TUESDAY OCT 15

AGENDA

		Room 1	Room 2	Room 3	Room 4	Room 5	Room 6		
9:00-1	10:00	O CHECK-IN							
10:00-1	12:00	Pipeline Pilot Fundamentals	Pipeline Pilot Analytics and Machine Learning	AI-Driven Drug Design	COSMO-RS: Reaction Modeling beyond DFT & Reactions in Solvents	Jupyter Notebook and Python Integration in Pipeline Pilot	1. Follow the Drug 2. Biologics Design		
12:00-	-1:00	00 LUNCH							
1:00-	-2:00	Pipeline Pilot Fundamentals (Continued)	Pipeline Pilot Analytics and Machine Learning (Continued)	ONE Lab Calculation Engine	COSMO-RS: Crystal Design in Pharmaceutical Development (Cocrystal Screening, Morphology, Solvent Screening)	Jupyter Notebook and Python Integration in Pipeline Pilot (Repeat)	Day in life of a Recipe Developer: A Food & Beverage Formulations Experience		
2:00-	-3:00						Development of Polymer Materials		
3:00-	-4:00						Battery Materials V+R Innovation		

WEDNESDAY OCT 16

MORNING AGENDA

	Lab of the Future	Regulatory, Quality and Manufacturing	Materials Innovation	Data Science and Informatics	Drug Discovery		
9:00 AM	KEYNOTE						
	Room 1	Room 2	Room 3	Room 4	Room 5		
10:00 AM	The Next Generation of ONE Lab on 3D EXPERIENCE BIOVIA	Future of Regulatory Kevin O'Leary BIOVIA	A Foundation Model for Atomic Scale Materials Chemistry Gabor Csanyi Cambridge University	Using Pipeline Pilot to Democratise Model Building lan Stott Unilever	Drug Discovery with AI Customer TBA		
10:25 AM	ONE Lab for Quality Control Labs BIOVIA	Intro and Overview of Structured Documents Margaux Soules BIOVIA	Optimizing Process Performance through Molecular Design and Predictive Thermodynamics Lukas Raßpe-Lange RWTH Aachen University	Data Science and AI in Biopharma Customer TBA	Application of Generative Therapeutic Design and CSD-GOLD for Discovery of Novel Anti-TB Molecules Rupesh CHIKHALE Cambridge Crystallographic Data Centre		
10:50 AM			BREAK				
11:10 AM	Biopharma Customer Presentation Customer TBA	CMC Dossiers Use Case & Demo of CMC Authoring Margaux Soules BIOVIA	Machine Learning (ML)Applications in Materials Innovation BIOVIA	AI/ML Use Cases with Pipeline Pilot David Nicolaides BIOVIA	Collaborative Solution for Small Molecule Therapeutics Design Alexandre Cabayé BIOVIA		
11:35 AM	UCB Biopharma 4.0 Smart Laboratory UCB	Customer TBA	A Quantum Computing Collection for Pipeline Pilot Quantinuum	Introduction to Virtual Companion Phil Cochrane BIOVIA	Enhanced Active Learning in Generative Design David Nicolaides BIOVIA		
12:00 PM			LUNCH				

WEDNESDAY OCT 16

AFTERNOON AGENDA

	Lab of the Future	Regulatory, Quality and Manufacturing	Modeling & Simulation in Pharma Development	Data Science and Informatics	Drug Discovery	
	Room 1	Room 2	Room 3	Room 4	Room 5	
1:30 PM	ELN Customer Presentation Customer TBA	Future of Quality Management – Industry is Transforming Part 1 Kevin O'Leary BIOVIA	Computer-Aided Solvent Selection to Control Nucleation and Resulting Product Quality Attributes in API Crystallization Jacek Zeglinski, APC Ltd.	Pipeline Pilot in Life Sciences Customer TBA	Retrosynthetic Analysis Laurent Naudin BIOVIA	
1:55 PM	BIOVIA Scientific Notebook ELN BIOVIA	Future of Quality Management – Industry is Transforming Part 2 Kevin O'Leary BIOVIA	Pharma Dev with COSMO-RS Customer TBA	Pipeline Pilot in Life Sciences Customer TBA	The Present and Future of BIOVIA Chemistry Matthew Sage BIOVIA	
2:20 PM	Effective Search for Scientific Data BIOVIA	Quality Document Manager Niamh Finn BIOVIA	Pharma Dev with Materials Studio Customer TBA	Pipeline Pilot in Life Sciences Customer TBA	Next-generation Materials Registration on 3D EXPERIENCE Platform Neil Eccles BIOVIA	
2:45 PM	POSTER SESSION & BREAK					
3:45 PM	Innovators for Instrument Integration BIOVIA	Introducing the New BIOVIA Biopharma Quality Management 3DEXPERIENCE Platform Niamh Finn BIOVIA	Pharma Dev with COSMO-RS Customer TBA	Introduction to Machine Learning Workbench and Pipeline Creator Clement Nardari BIOVIA	Optimization of Nek6 Inhibitors' Structure by Computer-assisted Design Maria Cristina De Rosa Catholic University of Rome	
4:10 PM	Drug Product Development BIOVIA	Exploring Next Gen Quality Customer TBA	Pharma Dev with Materials Studio Customer TBA	Predicting Prediction Accuracy David Nicolaides BIOVIA	Biologics Design with Deep Learning and Molecular Modeling and Simulation Anne Goupil BIOVIA	
4:35 PM	BIOVIA Professional Services: Your #1 Value Up Partner BIOVIA	Migrating Third-Party Quality Systems into the 3D EXPERIENCE Platform Kevin O'Leary BIOVIA	Pharma Development Customer Panel	Using LLMS and Foundation Models for Chemistry Gregory Price, Alena SHEVELEVA and David Nicolaides BIOVIA	Drug Discovery with Molecular Modeling Enhanced by OpenFold/AlphaFold in Discovery Studio Simulation BIOVIA	

