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SLab Data Manager

(Part of SLab HYDRA)

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1. Overview

1.1) What is SLab Data Manager?

The *SLab Data Manager* is a tool developed for helping activities in IAPS SLab structure. The app has the main goal of allowing researchers in processing and saving spectra saved during the acquisition sessions. Several kinds of processing tools have been made available to create a flexible and useful tool.

In this user manual it will be explained how to use the application for acquiring spectra, for processing them and saving raw and processed spectra into the SLab database (DB in the following).

1.2) SLab HYDRA (HYperspectral Data Reduction and Analysis)

SLab Data Manager is part of a set of informatic tools consisting of in:

- *SLab Data Manager*: UWP app discussed in this manual
- *SLab Web Data Manager*: web app that is being developed at this time
- *SLab DB*: the centralized database containing all the info about registered users and data.

These tools build up an integrated environment for easing and speeding up as much as possible the reduction and the analysis of spectra acquired during activities carried on @ IAPS SLab.

1.3) Software requirements

PFS Data Manager is a UWP (Universal Windows Platform) application which can only run on Windows 10/11. It is designed for being used with a mouse but also supports touch interactions, if runs on a touchscreen equipped device.

2. Installation

Installation and update of *SLab Data Manager* is pretty simple thanks to the ms-appinstaller protocol that has been realized by Microsoft to let developers creating the so-called LOB (Line Of Business) apps: apps developed for internal usage by companies that are not interested in publishing their apps on the Microsoft App Store.

When creating the app package in Visual Studio, an option is present to set an URL used by the app itself to search for an update when running. If this option is selected, an *index.html* file and a file with extension *.appinstaller* is created together with the app package.

Following the web page is shown.

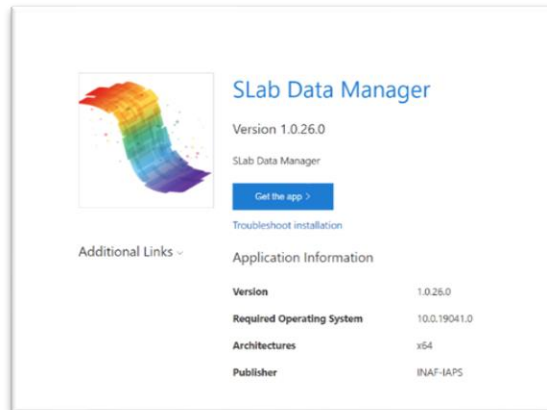


Figure 1 The web page for app installation.

By simply clicking on the *Get the app* button, a panel is shown, on top of the page, asking the user the authorization for installing the app.

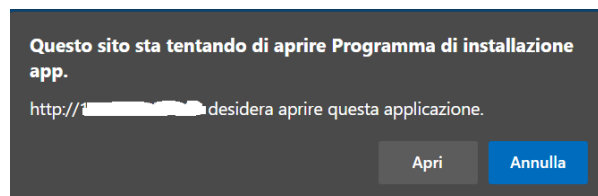


Figure 2 Alert asking user permission for starting the installation process.

Once pressed the *Open* button, the install process starts.

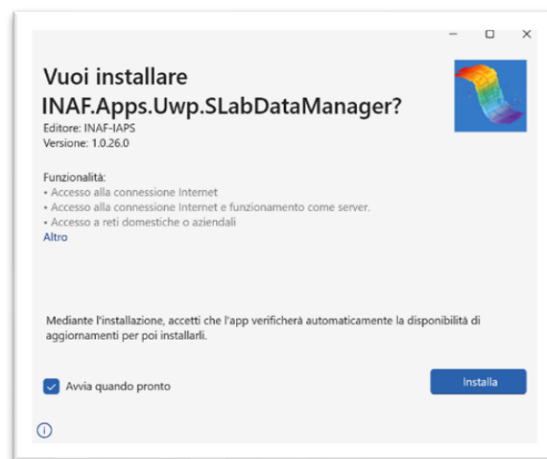


Figure 3 UI for starting installation process.

The UI for starting the installation process shows a few info about permissions required by the app for working and the option for starting the app once the installation is completed.

NB. Both the panel for authorization and the UI for installation are automatically localized by using the OS language.

2.1) Pre-installation

2.1.1) Enabling the ms-appinstaller protocol

The installation of apps following the method described in the earlier paragraph, called side-loading, is usually disabled on Windows since Microsoft discovered that a few viruses were propagated by using it. In order to enable this protocol, a few changes are required in the Windows registry.

2.1.2) Importing the certificate

Each UWP app installed in Windows needs a certificate which grants for the developer and the origin of the app itself. The OS must know the certificate used by the app in order to allow the installation. If the OS doesn't know it, the *Install* button in the UI shown in *Figure 3* is disabled and a warning is shown.

Usually, when apps are published on the Microsoft store, they are signed by Microsoft during the validation process. So, the apps contains a trusted certificate that allows the OS to run them.

When using the side-loading system, apps are not signed by Microsoft and a not-so-simple procedure is required to import the certificate, before trying to install the app, by using a Windows utility.

2.1.3) Pre-installation app

To **simplify the installation process** and avoid each user to waste a certain amount of time in changing the Windows registry and importing the certificate, a simple console application has been realized which does all the work.

By running the application, the OS is made ready for installing apps by using the side-loading system. This step is needed only one time, before the first installation of the app.

2.2) Updates

One of the greatest benefits of using the ms-appinstaller protocol is the easiness of the installation process, once the OS is ready for the protocol.

Another great advantage of the ms-appinstaller is the management of the software updates for the app users: each time the app is closed, it silently searches for an update at the URL specified when the app package has been created. If an updated version of the app is found, then it is silently downloaded and installed. The next time the user opens the app, the latest version is available.

3. Login

3.1) Why login is required?

SLab Data Manager app allows users to process public spectra and save data into the SLab DB. When any info is saved into the DB, an ID related to the user is recorded. This means the user must be logged into the system and an ID has already been created. Said this, inserting valid credential is required for starting using the app.

Following, the login view is shown.

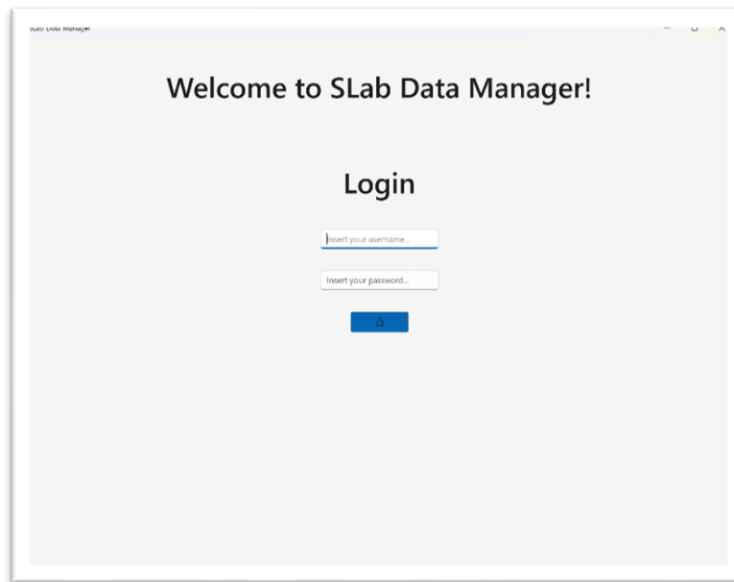


Figure 4 Login view.

