Application Note AN-NIR-054

Quality Control of Shampoo

Chemical-free and fast determination of surfactants in shampoo

Determination of sodium laureth sulfate (SLES), cocamidopropyl betaine (CABP), cocamidopropylamine oxide (CAW), cocamide diethanolamine (DEA), and carbopol in shampoo is a cost- and time-intensive process due to the use of large volumes of chemicals per analysis.

This application note demonstrates that the DS2500 Solid Analyzer operating in the visible and near-infrared spectral region (Vis-NIR) provides a **cost-efficient and fast solution** for a **simultaneous determination** of sodium laureth sulfate (SLES), cocamidopropyl betaine (CABP), cocamidopropylamine oxide (CAW), cocamide diethanolamine (DEA), and carbopol in shampoo. With n**o sample preparation or chemicals needed**, Vis-NIR spectroscopy allows for the analysis of these parameters in **less than a minute**.

EXPERIMENTAL EQUIPMENT

Shampoo samples were measured with a DS2500 Solid Analyzer in transflection mode over the full wavelength range (400–2500 nm). A DS2500 Slurry Cup was employed, which simplifies the positioning of the sample and cleaning of the sample vessel. The 1 mm gold diffuse reflector defines the same path length for all measurements to guarantee reproducible results. As displayed in Figure 1, samples were measured without any preparation. The Metrohm software package Vision Air Complete was used for all data acquisition and prediction model development.

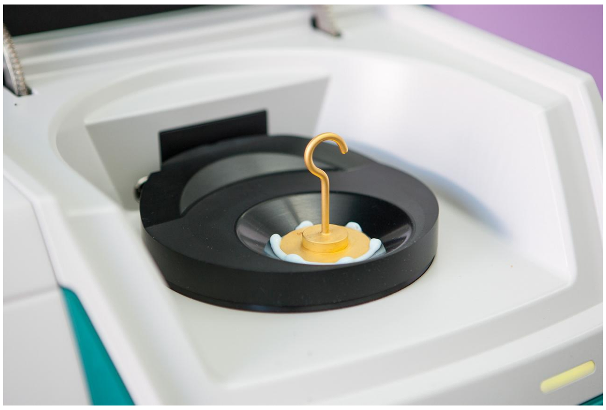

Figure 1. DS2500 Solid Analyzer and a shampoo sample present in the rotating DS2500 Slurry Cup.

Table 1. Hardware and software equipment overview

Equipment	Metrohm number
DS2500 Solid Analyzer	2.922.0010
DS2500 Slurry Cup	6.7490.430
Gold Diffuse Reflector 1 mm	6.7420.000
Vision Air 2.0 Complete	6.6072.208

RESULTS

The obtained Vis-NIR spectra (Figure 2) were used to create prediction models for quantification of the sodium laureth sulfate (SLES), cocamidopropyl betaine (CABP), cocamidopropylamine oxide (CAW), cocamide diethanolamine (DEA), and carbopol in shampoo. The quality of the prediction models was evaluated using correlation diagrams, which display the relationship between Vis-NIR prediction and primary method values. The respective figures of merit (FOM) display the expected precision of a prediction during routine analysis.

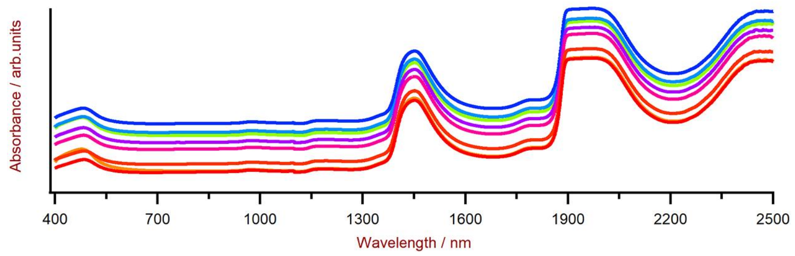

Figure 2. A selection of shampoo Vis-NIR spectra obtained using a DS2500 Analyzer and a DS2500 Slurry Cup. For display reasons a spectra offset was applied.

