ASD & Nicolet Spectra Processing Protocol

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This document details the steps necessary to process spectra from two instruments. The first collected using an Analytical Spectra Device (ASD) Full Range spectrometer which covers the 0.3 – 2.5 µm range with a sampling interval of 1 nm (Analytical Spectra Devices, Inc., Boulder, CO USA). The second collected using Nicolet Model 4700 Interferometer Spectrometer fitted with a Labsphere gold coated integrating sphere (model RSA N1 700D) which measured emissivity from 2.5 – 15.4 µm with a sampling interval of 1 nm (Thermo Electron Corp., Madison, WI, USA). This document details the steps necessary to convert and average spectra from the ASD and Nicolet sensors.

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Setting up the Code Project

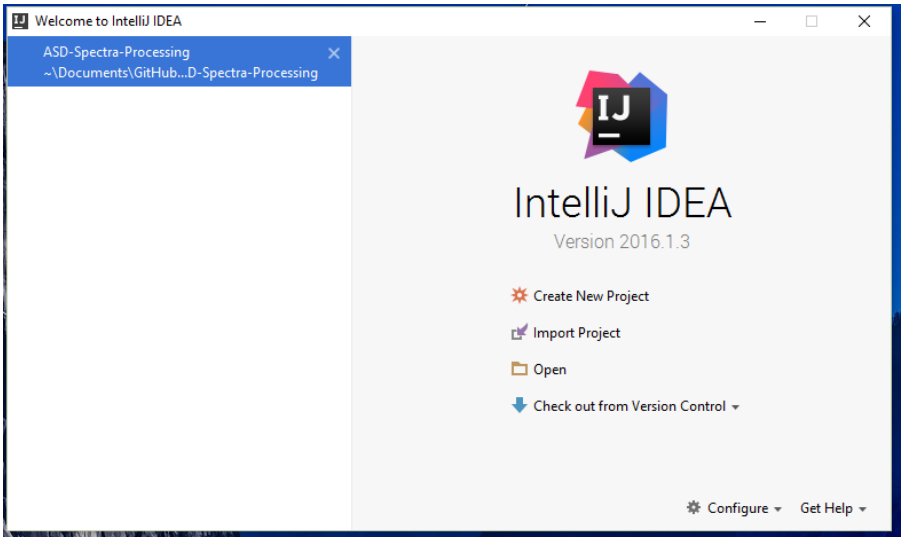
Java Requirements

The first step is to set up the program that will visualize and average spectra from the Nicolet and ASD. This program was developed using Java. You will need to have IntelliJ Idea which is a free

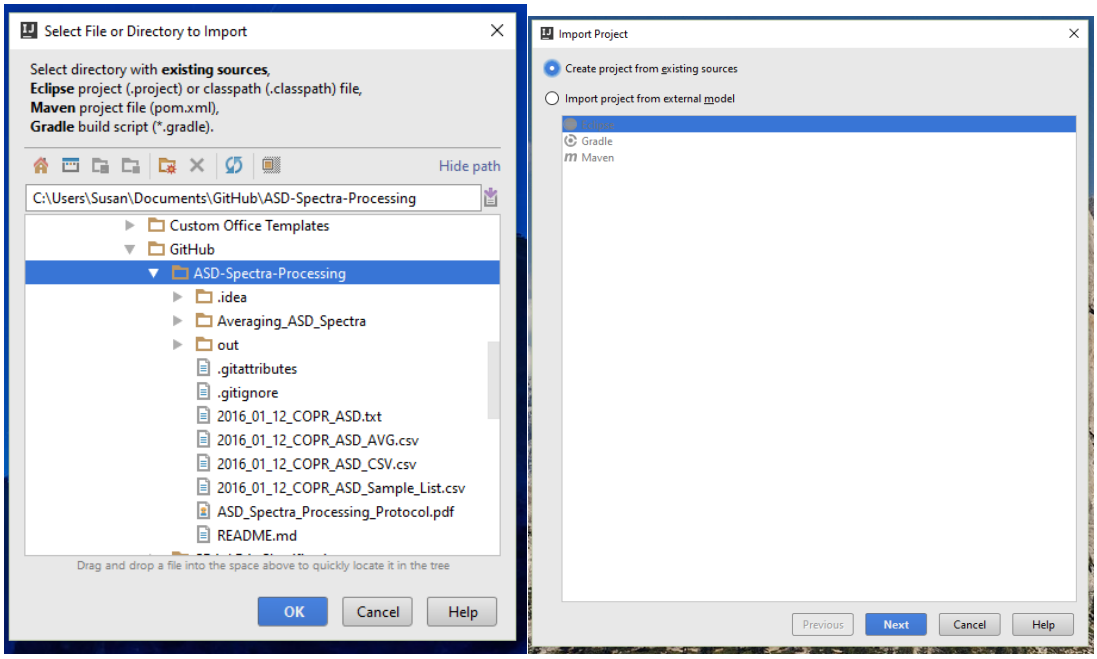
download (https://www.jetbrains.com/idea/). Additionally, you will need to have Java, which should already be installed. Specifically, you will need **Java JDK 1.8** to run this program. If not it is a free download from this website (http://www.oracle.com/technetwork/java/javase/downloads/jdk8-downloads-2133151.html).

Opening Code in IntelliJ

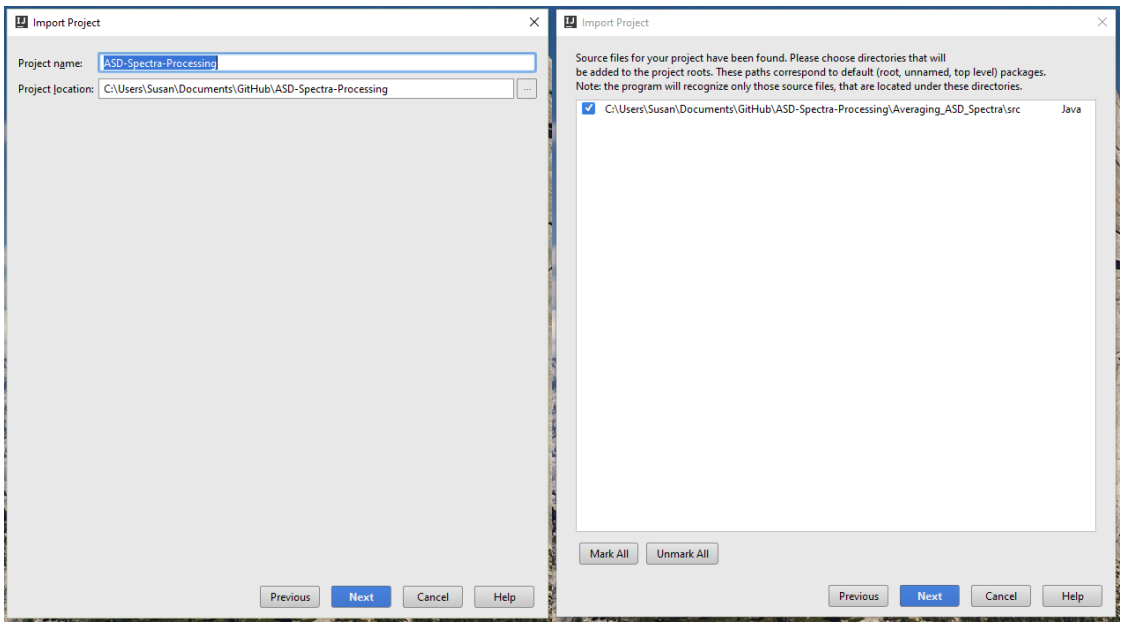
1. Open IntelliJ and click "Import Project" or File > Import Project.



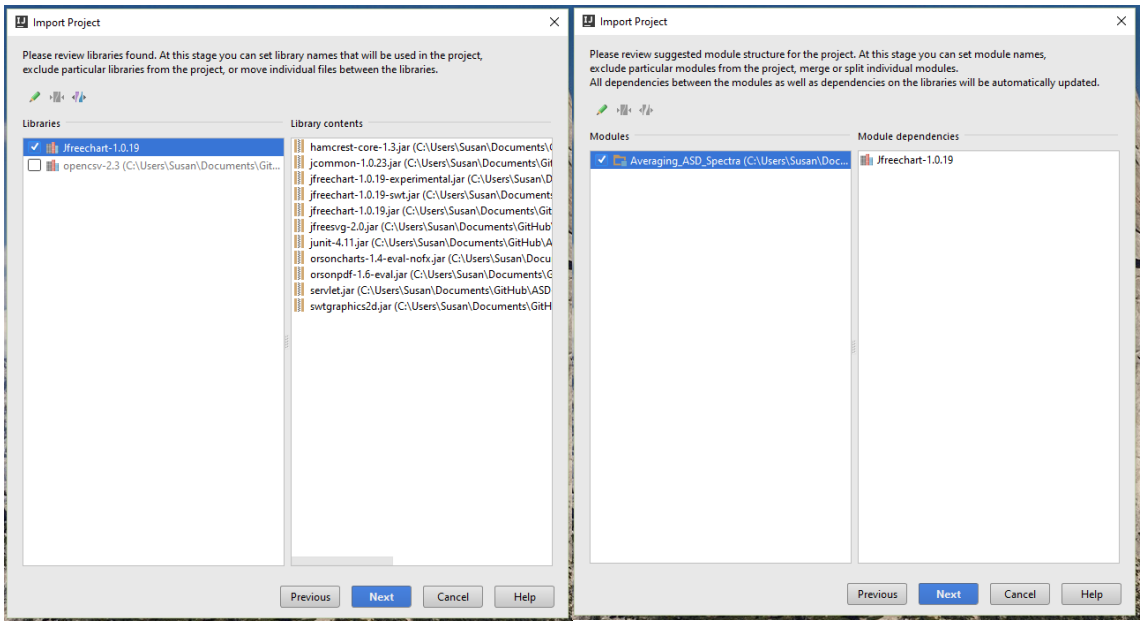
2. In the Import dialog box, select directory that contains the project. Once selected, hit OK. On the next dialog screen, select "Create project from existing sources". Hit Next.



