ASD Spectra Processing Protocol

Susan Meerdink

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This document details the steps necessary to process spectra 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). Spectra collected from the instrument are collected as .asd files. This document explains the steps of converting these files to .csv, fixing the joins, and averaging the spectra of a sample.

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Converting file formats

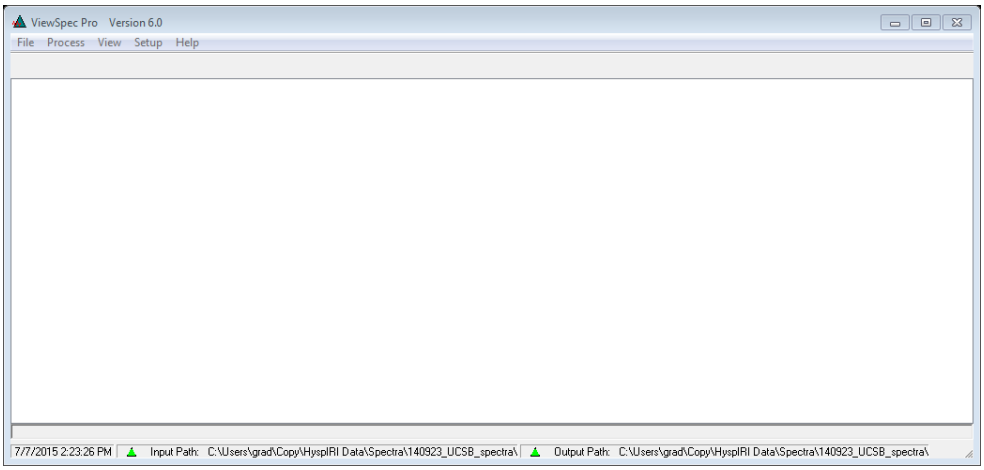
Background

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

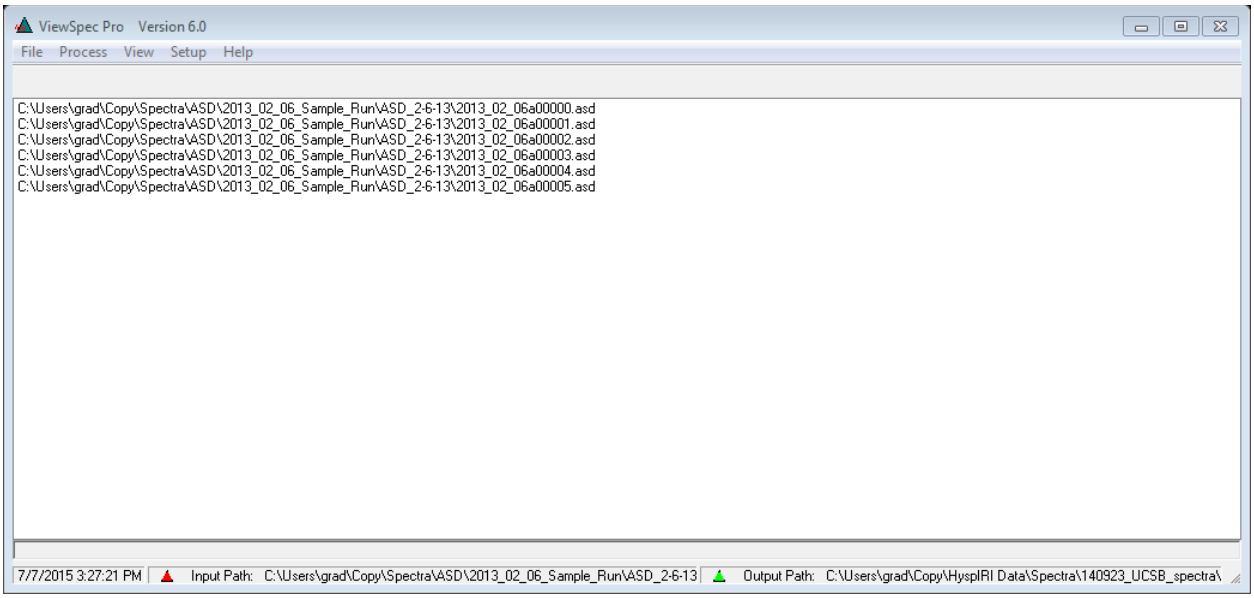
(http://discover.asdi.com/technical-support-for-asd-instruments-and-accessories/). The screenshots below are from Version 6.0.

Convert from ASD to Text

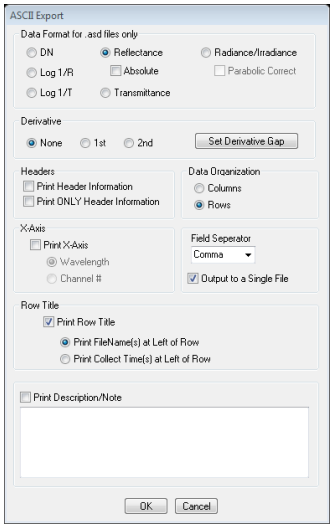
1. Open ViewSpecPro. Below is an example of what the program home screen looks like.



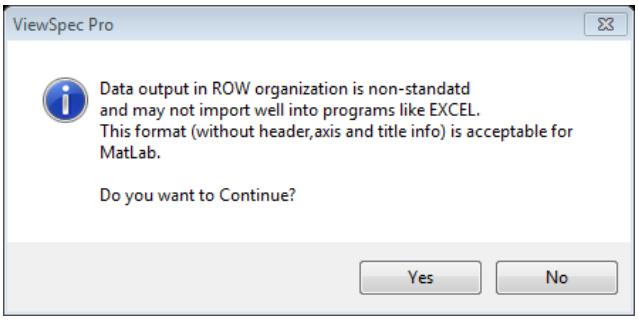
2. Go to File > Open and select the ASD files you want to convert. The filenames will show up on the main screen (seen below).



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, Do not Print X-Axis, No Description or Note, Print Row Title with FileName(s) to Left of Row. Once these settings are set, hit OK.



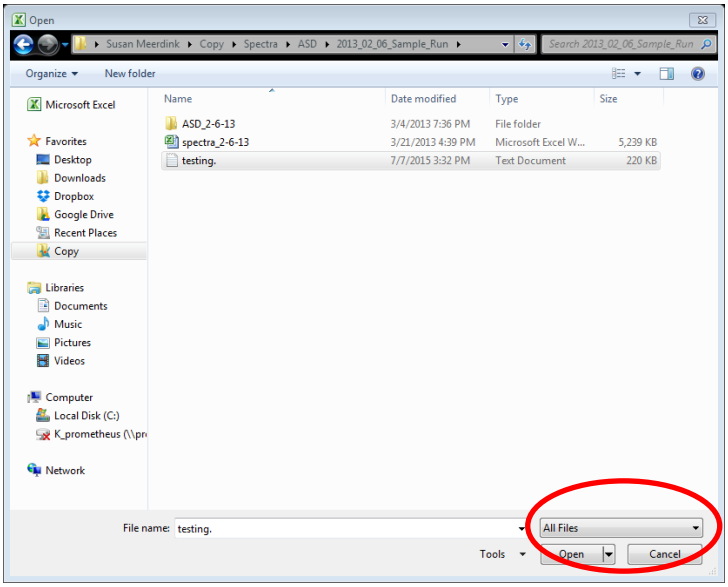
4. The following warning will appear and hit continue.



