Achieving More Efficient Data Review with OpenLAB CDS

Technical Note

Introduction

Separations have enjoyed major advances that have significantly reduced chromatographic run times. Ultra high performance liquid Chromatography (UHPLC), sub-2 micron particle-size LC columns, and dual-column gas chromatography (GC) systems allow for larger amounts of chromatographic data to be collected. As a result, labs now process and review very large chromatography data sets, which sometimes contain thousands of peaks. Data review tasks typically rely on manual interpretation of chromatograms, peak integration baselines, calibration curves, and calculated results to ensure they fall within specifications. Further, any incident or anomaly that negatively impacts production requires immediate investigation of these data to allow fast problem resolution. Together these factors create a compelling need for much more efficient data review and visualization.

Peak Explorer, an OpenLAB CDS data analysis capability, speeds up data review for complex samples by providing a new way of navigating and visualizing large data sets to find trends, missing or additional peaks, retention time shifts, integration problems, outliers, and artifacts. Peak Explorer also gives you the power to quickly evaluate your data during method development.

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The power of visualization

When presented in the correct manner, the human eye is powerful in its ability to identify anomalies in large data sets. Peak Explorer is specifically designed to present chromatographic data in a format optimized for visualization by the human eye.

As shown in Figure 1, Peak Explorer displays all peaks in a complex chromatographic data set (left) in a bubble chart (right) designed for easy scanning of anomalies. The X-axis is retention time and the Y-axis is the injection number of the data set loaded. The size of the bubble displayed represents a specific user-selected value related to the peak size. The value choices include area, height, area %, height %, width, amount, and concentration. Figure 2 shows a bubble chart where peak area was selected for display.

The Peak Explorer data presentation is highly customizable as the user can choose what to see and how it is shown. By default, the software displays a linear interpolation of the smallest to the largest value of all displayed peaks, though this setting can be turned on or off. Clicking on a specific bubble displays a tooltip that provides the analyst with more detailed information about a specific peak or selected injection (blue line shown in Figure 2). Identified peaks are shown in orange and unidentified peaks are shown in blue.

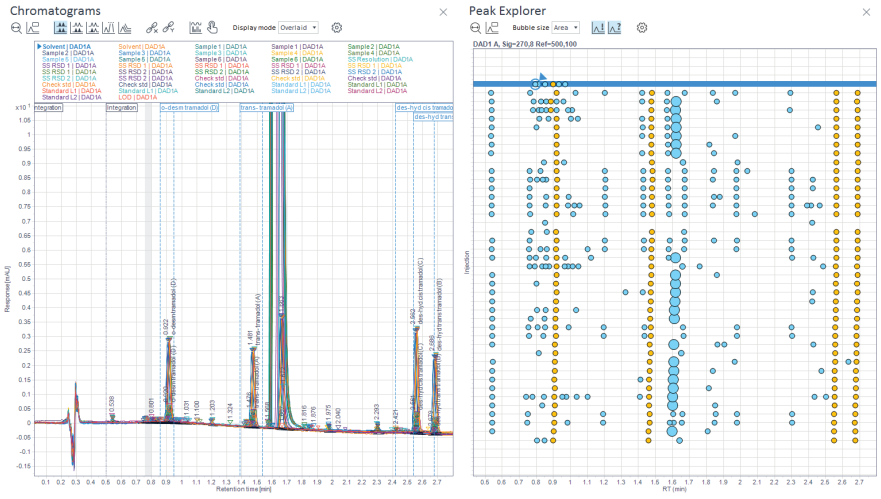

Figure 1. Chromatogram view (left) compared to Peak Explorer view (right).

