Managing Analytical Knowledge for Molecular Characterisation

Edward Milton-Harris, Advanced Chemistry Development, Inc (ACD/Labs)

Analytical data is at the heart of chemistry research. Almost every chemistry experiment involves one or more analytical tests. These results are then used to assess a synthetic route's performance or yield, determine possible impurities and their structures, or verify product safety.

Despite the importance of this information, many organisations lack the tools or infrastructure needed to properly manage their analytical data. Results are scattered across multiple systems in a variety of file formats. Chemists often feel they are spending more time handling data than doing experimental work.

Fortunately, there are solutions to this problem, but first, it is necessary to understand why analytical data management has become so challenging.

The State of Analytical Data Management

ACD/Labs recently ran a survey asking research chemists how they manage their analytical data. Over 90% of respondents said they use multiple types of analytical data, multiple instruments, or multiple applications to process their data.

Acquiring different types of data is often necessary for completing many research activities, such as elucidating the structure of unknown compounds or assessing the composition of a mixture. However, this diversity of methods often leads to multiple file formats. These file formats are often incompatible, leading to challenges when consolidating or comparing results.

Analytical data is also scattered across many systems. Our survey found that most scientists store their experimental results in at least two locations, such as Microsoft applications, instrument vendor software, and electronic laboratory notebooks, as shown in *Figure 1*.

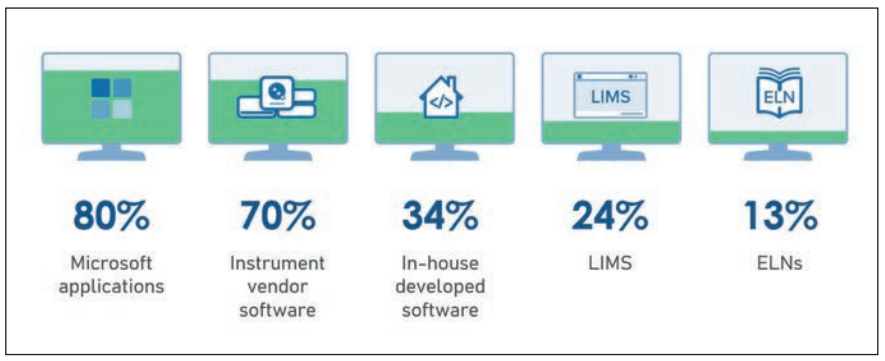

Figure 1. Where chemists store their analytical data, according to the Analytical Data Management Survey. Source: ACD/Labs.

Storing data in multiple places makes finding the results you need when you need them challenging, leading to wasted time searching for missing files. In some cases, scientists are forced to repeat experiments to replace lost data, which is a significant cost in both time and resources.

Effectively Manage Your Analytical Data

Researchers need an analytical data platform designed to meet their needs. At ACD/Labs, we have developed the Spectrus® platform that allows you to manage all your analytical data in one place, including NMR, LC/MS, Raman, and optical results. Consolidating multiple types of analytical data allows you to reach better insights while saving time since you won't need to switch between several applications.

You can also include contextual information such as chemical structures, the conditions used in the experiment, or the instrument used to run the analysis. This helps you have confidence when interpreting your analytical results in the future.

Spectrus is also a vendor-neutral platform, meaning it is compatible with all the major equipment vendors. Most laboratories want to use different instruments from various manufacturers due to scientific or cost considerations. This often means that each device uses its own software, which is incompatible with equipment made by other vendors, making it challenging to compare and consolidate results.

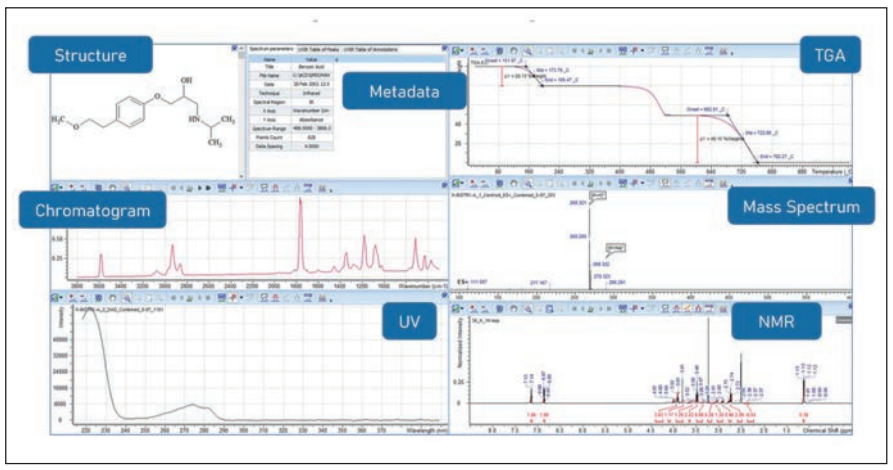

Figure 2. Connected, assembled analytical data in the Spectrus platform.

