UNIVERSITAT ROVIRA i VIRGILI

DEPARTAMENT D'ENGINYERIA QUÍMICA

OriginPro-Advanced Signal Analysis

Applications in Spectroscopic and Electrochemical Signals

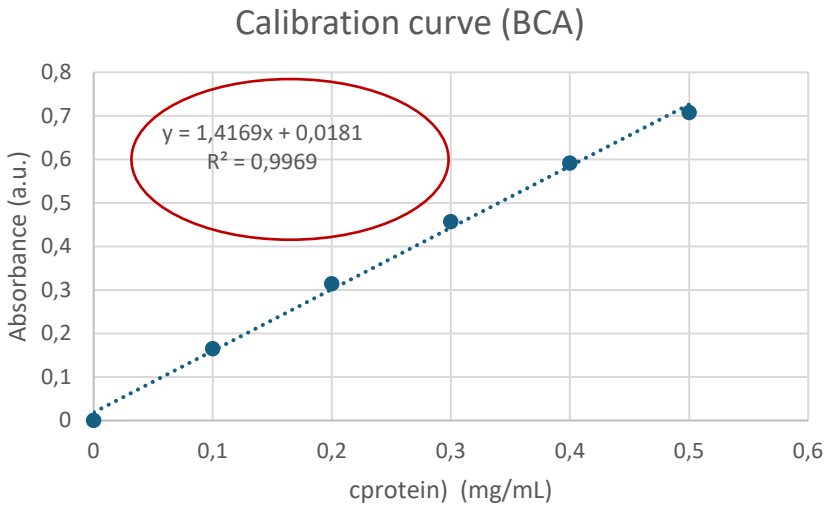
Dr. Mayreli Ortiz

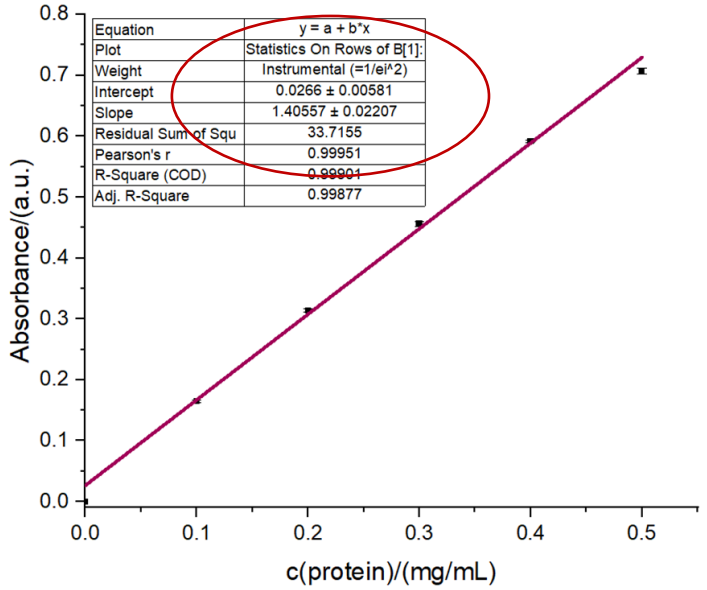
Tarragona, 24/02/2025

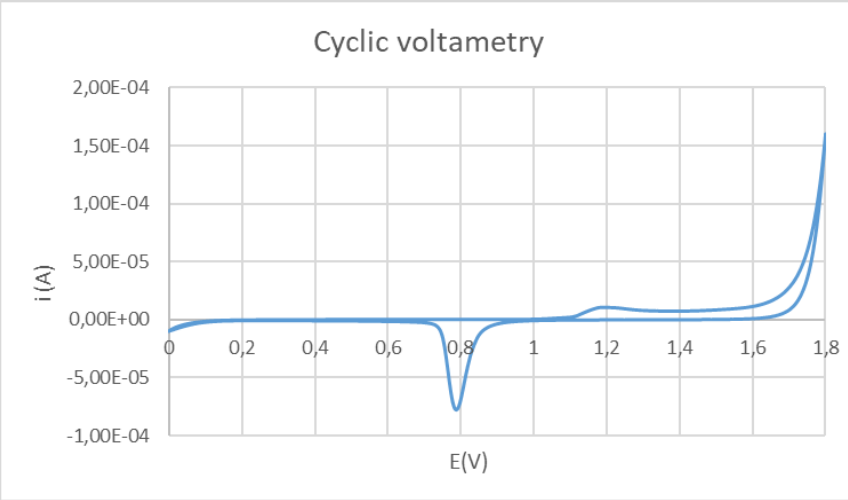
Origin vs Excel: an actual conflict?

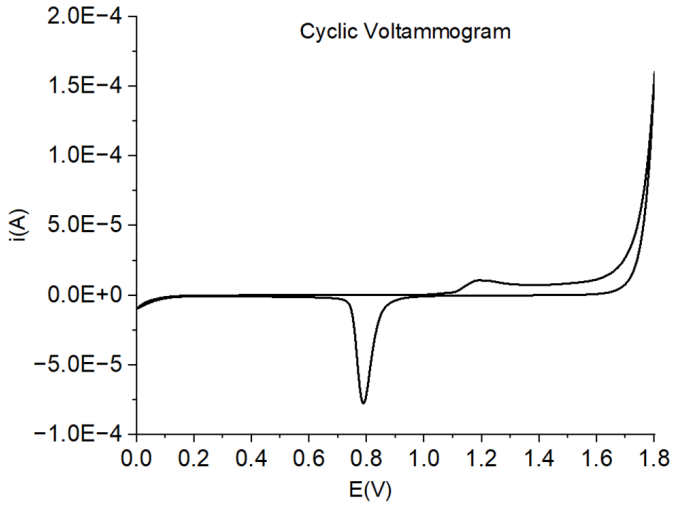
	Excel	Origin Pro
Data Handling	Suited for basic data entry, manipulation, and visualization; may struggle with large or complex datasets	Optimized for handling large datasets, offering advanced curve fitting, deconvolution, and statistical analysis
Analysis Tools	Provides basic charting, pivot tables, and limited statistical funcions	Includes specialized tools for peak analysis, curve fitting, and in-depth signal processing
Graphical Capabilities	Standard charts with moderate customization	Extensive customization, scientific plotting, and advanced visualization options
User Interface & Workflow	Familiar interface for general office tasks; less intuitive for specialized scientific data analysis	Tailored for research with dedicated workflows for experimental data analysis
Automation & Scripting	Uses VBA macros, which may require additional effort for complex tasks	Offers built-in analysis routines and scripting support designed for reproducibility in scientific research

Origin vs Excel: an actual conflict?

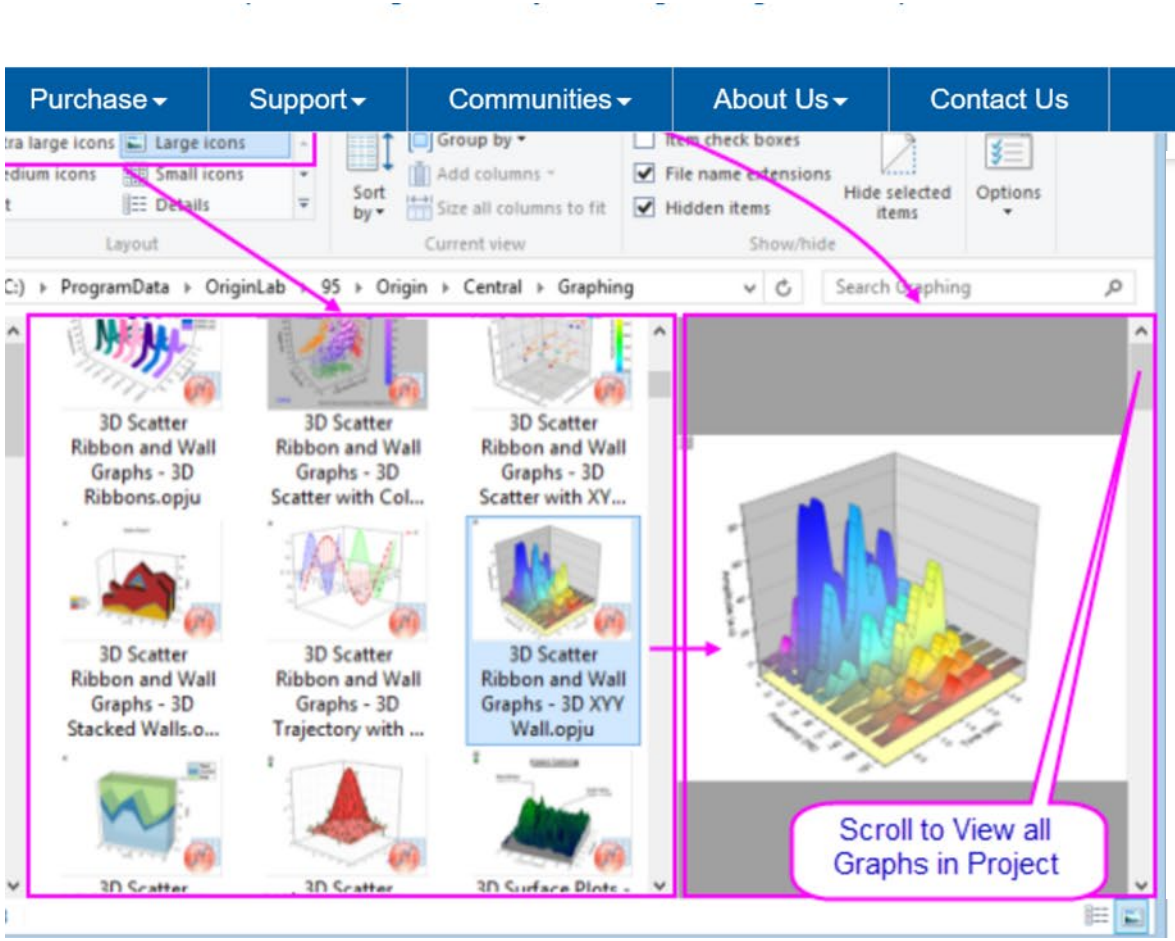


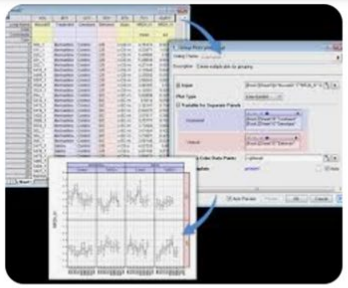






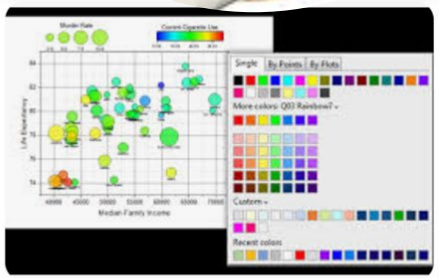
Origin offers a huge portfolio of graphical capabilities!



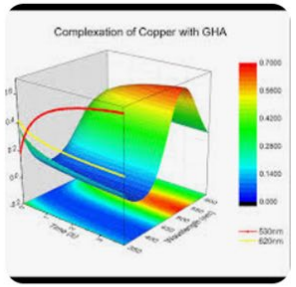


OriginLab
Origin: Data Analysis and Gra...

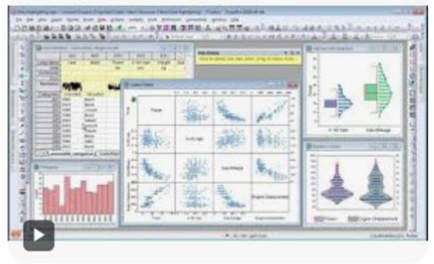
OriginLab
Origin: Data Analysis and Graphi...



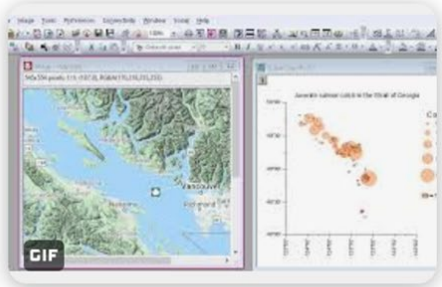
OriginLab
Origin: Data Analysis and Graphing Sof...



OriginLab
Origin: Data Analysis an...



YouTube
OriginPro - Graphing and Data Analysi...

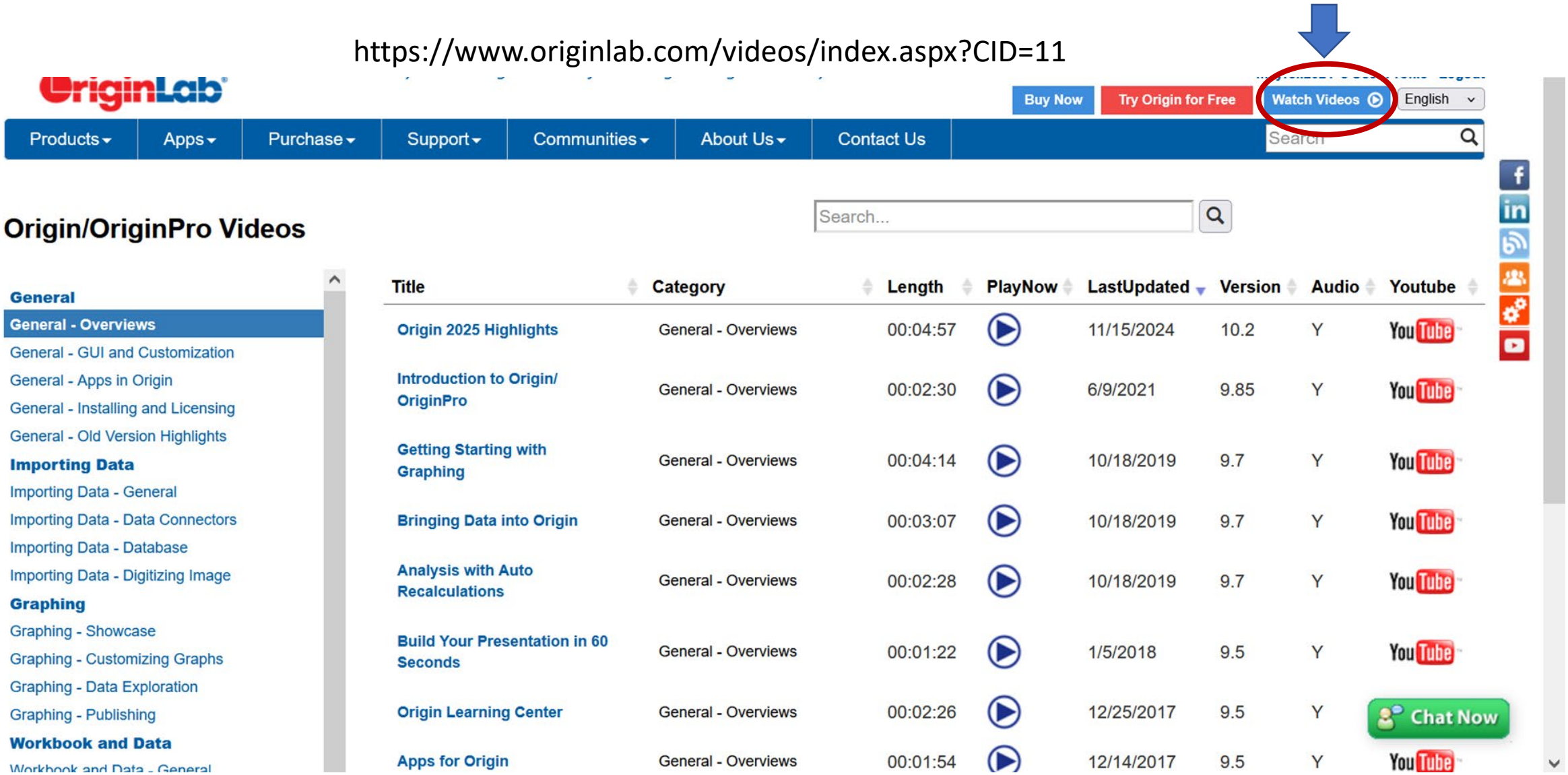


OriginLab
Origin: Data Analysis and Graphing Sof...

