Software User Guide

developed by

Daltonian Scientific

Contact: rawvision@daltonianscientific.com

SUM-121-RV01

Revision 1

05/14/2025

Installation 3
User Interface 4
File Menu 4
Settings Menu 5
Mass Resolution 5
Loading a File 6
Figure Behavior 6
Adjusting the Figures 7
Saving a Figure 8
Exporting Data 8
Importing a Reference Spectrum (PDA only) 8
Appendix A: Ion Binning 9

Installation

This program installs two separate executables:

RawVisionMS.exe: Tool for mass spectrometer analysis
RawVisionPDA.exe: Tool for photo-diode array detector analysis

Steps to Install

1. Download the installer from the official release page or distribution source.
2. Run the installer. You may be prompted for administrator privileges.
3. Choose installation options:
    a. Select the destination folder where both executables will be installed.
    b. Optionally, check the boxes to create desktop shortcuts for one or both programs.
4. Complete the installation by following the on-screen instructions.
5. Once installed, both RawVisionMS.exe and RawVisionPDA.exe will be available in the installation directory.

Notes

- You can launch either executable independently.
- If desktop shortcut creation was selected, you will find icons for RawVision MS and RawVision PDA on your desktop.
- The installer does not modify your system PATH.

User Interface

The main user interface of the MS and PDA programs are structured similarly, with a handful of unique features available for each. The following sections will explain many of the interface components individually. For reference, the UI for RawVision MS is shown in Figure 1.

