

November 13, 2025

10:00 AM

Plenary Sessions

PS

Opening remarks

Daiji Kani, **BIOVIA ASIA** Pacific, Sales Director

Nobutaka Sugaya, **BIOVIA** Japan Sales Senior Manager

Motohide Nishi, Life Sciences Japan Sales Vice President

Introduction and greetings of BIOVIA Live

10:05 AM – 10:35 AM

Plenary Sessions

PS

BIOVIA CEO SESSION

Jason Benedict, CEO, **BIOVIA**

Reza Sadeghi, CSO, **BIOVIA**

BIOVIA Vision and Direction

10:35 AM – 11:25 AM

Plenary Sessions

PS

R&D SESSION

Gene Tetreault, **BIOVIA** Portfolio Director

BIOVIA R&D: From Molecule to Manufacturing

11:25 AM – 11:45 AM

Plenary Sessions

PS

Key Note SESSION

Volume to Value, Scaling Compliance and Productivity: Our BIOVIA ONE Lab Journey

Ashok Nayak, **Ipca** Laboratories Limited

As a leading generics organization, Ipca manages a diverse portfolio of high-volume products while adhering to multiple global regulatory standards. To remain competitive and future-ready, digitization has become a strategic imperative. In this transformation journey, Ipca has adopted BIOVIA ONE Lab as its digital QC lab platform to streamline operations, ensure compliance, and drive efficiency.

11:45 AM – 12:15 AM

Plenary Sessions

PS

Key Note SESSION

The Early Challenges of Computational Chemistry - Celebrating the 25th Leader of Materials Studio -

Akira Miyamoto

Tohoku University, IRIC Corporation Professor Emeritus, Representative Director

Since the birth of computers in 1946, their use in chemistry has progressed, with applications including quantum chemistry calculations and reactor analysis. In the late 1980s, the introduction of computer graphics accelerated development beyond chemistry to a wide range of academic and industrial fields. This lecture will look back on the visualization research that began in 1987 and has led to collaborations with various fields, including automobiles, semiconductors, the environment, and nuclear power, since the 1990s. Specific examples will be used to introduce the results and significance of these efforts.

13:15 PM – 13:50 PM

Modeling & Simulation

M&S

Materials design and measurement data analysis using generative AI and machine learning potential

Teruyasu Mizoguchi

Institute of Industrial Science, The University of Tokyo

"In recent years, materials development utilizing machine learning has progressed rapidly. Machine learning potentials (MLPs), proposed by Behler and Parrinello in 2007, have been developed as a method that enables highly accurate and fast atomic-scale simulations, and in recent years, pre-trained general-purpose potentials (e.g., MACE) that can handle almost all elements in the periodic table have also appeared. On the other hand, generative AI, such as ChatGPT and Stable Diffusion, has also become widespread, and the application of these technologies to reverse design of materials and data analysis is attracting attention. In this presentation, we will introduce the ferroelectric simulation under electric fields using machine learning potentials, which the

presenter's research group has been working on in recent years, as well as methods for reverse design of materials and analysis of measurement data using generative AI.

13:55 PM – 14:30 PM

Modeling & Simulation

M&S

Computational Insights in CO₂ Capture: An Industrial Perspective

Dr. Anirban Bhaduri

Computational Chemistry and Materials Sciences -
Manager - **Shell Technology Center** – Bangalore, Shell Plc

Development of sustainable and efficient processes is a desired interest for industries. Understanding key technological bottlenecks in the process is thus essential. Molecular and atomistic scale simulations and computation provide key insights into chemical transformations. These lead towards actions associated with new material discovery, process optimization and eventually to enhanced yields. During the talk, three examples will be shared on how we utilize these approaches to optimize catalysts, screen new materials and evaluate process enhancement. The talk will reference how these approaches are being used to address and build decarbonization solutions.

