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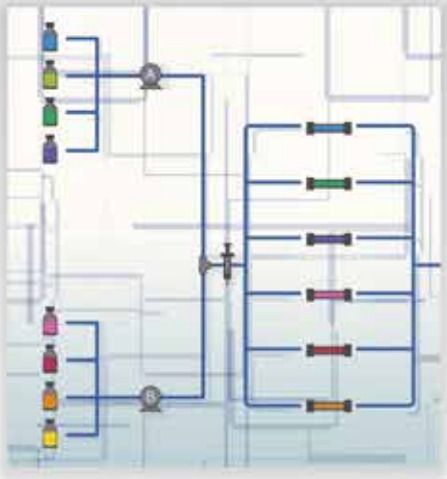
Excellence in Science

SEG-A-149

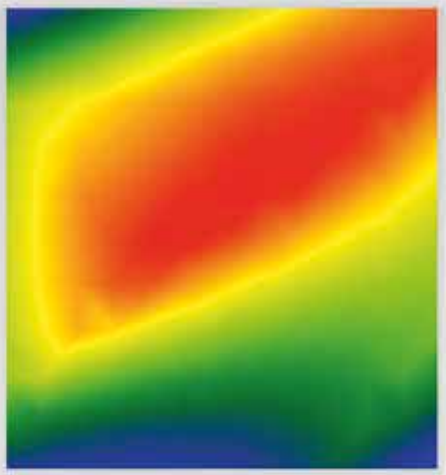
Nexera Method Scouting System – LabSolutions MD

The Fine Art of Method Development

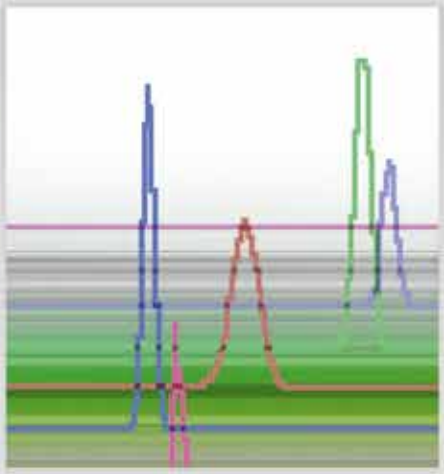
An automated solution following AQbD principles



- Screening -



- Optimization -



- Validation -

Maximizing Efficiency for HPLC Method Development

The design of the new Nexera Method Scouting System is based on the award-winning Nexera Series of ultra-high performance liquid chromatographs (UHPLC). It is equipped with two quaternary solvent pumps, a high-pressure-resistant column switching valve and patented analytical intelligence features to enable quick and reliable column and solvent screening. In combination with LabSolutions MD – a new support software for analytical HPLC method development and optimization that follows Analytical Quality by Design (AQbD) principles using Design of Experiments (DoE) – it provides an all-round solution for efficient and highly effective HPLC method development and implementation.

ANALYTICAL INTELLIGENCE

- 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.

Method Development Workflow according to AQbD principles

Screening
- Column and mobile phase screening
- Experiments to evaluate the most suitable combination of stationary and mobile phase

Optimization
- Computer aided method optimization
- Optimization of gradient conditions, temperature, flow rate, etc. using a design space.

Robustness
- Confirmation of robustness
- Evaluation of the effect of small variations in methods parameters on the chromatographic results

Analytical Quality by Design (AQbD) is recommended by the International Council for Harmonization (ICH) to emphasize rigorous scientific foundation and risk assessment in the development of analytical methods. It comprises a comprehensive evaluation of the analytical conditions without relying on an operator's experience or intuition. AQbD thus increases reliability and enables the efficient development of accurate, robust analytical methods. Using this systematic approach, analysts gain an understanding of the separation, which also enables informed decisions in troubleshooting and continuous improvement of test methods.

