

LabChrom-2 & TR-542a

Chemotron Instruments

1991-2011

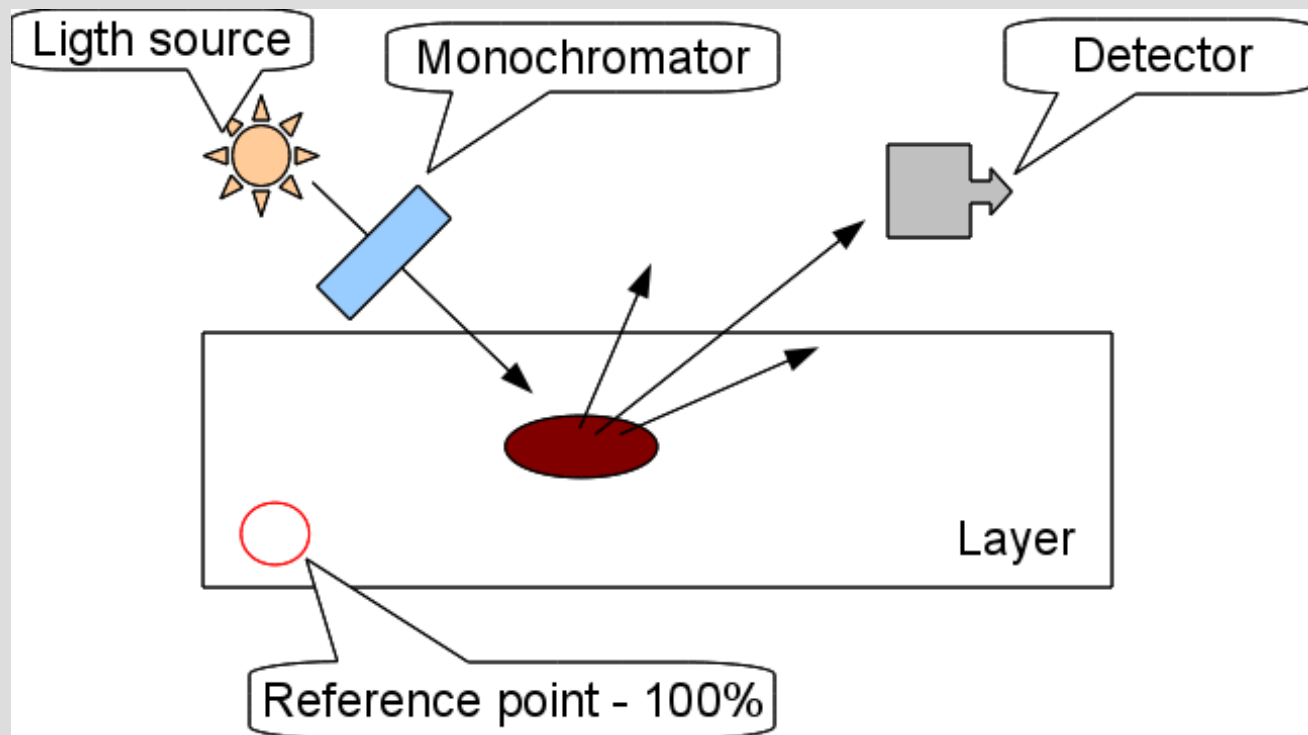
Measurement basics

Three types of measuring methods, by interaction of light

- ◆ Reflectance, TLC
- ◆ Fluorescence, mainly TLC
- ◆ Transmission, gel

Measurement basics

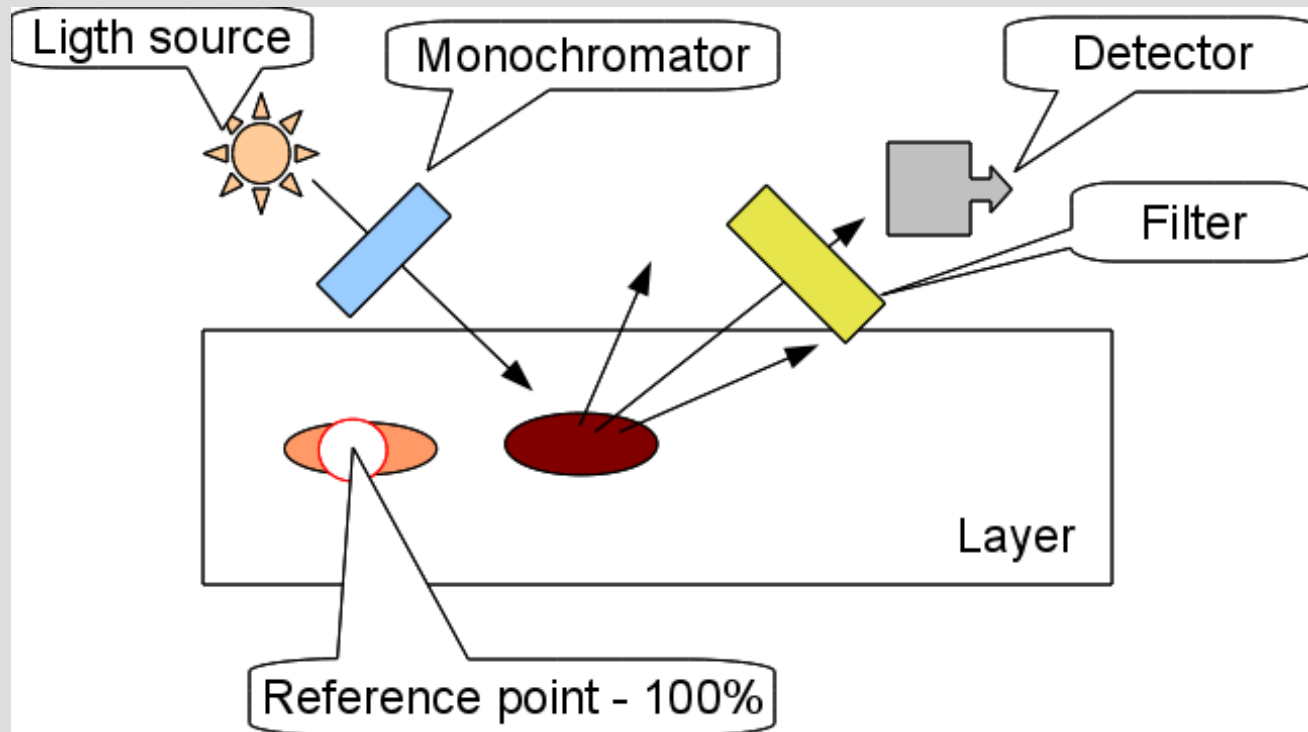
◆ Reflectance



The reference point is the „whitest” (lightest) area

Measurement basics

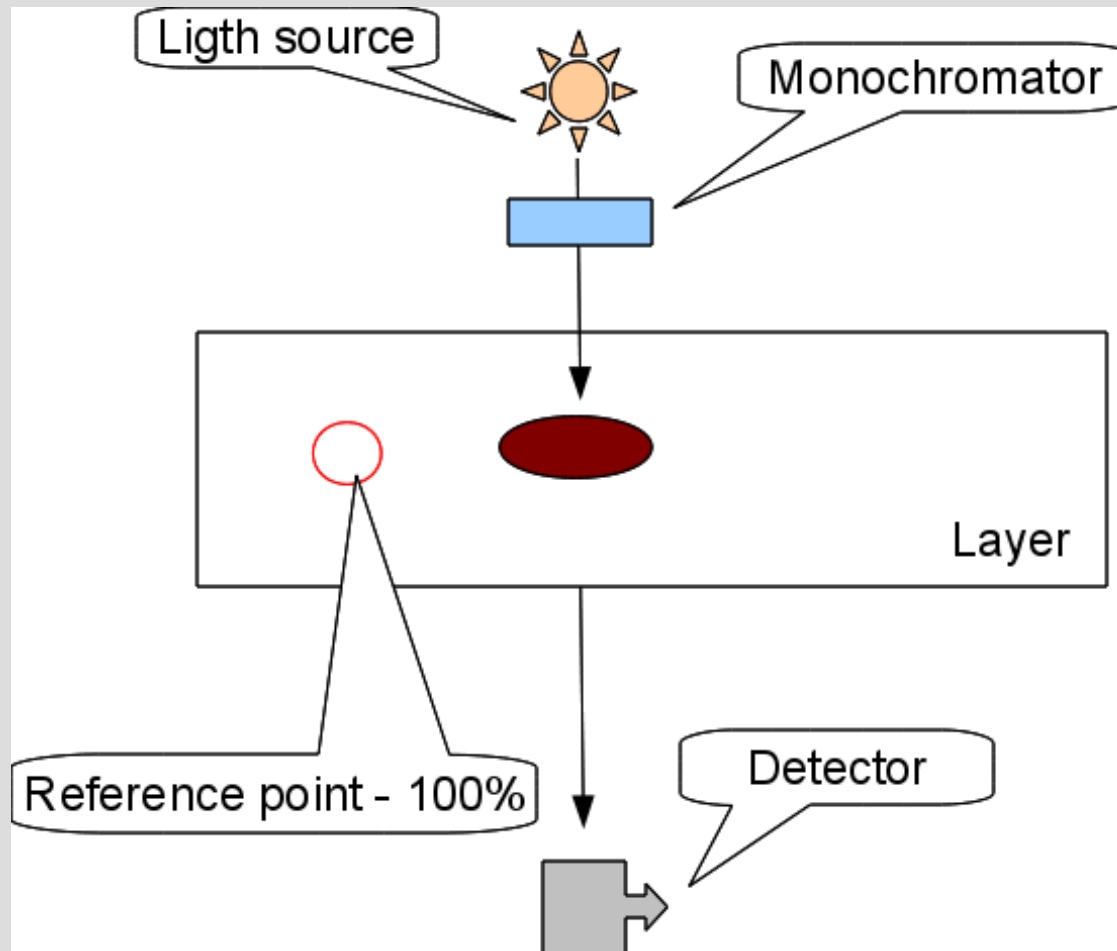
◆ Fluorescence



The reference point is the lightest spot on the layer

Measurement basics

◆ Transmission



Measurement settings

- ◆ Make a *Method* file
- ◆ Save it
- ◆ Set in *Preferences*
- ◆ Start measure
