

# Managing small molecule targeted mass spec assays using Skyline and Panorama

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## Overview

Panorama's new support for small molecule assays extends the features previously available for managing proteomics assays, including automated quality control workflows, data management and visualization, and secure sharing with internal and external collaborators. The popular Skyline targeted mass spec desktop application added support for small molecule assays in 2015. This recent work closely integrates Panorama, bringing its newly improved support for monitoring multiple mass spec instruments' performance at a glance. Additionally, Panorama adds capabilities to track revisions of the Skyline document for method building and similar uses. Developed as a module in the LabKey Server data management platform, Panorama is freely available, open source and may be installed and managed by any laboratory or organization. Free, hosted Panorama projects are also available on panoramaweb.org.

## Introduction

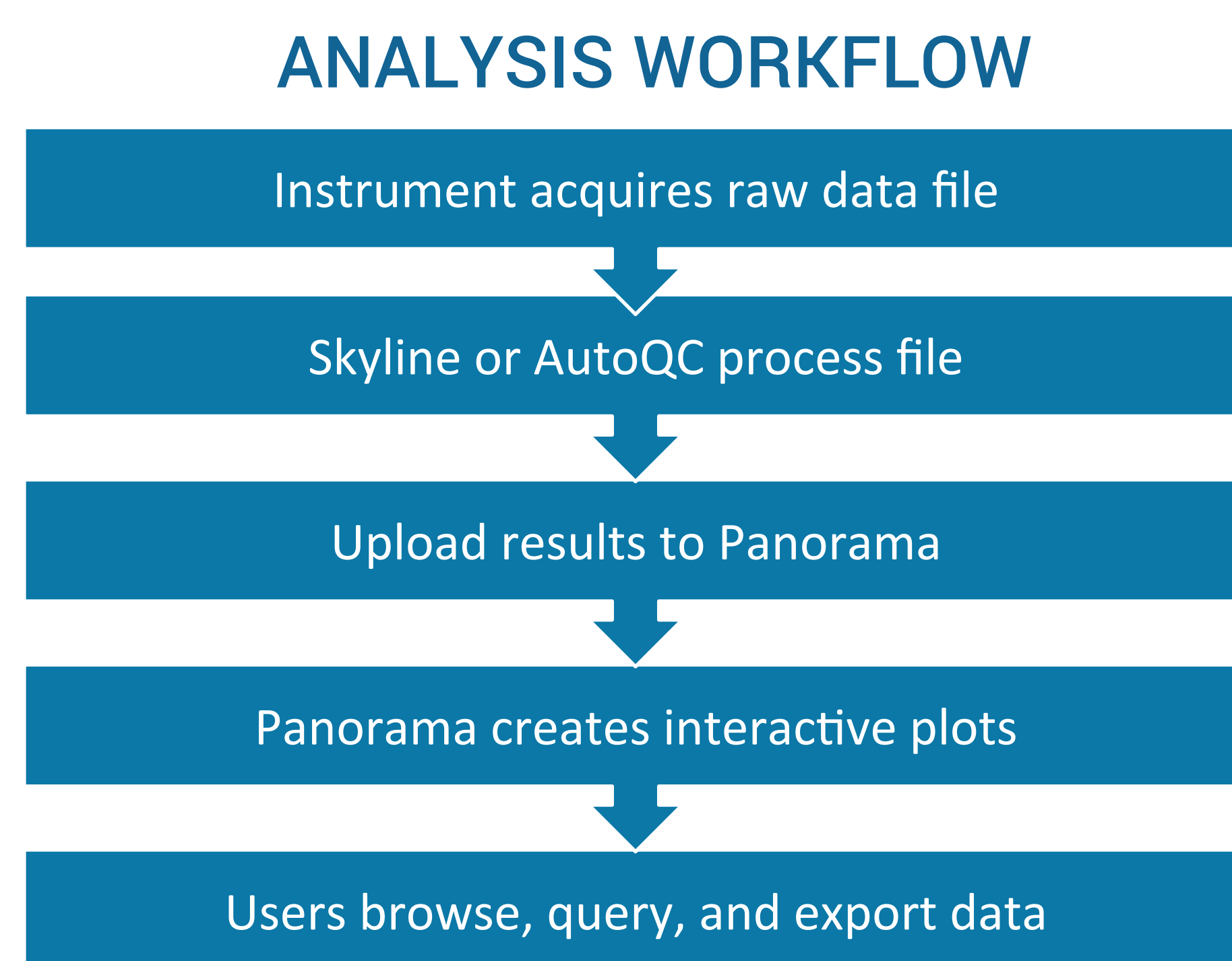


Figure 1: The workflow begins with data acquisition. For experimental assays, the user opens Skyline, analyzes the file, and then publishes to Panorama. For QC workflows, AutoQC monitors for newly acquired QC data files, and automatically analyzes the file and uploads to Panorama. Users can then interactively plot, query, and analyze the data.

