Protocol for exporting spectra data in Winisi from ASD (using ViewSpec Pro)

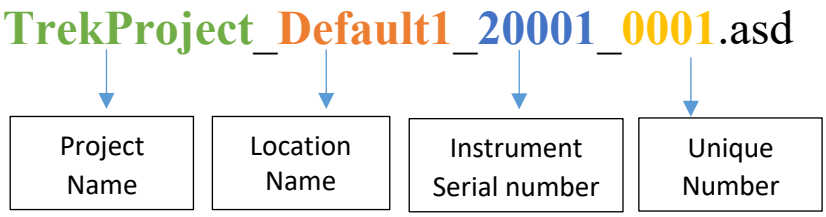
ASD QualitySpec® Trek is a portable hand-held, near infrared (NIR) contact spectrometer designed for fast and easy collection of spectra in a laboratory or in-situ field environments. Trek is a full-range instrument (350 nm to 2500 nm) that captures spectra in the visible, near infrared, and shortwave infrared range.

You can export spectral data for use with other software for further analysis. You can export the samples for use in the following software applications:

- Indico® Pro
- ENVI®
- The Spectral Geologist (TSG®)
- ViewSpec Pro®
- any other software that accepts ASD 1.0 format

The export process creates a spectral data file in ASD single vector format (.asd) for each sample.

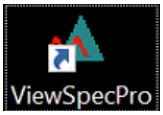
By default, the name for the exported files include the project name, location name, instrument serial number and sample number. For example



The ViewSpec™ application is a program used for post-processing spectra files that were saved using an ASD instrument

You can install ViewSpec pro from below link after registering
https://www.malvernpanalytical.com/en/support/product-support/software/ViewSpecProSoftwareInstall

After you download and install the software, you can initiate ViewSpec Pro by Clicking on the ViewSpec Pro icon from the desktop



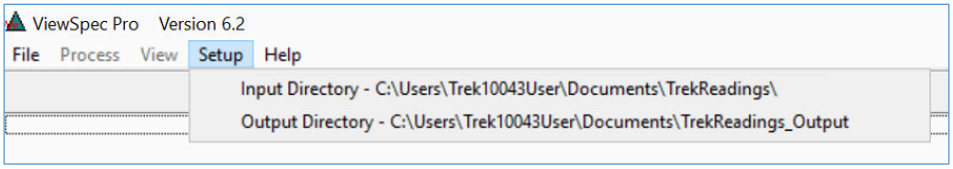
Step1

Select the input directory for the spectra files.

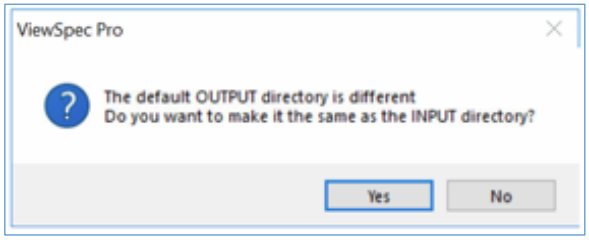
The input directory is the location where your spectra data files reside

For the input files, use:

• Setup->Input Directory... pull-down menu item.



When selecting a *new* input directory, a window will open asking if you want the output directory to be the same as the input directory.

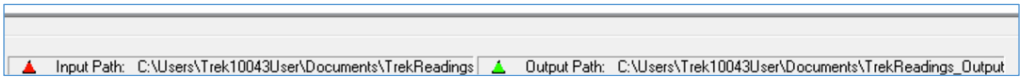


Step2 :

The input and output directories do not have to be the same directory. To select a different output directory for the spectra files.

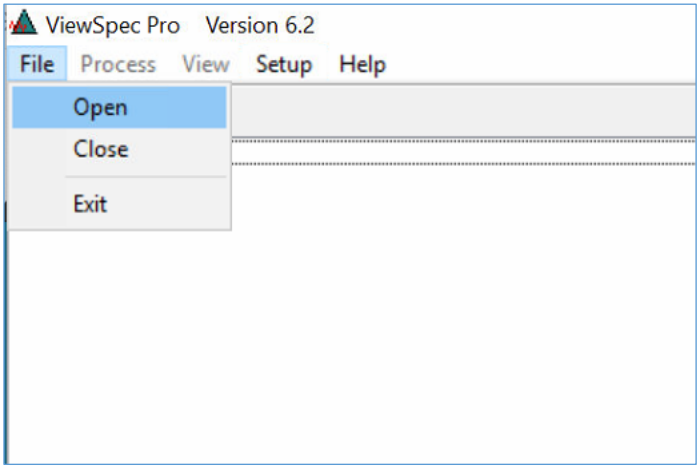
For the output files, use:

•Setup->Output Directory... pull-down menu item

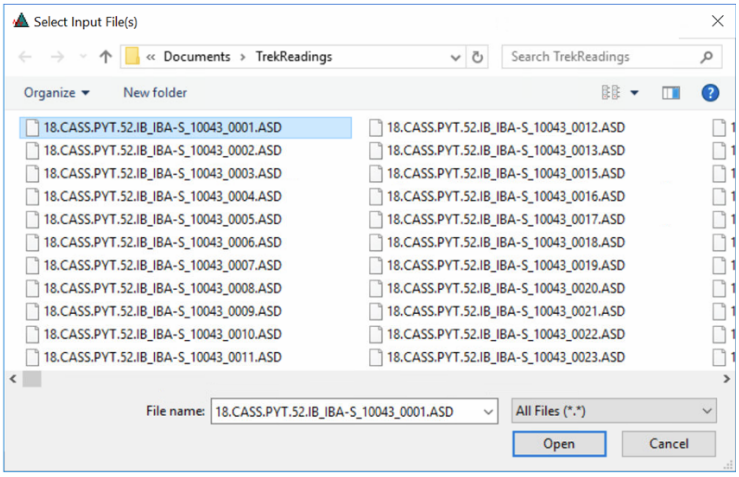


Step3 :

Select File->Open on the main menu bar and then choose the files for post-processing



The following dialog box will be displayed, automatically taking you to the directory selected in step 1.



