







R&D-driven industries talk a lot about progressing towards the paperless laboratory. Their ultimate aim is to capture and store all experimental, process, inventory and results data, from the earliest stages of discovery, through to manufacturing and QA/ QC in an electronic format.

While instrument and software vendors are developing the tools to facilitate hands-off laboratory workflows, what has been lacking is a unifying language for communication and standardized data formats. Laboratories today are typically disconnected: often there will be multiple method authoring systems and execution platforms, poor integration of existing electronic systems and equipment, and reliance on errorprone, manual activities and disparate data formats. This disconnection means that packets of data from a given workflow are commonly locked into different dead data silos and are not transferrable.

A basic analogy would be the evolution of printers. Twenty years ago, when someone bought a new printer they would have to plug it in, connect it to a PC, download and install specific drivers and hope that the computer's software and the printer software could understand each other. Every printer used different software, so it was often hit-and-miss. Things have progressed significantly since then: today, a printer can connect wirelessly with a laptop at the push of a button. The entire setup only takes a few minutes.

When it comes to laboratory informatics platforms, analytical software and hardware, we are still at the "early printer" stage of communication.

Instrument and software vendors develop their own data formats and languages. For some, these formats represent unique selling points and keep customers loyal. The software may offer a particular feature that isn't available using other packages, making it easier to stay with current software or instrument vendors since laboratory equipment is already set up to use their "language."

But using product-specific software can complicate the lab's operation. The range of software commonly used in a laboratory may span laboratory information management systems (LIMS), electronic laboratory notebooks (ELNs), enterprise resource planning (ERP), manufacturing execution systems (MES), product lifecycle management (PLM) and corrective and preventive action (CAPA) software, but they are often hard to interface together.

Having various informatics platforms grounded on the same language and data formats results in substantial efficiency improvements through the ability to search, mine and analyze collated data. Unfortunately, different software and informatics platforms from competing vendors commonly do not interface. This data disconnect is something that life science companies have long understood, recognizing that business processes in the laboratory were basically broken because everything was "non-standard:" data was collected in electronic format, but there was no common architecture.

A more seamless operational informatics infrastructure with standardized languages and data formats would enable scientific reproducibility and improve compliance, data integrity and context, while maximizing the ability to reuse data. With this capacity follows lower total cost of ownership, greater efficiency and faster time to value for implemented solutions.

With the understanding that standardization could help speed product development and time to market, while reducing attrition and repetition, a number of like-minded life science companies set up the Allotrope Foundation in 2012.

Their goal was to create a standardized data format for the acquisition, sharing, and management of structured procedural methodology and all experimental, analytical and process data. The impetus was all about enabling digital continuity, where the challenges were to bridge all the existing gaps between software, hardware, data management and reporting tools; to enable more compliant data tracking and better data integrity; to do away with dead data silos; and to simplify the overall laboratory operational landscape. Ultimately, data then becomes more transparent and accessible to scientists, managers and decision makers.

Allotrope's growing list of partners – the instrument and software vendors who are working together to shape this standardization, including BIOVIA – are driving development of the overarching Allotrope Framework which supports the standardization of industry-wide ontologies and languages.

As part of the framework, the Allotrope Data Format (ADF) is a single, unifying data format for managing all laboratory data and ancillary files. The ADF is underpinned by Allotrope Foundation Ontologies (AFO), which represent a common vocabulary of taxonomies and ontologies for describing tests, methods and processes. The Allotrope Foundation has now published publicly-available versions of both the ADF and AFO.

Allotrope data models then provide a route for using the ontologies and taxonomies to categorize and describe the laboratory's data holistically and reproducibly. Alongside the vendor partners, Allotrope Foundation members, including some of the world's largest pharma and biopharma companies, are working to implement Allotrope Framework solutions in real-world settings within their laboratories, while providing feedback to the partners so that the framework continually evolves. Since 2015, BIOVIA has worked as an Allotrope Foundation vendor partner to help develop a standardized data framework that other software vendors can plug into. As part of its own ongoing product development, BIOVIA had already been working towards an open laboratory system through which users could implement their own standards. Allotrope aligned perfectly with the company goal of enabling laboratory networks of software and hardware to communicate with the same language.

Vendors and developers are now working together on defining all the pieces and fitting them together. Once agreement on units, parameter names, process steps, measurement names, etc. is reached, there will be a common dictionary to make laboratories consistent, and so make equivalent data understandable and comparable. Standardization will help ensure data quality and integrity, as well as regulatory compliance, which are critical to any R&D or manufacturing environment.

In October 2017 BIOVIA released the latest version of the Dassault Systèmes ONE Lab solution. This is the first informatics solution developed to support the unified laboratory concept with ADF implemented throughout the laboratory workflow. The ONE Lab solution contains a variety of domain-specific tools and configurations to meet the needs of each type of laboratory operation: upstream research, development, and QA/QC.

As a platform for 'ideation to commercialization', ONE Lab is designed to allow organizations to operate as a unified lab, enabling comprehensive executive insight, faster cycle times and technology transfer, digital compliance, and a simpler IT environment.

ONE Lab facilitates total laboratory connectivity from research to manufacturing, streamlines external collaboration, guides more efficient use of manpower and resources, and provides better business insight. It effectively automates and standardizes everything – the test procedures, instrument connections, sample management and more – in small molecule or biologics research, development and quality control labs.

