

Solution for Efficient Method Development

Effortless Method Development with LabSolutions MD

—Automatic Optimization of Gradient Conditions with AI Algorithm—



The screenshot displays the LabSolutions MD software interface. It includes a 'Mobile Phase A' configuration table, a 'Mobile Phase B' configuration table, a 'Gradient' plot showing the percentage of Mobile Phase B over time, and a 'Chromatogram' showing the resulting peaks. The chromatogram includes a table of peak data.

Peak Name	pH	A (%)	B (%)	C (%)	D (%)
FB pH7.7	7.7	14	24	0	60
FB pH6.8	6.8	0	24	76	0

AcN Name	pH	A (%)	B (%)	C (%)	D (%)
ACN 100%	100	0	0	0	100
MeOH 100%	0	100	0	0	0
ACN-MeOH 50%-50	50	50	0	0	0
ACN-MeOH 30%-70	30	70	0	0	0
ACN-MeOH 40%-60	40	60	0	0	0

Time (min)	Conc. (%)
0.4	38
1.4	58
2	60
4.2	80
4.21	80
5.2	80
5.21	30
5.4	20

Compound Name	Ret. Time	Peak Width	Area
Compound 1 (PI Peak 01)	2.787	0.011	20.881
Compound 2 (PI Peak 02)	1.401	0.011	4.217
Compound 3 (PI Peak 03)	1.401	0.048	20.881
Compound 4 (PI Peak 04)	2.574	0.062	20.881
Compound 5 (PI Peak 05)	2.719	0.022	8.729
Compound 6 (PI Peak 06)	4.187	0.022	8.729



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

The screenshot displays the LabSolutions MD software interface, which is used for method development in chromatography. The interface is divided into several key sections:

- Method Development Solution (Analysis) MDS - (unsaved):** The main workspace showing the method configuration.
 - Mobile Phase A:** Set to Phosphate Buffer. Components include 50mmol/L Phosphoric acid Water, 50mmol/L Sodium dihydrogen phosphate, 50mmol/L Disodium hydrogen phosphate, and Water.
 - Mobile Phase B:** Set to Organic. Components include ACN and MeOH.
 - Columns:** A list of columns including Scepter-C18-120, Scepter-CB-120, Scepter-C4-300, Scepter-Phenyl-120, Scepter-PPFP-120, and GIST-C18-AQ.
 - Sample:** Configuration for sample type, volume, and multi-vial options.
 - Method:** Settings for flow rate (0.000 mL/min), oven temperature (40 °C), and gradient mode (Linear).
 - Default Settings:** Includes flow rate, oven temperature, and gradient mode.
 - Gradient Curve:** A graph showing the percentage of Mobile Phase B over time. The curve starts at 30% at 0 minutes, increases to 95% at 4.21 minutes, and then drops back to 30% at 5.21 minutes.
 - Measured Chromatogram:** Shows a single sharp peak at 2.904 minutes, identified as Compound 3 [11 Peak ID:3].
- Progress:** A section indicating the status of various steps: Initial Analysis (Completed), Initial Postion (Completed), and Initial Postion (Completed).
- Tables:**
 - Gradient Curve Table:**

Time (min)	Conc. (%)
0	30
0.4	30
1.4	50
2	50
4.2	80
4.21	95
5.2	95
5.21	30
5.8	30
 - Chromatogram Table:**