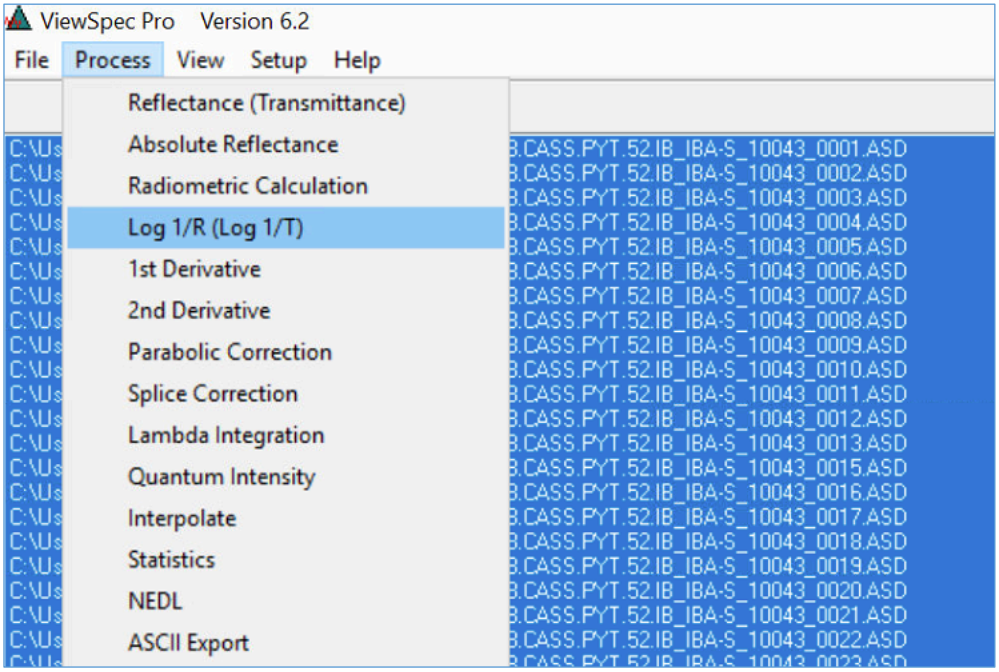
Select the file(s) from the list available in the directory.

- Use the **'Shift'** or **'Ctrl'** keys in conjunction with the mouse click to select multiple files.
- Use the **'Files of type'** combo box to show only files with certain file extensions.

When you have selected the files you desire, click '**Open**'.

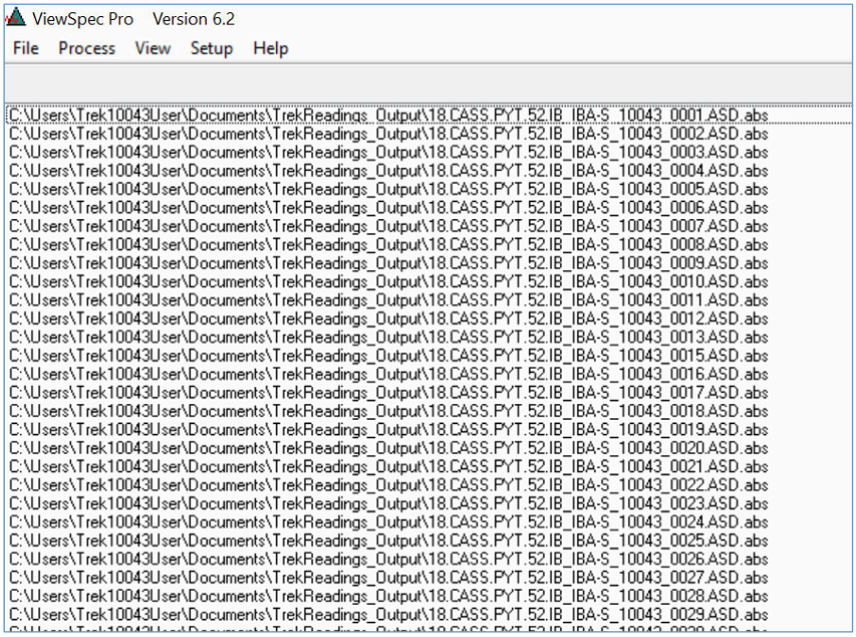
Step 4:

Select all the files and from **Process** pull-down menu, select log 1/R (1/T) option



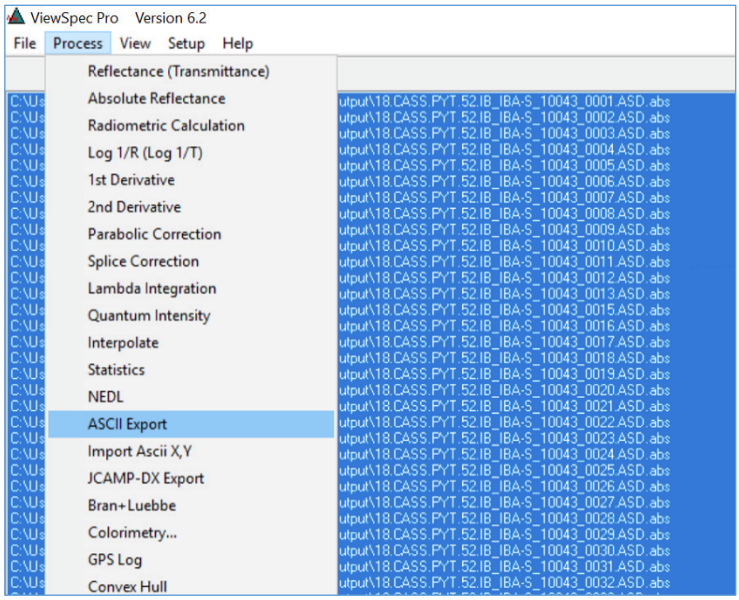
log 1/R (1/T) option Converts reflectance or transmittance to absorbance
Absorbance = log(1/Transmittance.)

