Aquaphotomics: Past, Present and Future

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水と光

Water and Light

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AQUAPHOTOMICS

Aqua - : water

Photo - : light

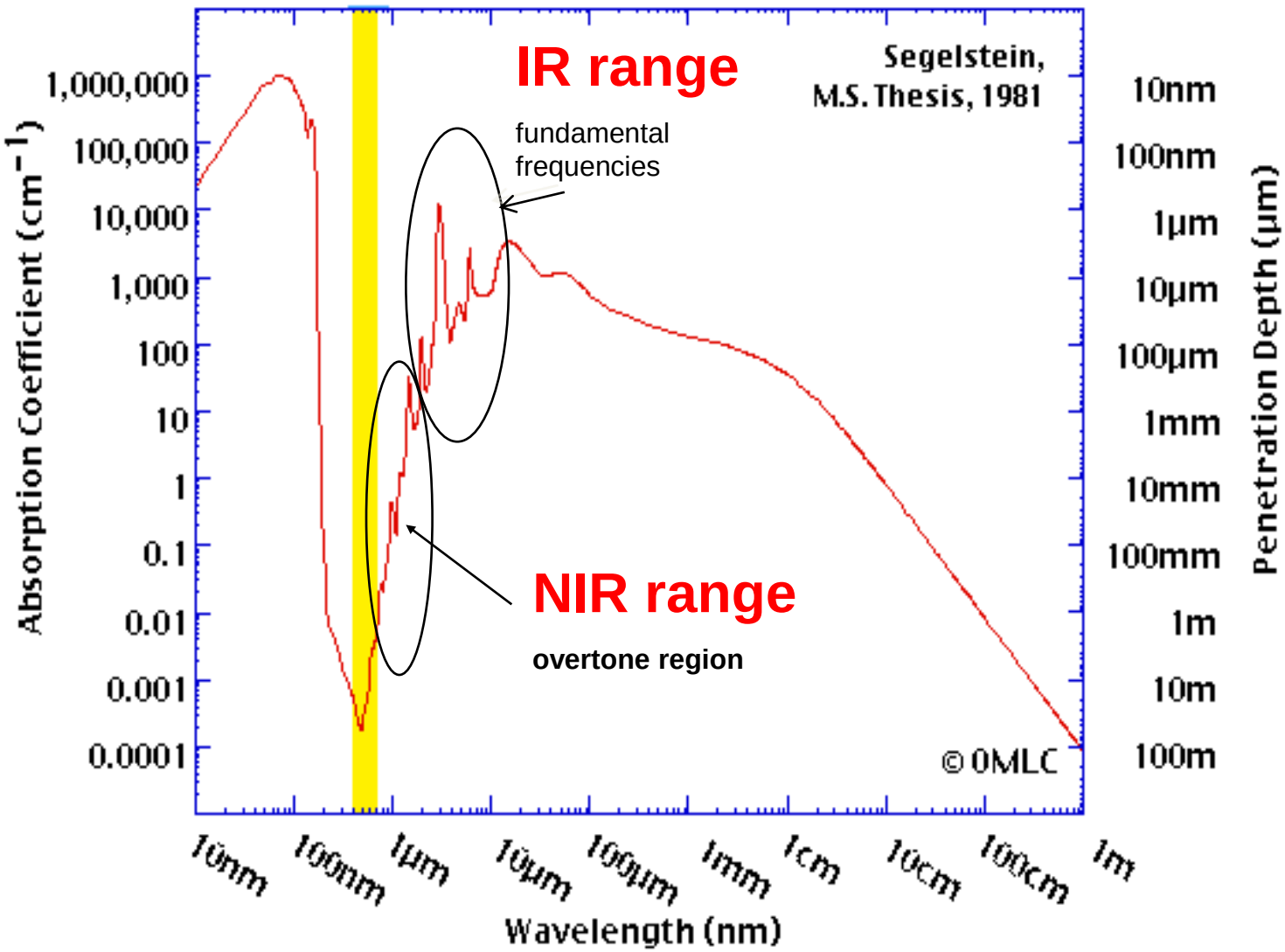
Omics - : all about,

complement of something

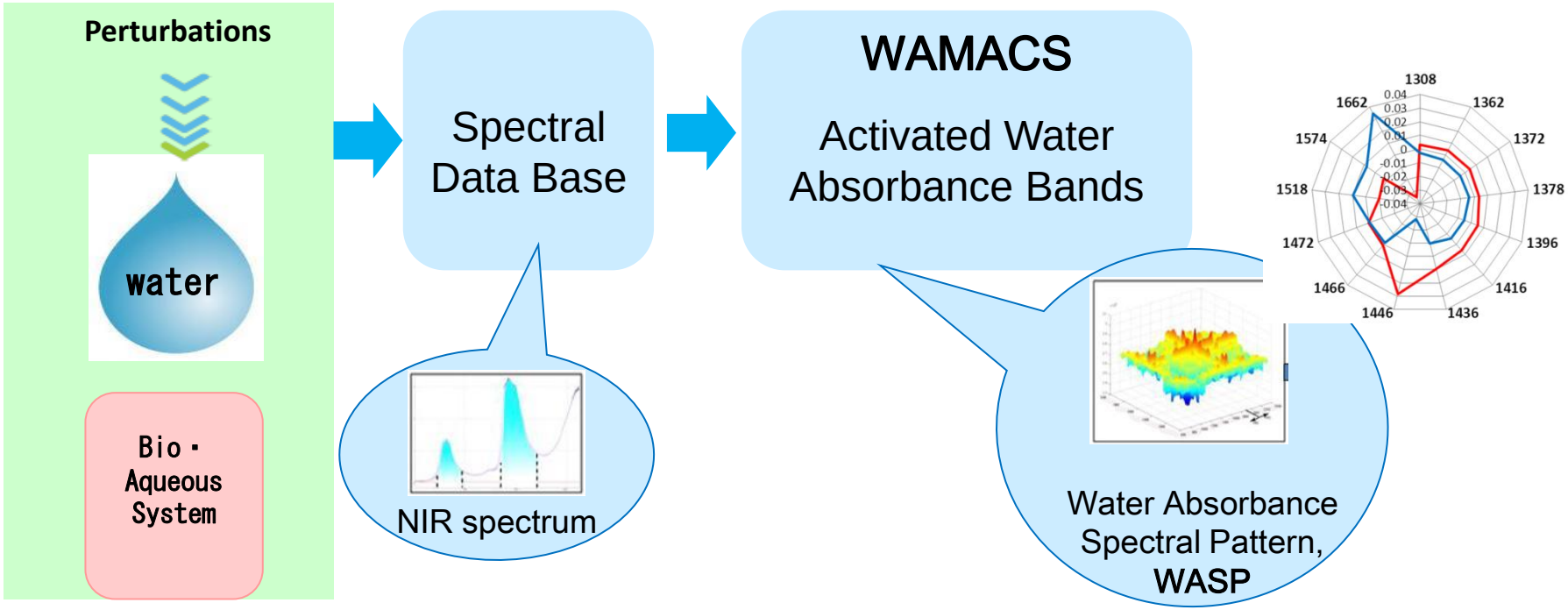
Aquaphotomics concept

Water as molecular mirror

WATER SPECTRUM



AQUAPHOTOMICS:
WATER as a
MOLECULAR MIRROR



WAMACS = Water Matrix Coordinates, i.e. water absorbance bands in VIS-NIR range

AQUAPHOTOME

AQUAPHOTOME

is

the entire complements of

water matrix coodinates

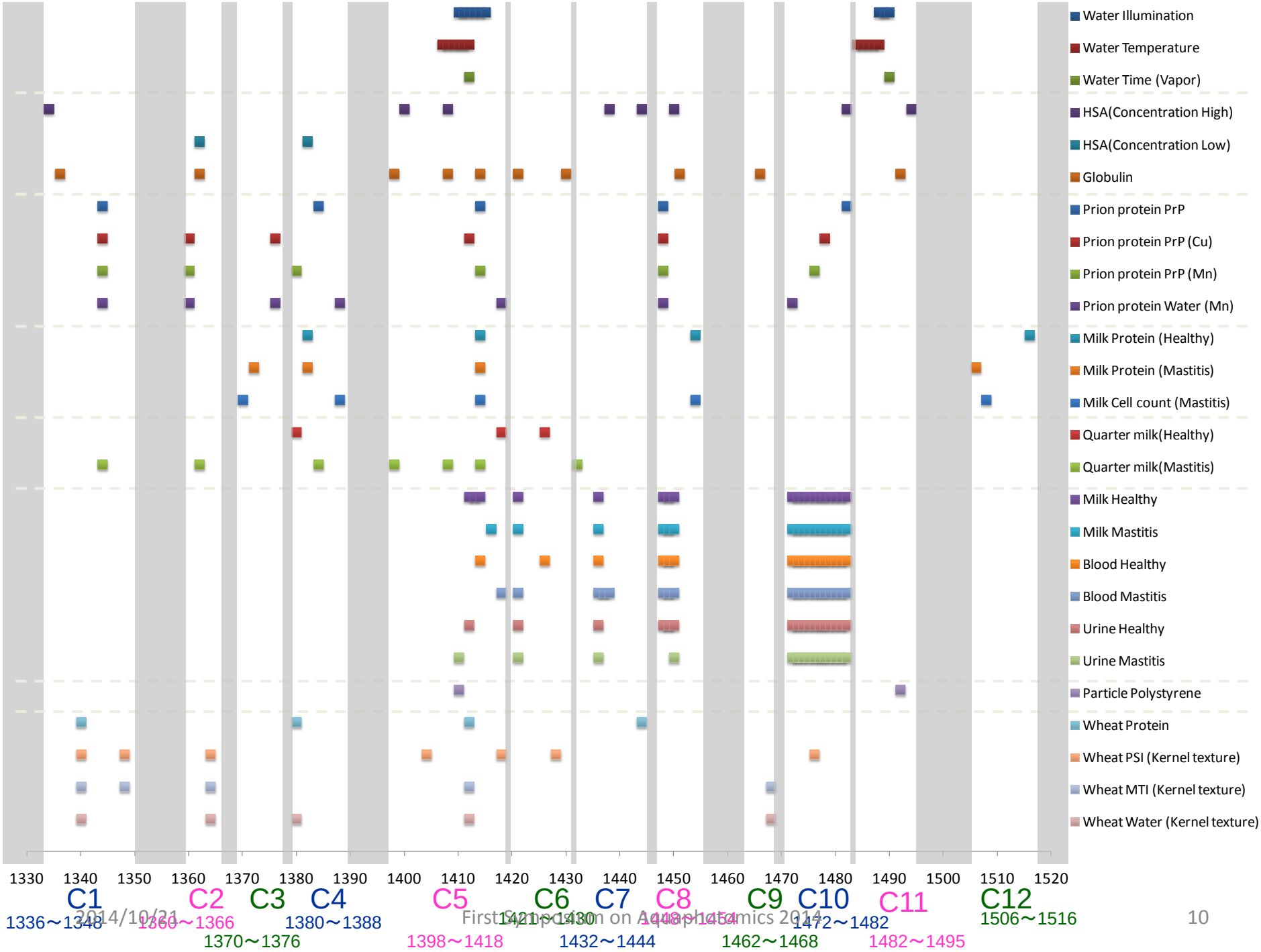
found under

various perturbations

WAMACS

Water Matrix Coordinates:

Water absorbance bands corresponding to pools of water molecules with the same vibration frequency


Water Illumination
Water Temperature
Water Time (Vapor)
HSA(Concentration High)
HSA(Concentration Low)
Globulin
Prion protein PrP
Prion protein PrP (Cu)
Prion protein PrP (Mn)
Prion protein Water (Mn)
Milk Protein (Healthy)
Milk Protein (Mastitis)
Milk Cell count (Mastitis)
Quarter milk(Healthy)
Quarter milk(Mastitis)
Milk Healthy
Milk Mastitis
Blood Healthy
Blood Mastitis
Urine Healthy
Urine Mastitis
Particle Polystyrene
Wheat Protein
Wheat PSI (Kernel texture)
Wheat MTI (Kernel texture)
Wheat Water (Kernel texture)
1330 1340 1350 1360 1370 1380 1390 1400 1410 1420 1430 1440 1450 1460 1470 1480 1490 1500 1510 1520
C1 1336～1348
C2 1360～1366
C3 1370～1376
C4 1380～1388
C5 1398～1418
C6 1421～1430
C7 1432～1444
C8 1448～1454
C9 1462～1468
C10 1472～1482
C11 1482～1495
C12 1506～1516

Assignment

<u>C1</u> - 1336-1348 (1342)nm – ν_3
1344nm H2O - 2 ν_3 (Siesler, Ozaki, Kawata, & Heise, 2001)*
1340nm liquid water/moisture (Williams, 2009)

<u>C2</u> - 1360-1366 (1364)nm – OH-$(H_2O)_1$, OH-$(H_2O)_2$, OH-$(H_2O)_4$
1360nm 1st overtone free OH stretch (OH-(H2O)4) - 3675cm^{-1} (Robertson, Diken, Price, Shin, & Johnson, 2003)
1366nm 1st overtone OH- stretch (OH-(H2O)2) - 3660cm^{-1} (Robertson et al., 2003)

<u>C3</u> - 1370-1379 (1374)nm – $\nu_1 + \nu_3$
1379.3nm H2O - v1 + v3 – 7250cm^{-1} (Siesler et al., 2001)
1379.3nm overtone of stretching vibration – 7250cm^{-1} (Kuroda, Hamano, Mori, Yoshikawa, & Nagao, 2000)
1373 nm first overtone of $2\nu_{OH}$ (Lakshmi Reddy, Padma Suvarna, Udayabhaska Reddy, Endo, & Frost, 2014)

<u>C4</u> - 1380-1388 (1384)nm – OH-$(H_2O)_1$, OH-$(H_2O)_4$, O_2-$(H_2O)_4$
1383.15nm 1st overtone interwater / DD stretch (OH-(H2O)4) - 3615cm^{-1} (Robertson et al., 2003)
1381nm H2O-ν_{1+} ν_3 (Cattaneo, Cabassi, Profaizer, & Giangiacomo, 2009)

Water Absorbance Pattern, WAP

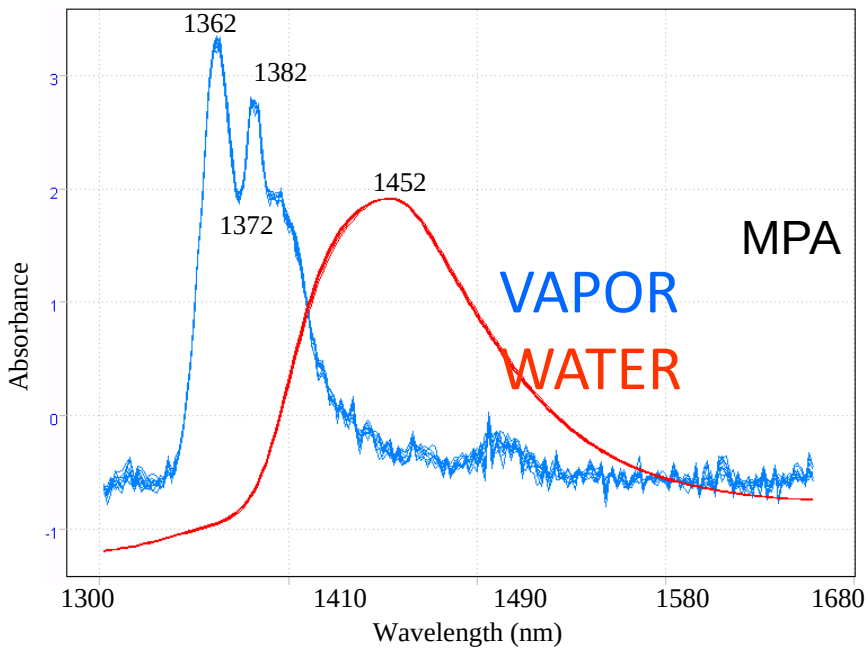
AQUAGRAM

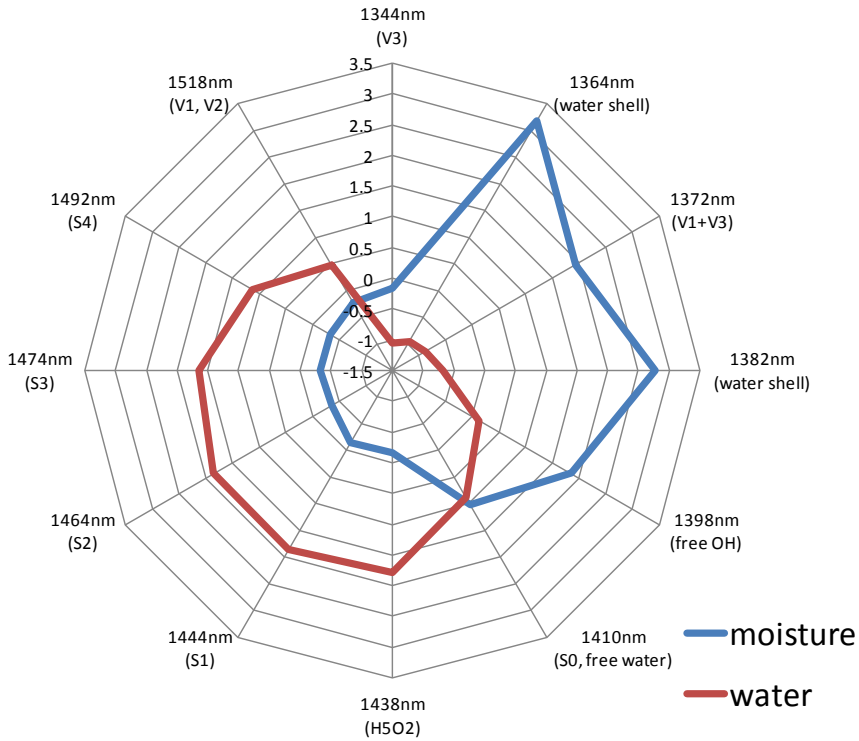
Aquagram was devised to **visualize the WASP.**

The aquagram displays **normalized absorbance values at specific water** bands on the axes originating from the center of the graph.

Absorbance values at the WAMACs are placed on the respective radial axes.

WATER and VAPOR SPECTRA and AQUGRAM



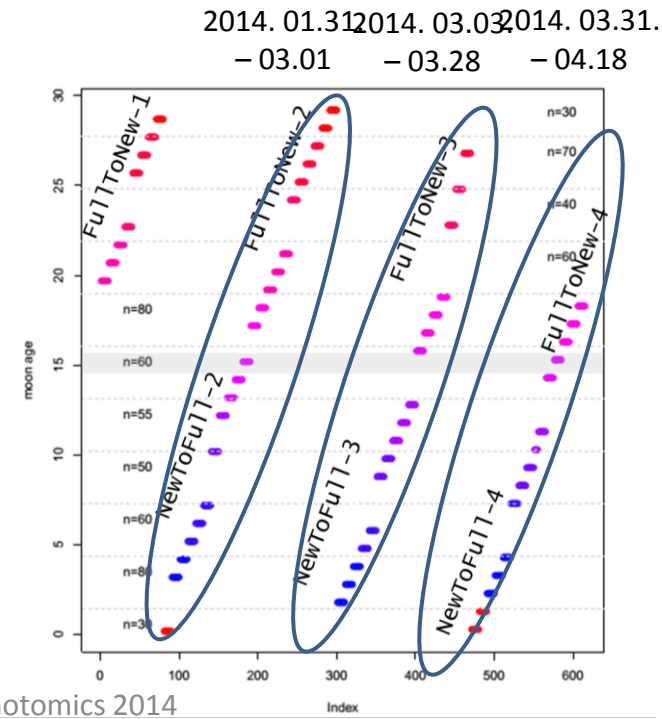


$$A'_{\lambda} = \frac{A_{\lambda} - \mu}{\sigma}$$

A : Absorbance after EMSC (1300-1600 nm)
μ : Mean of Averaged spectra
σ : SD of absorbance each wave length

