

Expertomica Metabolite Profiling Hi-Res

1. Introduction

EDA is Graphical User Interface and Matlab compiled application for analysis of both low and high resolution LC-MS datasets. The software works with several ascii and xml datafiles 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.

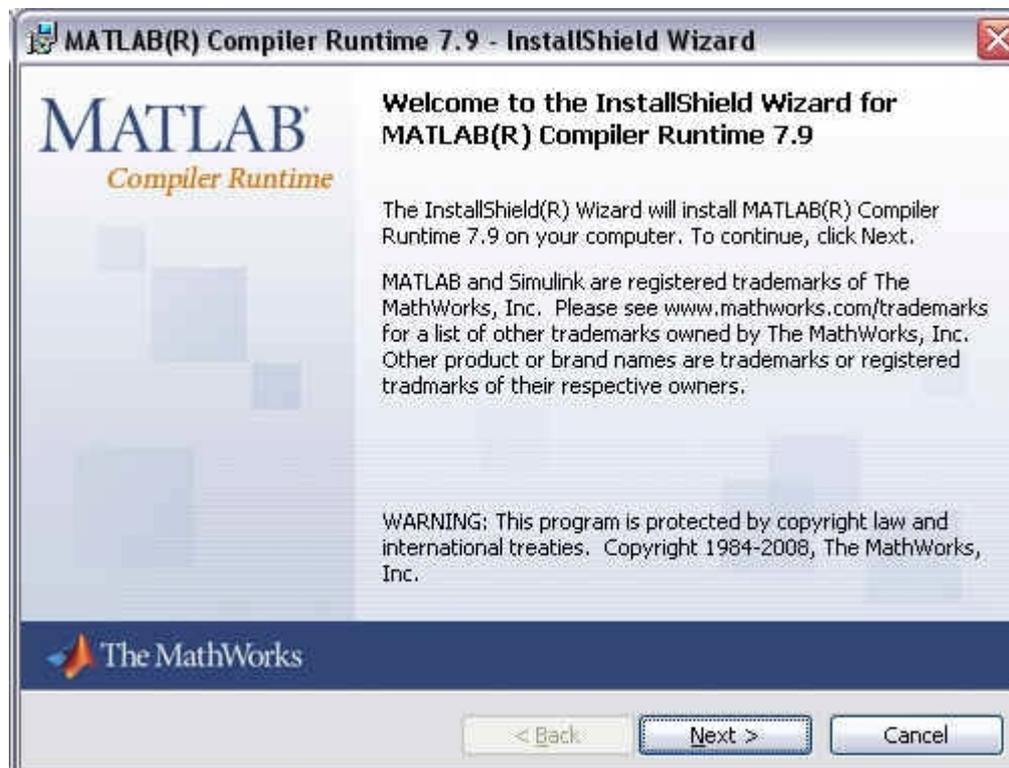
Optimal RAM size installed on computer is 1GB or higher, speed of computations decrease rapidly with less amount of memory (caused by swapping).

Blank analysis is not supported in version 1.7.

2. Install

a) Install Visual C++ 2005 Redistributable Package running vcredist_x86.exe

b) Install Matlab(R) Compiler Runtime 7.9 running MCRInstaller.exe.



and follow the instructions



c) Reboot your computer

d) Unpack all files from `eda.zip` into your folder.

e) Only if you want to read xml files:

I. Download OpenMS from www.openms.de and install

II. Create subdirectory 'fc' in your eda directory.

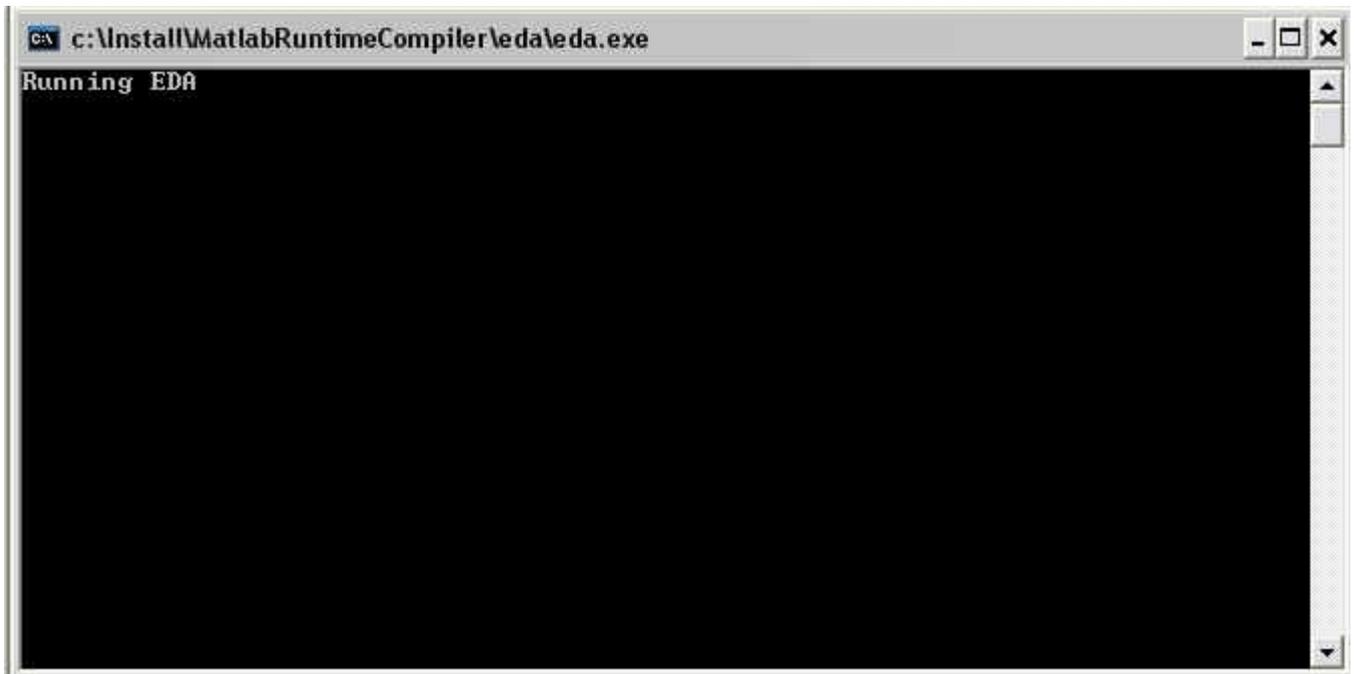
III. From `c:\Program Files\ OpenMS directory\bin`

copy files: `FileConverter.exe`; `QtCore4.dll`; and `QtGui4.dll` into your `eda\fc` directory

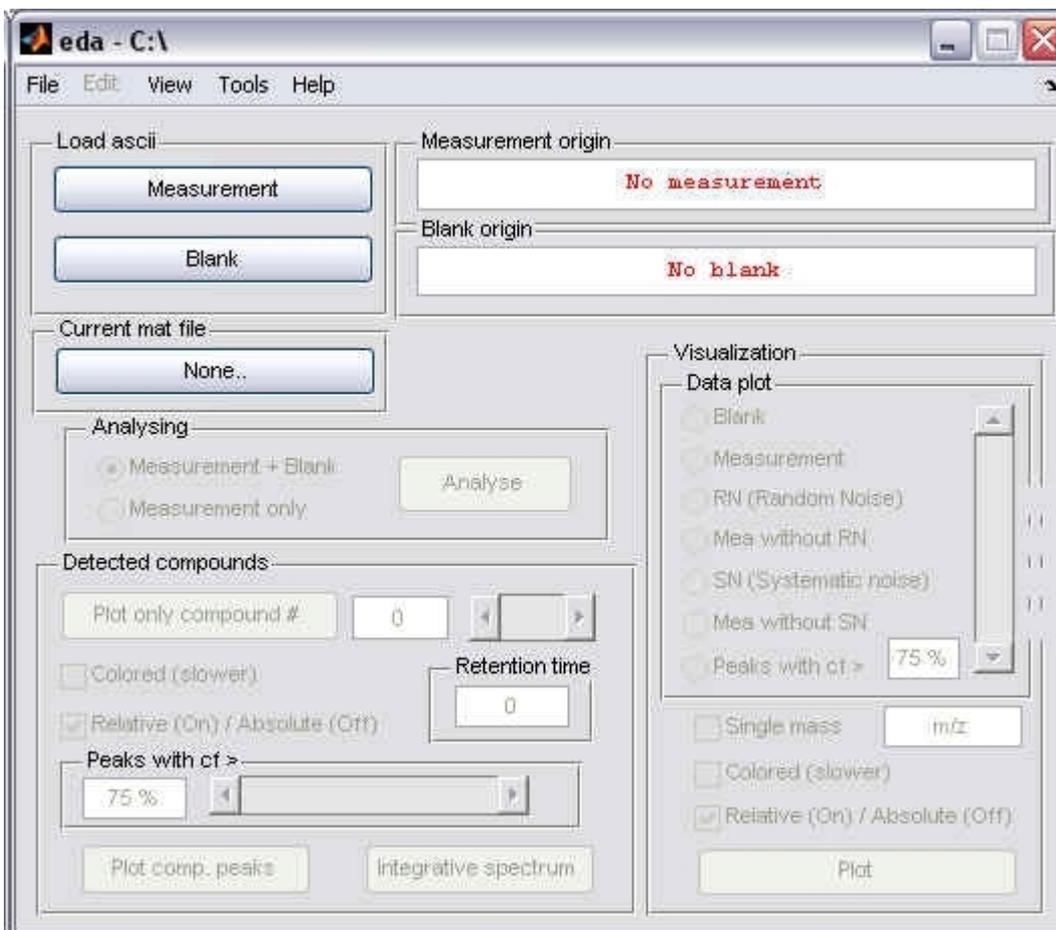
3. Start application

Run `eda.exe` and press Enter, You will see a command line window

(do not close - closing command line window will terminated whole application!)



and main window of EDA.



