

XPS & NEXAFS data analysis code: **Ctrl+Q**

- efficient and effective analysis ever experienced -

Hideki NAKAJIMA

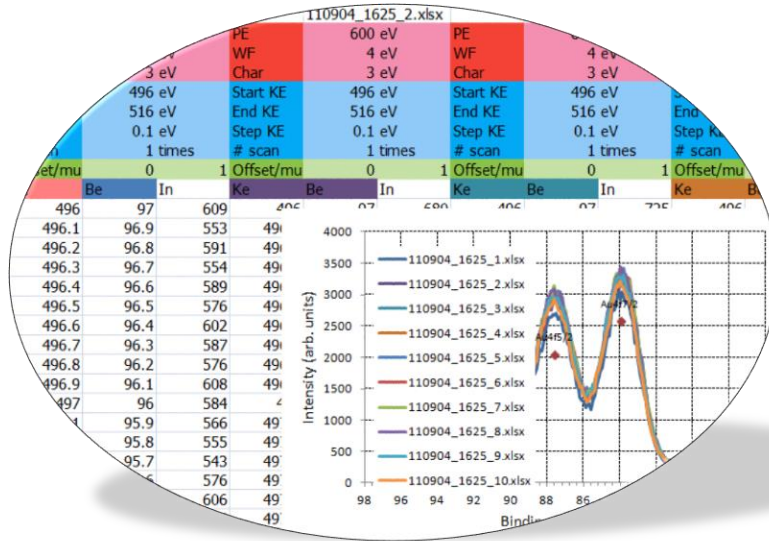
heitler@gmail.com

github: heitler/xps-excel-macro

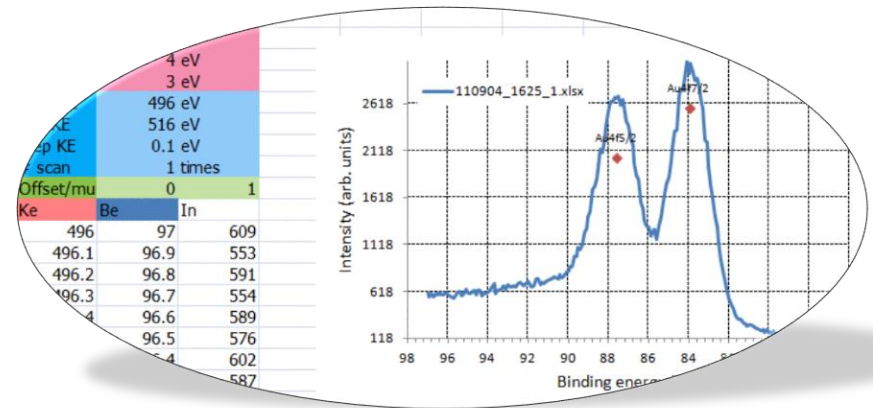
18 Oct. 2018

Brief

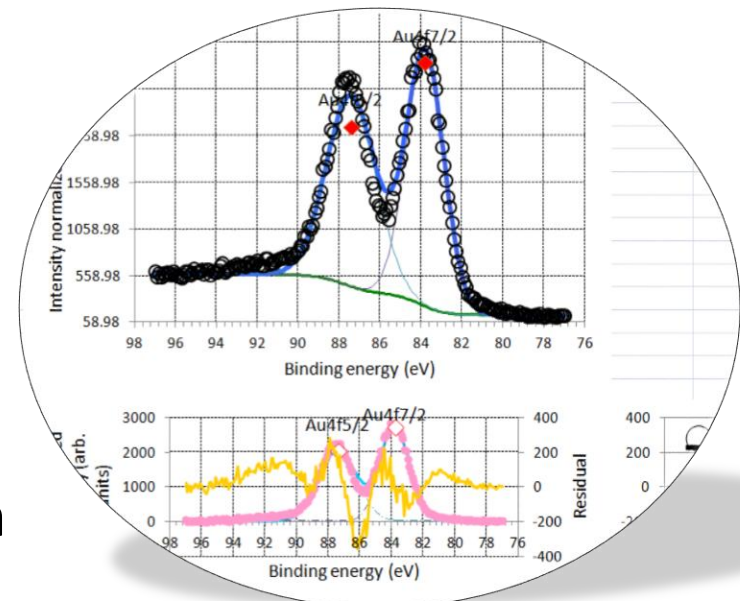
Plot with binding energy
Identify elements and states



Curve fitting and BG subtraction



Energy and intensity calibrations





Preface


- **Ctrl+Q** is the first comprehensive data-analysis code for **SR-XPS** and **XAS** working on Windows Office **Excel 2007 or later**. Mac **Excel 2016** works great now.
- Ctrl+Q will analyze the data by just pressing the shortcut key: **Ctrl + q**.
- It works great in publication quality.
 - Carbon, JPAP, ASS, ACS AMI, SAB, RCS Adv. etc. from the data obtained at BL3.2Ua and 5.3 in SPL
- **GitHub: xps-excel-macro** for updated info.

 [heitler / xps-excel-macro](#)


 Watch  Star  Fork

 Code

 Issues **0**

 Pull requests **0**

 Wiki

 Pulse

 Graphs

 Settings

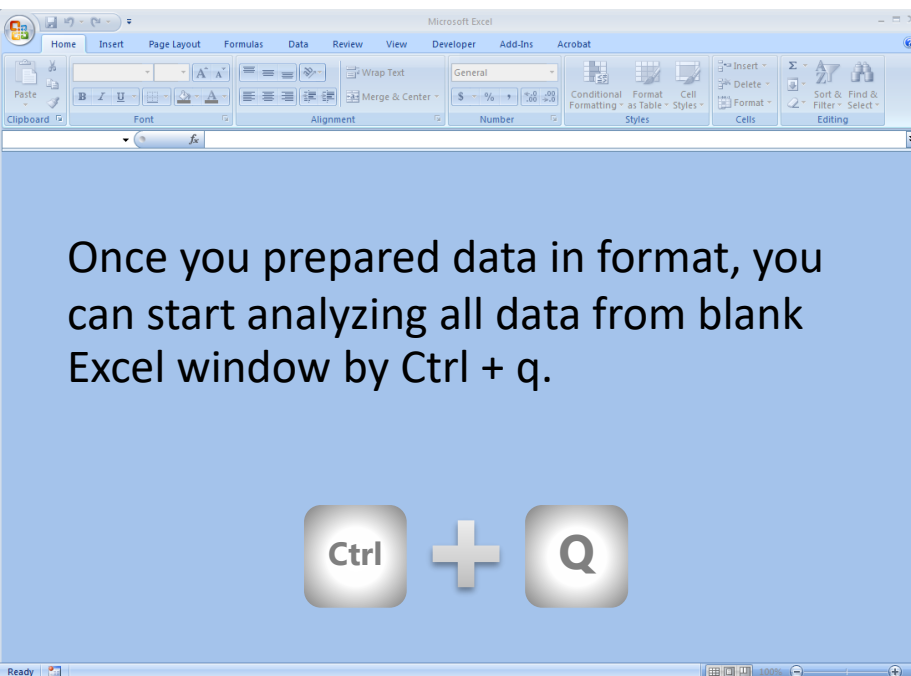
The VBA codes to be pasted in the personal macro workbook (Personal.xlsb) in Windows Office Excel 2007 - 2016 Visual Basic Editor (VBE) work with Solver for spectral analysis and curve fitting of the synchrotron-based soft x-ray photoemission (XPS) and absorption (XAS) spectra.

— Edit

Data preparation

	A	B
1	KE/eV	Scan#1
2	496	19.69872
3	496.1	17.95129
4	496.2	19.18263
5	496.3	18.03784
6	496.4	19.03867
7	496.5	18.80417
8	496.6	18.22572

- Two-column data in the spreadsheet format are analyzed in the code.
- Worksheet is named after workbook filename.
- Syntax in A1 cell corresponds to the following.



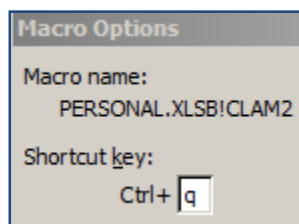
Once you prepared data in format, you can start analyzing all data from blank Excel window by Ctrl + q.

