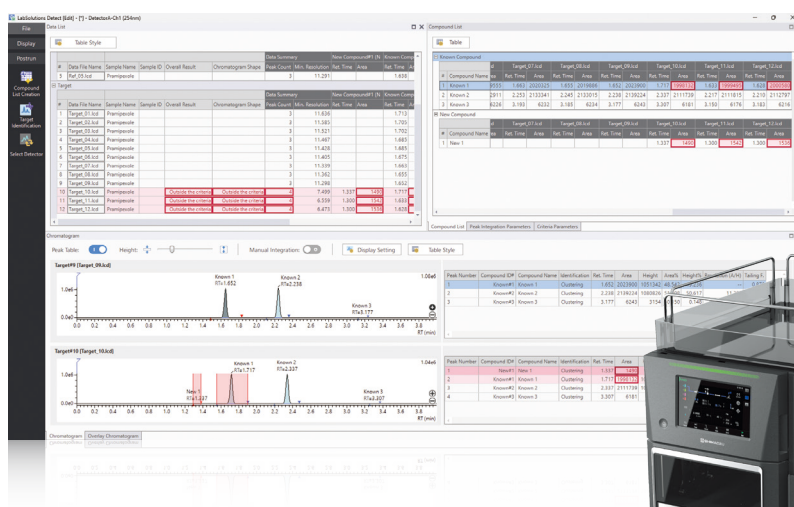# SHIMADZU
Excellence in Science

Anomaly Detection Support Software

LabSolutions Detect

LabSolutions Detect

Automating anomaly detection of analytical data with software

LabSolutions Detect software identifies unusual peaks, such as impurities or unexpected signals, making it easy to observe any differences between the correct data (reference data) and the analytical data (target data).

Accumulated reference data

Daily sample data
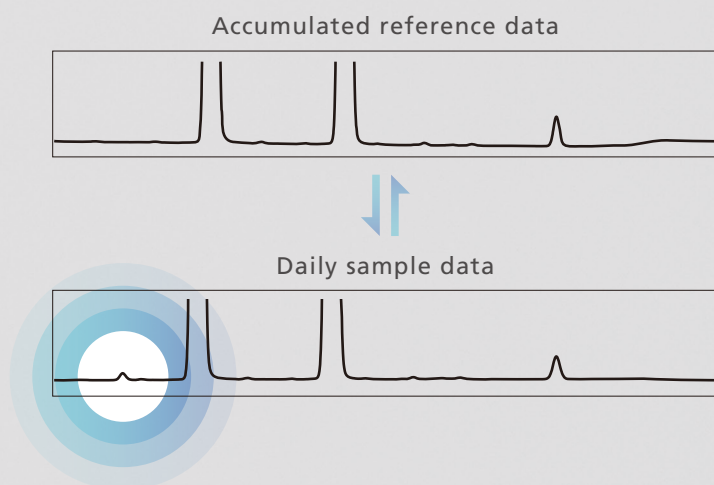
## Safe, Reliable Anomaly Detection

Quality control processes play a vital role in consistently delivering safe and effective pharmaceuticals and food products to the market. Liquid Chromatography (LC) is primarily used for quality control testing.

LabSolutions Detect transforms your LC data review process by visualizing differences between accumulated reference data and daily sample data.

Designed to support efficient quality control, it streamlines the entire workflow — from reviewing large amounts of analytical data and generating compound lists (including unknown peaks) to determining whether results meet predefined criteria.

Three Essential Features for Powerful Anomaly Detection
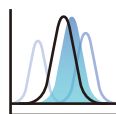
KEY 01
Alignment function

Enables easy comparison of chromatogram shapes by automatically correcting retention times.

KEY 02
Clustering function

Instantly detects common impurities across datasets by identifying similar peaks.

KEY 03
Reporting / data management function

Difference analysis results can be centrally stored in a database and reports can be generated with a single click.

ANALYTICAL INTELLIGENCE

- Automated support functions utilizing digital technology, 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.