Initialisation may take a while.

4. Insert measurement into application

EDA can currently read 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)

ASMS XML (*.mzML) - external convertor required (www.openms.de)

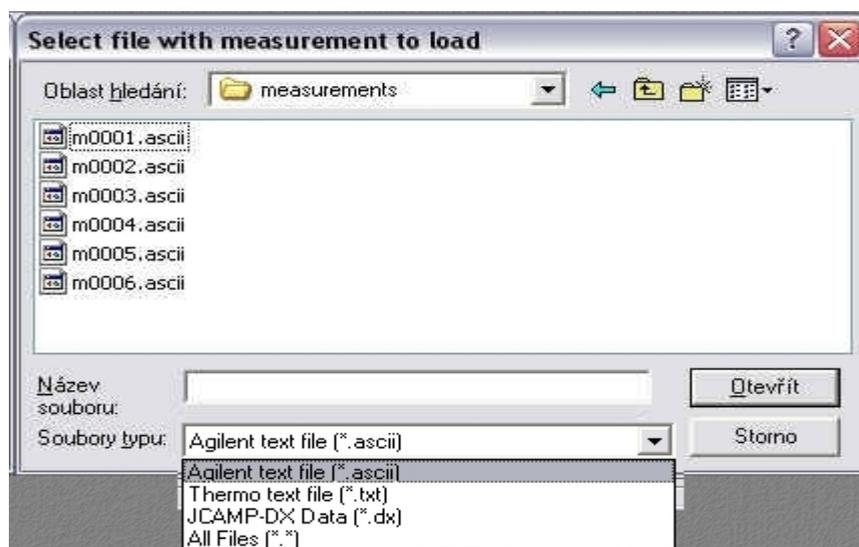
SPC/ISB XML (*.mzXML) - external convertor required (www.openms.de)

Thermo text file (*.txt)

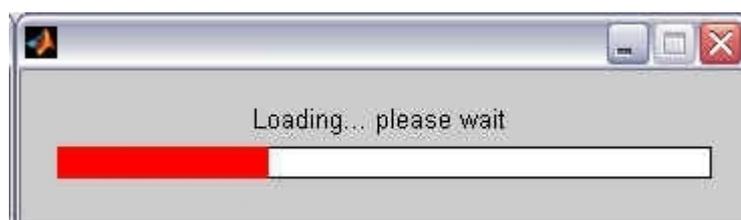
Matlab mat file (*.mat)

(see authors web page for new version or directly contact them for implementation of Your own file format).

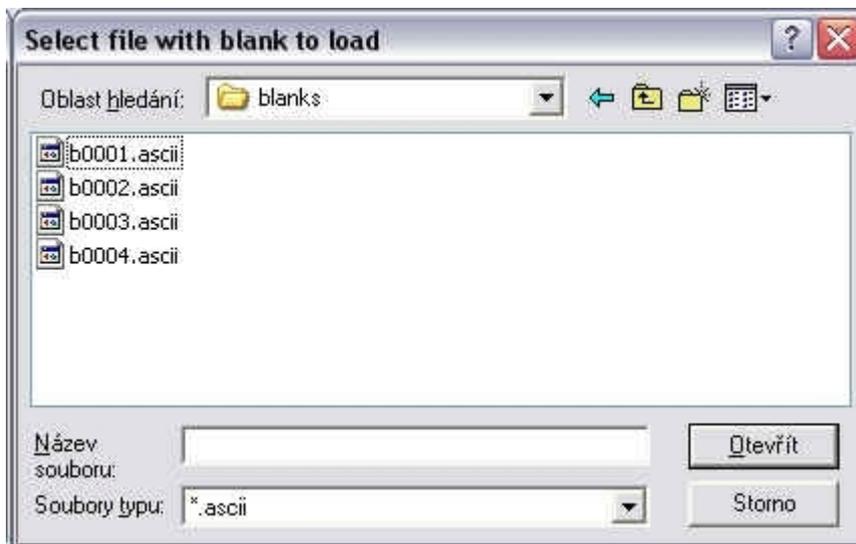
From menu `File \ Load Measurement` (or use button `Measurement` from panel `Load ascii` in EDA main window or hotkey **ctrl+m** instead) select ascii file with Your measurement in one of the supported formats and confirm.



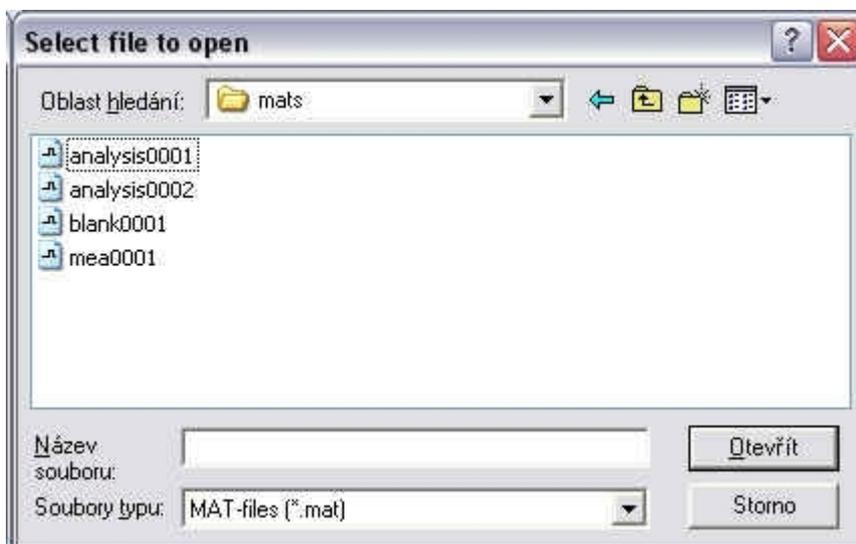
Loading ascii into data matrix takes a while, You will see a progress bar during process.



For loading blank (measurement without sample) use menu `File \ Load Blank` (or button `Blank` from panel `Load ascii` in EDA main window or hotkey **ctrl+b**), select Your ascii file and confirm. Again, You will see a progress bar.



Once You have saved the data in `mat` file (Matlab format, see **5. Save dataset** for details), You can also load it. From menu `File \ Open mat` (or button in panel `Current mat file` in EDA main window or hotkey **ctrl+o**) select `mat` file with Your dataset and confirm.

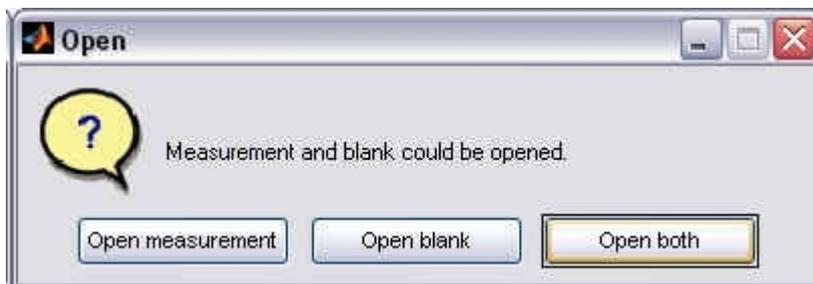


Application will check data integrity and content. Depending on Your decision during previous saving, can be opened one of this items:

- Data with Analysis - measurement (and blank, if available) with computed probabilities, list of segmented compounds and its peaks



- Data only - blank or measurement or both (if available).