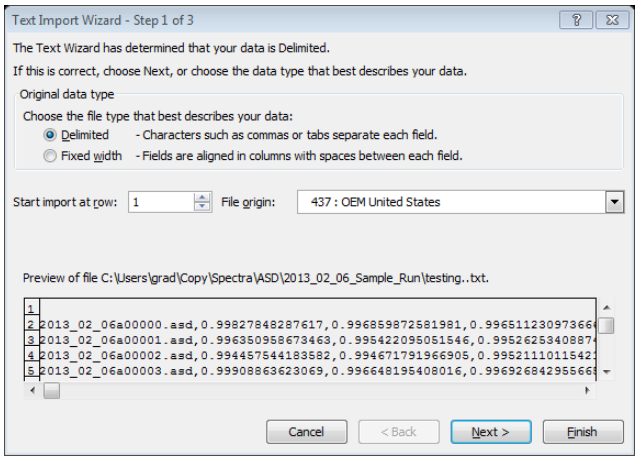
5. The Select ASCII file dialog window will appear. Navigate to the location you would like to have our output file placed and name the file. When finished hit OK. When the program has finished processing your file a dialog box will appear telling you how many files had been processed. The output file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

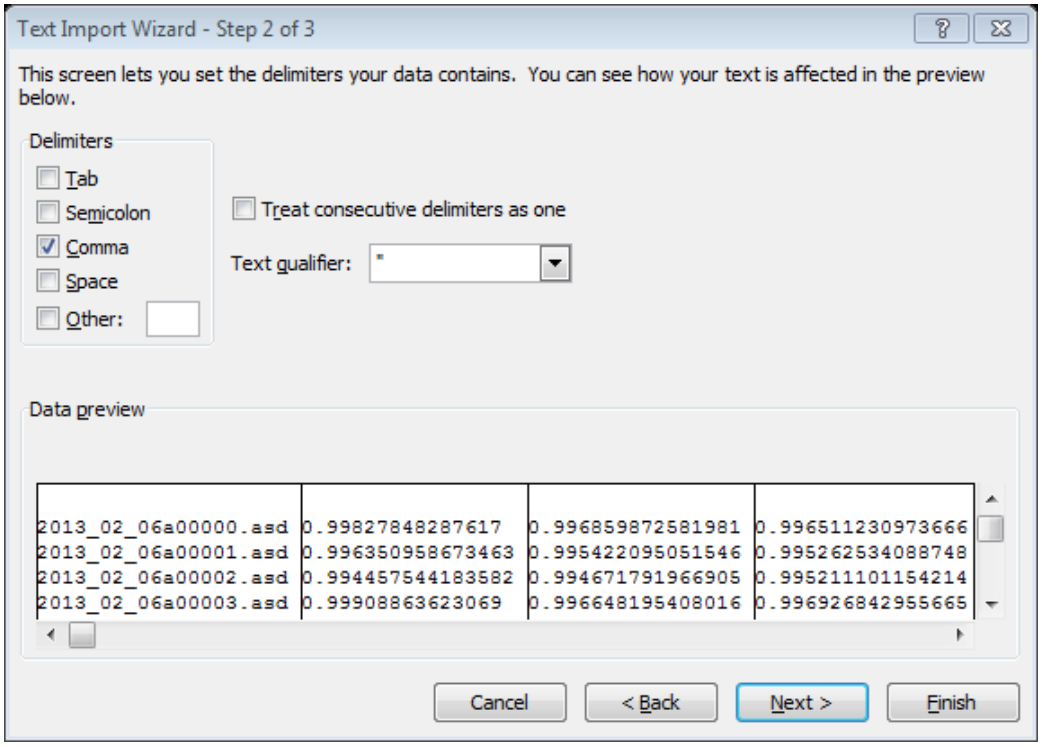
1. Open Microsoft Excel and go to File > Open. Navigate to the folder containing the output file. From the drop down menu select All Files (show with red circle) and select the output text file.



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.

