

“System Suitability Evaluation” / Skyline Ecosystem for Statistical Process Control

Wednesday, May 3 – 11:00am session

Targeted Proteomics with Skyline

objectives

- Gain exposure to Skyline ecosystem tools for quality control
- Assess implementing this or a similar QC pipeline for your own group

Agenda

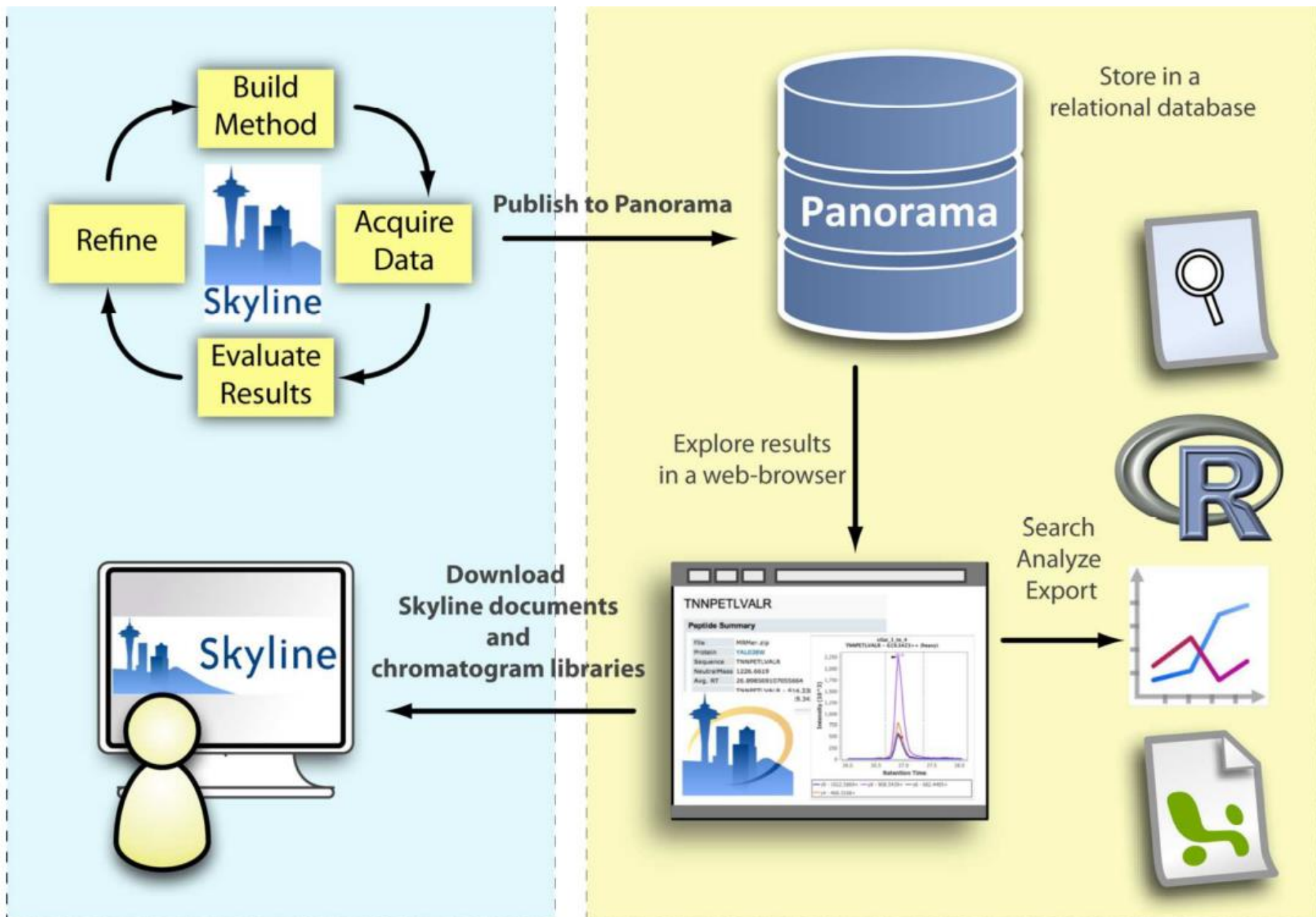
- Panorama for storing, sharing, analyzing, and reusing Skyline-based targeted assays
- SProCop for statistical process control of targeted assay quality
- AutoQC for automated system performance monitoring together with visualization in Panorama

