AN-NIR-054

Quality Control of Shampoo

Chemical-free and fast determination of surfactants in shampoo

Summary

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

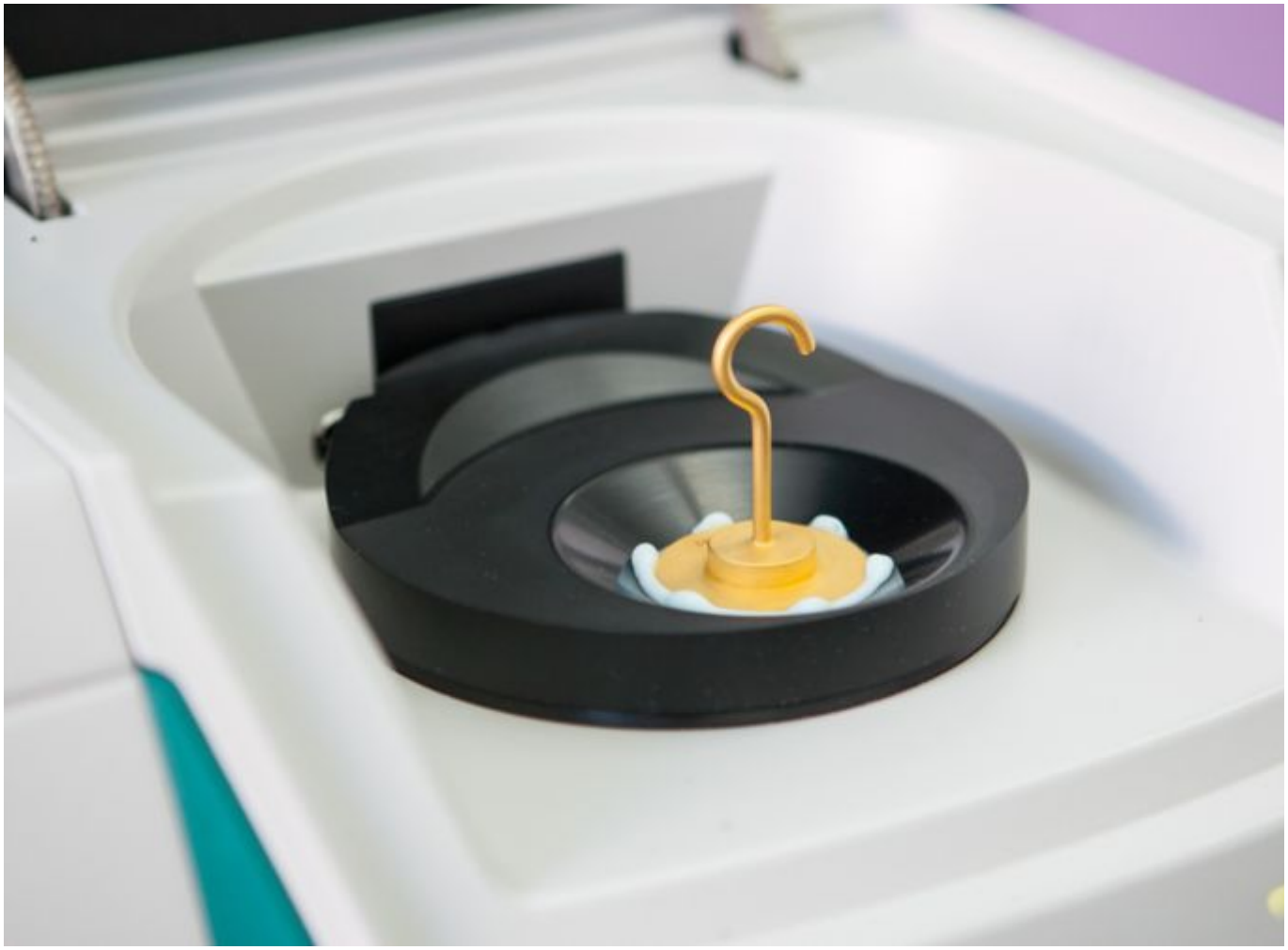

Figure 1. DS2500 Solid Analyzer and a shampoo sample present in the rotating DS2500 Slurry Cup.

