



Scientific / Metrology Instruments
Ultra-High Mass-Resolution MALDI-TOFMS System

Solutions for Innovation

JMS-S3000 SpiralTOF

Polymers & Materials Analysis Solutions



JEOL Ltd.

Analysis of Synthetic Polymers

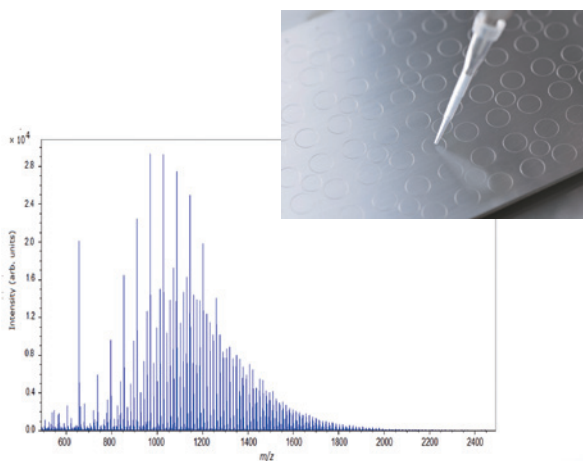
– from visualization to detailed analysis

Easy Ultra-High Mass-Resolution Measurement

A wide variety of target plates (384 or 96 spots, mirror finish or hairline finish, one time use) are available for a wide variety of samples (matrices, solvents, materials).

The msTornado Control instrument control and data acquisition software allows easy acquisition of ultra-high mass-resolution mass spectra.

The acquired data can be exported for further analysis using specialized polymer and material analysis software.



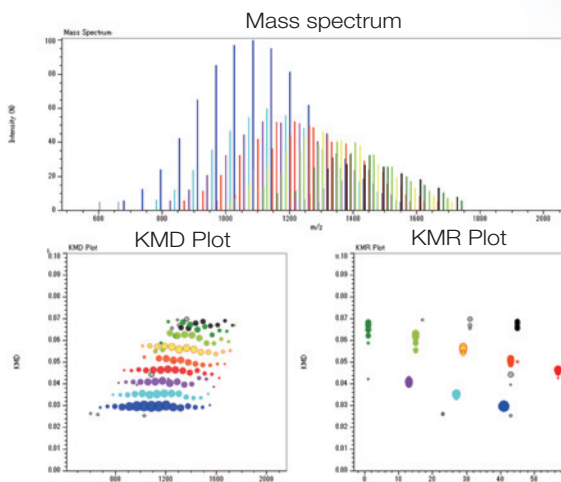
Visualize the details of the sample with a repeating structure without elucidating the elemental composition of every peak.

The **msRepeatFinder™** software is an application program for Kendrick mass defect (KMD) analysis.

A KMD plot visualizes the details of the sample with a repeating structure without elucidating the elemental composition of every peak.

A Kendrick Mass Remainder (KMR) plot helps with elucidating the end groups of homopolymer series.¹⁾

With the Grouping function, mass spectral peaks and KMD/KMR spots that belong to a homopolymer series with a specific end groups are displayed with the same color, facilitating the visualization of major as well as very minor components.



1) H. Sato, S. Nakamura, K. Teramoto, T. Sato, J. Am. Soc. Mass Spectrom. 25(8) 1346-1355 (2014)

Polymerix: a gold standard in synthetic polymer mass spectral analysis

Polymerix is a well established software package for polymer mass spectral analysis.

It calculates various average molar masses, polydispersity index, degree of polymerization, and helps with elucidating the elemental compositions of end groups.

It also presents the compositional distribution of a binary copolymer and calculates various statistics, including average molar masses, polydispersity index, and degree of polymerization, for various series in the binary copolymer.

