Application of Aquaphotomics to learn more about the rules of water

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Aquaphotomics: Understanding Water in Biology
2nd International Symposium

Kobe University, Faculty of Agriculture

Self introduction

CORVINUS UNIVERSITY of BUDAPEST
Faculty of Food Science

SZENT ISTVÁN UNIVERSITY

- 2000-2002 technical college:

  Baker and Confectioner Technician

- 2007 Diploma

  Food engineer

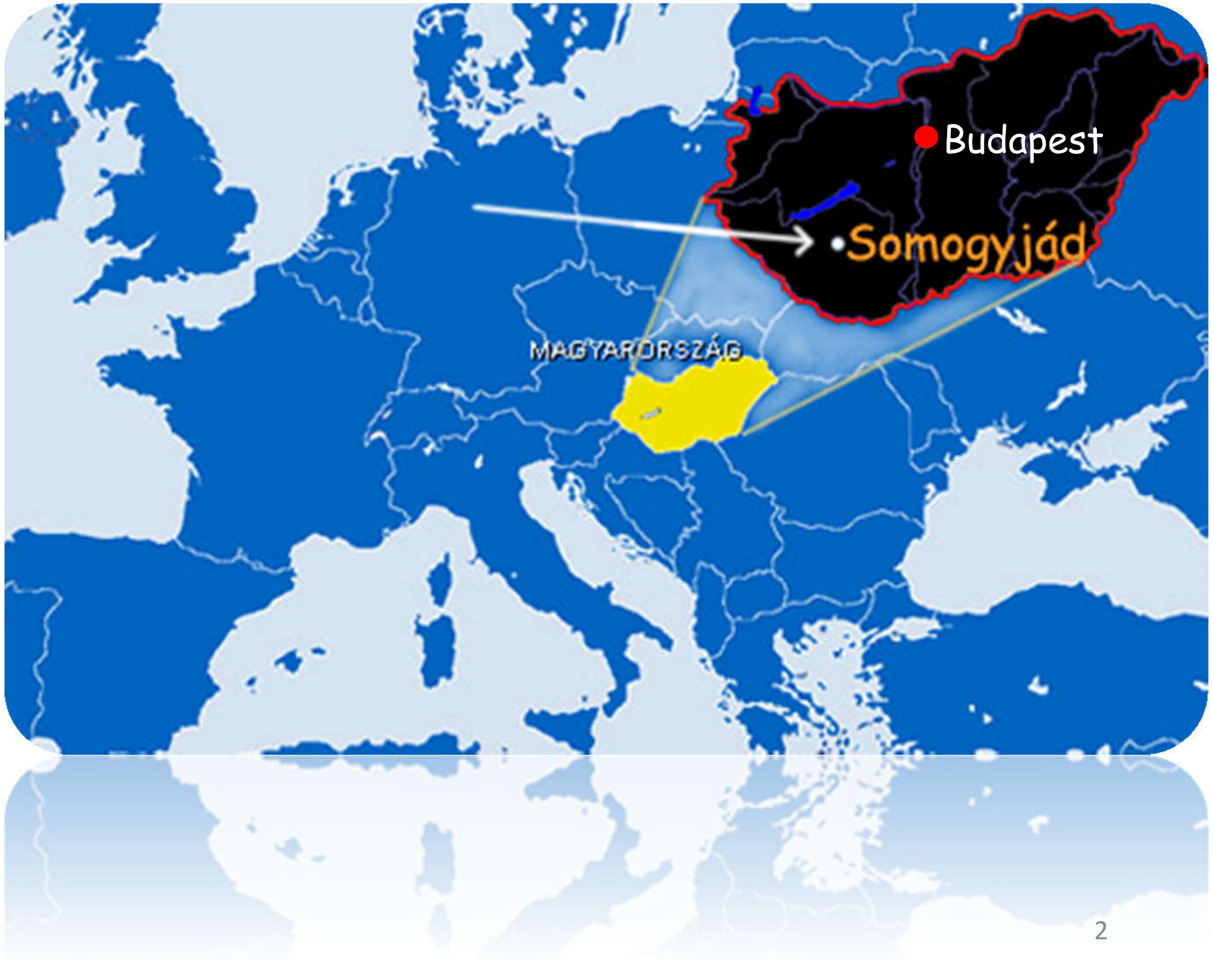
- 2012 PhD

  Food Science

chemometrics

- 2013-2016 Post-Doc

  Aquaphotomics



Agenda of the presentation

- Bacteria growing and Yogurt
- Plant cells growing
- Mineral Waters
- Calculation and presentation method of WASP

Application of Aquaphotomics to learn more about the rules of water

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Agenda of the presentation

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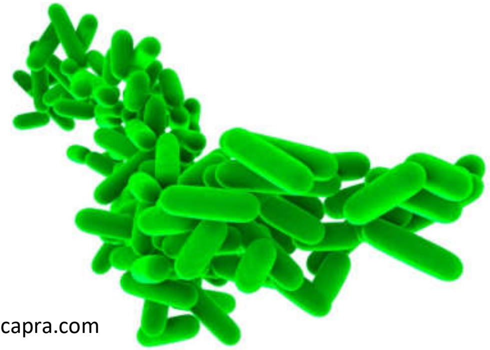
Experiments with bacteria



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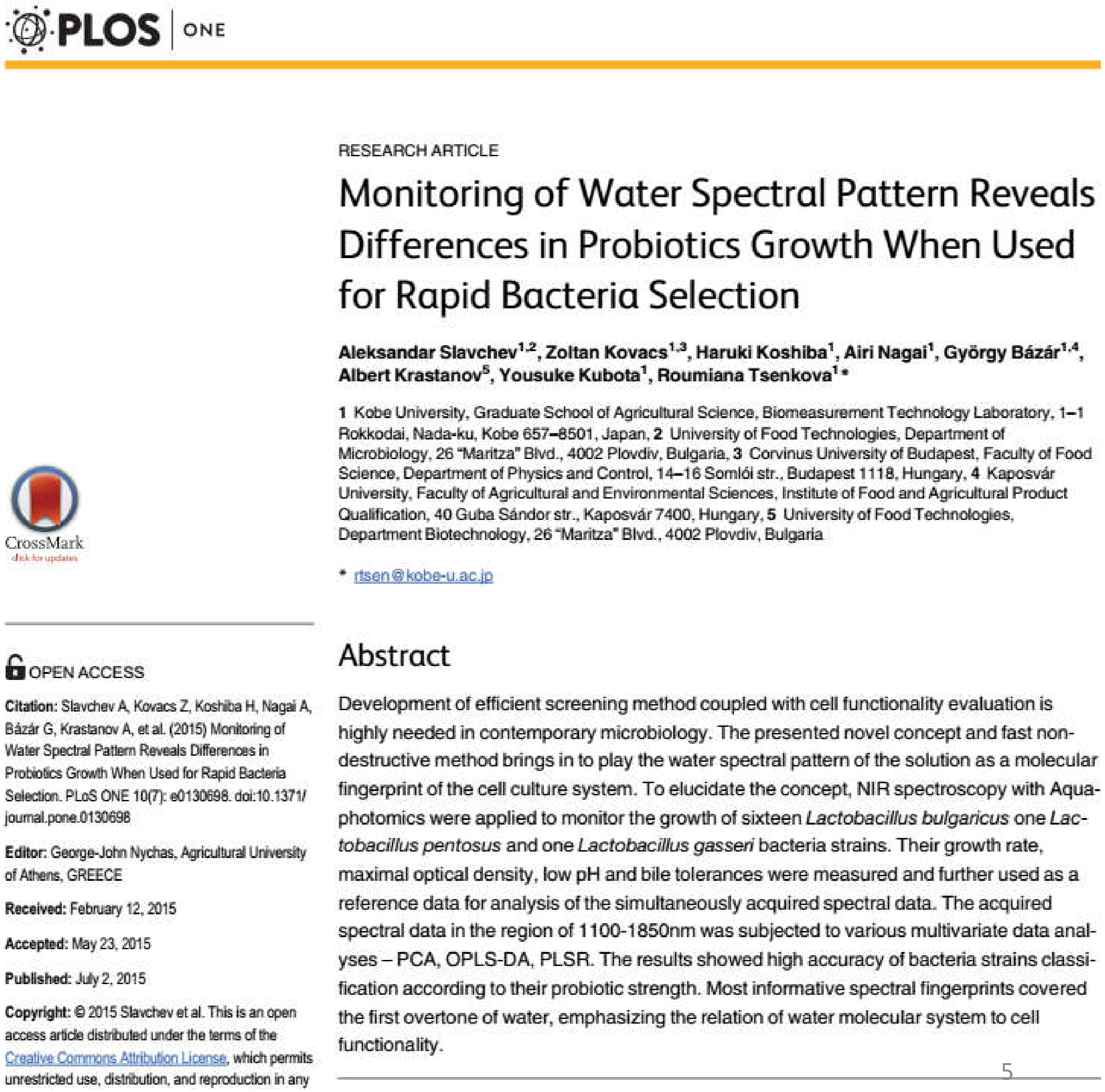

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RESEARCH ARTICLE

Monitoring of Water Spectral Pattern Reveals Differences in Probiotics Growth When Used for Rapid Bacteria Selection

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Abstract

Development of efficient screening method coupled with cell functionality evaluation is highly needed in contemporary microbiology. The presented novel concept and fast non-destructive method brings in to play the water spectral pattern of the solution as a molecular fingerprint of the cell culture system. To elucidate the concept, NIR spectroscopy with Aquaphotomics were applied to monitor the growth of sixteen *Lactobacillus bulgaricus* one *Lactobacillus pentosus* and one *Lactobacillus gasseri* bacteria strains. Their growth rate, maximal optical density, low pH and bile tolerances were measured and further used as a reference data for analysis of the simultaneously acquired spectral data. The acquired spectral data in the region of 1100-1850nm was subjected to various multivariate data analyses – PCA, OPLS-DA, PLSR. The results showed high accuracy of bacteria strains classification according to their probiotic strength. Most informative spectral fingerprints covered the first overtone of water, emphasizing the relation of water molecular system to cell functionality.

Slavchev, A. et al., 2015. Monitoring of Water Spectral Pattern Reveals Differences in Probiotics Growth When Used for Rapid Bacteria Selection. *PloS one*, 10(7), p.e0130698.

objectives

- to evaluate the application possibilities of **Aquaphotomics** in **rapid selection** and evaluation of bacterial strains possessing different **probiotic** properties
- to develop method for replacing the phenotypic and genetic approach for probiotic bacteria selection with Aquaphotomics
- to **learn more about living microorganisms and their functionality through** their **water spectral pattern**

Slavchev, A. et al., 2015. Monitoring of Water Spectral Pattern Reveals Differences in Probiotics Growth When Used for Rapid Bacteria Selection. *PloS one*, 10(7), p.e0130698.

Materials and methods I. – *samples* –

- Strains were cultivated in MRS broth for 24h at 37°C

Strain	OD max	MIC*, mg/ml	OD at 0.5 MIC	Corrected MIC (based on OD at 0.5MIC)	Yield of biomass after low pH stress	General PCA Score (probioticity)	Class
Lactobacillus bulgaricus S4	**0.84**	**0.16**	0.30	**0.10**	**0.07**	**-2.43**	Non probiotic
Lactobacillus bulgaricus S3	**1.34**	**0.31**	0.31	**0.20**	**0.05**	**-2.23**	
Lactobacillus bulgaricus S2	**1.52**	**0.16**	0.30	**0.10**	**0.06**	**-2.04**	
Lactobacillus bulgaricus S29	**1.44**	**0.63**	0.39	**0.43**	**0.05**	**-1.94**	
Lactobacillus bulgaricus S30	**1.36**	**0.63**	0.44	**0.45**	**0.06**	**-1.79**	
Lactobacillus bulgaricus S28	**2.770**	**0.313**	0.370	**0.214**	**0.025**	**-1.420**	Moderate
Lactobacillus bulgaricus S9	**2.880**	**0.156**	0.300	**0.101**	**0.029**	**-1.414**	
Lactobacillus bulgaricus S1	**1.690**	**0.625**	0.725	**0.539**	**0.038**	**-1.385**	
Lactobacillus bulgaricus Y12	**2.020**	**0.625**	0.303	**0.408**	**0.041**	**-1.349**	
Lactobacillus bulgaricus S7	**1.919**	**0.625**	0.790	**0.559**	**0.049**	**-1.274**	
Lactobacillus bulgaricus S6	**2.960**	**1.250**	0.307	**0.817**	**0.080**	**0.647**	Probiotic
Lactobacillus bulgaricus S22	**2.677**	**2.500**	1.230	**2.788**	**0.117**	**1.923**	
Lactobacillus gasseri S20	**3.030**	**2.500**	0.542	**1.928**	**0.114**	**2.145**	
Lactobacillus bulgaricus S11	**2.954**	**2.500**	1.600	**3.250**	**0.100**	**2.363**	
Lactobacillus bulgaricus S10	**2.950**	**2.500**	1.550	**3.188**	**0.126**	**2.569**	

Strains and their phenotypic characteristics

5 probiotic
5 moderate
5non-probiotic
+
L. bulgaricus S8
L. bulgaricus SR
L. pentosus SS

independent prediction

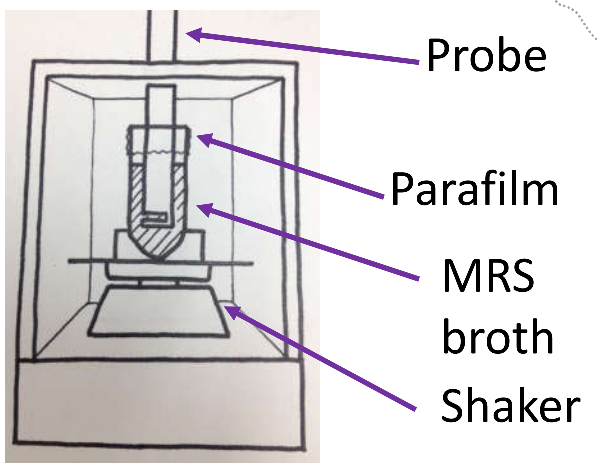
L. bulgaricus SR and *L. bulgaricus Y12*, *L. pentosus SS* were isolated , rest were provided by "Selur Pharma" Ltd. (Bulgaria).

Slavchev, A. et al., 2015. Monitoring of Water Spectral Pattern Reveals Differences in Probiotics Growth When Used for Rapid Bacteria Selection. *PloS one*, 10(7), p.e0130698.

*MIC (Minimal Inhibitory Concentration)

Materials and methods II.
– *instruments and conditions* –

- Spectra were acquired by XDS optiprobe module, imersion probe (transflectance mode) pathlenght 1 mm
- The cultivation in MRS broth for 24h at 37°C was monitored



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application you want to capture

ou going to capture a resource-demanding application like a modern game?

it is recommended to switch Debut to the "Fast Capture" mode. In this mode, the Debut overhead

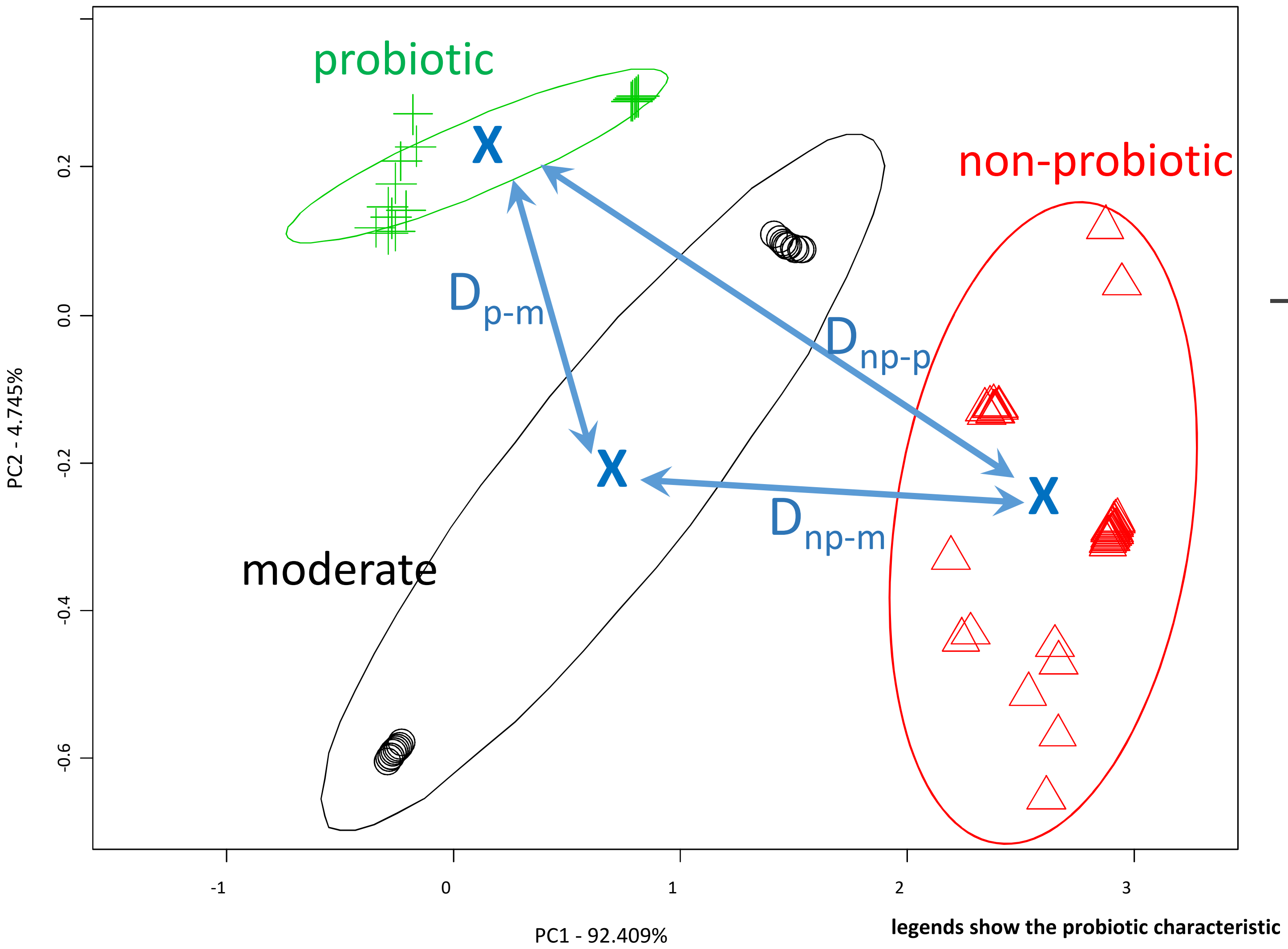
e minimal while keeping same video quality.

an always change the modes in "Record Screen as" list.

Results of mouving window PCA

Materials and methods III. – *chemometrics* –

PCA score plot (PC1-PC2) - from point x to point x+10



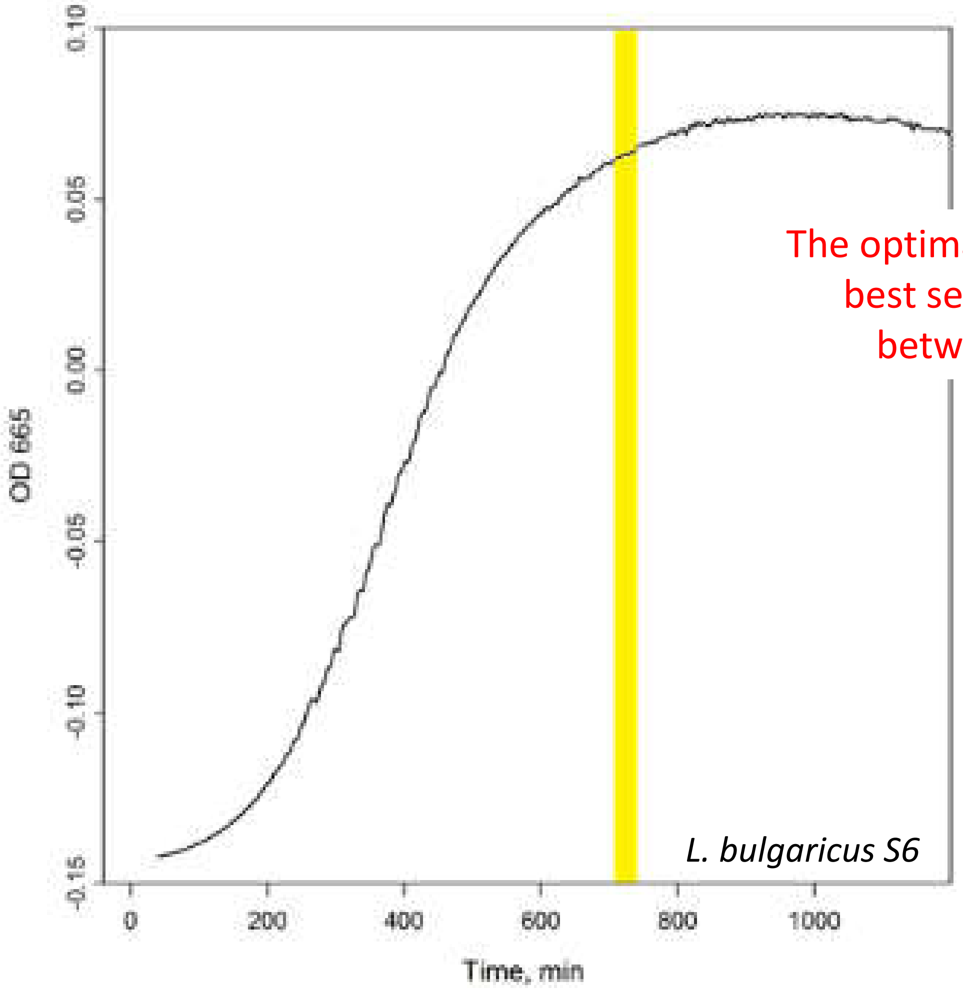
legends show the probiotic characteristic

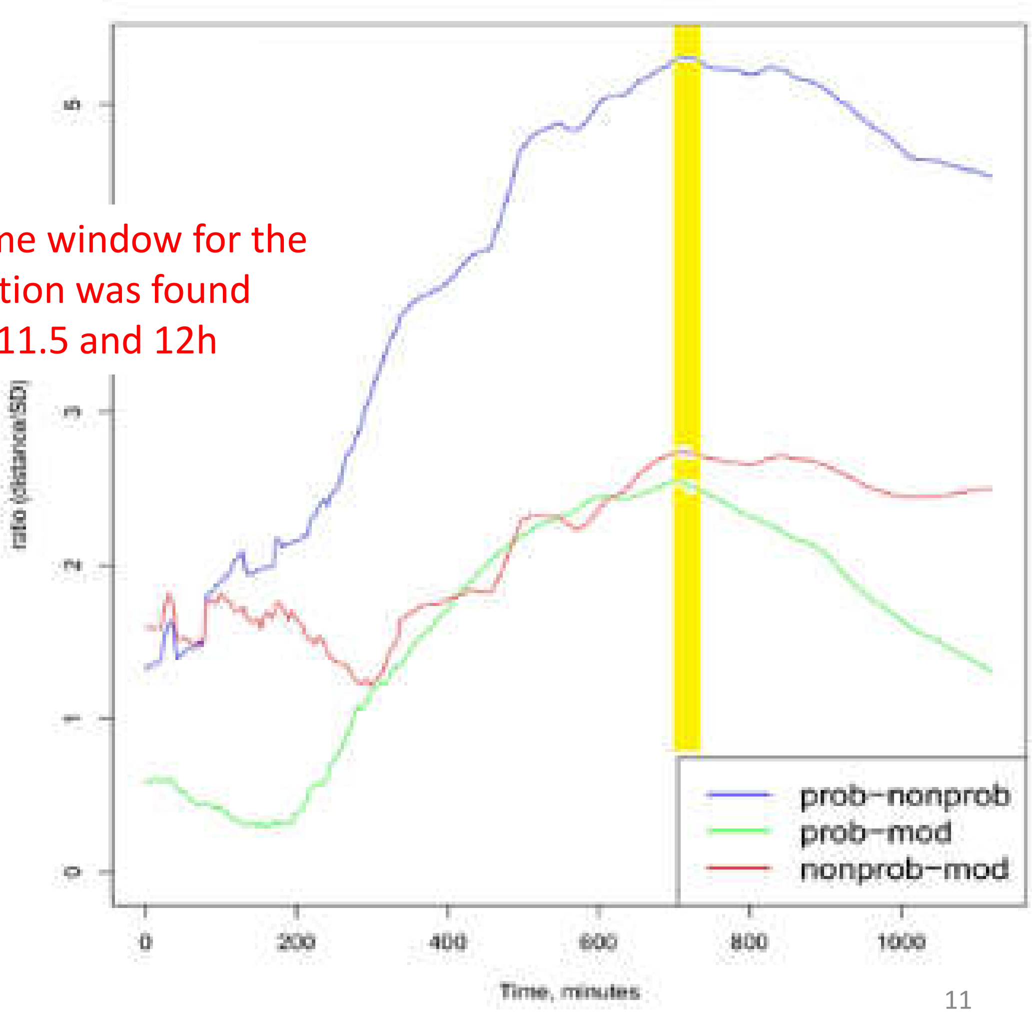
demonstration for moving window PCA (MW-PCA)

$$\frac{\text{distance between groups}}{\text{average standard deviation}}$$

to find the optimal time window for the best separation of probiotic, non-probiotic and moderate groups

Growing curve and results of MW-PCA





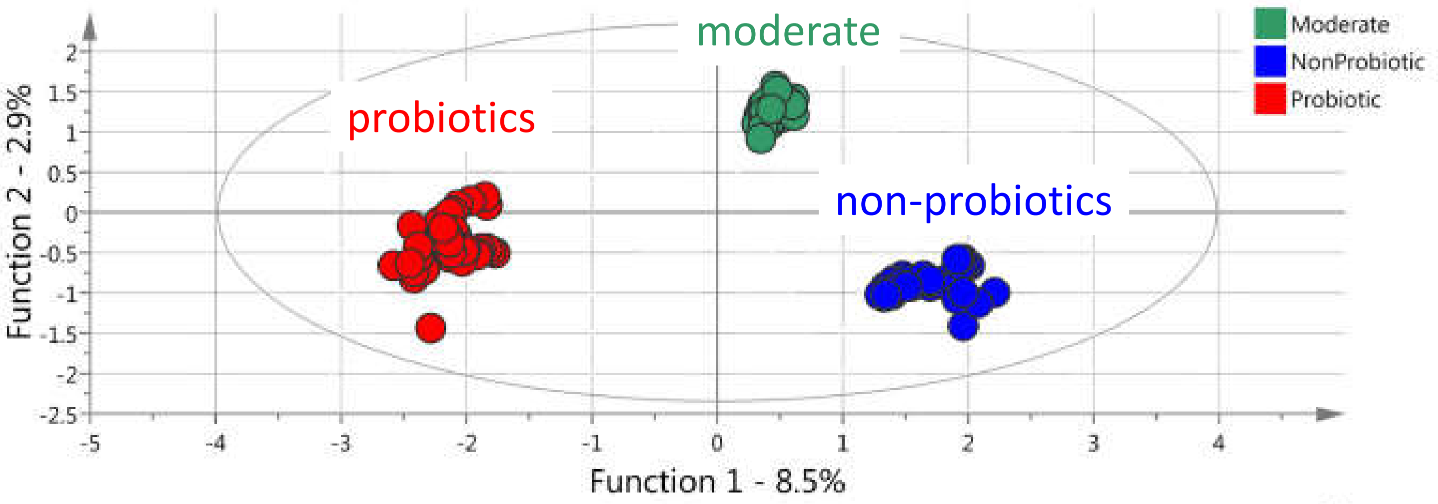
The optimal time window for the best separation was found between 11.5 and 12h

Slavchev, A. et al., 2015. Monitoring of Water Spectral Pattern Reveals Differences in Probiotics Growth When Used for Rapid Bacteria Selection. *PloS one*, 10(7), p.e0130698.

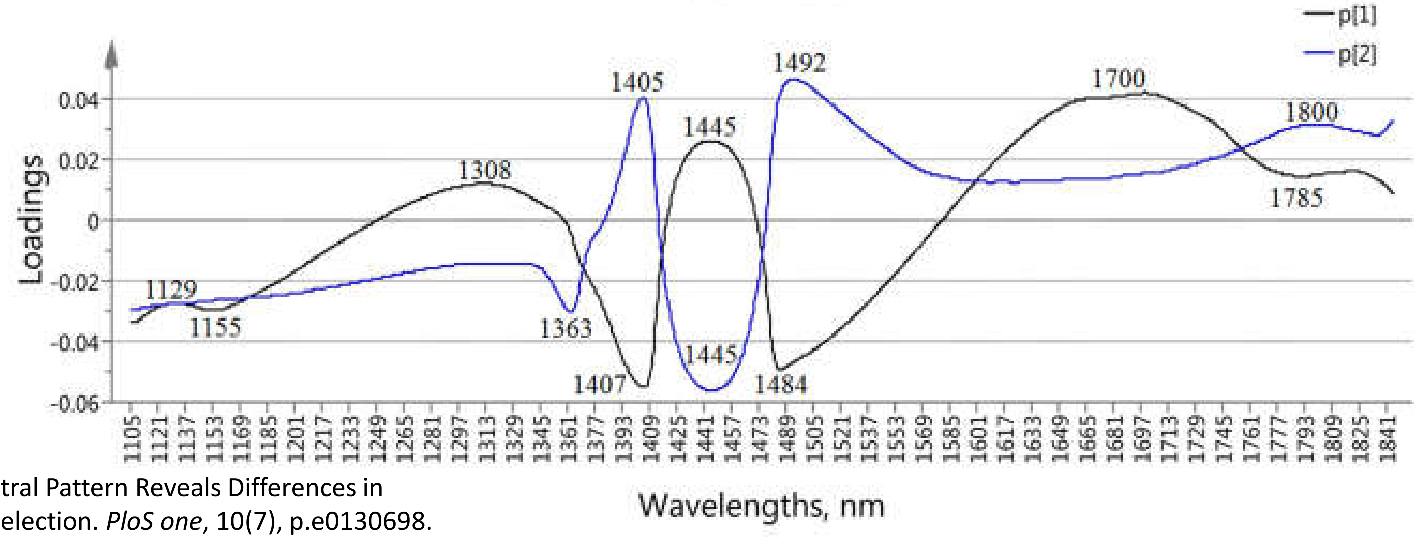
OPLS-DA of spectral data to discriminate groups

11.5 and 12h

100% correct classification of the three groups



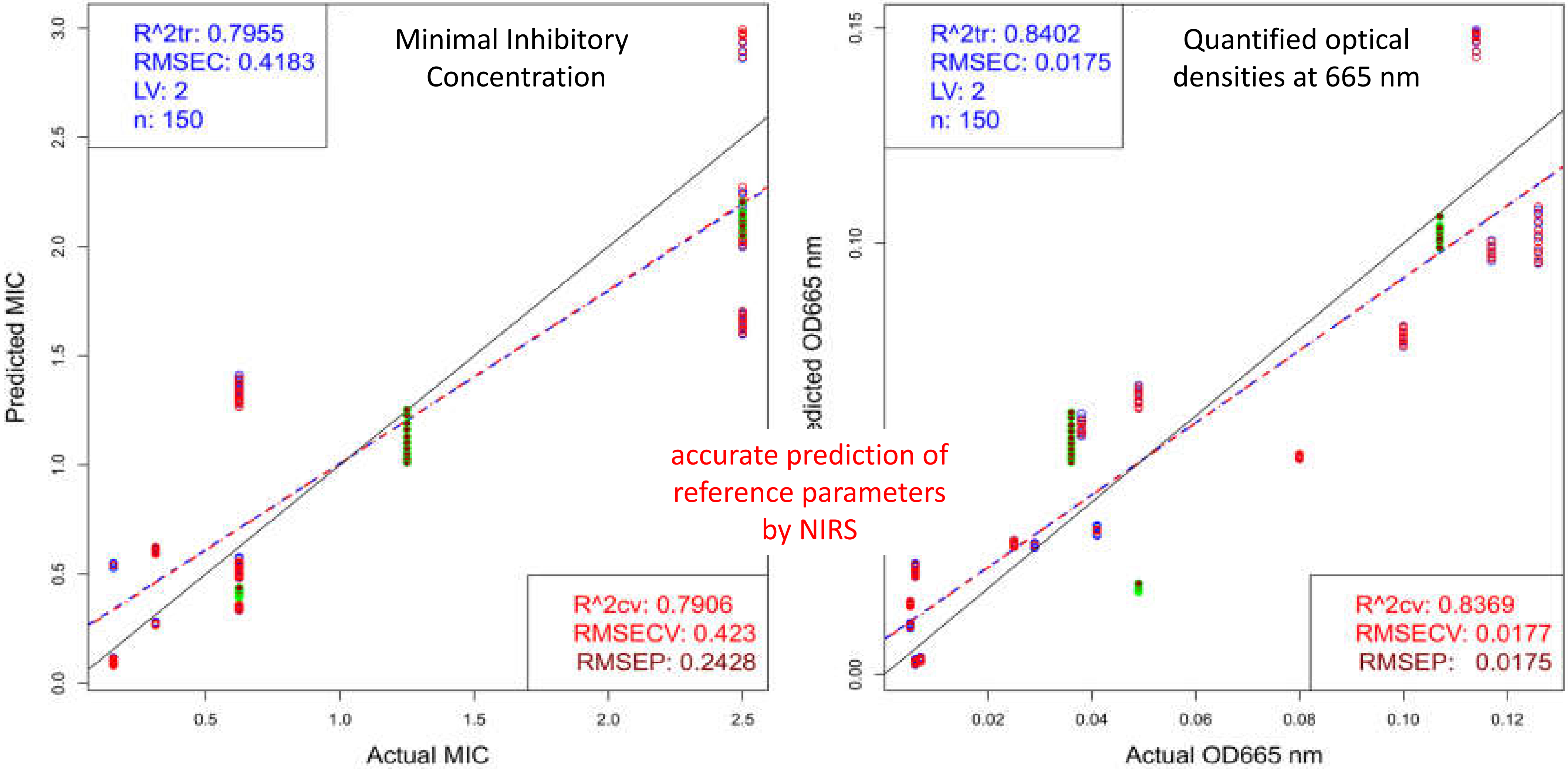
water bands important for separation



Slavchev, A. et al., 2015. Monitoring of Water Spectral Pattern Reveals Differences in Probiotics Growth When Used for Rapid Bacteria Selection. *PloS one*, 10(7), p.e0130698.

PLS regression to predict reference parameters

1100–1850nm



Minimal Inhibitory Concentration

Quantified optical densities at 665 nm

accurate prediction of reference parameters by NIRS

Slavchev, A. et al., 2015. Monitoring of Water Spectral Pattern Reveals Differences in Probiotics Growth When Used for Rapid Bacteria Selection. *PloS one*, 10(7), p.e0130698.

