

MASS SPECTROMETRY FOR PROTEOMICS COMPONENT COLLECTION

The Mass Spec for Proteomics Collection provides a data model for mass spec-based data within the Pipeline Pilot Enterprise Server, and provides methods to read, write, visualize, manipulate, analyze, compare, and publish results from mass spec experiments. The data model supports quick processing of large files and carries detailed information at multiple levels. Harnessing the power of the Pipeline Pilot graphical protocol-building capabilities, complex data analysis procedures, such as peptide and protein identification and differential profiling, can be easily constructed without the need to develop code. Built on top of the Analytical Instrument Collection and coupled with power of the Sequence Analysis and Gene Expression Collections, your mass spec data can be easily cross-validated and compared to other experiments for biomarker identification and verification.

WITH THE MASS SPEC FOR PROTEOMICS COLLECTION YOU CAN:

- Read in with .RAW*, .wiff, SEQUEST DTA, ANDI (netCDF), Mascot MGF, or mzXML files
- View your data with interactive chromatograms, 2D mass spec run charts, scan charts, feature peak charts, retention time drift charts, fragmentograms, peptide and protein viewers with drill down-down, and heat maps.
- Perform protein identification using X!Tandem to extract peptides and mapped proteins
- Use XCMS to extract, identify and align feature peaks for differential profiling
- Publish results in an interactive manner than can be deployed via web port with advanced reporting features

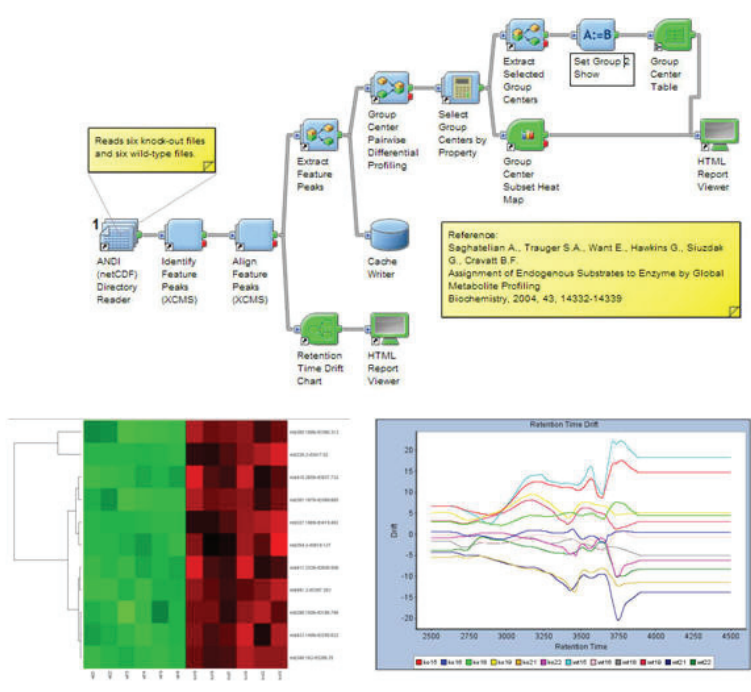
**extract_msn.exe is not included.*

MASS SPEC READERS AND WRITERS

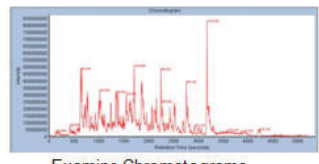
There is no agreed-upon standard format for mass spec-based data. Hence our component collection provides readers for SEQUEST DTA, ANDI (netCDF), Mascot MGF, and mzXML files. Our readers also wrap converters for .RAW and .wiff proprietary formats. Writers are provided for ANDI, Mascot MGF, and SEQUEST DTA.

MANIPULATORS AND CALCULATORS

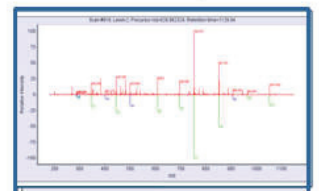
Components are provided that allow you to delete or extract specific scans, and reassemble later. Extract an interactive chromatogram from a mass spec run. Calculate peptide mass and fragment ion masses and display summaries. Precursor charge may be calculated using the 2to3 algorithm to speed up protein identification.



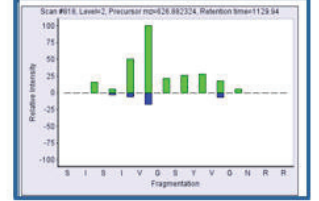
Perform differential metabolite profiling, automatically select features to separate populations, and examine drift in feature retention time



Examine Chromatograms



b+	bF	AA	Mod	yF	y+
86.0390	1	S	12	1251.6691	
204.1234	2	I	11	1164.6371	
250.1174	3	S	10	1511.1511	
452.2220	4	I	9	1047.2111	
520.3020	5	V	8	1114.6111	
557.3293	6	G	7	1121.3611	
644.3614	7	S	6	1002.1411	
807.4247	8	Y	5	1002.1111	
820.4220	9	V	4	1417.2311	
963.5146	10	G	3	1001.1111	
1077.5576	11	N	2	1001.1111	
1223.6506	12	R	1	175.1109	



Study details of fragmentation

ANALYSIS

The X!Tandem component is used for protein identification. You can also read output from Mascot directly. Other components extract peptides and proteins for reporting. Differential profiling between samples is accomplished through wrapping R and BioConductor functionality along with custom algorithms. Peaks that differentiate samples are identified and aligned using XCMS.

VIEWERS AND REPORTING TOOLS

A variety of static and interactive peptide and protein viewers are provided, including drill downs: chromatograms, 2D mass spec run charts, scan charts, feature peak charts, retention time drift chart, and heat maps streamline common inspection tasks.

INTEGRATION OF PROTEOMICS AND GENOMICS

The Mass Spec for Proteomics Collection is part of our Bioscience collections for Pipeline Pilot. Together they multiply your ability to cross-validate, correlate, and further research and publish your results. The Mass Spec Proteomics Collection is built on top of the Analytical Instrumentation Collection, which offers essential spectral informatics tools and algorithms for creating practical spectrum analysis workflows that complement laboratory research. Adding in the Sequence Analysis Collection, alignments or BLAST database searches are easily performed. The Gene Expression Collection allows the researcher seamless ability to automatically compare various experiments in a robust web-enabled environment.

To learn more about Pipeline Pilot, go to accelrys.com/pipeline-pilot