

For Master student in Physics Department

Mentoring Meet-up

Origin Data Analysis Tutorial

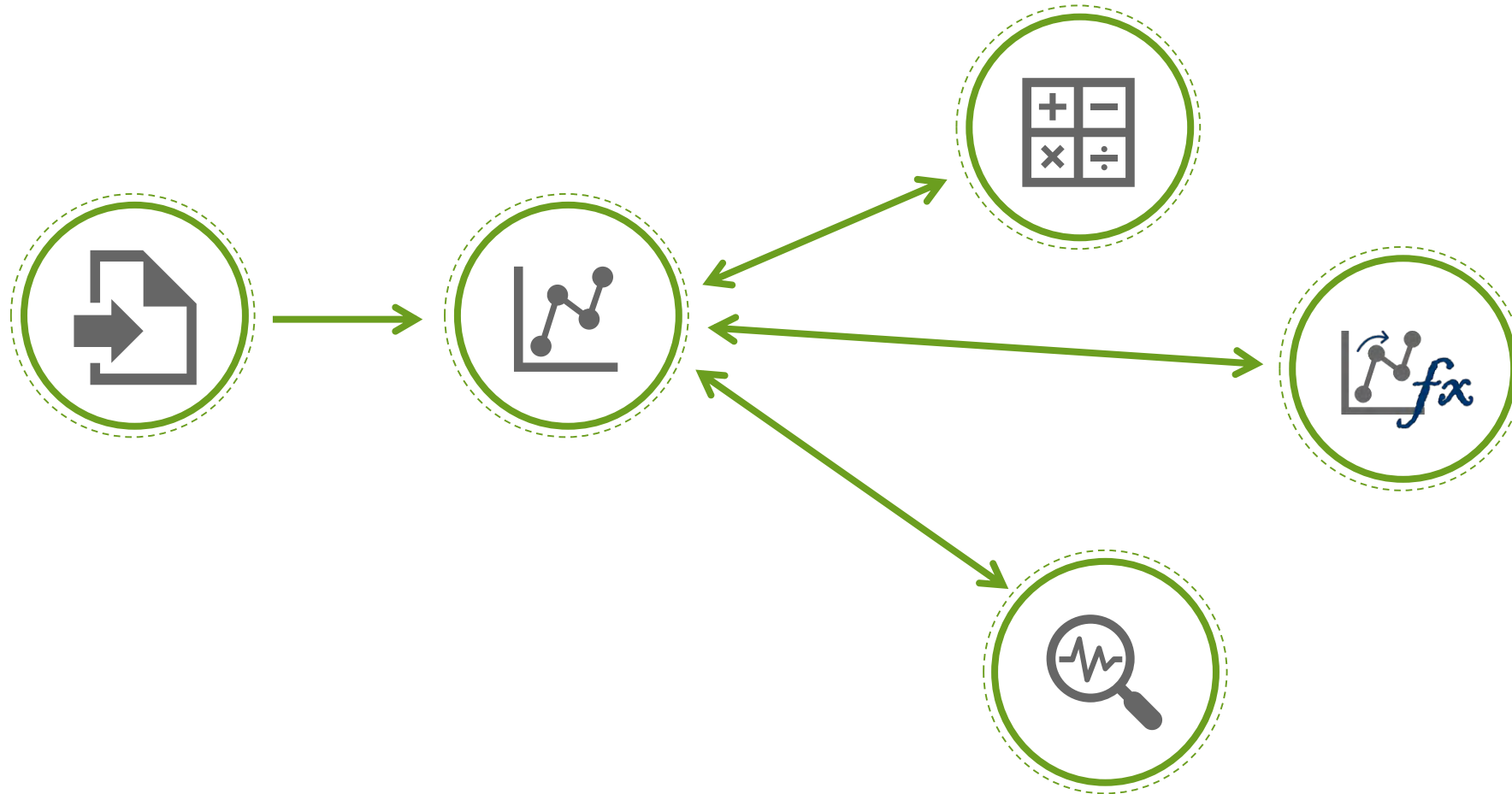


Origin Install Guide Page
(FU Physik software wiki)



ORIGIN® 2019

Graphing & Analysis



Data Import

DRAG & DROP
(on to a workbook)