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.

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

2.922.0010 - DS2500 Solid Analyzer

Robust near-infrared spectroscopy for quality control, not only in laboratories but also in production environments.The NIRS 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 NIRS DS2500 Analyzer resistant to dust, moisture, vibrations, and temperature fluctuations, which means that it is eminently suited for use in harsh production environments.The NIRS DS2500 covers the full spectral range from 400 to 2500 nm and delivers accurate, reproducible results in less than one minute. The NIRS 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 nine samples.

6.7490.430 - DS2500 Slurry Cup

The Slurry Cup is the ideal sample cup for analyzing high-viscosity substances with the DS2500. The positioning of pastes and creams in the Slurry Cup is made simple by its open design, which also permits rapid and effective cleaning.In combination with the Liquid Kit (6.7400.010), clear viscous samples can also be investigated.

6.7420.000 - NIRS gold diffuse reflector, 1 mm total pathlength

Gold diffuse reflector for the transflection measurement of liquids. Can be used in combination with the following instruments:NIRS DS2500 Analyzer (order number: 2.922.0010); NIRS XDS MasterLab Analyzer (order number: 2.921.1310); NIRS XDS MultiVial Analyzer (order number: 2.921.1120); NIRS XDS RapidContent Analyzer (order number: 2.921.1110); NIRS XDS RapidContent Analyzer - Solids (order number: 2.921.1210);

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 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.

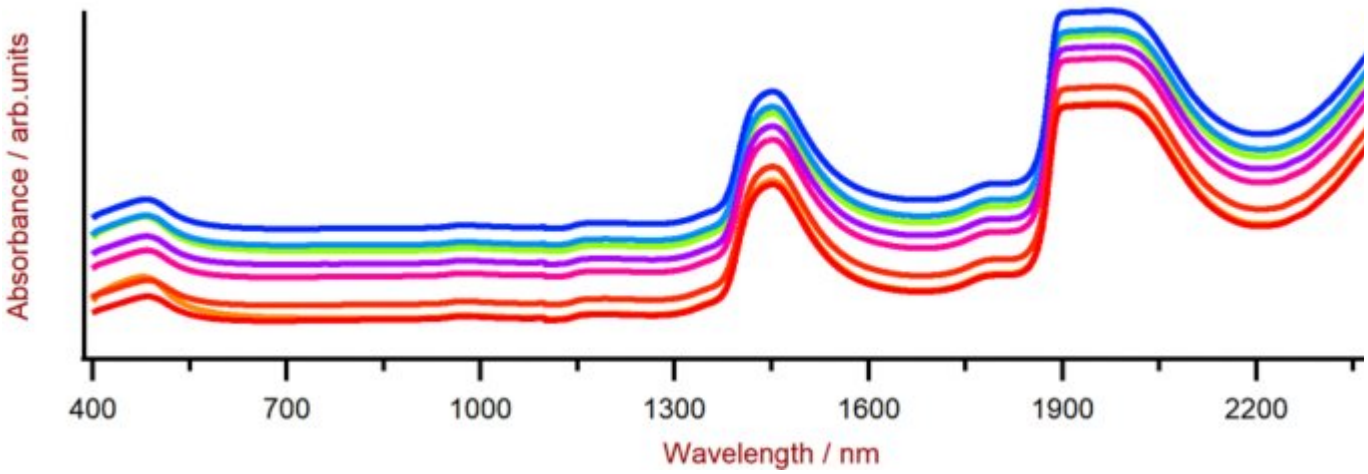

Figure 2. A selection of shampoo Vis-NIR spectra obtained using a DS2500 Analyzer and a DS2500 Slurry Cup. For display reasons a spectra offset was applied.

