BIOVIA Conference 2021

	Track: Laboratory Informatics	Track: Pipeline Pilot	Track: Life Sciences Modeling and AI	Track: Research Informatics	Track: Materials Innovation through Modeling and Simulation	Track: Formulations	Track: Manufacturing Intelligence	Track: Quality
	Day 1 09/14/21	Day 1 09/14/21	Day 1 09/14/21	Day 1 09/14/21	Day 1 09/14/21	Day 1 09/14/21	Day 1 09/14/21	Day 1 09/14/21
7:00 - 8:00 PST	**Welcome Opening Plenary** BIOVIA CEO, CSO and Head of R&D (40 min) Scott Bembenek, PhD. Founder, CEO, CSO, Denovicon Therapeutics and Reza Sadeghi, CSO BIOVIA (20 min)							
	Digitized Lab/Digital Experiments	**Drug Discovery Infrastructure I**	**AI Driven Drug Design I**	**Chemistry**	**Polymers & Composites**	**Formulations**	**Manufacturing Intelligence - Today and in the Future**	**Integrated Quality**
8:00 - 8:20	Huntsman, Florian Klunker - Introduction of Electronic Laboratory Notebook in Huntsman Corporation	GSK, Subhas Chakravorty - A One-prot Pipeline Pilot Reactor for Virtual Molecular Design Using a Traditional QSAR Approach	Denovicon Therapeutics, Scott Bembenek - AI–Molecular Modeling Platform for Enhanced Small-Molecule Drug Discovery	Roche, Gunther Doernen, Dieter Imark and Gerd Blanke - Wilberforce Normalize - Cheshire Replacement Using the Pipeline Pilot Chemistry SDK	WM York Consulting LLC, Michael York - Coarse-Grained Molecular Dynamic Simulations Can Predict Silica/Silanization Cluster Morphology	BIOVIA, Dale Pixley - Tips and tricks: Advance Topics in Enginuity	BIOVIA, Barbara Holtz - The Future of Manufacturing: Connecting the Virtual and the Real with Digital Twins	BIOVIA, Chris Frost - What's New and Coming with QUMAS?
8:20 - 8:40	Pfizer, Martin Berliner - What is a Web Section? Dynamic Dashboards and Displays in Workbook	Weizmann Institute of Science and GSI Technology, Dr. Efrat Ben-Zeev and Rudy Kirzhner - High Performance Similarity Search in Cheminformatics	Carnegie Mellon University, Olexandr Isayev - AI-accelerated Simulations and Molecular Design	BIOVIA, Moises Hassan - What's New in BIOVIA Pipeline Pilot Chemistry and SDK	BIOVIA, Reinier Akkermans - Multiscale Simulations of Polymer Composites	BIOVIA, Mary Beth Finnegan - Proactively Manage the Impact of Regulatory Changes in Process/Formulations Industries	UCB Biopharma, Jean-Etienne Fortier - Digital Frugality: What Is It? Example with Discoverant and Pipeline Pilot	BIOVIA, Conor Barry - QUMAS and BIOVIA ONE Lab - How to Connect QMS to the Laboratory
8:40 - 9:00	BIOVIA, Kirsten Gesenberg - What's New with BIOVIA Workbook	Galapagos NV, Miriam López-Ramos - Integrating Pipeline Pilot-based Chemoinformatics Tools in Medicinal Chemists' Workflows	Collaborations Pharmaceuticals, Sean Ekins - Applying Machine Learning to the Identification and Design of New Molecules		Université de Sherbrooke, Armand Soldera - Using Large-scale Simulations to Perform Dynamical Mechanical Analysis of Rubbers	Virtual Roundtable Discussion: What are the Biggest Challenges Facing Formulators Today? Leads: Mary Beth Finnegan/Dale Pixley	BIOVIA, Chris Andrews - Automatic Conversion of Process Recipes to Published Hierarchies	Pharmamar, Osvaldo Nestares - A Journey from Drug Discovery to e-Submission
