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CDD For Biologics

Harnessing the Additive Power of *In Silico* Tools for Biologics Development

Expert Speakers Include:

Anna Vangone
Postdoctoral Scientist
Roche

Vanita Sood
Senior Director, Global Head of Design, Structure, Prediction & Data science
EMD Serono

Stanley Krystek
Research Fellow, Molecular Structure & Design
BMS

Katrina Lexa
Pathway Leader
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Welcome to Computational Drug Development for Biologics 2019

What if you could improve on nature?

Biologics have always sought to exploit the ingenuity of the human body but now more than ever there is a chance to add to that. Powerful *in silico* tools exist to improve the selection of favorable molecules and optimize their attributes from early discovery through to ~~late stage~~ candidate optimization.

~~4th~~ **CDD for Biologics** gathers the computational thought leaders in biopharma, academia and software providers along with the ~~end users~~ in computational biology, structural biology and bioinformatics to debate how to add immediate value to biologics pipelines.

Join us to learn how to improve predictability of target ID and validation, better understand protein/protein interactions, enhance rational candidate selection and optimize developability characteristics. **How could your pipeline benefit?**

Testimonials from other Hanson Wade ~~CNS~~ events:

"Excellent conference and very well organized"

Kadmon

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

DNASTAR

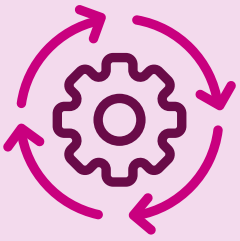
"I enjoyed this conference and look forward to future conferences around the developing field"

Macromoltek

5 INSIGHTS NOT TO MISS

Discover a suite of computational tools to aid assessment of CQAs and **augment overall developability attributes** for your molecule

Bristol-Myers Squibb



Evaluate workflows and novel algorithms to see you how your dataset can be **analyzed with faster throughput**

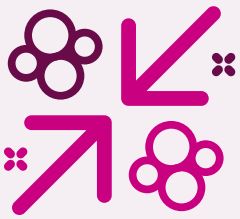
MERCK

Assess structure function relationships and affinity optimization for non-traditional biologics such as bispecifics, prodrugs and domain antibodies

DENALI THERAPEUTICS

Learn about new problem solving software to **aid the identification of tricky molecular signatures** such as charge patches and conformational flexibility

Roche



Develop a **predictive understanding of higher order structure liabilities** and minimize the risks of immunogenicity or off target binding

Voyager THERAPEUTICS

Your Expert Speakers

Pankaj Agarwal
Senior Member
ISCB

Marc Bailly
Associate Principal Scientist
Merck

Naresh Chennamsetty
Senior Scientist
BMS

Rafael Depetris
Principal Scientist I, Structure Based Drug Design
Kadmon

Yao Fan
Senior Scientist III, Biologics Generation Group
Abbvie

Monica Fernández-Quintero
PhD Student
University of Innsbruck

Dana Filoti
Senior Scientist, Analytical R&D,
AbbVie

John Gunn
Senior Research Scientist
Chemical Computing Group

Hubert Kettenberger
Senior Principal Scientist, Protein Engineering
Roche

Stanley Krystek
Research Fellow, Molecular Structure & Design
BMS

Vinodh Kurella
Senior Scientist II
Voyager Therapeutics

Katrina Lexa
Pathway Leader
Denali Therapeutics

Klaus Liedl
Professor, Theoretical Chemistry
University of Innsbruck

Johannes Maier
Principal Scientist
Schrodinger

Dea Shahinas
Director, Computational Biology
Aivie

Vanita Sood
Senior Director, Global Head of Design, Structure, Prediction & Data science
EMD Serono

Anna Vangone
Postdoctoral Scientist
Roche

Maria Wendt
Head, Biologics Research US
Sanofi

Pre-Conference Workshops
Tuesday November 19, 2019

Workshop A
9:00am – 12:00pm

Implementing Machine Learning and AI Technologies

It is undoubtable that AI and Machine Learning are the key technologies that have the potential of changing the course of *in silico* drug development. And as computational power increases, the depth to which teams will be able to interrogate their data to will be unmatched.

