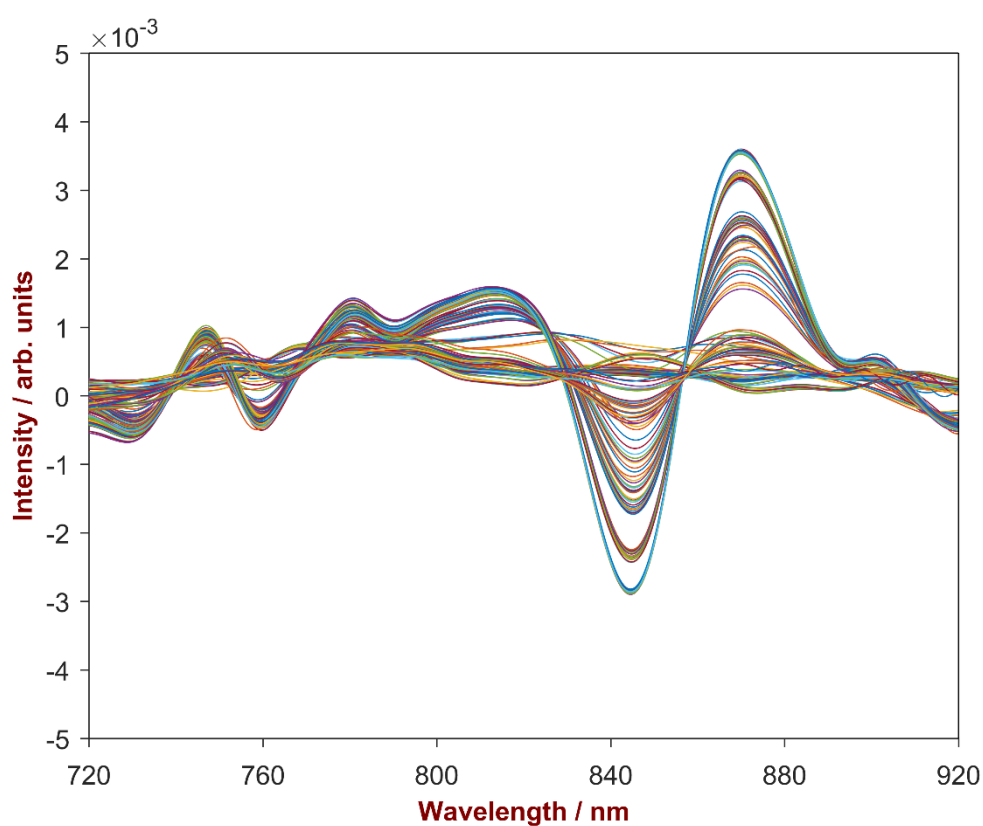# Quantification of Baicalin content in *scutuellaria baicalensis* powder (herbal supplements) by Vis-NIRS



This Application Note shows that visible near-infrared spectroscopy (Vis-NIRS) can be used for the quantification of Baicalin content in herbal supplements. Vis-NIRS is a good alternative to the conventional lab method (HPLC) and can save both cost and time.

**Ω Metrohm**
**NIRSystems**

# Method description

## Introduction

Lately, herbal medicines have been included in the International Conference on Drug Regulatory Authorities (ICDRA). Based on the World Health organization (WHO), the major objective of the Traditional Medicine Program is the integration of traditional medicine into national health care systems. These guidelines contain basic criteria for the assessment of quality, safety, and efficacy as well as important requirements for labelling and the package insert for consumers' information. Therefore, the same strict regulations apply as for synthetic medicines. [1]

One of the most widely used Chinese herbal extracts in Eastern and Western medicines is Baicalin, originally isolated from the roots of the species *scutellaria baicalensis* that has been shown to possess anti-inflammatory, anti-viral, and anti-tumor properties. [2]

Commonly, HPLC is used to quantify Baicalin concentration in *scutellaria baicalensis* powder, however this analysis technique involves time-consuming sample preparation and requires a well-trained operator, resulting in relatively high costs for routine analysis. In this application note, it is demonstrated that Vis-NIRS is a good alternative for saving both time and money.

## Experimental

In this study, 132 *scutellaria baicalensis* powder samples with the Baicalin concentration ranging from 11.54–15.40% were provided to evaluate the correlation between changes in spectral data and reference values.

