TUESDAY SEP 22 | VIRTUAL BIOVIA CONFERENCE 2020 AGENDA

	Quality Track begins 23-Sep				
	Laboratory Informatics	**Pipeline Pilot and Data Science**	**Discovery Studio**	**Materials Innovation**	**Manufacturing**
	7:15 -12 PT |10:15 - 15 ET| 16:15 - 21 CET				
SESSION TITLE	TRACK: **Laboratory Informatics**	TRACK: **Data Science**	TRACK: **Life Sciences Modeling**	TRACK: **Materials Innovation through Modeling and Informatics**	TRACK: **Manufacturing Intelligence**
7:15-8:00 PT 10:15-11:00 ET 16:15-17:00 CET	**PLENARY: BIOVIA and the 3DEXPERIENCE Platform: From New Modalities in Biopharma to Novel Materials and Formulations** Jason BENEDICT, BIOVIA CEO and Reza SADEGHI, BIOVIA CSO				
SESSION TITLE	**ELN**	**SARS-COV-2 CHARACTERIZATION & THERAPEUTICS**	**SARS-COV-2 CHARACTERIZATION & THERAPEUTICS**	**MACHINE LEARNING**	**MANUFACTURING**
8:00-8:20 PT 11:00-11:20 ET 17:00-17:20 CET	**What's New With BIOVIA ELNs** Kirsten GESENBERG, BIOVIA	**Broad-spectrum Antiviral Activity of Naproxen: From Influenza A to SARS-CoV-2 Coronavirus** Anny SLAMA-SCHWOK, Hôpital Saint-Antoine	**Broad-spectrum antiviral activity of naproxen: from Influenza A to SARS-CoV-2 Coronavirus** Anny SLAMA-SCHWOK, Hôpital Saint-Antoine	**Machine Learning for Materials and Formulations** Dana HONEYCUTT, BIOVIA	**Takeda Los Angeles' CPV Journey with BIOVIA Discoverant** Vivian MEDINA and Darren NG - Takeda
8:20-8:40 PT 11:20-11:40 ET 17:20-17:40 CET	**Unleashing the Power Of Pipeline Pilot: Design And Development Of A Next-Generation Balance Interface For Workbook** Marty BERLINER - Pfizer	**Integrative Methods for Structure-Determination: From Laptops to Exascale Supercomputers** Abhishek SINGHAROY, Arizona S.U.	**Integrative Methods for Structure-Determination: From Laptops to Exascale Supercomputers** Abhishek SINGHAROY, Arizona S.U.	**Machine Learned Force Fields and Potential Energy Surfaces** Gabor CSANYI, University of Cambridge	**The Integration of a Quality Management System in Discoverant** Carly MACNAB, UCB Pharma
8:40-9:00 PT 11:40-12:00 ET 17:40-18:00 CET	**Digitalizing Drug Transportation Protocols** Matt DUMOUCHEL, Amgen	**The Pandemic Experience: Using Computational and Experimental Approaches to Identify Inhibitors of SARS-CoV-2** Sean EKINS, Collaborations Pharmaceutical	**The Pandemic Experience: Using Computational and Experimental Approaches to Identify Inhibitors of SARS-CoV-2** Sean EKINS, Collaborations Pharmaceuticals	**Finding an Alternative Refrigerant Chemical Using Material Informatics** Abhijit CHATTOPADHYAY, BIOVIA	**Thermo Fisher Scientific's Multivariate Integrated Data Analytics Solution (MIDAS) Using Biovia's Discoverant** Chris ANDREWS, BIOVIA, Rob PERRY and Matt WESSEL, Thermo Fisher Scientific
9:00 - 9:20 PT 12:00-12:20 ET 18:00-18:20 CET	**Q/A Panel Lead:** Gene TETREAULT	**Q/A Panel Lead:** Hugues-Olivier BERTRAND	**Q/A Panel Lead:** Hugues-Olivier BERTRAND	**Q/A Panel Lead:** Stephen TODD	**Q/A Panel Lead:** Larry FIEGLAND
SESSION TITLE	**LAB TESTING**	**AI-DRIVEN DRUG DESIGN, PART I**	**AI-DRIVEN DRUG DESIGN, PART I**	**MODELING BATTERY MATERIALS**	**MANUFACTURING**
9:20 - 9:40 PT 12:20-12:40 ET 18:20-18:40 CET	**Lab Testing in 21st Century** Gene TETREAULT, BIOVIA	**Raising the Odds of Success in Multi-Objective Optimizations for Drug Discovery** Dana HONEYCUTT, BIOVIA	**Raising the Odds of Success in Multi-Objective Optimizations for Drug Discovery** Dana HONEYCUTT, BIOVIA	**Solvation and Desolvation vs. Electrolyte Design in Li-ion Batteries** Yue QI, Michigan State University	**Investigating Quality Issues in Tableting with BIOVIA Discoverant** Anand KRISHNAMURTHY, BIOVIA
9:40-10:00 PT 12:40-1:00 ET 18:40-19:00 CET	**Navigating the Data Lake** Hahdi PERFECT - Pfizer	**Molecular Modeling & Generative Strategies for the Design and Optimization of Lead Series** Scott BEMBENEK, Denovicon Therapeutics	**Molecular Modeling & Generative Strategies for the Design and Optimization of Lead Series** Scott BEMBENEK, Denovicon Therapeutics	**From Lithium Ions to Battery Cells** Johan CARLSSON, BIOVIA	**What's Next in Process Analytics** Larry FIEGLAND, Christopher ANDREWS, BIOVIA
10:00-10:20 PT 1:00-1:20 ET 19:00-19:20 CET	**NEXTLab (LES): Implementation of LES in QC for Roche** Lutz WILKE And Jessica JUSTICE, Roche	**Large Scale Application of Matched Molecular Pairs Analysis** Sandeep PAL, GSK	**Large Scale Application of Matched Molecular Pairs Analysis** Sandeep PAL, GSK	**Computational Design and Autonomous Discovery of Next-generation Battery Materials** Tejs VEGGE, Technical University of Denmark	**Golden Batch Analysis with Discoverant** Ryan HOLWAY, BIOVIA
10:20-10:40 PT 1:20-1:40 ET 19:20-19:40 CET	**Q/A Panel Lead:** Kirsten GESENBERG	**Q/A Panel Lead:** Ton VAN DAELEN	**Q/A Panel Lead:** Ton VAN DAELEN	**Q/A Panel Lead:** Felix HANKE	**Q/A Panel Lead:** Daniela JANSEN
SESSION TITLE	**MATERIALS MANAGEMENT**	**AI-DRIVEN DRUG DESIGN, PART II**	**AI-DRIVEN DRUG DESIGN, PART II**	**POLYMERS & COMPOSITES**	
10:40 - 11:00 PT 1:40-2:00 ET 19:40-20:00 CET	**What's New In BIOVIA Registration** Neil ECCLES, BIOVIA	**Bringing It All Together – Towards a Versatile Platform for Automated Ligand Design** Hans Briem, Bayer	**Bringing It All Together – Towards a Versatile Platform for Automated Ligand Design** Hans Briem, Bayer	**Multi-Scale Modeling of Polymer-Based Materials For Improved Tire Performance** Sebastien GARRUCHET & Benoit LATOUR, Michelin	
11:00- 11:20 PT 2:00-2:20 ET 20:00-20:20 CET	**Registering Small Molecules and Biologics at Pfizer** Steve TRUDEL, Pfizer, and Neil ECCLES, BIOVIA	**Automated Generation of Novel Fragments Using Screening Knowledge, a Hybrid Auto-encoder and Transfer Learning** Alan BILSLAND, Beatson Institute	**Automated Generation of Novel Fragments Using Screening Knowledge, a Hybrid Auto-encoder and Transfer Learning** Alan BILSLAND, Beatson Institute	**Local Dynamics In The Glass Transition Domain** Armand SOLDERA, Université De Sherbrooke	
11:20-11:40 PT 2:20-2:40 ET 20:20-20:40 CET	**Formulation Design on the 3DEXPERIENCE Platform** Chris STRASSEL, BIOVIA	**Antibody Developability Prediction with Machine Learning** Lei Jia, Amgen	**Antibody Developability Prediction with Machine Learning** Lei JIA, Amgen	**Modeling Chemical Reactions in the Fluid Phase** Rebecca SURE, BASF	
11:40 -12:00 PT 2:40-3:00 ET 20:40-21:00 CET	**Q/A Panel Lead:** Chris STRASSEL	**Q/A Panel Lead:** Lee Herman, SUNOVION	**Q/A Panel Lead:** Lee Herman, SUNOVION	**Q/A Panel Lead:** Jason DEJOANNIS	**Q/A**

WEDNESDAY SEP 23 | VIRTUAL BIOVIA CONFERENCE 2020 AGENDA

	Laboratory Informatics	Pipeline Pilot and Data Science	Discovery Studio	Materials Innovation	Quality
	8 -12 PT |11 - 15 ET| 17 - 21 CET				
SESSION TITLE	TRACK: **Laboratory Informatics**	TRACK: **Pipeline Pilot and Data Science**	TRACK: **Life Sciences Modeling**	TRACK: **Materials Innovation through Modeling and Informatics**	TRACK: **Quality**
SESSION TITLE	**ELN**	**DRUG DISCOVERY AI & CLINICAL TRIALS**	**SMALL MOLECULES - I**	**METALS AND ALLOYS**	**QUMAS PRODUCT FUNCTIONALITY**
8:00-8:20 PT 11:00-11:20 ET 17:00-17:20 CET	**ELN Roadmap to the 3DEXPERIENCE Platform** Kirsten GESENBERG, BIOVIA	**Using Pipeline Pilot Machine Learning Engine to Accelerate Discovery: Predictive Tier1 ADMET Models** Gennady PODA, Ontario Institute for Cancer Research	**Modeling and Validation, the Inseparable Partners** Francine ACHER, Université Paris Descartes	**Interfacing Ab Initio Calculations, Calphad Models,Thermodynamic Databases, Web Interfaces and Visualization Tools** Axel VAN DE WALLE, Brown University	**What's New / What's Next in QUMAS** Chris FROST, ENOVIA - Cyril WALSH, BIOVIA
8:20-8:40 PT 11:20-11:40 ET 17:20-17:40 CET	**iLab Project: Building the Foundation for Faster and Data-driven Product and Process Development** Claire VIRENQUE, Anne MARON, SANOFI	**Using Pipeline Pilot as an Integration Tool to Support Retrieval and Viewing of 3D Model and Structure** Mark KENNEY, Gilead	**Polarizable Force Field Based on the Classical Drude Oscillator** Alex MACKERELL, Univeristy of Maryland	**Tools for Metal Alloy Simulations** Martin PERSSON, BIOVIA	**A First Look at the new Learning Management System Integration** Cyril WALSH, ENOVIA
8:40-9:00 PT 11:40-12:00 ET 17:40-18:00 CET	**BIOVIA Workbook at Galapagos** Claire Meul, Veronique DeVroey, GALAPAGOS	**Precision Medicine in Research: Medidata Experience is From Medidata** Glen DE VRIES and Sastry CHILUKURI, Medidata	**Engineering Platforms for Infectious Disease Research** Joel FREUNDLICH, Rutgers University	**Simulations of Platinum Nanoparticle Catalysts with ONETEP** Chris-Kriton SKYLARIS University Of Southampton	**Planning a Successful Upgrade or Move to the Cloud** Conor BARRY, Noel O'BRIEN, BIOVIA
9:00 - 9:20 PT 12:00-12:20 ET 18:00-18:20 CET	**Q/A Panel Lead:** Laurent REBION	**Q/A Panel Lead:** Frank SCHAFFER	**Q/A Panel Lead:** Tien LUU	**Q/A Panel Lead:** Victor MILMAN	**Q/A Panel Lead:** Wesley FLAKE
SESSION TITLE	**FORMULATION DESIGN**	**DATA SCIENCE IN MATERIALS DESIGN**	**BIOTHERAPEUTICS DESIGN & DEVELOPMENT - I**	**PHARMACEUTICAL DEVELOPMENT**	**QUALITY & BEYOND - TRENDS, TECHNOLOGY ENABLERS AND INNOVATIONS**
9:20 - 9:40 PT 12:20-12:40 ET 18:20-18:40 CET	**Swipe Right on Product Ingredient Labeling** Dale PIXLEY, BIOVIA	**Machine Learning for Materials and Formulations** Dana HONEYCUTT, BIOVIA	**LIVE PRESENTATION: Machine Learning for Therapeutic Protein Developability and Formulation Design** Bernhardt TROUT, MIT	**Predictive Modeling in Process Development** Jacek ZEGLINSKI, AP Process	**Document Management in the 3DEXPERIENCE Platform** Ken HAYWARD, ENOVIA
9:40-10:00 PT 12:40-1:00 ET 18:40-19:00 CET	**Making Bread Part I** Patrick WHEELER, BIOVIA	**Multi-Objective Optimization of Formulations and Other Materials** Dana HONEYCUTT, BIOVIA	**Integrative Approach to T-cell Epitope Prediction** Andrej SALI, UCSF	**ssNMR CASTEP Predictions to Complement X-Ray Methods in Structure Determination of Crystalline Phases** Luca RUSSO, GSK	**Next generation Pharmaceutical Quality Systems (PQS)** Conor HAYES, ENOVIA
10:00-10:20 PT 1:00-1:20 ET 19:00-19:20 CET	**Making Bread Part II** Patrick WHEELER, BIOVIA	**Finding an Alternative Refrigerant Chemical Using Material Informatics** Abhijit CHATTOPADHYAY, BIOVIA	**The Impact of Proline Isomerization on Antigen Binding and the Analytical Profile of a Trispecific Anti-HIV Antibody** Alessandro MASIERO, SANOFI	**COSMO-RS in Practice During Drug Development** Anikó UDVARHELYI, Novartis	**Structured Document Management in the 3DEXPERIENCE Platform** Aidan QUILLIGAN, ENOVIA
10:20-10:40 PT 1:20-1:40 ET 19:20-19:40 CET	**Taking the Lab to the Cloud** John MCNEIL, BIOVIA	**Q/A Panel Lead:** Alex ORONA	**Q/A Panel Lead:** Anne GOUPIL-LAMY	**Q/A Panel Lead:** Karin WICHMANN	**Q/A Panel Lead:** Ken HAYWARD
SESSION TITLE	**LAB TESTING**	**ETL AND DATA SCIENCE IN THE FIELD, PART I**	**PHYSICS-BASED METHODS FOR LEAD OPTIMIZATION**	**SURFACES & CATALYSTS**	**QUALITY & BEYOND - TRENDS, TECHNOLOGY ENABLERS AND INNOVATIONS**
10:40 - 11:00 PT 1:40-2:00 ET 19:40-20:00 CET	**Solving the Problem of Today, Today. High Throughput COVID-19 testing with BIOVIA ONE Lab** Kanishka DESAI, BIOVIA, Benoit DARTIGUEMALLE, Kemika ALLOWAY, BIOVIA	**Communication to Your Future Self: Designing Pipeline Pilot Protocols for Reusability and Readability** Jennifer HEYMONT, Eisai	**Design, Development and Application of Ultra-High Throughput Free Energy Calculations Using CHARMM and Multi-Site λ Dynamics** Charlie BROOKS, University of Michigan	**Computational Chemistry in Materials Development for Semiconductors** Agnes DERECSKEI-KOVACS, Versum Materials Inc., a business of Merck KGaA	**Document Management in the 3DEXPERIENCE Platform** Ken HAYWARD, ENOVIA
11:00- 11:20 PT 2:00-2:20 ET 20:00-20:20 CET	**BIOVIA ONE Lab Equipment Class Ontologies with Allotrope** Mike WILSON, BIOVIA	**Training Pipeline Pilot Developers** Kip SHAFFER, P&G	**Evaluation of Multiple Free Energy and Null Methods to Assess Applicability in Drug Discovery** Kira ARMACOST, Merck	**Catalytic Platinum Nanoparticles Decorated with Subnanometer Molybdenum Clusters for Biomass Processing** Simon PODKOLZIN, Stevens Institute of Technology	**Next generation Pharmaceutical Quality Systems (PQS)** Conor HAYES, ENOVIA
11:20-11:40 PT 2:20-2:40 ET 20:20-20:40 CET	**Building Methods to Scale for QC** She YEN LOK	**Harmonized Tariff Schedule Classification of Chemicals** Bob SCHWARTZ, MyIslandBeach	**Physics-based Binding Affinity Calculations in Small Molecule Lead Optimization** Prabhu RAMAN, BIOVIA	**Perovskite Metal-Oxides for Automotive Three-Way Catalysis** Crispin COOPER, Johnson MATTHEY	**Structured Document Management in the 3DEXPERIENCE Platform** Aidan QUILLIGAN, ENOVIA
11:40 -12:00 PT 2:40-3:00 ET 20:40-21:00 CET	**Q/A Panel Lead:** Melissa STERRETT BARON	**Q/A Panel Lead:** Alex ORONA	**Q/A Panel Lead:** Adam GREEN	**Q/A Panel Lead:** Nick REYNOLDS	**Q/A Panel Lead:** Ken HAYWARD

