

BIOVIA NOTEBOOK AND BIG DATA ANALYTICS TURN DATA INTO KNOWLEDGE

HOW CHR. HANSEN EVOLVED BEYOND "PAPER ON GLASS"
CUSTOMER STORY

CUSTOMER: A LEADING GLOBAL PRODUCER OF FOOD INGREDIENTS

Since their founding in 1874, Chr. Hansen has consistently stood on the strength of its R&D team to create innovative, industry-leading ingredients for a wide variety of foods, dietary supplements, and pharmaceutical and agricultural products. They especially excel in the development of cultures, enzymes, probiotics and natural colors and maintain one of the largest commercial collections of bacteria in the world, with over 20,000 strains. Chr. Hansen employs over 2,800 employees in 30 countries around the world, each dedicated to producing natural solutions to promote the wellbeing of all.

THE CHALLENGE: SHARING AND LEVERAGING DEEPER INSIGHTS FROM EXPERIMENTAL DATA

The increasing pace of research and growing competition in their industry had compelled Chr. Hansen to explore new methods to extract every ounce of value from its historically strong R&D team. Previously, Chr. Hansen had undergone a very successful deployment of BIOVIA Notebook to centralize the storing and sharing of scientific information and create a scientific knowledge base for the R&D organization. However, forward-thinking scientists in R&D wished to derive deeper insights from their experimental data by utilizing Big Data analytics. Additionally, they wanted their Big Data tool to automatically collect data directly from laboratory instruments, aggregate it in a single data lake, and parse it into a standardized format to minimize the potential for human error as new data was generated and processed. Although solutions like Hadoop have these data management capabilities, implementing a Big Data tool alone exposed the R&D team to similar inefficiencies they had struggled with when they operated on paper but with a slight twist. Instead of scientists struggling to find "dark data," they would have an overabundance of "dark insights" if they did not have a centralized location to store the results of their analyses. Powerful data trends or predictive models could be isolated within individual labs or teams, with scientists needlessly redesigning and rerunning analytical protocols previously performed by their colleagues.



"The integration of BIOVIA Notebook with our Hadoop Big Data setup has provided a strong scientific data platform – a digital laboratory where we can explore data and share insights"

– Dr. Morten Meldgaard Innovation Data Architect,
Chr. Hansen

Challenge:

Effectively storing and sharing Hadoop Big Data analytics results throughout a global organization

Solution:

BIOVIA Notebook and Hadoop

Benefits:

- Automated preparation and combination of data
- Created a single, searchable location for storing and sharing of Big Data analytics results
- Streamlined the data management workflow from experimental design through analysis
- Increased innovation efficiency

THE SOLUTION: COMBINING HADOOP AND BIOVIA NOTEBOOK FOR A MORE POWERFUL R&D PLATFORM

Chr. Hansen's previous implementation of BIOVIA Notebook presented a unique opportunity to supplement their R&D Big Data initiatives. By automatically processing raw data into a common format directly from an experiment, Hadoop gave scientists the ability to conduct data searches and visualization, machine learning and predictive analytics to power data-driven innovation. By adding the flexible framework of BIOVIA Notebook, the R&D team has created a unified space for storing and sharing the outcomes of their analyses in BIOVIA Notebook, building a bridge between their database and knowledge base.

Additionally, Chr. Hansen was able to leverage the native functionalities of BIOVIA Notebook to create a global knowledge network, allowing teams from across the global R&D network to search for and share the enriched information Hadoop had created. BIOVIA Notebook's scalability assists in creating this global network, as its previous use had facilitated a culture of sharing and collaboration, further bolstering the utility of Hadoop.

