AvantageToPlot

Operating Manual

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AvantageToPlot

Operating Manual

Contents

This operating manual is intended for XPS users of the Thermo Scientific K alpha system who have exported their data in Excel files using the standard format provided by Thermo and wish to plot it professionally in the most efficient manner in a PowerPoint presentation.

Requirement

The followings must be installed to use the program:

- Python 3.6 or above
- Panda for python (Read Excel files)
- PPTX for python (Create PowerPoint presentation)
- Tkinter for Python
- Excel and PowerPoint
- ConfigXPS_10.xls file
- PowerPoint template file

Output Files (PPT, PNGs, SVGs)

AvantageToPlot provides a PPT file and images files of all the plotted data in PNG and SVG format. The PowerPoint file consists of the following slides:

- Individual Survey slide
- Individual Core levels slide
- Individual Shirley background subtracted core level slide
- Individual valence band slide
- Individual quantification slide
- Comparison Survey slide
- Comparison Core level slide
- Comparison valence band slide

An example is shown in the figures below:

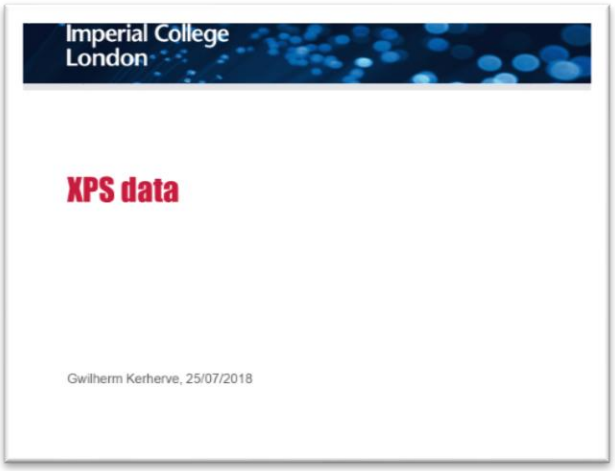


Figure 1:Title slide

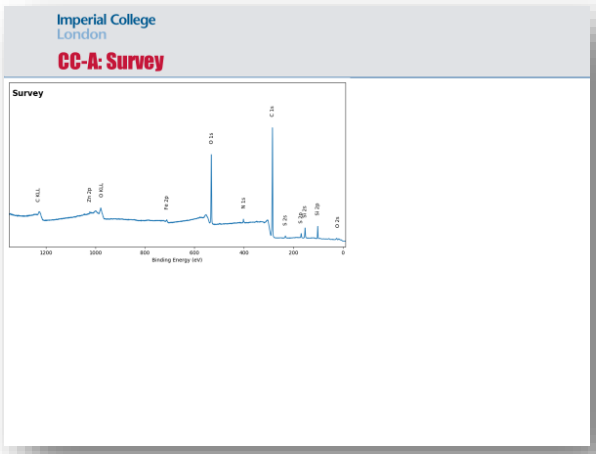


Figure 2: Survey slide of an individual file

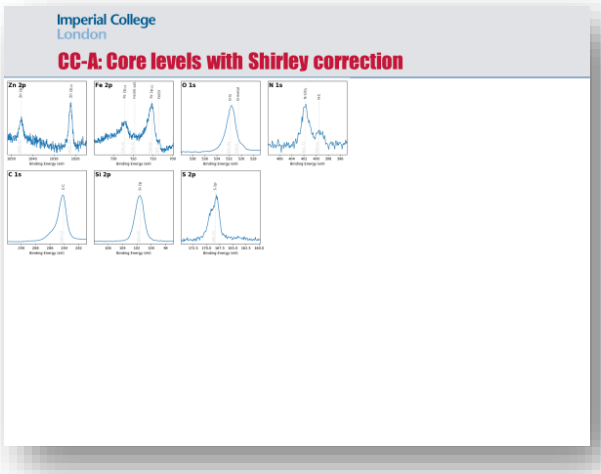


Figure 4: Bkg corrected slide of an individual slide

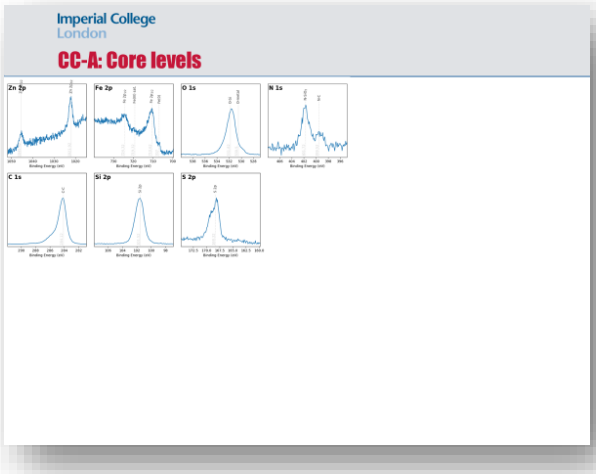


Figure 3: Core level slide of an individual slide

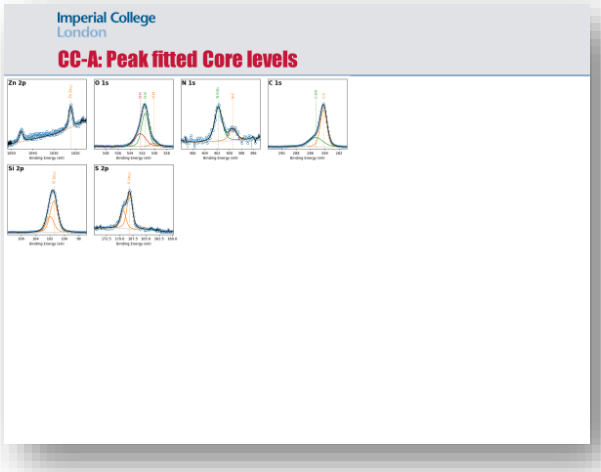
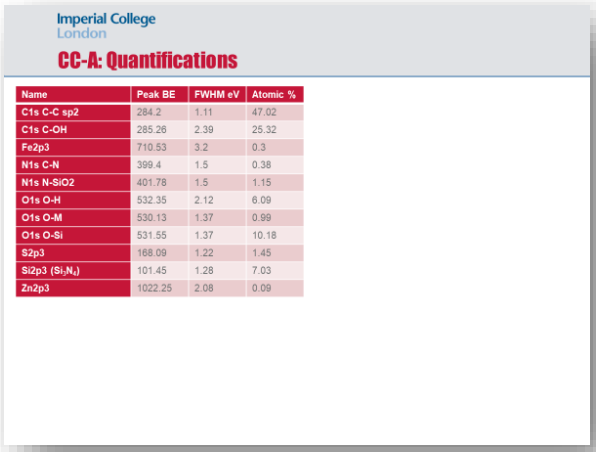


Figure 5: peak fitted core level slide of an individual file



Name	Peak BE	FWHM eV	Atomic %
C1s C-C sp2	284.2	1.11	47.02
C1s C-OH	285.26	2.39	25.32
Fe2p3	710.53	3.2	0.3
N1s C-N	399.4	1.5	0.38
N1s N-SiO2	401.78	1.5	1.15
O1s O-H	532.35	2.12	6.09
O1s O-M	530.13	1.37	0.99
O1s O-Si	531.55	1.37	10.18
S2p3	168.09	1.22	1.45
Si2p3 (Si_3N_4)	101.45	1.28	7.03
Zn2p3	1022.25	2.08	0.09

