

# The 4th Aquaphotomics International Conference

Kobe University, Centennial Hall (Rokko Hall)

March 20 - 22, 2021

SATURDAY March 20, 2021

On site & On line ( English & Japanese real-time interpretation)

## AQUAPHOTOMICS WORKSHOP

Chairperson: Roumiana Tsenkova

9:30	10:30	A closer look at preprocessing with focus on aquaphotomics	Federico Marini
10:30	12:00	Aquaphotomics tutorial - from experiment to interpretation	Jelena Muncan
12:00	13:00	☞ Lunch break	

## AQUAPHOTOMICS OPEN LECTURE

Chairperson: Masato Yasui

13:00	14:30	From non-invasive disease diagnostics to aquaphotomics	Roumiana Tsenkova
14:30	15:00	☞ Coffee break	

## LEADING EDGE OF SCIENCE

Chairperson: Christian Huck

15:00	15:40	Encounter with peculiarity in physical properties of water and expectation for definite developments of aquaphotomics	Mutsuo Iwamoto
15:40	16:20	Molecular spectroscopy studies of water from Far-ultraviolet to Far-infrared/Terahertz and Raman spectroscopy	Yukihiro Ozaki
16:20	16:50	Water biology and medicine - roles of aquaporins in biological system	Masato Yasui
16:50	17:20	☞ Coffee break	

## FURTHER DEVELOPMENTS

Chairperson: Zoltan Kovacs

17:20	17:50	Modern tools of NIR spectroscopy in water-related analysis. Miniaturized spectrometers, quantum chemistry and neural networks	Christian Huck <sup>※1</sup>
17:50	18:20	Aquaphotomics Laboratory in Yunosato	Shogo Shigeoka
18:20	18:50	Aquaphotomics science - looking at nature through water spectral patterns	Jelena Muncan
19:00		☞ Recess	

※1 The invitation is supported by Naito Foundation

**FROM WATER STRUCTURE AND SPECTRAL PATTERNS TO DIAGNOSTICS**

Chairperson: Jelena Muncan

9:00	9:30	Analyzing the water in chemical changes by Temperature-Dependent Near-Infrared Spectroscopy	Xuengang Shao
9:30	9:50	Aquaphotomics profiling of blood serum vs. plasma offers complementary modes of discriminating <i>Manheimia heamololytica</i> infection in dairy calves	Carry Vance
9:50	10:10	Aquaphotomics profile of near Infrared spectral signatures from four Anastomosis groups of the fungi <i>Rhizoctonia solani</i>	Mariana Santos Rivera
10:10	10:30	☞ Coffee break	

**QUANTUM BRAIN DYNAMICS - ROLE OF WATER**

Chairperson: Hiroshi Murakami

10:30	11:00	Modelling the measured microtubule conductivity and capacitance as a function of ionic concentrations	Jack Tuzsynski
11:00	11:20	Non-equilibrium quantum brain dynamics in 3+1 dimension with water dipoles and photons	Akihiro Nishiyama

**WATER AS A PART OF BIOLOGICAL PROCESSES**

Chairperson: Sae Tanaka

11:20	11:40	Studies on cryopreservation mechanism using Trehalose-transporter expressing cells	Tsutomu Uchida
11:40	12:00	Assessment of biological functions and metabolic activity during embryogenesis by water analysis using near-infrared spectroscopy	Mika Ishigaki
12:00	13:00	☞ Lunch break	

**HYDRATION & INTERFACIAL WATER**

Chairperson: Shigeaki Morita

13:00	13:30	Role of interfacial water in determining the interaction of proteins and cells with hydrated materials	Masaru Tanaka
13:30	13:50	Investigation on the reaction mechanism for dehydration of $Mg(OH)_2$ and hydration of $MgO$ by NIR spectroscopy	Masato Takeuchi
13:50	14:10	Water at biointerfaces: what makes surfaces bioinert?	Tomohiro Hayashi
14:10	14:30	Investigation of the electronic states of water in hydrate-melt	Yusuke Morisawa
14:30	15:00	☞ Coffee break	

