



Application Note AN-NIR-103

利用近红外光谱对巧克力棒进行质量控制

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.

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).

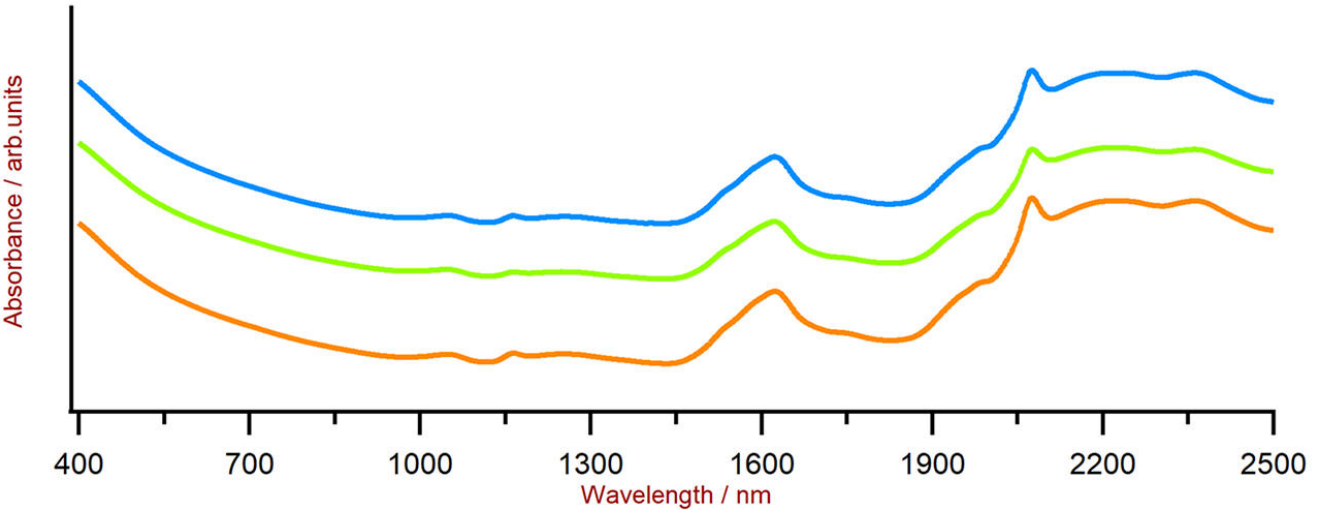
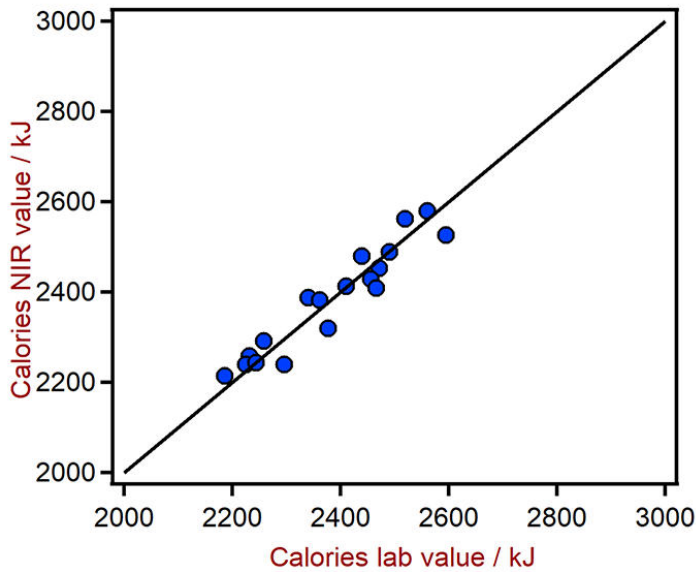


Figure 2. Selection of Vis-NIR spectra of chocolate bar samples. Data was obtained with a DS2500 Solid Analyzer. A spectra offset was applied for visualization purposes.