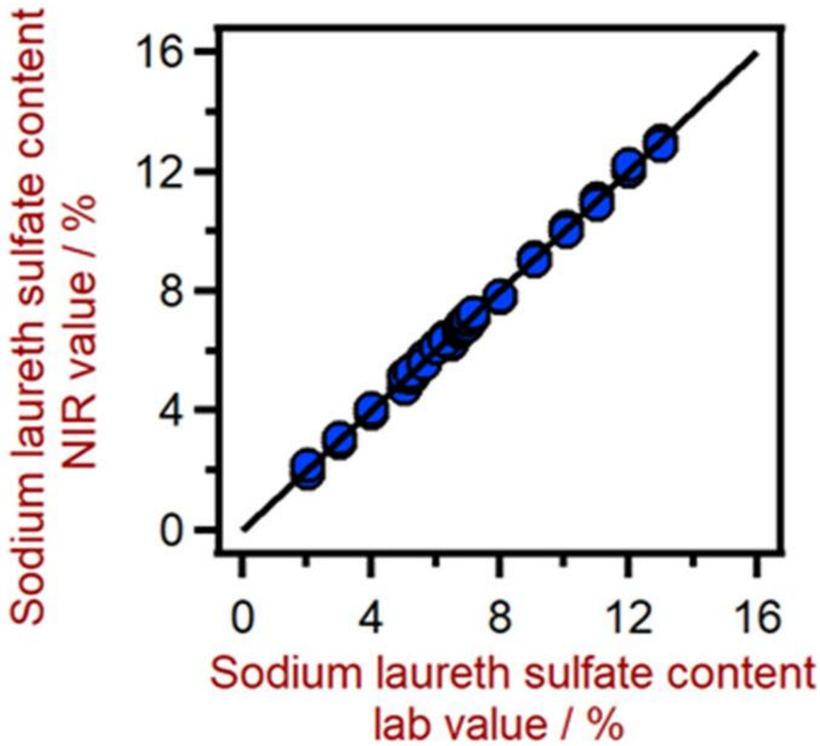

Figure 3. Correlation diagram for the prediction of the sodium laureth sulfate (SLS) content using a DS2500 Solid Analyzer. The SLS lab value was evaluated using titration.

Table 2. Figures of merit for the prediction of the sodium laureth sulfate (SLS) content in shampoo using a DS2500 Solid Analyzer.

Figures of merit	Value
R^2	0.998
Standard error of calibration	0.13%
Standard error of cross-validation	0.14%

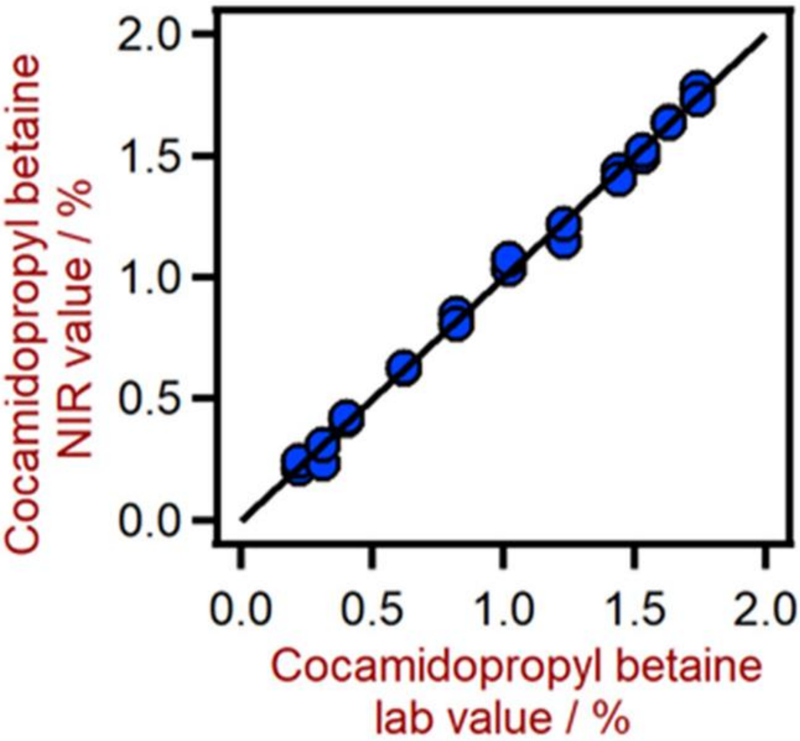

Figure 4. Correlation diagram for the prediction of the cocamidopropyl betaine (CABP) content using a DS2500 Solid Analyzer. The CABP was evaluated using titration.

Table 3. Figures of merit for the prediction of cocoamidopropyl betaine (CABP) content in shampoo using a DS2500 Solid Analyzer.

Figures of merit	Value
R^2	0.996
Standard error of calibration	0.04%
Standard error of cross-validation	0.05%

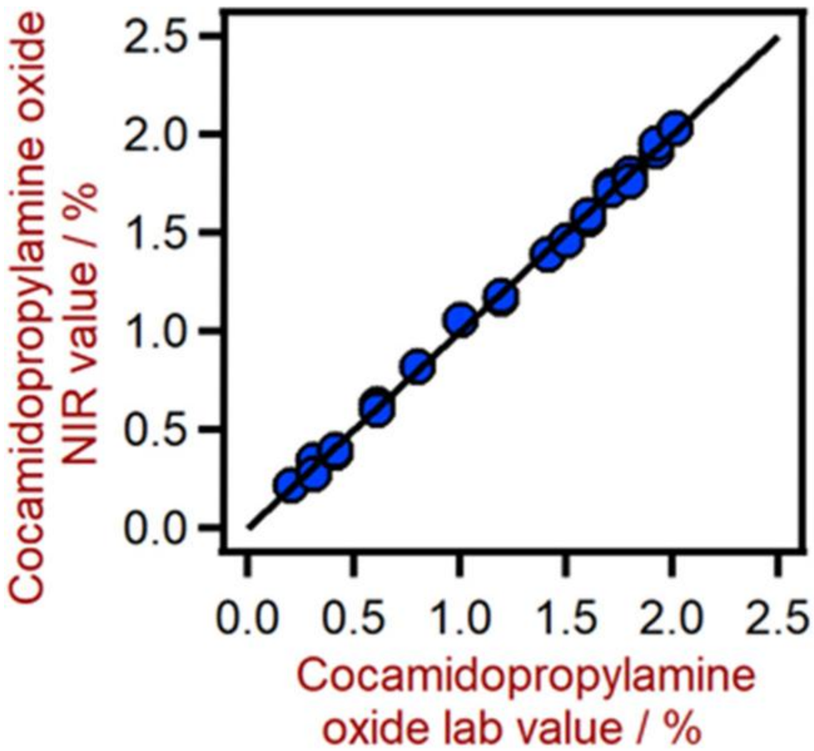

Figure 5. Correlation diagram for the prediction of cocamidopropylamine oxide (CAW) using a DS2500 Solid Analyzer. The CAW lab value was evaluated using titration.

Table 4. Figures of merit for the prediction of cocoamidopropylamine oxide (CAW) content in shampoo using a DS2500 Solid Analyzer.

