# Tutorial Part II: curve fitting

Background removal

1. Loading the files
2. Be sure that your x-axis are calculated !
3. Make a graph of the waves you want to fit
4. Think about reasonable functions and the number of them
… than start as followed

…first remove the background in your waves

1. Select the graph
2. Optimize the x-axis
3. Put both cursors (A and B) on the left and right site of your spectral feature - the background will be calculated between the boundaries and the cursor positions
4. Then start the BACKRAM macro
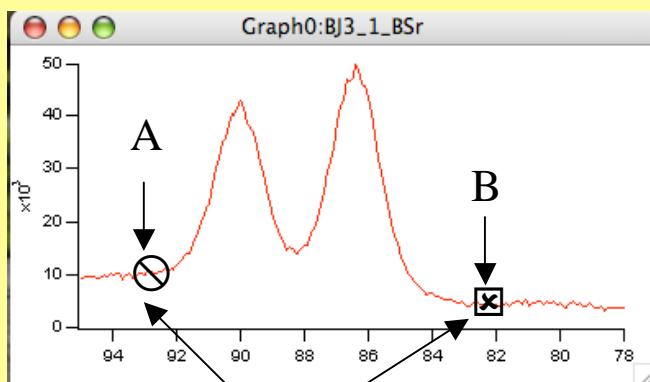
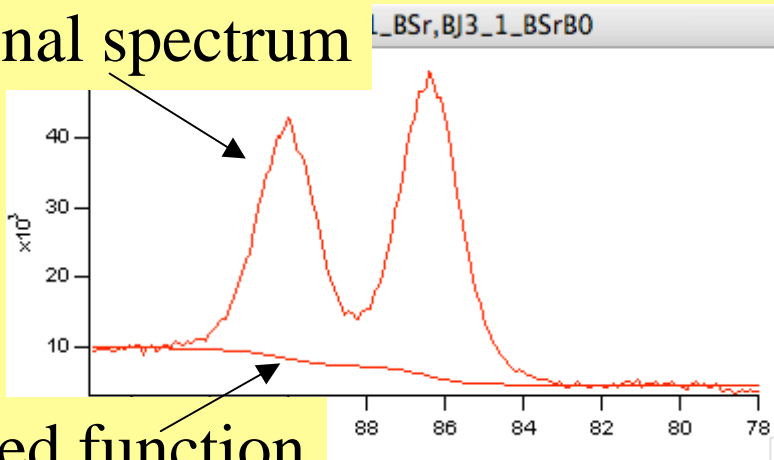background

Ruedi or poly-functions

BackRem

Modus ?

ruedi

Show ?

Nein

Versionsnummer ?

0

Quit Macro   Continue   Help
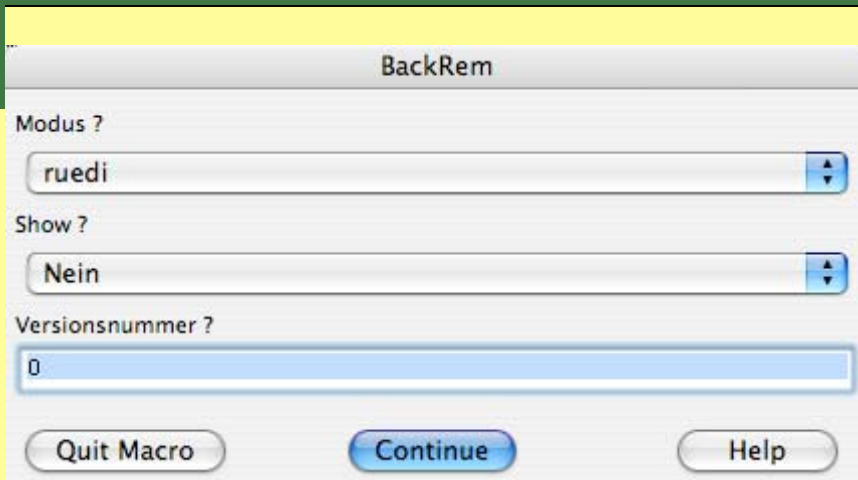
Here you can select differen background Functions (ruedi, line, and some polynom fuctions