**AQUAPHOTOMICS FOR FOOD QUALITY CONTROL**

Chairperson: Mika Ishigaki

15:00	15:30	Food quality and process investigated through water absorption variations in NIR range	Tiziana M.P. Cattaneo
15:30	15:50	Dairy products analysis - near-infrared spectroscopy and aquaphotomics approach	Stefka Atanassova
15:50	16:10	Recent applications of aquaphotomics in the field of food science	Zoltan Kovacs
16:10	16:30	Can aquaphotomics improve quality prediction of intact fruit?	Harpreet Kaur
16:30	16:45	☞ Coffee break	

## WATER STRUCTURE - NEW INSIGHTS & IMPLICATIONS

Chairperson: Krzysztof Bec

16:45	17:15	Extending the spectrum: NIR spectroscopy of crystalline H <sub>2</sub> O- ices	Christina Tonauer
17:15	17:35	Water structure and water mirror effect in NIR region. A perspective from the quantum chemical simulations.	Justyna Grabska
17:35	17:55	Detection of dissolved salts using the water spectrum	Herman Offerhaus
17:55	18:15	Near Infrared and aquaphotomic analysis of water absorption in lactate containing media	Nystha Baishya
18:15	19:00	<b>AQUAPHOTOMICS INTERNATIONAL ASSEMBLY</b>	
19:00	19:45	<b>POSTER SESSION I</b>	
19:45		☞ Recess	

MONDAY March 22, 2021

## WATER & OTHER BIOMOLECULES

Chairperson: Xuegang Shao

9:00	9:30	The role of water activity in the thermodynamic response of lipid interphases	E. Anibal Disalvo
9:30	9:50	Near infrared spectroscopy and multivariate analysis for the study of water in lipidic membranes	Jorge J. Wenz
9:50	10:10	Understanding hyaluronic acid induced variation of water structure by near-infrared spectroscopy	Hengchang Zang
10:10	10:30	Details of glucose solution near-infrared band assignment revealed using deuterium oxide and glucose isotopes	Sae Tanaka
10:30	10:40	☞ Coffee break	

## WATER STRUCTURE & HYDRATION

Chairperson: Masato Takeuchi

10:40	11:00	Recent and future X-ray measurements of pure water	Craig Schwartz
11:00	11:20	Concentration-dependent near-infrared spectra of water-aprotic organic solvents binary systems	Shigeaki Morita
11:20	11:40	Highly precise characterization of the hydration state upon thermal denaturation of globular protein	Keichiro Shiraga
11:40	12:00	Study on the dynamic state of free, hydrogen-bonded water with wood by near-infrared hyperspectral imaging	Te Ma
12:00	13:00	☞ Lunch break	

## POSTER SPECIALS

Chairperson: Jelena Muncan

13:00	13:15	NIR Spectroscopy and aquaphotomics in Carambola B10 Averrhoa	Siti Anis Dalila Muhammad Zahir
13:15	13:25	Water Changes Spectral Patterns When Perturbed by Sound Frequencies	Ryo Takagi
13:25	13:35	Understanding of Yogurt Bio-Functional Water	Alexander Stoilov
13:30	13:45	<b>SPONSORS</b>	
13:45	14:30	<b>POSTER SESSION II</b>	
14:30	15:00	<b>Post-workshop discussion / Questions &amp; Answers</b>	Jelena Muncan

## FORCES SHAPING THE WATER - BEYOND SENSING TO BIOMODULATION

Chairperson: Justyna Grabska

15:00	15:30	Microwaves and nanosecond electric pulses for analysis and influencing of microtubule systems	Michal Cifra
15:30	16:00	Heretics or pioneers: Viktor Schauburger and Wilhelm Reich - a fresh look	Pierre Madl
16:00	16:20	☞ Coffee break	

## SPECTRAL PATTERN OF BIOMATERIAL - WATER INTERACTION

Chairperson: Masaru Tanaka

16:20	16:50	Spectral imaging and spectroscopic methods for characterizing and monitoring biomaterial/water interactions	Aoife Gowen
16:50	17:10	Aquaphotomics for revealing the interaction between water molecular and surface: Potential applications to predict cell response and biofilm formation	Junli Xu
17:10	17:20	☞ Coffee break	