THURSDAY OCT 17

MORNING AGENDA

	Lab of the Future	Regulatory, Quality and Manufacturing	Materials Modeling & Simulation	Data Science and Informatics	Formulations		
9:00 AM	KEYNOTE						
	Room 1	Room 2	Room 3	Room 4	Room 5		
10:00 AM	Lab Workflows and Data Analytics for Battery Materials in Automotive BIOVIA	Discoverant: What's New and Maintaining Your Hierarchies (Gene / Tom Simons) BIOVIA	Interpreting X-ray Spectra from Li-ion Battery Cathode Materials Rebecca Nicholls Oxford University	Pipeline Pilot Applications Customer TBA Al	Streamline Formula and Recipe Development Workflows BIOVIA		
10:25 AM	Putting Your Lab Data to Work: Data Science Initiatives BIOVIA	Beyond Document Structured Content: APQR Use Case Stephane Vellay BIOVIA	Advanced Simulation for Next-gen Battery Materials Johan Carlsson BIOVIA	Pipeline Pilot Roadmap and What's New Clement Nardari BIOVIA	Virtual Formulation: Optimizing Your Designs for Success BIOVIA		
10:50 AM	BREAK						
11:10 AM	ELN and Inventory Management Customer TBA	Pharma 4.0: Achieving Agile Biomanufacturing Virtual Twin Experiences Mahaut De Villepin-Lambert BIOVIA	Material Studio as an Efficient Tool to Study Structure-property Relations of Novel Carbonates Prof. Bjoern Winkler Goethe University	Pipeline Pilot Pet Peeves Part 1 Clement Nardari BIOVIA	A Day in Life of Formulator BIOVIA		
11:35 AM	ELN and ONE Lab Customer TBA	Customer TBA	Hydrocarbon Membranes for Fuel Cell Applications: A DFT Stability Study Chris Perry Johnson Matthey	Pipeline Pilot Pet Peeves Part 2 Clement Nardari BIOVIA	Multi-Objective Formulation Optimization BIOVIA		
12:00 PM			LUNCH				

THURSDAY OCT 17

AFTERNOON AGENDA

	Lab of the Future	Regulatory, Quality and Manufacturing	Materials Modeling & Simulation	Workshop	
	Room 1	Room 2	Room 3	Room 4	Room 5
1:30 PM	Materials Inventory Management on 3D EXPERIENCE Platform BIOVIA	Customer TBA	Innovate Faster and Better with Materials Studio 2024 James Wescott BIOVIA		
1:55 PM	Synthetic Chemistry in ONE Lab BIOVIA	Customer TBA	Catalyst Modeling and Simulation Customer TBA	ONE Lab Calculation Engine BIOVIA	
2:20 PM	Customer Talk Customer TBA	Streamlining Templated Report Generation: Leveraging Discoverant Data Automation Stephane Vellay BIOVIA	The Chemistry of Sustainable Packaging Stephen Todd BIOVIA		
2:45 PM					
3:30 PM	Accelerating BIOVIA Deployment BIOVIA	Customer TBA	Molecular Modeling and Simulation Customer TBA		
3:55 PM	Controlled Substances in CISPro BIOVIA	Customer TBA	Reaction Modeling with COSMO-RS Customer TBA	ONE Lab Calculation Engine BIOVIA (Continued)	
4:20 PM	Drug Product Development BIOVIA	Customer Panel Discussion TBA	Industrial Applications with COSMO-RS BIOVIA		