Aquagrams of different waters at different moon stages

three repeats



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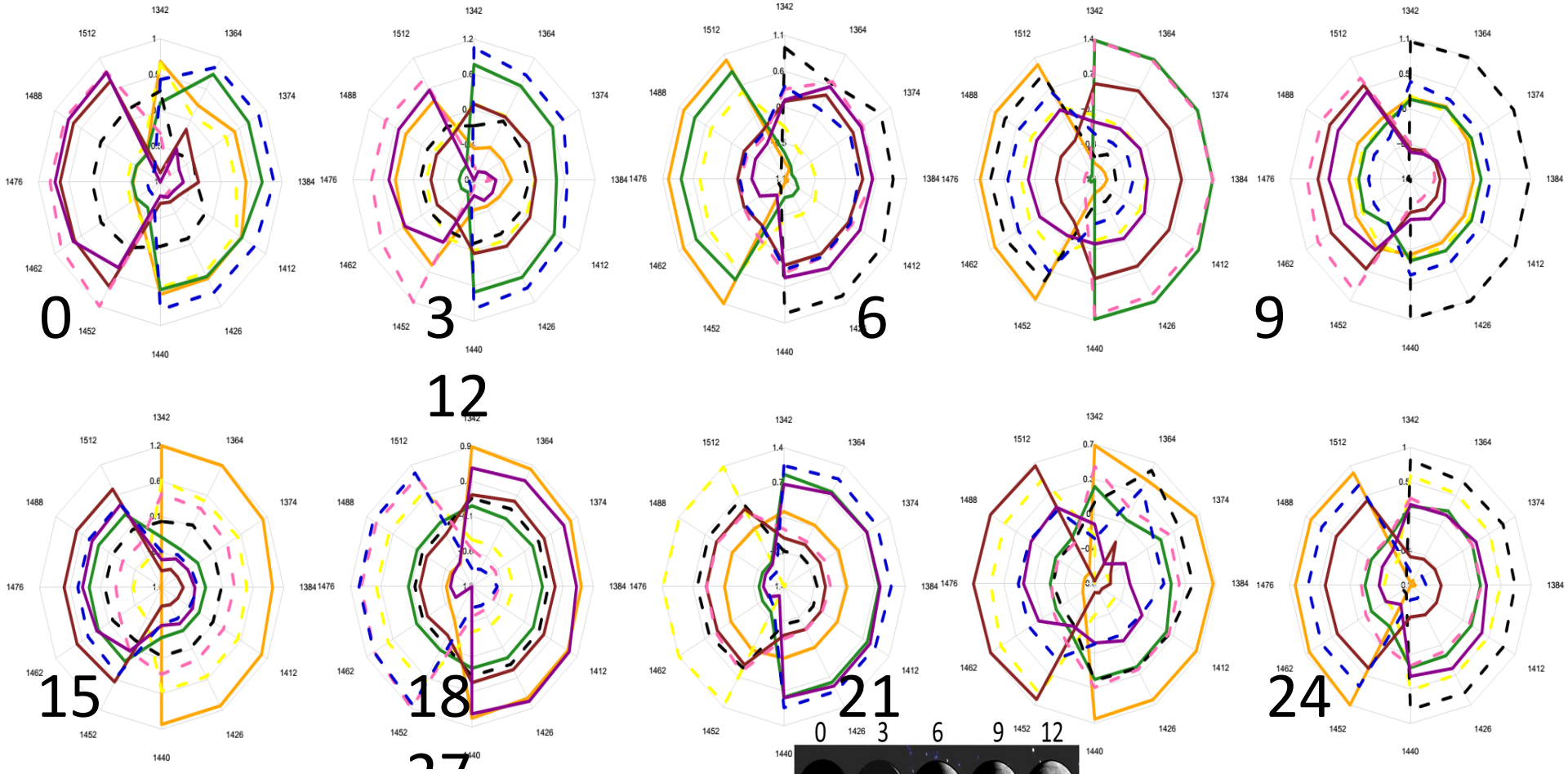
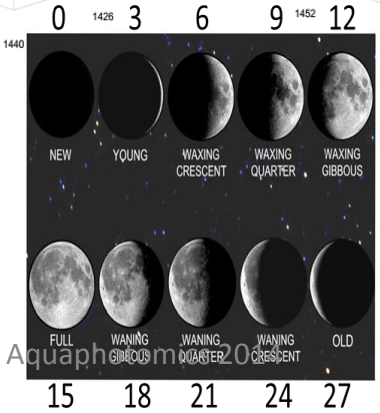
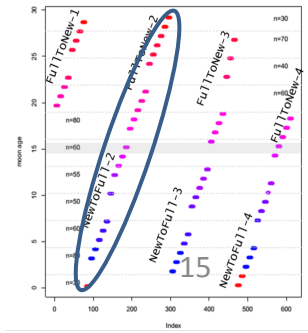
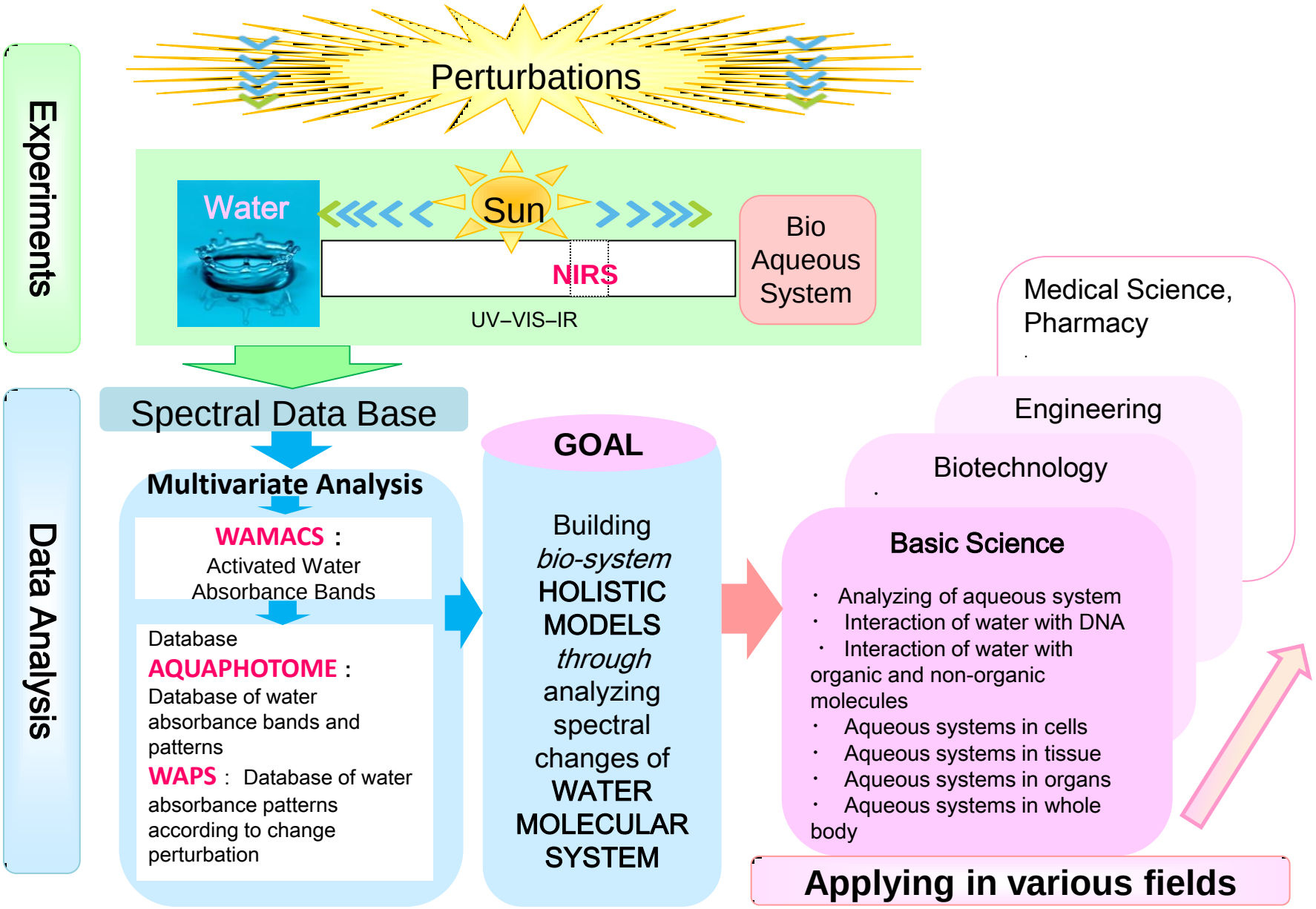


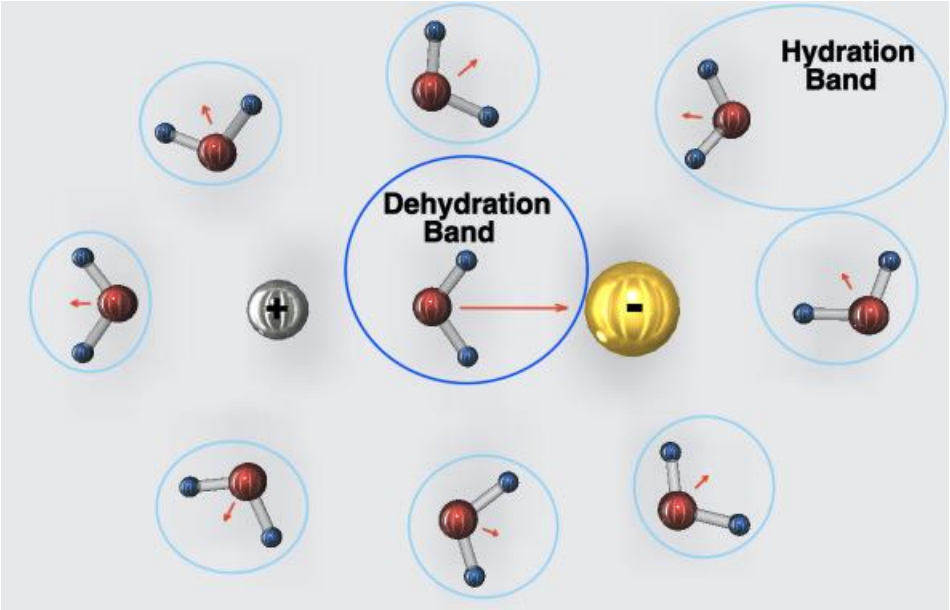
- Bronze Water
- Gold Water
- Kongo W1 (G:S:B=5:6:7)
- Kongo W2 (G:S:B=8:7:6)
- Kongo W3 (G:S:B=6:6:6)
- Purified Water
- Silver Water
- Tsukino Shizuku Water






Experiments
Perturbations
Water
Sun
NIRS
UV–VIS–IR
Bio Aqueous System
Data Analysis
Spectral Data Base
Multivariate Analysis
WAMACS : Activated Water Absorbance Bands
Database
AQUAPHOTOME : Database of water absorbance bands and patterns
WAPS : Database of water absorbance patterns according to change perturbation
GOAL
Building bio-system HOLISTIC MODELS through analyzing spectral changes of WATER MOLECULAR SYSTEM
Medical Science, Pharmacy
Engineering
Biotechnology
Basic Science
・ Analyzing of aqueous system
・ Interaction of water with DNA
・ Interaction of water with organic and non-organic molecules
・ Aqueous systems in cells
・ Aqueous systems in tissue
・ Aqueous systems in organs
・ Aqueous systems in whole body
Applying in various fields

Water dipole markedly altered for water molecules trapped in local field of ions



Kojić D., Tsenkova R, Tomobe K, Yasuoka K, and Yasui M., "Water confined in the local field of ions", ChemPhysChem, in press. [DOI : 10.1002/cphc.201402381R1]

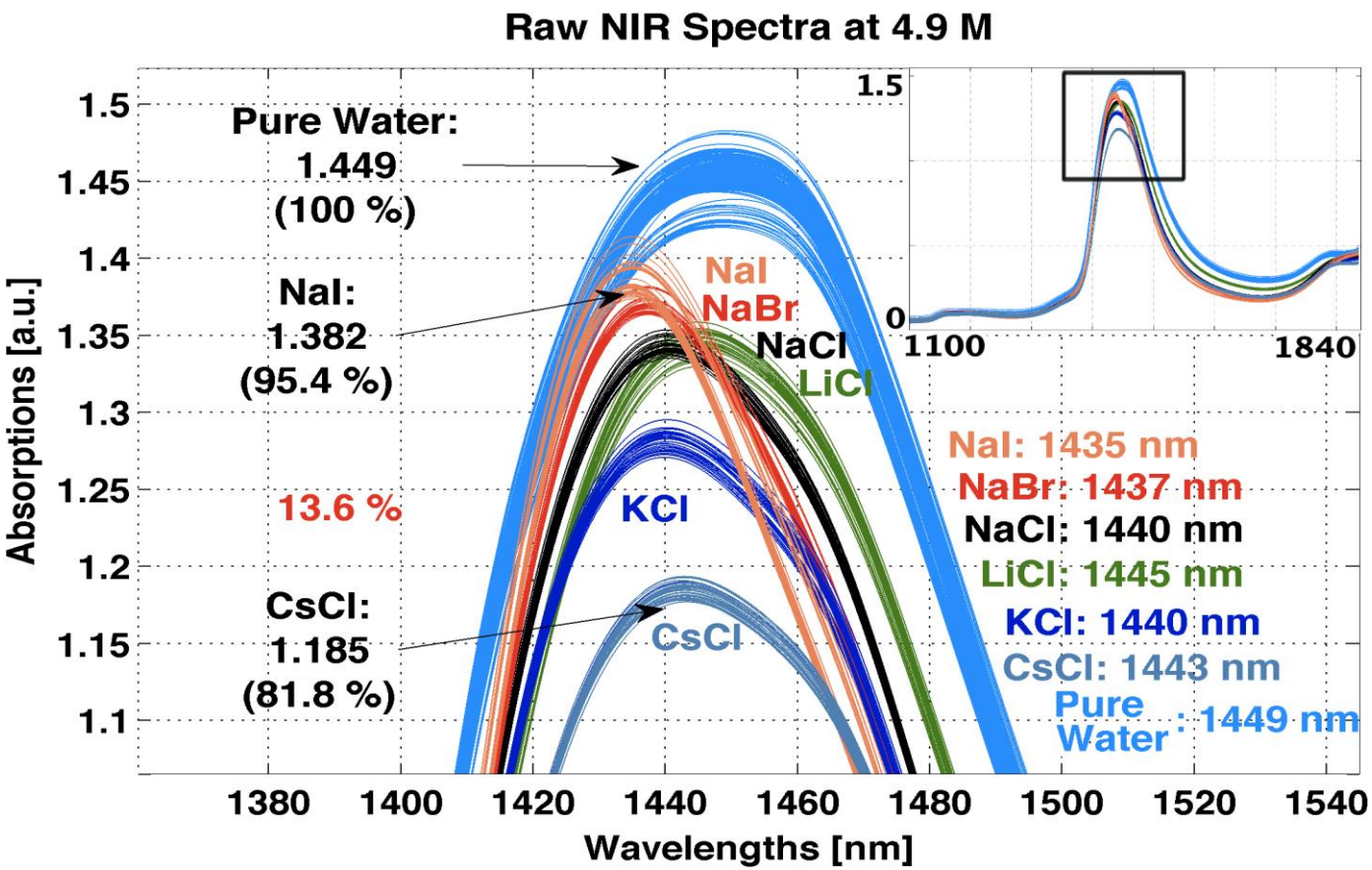


Figure : First overtone peak (raw spectra) of pure water and ionic solutions, at highest concentration level.
Difference in O—H bond absorption between highest (NaI) and lowest (CsCl) absorbing solution exhibits an unusual range of variation (13.6%, in red) which decreases with dilution.