THURSDAY SEP 24 | VIRTUAL BIOVIA CONFERENCE 2020 AGENDA

	Laboratory Informatics	Pipeline Pilot and Data Science	Discovery Studio	Materials Innovation
	8 -12 PDT |11 - 15 ET| 17 - 21 CET			
SESSION TITLE	TRACK: **Laboratory Informatics**	TRACK: **Data Science**	TRACK: **Life Sciences Modeling & Simulation**	TRACK: **Materials Innovation through Modeling and Informatics**
SESSION TITLE	**MATERIALS MANAGEMENT**	**ETL AND DATA SCIENCE IN THE FIELD, PART II**	**SMALL MOLECULES - II**	**ADVANCES IN MATERIALS MODELING**
8:00-8:20 PT 11:00-11:20 ET 17:00-17:20 CET	**What's New In BIOVIA CISpro** Anne SEFREID, BIOVIA	**What's New in Pipeline Pilot and Scientific Informatics?** Alex ORONA and Matt SAGE, BIOVIA	**Probing Protein-Ligand Interactions in Factor Xa using SAR and MD-based Free-Energy Calculations** Han SUN, Marc NAZARÉ, FMP Berlin	**Next Generation Surfactant Engineering Using COSMOplex** Johannes SCHWOEBEL, BIOVIA
8:20-8:40 PT 11:20-11:40 ET 17:20-17:40 CET	**CISPro Freezer Inventory: The Final Frontier** Jenna GANNON, Amgen		**Diving into the transport mechanism of a neurologic transporter: an explicit membrane molecular dynamics simulation approach** Alexandre CABAYÉ, Université Paris	**Democratising Virtual Product Simulation in a Large Consumer Goods Organisation – What Our Journey Has Taught Us** Andrew EVANS, Unilever
8:40-9:00 PT 11:40-12:00 ET 17:40-18:00 CET	**Tablet Formula: How to Control Final Composition** Dale PIXLEY, BIOVIA	**Introduction to Jupyter Notebooks in Pipeline Pilot** Alex ORONA and Ian KERMAN - BIOVIA	**Predicting Toxicity with TOPKAT for Regulatory Purposes** Stefan PUDENZ, Covance	**Accelerate Innovation through Collaborative Research** Lalitha SUBRAMANIAN, BIOVIA
9:00 - 9:20 PT 12:00-12:20 ET 18:00-18:20 CET	**Q/A Panel Lead:** Chris STRASSEL		**Q/A Panel Lead:** Hugues-Olivier BERTRAND	**Q/A Panel Lead:** James WESCOTT
SESSION TITLE	**DATA VISUALIZATION AND ANALYTICS**	**MATERIALS WORKSHOP**	**BIOTHERAPEUTICS DESIGN & DEVELOPMENT - II**	**FUTURE OF MATERIALS MODELING**
9:20 - 9:40 PT 12:20-12:40 ET 18:20-18:40 CET	**Visualizations for ONE Lab: Integrating Insight to Provide Data Review Capabilities** Chris PIERINI, Amgen	**Error Proof Assembly on Manufacturing Shop Floor with Data Science** Nick REYNOLDS, BIOVIA	**The Real Value & Opportunities in End-to-End Computational Drug Development for Biologics** Neeraj AGRAWAL, Amgen	**Molecular Simulation of Thermoset Curing: Application to 3D Printing Materials** James ELLIOTT, University Of Cambridge
9:40-10:00 PT 12:40-1:00 ET 18:40-19:00 CET	**Data Visualization in the Chemicals Industry** Frank SCHAFFER, BIOVIA	**Workshop: Utilizing IoT to Support Predictive Maintenance** Jason DEJOANNIS, BIOVIA	**Boosting Antibody Developability through Computational Protein Design** Qing CHAI, Lilly	**Applying Quantum Computers to the Study of Solid State Systems** Dr David MUÑOZ RAMO, Cambridge Quantum Computing
10:00-10:20 PT 1:00-1:20 ET 19:00-19:20 CET	**Extending ONE Lab using Pipeline Pilot** Shabbir KHERALUWALA, BIOVIA		**Predicting Protein Formulation Properties in BIOVIA Discovery Studio** Lisa YAN, BIOVIA	**Advances in Materials Studio** James WESCOTT, BIOVIA
10:20-10:40 PT 1:20-1:40 ET 19:20-19:40 CET	**Q/A Panel Lead:** Sean O'HARE		**Q/A Panel Lead:** Anne GOUPIL-LAMY	**Q/A Panel Lead:** Marc MEUNIER
SESSION TITLE		**ACCELERATING DRUG DISCOVERY**	**ADVANCING THERAPEUTICS DESIGN**	**POLYMERS & COMPOSITES**
10:40 - 11:00 PT 1:40-2:00 ET 19:40-20:00 CET		**Improved Lead Compounds from Generative Therapeutics Design** Ton VAN DAELEN, Adam GREEN, BIOVIA	**Promise and Challenges of AI for Therapeutic Target Identification** Niranjani IYER, BIOVIA	
11:00- 11:20 PT 2:00-2:20 ET 20:00-20:20 CET			**In-silico Biologics Design in 2020: Challenges and Perspectives** Anne GOUPIL-LAMY, BIOVIA	
11:20-11:40 PT 2:20-2:40 ET 20:20-20:40 CET		**Fogdesigner – towards an integrated design, make, test, analyze workflow platform for a small biotech** Johannes VOIGT, Foghorn Therapeutic	**Developments in Discovery Studio** Tien LUU, BIOVIA	
11:40 -12:00 PT 2:40-3:00 ET 20:40-21:00 CET		**Q/A Panel Lead:** Ton VAN DAELEN	**Q/A Panel Lead:** Niranjani IYER	**Q/A**

TUESDAY SEP 22 | VIRTUAL BIOVIA CONFERENCE 2020

8 -12 PT | 11 - 15 EST | 17 - 21 CET

Laboratory Informatics | TRACK: Laboratory Informatics

ELN

8:00-8:20 PT 11:00-11:20 ET 17:00-17:20 CET	**What's New With BIOVIA ELNs** Kirsten GESENBERG, BIOVIA	BIOVIA Workbook and BIOVIA Notebook have been the focus of continuous development as we work to enhance the connection between BIOVIA's Electronic Lab Notebooks and ONE Lab and Perfect Lab solutions. In this session we will provide an overview of the latest features in Workbook and Notebook.
8:20-8:40 PT 11:20-11:40 ET 17:20-17:40 CET	**Unleashing the Power Of Pipeline Pilot: Design and Development Of A Next-Generation Balance Interface For Workbook** Marty BERLINER - Pfizer	BIOVIA ONE Lab (Workbook, Hub, Foundation, Equipment, Pipeline Pilot, etc.) is a powerful environment for scientists, and it's also a very capable application development environment – for custom "Foundation Apps". These apps are easy to create and maintain, especially using Pipeline Pilot, and deliver substantial business value. This talk describes our first foray into the custom app space – the development and deployment of a "Balance Integration App" for Workbook. This app - which is a web app – was built almost entirely in Pipeline Pilot, and we will highlight learnings and best practices that can be applied to similar efforts.
8:40-9:00 PT 11:40-12:00 ET 17:40-18:00 CET	**Digitalizing Drug Transportation Protocols** Matt DUMOUCHEL, Amgen	Material entering Drug Product stability studies is often first exposed to a Drug Transportation simulation, which introduces representative shipping stress, prior to being placed into a stability chamber. In the initial state, the process for managing requests and executions of Transport protocols by the Drug Product and Transportation groups was paper and email based. The standard shipping protocol and the request process were digitalized using One Lab and Compose and Capture functionality, resulting in significant efficiency gains for both areas. This presentation will provide an overview of the initial and improved states for this request and execution process, including a review of key lessons learned and estimated return on investment.
9:00 - 9:20 PT 12:00-12:20 ET 18:00-18:20 CET	**Q/A Panel Lead:** Gene TETREAULT	

LAB TESTING

9:20 - 9:40 PT 12:20-12:40 ET 18:20-18:40 CET	**Lab Testing in 21st Century** Gene TETREAULT, BIOVIA	Labs in the 21st century are not working as they did in the past. Workflows are digital and connected, environments are harmonized and standardized, lab scientists are collaborating across borders. This requires an intelligent scientific platform that is aware of the context in which scientists operate. Within this framework, scientists should also be able to access and leverage supply, services and expertise within the internal and external networks. This framework will accelerate product design and development, while also saving time and costs for scientists. In this presentation, we will discuss how an intelligent scientific platform for the lab can accelerate innovation, leverage marketplaces and allow the labs of the 21st century to move to new heights of lab innovation and efficiency.
9:40-10:00 PT 12:40-1:00 ET 18:40-19:00 CET	**Navigating the Data Lake** Hahdi PERFECT - Pfizer	Over the past few years, migration of data from local storage to cloud-based solutions has taken off. While moving to a data lake solves storage capacity, finding relevant data can be an onerous task. This talk covers our journey of how we implemented our data lake and its integration with BIOVIA ONE Lab.
10:00-10:20 PT 1:00-1:20 ET 19:00-19:20 CET	**NEXTLab (LES): Implementation of LES in QC for Roche** Lutz WILKE And Jessica JUSTICE, Roche	
10:20-10:40 PT 1:20-1:40 ET 19:20-19:40 CET	**Q/A Panel Lead:** Kirsten GESENBERG	

MATERIALS MANAGEMENT

10:40 - 11:00 PT 1:40-2:00 ET 19:40-20:00 CET	**What's New In BIOVIA Registration** Neil ECCLES, BIOVIA	Learn what's new in Biological Registration and Chemical registration, then explore the future of Materials Registration on the 3DEXPERIENCE platform. The talk will include a demonstration of the latest updates, and an overview of what's in development.
11:00- 11:20 PT 2:00-2:20 ET 20:00-20:20 CET	**Registering Small Molecules and Biologics at Pfizer** Steve TRUDEL, Pfizer, and Neil ECCLES, BIOVIA	Registration plays a pivotal role in supporting the development of novel therapeutic entities. Having a modern system to enable the identification of chemical and biological substances remains an essential capability for any drug discovery operation. In this presentation we will discuss the challenges faced by Pfizer with their legacy registration system and describe the journey that led to the development of a new system using BIOVIA Biological and Chemical Registration that provides the ability to register small molecules and biologics in a single common platform.
11:20-11:40 PT 2:20-2:40 ET 20:20-20:40 CET	**Formulation Design on the 3DEXPERIENCE Platform** Chris STRASSEL, BIOVIA	Learn about the future of Formulations on the 3DEXPERIENCE platform. From a formula design experience that's tightly integrated with BIOVIA Materials Management to the availability of formulations on the cloud, this presentation will include a demonstration of the new Formulation Designer, as well as a preview of what's in development.
11:40 -12:00 PT 2:40-3:00 ET 20:40-21:00 CET	**Q/A Panel Lead:** Chris STRASSEL	

TUESDAY SEP 22 | VIRTUAL BIOVIA CONFERENCE 2020

8 -12 PT | 11 - 15 EST | 17 - 21 CET

7:15-8:00 PT 10:15-11:00 ET 16:15-17:00 CET	**Plenary** Jason BENEDICT, Reza SADEGHI	BIOVIA's Jason Benedict, BIOVIA CEO and Reza Sadeghi, BIOVIA CSO will discuss how BIOVIA can leverage the Dassault Systèmes3DEXPERIENCE platform (3DX) as a system of operation, as a business model and (most importantly) as a powerful platform for scientific collaboration. Bolstered by BIOVIA's 25-year record of scientific accomplishment, the BIOVIA portfolio and 3DX are well positioned to drive innovation in Life Sciences and Materials Sciences by connecting the Virtual and the Real (V+R). Hear how BIOVIA software accelerates drug design and development with "human-in-the loop", "AI-in-the-loop" and "lab-in-the-loop" learning. Gain a deeper understanding of how BIOVIA drives end-to-end digital continuity from materials designers to product makers. Discover how BIOVIA makes the lab of the future possible today and how our data-centric approach to quality, regulatory and operational management is transforming businesses across science- and process-driven industries.

