Differentiating between bottled water from different sources using near-infrared spectroscopy

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Summary

Water, as a medium, changes its absorbance pattern when adapting to physical or chemical changes within its respective environment. Near-infrared (NIR) spectroscopy can be used to show these changes in the vibrations of water molecules. Aquaphotomics, a scientific field that studies the interaction between water and light, provides the possibility to extract information from the water spectrum. Aquaphotomics provide a better understanding into the organisation of water molecules and the hydrogen-bond network in each of the water sources.

Introduction

Water is one of the most abundant components in biological systems and a complex subject which has been the focus of many studies over the years [1, 2]. Different scientific areas have been studying the properties, function and structure of water, but has provided only a limited picture of this unique substance. Recently, faster and more reliable testing methods have been explored, one such method being near infrared spectroscopy.

Near-infrared (NIR) spectroscopy is a non-destructive analytical method, which enables the simultaneous measurement of qualitative and quantitative parameters of a range of different products [3]. Water has always been considered as a hindrance in infrared spectroscopy since it absorbs across the entire frequency range [4]. However, aquaphotomics is an approach that uses NIR spectroscopy to extract information hidden in the water spectrum [5]. Hydrogen and covalent OH bonds are easily influenced by other molecules in the solution, this information can be extracted from the water spectrum using aquaphotomics [6].

Materials and Methods

Spring water from the same brand which was bottled at three different sources were obtained from a local supplier. The bottled water was stored at room temperature until analysis.

Spectra were acquired using a Buchi NIRFlex N-500 (BÜCHI Labortechnik AG, Flawil, Switzerland) with a liquid measurement cell. Spectra were obtained in the wavelength range of 1000 – 2500 nm with a quartz cuvette with a path length of 0.2 mm at a temperature of 32 ˚C. Each water sample was scanned 5 consecutive times. Differences between the three sources were visualised with aquagrams.

Results and Discussion

Absorbances in the 1342-1372 nm region correspond to free OH stretches, and the wavelength range between 1474 and 1518 nm is related to a strong hydrogen-bonded network of water molecules [7, 8]. The aquagrams (Figure 1) of the different sources indicates that source B has a stronger hydrogen-bonded network of water molecules than sources A and C. This is due to the higher absorbances of source B in the 1474 and 1518 nm wavelength region, compared to sources A and C. The absorbances in the region between 1342 and 1372 nm of sources A and C shows that there are more free water molecules present in the water than source B.

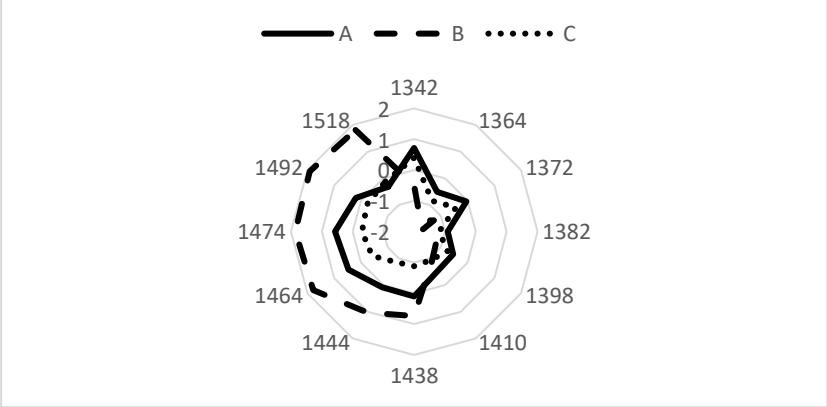

Figure 1 Aquagrams of spring water from three different sources

The different mineral content concentrations (Table 1) of the different sources, may contribute to the difference in the aquagrams. This is a result of the structure maker\breaker effect the different ions have on the hydrogen bond network of the water molecules.

Table 1 Nutritional information of the bottled water (mg/L)

Source	A	B	C
Calcium	2	0.4	5.9
Magnesium	1	0.2	2.4
Sodium	8	3.3	46.2
Potassium	1	<0.1	0.5
chloride	13.2	6.5	<5
sulphate	4.4	1.4	10.8
Alkalinity	5.4	3.4	104
Nitrate	0.2	<0.1	<0.1
Flouride	<1	<0.1	1
TDS	48	19	193
pH	6	5.1	8.5

Conclusion

The NIR spectra of bottled water can be used to distinguish between the different molecular conformations and the mineral content of the water molecules of the three different water sources. The study confirms that NIR spectroscopy can be used to differentiate between bottled water from different sources.

References

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