SHIMADZU
Excellence in Science

Solution for Efficient Method Development

Effortless Method Development with LabSolutions MD

—Automatic Optimization of Gradient Conditions with AI Algorithm—

ANALYTICAL INTELLIGENCE

Automatic Screening of Mobile Phases and Columns

Mobile phases and columns are automatically switched to find the optimal combination without human intervention.

Automatic Optimization of Gradient Conditions

Gradient conditions that satisfy criteria are automatically explored

Easy-to-Use Software

Easy creation of analysis schedules with various conditions. Chromatograms obtained can be ranked based on separation performance.

Software for Effortless Method Development
# LabSolutions™ MD

Effortless Method Development with LabSolutions MD

LabSolutions MD enables effortless exploration of optimal conditions through each phase of method development, such as screening and optimization. In the screening phase, LabSolutions MD allows selecting mobile phases and columns with a single click and analysis schedules are automatically generated. In the optimization phase, gradient conditions that meet the resolution criteria are automatically explored. This enables anyone to easily find optimal conditions without relying on experience.

Screening Phase

The optimal combination of mobile phases and columns is searched, utilizing parameters such as the pH of aqueous mobile phases, mixture ratios of organic mobile phases, and column types, which have a large effect on resolution and retention time.

Mobile phases ✕ Columns

?

Aqueous   Organic   ✕   Column

Optimal combination is screened
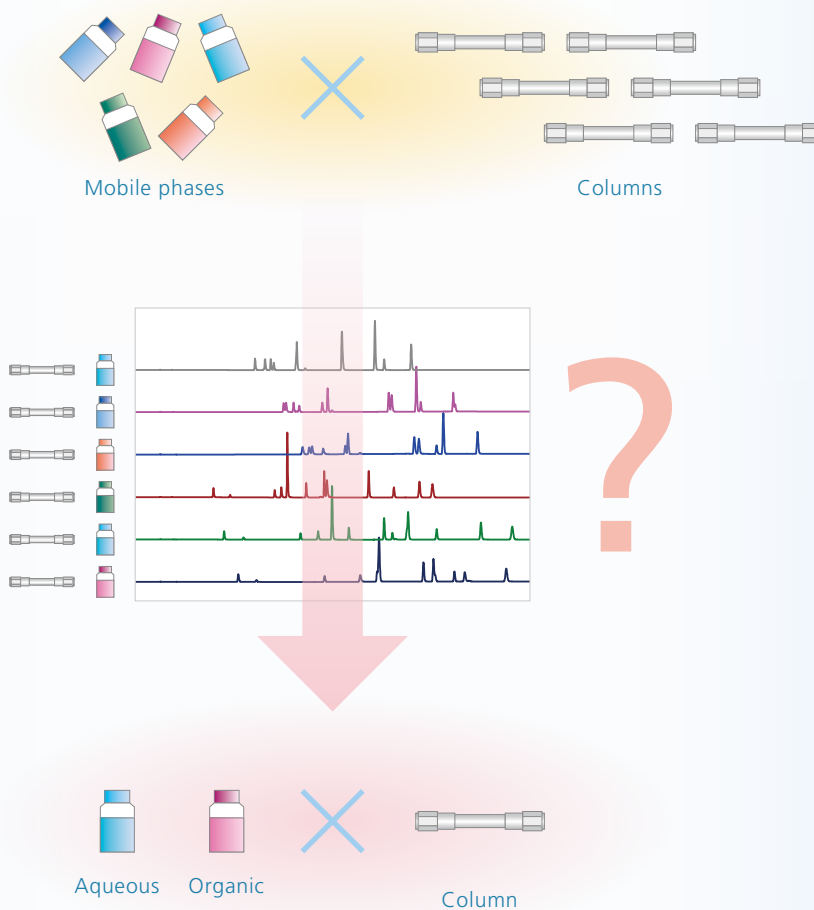
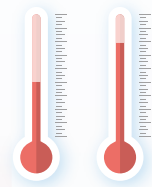## Automatic Screening of Mobile Phases and Columns ——— P.6