## Methods

Skyline and Panorama combine to provide a workflow for managing and analyzing LCMS-based small molecule experiments. For QC scenarios, AutoQC, a utility suitable for installing on instrument control computers, monitors for newly acquired small molecule QC runs, runs Skyline without a user interface, and automatically publishes them to Panorama. There, key instrument performance metrics can be viewed for multiple instruments in a single dashboard. New QC plotting options reveal additional metrics and allow users to more easily visualize instrument performance. For experimental data, Panorama now tracks a full history of document versions, allowing users to see how they have changed over time.

All tools are released under the Apache 2.0 open source license.

## Results

### VIEW PROTEOMICS AND SMALL MOLECULE DATA

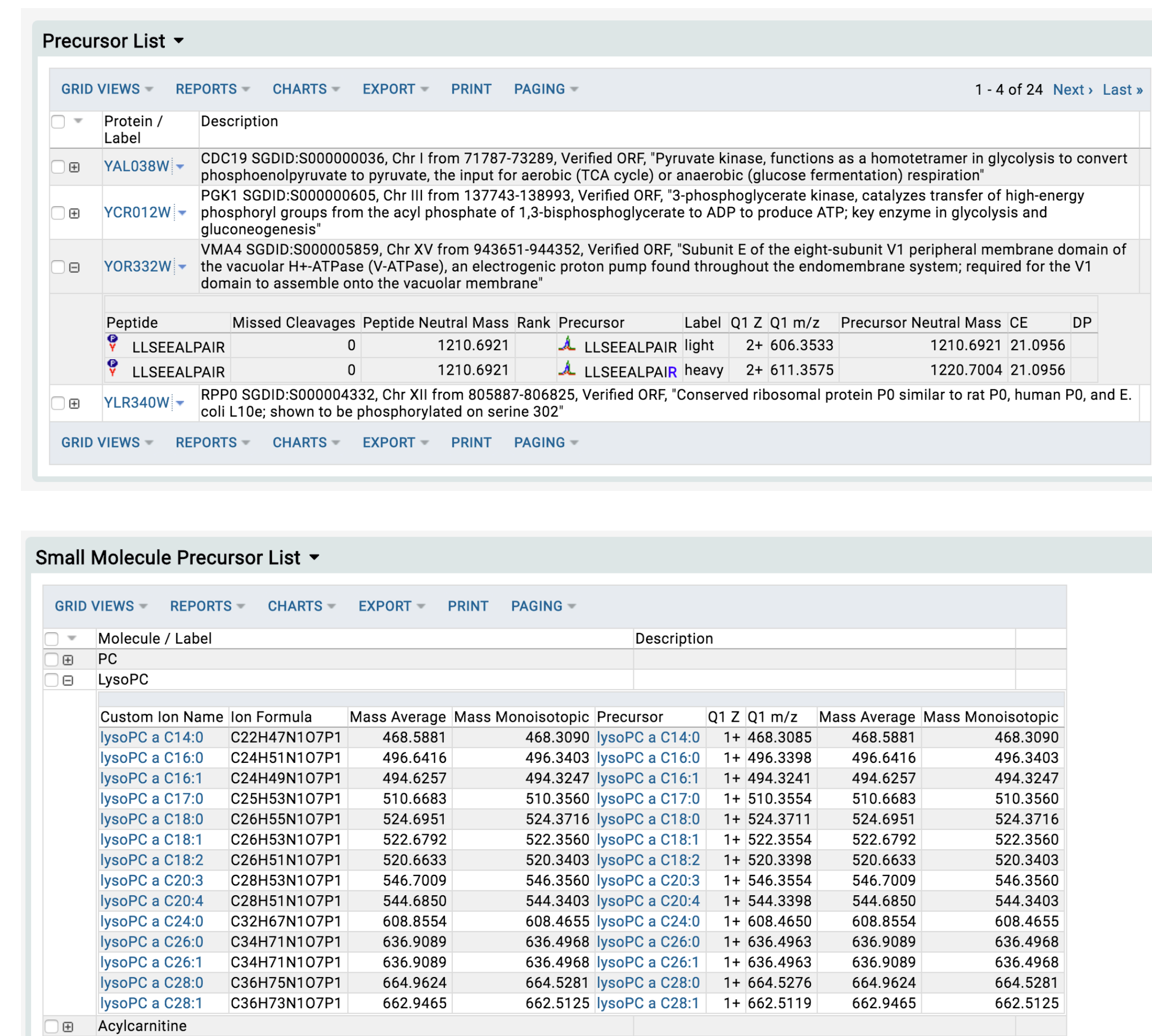


Figure 2: Panorama now shows proteomic and small molecule data as peers within a single document. As the different types have overlapping but different data fields available, they are shown in separate data grids.

