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VEMS: A TOOL TO QUANTIFY iTRAQ LABELED SAMPLES

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Introduction: The goal of many MS-based proteomics experiments nowadays is to quantify changes in the abundance of the proteomes across several samples of biological interest. The iTRAQ labeling method is a powerful relative quantitation technique that combined with liquid chromatography coupled to tandem mass spectrometry allows quantify up to eight different samples simultaneously. The transformation of the multiple spectra containing different protein expression values is a challenging task. We have developed an integrated tool for database dependent interpretation, quantitation and database storage for iTRAQ labeled samples able to handle various input data formats from instruments from different manufacturers. Users can download the Web Server from http://personal.cic.biogune.es/rmatthiesen/.

Results: The reference sample gave the expected ratios with a standard deviation on the peptide ratios in the range of 0.03-0.13. The accuracy of the calculated protein ratios was from 0.02-0.05% for the reference sample which contains the proteins mixed in known ratios.

To evaluate VEMS performance with large-scale proteomics data, the same amount of exosomes samples in three different conditions were labeled with iTRAQ and fractionated by SCX as explained in methods section. In the first experiment 326 proteins were identified while in the second experiment 243 proteins were identified. In total 191 proteins were identified commonly in the two replica experiments. From the total, 68.5% of these proteins were significantly quantified in the two replica experiments with an average 95% confidence interval of ±0.19 (Figure 1).

Innovative aspects

- Generalization of the quantitative algorithm provided in the program i-tracker (2).
- Integration of data search, quantitation and storage in one program in contrast TandTRAQ (3).
- Improved statistical analysis of result.

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References

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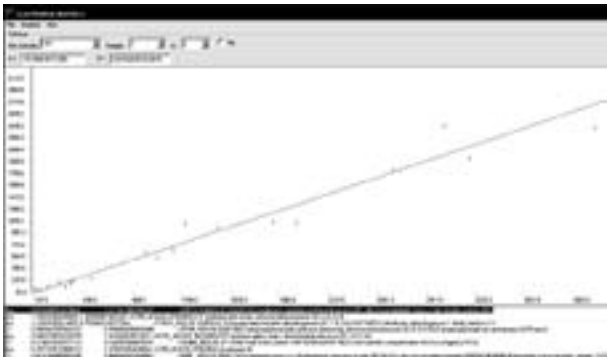

Figure 1
Manual validation of the protein quantitative values.
Peptide ratios considered to be outliers can be removed by clicking on the plot.