

P-006: NIRS based quantification of polyphenols in *Actaea racemosa* (L.) rhizome

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The rhizome of *Actaea racemosa* (L.), Ranunculaceae, is a relevant herbal drug used in manufacture of medicinal products. For quality control, plant specific constituents such as polyphenols need to be quantified. If quantification by NIRS would be possible on the powdered rhizome, laboratory effort could be reduced.

The aim of this study is to investigate whether a development of NIRS quantification models is possible [1]. We determined (LC-UV) *A. racemosa* polyphenols (fukinolic acid and cimicifugic acids) in a set of 157 individual rhizomes samples from cultivation (including 56 clone plants), as well as in 6 commercial batches from wild harvests in the U.S. The quantitative reference data for individual and total polyphenols was correlated with corresponding NIR spectra using PLSR. Resulting models were internally validated by tenfold cross-validation.

For total content of polyphenols, model development was generally possible, e.g. in the total sample set (n=163) with $R^2=0.95$ and RMSECV CV=9%. In homogeneous clone plants (n=56) prediction was even better with $R^2=0.98$ and RMSECV CV=5%. Quantification of individual polyphenols was only possible in clone plants, e.g. fukinolic acid with $R^2=0.96$ and RMSECV CV=5%. NIRS model development for quantification of fukinolic acid seems also possible for commercial batches (n=6) with $R^2=1.00$ and RMSECV CV=0.5%.

In summary, NIRS was proven a tool of interest for rapid quality control of *A. race-mosa* rhizomes, if polyphenols are considered. Depending on the sample set, even low concentrated individual constituents could be quantified. Nevertheless, control according to Pharmacopeia requires quantification of triterpene glycosides not polyphenols. NIRS model development for quantification of those was not possible in this study, potential reasons for this are discussed.

References

[1] BITTNER M., and A. KRÄHMER et al., 2017: *Planta Med*, **83**, 1085-1096.