### VIEW SMALL MOLECULE DETAILS

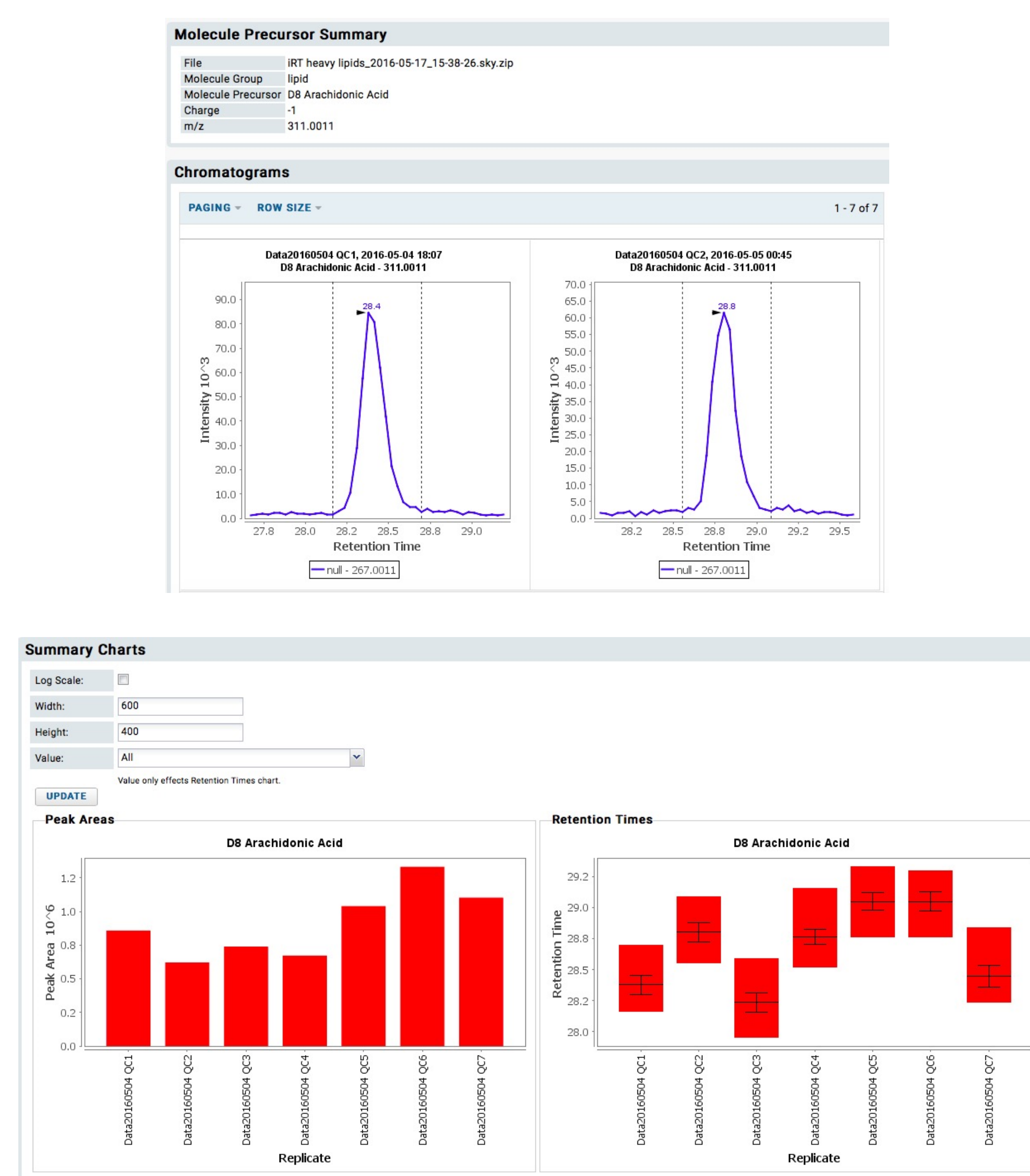


Figure 3: Familiar plots are available for small molecule data as well as proteomic data, including chromatograms and replicate comparison plots, here showing data for arachidonic acid.

