



Application Note AN-NIR-074

近红外光谱法对液体洗衣液的质量控制

Fast determination without using chemicals

Liquid laundry detergents contain fabric softeners, bleaching agents, surfactants, as well as enzymes. Out of these, the surfactant is the most important factor for the cleaning effect, as it breaks down the interface between polar and nonpolar compounds. This allows the detergent to be effective against greases as well as stains from soil or drinks.

Quantification of surfactant content is most

commonly performed by primary analyses (e.g., two-phase potentiometric titration). Disadvantages include manual sample preparation steps such as dilution and pH adjustment, and the method itself is time-consuming. In contrast, Vis-NIR spectroscopy has a time-to-result of less than 1 minute and does not require any sample preparation or chemicals for high quality data.

EXPERIMENTAL

A total of 37 samples with varying surfactant content were provided by a customer. The Vis-NIR spectra (**Figure 2**) were acquired on a Metrohm NIRS XDS RapidLiquid Analyzer equipped with 1 mm quartz cuvette (**Figure 1**). The samples were measured as-is, without any sample preparation steps. Data collection and model development was carried out with the Vision Air complete software package.



Figure 1. The NIRS XDS RapidLiquid Analyzer with a 1 mm quartz cuvette, used to collect the spectra of surfactant samples.

Table 1. Hardware and software equipment overview.

Equipment	Metrohm number
XDS RapidLiquid Analyzer	2.921.1410
NIRS 1mm quartz cuvette	6.7401.200
Vision Air 2.0 Complete	6.6072.208

RESULT

The obtained graph (**Figure 3**) displays a high correlation ($R^2 = 0.97$) between the values predicted by NIRS and the reference method.

The nearly perfect ratio of the SEC and SECV illustrates the validity of the model.

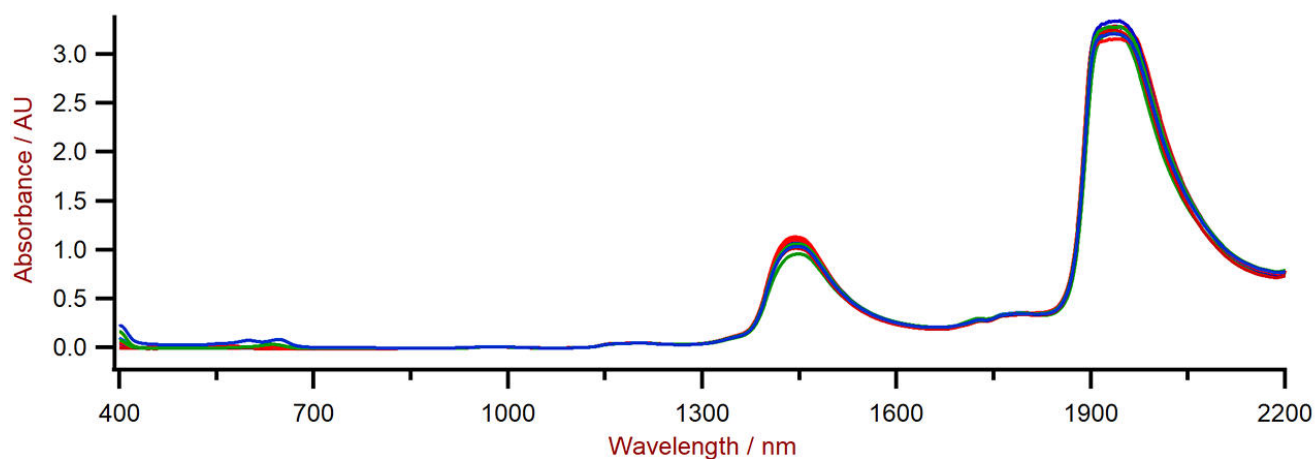


Figure 2 Selection of liquid detergent Vis-NIR spectra obtained using a XDS RapidLiquid Analyzer and a 1 mm quartz cuvette.

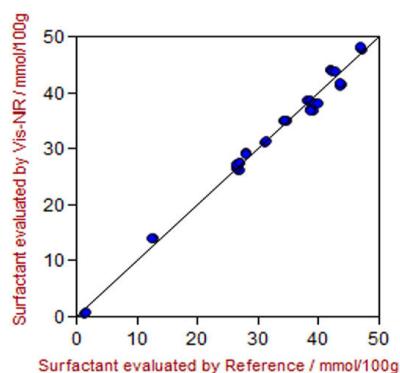


Figure 3 Correlation diagram and the respective figures of merit for the prediction of surfactant in liquid detergent using a XDS RapidLiquid Analyzer. The surfactant lab value was evaluated using HPLC.

Table 2. Figures of merit for the prediction of the surfactant content in liquid detergent using a XDS RapidLiquid Analyzer.

Figures of merit	Value
R^2	0.97
Standard error of calibration	2.20 mmol/100 g
Standard error of cross-validation	2.38 mmol/100 g

CONCLUSION

The results presented herein show that the Vis-NIR method is excellently suited for the fast quantification of surfactant concentration in

detergents. Using Vis-NIR for this application saves 10 minutes per sample compared to other methods (Table 3).

Table 3. Time to result overview for the different parameters

Parameter	Method	Time to result
Surfactant (anionic)	Potentiometric titration	10 min (adding solutions, stirring, pH-adjustments, determination)

CONTACT

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NIRS XDS RapidLiquid Analyzer 快速精确地分析各种液体和悬浮液.

NIRS XDS RapidLiquid Analyzer 分析仪可快速精确地分析液体制剂和物质。按下按钮即可得到精确的测量结果,NIRS XDS RapidLiquid Analyzer 是适用于实验室和工艺过程中质量控制的可靠且方便的解决方案。样品将被预置在可重复使用的石英比色皿或一次性玻璃瓶中;可控制温度的样品室确保可重现的分析条件,由此得到精确的测量结果。



1 mm

石英比色皿带有一个窗口,由高纯度和均质的石英玻璃制成。该比色皿在 200 nm - 2500 nm 波长范围中具有超过 80% 的透射性能。

兼容:

- NIRS Spacer,用于 12.5 mm 比色皿套件 (6.7403.180)
- DS2500 支架,用于 1 mm 比色皿 (6.7492.100)
- 支架 OMNIS NIR,比色皿,1 mm (6.07401.010)



Vision Air 2.0 Complete

Vision Air – 通用的光谱分析软件。

Vision Air Complete 是用于监管规范环境的先进易用的软件解决方案。

Vision Air 优点一览:

- 便捷的软件应用和经过适配的用户界面保证了直观简单的操作方式
- 操作过程的创建与维护方式简单
- SQL 数据库,可安全且简单地管理数据

Vision Air Complete (66072208) 版本包含所有用于可见近红外光谱分析质量保证过程的应用:

- 仪器和数据管理应用
- 方法开发应用
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其它 Vision Air Complete 解决方案:

- 66072207 (Vision Air Network Complete)
- 66072209 (Vision Air Pharma Complete)
- 66072210 (Vision Air Pharma Network Complete)