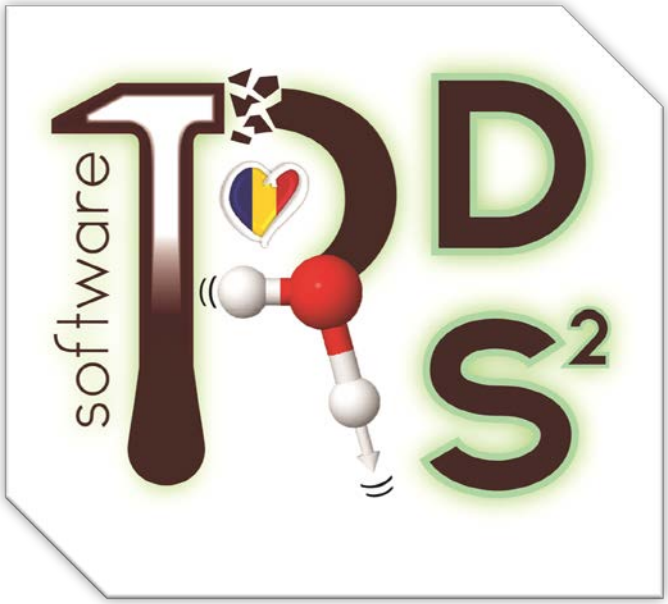
Raman Data Search and Storage (RDSS)

Complete Documentation

A Raman spectra library software using peaks position for fast and accurate identification of unknown inorganic compounds.



v2013.09.01

I wish you resonant, clean and non fluorescent spectra!

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RDSS website: http://rdss.sf.net
RDSS forum: http://rdrs.uaic.ro/forum/

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1. ABSTRACT

Raman spectroscopy is widely used in the field of geosciences because it is very fast, non-destructive, noninvasive and does not require sample preparation. The Raman spectra often provide unique fingerprint of the sample that can be used to identify any unknown minerals.

Raman Data Search and Storage (RDSS) software was developed as an analytical tool for a fast and accurate identification of unknown minerals by comparison of their spectra with the indexed library of data. **RDSS** is a freeware, user-friendly software, written in Java, not OS dependent, available for use by anyone who has an Internet connection and can be accessed at the following link: *http://rdss.sf.net*. A search function was implemented to enable users to find a specific peak value. Using the asterisk character (*) as a placeholder for one or more unknown peak value(s), the software will return the best match(es). Besides the search utility by the Raman band positions, which was proven to be priceless in the interpretation of Raman spectra, the **RDSS** software gives the user the ability to display and inspect the Raman spectra quickly and very efficiently. Users can zoom into the Raman spectrum, shift in any direction the wavenumber and the intensity axes, and if any part of the spectral display is clicked, that region will be highlighted and the specific wavenumber returned. A photo for every sample entry stored in the database is also available. For the raw Raman spectra, the **RDSS** software can open any .txt file format with XY data format, delimited by different delimiters: tab, space, comma, semicolon, and it can also ignore rows with ##comments.

The **RDSS** software allows users to easily find the Raman peaks of a raw spectrum obtained from a single crystal or from a mixture where multiple peaks are expected to arise. The only disadvantage encountered in most applications which use a spectral matching system is usually the insufficient number of spectra in the database. However, even with a limited number of records in the database, the user can obtain a first impression of the mineral class of the unknown compound.

2. GENERAL DESCRIPTION

2.1. Description

Raman Data Search and Storage (RDSS) software was developed as an analytical tool for a fast and accurate identification of unknown minerals by comparison of their spectra with the indexed library of data. This application derives from an online database entitled **Romanian Database of Raman Spectroscopy (RDRS)**. **RDSS** is freeware, enjoy!

2.2. System Requirements & Installation

2.2.1. Terms of Use / before start (takes 10 seconds)

Please, read *END-USER LICENSE AGREEMENT (EULA)* carefully before copying, installing or using the **RDSS** software. By using all or any portion of the Software you accept all the terms and conditions of this Agreement. If you do not agree, do not use this Software. You can read the *EULA* online, at this URL *http://rdss.sf.net/license.html*; or, you can read the full *EULA* which is in the root directory of the application (LICENSE.txt).

2.2.2. Download

You can download it from application website (*http://rdss.sf.net/download.html*), or from the sourceforge website (*http://sourceforge.net/projects/rdss/*).