Result sodium laureth sulfate

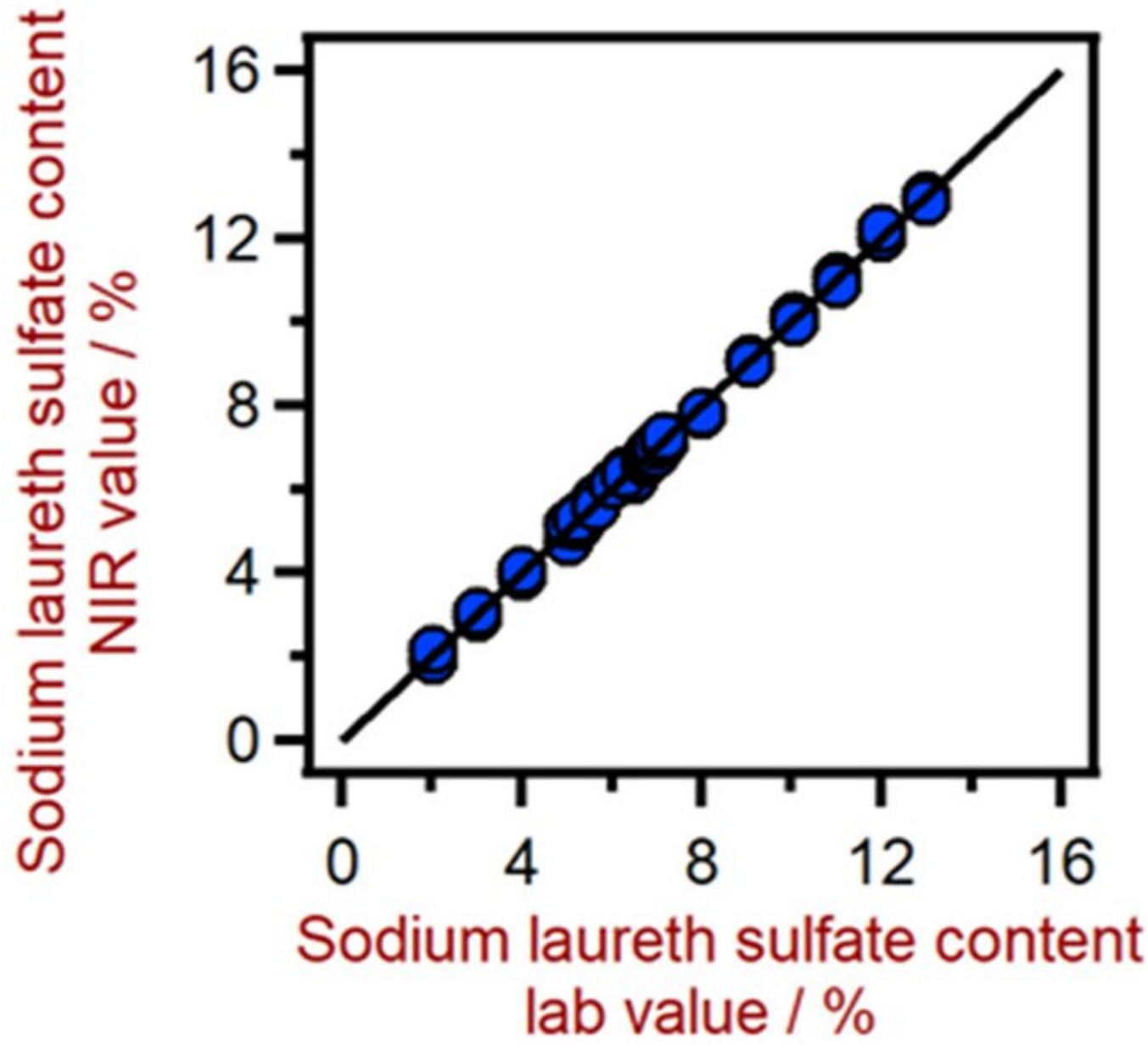

Figure 3. Correlation diagram for the prediction of the sodium laureth sulfate (SLS) content using a DS2500 Solid Analyzer. The SLS lab value was evaluated using titration.

