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PbS Detectors for Portable Near-Infrared Spectroscopy

Robert Lovrincic[1] , Michael Hanke[1], Daniel Kaelblein[1], and Wilfried Hermes[1]

[1]trinamiX GmbH, Industriestraße 35, 67063 Ludwigshafen am Rhein, Germany

Near-infrared spectroscopy (NIRS) has been a working horse in high-end analytics for decades. It covers the wavelength range from 0.9 to 2.5 µm (or 11000 to 4000 cm^{-1}). This spectral range allows to measure overtone (0.9 to 2 µm) and combination bands (2 to 2.5 µm) of molecular vibrations in organic materials. The overtone bands are 1st, 2nd, and 3rd order overtones:

	Range	Rel. intensities
1st overtones:	1700 - 2000 nm	1
2nd overtones:	1100 - 1700 nm	0.1
3rd overtones:	850 - 1100 nm	0.01

The combination bands carry very detailed information on the samples under test, e.g., the fatty acid composition in oilseeds or the amino acid profile in protein. Hence, laboratory spectrometers capable of measuring up to 2500 nm are widely used in agriculture for quality control and pricing.

Figure 1: trinamiX's mobile NIR spectrometer. The device is battery-powered, connects to smartphone or computer via *Bluetooth*®, and has an integrated lamp module for measurements in diffuse reflectance. The sensor unit consists of a 256-pixel PbS line array detector, fabricated in Ludwigshafen.

Fairly recently, NIR spectrometers have managed to break out of their well-controlled laboratory environment by becoming smaller, lighter, and scalable. In general, there are two approaches for handheld NIR spectrometers: (i) devices based on muti-pixel line array detectors, where the dispersive element splits the wavelength range in space and each pixel detects a certain wavelength; (ii) devices based on single-pixel detectors using an

interferometer with mechanically moving parts as dispersive element, such as MEMS Fourier-Transform (FT) or Fabry-Perot interferometers (FPI). Whereas the PbS detector technology is compatible with both approaches, InGaAs detectors are only used with option (ii) as extended InGaAs line array detectors are too scarce for widespread utilization in handheld devices. PbS is fabricated by chemical bath deposition, a process that is fast, scalable, and does not depend on lattice matched substrates.

trinamiX GmbH, a subsidiary of BASF SE based in Ludwigshafen, has introduced a portable NIR spectroscopy system to the market (see Fig. 1). This system consists of software, cloud-based NIR calibrations, and in-house developed spectrometer. The heart of the trinamiX spectrometer technology is its 256-pixel PbS line array detector, fabricated at cleanrooms in Ludwigshafen, Germany.

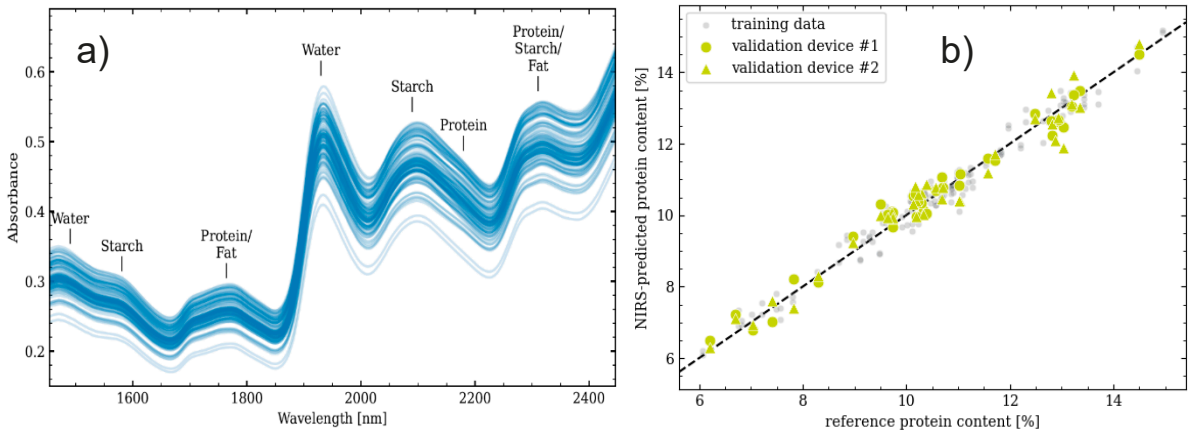

Figure 2: Portable NIRS of wheat. a) Spectra obtained from 108 wheat samples with the trinamiX handheld device. The chosen representation is absorbance (-log R) vs. wavelength in nm. To guide the eye, vertical black lines indicate the approximate positions and attributable species that are mainly responsible for the spectral appearance at those points. b) Reference crude protein content according to wet chemistry on the abscissa versus model predictions on the ordinate axis.

As an indication for the performance of the trinamiX NIRS system, Fig. 2 depicts the results of measurements on 108 wheat samples with known protein content and the subsequent data analysis. Fig. 2a) displays the raw NIR spectra of all samples measured with two trinamiX devices. Fig. 2b) shows how well the protein content of these samples can be predicted from their NIR spectra. The resulting standard error of prediction is 0.3 %, close to the accuracy that can be obtained by orders of magnitude larger and more expensive benchtop spectrometers.

Besides the classical NIRS application fields in the farm-to-fork environment, making the technology portable and affordable allows it to develop into markets far beyond the laboratory. Non-invasive biomarker monitoring is a huge trend in consumer electronics but still limited by the availability and affordability of detectors above 1000 nm detection range. PbS with its scalable and cost-effective production method (CBD) and broad wavelength detection range

enables consumers to track additional biomarker and therefore monitor their physical condition in real time. Seamless integration into consumer electronic devices, such as smartphones and watches, are in the focus.

Figure 3: Reference phone with an integrated NIR spectrometer module and a hydration application embedded in a health app.