2.2.3. Installation

This is written in Java, so you don't need to install it, just take care if you have JAVA Runtime Environment. You can find Sun's Java here (*http://java.com/download/*). By the nature of what it does and for what it's used, it is not portable at all, and only runs on Windows (tested on XP, Vista 32/64, Windows 7 32/64). It works on Linux OS, but not fully functional! Minimum hardware requirements: RAM 512 MB (1GB recommended).

2.3. Scientific citation

If you use RDSS in your scientific work, please reference to the software as:

"RDSS - A Raman spectra library software using peaks position for fast and accurate identification of unknown inorganic compounds", Version 201x.xx.xx, *http://rdss.sourceforge.net*.

Important! Please insert the current version number which is presented as date format yyyy.mm.dd.

3. THE GUI (GRAPHICAL USER INTERFACE)

3.1. Menus

General functions are accessed via the Menus.

Main Window //Menu			New Spectrum //Menu			
Function	**Shortcut**	**Action event**	**Function**		**Shortcut**	**Action event**
File > Login	F5	Disabled at this moment*	File > Clear Spectrum		Ctrl + R	Clear the spectrum from the ChartView
File > Open Spectrum	Ctrl + N	Open a new file spectrum	File > Exit		Ctrl + Q	Close the window
File > Save Spectrum	Ctrl + S	Save the current spectrum	Spectra > Properties		Ctrl + E	Properties of the spectrum
File > Refresh	Ctrl + Alt + R	Restart the application	Spectra > RIA	Baseline adjusted	Ctrl + B	Open 'baseline adjusted' tab for RIA
File > Exit	Ctrl + Alt + Q	Quit without prompt message		High fluorescence	Ctrl + H	Open 'high fluorescence' tab for RIA
Window > Reset Layout	F3	Reset all panels				
Help > Help	F1	Open this file				
Help > Quick Start Guide	Ctrl + G	Open a quick start guide				
Help > Support Forum	F11	Open the Forum webpage				
Help > License	Alt + L	Open License file				
Help > Change Log	F12	Open Change log				
Help > Roadmap		Open Roadmap page				
Help > Check for update	Ctrl + U	It checks for any updates				
Help > Donate		Open donation page				
Help > About	F2	Open About window				

* - Login function is disabled at this moment because administrator panel require some technical adjustments.

3.2. Main window

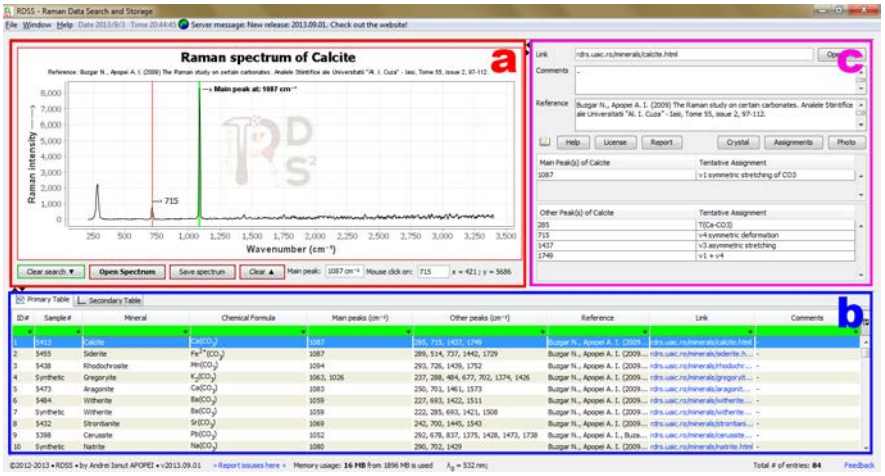

Figure 1 - Main window of the **Raman Data Search and Storage** application: a) – ChartView panel; b) – data entries panel; and c) – panel with the details of the selected entry from panel 2

3.2.1. Data entries, ChartView and tentative assignment of the Raman peaks

The core of the **RDSS** application GUI is the bottom, where two tabbed panels contain two tables. First tab named *Primary Table* contain a table designed to have commons columns like: sample no., mineral name, chemical formulae, main peaks, other peaks, reference, external link and comments. The second tab named *Secondary Table*, contain a table designed to have a more specific columns for specific domain search: mineral name, 200 - 600 cm^{-1}, 600 - 900 cm^{-1}, 900 - 1200 cm^{-1}, 1200 - 1500 cm^{-1}, 1500 - 2000 cm^{-1}, 2000 - 3000 cm^{-1}, 3000 - 4000 cm^{-1}, external link, comments and reference (see figure 1). The first and the last three columns are linked with those from Primary table for structure reasons.