Import Wizard

EASY & FAST

Sometimes imports files in a wrong way

Complicate

Manipulate import detail &
Import several files simultaneously

BEFORE IMPORT ANY DATA,
MAKE SURE YOU HAVE A **NEW WORKBOOK**



Graph Plot



Plot Type

Plot Design

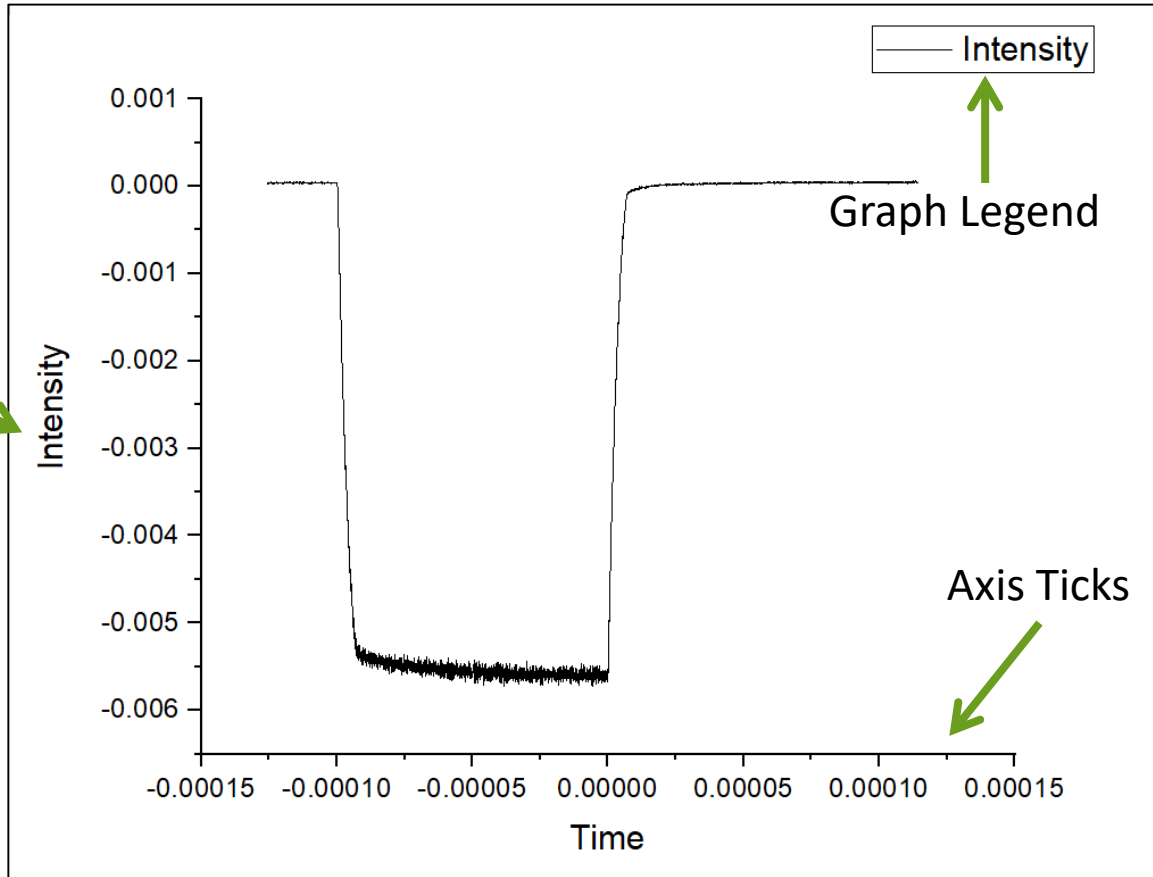
Frame Axis scale Graph Title
Color Grid

Multiple Graph

Linear vs Scatter

Axis information

Axis Title



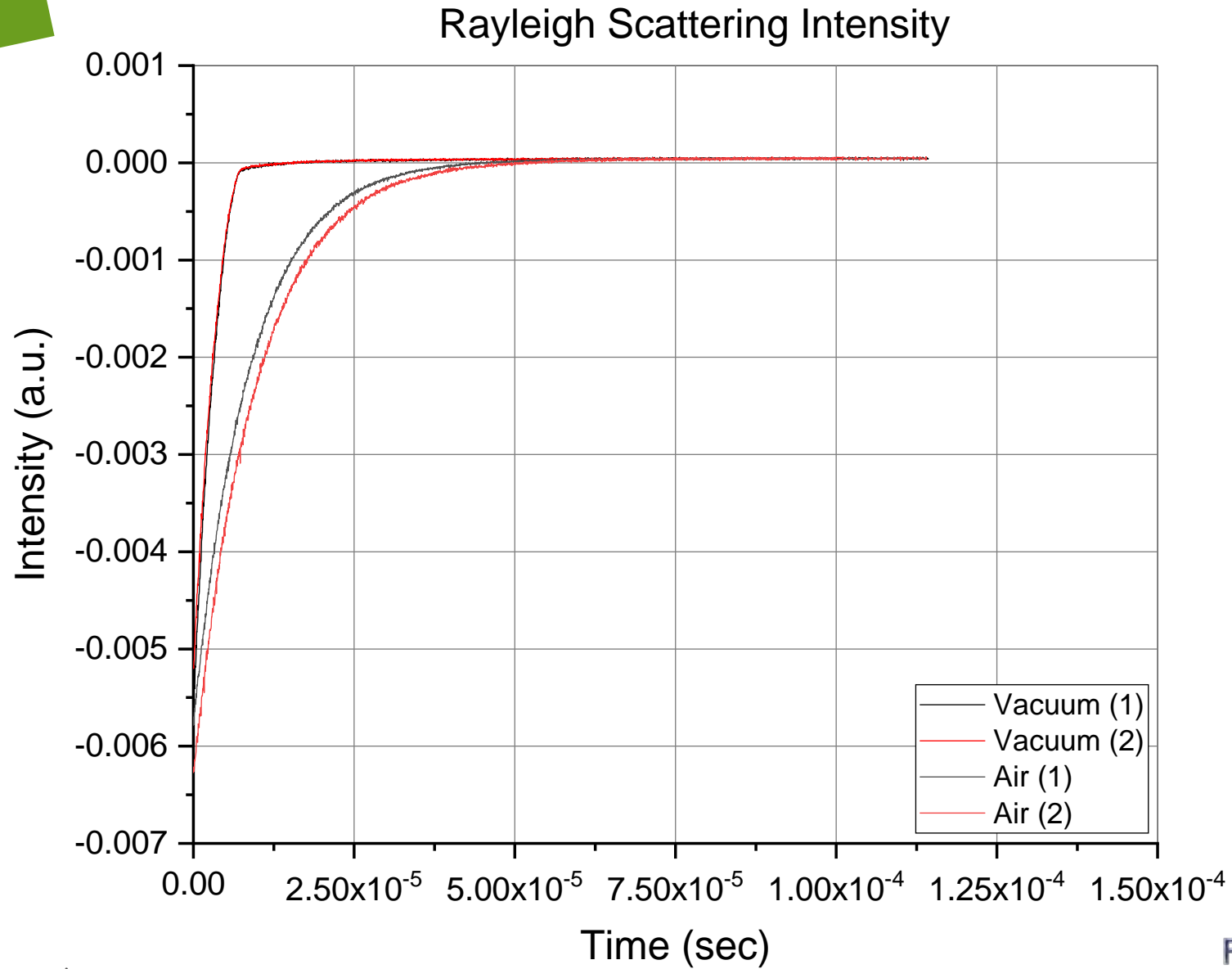
Graph Legend

Axis Ticks

Multiple Axis

Multiple Panel

Graph Overlap





Data Analysis

Curve Average

Average Multiple Curves: avecurves

Dialog Theme *

Average or concatenate multiple curves

Recalculate: Manual

Input: ((A"Time",B"Intensity"),(C"Time",D"Intensity"))

Method: Average

Averaged X: Same as Source X

Tolerance for Common X Values: 1E-8

Additional Output:

- Std Dev
- Std Err
- N
- Minimum
- Maximum
- SD times 2
- SD times 3

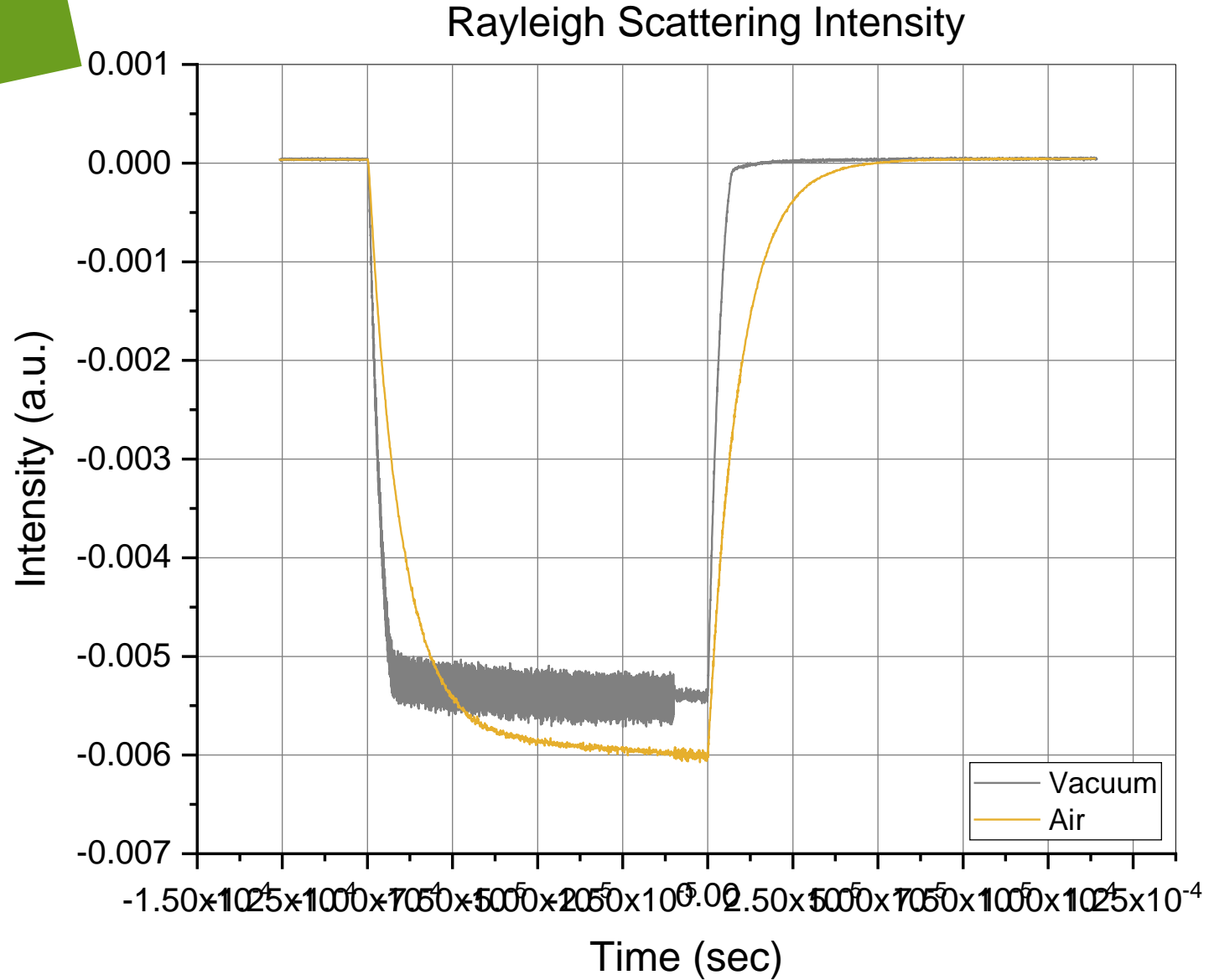
Output: [result1.txt]Vacuum!

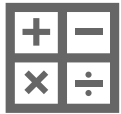
Auto Preview Preview OK Cancel

Preview: No Preview

Check the "Auto Preview" checkbox to display updated preview, or click "Preview" button when needed.

► After Average





Data Analysis



Normalization

Normalize Columns: normalize ? X

Dialog Theme *

Normalize a range of XY data

Recalculate Manual

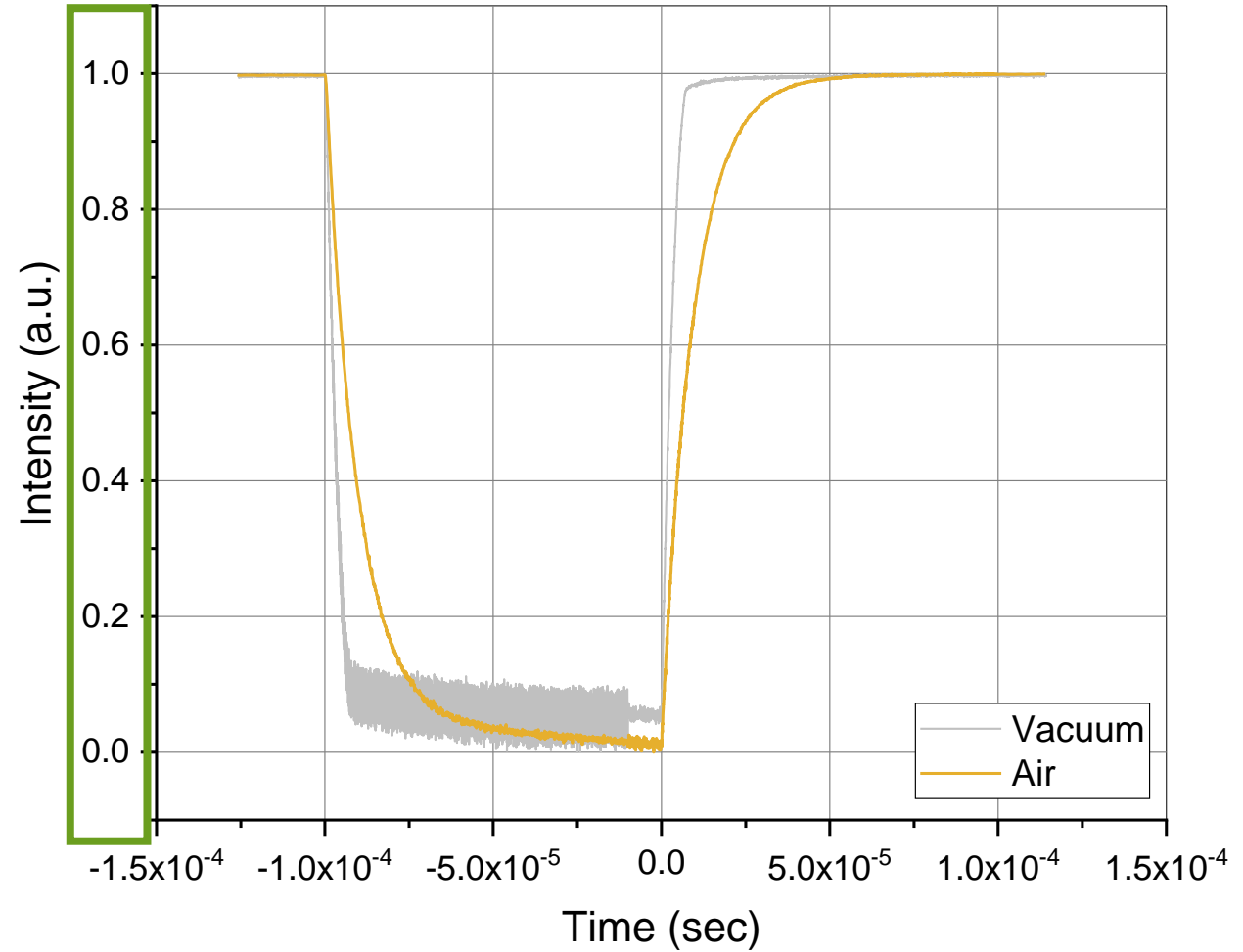
Input [result1.txt]Vacuum!5:6

Normalize Methods Normalize to [0, 1]

Output [result1.txt]Vacuum!7

OK Cancel

Rayleigh Scattering Intensity



Fitting Function

Data Range

Based on *Theory* & Own Idea

Gaussian vs Lorentzian

Types of Exponential Function

Trigonometric Function

...