3.2) How obtain a login

At the time this manual is being written (January 2023), valid credentials can be only obtained by contacting the administrator of the *SLab HYDRA* system: francesco.carraro@inaf.it. As mentioned at the beginning of this manual, anyway, a web application is under development which will, in the future, allow the self-registration of users by means of the ORCID ID.

N.B. Being both app and web app part of the same integrated system, as stated before, credentials are the valid everywhere.

3.3) User permissions

The *SLab Hydra* has been designed providing a wide set of features, each linked to permission, and a set of authorization levels. Each level is related to a sub-set of permissions. When a user is created in the system, an authorization level is assigned which grants a set of actions (permissions) to the user.

Currently three levels are available:

- *Admin*: all permissions are granted
- *User*: exploring the DB, processing and saving data are granted
- *Guest*: only exploring the DB and some processing levels are granted.

4. Getting started

4.1) App user interface

The common structure of the user interface (UI in the following) for modern apps consists in the division in *pages*. Each page is aimed to a single task or to a consistent set of tasks.

At the time this manual is being written (January 2023), the pages hosted in the *SLab Data Manager* app are the following ones:

- *Main* page: for opening input spectra
- *Charts* page: for displaying spectra and process them
- *Current user* page: for presenting permissions granted to the current user
- *Settings* page: for setting working folders, color associated to different level of processing, etc.

The overall look of the app is shown in Figure 5 below.

4.2) Pages usage

Each page of the app has a specific function and offers a set of features in order to accomplish its goal. Following a brief description of each page is given.

4.2.1) Main page

The *Main* page has the goal of loading input files to start working on spectra. It offers three different tabs aimed to opening different kinds of files.

4.2.2) Charts page

This is the page devoted to showing spectra and allowing user to process them by using the available tools.

4.2.3) Current user page

This page shows the user permissions and allows to log-out.

4.2.4) Settings page

Contains the following settings:

- Working settings: to define input and output folders
- Spectra colors: to define colors used for each level of processing
- UI settings: to select the theme used by the app.

5) Main page

SLab Data Manager offers several ways for loading input files. When logged into the app, the *Main* page is shown to the user which contains 3 tabs for starting loading of spectra in different ways.

The *Main* page at the 1st opening is shown below:

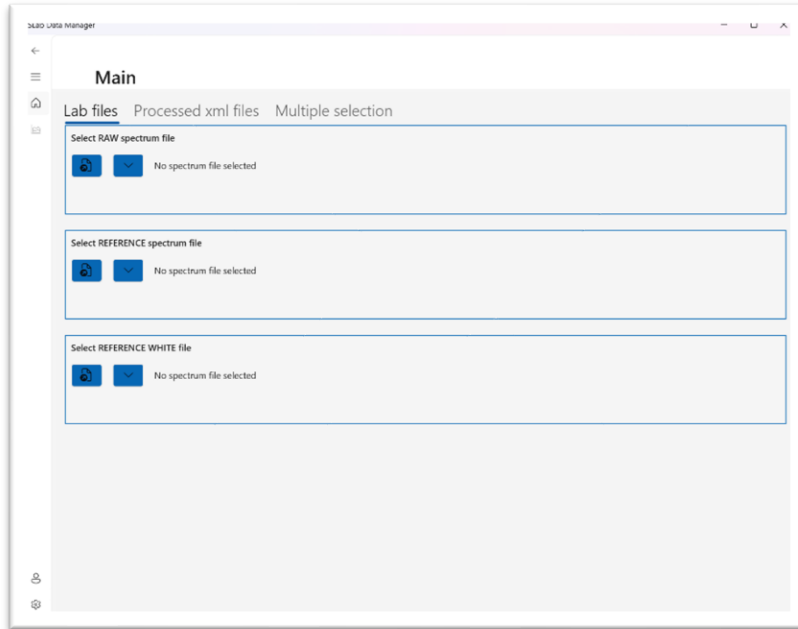


Figure 5 Main page at the 1st login.

The page offers 3 available tabs that correspond to the same amount of different kinds of input files:

- *Lab files*: for raw averaged spectra obtained after a first processing applied on several acquisitions
- *Processed XML files*: for spectra derived from raw spectra already processed by using the app
- *Multiple selection*: for raw spectra obtained by single acquisitions, not yet averaged.

5.1) Lab files

The default way for opening files is the one aimed to the already averaged spectra obtained by a pre-processing of single acquisitions.

Three files are required to enable processing features:

1. *Raw file*: the one that will be processed by the user
2. *White file*: the reference for calibration obtained in laboratory
3. *Reference white file*: the reference provided by the instrument manufacturer

For each selector a couple of buttons are available: the left one is for opening the standard UI for file selection; the right one opens a flyout (in place UI element created on the fly) for selection among the last selected files.

N.B. Given the peculiarity of the *Reference white* file, which is provided by the instrument manufacturer and is not usually updated, this file is automatically loaded at app start.

Once a file is loaded, the app automatically saves it onto the cloud, that means it saves the file into the *SLab HYDRA DB*. Each file and information saved into the DB, is marked with the user ID.

Also, for each file, a box with a summary about loaded spectrum is shown below the file path.

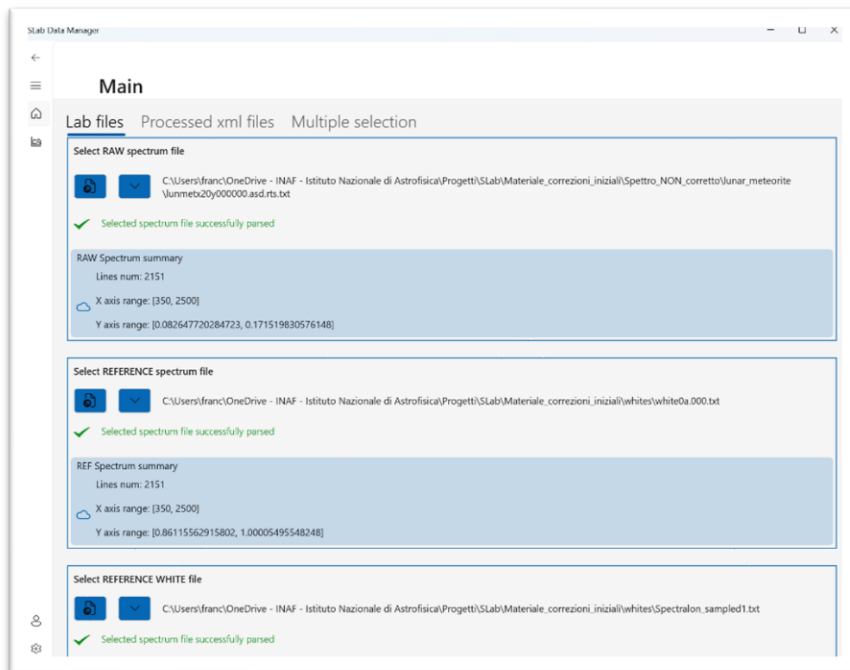


Figure 6 Lab files. All required spectra have been loaded. A cloud icon is shown for each files informing that file has been saved onto the cloud.