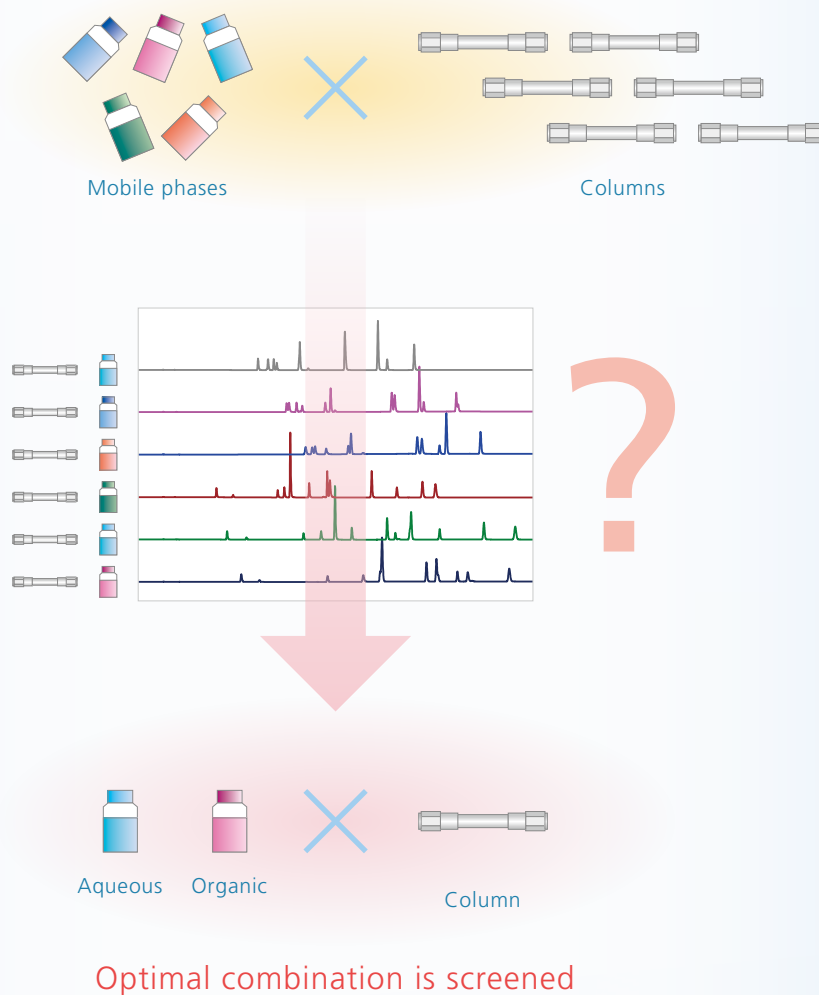
#	Compound Name	Ret. Time	Peak Width	Resolut
1	Compound 1 [11 Peak ID:1]	0.189	0.021	20.891
2	Compound 2 [11 Peak ID:2]	1.003	0.057	8.217
3	Compound 3 [11 Peak ID:3]	1.435	0.049	8.217
4	Compound 4 [11 Peak ID:4]	2.576	0.062	20.301
5	Compound 5 [11 Peak ID:5]	3.739	0.053	8.709
6	Compound 6 [11 Peak ID:6]	4.187	0.05	8.709

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.

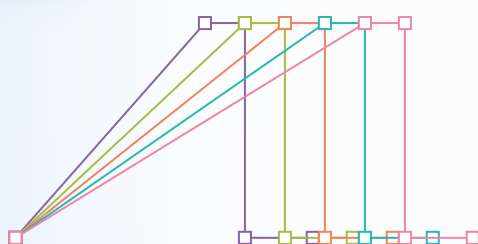
Screening Phase

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.



