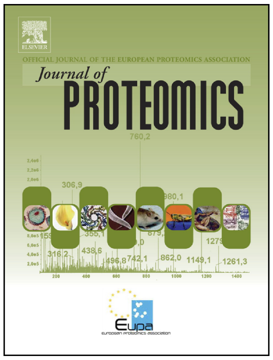

Experimental design and data-analysis in label-free quantitative LC/MS proteomics: A tutorial with MSqRob

Ludger J.E. Goeminne, Kris Gevaert, Lieven Clement

PII: S1874-3919(17)30123-9
DOI: doi: 10.1016/j.jprot.2017.04.004
Reference: JPROT 2820

To appear in: *Journal of Proteomics*

Received date: 1 March 2017
Revised date: 29 March 2017
Accepted date: 1 April 2017

Please cite this article as: Ludger J.E. Goeminne, Kris Gevaert, Lieven Clement , Experimental design and data-analysis in label-free quantitative LC/MS proteomics: A tutorial with MSqRob. The address for the corresponding author was captured as affiliation for all authors. Please check if appropriate. Jprot(2017), doi: 10.1016/j.jprot.2017.04.004

Title:

Experimental design and data-analysis in label-free quantitative LC/MS proteomics: a tutorial with MSqRob

Authors:

Ludger J. E. Goeminne[1,2,3,4], Kris Gevaert[2,3] and Lieven Clement[1,4*]

E-mail: ludger.goeminne@UGent.vib.be; kris.gevaert@UGent.vib.be; lieven.clement@UGent.be

Corresponding Author

* Tel.: +32 9 264 49 04. Fax: +32 264 49 95. E-mail: Lieven.Clement@UGent.be.

Affiliations:

[1] Department of Applied Mathematics, Computer Science and Statistics, Ghent University, Belgium

[2] VIB-UGent Center for Medical Biotechnology, VIB, Belgium

[3] Department of Biochemistry, Ghent University, Belgium

[4] Bioinformatics Institute Ghent, Ghent University, Belgium

Abbreviations:

CPTAC, Clinical Proteomic Technology Assessment for Cancer Network; DDA, data-dependent acquisition; DIA, data-independent acquisition; FC, fold change; FDR, false discovery rate; HCD, higher-energy collisional dissociation; IQR, interquartile range; KO, knock-out; MCAR, missingness completely at random; MDS, multidimensional scaling; MNAR, missingness not at random; PSM, peptide-to-spectrum match; SILAC, stable isotope labeling of amino acids in cell culture; TMT, tandem mass tags; UPS1, Universal Proteomics Standard 1; WT, wild type.

Keywords: differential protein abundance; biostatistics; label-free quantification; tandem mass spectrometry; experimental design; peptide-based linear model

Acknowledgements

Part of this research was supported by IAP research network “StUDyS” grant no. P7/06 of the Belgian government (Belgian Science Policy) and the Multidisciplinary Research Partnership “Bioinformatics: from nucleotides to networks” of Ghent University. L.G. is supported by a Ph.D. grant from the Flanders Innovation & Entrepreneurship agency, Flanders (Agentschap Innoveren & Ondernemen – Vlaanderen) entitled ‘Differential proteomics at peptide, protein and module level’ (141573).