



High Performance Liquid Chromatograph









# Finally, an LC as Smart and Flexible as You.

Amid increasing calls for improved work efficiency and a more flexible working style, ideas of LC analysis are changing. The time has come for an HPLC that delivers rugged, reliable results with less frequent interaction by the analyst. The new, integrated i-Series LC system maintains the excellent performance of its predecessor while addressing the need for automation efficiency.

## innovative

Remote instrument operation and monitoring allow analyses to be performed remotely, thereby reducing the time spent in the laboratory.

## intelligent

Software integration ensures both data reliability and improved work efficiency.

## intuitive

Intuitive operation ensures an efficient workflow.





## **Maximum Reliability and Stability**





#### Use of Multiple Detectors Expands Application Range

The i-Series can be equipped as standard with either a UV/VIS or photodiode array (PDA) detector. It can be expanded with a fluorescence detector, differential refractive index detector, the compact LCMS-2050 mass spectrometer, or other detectors.

# Excellent Baseline Stability Unaffected by Circumstances

The UV/VIS detector and the PDA detector employ dual-temperature control (TC-Optics and flow cell) and provide measurements with a stable baseline hardly affected by room temperature fluctuation.

#### Supports High-Speed Multi-Analyte Processing

A 14-second injection cycle maximizes the number of samples that can be processed. Moreover, a total of 1536 samples can be accommodated in right and left sample racks.

#### Autosampler Enhances Data Reliability

Excellent reproducibility for injection volumes less than 1  $\mu$ L, wide linearity range and ultra-low carryover (<0.0025%) improve the reliability of data, especially for analyses of precious biological samples and direct analyses of concentrated samples.

## Even if an Optional Detector is Added, the Installation Area Remains Small

Even if an optional detector is added, the installation area remains the same. That means a PDA detector, fluorescence detector, differential refractive index detector, or a compact mass spectrometer can be added to a UV detector model. Of course, data can be acquired simultaneously from the standard and added detectors. The i-Series offers excellent extendibility while still allowing easy operation due to its integrated configuration.





## **Refined Usability**

Control panel with a color LCD touch panel allows anyone to operate the instrument, regardless of experience level. Easily and reliably perform routine maintenance following onscreen instructions.

# Displays Chromatogram in Real Time

The chromatogram real-time monitor allows the user to immediately confirm the success or failure of data, even in a computer-less laboratory environment.

#### Large Capacity Column Oven with Ultra Wide Temperature Range

The forced-air circulation method is used to support temperatures up to 90 °C for sugar analysis or other applications that require high temperatures. By adding the optional unit, stability can be improved at lower temperatures to enable even analysis at 10 °C in a typical laboratory environment. A standard system fits either three 300 mm long columns or six 100 mm long columns.

## Quaternary Solvent Delivery Unit

A 10  $\mu$ L micro plunger ensures accurate quaternary gradient delivery. An optional reservoir switching valve further extends the solvent selection to seven so that the solvent for the flow path rinsing can be set.

#### Auto Shutdown Function Reduces Power Consumption

After analysis is complete, the auto shutdown function minimizes power consumption in standby mode and can reduce power consumption by at least 95% compared to normal standby mode.

# innovative

## Automation and Remote Operation/Monitoring Encourage a New Style of Work

Analytical Intelligence functions, such as FlowPilot and mobile phase monitoring, and LabSolutions<sup>™</sup> Direct can provide an automated workflow together with remote operation and monitoring from instrument startup to analysis completion.

Automated workflows incorporate the work-style habits of experienced analysts. The result is reliable data collected over extended periods.



#### Using Networks for More Improvements in Work Efficiency

LabSolutions CS allows remote operation and monitoring of all instruments on the analytical network from any location, even from home.\* Analysis data and reports are managed on a centralized database where administrative authorization allows managers to assign appropriate operational restrictions to operators, depending on their expertise and rank.

\* Must have a network in place that is appropriate for the workflow.



- Automated support functions utilizing digital technologies, 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.



# innovative





#### **Mobile Phase Monitoring**

## Advanced Real-Time Mobile Phase Monitoring

Making sure you have sufficient mobile phase in the system—before batch analysis—is critical to keeping your lab running smoothly. If you run out of mobile phase mid-batch, you have to stop the batch and take corrective action, resulting in costly workflow delays and potential loss of samples.

To overcome this challenge, the Mobile Phase Monitor<sup>\*1</sup> enables real-time, gravimetric monitoring of mobile phase levels to ensure maximum uptime. Levels for mobile phase or autosampler rinse solution may be monitored in up to six containers<sup>\*2</sup>. A large bottle version is also available. The containers can also be checked remotely from a smart device (PC/iOS/Android).