Show? Nomally: Ja=yes :)

If you want to try different background functions you must change the Versionsnumber 0➜1➜2➜3…
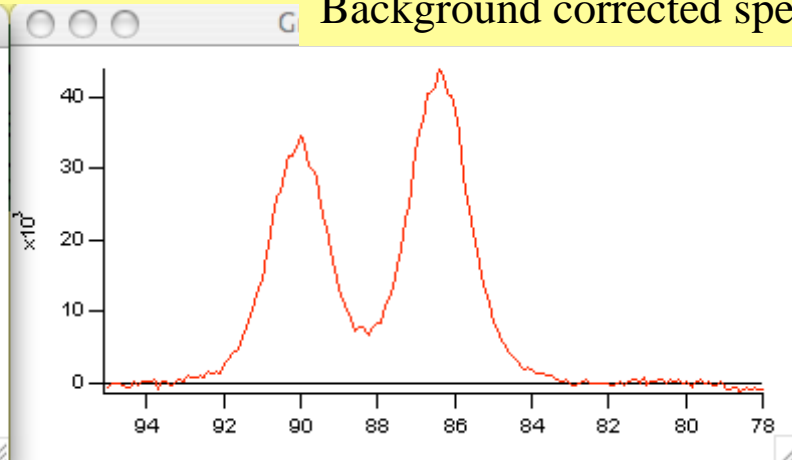
- Ruedi works fine with XPS-spectra, especially with doublets
-Poly's can be used for substracting e. g. a slope in the spectra (poly3 works normally)