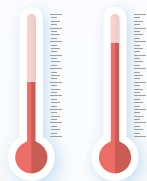
Optimization Phase

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



Optimize gradient condition

..* °C

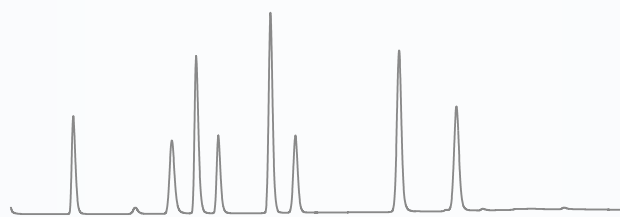


Optimize oven temperature

. mL/min



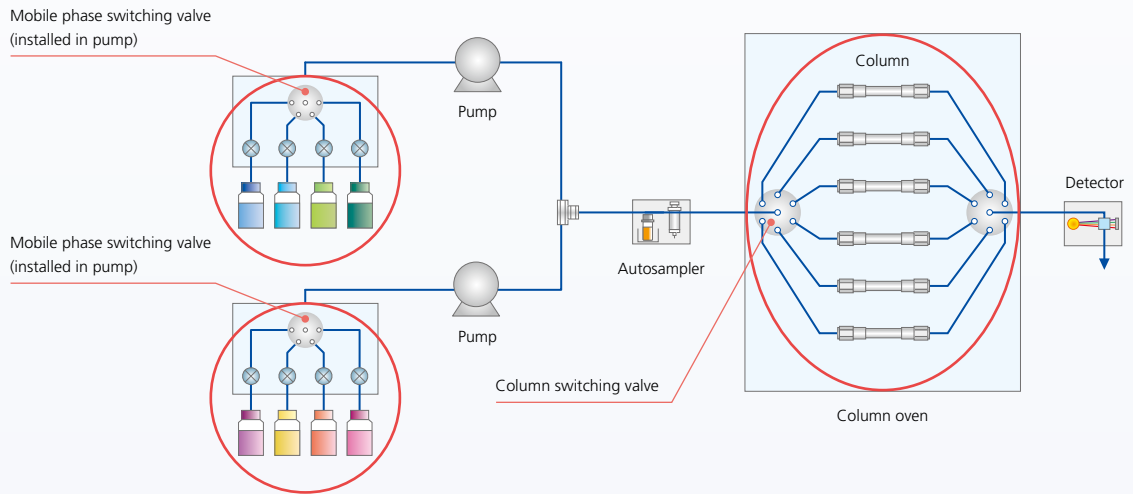
Optimize flow rate



Chromatogram at optimized condition

Automation of Mobile Phases and Columns Switching

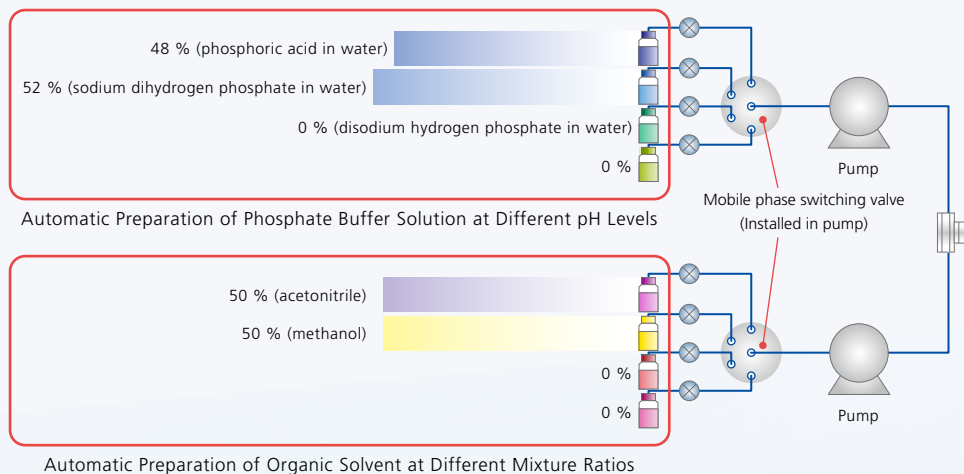
By installing a switching valve in a pump or column oven, several mobile phases and columns can be automatically switched without manually replacing them.



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.



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.

1 Select mobile phases

2 Select columns

3 Input sample information

4 Create 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.

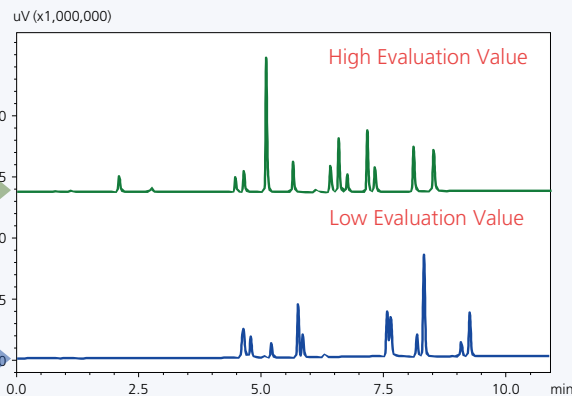
$$E = P \times (R_1 + R_2 + \dots + R_{P-1}) \dots \text{(Equation 1)}$$

