Application Note AN-NIR-115

Determination of iodine value and fatty acid profile in palm oil by NIRS

NIR spectroscopy offers fast, reliable results without chemicals

Palm oil is currently the most widely produced and consumed vegetable oil in the world. It has many uses as a raw material for both food and non-food industries (e.g., personal care and cosmetic products). The marketability of crude palm oil (CPO) is determined by many quality indicators such as iodine value (IV) and fatty acid composition.

This Application Note demonstrates how near-infrared (NIR) spectroscopy is an ideal alternative to traditional analysis techniques like gas chromatography. NIRS can provide results in less than one minute without requiring any sample preparation or chemical reagents, increasing the productivity and reducing costs.

EXPERIMENTAL EQUIPMENT

20 samples of crude palm oil (CPO) with varying iodine values (IV) were kept in a water bath at 60 °C for at least 30 minutes to liquify them. These samples were then measured at 60 °C on a Metrohm NIRS DS2500 Liquid Analyzer (Figure 1) in transmission mode over the full wavelength range (400–2500 nm) using 8 mm disposable vials. Data acquisition and prediction model development was performed with the Vision Air complete software package from Metrohm.

The reference method of gas chromatography (GC) was used after the methyl esterification of the fatty acids. The concentration of the fatty acids was derived from corresponding peak area. The iodine values were calculated from the combined concentrations of oleic acid and palmitic acid.

Table 1. Hardware and software equipment overview.

Equipment	Article number
DS2500 Liquid Analyzer	2.929.0010
DS2500 Holder 8 mm vials	6.7492.020
Vision Air 2.0 Complete	6.6072.208

Figure 1. Metrohm NIRS DS2500 Liquid Analyzer used for the determination of iodine value and fatty acid composition in crude palm oil samples.

RESULT

The measured Vis-NIR spectra (Figure 2) were used to create a prediction model for quantification of iodine value (IV), linoleic acid (18:2), oleic acid (18:1), and palmitic acid (16:0) in CPO. The quality of the prediction models was evaluated using correlation diagrams which display a high correlation between the Vis-NIR prediction and the GC results. The respective figures of merit (FOM) display the expected precision and confirm the feasibility during routine analysis (Figures 3–6)

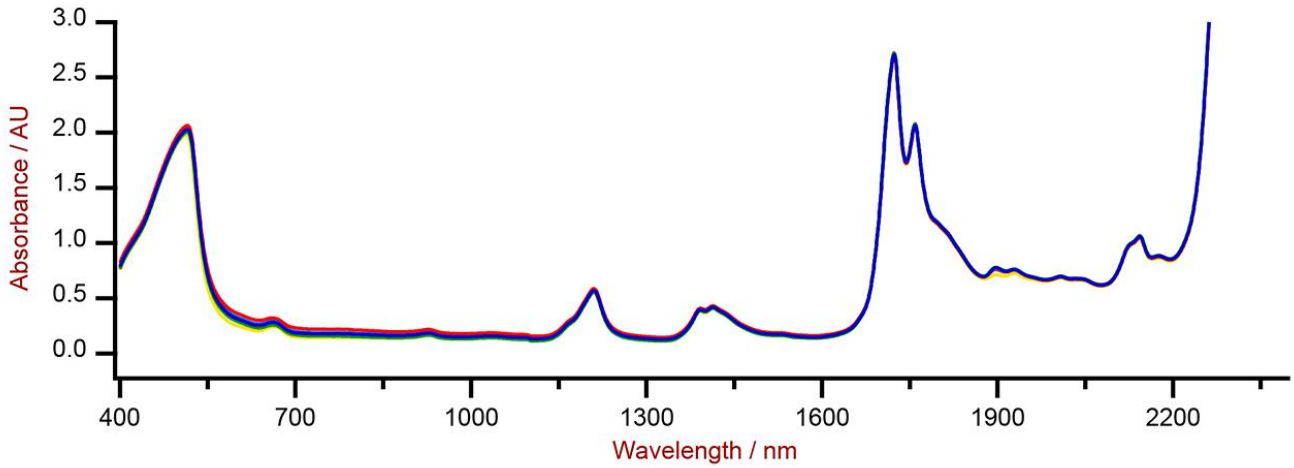

Figure 2. Selection of Vis-NIR spectra of crude palm oil samples analyzed on a Metrohm NIRS DS2500 Liquid Analyzer with 8 mm vials.