Now you can see that all the .ASD files are converted in to .abs files

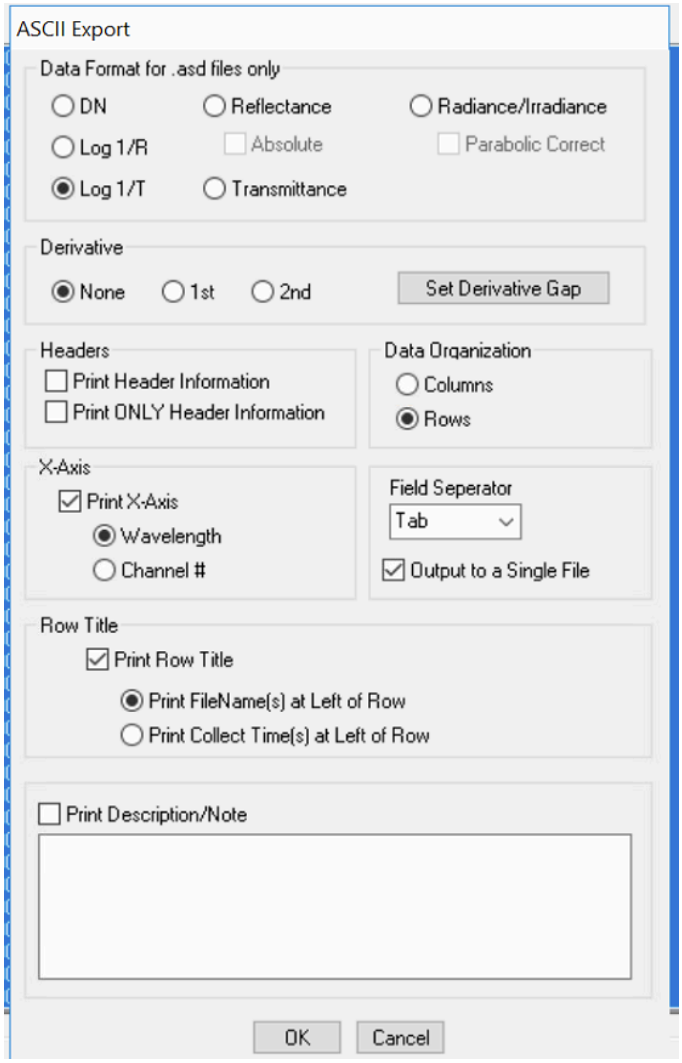


Step5:

Select all the. abs files and from **Process** pull-down menu, chose ASCII Export option This process converts data files into ASCII text files. Files can be exported Individually or similar files can be combined into an array and conveniently output as a single file.

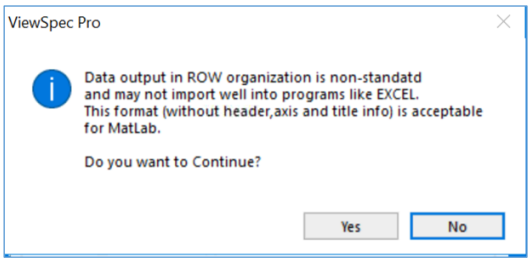


When ASCII Export is selected, the following Dialog Box is displayed:

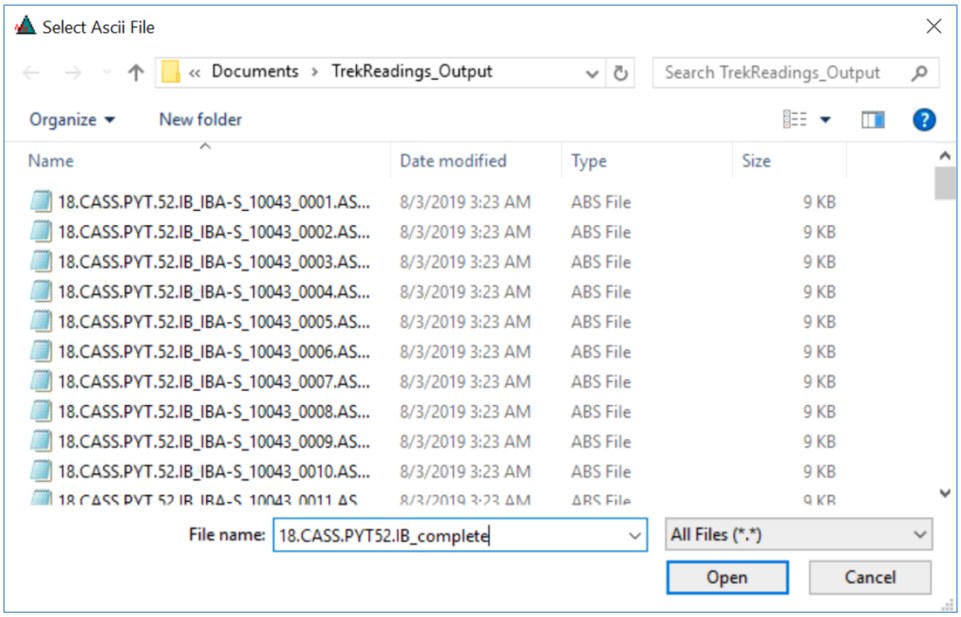


- Select log 1/T for Data Format for .asd files only
- Select None for Derivative
- Data organization should be Rows
- Under field separator check output to a single file option
- You can leave others as default
- Click ok

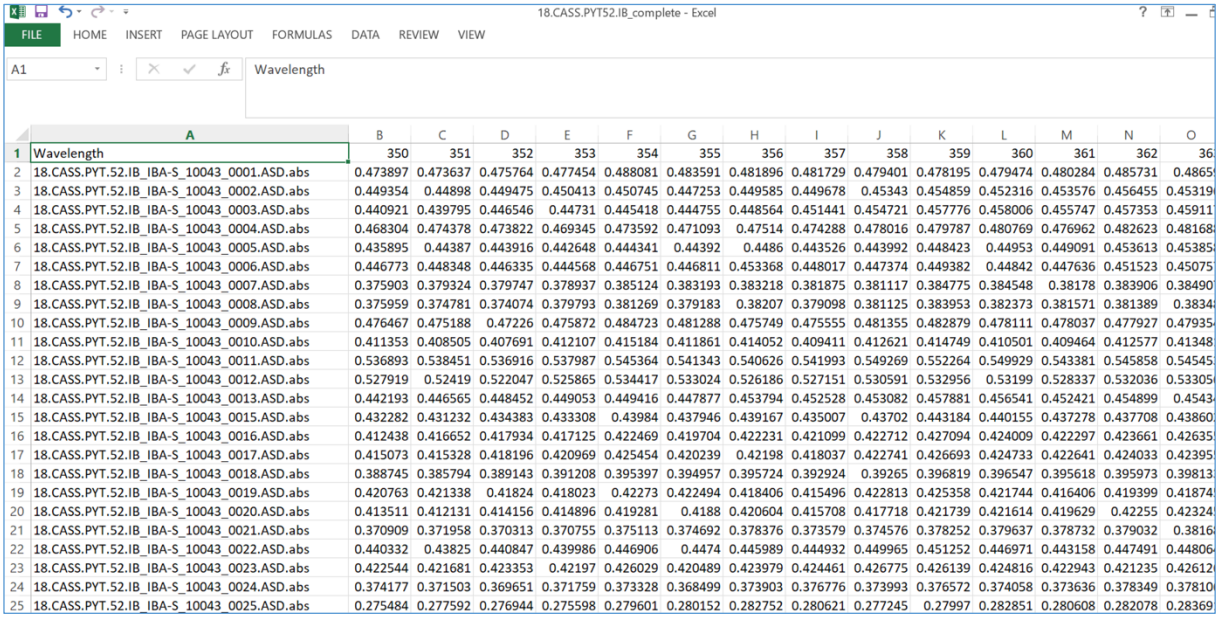
It gives a warning message, click yes.



