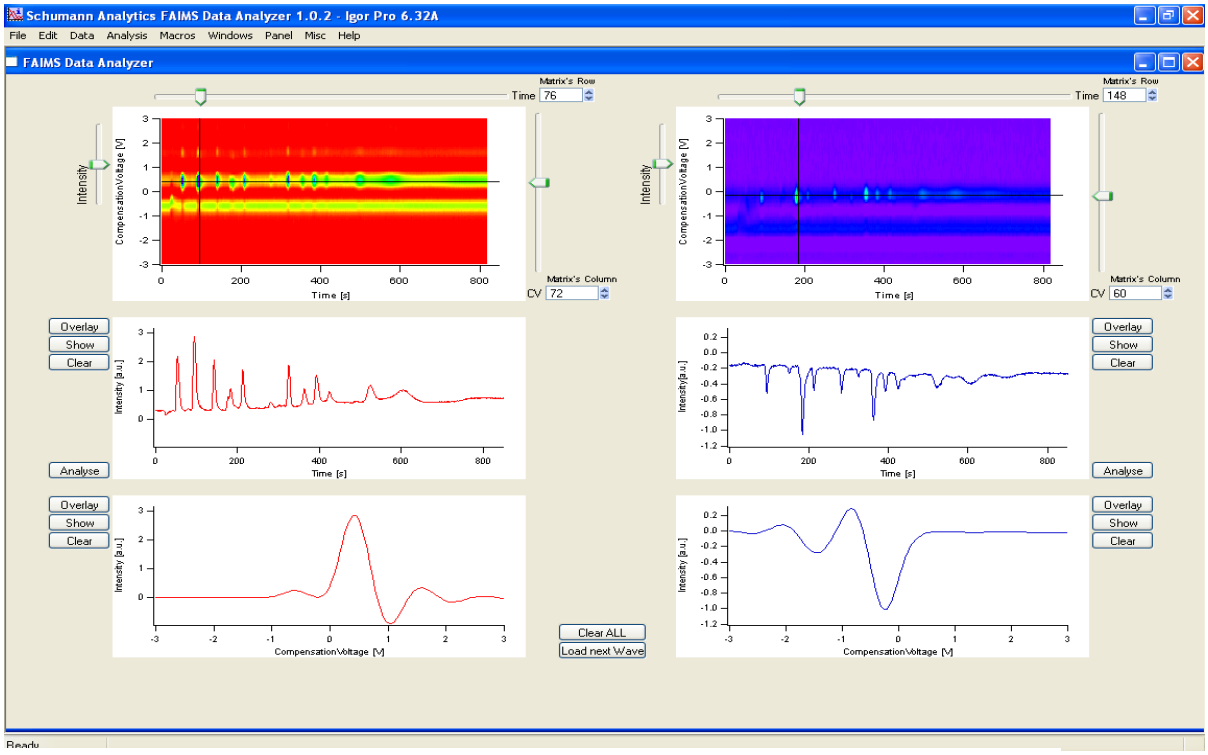
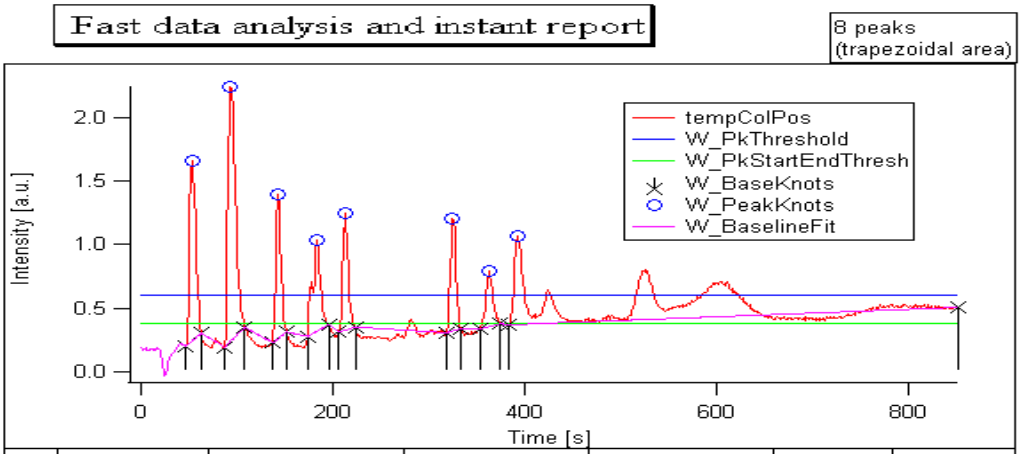
Operation Manual FAIMS Data Analyzer





Poin	W_PkCenters	W_PkAmps	W_PkFWHMs	W_PkAreas	W_PkX1	W_PkX2
0	52,8	1,4159	7,57137	10,7795	46,6	62,6
1	93,3	1,99798	8,72721	18,3869	87,2	108
2	142,4	1,1362	5,90956	7,00639	137,5	151,1
3	183	0,708923	6,9584	6,72357	173,2	195,3
4	212,5	0,918078	5,64054	5,76513	206,3	223,5
5	324,2	0,88684	6,48989	5,94603	318,1	332,8
6	362,3	0,440191	7,73348	3,58722	353,7	374,6
7	393	0,695313	8,50687	32,3173	383,1	851,2

Notices

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Content **Page**

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1. **Information about FAIMS Data Analyser**

The software "FAIMS Data Analyser" is an optional data analysis tool created with IGOR PRO from WaveMetrics, Inc. Portland, OR 97223, US.
To use the "FAIMS Data Analyzer" with all its functions it is necessary to install the program IGOR. You can download the fully-functional IGOR Pro 6.3 Demo and try it for 30 days after installation. After 30 days, the demo will lapse into limited functionality mode. The limitations of this mode are:

- Saving is disabled.
- The clipboard contents cannot be transferred to other programs.
- The printing output is lightly over-printed with Igor-related words.

To avoid these limitations, or to create your own procedures you can purchase an IGOR Pro license to restore the full functionality.

1.1 Preparing your data for analyse

Before starting the FAIMS Data Analyzer it is necessary to convert the format of your data. First create a txt-file with the Review Process File from the Lonestar software.

Export data from Review Process File Vsn

Initially load your lcbdf-file, choose File → Export Data and click “Ok” in the windows panel. Now the txt-file is created, close the Review Process File and start FAIMS Data Analyser.

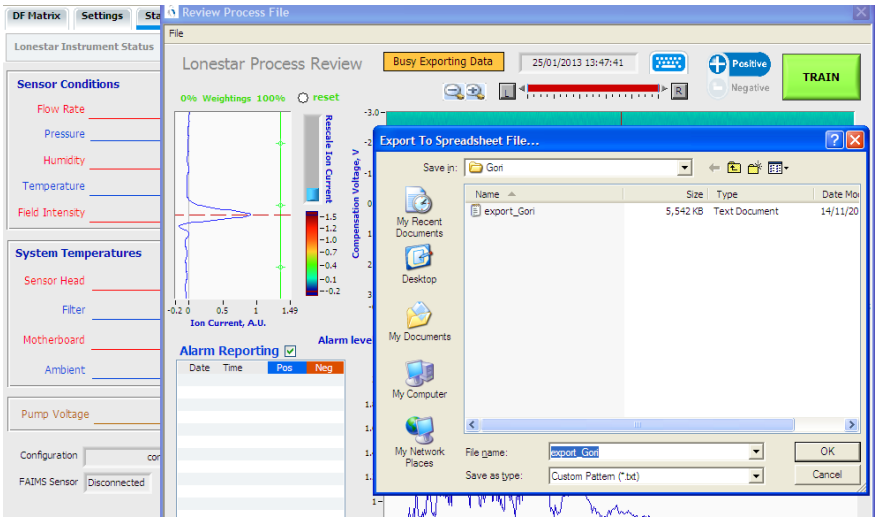


Fig. 1 Export the lcbdf-file to a txt-file

2. How to use FAIMS Data Analyser

If it is not installed, download and install Wavemetric's Igor Pro (http://www.wavemetrics.com/support/demos.htm). As described in the section "Information about FAIMS Data Analyzer" the demo version of Igor is completely sufficient.