And of course EXCEL is useful for many applications: it is a matter of selecting what you need at all times...

All information you would need about Origin Program is available.

https://www.originlab.com/videos/index.aspx?CID=11



Why do we need an Origin Pro licence?

OriginLab

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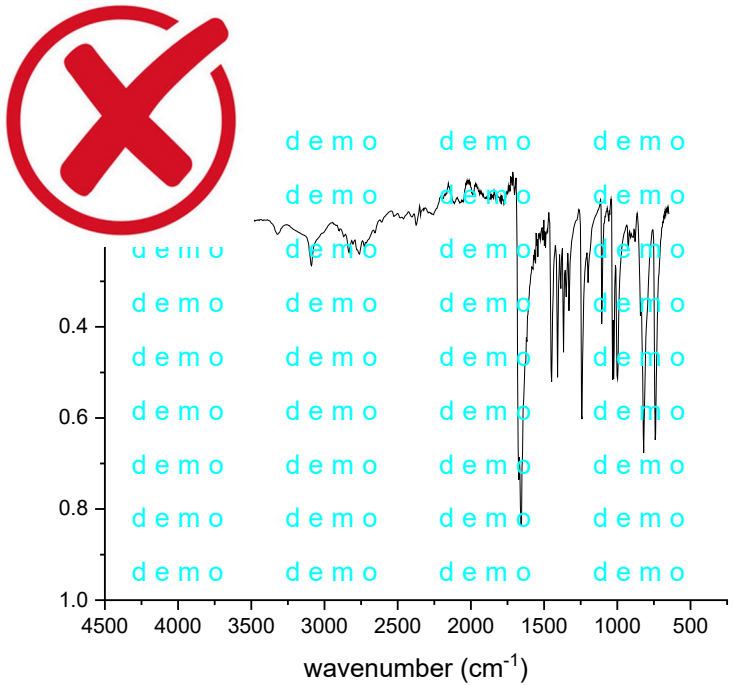
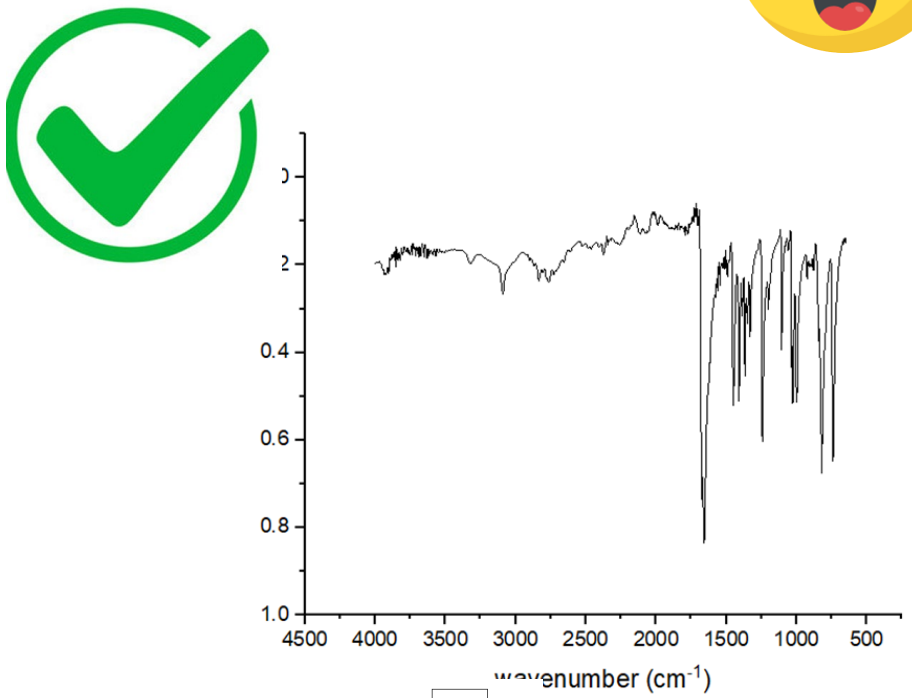
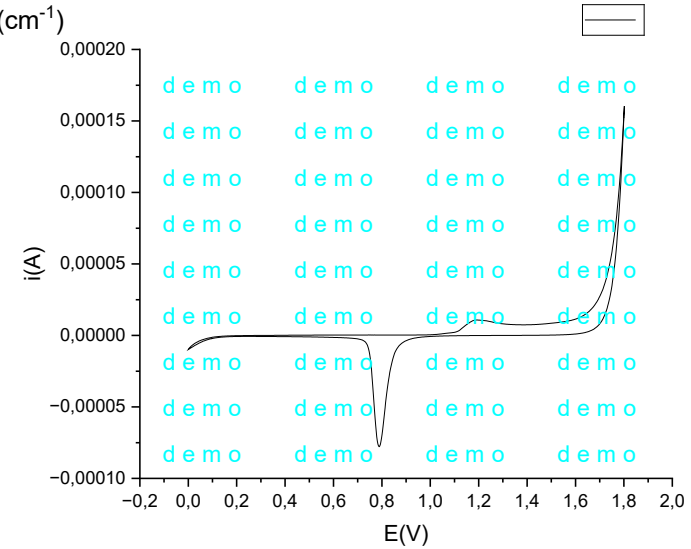
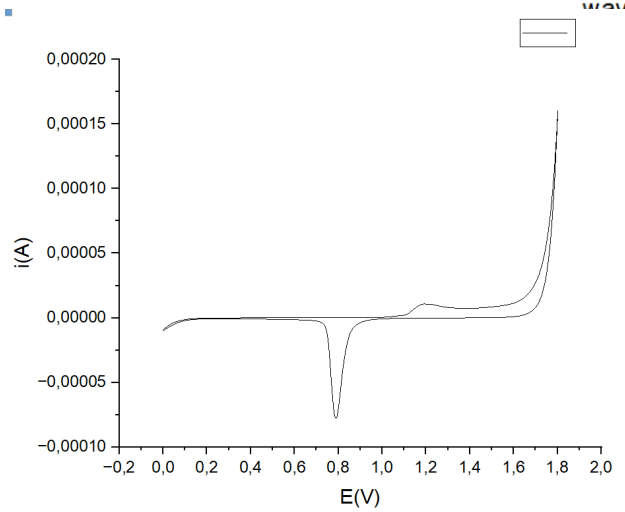
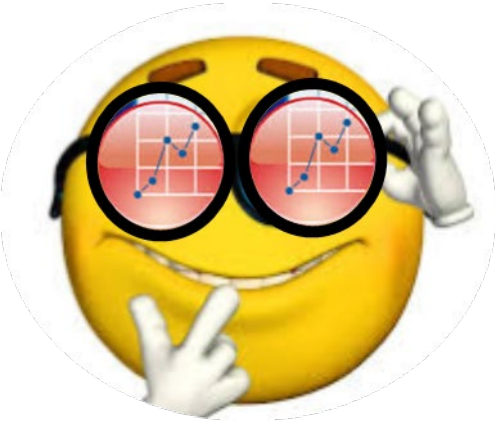




