

High Performance Liquid Chromatograph

Method Scouting System

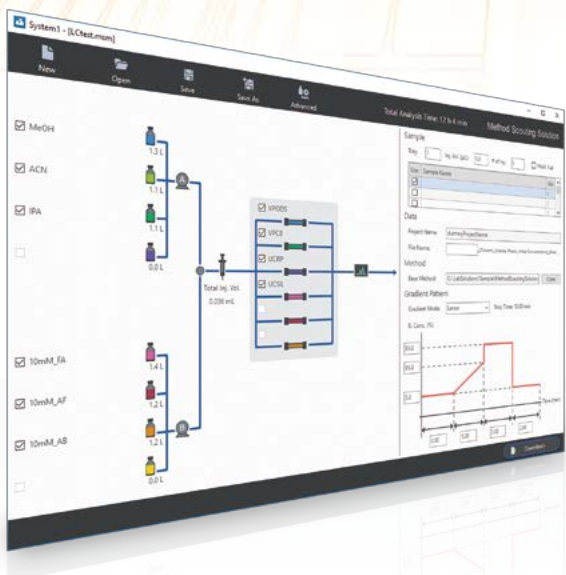


Maximizing Efficiency for Method Development

Fully Automated Method Scouting

Method Scouting System is an important system to improve efficiency in method development.

It uses Method Scouting Solution dedicated control software and a robust, high pressure-resistant column switching system to achieve a fast and accurate method scouting workflow and supports efficiency improvements in method development.



Method Scouting System

Supports scouting for optimized analytical conditions by automating the investigation of a vast number of conditions.

Improving the Productivity of Method Development Work by Freeing You from Tedious Analysis Work

Method Scouting System is the optimum system to use for analyses that involve tedious tasks, such as method scouting for new compounds or chiral compounds in the pharmaceutical and chemical fields, or standardizing a system for multiple official methods using mobile phase and column switching in the environmental field.

› Selectable System Line-Up

Method Scouting System is compatible with Shimadzu's diverse LC product line-up and allows you to select the LC system that matches your objective, whether it be ultra fast analysis, SFC analysis, or simple method assessment.

› Fully Automated Method Scouting

Method Scouting System is able to perform highly efficient and robust method scouting by automating entirely the switching between different combinations of mobile phases and columns.

› Simple Method Setting

Method Scouting Solution dedicated method scouting software can reduce substantially the tedious work of method and batch generation.

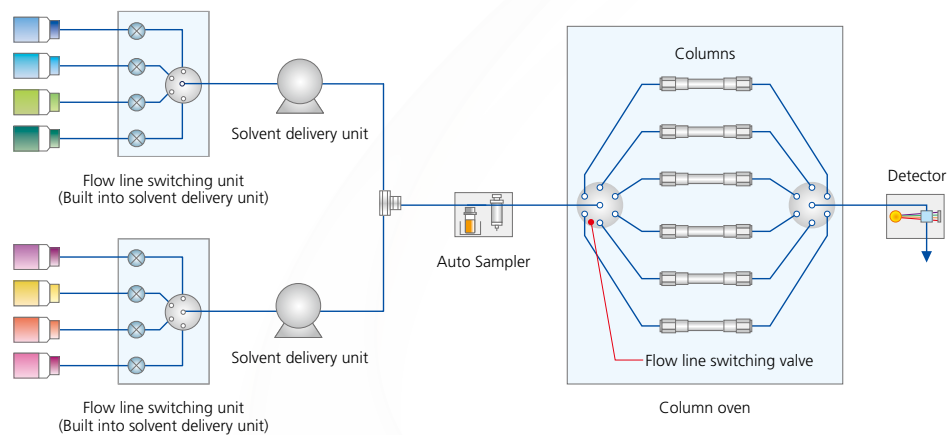


› Selectable System Line-Up

Method scouting can now be performed with Shimadzu's diverse LC product line-up. Choose the system suited to your laboratory environment, whether for SFC investigations or simple investigations on compact systems.

