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Simple Method Transfer from FOSS NIR to Antaris FT-NIR Analyzers

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Key Words

- Antaris
- Method Transfer
- NIR

Introduction

Concerns about method transferability between different near infrared (NIR) instrument models or technologies causes many NIR users to be reluctant to switch to a different NIR instrument model or technology. It is believed that the method transfer is too complicated, time consuming and fraught with issues that will result in an unsuccessful transfer of the method. In some cases, there is a mis-conception that the differences in instrument design, for example, dispersive versus Fourier Transform (FT) NIR, makes the spectra from the two instrument types incompatible with one another. This technical note will show how methods can be successfully transferred from FOSS dispersive instruments to Thermo Scientific Antaris FT-NIR analyzers (Figure 1) with very little effort. Antaris™ FT-NIR instruments are designed, built and tested to tight tolerances using certified standards to ensure system to system consistency resulting in excellent method transfer. Method transfer of both FOSS WinISI™ and Vision™ methods to the Antaris FT-NIR using a Standards Converter program combined with Thermo Scientific TQ Analyst software will be successfully demonstrated in this technical note.

Figure 1: Antaris II FT-NIR analyzer used to show successful transfer of FOSS NIR methods

Methods

NIR methods typically have many standards in them, and in the case of raw material libraries, this number can easily top 1000. The time and money invested in collecting spectra and performing primary laboratory analysis to develop these methods makes method transfer a requirement for many companies looking to change to a different instrument model. In this technical note, successful method transfer to the Antaris FT-NIR will be shown for the two most common NIR application types: raw material identification and multi-component PLS analysis.

The method transfer was accomplished quickly and easily using a Standards Converter program followed by TQ Analyst™ chemometric software. For both application types, the Standards Converter program served three functions that greatly simplified the method transfer. First, the program converted the more traditional NIR units of nanometers (nm) or microns into wavenumbers (cm^{-1}). Second, the program automatically converted all spectra into absorbance units from either transmittance or reflectance. Lastly, the program automatically launched TQ Analyst software and inserted all standards with their corresponding primary laboratory values into the TQ Analyst standards table. This three step process is a simple, repeatable procedure for transferring FOSS methods to a format that is directly compatible with Antaris FT-NIR spectra for easy method expansion. This seamless method transfer process has many time and resource saving benefits including eliminating the need to re-enter any primary laboratory values and avoiding the hassle of locating and loading multiple individual converted spectra into an unfamiliar software package.

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Multi-component PLS Method Transfer from FOSS WinISI Software

Methods developed using FOSS NIR instruments with WinISI software can be easily and quickly transferred to the Antaris FT-NIR. The steps for transferring a multi-component PLS model for a feed product containing a large number of standards are demonstrated below. The first step was to convert the existing WinISI calibration file into a format easily read by the Standards Converter program. This was accomplished by using the files converter option in WinISI to convert the calibration file into a single JCAMP Multifile (.jcp). The second step used the Standards Converter program to convert the JCAMP Multifile (.jcp) into JCAMP-DX Multifiles (.jdx), convert the spectra into wavenumber and absorbance units and import the converted spectra directly into TQ Analyst. Accomplishing this step inside the Standards Converter required the user to simply select File – Open from the menu bar then browse to their JCAMP Multifile (.jcp) and check the three boxes for automatic wavenumber conversion, automatic absorbance conversion and create TQ method (Figure 2). The Standards Converter program automatically launched TQ Analyst (Figure 3) and placed all standards with their corresponding primary laboratory results into the TQ Analyst standards table (Figure 4). The last step was to re-create the method in the TQ Analyst software using the original settings from the Foss WinISI method. TQ Analyst supports the most common spectral pretreatments such as 1st and 2nd derivative, standard normal variate (SNV), multiplicative signal correction (MSC) and smoothing which guarantees that the transferred method uses all the same method parameters as the original method. The method can now be inoculated with standards collected on an Antaris FT-NIR. It is common and beneficial to inoculate transferred methods since it often improves the accuracy of the transferred method.

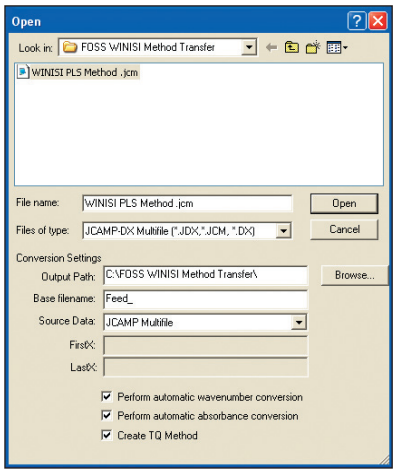

Figure 2: Standards Converter program showing the settings to transfer a FOSS WinISI method directly to an Antaris FT-NIR

Figure 3: Automatic launch of TQ Analyst chemometric package from the Standards Converter program simplifying transfer of FOSS methods

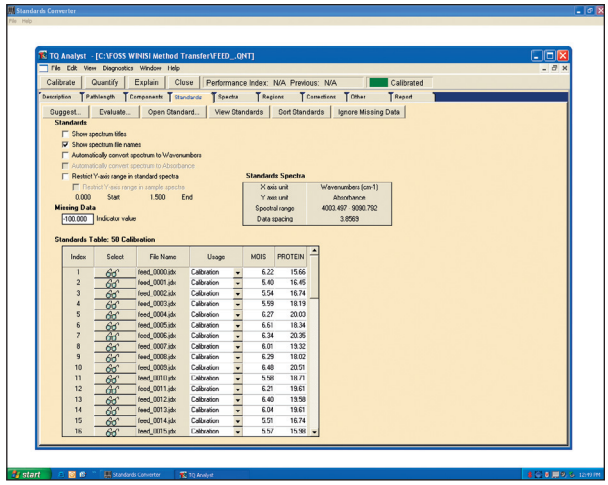

Figure 4: Standards table in TQ Analyst showing automatic import of primary laboratory values simplifying transfer of FOSS methods