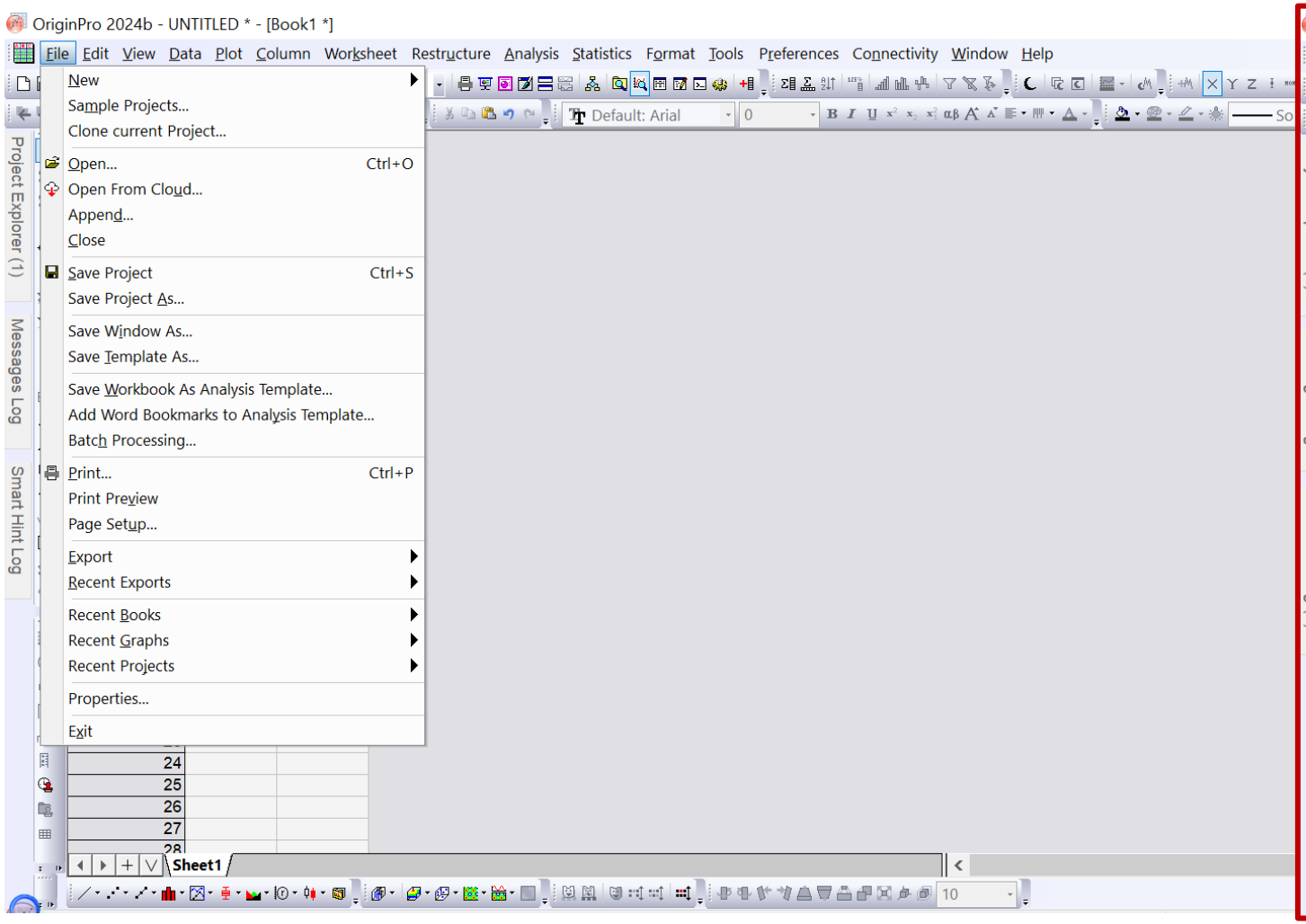


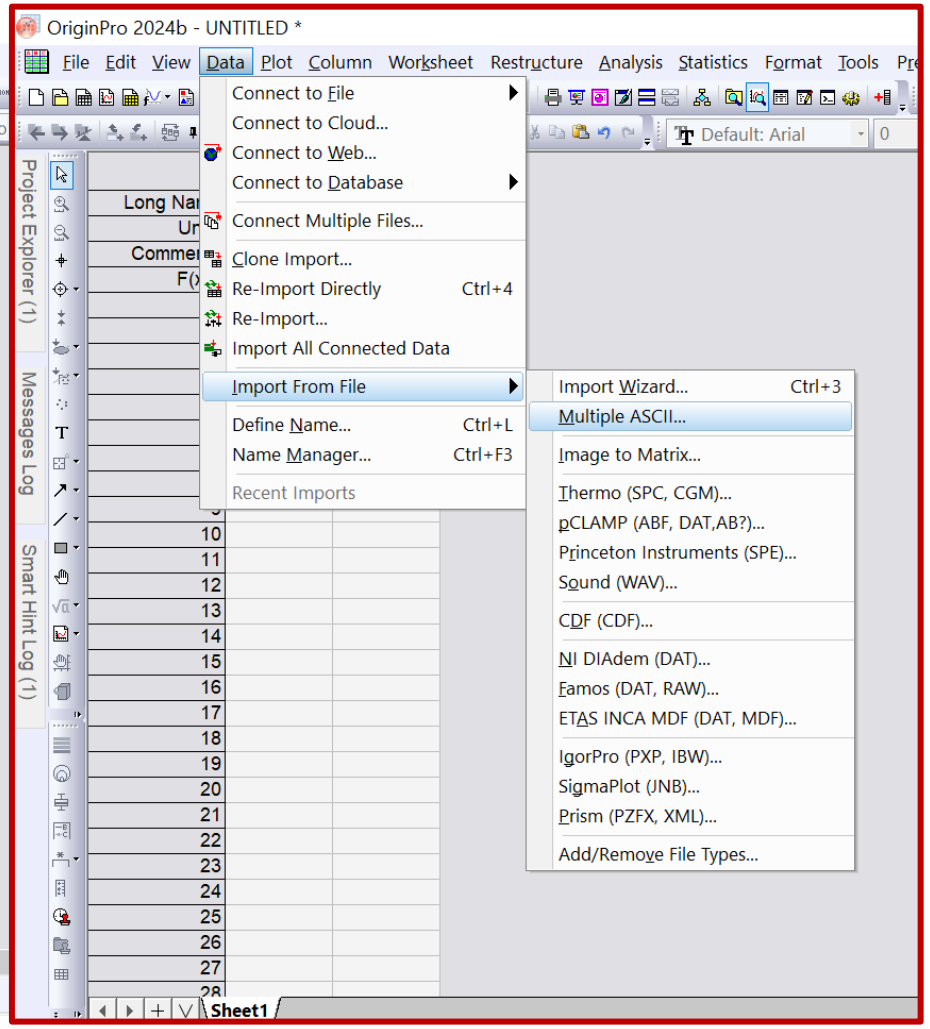


Some tips for starters in OriginPro…

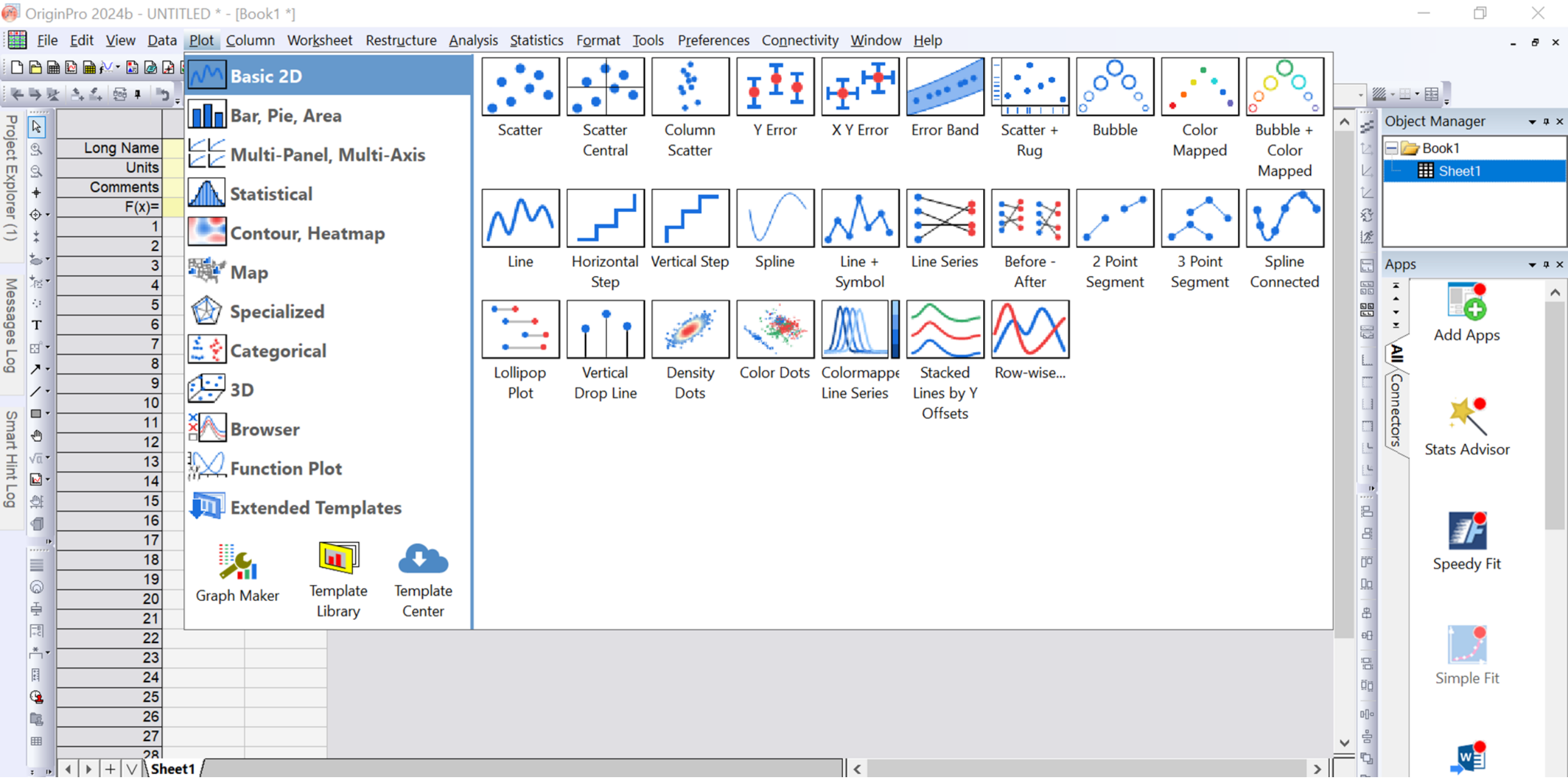


Some tips: the interface



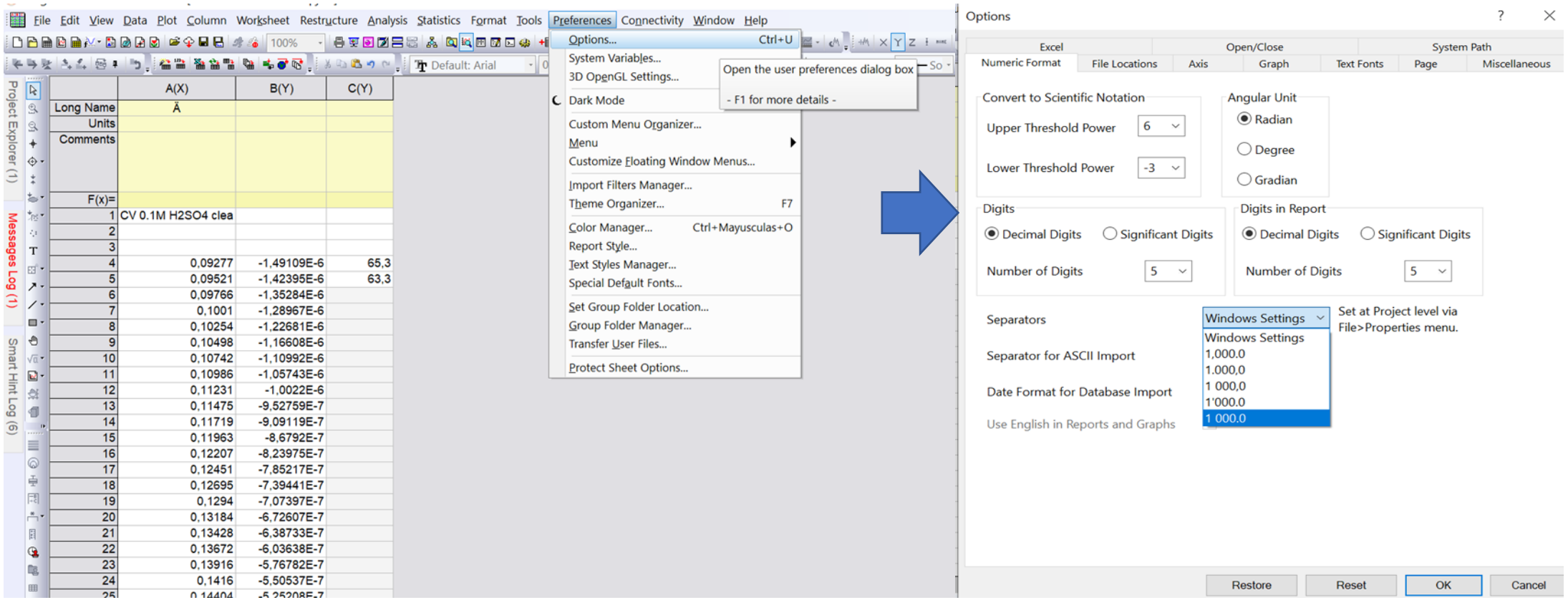


Some tips: the interface



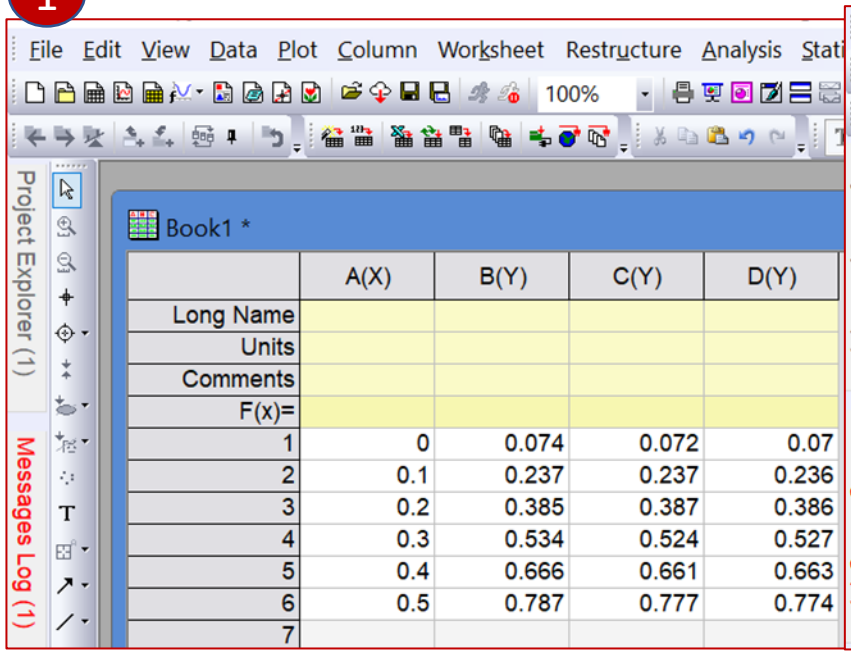
Some tips: Change “comma" for “dot" as decimal separator

The first thing to do when starting to use Origin…



I) Practical example: A calibration curve - Linear fitting

1



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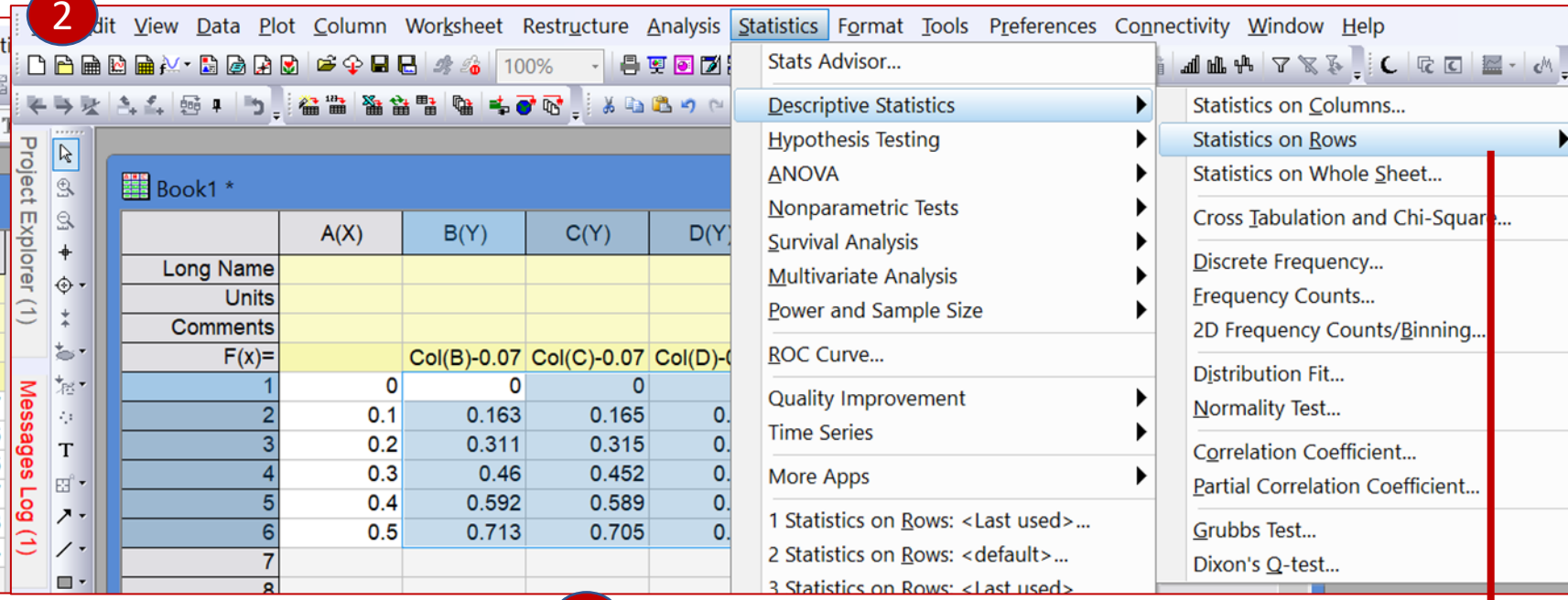

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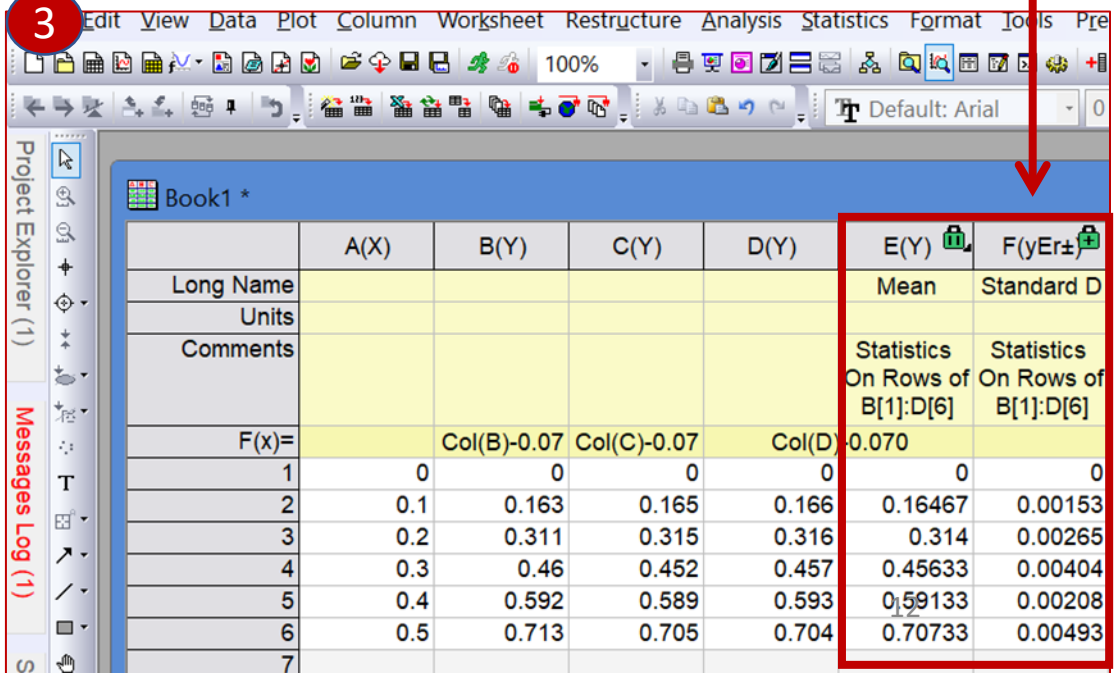

