

	Room D	Room E	Room A	Room H	Room M	Room J
9:00-10:00	<b>CHECK-IN</b>					
10:00-11:00	Pipeline Pilot Fundamentals Björn Loeprecht & Claire Mayo <b>BIOVIA</b>	Pipeline Pilot Analytics and Machine Learning David Nicolaides <b>BIOVIA</b>	Biologics Design (30 min) Anne Goupil, <b>BIOVIA</b>	COSMO-RS: Reaction Modeling beyond DFT & Reactions in Solvents Johan Carlsson & Marc Meunier <b>BIOVIA</b>	Jupyter Notebook and Python Integration in Pipeline Pilot Gregory Price <b>BIOVIA</b>	AI-driven Drug Design Alexandre Cabayé & João Inês <b>BIOVIA</b>
11:00-12:00			Follow the Drug <b>BIOVIA</b>			
12:00-1:30	<b>LUNCH</b>					
1:00-1:30	Pipeline Pilot Fundamentals (Continued) Björn Loeprecht & Claire Mayo <b>BIOVIA</b>	Pipeline Pilot Analytics and Machine Learning (Continued) David Nicolaides <b>BIOVIA</b>	ONE Lab Calculation Engine Benoit Dartiguemalle <b>BIOVIA</b>	COSMO-RS: Crystal Design in Pharmaceutical Development (Cocrystal Screening, Morphology, Solvent Screening) Johan Carlsson & Marc Meunier <b>BIOVIA</b>	Jupyter Notebook and Python Integration in Pipeline Pilot (Repeat) Gregory Price <b>BIOVIA</b>	Day in Life of a Recipe Developer: A Food & Beverage Formulations Experience Frank Schaffer, <b>BIOVIA</b>
1:30-2:00				Development of Polymer Materials Stephen Todd, <b>BIOVIA</b>		
2:00-3:00						Battery Materials Virtual+Real Innovation Johan Carlsson, <b>BIOVIA</b>
3:00-4:00						
4:30 - 5:30	<b>Welcome Reception</b>					

	Lab of the Future	Regulatory, Quality and Manufacturing	Materials Innovation	Data Science and Informatics	Drug Discovery & Development
9:00 AM	<b>KEYNOTE (Room B/C)</b>				
9:45 AM	<b>BREAK</b>				
	Room B	Room J	Room E	Room A	Room H
10:00 AM	The Next Generation of ONE Lab on the 3DEXPERIENCE Platform Gene Tetreault, <b>BIOVIA</b>	Future of Regulatory Kevin O'Leary, <b>BIOVIA</b> <b>AI</b>	Leverage AI and Large Language Models (LLMs) to Accelerate Materials Innovation Alena Sheveleva, <b>BIOVIA</b> <b>AI</b>	Machine Learning and Scientific Data Pipelining on the 3DEXPERIENCE Platform Clément Nardari, <b>BIOVIA</b> <b>AI</b>	Application of Generative Therapeutic Design and CSD-GOLD for Discovery of Novel Anti-TB Molecules Rupesh Chikhale <b>AI Cambridge Crystallographic Data Centre</b>
10:25 AM	ONE Lab in QC: A Journey from Paper to Digital Ricardo Gariso, <b>Hovione</b>	Beyond Documents: Introduction and Overview of Structured Documents Margaux Soulès, <b>BIOVIA</b> <b>AI</b>	A Foundation Model for Atomic Scale Materials Chemistry Gábor Csányi <b>AI University of Cambridge</b>	Democratized Science on the 3DEXPERIENCE Platform using Virtual Companion Phil Cochrane, <b>BIOVIA</b> <b>AI</b>	A Modeling Approach to Identify a New Inhibitory Mechanism of Glutamate Receptors Francine C. Acher <b>Université Paris Cité</b>
10:50 AM	<b>BREAK</b>				
11:10 AM	The Road to ONE Lab Pascal Maes, <b>Johnson &amp; Johnson Innovative Medicine</b>	Beyond Documents: Structured Content - CMC Dossiers Authoring Use Case Margaux Soulès, <b>BIOVIA</b>	Optimizing Process Performance through Molecular Design and Predictive Thermodynamics Lukas Raße-Lange <b>AI RWTH Aachen University</b>	Gene Expression Profiling Analysis with Pipeline Pilot Taoufiq Harach, <b>BIOVIA</b> <b>AI</b>	Collaborative Solution for Small Molecule Therapeutics Design Alexandre Cabayé, <b>BIOVIA</b> <b>AI</b>
11:35 AM	BIOVIA Notebook: An Important Piece of the Digital Transformation Puzzle Patrick Loffeld, <b>AkzoNobel</b>	Accelerating BIOVIA Deployment Tarkan Cevik, <b>BIOVIA</b>	Machine Learning (ML) Applications in Materials Innovation Johan Carlsson, <b>BIOVIA</b> <b>AI</b>	Using Large Language Models (LLMs) for Chemistry Gregory Price, <b>BIOVIA</b> <b>AI</b>	Retrosynthetic Analysis Alexandre Cabayé, <b>BIOVIA</b> <b>AI</b>
12:00 PM	<b>LUNCH</b>				