Provide name for the single file and click ok. It saves the file in the selected location.



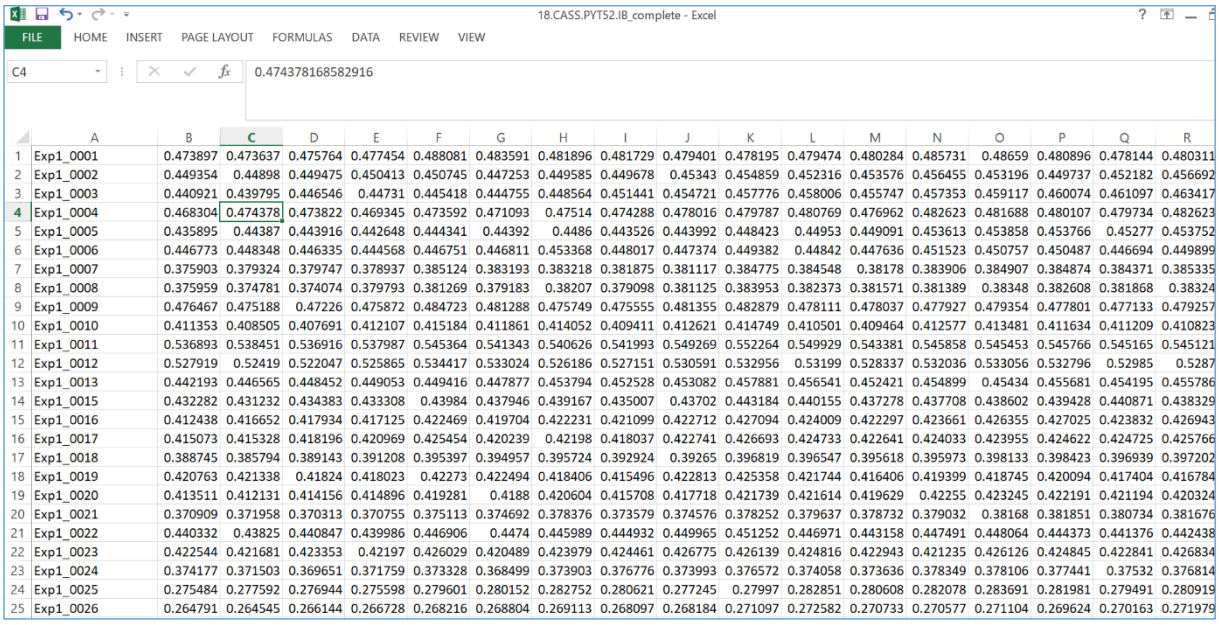
Open the saved file in excel, it will include Sample number in the first column and spectra data for wave length from 350 to 2500 in next coloumns as shown below. Each row correspondance to individual spectra you have selected.



	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O
1	Wavelength	350	351	352	353	354	355	356	357	358	359	360	361	362	36
2	18.CASS.PYT.52.IB_IBA-S_10043_0001.ASD.abs	0.473897	0.473637	0.475764	0.477454	0.488081	0.483591	0.481896	0.481729	0.479401	0.478195	0.479474	0.480284	0.485731	0.4865
3	18.CASS.PYT.52.IB_IBA-S_10043_0002.ASD.abs	0.449354	0.44898	0.449475	0.450413	0.450745	0.447253	0.449585	0.449678	0.45343	0.454859	0.452316	0.453576	0.456455	0.45319
4	18.CASS.PYT.52.IB_IBA-S_10043_0003.ASD.abs	0.440921	0.439795	0.446546	0.44731	0.445418	0.444755	0.448564	0.451441	0.454721	0.457776	0.458006	0.455747	0.457353	0.45911
5	18.CASS.PYT.52.IB_IBA-S_10043_0004.ASD.abs	0.468304	0.474378	0.473822	0.469345	0.473592	0.471093	0.47514	0.474288	0.478016	0.479787	0.480769	0.476962	0.482623	0.48168
6	18.CASS.PYT.52.IB_IBA-S_10043_0005.ASD.abs	0.435895	0.44387	0.443916	0.442648	0.444341	0.44392	0.4486	0.443526	0.443992	0.448423	0.44953	0.449091	0.453613	0.45385
7	18.CASS.PYT.52.IB_IBA-S_10043_0006.ASD.abs	0.446773	0.448348	0.446335	0.444568	0.446751	0.446811	0.453368	0.448017	0.447374	0.449382	0.44842	0.447636	0.451523	0.45075
8	18.CASS.PYT.52.IB_IBA-S_10043_0007.ASD.abs	0.375903	0.379324	0.379747	0.378937	0.385124	0.383193	0.383218	0.381875	0.381117	0.384775	0.384548	0.38178	0.383906	0.38490
9	18.CASS.PYT.52.IB_IBA-S_10043_0008.ASD.abs	0.375959	0.374781	0.374074	0.379793	0.381269	0.379183	0.38207	0.379098	0.381125	0.383953	0.382373	0.381571	0.381389	0.3834
10	18.CASS.PYT.52.IB_IBA-S_10043_0009.ASD.abs	0.476467	0.475188	0.47226	0.475872	0.484723	0.481288	0.475749	0.475555	0.481355	0.482879	0.478111	0.478037	0.477927	0.47935
11	18.CASS.PYT.52.IB_IBA-S_10043_0010.ASD.abs	0.411353	0.408505	0.407691	0.412107	0.415184	0.411861	0.414052	0.409411	0.412621	0.414749	0.410501	0.409464	0.412577	0.41348
12	18.CASS.PYT.52.IB_IBA-S_10043_0011.ASD.abs	0.536893	0.538451	0.536916	0.537987	0.545364	0.541343	0.540626	0.541993	0.549269	0.552264	0.549929	0.543381	0.545858	0.54545
13	18.CASS.PYT.52.IB_IBA-S_10043_0012.ASD.abs	0.527919	0.52419	0.522047	0.525865	0.534417	0.533024	0.526186	0.527151	0.530591	0.532956	0.53199	0.528337	0.532036	0.53305
14	18.CASS.PYT.52.IB_IBA-S_10043_0013.ASD.abs	0.442193	0.446565	0.448452	0.449053	0.449416	0.447877	0.453794	0.452528	0.453082	0.457881	0.456541	0.452421	0.454899	0.4543
15	18.CASS.PYT.52.IB_IBA-S_10043_0015.ASD.abs	0.432282	0.431232	0.434383	0.433308	0.43984	0.437946	0.439167	0.435007	0.43702	0.443184	0.440155	0.437278	0.437708	0.43860
16	18.CASS.PYT.52.IB_IBA-S_10043_0016.ASD.abs	0.412438	0.416652	0.417934	0.417125	0.422469	0.419704	0.422231	0.421099	0.422712	0.427094	0.424009	0.422297	0.423661	0.42635
17	18.CASS.PYT.52.IB_IBA-S_10043_0017.ASD.abs	0.415073	0.415328	0.418196	0.420969	0.425454	0.420239	0.42198	0.418037	0.422741	0.426693	0.424733	0.422641	0.424033	0.42395
18	18.CASS.PYT.52.IB_IBA-S_10043_0018.ASD.abs	0.388745	0.385794	0.389143	0.391208	0.395397	0.394957	0.395724	0.392924	0.39265	0.396819	0.396547	0.395618	0.395973	0.39813
19	18.CASS.PYT.52.IB_IBA-S_10043_0019.ASD.abs	0.420763	0.421338	0.41824	0.418023	0.42273	0.422494	0.418406	0.415496	0.422813	0.425358	0.421744	0.416406	0.419399	0.41874
20	18.CASS.PYT.52.IB_IBA-S_10043_0020.ASD.abs	0.413511	0.412131	0.414156	0.414896	0.419281	0.4188	0.420604	0.415708	0.417718	0.421739	0.421614	0.419629	0.42255	0.42324
21	18.CASS.PYT.52.IB_IBA-S_10043_0021.ASD.abs	0.370909	0.371958	0.370313	0.370755	0.375113	0.374692	0.378376	0.373579	0.374576	0.378252	0.379637	0.378732	0.379032	0.3816
22	18.CASS.PYT.52.IB_IBA-S_10043_0022.ASD.abs	0.440332	0.43825	0.440847	0.439986	0.446906	0.4474	0.445989	0.444932	0.449965	0.451252	0.446971	0.443158	0.447491	0.44806
23	18.CASS.PYT.52.IB_IBA-S_10043_0023.ASD.abs	0.422544	0.421681	0.423353	0.42197	0.426029	0.420489	0.423979	0.424461	0.426775	0.426139	0.424816	0.422943	0.421235	0.42612
24	18.CASS.PYT.52.IB_IBA-S_10043_0024.ASD.abs	0.374177	0.371503	0.369651	0.371759	0.373328	0.368499	0.373903	0.376776	0.373993	0.376572	0.374058	0.373636	0.378349	0.37810
25	18.CASS.PYT.52.IB_IBA-S_10043_0025.ASD.abs	0.275484	0.277592	0.276944	0.275598	0.279601	0.280152	0.282752	0.280621	0.277245	0.27997	0.282851	0.280608	0.282078	0.28369

