



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**)

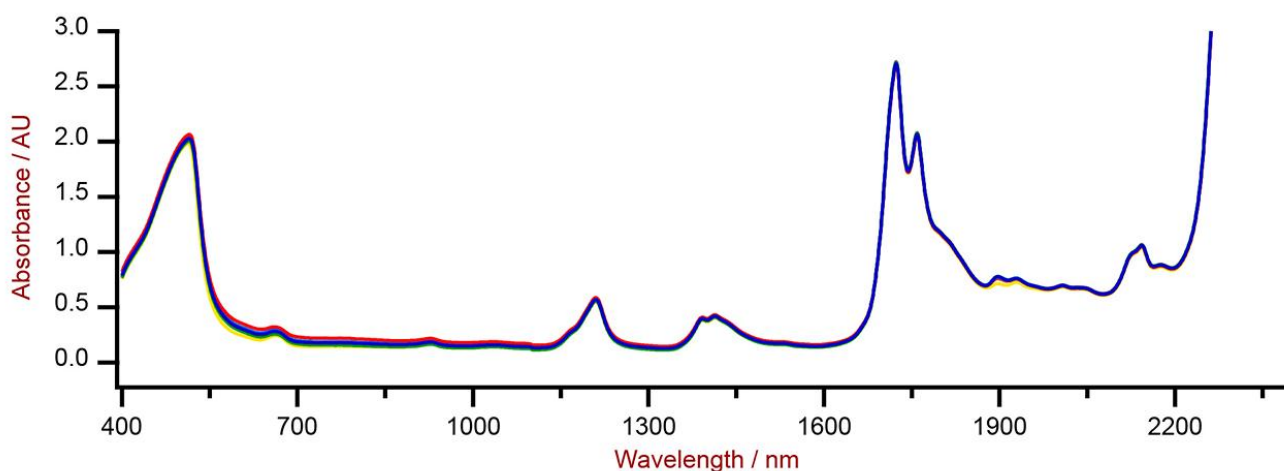


Figure 2. Selection of Vis-NIR spectra of crude palm oil samples analyzed on a Metrohm NIRS DS2500 Liquid Analyzer with 8 mm vials.

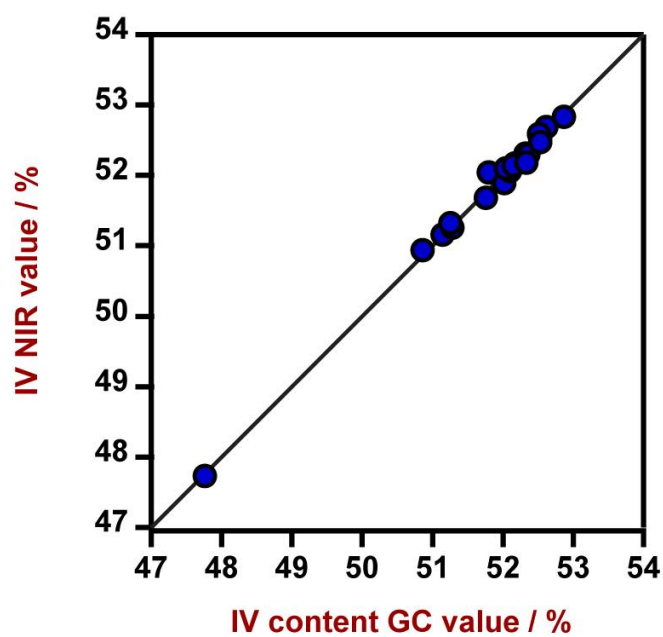


Figure 3. Correlation diagram and the respective figures of merit for the prediction of iodine value in CPO using a DS2500 Liquid Analyzer. The lab value was measured using GC.

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

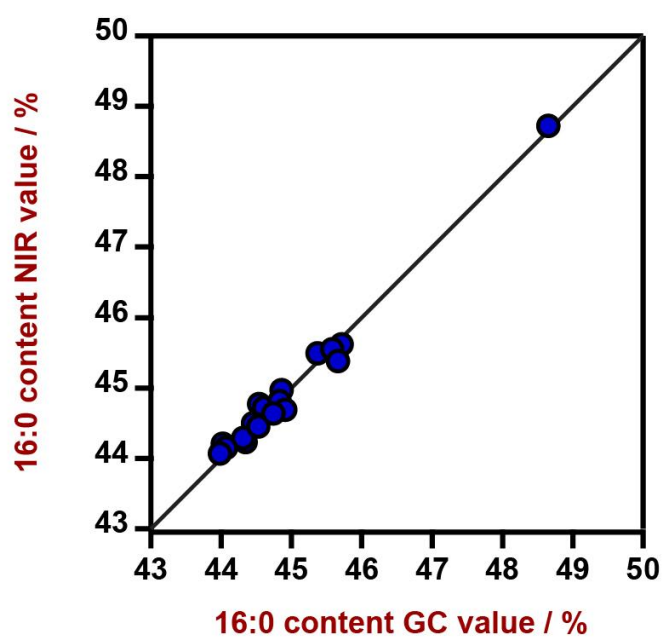


Figure 4. Correlation diagram and the respective figures of merit for the prediction of relative palmitic acid content in CPO using a DS2500 Liquid Analyzer. The lab value was measured using GC.