Optimization Phase

With the mobile phases and columns screened, LC parameters, such as gradient conditions, column oven temperature, and flow rate, are optimized.
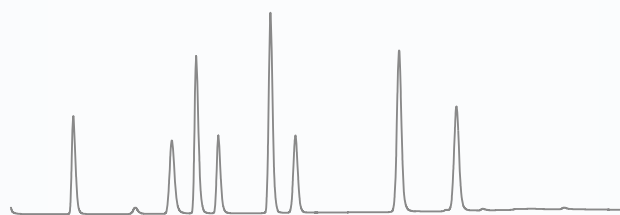
∗∗.∗ ℃

∗.∗ mL/min

Optimize gradient condition

Optimize oven temperature

Optimize flow rate

Chromatogram at optimized condition

Automatic Optimization of Gradient Conditions ——————— P.8

Automatic Screening of Mobile Phases and Columns
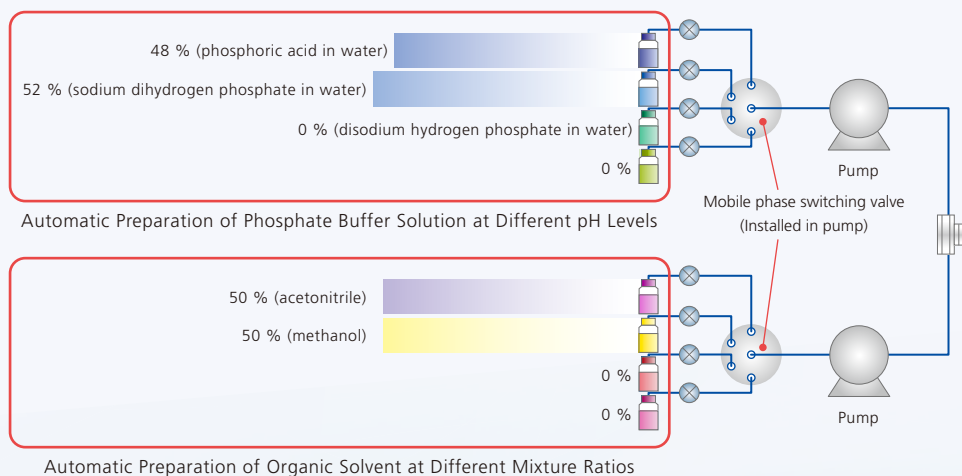
Automation of Mobile Phases and Columns Switching

By installing a switching valve in a pump or column oven, several mobile phases and columns can be automatically switched without manually replacing them.

Mobile phase switching valve
(installed in pump)

Pump

Mobile phase switching valve
(installed in pump)

Pump

Autosampler

Column switching valve

Column

Detector

Column oven
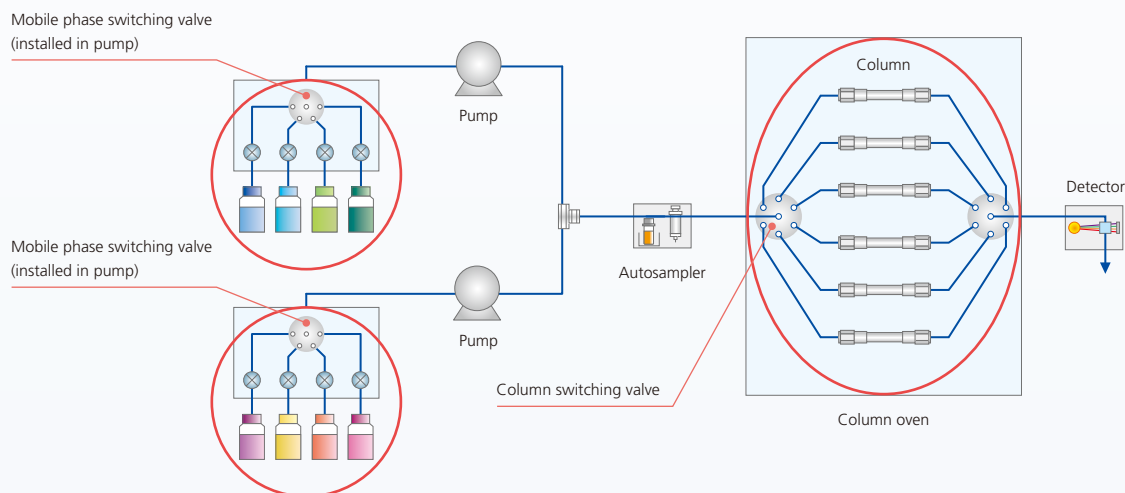
Automatic Mobile Phase and Column Switching

Automation of Mobile Phase Preparation with Mobile Phase Blending Function

The mobile phase blending function can improve the efficiency of mobile phase preparation by automatically preparing mobile phases based on factors such as the user-specified pH level or the mixture ratio of organic mobile phase, with only a few types of mobile phases prepared in advance. This not only greatly reduces the burden of manual preparation but also prevents human errors in blending.