Figure 6: Quantification slide of an individual file

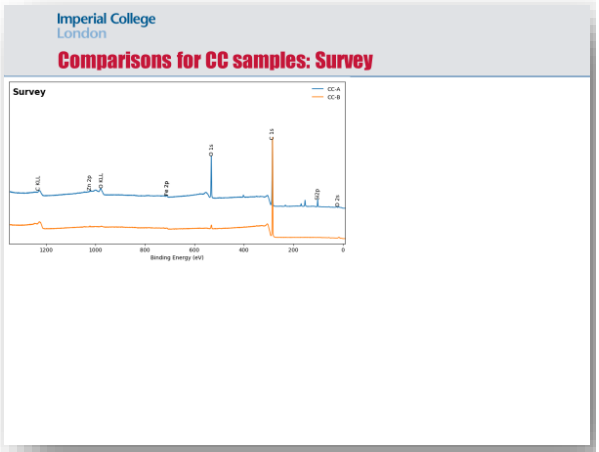


Figure 7: Comparison survey slide

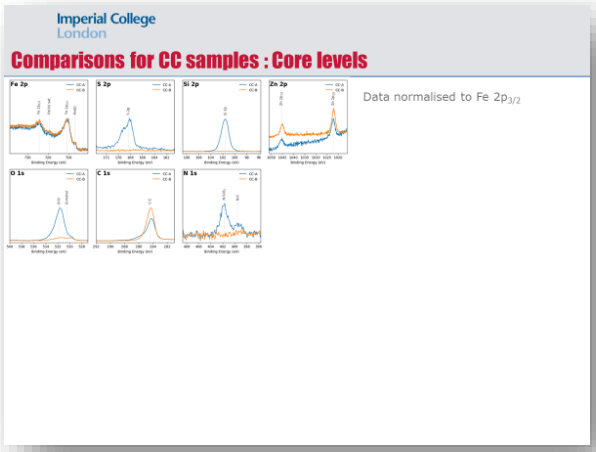


Figure 8: Comparison core levels slide

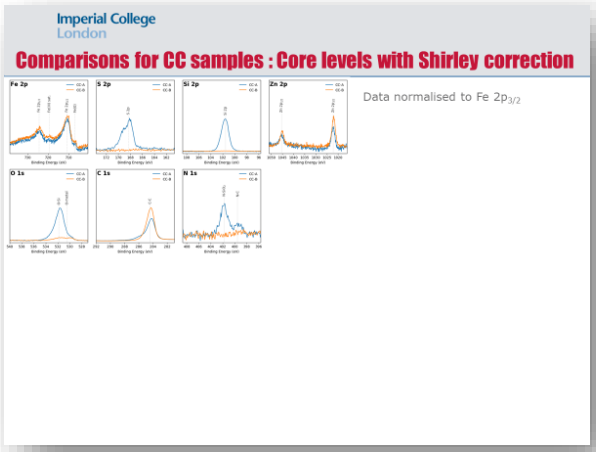


Figure 9: Comparison of bkg corrected core levels file

Quick Instruction

1. Create Excel datafiles of the samples that need to be plotted
2. In the samples Excel files
   a. Add the 'Carbon BE' value in the Title worksheet
   b. Add the 'Normalisation' value in the Title worksheet.
   c. Move all the worksheets that do not need plotting after the 'Title' or 'Quantifications' worksheets
3. In the ConfigXPS file

a. Choose the Config Tab number
b. Select the correct directory and files
c. Check if the followings are required:
    i. C-C correction
    ii. Quantifications
    iii. Automatic Shirley background

4. Compile the AvantageToPlot
5. On AvantageToPlot window, click 'Run' and look for possible error in the python compiler. Make sure the previously created PPT file is close before running the file

Exporting data to Excel

From the Avantage software, select all your data (survey, core levels and valence band) from the processing viewing window and export it to excel, see

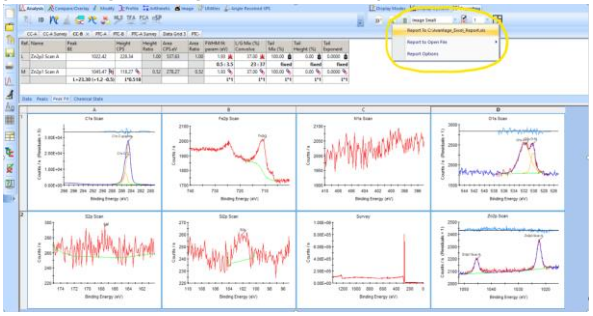


Figure 10. To avoid any unforeseen error in the AvantageToPlot it is best not to mess around with the exporting options provided by Avantage.