Ctrl + **Q**

Syntax in A1 cell	Data in column A	Data in column B
KE/eV	KE	XPS
BE/eV	BE	XPS
PE/eV	PE	XAS
GE/eV	PE	G scan
AE/eV	EE	Auger
QE/eV	mass	Q-mass
ME/eV	Position	Any

Installation of the code in Excel

- Generate **Personal Workbook Macro**
- Install **Solver** Add-in and setup its DLL
- Setup the **Shortcut key** in Macro Option



- Compile your own **database** for BE and sensitivities on UD.xlsx

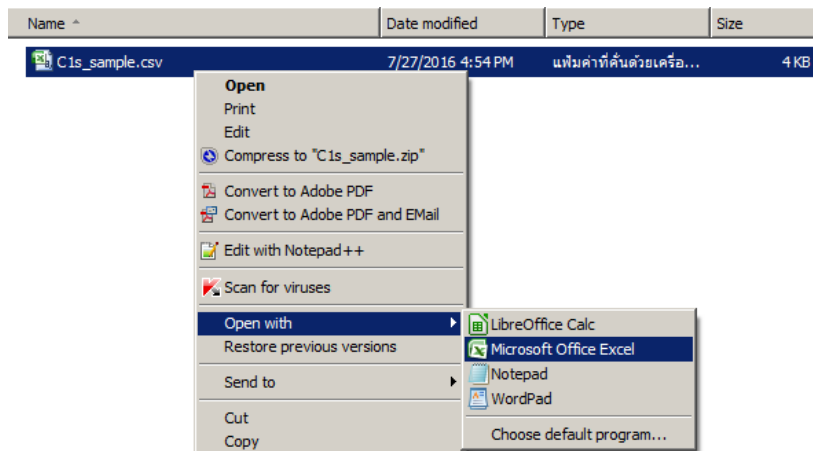
XPS worksheet

	A	B	C	D
1	Element	Orbit	BE(eV)	ASF
2	C	1s	284.6	1
3	O	1s	532	2.93

AES worksheet

	A	B	C	D
1	Element	Auger	KE(eV)	RSF
2	C	KLL	266	0.6
3	O	KLL	506	0.96

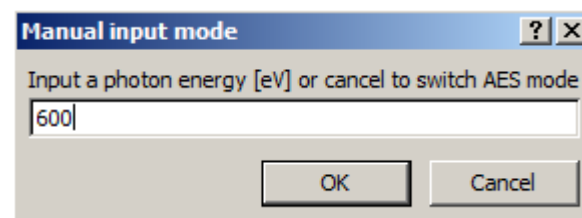
C1s sample csv



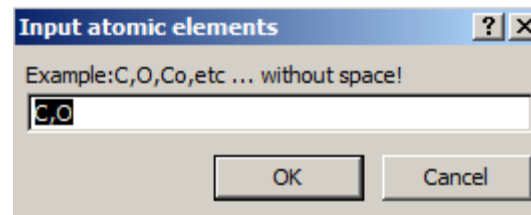
	A	B
1	KE/eV	PE: 600 eV
2	290	1709
3	290.1	1798
4	290.2	1845
5	290.3	1722
6	290.4	1729
7	290.5	1699
8	290.6	1727
9	290.7	1693
10	290.8	1647
11	290.9	1684
12	291	1650



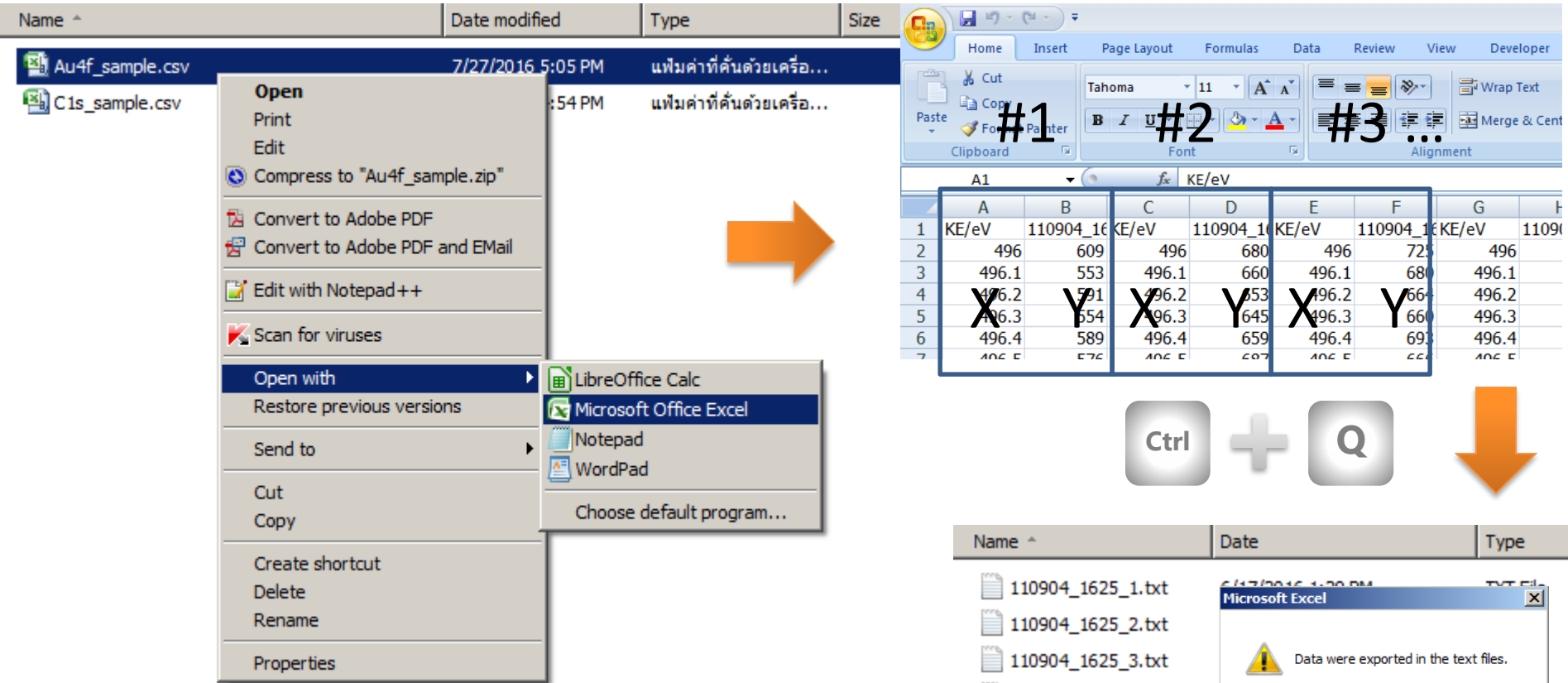
600 eV of photon energy














XPS: Carbon 1s spectrum



Sample file with multiple scans



- Download Au4f_sample.csv including 100 spectra.
- Open it with Excel as shown above.
- Export 100 text files by shortcut keys: Ctrl+Q.

Name ^	Date	Type
 110904_1625_1.txt	6/17/2016 1:29 PM	TXT File
 110904_1625_2.txt	6/17/2016 1:29 PM	TXT File
 110904_1625_3.txt	6/17/2016 1:29 PM	TXT File
 110904_1625_4.txt	6/17/2016 1:29 PM	TXT File
 110904_1625_5.txt	6/17/2016 1:29 PM	TXT File
 110904_1625_6.txt	6/17/2016 1:29 PM	TXT File
 110904_1625_7.txt	6/17/2016 1:29 PM	TXT File
 110904_1625_8.txt	6/17/2016 1:29 PM	TXT File
 110904_1625_9.txt	6/17/2016 1:29 PM	TXT File
 110904_1625_10.txt	6/17/2016 1:29 PM	TXT File
 110904_1625_11.txt	6/17/2016 1:29 PM	TXT File

Sample file includes single data

Name ^	Date modified	Type	Size
110904_1625_1.txt	7/27/2016 5:12 PM	TXT File	3 KB
110904_1625_2.txt		TXT File	3 KB
110904_1625_3.txt		TXT File	3 KB
110904_1625_4.txt		TXT File	3 KB
110904_1625_5.txt		TXT File	3 KB
110904_1625_6.txt		TXT File	3 KB
110904_1625_7.txt		TXT File	3 KB
110904_1625_8.txt		TXT File	3 KB
110904_1625_9.txt		TXT File	3 KB
110904_1625_10.txt		TXT File	3 KB
110904_1625_11.txt		TXT File	3 KB
110904_1625_12.txt		TXT File	3 KB
110904_1625_13.txt		TXT File	3 KB
110904_1625_14.txt		TXT File	3 KB
110904_1625_15.txt		TXT File	3 KB
110904_1625_16.txt		TXT File	3 KB
110904_1625_17.txt		TXT File	3 KB
110904_1625_18.txt		TXT File	3 KB

Open
Edit
Compress to "110904_1625_1.zip"
Convert to Adobe PDF
Combine supported files in Acrobat...
Edit with Notepad++
Scan for viruses

Open with
Restore previous versions

Send to

Cut
Copy

Create shortcut
Delete
Rename

Properties

Adobe Illustrator CS6
LibreOffice Calc
LibreOffice Writer
Mery
Microsoft Office Excel
Notepad
Notepad++ : a free (GNU) source co
WordPad

Choose default program...



