

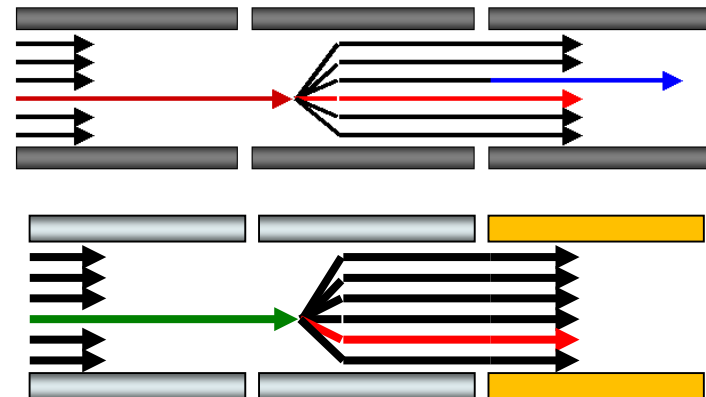


Skyline

Targeted Mass Spec Environment

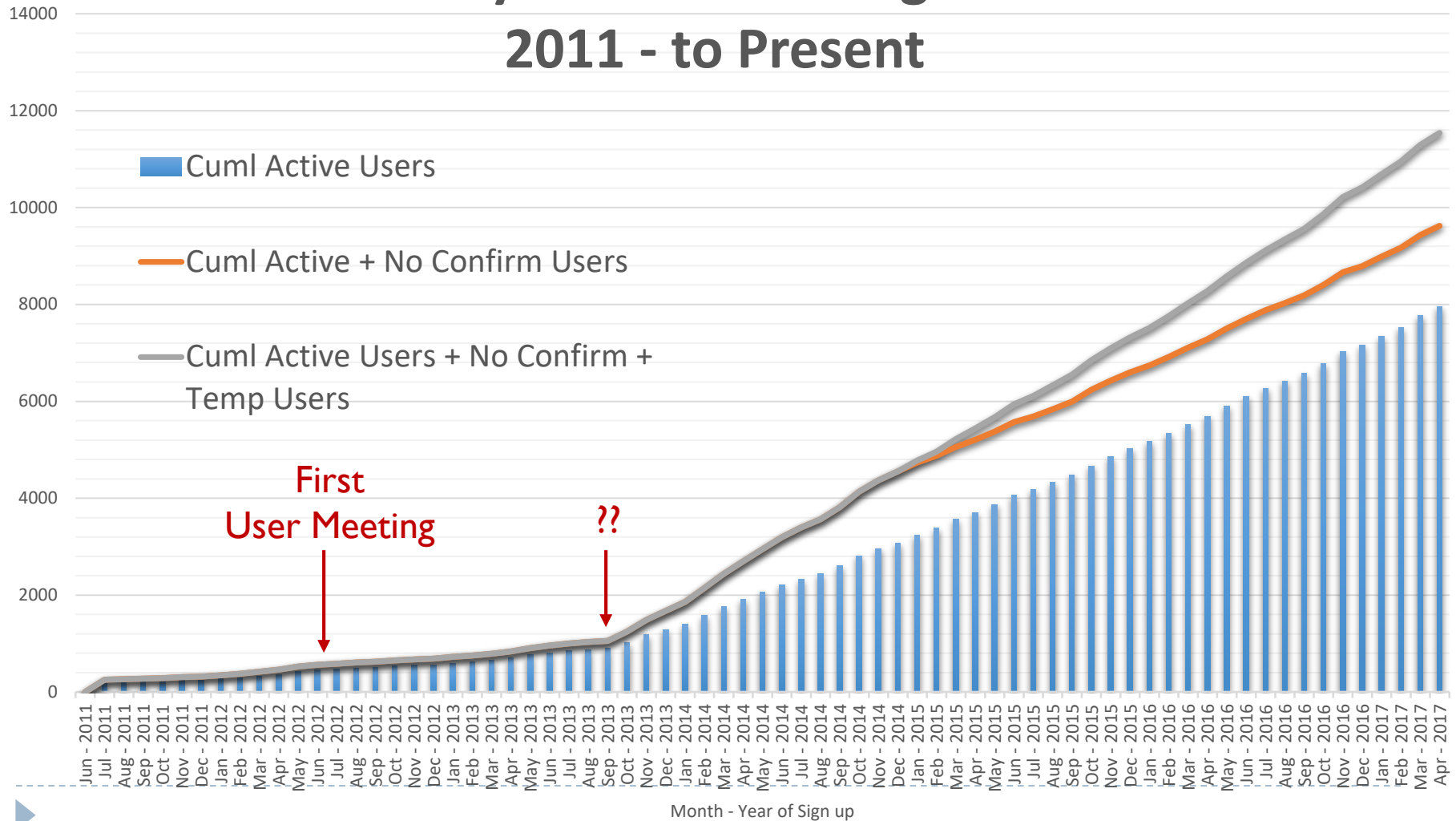
On year 9

Brendan MacLean



Viral Growth?

Cumulative Skyline Website Registrations from 2011 - to Present



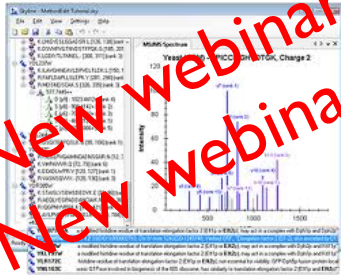
Teaching Targeted Proteomics

- ▶ **3 weeklong courses 2014**
 - ▶ Zurich, Seattle, Barcelona
- ▶ **7 workshops and short courses in 2014**
 - ▶ Albuquerque, Seattle, Baltimore, Brixen, Seoul, Kyoto, Mumbai
- ▶ **5 weeklong courses 2015**
 - ▶ Seattle, Boston, Zurich, Barcelona, Mumbai
- ▶ **5 workshops and short courses in 2015**
 - ▶ Tempe, St. Louis, Rio de Janeiro, Puerto Vallarta, Tokyo
- ▶ **5 weeklong courses 2016**
 - ▶ Zurich, San Francisco, Boston, Seattle, Barcelona
- ▶ **3 workshops and short courses in 2016**
 - ▶ Boston, Brixen, Johannesburg
- ▶ **5 weeklong courses 2017**
 - ▶ San Francisco, Boston, Zurich, Seattle, Barcelona
- ▶ **3 workshops and short courses in 2017**
 - ▶ San Diego, Indianapolis, Dublin

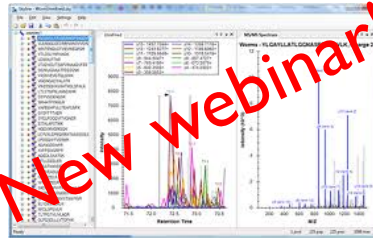


14 Tutorials (9 translated)

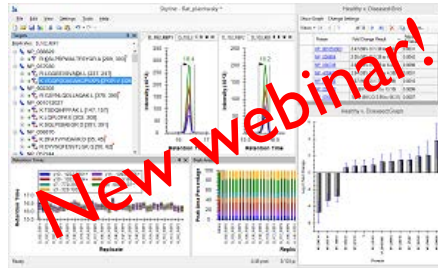
Method Editing



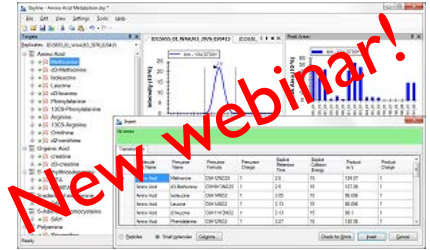
Method Refinement



Grouped Studies



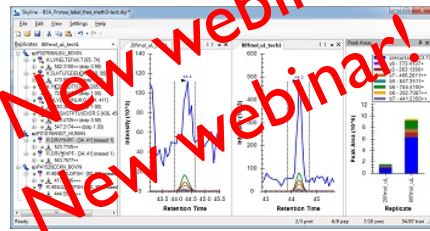
Small Molecule



MSI Filtering



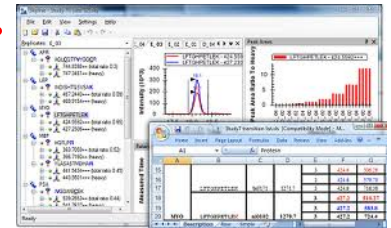
Targeted MS/MS (PRM)