- ◆ Make modifications if necessary

Measurement settings - Make a Method file

◆ Main window → Method

Instrument Par Data Proc Instrument Column/Layer

☐ Short ViewScan (100 mm)

Scan limits

Norm X 10 Norm Y 10

X start 1 X stop 1

Y start 1 Y stop 1

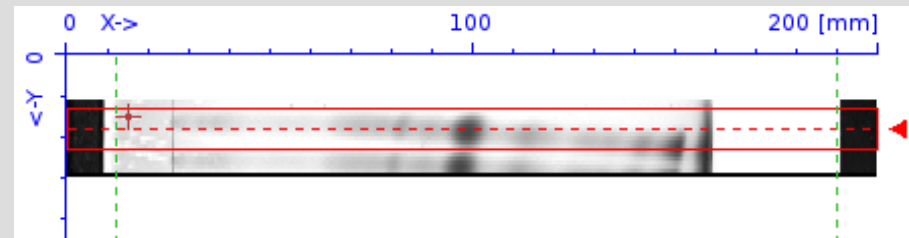
Scan parameters

Wavelength 614 nm

☐ Fluorescence

☒ Reflectance ☐ Transmittance

- Short ViewScan – for 100 mm wide layers
- Norm X,Y – coordinates for reference point, designated by a light red cross, usually in upper left corner
- X start, stop – chromatogram recording start-stop retentions (in mm unit)
- Y start, stop – upper and lower track limits