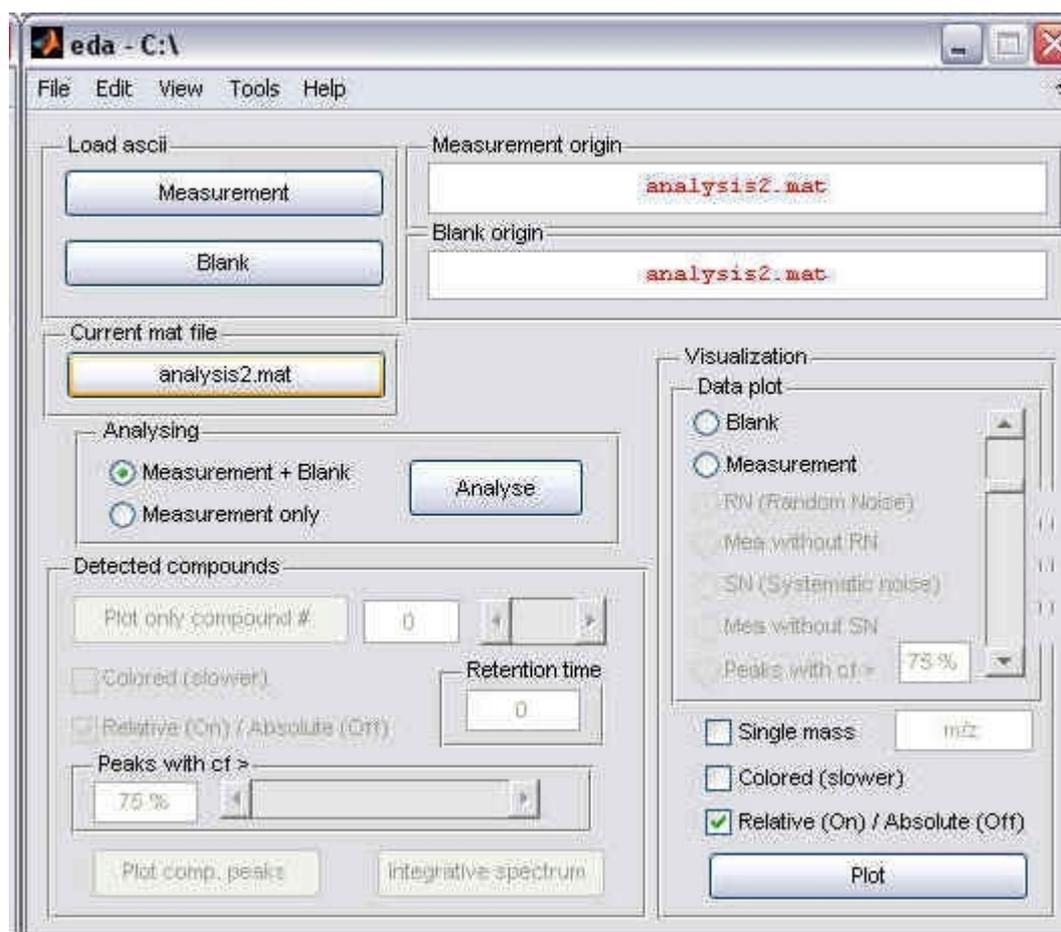


EDA will automatically ask You according to dataset presented in mat file.

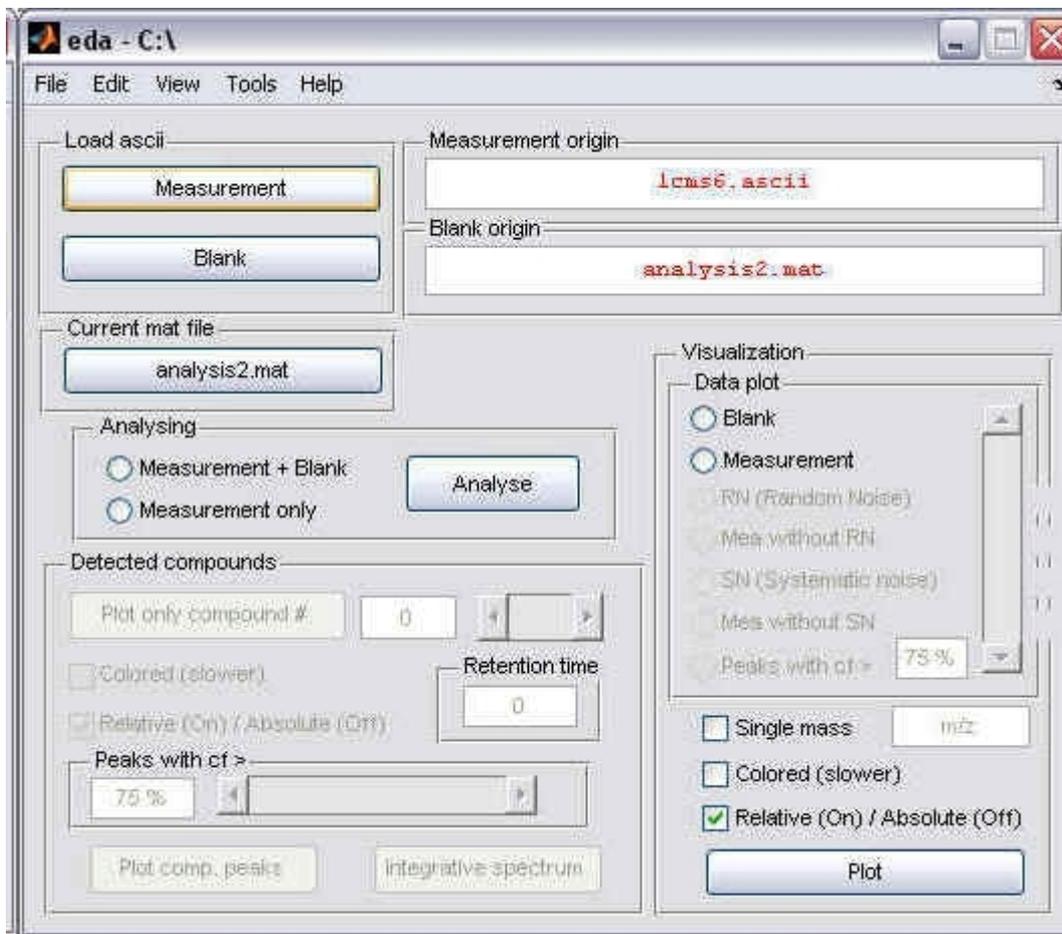
In panel Measurement origin You will see name of file with currently opened/loaded measurement (No measurement for none). Measurement can be loaded from ascii file or opened from mat file.

In panel Blank origin You will see name of file with currently opened/loaded blank (No blank for none). This option is not longer supported (see authors web page for new version).

On button in Current mat file panel You will see name of currently opened mat file (None . . . for none)



You can easily combine data from loading ascii and opening mat, for example: load measurement from ascii file and open only blank from mat file (mat file may include different measurement).

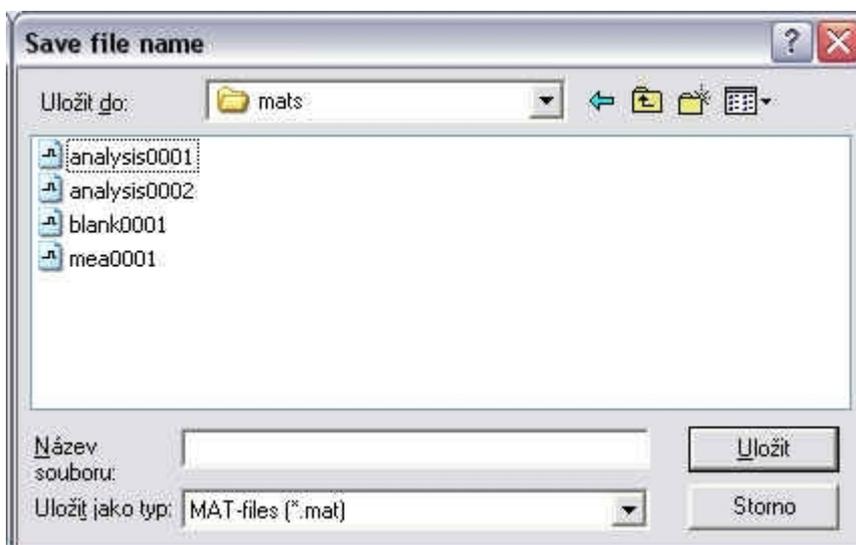


5. Save dataset

Loaded measurement or blank or both from ascii file can be simply saved in menu `File \ Save Data (M or B)` (or hotkey **ctrl+s**). Select name (default name is same as loaded ascii file, only extension is replaced by mat), where You want to have dataset stored and confirm.



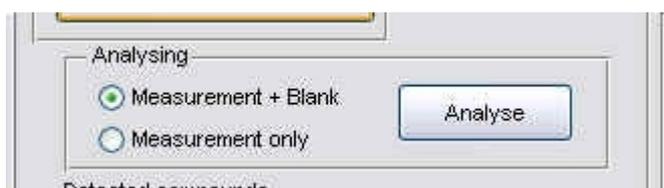
Computed analysis (see **6. Analysing**) of measurement (or measurement with blank) can be also saved as mat file. Measurement and blank (if available) used for analysing are stored together with analysis. From menu `File \ Save analysis (+Data)` as and select name for mat file to storage Your dataset and confirm.