Panorama: web-based application for Skyline documents



www.panoramaweb.org

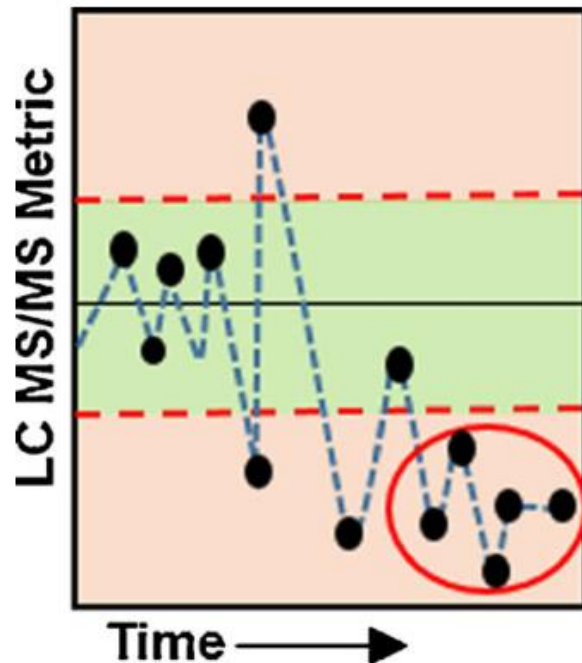
- **Problem:** time, effort, money poured into assay development is not usually “recycled” within labs, between labs, or across experiments
- **Solution:** a relational database storage system to aggregate and organize Skyline documents



Agenda

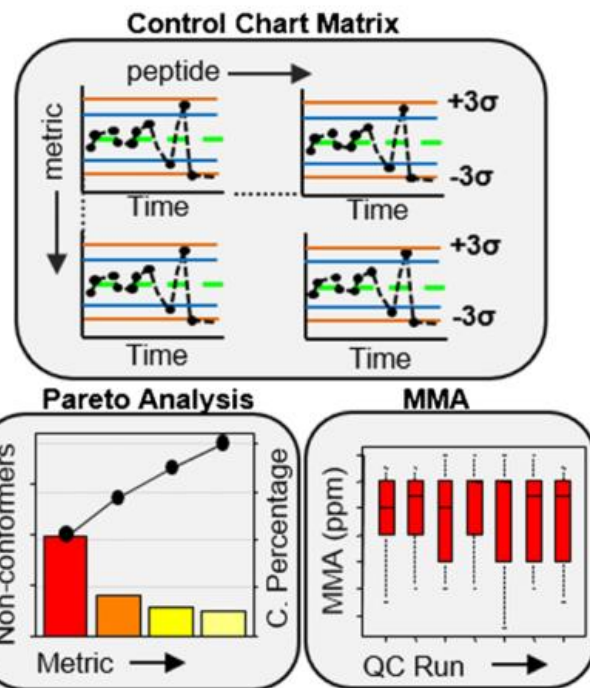
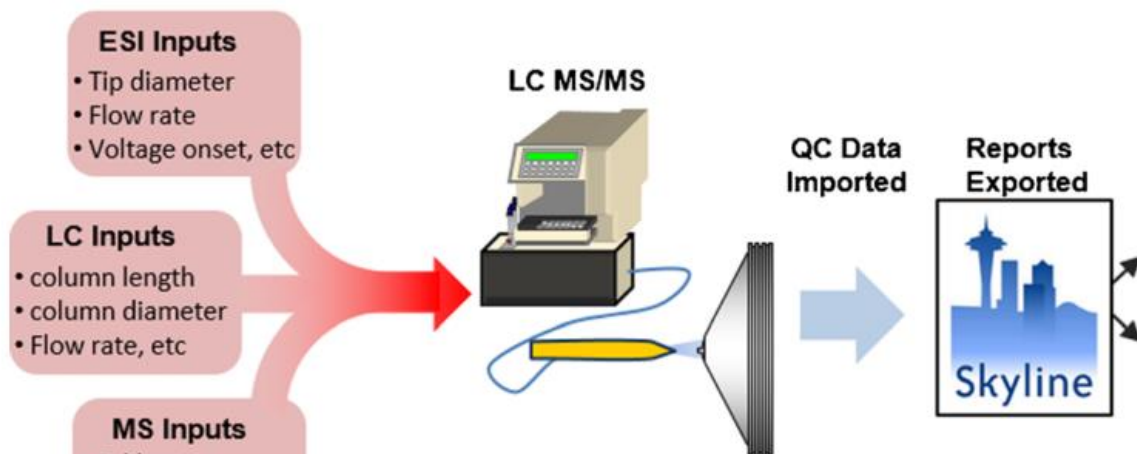
- Panorama for storing, sharing, analyzing, and reusing Skyline-based targeted assays
- **SProCop for statistical process control of targeted assay quality**
- AutoQC for automated system performance monitoring together with visualization in Panorama

