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Combined use of peptide ion and normalized delta scores to evaluate milk authenticity by ion-trap based proteomics coupled with error tolerant searching[☆]

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Abstract

A fundamental issue in proteomics is the peptide identification by database searching and the assessment of the goodness of fit between experimental and theoretical data. Despite the different number of ways to measure the quality of search results, the definition of a scoring criterion is still highly desirable in ion-trap based proteomics. Indeed, in order to fully take advantage of a low resolution MS/MS dataset, it is essential to strike a balance between greater information capture and reduced number of incorrect peptide assignments. In addition, the development of user-specified rules is a crucial aspect when very similar proteins of the same family are analyzed in order to infer the origin species.

In this study, a post-processing validation scheme is provided for the evaluation of proteomic data in shot-gun ion-trap proteomics, when a flexible database searching based on the error tolerant mode is adopted in combination with a low-specificity enzyme to maximize sequence coverage. To validate peptide assignments, we used standard β -casein digested with trypsin/chymotrypsin or trypsin alone and the popular search engine MASCOT to identify the relevant (known) peptide sequences. A linear combination between peptide ion score and normalized delta score (i.e. the difference between the best and the second best ion score, divided by the best score) is proposed to increase the accuracy in sequence assignments from low-resolution tandem mass spectra. Finally, the optimized post-processing database validation was successfully applied to the direct analysis of

[☆] Dedication in memory of Pier Giorgio Zambonin (Bari, Italy)

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