48 % (phosphoric acid in water)

52 % (sodium dihydrogen phosphate in water)

0 % (disodium hydrogen phosphate in water)

0 %

Automatic Preparation of Phosphate Buffer Solution at Different pH Levels

Pump

Mobile phase switching valve
(Installed in pump)

50 % (acetonitrile)

50 % (methanol)

0 %

0 %

Pump

Automatic Preparation of Organic Solvent at Different Mixture Ratios

Automatic Mobile Phase Preparation with Mobile Phase Blending Function

Easy Creation of Analysis Schedules

The process of creating an analysis schedule for screening can be completed quickly by following steps (1) to (6) below. The mobile phases and columns can be selected with a single click and the schedule, including column equilibration, is generated automatically. This not only improves operational efficiency, but also reduces human errors.

The screening system is also equipped with an automatic stop function, which terminates the search when conditions matching the preset criteria are detected.

❶Select mobile phases

▼

❷Select columns

▼

❸Input sample information

▼

❹Create analysis schedule

Quickly Find Optimal Conditions

Because screening generates as many chromatograms as the number of conditions considered, they need to be evaluated to determine the optimal one. If all the chromatograms had to be checked manually, it would take a lot of time.

LabSolutions MD can quickly and easily find optimal conditions using the equation (1) below to quantitatively evaluate the separation status based on each condition.

$$E = P \times (R_1 + R_2 + \ldots R_{P-1}) \ldots \text{(Equation 1)}$$

Evaluation Value (E) is calculated as the number of peaks detected (P) multiplied by the sum of the resolution (R) for all peaks.

Optimal combination of mobile phase and column

Column Nick Name	MPA pH	MPB A (%)	Response Evaluation Value
Scepter-Phenyl-120	6.8	50	546.000
Scepter-C8-120	6.8	0	469.894
GIST-C18-AQ	2.7	0	465.124
GIST-C18-AQ	6.8	50	443.580
Scepter-C8-120	6.8	50	436.241
Scepter-Phenyl-120	2.7	50	419.659
Scepter-C18	2.7	0	419.338
Scepter-C18	6.8	50	396.000
Scepter-C4-300	2.7	0	394.239
Scepter-C18	6.8	100	384.553

Ranking Each Condition
Based on Evaluation Value
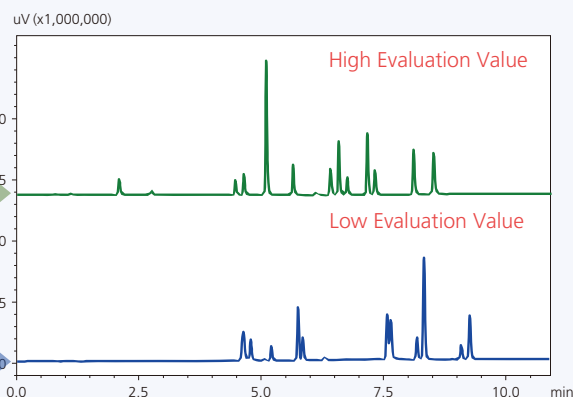
Comparison of Chromatograms
at High and Low Evaluation Value

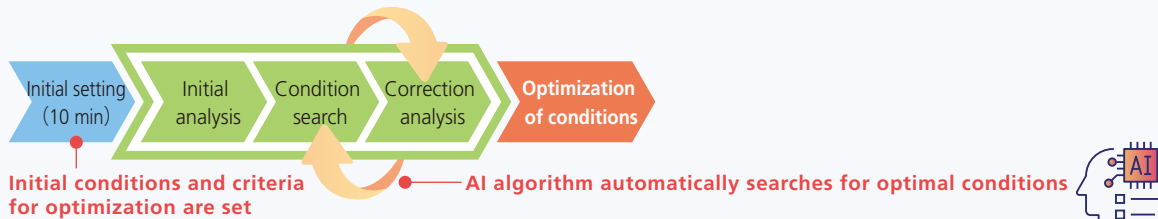# Automatic Optimization of Gradient Conditions

