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

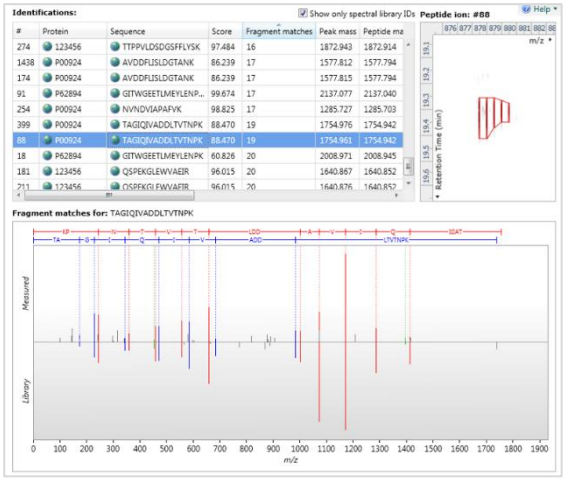
Version 4.0 and 4.1 | May 2018

The latest release of Progenesis® QI for proteomics helps scientists to overcome challenges in their research by offering some significant new developments. At the same time, attention has been paid to the usability of Progenesis QI for proteomics.

Spectral libraries: adding to database search flexibility

Progenesis QI for proteomics already has numerous options for database searching, interfacing with **14 different search engines**. Now we add to that flexibility by bringing the functionality of **spectral library searching**. Reclaim time traditionally spent identifying peptides and proteins already verified and quickly focus your efforts on new and interesting features. This means improved specificity, utilizing the knowledge that you already have, leading to **more accurate results** in **less time**.

In Progenesis QI for proteomics v4.1 you can:



- Build up a **library of verified identifications** from **DDA, MS^E, HDMS^E** and **SONAR data** including:
  - Fragmentation patterns seen in your own experiments and with your own instrumentation
  - Retention time information
  - Highlight overlapping ions to show potential interferences
  - You can also collaborate internally and externally by **sharing these libraries** with collaborators. This avoids duplication of effort within the Progenesis community.
- **Search the library first** in a new discovery experiment
  - Quickly find peptides that match something you've seen before
  - Hide strong spectral library matches
  - Submit the remaining unknowns for traditional search methods
  - Supports **NIST** and **Mascot .msp** files and **SWATH** Atlas .sptxt files
- **Append** any new verified identifications to the library

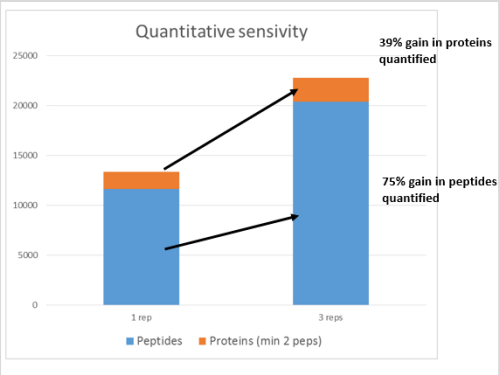
MS/MS Spectral clean-up tools during library creation

A new tool in the "Resolve conflicts" section indicates the identified peptides that have co-eluting peptides in close proximity. This gives the user the option to exclude the MS/MS spectra of these peptide ions from the spectral library export, thereby only exporting peptides which should give **cleaner matching in future identifications**.

Only identified fragments from the MS/MS spectra are included when you create a library, ensuring the MS/MS data used in the spectral library are **as "clean" as possible**.

Proteolabels - a solution for label-based proteomics quantification

Progenesis QI for proteomics now seamlessly integrates with Proteolabels Software, developed by Omics Analytics. Proteolabels is for quantitative proteomics, supporting studies involving stable isotope labels. Workflows include SILAC (two and three channels) and dimethyl (two and three channels).



Peak co-detection feature in Progenesis QI for proteomics gives a **75% gain** in the number of peptides quantified and a **39% gain** in the number of proteins in that sample, via a Proteolabels analysis of public data set PXD003284.

(http://www.proteomeexchange.org)

Use Progenesis QI for proteomics for data alignment, reliable feature measurement and identification. Then in Proteolabels auto-detect peptide pairs and triplets prior to protein-level quantification. Proteolabels offers a variety of QC metrics and plots to explore and optimise data quality, giving you visual confirmation your analysis results are correct.

Proteolabels features:

- SILAC and dimethyl-based proteome quantification
- Visualization of data at the feature level, peptide pair/triplet and protein-level to ensure reliable and sensitive quantifications
- Intelligent detection of labelled peptide pairs/ triplet when not all the labels were auto-detected

mzIdentML export

Progenesis QI for proteomics now supports **mzIdentML** export for Mascot and Ion Accounting searches, as developed by the **Proteome Xchange Consortium** for public sharing of data sets. This means that you can publish your papers in high ranking journals when the uploading of data to Proteome Xchange Consortium is a requirement.

Automatic peak detection thresholding to maximize identifications

It is now possible to utilize automatic peak detection thresholding for MS^e, HDMS^e and SONAR™ data. This maximizes the number and quality of protein identifications and saves operational time.

SONAR support

SONAR is a recently introduced data independent acquisition (DIA) mode for Waters HRMS instruments which provides additional specificity and clarity to DIA experiments. Data from this highly efficient workflow can now be analysed in Progenesis QI for proteomics v4.0.

Integration with Symphony – save data handling time

You can now initiate a Progenesis QI for proteomics experiment within the Symphony™ data pipeline. This means you can combine the efficiencies and flexibility of Symphony with the renowned user friendliness of Progenesis QI for proteomics. In real terms, this means that your MassLynx® controlled instrument can acquire data overnight, automatically transfer to a processing PC and initiate data import into a Progenesis QI for proteomics experiment. When you arrive in the morning, you'll be ready to get started on your data analysis!

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