

Comparison of the Iodine Value in Palm Oil With Two NIRS Systems

Accurate and precise determination in less than one minute

Summary

Determination of key quality parameters of palm oil, such as the iodine value (IV), are typically performed using time consuming and costly wet chemical methods.

This application note demonstrates that the Metrohm DS2500 Liquid Analyzer operating in the visible and near infrared spectral region (Vis-NIR) provides a **cost-efficient and fast solution** for the determination of these quality control parameters in palm oil. With **no sample preparation or chemicals needed**, Vis-NIR spectroscopy allows for the analysis of palm oil in **less than a minute** and **can be used by anyone**.

Experimental equipment



Figure 1. DS2500 Liquid Analyzer and a palm oil sample present in an 8 mm disposable vial.

Palm oil samples which have been refined, bleached, and deodorized (RBD palm oil) were measured in transmission mode with a DS2500 Liquid Analyzer over the full wavelength range (400–2500 nm). The highly viscous samples were liquefied using the Vial Heater. Reproducible spectrum acquisition was achieved using the built-in temperature control (at 60 °C) of the DS2500 Liquid Analyzer. For convenience, disposable vials with a path length of 8 mm were used, which made cleaning of the sample vessels unnecessary. The Metrohm software package Vision Air Complete was used for all data acquisition and prediction model development. The measurements were also conducted with a XDS RapidLiquid Analyzer to compare the analytical performance of both instruments.

Table 1. Hardware and software equipment overview

Equipment	Metrohm number
DS2500 Liquid Analyzer	2.929.0010
XDS RapidLiquid Analyzer	2.921.1410
Vial Heater	2.921.9010
Disposable vials, 8 mm diameter, transmission	6.7402.000
Vision Air 2.0 Complete	6.6072.208



2.929.0010 - 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.



2.921.1410 - NIRS XDS RapidLiquid Analyzer

Rapid, precise analyses of liquids and suspensions of all types. The NIRS XDS RapidLiquid Analyzer enables rapid, precise analyses of liquid formulations and substances. Precise measurement results at the push of a button make the NIRS XDS RapidLiquid Analyzer an equally reliable and simple solution for quality monitoring in laboratories and processes. The samples are transferred to quartz cuvettes designed for multiple use or disposable glass vials; a tempered sample compartment ensures reproducible analysis conditions and thus accurate measurement results.



2.921.9010 - NIRS XDS Vial Heater including 250 vials

The NIRS XDS Vial Heater Module enables analyses of samples at temperatures of up to 200 °C. The Vial Heater is used together with an NIRS XDS Transmission OptiProbe Analyzer. The Transmission Probes are fastened across from one another in the NIRS XDS Vial Heater. The NIRS disposable glass vials with 4 mm or 8 mm diameter are positioned between the two optical fibers in the heating block of the NIRS XDS Vial Heater. The temperature of the heating block can be regulated up to 200 °C. The sample and the optical fiber can be protected against ambient light with a lid. The spectral measurement of the sample takes place in transmission.



6.7402.000 - Disposable vials, 8 mm diameter, transmission

250 lockable disposable glass vials (borosilicate) with a diameter of 8 mm for analyses of liquid samples in transmission mode. Suitable for the following Analyzers: NIRS XDS RapidLiquid Analyzer NIRS XDS VialHeater + NIRS XDS Transmission OptiProbe Analyzer



6.6072.208 - Vision Air 2.0 Complete

Vision Air - Universal spectroscopy software. Vision Air Complete is a modern and simple-to-operate software solution for use in a regulated environment. Overview of the advantages of Vision Air: Individual software applications with adapted user interfaces ensure intuitive and simple operation; Simple creation and maintenance of operating procedures; SQL database for secure and simple data management; The Vision Air Complete version (66072208) includes all applications for quality assurance using Vis-NIR spectroscopy: Application for instrument and data management; Application for method development; Application for routine analysis; Additional Vision Air Complete solutions: 66072207 (Vision Air Network Complete); 66072209 (Vision Air Pharma Complete); 66072210 (Vision Air Pharma Network Complete);

Results

The obtained Vis-NIR spectra (**Figure 2**) were used to create prediction models for quantification of the individual key parameters. The quality of the prediction models was evaluated using correlation diagrams, which display the correlation between VisNIR prediction and primary method values. The respective figures of merit (FOM) display the expected precision of a prediction during routine analysis.