Statistical Process Control in Proteomics (SProCop)

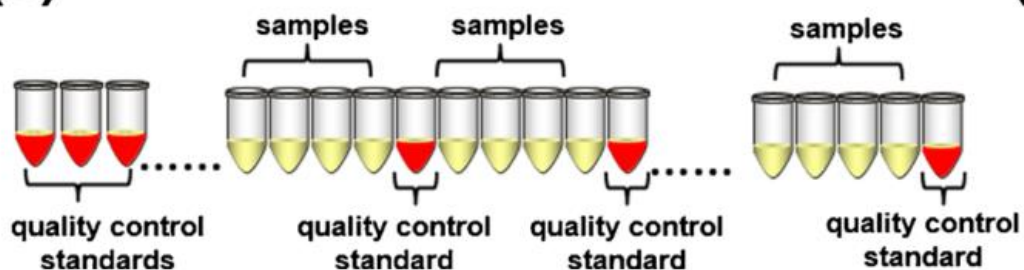


- **Problem:** data quality
- **Solution:** a relational database storage system to aggregate and organize Skyline documents

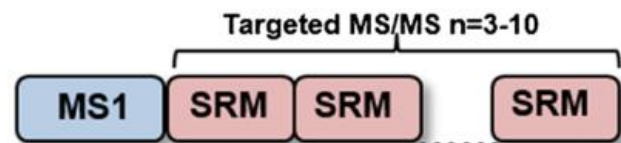
(a)



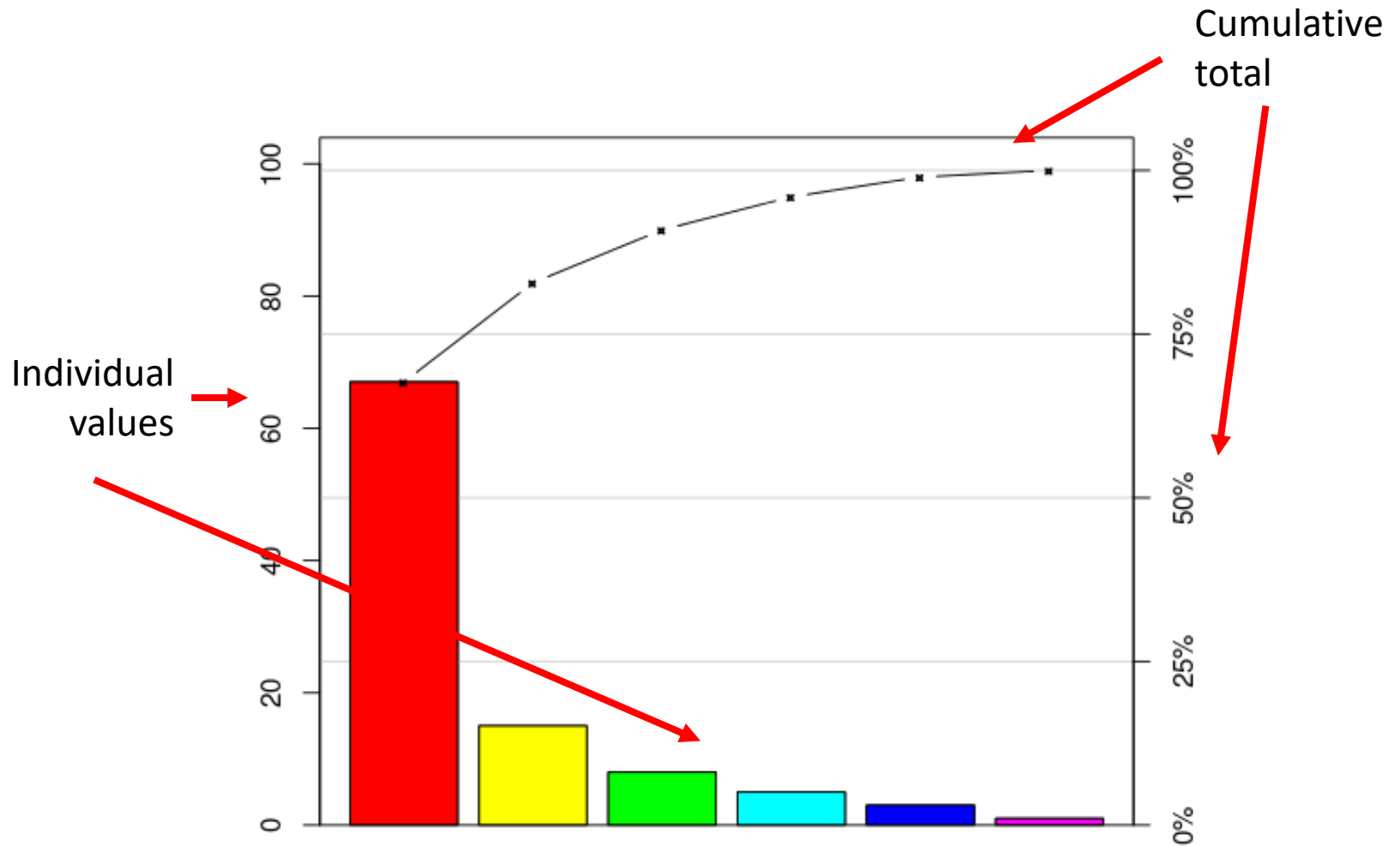
(b)