### LEVEY-JENNINGS PLOTS

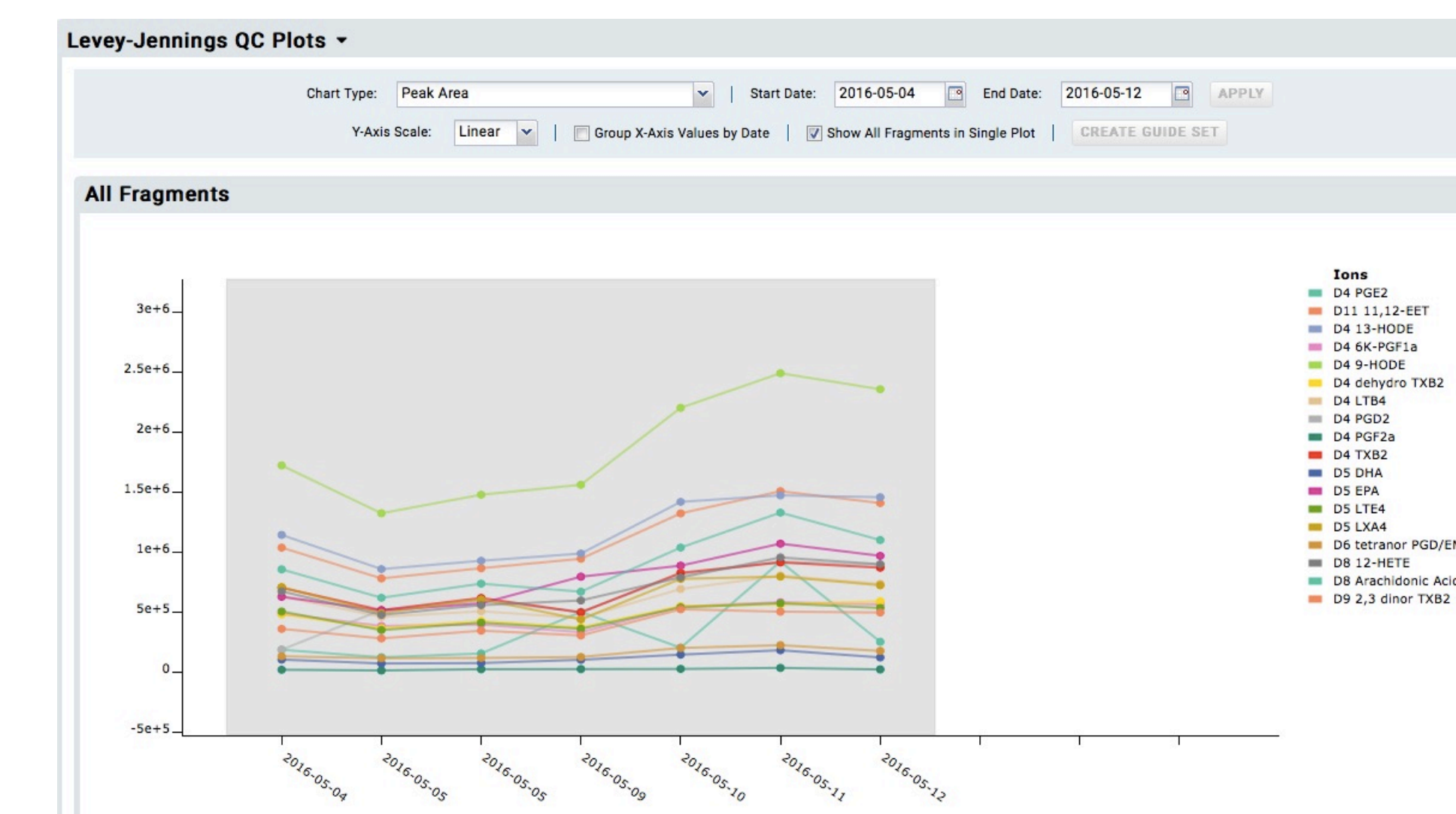


Figure 4: Panorama's Levey-Jennings plots now show small molecule data in addition to proteomics results. New metrics include mass accuracy and showing transition and precursor areas as separate series. Additionally, the plots now remember their most recently used settings, reducing repetitive UI configuration.

### VIEW QUALITY CONTROL STATUS ACROSS INSTRUMENTS

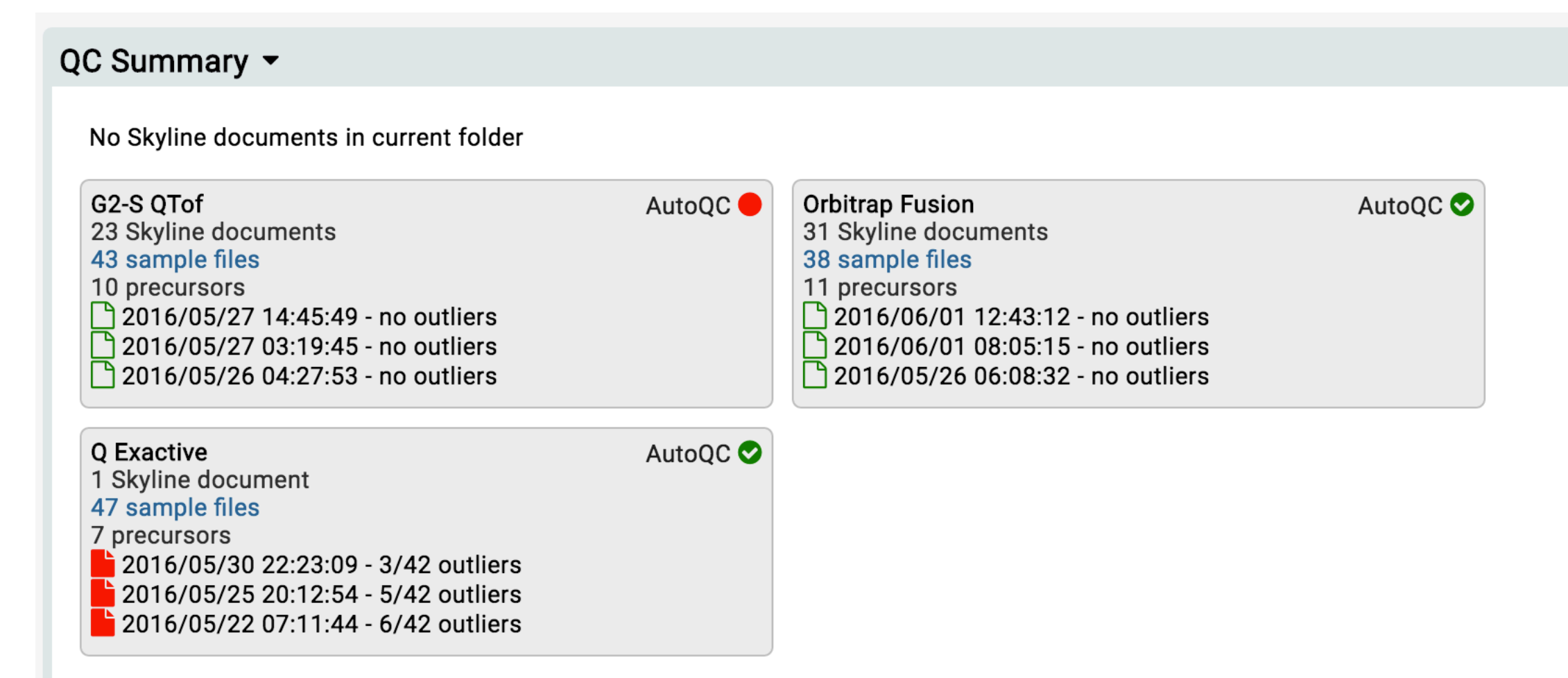


Figure 5: The new QC Summary component allows a quick visual check of quality control data across multiple folders. Here, there are three subfolders, each holding data for a single instrument. The three most recent QC sample files are summarized for each folder. The AutoQC status in the upper right shows if AutoQC is still running. A green check indicates that AutoQC is active for that instrument, while a red solid dot signifies that it is not running.

