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Application News

Anomaly Peak Detection Support Software
Gas Chromatograph

LabSolutions Detect™ for Automated Anomaly Detection in HS-GC-Based Pharmaceutical Residual Solvent Testing

Yu Nagao

User Benefits

- LabSolutions Detect™ anomalous peak detection functionality improves the reliability and productivity of quality control operations.
- Reporting functionality and compatibility with LabSolutions DB/CS help maintain data integrity and ensure analytical data can be recorded reliably.

■ Introduction

Pharmaceutical quality control is critically important for protecting human health and safety. For organic solvents that may adversely affect human health, pharmacopeias, such as the USP, EP, and JP, specify limits for residual solvent levels in pharmaceutical products, which requires stringent controls. In addition to controlling the content of known regulated substances, pharmaceutical quality controls increasingly require monitoring unexpected or unknown components and assessing their concentration levels. However, in quality control operations that involve analyzing large numbers of samples using the same test method, it can be difficult and time-consuming to inspect and manage vast amounts of data without overlooking anomalous results.

LabSolutions Detect (Fig. 1) is software that can automatically detect anomalies in sample data based on reference data. It can analyze large volumes of data in a single operation, providing efficient and robust support for quality control operations.

This Application News article describes an example of using LabSolutions Detect for data obtained using headspace gas chromatography (HS-GC; Fig. 2), a method used for pharmaceutical residual solvent testing.

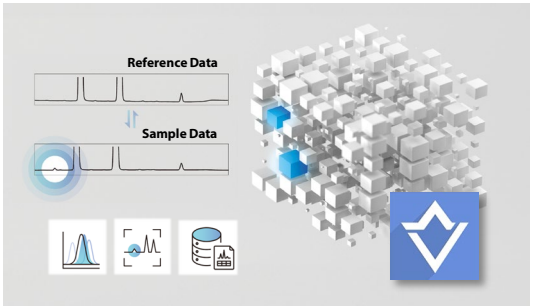


Fig. 1 LabSolutions Detect™



Fig. 2 Headspace sampler (HS-20 NX) and gas chromatograph (Nexis™ GC-2060)

■ LabSolutions Detect Software Features

LabSolutions Detect visualizes differences between accumulated reference data and target data acquired during routine testing and provides the following three functions for reviewing analytical results: (1) comparison of chromatogram shapes using automatic retention-time correction, (2) detection of potential impurities common to multiple data sets by identifying similar peaks, and (3) centralized management of difference-analysis results and report generation.

■ Analysis Using LabSolutions Detect

Reference data can be imported either with peaks already integrated or with peaks integrated after importing. LabSolutions Detect then automatically evaluates the detected peaks (Fig. 3). Next, the "Criteria Parameters" settings are configured for the target data (Fig. 4). The criteria parameters allow threshold values to be specified for peak attributes, including the intensity of known peaks, intensity criteria for unknown peaks, minimum and maximum peak counts, retention time, and tailing factor. That enables automatic determination of whether known peaks meet the specified intensity criteria and whether unknown peaks are present at levels that warrant investigation as impurities.

Fig. 5 shows a baseline-shifted comparison between the reference data and the average chromatogram. The maximum allowable range of variation in the chromatographic profile, as specified by the "Criteria Parameters" settings, is displayed as a light-blue band in Fig. 5.

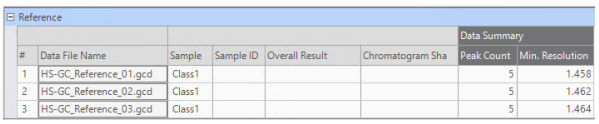


Fig. 3 Imported reference data

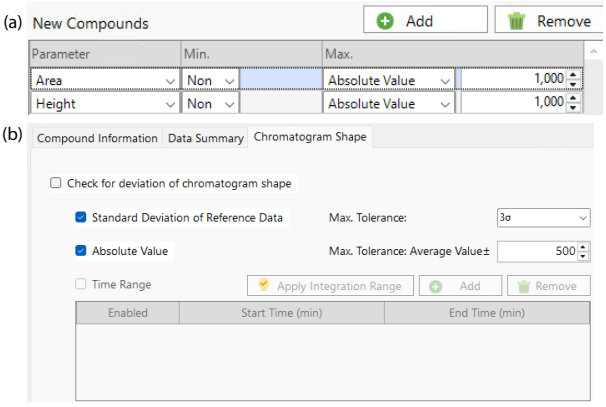


Fig. 4 Examples of criteria parameters: (a) criteria for new compounds (b) criteria for chromatogram shape

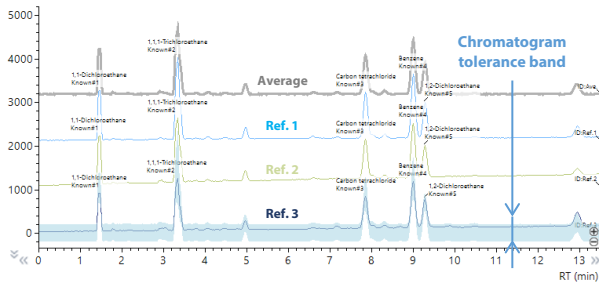


Fig. 5 Reference chromatograms and corresponding average (gray) chromatogram, shown with baselines shifted

■ Application Example Using a Class 1 Standard Solution for Residual Solvents in Pharmaceuticals

Reference and target chromatographic data was generated from the Class 1 standard solution for water-soluble articles using HS-GC and were analyzed with LabSolutions Detect. The evaluation results are shown in Fig. 6. Three sets of target data fell outside the predefined criteria, shown highlighted in red. In this example, the reference data contained five peaks, whereas each set of the target data that fell outside the predefined criteria contained six peaks.