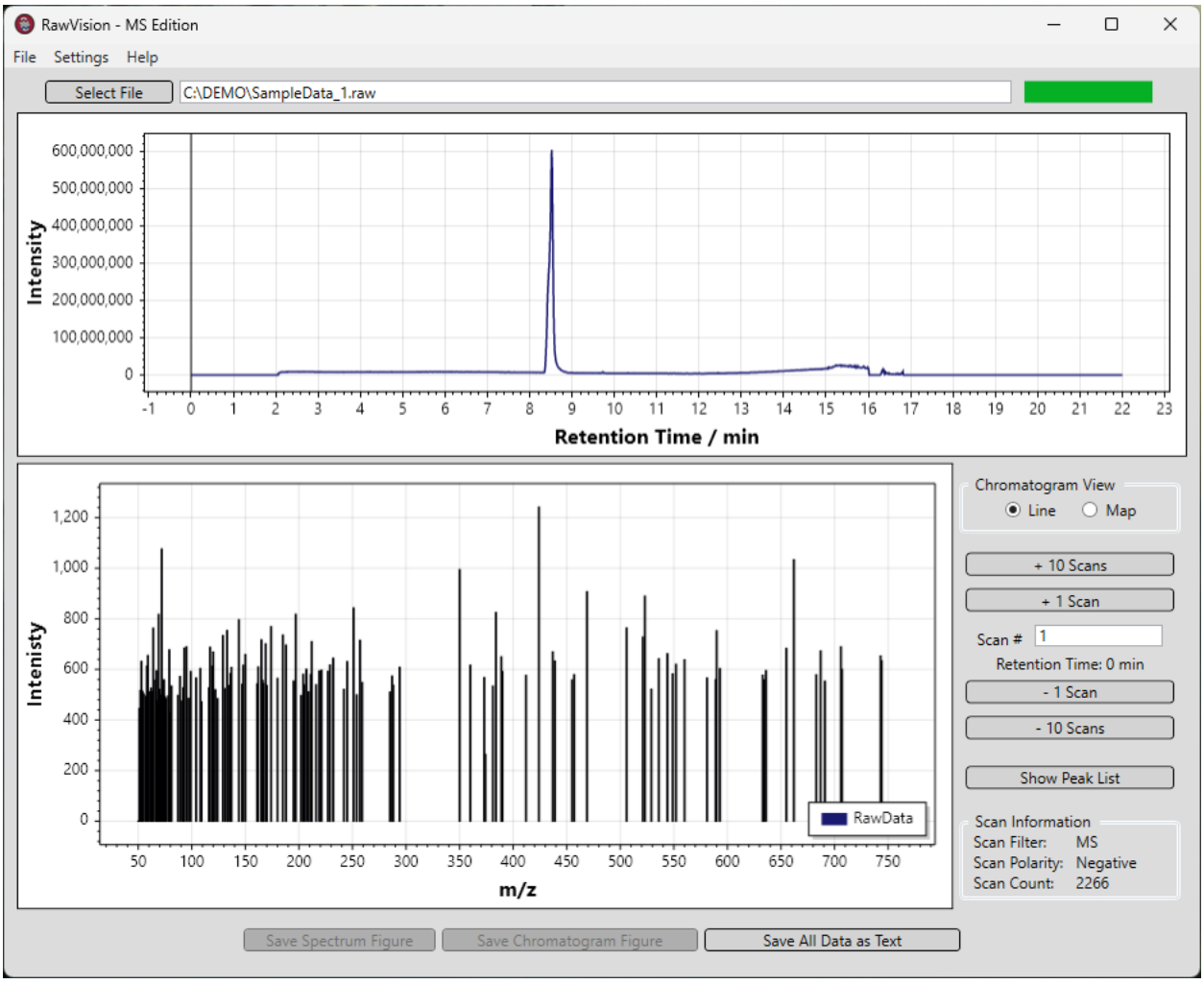

Figure 1. Main user interface of RawVision MS.

File Menu

The File Menu currently contains one option, “New”. **It is highly recommended that “New” be pressed prior to loading a second, third, etc. file.** This helps to ensure that the data from the prior .raw file is cleared.

Settings Menu

The Settings Menu contains various options related to Data Processing and Data Visualization. There are two options available in both the MS and PDA versions, “Map Scaling” and “Colormap”, with both altering the display of the 2-dimensional chromatogram map. Both options will open up a second window in which you will select your desired setting.

Note: These windows open to the left of the main window by default, meaning sometimes they may end up off screen depending on the position of the main window. This is a bug that will be fixed in later versions. To work around it, move the main window over to the left prior to opening the settings windows.

Another pair of similar settings in the MS and PDA programs are the “Mass Range” and “Wavelength Range” settings, respectively. Selecting this option will open up a window prompting you to type in the Min and Max values of your desired range. Clicking “Apply and Close Window” will filter the data to fit your specified range. To go back to the default (i.e. full measured) range, open the setting window again and click “Reset and Close Window”.

Mass Resolution

RawVision MS has a setting under the settings menu titled “Mass Resolution”. This setting is used to generate the common “mass axis” necessary for producing the ion map. **By default, the mass resolution is set to 0, meaning that the data from each scan is joined/rounded to each integer value observed on the mass scale, with their intensities being summed.** For more information on how the mass resolution joining procedure works, see *Appendix A: Ion Binning*.

On common PCs with typical HRMS datasets, the amount of time required to process a file in this manner increases 100-fold for each decimal step in mass resolution, mostly depending on your machine’s RAM. Furthermore, too granular data can result in ion maps with poor visibility of peaks due to pixel resolution of the figure itself.

Loading a File

For a file to be readable by RawVision, it must be in Thermo Scientific's .raw file format. After a file is selected the dialog will close and the file will begin to load. If successful, a popup window will appear confirming the file has been loaded. Load times are dependent on the specifications of your computer, and in the case of RawVision MS, on the Mass Resolution setting you use. A green progress bar is also part of the RV MS interface to provide further confirmation that the file has been completed processed. Doing anything in the program before the file is done loading *may* result in a crash.

If you are analyzing multiple files, it is **highly recommended** that you press "File" → "New" prior to selecting a new file.

Figure Behavior

The top figure in the UI is the chromatogram, and the bottom figure is the mass or UV/Vis absorption spectrum. These figures are built on a plotting library called ScottPlot, which means they have a variety of keyboard shortcuts that can be used to manipulate the data being displayed. A selection of the keyboard shortcuts available is in Table 1.

Table 1. Keyboard shortcuts for interacting with figures in RawVision.

Key	Mouse Action	Result
	Scroll Wheel	Scales both the x and y axis
CTRL	Scroll Wheel	Scales only the x axis
Shift	Scroll Wheel	Scales only the y axis
	Right Click	Drag to scale in all directions
CTRL	Right Click	Drag left/right to scale x axis
Shift	Right Click	Drag up/down to move along y axis
	Left Click	Drag to move in all directions
CTRL	Left Click	Drag left/right to move along the x axis
Shift	Left Click	Drag up/down to move along the y axis
Alt	Left Click	Opens a selection window

Adjusting the Figures

The plots in the figures are auto scaled to fit the data by default. Double-clicking on either figure will open up a "Plot Options" window for that figure. The options available are summarized in Table 2.

Table 2. Summary of plot manipulation options.

