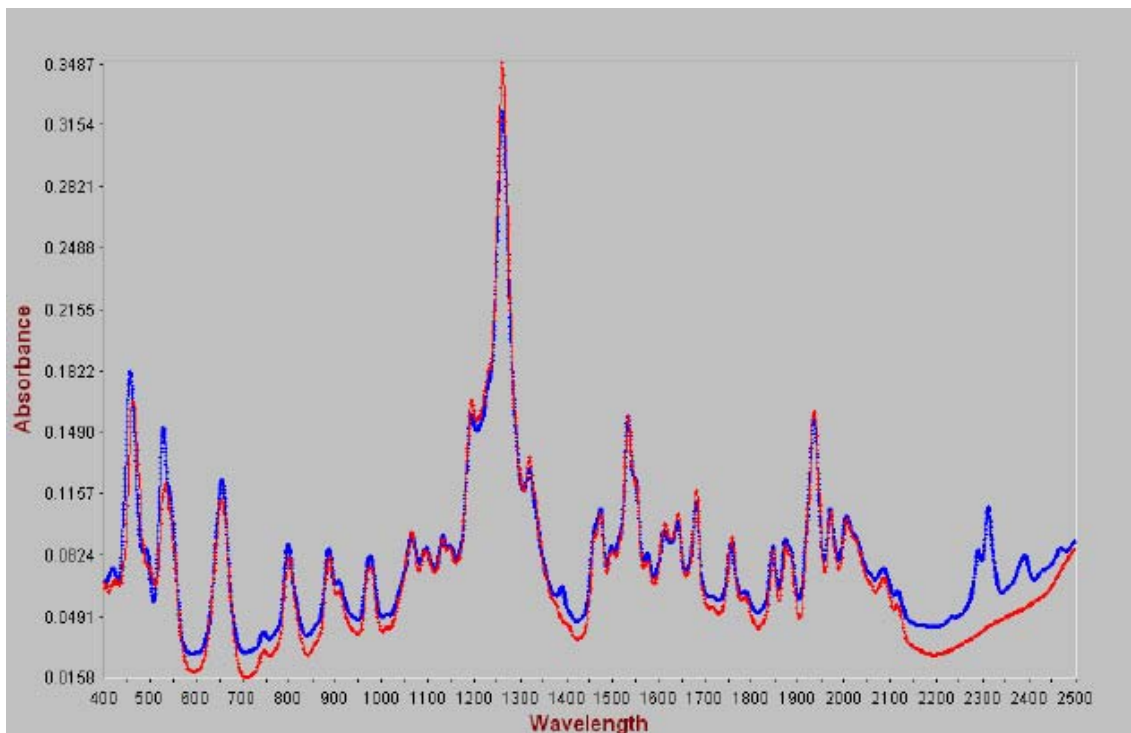


# Increase the accuracy of your NIR measurements with instrument calibration



This Application Note describes how the accuracy of your NIR measurements can be increased by using instrument calibration.

# Method description

## Introduction

Metrohm NIRSystems XDS instruments increase the accuracy of your NIR measurements and allow the seamless transfer of data, methods, and equations, in part through the use of certified external standards. These standards, traceable to the National Institute of Standards and Technology (NIST), and the Vision exclusive Instrument Calibration program, precisely align each instrument to the same wavelength and bandwidth accuracy. Instrument calibration is used on all NIRs XDS instruments (laboratory and process) performing reflectance, interactance immersion, and transmission measurements.

## Experimental

For reflectance and interactance immersion measurements, the external standard is scanned against the Reference Standardized internal reference of the instrument. The instrument wavelength response for each defined peak in the standard is measured and is then adjusted to that of the external standard. This assures accurate and reproducible wavelength registration between instruments. At the same time, bandwidth (band pass) is measured and is iteratively adjusted to an optimum value for the peaks being measured. The standard used for reflectance/interactance immersion measurement systems is traceable through a Master instrument, to NIST SRM 1920a (Fig. 1.). Talc has been added to provide additional measurements peaks above 2200 nm. This standard material is used for the XDS Rapid Content Analyzer series, XDS SmartProbe, XDS OptiProbe, and XDS Process instruments with interactance reflectance or immersion channels.

## Results and discussion

Instruments used to perform transmission measurements; XDS Liquid Analyzer, XDS OptiProbe transmission pair, and transmission pair XDS Process instruments, use "air" as the internal reference. An external standard of erbium oxide and samarium oxide glasses, and polystyrene, traceable to NIST SRM 2035 (Fig. 2.) through the use of a Master instrument, is scanned against the "air" reference. The instrument wavelength response for each of the defined peaks in the standard is measured. The instrument measurements are then adjusted to match those defined in the calibration standard.

The wavelength alignment established through Instrument Calibration, is applied to each subsequent sample scan collected on a calibrated instrument, yielding an accurate and reproducible spectrum.

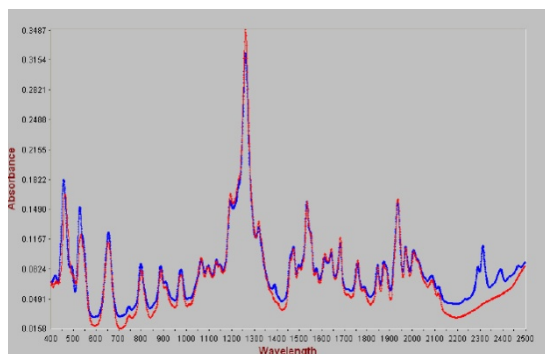


Fig. 1. SRM 1920a (red) vs XDS WSR Reflectance Standard (blue)

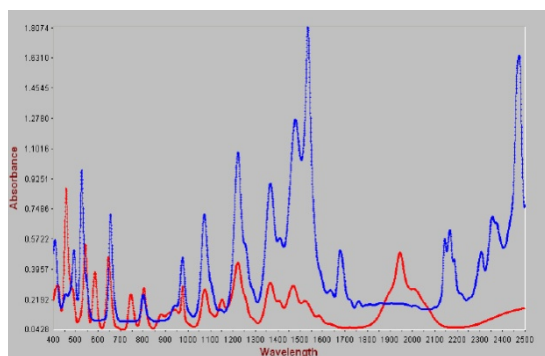


Fig. 2. SRM 2035 (red) vs XC-1300 Transmission Standard (blue)

Adjustments calculated during Instrument Calibration are stored on the motherboard of the instrument. The motherboard can store up to nine different adjustments. In XDS Laboratory instruments the sampling module serial number is linked to the adjustments of that particular sampling module. In XDS Process instruments it is the sample channel number that is linked to this information.

Results of the Vision Instrument Calibration program are more accurate and reproducible spectra. Multiple instruments of like configuration, will reliably report absorptions at the same location for the same sample making the transfer of data, methods, and calibration equations from instrument to instrument possible without the necessity of acquiring additional sample spectra or bias adjusting an equation.