

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. On the left, the 'Mobile Phase A' and 'Mobile Phase B' sections show various buffer and solvent compositions. The 'Gradient' section shows a plot of the gradient profile over time. The 'Chromatogram' section shows a chromatogram with several peaks. The 'Method Optimization' section shows a table of optimized conditions.

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

Run Name	pH	A (%)	B (%)	C (%)	D (%)
ACN: 100%	100	0	0	0	0
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

Run	Completed Name	Ret. Time	Peak Width	R _s
1	Compound 1 (PS) Peak (Q1)	2.344	0.739	2
2	Compound 2 (PS) Peak (Q2)	1.178	0.582	1
3	Compound 3 (PS) Peak (Q3)	1.232	0.296	1
4	Compound 4 (PS) Peak (Q4)	1.822	0.267	2
5	Compound 5 (PS) Peak (Q5)	1.388	0.272	2
6	Compound 6 (PS) Peak (Q6)	2.464	0.265	2
7	Compound 7 (PS) Peak (Q7)	2.584	1.057	2
8	Compound 8 (PS) Peak (Q8)	2.590	0.171	4
9	Compound 9 (PS) Peak (Q9)	4.738	0.149	2
10	Compound 10 (PS) Peak (Q10)	4.828	0.149	2



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 Progress:** A vertical sidebar on the left shows the status of various steps:
 - Program: **Completed**
 - Initial Analysis: **Completed**
 - Initial Position: **Completed**
 - Correction Analysis (1): **Completed**
 - Correction Analysis (2): **Completed**
 - Correction Analysis (3): **Completed**
 - Correction Analysis (4): **Completed**
 - Correction Analysis (5): **Completed**
 - Correction Analysis (6): **Completed**
 - Correction Analysis (7): **Completed**
 - Correction Analysis (8): **Completed**
 - Correction Analysis (9): **Completed**
 - Correction Analysis (10): **Completed**
 - Correction Analysis (11): **Completed**
 - Correction Analysis (12): **Completed**
 - Correction Analysis (13): **Completed**
 - Correction Analysis (14): **Completed**
 - Correction Analysis (15): **Completed**
 - Correction Analysis (16): **Completed**
 - Correction Analysis (17): **Completed**
 - Correction Analysis (18): **Completed**
 - Correction Analysis (19): **Completed**
 - Correction Analysis (20): **Completed**
- Mobile Phase Configuration:**
 - Mobile Phase A:** Phosphate Buffer. Components include 50mmol/L Phosphoric acid Water, 50mmol/L Sodium dihydrogen phosphate, and 50mmol/L Disodium hydrogen phosphate.
 - Mobile Phase B:** Organic. Components include ACN and MeOH.
 - Tables:** Two tables list buffer and solvent compositions with columns for Nick Name, pH, A (%), B (%), C (%), D (%), and E (%).
- Sample and Method Settings:**
 - Sample:** Includes fields for Name, Inj. Vol. (µL), Inj. Time (min), and # of Inj. (1).
 - Method:** Includes Project Name, File Name, and Default Settings for Flow Rate (0.0002 mL/min), Oven Temp. (40 °C), and Gradient Mode (Linear).
 - Gradient:** A graph shows the B. Conc. (%) over time, with a step change from 0% to 100% at 1.000 min.
- Chromatogram and Analysis:**
 - Gradient Curve:** A graph showing the gradient profile over time (0 to 16 minutes).
 - Measured Chromatogram:** Shows a single sharp peak at 2.196 minutes.
 - Table:** A table lists peak data:

Time (min)	Conc. (%)
0	20
3	20
12	100
12.01	20
16	20
 - Analysis Summary:**
 - Minimum Resolution: 1.045
 - Separated Peak Count: 10
 - Evaluation Value: 359.34
 - Table:** A table lists 10 compounds with their names, retention times, peak widths, and peak numbers.

