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Application News

Anomaly Peak Detection Support Software
Ultra High Performance Liquid Chromatograph

Streamlining Quality Control Operations with LabSolutions™ Detect

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User Benefits

- LabSolutions Detect enhances the reliability and productivity of quality control processes while minimizing the risk of errors or oversights associated with manual visual inspection.
- By overlaying chromatograms through alignment processing, the software enables rapid detection of abnormalities such as impurity contamination.

■ Introduction

In quality control of pharmaceuticals and functional foods, verification of impurities and active ingredient content is essential to ensure product efficacy and safety. These analyses are generally performed by qualitative and quantitative LC methods, with relevant guidelines including ICH Q3A, Q3B[1], and the GMP guidelines for functional foods scheduled to take effect in 2026[2]. In such verification, numerous chromatograms must be examined to identify peaks based on retention times, compare quantitative results with acceptance criteria, and confirm the presence or absence of impurities. When performed manually, these extensive tasks present a risk of human error and missed detections. LabSolutions Detect, an anomaly peak detection support software, addresses this issue by automatically analyzing differences between reference chromatograms representing impurity-free conditions (reference data) and chromatograms obtained in routine quality control (target data). This approach minimizes the risk of overlooking variations in active ingredient content or impurity contamination. As a result, LabSolutions Detect enables efficient, regulatory-compliant quality control operations. In this article, a case example of streamlining quality control processes is presented using a model sample of pramipexole hydrochloride, a compound listed in the USP.

■ Analytical Conditions and Target Samples

The analytical conditions for pramipexole hydrochloride in the system suitability test are summarized in Table 1. In this test, detection of both pramipexole and compound A (reference standard) is required (Fig. 1). LabSolutions Detect automatically evaluates chromatograms according to predefined criteria, confirming the presence of impurity peaks exceeding control thresholds and comparing the responses of specified compounds with their acceptance limits. In this study, the chromatogram shown in Fig. 1 was employed as the reference data, with the upper limit of the normalized peak area percentage of unknown impurities and the lower limits of the peak areas of pramipexole and compound A defined as control criteria (Table 1). Multiple target chromatograms were then automatically assessed for compliance with these criteria.

Table 1 Analytical Conditions [3]

System	: LC-2070C with compatibility kit
Sample	: Pramipexole dihydrochloride (1.5 mg/mL) and compound A (0.8 mg/mL)
Mobile phase	: A) 67 mmol/L (potassium) phosphate buffer containing 21 mmol/L 1-octanesulfonic acid sodium salt (pH 3.0) : B) Mobile Phase A / Acetonitrile = 50 : 50
Column	: Shim-pack Scepter™ C18-120 (150 mm × 4.6 mm I.D., 5 µm)*1
Injection Vol.	: 5 µL
Time program	: B Conc. 40%(0 min)→80%(15 min)→40%(15.1-20 min)
Column Temp.	: 40 °C
Flow rate	: 1.5 mL/min
Detection (UV)	: 264 nm
Criteria of peak detection :	
Upper limit of impurity (area %)	: 0.03
Lower limit of pramipexole (area)	: 7,700,000
Lower limit of compound A (area)	: 8,000,000

*1 P/N: 227-31020-05 (Shimadzu GLC product number)

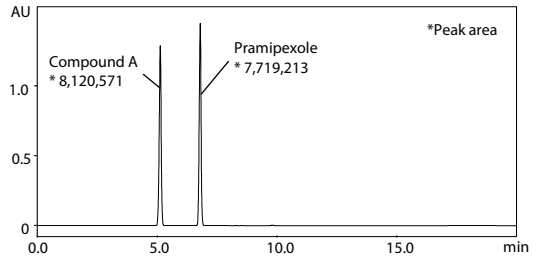

Fig. 1 Chromatogram of Pramipexole Hydrochloride

■ Abnormal Peak Detection Using LabSolutions Detect

LabSolutions Detect is operated according to the following two steps:

(1) Define control criteria for the reference data.

(2) Apply the predefined control criteria to the target data.

As an example, Fig. 2 illustrates the control criteria set for the reference data (chromatogram in Fig. 1), consisting of an upper limit for the normalized peak area percentage of unknown impurities (0.03%) and lower limits for the peak areas of pramipexole and compound A (7,700,000 and 8,000,000, respectively). Fig. 3 presents the results of applying these criteria to multiple target datasets. The target data comprised three manufacturing lots, each analyzed in triplicate (n = 3), yielding a total of nine (3 × 3) chromatograms.

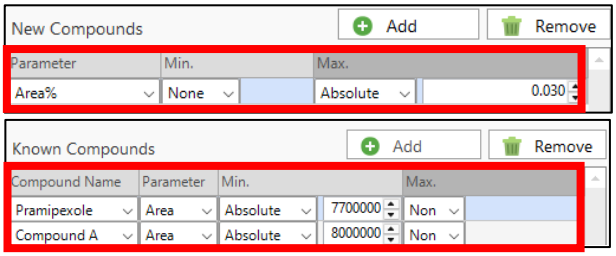

Fig. 2 Control Criteria for Unknown Impurities (upper) and for Pramipexole and Compound A (lower)

Reference

			New Compound#1 (Impurity)		Known Compound#1 (Pramipexole)		Known Compound#2 (Compound A)	
Reference data	mple Name	Overall Result	Area	Area%	Area	Area%	Area	Area%
1 Reference...	prami+compA				7719213	48.733	8120571	51.267
2 Reference...	prami+compA				7714090	48.738	8113503	51.262
3 Reference...	prami+compA				7718791	48.741	8117710	51.259

