Progenesis LC-MS v4.0 – benefits and features of the current release

Benefits

- Generate results at the protein level; necessary for biological studies and publications, which can also be easily integrated into wider bioinformatics projects and support a systems biology approach.
- Make confident conclusions based on reports of statistically valid, quality controlled, protein quantification and identification results.

Features

Version 4.0 of Progenesis LC-MS extends the workflow for quantification and identification of proteins including:

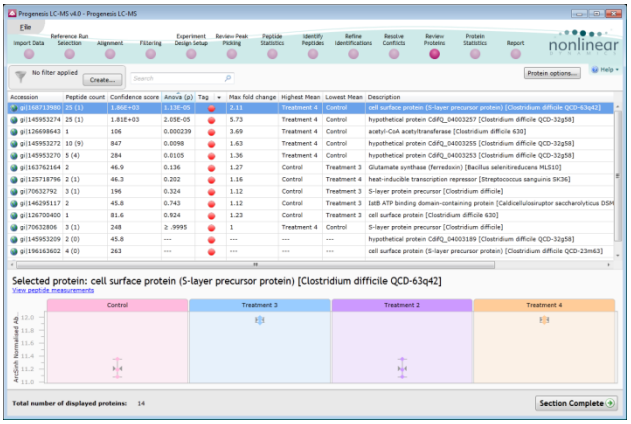
- A new step to review a final list of interesting proteins and their expression profiles from your experiments
- The ability to perform multivariate statistics on protein expression data
- Generate a protein-based (top-down) report of your results

The new protein features are available in both the fractionated workflow and unfractionated workflow. A summary of the new features and workflows are below:

Review Proteins

Automatically generate a tabular and graphical view for all the proteins of interest that you determine within your experiment. Results include:

- Graph of expression profile showing relative differences for each protein across the groups
- Peptide count for each protein
- Confidence Score calculated from the sum of the scores for each peptide from that protein
- Anova p-value for protein expression differences between groups
- Max fold change and the names of the groups that contain the highest and lowest protein expression measure
- Protein description returned from database searches



Protein tags

Tags allow you to display a selection of proteins according to the data associated with them (e.g. p-value, fold change, identity, up regulated in treatment). Directly list a sub-set of proteins in your experiment using quick tags, specific to protein results, for peptide sequence motif and/or modifications.

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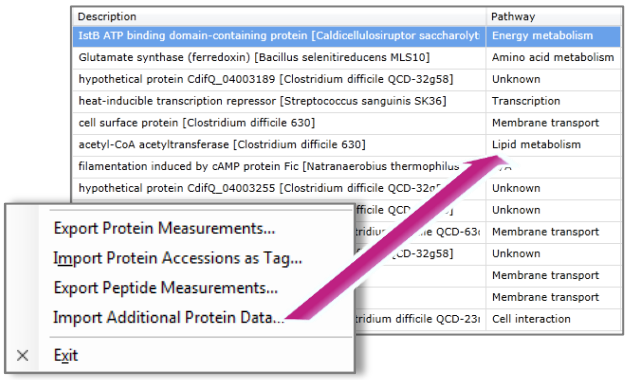
Import supplemental protein information

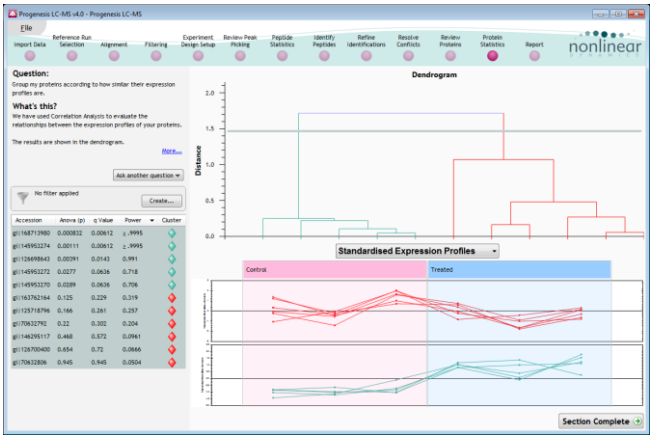
Export your list of interesting proteins, perform further analysis in any external bioinformatics package, and then import results generated externally, which become automatically added as extra columns in the Review Protein table.



