BioNumerics® FEATURED APPLICATIONS

MALDI-TOF MASS SPECTROMETRY
(MALDI-TOF MS)

Fast, robust and accurate strain typing

What is MALDI-TOF MS?

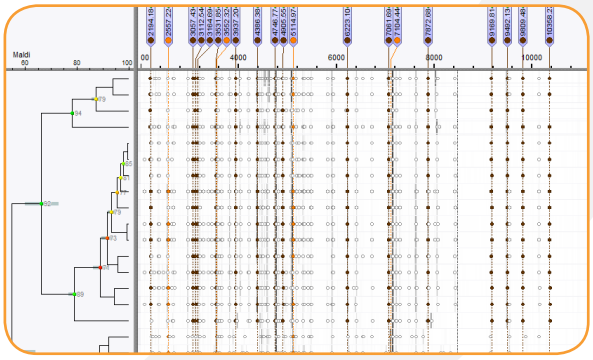
Mass spectrometry (MS), particularly Matrix Assisted Laser Desorption Ionization Time-Of-Flight (MALDI-TOF), is increasingly being used for routine identifications of bacterial and fungal isolates. It can be applied on intact cells or cell lysates. Starting from the biological material, a MALDI-TOF mass spectrum is generated within minutes and used for identification analysis.

For which applications?

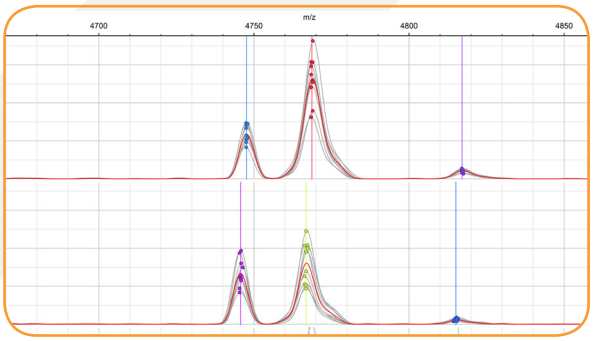
Because MALDI-TOF MS is quick and cost-effective, it is highly suitable for high-throughput applications such as pathogen identification in clinical laboratories, quality control in food industry or biomaterial validation in culture collections.

MALDI-TOF MS analysis in BioNumerics

1. Starting from biological material, a MALDI-TOF mass spectrum is generated in minutes
2. Import of MALDI-TOF MS data in BioNumerics
3. Automated spectra preprocessing including calculation of summary spectra
4. Identification analysis based on predefined peak sets or complete spectra
5. Advanced statistical analyses and data visualizations



Cluster analysis based on MALDI-TOF MS peak matching.



Summary spectra from averaging technical or biological replicates.

NOTE:
The minimal configuration consists of the "Fingerprint Data" module and the "Tree and Network Inference" module. We recommend having the "Dimensioning & Matrix Mining" and/or the "Classifiers and Identification" modules as well for additional functionality. Please contact us for more information.

YOUR ADVANTAGES

WHY USE **BioNumerics**
FOR YOUR MALDI-TOF MS ANALYSIS?

- ✓ A very flexible tool
- ✓ Automate your preprocessing
- ✓ Take control of your data
- ✓ Summarize replicate spectra
- ✓ Build your own database for identification

MALDI-TOF MS in BioNumerics®

A very flexible tool

Numerous import formats

Data formats from most hardware manufacturers are supported and can be imported in the same database. Both the import of raw data combined with automated preprocessing and the import of peak lists are possible.

Flexible analysis options

Single mass spectra and summary spectra can be analyzed with e.g. similarity-based cluster analysis, Principal Components Analysis (PCA) or Multidimensional Scaling (MDS). Peak matching allows to filter out common background peaks and focus on a set of discriminative peaks, drastically improving the sensitivity of the analysis. The matrix mining tools are very useful for identifying potential biomarkers.

Automate your preprocessing

With BioNumerics, you can automatically:

- Clean up raw spectra while importing
- Import with predefined or custom templates
- Get rid of technical variation by averaging replicates

Summarize replicate spectra

- Summarize several replicates into single spectra
- Define summary spectra on isolate, species, genus or any other level

Take control of your data

Perform a peak matching and identify specific peaks of interest, based on stochastics, statistics or results from more advanced analysis such as discriminant analysis and PCA.

Add different labels and colors to the peak sets according to your own needs and preferences.

Create a cluster analysis from your spectral data and have it visualized as a (circular) dendrogram, unrooted tree, network or 3D image. Add meta data on the tree and export the image in a wide variety of formats.

Use the built-in tools to calculate branch reliability and make confident interpretations based on your analysis.

Build your own database for identification

BioNumerics allows you to build your own reference databases. Reference sets based on mass spectra from organisms of your choice, using either complete spectra or custom peak classes, can be stored as identification projects. Identification of unknown isolates can then be performed using high-tech classifiers such as Support Vector Machines or Naive Bayesian classifiers.

CONVINCED? INTRIGUED? TRY IT FOR YOURSELF!

www.bionumerics.com

Scan the QR codes to access each step

1. Make sure you have a **BioNumerics** license (also see note on front page).

2. Watch tutorial movies or download sample data for use in **BioNumerics**.

Headquarters
Keistraat 120 • 9830 Sint-Martens-Latem • Belgium
+32 922 22 100 info@applied-maths.com

USA and Canada
11940 Jollyville Rd., Suite 115N • Austin, TX 78750 USA
+1 512 482 9700 info-us@applied-maths.com

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