JMSA2: Java Mass Sectrometry Analyzer

Bruno Henrique Meyer, Malton William Machado Cunico, Dieval Guizelini, Emanuel Maltempi de Souza, Fabio de Oliveira Pedrosa, Leonardo Magalhães Cruz

Federal University of Parana

Abstract

The use of MALDI-TOF mass spectrometry allows microorganism identification by generating mass spectra representing a characteristic profile of signals from ionized whole cell peptides or cell extracts. The microorganism identification by means of mass spectrometry is a recent technique, applied to different types of samples (i.e., clinic or environmental), with many advantages compared to classical approaches (e.g., amplification and sequence of genetic markes, such as 16S rRNA gene). It is time and cost effective. Comparing of mass spectra obtained from unknown microorganisms with a database of mass spectra for known microorganisms allows their identification. However, the spectra generated are complex data, being its interpretation and analysis difficult. Further, among few alternatives of software, there are proprietary code ones with limited environmental representative databases. The Java Mass Spectrometry Analyzer (JMSA) has been developed in open source code by the Nucleus of Nitrogen Fixation at Federal University of Paraná (UFPR) that facilitate the visualization, manipulation, creation of databases, and comparison of mass spectra for the purpose of microorganism identification, as well as include descriptive sample data. Here, we present JMSA version 2, developed in Java (platform independent), with the following main characteristics: i) clustering algorithm; ii) export results in many different file formats; iii) build superspectra that enhance comparison and identification; iv) creation of spectra database; v) pairwise-spectra comparison; vi) spectra database search tool for microorganism identification.

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