



# ProteolQ 2.70

## Opis produktu

# ProteolQ

## Features

### Statistical Validation

A user can validate protein identifications using False Discovery Rate (FDR) calculations at the protein and peptide level. FDR calculation is supported via concatenated or separate target and decoy databases. Plots based on Mascot or SEQUEST scores, discriminate scores or probabilities can be generated. The user also has the option to use probability based measurements for verifying protein assignments and use sensitivity and error plots to maintain an acceptable error rates as well.

### Label Free Quantification

Proteomic workflows can vary greatly from lab to lab. Regardless of your instrument type, database search engine format or chromatography settings, ProteolQ provides flexible parameters to ensure robust label free quantitation no matter how your experiment was performed. Control precursor m/z peak picking by defining retention shifts, precursor mass tolerance, and S/N thresholds. Further refine label free quantitation by applying smoothing algorithms and baseline subtraction.

### Spectral Counting

ProteolQ provides robust relative quantitation by spectral counting. Researchers have adopted the spectral counting method due to its scalability, ease of implementation and cost savings when compared to label based techniques. ProteolQ's spectral counting algorithms are based upon well established methodologies deployed in an intuitive and highly interactive software platform. ProteolQ easily supports small scale comparisons or complex clinical proteomic studies.

### Precursor Intensity (TIC)

For every identified peptide based on a user specified filter criteria, ProteolQ extracts precursor intensity values from the MS/MS database search result. The precursor ion intensities for all peptides matching a protein are then compared between replicates and groups to determine relative expression at the protein level. In addition to the intensity based relative quantitation, ProteolQ provides access to spectral count based quantitation within the same project. This allows for a quick comparison between intensity and spectral count based relative quantitation.

While spectral count quantitation provides an accurate estimation for high abundance proteins, it is limited in its ability to quantify low abundance species. This is due to the fact that proteins of low abundance often have less than five spectral counts. ProteolQ allows you to quickly filter proteins with low spectral counts and then apply the hybrid precursor intensity quantitation to derive relative expression values, thus adding confidence to quantitation for proteins with even a single peptide assignment. To improve protein quantitation a user may select one of the numerous normalization procedures provided and apply post quantitation statistics.

### Precursor Intensity (AUC)

ProteolQ's label free quantitation using area under the curve (LF-AUC) provides accurate and robust quantitation using intensities derived from extracted ion chromatograms for every precursor detected in the MS or MS/MS instrument files.

Isobaric Tag Quantitation iTRAQ, TMT, and Custom Reagents ProteolQ empowers isobaric label based quantitation, regardless of the labeling strategy employed. ProteolQ provides a feature rich software platform giving users the ultimate control over all aspects of quantitation. ProteolQ supports a wide array of experiment types including:

1. iTRAQ duplex
2. iTRAQ fourplex
3. iTRAQ eightplex
4. Tandem Mass Tags (TMT) duplex
5. Tandem Mass Tags (TMT) sixplex

Or even a custom reagent.

ProteolQ automatically removes peptide redundancy from multiple search engine results including Mascot, Sequest, X!Tandem and report accurate isobaric label quantitation for every peptide assignment regardless of the source of the identification. The peptide view displays all the quantitation metrics, reporter ion intensity, search scores and probabilities associated with each identified peptide.

### Isotopic Labeling Quantitation

SILAC, Dimethyl, and Custom Labeling ProteolQ enables accurate and rapid quantitation of isotopically labeled peptides in a vendor independent software platform. ProteolQ allows the user to define the type of isotopic label used

for the experiment making it extremely flexible for a wide array of experiment types including:

1. SILAC
2. ICAT
3. Dimethyl labeling
4.  $^{18}\text{O}$
5.  $^{15}\text{N}$
6. Acetylation

ProteolQ supports label based quantitation using any label and any instrument platform. To ensure accurate quantitation select from a wide array of quantitation parameters including, mass tolerance, retention time shifts to accommodate deuterated compounds, and S/N thresholds. Further refine label based quantitation by applying smoothing algorithms and baseline subtraction.

### Biological Annotation

For most proteomic studies the question is not what proteins change expression across samples rather what is the biological significance of those changes. ProteolQ provides a completely customizable interface to support any form of biological annotation. Users can easily compare protein quantitative results in relation to biological pathways, protein localization, protein function, or compare to transcript abundance. Every time a ProteolQ analysis is performed, access is provided to the biological terms associated with the protein identification.