Non-linear least squares fitting two Gaussians in Excel

The Gaussians are given by C column, which is plotted vs. the B column.
The initial guess for the parameters is given in the cells H7, I7, J7 and H8, I8 and J8

tutorial_6_gausTGA (week6) [Compatibility Mode] - Excel

FILE HOME INSERT PAGE LAYOUT FORMULAS DATA REVIEW VIEW ACROBAT

E2 =$H$7*NORMDIST(B2,$I$7,$J$7,0)+$H$8*NORMDIST(B2,$I$8,$J$8,0)

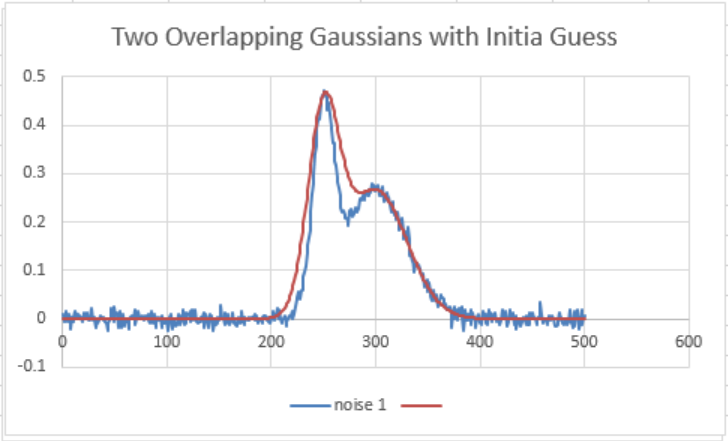
Fitting function

	A	B	C	D	E
1	**PEAK OVERLAP DATA**		noise 1	noise 2	
2		0	0.009773	-0.00093	5.1297E-23
3		1	0.00821	-0.00059	7.1551E-23
4		2	-0.00631	0.000472	9.9692E-23
5		3	0.004791	-0.00053	1.3875E-22
6		4	0.01636	0.000614	1.9288E-22
7		5	-0.00495	0.000613	2.6785E-22
8		6	0.010262	-0.00042	3.7153E-22
9		7	-0.00261	0.000746	5.1479E-22
10		8	-0.02278	-0.0006	7.1248E-22
11		9	0.002571	-0.00029	9.85E-22
12		10	-0.00437	-0.00027	1.3602E-21
13		11	0.002607	0.000603	1.8763E-21
14		12	0.015395	-0.00041	2.5854E-21
15		13	0.007243	0.000352	3.5585E-21
16		14	0.001776	0.000526	4.8923E-21
17		15	0.008453	0.000182	6.7186E-21
18		16	0.005783	-0.00031	9.2165E-21
19		17	-0.00068	0.000773	1.2629E-20
20		18	0.004804	0.000701	1.7286E-20
21		19	-0.0052	0.00044	2.3633E-20
22		20	0.013383	0.000968	3.2276E-20
23		21	0.002537	-0.00053	4.4031E-20
24		22	0.002272	0.000315	5.9999E-20
25		23	0.012812	-0.00051	8.1668E-20
26		24	0.010398	0.000281	1.1104E-19
27		25	-0.0024	0.000344	1.5081E-19

The two spectra represent the same signal but with a different noise level
Column A is e.g. elution time or scattering angle or frequency
First make a graph of both
Fit both data sets with a combination of two Gaussians using the solver