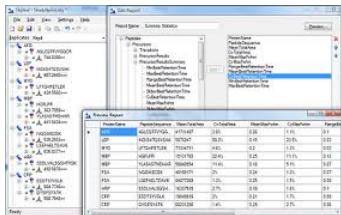
DIA with DDA



Existing Experiments



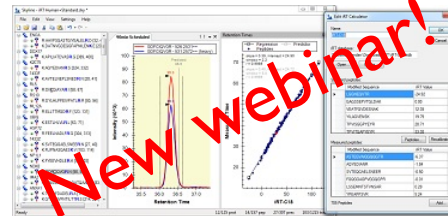
Custom Reports



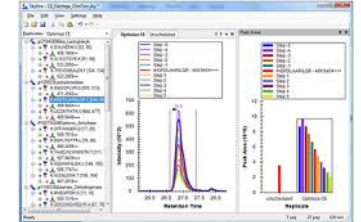
Advanced Peak Picking



iRT



CE Optimization

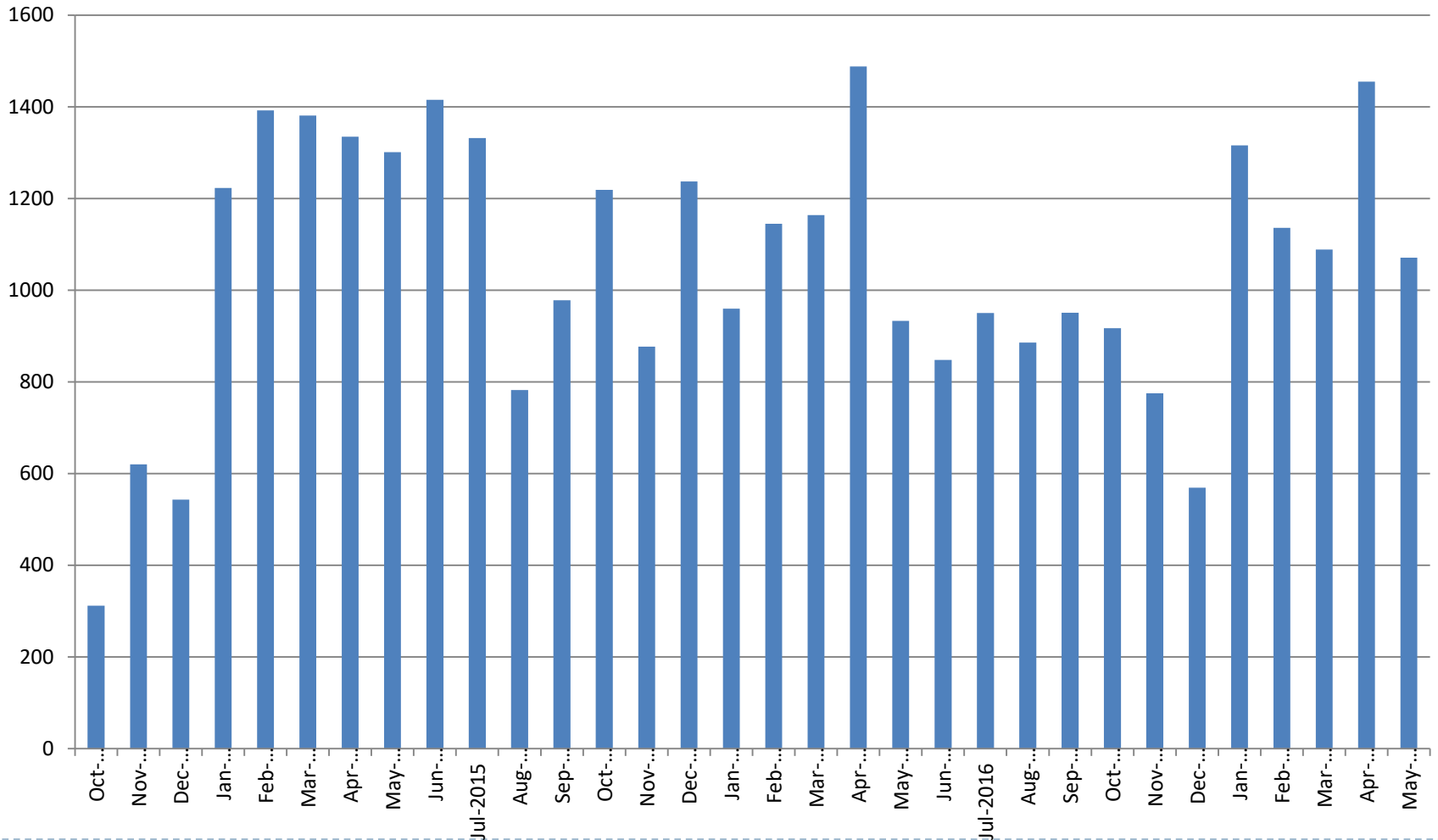


▶ 15 webinars

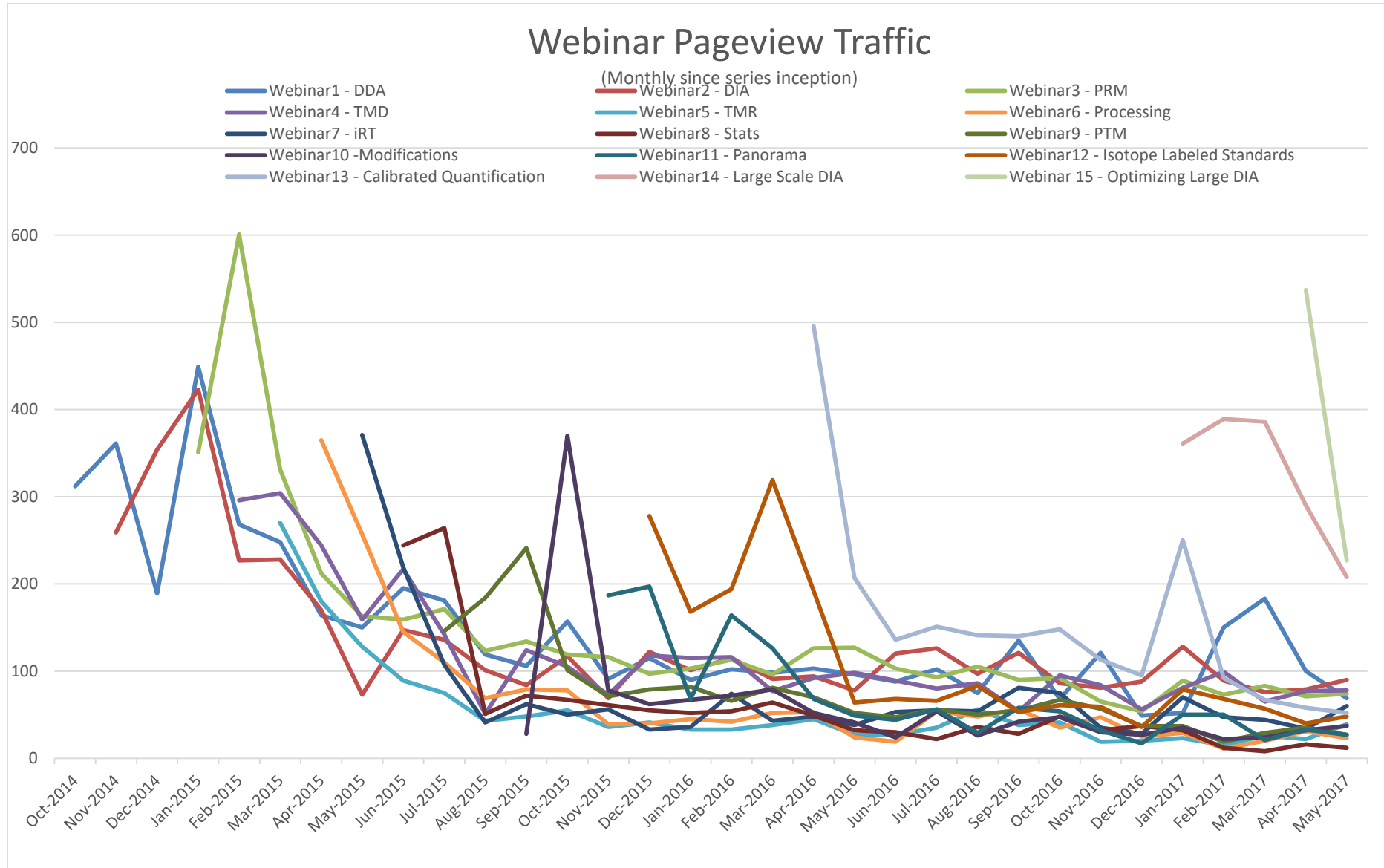
Growing...

Webinar Statistics

Total webinar pageviews



Webinar Statistics



2016-2017 Recap – Version 3.6

- ▶ **Improved results import:**
 - ▶ Parallel multi-file results import (in user and command-line interfaces)
 - ▶ New results import interface for improved unattended imports
 - ▶ Greatly improved import performance for Skyline documents on network drives
- ▶ **Calibrated quantification improvements:**
 - ▶ Surrogate standards for normalizing to explicit non-homologous molecules
 - ▶ Remove point right-click option in calibration curve graph
 - ▶ Explicit Global Standard Area added to replicates for explicit global normalization control with values like TIC
- ▶ **Group comparison additions and fixes to improve consistency with MSstats**
- ▶ **New Detection Q Value and Detection Z Score report columns for mProphet scored peak picking**
- ▶ **New Peak Rank By Level report value and Targets view showing separate peak rankings for MSI and MS/MS transitions**
- ▶ **Peptide uniqueness constraint added to Peptide Settings - Digestion tab (by protein, gene or organism)**
- ▶ **New Edit > Refine > Associate Proteins for adding protein associations for targeted peptides after they have been added to the targets list**
- ▶ **Ability to choose which modifications to use when showing a library in the Spectral Library Explorer**
- ▶ **New and improved plots:**
 - ▶ Mass error plots (replicate and peptide comparisons and 1D and 2D histograms)
 - ▶ Multi-peptide retention time plot
 - ▶ Point set selection in retention time regression plot



2016-2017 Recap – Version 3.6 (cont.)

- ▶ **Improved small molecule support:**
 - ▶ Improved support for negative ion mode
