



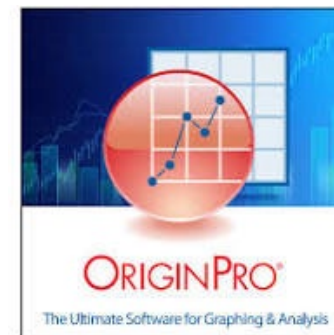
UNIVERSITAT ROVIRA I VIRGILI

DEPARTAMENT
D'ENGINYERIA QUÍMICA

OriginPro-Advanced Signal Analysis

Applications in Spectroscopic and Electrochemical Signals

Dr. Mayreli Ortiz



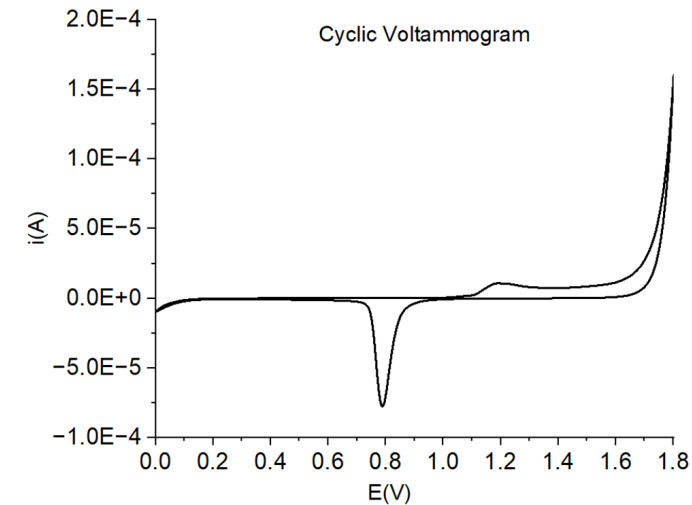
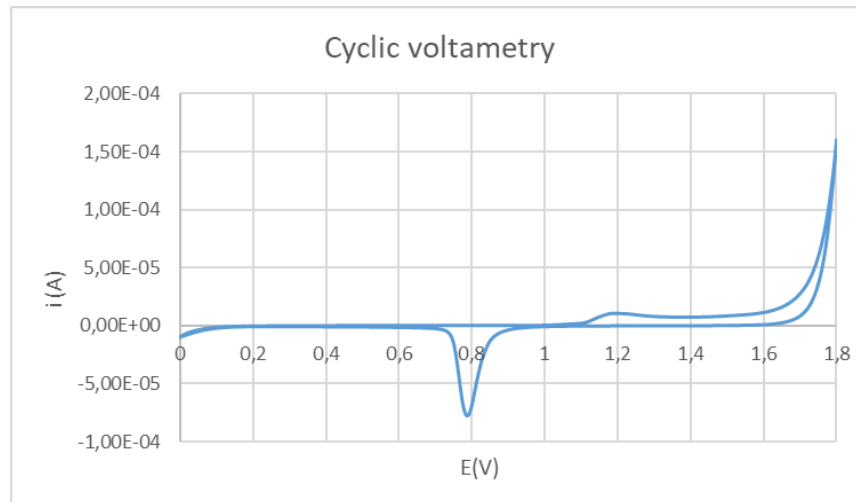
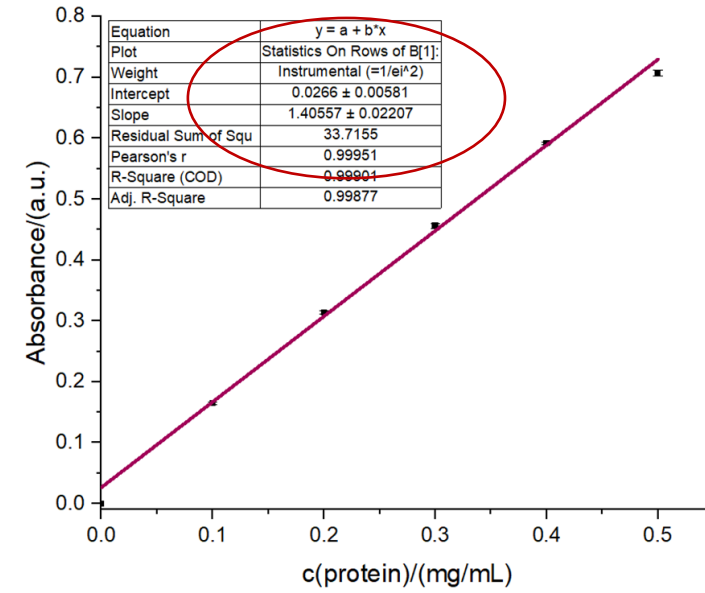
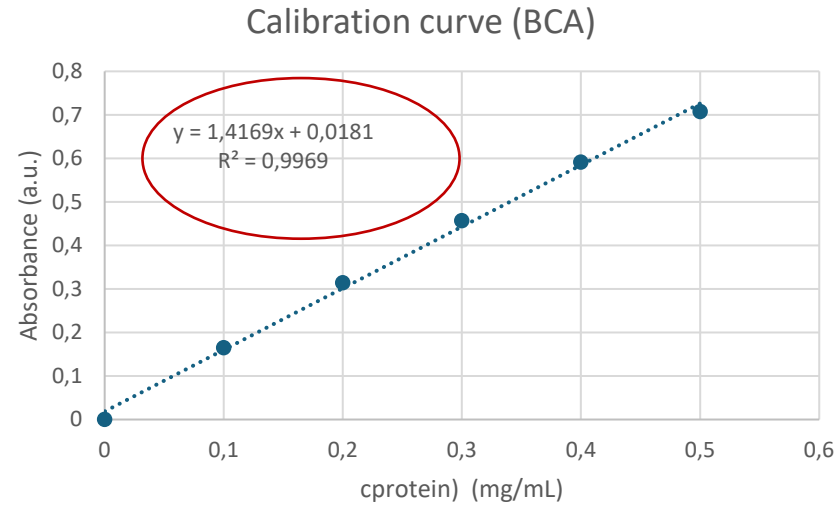
Origin vs Excel: an actual conflict?



	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 functions	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?



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C:\ProgramData\OriginLab\95\Origin\Central\Graphing Search Graphing

3D Scatter Ribbon and Wall Graphs - 3D Ribbons.opju
3D Scatter Ribbon and Wall Graphs - 3D Scatter with Col...
3D Scatter Ribbon and Wall Graphs - 3D Scatter with XY...
3D Scatter Ribbon and Wall Graphs - 3D Stacked Walls.o...
3D Scatter Ribbon and Wall Graphs - 3D Trajectory with ...
3D Scatter Ribbon and Wall Graphs - 3D XYY Wall.opju

3D Scatter 3D Scatter 3D Surface Plots

Scroll to View all Graphs in Project

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 Analy...
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>



OriginLab

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Origin/OriginPro Videos

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Importing Data - Database								
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Graphing								
Graphing - Showcase								
Graphing - Customizing Graphs								
Graphing - Data Exploration								
Graphing - Publishing								
Workbook and Data								
Workbook and Data - General								
	Origin 2025 Highlights	General - Overviews	00:04:57		11/15/2024	10.2	Y	YouTube
	Introduction to Origin/OriginPro	General - Overviews	00:02:30		6/9/2021	9.85	Y	YouTube
	Getting Starting with Graphing	General - Overviews	00:04:14		10/18/2019	9.7	Y	YouTube
	Bringing Data into Origin	General - Overviews	00:03:07		10/18/2019	9.7	Y	YouTube
	Analysis with Auto Recalculations	General - Overviews	00:02:28		10/18/2019	9.7	Y	YouTube
	Build Your Presentation in 60 Seconds	General - Overviews	00:01:22		1/5/2018	9.5	Y	YouTube
	Origin Learning Center	General - Overviews	00:02:26		12/25/2017	9.5	Y	
	Apps for Origin	General - Overviews	00:01:54		12/14/2017	9.5	Y	YouTube

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- ☒ I own/have used older version of Origin and I would like try Origin
- ☐ I have NEVER used Origin

What is your sector?

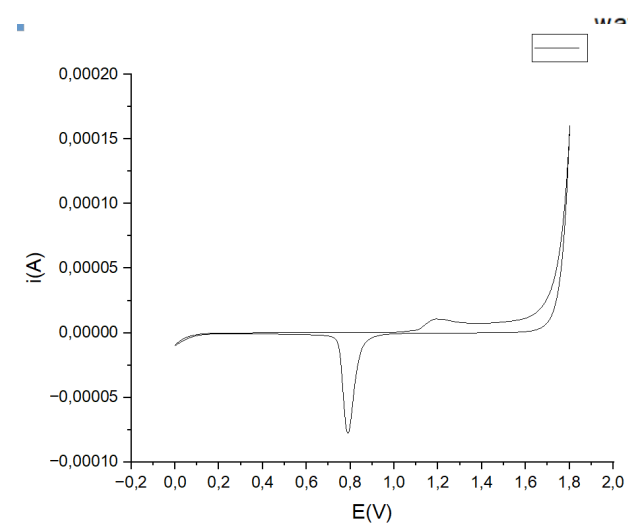
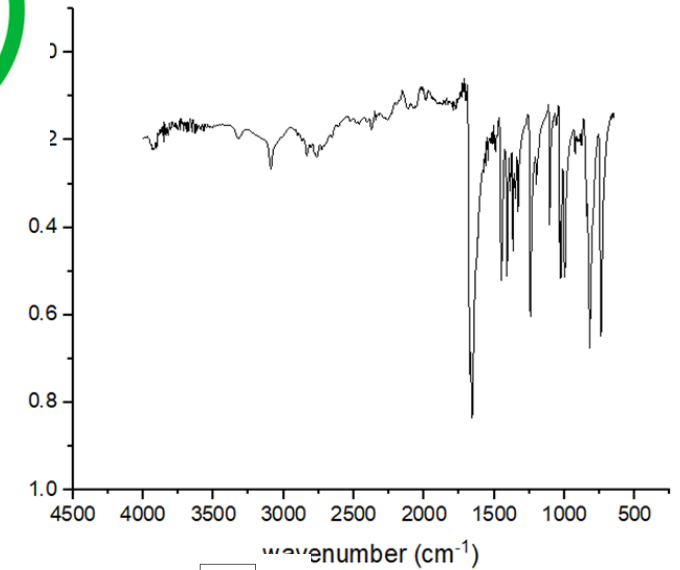
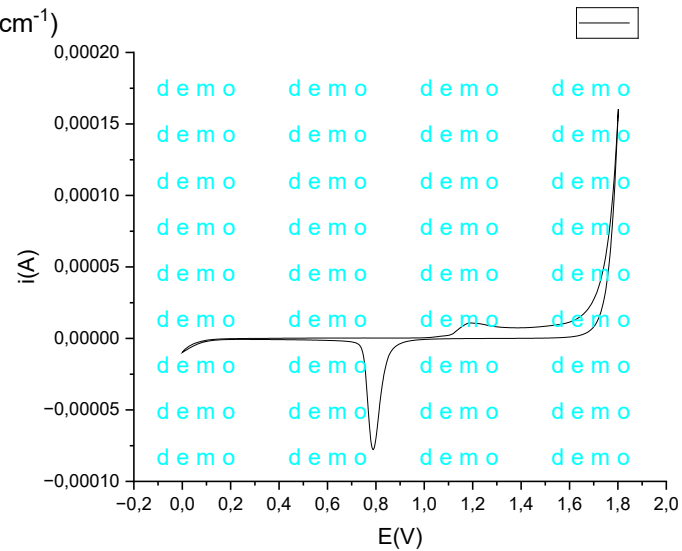
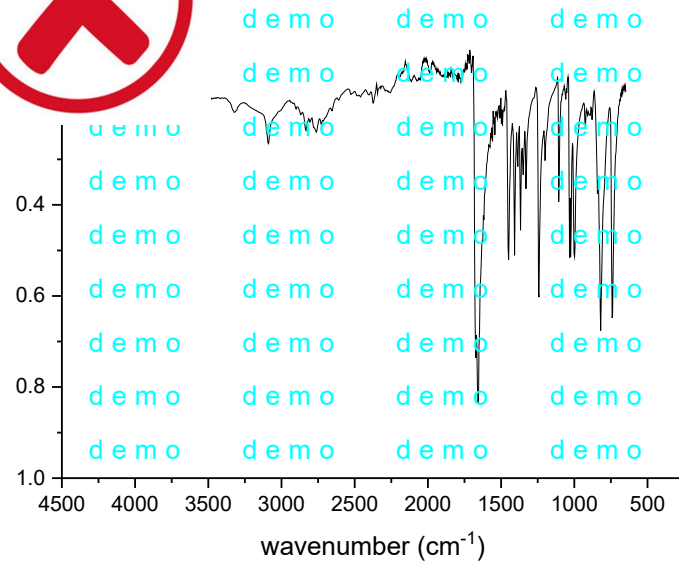
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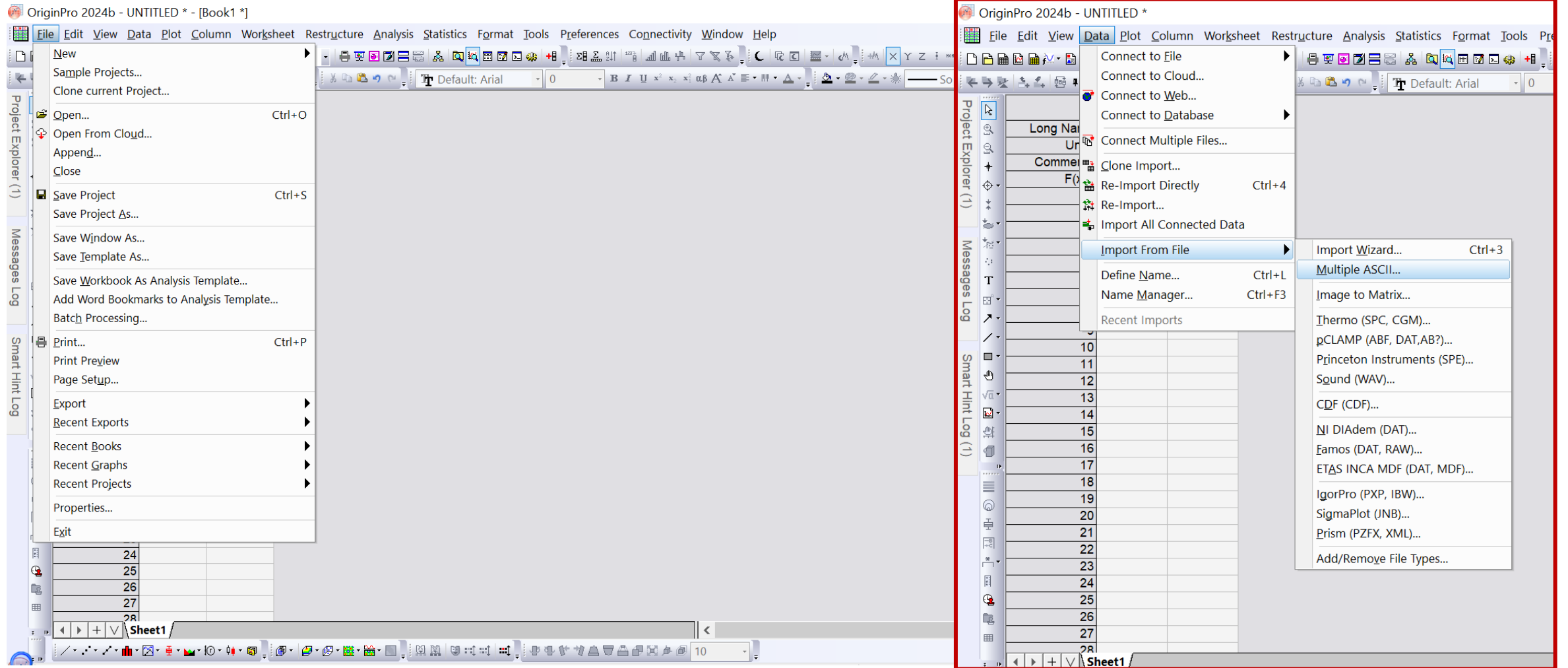
Why do we need an Origin Pro licence?



