Minora Feature Detection

Label-free quantification uses the Minora Feature Detection node in the processing workflow to detect features in individual raw data files and to map them to PSMs, if they are available. A feature is signal for a single molecule and charge state across the elution profile.

As a first step, the Minora Feature Detector node detects LC/MS peaks in the raw data files and then maps them to identified PSMs. It calculates the theoretical isotope pattern of a PSM, finds the LC/MS peaks mapping to the isotope pattern, and creates a feature from the fitting peaks.

After the Minora Feature Detector node maps all identified PSMs to features, it creates features from peaks that are not associated with any feature. To do this, it takes all LC/MS peaks within a small retention-time range and checks for peaks that build isotope patterns. Mass deviations and intensities of the peaks must fit a theoretical pattern of an averagine peptide.

For finding untargeted features, the node splits the complete retention-time range of a file into slices having the equal retention-time range width, although the time slices slightly overlap. The overlap is twice the value of the Pattern RT Tolerance parameter setting. The node takes all peaks within a time slice and searches for other peaks that build an isotope pattern for different charges. It searches the most intense peaks first. If it finds pattern peaks, it creates a feature from them and labels the peaks "used" to ensure that each peak is used only in a single pattern.

The Minora Feature Detector node creates LC/MS features for all identified patterns and stores them in a feature table where targeted features are already stored.

Retention-Time Alignment and Feature Mapping

Note Retention-time alignment is also called chromatographic alignment.

The Feature Mapper node in the consensus workflow performs retention-time alignment and feature linking across data sets. It first chromatographically aligns the input files in a sample set. Specifically, it uses the results from the Minora algorithm to find the most abundant features and then aligns them to have the same retention time across all sample files. It uses the file in which most of these features are found as the reference for the rest of the alignment. For each file, the node tries to find a matching feature for every feature from the reference file. For each of these feature matches, it records the retention time difference in the two files. Finally, it fits a regression curve into the (RT, ΔRT) points. The node uses this curve to correct the retention times of the file relative to the chosen reference file.