

Application Note AN-NIR-103

Quality control of chocolate bars by near-infrared spectroscopy

Simplified determination of calories, fat, saturated fat, carbohydrates, sugar, and protein

The production of foods requires strict quality control to guarantee their quality and protect the consumer. Confectionary products like chocolate are held to such standards—their final product control is mandatory to fulfill regulations and to ensure a consistent quality. The latter is especially critical for indulgent products.

Near-infrared spectroscopy (NIRS) is a fast, chemical-free analysis method for the determination of many important quality control parameters of chocolate bars without requiring any sample preparation. The NIRS solution is easy to use and can be utilized either atline or in a quality control laboratory.

EXPERIMENTAL EQUIPMENT

18 chocolate bars from different suppliers were analyzed on a Metrohm DS2500 Solid Analyzer (Figure 1). Chocolate bars were positioned directly onto the sample window and were measured in diffuse reflection mode. To include sample variety, each chocolate bar was measured at three different locations and the averaged spectra were used for model development. Data acquisition and prediction model development were performed with the software package Vision Air Complete (Table 1).

Table 1. Hardware and software equipment overview.

Equipment	Article number
DS2500 Solid Analyzer	2.922.0010
Vision Air 2.0 Complete	6.6072.208



Figure 1. Metrohm NIRS DS2500 Solid Analyzer with a chocolate bar covering the sample window.

RESULT

The obtained Vis-NIR spectra (Figure 2) were used to create prediction models for the different reference parameters. A leave one out validation procedure was used. Correlation diagrams which display the relation between the Vis-NIR prediction and the reference values are shown in Figures 3–8 together with the respective figures of merit (FOM).

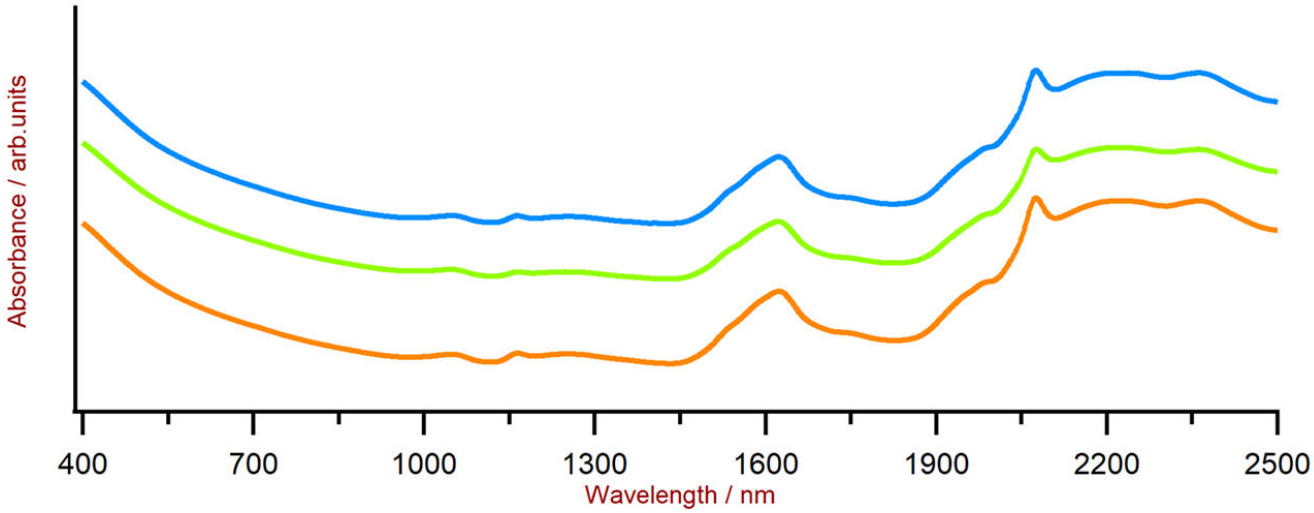
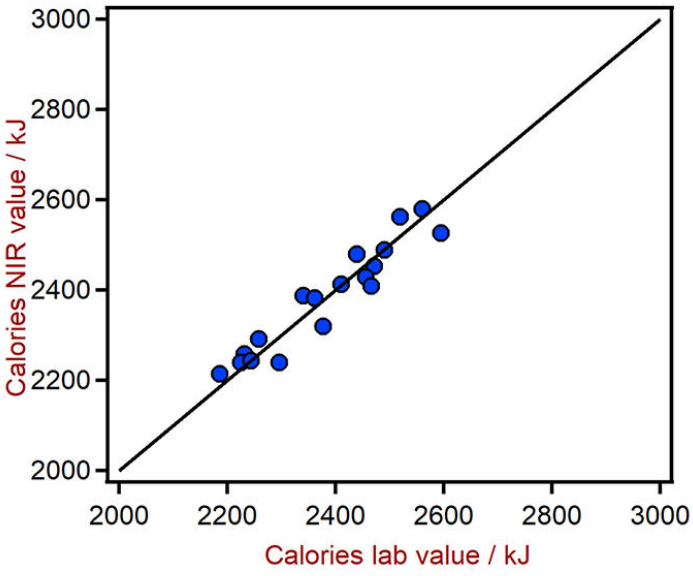


Figure 2. Selection of Vis-NIR spectra of chocolate bar samples. Data was obtained with a DS2500 Solid Analyzer. A spectra offset was applied for visualization purposes.