AI Algorithm Automatically Optimizes Gradient Conditions

LabSolutions MD has a unique AI algorithm for automatic optimization of gradient conditions. By setting resolution criteria, it automatically searches for the gradient conditions that meet the criteria. In a normal method development workflow, human intervention is required for creating analysis schedules and performing data analysis. In contrast, LabSolutions MD automatically generates and registers improved gradient conditions based on the data obtained, enabling exploration and optimization of gradient conditions without human intervention.
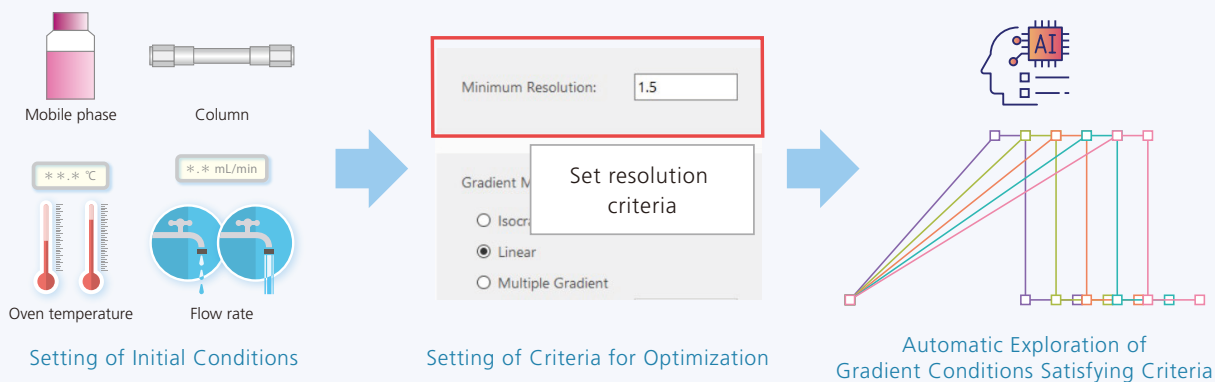
■ Normal Workflow of Gradient Optimization

Creation of analysis schedule (30 min) → Analysis → Data processing → Re-creation of analysis schedule (30 min) → Analysis → Data processing ⋯ Optimization of conditions

Intervention by human   **Intervention by human**   **Intervention by human**
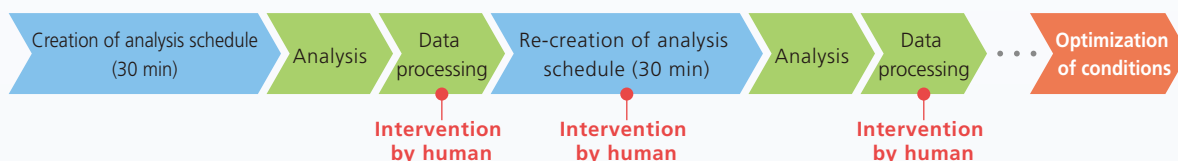
■ Automated Workflow of Gradient Optimization with LabSolutions MD

Initial setting (10 min) → Initial analysis → Condition search → Correction analysis → Optimization of conditions

Initial conditions and criteria for optimization are set   **AI algorithm automatically searches for optimal conditions**

Setting of Resolution Criteria for Automatic Optimization

By setting initial conditions of gradient curves and resolution criteria, the gradient conditions that meet the criteria can be automatically searched. With AI-driven automatic exploration, anyone can search for the conditions regardless of their chromatography experience.

Mobile phase   Column

Oven temperature   Flow rate

Minimum Resolution: 1.5

Set resolution criteria

Gradient M
○ Isocra
● Linear
○ Multiple Gradient

Setting of Initial Conditions   **Setting of Criteria for Optimization**   **Automatic Exploration of Gradient Conditions Satisfying Criteria**

Click the icon to access the Technical Report.▼

Technical Report

Capable of Selecting the Optimal Mode for the Application

There are two ways to perform automatic optimization of gradient conditions: all-peak resolution mode and specified peak resolution mode. They can be applied separately to suit the application.