15	250	15
20	300	30

Initial Guess

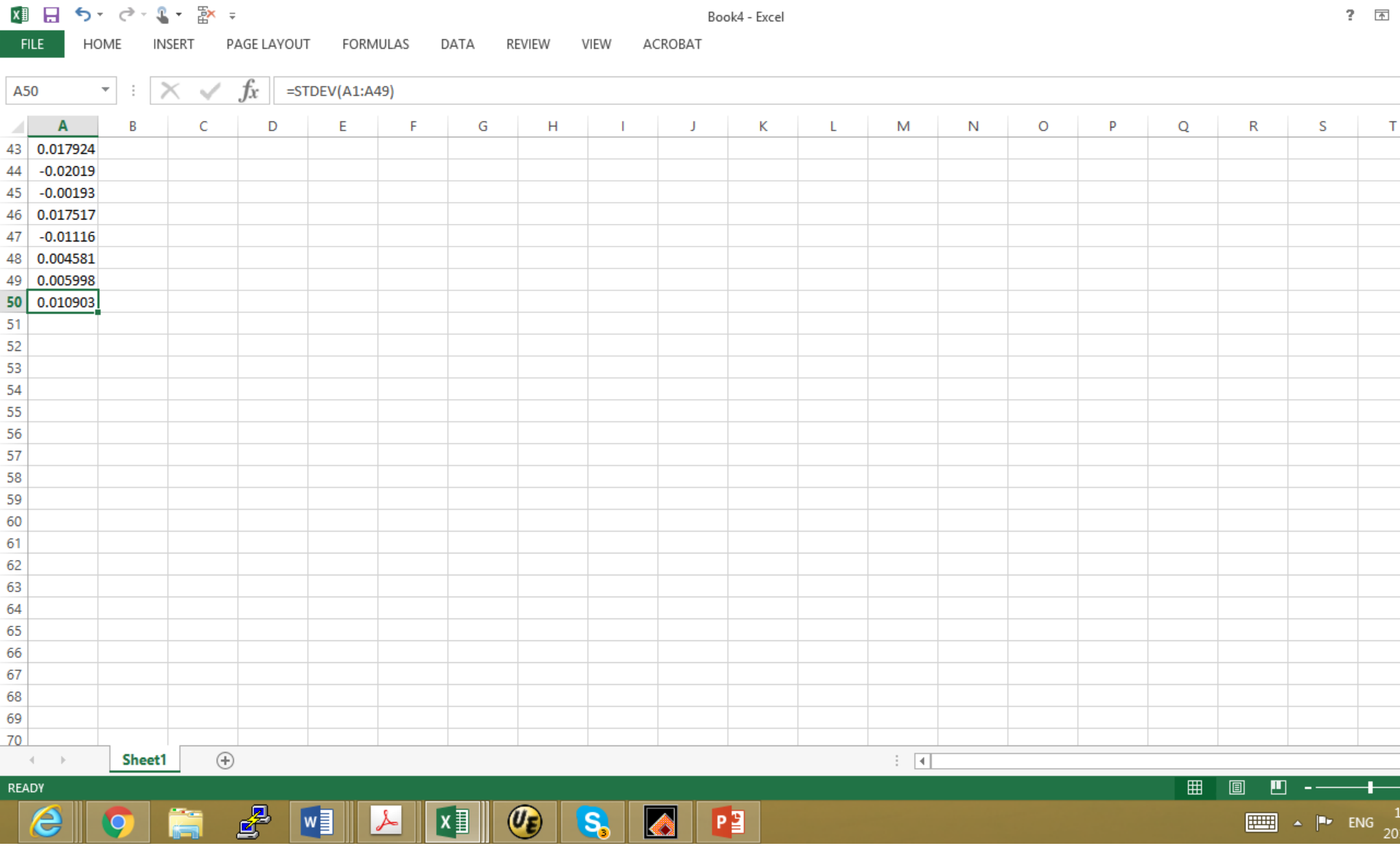


Peak overlap data | TGA data | Sheet3

READY

ENG

We can use the STDEV function (in another worksheet as needed) to calculate the noise in the data. This is shown below. Note that there are 50 data points in the file.