In the left-upper part of the main window of **RDSS** application, a Raman spectrum shows when a specific row is clicked in the Primary and Secondary Table. In other words, each mineral row is linked with its own Raman spectrum.

3.3. New Spectrum window

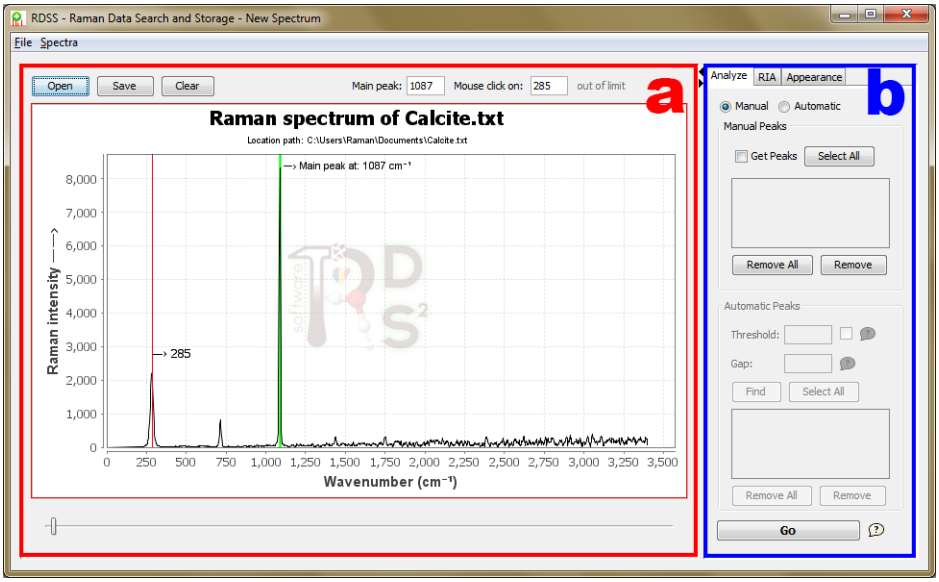

Figure 2 – New Spectrum window of the **Raman Data Search and Storage** application: a) – ChartView panel; and b) – a panel which contain tabs with specific functions

3.3.1. Analyze

In this tab user can manually extract the interested peaks or automatically which is a great function for Raman spectra with multiple peaks. See bellow discussions for both options.

3.3.1.1. Manual

When "Manual" radio button is pressed, a panel with manual search function of the Raman peaks becomes active (figure 3).

After the "Get Peaks" checkbox is checked, on the Raman spectra chart panel appear a crosshair which moves with the mouse crosshair. In other words it's like a real-time mouse tracing which help the user to get the exact peak position. Furthermore, the user can zoom in before get the desired peak. All peaks appear in a list with different options: delete a single peak, multiple or even all peaks from the list.

To compare selected peak(s), after selection, press "Go" button from the bottom of the entire panel.