Some tips for starters in OriginPro...



Some tips: the interface



Some tips: the interface

OriginPro 2024b - UNTITLED * - [Book1 *]

File Edit View Data Plot Column Worksheet Restructure Analysis Statistics Format Tools Preferences Connectivity Window Help

Project Explorer (1) Messages Log Smart Hint Log

Long Name
Units
Comments
 $F(x)=$
1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
16
17
18
19
20
21
22
23
24
25
26
27
28

Basic 2D

- Bar, Pie, Area
- Multi-Panel, Multi-Axis
- Statistical
- Contour, Heatmap
- Map
- Specialized
- Categorical
- 3D
- Browser
- Function Plot
- Extended Templates

Graph Maker Template Library Template Center

Scatter Scatter Central Column Scatter Y Error X Y Error Error Band Scatter + Rug Bubble Color Mapped Bubble + Color Mapped

Line Horizontal Step Vertical Step Spline Line + Symbol Line Series Before - After 2 Point Segment 3 Point Segment Spline Connected

Lollipop Plot Vertical Drop Line Density Dots Color Dots Colormapped Line Series Stacked Lines by Y Offsets Row-wise...

Object Manager

- Book1
- Sheet1

Apps

- Add Apps
- Stats Advisor
- Speedy Fit
- Simple Fit

Connectors

Sheet1

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

The first thing to do when starting to use Origin...

The screenshot shows the Origin software interface. The main window displays a worksheet with columns A(X), B(Y), and C(Y). The data in column A(X) is as follows:

Long Name	A(X)	B(Y)	C(Y)
Units	Å		
Comments			
F(x)=			
1	CV 0.1M H2SO4 clea		
2			
3			
4	0.09277	-1.49109E-6	65.3
5	0.09521	-1.42395E-6	63.3
6	0.09766	-1.35284E-6	
7	0.1001	-1.28967E-6	
8	0.10254	-1.22681E-6	
9	0.10498	-1.16608E-6	
10	0.10742	-1.10992E-6	
11	0.10986	-1.05743E-6	
12	0.11231	-1.0022E-6	
13	0.11475	-9.52759E-7	
14	0.11719	-9.09119E-7	
15	0.11963	-8.6792E-7	
16	0.12207	-8.23975E-7	
17	0.12451	-7.85217E-7	
18	0.12695	-7.39441E-7	
19	0.1294	-7.07397E-7	
20	0.13184	-6.72607E-7	
21	0.13428	-6.38733E-7	
22	0.13672	-6.03638E-7	
23	0.13916	-5.76782E-7	
24	0.1416	-5.50537E-7	
25	0.14404	-5.25208E-7	

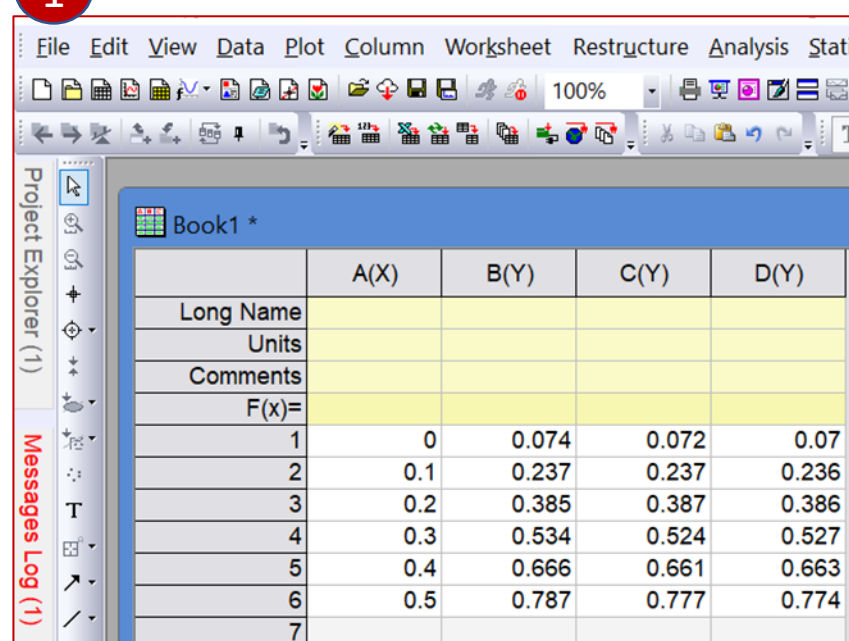
The Preferences dialog box is open, showing the Options tab. A blue arrow points from the Preferences dialog to the Options dialog. The Options dialog is also open, showing the Numerical Format tab. The Options dialog has several sections:

- Convert to Scientific Notation**: Upper Threshold Power (6), Lower Threshold Power (-3).
- Angular Unit**: Radian (selected), Degree, Gradian.
- Digits**: Decimal Digits (selected), Significant Digits. Number of Digits (5).
- Digits in Report**: Decimal Digits (selected), Significant Digits. Number of Digits (5).
- Separators**: Separator for ASCII Import (1,000.0), Date Format for Database Import (1,000.0), Use English in Reports and Graphs (1,000.0).

The Options dialog also has a dropdown menu for Windows Settings, which is currently set to 1,000.0. The OK button is highlighted.

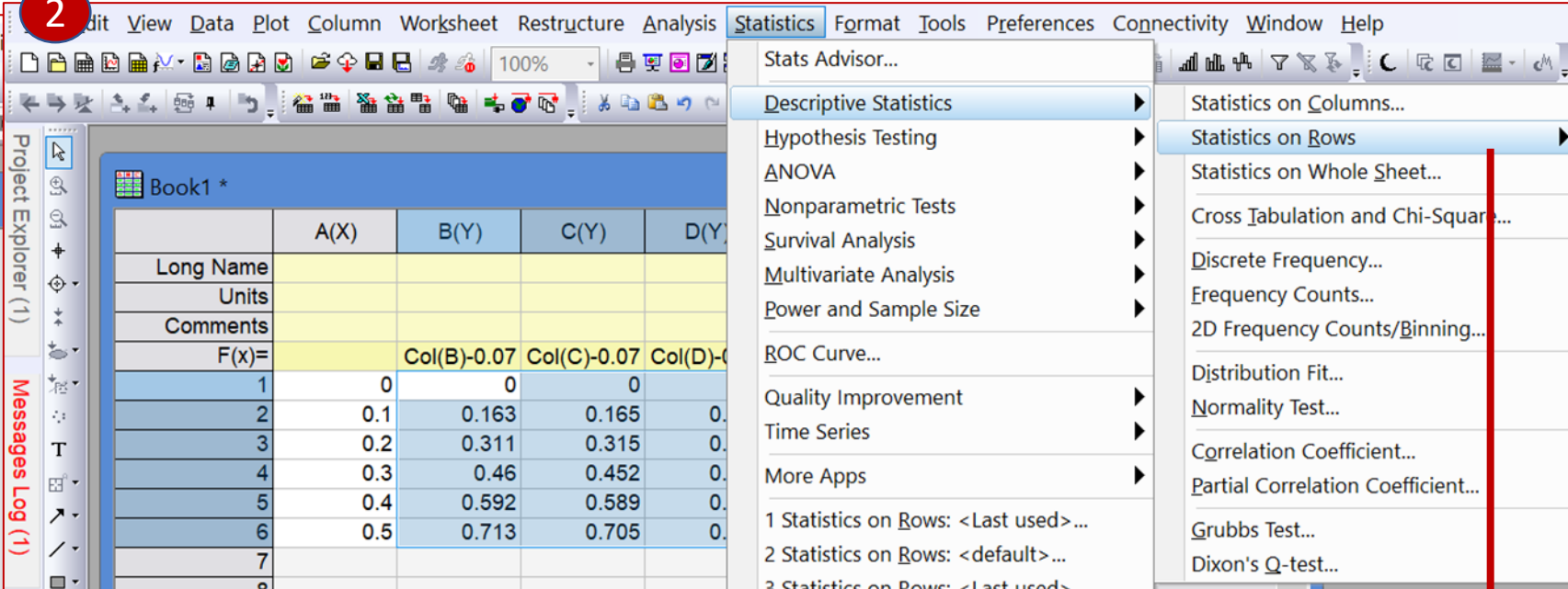
I) Practical example: A calibration curve - Linear fitting