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

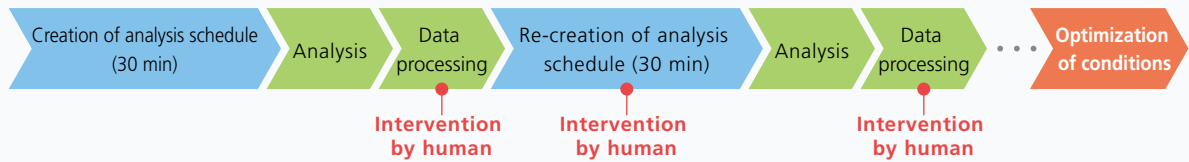


Comparison of Chromatograms at High and Low Evaluation Value

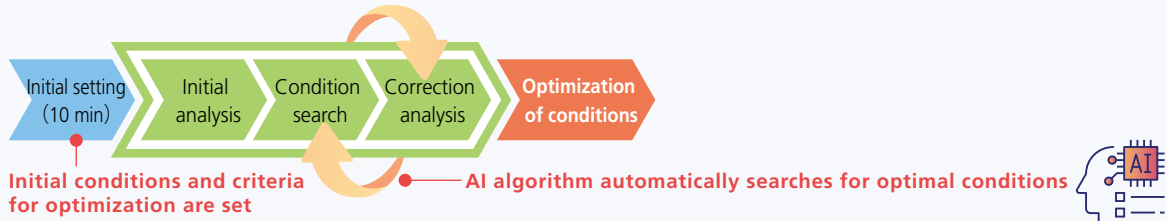
AI Algorithm Automatically Optimizes Gradient Conditions

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

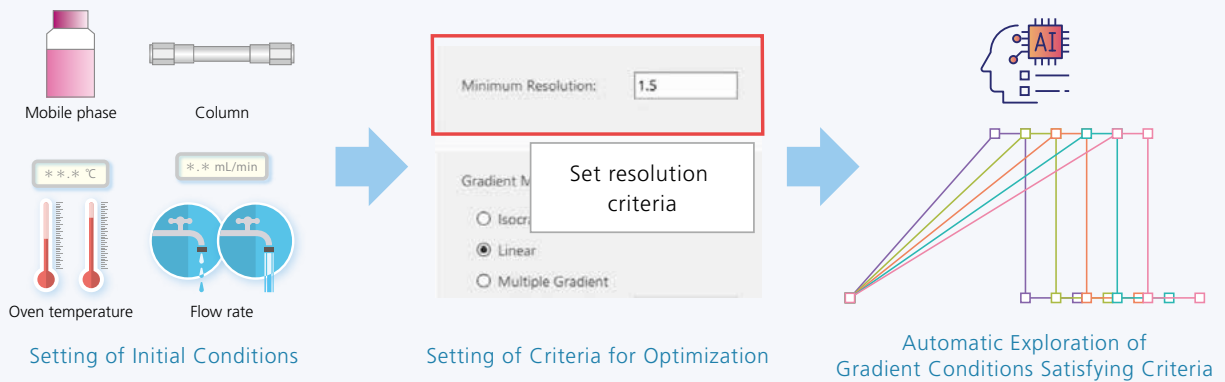


Automated Workflow of Gradient Optimization with LabSolutions MD



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.



Click the icon to access the Technical Report. ▾

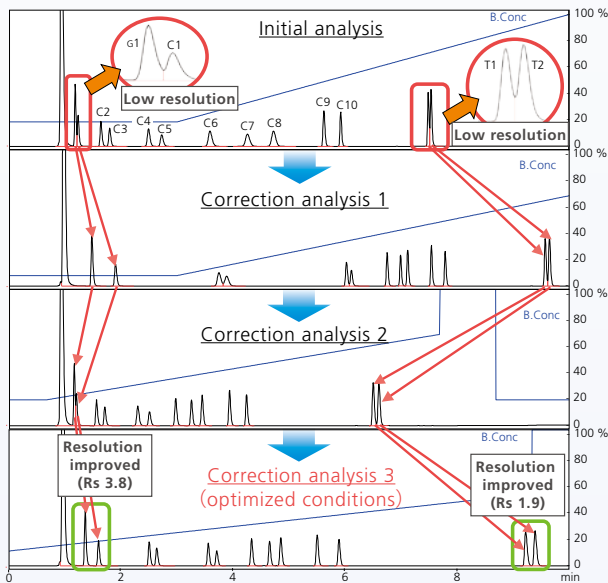
Technical Report

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

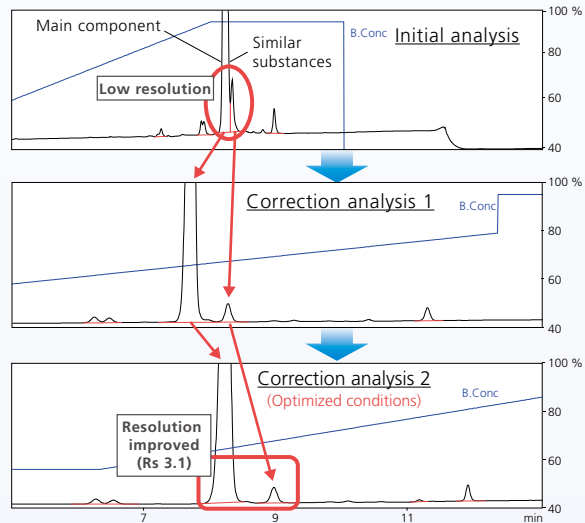
In this mode, the software searches for conditions satisfying the criteria for resolution configured for all the peaks detected. It is used when all the peaks must be resolved.



