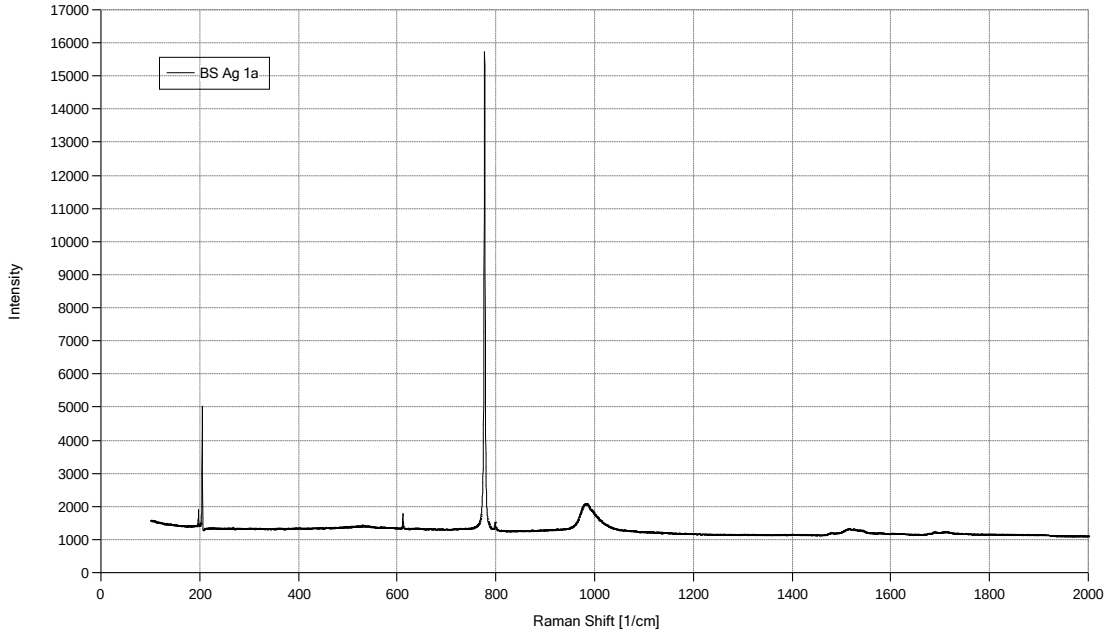
How to get Peak list and FWHM values for Raman spectrum

1. Importing Data

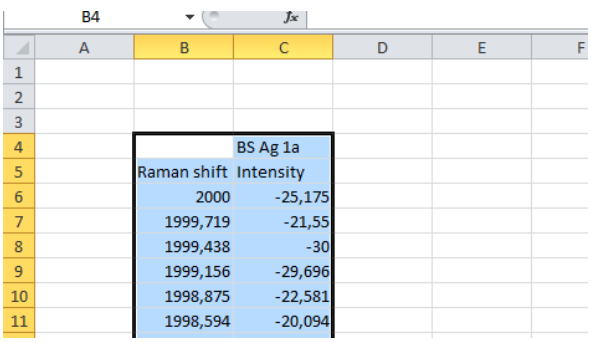
For import of arbitrary data which is not in a specific file format, it is your responsibility to get the axis types right. In case of Raman data, it is enough to write “Raman” in the first line of the data file (*.csv or *.fak file type), like this:

```
Raman
100,1594.754
100.281,1578.403
100.562,1574.144
100.843,1571.65
101.124,1565.265
```

This results in a spectrum plot with “Raman Shift” as x axis and “Intensity” as y axis:



In case you have your data in Excel anyhow, just select the data columns, and Copy&Paste (CTRL+C in Excel, then CTRL+V in Spekwin32) the data into Spekwin32 to get your plot.