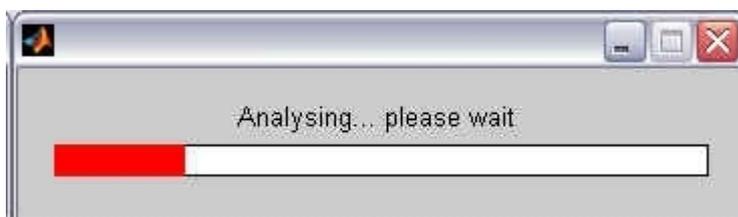
EDA may stop responding to other actions during saving process.

6. Analysing

After loading or opening measurement or measurement with blank or analysis dataset, EDA enables panel Analysing



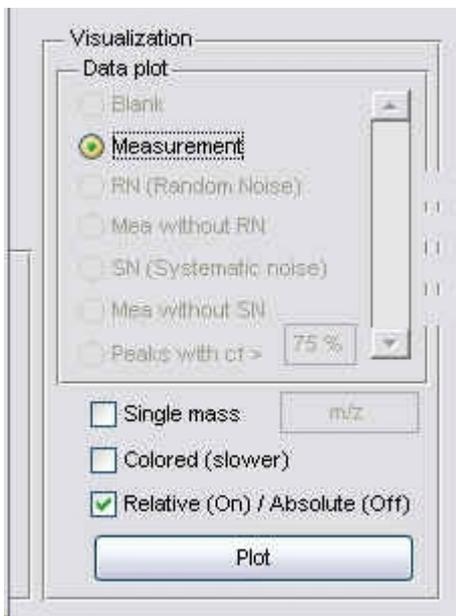
where You can choose by radiobuttons analysis of Measurement + Blank or analysis of Measurement only (depends on opened/loaded dataset). Analysis itself is started by clicking button Analyse in the panel. Computation of all analysing methods, filtration, probabilities computation, peaks and compound segmentation is indicated by progress bar. Speed depends on computer memory and processor frequency.



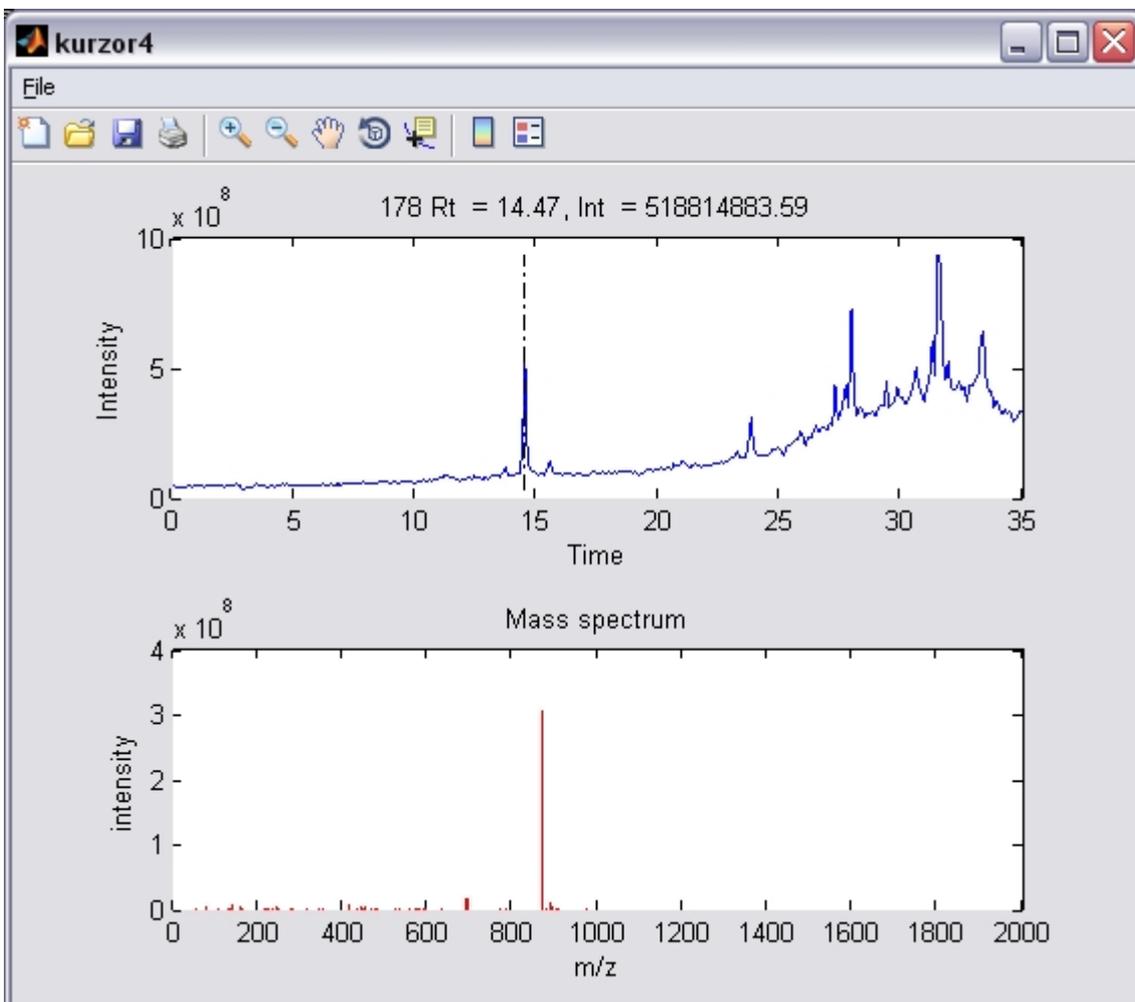
When analysing process finished, EDA enables two result panels - Detected compounds and Visualization (For detail information see 7. Visualization or 8. Peaks and Compounds).

7. Visualization

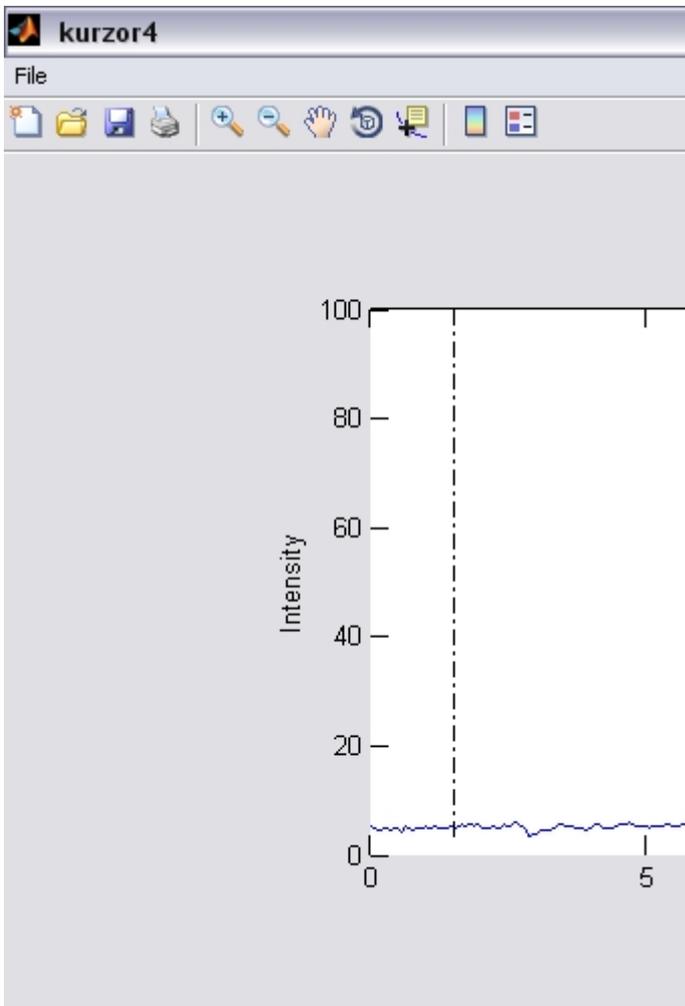
Loaded measurement or blank can be plotted using radio buttons in subpanel Data plot in panel Visualization, where you can also choose the type of data visualised from the measurement or blank.



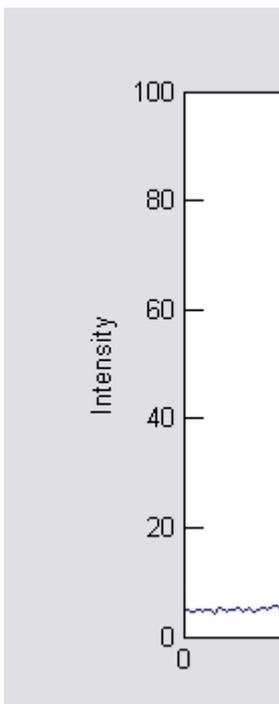
All plots are figured after clicking the button `Plot`. You will see a new figure with two subplots, upper one for TIC (Total Ion Chromatogram) and lower one for mass spectrum.