THE RESULT: CONVERSION OF SCIENTIFIC DATA INTO KNOWLEDGE

By combining Hadoop and BIOVIA Notebook, Chr. Hansen has created a modern data management and analysis culture by streamlining and enhancing the entirety of their experimental data management process from experimental design and data creation through the analysis of results. The previous implementation of BIOVIA Notebook constituted the first step towards a modern data landscape, as it promotes collaboration, automation, and data integrity and traceability. These aspects provide the framework for the back end of their Hadoop workflow, which automatically collects and processes data directly from laboratory instruments. Overall, this integration created a foundation for teams to innovate more quickly with faster access to historical insights and to think outside the box by comparing a variety of different data types and sources. The solution helps Chr. Hansen to identify the direction for future R&D endeavors by leveraging meaningful data insights sourced from their global R&D network, providing a transformational boost to innovation for an organization already renowned for its innovative culture.

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AKZONOBEL IMPLEMENTS LAB SAFETY STANDARD WITH BIOVIA CISPro

CHEMICAL INVENTORY MANAGEMENT SYSTEM STREAMLINES WORKFLOWS, CONTROLS COSTS, REDUCES RISK CUSTOMER STORY

CUSTOMER: A LEADING GLOBAL SUPPLIER OF SPECIALTY SURFACTANTS AND POLYMERS

AkzoNobel is a leading worldwide producer of decorative paints, performance coatings and specialty chemicals headquartered in Amsterdam, The Netherlands. They supply industries and consumers with innovative products in four key market segments: buildings and infrastructure, transportation, consumer goods and industrial applications. The company has approximately 50,000 employees in over 80 countries and more than 200 production sites.

AkzoNobel's Surface Chemistry division develops, manufactures and markets a unique spectrum of specialty surfactants, synthetic polymers and bio-polymers used in home and personal care products and in industrial and agricultural applications.

CHALLENGE: MANAGING CHEMICALS, ADDRESSING SAFETY REGULATIONS, CONTAINING ASSOCIATED COSTS

In 2012, AkzoNobel published a Laboratory Safety Standard addressing assets, procedures, people and substances within all R&D and QC laboratories across the enterprise. To meet this corporate safety standard, they conducted a comprehensive substance inventory to document existing chemical stores with substance names/labeling, quantities, amounts, dates, locations, owners, hazard ratings and safety data sheets for more than 10,000 containers. Student interns captured all this information on Excel spreadsheets, but this labor-intensive and time-consuming methodology was not sustainable for a company that is leading the way in sustainability, innovation and radical efficiency. For this reason, AkzoNobel opted to explore digital alternatives to managing chemicals and supplies in accordance with their Laboratory Safety Standard.



With CISPro, we know what hazardous materials we have, how much we have, where they're stored and who 'owns' them. Most importantly, we access our Safety Data Sheets directly from CISPro.

Jennifer Hergert, HSE Manager, AkzoNobel

Challenge:

Address critical workflow efficiency, risk management and cost control issues with a chemical inventory management system in a complex lab environment

Solution:

BIOVIA CISPro Cloud Chemical Inventory Management System

Benefits:

- Quick, accurate chemical inventory status and reporting
- Comprehensive hazard information for materials on site
- Reduced purchases of unnecessary chemicals
- Fewer chemicals in waste stream
- Faster experimentation, improved productivity
- Reduced chemical disposal costs

AkzoNobel's Surface Chemistry division decided to transition to a centralized chemical inventory system that would quantify and qualify all chemicals on site, provide transparency across multiple labs, reduce purchasing needs and disposal costs of unused chemicals, combine inventory and regulatory information and be easy to use with minimal IT support.

SOLUTION: ACCURATE, REAL-TIME CHEMICAL INVENTORY TRACKING AND REPORTING

AkzoNobel identified BIOVIA CISPro as a software system that could address lab safety challenges, but at that time, cost was an issue in deploying the system in a single lab location. After deploying CISPro at their Strongsville, Ohio R&D facility in 2012 (a multi-story, multi-building laboratory complex with more than 500 lab personnel), AkzoNobel subsequently began implementing the system at other R&D facilities including Surface Chemistry at Bridgewater, NJ in 2013.