Pipeline Pilot and Data Science | TRACK: Data Science

SARS-COV-2 CHARACTERIZATION & THERAPEUTICS

8:00-8:20 PT 11:00-11:20 ET 17:00-17:20 CET	**Broad-spectrum Antiviral Activity of Naproxen: From Influenza A to SARS-CoV-2 Coronavirus** Anny SLAMA-SCHWOK, Hôpital Saint-Antoine	There is an urgent need for specific antiviral drugs directed against SARS-CoV-2 both to prevent the most severe forms of COVID-19 and to reduce viral excretion and subsequent virus dissemination; in the present pandemic context, drug repurposing is a priority. Targeting the nucleoprotein N of the SARS-CoV-2 coronavirus in order to inhibit its association with viral RNA could be a strategy to impeding viral replication and possibly other essential functions associated with viral N. The antiviral properties of naproxen, belonging to the NSAID family, previously demonstrated against Influenza A virus, were evaluated against SARS-CoV-2. Naproxen binding to the nucleoprotein of SARS-CoV2 was shown by molecular modeling. Comparison with the binding of naproxen to the nucleoprotein of Influenza A virus will be also presented. In cellular and reconstituted human primary respiratory epithelium models of SARS-CoV-2 infection, naproxen inhibited viral replication and protected the bronchial epithelia against SARS-CoV-2 induced-damage. The benefit of naproxen addition to the standard of care is tested in an on-going clinical study.
8:20-8:40 PT 11:20-11:40 ET 17:20-17:40 CET	**Integrative Methods for Structure-Determination: From Laptops to Exascale Supercomputers** Abhishek SINGHAROY, Arizona State University	Accurate structure determination from medium to low-resolution experimental data necessitates a balance between extensive global and local sampling of atomistic models, yet with stereochemical correctness of backbone and sidechain geometries. Molecular Dynamics simulations, particularly through the application of enhanced sampling and Baysean inferencing schemes provide today a robust way of achieving this balance for hybrid structure determination. Engendering a high-throughput real space refinement approach, called molecular dynamics flexible fitting (MDFF), the protocol performs at scale from single-CPU/GPU machines unto 10000 nodes on national supercomputers. In this presentation, the capabilities of MDFF will be showcased with three distinct applications of imminent relevance to the BioXFEL community: (a) refinement of SARS-CoV-2 spike and envelope proteins, (b) elucidation of time-resolved minimum-free energy pathways from single particle images of calcium channels, and (c) finally, whole-cell models for determination of cooperative energy transfer in photosynthesis and respiration.The common theme that underlies these three applications is the role of large-scale conformational transitions within the functional cycle of the proteins. Information on the dynamics remain embedded within the diffraction, scattering, or single-particle data. Taking advantage of the highly efficient conformational search capabilities provided by MDFF, this dynamical information is revealed, uncertainty in the data is quantified, and inferences are drawn on the biological functions of the proteins. To this end, MDFF refinements deliver (a) pathways of viral infection, (b) mechanism of ion binding to the Calcium ion channel, and (c) molecular origins of ageing in cells.
8:40-9:00 PT 11:40-12:00 ET 17:40-18:00 CET	**The Pandemic Experience: Using Computational and Experimental Approaches to Identify Inhibitors of SARS-CoV-2** Sean EKINS, Collaborations Pharmaceutical Sean Ekins, Ana C. Puhl, Victor O. Gawriljuk, Thomas Lane, Daniel H. Foil and Kimberley M. Zorn.	The SARS-CoV-2 pandemic is an opportunity to showcase how technology can be applied to the discovery of a treatment to help humankind. In the space of a few months we have been involved with numerous international collaborations. We initially focused on docking molecules in the available protease structure and as published in vitro data became available in papers and preprints from groups globally, these data were used for machine learning models. We then used these models to select compounds for testing in vitro. In parallel we have been using NanoTemper microscale thermophoresis methods to test the binding affinity of compounds for the spike protein. As we had prior work on inhibitors of Ebola virus we prioritized these molecules for testing in vitro. One of these molecules was selected in a humanized mouse model. Two of these compounds have also made it to clinical trials after discussion with the companies involved. These include a phase II trial of pyronaridine in South Korea and a phase III trial of tilorone in the Ukraine. Our efforts show that we can prioritize approved drugs for testing and repurposing for COVID-19. This presentation will describe several of these collaborations and focus on the machine learning efforts using Assay CentralTM and other computational methods. Our experience of this pandemic has taught us that a small company can have an outsize impact by leveraging and integrating our computational and experimental approaches alongside those of a range of collaborators.
9:00 - 9:20 PT 12:00-12:20 ET 18:00-18:20 CET	**Q/A Panel Lead:** Hugues-Olivier Bertrand	

AI-DRIVEN DRUG DESIGN, PART I

9:20 - 9:40 PT 12:20-12:40 ET 18:20-18:40 CET	**Raising the Odds of Success in Multi-Objective Optimizations for Drug Discovery** Dana HONEYCUTT, BIOVIA	In the BIOVIA Generative Therapeutics Design project, we continue to extend and refine our approach to generating proposed small molecules that satisfy multiple competing objectives. This talk describes some of the methods developed and lessons learned during a recent lead optimization collaboration between BIOVIA and a major pharmaceutical company. The collaboration involves multiple cycles of compound synthesis, assay data acquisition, machine learning model building, and numerical optimization runs resulting in new proposed compounds for synthesis. We propose a way of performing multi-objective optimizations using desirability functions determined based on the concept of a model's positive predictive value (PPV). Incorporating the PPV into the method helps make successful optimization runs more interpretable and provides a systematic way to adjust the desirability profiles when an optimization run does not succeed.

Pipeline Pilot and Data Science | TRACK: Data Science

AI-DRIVEN DRUG DESIGN, PART I

9:40-10:00 PT 12:40-1:00 ET 18:40-19:00 CET	**Molecular Modeling & Generative Strategies for the Design and Optimization of Lead Series** Scott BEMBENEK, Denovicon Therapeutics	Scott Bembenek of Denovicon Therapeutics will discuss traditional drug discovery approaches that require some 5 years to identify and optimize molecules for clinical candidacy. In the end, several thousands of molecules will be made and less than a handful will move forward into clinical trials where 90% of molecules ultimately fail. Here, we overview a strategic combination of molecular modeling and generative approaches that allows for the identification of more viable chemical matter, which is then quickly transformed into lead series and, finally, optimized clinical candidates. Within this platform, we anticipate a much shorter timeline of around 2 years with only a few hundred molecules being synthesized in total. Moreover, molecules moving into clinical trials are expected to endure a much lower attrition rate.
10:00-10:20 PT 1:00-1:20 ET 19:00-19:20 CET	**Large Scale Application of Matched Molecular Pairs Analysis** Sandeep PAL, GSK	This presentation will describe the motivations behind Bradshaw, GSKs experimental automated design environment, our aspirations for it and our experience when applying the system to real medicinal chemistry projects.
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AI-DRIVEN DRUG DESIGN, PART II

10:40 - 11:00 PT 1:40-2:00 ET 19:40-20:00 CET	**Bringing It All Together – Towards a Versatile Platform for Automated Ligand Design** Hans BRIEM, Bayer	The early phase of drug discovery remains a complex endeavour which has to cope with multiple, sometime competing objectives (physicochemical and ADMET properties, target activity, selectivity, synthetic accessibility, patentability etc.) and rather limited amounts of heterogeneous experimental data. On the other hand, there is a vast space of drug-like compounds potentially active on a given target. In order to support ligand design under these circumstances, a variety of computational methods and tools have been developed over the last decades. Here, we will present an integrated molecular design platform developed inhouse, which combines a broad range of such computational components for successful ligand design: • Compound ideation methods, like rule-based and reaction-based transformations, scaffold-hopping, generative methods and screening of huge virtual compound databases • Machine-learning and structure-based methods to predict physicochemical, ADMET and target activity endpoints • Compound selection methods, taking into account multiple user-defined objectives • Strategies to actively learn from compound optimization cycles in order to constantly improve the models
11:00- 11:20 PT 2:00-2:20 ET 20:00-20:20 CET	**Automated Generation of Novel Fragments Using Screening Knowledge, a Hybrid Autoencoder and Transfer Learning** Alan BILSLAND, Beatson Institute	Fragment based drug discovery (FBDD) allows proportionately greater coverage of chemical space using fewer molecules than traditional high-throughput screening approaches. However, effective exploitation of this advantage is highly dependent on library design and this is a time-consuming task for medicinal chemists. Artificial neural networks have recently attracted considerable attention in automated de novo design applications for drug-like molecules and could also prove useful for fragment library design. Here we analysed several candidate architectures for automated fragment generation, comparing their performance across a range of properties including aromatic ring counts, heavy atom count, synthetic accessibility, and a new complexity score that we developed using Pipeline Pilot. Finally, we used the best-performing model to generate a library of novel candidate fragments with shape and complexity distributions to augment our existing screening collection.
11:20-11:40 PT 2:20-2:40 ET 20:20-20:40 CET	**Antibody Developability Prediction with Machine Learning** Lei JIA, Amgen	Monoclonal antibodies (Mabs) developability composes a set of biophysical and PKDM properties. It has become a major concern in the development of protein therapeutics due to its impact on drug manufacturing and patient experience. A set of developmental stage monoclonal antibodies were systematically produced and assayed. Predictive models are being developed with this high-quality data set. A key challenge is the small data size for machine learning purpose. To alleviate that, feature engineering was applied to select a set of predictive and biophysically meaningful features on in silico (sequence and structure) as well as experiment levels. In addition, a few machine learning algorithms were evaluated for training predictive models. Some models reach satisfactory level of accuracy so that we can deploy those models to help eliminate liable molecules in early stage of drug discovery. This can significantly save cost and shorten timeline of our antibody drug pipeline.
11:40 -12:00 PT 2:40-3:00 ET 20:40-21:00 CET	**Q/A Panel Lead:** Alex ORONA	

TUESDAY SEP 22 | VIRTUAL BIOVIA CONFERENCE 2020

8 -12 PT | 11 - 15 EST | 17 - 21 CET

Discovery Studio | TRACK: Life Sciences Modeling

SARS-COV-2 CHARACTERIZATION & THERAPEUTICS

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AI-DRIVEN DRUG DESIGN, PART I

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TUESDAY SEP 22 | VIRTUAL BIOVIA CONFERENCE 2020

8 -12 PT | 11 - 15 EST | 17 - 21 CET

Discovery Studio | TRACK: Life Sciences Modeling

AI-DRIVEN DRUG DESIGN, PART I

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TUESDAY SEP 22 | VIRTUAL BIOVIA CONFERENCE 2020

8 -12 PT | 11 - 15 EST | 17 - 21 CET

Materials Innovation | TRACK: Materials Innovation through Modeling and Informatics

MACHINE LEARNING

8:00-8:20 PT 11:00-11:20 ET 17:00-17:20 CET	**Machine Learning for Materials and Formulations** Dana HONEYCUTT, BIOVIA	We present capabilities in Pipeline Pilot for the modeling and optimization of materials properties using machine learning (ML). Using examples ranging from chocolate to steel, we discuss best practices for performing ML, and consider when it makes sense to use ML as opposed to the alternatives of experiment and simulation. Given that scientific and engineering data for a given problem are often scarce and expensive, we discuss active learning as a strategy for addressing the challenge of small training data sets.
8:20-8:40 PT 11:20-11:40 ET 17:20-17:40 CET	**Machine Learned Force Fields and Potential Energy Surfaces** Gabor CSANYI, University of Cambridge	There is a long tradition in computational chemistry and materials science of representing the Born-Oppenheimer potential energy surface of molecules, clusters of molecules and extended materials using empirical force fields on the one hand, and also, for small systems, using systematic expansions that have essentially arbitrary accuracy. The formalism of "machine learning" (non-parametric function fitting in high dimensions) unites these approaches. New kinds of parametrisations are the result, with a computational expense in between that of simple force fields and quantum chemistry, and leading to diverse applications. Notable work in my group include potentials for amorphous carbon, silicon with defects, as well as regression of molecular properties. I will outline my vision for the bright future of force field modelling.
8:40-9:00 PT 11:40-12:00 ET 17:40-18:00 CET	**Finding an Alternative Refrigerant Chemical Using Material Informatics** Abhijit CHATTOPADHYAY, BIOVIA	The a priori prediction of the thermodynamic behavior of mixtures of new compounds or of new mixtures of well-known compounds is a long-standing industrially important problem. Questions of this kind often appear in chemical engineering when new processes or alternatives for existing processes are considered, and in product design and development, when the quality or performance of a product depends on the solubility or partition behavior of compounds between different liquid phases. Refrigerant very commonly use fluorine-based compounds as the chemicals; for sustainability these chemicals need to be replaced with an alternative. This talk describes a workflow using a combination of molecular modeling and data science to find an alternative refrigerant to replace the existing one in a regulated marketplace in most timely manner.
9:00 - 9:20 PT 12:00-12:20 ET 18:00-18:20 CET	**Q/A Panel Lead:** Stephen TODD	