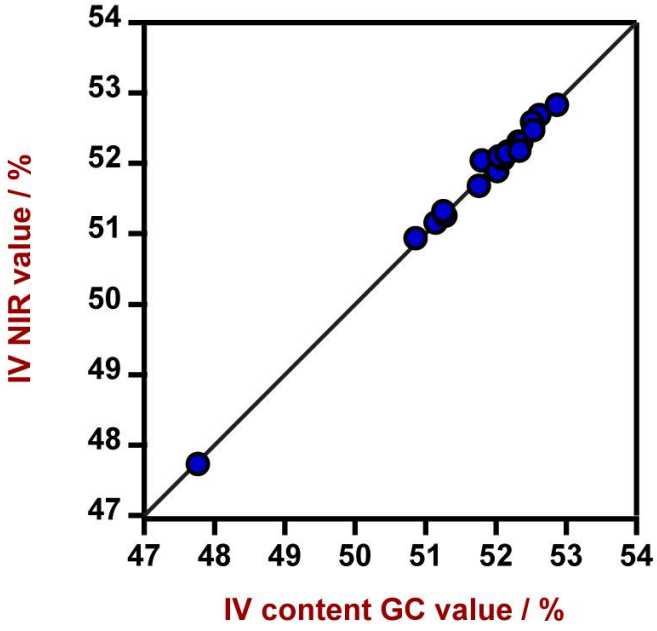

Figure 3. Correlation diagram and the respective figures of merit for the prediction of iodine value in CPO using a DS2500 Liquid Analyzer. The lab value was measured using GC.

Figures of Merit	Value
R^2	0.994
Standard Error of Calibration	0.10%
Standard Error of Cross-Validation	0.11%

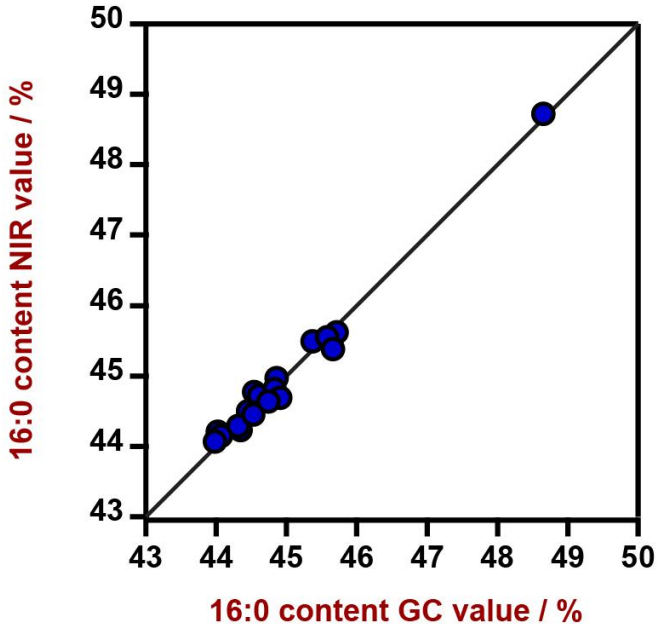

Figure 4. Correlation diagram and the respective figures of merit for the prediction of relative palmitic acid content in CPO using a DS2500 Liquid Analyzer. The lab value was measured using GC.

Figures of Merit	Value
R^2	0.9836
Standard Error of Calibration	0.15%
Standard Error of Cross-Validation	0.15%

