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Dotmatics Implements 'Data to Value' Initiative with BASF Agricultural Solutions

Research and development (R&D) are crucial to BASF's Agricultural Solutions division, leading to innovations that are essential to finding the right balance – for farmers, agriculture and future generations.

To cope with increasingly more complex and comprehensive data in R&D for new crop protection products, Dotmatics and BASF Agricultural Solutions worked together to enhance the division's R&D IT infrastructure.

With a 3-step phased approach, BASF Agricultural Solutions successfully reached the goals of the 'Data to Value' project. As a result, all steps of the data lifecycle – experiment planning, sample creation, testing, and scientific analysis – are handled by Dotmatics' unified data-centric platform.

*BASF creates chemistry for a sustainable future by combining economic success with environmental protection and social responsibility. More than 118,000 employees in the BASF Group actively contribute to the success of customers in nearly all sectors and almost every country. BASF's portfolio is divided into six segments: Chemicals, Materials, Industrial Solutions, Surface Technologies, Nutrition & Care and Agricultural Solutions. Innovations have made BASF the leading chemical company, with ~11,000 employees in R&D worldwide and more than 2 billion € R&D invested at ~70 R&D locations globally – resulting in ~1,000 new patents worldwide in 2019. As part of its corporate strategy, BASF has identified several strategic action areas including **Innovation** and **Digitalization** – both also of utmost importance for BASF's Agricultural Solutions division.*

Using digital technologies and data, BASF creates additional value for customers and increases the efficiency and effectiveness of its processes. The company can provide customers access to important information in real time using new digital services. The integrated use of internal and external data will strengthen BASF's innovation power. To that effect, a new supercomputer, Quriosity, maximizes the company's innovational potential.

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The BASF Group has a scientific history spanning over 150 years of R&D-led industry; its Agricultural Solutions division has more than 100 years of experience and an enviable market position as an integrated provider of crop protection products, seeds, and digital solutions. The portfolio comprises fungicides, herbicides, insecticides, and biological crop protection products, as well as seeds and seed treatment products, complemented by digital solutions and services. The strategy for the division is based on innovation-driven organic growth.
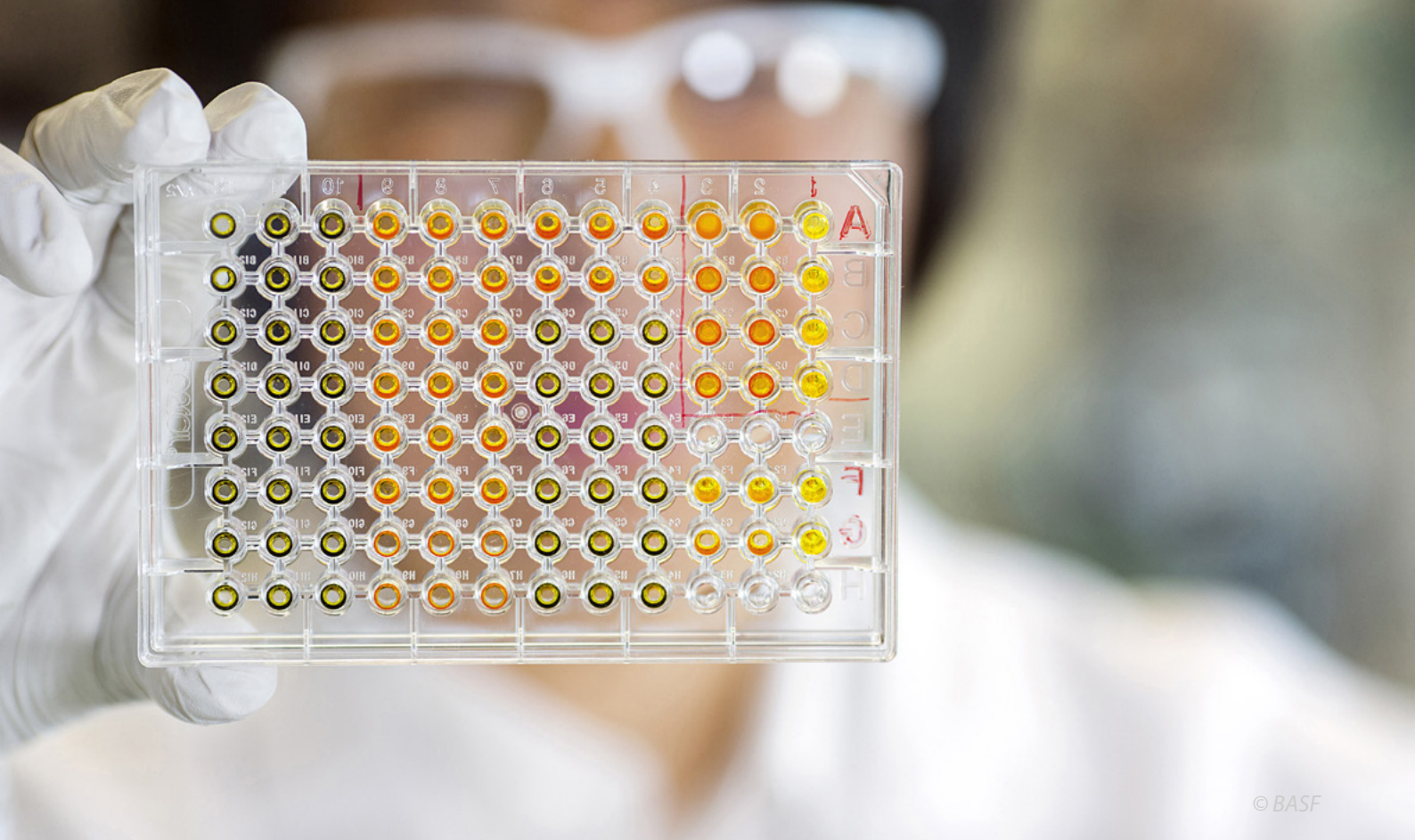
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BASF's innovative power is, among others, based on efficient research and development, building on the company's 'Verbund'.