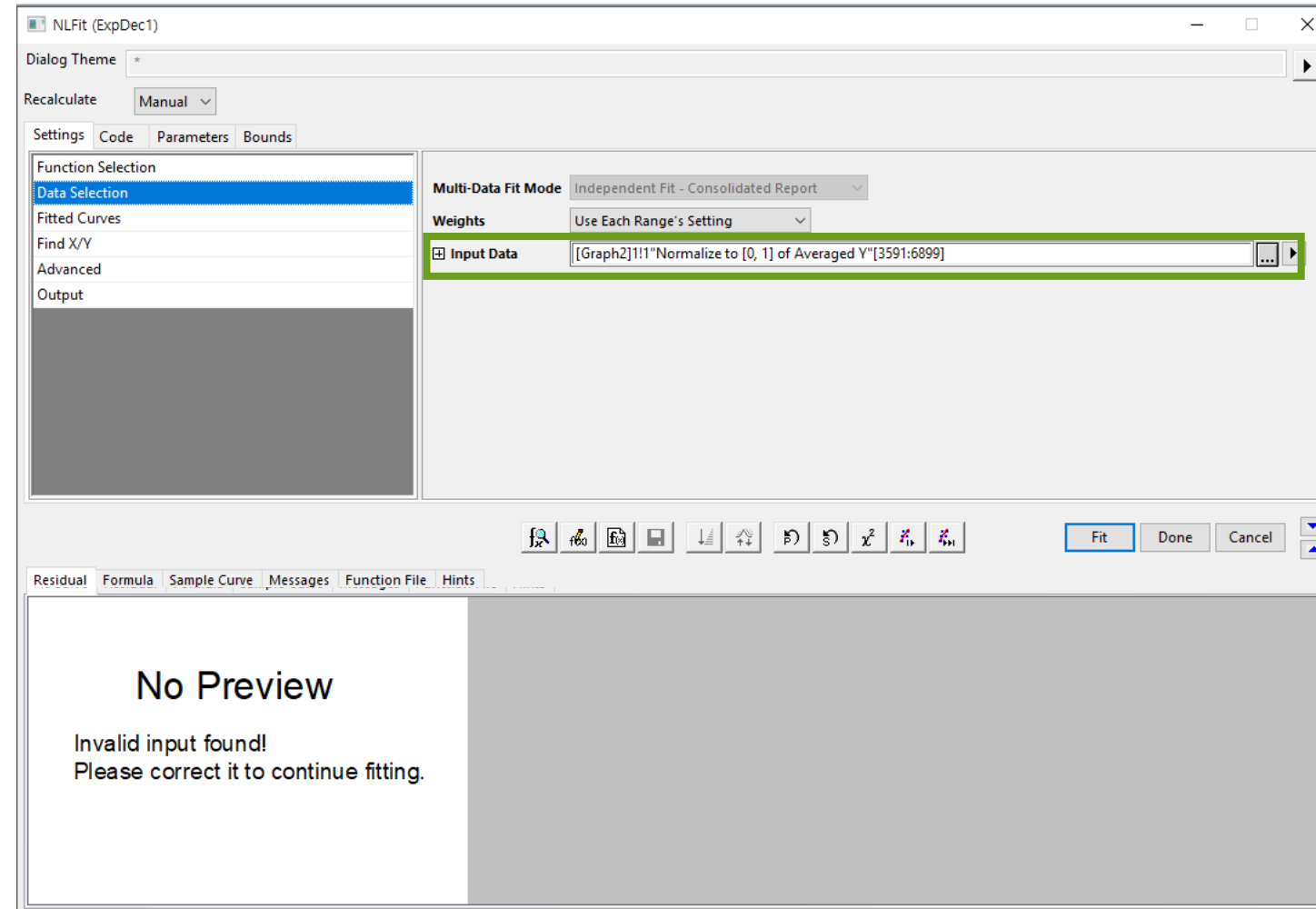
- Exponential Decay Function
- Time start form 0

Data Range

Make a new graph

Left Toolbar (Data Selector)

Fix the fitting range



The screenshot shows the NLFit (ExpDec1) dialog box. The 'Input Data' field is highlighted with a green border and contains the text: `[Graph2]!1!1"Normalize to [0, 1] of Averaged Y"[3591:6899]`. Below the dialog box, a message box displays the error: "No Preview Invalid input found! Please correct it to continue fitting."

Model	ExpDec1
Equation	$y = A1 \cdot \exp(-x/t1) + y$
Plot	Normalized Vacuum
y0	$0.99657 \pm 1.69015E-$
A1	-1.02552 ± 0.00223
t1	$2.69892E-6 \pm 8.5354$
Reduced Chi-	8.64896E-5
R-Square (CO	0.99179
Adj. R-Square	0.99178

Reduces Chi-Sqr

Scale Error with square, is equal to the residual sum of square (RSS) divided by the degree of freedom. (=Variations of residue)
Close to 1, Good fit.

R-Square (COD)

the coefficient of determination (COD).

A percentage of the response variable variation that explained by the fitted regression line, Always be between 0 and 1.
Close to 1 > Good fit.

Adj. R-Square

The Adj. R-square is a modified version of R-square, which is adjusted for the number of predictor in the fitted line.
Thus, it can be used to compare with the fitted lines with different numbers of predictors.

