

Statistical Analysis Software for Direct Ionization Mass Spectrometry

eMSTAT Solution



Enables Easy Statistical Analysis of MALDI/DPiMS™ Measurement Data by Anyone



eMSTAT Solution™

Easy Mass Spectrometric Statistical Solution for Matrix Assisted Laser Desorption Time of Flight Mass Spectrometry (MALDI-TOF MS) and Direct Probe Ionization Mass Spectrometry (DPiMS)

Features

Statistical Analysis Mode

Users can easily differentiate samples and identify marker peaks using univariate and multivariate analysis tools.

Discriminant Analysis Mode

Implement discoveries from Statistical Analysis Mode to discriminate unknown samples.

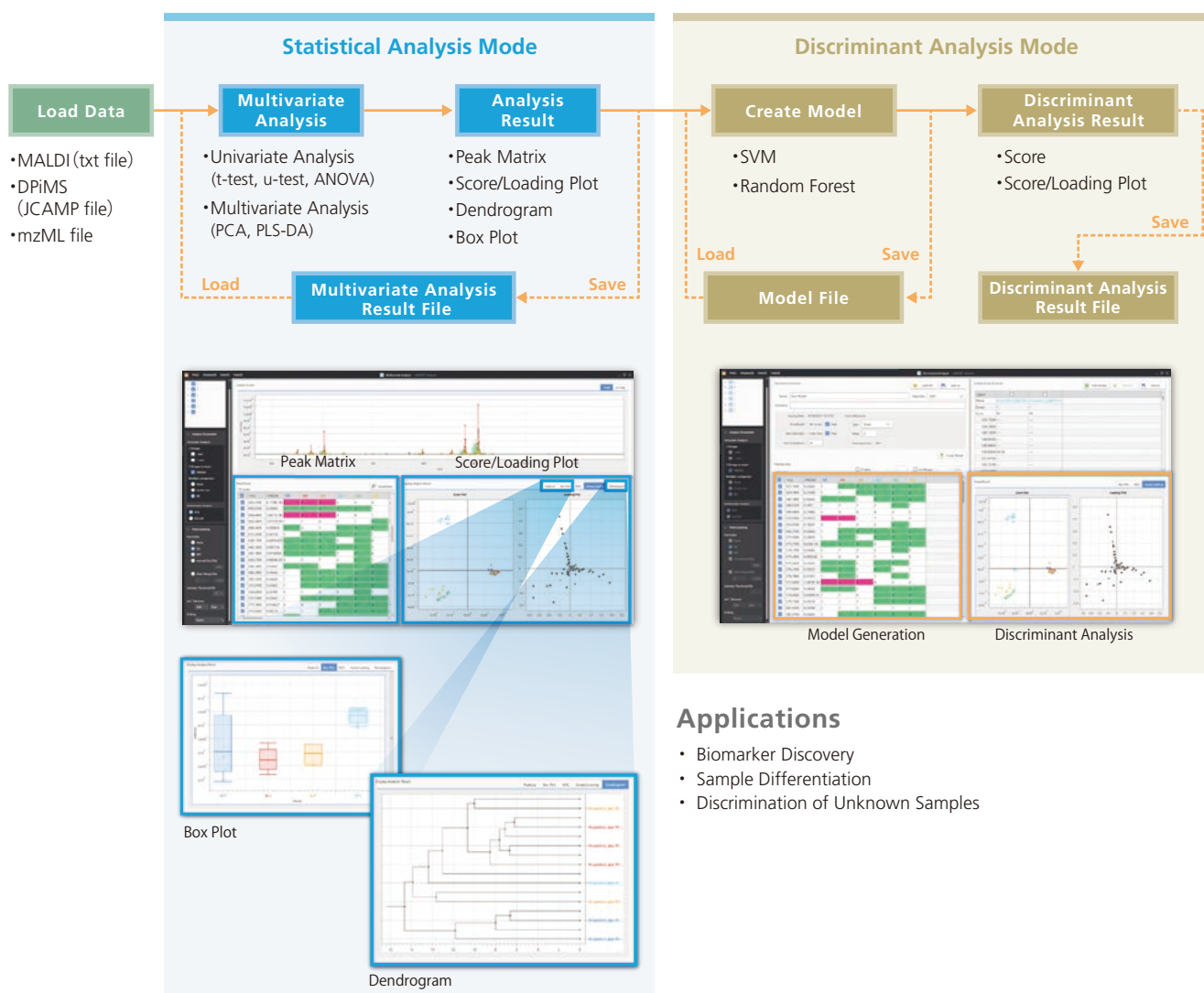
Flexible Dynamic Grouping Function

Flexible sample grouping based on registered quality information facilitates biomarker discovery.

Supports a Variety of Data Formats from MALDI-TOF and DPiMS Analyses