1



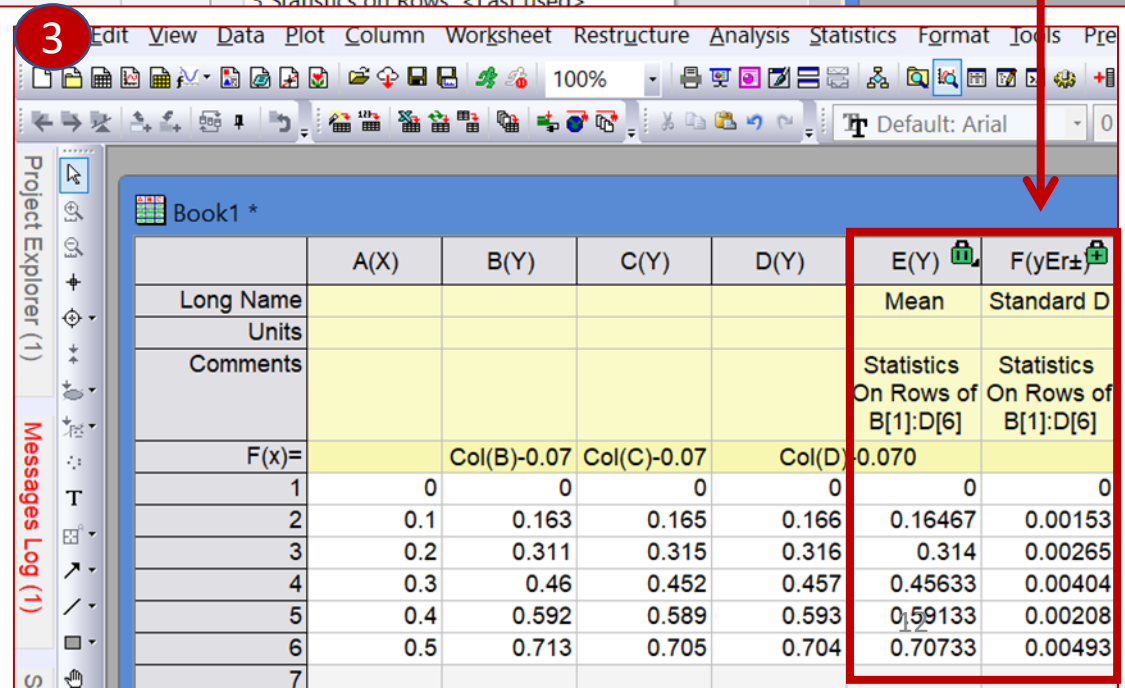
	A(X)	B(Y)	C(Y)	D(Y)
Long Name				
Units				
Comments				
F(x)=				
1	0	0.074	0.072	0.07
2	0.1	0.237	0.237	0.236
3	0.2	0.385	0.387	0.386
4	0.3	0.534	0.524	0.527
5	0.4	0.666	0.661	0.663
6	0.5	0.787	0.777	0.774
7				

2



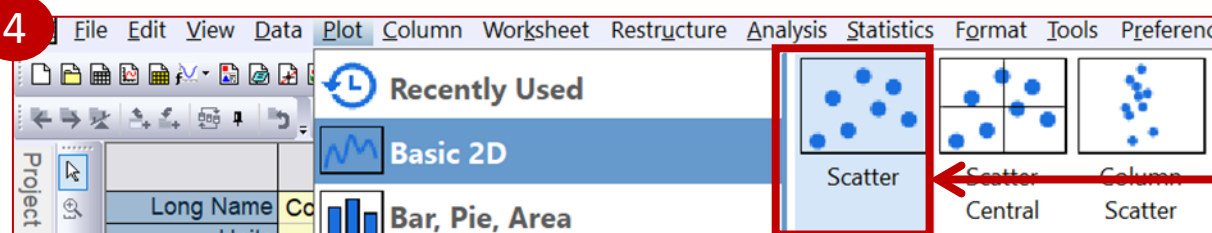
	A(X)	B(Y)	C(Y)	D(Y)
Long Name				
Units				
Comments				
F(x)=		Col(B)-0.07	Col(C)-0.07	Col(D)-0.07
1	0	0	0	0
2	0.1	0.163	0.165	0.166
3	0.2	0.311	0.315	0.316
4	0.3	0.46	0.452	0.457
5	0.4	0.592	0.589	0.593
6	0.5	0.713	0.705	0.704
7				
8				

3



	A(X)	B(Y)	C(Y)	D(Y)	E(Y)	F(Y)
Long Name					Mean	Standard D
Units						
Comments					Statistics On Rows of B[1]:D[6]	Statistics On Rows of B[1]:D[6]
F(x)=		Col(B)-0.07	Col(C)-0.07	Col(D)-0.07	0.070	
1	0	0	0	0	0	0
2	0.1	0.163	0.165	0.166	0.16467	0.00153
3	0.2	0.311	0.315	0.316	0.314	0.00265
4	0.3	0.46	0.452	0.457	0.45633	0.00404
5	0.4	0.592	0.589	0.593	0.59133	0.00208
6	0.5	0.713	0.705	0.704	0.70733	0.00493
7						

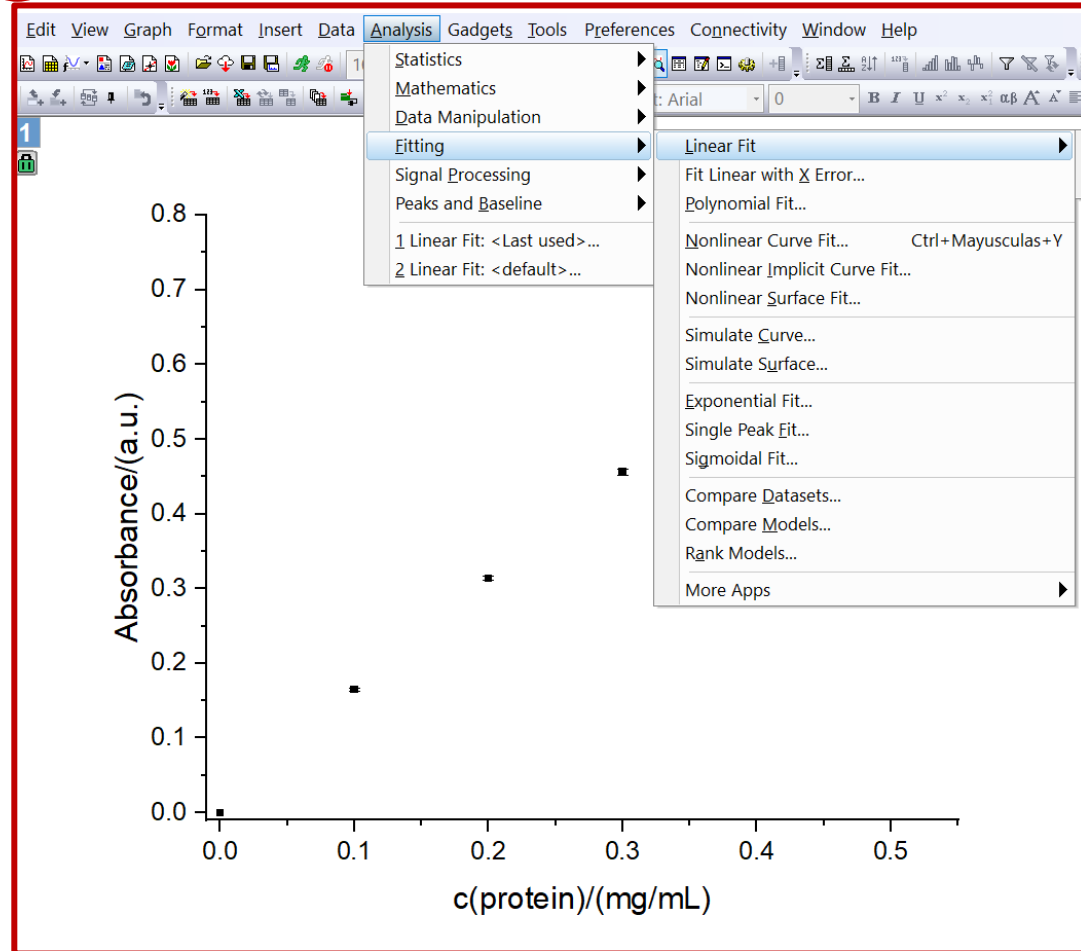
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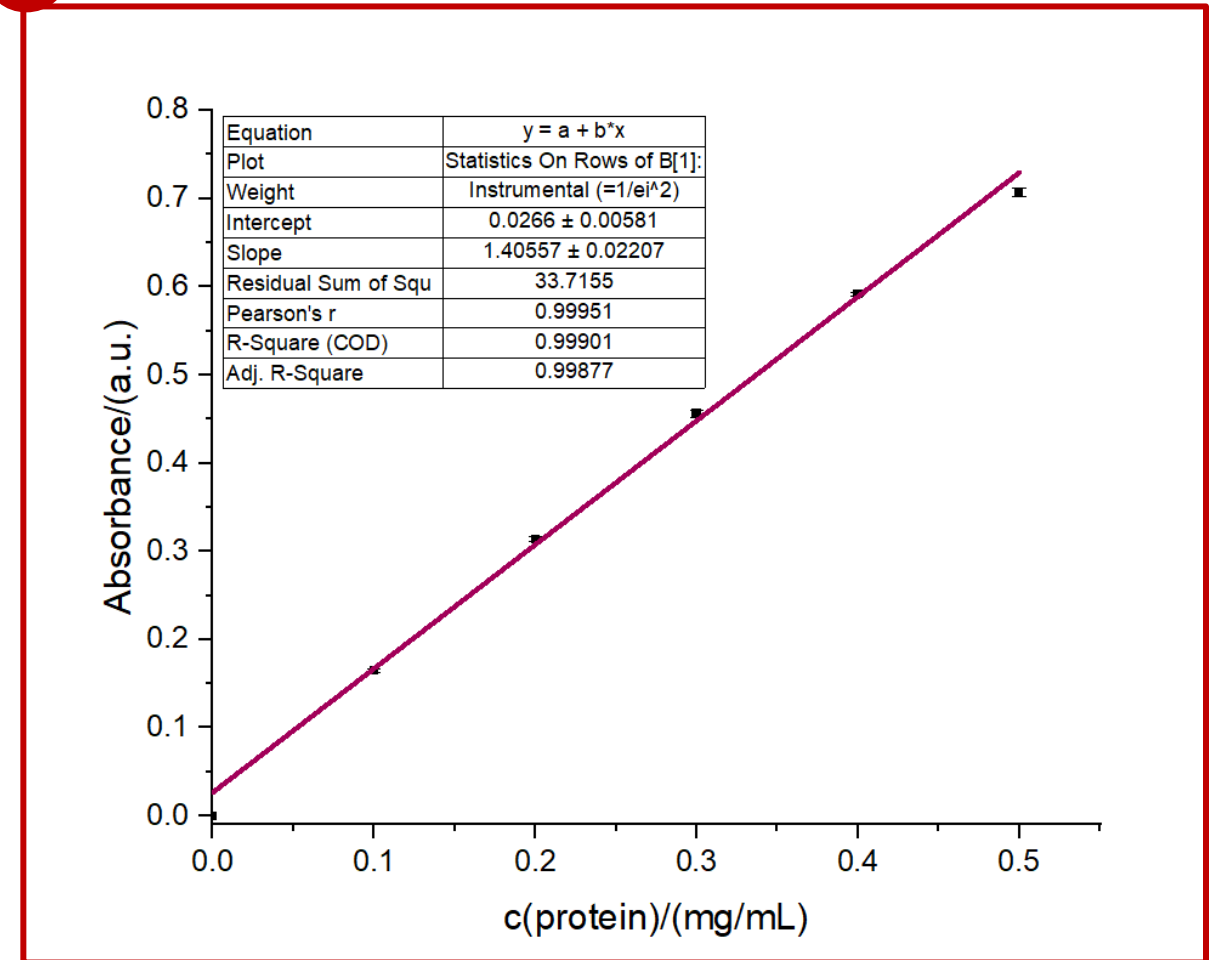
	A(X)	B(Y)	C(Y)	D(Y)
Long Name				
Units				
Comments				
F(x)=				
1	0	0.074	0.072	0.07
2	0.1	0.237	0.237	0.236
3	0.2	0.385	0.387	0.386
4	0.3	0.534	0.524	0.527
5	0.4	0.666	0.661	0.663
6	0.5	0.787	0.777	0.774
7				

