The BIOVIA Unified Lab offers research, development, analytical and QA/QC laboratories a unique opportunity to remove paper processes and better support end-to-end analytical and process workflows. Unified, harmonized and standardized laboratory/resource management and procedure execution can help achieve your business goals by improving collaborative innovation, increasing productivity, reducing regulatory compliance and safety risk and accelerating time to market. Cloud deployment of the Unified Lab increases security, while decreasing the necessary IT overhead and total cost of ownership, providing a dynamic infrastructure for your laboratory informatics.
In today’s competitive environment, science-based organizations need to optimize lab operations by improving efficiency, maximizing quality, complying with regulatory requirements and driving innovation. In the lab, these goals can be achieved by removing disconnected, paper-based and error-prone processes that often result in significant inefficiencies and compliance risks. They can also hinder data and technology transfer between research, development and manufacturing.

**BIOVIA UNIFIED LAB**

In daily laboratory workflows, experiments are planned, executed, and results recorded. The work needs to be planned and managed, which means that tasks such as the execution of tests is requested. The requests are reviewed, scheduled and confirmed, and the resources allocated. These resources include materials and equipment for testing, the personnel to execute the work and the samples that are actually tested. Methods and procedures are developed and adapted if required and need to be managed. These methods and specifications will be used for the execution of the lab work, where tests are prepared and performed. Then the raw data are collected and compiled and analyzed. The results are interpreted for decision making and reporting. Additionally, the data generated can be utilized for further interpretation through data science techniques.

With all these moving parts, any inefficiency can greatly slow down the overall process, majorly drive up operating costs, and significantly increase the bottleneck. With the Unified Lab from BIOVIA, daily workflows are truly digitalized, non-value added tasks are minimized and organization are able to transform their lab operations.

The suite of applications that comprise BIOVIA’s Unified Lab are all designed to integrate with each other, offering users a seamless user experience in the lab. The applications are all web-based and can be deployed in various combinations in the cloud or on-premise, depending on the specific needs of each organization, and can also integrate with existing lab informatics systems for a truly digital lab.

**CLOUD DEPLOYMENT**

The BIOVIA Unified Lab is available on the cloud to provide you with a secure, validation-ready laboratory informatics solution. In a cloud configuration, the BIOVIA Unified Lab is completely web-based and exists outside your firewall. Cloud deployment minimizes Information Technology (IT) overhead costs and frees up internal resources since it eliminates the need for internal IT staff to manage the applications and servers, keep track of upgrades, maintain performance, and manage security. Virtual machines can be quickly spun up or down according to changing project needs. Secure access is delivered via SSL encryption, ensuring system security regardless of user location. Authorized users anywhere in your company, anywhere in the world can access your secure laboratory informatics solution any time you want.

The BIOVIA Unified Lab leverages the infrastructure of BIOVIA ScienceCloud, a cloud-based information management and collaboration workspace that achieved and maintains ISO/IEC 27001:2013 Certification, as certified by Bureau Veritas Certification (http://www.bureauveritas.com). ScienceCloud is operated by certified security experts, and uses multiple layers of security to protect the sensitive information transmitted or stored by customers. On ScienceCloud, the BIOVIA Unified Lab is deployed using guidelines for GxP systems for use in regulated industries, with controlled update and upgrade schedules.

**Figure 1:** The Unified Lab enables digitalization of all aspects of lab procedures.
LAB EXPERIMENT DOCUMENTATION - ELECTRONIC LAB NOTEBOOKS

Electronic Lab Notebooks (ELNs) are the gateway for capturing lab data consistently and sharing data efficiently. ELNs streamline the documentation and protection of intellectual property, help scientists collaborate in increasingly global and networked activities from discovery to manufacturing and make scientific data and observations associated with experimentation easier to capture, search, find and use. BIOVIA provides two options for customers who are looking for ELN capabilities: one for simple easy-to-use experiment capture, documentation and sharing (BIOVIA Notebook) and one for more in-depth capabilities, mainly in the regulated areas for spaces like formulation or process development (BIOVIA Workbook).