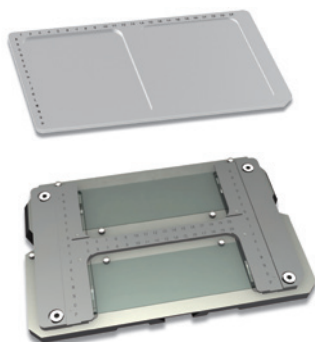
Compositional distribution of a binary copolymer

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Imaging Mass Spectrometry of Polymers and Materials

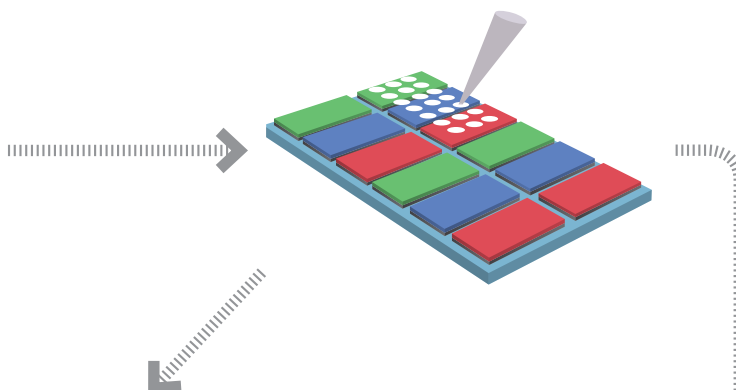


Holder for microscope slides and target plate for thick specimens (0.5 mm and 1 mm thick) available



2D Scanning Measurement

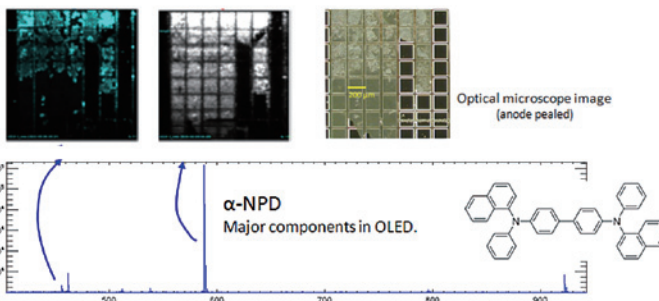
The msTornado Control software together with the MS Imaging Support Program perform 2D Scan data acquisition to obtain MS imaging data.



imzML – a common data format for MS imaging

The MS Imaging Support Program can convert the MS imaging raw data into imzML – a common data format for MS imaging, thus allowing the data acquired by the SpiralTOF to be processed by third party software, including BioMap and MALDIVision.

Anomalies observed by an optical microscopy can be compared with the MS images – highly effective for the analysis of foreign materials and defects.



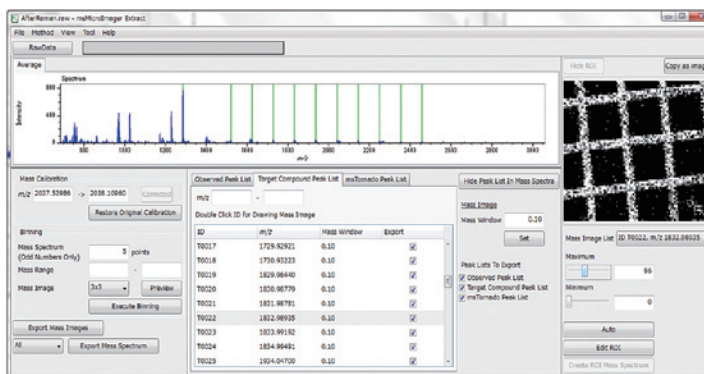
This data was acquired in a collaborative research effort with Asahi Glass Co., Ltd.