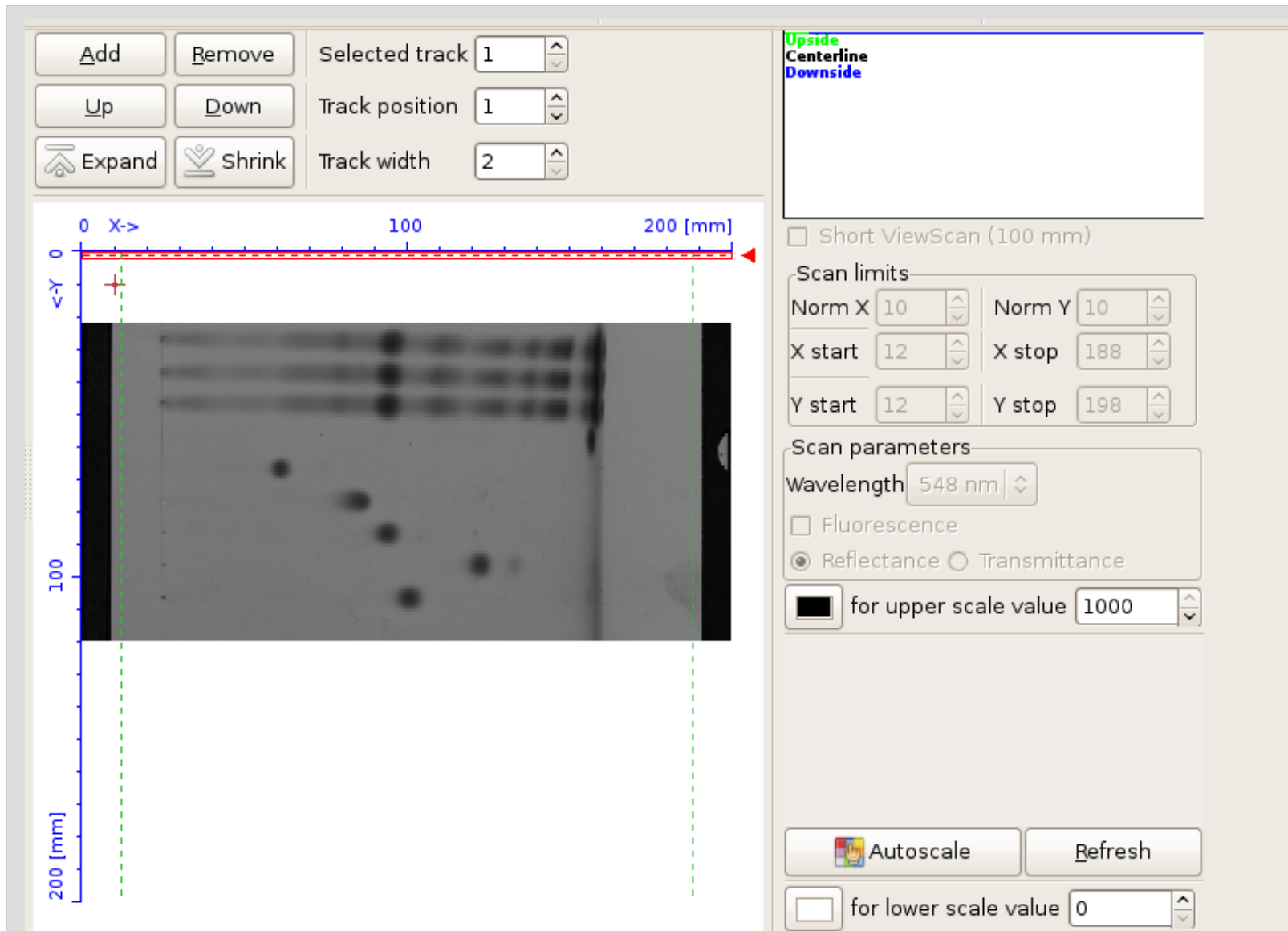
Measurement – The ViewScan

The ViewScan is a full resolution layer scan, between Y start/stop limits and in 200 mm (or 100 mm in case of short view) length of the layer.

The purpose: to get the whole layer data and in the next step you can easily select the desired tracks.

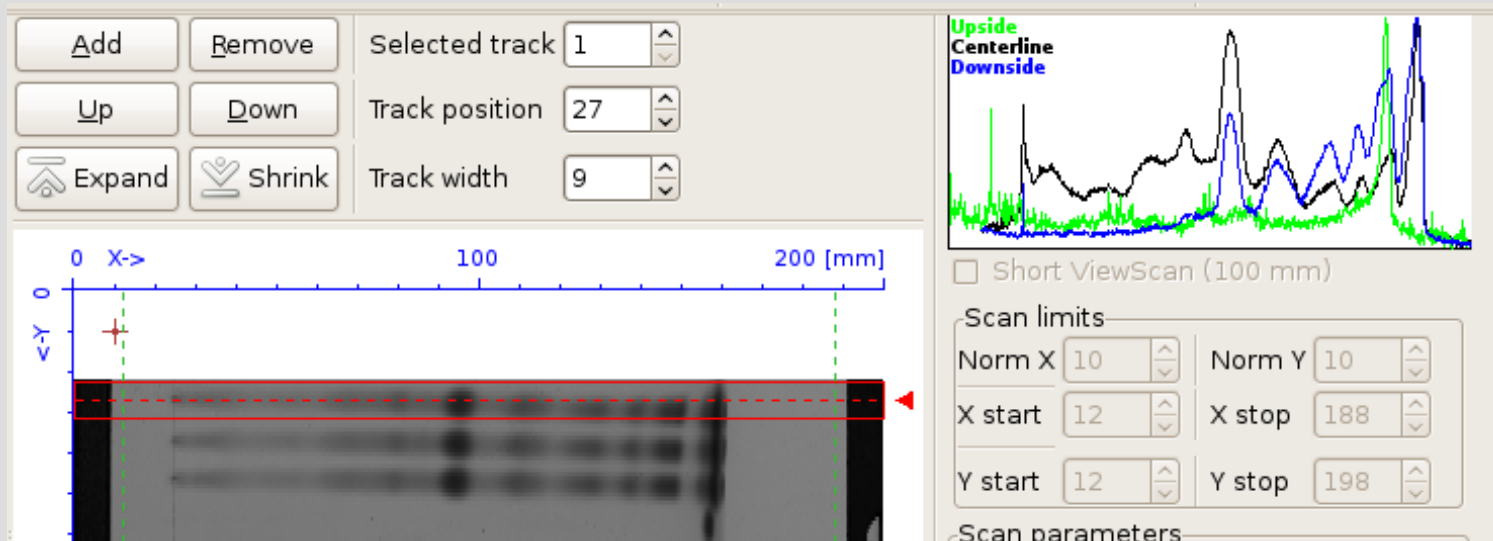
All the data is available now.

The ViewScan



Track handling

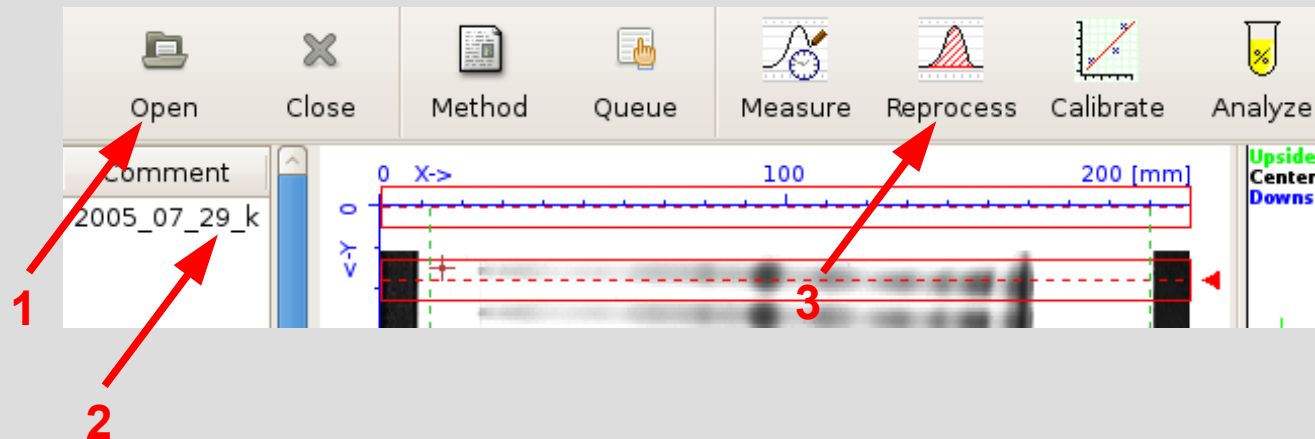
- ◆ After the ViewScan executing we can handle tracks:



- Add, remove tracks
- Modify their positions
- Modify the track width
- Visually detect the track side, if their width is too wide or too narrow

Main window - Open an existing layer

- ◆ Click on the **Open** button and select the „.lay” file which you need (1)
- ◆ Select the track from the list that you want to process (2)
- ◆ Go to **Reprocess** window (3)

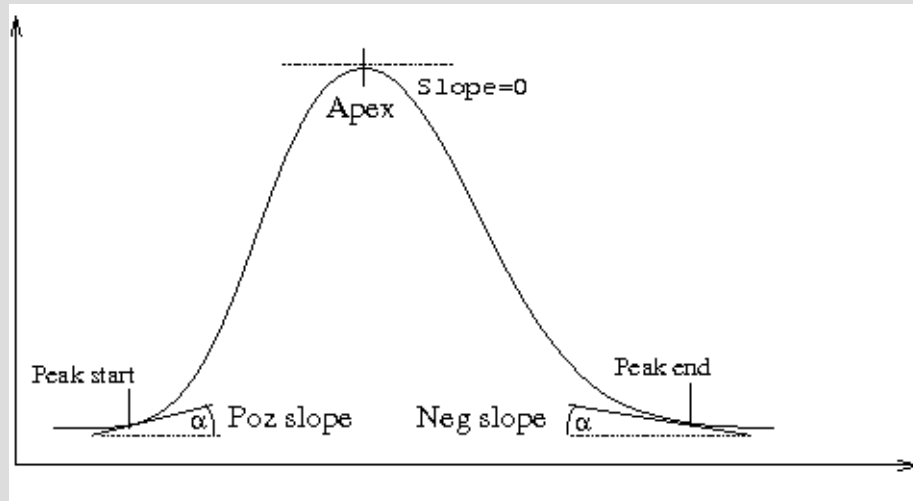


The Reprocess window

- ◆ Reintegrate
 - ◆ Compare / overlay
 - ◆ Save
 - ◆ Export
 - ◆ Print
- the chromatograms.
- The integration can be
- ◆ automatic (by parameter set)
 - ◆ manual

Integration basics

◆ How to detect a peak?

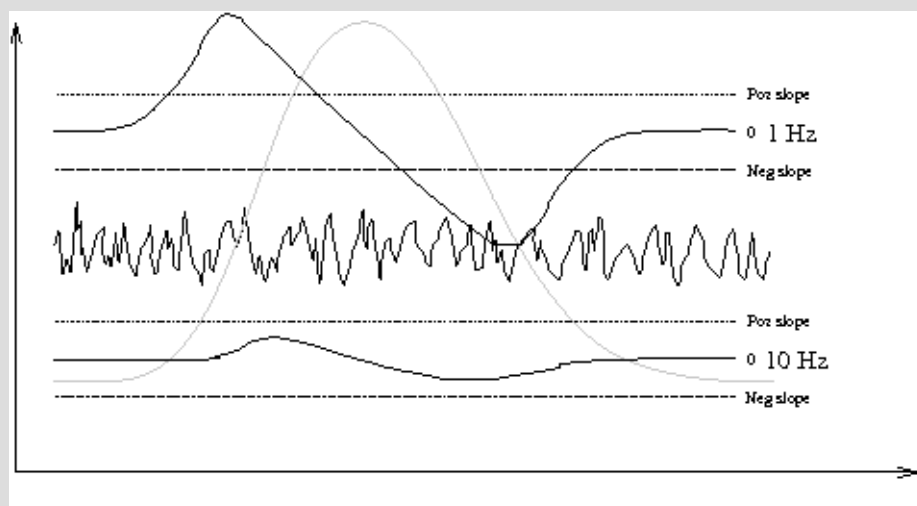


The software continuously calculates the derivative values of data stream. When the derivative value is higher than a previously set threshold value it detects as a peak start.

When this value's sign turns from positive to negative, this signals it is a peak apex. The peak end is detected by a negative slope threshold, similar to the peak start.


Peak detection - derivation

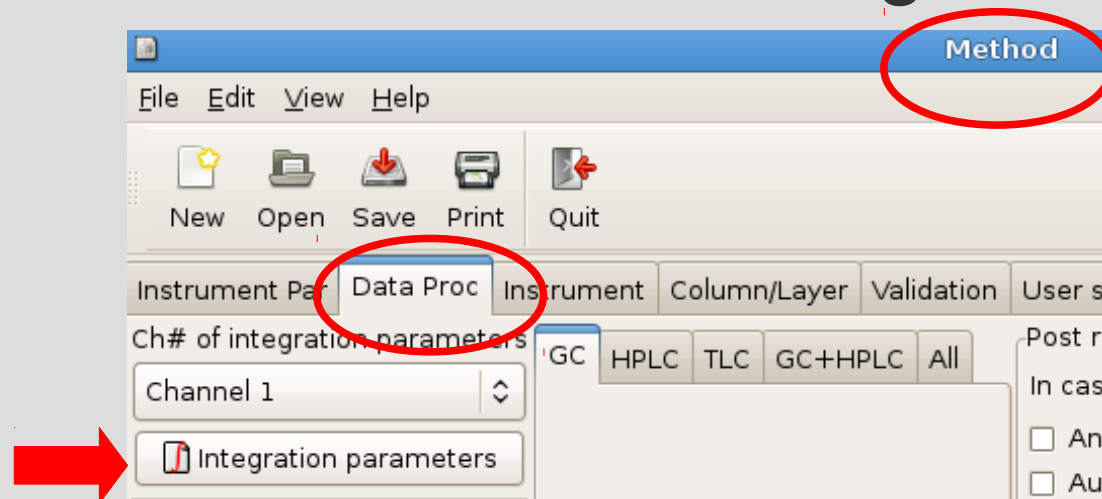
◆ Look, how does it work



When the sampling rate is not in concerning with peak width, the derivative data values can be too low, the peaks can not be detected.
In TLC scanning the sampling rate therefore is 0.2 mm, that give detectable peaks.

Integration parameters

- ◆ Select the integration button to set the parameters. 
- ◆ If the parameters give acceptable result, then you can store these parameters in the **Method** file and the next measure process will be finished with good automatic results



Integration parameter settings

◆ The detection parameters: slope and threshold

The screenshot shows a software window with the 'Detection' tab selected. It contains several sections for configuring peak detection parameters:

- Detection parameters:** Includes 'Up slope' (10.000) and 'Down slope' (-10.000).
- Thresholds:** Includes 'Area' (10000.000), 'Height' (1000.000), and 'Width' (0.100).
- Solvent peak detection parameters:** Includes 'Slope' (0.000), 'Area' (0.000), 'Height' (0.000), and 'Width' (0.000).
- Followers:** Includes 'Upside' (1), 'Apex' (1), and 'Downside' (1).