5.2) Processed XML files

SLab Data Manager offers several levels of processing, each level can be saved in both local XML file and cloud file: the file is saved onto the cloud (see 9) *Processed file savings and*).

Local XML files store several info about:

- local path
- parent files IDs. Parent files are the following ones:
 - ID of the file corresponding to the previous level of processing
 - White file ID
 - Reference White file Id
- info about current processing step
- spectrum values (wavelength, value, std-dev on y value)

The presence of the above-mentioned set of info allows the user to resume the work on a spectrum avoid starting again from the RAW level.

By opening XML files, the app automatically restores the status of the last time current file was processed: all parent files are loaded and the panel corresponding to the current kind of processing is filled with info contained in XML.

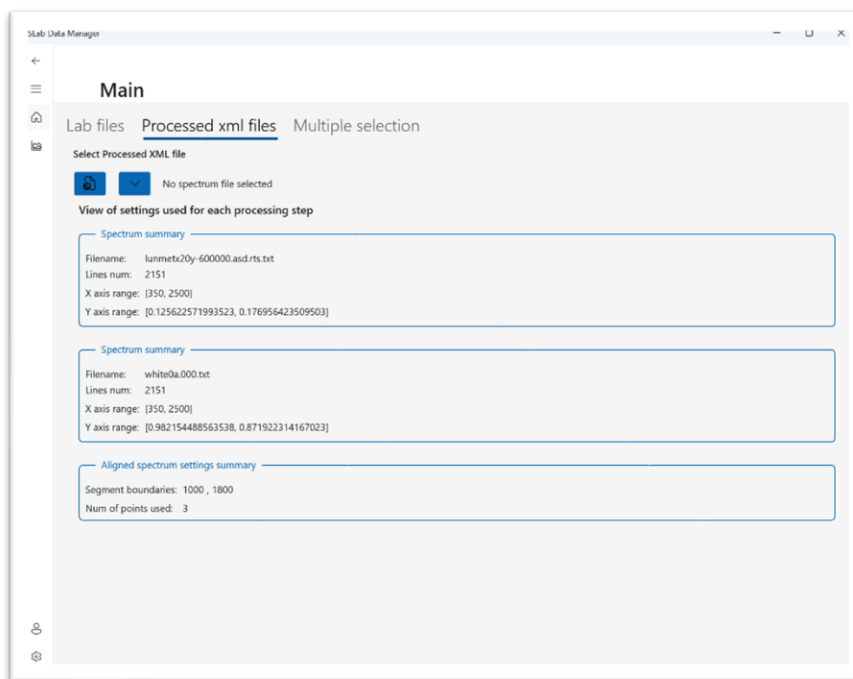


Figure 7 Processed XML files. Aligned file loaded. Below the spectrum summary, info about alignment is shown.

5.3) Multiple selection

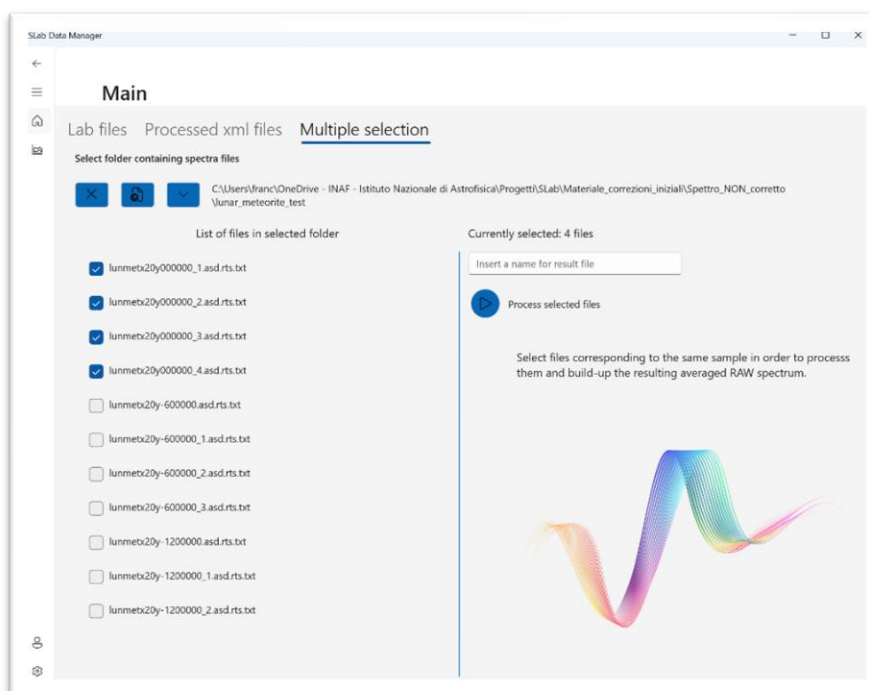


Figure 8 Multiple selection. Folder has been selected showing contained files. Spectra related to the same sample has been selected.

The main goal of this tab is allowing the user to create an averaged file, similar to the ones opened with the 1st tab, starting from set of acquisitions on the same sample.

The user is asked to select a folder containing one or more set of acquisitions, then the content of the folder is shown in the left panel as a list of files, each linked to a checkbox. The next steps are:

- the selection of the files being part of a series of acquisitions
- filling a name for the averaged file produced as output
- pressing the Play button to start the task that produces the output file.

At the end of the task, the output file is automatically loaded: its name is shown in the 1st tab as input raw file and spectrum is available in the *Chart* page.

6) Chart page

The *Chart* page is the real core of the *SLab Data Manager* app: is the *place* where spectra are processed and analyzed. The page after data have been loaded is shown below.