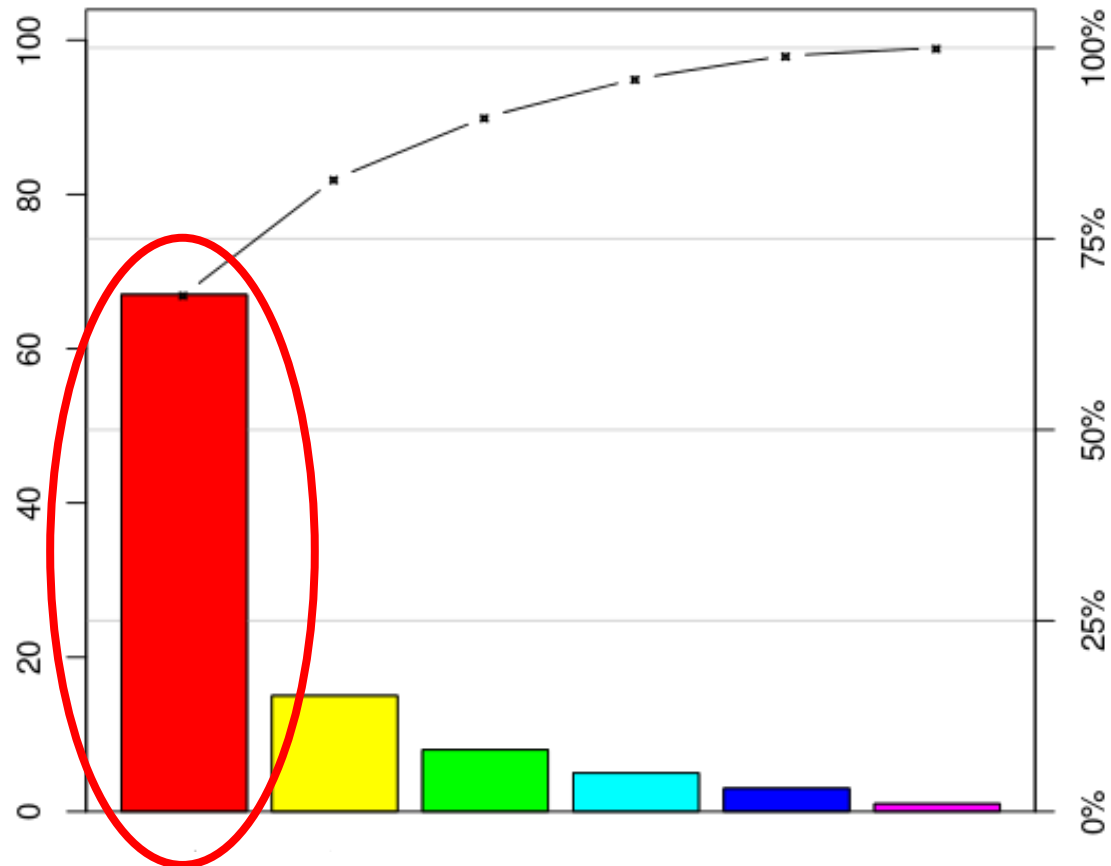
(c)