Nexera™ Method Scouting

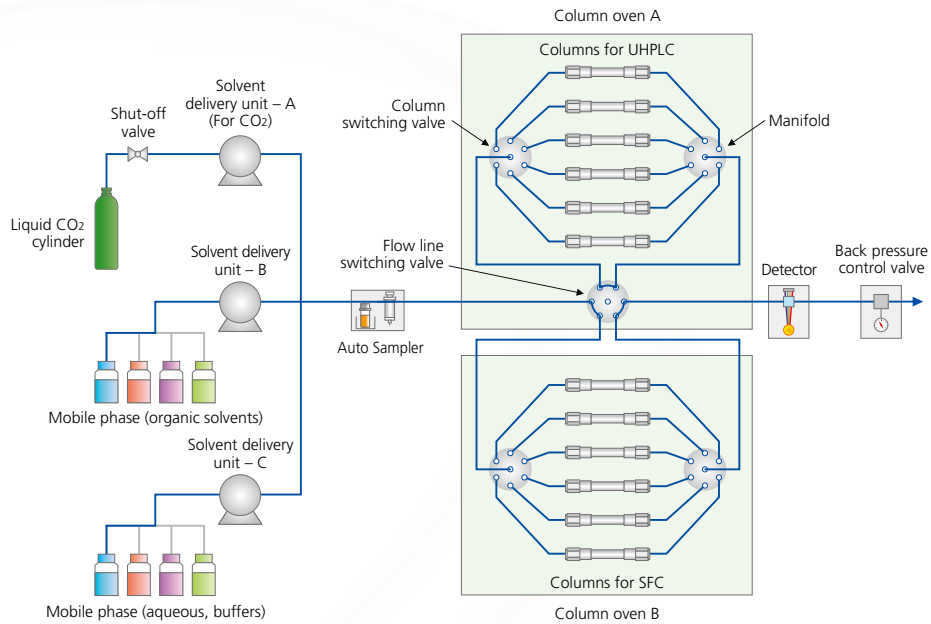
- Capable of automated investigation of conditions in the 130 MPa range, including 192 patterns of 8 mobile phases and 12 columns
- Also capable of investigating pH conditions with mobile phase blending*



*See page 11 for mobile phase blending.

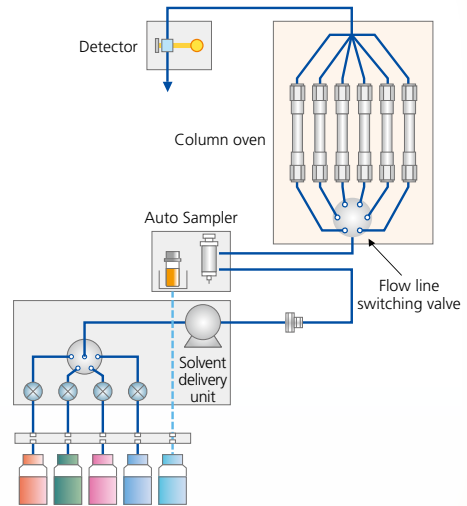
Supercritical Fluid Chromatograph Nexera/UCs UHPLC/SFC Switching System

- Optimized for method investigation of chiral compounds
- Also compatible with LC/SFC switching, for even greater efficiency improvements in method development



i-Series Method Scouting

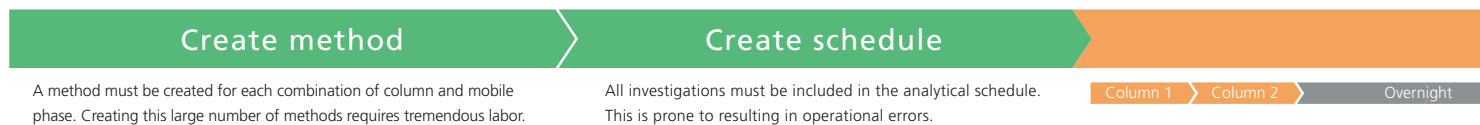
- Optimized for simple method development with a single pump
- Space-saving, low-cost design