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%

Result cocoamidopropyl betaine

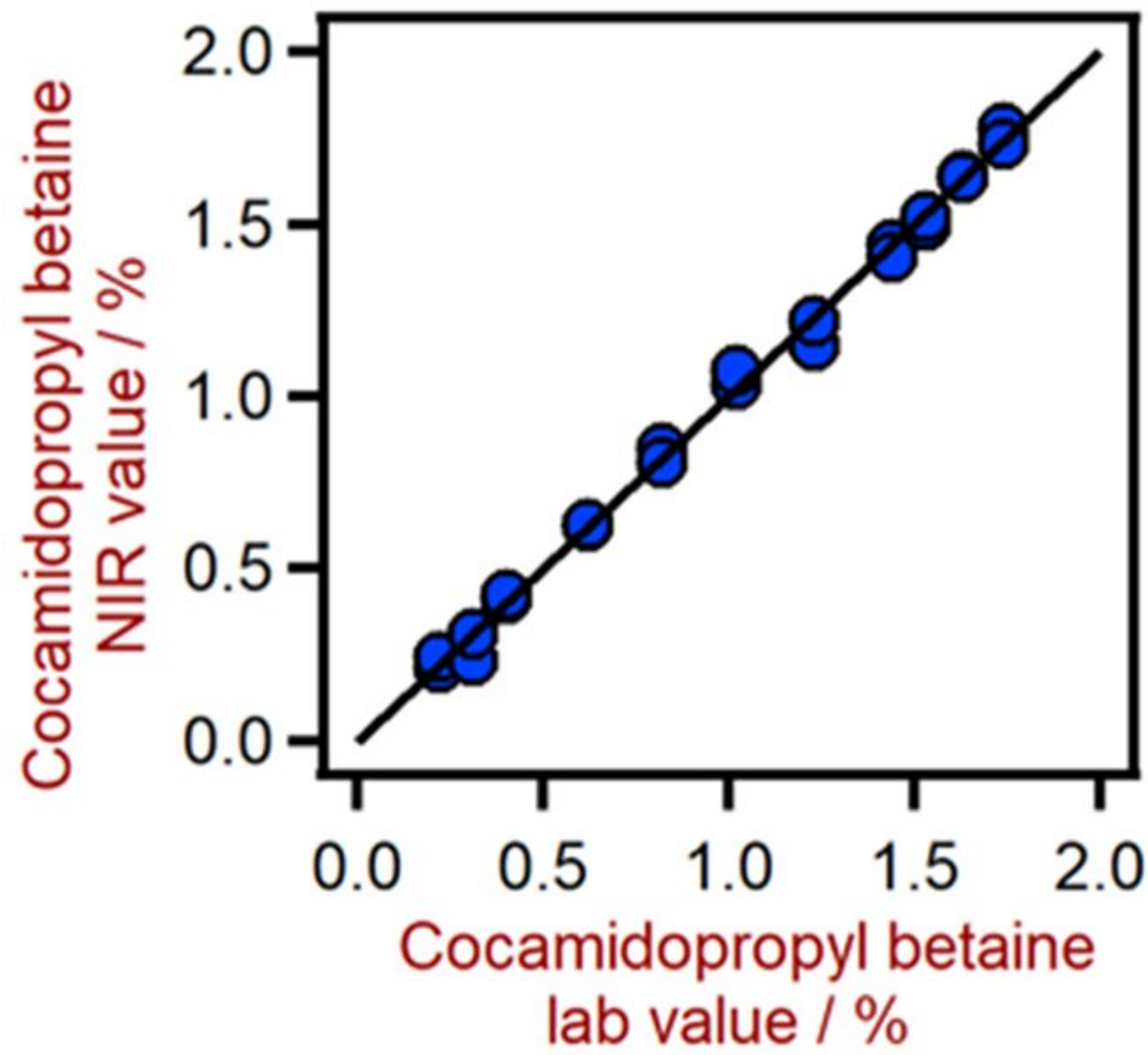

Figure 4. Correlation diagram for the prediction of the cocamidopropyl betaine (CABP) content using a DS2500 Solid Analyzer. The CABP was evaluated using titration.