2.1 Starting FAIMS Data Analyser

Double click the "FAIMS Data Analyser.pxp" file. Igor is going to start. If you will asked for a serial number and the user name, please fill in the information or click on limited function demo.

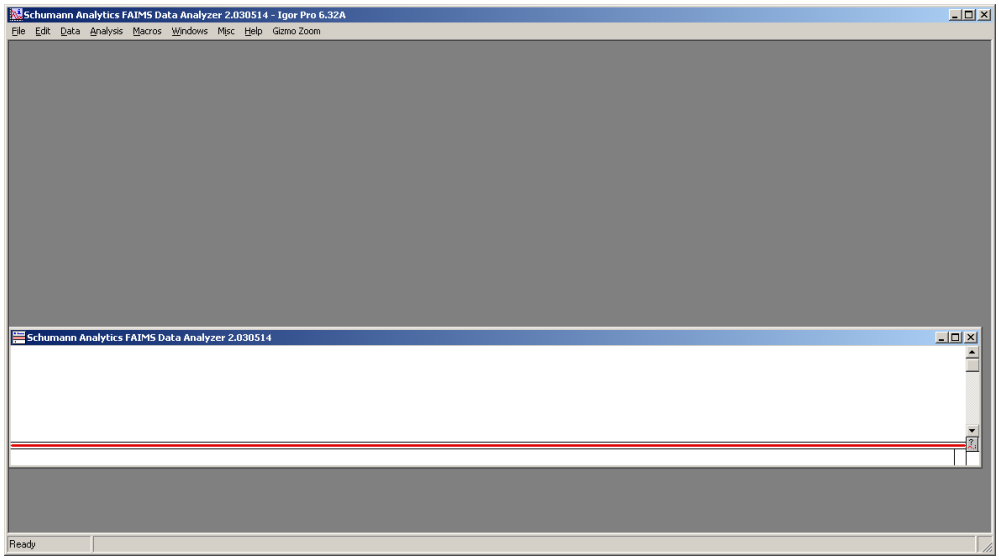


Fig. 2 Starting the FAIMS Data Analyser

Start your analysis by choosing "Macros" -> "Analyse Start".

Notice: Starting the "FAIMS Data Analyser" for the first time choose "Clear All and Use Default Options" before starting the analysis.

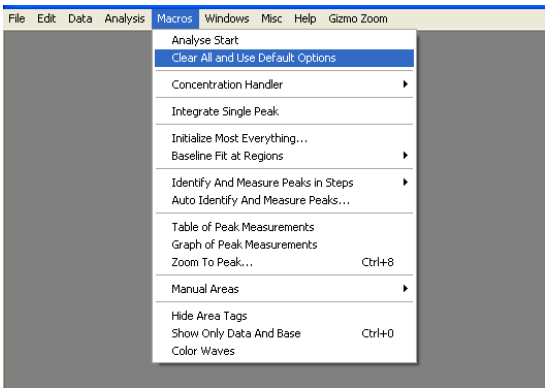


Fig. 3 Clear all Use default options when starting the first time

2.2 Loading Data

After launching FAIMS Data Analyser please load your data into the program. Select the folder, in which your ".txt"- file is saved. Mark this and click the "Load Data"-button. Now the program automatically opens the analysis panel and loads your measurements in the screens shown below:

2.3 Overview

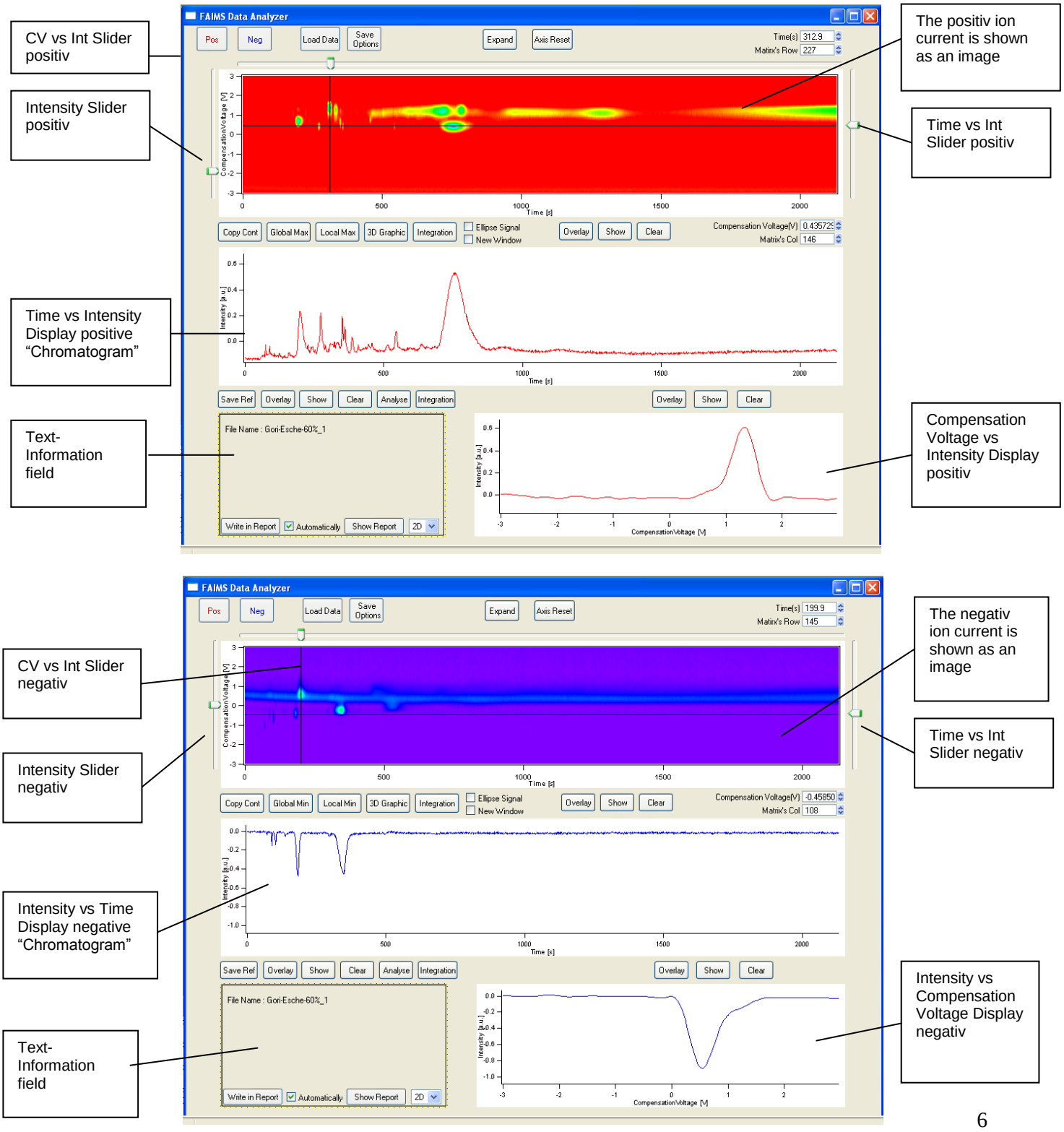


Fig. 4: Overview of the FAIMS-Data Analyser "Main-Displays" positive and negative mode

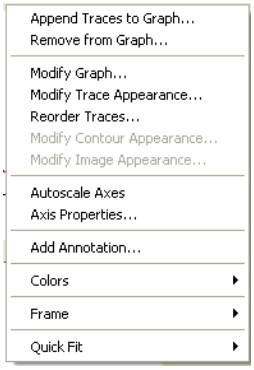
2.4 Display

The main displays in Fig 4 (positive and negative Ion currents) show your data as an image. The button axis is the time axis, the left axis is the compensation voltage axis and the ion current is illustrated by intensity similar to the “Lonestar Review”. Additional there are two black lines. The horizontal one belongs to the “Time vs Int” slider. The vertical line belongs to the “CV vs Int” slider. Both indicate the position, which is displayed in the “Time vs Int” display or “Compensation Voltage vs Int” display.