On the right side of the window, there are four buttons: 'OK', 'Cancel', 'Help', and 'Apply'.

- Slope: as shown on *Integration basics* slide
- Thresholds: **All** the three thresholds values have to be override to detect a peak. They have logical *AND* connection.
- Solvent: Do not care in TLC scanning, it is a GC speciality
- Followers: If the signal is too noisy, the peak detection can be unstable, try to increase the appropriate values to 2 or 3. Those are calculated in data points unit.

Integration parameter settings

◆ The lock table

Detection Advanced **Lock** Merge Timed events

Start lock 0.000 ☐ Drop truncated peaks

#	Lock ON	Lock OFF
1	1.000	46.000

1 Lock ON: 1.000 Lock OFF: 46.000

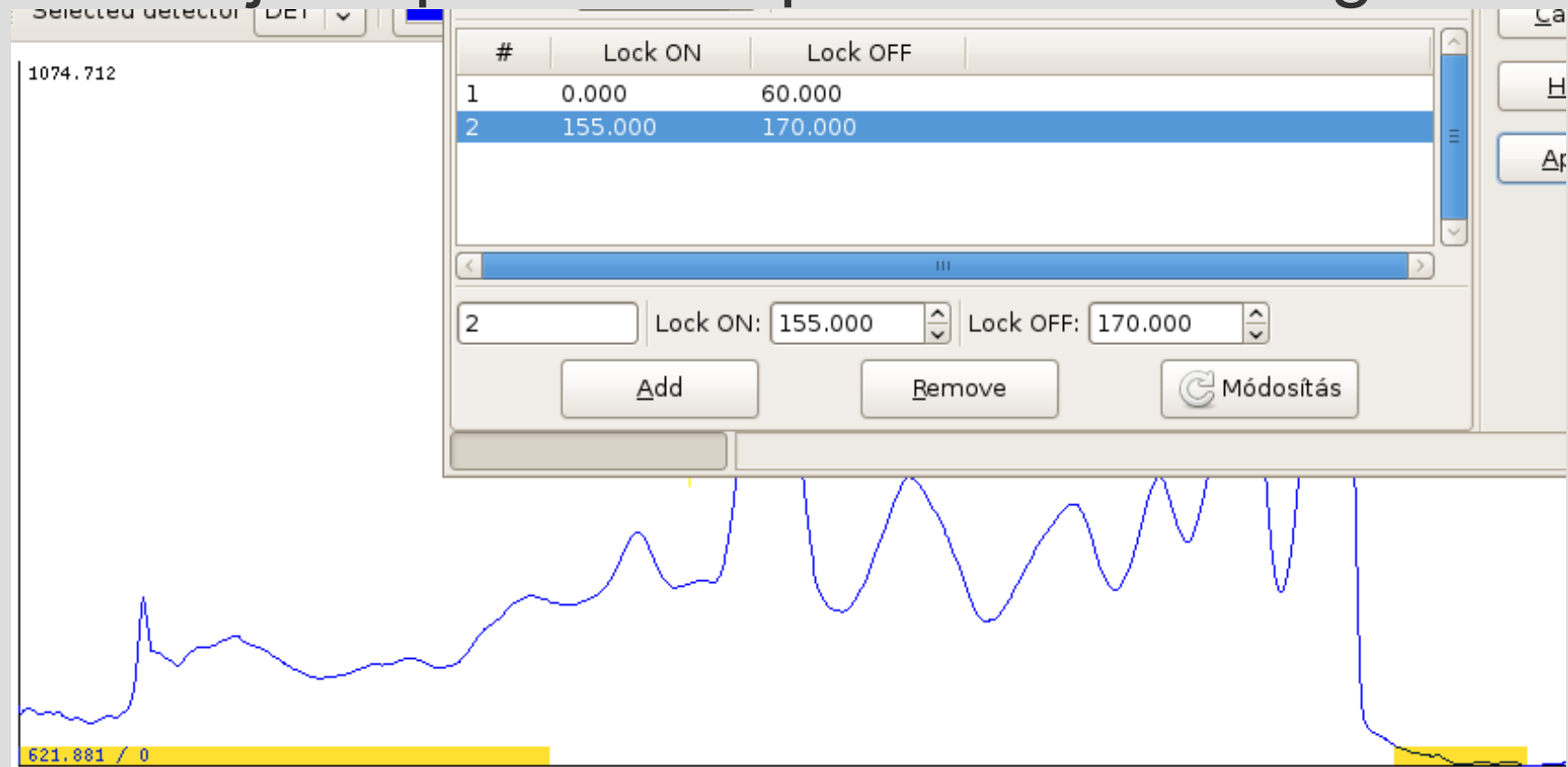
Add Remove Módosítás

OK Cancel Help Apply

You can add, remove and modify existing lock areas.

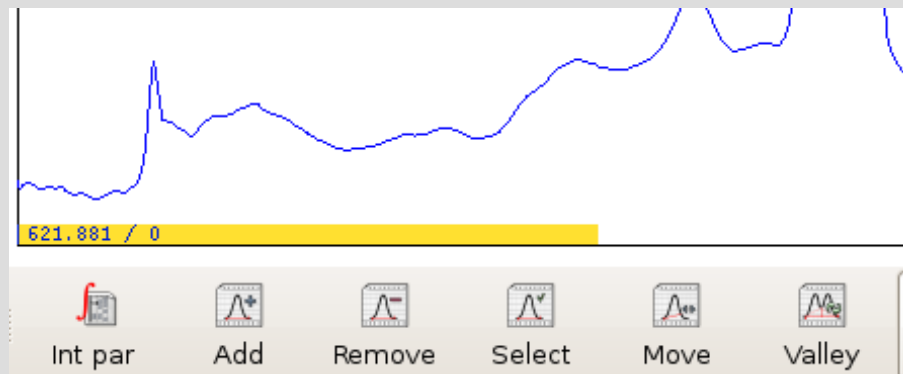
How lock works?

- ◆ The locked area are excluded (shown with yellow bars) from integration, it is very useful when junk peaks are present in the signal.



