

MSnbase, efficient R-based access and manipulation of raw mass spectrometry data

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Abstract

We present version 2 of the **MSnbase** R/Bioconductor package. **MSnbase** provides infrastructure for the manipulation, processing and visualisation of mass spectrometry data. Here we present how the new *on disk* infrastructure allows the handling of hundreds on commodity hardware and present some application of the package.

Introduction

What is **MSnbase**: **MSnbase**¹ offers a solution between low level libraries such as `jmzml`, exclusively for the development of new applications and GUI software, that provides a limited and fixed set of functionality.

Software functionality

On disk backend

Efficient low level access - in memory vs on disk mode (using mzR) - benchmarking - used in ms-based proteomics and metabolomics

Use cases

Example applications: visualisation, ...

Discussion

Collaborative development, 11 contributors since creation (see blog post).

Count packages depending on MSnbase.

Future developments.

Acknowledgement

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References

- (1) Gatto, L.; Lilley, K. S. MSnbase - an R/Bioconductor package for isobaric tagged mass spectrometry data visualization, processing and quantitation. *Bioinformatics* **2012**, *28*, 288–9.