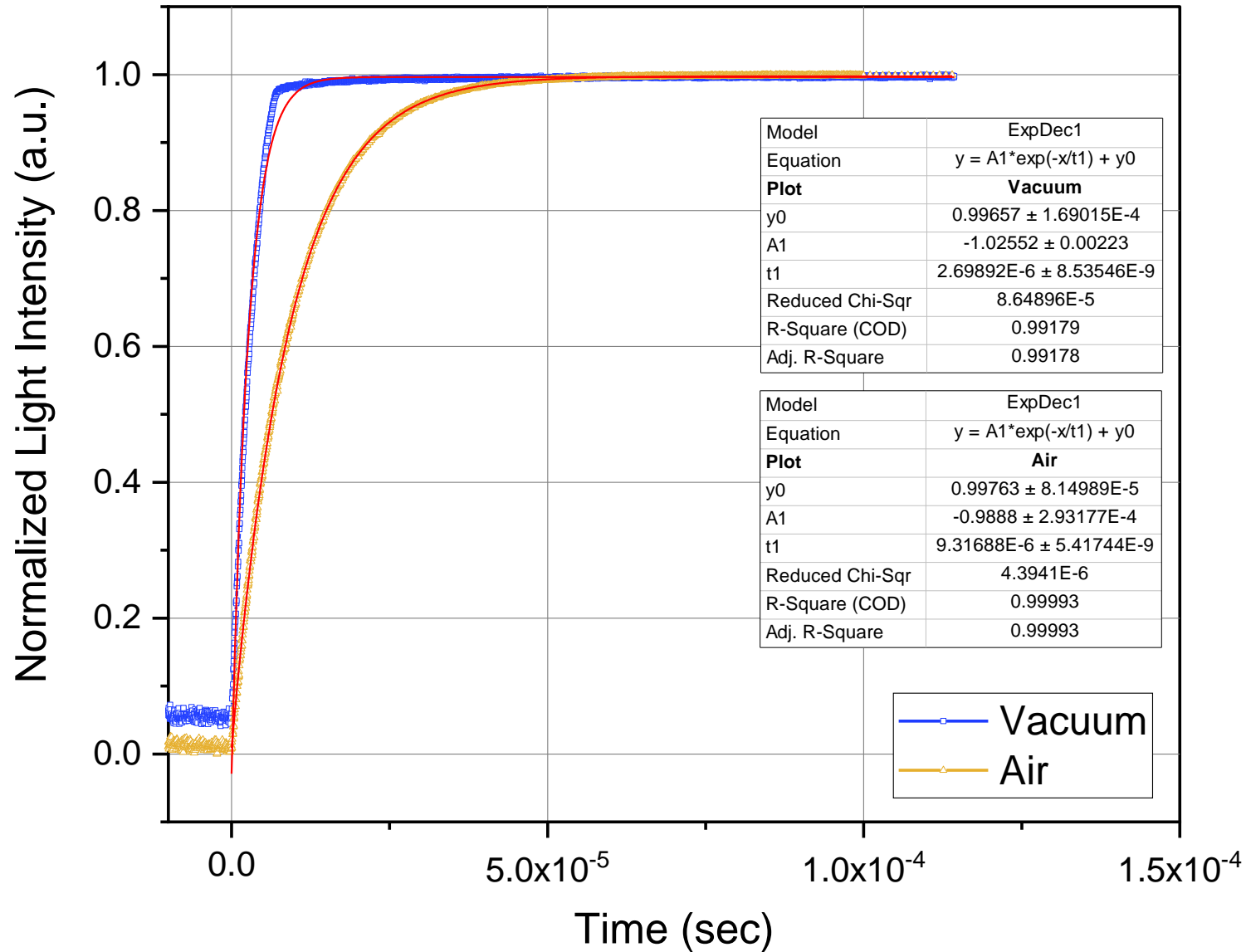
▶ Exercise 1



Plot this into a one graph:

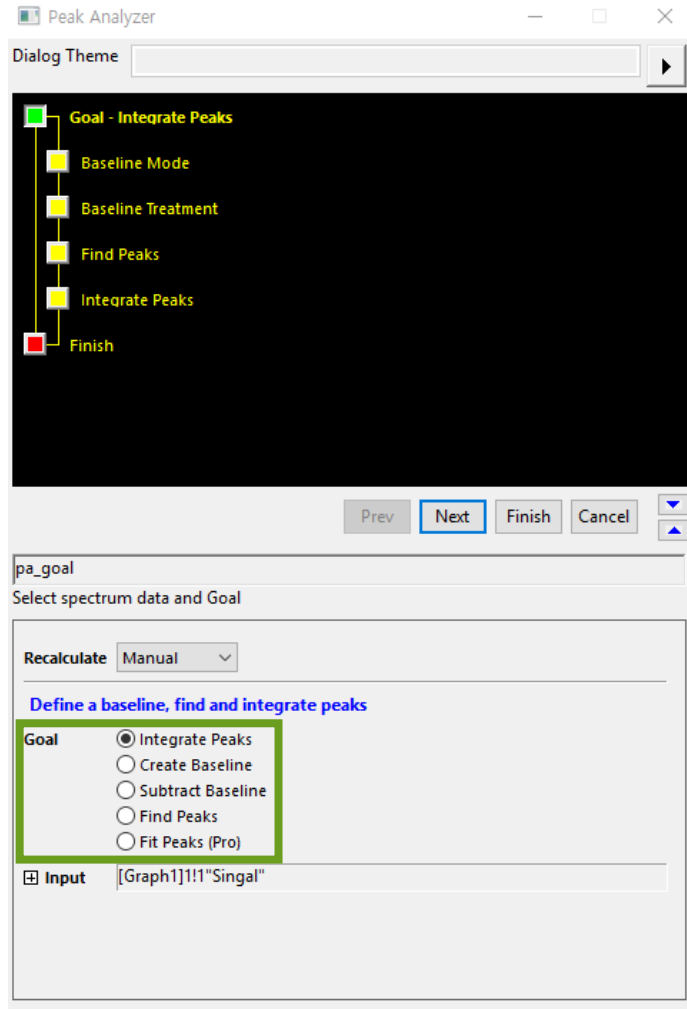
- Normalized Vacuum & Normalized Air data with each fitting function
- Find both decay function by using [Exp.Dic 1] function
- Determine each R-square value and decay constant(t_1)
- Compare both decay constant

Rayleigh Scattering Intensity in different conditions





Peak Searching



Peak Searching Mode

Integrate Peaks

Find Peaks

Fit Peaks (Pro)

Baseline Analyzing Mode

Create Baseline

Subtract Baseline

▶ Integrate Peaks



Peak Analyzer

Dialog Theme

- Goal - Integrate Peaks
 - Baseline Mode
 - Baseline Treatment
 - Find Peaks
 - Integrate Peaks
 - Finish

Prev Next Finish Cancel

pa_peaks

Current Number of Peaks 115

Enable Auto Find

Find Add Modify/Del Clear All Save... Load... Peaks Info...