JCAMP, ASCII and mzML data input are all supported.

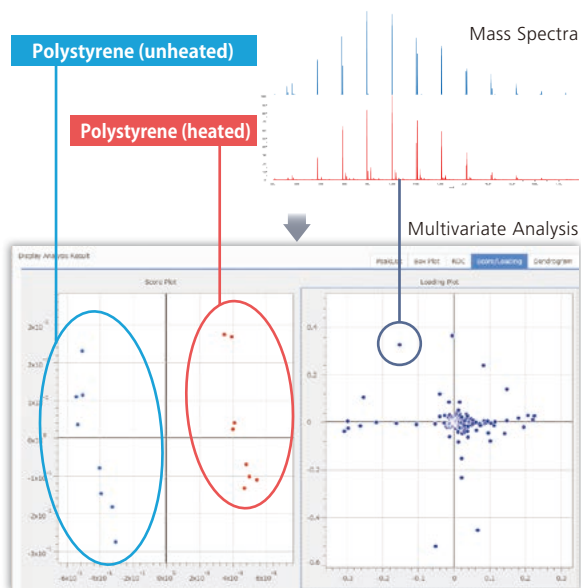
Workflow Using eMSTAT Solution



Applications

- Biomarker Discovery
- Sample Differentiation
- Discrimination of Unknown Samples

Identifying Degraded Synthetic Polymers



Polystyrene (heated and unheated) polymers were separated into two groups (heated or unheated) by multivariate analysis (PLS-DA) of the MALDI mass spectrum (Score Plot). A Loading Plot can be used to confirm which peaks (marker peaks) affect the differences between the two groups.



Experimental Conditions

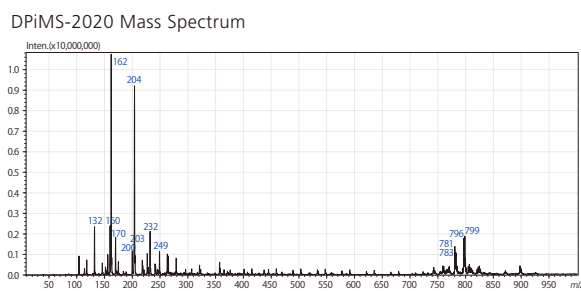
- Instrument: MALDI-8020
- Sample: Polystyrene 1,000 (heated for 2 hours at 200°C or unheated)
- Matrix: Dithranol
- Cationizing Agent: AgTFA
- Sample Preparation: The polystyrene (heated and unheated) dissolved in THF, matrix solution, and cationizing agent were spotted onto a sample plate.