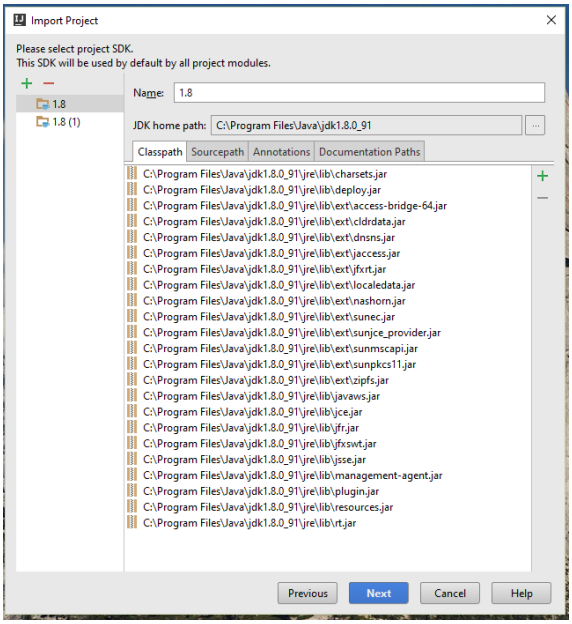
3. On the next dialog screen, enter the Project name and Project location. Hit Next. On the next screen, allow IntelliJ to add the source files for your project and hit next.



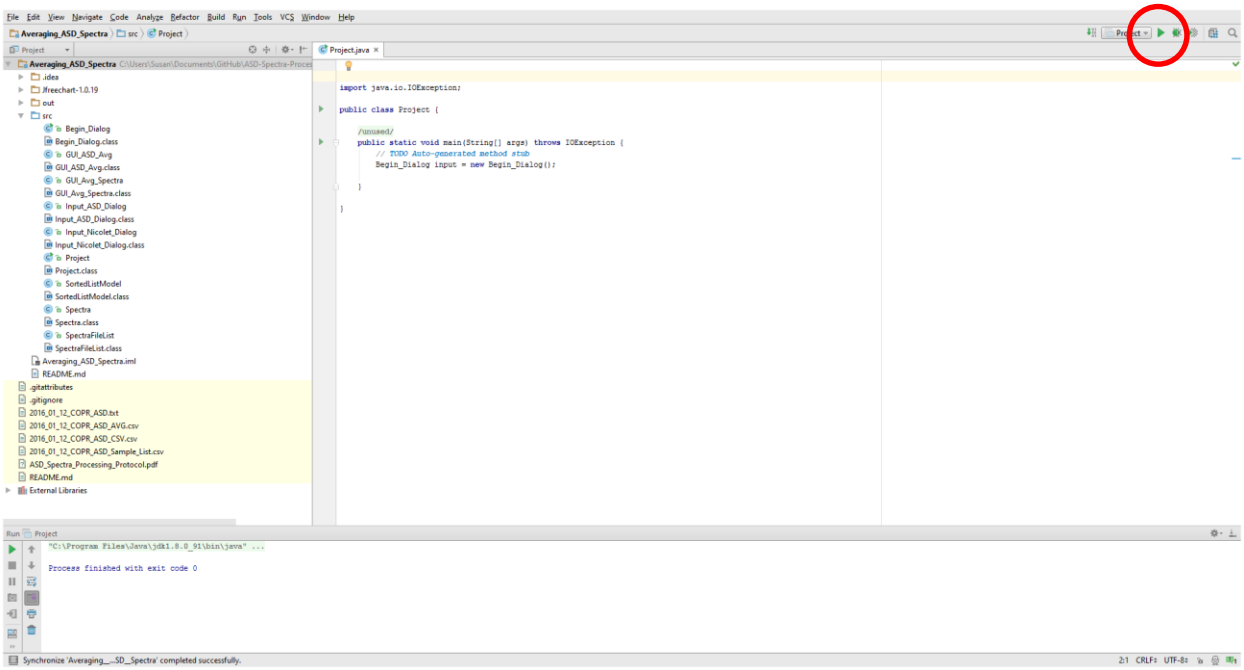
4. IntelliJ will automatically set up your libraries in the next dialog screen. Make sure the jfreechart library has been selected and then hit next. In the next dialog screen accept the defaults and hit next.



5. The next step is to select your Project SDK. If one is installed select that version and hit next. Especially for the first time you will need to navigate to the folder on your computer that contains the JDK. In that case, hit the green plus sign and navigate to that folder. Most cases it is located in C:\Program Files\Java\jdk1.8.0_91. On the next page, no frameworks will be detected. Hit Finish.



6. IntelliJ should be set up like the below photo. Double click the file called Project (not Project.class) and the code for this class will pull up (see below). Hit the green play symbol to run the code. If the green play symbol is not available, you may need to compile the code first. Right click and hit “Complied Project.java” and then right click and hit “Run Project.java”.