Winisi software input format requires

- No heading information – Delete the first row in the file
- Sample number is a 12-character alpha/numeric identifier - Include a new column with 12-character Sample number and delete the original Sample numbers. (note : It is recommended to save the original Sample number and changed Sample number in a seperate file for future reference)



18.CASS.PYT52.IB_complete - Excel

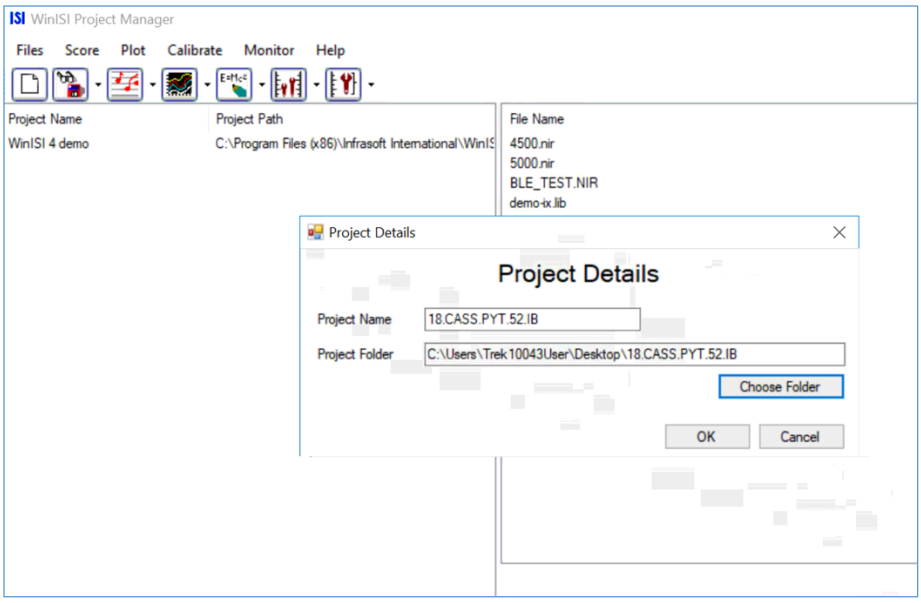
FILE HOME INSERT PAGE LAYOUT FORMULAS DATA REVIEW VIEW

C4 0.474378168582916

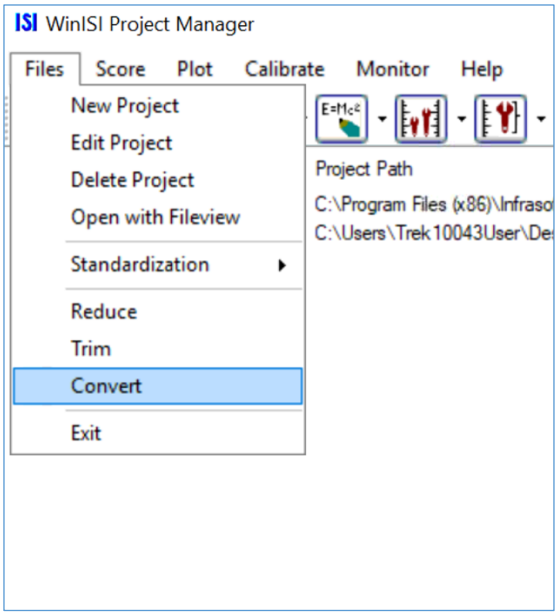
	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R
1	Exp1_0001	0.473897	0.473637	0.475764	0.477454	0.488081	0.483591	0.481896	0.481729	0.479401	0.478195	0.479474	0.480284	0.485731	0.48659	0.480896	0.478144	0.480311
2	Exp1_0002	0.449354	0.44898	0.449475	0.450413	0.450745	0.447253	0.449585	0.449678	0.45343	0.454859	0.452316	0.453576	0.456455	0.453196	0.449737	0.452182	0.456692
3	Exp1_0003	0.440921	0.439795	0.446546	0.44731	0.445418	0.444755	0.448564	0.451441	0.454721	0.457776	0.458006	0.455747	0.457353	0.459117	0.460074	0.461097	0.463417
4	Exp1_0004	0.468304	0.474378	0.473822	0.469345	0.473592	0.471093	0.47514	0.474288	0.478016	0.479787	0.480769	0.476962	0.482623	0.481688	0.480107	0.479734	0.482623
5	Exp1_0005	0.435895	0.44387	0.443916	0.442648	0.444341	0.44392	0.4486	0.443526	0.443992	0.448423	0.44953	0.449091	0.453613	0.453858	0.453766	0.45277	0.453752
6	Exp1_0006	0.446773	0.448348	0.446335	0.444568	0.446751	0.446811	0.453368	0.448017	0.447374	0.449382	0.44842	0.447636	0.451523	0.450757	0.450487	0.446694	0.449899
7	Exp1_0007	0.375903	0.379324	0.379747	0.378937	0.385124	0.383193	0.383218	0.381875	0.381117	0.384775	0.384548	0.38178	0.383906	0.384907	0.384874	0.384371	0.385335
8	Exp1_0008	0.375959	0.374781	0.374074	0.379793	0.381269	0.379183	0.38207	0.379098	0.381125	0.383953	0.382373	0.381571	0.381389	0.38348	0.382608	0.381868	0.38324
9	Exp1_0009	0.476467	0.475188	0.47226	0.475872	0.484723	0.481288	0.475749	0.475555	0.481355	0.482879	0.478111	0.478037	0.477927	0.479354	0.477801	0.477133	0.479257
10	Exp1_0010	0.411353	0.408505	0.407691	0.412107	0.415184	0.411861	0.414052	0.409411	0.412621	0.414749	0.410501	0.409464	0.412577	0.413481	0.411634	0.411209	0.410823
11	Exp1_0011	0.536893	0.538451	0.536916	0.537987	0.545364	0.541343	0.540626	0.541993	0.549269	0.552264	0.549929	0.543381	0.545858	0.545453	0.545766	0.545165	0.545121