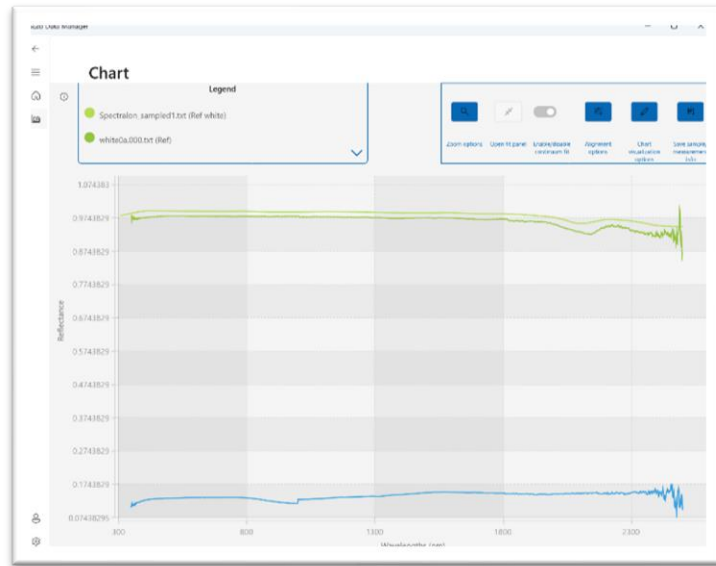


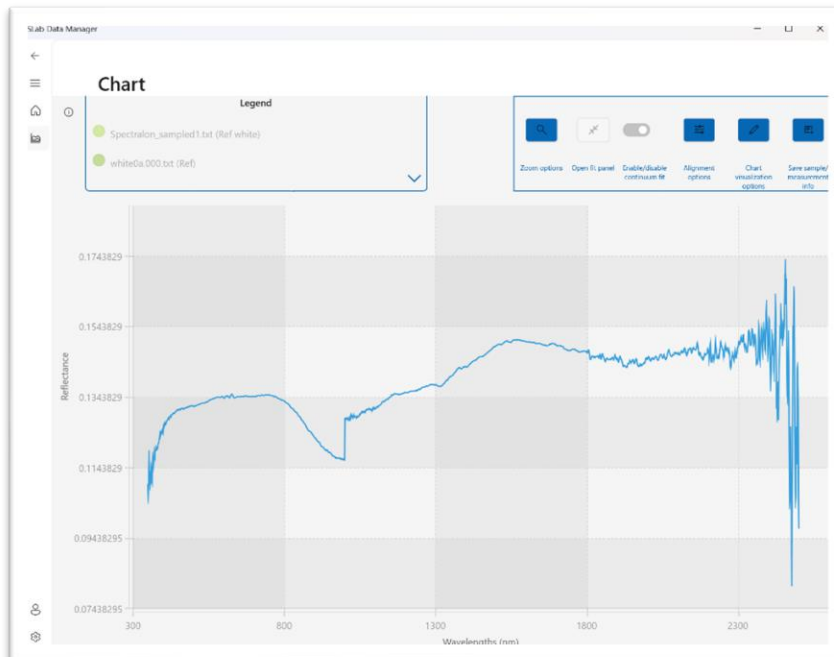
Figure 9 The Chart page when data have been loaded.

The page is divided in 3 main sections:

- The chart
- The legend on the top-left
- The toolbar (a set of buttons that enable the processing tools) on the top-right.

6.1) The legend

The chart legend, other than naming the lines visualized in the chart, offers the chance to show/hide each spectrum: by simply clicking on each colored circle, the related spectrum is shown or hidden. Also, the chart y-scale is updated each time a change in visibility of a spectrum happens, in order to have all spectra shown with the smallest possible y-scale. This means that hiding the white spectra correspond to a noteworthy enhancement of the visualization for the input spectrum, as shown in **Errore. L'origine riferimento non è stata trovata..**



In order to have the maximum wideness for the chart for a given size of the app window, the space reserved for legend and toolbar has been limited. This could lead to an issue regarding how many items in legend are shown. To prevent this issue a trick has been used: by moving the cursor above the legend, it is automatically expanded towards the bottom. This behavior is shown in Figure 11.

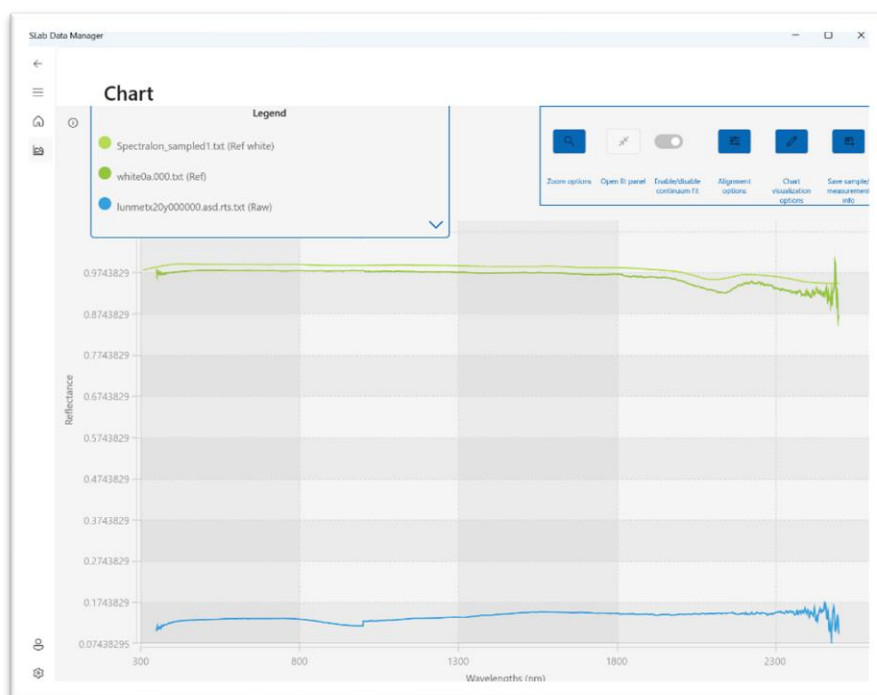


Figure 11 Expanded legend showing the complete list of loaded spectra.

6.2) The toolbar

The role of the toolbar is critical in analyzing and processing spectra, since the buttons contained in this area enable all the available features. The list of available features includes (from right to left):

- sample/measurement info
- visualization options
- alignment
- continuum fitting
- zoom

6.2.1) Save sample/measurement info

When processing a raw spectrum, saving info about the sample used for retrieving current data is crucial for subsequent analysis. Also, storing info about num of acquisitions, num of averaged spectra constituting the current one and geometry of acquisitions is relevant for a better understanding of spectrum when used in future studies.

The *sample/measurement panel* has been developed with the goal of letting users to save those information onto the cloud. The panel is shown in Figure 12.

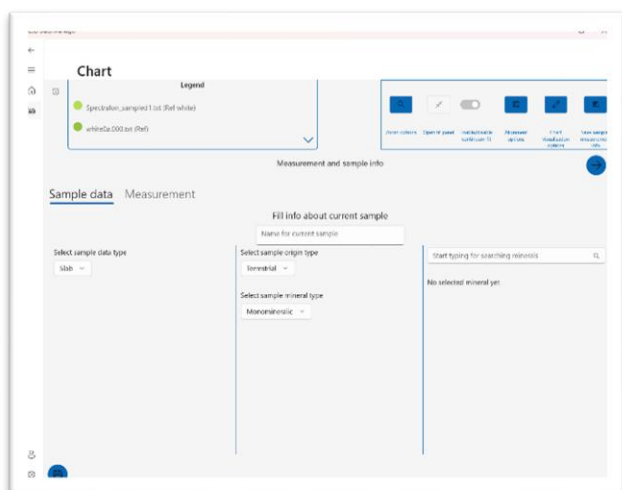


Figure 12 Sample/Measurement panel – sample data.