- \*1 Optional
- \*2 Monitors up to 6 liquids when using 1-liter bottles, and up to 3 liquids when using large-volume bottles (2- to 5-liter bottles).



→ Time

Previous model



When using the FlowPilot function

ANALYTICAL INTELLIGENCE

**Mobile Phase Flowrate Control Function** 

#### **Smart Flow Control Protects Columns**

UHPLC columns can be damaged by sudden pump starts and extreme gradient changes, especially true with polymeric packings. Smart Flow Control (FlowPilot) increases the flow rate gradually to the method set point according to the status of the column oven, extending the life of your columns.

# FlowPilot (Patent pending) The pump controls the flowrate based on oven temperature Image: Control of the flowrate based on oven temperature A Gradually increasing the flowrate B Maintaining the flowrate at half the method flowrate C When the oven temperature reaches the

configured temperature, the flowrate is gradually increased up to the configured flowrate





LabSolutions Direct

Web monitoring

**Remote Operation/Monitoring Function** 

# Take Control of Instruments from Outside the Laboratory

Using LabSolutions Direct, analysts can operate instruments remotely and implement pre-configured methods and batch analyses using the web browser of a computer or a smart device. Instrument status and chromatograms can also be monitored remotely to reduce the time and labor required to travel to and from the laboratory for improved work efficiency.





Analytical Intelligence is not limited to automating an analytical workflow or remote operations. By aggregating and automating the knowledge and skills of experienced analysts, Analytical Intelligence enables anyone to obtain reliable data and analytical results. Analytical Intelligence is also designed for high levels of compatibility with other instruments and comes with a method migration function, thereby providing an environment where anyone is equally able to obtain data without the need for complex procedures related to data compatibility between different systems.



i-PeakFinder<sup>™</sup> Automatic Peak Integration Function Process Large Volumes of Data with High Precision in a Single Step

The manual integration of un-resolved peaks is a labor-intensive process and prone to inconsistent results depending upon the experience level of the user. Shimadzu's proprietary i-PeakFinder peak integration algorithm is perfect for such situations. i-PeakFinder processes large volumes of data with high precision in a single step, saving a lot of time and increasing the consistency of results.



Baseline processing with no parameters specified



Baseline processing with complete separation



#### **ACTO Method Migration Support Function**

#### **Considering Instrument Replacement and Method Migration**

Migrating a test method (analytical conditions or method) from one instrument to another while obtaining the same chromatogram can be a challenging process. The i-Series is designed with the same internal system volumes as previous Shimadzu systems and competitor systems to ensure system compatibility and data reproducibility. An Analytical Condition Transfer and Optimization (ACTO) function also adjusts gradient start time automatically, so analysts can make adjustments to separations obtained by gradient analysis easily.

Note: The ACTO (Analytical Condition Transfer and Optimization) is the general name given to the method transfer/migration tools supplied by Shimadzu.



Migrating an analytical method from a previous Shimadzu system (LC-2010HT) to the LC-2050

Migrating an analytical method from a non-Shimadzu system to the LC-2050

![](_page_11_Picture_8.jpeg)

#### **Compatibility Through Software Control**

The ACTO function can be used to adjust gradient start times and allows analysis to be performed without worrying about the effects of piping volume.

ACTO allows you to adjust gradient timings without having to edit the gradient program itself, and as shown in the example below, the same sort of analytical results can be obtained using an existing analytical method with a larger system capacity to LC-2050. This gradient start time adjustment function can be used with all i-Series models.

![](_page_12_Figure_3.jpeg)

Using ACTO to Confirm Compatibility of LC-2050 and Previous Shimadzu System (LC-2010HT)

#### **Utilizing ACTO for US Pharmacopeia-Compliant Method Migration**

Maintaining method compatibility during gradient analysis can be difficult due to differences in gradient delay volumes between models. Adjustment of the initial hold time using the gradient start time adjustment function (ACTO) enables method transfer compatible with USP <621>. Even when instrument models have different gradient delay volumes, analysis can be performed without replacing piping, etc.

![](_page_12_Figure_7.jpeg)

HPLC Conditions				
Column	: Phenyl silyl silica gel column			
	(50 mm L. × 4.6 mm I.D., 1.8 μm)			
Mobile phase A	: Water/TFA = 2000/3			
Mobile phase B	: Acetonitrile/TFA = 2000/3			
Flowrate	: 1.2 mL/min			

 $\begin{array}{ll} \mbox{Gradient} & : B \mbox{ Conc. } 40\% \mbox{ (0 min)} \rightarrow 40\% \\ (3 \mbox{min)} \rightarrow 51\% \mbox{ (16 min)} \\ \mbox{Column temp.} & : 30^{\circ}\mbox{C} \\ \mbox{Injection volume} & : 10 \mbox{ \muL} \\ \mbox{Sample} & : \mbox{ Montelukast sodium} \\ \end{array}$ 