“The Time vs Intensity” displays (middle) show the current chosen intensity by Time vs Int slider.

“The Compensation Voltage vs Intensity” displays (bottom right) show the current chosen intensity by CV vs Int slider.

2.5 Modify Displays and Graphs



To modify a display right click on it. A popup shows your options. The core options are:

“Append Traces to Graph…” you can add other graphs into the display.

“Remove from Graph…” removes data from the graph.

“Modify Trace Appearance” opens a new panel. There you can change the colour, the mode (line, dots, markers) etc. of the displayed graphs.

“Modify Image Appearance…” (is useable at the top displays) opens a panel. There you can change the colour type of the image (e.g. to grays) or the intensity to a concrete value.

“Autoscale Axes” scales the axes as before, after you changed something by:

“Axis Properties…” opens a panel. There you can change the axis label, the axis range, the number of ticks etc.

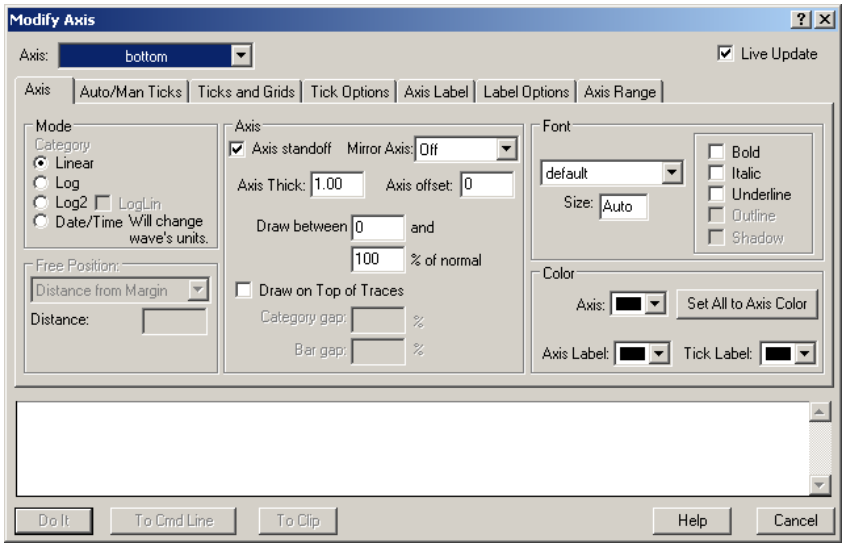


Fig. 5 Modifying the Axis properties

Slider

Intensity sliders

“The Intensity sliders” change the intensity of the image for a better peak detection. You can also do it manually by right click on the image and choose “Modify Image Appearance..”.

Time vs Int sliders

With this sliders you choose a constant compensation voltage (row of the matrix), which is extracted from the image and shown in the “Time vs Intensity Display”. The compensation voltage you have chosen and the exact matrix’s row for this voltage are displayed right below the image. The horizontal line displays which one is extracted, even when you have zoomed. The slider is not on the right position if you have expanded the window.

CV vs Int sliders

With this sliders you choose a constant time (column of the matrix), which is extracted from the image and shown in the “Compensation Voltage vs Intensity Display”. The time you have chosen and the exact matrix’s column for this time are displayed right above the image. The vertical line displays which one is extracted, even when you have zoomed. The slider is not on the right position if you have expanded the window.

Buttons

Pos / Neg buttons

With this buttons you can switch the recorded data between positive and negative ion mode.

Expand

The expand button zoom in the area, which you have to mark before, by pressed left mouse button. You can also expand manually by marking an area and right click in it.

Axis Reset

This button scales the axis to default, after expanding the image. You can also set the scale to default by right click on the image / graph and choose “Autoscale Axes”.

Copy Cont

This button opens a new window with the current shown image and the selected intensity so you can copy it and past to other programs (Ctrl-C).

Global Max / Min

The “Global Max / Min” button searches the whole image for the maximum value (positive ion current) or the minimum value (negative ion current). Both sliders are set to it and information about this point is displayed in the “Text – Information field”.

3D Graphic

The 3D Graphic button displays the current displayed image as a 3D surface in a new display.

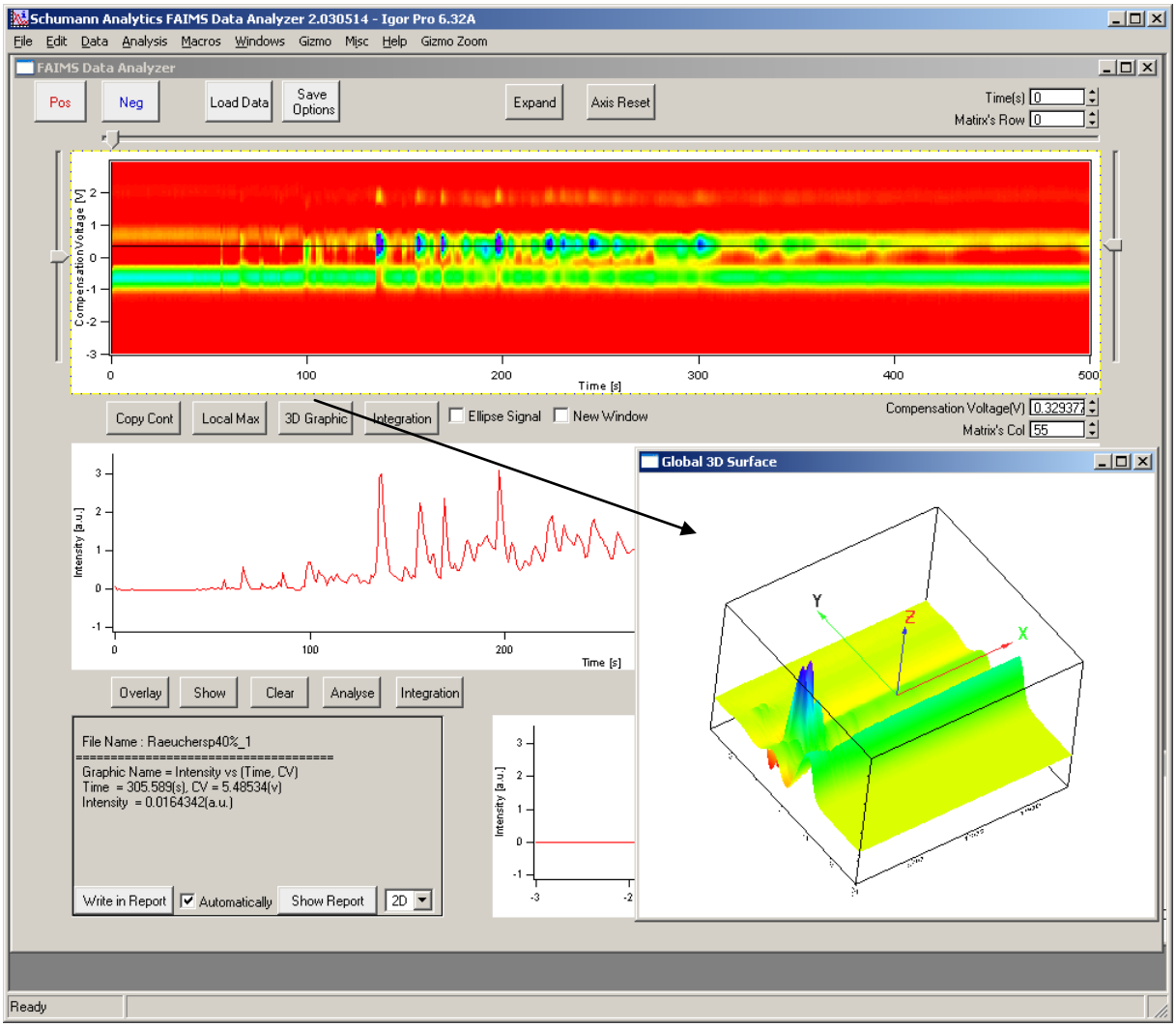


Fig. 6 Overview Display with activated 3 D graphic

You can rotate the global 3D surface as required by pressing and holding down the left mouse button and moving the mouse in the desired direction.