Measurement tab allows user to insert info about num of acquisitions, num of spectra used for retrieving the averaged one and a couple of angles related to the geometry of the acquisition.

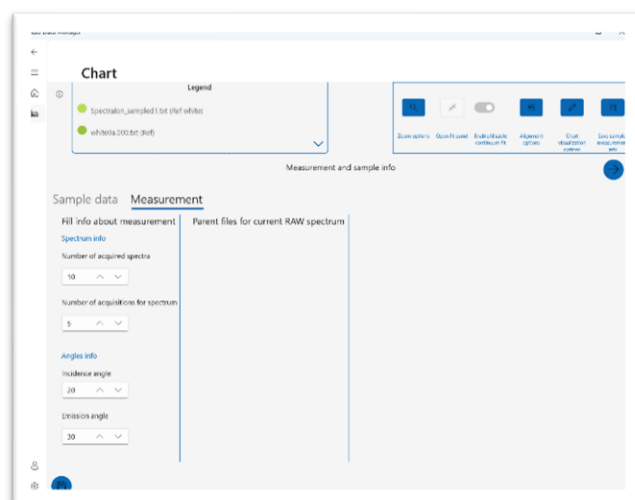


Figure 13 Sample/Measurement panel - measurement data.

6.3) Chart visualization options

A few customizations are allowed about how the chart is visualized. The *Chart visualization options* button shows a small panel containing the available customizations:

- unit of measure for wavelengths
- major lines visibility
- strip lines visibility
- pan mode
- zoom mode

The panel is shown in Figure 14.

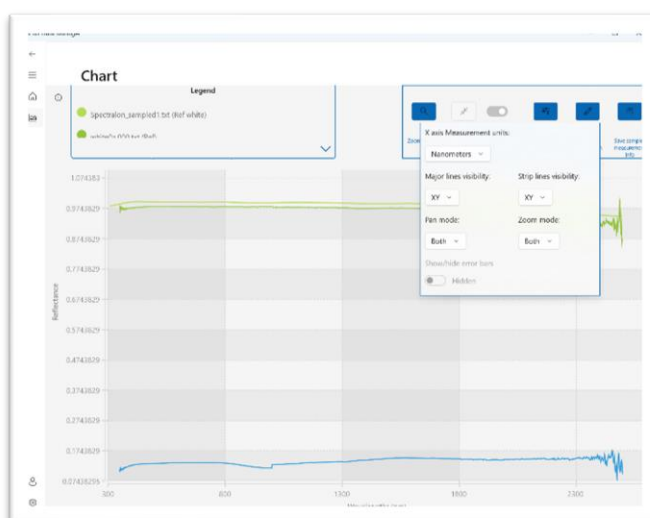


Figure 14 Chart visualization options panel.

6.4) Alignment options

Alignment options button shows a small panel with two options:

- *Align spectrum sections*: for immediately aligning spectrum
- *Open alignment settings panel*: for opening panel containing options for alignment

The panel is shown in Figure 15.

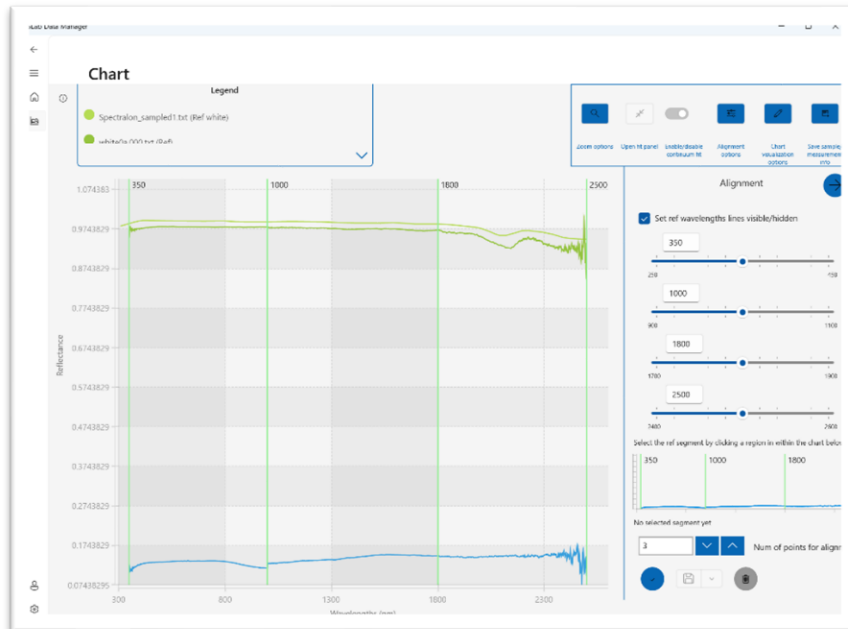


Figure 15 Alignment options panel, on the right of page. Also, separator lines are shown on chart.

Options for alignment basically consist in a few of settings:

- 1) The wavelengths where discontinuities between segments that constitute the raw spectrum occur
- 2) The reference segment the other ones are aligned to
- 3) The number of points are used in alignment procedure for calculating the difference in reflectance between the reference segment and the other 2 ones

The first time the app is used, no reference segment is chosen by default, so the selection is required to align spectrum. Tapping on the *align* button, at the bottom left of the panel, raises a warning message.

N.B. Once the reference segment has been selected, aligning the spectrum segments by simply tapping on the *Align spectrum sections* button is possible, with no need of opening the panel.

6.5) Continuum fitting

SLab Data Manager can help the user to fit the continuum for removing it.

N.B. The required condition for starting to fit the continuum is having an aligned spectrum.

Once the raw spectrum has been aligned, then *Enable/disable continuum fit* toggle button in the toolbar is automatically enabled. The continuum fitting procedure is pretty simple:

1. Tap on two or more points of the aligned spectrum (the app automatically generates lines connecting selected points)
2. Select the fit method, for each segment, among the available ones
3. Change the fitting parameter, when available, for each segment
4. Tap the remove continuum button at the bottom-left of the panel

The panel for fitting and removing continuum with the available settings is shown in Figure 16 below.