BIOVIA Notebook

BIOVIA Notebook is a web-based, easy-to-use and easy-to-deploy ELN for organizations focused on intellectual property capture, information sharing, process documentation and overall lower total cost of ownership. BIOVIA Notebook includes integration with the other Unified Lab applications like BIOVIA Compose, BIOVIA Capture, BIOVIA Samples, BIOVIA Task Plan, and the BIOVIA Pipeline Pilot data science solution. This powerful combination lets organizations integrate BIOVIA Notebook with their lab instruments and other data sources while also providing rich capabilities for scientific analytics, visualization and automated report generation.

Capabilities:

- Easily store, search and share entries from any location
- Digital signatures, experiment templates and workflow alerts
- Integration with instruments and data sources
- Scientific analytics, visualization and automated report generation when used with Pipeline Pilot

BIOVIA Workbook

For ELN needs that include deep capabilities for formulations or process development and stringent regulatory requirements users can opt for BIOVIA Workbook. BIOVIA Workbook is a multidisciplinary, enterprise solution for documenting and managing the flow of information, tasks and materials within and between labs, particularly in regulated environments. The Workbook ELN includes strong integration with the other Unified Lab applications, along with workflow support and authoring, collaboration and IP protection capabilities. BIOVIA Workbook efficiently manages the flow of information, tasks and materials among scientists, software and instruments within and between labs — improving personal productivity, collaboration and collective intelligence.

Capabilities:

- Customizable document workflows
- Secure document versioning, electronic signatures and audit trails
- Integration with instruments and systems
- Improved processes and documentation
- Improved collaboration and collective intelligence

Figure 2: BIOVIA Notebook

Figure 3: BIOVIA Workbook

RECIPE AND METHOD MANAGEMENT

BIOVIA Compose

BIOVIA Compose provides capabilities for the creation of recipes and methods from standardized libraries of operations and the storage. The application allows the right content to be input into processes from the beginning, so that organization can replicate production in similar ways globally. The standards put in place provide the system with a common language and a shared way of working. Recipes and methods can be included in BIOVIA Workbook, assigned to tasks with BIOVIA Task Plan, executed and reviewed using BIOVIA Capture.

Capabilities:

- Standardized interface for recipe/method design
- Recipe/method externalization and transfer via S88 standard
- Procedure and process flow views of the recipe/method
- Discipline-specific operation libraries fit individual user needs
• Support for customer and site-specific operation libraries
• Dynamic web-based user experience on desktop, laptop and mobile devices
• Integrated with material and equipment management

LAB PLANNING AND MANAGEMENT

BIOVIA Study Manager

BIOVIA Study Manager provides the tools to design and manage multiple study types that are performed in your scientific laboratories. Study Manager offers improved visibility of the experimental design (development) process to the organization. It minimizes the effort of defining the independent study arms by integrating the selection test criteria and parameters with your library of approved activities and activity plans. This ensures that a study design is implemented consistently, irrespective of the location of execution. Controls are in place to ensure study design approval follows an agreed lifecycle with appropriate management and e-signatures provide full traceability of author activities. Integration with the other Unified Lab applications ensures the materials and formulations tested have full traceability by using the correct IDs and labeling. Launching a study initiates a Task Plan with the necessary Tasks, Samples, and Results that will be used in the lab and linked to the target material. Using the tracking functionality, oversight of work progress is possible; allowing early identification of issues to allow mitigating actions and management of ongoing work in a study and portfolio.

Study types include, but are not limited to:
• Stability Testing
• Method Development/Validation
• Environmental Monitoring
• Process Development
• Excipient Compatibility

Capabilities:
• Easy Scientific Study Design
• Incorporate multiple dimensions of Study Parameters, Time Intervals, and Test Plans
• Select Tests and Specifications to characterize the material
• Automatically generate a linked Task Plan

BIOVIA Task Plan

BIOVIA Task Plan supports tasking out of activities along with sample and work management in the lab. Scientists can easily create tasks, assign them to colleagues, and request their completion directly within a single electronic laboratory environment. Additionally, scientists can digitally manage the submission, routing, receiving, tracking and reporting of results originating from laboratory work requests and test orders. BIOVIA Task Plan can be integrated directly into BIOVIA Workbook and BIOVIA Notebook to easily bring task management into the ELNs. BIOVIA Task Plan also functions as the central task management app for the other BIOVIA Unified Lab applications.