Using the estimate for the noise the value of chi-squared can be estimated and is given in cell L9 in this sheet. This step is essential for Solver to work.

tutorial_6_gaussians_B [Compatibility Mode] - Excel

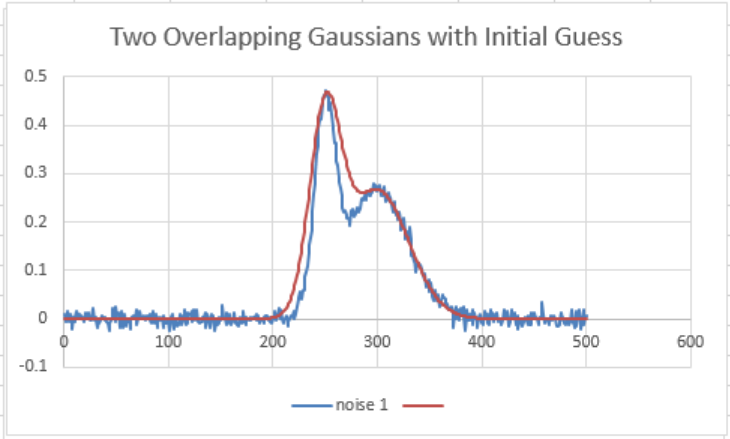
FILE HOME INSERT PAGE LAYOUT FORMULAS DATA REVIEW VIEW ACROBAT

L9 {=SQRT(SUM(F2:F502^2))/SQRT(500)/0.0109}

Formula Bar

	A	B	C	D	E	F	H	I	J	K	L	M	N	O	P	Q
1	PEAK OVERLAP DATA		noise 1	noise 2												
2		0	0.009773	-0.00093	5.1297E-23	-0.00977	The two spectra represent the same signal but with a different noise level									
3		1	0.00821	-0.00059	7.1551E-23	-0.00821	Column A is e.g. elution time or scattering angle or frequency									
4		2	-0.00631	0.000472	9.9692E-23	0.006312	First make a graph of both									
5		3	0.004791	-0.00053	1.3875E-22	-0.00479	Fit both data sets with a combination of two Gaussians using the solver									
6		4	0.01636	0.000614	1.9288E-22	-0.01636										
7		5	-0.00495	0.000613	2.6785E-22	0.004947	15	250	15							
8		6	0.010262	-0.00042	3.7153E-22	-0.01026	20	300	30							
9		7	-0.00261	0.000746	5.1479E-22	0.002614					2.791264					
10		8	-0.02278	-0.0006	7.1248E-22	0.02278										
11		9	0.002571	-0.00029	9.85E-22	-0.00257										
12		10	-0.00437	-0.00027	1.3602E-21	0.004368										
13		11	0.002607	0.000603	1.8763E-21	-0.00261										
14		12	0.015395	-0.00041	2.5854E-21	-0.01539										
15		13	0.007243	0.000352	3.5585E-21	-0.00724										
16		14	0.001776	0.000526	4.8923E-21	-0.00178										
17		15	0.008453	0.000182	6.7186E-21	-0.00845										
18		16	0.005783	-0.00031	9.2165E-21	-0.00578										
19		17	-0.00068	0.000773	1.2629E-20	0.000684										
20		18	0.004804	0.000701	1.7286E-20	-0.0048										
21		19	-0.0052	0.00044	2.3633E-20	0.005205										
22		20	0.013383	0.000968	3.2276E-20	-0.01338										
23		21	0.002537	-0.00053	4.4031E-20	-0.00254										
24		22	0.002272	0.000315	5.9999E-20	-0.00227										
25		23	0.012812	-0.00051	8.1668E-20	-0.01281										
26		24	0.010398	0.000281	1.1104E-19	-0.0104										
27		25	-0.0024	0.000344	1.5081E-19	0.002396										