	A	B
1	KE/eV	110904_16
2	496	609
3	496.1	553
4	496.2	591
5	496.3	554
6	496.4	589
7	496.5	576
8	496.6	602
9	496.7	587
10	496.8	576
11	496.9	608
12	497	594

Single data to plot in Graph sheet

	A	B
1	KE/eV	110904.16
2	496	609
3	496.1	553
4	496.2	591
5	496.3	554
6	496.4	589
7	496.5	576
8	496.6	602
9	496.7	587
10	496.8	576
11	496.9	608
12	497	594

KE/eV represents a kinetic energy scale.



600 eV of photon energy



Manual input mode ? X

Input a photon energy [eV] or cancel to switch AES mode

600

OK Cancel

Sample: Gold metal foil



Input atomic elements ? X

Example: C,O,Co,etc ... without space!

Au

OK Cancel

Note that Au4f sensitivity is not in database, so you have to input factors in database in a way below.

Au 4f BE and ASF
in XPS worksheet on UD.xlsx



	A	B	C	D
1	Element	Orbit	BE(eV)	ASF
2	C	1s	284.6	1
3	O	1s	532	2.93
4	Au	4f5/2	87.6	7.54
5	Au	4f7/2	84	9.58

[illegible]

Intensity (arb. units)

110904_1625_1.xlsx

Au4f5/2

Au4f7/2

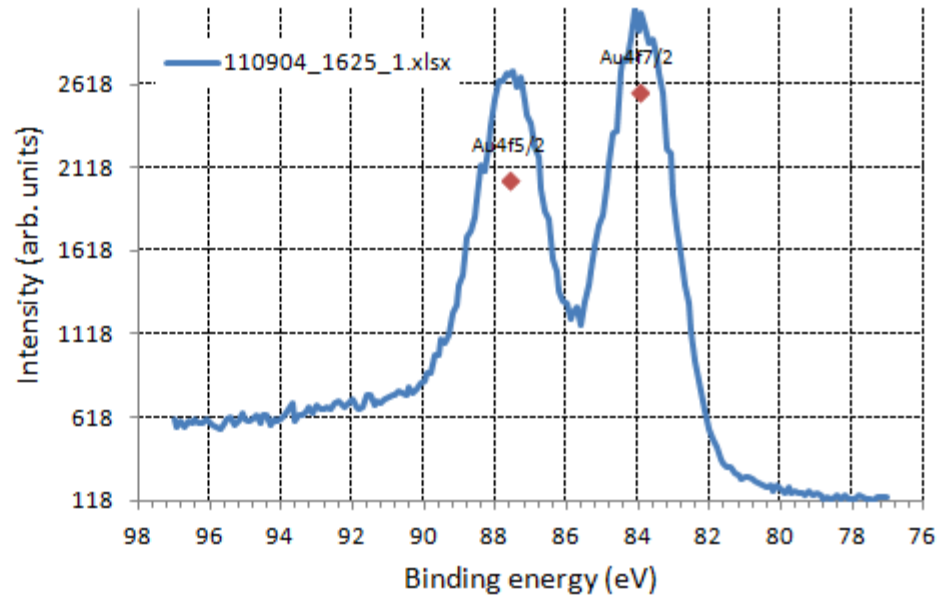
KE plot

Kinetic energy (eV)

Reference spectrum

Grating	0 lines/mm		
PE	600 eV		
WF	4 eV		
Char	3 eV		
Start KE	496 eV		
End KE	516 eV		
Step KE	0.1 eV		
# scan	1 times		
Offset/mu	0	1	
Ke	Be	In	
496	97	609	
496.1	96.9	553	
496.2	96.8	591	
496.3	96.7	554	
496.4	96.6	589	
496.5	96.5	576	
496.6	96.4	602	
496.7	96.3	587	
496.8	96.2	576	

Standard peak BE should be well-known and assumed to be identical with exp.

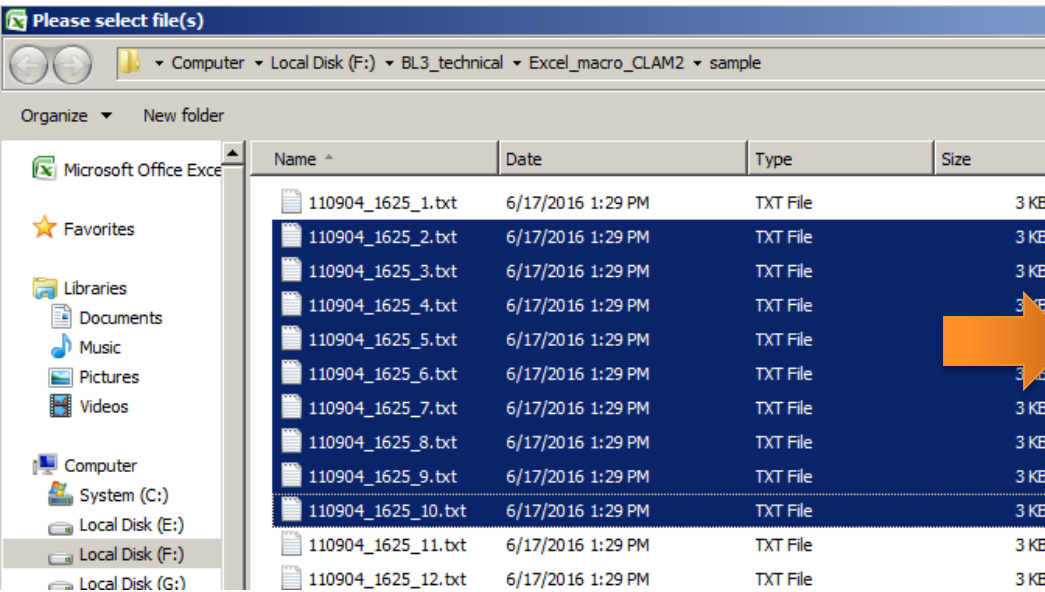


Next, apply these factors to another by “debug” in A1 cell then



	A	B	C
1	debug	0 lines/mm	
2	PE	600 eV	
3	WF	4 eV	
4	Char	3 eV	
5	Start KE	496 eV	
6	End KE	516 eV	
7	Step KE	0.1 eV	
8	# scan	1 times	
9	Offset/mu	0	1
10	Ke	Be	In

Multiple-file selection



Name	Date	Type	Size
110904_1625_1.txt	6/17/2016 1:29 PM	TXT File	3 KB
110904_1625_1.xlsx	6/17/2016 1:55 PM	แผ่นงาน Microsoft O...	53 KB
110904_1625_2.txt	6/17/2016 1:29 PM	TXT File	3 KB
110904_1625_2.xlsx	6/17/2016 2:02 PM	แผ่นงาน Microsoft O...	52 KB
110904_1625_3.txt	6/17/2016 1:29 PM	TXT File	3 KB
110904_1625_3.xlsx	6/17/2016 2:02 PM	แผ่นงาน Microsoft O...	12 KB
110904_1625_4.txt	6/17/2016 1:29 PM	TXT File	3 KB
110904_1625_4.xlsx	6/17/2016 2:02 PM	แผ่นงาน Microsoft O...	53 KB
110904_1625_5.txt	6/17/2016 1:29 PM	TXT File	3 KB
110904_1625_5.xlsx	6/17/2016 2:02 PM	แผ่นงาน Microsoft O...	53 KB
110904_1625_6.txt	6/17/2016 1:29 PM	TXT File	3 KB
110904_1625_6.xlsx	6/17/2016 2:02 PM	แผ่นงาน Microsoft O...	52 KB
110904_1625_7.txt	6/17/2016 1:29 PM	TXT File	3 KB
110904_1625_7.xlsx	6/17/2016 2:02 PM	แผ่นงาน Microsoft O...	52 KB
110904_1625_8.txt	6/17/2016 1:29 PM	TXT File	3 KB

Next, compare the spectra by “comp” in D1

	A	B	C	D
1	Grating	0 lines/mm	comp	
2	PE	600 eV		
3	WF	4 eV		
4	Char	3 eV		
5	Start KE	496 eV		
6	End KE	516 eV		
7	Step KE	0.1 eV		
8	# scan	1 times		
9	Offset/mu	0	1	
10	Ke	Be	In	
11	496	97	609	
12	496.1	96.9	553	
13	496.2	96.8	591	
14	496.3	96.7	554	
15	496.4	96.6	589	
16	496.5	96.5	576	
17	496.6	96.4	602	
18	496.7	96.3	587	