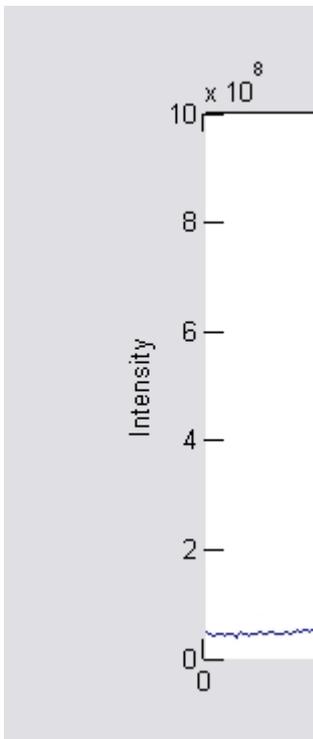


Use mouse right button in TIC to select exact time in upper figure for plotting related mass spectrum in lower figure.

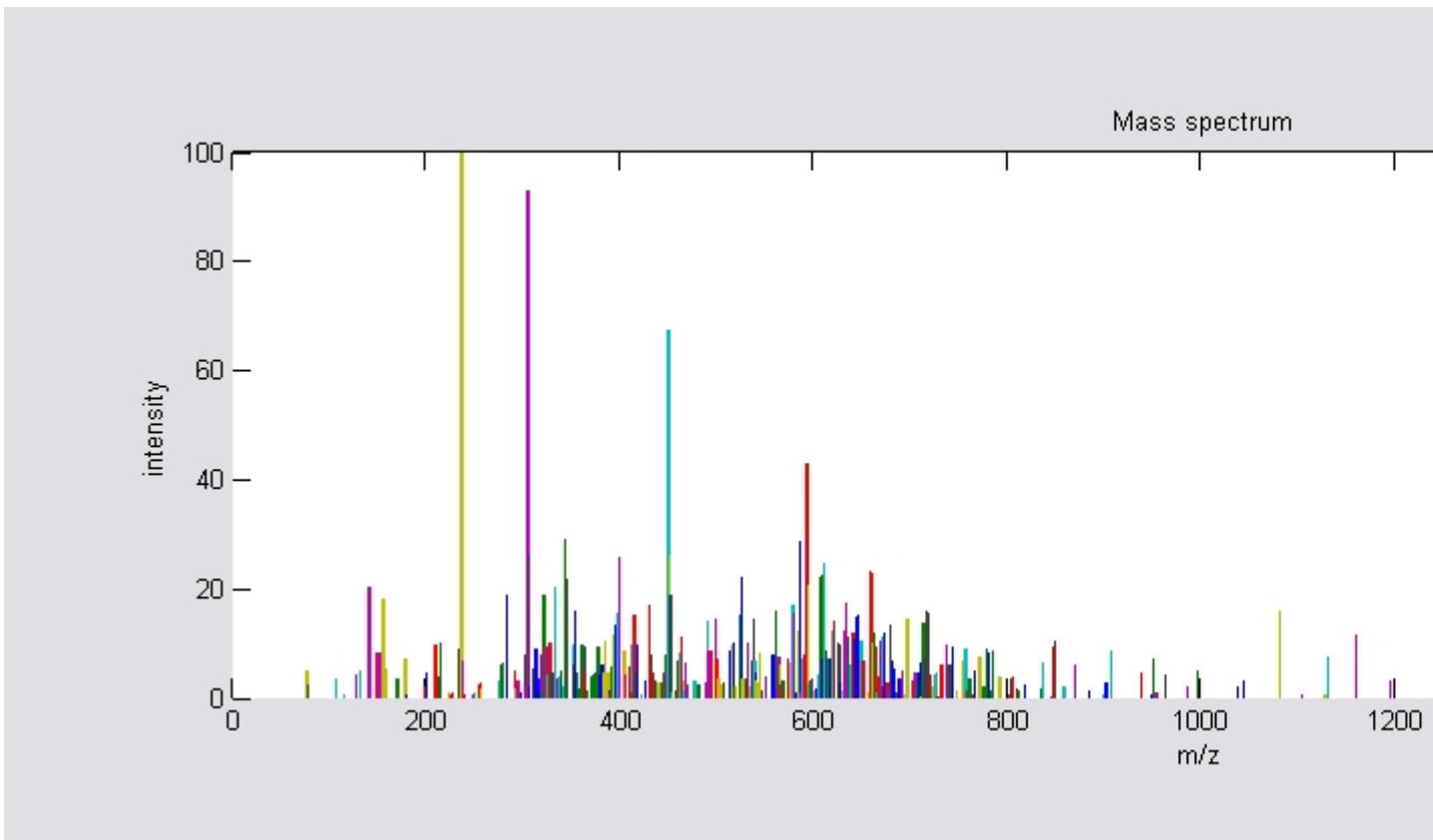


a) Check box Relative (On) / Absolute (Off) determine scale on y axis.





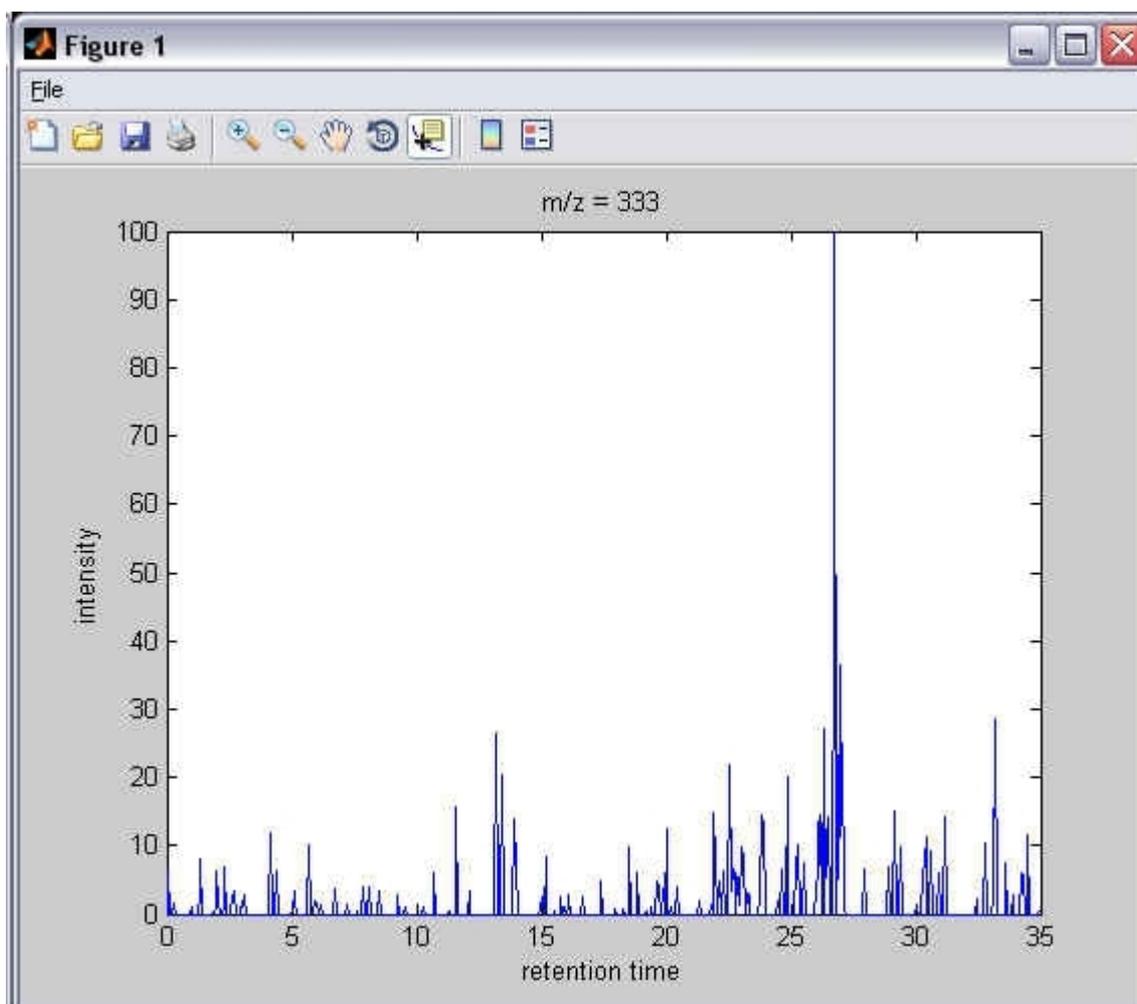
b) Check box Colored (Slower) determine using different colours for bars in mass spectrum. This option require little bit more computer memory to proceed.