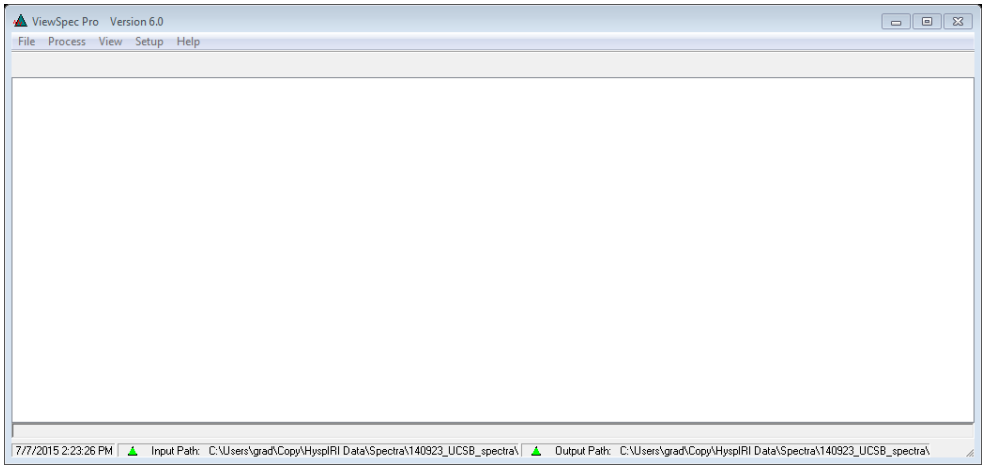
Averaging ASD Spectra

Converting ASD File Formats

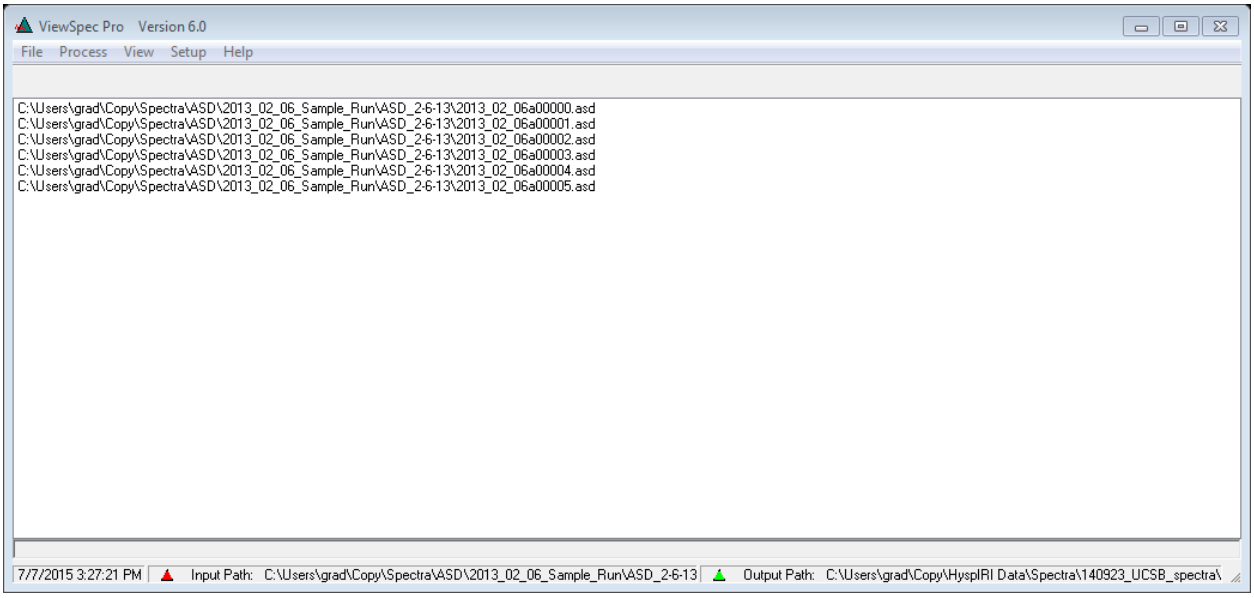
The files from the ASD are in a proprietary format that is called an ASD file (.asd). Due to the file being proprietary it is not easy to manipulate or work with the data. To convert this file type into something more manageable, use a program created by the ASD company called ViewSpecPro. This program can be downloaded from ASD's website (http://support.asdi.com/Products/Products.aspx). This software does require a password to install, but this password can be obtained freely by emailing ASD's support email (http://discover.asdi.com/technical-support-for-asd-instruments-and-accessories/). The screenshots below are from Version 6.0.

Convert from ASD to Text

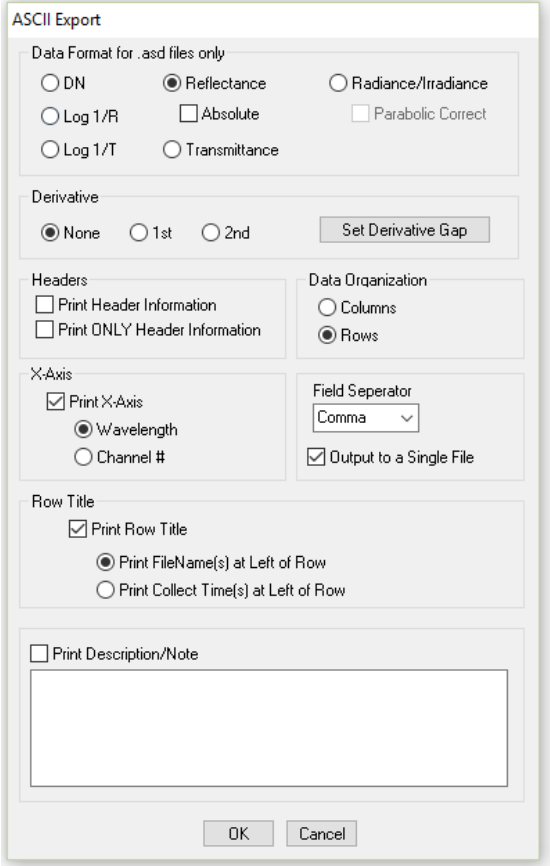
1. Open ViewSpecPro. Below is an example of what the program home screen looks like.



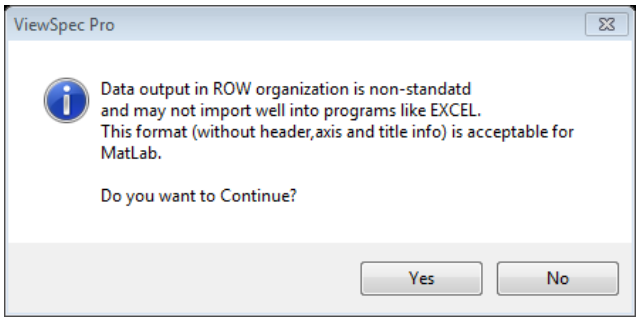
2. Go to File > Open and select the ASD files you want to convert. The filenames will show up on the main screen (see below).



3. Select all the files listed (or the ones you want to convert) and go to Process > ASCII Export. The ASCII Export window will appear (see below). When creating the file in ASCII Export make sure to set these settings: Data Format: Reflectance, Derivative: None, Data Organization: Row, Field Separator: Comma with Output to a Single File, No Header Information, Print X-Axis: Wavelength, No Description or Note, Print Row Title with FileName(s) to Left of Row. Once these settings are set, hit OK.



4. The following warning will appear and hit continue.



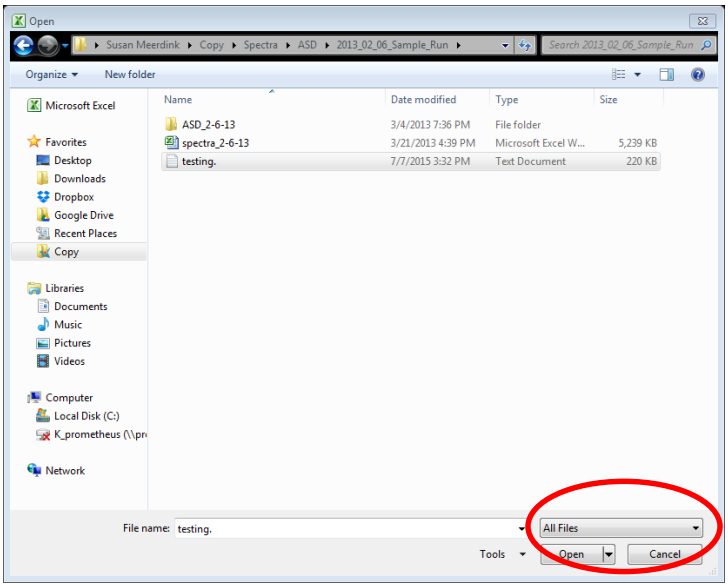
5. The Select ASCII file dialog window will appear. Navigate to the location you would like to have our output file placed and name the file. When finished hit OK. When the program has finished processing your file a dialog box will appear telling you how many files had been

processed. The output file will be a text document. This document can be used in the next section to fix the joins in ASD Spectra.

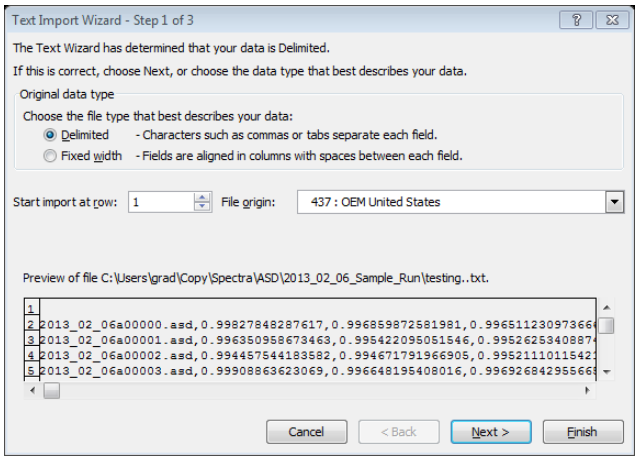
Optional: Convert from text to CSV

**You do not need to do this when using the Java program to analyze spectra!!

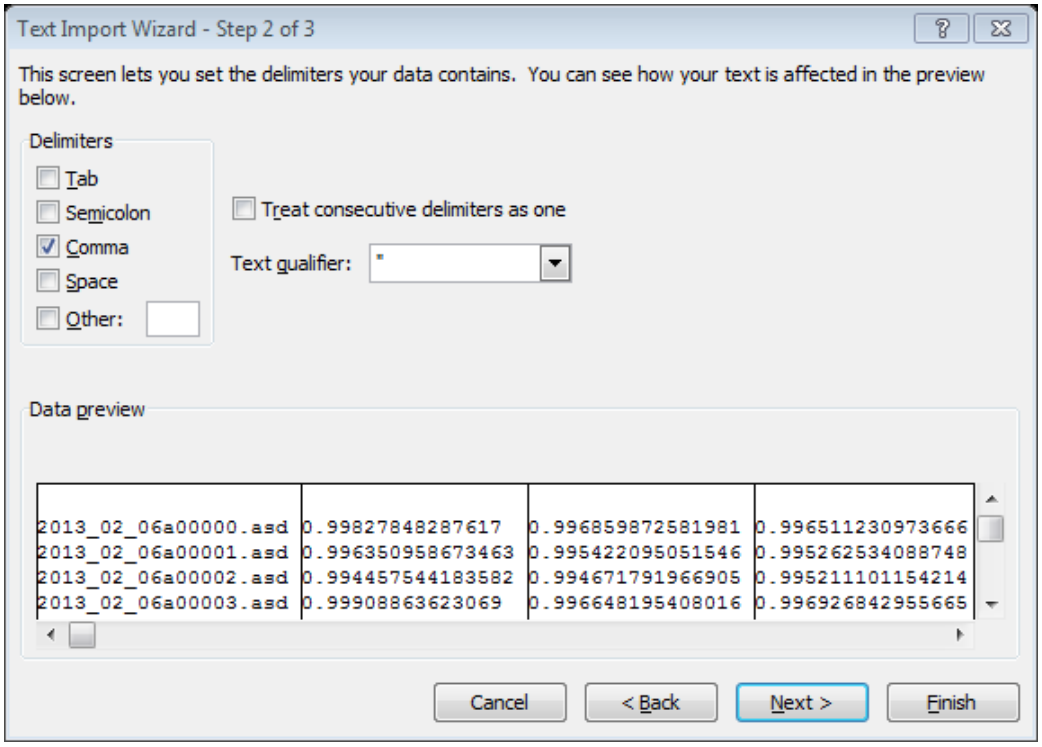
1. Open Microsoft Excel and go to File > Open. Navigate to the folder containing the output file. From the drop down menu select All Files (show with red circle) and select the output text file.



