



Skyline & Panorama: Key Tools for Establishing a Targeted LC/MS Workflow

Genentech
A Member of the Roche Group

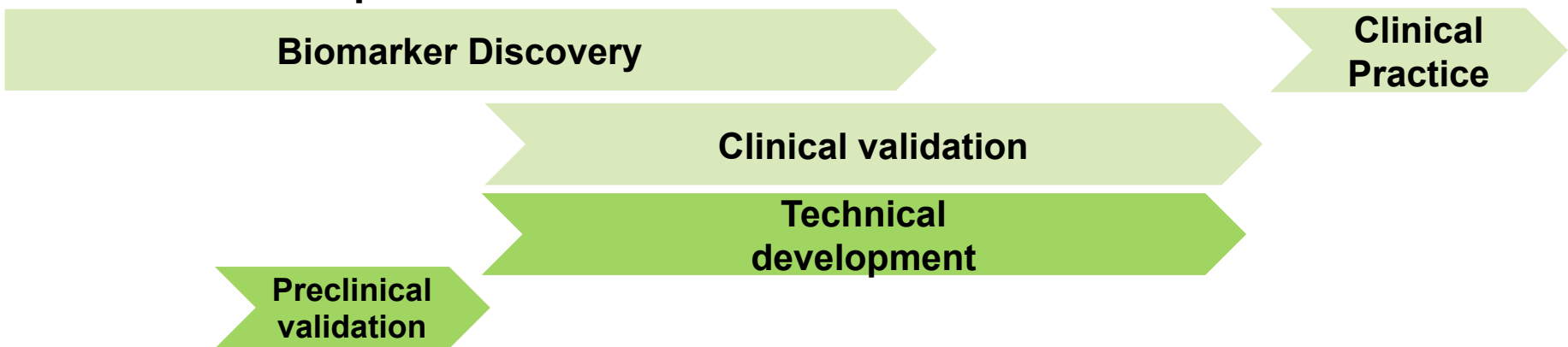
Kristin Wildsmith
Scientist, Biomarker Development
LabKey User Conference
October 6, 2016

Biomarkers enable drug development

Drug development

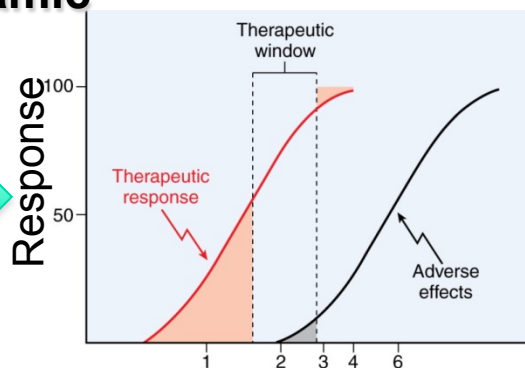


Biomarker development

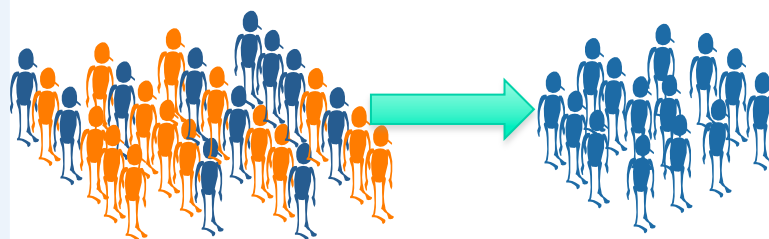


Pharmacodynamic

Therapeutic →



Diagnostic



Mass spectrometry is a quantitative tool for biomarker development and Labkey server is used for data management

Biomarker Discovery

- Discovery (unbiased)
- Targeted-discovery

Clinical validation

- Multiplex panel
- Single analyte quantitation

Clinical Practice



LTQ-Orbitrap
(High resolution)



Triple Quad
(High sensitivity)



LabKey Server

Create Folder in /gRED

Name:

Use name as title

Folder Type:

Assay

Collaboration

Flow

MS1

MS2

Microarray

Panorama

Study

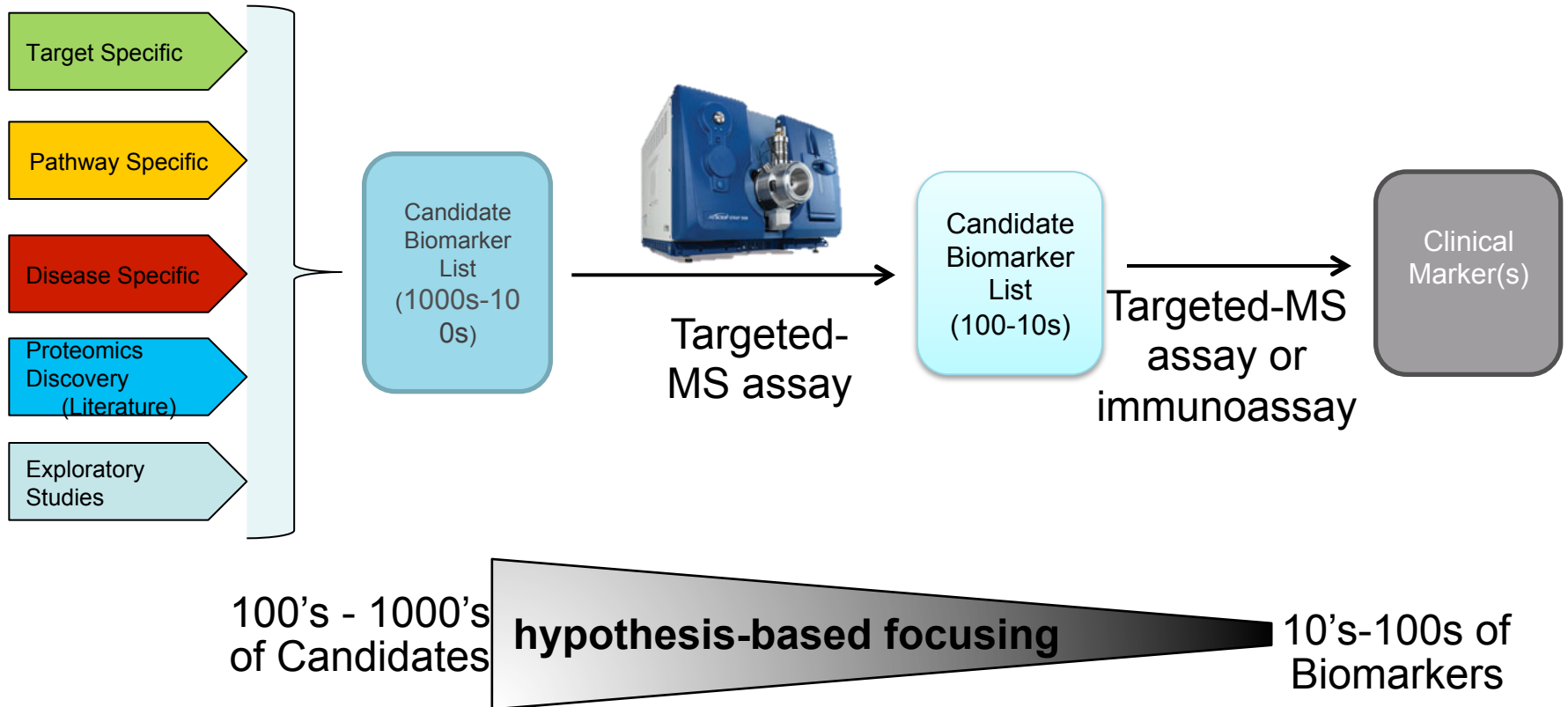
Custom

Create From Template Folder

Labkey is a data management solution for MS data

Development of customized folders accelerated Targeted MS assay development

New model for developing protein clinical biomarkers: Hypothesis driven multiplexing with mass spectrometry



**MS can provide a faster and more successful translation
of protein biomarkers to the clinic**

Multiplexed MRM assay developed for candidates



Candidate proteins
in CSF



↓ protease digestion

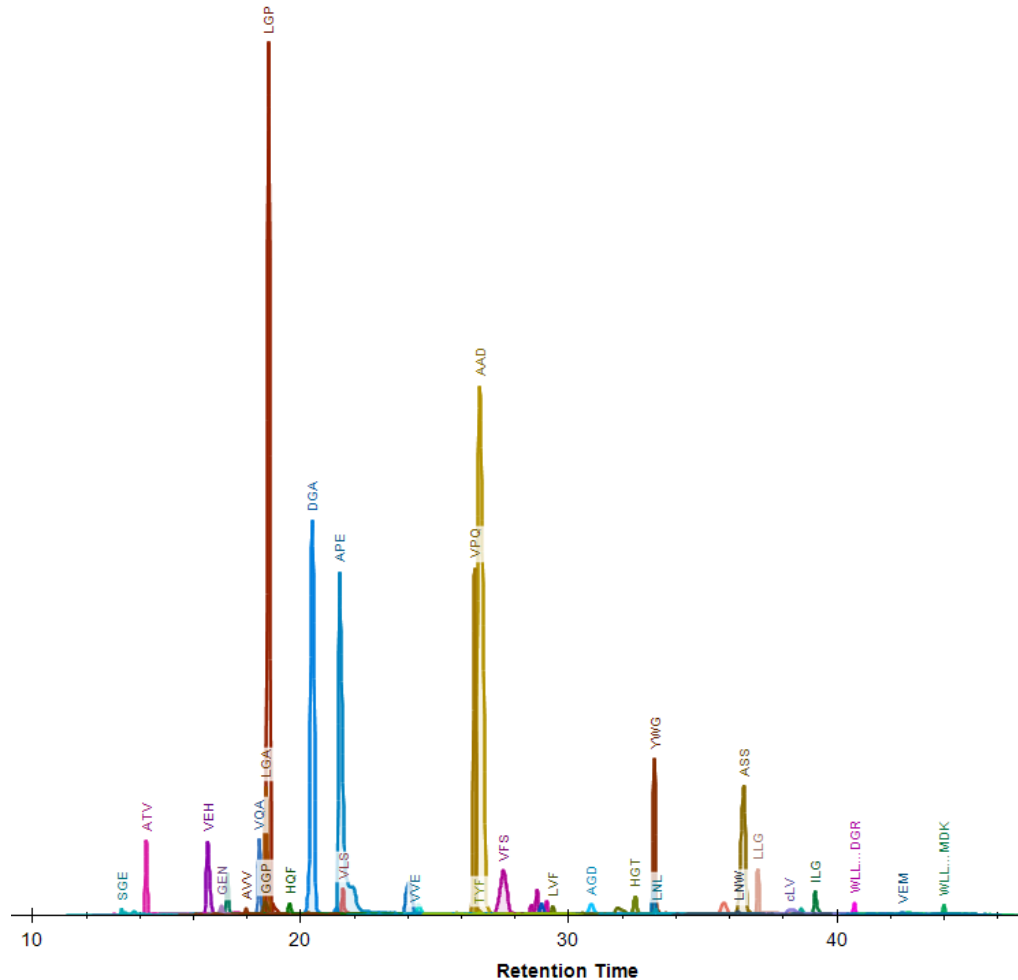
Signature peptides

+internal standards
(heavy peptides)

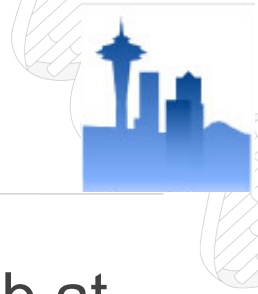


LC-MS/MS

Quantitation

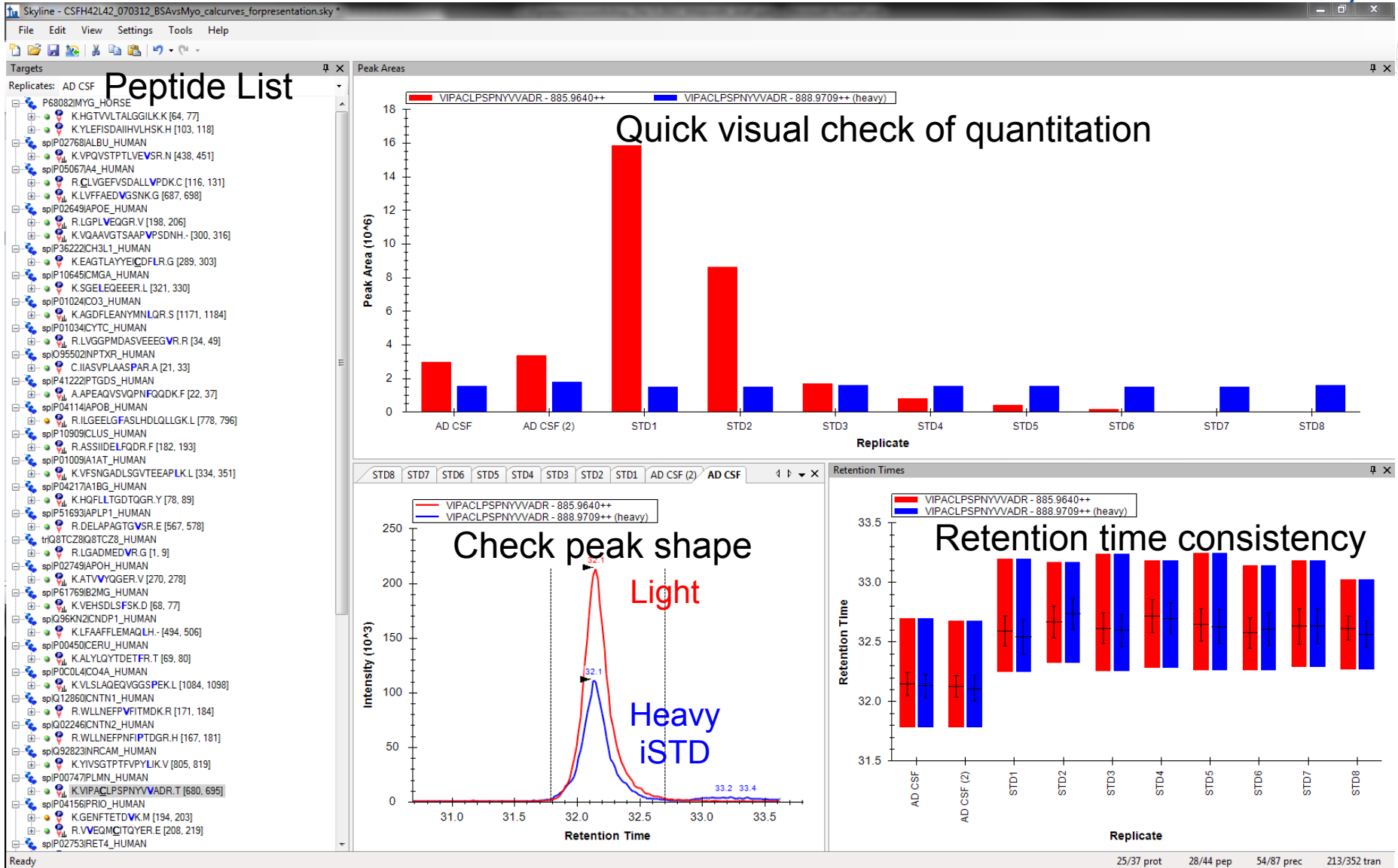


Skyline supports targeted MS techniques



- Skyline is an open-source software from MacCoss lab at University of Washington
- Vendor neutral
- Supports method development and data analysis:
 - Targeted MS/MS
 - Selected reaction monitoring (SRM, aka MRM)
 - Parallel reaction monitoring (PRM)
 - Data-independent-acquisition (DIA) / SWATH
 - Targeted discovery with MS¹ quantitative methods
 - Discovery proteomics with MS² methods

Multiplexing enabled by targeted-proteomics software



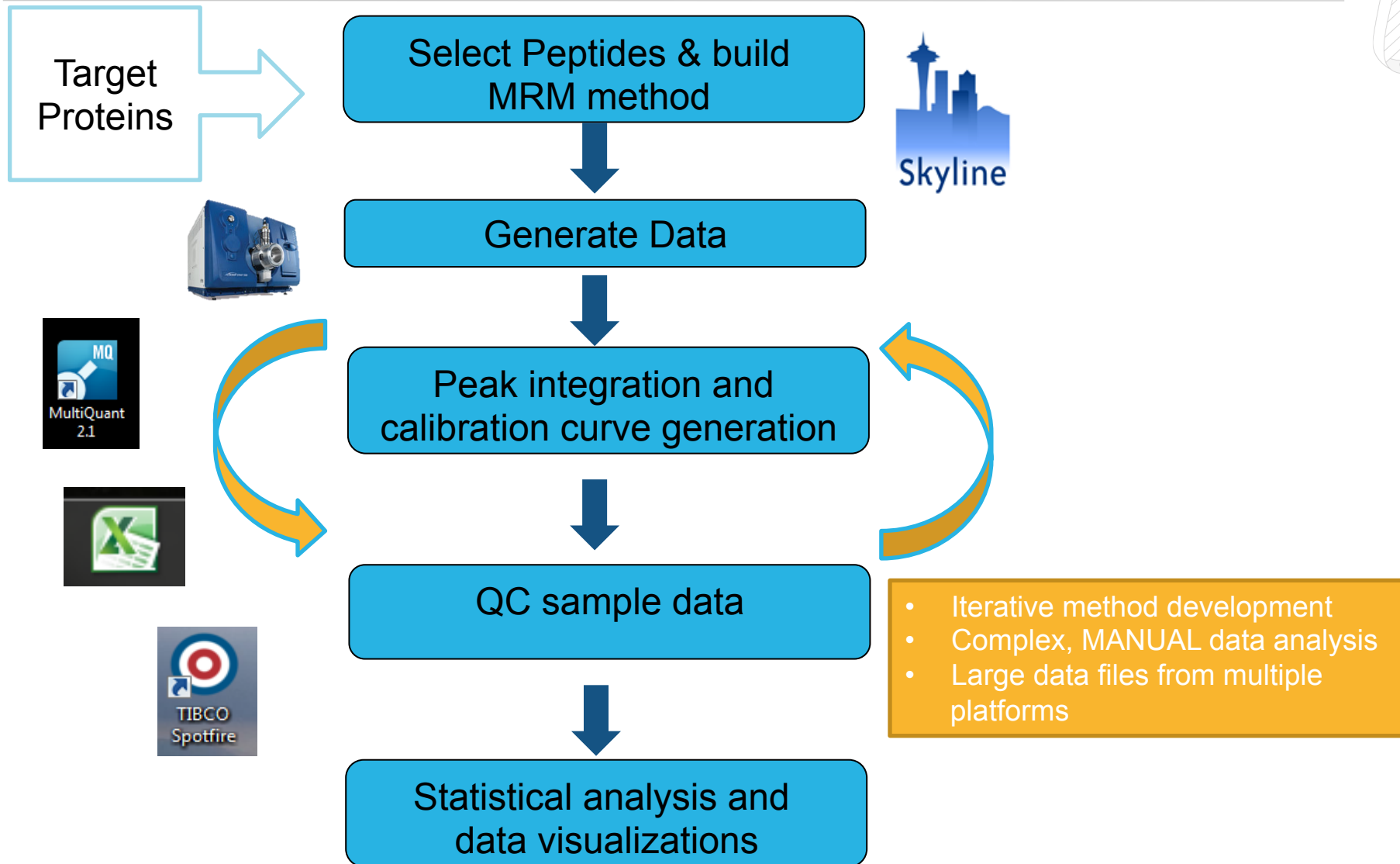
Quick visual check of quantitation

Check peak shape

Retention time consistency

Open-source software available from MacCoss lab at University of Washington:
<https://brendanx-uw1.gs.washington.edu/labkey/project/home/software/Skyline/begin.view>

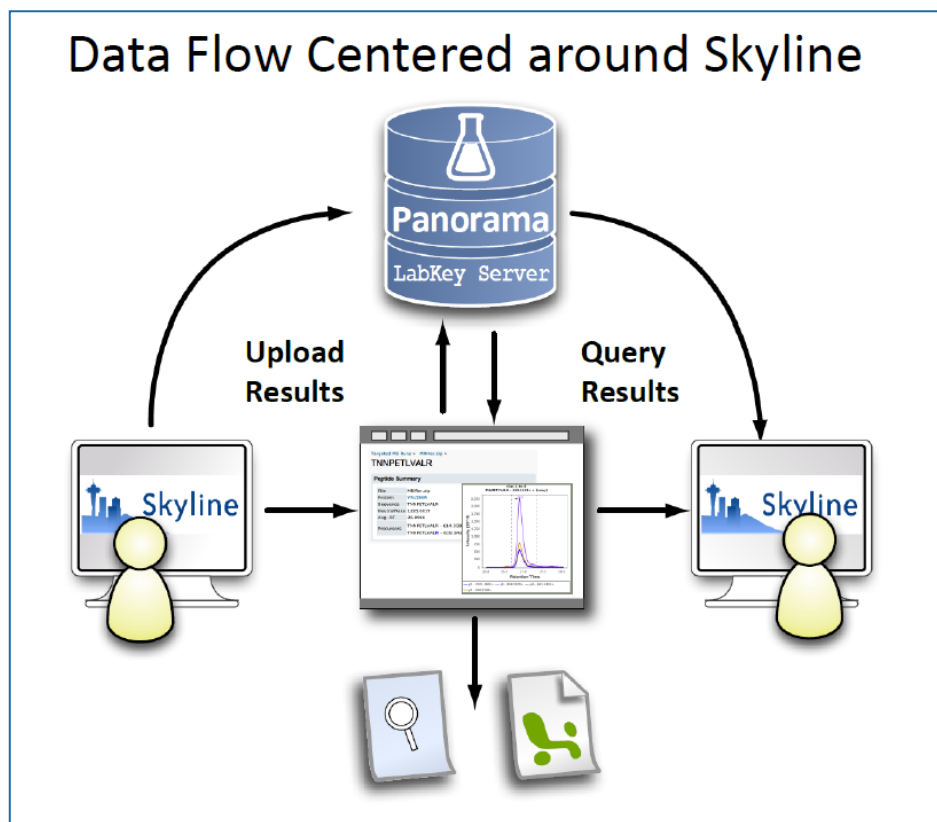
Old workflow for multiplexed MRM creates data management challenges





Panorama is a repository server application supporting Skyline

- Module within LabKey server
- Open-source bioinformatics data management platform
- Searchable database storing Skyline data files



Panorama increases rate of method development



- MacCoss-lab hosted instance (includes CPTAC, ABRF shared libraries)
- Shares read-only data to support publications
- Workflow for sharing data with reviewers and then general public

Panorama Public: A public repository for Skyline documents

Vagisha Sharma¹, Josh Eckels², Birgit Schilling³, Jacob D. Jaffe⁴, Michael J. MacCoss¹, Brendan MacLean¹
 University of Washington, Seattle, WA¹; LabKey Software, San Diego, CA²; Buck Institute for Research on Aging, Novato, CA³; The Broad Institute, Cambridge, MA⁴

<https://panoramaweb.org/>

Overview

Panorama[®] is an open-source repository software project for targeted proteomics data processed with Skyline that has been adopted by a number of laboratories and organizations. Panoramaweb (<https://panoramaweb.org>), the Panorama server hosted at the University of Washington, has become a popular choice with laboratories lacking the resources to set up their own Panorama servers. Users can request free projects on Panoramaweb where they can manage data access permissions. To fulfill journal submission requirements, researchers have used their own projects on Panoramaweb to provide public access to data. We present a new mechanism that allows users to publish their data to a public repository on Panoramaweb that provides a new central resource to the community for published data processed with Skyline.

Methods

Panoramaweb has become a popular choice with researchers for hosting Skyline documents associated with publications. However, these documents remain part of user projects on Panoramaweb where the user can make changes, including removing this supplementary data entry. When data contained in a user project is submitted to Panorama Public a snapshot of the data is created, to which the submitting authors have read-only access. Panorama Public provides a permanent location for supplementary data to reference in publications, in its original form as it was intended for publication. 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 upon publication.

Results

Publishing to Panorama Public

STEP 1 Upload documents to Panoramaweb: Skyline documents associated with a manuscript are uploaded to a researcher's project on Panoramaweb.

