

XMapsLab manual

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Introduction

XMapsLab is comprised of a set of programs that allow working with XRF, XRD, and other types of data. Its objective is to obtain relevant information about elements and pigments from spectral data obtained from scanning devices, as well as to produce graphical representations of the distribution of elements and pigments.

Currently, we have developed the program **XMapsLab** which can generate maps from validated data. This data includes elements and/or pigments extracted from the raw data produced by scanning devices and validated by experts in material sciences, painting conservation, and restoration. Additionally, we have created **Positions** a program that assists in defining measurement positions, and **Tools** a program that creates project folders and basic files. In future updates, we plan to deploy **Interpreter** a program to interpret raw information and generate values for elements and pigments.

1.1 The steps of the general process

The following steps outline the process of studying an artwork, such as a painting, using the XRF technique with the objective of producing maps:

1. The first step is to obtain a high-quality photograph of the artwork. This requires a good quality camera and lens, proper positioning and orientation, and uniform lighting. The photograph should capture enough detail and be processed to enhance the captured information. RAW format is recommended for saving the photos, and adjustments for white balance and colors should be made, including the use of a calibrated color table. Once processed, the image should be saved in a lossless format with an alpha channel option, such as PNG.

Regarding the appropriate size for the maps, there are no strict rules. **XMapsLab** offers real-time or interactive work capabilities with relatively large images, for example, 3000 pixels x 4000 pixels.

2. After obtaining the artwork, positions for measurements need to be decided. There are two approaches: selecting positions directly on the artwork or using a photograph of the artwork.
 - In the first case, different positions must be marked (non-invasively) and measured for later input into the project.
 - In the second case, using a high-quality photograph of the artwork, positions can be marked on the image using a program like **Positions**. The resulting image can be printed or displayed on a mobile device, enabling experts to identify and mark the positions for measurements.
3. Once the positions are marked, data capture is performed using the scanning device.
4. The scanning device produces data files that need to be processed and/or validated by the user to obtain information about the elements and/or pigments.
5. The data obtained in the previous step, along with the measurement positions and photograph, allow for the study and analysis of the artwork using **XMapsLab**.

It is important to note that this process assumes manual scanning in a few positions, as is typical with handheld devices. In the case of devices with mechanized positioning, there is less need for interpolation methods, and position selection is done directly using the software controlling the positioning.

1.2 Using **XMapsLab**

To utilize **XMapsLab** with the data of a specific artwork, it is necessary to create a project dedicated to that artwork. This project should contain all the relevant information needed to study the artwork, particularly for producing maps.

The required information to be saved in the project includes:

- A high-quality color photo of appropriate size.
- The positions where measurements were made.
- The data obtained from those positions.

All this information is stored in a project, which consists of a folder hierarchy and various files. The details of this hierarchy and the files will be explained further in the following chapter.

Creating a project for XMapsLab

2.1 The project

To be able to work with **XMapsLab** we must prepare a project: a structure of folders and files. The project contains all the data about an artwork that is studied and analysed.

The structure of a project is illustrated in Figure 2.1. The main folder, which includes the programs, contains two subfolders: one for personal databases (**pdb**), and another for projects (**projects**), where individual projects are stored. Each project is represented by a separate folder, such as **project_1**, typically named after the artwork being studied.

It is important to maintain the names and placement of the folders in the hierarchy for the proper functioning of the programs, as they rely on these specific locations to search for data. The folder structure and files can be created manually using standard operating system procedures and any text editor, or automatically generated using the **Tools** program.

Now let's describe the contents of each folder within a project:

- **images**

This folder contains the image file of the artwork. The image serves as a visual reference for the distribution of elements and/or pigments, and is also required for obtaining maps using the MHD method (see REF). The recommended format is PNG, but JPG can also be used. PNG format allows for the addition of a transparency channel, which can be utilized to exclude certain areas of the image from processing, particularly if the artwork shape is non-rectangular. Multiple images can be added, but only one can be loaded into the program. The **Tools** program can be used to copy any image to the appropriate folder.

- **positions**

This folder contains the image(s) generated by the **Positions** program.

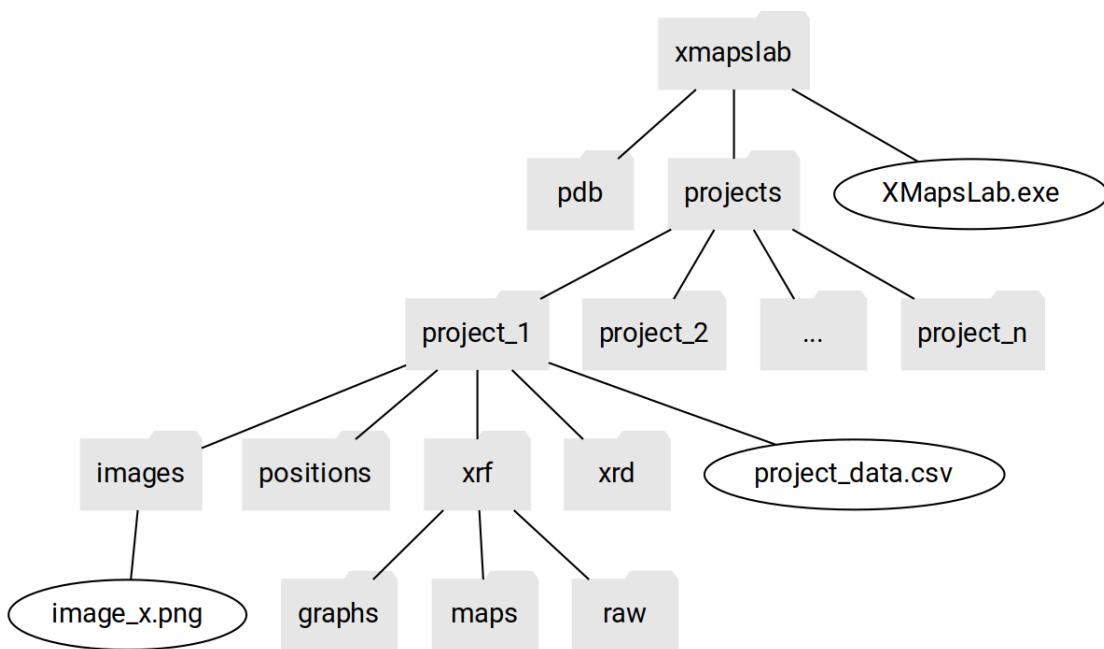


Figure 2.1: XMapsLab hierarchy

- **xrf**

This folder contains the data obtained by X-ray fluorescence. There are three folders to structure the data:

- **graphs (future work)**

This folder contains the graphs of the spectral data produced by **Interpreter** program.

- **maps**

This folder contains the maps produced by **XMapsLab** program.

- **raw (future work)**

This folder contains the files with the raw data produced by the scanning device and used by **Interpreter** to interpret the spectral data and produce elements and/or pigments.

- **xrd**

This folder contains the data obtained by X-ray diffraction. There are the same three folders as in **xrf** folder, with the same functionality.

Apart from the folder structure, the most important file to be able to run **XMapsLab** is the **project_data.csv** file. The information it should contain and how it can be created is described below.

2.2 The file with the project data

In addition to the folder structure, the most crucial file required to run **XMapsLab** is the [project_data.csv](#) file. This file contains all the information used by **XMapsLab** to generate the maps. It includes general details such as the project or artwork name, positions where measurements were taken, and the values of various elements and/or pigments measured and validated by the expert.

Here is an example of a [project_data.csv](#) file:

```
XML;1.0.0
PROJECT_NAME;Test
AUTHOR;DMP
DATE;18/05/20
DEVICE;DUETTO1
TUBE;CU
XRF_DATA_ADJUSTMENT;ATOMIC_NUMBER
WIDTH;2696
HEIGHT;3668
CS_ORIGIN;TOP_LEFT
POSITION; -;1;2;3;4;5;6;7
X; -;475;1273;1546;2365;2190;1294;1390
Y; -;2269;564;1369;2083;2512;2890;1844
XRF;Fe;0;62,344696;1314,839355;1685,118774;2614,584229;2015,744141;30,807642
XRF;Hg;926,384766;911,458984;3,695817;811,449341;7,174562;5,541962;776,76532
XRD;Calcita_Co;80,279877;259,103699;5,858643;291,345825;94,898193;97,665283;30,607697
```

The first thing to note is that there are certain words marked in blue. These words are mandatory and should be capitalized as shown. These keywords indicate the meaning of the data that follows. For example, after **AUTHOR**, we can input the name of the file's author. In some cases, as in the previous example, the text can be any text (following certain writing rules that will be discussed later), but for others, it will be necessary to choose from the available options.

It is important to mention that while the information in this file can be entered manually, it is more convenient to use the dedicated support programs: **Tools** for creating the file and entering basic information, as well as XRF and/or XRD data, and **Positions**, for specifying image dimensions and measurement positions.

In fact, for optimal execution of **XMapsLab** it is recommended to use the **Tools** program to copy the artwork image into the appropriate folder. This is because the image dimensions must meet certain restrictions (being a multiple of 4) for optimal memory usage. The **Tools**, program will adjust the image dimensions if necessary.

The fields that must be included in the [project_data.csv](#) file are as follows:

- **XML**

This is the first field/word that must appear. It tells the program that it is a **XMapsLab** file type. The parameter that follows is the version number. Currently it is "1.0.0".

- **PROJECT_NAME**

This field contains the name of the project.

- **AUTHOR**

This field contains the name of the project author.

- **DATE**

The date on which the file was created (or any date that is relevant to the author) should be entered here. The format can be any that is valid for the user, e.g. [DD/MM/YYYY](#).

- **DEVICE**

The used device. It can be any text that describes the device.

- **TUBE**

The type of tube used in device. It can be copper, [CU](#), or cobalt, [CO](#).

- **XRF_DATA_ADJUSTMENT**

This field contains if the XRF data should be adjusted. The possible values are: the atomic number, [ATOMIC_NUMBER](#) or without adjustment, [NONE](#).

- **WIDTH**

The width of the input image in pixels.

- **HEIGHT**

The height of the input image in pixels.

- **CS_ORIGIN**

The origin of the coordinate system. It can be [TOP_LEFT](#) or [BOTTOM_LEFT](#).

- **POSITION**

This is an auxiliary field that helps to know the number of each position. First you have to include the **POSITION** identifier, then the hyphen, and then the numbers for the positions, starting at 1, all of them separated by the separator.

- **X**

This field contains the information of the x coordinate of each position that was used to do the scanning. First you have to include the **X** identifier, then the hyphen, and then the values, all of them separated by the separator. The values must be in pixels. It is important to note that hyphen has no use but serves to align the information when it is imported by a spreadsheet. You can use the comma or the point as decimal separator.

- **Y**

This field contains the information of the y coordinate of each position that was used to do the scanning. The same conditions are used as with **X** field.

- **XRF**

This field contains the information of the XRF data. First you have to include the **XRF** identifier, then the name of the element, e.g. "Fe", "K", "Hg", and then the

values, all of them separated by the separator. The values must be any valid value, real or integer, but internally they are treated as reals. You can use the comma or the point as decimal separator. If no information is available for any position, 0 should be entered.

You can introduce as many values as you want but the important parameter is the number of positions, the number of X coordinates (the number of Y coordinates must be the same). If there are less values than positions, the added values will be 0. If there are more values than positions, they are not taken into account.



The names of the elements must be the names that appear in the database.



Since **XMapsLab** can enable and disable the positions desired by the user, it is much easier and more convenient to take more data captures when performing this process and then disable those that are not desired than to check for missing measurements once the data analysis has started.

- **XRD**

This field contains the information of the XRD data. First you have to include the XRD identifier, then the name of the compound, and then the values, all of them separated by the separator. The values must be any valid value, real or integer, but internally they are treated as reals. You can use the comma and the point as decimal separator. If no information is available for any position, 0 should be entered. If there are more values than positions, they are not taken into account.

The [CSV](#) file (comma-separated values) is a text file that utilizes a specific character, typically a comma, to separate values within a table. It is commonly used to store tabular data in plain text format. This format offers the advantage of being easily readable and writable using a regular text editor, while also being importable by spreadsheet software such as Microsoft Excel or LibreOffice Calc. Similarly, these spreadsheet programs can export data to [CSV](#) format. Consequently, it is an ideal format for working with the required data, providing program and operating system independence.

2.2.1 Entering the data with a spreadsheet

Using a spreadsheet is the easiest, most convenient, and least error-prone method for creating the [project_data.csv](#) file. The data should be arranged as explained in the previous section. When saving the file, it's important to select the semicolon as the separator.

2.2.2 Entering the data with a text editor

Using a text editor, such as Microsoft's Wordpad in Windows, is an option that doesn't require any additional installation. Text editors are easy to use and familiar to most users. However, they are primarily designed for entering text, and tabulating data (which is necessary for working with numbers) can be cumbersome.

Nevertheless, we will explain how to create the following example, focusing on the main issues that may arise.

```
XML;1.0.0
PROJECT_NAME;Test
AUTHOR;DMP
DATE;18/05/20
DEVICE;XRF pistol
TUBE;Cu
XRF_DATA_ADJUSTMENT;ATOMIC_NUMBER
WIDTH;1000
HEIGHT;1000
CS_ORIGIN;TOP_LEFT
POSITION;-1;2;3
X;-475;1273;1546
Y;-2269;564;1369
XRF;Fe;0.0;12.34;20.45
```

To begin, open the text editor and create a new file. Save it with the name [project_data.csv](#).



The text must be saved without any formatting. This ensures that the file contains only the characters you have typed. Using a different format can cause problems when programs try to read the file.

The reason behind this is quite straightforward. When working with a text editor, we can enter words and modify their appearance. For instance, you could type the text "XML" which consists of individual characters for each letter. However, you might choose to make it appear bold, like this: **XML**. In this case, the displayed text "XML" changes to appear bold. However, the crucial point is that the text editor introduces invisible control characters to indicate the bold formatting. Although these characters are not visible to us, they are present in the saved file. To illustrate, when we save the word "XML" in the file, it appears as follows:

```
XML
```

but if we indicate that it should be written in bold, what will be in the file is something like this:

```
<bold>XML<\bold>
```

or this

```
?A ‘XML’?A>
```

With this example, it should be clear that the file [project_data.csv](#) should be saved only in pure text format.

Now let's enter each line. Place the cursor on the first line, at the far left (which is the default position), and type [XML](#) in all capital letters. Then, add 1 separator, which is a semicolon (;), and after that, you can add the text "1.0.0". Since we will be writing more lines, press the return or new line key.

It is important to understand the writing rules:

- Separators cannot be placed at the begining of the identifiers.
- Use one and only one separator between two values. For example, [XML](#) and its value, “1.0.0”.
- No separators can be placed after the last value.
- No other separator can be used (e.g. comma, “,”, period, “.”, white space, “ ”, tabulator, etc.).
- Each line is finished by pressing the return/new line key.

As mentioned earlier, it is crucial to be careful when writing the file and follow all the provided rules to avoid creating files that may look correct but cannot be read by the program.

It's important to understand that although the information stored in the file is the same, the way it is displayed in a spreadsheet (Figure 2.2(a)) or a text editor (Figure 2.2(b)) is different. Pay special attention to the case of the text editor: you may notice rows with multiple semicolons. This is because the number of columns is indicated by the number of semicolons. In the example file shown in Figure 2.2(a), there are 16 rows, and some of them have 2 columns while others have up to 5 columns. This means that the resulting [CSV](#) file will have 16 rows, and each row will have 4 semicolons to indicate the presence of 5 columns. In rows with only 2 columns, which imply a single semicolon, 3 additional semicolons must be added to indicate the maximum number of columns.



Although the calculation of the number of semicolons required is straightforward, manually including them, especially in cases with many columns, can lead to errors. It is highly recommended to always use a spreadsheet to create or edit the file.

This example also demonstrates how numeric data can be saved as integers or real numbers, allowing the use of either a period or a comma as the decimal separator.