9:00 - 9:20	Q/A Panel Lead: Kirsten Gesenberg	Q/A Panel Lead: Ton van Daelen	Q/A Panel Lead: Dana Honeycutt, Tien Luu	Q/A Panel Lead: Matt Sage, Moises Hassan, and Gerd, Dieter, Gunther	Q/A Panel Lead: Marc Meunier	Q/A Panel Lead: Julian Willmott	Q/A Panel Lead: Stéphane Vellay	Q/A Panel Lead: Wesley Flake
	Process Optimization	**Drug Discovery Infrastructure II**	**AI Driven Drug Design II**	**Registration, Macromolecules &**	**Topic: Extending the Reach of**	**Topic: Formulations**	**Implementing Manufacturing**	**The Future of Quality**
9:20 - 9:40	Janssen, Shaun McWheeney, Koen Paeshuyse - tRex Recipe Builder Enables a Flexible Recipe-based Data Capture in Process Development Using BIOVIA Workbook	Sanofi, Florence Pernigotti, Sebastien Charneau - Sanofi R&D Compound Toolbox: A Web App for Advanced Computations and Analytics	BIOVIA, Dana Honeycutt - Predicting Prediction Quality	BIOVIA, Neil Eccles - BIOVIA Bio/Chem Registration Update	International Flavors & Fragrances, Haining Liu - Validation and Implementation of COSMOtherm to Calculate the Flashpoint of Flavor and Fragrance Formulae	BIOVIA, Ryan Cuprak - Enginuity 22x UI Refresh	BIOVIA, Anand Krishnamurthy - Discoverant APQR – Effective Quality Improvements for Pharma & Biotech.	BIOVIA, Ken Hayward - Structured Documents -- a New Way to Author Documents
9:40 - 10:00	BioPhorum, David Wallace - A Manifesto for the QC Lab of the F	AstraZeneca, Wolfgang Klute - Informatics Challenges in Early Clinical Development	Cambridge Crystallographic Data Centre, Dr. Vera Prytkova - GOLD Docking in Structure-based Drug Design Applications	BIOVIA, Guy Oshiro - Industry Process for Small Molecule Therapeutics Design	BIOVIA, James Wescott - What's New and What's Next in Materials Studio	BIOVIA, Akhil Kamma - Next Generation Formulation Design	Panel discussion: Discoverant best practices for implementation and maintenance	BIOVIA, Conor Barry - How to Get a Better Grip on Your GxP Risks with QUMAS EQMS Risk Management
10:00 - 10:20	BIOVIA, Graham Janson - Get Up and Running Quickly with Generic Template Methods	Roche, Gunther Doernen, Dieter Imark and Gerd Blanke - Wilberforce Normalize - Cheshire Replacement Using the Pipeline Pilot Chemistry SDK	University of Paris , Francine Acher - Modeling Elucidates Ligand Specificity of a Class C G-Protein Coupled Receptor	BIOVIA, Neil Eccles - BIOVIA Materials Registration Update	BIOVIA, Julian Willmott - Democratizing Simulation	BIOVIA, Julian Willmott - Democratizing Simulation	BIOVIA, Stéphane Vellay - Augmented Manufacturing Intelligence with External Data Access	BIOVIA, Noel O'Brien, Conor Barry - The Cloud and Validation Go Hand-in-Hand with BIOVIA ScienceCloud
10:20 - 10:40	Q/A Panel Lead: Graham Janson	Q/A Panel Lead: Ton van Daelen	Q/A Panel Lead: Anne Goupil	Q/A Panel Lead: Neil Eccles/Guy Oshiro	Q/A Panel Lead: Stephen Todd	Q/A Panel Lead: Mary Beth Finnegan	Q/A Panel Lead: Larry Fiegland	Q/A Panel Lead: Wesley Flake