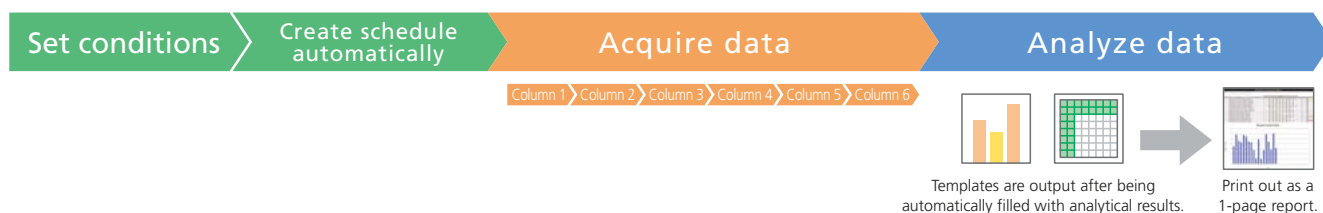
Fully Automated Method Scouting

Combine Method Scouting System with Method Scouting Solution dedicated software to achieve substantial efficiency improvements across all operations from method creation to data acquisition and analysis.

Previous Method

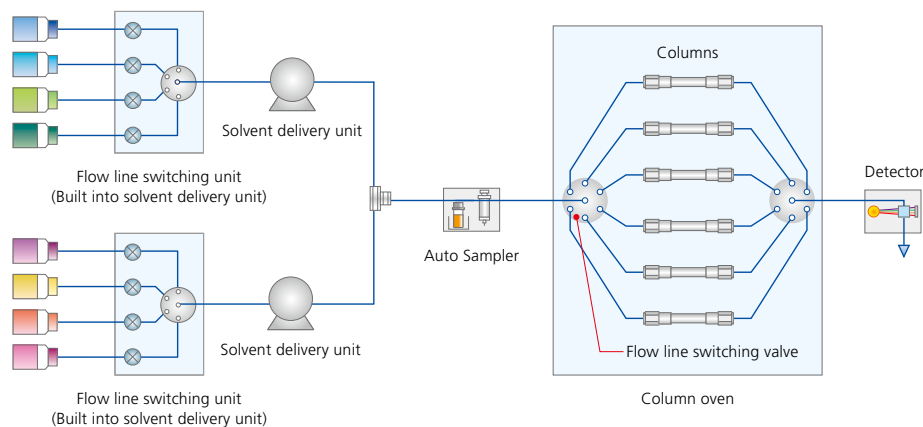


Method Scouting System + Method Scouting Solution



Continuous Overnight Analysis with Method Scouting System

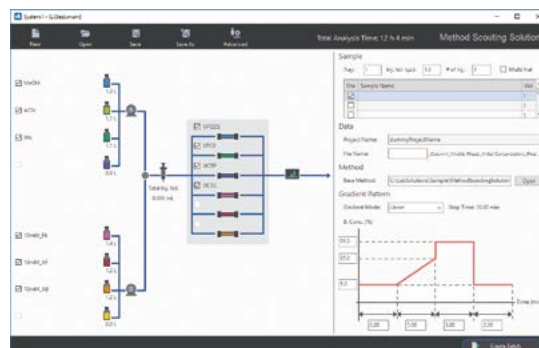
Automatic switching of columns and mobile phases reduces to zero the downtime seen with existing systems, and achieves a high throughput system capable of rapid method development.



Leaving Method and Analysis Schedule Creation to Method Scouting Solution

Previous method scouting requires preparation of a method every time the column or mobile phase is changed. Investigating 100 different conditions requires the creation of 100 different method files, which is a substantial use of labor hours.

Method Scouting Solution automatically creates methods with different columns, mobile phases, and gradient conditions from a single base method, allowing more effective use of your time.



Acquire data

Column 3 → Column 4 → Overnight → Column 5 → Column 6

Analyze data



Print out large volumes of analytical results.