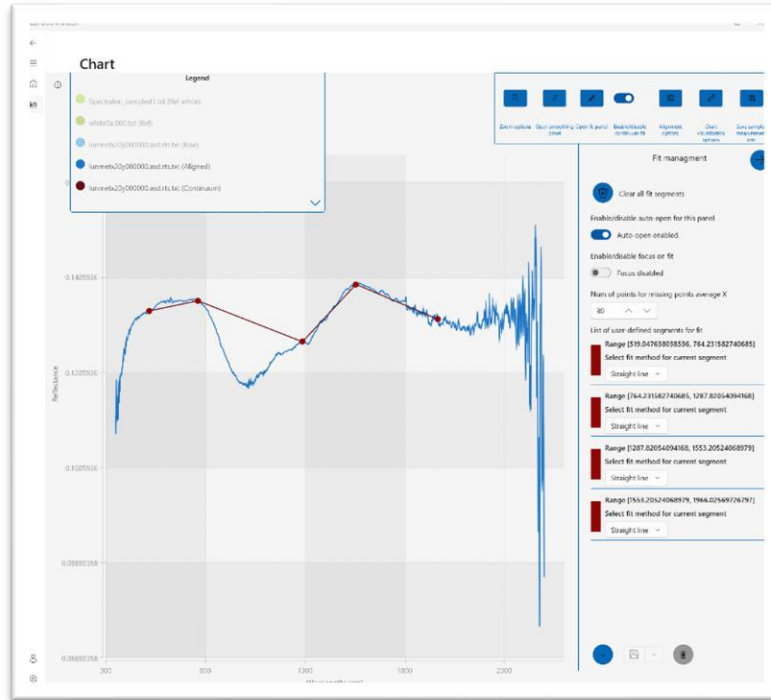


Figure 16 Continuum fitting panel on the right. The list of generated segments is visible in the middle of the panel. At the bottom-left of the panel the button for removing continuum is enabled. In this figure, the legend has been expanded to demonstrate how the list of all loaded or processed spectra is shown.

By tapping on the remove continuum button, the operation of continuum removal is executed and the new spectrum is added to the chart, as shown in Figure 17 below.

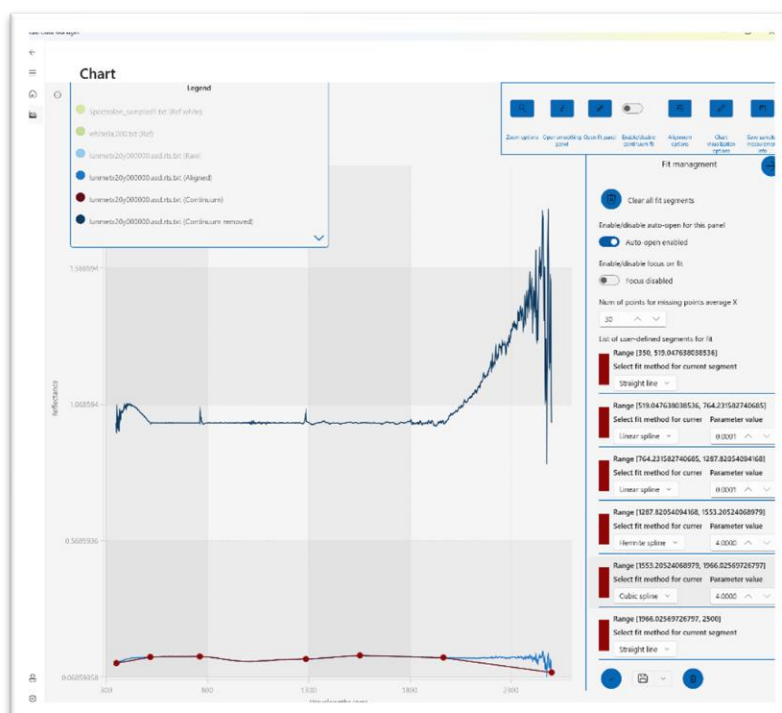


Figure 17 Continuum has been removed and the result is added to the chart.

N.B. Points in the previous figures 16 e 17 has been added with the only purpose of demonstrating the continuum fitting/removing features. No scientific evaluations have been used in selecting them. Also fitting methods used for segments have only purpose of showing the different available options.

6.5.1) About the generated segments

In Figure 16 and Figure 17 the list of options used for generating the continuum spectrum and for continuum removal process is shown. By comparing fitting methods used for each segment in Figure 16 and Figure 17 the customization used appears evident.

Some issues are worth to be listed in the following about how the app works for fitting continuum:

- when a line is automatically generated for connecting two points the *straight line* fit method is applied by default, anyway some available methods involving usage of splines are available in place of the default method
- by tapping on a selected point, it is removed and connecting lines are evaluated again in order to generate the correct fitting spectrum
- by adding a new point between two already existing points, connecting lines are evaluated again in order to generate the correct fitting spectrum
- when starting calculation of the removed continuum spectrum, the app automatically generates a point corresponding to the lowest wavelength and connect it to the leftmost user-generated point. In the same way, a point is generated in correspondence of the highest wavelength, and it is connected to the rightmost user-generated point. This ensures the accuracy of calculations while retrieving the continuum removed spectrum.
- A setting is available in the upper part of panel, to set how many points are used to obtain the average y-value of the couple of automatically generated points mentioned in the previous issue
- To generate a new version of continuum removed spectrum, in case of changed settings for one or more segments, only tapping again the *remove continuum* button is required.
- A button is available at the top of the panel for clearing all selected points and connecting segments.

6.6) Smoothing panel

In each phase of the spectrum processing, smoothing can be applied to reduce noise. The panel realized to achieve this task is shown in Figure 18.

Two main options are available, by selecting a tab in the panel, for smoothing the spectrum:

1. Smoothing by segments
2. Smoothing the whole spectrum

In both cases, the spectrum is smoothed by using the Savitzky-Golay filter. The only difference is in the choice of splitting spectrum in sections or not.

The filter requires two parameters for being applied: a num of points, called *window size*, and the order of polynomial to be used.

6.6.1) Smoothing by segments

The first tab offers a default split in three sections. Each section is identified by the spectral range. Default values for *window size* and *polynomial order* are 0.

The sub-panel containing values related to a spectral range contains a couple of buttons that can be used to edit the segmentation of the spectrum:

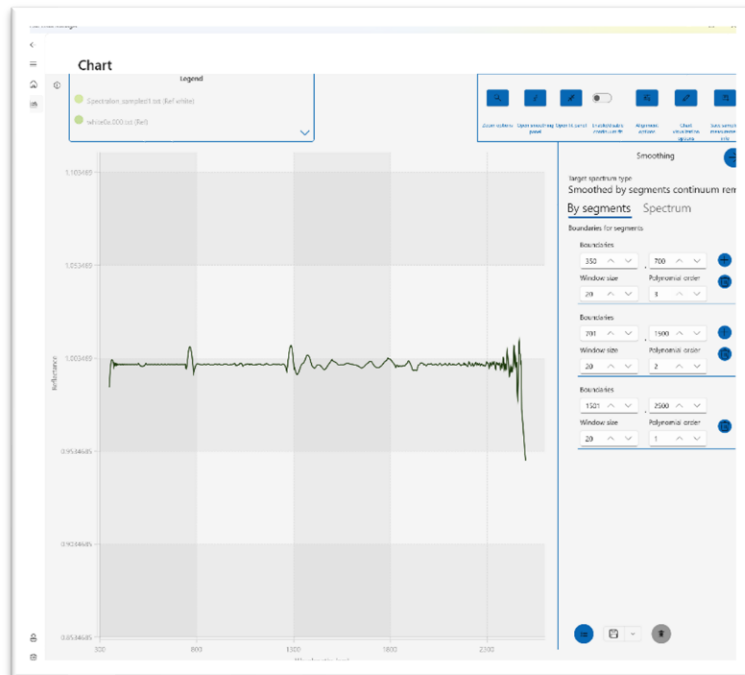


Figure 18 Panel for smoothing. The chart shows the result of smoothing algorithm applied to the continuum removed spectrum shown in Figure 17.