χ^2

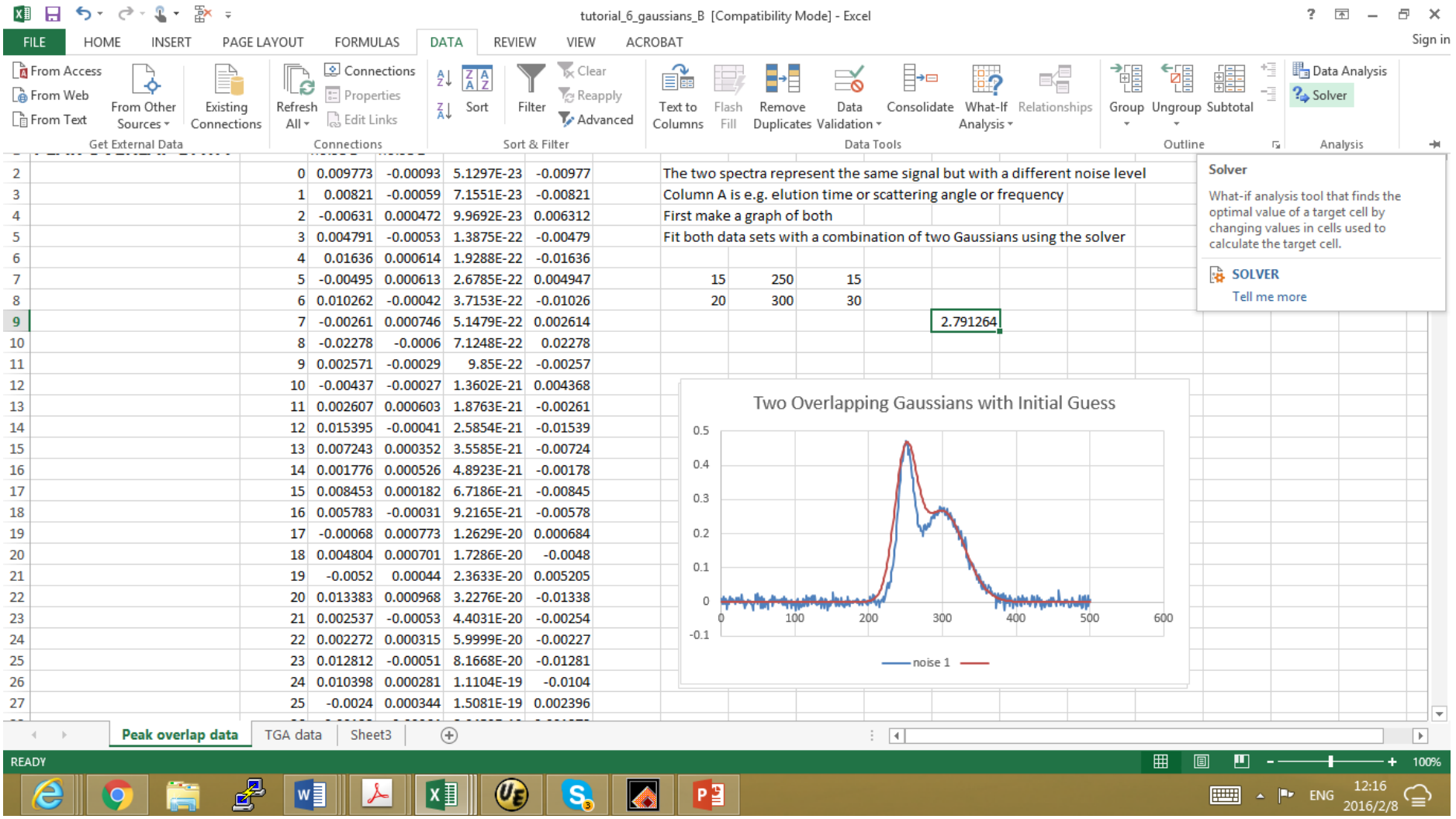


Peak overlap data | TGA data | Sheet3

READY

ENG

Then we run Solver, which will alter the parameters given in the 6 cells indicated previously to minimize the value of chi-squared. If you cannot find Solver then you need to install the Add-in as shown in a previous segment.



