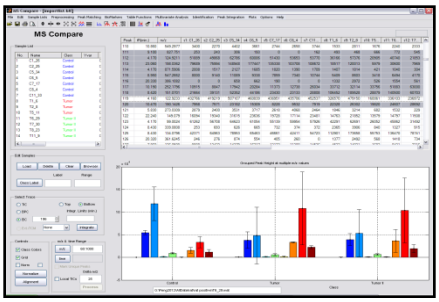
MsXelerator MsCompare v2.9

MsMetrix
Accelerating Data Analysis in LC/MS

LC/MS and GC/MS Data Processing Software

For BioMarker Discovery and Metabolomics Applications

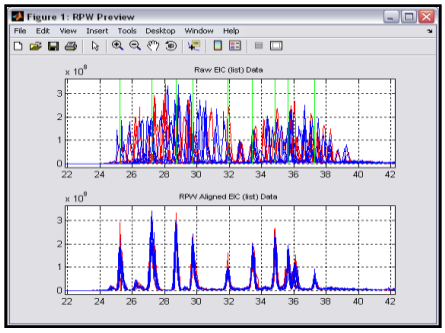
Mass Spectrometry (LC/MS) plays an increasingly important role in areas like BioMarker Discovery, Metabonomics and Metabolomics, due to its high sensitivity, rapid analysis and ease of identification. The **MsCompare™** software offers a large collection of tools, algorithms and visualization techniques for what in general could be called: **Comparative Analysis.** MsCompare offers all of the operations needed for processing LC/MS and GC/MS data sets and finding statistically significant differences between groups of samples:



Software Features:

Data Pre-Processing Tools

Quickly define your experiments and create multiple sample groups. All visualization tools in MsCompare offer coloring of individual samples based on group assignment. Pre-Processing Tools available are: baseline correction, smoothing, alignment etc. MsCompare offers visualization tools to decide whether normalization of your data will be necessary:

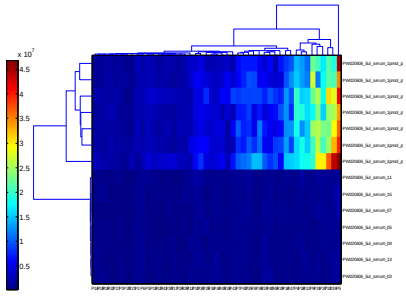


Alignment

Alignment of chromatograms will be necessary in cases that shifts between peaks in different samples are moderate or severe. Depending on the complexity of the samples, alignment can be very difficult and often results in non-optimal solutions. MsCompare offers 4 different alignment algorithms that can be used individually or sequentially.

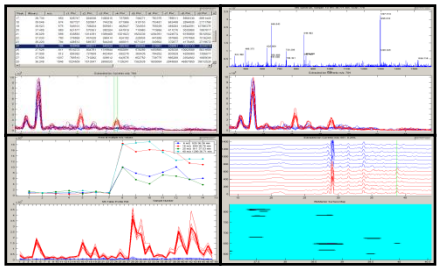
Peak Detection: Univariate & Multivariate Analysis

After Peak Picking or Peak Matching and clustering of all individual peaks from all samples, you can apply Univariate or Multivariate methods to find significant and relevant peaks that are different between samples from different groups. Apply univariate statistics like: p-and t- statistics, ratio group analysis, uniqueness values, Fisher Z-statistics or intensity weighted ratios. Create overview of all statistics in one table for all groups. Multivariate Analysis Tools include: PCA, PLS-DA, Support Vector Machines, ECVA, Hierarchical Clustering and Correlation Maps.



Visualization of results

Powerfull direct interactive viewing of extracted ion currents (EIC) and MS spectra from result tables produced by Peak Matching or Peak Picking. View data in overlay, stacked, normalized, raw or pre-processed. View results from the statistical analysis in many different graphical forms or as tables.



MsXelerator: ***Accelerating Data Analysis in LC-MS***

- **Drug Metabolite Profiling**
- **Differential Analysis**
- **Proteomics**
- **Biomarker Discovery**
- **GC-MS Data Processing**

MsMetrix

www.MsMetrix.com