

# Chromatography

## Digital transformation of the pharmaceutical industry: The role of chemistry software tools

Baljit Bains, Advanced Chemistry Development, Inc (ACD/Labs)

Over the last decade, there has been a big push in the pharmaceutical industry toward digital transformation. More recently, it has been fuelled by the COVID pandemic when there was a greater realisation that it was both necessary and possible to access data without physically being in a lab. The need to implement digitalisation of processes is further driven by the increasing gap between the demands of the industry and the capabilities of conventional systems.

Although digital transformation can be complicated to achieve, if implemented properly it can have transformative effects on drug discovery, development, and manufacturing processes. Digitalisation of data is key to navigating this dynamic landscape, as it enables the incorporation of appropriate knowledge management, data analytics, machine learning (ML), and artificial intelligence (AI) initiatives.

### Digitise vs. Digitalise - Why does the distinction matter?

The terms 'digitise' and 'digitalise' are fundamental elements for digital transformation. Although they possess unique definitions, they are often used interchangeably. To optimally leverage each approach, it is essential to grasp the difference between the two concepts.

Digitisation serves as the foundational step in the broader process of digitalisation. It involves the adoption of computerised tools to convert paper documents into digital formats. By digitising data, workflows are streamlined, data accessibility and sharing are enhanced, and the laborious, error-prone manual completion of tasks is eliminated. Digitisation of data empowers organisations to leverage advanced technologies and automation in their journey toward digitalisation.

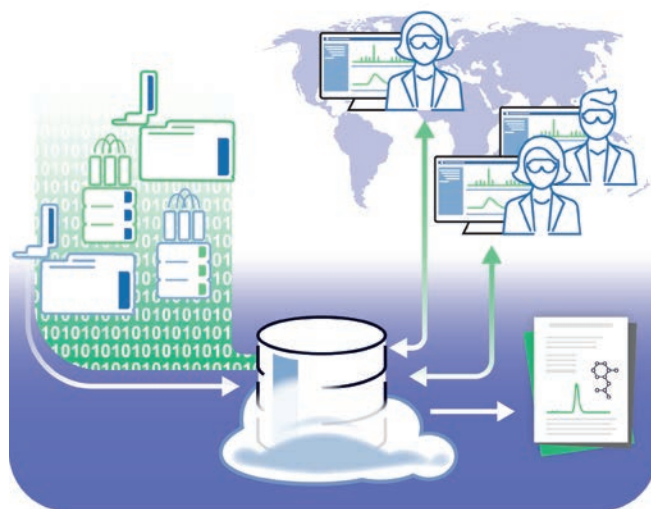
Digitalisation is the transformation of manual processes and operations into digital formats - encompassing tasks like the digitisation of documents, automation of manual tasks, and adoption of data-driven decision-making processes. It is achieved by integrating digital tools and advanced technologies, such as data analytics, cloud computing, ML, AI, etc., to optimise workflows.

### What is digital transformation

Digital transformation involves strategically integrating digital technologies throughout all aspects of a business's processes and operations to fundamentally change and optimise them. In the pharmaceutical industry, this can include everything from drug discovery to marketing products. It can be achieved by leveraging digitalised data through the integration of technologies like data analytics (including chemistry software tools), ML, and AI, among others.

Adopting digital transformation requires the evolution of an organisation's processes to create long-term sustainable digital solutions. To increase the digital capability of Research and Development (R&D) within pharmaceutical organisations, different components must be incorporated, including:

- Data Integration and Management - there must be a system in place to break down silos to collect and integrate data from all scattered sources
- Advanced Analytics - having tools in place (such as data science, AI, and machine learning) to analyse all the collated data and create predictive models to help support informed decision-making



## Challenges of digital transformation

Digital transformation is not as simple as adopting digital tools and assets - these tools must be deeply embedded within processes and IT environments for organisations to perform to their maximum potential. Successful implementation of digital transformation requires a significant investment of time and resources, and unfamiliarity with new technologies and resistance to change are among some of the challenges that must be overcome.

R&D in the pharmaceutical industry is characterised by strict regulations and complex processes that face unique digital transformation challenges.

### Scalability and adaptability of efficient processes

Industry standards and requirements heavily influence the long-established processes in the industry. However, this can often limit the scalability and adaptability of efficient processes. The capabilities of these conventional systems often struggle to meet the growing demands of the industry at a quick enough pace.

### Siloed and unstructured data

The masses of data generated by pharmaceutical companies are typically unstructured and unharmonised. In modern-day multi-instrument, multi-vendor labs, data processing with individual instrument software often results in data silos. Unstructured, siloed data poses a huge challenge in finding the right data when it's needed, making collaborative data-driven decision-making difficult.