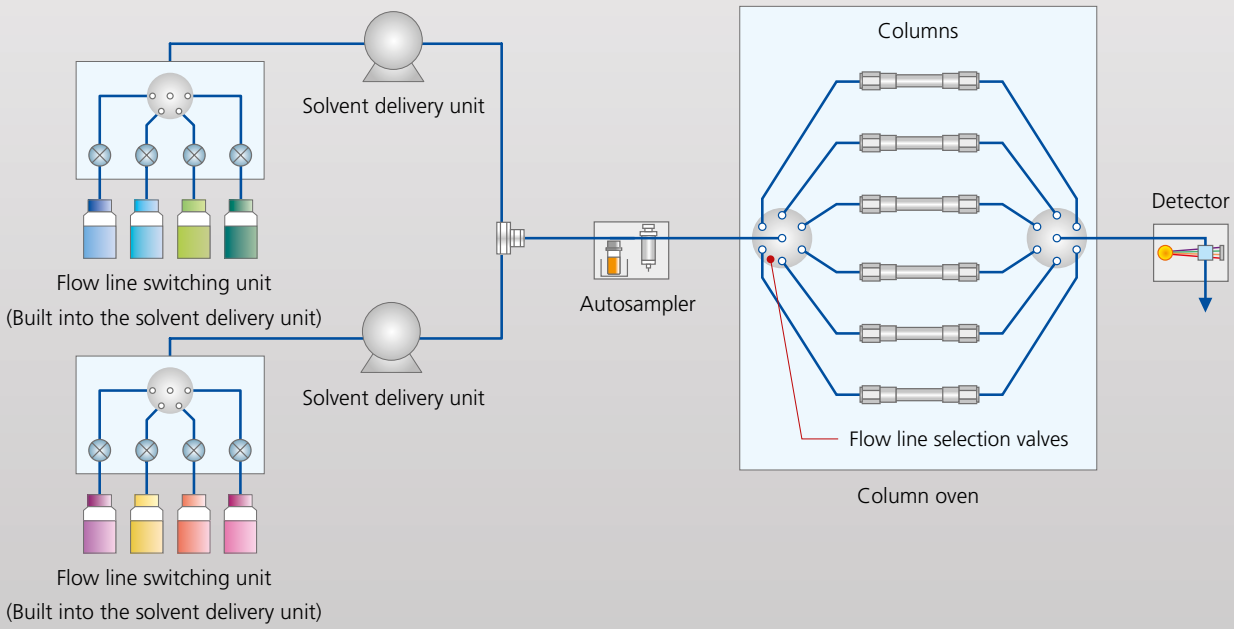
Intuitive operation and maintenance facilitate excellent instrument performance and ensure consistently reliable results.

The Nexera Method Scouting System

The Nexera Method Scouting System is based on the Nexera series UHPLC and its outstanding performance in ultra-high speed analysis. It features stable solvent delivery at ultra-high pressure and excellent injection repeatability, as well as virtually no carry-over. As a result, reliable method scouting data is efficiently produced.

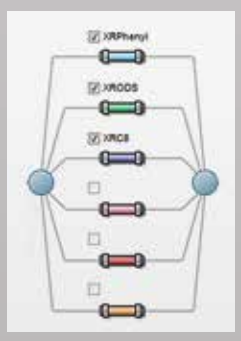
Basic configuration of the Nexera Method Scouting System

The Nexera Method Scouting System provides a choice of six or up-to-12 stationary phases by adopting a high-pressure-resistant column switching valve and a manifold. The two quaternary UHPLC solvent delivery units offer the possibility of sixteen different mobile phase combinations. In addition, the system features an auto-purging function that allows it to automatically flush the lines through the autosampler after a change in mobile phase, for quick and easy system equilibration and a continuous method scouting workflow.



Enabling graphical display of column connections

The column piping is color-coded and interlinked with the graphical user interface. This approach assists with system setup and reduces the risk of error in column placement.



