Panorama Public: A Public Repository for Quantitative Data Sets Processed in Skyline*

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To address the growing need for a centralized, community resource of published results processed with Skyline, and to provide reviewers and readers immediate visual access to the data behind published conclusions, we present Panorama Public (https://panoramaweb.org/public.url), a repository of Skyline documents supporting published results. Panorama Public is built on Panorama, an open source data management system for mass spectrometry data processed with the Skyline targeted mass spectrometry environment. The Panorama web application facilitates viewing, sharing, and disseminating results contained in Skyline documents via a web-browser. Skyline users can easily upload their documents to a Panorama server and allow other researchers to explore uploaded results in the Panorama web-interface through a variety of familiar summary graphs as well as annotated views of the chromatographic peaks processed with Skyline. This makes Panorama ideal for sharing targeted, quantitative results contained in Skyline documents with collaborators, reviewers, and the larger proteomics community. The Panorama Public repository employs the full data visualization capabilities of Panorama which facilitates sharing results with reviewers during manuscript review. *Molecular & Cellular Proteomics 17: 10.1074/mcp.RA117.000543, 1239–1244, 2018.

Skyline (1) is a widely used targeted proteomics software tool for processing mass spectrometry data from a range of acquisition techniques such as selected reaction monitoring (SRM)1, data-dependent acquisition (DDA) (2), parallel reaction monitoring (PRM) (3, 4) and data-independent acquisition (DIA) (5). A key strength of Skyline is its data visualization capabilities that include a vast array of interactive graphs for interrogating the underlying data. The Panorama (6) web-interface implements several Skyline graphs, including the annotated chromatogram views that are critical to evaluating the quality of quantitative results. These visualization capabilities enable viewers to get a quick overview of results contained in an uploaded Skyline document within a web-browser, without having to open the document in Skyline or even needing to install Skyline. Combined with the ability to easily upload documents to a Panorama server with the click of a button in Skyline, this makes Panorama an ideal data management system for Skyline documents. Additionally, the original Skyline documents uploaded to a Panorama server can also be downloaded and opened in Skyline making data sharing and dissemination easier and even aiding in reproducing results.

Many laboratories and organizations use Panorama as a repository of their Skyline-processed data. For researchers lacking the resources or inclination to set up their own server we have made available a Panorama server hosted by the Department of Genome Sciences at the University of Washington called PanoramaWeb (https://panoramaweb.org). This server is open to all researchers for storing and securely sharing experimental results contained in Skyline documents. Since its introduction in 2013, PanoramaWeb has become a popular repository choice among researchers who use Skyline to process their mass spectrometry data. As of February 2018, the server hosts data from 283 different laboratories (https://panoramaweb.org/dashboard.url). Researchers can request free projects for their laboratory or organization on PanoramaWeb, and are given full administrative control over their project space. This includes the ability to organize data in folders and configure access to the data contained in each folder for sharing with other researchers. Several researchers have used this flexibility to host Skyline documents associated with research manuscripts on PanoramaWeb. They have provided journals login access to the data while a manuscript is being reviewed and then made the data public once the manuscript was accepted for publication.

Although PanoramaWeb has enabled users to provide reviewers and the research community with access to published Skyline results within user projects, this capability has also exposed some shortcomings. Because the public data are dispersed over several user projects, it is not possible to provide a centralized, searchable location for data published...

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in this manner to the community. Additionally, the original authors retain control over the data making it difficult to guarantee the continued availability of the data exactly as they were originally published.

Panorama Public addresses the first concern by creating a central, searchable public resource of published data that can be explored using the same interface and data visualizing capabilities that are available in user projects on PanoramaWeb. We provide a simple mechanism for copying data from user projects on PanoramaWeb to Panorama Public. To address the second concern, once on Panorama Public, data cannot be modified by the original authors and remains available in its original form, in a permanent location. Panorama Public also facilitates manuscript review by keeping data private during the review process, with anonymous and secure access for reviewers. On notification that a paper has been accepted for publication the associated data is made publicly accessible.

Existing public repositories, such as the PeptideAtlas SRM Experiment Library (PASSEL) (7) are community resources of published data from SRM experiments. However, PASSEL only requires authors to submit transition lists describing the targeted analytes and, optionally, output from the tools used for analysis. Accompanying raw data submitted to PASSEL is reprocessed to provide a uniform view of all published data available on PASSEL. However, this loses any tool-specific processing information and creates a disconnect between the published results and the re-processed results available for viewing in the PASSEL interface. Unless authors provide visual output from their data processing and analysis tool, or another means of data visualization, it is difficult for readers to get insight into how well the chosen tools performed peak picking. It is also difficult to assess the reliability of the area under the curve (AUC) numbers around which the authors based their quantitative conclusions, now a critical requirement of the recently published Molecular & Cellular Proteomics (MCP) guidelines for targeted mass spectrometry experiments (8).