2. This will open the Text Import Wizard (shown below). Select delimited and hit next.



3. Deselect Tab and select Comma. The preview will automatically show the values separated into columns. Hit Finish.

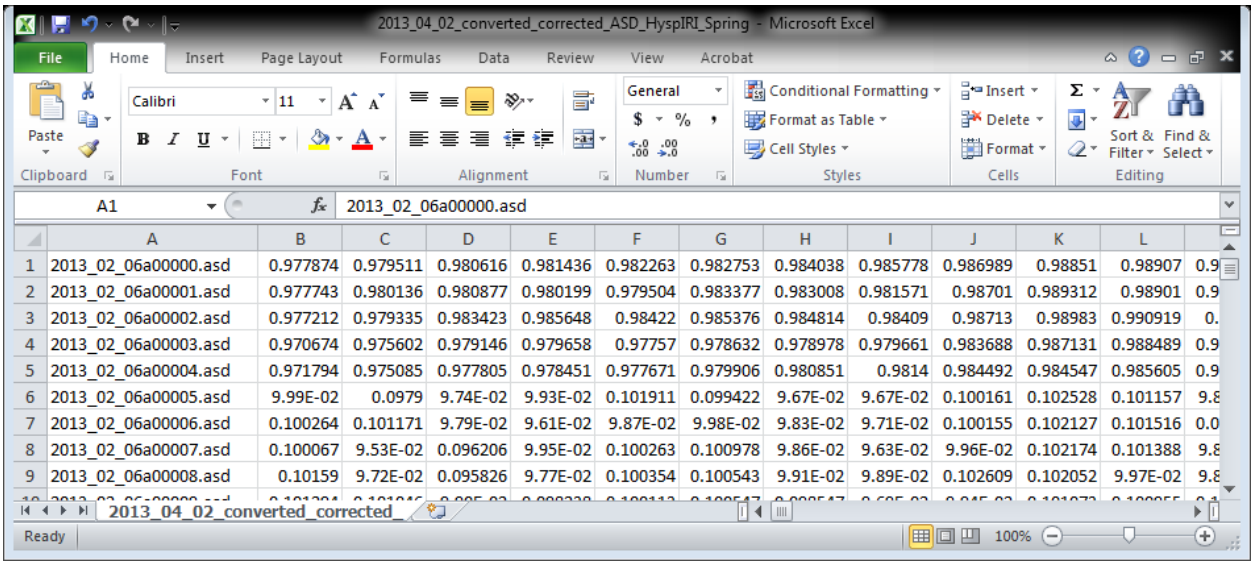


4. Go to File > Save As and select CSV (Comma delimited). Type in the new filename and hit save. Your spectra are now saved as .csv file and can be easily worked with in excel, ENVI, or code.

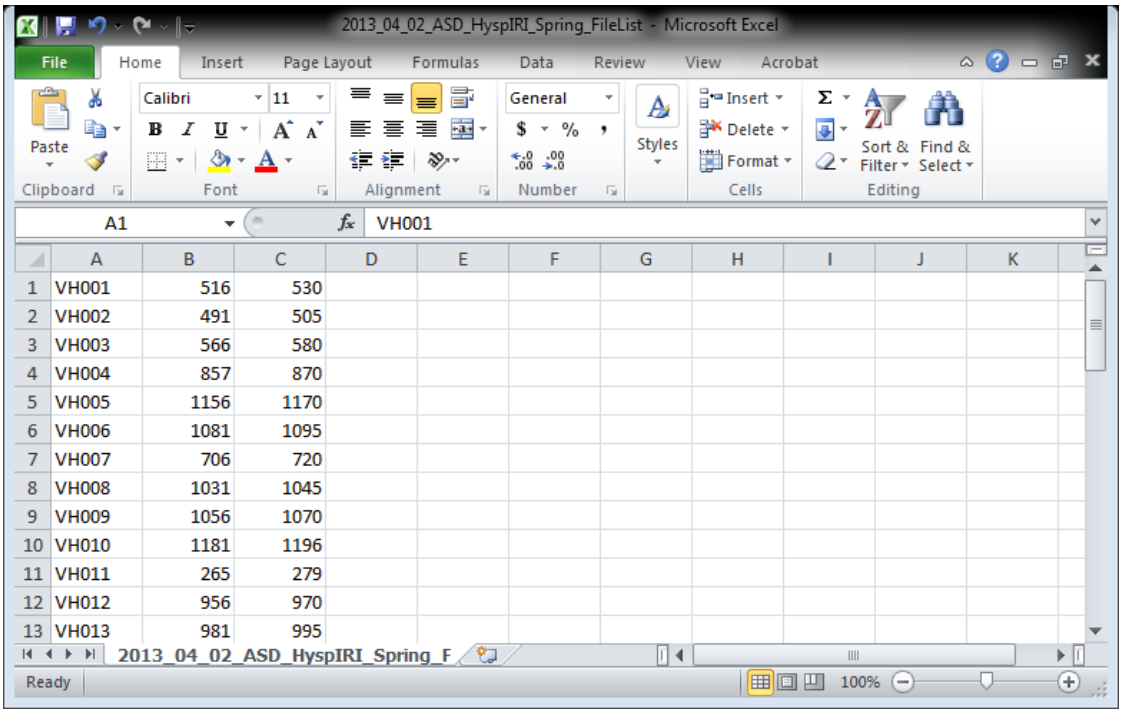
Inputs for Java Program

In most cases, it is common practice to collect multiple spectra for one sample. For example, when collecting the spectrum of a leaf it is common to collect 5 spectra then rotate the leaf and collect 5 more. Ultimately, the goal is to have one spectrum for a sample which is the average of all spectra collected. The collection of many spectra for one sample allows for the culling of bad collections. The code displays all spectra for one sample and allows the user to deselect the spectra that are undesired and average the remaining spectra. The output file will contain one spectrum for each sample.

1. ASD Spectra: This input is the text or csv file outputted from ASD's ViewSpecPro (see steps above). The file will look something like below and will have 2152 columns of data.



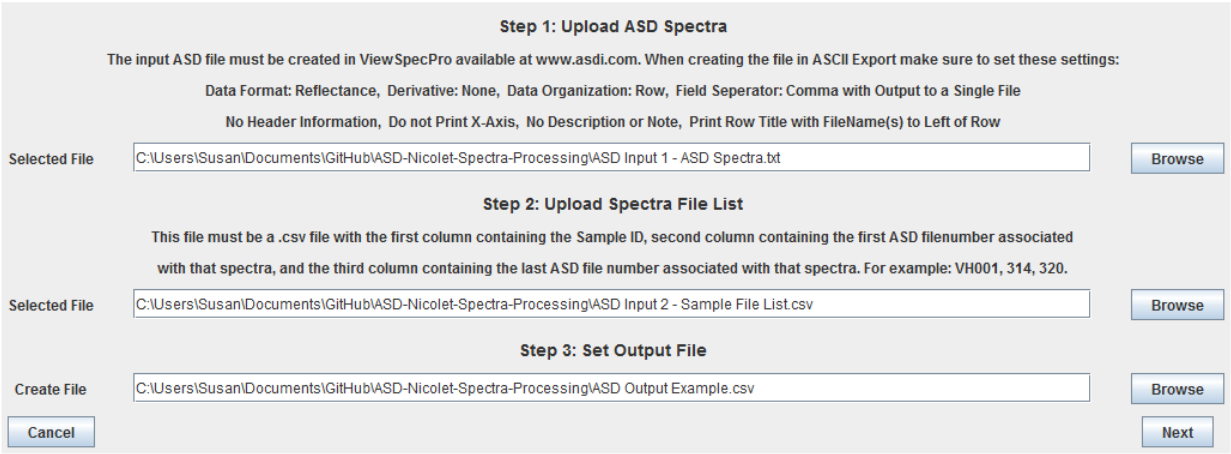
2. Sample File List: This input is a csv file that contains three columns of data. The first column contains the Sample ID or Name, the second column contains the first ASD file number associated with that sample, and the third column contains the last ASD file number associated with that sample. The numbers start at 0 and are referencing the index of the spectra in the ASD spectra file above. The code will take the first ASD file number and loop through the ASD spectra file pulling out lines of spectra that are related to that sample until it reaches the last ASD file number. So it is important to make sure all files are included in the ASD spectra file above and that a file number is not skipped. The number in columns two and three MUST match the end number of the file. **Do not** put commas in your Sample ID or Name (in the first column).