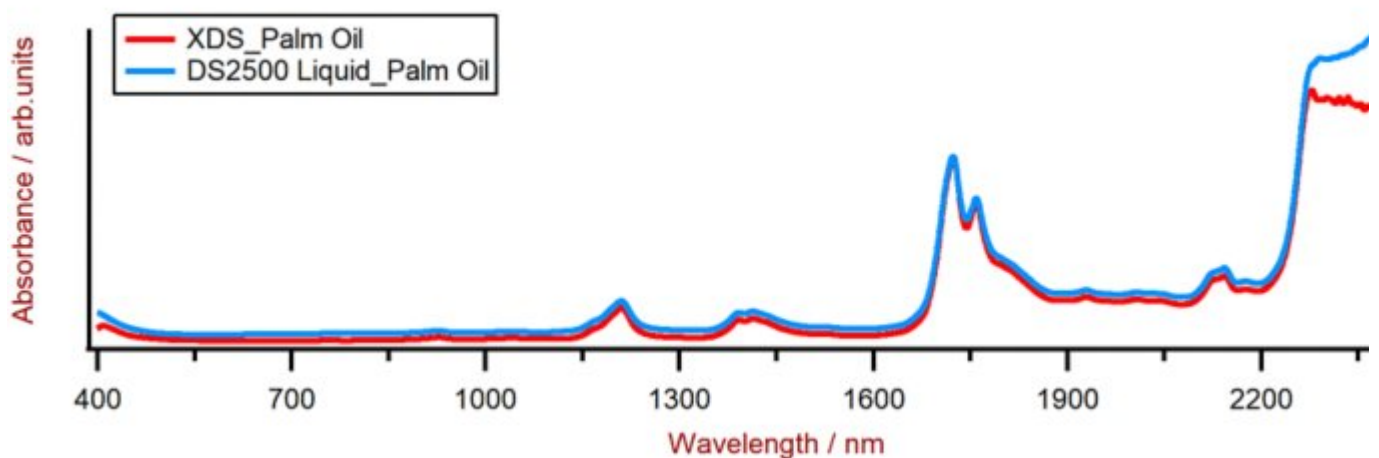


Figure 2. Vis-NIR spectra of palm oil obtained using a DS2500 Liquid Analyzer / XDS RLA and 8 mm disposable vials.

