Excel spectroscopic tools to visualize, analyze and manipulate remotely sensed data of planetary bodies.

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1. Introduction

In the context of the future and present missions, tools and techniques are needed to analyze new hyperspectral data of the surfaces of various bodies in the Solar System.
Here, we present an interactive Excel tool that provides a quick and easy way to visualize and manipulate laboratory spectroscopic data. The choice of an interactive Microsoft Excel environment was done to make the visualization and use of the manipulated data as simple and fast as possible by a large audience. Our tool works under three different operating systems: Microsoft Windows, MacOSX, and Linux using the opensource project Wine.

2. Overview

Our tool is meant to visualize and analyze the data of an Excel archive. This Excel archive is organized in two sheets. The first sheet contains different columns: *Sample name*, *Reference*, *DOI*, *Spectral range*, *Measured quantity* (e.g., reflectance, absorbance, transmittance, optical constants, etc.), *Lab/instrument*, *Temperature*, *Grain size*, *and Comments*. The second sheet contains the instrumental response of a number of spectrometers organized as follows: instrument names in the first row, and for each instrument two columns: the wavelength set and the spectral resolution (i.e., the full width at half maximum of each spectral channel).
In this sheet, one can put additional instrumental responses or update a given instrumental response if necessary.

Each row of the Excel archive represents a chemical compound for which laboratory measurements are available. When multiple temperatures of the measurements of a given sample are also available, a hyperlink under the *Temperature* column directly opens the related ASCII file. This allows a quick view and comparison of the spectra. To this aim, we prepared spectral tools written in Visual Basic for Application (VBA). These tools are easily accessible by right-clicking on specific cells in the Excel spreadsheet, and need no installation of separate add-ons (Figure 1).
The tools are the following:
The *Visualize* tool, which permits the quick-look of the spectral profile as found in the database.
The *Convolve* tool, which convolves the original spectral profile to a specific instrumental function available in a separate sheet of the Excel database.
The *Retrieve_k___Shkuratov_1999* tool, which calculates the absorption coefficient *k* starting from a reflectance spectrum, and making assumptions about the refractive index *n*, the porosity, and the grain size of the sample (Shkuratov et al., 1999). Error checks make sure this tool is used only when proper condition apply (for example, if the user attempts to derive *k* from absorbance, a warning pops up).
All of the three tools allow the user to save the result as a *.txt file or to plot the spectrum and save it as a *.png file.