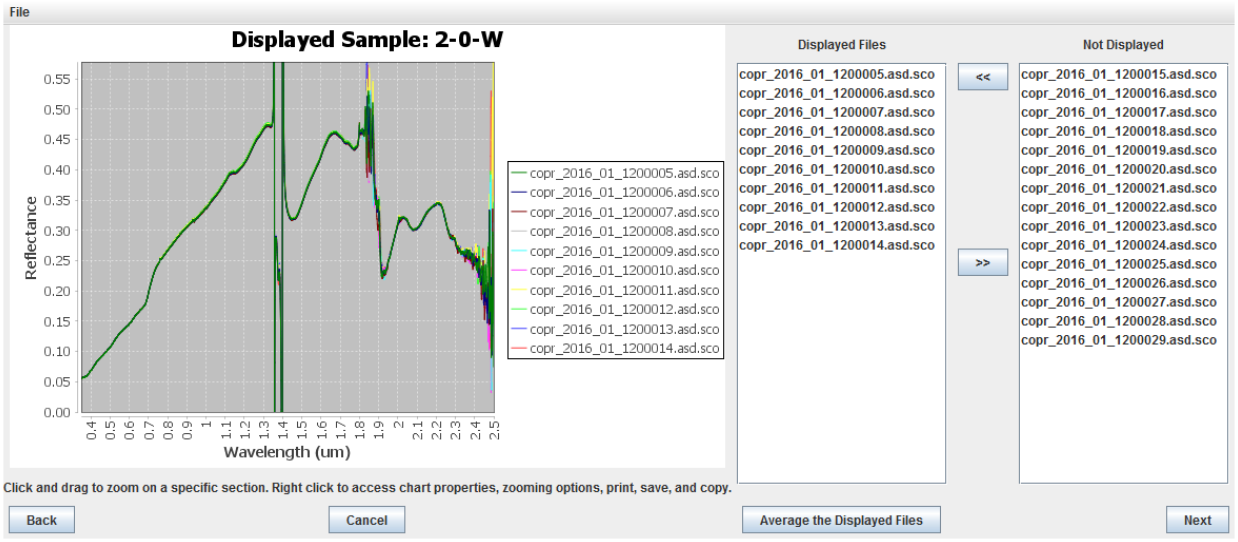
Running Java Program to Average ASD Spectra

1. The first GUI to appear allows the user to determine which sensor you have spectra from. In this case, we will be using ASD spectra, so select the ASD (VSWIR) button.

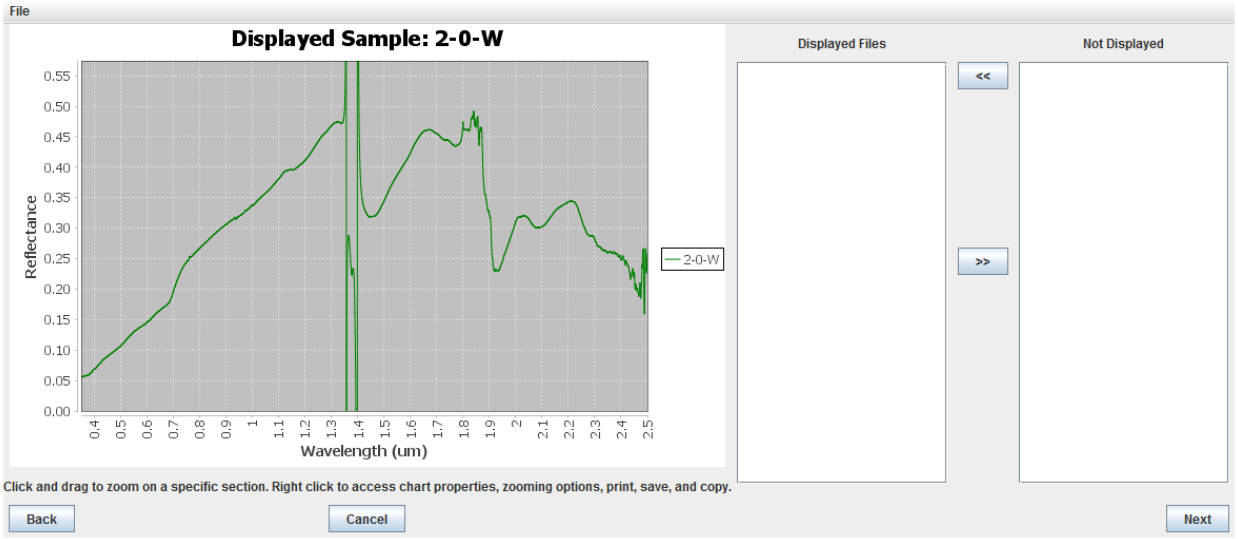
2. Next the "Program to batch average ASD Spectra" will open. Select the file created from the Join Correction code for Step 1. Navigate to the Sample File List for Step 2. Last navigate to the folder you want to output the file and name the file. Once these are completed, hit next.



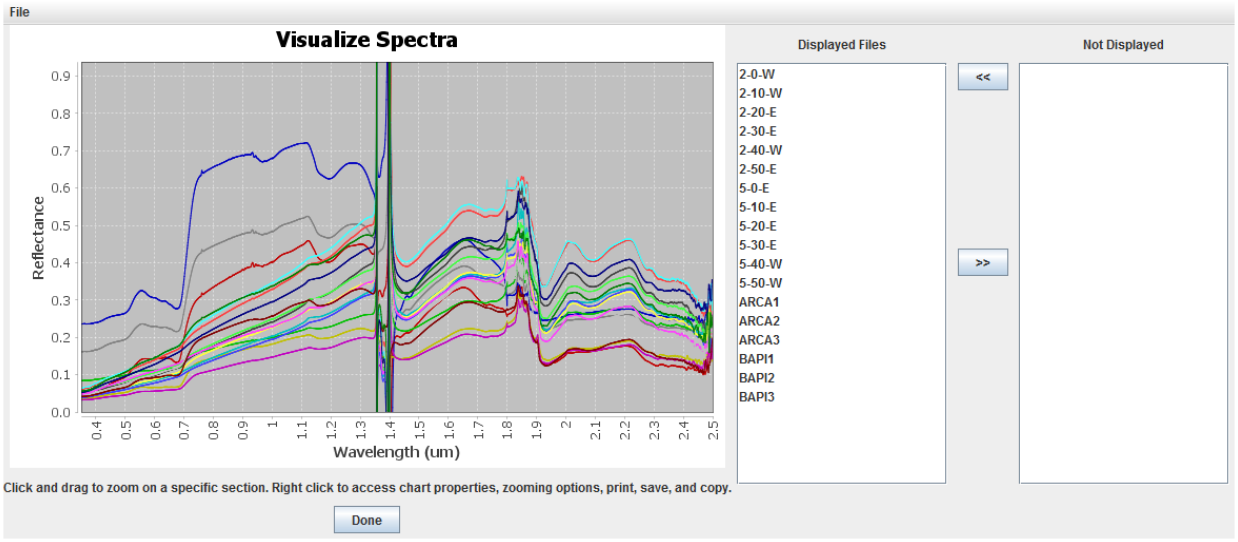
3. The "Visualizing ASD Spectra" dialog box will appear. The code will start with the first sample list in the Sample File List. At the beginning all spectra related to that sample will be displayed. If you do not want a file to be displayed and not included in the average, select the filename from the Displayed Files List and hit the >> button. All files displayed will be included in the averaging.



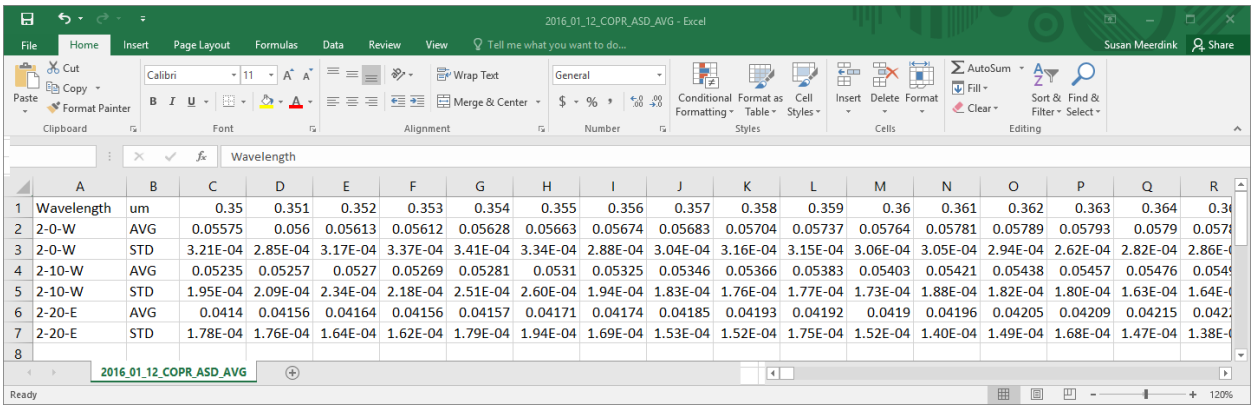
4. Once you have the spectra you want to average displayed, hit the “Average the Displayed Files” button. This will average the spectra, write it to the output file, and display the average spectrum. To continue onto the next sample, hit Next.



