i2MassChroQ: Software for Ion Mobility-Enabled Quantitative Proteomics in time TOF Data Format

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ABSTRACT

XITandemPipeline (Langella et al., 2017) is a free and open-source Java software program for proteomics initially designed to filter and group peptide/protein identifications from MS/MS mass spectra. After a complete rewrite in C++17, the new XITandemPipeline++ program features peptide/protein quantification, in particular with support for native timeTOF raw data.

XITandemPipeline++ performs peptide identifications and area-under-the-curve XIC-based quantifications using the Bruker’s native timeTOF raw data format. Using a common Hepa data set, published by Neier et al. (2018, PXD010012), we demonstrate that XITandemPipeline++ identifies and quantifies significantly more proteins than the MaxQuant and MS/fragger competitors, while being also significantly faster.

Please note that XITandemPipeline++ will soon be renamed to i2MassChroQ to reflect the Identification & Inference — mass chromatogram-based quantification capabilities.

RESULTS

Identification and protein inference

XITandemPipeline++ features high throughput and high resolution proteomics and metaproteomics features.

Thousands of DDA identification results can be loaded at once as part of the same project.

Our software supports Mascot, XITandem-generated identification data or any data set in mzIdentML and pepXML formats (from QemS, Comet, PepTidePhd). Its Occam’s razor-based grouping algorithm can infer protein groups very quickly, in particular by filtering out non informative redundancies (Van Den Bossche et al., nature communications, 2021).

Grouping might be performed by processing each sample separately or by creating a consensus protein list starting from multiple combined samples.

Quantitative analysis

Peptide quantification is handled by calculating extracted ion current chromatograms from precursor ion MS data (MassChroQ module).

Protein quantification is performed by the MQCR module that computes protein intensities by filtering and aggregating peptide intensities and carrying over cluster analysis, ANOVA, and comparisons between treatments.

TimsTOF PASEF quantification reproducibility

While quantifying more proteins than competitors (1 ion or more), XITandemPipeline still shows excellent correlations between replicates and very low median CV (H Hepa technical replicates, PXD010012)

Quantification accuracy

Plot of the 6428 proteins quantified (2 ions or more) and compared to ground truth ratio (2.1 for Yeast, 1:1 for Human, 1:4 for E coli, PXD01477)

AVAILABILITY

i2MassChroQ and its user manual are available as free software, licensed under the GNU General Public License (V3 +).

The user manual is available in PDF or HTML format. i2MassChroQ is developed on Debian GNU/Linux. Binary packages are built for GNU/Linux and MS Windows. Git repository: https://forge.mila.inra.fr/pappso/i2masschroq.

Main website

User manuals

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