Experiments with probiotic Yogurts

objectives

- to determine if there is any effect of the type of spring water on yogurt preparation
- to describe the interaction between different bacteria strains and spring waters

Materials and methods I. – *samples*

Preparation of the yogurt samples:

- soy milk & spring **Water*** mix with **probiotics bacteria****
- cultivate it and move to fridge

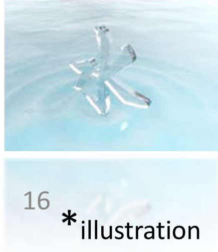
*Water:

- 2 types of water were used in different ratio:
  - Spring Water 1 (TSW) : Spring Water 2 (GoW) =
  - 100:0 or 70:30 or 50:50 or 30:70 or 0:100

**probiotics bacteria:

- 2 types of starter culture: probiotics with or without Yw

Resulting all together:
5 x 2 = **10**
different samples



*illustration

Materials and methods I./2 – *samples summary*

XDS
spectrometer

With Yw	Without Yw
1) Yw100G	6) noYw100G
2) Yw70G30TS	7) noYw70G30TS
3) Yw50G50TS	8) noYw50G50TS
4) Yw30G70TS	9) noYw30G70TS
5) Yw100TS	10) noYw100TS

five different combination of waters

two types of starter culture

http://www.welltechinc.com

Materials and methods II. – *instruments and conditions*

- XDS spectrometer with rapid content analyzer:
  - range: 400-2500nm
  - step 0.5nm
  - range used for data evaluation: 1300-1600nm
- <u>The yogurt samples were:</u>

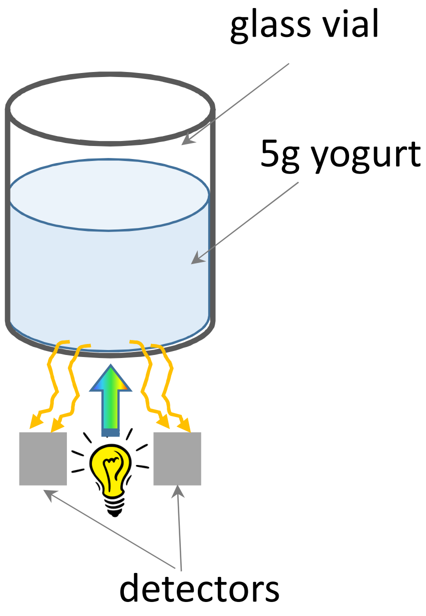
  measured with glass vials using reflectance mode from the bottom

  3 different repeats and MQ after every 5th sample

  using 5 consecutive scans

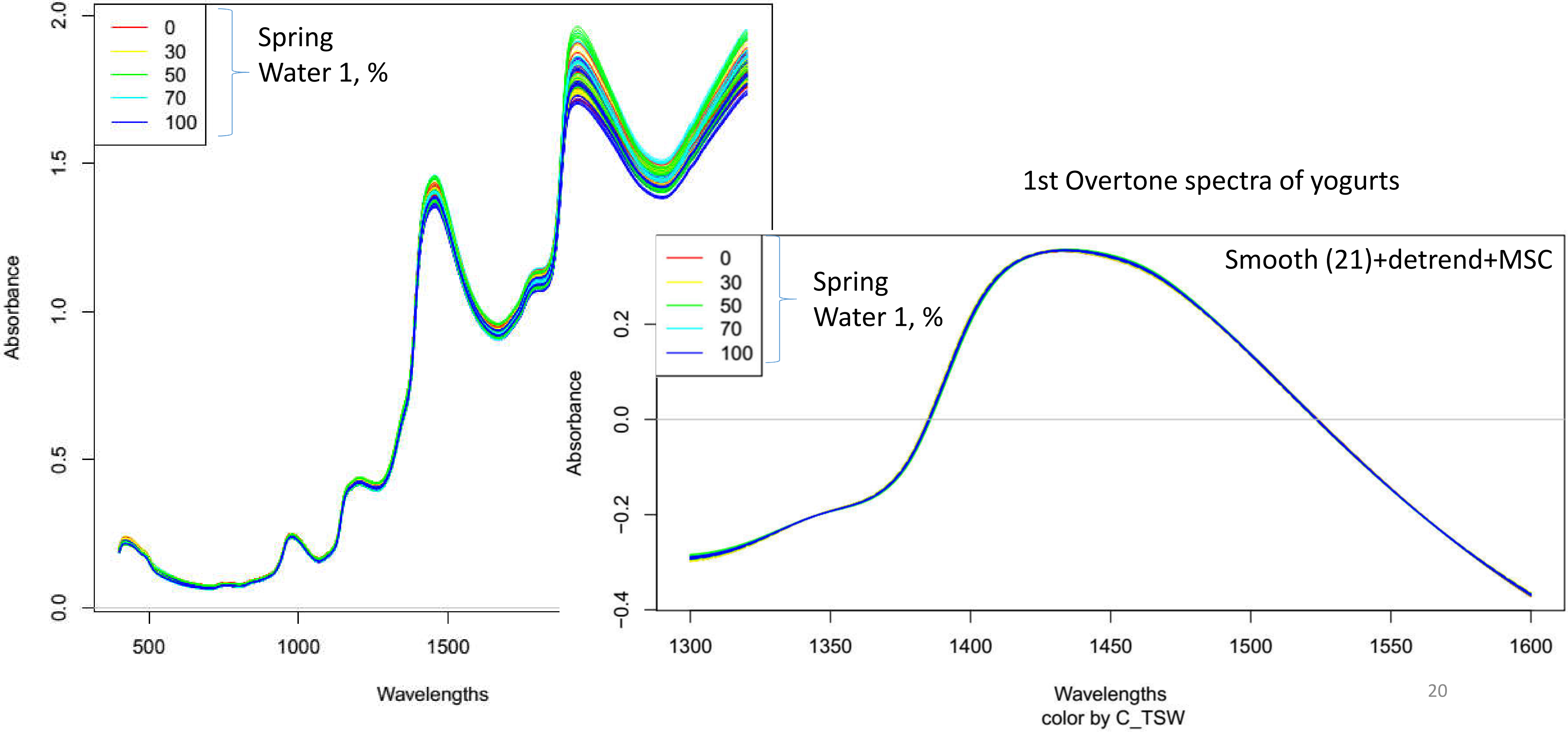
  5g yogurt sample was filled to the vial

  n = 185 (yogurt: 10x3x5 + MQ 7x5)



Results

Raw absorbance spectra of the samples



1st Overtone spectra of yogurts

Smooth (21)+detrend+MSC

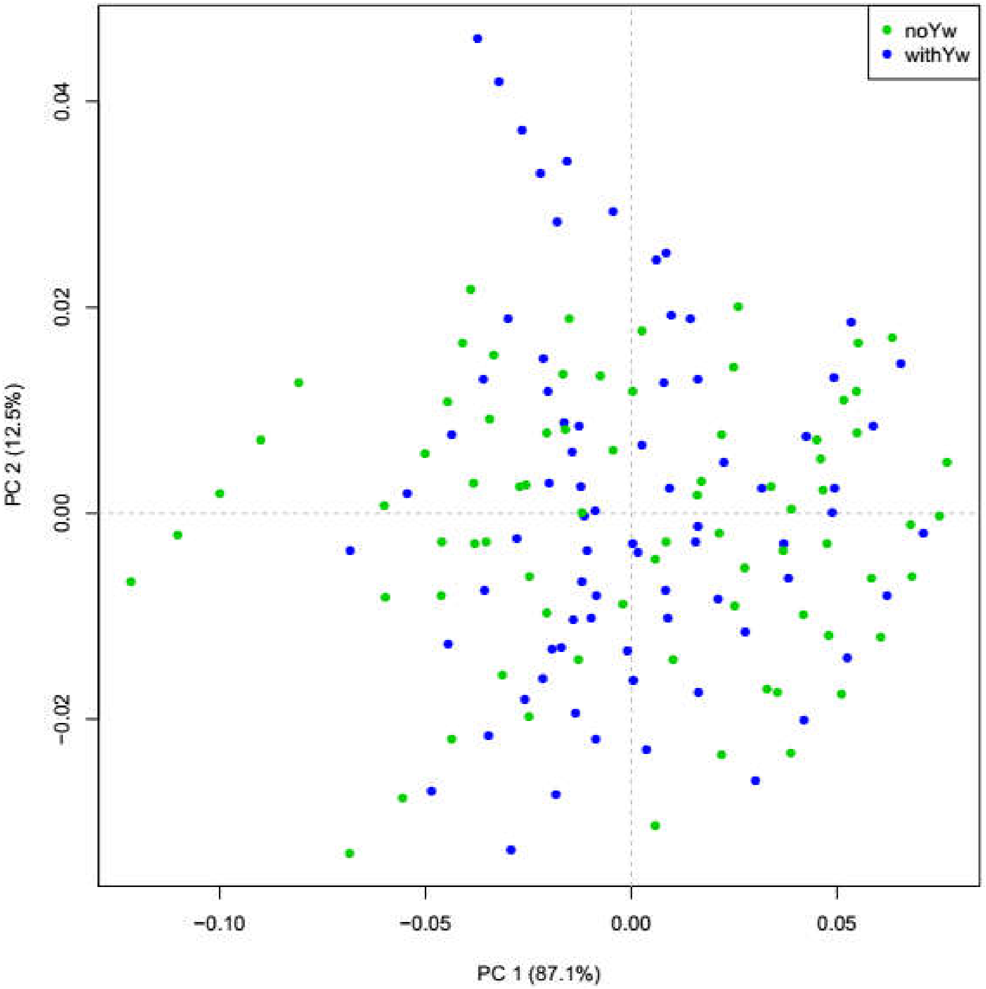
PCA plots of yogurts

(1300-1600nm, smooth 21)

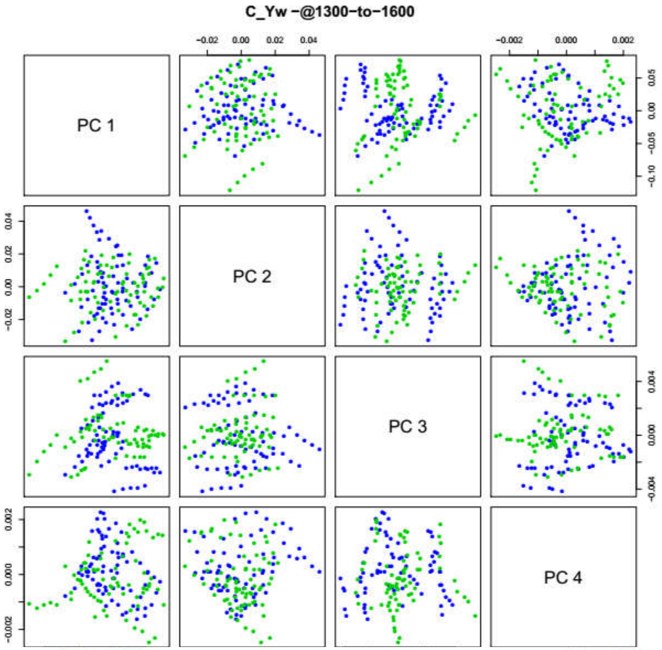
Mean-center

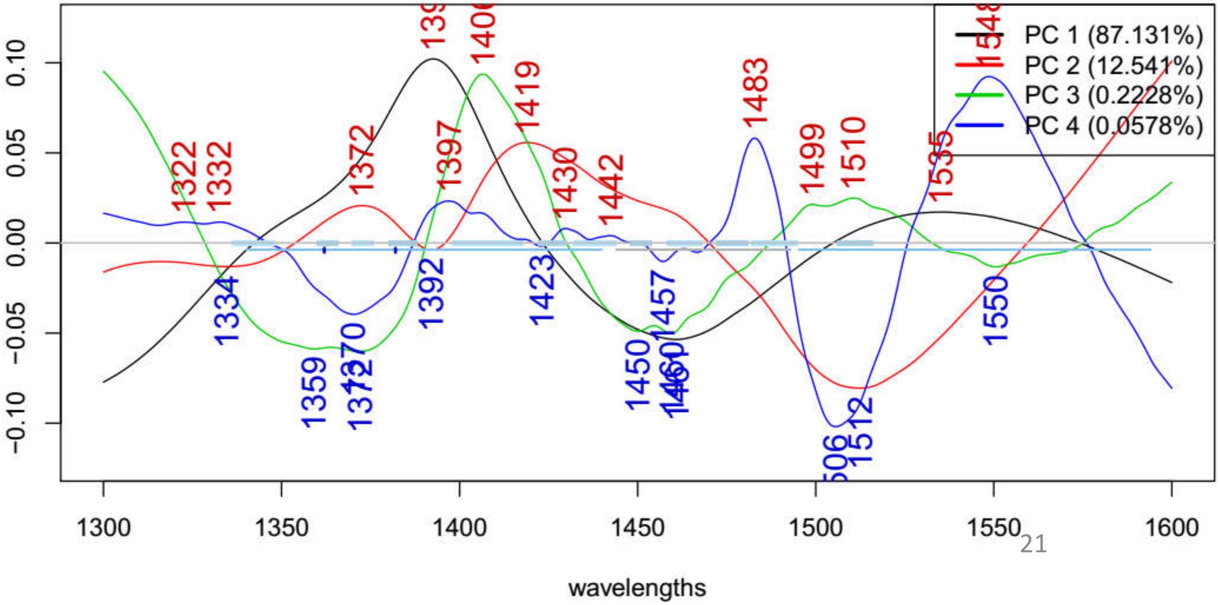
Colored by Yw

detrend
MSC



No obvious Separation based on the two types of starter culture





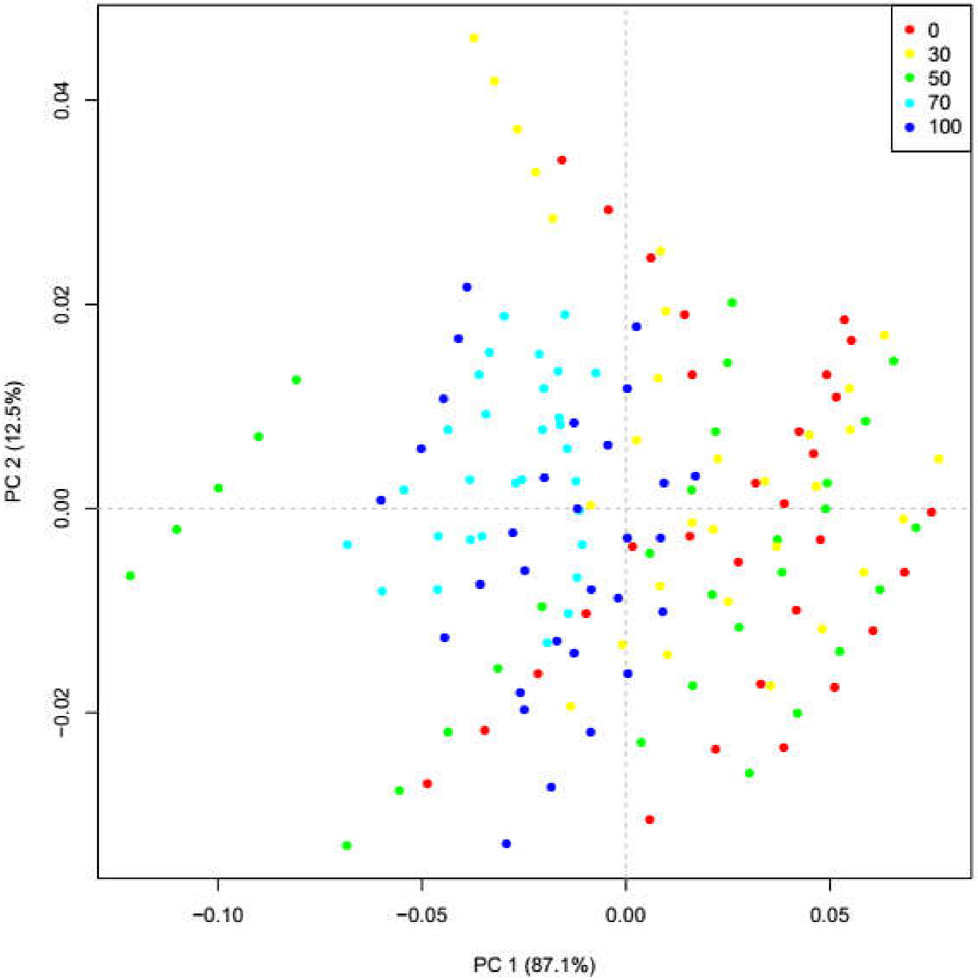
PCA plots of yogurts

(1300-1600nm, smooth 21)

Mean-center

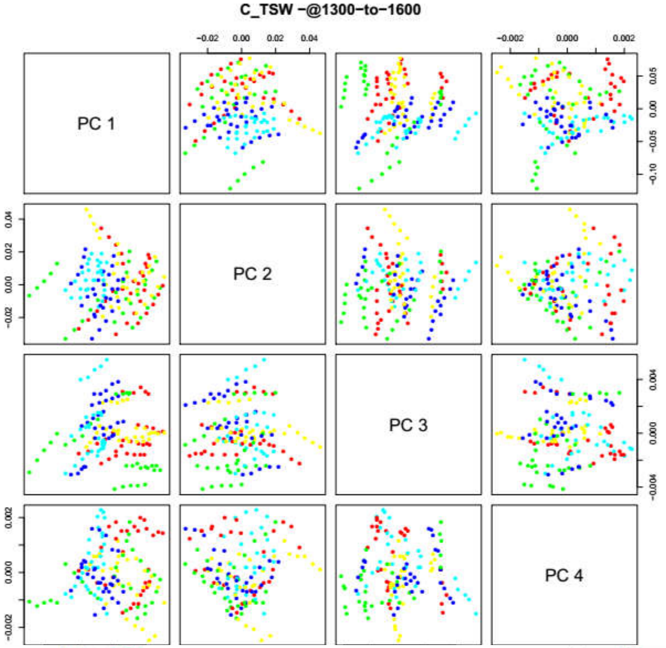
Colored by Water content

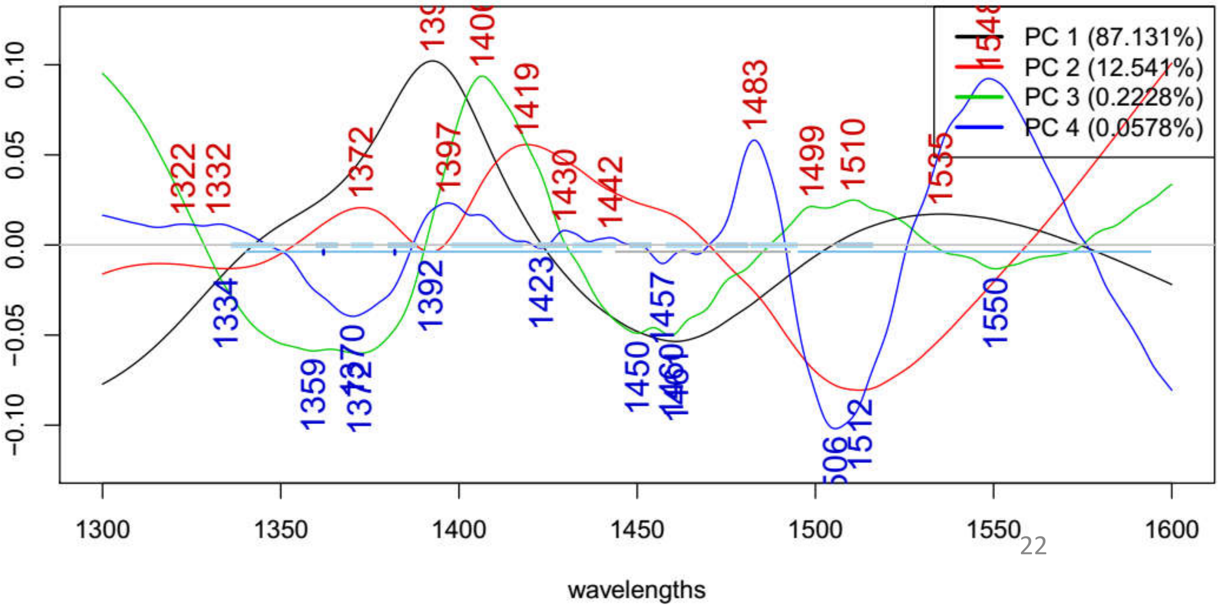
detrend
MSC



Some tendency on PC1

Effect of water stronger





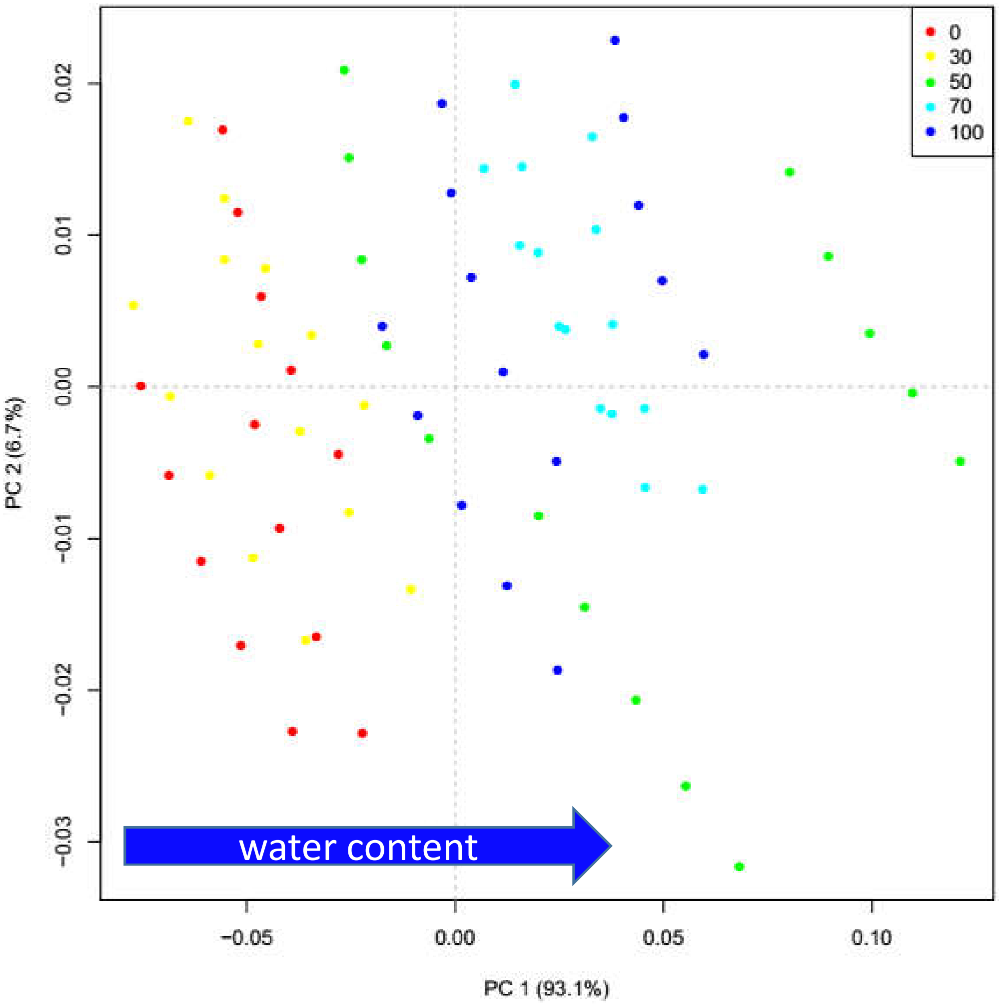
PCA plots of yogurts – only no Yw

(1300-1600nm, smooth 21)

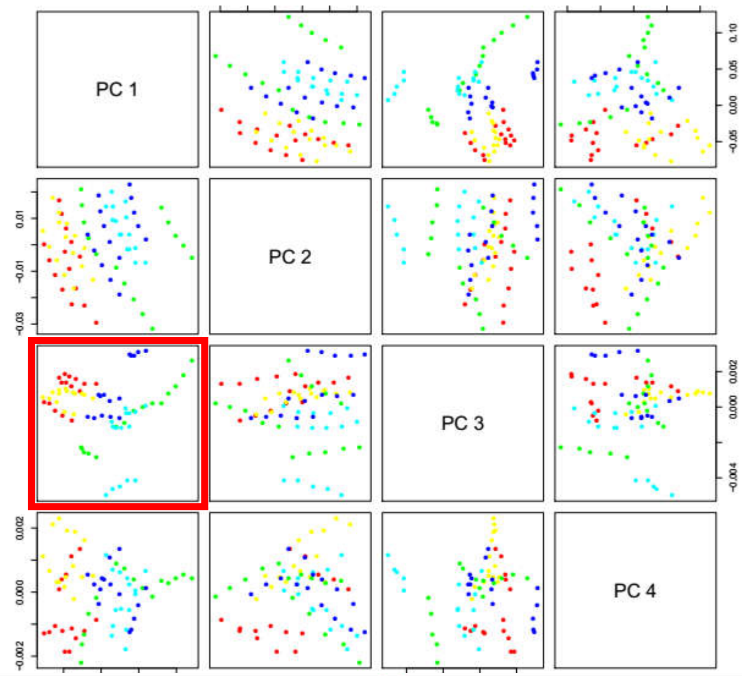
detrend
MSC

Mean-center

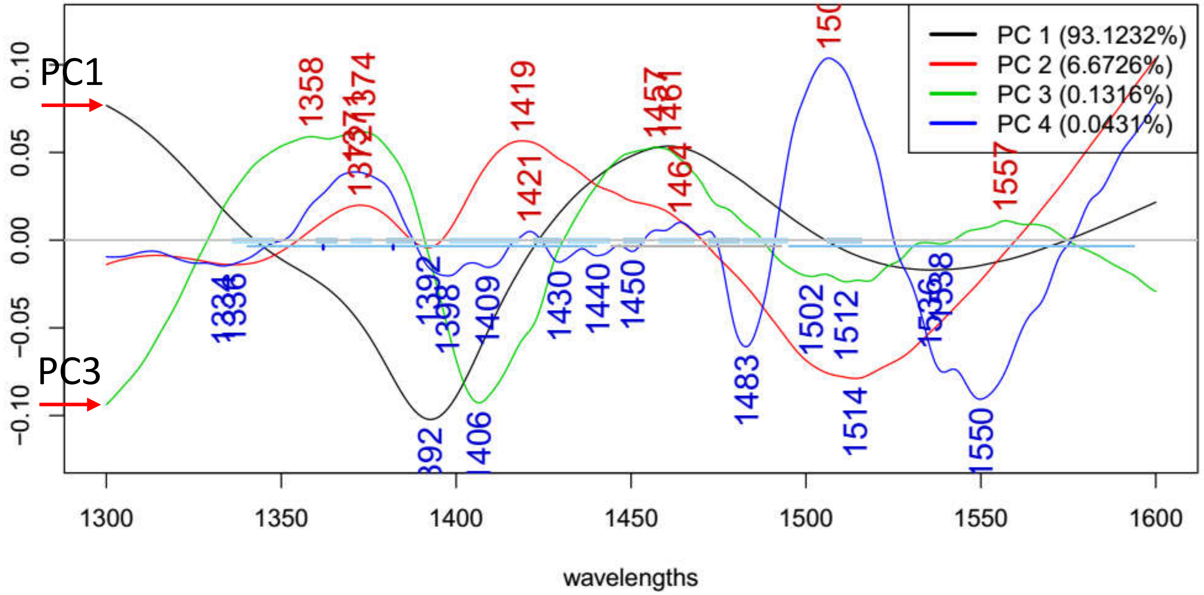
Colored by Water content



Yog6
Yog7
Yog8
Yog9
Yog10



Effect of water stronger



PCA plots of yogurts – only with Yw

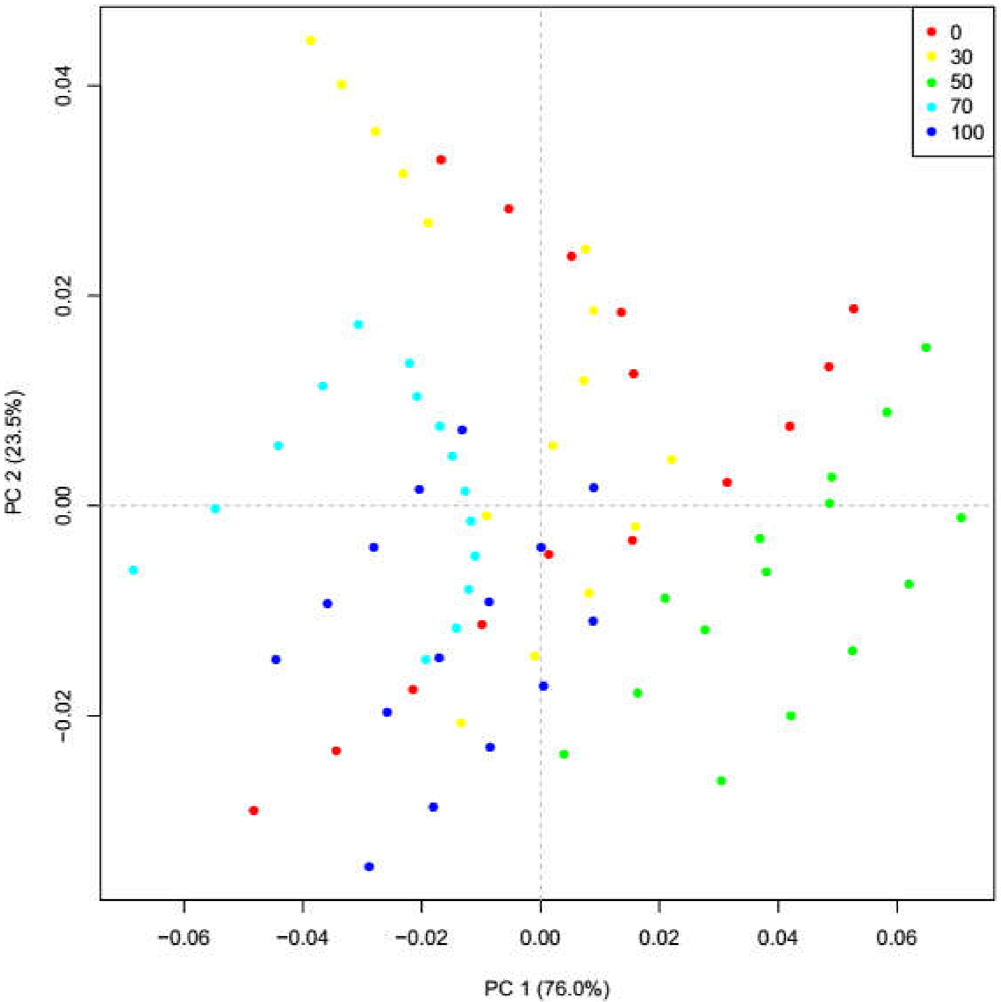
(1300-1600nm, smooth 21)

detrend

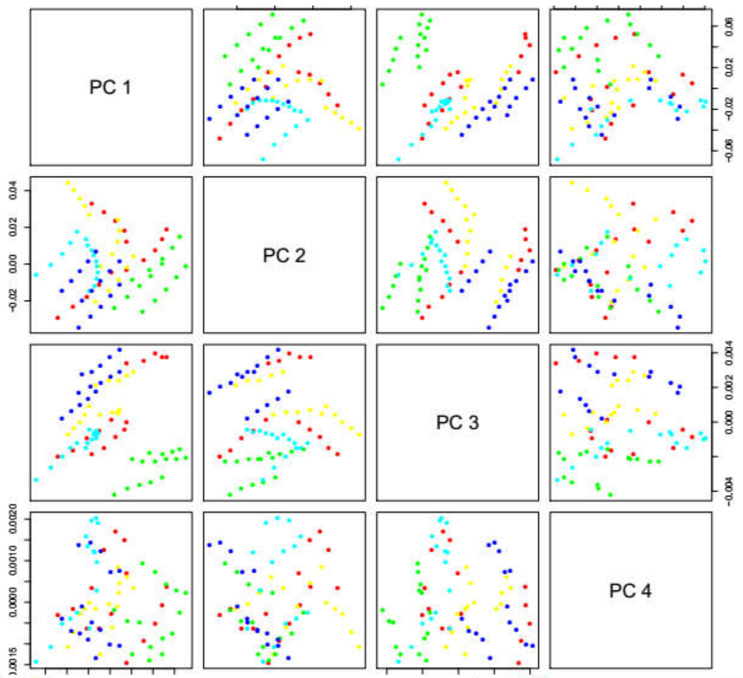
MSC

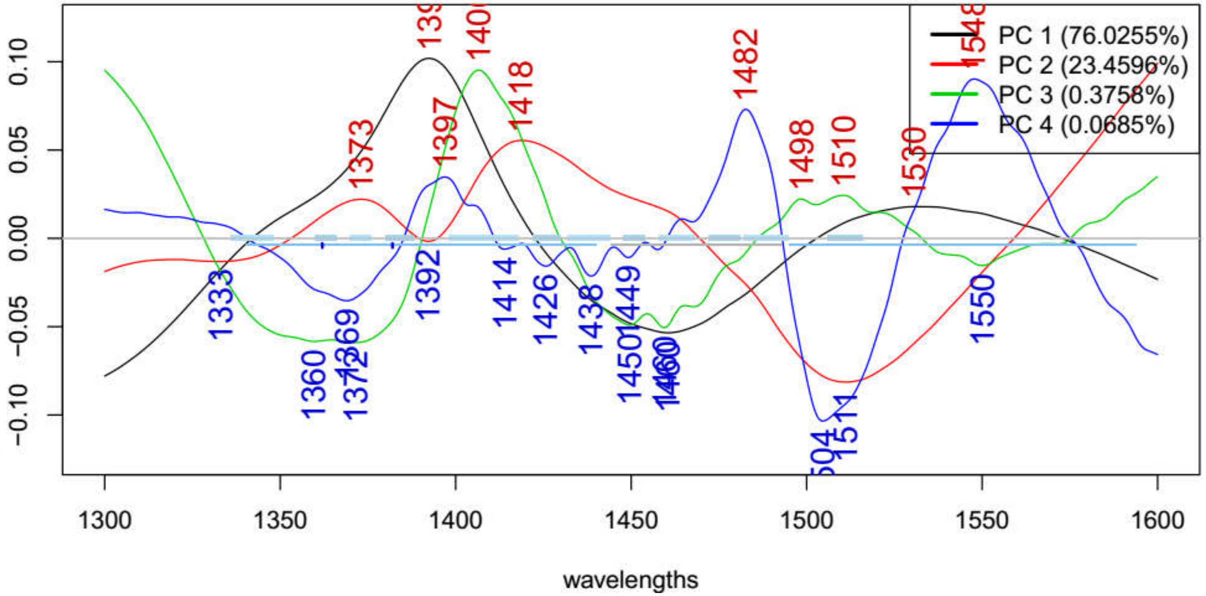
Mean-center

Colored by Water content



Effect of water stronger





Conclusion

- Water spectral pattern can be used as biomarker leading to highly accurate and fast classification and prediction of the different phenotypic properties of potential probiotic candidates of genus *Lactobacillus*
- Aquaphotomics could be used as rapid holistic approach in the screening and evaluation of probiotic microorganisms
- The type of water used for yogurt preparation has a significant effect on the spectral pattern of the final product

Agenda of the presentation

Application of Aquaphotomics to learn more about the rules of water

- Bacteria growing and Yogurt
- Plant cells growing
- Mineral Waters
- Calculation and presentation method of WASP

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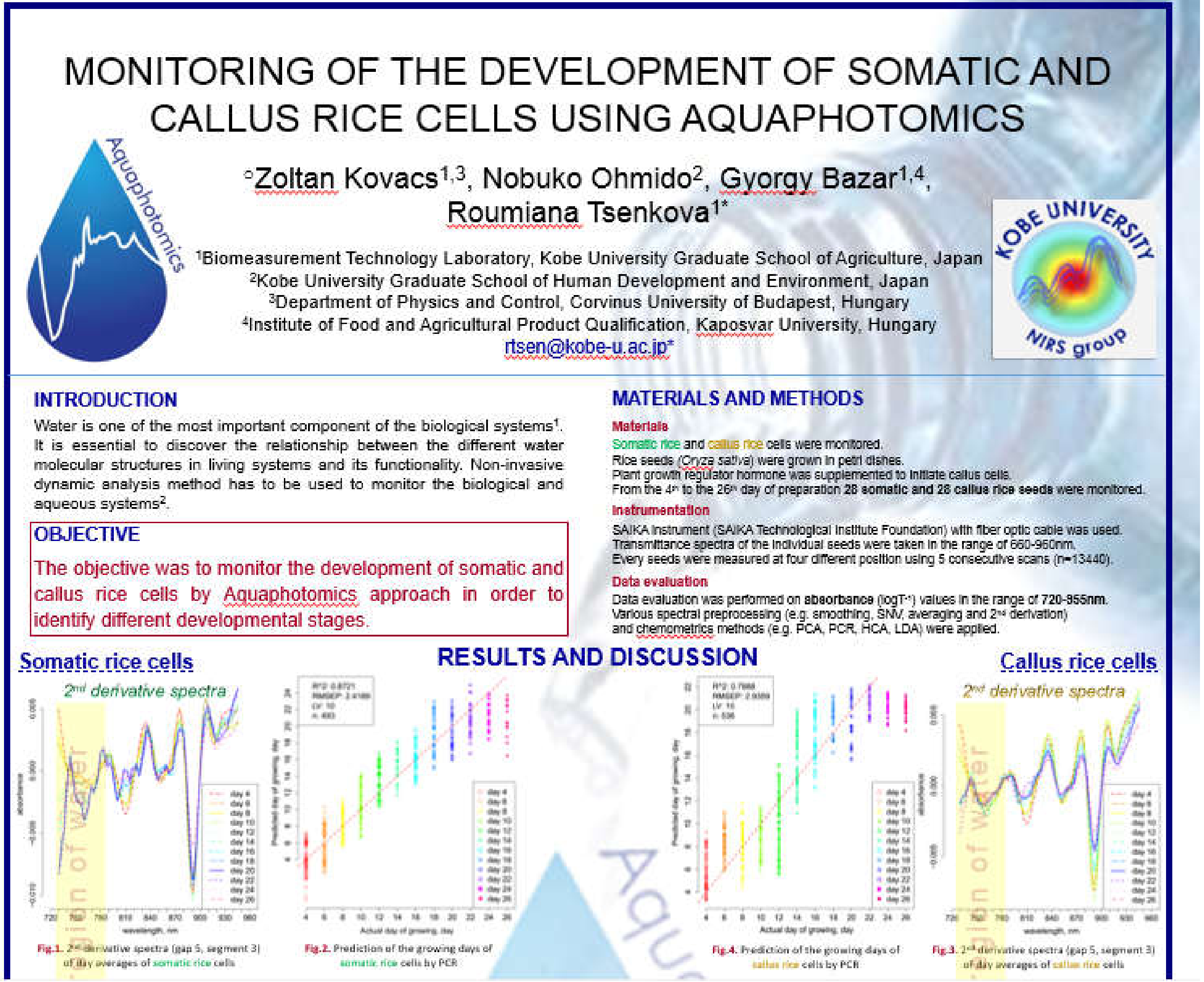
Experiments with plant cells



MONITORING OF THE DEVELOPMENT OF SOMATIC AND CALLUS RICE CELLS USING AQUAPHOTOMICS

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rtsen@kobe-u.ac.jp*

INTRODUCTION

Water is one of the most important component of the biological systems[1]. It is essential to discover the relationship between the different water molecular structures in living systems and its functionality. Non-invasive dynamic analysis method has to be used to monitor the biological and aqueous systems[2].