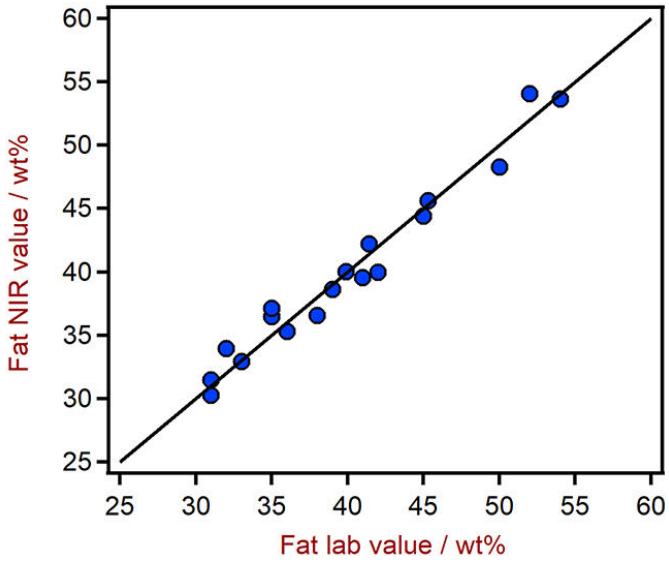
RESULT CALORIES IN CHOCOLATE BARS



Figures of Merit	Value
R^2	0.90
Standard Error of Calibration	43.5 kJ
Standard Error of Cross-Validation	50.5 kJ

Figure 3. Correlation diagram and the respective FOMs for the prediction of calories in chocolate bars using a DS2500 Solid Analyzer.

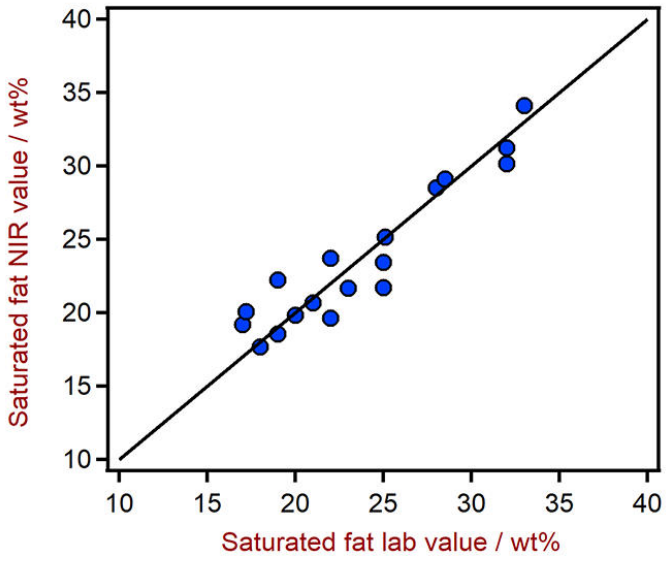
RESULT FAT IN CHOCOLATE BARS



Figures of Merit	Value
R^2	0.96
Standard Error of Calibration	1.38 wt%
Standard Error of Cross-Validation	1.73 wt%

Figure 4. Correlation diagram and the respective FOMs for the prediction of fat in chocolate bars using a DS2500 Solid Analyzer.

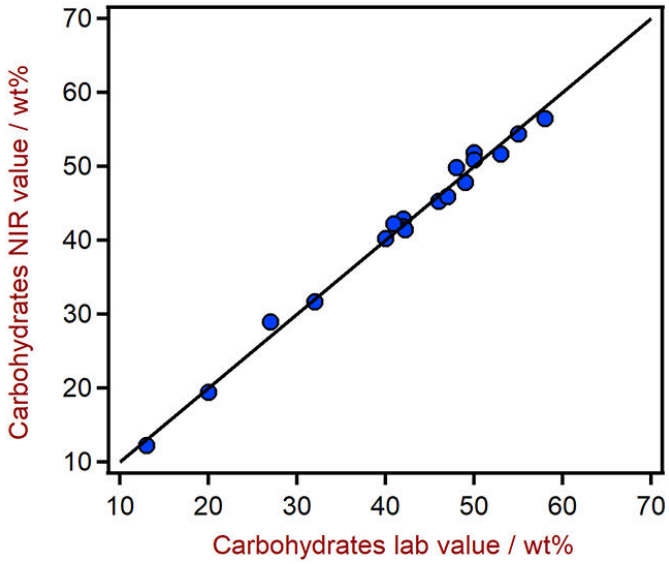
RESULT SATURATED FAT IN CHOCOLATE BARS



Figures of Merit	Value
R^2	0.88
Standard Error of Calibration	1.89 wt%
Standard Error of Cross-Validation	2.68 wt%

Figure 5. Correlation diagram and the respective FOMs for the prediction of saturated fat in chocolate bars using a DS2500 Solid Analyzer.

