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Intro to Panorama





Panorama Basics

- Web-based complement to Skyline
- Targeted mass spec data repository
- First released in 2012
- Joint development effort
 - MacCoss Lab, University of Washington
 - LabKey
- Installable in-house, or hosted in the cloud
- Previous Panorama webinars recordings available



- General purpose biomedical data management system
 - Assay (proteomics, flow cytometry, plate-based...)
 - Specimen
 - Demographic and clinical
- Collaboration tools
 - Files, wikis, issue trackers, message boards
- Originally released in 2003
- Panorama is one of a variety of modules

Skyline/Panorama Workflow



Panorama Usage Modes

- Experimental data
 - General purpose repository
- Quality control
 - Monitor instrument performance over time (system suitability)
- Chromatogram library
 - Curated precursor and product ions for designing and validating future experiments

Experimental Data Folders

- Secure place to store and share Skyline data
- Familiar Skyline views and plots
- Search by protein, peptide, etc

Prec	ursor List 👻												
VIE	WS V CHARTS V EXPORT V	PRINT PAGE SIZ	E▼							1 - 10	of 9	5 Next > Las	t »
	Protein / Label	Description				Protein Annotations							
•	B TAF11 - HsCD00301672 (1-A03)												
	Peptide	Peptide Annotations	Missed Cleavages	Peptide Neutral Mass	Rank	Precursor	Precursor Annotations	Label	Precursor Neutral Mass	Q1 m/z	Q1 Z	Transition Count	
	MDDAHESPSDK	Quality Score:	4 0	1230.4823		MDDAHESPSDK		light	1230.4823	616.2484	2+	7	A
	EAAAEEGELESQDVSDLTTVER	Quality Score:	4 0	2377.077		EAAAEEGELESQDVSDLTTVER		light	2377.0769	1189.5457	2+	11	A
	EDSSLLNPAAK	Quality Score:	1 0	1143.5771		EDSSLLNPAAK		light	1143.5771	572.7958	2+	7	A
	VDEDEIQK	Quality Score:	2 0	974.4556		VDEDEIQK		light	974.4556	488.2351	2+	4	A
	MQILVSSFSEEQLNR	Quality Score:	1 0	1779.8826		MQILVSSFSEEQLNR		light	1779.8826	890.9485	2+	10	A
	LIQSITGTSVSQNVVIAMSGISK	Quality Score:	1 0	2332.267		LIQSITGTSVSQNVVIAMSGISK		light	2332.2671	1167.1409	2+	12	A
	VFVGEVVEEALDVCEK	Quality Score:	1 0	1820.8866		VFVGEVVEEALDV <u>C</u> EK		light	1820.8866	911.4506	2+	11	A
	WGEMPPLQPK	Quality Score:	1 0	1181.5903		WGEMPPLQPK		light	1181.5903	591.8024	2+	6	A
	GQIPNSK	Quality Score:	4 0	742.39734		GQIPNSK		light	742.3973	372.2060	2+	3	A





Version Tracking

- Skyline and Panorama automatically connect subsequent versions of documents
- Retain history and context
- Add notes for specific versions

Document Versions							
Document Name	Imported	Imported By	Note	Protein	Precursor	Transition	
MethodBuildThird_2016-02-23_12-21-54.sky.zip	02/23/2016 12:22 PM	JEckels	Final version	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	Checkpoint for Vagisha	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	
MethodBuildThird_2016-10-26_11-57-19.sky.zip	10/26/2016 11:57 AM	JEckels		3	29	145	
MethodBuildThird_2017-01-24_10-02-02.sky.zip	01/24/2017 10:02 AM	JEckels	Initial version	3	29	145	

Quantitation and calibration curves

- New in Panorama 17.2
- Define curves in Skyline for absolute quant
- Import into Panorama
- Interactive plots
- Expanded reporting coming in 17.3



Quality Control Folders

- Monitor instrument performance over time
- Track a variety of metrics
 - Retention time, peak width, peak area, etc
- Inspired by SProCoP
- Establish normal ranges



Automating QC and System Suitability

- Define Skyline document with peptides and transitions to monitor
 * AutoQC Configuration
 * MatcoQC Configuration
- Install AutoQC and point to QC raw file location
- New files are automatically analyzed and imported

KatoQC Configuration	×
Settings Panorama Settings	
Configuration name	
DemoConfig	
Skyline file path:	
C:\Temp\AutoQC\TSQ2_autoQC.sk	y
Folder to watch:	
C:\Temp\AutoQC	
Include subfolders	
File filter:	
Al	
Populta time window:	
31 days	
Instrument type:	Expected acquisition duration:
Themo	75 minutes
	Save Cancel

9/21/17

- View multiple instruments at a glance
- Investigate outliers
- Drill in for details
- Exclude problematic samples and metrics

QC Summary	
QC Demo 47 sample files 7 precursors 2013/08/27 14:45:49 - 24/56 (Levey-Jennings), 13/56 (Moving Range), 1/56 (CUSUMv) outliers 2013/08/27 03:19:45 - 31/56 (Levey-Jennings), 21/56 (Moving Range), 2/56 (CUSUMv) outliers 2013/08/26 04:27:53 - 29/56 (Levey-Jennings), 21/56 (Moving Range), 1/56 (CUSUMv) outliers	AutoQC O
InstrumentA 5 sample files 52 precursors ¹ 2013/04/12 00:40:57 - no outliers ¹ 2013/04/11 21:35:37 - no outliers ¹ 2013/04/11 18:30:20 - no outliers	AutoQC O
InstrumentB 42 sample files 7 precursors 2013/08/25 18:55:36 - no outliers 2013/08/24 23:20:30 - no outliers 2013/08/22 10:59:40 - no outliers	AutoQC O



QC dashboards

Data Sharing

- Organize data in folders
- Grant access to users
 - Reader
 - Editor
 - Admin
- Manage users in groups
- Make available to public (if firewall allows)

APIs and Reporting

- R integration
 - Rlabkey package (in CRAN)
 - Query Panorama data from external systems
 - Provide R script to plot data and show to users

SQL queries

- Full Skyline data exposed via schemas and tables
- Plotting and charts

Next Steps

- Try using Panorama
 - Get an account on PanoramaWeb
 - Or, set up a local installation
- Use Panorama Public for sharing published data
- Join Panorama Partners Program
 - Joint effort with LabKey and MacCoss Lab
 - Expert assistance with Skyline and Panorama
 - Influence development plans



https://panoramaweb.org

Vagisha Sharma MacCoss Lab



PanoramaWeb

- Panorama server maintained by the department of Genome Sciences at the University of Washington
- Researchers can request free projects
- Project owners have complete control over their project
 - Create sub-folders
 - Add new users
 - Configure permissions on individual folders
 - Private
 - Access to select collaborators
 - Public

Panorama Public

- Public repository on PanoramaWeb for published data
 analyzed with Skyline
- Data already in a project on PanoramaWeb can be "published" to Panorama Public
 - Data can be private while manuscript is under review
 - Reviewer account provided
- Authors / submitters have read-only access
- Satisfies MCP guidelines for targeted mass spectrometry quantitative experiments
 - "provide all chromatograms used in quantification of analytes"