### MONITOR PROBLEMATIC QC METRICS

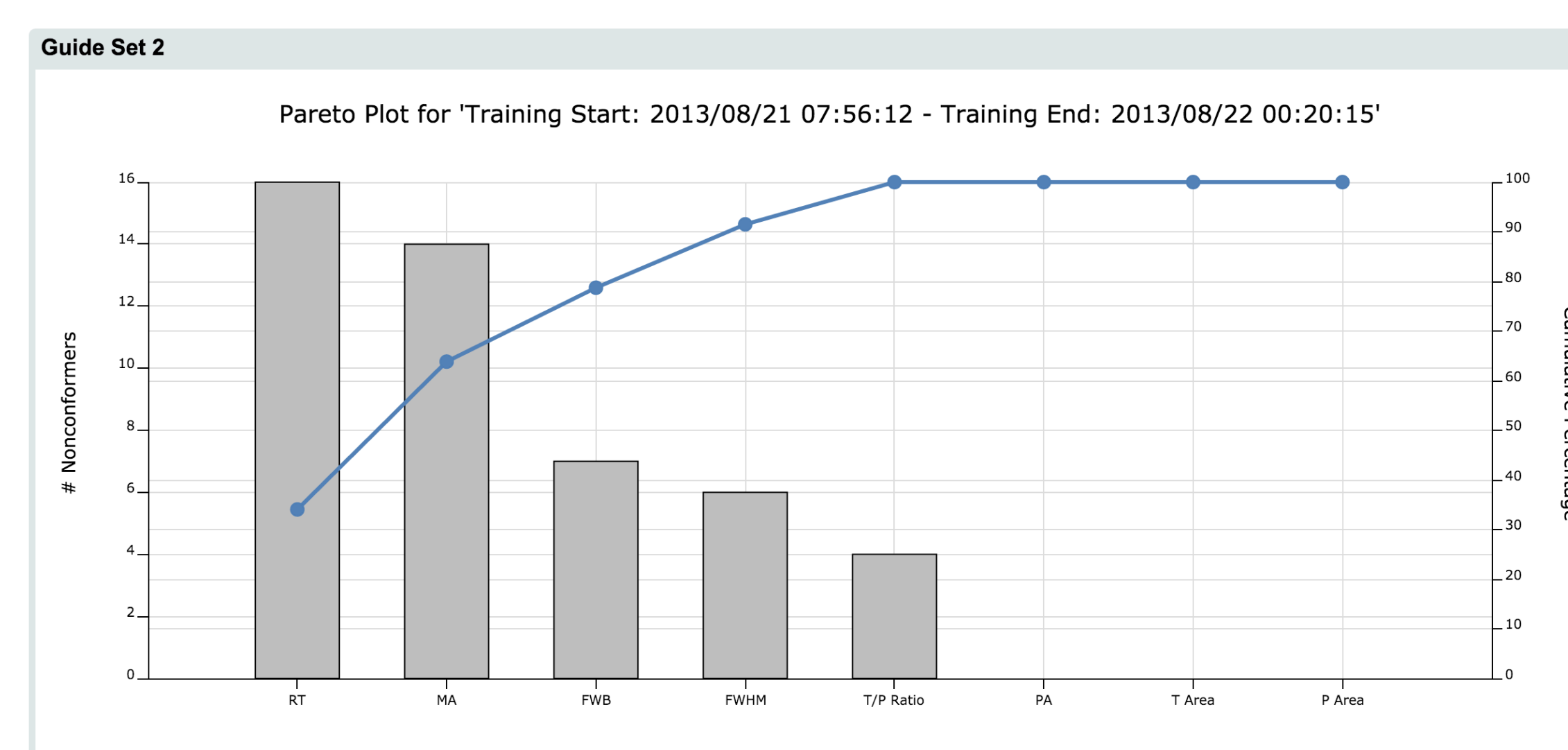


Figure 6: Pareto Plots indicate which metrics produce the most outliers, suggesting potential areas of corrective action in terms of instrument calibration and maintenance. Here, retention time (RT) is the most frequent outlier, followed by peak area (PA), and other metrics. Both small molecule and proteomic data is included.

