

Progenesis MALDI

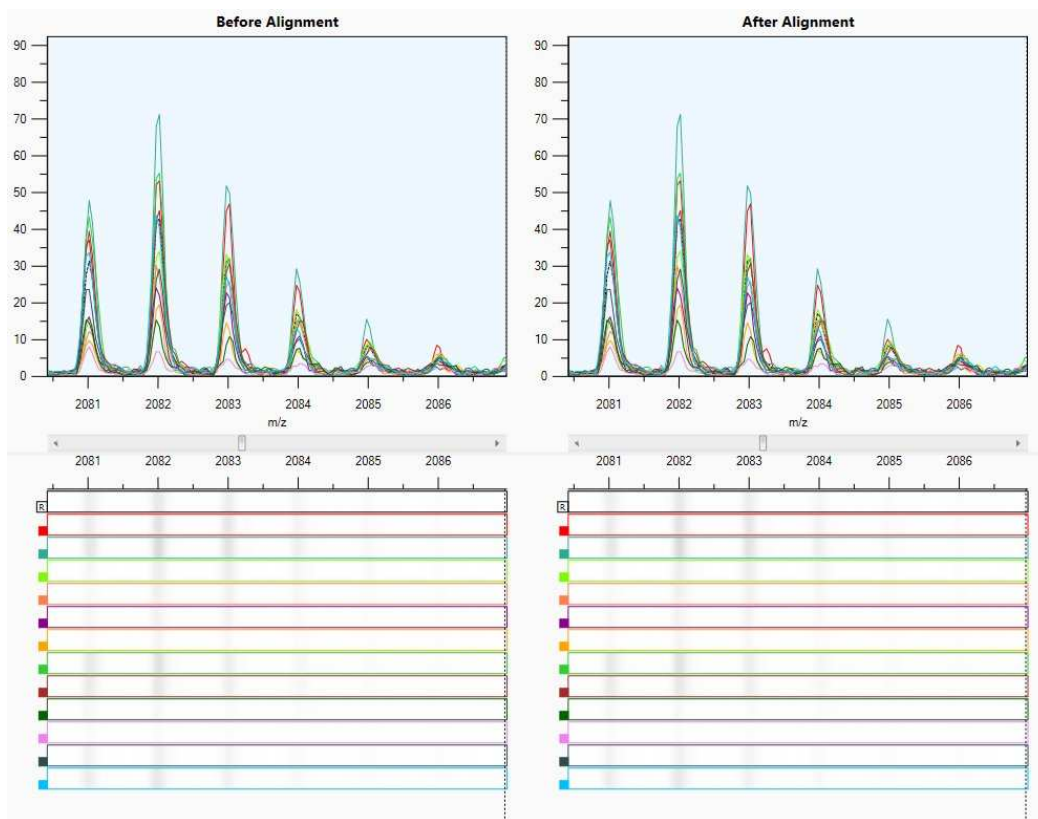
Fast & Easy Analysis of MALDI Mass Spectrometry Data