Kojić D., Tsenkova R, Tomobe K, Yasuoka K, and Yasui M., "Water confined in the local field of ions", ChemPhysChem, in press. DOI : 10.1002/cphc.201402381R1

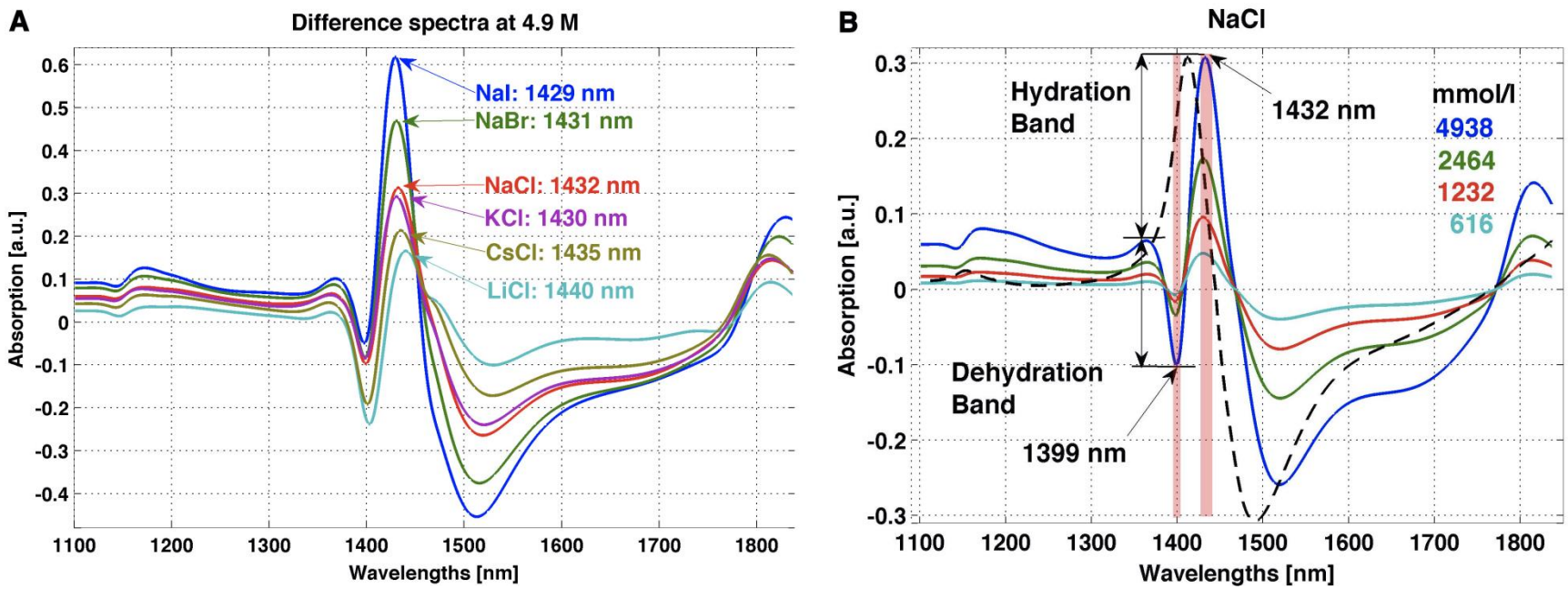


Figure : Panel A: difference spectra for all ions at 4.9 M.

Panel B: difference spectra of NaCl solution (averaged for each concentration level). Black dashed line: spectrum of pure water under thermal perturbation shows two common bands at 1412 and 1492 nm (elaborated in figure S1).

Solution spectra show two features:

1) band around 1432 nm, generated by shifting of pure water band (centered around 1412 nm) due to presence of ions named Hydration Band (HBand),

2) new band located between 1395-1403nm, named Dehydration Band (DBand), not observed in spectrum of pure water, generated at higher concentration levels, and previously reported in analysis of biological systems

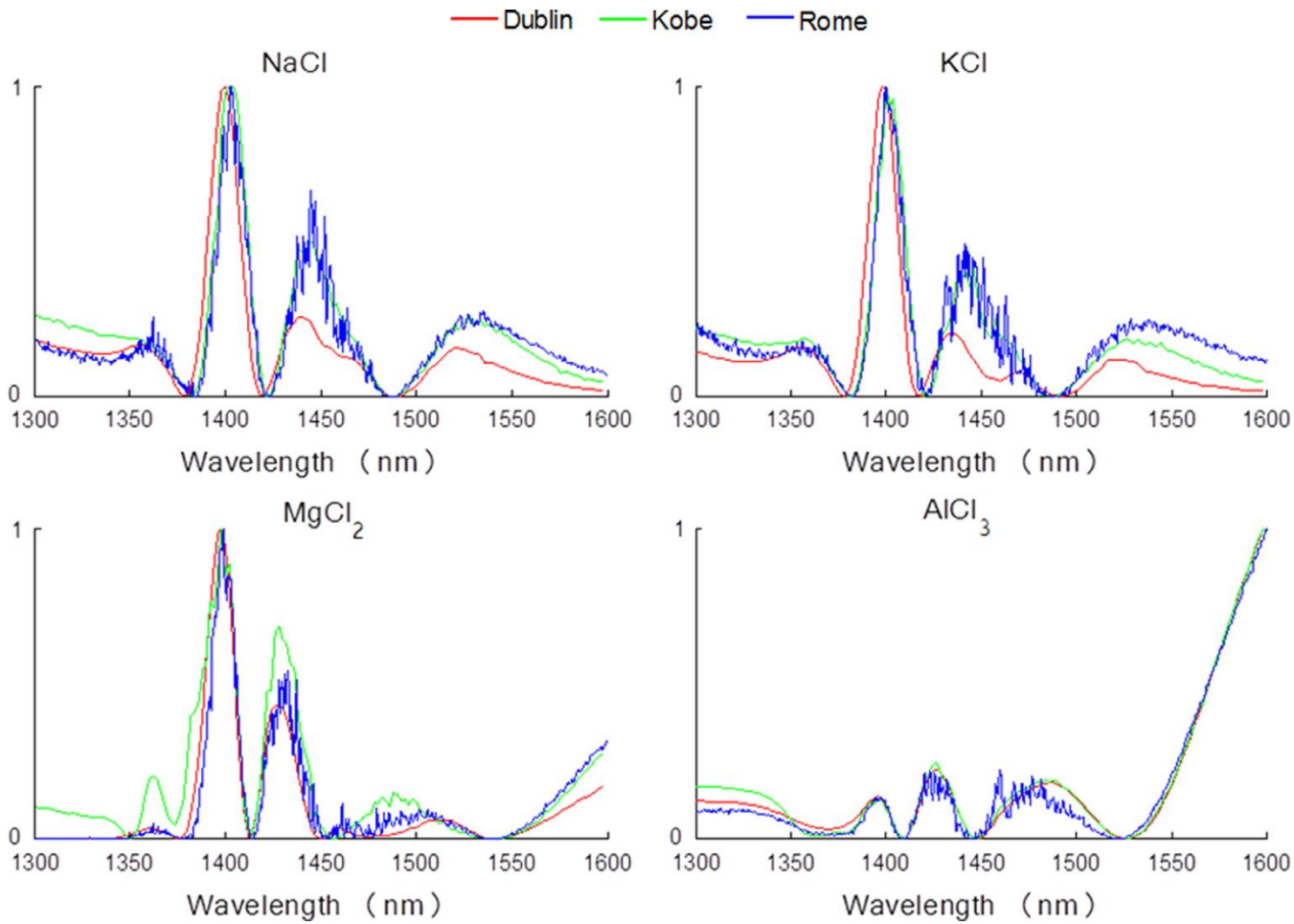
Kojić D., Tsenkova R, Tomobe K, Yasuoka K, and Yasui M., "Water confined in the local field of ions", ChemPhysChem, in press. [DOI : 10.1002/cphc.201402381R1]

Evaluation of quantitative models for prediction of salt concentration in solutions obtained at multiple geographical locations for testing

Concentration: 0.002–0.1molL
(equivalentto117–13,334ppm
0.0001–0.01%mass/mass)

A.A.Gowen et al./Talanta131(2015)609–618 615

- Aqueous solutions of 4 salts (NaCl, KCl, MgCl2, AlCl3) were prepared using Millipore water (Millipore,Molsheim,France, resistance20 m Ω).
- Ten concentrations (**0.002,0.004,0.006,0.008,0.01,0.02, 0.04, 0.06, 0.08, 0.1molL1**) were prepared for each salt.
- Three locations: Dublin, Kobe, Rome



First Principal component loading for salt solutions (afterSNV and EMSC pretreatment). The variations seen here (representing >85% of total variance in each data set) are related to changes in hydrogen bonding induced by the addition of salts

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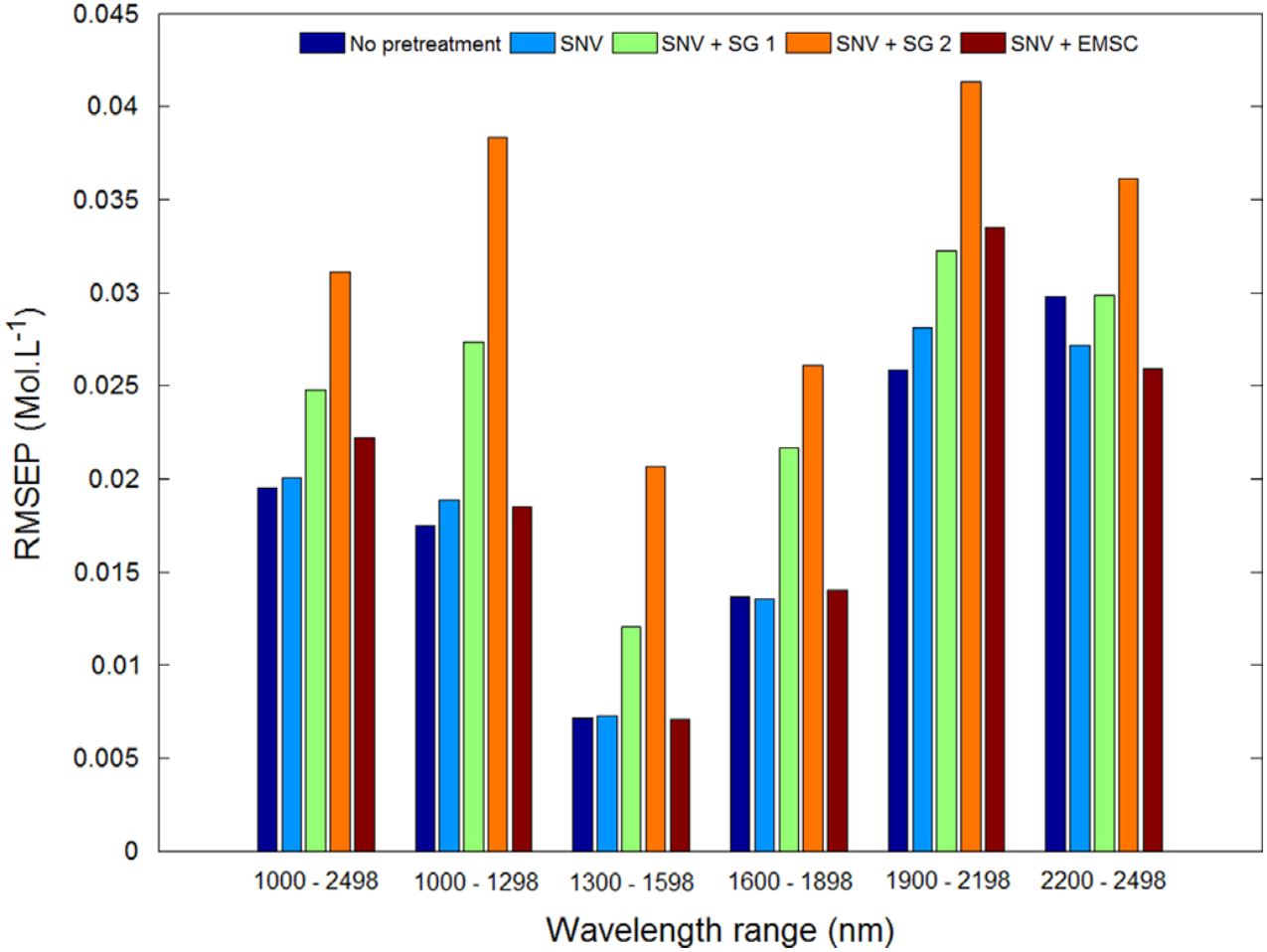


Root mean squared error of prediction(RMSEP) averaged over test locations, salt and permuted experimental test day, plotted as a function of pretreatment and wavelength range studied (SNV¼standard normal variate, EMSC extended multiplicative signal correction).