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%

Result cocoamidopropylamine oxide

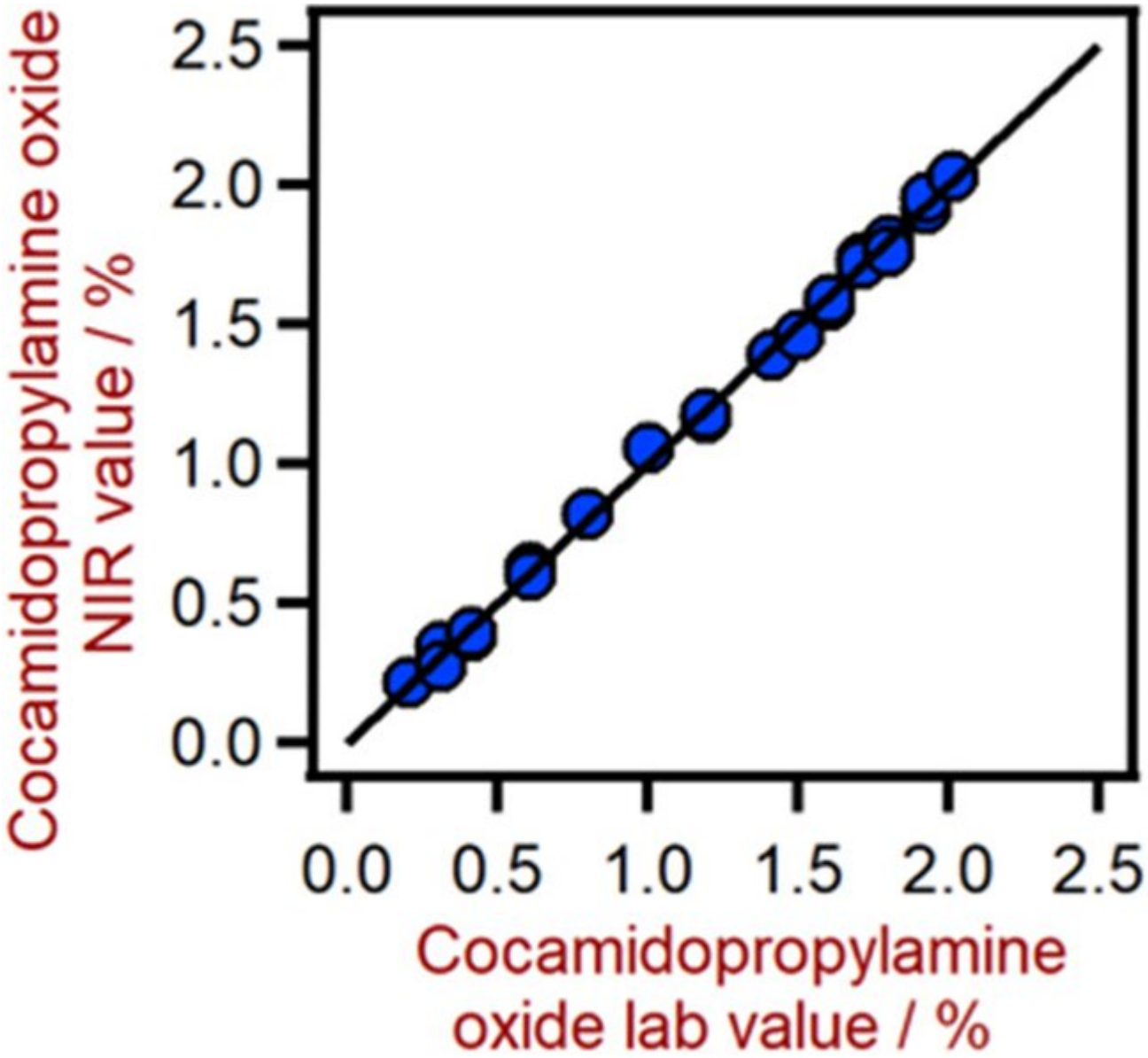

Figure 5. Correlation diagram for the prediction of cocamidopropylamine oxide (CAW) using a DS2500 Solid Analyzer. The CAW lab value was evaluated using titration.