 - ▶ Improved chromatogram matching for molecules with identical precursor m/z but different scheduled retention times
 - ▶ Parsing of chemical formula with adduct syntax in Edit > Insert > Transitions
 - ▶ Support for small molecule transition list import with Edit > Paste, File > Import > Transition List, external tools and with command-line
- ▶ **Improved Transition Settings for Full-Scan**
 - ▶ Centroided extraction with mass error tolerance made default, based on improvement seen with Thermo, Sciex and Bruker instruments
 - ▶ New high-selectivity extraction option (1/2 extraction width) for extraction from profile spectra, based on improvement seen with Thermo and Sciex raw data files
 - ▶ Easier import of existing data with improved isolation schemes based on raw data
 - ▶ Fixed support for importing from instruments using different high- and low-resolution between MSI and MS/MS
- ▶ **Ability to include ambiguously matched spectra in spectral libraries build by Skyline**
- ▶ **Improved support for iRT:**
 - ▶ Support for more iRT standard mixes
 - ▶ Automatic adding of iRT standard targets to document
 - ▶ More flexible iRT regression support (allowing 80% of standards at 0.995 correlation)
 - ▶ CiRT support
- ▶ **SkylineRunner command-line interface improvements:**
 - ▶ Command-line support for importing transition lists and assay libraries
 - ▶ Command-line support for exporting isolation lists
 - ▶ Command-line support for adding decoy peptides
 - ▶ Improvements made to support AutoQC
 - ▶ mProphet model generation output to console log
- ▶ **Initial support for Sciex MIDAS data**
- ▶ **Initial support fixes for Waters SONAR data**
- ▶ **Fix for File > Save As bug that disabled Edit > Refine > Re-import**
- ▶ **Many other smaller bug fixes**

Version 3.7 Coming Soon!



New External Tools

- ▶ **Cross-link Transition Calculator**

- ▶ **Coming soon...**
 - ▶ Garuda Integration (pipeline processing with Shimadzu)
 - ▶ TraceFinder Integration
 - ▶ Lipid Creator