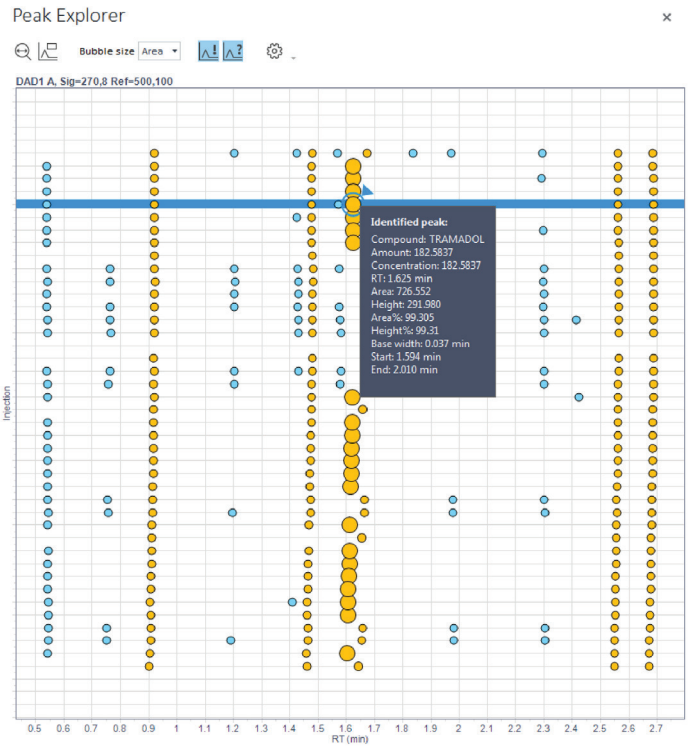

Figure 2. Peak Explorer data presentation detail. The X-axis is the retention time and the Y-axis is the injection number of the data set loaded. The size of the bubble represents peak area.

As shown in Figure 3, it's very easy to find additional peaks (green box), missing peaks (red box), and peaks not correctly identified (blue box) within seconds by comparing the fingerprints of chromatograms across all of the injections. Even in data sets with thousands of peaks, "holes" and patterns are easy to find.

As shown in Figure 4, when displaying the bubble chart results by concentration versus retention time, it is very easy to visualize and compare a detector's response to a specific compound. In this example, the electron capture detector (ECD) detected compounds around 3.5 minutes, while the nitrogen phosphorus detector (NPD) did not. This shows the selectivity of the two detectors and that they are both needed for the analysis.

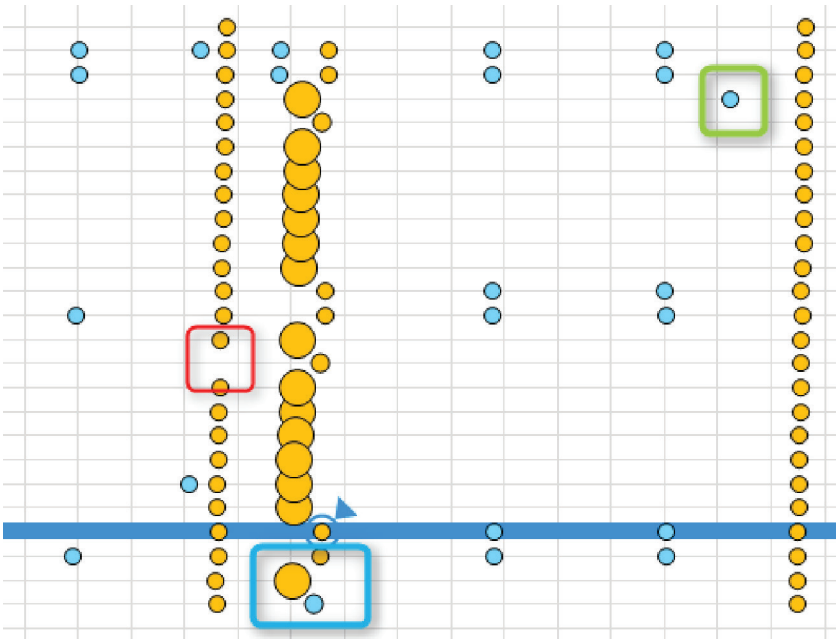

Figure 3. The Peak Explorer display allows rapid detection of additional (green box), unidentified (blue box), and missing (red box) peaks.