As this technology evolves into something more accessible and user-friendly it is important for you to know how to prepare for its arrival. Understand its true capability and advance your pipeline. Attendees will:

- Gain an understanding of the current landscape of computational tools available
- Dive deep on data – what sources, what volume and what processes to train your algorithms and boost predictive power
- Learn to optimize candidate screening, selection and design

Workshop Leader

Stanley Krystek
Research Fellow, Molecular Structure & Design
BMS

Additional workshop contributors:

Dana Filoti
Senior Scientist, Analytical R&D,
AbbVie

Dr. Krystek received his M.S. (1986) and PhD. in Biochemistry from Albany Medical College in 1989. Dr. Krystek joined Bristol-Myers Squibb (BMS) in 1989 and has remained at BMS throughout his 30 year career. Dr. Krystek focused his efforts developing computational methods for protein modeling and drug discovery. He applied computational methods to understanding protein-ligand interactions for important therapeutic targets such as GPCRs, proteases, and NHRs. Dr. Krystek has published over 65 papers in the area of protein structure and modeling including application of QSAR methods to drug discovery, structure-based drug design and GPCR modeling. He is the co-inventor on over 25 patents. Currently Dr. Krystek is a Research Fellow in the department of Molecular Structure and Design where he leads a team that is focused on design and engineering of protein therapeutics.

> "It's a great conference in the sense that we take home not only new methods and models, but more importantly the design and thinking process behind them"
>
> **Yao Fan, Boehringer Ingelheim**

Pre-Conference Workshops
Tuesday November 19, 2019

Workshop A
13:00pm – 16:00pm

In-silico Immunogenicity Predictions (Hands-on Session)

Computational immunogenicity predictions for ~~antibodies~~ as well as ~~pathogens~~ help in the rational design and re-engineering. This facilitates to minimize anti-drug antibodies (ADA) as well as better vaccine design. Latest in-silico tools can shorten the process from design to preclinical validations.

Topics to be covered:

- Computational prediction for T cell and B cell epitopes from primary sequences
- Antigen structure prediction via protein homology model
- Structure or homology model-based Vaccine/ antigen design
- Structural differences between MHC-I and MHC-II binding
- MHC class I and MHC class II predictions from peptide sequences
- Overview on the latest immunogenicity prediction programs

*All materials, including tutorials/exercises, will be available for users during and after the workshop. No prior programming experience necessary. Please bring your laptop for the workshop.

Workshop Leader

Vinodh Kurella
Senior Scientist II
Voyager Therapeutics

Vinodh Kurella currently is a Senior Scientist at Voyager Therapeutics within the Antibody discovery and design group in the Vector Engineering department. He is a protein engineer with a focus on antibody and antigen designs via structure guided computational modeling-based approach. At Merrimack Pharmaceuticals, he was team lead for structure guided antibody engineering, humanization designs and validations. At Intrexon corporation, lead the antibody CAR-T cell designs and optimizations in the Immuno_Oncology division at Intrexon Corporation. He completed his post-doctoral training at Dana Farber Cancer Institute and Harvard Medical school in Dr. Wayne Marasco laboratory and received Ph.D. in Dr. David Worthylake lab from Dept. of Biochemistry at LSU Health Sciences Center in the field of protein X-ray crystallography.

"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

Conference Day One
Tuesday November 20, 2019

8.00 **Registration, Coffee and Networking**

8.50 **Chair's Opening Remarks**

Maria Wendt
Head, Biologics Research US
Sanofi

9.00 **Keynote: Realizing Digitally Driven Drug Development – A Call to Action**

- Where is the field of computational drug development for biologics at?
- The cultural challenges of harmonizing internal departments and stakeholders
- Crunching the numbers; how can we assemble the magnitude of data required to develop more powerful prediction tools?

