

| | Room 1 | Room 2 | Room 3 | Room 4 | Room 5 | Room 6 |
|-------------|---|--|---|---|--|---|
| 9:00-10:00 | CHECK-IN | | | | | |
| 10:00-12:00 | Pipeline Pilot Fundamentals | Pipeline Pilot Analytics and Machine Learning | AI-Driven Drug Design | COSMO-RS: Reaction Modeling beyond DFT & Reactions in Solvents Johan Carlsson, Marc Meunier BIOVIA | Jupyter Notebook and Python Integration in Pipeline Pilot Gregory Price BIOVIA | Biologics Design Anne Goupil BIOVIA |
| 12:00-1:00 | LUNCH | | | | | |
| 1:00-2:00 | Pipeline Pilot Fundamentals (Continued) Björn Loeprecht, Claire Mayo BIOVIA | Pipeline Pilot Analytics and Machine Learning (Continued) David Nicolaidis BIOVIA | ONE Lab Calculation Engine Benoit Dartiguemalle BIOVIA | COSMO-RS: Crystal Design in Pharmaceutical Development (Cocrystal Screening, Morphology, Solvent Screening) Johan Carlsson, Marc Meunier BIOVIA | Jupyter Notebook and Python Integration in Pipeline Pilot (Repeat) Gregory Price BIOVIA | Day in life of a Recipe Developer: A Food & Beverage Formulations Experience Frank Schaffer, BIOVIA |
| 2:00-3:00 | | | | Development of Polymer Materials Stephen Todd, BIOVIA | | |
| 3:00-4:00 | | | | Battery Materials V+R Innovation Johan Carlsson, BIOVIA | | |
| 4:00 - 6:00 | Welcome Reception | | | | | |

| | Lab of the Future | Regulatory, Quality and Manufacturing | Materials Innovation | Data Science and Informatics | Drug Discovery & Development |
|----------|--|--|--|--|---|
| 9:00 AM | KEYNOTE | | | | |
| 9:45 AM | BREAK | | | | |
| | Room 1 | Room 2 | Room 3 | Room 4 | Room 5 |
| 10:00 AM | The Next Generation of ONE Lab on 3DEXPERIENCE Gene Tetreault, BIOVIA | Future of Regulatory Kevin O'Leary, BIOVIA AI | Leverage AI and Large Language Models (LLMs) to Accelerate Materials Innovation Alena Sheveleva, BIOVIA AI | Machine Learning and Scientific Data Pipelining on 3DEXPERIENCE Platform Clement Nardari, BIOVIA AI | Application of Generative Therapeutic Design and CSD-GOLD for Discovery of Novel Anti-TB Molecules Rupesh CHIKHALE AI Cambridge Crystallographic Data Centre |
| 10:25 AM | ONE Lab for Quality Control Labs Gene Tetreault, BIOVIA | Structured Document Authoring for CMC Dossiers Margaux Soules, BIOVIA AI | A Foundation Model for Atomic Scale Materials Chemistry Gabor Csanyi AI Cambridge University | BIOVIA Virtual Companion Phil Cochrane, BIOVIA AI | Enhanced Active Learning in Generative Design David Nicolaides, BIOVIA AI |
| 10:50 AM | BREAK | | | | |
| 11:10 AM | ONE Lab Implementation in QC Jason Walford, AstraZeneca | CMC Dossiers Use Case & Demo of CMC Authoring Margaux Soules, BIOVIA | Optimizing Process Performance through Molecular Design and Predictive Thermodynamics Lukas Raßpe-Lange AI RWTH Aachen University | AI/ML Use Cases with Pipeline Pilot David Nicolaides, BIOVIA AI | Retrosynthetic Analysis Alexandre Cabayé, BIOVIA AI |
| 11:35 AM | ONE Lab in QC: A Journey from Paper to Digital Ricardo Gariso, Hovione | Structured Document Authoring Customer TBA | Machine Learning (ML) Applications in Materials Innovation Johan Carlsson, BIOVIA AI | Using LLMs and Foundation Models for Chemistry Gregory Price, BIOVIA AI | Collaborative Solution for Small Molecule Therapeutics Design Alexandre Cabayé, BIOVIA AI |
| 12:00 PM | LUNCH | | | | |