Snap to Spectrum

Peak Finding Settings

Show 2nd Derivative

Smoothing Window Size 0 Auto

Direction Positive

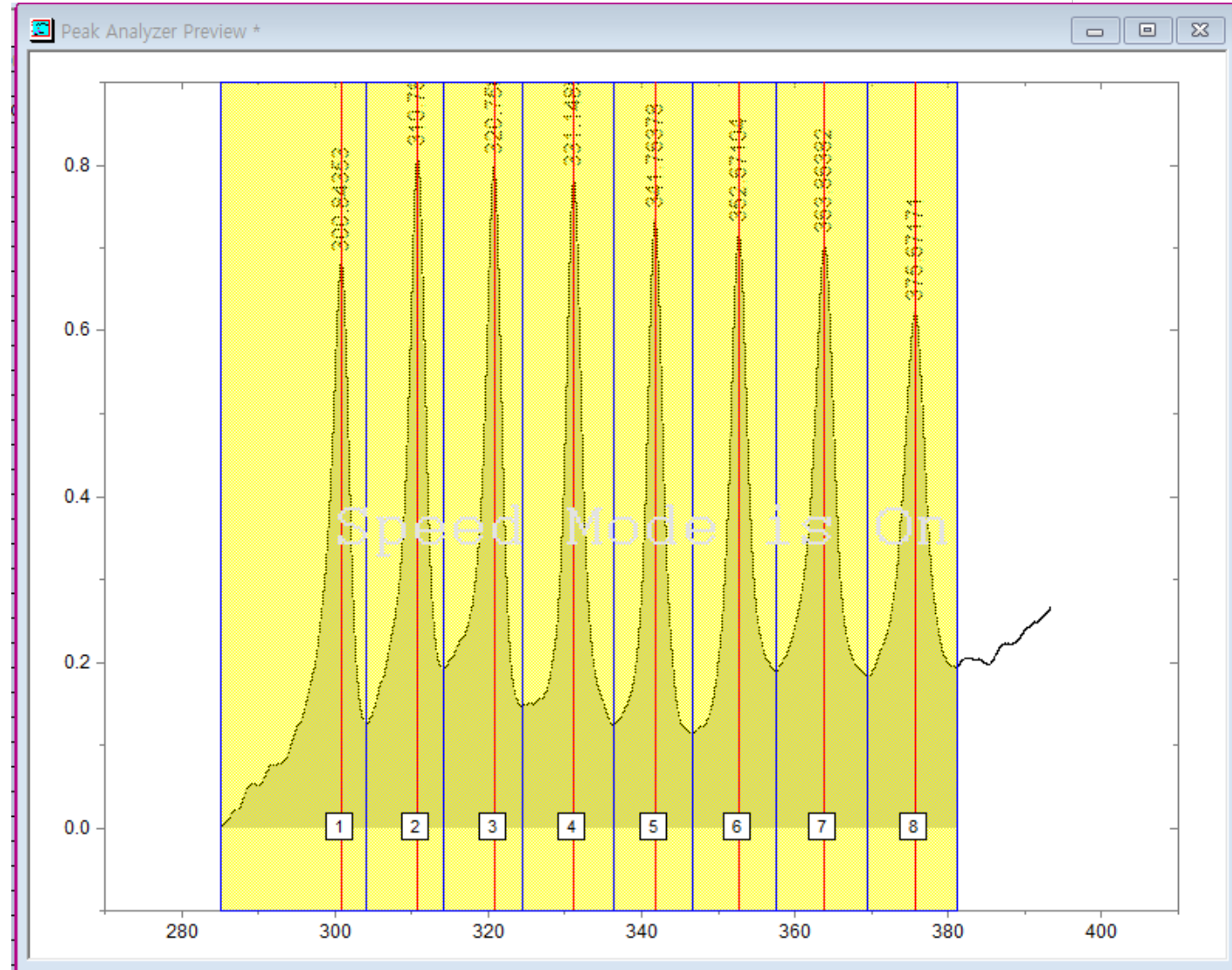
Method Local Maximum

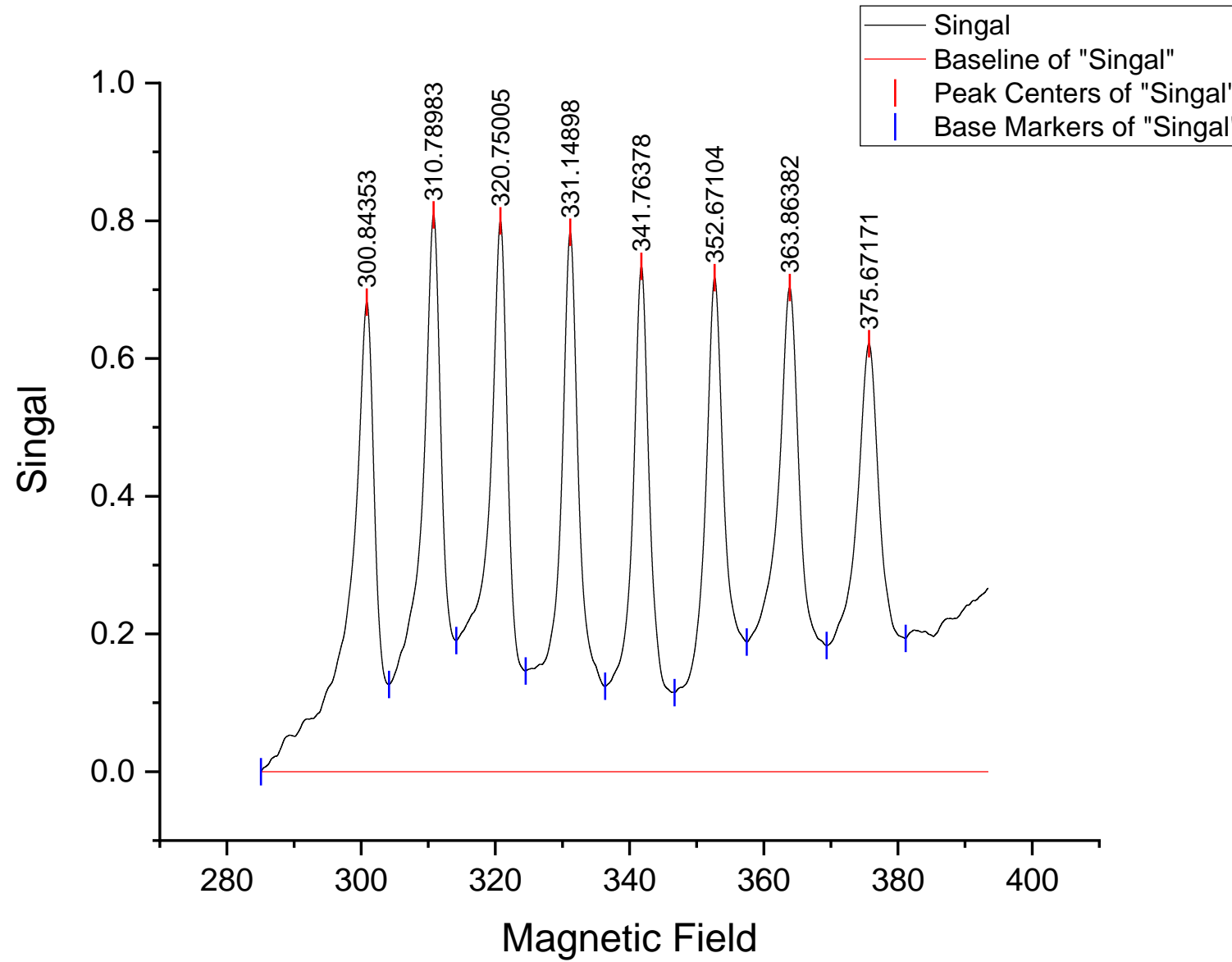
Local Points 50

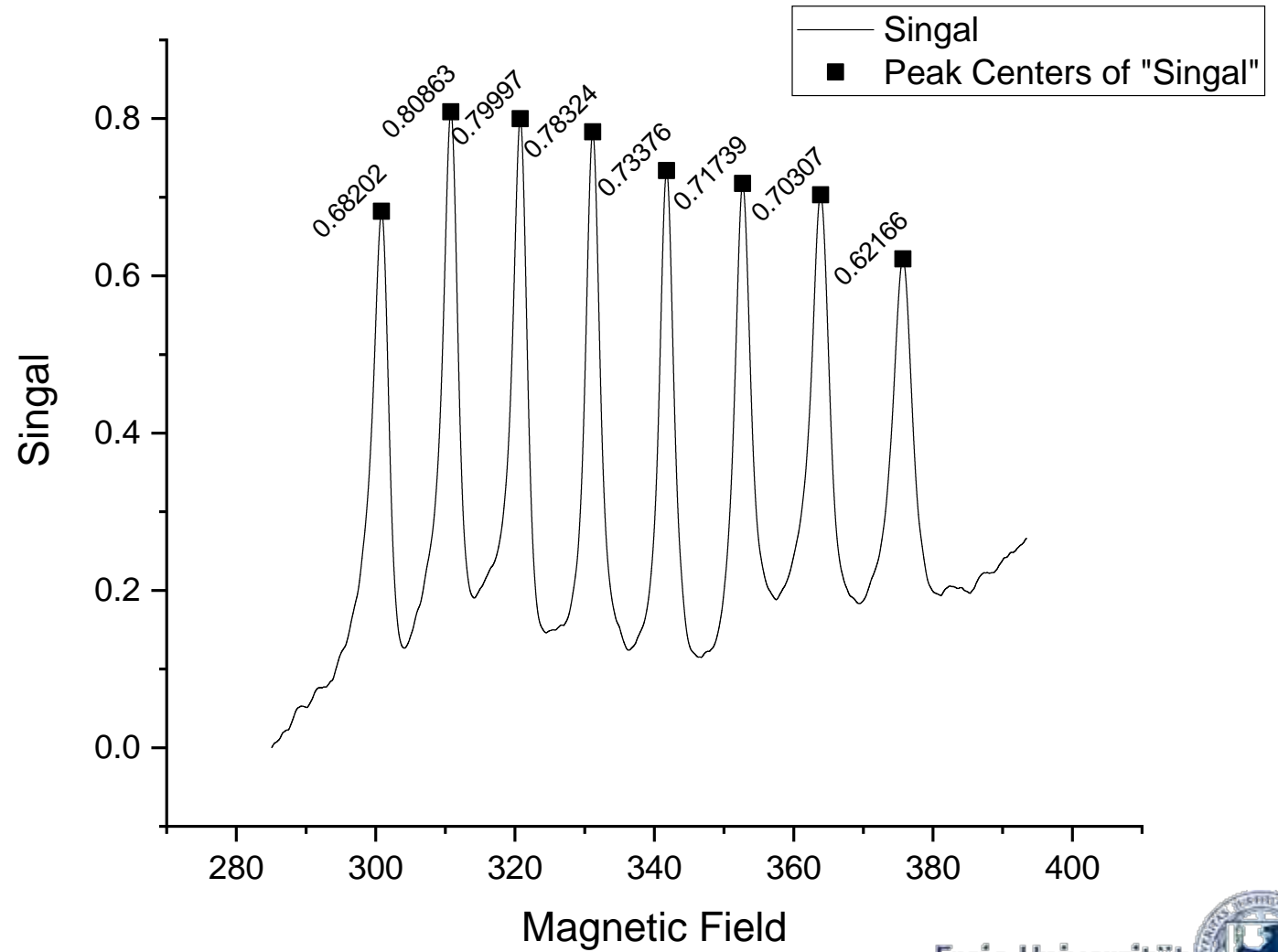
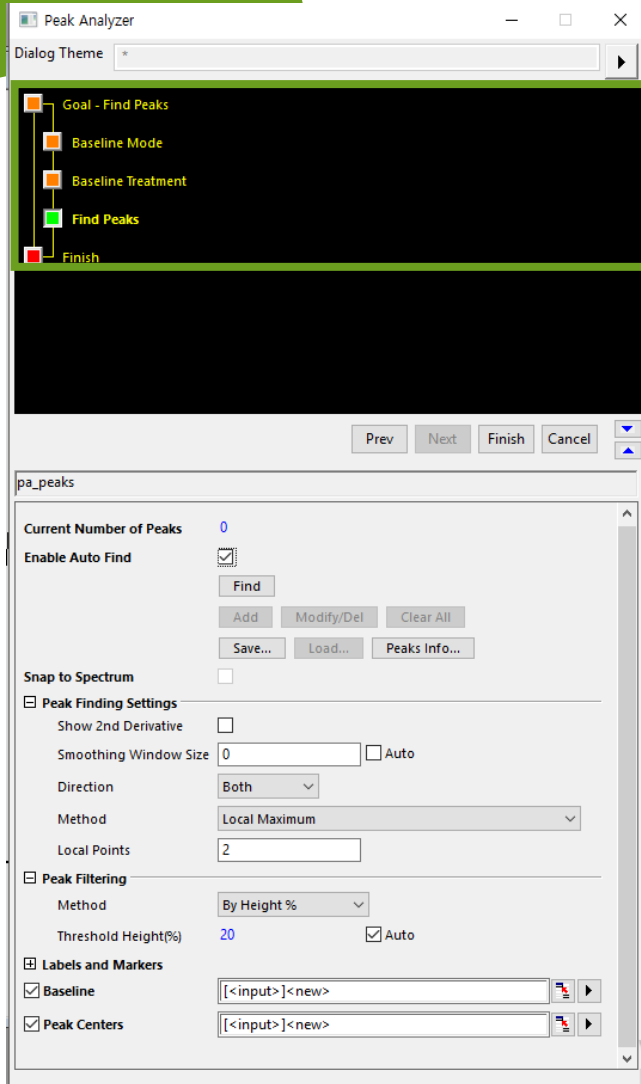
Peak Filtering

Method By Height %

Threshold Height(%) 50 Auto







► Find Peak (Pro)



Peak Analyzer

Dialog Theme *

- Goal - Fit Peaks (Pro)
 - Baseline Mode
 - Baseline Treatment
 - Find Peaks
 - Fit Peaks (Pro)**
 - Finish

Prev Next Finish Cancel

pa_fit

Snap to Spectrum

Peaks

Weight
Method: No Weighting

Show Residuals

Show 2nd Derivative

Result

- Output
- Configure Report
- Configure Graph

Generate Report from Current Fitting Result

Peak Fit Parameters

Auto Parameter Initialization

Parameters Bounds Fit Control

NO.	Peak Type	Param	Meaning	Share	Fixed	Value	Error	Dependency	Lower Conf Limits	Upper Conf Limits	Significant Digits
0	Constant	y0	unknown	0	<input type="checkbox"/>	0	--	--	--	--	System
1	Gaussian	xc_1	center	0	<input type="checkbox"/>	300.84353	--	--	--	--	System
1	Gaussian	A_1	area	0	<input type="checkbox"/>	1.1002	--	--	--	--	System
1	Gaussian	w_1	FWHM	0	<input type="checkbox"/>	1.51545	--	--	--	--	System
2	Gaussian	xc_2	center	0	<input type="checkbox"/>	310.78983	--	--	--	--	System
2	Gaussian	A_2	area	0	<input type="checkbox"/>	1.41833	--	--	--	--	System
2	Gaussian	w_2	FWHM	0	<input type="checkbox"/>	1.64777	--	--	--	--	System