MODELING BATTERY MATERIALS

9:20 - 9:40 PT 12:20-12:40 ET 18:20-18:40 CET	**Solvation and Desolvation vs. Electrolyte Design in Li-ion Batteries** Yue QI, Michigan State University	Yue Qi of Michigan State University will speak about electrolyte design for Li-ion batteries. This requires an integrated perspective, as the electrodes, electrolyte, and their interactions/reactions require consideration. Materials Studio offers a series of modeling tools such as Dmol3, DFTB and Forcite that can be integrated with thermodynamics framework to reveal the charge transfer reaction energetics at complex electrode/electrolyte interfaces and enable materials design. This talk will first demonstrate bulk electrolyte design for low temperature operations and durable Lithium-Sulphur batteries. Then a half-cell model will be introduced to reveal that at the experimentally defined zero voltage for Li+/Li0, the Li-metal surface is negatively charged to maintain the electrochemical equilibrium. The electric field created by the negatively charged surface can induce the electrolyte into an ordered structure and lower the Li+ ion desolvation energy barrier. This atomistic view of the lithium stripping/plating reaction.
9:40-10:00 PT 12:40-1:00 ET 18:40-19:00 CET	**From Lithium Ions to Battery Cells** Johan CARLSSON, BIOVIA	Today, it is hard to imagine a world without batteries as power sources. The performance may be sufficient for handheld devices, but it is still not sufficient to completely electrify the car fleet. This disruptive step requires a deep understanding of the materials in the battery cell down to the atomistic level -- both to increase the nominal charging capacity and to understand the aging processes. This can only be achieved by combining experiment and advanced simulations. This talk will give an introduction to the modelling of the materials in the battery cell, highlighting the recent developments at Dassault Systèmes for battery modelling. The specific focus will be on calculating the open cell potential and the lithium ion transport in the electrolyte. In addition, this information from the atomistic level may be propagated to the macroscopic level and incorporated as materials parameters into system level simulations of a cell. We establish a complete link from first-principles screening a database of potential additives for specific properties to calculating of the electrolyte performance and the subsequent simulation of battery cell behavior under realistic operating conditions. The initial tests with this multiscale approach shows promising results regarding simulating the I/V characteristics of a realistic cell model. This indicates that such a multiscale model can be utilized to get an understanding about how the atomistic properties influence the cell performance.

TUESDAY SEP 22 | VIRTUAL BIOVIA CONFERENCE 2020

8 -12 PT | 11 - 15 EST | 17 - 21 CET

Materials Innovation | TRACK: Materials Innovation through Modeling and Informatics

MODELING BATTERY MATERIALS

10:00-10:20 PT 1:00-1:20 ET 19:00-19:20 CET	**Computational Design and Autonomous Discovery of Next-Generation Battery Materials** Tejs VEGGE, Technical University of Denmark	Rechargeable batteries play a crucial role in the transition to a clean energy infrastructure, but the development of low-cost, high performance electrode materials, has been too slow. Understanding and controlling the complex and dynamic processes taking place in the electrodes, electrolyte and at the battery interfaces/interphases hold the key to develop more durable ultra-high performance batteries. Atomic-scale calculations have reached predictive accuracy in many critical areas of materials design and characterization, e.g. the identification of rate- and potential limiting reaction steps. Here, we provide a number of recent examples of how density functional theory (DFT) simulations supported by machine learning and cluster expansion techniques can been used efficiently to identify the limiting thermodynamic, ionic and electronic transport mechanisms in novel Li-ion electrode materials, Li-S and metal-oxygen batteries. Finally, we describe the "Battery Interface Genome – Materials Acceleration Platform" (BIG-MAP) project and Battery 2030+, which targets accelerated discovery and inverse design of future batteries using automated workflows and generative deep learning models by acquisition and utilization of data from large-scale multi-fidelity data sets, multi-scale computer simulations and databases, operando x-ray and neutron characterization from large-scale research facilities, high-throughput synthesis and laboratory testing.
10:20-10:40 PT 1:20-1:40 ET 19:20-19:40 CET	**Q/A Panel Lead:** Felix HANKE	

POLYMERS & COMPOSITES

10:40 - 11:00 PT 1:40-2:00 ET 19:40-20:00 CET	**Multi-Scale Modeling of Polymer-Based Materials For Improved Tire Performance** Sebastien GARRUCHET & Benoit LATOUR, Michelin	Michelin Group is constantly searching for innovative solutions to meet increasing expectations in terms of safety, performance over lifetime and environmental footprints (reduction of fuel consumption due to rolling resistance and greener composition of tires). Designing high-performance materials is thus a necessary step to answer both societal and environmental needs. Understanding local phenomena involved in our materials is crucial to better control their physical and chemical properties. To do so, methods and tools spanning from the atomistic scale to the mesoscale have been developed using BIOVIA suite to both understand the physical mechanisms occurring in our polymer-based materials and provide an efficient and ergonomic tool to the material designers. In this presentation, we will share several studies where BIOVIA software has been a key resource to design innovative materials.
11:00- 11:20 PT 2:00-2:20 ET 20:00-20:20 CET	**Local Dynamics In The Glass Transition Domain** Armand SOLDERA, Université De Sherbrooke	The glass transition refers to a change in dynamical properties of a material while keeping its amorphous structure. Experimentally it takes place over 3-5 K. From molecular dynamics simulation of polymers, an enlargement in order of 160 K was observed. Such a difference raises the question of the meaning of the glass transition temperature (Tg) captured by molecular simulation approach. To address this issue, local dynamics is investigated through the computation of the activation energy (Ea). This energy is deduced from the change in the rate of configurational transitions along the backbone chain with temperature. Thanks to an investigation of several polymers (PE, PS, PVDF), a chemical description of the glass transition was retrieved, both from quantitative and qualitative viewpoints. As a linear relationship between Ea and Tg was established, Tg can be computed from the knowledge of Ea stemming from the different components of a polymer. In fact, by correlating Tg with the dihedral potential graph, we were able to show that the outset of the glass transition corresponds to the moment where transitions from the gauche to the trans states begin.
11:20-11:40 PT 2:20-2:40 ET 20:20-20:40 CET	**Modeling Chemical Reactions in the Fluid Phase** Rebecca SURE, BASF	Quantum chemical methods can make predictions for molecules or small clusters of molecules in vacuum or gas phase within the experimental accuracy. However, most chemical processes are carried out in the condensed phase and quantum chemistry is still not able to treat molecules in fluid environments in an equally accurate manner. For a realistic modeling of reaction thermodynamics and kinetics solvation effects have to be taken into account. We will show examples for the application of COSMO-RS and COSMO-RS+microsolvation to model chemical reactions in the fluid phase.
11:20-11:40 PT 2:20-2:40 ET 20:20-20:40 CET	**Q/A Panel Lead:** Jason DEJOANNIS	

TUESDAY SEP 22 | VIRTUAL BIOVIA CONFERENCE 2020

8 -12 PT | 11 - 15 EST | 17 - 21 CET

Manufacturing | TRACK: Manufacturing Intelligence

MANUFACTURING

8:00-8:20 PT 11:00-11:20 ET 17:00-17:20 CET	**Takeda Los Angeles' CPV Journey with BIOVIA Discoverant** Vivian MEDINA and Darren NG - Takeda	In this session, we will provide an overview of Continued Process Verification (CPV) with BIOVIA Discoverant in today's dynamic, highly competitive biopharma environment, including success stories. We will also describe how Discoverant supported our entry into Quality by facilitating Product Quality Reviews (PQRs) and QC assay control monitoring.
8:20-8:40 PT 11:20-11:40 ET 17:20-17:40 CET	**The Integration of a Quality Management System in Discoverant** Carly MACNAB, UCB Pharma	Quality Management System (QMS) data is often undervalued and overlooked. Discoverant can help make QMS data more user-friendly and easy to visualize, allowing us to extract more value. In this talk I will describe how to develop generic QMS parameters which can be used in any product hierarchy. Once integrated in Discoverant, QMS data can be analyzed in a number of ways. By performing further analysis, we can gain clear insights, which help to improve process and product quality.
8:40-9:00 PT 11:40-12:00 ET 17:40-18:00 CET	**Thermo Fisher Scientific's Multivariate Integrated Data Analytics Solution (MIDAS) Using Biovia's Discoverant** Chris Andrews, BIOVIA, Rob Perry and Matt Wessel, Thermo Fisher Scientific	Thermo Fisher Scientific's Multivariate Integrated Data Analytics Solution (MIDAS) platform aims to reduce the systemic risk in the drug supply chain by predicting shifts in Critical Quality Attributes (CQAs) early in the manufacturing process. MIDAS leverages BIOVIA Discoverant, Python, R, cloud computing and other tools as a basis for its platform. Additionally, MIDAS uses advanced methods, including Random Forests (RF), Partial Least Squares (PLS), Principal Component Analysis (PCA) and other tools to build predictive models. Data capture, model execution, alerting and data visualization are automated along the pipeline from manufacturing instrument outputs to process engineers by the MIDAS platform. Chris Andrews from Dassault Systèmes will discuss the solution with Rob Perry and Matt Wessel from Thermo Fisher Scientific.
9:00 - 9:20 PT 12:00-12:20 ET 18:00-18:20 CET	**Q/A Panel Lead:** Larry FIEGLAND	

MANUFACTURING

9:20 - 9:40 PT 12:20-12:40 ET 18:20-18:40 CET	**Investigating Quality Issues in Tableting with BIOVIA Discoverant** Anand KRISHNAMURTHY, BIOVIA	In addition to Process Development and Process Monitoring, BIOVIA Discoverant enables Process Improvement through rapid investigations of quality issues and root cause analysis. In this session, we will demonstrate how we can get to the bottom of a "sticky" problem in a tableting manufacturing process.
9:40-10:00 PT 12:40-1:00 ET 18:40-19:00 CET	**What's Next in Process Analytics** Larry FIEGLAND, Christopher ANDREWS, BIOVIA	In this session we will cover the latest updates to BIOVIA Discoverant and introduce the concepts for the next generation of process analytics.
10:00-10:20 PT 1:00-1:20 ET 19:00-19:20 CET	**Golden Batch Analysis with Discoverant** Ryan HOLWAY, BIOVIA	BIOVIA Discoverant is customized for life science manufacturing. Small and large molecule manufacturing processes can be tracked in near-real time so manufacturers have more control over their process from start to finish. This presentation will focus on the analysis of continuous data, and how manufacturers can utilize BIOVIA Discoverant to ensure their continuous data analytics are easy to process, reliable and under control.
10:20-10:40 PT 1:20-1:40 ET 19:20-19:40 CET	**Q/A Panel Lead:** Daniela JANSEN	

WEDNESDAY SEP 23 | VIRTUAL BIOVIA CONFERENCE 2020

8 -12 PT | 11 - 15 EST | 17 - 21 CET

Laboratory Informatics | TRACK: Laboratory Informatics

ELN

8:00-8:20 PT 11:00-11:20 ET 17:00-17:20 CET	**ELN Roadmap to the 3DEXPERIENCE Platform** Kirsten GESENBERG, BIOVIA	This session will detail the roadmap and development strategy of our forthcoming cloud platform-based electronic lab notebook, BIOVIA Scientific Notebook. Get an advanced look at the features and workflows we are implementing in this next-generation ELN on the 3DEXPERIENCE platform.
8:20-8:40 PT 11:20-11:40 ET 17:20-17:40 CET	**iLab Project: Building the Foundation for Faster and Data-driven Product and Process Development** Claire VIRENQUE, Anne MARON, SANOFI	The Project Team will share the experience of implementing BIOVIA-OneLab Platform as a key enabler for Sanofi CMC labs digitization and automation: Expected core capabilities and benefits; Short demo; Implementation strategy; First learnings
8:40-9:00 PT 11:40-12:00 ET 17:40-18:00 CET	**BIOVIA Workbook at Galapagos** Claire MEUL, Veronique DeVroey, GALAPAGOS	This presentation outlines the implementation track of Biovia Workbook at Galapagos. We highlight challenges and lessons learned, and discuss how we approached testing and training.
9:00 - 9:20 PT 12:00-12:20 ET 18:00-18:20 CET	**Q/A Panel Lead:** Laurent REBION	

FORMULATION DESIGN

9:20 - 9:40 PT 12:20-12:40 ET 18:20-18:40 CET	**Swipe Right on Product Ingredient Labeling** Dale PIXLEY, BIOIVIA	Packaging plays an hugely important role in the purchase decision making process, so getting it right is imperative for manufacturers. Additionally, 85% of product recalls are due to incorrect ingredient labels. Product labels must be both optimized and accurate for a product to be successful. BIOVIA Enginuity has automated labeling tools which enable the simple creation of compliant labels that are updated on-the-fly as you adjust formulations.
9:40-10:00 PT 12:40-1:00 ET 18:40-19:00 CET	**Making Bread Part I** Patrick WHEELER, BIOVIA	In this detailed session we will take you on a journey of developing a recipe for bread, starting with optimizing the formula before working through all the requisite lab processes with Perfect Lab in Part 2.
10:00-10:20 PT 1:00-1:20 ET 19:00-19:20 CET	**Making Bread Part II** Patrick WHEELER, BIOVIA	In Part 2 of this detailed session we will continue the journey of developing a recipe for bread, working through all the requisite lab processes with Perfect Lab.
10:20-10:40 PT 1:20-1:40 ET 19:20-19:40 CET	**Taking the Lab to the Cloud** John MCNEIL, BIOVIA	Manage your samples, recipes, tests, equipment and experiments with zero footprint. We are taking the Unified Lab suite of applications to the cloud using the BIOVIA ScienceCloud infrastructure.