I) Practical example: A calibration curve - Linear fitting

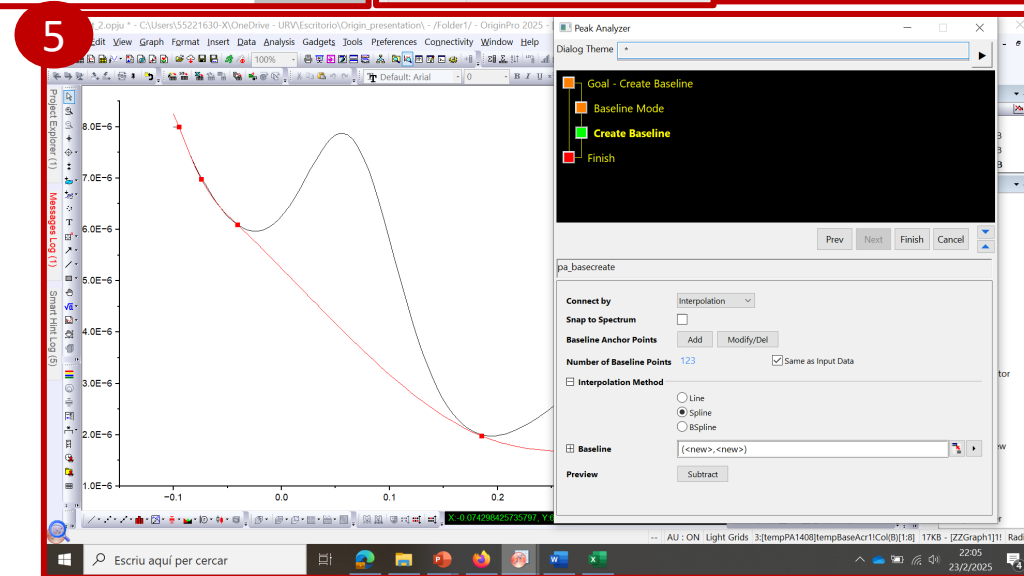
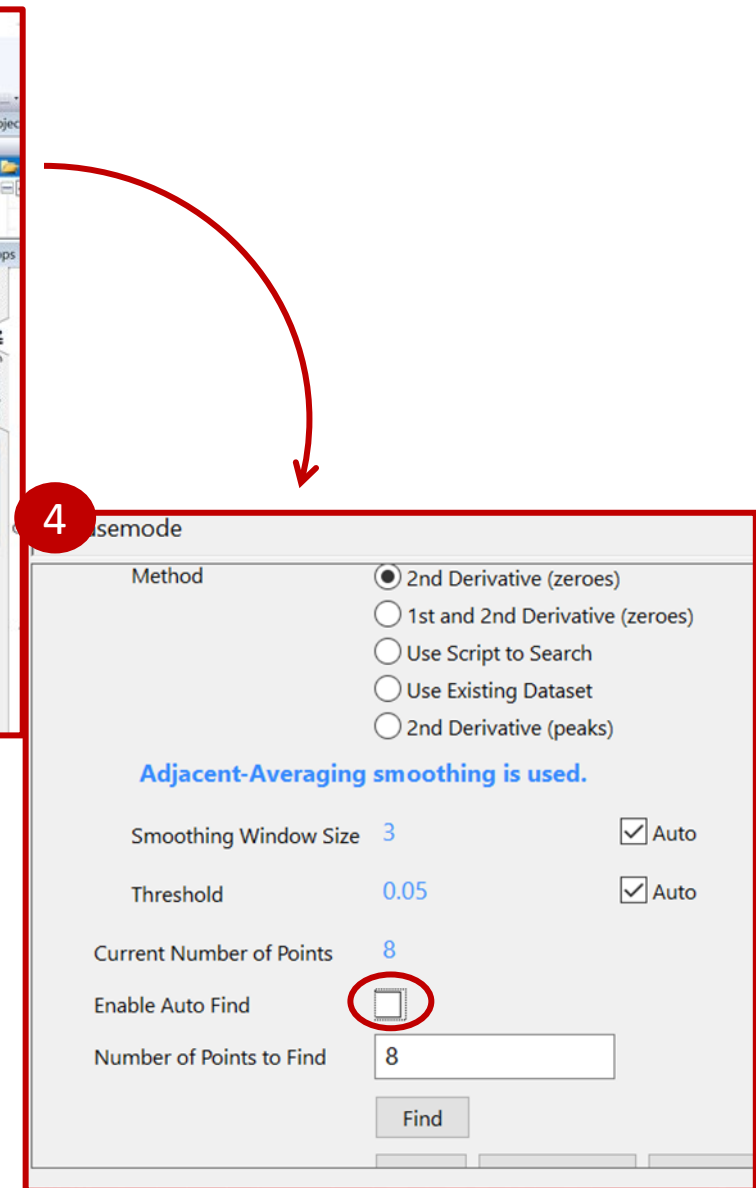
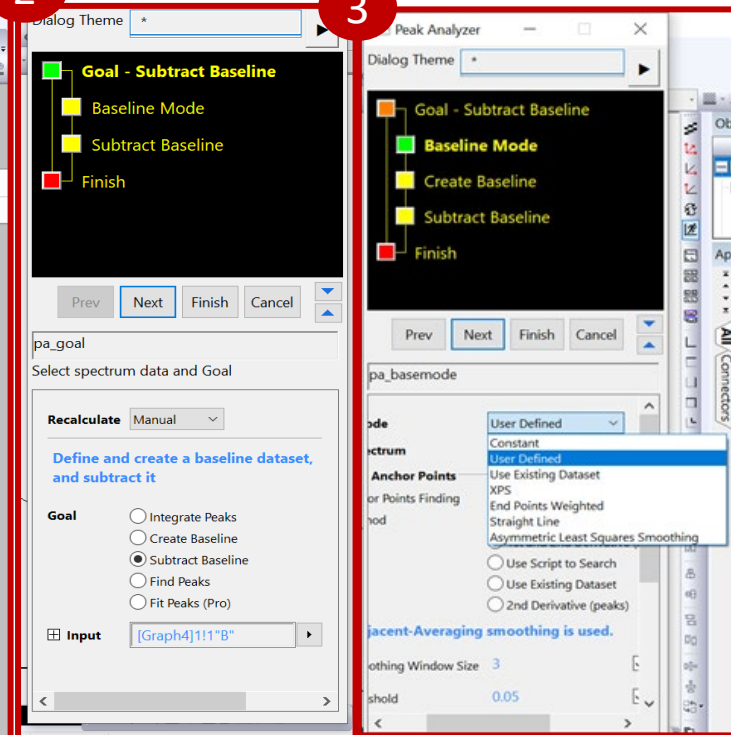
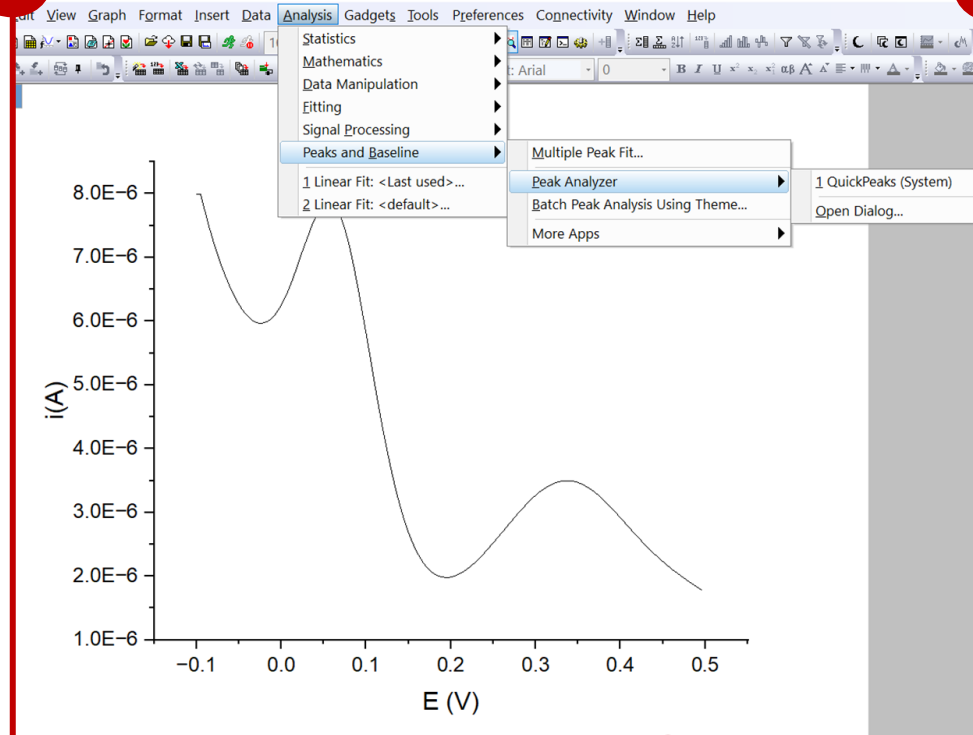
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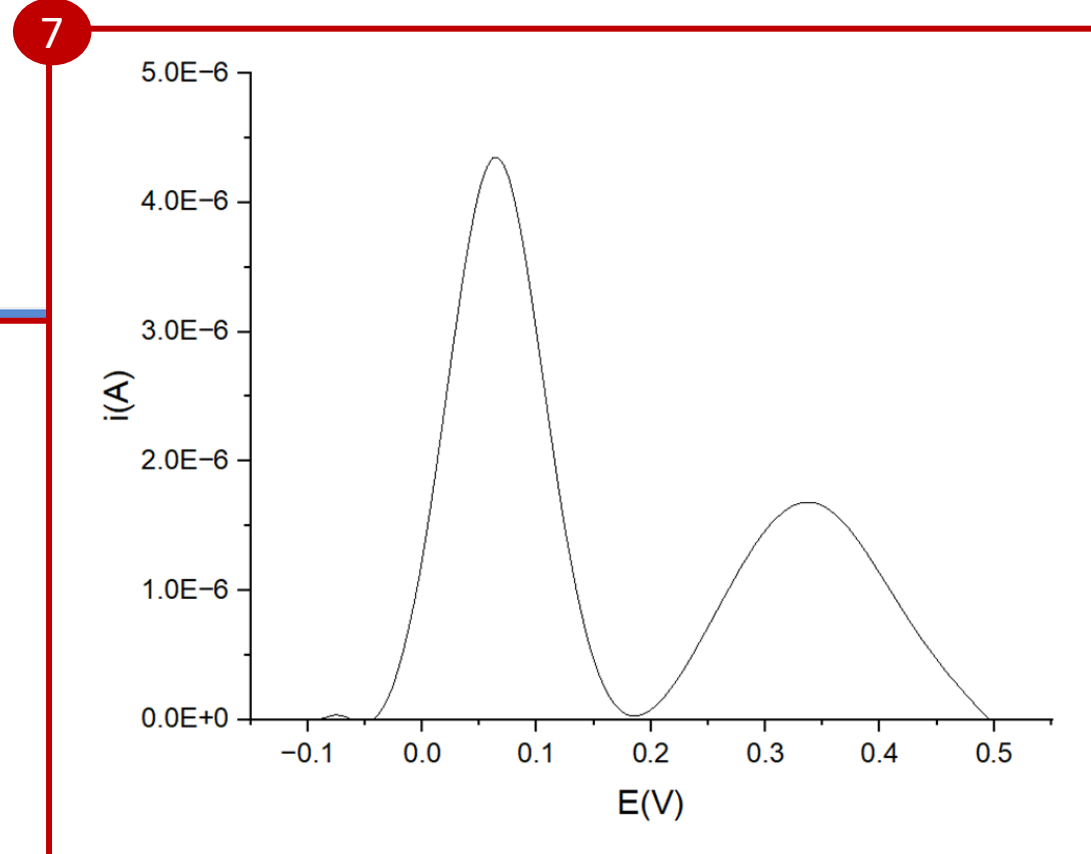
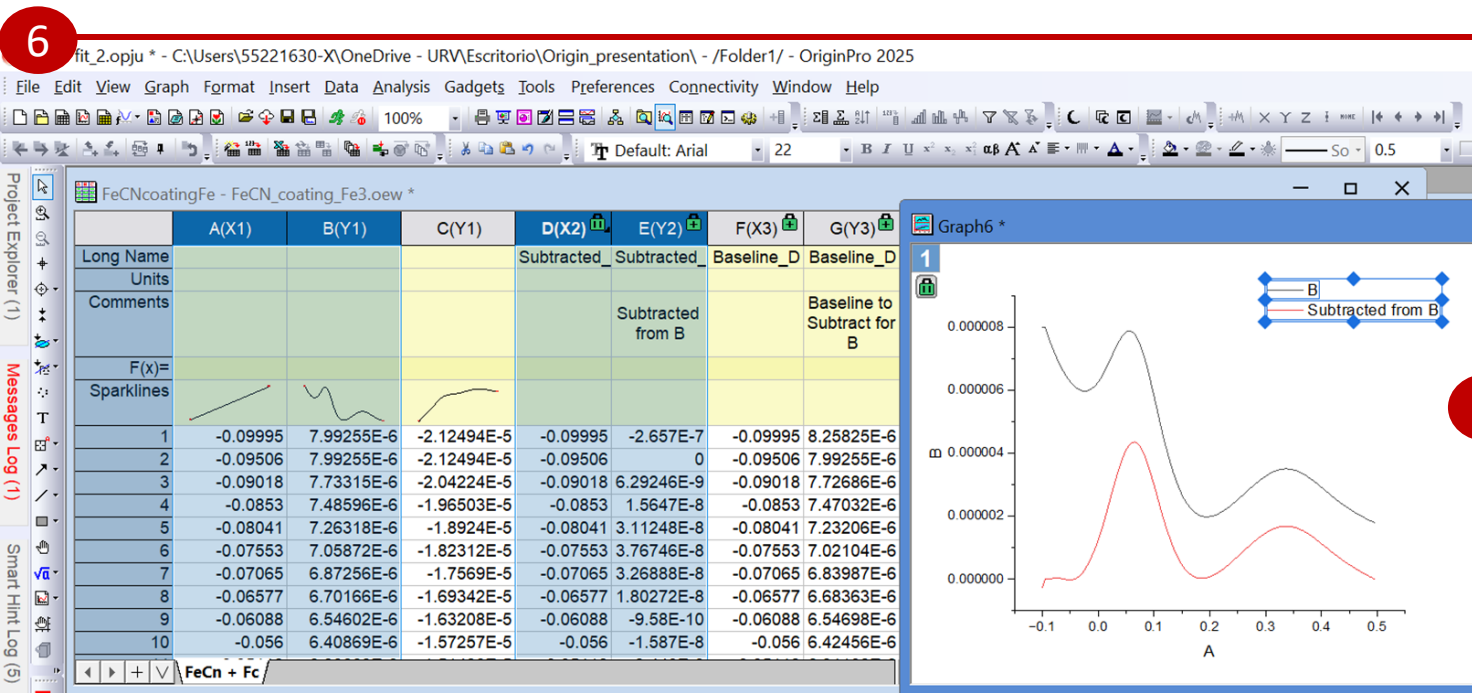
6



