

AQUAPHOTOMICS IN FOOD SCIENCE AND AGRICULTURE





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OUTLINE

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- □ Applications in food science:
 - Scattering and absorption
 - Just water
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The Research Unit for Food Processes (CRA-IAA) is a structure of the Consiglio per la Ricerca e la sperimentazione in Agricoltura (CRA), a National Institution of research and experimentation with a general expertise on agricultural and agroindustrial fields, fisheries and forests. Working under the supervision of the Italian Ministry of Agriculture and Forests.



ministero delle politiche agricole alimentari e forestali





- The CRA collects the expertises of 28 Research Institutes and agricultural experimentation, and of 54 operatives sites.
- Inside of CRA, The CRA-IAA is the only structure with the mission of the qualification of agro-food and agro-industrial systems.
- The main objective is to develop studies and projects for products and processes innovation, and at the same time for a sustainable SME's development and consumer's warranty.

The Aquaphotomics concept helps to positively evaluate the water changes occurring, after physical or chemical perturbations, in different and several bio-systems. The direct monitoring of food processes or/and chemical and physical changes in biological matrices is not often possible. These information can be collected through the study of water patterns in NIR region.



(a) At room temperature and atmospheric conditions, hydrogen (H) and oxygen (O) atoms in water exist predominantly as traditional H₂O molecules. (b) At 2,000 kelvins and a million times atmospheric pressure, the atoms begin to cluster, and water is in a superionic phase.

Water in extreme conditions (Lawrence Livermore National Laboratory, S&TR October 2005, 13-18.)

The liquid-air interface of water has an abundance of molecules whose hydrogen atoms are oriented into the air. The phenomenon, known as surface relaxation, may increase the reactivity of molecules in this region of water.





The changes in the water spectrum are comparable to variations due to changes in temperature, probably associated with a different H-bond content. The substances inducing a

change in the spectrum comparable to an increase in temperature are termed "structure-breakers".

The substances inducing a change comparable to a decrease of temperature are termed "structure-makers".

R. Giangiacomo, 2006, Food Chemistry, 96 (3), 371-379

Extracting scattering information and identify the wavelength ranges mainly influenced by particles distribution and size.

VIP coefficients for casein calibration on milk spectral data. Before (brillant blu line) and after (sweet blue line) EMSC correction.



Cattaneo, T.M.P.; Cabassi, G.; Profaizer, M.; Giangiacomo, R., 2009, JNIRS, 17 (6) 337-343

SPECTRUM OF DIFFERENCES AMONG WATER SAMPLES (Giangiacomo R. et al., 2010, 14th ICNIRS Proc., Thailand, 443-447)





Not only the mineral concentration, but also the types of minerals and their hydration capacities can affect water spectral response in the NIR range.

MSC pre-treated spectra

AQUAPHOTOMICS: WAVELENGTHS INVOLVED IN THE STUDY OF THE SPECIATION OF METAL IONS (Zn²⁺, Pb²⁺, Ag⁺) IN AQUEOUS SOLUTIONS. (Vero S. et al., 2010, NIRNews, 21 (8), 11-13)

The main differences

among spectra are detectable in the range 1340-1500, confirming the possibility to indirectly study cation solutions and their speciation by using water spectral modifications.

[20mM], pH 1.50



_____Zn2+, Ag+, Pb2+ _____Zn2+ ____Ag+ ____Pb2+

The study of the evolution of the spectra of individual ions at increasing pH values (Pb²⁺)



The spectral changes corresponding to pH variations are clearly visible in the selected NIR range. The water absorption bands seemed to be involved as possible descriptors of the presence of different cation species at each selected pH.

For increasing pH values from 3.00 to 5.15, it is possible to notice that the changes in the first derivative flexes and maxima can be interpreted as a function of the increased concentration of the species PbOH⁺ to 10^{-5} M. A further change was observed at pH 5.45, at which the presence of hydroxocomplex Pb₄(OH)₄⁴⁺ with a final concentration of 10^{-4} M becomes important.

The determination of the predominant components in spectra allowed the distinction between the different ways in which the water matrix is influenced by the presence of different cations at the different pH values.

These data can contribute to update the Aquaphotomics library in order to better understand which and what kinds of molecular bonds can modify water spectra, modifications that can also occur for the presence of natural or added compounds in very low concentrations.

THE USE OF NEAR INFRARED SPECTROSCOPY FOR MONITORING MILK-WHEY BIOTRANSFORMATION PROCESSES USING Lactobacillus plantarum

Remagni M.C. et al., 2012, (2012), 15th ICNIRS Proc., Cape Town, South Africa, 439-443



Relationship between microbial growth and fermentation trend:

Adaptability of *Lactobacillus plantarum* on the substrate tested: within 48 hours strains reached growth values of order 9 log CFU/mL demostrating how this species is able to multiply even in non-optimal growth conditions.









NUTRACEUTICAL PROPERTIES OF ITALIAN RICE Barzaghi S. et al., 2014, NIRItalia2014 Proceedings, 102-108

Total tocopherols content (RPD = 3,47; screening method)





Increase in tocopherols content corresponded to a decrease in water absorption



Natural dehydration during storage influenced Aquagram on the basis of an increased number of water-bonded molecules and a decreasing of free water molecules. At 21 days, no linear relationship with storage was detected. The maximum of variability was associated to this sampling point for weight loss calibration (*Cattaneo T.M.P. et al., 2014, NIRItalia2014 Proceedings, 118-123*), supporting Aquagram's results.

Days of storage





WAPS **The specific Water Spectral Absorbance** Patterns illustrated phase transitions in the system over the time on the basis of the increasing absorption intensity over the time, detected at 950, 970, 1200 nm.

INFLUENCE OF PACKAGING (MSC pretreated spectra)





SHELF LIFE OF WHITE MELON: INFLUENCE OF COATING (Cattaneo T.M.P. et al., 2014, NIRItalia2014 Proceedings, 118-123)



SKIN (surface)

PULP (inside)



Aquagrams showed differences ascribable to different coating permeability .

Each coating generates a specific fingerprint for the same product.

CONCLUSIONS

The chemical or physical perturbations applied to water (solution, suspension) disrupt the flickering cluster of water, breaking some water H-bonds and generating some new H-bonds, both

in the non-solvent water

and

in the water involved as solvent.

This higher number of water H-bonds, compared to those in the pure water, is more stable and with higher energy, giving rise to a new water spectrum.

The information provided support the use of Aquaphotomics as suitable tool in explaining and monitoring the evolution of biosystems through the study of water absorption pattern.

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Thank you for your attention!



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