With all the explanations provided, it should be clear how to enter the data for positions and the values of elements and/or pigments. For the X and Y coordinates of positions, it

A	B	C	D	E
1 XML	1.0.0			
2 PROJECT_Name	Test			
3 AUTHOR	DMP			
4 DATE	8/12/2021			
5 DEVICE	XRF PISTOL			
6 TUBE	CU			
7 XRF_DATA_ADJUSTMENT	ATOMIC_NUMBER			
8 WIDTH	1000			
9 HEIGHT	1000			
10 CS_ORIGIN	TOP_LEFT			
11 POSITIONS	-	1	2	3
12 X	-	250	500	750
13 Y	-	100	500	800
14 XRF	Cd	280,279	192,073	252,85
15 XRF	K	210	128,4	191,333
16 XRF	Sn	54,21	308	289,76
17 XRD	Calcite	3245	0	2435.5
18				
19				
20				

(a) Spreadsheet

```

project_data.csv — Kate
project_data.csv

1 XML;1.0.0;;
2 PROJECT_Name;Test;;
3 AUTHOR;DMP;;
4 DATE;8/12/2021;;
5 DEVICE;XRF PISTOL;;
6 TUBE;CU;;
7 XRF_DATA_ADJUSTMENT;ATOMIC_NUMBER;;
8 WIDTH;1000;;
9 HEIGHT;1000;;
10 CS_ORIGIN;TOP_LEFT;;
11 POSITIONS;-;1;2;3
12 X;-;250;500;750
13 Y;-;100;500;800
14 XRF;Cd;280,279;192,073;252,85
15 XRF;K;210;128,4;191,333
16 XRF;Sn;54,21;308;289,76
17 XRD;Calcite;3245;0;2435.5
18

```

(b) Text editor

Figure 2.2: Aspect of the `project_data.csv` file in a spreadsheet and a text editor.

is important to add a hyphen after the identifiers to align the values with the corresponding elements. When entering XRF and/or XRD data, simply start with the identifier, followed by the name of the element or compound, and then provide the corresponding values.

It's important to remember that positions and element/pigment values can be entered manually, but there is a simpler way to do it using the respective programs: **Positions** for positions and **Tools** for elements and/or pigments. For instructions on how to use these programs, refer to the corresponding chapters: **Positions** in [chapter 4](#) and **Tools** in [chapter 3](#).

Tools

Tools is a user-friendly program designed to simplify the process of creating a project. Its main purpose is to assist in creating the folder hierarchy for a project, adding the necessary [project_data.csv](#) file with all the project information, including the visible image, as well as facilitating the addition of XRF and XRD information. Each of these features is explained in more detail below.

Figure 3.1(a) depicts the initial state of the program, while Figure 3.1(b) illustrates the state after creating or opening a project.

- **Create project:** The first option allows you to create a project. If we click on this option, the program will request the following information:

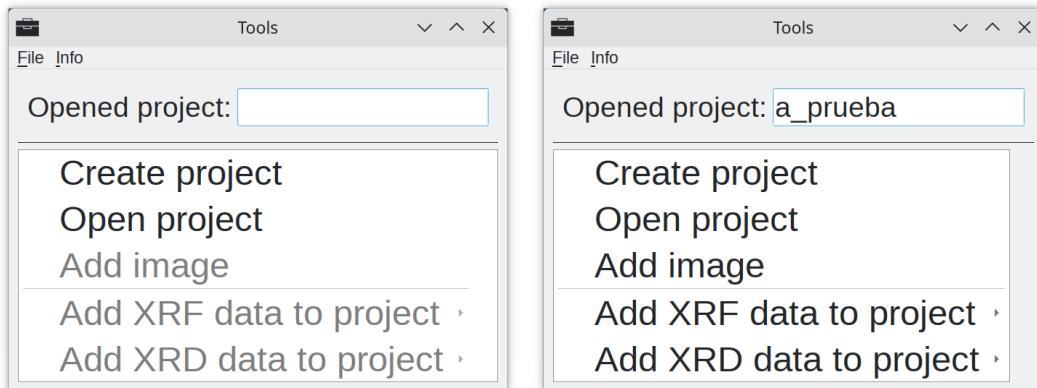


Figure 3.1: Tools

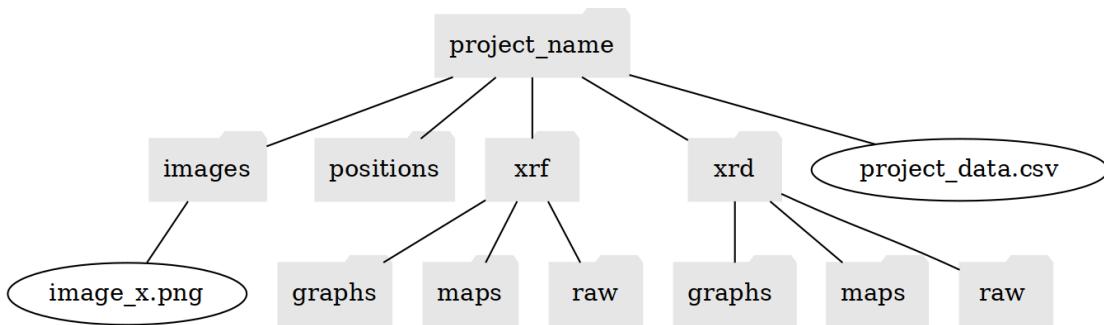


Figure 3.2: Project's structure

- **Project folder:** This is where you enter the name of the project folder that will contain all the other folders and files related to the project.
- **Project name:** This is where you enter the name of the project itself. This information, along with the details mentioned below, will be included in the [project_data.csv](#) file, which contains all the essential project information used as input by **XMapsLab**.
- **Author:** Here, you enter the name of the author of the project.
- **Date:** This field is used to specify the date of project initialization or any other representative date chosen by the user.
- **Device:** Enter the name of the scanning device used for data collection.
- **Tube:** Specify the type of tube used in the XRD scanning device. Currently, the options are copper (CU) or cobalt (CO).
- **XRF data adjustment:** This option allows you to adjust the saved XRF data by dividing the values by the atomic number. This adjustment takes into account the variations in captured information caused by differences in atomic number. Alternatively, you can choose to leave the data unchanged.

The hierarchy that is created is shown in [Figure 3.2](#). The [project_data.csv](#) file will be created with this content (the shown data is only for the example):

```

XML;1.0.0
PROJECT_NAME;Test
AUTHOR;DMP
DATE;18/05/20
DEVICE;DUETTO1
TUBE;CU
XRF_DATA_ADJUSTMENT;ATOMIC_NUMBER
WIDTH;0
HEIGHT;0
CS_ORIGIN;TOP_LEFT
POSITION;-
X;-
Y;-
  
```

	A	B	C	D	E	F	G	H	I	J	K
1	As	Ba	Ca	Cd	Co	Cr	Cu	Fe	Hg	K	Mn
2	4381155	281520	17249984	45900	0	0	2015392	3388950	261630	1945012	218408
3	4459950	353048	6232072	63495	0	70762	634185	2397510	113220	2436908	121252
4	6956528	626152	3531240	92565	0	0	668228	2656845	156825	1817258	0
5	8702258	862155	4048380	130050	0	0	574132	2015010	237532	1408748	0
6	9670342	1120342	4064456	173655	0	12622	184748	1400715	408128	1556392	0
7	7172640	839205	4094280	128138	0	0	30218	1501695	407362	2092658	0
8	6761452	705330	7060185	112072	0	100215	90270	1834088	167918	1692180	0
9	4688685	341572	5971972	60818	0	189720	440640	1635570	48195	2592968	0
10	2283525	203496	33492082	47812	1125698	12093502	281138	3181635	40928	7297718	0
11	2100690	320265	50715676	35955	765765	11217960	610470	2952135	28688	5239485	0
12	4860428	852592	21400876	96008	278078	3214530	1087830	5568435	196605	3029400	0
13	11359102	3061148	7269030	190102	314415	0	0	2083860	0	4505085	0
14	11897280	2626248	7697048	180540	367200	50490	70762	1454265	0	4375035	0
15	20965590	4111492	6150600	275400	410805	0	0	2555865	0	4142475	0
16	25871918	4451152	3807788	250538	386325	0	0	4443120	0	2732580	0
17	37088728	6479932	1815728	456512	0	0	0	3761888	0	1820318	0
18	47729116	8451720	989910	724072	0	0	0	5034848	0	913028	0
19	39745192	8147632	2820555	604732	0	0	0	2616300	0	1368202	0

(a) XLSX spreadsheet

1	4381155;1825128;17249984;...;0;1045012;1125698;12093502;281138;3181635;40928;7297718;0
2	4459950;353048;6232072;...;0;1945012;1125698;12093502;281138;3181635;40928;7297718;0
3	6956528;626152;3531240;...;0;1945012;1125698;12093502;281138;3181635;40928;7297718;0
4	8702258;862155;4048380;...;0;1945012;1125698;12093502;281138;3181635;40928;7297718;0
5	9670342;1120342;4064456;...;0;1945012;1125698;12093502;281138;3181635;40928;7297718;0
6	7172640;839205;4094280;...;0;1945012;1125698;12093502;281138;3181635;40928;7297718;0
7	6761452;705330;7060185;...;0;1945012;1125698;12093502;281138;3181635;40928;7297718;0
8	4688685;341572;5971972;...;0;1945012;1125698;12093502;281138;3181635;40928;7297718;0
9	2283525;203496;33492082;...;0;1945012;1125698;12093502;281138;3181635;40928;7297718;0
10	2100690;320265;50715676;...;0;1945012;1125698;12093502;281138;3181635;40928;7297718;0
11	4860428;852592;21400876;...;0;1945012;1125698;12093502;281138;3181635;40928;7297718;0
12	11897280;2626248;7697048;...;0;1945012;1125698;12093502;281138;3181635;40928;7297718;0
13	20965590;4111492;6150600;...;0;1945012;1125698;12093502;281138;3181635;40928;7297718;0
14	25871918;4451152;3807788;...;0;1945012;1125698;12093502;281138;3181635;40928;7297718;0
15	37088728;6479932;1815728;...;0;1945012;1125698;12093502;281138;3181635;40928;7297718;0
16	47729116;8451720;989910;...;0;1945012;1125698;12093502;281138;3181635;40928;7297718;0
17	39745192;8147632;2820555;...;0;1945012;1125698;12093502;281138;3181635;40928;7297718;0
18	1248832;3010275;5337842;...;0;1945012;1125698;12093502;281138;3181635;40928;7297718;0
19	2483128;3379012;53324899;...;0;1945012;1125698;12093502;281138;3181635;40928;7297718;0
20	3383522;3379012;53324899;...;0;1945012;1125698;12093502;281138;3181635;40928;7297718;0
21	2380698;238265;50715676;...;0;1945012;1125698;12093502;281138;3181635;40928;7297718;0
22	11897280;2626245;7697048;...;0;1945012;1125698;12093502;281138;3181635;40928;7297718;0
23	20965590;4111492;6150600;...;0;1945012;1125698;12093502;281138;3181635;40928;7297718;0
24	37088728;6479932;1815728;...;0;1945012;1125698;12093502;281138;3181635;40928;7297718;0
25	47729116;8451720;989910;...;0;1945012;1125698;12093502;281138;3181635;40928;7297718;0
26	39745192;8147632;2820555;...;0;1945012;1125698;12093502;281138;3181635;40928;7297718;0
27	1248832;3010275;5337842;...;0;1945012;1125698;12093502;281138;3181635;40928;7297718;0
28	2483128;3379012;53324899;...;0;1945012;1125698;12093502;281138;3181635;40928;7297718;0
29	3383522;3379012;53324899;...;0;1945012;1125698;12093502;281138;3181635;40928;7297718;0
30	2380698;238265;50715676;...;0;1945012;1125698;12093502;281138;3181635;40928;7297718;0
31	11897280;2626245;7697048;...;0;1945012;1125698;12093502;281138;3181635;40928;7297718;0
32	20965590;4111492;6150600;...;0;1945012;1125698;12093502;281138;3181635;40928;7297718;0
33	37088728;6479932;1815728;...;0;1945012;1125698;12093502;281138;3181635;40928;7297718;0
34	47729116;8451720;989910;...;0;1945012;1125698;12093502;281138;3181635;40928;7297718;0
35	39745192;8147632;2820555;...;0;1945012;1125698;12093502;281138;3181635;40928;7297718;0
36	1248832;3010275;5337842;...;0;1945012;1125698;12093502;281138;3181635;40928;7297718;0
37	2483128;3379012;53324899;...;0;1945012;1125698;12093502;281138;3181635;40928;7297718;0
38	3383522;3379012;53324899;...;0;1945012;1125698;12093502;281138;3181635;40928;7297718;0
39	2380698;238265;50715676;...;0;1945012;1125698;12093502;281138;3181635;40928;7297718;0
40	11897280;2626245;7697048;...;0;1945012;1125698;12093502;281138;3181635;40928;7297718;0
41	20965590;4111492;6150600;...;0;1945012;1125698;12093502;281138;3181635;40928;7297718;0
42	37088728;6479932;1815728;...;0;1945012;1125698;12093502;281138;3181635;40928;7297718;0
43	47729116;8451720;989910;...;0;1945012;1125698;12093502;281138;3181635;40928;7297718;0

(b) CSV data

Figure 3.3: Conversion from XLSX to CSV.

The [project_data.csv](#) file contains the basic information of the project that has been entered, such as the project name, author, date, device, tube type, and XRF data adjustment. However, it does not include the dimensions of the image, coordinates, XRF data, or XRD data, as those will be added in the next steps.

It is important to note that when a project is created, it remains open, allowing you to perform further operations and add more information to it.

- **Open project:** If you have previously created a project and want to perform additional operations on it, you can open it using this option. This allows you to identify the project on which the operations will be performed.

- **Add image:** To enable general visualization and create maps using **XMapsLab** with the MHD method, you need to include a color image in the project. This option allows you to select and add the desired image. It is recommended to use this option instead of manually placing the image in the appropriate folder. The program will not only copy the selected image to the images folder but also perform size adjustment for optimized calculations in **XMapsLab**. The image dimensions need to be multiples of 4 for hardware compatibility. If the image is manually copied without proper adjustment, it will be adjusted each time it is uploaded.
- **Add XRF data to project:** This option enables you to add XRF data to the [project_data.csv](#) file. XRF devices typically produce spreadsheets containing the measured results. The important information in these spreadsheets is the name of the detected element and the corresponding values obtained at each position. The data can be arranged in rows or columns. The common format used on Windows computers is usually XLSX.

For this option to work, the data needs to be saved in CSV format arranged by columns, as shown in Figure 3.3(b). You need to remove any unused values and keep only one column for each element, with the element name in the first row and the position values in subsequent rows.

To accomplish this with an XLSX spreadsheet, you simply remove irrelevant columns and export the data to CSV format, specifying the semicolon as the separator character. The saved file should be named [xrf_data.csv](#).

If the data is originally arranged in rows, it needs to be transposed before being processed.

By selecting this option, the program not only reads the information but also saves it in the appropriate format in the [project_data.csv](#) file. The XRF text is added to indicate that the included information is for XRF data. The resulting format is shown below.

```
XML;1.0.0
PROJECT_NAME;Test
AUTHOR;DMP
DATE;18/05/20
DEVICE;DUETTO1
TUBE;CU
XRF_DATA_ADJUSTMENT;ATOMIC_NUMBER
WIDTH;0
HEIGHT;0
CS_ORIGIN;TOP_LEFT
POSITION;-
X;-
Y;-
XRF;Fe;2345;145,33;28,9;1200;0;78
XRF;Hg;45;200,1,456;103,9;20;0;19,765
XRF;S;0;5,78,66;8,9;10;125;0
```

- **Add XRD data to project:** This option works the same as the previous one but for XRD data. Add the text "XRD" to identify the type of data. The name of the input file must be [xrd_data.csv](#). An example of the information added is shown below:

```
XML;1.0.0
PROJECT_NAME;Test
AUTHOR;DMP
DATE;18/05/20
DEVICE;DUETTO1
TUBE;CU
XRF_DATA_ADJUSTMENT;ATOMIC_NUMBER
WIDTH;0
HEIGHT;0
CS_ORIGIN;TOP_LEFT
POSITION;-
X;-  
Y;-
XRD;Cinnabar;2200;1500,22;998,4;1234;887;903,2
XRD;Lead_yellow;345;78;98;500,4;75;14,5
```


Positions

One of the most important tasks is to enter the coordinates of the measurement positions in the [project_data.csv](#) file. We have explained how to do this manually, but it can be a tedious and error-prone task, especially when dealing with a large number of positions. To address this, we have a solution: the **Positions** program (Figure 4.1). This program allows you to define measurement positions graphically and interactively. The position data can be saved to the [project_data.csv](#) file. Additionally, it provides the capability to generate an image with the marked positions, which can be printed and used as a guide for positioning the scanning device.