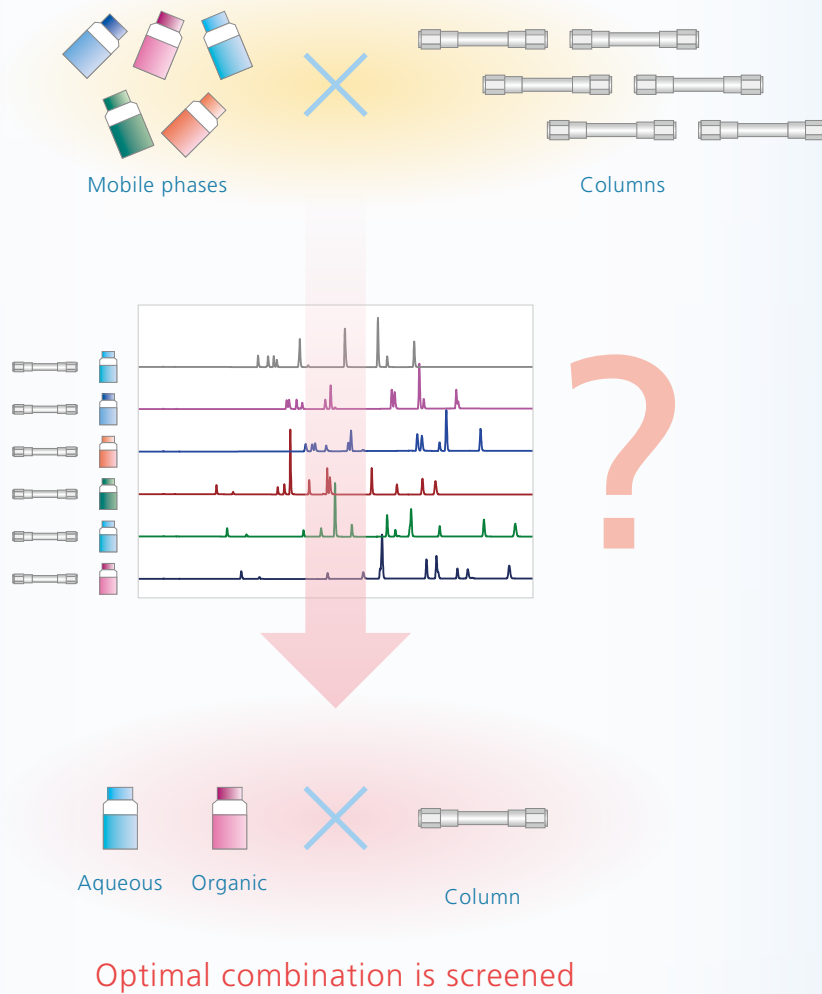
#	Compound Name	Ret. Time	Peak Width	R _s
1	Compound 1 [42 Peak ID:1]	0.044	0.109	2
2	Compound 2 [42 Peak ID:2]	1.176	0.052	1
3	Compound 3 [42 Peak ID:3]	1.232	0.056	1
4	Compound 4 [44 Peak ID:4]	1.632	0.067	2
5	Compound 5 [44 Peak ID:5]	1.784	0.072	2
6	Compound 6 [44 Peak ID:6]	2.404	0.095	2
7	Compound 7 [44 Peak ID:7]	2.884	0.097	2
8	Compound 8 [44 Peak ID:8]	3.596	0.12	4
9	Compound 9 [44 Peak ID:9]	4.228	0.149	2
10	Compound 10 [44 Peak ID:10]	4.656	0.149	2

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

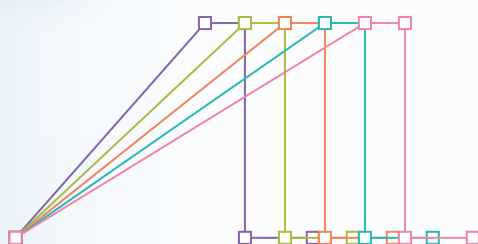
The optimal combination of mobile phases and columns is searched, utilizing parameters such as the pH of aqueous mobile phases, mixture ratios of organic mobile phases, and column types, which have a large effect on resolution and retention time.



