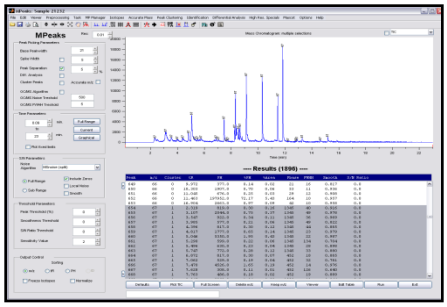
MsXelerator MPeaks v2.9

MsMetrix
Accelerating Data Analysis in LC/MS

LC/MS and GC/MS Data Processing Software

High Resolution Peak Picking and Differential Analysis: What are the differences between your samples

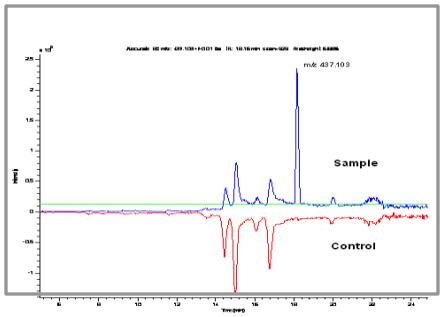
The core of the MPeaks Module are a number of high performance Peak Picking algorithms for LC/MS and GC/MS. MPeaks Peak Picking is extremely fast, easy to use and can be applied at any resolution and sensitivity. Peak Picking focuses on detection of *significant chromatographic peaks* from all Extracted Ion Currents (EIC). MPeaks results are clearly presented in peak tables, including many diagnostics on each detected peak. Results from MPeaks are the basis for many subsequent analysis tools available in the MPeaks Module, e.g. Differential Analysis and Identification.



Software Features:

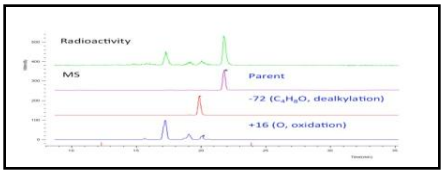
Fast and sensitive Peak Picking/Deconvolution

Determine accurate peak areas, peak heights, charge states and optionally convert all peaks to mono-isotopic mass. Group multiple charged ions, fragments and adducts into single components using fast clustering algorithms. Optimize High Resolution Peak Picking settings based on one single file. Next, run MPeaks on a large number of samples and output results to a combined peak picking list to be used for Comparative and Statistical Analysis.



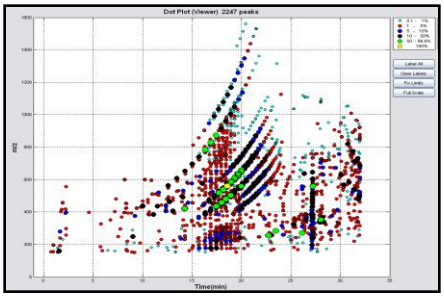
Comparative / Differential Analysis

Quickly find all differences between sample and control using Differential Analysis. Differential Analysis uses a shift tolerant algorithm to detect significant differences at any resolution. Ratios between sample and control, based on peak areas or peak height are reported and can be used for filtering results. Overlay detected differences from sample and control to validate results. Can be run on many controls simultaneously. Easy viewing of all MS spectra and extracted Ion currents.



Automatically identify all your detected Peaks

Link to existing or user created Metabolite ID data bases for Metabolomics applications, or with Mascot result files in case of Proteomics. Use pre-defined Biotransformation rules to identify potential metabolites from all detected peaks in drug metabolite profiling. Perform identification of deconvoluted MS spectra by direct linking to NIST MS Search libraries (GC/MS).



Pre-Processing and Post Processing Tools

Apply smoothing, baseline correction, Mass Defect Filtering or other filters to enhance the quality of the data. Remove isotopes, spikes and adducts. Run high resolution post-processing filters to get the answers you need.

Supports all major vendors: Thermo, Waters, Sciex, Bruker and Agilent.

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

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

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