The future of chromatography: How AI and automation are driving laboratory efficiency and decision-making

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The pressure on labs to perform has never been greater. Recent reports show that 60% of lab professionals are experiencing significant downtime due to equipment failures, missed calibration schedules and challenges in locating critical lab assets, highlighting the urgent need for smarter, more connected lab infrastructure. Compounding the challenge, 64% of labs have already implemented cost-cutting measures across Europe, with many also coming up against severe budget constraints and staff reductions.

However, balancing the mounting financial and human resource pressure with client expectations, regulatory demands and the need for faster turnaround times isn't easy. So how can labs improve efficiency and productivity while also ensuring accuracy and compliance? The answer is the application of advanced automation tools, including robots, and artificial intelligence (AI).

The concept – getting smart systems to carry out tasks with minimal direct human intervention – is straightforward; turning it into a reality requires a good understanding of the available technologies and a clearly defined set of objectives. For the best results, it's also important to be able to access siloed data and implement workflows capable of operating across a range of tools.

Turning concepts into reality

In the field of chromatography, collaborative robots, or 'cobots,' are transforming efficiency and precision. These advanced machines are engineered to work alongside human operators, enhancing their capabilities by taking on repetitive, time-consuming tasks.

The ability of cobots to execute complex analytical protocols that demand a high degree of accuracy and consistency enhances the reliability and precision of the processes. This is particularly critical in the pharmaceutical industry, where accuracy is paramount to ensure the safety and efficacy of products.

Also, by performing routine and labour-intensive tasks, cobots enable labs to process a higher volume of work, without compromising on quality, freeing up human operators to focus on more valuable scientific and problem-solving tasks.

Cobots can also provide economic benefits as the efficiencies gained from their use, and the consequent reduction in the need for manual labour, can result in significant cost savings. Their adaptability and flexibility – they can be easily reprogrammed and repurposed – enables them to seamlessly integrate into a variety of chromatography workflows, adapting as the demands of the industry evolve.

The power of AI

AI is also becoming an integral tool in chromatographic and mass spectrometric (MS) analysis, particularly in the fields of biopharmaceutical development and drug discovery. Its application not only enhances data processing, interpretation, and decision-making processes, it also makes them more efficient and accurate.

For example, AI-powered systems can now handle routine tasks, such as sample processing, data analysis and report generation, while also reducing the risk of human error, leading to more reliable results. Importantly, it frees up lab staff to focus on higher-value tasks that support innovation and value creation.

Ensuring peak performance

Increasing peak detection and quantification levels are one of the key areas where AI can make a substantial impact. Machine learning algorithms can be trained to

accurately identify and differentiate between peaks, even in complex chromatograms where peaks can co-elute.

This is further enhanced by AI's ability to optimise integration parameters, such as baseline correction and peak width, ensuring more accurate quantification results. It can also extract additional information from chromatography data, such as peak area, height and retention time, which further refines the accuracy of quantifications.

A collaborative environment

It's very hard to extract the maximum value from siloed data, which can occur when there is insufficient integration between departments, systems, or applications. This is particularly prevalent in industries that use a diverse range of data sources and proprietary technology formats spread across a number of geographical locations. As a result, there is a concerted drive to move away from vendor specific/proprietary technologies.

The Allotrope Foundation, an international consortium of pharmaceutical, biopharmaceutical, and other scientific research-intensive industries, is involved in breaking down these silos to enable seamless data integration. Its open-access data initiatives aim to create a more collaborative environment for data sharing and integration, particularly within the scientific community.

The foundation continues to promote the adoption of FAIR (Findable, Accessible, Interoperable, Reusable) data principles. By developing universal data formats and ontologies, Allotrope enables laboratories to enhance data integrity, improve quality, and enable the ability to provide real-time regulatory compliance – ultimately facilitating faster, more informed decision-making.

Through its work, Allotrope aims to make the intelligent analytical laboratory a reality – an automated environment where data, methods and hardware components are seamlessly shared among disparate platforms, and data integrity is built-in by design.

Workflow simplification

Scientific workflow systems have become a necessary tool for many applications, enabling the composition and execution of complex analysis on distributed resources. This is especially important as lab instruments and associated software can often be selected without fully understanding how and whether those instruments can be connected into an overall data and workflow ecosystem.

Step-by-step software guidance can therefore be very effective as it can help labs navigate complex workflows by providing clear instructions and automation for tasks, creating detailed model documentation, and streamlining data analysis. This guidance not only reduces the burden on scientists, it also improves reproducibility and supports communication and interoperability in scientific research.

SwissCAT+ on the EPFL Campus in Lausanne, Switzerland (SwissCAT+) is a new infrastructure project that offers a unique integrated technology platform for accelerating discoveries in sustainable catalytic technologies. It combines automated and high-throughput experimentation with advanced computational data analysis.

The company is collaborating with Agilent Technologies on a project to create a fully autonomous laboratory for the discovery, development, and optimisation of sustainable catalytic processes. The aim is to combine the OpenLab CDS system instrumentation and expertise with the SwissCAT+ platform to create a fully automated laboratory environment – one where robotic arms and cobots are seamlessly executing workflows.

A faster, more efficient future

Lab processes are already being transformed by the integration of automation and AI, which are increasingly being used in a multitude of areas in labs such as handling repetitive tasks and high-throughput screening, data analysis, process optimisation, and the design of new analytical methods.

This is enhancing efficiencies and increasing the accuracy of analytical processes, enabling new discoveries and advances across a variety of disciplines including drug discovery and food safety amongst many other domains.

The concept of the 'lights out' laboratory, where operations, including processes and data analysis, are largely or completely managed by automated systems with minimal or no human presence required, is becoming a reality. The power of AI and tech stacks, such as machine learning, cloud computing, and robotics, is revolutionising how labs operate, enhancing competitiveness and bottom-line performance.

Labs today are expected to deliver faster, more accurate results with fewer resources. With advanced automation, collaborative robotics, and AI-driven insights, labs can not only meet these rising expectations – but also exceed them.

About the author

John Beary is Associate Vice President of Product Marketing in Agilent's Productivity Solutions Division. With over 20 years of experience in laboratory instrumentation and data management, he has worked across a wide range of life sciences and applied markets globally. John holds a degree in Industrial Chemistry from the University of Limerick and earned his Masters in Business Administration from Henley Management College, UK, in 2011. His academic background, combined with his practical experience, equips him with a unique blend of technical knowledge and business acumen.