STEP 2 Annotate a folder for publication: Folders containing data intended for publication to Panorama Public must be annotated with a description of the experiment. This includes information such as an abstract, experiment and sample descriptions, organism, MS instrument used etc. The example shown above is from a published dataset¹ available on Panorama Public at <https://panoramaweb.org/Skyline/1study9.url>.

STEP 3 Submit the annotated folder for publication: Clicking on the "Publish" button in the experiment description brings up a form that lets users generate a permanent link to the data and submit the data for publication to Panorama Public. The permanent link can be included in manuscripts and given to journal editors during the manuscript review process.

Data on Panorama Public

Folder in researcher's project on Panoramaweb → **Folder on Panorama Public after copy**

Panorama allows users to create a rich interface around their data that can include web pages, charts and other supplementary files and images. These user interface elements are included in the copy of the data stored in Panorama Public. Submitting researchers have read-only access to data on Panorama Public.

Browse available data on Panorama Public by clicking on the link on the home page of Panoramaweb.

Introduction

Usage of Panoramaweb has grown since it became available in January 2013. As of May 2015, the server hosts projects for over 100 different laboratories.

Growth of projects on Panoramaweb.

Several projects on Panoramaweb contain Skyline documents associated with peer-reviewed publications that the project owners have made publicly available using the access control features implemented in Panorama. Google Scholar identifies around 18 publications that have references to data on Panoramaweb. However, these publicly accessible datasets are dispersed across several projects, which makes it difficult to provide a comprehensive listing and impossible to guarantee continued availability of the datasets in their original form. The availability of the Panorama Public repository on Panoramaweb allows users to submit their data to a central resource of data processed with Skyline that can be searched using various criteria.

Workflow for publishing to Panorama Public

Workflow for publishing to Panorama Public

Researcher uploads Skyline documents to a folder in their project on Panoramaweb → Researcher adds experiment annotations (abstract, organism, instrument etc.) to the folder → Researcher creates a permanent link to the data on Panoramaweb → Researcher submits the annotated folder for publication to Panorama Public → Panoramaweb administrators make a copy of the folder to Panorama Public

Researcher generated permanent link

Before copy: Researcher's project on Panoramaweb → After copy: Read-only copy on Panorama Public

The permanent link created by the researcher initially links to the researcher's folder on Panoramaweb. After a copy of the folder has been made to Panorama Public, the permanent link points to the new location of the copied data on Panorama Public.

Conclusions

Panorama Public provides a new community resource for published data processed with Skyline. Data is made available in its original form as it was intended for publication. Panoramaweb users may also submit data to Panorama Public during manuscript review process and request private access for reviewers until publication. A tutorial describing the process of publishing to Panorama Public is available at: https://panoramaweb.org/tutorials/tutorial_panorama_public.url

Future work: Fulfill the requirements for participating in the ProteomeXchange consortium as a data resource.

References

- Sharma V, MacLean B, et al. J. Proteome Res. 2014;13(8):1510-1519.
- Abdelhadi H, Carr SA et al. MCP 2014;4(2):10-13.

Funding: HD-082055 (PI: MacCoss) and USA-H102807 (BPI-Jaffe)

Panorama Public: CPTAC

Enabling data sharing



The CPTAC Assay Portal

https://assays.cancer.gov

National Cancer Institute

OFFICE OF CANCER CLINICAL PROTEOMICS RESEARCH Assay Portal

Available Assays About CPTAC Home

Assay Portal

Search the Assay Database by:

Search: Showing 1 to 50 of 1,068 entries

KEGG Pathways

Find assays to quantify proteins encoded in a specific chromosomal region

Chromosome Number

Chromosomal Location

Find assays to quantify proteins that interact with the following protein(s):

Proteins and peptides for which assays are available	Submitting Laboratory	Modification	Assay Type	Matrix	CPTAC ID
A18G - UniProt Accession ID: P04217					
LETPDFQLFK	Uvic-Genome BC Proteomics Centre	unmodified	direct	plasma	non-CPTAC-1064
A2M - UniProt Accession ID: P01023					
AIGYLNTGYQR	Uvic-Genome BC Proteomics Centre	unmodified	direct	plasma	non-CPTAC-1068
AARS - UniProt Accession ID: P49588					
AVFDETYPDVR	Fred Hutchinson Cancer Research Center	unmodified	direct	cell line lysate pool	CPTAC-2

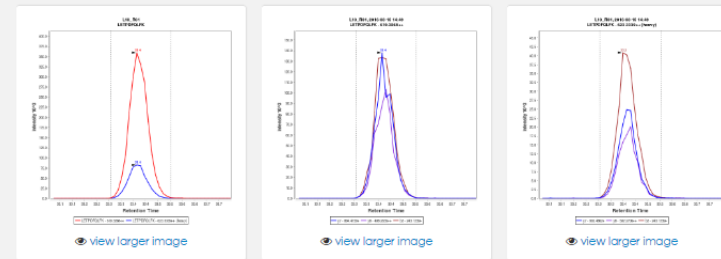
Assay Parameters

Data source: Panorama

Instrument 6490 Triple Quad (Agilent)	LC 1290 LC (Agilent)
Internal Standard synthetic peptide	Column Packing Zorbax Eclipse Plus C18, 1.8 µm
Peptide Standard Purity >95%	Column Dimensions 2.1 x 150 mm
Peptide Standard Label Type 13C and 15N at C-terminus K	Flow Rate 400 µL/min

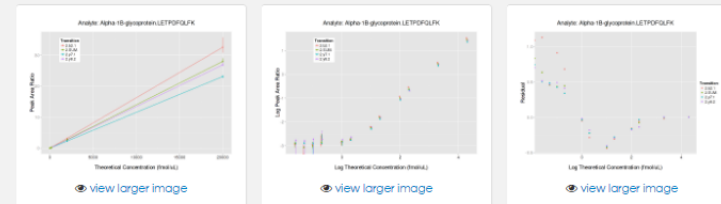
Chromatograms

Data source: Panorama



Response Curves

Data source: Panorama



Peptide	Transition	LOD (fmol)			LLOQ (fmol)		
		blank only	blank+low-conc	rsd limit	blank only	blank+low-conc	rsd limit
LETPDFQLFK	2.b2.1	4.5e-1	4.5e-1	4.5e-1	4.5e-1	4.6e-1	4.6e-1

Panorama Partnership enables use of Panorama in secure environment and expand capabilities



- Collaborate directly with MacCoss lab and LabKey teams
- Installed Labkey server on-site
- Guide Skyline & Panorama software development priorities
- All partners contribute to common development fund
- All partners give input on priorities and design decisions

- Genentech/Roche partners since Oct 2013 (1 of 4)

Field strongly supporting Skyline and Panorama development

Academic/Government: Industry:

2 R01s

1 P41

1 U01



<https://skyline.gs.washington.edu/labkey/wiki/home/software/Skyline/page.view?name=funding>

LabKey Server

gRED

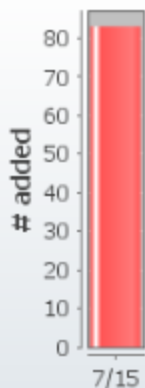
CSF peptide library

CSF peptide library

Targeted MS Runs > CSF_V1 and V2 with IRT_using scheduled CSF result_2014-07-15_08-53-03.sky.zip >

LSSPAVITDK

Chromatogram Library Download ▾



CSF peptide library Library

Download

CSF peptide library_rev1.clib (185 KB)
Revision 1

ARCHIVED REVISIONS ▸

Peptides

Library Statistics:

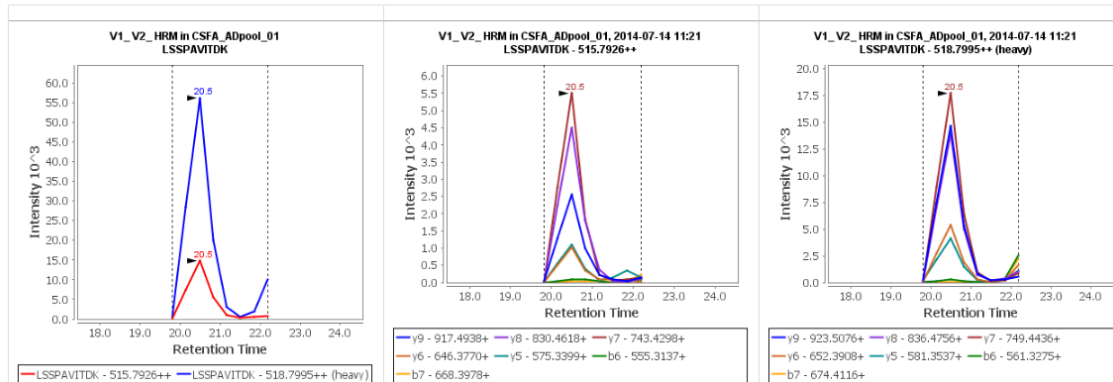
The library contains 83 peptides with 605 ranked transitions.

Peptide Summary

Name	CSF_V1 and V2 with IRT_using scheduled CSF result_2014-07-15_08-53-03.sky.zip
Protein	sp P00747 PLMN_HUMAN
Sequence	LSSPAVITDK
NeutralMass	1029.5707
Avg. RT	20.6571
Predicted RT	20.7100
RT Score	10.2096
Precursors	LSSPAVITDK - 515.7926++ LSSPAVITDK - 518.7995++ (heavy)

Chromatograms

Display Chart Settings

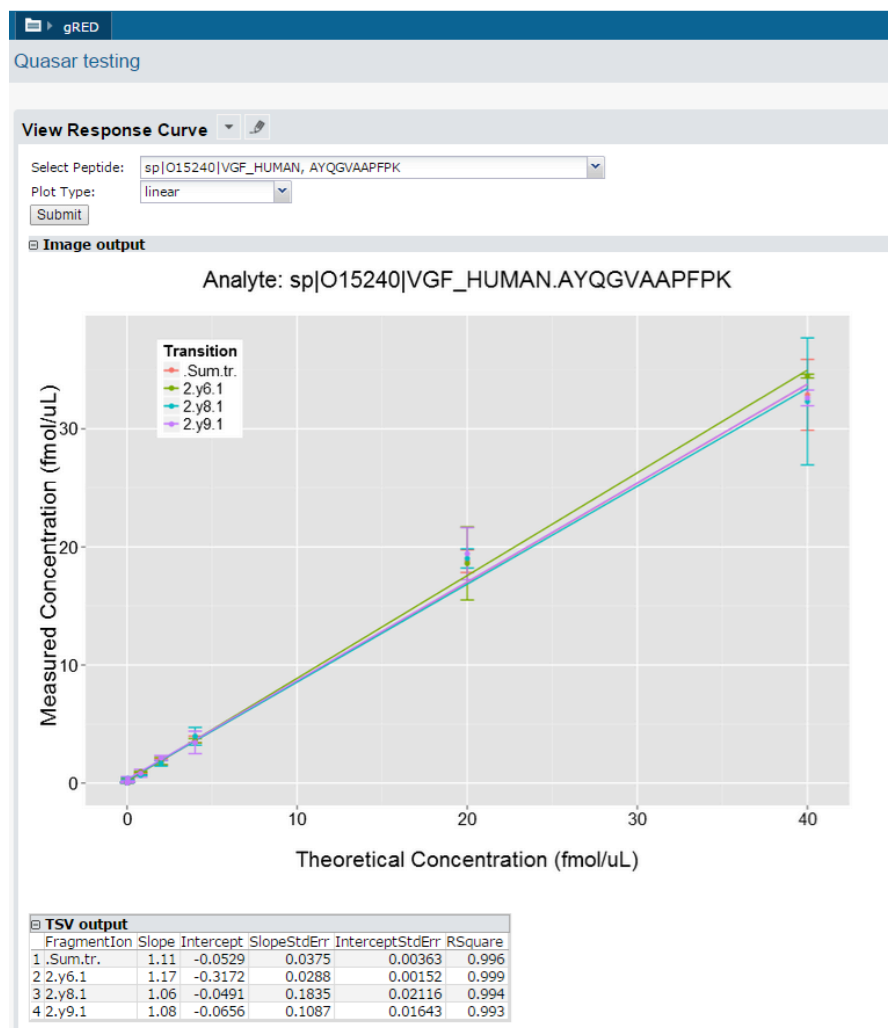


Key areas of focus for Panorama Partnership

Vision: Data analysis directly in Panorama



- Tracking method development (versioning)
- Implementing data analysis tools directly in Panorama
 - Quality Control folder
 - AutoQC
 - Statistics