LAB TESTING

10:40 - 11:00 PT 1:40-2:00 ET 19:40-20:00 CET	**Solving the Problem of Today, Today. High Throughput COVID-19 testing with BIOVIA ONE Lab** Kanishka DESAI, BIOVIA, Benoit DARTIGUEMALLE, Kemika ALLOWAY, BIOVIA	COVID-19 is still a novel disease with new information, standards of care, and diagnostic technologies becoming available at a very rapid rate. Daily testing requirements in the US are estimated to be in the millions of samples per day at peak across multiple testing platforms. BIOVIA ONE Lab provides a rapidly configurable, compliant, secure and integrated technology for addressing this problem of today.
11:00- 11:20 PT 2:00-2:20 ET 20:00-20:20 CET	**BIOVIA ONE Lab Equipment Class Ontologies with Allotrope** Mike Wilson, BIOVIA	In this presentation we will delve into the way BIOVIA ONE Lab leverages ontologies such as those provided by Allotrope to standardize the data acquired from lab instruments, and the management of lab equipment.
11:20-11:40 PT 2:20-2:40 ET 20:20-20:40 CET	**Building Methods to Scale for QC** She YEN LOK	One of the main challenges of implementing a Laboratory Informatics solution in QC labs is digitizing the test method to run electronically in the QC lab. It can be very time consuming to create digital versions of each test that needs to be run on each product, and then qualify the tests as well. With BIOVIA ONE Lab, scientists can create generic master method templates which are first validated, and then can be cloned with only the parameter values changing as necessary. In this way efforts are reduced, and method standardization is enforced across all labs using the solution.
11:40 -12:00 PT 2:40-3:00 ET 20:40-21:00 CET	**Q/A Panel Lead:** Melissa STERRETT BARON	

WEDNESDAY SEP 23 | VIRTUAL BIOVIA CONFERENCE 2020

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Pipeline Pilot and Data Science | TRACK: Pipeline Pilot and Data Science

DRUG DISCOVERY AND CLINICAL TRIALS

8:00-8:20 PT 11:00-11:20 ET 17:00-17:20 CET	**Using Pipeline Pilot Machine Learning Engine to Accelerate Discovery: Predictive Tier 1 ADMET Models** Gennady PODA, Ontario Institute for Cancer Research	A set of in vitro Tier 1 ADMET assays is paramount for deciding which compounds to advance to in vivo PK and efficacy models. Quality ADMET models are instrumental in compound design and, along with other computational methods to improve potency and selectivity, accelerate the drug discovery process. A suite of self-evolving, predictive (with >95% accuracy) Caco2 permeability and efflux and human and mouse liver metabolic stability (HLM and MLM) phase I machine learning models will be presented along with the best practices to build them.
8:20-8:40 PT 11:20-11:40 ET 17:20-17:40 CET	**Using PipelinePilot as an Integration Tool to Support Retrieval and Viewing of 3D Model and Structure** Mark KENNEY, Gilead	Structure enabled project teams require ways of viewing three dimensional structures of ligand-protein complexes. These structures often involve interactions with ligands not yet synthesized, and thus not present in core workflow systems that track small molecule registration and activity. The Gilead Sciences Structure Portal is used to allow access to this data in an easy to use interface that also provides access to other relevant data and an easy entry point into PyMOL sessions and comparison between related molecules. Prospective structures are automatically connected to synthesized molecules when possible. The benefits and challenges of using Pipeline Pilot to maintain the underlying portal database, to provide a convenient search and display interface, and to allow simplified interactions with 3D visualizers such as PyMOL will be discussed.
8:40-9:00 PT 11:40-12:00 ET 17:40-18:00 CET	**Precision Medicine in Research: Medidata Experience is From Medidata** Glen DE VRIES and Sastry CHILUKURI, Medidata	
9:00 - 9:20 PT 12:00-12:20 ET 18:00-18:20 CET	**Q/A Panel Lead:** Frank SCHAFFER	

DATA SCIENCE IN MATERIALS DESIGN

9:20 - 9:40 PT 12:20-12:40 ET 18:20-18:40 CET	**Multi-Objective Optimization of Formulations and Other Materials** Dana HONEYCUTT, BIOVIA	Computational generation of new optimized materials reduces to two basic issues: (1) how to explore the design space to generate new proposed materials, and (2) how to rank the proposals in a way that accounts for multiple competing objectives Through the use of specific examples, this talk shows the ways you can use Pipeline Pilot to address these issues and solve multi-objective problems in formulation and materials design. Examples include high-performance concrete, automobile tires, and polymer structure.
9:40-10:00 PT 12:40-1:00 ET 18:40-19:00 CET	**Machine Learning for Materials and Formulations** Dana HONEYCUTT, BIOVIA	We present capabilities in Pipeline Pilot for the modeling and optimization of materials properties using machine learning (ML). Using examples ranging from chocolate to steel, we discuss best practices for performing ML, and consider when it makes sense to use ML as opposed to the alternatives of experiment and simulation. Given that scientific and engineering data for a given problem are often scarce and expensive, we discuss active learning as a strategy for addressing the challenge of small training data sets.
10:00-10:20 PT 1:00-1:20 ET 19:00-19:20 CET	**Finding an Alternative Refrigerant Chemical Using Material Informatics** Abhijit CHATTOPADHYAY, BIOVIA	The a priori prediction of the thermodynamic behavior of mixtures of new compounds or of new mixtures of well-known compounds is a longstanding industrially important problem. Questions of this kind often appear in chemical engineering when new processes or alternatives for existing processes are considered, and in product design and development, when the quality or performance of a product depends on the solubility or partition behavior of compounds between different liquid phases. Refrigerant very commonly use fluorine based compounds as the chemicals; for sustainability these chemicals need to be replaced with an alternative. This talk describe a workflow using a combination of molecular modeling and data science to find an alternative refrigerant to replace the existing one to serve the community in a regulated market place in most timely manner.
10:20-10:40 PT 1:20-1:40 ET 19:20-19:40 CET	**Q/A Panel Lead:** Alex ORONA	

ETL AND DATA SCIENCE IN THE FIELD, PART I

10:40 - 11:00 PT 1:40-2:00 ET 19:40-20:00 CET	**Communication to Your Future Self: Designing Pipeline Pilot Protocols for Reusability and Readability** Jennifer HEYMONT, Eisai	With great power comes great responsibility ... and in Pipeline Pilot it comes with the ability to make a huge mess. We all know about making user interfaces user-friendly, but on the back end usability is important too – it drives the ability to easily maintain and reuse protocols and pieces of protocol workflows. If you're just doing something quick and dirty that you'll never use again then finishing with a protocol that looks like a pile of spaghetti is fine, but if you're writing code that will be used over a period of months or years then the strategies and tips in this talk are for you.
11:00- 11:20 PT 2:00-2:20 ET 20:00-20:20 CET	**Training Pipeline Pilot Developers** Kip SHAFFER, P&G	Pipeline Pilot makes it easier than ever for people to create powerful protocols, but not everyone will become a successful protocol author. In this presentation we look at some of the factors that may predict if someone has what it takes to become a successful protocol developer. We will also discuss several tips to help shape the mindset of new protocol developers so they can maximize their potential.

Pipeline Pilot and Data Science | TRACK: Pipeline Pilot and Data Science

ETL AND DATA SCIENCE IN THE FIELD, PART I

11:20-11:40 PT 2:20-2:40 ET 20:20-20:40 CET	**Harmonized Tariff Schedule Classification of Chemicals** Bob SCHWARTZ, MyIslandBeach	Assigning Harmonized Tariff Schedule Classification to chemicals for importation requires an understanding of chemistry, as well as legal and treaty considerations. Complex, ambiguous and sometimes controversial classifications, not specifically covered by the Harmonized Tariff Schedule, are the biggest challenge. Effectively dealing with these challenges and providing guidance to end-users in an efficient and user-friendly manner, requires a combination of chemical tools, and access to expertise, both automated and personal. Pipeline Pilot provides the ideal tool for all chemical issues and, in addition, delivery of automated expertise and guidance. Personal expertise is available via direct consultation, modeled after the Dassault Systemes helpdesk.
11:40 -12:00 PT 2:40-3:00 ET 20:40-21:00 CET	**Q/A Panel Lead:** Kip SHAFFER	

Discovery Studio | TRACK: Life Sciences Modeling

SMALL MOLECULES - I

8:00-8:20 PT 11:00-11:20 ET 17:00-17:20 CET	**Modeling and Validation, the Inseparable Partners** Francine ACHER, Université Paris Descartes	F. Acher,1 A. Cabayé,1,4 I. Brabet, 2 R. Glatthar,3 N. Cristiano,1 I. McCort,1 C. Goudet,2 PJ. Flor,4,3 JP. Pin,2 A. Goupil,4 HO. Bertrand4 1 UMR8601-CNRS, Université de Paris, Paris06, France 2 Institut de Génomique Fonctionnelle, Montpellier, France 3 Novartis Institutes for BioMedical Research, CH-4002 Basel, Switzerland 4 Present address: University of Regensburg, D-93053 Regensburg, Germany 5 BIOVIA Dassault Systèmes, Velizy, France The lack of efficient drugs against the Covid-19 shows that scaling down medicinal chemistry programs in many pharmaceutical companies, was not the right choice. In addition, 60 to 70% of new drugs approved yearly by the FDA are still small molecules. In this context, we may anticipate a renewal of interest in this neglected domain of drug discovery and in silico drug design is expected to play a major role. In this presentation, we will point out the critical role of computation to decipher the action mechanism of a biologically active molecule but also the essential validation of models. The mGlu7 receptor is a promising therapeutic target for several central nervous diseases and disorders (e.g. epilepsy, anxiety, depression and addiction). XAP044 is an mGlu7receptor allosteric modulator discovered by Novartis.1 The challenging search for its binding to the receptor reveals how 3D-model validation is critical to provide a significant model that will allow further drug development. 1. Gee, C. E.et al. J Biol Chem 2014, 289, 10975-87..
8:20-8:40 PT 11:20-11:40 ET 17:20-17:40 CET	**Polarizable Force Field Based on the Classical Drude Oscillator** Alex MACKERELL, Univeristy of Maryland	The inclusion of the explicit treatment of electronic polarizability in empirical force fields offers the potential to significantly improve the accuracy of molecular simulations of chemical, biological and pharmacological systems in condensed phases. Towards this goal we have developed a polarizable force field based on the classical Drude oscillator model. The Drude force field encompasses proteins, nucleic acids, lipids, carbohydrates and a limited range of drug-like molecules allowing for simulation studies of heterogeneous systems. An advantage of the Drude approach over other methods to model polarization is the inclusion of an explicit particle to model the electronic degrees of freedom allowing for steric contributions associated with electronic polarization to be modeled, a capability that has been used in the Drude Mg2+ ion and halogen parameters. The utility of the model over the additive CHARMM36 force field has been shown in the treatment of the cooperativity of helix formation of the (AAQAA)3 peptide and in the unfolding of Amyloid peptides, on base flipping in DNA and on the interactions of ions with DNA. An overview of the model will be presented along with ongoing developments and applications of the force field.
8:40-9:00 PT 11:40-12:00 ET 17:40-18:00 CET	**Engineering Platforms for Infectious Disease Research** Joel FREUNDLICH, Rutgers University	Infectious diseases caused by bacteria are responsible for millions of new infections and deaths per year. The continued spread of drug resistance, both in terms of geography and extent of resistance to approved therapies, represents a global health pandemic. To address this issue we have focused on novel approaches to discover antibacterial small molecules and probe their mechanism of action. We have sought to learn about the ideal characteristics of an antibacterial drug and its companion bacterial drug target/s. A new antibacterial critically must modulate the activity of a primary target distinct from those perturbed by current drugs. To translate toward successful outcomes, we have developed a novel platform in machine learning which has been blended with medicinal chemistry and mechanistic biology to validate novel therapeutic approaches (e.g., molecule and target). In this presentation, I will highlight the application of such an approach to the discovery of a hit compound that achieves bactericidal activity versus Mycobacterium tuberculosis through the release of NO• and inhibition of an enoyl-ACP reductase, while discussing recent advances that have enabled extension of this general approach to address ADME issues and discover novel inhibitors of Staphylococcus aureus.
9:00 - 9:20 PT 12:00-12:20 ET 18:00-18:20 CET	**Q/A Panel Lead:** Tien LUU	

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Discovery Studio | TRACK: Life Sciences Modeling