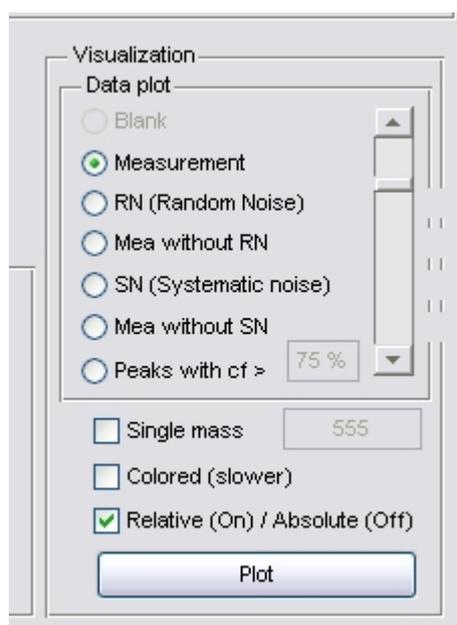
c) Check box Single mass allow to plot selected m/z value in time.



No mass spectrum will be plotted for single mass (it is nonsense).



After finishing analysis of Your data, more radio buttons will be enabled in Data plot subpanel.



All check boxes are the same as in previous case. Using different radio buttons You can plot contribution of Random noise or Systematic noise (base line) in Your measurement as well as Measurement without random noise or Measurement without systematic noise (means without both noises, random noise was removed before the algorithms for systematic

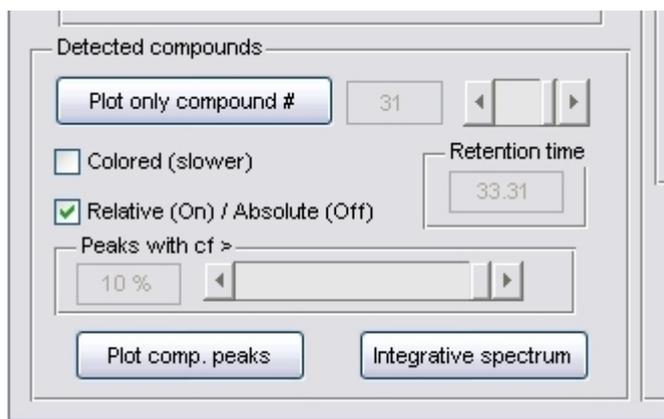
noise were applied).

You can also plot only masses, that have peak behaviour in time with certain level of probability (*cf*). For selecting the minimal *cf* value of plotted peaks use the slider in subpanel *Data plot*. Default value is 75% and maximal value is equal to maximal probability in the whole measurement.

All plots are figured after clicking the button *Plot*.

8. Peaks and Compounds

After analysing process finished, EDA enables *Detected compounds* panel.

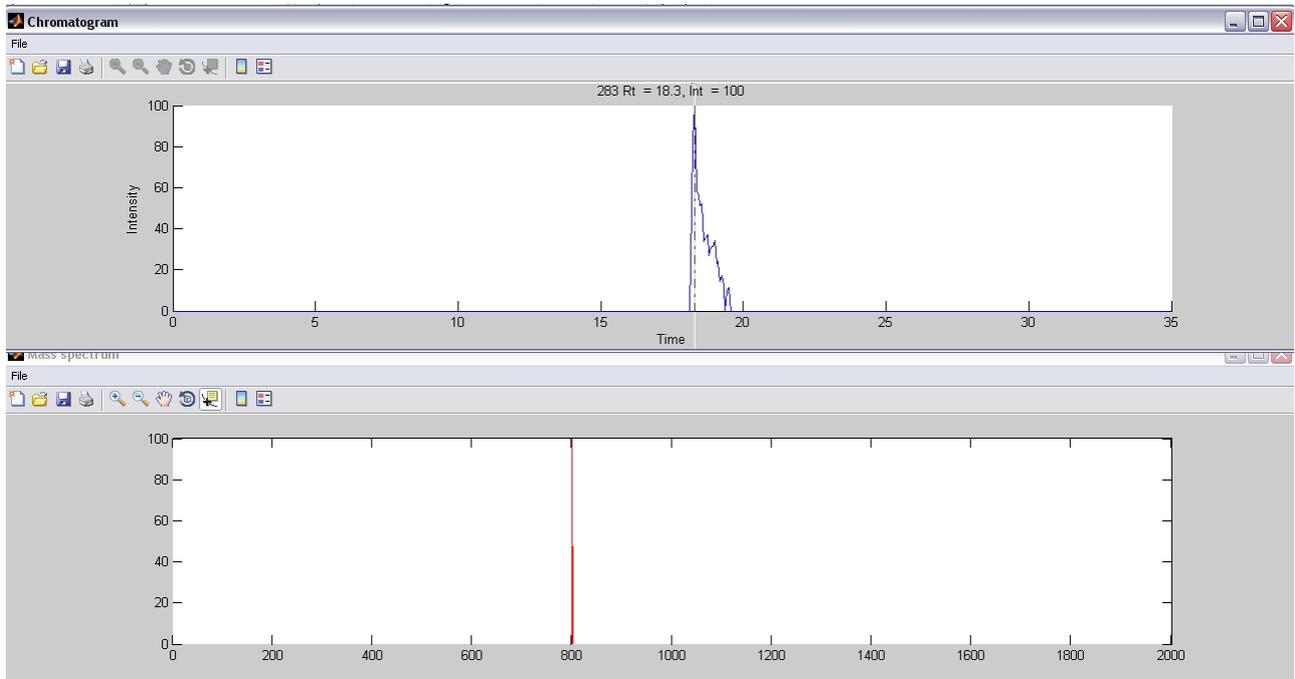


Between button *Plot only compound #* then You will see number of detected compounds. Using slider on the right-top will select which one of detected compounds You want to see in detail. Also the *Retention time* of compound intensity maximum will be displayed in window below



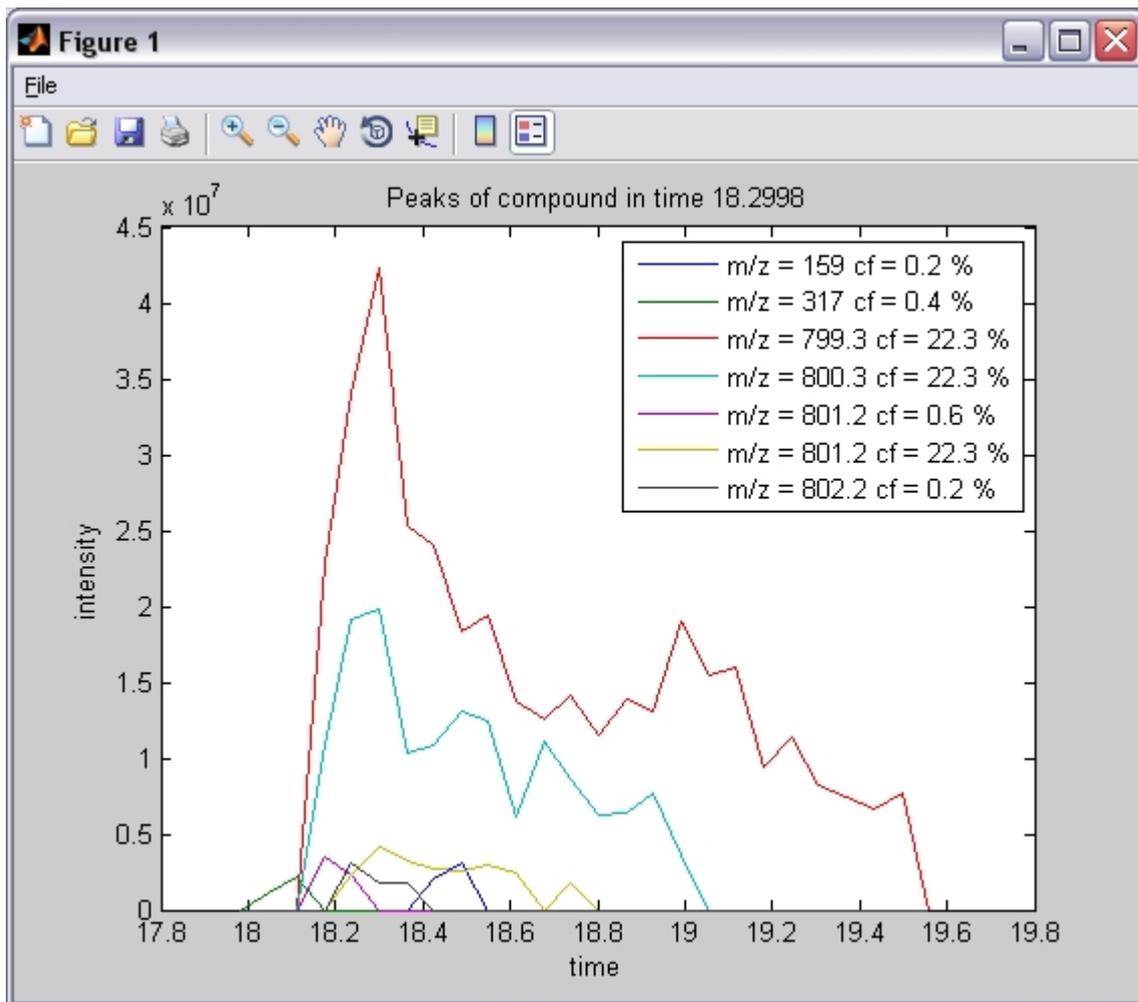
Check boxes *Colored (Slower)* and *Relative (On) / Absolute (Off)* have exactly the same function as in previous case (7. Visualization).