9.30 **Speed Networking**

This session is the ideal opportunity to meet face-to-face with the key thought leaders working in the neuromuscular field. Specifically designed to connect you with new contacts from the most active companies in the field, the renowned Speed Networking session will be one of the most valuable hours you will spend at CCD for Biologics.

10.30 **Morning Refreshments**

Computationally-Driven Identification of Antibody Epitopes and Enhancement of Binding Affinity

Johannes Maier
Principal Scientist
Schrodinger

11.00 **Improved Scoring Function to Reliably Detect Antigen Binding Sites**

- The progress of genomics and proteomics has provided a great deal of information on the sequences, thermodynamics, kinetics, biological functions, and structures of an ever-growing number of protein complexes. However, these techniques can be expensive and time-consuming
- Although the reliable detection of ~~antigen binding~~ sites has proven to be a severe computational challenge, we introduce an improved scoring function based on the well-established PIPER protein-protein docking engine that factors in terms specific to the binding of antibodies to antigens
- The method was benchmarked on more than 300 publicly available antibody/antigen structures revealing a success rate of more than 90%

Anna Vangone
Postdoctoral Scientist
Roche

11.30 **Roche Antibody Formats: Predict the Epitope to Generate Adequate Bi-specifics or Bi-paratopics**

- A challenge in antibody discovery is to identify, among generated binders, the ones which will hold therapeutic properties
- In silico studies and modelling can provide fundamental help in order to focus on binders and formats with ~~desired~~ (therapeutic) mode of action
- A combination of docking and epitope prediction approaches can successfully drive the design of potential drugs candidates though effective formats

12.00 **Lunch and Networking**

Predicting Immunogenicity and the Impacts of Other On and Off Target Binding

Vinodh Kurella
Senior Scientist II
Voyager Therapeutics

13.00 **Structure Guided Homology Model-Based Humanization of a Mouse Antibody Against Leukemia(B-CLL)**

- Generation of a humanized antibody that specifically targets ~~unique~~ population of leukemic cells that are ~~over expressed~~ in certain B-CLL patients
- Homology model-based humanization designs were successful over sequence-based approaches
- Case study data will be provided with key lessons learned

Stanley Krystek
Research Fellow, Molecular Structure & Design
BMS

13.30 Engineering Safer Antibodies: In Silico Design of Antibody Prodrugs

- X
- X
- X

14.00 Afternoon Refreshments, Networking and Poster Session

Dig into the data during the poster session. Discuss new approaches, assess a variety of case studies and learn from those at the cutting edge of in silico research.

Striving for More Accurate Computer-Aided Prediction of Structure and Function

Hubert Kettenberger
Senior Principal Scientist, Protein Engineering
Roche

15.00 Scope and Limitations of In Silico Feature Prediction in Therapeutic Proteins

- During the discovery process of new biologics, there is a need for identifying molecules with optimal developability properties such as chemical stability, solubility, pharmacokinetics etc
- There is a large number of tools and algorithms out there which can help to identify the root-causes for certain "problems", e.g. charge patches
- Finding algorithms to compare and rank different, unrelated molecules, however, remains challenging

Vanita Sood
Senior Director, Global Head of Design, Structure, Prediction & Data science
EMD Serono

15.30 Designing Superior Scaffolds Using Genetic Algorithms

- More details to be disclosed

Rafael Depetris
Principal Scientist I, Structure Based Drug Design
Kadmon

Yao Fan
Senior Scientist III, Biologics Generation Group
Abbvie

Dea Shahinas
Director, Computational Biology
Aivie

16.00 Panel Session: Predictive Tools for Optimizing Antibody Structure Function and Developability Attributes

- What are the current predictive limits of our technology
- What is more needed; greater computational power or biological understanding
- mAb-ye too difficult? Can more complex biologics (bispecifics, CAR-T etc) be tamed or are they one step too far
- multi-variant optimization –are there "golden rules" which for developability characteristics have the greatest priority

