

Leveraging Visualizations in Analytical Studio for Efficient Chiral Method Selection

Introduction

Analytical Studio Professional enhances high-throughput purification (HTP) workflows by automating data analysis and decision-making. A key feature within the platform is its visualization capability, a powerful tool that transforms complex chromatographic data into actionable insights. This application note illustrates how a scatter plot visualization accelerated method development for chiral separations by allowing scientists to identify trends and patterns across large datasets that would be difficult to discern through traditional data review methods.

Background

Chiral purification campaigns often require systematic screening of multiple stationary phases and mobile phase modifiers. Here, the objective was to identify conditions that reliably provide adequate resolution between isomers while maintaining fast cycle times. Traditional review methods, manually inspecting chromatograms, are time-consuming and prone to variability.

Analytical Studio addresses this challenge through its integrated visualizations, allowing users to assess performance across many column-modifier combinations in a fraction of the time. This visual approach brings key parameters into focus and highlights trends that would be difficult to detect through serial review. There are several different visualizations available in Analytical Studio, as shown in Figure 1. For this work, a scatter plot visualization was used to determine the best separation techniques for the selected chiral compounds.

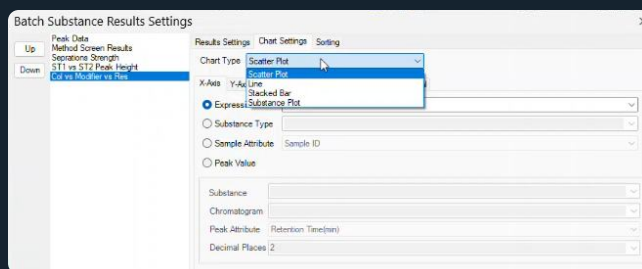


Figure 1

Analytical Studio offers several different types of visualizations to help dig deeper into your data, finding patterns that aren't obvious when reviewing chromatograms and mass spectra individually.

Experimental

In this example, a representative subset of three chiral compounds was screened via supercritical fluid chromatography-mass spectrometry (SFC-MS) across eight columns and four modifiers, resulting in 32 unique conditions. Instead of manually evaluating 96 chromatograms (4 modifiers x 8 columns x 3 compounds) resulting from these 3 samples, the data were processed in Analytical Studio and then viewed using the scatter plot visualization.

Data points were plotted in a two-dimensional space, with modifiers on the x-axis and columns on the y-axis. Key parameters were defined using color and shape which provide an immediate picture of which combinations met both criteria:

- Point color represented whether the resolution between isomers met a predefined threshold (e.g., green if $R_s \geq 2.0$, red if $R_s < 2.0$)
- Point shape indicated whether the retention time of the first-eluting isomer met a throughput threshold (e.g., circle if $R_t \leq 2.0$ min, cross if $R_t > 2.0$ min).

Selecting any point on the chart showed the underlying chromatogram and mass spectrum, ensuring that conclusions drawn from the visual summary could be validated against the source data.

Results

The visualization shown in Figure 2 revealed clear performance patterns:

- Several column-modifier pairs met both the resolution and retention criteria.
- Some pairs offered good resolution but failed to meet retention time requirements, indicating potential bottlenecks for HTP.
- One column, the ChiralPak® IG, consistently underperformed regardless of modifier, as indicated by the red box around the results from this column.
- Another column, the ChiralPak® IB, met both criteria across all modifiers, indicating a strong candidate for full library analysis, as highlighted by the green box around the results from this column.

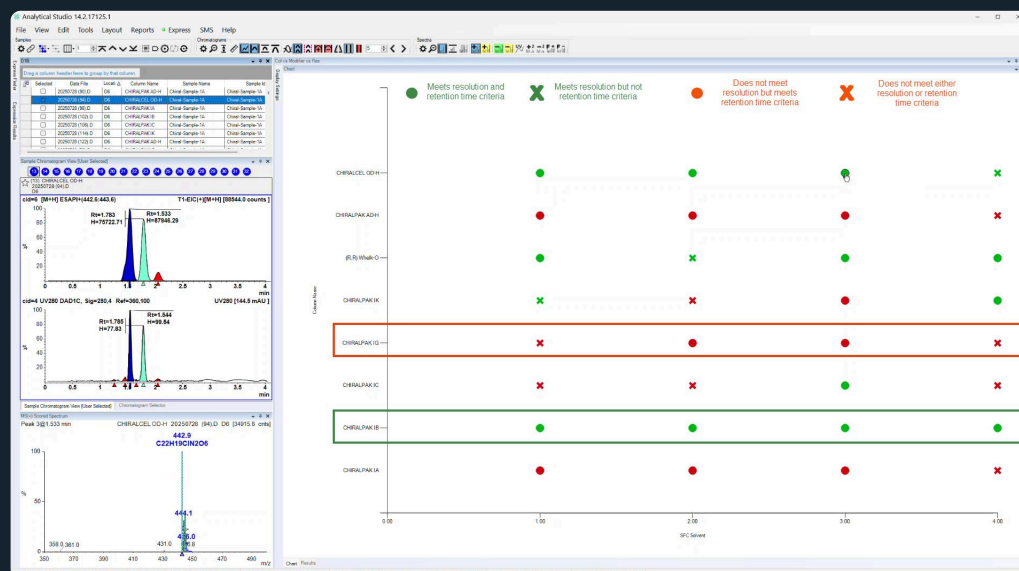


Figure 2

The visualization created by Analytical Studio clearly displays which column/modifier pairs met both the resolution and retention time criteria. The interactive nature of the visualization allows you to view the chromatogram and mass spectrum for any selected point.

This rapid, visual comparison enabled confident selection of optimal conditions for purification of the full chiral library, eliminating ineffective options early in the process.

Conclusion

Analytical Studio's visualizations streamline the method development process by turning complex chromatographic data into structured, decision-ready summaries. In this example, Analytical Studio reduced a task that would normally take hours of expert review into a few minutes, while improving consistency and auditability.

Here, visualizations made it easy to identify poor-performing columns, high-potential modifier combinations, and robust conditions that met multiple criteria. The ability to capture and reuse visualization configurations promotes standardization across teams and projects, turning expert workflows into scalable best practices.

By integrating batch processing with interactive visuals, Analytical Studio empowers scientists to make faster, more reliable decisions, ensuring that purification workflows are optimized not only for quality, but also for speed and reproducibility.

How can Analytical Studio's visualizations help you reimagine your workflow?

Contact us today to see for yourself.