OBJECTIVE

The objective was to monitor the development of somatic and callus rice cells by Aquaphotomics approach in order to identify different developmental stages.

MATERIALS AND METHODS

Materials

Somatic rice and callus rice cells were monitored.
Rice seeds (*Oryza sativa*) were grown in petri dishes.
Plant growth regulator hormone was supplemented to initiate callus cells.
From the 4th to the 26th day of preparation **28 somatic and 28 callus rice seeds** were monitored.

Instrumentation

SAIKA Instrument (SAIKA Technological Institute Foundation) with fiber optic cable was used.
Transmittance spectra of the individual seeds were taken in the range of 660-960nm.
Every seeds were measured at four different position using 5 consecutive scans (n=13440).

Data evaluation

Data evaluation was performed on **absorbance** ($\log T^{-1}$) values in the range of **720-955nm**.
Various spectral preprocessing (e.g. smoothing, SNV, averaging and 2nd derivation)
and chemometrics methods (e.g. PCA, PCR, HCA, LDA) were applied.

RESULTS AND DISCUSSION

Somatic rice cells

2nd derivative spectra

Fig.1. 2nd derivative spectra (gap 5, segment 3) of day averages of somatic rice cells

Fig.2. Prediction of the growing days of somatic rice cells by PCR

Callus rice cells

2nd derivative spectra

Fig.4. Prediction of the growing days of callus rice cells by PCR

Fig.3. 2nd derivative spectra (gap 5, segment 3) of day averages of callus rice cells

Kovacs, Z. et al., 2014. Monitoring of the development of somatic and callus rice cells using aquaphotomics. In *73th Annual Meeting of the Japan Society of Agricultural Machinery and Food Engineers*. Okinawa, Japan, p. 267.

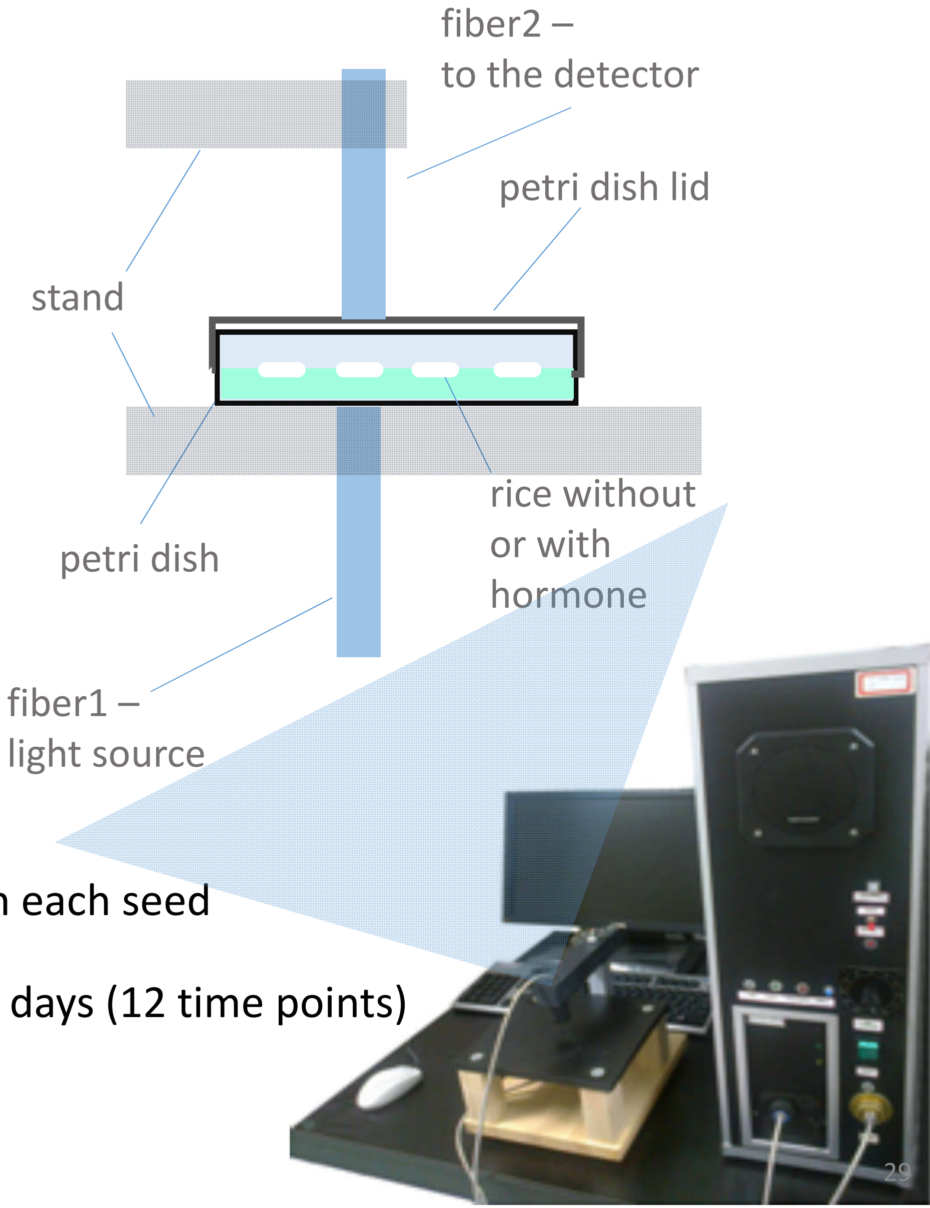
objectives

- to monitor the development of cells in somatic and callus rice cells
- to determine the water structural changes during the cell development
- to describe the wavelengths activated during the cell development

Kovacs, Z. et al., 2014. Monitoring of the development of somatic and callus rice cells using aquaphotomics. In 73th *Annual Meeting of the Japan Society of Agricultural Machinery and Food Engineers*. Okinawa, Japan, p. 267.

Materials and methods

- the experiment was performed with SAIKA instrument
- the instrument was connected with fiber in transmittance arrangement
- the fiber probe was fixed by a stand
- the samples were measured in the petri dish (without opening it)
- the seeds were measured using 5 consecutive scans and the petri dish was turned with 90° (4 positions) resulting 20 spectra from each seed
- 28 somatic and 28 callus rice seeds were monitored for 24 days (12 time points)
- total number of spectra 13 440 scans

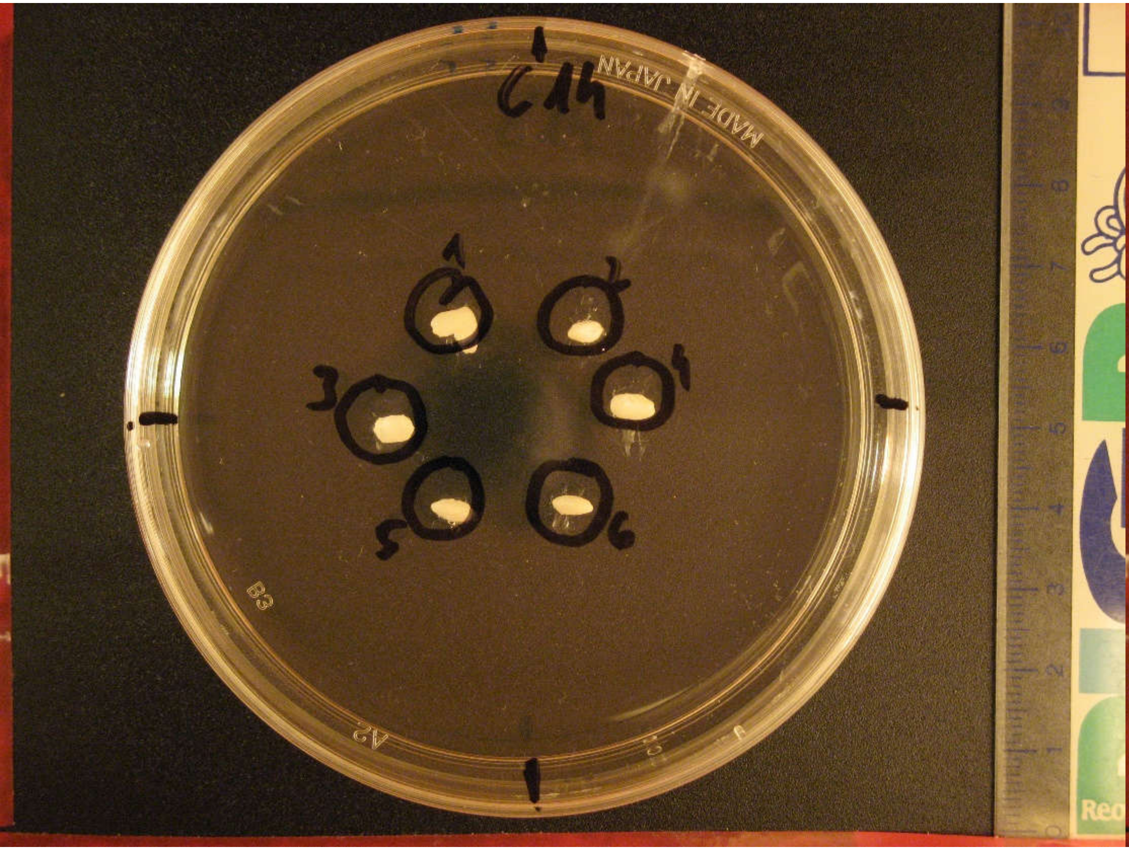


Kovacs, Z. et al., 2014. Monitoring of the development of somatic and callus rice cells using aquaphotomics. In *73th Annual Meeting of the Japan Society of Agricultural Machinery and Food Engineers*. Okinawa, Japan, p. 267.

20140221

day 2

somatic cells

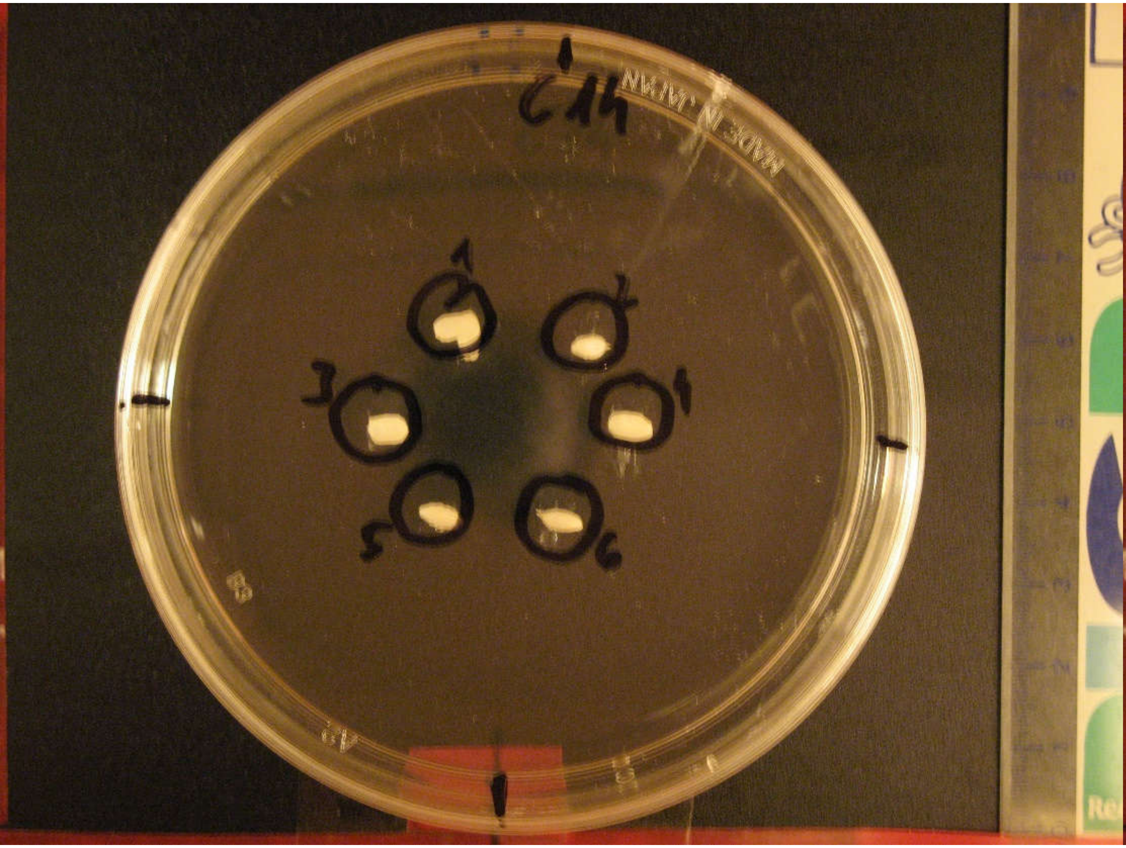


callus cells

20140223

day 4

somatic cells

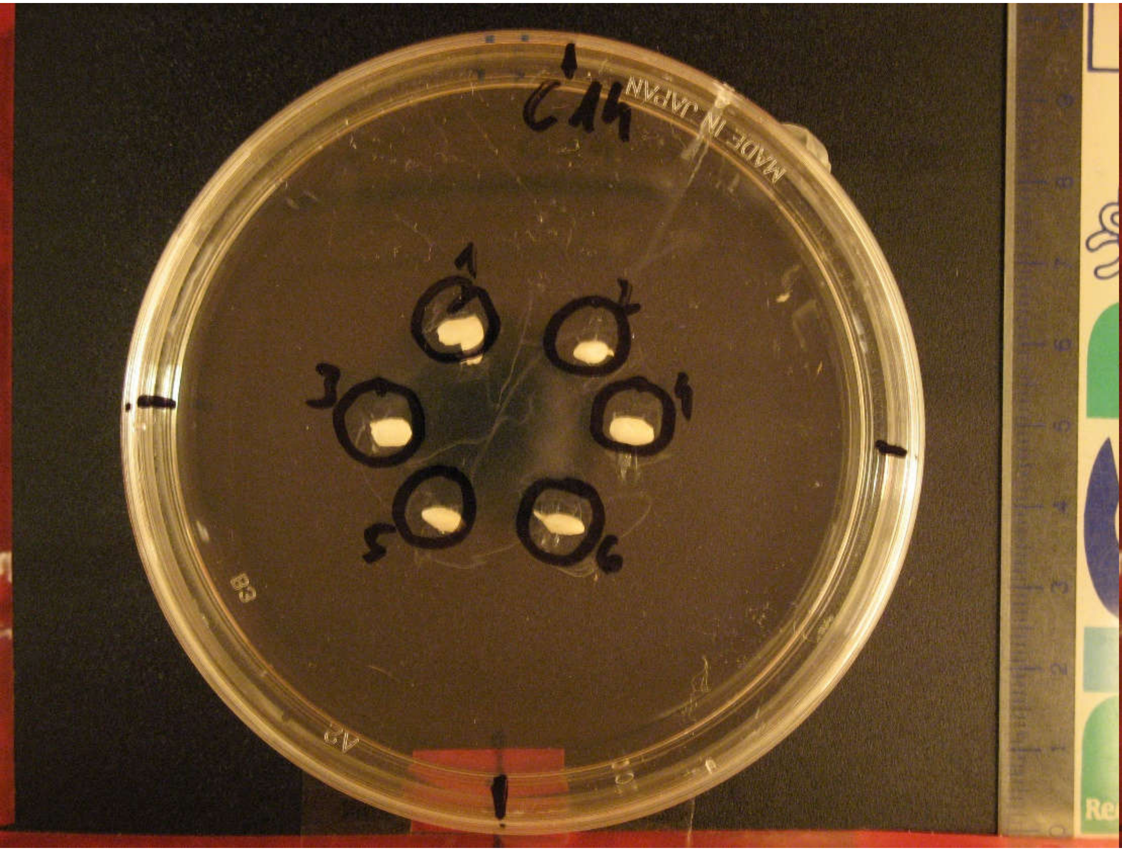


callus cells

20140224

day 5

somatic cells



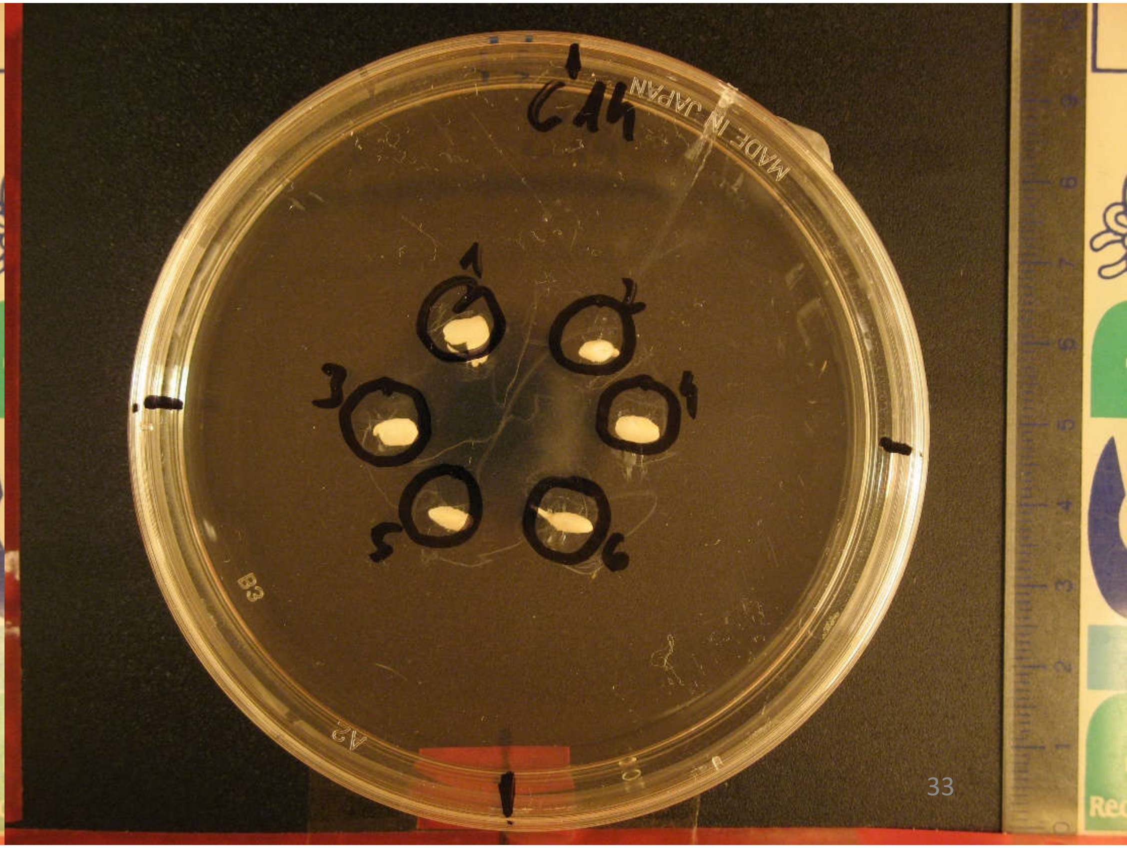
callus cells

20140225

day 6

somatic cells

callus cells



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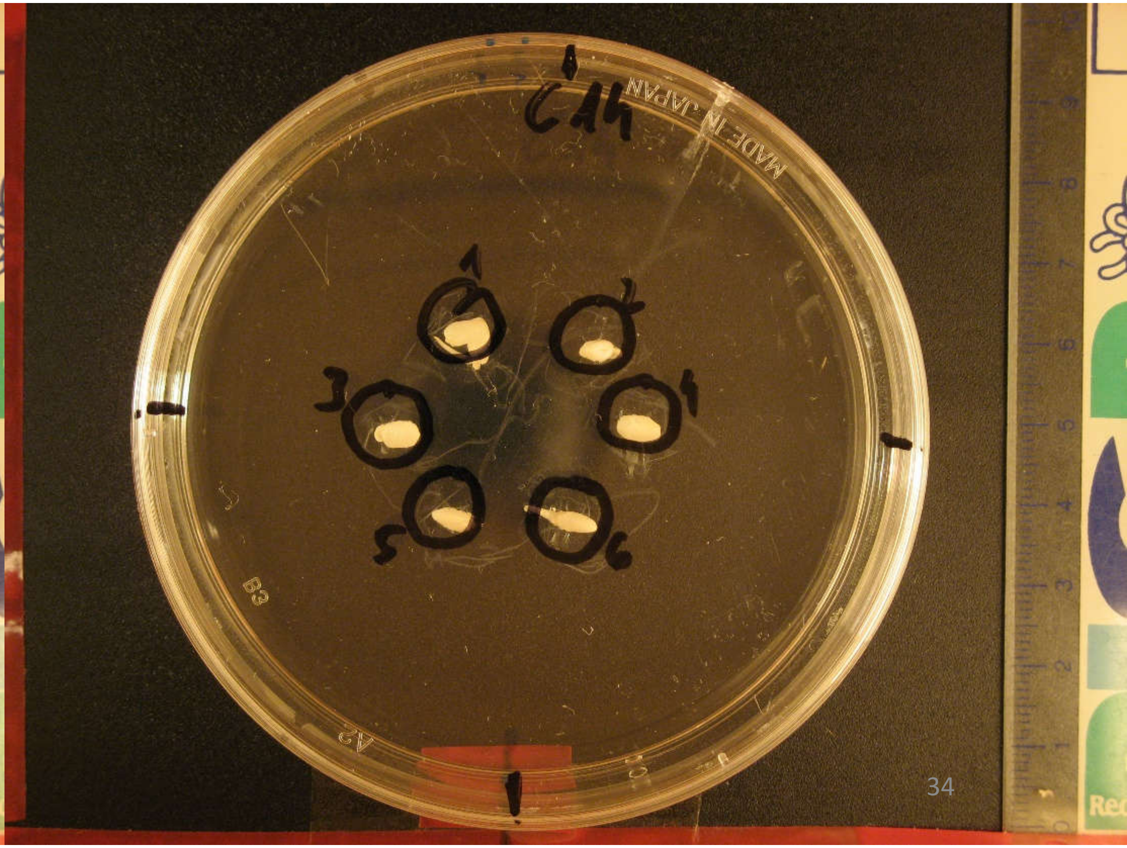
day 7