15:10 PM – 15:45 PM

Modeling & Simulation

M&S

Evaluation of magnetic degradation of soft magnetic material FeCo-V using a multi-scale, multi-physics approach: GRIT (grit) x first-principles calculations for material design (first-principles analysis)

Haruki EGUCHI

IHI Corporation - IHI Group Advanced Expert
(Physics/Materials)

In this presentation, I will introduce the evaluation of magnetic degradation in an FeCo-V alloy as an example of the application of a multi-scale, multi-physics approach in the field of soft magnetic materials. By combining elastic stiffness analysis and micromagnetic simulation, I analyzed the magnetic flux density-magnetic field (B-H) curve and the magnetic flux density-

magnetostriction (B - ε) curve, and found that pre-straining leads to a decrease in magnetic flux density and an increase in magnetostriction. In materials development, it is important to understand the discrepancy between calculations and experiments and use it to move forward. I consider how the perspective of researchers with grit (the ability to see things through) is directly linked to maximizing technological value. Reference: Haruki Eguchi, Natsuki Yoneyama, Masakazu Hara, Shinnosuke Nakai, Hiroyuki Nose, Hiroki Yoshizawa, Evaluating magnetic degradation in FeCo-V alloys for high-output and compact electric motors: A multiscale-multiphysics approach, Materials Letters, 382 (2025) 137937, <https://doi.org/10.1016/j.matlet.2024.137937>

15:50 PM – 16:25 PM

Modeling & Simulation



Advanced in Materials Modeling: Focus on Glasses

SungHoon Lee

Principal Research Scientist, Ph.D. - **Corning Precision Materials**

This presentation aims to explore the latest advancements in glass technology, emphasizing the development of antimicrobial glass and the enhancement of glass-polymer adhesion. By delving into these two key topics, we will highlight the role of materials modeling in driving these innovations and their potential applications. The research utilizes density functional theory and molecular dynamics techniques to simulate the properties and interactions of glass at the molecular level. In the realm of antimicrobial glass, structural analyses of various glass compositions are conducted to identify effect of glass former that effectively enhance chemical durability. The study of glass-polymer adhesion emphasizes interfacial chemistry and surface roughness, aiming to optimize bonding between these materials for improved durability and performance.

16:30 PM – 17:05 PM

Modeling & Simulation

M&S

Application of quantum chemical calculations to automobile exhaust gas purification catalysts

Kazuya Miura

SUZUKI MOTOR CORPORATION - Environment, Materials and Production Technology Development

I will introduce two research examples that utilize quantum chemical calculations targeting exhaust gas purification catalysts (three-way catalysts) for gasoline engine automobiles. The first introduces a technology for designing new three-way catalyst materials, using coupled analysis that combines quantum chemical calculations with chemical reaction kinetics simulations to predict purification rate curves. The second introduces a basic research example that provides a detailed examination of Temkin-type adsorption, the empirical rule that the adsorption energy of molecules on a material surface can be approximately expressed as a linear equation for the coverage rate.

17:10 PM – 17:30 PM

Modeling & Simulation

M&S

Molecular Modeling 2026

Stephen Todd, **BIOVIA**

In recent years, there has been a growing integration of physics-based models with machine learning approaches to enhance the speed and accuracy of existing computational methods. This presentation will explore the latest improvements in Materials Studio and Discovery, focusing on new methodologies and important updates to existing solvers. We will also discuss a collaborative effort involving quantum computing. As these solvers continue to advance, the way we interact with the tools also evolves. Last year, a key functionality called "Virtual Lab" within the 3DEXperience platform was introduced, and this session will present the new enhancements to that system.

13:15 PM – 13:55 PM

D&I

Accumulating Experimental Data and Accelerating Materials Development Using Electronic Laboratory Notebooks

Yuta SHIMAZU

Nitto Denko Corporation - Research and Development Headquarters, Core Technology Research Center

This presentation will introduce the construction and operation of a data infrastructure at Nitto Denko that is based on electronic experiment notebooks and Pipeline Pilot. Our company has implemented a system that structures experimental data in Excel format, preprocesses and automatically stores the data in Pipeline Pilot, and links it to an analysis platform. This is expected to significantly reduce the man-hours and errors involved in recording, searching, and processing, as well as to accelerate decision-making in materials development by utilizing accumulated data across multiple disciplines. In this presentation, we will share specific efforts and the results achieved.