Comparison of Retention Time Difference (%) With and Without ACTO Adjustment

Component	Without ACTO Adjustment	With ACTO Adjustment
1 impurity A	1.3	1.1
2 impurity B	2.7	0.3
3 impurity C, D	3.1	0.2
4 Montelukast Sodium	2.7	-0.1
5 impurity E	2.8	-0.1
6 impurity F	2.5	-0.3

\* Excerpt from USP 40 <621> CHROMATOGRAPHY

![](_page_13_Picture_0.jpeg)

#### **User Interface**

## Simple in Operation

The user interface replicates the system flow channel and is used to visually check the operating status of the system. Method editing can also be performed from the same screen. With its intuitive design, even users who are completely new to liquid chromatography can navigate the user interface with minimal training.

![](_page_13_Picture_4.jpeg)

#### Instructional maintenance videos

**Maintenance Videos** 

# Supporting the Replacement of Consumables

Reading a QR Code<sup>®</sup> shown on the touch panel directs the user to a website with instructional videos on maintenance. This feature helps improve system availability and increases efficiency.

![](_page_13_Figure_9.jpeg)

![](_page_14_Picture_0.jpeg)

#### **Auto-Validation Function**

#### Stable Operation Assured with Smart System Startup

An auto-validation function means anyone can follow a set procedure and verify the instrument condition easily. The auto-validation function examines solvent delivery stability, wavelength accuracy, absorbance accuracy, gradient accuracy, the presence of any drift/noise, and other parameters. Also, an instrument check function automatically carries out the routine inspections performed before instrument operation and creates a report showing system self-diagnostic results along with a record of consumables usage, including total solvent volume delivered by the delivery pump, total number of injections performed by the autosampler, and the number of hours the lamp has been illuminated. The system check function also manages auto-validation results, making it easy to accurately determine the operating status of the instrument.

![](_page_14_Picture_4.jpeg)

#### **Starting Auto-validation**

Procedures, mobile phases, and other information necessary for validation are displayed on the screen, allowing you to perform inspections by simply following the instructions.

#### **Creating a System Check Report**

Validation results can be viewed from the i-Series main unit. Validation results can also be output in a report format from a workstation.

![](_page_15_Picture_0.jpeg)

Packed with advanced technologies developed by Shimadzu, the i-Series offers even easier operability in addition to high core performance.

A column oven that can be controlled to a wider range of temperatures, an autosampler with automatic pretreatment functionality for co-injecting internal standard substances, and other features not only increase analysis throughput, but also help increase work efficiency by automating various manual tasks.

#### **Automatic Pretreatment Functionality Increases Work Efficiency**

i-Series autosamplers include easy-to-use automatic pretreatment functionality. For example, co-injecting samples together with the diluent solvent (co-injection) ensures reliable analysis even when using sample solvents that tend to cause peak distortion. That functionality can also be used to react samples with reagents inside the sample loop. The chromatogram below shows results from using this function to pre-label amino acids with a pre-labeling reaction with OPA/FMOC reagents. Analyzing the entire aspirated sample quantity enables high-sensitivity analysis while minimizing reagent and sample quantities required.

![](_page_15_Figure_5.jpeg)

Example of peak shape improvement by co-injection of diluent solvent

![](_page_15_Picture_7.jpeg)

![](_page_15_Figure_8.jpeg)

Amino acid analysis by automatic pre-column derivatization

#### **Dual-Temperature Control with TC-Optics and Flow Cells**

#### **Excellent Baseline Stability**

![](_page_16_Figure_2.jpeg)

In addition to the temperature control function for flow cells, the i-Series employs new temperature control technology for detector optical systems, known as TC-Optics (Temperature Controlled Optics). This ensures a more stable baseline that is less susceptible to room temperature variation and increased precision during verification testing and quantitative testing of trace components.

#### Ultra-Low Carryover Performance Enables High-Sensitivity Analysis

![](_page_16_Figure_5.jpeg)

#### Improved Reliability of Trace Component Analysis

Shimadzu's proprietary flow channel design, parts, and materials reduce the carryover effects of sample residue to almost zero. Ultra-low carryover performance has been improved to 0.0025% (chlorhexidine, assigned conditions), thereby providing highly precise quantitative performance when analyzing complex samples.

#### Support for Low-Temperature Analysis (Optional)

Pharmaceutical analysis can sometimes require analysis at lower temperatures. Therefore, the i-Series includes an optional low-temperature analysis unit for supporting such analytical conditions. With the optional low-temperature analysis unit installed, the oven temperature can be controlled down to a room temperature of -15 °C. The following is an example of analyzing valaciclovir, a drug listed in the 18th Edition of the Japanese Pharmacopoeia. It specifies a temperature of 10 °C in analytical conditions for quantitative testing.