	Lab of the Future	Regulatory, Quality and Manufacturing	Materials Innovation	Data Science and Informatics	Drug Discovery & Development
	Room B	Room J	Room E	Room A	Room H
1:30 PM	BIOVIA Workbook Modifications for Process Chemistry Tobias Brüttsch, <b>DOTTIKON</b>	Future of Quality Management – Industry is Transforming <b>Part 1</b> <b>AI</b> Kevin O’Leary, <b>BIOVIA</b>	Industrial Applications with COSMO-RS Marc Meunier, <b>BIOVIA</b>	Next-generation Materials Registration on the <b>3DEXPERIENCE</b> Platform Neil Eccles, <b>BIOVIA</b>	Optimization of Nek6 Inhibitors' Structure by Computer-assisted Design Maria Cristina De Rosa, <b>CNR</b>
1:55 PM	Reinventing Analytical Methods in the Digital Era Thomas Neefs, <b>Johnson &amp; Johnson Innovative Medicine</b>	Future of Quality Management – Industry is Transforming <b>Part 2</b> <b>AI</b> Kevin O’Leary, <b>BIOVIA</b>	Validation of Conformer Search Strategies Volker Settels, <b>BASF</b>	Enhancing Generative Design <b>AI</b> David Nicolaides, <b>BIOVIA</b>	Biologics Design with Deep Learning and Molecular Modeling <b>AI</b> Anne Goupil, <b>BIOVIA</b>
2:20 PM	Reimagining the Management of HPLC Test Methods Martin Strachon & Lucy Morgan <b>Pfizer</b>	Quality Document Manager Niamh Finn, <b>BIOVIA</b>	Solubility Prediction of Complex Mixture: a Bayesian Optimization Approach Sophie Loehlé, <b>TotalEnergies</b>	The Present and Future of BIOVIA Chemistry João Inês, <b>BIOVIA</b>	Accelerating Drug Discovery with Discovery Studio Simulation <b>AI</b> Anne Goupil, <b>BIOVIA</b>
2:45 PM	<b>POSTER SESSION, DEMOS &amp; BREAK</b>				
3:45 PM	Introduction of a Laboratory Notebook at Huntsman Florian Klunker, <b>Huntsman</b>	Quality Process Management on the <b>3DEXPERIENCE</b> Platform <b>AI</b> Niamh Finn, <b>BIOVIA</b>	Innovate Faster and Better with Materials Studio James Wescott, <b>BIOVIA</b>	Solving Informatics Challenges with Pipeline Pilot: Present and Future <b>AI</b> Clément Nardari, <b>BIOVIA</b>	Computer-aided Solvent Selection to Control Nucleation and Resulting Product Quality Attributes in API Crystallization Jacek Żegliński, <b>APC Ltd.</b>
4:10 PM	Innovators for Instrument Integration She Yen Lok, <b>BIOVIA</b>	Migrating Third-party Quality Systems into the <b>3DEXPERIENCE</b> Platform <b>AI</b> Kevin O’Leary, <b>BIOVIA</b>	Hydrocarbon Membranes for Fuel Cell Applications: A DFT Stability Study Christopher Perry <b>Johnson Matthey</b>	Pipeline Pilot Pet Peeves <b>Part 1</b> Clément Nardari, <b>BIOVIA</b>	Get It Before You Need It: A Fully-automated Data Pipeline for Physical Property Predictions Maxime Tarrago, <b>AstraZeneca</b>
4:35 PM	Drug Product Development Kirsten Gesenberg, <b>BIOVIA</b>	BIOVIA Professional Services: Your #1 Value Up Partner Tarkan Cevik, <b>BIOVIA</b>	The Chemistry of Sustainable Packaging Stephen Todd, <b>BIOVIA</b>	Pipeline Pilot Pet Peeves <b>Part 2</b> Clément Nardari, <b>BIOVIA</b>	Accelerating Pharmaceutical Development with Materials Studio Marc Meunier, <b>BIOVIA</b>

