

PEAKPLOT: Visualizing Fragmented Peptide Mass Spectra in Proteomics

Christian Panse^{1,*} Bertran Gerrits¹ Ralph Schlapbach¹

1. Functional Genomics Center Zurich (FGCZ)

* Contact author: cp@fgcz.ethz.ch

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The goal of proteomics research in general is to identify and quantify proteins on a defined biochemical state. Mass spectrometry is the method of choice for protein identification and post-translational modification assignment in proteomic studies [Roepstorff, P. and Fohlman, J. (1984)]. Due to the advent of accurate and fast sampling mass spectrometers, proteomic experiments often contain thousands of peptide fragmentation spectra. Although it is commonly accepted that no manual validation of individual spectra in such experiments is feasible, annotated spectra of the peptides assignments with their modifications are required for publication and reviewing purposes. Hand-drawn approaches as shown in Figure 1(a) are effective and attractive visualizations. However, their production is very time consuming. The routines provided by [Matrix Science (2009)] are limited by bitmap graphics by the GraphGD library and difficult to customize. Here, we demonstrate a software package called *peakplot*. The software *peakplot* labels the spectra from a peptide sequence assignment by the Mascot search algorithm [Matrix Science (2009)] retrospectively with the appropriate fragment ion labels. The software can be used either via an easy-to-use web interface or a command line version (for advanced users). We also demonstrate how we embedded our application into existing LIMS (Laboratory Information Management System) infrastructure at our research center. The *peakplot* application consists of two steps. First, the Mascot Server result file is parsed and the data are processed for the subsequent visualization step. Furthermore, our aim was to provide 'first' visualization functions, which can be easily extended upon individual demands. The difficulty on the 'large-scale, high-throughput' automatic labelling is to avoid overlapping of the labels on each plot. Our heuristic tries to solve this problem by determining the importance of each putative label and drawing only the most important of them. *Peakplot* greatly facilitates the visualization of peptide fragmentation spectra and improves quality assessment of modification sites such as phosphorylation. Availability: <http://fgcz-peakplot.uzh.ch/>

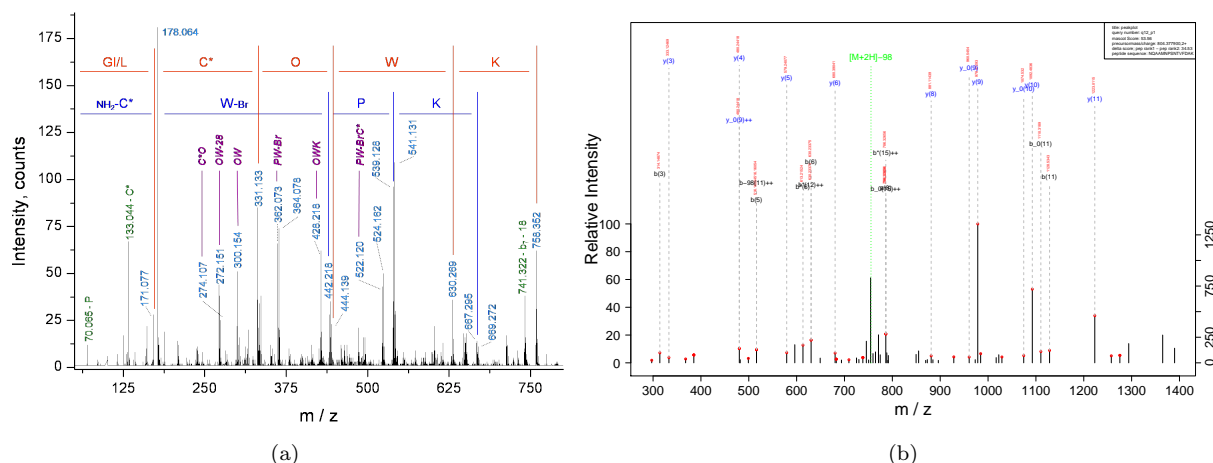


Figure 1: The picture displays two labeled mass spectra of two different peptides. (a) hand-drawn by an author, (b) generated from the proposed *peakplot* application.

References

- Matrix Science (2009). Mascot Server, <http://www.matrixscience.com/server.html>.
- Roepstorff, P. and Fohlman, J. (1984). Proposal for a common nomenclature for sequence ions in mass spectra of peptides. *Biomed Mass Spectrom*, 11, p601.