somatic cells

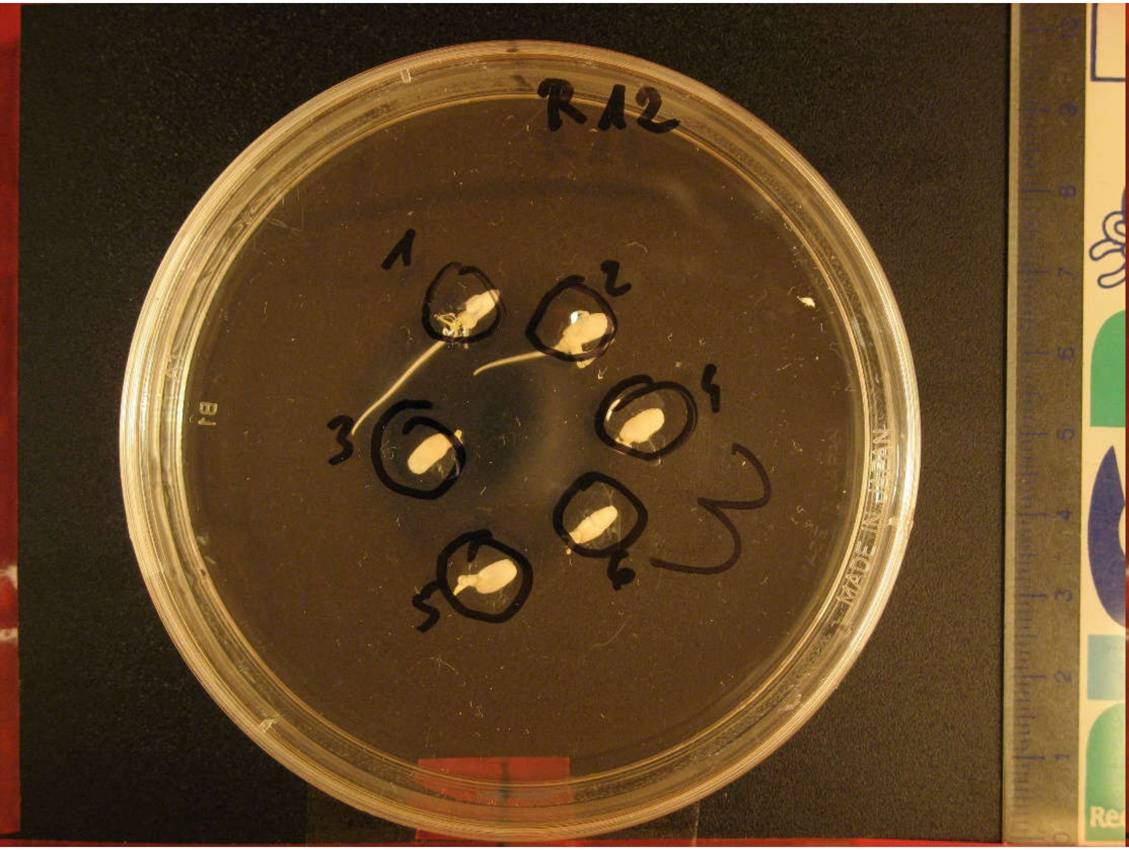
callus cells



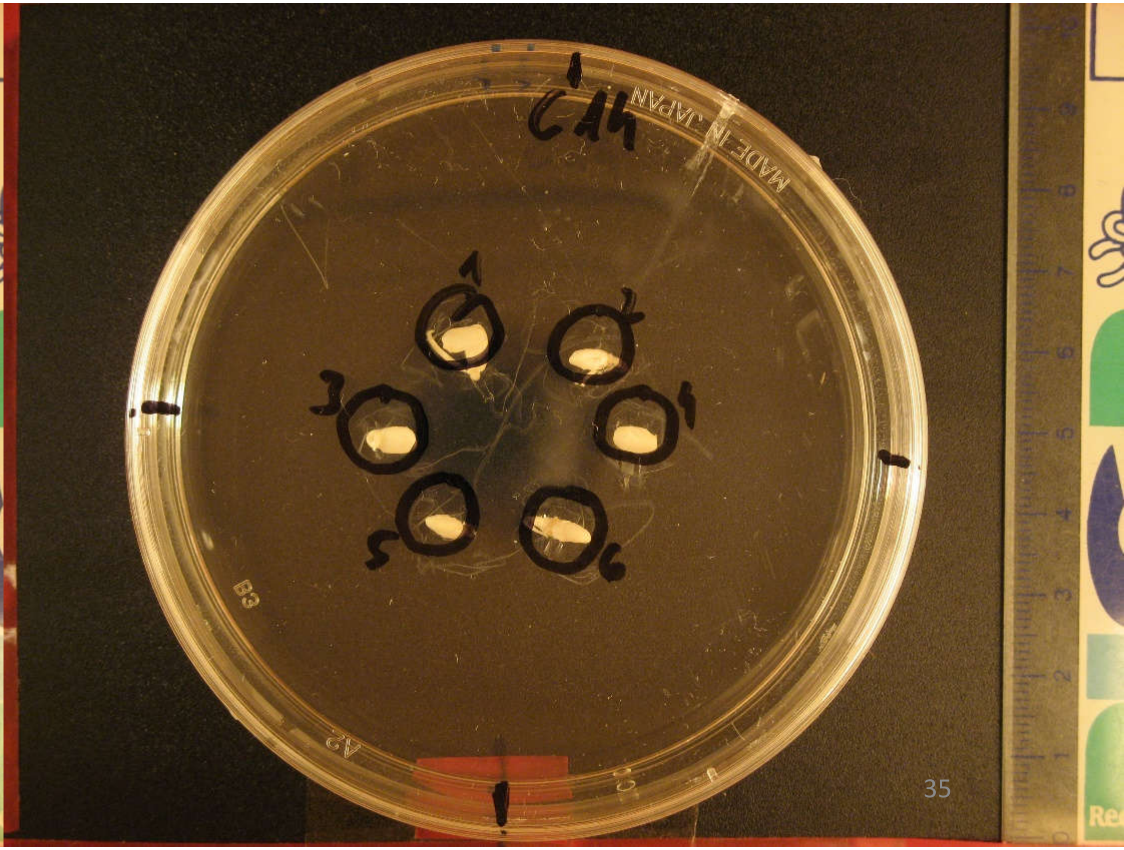
20140227

day 8

somatic cells



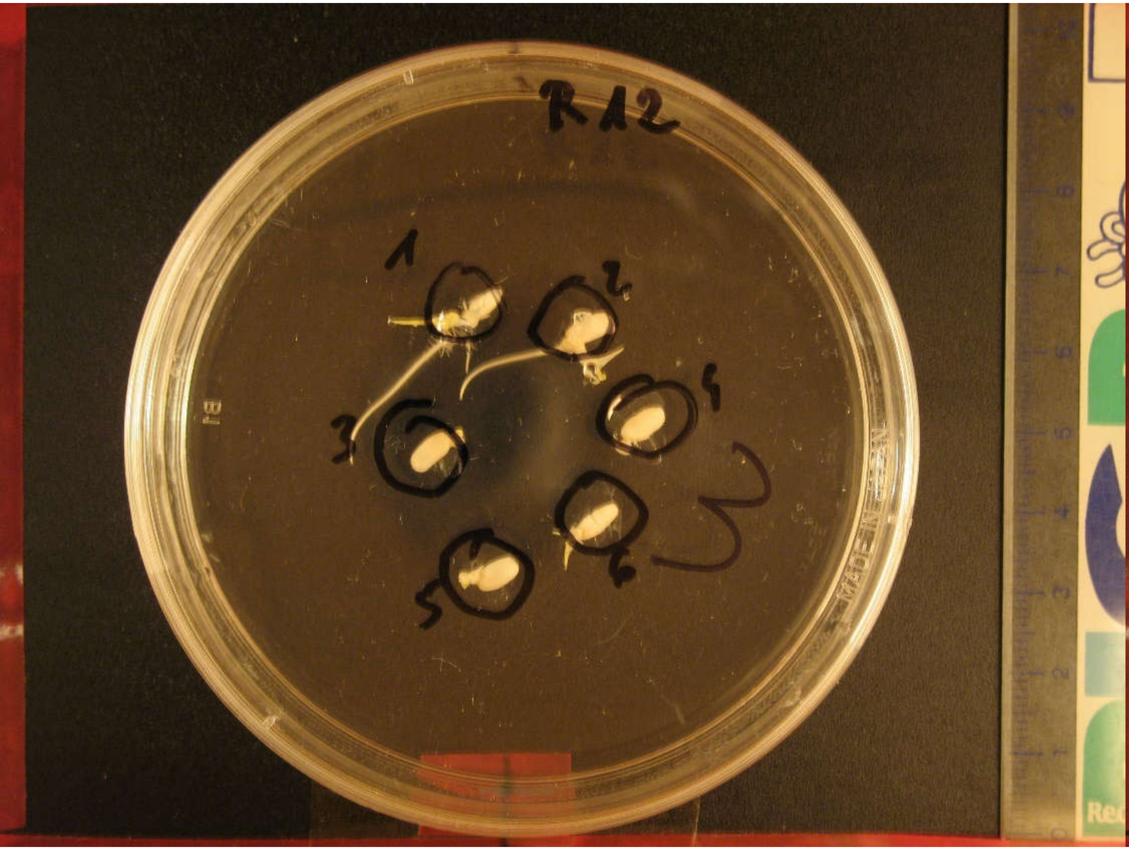
callus cells



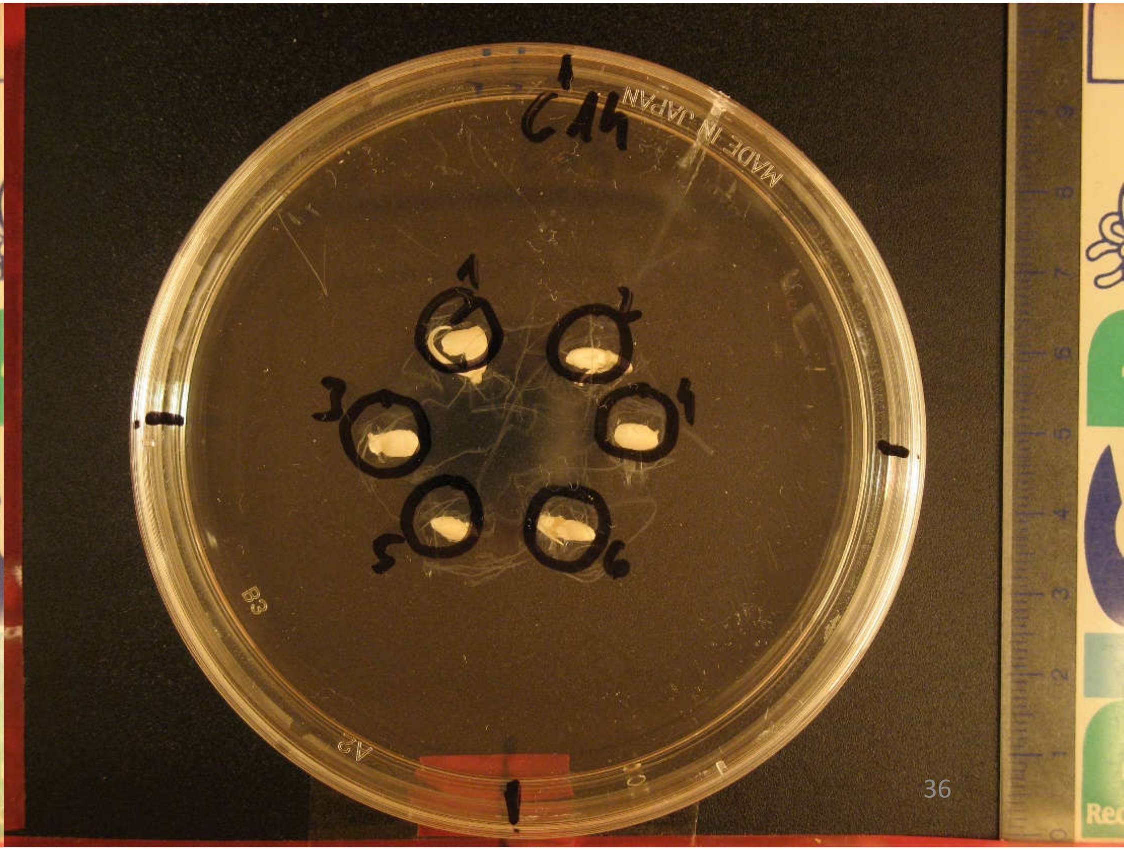
20140301

day 10

somatic cells



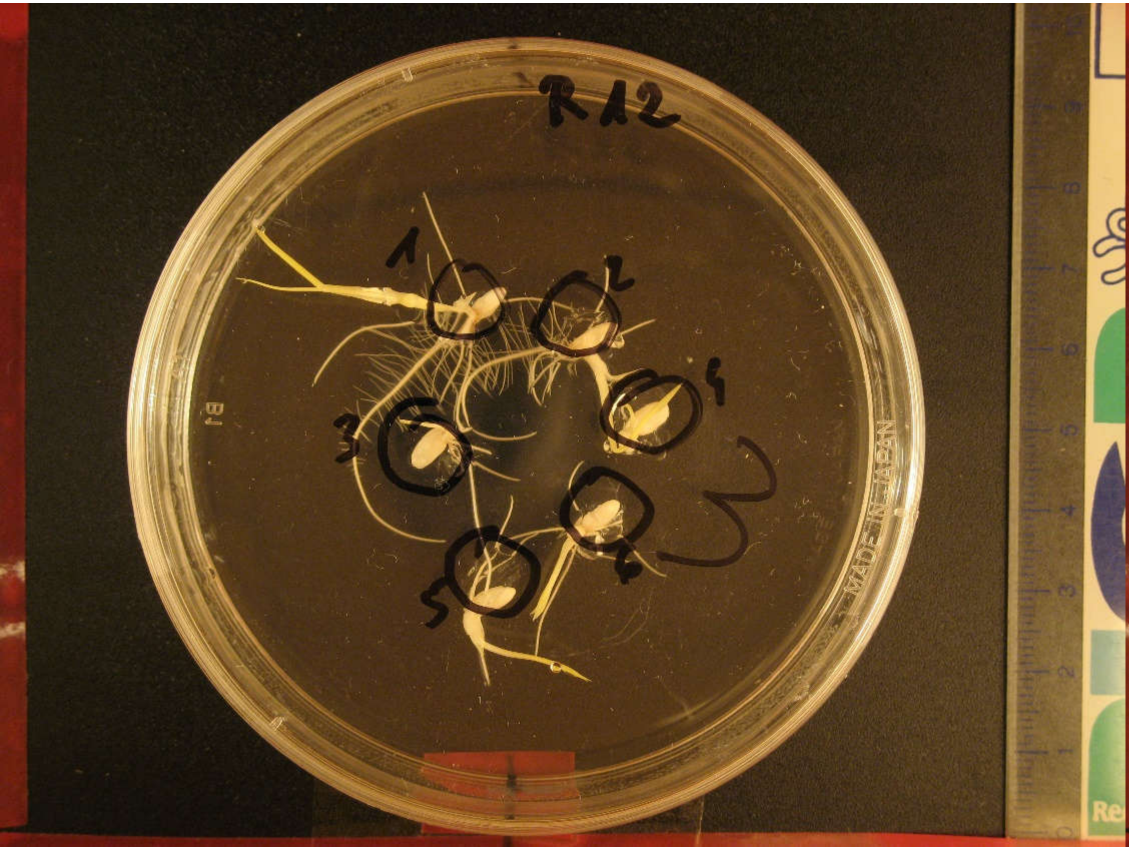
callus cells



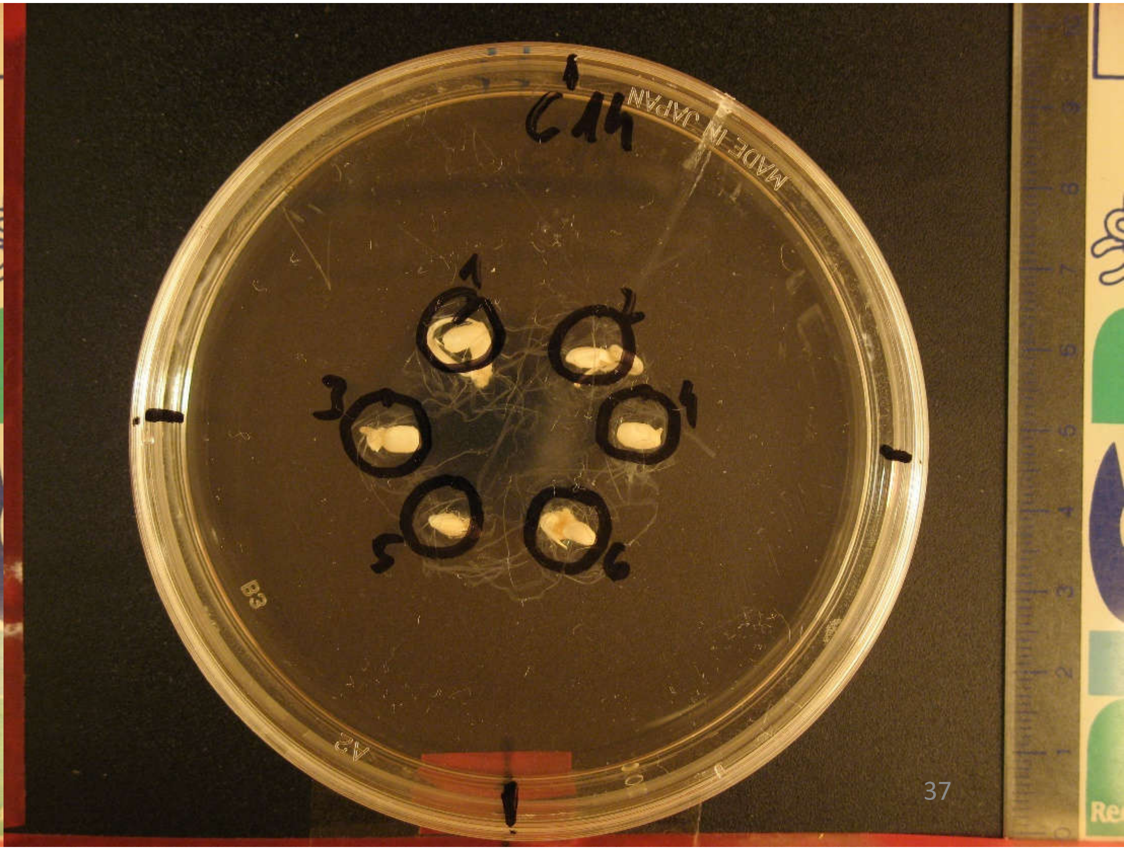
20140303

day 12

somatic cells



callus cells

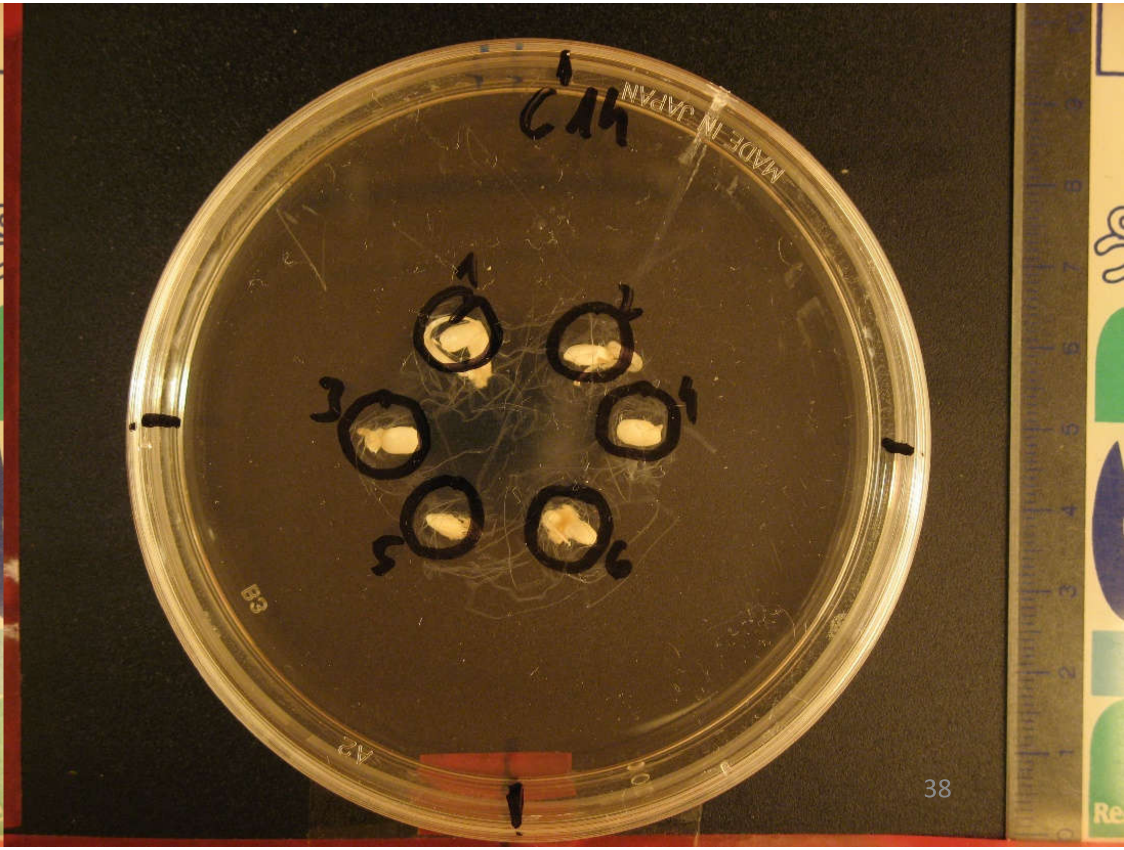


20140305

day 14

somatic cells

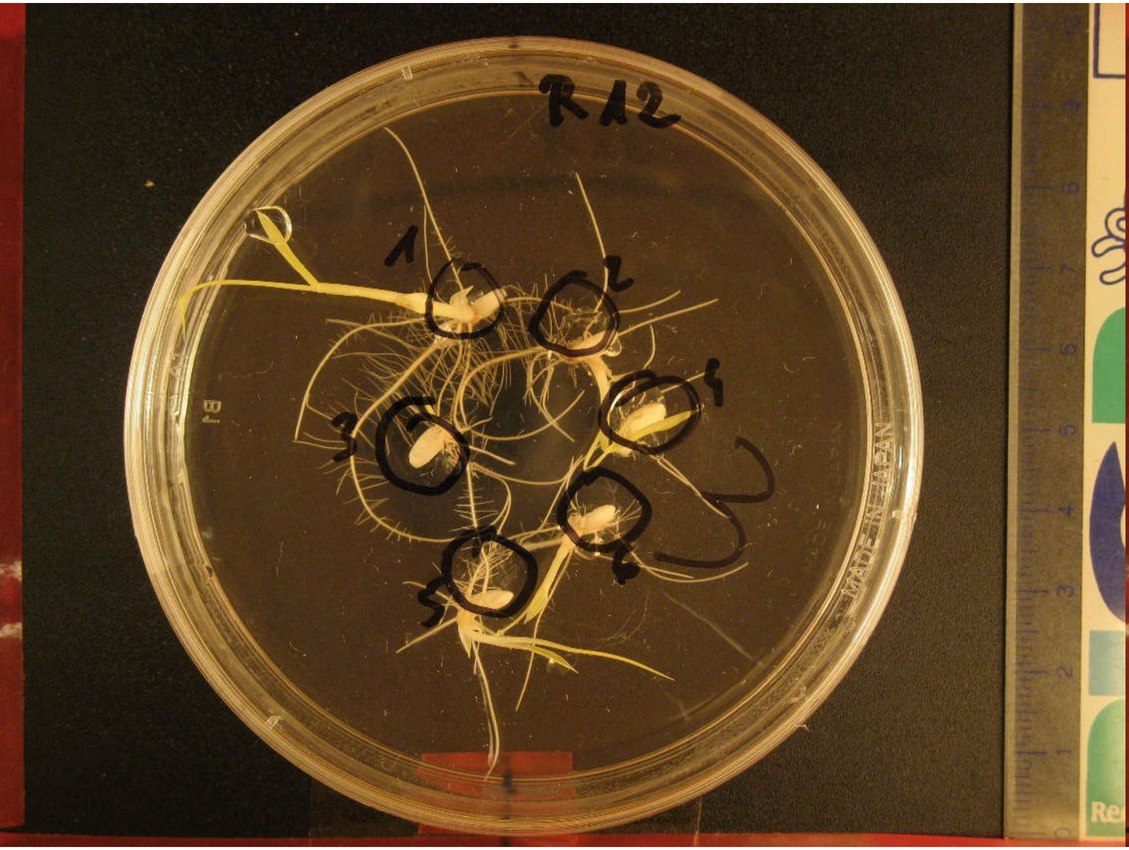
callus cells



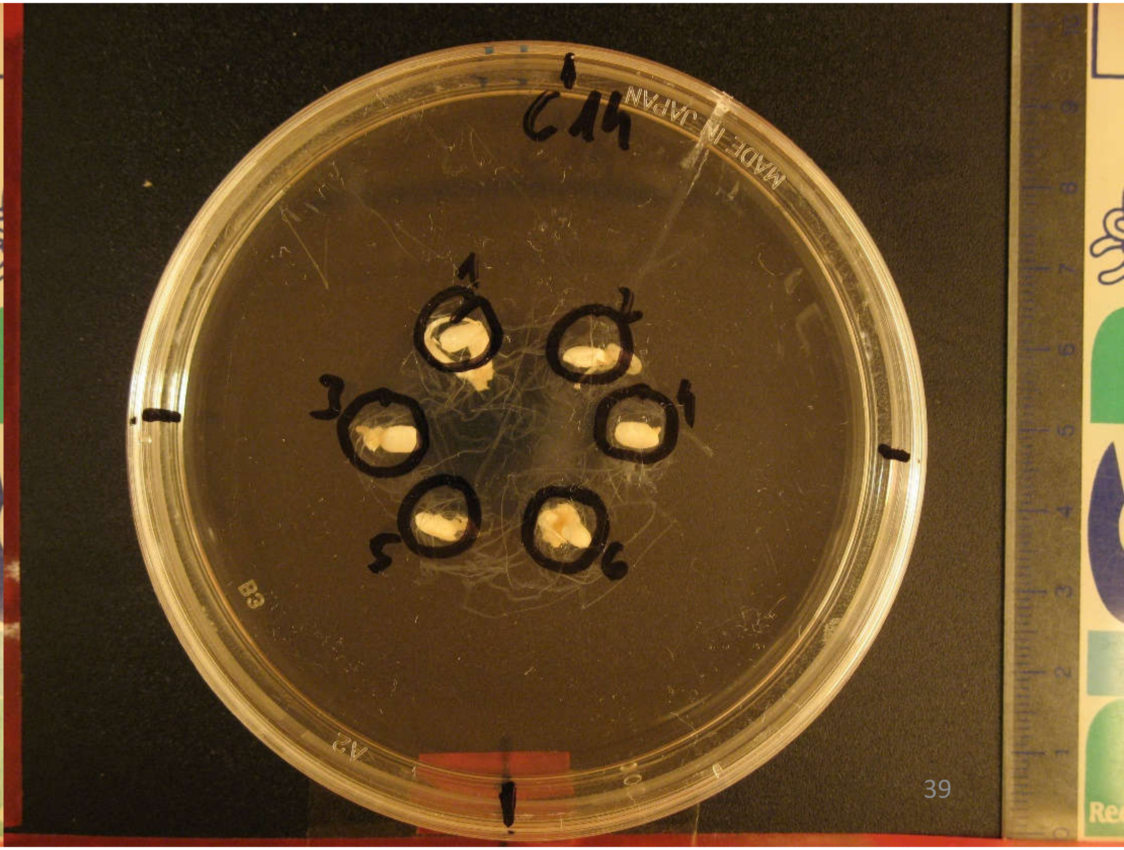
20140307

day 16

somatic cells



callus cells

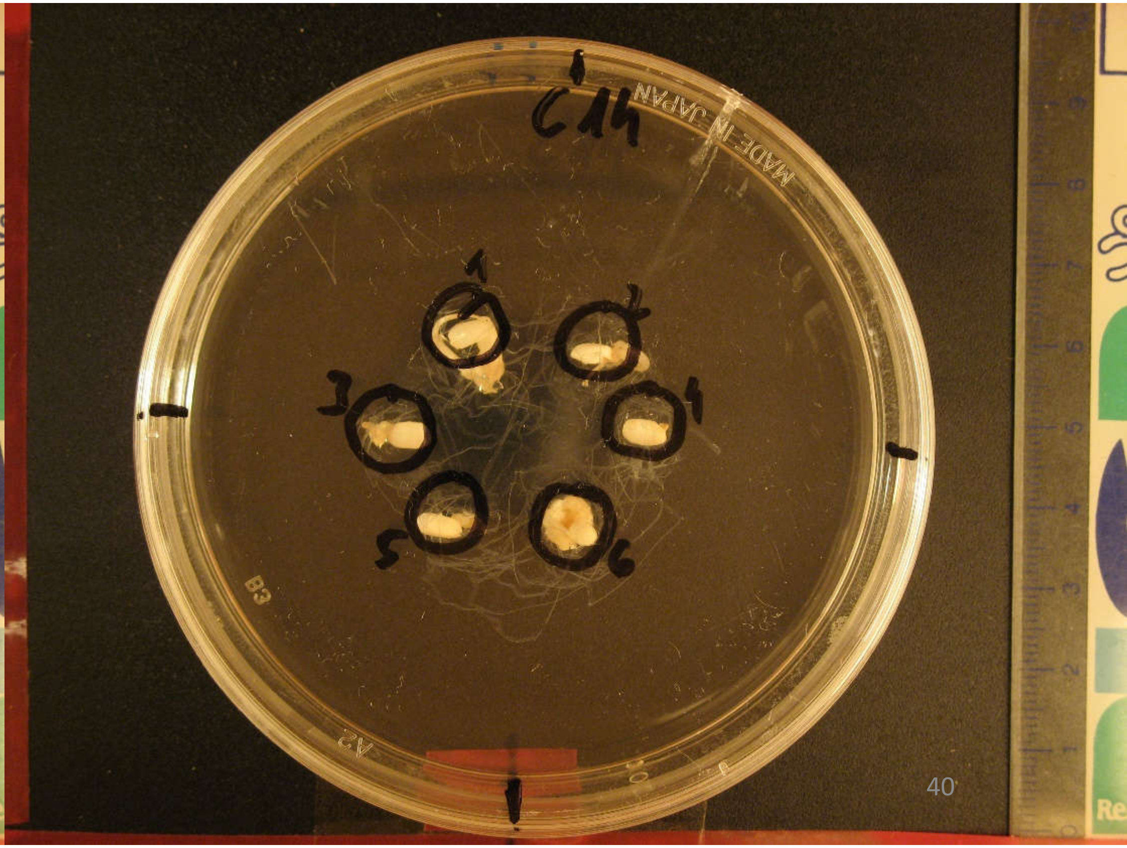


20140309

day 18

somatic cells

callus cells

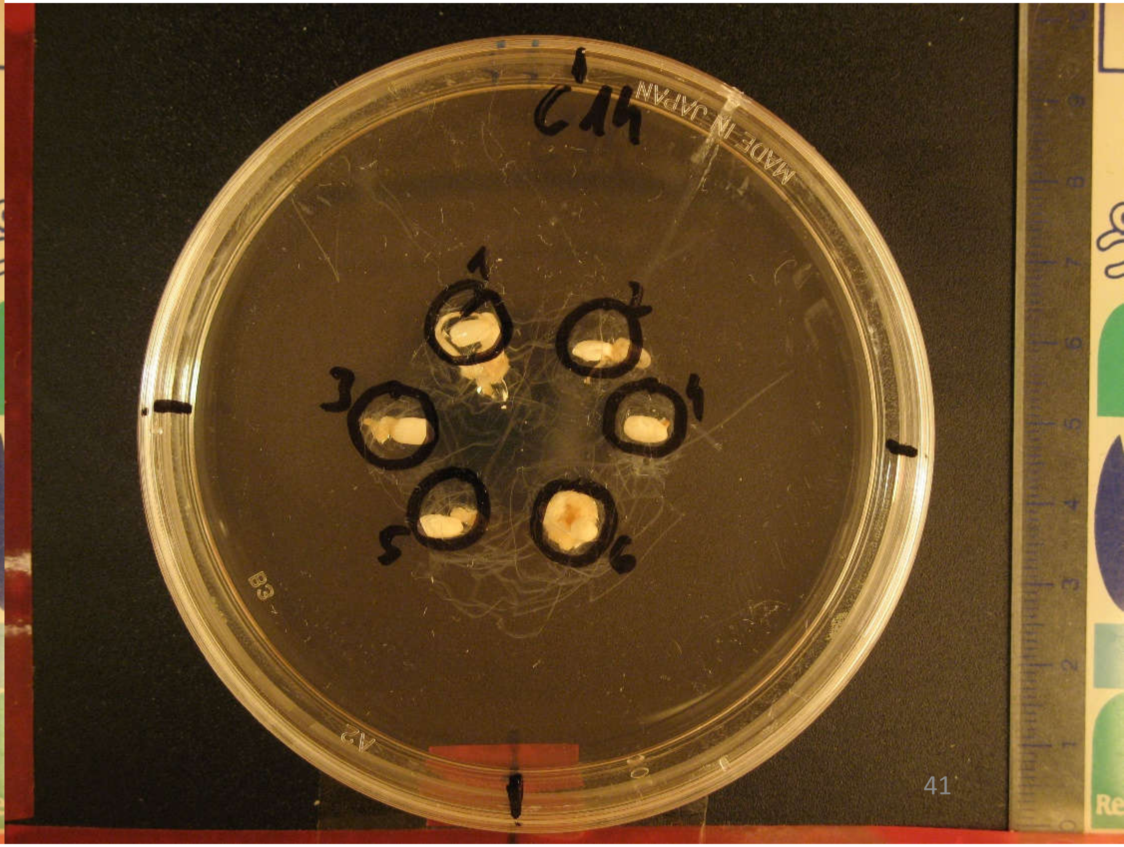


20140311

day 20

somatic cells

callus cells

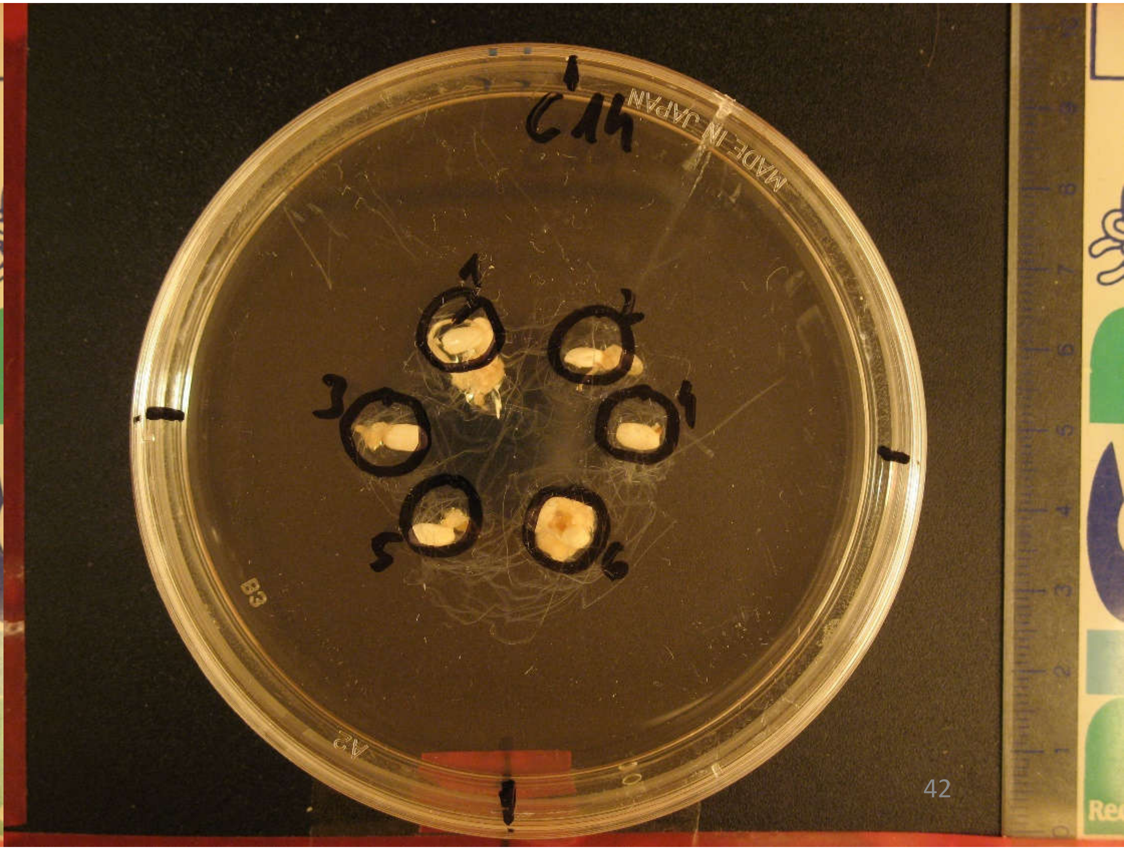


20140313

day 22

somatic cells

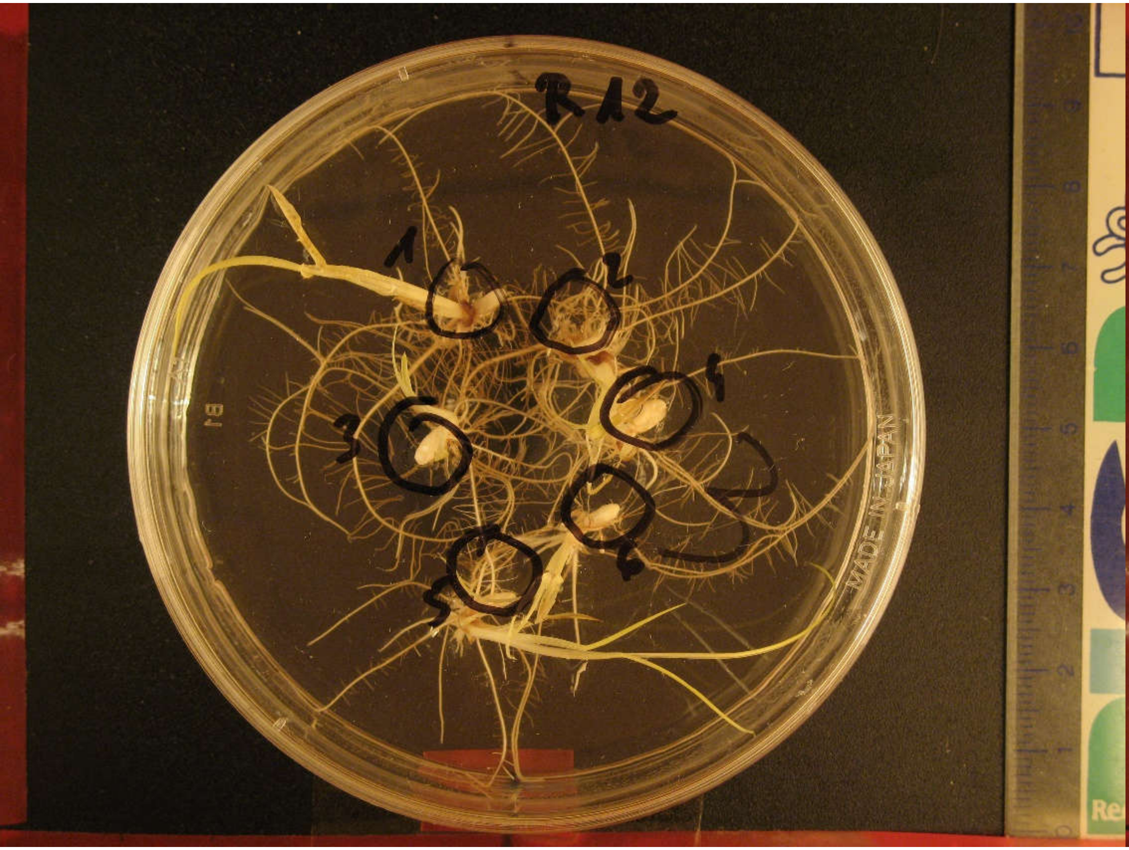
callus cells



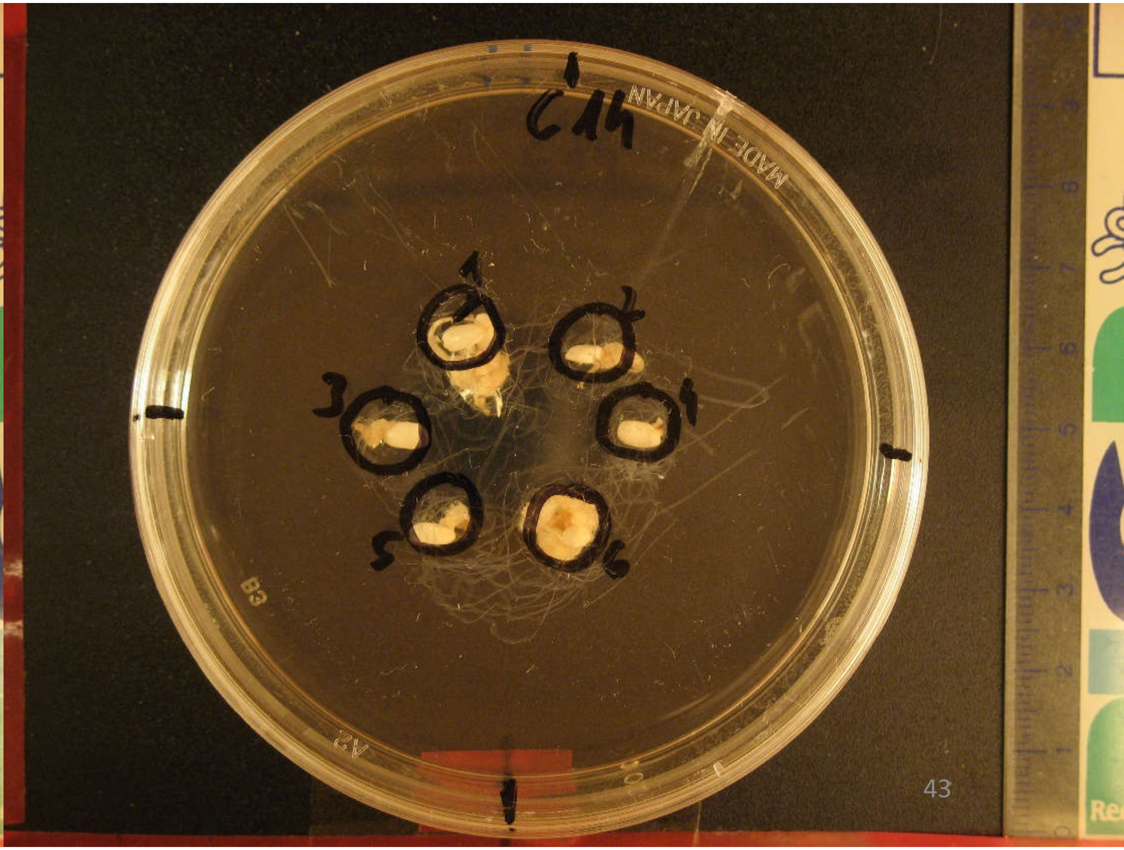
20140315

day 24

somatic cells



callus cells

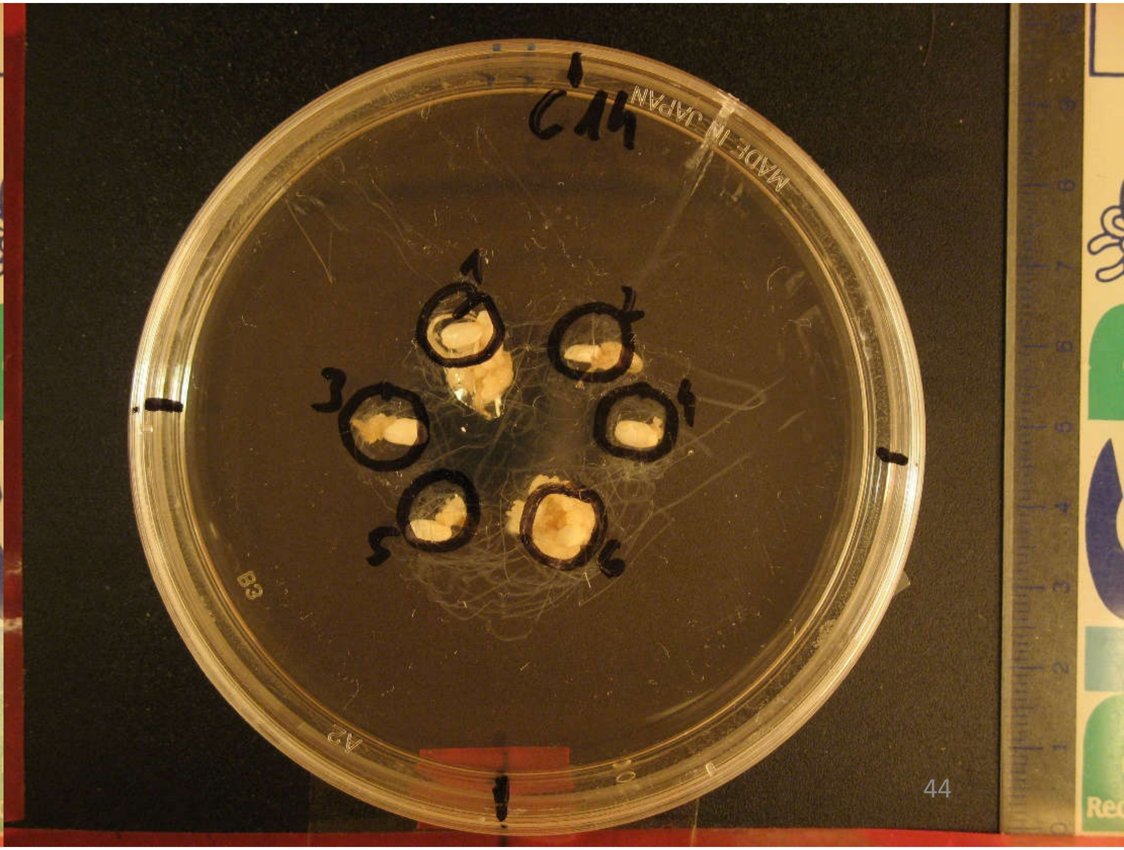


20140317

day 26

somatic cells

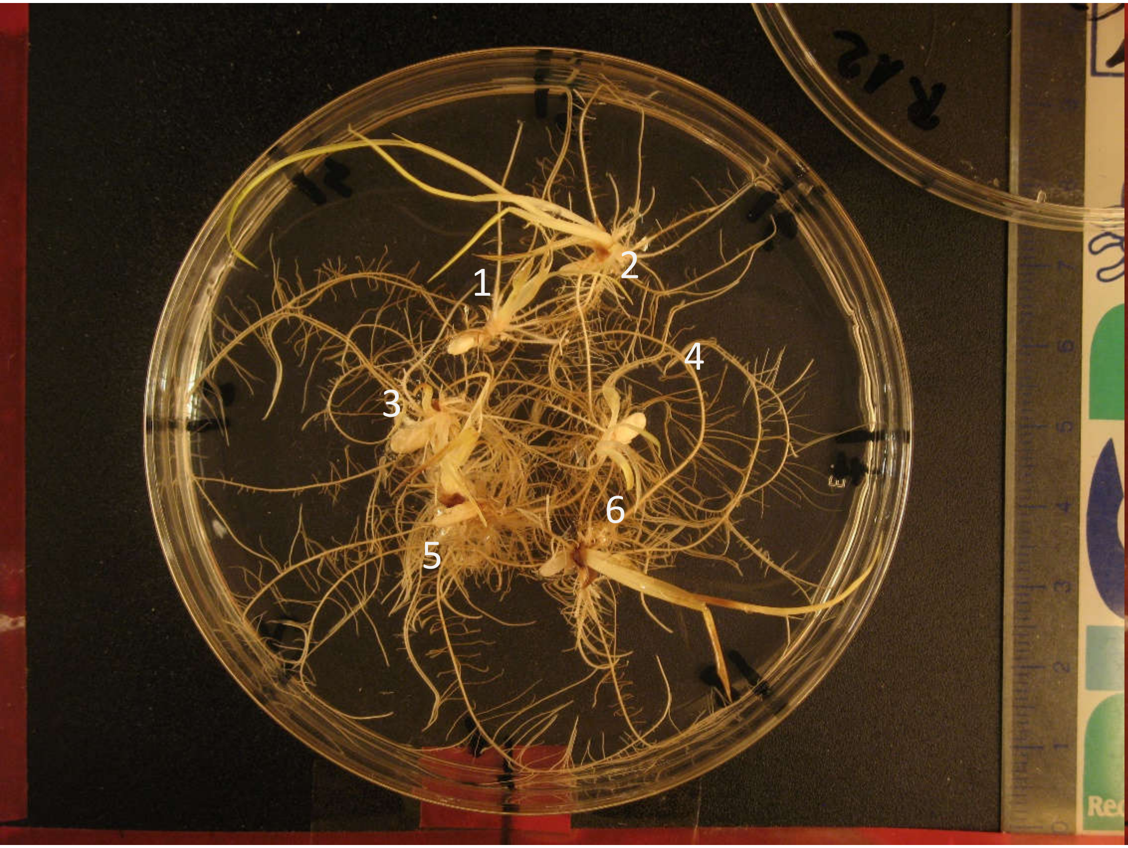
callus cells



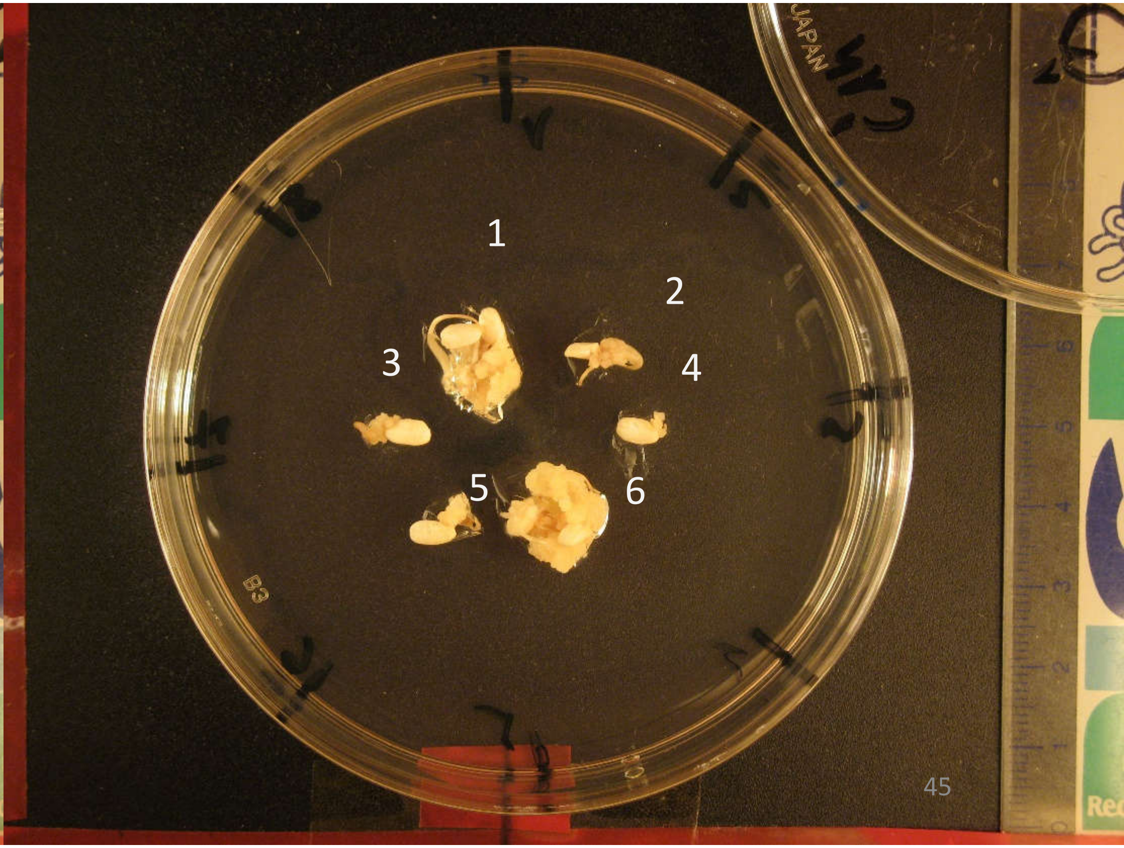
20140319

day 28

somatic cells

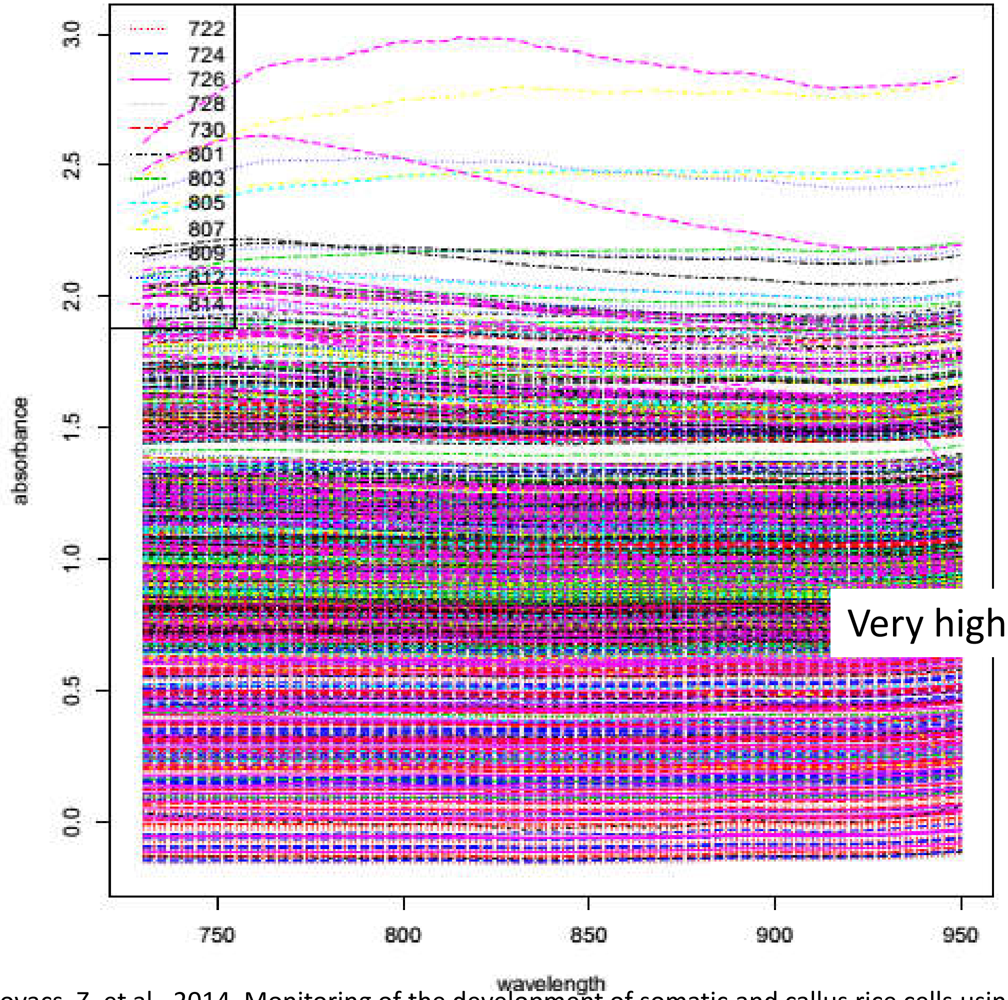


callus cells