![](_page_16_Figure_10.jpeg)

 Column
 : DAICEL CROWNPAK\* CR(+) 150 mm x 4 mm I.D., 5 µm

 Mobile Phase
 : Water / Perchloric acid / Methanol = 950:5:30

 Flow Rate
 : 1.6 ml/min

 Column Temp.
 : 10 °C

 Injection Volume: 10 µL
 Detection

 UV at 254 nm
 : UV at 254 nm

#### System suitability test results (quantitation method)

Test item	Criteria	Result	Judgement
Theoretical plate number	≥ 700	1849	PASSED
Symmetry factor	≤ 1.5	1.22	PASSED
Area %RSD (N = 6)	≤ 1.0%	0.02%	PASSED

# Dedicated Software Improves Method Development Efficiency

Using LabSolutions MD method development software, methods can be developed using an i-Series system. LabSolutions MD enables efficient analysis method development using an "Analytical Quality by Design" (AQbD) approach for designing analysis methods based on science and risk. LabSolutions MD can be used for the entire workflow, from creating an analysis schedule based on the experimental design, automating acquisition by switching

between mobile phase, column, and LC parameters, and determining optimal analytical conditions by creating a design space, to performing validation. For more information about the LabSolutions MD, also refer to the following.

![](_page_17_Picture_4.jpeg)

## Automatically Tracking Chromatogram Peaks

LabSolutions MD includes functionality for identifying peaks based on a combination of parameters. In the example on the right, the fumaric acid retention time varies significantly more than other peaks depending on the acid concentration and column oven temperature. To automatically identify each peak despite the elution order of fumaric acid changing with respect to other peaks, only the maleic acid peak, which does not change order with fumaric acid, was filtered based on both peak height percent and elution order, whereas the peaks for other components were identified based on elution order only.

![](_page_17_Figure_7.jpeg)

For initial screening, multiple parameters in analytical conditions, such as the organic solvent concentration used for the mobile phase and the column oven temperature, are specified automatically. Then the effects on separation due to variation of each parameter determined from that process can be displayed visually. For example, the design space on the right shows organic solvent concentration of mobile phase B plotted on the vertical axis and column oven temperature on the horizontal axis. That makes it easy to see at a glance that an organic solvent mixture ratio of 50 % and a column oven temperature of 39 °C are the most robust analytical conditions.

![](_page_17_Figure_9.jpeg)

![](_page_17_Figure_10.jpeg)

Design Space for Minimum Separation Level (given a gradient with 80 % final concentration) By entering the allowable fluctuation range in response to parameter (factor) changes, the software can suggest robust analytical conditions that satisfy

that allowable range (black box

in figure to the left).

## Predicting Chromatograms from a Design Space

The effect of analytical condition changes on chromatograms can be visually estimated by clicking on any corresponding point in the design space. That means changes in separation behavior in response to any particular change in analytical conditions can be checked before starting an analysis.

![](_page_17_Figure_15.jpeg)

# i-Series **Data Management**

#### **Compliant with ER/ES Guidelines and Data Integrity**

LabSolutions has a variety of functions to ensure compliance with FDA 21 CFR Part 11 and Japanese Ministry of Health, Labour and Welfare guidelines on electronic records and electronic signatures. LabSolutions also includes functions that address and support data integrity.

# Centralized Management of Data and User Information

Data and user information are managed on a database with restrictions on data file deletion and a version number management function that ensures safe storage. Furthermore, fine-grained division of operational restrictions allows optimum user management based on role, such as system administrator, analysis operator, etc. LabSolutions records the access status of the system, changes to data and methods, operations performed during analysis and re-analysis, changes to system settings, etc.

![](_page_18_Figure_5.jpeg)

An "audit trail" that records all operations

## **Review of Operation Logs**

A report set function compiles analytical conditions or analytical results/conditions for sets of analysis (batch analysis) and also compiles operation logs from start to completion of analysis. The report set function automatically collects information, prevents the accumulation of arbitrary reports and prevents operational errors.

![](_page_18_Picture_9.jpeg)

## Seamless Integration of Testing and Analysis

LabSolutions i-QLinks<sup>™</sup> can create test plans and test items, incorporate results from tests performed on HPLC systems and other analytical instruments, automatically create test reports based on test results from all kinds of analytical instruments and manage the progress status of quality testing.

The Analytical Intelligence logo, LabSolutions, i-PeakFinder and i-QLinks are trademarks of Shimadzu Corporation or its affiliated companies in Japan and/or other countries. Crownpak is a registered trademark of Daicel Corporation.

![](_page_19_Picture_3.jpeg)

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