Boosting Efficiency in Data Review with Difference Analysis

LabSolutions Detect enhances quality control by visualizing differences between accumulated reference data and daily sample data. By treating reference data as the standard, the software supports the detection and confirmation of distinctive peaks, including potential impurities. This streamlines impurity monitoring tasks in quality management, increasing workflow efficiency and contributing to the development of safe, reliable products.
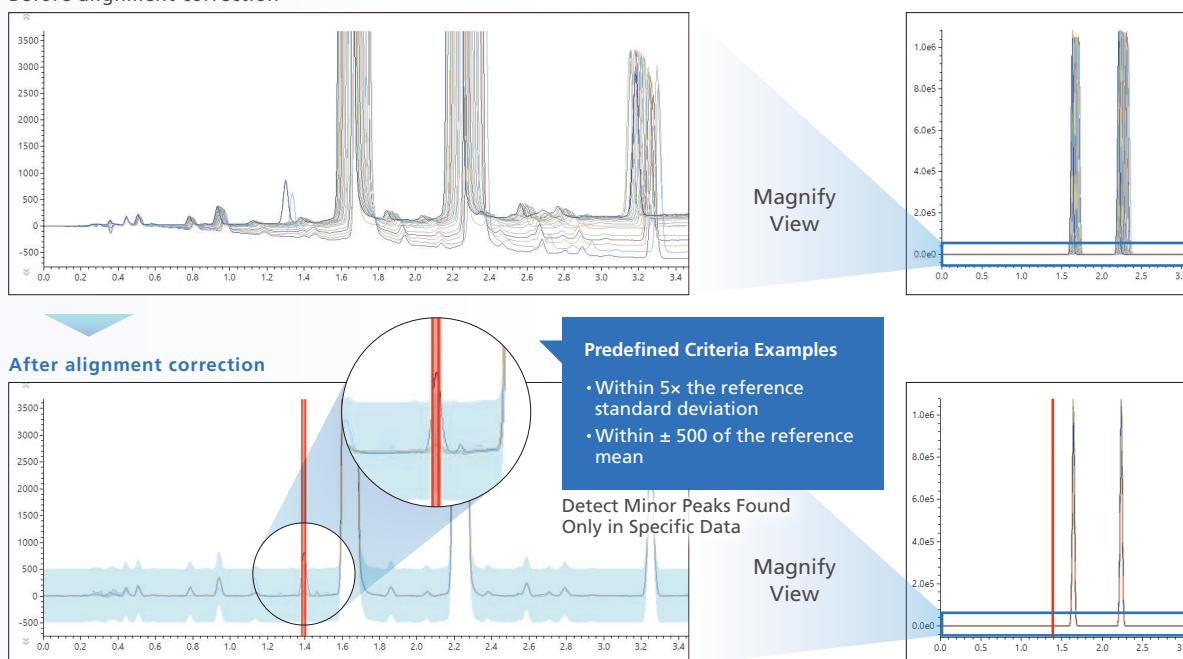
Analyzing Differences in Chromatogram Shapes and Detected Peaks

Accumulated reference data

Detect differences!

Daily sample data

Efficient extraction of data containing differences
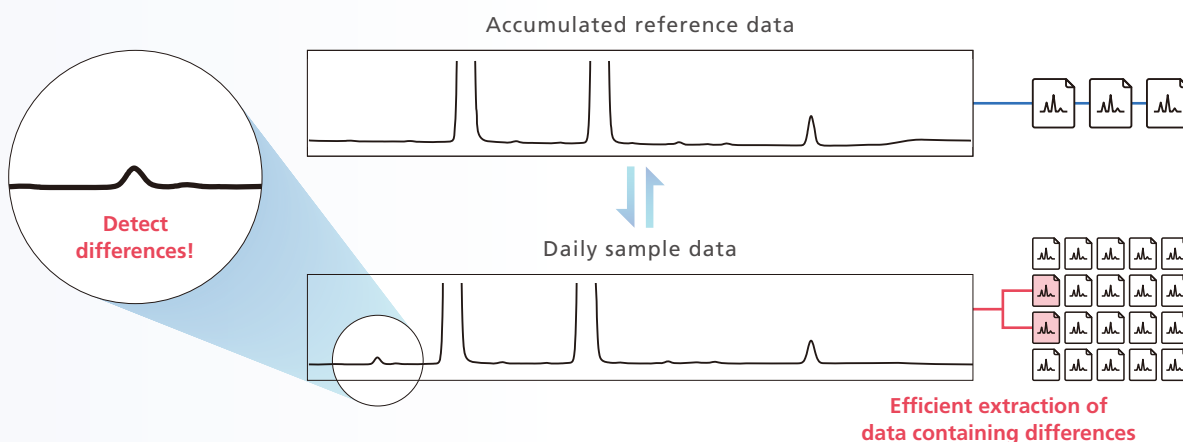
Smarter Chromatogram Comparison Through Retention Time Alignment