Application

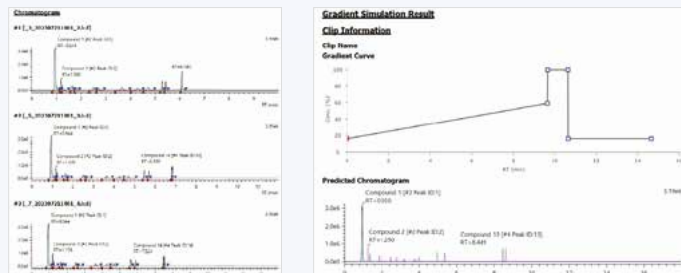
Specified peak resolution mode **NEW**

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.



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.

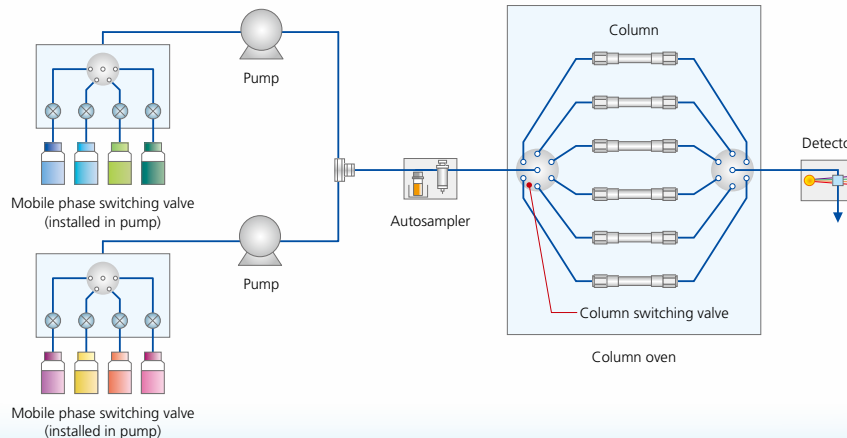
Instrument Parameters					# Sample Name			
Parameter	Enabled	Center Value	Step Size	Steps	Inj. Vol.	Oven Temp. (°C)	Flow Rate (mL/min)	
Flow Rate (mL/min)	<input checked="" type="checkbox"/>	1.0	0.1000	1	1	35	0.9	Sample1
Oven Temp. (°C)	<input checked="" type="checkbox"/>	40	5	1	2	35	1	Sample1
Inj. Vol. (µL)	<input type="checkbox"/>		1.0	1	3	35	1.1	Sample1
					4	40	0.9	Sample1
					5	40	1	Sample1

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.