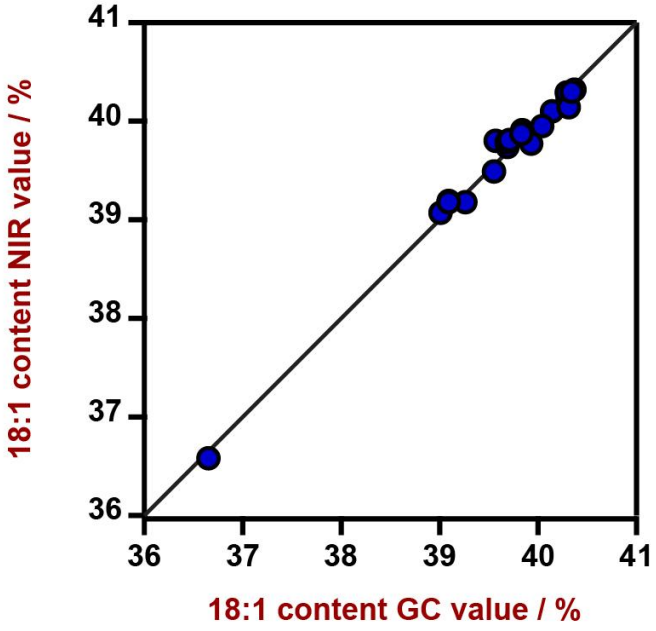

Figure 5. Correlation diagram and the respective figures of merit for the prediction of relative oleic acid content in CPO using a DS2500 Liquid Analyzer. The lab value was measured using GC.

Figures of Merit	Value
R^2	0.9851
Standard Error of Calibration	0.11%
Standard Error of Cross-Validation	0.12%

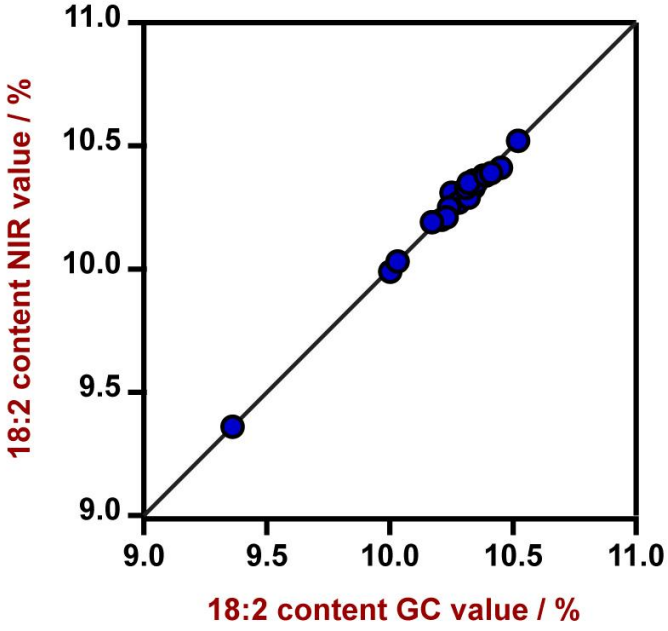

Figure 6. Correlation diagram and the respective figures of merit for the prediction of relative linoleic acid content in CPO using a DS2500 Liquid Analyzer. The lab value was measured using GC.

Figures of Merit	Value
R^2	0.9916
Standard Error of Calibration	0.03%
Standard Error of Cross-Validation	0.04%

CONCLUSION

This Application Note displays the benefits of using the Metrohm NIRS DS2500 Liquid Analyzer for routine quality control analysis of crude palm oil. Compared to conventional methods, the determination with Vis-NIR spectroscopy does not need any sample preparation. Consequently, this leads to a reduction of workload (Table 2) and operating costs.

Table 2. Time to result overview for the determination of iodine value and fatty acid composition in palm oil by standard methods.

Parameter	Method	Time to result
Iodine value, Fatty acid composition	Gas Chromatography	40 min sample preparation (methyl esterification + sample preparation) + 20 min GC

Internal reference: AW NIR CH-0066-042023

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CONFIGURATION

DS2500 Liquid Analyzer

Robust near-infrared spectroscopy for quality control, not only in laboratories but also in production environments.

The DS2500 Liquid Analyzer is the tried and tested, flexible solution for routine analysis of liquids along the entire production chain. Its robust design makes the DS2500 Liquid Analyzer resistant to dust, moisture and vibrations, which means that it is eminently suited for use in harsh production environments.

The DS2500 Liquid Analyzer covers the full spectral range from 400 to 2500 nm, heats samples up to 80°C and is compatible with various disposable vials and quartz cuvettes. The DS2500 Liquid Analyzer is thus adaptable to your individual sample requirements and helps you obtain accurate and reproducible results in less than one minute. The integrated sample holder detection and the self-explanatory Vision Air Software also ensure simple and safe operation by the user.

In the case of larger-sized sample quantities, productivity can be considerably increased by using a flow-through cell in combination with a Metrohm sample robot.