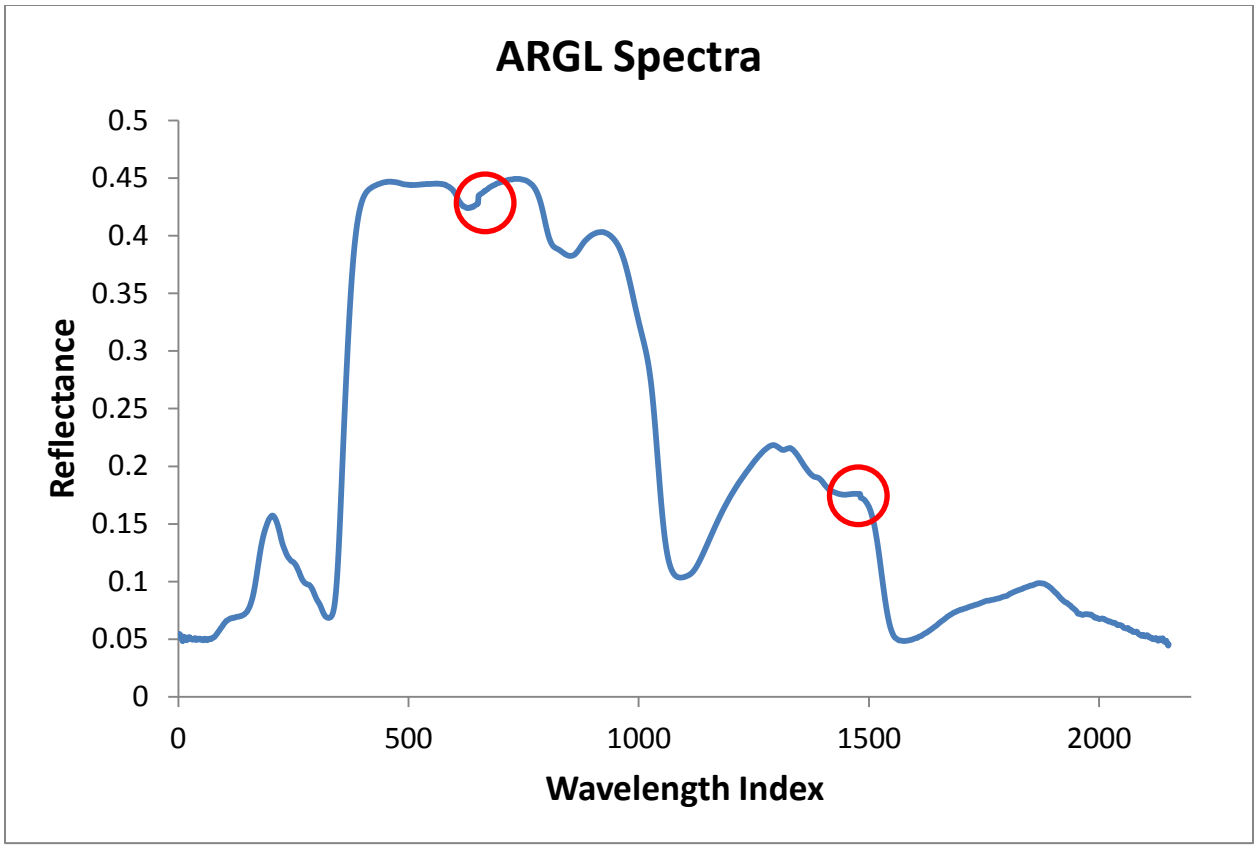


4. Go to File > Save As and select CSV (Comma delimited). Type in the new filename and hit save. Your spectra are now saved as .csv file and can be easily worked with in excel, ENVI, or code.

Fixing Join in ASD Spectra

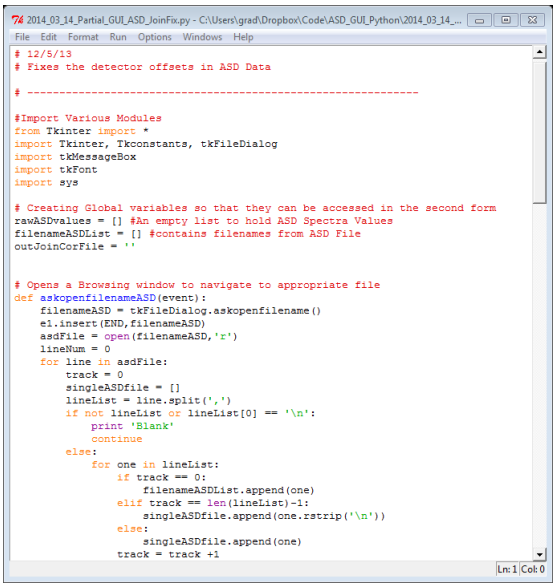
Background

The ASD uses three sensors to collect the spectrum of a sample from 0.35 – 2.5 μm. Each sensor collects a different region of the spectrum, but the values collected at the extent of the range for one sensor do not always match with the values collected by the following sensor. This creates a jump or disjointed features in the spectra as shown in the figure below. Code has been adapted to smooth out these features at the joins of the sensors. The code reads through the spectra and finds the reflectance values on each side of the join. The average of these two values is found and replaces the reflectance at the join. The output is a csv file that contains the corrected spectra.

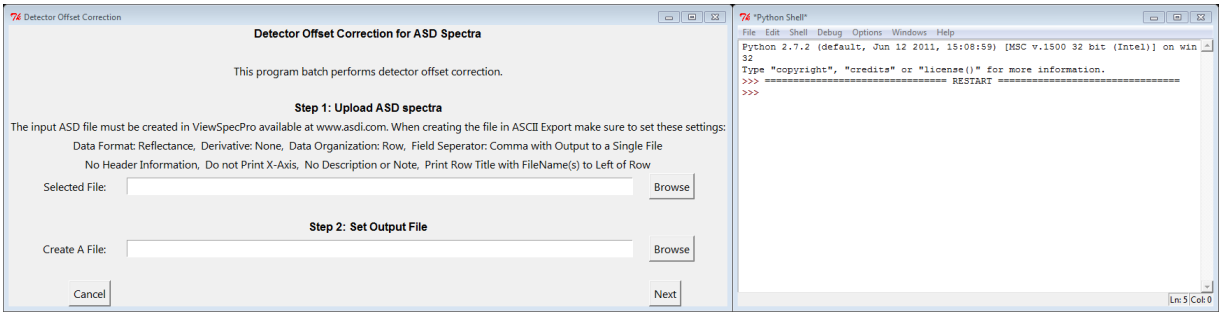


Fixing Joins using Python Code

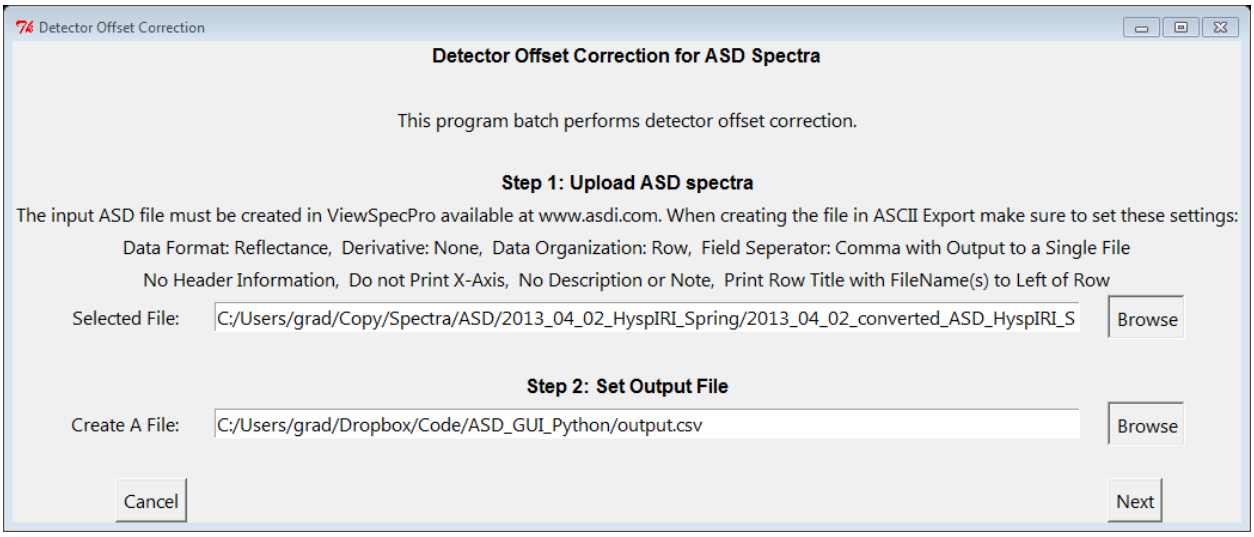
1. Right click on 2014_03_14_Partial_GUI_ASD_JoinFix.py and choose 'Edit with IDLE'. This option should be available when ENVI is installed on the computer. The IDLE editing window will appear (see below).