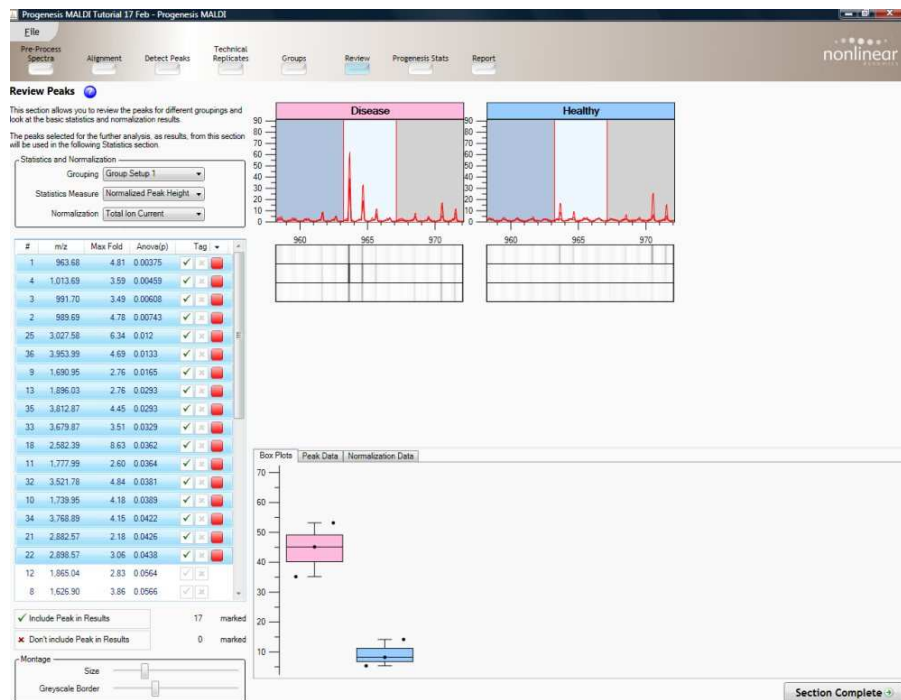
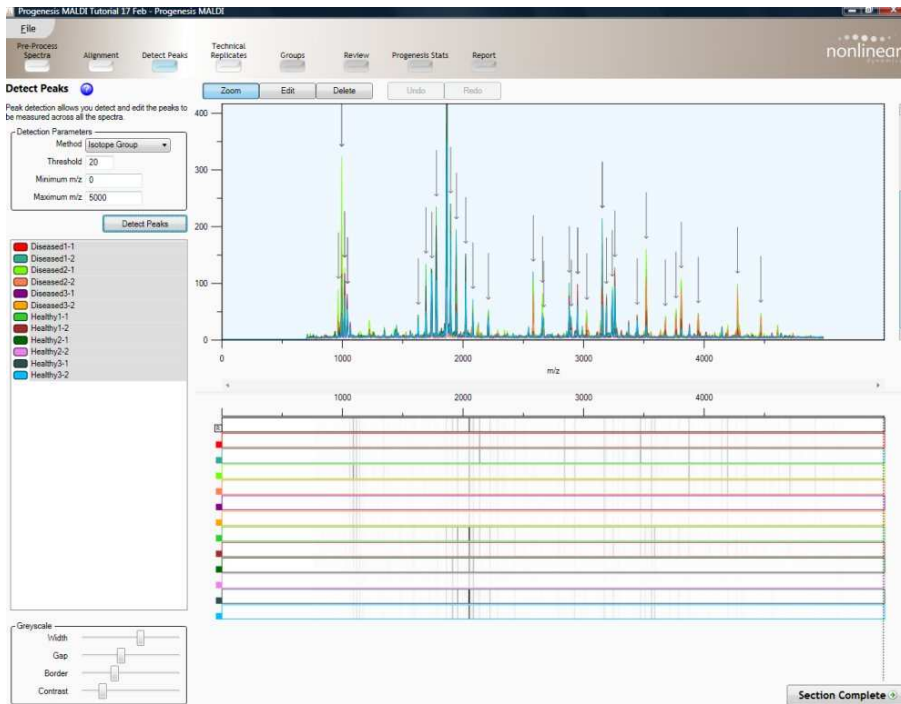
Discover the biomarkers in your proteomics data...

Progenesis MALDI is a simple to use application that gives you high quality proteomics data for biomarker discovery using MALDI-TOF or SELDI analysis. It uses the unique Progenesis workflow and technology to provide:

- **Speed** - Simple, rapid analysis of large data sets makes it easy for you to run enough replicates in order to minimise false discovery rates
- **Objectivity** - Guided workflow that helps you apply an objective, statistical-based analysis and run reproducible experiments
- **Statistics** - Unique spectra alignment process delivers a complete data set for multivariate statistical analysis

The first version of Progenesis MALDI allows you to try a unique workflow for biomarker discovery. Future versions will incorporate features based on your feedback; [contact us](#) to try it on your own data today.

