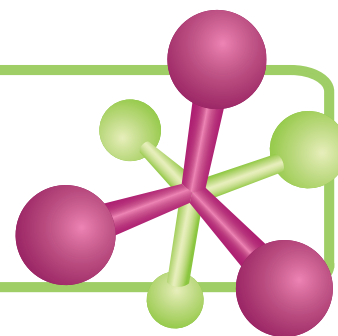


# Progenesis LC-MS



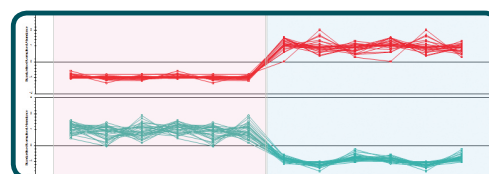
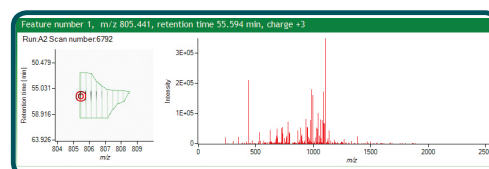
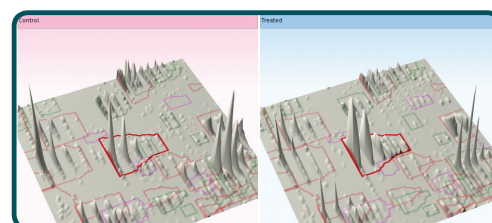
A unique approach for label-free LC-MS data analysis  
Quantify and identify the significant proteins in your experiment...

Progenesis LC-MS quantifies peptides so you can obtain identifications for those that are significantly changing between runs. Identified peptides are then combined to report protein expression and measure relative differences within your experiment.

Protein quantification and identification data, necessary for biological studies and publications, can be easily integrated into wider systems biology projects.

## Why Progenesis LC-MS?

- Increase protein and proteome coverage with support for generating additional fragmentation spectra using inclusion lists or gas-phase fractionation
- Reliably quantify the same peptide in all your runs with no missing values for valid multivariate statistics
- Reduce instrument time and research costs with the analysis of label-free complex samples
- Analyse fractionated samples and recombine them to measure protein expression changes



## What you say:

### Prof. Steve Pennington, UCD Conway Institute, Ireland

"The inclusion of embedded statistics functions and simple data reporting and export make integrating label free LC-MS datasets into established workflows considerably more straightforward."

### Dr Friedrich Lottspeich, Max Planck Institute of Biochemistry, Protein Analysis, Martinsried, Germany

"The intuitive and unbiased workflow of Progenesis LC-MS makes the labor-intensive [label-free] data evaluation much more efficient."

### Dr Leslie Hicks & Dr Sophie Alvarez, Proteomics & Mass Spectrometry Facility, Donald Danforth Plant Science Center, St. Louis, USA

"Progenesis LC-MS software has significantly improved our data analysis platform, as it allows us to do label-free quantitative proteomics acquired on instruments from various vendors."

### Dr Duncan Smith, Paterson Institute for Cancer Research, University of Manchester, England,

"Progenesis LC-MS allows rigorous global analysis of multiple datasets in an unbiased manner which is incredibly powerful."

### Dr Theo Luider, Erasmus University, Netherlands

"...large numbers of LC-MS runs can be compared in a relative fast way. The results of Progenesis are of high standard. It leads to results that can be verified by independent technology."

# The quantify-then-identify approach of Progenesis LC-MS

## Quantify

### Import runs

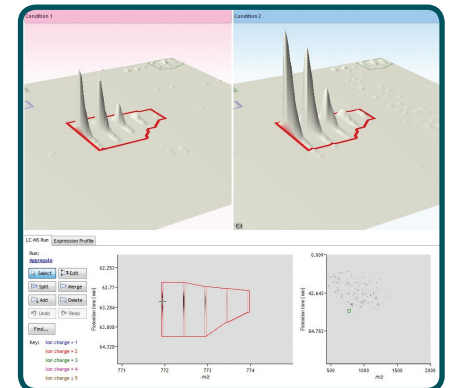
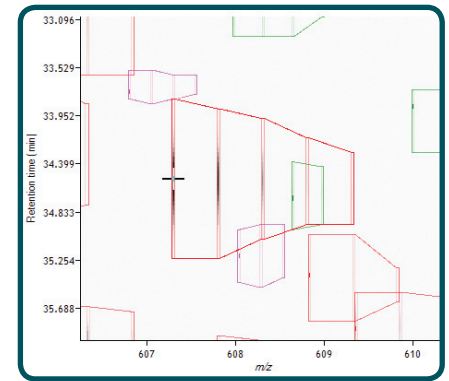
- Platform independent with support for all major hardware vendors as well as mzXML and mzML
- Peak modelling and data reduction for fast analysis without affecting quantification
- Generate ion intensity maps of each run representing RT vs. m/z vs. ion intensity to review LC-MS data quality prior to analysis

### Retention time alignment

- Correct for retention time differences between runs
- Create a single "aggregate run" containing all peptide ions
- Confidently detect and quantify the same feature across all samples
- No missing values no matter how many replicates you run

### Quantify peptide ions

- Ion abundance is measured from the same isotope peak detection applied to the same feature across every run in your experiment
- Automatic normalisation accounts for sample loading variation and direct comparison of up or down regulation between runs
- Option to normalise using known peptides and proteins in your sample
- Quickly compare the same feature across multiple groupings within your experiment
- Validate peptide ion quantification and expression differences using data tables linked to visual displays
- Explore complex data by selecting and grouping peptide ions in multiple ways using the simple but powerful tags feature
- Easy-to-use multivariate statistics applied to **peptide ion** measurements including q-values to control False Discovery Rates, Principle Components Analysis (PCA), Correlation Analysis and Power Analysis