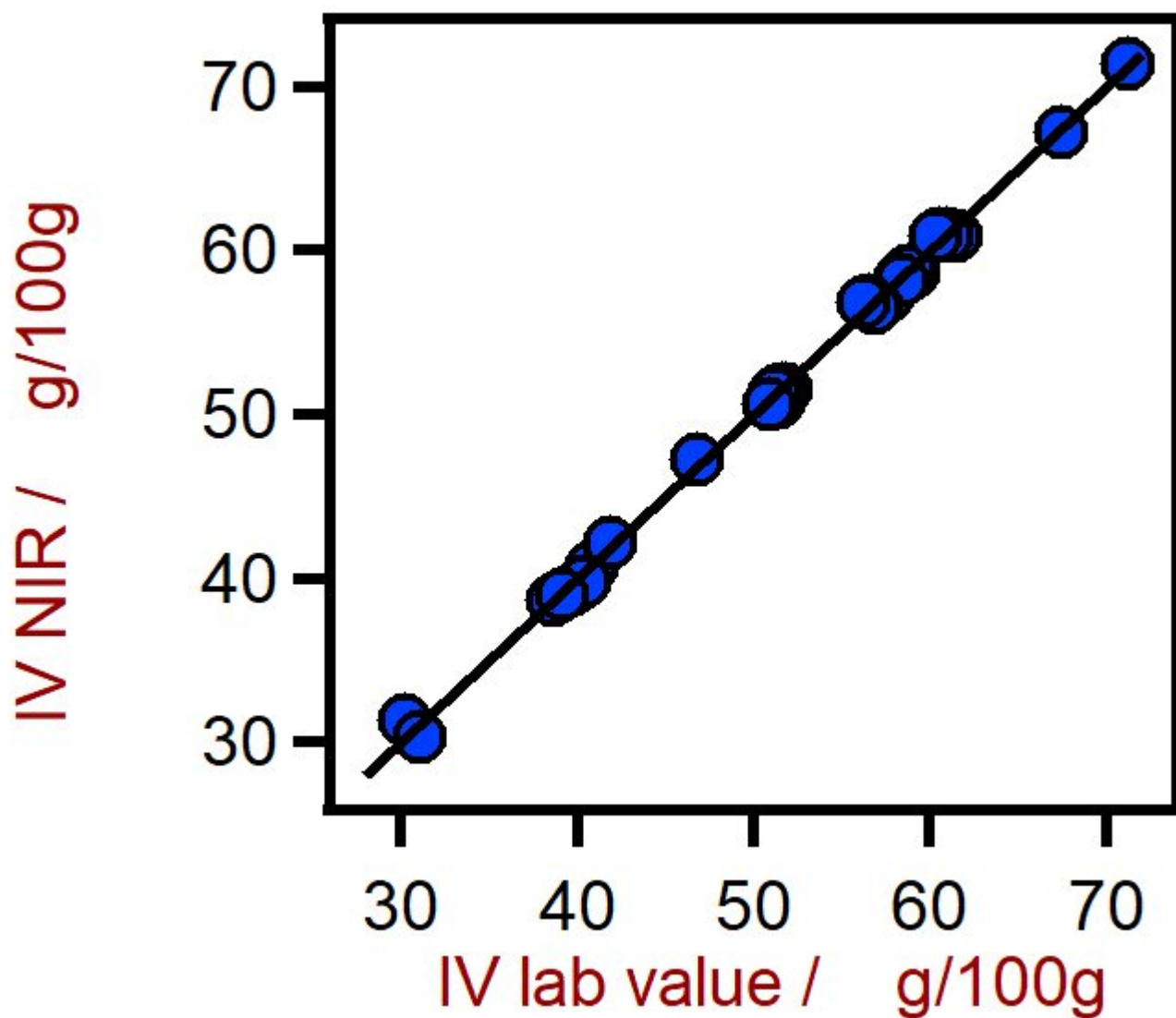


Figure 3. Correlation diagram for the prediction of the iodine value (IV) in palm oil using a DS2500 Liquid Analyzer. The iodine lab value was evaluated using titration.

Table 2. Figures of merit for the prediction of the iodine value (IV) in palm oil using a DS2500 Liquid Analyzer.

Figures of merit	Value
R^2	0.998
Standard error of calibration	0.49 g/100g
Standard error of cross-validation	0.49 g/100g

