# Aquaphotomics tutorial – from experiment to interpretation

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"If you want to find the secrets of the universe, think in terms of energy, frequency and vibration."
Nikola Tesla

## Introduction

There are many articles, webpages, and book chapters written about what aquaphotomics is, what exciting new discovery it made, for what purposes it can be used and how it can be applied. It sounds exciting and as if it can really bring better understanding! Until…you acquire spectra, you look at them. And you see nothing!

You go over material and methods of the scientific papers, if you are lucky enough you understand the half of the new preprocessing and data analysis methods, you repeat the experiment, try this and that analysis. You create nice aquagrams. And yet the spectra stubbornly refuse to cooperate. You feel stuck trying to understand what BIG words like WAMACS, WASP or WABS mean. And I do not even want to mention the words which are so commonly used, like moisture content, water content, bulk water, bound water which despite their simplicity remain elusive.

I know that in the beginning of my aquaphotomics experience the water did not look like mirror to me, and the spectra looked like a bunch of similar looking lines. Many of us have been there. I have spent almost 2 years at "that place", where aquaphotomics seemed like a closed world I did not have access to. This workshop will show you how to find your way through.

## Aquaphotomics – a survivial guide

At the beginning of my aquaphotomics journey, I spent one month in the Bio measurement Technology Lab at Kobe University, Japan , doing the standard "beginner`s experiment" – measurement of near infrared spectra of several tap, spring and commercial mineral waters. My objective was to use the spectra to identify each water. After 5 days of morning and afternoon measurements of 10 different waters, I had enough data to analyze. I learned few things, how to subtract the spectra, create aquagrams and make a lot of nice-looking graphs. However, I was far from reaching my objective and I understood nothing.

Looking back to this experience, even though at that time I was not aware of it, I left the Lab of prof. Tsenkova equipped with only 3 things:

1) Good data! I knew how the water spectra should look like. And this is the most important step. It depends on the instrument, measurement technique and acquisition software. Not all instruments are designed with the precision needed for aquaphotomics analysis, nor they provide the spectra in the form which can usually be seen in the papers. But if you know how the spectra should look like, it is enough. In the visible near-infrared range the spectra must be smooth across the entire 400 – 2500 nm region, with clearly recognizable 4 peaks (Fig.1). Whichever part you zoom in, like presented in the Fig. 1, even when you subtract the average spectrum or pure water spectrum, the spectra still must look smooth enough. This is important step to learn to recognize what is noise and what is spectral response, which in the case of water is very subtle. There will be occasions when good signal is not possible to achieve in the whole region, but in that case look for any usable parts.
2) The second thing I had was a corner-stone paper "Aquaphotomics – Dynamic spectroscopy of aqueous systems describes peculiarities of water" [1]. This paper is aquaphotomics in a nutshell, a perfect introduction to the basics of water structure, different water species, conformations and their functionality

in different systems. It also contains the fundamental table with the 12 best known water absorbance bands in the area of 1st overtone of water (1300 – 1600 nm).

3) Lastly, I had one more paper "Prion protein governed by metal binding" [2], written by prof. Tsenkova back in pre-aquaphotomics era. This paper tends to be overshadowed by later publications, but it is one of the best written papers from which I have learned how to "read" the graphs and do basic analysis like Principal Components Analysis and SIMCA, and I always recommend it as a great paper for beginners.

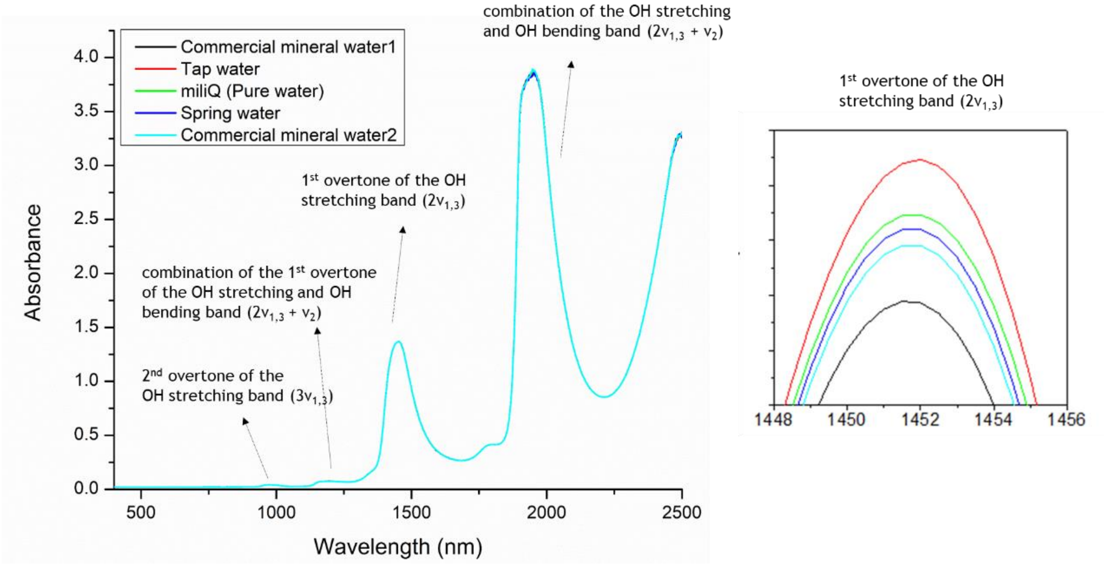


**Figure 1. Visible-near infrared spectra of several types of water**

These three simple things provided me in the following years with much more than I initially intended. And now I often feel overwhelmed by how many lovely interesting things can be seen from only one dataset!
With so many on-line materials now available like open access papers, free software and programming tools, YouTube video instructions, it is easy to build on the knowledge after laying down the good foundation. Starting from scratch, can sometimes be difficult, especially when it comes to performing the experiment. Materials & methods sections of the papers do not provide sufficient enough details because they are often considered unimportant or trivial. This is the reason why we specifically wrote "Essentials of aquaphotomics and its chemometric approaches" [3] in which we addressed many of such issues.

## What will be learned

Aquaphotomics is still an uncharted territory, and what may seem as an obstacle in the analysis will in most cases reveal something new which builds your experience, a valuable contribution that can be shared with other aquaphotomics researchers. Each step matters. The workshop will present all the steps needed for successful performance of experiment and analysis. A variety of different scenarios, working with different samples and measurement techniques will be presented and explained in an easy to understand manner. You will be guided how to find solutions for obstacles and difficult cases which might happen when you are doing the preprocessing and/or analysis. Lastly, in the interpretation part you will learn how to read the story the water mirror is telling you using WAMACs as letters and WASPs as words.


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