- ▶ **And... MSstats over 10,000 downloads!**



What you see is what you believe

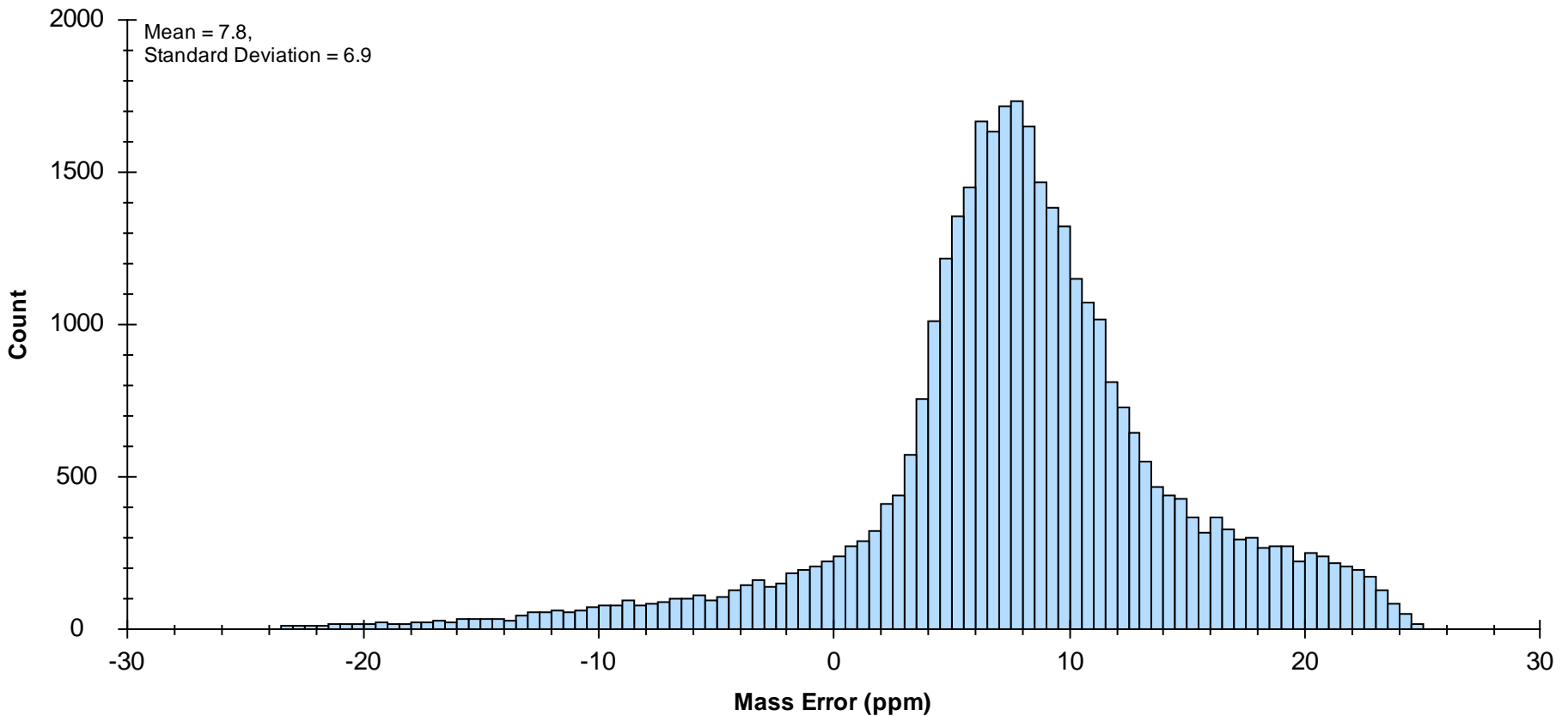
See **MORE!!**

with



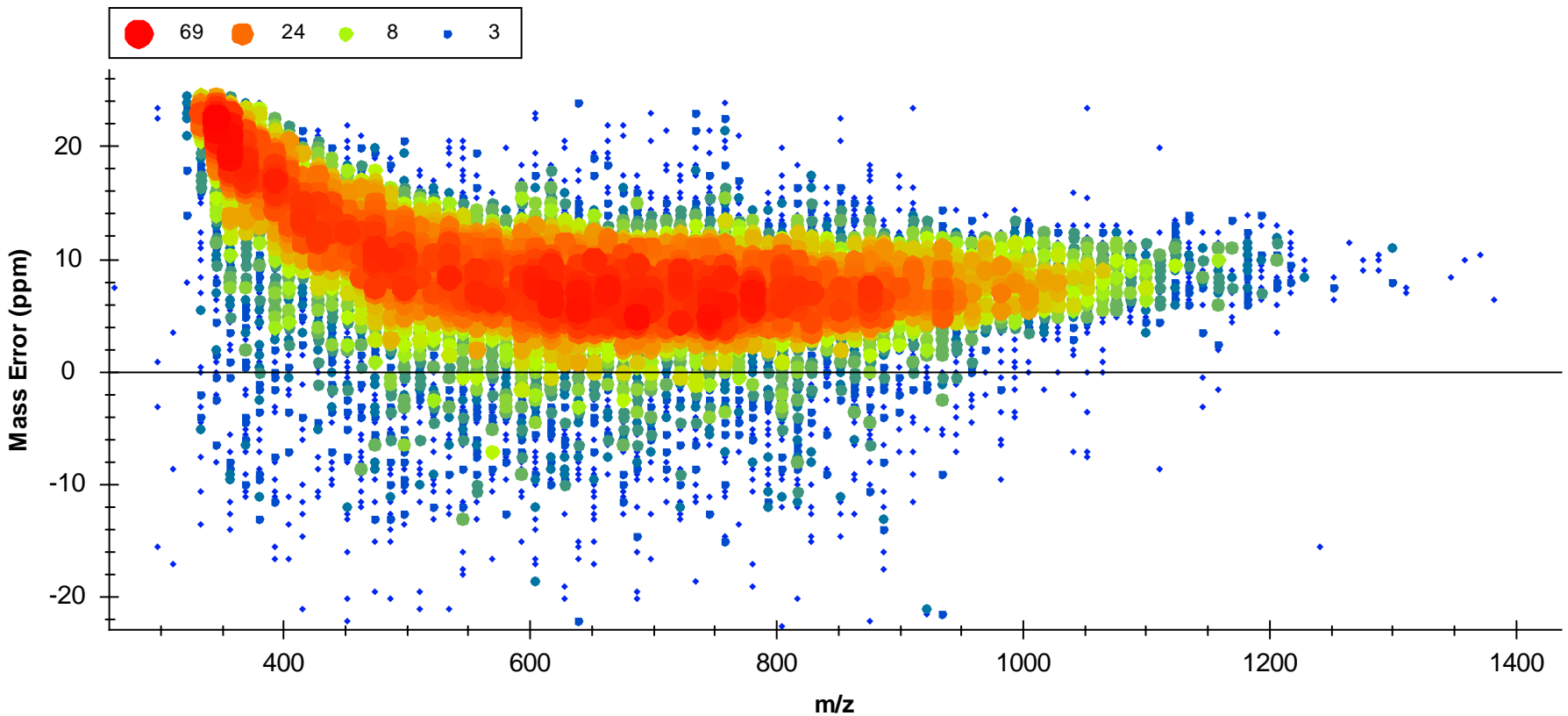
New Mass Error Graphs