Integration

The “Integration” button starts the fast integration for one peak. Just follow the instructions in the “Text – Information field”. For the 3D integration you have two more options:

- if your peak you want to integrate is an ellipsoid mark the “Ellipse Signal” checkbox
- if you want to see the image in a new window while integration (not advised) mark “New Window” checkbox.

Save Ref

This button allows you to save the current “Int vs Time” graph. It is useful to create a library with substances. You can load the saved file into the “Overlay Panel” to compare to your measurements. A new window is opened, this function is detailed described in the chapter “Creating a Reference”.

Write in Report

This button, located in the “Text – Information field”, writes the integration data into a table. If the checkbox “Automatically” is marked, you don’t have to press the button. There two different tables for each integration button one.

Show Report

This button shows the table with your integration data. The table according to the popup menu next to the button is shown.

Local Max / Min

Same as “Global Max / Min”, but only for the area you have marked before.

Overlay buttons

The “Overlay”-buttons temporarily store the current displayed image, CV vs Int or Time vs Int depending on the location of the button. It will not be deleted by pressing “Load Data”, but they are all deleted by choose “Macros” -> “Clear All and Use Default Options”.

Show buttons

The “Show”-buttons display the stored data by “Overlay” in a new panel, but each one only shows the data for the display they are next to.

Clear buttons

Whit the “Clear”-buttons you delete the temporarily stored data by “Overlay”. Only the data they are next to.

Load Data

This button opens the load panel where you choose the next “.txt”-file you want to load.

Analysis button

The “Analysis” –buttons opens the current selected “Time vs Int” in a new window and initiate everything for data analysis.

Raw Data

To edit the raw data of a chromatogram or a individual spectra, place the cursor near the curve and press the right mouse button, a submenu is displayed in which you can choose the point “edit tempColPos” or “tempColNeg” for the data in the negative mode. (Fig. 7 and Fig.8)

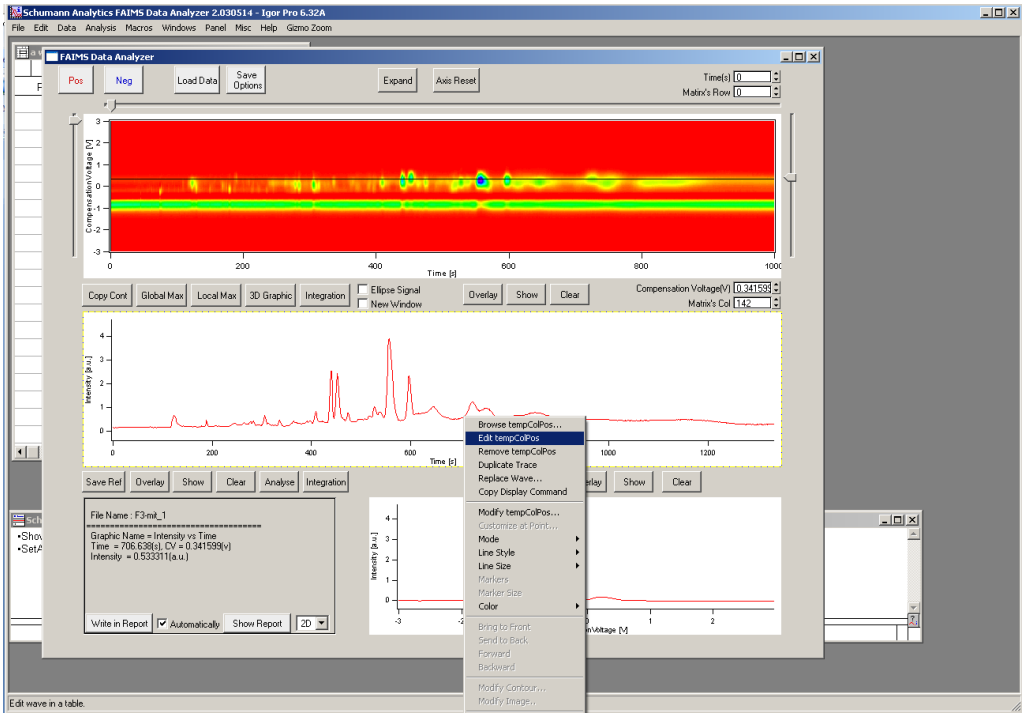


Fig. 7 To display the raw data of a curve, press the right mouse button near the curve

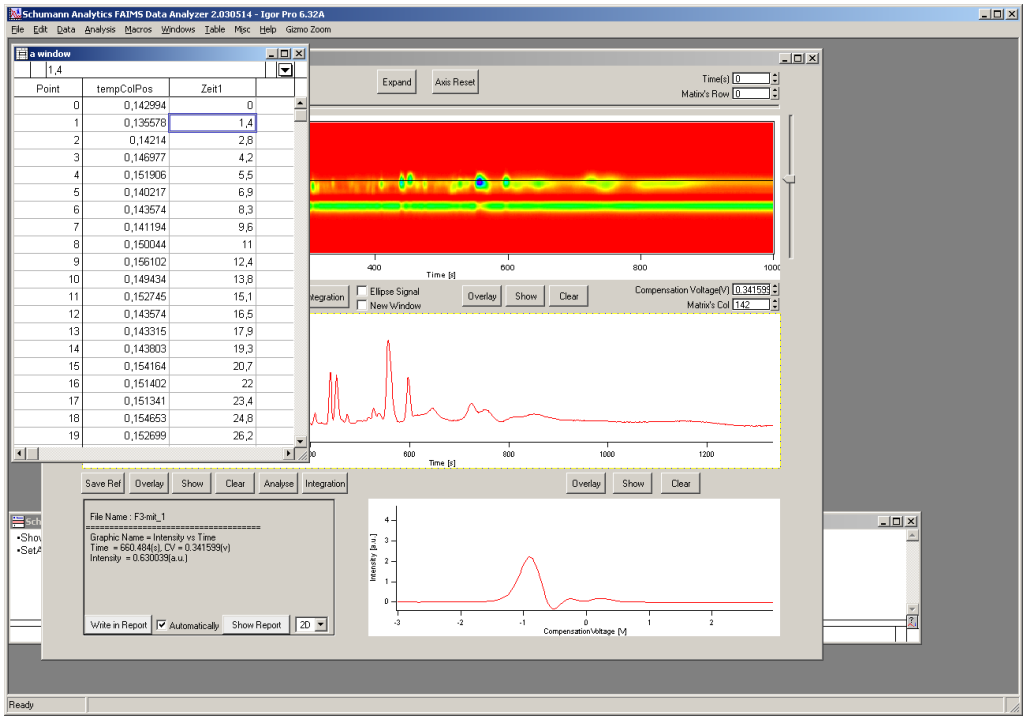


Fig. 8 Table of the raw data

3. Data Analysis

3.1 Overlaying chromatograms

To be able to compare different measuring chromatograms with each other it is possible to overlay them as shown in figure 9.

Select the first chromatogram to compare and press the “Overlay button” left under the chromatogram window. Select the next chromatogram you want to compare and press again the “Overlay button”. Press the “Show” button and enable the names of the curves in the text box under the graph window. A click on the “Annotation-Button” will display the legend of the curves with the selected compensation voltages.