Button *Plot only compound #* will plot two figures, upper one for TIC (Total Ion Chromatogram) and lower one for mass spectrum. Both only for selected compound.

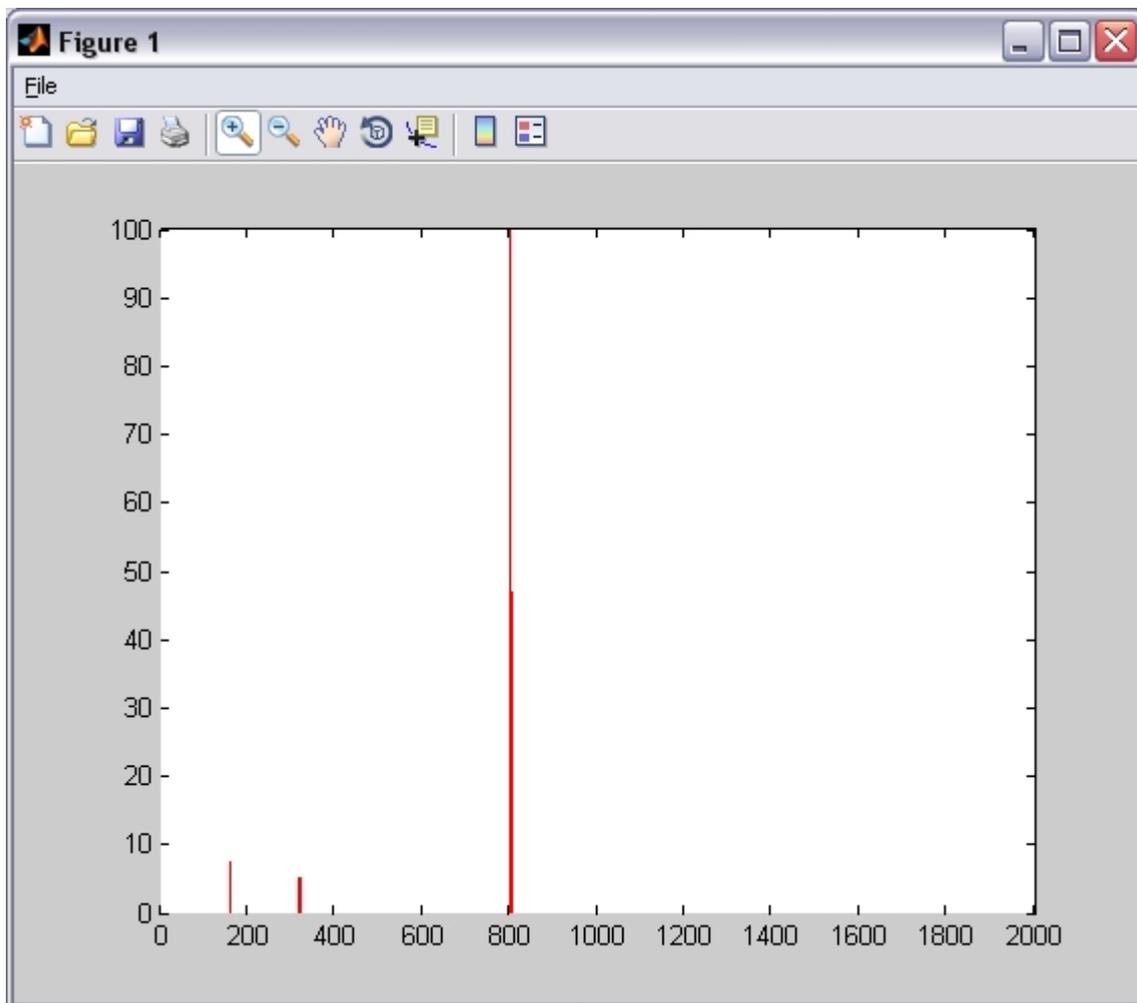


Slider for Peaks with `cf` determine value of probability for plotting TIC and mass spectrum.

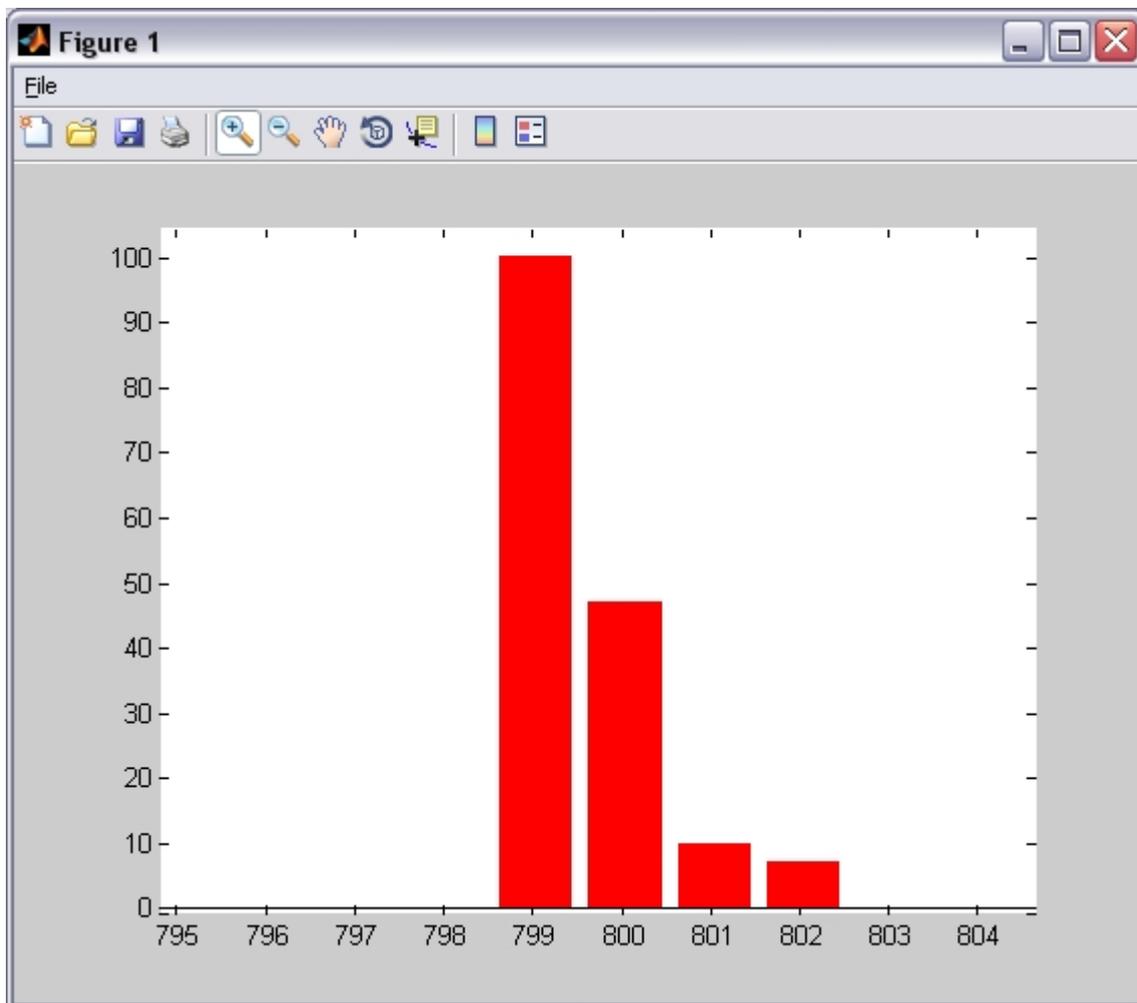
Button Plot comp. peaks will plot time behaviour of **all** masses in selected compound.