It doesn't have a direct English translation, but the concept of the Verbund emphasizes the intelligent interlinking of research and development, production plants, energy flows and infrastructure. The Agricultural Solutions division is no exception and has benefitted greatly from the Verbund's many possibilities.

Quriosity:

BASF's supercomputer has computing power of 1.75 petaflops. Research and development play a key role in expediting digitalization at BASF. With Quriosity, much more complex models are possible, in which significantly more parameters can be varied. This could not only result in substantially reduced development times, but also previously unknown relationships can be recognized and used to advance completely new research approaches. An example project is studying the performance of molecules as related to their properties. With the help of Quriosity, a huge database with computed molecular properties has been created. These properties can be linked to the performance of BASF products by use of machine learning. Using this approach, the database enables scientists to find promising molecules for innovative BASF products.

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How to Extract Value from Data

In the first instance, designing the most suitable molecule with desirable properties is not trivial. Then, once a molecule is determined, scientists go on to design and carry out experiments. The resulting data is collected and evaluated to enable conclusions to drive decisions. This well-established scientific workflow, Design, Make, Test, Analyze (DMTA), normally requires several iterations of the cycle to optimize the desired property.

With a strong mandate for continuous innovation and digitalization, the Agricultural Solutions R&D team sought to optimize workflows involved in this design cycle. This ultimately led to the project name, 'Data to Value' or in short, D2V.

FIND STARTING POINT
DESIGN EXPERIMENT
DO EXPERIMENT
EVALUATE DATA
DRAW CONCLUSIONS
MAKE DECISIONS
OPTIMIZED PRODUCT

Joachim Dickhaut is responsible for the Dotmatics implementation project at BASF and is dedicated to providing chemists with access to all data they need to make informed decisions in addition to working seamlessly with expert informatics teams tasked with data management, machine-learning and application development for R&D. Joachim has over 20 years' experience in agricultural science research. He was awarded a Doctorate in Chemistry by the University of Basel.

Dr. Joachim Dickhaut

Senior Principal Scientist
Agricultural Research

BASF

Mapping Digital Workflows and Understanding the Needs of Research Data Stakeholders

The digitalization team invested time mapping and analyzing their R&D digital workflow - who generates and who uses the data?

- Bench chemists use data, such as analytical data or yields, to run individual experiments.
- Lab leaders use the data of several experiments to plan a series of new experiments.
- Senior Scientists use the data from many different sources to manage projects and support next-step decisions.

The team then established the requirements for a system to support both data capture and its subsequent application to decision-making.

- Data Capture and Acquisition: Bench chemists need an electronic lab notebook (ELN) to capture experimental data and store it securely in a computationally usable format. Curation of input data to maintain data quality is key.
- Data Search and Aggregation: A scientific data management platform to enable the seamless data flow between different sources, and across a variety of managed workflows.
- Data Analysis: support workflows and decisions through visualization and machine learning. Use advanced analytics, automation, and artificial intelligence to build on all available data. Connect data and methods, in new ways not feasible for humans due to the volume and variety of data, and extract knowledge.

"It's not good enough to reduce digitalization to simply introducing new systems which bench chemists have to find work-arounds to in order to make work for them. A good system will make life easier for our scientists by supporting their workflows and allowing them to concentrate on research, which is already complex enough!"

Dr. Joachim Dickhaut

What are the qualities of a good R&D informatics platform?

Flexibility: In a good R&D environment the process is under continuous improvement so the system should be adaptable.

Performance: The system should allow scientists to retrieve information and results as fast as possible.

Usability: The system needs to be intuitive and should support the research workflow, making life easier for scientists.