	Lab of the Future	Regulatory, Quality and Manufacturing	Materials Modeling & Simulation	Workshop	CPG & Formulations
9:00 AM	<b>KEYNOTE</b>				
9:50 AM	<b>BREAK</b>				
	Room B	Room J	Room C	Room H	Room A
10:20 AM	UCB Smart Laboratory: Establishing Our Digital Sciences Backbone Philippe Huberts & Phu Nguyen <b>UCB</b>	Discoverant: What's New and Maintaining Your Hierarchies Stéphane Vellay, <b>BIOVIA</b>	Advanced Simulation for Next-gen Battery Materials Johan Carlsson, <b>BIOVIA</b>	ONE Lab Calculation Engine Benoit Dartiguemalle, <b>BIOVIA</b>	Accelerate Science-Based Innovation in Consumer Packaged Goods Industry with Virtual Twins Experiences Walid Darghouth <b>Dassault Systèmes</b>
10:45 AM	Biologics Purification Workflow Frederico Nardi, <b>Sanofi</b>	Beyond Document Structured Content – The APQR Use Case Stéphane Vellay, <b>BIOVIA</b>	Interpreting X-ray Spectra from Li-ion Battery Cathode Materials Rebecca Nicholls <b>University of Oxford</b>		Navigating Digital Transformation: Aboca's R&D Innovation Riccardo Conti, <b>Aboca</b>
11:10 AM	Padagis E-volution Natanel Sela, <b>Padagis</b>	Unlocking Synergy: Integrating Tools with Pipeline Pilot Ilyes Boussama, <b>UCB</b>	Battery Lab and Recipe Management Björn Loeprecht, <b>BIOVIA</b>		Streamline Formula and Recipe Development Workflows Frank Schaffer, <b>BIOVIA</b>
11:35 AM	A Day in Life of a Formulator Frédéric Barbéris, <b>BIOVIA</b>	Pharma 4.0: Achieving Agile Biomanufacturing Virtual Twin Experiences Gene Tetreault, <b>BIOVIA</b>	Modelling the Effect of Polymer Stiffness on Interfacial Failure Behaviour of Isotactic Polypropylene and Hydroxylated $\gamma$ -Al <sub>2</sub> O <sub>3</sub> James A. Elliott <b>University of Cambridge</b>		Using Pipeline Pilot to Democratise Model Building Ian Stott, <b>Unilever</b>
12:00 PM	<b>LUNCH</b>				



	Lab of the Future	Additional Sessions	Materials Innovation	CPG & Formulations
	Room B	Room A	Room C	Room J
1:00 PM	<p>What Do ONE Lab Administrators Really Do?</p> <p>Marty Berliner, <b>Pfizer</b></p>	<p>Streamline Tech Transfer with BIOVIA</p> <p>Isabella Telò <b>Dassault Systèmes</b></p>	<p>Lab Workflows and Data Analytics for Battery Materials in Automotive</p> <p>Gregory Price, <b>BIOVIA</b></p>	<p>Virtual Formulation: Optimising Your Designs for Success</p> <p>Phil Cochrane, <b>BIOVIA</b></p> <p>AI</p>
1:25 PM	<p>Materials Inventory Management on the 3DEXPERIENCE Platform</p> <p>Frank Schaffer, <b>BIOVIA</b></p>	<p>ONE Lab for Quality Control Labs</p> <p>Gene Tetreault, <b>BIOVIA</b></p>	<p>Materials Studio as an Efficient Tool to Study Structure-property Relations of Novel Carbonates</p> <p>Prof. Bjoern Winkler <b>Goethe University</b></p>	<p>AI-powered Generative Formulation</p> <p>Badis Mohamed Jaouani <b>Dassault Systèmes</b></p> <p>AI</p>
1:50 PM	<p>Synthetic Chemistry in ONE Lab</p> <p>Frédéric Barbéris, <b>BIOVIA</b></p>	<p>Effective Search for Scientific Data</p> <p>Kirsten Gesenberg, <b>BIOVIA</b></p>	<p>A Quantum Computing Collection for Pipeline Pilot</p> <p>Irfan Khan, <b>Quantinuum</b></p>	<p>Large Language Models (LLMs) for Formulation Design</p> <p>Alena Sheveleva, <b>BIOVIA</b></p> <p>AI</p>
2:10 PM	<b>B R E A K</b>			
3:00 PM	<p>Controlled Substances in CISPro</p> <p>Claire Mayo, <b>BIOVIA</b></p>	<p>Battery Materials Virtual+Real Innovation</p> <p>Johan Carlsson, <b>BIOVIA</b></p>	<p>Development of Polymer Materials</p> <p>Stephen Todd, <b>BIOVIA</b></p>	<p>Multi-objective Formulation Optimisation</p> <p>Gregory Price, <b>BIOVIA</b></p> <p>AI</p>
3:25 PM	<p>BIOVIA Scientific Notebook ELN</p> <p>Kirsten Gesenberg, <b>BIOVIA</b></p>			<p>Day in Life of a Recipe Developer: A Food &amp; Beverage Formulations Experience</p> <p>Frank Schaffer, <b>BIOVIA</b></p>