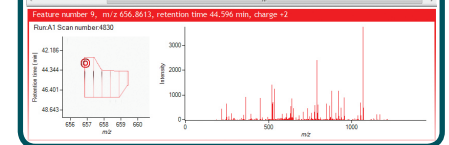


Feature intensity	Protein intensity (%)	Chai	Protein m/z	Is score	Peptide	Protein description	
1.2e+005	4.8e-004	403	2	936.5140	55.0	AGAGDFDEEPPVPAK	actin/Cytoskeletal thymosin beta 4 (Clonidium dff)
8.5e+005	5.3e-005	918	2	936.5096	106.1	AGAGDFDEEPPVPAK	actin/Cytoskeletal thymosin beta 4 (Clonidium dff)
5.6e+005	5.1e-005	904	2	936.5081	76.6	AGAGDFDEEPPVPAK	actin/Cytoskeletal thymosin beta 4 (Clonidium dff)
1.7e+006	2.3e-005	124	3	976.4843	50.9	TYFNQYDNEVAGEDR	cell surface protein (S-layer precursor protein)
1.6e+007	3.3e-006	662	3	976.4853	80.6	TYFNQYDNEVAGEDR	cell surface protein (S-layer precursor protein)
1.7e+006	1.2e-005	6.9	3	976.4822	20.9	TYFNQYDNEVAGEDR	cell surface protein (S-layer precursor protein)
1.6e+007	5.7e-006	39.1	3	976.4847	53.6	TYFNQYDNEVAGEDR	cell surface protein (S-layer precursor protein)
1.6e+007	4.5e-005	4.6	3	976.4839	88.2	TYFNQYDNEVAGEDR	cell surface protein (S-layer precursor protein)
1.7e+006	1.5e-005	9.2	3	976.4838	62.8	TYFNQYDNEVAGEDR	cell surface protein (S-layer precursor protein)
1.6e+006	1.5e-005	224	3	976.4839	50.0	TYFNQYDNEVAGEDR	cell surface protein (S-layer precursor protein)
4.6e+006	1.6e-005	284	3	976.4842	72.1	TYFNQYDNEVAGEDR	cell surface protein (S-layer precursor protein)
1.7e+006	4.2e-005	251	3	976.4842	65.3	TYFNQYDNEVAGEDR	cell surface protein (S-layer precursor protein)
4.6e+006	1.6e-005	401	3	976.4843	58.0	TYFNQYDNEVAGEDR	cell surface protein (S-layer precursor protein)

## Identify

### Identify peptides and proteins

- A simple, visual approach to validate and select MS/MS spectra for export and query using common search engines
- Automatically display imported search results alongside parent ion measurements and filter prior to produce a peptide-based view of proteins in your experiment
- Quantify based on unique peptides only, with the ability to resolve conflicts when a peptide sequence is associated with more than one protein
- Easily tag unique peptides and select the best ones as candidates for future MRM studies



Protein	Protein description	Protein m/z	Protein score	Protein p-value	Protein q-value
1	actin/Cytoskeletal thymosin beta 4 (Clonidium dff)	936.5140	55.0	1.2e-005	4.8e-004
2	actin/Cytoskeletal thymosin beta 4 (Clonidium dff)	936.5096	106.1	8.5e+005	5.3e-005
3	actin/Cytoskeletal thymosin beta 4 (Clonidium dff)	936.5081	76.6	5.6e+005	5.1e-005
4	cell surface protein (S-layer precursor protein)	976.4843	50.9	1.7e+006	2.3e-005
5	cell surface protein (S-layer precursor protein)	976.4853	80.6	1.6e+007	3.3e-006
6	cell surface protein (S-layer precursor protein)	976.4822	20.9	1.7e+006	1.2e-005
7	cell surface protein (S-layer precursor protein)	976.4847	53.6	1.6e+007	5.7e-006
8	cell surface protein (S-layer precursor protein)	976.4839	88.2	1.6e+007	4.5e-005
9	cell surface protein (S-layer precursor protein)	976.4838	62.8	1.7e+006	1.5e-005
10	cell surface protein (S-layer precursor protein)	976.4839	50.0	1.6e+006	1.5e-005
11	cell surface protein (S-layer precursor protein)	976.4842	72.1	4.6e+006	1.6e-005
12	cell surface protein (S-layer precursor protein)	976.4842	65.3	1.7e+006	4.2e-005
13	cell surface protein (S-layer precursor protein)	976.4843	58.0	4.6e+006	1.6e-005

### Report interesting proteins

- Protein abundance is calculated from the sum of all unique normalised peptide ion abundances
- Automatic normalisation allows direct comparison of protein expression between groups
- Display expression profiles for selected proteins of interest
- Easy-to-use multivariate statistics applied to **protein** measurements including q-values to control False Discovery Rates, Principle Components Analysis (PCA), Correlation Analysis and Power Analysis
- Correlation analysis allows you to find all the proteins sharing a common expression pattern
- Export protein data for further analysis in any external bioinformatics package and then import any additional results as extra columns in the Review Proteins table
- Report a protein (top-down view) as well as a peptide (bottom-up) view of your proteomics experiment



Find out more at: [www.nonlinear.com/lc-ms](http://www.nonlinear.com/lc-ms)

Version 4.0