5. The program will continue until it finishes with the last sample in the Sample File List. At the last sample, all the samples that were averaged will be displayed.



The output file will be a csv with the first column being the sample ID, second column stating whether it is the average or standard deviation, and the following columns the spectra (see below). The top row is the wavelengths in micrometers.



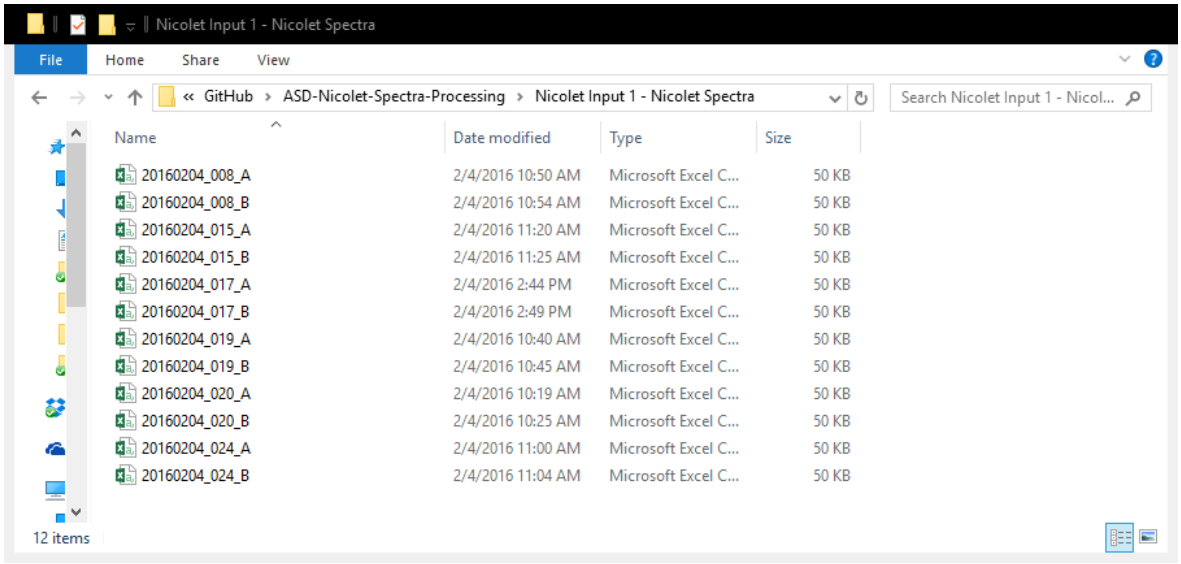
	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R
1	Wavelength	um	0.35	0.351	0.352	0.353	0.354	0.355	0.356	0.357	0.358	0.359	0.36	0.361	0.362	0.363	0.364	0.3
2	2-0-W	AVG	0.05575	0.056	0.05613	0.05612	0.05628	0.05663	0.05674	0.05683	0.05704	0.05737	0.05764	0.05781	0.05789	0.05793	0.0579	0.057
3	2-0-W	STD	3.21E-04	2.85E-04	3.17E-04	3.37E-04	3.41E-04	3.34E-04	2.88E-04	3.04E-04	3.16E-04	3.15E-04	3.06E-04	3.05E-04	2.94E-04	2.62E-04	2.82E-04	2.86E-
4	2-10-W	AVG	0.05235	0.05257	0.0527	0.05269	0.05281	0.0531	0.05325	0.05346	0.05366	0.05383	0.05403	0.05421	0.05438	0.05457	0.05476	0.054
5	2-10-W	STD	1.95E-04	2.09E-04	2.34E-04	2.18E-04	2.51E-04	2.60E-04	1.94E-04	1.83E-04	1.76E-04	1.77E-04	1.73E-04	1.88E-04	1.82E-04	1.80E-04	1.63E-04	1.64E-
6	2-20-E	AVG	0.0414	0.04156	0.04164	0.04156	0.04157	0.04171	0.04174	0.04185	0.04193	0.04192	0.0419	0.04196	0.04205	0.04209	0.04215	0.042
7	2-20-E	STD	1.78E-04	1.76E-04	1.64E-04	1.62E-04	1.79E-04	1.94E-04	1.69E-04	1.53E-04	1.52E-04	1.75E-04	1.52E-04	1.40E-04	1.49E-04	1.68E-04	1.47E-04	1.38E-
8																		

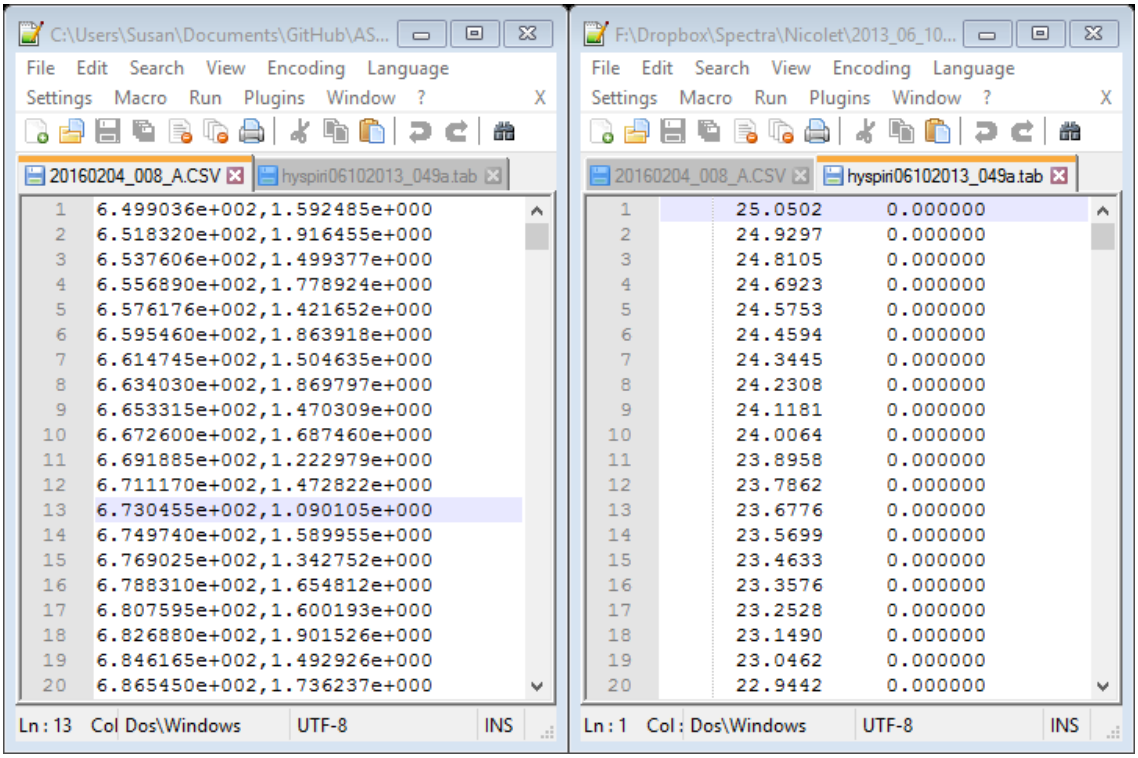
Averaging Nicolet Spectra

Inputs for Java Program

In most cases, it is common practice to collect multiple spectra for one sample. For example, when collecting the spectrum of a leaf it is common to collect a spectrum of a sample then rotate the leaf and collect another. Ultimately, the goal is to have one spectrum for a sample which is the average of all spectra collected. The collection of many spectra for one sample allows for the culling of bad collections. The code displays all spectra for one sample and allows the user to deselect the spectra that are undesired and average the remaining spectra. The output file will contain one spectrum for each sample.

1. Nicolet Spectra: This input is the directory that contains either .tab or .csv files for each spectrum collected. For example, in this folder there are 12 .csv files with each file containing a single spectrum. This folder contains spectra for 6 samples. The .csv file has columns separated with a comma. Column one is wavenumbers while column 2 is reflectance (see example below). The .tab file has columns separated by tabs with the first column being empty, second column as wavelengths, and third column as reflectance. The .csv file will only have wavelengths 2.5 – 15.384 µm, while the .tab file will have 2.49898 - 25.0502 µm. These values will be listed in descending order. It is important that your files are set up the same, so that the program reads in the files correctly.