Manual integration

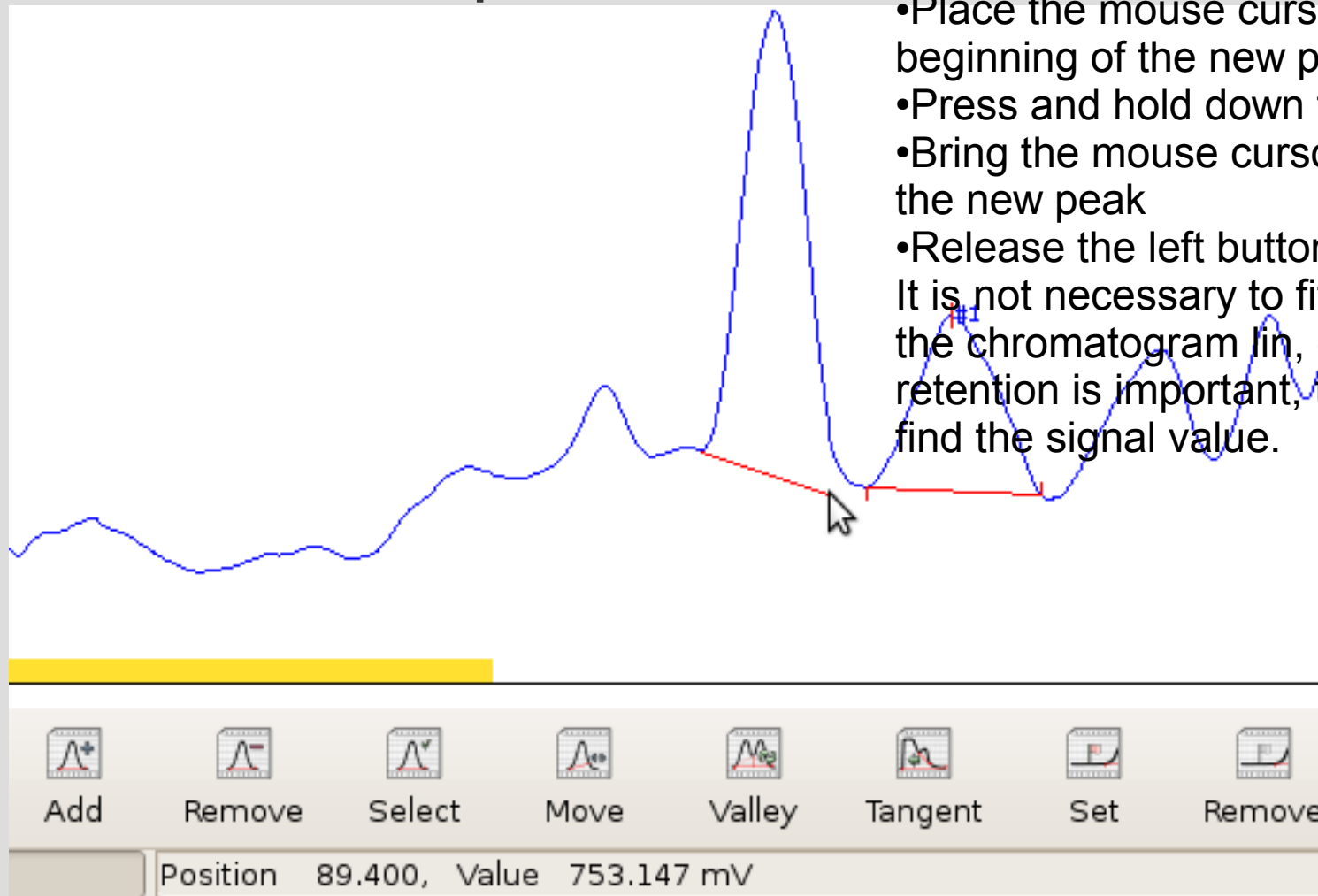
- ◆ You can add, remove, modify peaks manually



Add peak

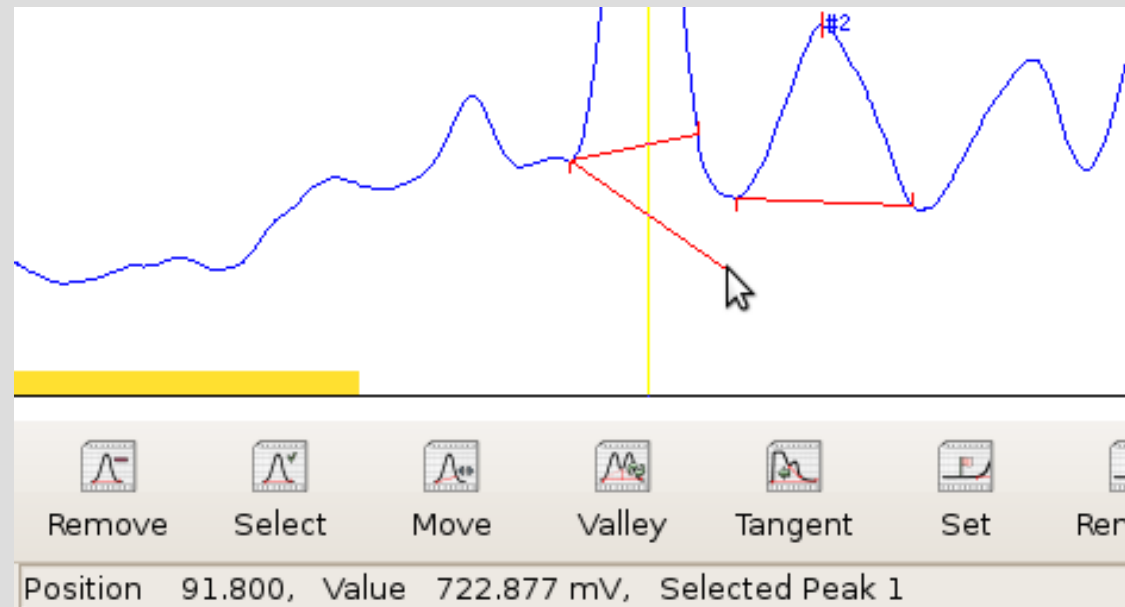
◆ How to add peaks?

- Press „**Add**” button
 - Place the mouse cursor to the beginning of the new peak
 - Press and hold down the left button
 - Bring the mouse cursor to the end of the new peak
 - Release the left button
- It is not necessary to fit the points to the chromatogram line, only the retention is important, the software will find the signal value.



Delete - Move

- ◆ To delete a peak from the list, first click in the peak area, the yellow cursor line will be placed there. Then press **Remove** button.
- ◆ To move a basepoint, press **Move** button, drag the basepoint and drop to the new place.