BIOTHERAPEUTICS DESIGN & DEVELOPMENT

9:20 - 9:40 PT 12:20-12:40 ET 18:20-18:40 CET	**LIVE PRESENTATION: Machine Learning for Therapeutic Protein Developability and Formulation Design** Bernhardt TROUT, MIT	We discuss cutting-edge approaches for developability and formulation design based on physical understanding and machine learning. Connection between experimental data and model-based predictions will be discussion, in addition to consequences for biotherapeutic process development.
9:40-10:00 PT 12:40-1:00 ET 18:40-19:00 CET	**Integrative Approach to T-cell Epitope Prediction** Andrej SALI, UCSF	Accurate predictions of T-cell epitopes would be useful for designing vaccines, immunotherapies for cancer and autoimmune diseases, and improved protein therapies. The humoral immune response involves uptake of antigens by antigen presenting cells (APCs), APC processing and presentation of peptides on MHC class II (pMHCII), and T-cell receptor (TCR) recognition of pMHCII complexes. Most in silico methods predict only peptide-MHCII binding, resulting in significant over-prediction of CD4 T-cell epitopes. We present a method, ITCell, for prediction of T-cell epitopes within an input antigen sequence for given MHCII and TCR sequences. The method integrates information about three stages of the immune response pathway: antigen cleavage, MHCII presentation, and TCR recognition. First, the antigen cleavage sites are predicted based on the cleavage profiles of cathepsins S, B, and H. Second, for each 12-mer peptide in the antigen sequence we predict whether it will bind to a given MHCII sequence, based on the scores of modeled peptide-MHCII complexes. Third, we predict whether or not any of the top scoring peptide-MHCII complexes can bind to a given TCR, based on the scores of modeled ternary peptide-MHCII-TCR complexes and the distribution of predicted cleavage sites. Our benchmarks consist of epitope predictions checked against 20 known peptide-MHCII-TCR crystal structures, as well as epitope predictions for four peptide-MHCII-TCR complexes with known epitopes but without crystal structures. ITCell successfully identified the correct epitopes among 20 top scoring peptides for all but two of these 20 benchmark cases. To validate the method using a clinically relevant application, we utilized five factor VIII-specific TCR sequences from hemophilia A subjects who developed an immune response to factor VIII replacement therapy. ITCell predicted the known factor VIII epitope among the six top-scoring factor VIII peptides predicted to bind all five TCRs. Our integrative approach has a higher accuracy than current single-stage models applied to the same benchmarks. It is freely available as a web server (http://salilab.org/itcell)
10:00-10:20 PT 1:00-1:20 ET 19:00-19:20 CET	**The Impact of Proline Isomerization on Antigen Binding and the Analytical Profile of a Trispecific Anti-HIV Antibody** Alessandro MASIERO, SANOFI	Proline cis-trans conformational isomerization is a mechanism that affects different types of protein functions and behaviors. Using analytical characterization, structural analysis, and molecular dynamics simulations, we studied the causes of an aberrant two-peak size-exclusion chromatography profile observed for a trispecific anti-HIV antibody. We found that proline isomerization in the tyrosine-proline-proline (YPP) motif in the heavy chain complementarity-determining region (CDR)3 domain of one of the antibody arms (10e8v4) was a component of this profile. The pH effect on the conformational equilibrium that led to these two populations was presumably caused by a histidine residue (H147) in the light chain that is in direct contact with the YPP motif. Finally, we demonstrated that, due to chemical equilibrium between the cis and trans proline conformers, the antigen-binding potency of the trispecific anti-HIV antibody was not significantly affected in spite of a potential structural clash of 10e8v4 YPtransPtrans conformers with the membrane-proximal ectodomain region epitope in the GP41 antigen. Altogether, these results reveal at mechanistic and molecular levels the effect of proline isomerization in the CDR on the antibody binding and analytical profiles, and support further development of the trispecific anti-HIV antibody.
10:20-10:40 PT 1:20-1:40 ET 19:20-19:40 CET	**Q/A Panel Lead:** Anne GOUPIL-LAMY	

WEDNESDAY SEP 23 | VIRTUAL BIOVIA CONFERENCE 2020

8 -12 PT | 11 - 15 EST | 17 - 21 CET

Discovery Studio | TRACK: Life Sciences Modeling

PHYSICS-BASED METHODS FOR LEAD OPTIMIZATION

10:40 - 11:00 PT 1:40-2:00 ET 19:40-20:00 CET	**Design, Development and Application of Ultra-High Throughput Free Energy Calculations Using CHARMM and Multi-Site λ Dynamics** Charlie BROOKS, University of Michigan	Charles L. Brooks III Cyrus Levinthal Distinguished University Professor of Chemistry and Biophysics Warner-Lambert/Parke-Davis Professor of Chemistry Professor of Chemistry and Professor of Biophysics Chair of Biophysics Departments of Chemistry and Biophysics University of Michigan In this talk I will discuss the approaches used to address the problem of developing methods for ultra-high throughput free energy methods that build from the past two decades of development in our group to establish a rigorous statistical mechanical framework for the exploration of free energy landscapes associated with changes in the chemical constituency of molecules with a particular emphasis on biomolecules and their small molecule partners. These developments are relevant to the discovery and refinement of small molecules that bind in a targeted and specific manner to biological receptors (drug design and refinement). I will provide an overview of our λ-dynamics and multi-site λ-dynamics, which facilitate ultra-high throughput free energy-based calculations of ligand binding affinities and protein. These theoretical and methodological developments will be illustrated by recent applications to significant biological and biomedical questions.
11:00- 11:20 PT 2:00-2:20 ET 20:00-20:20 CET	**Evaluation of Multiple Free Energy and Null Methods to Assess Applicability in Drug Discovery** Kira ARMACOST, Merck	Kira A. Armacost, Zhuyan Guo, Essam Metwally, Xin Cindy Yan, Song Yang Free energy calculations are widely used in the pharmaceutical industry to advance lead optimization efforts. While there are many flavors of free energy calculations being used, many are limited by scalability and selection of the most appropriate method for a given target. An internal evaluation of multiple free energy workflows on a variety of targets is underway to address some of these concerns. Currently, we are evaluating many free energy methods to assess scalability, via BIOVIA's implementation of the multi-site lambda dynamics (MSλD) method, robustness, via methods like FEP+, and speed via the Movable Type implementation by QuantumBio. In this talk, I will describe these various methods and their application to a few targets of interest in drug discovery.
11:20-11:40 PT 2:20-2:40 ET 20:20-20:40 CET	**Physics-based Binding Affinity Calculations in Small Molecule Lead Optimization** Prabhu RAMAN, BIOVIA	This talk will focus on physics-based computational methods to assist in small molecule lead optimization (LO). Attention will be placed on new tools implemented in BIOVIA Discovery Studio for protein-ligand binding affinity calculation and their applicability domains in early and late-stage LO. Early LO can benefit from the rapid screening of a large number of design ideas; toward this goal, the utility of a recently implemented end-point method to screen congeneric ligands will be discussed. Complimentary to this, the development and validation of an accurate explicit solvent-free energy perturbation (FEP) workflow for late-stage LO will be presented. Addressing the relatively higher computing time of FEP, a newly deployed alternative free energy method called Lambda Dynamics will be presented that allows for efficient R-group chemical space exploration. Addressing different domains of applicability, these methods together have the potential to bring significant efficiency and effectiveness to small molecule lead optimization.
11:20-11:40 PT 2:20-2:40 ET 20:20-20:40 CET	**Q/A Panel Lead:** Adam GREEN	

WEDNESDAY SEP 23 | VIRTUAL BIOVIA CONFERENCE 2020

8 -12 PT | 11 - 15 EST | 17 - 21 CET

Materials Innovation | TRACK: Materials Innovation through Modeling and Informatics

METALS AND ALLOYS

8:00-8:20 PT 11:00-11:20 ET 17:00-17:20 CET	**Interfacing Ab Initio Calculations, Calphad Models,Thermodynamic Databases, Web Interfaces and Visualization Tools** Axel VAN DE WALLE, Brown University	We present an array of software tools facilitating the combination of ab initio data, Calphad tools and databases, structural databases, web interfaces and 3D visualization tools. We present high-throughput methods that properly model non-stoichiometric phases at finite temperatures (including short-range order effects), lattice vibrations, mechanical instabilities and liquid phases, and that yield data that is directly compatible with the widely used elemental SGTE data. We also describe a recently developed extensive database of nearly all freely available Calphad thermodynamic databases that is web-accessible interactively or via an application programming interface. We finally showcase a simple front-end to OpenCalphad that enables 3D visualization of multicomponent phase diagrams and interfacing with standard 3D tools such as Paraview. An example of application of these tools to the design of a multicomponent alloy that is a viable inexpensive rhenium substitute for the aerospace industry is given.
8:20-8:40 PT 11:20-11:40 ET 17:20-17:40 CET	**Tools for Metal Alloy Simulations** Martin PERSSON, BIOVIA	We present tools and workflows for prediction of metal alloy thermodynamics and properties for disordered alloys. The Materials Studio Collection in Pipeline Pilot has a set of protocols geared towards metal alloy modelling. The protocols are based around the ATAT tool set by Axel van de Walle at Brown University. To enable prediction of properties for disordered alloys, we have created a protocol which generates special quasi-random structures (SQS). These SQSs can be used to predict a wide variety of properties. Additionally we present a set of protocols that target thermodynamics of alloy systems using first principle data. The first protocol predicts the convex hull and meta-stable phases for an alloy system using cluster expansion. The protocol can also create cluster expansions for other properties such as mechanical and magnetic. A second protocol uses the result from the convex hull prediction to create a CALPHAD database. The CALPHAD database can be used for thermodynamic modelling such as the prediction of phase diagrams and solidification simulations. We will show some examples of convex hull calculations and results from thermodynamic modelling using CALPHAD databases produced by our protocols. We will also show some examples of property calculations using both the SQS approach and the cluster expansion approach.
8:40-9:00 PT 11:40-12:00 ET 17:40-18:00 CET	**Simulations of Platinum Nanoparticle Catalysts with ONETEP** Chris-Kriton SKYLARIS University Of Southampton	I will present an overview of the ONETEP program which is based on a linear-scaling reformulation of DFT that retains the same high level of accuracy as conventional cubic-scaling DFT. Our new developments have allowed us to extend ONETEP to metallic systems opening the way for technologically relevant applications such as heterogeneous catalysis and electrochemistry. We have used these capabilities to perform large-scale simulations of Pt nanoparticles to study the adsorption of oxygen which controls the oxygen reduction reaction (ORR), a rate-determining step in fuel cell operation. We have investigated the effects of size, support and coverage of the nanoparticle. While most simulations make use of idealized structures such as extended surfaces or regular polyhedral nanoparticles, we have been able to work with real 3D nanoparticle structures obtained from high-precision electron microscopy. We find significant differences between the real and idealised geometries and by using electronic and geometric descriptors we can determine the optimum nanoparticle size and shape for increased performance of potential catalysts.
9:00 - 9:20 PT 12:00-12:20 ET 18:00-18:20 CET	**Q/A Panel Lead:** Victor MILMAN	

PHARMACEUTICAL DEVELOPMENT

9:20 - 9:40 PT 12:20-12:40 ET 18:20-18:40 CET	**Predictive Modeling in Process Development** Jacek ZEGLINSKI, AP Process	In this contribution, several case studies will be presented to demonstrate how computational modelling can aid development of manufacturing processes of active pharmaceutical ingredients (APIs). A typical workflow for in silico solubility screening using COSMO-RS will be presented, and a level of accuracy of the predictions will be demonstrated for a model API. In addition, different strategies of accessing theoretical crystal morphology of APIs, both in vacuum and in solvent environment will be discussed.
9:40-10:00 PT 12:40-1:00 ET 18:40-19:00 CET	**ssNMR CASTEP Predictions to Complement X-Ray Methods in Structure Determination of Crystalline Phases** Luca RUSSO, GSK	When suitable single crystals for X-ray Diffraction (SC-XRD) structure determination cannot be easily grown, a structure determination from X-ray Powder Diffraction (XRPD) can be attempted on molecular crystals of relevant complexity to pharmaceutical R&D. Following the CASTEP-based methodology published by the CCPNC network (Collaborative Computational Project for NMR Crystallography; https://www.ccpnc.ac.uk/), is possible to improve partial or ambiguous structural models that may be obtained by a pure XRPD determination. At GSK, using this methodology, we have been able to improve both chemical likelihood and consistency with XRPD data of a number of XRPD-refined models.

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Materials Innovation | TRACK: Materials Innovation through Modeling and Informatics

PHARMACEUTICAL DEVELOPMENT

10:00-10:20 PT 1:00-1:20 ET 19:00-19:20 CET	**COSMO-RS in Practice During Drug Development** Anikó UDVARHELYI, Novartis	In this talk, I will focus on practical aspects on how we use COSMO-RS during drug development at Novartis. The first part of the talk will deal with conformer selection in the context of phys-chem property predictions, including several case studies. In the second part, I will discuss solubility prediction, again focusing on practical considerations as well as using excess enthalpies for cocrystal prediction. The talk will close with an assessment of drug-polymer mixing enthalpies as an in silico pre-screening tool for precipitation inhibitors during amorphous solid dispersion development.
10:20-10:40 PT 1:20-1:40 ET 19:20-19:40 CET	**Q/A Panel Lead:** Karin WICHMANN	