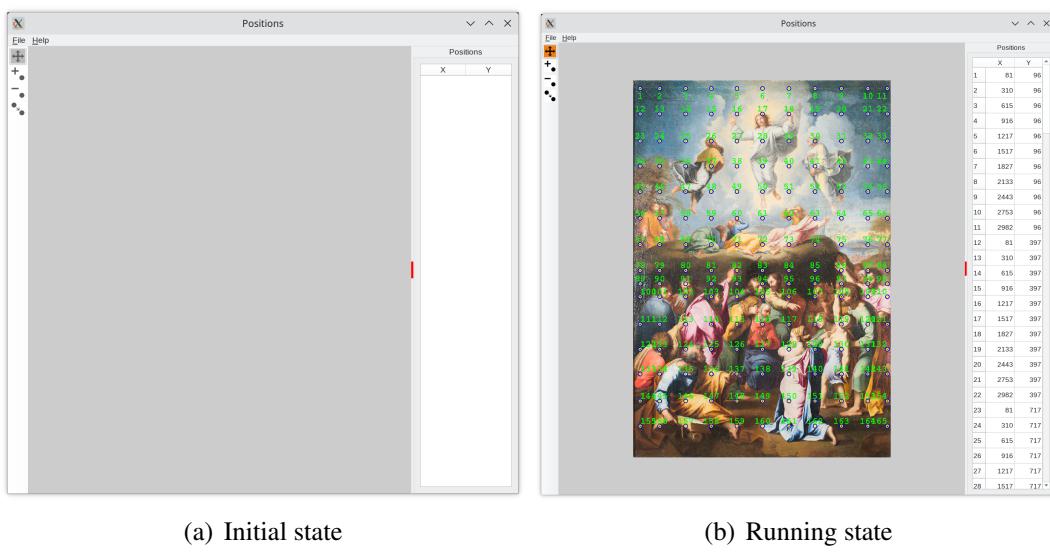


Figure 4.1: Two captures of the **Positions** program in the initial state and when the positions are introduced.

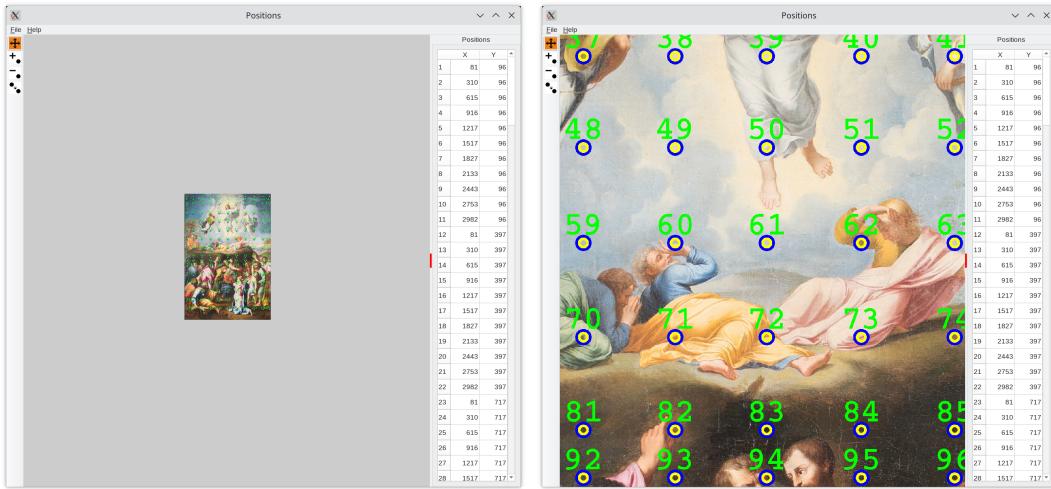


Figure 4.2: The mouse wheel allows to do zoom.

The images in [Figure 4.1](#) depict the program's information structure, with the toolbar on the left, the image display in the center, and the position information on the right. The initial state of the program when executed is shown in [Figure 4.1\(a\)](#).

The first two steps are as follows: indicating the project you want to work with and selecting the image that will be used to define the positions.

To select the project, go to the [File](#) menu and choose the [Open project](#) option. From the list of project names displayed, click on the desired project.

Once the project has been successfully loaded, the [Load image](#) option for the project will become active. Typically, there will be a single image used for all stages of the study, but the user has the flexibility to choose any image associated with the project.

After loading the image, the user can edit the positions where the measurements were or will be taken. If the project already has pre-defined positions, they will be displayed (as shown in [Figure 4.1\(b\)](#)). Otherwise, the image will be displayed without any markings.

The program offers various operations, including the following:

- Move the image

By default, the program is in a mode that allows you to move the image and zoom in or out for easier manipulation.

To move the image, simply press and hold the left mouse button, then move the mouse to adjust the position of the image accordingly.

To zoom in or out, you can use the mouse wheel. Scroll the wheel forward to zoom in and make the image larger, or scroll it backward to zoom out and make the image smaller. This zooming effect helps in performing various operations on the image ([Figure 4.2](#)).

- Add points 

To enter positions using the program, select this option by clicking on the corresponding icon with the mouse. Once selected, you can start adding positions to the image.

To add a position, move the cursor to the desired location on the image and press the right mouse button. This will create a circle to mark the position, and a position number will be assigned to it. The position number, as well as the X and Y coordinates, will be displayed in the right panel of the program.

It's important to note that the positions are given and stored in pixels, which correspond to the units of the image.

You can add as many positions as you need using this procedure. Additionally, while adding positions, you can also move the image or zoom in to make the selection process easier and more accurate.

- Remove points 

By selecting the option to delete positions, which can be done by clicking on the corresponding icon with the mouse, the user can remove positions from the image.

To delete a position, simply move the cursor to the desired position and press the right mouse button. This action will erase the circles and the corresponding number from the image. The position will also be removed from the right panel of the program.

It's important to note that there is a specific order for deleting positions. To avoid the complexity of renumbering positions if an intermediate position is deleted, it has been established that only the last position entered can be deleted. In other words, positions can only be deleted in the reverse order in which they were added.

- Move points 

By selecting the option to move positions, which can be done by clicking on the corresponding icon with the mouse, the user can relocate positions to new coordinates. This process involves two steps: selecting the position to be moved and then marking and moving it to the new position.

To select a position for moving, place the cursor near it and press the right mouse button. If the position is found, it will be highlighted with circles of a different color to indicate that it has been selected. Once the position is selected, simply move the cursor to the new desired position and select it by pressing the right mouse button. The position will then be marked at the new coordinates, and the point will be moved accordingly.

This allows the user to easily adjust the positions by dragging them to different locations on the image.

The right panel not only displays the order, x-coordinate, and y-coordinate of each position, but it also provides a convenient way to locate a specific position on the image. To find a position, simply click on any cell in the position's row, whether it's the order, x-coordinate, or y-coordinate. The entire row will change color to indicate that it has been selected, and the image will display large circles to highlight the corresponding position.

Once the positions have been marked and reviewed, the program offers two options to save the information:

- [Save image](#)

This option allows you to save an image with the position marks in the [positions](#) folder.

- [Save positions](#)

This option allows saving the data of the selected positions in the [project_data.csv](#) file. The x and y coordinates are stored for each position. It also saves the width and height data of the image. As previously indicated, the values that are saved are in pixels. Additionally the numbers of the positions are added using the field [POSITION](#). An example of the result is shown below:

```
XML;1.0.0
PROJECT_NAME;Test
AUTHOR;DMP
DATE;18/05/20
DEVICE;XRF pistol
TUBE;CU
XRF_DATA_ADJUSTMENT;ATOMIC_NUMBER
WIDTH;1000
HEIGHT;1000
CS_ORIGIN;TOP_LEFT
POSITION;-;1;2;3
X;-;475;1273;1546
Y;-;2269;564;1369
XRF;Fe;0.0;12.34;20.45
```



It is important that the image used to define the positions is the same as the one used by **XMapsLab**. As previously stated, it is convenient that this image has been processed and placed in the appropriate folder by the **Tools** program to optimize its use.

The option [Options](#) allows to change the parameters that control how the marks are shown: colors, font size, etc. ([Figure 4.3](#)).

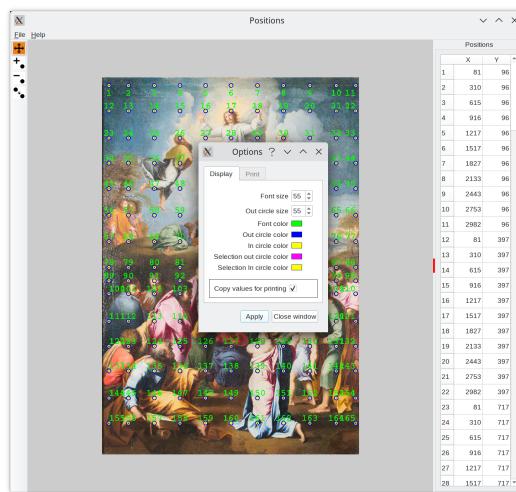


Figure 4.3: Widget to change the options

XMapsLab

XMapsLab is the program that allows you to generate maps from the information stored in the project folder, including the image and the data stored in the [project_data.csv](#) file.

Firstly, let's explain the general usage, and later we'll delve into the details and possibilities of the program.

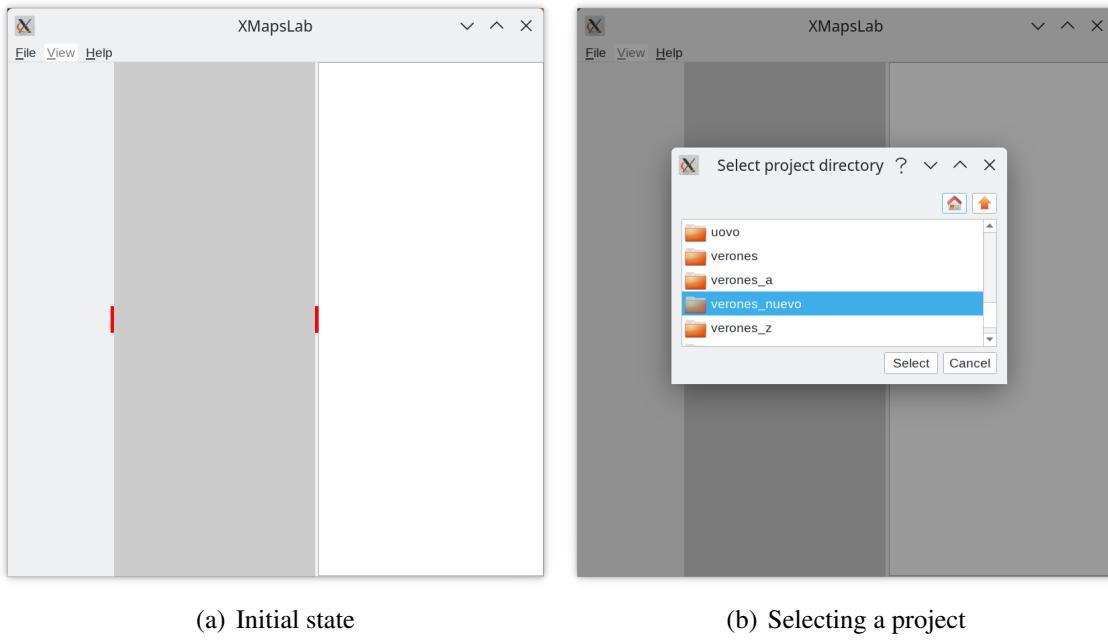
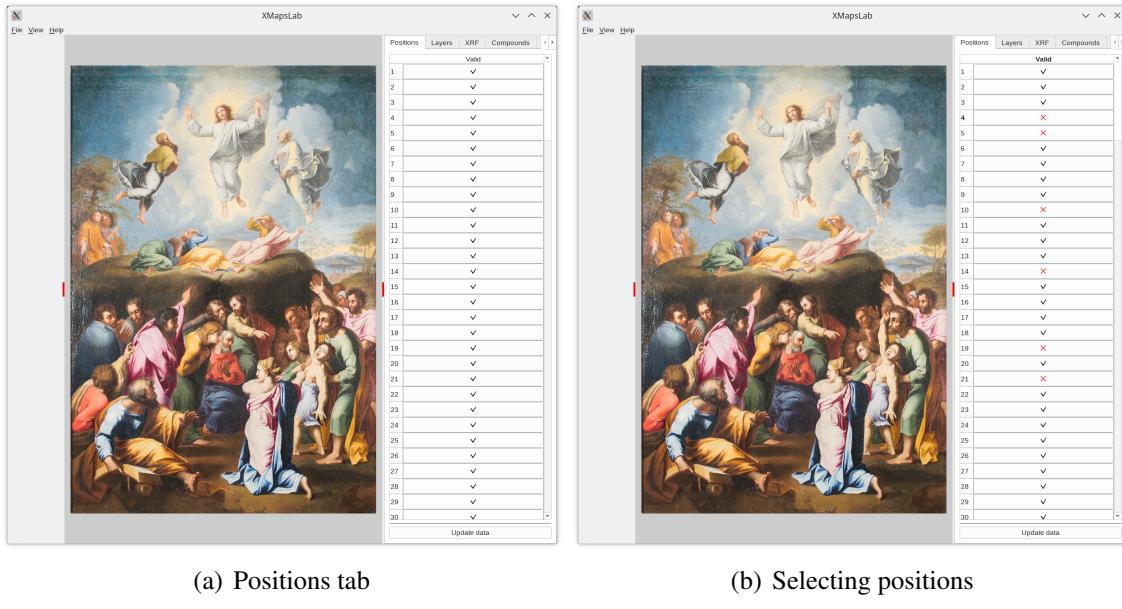


Figure 5.1: Two captures of the **XMapsLab** program in the initial state and selecting a project.



(a) Positions tab

(b) Selecting positions

Figure 5.2: The selection of positions that will be used to create the maps.

As mentioned earlier, it is necessary to have a properly created project, as explained in the previous chapters. In such a case, running the **XMapsLab** program is straightforward. The steps are as follows: load a project, select the positions to be used for creating the maps, choose the elements, select the interpolation method, and finally generate the maps. Once the maps are created, the program provides tools to visualize them. Let's follow this sequence of steps to explain the program's usage quickly.

When the program is executed, a window with a menu and three display areas will appear. Click on the [File](#) option from the menu, and then select [Load project data](#) (Figure 5.1(a)).

Select the project you want to work with by clicking on its name and then clicking on the [Select](#) button (Figure 5.1(b)). The program will display the color image in the central area, and the Positions tab will be selected (Figure 5.2(a)).

Next, we need to select the positions that will be used to create the maps. By default, all positions are selected, but the user can click on any of the rows shown in the right area to mark a position as invalid (Figure 5.2(b)). Similarly, clicking on a row that is marked as invalid will make it valid again. If there are many positions, this task can be tedious. In such cases, the workload can be reduced by changing the status of all positions at once. To do this, simply click on the header of the list where it says [Valid](#). To avoid multiple updates while selecting or deselecting positions, the changes are not applied for map creation until the [Update data](#) button is pressed.

The next step is to create the maps. To do this, we need to select the XRF tab (Figure 5.3(a)). Here, we can choose the image we want to use and the elements for which we want to create the maps. There are two options: select all elements or select specific ones.

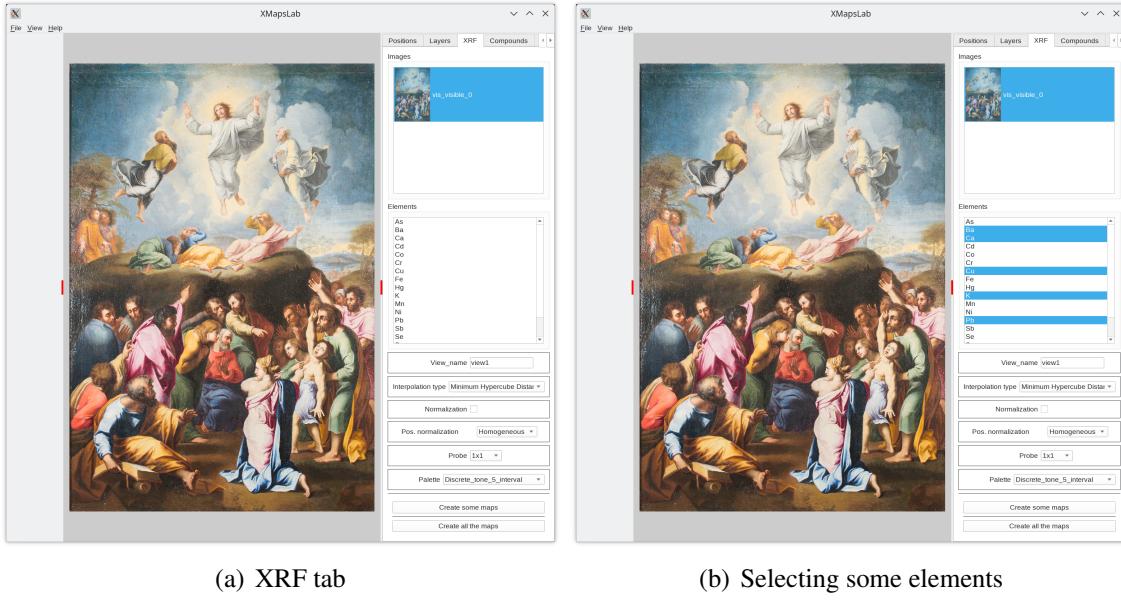


Figure 5.3: The XRF tab allow to select the elements for which the maps will be created, the method to be used and its parameters.