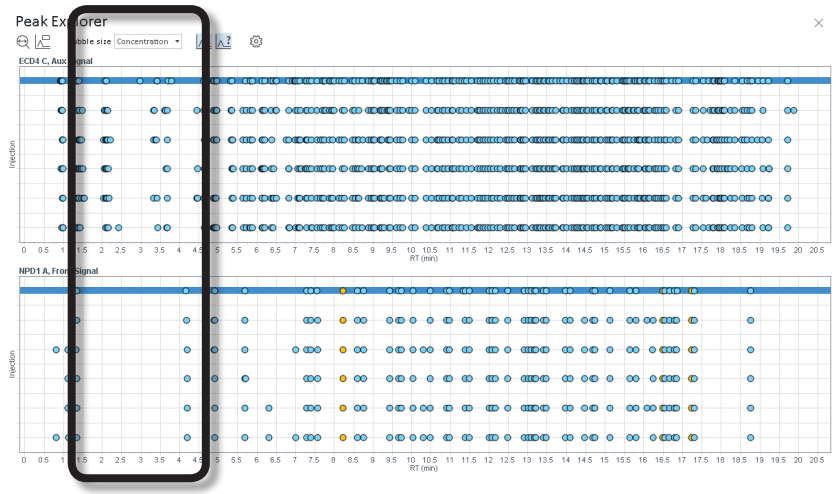

Figure 4. The Peak Explorer display allows easy visualization of detector response. Top: ECD response. Bottom: NPD response.

Retention time shifts–a pump or column problem?

The stability of an LC or GC system is critical to producing accurate and reproducible results. Retention time is a fundamental qualitative measurement of a compound's chromatographic properties and retention time stability is an important parameter for measuring system health. Shifts in retention time occur due to routine maintenance procedures such as column trimming. In a multi-instrument laboratory running duplicate methods, the retention times for each instrument will differ from each other, even when run under seemingly identical conditions. Differences in retention time also complicate comparison of data between instruments and over time.

There are several ways to determine retention time reproducibility. One is to calculate the relative standard deviation (RSD) of a compound's retention time across a set of injections. Or, overlaid chromatograms can be visually compared as shown in Figure 5.

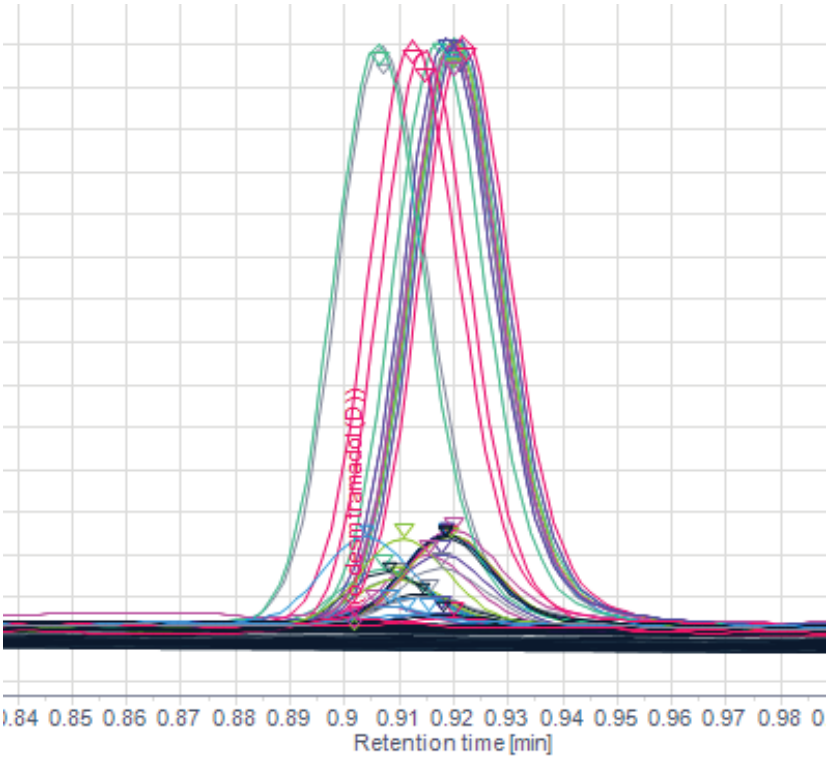

Figure 5. Retention time reproducibility can be reviewed visually using a chromatographic overlay.