Data Science &
Informatics

14:00 PM – 14:40 PM

D&I

Virtual Twin Experiences & Predictive Modeling

Evaluating Large Language Models vs. Physics for Antibody Optimization

Reza Sadeghi, **BIOVIA**

Amit Kulkarni, **BIOVIA** Industry Process Consult , Senior Director

Anne Goupil-Lamy, **BIOVIA**

Virtual Twin Experiences & Predictive Modeling

Virtual Twin Experiences (VTEs) are transforming innovation across industries by enabling a connected, predictive, and sustainable approach to design and development. This presentation will demonstrate how VTEs, powered by the accessible, subscription-

based 3DEXPERIENCE cloud platform, integrate advanced AI-driven modeling and multiscale simulations to revolutionize traditional workflows in both Materials and Life Sciences. In materials innovation, VTEs accelerate the entire lifecycle—from selection and design to utilization and recycling—driving efficiency and sustainability. In Life Sciences, VTEs redefine the drug lifecycle, integrating validated Virtual Twins and predictive models to enhance discovery, development, manufacturing, and delivery. Together, these examples showcase how VTEs unify data, modeling, and collaboration to foster innovation, improve decision-making, and enable a more sustainable and patient-centered future.

Evaluating Large Language Models

vs. Physics for Antibody Optimization

The application of large language models (LLMs) created a lot of attention, with many models being created for in-silico antibody design, particularly for generating diverse sequence libraries. However, their efficacy in guiding affinity maturation, a process dependent on subtle energetic trade-offs, remains uncertain. We conducted a rigorous head-to-head validation, comparing the predictive power of state-of-the-art LLMs against a physics-based virtual mutagenesis protocol within Discovery Studio. Our study involved introducing a series of mutations into a model antibody-antigen complex, predicting their impact on binding affinity using both computational methodologies, and benchmarking these predictions against experimentally determined values. This work provides a critical, data-driven comparison of these two leading computational paradigms in antibody engineering, offering insights into their respective strengths and weaknesses and paving the way for a more efficient and reliable synergistic workflow for engineering best-in-class antibody therapeutics.

15:10 PM – 15:50 PM

D&I

Kaneka accelerates research digital transformation with company-wide ELN implementation

Akihisa Kanda, Executive, **Kaneka Corporation**,
R2B Strategy Office and Discover Planning Group,
R2B Headquarters

Kaneka is accelerating digital transformation across the company, and has been gradually introducing BIOVIA Notebook in its research department since fiscal 2020. As the company has diverse business fields, including life sciences, polymers, and food, it is necessary to propose usage methods that are suited to each. Furthermore, when developing tools using Pipeline Pilot, the key is to incorporate generative AI and machine learning libraries in a way that can be commonly used by many departments.

Today, I will discuss the challenges of introducing a company-wide ELN, efforts to further utilize generative AI, and future prospects.

Data Science &
Informatics

16:00 PM – 16:40 PM

D&I

The Logic of Chemical Optimization

Model-Based Virtual Twins Driving Outcomes through BIOVIA Deep Science

David Kombo, **Sanofi**

Reza Sadeghi, BIOVIA

The Logic of Chemical Optimization

During multi-parameter chemical optimization, hits evolve into leads and development candidates with increasing molecular capabilities. We introduce retro-optimization analysis, transforming candidates into simpler leads and hits to understand optimization logic. By mapping a matched molecular pair network, we compared actual optimization routes to theoretical alternatives, identifying differences in lead properties and "optimizons" (key substructures). Expanding this method across

multiple projects and datasets, we define optimization logic to guide future discovery campaigns.