12	Exp1_0012	0.527919	0.52419	0.522047	0.525865	0.534417	0.533024	0.526186	0.527151	0.530591	0.532956	0.53199	0.528337	0.532036	0.533056	0.532796	0.52985	0.5287
13	Exp1_0013	0.442193	0.446565	0.448452	0.449053	0.449416	0.447877	0.453794	0.452528	0.453082	0.457881	0.456541	0.452421	0.454899	0.45434	0.455681	0.454195	0.455786
14	Exp1_0015	0.432282	0.431232	0.434383	0.433308	0.43984	0.437946	0.439167	0.435007	0.43702	0.443184	0.440155	0.437278	0.437708	0.438602	0.439428	0.440871	0.438329
15	Exp1_0016	0.412438	0.416652	0.417934	0.417125	0.422469	0.419704	0.422231	0.421099	0.422712	0.427094	0.424009	0.422297	0.423661	0.426355	0.427025	0.423832	0.426943
16	Exp1_0017	0.415073	0.415328	0.418196	0.420969	0.425454	0.420239	0.42198	0.418037	0.422741	0.426693	0.424733	0.422641	0.424033	0.423955	0.424622	0.424725	0.425766
17	Exp1_0018	0.388745	0.385794	0.389143	0.391208	0.395397	0.394957	0.395724	0.392924	0.39265	0.396819	0.396547	0.395618	0.395973	0.398133	0.398423	0.396939	0.397202
18	Exp1_0019	0.420763	0.421338	0.41824	0.418023	0.42273	0.422494	0.418406	0.415496	0.422813	0.425358	0.421744	0.416406	0.419399	0.418745	0.420094	0.417404	0.416784
19	Exp1_0020	0.413511	0.412131	0.414156	0.414896	0.419281	0.4188	0.420604	0.415708	0.417718	0.421739	0.421614	0.419629	0.42255	0.423245	0.422191	0.421194	0.420324
20	Exp1_0021	0.370909	0.371958	0.370313	0.370755	0.375113	0.374692	0.378376	0.373579	0.374576	0.378252	0.379637	0.378732	0.379032	0.38168	0.381851	0.380734	0.381676
21	Exp1_0022	0.440332	0.43825	0.440847	0.439986	0.446906	0.4474	0.445989	0.444932	0.449965	0.451252	0.446971	0.443158	0.447491	0.448064	0.444373	0.441376	0.442438
22	Exp1_0023	0.422544	0.421681	0.423353	0.42197	0.426029	0.420489	0.423979	0.424461	0.426775	0.426139	0.424816	0.422943	0.421235	0.426126	0.424845	0.422841	0.426834
23	Exp1_0024	0.374177	0.371503	0.369651	0.371759	0.373328	0.368499	0.373903	0.376776	0.373993	0.376572	0.374058	0.373636	0.378349	0.378106	0.377441	0.37532	0.376814
24	Exp1_0025	0.275484	0.277592	0.276944	0.275598	0.279601	0.280152	0.282752	0.280621	0.277245	0.27997	0.282851	0.280608	0.282078	0.283691	0.281981	0.279491	0.280919
25	Exp1_0026	0.264791	0.264545	0.266144	0.266728	0.268216	0.268804	0.269113	0.268097	0.268184	0.271097	0.272582	0.270733	0.270577	0.271104	0.269624	0.270163	0.271979