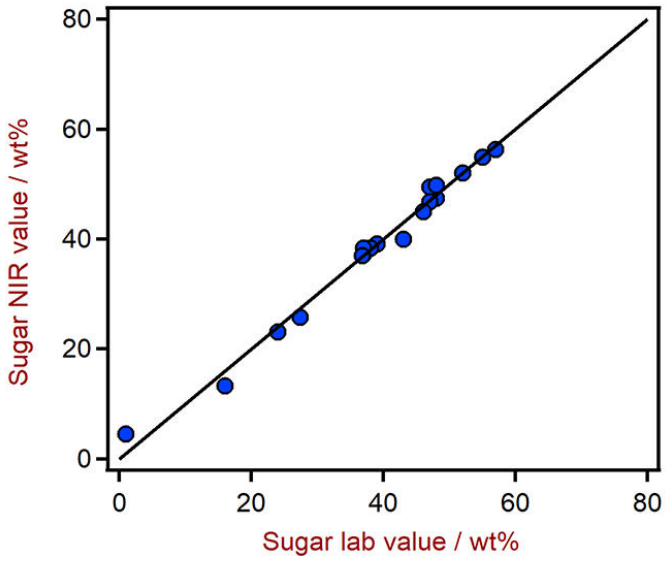
RESULT CARBOHYDRATES IN CHOCOLATE BARS



Figures of Merit	Value
R^2	0.99
Standard Error of Calibration	1.23 wt%
Standard Error of Cross-Validation	1.33 wt%

Figure 6. Correlation diagram and the respective FOMs for the prediction of carbohydrates in chocolate bars using a DS2500 Solid Analyzer.

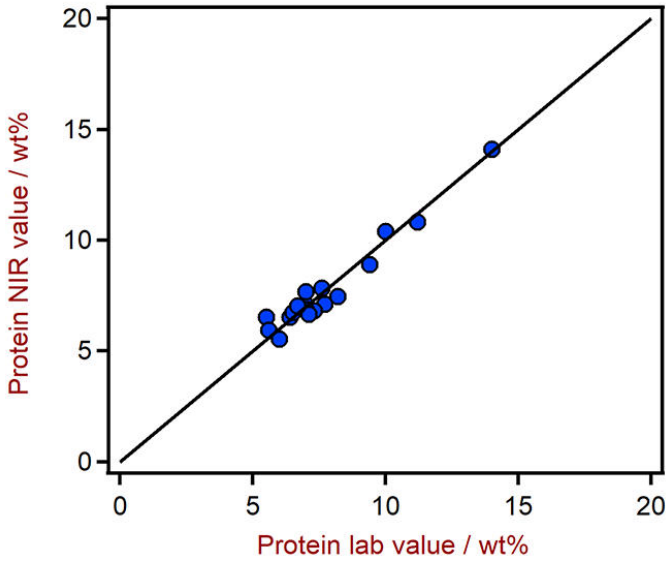
RESULT SUGAR IN CHOCOLATE BARS



Figures of Merit	Value
R^2	0.99
Standard Error of Calibration	1.81 wt%
Standard Error of Cross-Validation	2.56 wt%

Figure 7. Correlation diagram and the respective FOMs for the prediction of sugar in chocolate bars using a DS2500 Solid Analyzer.

RESULT PROTEIN IN CHOCOLATE BARS



Figures of Merit	Value
R^2	0.95
Standard Error of Calibration	0.53 wt%
Standard Error of Cross-Validation	0.65 wt%

Figure 8. Correlation diagram and the respective FOMs for the prediction of protein in chocolate bars using a DS2500 Solid Analyzer.

CONCLUSION

This Application Note shows the feasibility of near-infrared spectroscopy for the analysis of calories, fat, saturated fat, carbohydrates, sugar, and protein content in chocolate bars. Compared to the conventional analysis techniques used to determine all of these quality parameters, NIRS saves a considerable amount of time and costs. With NIRS, these analyses can be conducted without using any chemical reagents, giving users reliable results in seconds.

Internal reference: AW NIR CH-0067-042023

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CONFIGURATION



DS2500 Solid Analyzer

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

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

The DS2500 covers the full spectral range from 400 to 2500 nm and delivers accurate, reproducible results in less than one minute. The DS2500 Analyzer meets the demands of the pharmaceutical industry and supports users in their day-to-day routine tasks thanks to its simple operation.

Thanks to accessories tailored perfectly to the instrument, optimum results are achieved with every sample type, no matter how challenging it is, e.g. coarse-grained solids such as granulates or semi-solid samples such as creams. The MultiSample Cup can help improve productivity when measuring solids, as it enables automated measurements of series containing up to 9 samples.