Model-Based Virtual Twins Driving Outcomes through BIOVIA Deep Science

Model-based Virtual Twins are redefining how science and industry connect data, models, and experimentation to achieve real-world outcomes. By leveraging BIOVIA's deep scientific foundation in molecular modeling, materials science, chemistry, and biology, organizations can move from descriptive analytics toward predictive and generative intelligence. The Virtual Twin provides a continuously learning representation of physical systems—from molecules and formulations to manufacturing processes—built on validated models and experimental data. Through integration with laboratory automation, simulation, and AI-driven analytics, BIOVIA's Virtual Twin framework enables scientists and engineers to explore scenarios, optimize performance, and accelerate innovation while reducing risk and cost.

Combined with machine learning and data connectivity across R&D and manufacturing, they form an intelligent ecosystem that supports faster decision-making and higher success rates. From drug discovery and biologics development to formulated products and sustainable materials, model-based Virtual Twins powered by BIOVIA deep science are driving measurable business and scientific outcomes—transforming experimentation into a continuous cycle of prediction, validation, and improvement across the value chain.

**Data Science &
Informatics**

16:50 AM – 17:30 AM



Pipeline Pilot and Large Language Modules (LLMs) in 2026

Gregory Price, **BIOVIA** Industry Process Consultant

Large Language Models (LLMs) have recently received significant interest from researchers in chemical and materials science.[1,2] However, using LLMs in scientific pipelines presents a challenge for general models due to the specialized terminology and diverse reporting formats used in scientific domains.

In this work, we demonstrate several approaches for using LLMs within BIOVIA Pipeline Pilot to perform scientific tasks. We show how machine learning approaches can leverage experimental data to support formulation experts. We will also present results using

LLMs to extract and parse data stored in the BIOVIA Notebook and BIOVIA Workbook electronic lab notebooks (ELNs). Overall, our findings highlight the potential for LLMs to aid scientists in the extraction and structuring of data and predictive model development.

This talk will also outline some of the recent updates to Pipeline Pilot.

References

[1] Z. Xie, X. Evangelopoulos, Ö. H. Omar, A. Troisi, A. I. Cooper, L. Chen, Fine-tuning GPT-3 for machine learning electronic and functional properties of organic molecules, *Chem Sci* 2023, 15, 500–510.

[2] K. M. Jablonka, P. Schwaller, A. Ortega-Guerrero, B. Smit, Leveraging large language models for predictive chemistry, *Nat Mach Intell* 2024, 6, 161–169

Laboratory &

Data Management

13:15 PM – 13:55 PM

L&D

BIOVIA Notebook Implementation: Achieving an Uptime Rate of Over 90%

Tomohiro Ono

Lonseal Corporation - Research and
Development Group Leader

The Research and Development Department of Lonseal Corporation introduced BIOVIA Notebook in 2024 as part of its digitalization and digital transformation efforts. The utilization rate of BIOVIA Notebook licenses has remained at a high level of over 90% since the introduction. In this presentation, I will introduce 1) the implementation process utilizing the "Innovator Theory" that achieved a high utilization rate of over 90% immediately after the introduction, and 2) efforts centered on system construction and tuning. "Innovator theory" is a marketing theory that classifies and analyzes the process by which new products and services become popular in the market into five types based on the timing at which consumers accept new products and services.

14:00 PM – 14:40 PM

L&D

Initiatives to introduce and popularize electronic laboratory notebooks

Yuki Takei

Asahi Kasei Corporation - Research and Development Headquarters

At our Basic Technology Research Institute, we have been introducing electronic lab notebooks with the goal of "preserving as much information as possible." However, when we first introduced them, we experienced some setbacks, as they were not widely adopted due to issues with the introduction process and operation. We are currently rolling them out in stages, carefully listening to feedback from the field, and although we are still in the middle of this process, we are beginning to see signs that they are gradually taking root. In this presentation, I will talk about the trial and error involved in introducing and popularizing the system and the lessons learned from that process.