LabKey Server

TargetedMS

Method Build

Targeted MS Runs >

MethodBuildThird_2016-03-24_08-16-29.sky.zip

Document Summary

Name	MethodBuildThird_2016-03-24_08-16-29.sky.zip RENAME DOWNLOAD		
Protein Count	3	Peptide Count	30
Precursor Count	30	Transition Count	155

Document Versions

Document Name	Imported	Imported By	Note	Proteins	Precursors	Transitions
MethodBuildThird_2016-02-23_12-21-54.sky.zip	02/23/2016 12:22 PM	JEckels		4	49	313
MethodBuildThird_2016-02-23_12-22-33.sky.zip	02/23/2016 12:22 PM	JEckels		4	45	287
MethodBuildThird_2016-02-23_12-22-47.sky.zip	02/23/2016 12:22 PM	JEckels		4	45	279
MethodBuildThird_2016-02-23_13-41-10.sky.zip	02/23/2016 1:41 PM	JEckels		3	36	208
MethodBuildThird_2016-02-24_11-00-03.sky.zip	02/24/2016 11:00 AM	JEckels		3	33	180
MethodBuildThird_2016-02-24_11-30-52.sky.zip	02/24/2016 11:30 AM	JEckels		3	31	169
MethodBuildThird_2016-02-26_14-28-57.sky.zip	02/26/2016 2:29 PM	JEckels		3	31	169
MethodBuildThird_2016-03-23_22-00-40.sky.zip	03/23/2016 10:00 PM	JEckels		3	30	159
MethodBuildThird_2016-03-24_08-16-29.sky.zip	03/24/2016 8:16 AM	JEckels		3	30	155

Panorama Partners QC folder Development of QC folder to monitor instrument performance



The screenshot displays the Panorama Dashboard interface. At the top, there's a navigation bar with 'LabKey Server', 'TargetedMS', and 'QC Demo'. A search bar is visible on the right. Below the navigation, the 'QC Summary' section shows '2 Skyline documents uploaded containing 47 sample files' and '7 precursors tracked'. The 'QC Plots' section features a 'Retention Time' chart for 'ATEEQLK' from 2013-08-09 to 2013-08-27. The chart shows a baseline around 14.5 minutes with a significant peak at approximately 16.8 minutes. A legend indicates 'Technician Change' (blue asterisk), 'Reagent Change' (green asterisk), and 'Instrumentation Change' (red asterisk). A yellow callout bubble points to the chart with the text 'View retention time, peak area, H/L ratio, etc.'. To the right, a 'Precursor Chromatograms' window shows a grid of chromatograms for various precursors. A yellow callout bubble points to this window with the text 'Add notes'. A third yellow callout bubble points to a zoomed-in view of a precursor chromatogram with the text 'Zoom to details'.

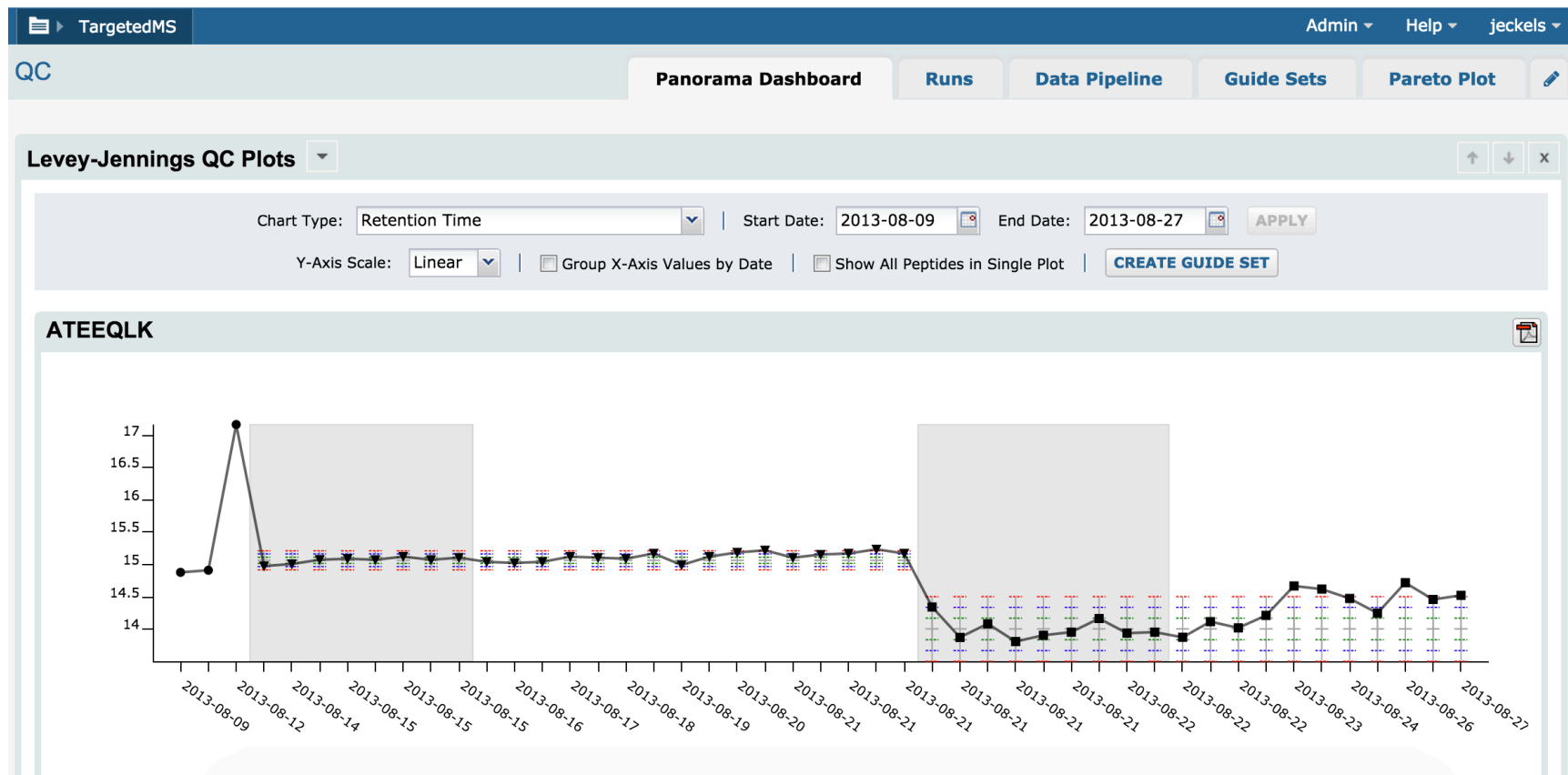
View retention time, peak area, H/L ratio, etc.