Name	Date modified	Type	Size
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110904_1625_2.xlsx	6/17/2016 2:02 PM	แผ่นงาน Microsoft O...	53 KB
110904_1625_3.xlsx	6/17/2016 2:02 PM	แผ่นงาน Microsoft O...	53 KB
110904_1625_4.xlsx	6/17/2016 2:02 PM	แผ่นงาน Microsoft O...	53 KB
110904_1625_5.xlsx	6/17/2016 2:02 PM	แผ่นงาน Microsoft O...	53 KB
110904_1625_6.xlsx	6/17/2016 2:02 PM	แผ่นงาน Microsoft O...	52 KB
110904_1625_7.xlsx	6/17/2016 2:02 PM	แผ่นงาน Microsoft O...	52 KB
110904_1625_8.xlsx	6/17/2016 2:02 PM	แผ่นงาน Microsoft O...	52 KB
110904_1625_9.xlsx	6/17/2016 2:02 PM	แผ่นงาน Microsoft O...	52 KB
110904_1625_10.xlsx	6/17/2016 2:02 PM	แผ่นงาน Microsoft O...	53 KB
sample.xlsx	6/17/2016 1:55 PM	แผ่นงาน Microsoft O...	181 KB

Compared spectra

Grating	0 lines/mm			110904_1625_2.xlsx			110904_1625_3.xlsx			110904_1625_4.xlsx	
PE	600 eV			PE	600 eV			PE	600 eV		
WF	4 eV			WF	4 eV			WF	4 eV		
Char	3 eV			Char	3 eV			Char	3 eV		
Start KE	496 eV			Start KE	496 eV			Start KE	496 eV		
End KE	516 eV			End KE	516 eV			End KE	516 eV		
Step KE	0.1 eV			Step KE	0.1 eV			Step KE	0.1 eV		
# scan	1 times			# scan	1 times			# scan	1 times		
Offset/ μ	0	1		Offset/ μ	0	1		Offset/ μ	0	1	
Ke	Be	In		Ke	Be	In		Ke	Be	In	
496	97	609		496	97	609		496	97	609	
496.1	96.9	553	496	96.9	553	496	96.9	553	496	96.9	553
496.2	96.8	591	496	96.8	591	496	96.8	591	496	96.8	591
496.3	96.7	554	496	96.7	554	496	96.7	554	496	96.7	554
496.4	96.6	589	496	96.6	589	496	96.6	589	496	96.6	589
496.5	96.5	576	496	96.5	576	496	96.5	576	496	96.5	576
496.6	96.4	602	496	96.4	602	496	96.4	602	496	96.4	602
496.7	96.3	587	496	96.3	587	496	96.3	587	496	96.3	587
496.8	96.2	576	496	96.2	576	496	96.2	576	496	96.2	576
496.9	96.1	608	496	96.1	608	496	96.1	608	496	96.1	608
497	96	584	497	96	584	497	96	584	497	96	584
497.1	95.9	566	497	95.9	566	497	95.9	566	497	95.9	566
497.2	95.8	555	497	95.8	555	497	95.8	555	497	95.8	555
497.3	95.7	543	497	95.7	543	497	95.7	543	497	95.7	543
497.4	95.6	576	497	95.6	576	497	95.6	576	497	95.6	576
497.5	95.5	606	497	95.5	606	497	95.5	606	497	95.5	606
497.6	95.4	614	497	95.4	614	497	95.4	614	497	95.4	614
497.7	95.3	575	497	95.3	575	497	95.3	575	497	95.3	575

Intensity (arb. units)

Binding energy (eV)

Au 4f5/2

Au 4f7/2

110904_1625_1.xlsx

110904_1625_2.xlsx

110904_1625_3.xlsx

110904_1625_4.xlsx

110904_1625_5.xlsx

110904_1625_6.xlsx

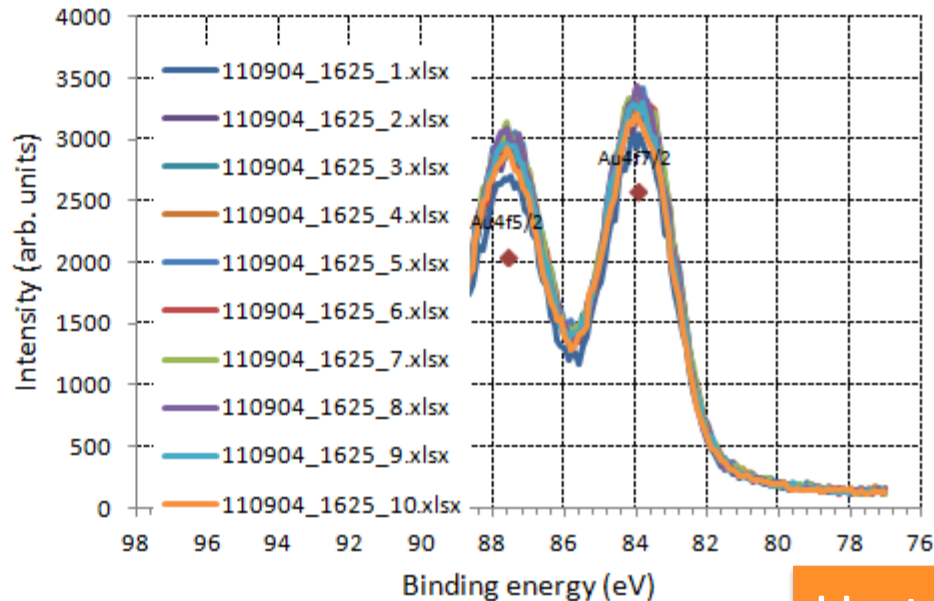
110904_1625_7.xlsx

110904_1625_8.xlsx

110904_1625_9.xlsx

110904_1625_10.xlsx

Up to



Up to 100 spectra
for BE&KE plots

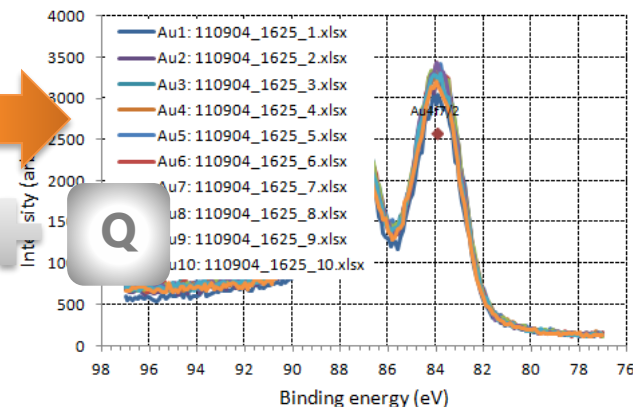
Analysis on spectra compared

- Automatically scaled spectra for comparison
 - “auto” in A1 cell to scale at the both ends
 - “auto[x1:x2,x3:x4]” in A1 cell to scale in the ranges of (x1, x2) for offset (0) and (x3, x4) for multiple (1).
 - “auto{284.6}” in A1 cell to shift the maximum intensity to 284.6 eV in BE scale.
 - “auto’-7.8” in A1 cell to set all char factor to be -7.8 eV.
- Annotate legends in each plot
 - “leg” in A1 cell to generate Sample sheet
 - Describe sample or spectrum name in the sheet
 - “leg” in A1 cell to run the code again.
- Normalize spectra with ref. spectrum by “norm” in A1 cell.
 - Second set of data will be selected for ref. and third set to be normalized data.
 - Norm sheet appears from the data normalized.

Every single step needs



	A	B	C		A	B	C	D	E
1	leg	0	lines/mm	1	No.	Name	Sep.	File name	
2	PE	600	eV	2	1	Au1	:	110904_1625_1.xlsx	
3	WF	4	eV	3	2	Au2	:	110904_1625_2.xlsx	
4	Char	3	eV	4	3	Au3	:	110904_1625_3.xlsx	
5	Start KE	496		5	4	Au4	:	110904_1625_4.xlsx	
6	End KE	516		6	5	Au5	:	110904_1625_5.xlsx	
7	Step KE	0.1	eV	7	6	Au6	:	110904_1625_6.xlsx	
8	# scan	1	times	8	7	Au7	:	110904_1625_7.xlsx	
9	Offset/mu	0		9	8	Au8	:	110904_1625_8.xlsx	
10	Ke	Be	In	10	9	Au9	:	110904_1625_9.xlsx	
11				11	10	Au10	:	110904_1625_10.xlsx	



