# Determination of artemisinin content by hand-held NIR and FT-NIR spectroscopy: A promising tool for breeding.

C. Camps, P. Rauscher, J. Henkel, X. Simonnet, M. Toussirot, M. Quennoz

[1]Agroscope, Centre de recehrche conthey, CH-1964 Conthey, Switzerland; [2]Hochschule Hannover, University of Applied Sciences and Arts, Germany.
cedric.camps@acw.admin.ch

## Introduction

Artemisinin is a drug used to treat malaria. It is a sesquiterpene lactone with an endoperoxide bridge which is difficult to synthesize in a cost-effective manner, so direct extraction from the leaves of *A. annua* remains an essential step in drug manufacture. The aim of the present study, models aiming at determining the artemisinin content (AC) were evaluated using a 2 NIR spectrometers: a hand-held (phazir 10-18, polychromix)[1] and a lab unit (FT-NIR, MPA Bruker Optics).

## Calibration

A set of 60 samples of A. annua dried leaves were used for calibrations. PLS regressions including cross-validation were used to correlate NIR data and references AC-values. Reference AC-values have been determined by thin layer chromatography. The table 1 presents the calibration (with cross-validation) results and the figure 1 shows how the reference and the predicted values fit in the calibration step using the handheld device.

**TABLE 1**. PLS-values of cross-validation obtained with the two NIR devices.

| PLS paramters | Calibration with Cross-validation | | | | |
| --- | --- | --- | --- | --- | --- |
| | $R^2$ | SECV | LV | $\lambda$ range | RPD |
| Hand-held NIR | 0.94 | 0.1 | 6 | 948-1781 nm | 2.32 |
| FT-NIR | 0.92 | 0.03 | 10 | 7506-6094; 5454.1-4597.8 cm$^{-1}$ | 3.49 |

*R2: coefficient of determination, SECV: standard error of cross-validation, LV: number of latent variables, $\lambda$ range: the range of wavelenghts used in the model, RPD: ration performance to deviation.*
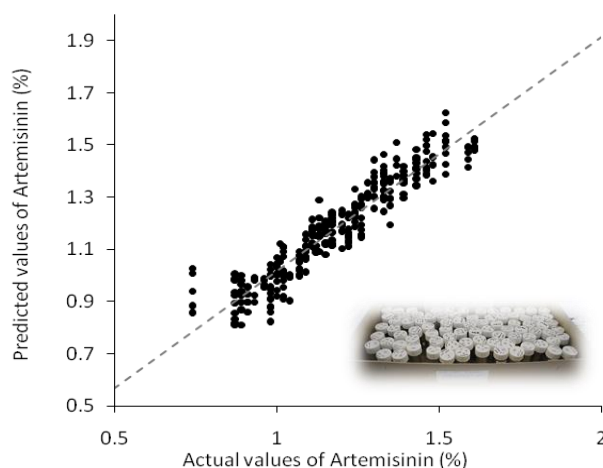


**Fig.1.** Actual vs. Predicted values of AC (%) using the handheld NIR device (cross-validation).

## Validation

Validations were performed for both devices. SEP-values have been calculated without and with bias correction. PLS-values of validation steps are presented in the table 2. Figure 2 shows a measurement performed with the hand-held device and the display of the content of artemisinin.

**TABLE 2**. PLS-values of validation obtained with the two NIR devices.

| PLS paramters | Validation | | |
| --- | --- | --- | --- |
| | SEP | bias | SEPc |
| Hand-held NIR | 0.103 | -0.006 | 0.103 |
| FT-NIR | 0.062 | 0.02 | 0.060 |

*SEP: standard error of prediction, bias: bias value, SEPc: SEP corrected from bias.*



**Fig.2.** Actual vs. Predicted values of AC (%) using the FT-NIR device (validation).

## Conclusion

- Prediction with the FT-NIR is satisfactory.
- The results obtained with the hand-held NIR spectrometer are promising but not ready for use in practice because the values of RPD and SEP.
- Develop an accurate and robust calibration with the hand-held device requires a larger number of samples and a much larger time labor and work compare to F-NIR device.
- Within the framework of a breeding program aiming at selecting high content hybrids, FT-NIR and hand-held NIR spectroscopy remain interesting methods compared to chemical analyses (TLC, HPLC).

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