Aquaphotomics Course
Data analysis and Software

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The primary goal of the course is to introduce chemometrics methods most commonly used in NIRS, and Aquaphotomics data evaluation techniques coupled with dedicated software applications. The introduced tools are not limited to the use only in the field of Aquaphotomics or NIRS, but can be used in a much wider range of applications.

Water is one of the most important components of biological and aqueous systems, but it has been generally considered as disturbing factor in NIRS when the main target has been other molecules. On the other hand, water can be analyzed in very small details only in the NIR region as its absorption is optimal in this region to get useful and informative signals.

In Aquaphotomics, water is analyzed under various perturbations, and specific narrow wavelength regions ("water bands" or WAter MAtrix CoordinateS – WAMACS) have been assigned on the basis of the loadings and regression vectors of the multivariate data analysis techniques, such as Principal Component Analysis (PCA), Partial Least Squares Regression (PLSR) and Soft Independent Modeling of Class Analogy (SIMCA) etc.

The chemometrics techniques mentioned above, together with various spectral pretreatment methods, will be presented in theory and practice through real case studies by introducing a self-developed, easy to use dedicated software package called ‚**aquap2'**, developed entirely in R project environment and specifically oriented towards facilitating and speeding up general NIRS analysis and additionally facilitating specialized Aquaphotomics calculations like e.g. the Aquagram. While the first part of the course will provide the theoretical background and a general introduction and an overview of the possibilities of the package aquap2, in the second part participants are welcome to join with their own computers (*) in an interactive way to take part in the discovery of the numerous possibilities of the **aquap2** package.

Beside the introduction of the above mentioned tools, an other purpose of this course is to give some additional knowledge eventually pointing to new directions in the evaluation of spectroscopic data.

(*)To save time, please see www.pollner-research.eu for a list of requirements and the required R-packages to install.