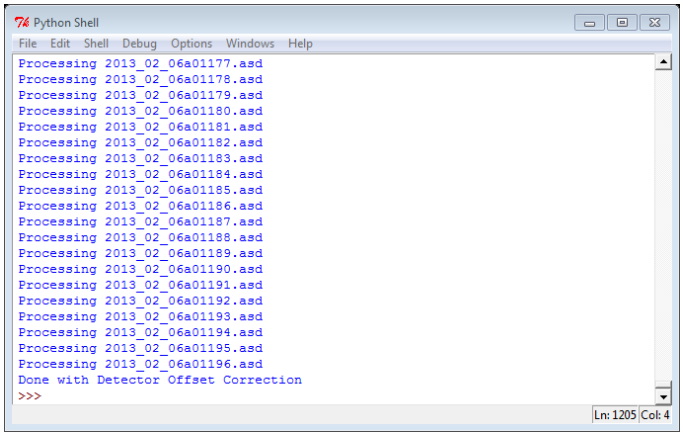
2. Go to Run > Run Module and the Python Shell window will appear along with the GUI interface (see below).



3. Select the Browse button for Step 1 and select the text or csv file you created in this first section. Select the Browse button for Step 2 and navigate to the folder you want to output the corrected file and name the file with .csv at the end. Once inputs and outputs are set select the next button.



4. The GUI dialog will disappear and output text will appear on the Python Shell window. The Python Shell window will contain a line for each spectra processed. At the end of processing the program will output “Done with Detector Offset Correction”. You have now successfully corrected your spectra from join disjoints.



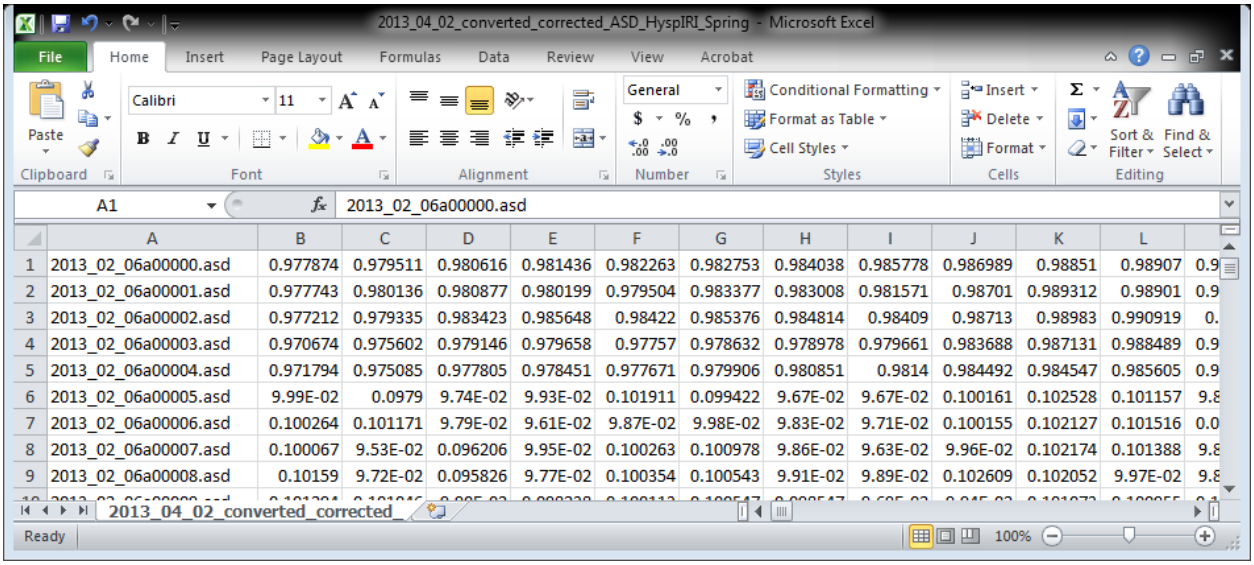
Averaging Spectra

Background

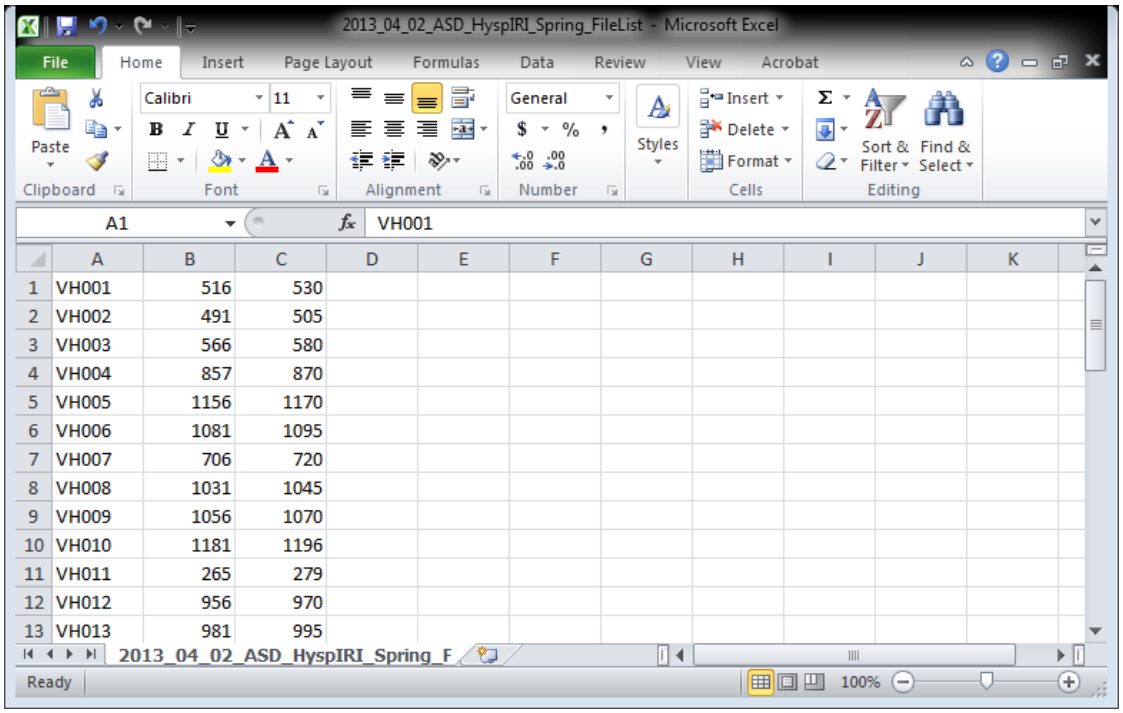
In most cases, it is common practice to collect multiple spectra for one sample. For example when collecting the spectrum of a leaf it is common to collect 5 spectra then rotate the leaf and collect 5 more. Ultimately, the goal is to have one spectrum for a sample which is the average of all spectra 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. This program was developed using Java. You will need to have Eclipse which is a free download (https://www.eclipse.org/downloads/). Additionally you will need to have Java, which should already be installed. If not it is a free download from this website (http://www.oracle.com/technetwork/java/javase/downloads/jdk8-downloads-2133151.html).