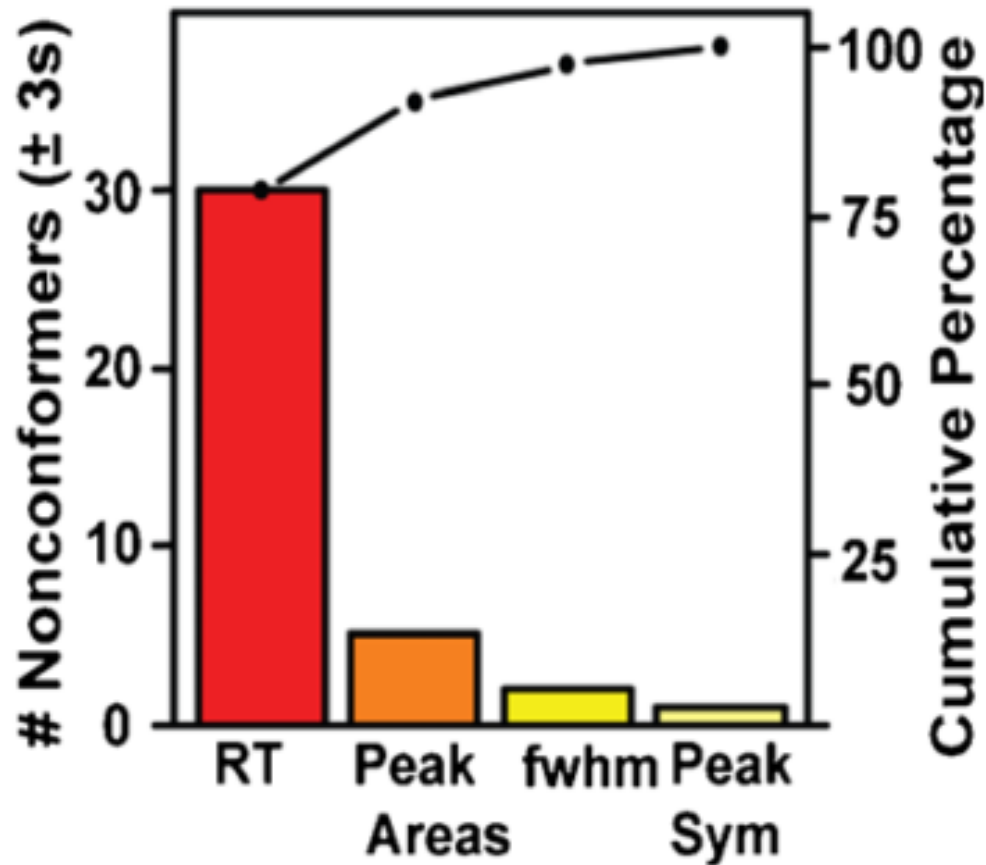
Viewing general Pareto plots



Viewing general Pareto plots



Viewing SProCop's Pareto plots



Agenda

- Panorama for storing, sharing, analyzing, and reusing Skyline-based targeted assays
- SProCop for statistical process control of targeted assay quality
- **AutoQC for automated system performance monitoring using SProCop analyses and stored in Panorama**

Panorama AutoQC

The screenshot displays the Panorama AutoQC interface. At the top, a 'QC Summary' section shows the 'Panorama Demo Project' with an 'AutoQC' status and a green checkmark. Below this, it lists '1 Skyline document', '47 sample files', and '7 precursors'. Three sample files are listed with their acquisition times and outlier status: '2013/08/27 14:45:49 - no outliers', '2013/08/27 03:19:45 - no outliers', and '2013/08/26 04:27:53 - 25/56 (Levey-Jennings), 16/56 (Moving Range) outliers'. Below the summary, a 'QC Subfolder 1' section shows 'No sample files imported' and an 'AutoQC' status with a grey circle icon.

QC Summary ▾

Panorama Demo Project AutoQC ✓

1 Skyline document
47 sample files
7 precursors

2013/08/27 14:45:49 - no outliers
2013/08/27 03:19:45 - no outliers
2013/08/26 04:27:53 - 25/56 (Levey-Jennings), 16/56 (Moving Range) outliers

QC Subfolder 1 AutoQC ○

No sample files imported

- **Problem:** data quality monitoring must be continuous for best QA
- **Solution:** a small program that automatically monitors a directory for QC acquisitions, analyzes the QC, and uploads the results to Panorama for visualization

For more information...

PanoramaQC pipeline:

<https://www.labkey.org/Documentation/wiki-page.view?name=panoQCdash#summary>



Hands on: Setting up AutoQC and viewing SProCop output

- Take home:
 - initializing an automated QC monitoring system
 - familiarizing with Levey-Jennings and Pareto plots