Objective
Recent generation high-resolution mass spectrometers supporting ion-mobility separation (IMS) combined with advanced acquisition schemes such as UDMS\(^5\) enable the reliable identification and quantification of over 4,000 proteins in a single nanoUPLC-MS run [1]. Large amounts of generated data induce new requirements for the data processing software. MS\(^2\)/HDMS\(^5\)/UDMS\(^5\) data require processing by proprietary vendor software ProteinLynx GlobalSERVER (PLGS) [2]. Preprocessed data require further analysis to confidently identify and quantify regulated proteins, typically done by stepwise application of different dedicated algorithms and exporting to common data formats for result interpretation and sharing with the community. We present ISOQuant, an integrated open source software pipeline for in-depth evaluation and standardized reporting of MS\(^2\)/HDMS\(^5\)/UDMS\(^5\) based label-free proteomics data [1].

Methods
Tryptic HeLa cell lysate was analyzed in MS\(^2\)/HDMS\(^5\) and UDMS\(^5\) acquisition modes on a Waters Synapt G2-S mass spectrometer using 90 and 180 min gradients. PLGS (version >2.5, Waters Corporation) was used for raw data processing and for peptide and protein identification. ISOQuant was used for downstream analysis.

Data Analysis Workflow

Reports
ISOQuant exports analysis results to a set of uniform report formats. Generated MS Excel and CSV spreadsheets, as well as HTML reports allow to easily browse and share analysis results and display basic data quality metrics. Additionally, HUPO PSI standardized mzIdentML files are generated for an easy submission to PRIDE Archive - proteomics data repository [3][4].

Availability
Please visit www.isoquant.net to obtain current version of ISOQuant. Installation packages are available for Windows, Mac OSX and UNIX/Linux operating systems.

Bibliography

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