A.A.Gowen et al./ Talanta 131 (2015) 609–618

Unique transformations of water structure for the amyloidogenic nucleation

Chatani E, Tsuchisaka Y, Masuda Y, Tsenkova R (2014) Water molecular system dynamics associated with amyloidogenic nucleation as revealed by real time near infrared spectroscopy and aquaphotomics.PLoS ONE 9(7): e101997. doi:10.1371/journal.pone.0101997

Human insulin dissolved in 25 mM HCl containing 100 mM NaCl at a concentration of **0.5 - 3.0 mg/ml**.

The fibrillation reaction was initiated by jumping the temperature of the protein solution sealed inside a quartz liquid sample cell with a 1-mm optical path length to 75° C, and then was kept constant until the completion of the NIR measurement.

NIR transmission spectra were monitored in the range of 400-2500 nm region every 1 min in transmittance mode with a step size of 2 nm by NIR spectrophotometer (MPA, Bruker Optics, Germany).

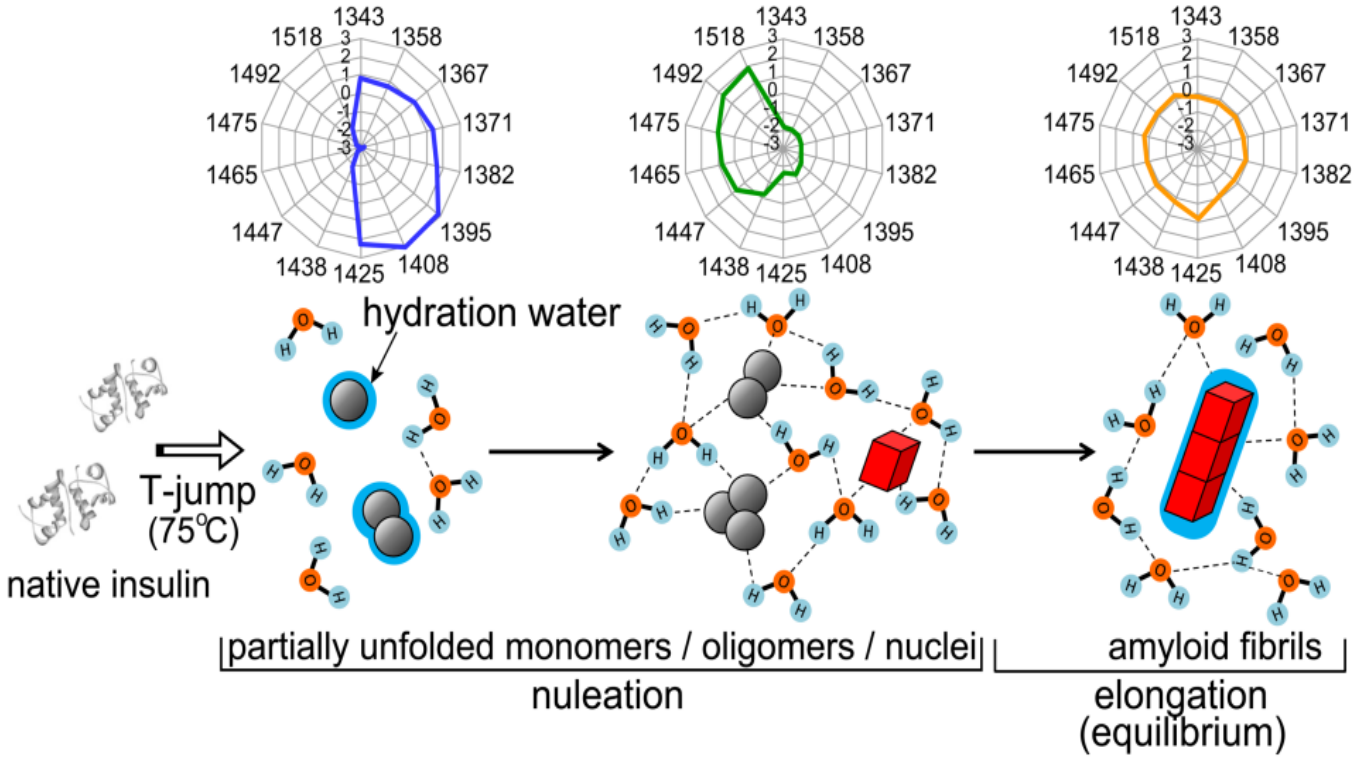
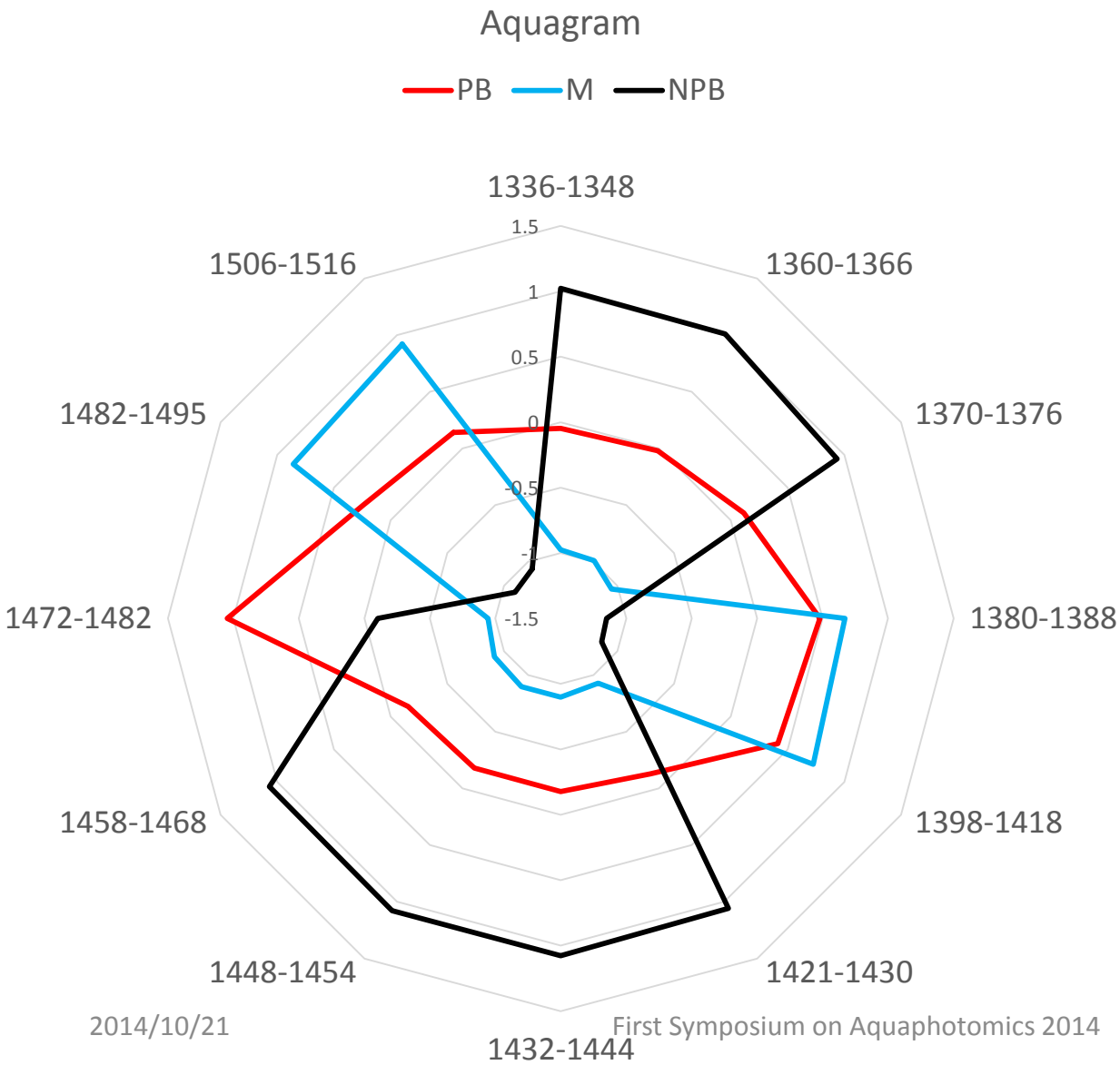


Figure: Schematic illustration representing multi-step transformation of water structures during thefibril formation.

In the **nucleation phase**, **free water molecules and hydrating water** onto protein molecules are dominated initially, but **afterwards hydrogen-bonded water networks are developed**, which is considered essential for nucleation by interlinking protein molecules softly. In the **elongation phase**, the **hydrogen bonds were decayed** gradually towards the state observed in bulk water, and **slight increasing of hydrated water onto amyloid fibrils** was also observed.

Chatani E, Tsuchisaka Y, Masuda Y, Tsenkova R (2014) Water molecular system dynamics associated with amyloidogenic nucleation as revealed by real time near infrared spectroscopy and aquaphotomics.PLoS ONE 9(7): e101997. doi:10.1371/journal.pone.0101997

Probiotic (PB) Medium (M) Non Probiotic (NPB) Lactic Acid Bacteria



Average spectra of every strain

↓

MSC transformation

↓

Averaging absorbance based on WAMACS, which means absorbances were averaged in every wavelength range defined in WAMACS