► Webinar 15 – troubleshooting Bruker data



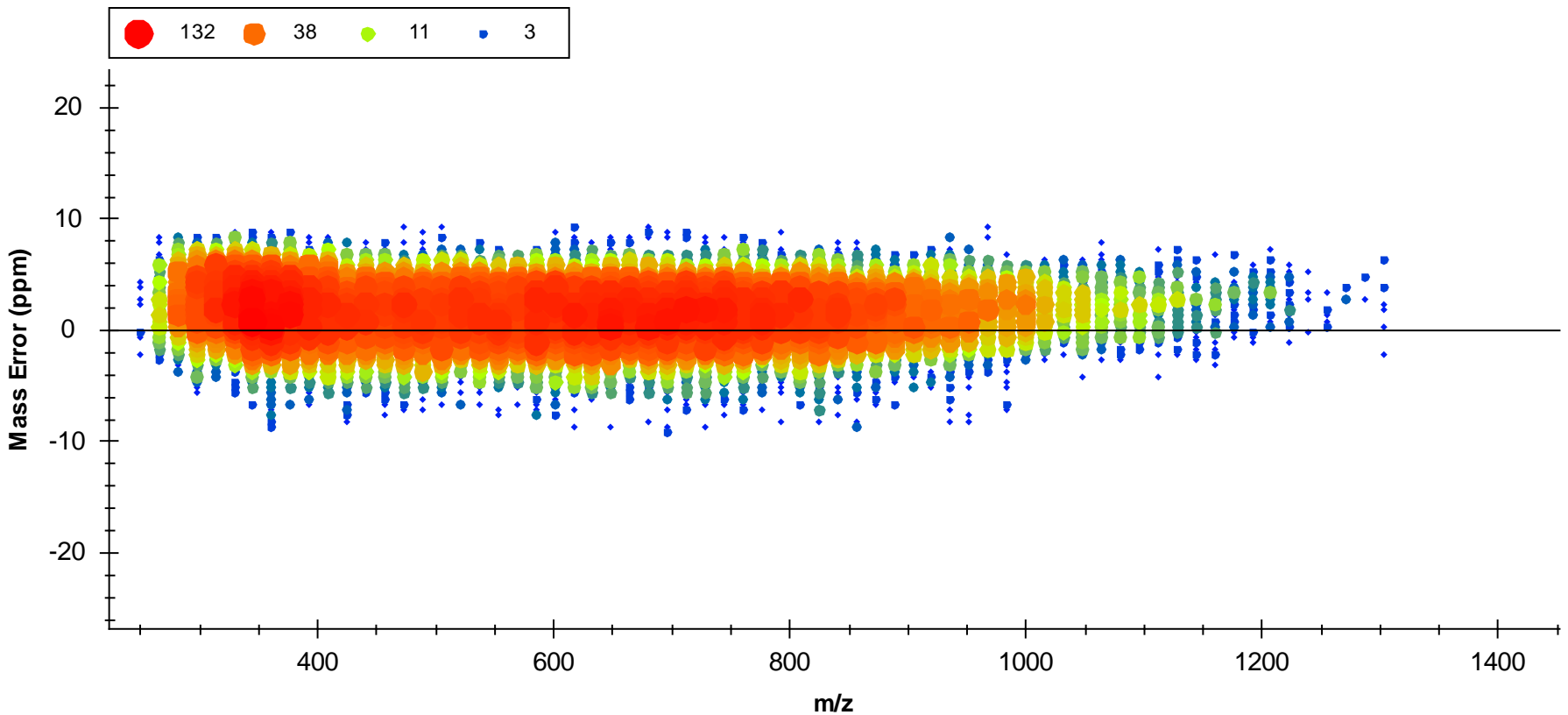
New Mass Error Graphs

► Webinar 15 – troubleshooting Bruker data

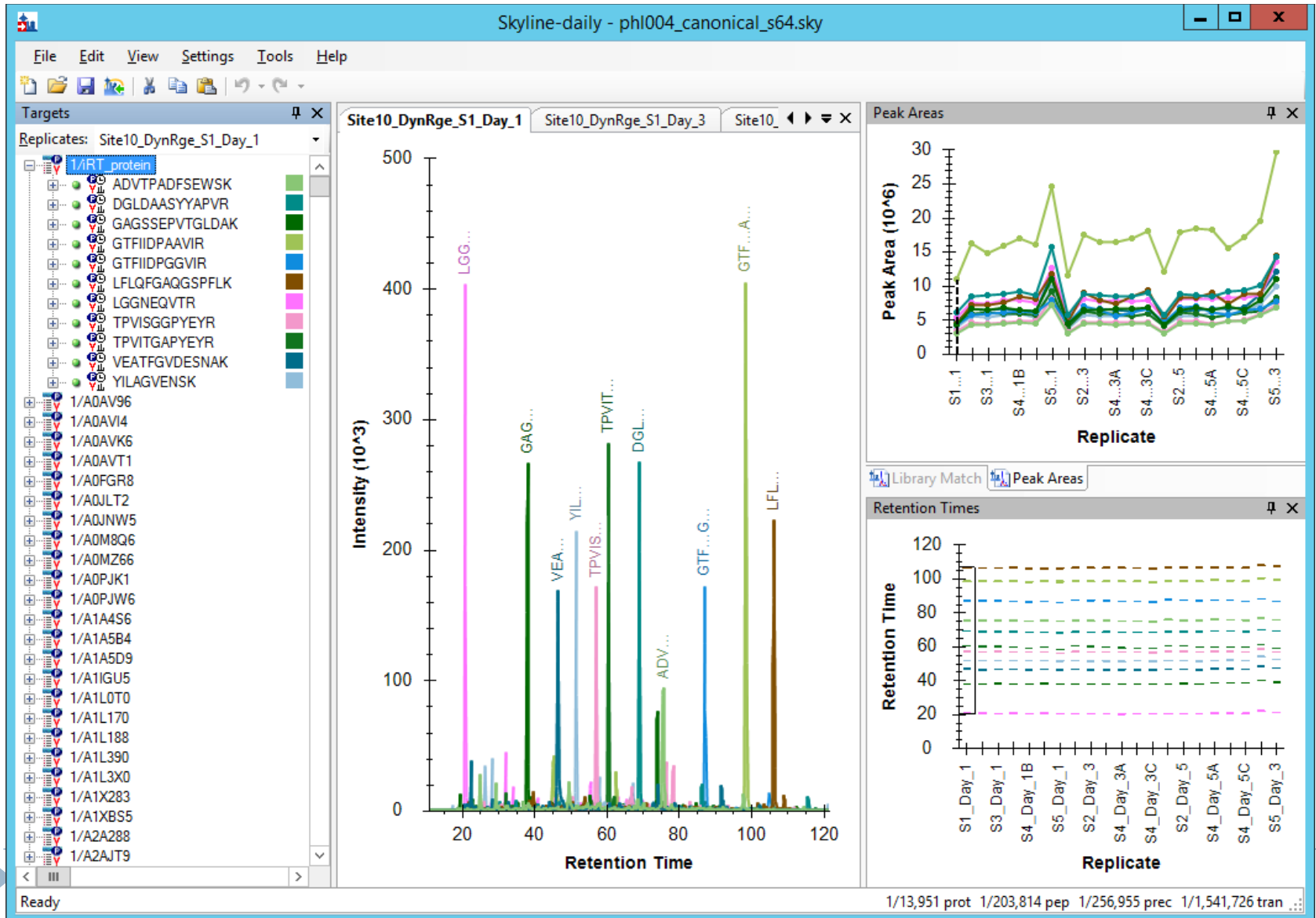


New Mass Error Graphs