Capabilities:
• Create a library of lab activities - single lab procedures such as performing a pH measurement, a chromatographic measurement, weighing etc.
• Create tasks from available activities – either a single activity or a group of related activities
• Assign tasks to be executed on available samples
• Assign tasks to other scientists in the lab, or execute the tasks directly
• Request execution of tasks with different priority levels and due dates
LAB PROCEDURE EXECUTION

BIOVIA Capture

BIOVIA Capture is an intuitive, easy-to-use, mobile-friendly application supporting the efficient, standardized and paperless execution of recipes and methods in the lab as well as secure, structured data collection at the bench. The application increases efficiency, reduces transcription errors and improves both standardization and compliance. And just makes the lives of scientists so much easier!

Capabilities:

• Support of lab workflows – free flow as well as defined procedures
• Optimized for tablet devices, supporting iOS, Android and Windows devices
• Stepwise execution of procedures with ability to enforce limits and tolerances
• Integrated with materials inventory and equipment
• Modify and create new actions, operations, stages and procedures
• Access Operation Libraries to edit procedures during execution
• Designed for mobility with e-signature control

BIOVIA Capture also includes the ability to quickly review experimental results, with flexible filters in a mobile-friendly design.

LAB RESOURCE AND INVENTORY MANAGEMENT

BIOVIA CISPro

BIOVIA CISPro is a chemical inventory management system that makes current, real-time chemical safety and inventory data available on-demand, helping to drive the safe handling, storage and management of chemicals and other inventory materials. Scientists get immediate information about available quantities and locations of chemicals and other materials required for their lab activities. This avoids delays and costs due to unnecessary purchase.

Capabilities:

• Real-time overview of chemicals inventory and other materials required in the lab
• Barcode labeling and remote inventory control
• Integrated Safety Data Sheets (SDS) management
• Comparison of chemicals and chemical inventory with hazard and regulatory criteria

Review Capabilities:

• Interactive review by exception with flagging of deviations
• Quick filters for events and signatures
  • Data Entry, Data Modification
  • Observations
  • Out of Limits
  • Values collected by Instruments
  • System-calculated values
  • Manually-entered data
  • Drill-down into metadata, signatures and audit trails
**BIOVIA Samples**

BIOVIA Samples provides capabilities for sample management that can be readily configured to meet specific needs without the extensive and expensive modifications traditionally seen with Laboratory Information Management System (LIMS) modules. Designed to manage the creation, receipt, collection, labeling, splitting and disposal of samples within the lab, the application integrates with other BIOVIA Unified Lab apps to improve documentation efficiency, ensure compliant procedure documentation and reduce manual transcription errors. The sample Chain of Custody can be viewed to track its whereabouts including who handled it, where it went and under what storage conditions it was kept for different time periods.

**Capabilities:**
- Create samples with auto-generated or customized names
- Print appropriate sample labels
- Group related samples together
- Split (aliquot) samples and specify handling and storage conditions
- Mark samples as received or collected
- Execute planned tests for samples, and enter results through integration with BIOVIA Capture
- Mark samples for disposal

**Figure 10: BIOVIA Samples**

**BIOVIA Equipment**

BIOVIA Equipment is a comprehensive application for automated instrument data acquisition and the management of instrument-related data and workflows. It provides scientists with easy and intuitive transfer of instrument data into experiments in a BIOVIA ELN, or to other applications such as BIOVIA Capture and BIOVIA Task Plan. BIOVIA Equipment can be configured to automatically parse data from instrument data files to make results available when the scientist needs them. Auto-mapping of measurements to samples makes the import of results easy for the scientist and reduces transcription errors. Additionally, metrology “fit-for-use” checks directly from BIOVIA Capture makes lab workflows efficient and reliable.