Sample sheet

Edge correction in NEXAFS

	1	2	3	4	5	6	7	8	9
1	edge	1200	lines/mm		Pre edge	Post edge		170330_1456_Is_edge	
2	PE shifts	-0.17 eV		Start, eV	392	415	PE shifts	0 eV	
3	Smoothing	4 points		End, eV	397	429			
4					Polynomial coeff				
5	Start PE	390 eV		a0	0.078983	0.085857	Start PE	389.83 eV	
6	End PE	430 eV		a1	0.003787	0.001334	End PE	429.83 eV	
7	Step PE	0.1 eV		a2	-0.00071	0.002589	Step PE	0.1 eV	
8	# scan	1 times		a3	0	0			
9	Offset/mu	0	1	chi^2	7.03E-08	9.53E-07	Offset/mu	0	1
10	PE	Ab	De	PE	Pre-edge	Post-edge	Pe	Ab	De

Post-edge region to be 1

New spline edge correction

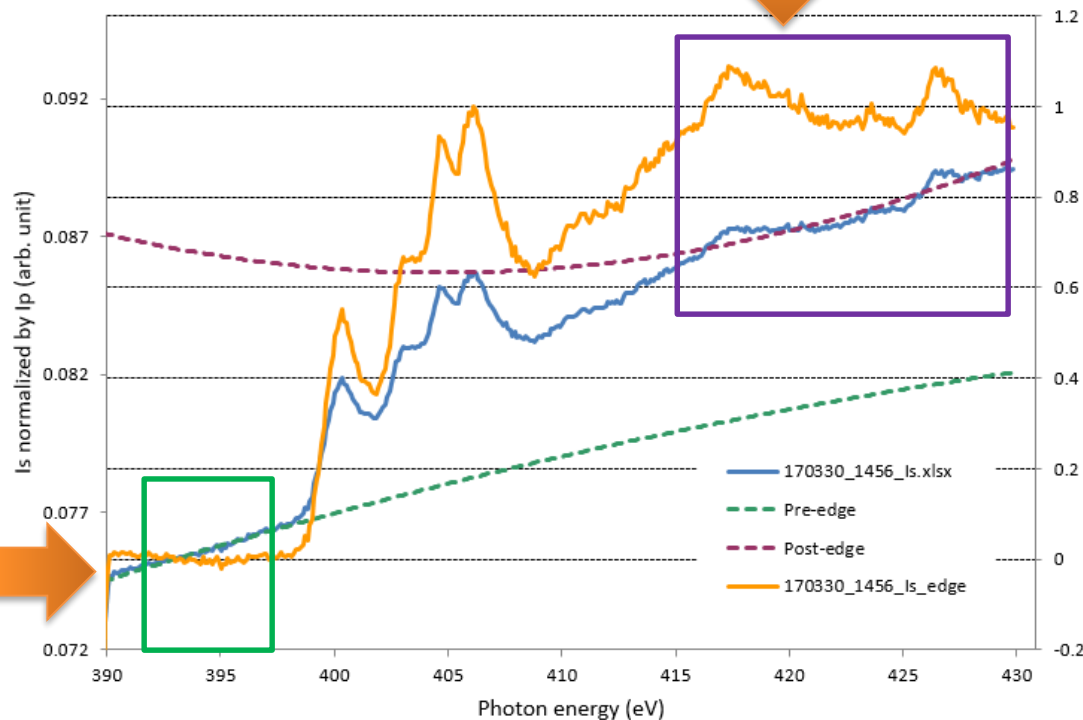
A1 cells: "edge"

New Linear combination

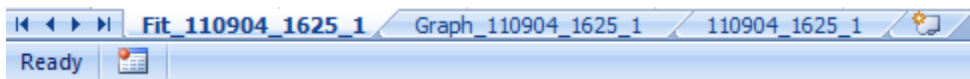
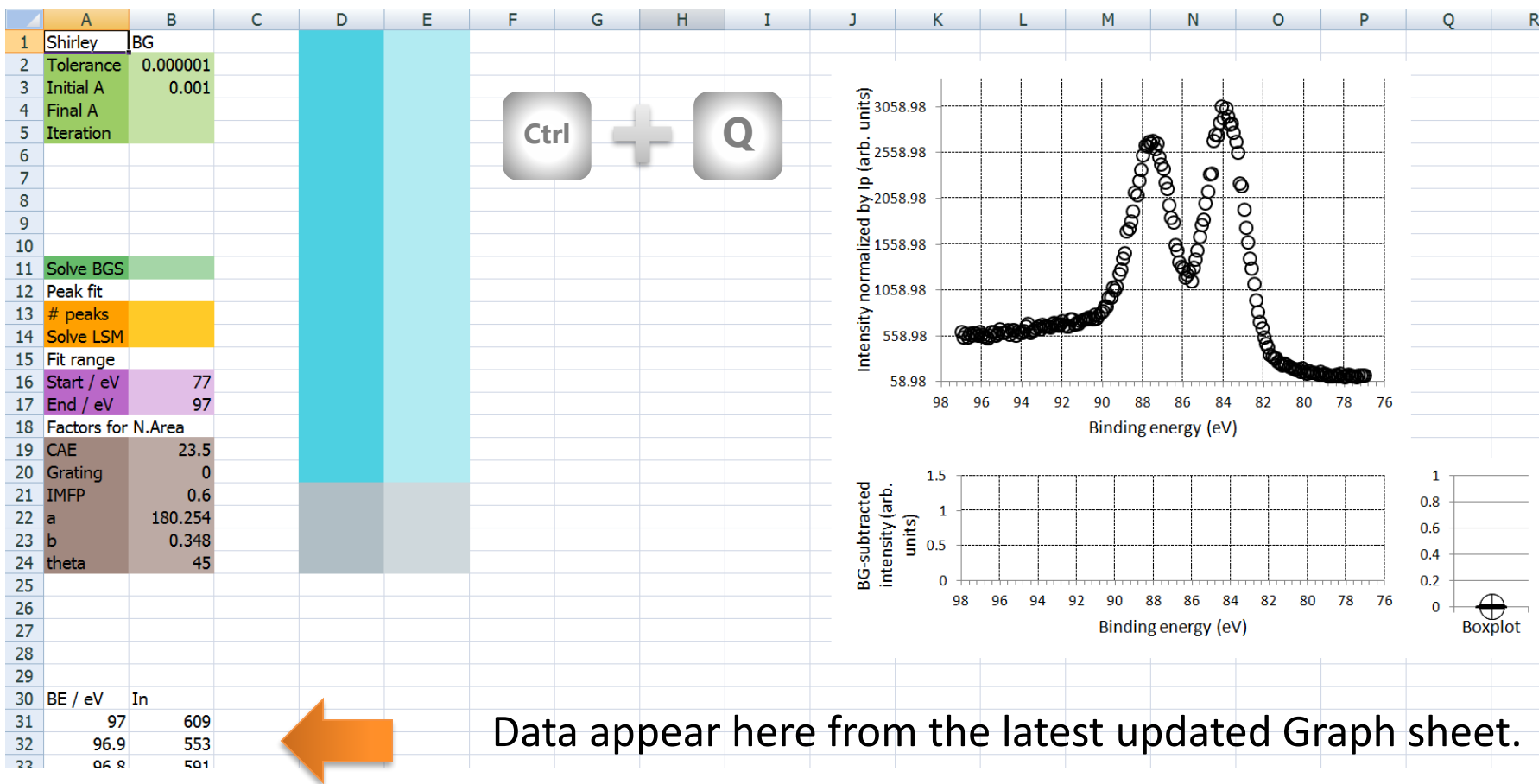
A1 cells: "lcmb"

After two references added.