For the first case, simply click on the [Create all maps](#) button. For the second case, first select the elements by clicking on them, and then click on the [Create some maps](#) button (Figure 5.3(b)).

The program also allows us to select the type of interpolation and modify the parameters for each method. There is a field where we can add an identifier to the map's name, which can be useful for distinguishing different studied situations. Additionally, we can change the color palette used to assign colors to numerical values.

After clicking on one of the buttons to create the maps, the program will switch to the Layers tab (Figure 5.4(a)). Each created map is placed on a layer, and the layers are ordered in depth. The layer displaying the color image is at the top of the list, while the closest layer is at the bottom. This depth ordering allows for transparency and blending operations between layers.

Once the maps are created, the program automatically selects the closest layer. The color bar of the selected layer will be displayed on the left side of the application. The color bar illustrates the relationship between numerical values and colors. The appearance of the color bar changes depending on the selected palette. The program assigns a color to each element automatically, but this can be changed by the user. The values on the color bar can be displayed in various ways, which will be explained below.

Each layer is assigned a name that is automatically generated and provides information about how the map was created. The name includes the name of the element, the interpolation method used, and the parameters applied. Additionally, a number indicating the order of

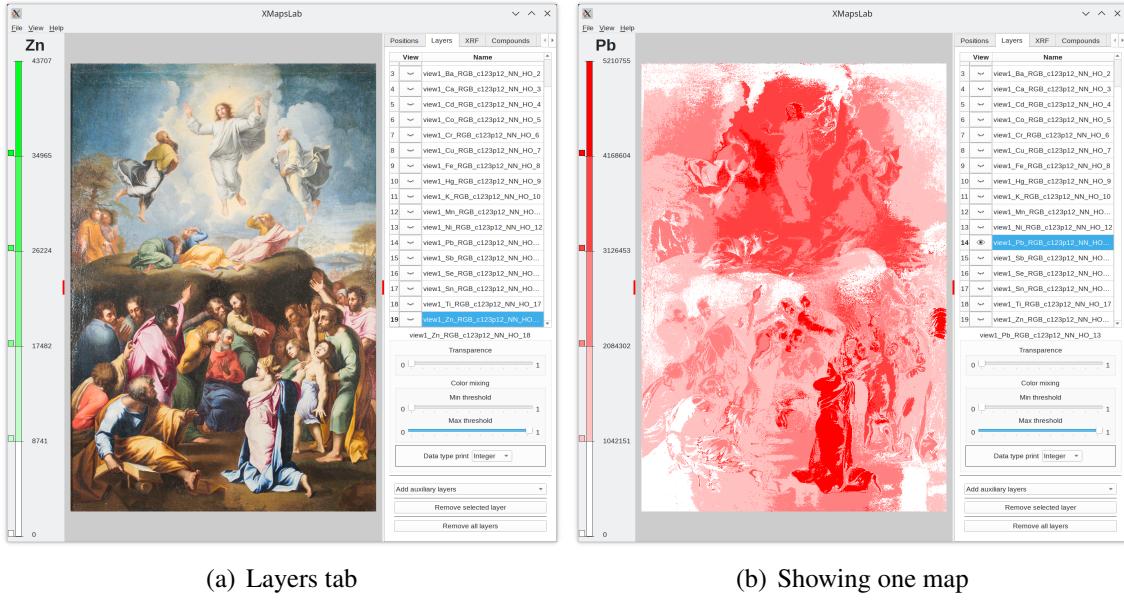


Figure 5.4: The Layers tab allows you to select the displayed map and apply effects such as transparency and blending to it.

layer creation is included. This ensures that all layers can be identified, even if they have the same values (for example, it is possible to create two layers with exactly the same values).

The next operation is to select the layer/map that we want to display in the display area. This can be done by clicking on the closed eye icon of the desired layer. When clicked, the map associated with the layer will be displayed, the selected layer will be highlighted, and the icon will change to an open eye (Figure 5.4(b)).

We can select any layer, and it is possible to select multiple layers (up to 8). However, it's important to note that there is an ordering based on depth, which means that the closest layer that is activated will be visible. When a layer is selected, the color bar for that layer will be displayed. By activating multiple layers, we can combine the results of the selected layers using transparency and color mixing.

Each layer can adjust the transparency, color mixing, and display of numbers on the color bar.

To change the transparency, simply move the **Transparency** slider. The default value makes the layer opaque, but moving the slider to the right increases transparency, allowing the layers below the selected layer to become visible. If the next visible layer at a lower depth has no transparency, color mixing will occur between the selected layer and that layer. However, if the next layer also has transparency, the layers will blend consistently, up to a maximum of 8 layers. It's worth noting that with more than 3 layers, it can become difficult to distinguish the contribution of each individual layer. An example of the transparency effect is shown in Figure 5.5(a).

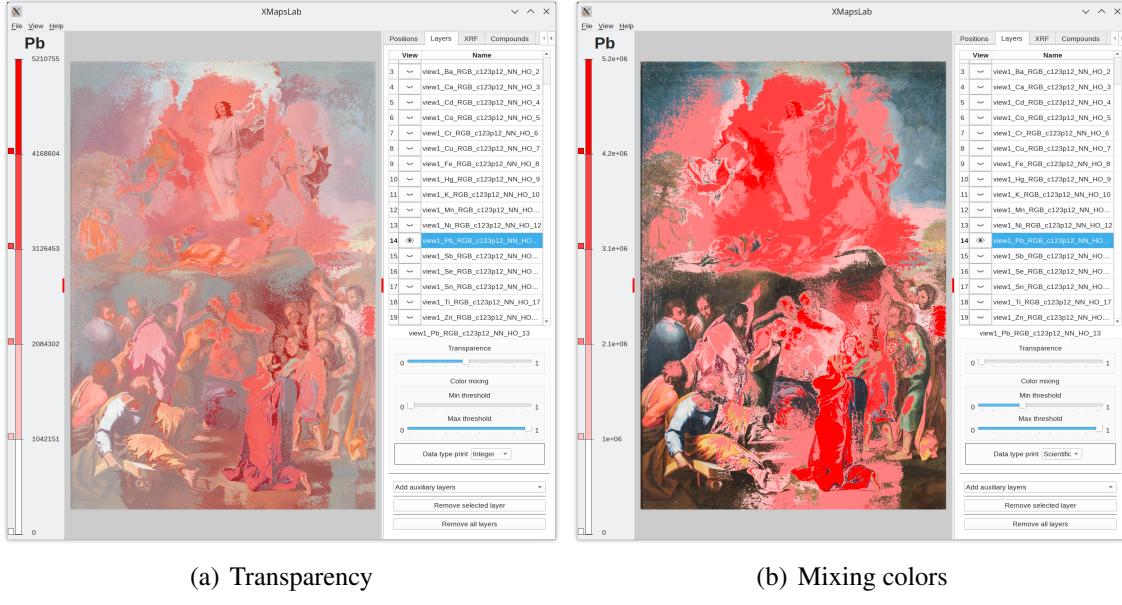


Figure 5.5: It is possible to change the transparency and the mixing colors attributes of the maps.

Another combination possibility is color mixing. For this, we have two sliders: one for the minimum threshold and another for the maximum threshold. Here's how it works:

- The minimum threshold determines the minimum value from which the layer's values will be displayed. Any values below this threshold will result in full transparency, allowing the next visible layer to show through.
- The maximum threshold works similarly, but in reverse. Values below the maximum threshold will display the selected layer, while values greater than the maximum threshold will result in total transparency.

This color mixing effect allows for more selective display of specific value ranges within a layer. An example of the color mixing effect is shown in Figure 5.5(b). It's important to note that you can combine multiple layers with transparency, multiple layers with color mixing, or any combination of these attributes.

By adjusting the thresholds and transparency settings for each layer, you have the flexibility to create complex and visually informative combinations of maps.

5.1 A detailed explanation

In this section, we will provide a detailed explanation of the different sections and functionalities of the **XMapsLab** program.

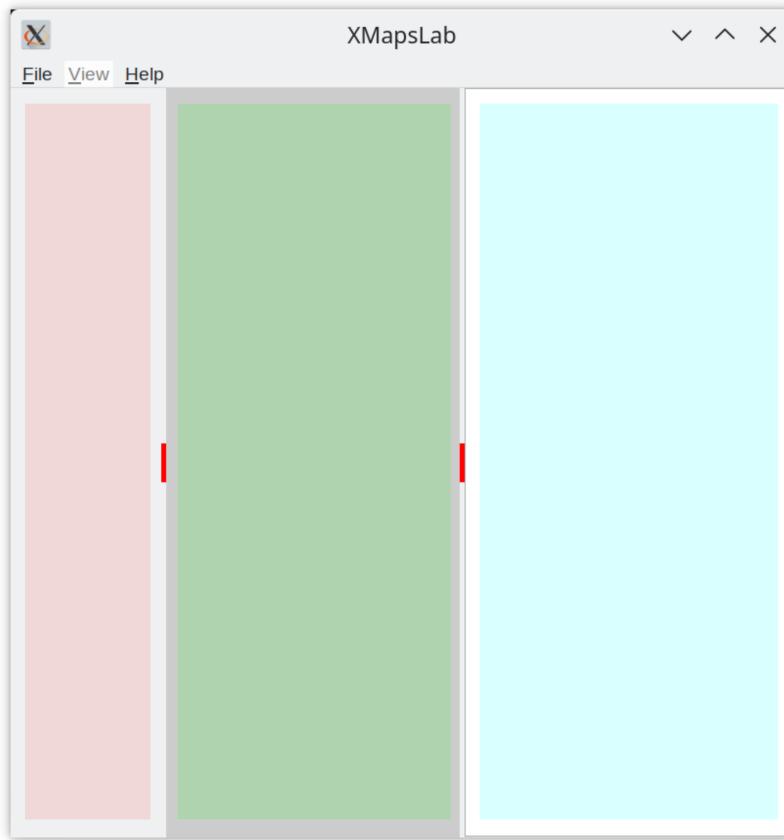


Figure 5.6: The main zones of the program: Color bar zone (red color), Display zone (green color) and Control zone (blue zone).

The program consists of three main sections, as shown in Figure 5.6. Let's explore each section in more detail:

- **Left Zone:** This area displays the color bar and associated numerical information of the selected layer. If the selected layer represents an element or compound map, the color bar will provide a visual representation of the numerical values. This section is particularly useful for understanding the color-coding scheme used in the maps.
- **Middle Zone:** This area displays the resulting image, which can be a single layer or a combination of up to eight layers. You can manipulate the image in this area by changing the observer's position and adjusting the zoom level. These operations allow you to explore the maps from different perspectives and magnifications, providing a more detailed view of the data.
- **Right Zone:** This area is the control area, where you can define the parameters and settings for the calculations and display. It is organized into different tabs, each serving a specific purpose. The tabs provide access to various functionalities and options related to map generation, visualization, and customization.

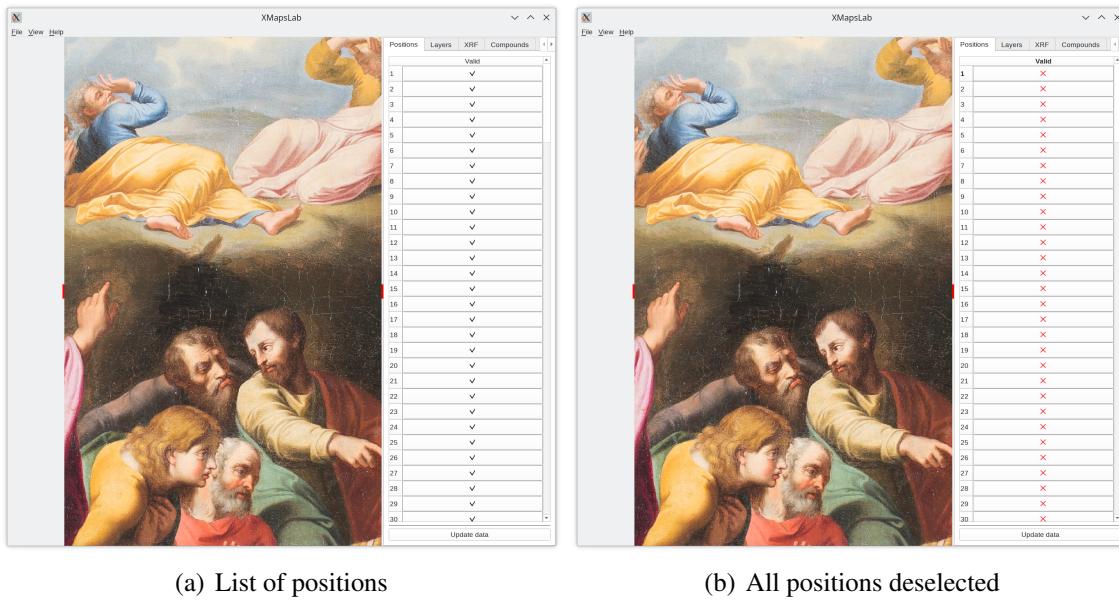


Figure 5.7: The positions tab shows the list of positions and their state, selected or unselected. They can be changed individually or all at the same time.

Understanding the layout and functionalities of these three sections is crucial for effectively using the **XMapsLab** program. It allows you to interact with the maps, explore different visualizations, and customize the display according to your needs.

5.1.1 Control zone

In the right zone of the program, you will find tabs that enable you to access different types of actions and functionalities. Let's explore each tab in more detail:

- **Positions** tab

When the "Positions" tab is selected, a list of all the positions stored in the "project_data.csv" file is displayed (5.7(a)). Each position is represented by a row, and there is a button indicating whether the position is active or deactivated. By clicking on each button, the user can change the state of the position, and clicking it again will revert it to its original state. The status of all positions can be changed at once by clicking on the header of the list, specifically on the text **Valid** (5.7(b)). To ensure that all the changes are applied and the positions are updated, it is necessary to click on the **Update data** button.

- **Layers** tab

When this tab is selected, all the information about the created layers is displayed, arranged in a stack (Figure 5.8). It's important to understand the concept of a layer

and a layer stack. A layer represents a 2D image along with its associated parameters. A layer stack represents a collection of images stacked on top of each other, with a specific depth order. The layers are ordered such that the topmost layer is at the bottom of the list, and the bottom layer (initial image) is at the top of the list. The user's perspective is positioned at the bottom of the screen, looking towards the top part of the screen. The layers are displayed from bottom to top of the stack (top to bottom of the list).

To modify the order of the layers, a click-and-drag operation can be performed. Simply click on a row to select the layer, hold down the left mouse button, and move the mouse up or down to reposition the layer within the stack. It's worth noting that the initial image layer, which represents the bottom layer, cannot be moved and always remains at the bottom of the stack.

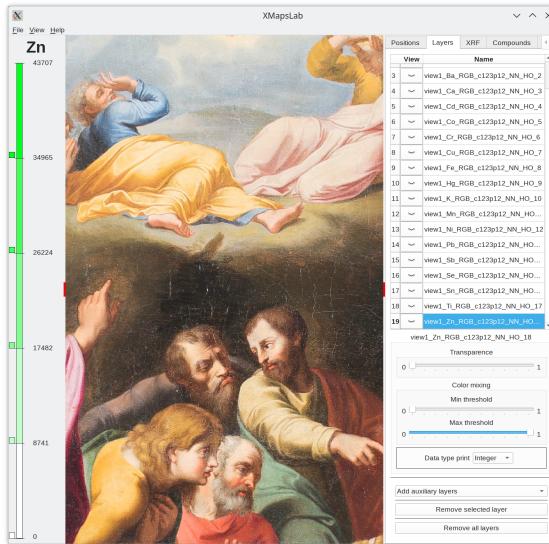


Figure 5.8: Once all the selected maps are created they appear as layers in a stack. The top layer is selected but is not visible. Its color bar is shown.

