

Progenesis QI for proteomics– What's new in the latest release?

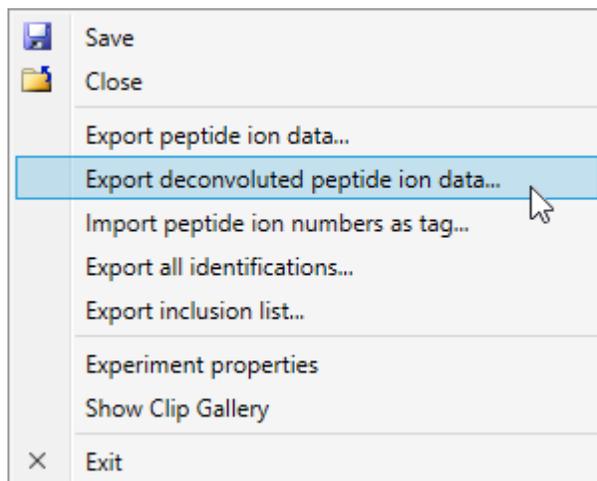
Version 3.0, May 2016

Progenesis® QI for proteomics software enables you to **Quantify** and then **Identify** the proteins that are significantly changing in your complex samples using the advantages of label-free analysis. With support for all common vendor data formats and a highly intuitive, visually guided workflow, Progenesis QI for proteomics helps you to rapidly, objectively and reliably discover proteins of interest. These can be from single or fractionated samples, using multi-group experimental designs, with the capability to handle the large sample sets typical of today's experiments. As well as conventional data-dependent analysis (DDA), Progenesis QI supports Waters MS^E and HDMS^E data independent analysis (DIA). Uniquely, the software also takes advantage of the additional dimension of resolution offered by Ion Mobility separations increasing peak capacity to give improvements in accuracy and precision of quantification and identification.

New Features

Improved access to peptide-level information

In v3.0 the charge deconvoluted peptide quantification results are reported, making it much easier to review and report peptide level quantification. New export options make this data readily available. Additional data drilldowns from the protein to peptide level and then to individual peptide ions have been added. The new peptide correlation scores in the tables also provide a more informed assessment of your results, as does the addition of the unique peptide column enabling tagging and filtering of proteins based on the number of unique peptides observed.



Easy export of deconvoluted peptides

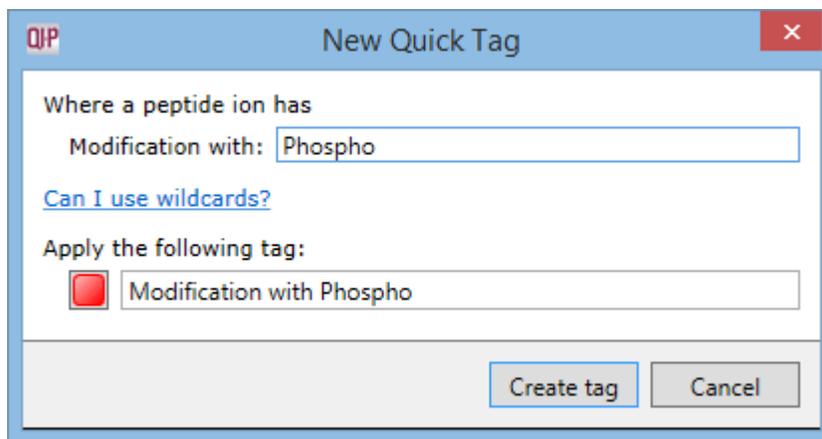
Nonlinear Dynamics

Keel House, Garth Heads, Newcastle upon Tyne, NE1 2JE, UK [T] +44 (0) 191.230.2121 [F] +44 (0) 191.230.2131

Nonlinear Dynamics, Americas Sales Office

2530 Meridian Parkway, 3rd Floor, Durham, NC 27713 U.S.A.

[T] +1 919.806.4401 [TOLL FREE] +1 866.435.7872 [F] +1 919.806.4301 [E] info@nonlinear.com [W] www.nonlinear.com



*Creation of a quick tag e.g. for phospho modification:
to highlight all the peptides modified with phospho from the overall peptide list.*

Review selected protein
Review the selected protein's identified peptides and validate their expression patterns.

1 Choose the level of detail
View the properties and expression profiles of either peptides or individual peptide ions:
Show: Peptides Peptide ions
Tip: you can also double-click a peptide to select and view its component ions.

2 Compare expression profiles
Select peptides in the table to show their expression profiles in the chart below.

Correlation values for the expression profiles can also be seen in the table.

3 Resolve any quantitative outliers
Tag any peptide ions whose expression profile is an outlier for this protein.
[Learn about tagging and filtering](#)
You can then review their identifications in more detail at the [Refine Identifications](#) step.

Experiment design
Review your data from a different perspective:
Current design:

Σ	Identifier	Ions	Score	Correlation	Anova (p)	Max Fold Change	Highest Mean	Lowest Mean	Peptide Sequence	Modifications
○	49.27_1718.8841n	1	92.430	-0.976	6.23E-05	2.91	C	A	IQLVGGDLFVTNTER	
●	33.96_1606.7422n	2	0.680	0.990	7.27E-06	6.65	A	C	MAHKAGYIAVVSHR	[8] Phospho (ST)
●	28.27_1728.8584n	1	6.660	0.994	0.000156	3.71	A	C	SKFGANAVLAVSIACAK	[1] Phospho (ST)
●	47.24_1614.8817n	2	16.910	0.997	2.89E-06	64.9	A	C	LNQIGTVSETLEAIK	

Standardised Expression Profiles

Peptide profiles: ■ Contributes to protein measurements ■ Does not contribute to protein measurements

*Peptide correlation at protein view helps you to see correlated peptides
and enables better judgement of modifications and assignments within the data*

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Description: SPTEYHEPVpYANPFYRPTpTPQR

Σ	Ions	Peptide Sequence	Score	Correlation	Tag	Max Fold Change
●	3	SPTEYHEPV \bar{Y} ANPF \bar{Y} RPTTPQR (+1)▶	26.330	-0.190	■	278
●	3	SPTEYHEPV \bar{Y} ANPF \bar{Y} RPTTPQR \bar{R}	13.350	0.742	■	41.2
●	2	SPTEYHEPVYANPFYRPTTPQR \bar{R} (+1)▶	14.410	0.950	■	6.2

The table indicates the number of ions per peptide and the locations of any modifications

Performance improvements

Our users tell us that responsiveness and processing speed are important to them, in this version many small but significant general improvements have been made to increase responsiveness and improve areas of the workflow to give an overall improved user experience.

In addition, for users working with large Waters MS^E experiments, improved communications with PLGS make for a much smoother experience and our internal testing has even shown processing time to be reduced by three-fold on some datasets.

Improved support of functionality for data from multiple vendors

In continuity with Progenesis QI for proteomics' vendor neutral strategy, we have created a new plugin for our SCIEX users of ProteinPilot v5.0 and improved support for the generic mzML data format.

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