Add notes

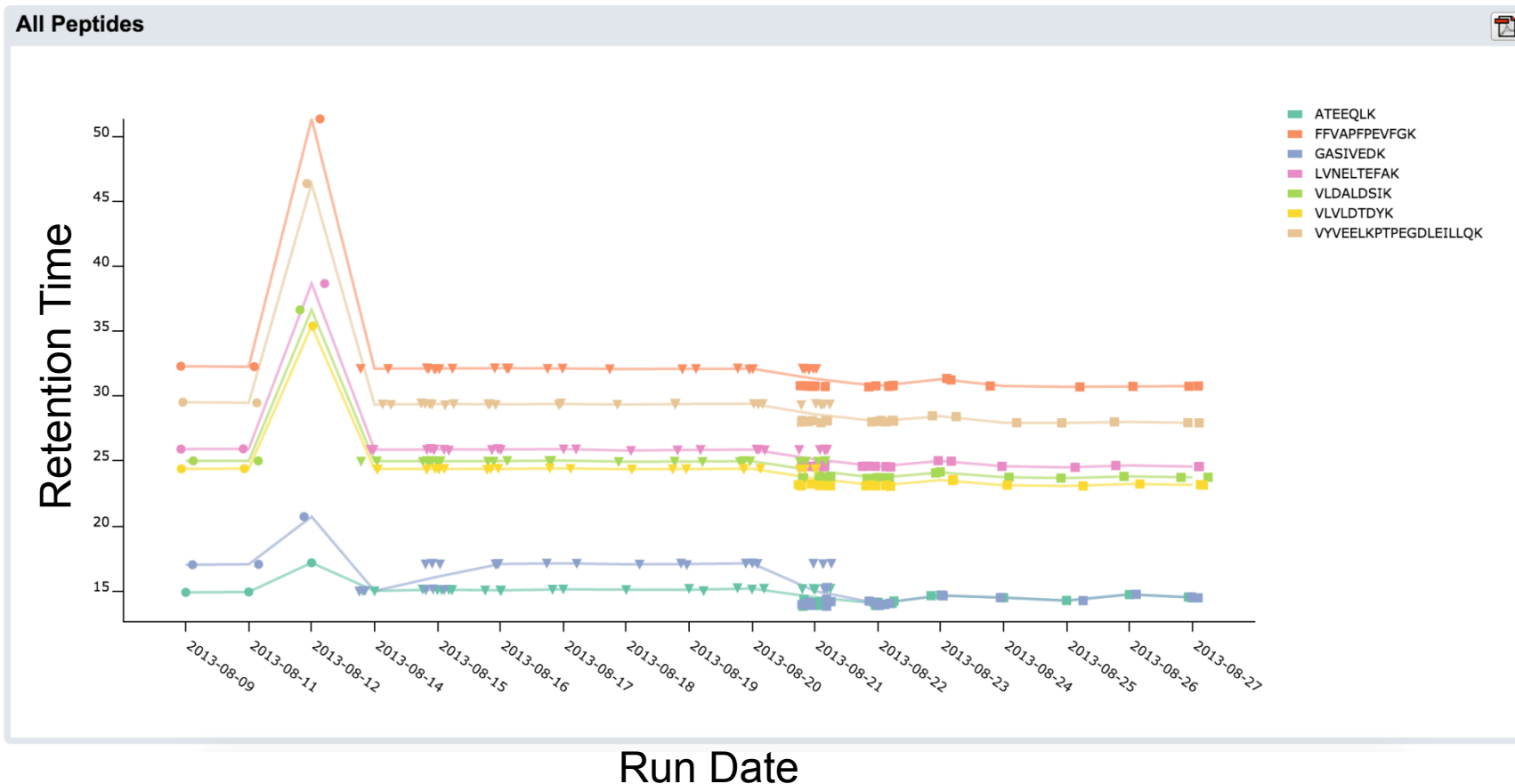
Zoom to details



QC – Levey-Jennings Plots

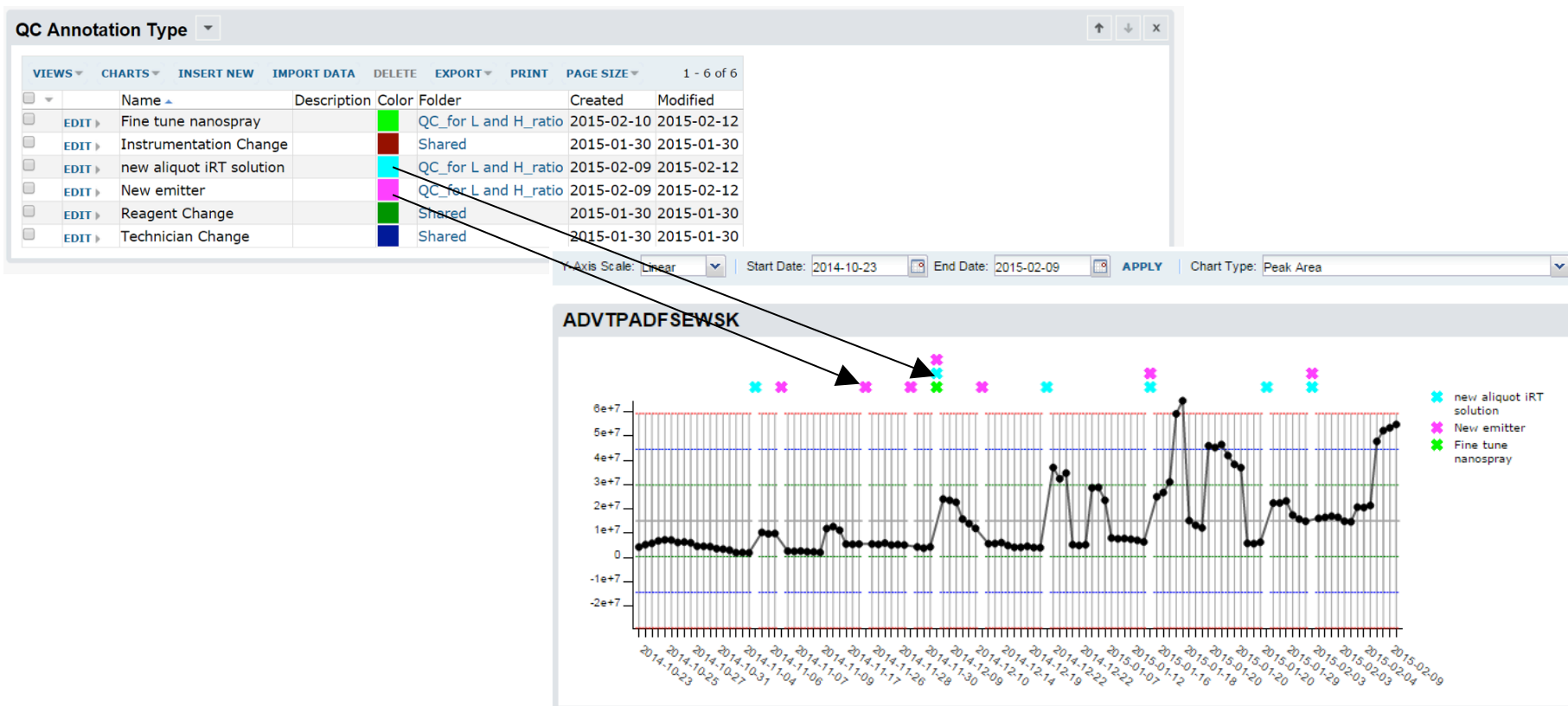


Evaluate performance of multiple peptides



Panorama Partners QC folder

Track instrument performance

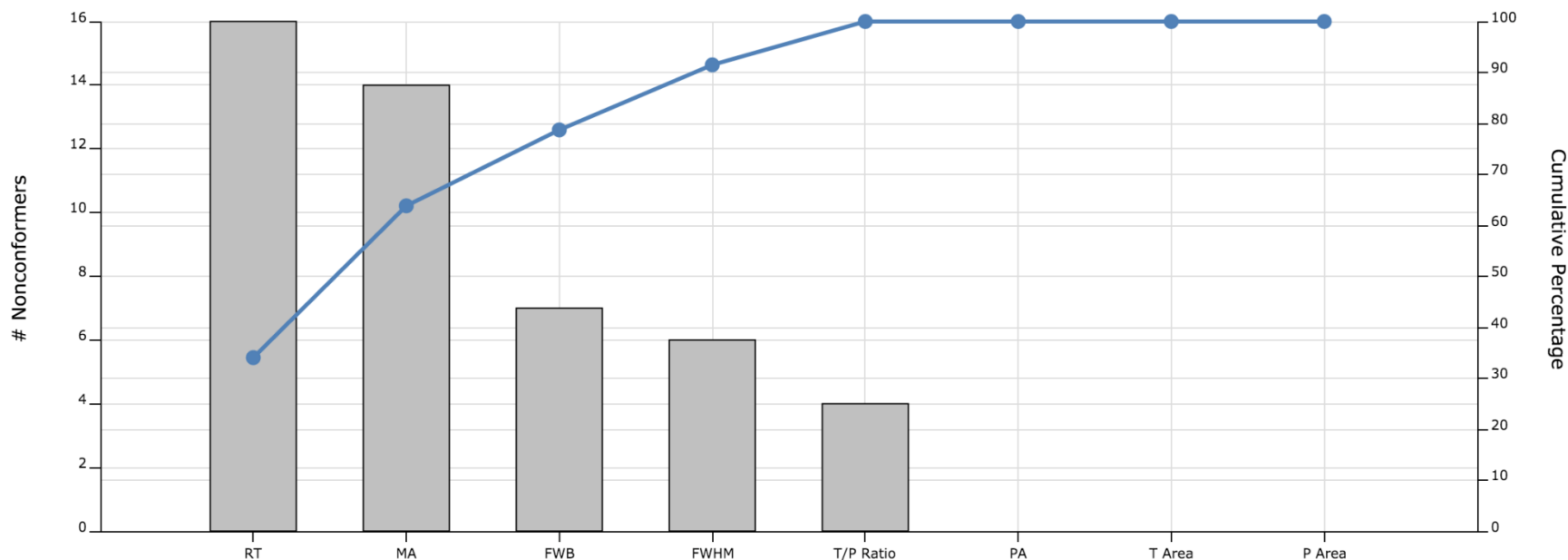


Determine which feature drives variability in method



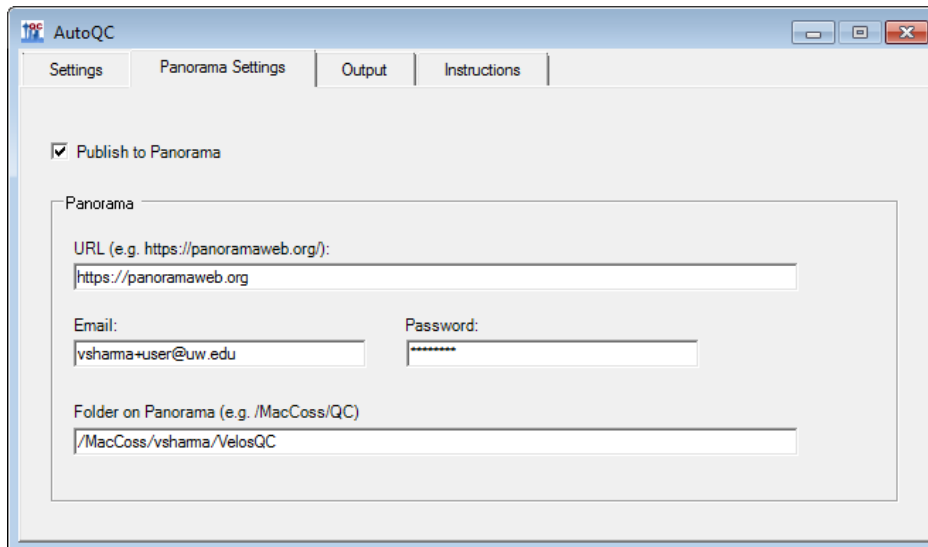
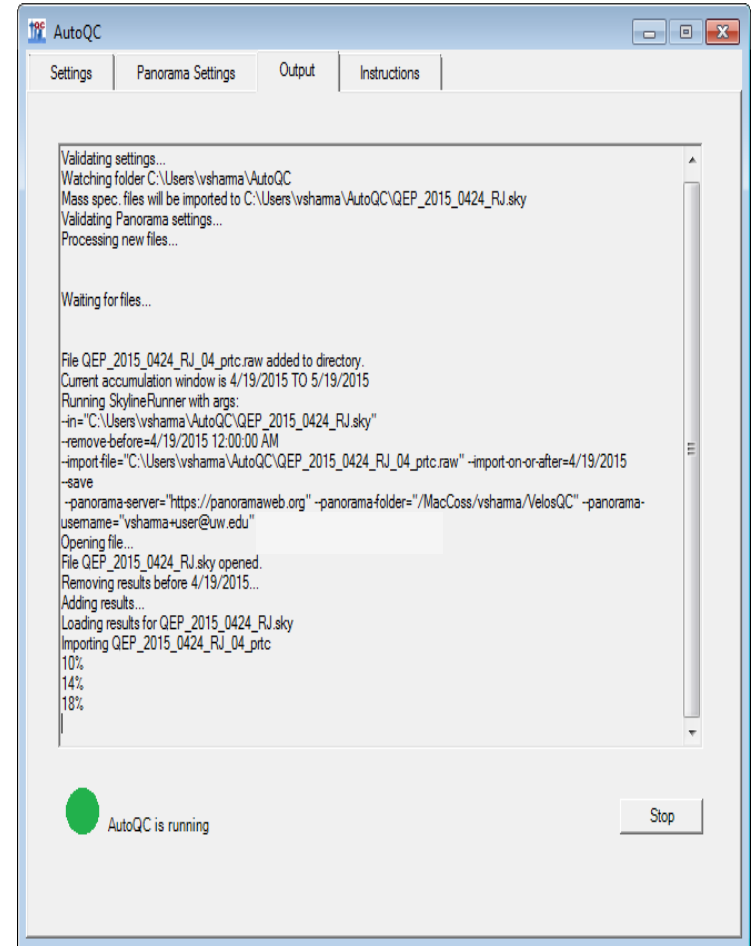
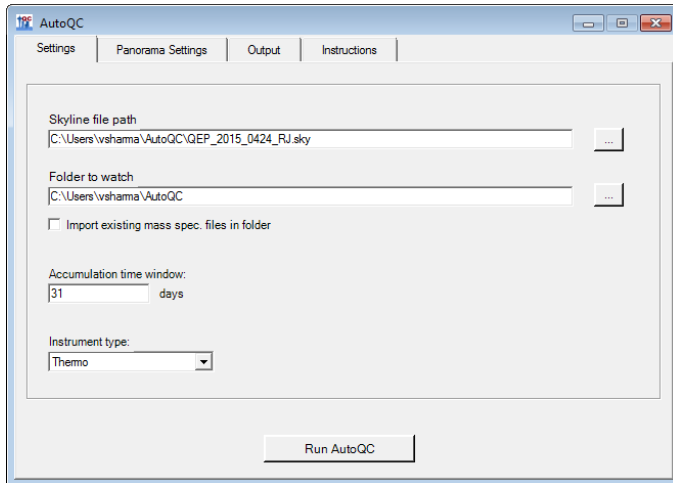
Guide Set 2

Pareto Plot for 'Training Start: 2013/08/21 07:56:12 - Training End: 2013/08/22 00:20:15'



Retention time variable

Automatically upload QC runs to Panorama



Monitor active instruments using QC summary view

QC Summary ▾

No Skyline documents in current folder

4000 No Skyline documents AutoQC ○	5500a 5 Skyline documents 12 sample files 11 precursors 2015/09/11 07:39:48 - no outliers 2015/09/11 06:47:35 - no outliers 2015/09/11 05:55:22 - no outliers AutoQC ○
5600 No Skyline documents AutoQC ○	6500 No Skyline documents AutoQC ○
QEHF 206 Skyline documents 300 sample files 11 precursors 2016/08/10 01:19:10 - 25/66 outliers 2016/08/08 17:08:12 - 33/66 outliers 2016/08/06 12:33:06 - 28/66 outliers AutoQC ○	

Skyline and Panorama expansion in 2016

Small molecule support



Small Molecule Precursor List

GRID VIEWS ▾ REPORTS ▾ CHARTS ▾ EXPORT ▾ PRINT PAGING ▾

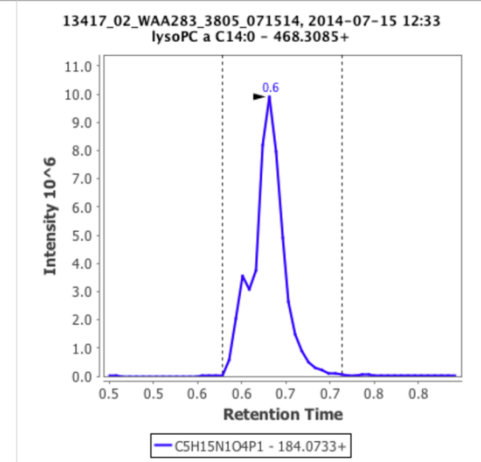
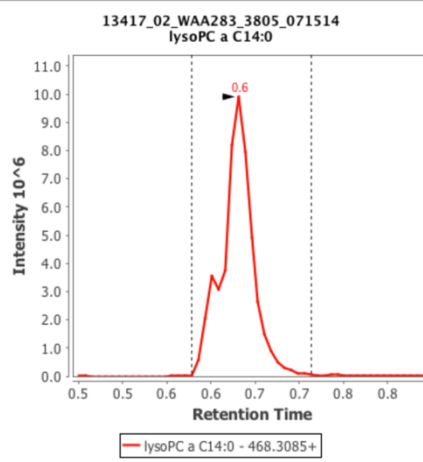
Molecule / Label Description