Three Projects Commencing with Data Analysis, Followed by Data Aggregation, and Finally Data Capture

Like many Dotmatics customers, BASF Agricultural Solutions had an existing IT and data landscape to incorporate in their digitalization plans. If starting a research organization from scratch, such as at a biotech start-up, then the ideal order of steps for digitalization would be data capture followed by the establishment of workflows and only afterwards, data analysis. However, the R&D project team sought to move to a web-based solution without disrupting the existing workflow. Thus, the D2V project was initiated with data analysis; bench chemists had identified a need for enhanced tools to deal with ever-increasing data volumes.

Project 1 | Data Visualization

The first project involved making Dotmatics Vortex the default R&D data analytics tool, a move away from analytics in freely available Excel spreadsheets. Although a great deal can be done with spreadsheets, they are not designed for chemistry data nor chemical structures. A typical research project has huge amounts of data associated with structure which needs to be represented visually in order to be analyzed and interpreted. The lab leaders and project scientists were very pleased to be able to look at the data in many different ways and supported the decision to invest in Vortex.

Project 2 | Search & Aggregation

BASF Agricultural Solutions already had an older project, in which a data warehouse was created to gather all legacy R&D data from different sources and different organizations, this insured good data curation and data quality. A custom-made client was also built. This was very powerful at the time because it supported searching all data in a flexible way, and also supported workflows.

However, after some years, this system could not handle the enormous amount of data in the way it is assembled in modern research projects. The digitalization experts recognized the need to give enhanced search and aggregation capability to all of their scientists.

Following on from the Data Analysis success with Vortex, the team introduced Dotmatics Browser as a client on the data warehouse. This was very much in line with a digitalization strategy of giving scientists access to all of their data and the creativity to innovate. BASF data scientists can now rapidly generate their own individual forms and the web client is more performant than the previous one. An additional benefit is that web-based updates are more efficient to manage.

The D2V project started with a need from the chemists. They said, "We need something better to cope with our data. With data volume growing and growing, we have to find a better way to work with that."

Dr. Joachim Dickhaut

"High quality data is the basis for good business decisions."

"We came to the point where accessing the data was becoming slower, and colleagues were asking for similar features to those in their personal apps but these couldn't be implemented within the architecture. It had been designed as a one size fits all, and although very robust wasn't flexible enough for end users who didn't know the structure of the underlying database."

Dr. Joachim Dickhaut

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Project 3 │ ELN Roll Out

The Agricultural Solutions division of BASF already had in place an ELN which was in its third generation. Many organizations approach Dotmatics with a view to enhancing specific functionality of legacy ELNs which were not designed with the web-based data aggregation capability on which Dotmatics is founded. Over time, scientists using legacy systems find it increasingly difficult to handle large numbers of experiments and carry out rapid structure searches, and IT teams find supporting proprietary data formats without APIs a challenge.

The digitalization team initiated a project to build a new ELN, which is based on Dotmatics Studies Notebook. Although it may have been tempting for the overall organization to insist on implementing a one-size-fits-all solution across all divisions, BASF understood the challenge of defining a single system across all research areas, given the breadth of science involved. The new ELN, has recently been implemented with scientists enjoying the ability to rapidly search across all their experiments.

"Scientists need the ability to do a variety of searches, looking over multiple experiments or across many projects, if they have required permissions."

"The early involvement of end users is crucial for the success of new solutions such as the ELN. Our power users built the system together with the Dotmatics experts which made it "their" solution. This contributed to the fact that they were very open to the new system and had a positive attitude towards it."

Dr. Joachim Dickhaut

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Enhanced Access to R&D Data and Analytics to Support Innovation

The result of the three projects Data Analysis, Data Search and Aggregation, and Data Capture, is that scientists of BASF's Agricultural Solutions division are building on the organization's solid data foundation.

- Lab technicians and bench scientists add to the corporate knowledge base by capturing experimental data and storing it in a usable format, as part of their natural workflow. Their day-to-day work also benefits from enhanced access to experimental results.

- Team and Project leaders efficiently access and manage results and workflows.

- Data scientists use enhanced analytics to support data-driven decisions by using all available results and information to extract knowledge. Unhindered access to high quality and curated data combined with advanced analytics and automation means they can connect data and methods to gain insights not previously possible.

- The R&D IT team of the Agricultural Solutions division manage updates more efficiently with a web-based platform: updates for web-based solutions are automatically pushed into the system; APIs enable on-top updates.

Dotmatics was able to deliver these benefits to BASF due to three main reasons:

- A unified platform

- Focus on data access – "giving researchers access to all of their data, all the time"

- A collaborative approach to working with customers combined with a continuous drive to innovate.

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"When implementing our new ELN, one thing became clear very quickly: with the new software, the data we accumulated over the years became much more visible to our researchers. That was a big eye opener for us. Our data scientists got much better access to our data and are already supporting several other projects."

Dr. Joachim Dickhaut

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About Dotmatics

Dotmatics is a global organization supporting science-driven research around the world.

Dotmatics offices are situated to allow real-time support at any time, ensuring your collaborative research can proceed at full speed.

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