## SPECTRAL PREPROCESSING FOR AQUAPHOTOMICS

Chairperson: Federico Marini

17:20	17:50	New trends in the pre-processing of near-infrared spectra	Jean Michelle Roger
17:50	18:10	Non-linear regression and artificial neural networks in NIR spectroscopy: insights into fundamental phenomena and impact on practical applications in water-related scenarios	Krzysztof Bec
18:10	18:30	The effects of water on scattering: taking into account path-length modifications	Alexander Mallet
18:30	19:00	<b>POSTER AWARD CEREMONY &amp; CLOSING SPEECH</b>	Roumiana Tsenkova
19:00		☞ Goodbye	

*Until we meet again!*



1

## 2 Near infrared spectroscopy and multivariate analysis for the study of 3 water in lipidic membranes

4 **Jorge J. Wenz** <sup>1,2,\*</sup>

5 <sup>1</sup> Instituto de Investigaciones Bioquímicas de Bahía Blanca, UNS-CONICET, Bahía Blanca, Argentina;

6 <sup>2</sup> Departamento de Biología, Bioquímica y Farmacia, UNS, Bahía Blanca, Argentina.

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8 **Keywords:** Membranes; Water; Near Infrared Spectroscopy; Principal Component Analysis.

### 9 Introduction

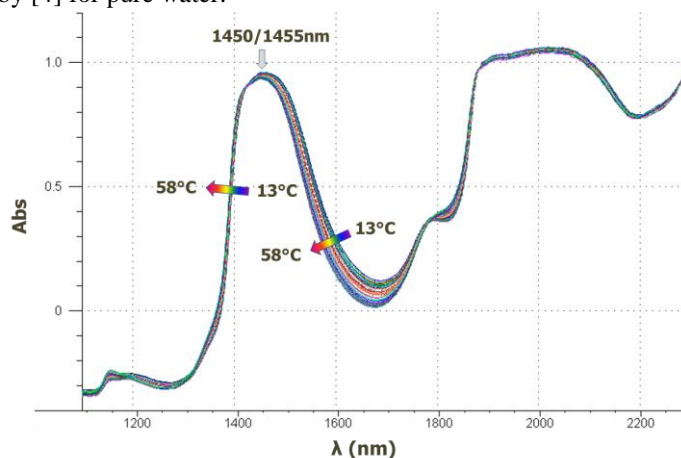
10 The ability of near infrared spectroscopy to inform about the vibrations of the covalent O-H, by means of the  
11 first overtone of water around 1450/55 nm, was exploited to examine the water in membranes and the influence  
12 of the constitutive phospholipids on hydrogen bonding. The less the number and/or the strength of H-bonds, the  
13 more the strength of the O-H bonds and so they vibrate and absorbs radiation at higher frequencies. This shift is  
14 employed to evaluate the water status in membranes composed of two phospholipids having the same acyl chain  
15 but different polar head, the part of the molecule typically associated in the interaction with water.

### 16 Materials and Methods

17 Membrane production: solvent from phospholipids solution was removed with nitrogen flux while rotating the  
18 container, in order to obtain a thin film. MilliQ water was next added, vortexing and sonicating to form the  
19 vesicles, working at temperatures higher than the highest transition temperature of the lipids. NIR spectra and  
20 analysis: absorbance of the suspensions was registered in the 1100-2300 nm interval, between 13-58 °C every  
21 5°C. Principal Components Analysis was employed to disclose the spectral changes [1].

### 22 Results

23 Figure 1 shows the sixty spectra, quite overlapped and unfeasible to discriminate according to phospholipid  
24 (DMPA or DMPC) or concentration (250 or 500 µM). Only the effect of temperature can be barely advised in  
25 some regions (shown by arrows). The localization of the first overtone of water (1450/55 nm) matches with  
26 previous reports [2-4]. The isosbestic region at 1425-1430 nm, is not far from the 1440-1442 nm reported by [5]  
27 and 1446 nm reported by [4] for pure water.