With Spectrus, your team can use the instruments they want, and review results acquired in different laboratories using one application. Scientists are also not limited to using processing software only available on a dedicated lab workstation. This gives them the freedom to process their data whenever and wherever they like.

Another common challenge for chemists is finding their data. This is particularly true in pharmaceutical research, where results that are several years old may need to be used to complete regulatory filings. Without search functionality, finding the file you need can be nearly impossible. The Spectrus platform allows you to query by chemical structure, sub-structure, retention time, molecular formula, and more, allowing you to quickly locate the results you need.

Boost Your Productivity with Automation

Time is a valuable resource, especially in research and development. One of the most powerful tools for increasing efficiency is automation. By delegating routine tasks to computers and robots, it is possible to increase the work each scientist can accomplish, meaning faster results and shortened time to market.

The analytical lab has many opportunities for automation. Using NMR processing as an example, what tasks can be automated with Spectrus applications?

Processing: Software can quickly and accurately pick peaks, integrate areas, and summarise peaks into a list.

Interpretation: Software suggests a structure based on the analytical data—unbiased by what the scientist expects to find.

Reporting: The analytical data, structure, and relevant contextual information are compiled into a pre-built document. This improves efficiency and re-usability, while simplifying the completion of filings for regulatory agencies.

Databasing: Results are saved in the appropriate file format, along with any metadata necessary for retrieval or re-use.

These operations can save considerable time for analytical chemists, allowing them to be more productive and focus on more challenging problems. The effect of these efficiency gains is magnified when combined, as shown in the case of Novartis.

Case Study: Automation of Structure Verification at Novartis

Novartis improved efficiency by implementing automation. The company has implemented an automatic structure verification (ASV) system developed by ACD/Labs, which uses NMR data to determine chemical structures. An internal study completed in 2020 found that each manual analysis took approximately 20 minutes to process manually, while automated verification took 1-2 minutes.

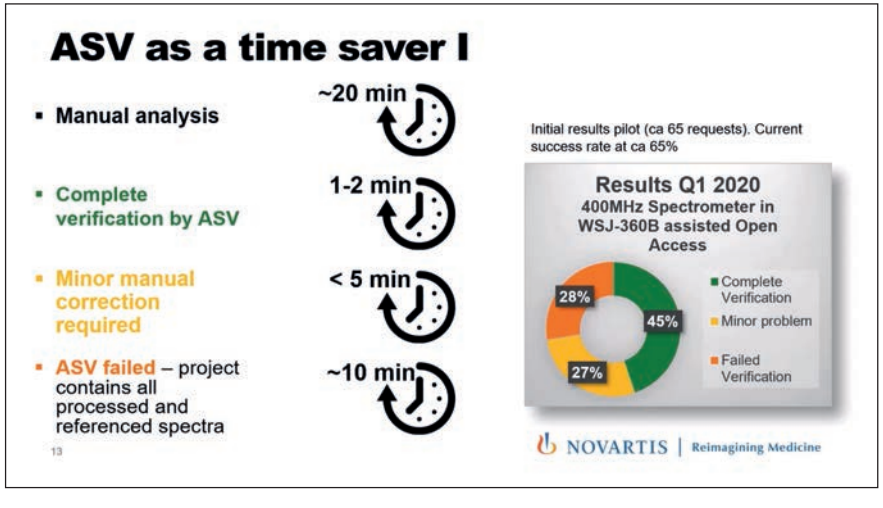

Figure 3. Novartis is using Automated Structure Verification (ASV) to increase the efficiency of analytical chemists. Source: Novartis

Even in the cases where correction was required, time savings of 50-75% were observed. The effectiveness of an ASV will also improve over time as the training set is expanded.

Realising the Power of Your Analytical Data

There are many benefits from implementing technology, such as the Spectrus platform, including:

Simplify identification of known and similar structures. Where have we seen these molecules before? How do we make them? Where did they come from? If somebody made this 20 years ago, how did they improve the yield? All this information is stored within a database that can be searched, by relevant chemical and analytical parameters, quickly and easily.

Use your experimental data to train spectral prediction algorithms. You can create a master database with all your chemical data or smaller training databases for libraries of similar compounds.

Share data and collaborate with others. Anything updated can be rolled out to everybody within the blink of an eye, so the system is always current and has the latest information.

As we enter an age of artificial intelligence and machine learning, data is more vital than ever. However, not all data is equally valuable. Organisations need to implement the necessary infrastructure to manage their data effectively, without burdening experimental scientists with endless file management and extra work.

The Spectrus platform is critical for getting the most out of your analytical data, combining multi-technique and vendor-neutral processing with automated workflows and state-of-the-art databasing technology.

For more information, visit: www.acdlabs.com/products/spectrus-platform/