

BITS :: Call for Abstracts 2019 - Oral communication

<i>Type</i>	Oral communication
<i>Session</i>	Proteomics
<i>Title</i>	FROM GEENA2 TO GEENAR: A USER FRIENDLY WEB TOOL FOR MALDI-TOF MASS SPECTRA MANAGEMENT
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Motivation

Matrix Assisted Laser Desorption Ionization - Time Of Flight (MALDI-TOF) is a robust mass spectrometry technology well-known for the analysis of proteomics data, widely used in research studies, such as in clinical applications for discovering biological biomarkers related to different phenotypes [1].

Geena2 is a web tool for raw MALDI-TOF mass spectra management, designed to help scientists in filtering, aggregating and analysing their data from spectrometer. Geena2 structure is conceived to be a user friendly interface with three different levels of parameters tuning [2]. Different protocols for its application are described in [3].

Starting from the results obtained in [4] by using MALDIquant R package [5], GeenaR is designed as a parallel web tool, which combines the structure of Geena2 with the R environment for the pre-processing, analysis, visualisation and comparison of MALDI-TOF mass spectra. The aim of GeenaR is the same of Geena2: to help the scientists in managing mass spectra, without the constraints that comes from programme languages knowledge. The pipeline of GeenaR consists of different modules for each tasks, with particular emphasis on that tasks complementary to Geena2, such as the reporting for the sake of the reproducible research.

Methods

The background system of Geena2 and GeenaR is a Linux-Apache-MySQL-PHP (LAMP) environment, which is the box of a three layers pipeline:

- a developer layer, consisting of parallel scripts in Perl language for Geena2 and in R language for GeenaR;
- an interconnection layer, which provides the user's choices in form of parameters to be interpreted by Perl and R scripts;
- a user layer, two HTML masks that help the user in selecting the steps for the treatment of the raw mass spectra and the required results.

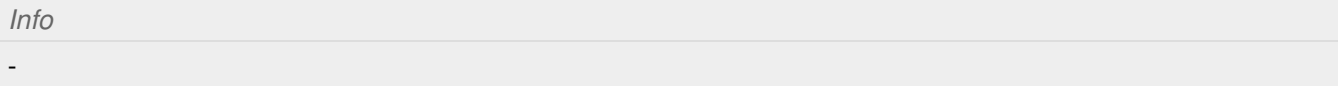
The user layers for Geena2 and GeenaR are shown in Figure 1. For example, the possibility to copy with isotopic peaks is provided in Geena2 (A), while a plethora of alternative methods for cleaning and aligning mass spectra is provided in GeenaR (B).

The main result is the peaks list, both for Geena2 and GeenaR. The added value from GeenaR is the possibility to show an example of tidy mass spectrum after the cleaning step and a graph of the peaks lists after the aligning step, and to suggest the number of clusters for the different experimental samples by means of gap statistic method, together with a dendrogram representative of the clustering. These methodologies are provided by means of R packages, called in different scripts that preserve a sort of modularity for the tasks.

Results

GeenaR inherits the concept of flexibility from Geena2, because the parameters are under the control of the users by means of a clear html interface and the underground LAMP environment. GeenaR pipeline supports all the issues related to the MALDI-TOF mass spectra, such as cleaning data, aggregation of mass spectra (in presence of multiple replicas per sample), peak extraction, and mass spectra clusterization. R scripts call several R packages for the augmentation of Geena2 methodologies: nevertheless, the parallelism with Geena2 ensures again the flexibility for the scientists, selecting the typology of results, tables or graphs, according to their preferences.

An important added value from GeenaR is the possibility to obtain a report, both in html and pdf format, which keeps track of the used R packages, selected parameters, descriptive and graphical results, generated from the R developer layer. In this way, the philosophy of reproducible research is favoured for non-expert and expert users, in order to repeat the analysis on different data with the same methods or parameters, or to tune them according to personal knowledge.



Figure

A

Geena 2
Build March 10, 2015.

This system is under active development, please forgive us for possible errors and send us your comments, criticisms and congratulations, if any.