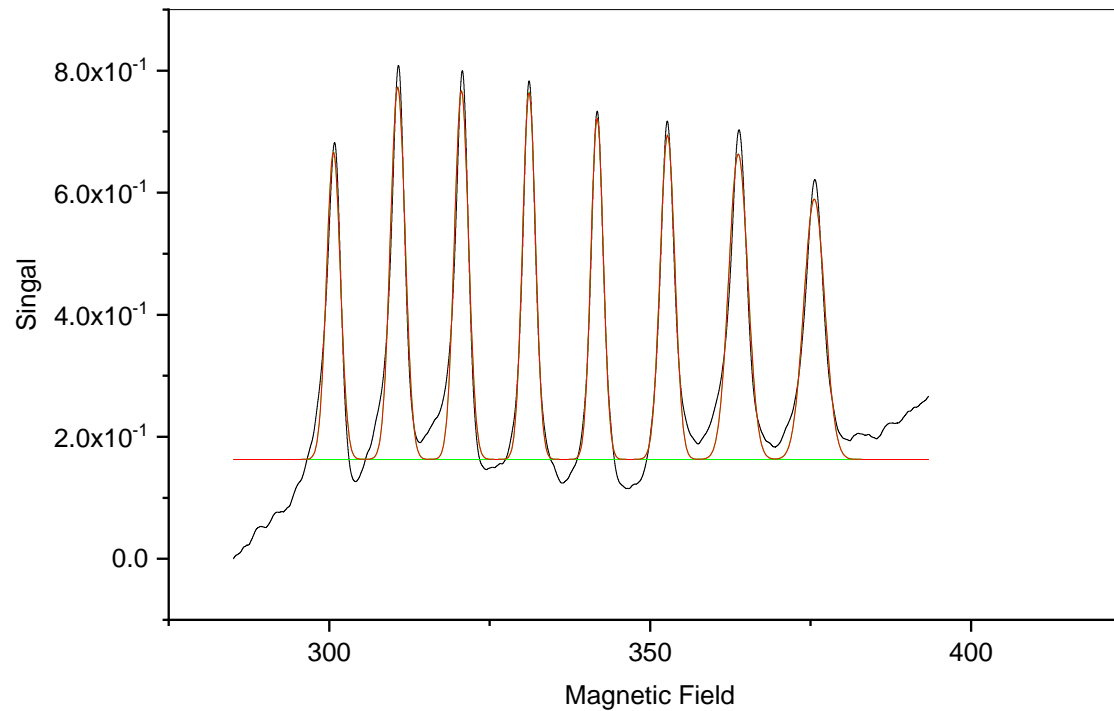
Gaussian

Messages Formula Sample Curve Function File

Peak Analysis



Data Set:[Book1]"Result 5"!B"Singal" Date:2019-11-04
 BaseLine:Constant
 Chi²=2.34301E-003 Adj. R-Square=9.30068E-001 # of Data Points=46700
 SS=1.09360E+002 Degrees of Freedom=46675



Fitting Results

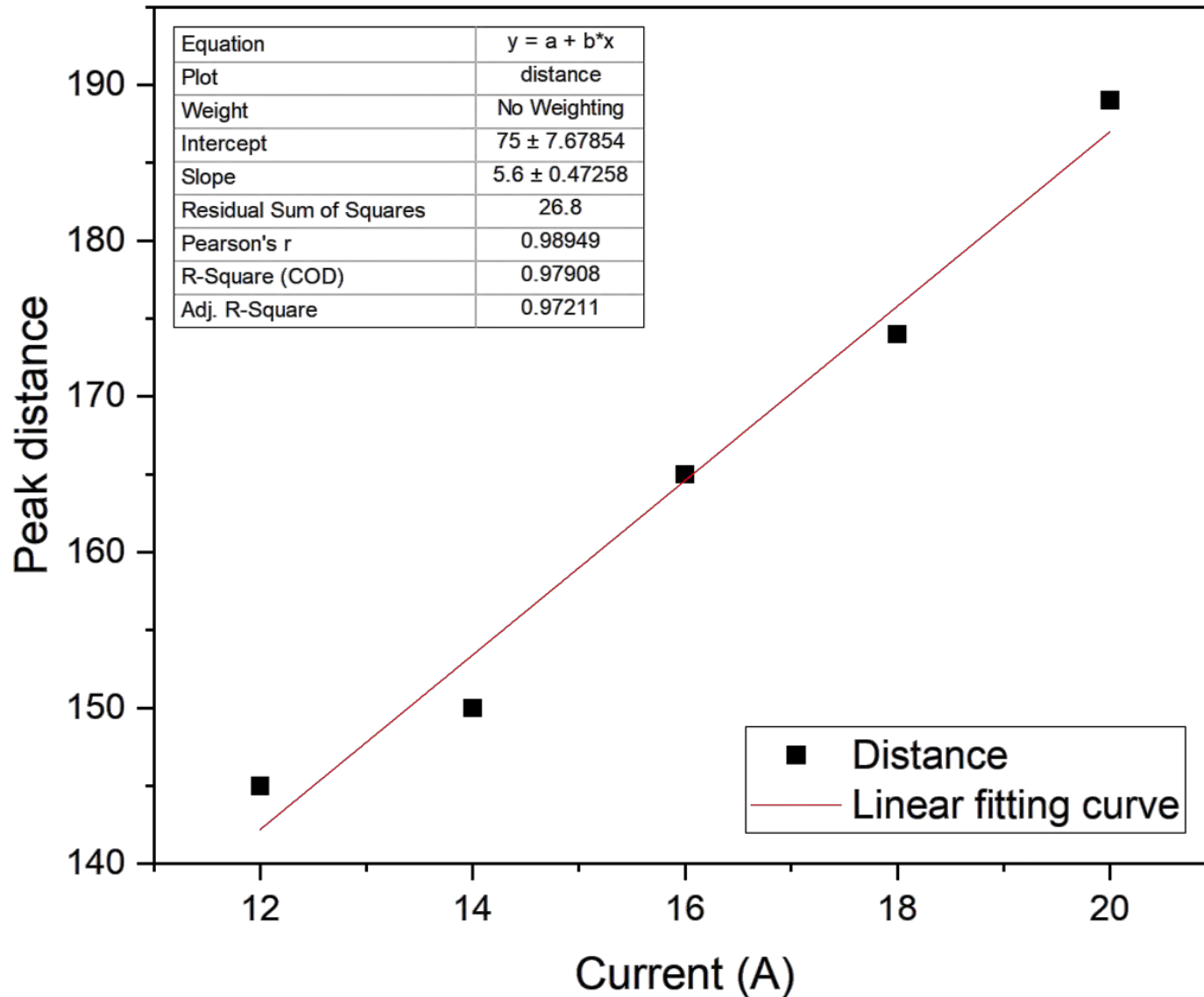
Peak Index	Peak Type	Area Intg	FWHM	Max Height	Center Grvty	Area IntgP
1	Gaussian	1.3575	2.53025	0.50402	300.66805	10.65831
2	Gaussian	1.7473	2.68978	0.61027	310.68673	13.71877
3	Gaussian	1.6581	2.57992	0.60377	320.61497	13.0184
4	Gaussian	1.51755	2.37026	0.60147	331.14266	11.91487
5	Gaussian	1.34899	2.26652	0.55914	341.75308	10.59149
6	Gaussian	1.5186	2.68511	0.53131	352.71792	11.92311
7	Gaussian	1.85749	3.48809	0.50027	363.73993	14.58391
8	Gaussian	1.73104	3.81096	0.42672	375.58757	13.59113

▶ Exercise 2



Find peaks and compare

- Import Result 6
- Find peaks for each data set
- Compare peaks in between 160-400 pixels
- Find the relationships between peak position and current



Distance = peak2-peak1

Peak 2 = late peak in 160-400 range

Peak1 = first peak in 160-400 range



Read a code,
share your question

Future Plan: Regularly meeting for data analyzing?
Study & Life tips in Berlin?
Christmas market?