MS-Viewer – A Web Based Spectral Viewer For Database Search Results



Peter R. Baker¹, Alma L. Burlingame¹ and Robert J. Chalkley¹ ¹Mass Spectrometry Facility, Dept. of Pharmaceutical Chemistry, University of California, San Francisco, USA

pkl, etc) are supported.

the relevant report column

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Link to the MS-Product

interactive spectral display program. This supports

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MS-Viewer Report

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Introduction

Many academic journals require annotated spectra to be made available to support identifications in manuscripts. As some articles now report upwards of 10000 phosphorylation site assignments, submission of annotated spectra directly to the journal is becoming impractical. Also, if the spectral submissions are static documents it is often difficult to assess the assignments. Another common requirement is for researchers remote from each other to want to share results

Submission of results to a public repository is often the most practical option, although many of these repositories have strict and complex formatting requirements for submissions. A spectral viewer has now been added to the Protein Prospector web site that allows annotated spectra from database search results to be viewed interactively using simple tab-delimited or comma separated text files as input. Once the data has been uploaded and the report formatted, other internet users can access the data via a keyword. The spectral viewer is also freely available for local installation.

Methods

The program input is either a single peak list file or an archive of peak list files and a database search results file. The results file is expected to be in tabular form with columns containing peotides, spectrum identifiers and precursor charges. A fraction column is also required if multiple peak lists are uploaded. An arbitrary number of other columns containing other information may also be present. Individual spectra in the report can be viewed by clicking on entries in the peptide column. There is also a facility for re-searching individual spectra using the MS-Tag program. Data from up to four columns can be used for sorting the table. Reports can be saved and then viewed in the future by other web users who enter a 10 digit randomly generated code.

Apart from Protein Prospector results the software currently supports Mascot CSV and X!Tandem Tab Delimited results files via conversion scripts. Users can write their own scripts for automatic results file conversion.

Other unique features of the spectral viewer are the ability to deal with ambiguous site assignments for modified amino acids¹ and cross-linked peptides and the ability to visually compare different assignments to the same spectrum

The software is available for use on the Protein Prospector web site and for local installation.

Conclusion

MS-Viewer is available at http://prospector.ucsf.edu/prospector/cgi-bin/msform.cgi?form=msviewer or for local installation by emailing ppadmin@cgl.ucsf.edu.

A video explaining MS-Viewer is available at http://vimeo.com/30462677.

References

1. Baker P. R., Trinidad J. C. and Chalkley R. J., Modification Site Localization Scoring Integrated into a Search Engine. Molecular and Cellular Proteomics, doi: 10.1074/mcp.M111.008078

Acknowledgements

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To deal with other results file formats the user needs to specify the columns containing the peptide hits, the spectral identifiers and the precursor charges.

Last 4 columns of a Mascot CSV report displayed in MS-Viewer