Inputs

1. ASD Spectra: This input is the csv file created from the join correction code above. The file will look something like below and will have 2152 columns of data.

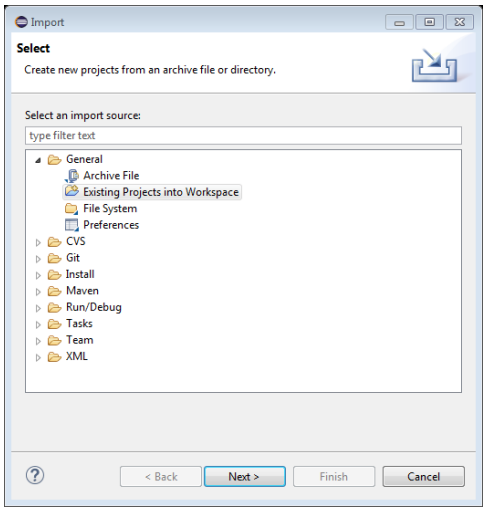


2. Sample File List: This input is a csv file that contains three columns of data. The first column contains the Sample ID, the second column contains the first ASD file number associated with that sample, and the third column contains the last ASD file number associated with that sample. The numbers 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.

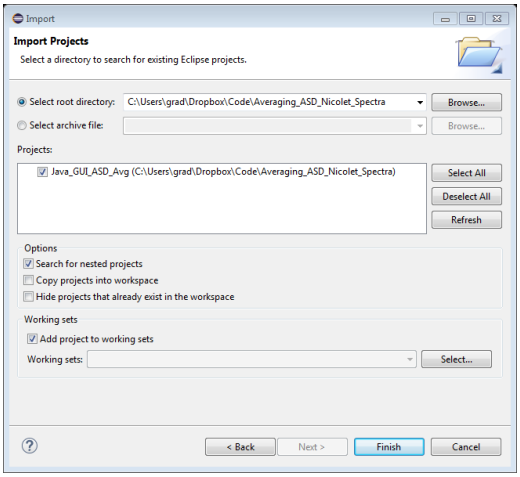


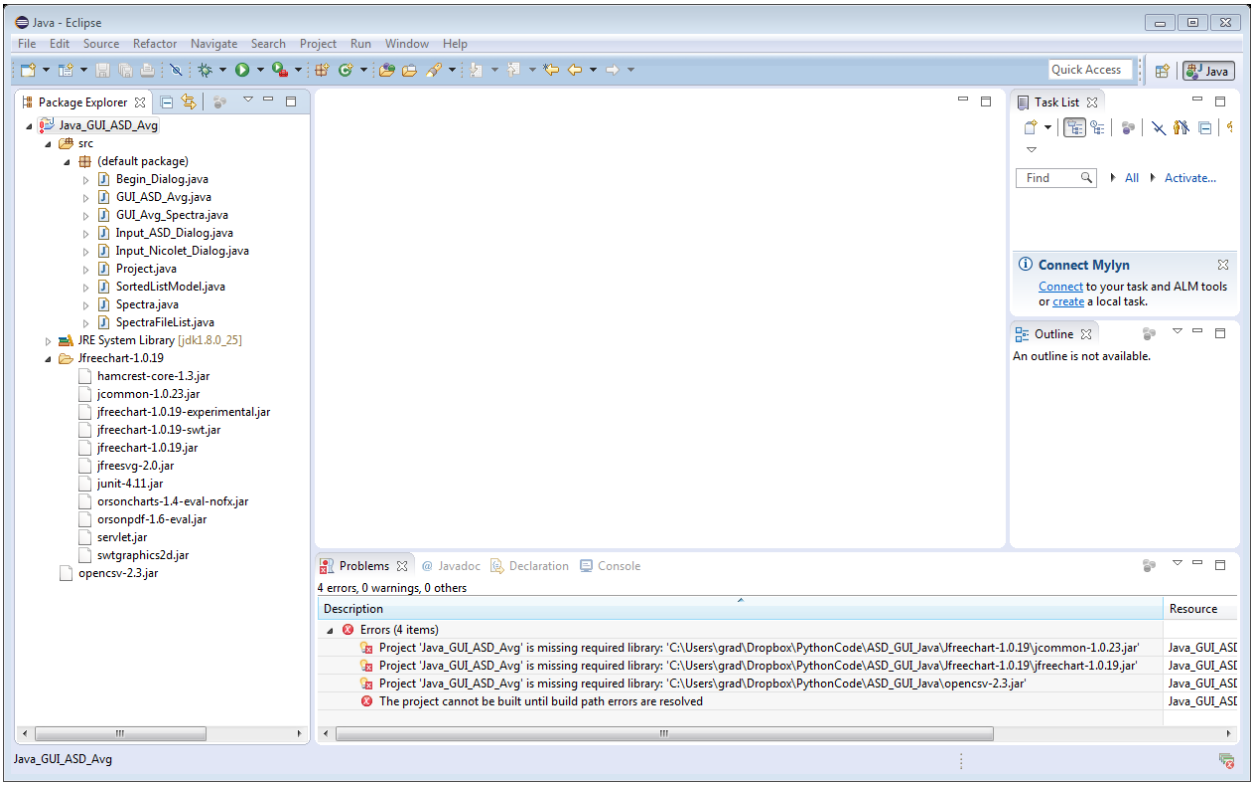
Opening Code in Eclipse

1. Open Eclipse and navigate to File > Import. In the Import dialog box, click on General and then Existing Projects into Workspace. Select Next.