| | Lab of the Future | Regulatory, Quality and Manufacturing | Materials Innovation | Data Science and Informatics | Drug Discovery & Development |
|---------|---|---|--|--|--|
| | Room 1 | Room 2 | Room 3 | Room 4 | Room 5 |
| 1:30 PM | BIOVIA Notebook ELN Florian Klunker, Huntsman | Future of Quality Management – Industry is Transforming Part 1 AI Kevin O’Leary, BIOVIA | Industrial Applications with COSMO-RS Marc Meunier, BIOVIA | Predicting Prediction Accuracy AI David Nicolaides, BIOVIA | Optimization of Nek6 Inhibitors’ Structure by Computer-assisted Design Maria Cristina De Rosa, SCITEC |
| 1:55 PM | BIOVIA Scientific Notebook ELN Kirsten Gesenberg, BIOVIA | Future of Quality Management – Industry is Transforming Part 2 AI Kevin O’Leary, BIOVIA | Validation of Conformer Search Strategies Volker Settels, BASF | The Present and Future of BIOVIA Chemistry Frederic Barberis, BIOVIA | Biologics Design with Deep Learning and Molecular Modeling and Simulation AI Anne Goupil, BIOVIA |
| 2:20 PM | BIOVIA Workbook Modifications for Process Chemistry Tobias Bruitsch, Dottikon | Quality Document Manager Niamh Finn, BIOVIA | Solubility prediction for product formulation Sophie Loehlé, TotalEnergies | Next-generation Materials Registration on 3DEXPERIENCE Platform Neil Eccles, BIOVIA | Drug Discovery with Molecular Modeling Enhanced by OpenFold/AlphaFold in Discovery Studio Simulation AI BIOVIA |
| 2:45 PM | POSTER SESSION, DEMOS & BREAK | | | | |
| 3:45 PM | Notebook Lab 4.0 Patrick Loffeld, AkzoNobel | Introducing the New BIOVIA Biopharma Quality Management 3DEXPERIENCE Platform AI Niamh Finn, BIOVIA | Innovate Faster and Better with Materials Studio 2024 James Wescott, BIOVIA | Pipeline Pilot Roadmap and What’s New AI Clement Nardari, BIOVIA | Computer-Aided Solvent Selection to Control Nucleation and Resulting Product Quality Attributes in API Crystallization Jacek Zeglinski, APC Ltd. |
| 4:10 PM | Innovators for Instrument Integration Kirsten Gesenberg, BIOVIA | Exploring Next Gen Quality Customer TBA | Hydrocarbon Membranes for Fuel Cell Applications: A DFT Stability Study Chris Perry, Johnson Matthey | Pipeline Pilot Pet Peeves Part 1 Clement Nardari, BIOVIA | Get It Before You Need It: A Fully-automated Data Pipeline for Physical Property Predictions Simone Tomasi, AstraZeneca |
| 4:35 PM | Drug Product Development Kirsten Gesenberg, BIOVIA | Migrating Third-Party Quality Systems into the 3DEXPERIENCE Platform AI Kevin O’Leary, BIOVIA | The Chemistry of Sustainable Packaging Stephen Todd, BIOVIA | Pipeline Pilot Pet Peeves Part 2 Clement Nardari, BIOVIA | Accelerating Pharmaceutical Development with Materials Studio Marc Meunier, BIOVIA |