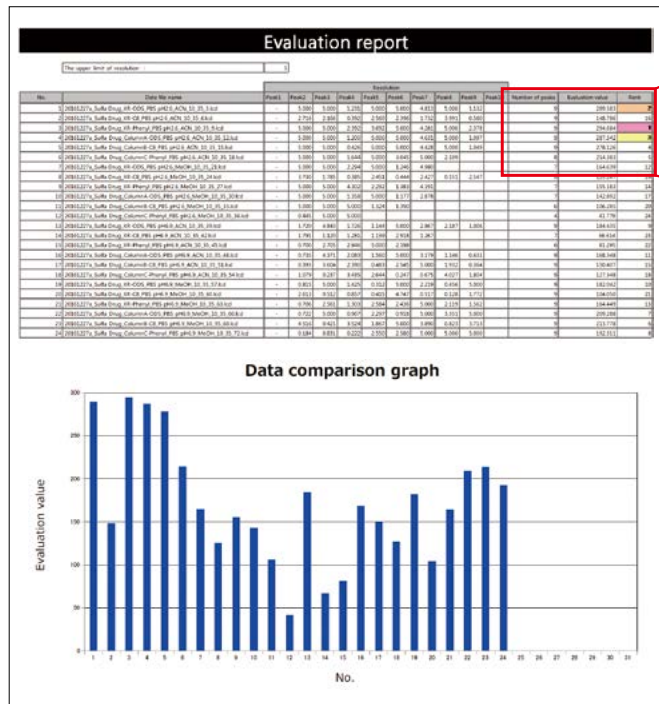
Manually transcribe the necessary values into spreadsheet software.



Print out as a 1-page report.

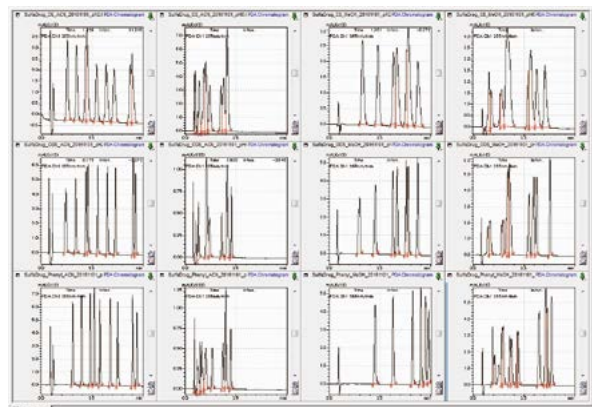
Seamless Evaluation of Results in a Multi-Data Report

Data obtained by method scouting can be evaluated quantitatively with a multi-data report. By employing the evaluation method proposed by Shimadzu that uses resolution and peak detection number, chromatograms can be examined quantitatively and so help the user obtain an optimum method. When templates provided by Shimadzu are registered to Method Scouting Solution, reports are created and output simultaneous with completion of analysis, which allows rapid verification for optimum conditions.



Number of peaks	Evaluation value	Rank
9	289.583	2
9	148.786	16
9	294.684	1
9	287.342	3
9	278.126	4
8	214.383	5
7	164.639	12

Ordered by evaluated score



A browser also allows for visual evaluation of multiple chromatograms.

Simple Method Setting

Method scouting can involve tedious work during method and batch generation, which is prone to resulting in operational errors. The Method Scouting Solution graphical user interface is tailored to the system configuration and allows for intuitive and easy creation of method and batch schedules.

Graphical Information That Supports Proper Analysis

(1) Select mobile phase.

(2) Select column.

(3) Input sample information.

(4) Input gradient conditions.

(5) Create analysis schedule. → Scouting start.

Note: Conditions can also be saved and used later.

(1) Select a mobile phase and (2) select a column.

Select the column and mobile phase from those columns and mobile phases already added to the database. Methods will be generated automatically based on the number of selected conditions.



(3) Input sample information.

Injection volume and number of injections can be set for each sample.



(4) Input gradient conditions.

Gradient conditions can be configured simply by entering duration and concentration parameters. Investigations of gradient speed are also easy to configure.



(5) Create an analysis schedule.

An analysis schedule is generated automatically based on the conditions set above. This saves substantial labor over manual setting of conditions, and allows analysis to start immediately.

Improved Operating Rates Due to Automation of Analysis Sequences

Purge conditions and equilibration during automatic switching of mobile phases and columns are key issues in method scouting. With Method Scouting Solution, these and all laboratory operations can be performed automatically based on conditions set in advance, from automated control to system checks and system shutdown.