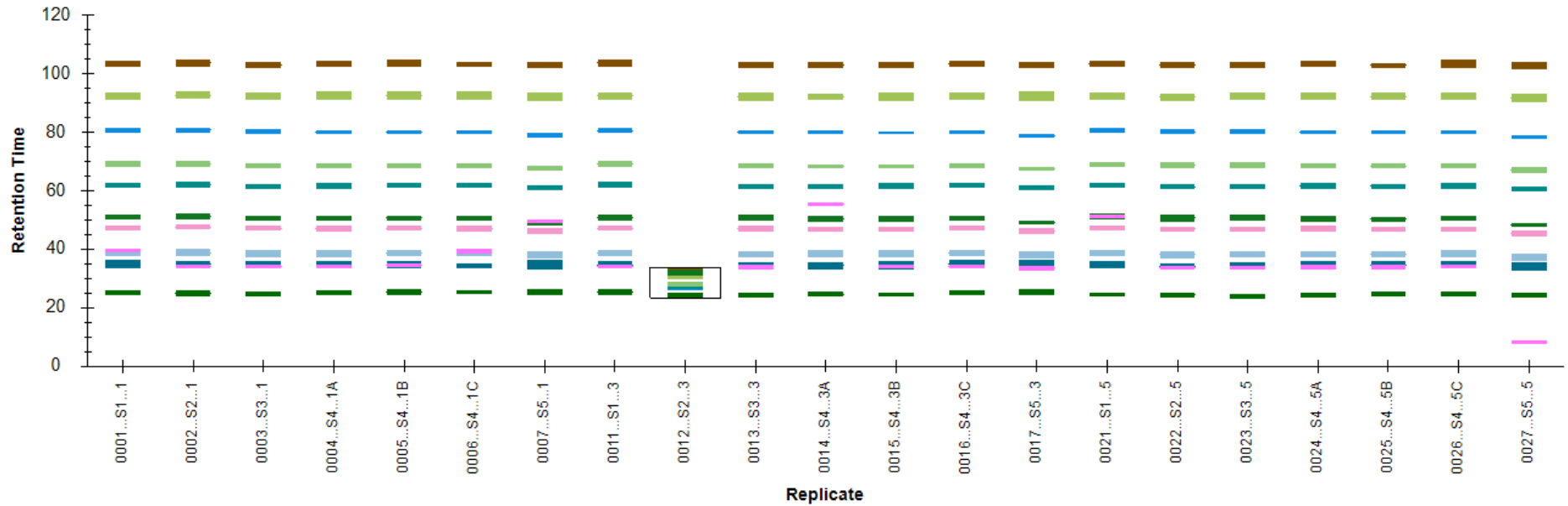
► Webinar 15 – Bruker data recalibrated



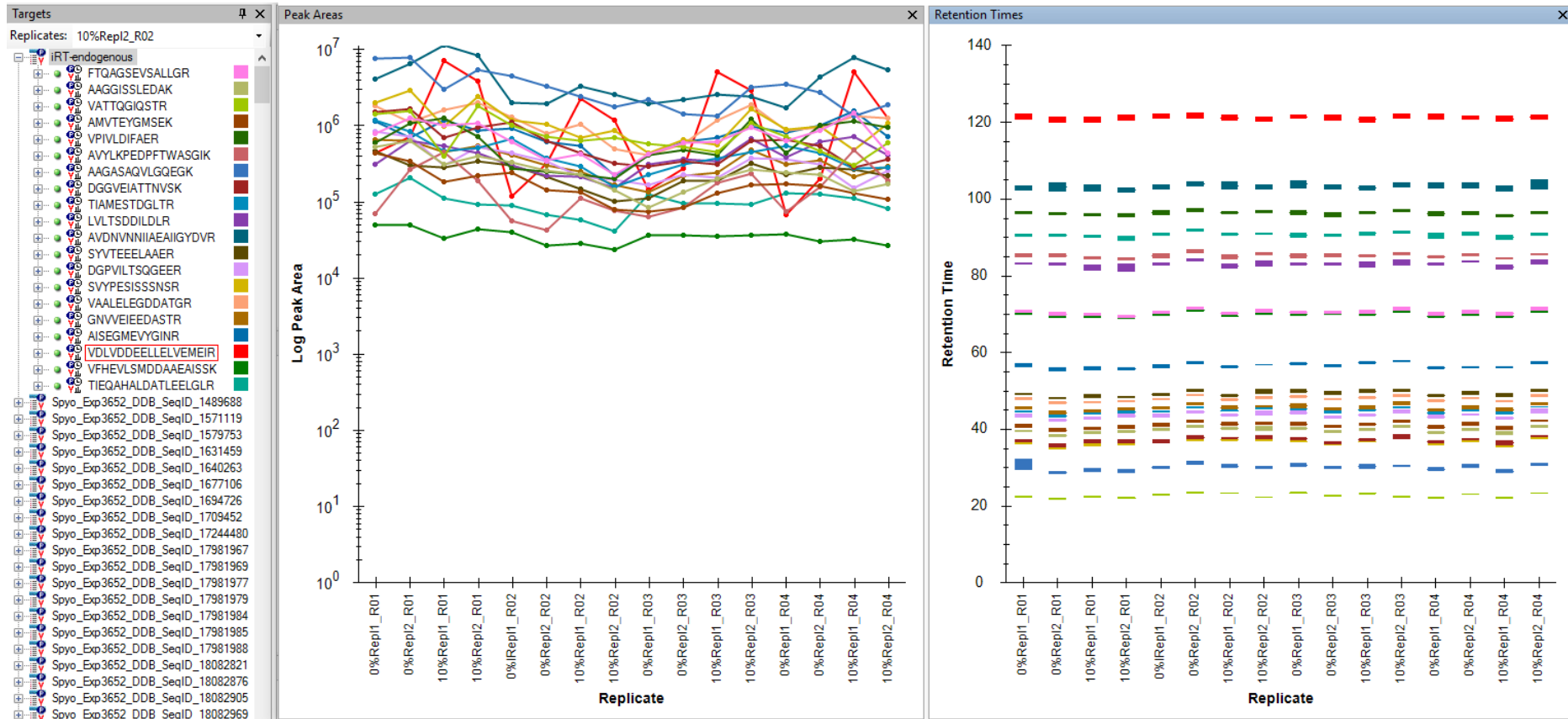
New Multi-Peptide Plots



New Multi-Peptide Plots

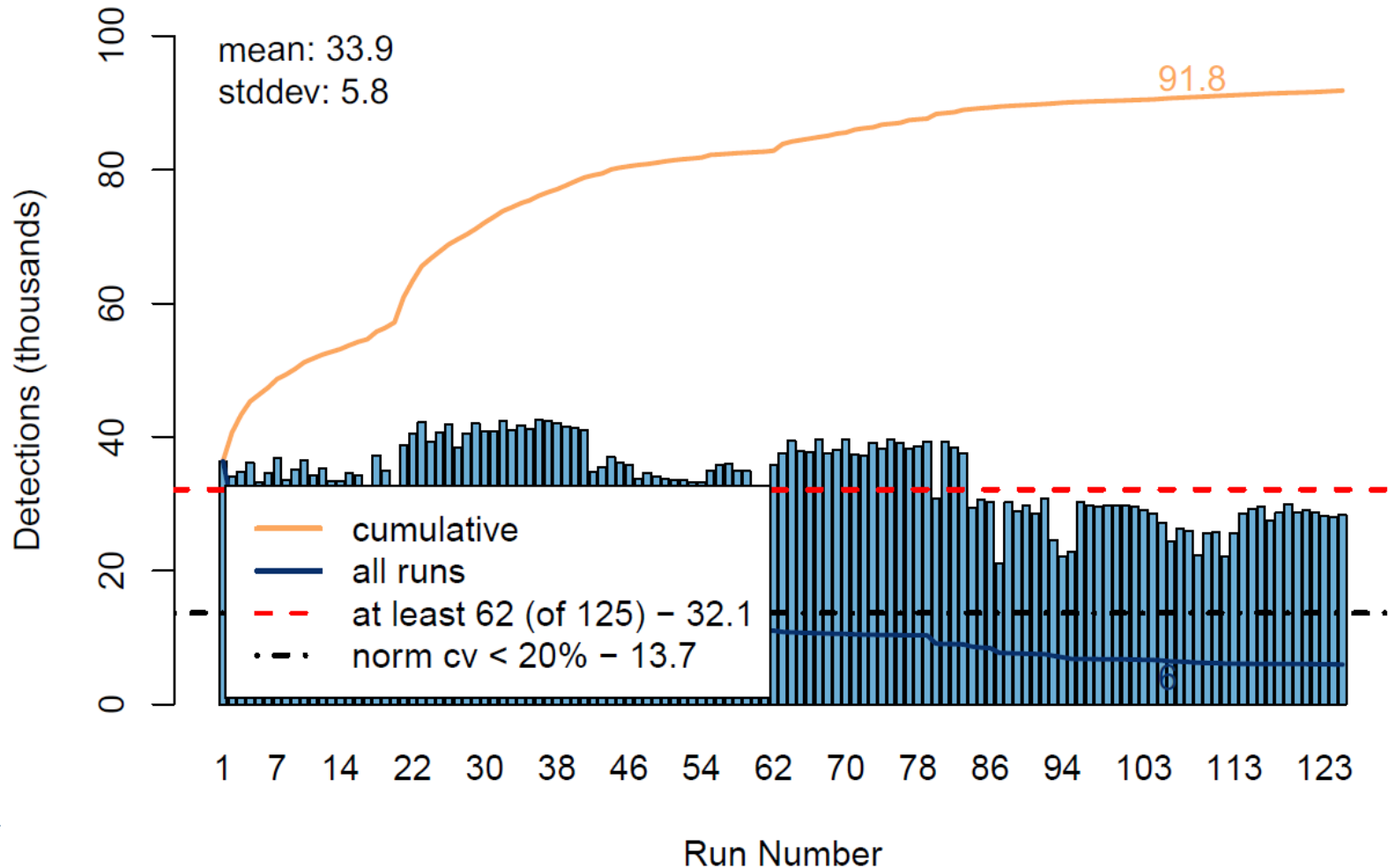