Figures of merit	Value
R^2	0.998
Standard error of calibration	0.031%
Standard error of cross-validation	0.058%

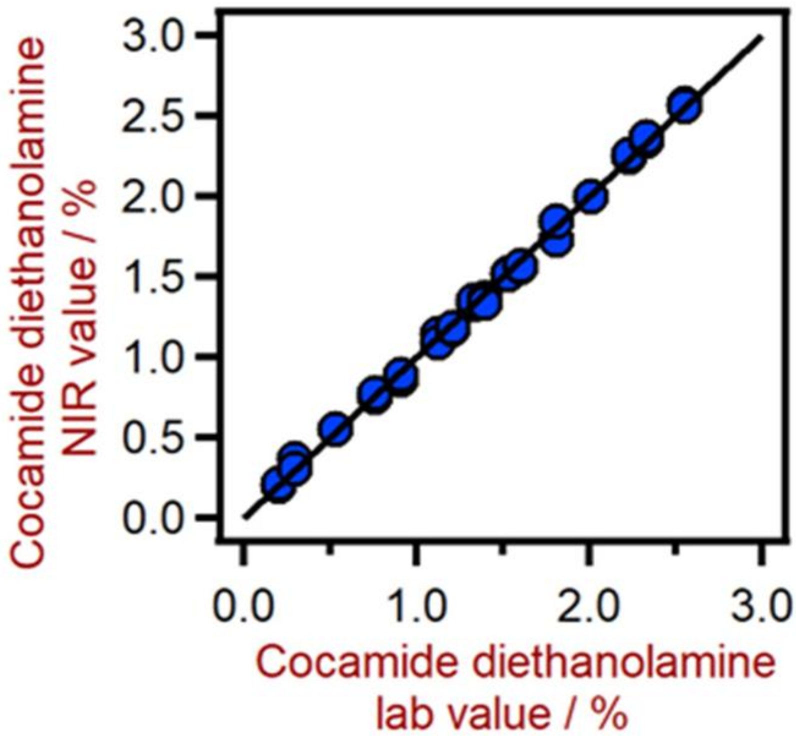

Figure 6. Correlation diagram for the prediction of the cocamide diethanolamine (DEA) using a DS2500 Solid Analyzer. The DEA lab value was evaluated using titration.

Table 5. Figures of merit for the prediction of cocoaminde diethanolamine (DEA) content in shampoo using a DS2500 Solid Analyzer.

Figures of merit	Value
R^2	0.998
Standard error of calibration	0.034%
Standard error of cross-validation	0.036%

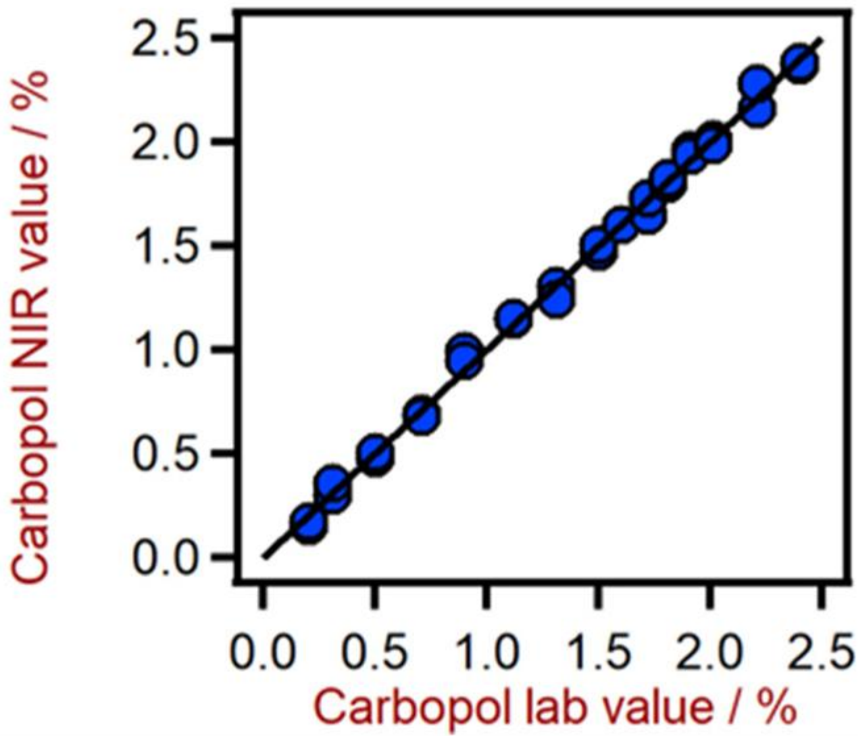

Figure 7. Correlation diagram for the prediction of the carbopol content using a DS2500 Solid Analyzer. The carbopol lab value was evaluated using titration.