II) Practical example: Baseline correction - SWV

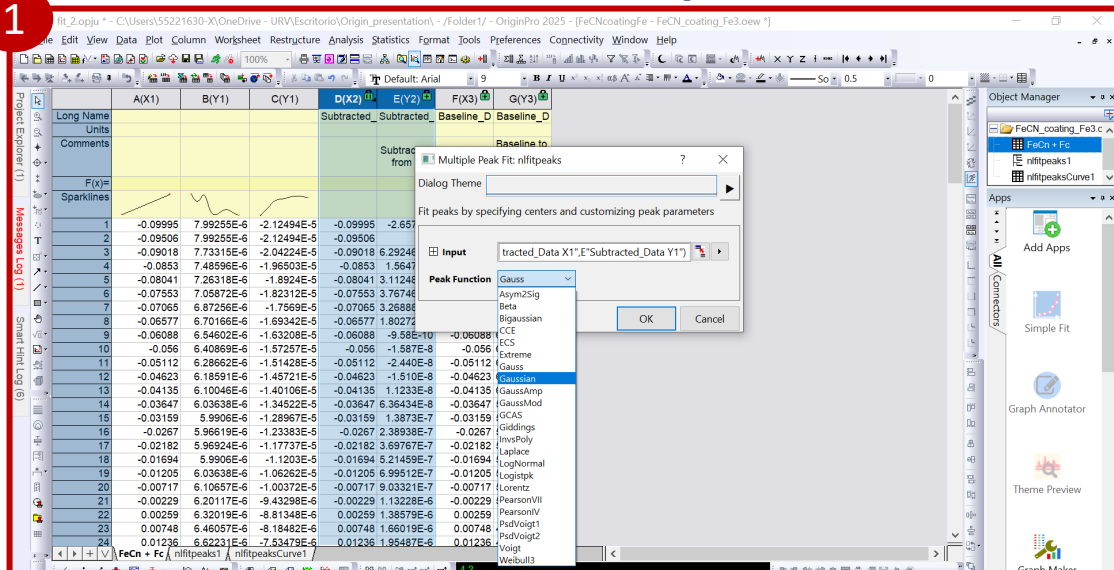


II) Practical example: Baseline correction

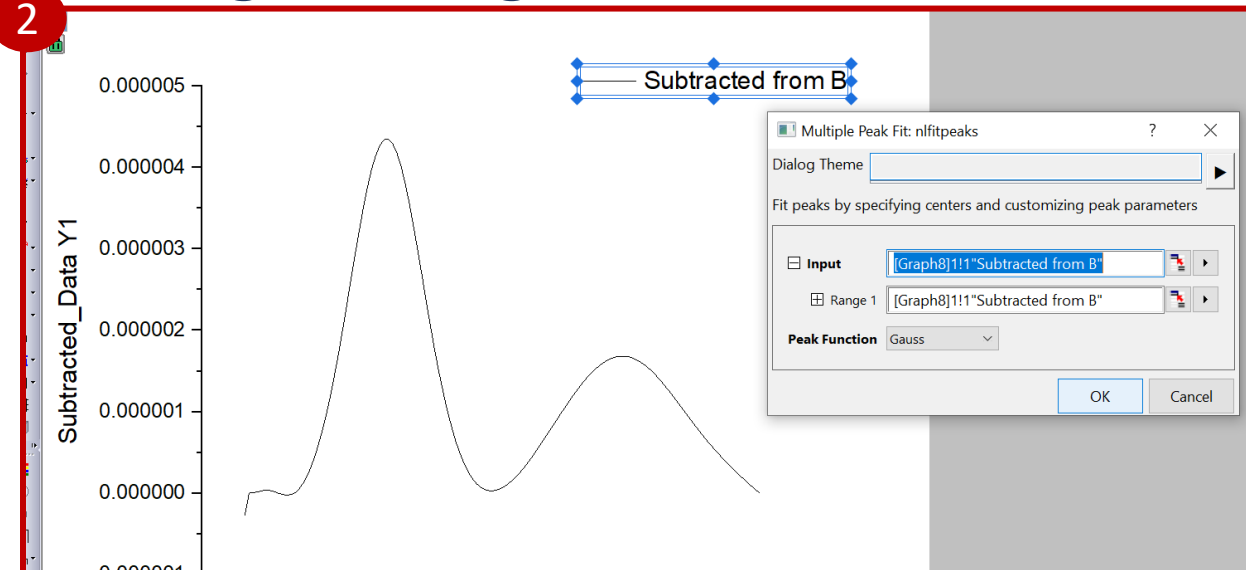


II) Practical example: Signal integration

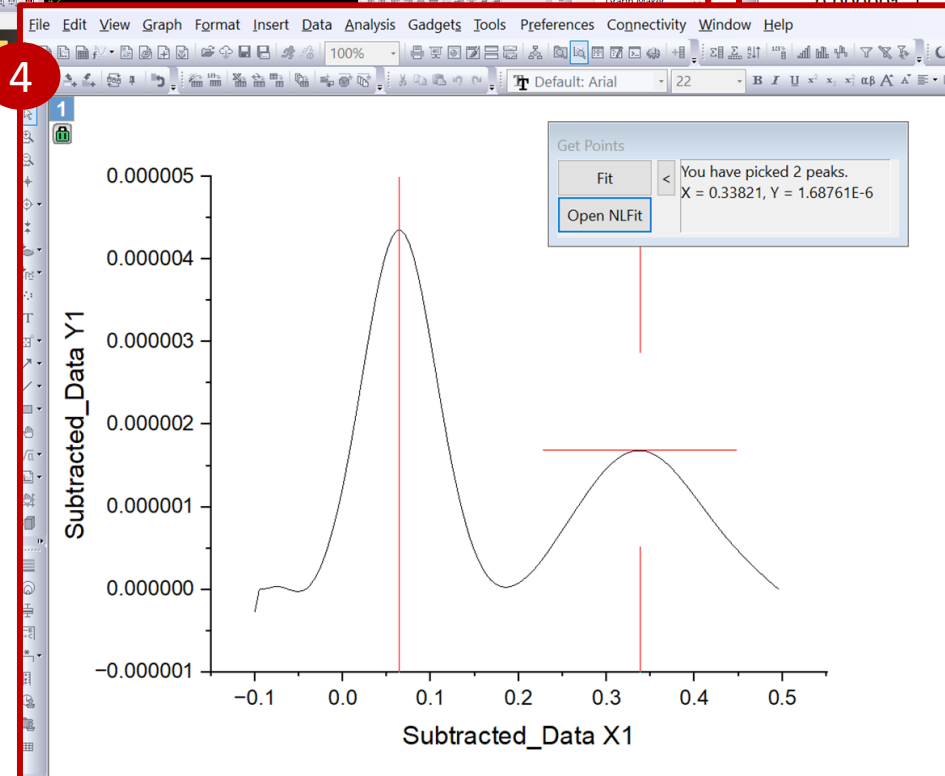
1