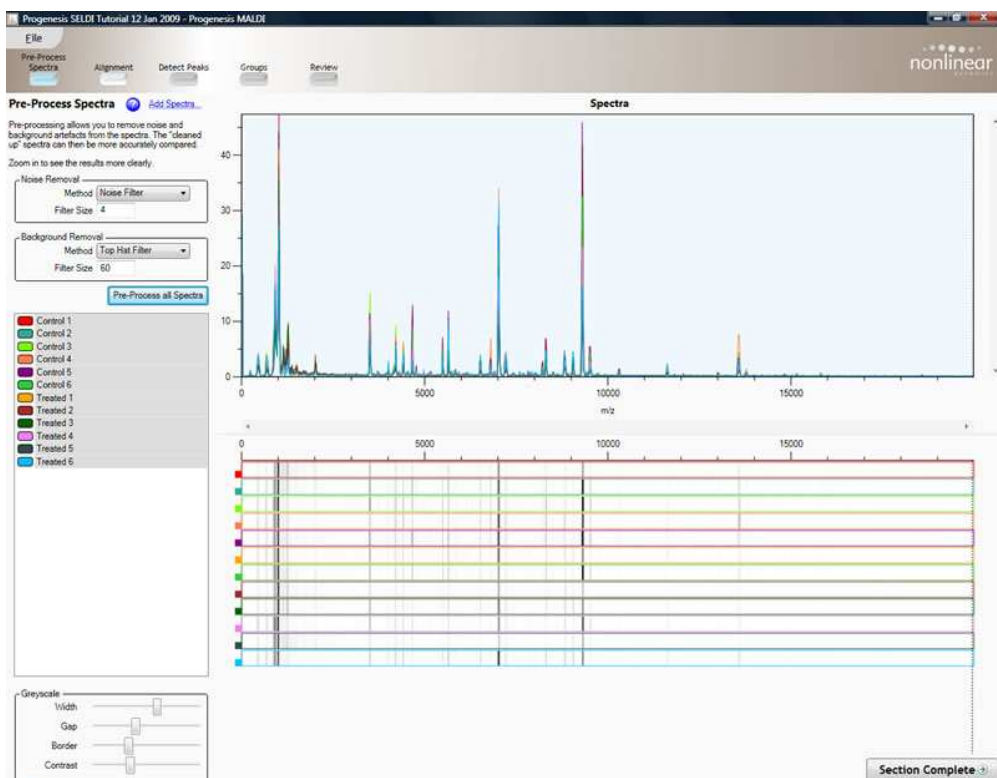
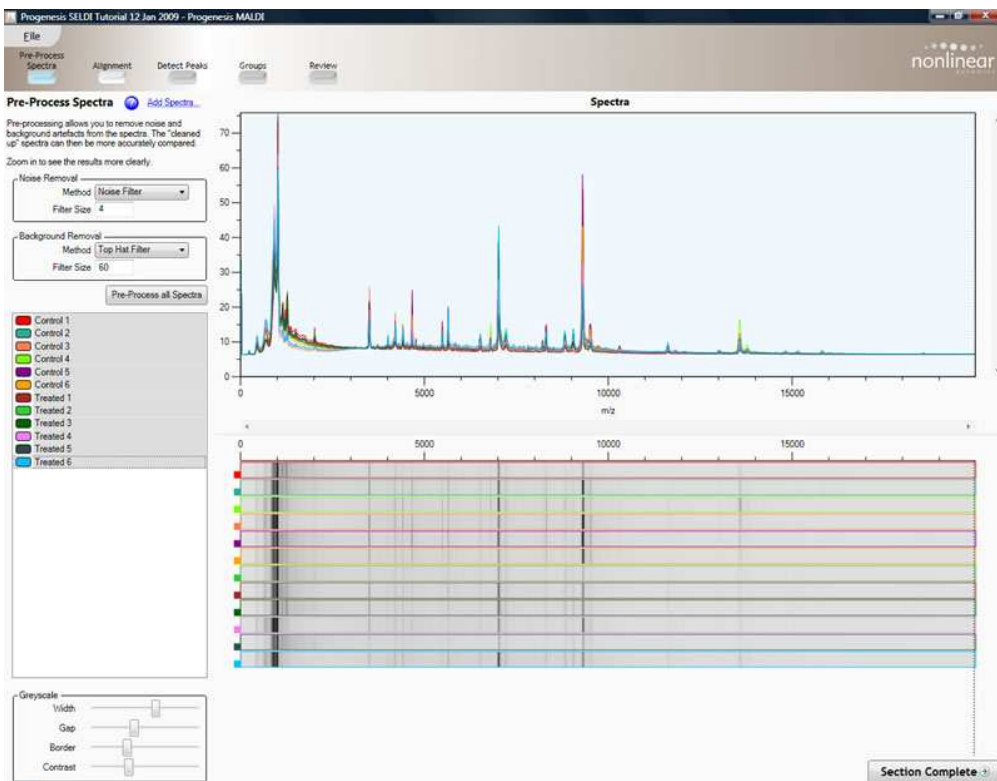