All-peak resolution mode

In this mode, the software searches for conditions satisfying the criteria for resolution configured for all the peaks detected. It is used when all the peaks must be resolved.
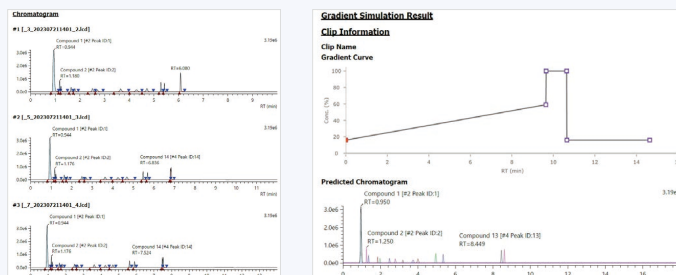

Automatic Gradient Optimization by AI (Catechin and Theaflavin)
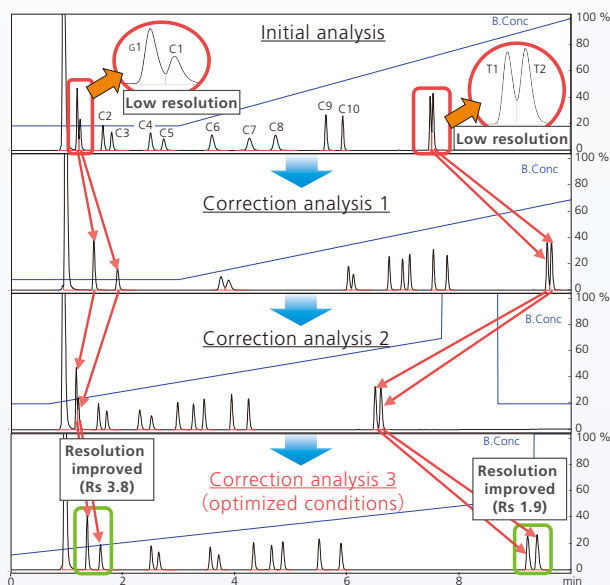
Application

Specified peak resolution mode (NEW)

In this mode, the software searches for conditions satisfying the criteria for resolution configured for any peaks selected. It is used when specific peaks must be separated.

Automatic Exploration of Gradient Conditions Using AI (the Pharmaceutical Montelukast)
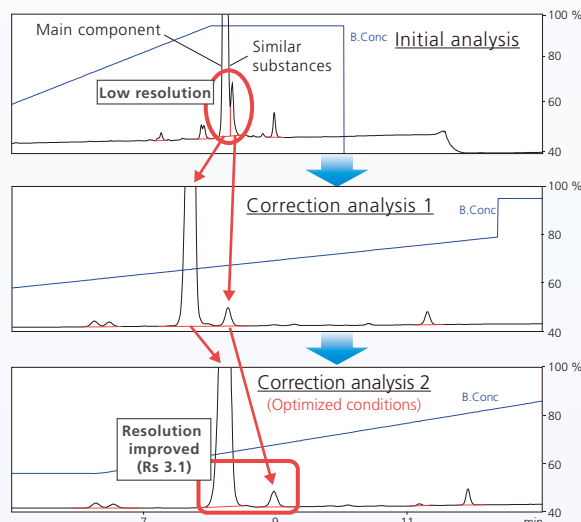
Application

During the process of optimizing gradient conditions, all of the chromatograms and gradient conditions obtained during the exploration are also saved. These results can be utilized if needed. Also, a report with these results can be output (as shown in the figure below).

Automatic Gradient Optimization by AI (Catechin and Theaflavin)

LabSolutions MD not only offers automatic optimization of gradient conditions but also supports the efficient creation of analysis schedules to optimize column oven temperature and flow rate. For instance, in the case of column oven temperature, by simply inputting the central value (40°C), step size (in 5°C increments), and the number of steps, a schedule that includes column equilibration is generated automatically.

Supporting Various System Configurations

LabSolutions MD is compatible with the Nexera series, i-Series, and supercritical fluid chromatography (SFC). It is compatible with all LC detectors (UV, PDA, RID, RF, ELSD, and (AD) and, when used in combination with PDA and single quad LCMS, enables more accurate data analysis.