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%

Result cocoamide diethanolamine

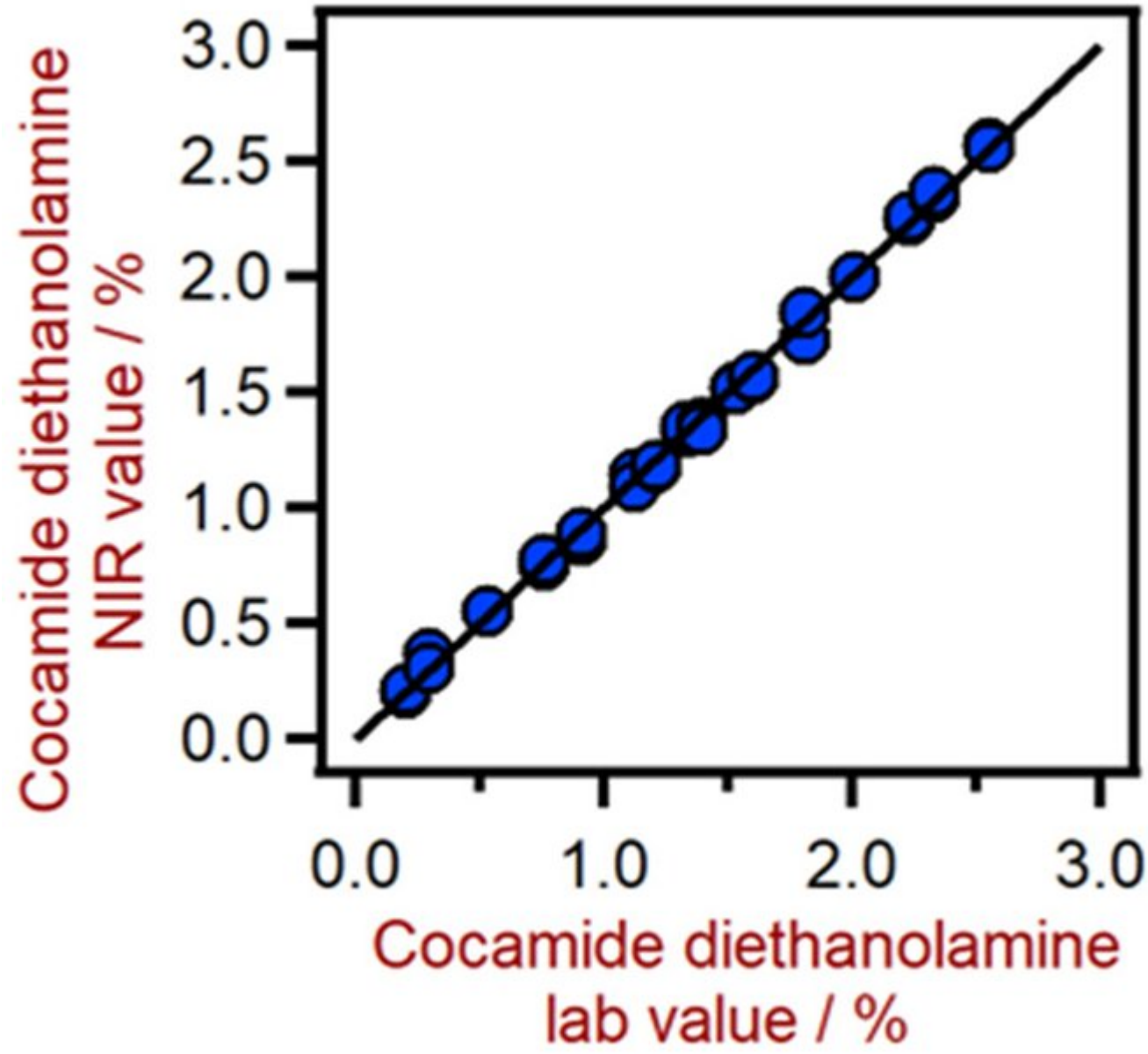

Figure 6. Correlation diagram for the prediction of the cocamide diethanolamine (DEA) using a DS2500 Solid Analyzer. The DEA lab value was evaluated using titration.

