



TRANSFORM YOUR LAB LEVERAGE A UNIFIED ECOSYSTEM WITH BIOVIA ONE LAB Datasheet

BIOVIA ONE 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 ONE 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.



Figure 1: BIOVIA ONE Lab enables digitalization of all aspects of lab procedures.

BIOVIA ONE 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 lab bottlenecks. With BIOVIA ONE Lab, daily workflows are truly digitalized, non-value added tasks are minimized and organization are able to transform their lab operations.

BIOVIA ONE Lab offers a seamless user experience to lab scientists as they move through their daily tasks. The web-based solution can be deployed on 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. Instead of compartmentalized point solutions, ONE Lab leverages natively integrated capabilities of traditional ELN, LIMS, and LES solutions for seamless workflows within a single, unified software environment.

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 Scientific Notebook provides ELN capabilities for ONE Lab, enabling powerful documentation tools, workflow simplification, and data parameterization to leverage experimental data like never before. But it is also more than an ELN, enabling scientists to document and leverage knowledge from across the lab in a centralized location. BIOVIA Scientific Notebook is a cloud-native ELN that is centered on the needs of scientists in the lab. It boasts a flexible, easy-touse and mobile friendly design that makes it easy for scientists to quickly adopt into their workflows. Existing experiments can be searched by various parameters, including experimental maturity states. Searches also leverage 6W tagging: Who, What, When, Where, Why, and How.

Scientific Notebook leverages a knowledge graph data of experimental data, enabling a much deeper connection between various lab data. In addition, Scientific Notebook integrates with other ONE Lab workflows, becoming a central hub for lab data and activities.

Capabilities

- Capture of structured and unstructured data
- RDF data model for bi-directional linking and actionable data objects
- Dynamic, user-based templates for flexibility while enabling consistency
- Search records by full-text or chemical structure or substructure
- Built-in synthetic chemistry support
- Integration for formulation testing and experimentation
- Integrate experimental data from BIOVIA Workbook, BIOVIA Notebook, and 3rd party ELNs

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REMOVING THE BARRIER BETWEEN LIMS AND LES

BIOVIA ONE Lab incorporates a highly advanced range of lab informatics capabilities which encompass the traditional capabilities of both a Laboratory Information Management System (LIMS) and a Laboratory Execution System (LES), as well as instrument integration and materials inventory management. By eliminating the barriers between these traditionally separate systems, and unifying the underlying data model, ONE Lab delivers seamless workflows for scientists, greatly simplifying their digital life in the lab.

Recipe and Method Management

BIOVIA ONE Lab provides capabilities for the creation of recipes and methods from standardized libraries of operations. This allows the right content to be input into processes from the beginning, so that the organization can replicate production in similar ways globally. The standards put in place provide the solution with a common language and a shared way of working. Recipes and methods can be included experiments, assigned to tasks for scientists, who can then execute and review the results.

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



Figure 3: Recipe and Method Management in ONE Lab

Lab Planning and Management

BIOVIA ONE Lab supports the 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.

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

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Figure 4: Task Planning in ONE Lab

Sample Management

BIOVIA ONE Lab provides full-featured 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, sample management is integrated with the other aspects of ONE Lab 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

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Figure 5: Sample Management in ONE Lab

Lab Procedure Execution

BIOVIA ONE Lab also incorporates the capabilities of a fully-featured Laboratory Execution System (LES), enabling intuitive, easy-to-use, and mobile-friendly lab procedure execution. The solution supports the efficient, standardized and paperless execution of recipes and methods in the lab as well as secure, structured data collection at the bench. ONE Lab increases efficiency, reduces transcription errors and improves both standardization and compliance. And by removing the traditional barriers between a LIMS and LES, ONE Lab simplifies the daily life of lab scientists.

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

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Automated Review-by-Exception

BIOVIA ONE Lab also enables automated Review-by-Exception, so that completed procedures which have no flags for review can be automatically released without the need for manual review. Batch release can become instantaneous, greatly increasing scientific efficiency. The parameters for automated review are completely configurable, enabling the process to match operational business rules.

Capabilities:

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

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Figure 7: Review-by-Exception in ONE Lab

Lab Resource and Inventory Management

BIOVIA ONE Lab includes a powerful 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. Scientist 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



Equipment Integration

With BIOVIA ONE Lab, data can be captured directly from networked instruments in the lab using an IoT approach. Data can be captured in its original format, and also parsed into standardized formats with agreed taxonomies and ontologies. On premise instruments can be easily connected to the cloud for ease of access regardless of location.

Equipment integration with ONE Lab provides scientists with easy and intuitive capture of instrument data. ONE Lab 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 make 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

BIOVIA CHROMATOGRAPHIC DATA SYSTEM (CDS) ADD-INS

BIOVIA's CDS Add-Ins for ONE Lab enable scientists to import sample information from ONE Lab (including recipes) to the CDS, and send CDS result data back to the measurement store in ONE Lab to be used in task plans and procedure execution. 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
- Attach CDS report to measurement
 - Select from reports available in the Empower project
 - Designated "Electronic Report" from Chromeleon

CLOUD DEPLOYMENT

BIOVIA ONE Lab is available on the cloud to provide you with a secure, validation-ready laboratory informatics solution. BIOVIA ONE Lab is completely web-based and when deployed on the cloud, exists outside your firewall. Instrument connectivity is delivered through a secure integration gateway, where connections are initiated from a lightweight on premise client.

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.

COMPUTER SYSTEM VALIDATION

BIOVIA supports computer system validation for ONE Lab, providing validation testing kits and working closely with customers to validate deployments efficiently. With cloud deployment, BIOVIA utilizes automation to perform the initial validation steps, delivering production environments to customers ready for final validation.

DATA SCIENCE IN THE LAB

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 ONE Lab can leverage BIOVIA Pipeline Pilot to provide 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.



Figure 9: 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 ONE 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.

With BIOVIA ONE Lab, organizations can unify, harmonize and standardize lab/resource management and procedure execution to help improve collaboration, increase productivity, and reduce regulatory compliance and safety risks while accelerating time to market.

LEARN MORE



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