Comprehensive reference guide for LabChrom-2 chromatographic software TR-542a TLC scanner edition Version 2.0 - 2.1

Chemotron Inc.

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Basics

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Central setup

The LabChrom2 chromatographic software is already installed to the computer. If you reinstall the system, the settig up of the software may be necessary. If you start the program and you see the window without an installed instrument (picture 2.1), this is that case. If your instrument is installed (usually only one piece) and works properly, you should jump to the section 2.1, see picture 2.2.

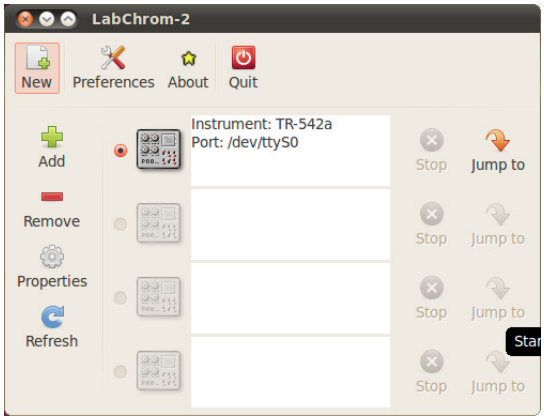

Figure 2.1: The Central setup window

When you made every settings, quit from the central window, then restart the program.

2.1 Preferences for the whole software

These settings are software-wide, that means those are common for all the part of the software system.

2.1.1 Central window closing

If all your central settings are good, no other change is necessary, you can check this button (see picture 2.2), at the next start will not appear this window. This option

depends on `Auto start` option, see section 2.2.

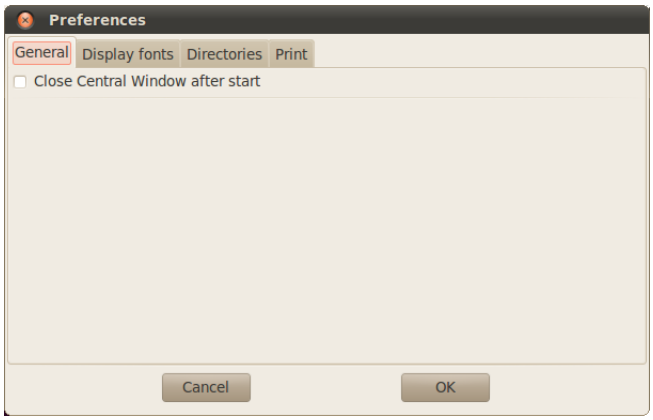

Figure 2.2: Close this window at startup

2.1.2 Central directories

The software generates a log file that contains internal information due to backtracing the misbehavior of it. This file is placed into a directory, can be set here. This directory (subfolder) is usually the `/home/labor/LabChrom2`.

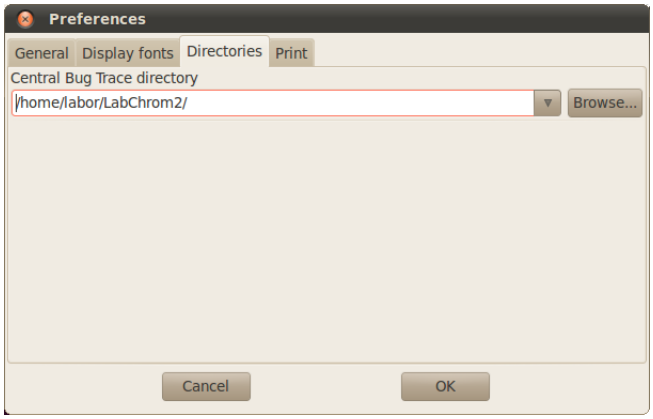

Figure 2.3: Log directory

2.1.3 Print settings

The inkjet printer usually can not use the whole area of the paper, but the printer driver. Therefor we have to set margins, on this way the printer will print our data in the printable area, not outside of it. Usually the applicable value is 10 (ten) for each side.

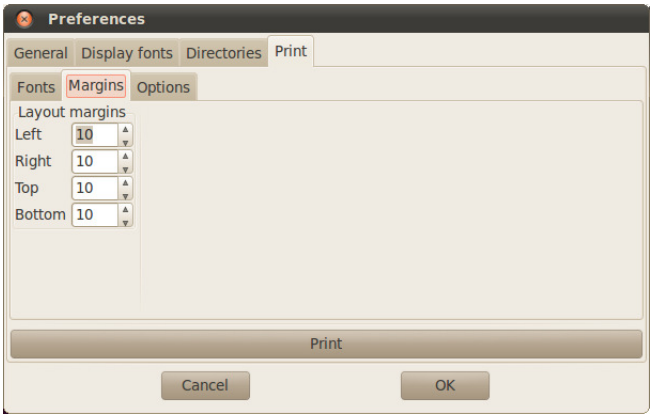

Figure 2.4: Print margins

2.2 Properties of an instrument

2.2.1 Instrument settings

The LabChrom2 software can handle some different type of instruments. You must set here your instrument parameters. For TLC scanner you must select the TR-541 instrument (not the TR542!). A name can be given to the instrument, for example *Bio labor scanner 1* or anything else. It is recommended to check the `Auto start` checkbox, it is necessary when you check the centrak window closing option. By clicking to the icon button you can select an icon for the instrument.

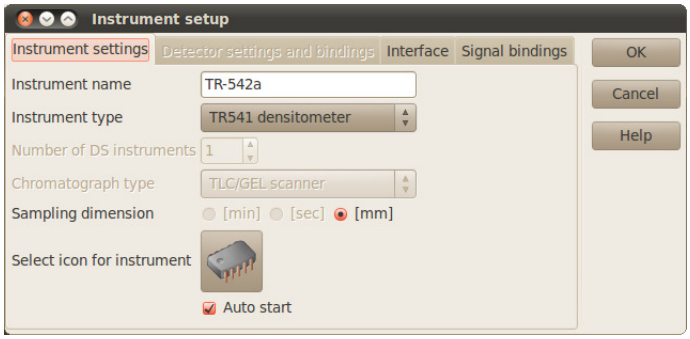

Figure 2.5: The instrument setting

2.2.2 Detector

This instrument has one (1) detector, therefore you must fill only the first row. The recommended setting can be seen on the picture 2.6.

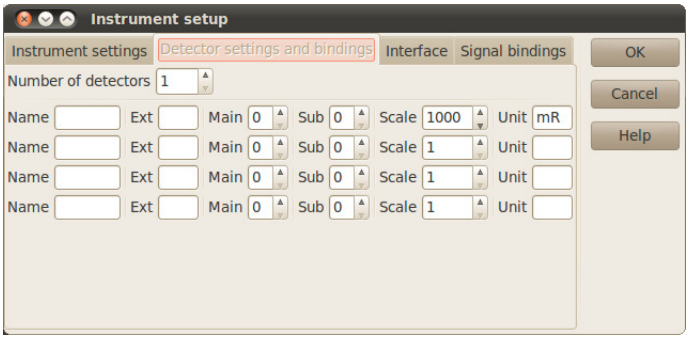

Figure 2.6: The detector sttings

2.2.3 Interface

The communication interface is usually `Com1`, in some special cases is `Com2` but this is noted on the back of the computer.