While both approaches can indicate the stability of the system, neither offers clues as to the cause of the instability. Unstable LC retention times can be due to air in the pump, solvent mixing problems, and the condition of the column. Peak Explorer provides a unique view of the retention time stability, enabling the user to identify the source of the instability faster.

As shown in Figure 6, a compound appears to elute earlier and earlier over the series of injections. Zooming in on the specific peak clearly shows the instability of the compound's retention time. Earlier elution is indicative of a problem with the column or solvent mixing. Air in the pump typically produces unstable retention times without any trend toward earlier or later elution. Using peak overlays or RSD calculations, this trend would likely be overlooked. Focusing on correcting the column and solvent mixing expedites troubleshooting so the chromatographic system can rapidly be up and running samples again.

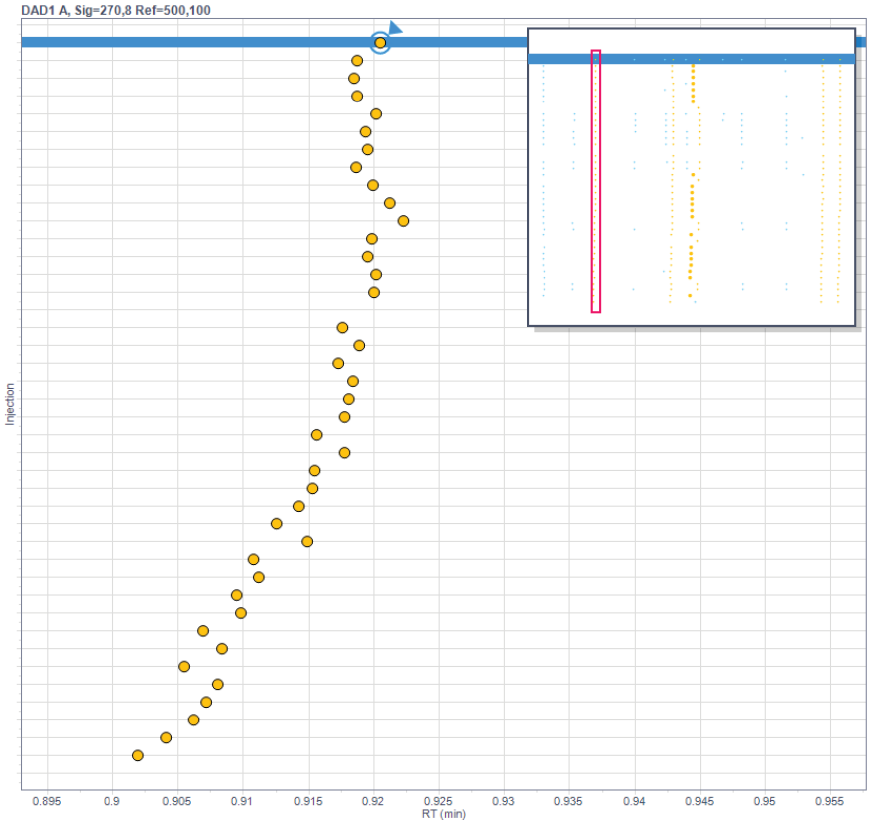

Figure 6. Zooming in on a single compound peak clearly shows the change in retention time for a set of runs.

Ensure correct peak integration, quickly and easily

Ensuring that all peaks are correctly integrated is a tedious data review task. “Correctly integrated” typically means that a peak has been integrated as prescribed by the standard method. In addition, the user wants the peaks integrated consistently even when the baseline between injections changes due to noise or drift. Without Peak Explorer, the user must check integrations using a time-consuming manual process.

Peak Explorer eliminates this manual task. In the example shown in Figure 7, the value for defining the bubble size is first set to base width, which makes it easy to see whether the baseline allocation of peaks are the same in all injections displayed. When selecting one of the outliers, the software automatically displays the zoomed peak in “Peak Details” (Figure 8). The integration problem can be resolved easily by changing the integration parameters in the processing method or by correcting the baseline using the manual integration tool.