**EXPERIMENTAL PROCEDURES**

Support for uploading documents to a Panorama server has been available in Skyline since version 1.4 (released on 11/12/2012). The current version of Skyline can be downloaded from the Skyline website (https://skyline.ms). To submit results to Panorama Public, authors must first upload Skyline documents to their own project on PanoramaWeb (https://panoramaweb.org). If a laboratory or organization does not already have a project on PanoramaWeb, a new project can be requested by filling a simple form on this page: https://panoramaweb.org/signup.url. Before uploading documents from Skyline to PanoramaWeb a one-time configuration step is required in

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1 The abbreviations used are: SRM, selected reaction monitoring; DDA, data-dependent acquisition; PRM, parallel reaction monitoring; DIA, data-independent acquisition; AUC, area under the curve; PASSEL, PeptideAtlas SRM Experiment Library; MCP, Molecular & Cellular Proteomics.
abstract, experimental and sample descriptions, the organism(s) studied, and the mass spectrometry instrument(s) used to collect data (Fig. 1, step 2). After all the Skyline documents and any other related data have been uploaded to PanoramaWeb, to complete step 3 of the workflow, the user clicks a button (Fig. 2A) to request that the data be copied to Panorama Public. In the resulting form, the user creates a custom link to their data (Fig. 2B) on Panorama Public. The user may choose a custom name for their link that is relevant to their data, making it more memorable. This becomes the permanent access link to the data on Panorama Public and can be referenced in manuscripts and published papers. In the same form the user may check a box (Fig. 2C) to request that their data on Panorama Public be kept private by checking a box in the form (C). Keeping data private may be suitable if it is associated with a manuscript under review. If this option is checked, the copy on Panorama Public is private with read-only access to submitters. An additional account is created with read-only access to the data, and account details are included in the confirmation E-mail sent to submitters after the data has been copied. These account details can be conveyed to journal editors at the time of manuscript submission and can be used by reviewers.

When data contained in a user folder on PanoramaWeb is submitted to Panorama Public a snapshot of the folder is created that is identical in all respects to the source folder. In addition to the uploaded Skyline documents, this snapshot also includes all other page components and folder layout (Fig. 3). The snapshot on Panorama Public cannot be edited by the original authors. If the authors need to make updates to address reviewer feedback, they can make changes in their own folder on PanoramaWeb and click a link to request an update to the snapshot on Panorama Public. It is common for data to be added or modified during the manuscript review process and having the ability to easily update data in the repository is important for an efficient workflow for authors and the journal. Requests to copy data to Panorama Public, or update an existing copy are handled by the Panorama Public administrators. After receiving a request, the administrators initiate the copy process and on successful completion send a confirmation E-mail to the authors. If the option to keep data private on Panorama Public was checked in the submission form, reviewer account details are included in the confirmation E-mail sent to submitters. These account details can be conveyed to journal editors at the time of manuscript submission and can be used by reviewers.

While the manuscript is under review, reviewers can use the permanent access link created by the authors in step 3 of the publication process to login and view the data with the full web browsing experience presented by Panorama. Reviewers can view details of each uploaded Skyline document along with any other supplementary information made available by the authors. They can either view details of the available Skyline documents within a web-browser directly in Panorama or download the documents to open them in Skyline on their computer. Within Panorama they can view a list of the
targeted analytes along with chromatograms and marked peak boundaries for each analyte in all the replicates (Fig. 4). Chromatograms of light and heavy isotopically labeled peptides in a single replicate are displayed side-by-side for quick comparison.

The number of independent projects on PanoramaWeb has been growing steadily since its launch in 2013. As of February 2018, the server hosts projects for over 283 different labs. We have implemented a simple mechanism for PanoramaWeb users to make their data available on Panorama Public. A growing number of researchers with projects on PanoramaWeb have published their results to Panorama Public since it was made available in early 2015. There are 71 public data sets available as of February 2018, with over 13,000 page views and around 800 download requests representing a broad geographical distribution (https://panoramaweb.org/public-usage.url).

In summary, Panorama Public provides a permanent location for supplementary data in its original form as intended for publication. It also provides a central resource of published Skyline results to the proteomics research community. Access to data in the repository is managed as required. If requested, data can be private with access only to authors and reviewers during the manuscript review process. Data is made publicly accessible on publication. Open access to published, quantitative data sets in Panorama Public provides a useful source of information and knowledge to the research community.

DISCUSSION
Panorama Public is a repository specifically designed for publishing data generated through Skyline-based targeted proteomics workflows, and sharing them with reviewers and the public. While the Skyline - Panorama workflow provides end-to-end support for the MCP guidelines for targeted mass spectrometry experiments (http://www.mcponline.org/site/misc/MCP_Targeted_Mass_Spec_Guidelines_1.27.17.pdf), publications to all journals are supported. Results contained in Skyline documents are uploaded through a point-and-click operation to user projects on PanoramaWeb where researchers can also provide additional context and other supplementary information relevant to their studies. Tools available in Panorama let researchers add additional content and create a customized micro-website for their data which is then copied in its entirety to Panorama Public. The copy on Panorama Public becomes the permanent location of the data that can be private during peer review and made public after the manuscript is accepted for publication. The copy on Panorama Public protects against accidental deletion or data alteration. Reviewers and readers can easily browse data underlying published conclusions within the Panorama Public interface or download the original Skyline documents and explore them with the complete data interrogation and reprocessing features available in Skyline. Readers get vis-
ibility into all the extracted chromatograms and the actual peak boundaries used for calculating peak areas that can help them to evaluate the reliability of reported results.

A growing number of data sets are already publicly available on Panorama Public, and we hope that the simplicity of submitting to Panorama Public as well as the ability to quickly explore data within a web browser will encourage more researchers to share their Skyline documents on Panorama Public.

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