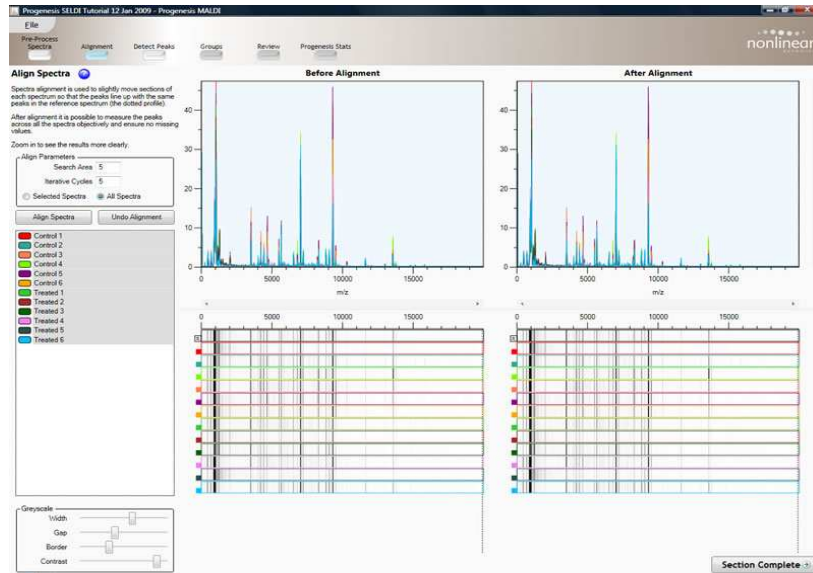
Progenesis MALDI v1.2 - unique analysis workflow

Import data - Load mzXML files, standard text file of mass vs. intensity data and ProteinChip® SELDI System XML files for simple integration into your existing workflow. The software allows hundreds of spectra to be analysed within a single experiment, so you can easily run enough replicates for biologically relevant conclusions.

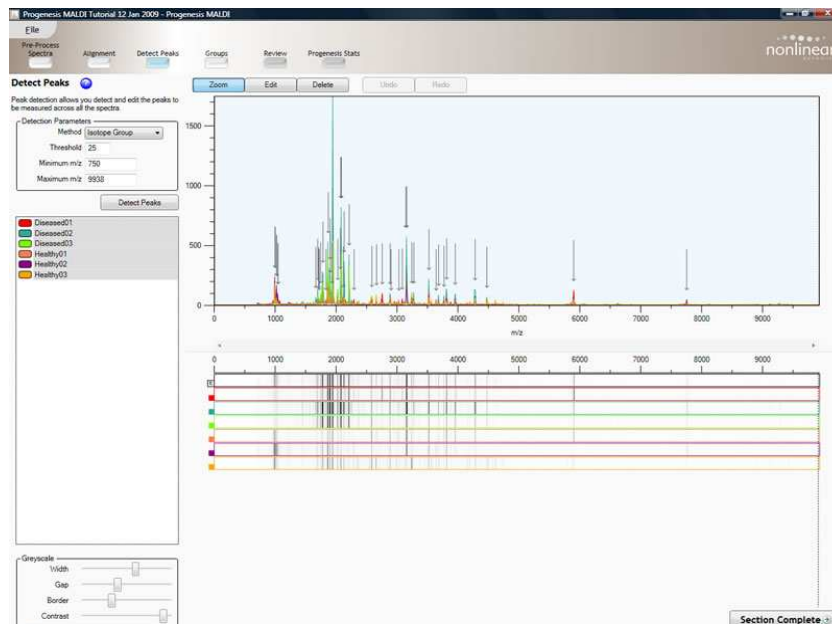
Pre-Process Spectra - This first stage of analysis removes noise and background from your spectra. Progenesis MALDI includes a noise filter and background removal methods using simple parameter settings to improve the input data for analysis.



Alignment - This unique step allows you to quickly align the peaks of your spectra. MALDI data is usually very well aligned in but there is the possibility that data from different labs or from later batches of spectra will have the mass of the peaks unaligned. Performing this step prior to analysis allows you to overcome any variation that can occur and generate a complete data set with no missing values for robust statistical analysis.