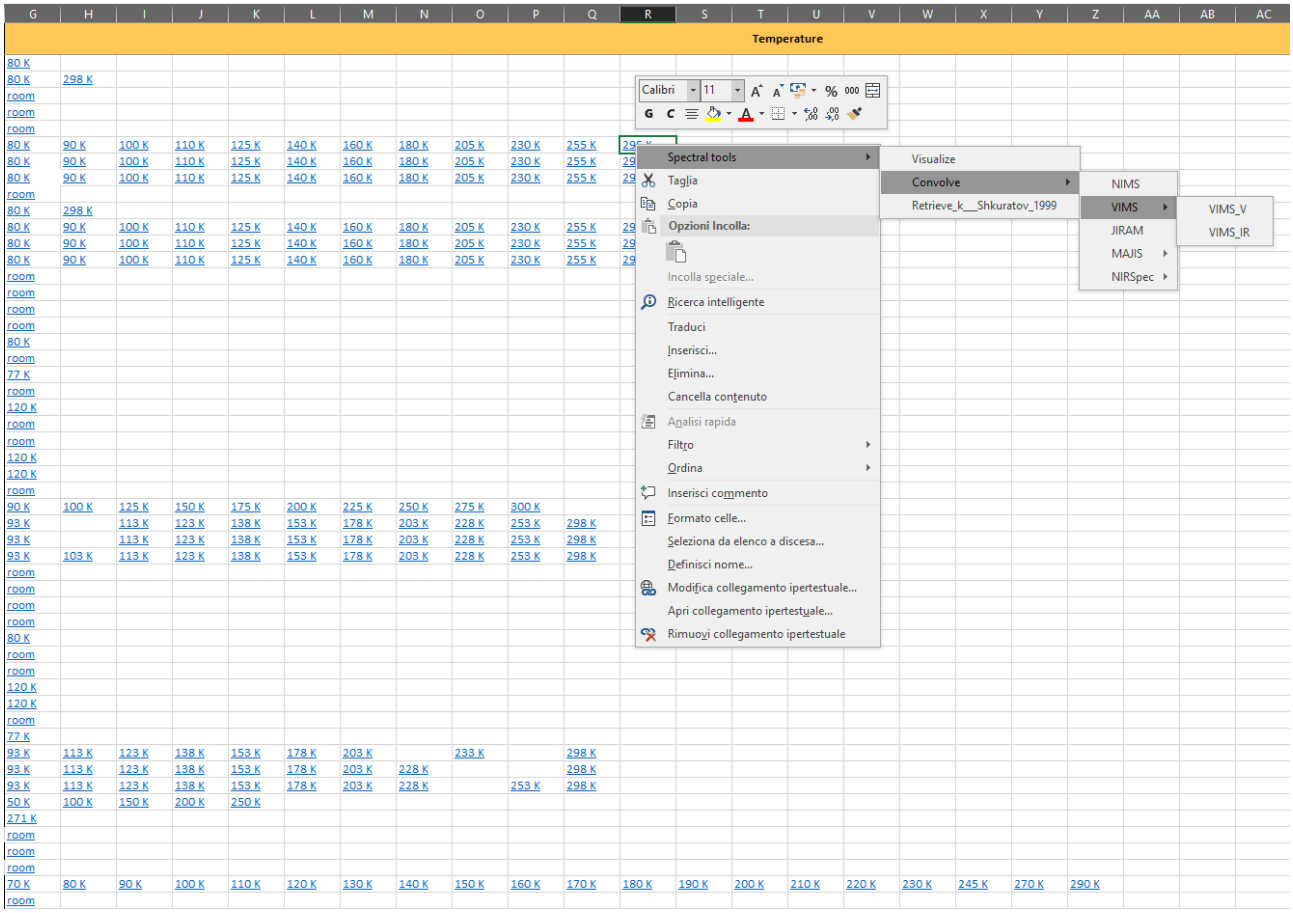

Figure 1. The right click menu Spectral Tools created with VBA Excel.

3. Methods

These tools are Excel macros written in the Visual Basic for Applications (VBA) language. Any user opening this spreadsheet for the first time will need to authorize the use of macros within the Excel environment.

The first tool, *Visualize*, is meant to just display the data as they are in the archive. In this case, the user shall place the mouse on the cell corresponding to a specific chemical compound and temperature value (if multiple temperature values are available). By right-clicking on the cell, a new menu appears among the various existent entries, the Spectral tools menu.

By choosing the Visualize entry (Figure 1), a new Excel Window opens (Figure 2). The new window is the ASCII file visualized in Excel format with the relative plot.

The second tool, *Convolve*, applies a spectral convolution to the laboratory data present in the archive. This is crucial whenever a direct comparison between remotely sensed spectra (e.g., acquired by an imaging spectrometer onboard a spacecraft or by JWST/NIRSpec) and laboratory spectra is needed, or to perform spectral unmixing based on a number of spectral endmembers.

In this tool, the user must first place the mouse on a specific cell representing a given chemical compound and temperature, then choose the Convolve menu by right-clicking the mouse. There the user can choose between several imaging spectrometers

relevant for the exploration of the outer Solar System plus JWST/NIRSpec (Figure 1), and among specific channels (e.g., VIS or IR) if the instrument has more than one.

After the desired option is selected, the program performs a convolution of the laboratory spectrum to the wavelength set and spectral resolution of the instrument (as found in the second sheet of the main Excel archive). Once the convolution is completed, the result is displayed in a new window. Figure 3 shows an example of what can be obtained.

	A	B	C	D	E	F	G
1	MgCl2 · 6H2O (bischofite)	De Angelis 2022	0.5 - 4.7 µm	Reflectance	SSHADE/REFL_SLAB - OSU(	125 K	500-800 µm
2	Wavelength (micron)	Reflectance					
3	0.50000	0.78926					
4	0.52000	0.79199					
5	0.54000	0.78944					
6	0.56000	0.78794					
7	0.58000	0.79611					
8	0.60000	0.79323					
9	0.62000	0.79362					
10	0.64000	0.78982					
11	0.66000	0.79531					
12	0.68000	0.77115					
13	0.70000	0.77357					
14	0.72000	0.76279					
15	0.74000	0.73957					
16	0.76000	0.72098					
17	0.78000	0.73168					
18	0.80000	0.73960					
19	0.82000	0.74132					
20	0.84000	0.74087					
21	0.86000	0.72593					
22	0.88000	0.72583					
23	0.90000	0.71445					
24	0.92000	0.68837					
25	0.94000	0.64363					
26	0.96000	0.55509					