	Inventory Management	**Pipeline Pilot Strategies**	**Materials Science in Life Sciences**	**Registration, Macromolecules & Biologics**	**Topic: Pharmaceutical Development (Shared with LS**		**Best practices of Manufacturing Analytics**	**Quality and Collaboration**
10:40 11:00	Merck, Jessie Bin Song - Regulated Substance Inventory Management based on Standard BIOVIA CISPro Platform	P&G, Kip Shaffer - Designing and Initiating Asynchronous Jobs in Pipeline Pilot	Vertex Pharmaceuticals, Satish Kumar Iyemperumal - Speeding Up Drug Development with Workflows Involving Quantum Mechanical Calculations: Case Study of Cocrystal and Solubility Screening of Drug Molecules	BIOVIA, Martin Hornig - BIOVIA Draw Updates	*** SAME AS Life Sciences Track		UCB, Valentin Salvia-Prats - The Impact of Master Data on Discoverant Hierarchy Configuration	BIOVIA, Wesley Flake - CMC Authoring -- Transfering Data to Documents for Technical Reporting
11:00 - 11:20	BIOVIA, Anne Sefried - What's New and What's Next in BIOVIA CISPro	Eisai, Jennifer Heymont - Leaf, Tree, Forest: Choosing the Right Zoom Level for Solution Development	BIOVIA, Stephen Todd - Towards in-silico Prediction of Solvent Effect on Crystal G	Janssen, Danny Verbinnen - Maximizing the Power of Molfile Format and BIOVIA Products BIOVIA Draw & BIOVIA Direct with GCRS	*** SAME AS Life Sciences Track		BIOVIA, Larry R. Fiegland - BIOVIA Discoverant 2022 Release Coming Soon!	BIOVIA, Hugh Madden - How to Solve Your Third-party Collaboration Challenges with BIOVIA ScienceCloud
11:20 - 11:40	Virtual Roundtable and Q/A Q/A Lead: Kirsten Gesenberg	Virtual Roundtable and Q/A Q/A Lead: Lee Herman	BIOVIA & SIMULIA, Marc Meunier & Christina Foley - Multi-scale Simulation of Tableting Processes	AstraZeneca, Wolfgang Klute - Informatics Challenges in Early Clinical Development	*** SAME AS Life Sciences Track		Q/A Panel Lead: Chris Andrews	Q/A Panel Lead: Wesley Flake

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11:40 - Noon			Q/A Panel Lead: Jason DeJoannis	Q/A Panel Lead:Matt Sage, Martin, Danny, Wolfgang	*** SAME AS Life Sciences Track			
	DAY 2 Sep 15	**DAY 2 Sep 15**	**DAY 2 Sep 15**	**DAY 2 Sep 15**	**DAY 2 Sep 15**		**DAY 2 Sep 15**	
	Topic: Data Acquisition	**Pipeline Pilot in Practice**	**Biologics Design**	**Topic: Chemistry in Practice**	**Topic: Sustainable Energy**		**Leveraging Manufacturing Data**	
8:00 - 8:20	BIOVIA, Graham Janson - Sequenced Compose and Capture Recipes	Scitegrity, Joe Bradley - Automating Regulatory Compliance for Compound Logistics	MIT, Bernhardt Trout - Machine Learning for Bioformulation Development	*** SAME AS Pipeline Pilot	Johnson Matthey, Misbah Sarwar - Exploring Fuel Cell cathode materials: Towards more representative models		BMS, June Axelson - Centralized Management of Data Mappings Consumed by Discoverant	