Target

				New Compound#1 (Impurity)		Known Compound#1 (Pramipexole)		Known Compound#2 (Compound A)	
#	Data File Na	Sample Name	Overall Result	Area	Area%	Area	Area%	Area	Area%
Lot 1	_001.lcd	prami+compA				7719213	48.733	8120571	51.267
	_002.lcd	prami+compA				7714090	48.738	8113503	51.262
3	Lot1_003.lcd	prami+compA				7718791	48.741	8117710	51.259
Lot 2	_001.lcd	prami+compA	Outside the criteria	6312	0.039	7820010	48.683	8236841	51.278
	_002.lcd	prami+compA	Outside the criteria	6299	0.039	7819240	48.683	8235879	51.277
6	Lot2_003.lcd	prami+compA	Outside the criteria	6350	0.040	7819990	48.683	8236585	51.277
Lot 3	_001.lcd	prami+compA	Outside the criteria	70970	0.457	7530284	48.460	7938045	51.084
	_002.lcd	prami+compA	Outside the criteria	70986	0.457	7532826	48.464	7939264	51.079
9	Lot3_003.lcd	prami+compA	Outside the criteria	70904	0.456	7532244	48.461	7939836	51.083

Fig. 3 Results of Pass/Fail Decisions by LabSolutions Detect (red boxed values indicate items that did not meet the control criteria)

The orange box at the top of Fig. 3 shows the normalized peak area percentages and peak areas of each compound (pramipexole and compound A) detected in the reference data. The analysis results of the target data are displayed in the blue box for lot 1, the green box for lot 2, and the red box for lot 3. Values that do not meet the control criteria are highlighted in red, allowing for quick visual confirmation. For lot 2 and lot 3, unknown impurities exceeding the upper limit (0.03%) of normalized peak area percentage were detected. In addition, for lot 3, the peak areas of pramipexole and compound A were below the lower limit of the respective control criteria. Thus, by simply loading the target data into LabSolutions Detect, the presence of impurities, as well as the identification and pass/fail assessment of target compounds, can be performed automatically. This approach not only reduces human errors in decision-making but also streamlines quality control workflows.

■ Easy Confirmation of Chromatographic Differences

LabSolutions Detect enables easy and visual confirmation of differences between chromatograms by using overlaid plots and alignment processing (automatic correction of retention time and baseline). Overlaying the chromatograms of the nine target data sets (Fig. 4) allows intuitive assessment of the peak areas and retention times of unknown impurities. Furthermore, by applying alignment processing to overlaid plots (Fig. 5), differences between data can be confirmed visually without being affected by retention time shifts or baseline fluctuations.

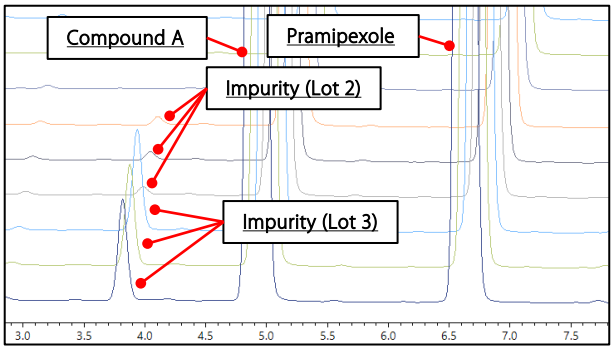

Fig. 4 Visualization of Impurity Peaks Using Overlaid Chromatograms

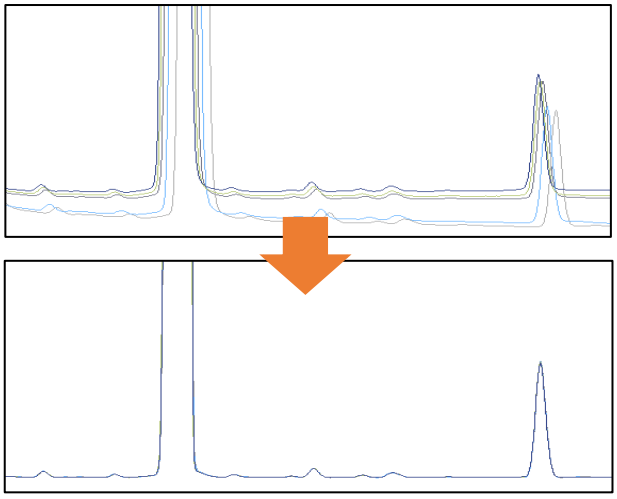

Fig. 5 Clear Comparison of Chromatograms Using Alignment Processing
Before alignment (upper), After alignment (lower)

■ Conclusion

In quality control, ensuring product efficacy and safety is essential. LabSolutions Detect automatically analyzes the differences between reference and target data, enabling automated detection of unknown impurities and pass/fail assessment against control criteria. This helps streamline quality control workflows while maintaining high reliability.

<References>

1) International Council for Harmonisation of Technical Requirements for Pharmaceuticals for Human Use (ICH) : Q3A, Q3B
2) Consumer Affairs Agency, Food Labeling Division. (only in Japanese)
3) US Pharmacopeia 43-NF38, 2022
"Pramipexole Dihydrochloride"

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