### TRACK SKYLINE DOCUMENT VERSIONS

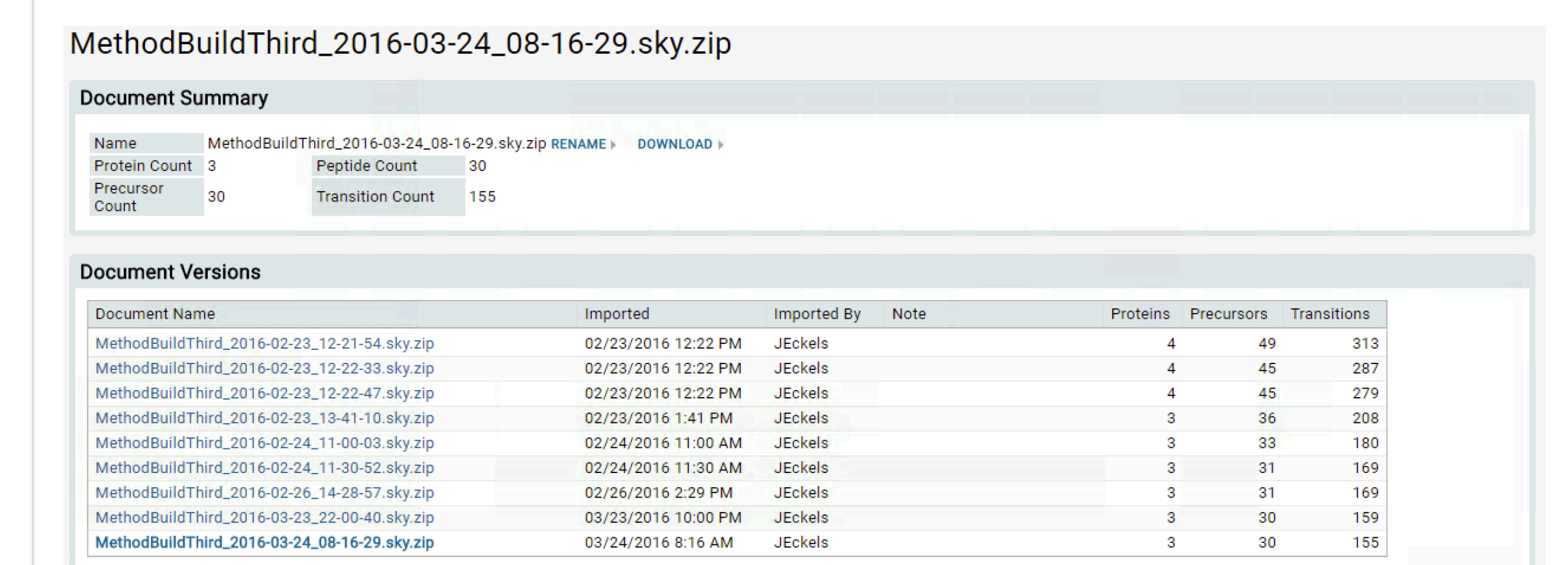


Figure 7: Panorama now tracks and links successive versions of Skyline documents. When publishing to Panorama, Skyline automatically includes a unique document ID, which allows Panorama to accurately identify it as a new version of a previously imported document. Each version of the document is summarized, and users can click to jump to a different version.

## Conclusions

As of May 2016, more than 160 labs are already using PanoramaWeb, a server hosted by the University of Washington. Additionally, major pharmaceutical companies and other organizations are using in-house Panorama deployments. With the release of LabKey Server version 16.1 (March 2016), Panorama added support for small molecule data, and the upcoming 16.2 release (July 2016) adds new capabilities. Allowing a mix of proteomics and small molecule data in all contexts allows labs to use Panorama's convenient QC work and data flows. Exposing the Levey-Jennings plots in an interactive, secure, web-based interface, gives all authorized users immediate access to both historic and just-acquired assays, and also makes it available via HTTP-based APIs (including R, Perl, Python, Java, and JavaScript) in external tools and reporting.

## References

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Sharma V, MacLean B, et al. J. Proteome Res. 2014/08; 10.1021/pr5006636.  
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