

Product Specification:

Progenesis MALDI v1.4

Data Import Specifications

- Supports the following data formats:
 - .mzXML
 - generic .txt files (mass and intensity)
 - Waters .RAW
 - Perkin Elmer pTOF data
 - Thermo .RAW
 - ProteinChip SELDI-TOF XML
- Ability to add/remove spectra after starting experiment
- Binning option to reduce data size for high resolution MALDI-TOF spectra

Spectra Pre-Processing

- Noise removed before alignment using the Savitzky-Golay filter
- Background removed before alignment using Top-Hat morphology filter or a Loess Smoothing algorithm
- Spectra displayed individually with before and after pre-processing profiles
- Multiple spectra display overlaid with processed profiles
- Greyscale representation of selected spectra under profiles
- Zoom in on pre-processing results

Spectra Alignment

- Unique alignment algorithm to create geometrically corrected spectra and generate consistent peak measurements between runs
- Multiple spectra displayed overlaid with processed profiles
- Greyscale representation of selected spectra under profiles
- Contrast control to highlight greyscale differences
- Before and after alignment spectra displayed side by side for visual comparison
- Zoom in on alignment changes

Peak Detection

- Automatic peak detection of aligned spectral data that creates a complete table of comparative intensities across all spectra, which means no missing values when calculating the statistical results
- Detection run on weighted average of all the aligned spectra

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- Special Isotope group detection method which highlights the mono-isotopic peak for high resolution spectra
- Manual peak editing
 - Additional peaks can be added
 - Peak edges can be moved
 - Superfluous peaks can be deleted
 - Move mono-isotopic peak position
 - Undo / redo editing
- Multiple spectra displayed overlaid with processed profiles
- Greyscale representation of selected spectra under profiles
- Contrast control to highlight greyscale differences
- Zoom in on peaks for editing

Analysis and Review Specifications

Technical Replicates

- Group spectra into samples according to experiment structure
- Name search facility to assist with replicate set up in large experiments
- Rename experimental samples
- Ability to add and remove spectra from experimental samples
- Ability to delete samples

Experimental group set-up

- Group samples according to experiment structure
- Ability to set up multiple experimental groupings, e.g. male v female, control v treated
- Name search facility to assist with group set up in large experiments
- Rename experimental groups
- Colour coding of experimental groups
- Ability to add and remove samples from experimental groups
- Ability to delete groups

Review peaks of interest

- Automatic highlighting of interesting peaks according to ANOVA p-values
- Peaks ranked by ANOVA p-value or fold change
- Switching between experimental groupings automatically updates all views
- Peak ID numbers remain consistent when experiment groupings are changed
- Tick / cross buttons to individually include / excluding interesting peaks
- Click and drag to select multiple peaks to be ticked / crossed
- Visible count of number of peaks ticked / crossed
- Automatically advance through peak list

Normalisation

- Optional normalisation of peaks using
 - Total Ion Current (TIC) of each spectra
 - Measurement of a single peak
- Normalisation data table showing TIC and normalisation factor

Peak tags

- Colour coded tags to assist with data exploration
- Right click on highlighted group of peaks to tag
- Add name label to peaks tag
- Filter peaks list by tags
- Tag editing
- Peaks can be tagged multiple times
- Peaks tags maintained throughout the workflow

Viewing options

- View montage of peak values per groups across the experiment
- Box plot of results for selected peak
- Data views / pictures can be sent to clipboard

Reporting

- Peaks selected for reporting using tag filtering
- Report title
- Report creation date
- Customisable reporting options include
 - Experiment design
 - Peak table
 - Peak number
 - ANOVA p-value
 - Fold change
 - Tags
 - Average Normalised Volumes
 - m/z
 - Peak details
 - Tags
 - Box Plot
 - Peak Montage
- Open report to view and print
- Save report to PDF format
- Export of measurements as .csv (commas separated value) file via File menu