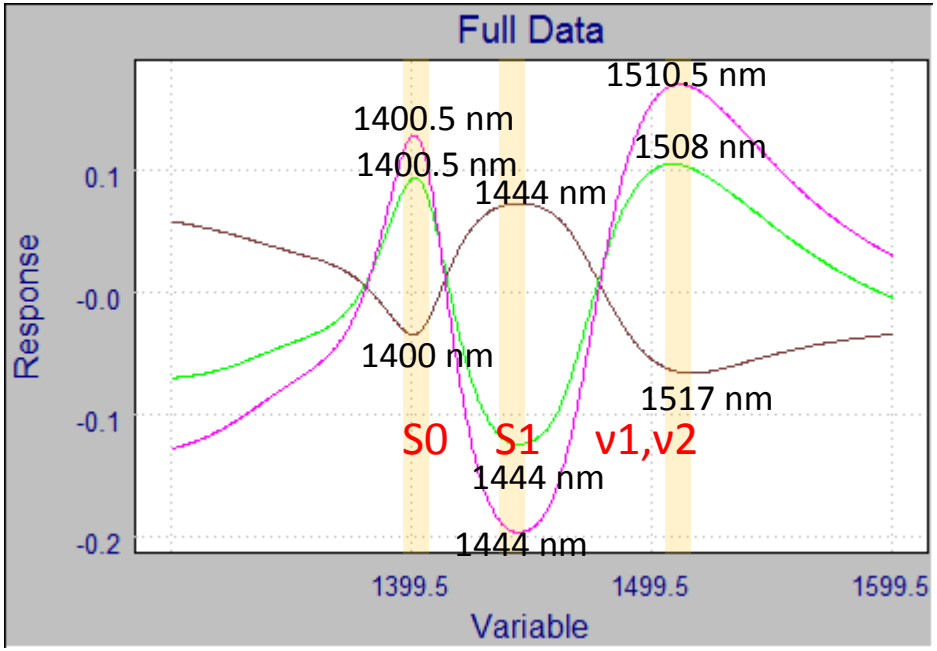
↓

Aquagram culculation

$$Aqg = \frac{X_{MSC,mean} - \overline{X_{MSC,mean}}}{SD}$$

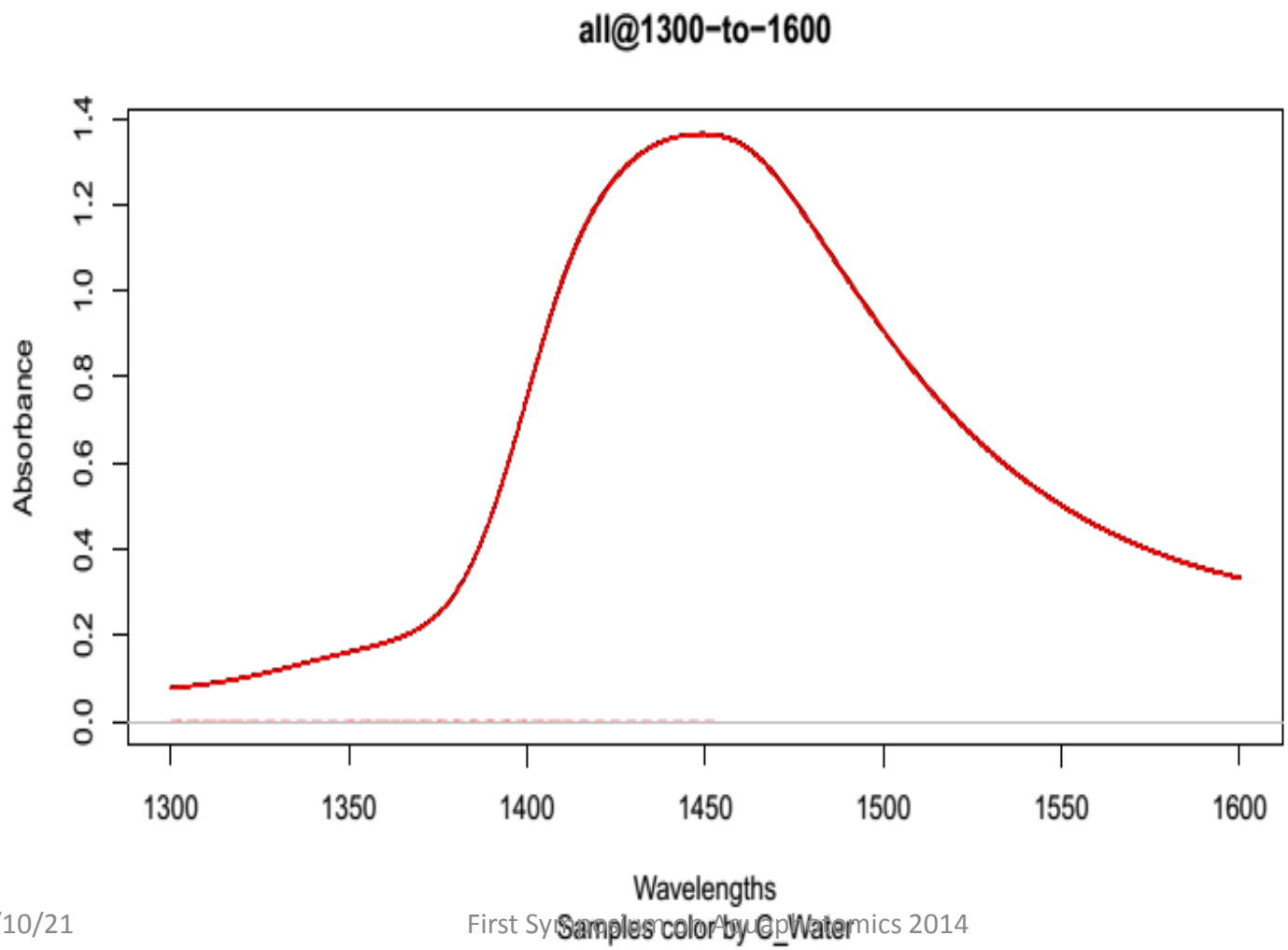
Probiotic (PB) Medium (M) Non Probiotic (NPB) Lactic Acid Bacteria

PB-M
PB-NPB
M-NPB



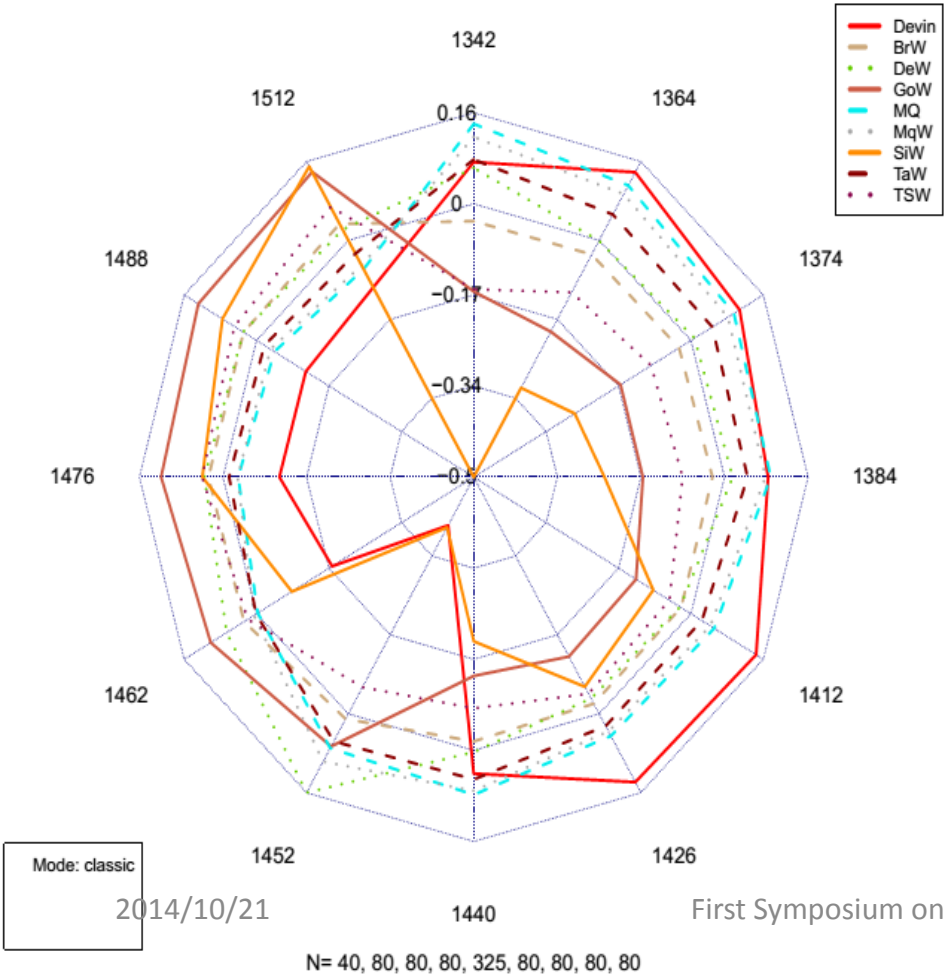
Spectra showed specific pattern derived from S0, S1, v1, v2 and they can be the main difference between bacterial tolerance to digestive fluids.

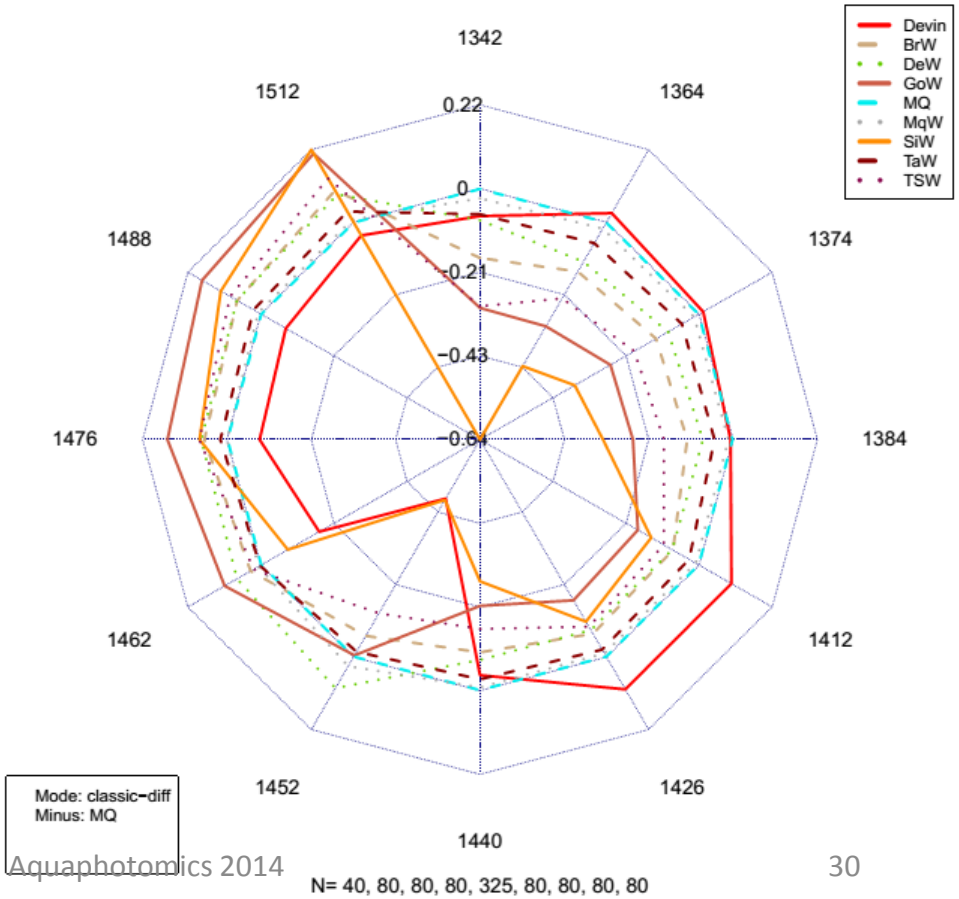
First overtone raw absorbance spectra of Mineral Water and MQ water