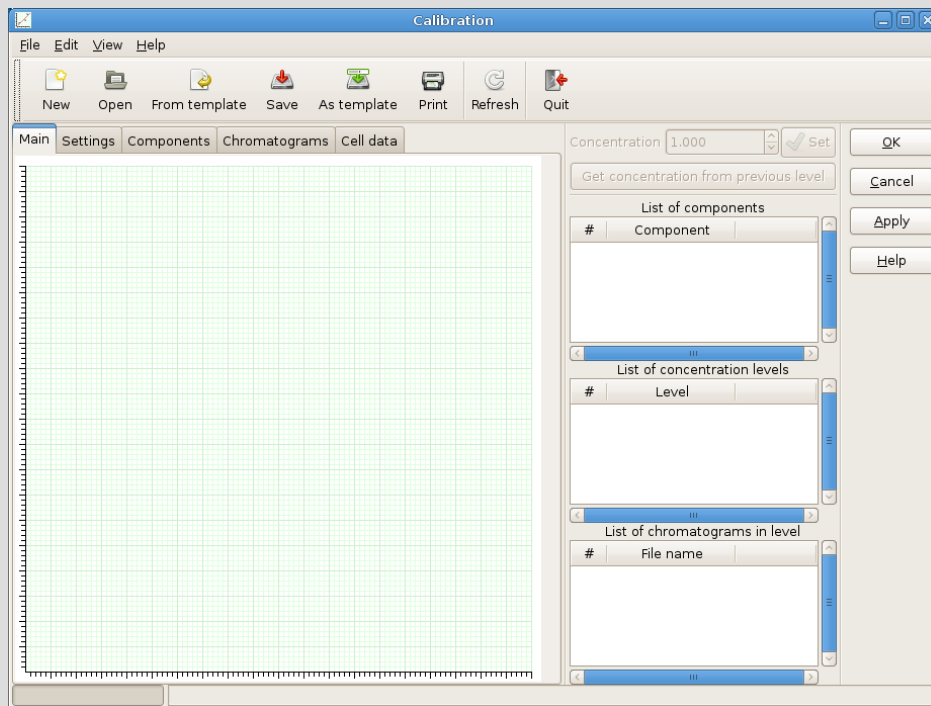


Print

- ◆ To print the results press ***Print*** button.
- ◆ Select the printer.
- ◆ Press Print button.
- ◆ Before you print, in the menupoint „***Printer settings***” you can set the graphical parameters for the print.
- ◆ The report can be directly print to a PDF file.

Calibration

- ◆ Multi component
- ◆ Multi level (concentrations levels)
- ◆ Multi chromatogram (parallel chromatograms inside in one level)



Component settings

◆ Fill the component list

Concentration 1.000

Get concentration from previous level

Template chromatogram to find easier the retentions

Name ☐ Internal standard Detector:

ID num

ID

Detector

Retention

#	Retention
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List of components

#	Component
1	Comp-1
2	Comp-2

When you filled the fields, press **Add** button.

Level settings

◆ Add level names

Main Settings Components **Chromatograms** Cell data

Add / Delete / Modify levels if necessary

Level name

Amount Volume Factor

Inj.vol. IST conc

Temper. Pressure

Add (Delete / Modify) chromatogram to the selected level if necessary

Concentration

List of components

#	Component
1	Comp-1
2	Comp-2
3	Comp-3

List of concentration levels

#	Level
1	Level-1

Fill levels with chromatograms

- ◆ Select a level and **Select/Add** the chromatogram in to the level.

The screenshot shows a software interface with a main window and a modal dialog box.

Main Window:

- Header: "Add (Delete / Modify) chromatogram to the selected level if necessary"
- Text input field: `/home/labor/LabChrom2/Data/2005/07/29/2005_07_29_kamilla K32.001`
- Buttons: "Add", "Remove", "Módosítás", and "Select" (with a magnifying glass icon).
- Form fields: "Chromatogram name", "Comment", "Amount" (0.001), and "Inj.vol." (0.001).

Modal Dialog: "Select chromatogram"

#	Type	Name
1	Sample	2005_07_29_kamilla K32.001.chr
2	Sample	.
3	Sample	.
4	Sample	.
5	Sample	.

Right Panel:

- Section: "List of concentration levels"
- Table:

#	Level
1	Level-1
- Section: "List of chromatograms in level"
- Table:

File name
2005_07_29_kamil

Set concentrations

- ◆ Select a Component **and** a Level, now you can fill the Concentration field.

The screenshot shows a software interface for setting concentrations. At the top, there is a 'Concentration' input field with the value '0.001' and a 'Set' button with a green checkmark. Below this is a button labeled 'Get concentration from previous level'. The interface is divided into two main sections: 'List of components' and 'List of concentration levels'. The 'List of components' section contains a table with three rows: '#', 'Component', and a list of '1 Comp-1', '2 Comp-2', and '3 Comp-3'. The 'List of concentration levels' section contains a table with two rows: '#', 'Level', and a list of '1 Level-1'. On the left side of the interface, there are several buttons and labels, including 'itás', 'essary', '01', 'Select', and 'itás'.

#	Component
1	Comp-1
2	Comp-2
3	Comp-3

#	Level
1	Level-1

Fill cells

- ◆ If you filled all the component names, all the level names, assigned all the chromatograms to their levels, you can fill the cells.

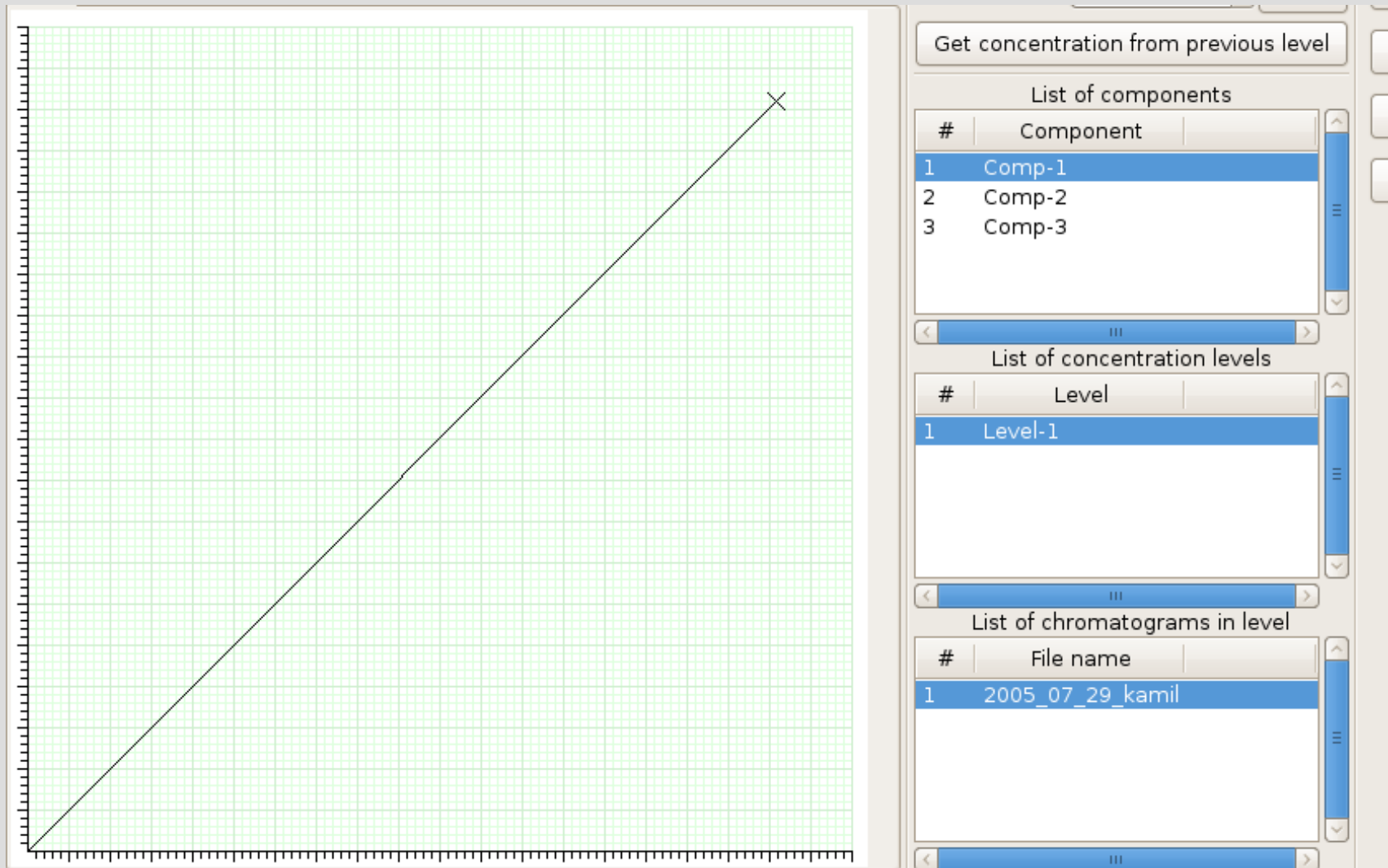
This filling means you must select the Component, the Level, the Chromatogram (each of them), the peak from the chromatogram (in the middle block) and pressing the button **Set to cell**. This process must be repeated to each of the components, levels, chromatograms.