SURFACES & CATALYSTS

10:40 - 11:00 PT 1:40-2:00 ET 19:40-20:00 CET	**Computational Chemistry in Materials Development for Semiconductors** Agnes Derecskei-Kovacs, Versum Materials Inc.	With the always shrinking size of semiconductor devices and the increasing complexity of the architecture, advanced specialty materials to deposit, etch, polish, clean, package, etc. the wafers during manufacturing are also more and more in demand as the nodes advance. The materials used range from small molecules to complex liquid phase formulations and contain almost all elements in the periodic table. To improve the general understanding of the underlying mechanisms of the different processes, and to speed up the development cycle of new materials, computational chemistry (also supported by other modeling tools) has been found to be useful and widely practiced. The computational approaches need to be flexible in order to match the variety of chemical systems to be treated. Model systems range from small gas phase molecules treated by highly accurate traditional ab initio methods and polymeric systems characterized by molecular mechanics, to complex multiphase systems for which QSAR approaches could be the most useful. The presentation covers real life industrial examples along with the contribution of computational chemistry to the solution, all related to advanced materials used in the semiconductor industry.
11:00- 11:20 PT 2:00-2:20 ET 20:00-20:20 CET	**Catalytic Platinum Nanoparticles Decorated with Subnanometer Molybdenum Clusters for Biomass Processing** Simon PODKOLZIN, Stevens Institute of Technology	DMol^3 calculations in Materials Studio were used to determine properties of a new catalytic material and evaluate the mechanism of chemical reactions on its surface. Development of improved technologies for biomass processing into transportation fuels and industrial chemicals is hindered due to a lack of efficient catalysts for selective oxygen removal. In this study, we report that platinum nanoparticles decorated with subnanometer molybdenum clusters can efficiently catalyze hydrodeoxygenation of acetic acid, which serves as a model biomass compound. In contrast with monometallic Mo catalysts that are inactive and monometallic Pt catalysts that have low activities and selectivities, bimetallic Pt-Mo catalysts exhibit synergistic effects with high activities and selectivities. The maximum activity occurs at a Pt to Mo molar ratio of three. Although Mo atoms themselves are catalytically inactive, they serve as preferential binding anchors for oxygen atoms while a catalytic transformation proceeds on neighboring surface Pt atoms. Beyond biomass processing, Pt-Mo nanoparticles are promising catalysts for a wide variety of reactions that require a transformation of molecules with an oxygen atom and, more broadly, in other fields of science and technology that require tuning of surface-oxygen interactions.
11:20-11:40 PT 2:20-2:40 ET 20:20-20:40 CET	**Perovskite Metal-Oxides for Automotive Three-Way Catalysis** Crispin COOPER, Johnson MATTHEY	Perovskite oxides have long been the subject of study and speculation as possible base-metal alternatives to precious metals in catalytic application. Here we present results and conclusions from a study of these materials for application to three-way emissions control catalysis (TWC) as well as wider catalytic functions. Key predictions are compared with experimental results. Traditional TWC materials are typically noble metals supported on redox-active supports such as doped ceria-zirconias. Noble and other metals can likewise be supported on, or incorporated in to, the perovskite oxides. The thermodynamic preference for a wide range of metals to segregate to the surface or dissolve in to the bulk of the supporting perovskite has been studied by application of theoretical methods and expands on the previously known literature results for these system. This includes the effects of reducing or oxidising environment on the segregation of components. The mechanisms of CO oxidation and NO reduction with and without supported metal particles are discussed. The effects of metal ad-atoms and larger supported particles are studied and results resented in terms of NO activation, competitive adsorption and effects on oxygen behaviour. We draw conclusions as to the potential and limits of these systems and briefly outline the scope for future study.
11:20-11:40 PT 2:20-2:40 ET 20:20-20:40 CET	**Q/A Panel Lead:** Nick REYNOLDS	

WEDNESDAY SEP 23 | VIRTUAL BIOVIA CONFERENCE 2020

8 -12 PT | 11 - 15 EST | 17 - 21 CET

Manufacturing | TRACK: Quality

QUMAS PRODUCT FUNCTIONALITY

8:00-8:20 PT 11:00-11:20 ET 17:00-17:20 CET	**What's New / What's Next in QUMAS** Chris FROST, ENOVIA, Cyril WALSH, BIOVIA	What has R&D been working on? Let's kick off with an update from the QUMAS product manager including release dates and product road maps for QUMAS EDMS and QUMAS EQMS. The new EQMS Search and Export will be covered in depth.
8:20-8:40 PT 11:20-11:40 ET 17:20-17:40 CET	**A First Look at the new Learning Management System Integration** Cyril WALSH, ENOVIA	Learning Management Systems (LMS) are not always suitable for recording training for GMP processes. Linking the LMS training task to the effective procedure in the controlled document management system is the first step to ensuring compliance. This talk will show how the integration should go further to enable the training manager to go beyond managing training per SOP to coordinating competencies and job profiles.
8:40-9:00 PT 11:40-12:00 ET 17:40-18:00 CET	**Planning a Successful Upgrade or Move to the Cloud** Conor BARRY, Noel O'BRIEN, BIOVIA	Thinking about a move to the cloud? BIOVIA services leaders will discuss considerations for planning a move to ScienceCloud.
9:00 - 9:20 PT 12:00-12:20 ET 18:00-18:20 CET	**Q/A Panel Lead:** Wesley FLAKE	

QUALITY & BEYOND - TRENDS, TECHNOLOGY ENABLERS AND INNOVATIONS

9:20 - 9:40 PT 12:20-12:40 ET 18:20-18:40 CET	**Document Management in the 3DEXPERIENCE Platform** Ken HAYWARD, ENOVIA	Document Management in the 3DExperience platform provides intuitive, consistent platform-wide access to document capabilities transforming your ability to manage documents fully integrated with product lifecycle management, projects and enterprise change management. Discover how the platform can enable collaboration and sharing of documents together with new approaches to document authoring and publishing.
9:40-10:00 PT 12:40-1:00 ET 18:40-19:00 CET	**Next generation Pharmaceutical Quality Systems (PQS)** Conor HAYES, ENOVIA	Quality management has long been an exercise involving the manual capture of data about Quality events or changes and the control of the flow of that data through the pre-defined process. Using the 3DEXPERIENCE platform to move from this corrective to a preventative approach allows us to warn of issues as – or even before – they occur. We augment the manual activity, this can reduce instances of duplication of changes, repeat deviations and move us from 'human data assembly' to capture of realtime evidence to improve product quality and lower cost.
10:00-10:20 PT 1:00-1:20 ET 19:00-19:20 CET	**Structured Document Management in the 3DEXPERIENCE Platform** Aidan QUILLIGAN , ENOVIA	Structured Document Management combines in-browser authoring with content re-use and data connectivity to change how you can create and manage documents. By leveraging re-usable content topics included in one or more document maps, Structured Documents allow you to reduce content duplication, manage change centrally and drive consistency and standardization. A flexible publishing pipeline means you can produce output in a variety of formats, with centralized control over layout, format and overall appearance. Our Structured Document Editor also supports Data-to-Document, allowing you to include application data directly within the content, without having to duplicate or copy the data.
10:20-10:40 PT 1:20-1:40 ET 19:20-19:40 CET	**Q/A Panel Lead:** Ken HAYWARD	

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11:40 -12:00 PT 2:40-3:00 ET 20:40-21:00 CET	**Q/A Panel Lead:** Ken HAYWARD	

THURSDAY SEP 24 | VIRTUAL BIOVIA CONFERENCE 2020

8 -12 PT | 11 - 15 EST | 17 - 21 CET

Laboratory Informatics | TRACK: Laboratory Informatics

MATERIALS MANAGEMENT

8:00 - 8:20 PT 11:00 EST	**What's New in BIOVIA CISPro** Anne SEFREID, BIOVIA	Join us as we explore What's New for CISPro 2020. Check out new container management workflows and the upcoming changes that will both enhance and simplify the end user experience. Be the first to preview the new freezer inventory management features built to address complex the
8:20-8:40 PT 11:20-11:40 ET 17:20-17:40 CET	**CISPro Frozen Inventory: Older Database? Let it go.** Jenna GANNON, Jonathan RICE, Amgen	Managing freezer inventory is what the Amgen Critical Reagent Group (CRG) lives and breathes. Join Jenna Gannon, one of the 5 scientists of the CRG team, and Jonathan Rice, their digital guru, as they explain the challenges they faced with their legacy system and how CISPro Freezer Inventory has addressed those issues.
8:40-9:00 PT 11:40-12:00 ET 17:40-18:00 CET	**Tablet Formula: How to Control Final Composition** Dale PIXLEY, BIOVIA	Modern multi-layered therapeutic tablets contain separate compositions for each layer. In designing such a tablet, scientists need to be able to track the formulations of each layer, and how the amounts needed are linked together. In this presentation we will delve into how BIOVIA Enginuity simplifies this process and ensures consistency throughout the process.
9:00 - 9:20 PT 12:00-12:20 ET 18:00-18:20 CET	**Q/A Panel Lead:** Chris STRASSEL	

DATA VISUALIZATION AND ANALYTICS

9:20 - 9:40 PT 12:20-12:40 ET 18:20-18:40 CET	**Visualizations for ONE Lab: Integrating Insight to Provide Data Review Capabilities** Chris PIERINI, Amgen	BIOVIA ONE Lab provides a robust set of data capture and user controls to enable various scientific workflows. However, visualization capability such as graphing is not a currently supported feature in ONE Lab. Our Proof-of-Concept (POC) work demonstrates integrating BIOVIA Insight as a visualization layer for data captured through ONE Lab can provide end-to-end documentation for scientists while maintaining GMP controls.
9:40-10:00 PT 12:40-1:00 ET 18:40-19:00 CET	**Data Visualization in the Chemicals Industry** Frank SCHAFFER, BIOVIA	Many science-based companies face experiment summaries that are stored in Excel, locally or on Sharepoint, and raw data files scattered in silos. But this is not FAIR data - that which is Findable, Accessible, Interoperable, and Reuseable. Scientists need data which is standardized and can be easily found and reused to visualize results and make better decisions, faster. In this presentation we will demonstrate how Dassault Systemes and BIOVIA are combining data into flexible visualization reports for formulators and decision makers.
10:00-10:20 PT 1:00-1:20 ET 19:00-19:20 CET	**Extending ONE Lab using Pipeline Pilot** Shabbir KHERALUWALA, BIOVIA	In BIOVIA ONE Lab, scientists can utilize BIOVIA Pipleline Pilot to create custom protocols that are accessible to users via simple buttons in the normal ONE Lab interfaces. In this presentation we will demonstrate how to create and implement these controls to extend and customize ONE Lab functionality.
10:20-10:40 PT 1:20-1:40 ET 19:20-19:40 CET	**Q/A Panel Lead:** Sean O'HARE	

THURSDAY SEP 24 | VIRTUAL BIOVIA CONFERENCE 2020

8 -12 PT | 11 - 15 EST | 17 - 21 CET

Pipeline Pilot and Data Science | TRACK: Data Science

ETL AND DATA SCIENCE IN THE FIELD, PART II

8:00-8:40	**What's New in Pipeline Pilot and Scientific Informatics?** Alex ORONA and Matt SAGE, BIOVIA	The Pipeline Pilot and broader Research Informatics team has been busy at work. This session reviews the latest additions from Pipeline Pilot to Scientific Intelligence to Insight. Learn about our recent work and our roadmap for the future.
8:40-9:20	**Introduction to Jupyter Notebooks in Pipeline Pilot** Alex ORONA and Ian KERMAN - BIOVIA	Jupyter Notebooks are commonly used in data science development today. In this session, you will learn the basics of the new Python Jupyter Notebook (on Server) component in Pipeline Pilot 2020. We will also show you how to enable GPU support in TensorFlow 2.0 on your machine (if you have a compatible NVIDIA GPU).

MATERIALS WORKSHOP

9:20 - 9:40 PT 12:20-12:40 ET 18:20-18:40 CET	**Error Proof Assembly on Manufacturing Shop Floor with Data Science** Nick REYNOLDS, BIOVIA	The use of data science in supporting error proof manufacturing will be described. Working with an automobile manufacturer, a solution based on Pipeline Pilot has been developed to identify when manufacturing steps are done incorrectly, or in the wrong order, in order to quickly identify problems and increase manufacturing quality.
9:40-10:40	**Workshop: Utilizing IoT to Support Predictive Maintenance** Jason DEJOANNIS, BIOVIA	We will use Pipeline Pilot to engineer machine learning descriptors from time series data coming from equipment in the field. We will build predictive maintenance models to tell us when to perform maintenance on each machine. Participants can follow along if they have Pipeline Pilot 2019 or 2020 installed. Prior to arriving, the organizer will send you a link with the data, which you can download before the session.

ACCELERATING DRUG DISCOVERY

11:00 - 11:20	**Improved Lead Compounds from Generative Therapeutics Design** Ton VAN DAELEN, BIOVIA	The drug discovery phase typically takes around four years and, in the case of small molecule therapeutics, can require the synthesis and screening of over 4,000 compounds. We will discuss an approach that applies AI and machine learning to design, test and optimize lead molecules rapidly in silico and to suggest what compounds to synthesize and screen next in an 'active learning' process. The Dassault Systèmes' 3DEXPERIENCE platform offers tight integration between the virtual and real cycles (V+R). This shortens timelines by reducing turnaround time for laboratory synthesis and screening, while also reducing the number of V+R cycles. 3D modeling and simulation methods can enhance the accuracy of predictions for drug potency, efficacy and selectivity, while also addressing multi-target effects. This approach can help identify the best synthesis routes, taking into consideration availability of chemicals, published synthetic routes and reagent availability from commercial vendors and contract research organizations (CROs). Furthermore, by building better predictive models for target activity, anti-target effects and ADME/TOX effects, teams can improve success rates in the clinical phase and bring therapeutics to market faster.
11:20 - 11:40	**Fogdesigner – Towards an Integrated Design, Make, Test, Analyze Workflow Platform for a Small Biotech** Johannes VOIGT, Foghorn Therapeutics	Hypothesis guided drug design requires access to all relevant in vitro, in vivo, chemistry and structural data, and should be aided by state-of-the-art data analysis, visualization, and in silico prediction approaches. To that end Foghorn Therapeutics has developed a design and workflow management platform based on Biovia's Pipeline Pilot. Chemists can interactively design and in silico profile ideas in the context of all existing bioassay and structural data. Synthesis in house or at CROs is managed through this tool and once synthesis is complete the compound is linked back to the design idea record and all the relevant experimental data is captured in a datamart. The datamart centrally aggregates all individual assay data points and provides summarized averages considering all relevant protocols and protocol conditions. The datamart also enables seamless integration with Vortex, Excel, ChemDraw, and Fogbrowser – an in house developed web-based data browser also realized through Pipeline Pilot.
11:40-12:00	**Q/A Panel Lead:** Ton VAN DAELEN	