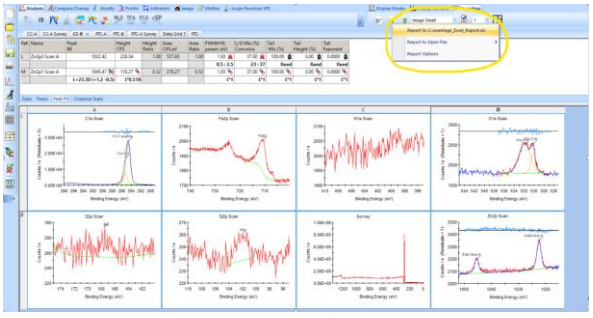


Figure 10: Exporting data to Excel in Avantage software

The Excel exported data consists of several worksheets containing the binding energies, intensity and background values of the different core levels valence band and survey data. The Excel file also MUST contain a 'Peak Table' and 'Titles' worksheets, see

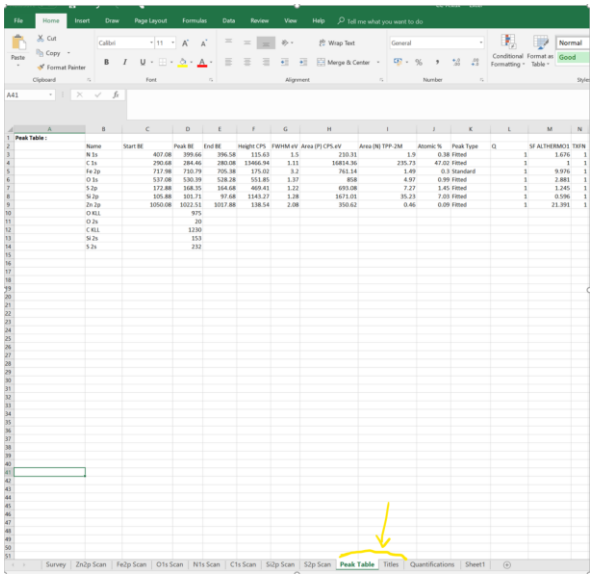


Figure 11.