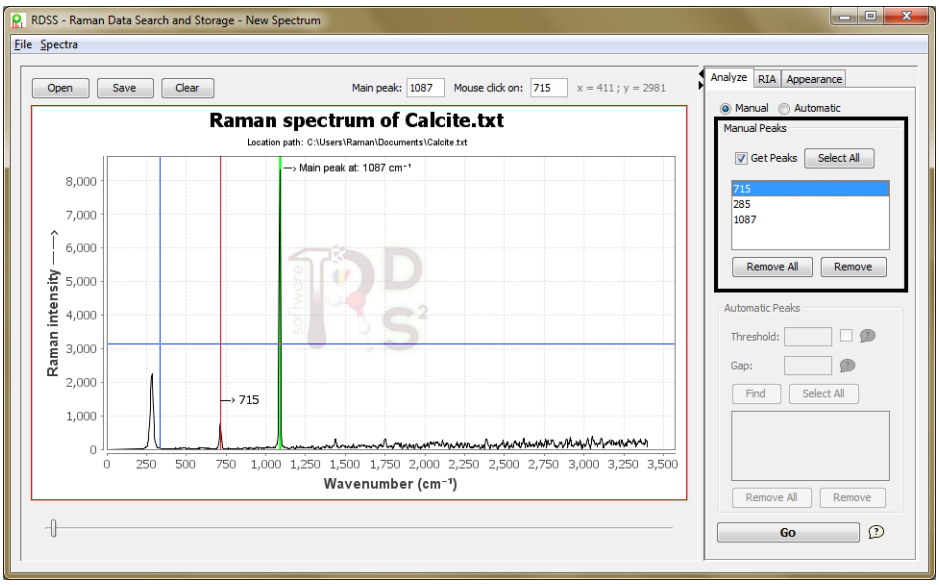

Figure 3 – Manual search function of the Raman peaks

3.3.1.2. Automatic

When "Automatic" radio button is pressed, a panel with automatic search function of the Raman peaks becomes active (figure 4).

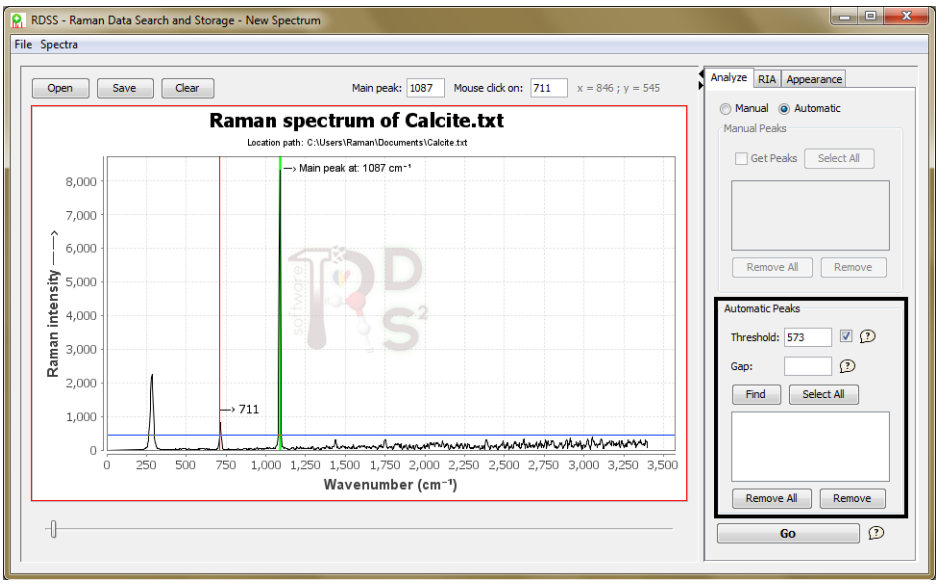

Figure 4 – Automatic search function of the Raman peaks while set the value of the "Threshold"

To use the automatic search function, the user needs to fill two variables before obtaining peak values.

First variable is the "threshold". Specify the 'threshold' heigh, 'findpeaks' only returns peaks that exceed at least the Y-value of 'Threshold' (figure 4).

Second variable is the "Gap". Specify the 'gap' width. This function affects number of peaks. Density of the peaks is directly correlated with this variable. Most recommended values are

between 50 and 300. In this example (figures 4 and 5), was used a value of 200. Don't forget to press "Find" button after you filled the second variable.

All peaks appear in a list with different options: delete a single peak, multiple or even all peaks from the list. To compare selected peak(s), after selection, press "Go" button from the bottom of the entire panel.