msMicrolmager™

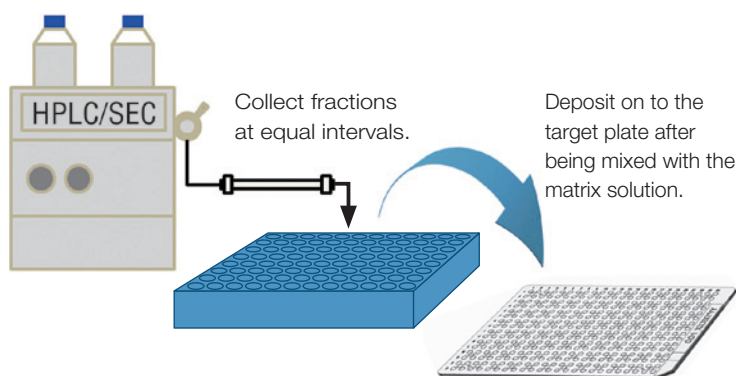
– software specifically designed for ultra-high mass-resolution imaging data

msMicrolmager™ can directly read and visualize very large, ultra-high mass-resolution MS imaging raw data acquired by the SpiralTOF.

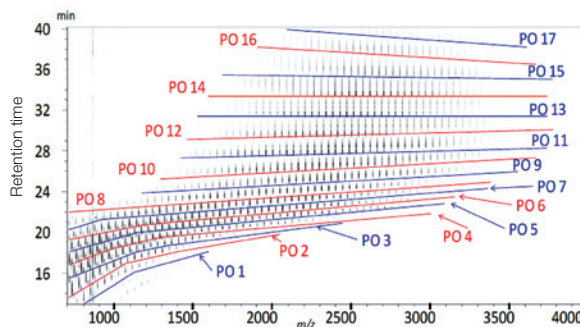
msMicrolmager can extract more than 100 MS images at once from a data set by giving a list of target m/z 's – making it convenient for the MS imaging of synthetic polymer samples.



LC-MALDI Applications



Analysis of EO-PO random copolymer



The msTornado™ Analysis software allows for the visualization and analysis of a series of mass spectra measured for HPLC and SEC fractions collected at equal intervals.

Fractionating a highly complex mixture sample with HPLC/SEC reduces ion suppression effects, thus facilitating the detection of many more components in the sample.

With a reversed phase HPLC separation, components were separated according to the number of PO units in each component.

List of software for polymers and materials analysis

Model Name		Description
msTornado™ MS-56510MP Main Program	Control	Manual and automated data acquisition. Automated data acquisition for a series of HPLC/SEC fractions (LC-MALDI). Data export.
	Analysis	Elemental composition elucidation. Isotope peak simulation. Mass spectral processing and annotation. Mass spectral comparison (stacking and overlay). Visualizing LC-MALDI data (the Survey View).
msRepeatFinder™ MS-56560REP Repeating Structure Analysis Program		Import peak list (centroided mass spectrum). Display a centroided mass spectrum. Display Kendrick mass defect (KMD) and Kendrick mass remainder (KMR) plot. Elucidate the mass of the end group.
Polymerix (Sierra Analytics, Inc.)		Elucidate elemental compositions of end groups. Calculate average molar masses, polydispersity index, and degree of polymerization of homopolymers. Display compositional distribution of the binary copolymer. Calculate average molar masses, polydispersity index, degree of polymerization, of various series in the binary copolymer.
MS-56530MSI MS Imaging Support Program		1D (line) scan and 2D scan (imaging) data acquisition. Convert MS imaging raw data into imzML format.
msMicrolImager™ MS-56550MSIV MS Imaging Viewer Program	Extract	Read MS imaging raw data acquired by msTornado Control. Perform pixel binning. Extract and export MS images. Export mass spectra of the regions of interest.
	View	Browse MS images. Change color map of the images. Perform arithmetic operations between MS images. Overlay MS images.
BioMap		BioMap is developed by and ©Novartis Institute for BioMedical Research (Basel, Switzerland) and available from the MALDI Mass Spectrometry Imaging Interest Group (MALDI MSI IG) web site at http://www.imzml.org/ .
MALDIVision		MALDIVision is a product of PREMIER Biosoft.

* Specifications subject to change without prior notice.

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