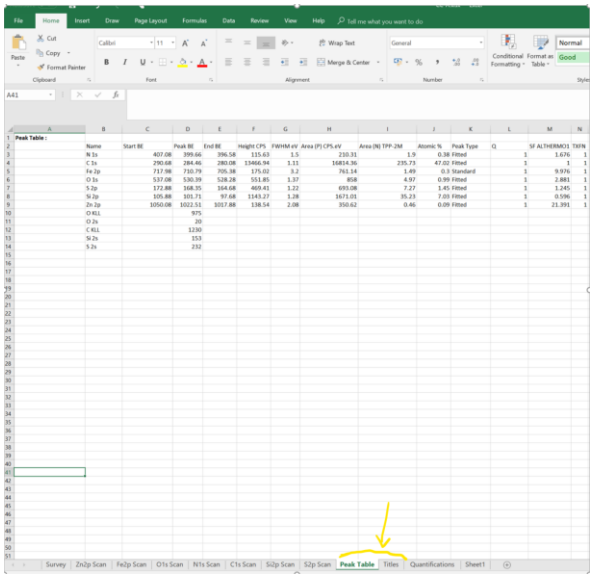


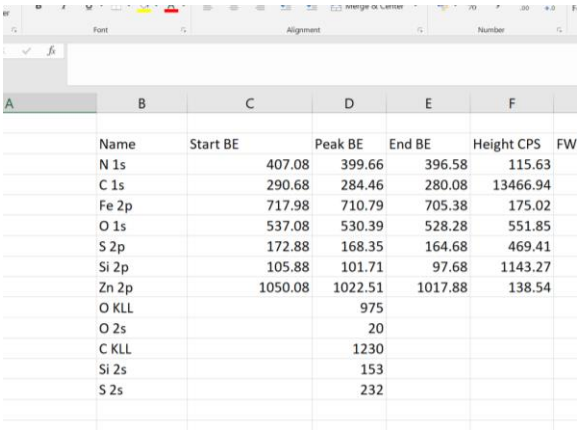
Figure 11: Example of an Excel file produced

Explanation of the Excel datafile

To get the correct output from the AvantageToPlot program, the following worksheet need to be in the Excel datafile:

- 'Peak Table' worksheet
- 'Title' worksheet
- 'Quantifications' worksheet (Optional)

The 'Peak Table' worksheet is used by AvantageToPlot to label the survey spectrum (if available). An example of a Peak Table is shown in Figure 12. The user can add or remove peak labels and Peak BE if required.



	Name	Start BE	Peak BE	End BE	Height CPS	FW
	N 1s	407.08	399.66	396.58	115.63	
	C 1s	290.68	284.46	280.08	13466.94	
	Fe 2p	717.98	710.79	705.38	175.02	
	O 1s	537.08	530.39	528.28	551.85	
	S 2p	172.88	168.35	164.68	469.41	
	Si 2p	105.88	101.71	97.68	1143.27	
	Zn 2p	1050.08	1022.51	1017.88	138.54	
	O KLL		975			
	O 2s		20			
	C KLL		1230			
	Si 2s		153			
	S 2s		232			

Figure 12: Example of a Peak Table worksheet

The 'Title' worksheet is used by AvantageToPlot to read the name of the sample, the position of the adventitious carbon C 1s and the number used in the normalization. An example of the 'Title' worksheet is shown in Figure 13. Note that the program will hang if the word 'Carbon BE' together with a value for the C-C bond position is not provided. If a normalization is used, the program will also require having the word 'Normalisation' together with a value at the column and row position shown in the figure below.

	A	B	C
1	17:26:23 Monday, July 02, 2018		
2			
3	C:\Avantage_Excel_Report.xls		
4	Normalisation	45714.79	Zr3d5
5	Ref. (interface)	Interface	
6	Carbon BE	284.46	
7	Data Files :	Title	File Name
8		Zr3d Scan	C:\...\Data\20180531_NewClean\LAC
9		Y3d Scan	C:\...\Data\20180531_NewClean\LAC
10		Survey	C:\...\Data\20180531_NewClean\LAC
11		O1s Scan	C:\...\Data\20180531_NewClean\LAC
12		Mn2p Scan	C:\...\Data\20180531_NewClean\LAC
13		La3d Scan	C:\...\Data\20180531_NewClean\LAC
14		Fe2p Scan	C:\...\Data\20180531_NewClean\LAC
15		Cr2p Scan	C:\...\Data\20180531_NewClean\LAC
16		Ce4d Scan	C:\...\Data\20180531_NewClean\LAC
17		Ce3d Scan	C:\...\Data\20180531 NewClean\LAC

Figure 13: Example of a Title worksheet

A quantification table can also be added in a new worksheet called 'Quantifications'. To add this quantification table in the ppt presentation, the user must also tick the quantification in the ConfigXPS spreadsheet.

Explanation of ConfigXPS file

ConfigXPS is an excel file used by the user to configure all the settings of AvantageToPlot. It consists of 3 worksheets:

- Main Settings
- Plot Settings
- Line Settings

Main Settings worksheet

The 'Main Settings' worksheet contains all the general configurations of AvantageToPlot. Figure 14 shows a view of the ConfigXPS files provided. The sections below described all the possible configurations.