PC

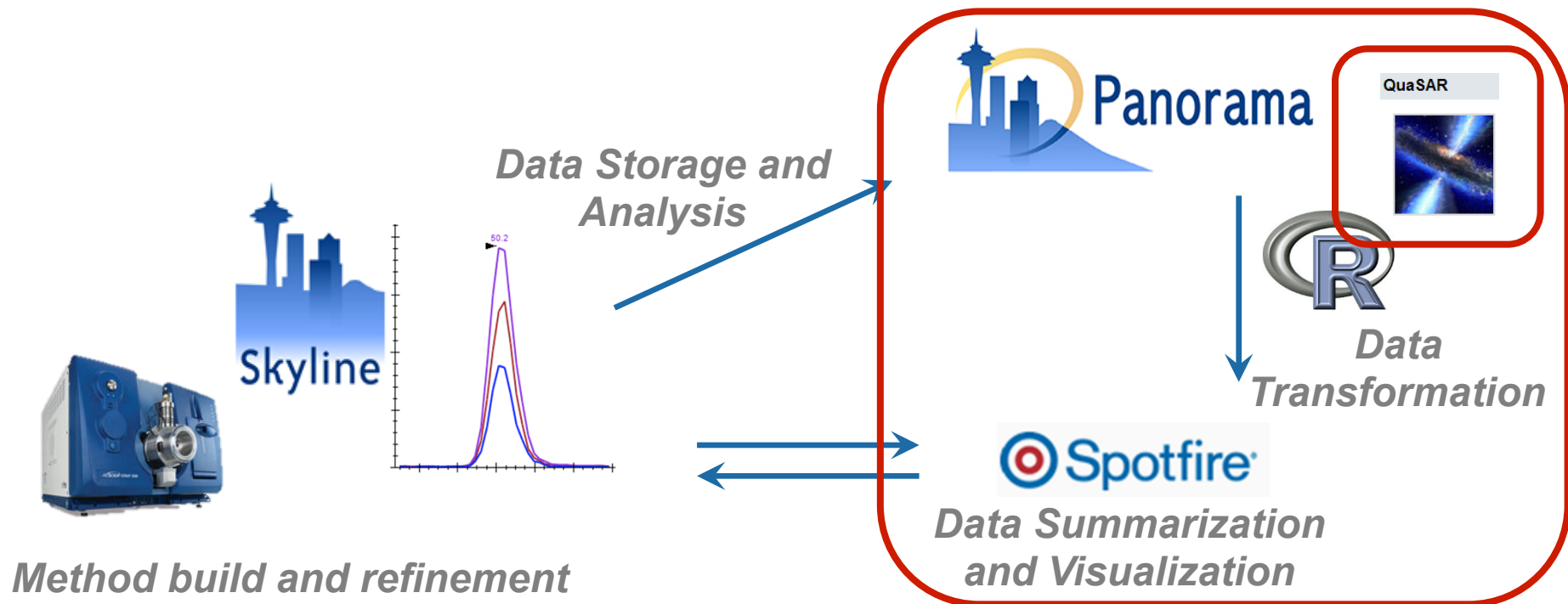
LysoPC

Custom Ion Name	Ion Formula	Mass Average	Mass Monoisotopic	Precursor	Q1 Z	Q1 m/z	Mass Average	Mass Monoisotopic
lysoPC a C14:0	C22H47N107P1	468.5881	468.3090	lysoPC a C14:0	1+	468.3085	468.5881	468.3090
lysoPC a C16:0	C24H51N107P1	496.6416	496.3403	lysoPC a C16:0	1+	496.3398	496.6416	496.3403
lysoPC a C16:1	C24H49N107P1	494.6257	494.3247	lysoPC a C16:1	1+	494.3241	494.6257	494.3247
lysoPC a C17:0	C25H53N107P1	510.6683	510.3560	lysoPC a C17:0	1+	510.3554	510.6683	510.3560
lysoPC a C18:0	C26H55N107P1	524.6951	524.3716	lysoPC a C18:0	1+	524.3711	524.6951	524.3716
lysoPC a C18:1	C26H53N107P1	522.6792	522.3560	lysoPC a C18:1	1+	522.3554	522.6792	522.3560
lysoPC a C18:2	C26H51N107P1	520.6633	520.3403	lysoPC a C18:2	1+	520.3398	520.6633	520.3403
lysoPC a C20:3	C28H53N107P1	546.7009	546.3560	lysoPC a C20:3	1+	546.3554	546.7009	546.3560
lysoPC a C20:4	C28H51N107P1	544.6850	544.3403	lysoPC a C20:4	1+	544.3398	544.6850	544.3403
lysoPC a C24:0	C32H67N107P1	608.8554	608.4655	lysoPC a C24:0	1+	608.4650	608.8554	608.4655
lysoPC a C26:0	C34H71N107P1	636.9089	636.4968	lysoPC a C26:0	1+	636.4963	636.9089	636.4968
lysoPC a C26:1	C34H71N107P1	636.9089	636.4968	lysoPC a C26:1	1+	636.4963	636.9089	636.4968
lysoPC a C28:0	C36H75N107P1	664.9624	664.5281	lysoPC a C28:0	1+	664.5276	664.9624	664.5281
lysoPC a C28:1	C36H73N107P1	662.9465	662.5125	lysoPC a C28:1	1+	662.5117	662.9465	662.5125

Acylcarnitine



Connecting Labkey's Panorama to data analysis tools



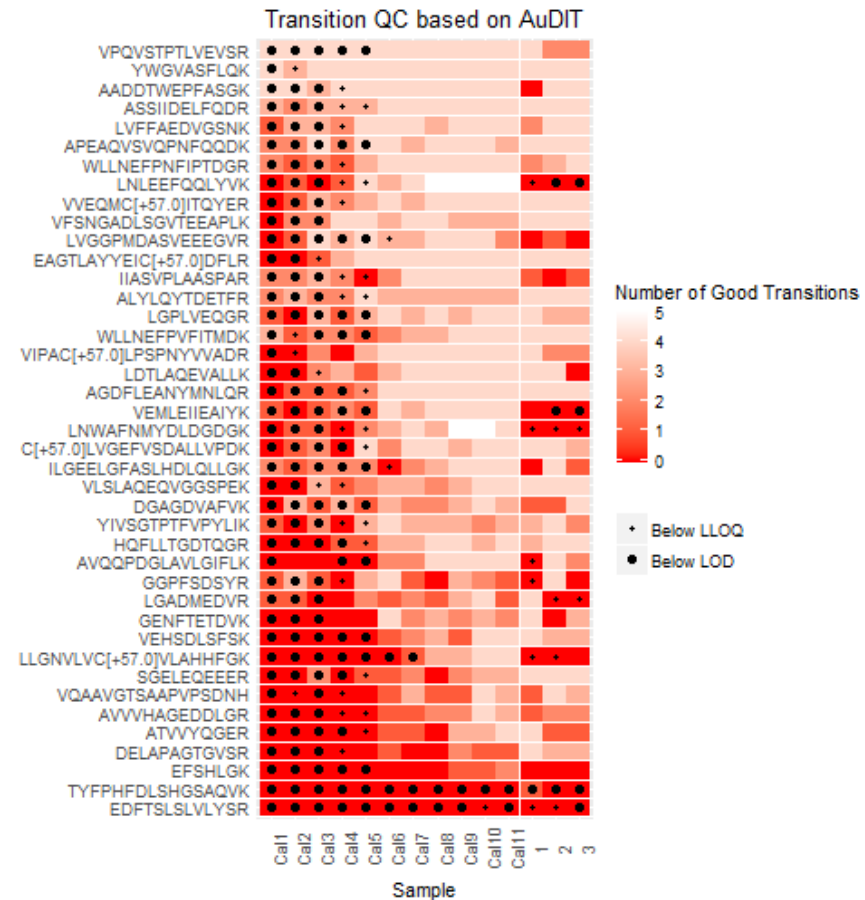


QuaSAR processes SRM/MRM-MS data calculating:

- limits of detection and quantification (LOD and LOQ),
- Mean and Coefficient of variation (CV) for all transitions of each peptide in a set of samples
- Peptide analyte concentration in unknown samples
- Runs the AuDIT algorithm to evaluate the transition quality and detect interference

Reports

Transitions QC Plot: AuDIT



Panorama Partners Progress: Data Summarization

Connecting LabKey's Panorama to Spotfire for visualization



LabKey Template TT8 - Tibco Spotfire

File Edit View Insert Tools Help

Reporting data Data with annotations Heatmap Treemap 3D QC data (pivot) Histogram analysis (pivot) Raw LabKey data

LOAD REPORTING DATA FROM LABKEY

LabKey Database
Roche Prod

Load Server Projects

Project
/pRED/HTRA1/HTRA1 RO620 6

Domain
Targeted Proteomics (Skyline)

Query
Reporting data with annotations

Load LabKey Data

LabKeyData

Server	Path	Schema	Query
https://labkey-pr...	/pRED/Carine/TNBC/peptide_selecto...	auditLog	QueryExportAud...
https://labkey-pr...	/pRED/Carine/TNBC/peptide_selecto...	auditLog	QueryUpdateAu...
https://labkey-pr...	/pRED/Carine/TNBC/peptide_selecto...	auditLog	SampleSetAuditE...
https://labkey-pr...	/pRED/Carine/TNBC/peptide_selecto...	auditLog	SearchAuditEvent
https://labkey-pr...	/pRED/Carine/TNBC/peptide_selecto...	auditLog	AppPropsEvent
https://labkey-pr...	/pRED/Carine/TNBC/peptide_selecto...	auditLog	SpecimenComme...
https://labkey-pr...	/pRED/Carine/TNBC/peptide_selecto...	auditLog	TargetedSRpr...
https://labkey-pr...	/pRED/Carine/TNBC/peptide_selecto...	auditLog	UserAuditEvent
https://labkey-pr...	/pRED/Carine/TNBC/peptide_selecto...	wiki	AWikiVersions

Protein
Type to search in list
(A1) 91 values
RT
spiA8MV23SERP3_HUMAN
spi000299CLC1_HUMAN
spi015230LAMA5_HUMAN
spi094985CSTN1_HUMAN
spi095987FBLN4_HUMAN

Peptide
Type to search in list
(A1) 3 values
ADRPFIYFLR
ASGATALLLK
GISQDGFVSEAHK

Replicate
Type to search in list
(A1) 10 values
160615_S01
160615_S02
160615_S04
160615_S07
160615_S09
160615_S03

Areas

spiA8MV23SERP3_HUMAN

Peptide	Avg(Total Area)
ADRPFIYFLR	890119.57
ASGATALLLK	2297083.70
ASGATALLLK	2360469.50
ASGATALLLK	1659671.62
GISQDGFVSEAHK	536980.77
GISQDGFVSEAHK	1409229.00

Retention Times

spiA8MV23SERP3_HUMAN

Peptide	Avg(Best RT)
ADRPFIYFLR	73.23
ADRPFIYFLR	73.24
ASGATALLLK	70.42
ASGATALLLK	70.43
GISQDGFVSEAHK	56.44
GISQDGFVSEAHK	56.45

Areas

ADRPFIYFLR

Retention Times

ADRPFIYFLR

60 of 4 690 rows | 40 marked | 37 columns | data

EN 18:01 05.10.2015

Labkey helping to accelerate biomarker development through support of MS data management

Biomarker Discovery

- Discovery (unbiased)
- Targeted-discovery



LTDQ-Orbitrap
(High resolution)