Save file as .txt

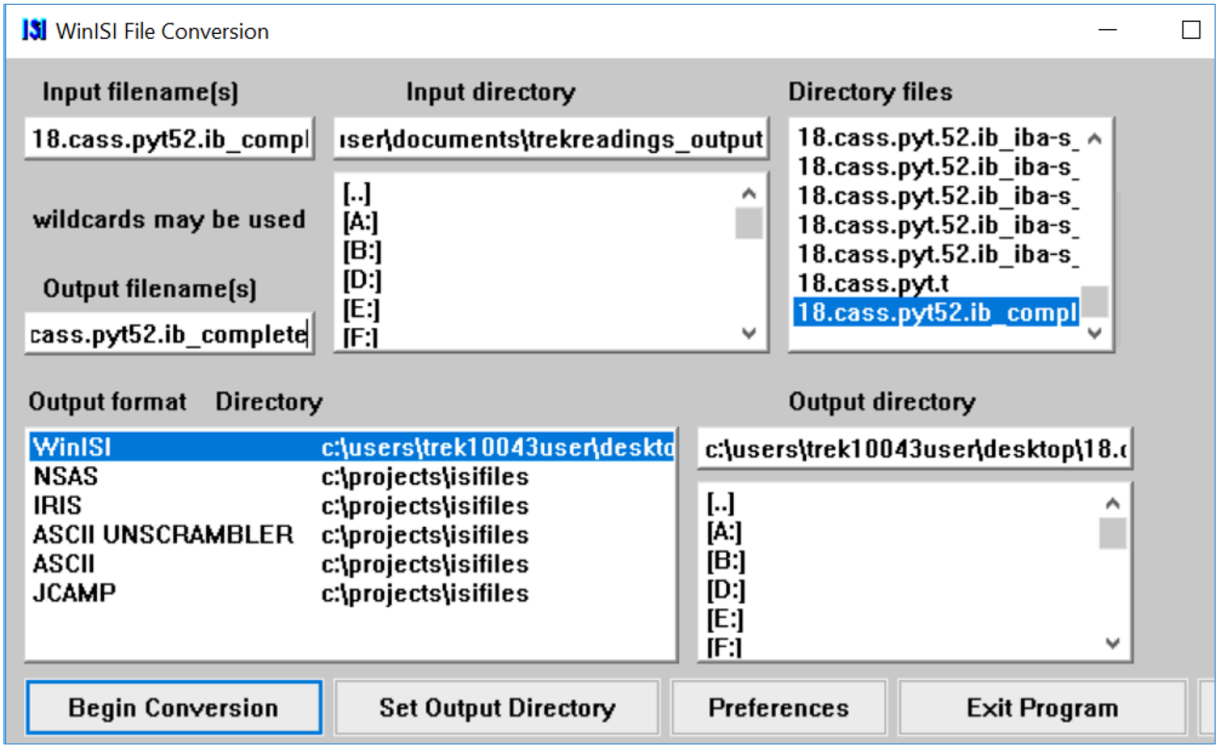
Open the Winisi software, create a new project



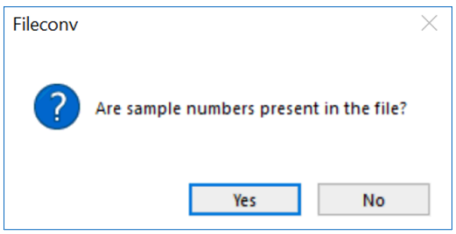
Select **Convert** from Files pull-down menu



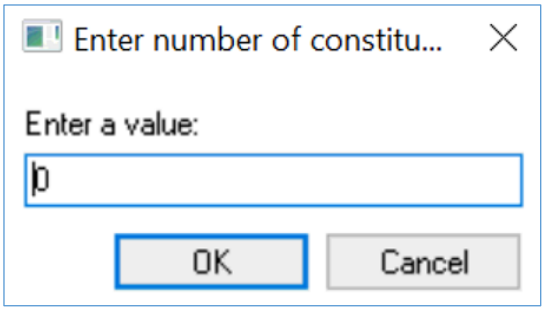
Select the input file (.txt) and give output file name and directory to save



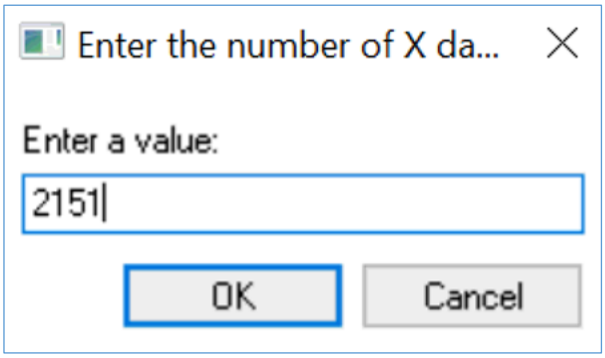
It will prompt to check if the sample number is present in the file, select Yes



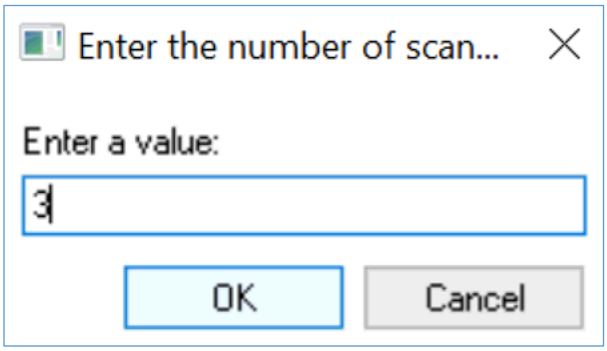
Enter number of Constituents - **0**



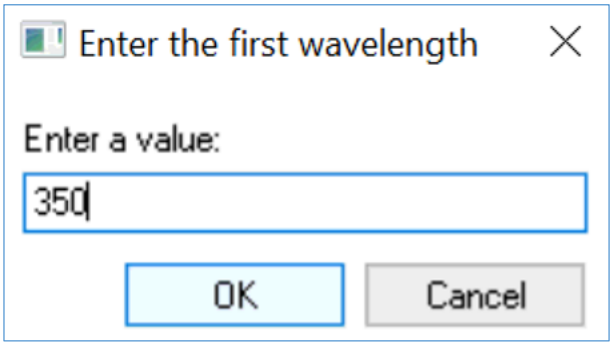
Enter the number of X data (wave length) : **2151** (as it is from 350 to 2500)