BIOVIA CISPro is currently supporting AkzoNobel's Laboratory Safety Standard at Surface Chemistry by providing a complete, up-to-date substance register with all chemicals entered into CISPro before delivery to the laboratory. It is now easy to determine types and quantities of chemicals and other items held in different lab locations, and Safety Data Sheets (SDS) are also available within a single inventory system. CISPro supports

container labeling, chemical storage/disposal and annual inventory audits in accordance with regulatory requirements. The system also encourages lab personnel to share inventory, thereby minimizing the quantities of chemicals held on site, avoiding duplicate orders and reducing disposal of partially used chemicals. Previously, when using spreadsheets to track substances, it was not as easy to share chemicals across labs and files were not kept up to date.

RESULTS: WORKFLOW PROCESS EFFICIENCIES, LOWER CHEMICAL COSTS AND IMPROVED COMPLIANCE TO REDUCE RISK

One year after implementing BIOVIA CISPro, chemical inventory data clean-up and uploading of current hazard information (Safety Data Sheets) continues. Lab personnel have noted reduced ordering of new chemicals, easier transfer of chemical stocks to new owners and other operational efficiencies made possible through the use of barcode scanners to track containers. The CISPro system supports a consistent Hazardous Materials Identification System in which pre-printed barcode labels clearly identify both purchased chemicals and laboratory-created samples. This approach has streamlined workflows for the receipt, storage, tracking, reconciliation, disposal and reporting of chemicals and SDS management.

Since the deployment of CISPro, the number of chemical purchases and chemical disposals has decreased and overall lab productivity has improved. In some instances, chemists have saved several days in starting an experiment because they were able to determine through CISPro that required chemicals were already in the lab, so there was no need to order materials.

By efficiently tracking chemicals and other laboratory assets from receipt to disposal, BIOVIA CISPro is helping AkzoNobel's Surface Chemistry division to control both chemical inventory and laboratory costs, while also managing health, safety and regulatory compliance risks in accordance with Local, State, Federal and International EH&S regulations and Fire Code safety/reporting standards. An easy-to-use, real-time, barcode-based chemical inventory management system creates a firm foundation for accurate hazardous materials reporting and compliance.

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STREAMLINING SMALL MOLECULE R&D WITH BIOVIA PIPELINE PILOT STRATEGIES TO MODERNIZE COMBINATORIAL CHEMISTRY

Use Case



Challenge:

Technological and operational complexities in managing an enterprise small molecule combinatorial library made selecting new drug leads slow and prohibitively expensive

Solution:

BIOVIA Pipeline Pilot to automate screening of compound libraries for candidate selection

Results:

- Automated and enhanced input processes for determining chemical compounds
- Increased compound library by 55% while reducing overall operating costs by over 50%
- Efficient and effective access to chemical compound screening

CUSTOMER: A GLOBAL PHARMACEUTICAL PRODUCER

This BIOVIA customer is one of the world's largest pharmaceutical producers, touting a diverse global network of research groups and manufacturing sites. Their aim as an organization is to research, develop and manufacture a diverse pipeline of pharmaceuticals, vaccines and consumer healthcare products. They continually lead the pack in adopting new approaches to improve their R&D capabilities, increasing their R&D productivity and efficiency and supporting their mission to take on some of the most complex problems in medicinal chemistry.

CHALLENGE: EFFICIENTLY SELECTING NEW LEAD COMPOUNDS

The space of drug-like molecules is vast, and determining which to use as a jumping off point for a new lead compound remains a key challenge for medicinal chemists across the life science industry. These candidates must satisfy a number of key parameters, from size to synthesizability to safety. Combinatorial chemistry has allowed pharmaceutical companies to create virtual libraries of related compounds, helping researchers to narrow their focus on those which best suit their needs. Previously, this BIOVIA customer had devoted a large team of medicinal and computational chemists to oversee their combinatorial library, which contained tens of thousands of unique entities. This library needed to be updated frequently to capture the latest regulatory and R&D strategy changes. As a result, the management team would need to assess the millions of compounds available from their various suppliers and filter them down to match the customer's desired specifications. To ensure candidate compounds met researcher's needs, the customer maintained a highly-selective, three-phase process for potential purchase of new compounds. Their efforts focused on screening candidates via a variety of business goals (i.e. cost) and specific physicochemical descriptors. This process was repeated annually.