Each layer has an important attribute: visibility. When a layer is activated, it becomes visible, while deactivating it makes the image invisible (Figure 5.9). To activate the visibility of a layer, simply click on the eye icon. The eye icon is closed if the layer is currently invisible, and it is open if the layer is visible.

The order of the layers directly affects their visibility (Figure 5.10). Assuming that no transparency or color mixing effects have been applied to the layers, only the layer with active visibility at the top of the stack will be visible. If we want to see a layer that is currently hidden by other layers, we need to either make the layers above it invisible or rearrange the stack by moving it to a position higher than the other visible layers.

To display the information from multiple layers simultaneously, the program provides operations to adjust the transparency and color mixing of each layer individually.

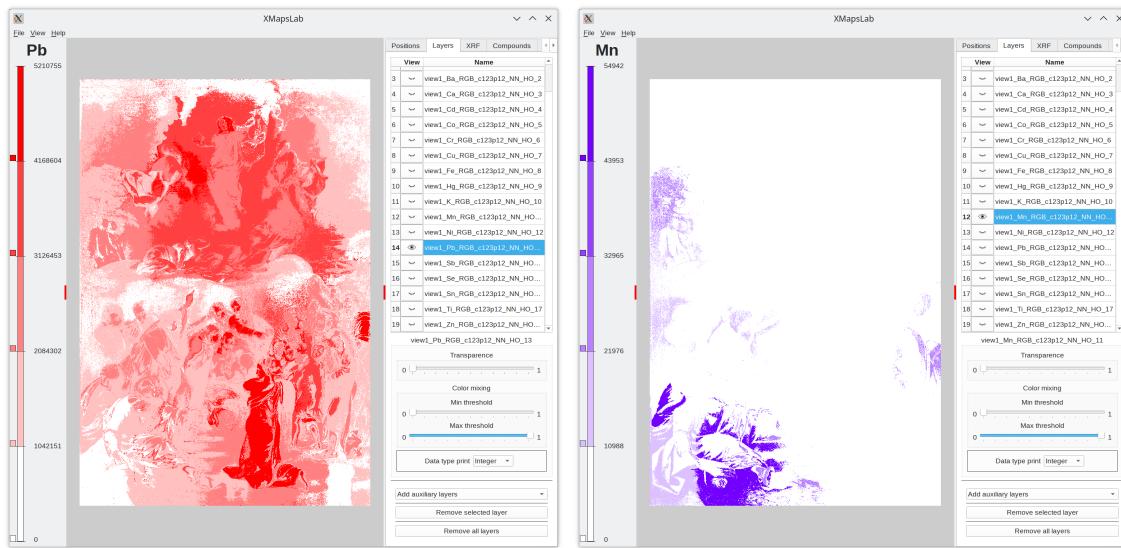


Figure 5.9: Making visible one layer. Its color bar is shown. Two examples with only one layer visible.

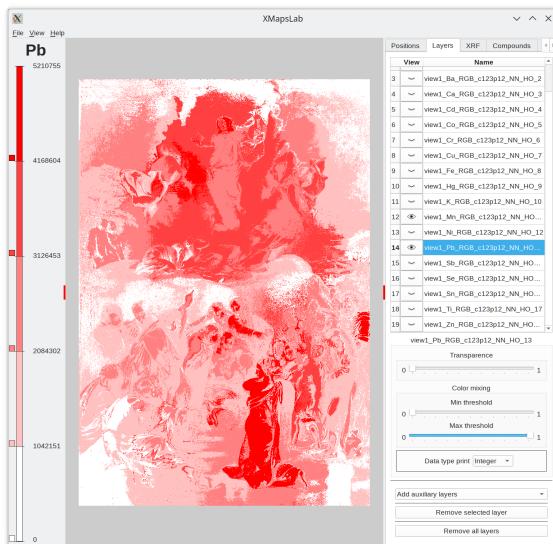


Figure 5.10: The order in the stack affects the final result. The top layer hiddens the one that is below.



These operations are carried out on the layer that is selected.

Adjusting the transparency level using the slider allows us to control the visibility of a layer. By increasing or decreasing the transparency, we can make the layer partially visible. For example, if there are two visible layers and we adjust the transparency

of the top layer, we will be able to see the layer below it. However, if we adjust the transparency of the bottom layer, there will be no visible change because the top layer is opaque. The same principles apply when working with more than two visible layers. It's important to note that transparency represents a linear combination of colors, where the slider determines the proportion of the image to be combined.

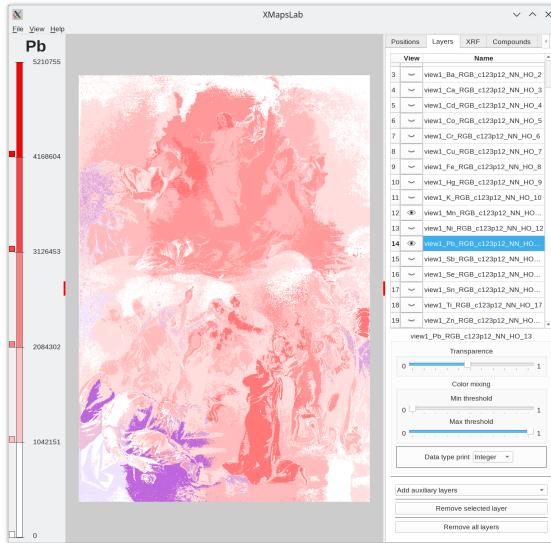


Figure 5.11: Applying transparency to the top layer allows to see the layer that is below.

Color mixing involves a substitution operation based on thresholds. It requires setting a minimum threshold and a maximum threshold. The substitution operation works as follows.

For the minimum threshold, if the value of a pixel in the selected image is less than or equal to the minimum threshold value, it is replaced with the corresponding pixel value from the next visible layer. However, if the pixel value exceeds the minimum threshold, the pixel value remains unchanged.

Similarly, for the maximum threshold, if the pixel value is less than or equal to the maximum threshold, it remains unchanged. But if the pixel value exceeds the maximum threshold, it is replaced with the pixel value from the next visible layer.

This process allows for color substitution based on the defined thresholds, resulting in a mixed color effect where pixel values from different layers are combined (Figure 5.12).



Transparency and color blending operations can be used without any limitations.

The last parameter that can be changed individually for each layer is the type of numerical data that is shown in the color bar, the possibilities being integer, real, scientific or percentage.

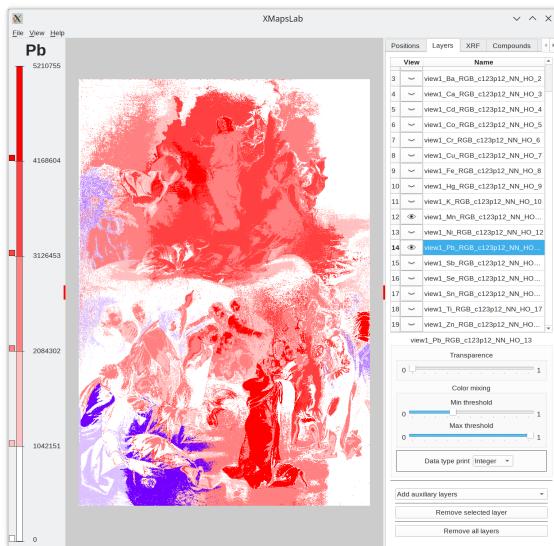


Figure 5.12: Applying color mixing to the top layer allows to combine it with the layer that is below.



The default type can be changed in [Options](#).

In the bottom part of the Layers tab, there are buttons available to perform certain actions on the layers. The first button, [Remove selected layer](#), allows you to delete the currently selected layer. If you want to remove all the layers at once, you can click on the [Remove all layers](#) button.

Additionally, there is a feature that allows you to add auxiliary layers that are not related to specific elements or compounds. Currently, the only available option is to create a layer using the "Difference of Gaussians" method. This method generates an image that highlights contours, which can be useful for identifying different regions or boundaries. Similar to other layers, you can apply transparency operations to this auxiliary layer.

The "Difference of Gaussians" layer also has its own set of parameters that can be modified to adjust the resulting image. These parameters include the Gaussian threshold, Big Gaussian size, and Small Gaussian size. Changing these parameters will produce different visual outcomes, allowing you to explore and fine-tune the appearance of the image.



Normally only the parameters that change the sizes of the Gaussians will be changed

The [Pixel transparency](#) option is a unique feature that distinguishes it from the regular transparency option. It specifically targets the pixels in the image that represent

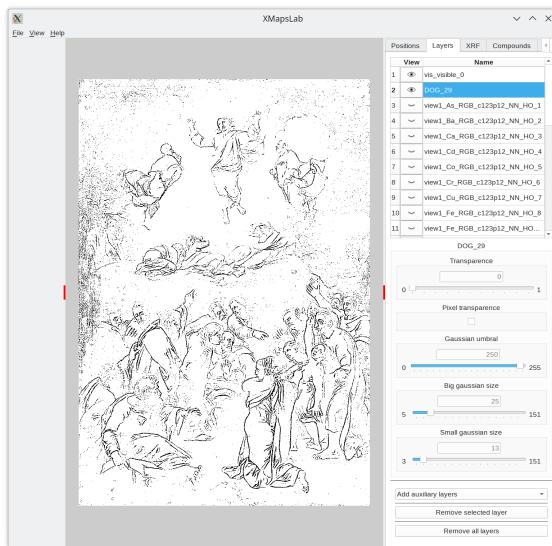


Figure 5.13: It is possible to create an image with the contours of the selected layer. The normal use is with the color image, which must be selected.

contours. In this case, white pixels are considered as non-contour areas and will be fully transparent, while black pixels are considered as contour areas and will be fully opaque. This allows for a clear visualization of the contours while maintaining transparency for the non-contour regions.

When creating a layer with contours using the "Difference of Gaussians" method, it is typically applied to the active layer. While it can be applied to map layers, it is more commonly used on the initial image layer ([Figure 5.13](#)). The resulting layer with contours is placed just above the selected layer in the layer stack. To see the effect of the contours in relation to the map layers, it is necessary to move the contours layer to the top of the stack so that it is displayed above the map layers. This will allow you to observe the contours in combination with the map data ([Figure 5.14](#)).

- [XRF tab](#)

In the XRF tab, you have the option to define the image and elements for which the interpolation operations will be performed. To select the image, you can simply click on it in the list of available images ([Figure 5.16](#)). This will indicate which image will be used for the interpolation calculations.



In the current implementation, there is only one image available to select

Once the image is selected, you can proceed with selecting the elements for which the interpolation will be performed. There are two possibilities: selecting all elements or selecting specific elements. To select all elements, click on the [Create all maps](#) button. This will generate maps for all elements present in the selected image.

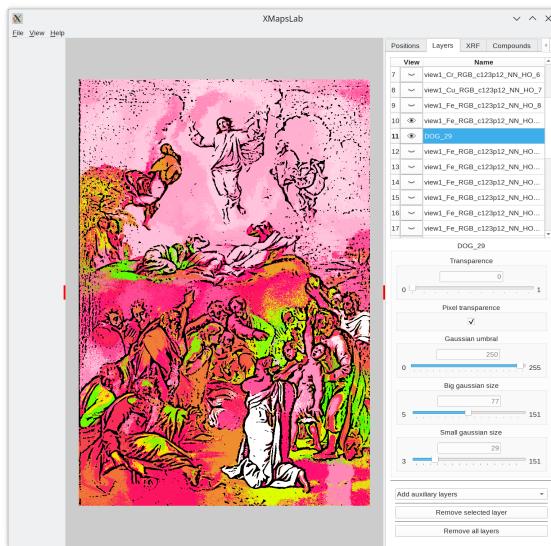


Figure 5.14: The layer with the contours image is moved above one map and the [Pixel transparency](#) is active to show the map.

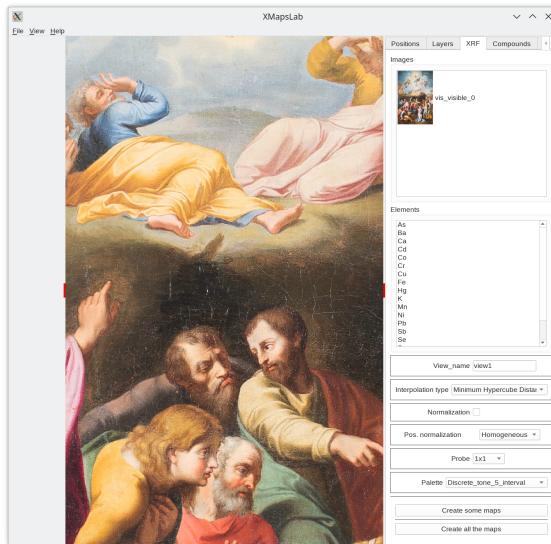


Figure 5.15: The initial state of the XRF tab.

For the selection of elements, you have two options: selecting a few or selecting all. To select an element, simply click on its name. Clicking again will deselect it. You can select as many elements as you want using this mechanism. If you only want to create the map for one or a few elements, once they are selected, click on the [Create some maps](#) button.

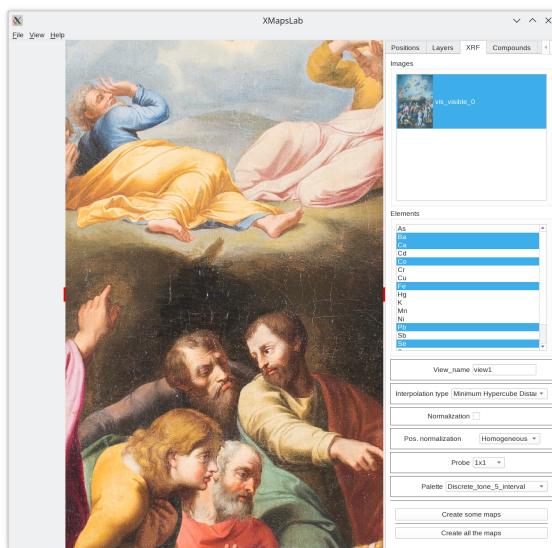


Figure 5.16: One image must be selected and also the elements that will be computed. One possibility is to not select any element and click on [Create all the maps](#) button. The other possibility is to select some of them by clicking on their names and then click on the [Create some maps](#) button. In the image, some of the elements have been selected. The interpolation method is Minimum Hypercube Distance, so its parameters are shown (they are the same for Minimum 2D cartesian distance method).



The layers that are created are placed on top of the one that is selected. In the first time only the color image is in the stack.

In the case where you want to obtain the maps of all the elements, you could select all the elements and then click on the [Create some maps](#) button. However, it is easier and faster to click on the [Create all the maps](#) button. In this case, it is not necessary to select any element individually since it is understood that all elements are selected by default.

To create each map, you have the following options:

- [View_name](#).

When creating a layer, a unique name is assigned to each layer, which provides information about the parameters that have been used. This is important not only for display purposes in the application but also for naming files if layer images are saved. To personalize the name, this field allows you to add text at the beginning of the name.

- [Interpolation type](#).

This parameter enables you to modify the type of interpolation function that will be utilized. Depending on the selected type, its specific parameters will be displayed for further customization.

* **Minimum Hypercube Distance (Figure 5.16)**

For this method the following parameters can be changed:

- **Normalization:** This parameter enables or disables the normalization of the calculated values. When activated, the assigned value is influenced by the variation in the calculated distance. On the other hand, when deactivated, the assigned value remains constant regardless of the variation in the calculated distance.



The original method applies normalization.

- **Pos. normalization:** This parameter controls whether positions are normalized for both x and y coordinates, regardless of the ratio of the image's width to height. When enabled, this normalization can cause deformation in non-square images, where a circle may appear as an ellipse due to the distortion introduced by the normalization process.



The original method applies normalization.

- **Probe:** This parameter specifies the number of pixels used to calculate the color of the pixel being processed. If the “1x1” option is chosen, it indicates that only the color of the current pixel is considered. When selecting the “3x3” option, the color is calculated by including the 8 neighboring pixels. The final color is obtained as the average of these 9 pixels. Similarly, with the “5x5” option, the color is generated using 25 pixels following the same process. This continues for the remaining options, up to “49x49”. The purpose of this operation is to reduce any noise present in the image.

* **Minimum 2D Cartesian Distance**

The parameters are the same as the previous method.