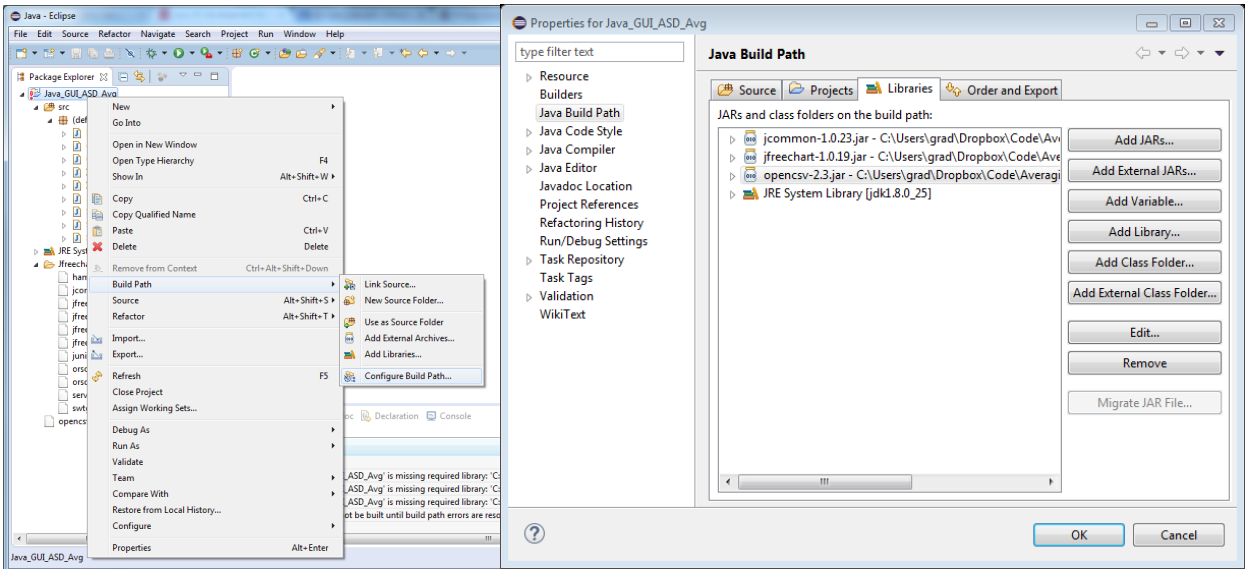


2. Navigate to the folder titled Averaging_ASD_Nicolet_Spectra. The Projects should have Java_GUI_ASD_Avg show up and selected. Select Finish. The project should then show up on the left side in the package explorer (see below).

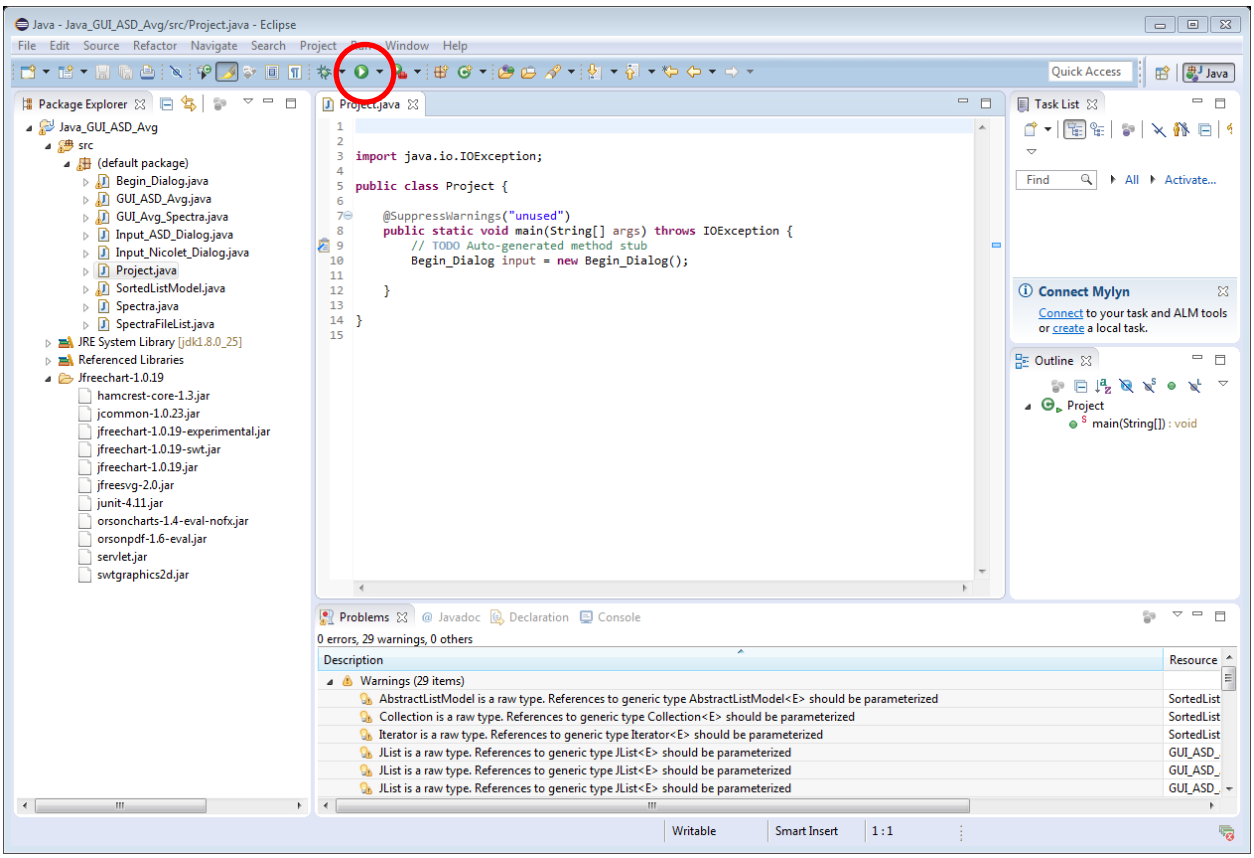




3. There will be a large red ! on the project folder. In order to fix these errors, some external libraries need to be imported. Right click on Java_GUI_ASD_Avg and select Build Path > Configure Build Path. The Properties for Java_GUI_ASD_Avg dialog box will open. Navigate to the Libraries Tab where 3 libraries will be listed with a red X. Double click on jcommon-1.0.23.jar and the Edit Jar dialog will open. Navigate to the Jfreechart-1.0.19 folder and select the jcommon-1.0.23.jar file. Continue to double click on jfreechart-1.0.19.jar and select it from the Jfreechart-1.0.19 folder. The opencsv-2.3.jar file is located in the Averaging_ASD_Nicolet_Spectra folder. Once all three libraries have been updated select OK.



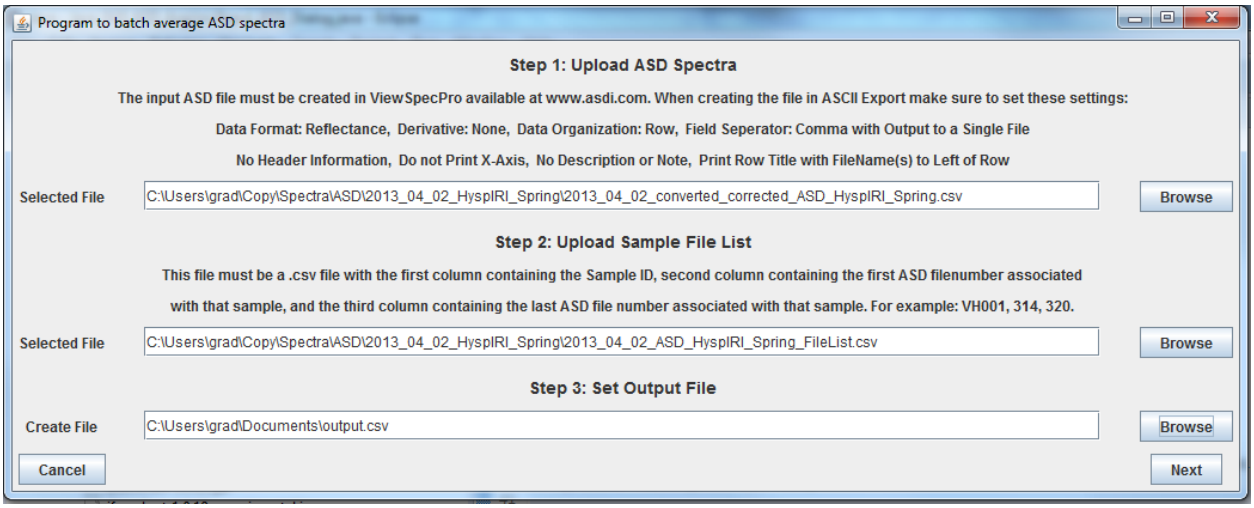
4. Double click the file called Project.java and the code for this class will pull up (see below). Hit the green circle with a play symbol to run the code.