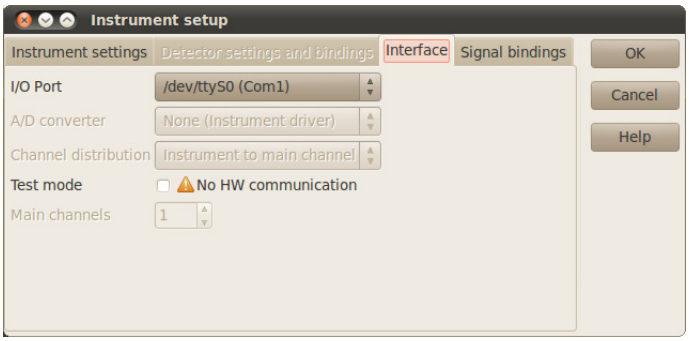

Figure 2.7: The interface settings

Chapter 3

Preferences

The preferences of the chromatographic software can be set in the Main Window, selecting menu item Edit→Preferences.

3.1 File locations

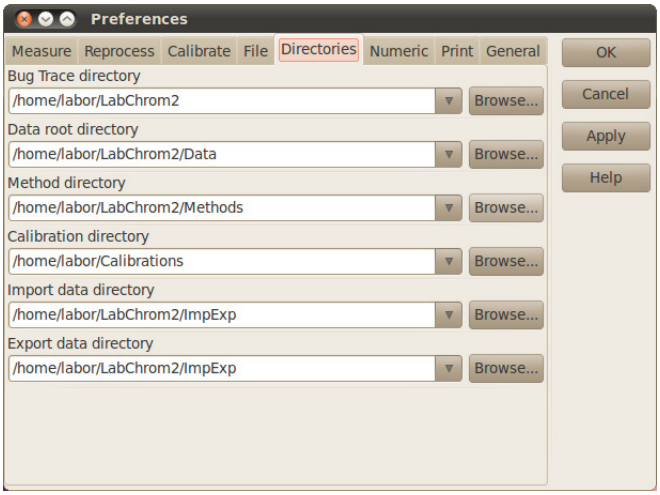

Figure 3.1:

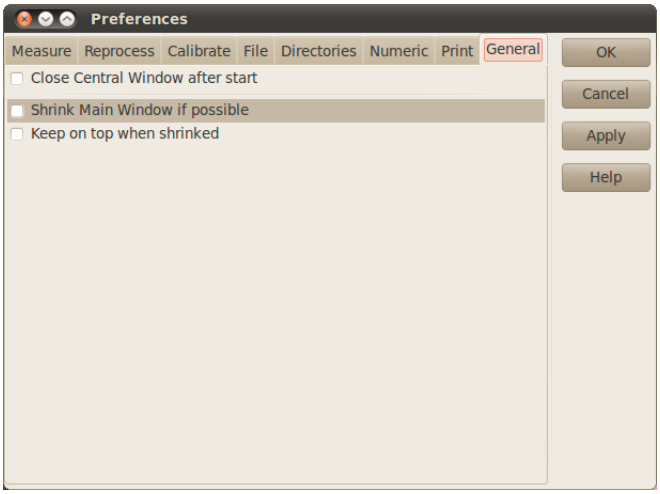

Figure 3.2:

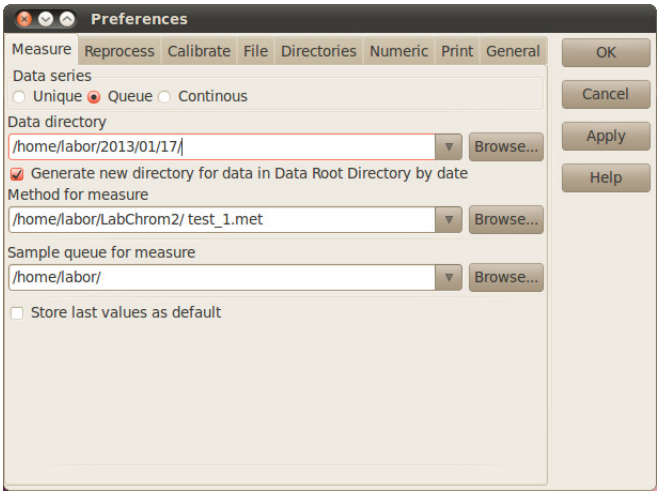

Figure 3.3:

3.2 System-wide

3.3 Measure

3.4 Numeric format

3.5 Printing

3.6 Encoding

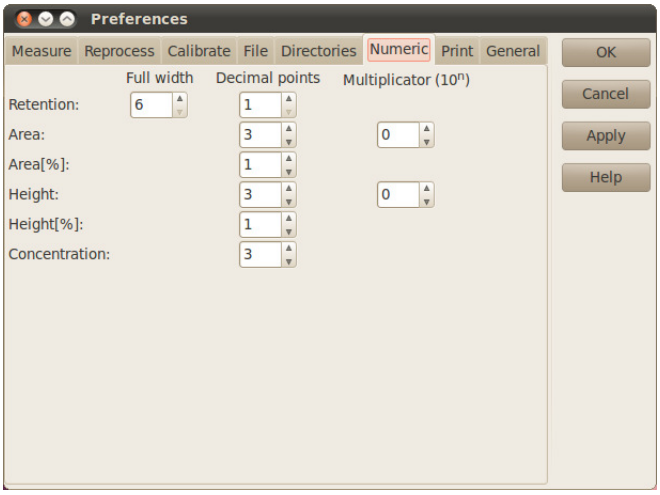

Figure 3.4:

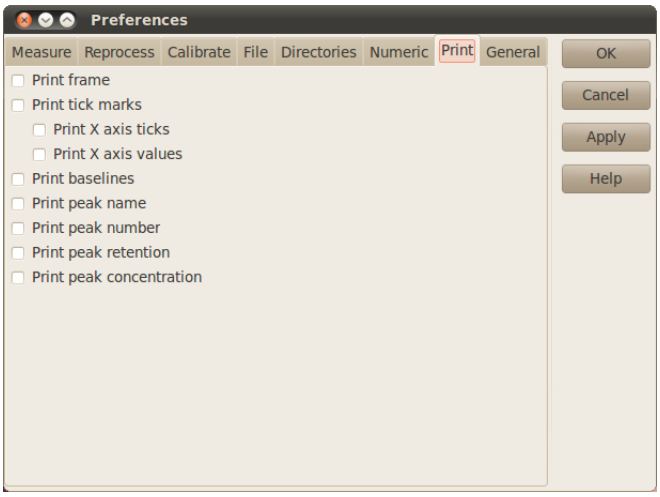

Figure 3.5:

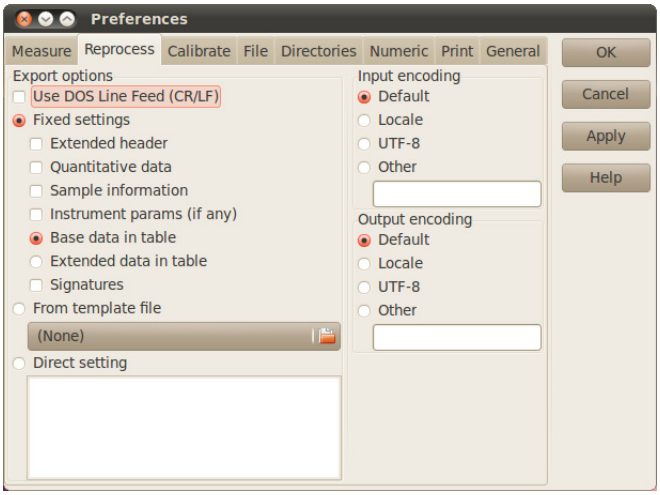
Preferences
Measure
Reprocess
Calibrate
File
Directories
Numeric
Print
General
OK
Cancel
Apply
Help
Export options
Use DOS Line Feed (CR/LF)
Fixed settings
Extended header
Quantitative data
Sample information
Instrument params (if any)
Base data in table
Extended data in table
Signatures
From template file
(None)
Direct setting
Input encoding
Default
Locale
UTF-8
Other
Output encoding
Default
Locale
UTF-8
Other

