Sustainable chromatography: Embracing software for greener methods

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

Chromatographic methods are crucial for separating and analysing complex mixtures and are widely used across industrial R&D - from pharmaceuticals to environmental science. With such a range of potential applications, these methods provide insights that are essential for quality control, and research and development. Although chromatography techniques are indispensable in modern laboratories, they typically have a large environmental footprint.

As the push for sustainability intensifies across all sectors, chromatography seems to be at the forefront of efforts. Although certain levels of waste are unavoidable and there are several challenges in making chromatographic processes greener, sustainability can be improved without compromising operational efficiency and accuracy using readily available software tools.

Adopting green chemistry principles for more sustainable chromatography

The 12 principles of green chemistry formulated by Paul Anastas and John Warner [1], aim to minimise the environmental impact of chemical processes. While green chemistry offers numerous benefits for sustainability and environmental protection, it also faces several challenges such as economic constraints, regulatory issues, technical challenges, and scalability, among others, that must be addressed for broader adoption and effective implementation.

Green chemistry principles inspire the concept of green chromatography - shifting existing practices to minimise the environmental impact of chromatographic processes. Adapting green chemistry principles to chromatography involves several strategies, including but not limited to, solvent reduction and replacement, improving energy efficiency through the design of more sustainable workflows, and minimising waste with in silico experiments. Chemistry software plays a crucial role in overcoming some of the challenges faced in the implementation of green chromatography practices. Software tools offer predictions and can simulate methods so they can be optimised with fewer experiments - supporting greener practices and allowing for smarter decision-making.

Leveraging software tools for sustainable chromatography

Chemistry experiments inevitably produce waste. The 'greenest' experiments are those run on a computer. The sustainability of chromatographic experiments can be enhanced using appropriate software solutions. These tools can also be used to design and optimise methods that adhere to green chemistry principles.

Avoid unnecessary experiments with predictive technology

Understanding the physicochemical properties of a molecule can help better understand its likely behaviour, allowing methods to be created and refined without trial-and-error experimentation. Prediction software like ACD/Labs' PhysChem Suite is a computational approach that uses quantitative structure-property relationship (QSPR) calculations and complex algorithms to predict physicochemical properties like logP, logD, pKa, and more. Additionally, Method Selection Suite, an analytical prediction and optimisation software is equipped with Quality by Design (QbD) tools such as column selection, column comparison, and pH selection which can be used to predict a better starting point for method development.

These tools help scientists take a systematic and rational approach to quickly identify and select optimal chromatographic parameters (e.g., pH or solvent) - reducing the number of runs necessary to achieve the optimal method, thereby minimising waste and conserving resources.

Reduce waste and save time with in silico modelling to optimise chromatographic simulations

ACD/Labs' expert method development software, AutoChrom®, allows users to optimise chromatographic conditions (like pH, gradient, etc.) using 1D, 2D, or 3D models for better peak separation. The software ranks screened experiments by different mathematical parameters, helping scientists quickly select parameters that best meet their defined success criteria (k', run time, resolution, and peak relevance). By fine-tuning these parameters in silico, scientists can generate better methods with fewer injections. This reduces instrument and column wear per method, and saves time, energy, and resources required to develop efficient and robust separations.

Enhance data management - Reduce Duplicated Experiments, Preserve Knowledge, and Make Informed Data-Driven Decisions Faster

Typically, labs are multi-instrument and multi-vendor with masses of unstructured and unharmonised siloed data. This poses several challenges, including increased susceptibility to error, and loss of data that leads to duplication of experiments. Effective data integration and management is crucial for more sustainable R&D.

Vendor-neutral and platform-agnostic tools like Method Selection Suite and AutoChrom, provide a standardised solution to capture, process, and analyse multiple file formats and data types into a single standardised data format, within a single interface. Having standardised files and formats reduces the time scientists spend assembling and processing data. Furthermore, the creation of centralised and easily searchable databases containing live analytical and chemical information (i.e., structures, metadata, methods, etc.) gives scientists access to all pertinent information so they can make informed data-driven decisions. These chemically intelligent databases connect data to original experiments for simplified review and verification and ensure that knowledge is preserved and leveraged for reproducible research.

The potential of artificial intelligence (AI) to improve sustainability

The quality of data is a key driver in maximising the potential of AI. Good quality datasets should be homogenised, comprehensive, and prepared for further use by advanced analytical tools (such as data science, AI, or ML). The carefully curated databases created with ACD/Labs' Spectrus applications supplement AI, as the data can be exported in machine readable formats (i.e., JSON), ready for integration into AI and ML applications.

As the number and diversity of datasets increases, so does the need for efficient and effective data analysis. Having data that is ready for use by advanced analytical tools to analyse collated data and create predictive models is necessary to accelerate the prediction and optimisation of in silico experiments.

Advancing sustainability in analytical labs through green chromatography

As sustainability is increasingly prioritised, the adoption of green chemistry principles is essential. As chromatography remains a critical analytical tool, adopting green chromatography practices is crucial to minimising the environmental impact of analytical labs. Despite the inherent challenges, sustainable practices can be integrated without sacrificing efficiency and accuracy. Leveraging enhanced software tools like predictive technology and in silico modelling support green chromatography principles - allowing scientists to conduct fewer experiments thus reducing waste and saving resources. Integration of these software tools into workflows and laboratory processes support and streamline effective data management and ensure that data is prepared for further use by AI or ML tools. This ensures that scientists have access to comprehensive and historical data across their organisations so they can manage, analyse, and extract relevant insights from this data, while minimising duplication of experiments and preserving knowledge. By embracing green chromatography, scientists can continue to achieve high-quality results while contributing to a more sustainable future.

References

1. Anastas, P. T.; Warner, J. C. (1998). Green Chemistry: Theory and Practice. Oxford University Press.