Automatic Screening of Mobile Phases and Columns ——— P.6

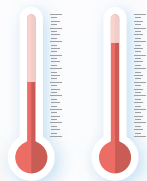
Optimization Phase

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



Optimize gradient condition

..* °C

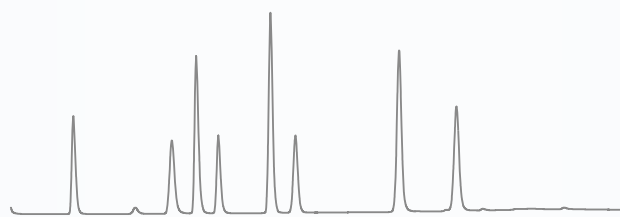


Optimize oven temperature

. mL/min



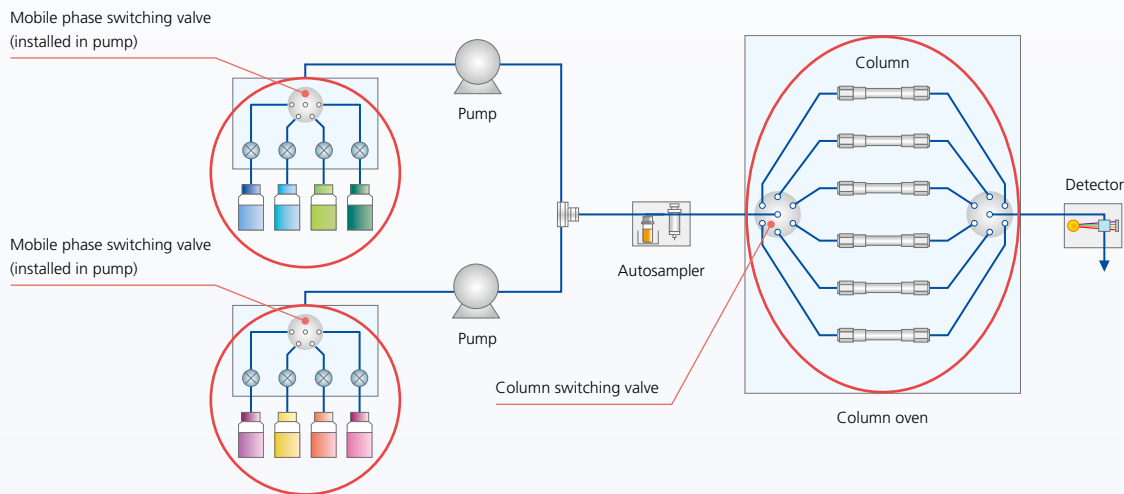
Optimize flow rate



Chromatogram at optimized condition

Automation of Mobile Phases and Columns Switching

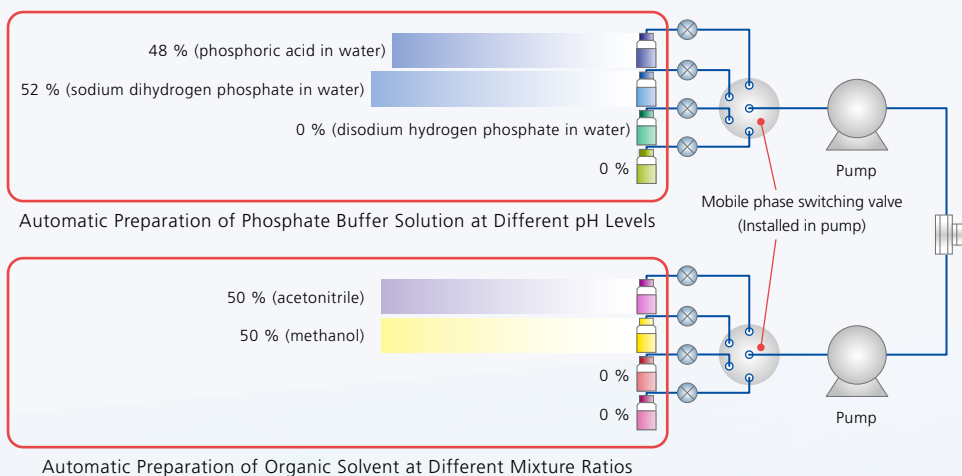
By installing a switching valve in a pump or column oven, several mobile phases and columns can be automatically switched without manually replacing them.



Automatic Mobile Phases and Columns Switching

Automation of Mobile Phases Preparation with Mobile Phase Blending Function

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 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.

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.