Figure 3.6:

Chapter 4

Main window

All the software functionality can be accessed from the Main window. You can

- recall and store again existing, previously measured layer data
- print a layer data set, print the chromatograms, the results
- reintegrate the chromatograms
- make a calibration
- do calculations

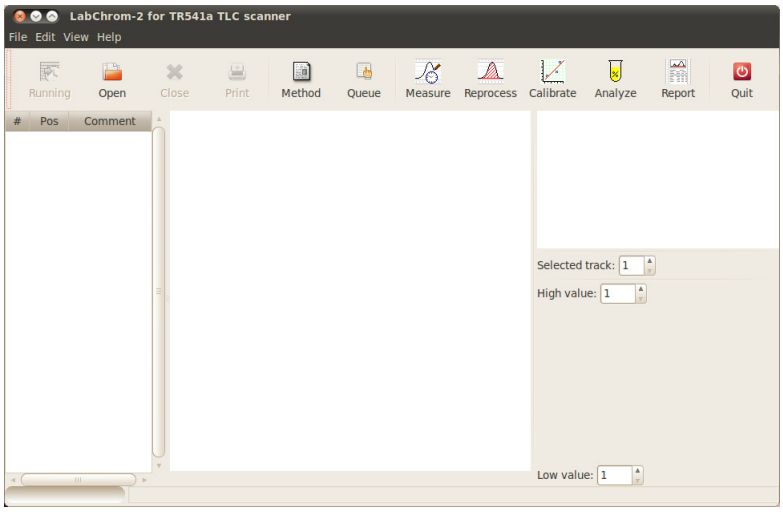

Figure 4.1: The Main window

The toolbar can be divided to four parts:

- Recall related buttons
- Prepare method templates

- Functions from measure to analysis
- Exit

The first four buttons control the handling of an existing layer, the functions are detailed in section 4.2.

With the next two buttons you can assemble method and sample queue templates for themeasures that will be executed later, see section 4.3.

4.1 Preferences

4.2 Recall an existing layer

If the user wants to open an existing — previously measured — layer, should press the `Open` button. A file opening window will appear and can be selected the necessary layer.

- You need the file which has extension "`.lay`" only, *not* the "`.lay.raw`".
- Usually you find your structured (by date) data in `/home/labor/LabChrom2/Data` folder.
- You have to select only the layer file, the additional files (chromatograms, calibration, settings) will be loaded automatically.

Figure 4.2: File selector

When you opened an existing (previously measured) layer, there will be three areas on the screen:

- Left side - the list of the chromatograms on the layer

- Middle - the photographic look image of the layer, graphically noted with tracks, limits, etc.
- Right side - the visualized raw chromatographic data, similar as in the measuring screen

For reintegration you can select an individual chromatogram from the list and double click on it or press the `Reprocess` button.

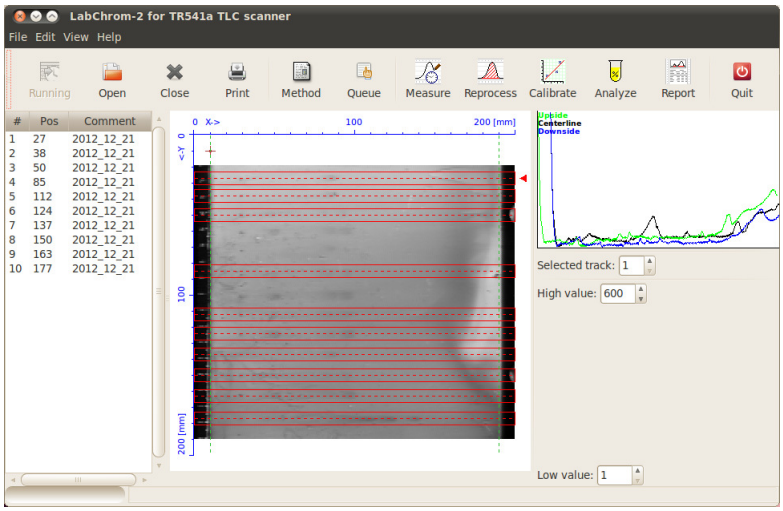

Figure 4.3: Opened layer

A very important function is the printing. Pressing the `Print` button a window pops upwhere we can print the layer image and other data.

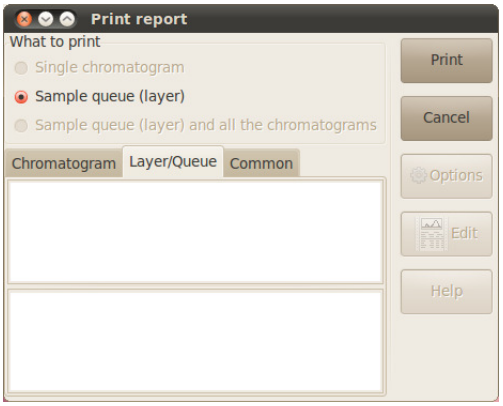

Figure 4.4: Print function

When we press the Print button in window (see picture 4.4) we get a selector window, where we can choose the printing destination. Usually we print to the printer az shown on picture 4.5.

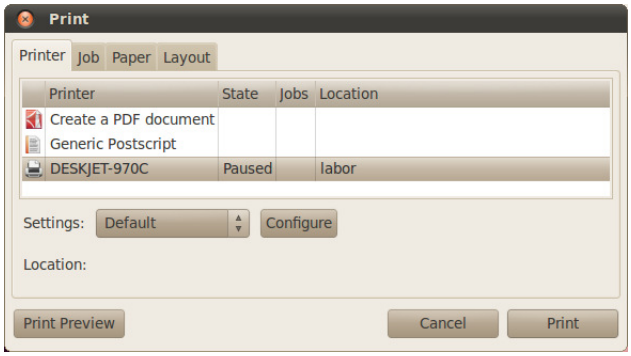

Figure 4.5: Printing to printer

For other purposes we can print to electronic form our data, especially into PDF (Portable Document Format) file as shown on picture 4.6. In that case we should type the output file name and the destination subfolder.

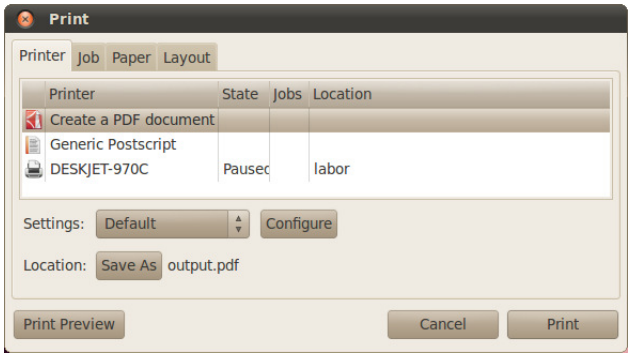

Figure 4.6: Print to PDF file

Before we execute the printing command, we can look the the result (picture 4.7) that we will print by pressing `Print preview` button.

