Panorama: A Private Repository of Targeted Proteomics Assays for Skyline

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Overview:

The Skyline Targeted Proteomics Environment has enabled researchers to rapidly generate and evaluate assays for targeted proteomics experiments on a wide range of instrumentation. The ability to easily produce and refine targeted methods has created a need for a database of validated assays that can benefit future investigations. We present Panorama, an open-source and freely available repository server application for targeted assays that integrates seamlessly into a Skyline-based proteomics workflow. Scientists can access a Panorama server via a web-browser interface to upload Skyline documents, and query available results. We present the current state of the project and discuss plans for future work.

Introduction:

Skyline is fast becoming the standard tool for targeted proteomics experimentation. Experience in our own lab as well as communication with many of the labs using Skyline has proven that a large collection of personal Skyline documents makes using previous results to inform new experiments cumbersome.

We started developing Panorama with the following goals:

- Help labs aggregate curated results
- Store the complete Skyline document data model
- Use previous experiments to inform new experiments
- Make it easy to search and review a large body of experiments
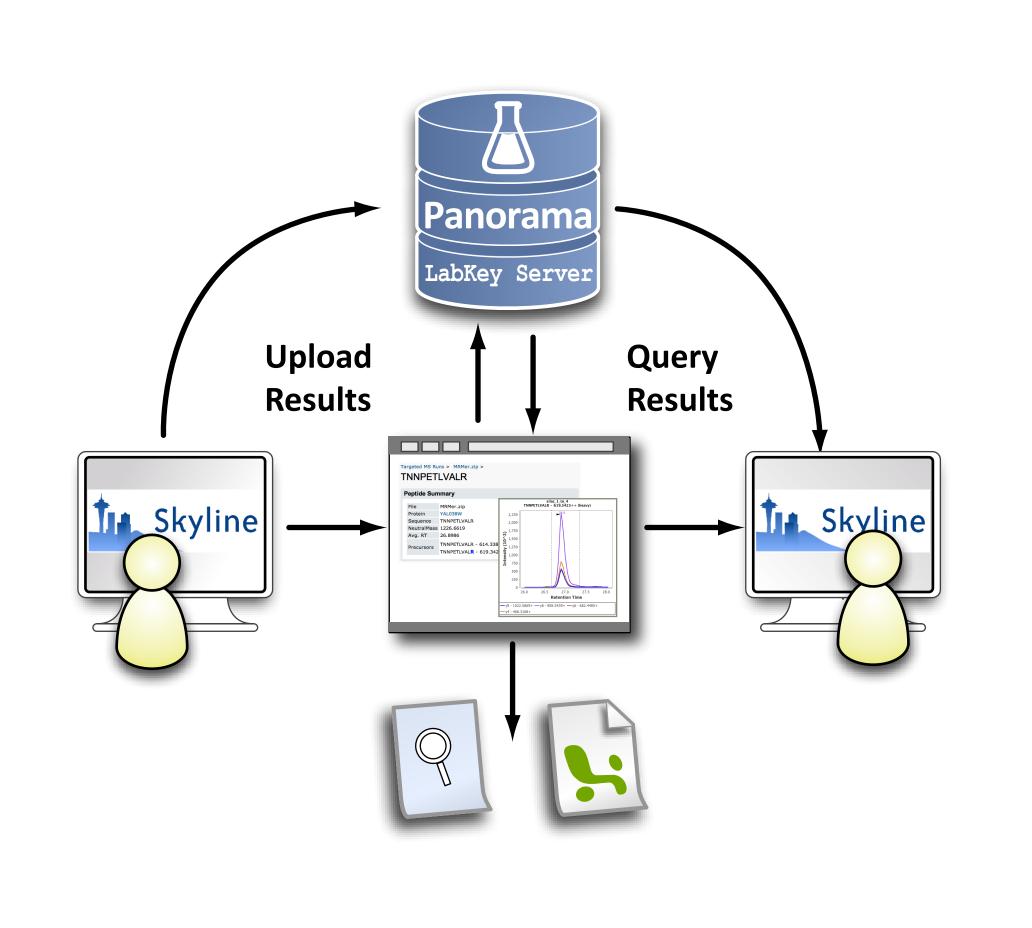- Facilitate sharing results
- Keep private data secure

Figure 1: Panorama data flow

Methods:

Panorama has been implemented as a module within LabKey Server, a general-purpose open source bioinformatics data management platform with rich support for proteomics data, and a security model that currently support clinical studies.

LabKey Server was the perfect base platform for Panorama for the following reasons:

- Open source under Apache 2.0 License
- Rich set of customizable core functionality
- Modular design
- Existing support for mass spectrometry-based proteomics
- Easy deployment into most lab environments
- Powerful security model
- Ability to integrate with other assay, specimen, clinical, and other information supported within the LabKey environment

Skyline documents are uploaded into the repository via the Panorama web-browser interface. Efforts are underway to enable upload of documents directly from Skyline. Data are stored in a relational database supporting the full information content available in Skyline documents.