16.45 Chair's Closing remarks and Poster Session Resumes

18.30 End of Day One

Conference Day Two
Wednesday November 21, 2019

8.50 Chair's Opening Remarks

Utilising Current and Novel Predictive Models for Enhanced Forecasting of Developability and Manufacturability

9.00 Computational Tools to Aid in Developability and Early Risk Assessment of Biologics

Naresh Chennamsetty
Senior Scientist
BMS

- Overview of the in silico tools developed to aid in assessing physical and chemical liabilities of biologics such as aggregation, oxidation, deamidation etc
- Demonstrate the use of these tools both in Discovery and Development for developability assessment and in ~~identification~~ of key critical quality attributes (CQAs) during manufacturing
- Case studies will be discussed to showcase the use of computational tools to aid in mechanistic understanding of degradation as well as ~~higher order~~ structural characterization

9.30 Modeling Protein Properties using pH-dependent Conformational Sampling

John Gunn
Senior Research Scientist
Chemical Computing Group

- Sampling protein conformational and charge states using grand-canonical dynamics
- Calculating ensemble-averaged properties and descriptors in a variable-pH ensemble
- Developing models for biologics developability assessment and liability prediction

10.00 Building a Computational Pipeline for Early Developability Assessment and Optimization

Katrina Lexa
Pathway Leader
Denali Therapeutics

- Overview ~~of~~ developability funnel at Denali and impact of structural analysis on predicting aggregation propensity
- Introducing an ML tool for experimentalists to quickly glean insight from their sequence-"activity" data and rationally design next round of variants with improved developability characteristics
- Examples from integrating a design-predict-make-test cycle for antibody engineering and hit triage

10.30 Morning Refreshments and Networking

Implementing the Capabilities of AI and Machine Learning into the Process of Engineering Complex Biologics

11.30 Modifying Discovery Workflow to Utilize Machine Learning Algorithms for Better and Faster Optimization of Biologics

Marc Bailly
Associate Principal Scientist
Merck

- Merck's biologics developability discovery platform
- High throughput analytical characterization data management
- Example of analytical characterization data overview; looking for patterns and correlations in analytical characterization data
- Case study 1: Hydrophobicity and developability profiles
- Case study 2: Thermal stability and developability profiles

Pankaj Agarwal
Senior Member
ISCB

12.00 AI & Machine Learning for High Quality Targets and Disease Indications for Both Biologics and Small Molecules

- Practical and strategic bioinformatics to enable drug discovery
- Published examples of how to use AI and ML to predict clinical successes
- How to find the first and additional disease indications for your assets leveraging ~~computational~~ solutions

12.30 Mastermind Session

This is an interactive session designed to help broaden your understanding of the challenges with the field and potential opportunities. Engage with different industry stakeholders and develop a deeper ~~appreciate~~ for how the field can move forward.

13.00 Lunch and Networking

Computational Tools for Accelerating Antibody Discovery & Lead Selection

Dea Shahinas
Director, Computational Biology
Aivie

14.00 Computational Design of Single Domain Antibodies

- Challenges in the computational design of single domain antibodies
- Selection of scaffolds for single domain antibody design
- Utilization of machine learning and molecular dynamic simulations for single domain antibody design

Klaus Liedl
Professor, Theoretical Chemistry
University of Innsbruck

14.30 Antibody Dynamics from the Nanosecond to Millisecond Timescale – Implications for Affinity Maturation and Humanization

- Linking loop flexibility and affinity maturation
- Relative VH-VL interdomain dynamics
- Kinetics vs. thermodynamics

Monica Fernández-Quintero
PhD Student
University of Innsbruck

15.00 CDR-H3 Loop Dynamics – Implications for Antibody Design and Structure predictions

- Conformational ensembles of CDR-H3 in solution vs. crystal structures
- Induced fit and Conformational selection as paradigms for binding
- Timescales of conformational transitions of loops