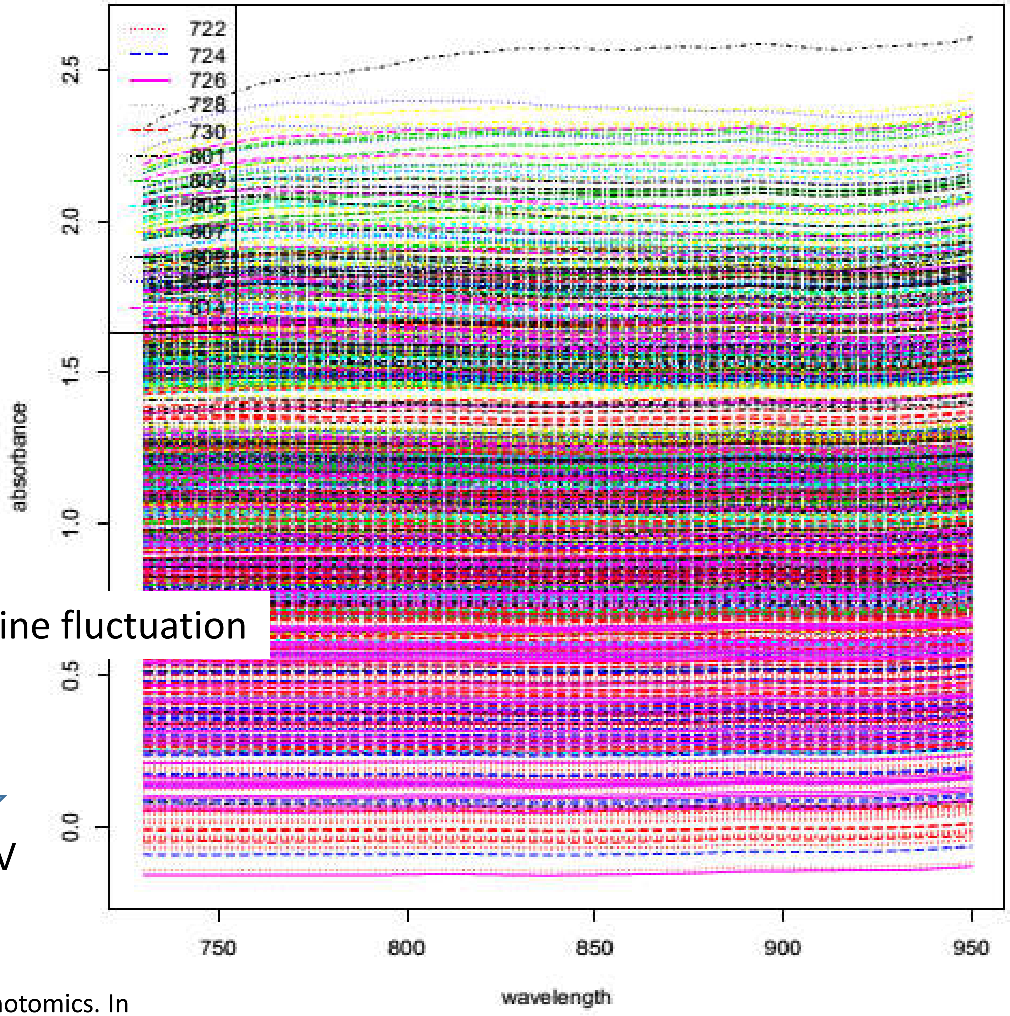


Calculated absorbance spectra

callus cells



somatic cells



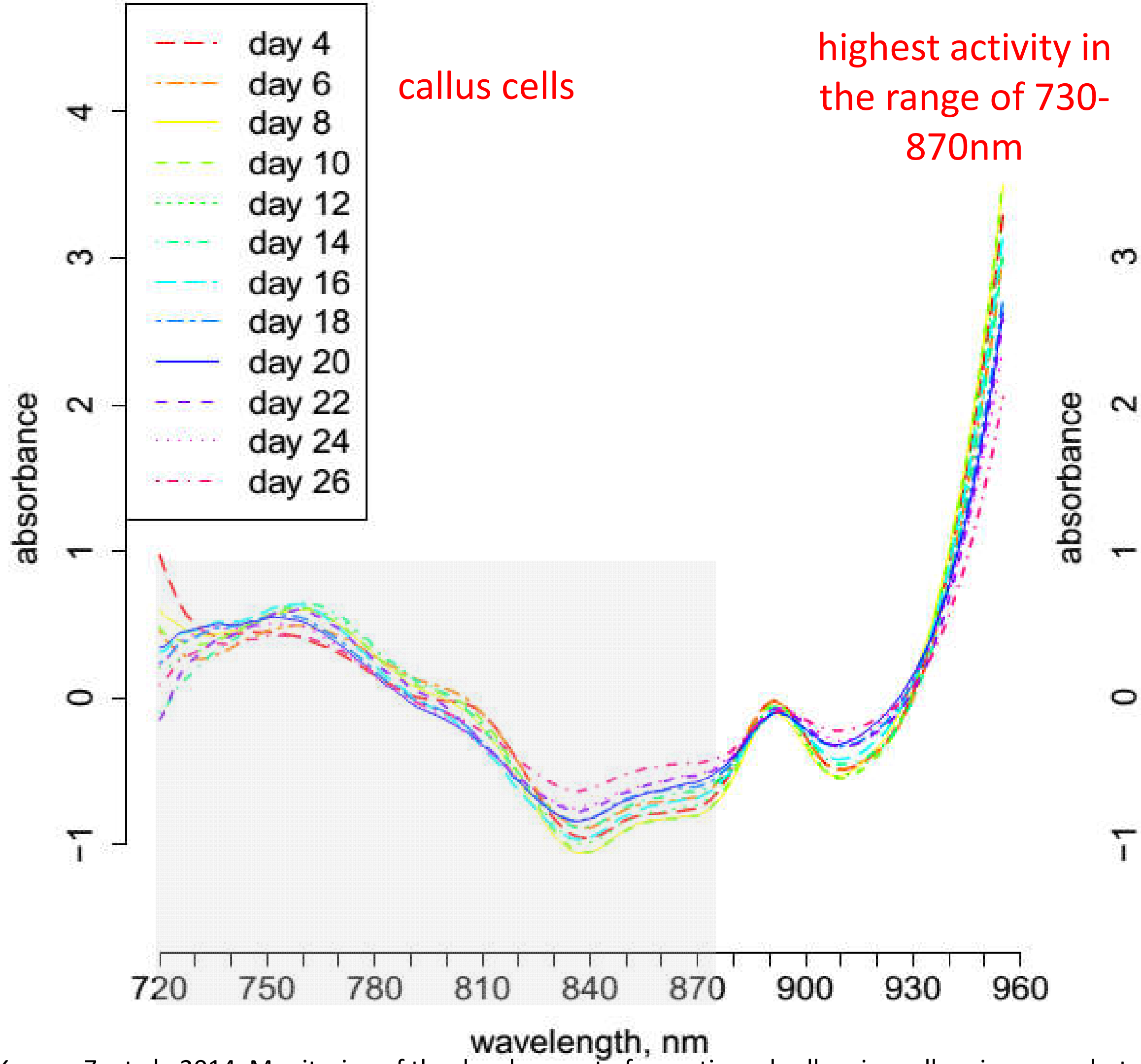
Very high baseline fluctuation

SNV

Kovacs, Z. et al., 2014. Monitoring of the development of somatic and callus rice cells using aquaphotomics. In *73th Annual Meeting of the Japan Society of Agricultural Machinery and Food Engineers*. Okinawa, Japan, p. 267.

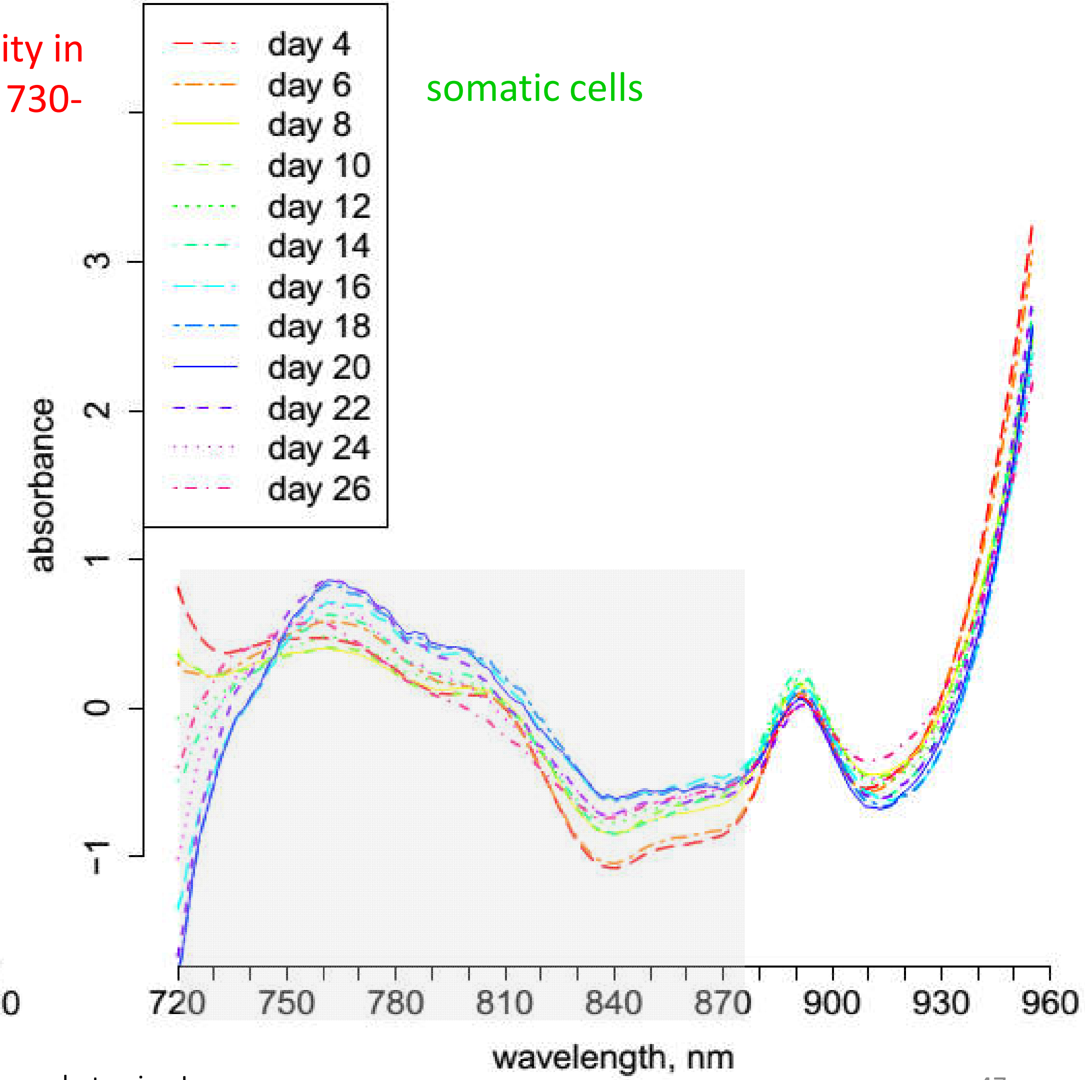
Daily average absorbance spectra

SNV + linear detrend



callus cells

highest activity in the range of 730-870nm



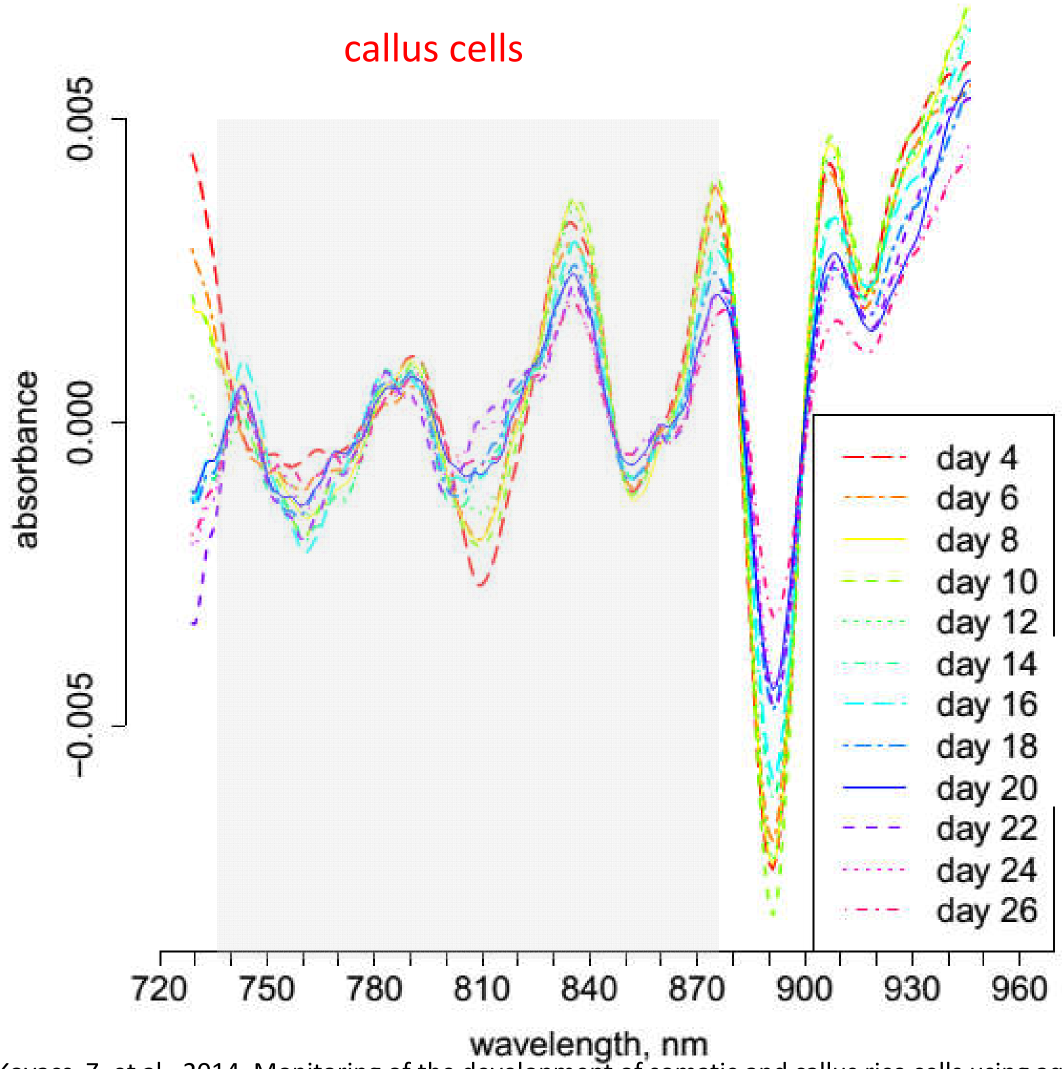
somatic cells

Kovacs, Z. et al., 2014. Monitoring of the development of somatic and callus rice cells using aquaphotomics. In *73th Annual Meeting of the Japan Society of Agricultural Machinery and Food Engineers*. Okinawa, Japan, p. 267.

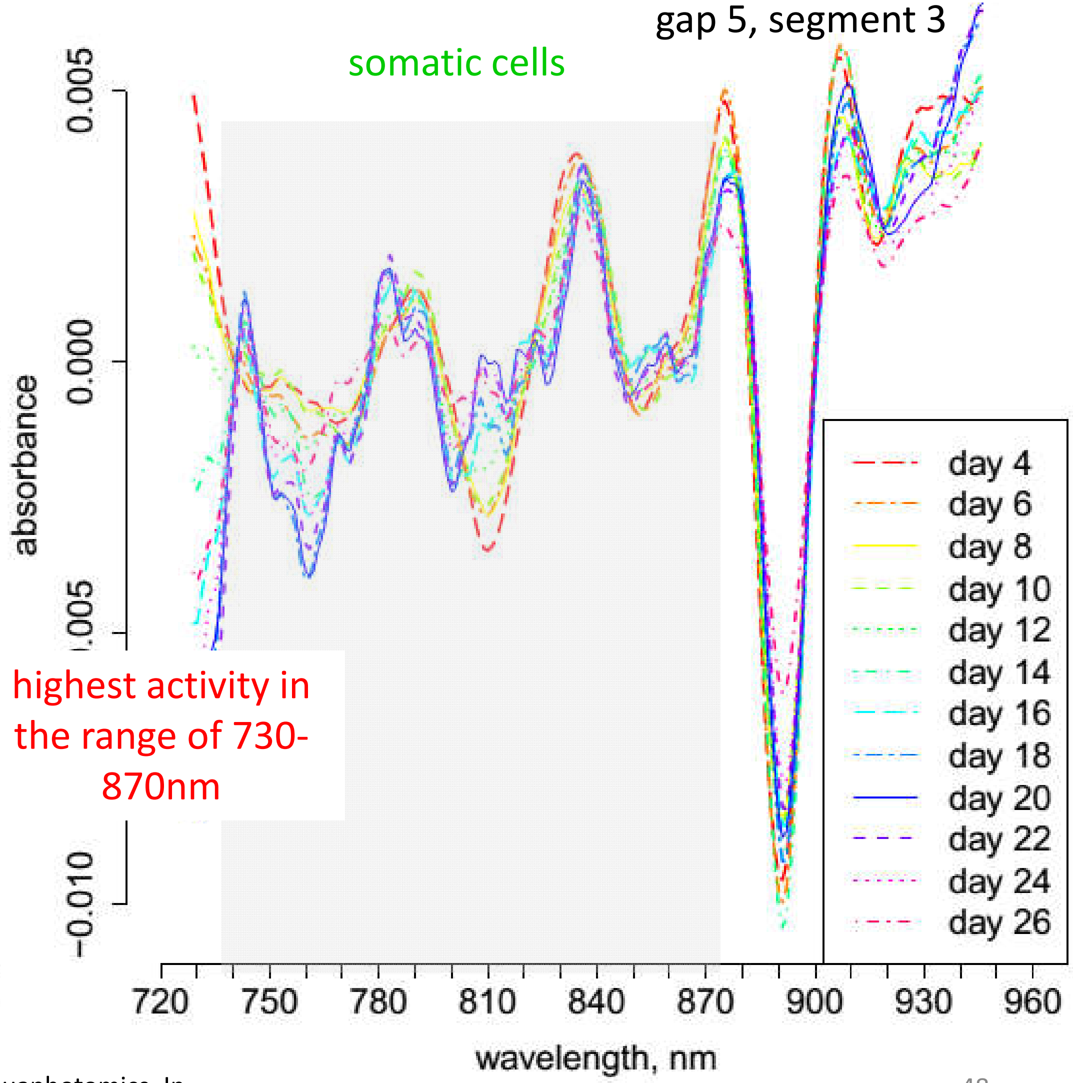
Daily average absorbance spectra

SNV + linear detrend
2nd derivative
gap 5, segment 3

callus cells



somatic cells

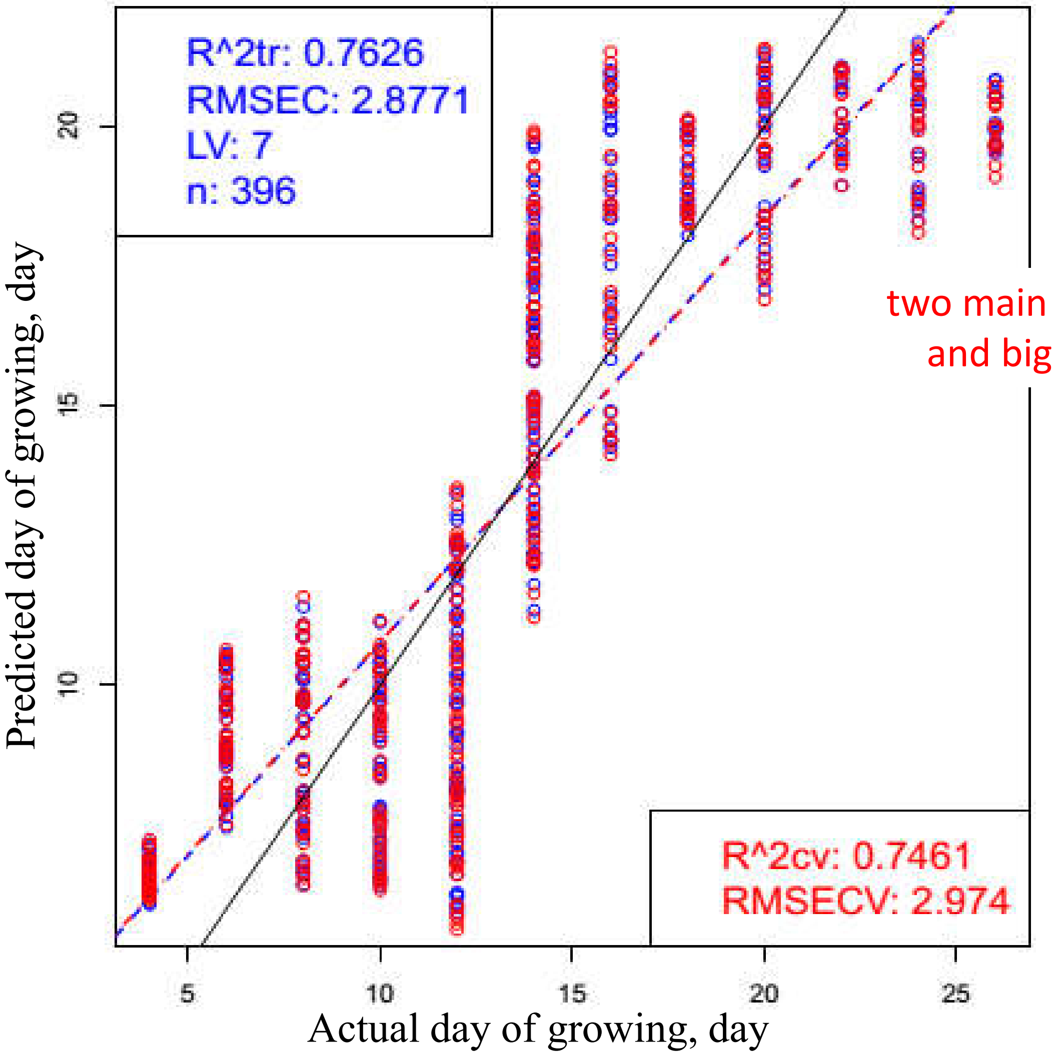


highest activity in the range of 730-870nm

Kovacs, Z. et al., 2014. Monitoring of the development of somatic and callus rice cells using aquaphotomics. In *73th Annual Meeting of the Japan Society of Agricultural Machinery and Food Engineers*. Okinawa, Japan, p. 267.