2	0	0.009773	-0.00093	5.1297E-23	-0.00977
3	1	0.00821	-0.00059	7.1551E-23	-0.00821
4	2	-0.00631	0.000472	9.9692E-23	0.006312
5	3	0.004791	-0.00053	1.3875E-22	-0.00479
6	4	0.01636	0.000614	1.9288E-22	-0.01636
7	5	-0.00495	0.000613	2.6785E-22	0.004947
8	6	0.010262	-0.00042	3.7153E-22	-0.01026
9	7	-0.00261	0.000746	5.1479E-22	0.002614
10	8	-0.02278	-0.0006	7.1248E-22	0.02278
11	9	0.002571	-0.00029	9.85E-22	-0.00257
12	10	-0.00437	-0.00027	1.3602E-21	0.004368
13	11	0.002607	0.000603	1.8763E-21	-0.00261
14	12	0.015395	-0.00041	2.5854E-21	-0.01539
15	13	0.007243	0.000352	3.5585E-21	-0.00724
16	14	0.001776	0.000526	4.8923E-21	-0.00178
17	15	0.008453	0.000182	6.7186E-21	-0.00845
18	16	0.005783	-0.00031	9.2165E-21	-0.00578
19	17	-0.00068	0.000773	1.2629E-20	0.000684
20	18	0.004804	0.000701	1.7286E-20	-0.0048
21	19	-0.0052	0.00044	2.3633E-20	0.005205
22	20	0.013383	0.000968	3.2276E-20	-0.01338
23	21	0.002537	-0.00053	4.4031E-20	-0.00254
24	22	0.002272	0.000315	5.9999E-20	-0.00227
25	23	0.012812	-0.00051	8.1668E-20	-0.01281
26	24	0.010398	0.000281	1.1104E-19	-0.0104
27	25	-0.0024	0.000344	1.5081E-19	0.002396

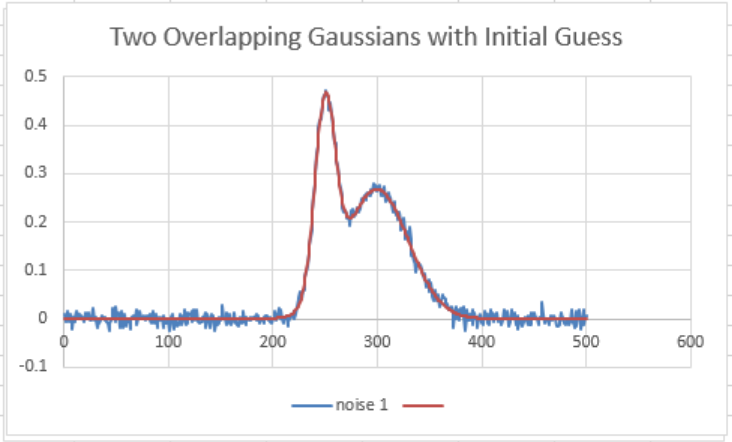
Note that the Gaussians have been fit reasonably well and the value of chi-squared is 0.9. If the estimate for the noise were perfect then chi-squared should be 1.0

