

Problem-Oriented Introduction to *aquap2*, a Free Multivariate Data Analysis Tool with Aquaphotomics Methods

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In the last decade, the concept of Aquaphotomics has constantly picked up momentum and broadened its scientific user-base. Initially introduced by Prof. Roumiana Tsenkova, Aquaphotomics aims to describe the functional state of a living / aquatic system via closely examining its water-phase utilizing spectroscopic approaches. Near-infrared spectroscopy has been shown to be of special value to characterize the systems under scrutiny, with water not being seen as an enemy of spectroscopy, but as a “molecular mirror”, where the entirety or big parts of the perturbances a system has been or is experiencing is reflected in the spectroscopic properties of water.

A profound and often custom-tailored data analysis forms the second part of the typical Aquaphotomics workflow, and it is the purpose of this workshop to provide a problem-oriented hands-on introduction to the freely available R-package *aquap2* that the authors developed over the course of the last years: While *aquap2* can be seen as a versatile and fully scriptable multivariate data analysis tool, it also incorporates and facilitates the usage of some specialized Aquaphotomics methods like the Aquagram. The workshop covers a basic introduction to the architecture of the *aquap2* package, visualization of raw data, principal component analysis, regression analysis and the usage of the bootstrapped linearized Aquagram. In all topics, an emphasis will be placed on utilizing the built-in documentation to solve problems, with the goal to empower the user to efficiently help herself.

Please note that as the time for the workshop is limited we cannot assist participants in installing *aquap2*. You are urgently asked to please install the package prior to the workshop by following the instructions as given in <https://github.com/bpollner/aquap2>. Please also download and prepare the *aquap2_courseMaterial* referenced therein.