	A	B	C	D	E
1	**Main Settings**				
2			**SAMPLE 1**	**SAMPLE 2: SLA**	**SAMPLE 3: LSCM**
3	**Name**	**Values**	**Values**	**Values**	**Values**
4	**Config Tab Number**	9			
5					
6					
7	**Folder**		C:\Users\gwilh\Google Drive\	C:\Users\gwilh\Google Drive\	C:\Users\gwilh\Google Drive\
8			XPS Others\Milly\Analysis	SOFC\Analysis\Celeste_SLAO\Ana	SOFC\Analysis\LSCM & YSZ St An
9	**Files**		Fe16CR.xlsx	SLA_180531_0.xlsx,SLA_180531_	S1_CeO2.xlsx,S5_NiCeO2.xlsx, R1
10					
11					
12	**General**				
13	Peak line & value		TRUE	TRUE	TRUE
14	Visible Y values		FALSE	FALSE	FALSE
15	Automatic Shirley		TRUE	TRUE	TRUE
16	Do quantification		TRUE	FALSE	FALSE
17	Do C-C correction		TRUE	TRUE	TRUE
18					
19	Auto height comp		FALSE	FALSE	FALSE
20	Manual Height comp		1.95	1.95	1.95
21					
22	Do normalisation by val		TRUE	TRUE	TRUE
23	Normalisation value		file, file, file, file,file,file	file, file, file, file,file,file	file, file, file, file,file,file
24					
25	Show Figure in Python		FALSE	FALSE	FALSE
26	Plot settings sample number		1	2	3
27	Lines settings sample number		1	2	3
28					
29	**Powerpoint**				
30	Do a presentation		TRUE	TRUE	TRUE
31	Filename		XPS_Data_by_GK.pptx	XPS_Data_by_GK.pptx	XPS_Data_by_GK.pptx
32	Title		XPS data	XPS data	XPS data
33	Template Filename		ICL_template.pptx	ICL_template.pptx	ICL_template.pptx
34					
35	**Pictures**				
36	Save Images		TRUE	TRUE	TRUE
37	DPI level		200	200	100
38					
39	**Comparison plots**				
40	Change Legend default location?		FALSE	FALSE	FALSE
41	Legend position		upper left	upper left	upper left
42	Legend Offset X		0	0	0
43	Legend Offset Y		0.94	0.94	0.94
44	Autoheight for labelling		TRUE	TRUE	TRUE
45	File number for labelling		2	2	2
46					
47	Offset in Survey		-0.3	-0.3	-0.3
48	Offset plots		FALSE	FALSE	TRUE

Figure 14: Overview of the Main Settings worksheet

Config Tab Number

Value: 1-9

The config Tab Number consists of the sample configuration number that the user has chosen to use. As AvantageToPlot is aimed for the heavy XPS user, it is expected that the user would study different types of samples in the XPS in which a sample configuration number would be dedicated. The original ConfigXPS contains 9 types of samples but this can be extended indefinitely.

Folder

Value: String

It consists of the path of the files. Note that it contains of 2 lines which are concatenated by AvantageToPlot to get the whole path. The first line of the path is expected to be the same for all the samples configuration. The second line of the path is more specific to the project.

Files

Value: List of strings

This line contains the list of filenames (samples) that AvantageToPlot will plot. An indefinite number of files can be plotted at the same time. The user must note that all files will be plotted individually and together in a comparison plot at the end of the PPT presentation. Each file is separated by a coma. An example is shown below:

```
STO_1.xlsx, NGO_2.xlsx, STO_3.xlsx, NGO_4.xlsx
```

Peak line & value

Value: True / False

Visible line and its corresponding value in binding energy for a known peak. The configuration of each line (Label and value) is done in the 'Line Settings' worksheet

Visible Y values

Value: True / False

The user can decide to show the intensity of the data.

Automatic Shirley

Value: True / False

A Shirley background can be applied to the data which provide an extremely fast way of plotting background corrected data. Note that in contrast to the Avantage software, this is not a smart background correction.