* **RBF (Figure 5.17)**

If we select the RBF method we can change the following parameters:

- **Function:** This parameter enables you to select the type of radial function that will be utilized. You can choose from different options available, such as Gaussian, Multiquadratics, Inverse Multiquadratics, etc. Each radial function has its own characteristics and behavior, allowing you to customize the interpolation process based on your specific needs.
- **Radius:** Through this parameter, you can adjust the extension of the Gaussian, Multiquadratics, and Inverse Multiquadratics functions. It allows you to modify the shape or range of these functions according to your specific requirements.

* **Triangulation (Figure 5.18)**

For this type we only have the possibility of adding or not the corners.

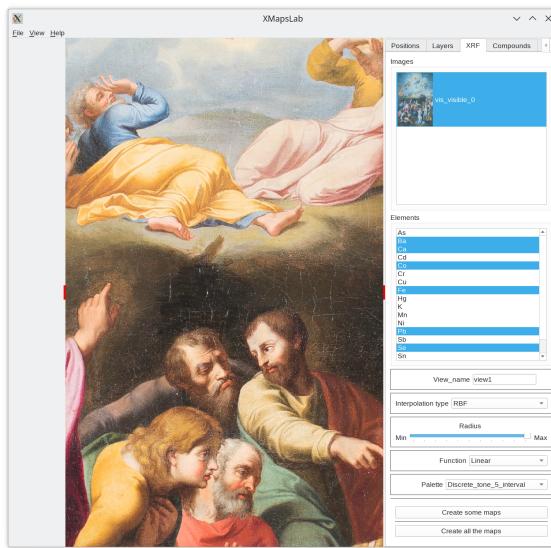


Figure 5.17: The parameters of the Radial Basis Function method are shown.

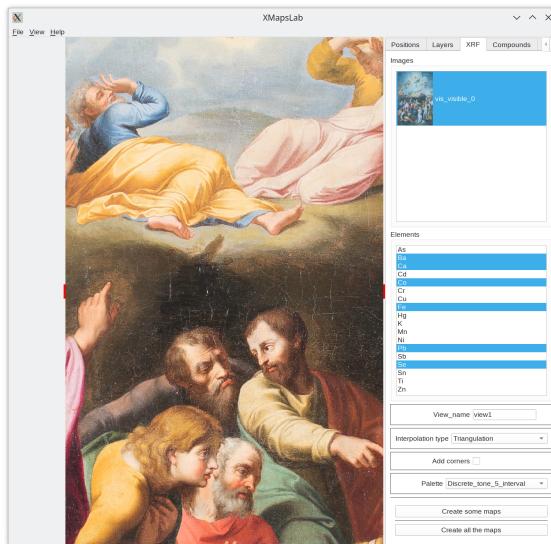


Figure 5.18: The parameters of the Triangulation method are shown.

– Palette

The creation of the maps involves calculating the value of an element for each pixel. These calculated values need to be matched with a color table, which is referred to as a palette. Different palettes are available, each catering to various scenarios. Some palettes include options such as using a single color, multiple colors, continuous gradients, or sectioned gradients. The default palette can be modified in the [Options](#) submenu.

- [Compounds](#) tab

By clicking on this tab, you can generate maps of potential compounds that are viable

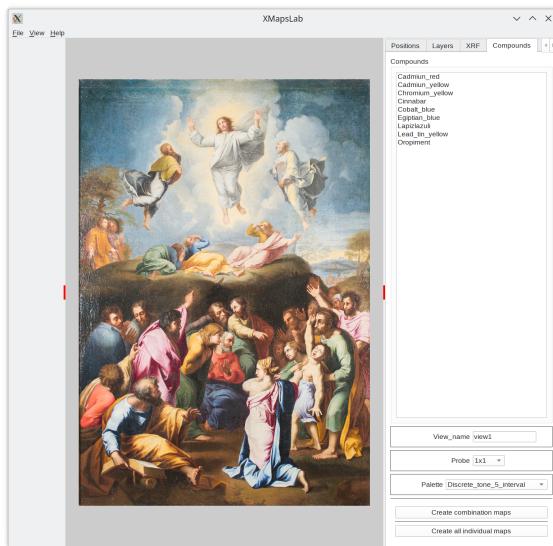


Figure 5.19: The initial state of the [Compounds](#) tab.

based on the selected elements. This process involves utilizing the formulas that define each compound and conducting a search to verify which formulas are fulfilled. When a match is found, a map is created using the selected element maps. For instance, if you want to determine if cinnabar is possible, the program will first check for the existence of the elements Hg and S. If they are present, the cinnabar map is generated using the Hg and S maps.

The tab displays a list of compounds that can be searched. You can select the compounds you wish to search for by clicking on their respective names.

The parameters that can be modified include [View_name](#) [Probe](#) and [Palette](#), which we have already explained previously.

Finally, there are two buttons provided to create the maps:

- [Create combination maps](#): This option enables you to create compound maps by considering ALL the selected compounds. It attempts to find the proportions of the elements in such a way that all the compounds can be defined based on the information provided in their formulas. This means that the program will try to determine the appropriate ratios of elements to satisfy the formulas of all the selected compounds simultaneously. By utilizing this option, you can obtain compound maps that encompass all the chosen compounds.
- [Create all individual maps](#): This option generates maps for all the compounds, regardless of whether they have been selected individually. It treats each compound as if it were the only one found in the data. In other words, the program creates separate maps for each compound, isolating its presence and properties as if it were the sole compound in the dataset. This allows you to visualize and analyze the characteristics of each compound independently.

5.1.2 Display Zone

The display zone is utilized to showcase the resulting image after selecting, activating, and performing operations on the layers. It also provides supplementary information such as the positions where measurements were taken and the triangulation obtained from these positions (excluding the corners).

Moreover, you can adjust the position of the observer by clicking the left mouse button and dragging it. Zooming in or out of the image can be accomplished using the mouse wheel.

A double click with the left mouse button centers the camera.

A double click with the right mouse button resets the camera to the initial distance.

5.1.3 Color Bar Zone

The color bar zone displays the color bar corresponding to the selected layer (see Figure [ref:xml:colormap1]) if it has a map of an element or compound. Otherwise, it remains empty.

The color bar visually represents the assignment of colors to values. This assignment depends on the chosen palette in the XRF tab. The numerical values on the color bar can be displayed in four formats: integers (see Figure 5.21(a)), real numbers (see Figure 5.21(b)), scientific notation (see Figure 5.22(a)), and percentage values (see Figure 5.22(b)).

The number of steps chosen when selecting the palette determines the number of color boxes that represent the same range of values. The minimum number of steps that can be selected is 2, representing the minimum and maximum values. If the number of steps is increased, they are evenly distributed across the entire range. For example, if 3 steps are chosen, the color bar will display the minimum value, the average value between the minimum and maximum, and the maximum value. The same principle applies to 4 or 5 steps.

To obtain the colors, we distinguish between palettes that use tones and those that use colors.

For tone-type palettes, a gradient of a single color is used based on the base color assigned to the minimum value. The base color can be white or black, and this parameter can be modified in the [Options](#) submenu.

Within tone-type palettes, there are two assignment options: gradual assignment or step assignment. In gradual assignment, the tone varies linearly between each pair of steps. In step assignment, the tone corresponds to the value of the specific color box and extends to the next box.

For color-type palettes, the same options as tone-type palettes are available, but with different colors.

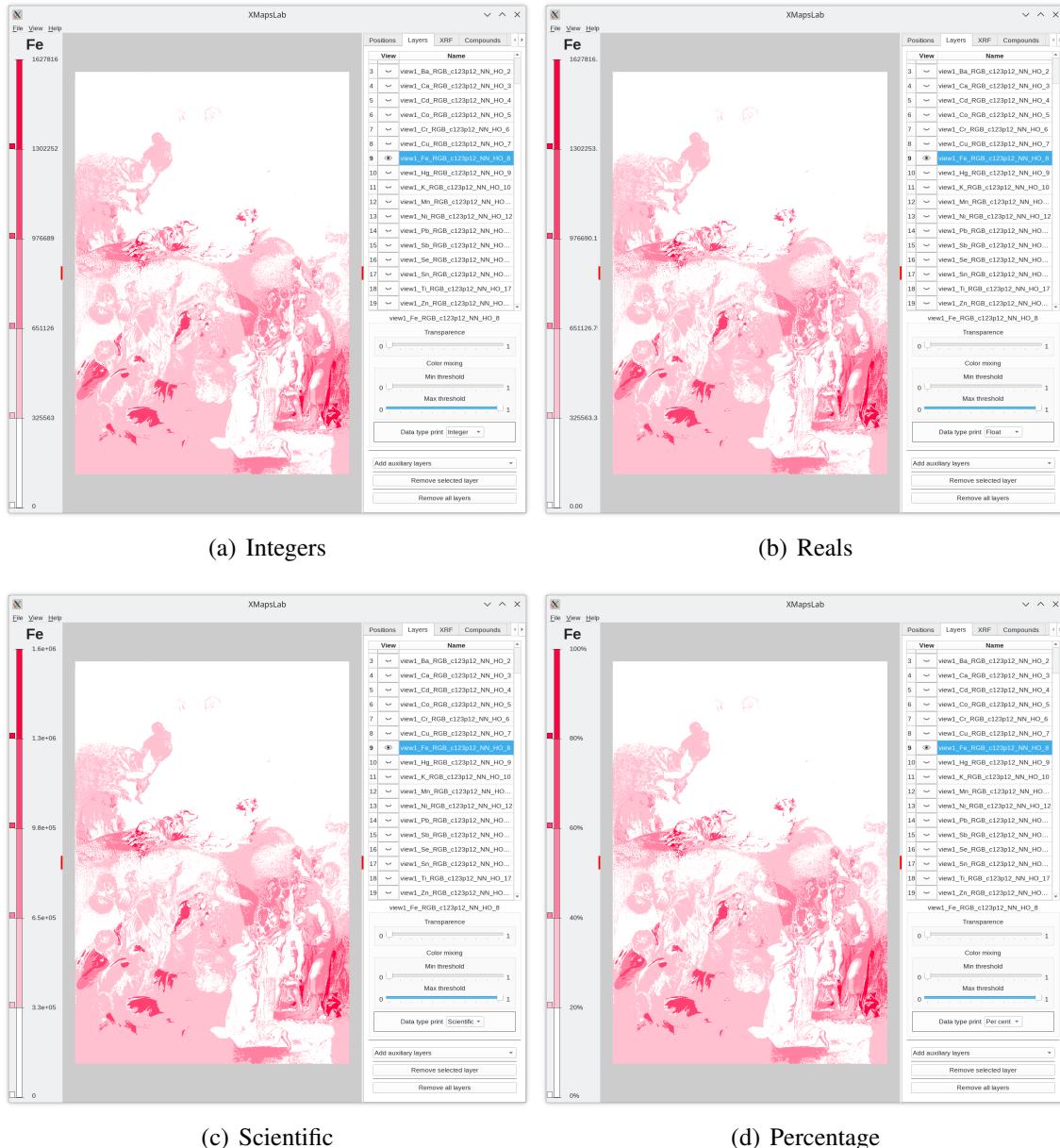


Figure 5.20: The color bar of the selected layer is shown in the left zone. The type of color bar depends on the selected palette. The numerical values can be shown in four types.

Now that we have explained the components of the color bar and how they are obtained, let's move on to the changes that can be made.

- To change the color of a color box:

1. Double click on the desired color box.

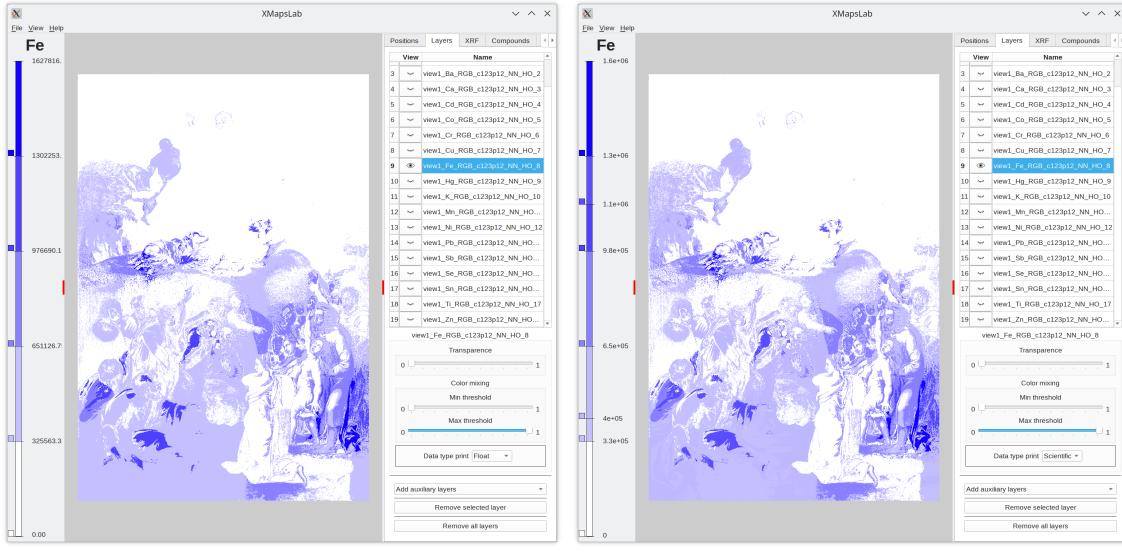


Figure 5.21: Different operations on the color bar that uses a discrete palette with 5 steps.

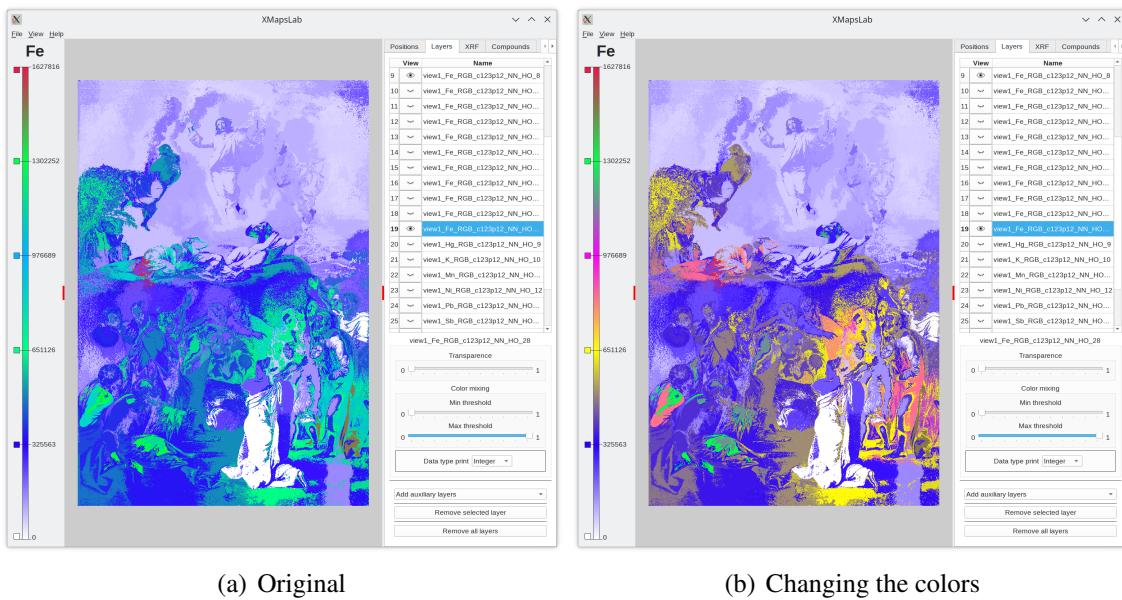


Figure 5.22: Different operations on the color bar that uses a continuous palette with 5 steps.

2. A window will appear, allowing you to select the tone or color, depending on the type of palette.
3. In the case of shaded palettes, make sure to select the box at the upper end of the color bar.

By following these steps, you can modify the color of a specific color box in the color bar.

- To add a step/color box:
 1. Double click with the left mouse button on the color bar at the desired position where you want to add the new box.
 2. The assigned value will be calculated automatically based on the position.
 3. The color of the new box will depend on whether the palette is tone or color. For tone palettes, it will assign the corresponding tone. For color palettes, it will assign a random color.

By following these steps, you can add an intermediate step or color box to the color bar.

- To delete a step/color box:
 1. Double click with the right mouse button on the color box that you want to delete.
 2. The selected box will be removed from the color bar.

By double-clicking with the right mouse button on a color box, you can delete a specific step/color box.

- To move a step/color box:
 1. Left-click and hold the mouse button on the color box that you want to move.
 2. While holding the mouse button down, move the mouse to the new position where you want to place the box.
 3. Release the mouse button to drop the box in the new position.