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%

Result carbopol

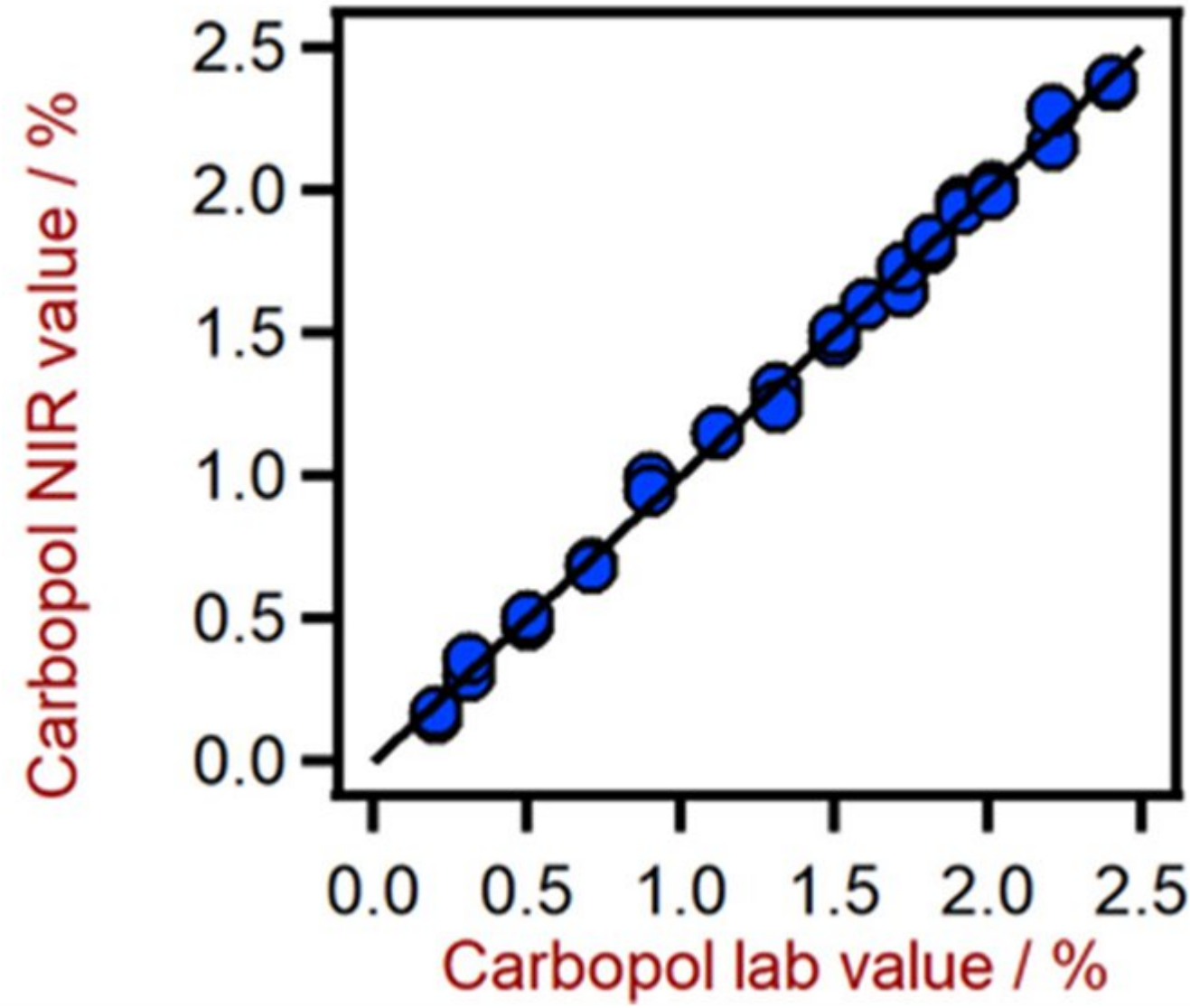

Figure 7. Correlation diagram for the prediction of the carbopol content using a DS2500 Solid Analyzer. The carbopol lab value was evaluated using titration.