Do quantification

Value: True / False

Provide a quantification table in the PPT file. Note that the 'Quantifications' worksheet must be added manually in the Excel file.

Do C-C correction

Value: True / False

If True, AvantageToPlot correct each core level and valence band provided so that the C-C bond is at 284.8 eV

Auto height comp

Value: True / False

If True, AvantageToPlot makes the data…. Default is False

Manual Height comp

Value: 1 (Max) to infinite (Min). Float number e.g. 1.95

Value used by AvantageToPlot if 'Auto height comp' is set to 'False' so that the data is divided by the given value. This enable the user to define the correct height so that the label of the 'Peak line' is not out of the plot.

Do normalisation by val

Value: True / False

If True, AvantageToPlot uses the values in 'Normalisation value' to normalize the data of each core level of the comparison plots.

If False, AvantageToPlot normalize each core level to the maximum height.

Normalisation value

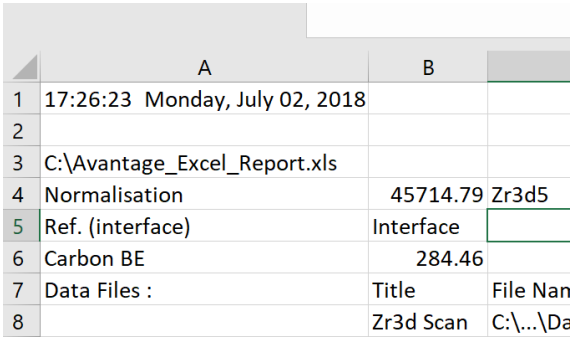
Value: list of numbers or string

The values can be a list of numbers, then the data from each core level will be divided (normalized) by it. Note that there should be at least the same amount of numbers as there are files to compare. An example is shown below if the user wants to compare 4 files or less:

```
1456, 759.1, 546, 795
```

The values can also be a list of strings with the string being 'file'. This is the preferential option as it avoids mistake in the normalization value. AvantageToPlot looks for the normalization value in the 'Title' worksheet of the excel sample file in row B4. Note that row A4 must be filled with 'Normalisation' otherwise the number in B4 is ignored. An example of the normalization is shown in Figure 15. An example is shown below if the user wants to compare 4 files or less:

```
file, file, file, file
```



	A	B	
1	17:26:23 Monday, July 02, 2018		
2			
3	C:\Avantage_Excel_Report.xls		
4	Normalisation	45714.79	Zr3d5
5	Ref. (interface)	Interface	
6	Carbon BE	284.46	
7	Data Files :	Title	File Nan
8		Zr3d Scan	C:\...\Da

Figure 15: Example of the Normalisation value in a excel sample file

Show Figure in Python

Value: True / False

Leave this value to False

Plot settings sample number

Value: 1 to 9

Similar to 'Config Tab Number', it represents the plot settings numbers that will be used by AvantageToPlot

Lines settings sample number

Value: 1 to 9

Similar to 'Config Tab Number', it represents the line settings numbers that will be used by AvantageToPlot

Do a presentation

Value: True / False

Default value is True.

During the compilation of AvantageToPlot the data is plotted with PNG and SVG files saved into the 'PNGs' folder. AvantageToPlot can also save a PowerPoint presentation listing all the surveys, core levels and valence band.

Note 1: If the PowerPoint file is already opened then AvantageToPlot will not be able to compile.

Note 2: 'Save Images' must be set to 'True' for the powerpoint file to be created

Title

Value: String

Name of the PowerPoint file

Template Filename

Value: String

Name of the PowerPoint template file used to create the PowerPoint presentation

Save Images

Value: True / False

Default value is 'True'. Save the images in the 'PNGs' folder. Note that AvantageToPlot saves images in the PNG format but ALSO in the vectoriel SVG format. While the PNG formatted is intended for the PowerPoint presentation, the SVG format is intended to be used for the Publishing of the plots. Tools like 'Inskape' can be used to manipulate SVG files

DPI level

Value: number

Quality of the PNG

Change Legend default location?