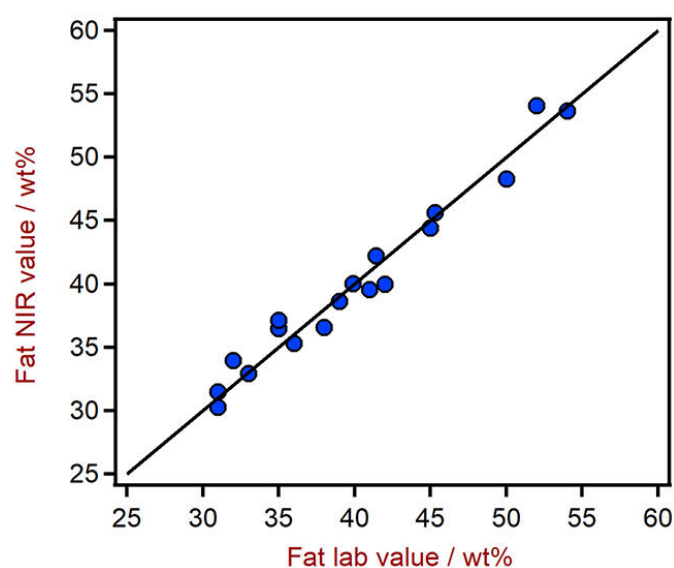
RESULT CALORIES IN CHOCOLATE BARS



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.

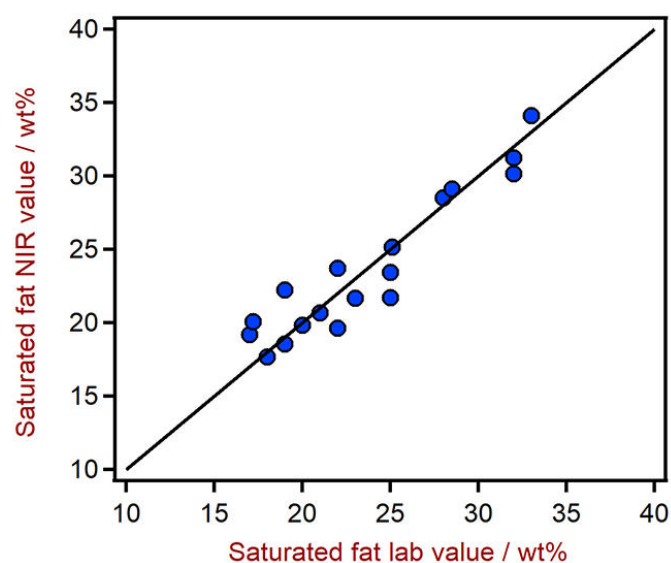
RESULT FAT IN CHOCOLATE BARS



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.

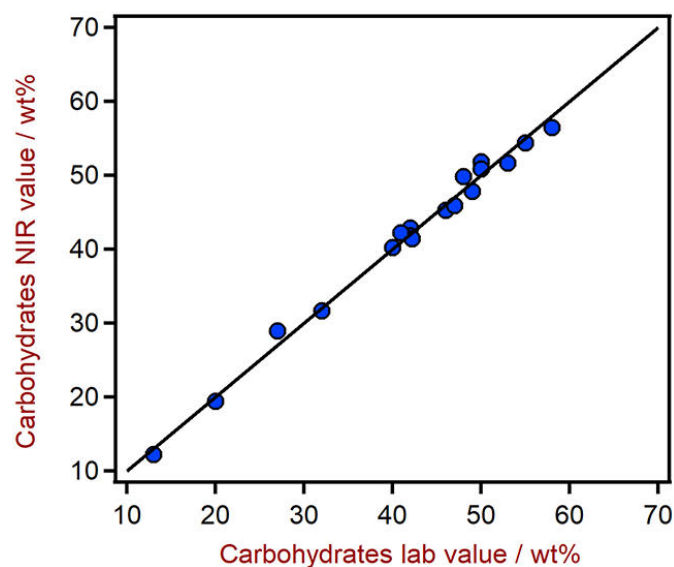
RESULT SATURATED FAT IN CHOCOLATE BARS



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.