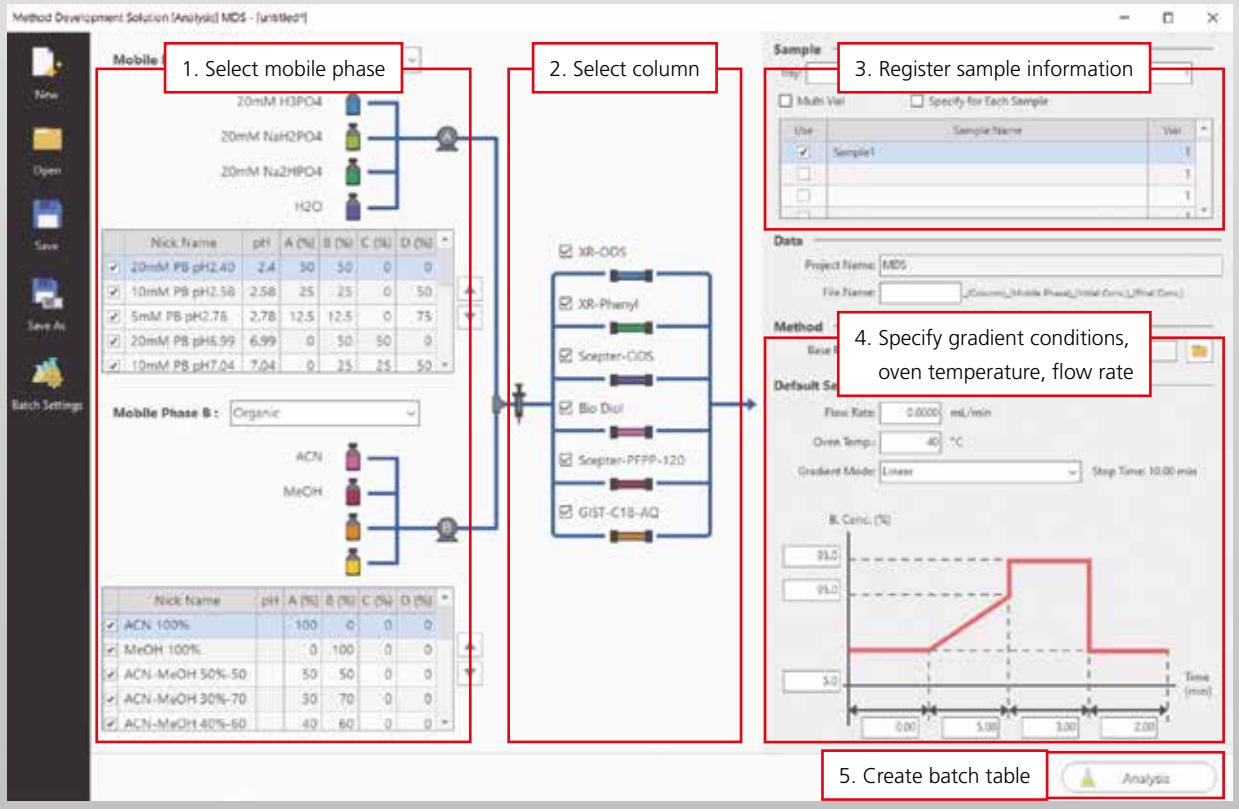
LabSolutions MD –
Method Development Solution Software

AQbD requires efficient data acquisition, and in accordance with the experimental design. Factors which affect analytical results are identified by statistical methods, and the effective range of parameter settings is visualized as a design space. This science and risk-based approach ensures the development of robust, reliable analytical methods without relying on operator experience or intuition.

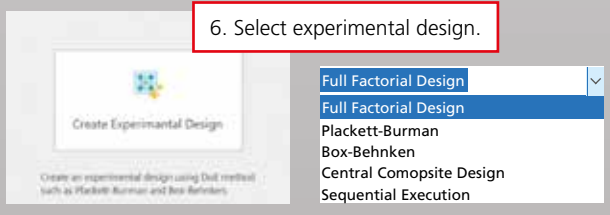
LabSolutions MD allows for automation of the three phases of the method development workflow: screening, optimization and the evaluation of robustness.

Screening Phase

The process of creating a large number of different gradient method files and the corresponding batch table can be completed quickly by simply following steps (1) to (6) in the easy-to-use graphical user interface (GUI), as shown below. Mobile phases and columns to be tested can be selected with a single click, and a comprehensive sequence table including column equilibration and blank runs is generated automatically. This not only improves operational efficiency, but also helps to reduce the risk of human error. The experimental design to be used can also be selected with a single click.