Value: True / False

The default value is False. The default place of the legend is in the UPPER RIGHT border of the comparison plot. If the legend obstructs the label of the line then the legend can be placed in the UPPER LEFT border of the comparison plot.

Legend position

Value: String

The only working value is UPPER LEFT. If UPPER RIGHT is preferred, add False to 'Change Legend default location?'

Legend Offset X

Value: Number

X value of the offset legend

Legend Offset Y

Value: Number

Y value of the offset legend

Autoheight for labelling

Value: True / False

If True, then the label for the line is inserted above the peak from the data with the maximum intensity.

If False, then the label for the line is inserted above the peak from the data chosen in 'File number for labelling'

File number for labelling

Value: 1 to Max file/sample number

File/sample number chosen for the height of the labelling. Note that this function is only used if autoheight for labelling is False

Offset in Survey

Value: 0 to 1

Offset used between the different surveys of the comparison survey plot.

Offset plots

Value: True / False

Offset between each data in the comparison core levels plots

Files per offset

Value: 1,2,3,4

Value used in the offset of core level comparison plots

Offset Maximum Percentage

Value: 0 to 1

Value used in the offset of core level comparison plots

Offset Gap in Percentage

Value: 0 to 1

Value used in the offset of core level comparison plots

Plot Settings

The 'Plot Settings' worksheet is a configuration page used to define the minima and maxima in B.E. of all plotted core levels. If 'use it?' is set to False, AvantageToPlot plots all the data provided in the Excel spreadsheet.

Note 1: If a core level is not specified in the spreadsheet, the user would have to amend the code of AvantageToPlot. To do this, an existing element can be used as an example.

Note 2: The 'Plot Settings' worksheet has 9 sample 'Plot Settings' configuration number available. As AvantageToPlot is aimed for the heavy XPS user, it is expected that the user would study different types of samples in the XPS in which a sample configuration number would be dedicated. The sample number used by AvantageToPlot is set in the 'Main Settings' worksheet in 'Plot settings sample number'.

Line Settings

The 'Lines Settings' worksheet is a configuration page used to define the labelling in the core level plots. The variables are available to the user:

BE Line

Value: Number

Position of the line in B.E.

Note: If 'Look for Position' is set to True, AvantageToPlot will look for the maximum around the position

Name

Value: String

Name of the label. The code used in the labelling is identical to the one used in 'Latex' subscripts and superscripts are shown in the following manner: '$_{2}$' or '^{2}'.

Look for Position

Value: True / False

If True, AvantageToPlot sets the labeling at the B.E. position with the maximum intensity. The maximum intensity search is done around the position of the line +/- 7 datapoints.

Running AvantageToPlot Interface

AvantageToPlot has a simple window interface (see Figure 16) to avoid opening the PPT file each time a change is made.

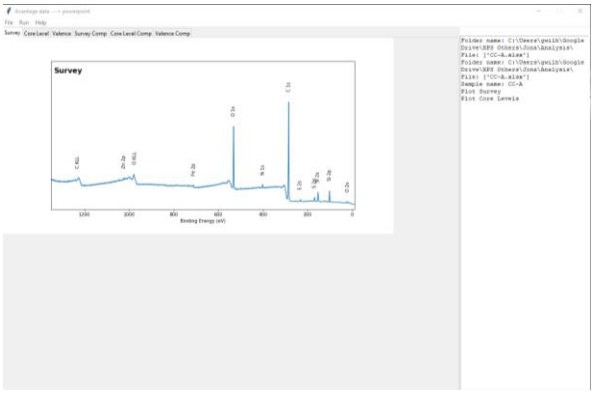


Figure 16: AvantageToPlot Front Interface

Files

Open

Not available yet

Save

Not available yet

Quit

Quit the program

Run

Run AvantageToPlot as specified in ConfigXPS file.

Help

Not available yet. Link to this document