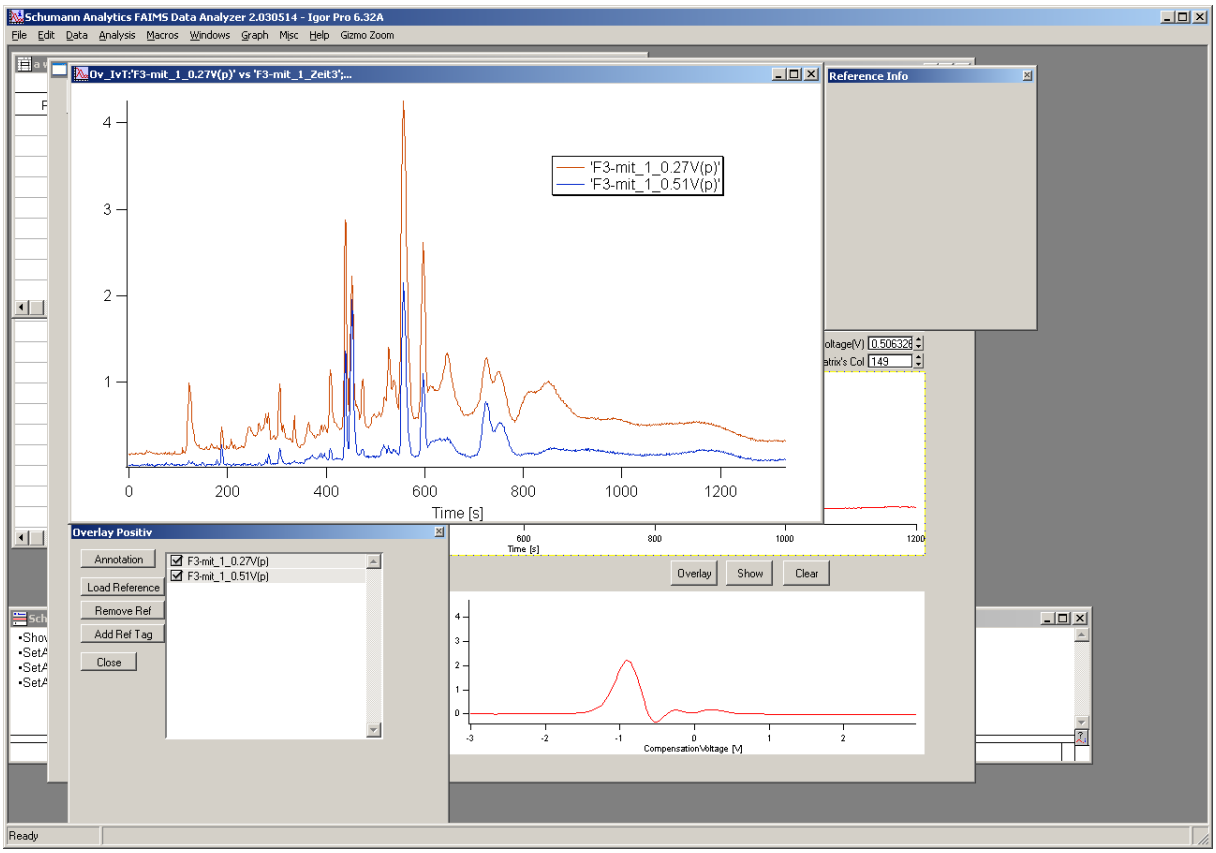


Fig. 9 Overlaying different chromatograms

A click on the “Close-button” will not delete the overlayed chromatograms it will only close the current window. You can display the compared chromatograms again with a click on the “Show-button” left under the chromatogram in the main window. To clear these data from the temporary storage please press the “Clear-button” left under the chromatogram in the main window.

3.2 Creating and Using the Reference

The save reference option is useful to create a library for chemicals you want to detect in an unknown sample.

Creating a Reference spectra

First record a “Continuous Mode file” with a pure substance with the Lonestar software. Then load it into the FAIMS Data Analyzer. Choose a compensation voltage with the “Time vs Int” slider, where your substance has a perfect peak. Press the “Overlay button” left under the chromatogram window. After that please press the “Show button” the and the current “Int vs Time“ graphic is shown in a new window. Here you have the ability to add tags on the graph:

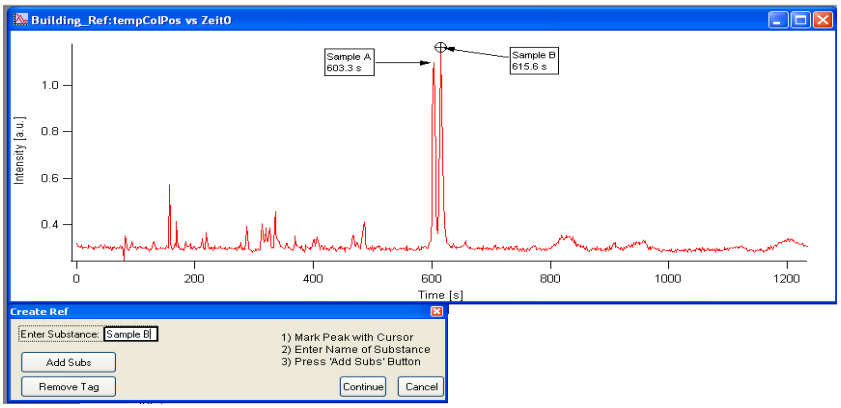


Fig.10 „Creating a Reference spectra“

- Place the cursor (initially placed bottom left) at this place, where you want to add the tag

- In the subwindow below enter a substance name

- Confirm with “Add Subs” button

- Your tag is shown in the graph window

- Add as much tags as you like

- To delete the last tag, press “Remove Tag” button

Confirm with “Continue Button”, if all tags are right set or use “Cancel” to quit “Creating a Reference”.

A new window is shown (Fig. 7), it contains data according to your loaded measurement. You can change the “Sample Name” and add “Additional Note”.

Please fill in the right parameter at “GC Parameter”. Confirm with the “Continue” button and choose a data folder and the save the name of the data.

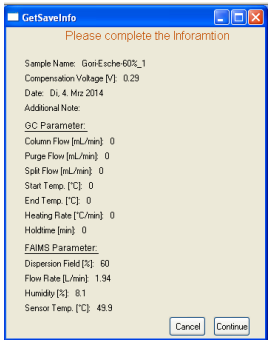


Fig. 11: Editor to set GC-Parameters

Loading a Reference file

Press the “Show” button below the “Int vs Time” graph. Notice: You can display the Reference file even without having data “overlayed” by “Overlay” button. The “Overlay” window appears. Now press the “Load Reference” button. A “Load Dialog Window” is opend, choose the Reference, you want to open, confirm with “Load”. The Reference file is append to the graph window and automatically the common-, GC- and FAIMS- parameter are displayed in a subwindow on the right hand side. To display the tags, you have added during “Create a Reference”, press “Add Ref Tag”, all tags are automatically added to the graph. To remove the “Reference” press the “Remove Ref” button. If you want to load another Reference file, use the “Load Reference” button, you don’t have to use the “Remove Ref” button before. If you press the “Close” button, the Reference is automatically removed.