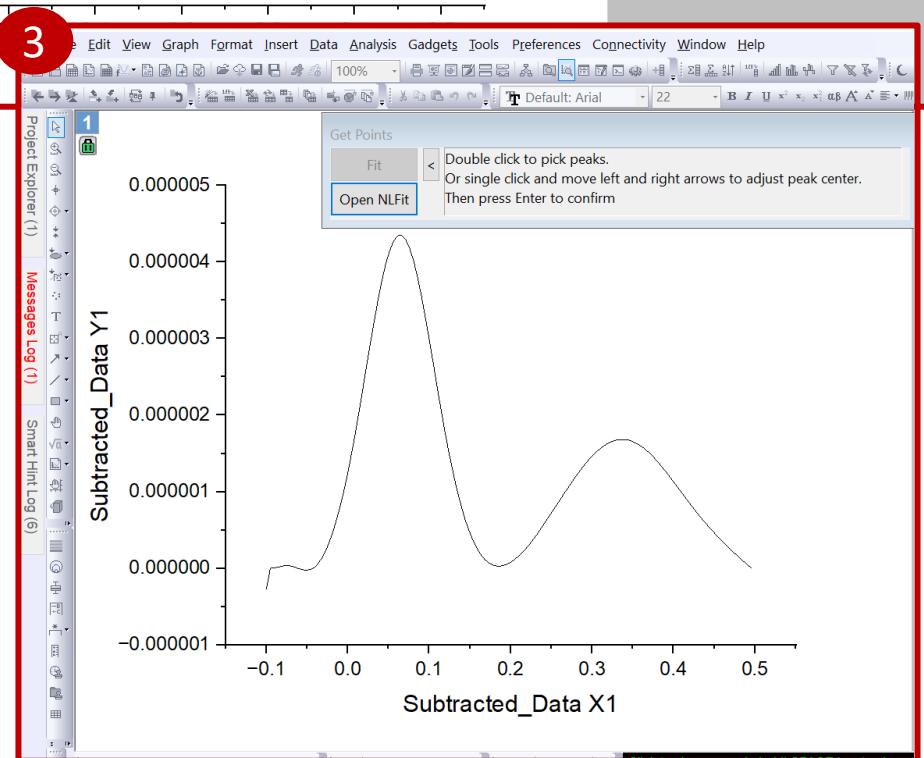
2



4

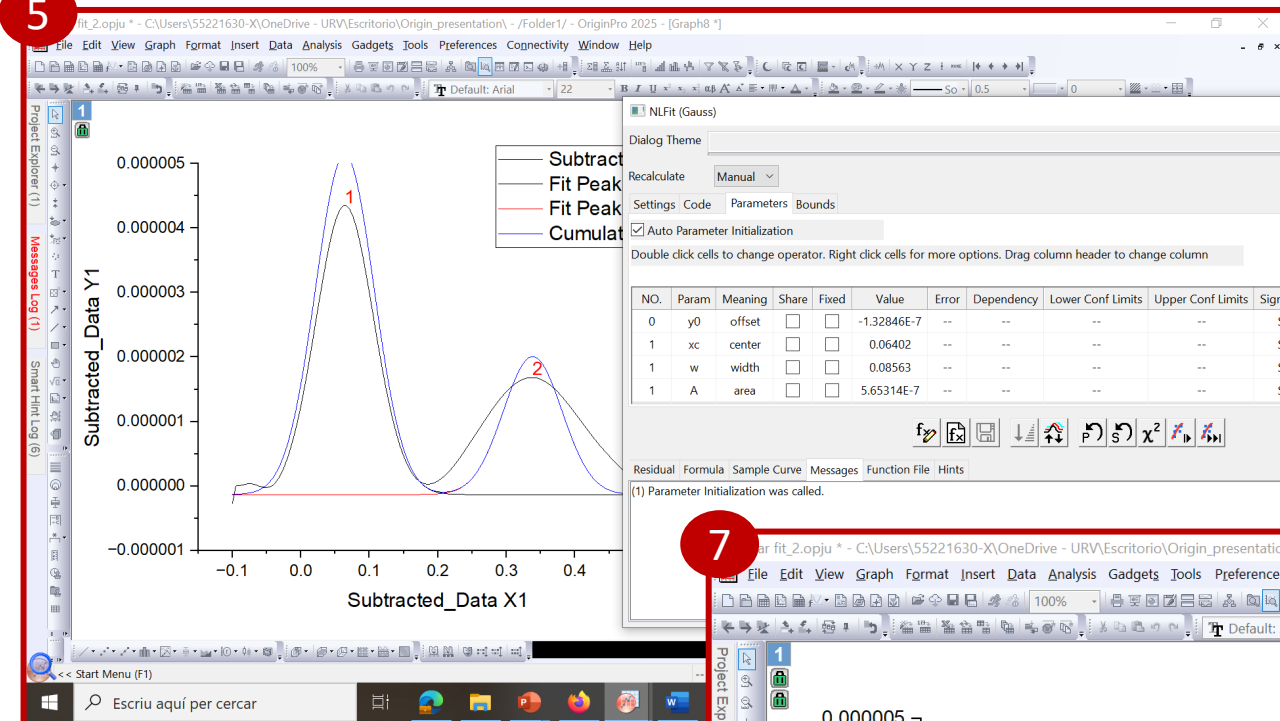


3

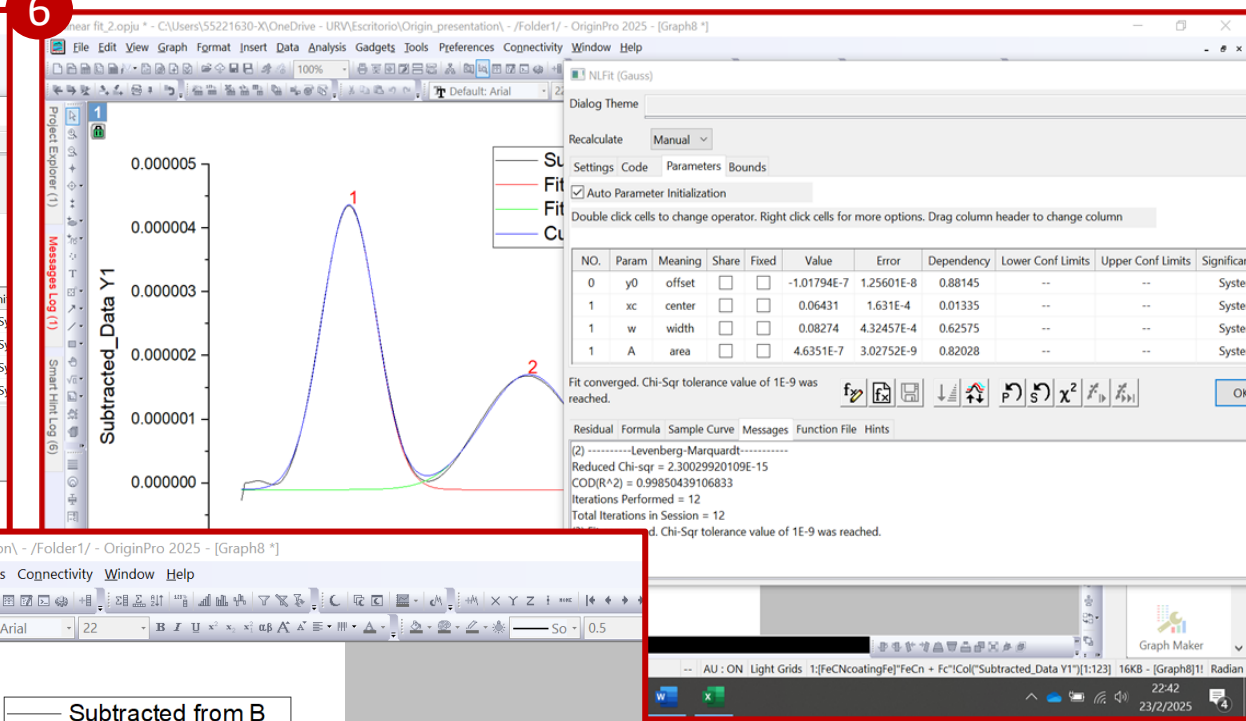


II) Practical example: Signal integration

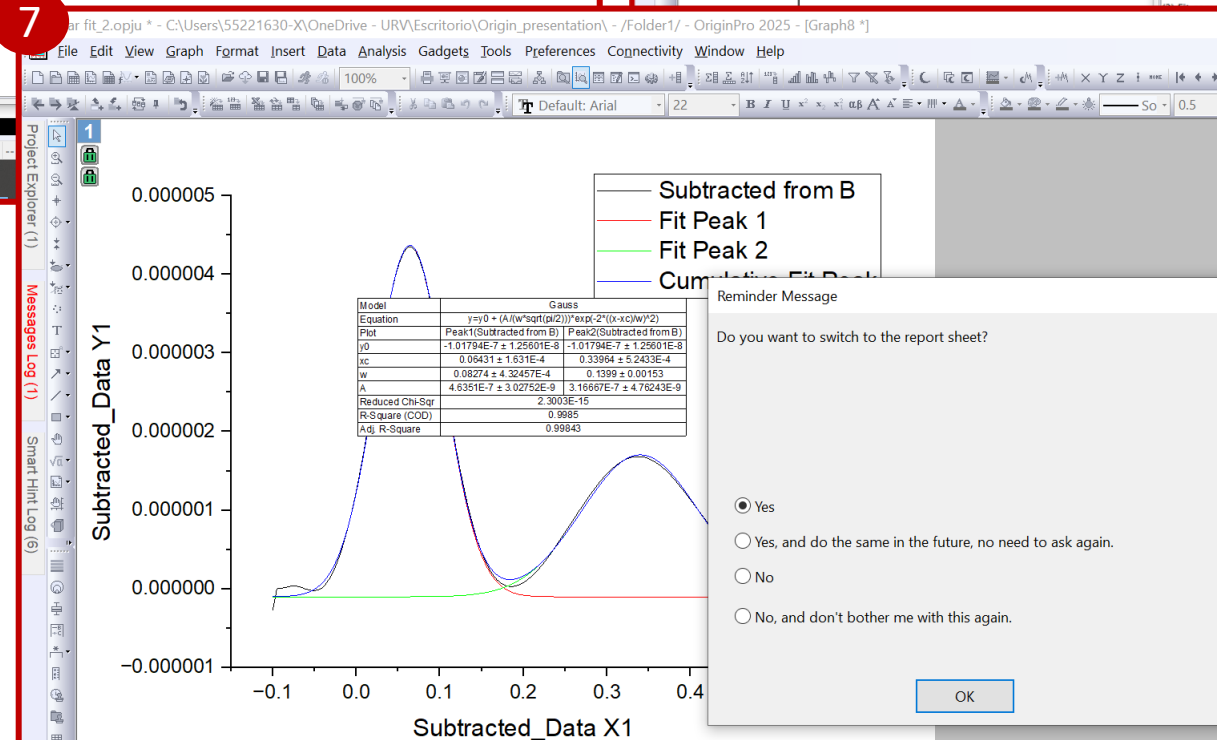
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6

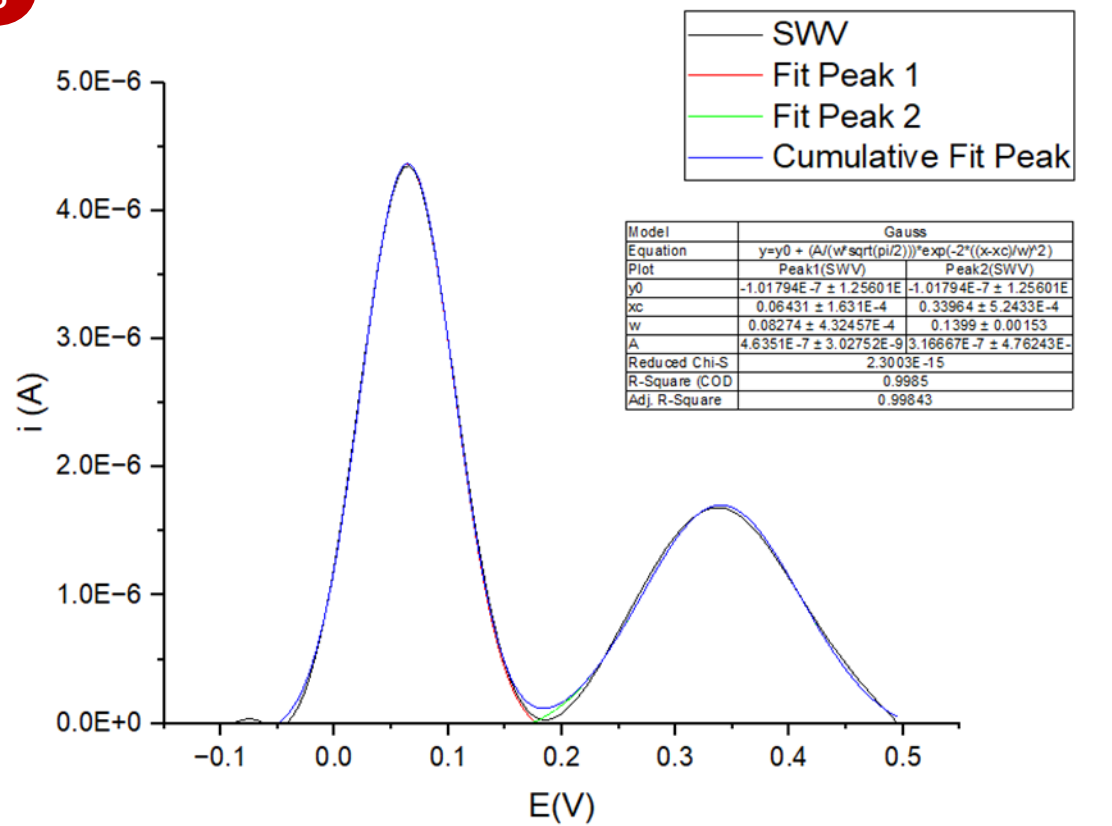


7

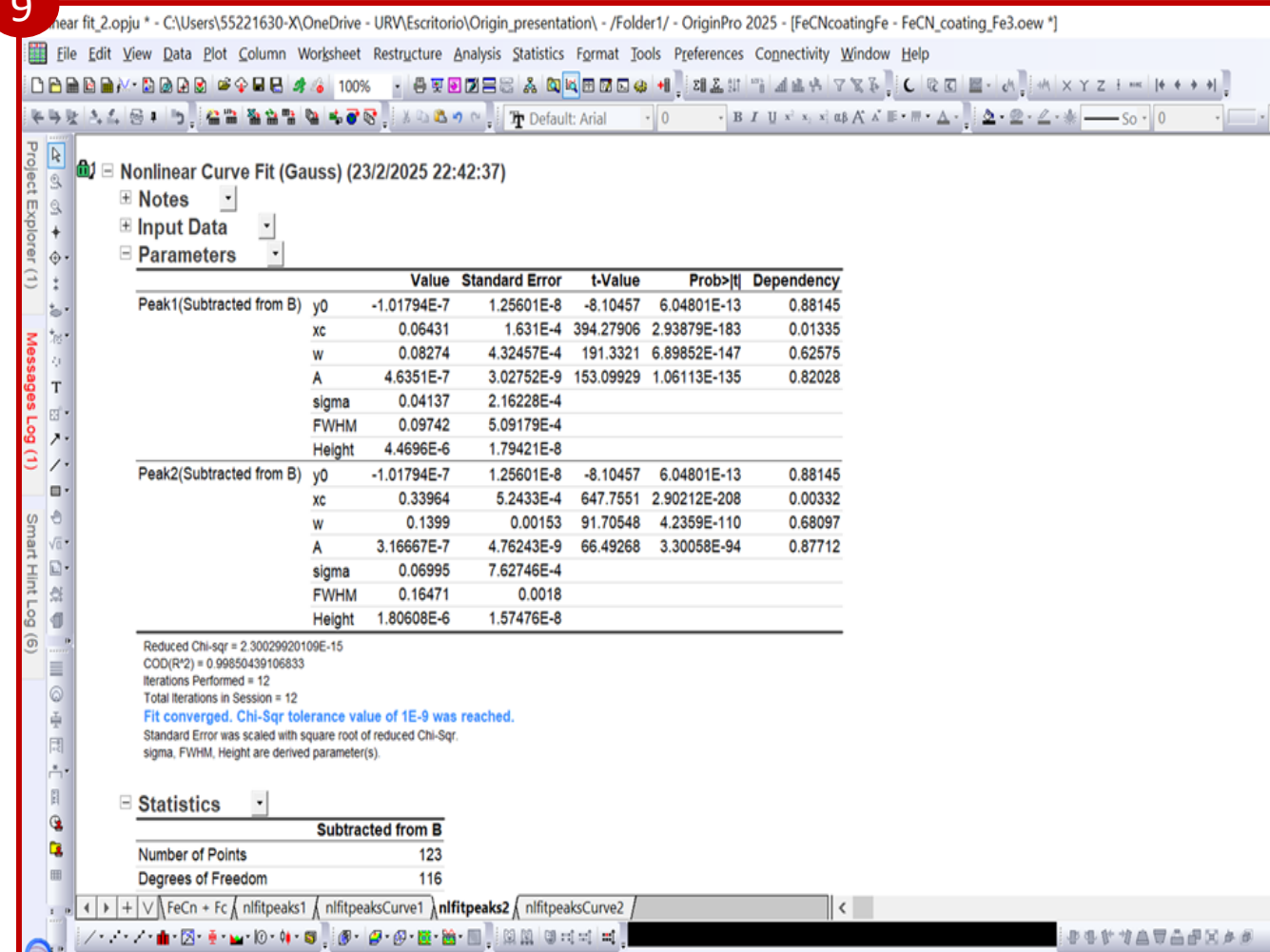


II) Practical example: Signal integration

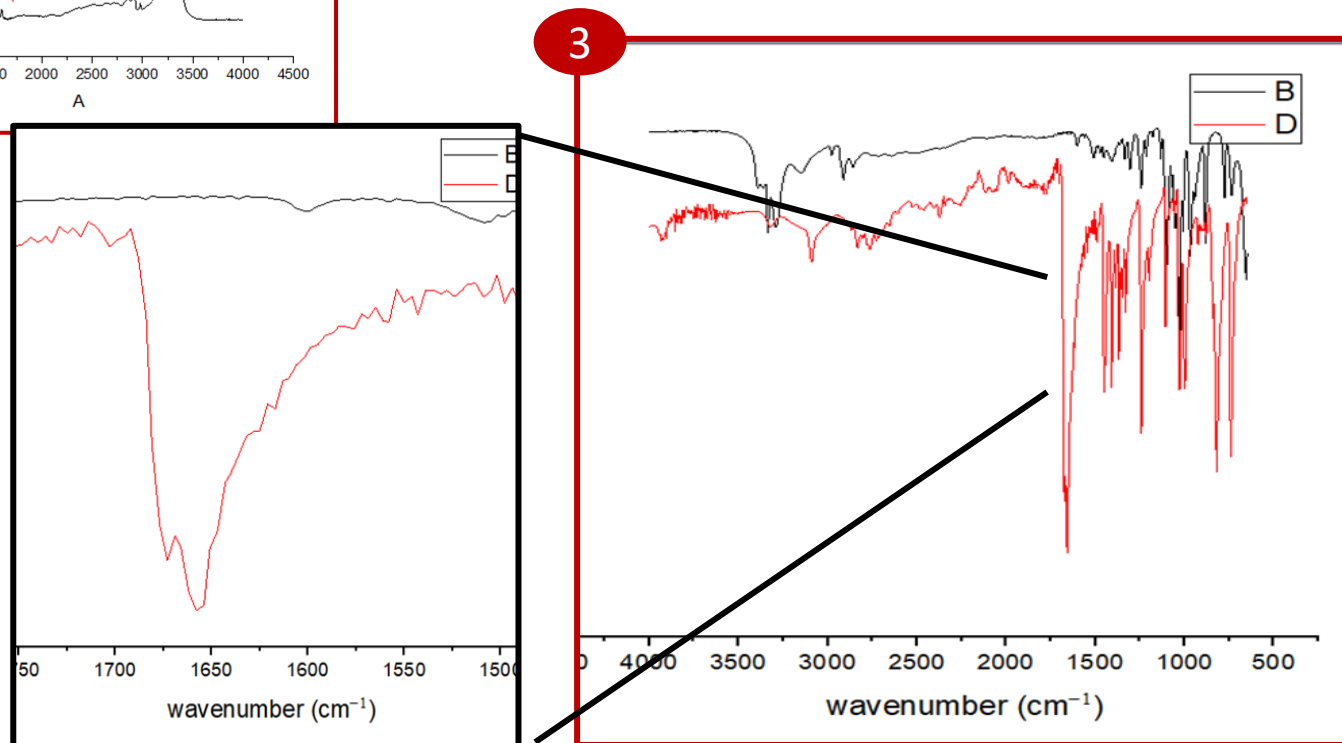
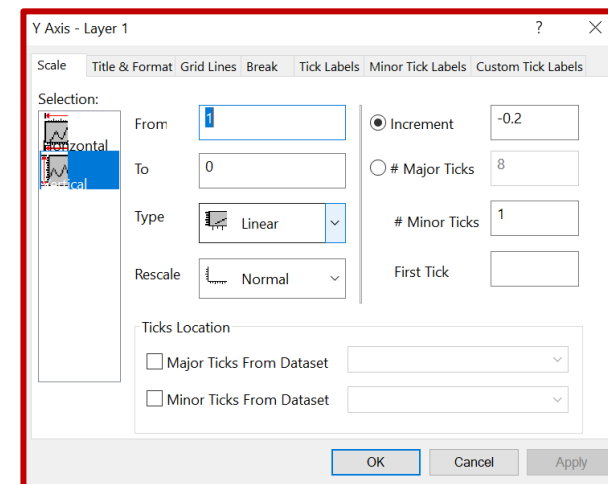
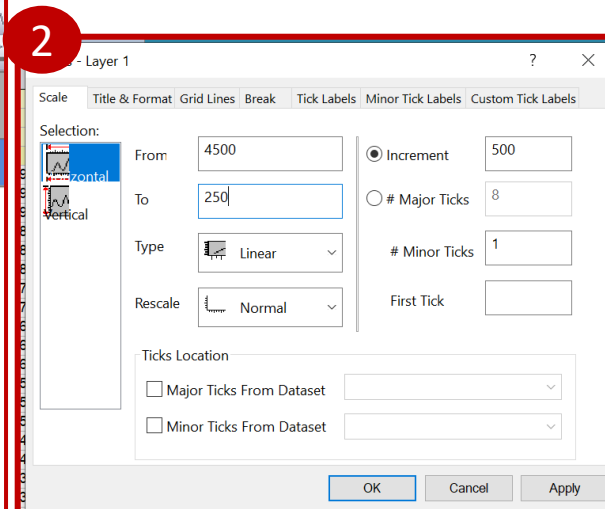
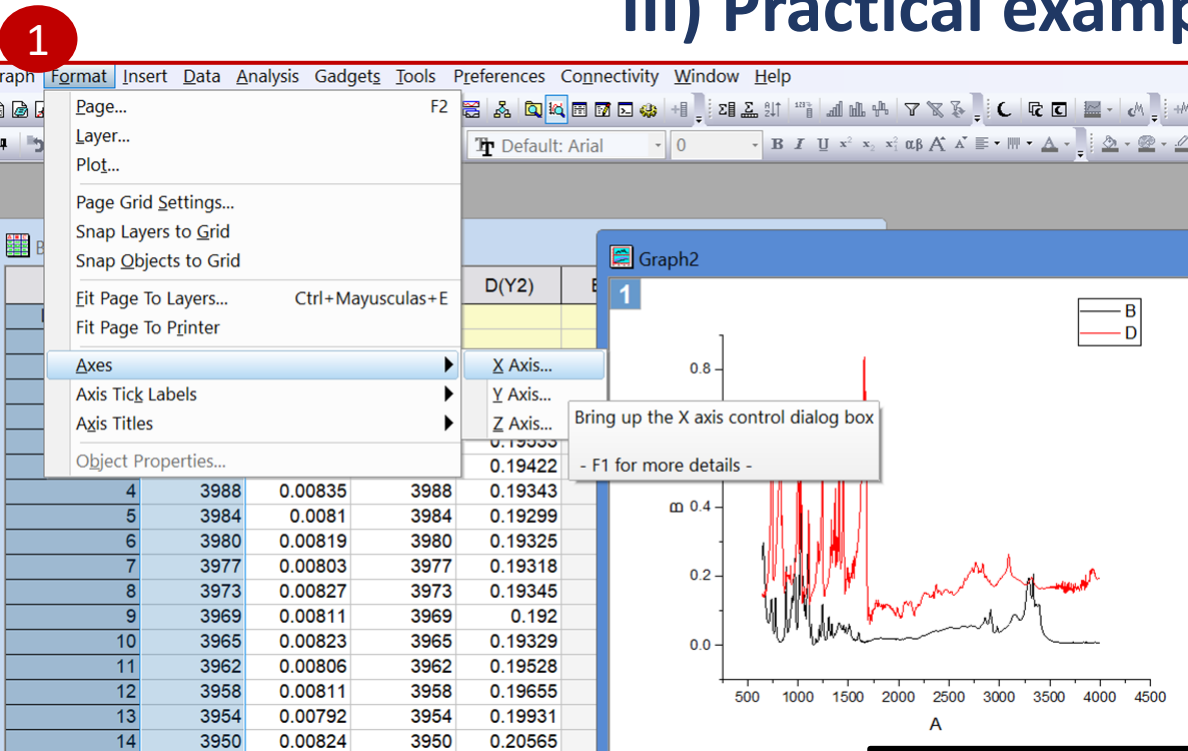
8



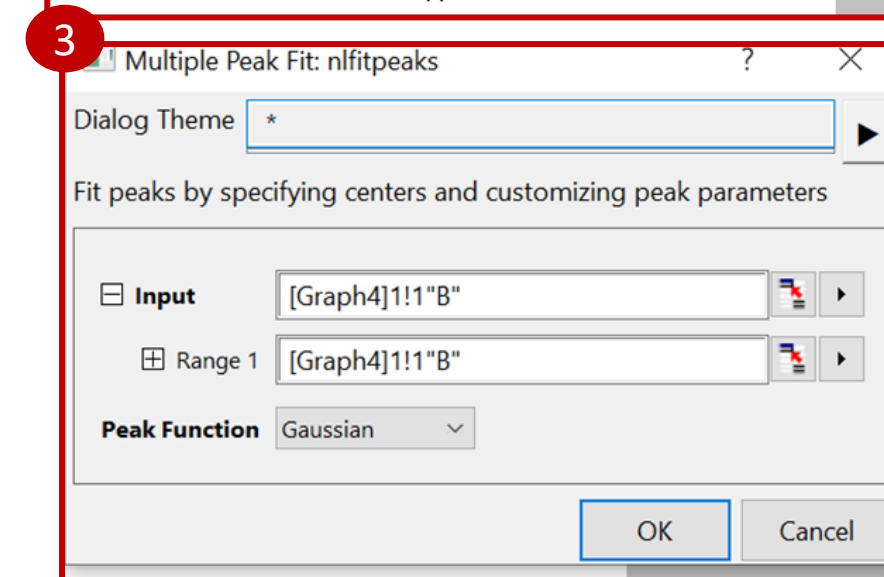
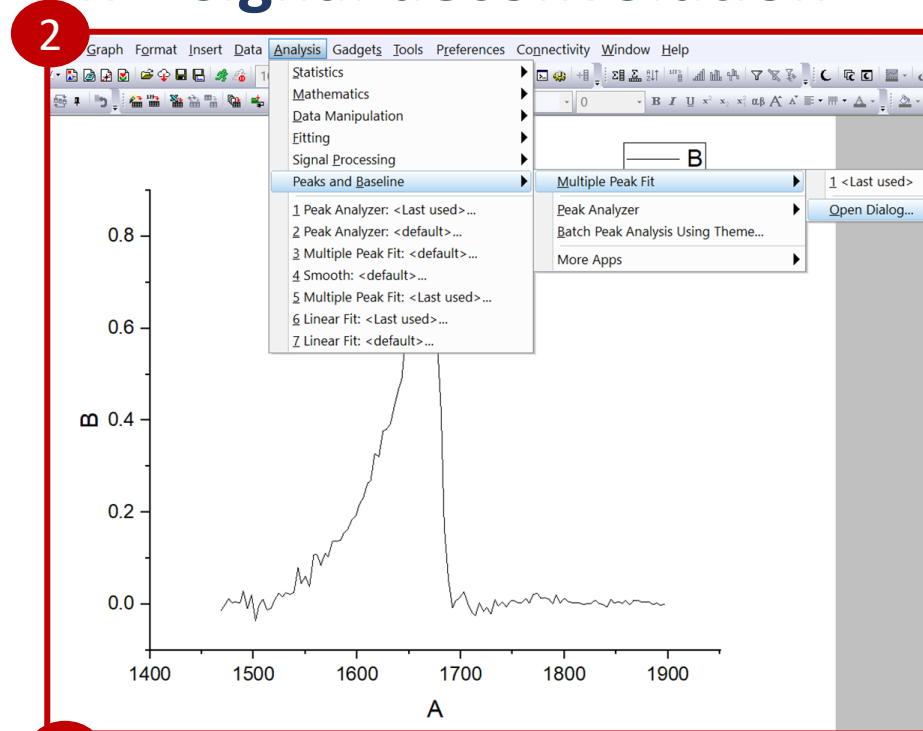
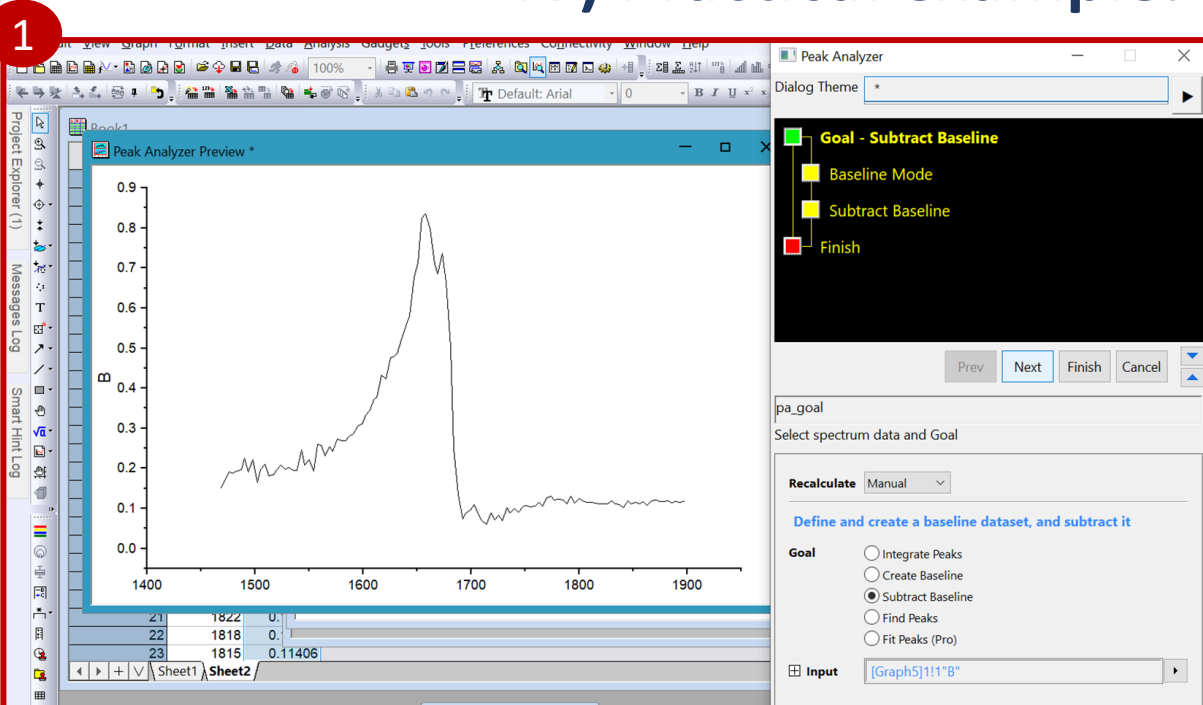
9



III) Practical example: plotting FTIR spectra

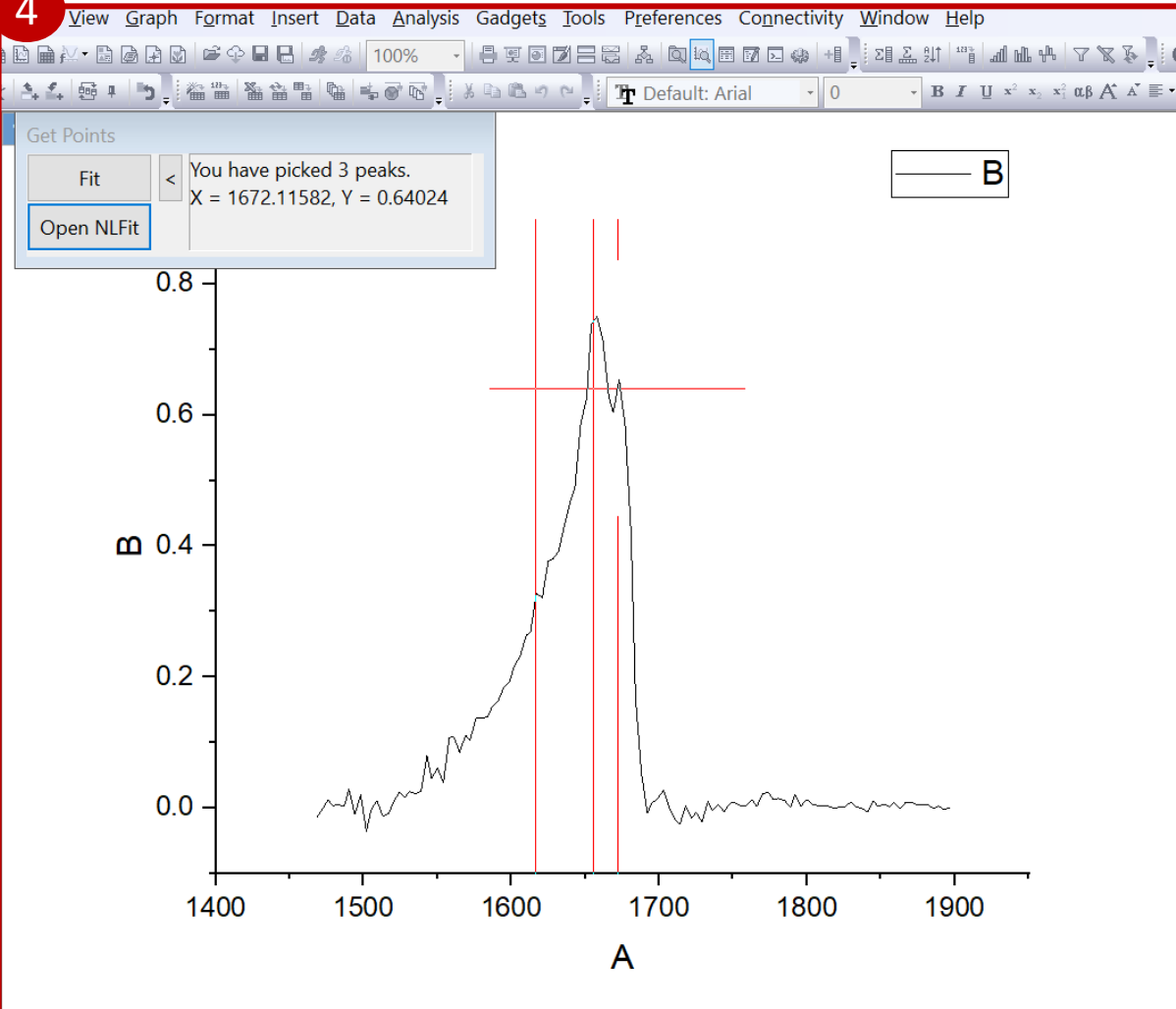


IV) Practical example: FTIR – signal deconvolution

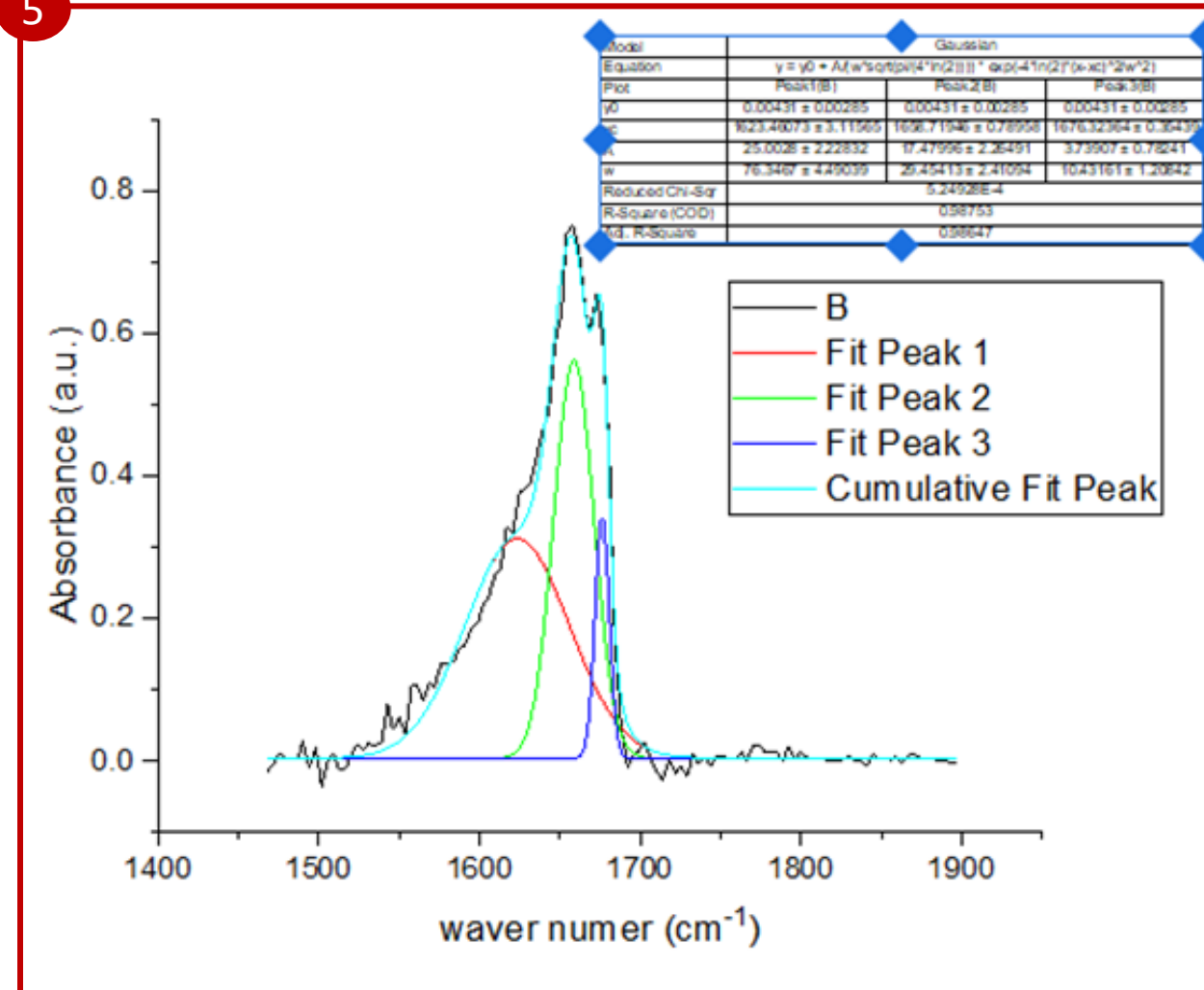


IV Practical example: FTIR – signal deconvolution

4



5



V) Practical example: Statistics by ANOVA

1

2

3

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.

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.

Means Comparisons

☒ 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.



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!