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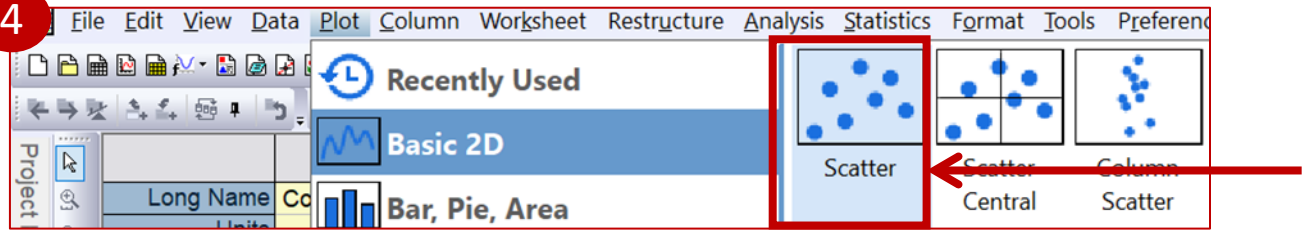
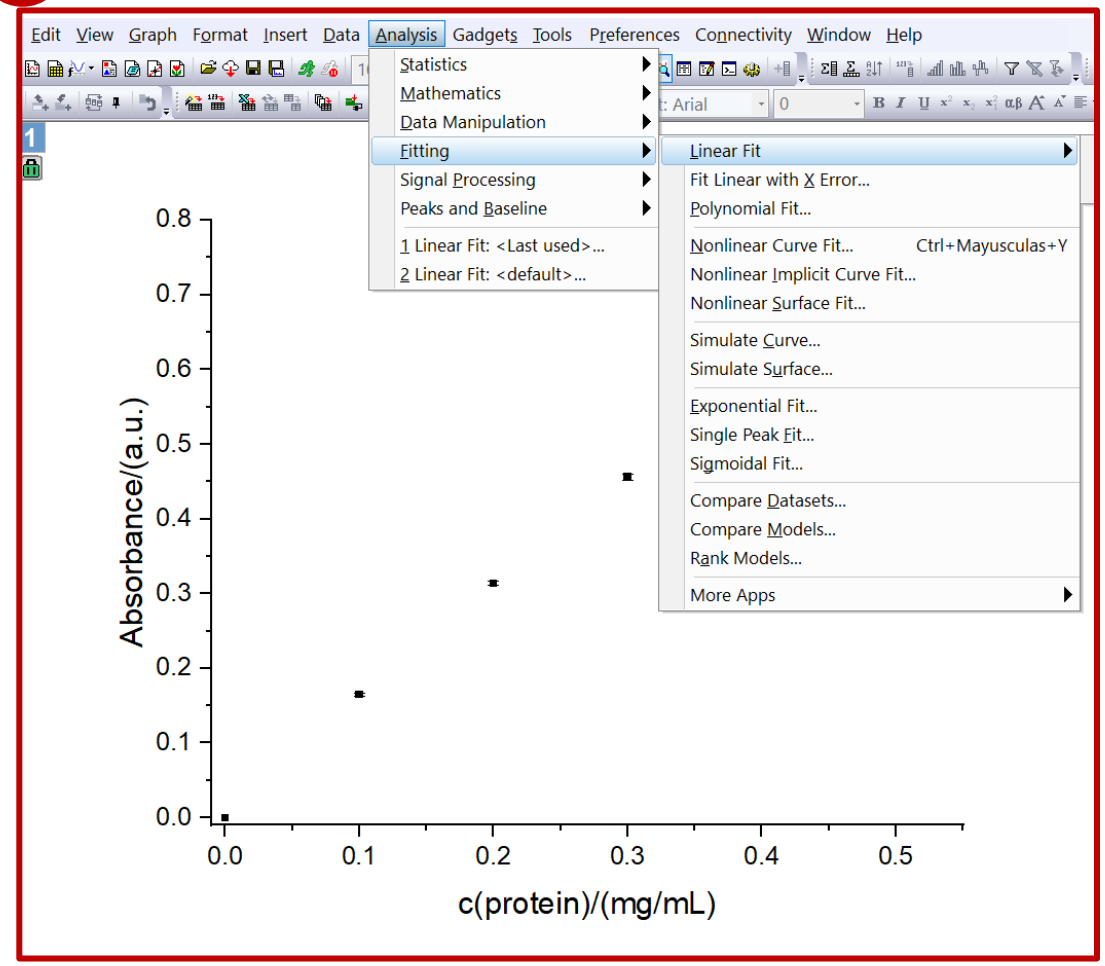


I) Practical example: A calibration curve - Linear fitting

5



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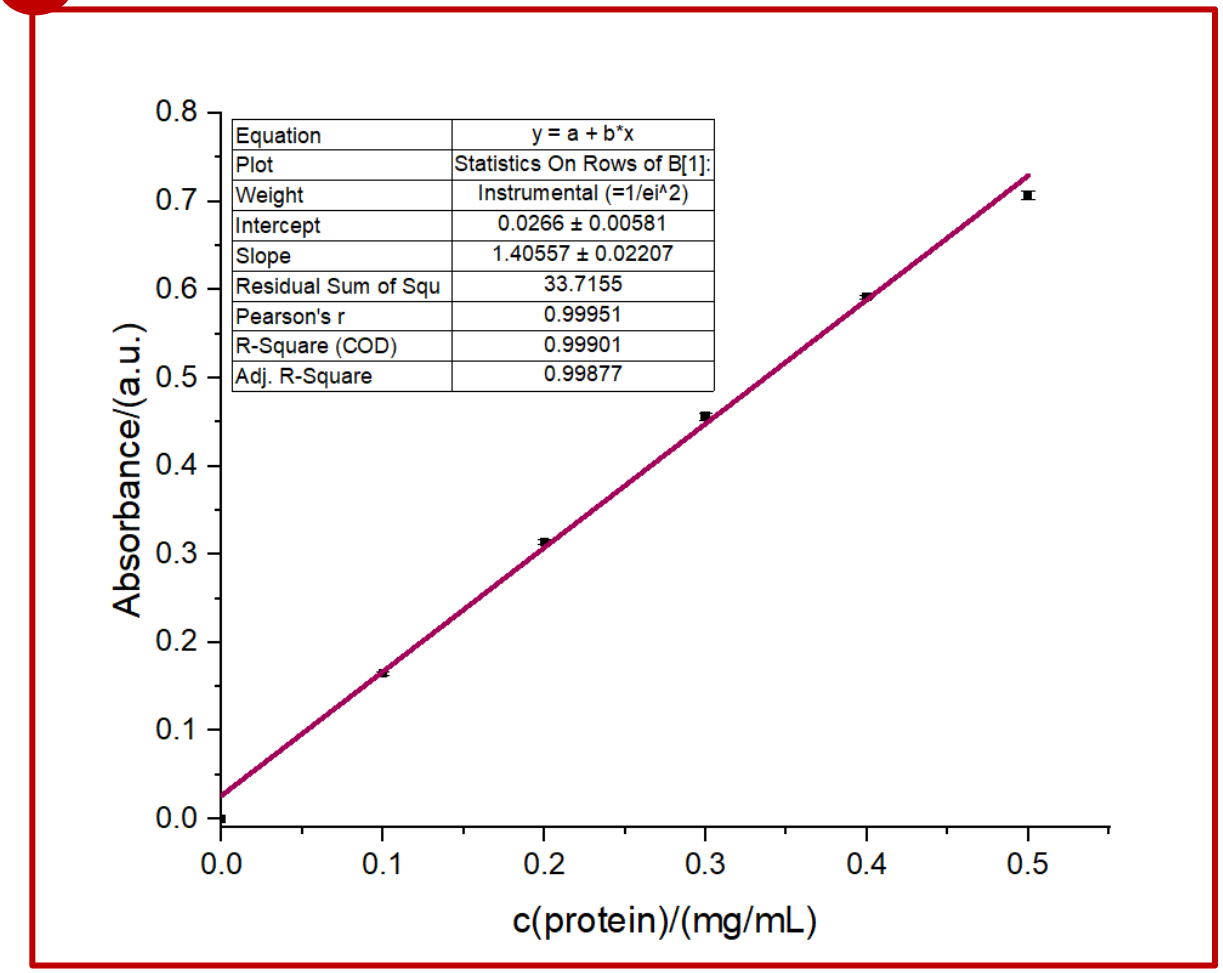
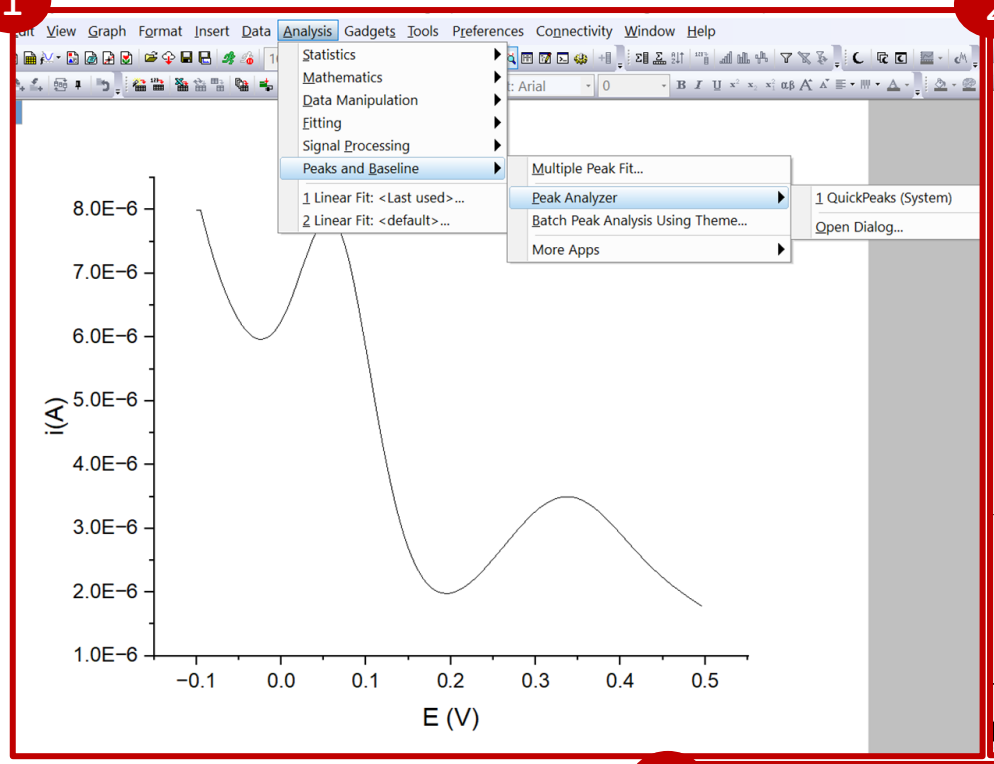
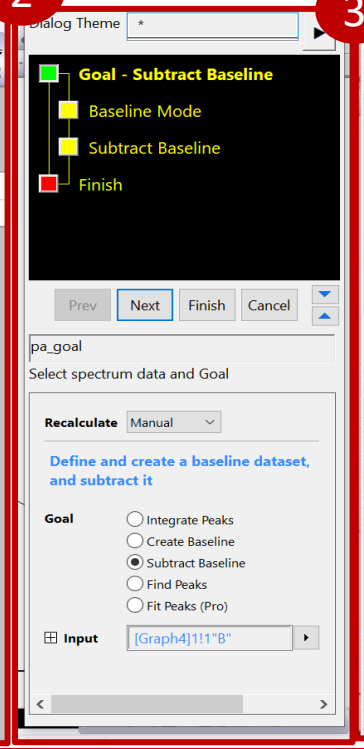
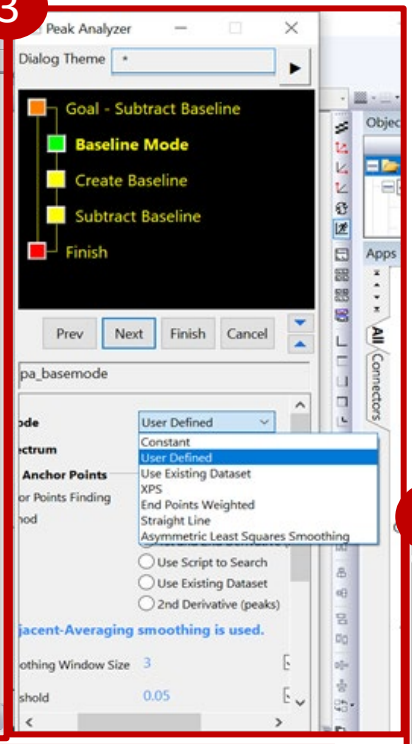
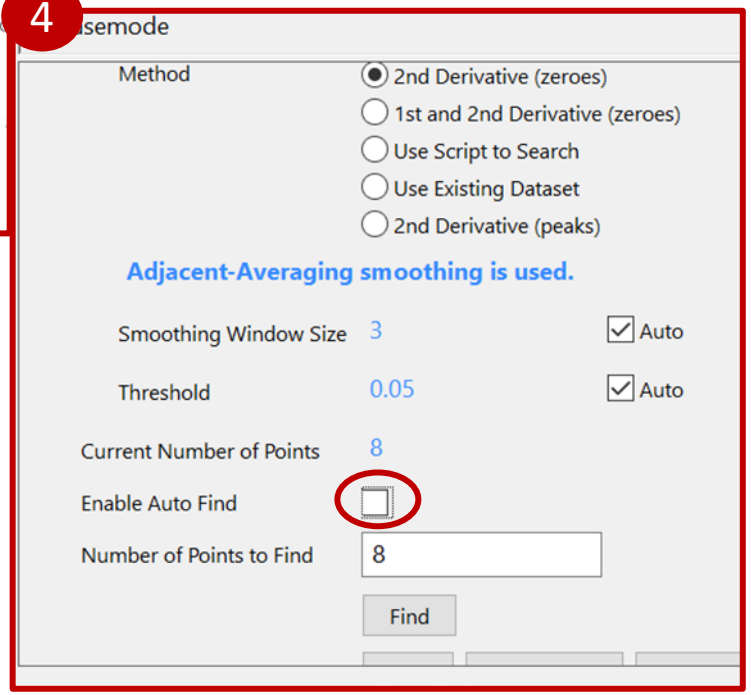


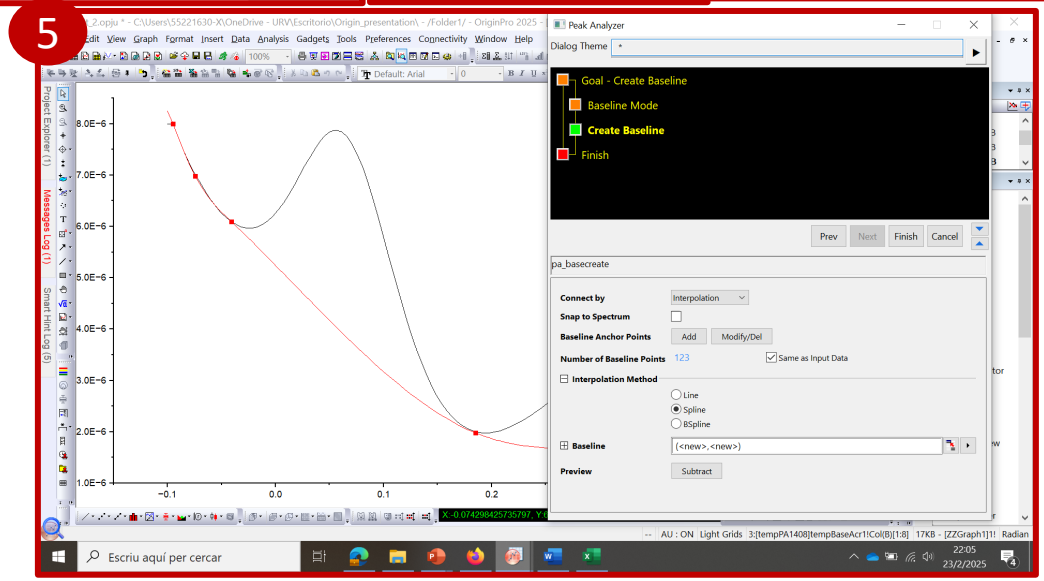
II) Practical example: Baseline correction - SWV











II) Practical example: Baseline correction

6

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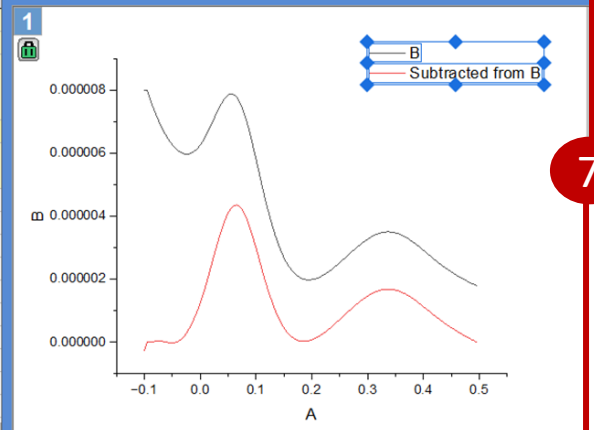
File Edit View Graph Format Insert Data Analysis Gadgets Tools Preferences Connectivity Window Help