2. Nicolet Correction: Corrections are made for imperfections of the sphere, the incoming & exiting ports, and imperfections in the gold coating. These corrections are based on Generalized Integrating-Sphere Theory, David G. Goebel, Applied Optics, v. 6, no. 1, Jan. 1967, pp. 125-128 cap on – cap off approach. The correction factors have been calculated by JPL for the specific model that is housed at JPL. These corrections will not be applicable to other instruments. Generally speaking, .tab files have correction already applied, while .csv files do not have correction applied. Selecting 'No' will automatically apply correction. Selecting ‘Yes’ will not apply correction to spectra.

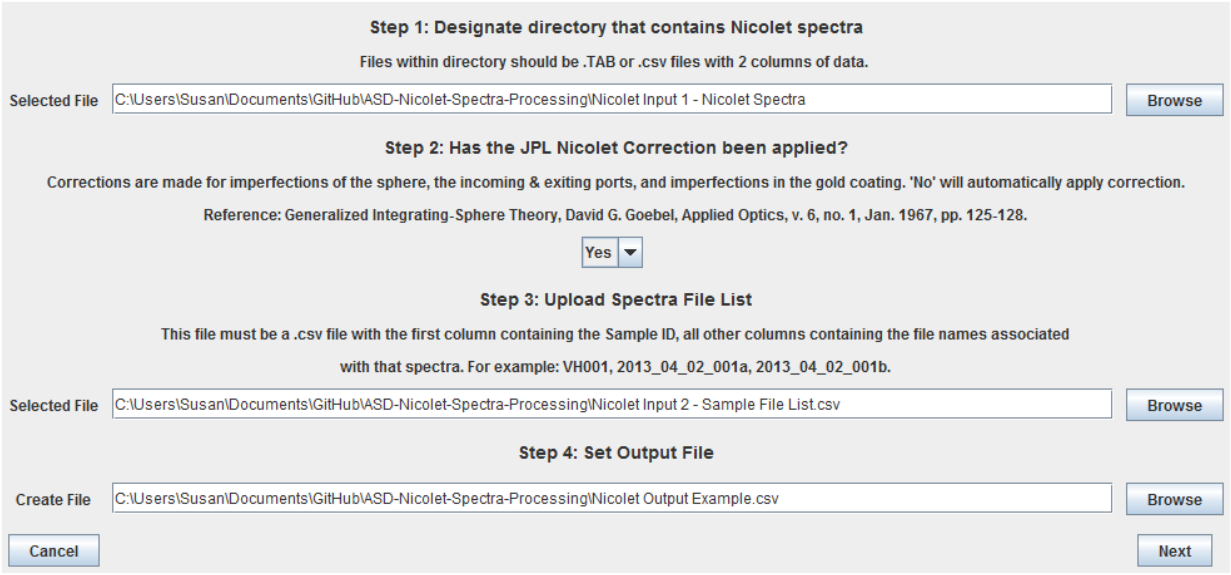
3. Sample File List: This input is a csv file that contains three columns of data. The first column contains the Sample ID or Name and the subsequent columns contains the file name of the sample spectrum. If your same has two spectrums to average, there will be a total of three columns for that line: Sample1, file1, file2. If you sample has three spectrums to average, there will be a total of four columns for that line: Sample2, file1, file2, file3. See example below. **Do not** put commas in your Sample ID or Name (in the first column) or file extensions (.csv & .tab) on the end of filenames.

	A	B	C	D	E
1	JPL084	20160204_020_A	20160204_020_B		
2	JPL085	20160204_024_A	20160204_024_B	20160204_024_C	
3	JPL091	20160204_019_A	20160204_019_B		
4	JPL092	20160204_017_A	20160204_017_B	20160204_017_C	20160204_017_D
5	JPL099	20160204_015_A	20160204_015_B		
6	JPL100	20160204_008_A	20160204_008_B		
7					

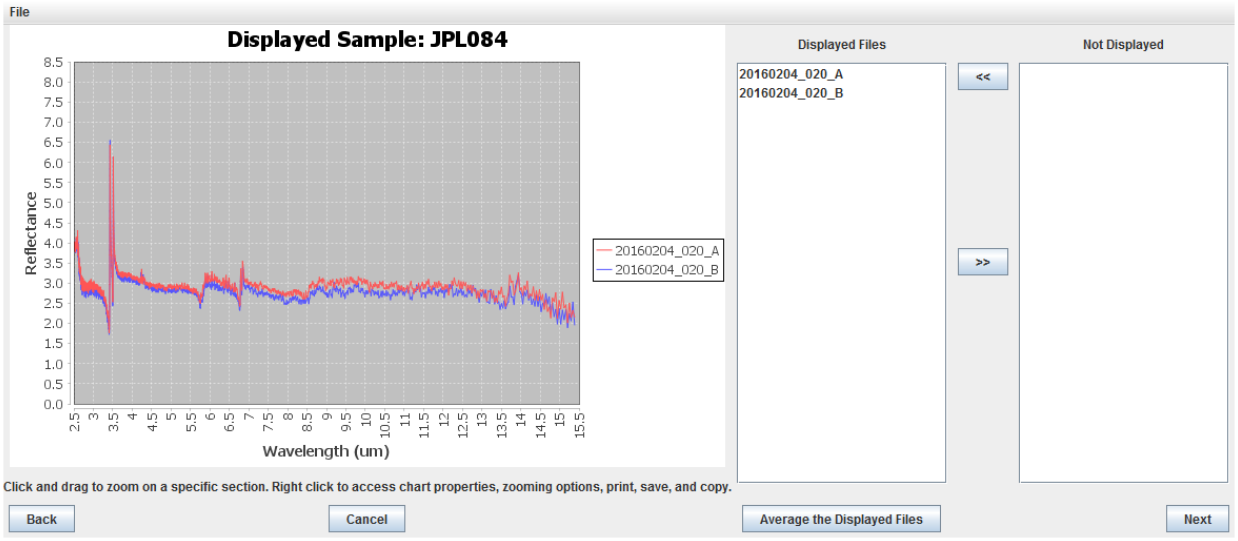
Running Java Program to Average Nicolet Spectra

1. The first GUI to appear allows the user to determine which sensor you have spectra from. In this case, we will be using Nicolet spectra, so select the Nicolet (TIR) button.

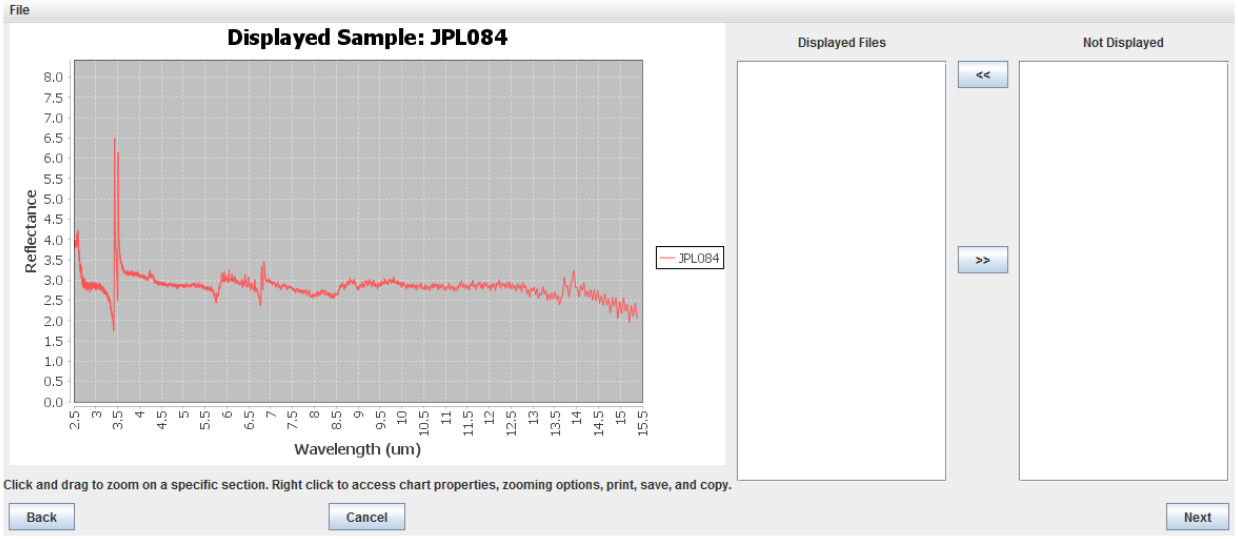
2. Next the "Program to batch average Nicolet Spectra" will open. Select the directory of your spectra for Step 1. For Step 2, select yes or no to determine if a correction will be applied to the input spectra. Navigate to the Sample File List for Step 3. Last navigate to the folder you want to output the file and name the file. See section above on Inputs for Java Program for more details. Once these are completed, hit next.