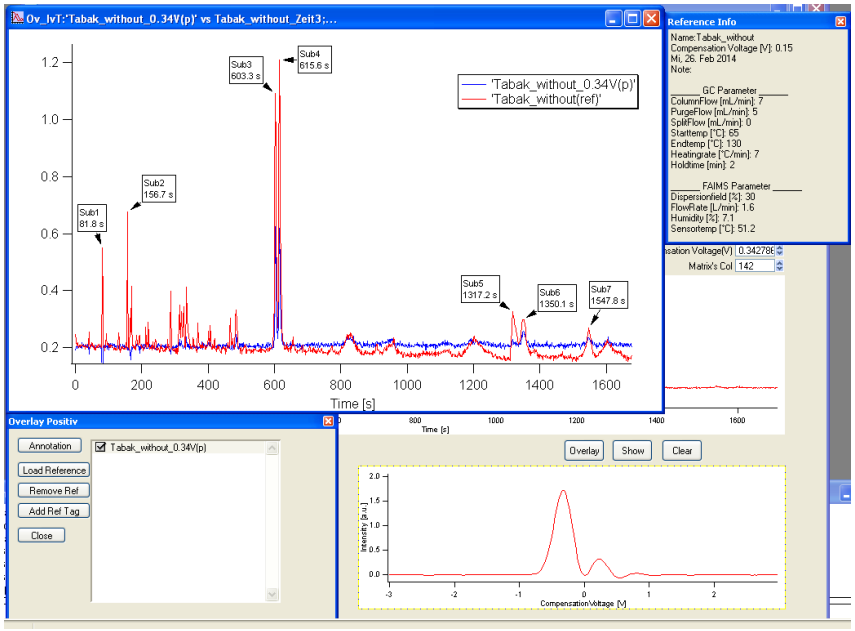
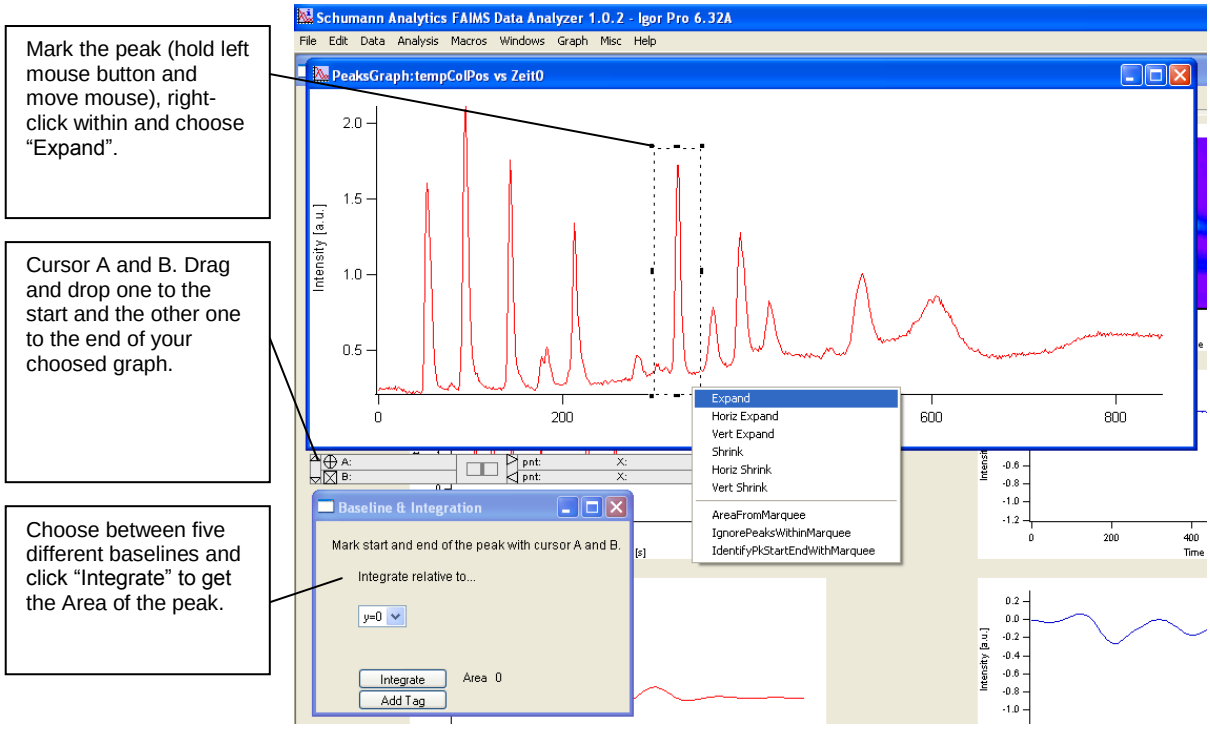


Fig. 12 Comparison of an unknown substance with a reference spectra

3.3 Integrate Single Peak

Choose “Macros → Integrate Single Peak”. A panel appears below the displayed graph. Now you have to place cursor A at the start and cursor B at the end of the peak by drag and drop. Therefore it is easier if you first expand the peak and then put the cursors on it.



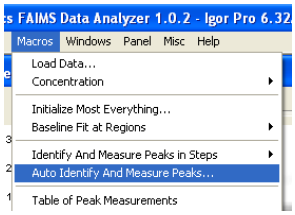
Then you have to pick a baseline for your integration. Click the popup and choose between five baseline-types:

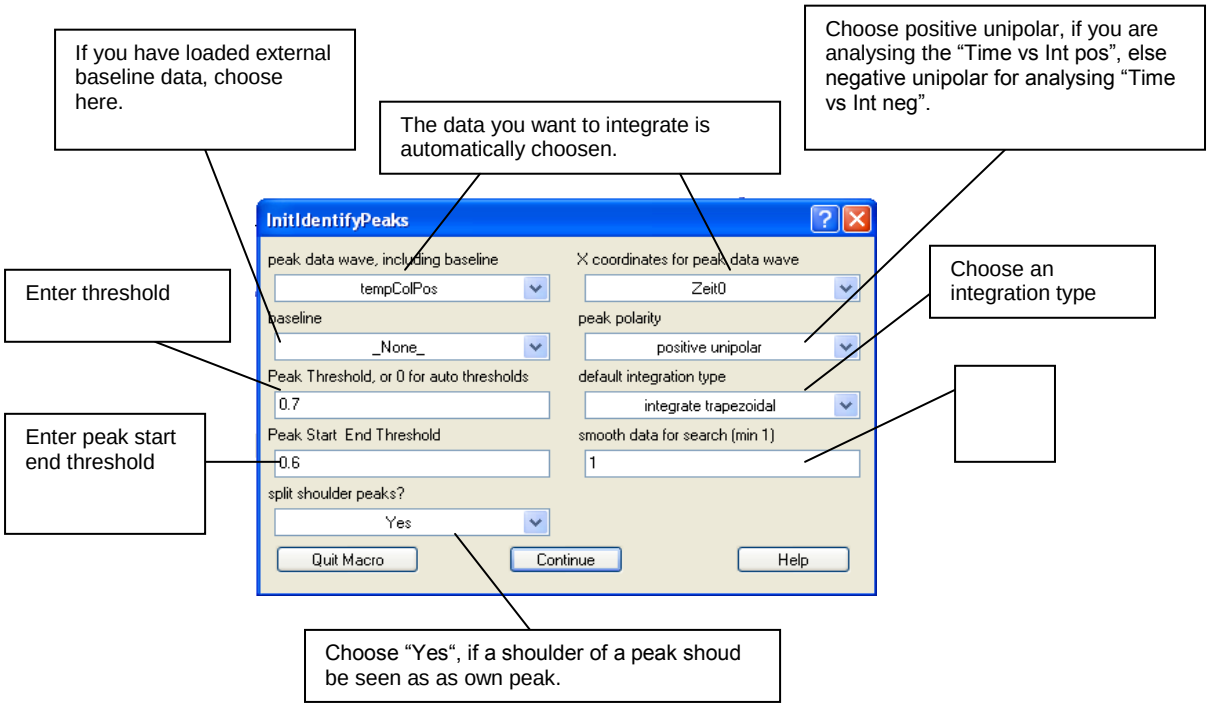
- “y=0” – the area between y=0 and the graph is calculated.
- “y=…” – an input area appears. You set a constant line as baseline. E.g. you set 0, this would be the same as « y=0 »
- “Constant line through cursor A” – the same as “y=…”, but the program sets the constant line at the high of cursor A
- “Line between Cursor A and Cursor B” – a line between both cursors is drawn.
- “Create own Baseline” – a cursor (named “C”) appears in the middle of the display. Set this cursor to the start point of your baseline. Click the appeared “Add cursor”-button to display the next cursor in the middle of the display. You can work with up to eight cursors. They were connected alphabetical, after pressing the “Construct Baseline”-button.