By following these steps, you can move a step/color box to a different position on the color bar.

5.1.4 Menu options

The different menu options are listed below:

- [File](#)
 - [Load project data](#): This option opens the selected project, loading all its data.
 - [Close project](#): This option closes the current project, allowing you to load a new one.

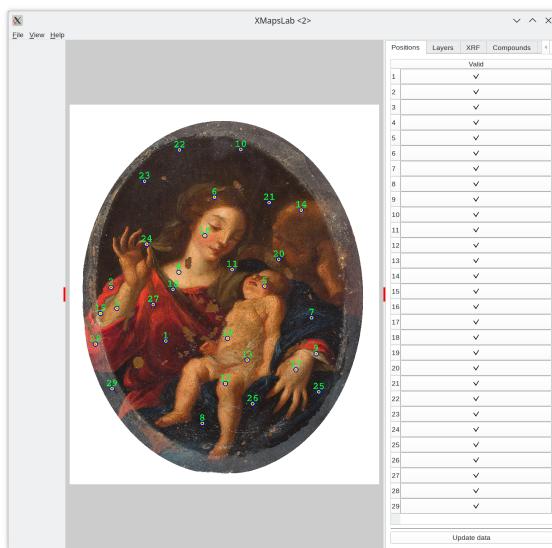


Figure 5.23: The positions are shown.

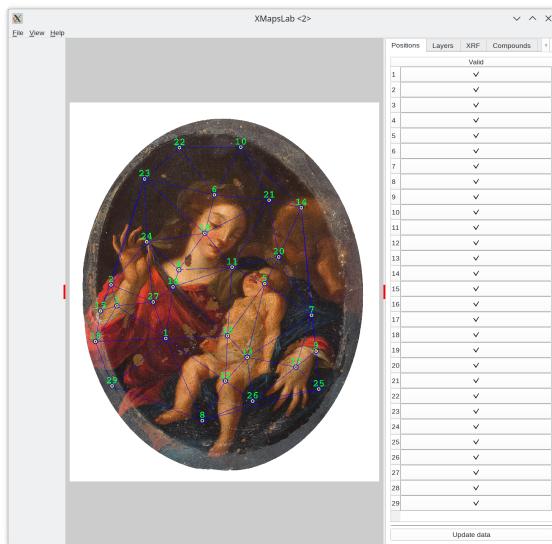


Figure 5.24: The triangulation is shown.

- **Save selected layer:** This option enables you to save the map of the selected layer. It is possible to select between saving only the map or adding the color bar to it.
- **Save all layers:** This option allows you to save the maps of all layers in the project. It is possible to select between saving only the map or adding the color bar to it.

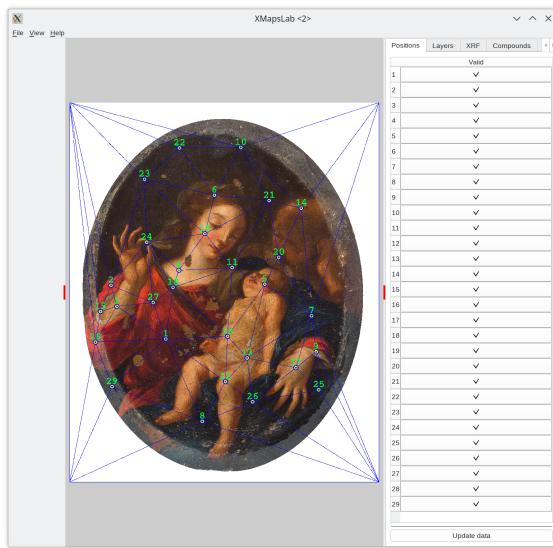


Figure 5.25: The triangulation with the added corners is shown.

- **Save composed image:** This option allows you to save the image displayed in the Display Zone, which may involve transparency and color mixing operations. This image represents the result of various layer operations and adjustments.
- **Options:** This option opens a window where you can modify various program settings, including:
 - * **P. display:**
 - **Font size:** This option allows you to adjust the font size of the text and circles used to indicate positions on the display. Two circles are used to ensure visibility of the positions regardless of the color scheme of the image. You can customize the size and color of the circles, as well as the color and size of the text that shows the position order. The measurement position is located at the center of the concentric circles.
 - **P. print:** This option allows you to change the scaling factor applied to the text when printing, relative to the size defined for the screen.
 - **Layers:** This option allows you to specify the default format for displaying numerical values in the color bar. You can choose between integer, real, scientific, and percentage formats.
 - **Palettes:** This option allows you to define the color that corresponds to the value 0 in the color bar. You can choose between the colors black and white.
 - **View**

By accessing the "Options" menu and navigating to these specific sections, you can customize the display, printing, layer formatting, and color palette settings according to your preferences and requirements.

- **Show positions:** This option enables you to display the positions where the measurements were made. This helps visualize the spatial distribution of measurements ([Figure 5.23](#)).
- **Show triangulation:** This option allows you to display the Delaunay triangulation obtained from the measured positions. There are two options:
 - * **Normal:** This option displays the Delaunay triangulation without including the corners ([Figure 5.24](#)).
 - * **With corners:** This option displays the Delaunay triangulation including the corners, which are assigned a value of 0 ([Figure 5.25](#)).

Interpolation methods

Among the various methods available for interpolating spatial data, we have implemented several methods capable of handling scattered positions rather than a grid, which can also produce values outside the convex hull (the smallest convex polygon that includes all the measured points [Graham and Frances Yao, 1983]).

XMapsLab includes four interpolation methods:

- Minimum Hypercube Distance (6.2(a))

This method, developed by Martín-Ramos and Chiari [2019], utilizes both the normalized RGB color values (R, G, B) (with R, G, B ranging from 0 to 1) and the normalized position coordinates (x, y) (with x, y ranging from 0 to 1) to calculate the distance. Each non-measured position has five known parameters (RGB and position coordinates) and one unknown parameter (the value, $(R, G, B, x, y, ?)$). The method calculates the distance between the unknown position and all the known positions using the formula $d = \sqrt{(R - R_i)^2 + (G - G_i)^2 + (B - B_i)^2 + (x - x_i)^2 + (y - y_i)^2}$. The value of the known measurement that produces the smallest distance is assigned to the non-measured position. Additionally, a modulation factor can be applied to the value by computing the ratio between the minimum computed distance and the maximum distance of the hypercube: $f = \frac{Max_{distance} - d}{Max_{distance}}$. Since the method described by Martín-Ramos and Chiari [2019] does not have an assigned name, we label it as Minimum Hypercube Distance (MHD).

- Minimum 2D cartesian distance (6.2(b))

Another interesting method for obtaining interpolation is the Voronoi diagram [Aurenhammer, 1991]. This method works by classifying the rest of the positions based on the nearest distance criteria, given a set of n seed positions. The distance between each unknown position and each seed is computed, and the value of the unknown position is set to that of the nearest seed. It is important to note that any accompanying values with the seeds will be transmitted to the unknown positions. In this case, the measured values are transmitted and then mapped to colors. From this explanation, it is evident

that the Minimum Hypercube Distance (MHD) method is actually an extension of the Voronoi diagram to 5 dimensions, incorporating color into the position coordinates and transmitting the measured value.

In terms of visualization, we can think of it as simulating a process where a different colored paint has been poured into each seed position and spreads until colliding with the other paints. It is also possible to simulate a gradual change as the paint spreads.

We have included this method as it is a simplified version of MHD and can complement the other methods available.

- Radial Basis Function ([6.2\(c\)](#))

The interpolation using radial basis functions (RBF) involves constructing an interpolant by taking the weighted sum of RBFs. A radial basis function, as defined by [[Hardy, 1971](#)], is a function that depends on the distance to a fixed point. For example, a Gaussian function satisfies this definition. The basic idea is to place a radial function at each point, adjust the weights of the functions, and then combine them to form the interpolant. The parameter ϵ for Gaussian or multiquadric functions defaults to the average distance between known points. Additionally, there is a smoothness parameter that controls the smoothness of the approximation. By default, the interpolation is performed at the known points.

In our implementation, we have tested several radial basis functions, including Multiquadric, Inverse, Gaussian, Linear, Cubic, Quintic, and Thin plate functions. These functions provide different behaviors and characteristics, allowing for flexibility in the interpolation process.

We have tested these radial functions: Multiquadric, Inverse, Gaussian, Linear, Cubic, Quintic and Thin plate.

- Triangulation ([6.2\(d\)](#))

We have implemented the interpolation method using normalized barycentric coordinates with triangles. This type of coordinates was introduced by [Möbius and Barth \[1827\]](#) and allows us to compute the value of any position within a triangle given at least three measurements (V_1, V_2, V_3) at three different positions $P_1(x_1, y_1)$, $P_2(x_2, y_2)$, and $P_3(x_3, y_3)$. The absolute barycentric coordinates (α, β, γ) of the triangle are used in this computation.

The absolute barycentric coordinates satisfy the following conditions:

$$\begin{aligned}\alpha + \beta + \gamma &= 1 \\ 0 \leq \alpha, \beta, \gamma &\leq 1\end{aligned}$$

To compute the position within the triangle, we use the following formulas:

$$\begin{aligned}x &= \alpha x_1 + \beta x_2 + \gamma x_3 \\ y &= \alpha y_1 + \beta y_2 + \gamma y_3\end{aligned}$$

These formulas allow us to interpolate the value at any position within the triangle based on the known measurements at the three vertices. For example, if the values at the three positions were (1000, 500, 600), then the value at the center of the triangle would be $\frac{1}{3} \times 1000 + \frac{1}{3} \times 500 + \frac{1}{3} \times 600 = 700$.

To apply this interpolation method to a set of samples, we first convert the positions into a set of triangles using the Delaunay method [Delaunay, 1934]. This triangulation method ensures that the triangles have desirable properties, such as maximizing the minimum angle and avoiding sliver triangles.

It's worth noting that if there are missing corner samples, the resulting triangulation may not cover the entire image. In such cases, artificial corners can be added with a value of 0 to ensure full coverage.

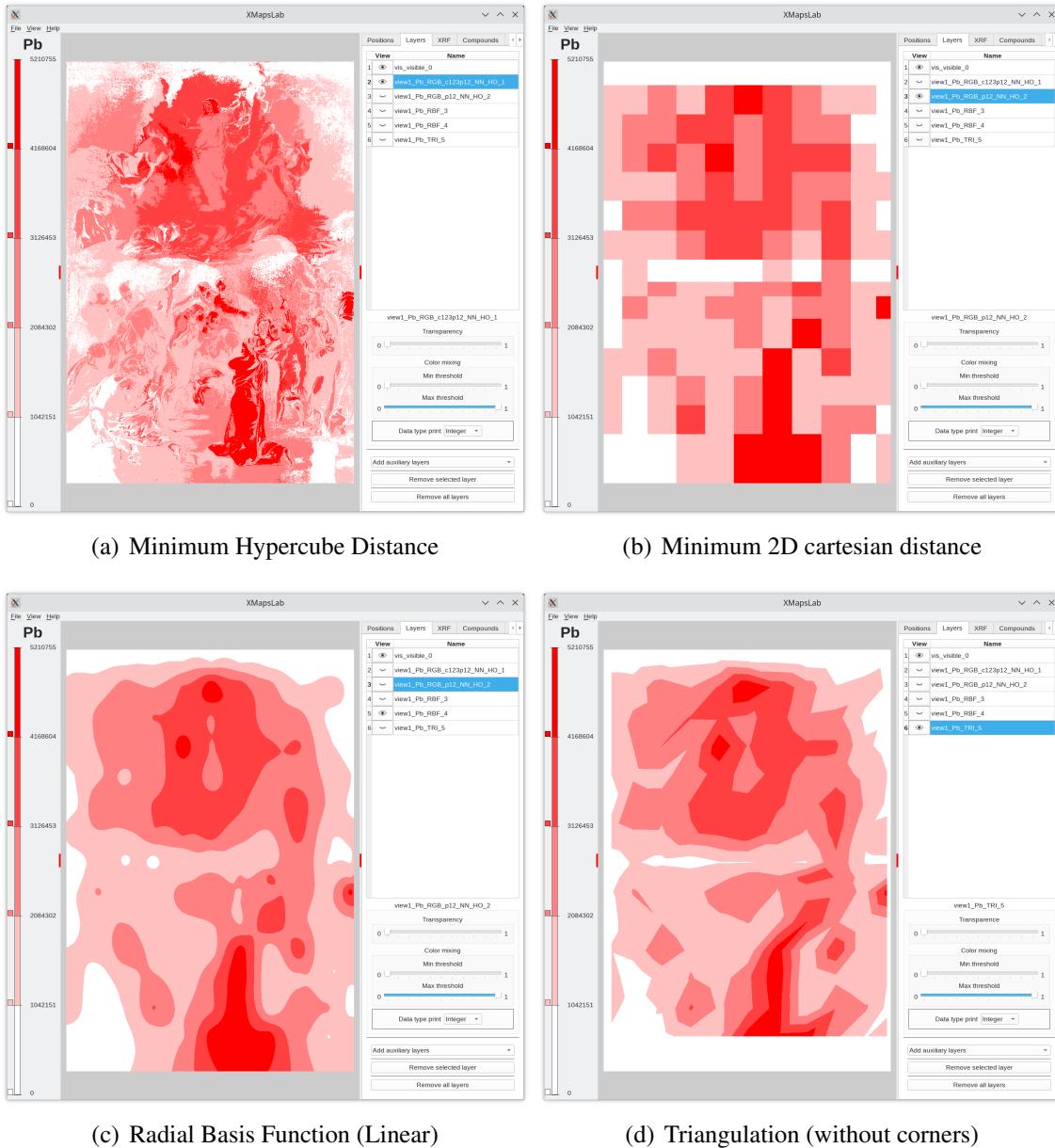


Figure 6.1: Results of the four interpolation methods using the same data with example A.

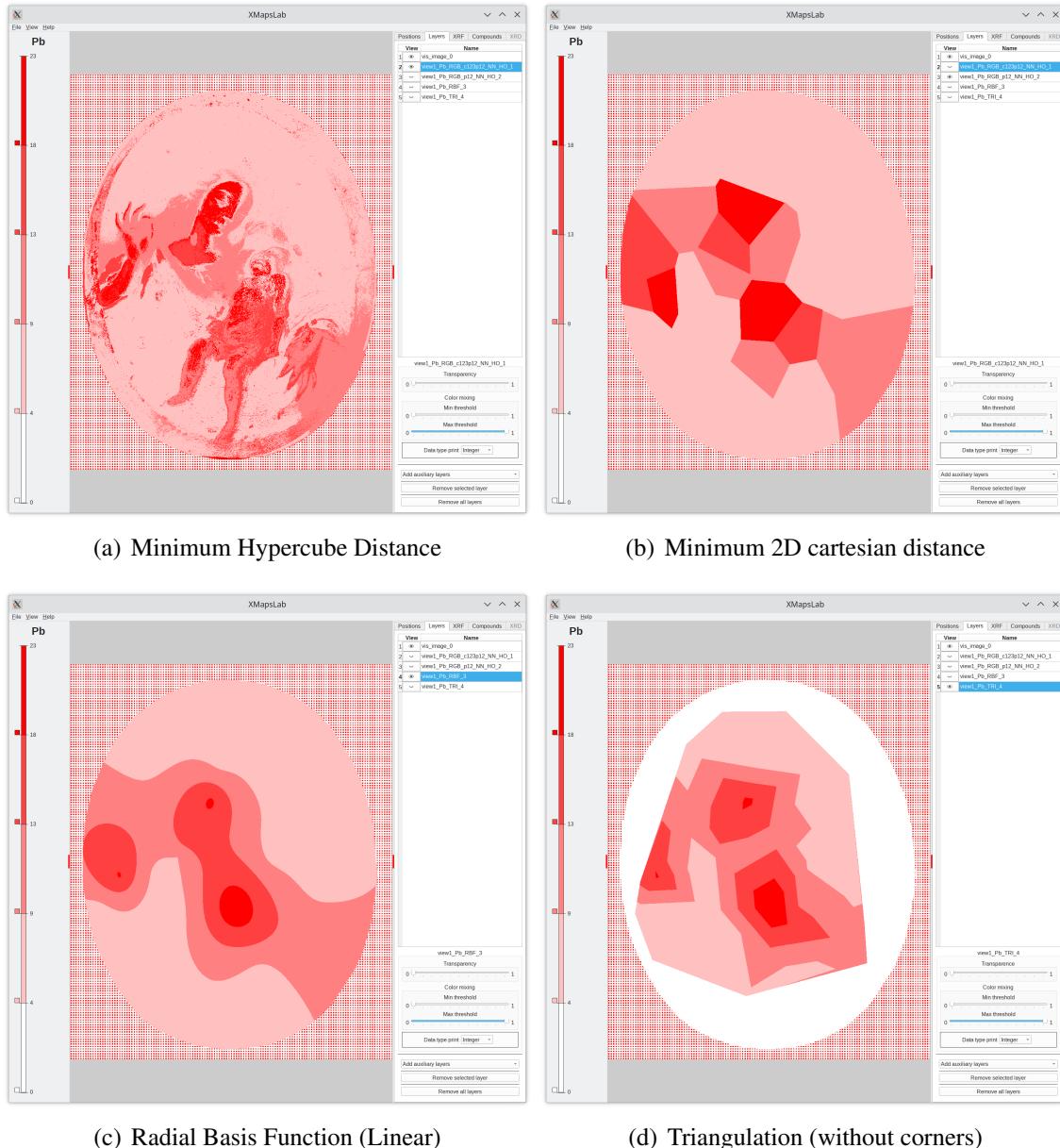


Figure 6.2: Results of the four interpolation methods using the same data with example B.