Aquagram of water samples and mQ

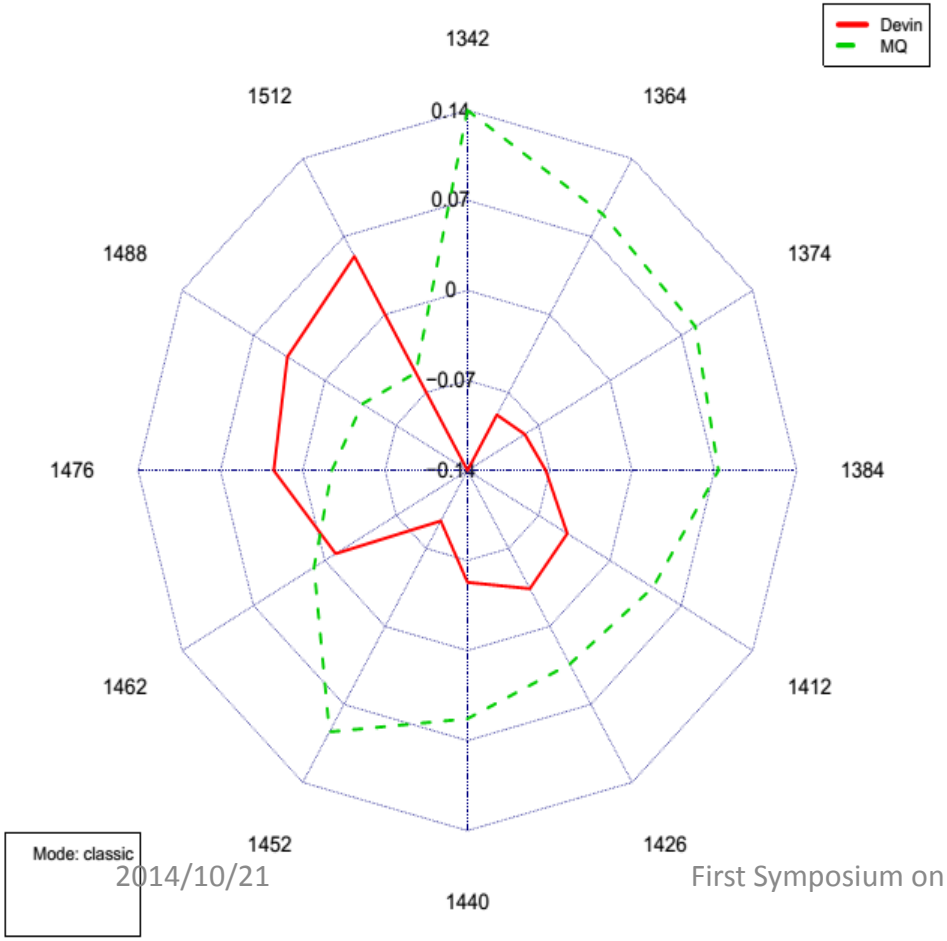
All dates

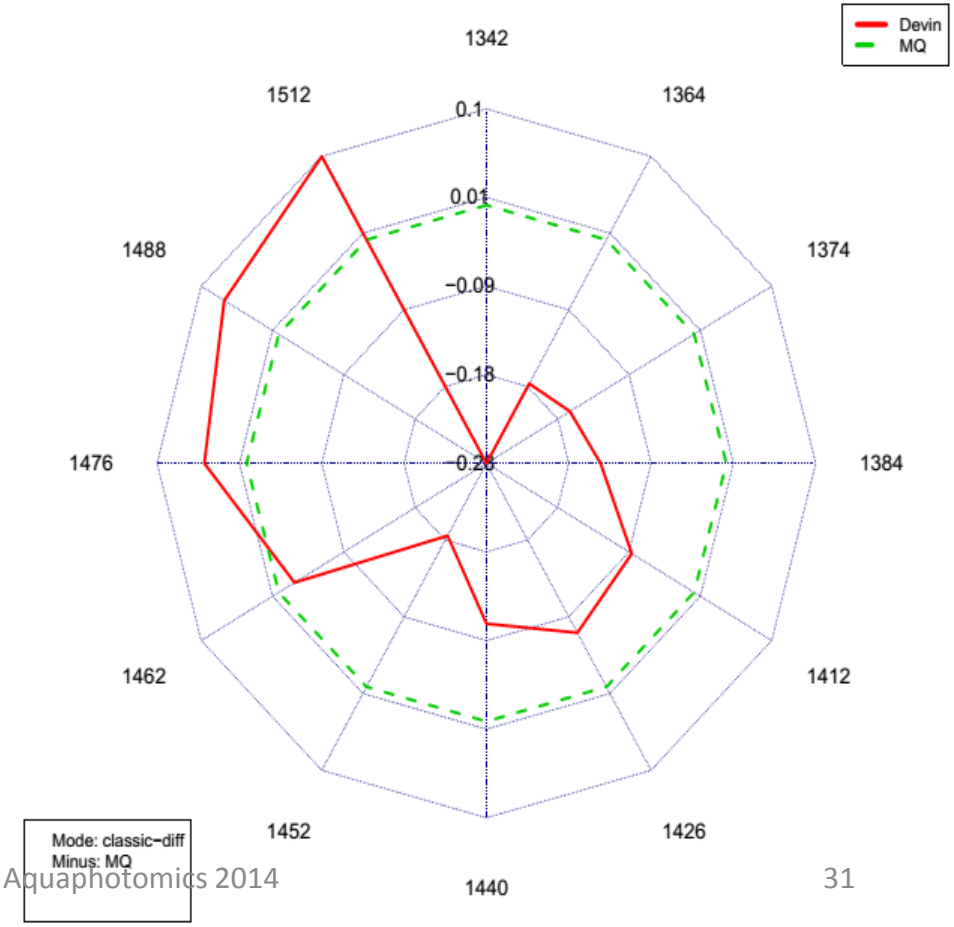




Aquagram of Mineral Water and mQ

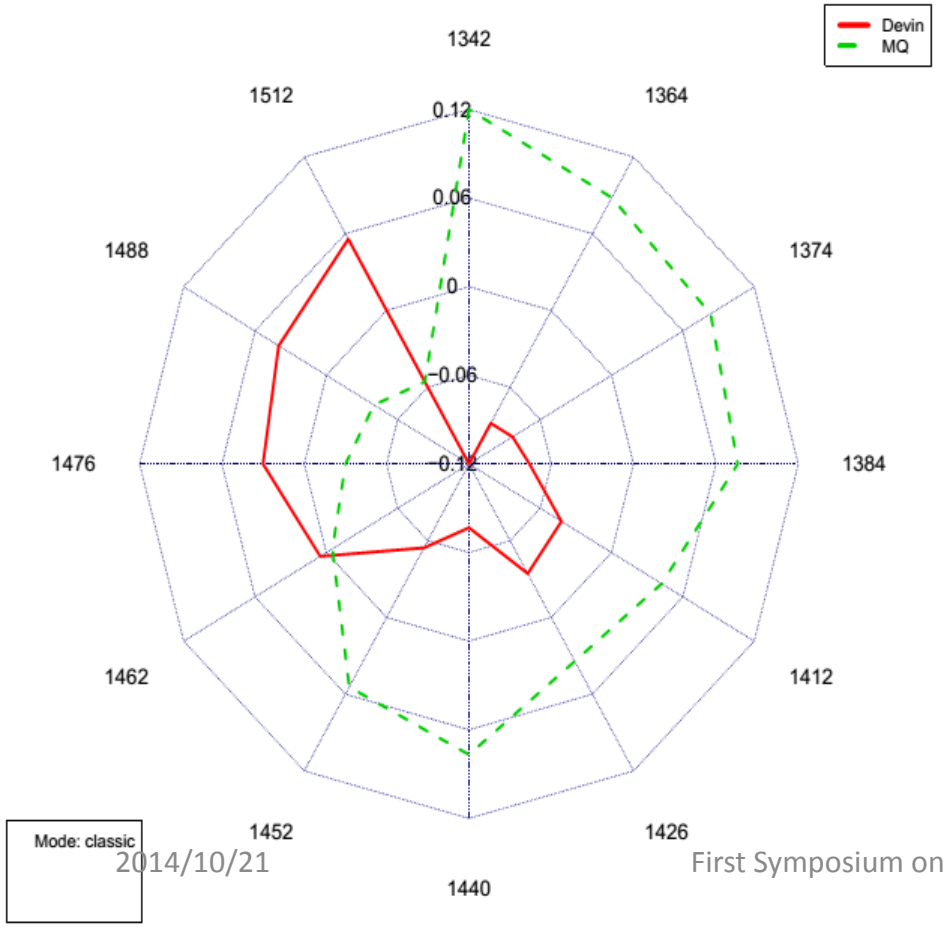
Sept 22

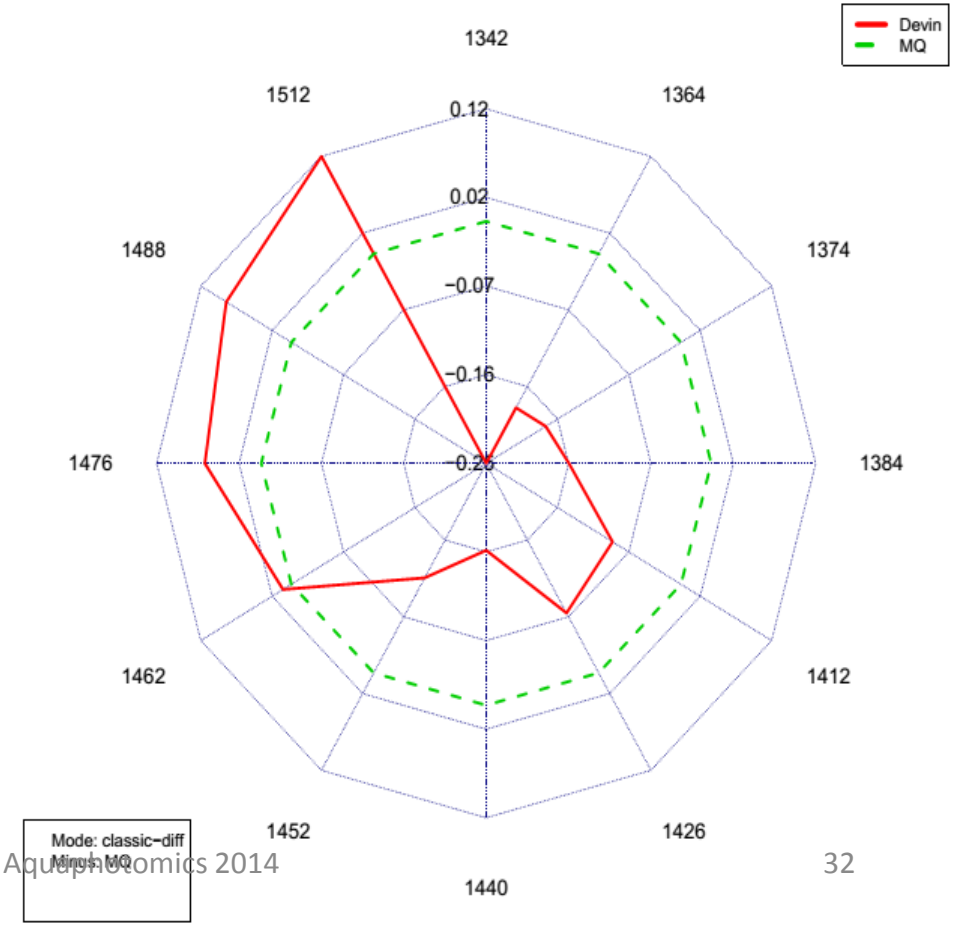




Aquagram of Mineral Water and mQ

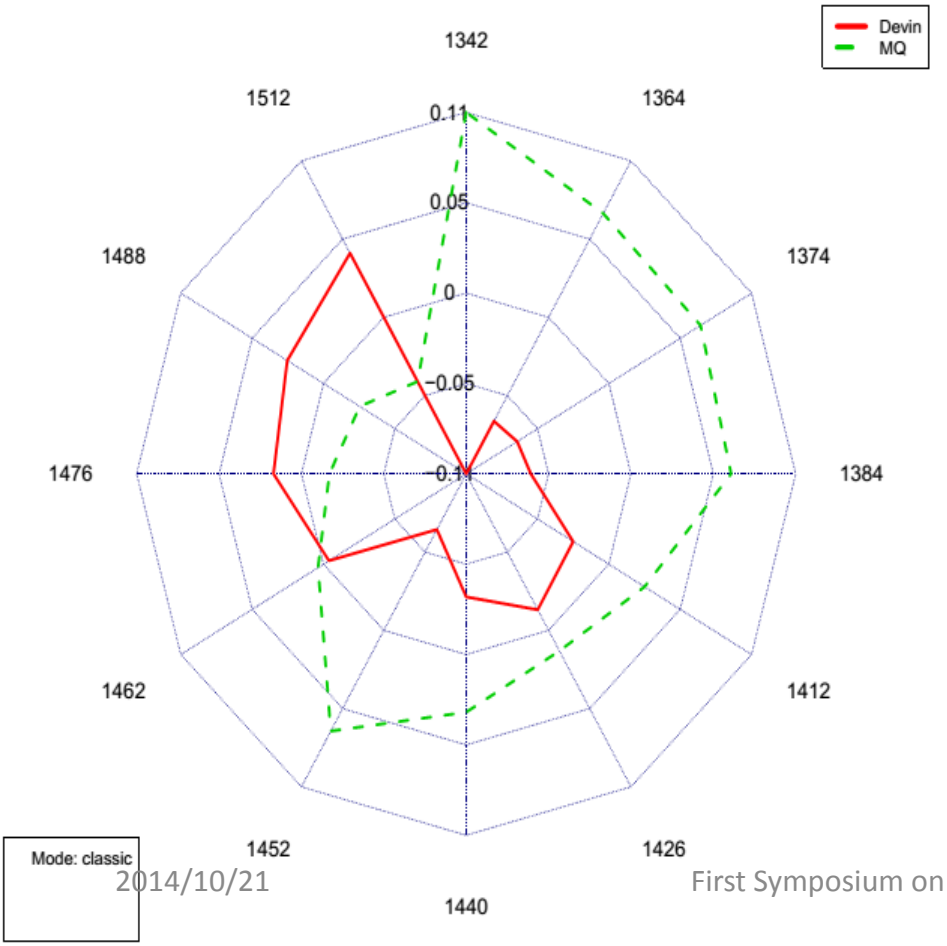
Sept 23

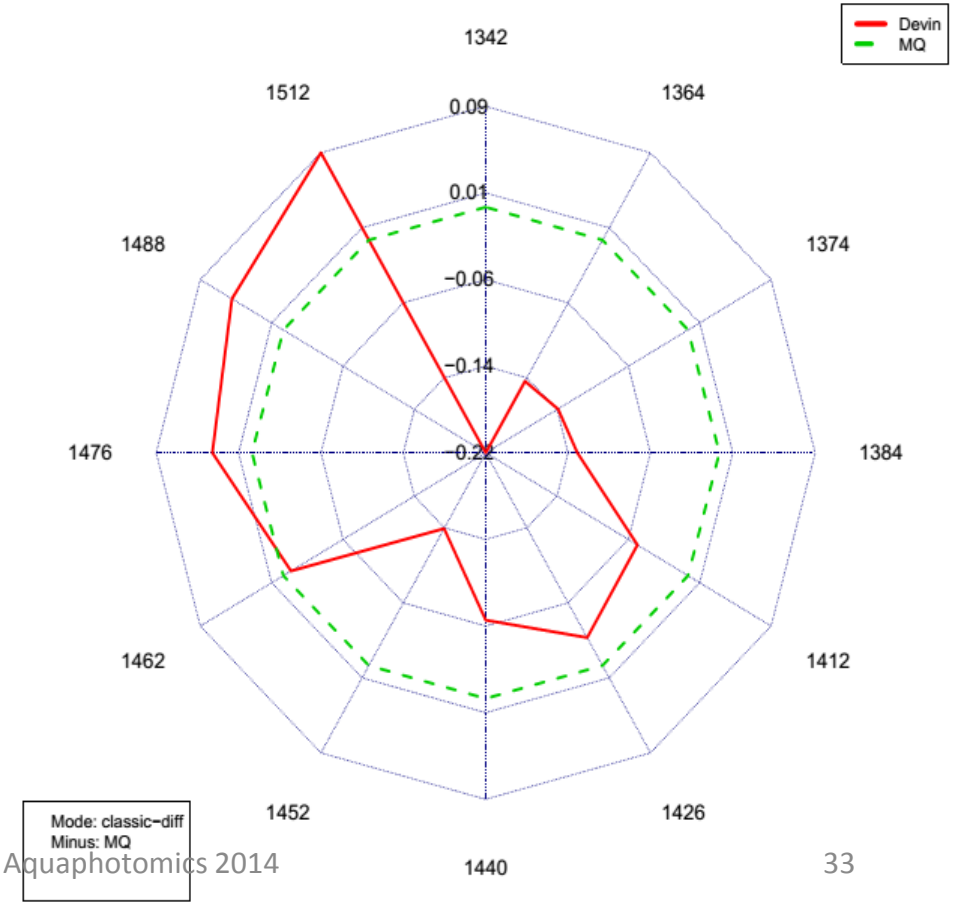




Aquagram of Mineral Water and MmQ

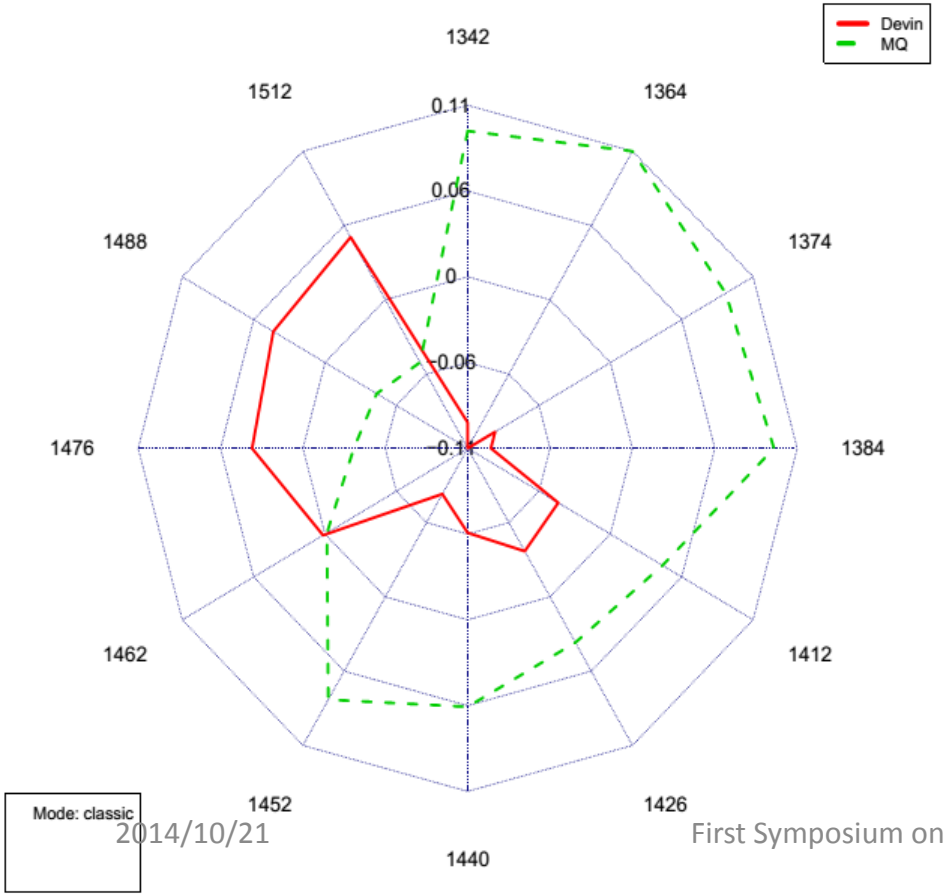
Sept 24

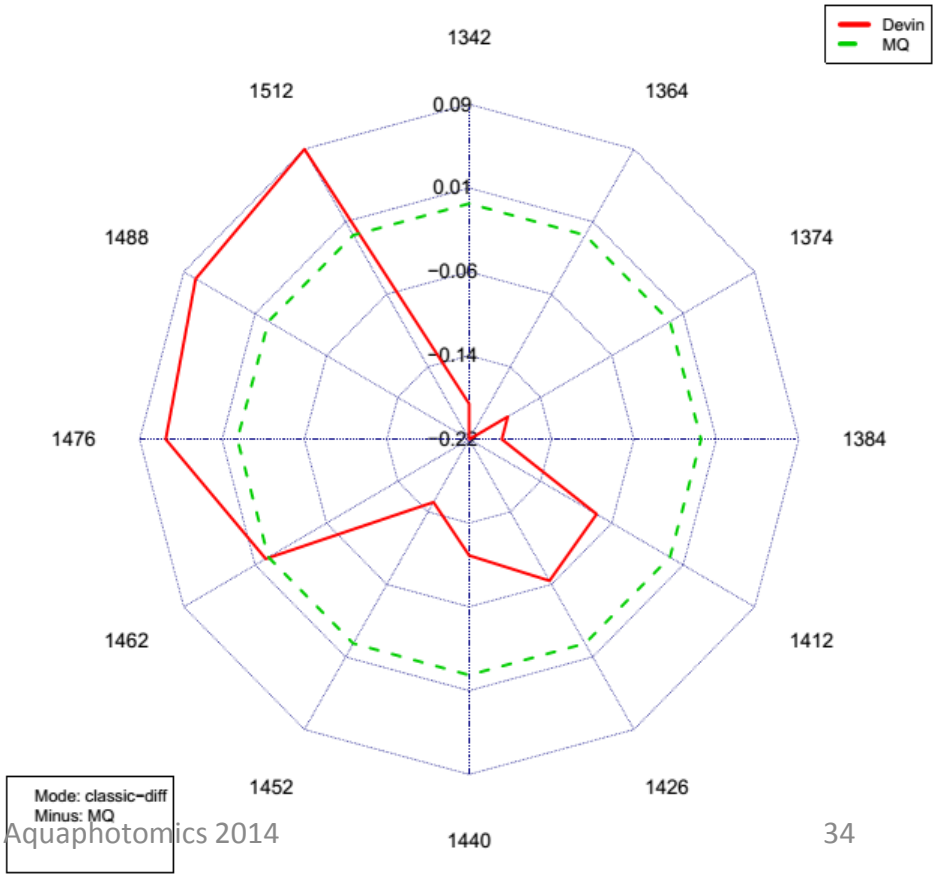




