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1 Data analysis with the "aquap2" R-package: a free multivariate

2 data analysis framework

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10 Since the early 2000s, the field of aquaphotomics has gained increasing traction and expanded its

11 scientific community. Introduced by Professor Roumiana Tsenkova, aquaphotomics seeks to

12 characterize the functional state of living and/or aqueous systems by examining their water phase

13 through spectroscopic techniques [1]. Notably, near infrared spectroscopy has proven particularly

- 14 effective for such analyses. In this context, water is treated as a "molecular mirror" that reflects
- 15 perturbations from different sources affecting the system, as captured in its spectral properties.

16 Comprehensive, often bespoke data analysis constitutes the second core component of the typical

aquaphotomics workflow. To facilitate this, the authors of the abstract are developing a problem-

18 oriented, continuously evolving R-package called "aquap2", which will be presented as part of this

workshop [2]. This package functions as a flexible and fully scriptable multivariate data analysis

toolkit, it also supports key aquaphotomics-specific methods. The workshop will guide participants

through theoretical background and the foundational architecture of "aquap2" followed by an

22 interactive demonstration of basic application functions, i.e., evaluation examples.

Participants of the workshop gains insight into how "aquap2" can help in the design of experiments,
 flexible data import and spectral preprocessing. This is complemented by the potential use of
 advanced chemometrics such as principal component analysis, regression modelling, and using
 different visualisation techniques [3]. After installing the appropriate versions of RStudio and RTools

for their operating system, interested users are encouraged to install the "aquap2" package by

- 28 following the instructions available at the link below:
- 29

https://github.com/bpollner/aquap2

30 The workshop will provide a comprehensive demonstration of how to carry out investigations for 31 both available and in-preparation samples - whether spectroscopic or not. It will cover how to import 32 data of various origin and formats (e.g., ".da", ".pir", ".txt"), filter full spectral datasets according 33 to specific sample groups and how to examine spectral data within targeted wavelength ranges. A key 34 component of the workshop is the application of widely used data preprocessing techniques and 35 chemometric methods in spectroscopic analysis (i.e., PCA, PLSR), all accessible with just a few 36 clicks. A particularly notable feature of the package is its user-oriented implementation of aquagrams, 37 illustrating water absorbance patterns at specific water matrix coordinates - essential elements of 38 aquaphotomics-related research. In addition to mastering core commands, the workshop will also 39 explore effective strategies for visualising results.

40 The presented software and tools are not restricted to aquaphotomics or near infrared spectroscopy;

41 rather, they are broadly applicable across diverse scientific disciplines, offering powerful and efficient

42 support for data analysis in a wide range of contexts.

44 **References**

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