Original spectrum
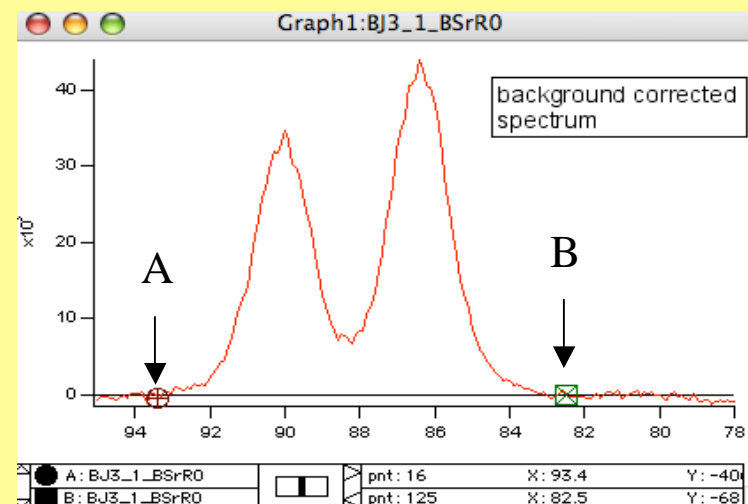
L_BSr,BJ3_1_BSrB0

removed function
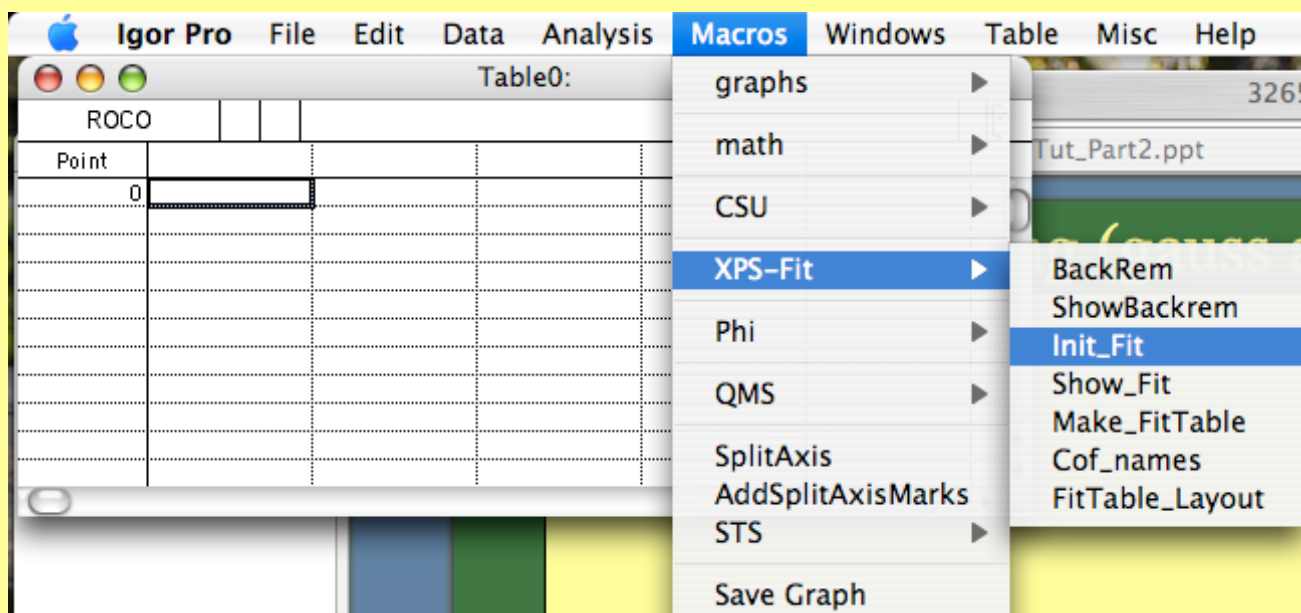
Background corrected spectrum

Curve Fitting

The fitting macros are mostly from A. Klein

1. Bring cursors A and B on the graph, they define the region for the fitting procedure

2. Start INIT_Fit macro

Fit pannel

This botton starts the fitting procedure

Here you can select the Window you want to do the fitting

Here you can load user defined fit-functions !! Very important!!

Use this function, if you want to run the fit two time with different fixed settings

Shows you a preview of the fit with the settings you entered in the "Start-panel"

Igor Pro   File   Edit   Data   Analysis   Macros   W

Fit_Panel

GO

Fitwindow
Graph1

Funktion :
f_gl1

Load function
Version : 0
Start(n+1) = Fit(n)
Ann%herung

Startwerte =
none
show Nein
Load glwave
Save glwave

Start_Panel

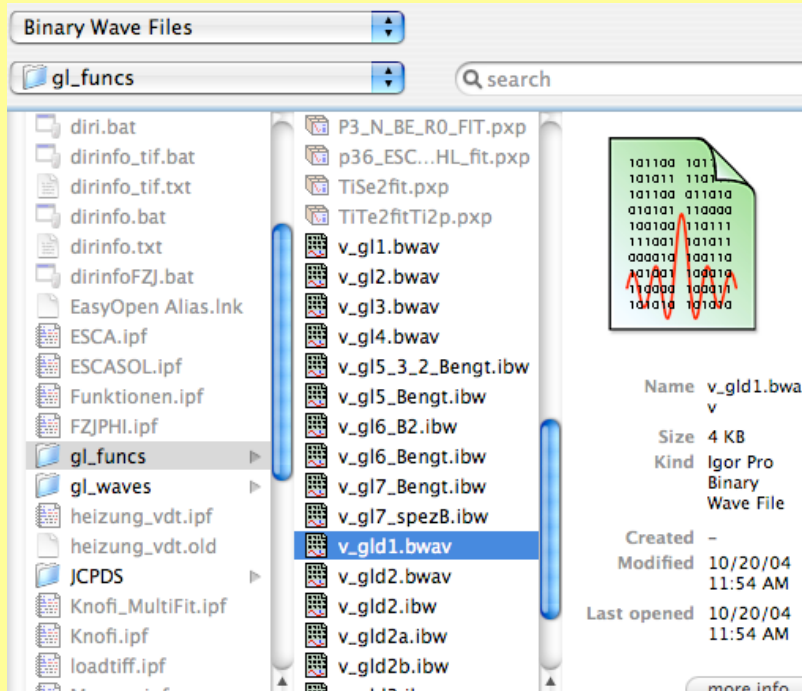| Variable	Wert	1st	Tbl
BE :	0.000	☑	☐
Int :	0.000	☑	☐
FWHM :	0.000	☑	☐
alfa :	0.000	☑	☐
G/L :	0.000	☑	☐