Raw Material Identification Method Transfer from FOSS Vision Software

Raw material libraries often have many classes of compounds; it is not uncommon to have over 100 classes in the library. These libraries can contain over a thousand standard spectra; so recollecting spectra in order to recreate the library is not an option for most users. The steps for seamless transfer of a raw material identification method out of FOSS Vision software is described in this second application. FOSS Vision identification libraries are held in a database format. Identification libraries are built by creating 'products' containing a number of standards of each raw material. The equivalent FOSS 'product' is called a 'class' in TQ Analyst software. The process of transferring the FOSS Vision library method involved not only transferring the spectral information but also converting each 'product' in the Foss library to a 'class' in the TQ Analyst method. The first step to transfer the FOSS Vision library was to export the library using the ASCII file conversion option in Vision. This converted the Vision library into ASCII (.txt) format that was directly read into the Standards Converter program. The program

converted the ACSII (.txt) file into JCAMP-DX Multifiles (.jdx) which were imported directly into TQ Analyst. (Figure 5) As shown in Figure 5, selections were made in the Standards Converter to perform automatic wavenumber and absorbance conversion and automatically create a TQ Analyst method. Raw spectra from the FOSS Vision library that were converted to wavenumber and absorbance units and directly imported into TQ Analyst are shown in Figure 6. The library was then re-created in TQ Analyst software using the spectral data transferred from the Foss instrument and the original method settings from the FOSS method. The library method is now ready for expansion with standards collected on an Antaris FT-NIR.

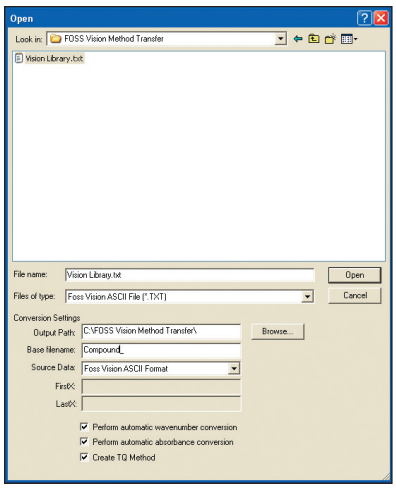

Figure 5: Standards Converter program showing the settings to transfer a FOSS Vision method directly to an Antaris FT-NIR

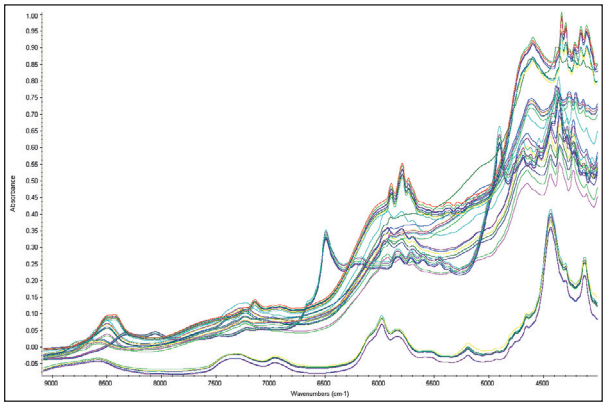

Figure 6: Successful wavenumber and absorbance conversion of FOSS spectra that were automatically imported into TQ Analyst software for method transfer to Antaris FT-NIR

As a validation of the successful transfer of FOSS methods to the Antaris systems, the material identification library transferred from the FOSS instrument had positive challenge samples analyzed on the Antaris FT-NIR. Thermo Scientific RESULT software for instrument control, monitoring and operation was used to collect spectra and report validation results for the transferred library method. The raw material identification report from RESULT™ for a positive challenge sample of caffeine showed proper identification with an excellent match value (Figure 7). This proper identification, using a transferred FOSS method, demonstrated that methods created using a FOSS instrument can be successfully transferred to the Antaris FT-NIR analyzer without loss in method performance.

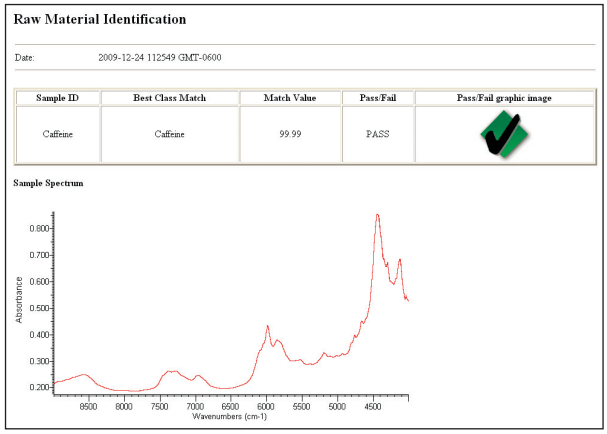

Figure 7: Antaris FT-NIR material identification report showing positive identification of caffeine, a compound present in the transferred FOSS material identification library

Conclusion

The transfer of methods from different NIR instrument models or technologies was thought to be an insurmountable obstacle to NIR users that wanted to change to a different NIR instrument. These NIR users thought they were locked into their current instrument or technology. This technical note proves that this is not the case and that transfer of methods from FOSS, as well as other instruments and technologies, is easily accomplished using the Thermo Scientific Standards Converter and TQ Analyst software packages. Simple and quick method transfer was demonstrated using software that requires very few steps in order to successfully transfer both FOSS WinISI and Vision methods to Thermo Scientific Antaris FT-NIR.

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