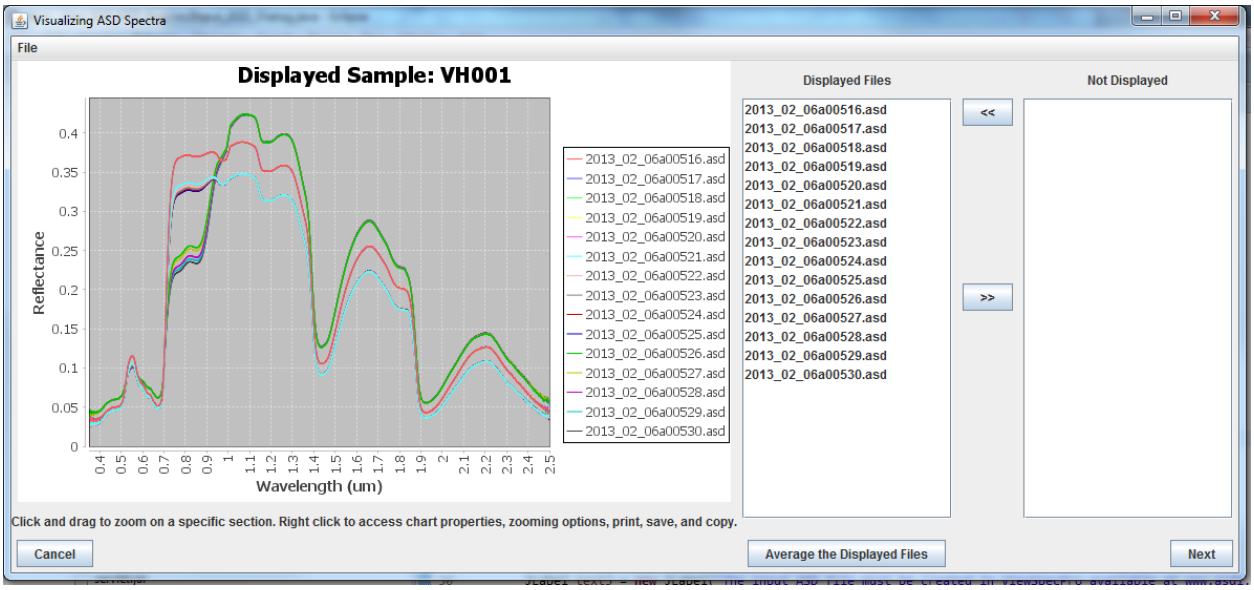
Averaging ASD Spectra

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.

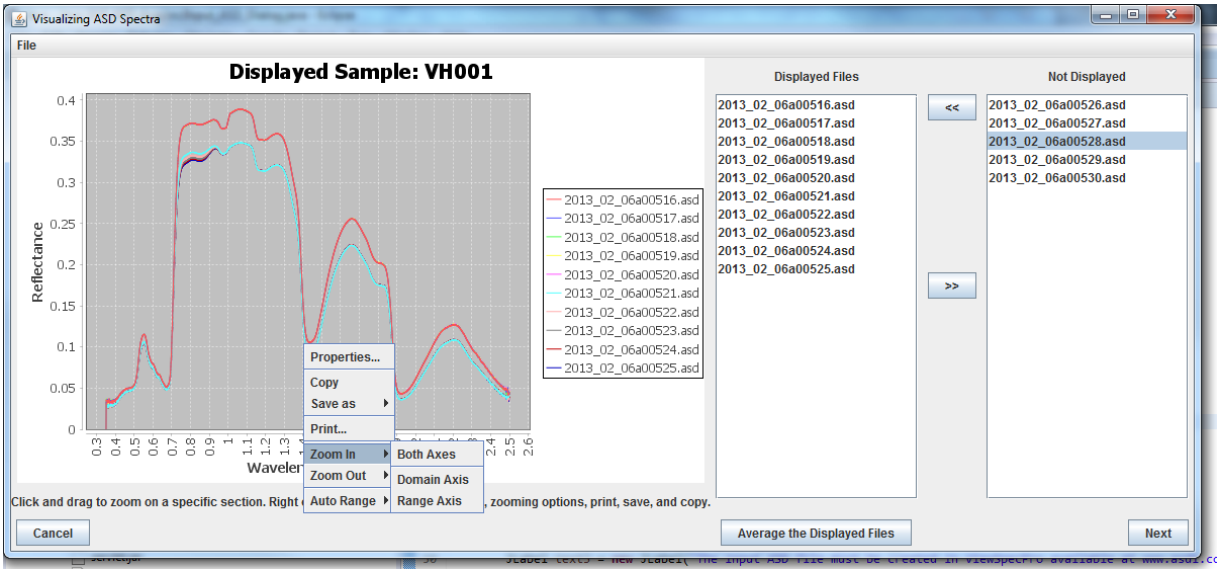
2. Next the "Program to batch average ASD Spectra" will open. Select the file created from the Join Correction code for Step 1. Navigate to the Sample File List for Step 2. Last navigate to the folder you want to output the file and name the file. Once these are completed, hit next.