Overlaying chromatograms is an effective way to identify waveform differences. However, lot variations, instrument conditions, laboratory environments, and other factors may cause retention times and baselines to fluctuate. As a result, even when chromatograms are overlaid, it may not be possible to accurately detect differences. LabSolutions Detect enables overlay display after performing alignment (automatic retention time correction), allowing users to compare chromatograms without being affected by retention time shifts or baseline fluctuations. Additionally, the software can determine whether peaks fall outside the reference criteria range, making it easier to detect anomalies.

Before alignment correction

Magnify View

After alignment correction

Predefined Criteria Examples
- Within 5× the reference standard deviation
- Within ± 500 of the reference mean

Detect Minor Peaks Found Only in Specific Data

Magnify View

Automatically Match Similar Peaks to Instantly Detect Common Impurities

Traditionally, checking for anomalies in the quantity of controlled compounds or for the presence of unexpected impurities required a multi-step process: first identifying the target compounds and reviewing their peak information, then manually comparing unidentified peaks across multiple datasets based on retention time to determine whether they represented the same impurity.
LabSolutions Detect automates this complex matching process with its clustering function, which groups similar peaks and instantly detects impurities common across datasets. The matching results are clearly visualized in both the chromatogram overview and the peak table, enabling immediate review and streamlined analysis.

Reference

#	Data File Name	Sample Name	Overall Result	Chromatogram Shape	Data Summ Peak Count	New Compound#1 (N Ret. Time	Area	Known Compound#1 (K Ret. Time	Area	Known Compound#2 (Kn Ret. Time	Area	Known Compound#3 Ret. Time	Area
1	Ref_01.lcd	Pramipexole			3			1.717	2018649	2.320	2131863	3.277	6229
2	Ref_02.lcd	Pramipexole			3			1.692	2015791	2.288	2127991	3.298	6235
3	Ref_03.lcd	Pramipexole			3			1.668	2020239	2.260	2133634	3.202	6233
4	Ref_04.lcd	Pramipexole			3			1.645	2020959	2.233	2158282	3.250	6242
5	Ref_05.lcd	Pramipexole			3			1.638	2020309	2.223	2132926	3.158	6236

Target

#	Data File Name	Sample Name	Overall Result	Chromatogram Shape	Data Summ Peak Count	New Compound#1 (N Ret. Time	Area	Known Ret. T	Area	Ret. Time	Area	Ret. Time	Area
1	Target_01.lcd	Pramipexole			3								
2	Target_02.lcd	Pramipexole			3								
3	Target_03.lcd	Pramipexole			3								
4	Target_04.lcd	Pramipexole			3								
5	Target_05.lcd	Pramipexole			3								
6	Target_06.lcd	Pramipexole			3								
7	Target_07.lcd	Pramipexole			3								
8	Target_08.lcd	Pramipexole			3			1.655	2019888	2.243	2133015	3.185	6234
9	Target_09.lcd	Pramipexole			3			1.652	2023900	2.238	2139224	3.177	6243
10	Target_10.lcd	Pramipexole	Outside the criteria	Outside the criteria	4	1.337	1490	1.717	1998132	2.337	2111739	3.307	6181
11	Target_11.lcd	Pramipexole	Outside the criteria	Outside the criteria	4	1.300	1542	1.633	1999495	2.217	2111815	3.150	6176
12	Target_12.lcd	Pramipexole	Outside the criteria	Outside the criteria	4	1.300	1536	1.628	2000580	2.210	2112797	3.183	6216

Predefined Criteria Examples

- Number of peaks: 3 or fewer
- Area of unknown impurities: 1,000 or less
- Area of Compound A: reference value – 10,000 or more

Based on predefined criteria, the software evaluates whether the results of detected peaks fall within acceptable limits. It enables users to check for the presence of impurity peaks that exceed control thresholds, as well as verify the intensity values of target compounds.