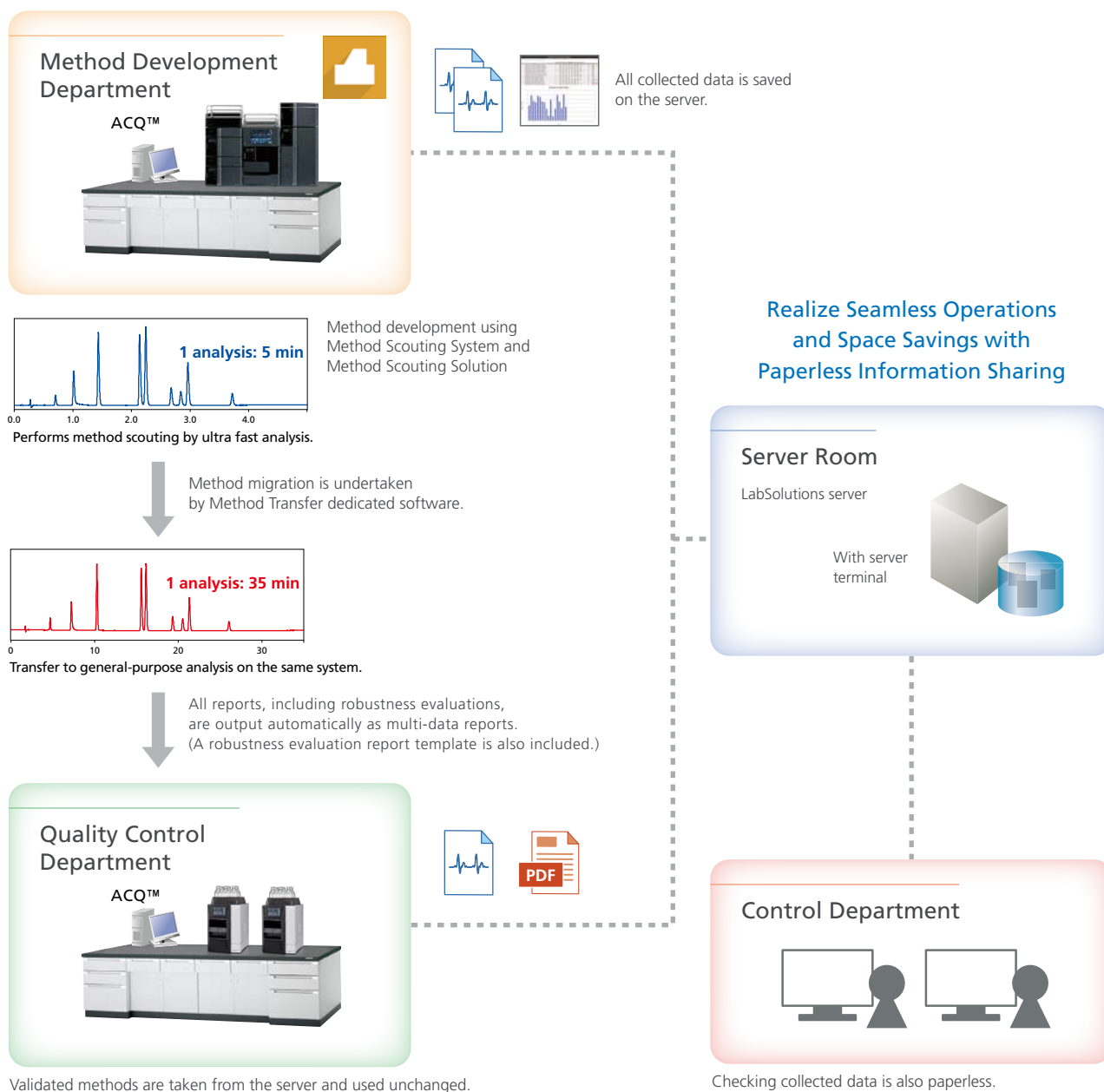


Repeats pattern automatically.