Table 6. Figures of merit for the prediction of carbopol content in shampoo using a DS2500 Solid Analyzer.

Figures of merit	Value
R^2	0.969
Standard error of calibration	0.290%
Standard error of cross-validation	0.410%

CONCLUSION

This application note demonstrates the feasibility of NIR spectroscopy for the analysis of sodium laureth sulfate (SLES), cocamidopropyl betaine (CABP), cocamidopropylamine oxide (CAW), cocamide diethanolamine (DEA), and carbopol in shampoo. In comparison to wet chemical methods running costs are significantly lower when using NIR spectroscopy (Tabel 7 and Figure 8).

Table 7. Comparison of running costs for the determination of the key quality parameters in shampoo with titration/HPLC and NIR spectroscopy.

	Lab method	NIR method
Number of analyses per day	10	10
Cost of operator per hour	$25	$25
Costs of consumables and chemicals (SLS, CABP, CAW, DEA, carbopol)	$5	$1
Time spent per analysis (SLS, CABP, CAW, DEA, carbopol)	5 min	1 min
Total running costs (per year)	$18,188	$2,063

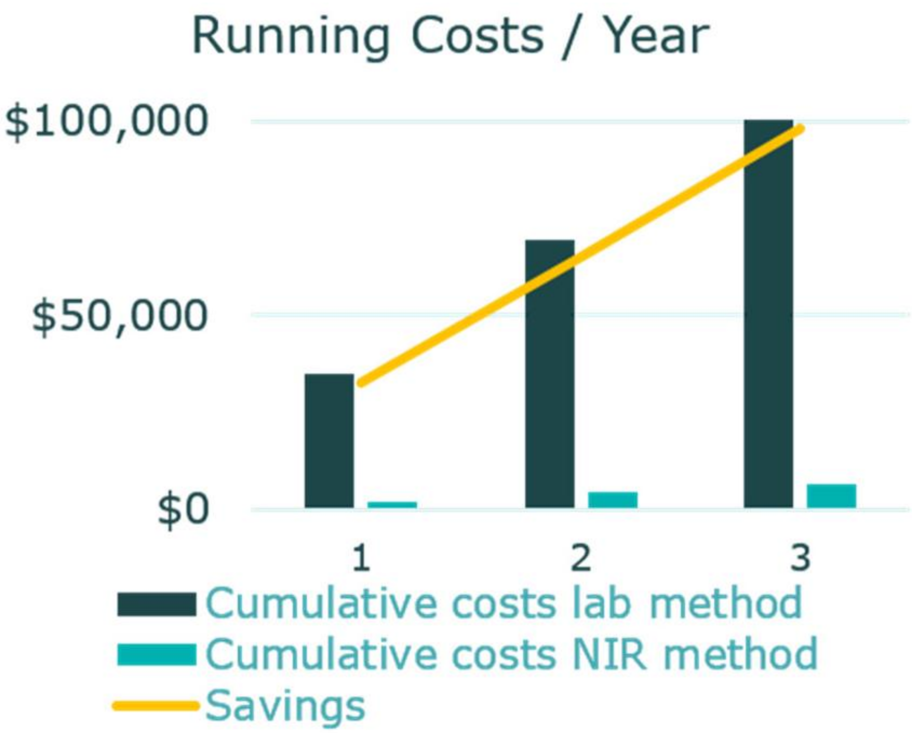

Figure 8. Comparison of the cumulative costs costs for the determination of key quality parameters in shampoo with titration/HPLC and NIR spectroscopy.

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