Protein Statistics

Multivariate statistics applied to protein measurements including q-value to control False Discovery Rates, Principle Components Analysis (PCA), Correlation Analysis and Power Analysis.

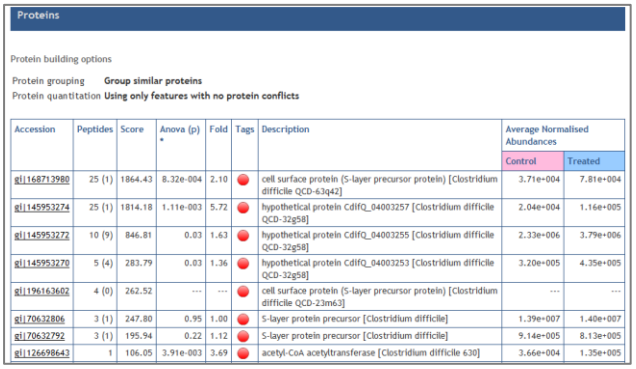
Correlation analysis gives you the first step towards taking a systems biology view. It does this by allowing you select a node and instantly report all the proteins that share a common expression pattern.



Protein Reports

Report a protein (top-down) as well as a peptide (bottom-up) view of your proteomics experiment. Protein report details can include, but are not limited to:

- Ion intensity map showing feature positions
- Table of protein measurements summarised
- Table of peptide measurements relating to each specific protein
- Expression profile graphs



Accession	Peptides	Score	Anova (p) *	Fold	Tags	Description	Average Normalised Abundances	
							Control	Treated
gi|168713980	25 (1)	1864.43	8.32e-004	2.10		cell surface protein (S-layer precursor protein) [Clostridium difficile QCD-63q42]	3.71e+004	7.81e+004
gi|145953274	25 (1)	1814.18	1.11e-003	5.72		hypothetical protein CdifQ_04003257 [Clostridium difficile QCD-32g58]	2.04e+004	1.16e+005
gi|145953272	10 (9)	846.81	0.03	1.63		hypothetical protein CdifQ_04003255 [Clostridium difficile QCD-32g58]	2.33e+006	3.79e+006
gi|145953270	5 (4)	283.79	0.03	1.36		hypothetical protein CdifQ_04003253 [Clostridium difficile QCD-32g58]	3.20e+005	4.35e+005
gi|196163602	4 (0)	262.52	---	---		cell surface protein (S-layer precursor protein) [Clostridium difficile QCD-23m63]	---	---
gi|70632806	3 (1)	247.80	0.95	1.00		S-layer protein precursor [Clostridium difficile]	1.39e+007	1.40e+007
gi|70632792	3 (1)	195.94	0.22	1.12		S-layer protein precursor [Clostridium difficile]	9.14e+005	8.13e+005
gi|126698642	1	106.05	3.91e-003	3.69		acetyl-CoA acetyltransferase [Clostridium difficile 630]	3.66e+004	1.35e+005

Additional new features and enhancements

Gas-phase fractionation feature

Support for increasing protein and proteome coverage using a gas-phase fractionation approach. Enter the desired number of fractions and the software automatically calculates the m/z ranges to give an even distribution of features across the fractions. Export these ranges to generate fragmentation spectra across each m/z bin using your MS instrument.

Data formats

Now supports **direct loading of Agilent .d data** as well as the **mzML file format**. Progenesis LC-MS is platform independent and supports all the major MS instruments in use today.

Import data view

Improved usability based on user feedback, including:

- Large ion maps that you can instantly use to review chromatography quality prior to analysis
- You can delete runs at the import data step for improved experiment data file management
- Software no longer re-evaluates each run when you enter the import data screen