunity to network. I normally go to major scientific meetings and have always been skeptical that smaller meetings like this could add anything useful – I have been proved wrong!"
>
> **Aquila, previous partner**

> "First class meeting – incredible opportunity to meet directly with a broad range of decision makers in this growing field."
>
> **Quanta Biodesign, previous partner**

Partner With Us

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Pricing

Register

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Team Discounts*

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

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

Top 3 Benefits of Attending

1. Learn how computational tools can enhance library design and candidate selection
2. Investigate how the developability of biologics can be improved using the latest computational approaches
3. Understand how the industry leaders have applied computational tools to benchmark against their progress

Standard Pricing

	Register & Pay before October 7th, 2016	Register & Pay before November 11th, 2016	Standard Prices
Conference + 2 Workshops	$3597 **(save $500)**	$3697 **(save $400)**	$3797 **(save $300)**
Conference + 1 Workshop	$2998 **(save $400)**	$3098 **(save $300)**	$3198 **(save $200)**
Conference Only	$2399 **(save $300)**	$2499 **(save $200)**	$2699
Workshops (each)	$699		

Academic Pricing

	Register & Pay before October 7th, 2016	Register & Pay before November 11th, 2016	Standard Prices
Conference + 2 Workshops	$2197 **(save $400)**	$2297 **(save $300)**	$2397 **(save $200)**
Conference + 1 Workshop	$1798 **(save $300)**	$1898 **(save $200)**	$1998 **(save $100)**
Conference Only	$1399 **(save $200)**	$1499 **(save $100)**	$1599
Workshops (each)	$499		

Venue

Aloft Boston Seaport
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"All talks were divergent and complimented each other well. Venue great, organisers brilliant and friendly."

GSK

Code: 7961