8:20 - 8:40	BIOVIA, Patrick Wheeler - Mobile Execution in your Kitchen	Southern Research Institute, Sixue Zhang - BIOVIA Pipeline Pilot in Computer-Aided Drug Discovery of Anti-Alphavirus Agents	BIOVIA, Anne Goupil-Lamy - A Nanobody Activating Metabotropic Glutamate Receptor 4 Discriminates Between Homo and Heterodimers	*** SAME AS Pipeline Pilot	BIOVIA, Felix Hanke - Electrolyte Decomposition in Lithium Ion Batteries		Merck KGaA, Valerie Dayer, Florence Monard, and Coline Monnard - Leveraging manufacturing data with Discoverant and Pipeline Pilot at Merck KGaA	
8:40 - 9:00	BIOVIA, Mike Wilson - Ontology-based Reference Data and Administration of Equipment	GSK, Baptiste Canault - Pipeline Pilot Enabling and Connecting Computational Science Applications	VITRUVIAE, Mahiuddin Ahmed - In Silico Engineering of Therapeutics for Oncology and Infectious Diseases	*** SAME AS Pipeline Pilot	University of Birmingham, Andrew J. Morris - The Wadsley-Roth Niobates for Stable, Fast Lithium-ion Diffusion Battery Anodes: First Principles Modelling Combined with Experiment			
9:00 - 9:20	BIOVIA, Nick Reynolds - Lab Scheduling with Task Planner	Q/A Panel Lead: Alexander Orona	Q/A Panel Lead: Anne Goupil, Tien Luu	*** SAME AS Pipeline Pilot	BIOVIA, Abhijit Chatterjee - Quasi-Solid State Electrolyte with Nanoparticles for LiO2 Battery Applications		BIOVIA, Larry R. Fiegland - Introducing Bioprocess Intelligence in the Cloud	
9:20 - 9:40	Q/A Panel Lead: Patrick Wheeler		Panel Topic: AlphaFold2 and How It Will Change Drug Discovery Neeraj Agrawal, Amgen Abhishek Singharoy, Arizona State University Brian G. Pierce, University of Maryland Jason Cole, Cambridge Crystallographic Data Centre Lisa Yan, BIOVIA Anne Goupil, BIOVIA		Q/A Panel Lead:Johan Carlsson		Q/A Panel Lead: Chris Andrews	
		Data Science Use Cases with Pipeline Pilot	**SARS-CoV-2**	**Topic: Decision Support**	**Topic: Data Science for Materials**			
9:40 - 10:00	BIOVIA, Mike Wilson - Control Access to Task Planner Content using Collaborative Spaces	BIOVIA, Kevin Grogan - Segmentation of Medical Images in Pipeline Pilot with Deep Learning	Vrije Universiteit Amsterdam, Jakub Tomczak - Identification of Ebselen and Its Analogues as Potent Covalent Inhibitors of Papain-like Protease from SARS-CoV-2	BIOVIA, Matthew Sage - What's New in BIOVIA Insight and Insight for Excel	Key To Metals AG, Natalija Scepanovic, Viktor Pocajt - Introduction to Total Materia			
10:00 - 10:20	** Same as Research Informatics	BIOVIA, Niranjani Iyer - Biological Sequence: Machine learning and Embedding using Pipeline Pilot	National Research Council of Canada, Sergey Gusarov - Modeling the Interaction of SARS-CoV-2 Binding to the ACE2 Receptor by Molecular Dynamics and Integral Equation Theory	BIOVIA, Frederic Barberis - Finding and Searching Lab Data Quickly	Materials Platform for Data Science, Evgeny Blokhin - Quantitative Trends in Physical Properties of 115000 Inorganic Compounds Gained by Machine Learning			
10:20 - 10:40	BIOVIA, Kanishka Desai - Analytics with BIOVIA Insight	SIMULIA, Jing Bi and Victor Oancea - Machine Learning Applications in Additive Manufacturing and Health Science	Q/A Panel Lead: Abhigna Polavarapu	BIOVIA, Kanishka Desai - Analytics with BIOVIA Insight	Virtual Roundtable: Data Science for Materials - Patricia Gestoso			