The spectra were collected in reflection on a NIRS DS2500 Analyzer (**Fig. 1, Tab. 1**) over the full wavelength range (400–2500 nm). The samples were filled in flat quartz glass vessels and measured as triplicates. The software package Vision Air 2.0 Complete was used for data acquisition, data management and development of the quantification method.

**Tab. 1:** Used equipment and software.

| Equipment | Metrohm number |
|---|---|
| NIRS DS2500 | 2.922.0010 |
| NIRS transflection vessel, optically flat | 6.7401.000 |
| Vision Air 2.0 Complete | 6.6072.208 |



**Fig. 1:** The NIRS DS2500 Analyzer was used for spectral data acquisition over the full range from 400 nm to 2500 nm.

## Results

A Partial Least Squares regression (PLS) was performed on 90 *scutellaria baicalensis* powder samples using 2nd derivative as data pre-treatment to correct for spectral baseline shifts. **Fig.2** shows the wavelength region of 720–920 nm, were the correlation between absorbance change and concentration change is obvious, even for the human eye. Internal cross-validation and external validation on an independent data set of 42 samples was applied to verify the performance of the derived quantitative models during method development.
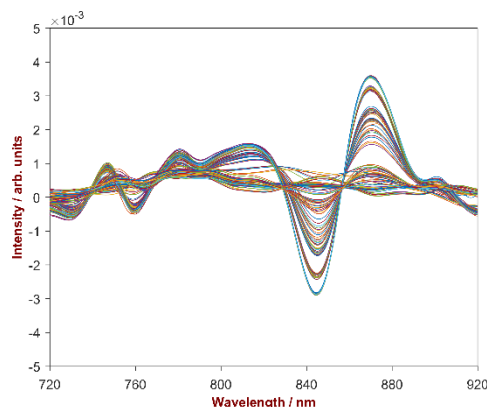


**Fig. 2:** 2nd derivative spectra of 132 *scutellaria baicalensis* powder samples with the Baicalin concentration differing from 11.54–15.40%. Displayed is the wavelength region of 720–920 nm were the correlation between absorbance change and concentration change is obvious.

For the quantification of Baicalin in *scutellaria baicalensis* powder, a 3-factor-model with a Standard Error of Calibration (SEC) of 0.35%, a Standard Error of Cross Validation (SECV) of 0.48% and a Standard Error of Prediction (SEP) of 0.53% was developed. A high correlation between the provided reference values and the calculated values ($R^2 = 0.75$) was achieved, see **Fig. 3**.

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# Method description

Parameters used for method development and the Figures of Merit (FoM) are listed in **Tab. 2**.
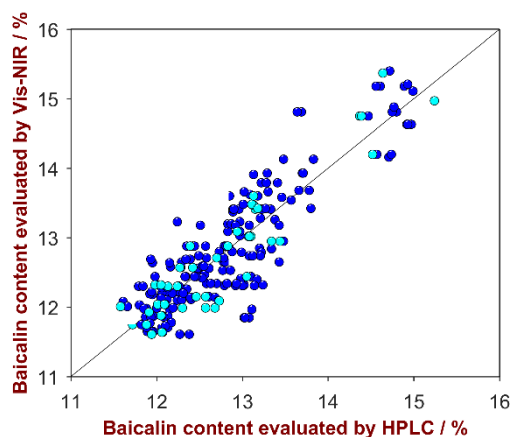


**Fig. 3:** Correlation plot of the predicted Baicalin product strength by NIRS versus the HPLC reference values. Displayed are the calibration (blue) and validation data (turquois).

**Tab. 2:** Results of the quantitative method development for Baicalin content.

| Regression model | PLS with 3 factor |
|---|---|
| Pre-treatment | $2^{nd}$ derivative |
| Wavelength range | 780–1080 nm<br>1120–2500 nm |
| $R^2$ | 0.75 |
| SEC | 0.36% |
| SECV | 0.48% |
| SEP | 0.53% |

## Summary

This application note shows that quantification of Baicalin content in a *scutellaria baicalensis* powder can be conveniently done with Vis-NIR spectroscopy. The calculated standard errors are similar to the HPLC reference method highlighting the suitability of Vis-NIR spectroscopy as a highly reliable and much faster quality control method for herbal medicine manufacturers.

## References

[1] https://nccih.nih.gov/health/whatiscam/chinesemed.htm
[2] https://en.wikipedia.org/wiki/Baicalein