New Multi-Peptide Plots



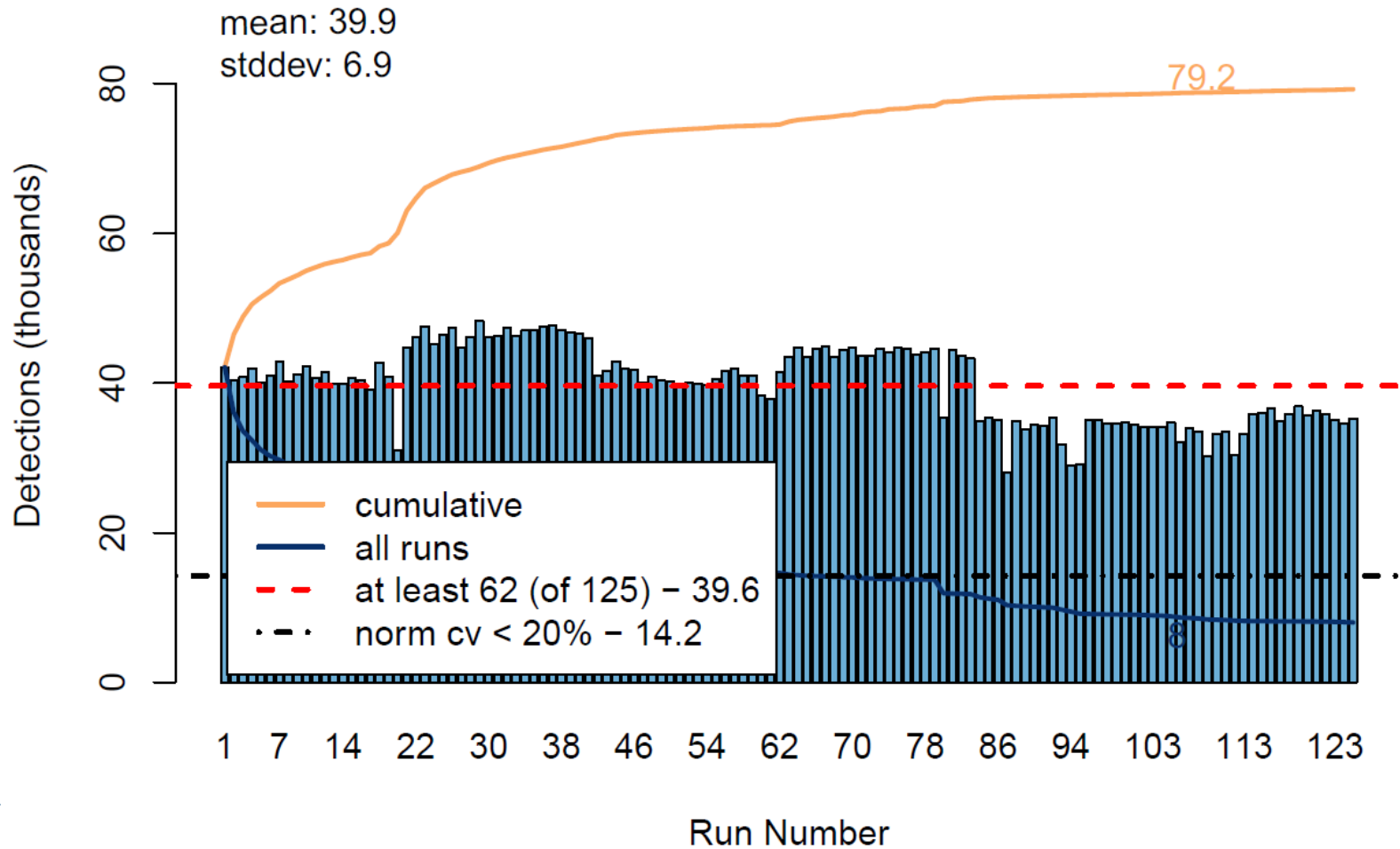
Pan Human DIA: “1 billion peaks”

Precursors Detections by Run



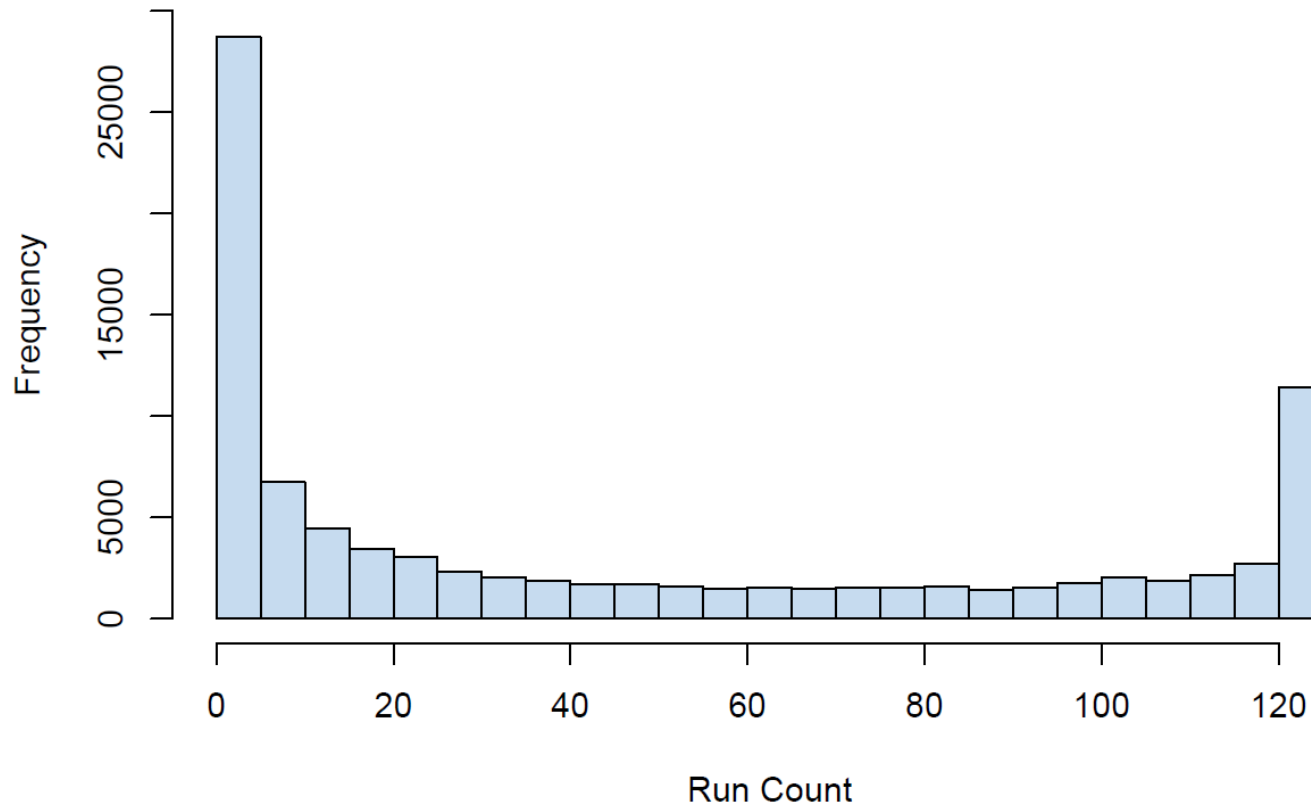
With Alignment (early)