Pre-edge regions to be 0



Fit sheet

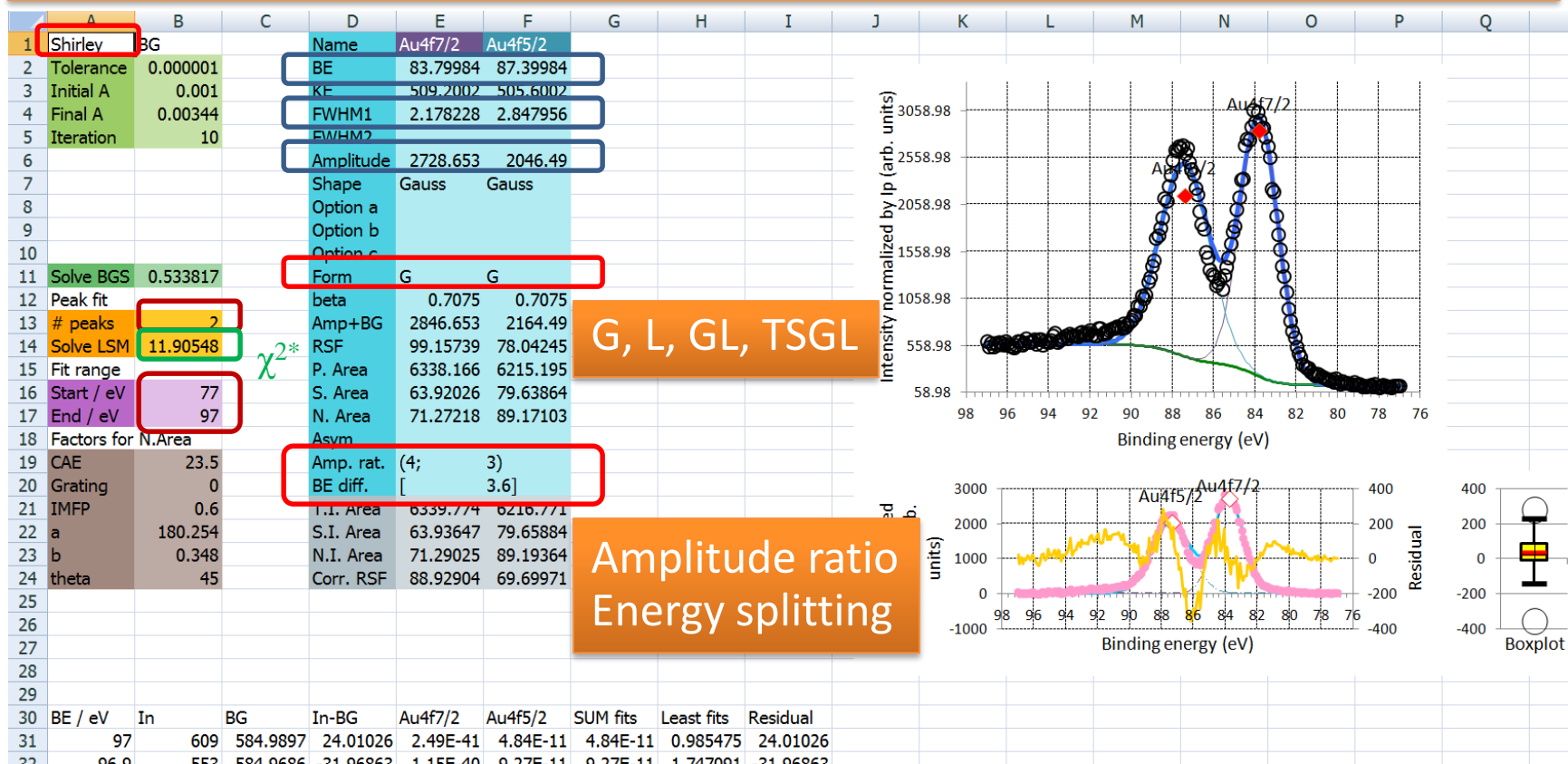


Switch the worksheet

Note that offset/multiple factors should be aligned for all spectra in Graph sheet to evaluate the peak area in Fit sheet.

Fitting functions and parameters

Shirley, Tougaard, Polynomial, Poly Shirley, Poly Tougaard, Victoreen, Arctan



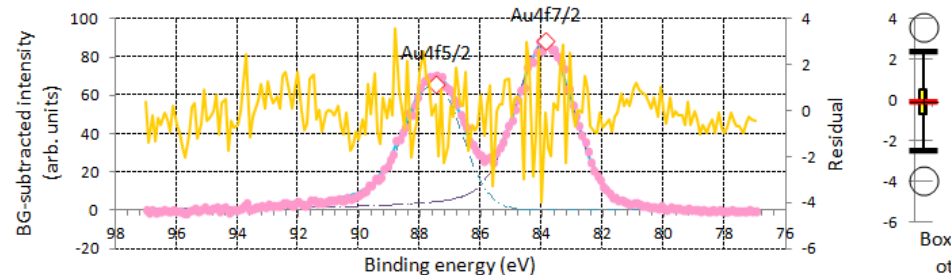
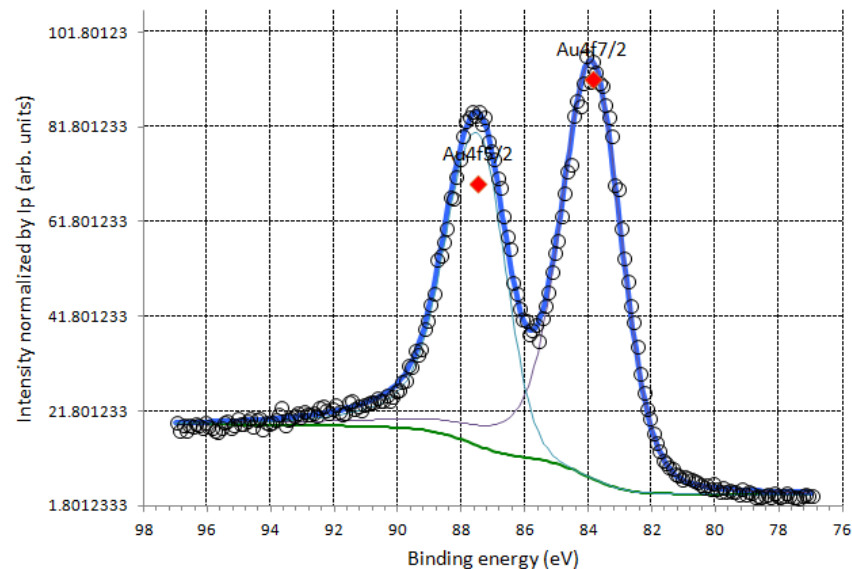
Update results by setup **constraints with bold font style**, various BGs or Forms



FWHM ranges can also be setup.