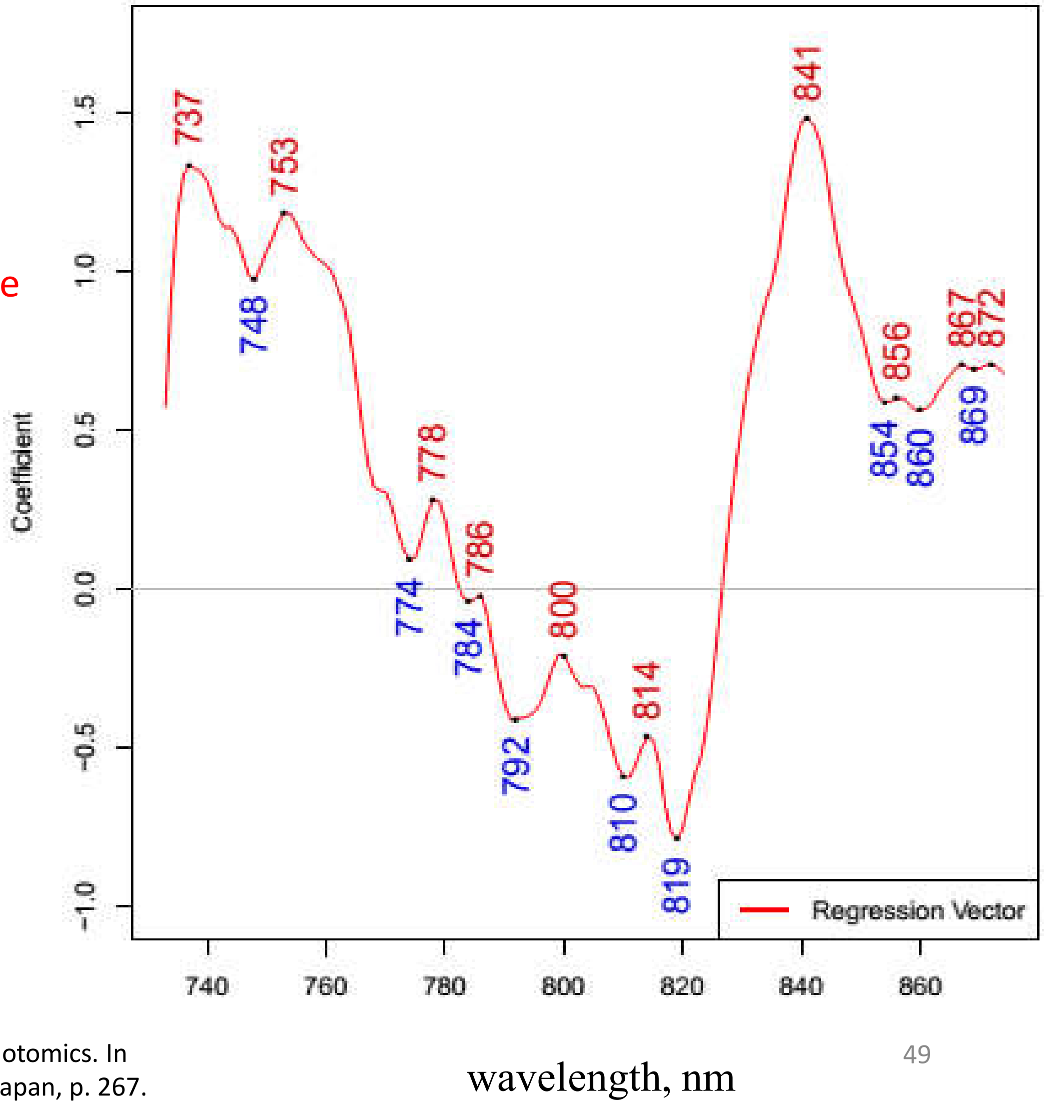
PLS regression on the growing days

callus cells



two main stage
and big SD

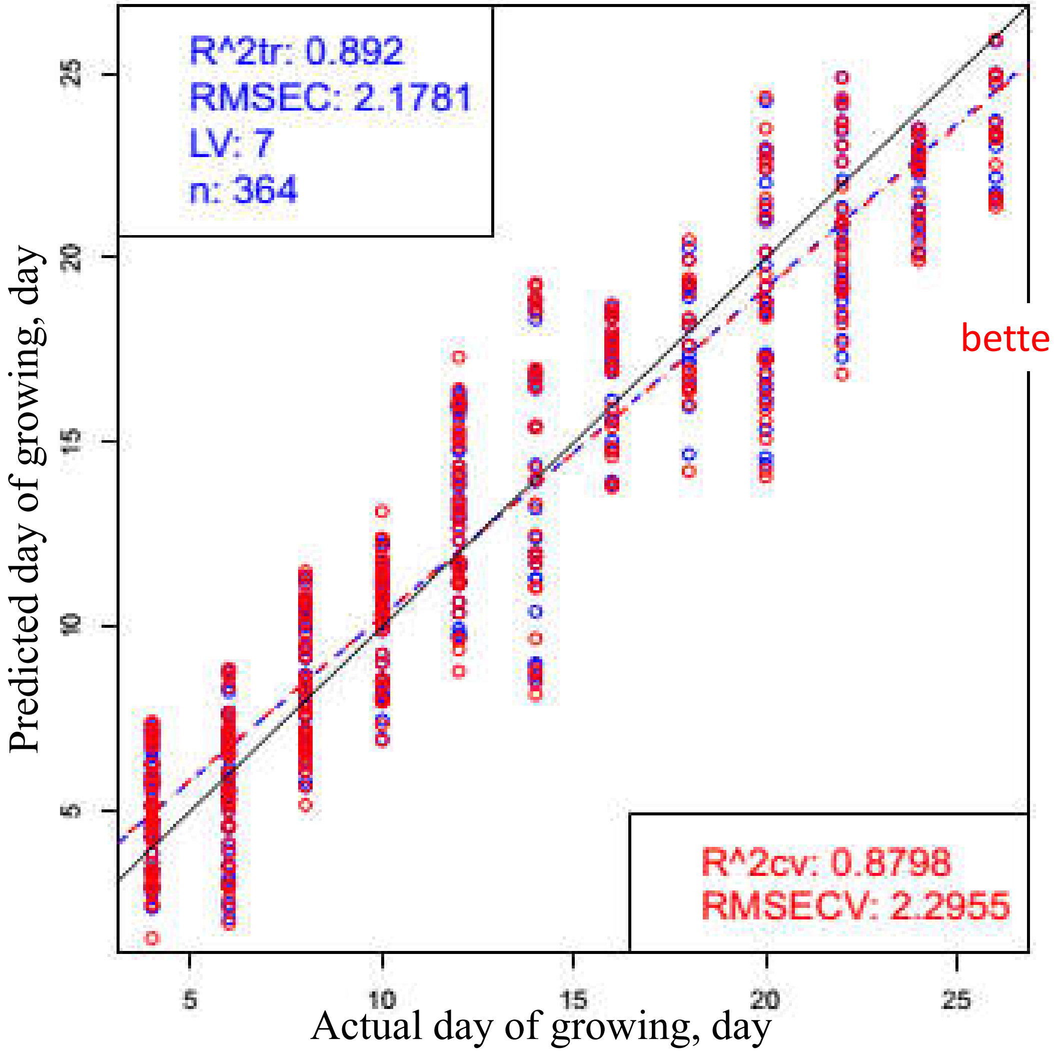
730-870nm



Kovacs, Z. et al., 2014. Monitoring of the development of somatic and callus rice cells using aquaphotomics. In *73th Annual Meeting of the Japan Society of Agricultural Machinery and Food Engineers*. Okinawa, Japan, p. 267.

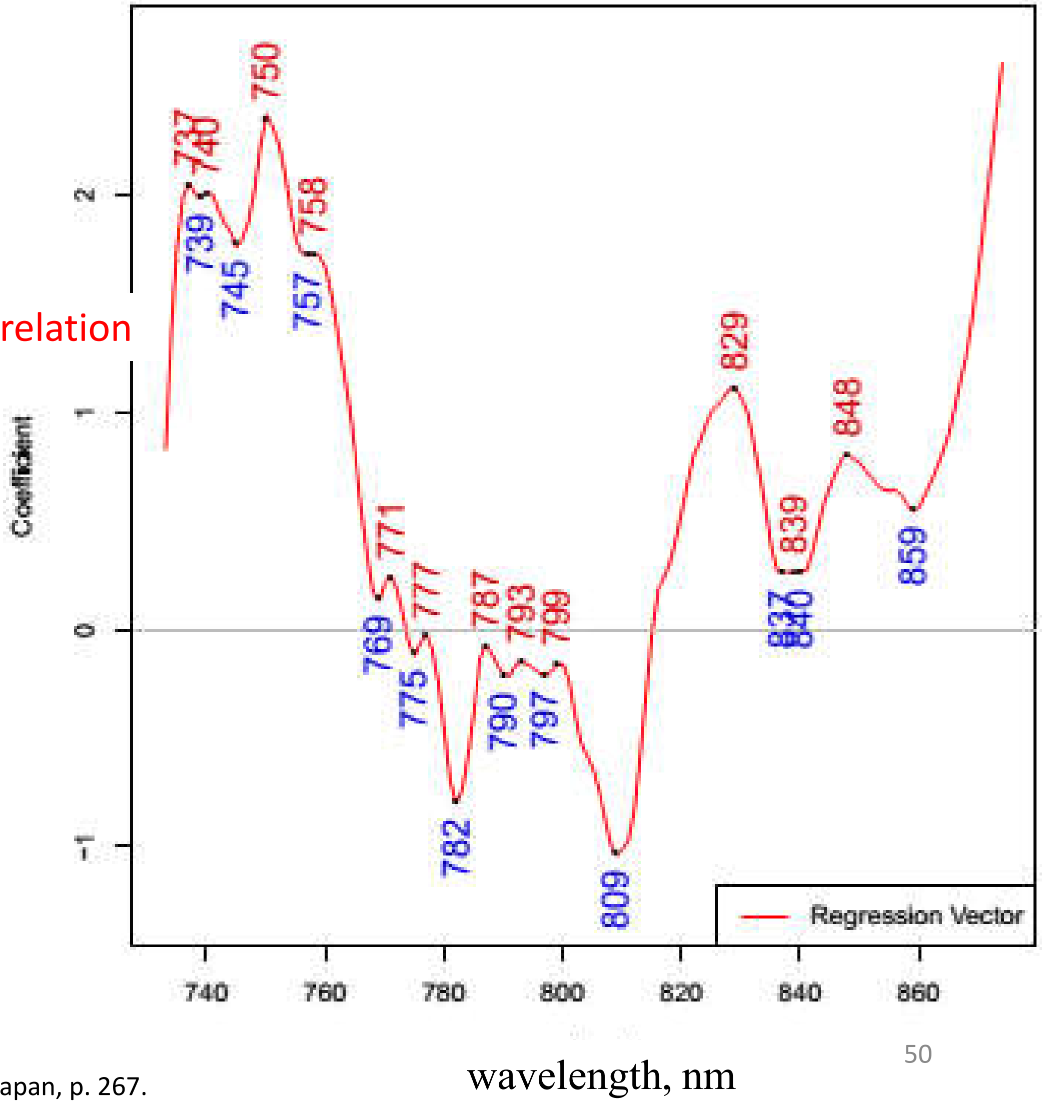
PLS regression on the growing days

somatic cells



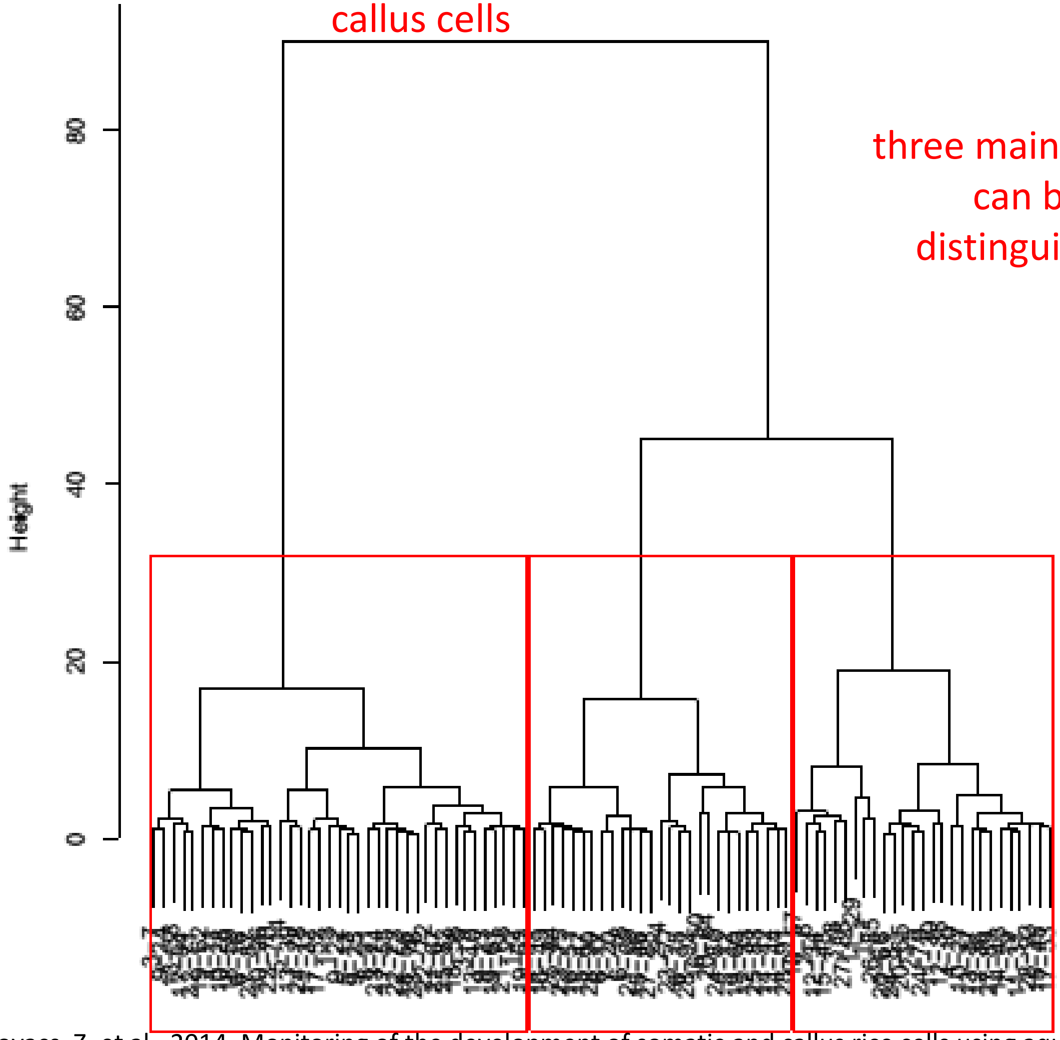
better correlation

730-870nm

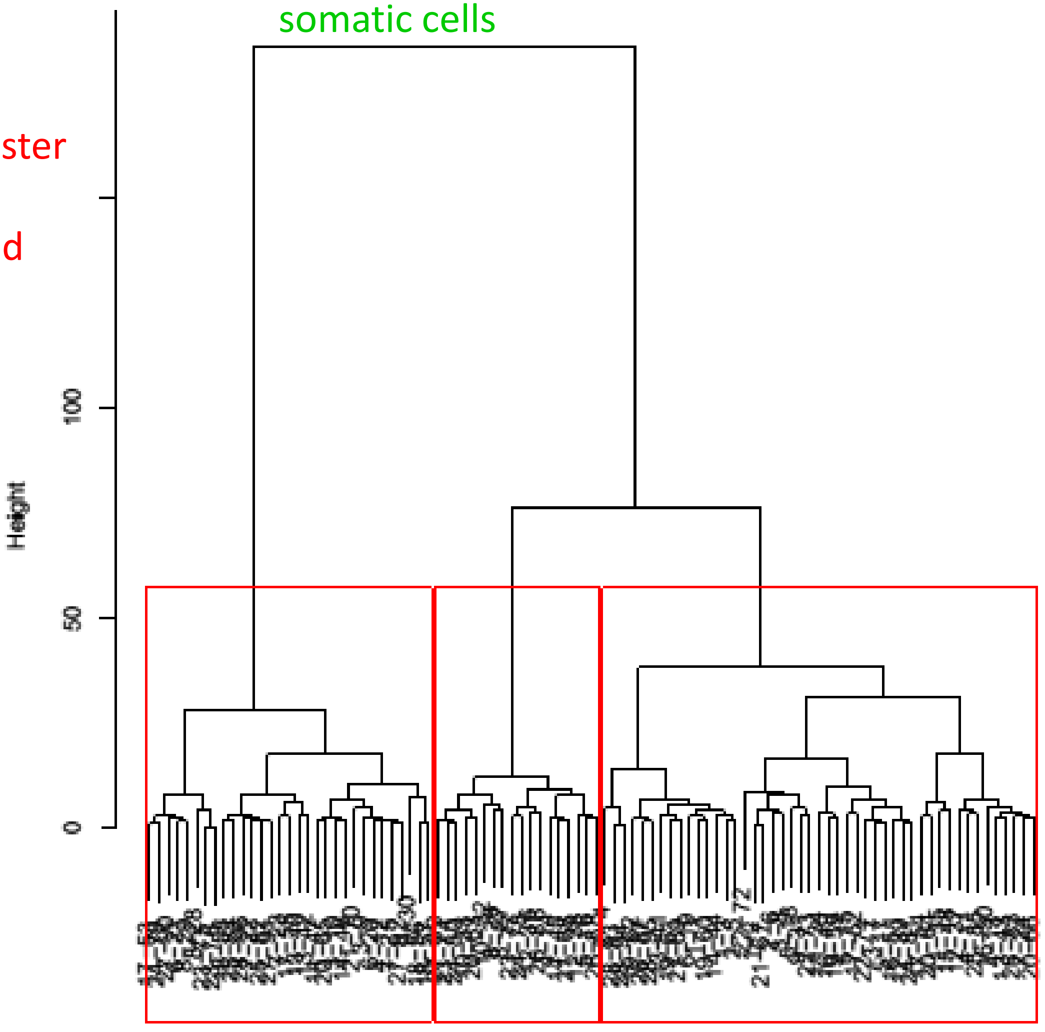


Kovacs, Z. et al., 2014. Monitoring of the development of somatic and callus rice cells using aquaph
73th Annual Meeting of the Japan Society of Agricultural Machinery and Food Engineers. Okinawa, Japan, p. 267.

HCA to determine groups



three main cluster can be distinguished

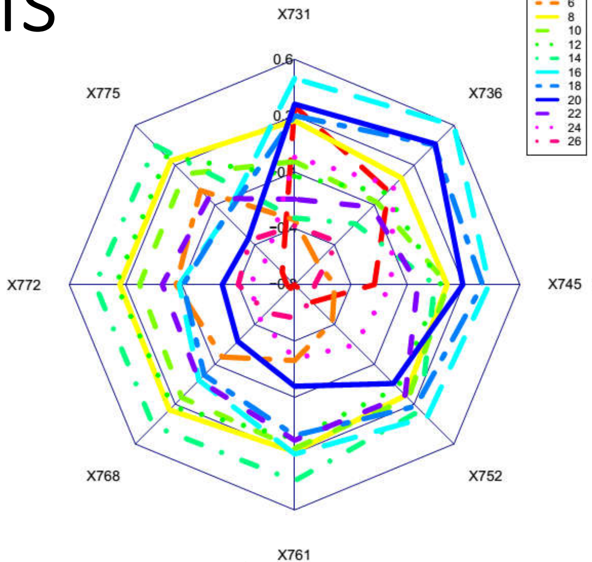


Kovacs, Z. et al., 2014. Monitoring of the development of somatic and callus rice cells using aquaphotomics. In 73th *Annual Meeting of the Japan Society of Agricultural Machinery and Food Engineers*. Okinawa, Japan, p. 267.

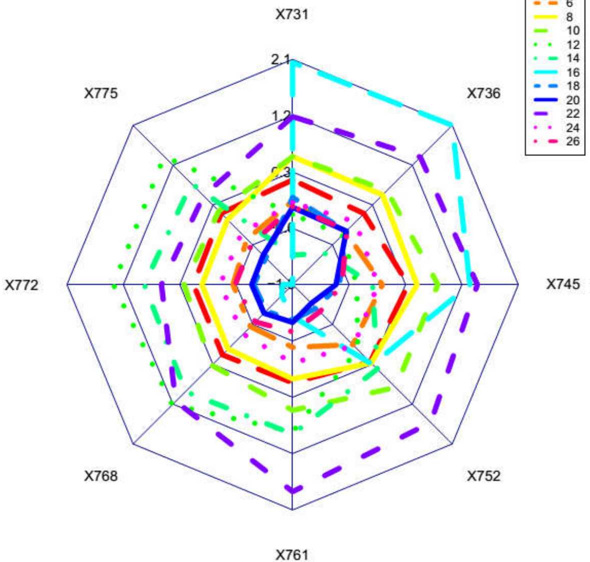
Aquagrams

callus cells

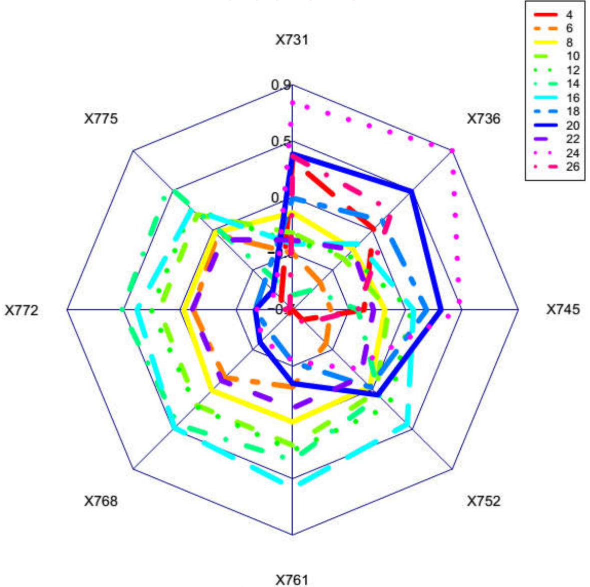
cluster 1



cluster 2

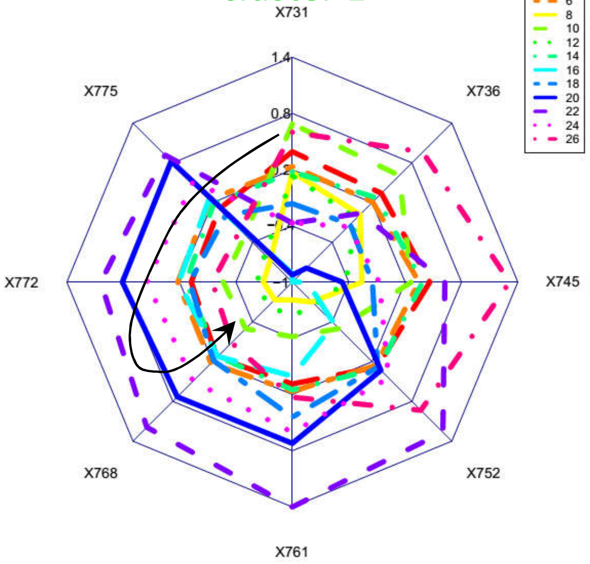


cluster 3

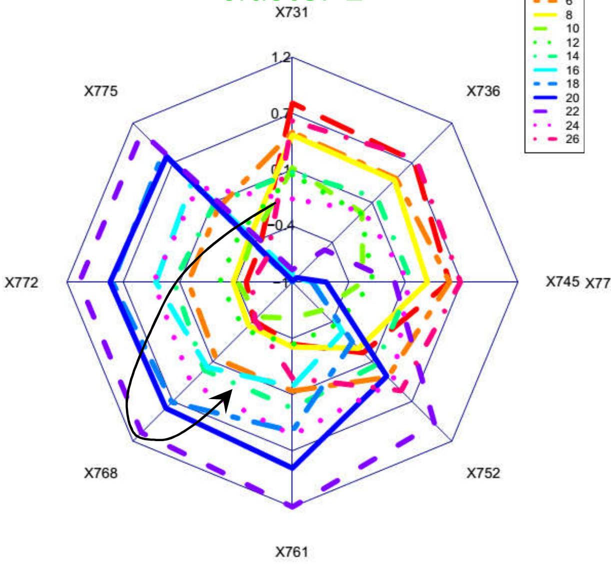


somatic cells

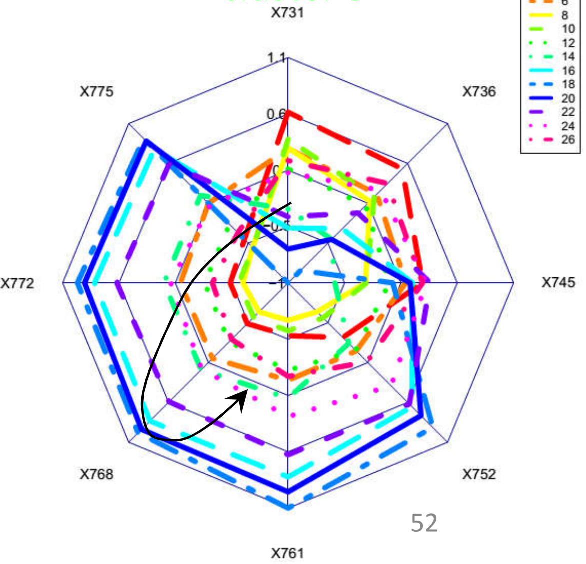
cluster 1



cluster 2



cluster 3



spectral patterns of the callus cells do not show as systematic tendency as spectral patterns of somatic cells

Agenda of the presentation

- Bacteria growing and Yogurt
- Plant cells growing
- **Mineral Waters**
- Calculation and presentation method of WASP

Application of Aquaphotomics to learn more about the rules of water

http://www.dreamstime.com

objectives

- to compare the water spectral pattern of different mineral water samples
- to determine the applicability of NIRS and Aquaphotomics in mineral water analyses
- to **introduce a new complimentary concept of water quality** evaluation:
  - easy-to-use
  - time and cost effective
  - fast monitoring of water molecular system changes
  - provide information about the multitude of water structural changes
- method **can warn at any irregular changes of abnormal water quality**

Materials and methods
– *instruments and conditions* –

- NIR Gun with 10mm pathlength cuvette cell in transflectance mode
- Ground Water samples has been Analyzed every day for more than three years
- 3 consecutive spectra were taken every day

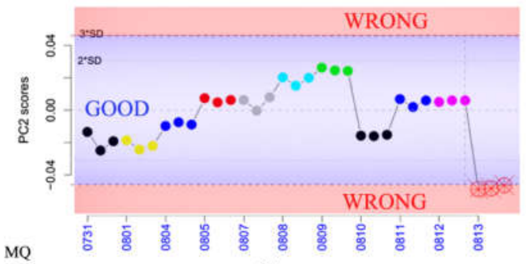
http://www.nirsresearch.com/NP-15967-fqa_nir_gun.html

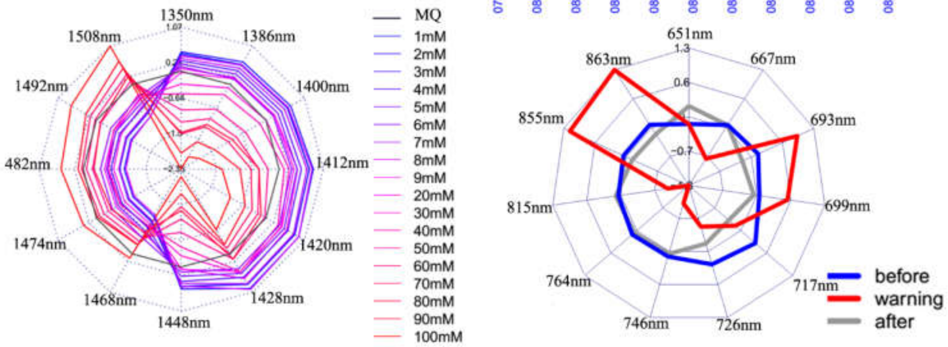
Experiments with aqueous solutions and ground water

Monitoring of individual parameters is not always satisfactory

↓

Examination of water at specific wavelengths provides more information





Kovacs, Z. et al., 2016. Water spectral pattern as holistic marker for water quality monitoring. *Talanta*, 147, pp.598–608.

Talanta 147 (2016) 598–608

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Water spectral pattern as holistic marker for water quality monitoring

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[b] Corvinus University of Budapest, Faculty of Food Science, Department of Physics and Control, 14-16 Somlói str., Budapest 1118, Hungary
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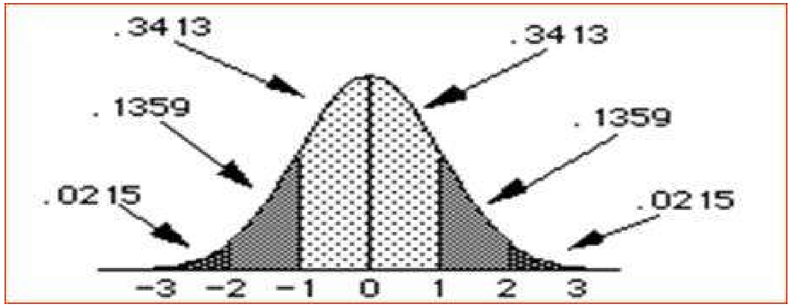
Spectral monitoring
Water molecular system

ABSTRACT

Online water quality monitoring technologies have been improving continuously. At the moment, water quality is defined by the respective range of few chosen parameters. However, this strategy requires sampling and it cannot provide evaluation of the entire water molecular system including various solutes. As it is nearly impossible to monitor every single molecule dissolved in water, the objective of our research is to introduce a complimentary approach, a new concept for water screening by observing the water molecular system changes using aquaphotomics and Quality Control Chart method. This approach can continuously provide quick information about any qualitative change of water molecular arrangement without taking into account the reason of the alteration of quality. Different species and concentrations of solutes in aqueous systems structure the water solvent differently. Aquaphotomics investigates not the characteristic absorption bands of the solute in question, but the solution absorption at vibrational bands of water's covalent and hydrogen bonds that have been altered by the solute. The applicability of the proposed concept is evaluated by monitoring the water structural changes in different aqueous solutions such as acid, sugar, and salt solutions at millimolar concentration level and in ground water. The results show the potential of the proposed approach to use water spectral pattern monitoring as bio marker of water quality. Our successful results open a new venue in water quality monitoring by offering a quick and cost effective method for continuous screening of water molecular arrangement. Instead of the regular analysis of individual physical or chemical parameters, with our method – as a complementary tool – the structural changes of water molecular system used as a mirror reflecting even small disturbances in water can indicate the necessity of further detailed analysis by conventional methods.

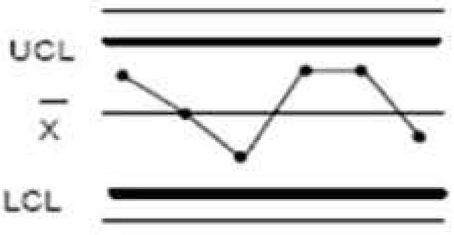
Materials and methods IV.
– *statistics* –



Model built based on the natural variability of the system

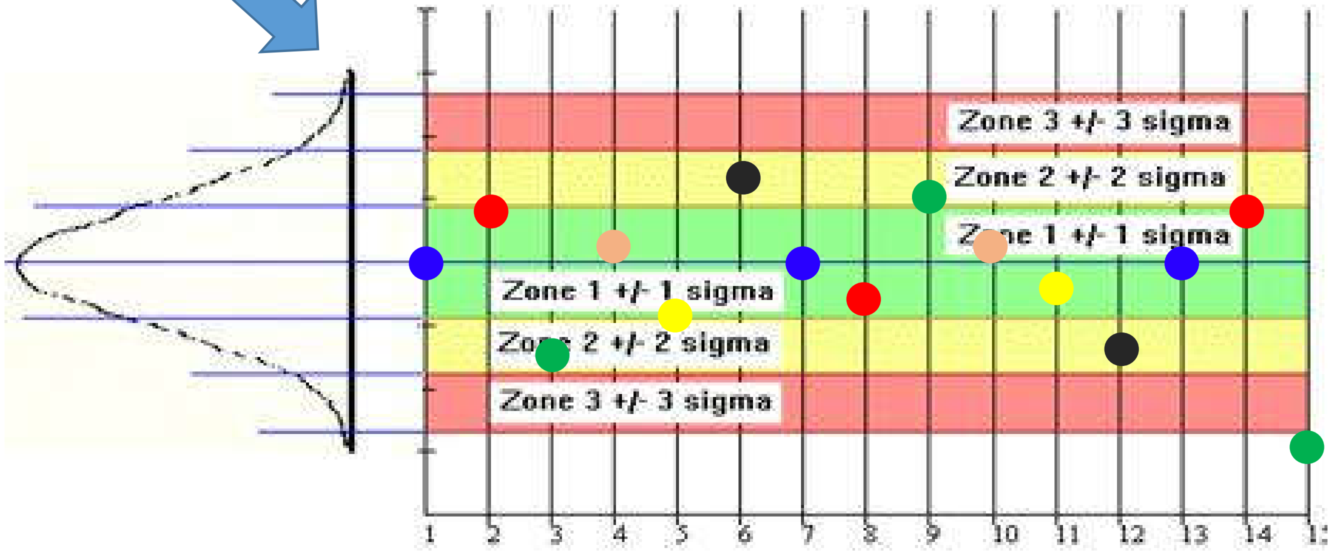
↓

New sample variation tested



Control Charts

PCA-QCC



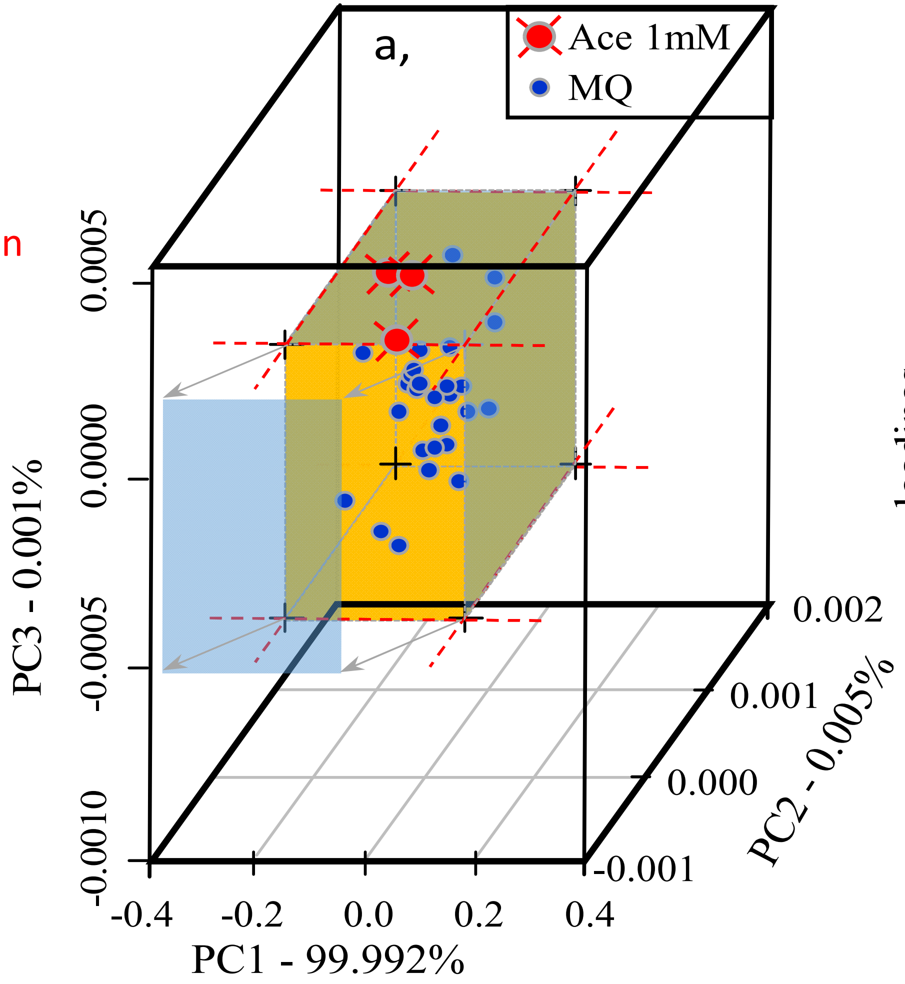
Kovacs, Z. et al., 2016. Water spectral pattern as holistic marker for water quality monitoring. *Talanta*, 147, pp.598–608.