values

Fixed or open ☑ parameters

Tablefunction
(useful, if you have more the 3 waves to fit)

The parameters of the fit-panel varies by changing the fit-function.

1. Choose function: click on "LOAD Function"
2. Select a function from the list (folder: gl_functions = default)

Names:
- "v" Voigt-functions are included
- "c" and "f" FWHM and an
   assymetric parameter is included
- "g" Gauss
- "l" Lorenzian
- "d" doublet
- # number e.g. of doublets

3. Choose e. g. v_gld1.bwav to fit a doublet into the selected graph
4. Select the loaded function in the Fit-panel
   ➔ The parameter in the Start-panal will chance

Vallues and Preview

1. Click on Show and select "SPEZ" ➔ an new graph will appear
2. Enter reasonalbe values in the Start-panel

   ➔during entering values the "startgraph" will show you the result of your entries

3. Optimize the values

If your cursors are on the selected graph

Click on "GO"

➔ The startgraph will disappera
➔ A panel appears with running numbers (do nothing !)
➔ Depending on your start values and the number of waves the fit takes some seconds

Red Dots: data
Blue line: FIT
Green line: error-curve

Displaying results

1. After the fit in the command window the fitted wave and chi^2 is logged

2. For displaying the graph start the "Show_Fit"-macro
3. A new window with display options appear
   -select Fehlerkurve=Errorcurve➜ Ja or x3
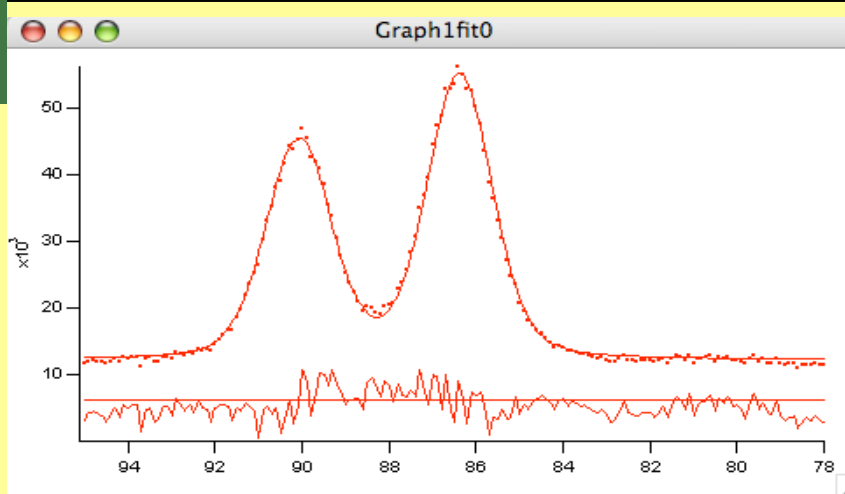   ➜Continue

Show_Fit

enter y-offset (Auto=0)

0

Versionsnummer

0

Fehlerkurve zufuegen?