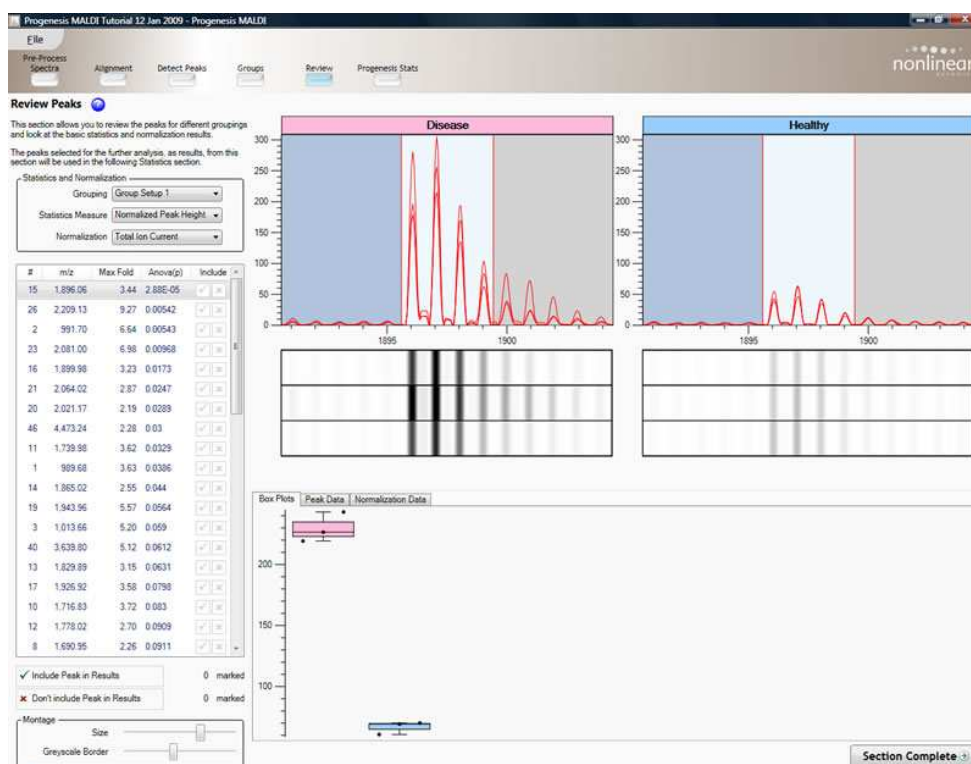
Peak Detection - With all the spectra aligned peak detection takes place on the average spectrum and you can specify the threshold for detecting the features you want to compare. Progenesis MALDI uses isotope patterns to detect the mono-isotopic peaks. The entire isotope pattern for each peak is then measured in the same position on each spectrum to ensure no missing values in the final analysis. You can also select whole protein detection for low resolution MALDI data. Editing options mean you can define the edges of peaks, merge peaks and optimize the m/z value for a peak.



Technical Replicates - Account for the technical variation within your MALDI-TOF analysis by creating an average spectrum from any technical replicates run for each sample.