Peak shape: Tailed pseudo-Voigt

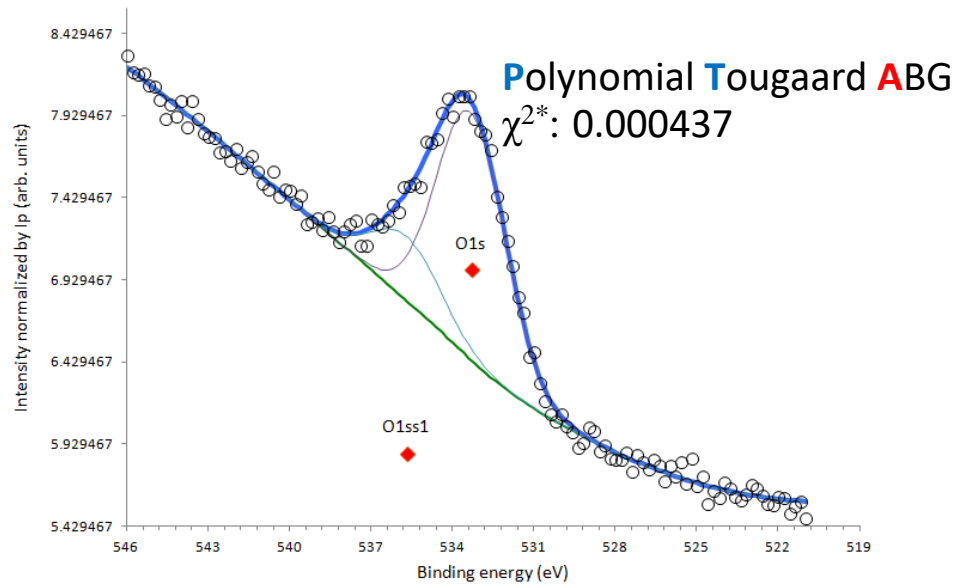
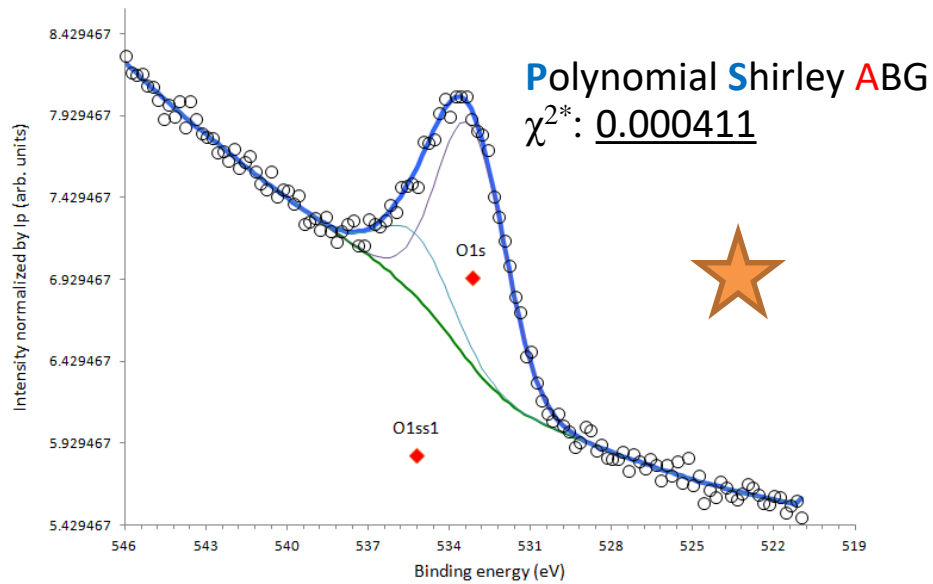
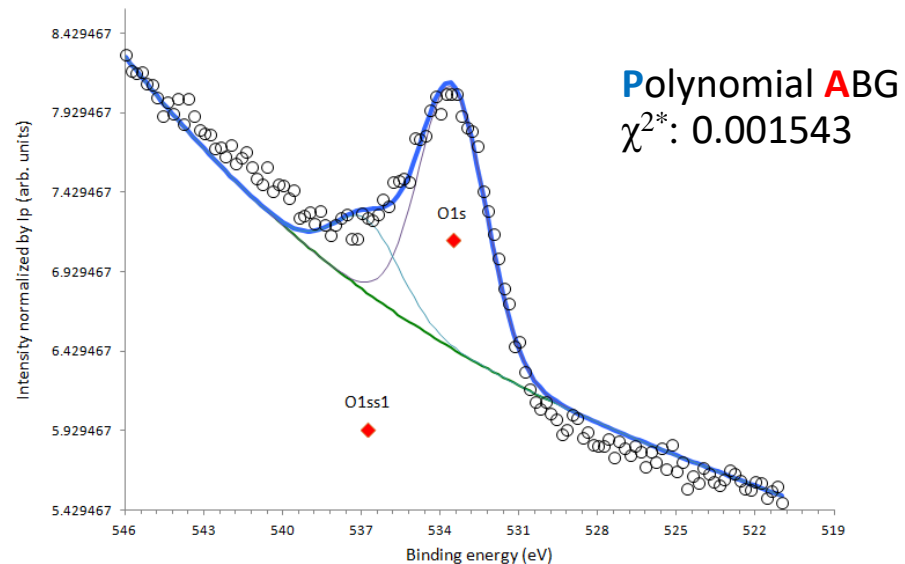
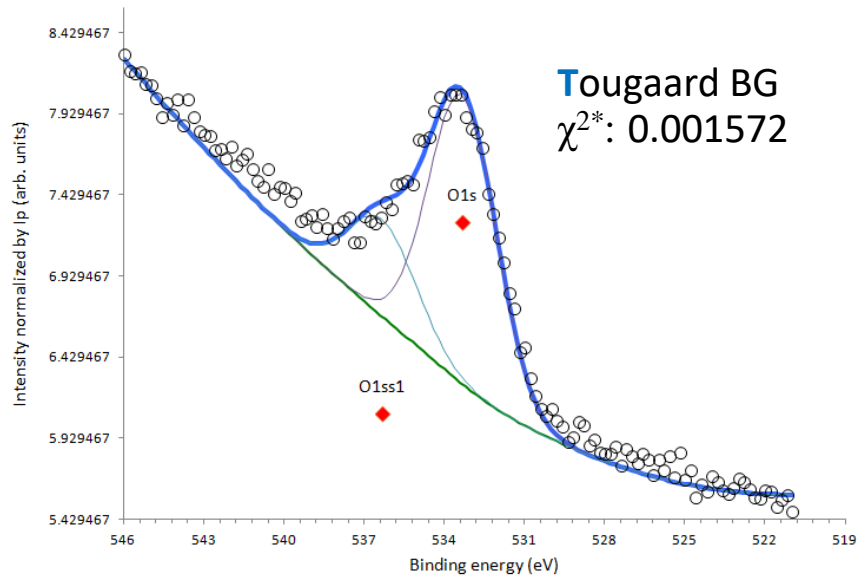
	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R	S
1	Shirley	BG		Name	Au4f7/2	Au4f5/2													
2	Tolerance	0.000001		BE	83.89177	87.49177													
3	Initial A	0.001		KE	509.1082	505.5082													
4	Final A	0.0036		FWHM1	2.192026	2.036631													
5	Iteration	3		FWHM2															
6				Amplitude	88.24273	66.18205													
7				Shape	0.207135	0.001													
8				Option a	0.0927	0.442394													
9				Option b	20.46306	11.55928													
10				Option c															
11	Solve BGS	0.01586		Form	TSGL	TSGL													
12	Peak fit			beta	0.7075	0.7075													
13	# peaks	2		Amp+BG	91.91117	69.85049													
14	Solve LSM	0.045204		RSF	99.15739	78.04245													
15	Fit range			P. Area	226.4484	143.8036													
16	Start / eV	77		S. Area	2.283727	1.842633													
17	End / eV	97		N. Area	2.546665	2.063409													
18	Factors for N.Area			Asym															
19	CAE	23.5		Amp. rat.	(4;	3)													
20	Grating	0		BE diff.	[3.6]													
21	IMFP	0.6		T.I. Area	240.0941	171.4606													
22	a	180.254		S.I. Area	2.421343	2.197018													
23	b	0.348		N.I. Area	2.700126	2.460255													
24	theta	45		Corr. RSF	88.91957	69.69223													
25																			
26																			
27																			
28																			
29																			
30	BE / eV	In	BG	In-BG	Au4f7/2	Au4f5/2	SUM fits	Least fits	Residual										
31		97	19.69872	18.94799	0.750731	0.271886	0.111915	0.383802	0.006965	0.36693									
32		96.9	17.95129	18.94713	-0.99584	0.278361	0.118642	0.397003	0.100289	-1.39284									
33		96.8	19.18263	18.94387	0.238762	0.285022	0.125775	0.410797	0.001529	-0.17204									
34		96.7	18.03784	18.94352	-0.90568	0.291876	0.133338	0.425214	0.091451	-1.3309									
35		96.6	19.03867	18.94303	0.095641	0.298928	0.141357	0.440284	0.006128	-0.34464									
36		96.5	18.80417	18.94164	-0.13747	0.306184	0.149859	0.456043	0.01816	-0.59352									



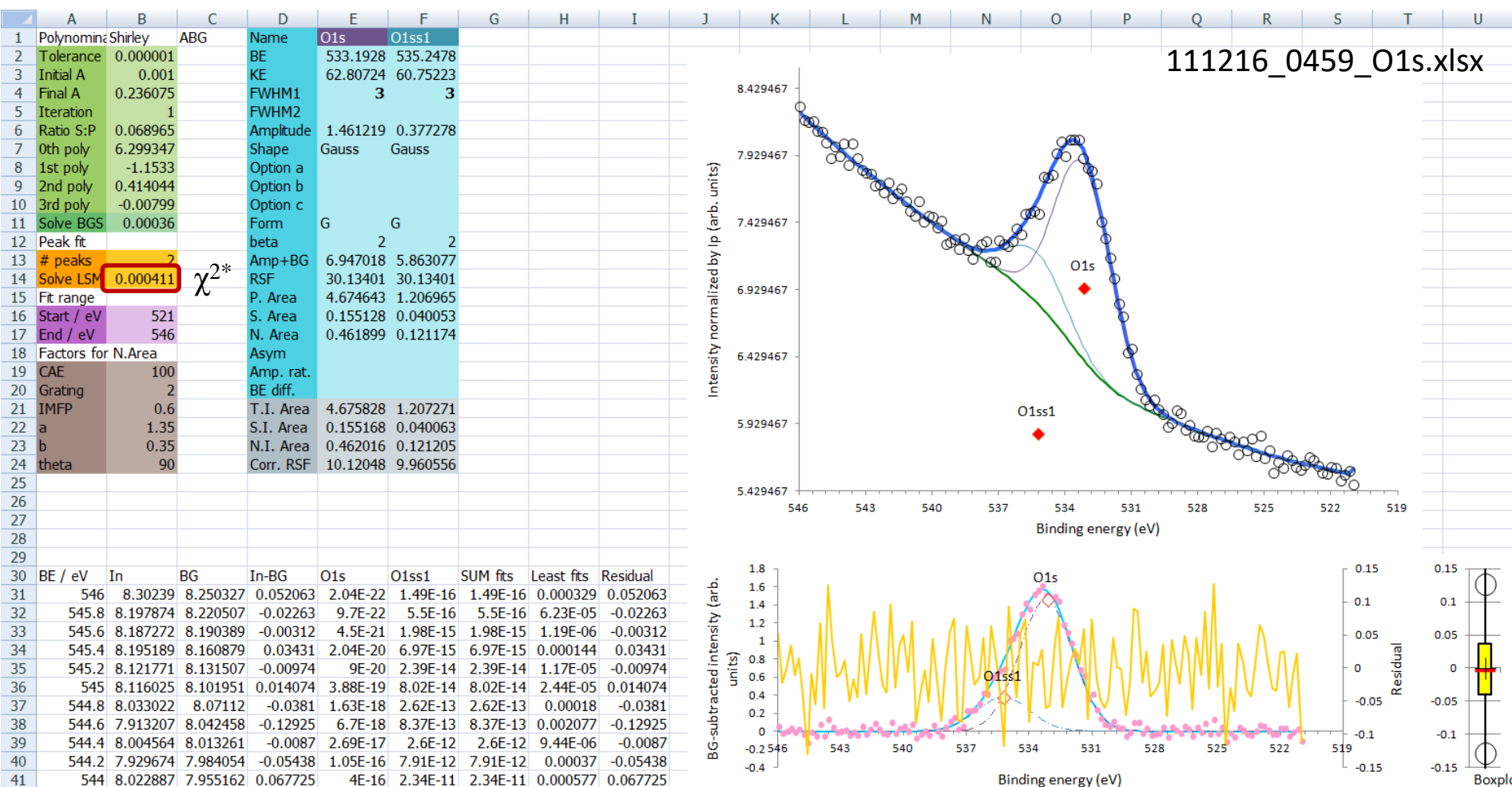
Shirley's BG, Tailed Voigt, Doublet 4f (4:3), Δ SO Au4f: 3.6 eV are used for above fitting. User-defined peak and BG functions can be easily implemented in your Visual Basic code.