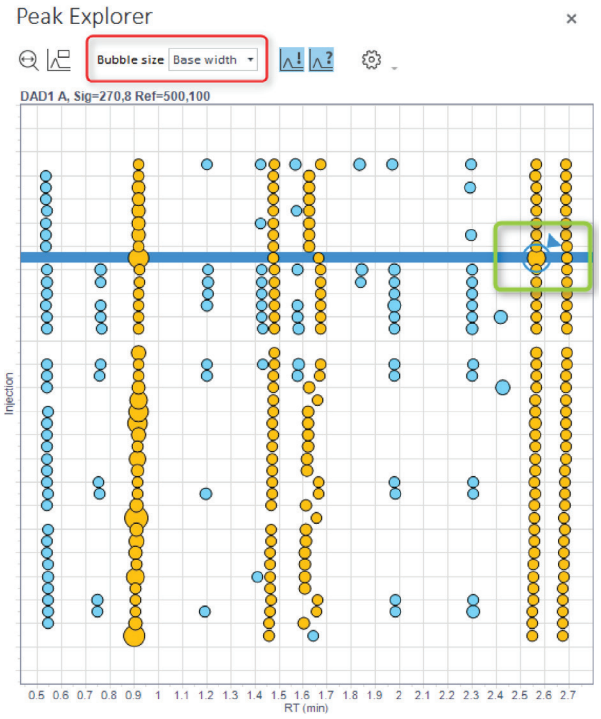

Figure 7. Peak Explorer makes it possible to quickly identify poorly integrated peaks. The bubble size is set to reflect peak base width (red box). Outliers can be selected (green box) for further review.

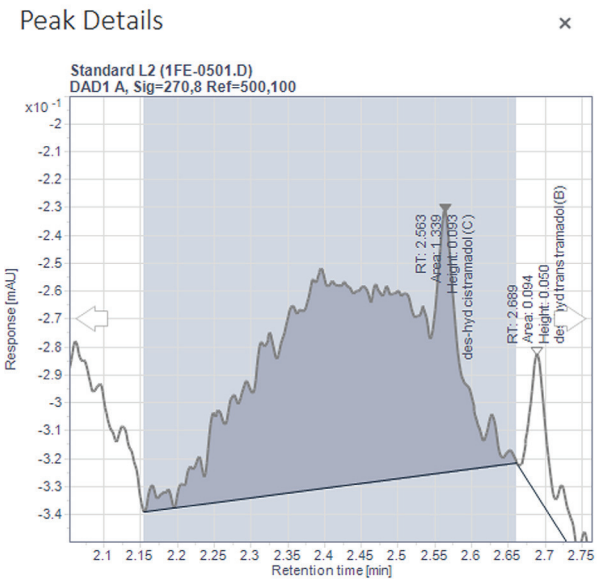

Figure 8. The Peak Details window displays the integration of the selected outlier. Using the forward or back arrows allows the user to review the next or previous peak for comparison.

Speed review of method optimization data

Chromatographic optimization can require hundreds of injections with large data sets generated. Peak Explorer used with the LC Method Scouting Wizard (an add-on to OpenLAB CDS ChemStation Edition) provides an easier way to find the optimal solvent, pH and column for optimal separation of compounds in the shortest run time. As shown in Figure 9, Peak Explorer provides an overview of the separations. Selecting a peak from a specific injection displays the acquisition conditions in the Sample Information window (see Figure 10) as set by the LC Method Scouting Wizard. Very large bubbles indicate large peak areas. The results of method optimization experiments can be summarized using predefined report templates in OpenLAB CDS.

Conclusion

In combination with the full set of capabilities provided by OpenLAB CDS, Peak Explorer is designed to boost sample throughput for laboratories processing large numbers of complex samples. Peak Explorer increases the efficiency of reviewing complex data sets. By presenting chromatographic data and results in a single view, users can easily and rapidly detect artifacts, outliers and patterns. If the user finds an anomaly, Peak Explorer makes it easy to dig deeper into the data in order to determine the cause of the problem so it can quickly be corrected.