### Inefficient data management

Given the vast amounts of data that pharmaceutical organisations generate, it is challenging for traditional methods to manage, analyse, and extract relevant insights from this data. As sources of data increase, so does the incompatibility of files, and the time spent tracking down results. These traditional data management methods are time-consuming with an increased susceptibility to error and loss of data. Without access to historical data across the organisation, experiments and mistakes will likely be repeated.

Incorporating a cultural shift and appropriate digital tools can help to overcome these challenges, and successfully implement digital transformation in the pharmaceutical industry.

## The role of chemistry software in digital transformation

Digitalisation involves optimising data analytics with software tools to extract maximal value from the data - ensuring that it is findable, accessible, interoperable, and reusable. Vendor-neutral and platform-agnostic tools like ACD/Labs' chromatographic method development software, Method Selection Suite, provide a standardised solution to capture, unify, store, and access analytical data.

The scope and potential of such software tools are immense, playing a role in the prediction of structures, modeling, and simulation to develop robust chromatographic methods, and the interpretation of experimental results. Leveraging this digital tool empowers pharmaceutical organisations to harmonise and manage data more effectively, enables easier accessibility to data, and allows informed data-driven decisions to be made faster.

### Harmonise data for easier retrieval

Using Method Selection Suite, multiple file formats and data types can be harmonised into a single standardised data format, preparing it for further use by humans or machines. All analytical techniques used to characterise compounds and formulations can be analysed and processed within a single interface - allowing data continuity and eliminating data silos. Integration of this tool into method development processes allows consolidation and standardisation of data - ensuring that the right data is found at the right time.

### Make informed data-driven decisions faster with better data management

Data management includes the secure and efficient collection, storage, and use of data. To reduce the time spent assembling, processing, and finding data, files and formats must be standardised. Method Selection Suite is an example of a software solution that can homogenise data, and store it in a centralised, easily accessible database.

These chemically intelligent databases contain chemical context (i.e., structures, metadata, methods, etc.), connect data to the original experiments for simplified review and verification, and enable reproducible research. Live analytical and chemical information in these centralised databases can be easily searched by structure, spectra, or text-based queries, providing information about the origin and details supporting the confidence or validity of experiments. These archives of carefully curated knowledge give scientists access to all pertinent information at their fingertips - empowering them to gain new insights into their analytical data and make confident, informed decisions.

Incorporation and implementation of this software tool ensures that data integrity is maintained - increasing the efficiency of data collection, minimising duplication of experiments, and reducing the risk of repeating past mistakes.

### Easier collaboration

Digital transformation is required to connect different operational areas and improve communication and collaboration across teams, facilities, and partners. Tools like Method Selection Suite digitalise data and ensure it is consistent, reproducible, and readily accessible - making collaboration easier and faster. Searchable data assets allow scientists to access real-time data to avoid duplication of experiments and minimise transcription errors. Creating customised reports allows researchers to easily share scientific insights to enable informed decision-making.

## The role of AI and ML

AI has the potential to transform the future of the pharmaceutical industry. As datasets grow in number and diversity, the need for efficient and effective analysis is paramount, highlighting the significance of AI and ML technologies. AI can analyse masses of data, in a fraction of the time of conventional approaches without the risk of human error. These tools can be used to accelerate the prediction and optimisation of experiments, quickly identify anomalies, and empower decision-making.

Adequately engineered, quality data and an infrastructure for facile data management are key factors in the successful implementation of AI in pharmaceutical workflows. The maximal potential of AI can only be achieved if it is properly trained with good-quality datasets. Implementation and integration of appropriate chemistry software tools, like Method Selection Suite, can help create comprehensive and curated databases that can be used to supplement AI tools.

The software prepares data for machine use by homogenising and storing it with its chemical context - further enabling integration into AI initiatives by exporting the data in machine-readable format (i.e., JSON) ready for AI and ML applications.

## Conclusion

Data analysis software tools are increasingly being leveraged to integrate and manage the vast amounts of data generated by pharmaceutical organisations, helping to eliminate siloed systems and empowering data accessibility. With the correct digital tools, collaboration is easier and scientists can preserve and leverage knowledge for future projects, data science, and deeper insights.

Digital transformation offers pharmaceutical organisations great potential. When done right, it should enhance processes to efficiently collect, analyse, and manage data, offer greater accessibility of data, and ensure that value can be extracted from the data to support informed data-driven decision-making.



***Read, Share and Comment on this Article, visit: [www.labmate-online.com](http://www.labmate-online.com)***