Description of DDA:Choi2017 - Choi et al., 2017[1]

Data processing and quantification

Dataset was processed and quantified with Skyline (3.5.0.9319).

Details for data processing are described in Choi, et al., 2017 and Panorama Web (https://panoramaweb.org/iPRG-2015.url) for iProphet cut-off 0.15. The MSstats report was exported for further analysis.

Statistical analysis

The MSstats report from Skyline and annotation for condition and biological replicate were used for SkylinetoMSstatsFormat function in MSstats v3.13.5, in order to pre-process before statistical analysis. Truncated peaks are replaced with NA missing value. Only unique peptides were used and shared peptides are removed (useUniquePeptide=TRUE). Features that have less than 3 measurements across MS runs were removed (fewMeasurements="remove"). Proteins which have only one PSM were removed (removeProtein_with1Feature=TRUE). Three isotopic peaks per feature and run were summed. Medians of log2 intensnties across MS runs were equalized for normalization (Normalization='equalizeMedians'). Intensity=0 was considered as censored missing values (censoredInt='0'). Differential abundance analysis for all possible pairwise comparisons was performed. R script for statistical analysis with MSstats is available (Choi2017_DDA_Skyline_Rscript.R).

1   Choi, M. *et al.* ABRF Proteome Informatics Research Group (iPRG) 2015 Study: Detection of Differentially Abundant Proteins in Label-Free Quantitative LC-MS/MS Experiments. *J Proteome Res* **16**, 945-957, doi:10.1021/acs.jproteome.6b00881 (2017).