How to use CSV files with a spreadsheet

In this chapter, we will guide you on how to use a spreadsheet to create or edit CSV files. While most spreadsheets have this capability, we will focus on using LibreOffice, a widely-used spreadsheet program that offers compatibility with Excel and is available for various operating systems including Windows, Linux, and Mac.

If you don't have LibreOffice installed on your machine, you can visit their website by searching for "libreoffice.org". From there, select the download option and proceed with the installation.

Once LibreOffice is installed, you can follow the steps below to create a CSV file.

1. Launch the LibreOffice program. Upon opening, you will see the initial state of the application, as shown in [Figure 7.1](#). A blank spreadsheet will open, where you can enter your data.
2. Fill in the cells with the desired values and organize them into columns and rows according to your requirements. We are going to introduce the data of a very simple project. The meaning of each field was explained in [chapter 2, page 13](#). The result is shown in [Figure 7.2](#).
3. Once you have entered your data, navigate to the [File](#) menu and select the [Save As](#) option. This spreadsheet can be saved in various formats, such as ODS, XLSX, and more. If you intend to perform operations with the data, it is essential to save it in one of these formats since they provide the necessary functionality. However, for **XMapsLab** it is mandatory to save the spreadsheet in CSV format.

By default, the program saves the file in the folder where it is run, with the name [Untitled 1](#) and the format as ODS ([Figure 7.3](#)). To save the file in a specific folder, we need to navigate to that folder first. Then, we can click on the [Name](#) field to change the name to [project_data.csv](#). As we type the [.csv](#) characters, the format will automatically change accordingly. Before clicking the [Save](#) button, it is important to select the option

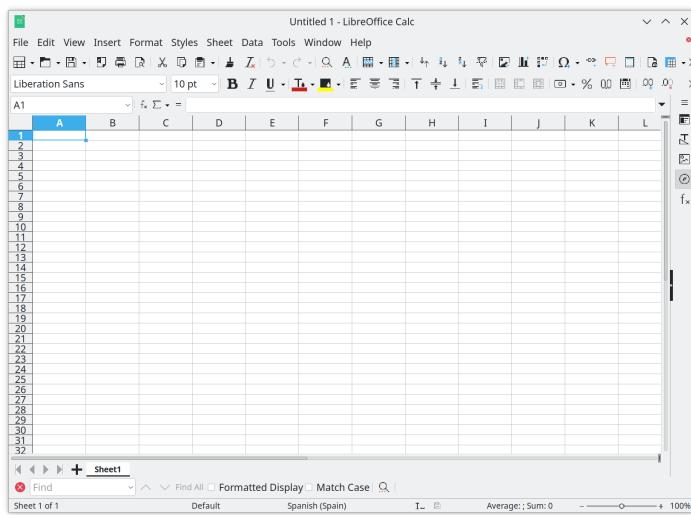


Figure 7.1: Initial state of LibreOffice

	A	B	C	D	E	F
1		XRF pistol				
2	XML	1.0.0				
3	PROJECT_NAME	Example				
4	AUTHOR	DMP				
5	DATE	22/05/23				
6	DEVICE	XRF pistol				
7	TUBE	CU				
8	XRF_DATA_ADJUSTMENT	ATOMIC_NUMBER				
9	WIDTH	3020				
10	HEIGHT	4456				
11	CS_ORIGIN	TOP_LEFT				
12	POSITION	-	1	2	3	
13	X	-	81	310	615	
14	Y	-	96	96	96	
15	XRF	As	4381155	4459950	6956528	
16	XRF	Ba	281520	353048	626152	
17	XRF	Ca	17249984	6232072	3531240	
18						
19						
20						

Figure 7.2: Inserting the data in the table.

Edit filter settings to define the separator character. Once all the necessary settings are in place, we can proceed to click the Save button (Figure 7.4).

4. A window will appear, notifying us about the format in which the file will be saved. In this window, we need to click on the option Use text CSV format (Figure 7.5).
5. The following window will display the options for saving the data. We need to select the option Unicode (UTF-8) for the Character set field. The crucial field is Field delimiter, which determines the character used to separate the tabular data. In our case, we

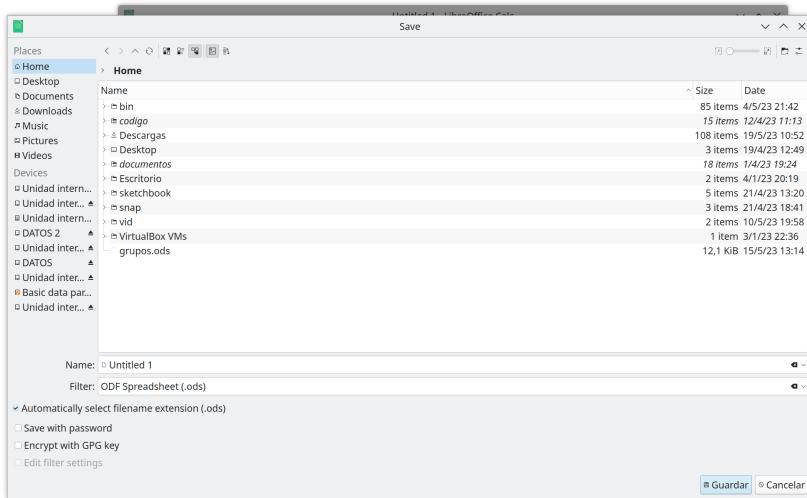


Figure 7.3: Save options.

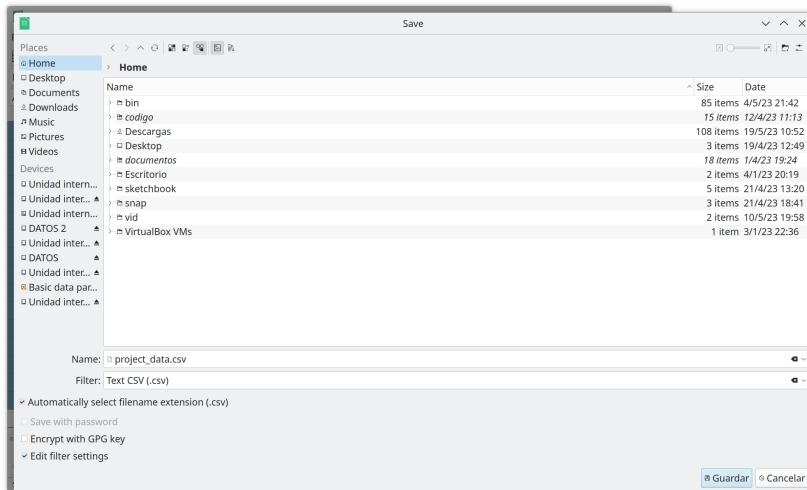


Figure 7.4: The values that must be changed.

want to use the semicolon character. Once the fields are filled, we can click on the **OK** button to save the file ([Figure 7.6](#)). And that's it!

Loading a CSV file in the spreadsheet is even easier. One option is to double-click on the file name. LibreOffice will launch, and a window will open displaying information for importing the data. At the bottom of the window, there will be a preview of the importation. The important parameters are found in the **Separator Options** section. We need to select the **Semicolon** option and uncheck the other boxes ([Figure 7.7](#)). Once we have verified that the preview is correct, we can click the **OK** button, and the file will be loaded correctly.

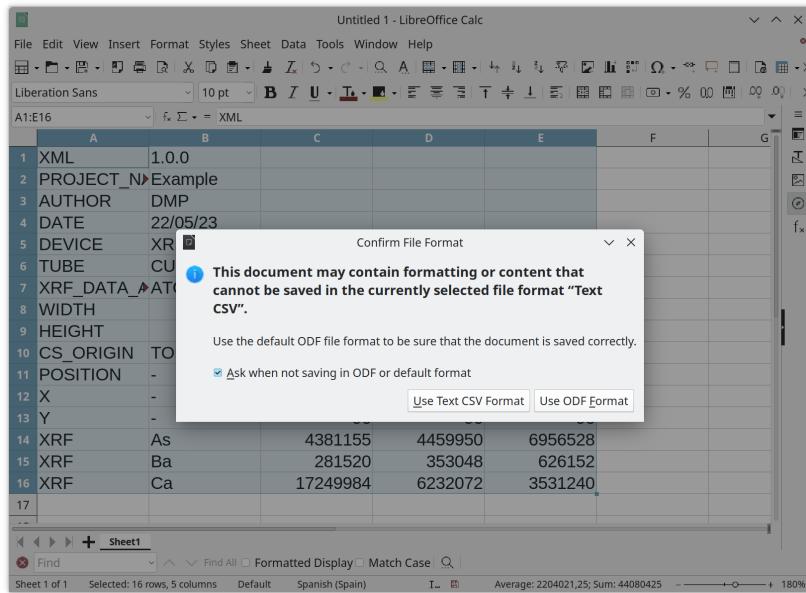


Figure 7.5: Window to confirm the type of the file. It must be CSV.

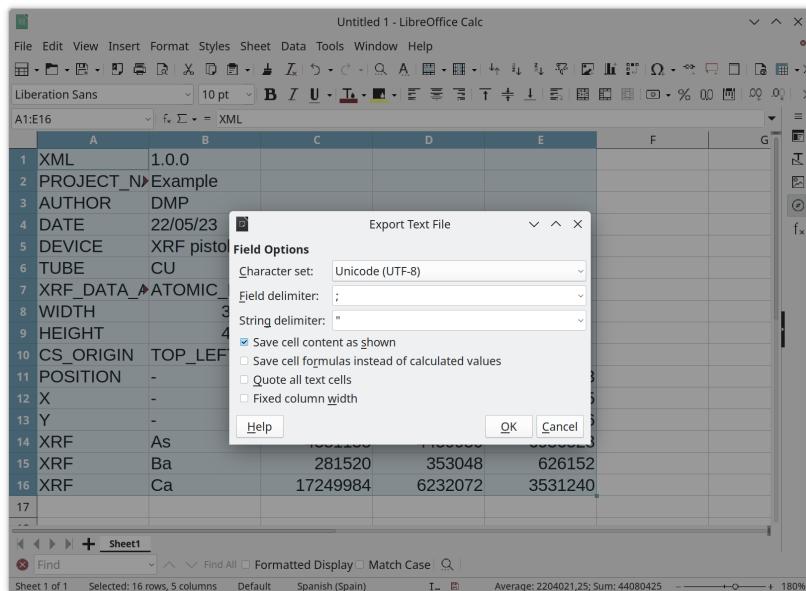


Figure 7.6: Window with the saving options. The most important is the Field delimiter.

In the case of having Excel or another spreadsheet software as the primary spreadsheet program on the system instead of LibreOffice, we will need to follow different steps to load the file. First, we need to launch the LibreOffice program. Then, we will navigate to the **Open** option, which can be found under the **File** menu. This will open a window displaying the files in the folder where LibreOffice is located ([Figure 7.8](#)).

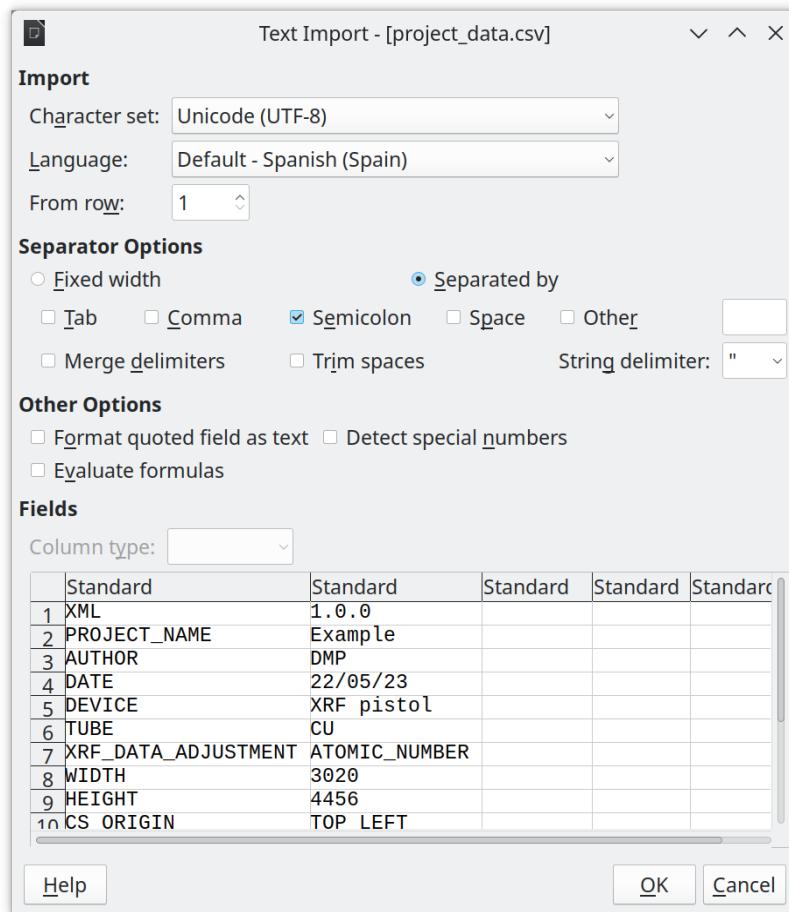


Figure 7.7: Window with the import options. The most important is the Separator Options.

We will navigate to the folder where our CSV file is located and click on its name. This action will open the load options window, similar to the one shown in [Figure 7.7](#). From there, the process is the same as explained previously.

If you are using Excel, the operations for working with CSV files should be similar. You can open the program and navigate to the [Open](#) option, which allows you to select the CSV file from the desired folder. Excel will prompt you with import options, including the choice of delimiter and character encoding. Once you have specified the appropriate settings, you can proceed with opening the file and working with the data in the spreadsheet.

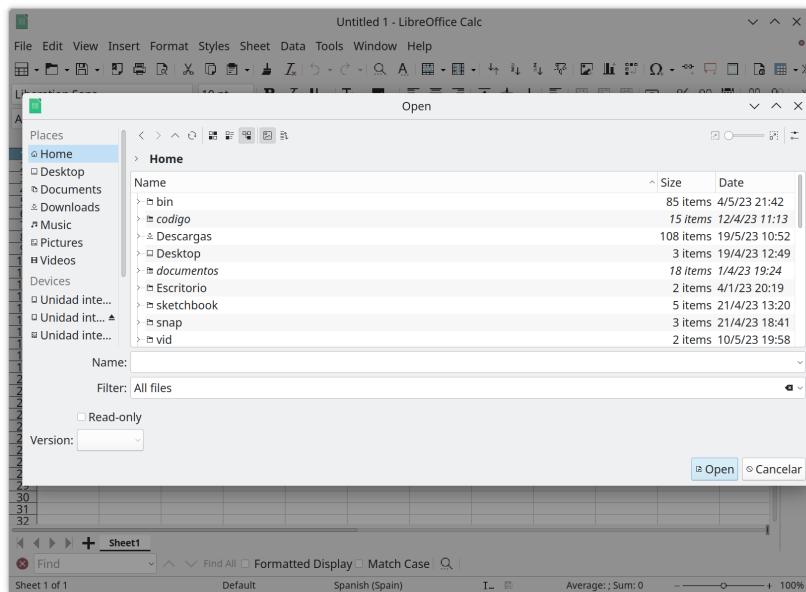


Figure 7.8: Window for selecting the file that is opened

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