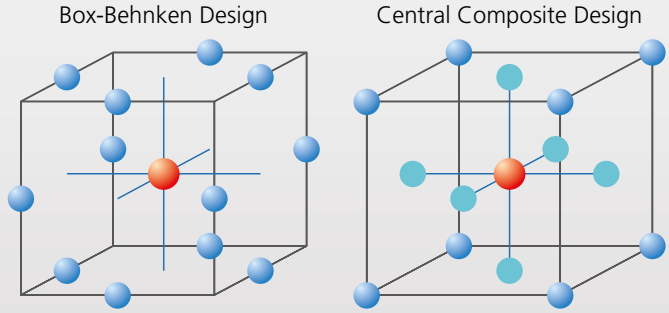


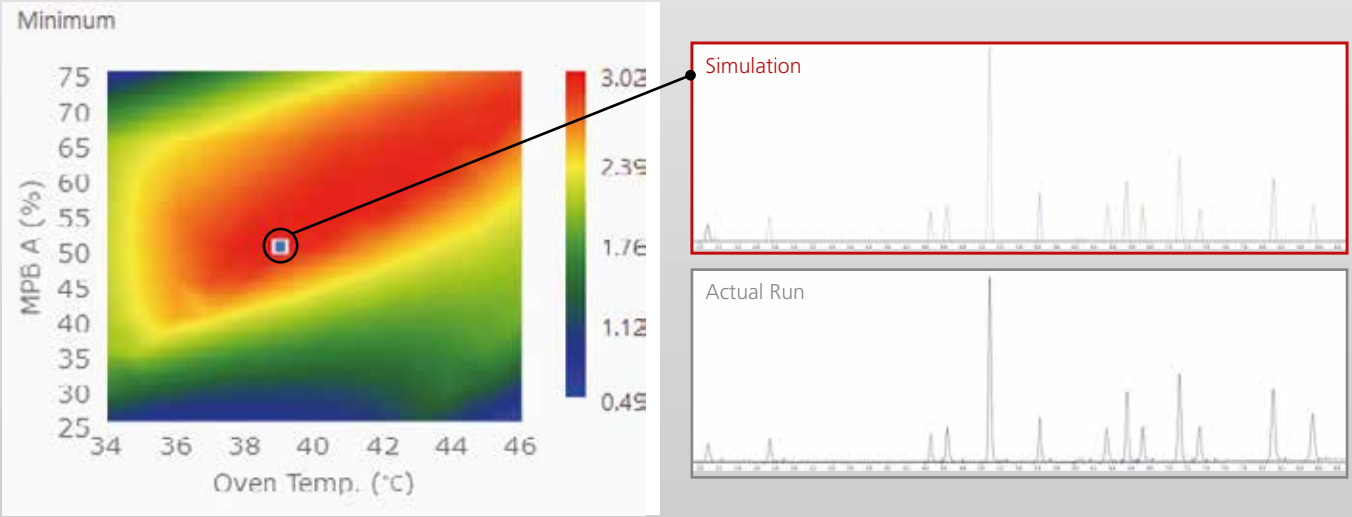
How much each screening parameter affects separation can be confirmed by variance analysis. Identifying the parameters with a large effect on separation can reduce the number of target parameters to be optimized, which enables even more efficient experiments.



Optimization Phase

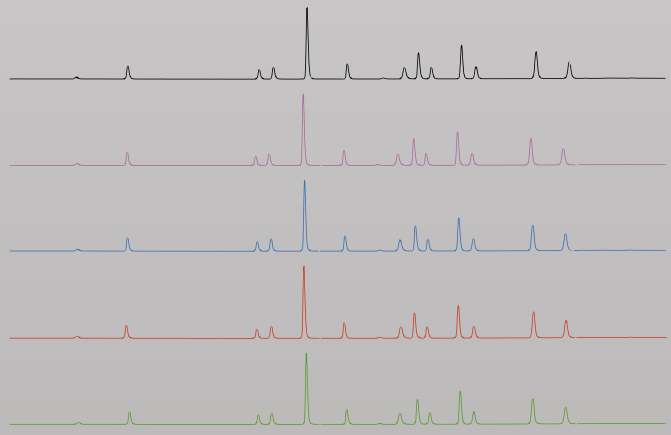
Using Experimental Design for method optimization significantly reduces the number of data points, and consequently the time and effort required. For example, when screening for optimum levels for % organic modifier in the mobile phase, gradient conditions and column oven temperature, full factorial design requires 27 data points (3 × 3 × 3) for optimization. On the other hand, a Box-Behnken design requires 13 points and a Central Composite design requires 15 points to create a design space. From these initial experiments LabSolutions visualizes the factor-response relationship in color coded "heat-maps" that allow identification of optimum separation conditions at a glance. Computer simulation of chromatograms at any given point in the design space allows for confirmation of separation behavior in response to arbitrary changes in analytical conditions, offering prediction of the robustness of the method used.