Nein

Spezial?

v_gld1

Quit Macro   Continue   Help

Macros   Windows   Graph   Misc   Help

graphs   ▶

math   ▶

CSU   ▶

XPS-Fit   ▶   BackRem
                       ShowBackrem
Phi   ▶   Init_Fit
                       Show_Fit
QMS   ▶   Make_FitTable
                       Cof_names
SplitAxis   FitTable_Layout
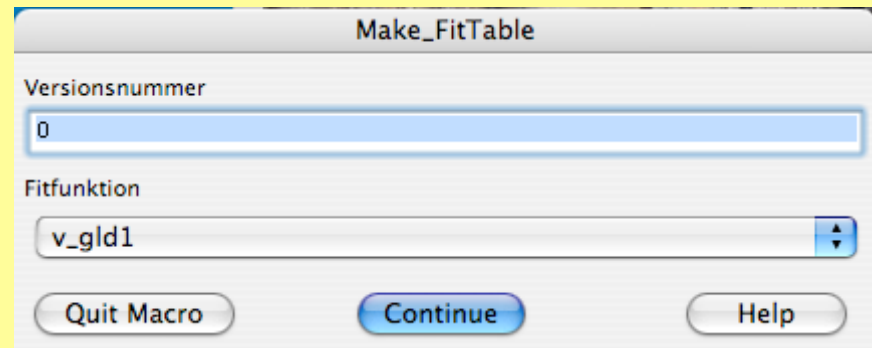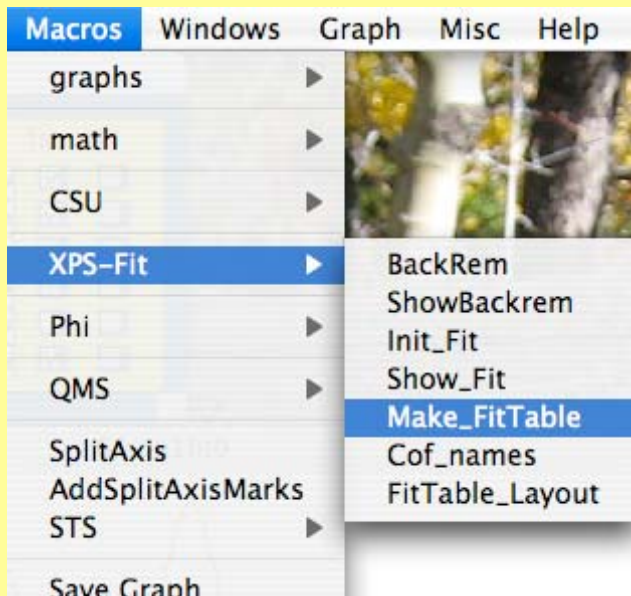AddSplitAxisMarks
STS   ▶