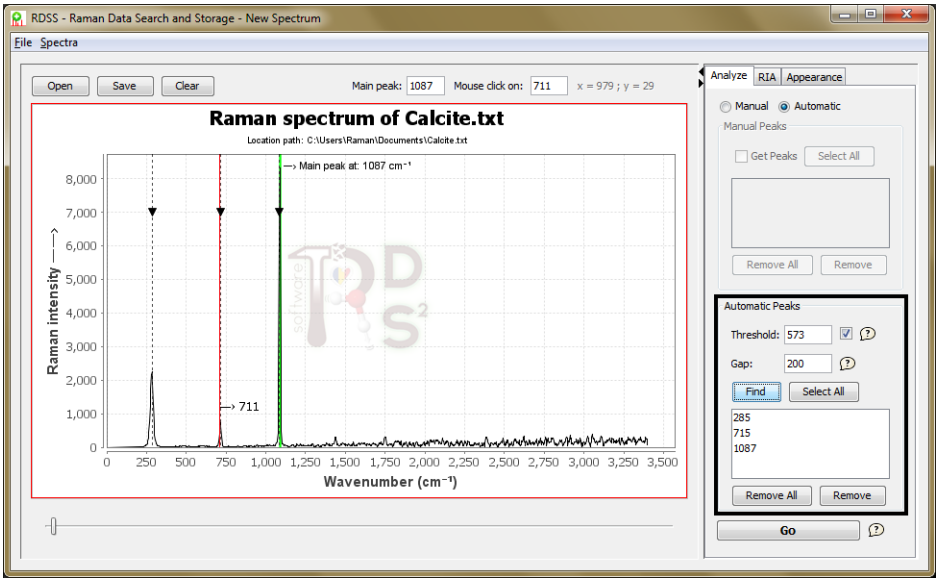

Figure 5 – Automatic search function of the Raman peaks after was set the value of the "Gap" and "Find" button was pressed

3.3.2. Relative Intensity Assignment (RIA)

This function is performed for both the Baseline Adjusted Raman spectra and for Raman spectra with High fluorescence. For both functions is used a 5 steps of intensity assignment and are divided as follow:

Intensity	Assignment
between 0 – 10%	very weak (vw)
between 10 – 30%	weak (w)
between 30 – 60%	medium (m)
between 60 – 90%	strong (s)
between 90 – 100%	very strong (vs)

The Baseline adjusted Raman spectra (figures 6 and 7) works very well with baseline-removed spectra. After the checkbox "On/Off | Intensity Assignment" is checked, the user must extract the strongest peak by moving the crosshair and press first mouse-button on that peak (figure 6). Afterwards, the lowest peaks (in terms of intensity) can be assignet based on the strongest peak.

The High fluorescence Raman spectra (figures 8 and 9) works very well with the Raman spectra which has no baseline-removed spectra. After checkbox "On/Off | Intensity Assignment" is checked, the user must extract the strongest peak in two steps:

(i) first identify the highest peak from the Raman spectrum and check the "Min" (which stands from "minimum") radiobutton, afterwards the user must extract the minimum of the strongest peak by moving the crosshair and press first mouse-button on that minimum of the peak (figure 8);

(ii) the second step is similar to the first, the difference being that the user must to check the "Max" (which stands from "maximum") radiobuutton, afterwards the user must extract the maximum of the strongest peak by moving the crosshairr and press first mouse-button on the maximum of the peak.

For the Peak 1 assignment, the procedure is similar to that of the extraction intensity value for the "Strongest peak" (discussed above).

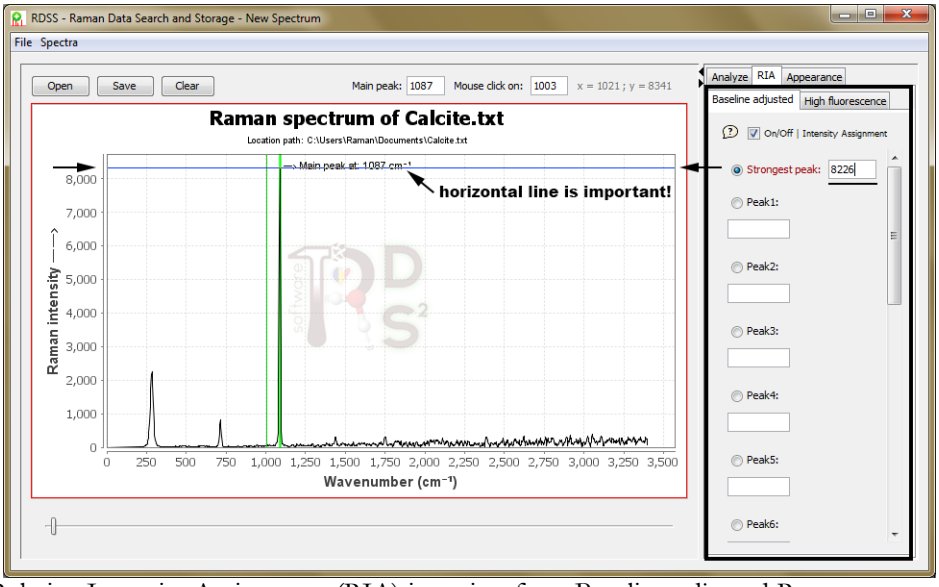

Figure 6 – Relative Intensity Assignment (RIA) in action for a Baseline adjusted Raman spectrum. Obtaining the "Strongest peak" intensity value