All automated

Seamless Method Migration with LabSolutions™ CS

Optimum conditions obtained by method scouting can be applied to general-purpose analytical conditions and migrated to related departments. In doing so, it is desirable for this data to be retained in the medium to long term, and be easily accessible when required. The combination of LabSolutions CS and Method Scouting Solution realizes labor savings and efficiency improvements for all analytical tasks, not only during method development operations but from method migration to reporting of results to other departments.



Application

Productivity Improvements for Method Scouting Process

When looking for the optimum mobile phase, column, and gradient conditions for a simultaneous analysis of multiple components, it is more efficient to break down the process into a number of steps. In the example shown below, simultaneous analysis conditions for a 13-component mixture of cephem antibiotics are determined by first narrowing down the mobile phase and column to items that are suited to the type of analysis (STEP 1) then optimizing the gradient conditions (STEP 2). This sequence of steps allows for efficient method scouting with reduced mobile phase consumption.

13-Component Mixture of Cephem Antibiotics

1. Cefsulodin
2. Cefadroxil
3. Cephapirin
4. Cefaclor
5. Cephalixin
6. Cephadrine
7. Cefotaxime
8. Cefazolin
9. Cefuroxime
10. Cefmetazole
11. Cefoxitin
12. Cefoperazone
13. Cephalothin

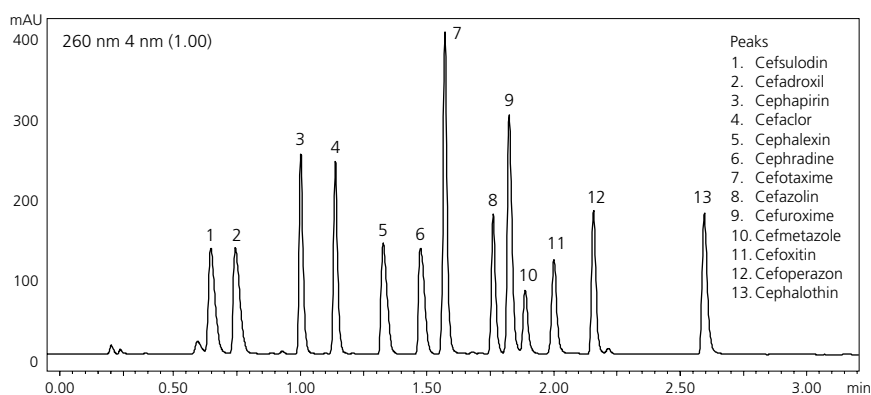
Preparation of Mobile Phases and Columns

- Mobile Phase: (A) (a) Phosphoric acid (sodium) buffer solution (pH 2.6)
 (b) Citric acid (sodium) buffer solution (pH 3.1)
 (c) Acetic acid (ammonium) buffer solution (pH 4.7)
 (d) Acetic acid (ammonium) aqueous solution (pH 6.7)
- (B) (a) Acetonitrile
 (b) Methanol
 (c) Acetonitrile/Methanol = 1/1 (v/v)
- Column: (1) Reversed phase column A (50 mm L. × 3.0 mm i.d., 2.2 mm)
 (2) Reversed phase column B (50 mm L. × 3.0 mm i.d., 2.2 mm)
 (3) Reversed phase column C (50 mm L. × 3.0 mm i.d., 2.2 mm)
 (4) Reversed phase column D (50 mm L. × 3.0 mm i.d., 2.6 mm)
 (5) Reversed phase column E (50 mm L. × 3.0 mm i.d., 2.6 mm)
 (6) Reversed phase column F (50 mm L. × 3.0 mm i.d., 2.6 mm)
- 4 aqueous mobile phases
 3 organic mobile phases
 6 columns

STEP 1 Select mobile phase and column.

STEP 2 Investigate gradient conditions.

Determine conditions for simultaneous analysis.



