

	Room A	Room B	Room C	Room D	Room E	Room F
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>	AI-Driven Drug Design Alexandre Cabayé Joao Ines <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>	Biologics Design (30 min) Anne Goupil, <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 V+R 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</b>				
9:45 AM	<b>BREAK</b>				
	Room A	Room B	Room C	Room D	Room E
10:00 AM	The Next Generation of ONE Lab on <b>3DEXPERIENCE</b> 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 <b>3DEXPERIENCE</b> 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>Cambridge Crystallographic Data Centre</b> <b>AI</b>
10:25 AM	ONE Lab in QC: A Journey from Paper to Digital Ricardo Gariso, <b>Hovione</b>	Structured Document Authoring for CMC Dossiers Margaux Soules, <b>BIOVIA</b> <b>AI</b>	A Foundation Model for Atomic Scale Materials Chemistry Gabor Csanyi <b>University of Cambridge</b> <b>AI</b>	Democratized Science in the <b>3DEXPERIENCE</b> 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>	CMC Dossiers Use Case & Demo of CMC Authoring Margaux Soules, <b>BIOVIA</b>	Optimizing Process Performance through Molecular Design and Predictive Thermodynamics Lukas Raße-Lange <b>RWTH Aachen University</b> <b>AI</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 A	Room B	Room C	Room D	Room E
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 <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 for Product Formulation Sophie Loehlé, <b>TotalEnergies</b>	The Present and Future of BIOVIA Chemistry João Ines, <b>BIOVIA</b>	AI-powered Biologics Discovery with BIOVIA <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 2024 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 Zeglinski, <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 Chris 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 A	Room B	Room C	Room D	Room E
10:20 AM	UCB Smart Laboratory: Establishing Our Digital Sciences Backbone Philippe Huberts, <b>UCB</b>	Discoverant: What's New and Maintaining Your Hierarchies Stephane 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 Stephane Vellay, <b>BIOVIA</b>	Interpreting X-ray Spectra from Li-ion Battery Cathode Materials Rebecca Nicholls <b>Oxford University</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 Frederic Barberis, <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 A	Room B	Room C	Room E
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 Telo, <b>BIOVIA</b></p>	<p>Lab Workflows and Data Analytics for Battery Materials in Automotive</p> <p>Gregory Price, <b>BIOVIA</b></p>	<p>Virtual Formulation: Optimizing Your Designs for Success</p> <p>Phil Cochrane, <b>BIOVIA</b></p>
1:25 PM	<p>Materials Inventory Management on 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>Material 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>
1:50 PM	<p>Synthetic Chemistry in ONE Lab</p> <p>Frederic Barberis, <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>
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 V+R 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 Optimization</p> <p>David Nicolaides, <b>BIOVIA</b></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>

# Hands-on Session Abstracts

**15-Oct**

**10:00 AM - 12:00 PM**  
**01:00 PM - 04:00 PM**

Room 5

## Unlocking the Power of Jupyter Notebook and Python Integration in Pipeline Pilot

Gregory Price, **BIOVIA**

Python is the go-to language for innovation. See how you can leverage its considerable capabilities via Pipeline Pilot. Do data analysis, visualization, AI, etc., and access the latest scientific algorithms (e.g. Bayesian Experimental Design) for advancing your R&D”

\*Please bring your own laptop.

**15-Oct**

**10:00 AM - 12:00 PM**  
**01:00 PM - 04:00 PM**

Room 1

## Pipeline Pilot Fundamentals

Björn Loeprecht, Claire Mayo

**BIOVIA**

Learn how to build and utilize protocols (process steps) in Pipeline Pilot. Rapidly create, test and publish scientific services and automate the process of accessing, analyzing and reporting scientific data.

This course is for beginners to BIOVIA Pipeline Pilot. Session includes lunch.

\*Please bring your own laptop.

**15-Oct**

**10:00 AM - 12:00 PM**  
**01:00 PM - 04:00 PM**

Room 2

## Pipeline Pilot Analytics and Machine Learning

David Nicolaidis, **BIOVIA**

Learn how to use Pipeline Pilot for analytics and machine modeling. In this session you will learn how to characterize the variables in a data set, clean the data, group the data into clusters, build and validate predictive machine learning models from your data and apply your models to make new predictions and optimizations.

Requires a knowing how to create and run a protocol and how to use components.

\*Please bring your own laptop

**15-Oct**

**01:00 PM - 04:00 PM**

Room 3

## ONE Lab Calculation Engine

Benoit Dartiguemalle, **BIOVIA**

A popular session in Americas BIOVIA Live, this is a hands-on session best designed for ONE Lab Recipe Authors who are ready to take their use of Compose expressions to the next level. The session will be Instructor led, but paced for you to follow along on your own laptop and to leave time for questions as you proceed through the curated examples. The session is roughly divided into two parts that will run consecutively:

**Part 1:** Fun with Summary Expressions in this session, harness the power of advanced data manipulation techniques like variable-length statistical analysis, multi-point filtering and selection.

**Part 2:** Automating Decisions and Other Important Tricks Learn to simplify value searches with partial string matching and conquer repetitive tasks with loops.

\*Please bring your own laptop.

**15-Oct**

**10:00 AM - 12:00 PM**

Room 4

## COSMO-RS: Reaction Modeling beyond DFT & Reactions in Solvents

Johan Carlsson, Marc Meunier

**BIOVIA**

Join our workshop on COSMO-RS, where you'll explore advanced reaction modeling techniques beyond Density Functional Theory (DFT) and learn how to predict chemical reactions in solvents. Enhance your understanding of computational chemistry and gain practical insights into predictive modeling for complex chemical systems.

\*Please bring your own laptop.

**15-Oct**

**01:00 PM - 03:00 PM**

Room 4

## COSMO-RS: Crystal Design in Pharmaceutical Development

Johan Carlsson, Marc Meunier

**BIOVIA**

Join our 2-hour workshop on COSMO-RS: Crystal Design in Pharmaceutical Development. Dive into cocrystal screening, morphology, and solubility screening to enhance your understanding of crystal design and its applications in pharmaceuticals. Perfect for professionals aiming to optimize drug development processes.

\*Please bring your own laptop..