However, keeping the appropriate balance between these business and scientific goals often resulted screens needing to be run multiple times. These failed runs thus led to increased pressure to meet deadlines and cost efficiency, driving down productivity and increasing the risk for errors in analysis. As a result, managing the library was costing this customer tens of millions of dollars per year. To address this issue, company leadership decided to explore methods to automate the labor-intensive, non-value added steps of the process to streamline compound selection for the library.

"We wrote screening templates and tools within [BIOVIA Pipeline Pilot]. This is the most cost-effective tool I've ever had... It completely saved our sanity."

— Director of R&D,
Global Pharmaceutical Producer

SOLUTION: PIPELINE PILOT TO AUTOMATE CANDIDATE SCREENING

For the customer's high-throughput screening processes, BIOVIA Pipeline Pilot compartmentalizes their data on their extensive variety of chemical compounds and controlled substances. This has helped alleviate any foreseeable issues with legislative shifts and allotted for a pharmacophoric approach to candidate selection. Pipeline Pilot allows this customer to meet their goals of archiving compound collections based on a variety of parameters, including desired physicochemical properties, molecule complexity, and synthesis cost, among others.

By developing a mathematical model within BIOVIA Pipeline Pilot that parameterized historical screening data, the customer was able to determine—based on a particular portfolio of targets and possible compounds—which compound in their extensive library would give the maximum return. They are able to manage their supply chain of external companies with greater ease. Through filters and caches created in Pipeline Pilot, the team has removed mistakes in their acquisition processes and compound collection protocols. By alleviating the often painstaking difficulties involved in these processes, they have stemmed employee turnover and streamlined processes. This, according to one team member, has "completely saved their sanity."

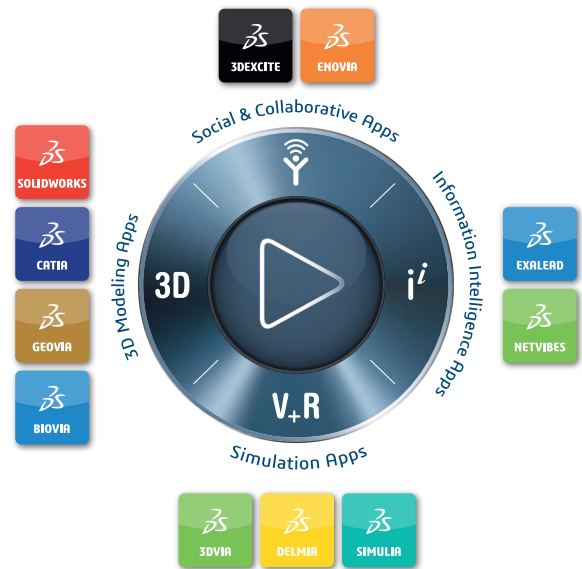
RESULT: A STREAMLINED PROCESS FOR COMBINATORIAL CHEMISTRY

BIOVIA Pipeline Pilot has helped the customer create effective protocols to streamline their chemical compound collection processes. In addition to reducing overall operational costs, they were able to overcome many bottlenecks in their automation facilities, eventually changing the scope of their processes

entirely. They were not only able to increase their compound library by 55% with these transitional changes in place; they also reduced costs to maintain this increased library by more than 50%. The team that works today at this BIOVIA customer now has efficient and effective access to high-throughput screening data, along with automated and enhanced input process for determining chemical compound collection. This has led to improved synchronization and continued vetting of their compound collection processes.

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