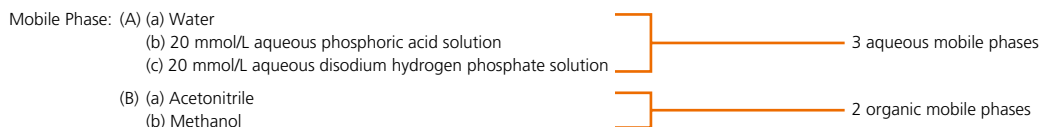
Mobile Phase : (A) Phosphoric acid (sodium) buffer solution (pH 2.6)
 (B) Acetonitrile
 Column : Reversed phase column E (50 mm L. × 3.0 mm i.d., 2.6 μm)
 Time Program : B. Conc. 5% (0 min) → 65% (5 min) → 90% (5.01–7 min)
 Flowrate : 1.0 mL/min
 Injection Volume : 5 μL
 Column Temp : 40°C
 Detection Wavelength : 260 nm (SPD-M20A)

Method Scouting Example for 13-Component Mixture of Cephem Antibiotics

Reducing the Labor Involved in Mobile Phase Blending

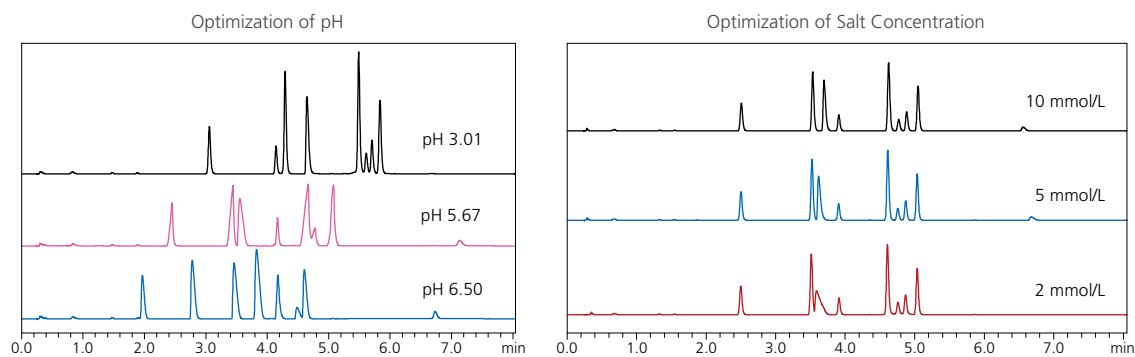
Method development for HPLC requires the selection of mobile phases and columns that are suited to the type of analysis. Mobile phase optimization has a particularly large influence on separation, and is therefore treated as important. However, mobile phase optimization requires the examination of a wide variety of parameters, including salt concentration, pH, and proportions of organic solvents. Because of this, mobile phase optimization commonly requires substantial time, effort, and skill.

Nexera Method Scouting has a mobile phase blending function that adjusts salt concentration, pH, and proportions of organic solvent on-line from multiple solvents that have been prepared in advance, and is quickly able to find conditions suited to a given type of analysis. This function can not only reduce considerably the time required to prepare and investigate mobile phases, it can also reduce solvent consumption.

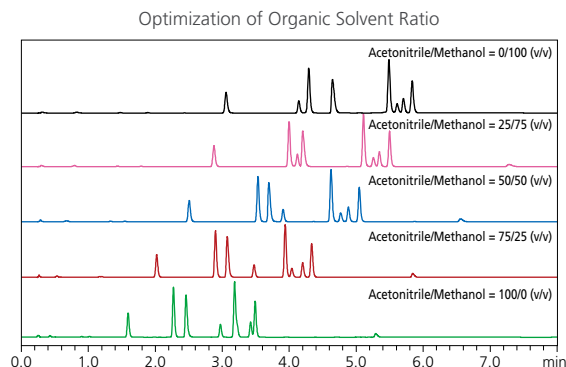


Water, aqueous phosphoric acid solution, and aqueous disodium hydrogen phosphate solution are connected to solvent delivery unit A, and the pH and salt concentration can be adjusted at will by changing the mixing ratio.

Pump A Mixing Ratio (a/b/c)		Buffer Concentration (mmol/L)		
		2	5	10
pH	3.01	90/6/4	75/15/10	50/30/20
	5.67	90/5/5	75/12.5/12.5	50/25/25
	6.50	90/4/6	75/10/15	50/20/30



In reversed-phase chromatography, the type of organic solvent used affects retention behavior and peak shape. When a single organic solvent is used and a component cannot be separated or there is a desire to improve peak shape, mixing more than one organic solvent can resolve the problem.



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