15.30 Chair's Closing Remarks

"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

Partnership Opportunities

Program Partner

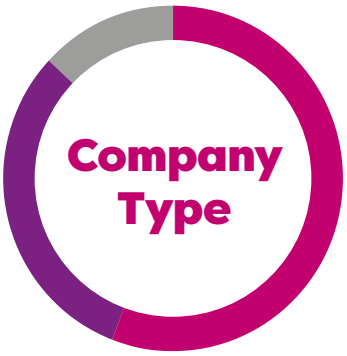
CCG (Chemical Computing Group) is a leading supplier of software solutions for life sciences. With a proven track record in scientific innovation, CCG continues to provide state-of-the-art applications in drug discovery to pharmaceutical, biotechnology and academic researchers. CCG's software platform 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. CCG has a very strong reputation for collaborative scientific support, maintaining support offices in both Europe and North America. Founded in 1994, CCG is headquartered in Montreal, Canada. **www.chemcomp.com**

Program Partner

Schrödinger is a leading provider of advanced molecular simulations and enterprise software solutions that accelerate and increase the efficiency of drug discovery and materials design. Founded in 1990, Schrödinger has nearly 400 employees and operations across the world. For more information, please visit **www.schrodinger.com**

Typical breakdown of Audience:

By Organization Type



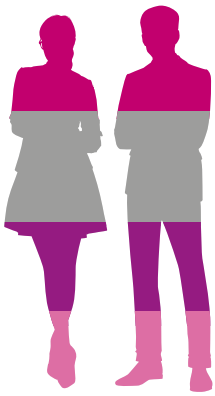
56% Pharma/Biotech

31% Software & Service Providers

13% Academia

* Based on representative attendance from CDD for Biologics 2018

By Function



25% Director & Above

35% Senior/Principal Scientist

31% Scientist

20% Professor

* Based on representative attendance from CDD for Biologics 2018

Companies already attending:

abbvie, Biogen, Chemical Computing Group, distributed bio, EMD Serono, Fox Chase Cancer Center, Genentech, Kadmon, MedImmune, Johns Hopkins School of Medicine, University of Delaware, Amgen, Arzeda, Just, NIH NIAID, Rutgers, Sanofi, The University of Alabama in Huntsville, zymeworks

Get Involved

Diane McKenna
Commercial Director
Tel: +1 508 869 4452
Email: diane.mckenna@hansonwade.com

Ready to Register?

3 Easy Ways To Book

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1. Improve the design, developability and manufacturability of your biologics pipeline
2. Learn and benchmark against industry leaders
3. Leave with clear actionable insights to enhance the integration of computational tools within your organization

Team Discounts*

- **10% discount – 2-3 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.

Discounts cannot be used in conjunction with any other offer or discount. Only one discount offer may be applied to the current pricing rate.

Contact: register@hansonwade.com

SECURE YOUR PLACE

Industry Pricing	Register and Pay before Friday, ~~September 27~~	Standard Rate
Conference + 2 Workshops	$3,299 **(save $600)**	$3699 **(save $200)**
Conference + 1 Workshop	$2,799 **(save $500)**	$3,199 **(save $100)**
Conference Only	$2,299 **(save $400)**	$2,699
Workshop Only	$599	

Academic and Small Biotech	Register and Pay before Friday, ~~September 27~~	Standard Rate
Conference + 2 Workshops	$1,899 **(save $600)**	$2,299 **(save $200)**
Conference + 1 Workshop	$1,599 **(save $500)**	$1,999 **(save $100)**
Conference Only	$1,299 **(save $400)**	$1,699
Workshop Only	$599	

A 40% registration discount is available to allow academicians and newer, less established drug developers to attend this meeting. Email info@hansonwade.com to enquire about the rate or apply.

Eligibility criteria for small biotechs states that the company needs to be less than 10 years old or have fewer than 30 full time employees. Software and service providers are excluded. All bookings at this rate are subject to organizer approval. T&Cs apply.

VENUE

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