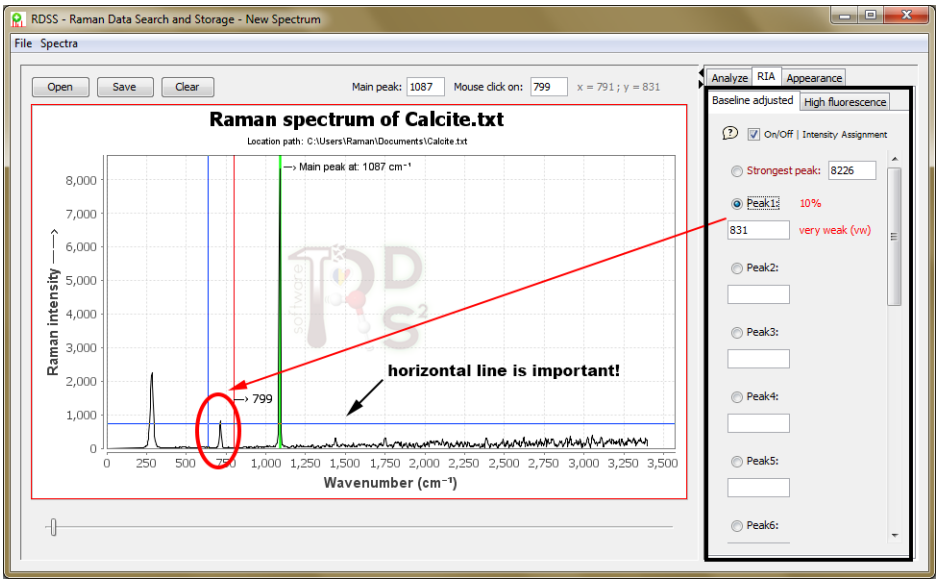

Figure 7 – Relative Intensity Assignment (RIA) in action for a Baseline adjusted Raman spectrum. Obtaining the "Peak 1" Intensity Assignment based on the "Strongest peak" intensity

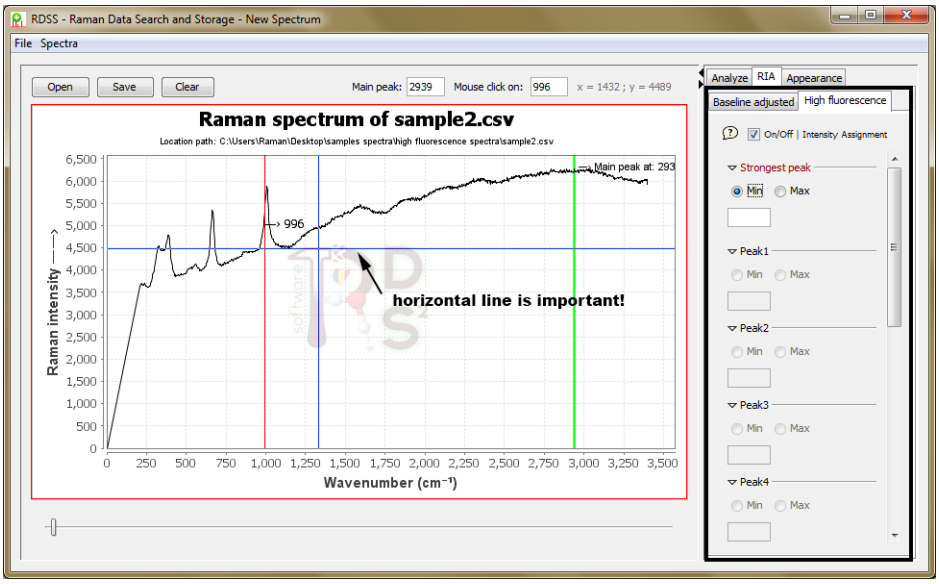

Figure 8 – Relative Intensity Assignment (RIA) in action for a High fluorescence Raman spectrum. Obtaining the minimum intensity value of the "Strongest peak"