FeCNcoatingFe - FeCN_coating_Fe3.oew *

	A(X1)	B(Y1)	C(Y1)	D(X2)	E(Y2)	F(X3)	G(Y3)
Long Name				Subtracted_	Subtracted_	Baseline_D	Baseline_D
Units							
Comments					Subtracted from B		Baseline to Subtract for B
F(x)=							
Sparklines							
1	-0.09995	7.99255E-6	-2.12494E-5	-0.09995	-2.657E-7	-0.09995	8.25825E-6
2	-0.09506	7.99255E-6	-2.12494E-5	-0.09506	0	-0.09506	7.99255E-6
3	-0.09018	7.73315E-6	-2.04224E-5	-0.09018	6.29246E-9	-0.09018	7.72686E-6
4	-0.0853	7.48596E-6	-1.96503E-5	-0.0853	1.5647E-8	-0.0853	7.47032E-6
5	-0.08041	7.26318E-6	-1.8924E-5	-0.08041	3.11248E-8	-0.08041	7.23206E-6
6	-0.07553	7.05872E-6	-1.82312E-5	-0.07553	3.76746E-8	-0.07553	7.02104E-6
7	-0.07065	6.87256E-6	-1.7569E-5	-0.07065	3.26888E-8	-0.07065	6.83987E-6
8	-0.06577	6.70166E-6	-1.69342E-5	-0.06577	1.80272E-8	-0.06577	6.68363E-6
9	-0.06088	6.54602E-6	-1.63208E-5	-0.06088	-9.58E-10	-0.06088	6.54698E-6
10	-0.056	6.40869E-6	-1.57257E-5	-0.056	-1.587E-8	-0.056	6.42456E-6

FeCn + Fc

Graph6 *



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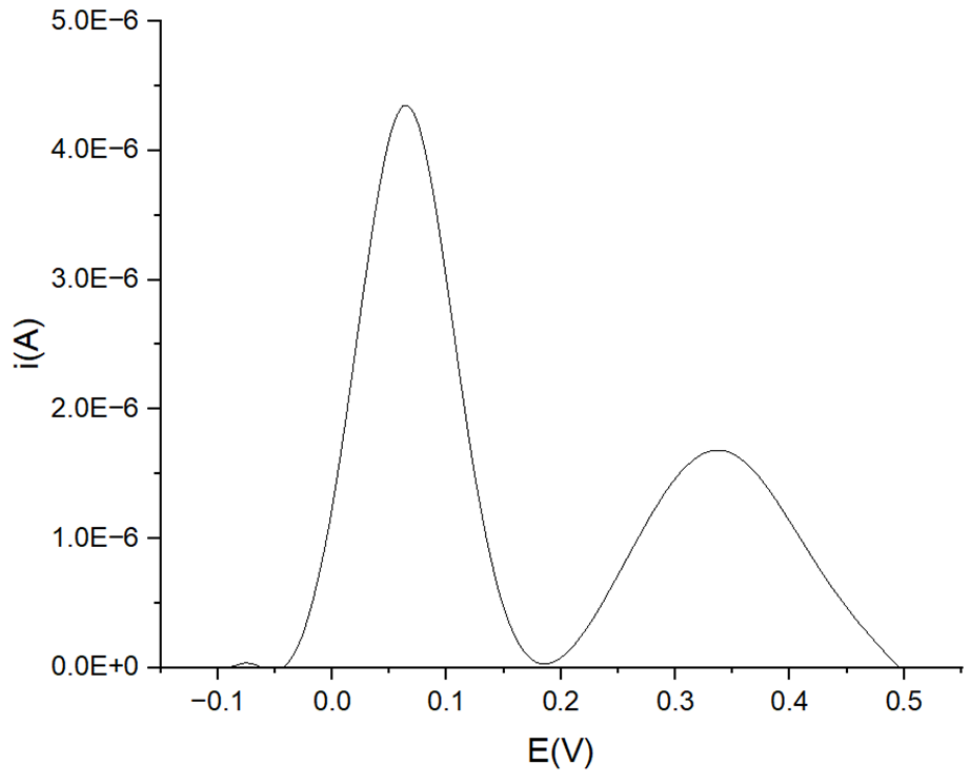
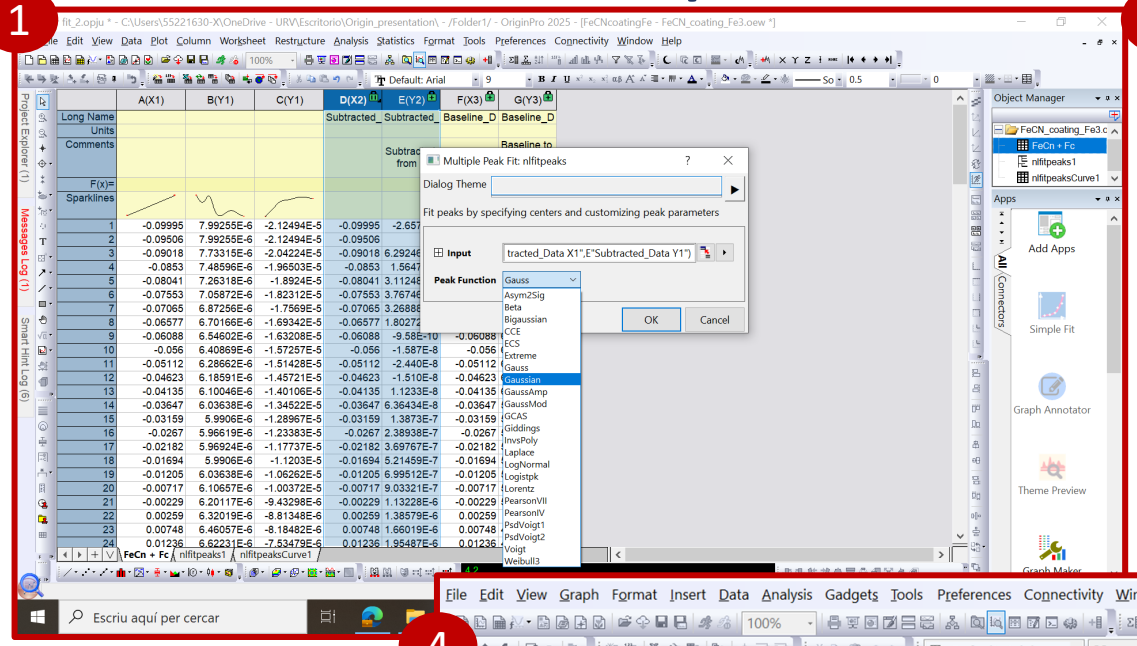


II) Practical example: Signal integration

1



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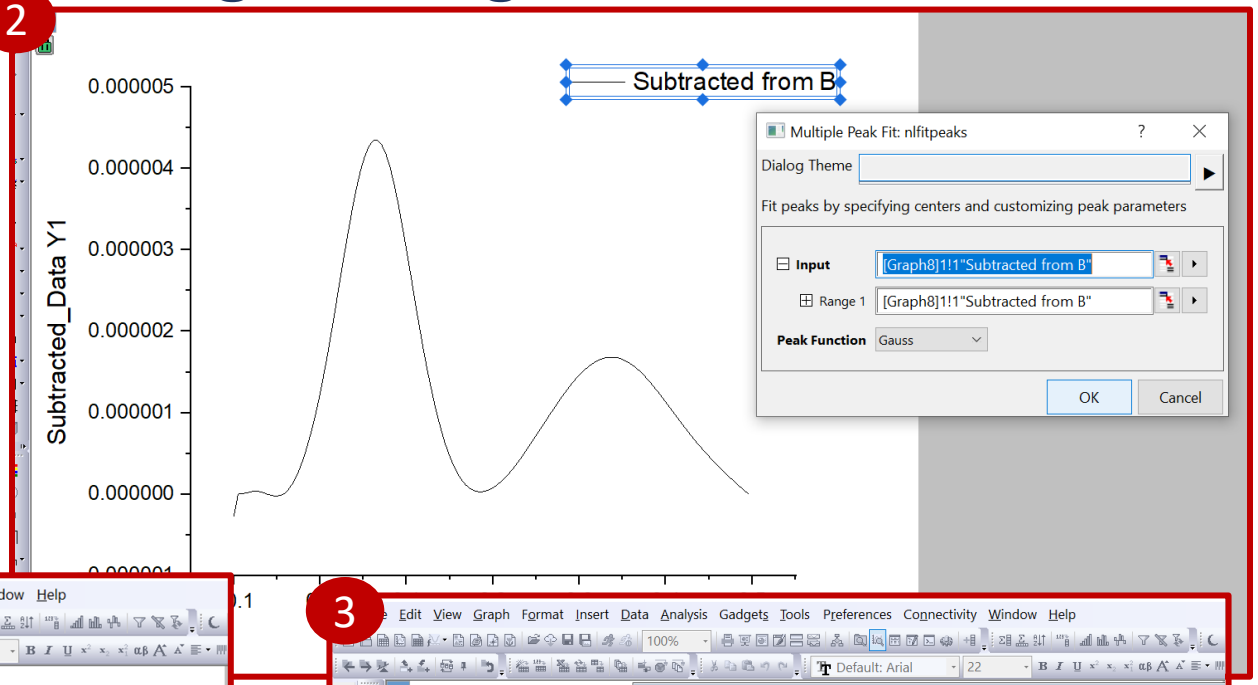

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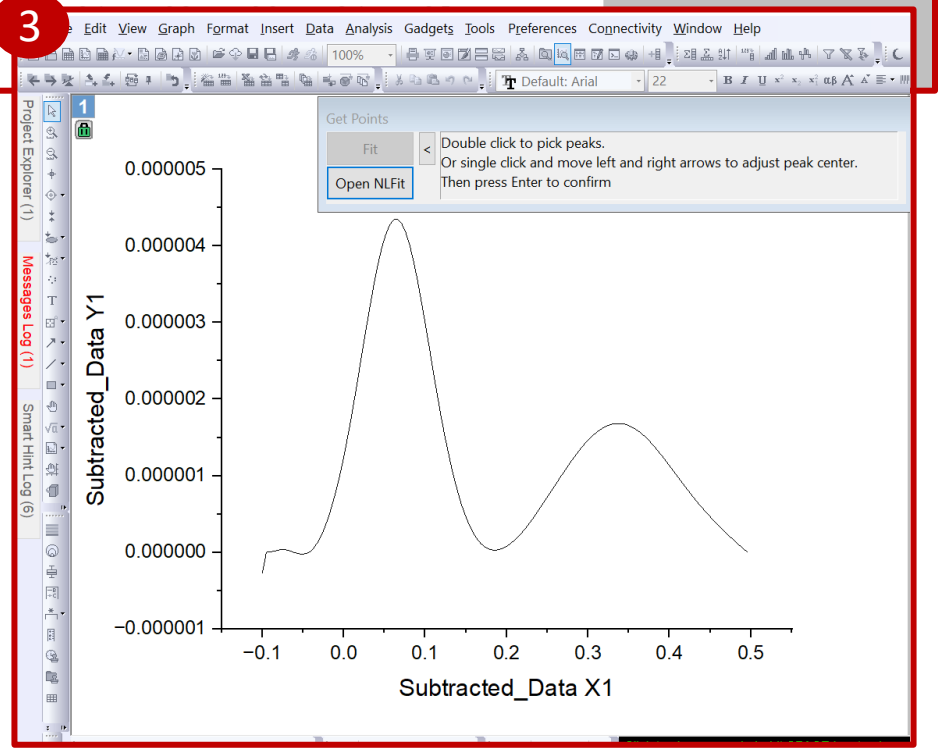

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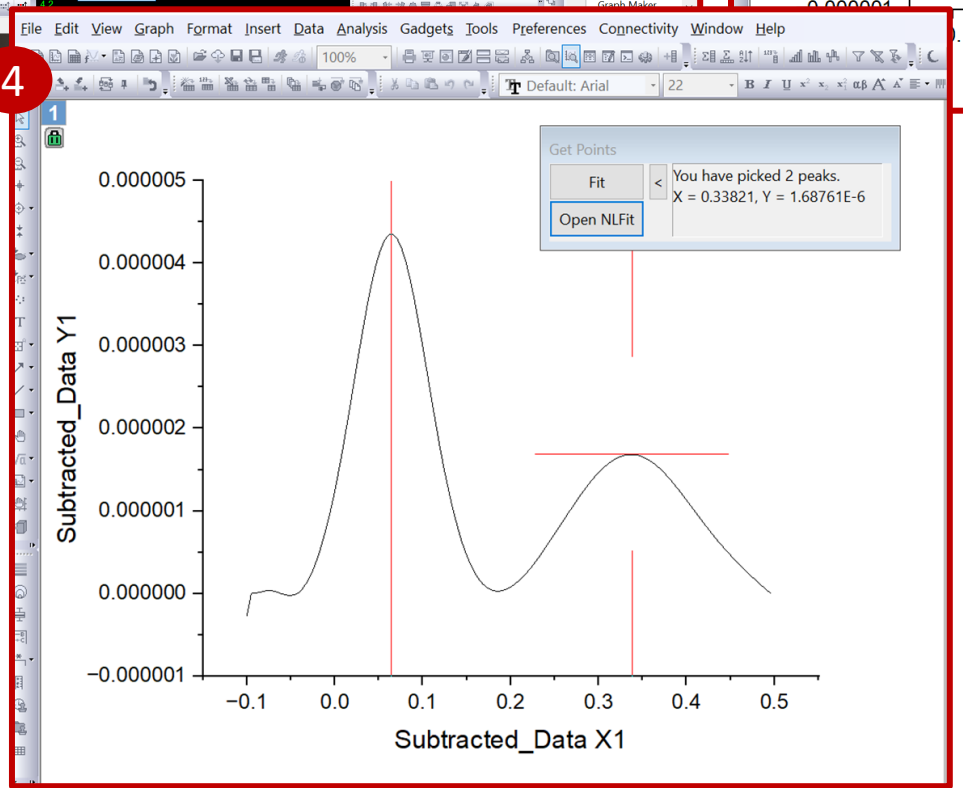
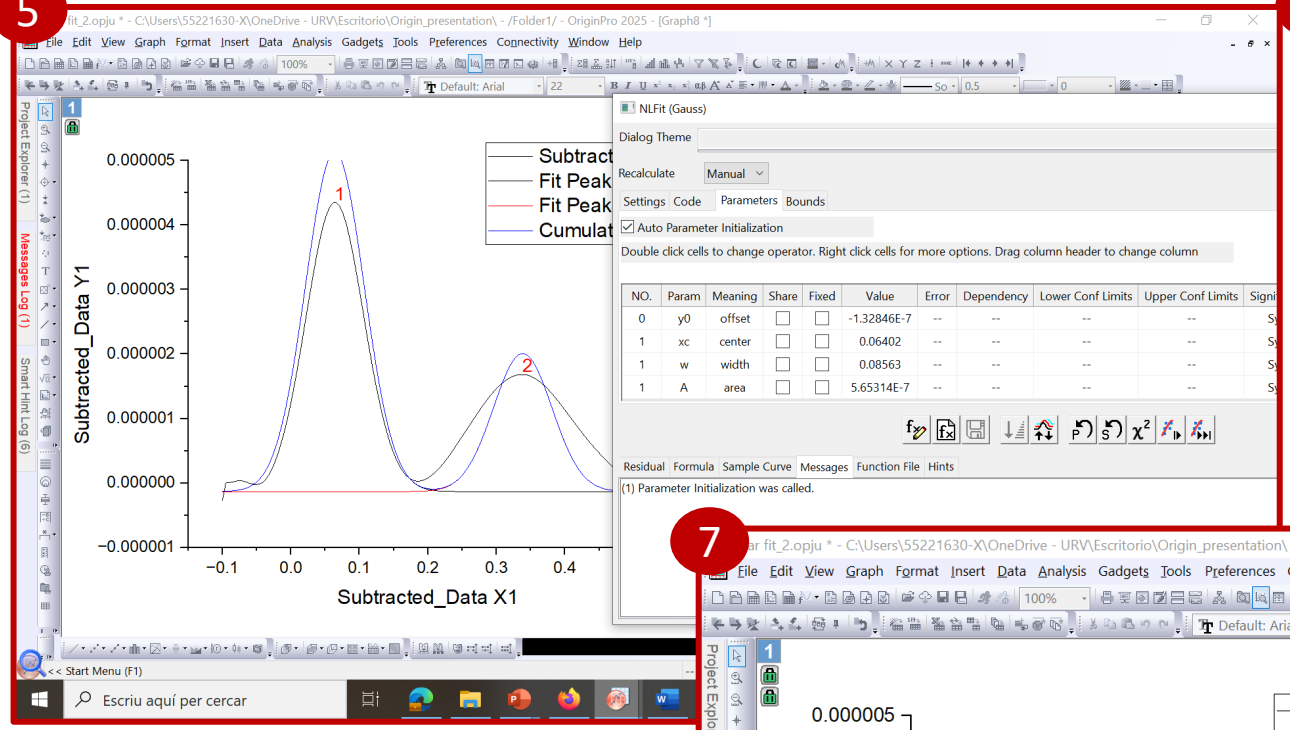