Polynomial (Shirley or Tougaard)

Active-BGs



Poly Shirley ABG



3-eV FWHM Gaussian fit

Lists of fitting functions

Peak shapes (total 4 forms)

Code (form)	Shape	Option a	Option b
G (0)	Gauss		
L (1)	Lorentz		
<u>TSGL</u>	Exponential blend SGL	Tail scale	Tail length at half max
GL (0 < shape < 1)	G + L with the same FWHM		

Backgrounds (total 8 BGs)

BG (A1)	BG (B1)	BG (C1)	Technique	Optimization
Shirley	BG		XPS	Static
Tougaard	BG		XPS	Static
Polynomial	BG		XPS/XAS	Static
Polynomial	ABG		XPS/XAS	Active
Polynomial	Shirley	ABG	XPS	Active
Polynomial	Tougaard	ABG	XPS	Active
Victoreen	BG		XAS	Static
ArcTangent	BG		XAS	Active

Multiple data-fit

	A	B	C	D	E	F
1	Shirley	BG		debug	Au4f7/2	Au4f5/2
2	Tolerance	0.000001		BE	83.89131	87.49132
3	Initial A	0.001		KE	509.1087	505.5087
4	Final A	0.00344		FWHM1	2.196802	2.052602
5	Iteration	6		FWHM2		

“debug”/“debuga” in D1 cell

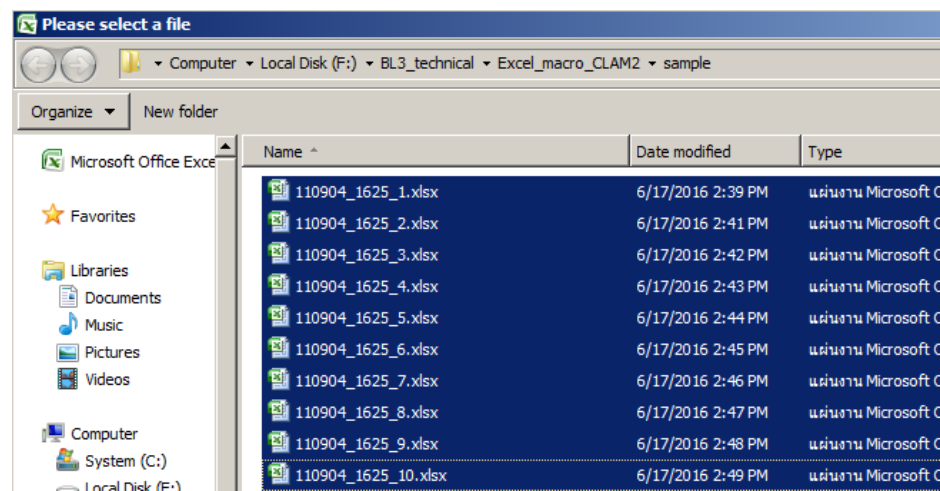
- debug: apply the original fit parameters
- debuga: apply those used just before



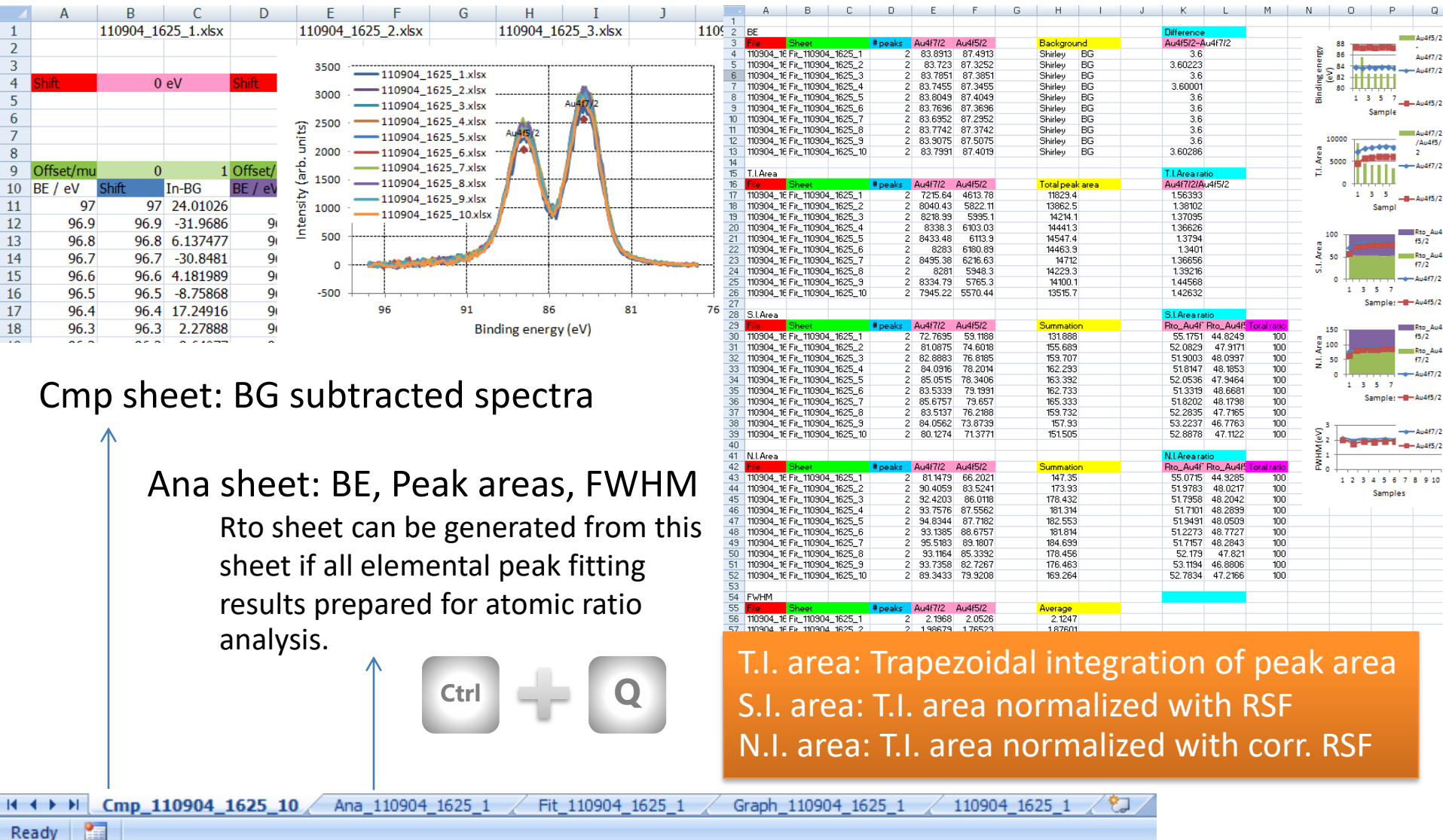
Once fitting process above done, “ana” in D1 cell to compare those fitted xlsx files.



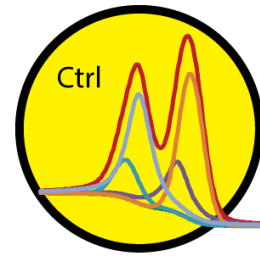
	A	B	C	D	E	F
1	Shirley	BG		ana	Au4f7/2	Au4f5/2
2	Tolerance	0.000001		BE	83.89131	87.49132
3	Initial A	0.001		KE	509.1087	505.5087
4	Final A	0.00344		FWHM1	2.196802	2.052602
5	Iteration	6		FWHM2		



Summary of fitting results



Enjoy!



Depth-profile XPS: RSC Adv. 6, 94905 (2016).