After pressing “Integrate” the area is calculated and shown next to the button. Now note the area by Concentration Handler or use the “Add Tag”-button.

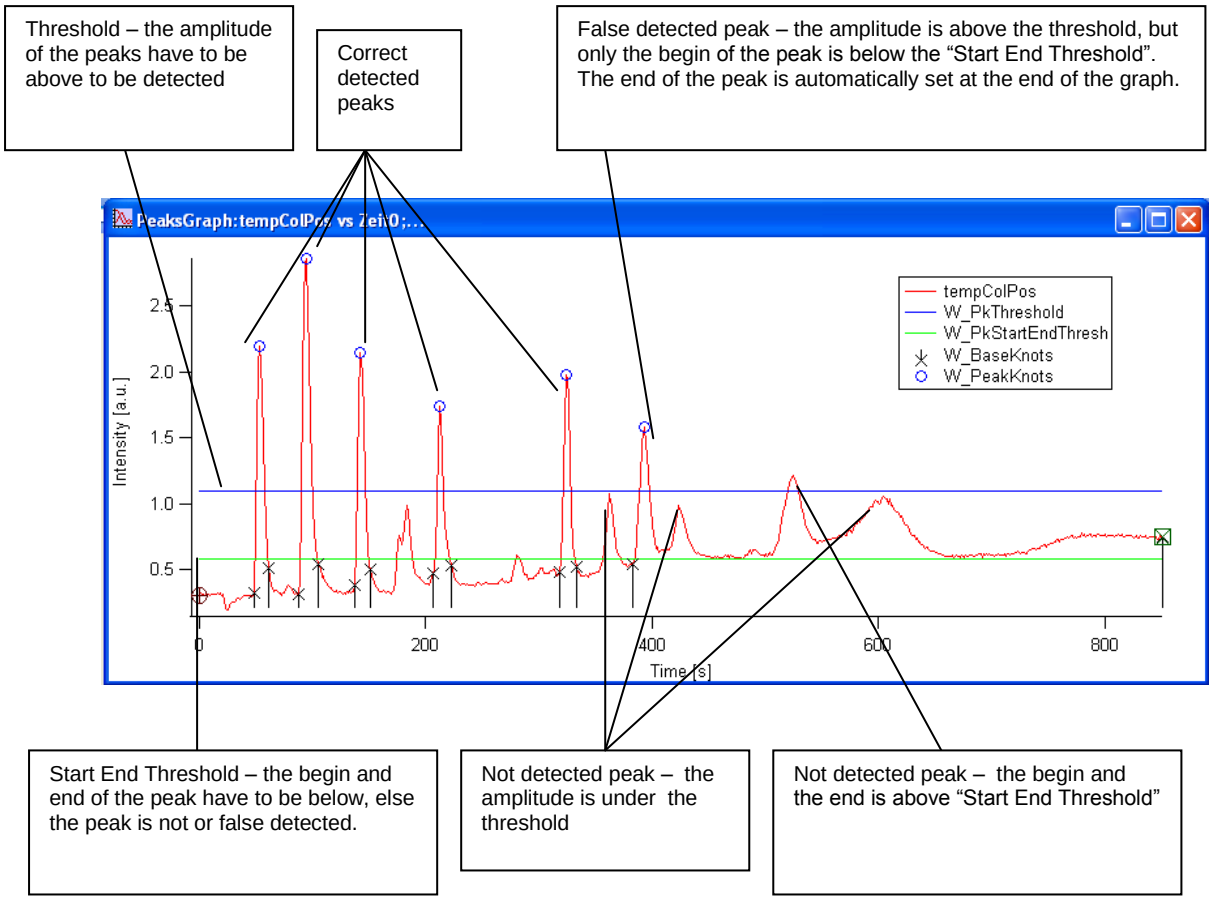
Auto Identify and Measure Peaks

To start the automatic peak analyse choose “Macros → Auto Identify And Measure Peaks…”. A new panel is shown. There you declare the parameters for peak integration:

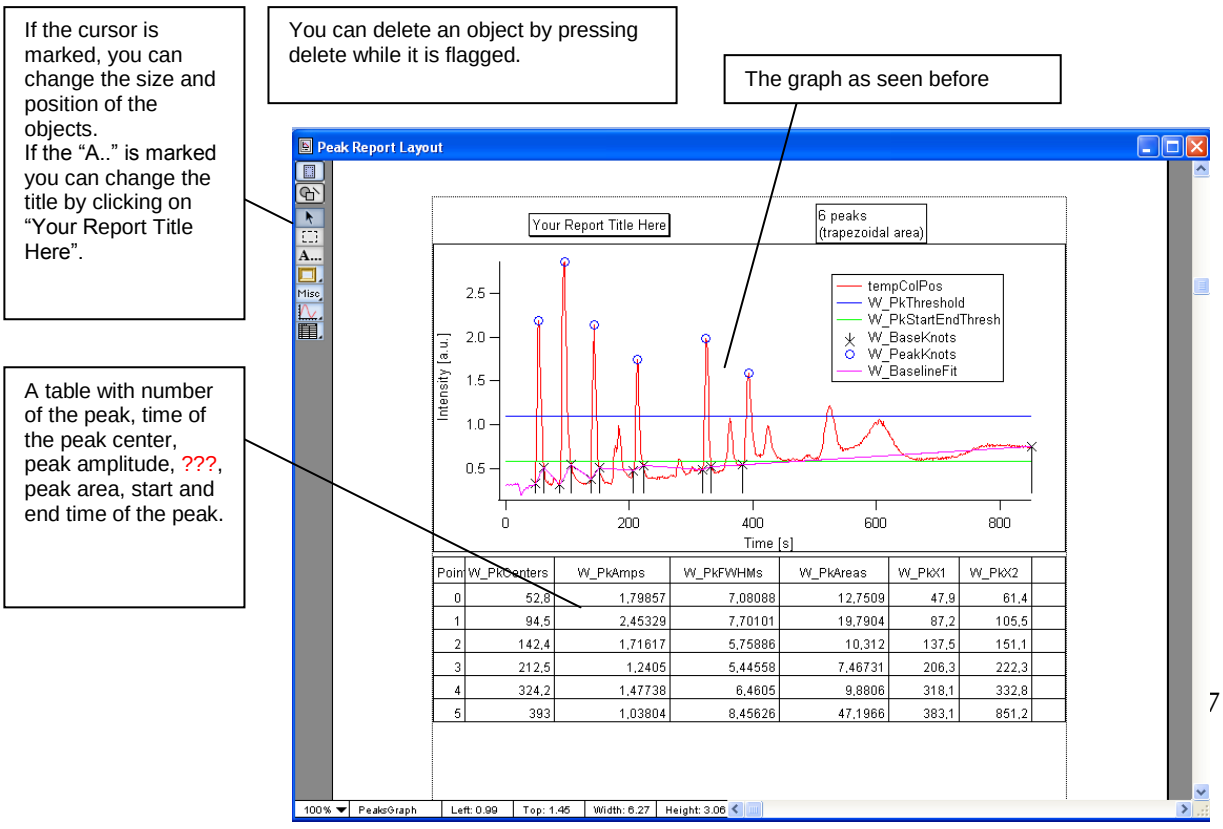




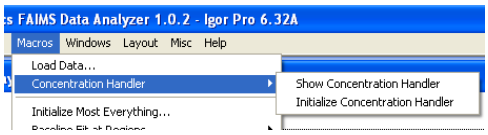
Press “Continue”, if you have finished entering the settings. You were asked, if you want to construct a baseline from the “BaseKnots”. In the background you see is updated “Analyse”-panel:



If you choose “Yes” for “Construct Baseline from W_Baseknots”, a line through the “Baseknots” (cross at start and end of a peak) is drawn. In the next panel you choose either the area should be detected in relation to the baseline or to y=0 and you choose the measure period. After pressing continue an automatically created report appears.