Aquagram of Mineral Water and mQ

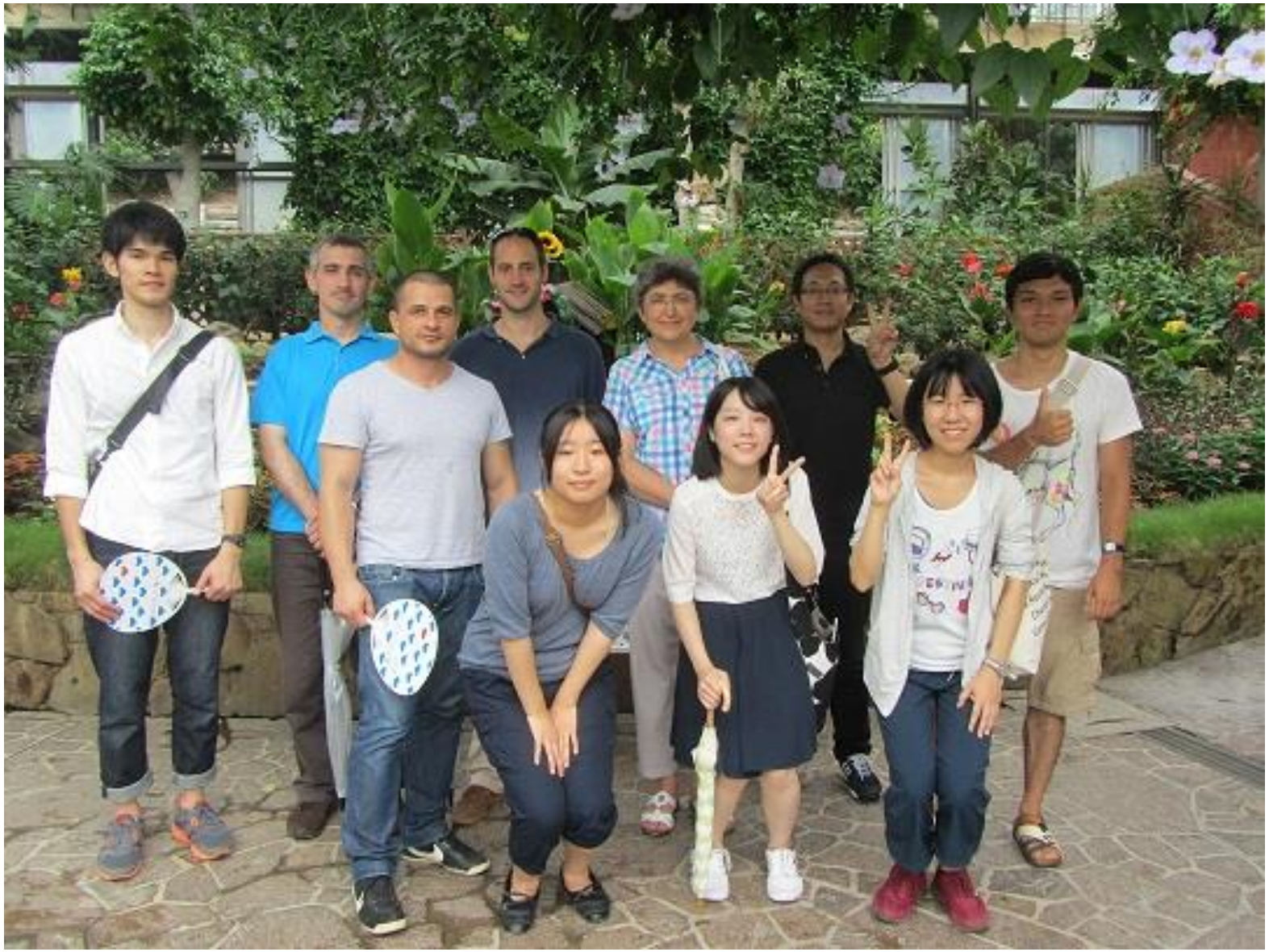
Sept 25





FUTURE

- Water Vocabulary: letters (water bands), words (spectral patterns), sentences (water functionality)
- Basic well known phenomena and reactions should be explained with added knowledge about water
- Education about water on a large scale



水の音
光の遊び
生きている

Sound of a stream,
Sunlight dancing on waters,
Life wakes up again.

R. Tsenkova, 2004


Aquaphotomics
WATER AS MOLECULAR MIRROR