MSnbase input/output capabilities

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Abstract

This vignette describes **MSnbase**'s input and output capabilites. *Keywords*: Mass Spectrometry (MS), proteomics, infrastructure, IO.

1 Overview

MSnbase's aims are to facilitate the reproducible analysis of mass spectrometry data within the R environment, from raw data import and processing, feature quantification, quantification and statistical analysis of the results. Data import functions for several formats are provided and intermediate or final results can also be saved or exported. These capabilities are presented below.

2 Data input

Raw data Data stored in one of the published XML-based formats. i.e. mzXML (Pedrioli et al., 2004), mzData (Orchard et al., 2007) or mzML (Martens et al., 2010), can be imported with the readMSData method, which makes use of the mzR package to create MSnExp objects. The files can be in profile or centroided mode. See ?readMSData for details.

Peak lists Peak lists in the mgf format¹ can be imported using the readMgfData. In this case, the peak data has generally been pre-processed by other software. See **?readMgfData** for details.

Quantitation data Third party software can be used to generate quantitative data and exported as a spreadsheet (generally comma or tab separated format). This data as well as any additional metadata can be imported with the readMSnSet function. See ?readMSnSet for details.

MSnbase also supports the mzTab format², a light-weight, tab-delimited file format for proteomics data developed within the Proteomics Standards Initiative (PSI). mzTab files can be read into R with readMzTabData to create and MSnSet instance.

¹http://www.matrixscience.com/help/data_file_help.html#GEN

²http://code.google.com/p/mztab/

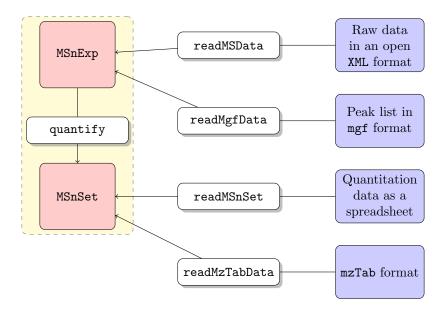


Figure 1: Illustration of MSnbase input capabilities. The white and red boxes represent R functions/methods and objects respectively. The blue boxes represent different disk storage formats.

3 Data output

RData files R objects can most easily be stored on disk with the **save** function. It creates compressed binary images of the data representation that can later be read back from the file with the **load** function.

Peak lists MSnExp instances as well as individual spectra can be written as mgf files with the writeMgfData method. Note that the metadata in the original R object can not be included in the file. See ?writeMgfData for details.

Quantitation data Quantitation data can be exported to spreadsheet files with the write.exprs method. Feature metadata can be appended to the feature intensity values. See ?writeMgfData for details.

MSnSet instances can also be exported to mzTab files using the writeMzTabData function.

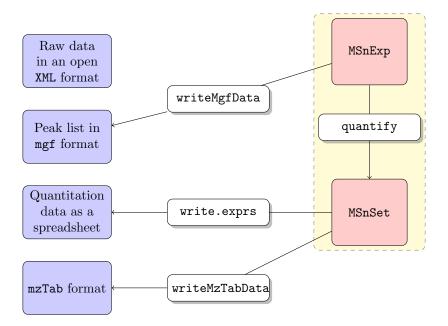


Figure 2: Illustration of MSnbase output capabilities. The white and red boxes represent R functions/methods and objects respectively. The blue boxes represent different disk storage formats.

References

- Lennart Martens, Matthew Chambers, Marc Sturm, Darren Kessner, Fredrik Levander, Jim Shofstahl, Wilfred H Tang, Andreas Rompp, Steffen Neumann, Angel D Pizarro, Lu isa Montecchi-Palazzi, Natalie Tasman, Mike Coleman, Florian Reisinger, Pune et Souda, Henning Hermjakob, Pierre-Alain Binz, and Eric W Deutsch. mzml - a community standard for mass spectrometry data. *Molecular* & Cellular Proteomics : MCP, 2010. doi: 10.1074/mcp.R110.000133.
- Sandra Orchard, Luisa Montechi-Palazzi, Eric W Deutsch, Pierre-Alain Binz, Andrew R Jones, Norman Paton, Angel Pizarro, David M Creasy, Jérôme Wojcik, and Henning Hermjakob. Five years of progress in the standardization of proteomics data 4th annual spring workshop of the hupoproteomics standards initiative april 23-25, 2007 ecole nationale supérieure (ens), lyon, france. Proteomics, 7(19):3436–40, 2007. doi: 10.1002/pmic.200700658.
- Patrick G A Pedrioli, Jimmy K Eng, Robert Hubley, Mathijs Vogelzang, Eric W Deutsch, Brian Raught, Brian Pratt, Erik Nilsson, Ruth H Angeletti, Rolf Apweiler, Kei Cheung, Catherine E Costello, Henning Hermjakob, Sequin Huang, Randall K Julian, Eugene Kapp, Mark E McComb, Stephen G Oliver, Gilbert Omenn, Norman W Paton, Richard Simpson, Richard Smith, Chris F Taylor, Weimin Zhu, and Ruedi Aebersold. A common open representation of mass spectrometry data and its application to proteomics research. *Nat. Biotechnol.*, 22(11):1459–66, 2004. doi: 10. 1038/nbt1031.