1. The *Add* button causes the split of the next segment into two new segments containing the same number of wavelengths.
2. The *Remove* button causes the removal of the selected segment and the assignment of the wavelengths contained in the removed segments to the remaining segments located at the boundaries of the removed one.

6.6.2) Smoothing by spectrum

The second tab is designed for simple smoothing, when no segmentation is required. This offers customization only for *window size* and *polynomial order* parameters.

6.7) Zoom options

Three buttons are shown when tapping on Zoom options button in toolbar:

- Enable/disable drawing area for zoom
- Open zoom settings panel
- Reset zoom (disabled by default)

The first button allows the user to manually select a region of the chart and zoom in; the second button opens a panel with a set of settings related to the zoom; the third one reset the zoom and restore the visualization of the complete spectrum.

To start the procedure for the manual selection of the region to be zoomed, user has just to:

1. Tap on the *Enable/disable drawing area for zoom* button

2. Draw a region on the chart by using the mouse on traditional monitors or finger/pen on touch monitor

An example of the region selection for zooming in the spectrum in a user-defined region is shown in Figure 19.

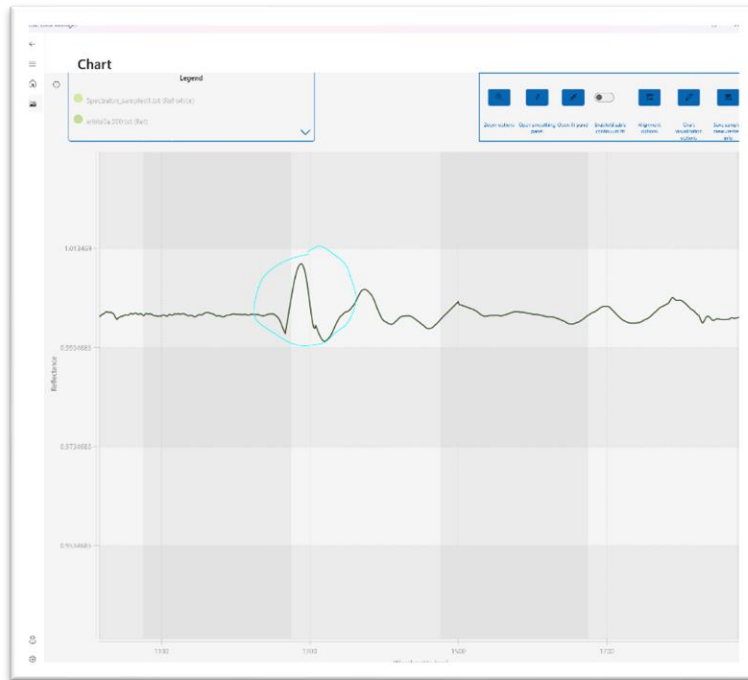


Figure 19 Manual selection of region for zooming-in the spectrum in a user-defined region.

The result of the selection of a region within the chart area, is the visualization of the selected area and the opening of a panel with tools for navigating the zoom. The panel is shown in Figure 20 below.

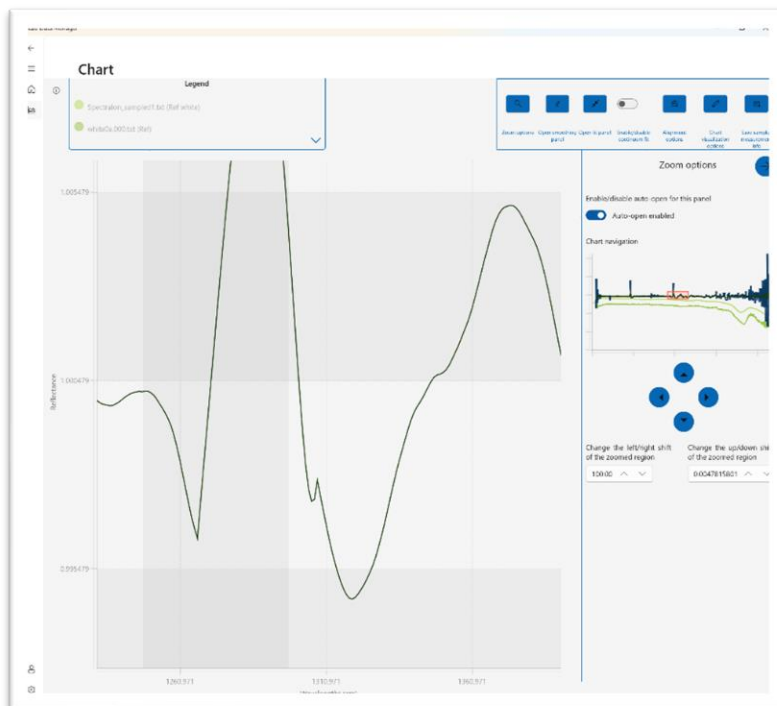


Figure 20 Zoomed region of the spectrum and, on the right, the panel with tools for navigating the chart.

The zoom options panel presents a couple of key features:

1. the chart miniature
2. the set of arrow buttons.

The chart miniature shows the whole chart highlighting the zoomed region with a small red rectangle. It allows a fast navigation across the chart: by simply tapping on a point within the chart miniature, the zoomed region is moved to the selected area.

The arrow buttons allow a fine tuning of the position of the zoomed region.

7) Current user

The page simply shows information about the name, the role and the permission granted to the user. An example is shown in Figure 21. At the bottom of the page is also present a log-out button.