Welcome to **Geena 2**, a tool for MS spectra filtering, averaging and aligning.
(SSI - Standard Search Interface)

This is the **Standard Search Interface (SSI)**. You may be interested in using the **Quick Search Interface (QSI)** that simplifies the use of Geena 2 by reducing the number of parameters to a very minimum or the **Bright Search Interface (BSI)** that allows you to tune averaging and alignment parameters, while leaving all remaining to their default values.

Using Geena 2 should be straightforward. Input and output data use a simple format. Nevertheless, should you have any problem, see the [help](#) or the [information on data formats](#) pages.

NB! This version includes a new feature. When a normalization peak is provided, it is used to calibrate m/z values. In practice, for each spectrum all m/z values are recomputed by taking into account the difference between the theoretical and the actual m/z values of the normalization peak.

NB! Move your mouse over the icon for a contextual help.

Job information

Job name:

Your email:

Country:

Input data

Data origin: Upload file Spectra data store

Data file: Nessun file selezionato.
(see [information on data file format](#) and an [example file](#))

Samples from spectra data store: All Some

Which samples (only if Some is checked):
CRC_Case02
CRC_Case03
CRC_Case04

Filter and isotopic peaks join

Analysis range: From m/z to m/z

Normalization peak: No Yes, at m/z

First abundance threshold: at lowest m/z (absolute value)

Last abundance threshold: at highest m/z (absolute value)

Intermediate thresholds: at m/z

Computation and alignment of average spectra

Maximum delta for aligning replicates: Da

Minimum number of signals in replicates:

Maximum delta for aligning average spectra: Da

Minimum number of signals in average spectra:

B

Geena R
Build January 23, 2018.

This system is under active development, please forgive us for possible errors and send us your comments, criticisms and congratulations, if any.

Welcome to **GeenaR**, a tool for MALDI/ToF MS spectra analysis.

Using GeenaR should be straightforward. Nevertheless, should you have any problem, see the [help page](#), the page on [information on format](#) or the [example file](#).

NB! Move your mouse over the icon for a contextual help.

Job information

Job name:

Email:

Country:

Input data

List of spectra file names: Nessun file selezionato.

File contents are: Spectra Peaks

File with tasks and related parameters: Nessun file selezionato.

Tasks

Task (select to execute)	Step (select to execute)	Method	Parameters
<input type="checkbox"/> Select/unselect all tasks	<input type="checkbox"/> Select/unselect all steps	<input type="checkbox"/> Restore default parameters	<input type="checkbox"/> Restore default parameters
Quality control <input type="checkbox"/>			Display example <input type="checkbox"/> Report log file <input type="checkbox"/>
Trimming <input type="checkbox"/>			Lower m/z value: <input type="text"/> Upper m/z value: <input type="text"/>
Cleaning and Smoothing <input type="checkbox"/>	Variance stabilization <input type="checkbox"/> <input type="radio"/> SQRT <input type="radio"/> LOG <input type="radio"/> LOG2 <input type="radio"/> LOG10		Half window size: <input type="text"/>
	Smoothing <input type="checkbox"/> <input type="radio"/> Savitsky-Golay <input type="radio"/> Moving average		Number of iterations: <input type="text"/>
	Baseline removal <input type="checkbox"/> <input type="radio"/> SNIP <input type="radio"/> TopHat <input type="radio"/> Convex-Hull <input type="radio"/> Median		
	Normalization <input type="checkbox"/> <input type="radio"/> TIC <input type="radio"/> PQN <input type="radio"/> Median		
Aligning <input type="checkbox"/>	Filtering <input type="checkbox"/> <input type="radio"/> MAD <input type="radio"/> SuperSmother		Half window size: <input type="text"/> SNR: <input type="text"/> Tolerance: <input type="text"/>
	Smoothing <input type="checkbox"/> <input type="radio"/> Lowess <input type="radio"/> Linear <input type="radio"/> Quadratic <input type="radio"/> Cubic		Half window size: <input type="text"/> SNR: <input type="text"/> Tolerance: <input type="text"/>
	Binning <input type="checkbox"/> <input type="radio"/> Strict <input type="radio"/> Relaxed		Display example <input type="checkbox"/>
Peak detection <input type="checkbox"/>			Display example <input type="checkbox"/>

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