Nexera™ Series

These ultra-high-performance liquid chromatographs have a maximum pressure capacity of 130 MPa and support up to 8 types of mobile phases and 12 types of columns.
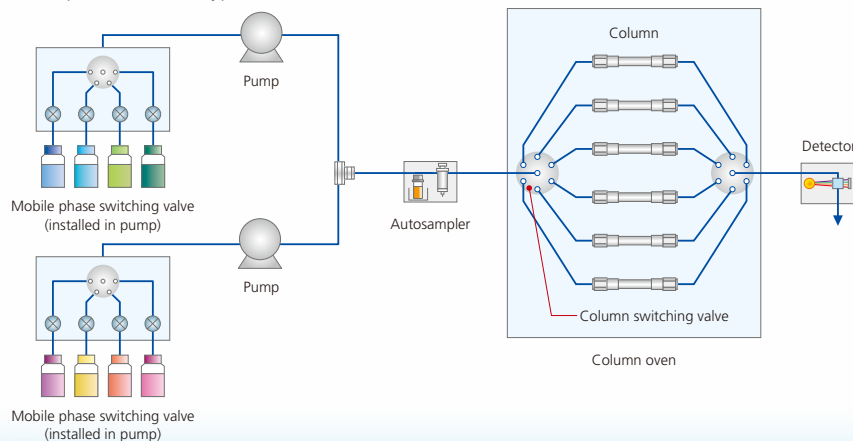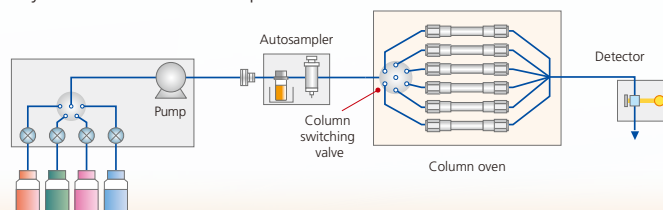

Nexera UC
UHPLC/SFC Switching System

By switching between LC and SFC in a single system, the optimum conditions can be determined more efficiently. In SFC analysis, mobile phases can be automatically switched up to seven lines.
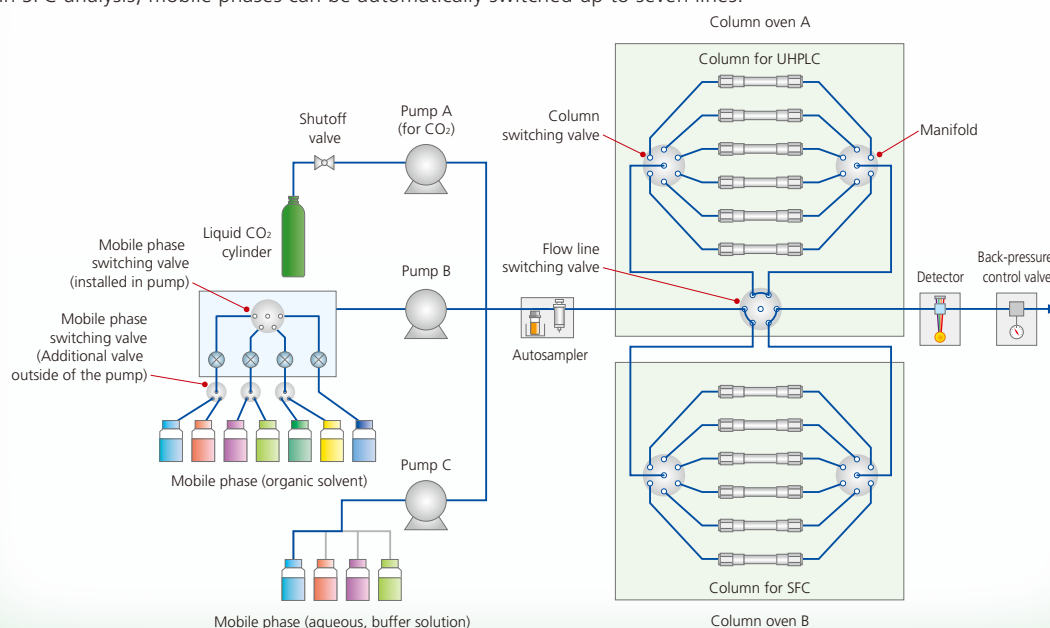
i-Series

This is an integrated LC system with a maximum pressure resistance of 70 MPa.