Concentration Handler



The “Concentration Handler” is an easy way to take a concentration curve. Open the “Concentration Handler” by pressing “Macros → Concentration Handler →” either “Initialize Concentration Handler”, if you want to create a new concentration curve or “Show Concentration Hander”, if you want to add a point or see the last concentration curve you have taken.

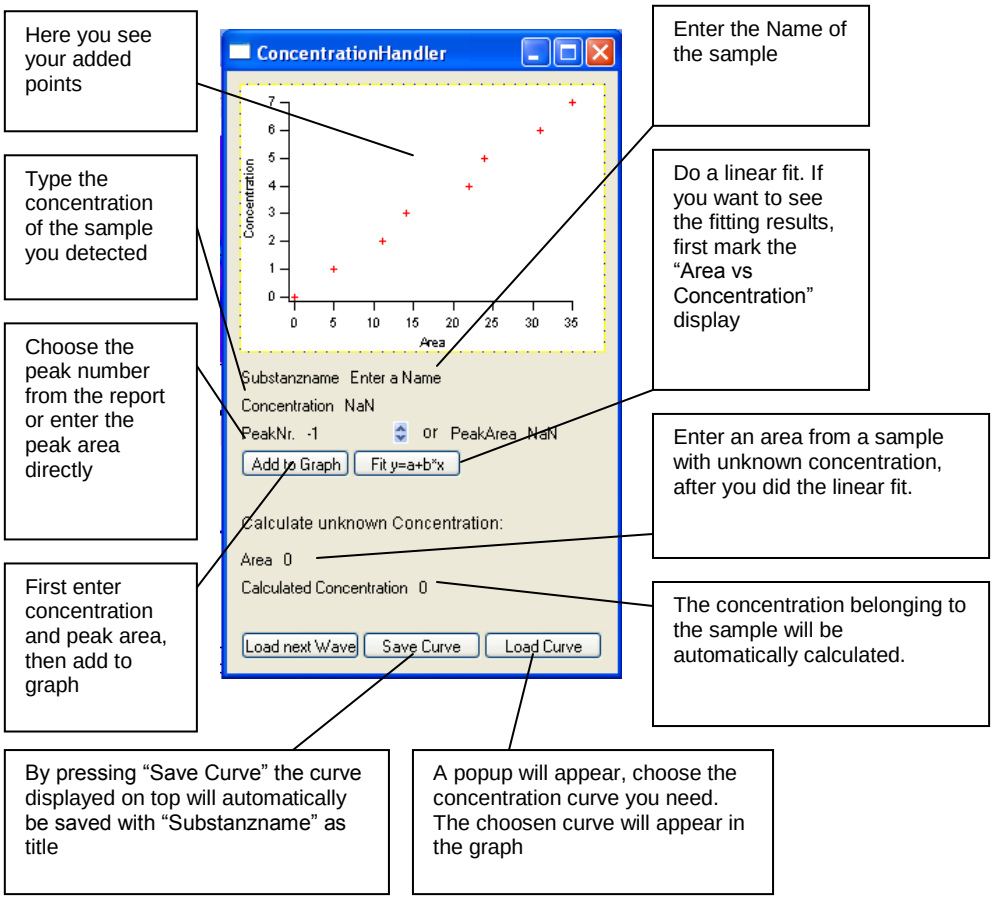
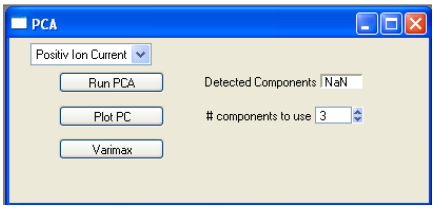


Fig. 17: Concentration Handler

4. PCA – Principal component analysis

There is the possibility to arrange a PCA. Therefore choose “Start PCA” in the submenu of Macros.

A new window will open, where you can choose with which matrix (positive or negative) you want to start the PCA.



Then press the “Run PCA” button. The process may take several minutes. Afterwards the number of detected components are shown in the display next to the button. In the display below you can now enter the number of components you want to displayed by “Plot PC” or “Varimax”. The PCA operation and procedures follow the text by E.R. Malinowski: Factor Analysis in Chemistry, John Wiley and Sons (1991).

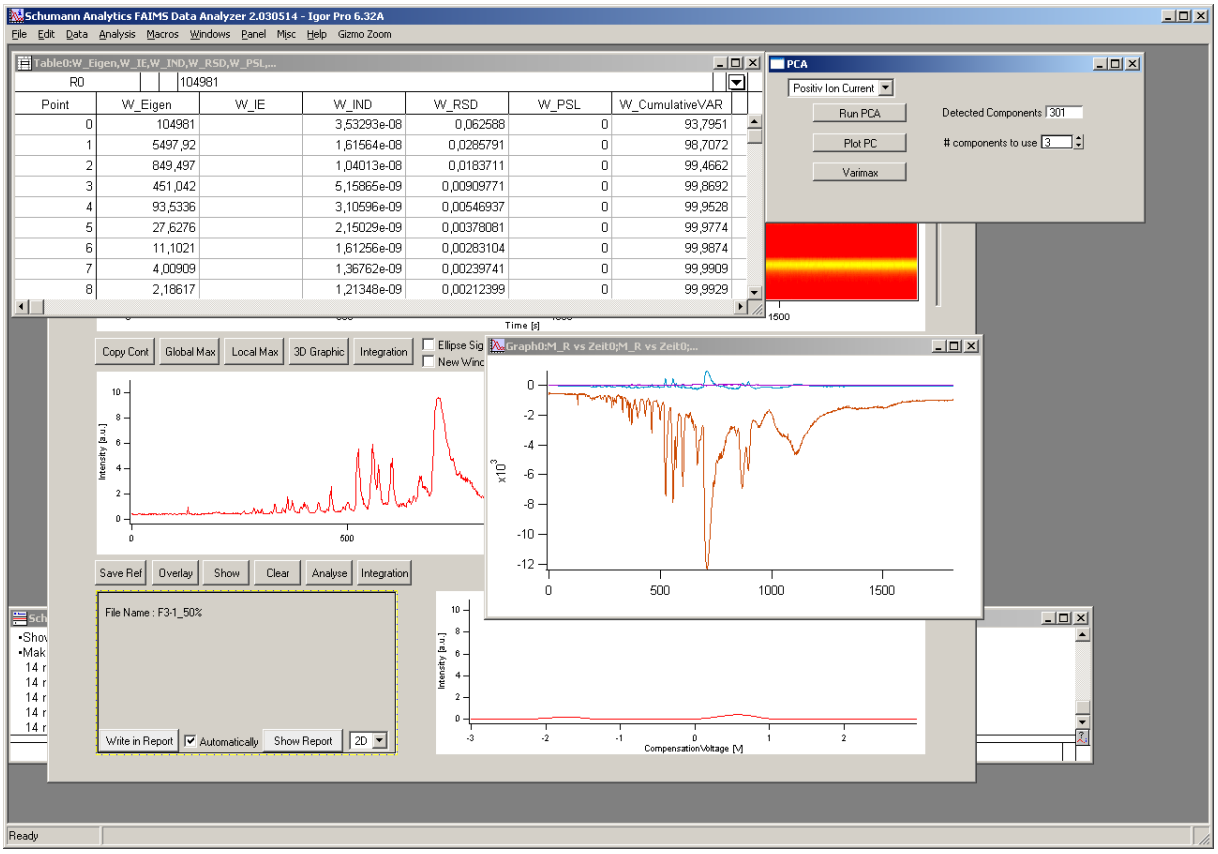


Fig. 18 Example for Principal Component Analysis (PCA)