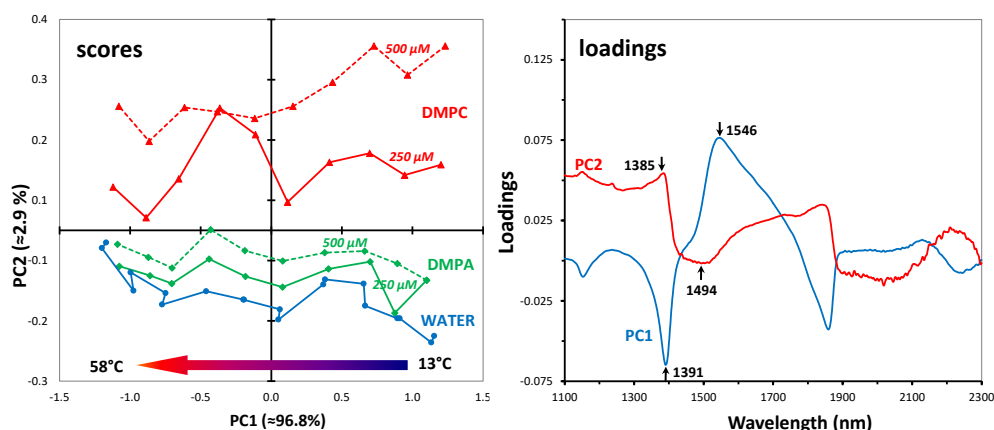
28

29 **Figure 1.** The sixty NIR spectra includes: two water control samples (Milli-Q), a sample of DMPA  
30 (1,2-dimyristoyl-sn-glycero-3-phosphate) and a sample of DMPC

31 (1,2-dimyristoyl-sn-glycero-3-phosphocholine) at two concentrations (250 and 500  $\mu\text{M}$ ). All samples measured  
32 at ten temperatures (every 5°C in the 13-58 °C interval).

33 The simultaneous analysis of scores (Figure 2, left) and loadings (Figure 2, right) discloses useful information.  
34 Scores along PC1 capture the effect of temperature on the hydrogen bonding, whereas scores on PC2 capture  
35 the effect of phospholipids. By far, temperature in the assayed range is the dominating affecting factor (PC1  $\approx$   
36 97 %). As temperature increases, the differences in the effect of phospholipids become smaller, as series  
37 become closer at the highest temperatures.

38 Loadings reveal that increasing temperatures and the presence of phospholipids (particularly DMPC) weaken  
39 water H-bonds, as the O-H vibration band (first overtone) shift to higher frequencies, i.e. higher energy. As  
40 temperature increase, the absorbance increases at shorter (1391 nm) and it decreases at longer (1546 nm)  
41 wavelengths of the water band. To a lesser extent, phospholipids cause similar changes around 1385 and 1494  
42 nm, respectively.



43  
44 **Figure 2.** Output of the PCA, considering the first two PCs. Left panel: scores, where the connecting lines  
45 denote the evolution of samples with temperature, increasing from right to left every 5°C, as indicated by the  
46 arrow. Right panel: loadings plotted against the original variables.

## 47 Conclusions

48 As occurs with increasing temperature, DMPA and DMPC disrupt H-bonding in membranes, and the effect  
49 increases with the concentration.

50 Having identical acyl chain (myristoyl), the absence of OH in the polar head of DMPC may explain why it has  
51 a stronger disrupting effect on H-bonds than DMPA (OH acts as a H-bond donor).

## 52 References

- 53 1. Beeve KR, Pell RJ, Seasholtz MB (1998) Chemometrics: A Practical Guide 1998, John Wiley & Sons,  
54 New York.
- 55 2. Maeda H, Ozaki Y, Tanaka M, Hayashi N, Kojima, T (1995) Near infrared spectroscopy and  
56 chemometrics studies of temperature-dependent spectral variations of water: relationship between  
57 spectral changes and hydrogen bonds. Journal of Near Infrared Spectroscopy 3:191-201.
- 58 3. McCabe WC, Subramanian S, Fisher HF (1970) Near-infrared spectroscopic investigation of the effect  
59 of temperature on the structure of water. The Journal of Physical Chemistry 74(25):4360-4369.
- 60 4. Segtnan VH, Sasic S, Isaksson T, Ozaki Y (2001) Studies on the structure of water using  
61 two-dimensional near-infrared correlation spectroscopy and principal component analysis. Anal Chem  
62 73(13): 3153-3161.
- 63 5. Gowen A.A., Amigo jM, and Tsenkova R (2013) Characterisation of hydrogen bond perturbations in  
64 aqueous systems using aquaphotomics and multivariate curve resolution-alternating least squares. Anal  
65 Chim Acta 759: 8-20.