10:40 - 11:00	Go to ..Research Informatics TRACK	Q/A Panel Lead: Jason DeJoannis		Q/A Panel Lead: Sean O'Hare or Frederic Barberis, Kanishka, Mike,	Virtual Roundtable Continued : Patricia Gestoso			
	Day 3 Sep 16	Day 3 Sep 16	Day 3 Sep 16	Day 3 Sep 16	Day 3 Sep 16			
	ELN: BIOVIA Notebook	**Pipeline Pilot: What's New**	**Topic: Simulations**	**What's New**	**TOPIC: Chemical Reactions**			
8:00 - 8:20	Dow, Todd Senecal - BIOVIA Electronic Laboratory Notebook Implementation at Dow: Documentation, Data Repository, and Integration with High-Throughput Workflows	BIOVIA, Alexander Orona - What's New and What's Next in Pipeline Pilot	University of Maryland , Alex MacKerell - Drude General Force Field (DGenFF): Extension of the Drude Polarizable Force Field to Drug-like Molecules using Machine Learning	*** SAME AS Pipeline Pilot	University of Cambridge, David Wales - Energy Landscapes and Reaction Pathways			

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8:20 - 8:40	BIOVIA, Mats Kihlen - High-performance Voice Dictation in BIOVIA Notebook		University of Michigan, Xiaorong Liu - Rapid Calculation of Relative Binding Free Energies for TSSK1B Using Multisite λ Dynamics		BIOVIA, Abhijit Chatterjee - Selectivity-controlled Transformation of Carbon Dioxide into a Multi-carbon Oxygenate			
8:40 - 9:00	BIOVIA, Patrick Wheeler - USP Methods		FMP Berlin, Han Sun & Marc Nazare - Prediction of Factor Xa - Inhibitor Binding Affinities Using Multisite Lambda Dynamics		Shell India, Nishant Sinha - Molecular Modelling for Improved Catalysis			
9:00 -	Q/A Panel Lead: Stephen Hayward	Q/A Panel Lead: Alexander Orona	Q/A Panel Lead: Hugues-Olivier	*** SAME AS Pipeline Pilot	Q/A Panel Lead: -Felix Hanke			
	Lab	**Topic Data Science**	**Topic: Modeling and Simulations for Life**	**TOPIC: Moving to Cloud**	**TOPIC: Industry Innovation**			
9:20 - 9:40	Janssen, Steve Jadczak, Brian Rakowiecki - ONE Lab-based Stability Study Workflow	**Workshop: Data Science with Pipeline Pilot**	BIOVIA, Rohith Mohan - Force Field Parametrization: Charge Assignment Powered by Machine Learning	BIOVIA, Matthew Sage - New BIOVIA Sketcher	BIOVIA, Johan Carlsson - Simulations of Corrosion			
9:40 - 10:00	BIOVIA, Kirsten Gesenberg - Running More Efficient Stability Studies		University of Paris Descartes, Alexandre Cabaye - Exploring the Activation Mechanism of a Class C GPCR	BIOVIA, Matthew Sage - Scaling Structure and Similarity Search for BIG Chemical Data in the Era of Cloud Computing	BIOVIA, Lalitha Subramanian - Chemical Drivers for Sustainability – Key Insights from 3D Virtual Twin Case Studies			
10:00 - 10:20	BIOVIA, Kirsten Gesenberg - Connecting Next-Generation Labs on the 3DEXPERIENCE Platform		BIOVIA, Tien Luu - What's New and What's Next in BIOVIA Discovery Studio	Q/A Panel Lead:Sean O'Hare (TBC), Matt Sage	BIOVIA, Arvin Kakekhani - How to Address Selective Direct Methane to Methanol Challenge: Insights from Density Functional Theory			
10:20 - 10:40	Q/A Panel Lead: Stephen Hayward	Q/A Panel Lead: Alex Orona, Alta Fang	Q/A Panel Lead: Patricia Gestoso		Q/A Panel Lead: Sabine Schweizer + Kwan Skinner			