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Seamless Transfer of Bruker Spectra and Methods to an Antaris FT-NIR analyzer

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Key Words

- Antaris
- Chemometrics
- Methods Transfer
- Near-infrared

One of the hurdles for users of production near-infrared (NIR) systems is that they believe they are locked into the technology and instrument model they are currently using. Consistency is a critical parameter for NIR analysis and it is commonly thought that spectra and chemometric methods developed on one system are difficult to successfully transfer to another system. Transferring methods and spectra between different manufacturer's NIR systems is thought to be even more difficult since they are of such different designs. The Thermo Scientific Antaris FT-NIR analyzer product line (Figure 1) is designed such that transferability from one Antaris™ instrument to another Antaris instrument is virtually guaranteed. Transferability of spectra and methods from other manufacturer's instruments to the Antaris line is easy and is not the intractable problem it is thought to be. The design of the Thermo Scientific instruments coupled with its associated chemometric software greatly reduce the issue of transferability to the Antaris FT-NIR analyzers. To demonstrate this capability, methods were created for the Antaris analyzers using Thermo Scientific TQ Analyst software loaded only with spectra collected from a competing Bruker® MATRIX™-F FT-NIR system. This technical note describes the simple steps needed to easily convert the spectra into a TQ Analyst™ method and deploy it on the Antaris instrument.

Figure 1: Antaris II FT-NIR analyzer with SabIR probe. This instrument was successfully used to test the transferability of spectra and methods from a competing instrument.

Methods

Approximately 150 separate raw material methods, each with at least 10 separate Bruker spectra, were obtained from a nutraceutical company wishing to replace their Bruker NIR instrument with an Antaris II FT-NIR analyzer. The company wished to upgrade to a more reliable instrument that was easier for the operator to use. However, there was concern that their previously collected spectra and methods would be unusable with the Antaris system and that they would have to re-analyze their training set standards and collect and save the new spectra in the Antaris format. This would be a particularly daunting task, since there were over 4000 standards spectra collected over several years with the Bruker instrument.

TQ Analyst software is configured such that it can easily incorporate the Bruker spectra and use them for chemometric methods. TQ Analyst is able to load many different spectral data formats including Bruker, JCAMP, PCIR, CSV Text, PerkinElmer®, GRAMS/32, FOSS® and others. Figure 2 shows a screen capture of some of the file types that can be loaded directly into TQ Analyst without any further manipulation.

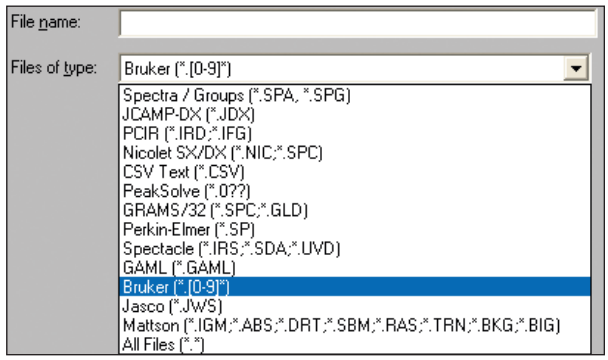

Figure 2: Screen capture showing the spectral formats that can be directly loaded into TQ Analyst software. Any of these file types can be used with TQ Analyst and subsequently used with the Antaris NIR analyzers.

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The loaded spectra were to be used for identification and quality confirmation of samples from over 150 raw materials used by the company. The company had used the Bruker instrument to generate match values between the incoming raw materials and accepted standards. The acceptance criterion was a match value of 95 or greater for each of the materials compared to their standards. Samples with match values less than 95 would be rejected while those greater than 95 would be accepted.

Chemometric methods were built in TQ Analyst using the same treatments as the Bruker methods. These methods used the Similarity Match algorithm with a Standard Normal Variate (SNV) pathlength type. The raw spectra were analyzed without any smoothing or derivative filters. The entire spectral region was included in the analysis from 9000 to 4000 wavenumbers, and no baseline treatment was performed.

Thermo Scientific RESULT software was used to interface with the Antaris instruments and collect, monitor and report results from the spectra. RESULT™ operates using workflows that allow a great deal of flexibility for the end user. Additionally, RESULT software is configurable so that the operator needs only click on one button to perform an analysis and report data. The ease of software usage was a key desire for the company for rapidly testing their incoming materials. Loading the over 4000 Bruker formatted spectra and creating the chemometric methods and workflows for the 150 individual materials required approximately three work days to accomplish.

As a validation of the success of the transfer to the Antaris system, new incoming materials were tested. The samples were directly analyzed using the SabIR™ probe on the Antaris system. An example result is shown in Figure 3. A vitamin B12 sample was analyzed and produced a match value of 99.91. This is a correct match for the material and demonstrates that spectra collected on the competing Bruker instrument can be successfully transferred to the Thermo Scientific Antaris analyzer without loss of method performance. Other tested materials also performed as expected.

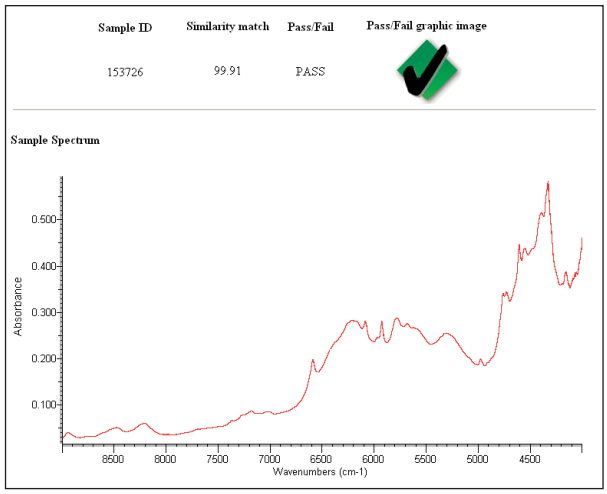

Figure 3: Part of a report showing the results of validating the Antaris NIR instrument using standard spectra obtained from a competing instrument. The standard spectra were used to develop a chemometric method and the validating spectrum was collected with the Antaris instrument. The Similarity Match value for this example was 99.91, showing exceptional transferability of previously collected Bruker spectra to the Antaris instrument.

Transferring previously built methods from one competing NIR instrument to another has previously been a roadblock for users wishing to upgrade or replace their existing systems. This is no longer a problem if the new system can automatically read in, measure against and create chemometric algorithms from several different spectral formats. The Antaris line of FT-NIR analyzers is capable of performing these functions successfully using Bruker spectra as well as other competing formats. The application described above demonstrates that the Antaris instruments can be seamlessly integrated into existing process systems using previously developed spectral training sets from other instrument brands.

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