Discriminant Analysis

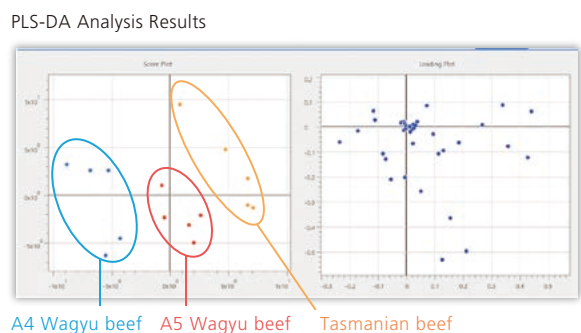
Sample Name & Result	Add Sample			
Select	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
Name	ps1000_test1_	ps1000_test2_	ps1000_test3_	ps1000_test4_
Group	ps1000	ps1000-heated	ps1000-heated	ps1000
Score	50	100	100	50
1013.7900	---	3985.4	88622.56	---
1117.9800	---	4164.21	88551.29	---
1222.1900	---	3538.89	73778.07	---
1326.5400	---	2200.28	54638.13	---
1430.8300	---	1174.1	36868.51	---
1535.1200	---	576.84	22255.33	---

Using marker peaks identified by multivariate analysis to create a discriminant model and discriminate (SVM) between heated and unheated polymers in a polystyrene mass spectrum, obtained separately, resulted in correct discrimination of all polymers. By using eMSTAT Solution in combination with MALDI mass spectrometry, which can easily measure samples with large molecular weight, in addition to synthetic polymers, a wide variety of samples, such as protein, fat, or sugar samples, can be easily differentiated.

Easy Differentiation for Beef Classification



Extracts from commercial beef (Tasmanian and A5/A4 grade Wagyu beef) were analyzed in a DPIMS-2020 mass spectrometer. The resulting spectra were then analyzed by PLS discriminant analysis. A Score Plot confirms grouping into three groups and a Loading Plot confirms which metabolite peaks affect grouping.



With eMSTAT Solution, spectra obtained by convenient metabolite analysis in a DPIMS-2020 spectrometer can be used to easily differentiate between differences in food, plant, and other samples, and screen for information about metabolites that contribute to differentiation.

Experimental Conditions

- Instrument: DPIMS-2020
- Sample: Edible beef
- Ionization Solution: 50% aqueous ethanol solution
- Sample Preparation: 10 µL of the suspension from homogenizing the beef for human consumption in the 50% aqueous ethanol solution was dripped onto a sample plate.

Specifications

	Item	Description
Analysis functions	Univariate analysis	t-test Mann-Whitney U test ANOVA (analysis of variance)
	Multivariate analysis	PCA (Principal Component Analysis) PLS-DA
	Discriminant analysis	Support Vector Machine (SVM) Random Forest
	Other	Dynamic grouping
Display functions	Multivariate analysis	Peak Matrix Box Plot ROC AUC Score/Loading Plot Dendrogram
	Discriminant analysis	Discriminant analysis results (group and score) Unknown samples superimposed on Score Plot
Input-output data	Input	ASCII format peak lists JCAMP format peak lists mzML format peak lists (only supports Centroid mode, 1 scan/per file, data uncompressed) <small>Note: File name must only contain half-width alphanumeric characters.</small>
	Output	Peak lists (txt format) Analysis results (xlsm format) Graph screenshot
Operating system	OS	Windows® 10 Pro, 64-bit (English/Chinese)



Visit MALDI-TOF MS series website:
<https://www.shimadzu.com/an/lifescience/maldi/index.html>



eMSTAT Solution and DPIMS are trademarks of Shimadzu Corporation.
 Windows is either a registered trademark or a trademark of Microsoft Corporation in the United States and/or other countries.



For Research Use Only. Not for use in diagnostic procedure.
 This publication may contain references to products that are not available in your country. Please contact us to check the availability of these products in your country.
 Company names, product/service names and logos used in this publication are trademarks and trade names of Shimadzu Corporation or its affiliates, whether or not they are used with trademark symbol "TM" or "®". Third-party trademarks and trade names may be used in this publication to refer to either the entities or their products/services. Shimadzu disclaims any proprietary interest in trademarks and trade names other than its own.

The contents of this publication are provided to you "as is" without warranty of any kind, and are subject to change without notice. Shimadzu does not assume any responsibility or liability for any damage, whether direct or indirect, relating to the use of this publication.

Shimadzu Corporation

www.shimadzu.com/an/