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

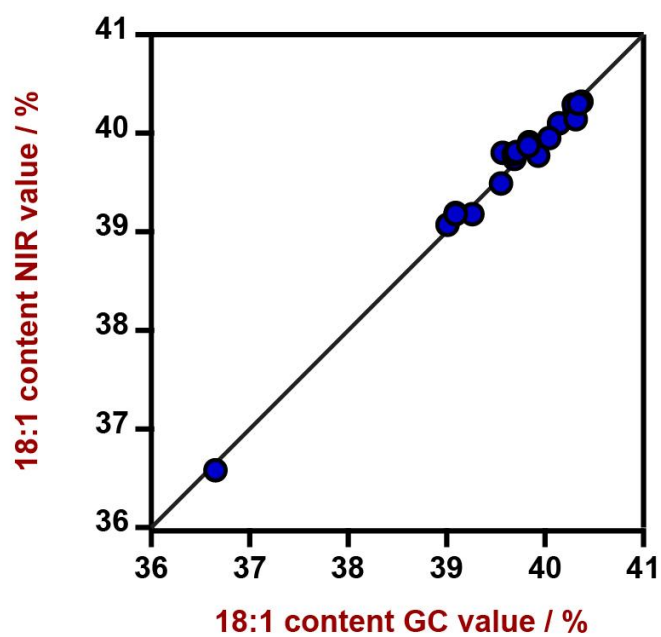


Figure 5. Correlation diagram and the respective figures of merit for the prediction of relative oleic acid content in CPO using a DS2500 Liquid Analyzer. The lab value was measured using GC.

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

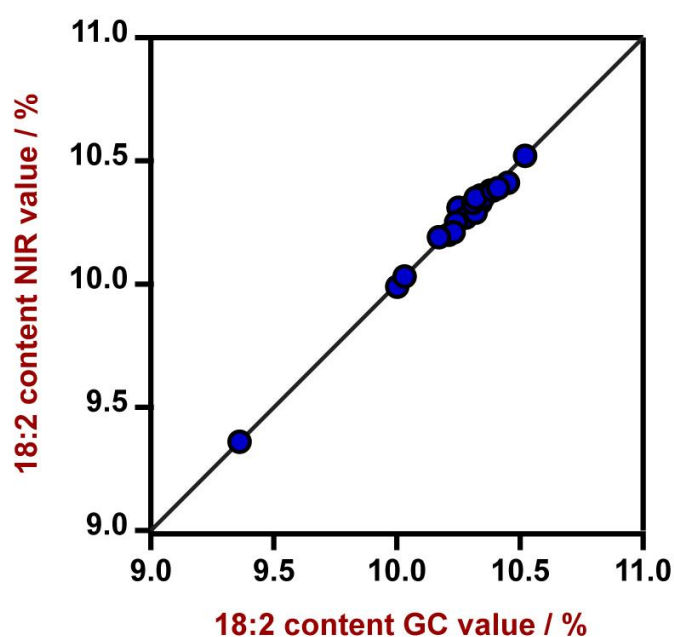


Figure 6. Correlation diagram and the respective figures of merit for the prediction of relative linoleic acid content in CPO using a DS2500 Liquid Analyzer. The lab value was measured using GC.

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

ラボおよび生産環境における品質管理用の堅牢な近赤外分光法。

NIRS DS2500 Liquid Analyzerは、生産チェーン全体に沿った液体のルーチン分析に実績のあるフレキシブルなソリューションです。頑丈な仕様により、NIRS DS2500 Liquid Analyzerは粉塵、湿気、および振動に強い為、過酷な生産環境での使用に理想的です。

DS2500 Liquid Analyzer は400~2500 nmのスペクトル範囲全体をカバーし、サンプルを80° Cまで加熱し、様々な使い捨てハイアルやクォーツキュベットとの互換性を有します。このようにして個々のサンプル要件に対応し得るDS2500 Liquid Analyzerは、1分未満で正確かつ再現性ある結果を得られるようサポートします。さらに一体型のサンプルホルダー検出、および説明不要のVision Airソフトウェアを用いることで、ユーザーが簡単かつ安全に操作できることが保証されます。

サンプル量が多い場合、Metrohmサンプルロケットと組み合わされたフローセルの導入によって、生産性を著しく向上させることができます。