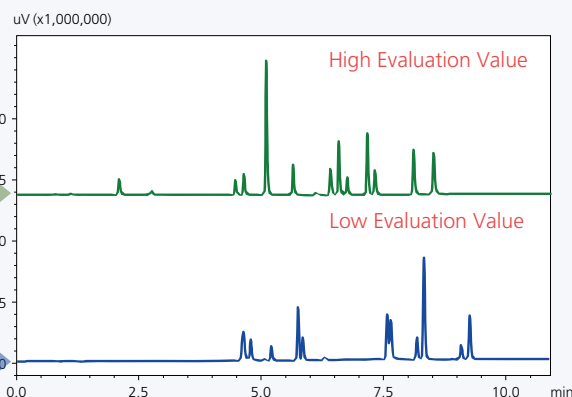
$$E = P \times (R_1 + R_2 + \dots + R_{P-1}) \dots \text{(Equation 1)}$$

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

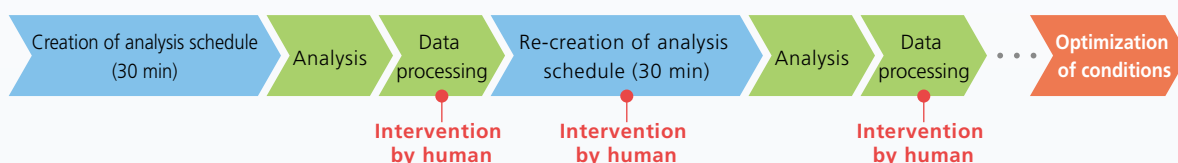


Comparison of Chromatograms at High and Low Evaluation Value

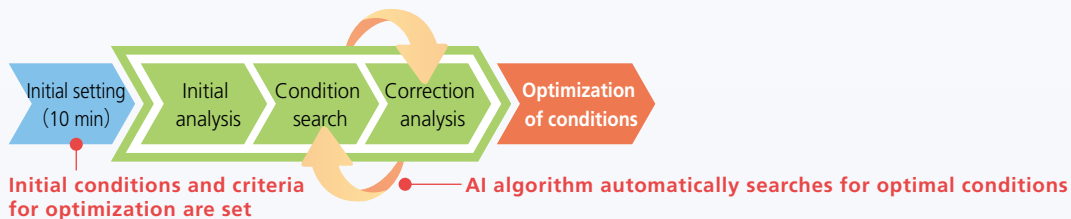
AI Algorithm Automatically Optimizes Gradient Conditions

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

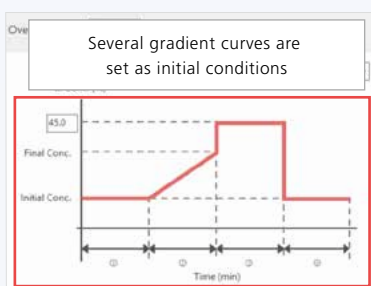


Automated Workflow of Gradient Optimization with LabSolutions MD



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.



Setting of Initial Conditions



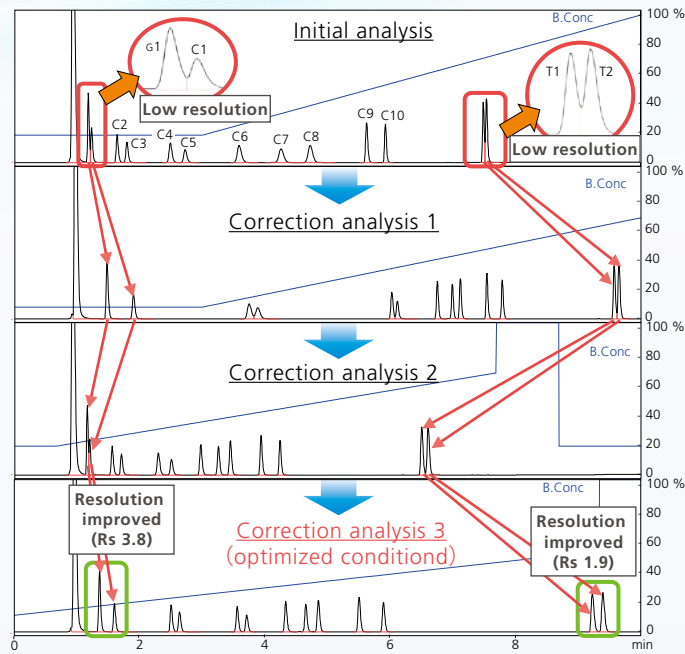
Setting of Criteria for Optimization

Application to Functional Components in Food

On the next page, a case study demonstrates the application of automatic optimization of gradient conditions for the simultaneous analysis of catechins and theaflavins. At first, the resolution between G1 and C1 as well as T1 and T2 (highlighted in red in the figure) was not sufficient. However, by using AI to conduct a series of searches, gradient conditions meeting the criteria (minimum resolution : 1.5) were automatically discovered (highlighted in green in the figure). The blue lines in the figure represent the gradient conditions for each analysis.