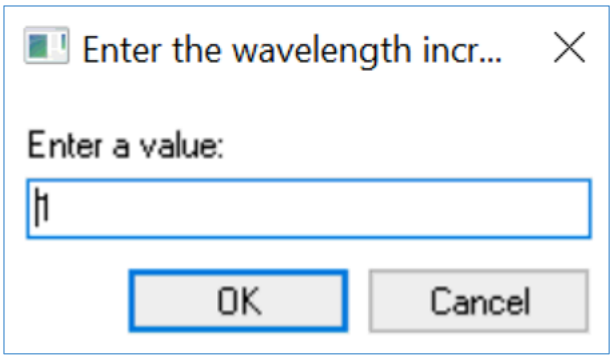
Enter the number of scannings : **3**



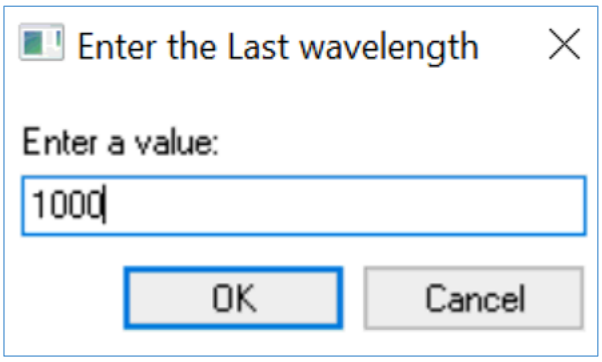
Enter the first wavelength : **350**



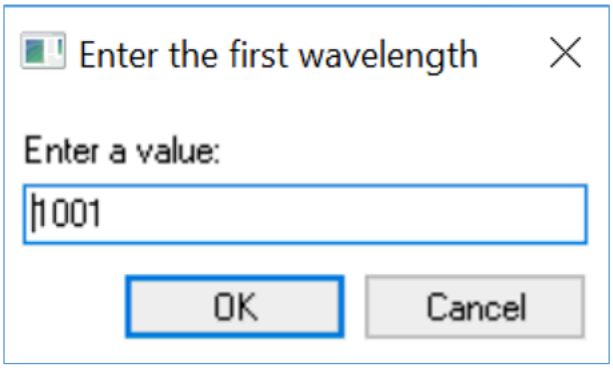
Enter the wavelength increment : **1**



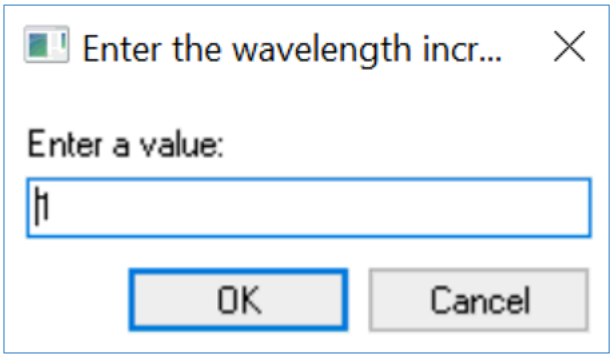
Enter the last wavelength : **1000**



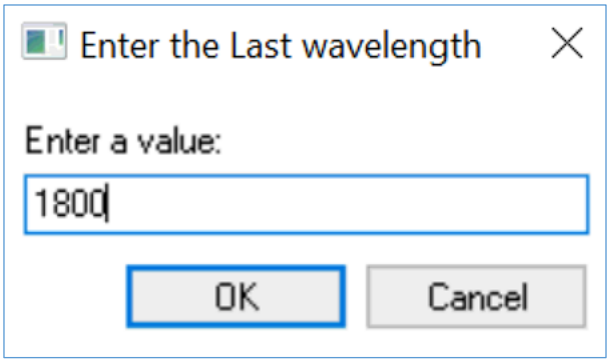
Enter the first wavelength : **1001**



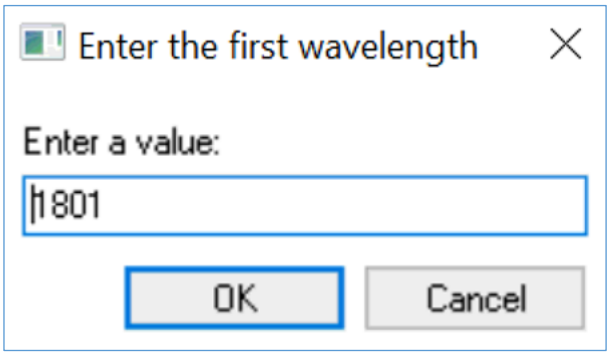
Enter the wavelength increment : **1**



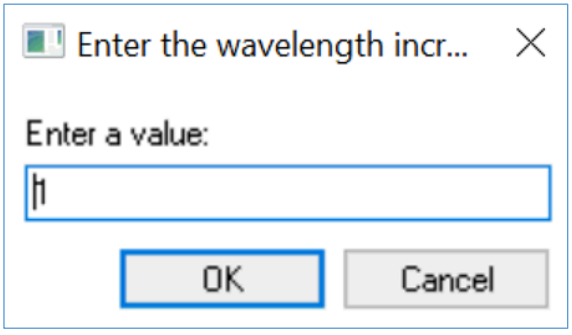
Enter the last wavelength : **1800**



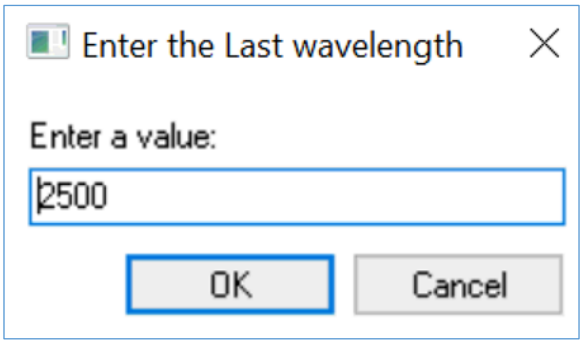
Enter the first wavelength : **1801**



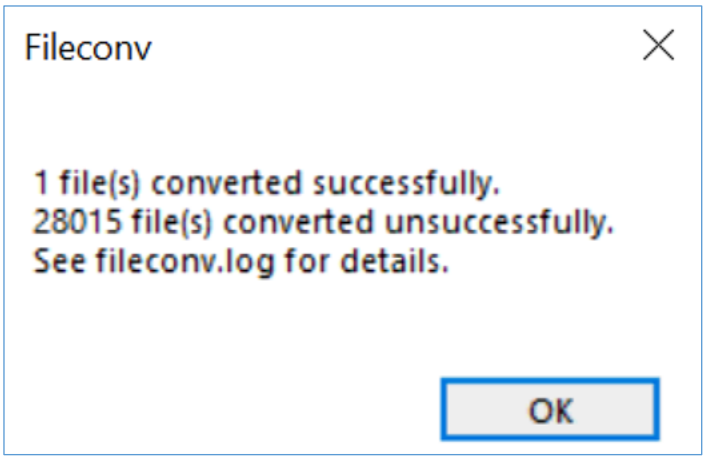
Enter the wavelength increment : **1**



Enter the last wavelength : **2500**



File converted prompt



Winisi showing the whole spectra data :