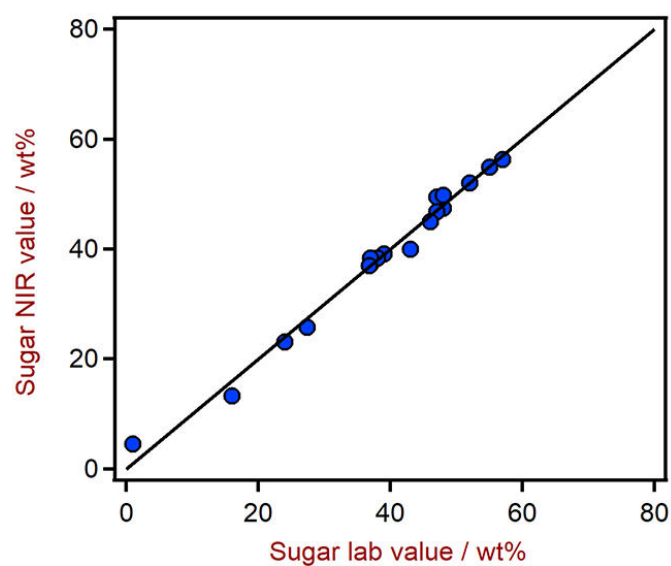
RESULT CARBOHYDRATES IN CHOCOLATE BARS



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.

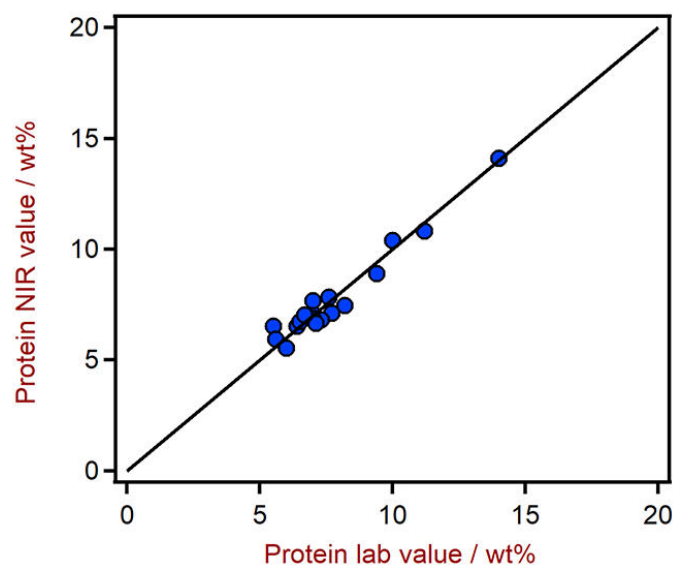
RESULT SUGAR IN CHOCOLATE BARS



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

坚固结实的近红外光谱仪,用于生产环境和试验室中的质量检查。

DS2500 分析仪是经过验证的灵活解决方案,用于对整个生产链过程中的固体、乳膏和液体进行常规分析。其坚固结实的设计使 DS2500 Analyzer 分析仪不受灰尘、湿度、振动和温度波动的影响,因此非常适用于在恶劣的生产环境中使用。

DS2500 涵盖了从 400 到 2500 nm 的整个光谱范围,并能在不到一分钟时间内提供准确和可再现的结果。DS2500 Analyzer 满足制药行业的要求,并由于操作简便而能帮助用户完成其日常工作任务。

由于与设备匹配,附件可以承受任何具有挑战性的样品类型,例如:粒料之类的粗颗粒固体或乳膏之类的半固体样品,可获得结果。测量固体的时候,使用 MultiSample Cup 可以提高生产率,可以自动批量测量多 9 个样品。