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

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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 peptides, 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 acids[1] 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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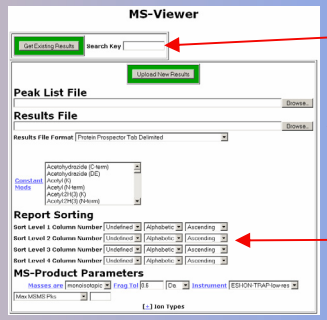
MS-Viewer Form



The peak list file can either be a single file or a file archive (zip, rar, 7z, etc) containing multiple peak list files. Most of the common peak list formats (mgf, mzXML, mzML, dta, pkl, etc) are supported.

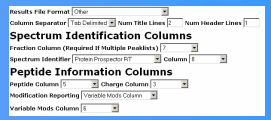
Constant amino acid modifications need to be specified if they are not present in the relevant report column.

Parameters for the spectral viewer.

Once a report has been formatted it can be saved and subsequently recalled by another web user entering a 10 digit code.

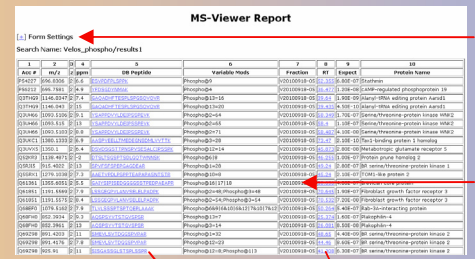
The results file can either be a Protein Prospector or X!Tandem Tab Delimited Text file, a Mascot CSV file or a tabular file with an arbitrary number of columns (see right).

Reports can be sorted based on the contents of up to 4 columns.



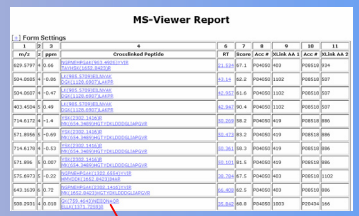
To deal with other results file formats the user needs to specify the columns containing the peptide hits, the spectral identifiers and the precursor charges.

MS-Viewer Report



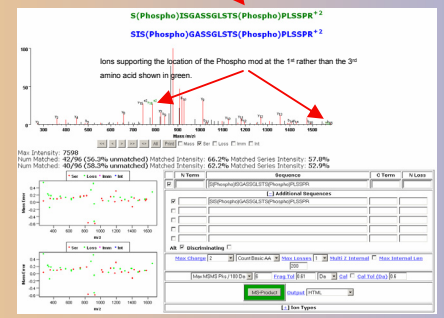
Click the + to show the MS-Viewer form. This can be used to reformat the report without uploading the data again.

The fraction column denotes which peak list the spectrum comes from.

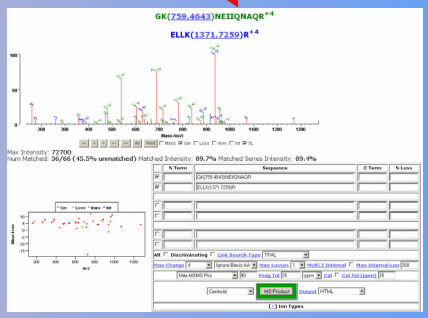


Link to the MS-Product interactive spectral display program. This supports SLIP (Site Localization in Peptide) scoring[1] and ambiguous site localization.

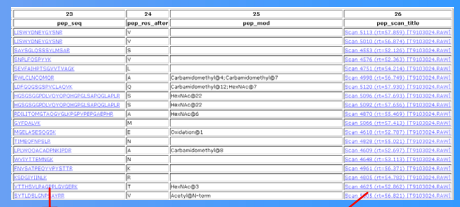
Link to Protein Prospector MS-Tag form to re-search the spectrum.



MS-Viewer can also deal with cross-linked peptides.



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



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