From the perspective of supporting an Allotrope Foundation framework for complete laboratory standardization, the ONE Lab infrastructure allows laboratories to adopt a unified standard and language, while still using different software applications, because resulting data can be converted into the standard format.

BIOVIA has also incorporated both reader and writer functionality components in BIOVIA Pipeline Pilot to read and

to write ADF files. In addition, BIOVIA solutions have the ability to synchronize with Allotrope taxonomy and ontology data for material, process, equipment and result data.

This means that practically every ad hoc or repeated process is carried out according to validated procedures, recorded using the same language and reported under that single framework. Laboratories can adopt standard Allotrope Foundation vocabularies, taxonomies and ontologies, so as scientists develop an experiment or procedure, take a measurement, or describe materials or an operation in the laboratory, they are doing it in a common language.

These are critical capabilities which enable the industry to generate information-rich data acquisition layers. So when data is acquired from systems, it can be transformed into the ADF format, but on top of that, every procedure executed in the lab can be standardized, including the most mundane or common processes such as compound registration, making solutions, or using and calibrating equipment.

All of those procedures can now be based on building blocks of standard nomenclature and process steps, which are all configured around the S88 industry standard for authoring and defining processes, and for defining the materials and equipment associated with those processes. The experiments and studies that use these standard procedures, standard data and standard language can then be layered on top. And all of that can now be stored in and retrieved from a cloud-based data lake that can be indexed and accessed by people from anywhere in the world.

Laboratory-wide standardization creates huge value within an organization, above and beyond just sticking to standard



operating procedures (SOPs) and ensuring data integrity. Inefficiencies and data utility challenges are reduced through consistency. The ability to easily access both current and historical data enables scientists and business managers to avoid repeating experiments, while the ability to rapidly compare results informs scientific and operational decision making and aids regulatory review and audit. Processes and data are easier to understand, and laboratory integration is easier to perform. Ultimately every process becomes more efficient and effective.

Standardization also makes it easier to collaborate with partners or service providers. If everyone is using the same language and data format, then internal scientists can easily communicate and exchange information with a partner, contract research organization (CRO), contract manufacturer or other service provider. And they can do that without having to translate data or provide summaries in flat files such as PDFs.

While an increasing number of vendors and life science companies are joining Allotrope as members to help develop the framework and demonstrate its utility in industrial settings, there is still work to be done. BIOVIA is collaborating with instrument vendors to align equipment with its ONE Lab infrastructure, so that laboratories can effectively purchase new equipment and interface directly through BIOVIA's standard lab services without facing communication issues.

BIOVIA looks at a laboratory workflow from end to end and provides solutions for the logistic functions of the lab such as the documentation of experiments, and the execution of procedures and the management of equipment. But instead of selling equipment directly, BIOVIA works with equipment vendor partners to make sure their equipment fits into the customer's workflows using the ADF standard.



Out of the box, the BIOVIA software is effectively empty of defined content; as an example, it's a bit like opening up a dictionary in which every page is blank, and then being able to press a button and pull in all of the language, or all of the words, the vocabularies that would go into that dictionary. The customer is then working with a full dictionary of terms for every laboratory process. There is no uncertainty about how to name or describe things; the terminology is clear.

A growing number of partner software and instrument vendor companies are joining the Allotrope Foundation to continue developing the framework. Similarly, there is a broad spectrum of member companies that represent the end users, and this now includes many of the world's major pharma and biopharma companies, who are working alongside the Allotrope Foundation on implementations of the ADF data standard, taxonomies and ontologies.

Firms don't need to be members to take advantage of the ADF standard and language, but there's a lot of motivation for vendors to join as partners. Members whose implementations are supported by Allotrope Foundation partners will receive direct feedback into how the framework evolves.

Some of those member companies now have hundreds of thousands of data points in their data lakes that are being accessed by thousands of scientists on a daily basis, and they are already starting to realize major savings from not having to search for, or recreate data, because it is all accessible. Scientists are able to work more efficiently, and are deriving more value from their experiments and analyses. Ultimately, data can not only be captured as part of every experiment and procedure, but it can be reused over and over again, so researchers won't have to do as many tests or as many experiments in the future.

The industry is now working together to define that language and make compromises, so that the language is as relevant as possible to everyone.

Now there is tremendous value in coming to a compromise, because when everyone agrees on units, on parameter names, on what to call process steps, then that dictionary is useful to everyone and it is easy to find all their data using standard terms. Customers can exchange data both internally and with external partners, access and read it. BIOVIA is playing a key role in making this possible by adopting an underlying architecture to capture and store data, and to implement standards.



## Our **3D**EXPERIENCE® platform powers our brand applications, serving 12 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**.

## Europe/Middle East/Africa Dassault Systèmes 10, rue Marcel Dassault CS 40501 78946 Vélizy-Villacoublay Cedex France

Asia-Pacific Dassault Systèmes K.K. ThinkPark Tower 2-1-1 Osaki, Shinagawa-ku, Tokyo 141-6020 Japan Americas Dassault Systèmes 175 Wyman Street Waltham, Massachusetts 02451-1223 USA