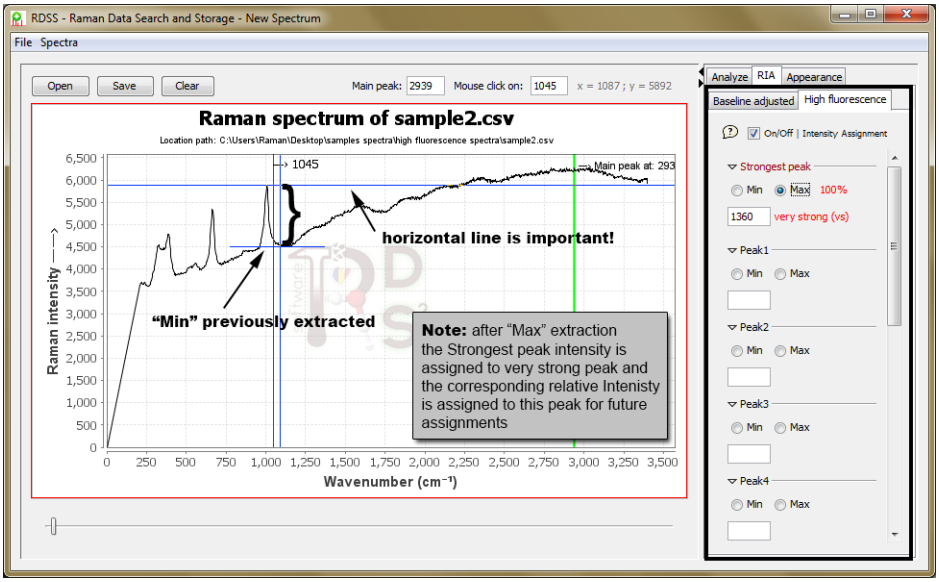

Figure 9 – Relative Intensity Assignment (RIA) in action for a High fluorescence Raman spectrum. Obtaining the maximum intensity value of the "Strongest peak"

3.3.3. Appearance

The Appearance panel (figure 10) contains a lot of tools to manipulate the Raman spectrum in terms of appearance. These tools are described in the following table:

Tool	Action
Tick spacing	Fill the textbox with the desired space between ticks for both axes (Wavenumber and Intensity)
Gridlines	Check or uncheck the checkboxes for the desired axis to show or hide the gridlines
Range	Fill the textboxes from x (start number) to y (end number). Don't confuse y with Y axis. This range can be used just for the Wavenumber axis.
Spectrum color	User can choose a color from 7 available colors (black, red, green, blue, orange, yellow and cyan). Default is black.

Spectrum width	Width of the Spectrum line
Spectrum points/lines	Convert the Raman spectrum line in points linked by a thin line and default Raman spectrum line
Reverse axes	Checkbox to reverse X-axis (Wavenumber) and checkbox to reverse Y-axis (Intensity)