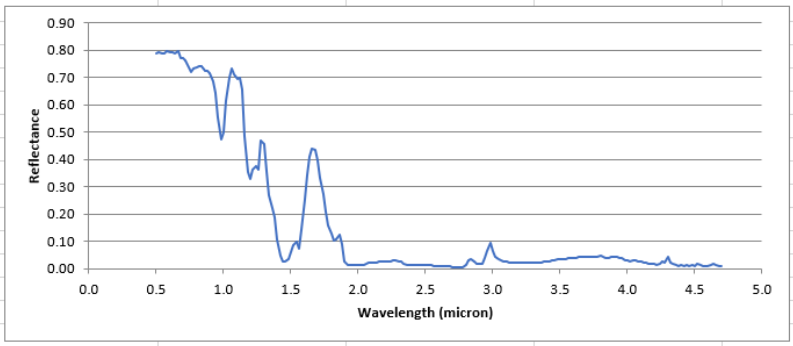

Figure 2. An example of the Visualize output.

	A	B	C	D	E	F	G	H	I	J	K	L
1	MgCl2 · 6H2O (bischofite)	De Angelis 2022	0.5 - 4.7 µm	Reflectance	SSHADE/REFL_SLAB - OSUG Data Center	110 K	500-800 µm					
2	Wavelength (micron)	Reflectance	NIMS wavelenght (nm)	Convolution								
3	500.00000	0.78568	710.10000	0.7674869388								
4	520.00000	0.79149	723.10000	0.7582269169								
5	540.00000	0.78736	736.10000	0.7441305019								
6	560.00000	0.78662	749.10000	0.7308878123								
7	580.00000	0.79520	762.10000	0.7232236088								
8	600.00000	0.79285	775.20000	0.7281649084								
9	620.00000	0.79313	788.20000	0.7342772366								
10	640.00000	0.78893	801.20000	0.7389616597								
11	660.00000	0.79476	814.20000	0.7403523737								
12	680.00000	0.77074	827.20000	0.7409855201								
13	700.00000	0.77291	840.30000	0.7396616455								
14	720.00000	0.76231	853.30000	0.7313097319								
15	740.00000	0.73957	849.00000	0.7344161861								
16	760.00000	0.72032	862.10000	0.7267852126								
17	780.00000	0.73069	875.10000	0.7253778326								
18	800.00000	0.73949	888.10000	0.7208954088								
19	820.00000	0.74072	901.20000	0.7115139260								
20	840.00000	0.74150	914.20000	0.6953203266								
21	860.00000	0.72588	927.30000	0.6714865229								
22	880.00000	0.72557	940.30000	0.6379713333								
23	900.00000	0.71427	953.30000	0.5865493052								
24	920.00000	0.68808	966.40000	0.5324164797								
25	940.00000	0.64320	979.40000	0.4894359567								
26	960.00000	0.55794	992.40000	0.4914496253								
27	980.00000	0.47779	1002.80000	0.5286685531								
28	1000.00000	0.49839	1028.80000	0.6486142503								
29	1020.00000	0.61397	1054.80000	0.7183681200								
30	1040.00000	0.70161	1080.80000	0.7131280129								
31	1060.00000	0.73301	1106.70000	0.6989843211								
32	1080.00000	0.71375	1132.70000	0.6650345366								
33	1100.00000	0.69538	1158.70000	0.5094422659								
34	1120.00000	0.70355	1184.70000	0.3611134869								

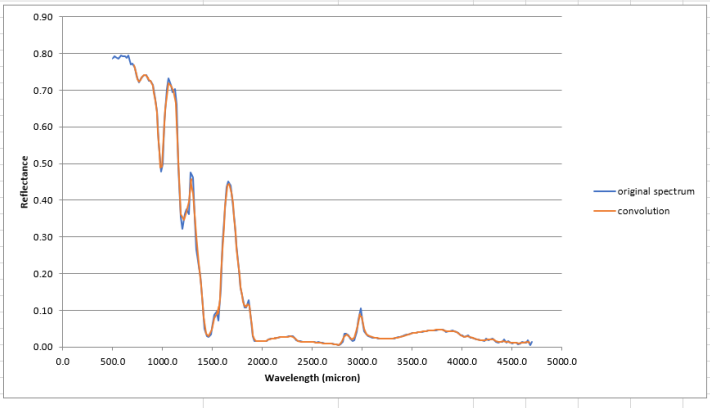

Figure 3. An example of the Convolve output.