Precursors Detections by Run



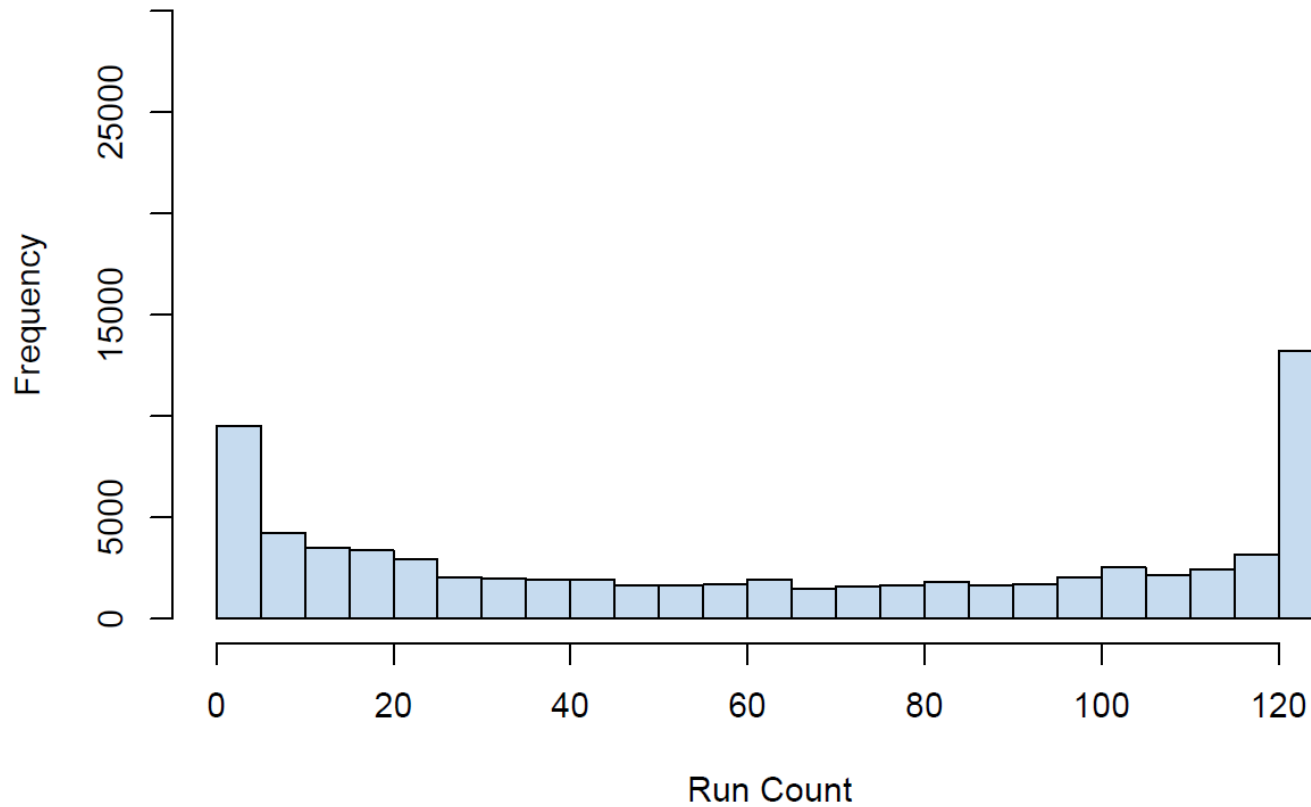
Pan Human DIA: Peak-only q values

MultiSite Precursors Detected in Runs



With Alignment (early)

MultiSite Precursors Detected in Runs



Processing with SkylineRunner

- ▶ NUMA Server (24 cores, 196 GB of RAM)
- ▶ `--import-process-count=12`
- ▶ 1.5 million transitions (with decoys), 21 files per site
- ▶ 1 hour per site (11 sites)
- ▶ 5 hours per site on i7 (4 cores) with 32 GB RAM



More Posters to See

- ▶ Brian Pratt – Small Molecule & IMS
- ▶ Nick Shulman – Peak Integration Improvements
- ▶ Josh Eckels – Panorama Absolute Quantification
- ▶ Jarrett Egertson – AWS Automated Pipeline
- ▶ Brian Searle – EncyclopeDIA Progress for Phospho Study



Skyline Team

▶ Nick Shulman



▶ Don Marsh



▶ Brian Pratt



▶ Max
Horowitz-Gelb



▶ Vagisha Sharma



▶ Nat Brace



▶ Kaipo Tamura



▶ Yuval Boss



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- ▶ Jarrett Egertson
- ▶ Clark Henderson
- ▶ Andy Hoofnagle
- ▶ Lindsay Pinot
- ▶ Brian Searle
- ▶ SoniaTing

▶ Broad Institute

- ▶ Steve Carr
- ▶ Jake Jaffe

▶ Buck Institute

- ▶ Birgit Schilling
- ▶ Brad Gibson

▶ Duke

- ▶ Will Thompson
- ▶ Arthur Moseley

▶ FHCRC

- ▶ Amanda Paulovich
- ▶ Jeffrey Whiteaker

▶ InfoClinika

- ▶ Andrey Bondarenko
- ▶ Oleksii Tymchenko

▶ IMSB

- ▶ Rudolph Aebersold
- ▶ Ben Collins
- ▶ Ludovic Gillet
- ▶ Christina Ludwig
- ▶ Hannes Röst
- ▶ George Rosenburger

▶ LabCorp

- ▶ Chris Shuford
- ▶ Russ Grant

▶ LabKey

- ▶ Josh Eckels

▶ PNNL

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- ▶ Yehia Ibrahim
- ▶ Tao Liu
- ▶ Sam Payne

▶ Northeastern

- ▶ Meena Choi
- ▶ Olga Vitek

▶ Stanford

- ▶ Dario Amodei
- ▶ Parag Mallick

▶ Vanderbilt

- ▶ Matthew Chambers



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- ▶ Joe Roark
- ▶ Ed Darland
- ▶ Yinghang Yang



Agilent Technologies

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- ▶ Mark Cafazzo
- ▶ David Cox
- ▶ Christie Hunter



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- ▶ Neil Loftus
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▶ Thermo-Scientific

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- ▶ Andreas Kuehn
- ▶ Rajiv Rawal
- ▶ Jim Shofstahl
- ▶ Vlad Zabrouskov



▶ Waters

- ▶ James Langridge
- ▶ Martin Lunt
- ▶ Keith Richards
- ▶ David Varley
- ▶ Hans Vissers