THURSDAY SEP 24 | VIRTUAL BIOVIA CONFERENCE 2020

8 -12 PT | 11 - 15 EST | 17 - 21 CET

Discovery Studio | TRACK: Life Sciences Modeling & Simulation

SMALL MOLECULES - II

8:00-8:20 PT 11:00-11:20 ET 17:00-17:20 CET	**Probing Protein-Ligand Interactions in Factor Xa using SAR and MD-based Free-Energy Calculations** Han SUN, Marc NAZARÉ, FMP Berlin	1. Structural Chemistry and Computational Biophysics, Leibniz-Forschungsinstitut für Molekulare Pharmakologie, 13125, Berlin, Germany. 2. Medicinal Chemistry, Leibniz-Forschungsinstitut für Molekulare Pharmakologie, 13125, Berlin, Germany. Free energy calculations of protein ligand binding are of great interest to medicinal chemists, because they can be used to guide structure-based drug design. Among the existing computational techniques, molecular dynamics-based alchemical free energy calculations are unique in their accuracy and solid theoretical basis, and therefore show great potential for a widespread use in pharmaceutical drug discovery. In this study, we adopted alchemical relative free energy calculations for evaluating and predicting binding affinities of a series of 2-carboxyindole-based inhibitors of serine protease factor Xa, which plays an important role in the blood coagulation cascade. The binding mode and structure-activity relationship of 2-carboxyindole-based inhibitors including biaryl and phenylacetamide substituents have been systematically investigated, providing an excellent experimental basis for our computational study. Using a combination of free energy calculations and experimental validation, a large perturbation in the binding affinity of several congeneric new fXa ligands could be identified. Moreover, analysis and comparison of inhibitors with different substituents and scaffolds from the calculations provide a basis for better understanding of the underlying interactions and energetics of fXa inhibitors and the enzyme's active site.
8:20-8:40 PT 11:20-11:40 ET 17:20-17:40 CET	**Diving into the transport mechanism of a neurologic transporter: an explicit membrane molecular dynamics simulation approach** Alexandre CABAYÉ, Université Paris	Amino-acid transporters play an important role in the regulation of the synaptic availability of amino-acid agonists. Here we explore the first steps of the transport mechanism of the Asc-1 transporter, using molecular dynamic simulations with an explicit environment (water and lipid bilayer). Understanding this mechanism opens the door for rational design of potential inhibitors, which could play an important role for treating neurological disorders like schizophrenia.
8:40-9:00 PT 11:40-12:00 ET 17:40-18:00 CET	**Predicting Toxicity with TOPKAT for Regulatory Purposes** Stefan PUDENZ, Covance	International and national regulatory authorities identified quantitative structure activity-relationship (QSAR) modelling as an alternative to toxicity testing of animals to identify potential health and safety hazards of chemicals. Over the last years the author conducted numerous QSAR studies of predicting toxicity using TOPKAT and other QSAR models for submission to regulatory bodies. Unlike many other models TOPKAT provides the possibility of model extension by including additional compounds in the training set. This feature has been extensively used and its effects on the prediction of specific compounds and endpoints will be discussed. Furthermore, regulatory requirements on QSAR studies are mainly based on the OECD guidance document on the validation of QSAR models. We will report about our experience and challenges of submitting QSAR studies according to the five OECD principles.
9:00 - 9:20 PT 12:00-12:20 ET 18:00-18:20 CET	**Q/A Panel Lead:** Hugues-Olivier BERTRAND	

BIOTHERAPEUTICS DESIGN & DEVELOPMENT - II

9:20 - 9:40 PT 12:20-12:40 ET 18:20-18:40 CET	**The Real Value & Opportunities in End-to-End Computational Drug Development for Biologics** Neeraj AGRAWAL, Amgen	Computational tools are gaining popularity within biopharmaceutical industry and have been applied to drug discovery, development and manufacturing with a net positive impact on the efficiency and agility of these processes. These computational tools span from first principle modeling tools such as molecular dynamics to semi-empirical tools to big data based "trained models" tools. Within Amgen Process Development, we have applied some of these computational tools to understand and monitor the critical quality attributes (CQAs). The improved understanding of these CQAs through first principle and semi-empirical tools have led to enhanced biotherapeutic molecule design and molecule selection. Similarly, the real time monitoring of these attributes (during the manufacturing phase & within the framework of continued process verification) through data engineering and analytics has improved our reliability and reduced the manufacturing lot-to-lot variability in the product quality. Overall, we believe that advanced computational approaches are an essential complement to experimental approaches and their joint deployment is necessary for the selection and commercialization of a biotherapeutic that comprehensively satisfies an unmet medical need.
9:40-10:00 PT 12:40-1:00 ET 18:40-19:00 CET	**Boosting Antibody Developability through Computational Protein Design** Qing CHAI, Lilly	
10:00-10:20 PT 1:00-1:20 ET 19:00-19:20 CET	**Predicting Protein Formulation Properties in BIOVIA Discovery Studio** Lisa YAN, BIOVIA	Formulation issues, including aggregation, protein stability, high viscosity, and low solubility put biologic design projects at high risk and cause failure in late-stage development. BIOVIA Discovery Studio provides computational tools to predict protein formulation properties which allow quick ranking and screening of the antibody candidates in the early stage of biologics design to help to reduce the downstream risks. This presentation will explore the newest functionality for predictions of viscosity (based on the SCM algorithm from MIT) and solubility in the latest Discovery Studio release.
10:20-10:40 PT 1:20-1:40 ET 19:20-19:40 CET	**Q/A Panel Lead:** Anne GOUPIL-LAMY	

THURSDAY SEP 24 | VIRTUAL BIOVIA CONFERENCE 2020

8 -12 PT | 11 - 15 EST | 17 - 21 CET

Discovery Studio | TRACK: Life Sciences Modeling & Simulation

ADVANCING THERAPEUTICS DESIGN

10:40 - 11:00 PT 1:40-2:00 ET 19:40-20:00 CET	**Promise and Challenges of AI for Therapeutic Target Identification** Niranjani IYER, BIOVIA	Identifying potential targets for developing new drugs is the first major step in the arduous quest for curing a disease. With the high attrition rates involved in the drug development process, judicious science-based decisions are essential to minimize costly failures. Scientists use multiple approaches and technology platforms to understand the cellular, molecular, biochemical complexities associated with a disease. These approaches heavily rely on high throughput omics-datasets such as genome wide association scans, gene expression analysis from tissue to single cell, miRNA analysis, proteomics, post-translational modifications, cellular imaging to name a few. For a holistic analysis, information from several multi-dimensional datasets (Omics, text and image analytics, public databases, systems biology) needs to be integrated. AI and machine learning technologies are gaining popularity in extracting knowledge from a multitude of resources and thus enabling precision medicine. This talk will focus on Biovia's tool sets that will empower scientists to harmonize and cogently retrieve the valuable information from numerous datasets.
11:00- 11:20 PT 2:00-2:20 ET 20:00-20:20 CET	**In-silico Biologics Design in 2020: Challenges and Perspectives** Anne GOUPIL-LAMY, BIOVIA	The world of "biologic" therapeutics has rapidly expanded over the last decade: what once started with repurposed IgG antibodies has grown to include a seemingly limitless range of modalities. This in turn has made developing treatments for previously intractable diseases safer and more effective. At the same time, each new approach introduces a layer of complexity that must be accounted for. For example, can the chimeric antigen receptor in a CAR-T cell be modified to increase overall T cell potency? While physical experimentation can shed light onto this and other processes, in silico methods can guide and augment this work to foster a deeper understanding of how these approaches work and how they can best be optimized. This talk will cover strategies for improving the performance of new antibody modalities, CAR-T therapeutics, CRISPR-Cas9 and rational vaccine design within BIOVIA Discovery Studio 2020.
11:20-11:40 PT 2:20-2:40 ET 20:20-20:40 CET	**Developments in Discovery Studio** Tien LUU, BIOVIA	BIOVIA Discovery Studio 2021 is an exciting major release building on the software's decades-long legacy of scientific development in life science modeling and simulation. This talk presents the latest new science, features and enhancements, and provides a preview of plans for the future roadmap.
11:20-11:40 PT 2:20-2:40 ET 20:20-20:40 CET	**Q/A Panel Lead:** Niranjani IYER	

THURSDAY SEP 24 | VIRTUAL BIOVIA CONFERENCE 2020

8 -12 PT | 11 - 15 EST | 17 - 21 CET

Materials Innovation | TRACK: Materials Innovation through Modeling and Informatics

ADVANCES IN MATERIALS MODELING

8:00-8:20 PT 11:00-11:20 ET 17:00-17:20 CET	**Next Generation Surfactant Engineering Using COSMOplex** Johannes SCHWOEBEL, BIOVIA	During the past 20 years, the efficient combination of quantum chemical calculations with the statistical thermodynamics method COSMO-RS has become an important and efficient alternative to force-field based simulations for the accurate prediction of free energies of molecules in liquid systems. While COSMO-RS was restricted to homogeneous liquids, it has been extended to the self-consistent prediction of the structure and free energies of molecules in complex, self-organizing inhomogeneous systems. This new COSMOplex method extends the application range to many new areas and is 10,000 times faster than comparable molecular dynamics calculations, thus enabling many applications at significantly lower computational costs while also achieving better agreements with experiments.
8:20-8:40 PT 11:20-11:40 ET 17:20-17:40 CET	**Democratising Virtual Product Simulation in a Large Consumer Goods Organisation – What Our Journey Has Taught Us** Andrew EVANS, Unilever	Unilever is one of the world's largest consumer goods companies, making many of our consumers most favourite brands. With a stated purpose of making sustainable living commonplace and big goals around improving health and well being, halving our environmental footprint and enhancing the livelihoods of millions of people, it is clear that innovation must be at the core of Unilever's processes and in particular within R&D. Unilever is not new to Virtual Product Simulation, however from 2017 a step change has been made to transform the use of simulation and optimisation from a specialist, expert activity, to one that is in the everyday reach of its thousands of R&D professionals. This presentation describes the lessons learned during this journey , and concludes that focussing purely on technology will not deliver a successful outcome. Instead, a multi-pronged approach is essential, incorporating seamlessly connected digital tools, trusted data and digitally skilled and empowered people.
8:40-9:00 PT 11:40-12:00 ET 17:40-18:00 CET	**Accelerate Innovation through Collaborative Research** Lalitha SUBRAMANIAN, BIOVIA	As a trusted partner for 25 years, we are continuing to provide solutions to numerous business-critical industry challenges. These range from product performance enhancement, process optimization, manufacturing failure remediation, therapeutics discovery, development, and delivery. Working in direct collaboration on proprietary projects with our industry customers as well as via consortium-style engagements on pre-competitive topics, our digital solutions enable our customers to improve productivity, obtain competitive edge, and achieve sustainability goals. With several case studies, this talk will cover application of multiscale modeling and simulations and machine learning methods applied to challenging problems in industries spanning Energy & Materials, Transportation & Mobility, Aerospace & Defense, Consumer Packaged Goods, Industrial Equipment, and Pharmaceuticals.
9:00 - 9:20 PT 12:00-12:20 ET 18:00-18:20 CET	**Q/A Panel Lead:** James WESCOTT	

THURSDAY SEP 24 | VIRTUAL BIOVIA CONFERENCE 2020

8 -12 PT | 11 - 15 EST | 17 - 21 CET

Materials Innovation | TRACK: Materials Innovation through Modeling and Informatics

FUTURE OF MATERIALS MODELING

9:20 - 9:40 PT 12:20-12:40 ET 18:20-18:40 CET	**Molecular Simulation of Thermoset Curing: Application to 3D Printing Materials** James ELLIOTT, University Of Cambridge	Conventional three-dimensional (3D) printing uses a feedstock of pellets or filaments made of thermoplastic material, which can be melted and extruded before solidifying in their final shape. Printing of thermosetting polymers however represents a much greater challenge, as these materials need to be cured during or after printing to retain their shape, over timescales that generally exceed those of the rapid 3D printing process. Being able to print thermosets is highly desirable due to the superior properties these materials offer over thermoplastics, and the costs and energy-intensity of the traditional moulding process used to fabricate 3D architectures. Bismaleimide (BMI) resins are a new class of high-performance thermosetting polymers that have excellent chemical and thermal stability and outstanding mechanical properties, making them attractive for industrial 3D printing applications. There is a great demand for tailoring properties of thermosets, but there are significant challenges in the detailed modelling of these materials using conventional methods. Among these is the lack of direct access to the structure of the polymer network on the length scale of monomers. Using a Pipeline Pilot workflow combining Random Graph Theory (RGT) and Guided Reactive Molecular Dynamics (GRMD), we have carried out computer simulations of the polymerisation process which provide detailed information on the topological evolution of the system in the polymerisation process, and can help gain a better understanding of the structure property relationship, with a potential to guide materials design.
9:40-10:00 PT 12:40-1:00 ET 18:40-19:00 CET	**Applying Quantum Computers to the Study of Solid State Systems** Dr David MUÑOZ RAMO, Cambridge Quantum Computing	The simulation of molecules and materials has been identified for a long time as one of the key areas that will benefit from quantum computing. This is due to the natural way in which electron correlations may be implemented on quantum hardware, with an exponential reduction in the memory required to express the correlated wavefunction. Most of the research done in this field involves the modeling of molecular systems, while research on solid state systems has been mostly restricted to Hubbard-like simple models. In this talk, we present our investigations in the area of quantum algorithms for solid state quantum simulation, with two strategies being pursued. First, we show our efforts in creating a variational quantum algorithm with a Unitary Coupled Cluster ansatz that is compatible with periodic boundary conditions. Then, we present our work on a quantum implementation of Dynamical Mean Field Theory. Strengths and challenges of each approach are discussed.
10:00-10:20 PT 1:00-1:20 ET 19:00-19:20 CET	**Advances in Materials Studio** James WESCOTT, BIOVIA	As BIOVIA Materials Studio moves into its third decade we reflect on the many contributions made by our customers to materials research across multiple industries, as evidenced by literally tens of thousands of literature citations. Nevertheless, development of scientific capability continues unabated and in this talk we will review some of the recent features of the 2020 release supporting new materials development for batteries, polymers, metals and more. Further, in the 2021 release we will soon be leveraging features of the 3DEXPERIENCE platform to provide new ways to execute molecular simulations in what promises to be a landmark release for Materials Studio.
10:20-10:40 PT 1:20-1:40 ET 19:20-19:40 CET	**Q/A PANEL LEAD:** MARC MEUNIER	