II) Practical example: Signal integration

5



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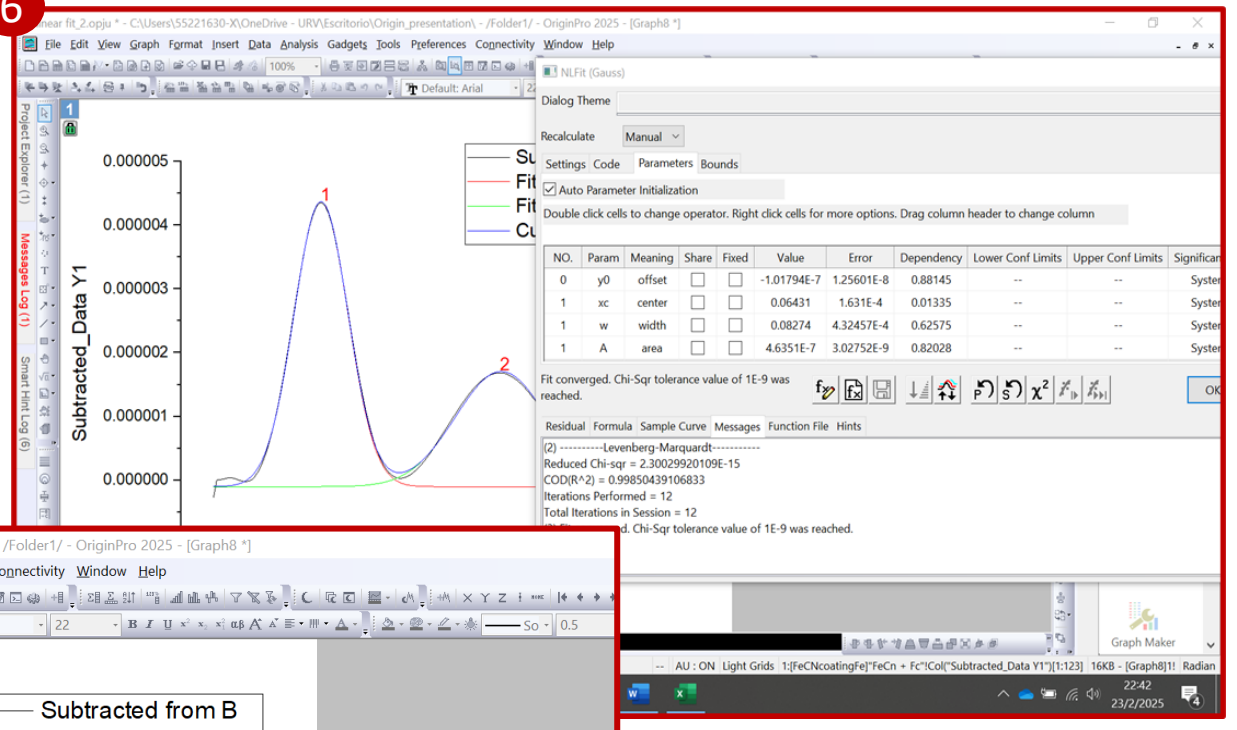

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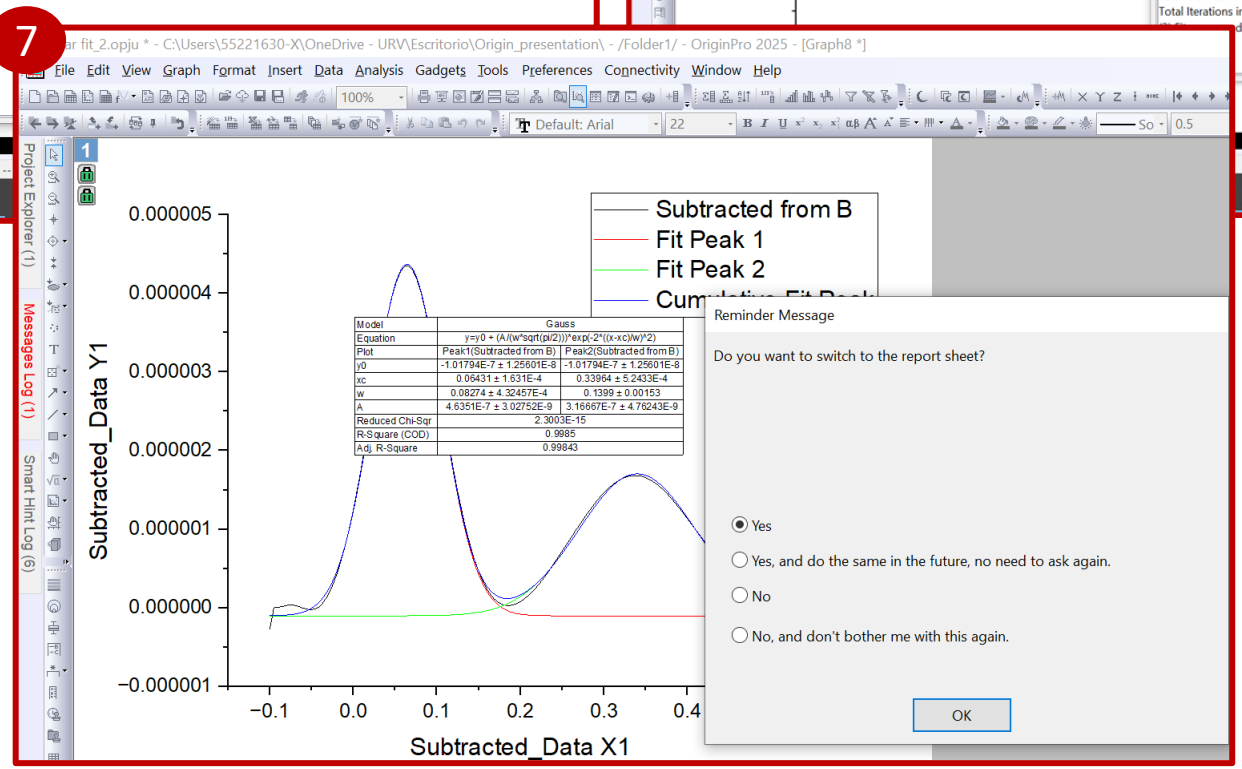
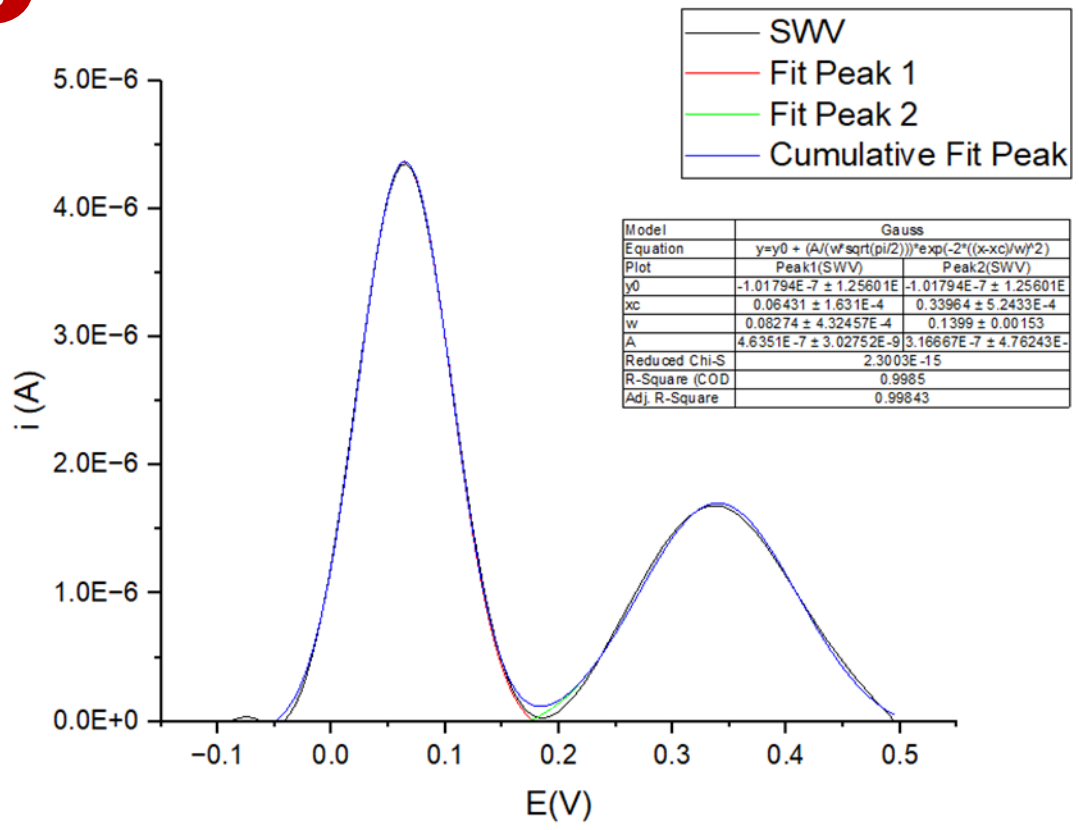


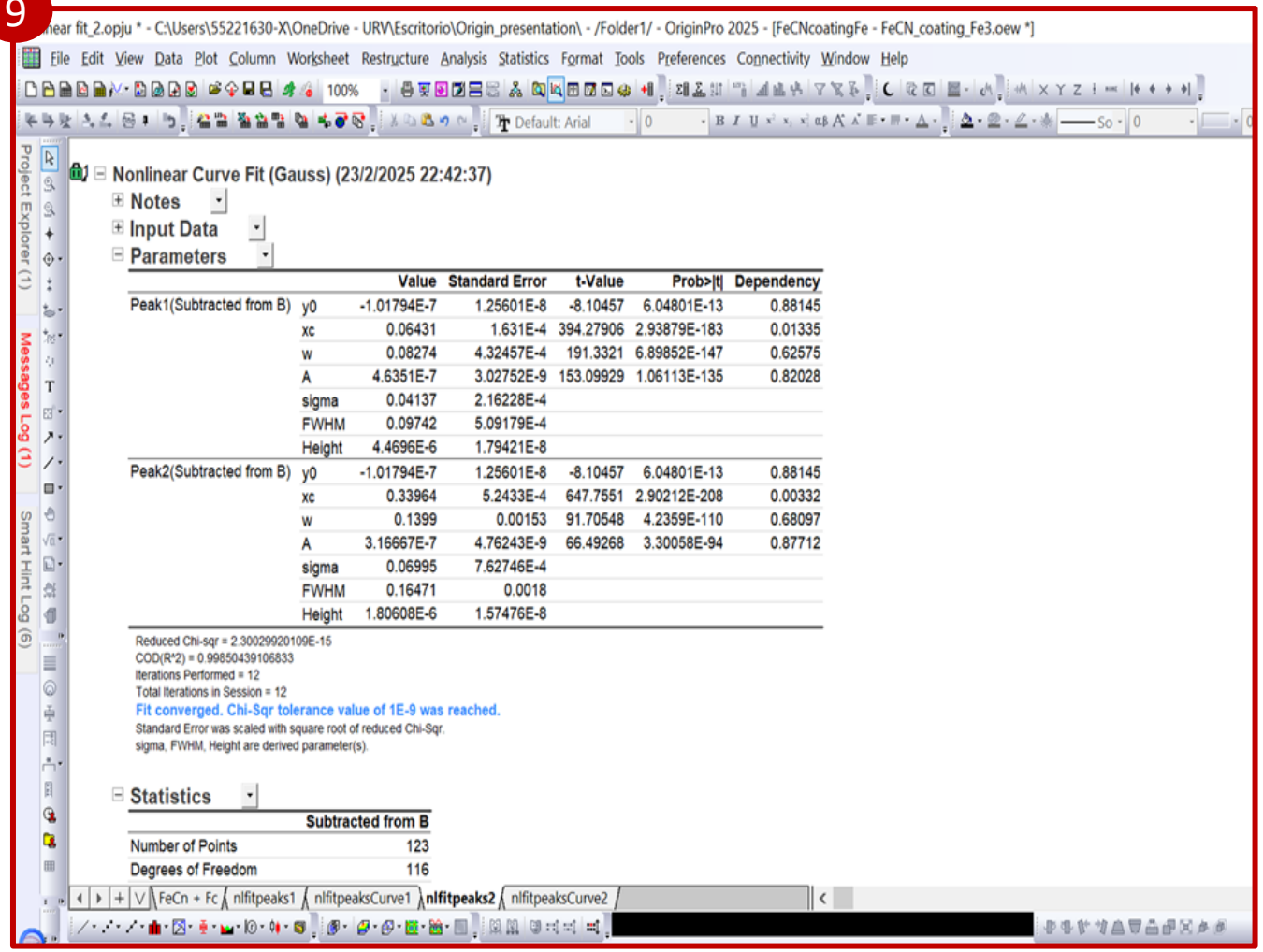
II) Practical example: Signal integration

8



Model	Gauss	
Equation	y=y0 + (A/(w*sqrt(pi/2)))*exp(-2*((x-xc)/w)^2)	
Plot	Peak1(SWV)	Peak2(SWV)
y0	-1.01794E-7 ± 1.25601E	-1.01794E-7 ± 1.25601E
xc	0.06431 ± 1.631E-4	0.33964 ± 5.2433E-4
w	0.08274 ± 4.32457E-4	0.1399 ± 0.00153
A	4.6351E-7 ± 3.02752E-9	3.16667E-7 ± 4.76243E-
Reduced Chi-S	2.3003E-15	
R-Square (COD	0.9985	
Adj. R-Square	0.99843	