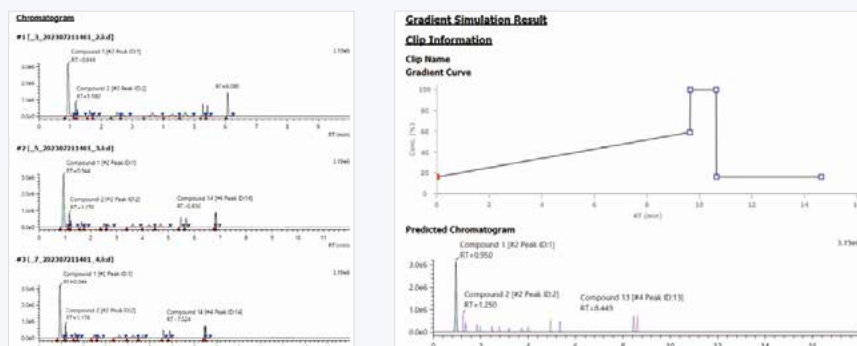
[Click the icon to access the Technical Report.](#)

Technical Report



Automatic Gradient Optimization by AI (Catechin and Theaflavin)

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).



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.

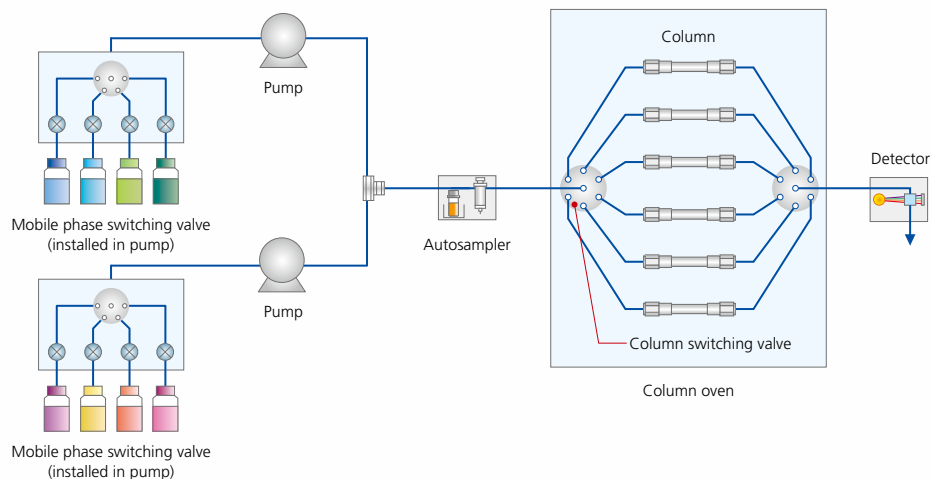
Instrument Parameters					Analysis Schedule				
Parameter	Enabled	Center Value	Step Size	Steps	#	Sample Name	Inj. Vol.	Oven Temp. (°C)	Flow Rate (mL/min)
Flow Rate (mL/min)	<input checked="" type="checkbox"/>	1.0	0.1000	1	1	Sample1	1	35	0.9
Oven Temp. (°C)	<input checked="" type="checkbox"/>	40	5	1	2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

Supporting Various System Configurations

LabSolutions MD supports the Nexera series, i-Series, and supercritical fluid chromatography (SFC).

