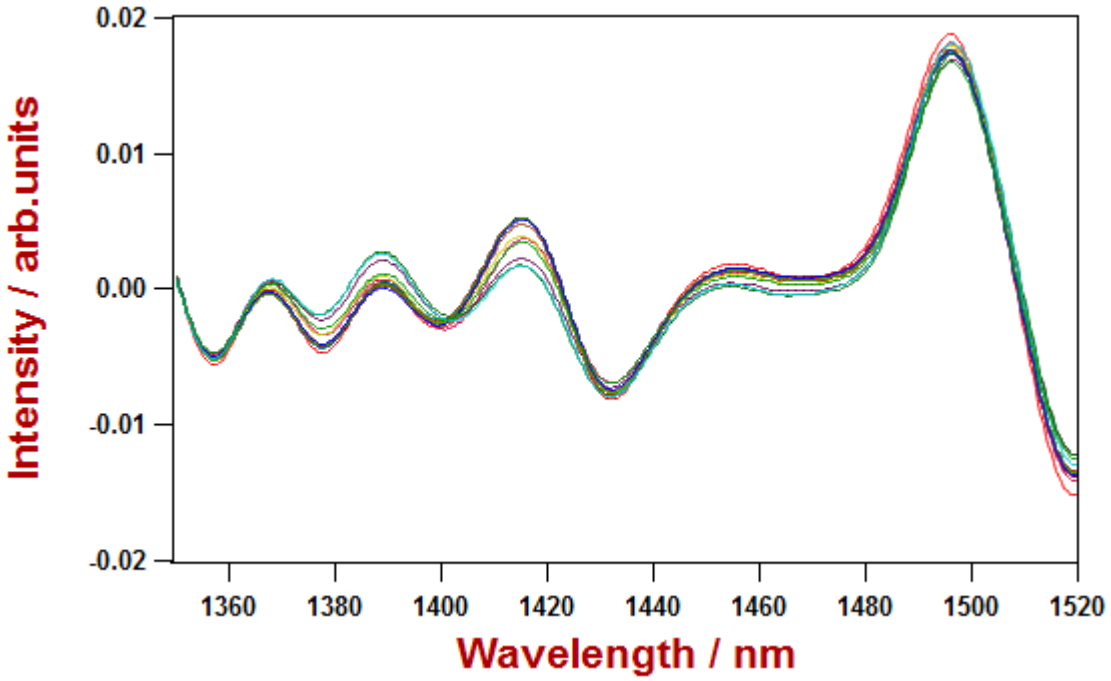
NIR Application Note AN-NIR–073

Water Activity measurement using Vis-NIR spectroscopy

Rapid determination within a few seconds



Water Activity is a critical parameter in determining the safety and quality of pharmaceutical products. Measuring Water Activity in the pharma environment is described in USP<1112>. It is used as an indicator for chemical hydrolysis and microbial growth. Water Activity is defined by the partial vapor pressure of water in a substance divided by the vapor pressure of water in standard state, expressed either as 0–100% equilibrium relative humidity (erh) or scaled to 0–1 water activity units (aw).

Dedicated instruments that measure Water Activity require up to 30 minutes for a single measurement. Using the XDS Masterlab Analyzer and Visible-Near Infrared Spectroscopy (Vis-NIRS), reliable results are now available in just a few seconds.

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Method description

Samples & Sample preparation

16 tablets samples were measured on an XDS Masterlab in transmission mode without any sample preparation.

Configuration

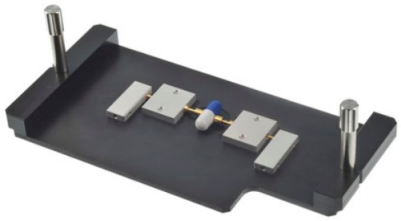
NIRS XDS Masterlab Analyzer	2.921.1310
NIRS FlexiTray	6.7410.110
Vision Air 2.0 Complete	6.6072.208
Novasina (Reference instrument)	LabMaster-aw neo

Experimental

Samples with varying (aw) values were positioned on the NIRS FlexiTray, which enables the measurement of tablets with a variety of different shapes and sizes. Data acquisition and method development was carried out with the software package Vision Air 2.0 Complete.

Figure 1. NIRS XDS Masterlab Analyzer used for spectral data acquisition.

Figure 2. NIRS FlexiTray used for tablet measurements.

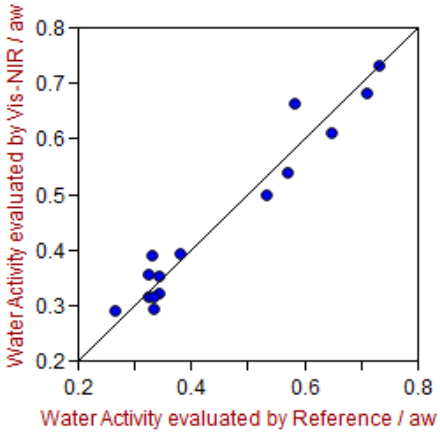


Method development

Spectral offset caused by particle size variation was excluded during the method development process by Standard Normal Variate pre-treatment. Internal cross-validation was applied on the data set to verify the performance of the PLS model. The model was optimized using the following parameters:

Regression model	PLS
Pretreatment	2nd Derivative + SNV
Validation	Cross validation

Results



Range	0.26–0.73 aw
No. of factors	2
R^2	0.95
SEC	0.039
SECV	0.041

This Application Note describes the determination of Water Activity in Acetaminophen tablets. Although only two factors were used to describe the model, satisfying values for Standard Error of Calibration (SEC) and Standard Error of Cross-validation (SECV) were achieved. Additionally, it should be pointed out, that similar Vis-NIR methods can be developed for other pharmaceutical products.

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