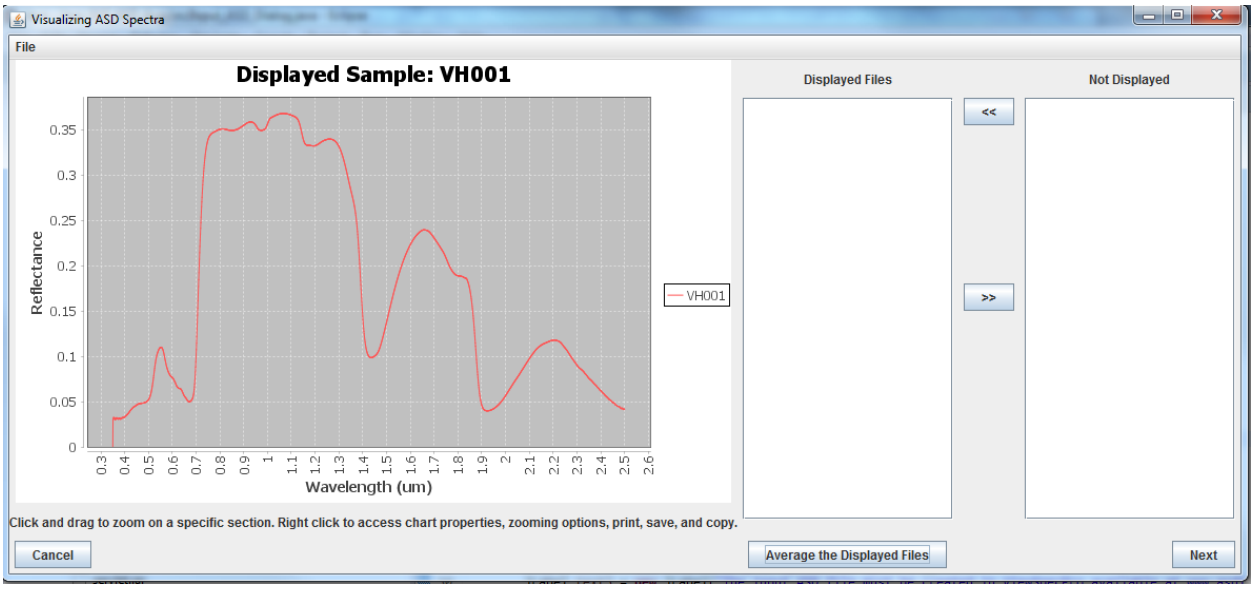
3. The "Visualizing ASD Spectra" dialog box will appear. The code will start with the first sample list in the Sample File List. At the beginning all spectra related to that sample will be displayed. If you do not want a file to be displayed and not included in the average, select the filename from the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



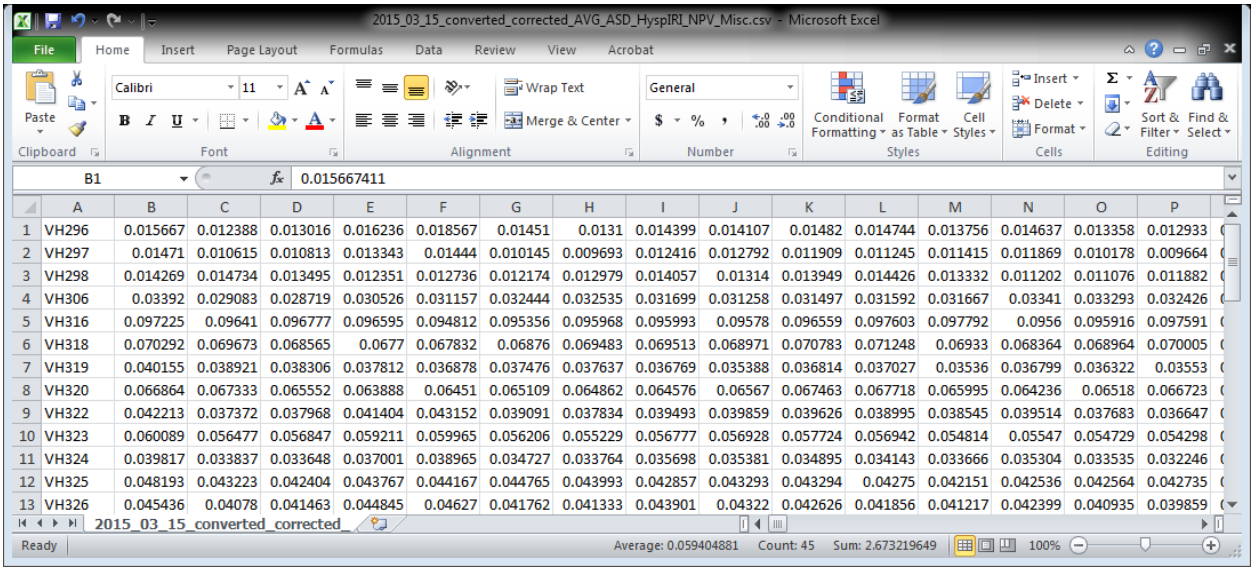
The graph itself has options to change font, zoom, print, save, copy, etc. You can access these by right clicking on the graph.



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 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. Hitting the Next button will always continue on to the next sample even if the current sample has not been averaged. The output file will be a csv with the first column being the sample ID and the following columns the spectra (see below).



	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P
1	VH296	0.015667	0.012388	0.013016	0.016236	0.018567	0.01451	0.0131	0.014399	0.014107	0.01482	0.014744	0.013756	0.014637	0.013358	0.012933
2	VH297	0.01471	0.010615	0.010813	0.013343	0.01444	0.010145	0.009693	0.012416	0.012792	0.011909	0.011245	0.011415	0.011869	0.010178	0.009664
3	VH298	0.014269	0.014734	0.013495	0.012351	0.012736	0.012174	0.012979	0.014057	0.01314	0.013949	0.014426	0.013332	0.011202	0.011076	0.011882
4	VH306	0.03392	0.029083	0.028719	0.030526	0.031157	0.032444	0.032535	0.031699	0.031258	0.031497	0.031592	0.031667	0.03341	0.033293	0.032426
5	VH316	0.097225	0.09641	0.096777	0.096595	0.094812	0.095356	0.095968	0.095993	0.09578	0.096559	0.097603	0.097792	0.0956	0.095916	0.097591
6	VH318	0.070292	0.069673	0.068565	0.0677	0.067832	0.06876	0.069483	0.069513	0.068971	0.070783	0.071248	0.06933	0.068364	0.068964	0.070005
7	VH319	0.040155	0.038921	0.038306	0.037812	0.036878	0.037476	0.037637	0.036769	0.035388	0.036814	0.037027	0.03536	0.036799	0.036322	0.03553
8	VH320	0.066864	0.067333	0.065552	0.063888	0.06451	0.065109	0.064862	0.064576	0.06567	0.067463	0.067718	0.065995	0.064236	0.06518	0.066723
9	VH322	0.042213	0.037372	0.037968	0.041404	0.043152	0.039091	0.037834	0.039493	0.039859	0.039626	0.038995	0.038545	0.039514	0.037683	0.036647
10	VH323	0.060089	0.056477	0.056847	0.059211	0.059965	0.056206	0.055229	0.056777	0.056928	0.057724	0.056942	0.054814	0.05547	0.054729	0.054298
11	VH324	0.039817	0.033837	0.033648	0.037001	0.038965	0.034727	0.033764	0.035698	0.035381	0.034895	0.034143	0.033666	0.035304	0.033535	0.032246
12	VH325	0.048193	0.043223	0.042404	0.043767	0.044167	0.044765	0.043993	0.042857	0.043293	0.043294	0.04275	0.042151	0.042536	0.042564	0.042735
13	VH326	0.045436	0.04078	0.041463	0.044845	0.04627	0.041762	0.041333	0.043901	0.04322	0.042626	0.041856	0.041217	0.042399	0.040935	0.039859