The third and last tool derives the absorption coefficient *k* of a chemical compound with the semi-empirical approach of Shkuratov et al. (1999), starting from the knowledge of the reflectance spectrum and making assumptions on the refractive index *n*, the porosity, and the grain size of the sample.

In this case, the user must choose the *Retrieve_k___Shkuratov_1999* option in the right-click menu. This will open an interactive Excel window (Figure 4).
There, the user can specify the grain size (in microns), the porosity, and the scalar value of the refractive index (assumed to be constant throughout the spectral range) following the red arrow, and then pressing the button "Calculate *k*" on the right.

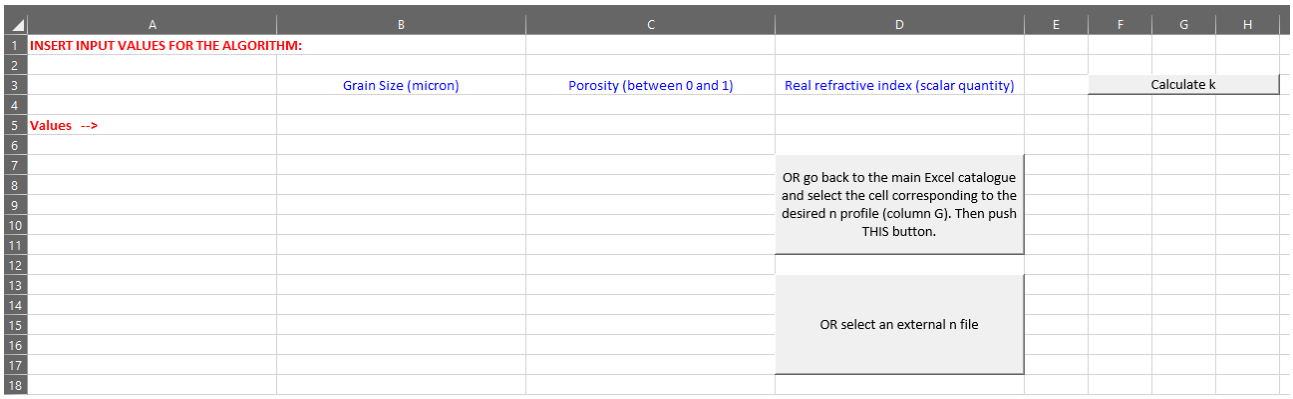

Figure 4. This new calculation sheet opens after clicking Retrive_k___Shkuratov_1999.

Two other buttons offer an alternative to using a scalar value for the refractive index *n*. The first button allows the user to choose a refractive index file available in the archive, while the second button opens and reads an external *n* ASCII file (provided that it has the same formatting used for all the ASCII files in our archive).
In the first case, the user must go back to the main Excel catalogue and place the mouse on the cell corresponding to the desired *n* profile (column G). Then the user must switch to the interactive windows and push the button named: "OR go back to the main Excel catalogue and select the cell corresponding to the desired n profile (column G)".
In the second case, a "Open Folder and Select File" window pops up, allowing the user to choose an external ASCII file.
In both cases, the selected refractive index spectrum is first interpolated to the same wavelength set of the laboratory data, then the absorption coefficient *k* is derived using the refractive index spectrum instead of a scalar value of *n* in the Shkuratov approach.
In all cases, the *k* value is tabulated next to the *n* column (Figure 5). In the second sheet (Figure 6), a dialog box will appear saying: "*k* retrival is completed. Do you want to calculate *k* again with other parameters? If you choose no and you want to calculate *k* later, cancel the *n* and *k* column in the first sheet and insert new parameters in this second sheet."

