



South Bohemian  
Research Center  
of Aquaculture  
and Biodiversity  
of Hydrocenoses



**This work was supported and co-financed by project Aquaexcel.**

**Name of software (Czech):** Expertomica Metabilite Profiling Hi-Res

**Name of software (English):** Expertomica Metabilite Profiling Hi-Res

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## Description

The software was developed for analysis of datasets with high resolution from Liquid chromatography – mass spectrometry. It works with several ascii and xml datafiles. Native Matlab and specified cdf files are also supported. Application performs precision and resolution estimation, mass peaks centroidisation, unsupervised noise and mobile phase removal, iterative peak deconvolution and confidence factors evaluation. No information is lost during the processing. Program enables graphical user interface with basic plotings (Total Ion Current chromatograms and Mass spectra) of raw, processed and resulted data.

## Input Data

The software processes the Liquid chromatography – mass spectrometry datasets from following file formats:

Bruker Daltonics text file (\*.ascii)

ANDI-MS netCDF (\*.cdf)

Tab separated values (\*.csv)

Data analysis file (\*.dta2d)

JCAMP-DX Data (\*.dx)

HUPO-XML (\*.mzdata) - external convertor required ([www.openms.de](http://www.openms.de))

ASMS XML (\*.mzML) - external convertor required ([www.openms.de](http://www.openms.de))

SPC/ISB XML (\*.mzXML) - external convertor required ([www.openms.de](http://www.openms.de))

Thermo text file (\*.txt)

Matlab mat file (\*.mat)

## Output

Ascii table of detected peaks information (\*.prt).

## Installation

You can download the last version of the software from [here](#) and unpack to selected directory. Please open in your favorite browser and read the included 'edahelp.html' instalation and user guide file.

### **The installation contains:**

eda.exe - the software

vc redistrib\_x86.exe - Visual C++ 2005 Redistributable Package

edahelp.html – instalation help and user guide

Yuo can also downlad testing dataset from

[http://pepkac.sweb.cz/e2737n17\\_nystatin0.05mg\\_ml.mat](http://pepkac.sweb.cz/e2737n17_nystatin0.05mg_ml.mat)

## Requirements

**Operation system:** Windows XP, Vista (32 bit) and 7 (32 bit)

**Software:**

Visual C++ 2005 Redistributable Package (included in installation)

Matlab Compiler Runtime 7.9 (available at <http://sourceforge.net/projects/expertomica-eda/files/Matlab%20R%29%20Compiler%20Runtime%207.9/7.9%20Win32/MCRInstaller.exe/download>)

## **Hardware**

The software require at least 1 GB of memory (exact amount depend on the size of datafiles) and space for temporary files at drive c:\. The amount of temporal space required equals approximately the double size of raw input file.