One-Click Anomaly Analysis Report Generation

LabSolutions Detect allows users to generate anomaly analysis reports without complex settings.
The report includes overlayed chromatogram displays as well as lists of compounds and impurities. It also highlights results that fall outside the predefined criteria — enabling users to review difference analysis results at a glance.
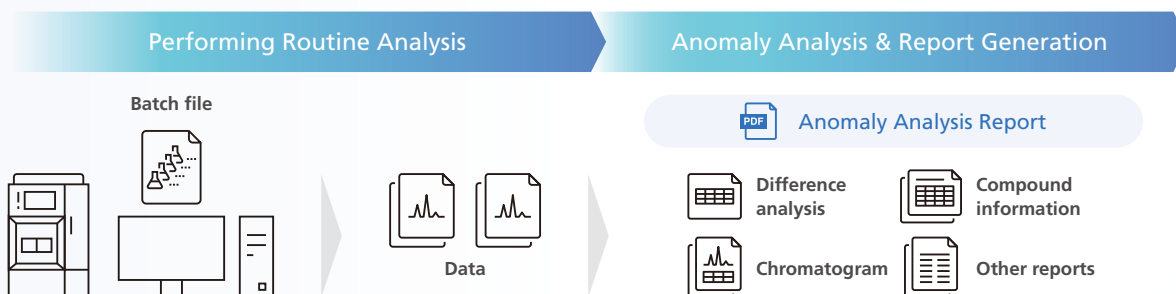
Example of a Anomaly Analysis Report

Magnify View

Highlight results that do not meet the following predefined criteria:

- Number of peaks: more than 3
- Area of unknown impurities: greater than 1,000
- Area of Compound A: reference value – 10,000 or more

Magnify View

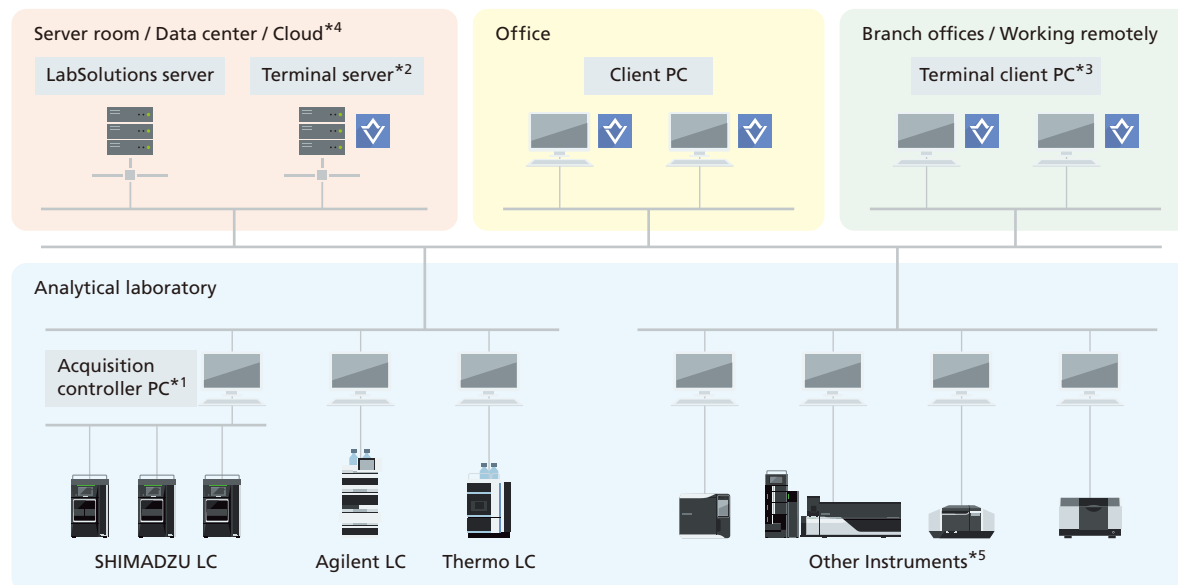# Store All Difference Analytical Results in an Integrated Database

LabSolutions Detect supports data management within the LabSolutions database, allowing users to manage difference analysis reports together with the original data files — ensuring data integrity.
Because it integrates seamlessly with LabSolutions, reports can be generated without the need to export or import data or method files.