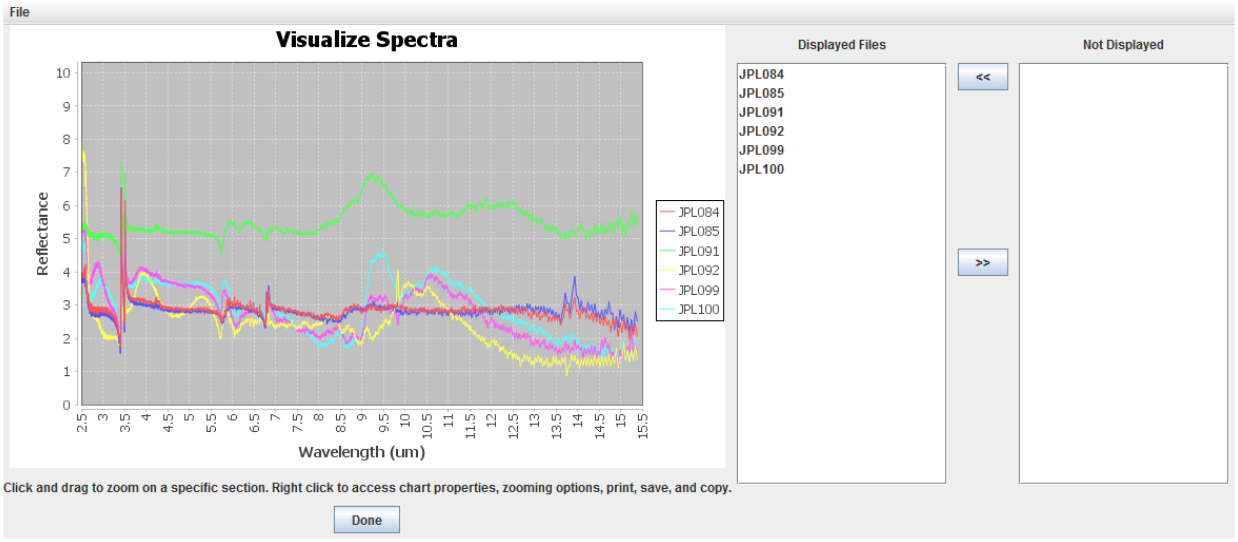
3. The “Visualizing Spectra” dialog box will appear. The code will start with the first sample list in the Sample File List. At the beginning all spectra related to that sample will be displayed. If you do not want a file to be displayed and not included in the average, select the filename from the Displayed Files List and hit the >> button. All files displayed will be included in the averaging.



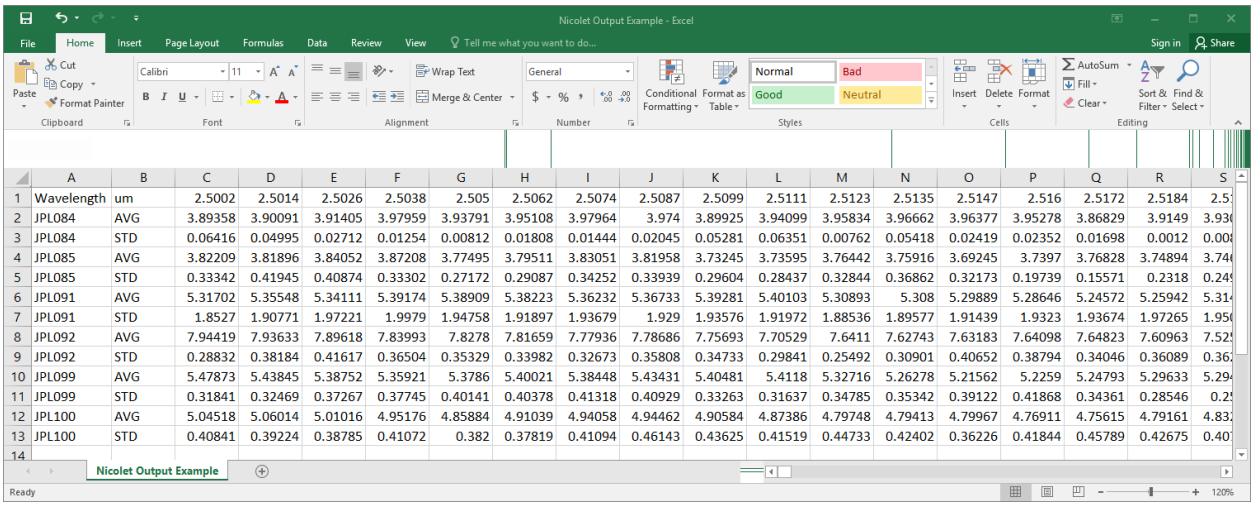
4. Once you have the spectra you want to average displayed, hit the “Average the Displayed Files” button. This will average the spectra, write it to the output file, and display the average spectrum. To continue onto the next sample, hit Next.



5. The program will continue until it finishes with the last sample in the Sample File List. At the last sample, all the samples that were averaged will be displayed.



The output file will be a csv with the first column being the sample ID, second column stating whether it is the average or standard deviation, and the following columns the spectra (see below). The top row is the wavelengths in micrometers.



	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R	S
1	Wavelength	um	2.5002	2.5014	2.5026	2.5038	2.505	2.5062	2.5074	2.5087	2.5099	2.5111	2.5123	2.5135	2.5147	2.516	2.5172	2.5184	2.5
2	JPL084	AVG	3.89358	3.90091	3.91405	3.97959	3.93791	3.95108	3.97964	3.974	3.89925	3.94099	3.95834	3.96662	3.96377	3.95278	3.86829	3.9149	3.93
3	JPL084	STD	0.06416	0.04995	0.02712	0.01254	0.00812	0.01808	0.01444	0.02045	0.05281	0.06351	0.00762	0.05418	0.02419	0.02352	0.01698	0.0012	0.00
4	JPL085	AVG	3.82209	3.81896	3.84052	3.87208	3.77495	3.79511	3.83051	3.81958	3.73245	3.73595	3.76442	3.75916	3.69245	3.7397	3.76828	3.74894	3.74
5	JPL085	STD	0.33342	0.41945	0.40874	0.33302	0.27172	0.29087	0.34252	0.33939	0.29604	0.28437	0.32844	0.36862	0.32173	0.19739	0.15571	0.2318	0.24
6	JPL091	AVG	5.31702	5.35548	5.34111	5.39174	5.38909	5.38223	5.36232	5.36733	5.39281	5.40103	5.30893	5.308	5.29889	5.28646	5.24572	5.25942	5.31
7	JPL091	STD	1.8527	1.90771	1.97221	1.9979	1.94758	1.91897	1.93679	1.929	1.93576	1.91972	1.88536	1.89577	1.91439	1.9323	1.93674	1.97265	1.95
8	JPL092	AVG	7.94419	7.93633	7.89618	7.83993	7.8278	7.81659	7.77936	7.78686	7.75693	7.70529	7.6411	7.62743	7.63183	7.64098	7.64823	7.60963	7.52
9	JPL092	STD	0.28832	0.38184	0.41617	0.36504	0.35329	0.33982	0.32673	0.35808	0.34733	0.29841	0.25492	0.30901	0.40652	0.38794	0.34046	0.36089	0.36
10	JPL099	AVG	5.47873	5.43845	5.38752	5.35921	5.3786	5.40021	5.38448	5.43431	5.40481	5.4118	5.32716	5.26278	5.21562	5.2259	5.24793	5.29633	5.29
11	JPL099	STD	0.31841	0.32469	0.37267	0.37745	0.40141	0.40378	0.41318	0.40929	0.33263	0.31637	0.34785	0.35342	0.39122	0.41868	0.34361	0.28546	0.2
12	JPL100	AVG	5.04518	5.06014	5.01016	4.95176	4.85884	4.91039	4.94058	4.94462	4.90584	4.87386	4.79748	4.79413	4.79967	4.76911	4.75615	4.79161	4.83
13	JPL100	STD	0.40841	0.39224	0.38785	0.41072	0.382	0.37819	0.41094	0.46143	0.43625	0.41519	0.44733	0.42402	0.36226	0.41844	0.45789	0.42675	0.40
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Features & Notes

Next Button: Hitting the Next button will always continue on to the next sample even if the current sample has not been averaged.

Back Button: You may at any time hit the Back button to go to a previous sample. However, if you have averaged that sample already, it will already be written to the averaged output file. If you average the sample again, that line in the file will NOT be overwritten. Instead an additional line of text will be added to the file, so you will have duplicate sample IDs.

Cancel Button: At any point you can close the program by going to File>Exit or Cancel. This will save the samples that have already been averaged in the output file and close the program.

Graphing Features: The graph itself has options to change font, zoom, print, save, copy, etc. You can access these by right clicking on the graph.