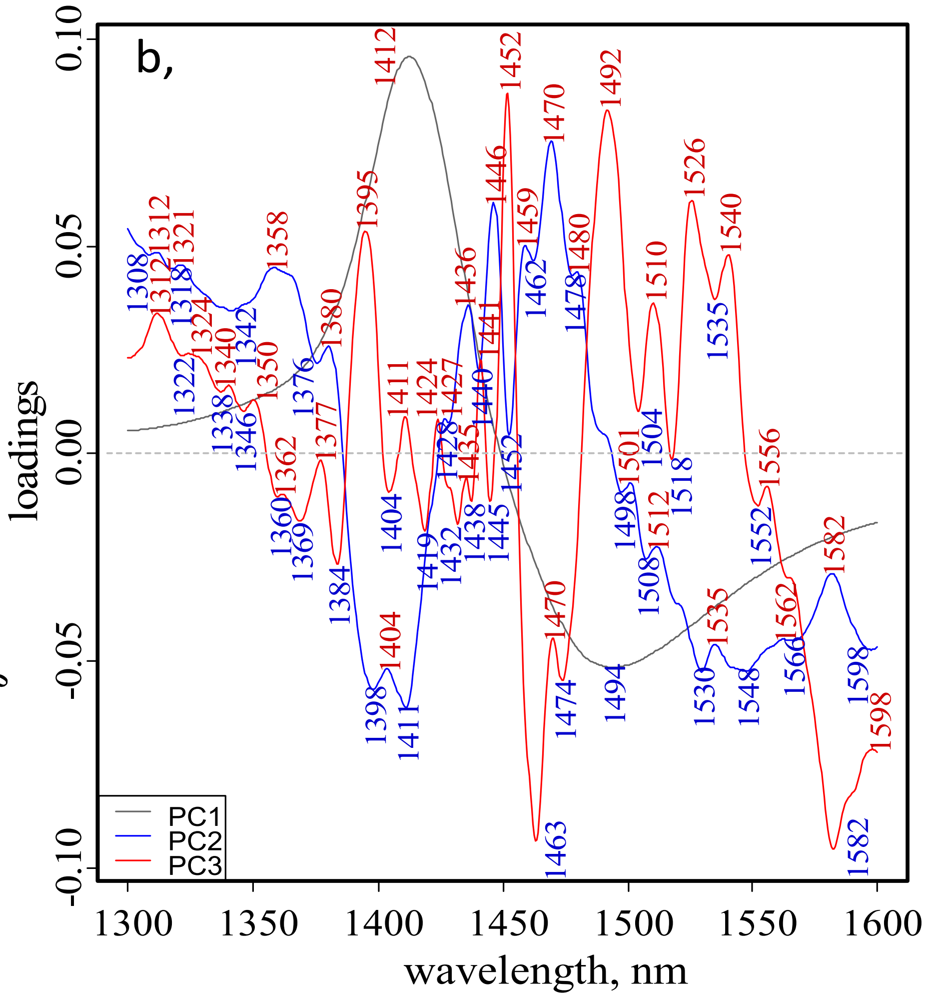
PCA score and loadings plots (1-3) of **MQ** and **1mM** Aqueous solution of **acetic acid**

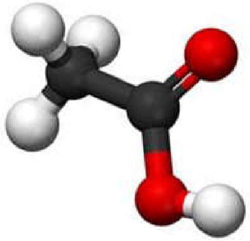
Difference between 1mM acetic acid and MQ on PC3 only

3D

difficult picture







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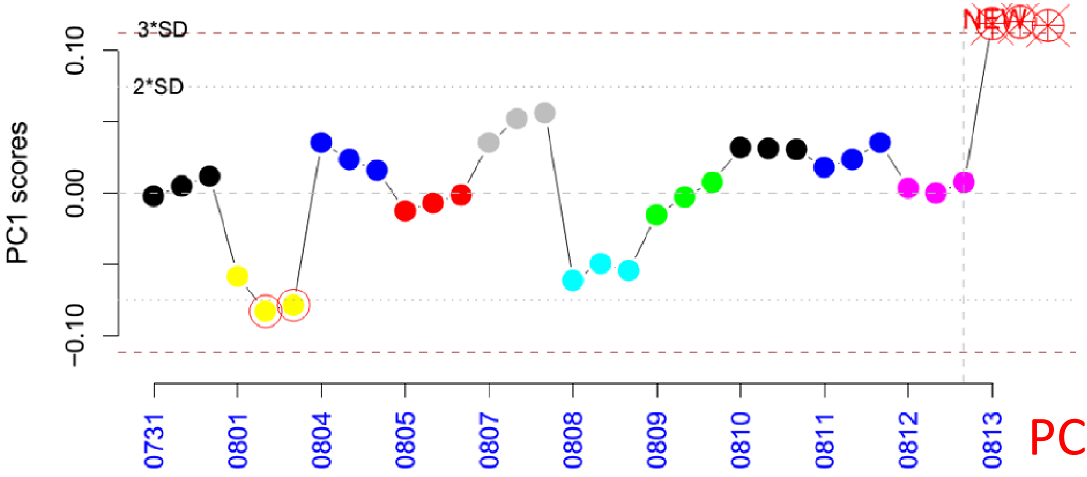
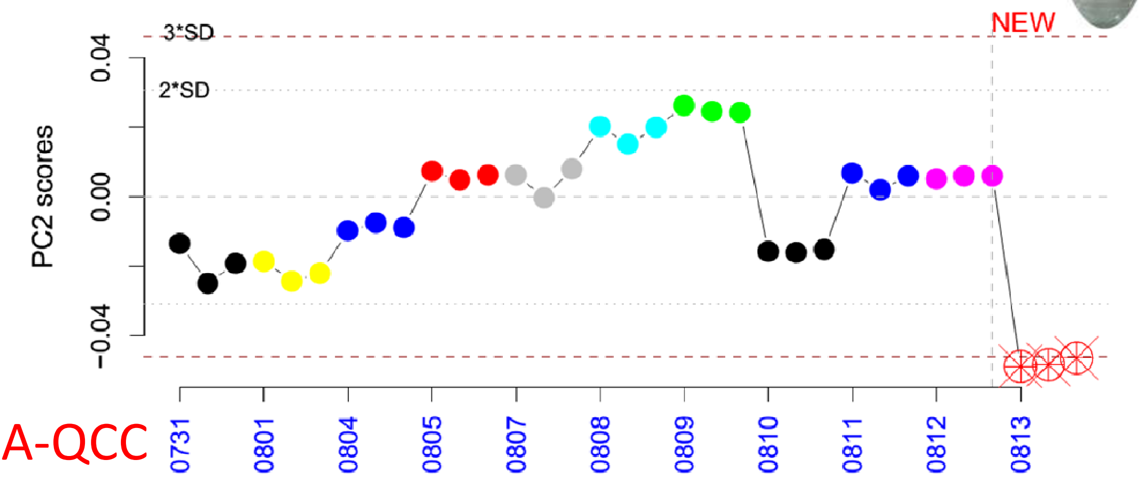
PCA-QCC of Ground Water monitoring (PC1-PC2)

PC1 scores with 95 and 99% confidence intervals



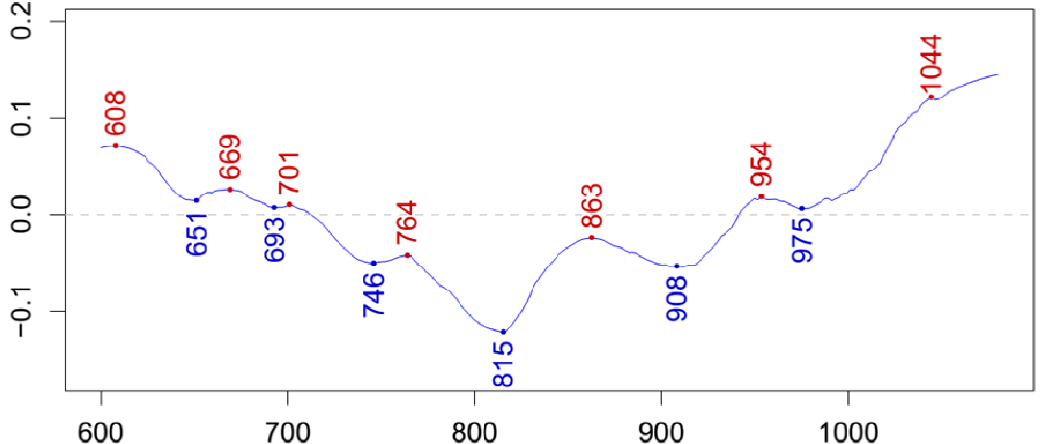
PC2 scores with 95 and 99% confidence intervals



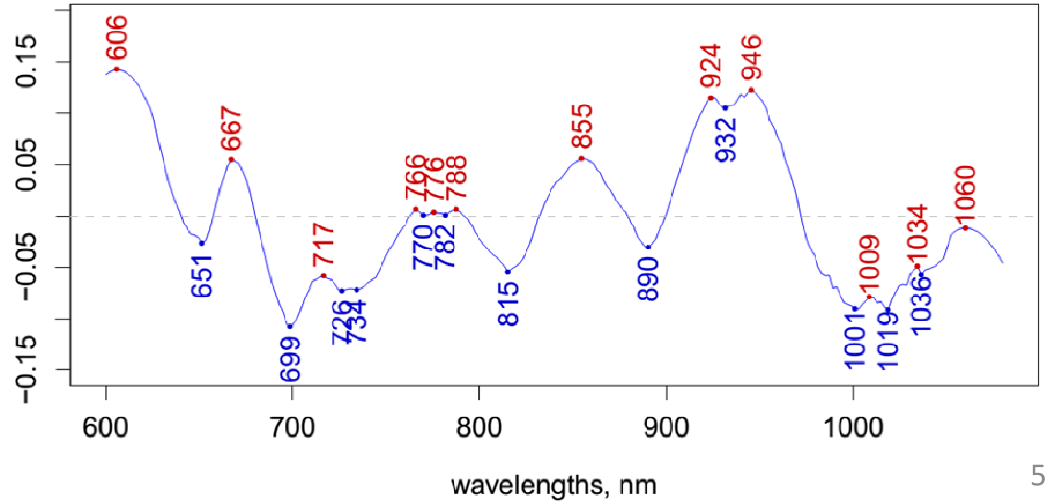
PCA-QCC

gave warning for quality change of ground water

PCA loading of PC1 – 71.581%



PCA loading of PC2 – 12.072%



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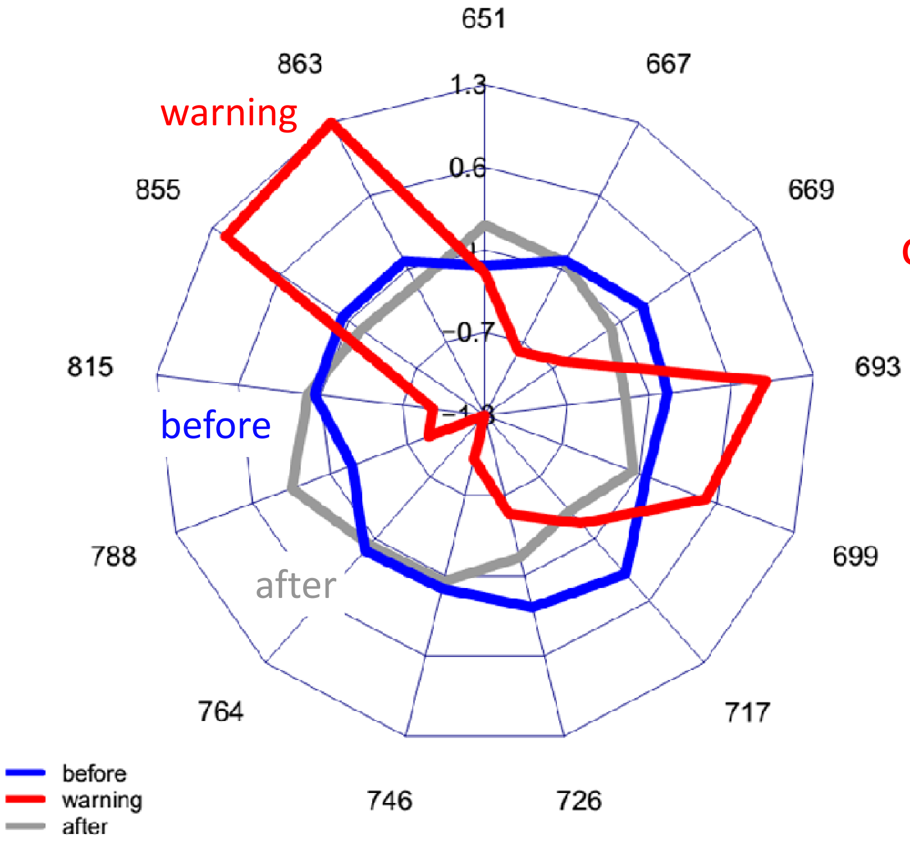
Aquagrams of ground waters

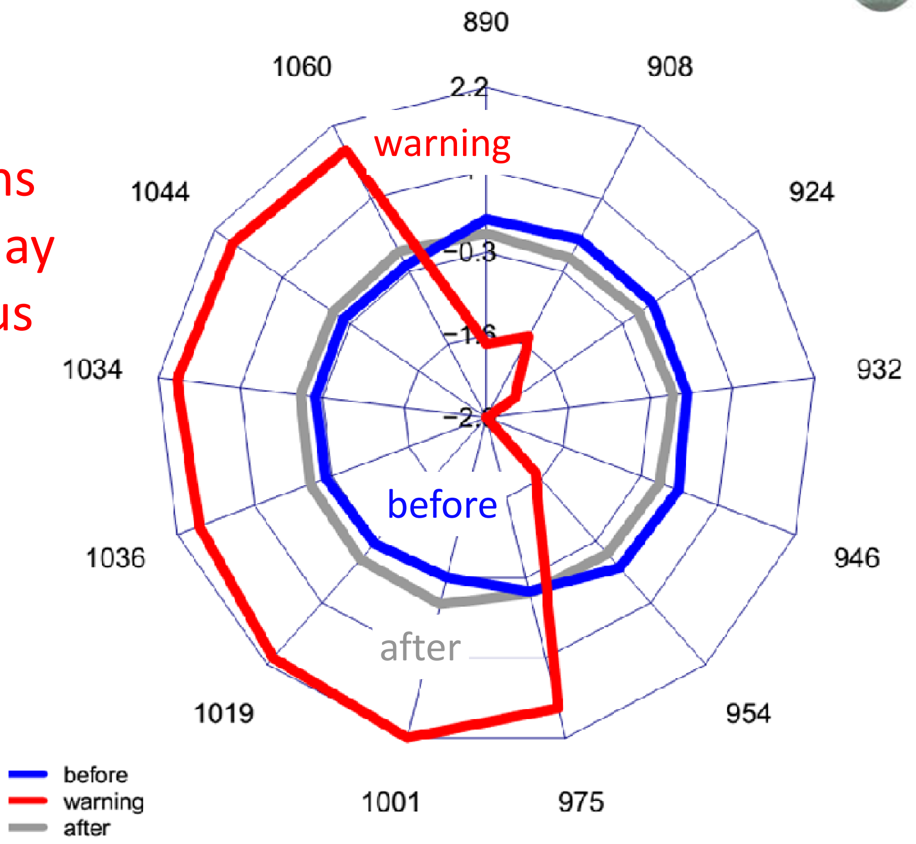
spectra of warning day compared to previous
10 days and the following 10 days

3rd overtone



Spectral patterns
of the warning day
and the previous
and following
periods are
different

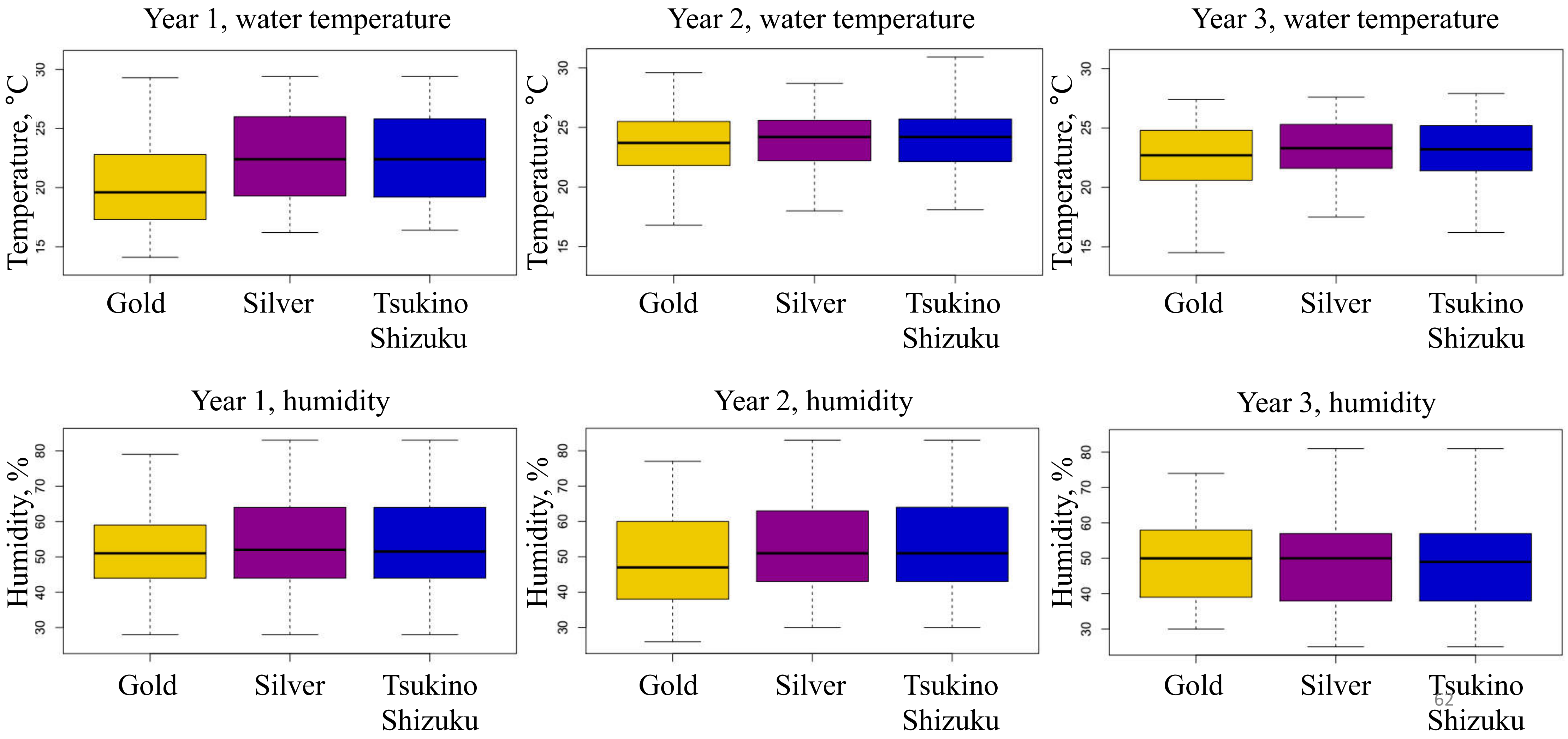
2nd overtone



Kovacs, Z. et al., 2016. Water spectral pattern as holistic marker
for water quality monitoring. *Talanta*, 147, pp.598–608.

wavelengths found important
in PCA-QCC were used

Distribution of water temperature and relative humidity along the three years


Year 1, water temperature

Year 2, water temperature

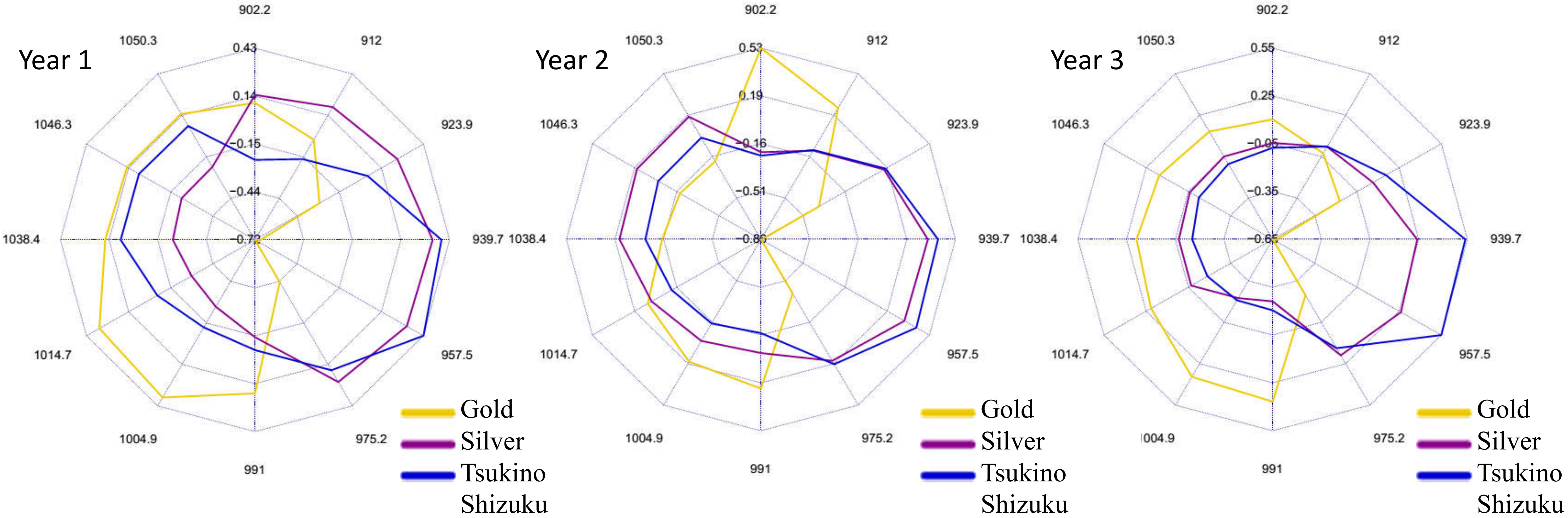
Year 3, water temperature

Year 1, humidity

Year 2, humidity

Year 3, humidity

Aquagrams of ground water samples in three different years



calculated at wavelengths found important
in PCA, PLSR and subtracted spectra

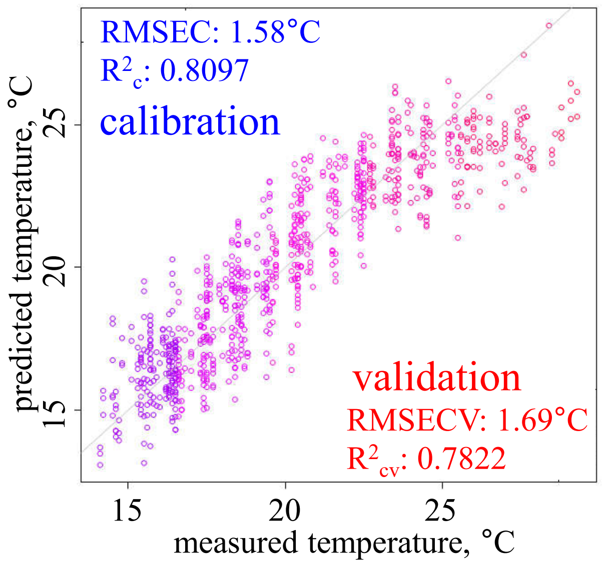
PLSR models of ground water samples for water temperature

Smooth (2nd order polynomials, n = 11 points)
MSC transform
Range 600-1060 nm
latent variable: 10

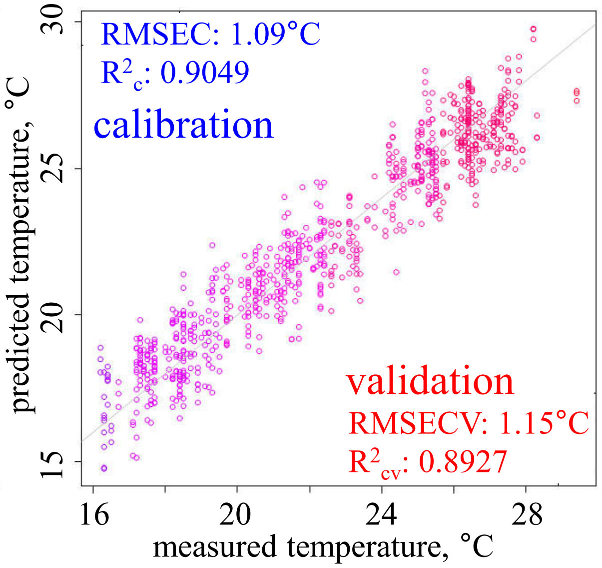
Year 1

leave-one-temperature level-out cross-validation

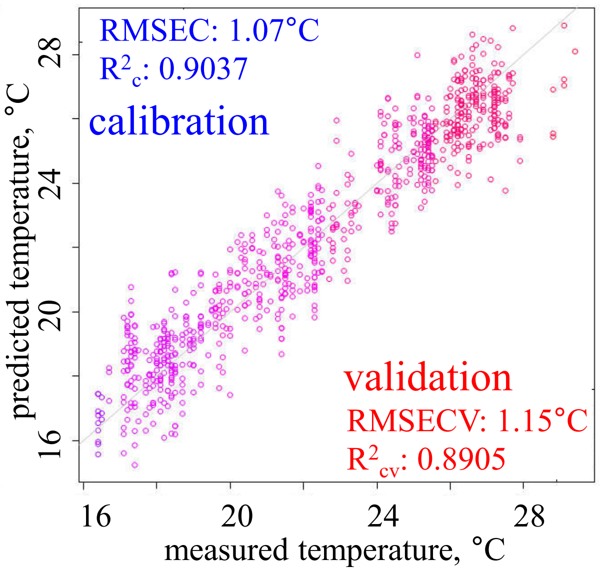
Gold Water



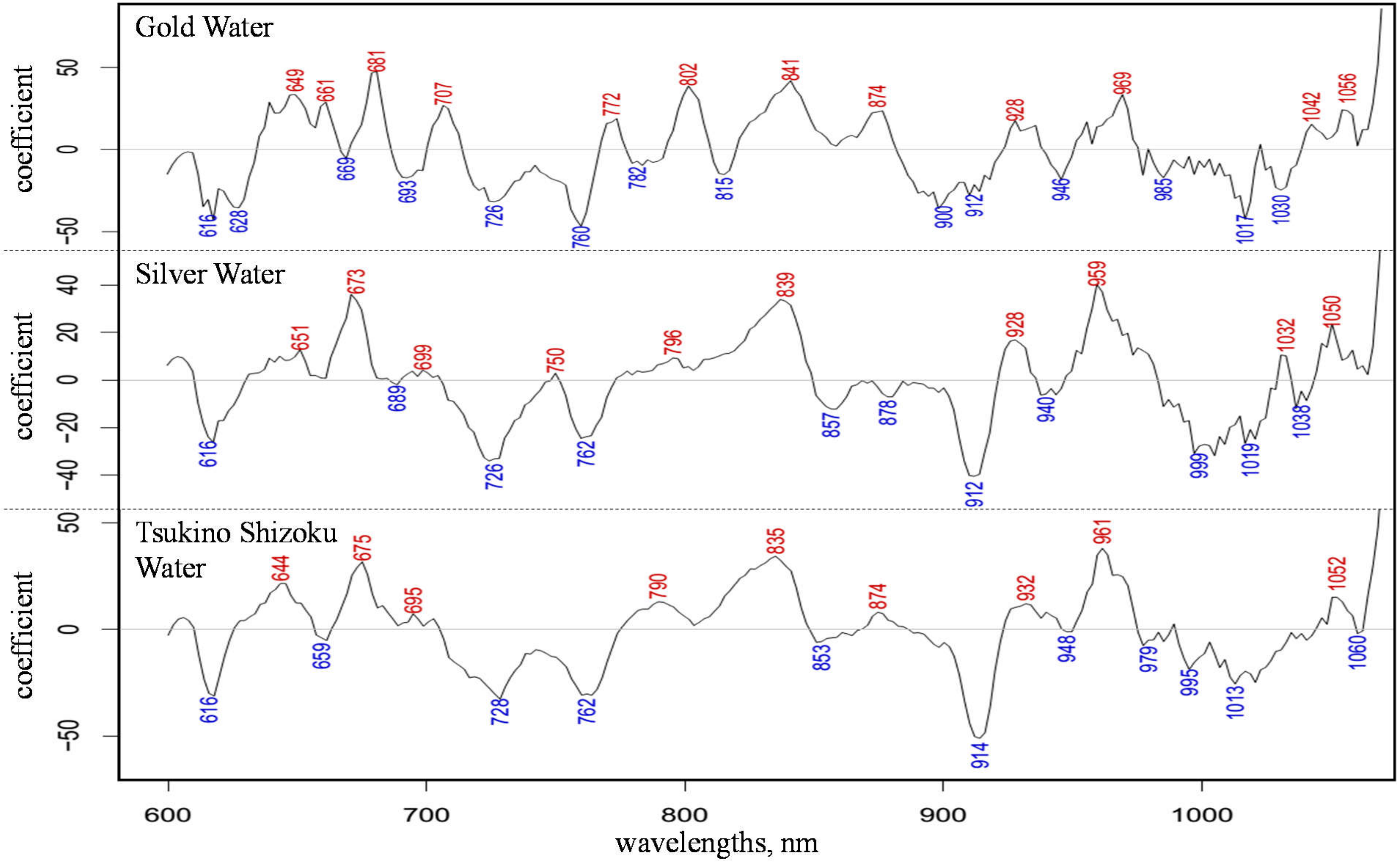
Silver Water



Tsukino Shizuku Water



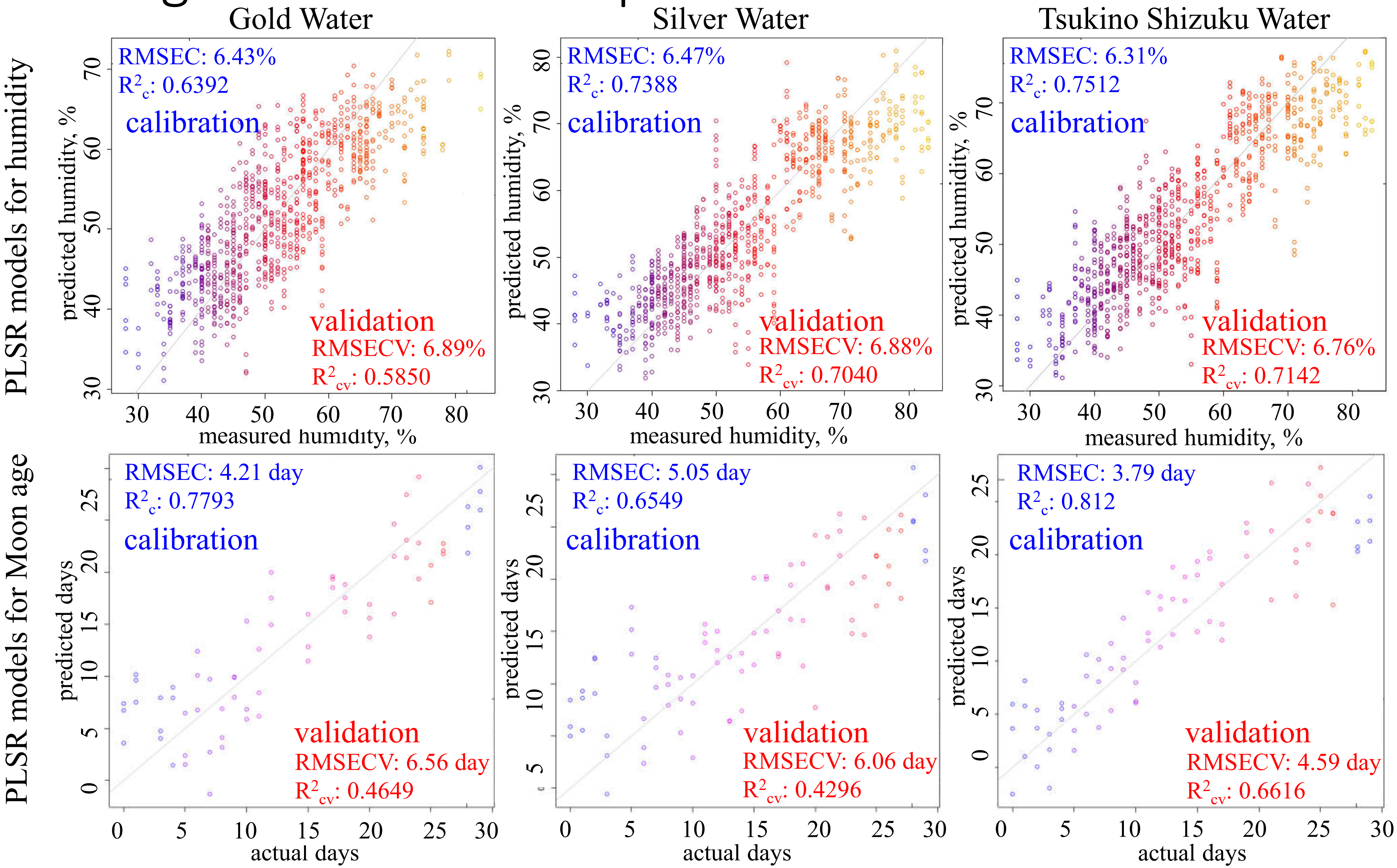
Regression vectors of PLSR models fitted on water temperature
Year 1



PLSR models of ground water samples

Smooth (2nd order polynomials, n = 11 points)
MSC transform
Range 600-1060 nm
latent variable: 10

leave-one-level-out cross-validation



Conclusion

- The application of NIRS and Aquaphotomics in the evaluation of ground water samples showed:
  - spectral pattern of the water samples can be used for quality monitoring
  - spectral pattern of the water samples can be used to compare the different samples using different perturbations

Agenda of the presentation

Application of Aquaphotomics to learn more about the rules of water

- Bacteria growing and Yogurt
- Plant cells growing
- Mineral Waters
- Calculation and presentation method of WASP

http://www.dreamstime.com

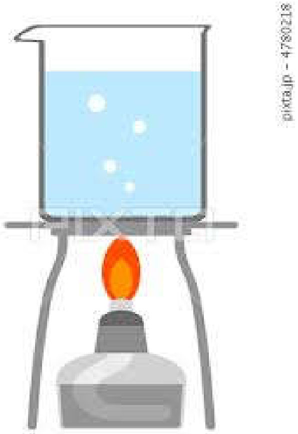
objectives

- to develop a calculation and presentation method
  - to be able to **provide information about the ratio of the water species**
  - to be able to compare samples **in an absolute scale**:
    - if we have only one sample
    - if we have samples with different composition
  - to have **expressive unit** on the **scale**

