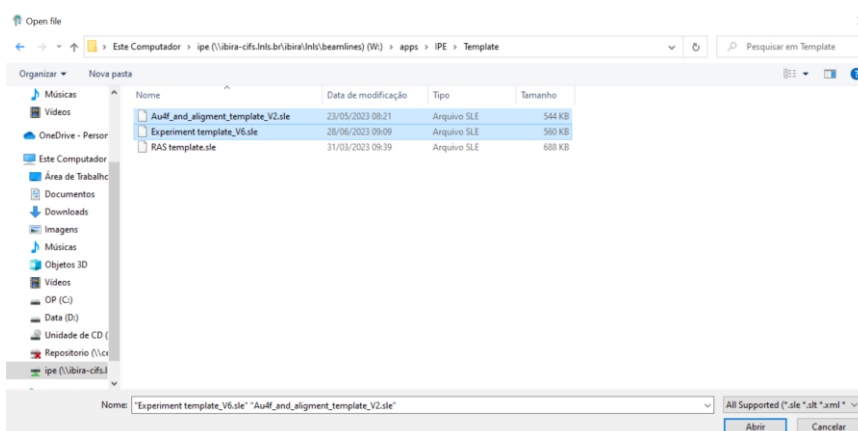
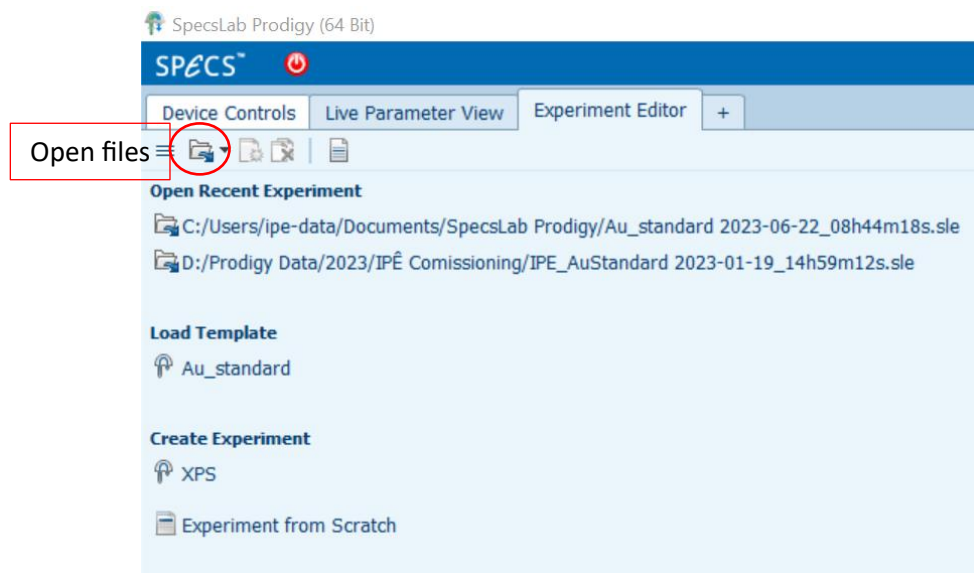
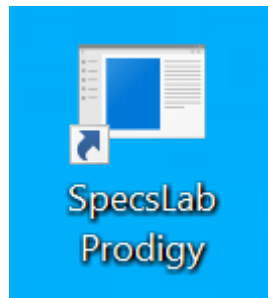


XPS data visualization and acquisition

v1.0

1 – Opening the software with the templates

Open the SpecsLab Prodigy. With the software already opened, click in “open file” and select both templates: alignment and experiment (this step should be ready before the user comes in).



2 – Alignment the sample

After opening both templates, the sample should be aligned with the electron analyzer. To align the sample, we use the “Fixed Energy” mode on the alignment template. After choosing the energy (Ebin), select the spectra and press “play” on the top of the file.

Play

ID	Name	Eexc	Scans	Start (Ebin)	End (Ebin)	Step	Values	Dwell	Lens	Epass	Duration	Acquisition Time	Comment
	Au_Survey	930	1	880	-10	1	891	0.25	SA	40	03:43		
	Au4f	250	1	95	77	0.05	361	0.25	SA	20	01:31		

Fixed energy mode

ID	Name	Eexc	Scans	Values	Ebin	Dwell	Lens	Epass	Duration	Acquisition Time	Comment
	Spectrum	1253.6	1	10000	764	0.1	SA	20	16:40		
	Spectrum	1253.6	1	10000	768	0.1	SA	20	16:40		
	Spectrum	1253.6	1	10000	846	0.1	SA	40	16:40		
	Spectrum	1253.6	1	10000	846	0.1	SA	40	16:40		
	Spectrum	1253.6	1	10000	846	0.1	SA	40	16:40		
	Spectrum	1253.6	1	10000	768	0.1	SA	40	16:40		

Changes the energy

Selects the spectrum to be measured

After the electron analyzer starts to count, move the XPS manipulator on “Z” axis until increasing the signal (the alignment procedure will be explained in detail after the user arrives).

Manipulator Motors

XPS - eixo X
0.00000 | 1 | STOP
0.00000 mm

XPS - theta
0.00000 | Step (VAL) | STOP
0.00000 deg

XPS - eixo Y
24.00002 | 10 | STOP
24.00002 mm

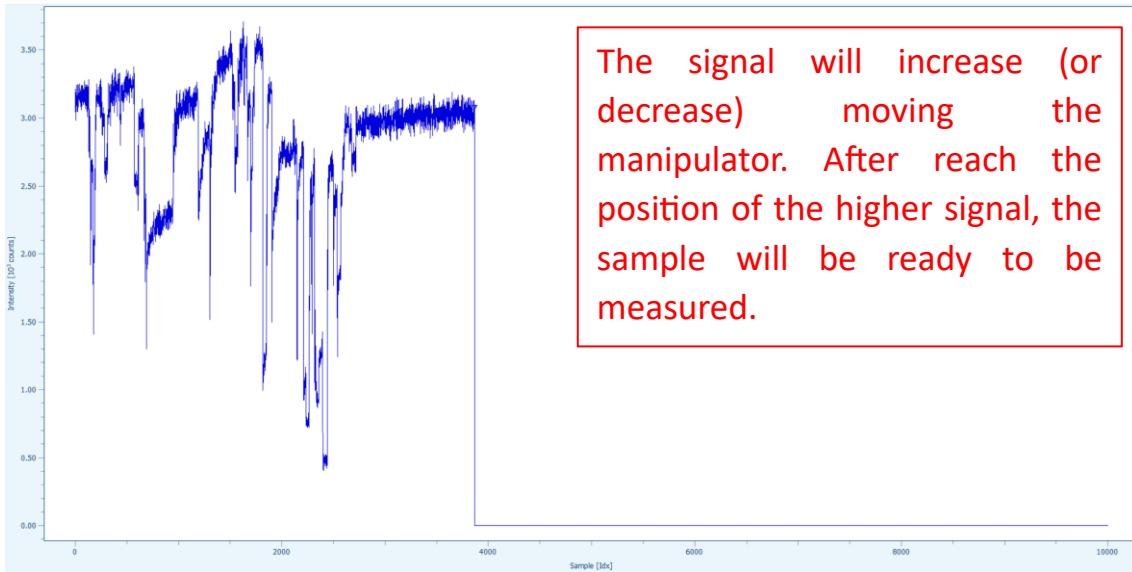
Photo Diode
0.00000 | Step (VAL) | STOP
0.00000 mm

XPS - eixo Z
1.50005 | 1 | STOP
1.50005 mm

LED
LASER
PD safety

Stop XPS

Positioners
Zero Position
Transfer Position



The signal will increase (or decrease) moving the manipulator. After reach the position of the higher signal, the sample will be ready to be measured.

3 – Measuring the XPS spectra

After the alignment step, go to the “Experiment template” and select the spectra that you wish to obtain. In the “XPS spectra 1” is there three spectrum group: **Sample 1 different spots** (in order to check the sample’s homogeneity, a fast scan is acquired in different positions of the sample), **Sample 1 composition** (in this group a complete spectrum survey is made as well the spectra of the element composition in the sample) and **Sample 1 depthprofile** (in order to investigate the composition in different depths is possible to change the excitation energy).

Sample 1 different spots

ID	Name	Excc	Scans	Start (Ebin)	End (Ebin)	Step	Values	Dwell	Lens	Epass	Duration	Acquisition Time	Comment
<input type="checkbox"/>	Spot1	1253.6	1	800	200	1	601	0.1	SA	40	01:01		
<input type="checkbox"/>	Spot2	1253.6	1	850	250	1	601	0.1	SA	40	01:01		
<input type="checkbox"/>	Spot3	1253.6	1	850	250	1	601	0.1	SA	40	01:01		
<input type="checkbox"/>	Spot4	1253.6	1	850	250	1	601	0.1	SA	40	01:01		

Sample 1 composition

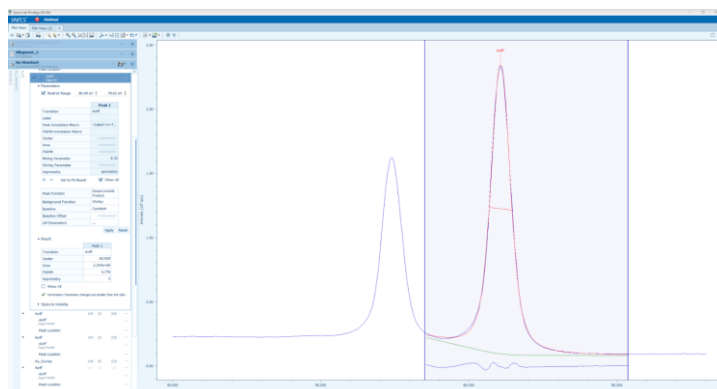
ID	Name	Excc	Scans	Start (Ebin)	End (Ebin)	Step	Values	Dwell	Lens	Epass	Duration	Acquisition Time	Comment
<input type="checkbox"/>	Survey	1253.6	2	1200	-5	0.5	2411	0.1	SA	40	08:03		
<input type="checkbox"/>	Sm3d	1481	≤10	1128	1071	0.1	571	0.1	SA	20	≥00:58		
<input type="checkbox"/>	Co2p	1180	≤10	814	768	0.1	461	0.1	SA	20	≥00:47		
<input type="checkbox"/>	Y3d	556	≤10	179	146	0.1	331	0.1	SA	20	≥00:34		
<input type="checkbox"/>	O1s	930	≤10	538	525	0.1	131	0.1	SA	20	≥00:14		
<input type="checkbox"/>	C1s	684	≤10	290	275	0.1	171	0.1	SA	20	≥00:08		

Sample 1 depthprofile

ID	Name	Excc	Scans	Start (Ebin)	End (Ebin)	Step	Values	Dwell	Lens	Epass	Duration	Acquisition Time	Comment
<input type="checkbox"/>	Co3p	280	≤10	81	50	0.1	311	0.1	SA	20	≥00:32		
<input type="checkbox"/>	Co3p	460	≤10	81	50	0.1	311	0.1	SA	20	≥00:32		
<input type="checkbox"/>	Co3p	860	≤10	81	50	0.1	311	0.1	SA	20	≥00:32		
<input type="checkbox"/>	Co3p	1360	≤10	81	50	0.1	311	0.1	SA	20	≥00:32		
<input type="checkbox"/>	Y3d	376	≤10	179	146	0.1	331	0.1	SA	20	≥00:34		
<input type="checkbox"/>	Y3d	556	≤10	179	146	0.1	331	0.1	SA	20	≥00:34		
<input type="checkbox"/>	Y3d	956	≤10	179	146	0.1	331	0.1	SA	20	≥00:34		
<input type="checkbox"/>	Y3d	1456	≤10	179	146	0.1	331	0.1	SA	20	≥00:34		
<input type="checkbox"/>	Sm4d	349	≤10	150	119	0.1	311	0.1	SA	20	≥00:32		
<input type="checkbox"/>	Sm4d	529	≤10	150	119	0.1	311	0.1	SA	20	≥00:32		
<input type="checkbox"/>	Sm4d	929	≤10	150	119	0.1	311	0.1	SA	20	≥00:32		
<input type="checkbox"/>	Sm4d	1429	≤10	150	119	0.1	311	0.1	SA	20	≥00:32		

4 – Visualizing the data

In the “plot view”, double click in the spectra of interest. The spectra must appear during the measuring.



5 – Exporting the data

The data is automatically exported into two forms “x, y” (Binding energy x cps) or “.VMS” (format used in the “CasaXPS” software) and different files for each group. The experiment can be exported in a single file as well. Click in “Export” and select the format.

Opening .VMS files

The export data in .VMS format can be opened and treated using the following software:

CasaXPS: available in <http://www.casaxps.com/> (Free version)

Useful guides for CasaXPS:

- Systematic and collaborative approach to problem solving using X-ray photoelectron spectroscopy - <https://doi.org/10.1016/j.apsadv.2021.100112>
- <http://www.casaxps.com/casaxps-training/training-events.htm>
- http://www.casaxps.com/help_manual/

***CasaXPS Demo version doesn't allow to save treated data!!**

Opening .SLE files

.SLE files can be opened using the same software used for data acquisition (Specs Lab Prodigy).

The specs Lab prodigy allows to visualize, treat data and export the data in different formats.

All the features are available in free version such as: peak finding, peak fitting, different types of line shapes, among others. The example of a quick fitting is shown on the next figure:

Prodigy: available in <https://www.specs-group.com/nc/specs/products/detail/prodigy/> (Free version)