**Capabilities:**
- Manage registry of equipment including metrology status
- Automatically acquire and parse equipment data for later use
- Easily bring equipment measurement data into the scientist’s experiment session
- Maintain traceability of equipment data from the source to the system where data are recorded or consumed
- Track metrology events including required preventative maintenance, calibration and verification events
- Link metrology events to methods and recipes like in BIOVIA Capture to ensure the correct procedure is followed
- Audit trail for all equipment records
- Electronic logbook of equipment use and metrology events

**Figure 11: BIOVIA Equipment includes comprehensive metrology capabilities, providing users with an overview of events and allowing them to perform scheduled as well as unscheduled maintenance of the equipment.**

**BIOVIA Chromatographic Data System (CDS) Add-Ins**

BIOVIA’s CDS Add-Ins enable scientists to import sample information from BIOVIA Task Plan (including recipes) to the CDS, and send CDS result data back to the measurement store in BIOVIA Equipment, where it is available for further use in BIOVIA Capture and Task Plan. BIOVIA offers two optional CDS add-ins, for Waters Empower and for Thermo Fisher Scientific Chromeleon. The add-ins are extensions to the Empower and Chromeleon clients making it convenient for scientists as they work in their existing CDS.

**Capabilities:**
- Sample Related Import into CDS
- Use existing sequence layouts for new sequence to control bracketing and injection types
- Import information of sample, control, and standard preparation tasks into Empower or Chromeleon supporting standard and custom data fields
- Control placement of imported data within the sequence or auto-replace by injection type
- Results Export from CDS
- Send peak data to BIOVIA including
  - All Empower data fields
  - A configurable list of Chromeleon data fields
  - Custom CDS fields

**Figure 12: BIOVIA Chromatographic Data System (CDS) Add-Ins**
• Attach CDS report to measurement
• Select from reports available in the Empower project
• Designated “Electronic Report” from Chromeleon

DATA SCIENCE IN THE LAB

BIOVIA Pipeline Pilot

Digital data offers more than just integrated workflows, automated data capture, and data standardization. Artificial intelligence, machine learning, data visualization and a cohesive data science strategy allow organizations to go beyond operational efficiency. Today’s lab operations are generating a vast amount of data from a plethora of different data sources. By effectively leveraging this data, organizations can avoid redundant work, increase lab efficiency and improve decision-making. BIOVIA Pipeline Pilot provides the scalable framework necessary to transform your lab into an intelligent, data-centric machine.

BIOVIA Pipeline Pilot is a graphical application that automates the analysis of scientific data, enabling users across the enterprise to rapidly explore, visualize and report research results without needing to write a single line of code. It optimizes the innovation process, increases operational efficiency and reduces costs for both the lab and IT.

One of the major obstacles to an effective data science initiative at any organization has been maintaining the quality of the models available to end users. Often, teams rely on fads over sound fundamentals. BIOVIA Pipeline Pilot ensures that best practices are easily captured, deployed and shared across your organization, maximizing the value of your data science team and allowing them to focus their work on value-added tasks.

BIOVIA ScienceCloud allows Pipeline Pilot protocols to be deployed alongside the BIOVIA Unified Lab applications in the cloud. In this way, the standardized protocols are readily available to all authorized users throughout your organization, enabling rapid deployment, ensuring best practices are followed, and accelerating the use of data science techniques to maximize lab efficiency.

Figure 12: An example machine learning protocol

Capabilities:
• Data management, analysis and reporting for text, numeric and complex scientific data, including chemical structures, biological sequences and scientific images
• Rapid application development environment for engineers, developers and scientists with a standard software development processes using a graphical design interface
• More than 2000 “scientific building blocks” – components that snap together, allowing rapid creation of all aspects of data processing, including data retrieval, manipulation, computational analysis, filtering, and display
• Validated scientific components and best practice workflows that cover a broad range of scientific disciplines

SUMMARY

With BIOVIA’s Unified Lab, companies can harness the power of a common software environment that manages most aspects of today’s laboratories, while also integrating with other existing lab informatics systems. The web-based applications are lightweight and easy-to-deploy, and allow for a custom-built solution best suited to each customer’s needs. Deployment on the cloud further lowers IT requirements, while enhancing overall security and IP protection.

Learn more at 3dsbiovia.com/UnifiedLab

Our 3DEXPERIENCE® platform powers our brand applications, serving 11 industries, and provides a rich portfolio of industry solution experiences.

Dassault Systèmes, the 3DEXPERIENCE® Company, provides business and people with virtual universes to imagine sustainable innovations. Its world-leading solutions transform the way products are designed, produced, and supported. Dassault Systèmes’ collaborative solutions foster social innovation, expanding possibilities for the virtual world to improve the real world. The group brings value to over 210,000 customers of all sizes in all industries in more than 140 countries. For more information, visit www.3ds.com.