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**

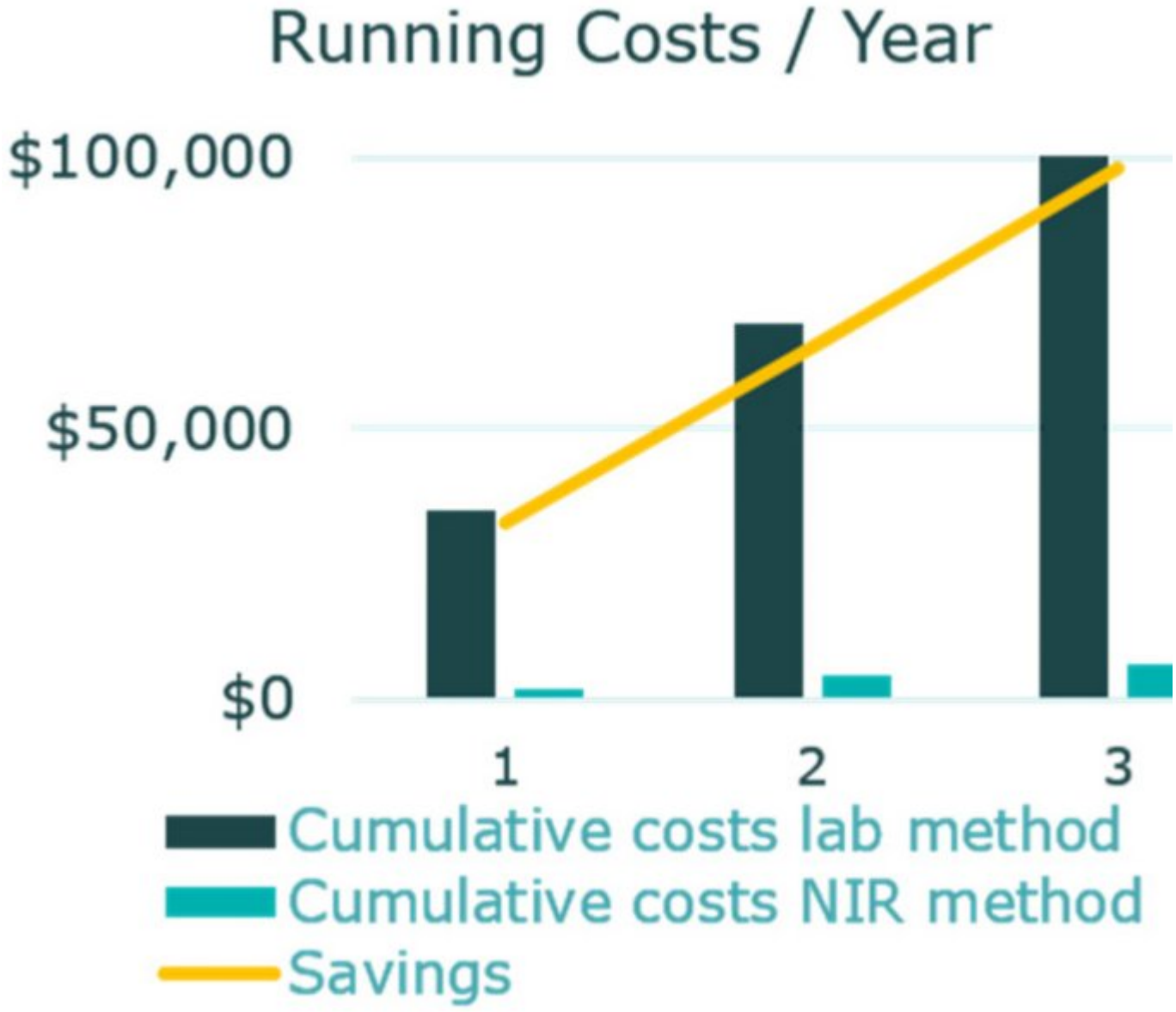

Figure 8. Comparison of the cumulative costs costs for the determination of key quality parameters in shampoo with titration/HPLC and NIR spectroscopy.

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