tutorial_6_gaussians_B [Compatibility Mode] - Excel

FILE HOME INSERT PAGE LAYOUT FORMULAS DATA REVIEW VIEW ACROBAT

{=SQRT(SUM(F2:F502^2))/SQRT(500)/0.0109}

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q
1	**PEAK OVERLAP DATA**		noise 1	noise 2													
2		0	0.009773	-0.00093	1.8637E-22	-0.00977		The two spectra represent the same signal but with a different noise level									
3		1	0.00821	-0.00059	2.5791E-22	-0.00821		Column A is e.g. elution time or scattering angle or frequency									
4		2	-0.00631	0.000472	3.5652E-22	0.006312		First make a graph of both									
5		3	0.004791	-0.00053	4.923E-22	-0.00479		Fit both data sets with a combination of two Gaussians using the solver									
6		4	0.01636	0.000614	6.7906E-22	-0.01636											
7		5	-0.00495	0.000613	9.3565E-22	0.004947		9.747989	249.8944	9.839749							
8		6	0.010262	-0.00042	1.2878E-21	-0.01026		20.39415	299.4154	30.33281							
9		7	-0.00261	0.000746	1.7706E-21	0.002614						0.9195					
10		8	-0.02278	-0.0006	2.4316E-21	0.02278											
11		9	0.002571	-0.00029	3.3359E-21	-0.00257											
12		10	-0.00437	-0.00027	4.5715E-21	0.004368											
13		11	0.002607	0.000603	6.258E-21	-0.00261											
14		12	0.015395	-0.00041	8.5573E-21	-0.01539											
15		13	0.007243	0.000352	1.1689E-20	-0.00724											
16		14	0.001776	0.000526	1.5949E-20	-0.00178											
17		15	0.008453	0.000182	2.1738E-20	-0.00845											
18		16	0.005783	-0.00031	2.9595E-20	-0.00578											
19		17	-0.00068	0.000773	4.025E-20	0.000684											
20		18	0.004804	0.000701	5.4681E-20	-0.0048											
21		19	-0.0052	0.00044	7.4205E-20	0.005205											
22		20	0.013383	0.000968	1.0059E-19	-0.01338											
23		21	0.002537	-0.00053	1.3621E-19	-0.00254											
24		22	0.002272	0.000315	1.8424E-19	-0.00227											
25		23	0.012812	-0.00051	2.4894E-19	-0.01281											
26		24	0.010398	0.000281	3.36E-19	-0.0104											
27		25	-0.0024	0.000344	4.53E-19	0.002396											

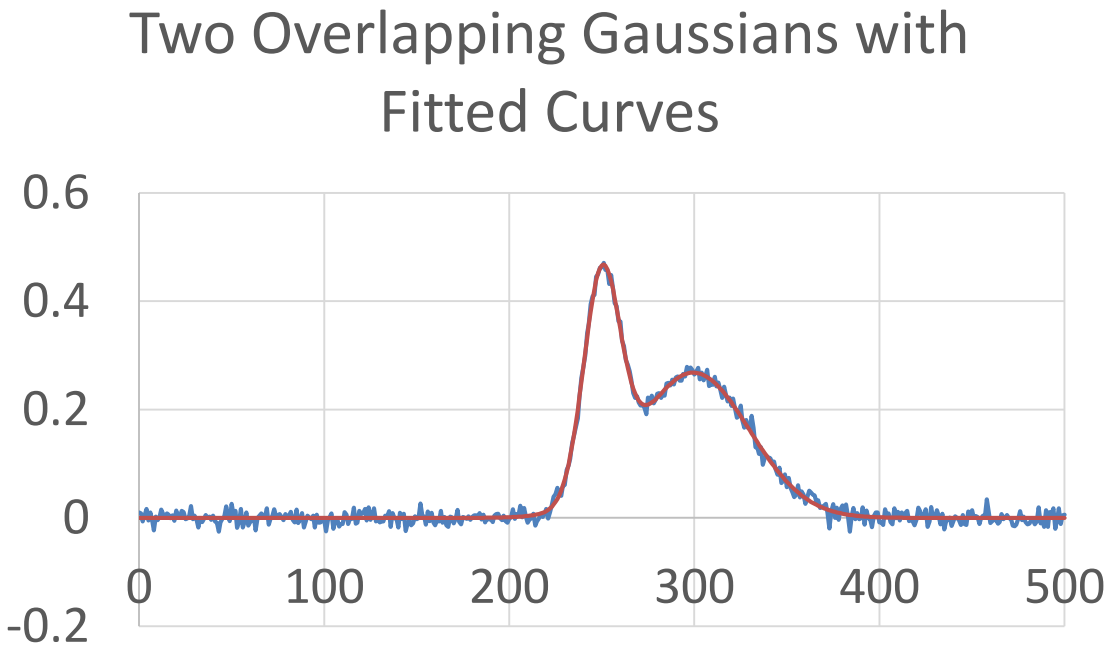


Peak overlap data | TGA data | Sheet3

READY

ENG

We focus on the fit. Now if we subtract the fitted function from the data we will obtain the residuals.



Amplitude	Position	Width
9.75	250.0	9.84
20.4	299.0	30.3

In this case the residuals have the appearance of noise. They have no structure. This is an indication of a good fit as well.