Combine with a Mass Spectrometer for Even More Productivity
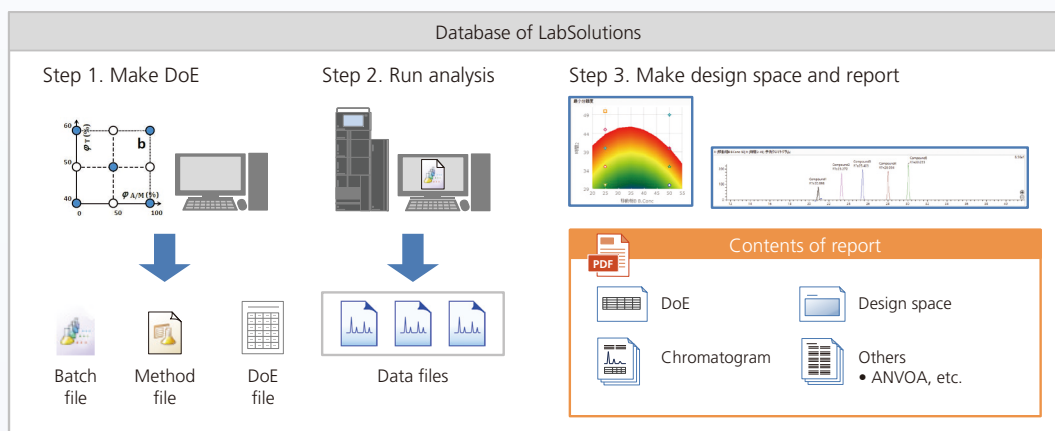

Single Quadrupole
Mass Spectrometer

Triple Quadrupole
Mass Spectrometer

With LabSolutions MD, peak tracking is possible using scan data from single quadrupole and triple quadrupole mass spectrometers.

By taking advantage of the excellent selectivity of mass spectrometers, analysis method development for chromatograms with many eluted peaks can be carried out more efficiently.

Ensure Data Integrity by Database Management

LabSolutions MD ensures data integrity by managing all the data in a single database of LabSolutions. This database also enables seamless operation, from creating an analysis schedule and running the analysis to data processing using design space, and eliminates time-consuming file importing or exporting steps.

Database of LabSolutions

Step 1. Make DoE

Step 2. Run analysis

Step 3. Make design space and report

Batch file   Method file   DoE file

Data files

Contents of report

DoE   Design space

Chromatogram   Others
• ANVOA, etc.

Column Kits for Reverse-Phase Analysis Method Development

C18 (ODS) columns have different resolution properties. A variety of C18 columns are included in the Shimadzu Shim-pack series of LC columns. Shimadzu has bundled columns with different resolution characteristics into kits to make selecting candidate columns easier. These column kits are intended for reversed-phase analysis method development applications. In combination with LabSolutions MD, they enable more efficient column selection.

Kit types	HPLC	UHPLC	HPLC (LC-MS)	UHPLC (LC-MS)
① L1 Kit for HPLC (C18 only)	◎			
② L1Kit for HPLC / UHPLC (LC-MS) (C18 only)	◎	◎	◎	◎
③ Maximum Selectivity RP Kit for HPLC / UHPLC Type A	◎	◎	○	○
④ Maximum Selectivity RP Kit for HPLC / UHPLC Type B	◎	◎	○	○
⑤ Maximum Selectivity RP Kit for HPLC / UHPLC (LC-MS)	○	○	◎	◎

*These column kits do not guarantee the appropriate separation for customer analyses.

◎: Most suitable
○: Compatible

Brochure

List of LabSolutions MD Applications

Efficient Method Development on Pharmaceutical Impurities Using Single Quadrupole Mass Spectrometer ▶

Efficient Method Development through Design Space Evaluation on Different Brands of Columns ▶

Efficient Method Development by Automated pH Screening with LabSolutions MD ▶

Efficient Method Development Based on Analytical Quality by Design with LabSolutions MD Software ▶

Efficient Method Development of Oligonucleotides by Reversed-Phase Ion-Pair Chromatography ▶

Efficient Method Development on Pharmaceutical Impurities Based on Analytical Quality by Design ▶

Efficient Method Development of Monoclonal Antibody Size Variants by Size Exclusion Chromatography ▶

LabSolutions MD Package Contents

Method Development Solution license set

Installation CD (electronic operation guide and technical explanation)

Click the icon to access the brochure of LabSolutions MD-
Solution for Method Development and Analytical Quality by Design-▼

Brochure

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