Figure 2: Above: Panorama relational database schema to support the rich variety of information available in the Skyline custom reports. Below: The Skyline custom report editor for a single Skyline document.
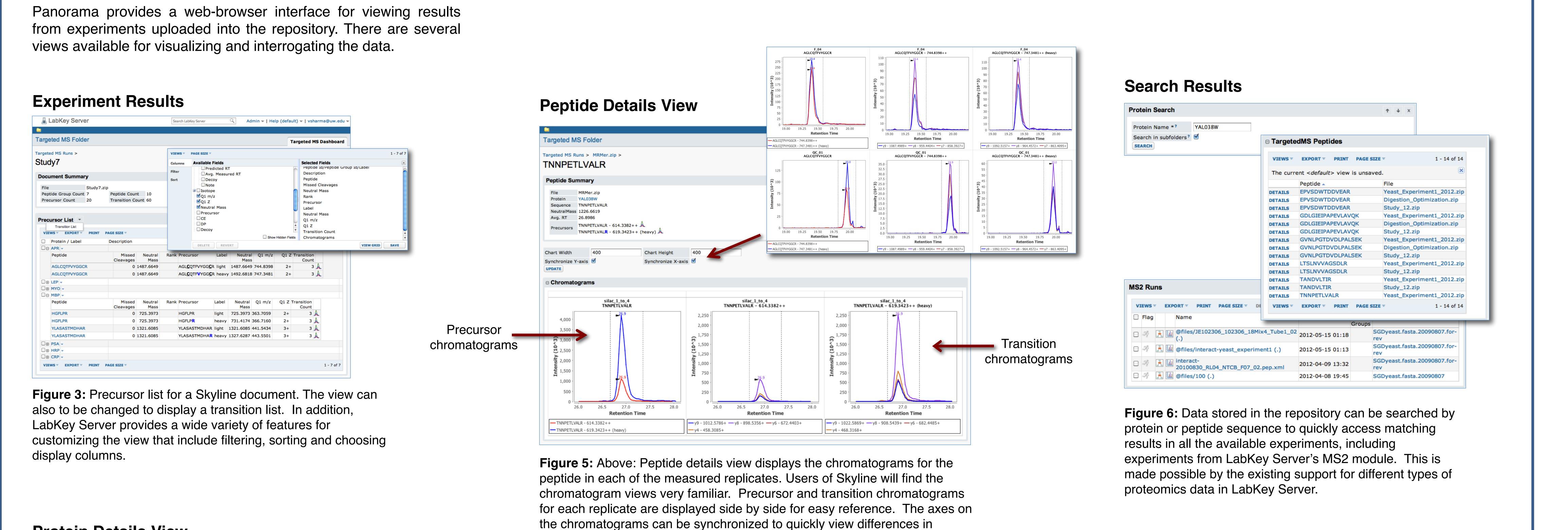
Results:

Panorama provides a web-browser interface for viewing results from experiments uploaded into the repository. There are several views available for visualizing and interrogating the data.

Experiment Results

Figure 3: Precursor list for a Skyline document. The view can also to be changed to display a transition list. In addition, LabKey Server provides a wide variety of features for customizing the view that include filtering, sorting and choosing display columns.

Protein Details View

Figure 4: Protein overview showing sequence coverage along with peak areas of the peptides measured for the protein. This relative peptide response can help in choosing the best peptides to monitor for a protein in targeted experiments.

Peptide Details View

Figure 5: Above: Peptide details view displays the chromatograms for the peptide in each of the measured replicates. Users of Skyline will find the chromatogram views very familiar. Precursor and transition chromatograms for each replicate are displayed side by side for easy reference. The axes on the chromatograms can be synchronized to quickly view differences in intensity and retention times within precursors in a single replicate or across multiple replicates. Below: A library spectrum for the peptide above is also displayed, as in Skyline, when one is available.

Precursor chromatograms

Transition chromatograms

Search Results

Figure 6: Data stored in the repository can be searched by protein or peptide sequence to quickly access matching results in all the available experiments, including experiments from LabKey Server's MS2 module. This is made possible by the existing support for different types of proteomics data in LabKey Server.

http://proteome.gs.washington.edu/software/skyline

Conclusions:

Panorama manages results processed with Skyline from targeted proteomics experiments within a lab or a multiple lab consortium. Results in the repository can be kept secure or made publicly available. Results are easy to search and review. They can be used to inform future experiments. Leveraging the LabKey Server platform has accelerated development and given Panorama the benefit of an extremely rich set of base functionality hardened over 9 years of development and use.

Future work includes:

- Direct file export from Skyline into Panorama.
- Real-time access to Panorama results in Skyline:
  - Choose optimal peptides for proteins
  - Choose optimal product ions for peptides
  - Compare acquired results to repository results