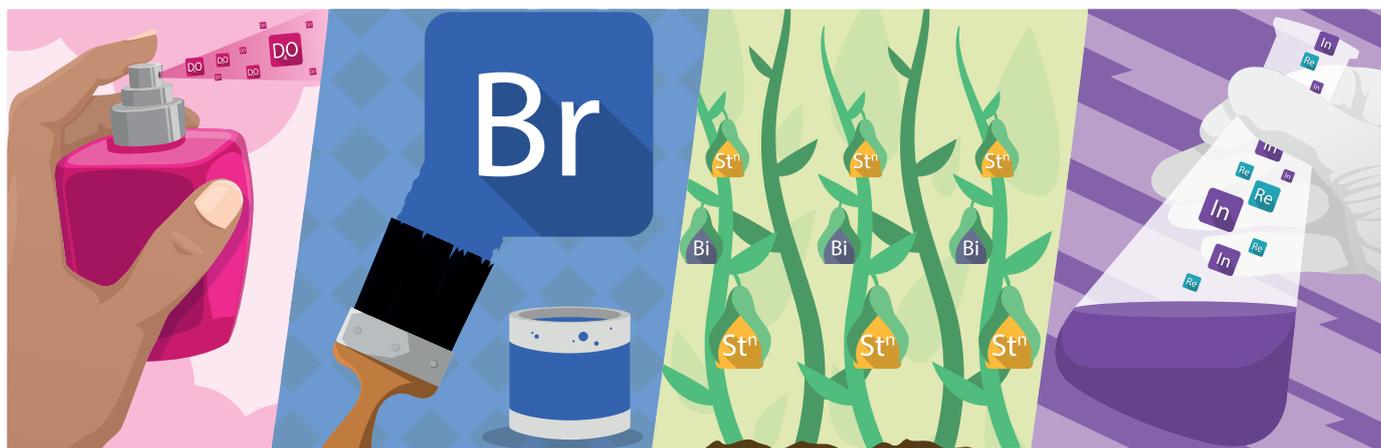


# TURNING SCIENTIFIC DATA INTO VALUE

## DOTMATICS FOR CHEMICALS & MATERIALS INNOVATION



The Chemicals & Materials industry is at the center of many of today's innovation challenges, including energy storage for e-mobility, lightweight and high performance materials for increased energy efficiency and miniaturization for mobility applications. As a part of a larger innovation value chain, they are driven to globalize their research teams to work more closely with key customers that require faster innovation cycles to meet product development timelines. Digitalizing R&D has become a key component of Chemicals & Materials R&D strategies, aiming to innovate faster, by leveraging existing research data, IP and knowledge

- Innovate faster - Leverage existing research data, IP and knowledge
- Do more with less - Ensuring throughput, avoiding duplication and distributing workloads while monitoring projects for their chances of success
- Empower globalized innovation networks: Enable free flow of information across customers, suppliers, partners and in-house teams while keeping proprietary IP safe and proprietary

At the core of these objectives sits the need to handle research data in a more effective way. When data can be easily accessed, it can become the basis for decision support and predictive data modeling applications. And if data is easy to capture and process, it helps eliminate tedious non-value added tasks, accelerating turnaround times and increasing experimental throughput. To do so, digitalization requires dealing with the data complexity found in Chemicals & Materials innovation.



### DEALING WITH DATA COMPLEXITY

Materials innovation typically combines a multitude of scientific disciplines, including: synthetic chemistry, polymer science, formulation and process development. As a result, digitalizing materials innovation fundamentally requires an inclusive view on all research data associated with any given project, as opposed to a siloed view in which each scientific discipline deals with their data in separate IT environments.

At the application level the implications are immediately apparent, for example, the performance of an inorganic catalyst will depend on

compositional data as well as processing data, or an engine oil additive will depend on functionalization (chemical activity), polymeric tails (solubility) as well as the overall base-oil formulation.

To deal with this complexity, any successful digitalization project needs to address these two challenges: implement the correct domain models and provide these domain models on a data-centric platform that allows all stakeholders in the innovation process to access and capture data. Dotmatics is uniquely positioned to address these challenges with its data-centric platform approach to the digitalize in Chemicals & Materials innovation.

