

## MsXelerator Tutorials Overview

### Introduction:

Below a list of Tutorial Documents is presented, divided into main topics of LC/MS Data Processing. The tutorials are in addition to the tutorials found in the manual. The main manual can be found by clicking on the Help Menu in the Browser. The Tutorial documents are available from the zip file.

### Overview MsXelerator:

**Document: 1. MsXelerator2014**

PDF Presentation showing different applications of MsXelerator. Differential Analysis, Isotope Peak Matching, Searching for Biomarkers, MsX Quant Module, GC/MS QC-Quant and some Custom Applications.

### Metabolite Drug Profiling:

**Document: 2. MsX Metabolite\_Profiling\_Demo**

Drug Metabolite Profiling Examples: detection of Chlorine containing metabolites using IPeaks nominal search. Species Comparison using MsCompare and Multivariate Analysis.

**Document: 3. MsX Reactive Metabolite Detection\_Tutorial\_IPF\_II and Postprocessing Filters**

High Resolution Isotope Pattern Filtering using the IPF II algorithm (directly search raw ms spectra) based on GSH labeling pattern (labeled/un-labeled GSH). This tutorial also demonstrates how to use High Resolution Post Processing to remove false positives, e.g. peaks that are also found in a control sample. Includes Identification based on common Biotransformation rules. See also the Differential Analysis Section.

### Differential Analysis: comparing Sample/Control or Groups of Samples

**Document: 4. MsX Differential Analysis two samples**

Demonstrates how to use MPeaks for finding relevant differences between two samples, typically applied when comparing a sample and control. MPeaks contains four different algorithms that are explained, from nominal to high resolution. Includes examples how to use alignment in cases where the sample and control show severe shifts between peaks.

**Document: 5. MsX Differential Analysis two Groups/Classes**

Example of Biomarker Discovery/Comparative Analysis using MsCompare. Shows example how to detect significant differential peaks between two groups or classes, e.g. control/disease or treated/non-treated. Includes alignment of samples that show severe shifts.

**Document: 6. MsX High Resolution Peak Matching using MsCompare**

Targeted Analysis of any number of ions and samples in High Resolution Mode. List of ions is based on Peak Picking

done in MPeaks a from a user imported list of ions. Includes alignment of samples. Then apply Univariate and Multivariate tools to find differences between the sample groups.

## Proteomics (Quantitative):

See the documents on Differential Analysis:

**Document:** 7. *MsX MS Protein Deconvolution*

Tutorial on how to use MS Spectrum Deconvolution Tool to estimate the molecular weight of multi charged protein peaks . Show nice overview of all calculated charge states and Molecular Weights. Also determines the deconvoluted MS spectrum in detail.

**Document:** 8. *MSX Quant.pdf*

Tutorial on how to use MsX Quant (IPeaks) for relative quantitation of SILAC Labeled Peptides.

## Chromatographic Alignment:

**Document:** 9. *MsX Demo\_Reference\_Peak\_Warping LC/MS I*

Updated version of Reference Peak Warping. Demonstrates how to use automatic Selection of reference peaks to be used for alignment in MsCompare.

## Impurity Profiling LC/MS and GC/MS:

**Document:** 10. *MSX Tutorial\_ImpProfiling*

Examples of how to use MPeaks for impurity profiling and peak purity analysis, including identification and MPeaks graphics features for comparing of peaks.

**Document:** 11. *MSX Tutorial\_ImpProfiling\_II*

Additional examples of impurity profiling and peak purity analysis.

## GC/MS Data Processing:

**Document:** 12. *MsX GCMS\_Features*

Demonstrates the use of MPeaks for impurity profiling of GC/MS data. Includes Peak Picking, Clustering of fragments into components. Also demonstrates a Metabonomics example using MsCompare to detect differential peaks between two groups of samples. Ask for the Manual on GC/MS QC Quant.

**Document:** 13 *MsX GCMS QC-Quant*

Manual of GC/MS QC Quant Module: demonstrates GCMS Quant for Metabolomics; Quality Control and Data Processing, see website for more information.