




Army Educational Outreach Program
(AEOP)
Summer Research Camp 2017
Nuclear and Surface Physics Lab/UTEP

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I. How To Use CASA XPS for Peak Fitting and Chemical Analysis:

- 1) To view a text document in CASA XPS, you must first convert the .txt file to a(.vms) file, by clicking the purple folder  icon, then you can see the XPS's spectrum (for more detailed see figure 1).

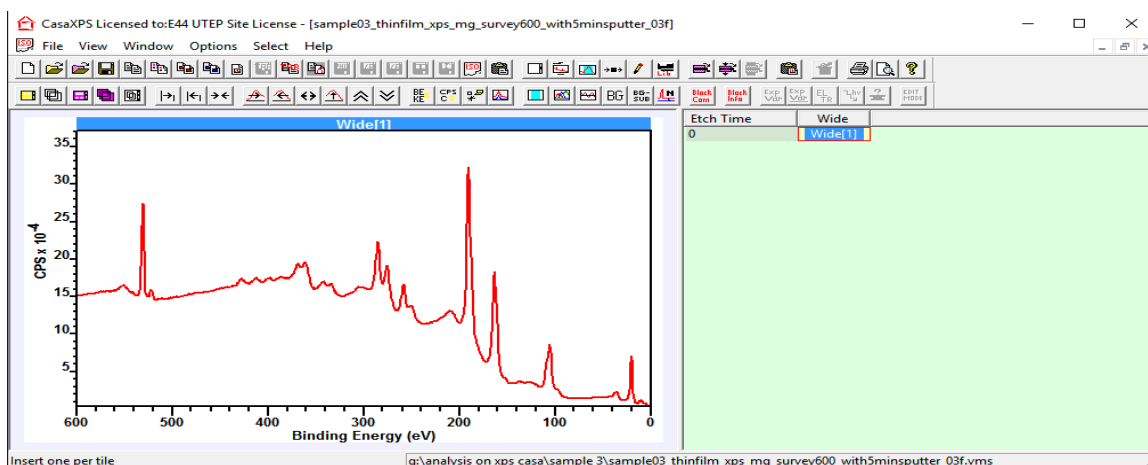




Figure 1

- 2) Once this is done, open the file by clicking the yellow folder icon  or pressing (CTRL + O) and search for the .vms file.
- 3) To analyze the (.vms) file, click on the icon labeled as “Quantify” or press F7, a window titled “Quantification Parameters” should appear. 

By clicking “Create” a background line is drawn over the region. To specify the region for the background line, click and drag from each end of the vertical axis (see figure 2).

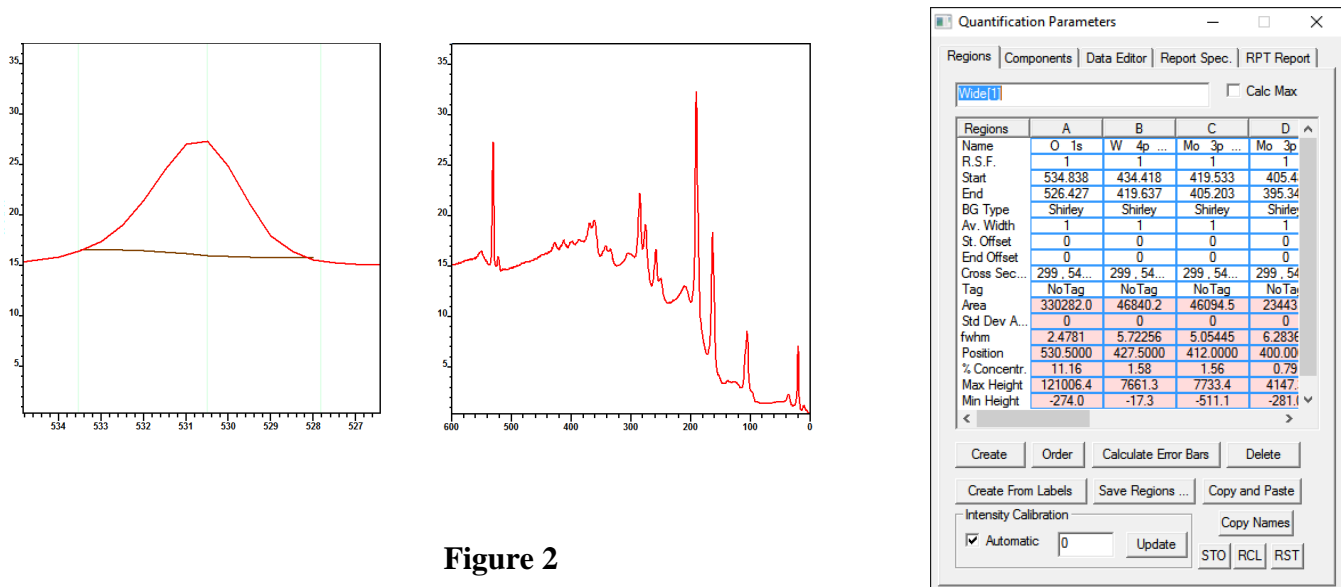


Figure 2

The Blue vertical lines indicate the boundaries for the background line, and will allow us to fit the peak.

- To identify the chemical composition of the sample, search for peaks along the Counts per Second vs Binding Energy graph, obtain the Binding Energy value for the peaks and search through the NIST XPS Database to determine which elements are present. Once this is done, label the region created in Step 3 by changing the “Name” space in the column created. Once this is done, the peak will be labeled with the name given as shown in figure 3.

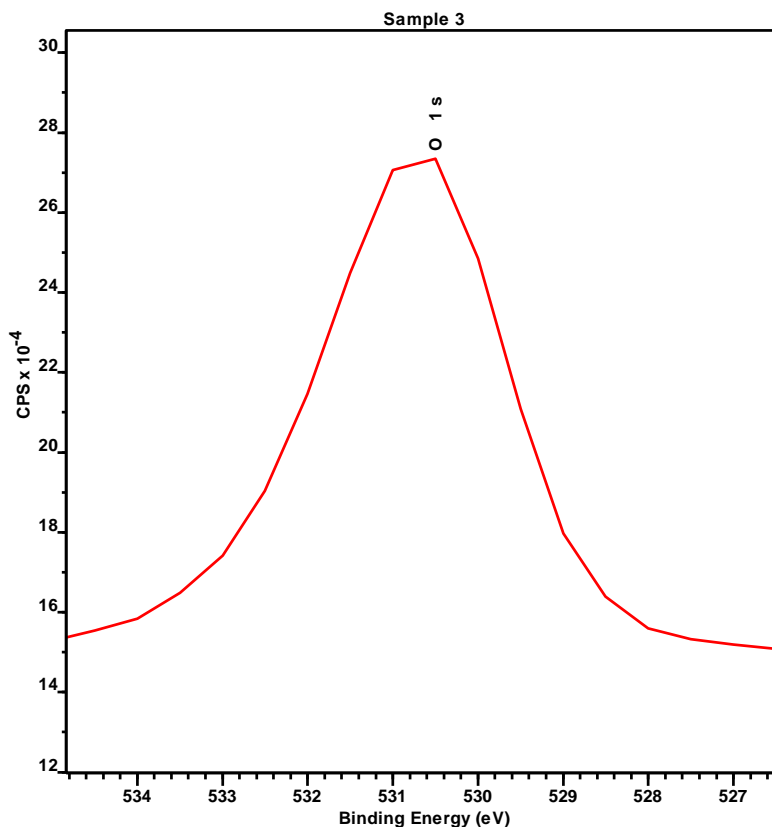



Figure 3

- 5) To display data, such as the area underneath a curve, click on the “Title Annotation” icon  or press F9. Once this is done, a window titled “Annotation” will appear. Click on the “Regions” option from this window, and click “Apply” as shown in figure 4.

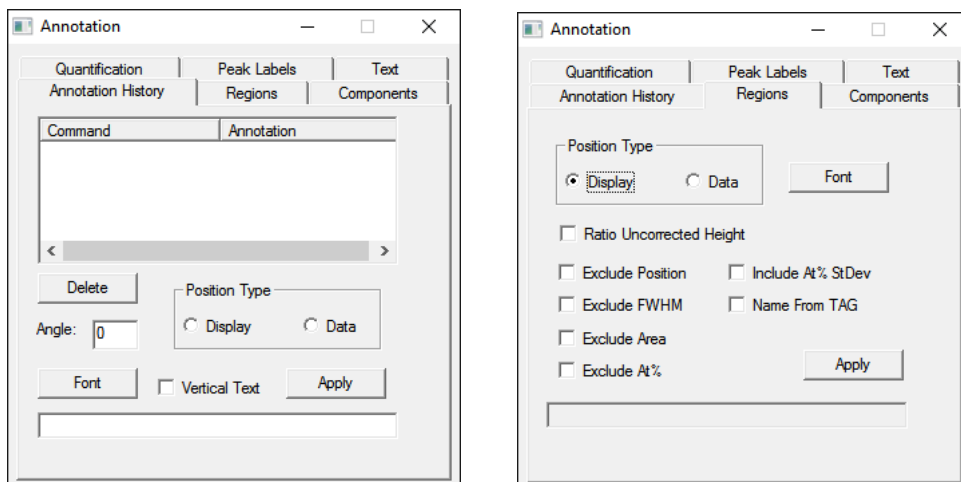
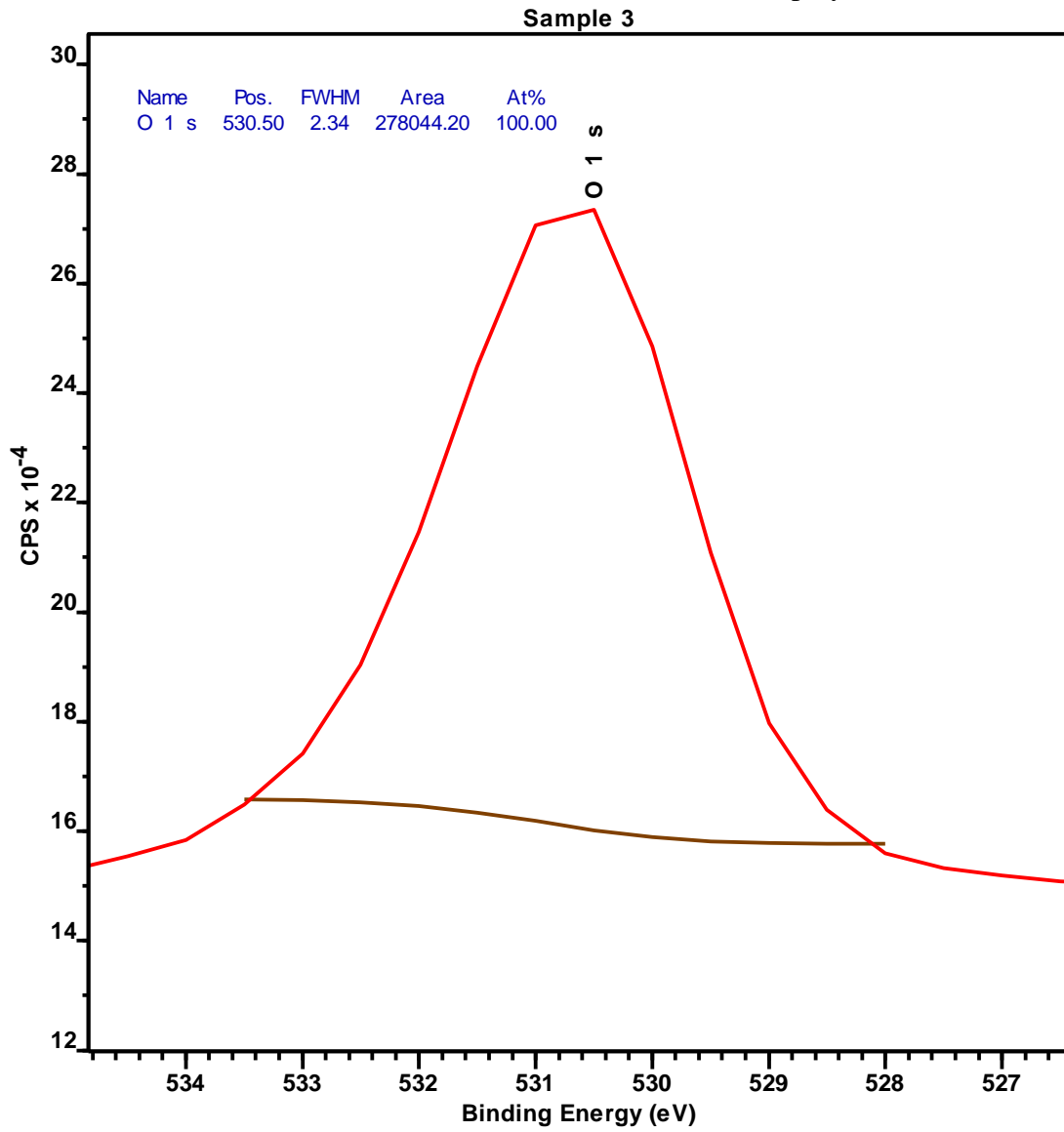
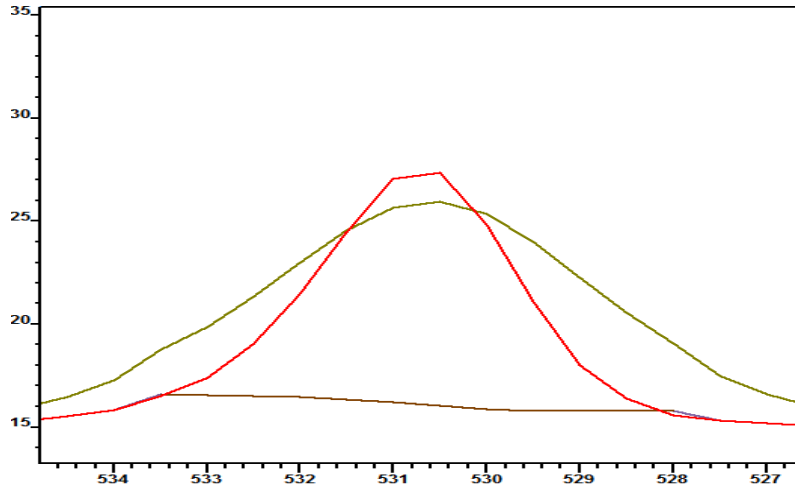


Figure 4

Once this is done, data such as area under the curve, will be displayed.



- 6) To fit the peak, click on the “Components” option from the “Quantification Parameters” window and click “Create”. A curve will be formed, as the one shown below in green. To have this curve fitted to the peak, simply click the “Fit Components” option.



Quantification Parameters

Regions Components Data Editor Report Spec. RPT Report

Wide[1] [RMS = 104413; D. of F. = 201] [Eff. RSF = 1] [Eff. Mass

Component	A	B	C
Name	Wide	Wide	Wide
R.S.F.	1	1	1
Line Shape	LF(1,1,25,2...	LF(1,1,25,2...	LF(1,1,25,2...
Area	339057.5	48505.1	46034.0
Area Constr.	0.0, 10000...	0.0, 10000...	0.0, 10000...
fwfm	2.40675	5.76043	5.46831
fwfm Constr.	0.9992, 24...	0.4812, 12...	1.321, 33.03
Position	530.7490	427.6675	412.6187
Pos. Constr.	534.838, 5...	434.418, 4...	419.533, 4...
Tag	No Tag	No Tag	No Tag
Comp Index	-1	-1	-1
Asymmetry In...	-0.0000	-0.0000	-0.0000
% Concentr.	10.79	1.54	1.47

Marquardt

Simplex

Use RMS