	A	B	C	D	E	F	G	H	I	J	K
1	CaCO3 (calcium c	ReLab Database(	0.3 - 2.8 µm	Reflectance	Brown Un	room	0 - 45 µm	sample path name: SF-BFJ-002/C1SF02			
2	Wavelength(mic	Reflectance	n	k							
3	0.3	0.82956	1.72139032	1.2097476E-06							
4	0.305	0.81655	1.718164862	1.4496101E-06							
5	0.31	0.825	1.715338939	1.3298333E-06							
6	0.315	0.82604	1.712513017	1.3359526E-06							
7	0.32	0.82441	1.709687094	1.3877324E-06							
8	0.325	0.82907	1.707202061	1.3303548E-06							
9	0.33	0.82988	1.704963879	1.3385956E-06							

Figure 5. An example of the Retrive_k___Shkuratov_1999 output in the first sheet.

After having obtained the absorption coefficient *k*, new buttons will appear, which will allow the user to convolve the spectral profile of k with some specific instrumental profiles among those available (imaging spectrometers and JWST/NIRspec), without the need to save an ASCII file and put it in the database.

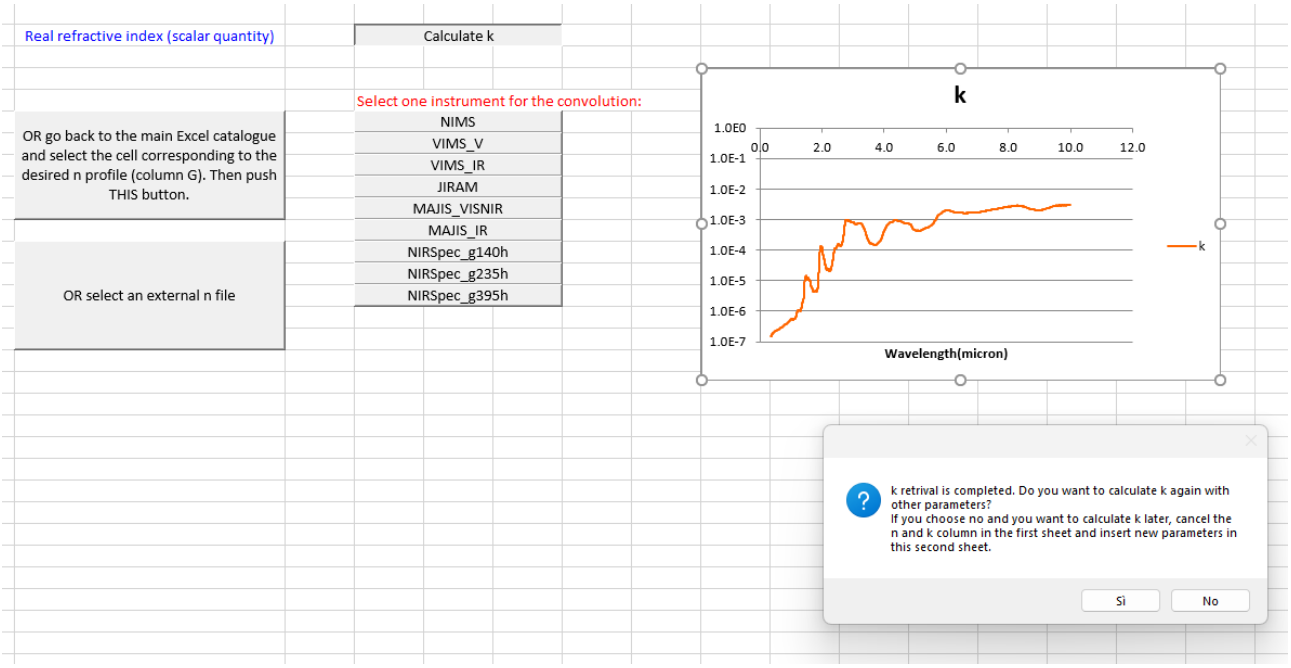

Figure 6. An example of the Retrive_k___Shkuratov_1999 output, second sheet.

At the end of these computations, that is after Visualize, Convolve and Retrieve, a new menu appears in the right-click menu on the output sheet: “Save calculation” (Figure 7). It gives the user the possibility to save the data as an ASCII file or as a plot in the *.png file format. When the user selects an option, a folder window opens, allowing one to save the file in the desired local directory.