Reference

#	Data File Name	Sample Name	Sample ID	Overall Result	Chromatogram Shape	Data Summary: Peak Count	Data Summary: Min. Resolution
3	HS-GC_Reference_03.gcd	Class1				5	1.464
2	HS-GC_Reference_02.gcd	Class1				5	1.462
1	HS-GC_Reference_01.gcd	Class1				5	1.458

Target

#	Data File Name	Sample Name	Sample ID	Overall Result	Chromatogram Shape	Data Summary: Peak Count	Data Summary: Min. Resolution
1	HS-GC_Target_01.gcd	Class1				5	1.468
2	HS-GC_Target_02.gcd	Class1		Outside the criteria	Outside the criteria	6	1.444
3	HS-GC_Target_03.gcd	Class1		Outside the criteria	Outside the criteria	6	1.453
4	HS-GC_Target_04.gcd	Class1				5	1.472
5	HS-GC_Target_05.gcd	Class1		Outside the criteria	Outside the criteria	6	1.452

Fig. 6 Evaluation results for the target data sets

Fig. 7 compares overlaid chromatograms for the sets of target data that fell outside the predefined criteria in Fig. 6. Anomalous peaks that did not correspond to any of the five compounds defined in the reference data were observed in those sets of target data. Although a comparable assessment can be performed using conventional workflows that involve visually inspecting all chromatograms, LabSolutions Detect allows up to 200 data sets to be displayed simultaneously at this stage of the analytical workflow, thereby facilitating the efficient identification of data sets containing unexpected anomalies.

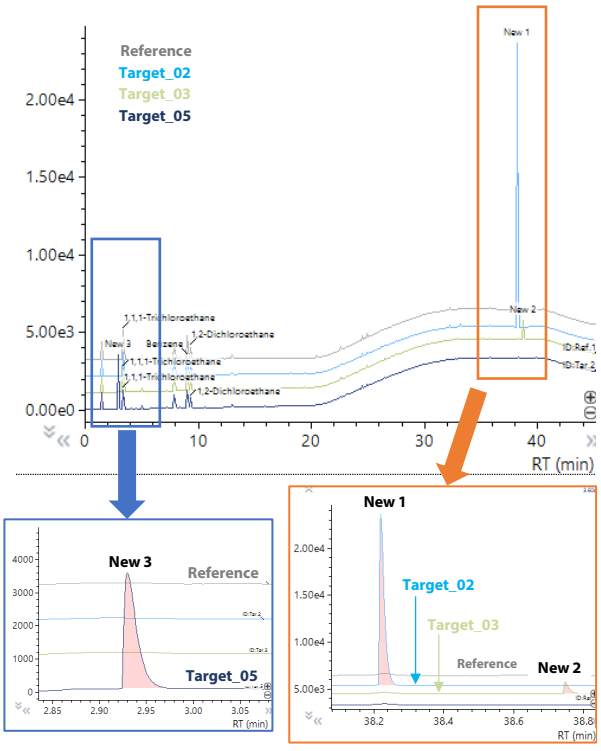


Fig. 7 Comparison of chromatograms for reference data (gray) and target data that fell outside the predefined criteria. Insets show enlarged views. New 1 to 3 indicate peaks detected and flagged as anomalous.

LabSolutions Detect also supports report generation, allowing various analytical results to be compiled into a single report. Fig. 8 shows a report for a target data set in which anomalous peaks were observed (Fig. 7). In addition to the results for the target analytes, the report also includes other information, such as the intensities of peaks identified as anomalous (red boxes in Fig. 8). That helps maintain a complete record of the quality control results for each sample. Furthermore, LabSolutions Detect is compatible with LabSolutions DB/CS analytical data management software, which helps ensure compliance with data integrity requirements for instrumental analysis.

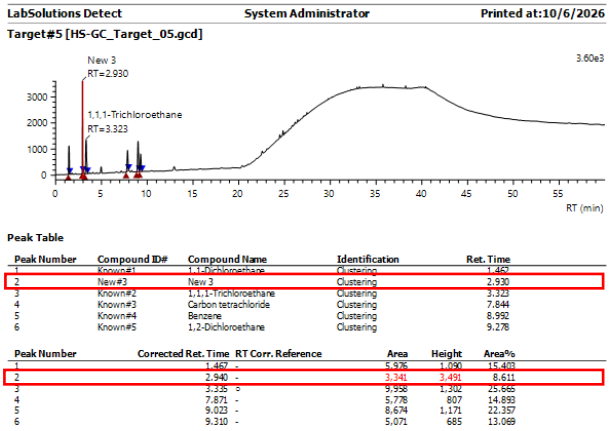


Fig. 8. Example of a report generated by LabSolutions Detect. The red boxes indicate information on newly detected peaks flagged as anomalous.

■ Conclusion

LabSolutions Detect was used to automate anomaly detection in data from HS-GC analysis of residual solvents in pharmaceuticals. By automating data analysis, LabSolutions Detect streamlines the manual visual review process traditionally required for rigorous pharmaceutical quality control, even for large data sets. Furthermore, its reporting functionality and compatibility with LabSolutions DB/CS enable the reliable recording and reporting of results while supporting compliance with data integrity requirements.

Related Applications

1. Streamlining Quality Control Operations with LabSolutions Detect, Application News No. 01-01014-EN
2. Streamlining Impurity Management Using LabSolutions Detect, Application News No. 01-01221-EN

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