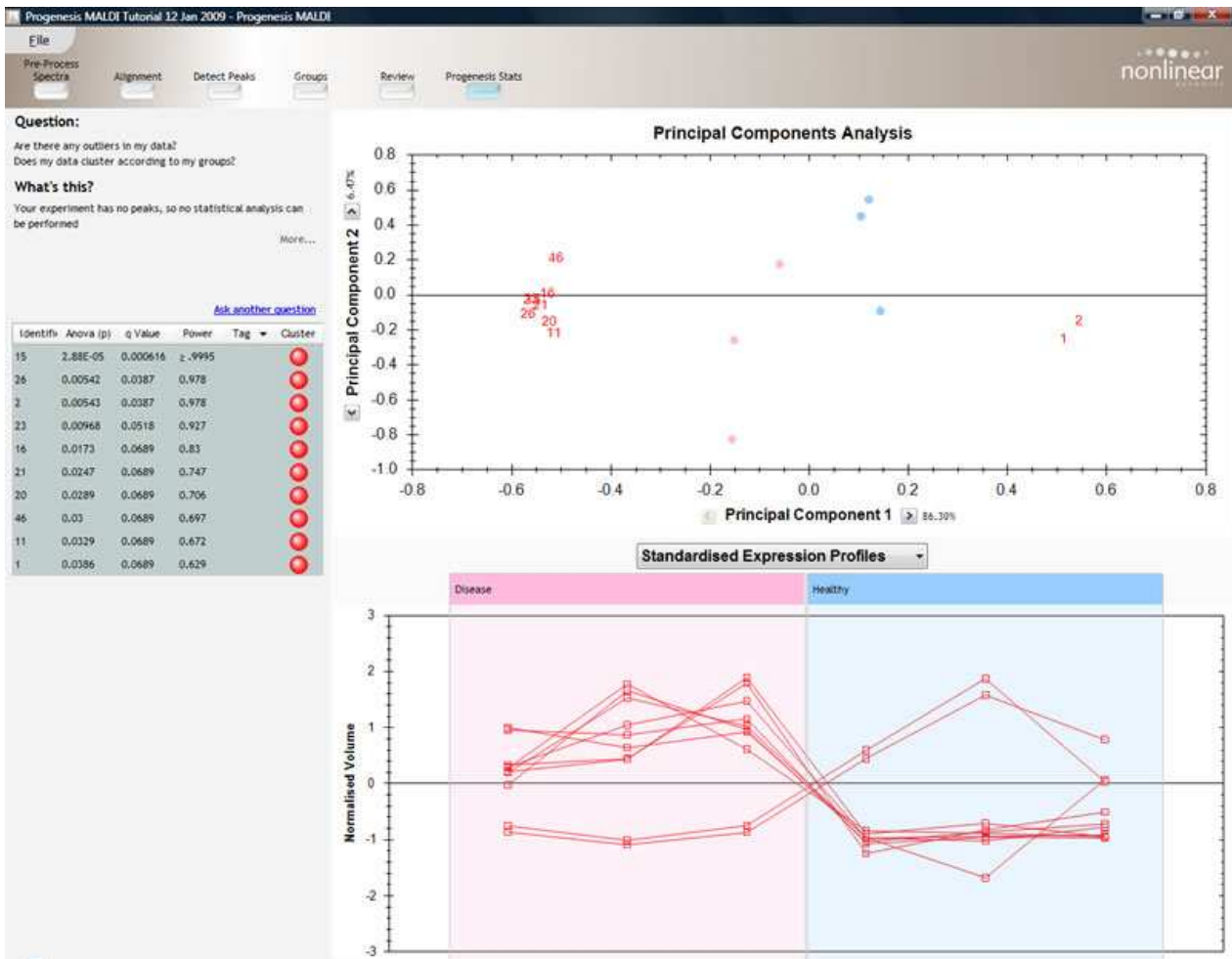
Create experimental groups - Create different groupings of the same data set to measure significant differences within the experiment based on user define criteria such as control vs. treated, male vs. female.

Review analysis results - The review stage allows you quickly review the features that have been measured as statistically significant within any groups you choose to compare. Box plots graphically represent the differences between the spectra for a selected peak. All the data at this stage can be copied or exported for you to generate presentations or for lab book information. Following the review stage, you can select peaks of interest for further investigation in Progenesis Stats.



Statistical Analysis - Progenesis Stats is a simple-to-use tool that allows you to easily apply powerful statistical analysis and make reliable conclusions. Principle Components Analysis (PCA), Correlation Analysis and Power Analysis are included to explore the trends in your data. The tests enable you to measure,

- How your data clusters within your experiment. This can validate the hypothesis used to create the experimental groups and indicate any outliers in your data.
- How similar features are in terms of their expression profile. This can help you find additional drug targets or other proteins involved in processes related to the one you're studying.
- The power of your experiment. This will tell you if you've run enough replicates for valid results and is increasingly becoming a requirement for publishing research in journals.



What is Biomarker discovery?

The major goal of biomarker discovery (or protein profiling) is to identify disease specific proteins/peptides, primarily from easily accessible bodily fluids such as serum, plasma and saliva. The technique of MALDI-TOF mass spectrometry is a reliable and efficient method of acquiring highly sensitive proteomic data from complex biological samples and is increasingly being used to gain insights into the mechanisms of disease and to monitor the success of a therapy. Widespread implementation of this technique is hampered by the lack of accurate, platform independent software available to researchers. Progenesis MALDI has been developed specifically for this application and simplifies the process of discovering specific and sensitive biomarkers from this abundance of MALDI-TOF spectral data.

Progenesis MALDI - Specifications

Data Import Specifications

- Supports the following data formats:
 - .mzXML
 - Generic .txt files (mass and intensity)
 - ProteinChip® SELDI-TOF XML
 - Waters instrument data
 - Perkin Elmer prOTOF™ data
- 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
- 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 alignment changes

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 and 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