## DATA-CENTRIC PLATFORM

Traditionally, R&D IT digitalization focuses on lab data capture via LIMS (Lab Information Management Systems) or the replacing lab notebooks with their digital equivalent, an ELN (Electronic Lab Notebook). These efforts generally aim at streamlining lab processes and gain efficiency by eliminating non-value-added work (reporting, data pre- and post-processing), improving resource allocation or accelerating work processes. While lab digitalization undoubtedly creates value by reducing operational expenses, it does little to accelerate innovation itself as it produces no new scientific insights or increases the understanding of the problem. Research data not only needs to be captured, but also made available to researchers to widen their research understanding, help them make better decisions, or provide them with a foundation for data-sciences approaches, including machine learning (ML) and artificial intelligence (AI) applications.

Dotmatics' approach to providing a data-centric for Chemicals & Materials R&D is to allow a data intelligence layer on top of its lab digitalization infrastructure. While the data intelligence layer can be implemented on-top of any existing lab digitalization infrastructure, Dotmatics' integrated IT infrastructure provides unique opportunities to simplify R&D IT. The most important components and aspects of the Dotmatics platform are:

### DATA INTELLIGENCE

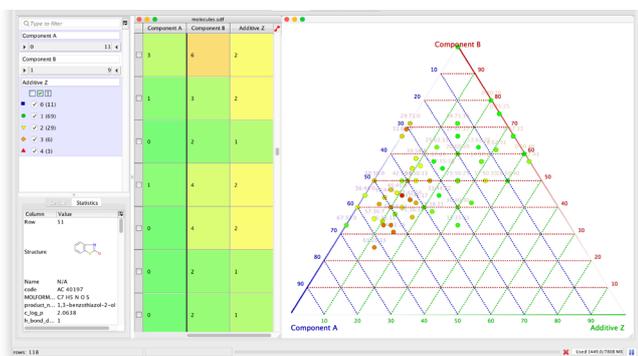
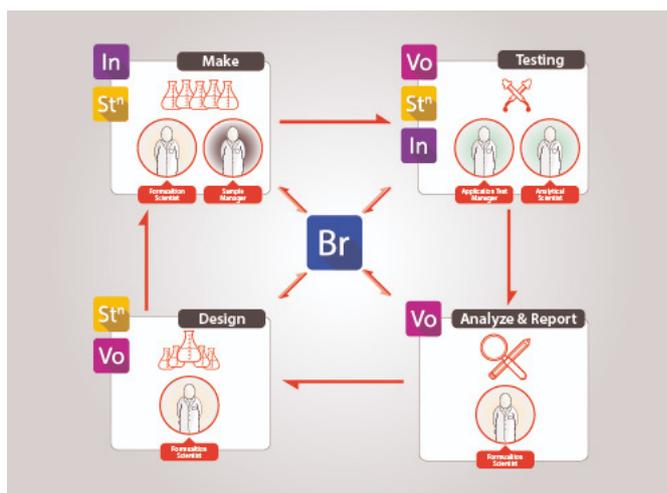
- Dotmatics Browser: search and query interface to Dotmatics and other 3rd party data sources
- Dotmatics Vortex: Data visualization and decision support tool

### LAB DIGITALIZATION

- Dotmatics Studies Notebook: Experiment capture for synthetic chemistry, formulations, process development and analytical/application testing
- Dotmatics Cascade: Request management system that brokers the interaction between project management, scientists and lab technicians
- Dotmatics Inventory: Organizes labs by managing samples and consumables
- Dotmatics Register: Defines experimental entities and establishes uniqueness rules

### R&D IT INFRASTRUCTURE SIMPLIFICATION

- Configuration-based: Simplifies maintenance and minimizes TCO
- Consistent deployment model: On-prem, cloud-based or hosted - all from the same code base
- Open: Allows for application integration and connection to a wide array of data sources, including web services, semantic and highly structured data sources (LIMS, ELN, ...)



## SCIENTIFIC DATA SOLUTIONS

Using Dotmatics Browser within the Dotmatics Platform, scientists break down data silos by aggregating searches across in-house and external databases into single searchable project views. Structure-searching capability across multiple projects allows teams to re-apply corporate experience. Easy-to-use analytics tools, such as Dotmatics Vortex, allow project teams to analyze and visualize their data on a common platform for integrated decision-making giving faster product turn-around.

Dotmatics capabilities including ELN for synthesis, analytical and formulation, registration, inventory management, test data management, work request systems, federated search and visual data analytics which can all be leveraged within workflows.