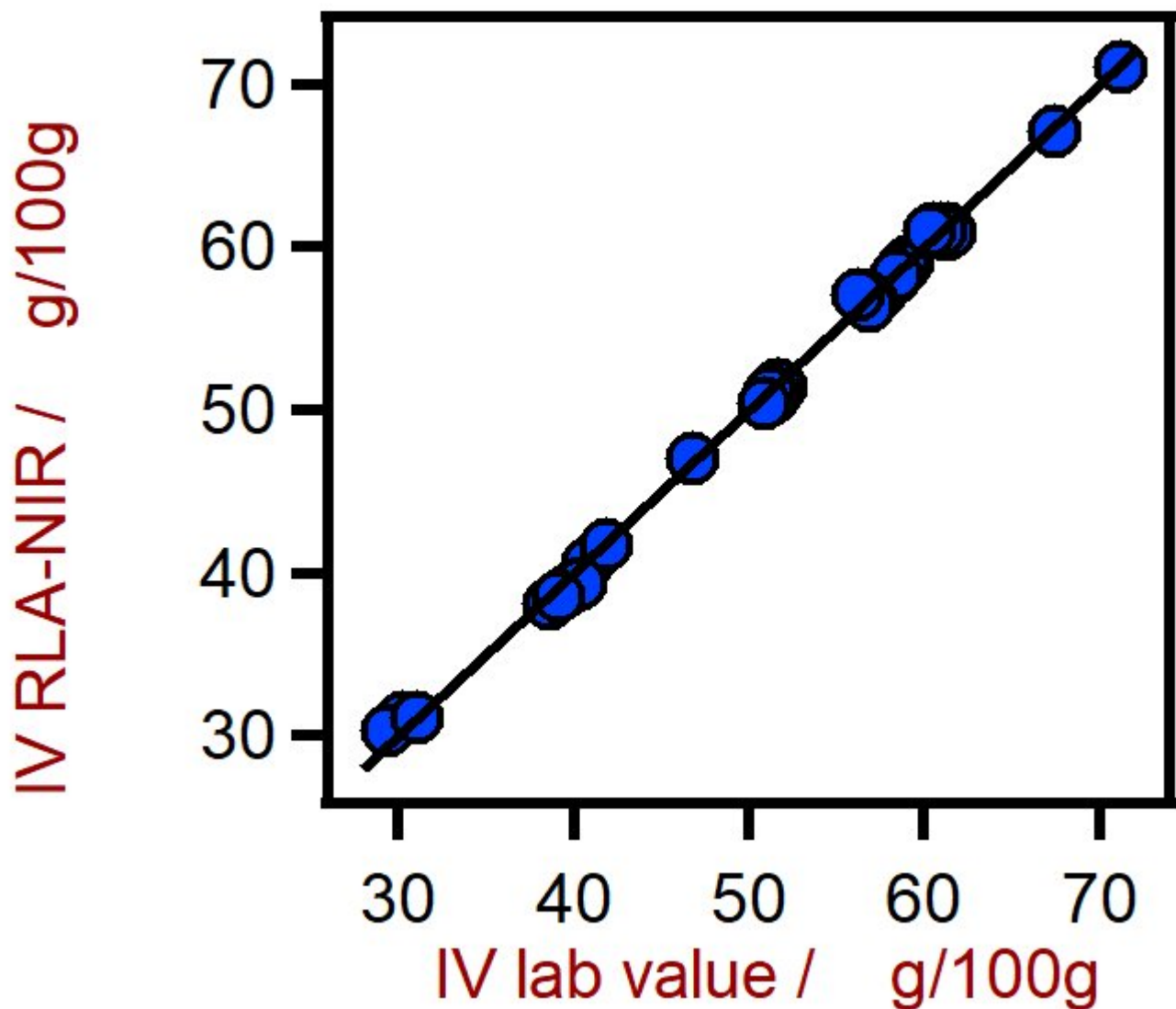


Figure 4. Correlation diagram for the prediction of the iodine value (IV) in palm oil using a XDS RapidLiquid Analyzer. The iodine lab value was evaluated using titration.

Table 2. Figures of merit for the prediction of the iodine value (IV) in palm oil using a XDS RapidLiquid Analyzer.

Figures of merit	Value
R ²	0.998
Standard error of calibration	0.55 g/100g
Standard error of cross-validation	0.54 g/100g

Conclusion

This application note demonstrates the feasibility of the DS2500 Liquid Analyzer for the analysis of the iodine value in palm oil. Compared to the older generation XDS RLA, the observed accuracy is slightly better, yet within statistical relevance.

In a previous application note (AN-NIR-044), the XDS RLA was used to determine **additional quality parameters in palm oil**, including **free fatty acids, moisture content**, and the **deterioration of bleachability index (DOBI)**. Due to the demonstrated comparability between the DS2500 Liquid Analyzer and XDS RapidLiquid Analyzer, it is clear that those parameters can also be determined with the DS2500 Liquid Analyzer.

The main advantages of NIR spectroscopy over wet chemical methods are that, **running costs are significantly lower and time-to-result is significantly reduced**.

AN-NIR-044 - Quality Control of Palm Oil – Environmentally friendly determination of FFA content, iodine value, moisture, DOBI, and carotene content

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