LabSolutions Database

Performing Routine Analysis	Anomaly Analysis & Report Generation
Batch file	Anomaly Analysis Report
Data	Difference analysis / Compound information / Chromatogram / Other reports

Network Management with LabSolutions CS

By integrating LabSolutions Detect with LabSolutions CS, users can streamline quality testing operations.
All analytical data is managed within a server-based database, allowing access from any PC on the network. Even client PCs that are not directly connected to analytical instruments can perform analysis using LabSolutions Detect.

Server room / Data center / Cloud*4 — LabSolutions server, Terminal server*2
Office — Client PC
Branch offices / Working remotely — Terminal client PC*3

Analytical laboratory
Acquisition controller PC*1

SHIMADZU LC   Agilent LC   Thermo LC   Other Instruments*5

*1 The acquisition controller PC controls analytical instruments.
*2 A terminal server is a server for using terminal services. Users can generate data reports using LabSolutions Detect through terminal services.
   It is also ideal for remote connections due to its low network load.
*3 If a terminal service is used, then LabSolutions and LabSolutions Detect software do not need to be installed on client PCs
*4 Servers can be built on various clouds (IaaS). AWS (Amazon Web Services), Azure (Microsoft Azure), GCP (Google Cloud Platform)
*5 LabSolutions Detect only supports LC data.

Streamlining Analytical Workflows with Shimadzu LC

LabSolutions Detect supports differential analysis across all Shimadzu LC systems.
Building on the exceptional performance of Shimadzu's LC technology, it meets the evolving needs of modern laboratories — where people, environments, and working styles are increasingly diverse — while consistently delivering reliable, high-quality results.
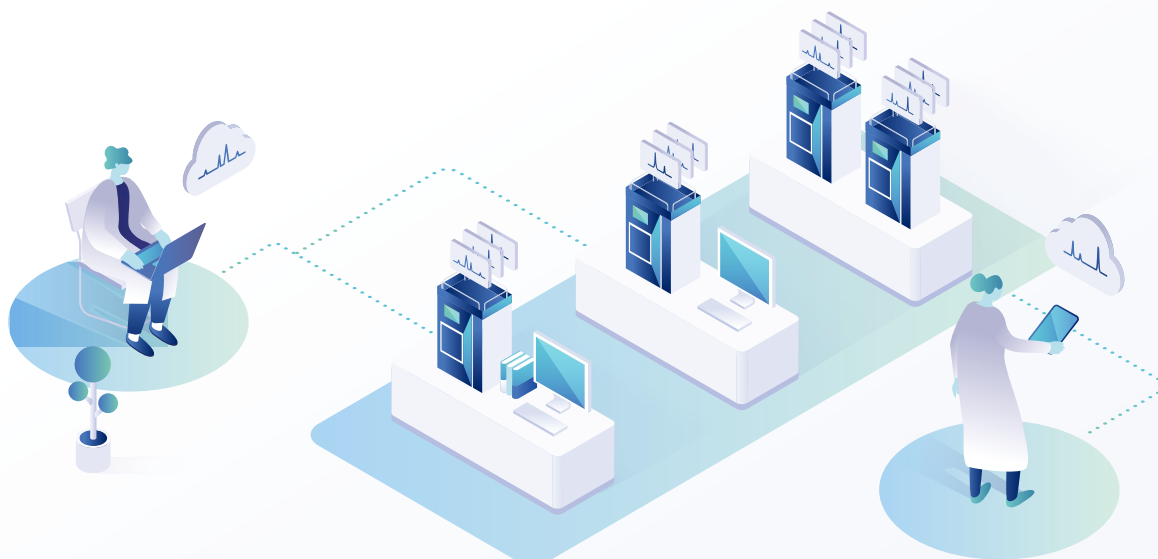
License Types

• 1st year pack
• 1-year licecse

Application

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