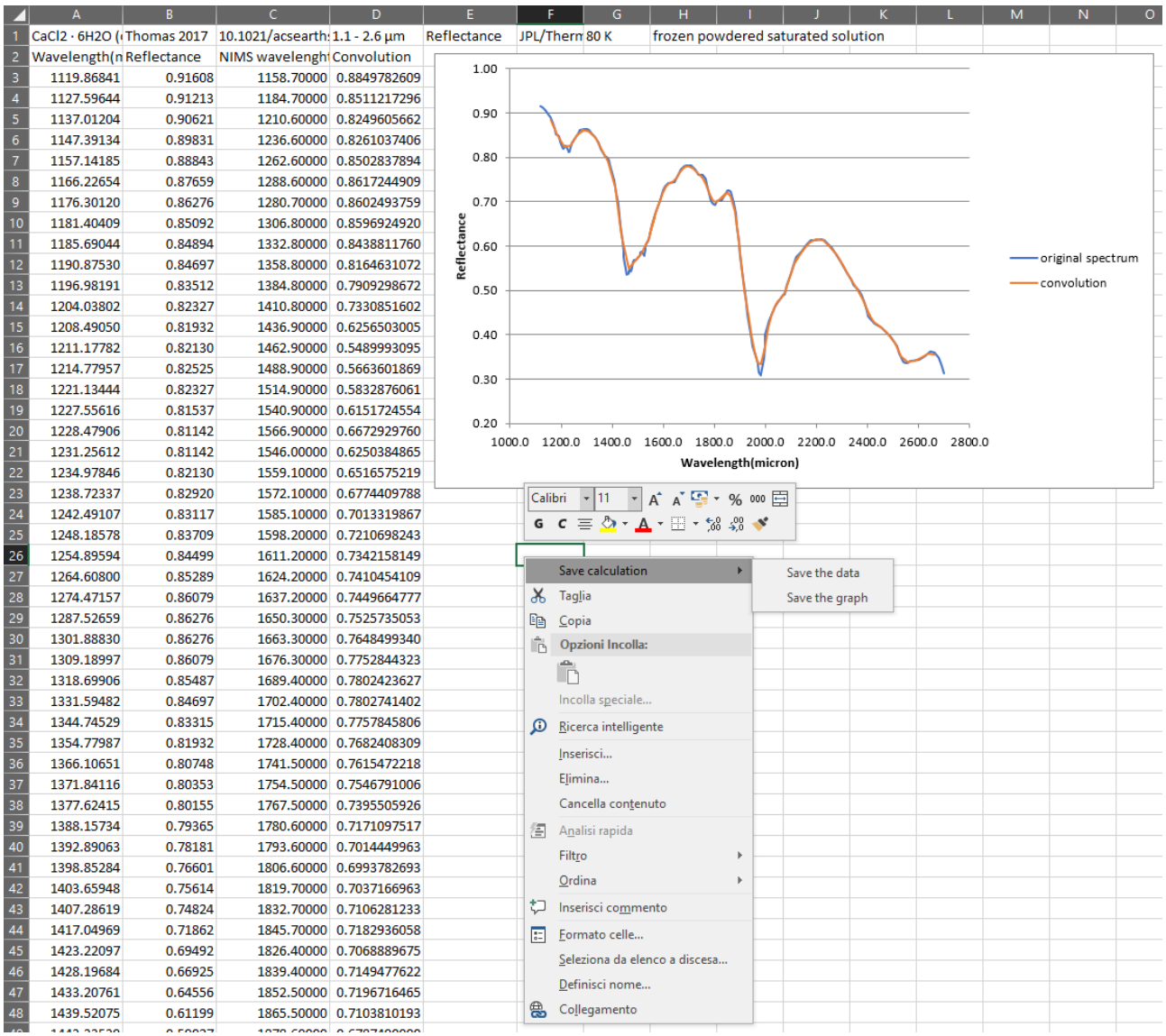

Figure 7. Once the computation is done, the save options appear in the menu in the new Excel file.

4. Installation

To use this Excel archive there is no need to install separate add-ons. The package is self-consistent and provided in the form of an Excel sheet with macros. It includes examples in the first and second Excel sheets on how to set up the data.
The tools are ready to be distributed and they are available sending an email to alessandra.cofano@inaf.it. When used for publications, it is kindly requested to cite its DOI.

5. Conclusions

These spectroscopic tools in Excel provide a quick and easy way to manipulate data. To validate the outputs, the results from the convolution tool were compared with a convolution tool existing in the Harris ENVI software, while the derivation of *k* using

the Skhuratov approach was double-checked with other studies such as Roush et al. (2007).

6. References

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