Clinical validation

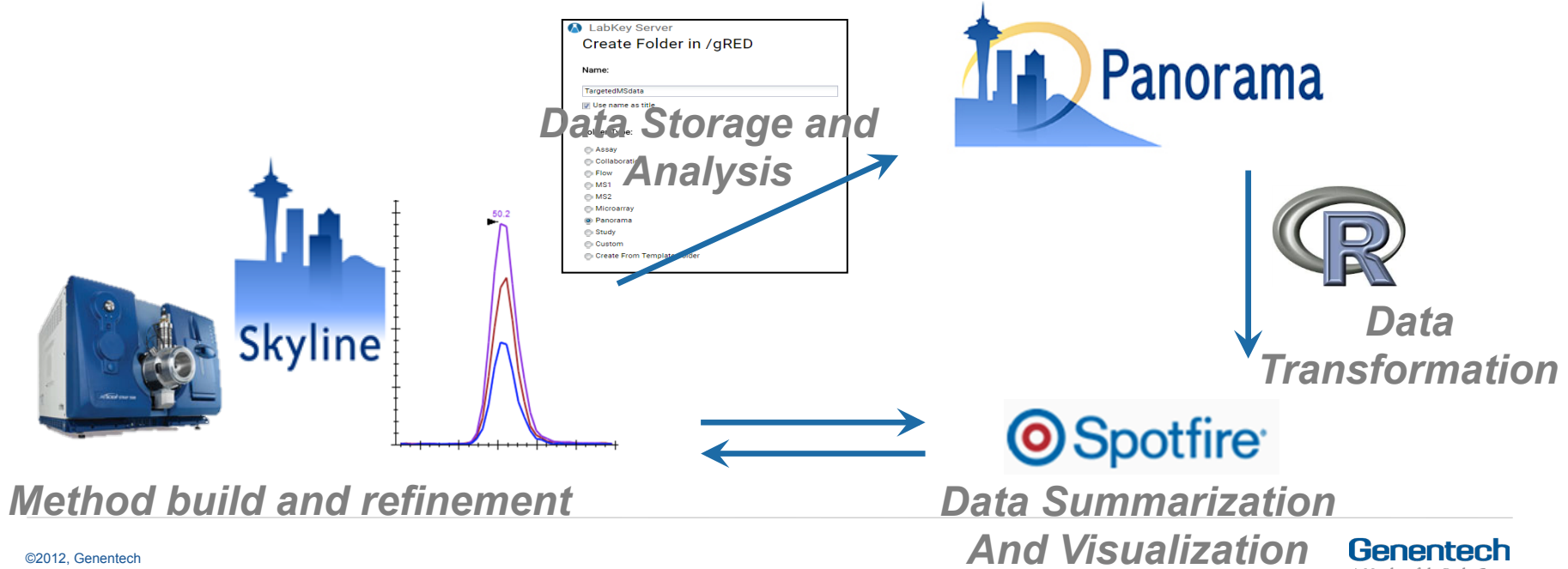
- Multiplex panel
- Single analyte quantitation



Triple Quad
(High sensitivity)

Clinical Practice

Developing customized features within Labkey to simplify method development and data analysis



Acknowledgements

Genentech

OMNI Biomarker Development

Paul Auger

Veronica Anania

Shadi Eshghi

Rod Mathews

Lee Honigberg

gRED IT

Jon Sasano

Spotfire

Laura Harris

Joshua Haznedar

Panorama Partners

Josh Eckels (Labkey)

Brendan MacLean (UW)

Vagisha Sharma (UW)

Tom Dunkley (Roche)

Michel Petrovic (Roche)



UW Targeted Proteomics Course 2014

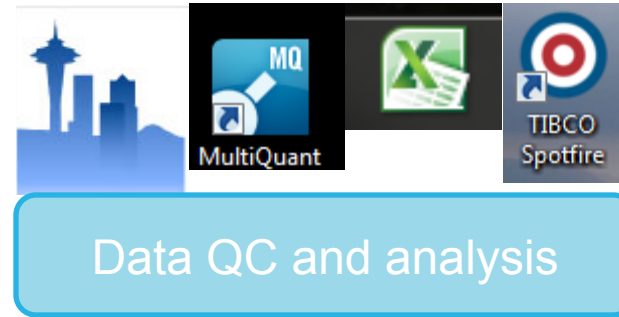




Genentech
A Member of the Roche Group

Appendix

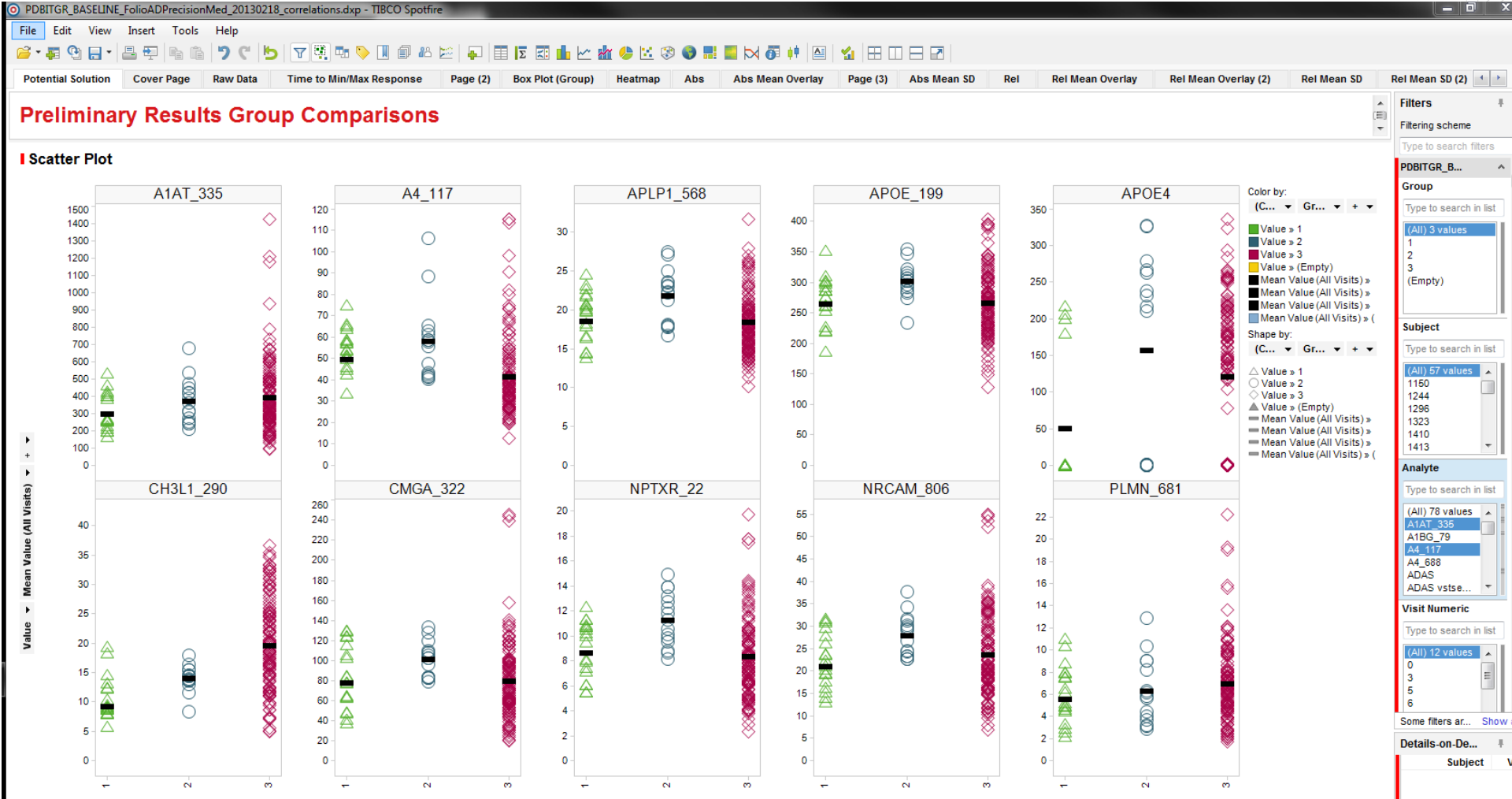
Large data files from multiple platforms creates data management challenges



Types of files generated:

- Skyline method and data visualization files
- Instrument method file
- Raw MS data
- Quantitation file
- Excel spreadsheets for import to Spotfire
- Spotfire QC file
- Spotfire biomarker result file
- Additional (externally generated) biostats *.csv files and R plots

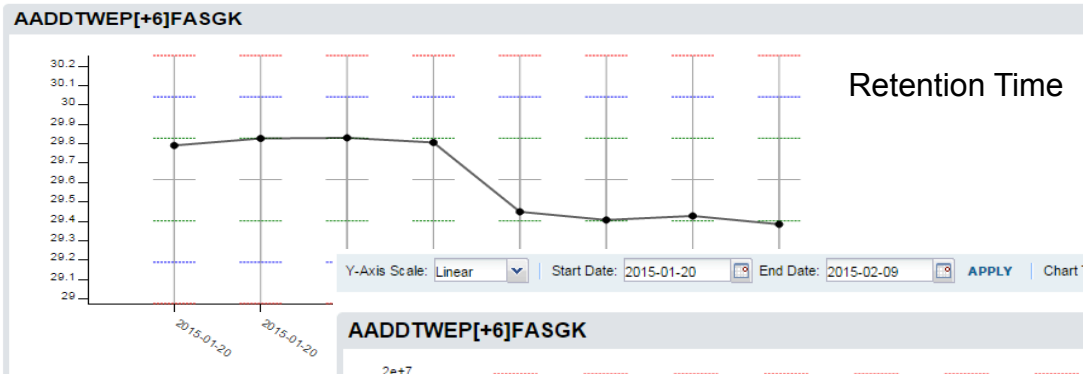
Spotfire visualization of multiplex results



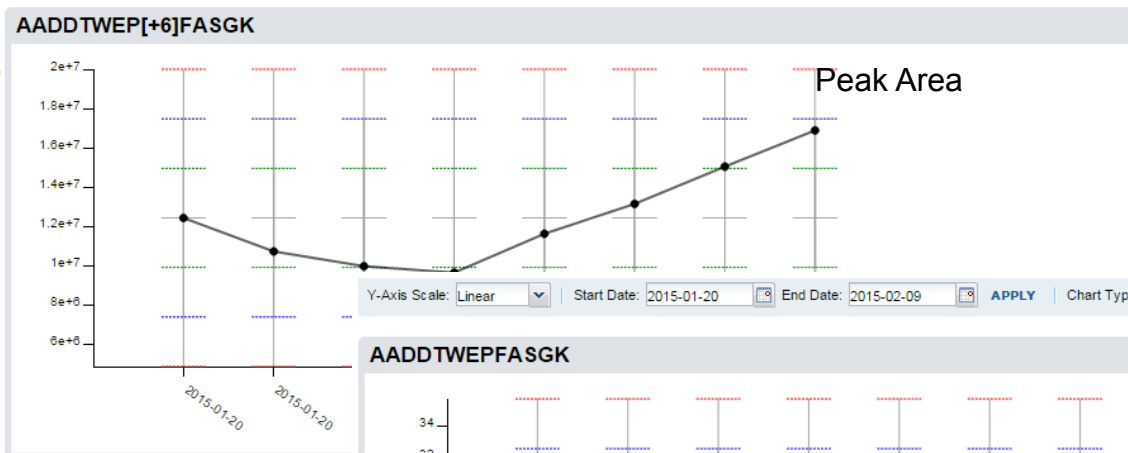
Development of QC folder to monitor instrument performance