## LAB DIGITALIZATION

Chemicals & Materials product innovation workflows are complex, iterative and require multiple handoffs between scientific and manufacturing teams within an organization or collaborators. Dotmatics provides a comprehensive solution which can map to all stages of an innovation workflow, such as the formulation workflow shown.

Scientists plan and record experiments in Dotmatics Studies Notebook with templates configured to each experiment type. These can be highly structured, for example to capture the synthetic route of an active ingredient, or much more ad hoc performance-related experiments. Scientist are able to capture files such as spreadsheets, documents, images and video to assemble a notebook page.

FORMULATIONS											
FORMULATION EXPERIMENT DETAILS											
Name	Experiment ID	Description	User	Created Date	Completed Date	Countersigned Date	Countersigned	Customer	Application	Project	
Formulation D	138959	Control Example with New Formulation Interface	bill_jack	18/06/2019				CUSTOMER B	Personal Care	PROJECT B	
FORMULATION SUMMARY											
Name	Description	Amount Required	Amount Actual	Mass % Planned	Mass % Actual	Amount Units					
Formulation D	Formulation D	50	15.5	100	100	0					
FORMULATION INGREDIENTS											
Seq	Address Order	Name	Ingredient Name	Batch ID	Rate	Active %	Amount Planned	Amount Actual	Units	Mass % Planned	Mass % Actual
1	1	Formulation D	DCOT-000000011	DCOT-00000010-001	100	100	1.5	1.4	g	7.023	7.2476
1	2	Formulation D	DCOT-000000019	DCOT-00000010-001	Solvent	100	18	18	g	31.282	34.564
1	3	Formulation D	Water	3300013-4932-01	Water	100	5	6	g	25.641	32.432
1	5	Formulation D	DCOT-000000179	null	Default	0	2	g	g	10.256	g
1	6	Formulation D	138865-2-1	138865-2-1	Resin	99	1	1.1	g	5.1382	5.9459
1	1	138865-2-1	DCOT-000000002	DCOT-00000000-001	Default	100	0.5000	0.5000	g	50	50
1	2	138865-2-1	Water	3300013-4932-01	Oil	100	0.5000	0.5000	g	50	50
FORMULATION SAMPLES											
Sample ID	Barcode	Location Barcode	Container Location	Quantity	Units	Comments					
Formulation D-3	BYV-02345	BOX 5	> US Store- Room 1- Box 5	3	g						
Formulation D-3	BYV-02345	BOX 1	> UK Store- Chem 1- Box 1	3	g						
Formulation D-2	BYV-02261	BOX2	> UK Store- Chem 1- Box2	10	g						
ANALYTICAL RESULTS											
Sample ID	Service Experiment ID	Files	File Name	Analytical Technique	Date of Analysis						
Formulation D-2	138120	IR.jpg	IR.jpg	IR	30/07/2019						
Formulation D-2	138120	IR.jpg	IR.jpg	IR	30/07/2019						
APPLICATION TESTING											
Sample ID	Barcode	Experiment ID	Comments	Result Name	Result Type	Modifier	Result	Parameter Type	Parameter Value	Flag	
Formulation D-2	123	138145	High stability observed	pH	Stability	+	99	pH	7.5	none	

An SDMS (Scientific Data Management System) allows files from remote instruments to be uploaded to the server for easy consumption within Dotmatics Studies Notebook pages.



## R&D IT INFRASTRUCTURE SIMPLIFICATION

Working with Dotmatics offers several unique advantages while tackling your digital transformation project:

- Consistent deployment model: cloud, hosted or on-prem solutions operate all from a single code base
- Configuration-based implementation: simplifies maintenance and minimizes TCO
- Browser-based UI: mobile support, OS/device agnostic
- Open: connects to existing infrastructure, e.g. LIMS, ERP and PLM

## CUSTOMER EXPERIENCES

A large fragrances and flavours company has made the transition from a legacy vendor ELN which had reached end of life and was no-longer scalable nor appropriate for a global collaborative environment. Researchers are now able to share data across projects in real time enabling rapid, informed decision-making.

A major chemicals company moved from a diverse departmental system of both paper and scattered legacy digital systems. The move from error-prone paper was expected to show increased efficiencies but integrated searchability was the most valued aspect of streamlining their innovation workflow.

A global materials company updated a legacy in-house developed solution which was not maintainable or scalable for modern data management. The Dotmatics implementation team advised on a Cloud-hosting strategy for deploying software and best practice for structured data capture. Dotmatics skill in Change Management helped the organization adopt standardized new systems and workflows to improve their processes.

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