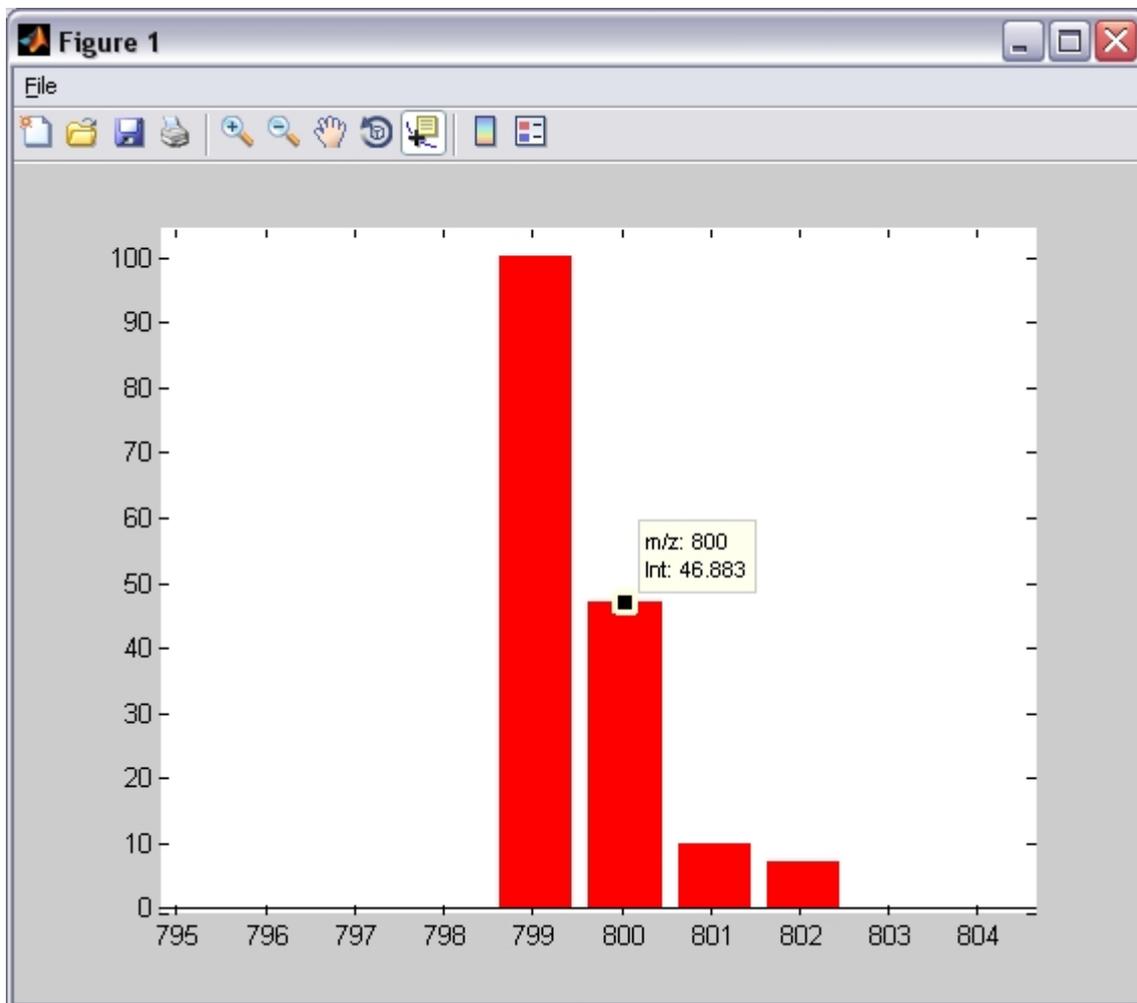
Button Integrative spectrum will plot mass spectrum across whole compound.



All mass spectrum plots may be zoomed using icon of magnifying glass and selection of region of interest. For zoom reset use double click of left mouse button.

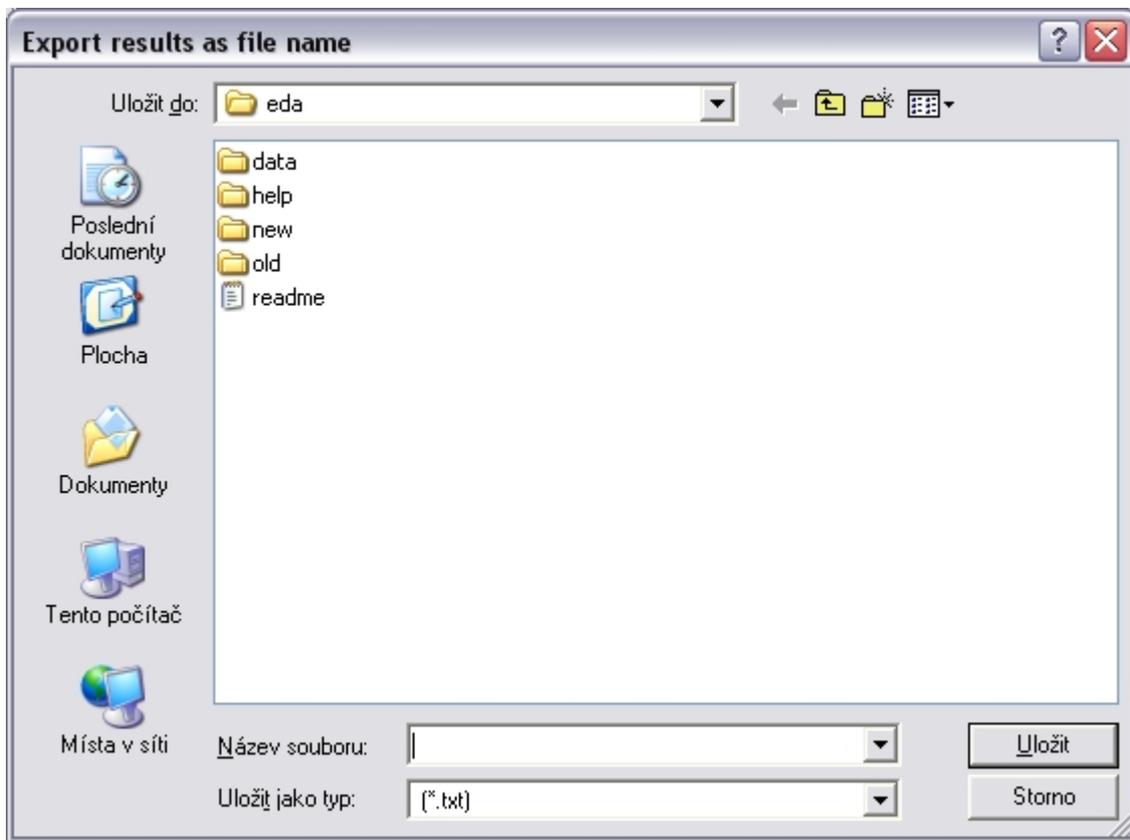


Another icon Data cursor allow to describe plot points. Hold alt on Your keybord to allow multiple data cursors.



9. Export Data

From menu File/Export Data create a txt file with the results of Analysis (table of compounds, peaks and their properties)



10. Main menu

In left upper corner You can find menu toolbar



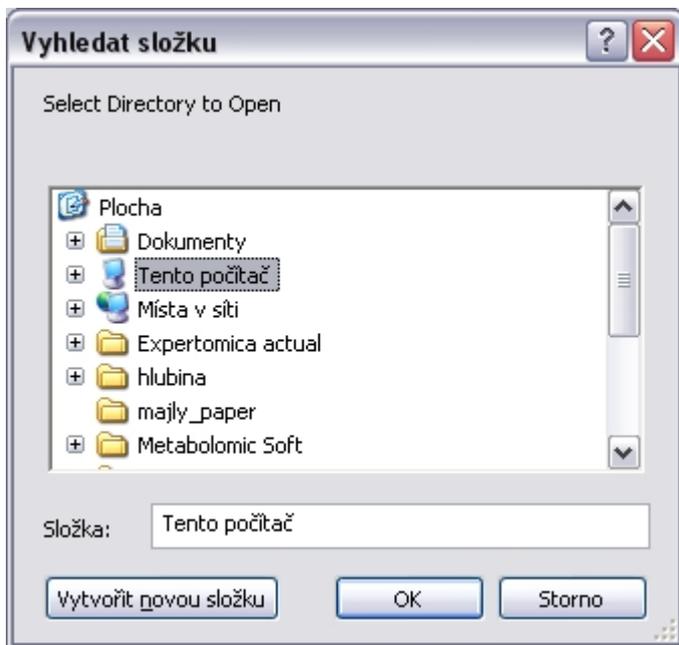
where

- `File` contains items for Open mat, Load Measurement, Save Data, Save Analysis, Export Data and Quit (see 4. Insert measurement into application and 5. Save dataset for details)

Before `Quit` You willbe asked for saving data.



- `Edit` contains items for Clear measurement, Clear analysis or Clear all from the computer memory.
- `Tools` contains items for Analysis (see 6. Analysing for details) and Set Current directory



- Help allows to read this help and some basic informations about the program.

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