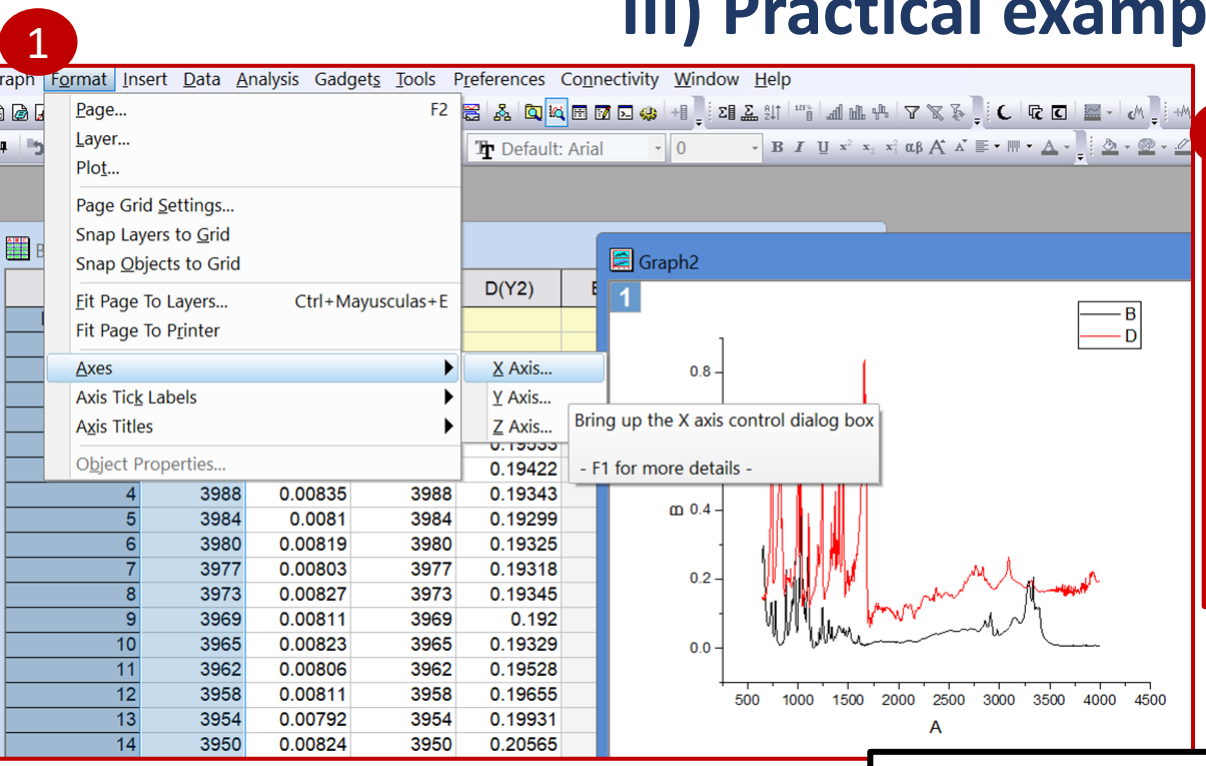
9

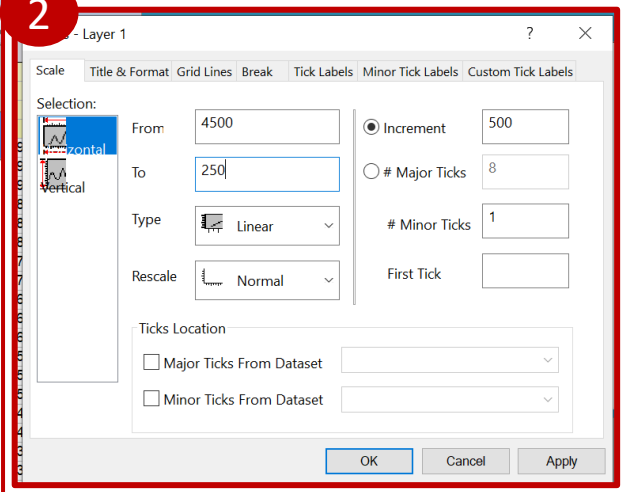


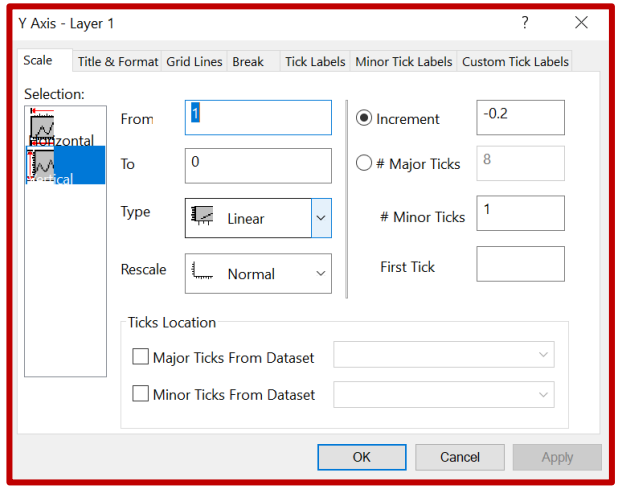
		Value	Standard Error	t-Value	Prob>|t|	Dependency
Peak1(Subtracted from B)	y0	-1.01794E-7	1.25601E-8	-8.10457	6.04801E-13	0.88145
	xc	0.06431	1.631E-4	394.27906	2.93879E-183	0.01335
	w	0.08274	4.32457E-4	191.3321	6.89852E-147	0.62575
	A	4.6351E-7	3.02752E-9	153.09929	1.06113E-135	0.82028
	sigma	0.04137	2.16228E-4			
	FWHM	0.09742	5.09179E-4			
	Height	4.4696E-6	1.79421E-8			
Peak2(Subtracted from B)	y0	-1.01794E-7	1.25601E-8	-8.10457	6.04801E-13	0.88145
	xc	0.33964	5.2433E-4	647.7551	2.90212E-208	0.00332
	w	0.1399	0.00153	91.70548	4.2359E-110	0.68097
	A	3.16667E-7	4.76243E-9	66.49268	3.30058E-94	0.87712
	sigma	0.06995	7.62746E-4			
	FWHM	0.16471	0.0018			
	Height	1.80608E-6	1.57476E-8			

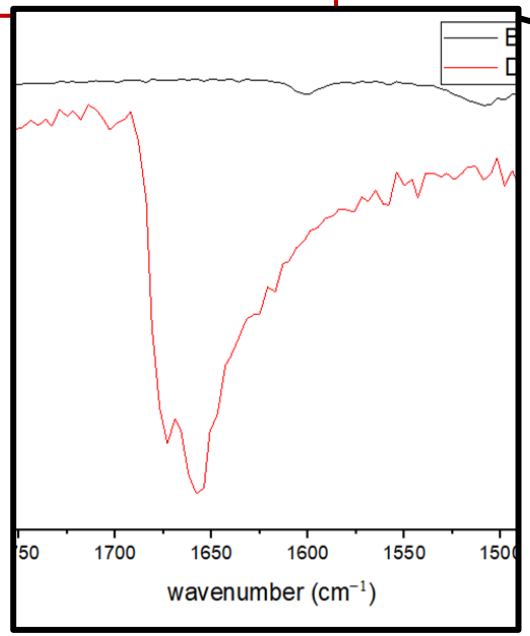
	Subtracted from B
Number of Points	123
Degrees of Freedom	116

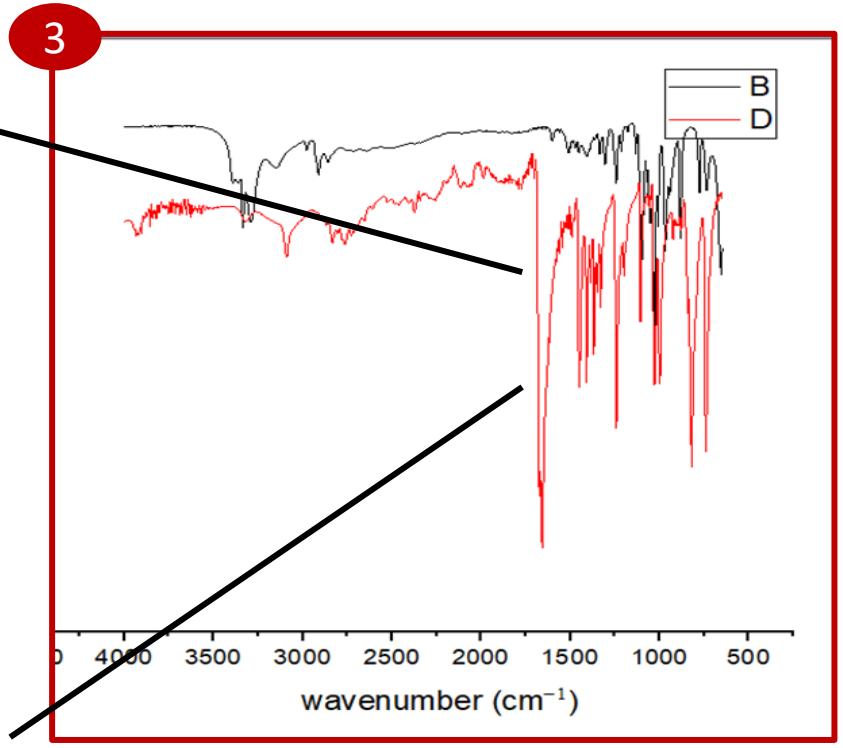
III) Practical example: plotting FTIR spectra