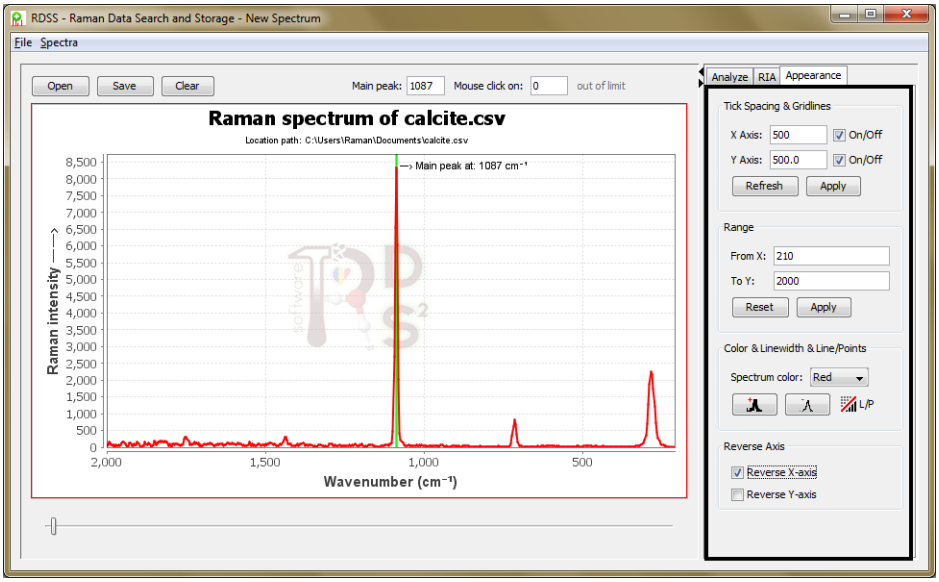

Figure 10 – Functions from the Appearance panel tab in action

3.4. Spectra menu and properties

The Chart Panel where is shown the Raman spectrum has some functionalities and properties which can be archieved by mouse actions.

Right mouse click activates a popup menu with the following items:

Item	Action
Copy	Copy the Raman spectrum (you can paste it in photo editors)
Save as…	Save the Raman spectrum in .png format
Print…	Print it
Zoom in > Both Axes	Zoom in perserving the ratio of both axes
> Domain Axis	Zoom in perserving just the Intensity ratio
> Range Axis	Zoom in perserving just the Wavenumber ratio
Zoom out > Both Axes	Zoom out perserving the ratio of both axes
> Domain Axis	Zoom out perserving just the Intensity ratio
> Range Axis	Zoom out perserving just the Wavenumber ratio
Auto Range > Both Axes	Auto Range both axes
> Domain Axis	Auto Range Wavenumber axis
> Range Axis	Auto Range Intensity axis
Reverse X-axis	Reverse Wavenumber axis
Help/Shortcuts	Opens a window with explainations of how to use mouse for a fast and easy controlls of the Raman spectrum

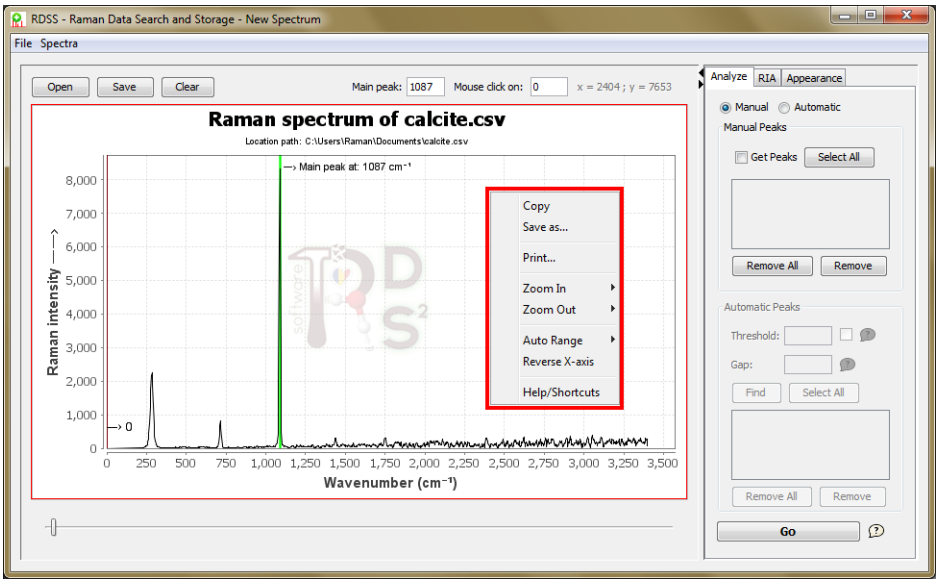

Figure 11 – Spectra menu and properties

Action	How to do it
Zoom in/out	Use the scroollwheel-up/down of the mouse
Zoom in on a desired region	Use the left mouse button to drag a selection rectangle
Restore X-axis / Y-axis	Press right mouse button and drag the mouse up/down
Translate X-axis / Y-axis	Ctrl + left mouse button and drag the mouse to move the whole Raman spectrum
Get X value	press left mouse button on the Raman spectrum and hover the mouse to see the specific value of the X axis

4. FUTURE DEVELOPMENT

- to populate the application with new Raman spectra;
- integrate 3D crystal structure for every entry;
- save spectra in .csv / .xls format
- drag and drop spectrum file;
- add clear button for RIA panel;
- mineral classes description;
- Raman introduction/tutorial/short presentation;
- google maps api, for GIS coordinates of the samples.