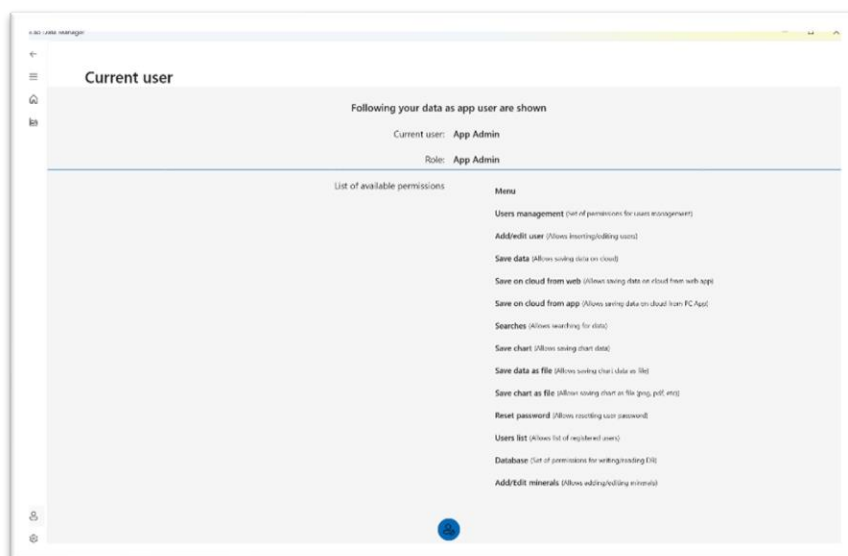
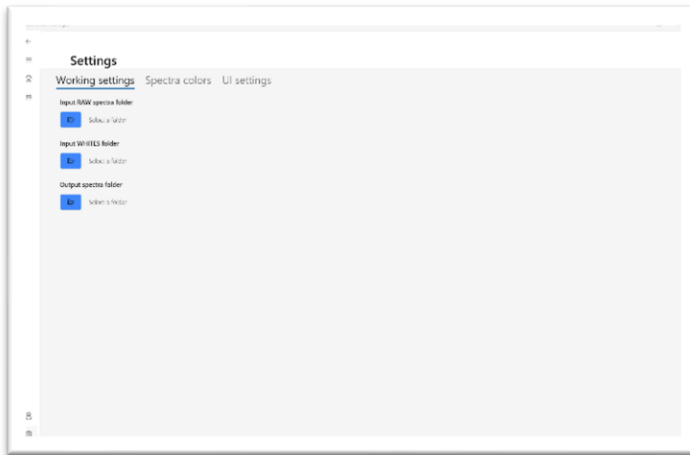


Figure 21 Current user page. Name, role and user permissions are listed

8) Settings

The page consists of three main tabs hosting different kind of settings:

1. working folders
2. spectra colors
3. app theme



The *working folders* tab hosts the selection of the app working folders. These are folders commonly used by the app for opening the white spectra, opening the input raw spectra and for saving the processed output spectra.

The tab is shown on the left, in Figure 22

Figure 22 Settings - working folders.

The *spectra colors* tab allows the selection of color used for visualizing the different processed spectra. The tab is shown here in Figure 23

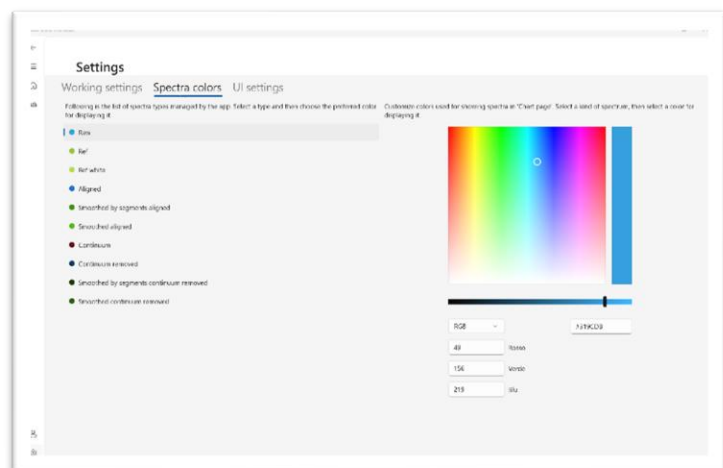
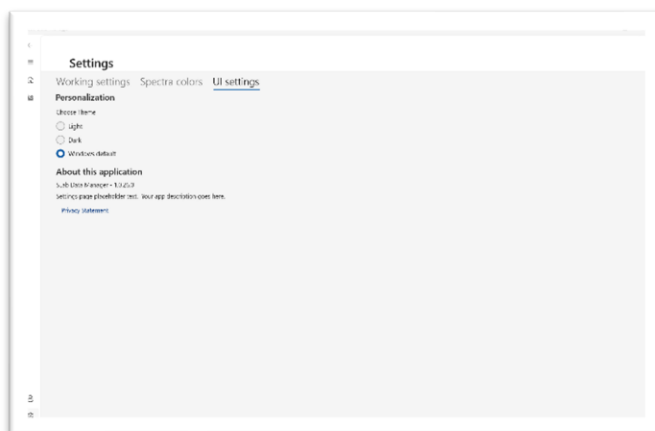


Figure 23 Settings - spectra colors.



The *UI settings* allows the selection of the app theme: available options are light (light background white black text) and dark (dark background with white text). The tab is show here in Figure 24.

Figure 24 Settings - UI settings.

9) Processed file savings and deletion

Saving processed spectra and deleting them is a feature common to all the panels aimed at manipulating the input spectrum, which means the *alignment panel*, the *continuum removal panel* and the *smoothing panel*.

At the bottom of each panel, a set of buttons is available. An example of those buttons, taken from the *alignment panel*, is shown below, in Figure 25.

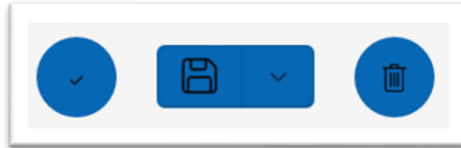


Figure 25 Example of buttons at bottom of processing panels.

The leftmost button is panel dependent and it is not of interest in this chapter. The central one, for saving spectra, and the rightmost, for deleting them represent a common feature explained in this section.

9.1) Saving button

Saving a spectrum is a permission granted to users in different ways, depending on the role of the single user. *Admin* and *user* users have permission to save locally and on cloud.

The save button shown to those kinds of users is the one visualized in Figure 25. By tapping on the *expand* icon, the button is expanded showing two options for different savings, as shown in Figure 26.

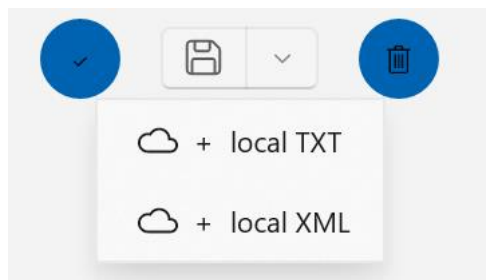


Figure 26 Expanded save button.

Both options allow user to save spectrum on cloud but differ from the kind of local saving offered. Different users may be interested in saving spectrum as a TXT file (comma separated values) for open it in a spreadsheet or in saving it as a information-rich XML format.

TXT files contain only columns with wavelength and related reflectance.

XML files contains also information about parent files and settings used for retrieving the current level of processing. XML files are also eligible for being opened by using the 5.2) *Processed XML files* tab in the *Main* page.

In both cases, the spectrum is saved on cloud as a XML file.

9.2) Delete button

When the result of a processing step is not the expected one or anyway not satisfying, it can be simply removed by using the delete button. The user is also asked whether the spectrum saved on cloud, if existing, is to be deleted or not.

10) Acknowledgments

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