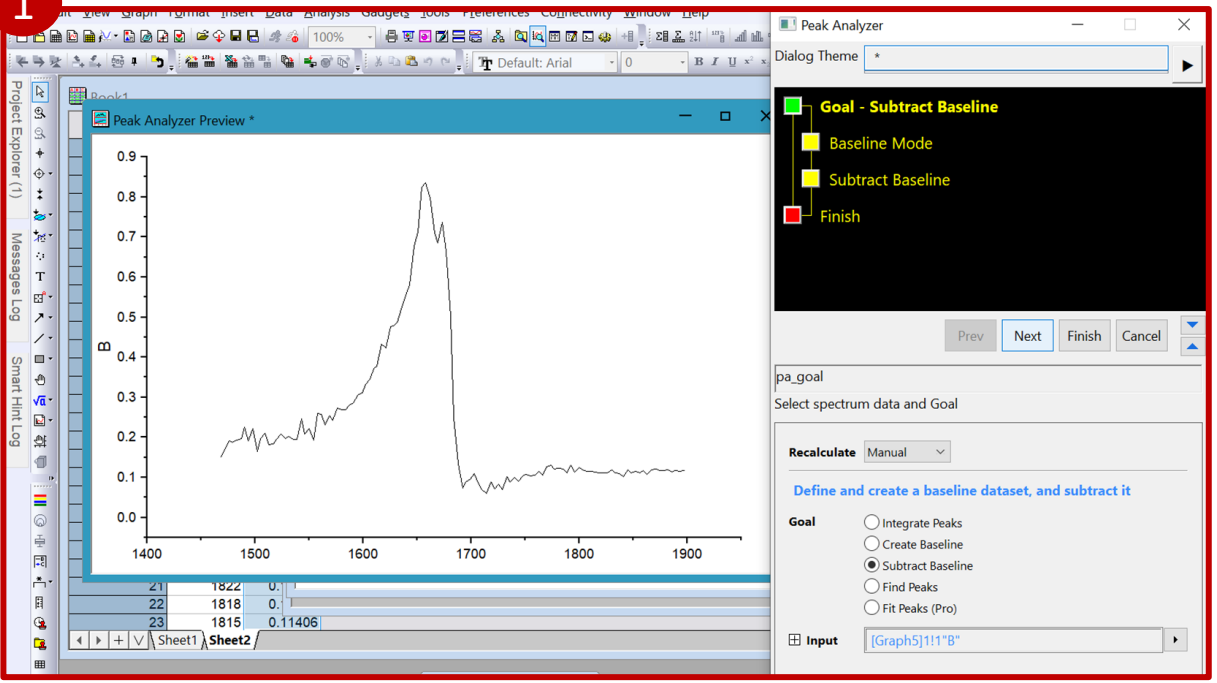




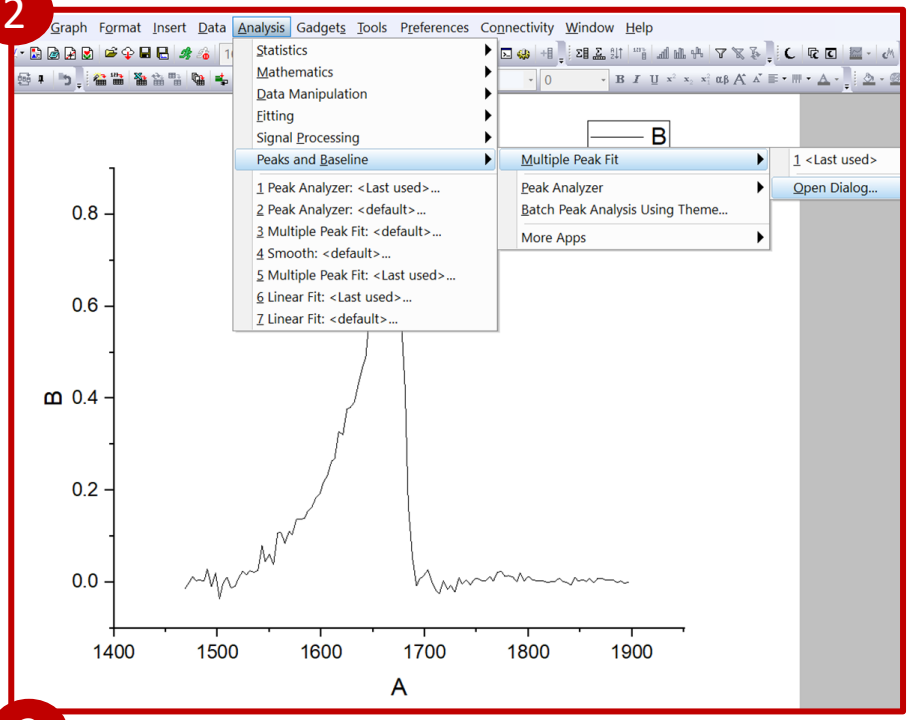


IV) Practical example: FTIR – signal deconvolution

1



2



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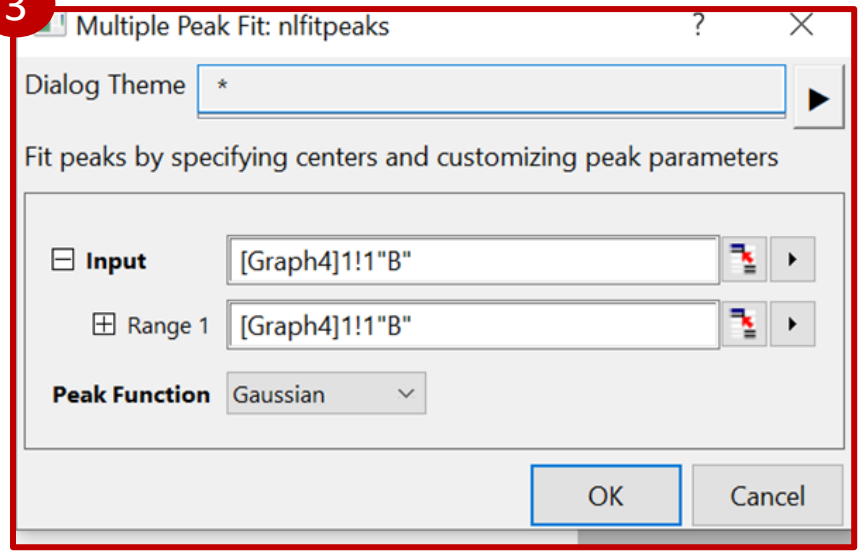
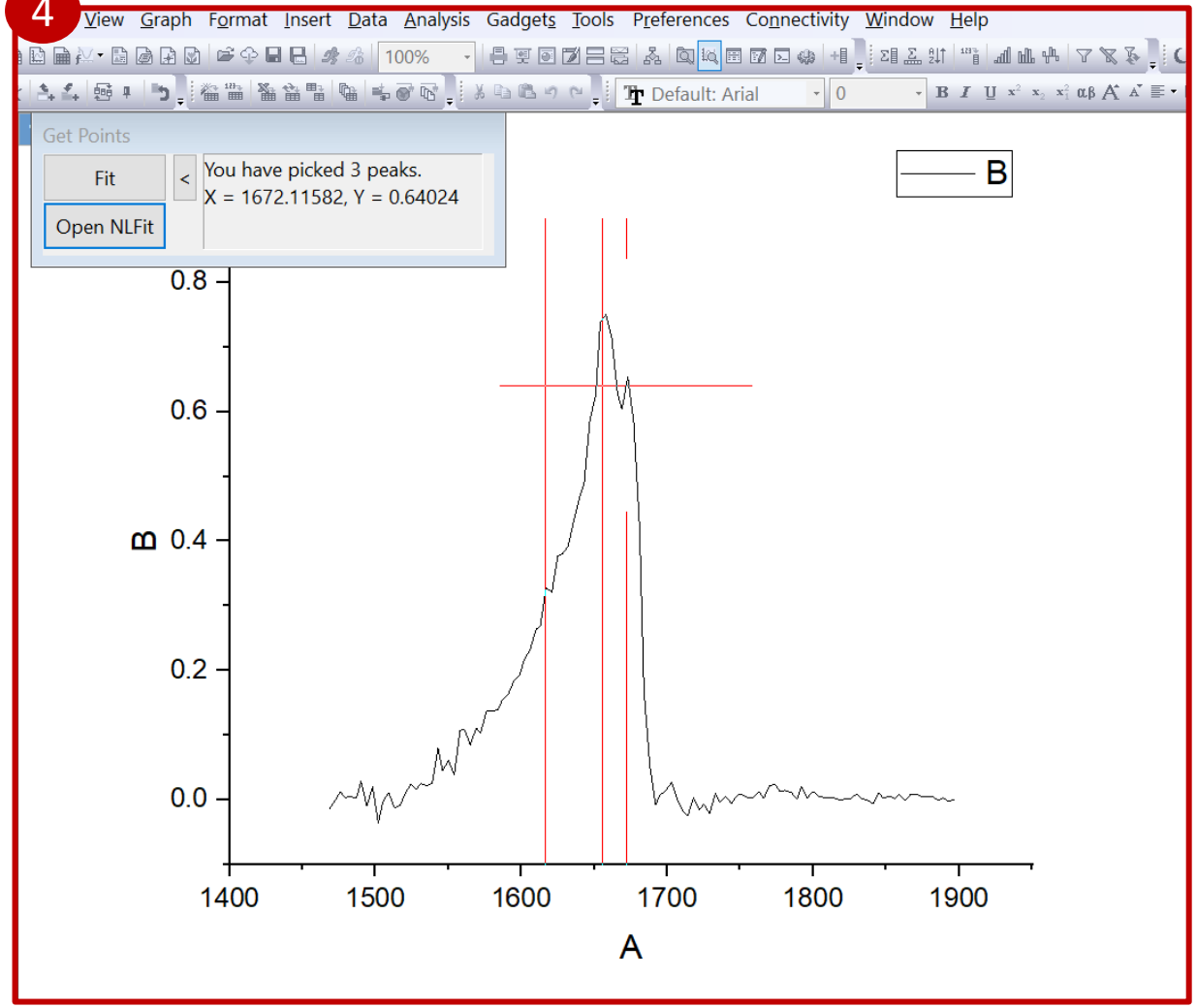
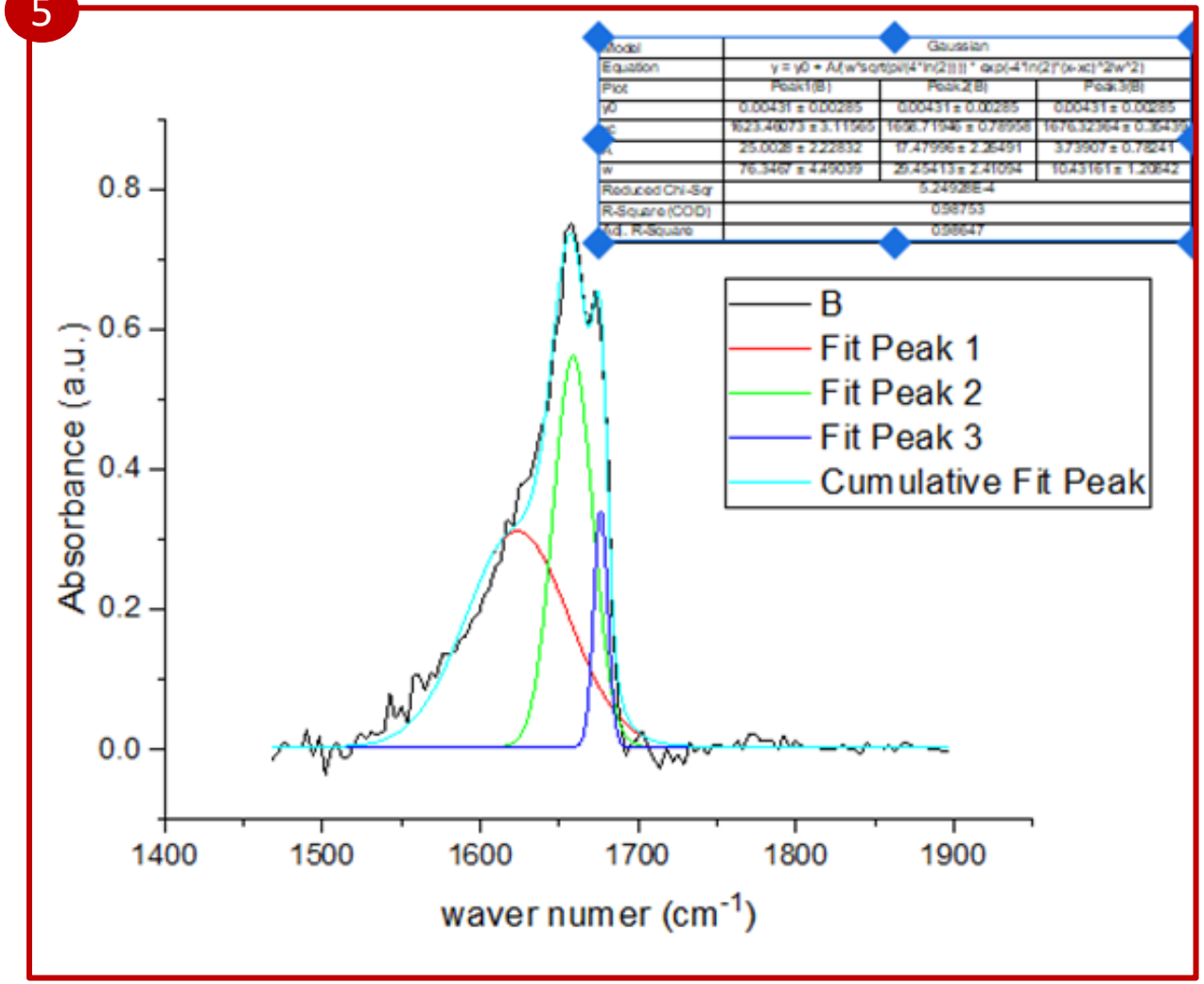


IV Practical example: FTIR – signal deconvolution

4

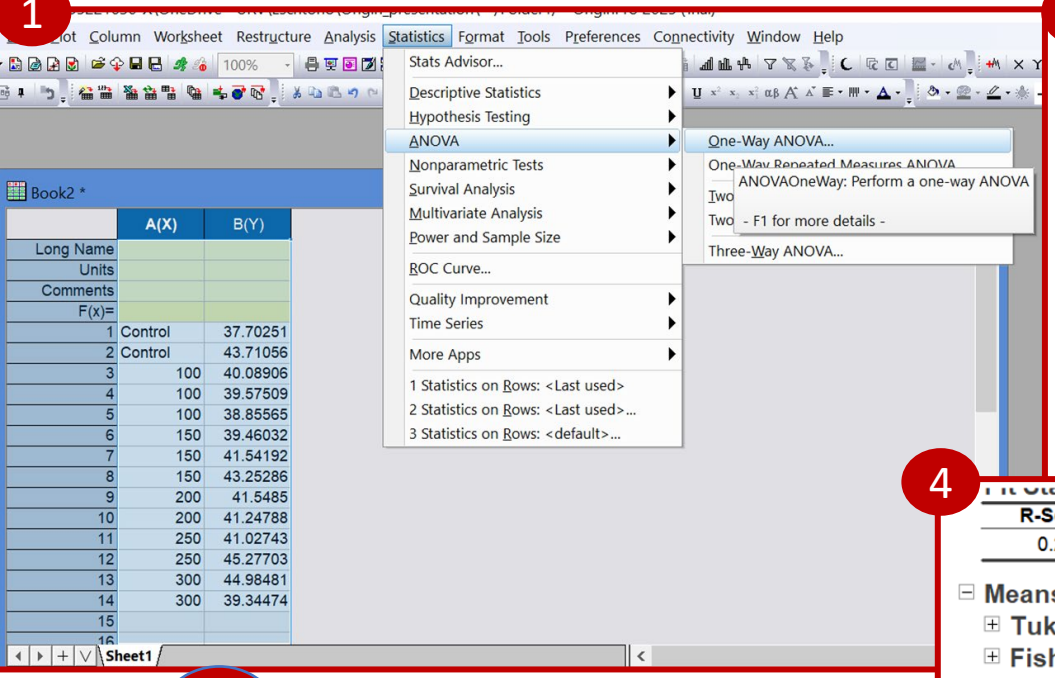


5

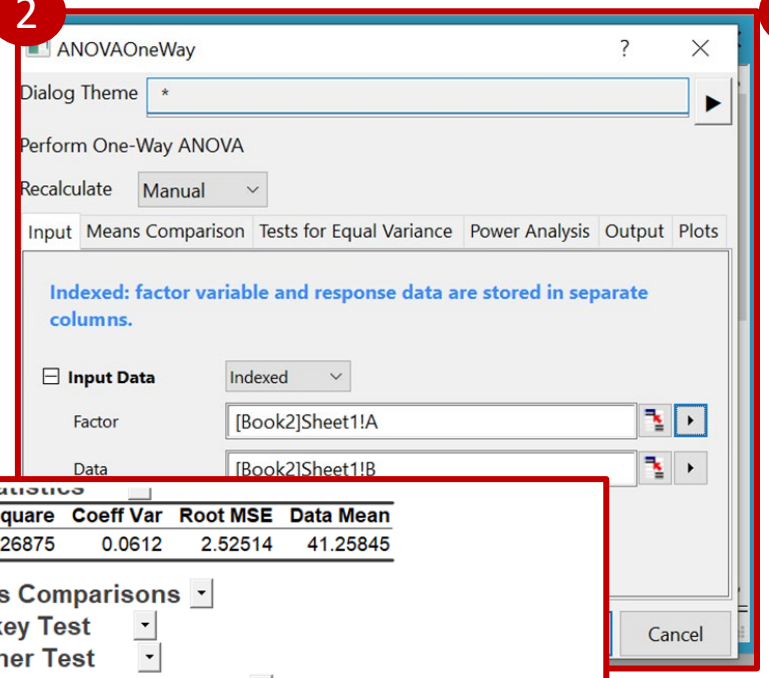


V) Practical example: Statistics by ANOVA

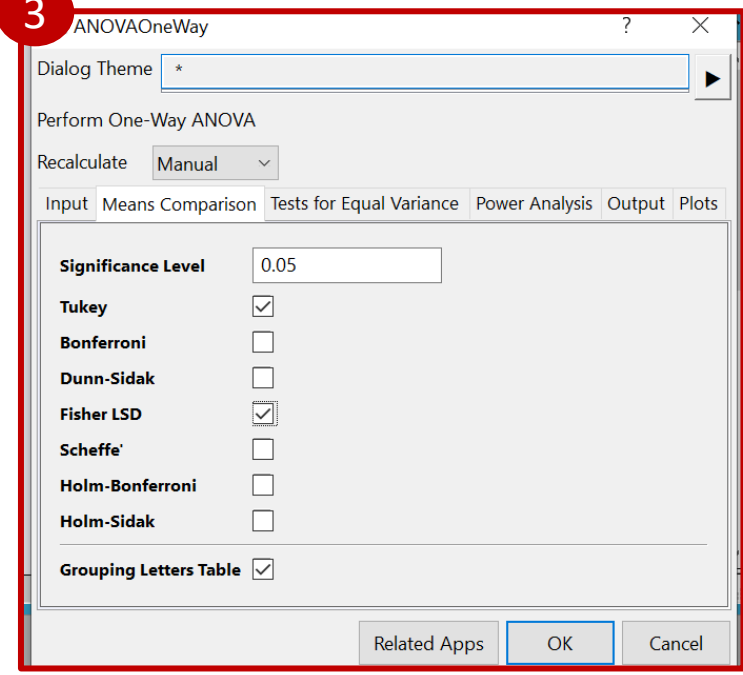
1



2



3



4

R-Square	Coeff Var	Root MSE	Data Mean
0.26875	0.0612	2.52514	41.25845

Means Comparisons

Tukey Test

Fisher Test

Grouping Letters Table

Tukey Test

	Mean	Groups
250	43.15223	A
300	42.16477	A
150	41.41837	A
200	41.39819	A
Control	40.70654	A
100	39.5066	A

Means that do not share a letter are significantly different.

Fisher Test

	Mean	Groups
250	43.15223	A
300	42.16477	A
150	41.41837	A
200	41.39819	A
Control	40.70654	A
100	39.5066	A

Means that do not share a letter are significantly different.

Sig equals 1 indicates that the difference of the means is significant at the 0.05 level.
Sig equals 0 indicates that the difference of the means is not significant at the 0.05 level.

4a

Means Comparisons

Tukey Test

Fisher Test

Grouping Letters Table

Tukey Test

	Mean	Groups
200	50.63666	A
250	45.15223	A B
300	42.16477	B
150	41.41837	B
Control	40.70654	B
100	39.5066	B

Means that do not share a letter are significantly different.

To conclude:

Origin offers a huge portfolio of graphical capabilities!

And of course EXCEL is useful for many applications:

it is a matter of selecting what you need at all times...

They are worth exploring.

Thank you!