4.3 Setting the method and sample queue

When we start a measure process, the software needs a pre-set method and queue file for preparing of measure.

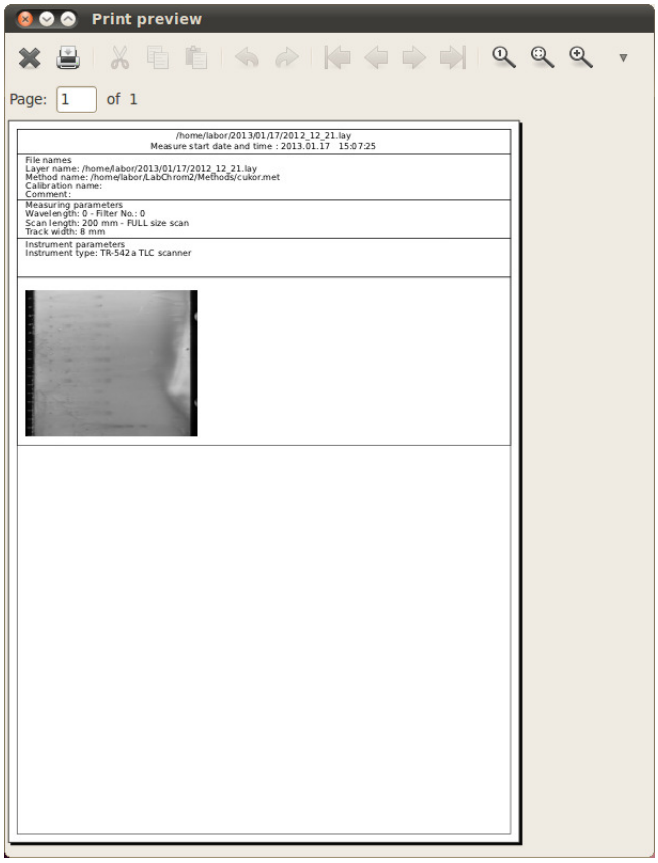

Figure 4.7: Print preview

4.3.1 Method settings

4.3.2 The sample queue

4.4 From measure to report

The purpose of the software is measure, process and print the chromatographic data. In this group of buttons we can select these functions:

- Measure the layer
- Reprocess (reintegrate) the chromatograms on the layer
- Make a calibration table
- Calculate the quantitative results
- Set parameters for report printing

Each of them are detailed in the appropriate section.

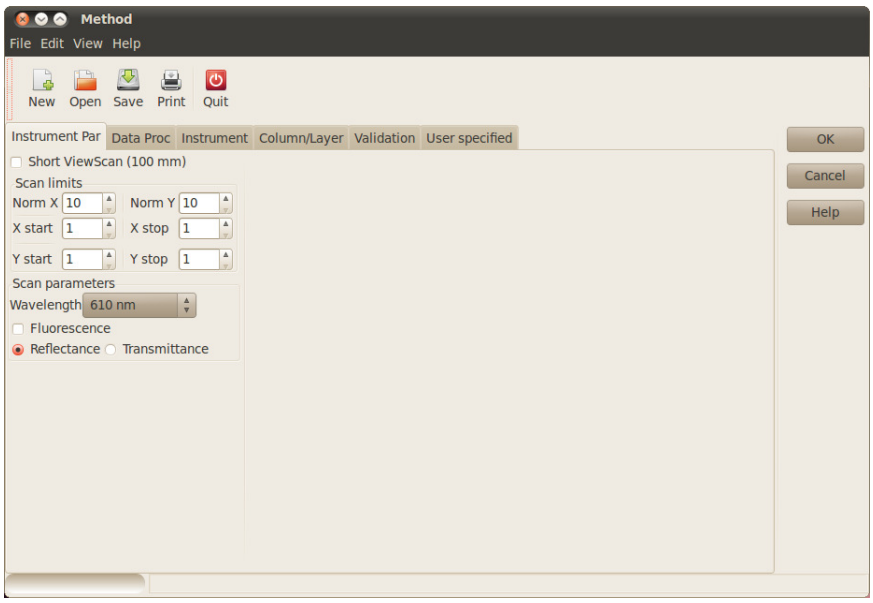

Figure 4.8: Method settings - instrument parameters

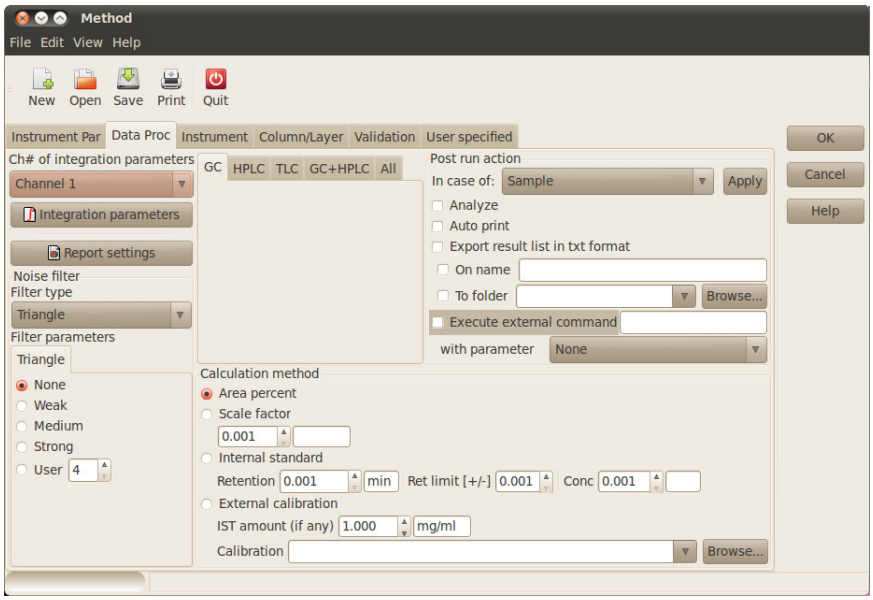

Figure 4.9: Method settings - data processing parameters

4.5 Exit

If you want to leave the program, press `Quit` button, a confirmation window will appear and program can be closed. Do not forget:

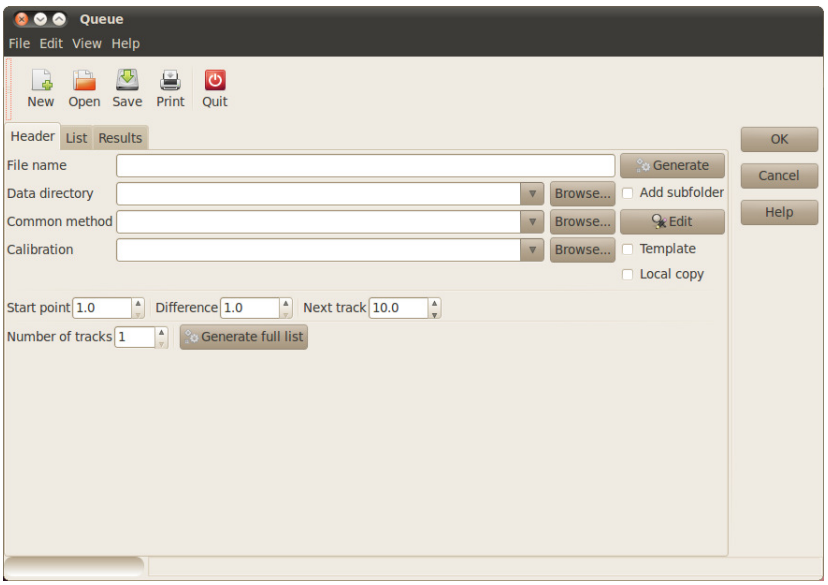

Figure 4.10: Sample queue - header

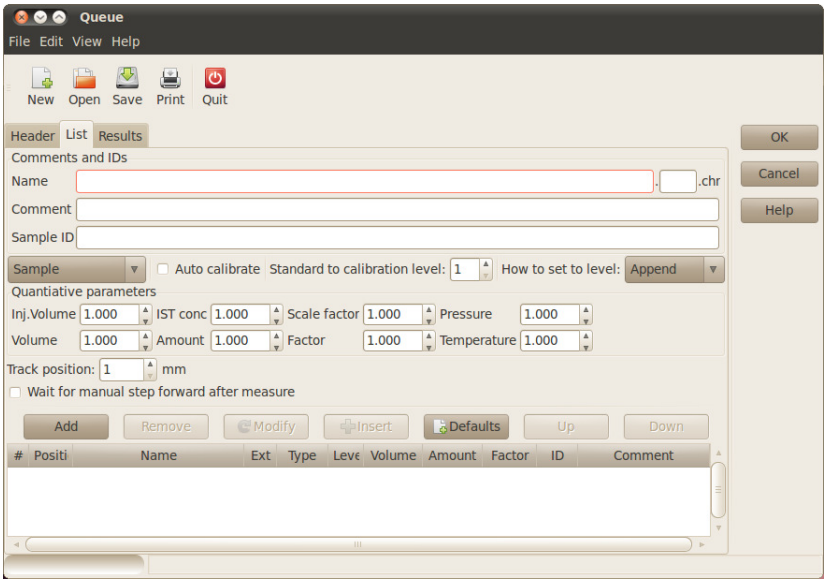

Figure 4.11: Sample queue - list

- Save your unsaved items, for example chromatograms
- To finish (wait the end) of your running measurement process if any

If you modified any settings, preferences, they will be saved now, no user interaction need.

Chapter 5

Reprocess

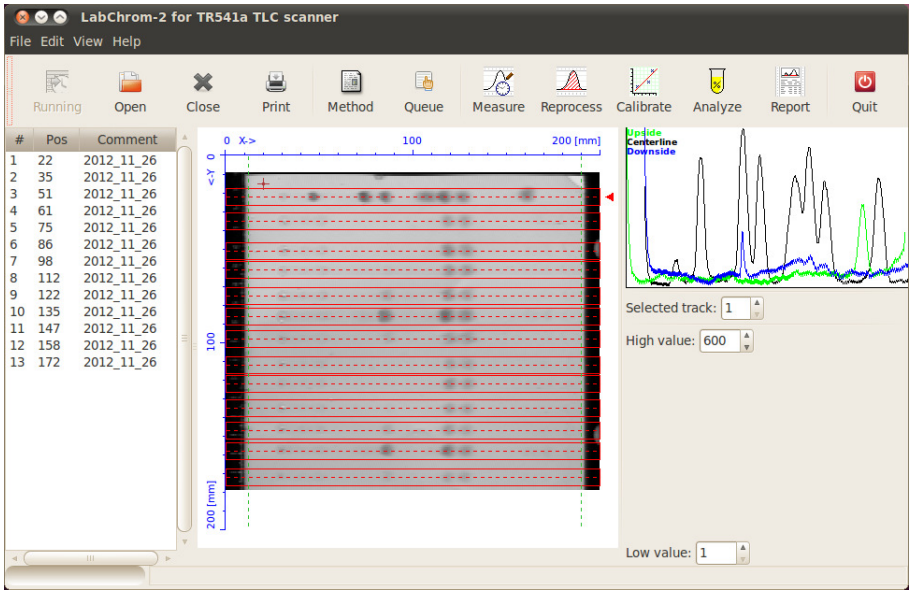

Figure 5.1: Open an existing layer for reintegration

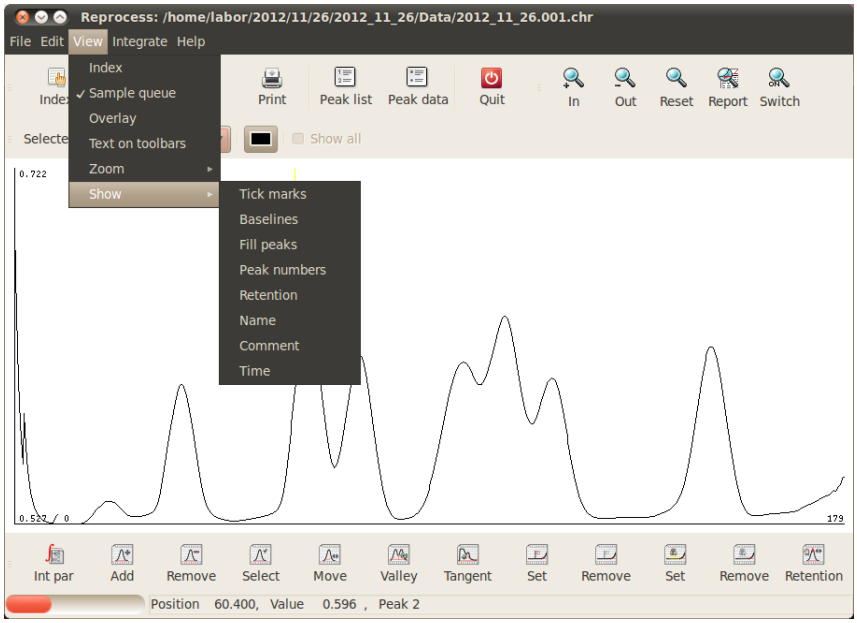

Figure 5.2:

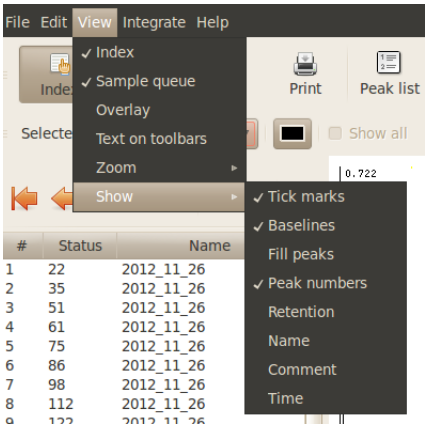

Figure 5.3:

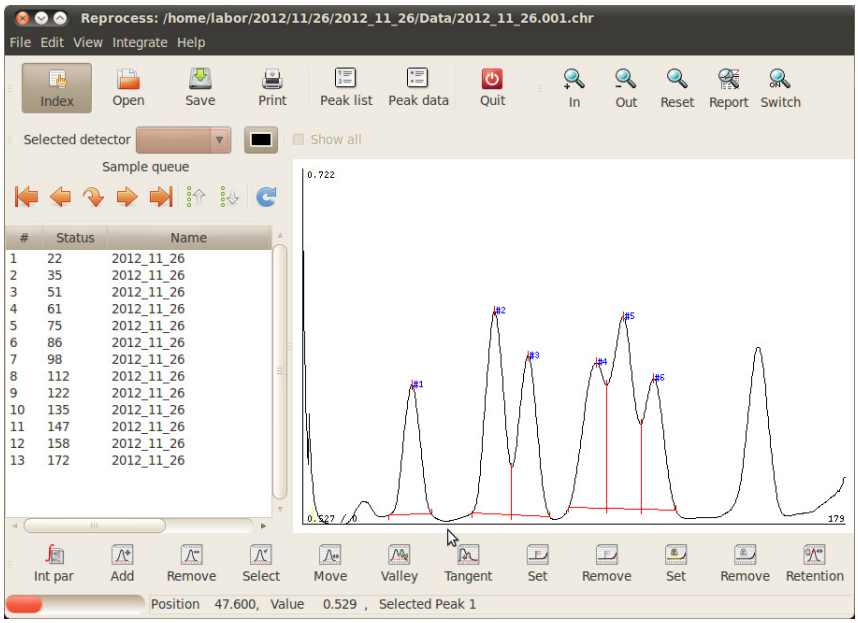

Figure 5.4:

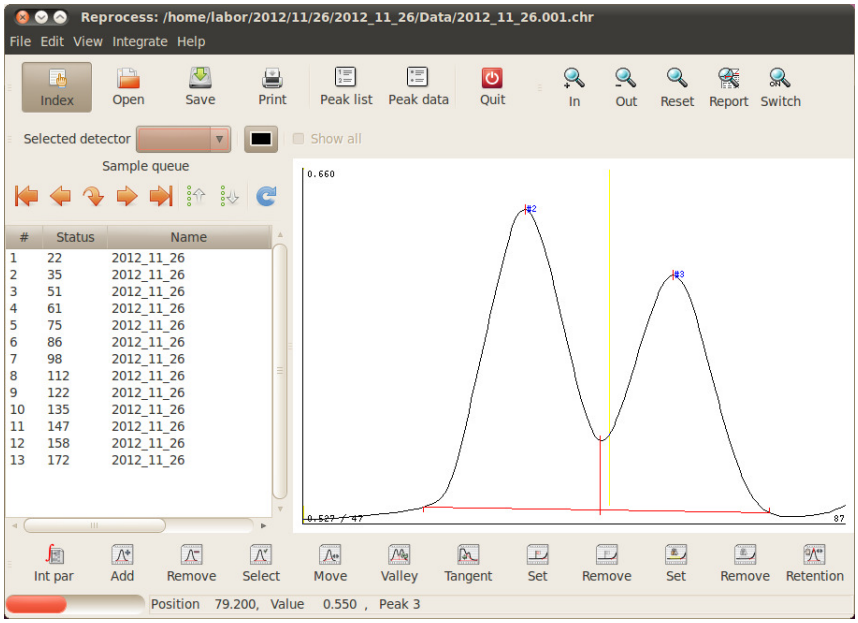

Figure 5.5:

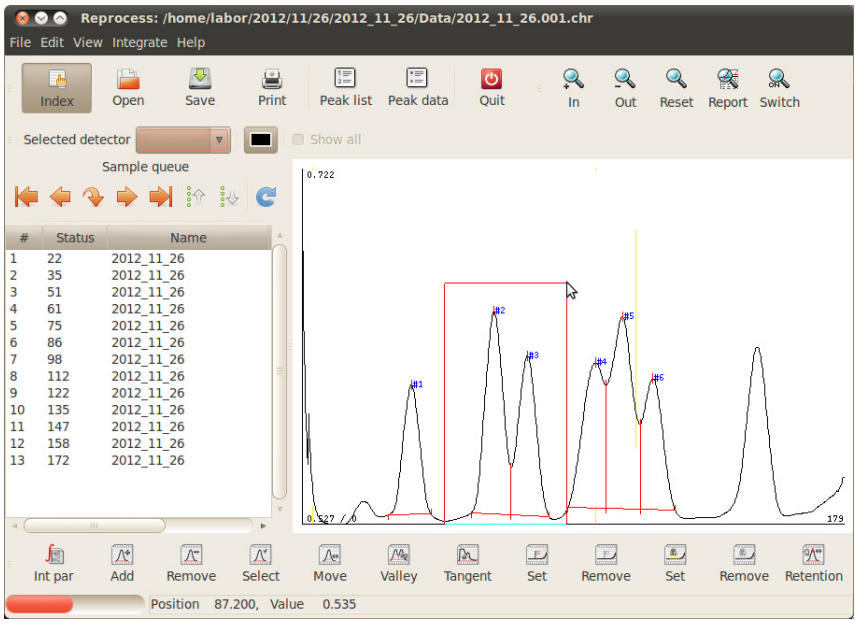

Figure 5.6:

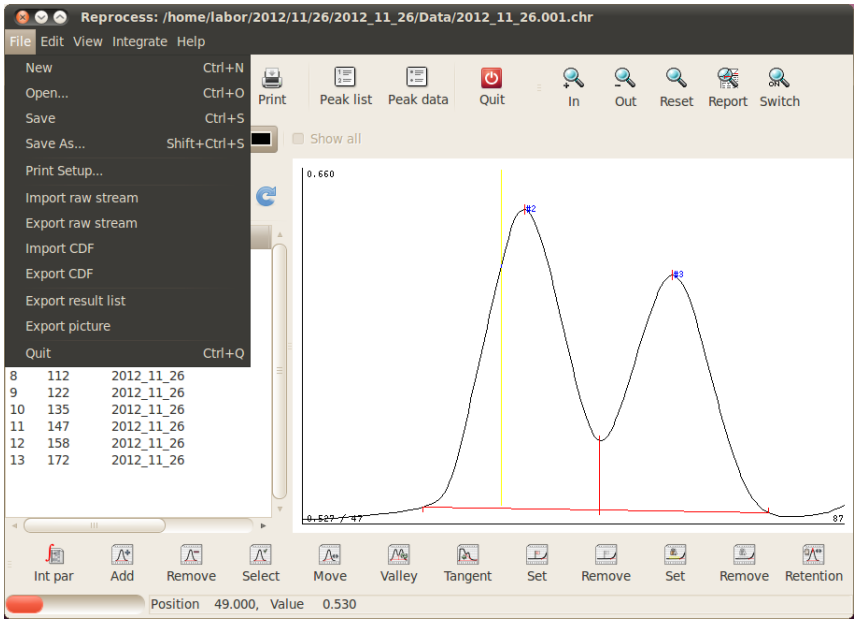

Figure 5.7:

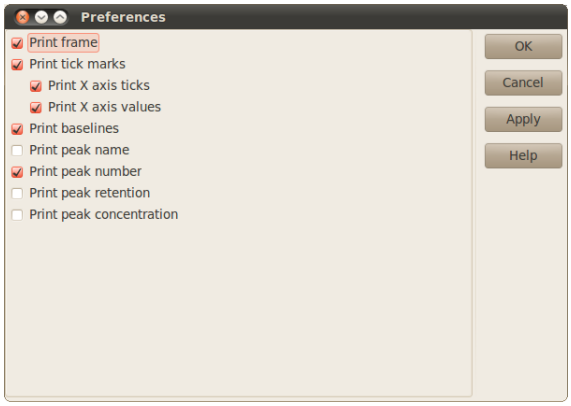

Figure 5.8:

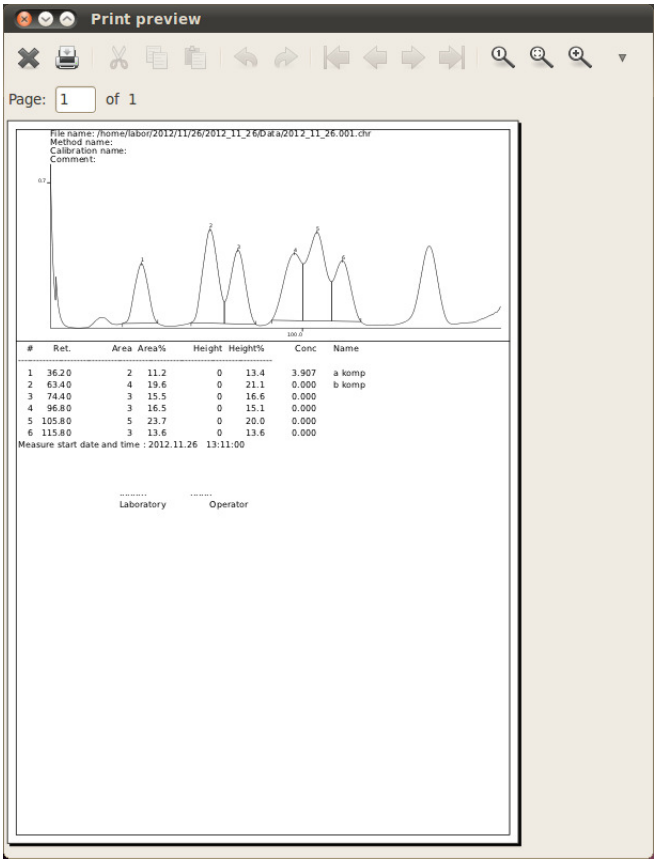

Figure 5.9:

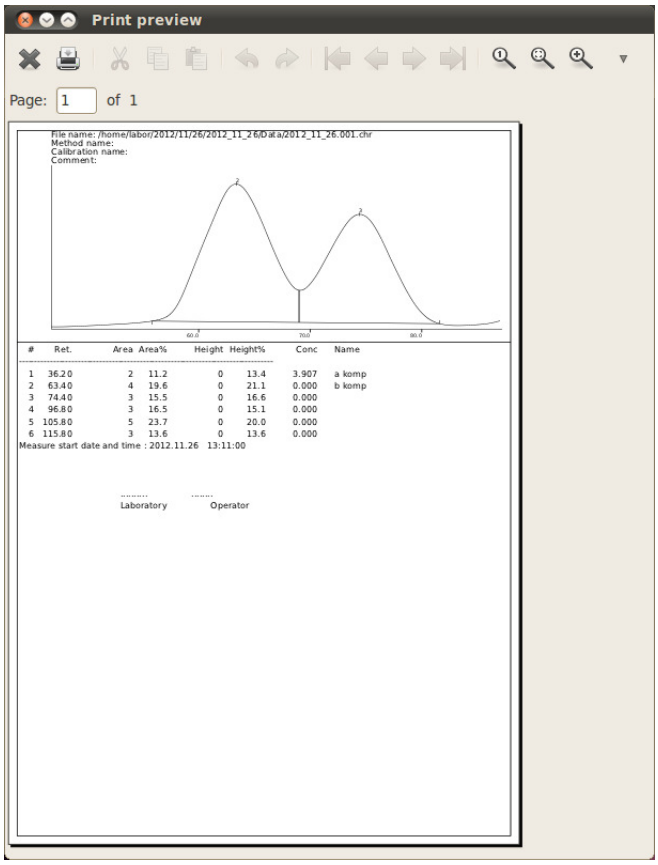

Figure 5.10:

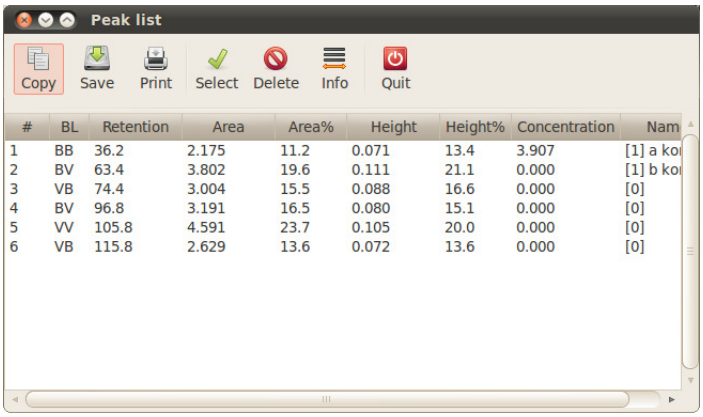

Figure 5.11:

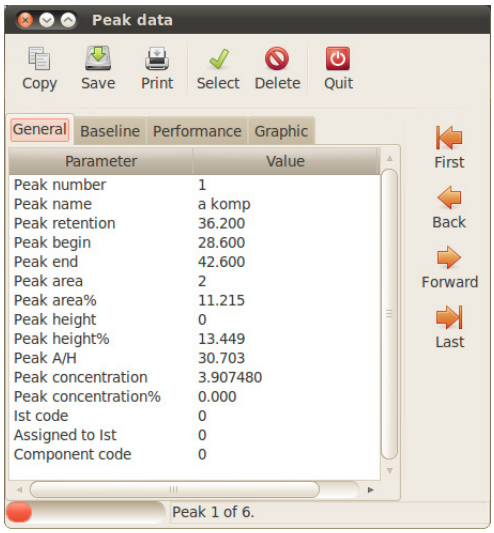

Figure 5.12:

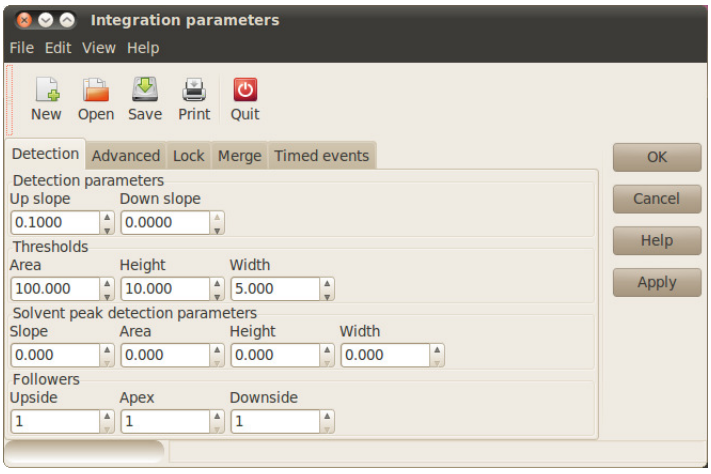

Figure 5.13:

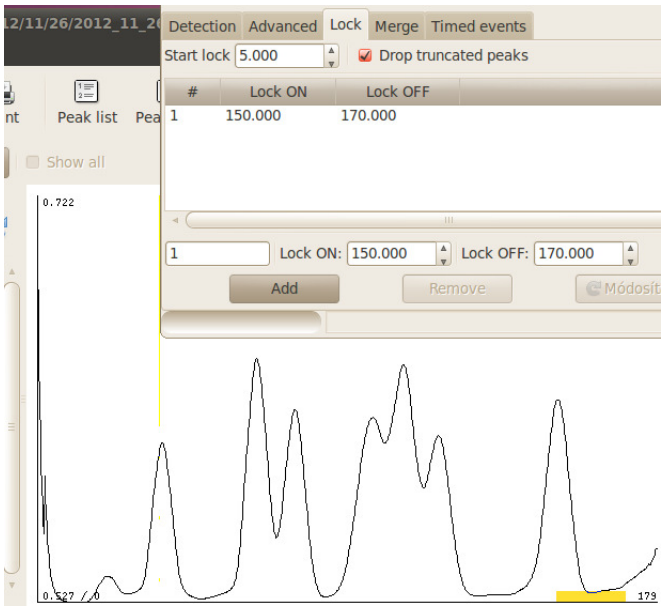
Detection
Advanced
Lock
Merge
Timed events
Start lock 5.000
Drop truncated peaks
Lock ON Lock OFF
1 150.000 170.000
Peak list
Show all
0.722
1
Lock ON: 150.000
Lock OFF: 170.000
Add
Remove
Módosít
179

Figure 5.14:

Chapter 6

Analysis

When we reintegrated the chromatograms and made the calibration table, we can do the concentration calculation. Press the `Analyze` button in the main window, you will get asmall window (see picture 6.1) and press OK button. The results can be seen in Reprocess window (Peak list button) or in the Report print.

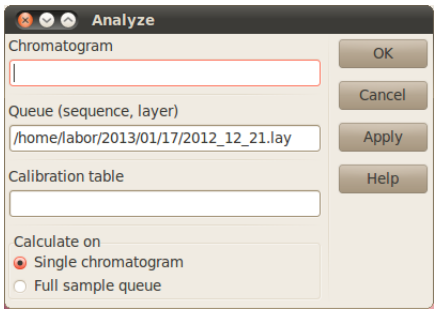

Figure 6.1: Analysis window

Chapter 7

Report edit

The final step in a measure process is the printing the results. There are three printing possibilities:

- Layer report
- Chromatogram report
- Calibration report

In this chapter we can set the layer report parameters.

7.1 The layer report settings

There is a common option for the reports: `Draw frame` checkbox. If you check it, the different parts of the report will be separated by a frame and you can set the frame line width.

7.1.1 The header settings

On the `Header` tab there are options for the report header settings:

- `Print graphic` - turns on/off the layer image printing
- `Print file names` - turns on/off the printing of essential file names that controlled the measure process
- `Instrument description` - turns on/off the printing of instrument parameters were set in measuring process
- `Measuring parameters` - turns on/off the printing of measuring parameters were set in measuring process

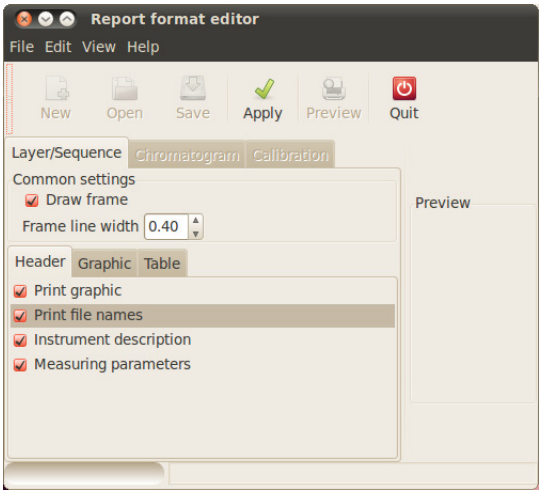

Figure 7.1: The layer report header settings

7.1.2 The graphic settings

If you chechk the `Print graphic` on the `Header` tab, you can set detailed otions for the layer image printing. The following options are available:

- `Rulers` - turns on/off the printing of rulers by other word the scale in millimeters
- `Track limits, reference coords` - turns on/off the printing of begin/end coordinates for X and Y axis and the normalization (white reference) point.
- `Draw chromatograms` - turns on/off the printing of chromatograms (of course in small size) near the layer image
- `Only scanned image` - turns on/off the printing of reduced size of image. The layer size is 200×200 mm and the layer image is set to this size independently the scanned area. If you chceck this option the image area will be fitted to the scanned image size only, will occupy smaller area on the report.
- `Frame around layer image` - turns on/off the printing of a weak frame (quadratic line) around the layer image. This option is independent from `Draw frame` checkbox.
- `Scale image` - turns on/off the printing of scaling the image. You can shrink or magnify the printed layer image by multiplying a value.

7.1.3 The table settings

There are two options and some selector and parametersthat control the result table generating.

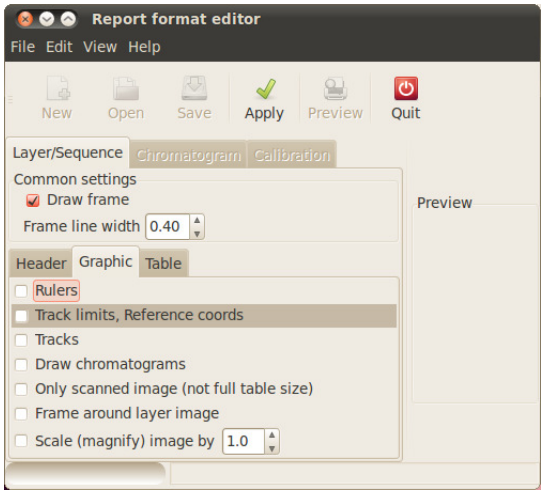

Figure 7.2: The layer report graphic settings

- `Print result table` - turns on/off the printing the result table
- `Start at new page` - turns on/off a form feed before printing the result table

When the software assembles the table,there are some important parameters that controls, how to select the relevant peaks across the chromatograms on the layer. You must give a retention range in which the peaks will be found. Its value is usually between 2-10 mm, depends on smallest distance between peaks (spots) on the layer. The number of selected/printed peaks in the table depend on the following seletor:

- `All` - the software tries to sort the peaks to one (sometimes big) table.
- `Only relevant` - the softwareselects only the relevant peaks, the number of peaks can be set in the numeric field.
- `From reference` - if you have a chromatogram (track) that contains all the peaks that you want to report, this is the useful selection but you should ensure, that this chromatogram must not contain any other (for example noise origin) peaks.

Generally we can advice, the chromatogram should not contain any junk peaks, only the real, purposeful ones. You can clean the chromatograms in the Reprocess/Reintegrate window if necessary.

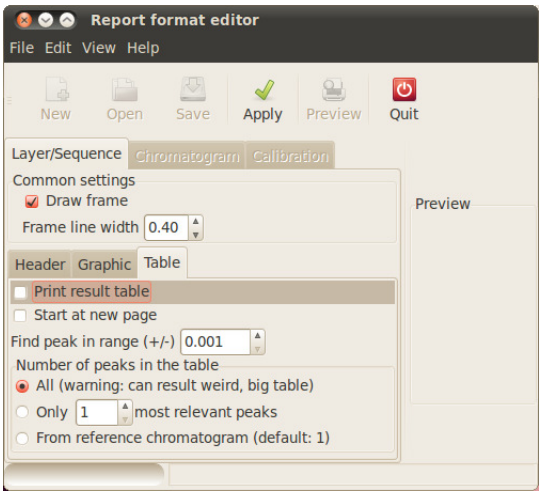

Figure 7.3: The layer report table settings

Part III

Appendix

Chapter 8

Recover damaged layer data

Chapter 9

Upgrade

List of Figures

List of Tables