1 Peptide Identification

The content of proteins in the proteome is a protein. Proteins, which are depicted to be called peptides since proteins are much easier to handle biochemically than proteins. Peptides are very different each other and very similar with others. Wu and al. has studied a series of peptides and are known to be measured with the mass spectrometer. This step introduces another problem, the so-called protein inference problem. In this case, we do not look at all the peptides within the protein inference.

1.1 Computing the Parent Ion Mass

The function parentIonenMass determines the mass of a peptide and sequence while the function parentZoom returns a hydrophilicity for a given sequence of amino acids which can be used to predict the retention times [3].

For an overview of Quantitative Proteomics read [1, 2]. The data set

This left figure below shows the correlation between runs of each fragment ion. The two sets of data either differ across conditions using the four biological replicates.

1.2 In-silico Peptide Fragmentation

The fragment ions of a peptide can be computed following the rules proposed in [3]. Below the text and the ion, the FDR argument of fragmentation defines which ions are computed. The default one being computed are defined in the function definition. There are no limits for defining other forms of fragmentation ions for ETD (c and z ions) CD (b and y ions).

function (b, y)
{
  Hydrogen <- c(1.007825)
  Oxygen <- 15.9994
  Carbon <- 12.0111
  Nitrogen <- 14.0067
  Sulfur <- 32.065
  findions <- c(Carbon, Hydrogen)
  x <- 8 * findions + Hydrogen
  y <- -x
  z <- 2 * x + Hydrogen
  return(findions, c(x, y, z))
}

Theoretical Quantiles
Sample Quantiles

The plot shows the normalized signal intensity distribution (Log2 scale) on the 24 LCMS runs aligned in this experiment.

1.4 MS2 Labeling

The above-described peptide assignment is handled by the peakfinder function.

p <- peakplot(LCMSSpec, yrange = c(0, 1))

The plot below graphs a peptide-spectrum match of the "HILICQYQ2." peptide.

The right figure above shows the correlation between runs of each fragment ion. The two sets of data either differ across conditions using the four biological replicates.

2.1 Absolute Label-Free

The data set contains data of a protein mass spectrum and a peptide spectrum. In this case, a protein mass spectrum is used to identify the protein sequence with the help of a peakfinder function.

2.2 Relative Label-Free

LCMS based label-free quantification is a very popular method to extract relative quantitative information from mass spectrometry experiments. At the FCZG we use the software ProgenesisLCMS for this workflow [http://www.progenesis.com]. The plot below shows the alignment and extracting signals intensities from LCMS maps.


default

This figure shows a protein which is tested using the test command. It does not differ across conditions using the four biological replicates.

References


This poster has been produced using the R. O. D. Source: RStudio, version 3.5.6 (2017-10-30), and progenesis package version 0.6-4.

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