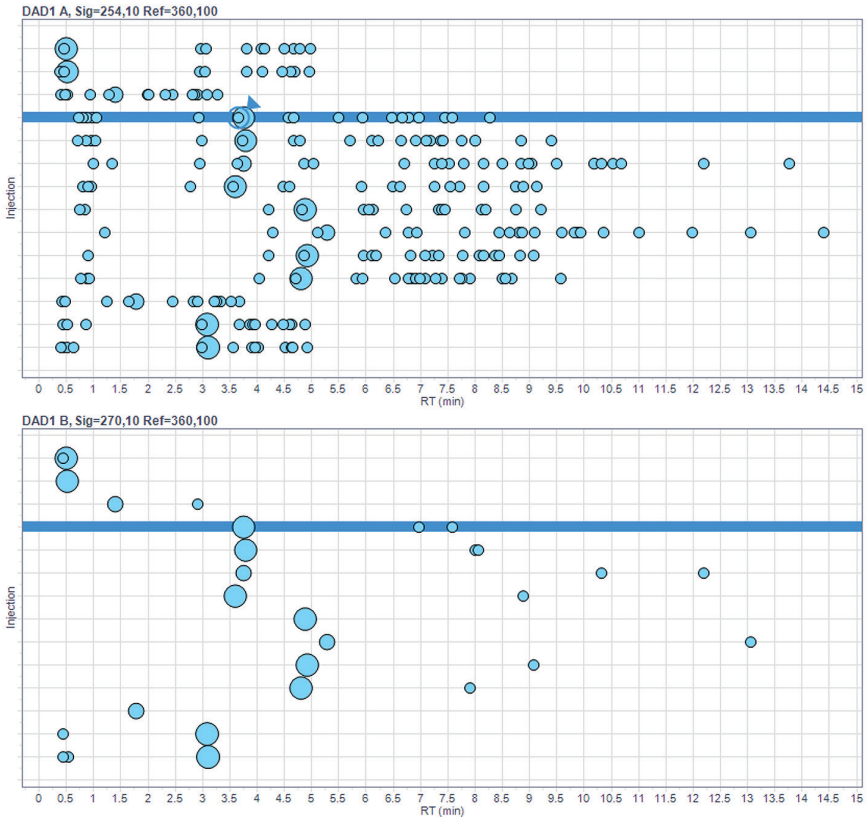

Figure 9. Peak Explorer with the LC Method Scouting Wizard allows rapid review of optimization experiments even when more than one signal is acquired.

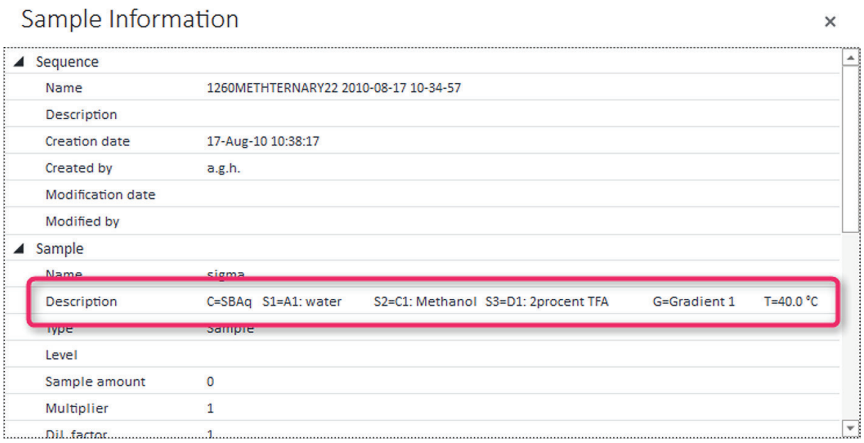

Figure 10. Selecting a peak from a specific injection shown in Figure 9 displays the acquisition conditions in the Sample Information window.

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