Digital Transformation of the Mass Spectrometry Laboratory

Toshinobu Yanagisawa[A], Koji Ono[A], Takeshi Yoshida[A], Yuji Maeda[A], Kyoko Watanabe[A], Takashi Inoue[A] and Scott Kuzdzal[B]
[A]Shimadzu Corporation, Kyoto, Japan, [B]Shimadzu Scientific Instruments, Columbia, MD, USA

1. Introduction

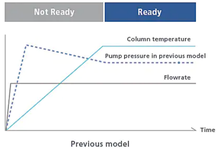
Applications of artificial intelligence (AI) are reshaping entire industries, including transportation and telecommunications, with innovations that improve how humans and technology can work together. The scientific research laboratory is no exception. AI has opened the door for the lab of the future and introduced transformative changes in how scientists approach research. Below we share examples of AI, IoT and M2M functionality designed to improve remote laboratory operation and define a new concept of '**ANALYTICAL INTELLIGENCE'.**

ANALYTICAL INTELLIGENCE is defined as...

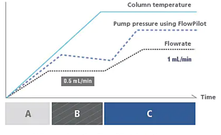
- ✓ Automated support functions utilizing digital technology, such as M2M, IoT, and Artificial Intelligence (AI), that enable higher productivity and maximum reliability.
- ✓ Allows a system to monitor and diagnose itself, handle any issues during data acquisition without user input, and automatically behave as if it were operated by an expert.
- ✓ Supports the acquisition of high-quality, reproducible data regardless of an operator's skill level for both routine and demanding applications.

2.1 Smarter, Self-protecting LC Systems

UHPLC columns can be damaged by sudden pump starts and extreme gradient changes, especially true with polymeric packings. Integrating an automated, smart flow control program like the one illustrated below increases the flow rate gradually to the method set point according to the status of the column oven, extending the life of your HPLC columns.



Previous model



When using the FlowPilot function

FlowPilot (Patent pending)

The pump controls the flowrate based on oven temperature

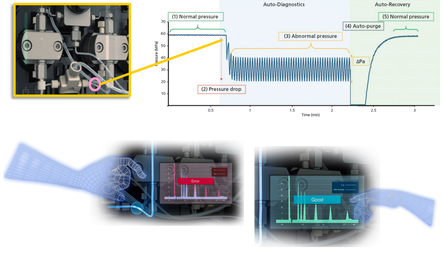
- A Gradually increasing the flowrate
- B Maintaining the flowrate at half the method flowrate
- C When the oven temperature reaches the configured temperature, the flowrate is gradually increased up to the configured flowrate

2.2 Remote, Real-time Monitoring

A mobile phase monitor system enables real-time, gravimetric monitoring of mobile phase levels to ensure maximum uptime. Mobile phase or autosampler rinse solution levels can be monitored remotely. The containers can also be checked remotely from a smart device (PC/iOS/Android) to better facilitate remote operation.

2.3 Advanced Self-diagnostics

Flow anomalies such as HPLC air bubbles can cause a drop in the flow rate, resulting in irreproducibility and inaccuracy. Because these events are spurious, they are difficult to predict. AI can detect and correct such adverse events. When the ***Analytical Intelligence*** engine detects an unusual fluctuation, it pauses the batch, applies a corrective purge and restarts the run—all automatically.



Auto-diagnosis and fully automated recovery of a flow anomaly (air bubble) using advanced, remote AI features.

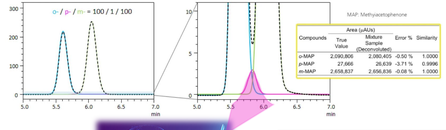
2.4 Remote Control Access

New AI and IoT technology allows you to remotely monitor, control, and analyze your instruments, and view results using a web browser / VPN. Researchers can monitor the analysis progress remotely and check the report of the analysis results. Furthermore, all lab instruments are on a single, unified lab informatics platform called LabSolutions.

LabSolutions Direct Web monitoring

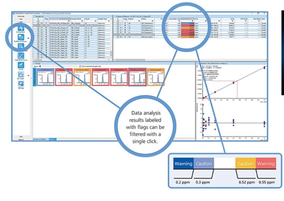
2.5 Intelligent Peak Deconvolution

Intelligent Peak Deconvolution Analysis (i-PDeA) is a data analysis technique that extracts a single peak from co-eluted HPLC peaks and quantitates it by exploiting the differences in spectra between each compound. i-PDeA II enables users to visualize and detect a minor single impurity even when the impurity is co-eluted with an analyte. Advanced i-PDeA II peak deconvolution functionality uses a multivariate curve resolution alternating least squares (MCR-ALS) method to enable qualitative and quantitative analysis of LC peaks not fully separated by the column.



2.6 Automated QA/QC & MS Peak Flagging

Due to increasingly sophisticated automation, large quantities of high-quality mass spectrometer data are obtained day and night. However, checking and analyzing all that data can be extremely time-consuming, which significantly decreases the efficiency of research and investigation work. Therefore, multi-analyte quantitation software for LC-MS/MS and GC-MS helps analyze data more conveniently and more efficiently.



This presentation shows how advanced application of AI, IoT and M2M technologies are resulting in a digital transformation of laboratories and contributing to the implementation of a new, remote working style in labs.

The pandemic has enhanced the need for smarter, remote functionality for laboratory operation. A digital transformation has occurred over the past years, wherein smarter, self-diagnosing and auto-recovering systems have been developed with advanced monitoring (and correcting) capabilities. We have incorporated ANALYTICAL INTELLIGENCE into LC, LCMS and GC platforms and will be continuing to expand remote operation, self-diagnostic / auto recovery functions and smarter M2M capabilities.