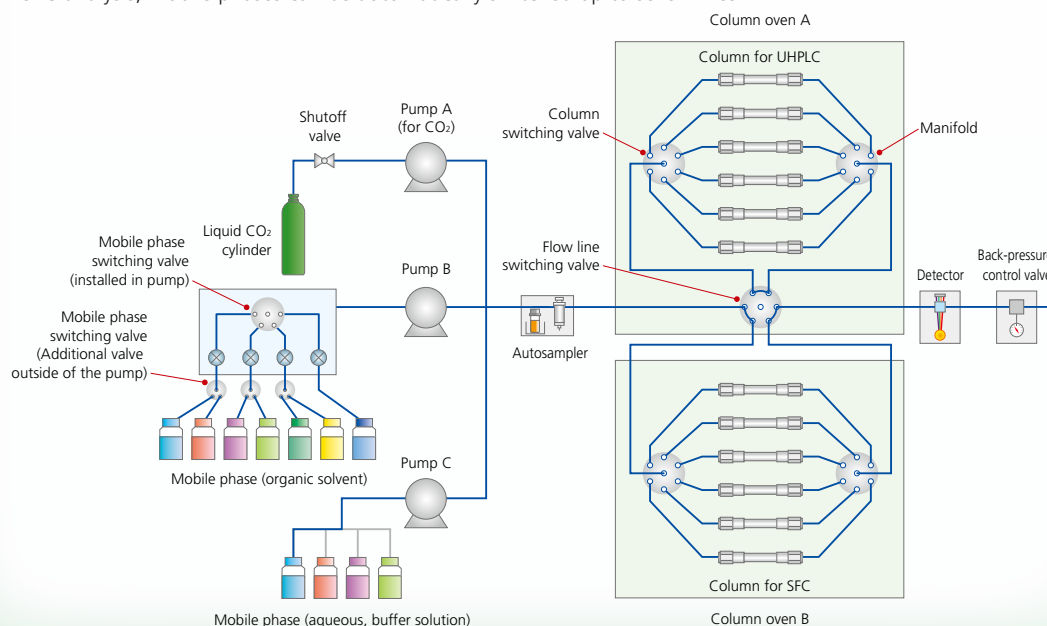
Nexera™ Series

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.



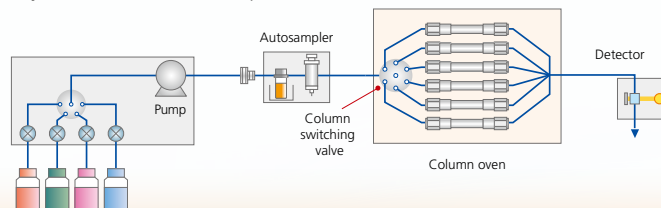
Nexera UC UHPLC/SFC Switching System

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.



Maximizing Productivity with LCMS-2050



The single quadrupole LCMS-2050 combines revolutionary technology with the ease of use of an LC detector. This system features a wide mass range (m/z 2 to 2,000), a quick start as fast as six minutes, and easy, tool-free maintenance. It can fit into basic LC systems with its space-saving design. For details, refer to the catalog "LCMS-2050 Liquid Chromatograph Mass Spectrometer (C146-2256)".

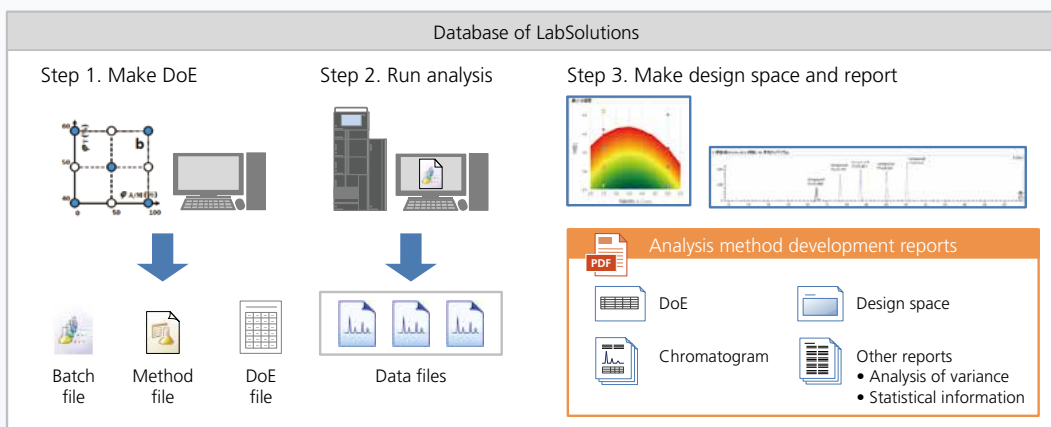
Click the icon to access the LCMS-2050 catalog. ▶

Brochure



Ensure Data Integrity by Database Management

Not only can LabSolutions MD ensure data integrity by managing all the data in a single database of LabSolutions, but it enables seamless operation, such as creating analysis schedules, running the analysis, and data processing using design space, to eliminate time-consuming file importing and exporting steps.



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 LC column Shim-pack series lineup. 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

Automatic Optimization of Gradient Conditions Using AI



Automatic Optimization of Gradient Conditions by AI Algorithm for Impurity Analysis



Automatic Optimization of Gradient Conditions by AI Algorithm – Application to Functional Components in Foods –



AI-Driven Automated Column Screening and Gradient Optimization for LC Method Development



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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