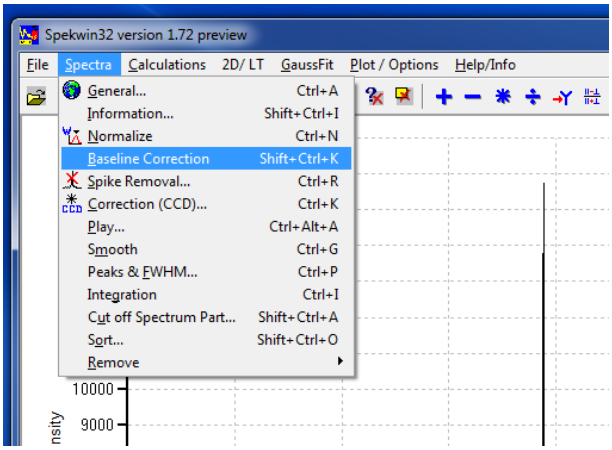


B4

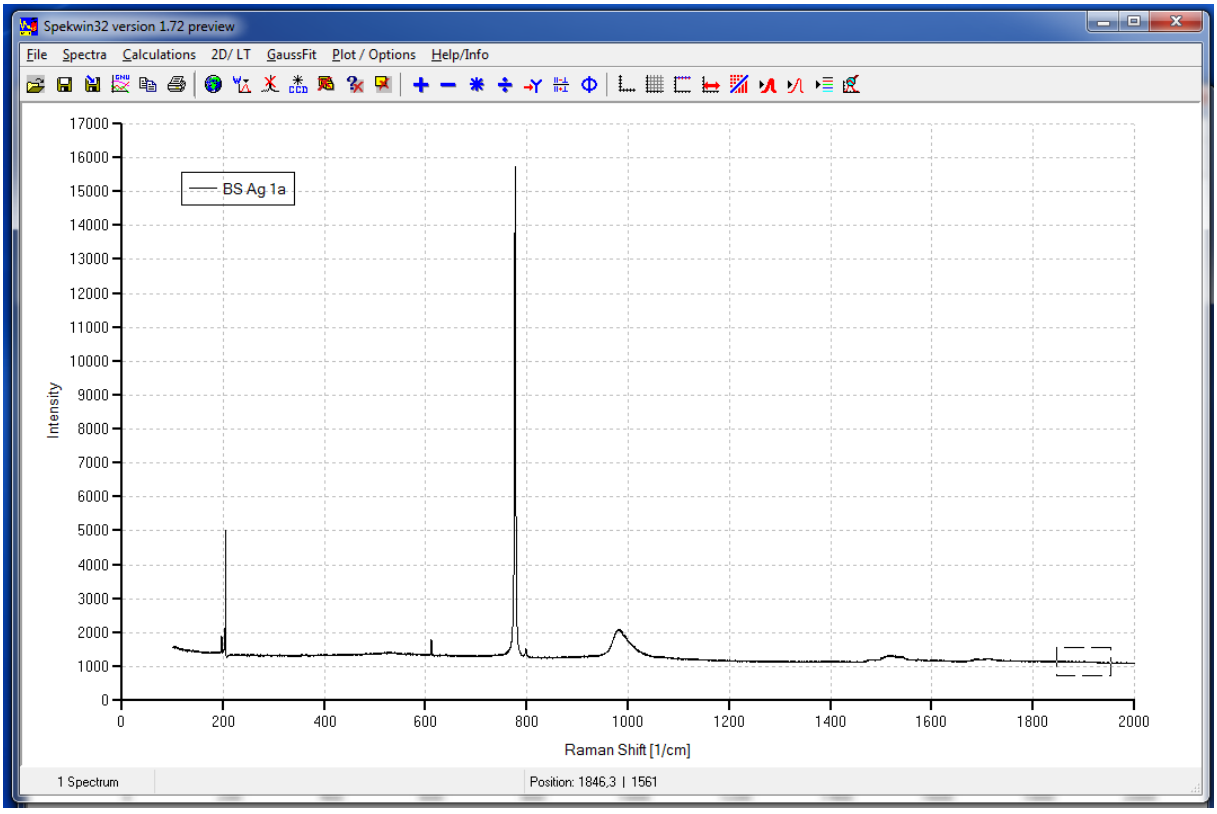
	A	B	C	D	E	F
1						
2						
3						
4			BS Ag 1a			
5		Raman shift	Intensity			
6		2000	-25,175			
7		1999,719	-21,55			
8		1999,438	-30			
9		1999,156	-29,696			
10		1998,875	-22,581			
11		1998,594	-20,094			

2. Correcting Baseline

As can be seen from the plot above, the baseline sits around 1100 counts. However, it should be zero. This can be done with the menu item “Baseline correction” from the “Spectra” menu:

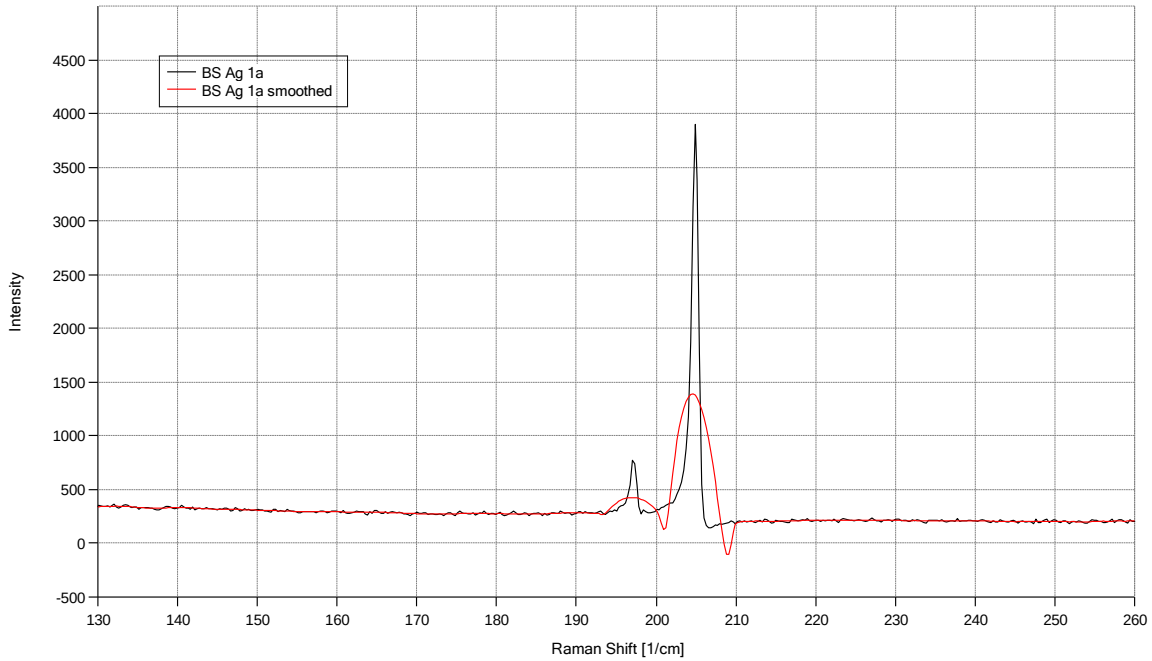


After calling the function, just use the left mouse button to zoom the baseline region which should be set to zero.



3. Smoothing necessary?

For this example's spectrum, it is better to not use the simple Smooth function: it's Raman peaks are prominent, well resolved and high above the baseline. Simple smoothing would introduce artifacts, as can be seen below.

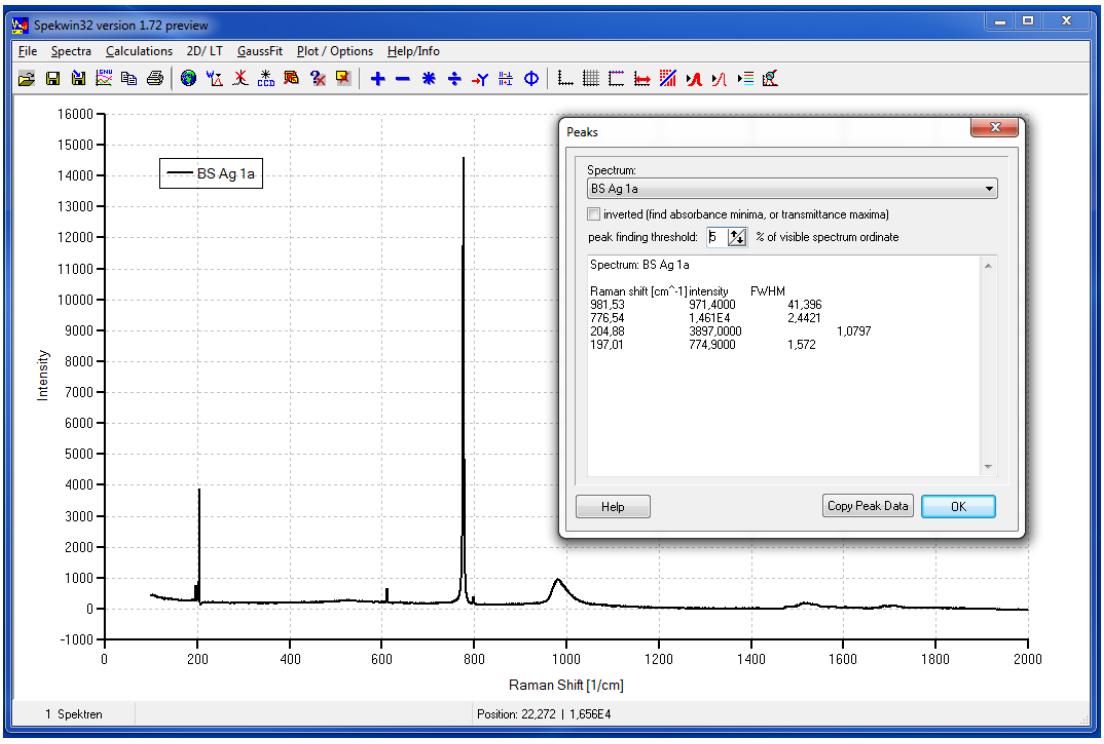


However, by using the "Advanced Smoothing" function, working smoothing parameters could be found for smoothing without spectrum distortion.

4. Peak finding + peak's FWHM

Is quite straightforward by using the "Peaks & FWHM" function from the "Spectra" menu. Never use the "inverted" option for Raman spectra, as there are no minima to find. There is just the baseline at the bottom, the interesting thing are the peak maxima and perhaps their bandwidth.

By varying the threshold, the peak finding sensitivity can be adapted.



You might also want to try out the Peak Labeling function from the “Plot/Options” menu; this will label your peaks within the plot: