



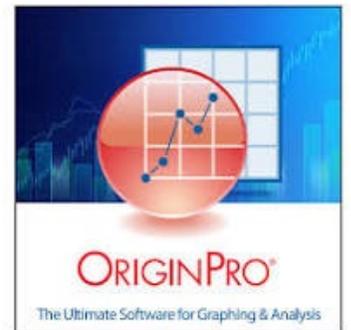
UNIVERSITAT ROVIRA I VIRGILI

DEPARTAMENT
D'ENGINYERIA QUÍMICA

OriginPro-Advanced Signal Analysis

Applications in Spectroscopic and Electrochemical Signals

Dr. Mayreli Ortiz



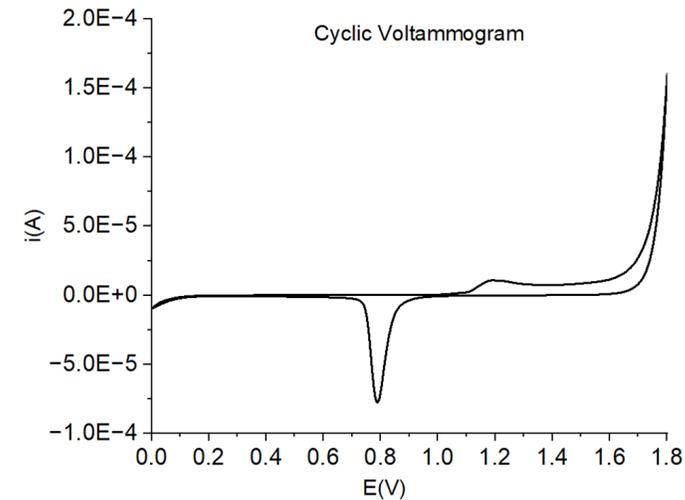
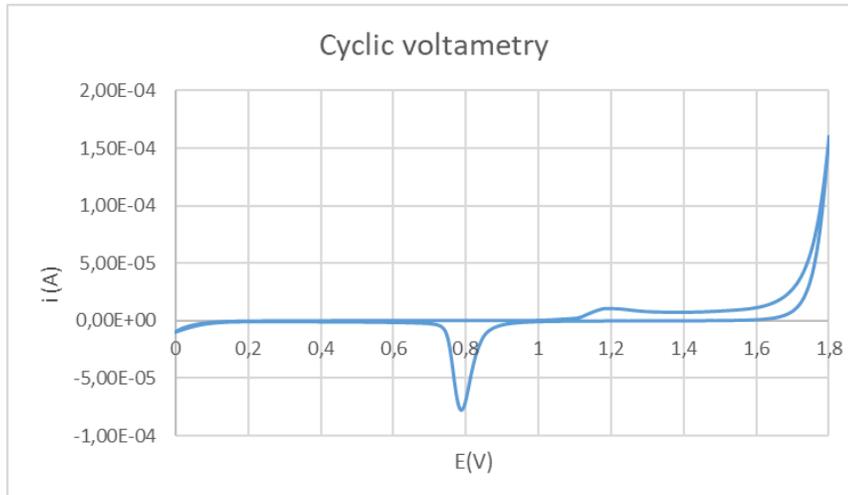
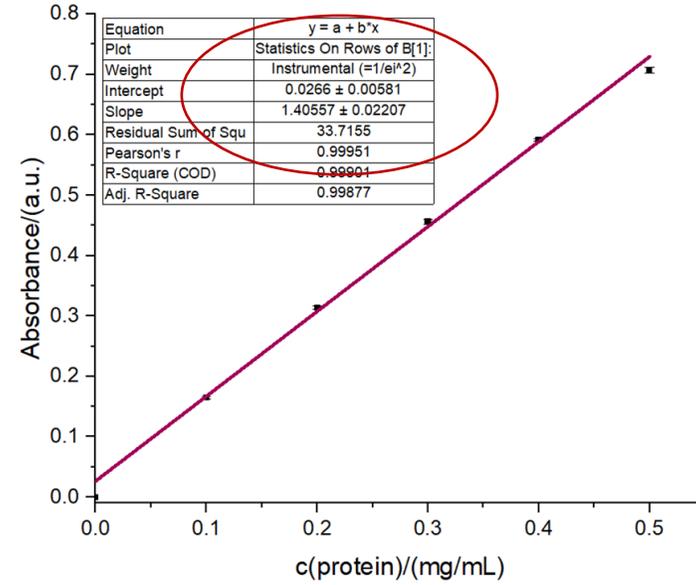
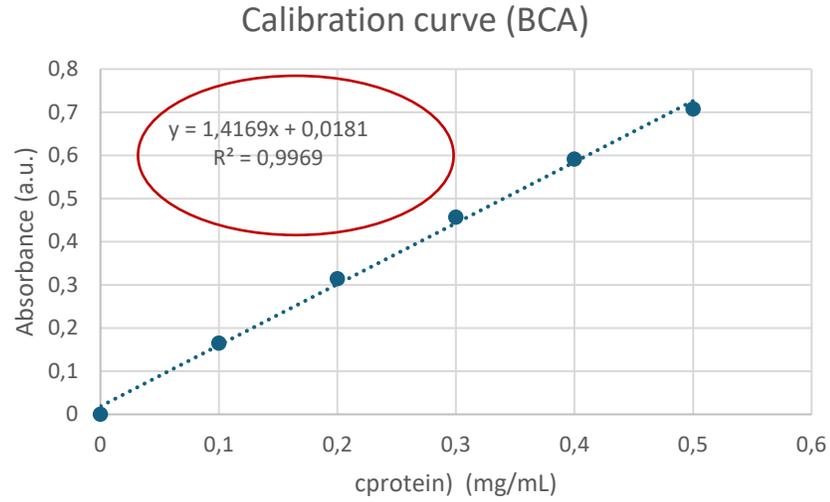
Origin vs Excel: an actual conflict?



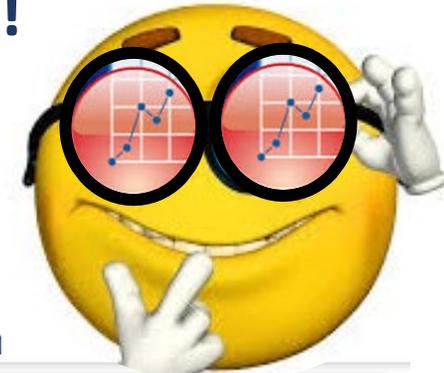
	Excel	Origin Pro
Data Handling	Suited for basic data entry, manipulation, and visualization; may struggle with large or complex datasets	Optimized for handling large datasets, offering advanced curve fitting, deconvolution, and statistical analysis
Analysis Tools	Provides basic charting, pivot tables, 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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Extra large icons Large icons Medium icons Small icons Details

Group by Add columns Item check boxes File name extensions Hidden items Hide selected items Options

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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...

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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>



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

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- I own/have used older version of Origin and I would like try Origin
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What is your sector?

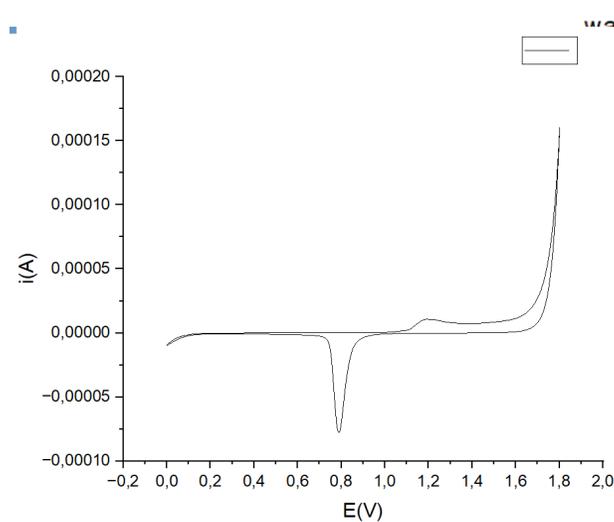
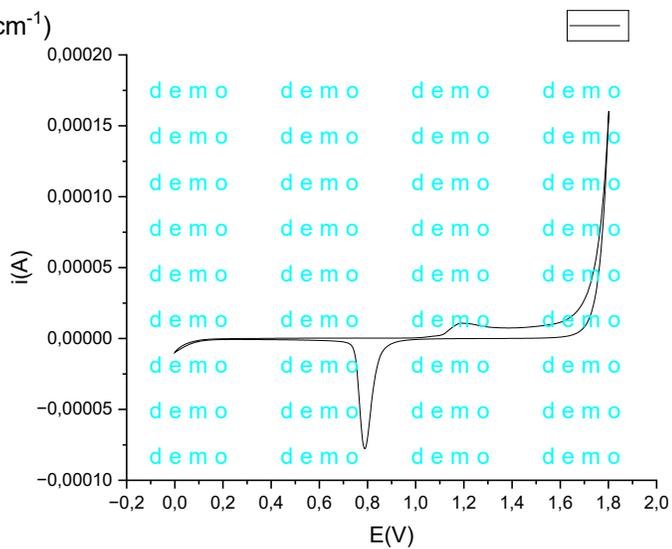
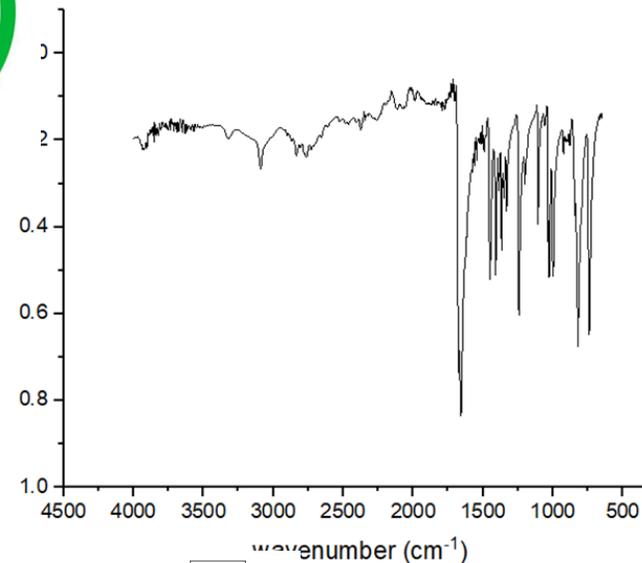
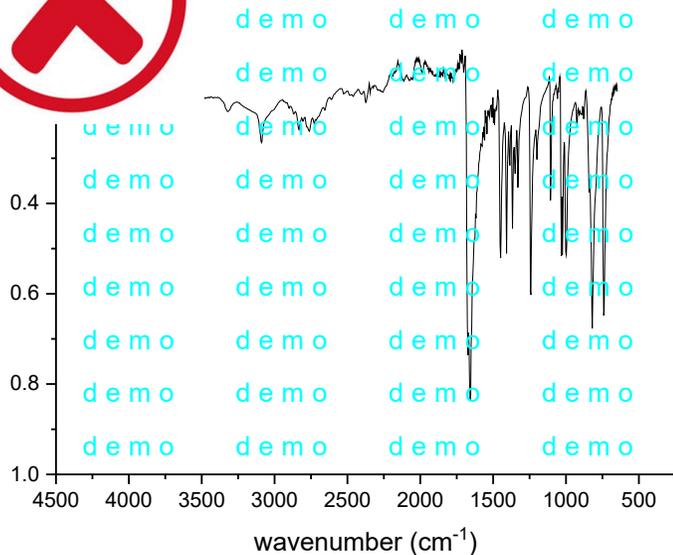
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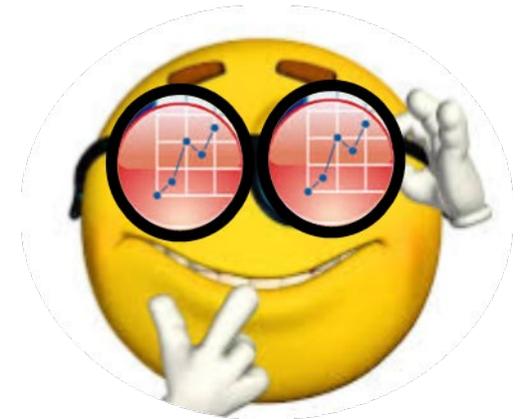
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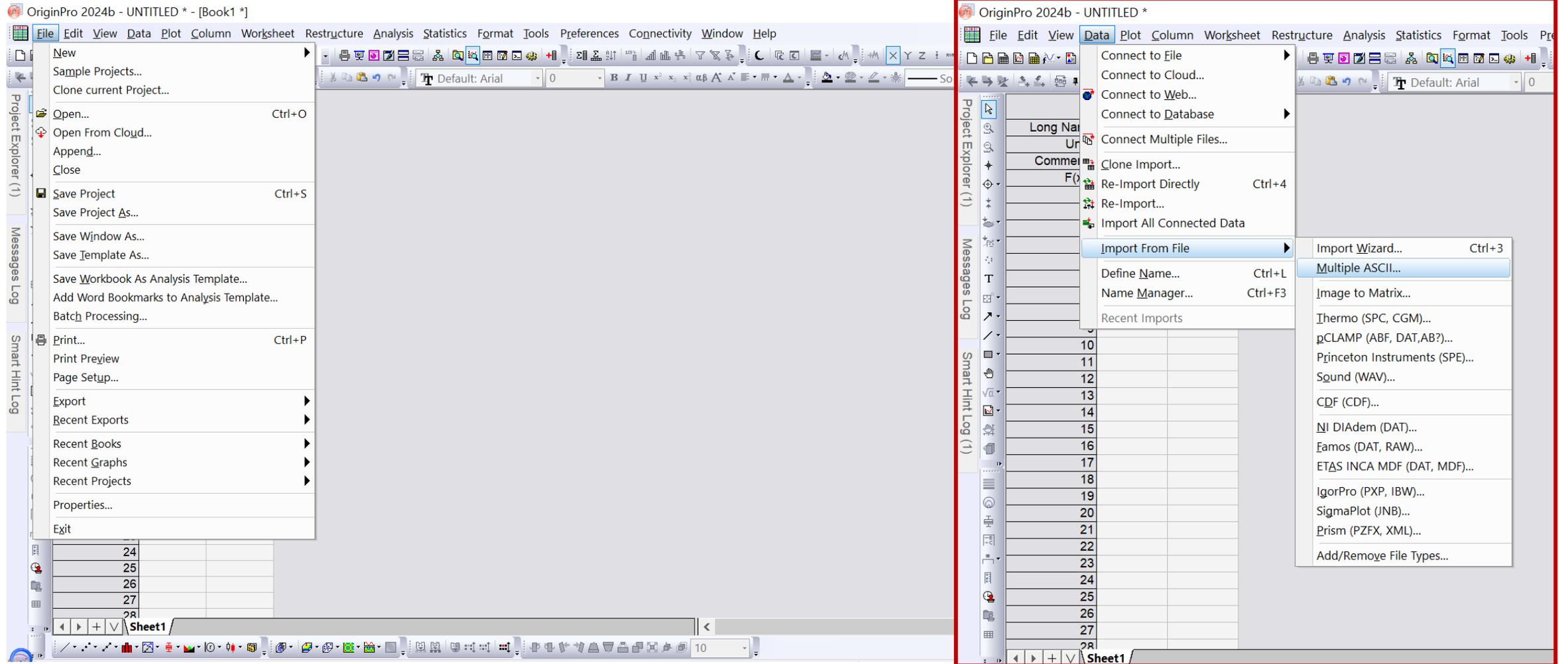
Why do we need an Origin Pro licence?



Some tips for starters in OriginPro...



Some tips: the interface



Some tips: the interface

The screenshot displays the OriginPro 2024b software interface. The main window shows the 'Plot' menu, which is open, revealing a grid of chart types. The menu is organized into several categories:

- Basic 2D**: Scatter, Scatter Central, Column Scatter, Y Error, X Y Error, Error Band, Scatter + Rug, Bubble, Color Mapped, Bubble + Color Mapped.
- Bar, Pie, Area**: (Icon for bar chart)
- Multi-Panel, Multi-Axis**: (Icon for multiple panels)
- Statistical**: (Icon for statistical distribution)
- Contour, Heatmap**: (Icon for contour plot)
- Map**: (Icon for map)
- Specialized**: (Icon for specialized chart)
- Categorical**: (Icon for categorical chart)
- 3D**: (Icon for 3D chart)
- Browser**: (Icon for browser chart)
- Function Plot**: (Icon for function plot)
- Extended Templates**: (Icon for extended templates)

At the bottom of the 'Plot' menu, there are three icons: Graph Maker, Template Library, and Template Center.

The main window also shows the 'Object Manager' on the right, which displays the current project structure: Book1 > Sheet1. Below the Object Manager is the 'Apps' panel, which contains several application icons: Add Apps, Stats Advisor, Speedy Fit, Simple Fit, and a Microsoft Word icon.

The interface includes a menu bar at the top with options: File, Edit, View, Data, Plot, Column, Worksheet, Restructure, Analysis, Statistics, Format, Tools, Preferences, Connectivity, Window, and Help. The status bar at the bottom shows 'Sheet1'.

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

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

The image shows the Origin software interface with the Preferences dialog box open to the 'Options...' tab. A blue arrow points from the 'Options...' tab in the Preferences dialog to the 'Numeric Format' tab in the Options dialog. The Options dialog box shows the 'Separators' section with a dropdown menu open, showing 'Windows Settings' selected. The 'Separator for ASCII Import' is set to '1,000.0'. The 'Date Format for Database Import' is set to '1 000.0'. The 'Use English in Reports and Graphs' checkbox is checked.

	A(X)	B(Y)	C(Y)
Long Name	Å		
Units			
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	

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

Statistics

- Stats Advisor...
- Descriptive Statistics
- Hypothesis Testing
- ANOVA
- Nonparametric Tests
- Survival Analysis
- Multivariate Analysis
- Power and Sample Size
- ROC Curve...
- Quality Improvement
- Time Series
- More Apps

Statistics on Columns...

Statistics on Rows

Statistics on Whole Sheet...

Cross Tabulation and Chi-Square...

Discrete Frequency...

Frequency Counts...

2D Frequency Counts/Binning...

Distribution Fit...

Normality Test...

Correlation Coefficient...

Partial Correlation Coefficient...

Grubbs Test...

Dixon's Q-test...

3

	A(X)	B(Y)	C(Y)	D(Y)	E(Y)	F(Y)
Long Name					Mean	Standard D
Units						
Comments					Statistics	Statistics
F(x)=		Col(B)-0.07	Col(C)-0.07	Col(D)-0.070	On Rows of B[1]:D[6]	On Rows of B[1]:D[6]
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						

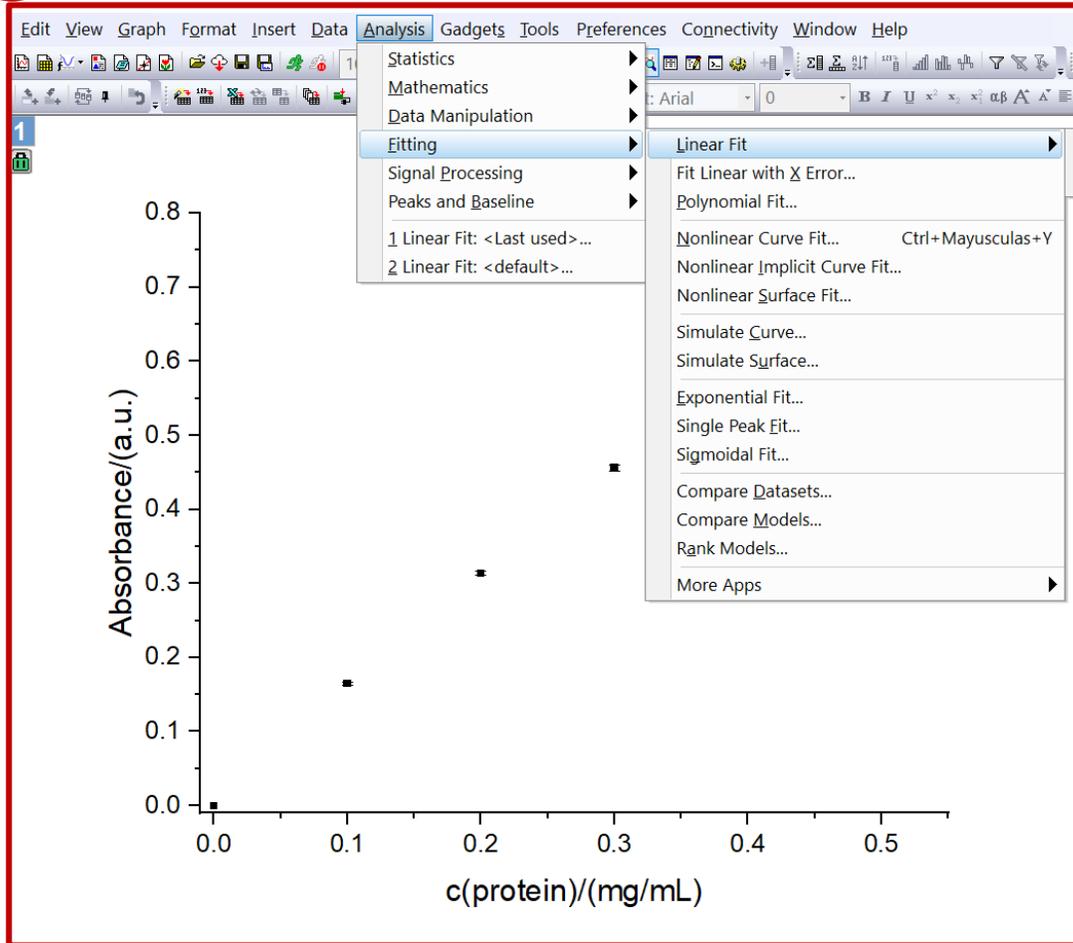
4

Statistics

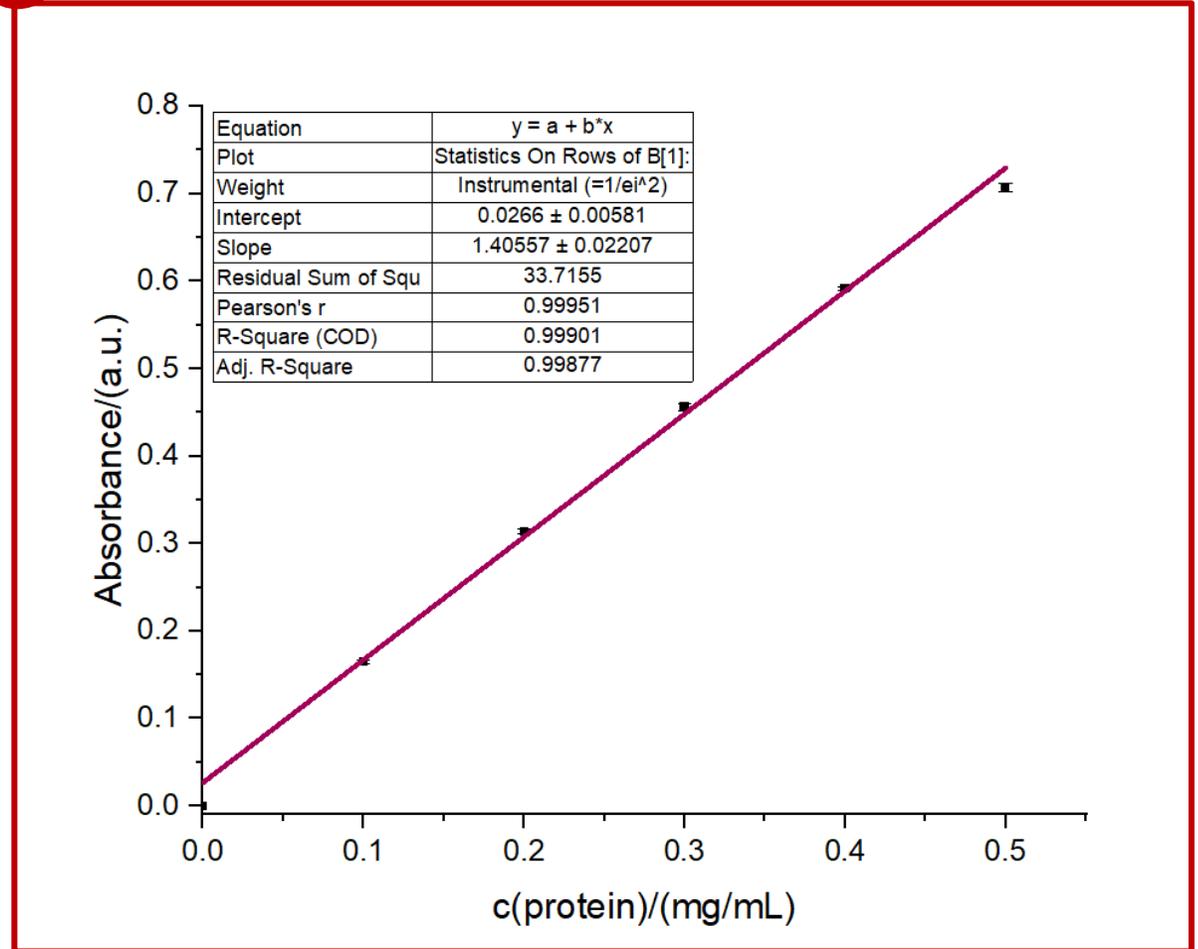
- Recently Used
- Basic 2D
- Bar, Pie, Area
- Scatter
- Central
- Scatter

I) Practical example: A calibration curve - Linear fitting

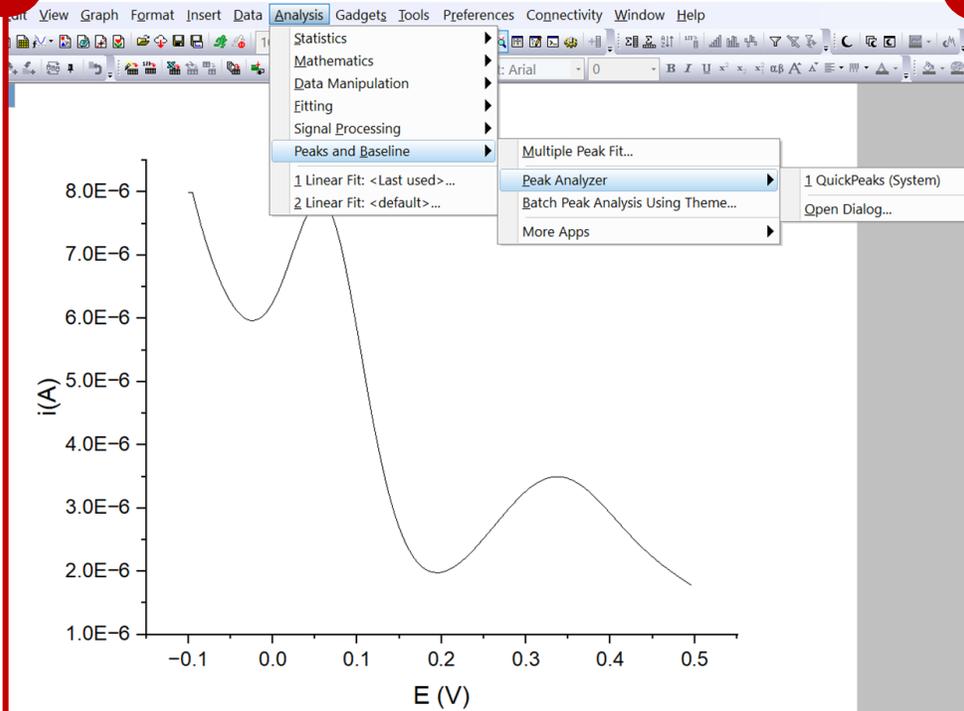
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6



II) Practical example: Baseline correction - SWV



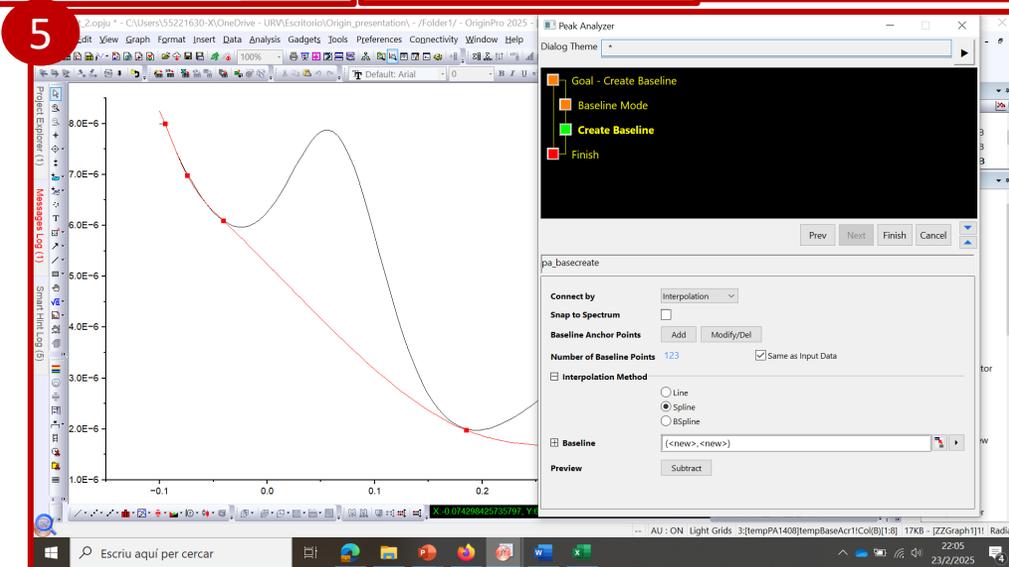
2

3

Dialog boxes for 'Goal - Subtract Baseline' and 'Baseline Mode'. The 'Baseline Mode' dialog shows options for 'Method' (User Defined, Constant, Use Existing Dataset, XPS, End Points Weighted, Straight Line, Asymmetric Least Squares Smoothing) and 'Smoothing' (Use Script to Search, Use Existing Dataset, 2nd Derivative (peaks)).

4

Baseline Mode dialog box. Method: 2nd Derivative (zeroes). Smoothing Window Size: 3. Threshold: 0.05. Current Number of Points: 8. Number of Points to Find: 8. Find button.



II) Practical example: Baseline correction

6

fit_2.opju * - C:\Users\55221630-X\OneDrive - URV\Escritorio\Origin_presentation\ - /Folder1/ - OriginPro 2025

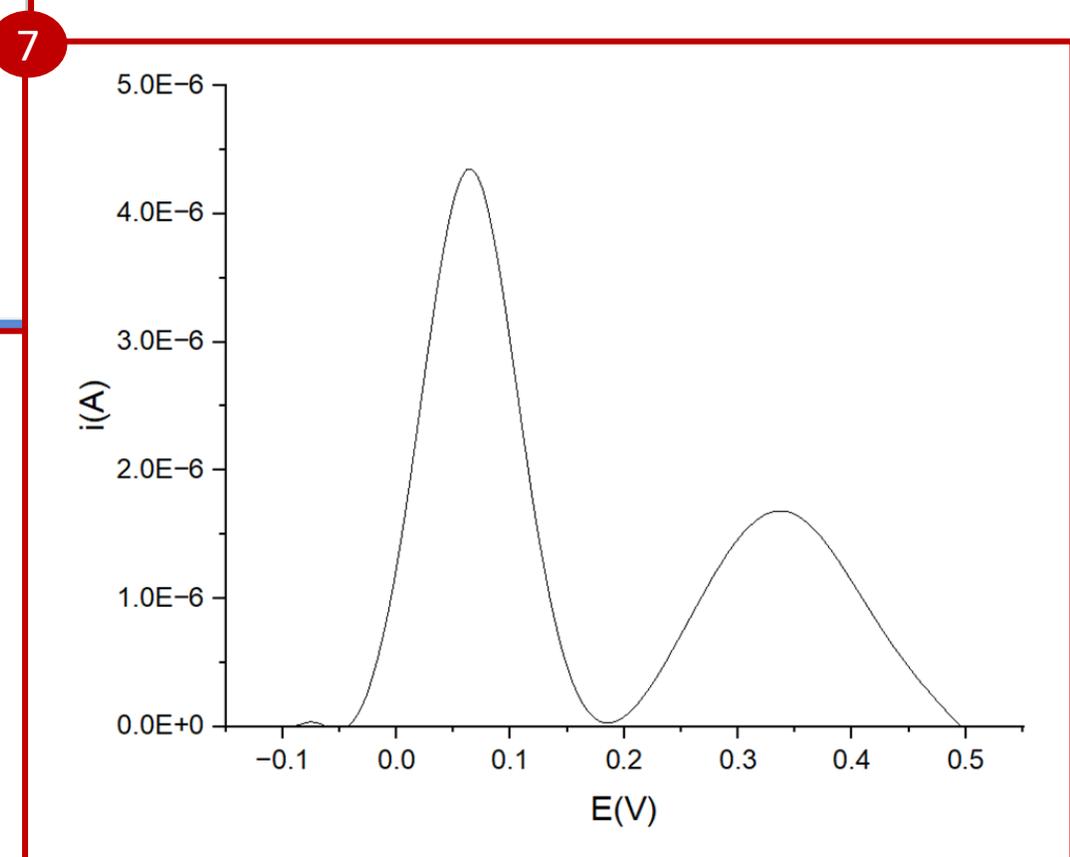
File Edit View Graph Format Insert Data Analysis Gadgets Tools Preferences Connectivity Window Help

100%

Default: Arial 22

FeCNcoatingFe - FeCN_coating_Fe3.ow * Graph6 *

	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



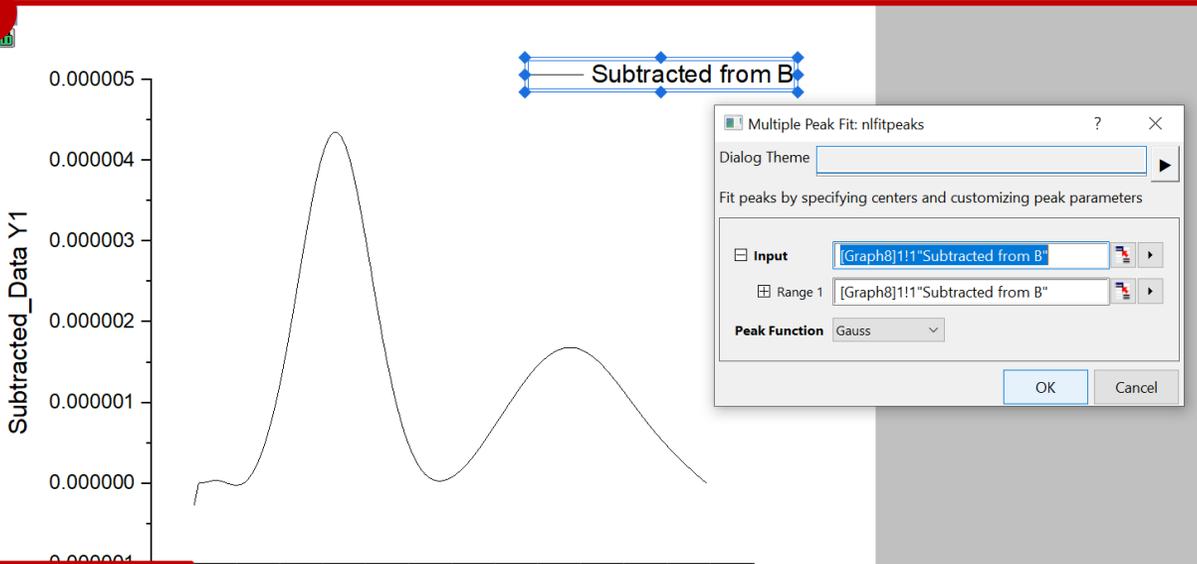
II) Practical example: Signal integration

1

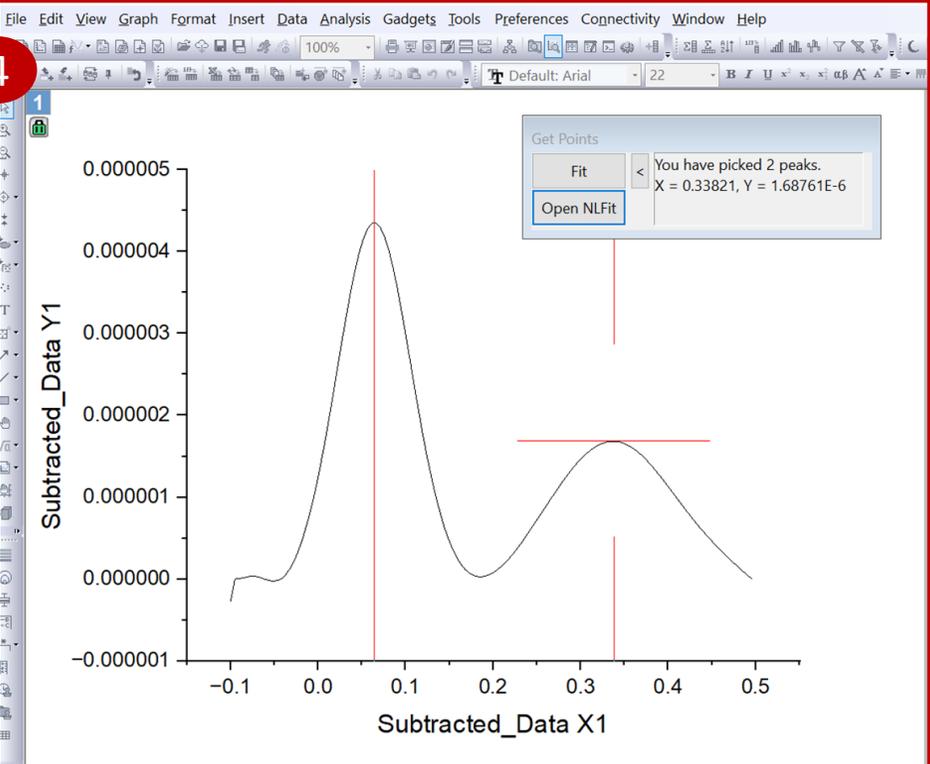
The screenshot shows the Origin software interface with a data table and a dialog box for multiple peak fitting. The data table has columns A(X1), B(Y1), C(Y1), D(X2), E(Y2), F(X3), and G(Y3). The dialog box is titled 'Multiple Peak Fit: nfitpeaks' and includes fields for 'Input' (traced_Data X1:E:Subtracted_Data Y1), 'Peak Function' (Gauss), and 'Range 1'.

	A(X1)	B(Y1)	C(Y1)	D(X2)	E(Y2)	F(X3)	G(Y3)
1	-0.09995	7.99255E-6	-2.12494E-5	-0.09995	-2.657	-0.09995	-2.657
2	-0.09506	7.99255E-6	-2.12494E-5	-0.09506	-0.09506	-0.09506	-0.09506
3	-0.09018	7.73315E-6	-2.04224E-5	-0.09018	6.2924E-6	-0.09018	6.2924E-6
4	-0.0853	7.48836E-6	-1.96303E-5	-0.0853	1.5647	-0.0853	1.5647
5	-0.08041	7.26318E-6	-1.8924E-5	-0.08041	3.1124E-6	-0.08041	3.1124E-6
6	-0.07553	7.05872E-6	-1.82312E-5	-0.07553	3.7674E-6	-0.07553	3.7674E-6
7	-0.07065	6.87256E-6	-1.75698E-5	-0.07065	3.2688E-6	-0.07065	3.2688E-6
8	-0.06577	6.70166E-6	-1.69342E-5	-0.06577	1.8027E-6	-0.06577	1.8027E-6
9	-0.06088	6.54602E-6	-1.63208E-5	-0.06088	-9.58E-10	-0.06088	-9.58E-10
10	-0.056	6.40869E-6	-1.57257E-5	-0.056	-1.587E-8	-0.056	-1.587E-8
11	-0.05112	6.28662E-6	-1.51428E-5	-0.05112	-2.440E-8	-0.05112	-2.440E-8
12	-0.04623	6.18591E-6	-1.4571E-5	-0.04623	-1.510E-8	-0.04623	-1.510E-8
13	-0.04135	6.10046E-6	-1.40106E-5	-0.04135	1.1233E-8	-0.04135	1.1233E-8
14	-0.03647	6.03638E-6	-1.34522E-5	-0.03647	6.3634E-8	-0.03647	6.3634E-8
15	-0.03159	5.9906E-6	-1.28967E-5	-0.03159	1.3873E-7	-0.03159	1.3873E-7
16	-0.0267	5.9619E-6	-1.23383E-5	-0.0267	2.3893E-7	-0.0267	2.3893E-7
17	-0.02182	5.96924E-6	-1.17737E-5	-0.02182	3.69767E-7	-0.02182	3.69767E-7
18	-0.01694	5.9906E-6	-1.1203E-5	-0.01694	5.21459E-7	-0.01694	5.21459E-7
19	-0.01205	6.03638E-6	-1.06262E-5	-0.01205	6.9912E-7	-0.01205	6.9912E-7
20	-0.00717	6.10657E-6	-1.00372E-5	-0.00717	9.03321E-7	-0.00717	9.03321E-7
21	-0.00229	6.20117E-6	-9.43298E-6	-0.00229	1.13228E-6	-0.00229	1.13228E-6
22	0.00259	6.32019E-6	-8.81348E-6	0.00259	1.38579E-6	0.00259	1.38579E-6
23	0.00748	6.46057E-6	-8.18482E-6	0.00748	1.66019E-6	0.00748	1.66019E-6
24	0.01236	6.62231E-6	-7.53479E-6	0.01236	1.95487E-6	0.01236	1.95487E-6

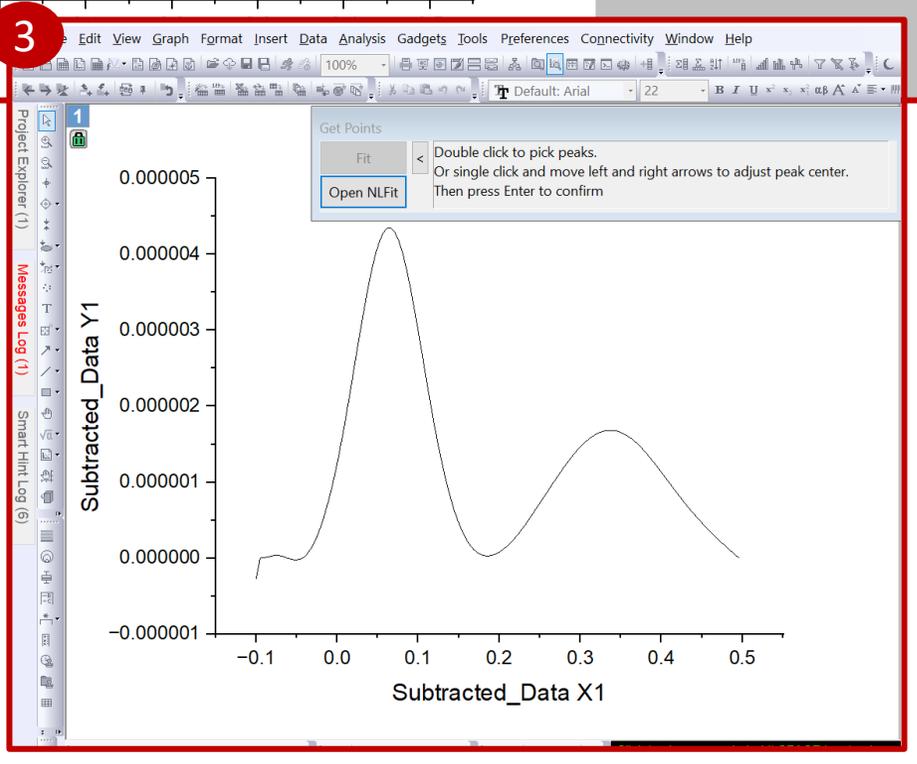
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4

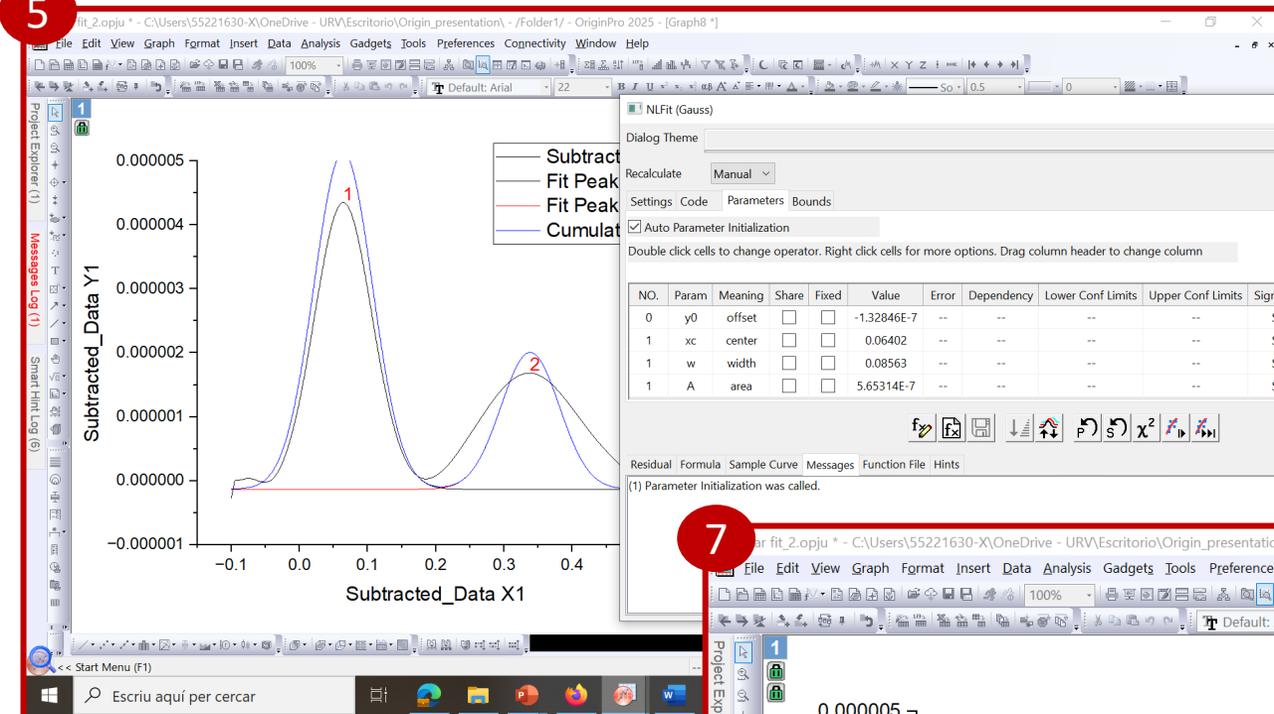


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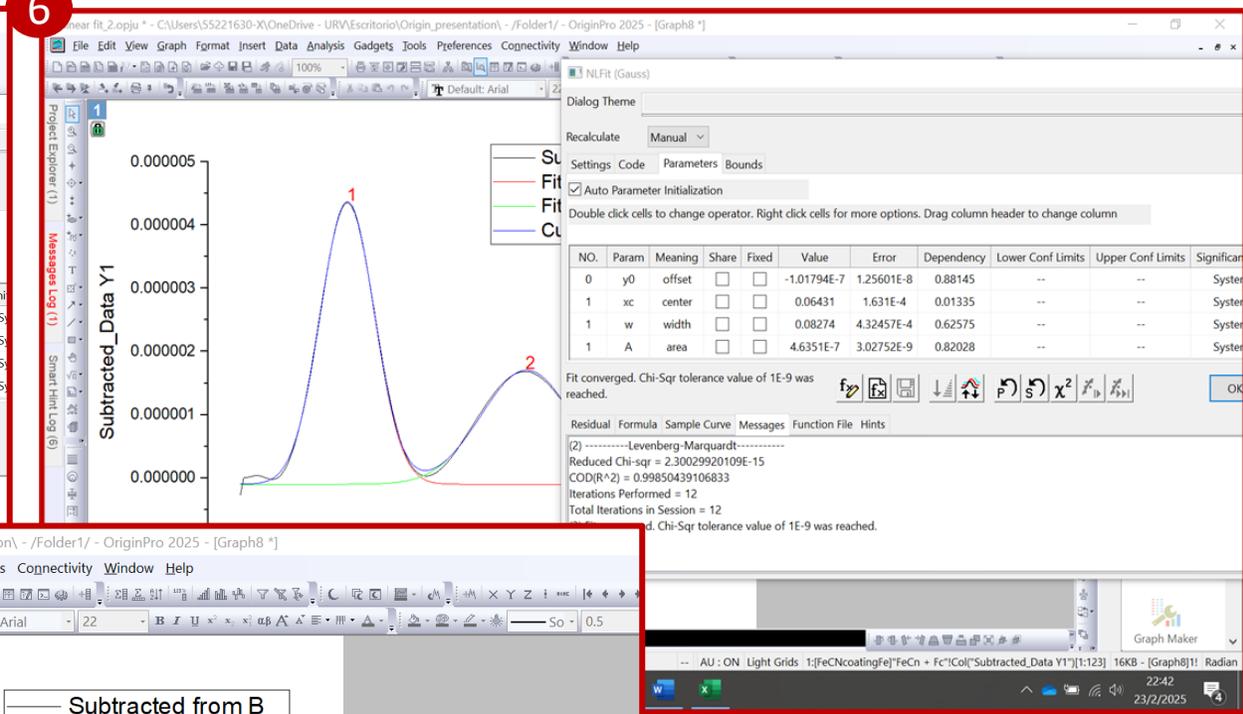


II) Practical example: Signal integration

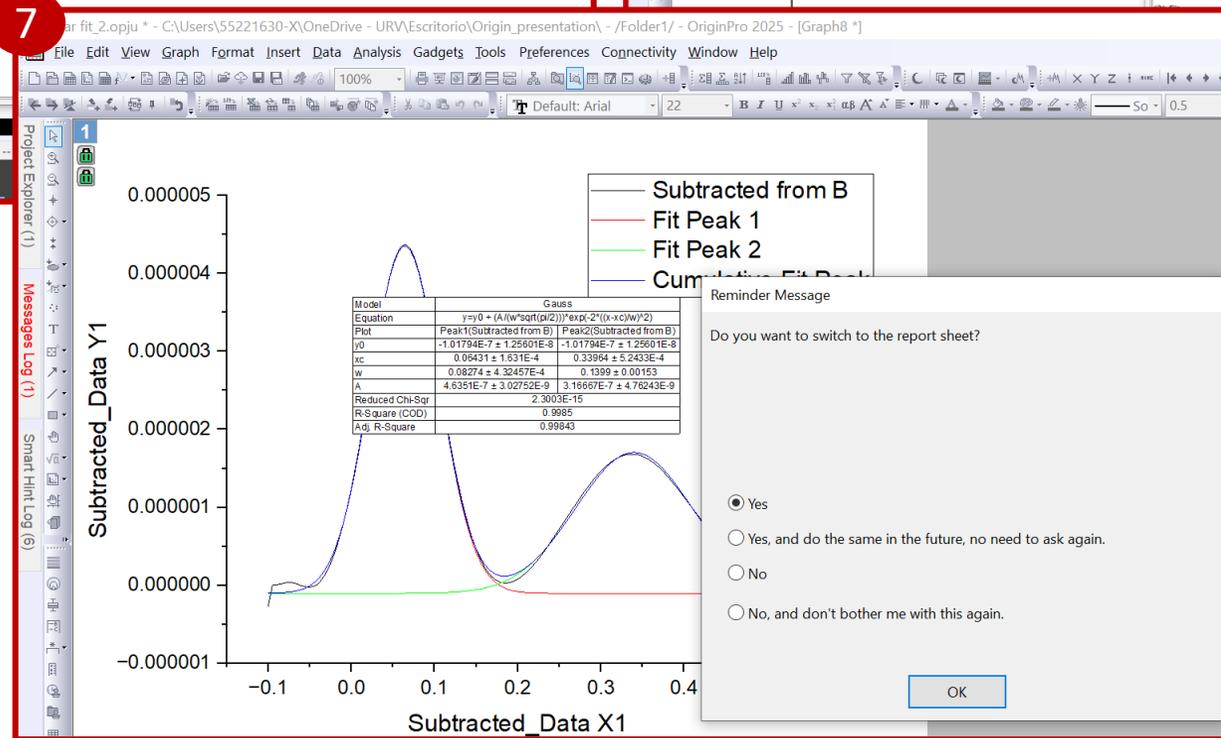
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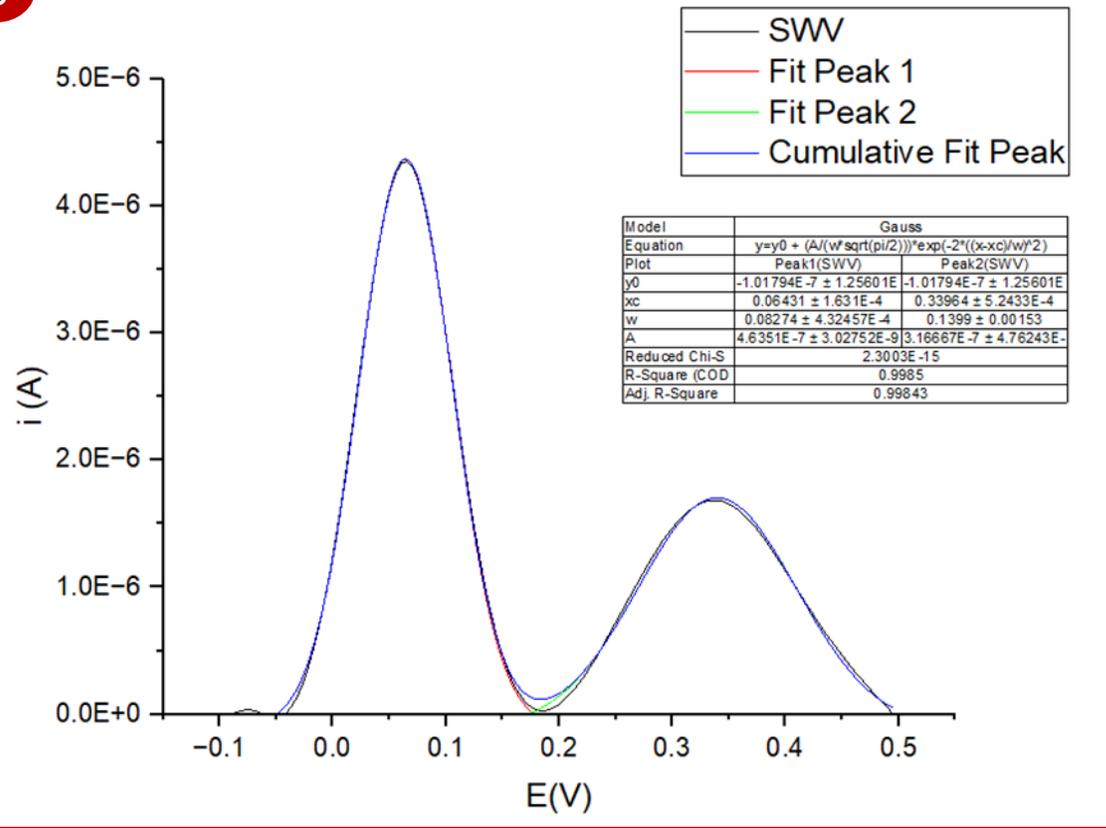


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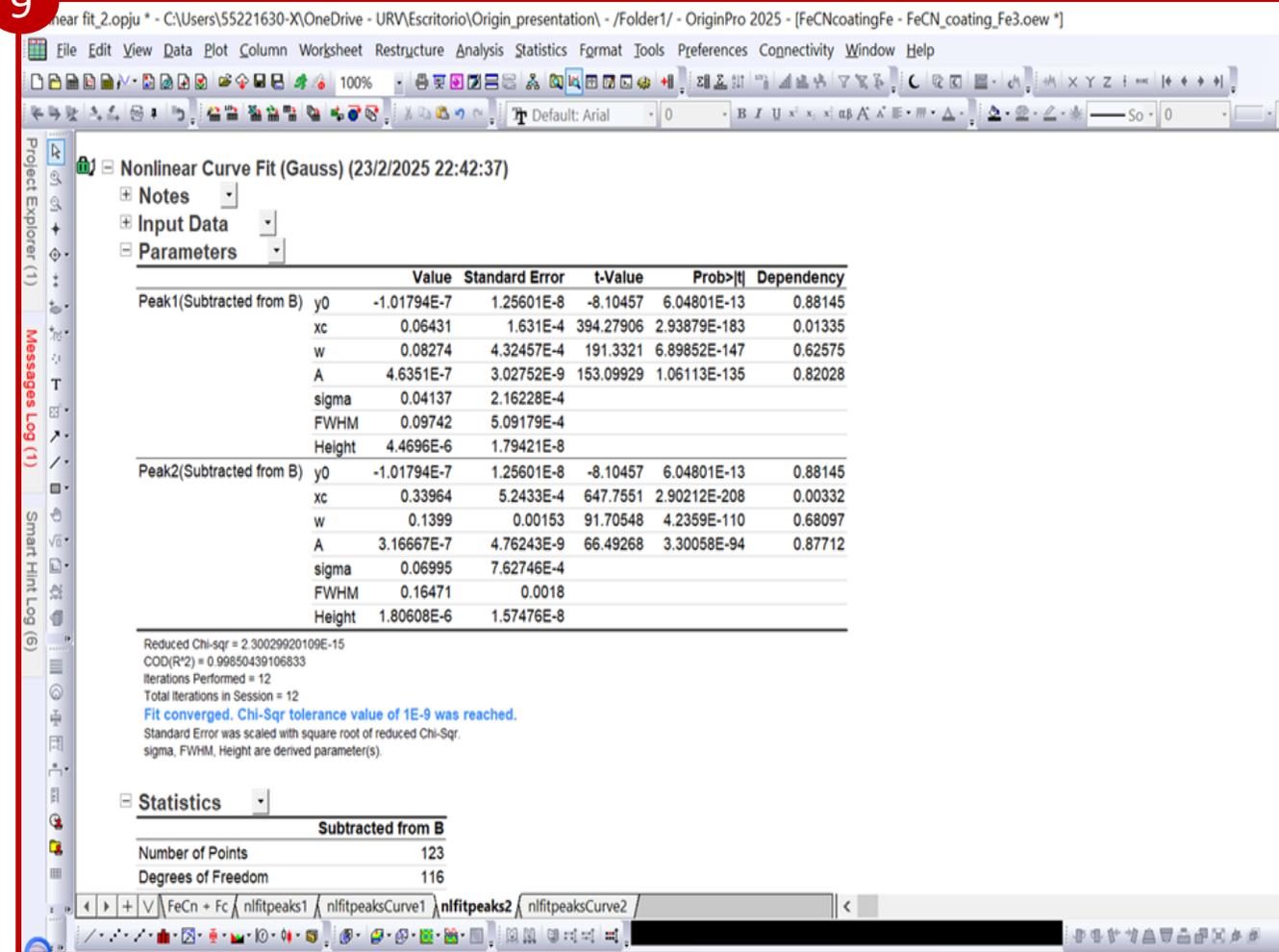


II) Practical example: Signal integration

8



9



III) Practical example: plotting FTIR spectra

1

Bring up the X axis control dialog box
- F1 for more details -

	D(Y2)	E
4	3988	0.00835
5	3984	0.0081
6	3980	0.00819
7	3977	0.00803
8	3973	0.00827
9	3969	0.00811
10	3965	0.00823
11	3962	0.00806
12	3958	0.00811
13	3954	0.00792
14	3950	0.00824

2

X Axis - Layer 1

Selection: Horizontal Vertical

From: 4500 To: 250

Type: Linear

Rescale: Normal

Increment: 500

Major Ticks: 8

Minor Ticks: 1

First Tick:

Ticks Location

Major Ticks From Dataset

Minor Ticks From Dataset

OK Cancel Apply

Y Axis - Layer 1

Selection: Horizontal Vertical

From: 1 To: 0

Type: Linear

Rescale: Normal

Increment: -0.2

Major Ticks: 8

Minor Ticks: 1

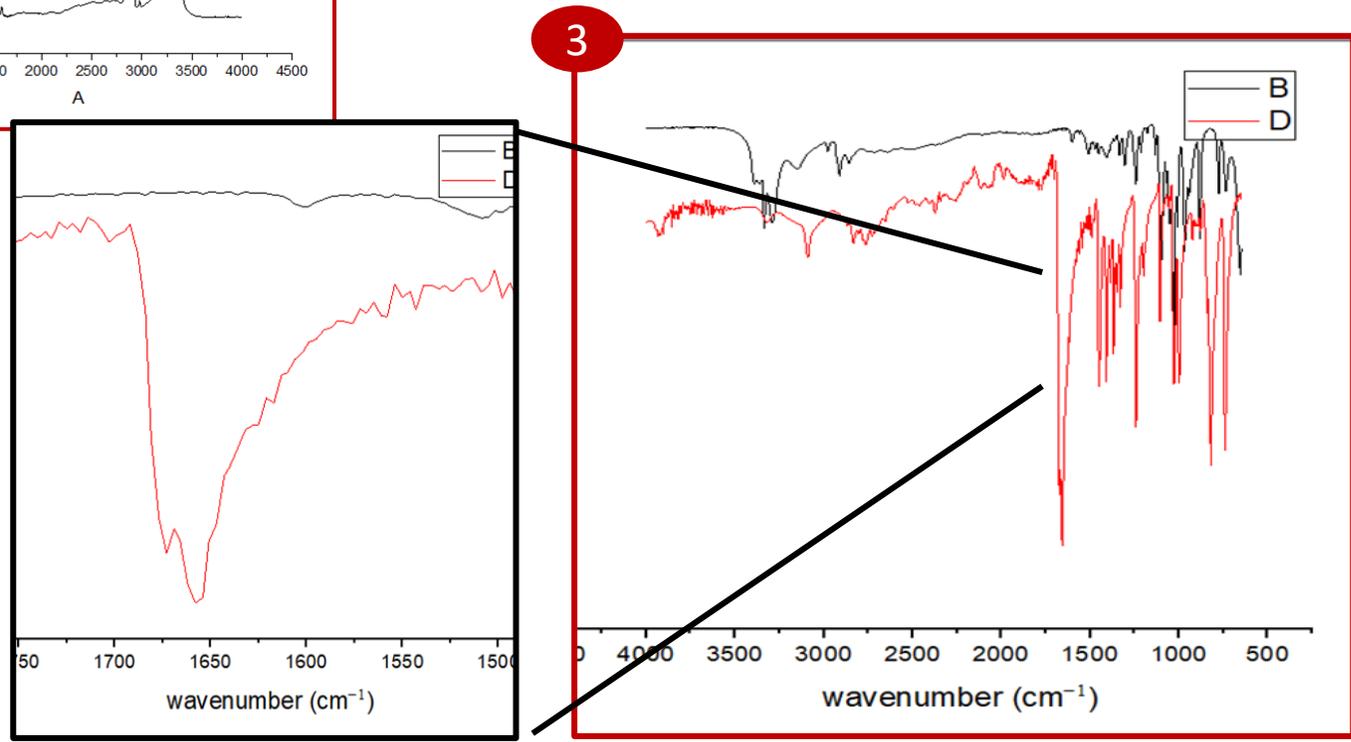
First Tick:

Ticks Location

Major Ticks From Dataset

Minor Ticks From Dataset

OK Cancel Apply



IV) Practical example: FTIR – signal deconvolution

1

The screenshot shows the Peak Analyzer software interface. On the left, a graph displays a spectrum with a prominent peak around 1650 cm⁻¹. The y-axis is labeled 'B' and ranges from 0.0 to 0.9. The x-axis ranges from 1400 to 1900. On the right, a 'Goal' panel is active, showing a tree view with 'Goal - Subtract Baseline' selected. Below this, there are buttons for 'Prev', 'Next', 'Finish', and 'Cancel'. A 'Recalculate' dropdown is set to 'Manual'. The 'Goal' section has radio buttons for 'Integrate Peaks', 'Create Baseline', 'Subtract Baseline' (which is selected), 'Find Peaks', and 'Fit Peaks (Pro)'. The 'Input' field contains the formula '[Graph5]!1"B"'. A small data table is visible at the bottom left of the graph area.

21	1822	0.1
22	1818	0.1
23	1815	0.11406

2

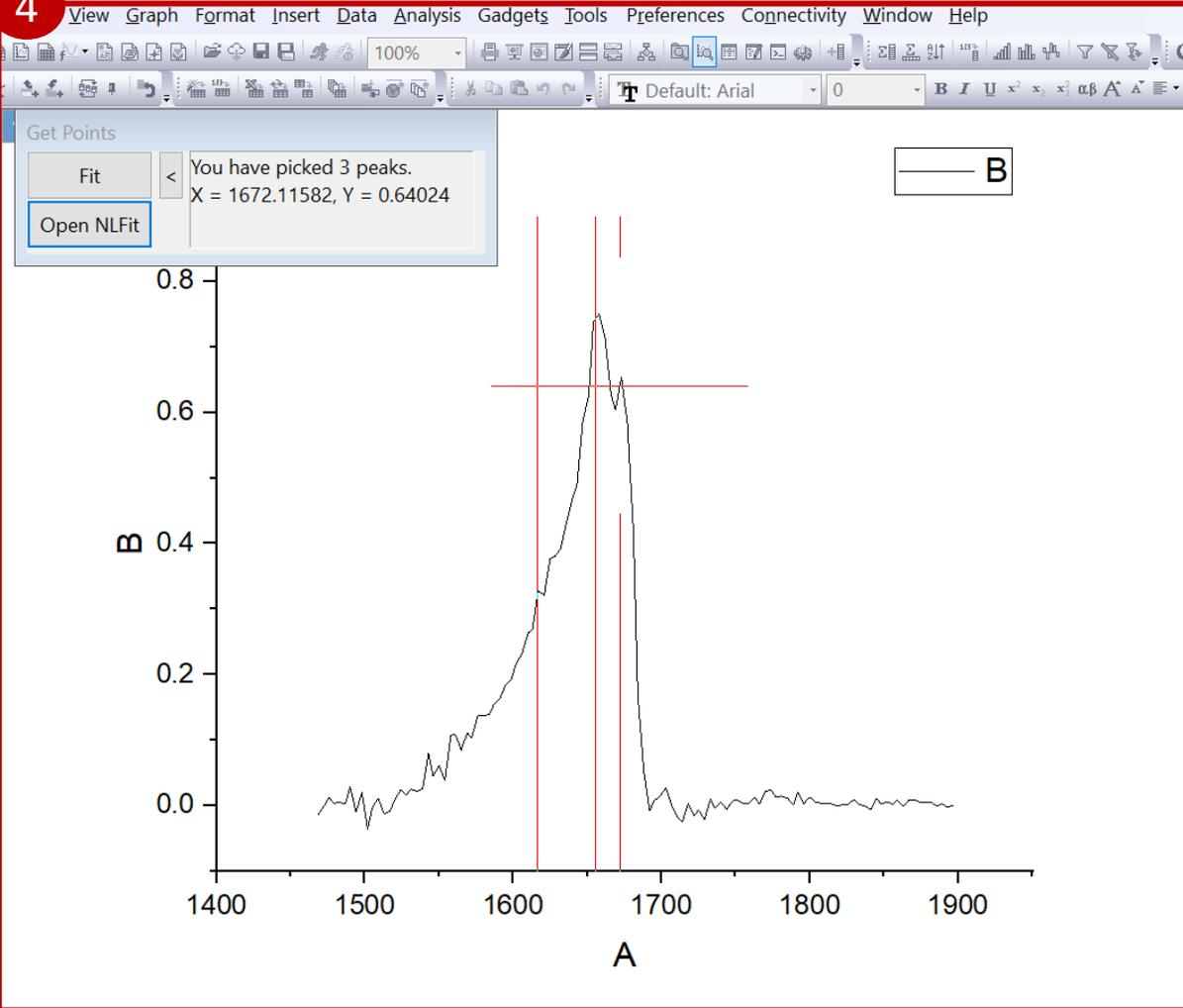
The screenshot shows the Peak Analyzer software interface with the 'Analysis' menu open. The 'Peaks and Baseline' submenu is also open, showing options like 'Multiple Peak Fit', 'Peak Analyzer', and 'Batch Peak Analysis Using Theme...'. The 'Multiple Peak Fit' option is selected. The background graph is the same as in the first screenshot, showing a spectrum with a peak around 1650 cm⁻¹. The y-axis is labeled 'B' and ranges from 0.0 to 0.8. The x-axis is labeled 'A' and ranges from 1400 to 1900.

3

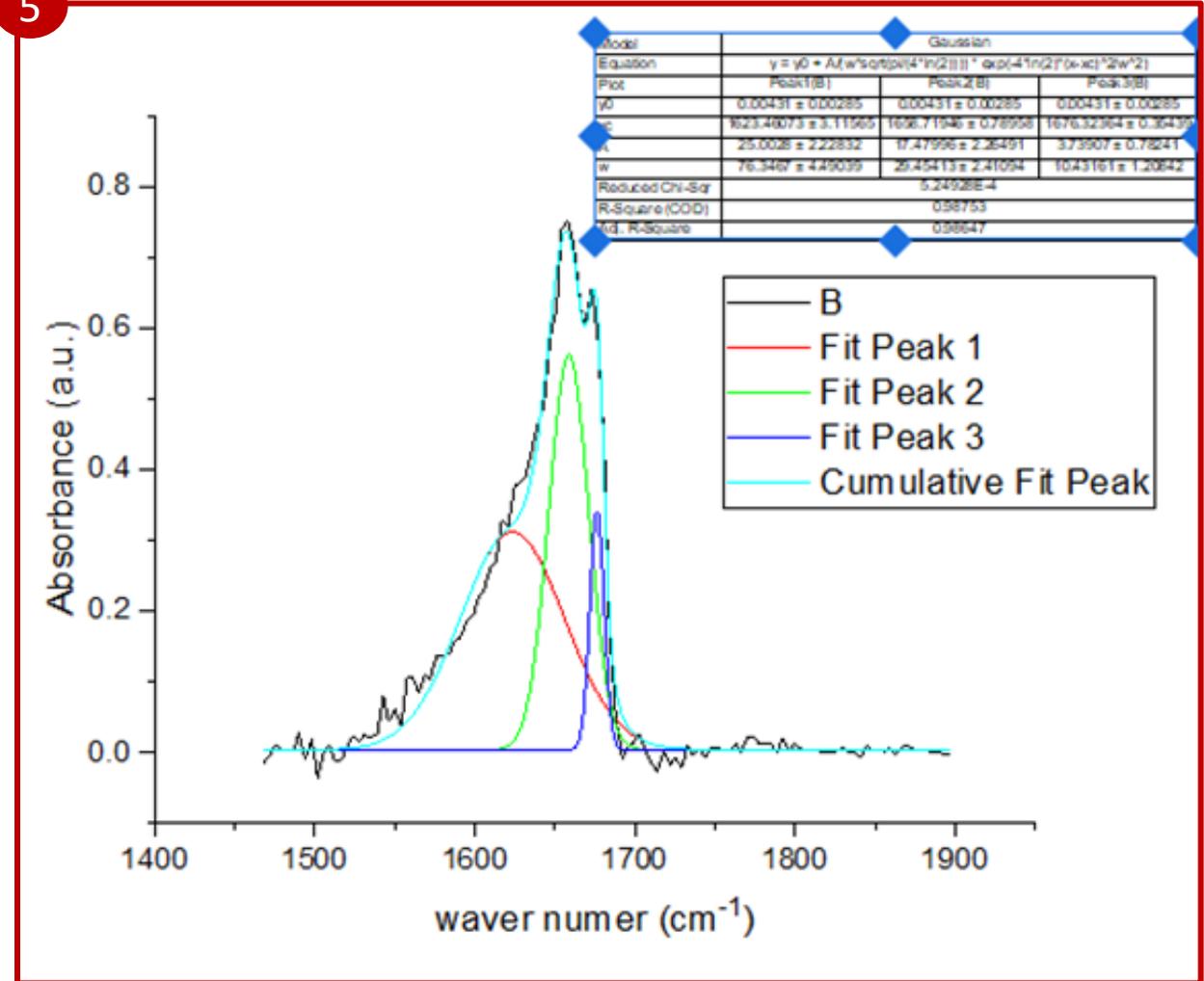
The screenshot shows the 'Multiple Peak Fit: nlfiteaks' dialog box. The 'Dialog Theme' is set to '*'. The text 'Fit peaks by specifying centers and customizing peak parameters' is displayed. The 'Input' field contains '[Graph4]!1"B"'. The 'Range 1' field also contains '[Graph4]!1"B"'. The 'Peak Function' dropdown is set to 'Gaussian'. There are 'OK' and 'Cancel' buttons at the bottom right.

IV Practical example: FTIR – signal deconvolution

4



5



V) Practical example: Statistics by ANOVA

1

Book2 *

	A(X)	B(Y)
Long Name		
Units		
Comments		
F(x)=		
1	Control	37.70251
2	Control	43.71056
3	100	40.08906
4	100	39.57509
5	100	38.85565
6	150	39.46032
7	150	41.54192
8	150	43.25286
9	200	41.5485
10	200	41.24788
11	250	41.02743
12	250	45.27703
13	300	44.98481
14	300	39.34474
15		
16		

2

ANOVAOneWay
 Dialog Theme *
 Perform One-Way ANOVA
 Recalculate Manual
 Input Means Comparison Tests for Equal Variance Power Analysis Output Plots
 Indexed: factor variable and response data are stored in separate columns.
 Input Data Indexed
 Factor [Book2]Sheet1!A
 Data [Book2]Sheet1!B
 Cancel

3

ANOVAOneWay
 Dialog Theme *
 Perform One-Way ANOVA
 Recalculate Manual
 Input Means Comparison Tests for Equal Variance Power Analysis Output Plots
 Significance Level 0.05
 Tukey
 Bonferroni
 Dunn-Sidak
 Fisher LSD
 Scheffe'
 Holm-Bonferroni
 Holm-Sidak
 Grouping Letters Table
 Related Apps OK Cancel

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.

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.

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!