| | Lab of the Future | Regulatory, Quality and Manufacturing | Materials Modeling & Simulation | Workshop | CPG & Formulations |
|----------|---|--|---|---|---|
| 9:00 AM | KEYNOTE | | | | |
| 9:45 AM | BREAK | | | | |
| | Room 1 | Room 2 | Room 3 | Room 4 | Room 5 |
| 10:00 AM | UCB Biopharma 4.0 Smart Laboratory Philippe Huberts, UCB | Discoverant: What's New and Maintaining Your Hierarchies Stephane Vellay, BIOVIA | Advanced Simulation for Next-gen Battery Materials Johan Carlsson, BIOVIA | ONE Lab Calculation Engine Benoit Dartiguemalle, BIOVIA | Consumer Trends and the Emerging Innovation Gap Walid Darghouth BIOVIA |
| 10:25 AM | Biologics Purification Workflow Frederico Nardi, Sanofi | Beyond Document Structured Content: APQR Use Case Stephane Vellay, BIOVIA | Interpreting X-ray Spectra from Li-ion Battery Cathode Materials Rebecca Nicholls Oxford University | | Navigating Digital Transformation: Aboca's R&D Innovation Riccardo Conti, Aboca |
| 10:50 AM | BREAK | | | | |
| 11:10 AM | ONE Lab Natanel Sela, Padagis | Pharma 4.0: Achieving Agile Biomanufacturing Virtual Twin Experiences Gene Tetreault, BIOVIA | Battery Lab and Recipe Management Johan Carlsson, BIOVIA | ONE Lab Calculation Engine Benoit Dartiguemalle, BIOVIA (Continued) | Streamline Formula and Recipe Development Workflows Frank Schaffer, BIOVIA |
| 11:35 AM | Materials Inventory Management on 3DEXPERIENCE Platform Frank Schaffer, BIOVIA | Manufacturing in Life Sciences Customer TBA | Modelling the effect of polymer stiffness on interfacial failure behaviour of isotactic polypropylene and hydroxylated γ -Al ₂ O ₃ James A. Elliott University of Cambridge | | Using Pipeline Pilot to Democratise Model Building Ian Stott, Unilever |
| 12:00 PM | LUNCH | | | | |

| | Lab of the Future | Regulatory, Quality and Manufacturing | Materials Innovation | CPG & Formulations |
|---------|---|--|--|---|
| | Room 1 | Room 2 | Room 3 | Room 5 |
| 1:30 PM | ELN and Inventory Management Customer TBA | Customer TBA | Lab Workflows and Data Analytics for Battery Materials in Automotive Johan Carlsson, BIOVIA | AI Virtual Formulation: Optimizing Your Designs for Success Phil Cochrane, BIOVIA |
| 1:55 PM | Synthetic Chemistry in ONE Lab Frederic Barberis, BIOVIA | Unlocking Synergy: Integrating Tools with Pipeline Pilot Ilyes Boussama, UCB | Material Studio as an Efficient Tool to Study Structure-property Relations of Novel Carbonates Prof. Bjoern Winkler Goethe University | AI Multi-Objective Formulation Optimization David Nicolaidis, BIOVIA |
| 2:20 PM | Controlled Substances in CISPro Frank Schaffer, BIOVIA | Streamlining Templated Report Generation: Leveraging Discoverant Data Automation Stephane Vellay, BIOVIA | Customer TBA | AI Large Language Models (LLMs) for Formulation Design Alena Sheveleva, BIOVIA |
| 2:45 PM | B R E A K | | | |
| 3:30 PM | Effective Search for Scientific Data She Yen Lok, BIOVIA | BIOVIA Professional Services: Your #1 Value Up Partner Tarkan Cevik, BIOVIA | Battery Materials V+R Innovation Johan Carlsson, BIOVIA | Customer TBA |
| 3:55 PM | Accelerating BIOVIA Deployment Tarkan Cevik, BIOVIA | Customer TBA | | A Day in Life of Formulator Frederic Barberis, BIOVIA |
| 4:20 PM | Putting Your Lab Data to Work: Data Science Initiatives She Yen Lok, BIOVIA | AI The Future of Bioprocess Intelligence - Customer Panel Discussion TBA | Development of Polymer Materials Stephen Todd, BIOVIA | |

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 Pancrace

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

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..