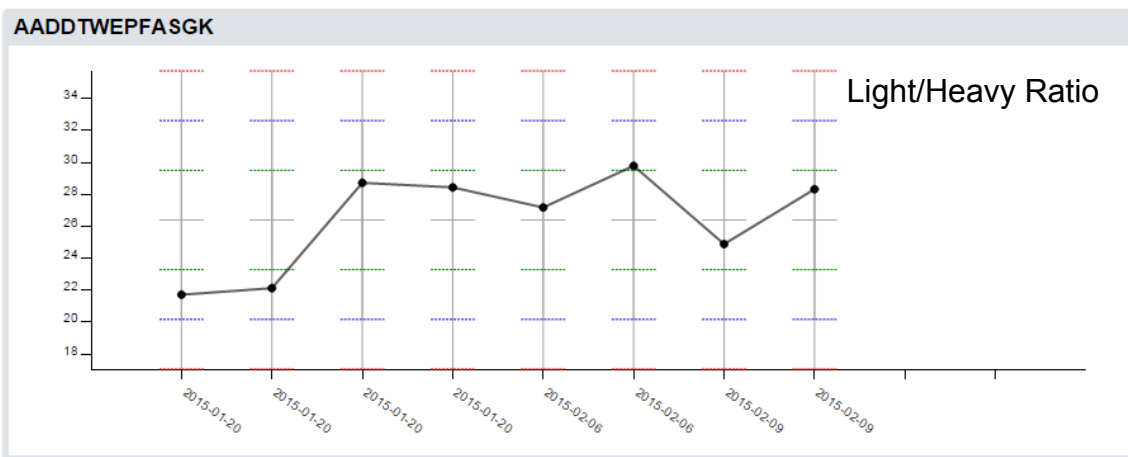
Y-Axis Scale: Linear Start Date: 2015-01-20 End Date: 2015-02-09 APPLY Chart Type: Retention Time



Y-Axis Scale: Linear Start Date: 2015-01-20 End Date: 2015-02-09 APPLY Chart Type: Peak Area



Y-Axis Scale: Linear Start Date: 2015-01-20 End Date: 2015-02-09 APPLY Chart Type: Light/Heavy Ratio





Research • Technology
Communication • Education

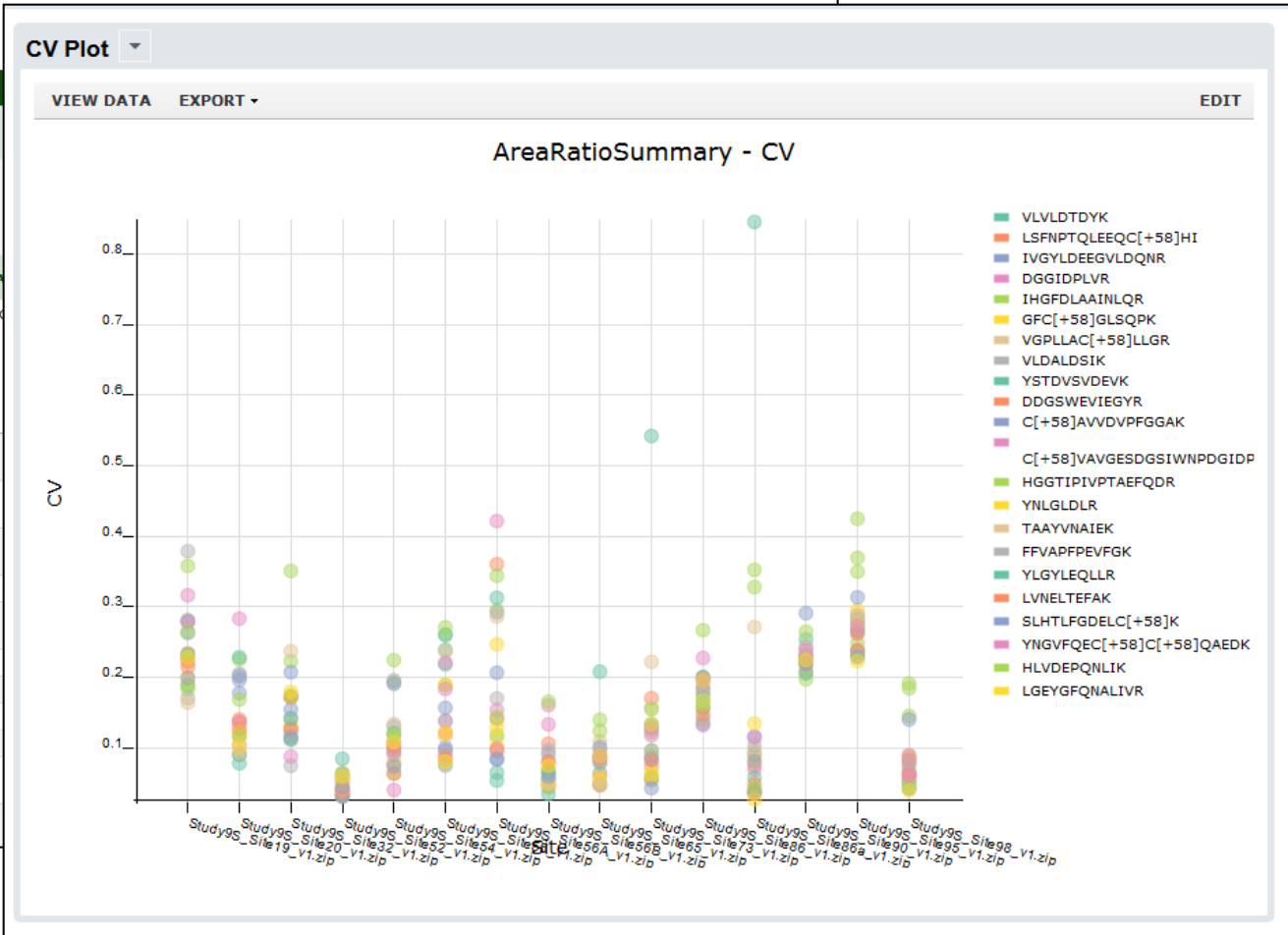
Search ABRF Standards Proteome Research Group

ABRF sPRG Study Results

ABRF sPRG 2013 Study Results

Lists >
Results

VIEWS	CHARTS	INSERT NEW	IMPORT DATA	Sample ID	MSManufact
<input type="checkbox"/>					
<input type="checkbox"/>	EDIT	DETAILS		AS6842-01	Thermo
<input type="checkbox"/>	EDIT	DETAILS		MFIG13	Thermo
<input type="checkbox"/>	EDIT	DETAILS		56365A	Thermo
<input type="checkbox"/>	EDIT	DETAILS		BMS161	
<input type="checkbox"/>	EDIT	DETAILS		AS6842-02	Thermo
<input type="checkbox"/>	EDIT	DETAILS		FR5411_1	
<input type="checkbox"/>	EDIT	DETAILS		12358f	Bruker
<input type="checkbox"/>	EDIT	DETAILS		02940a	Thermo
<input type="checkbox"/>	EDIT	DETAILS		10140s	Thermo
<input type="checkbox"/>	EDIT	DETAILS		80232a	Thermo
<input type="checkbox"/>	EDIT	DETAILS		p7iac1	Thermo



Point-and-Click Visualizations

Box Plot Report

Box Plot Report

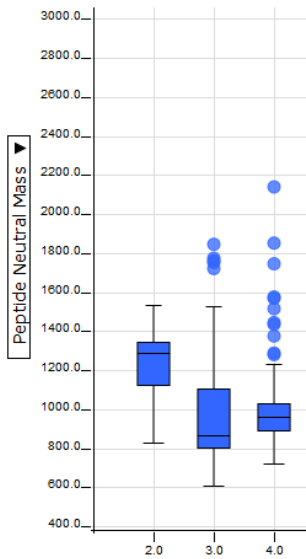
VIEW DATA EXPORT

Box Plot Report

Box Plot Report

VIEW DATA EXPORT OPTIONS GROUPING DEVELOPER

HELP SAVE



Box Plot Report

Box Plot Report

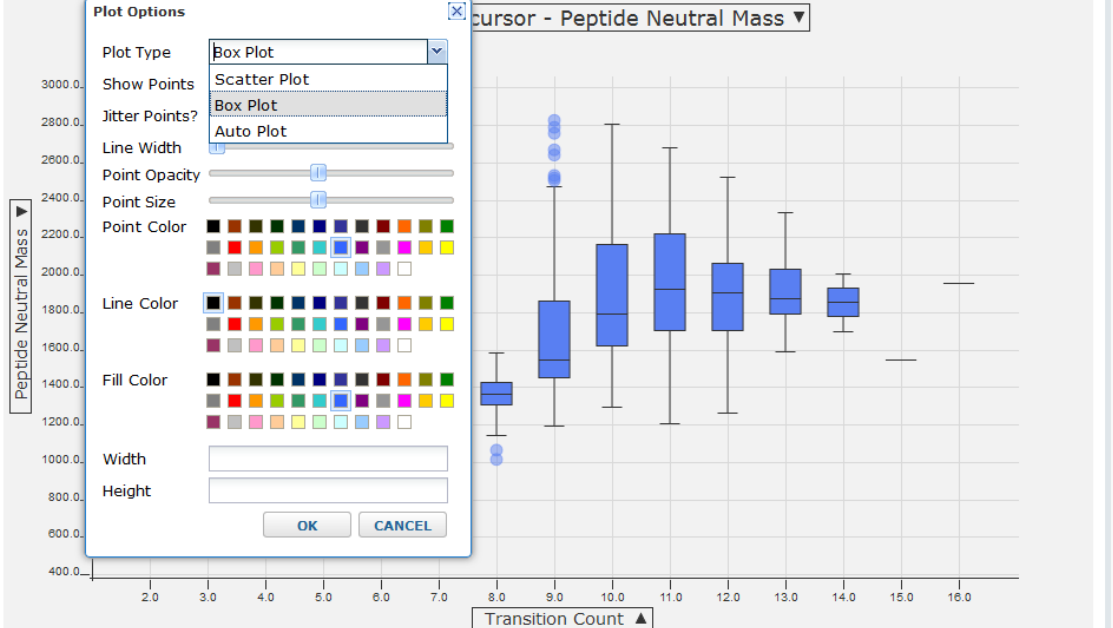
VIEW DATA EXPORT OPTIONS GROUPING DEVELOPER

HELP SAVE

Plot Options

- Plot Type: Box Plot
- Show Points: Scatter Plot
- Jitter Points?: Box Plot
- Auto Plot:
- Line Width: [Slider]
- Point Opacity: [Slider]
- Point Size: [Slider]
- Point Color: [Color palette]
- Line Color: [Color palette]
- Fill Color: [Color palette]
- Width: [Text box]
- Height: [Text box]

OK CANCEL



Panorama Software

- ▶ **Module in LabKey Server**
 - ▶ Open source (Apache 2.0 license)
 - ▶ Easy to install
 - ▶ Tested and in production over 5 years
 - ▶ Extensive core features
 - ▶ Projects and folders
 - ▶ Powerful security model
- ▶ **Relational database supports full Skyline document model**
- ▶ **Integration with Skyline**
 - ▶ Publish files directly to a Panorama server
- ▶ **Web browser interface**
 - ▶ Several data views familiar to Skyline users

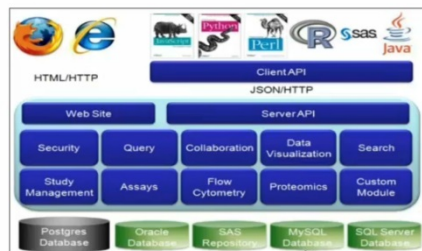
Aggregating and Publishing

- ▶ **Publish fully annotated Skyline documents**
- ▶ **Build chromatogram libraries**
- ▶ **Aggregate lab QC data (future)**
- ▶ **Free hosted version (<http://panoramaweb.org>)**
 - ▶ 25 separate projects so far (CPTAC and ABRF sPRG)
 - ▶ User controlled security
- ▶ **Locally installable server application**
- ▶ **Free and open source (Apache 2.0)**



Proteomics Standards
Research Group (sPRG)

Back End Panorama (Labkey)



- Final datasets (estimate ~40-60)
- Perform Java/SQL Queries for downstream analyze data
- Generate report for 2014 ABRF Meeting and Manuscripts
- Build and Host Spectral Library directly through Panorama for future proteomic experiments

CPTAC MRM Assay Web Portal

- ▶ **Goals**
 - ▶ Promote the development and dissemination of MRM-based proteomic assays with high quality standards
 - ▶ Facilitate user community access to CPTAC assay development efforts
- ▶ **Integration with Panorama**
 - ▶ Use Panorama as a data repository
 - ▶ Use LabKey's Client APIs to pull data out of Panorama for viewing in the web portal
 - ▶ Provide access to chromatogram libraries built in Panorama