Validation of Robustness

It is important to validate the robustness of the chosen conditions to evaluate how small changes will affect the chromatographic result, and to ensure reliability of the analytical method. Iterative experimental design automatically generates a batch table for analyzing a small range of variations in each of the parameters that are determined to have a distinct effect on the separation, such as % organic modifier or oven temperature. The resulting chromatograms show whether the chosen variations result in acceptable (or any) changes in retention of the analytes.



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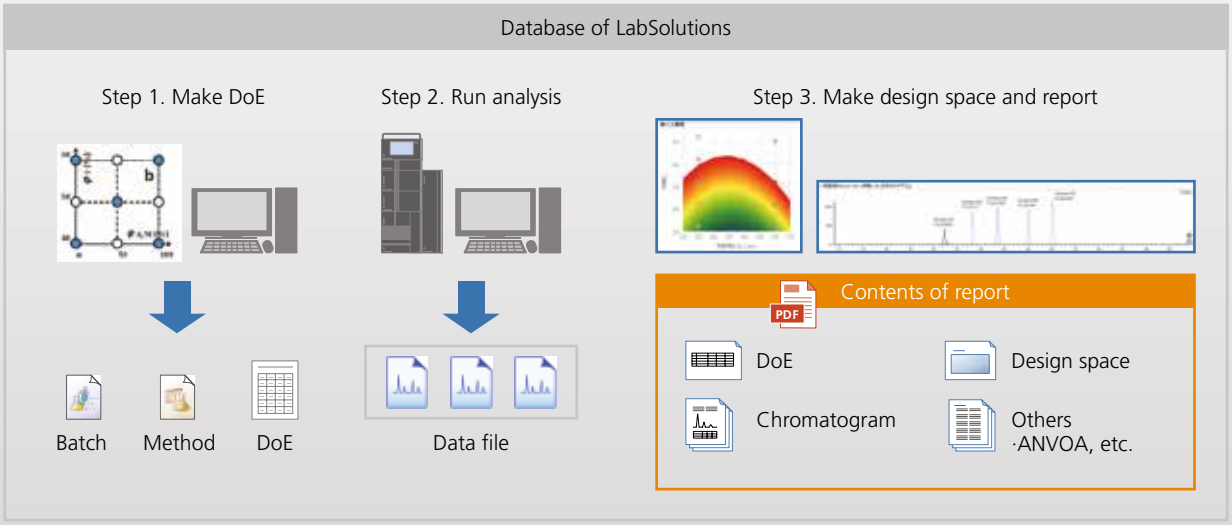
Ensure Data Integrity by Database Management

It is easy to check analysis results using LabSolutions MD because all associated information –the experimental design, design space, chromatograms, etc. – are output in a report. It also ensures data integrity by managing outputted reports together with the corresponding experimental design file, method file, batch file, and data file within a LabSolutions database. Due to the seamless integration of all process steps (including creating an experimental design, acquiring data, and all method development steps in the design space), LabSolutions MD eliminates the need for any time-consuming file importing or exporting steps.



Shimadzu LC column line-up

Excellent stability, selectivity and performance for diverse separation needs

Retention behavior can vary significantly depending on the type of stationary phase. During method development, a variety of columns should be tested to achieve optimum separation. The Shim-pack series of UHPLC columns offers a wide range of different selectivities and available column sizes to enable seamless scale-up from analytical to preparative applications.

Get more information:
https://www.shimadzu.eu/columns-and-consumables

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