

Workshop – Aquaphotomics Data Analysis

The R-Package “aquap2”: A Multivariate Data Analysis Framework
with a Focus on Aquaphotomics Techniques

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Water is one of the most important components of biological and aqueous systems, but it has been generally considered as disturbing factor in the conventional use of NIRS due to its immense absorption in the NIR spectral region. In the Aquaphotomics evaluation methodology, a contrary approach is employed: Water is used as “molecular mirror” providing indirect information about even small quantities or structural changes of other molecules present in the aqueous systems.

The *aquap2* software package dedicated to the Aquaphotomics data evaluation approach has been developed since 2014 in the R-project programming environment. The primary goal of this Data Analysis workshop is to introduce some key features of the *aquap2* software package through hands on evaluation examples. The introduced software and tools are not limited to the use of Aquaphotomics or NIRS, but can be used in a much wider range of applications providing a great help to perform data evaluation in various field of science in very efficient way.

In the frame of the workshop the main benefits of the use of the *aquap2* software will be introduced including but not limited to the **preparation of experimental design**, efficient and flexible ways of **data import**, use of various **spectral pretreatment** methods and application of some **chemometrics techniques** used in Aquaphotomics using an illustrative dataset.

The first part of the course will provide theoretical background and a general introduction and short overview of the possibilities of *aquap2*, in the second part participants are welcome and highly encouraged to join with their own computers¹ to discover, with our help of course, the numerous possibilities of the *aquap2* software as outlined above.

¹ Detailed information of the requirements and installation steps of the necessary programs are available on the Aquaphotomics website: <http://www.aquaphotomics.com/resources/aquap2/>
We will be available already before the workshop (from about 11:00 on; please feel free to contact us) and of course at the beginning of the workshop to assist with the installation of *aquap2*.