CASE STUDY

Use Your Existing NIR Spectral Database on a New Platform

Introduction

Everyone knows the value of data these days. The value of NIR calibration data (spectral data, it's associated reference chemistry, that spans multiple crop years and production runs) is often a major inhibiting factor to upgrading old spectrometers or changing from an ill-suited vendor. This short case study demonstrates the ability to transfer calibration databases across an instrument/vendor platform to take advantage of the latest technology while working with a supplier who can meet the majority of food and agri analysis requirements.

Benefits of Upgrading to a New High Performance FT-NIR Analyzer

When comparing to old scanning monochromator and FT NIR instruments developed in the eighties or nineties, the FT 9700™ provides many advantages. The FT 9700™ is a recently launched high performance Fourier Transform NIR instrument based on the PerkinElmer DynaScan™ interferometer. The FT 9700 analyzes a sample in 30 seconds using a temperature stabilized InGaAs detector covering the 700 - 2500 nm, (ca 14700 - 4000 cm^{-1}) wavelength region. Samples are analyzed using an up-view NIR reflectance module using sapphire glass bottom cups which are rotated via a magnetic coupled spinner. The FT 9700 is a stand-alone analyzer driven by a Windows 10 computer, operated via a touch screen, using ResultsPlus user interface. Systems can be networked through the NetPlus™ cloud solution providing remote maintenance, administration, calibration support, and report generation. The modern FT-NIR technology platform provides better technical performance, improved calibration transferability, and allows for use of advanced calibration algorithms such as Artificial Neural Network (ANN) or PerkinElmer developed Hongis Regression™ (HR). There are also benefits associated with ease of use and flexibility with simple sample handling, integrated computer, and touch screen operation.

Figure 1: FT 9700 NIR Analyzer.

PerkinElmer®
For the Better

NIR Data Transfer from Old to New Unit

As mentioned, the ability to re-use historical NIR data collected on an old NIR platform as the basis of calibrations for the new platform has tremendous value. It avoids the need to essentially start from scratch and speeds dramatically speeds implementation of the newest technology.

Studies were performed transferring calibrations based on data collected both on dispersive scanning monochromator and non-PerkinElmer branded FT-NIR instruments to the new FT 9700 analyzer. Successful model transfers have been made from various NIR models, from various vendors, and include older and newer NIRS instruments. Sample matrices for these transfers include various grains, forages, other feed materials, dairy powders, fermentation slurries, and more.

The calibration transfer process involves analysis of the actual wavelength scale of the old NIR units, realignment of existing data, followed by development and implementation of new calibrations. The steps involved include:

1. Analyzing a set of common samples on the old NIR unit and FT 9700.
    a. Wavelength standard samples
    b. Followed by a set of 10-30 real samples (no reference chemistry values required)
2. Realignment of existing database with standardization to match FT 9700.
3. Development of new calibration models on the standardized data using Unscrambler X or PerkinElmer calibration tools.
4. Validation of new calibrations using a set of ~20 samples with reference values.

PerkinElmer has developed a spectra transfer tool including various tuning and data alignment functions to facilitate the process.

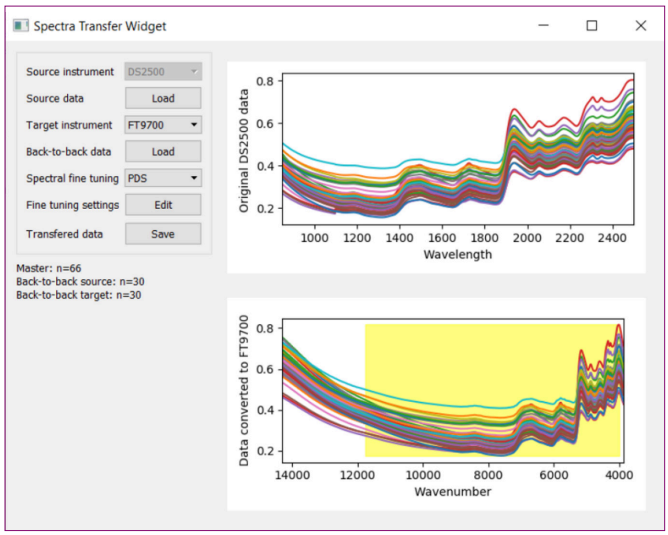

Figure 2: Spectra graph of data transferred from dispersive unit to new FT 9700 analyzer.

Results

Results from the studies showed that successful calibration transfer was possible and straightforward provided that the old platform covered a similar wavelength range as the FT 9700. The transfers worked whether the original data was collected on scanning monochromator instruments or other FT-NIR models. The prediction accuracy after transfer was nearly identical to performance on the older platforms. The final accuracy is limited by the original spectra quality, the data transfer process and reference value accuracy on the original data.

To further improve accuracy and fully benefit from the capabilities of the modern FT-NIR unit, it was beneficial to add additional samples collected on the FT 9700 to calibrations. Adding samples allowed for the benefits of improved spectra quality to be utilized and make the advanced calibration types such as ANN and HR perform at their best.

Table 1 shows calibration results on FT 9700 models on dry grass silage and forage calibration models from databases collected on dispersive scanning monochromator instruments. Transfer was done by Walloon Agricultural Research Centre, CRA-W, Gembloux Belgium. N = number of sample spectra in models, Range = lowest to highest value of included samples, RSQ = determination coefficient, SEC = Standard Error of Calibration, and SECV = Standard Error of Cross Validation estimated accuracy. Accuracy of transferred models was similar to the original performance.

Table 1: Calibration performance example, transferring dry grass and forage calibrations from scanning monochromator unit collected database to new FT-NIR technology based FT 9700.

Constituent	N	Range %	RSQ	SEC	SECV
Dry matter	2835	87.9 - 98.5	0,74	0,89	0,90
Protein	2497	0.9 - 29.8	0,97	0,82	0,83
Fiber	1926	11.5 - 40.7	0,93	1,28	1,31
Ash	2773	3.4 - 17.3	0,85	0,88	0,90
NDF	956	28.6 - 67.3	0,95	1,46	1,54
ADF	818	15.3 - 40.0	0,95	0,88	0,94
ADL	683	0.0 - 4.9	0,89	0,27	0,30
Dry Matter Digestibility	140	31.8 - 103.6	0,97	2,09	2,44
Total Soluble Sugar	821	0.0 - 33.3	0,98	0,93	1,02

* Results calculated on database that Includes only 20 additional calibration samples from FT 9700.

Conclusion and Importance of Planning Ahead

In summary, it was concluded that a transfer of existing NIR data can be readily and simply used to generate calibrations suitable to the FT 9700. The hundreds of samples in the historical databases were able to be used with good result. It is important to note however, that the calibration transfer requires the spectra be collected on a common set of samples on both the old instrument and the FT 9700. This procedure should take place before the older platform is inoperable and is still producing quality data.

PerkinElmer, Inc.
940 Winter Street
Waltham, MA 02451 USA
P: (800) 762-4000 or
(+1) 203-925-4602
www.perkinelmer.com

408794 PKI