Peaks, Peptides, Computers -- Bioinformatics in the Analysis of HPLC/MS Proteomics Data

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Abstract

Differential analysis of proteome expression levels has been developing rapidly over the last years. While 2D-gel-based techniques are still the standard in the field, HPLC/MS-based approaches have gained considerable interest due to their larger potential for full automation. Consequently, this approach is being developed in industrial settings but also in larger biomedical research settings. The acceptance as well as the impact of these techniques is however bounded by the ability to efficiently handle and analyze the tremendous volume of data produced by these techniques. the inevitable flip-side of automation. Overcoming these problems, and thus enabling the full potential of the method, can only be achieved by new developments in algorithmics, data management, and software engineering. These developments have to take place in tight integration with the method development in HPLC/MS, which is currently a very rapidly evolving field. We propose a number of new strategies centered around HPLC/MS-based proteomics that will fully enable the potential of these techniques in high-throughput settings by automatically reducing the data volume and annotating this data with the relevant information.