The screenshot displays a chromatogram software interface with several panels:

- Component status:** A table with columns #, Status, Retention, and Name. It is currently empty.
- Detector:** A dropdown menu showing 'DET'.
- Set to cell:** A button with a magnifying glass icon.
- Identify:** A button with a magnifying glass icon.
- Find & set:** A button with a magnifying glass icon.
- Unfilled components:** Radio buttons for 'Do nothing' (selected), 'Highlight them', and 'Show only them'.
- Cell data at selection:** Displays data for 'Comp: 1', 'Level: 1', and 'Chrom: 2005_07_29_kamilla k'.
- Alaphelyzet:** A button with a magnifying glass icon.
- Peak list of selected chromatogram:** A table with columns #, Retention, and Area. It lists 9 peaks, with the first peak (14.000) highlighted.
- Unidentified peaks:** Radio buttons for 'Do nothing' (selected), 'Highlight them', and 'Show only them'.
- Selected peak's data:** Displays data for the selected peak: Retention: 14.000, Height: 3328.857, Area: 30854.000.
- Get concentration from previous level:** A button.
- List of components:** A table with columns # and Component. It lists 3 components: Comp-1, Comp-2, and Comp-3.
- List of concentration levels:** A table with columns # and Level. It lists 1 level: Level-1.
- List of chromatograms in level:** A table with columns # and File name. It lists 1 chromatogram: 2005_07_29_kamil.

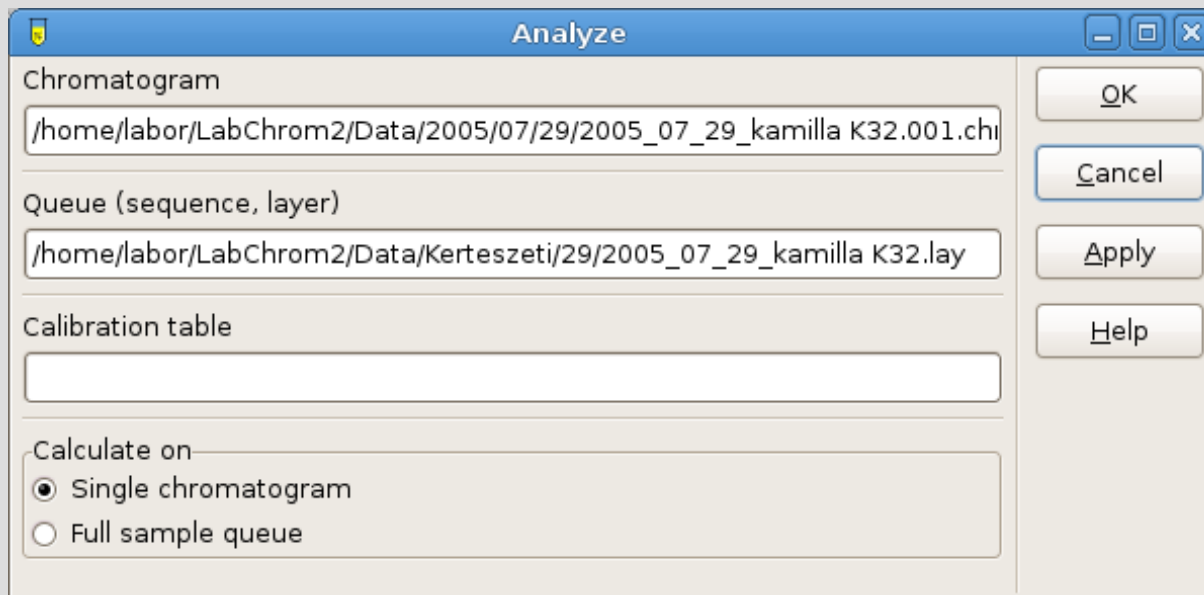
Curve

- ◆ Then you can see the calibration curve



Analysis

- ◆ If you finished the calibration table, you can select the **Analyze** function.



The screenshot shows a dialog box titled "Analyze" with a standard Windows-style title bar (minimize, maximize, close buttons). The dialog is divided into several sections:

- Chromatogram:** A text field containing the path `/home/labor/LabChrom2/Data/2005/07/29/2005_07_29_kamilla K32.001.chi`.
- Queue (sequence, layer):** A text field containing the path `/home/labor/LabChrom2/Data/Kerteszeti/29/2005_07_29_kamilla K32.lay`.
- Calibration table:** An empty text field.
- Calculate on:** A section with two radio buttons:
 - ☒ Single chromatogram
 - ☐ Full sample queue

On the right side of the dialog, there are four buttons: **OK**, **Cancel**, **Apply**, and **Help**.

You can analyze either a single chromatogram or the full table. Analysis means the component identification and the calculation of the concentrations.

More information

www.chemotron.hu/service

- ◆ New software versions
- ◆ Presentations
- ◆ Upgraded user manuals
- ◆ Application notes