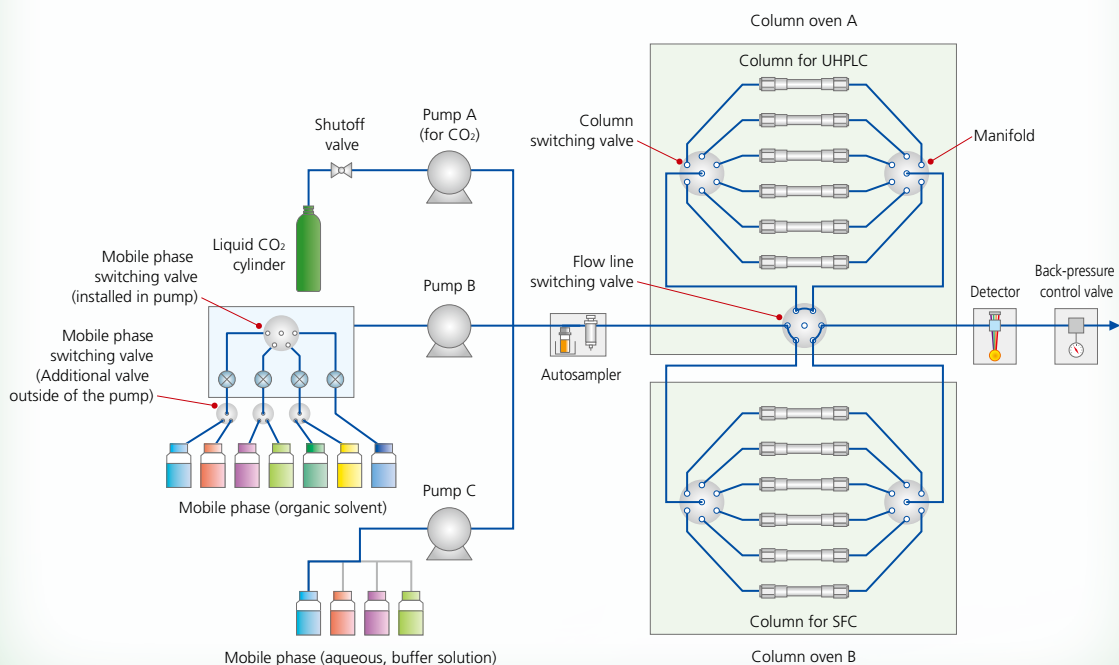
Nexera™ Series

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.



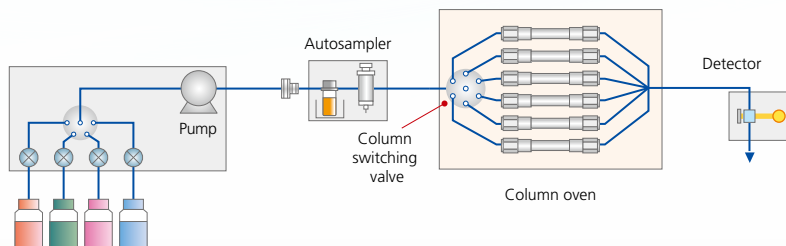
Nexera UC UHPLC/SFC Switching System

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)".

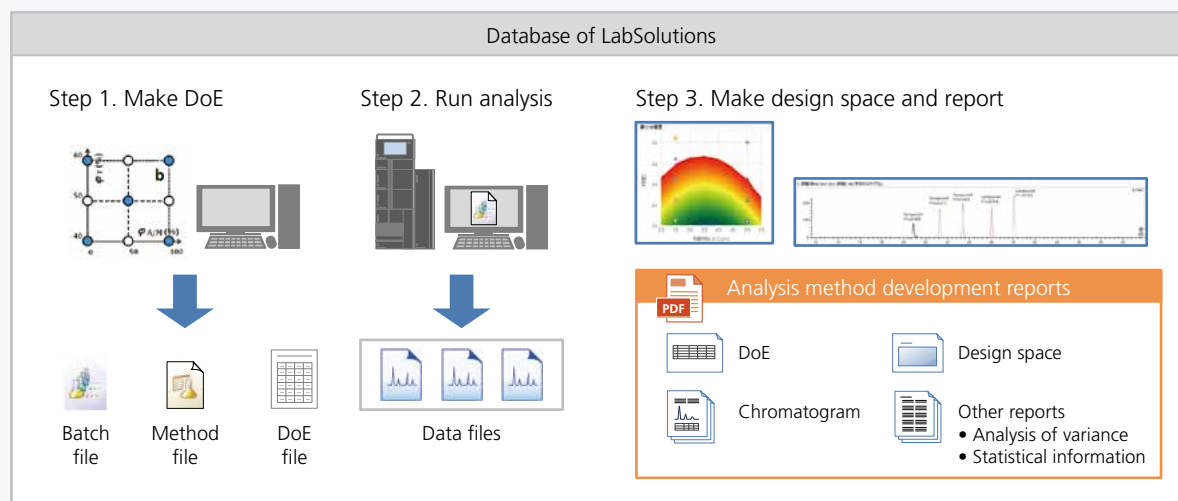
[Click the icon to access the LCMS-2050 catalog.](#)

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.



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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