Save Graph

Fit and Fitparameter

Dots: data
Line in the dots: Fit
Lower curve: Error-curve
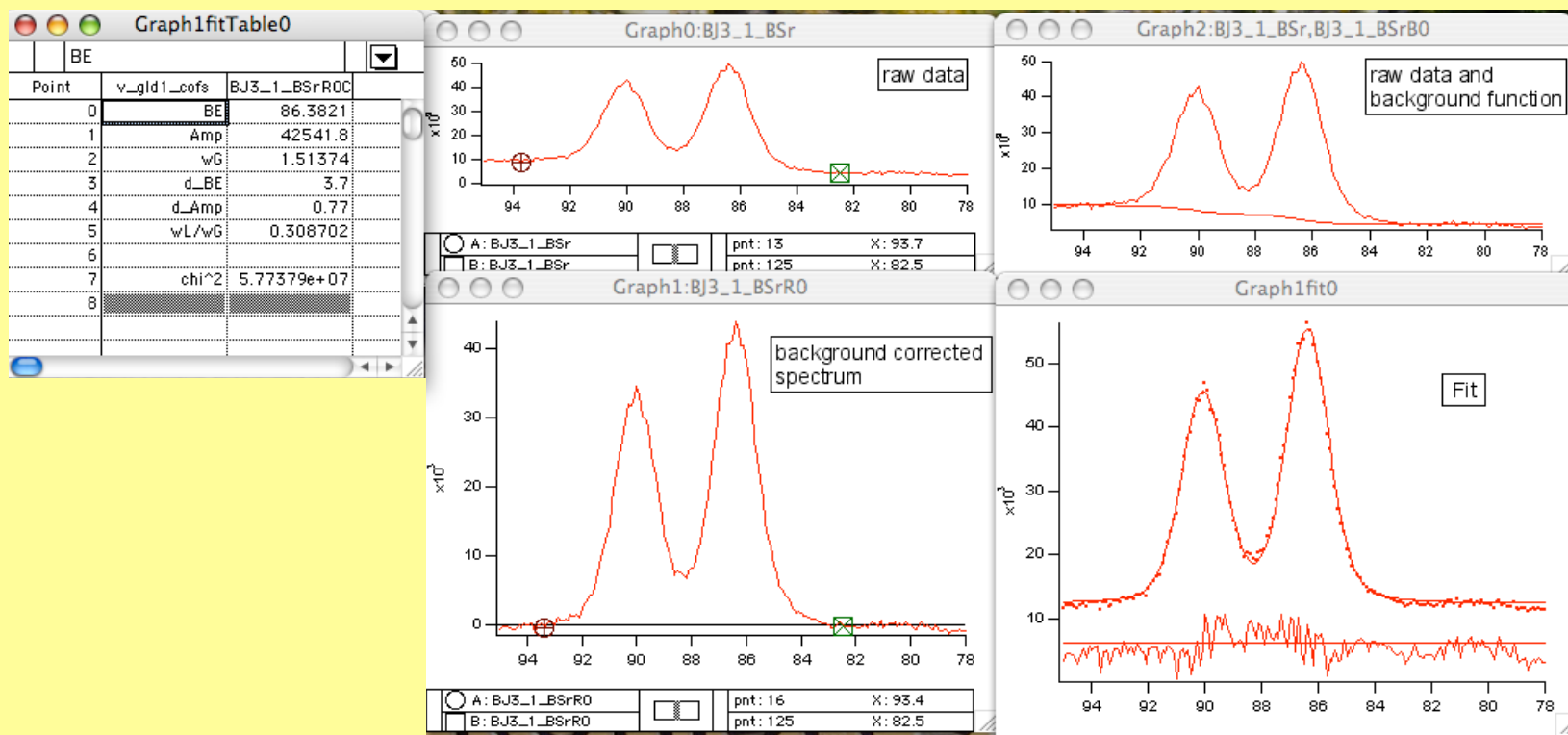
To see the Fit-parameter start the "Make_FitTable"-marco
➔ be sure that you have selected you raw-date window!
➔ select the Fitfunctions you had used for the fit and continue

➔

Fittable

After running the "Make_FitTable"-marco a table with the fitparameters appear

Summary:

If you have more then one wave in the window…

….this is no problem

… do basically the same

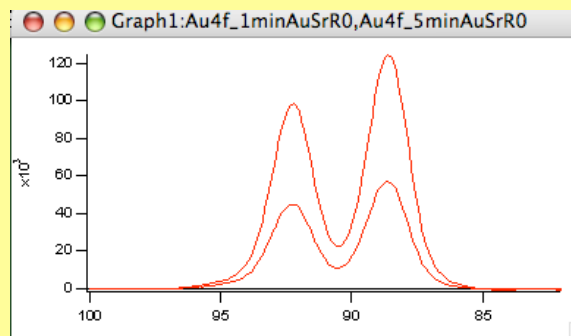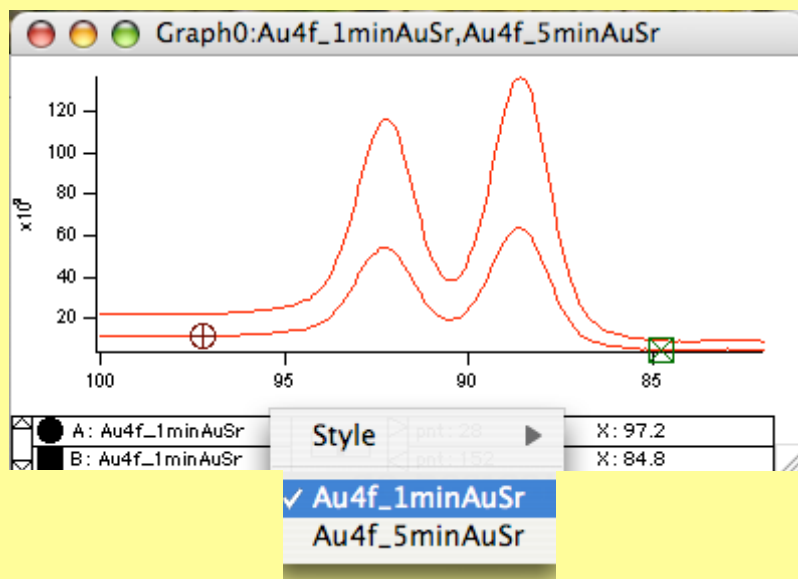1. Remove background:

   1. Set Cursors A and B on the lowest graph
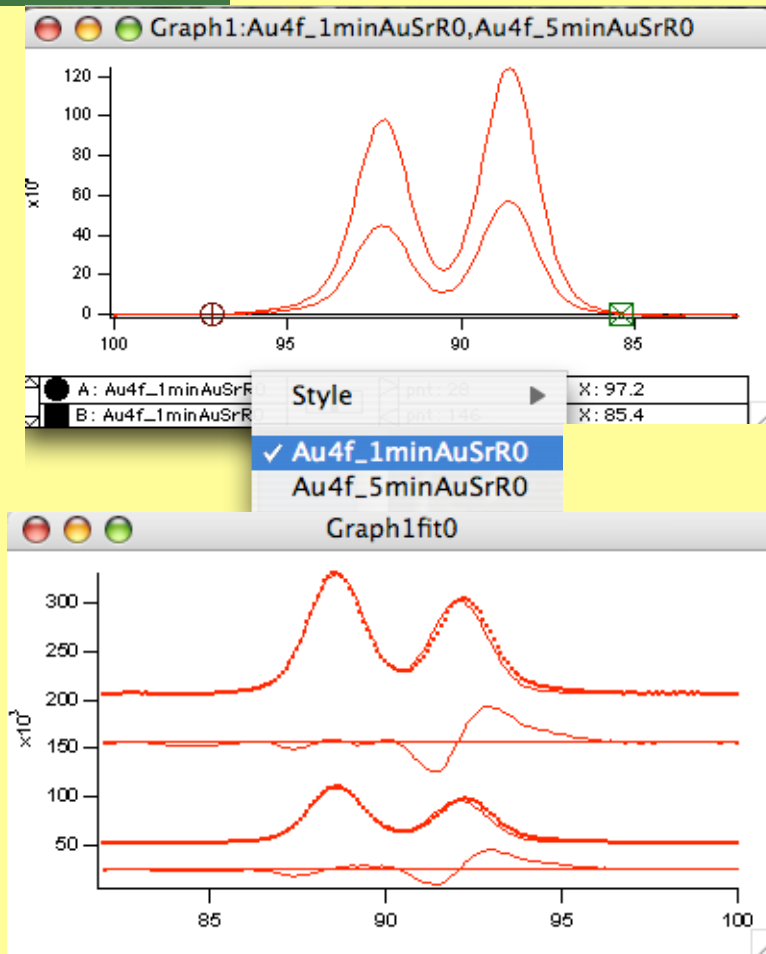
     (you can change the order of the traces Graph-Menu)

   2. Start the Backrem macro

   3. Select function ….

   ➔ the background of both (3,4…) waves will be substracted

Fit, Display and Values

1. Put Cursors A and B on the lowest wave !! (in the list the topmost graph!)
2. Start Init_Graph (if you haven't start it yet)
3. Load and Select function
4. Select Window to fit
5. Enter reasonable values
6. In the Startgraph only the graph of the lowest wave will be displayed
7. Klick on "GO" and both (3..) waves will be fitted
8. Display result: Show_Fit and MakeFitTable

Have fun and save time…