Chromatogram Figure

Option	Description
Axis Limits	Sets the min/max of the chromatogram
Autoscale	Resets the axis limits to fit the whole dataset
Show Vertical Line for Scan Number	Provides a visual for the position of the current spectrum being shown in the Spectrum Figure
Show Grid in Plot	Shows/hides gridlines in the figure
Allow Mouse to Edit Axes	Enables/disables click and drag manipulation of the plot
Line Color	Changes the color of the chromatogram line
Color Axis Limits	Sets the limits for the map view of the chromatogram, lowering the upper limit will help emphasize intense regions
Save Settings	Closes the options window and keeps any changes
Close Without Saving	Closes the options window and reverts changes

Spectrum Figure

Option	Description
Axis Limits	Sets the min/max of the chromatogram
Autoscale	Resets the axis limits to fit the whole dataset
Show Grid in Plot	Shows/hides gridlines in the figure
Allow Mouse to Edit Axes	Enables/disables click and drag manipulation of the plot
Line Color	Changes the color of the spectrum line(s)
Disable Autoscale on New Spectrum	Disable automatic adjustment of axis limits when new spectrum is displayed
Save Settings	Closes the options window and keeps any changes
Close Without Saving	Closes the options window and reverts changes

Saving a Figure

To save a figure, right-click on the figure you want to save, and a new menu will appear. Figures can be either saved to files or copied to the clipboard.

Exporting Data

The “Save Data as Text” button on the bottom right will export three files to the original location of your .raw file, depending on which version you are using. For RawVision PDA, the three files will append “_PDA_wavelengths.csv”, “_PDA_times.csv”, and “_PDA_spectra.csv”. The “wavelengths” and “times” files are single column arrays, and “spectra” contains the 2-dimensional chromatogram data.

The same will occur in RawVision MS, with “MS” in place of “PDA”, and with “_masses.csv” in place of “_wavelengths.csv”. The 2-dimensional mass spectra correspond to the data processed by RawVision aligned to the masses resulting from the Mass Resolution setting.

An individual spectrum can be accessed by pressing the “Show Peak List” button or the “Show Spectrum Table” button in RawVision MS and PDA, respectively. This will open up a small window containing a tabular version of the data currently displayed in the spectrum plot. This table can be copied into an Excel or CSV file and saved individually.

Importing a Reference Spectrum (PDA only)

RawVision PDA currently supports importing a reference UV/Vis spectrum to overlay on the spectra from the .raw file. The imported spectrum must be in CSV format with only two columns; the first column should contain wavelength values and the second column should contain absorbance values. One row of column headers is okay, but not necessary.

After importing a spectrum, the Plot Options window will provide the ability to scale your reference spectrum if needed.

Appendix A: Ion Binning

Making a 2-dimensional chromatogram, or an ion map, requires the spectra recorded at each retention time to share a common mass axis. Unlike a diode array detector, which measures the same wavelengths with every scan, most mass spectrometers in liquid chromatography systems only measure the intensity of masses that are physically present at the moment of each scan. This results in mass spectra of difference lengths at each retention time.

RawVision aligns the mass spectra to a common mass axis based on the user-specified Mass Resolution. "Mass Resolution" in RawVision refers to the number of decimal points used for masses in the common mass axis. The default setting is 0, meaning masses are rounded to the nearest integer number. The reason for this being the default is two-fold: relatively fast processing times and producing the most "visually appealing" ion maps.

An example of how a spectrum is aligned to integer numbers is provided below. In short, the masses themselves are rounded to the nearest integer value, and then the intensities of each occurrence of that integer are summed.

Mass	Intensity
154.0146	2000
154.2315	500
154.3561	100
157.6243	800
158.0245	200
158.1342	200
159.0912	750

rounds to

Mass	Intensity
154	2000
154	500
154	100
158	800
158	200
158	200
159	750

resulting in

Mass	Intensity
154	2600
158	1200
159	750

Changing the Mass Resolution changes how granular this binning procedure becomes. For high-resolution instruments, increasing the number of decimals included in the binning procedure drastically increases processing times, as one high-resolution .raw file can contain 10^7 or more unique masses.

Data with high Mass Resolution may also not appear very intense in this program. The plotting library used in RawVision generates a Bitmap image for the figures that are displayed in the program. In this image, each measured mass is effectively one row of pixels. Decreasing the number of masses in the final array (i.e. minimum Mass Resolution) can actually help spread some of the intensity out, yielding ion maps that are easier to see without scaling into individual features of the plot.