15:10 PM – 15:50 PM

L&D

Discoverant and Pharmaceutical Data

Discoverant-to-Discoverant Data Transfer

Sam Watson, **ThermoFisher Scientific**Abha Ramchandani, **Gilead Sciences**

Discoverant and Pharmaceutical Data

In the rapidly evolving pharmaceutical industry, the integration and management of shop floor and lab data are critical for ensuring product quality and regulatory compliance. This presentation will explore how ThermoFisher Scientific leverages BIOVIA Discoverant to revolutionize Continuous Process Verification (CPV) and Annual Product Review (APR) report generation. We will delve into the benefits of single-source system builds, emphasizing the seamless integration of data from

Laboratory Information Management Systems (LIMS) and equipment for Environmental Monitoring. Additionally, we will discuss how ThermoFisher Scientific, as a Contract Development and Manufacturing Organization (CDMO), enhances client data sharing and validated data transfer services using Discoverant. Finally, we will cover the application of Discoverant in Statistical Process Control (SPC), focusing on golden batch analysis and the potential for product loss prevention and process improvements.

Discoverant-to-Discoverant Data Transfer

The presentation outlines the business case when data needs to be migrated from one organization to another, both with a strong implementation of BIOVIA Discoverant. Why enter the same data into two different PRIMR templates? This presentation will cover how the data transfer from one Discoverant implementation to the other was automated, its benefits and the technological limitations that must be accounted for.

Laboratory &

Data Management

16:00 PM – 16:40 PM

L&D

Solution for Formulated Goods with AI for Food, Beverage, and Cosmetics

Suchaya (Pam) Leelapatranurak, Manager, **FoodChain ID**

Amit Kulkarni, **BIOVIA** Industry Process Consult, Senior Director

Gregory Price, **BIOVIA** Industry Process Consultant

AI and Machine Learning are redefining how food, beverage, and cosmetic companies design and deliver formulated products. Traditional trial-and-error approaches are giving way to data-driven innovation powered by predictive modeling, scientific AI, and unified lab informatics. Dassault Systèmes' Virtual Twin Experience connects real and virtual labs to accelerate formulation design—optimizing ingredient selection, performance, stability, and sustainability before physical testing. Leveraging advances such as BIOVIA's Chemical Language Model (CLM), which applies large language model (LLM) principles to chemical data, organizations can now capture the "language of formulation" to predict outcomes, uncover novel ingredient combinations, and shorten development cycles. This session highlights how AI-powered formulation and digital continuity are transforming R&D

efficiency, compliance, and speed to market—enabling companies to innovate smarter and more sustainably.

Laboratory &

Data Management

16:50 PM – 17:30 PM

L&D

Update of our LAB portfolio 2026 and the journey to a *Connected Science in the Cloud*

Gene Tetreault, **BIOVIA** Roles Portfolio Director

The future of laboratory innovation lies in connection—connecting people, data, and processes across every stage of scientific discovery. In this 40-minute session, we'll explore how our current portfolio is adding functionality based on your input and as well show how BIOVIA ONE Lab and Scientific Notebook come together on the data-centric 3DEXPERIENCE platform cloud to deliver a unified, intelligent laboratory environment.

Attendees will see how experiment design, execution, inventory, registration, and reporting can now flow seamlessly across disciplines—removing the friction between ELN, LIMS, and LES systems. Scientific Notebook becomes the digital workspace for capturing structured scientific knowledge, while ONE Lab orchestrates the broader workflow, ensuring data continuity and compliance from bench to enterprise.

We'll demonstrate how this integration simplifies day-to-day lab operations, supports regulatory confidence, and opens new possibilities for AI-driven insight, as historical ELN data fuels next-generation predictive models. Discover how connected science on the cloud is transforming the way modern R&D organizations think, work, and innovate.