Materials and methods for **temperature** experiment

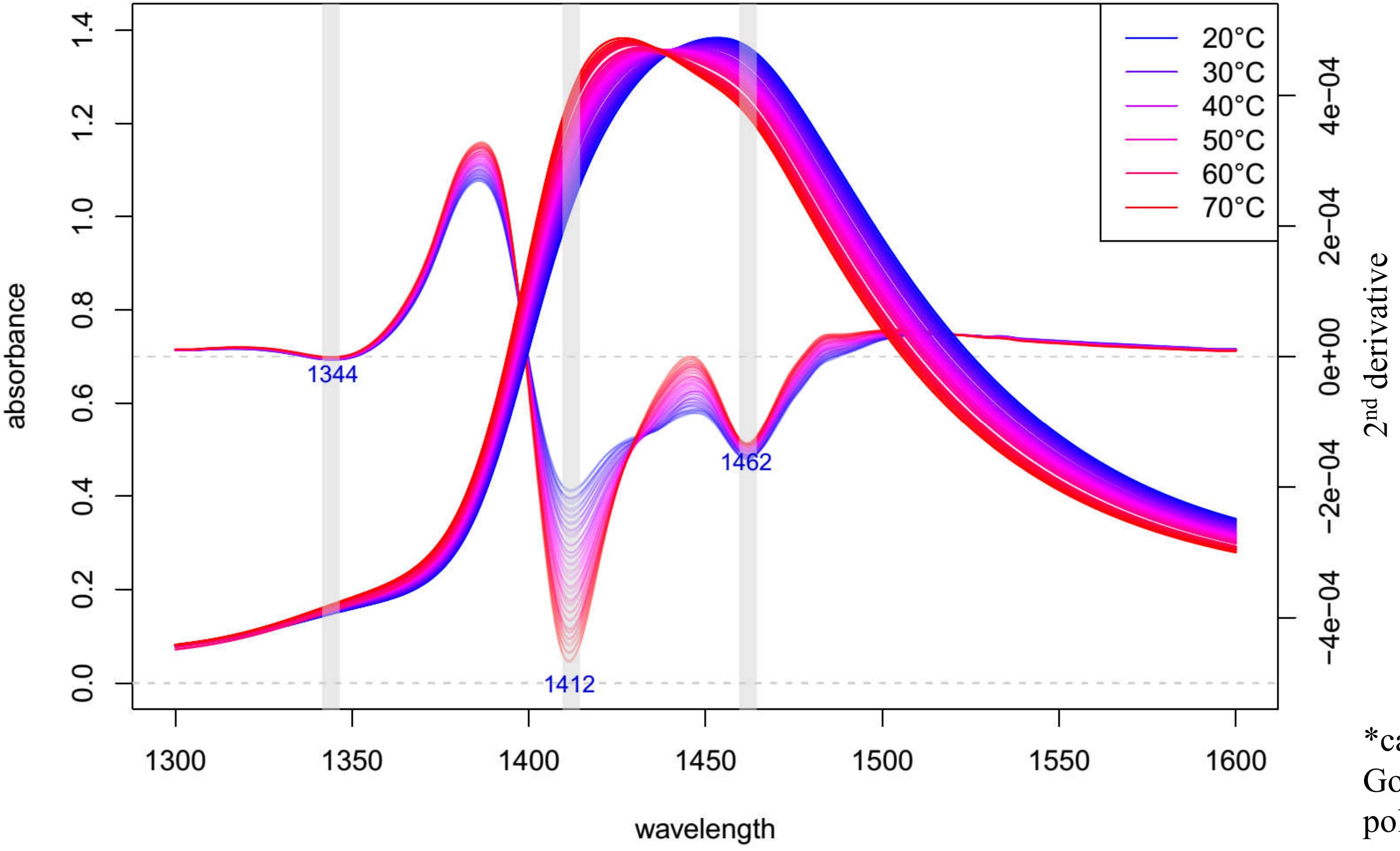
Samples and instrumentation:

- spectra of
  - MQ,
  - distilled water (DW) and
  - tap water were taken
- in the temperature range
  - from 20
  - to 70°C
  - at every 2nd °C
- the experiment was performed by XDS



Raw and 2nd derivative* absorbance spectra of Milli-Q water in the temperature range of 20-70°C

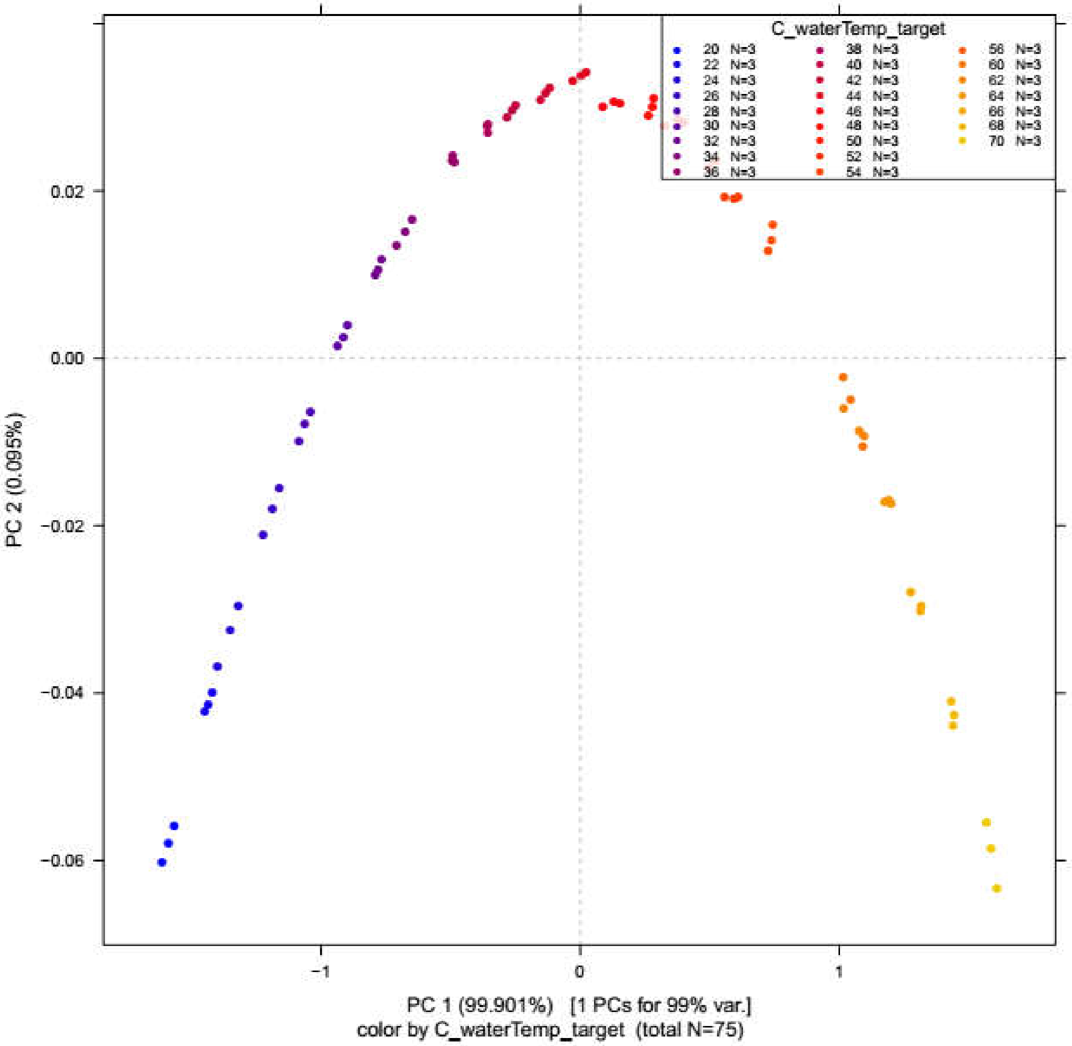
n = 78

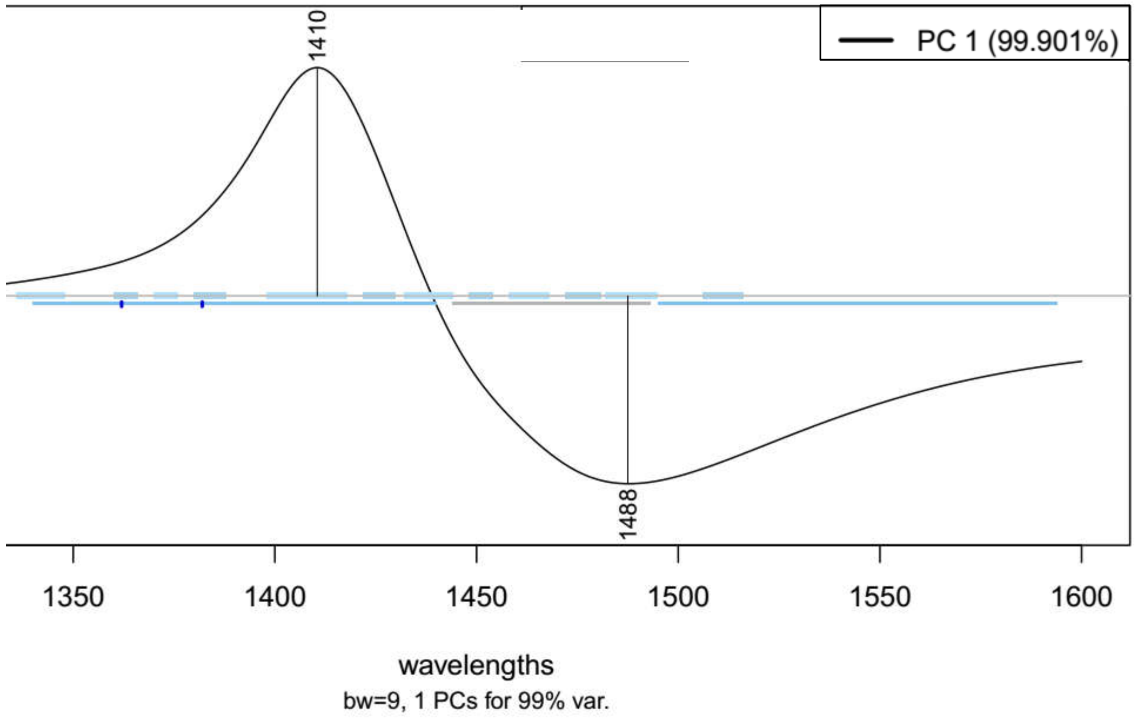


blue shift with increasing temperature

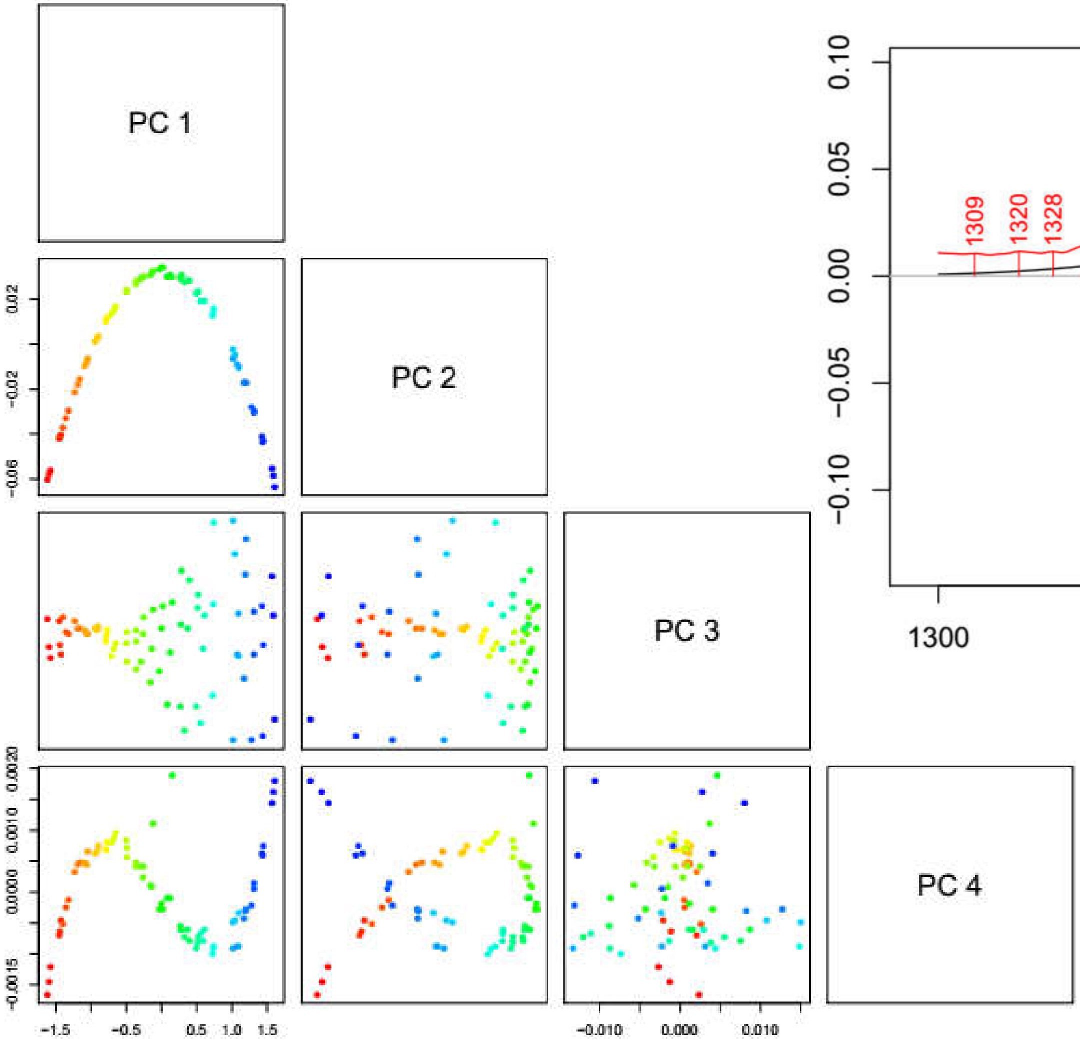
*calculated with Savitzky-Golay filter using 2nd order polynomial and 21 points

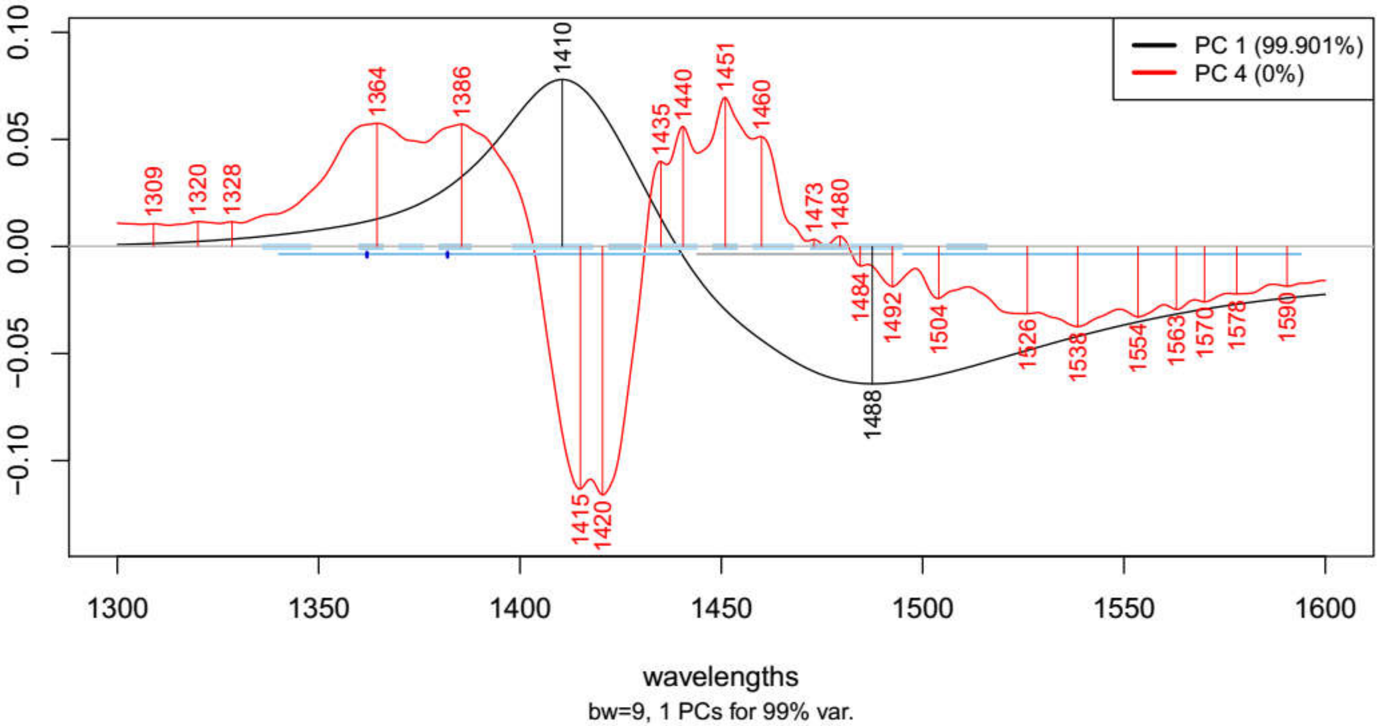
PCA score and loadings plots of MQ water in the temperature range of 20-70°C



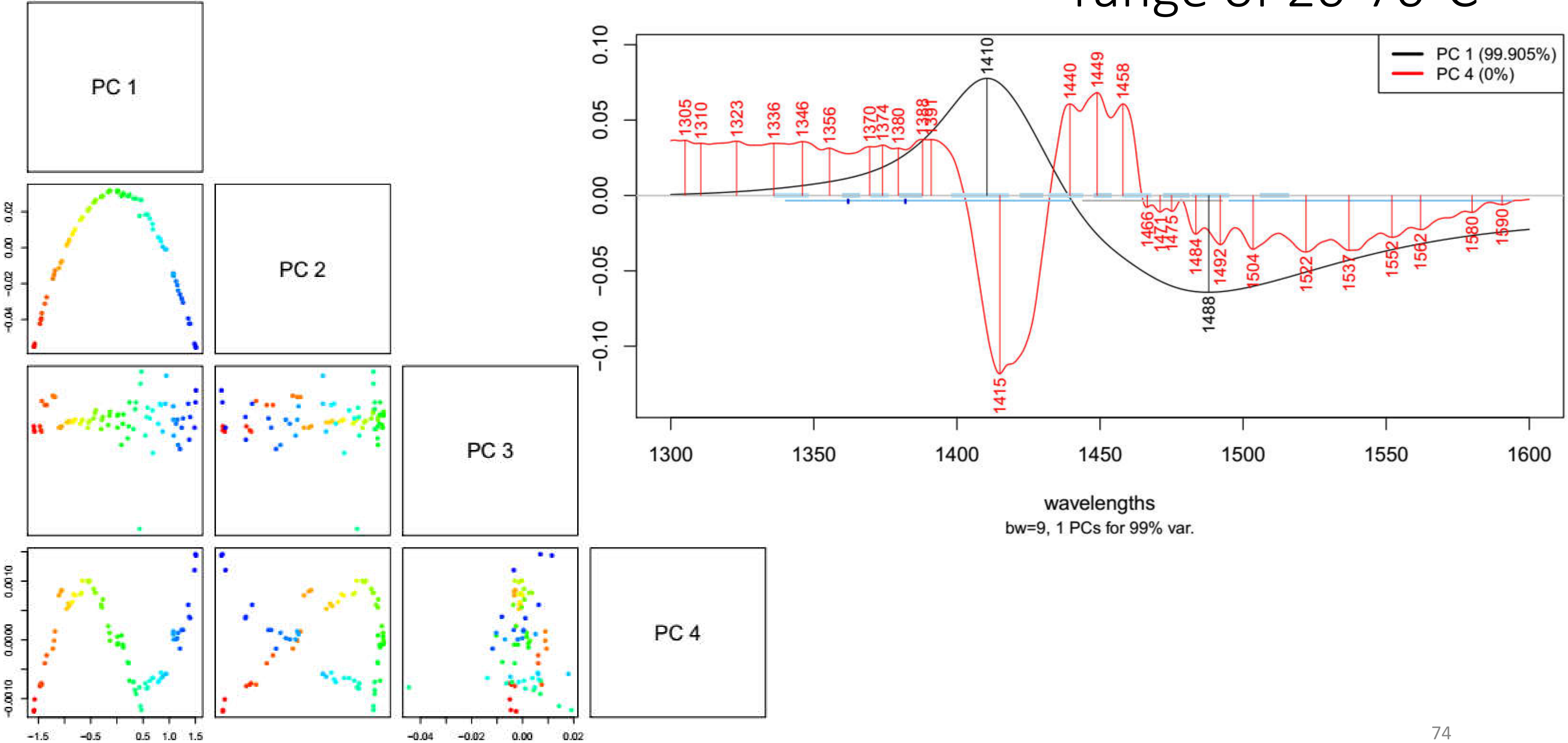


PCA score and loadings plots of MQ water in the temperature range of 20-70°C

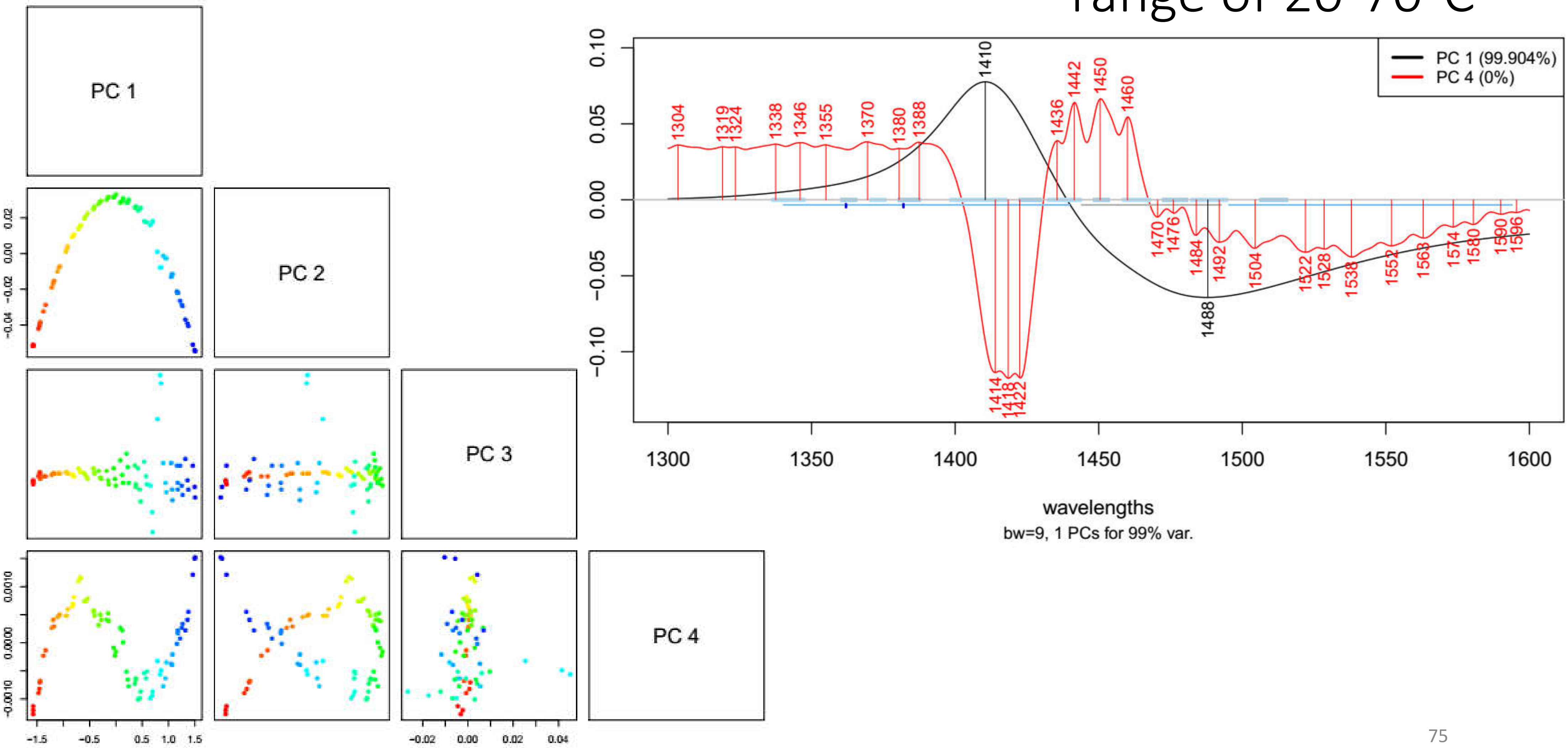




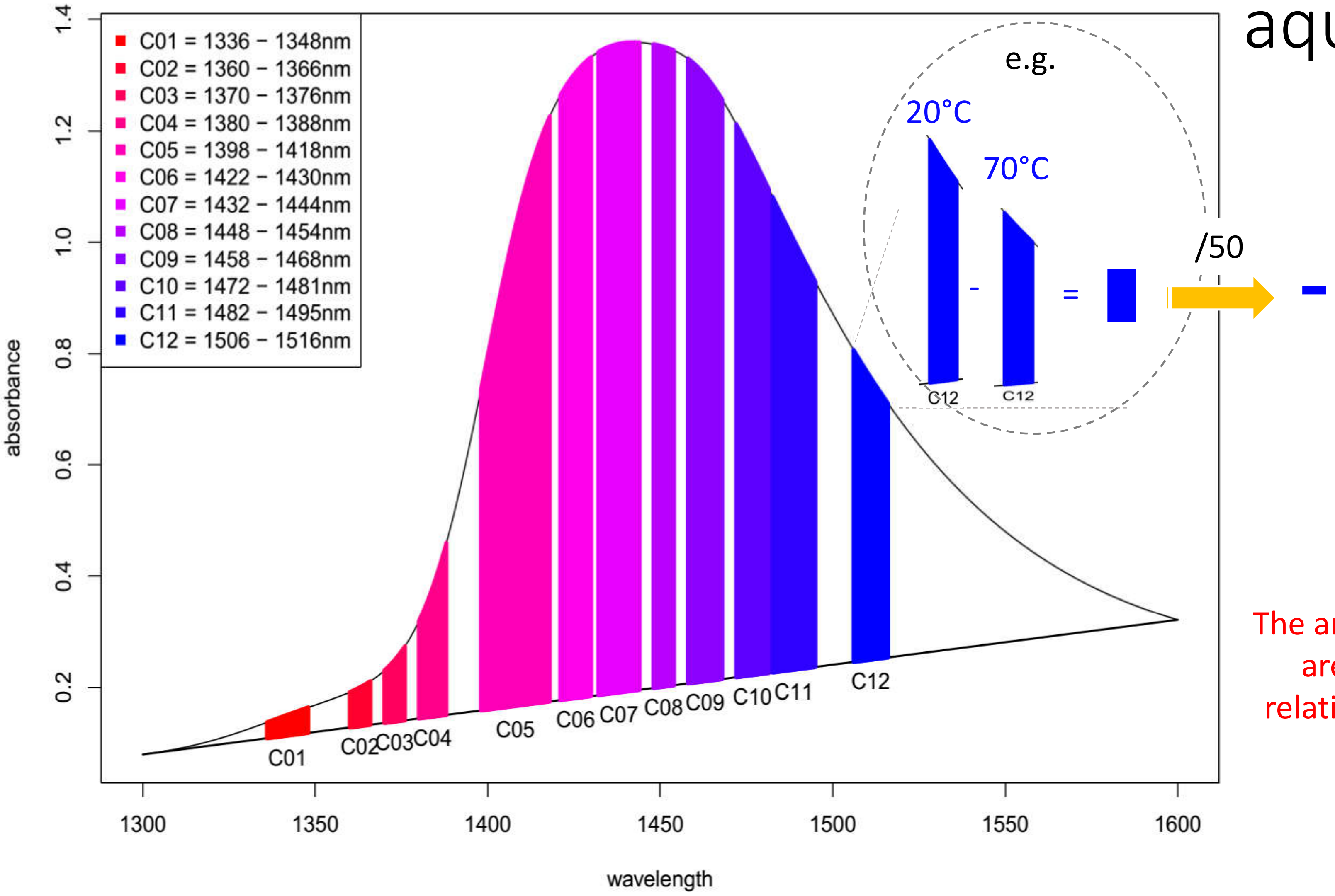
PCA score and loadings plots of DW in the temperature range of 20-70°C



PCA score and loadings plots of tap water in the temperature range of 20-70°C



Scheme of the calculation for Area under the curve (AUC) aquagram method

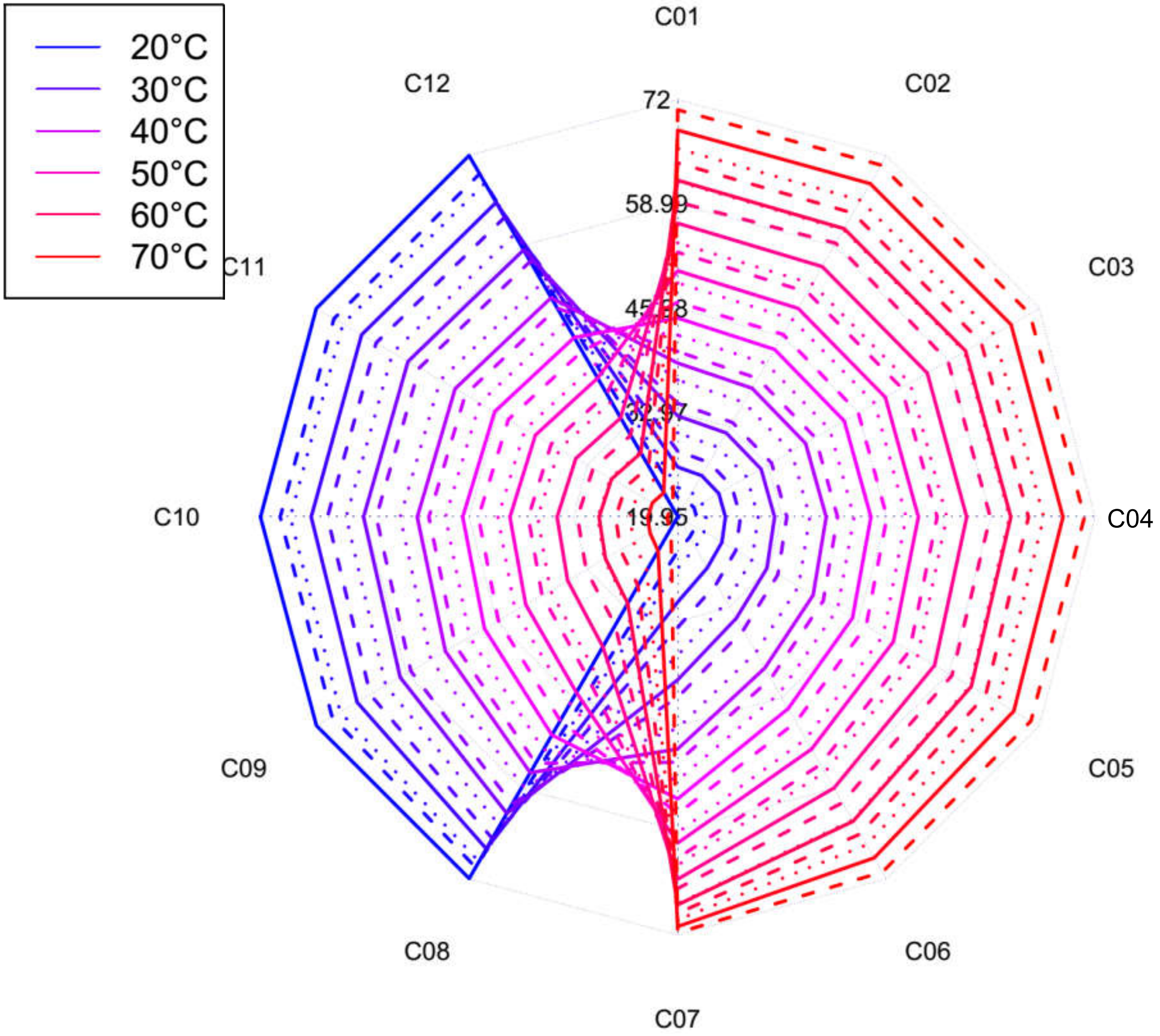


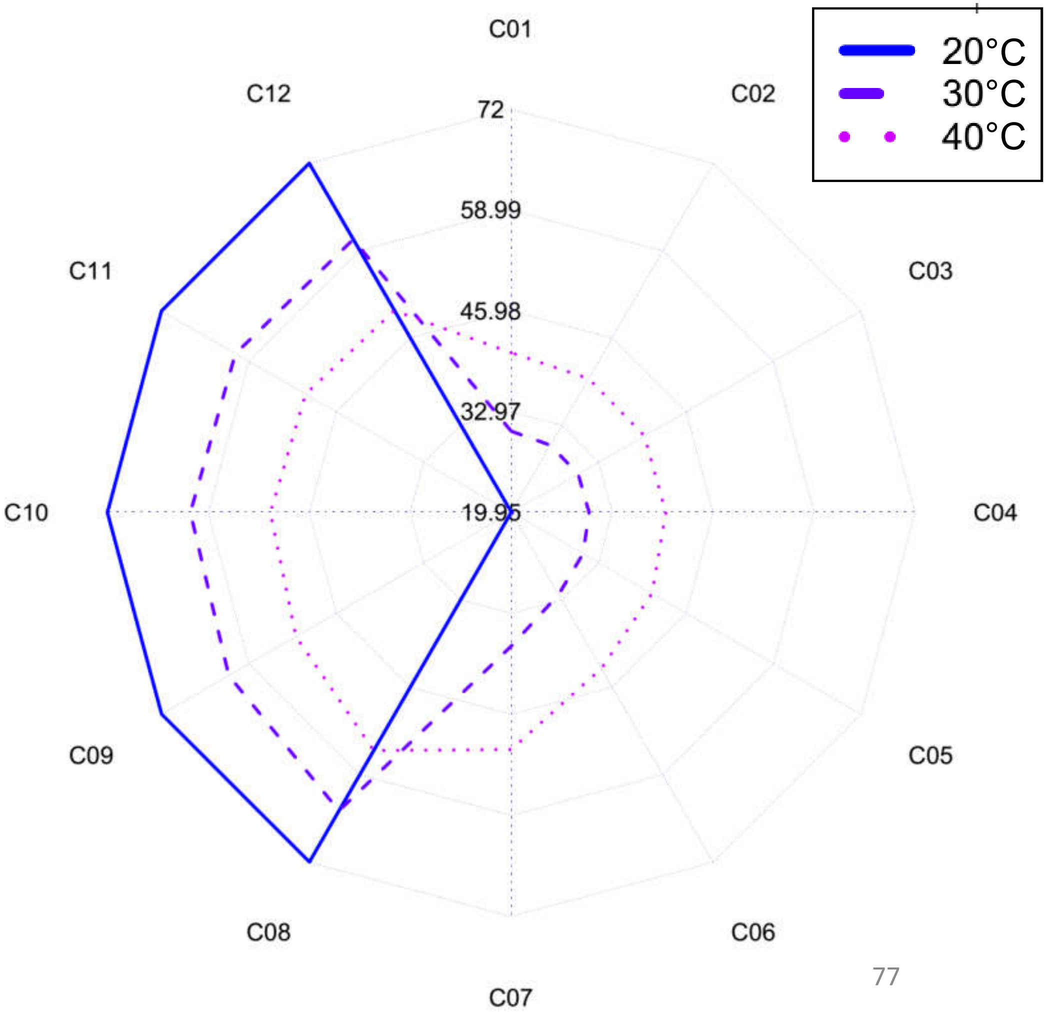
area change at C12 by 1°C

compare to the change of perturbation

The areas under the specific WAMACS are calculated and expressed in relation to the area change occurred by different temperature

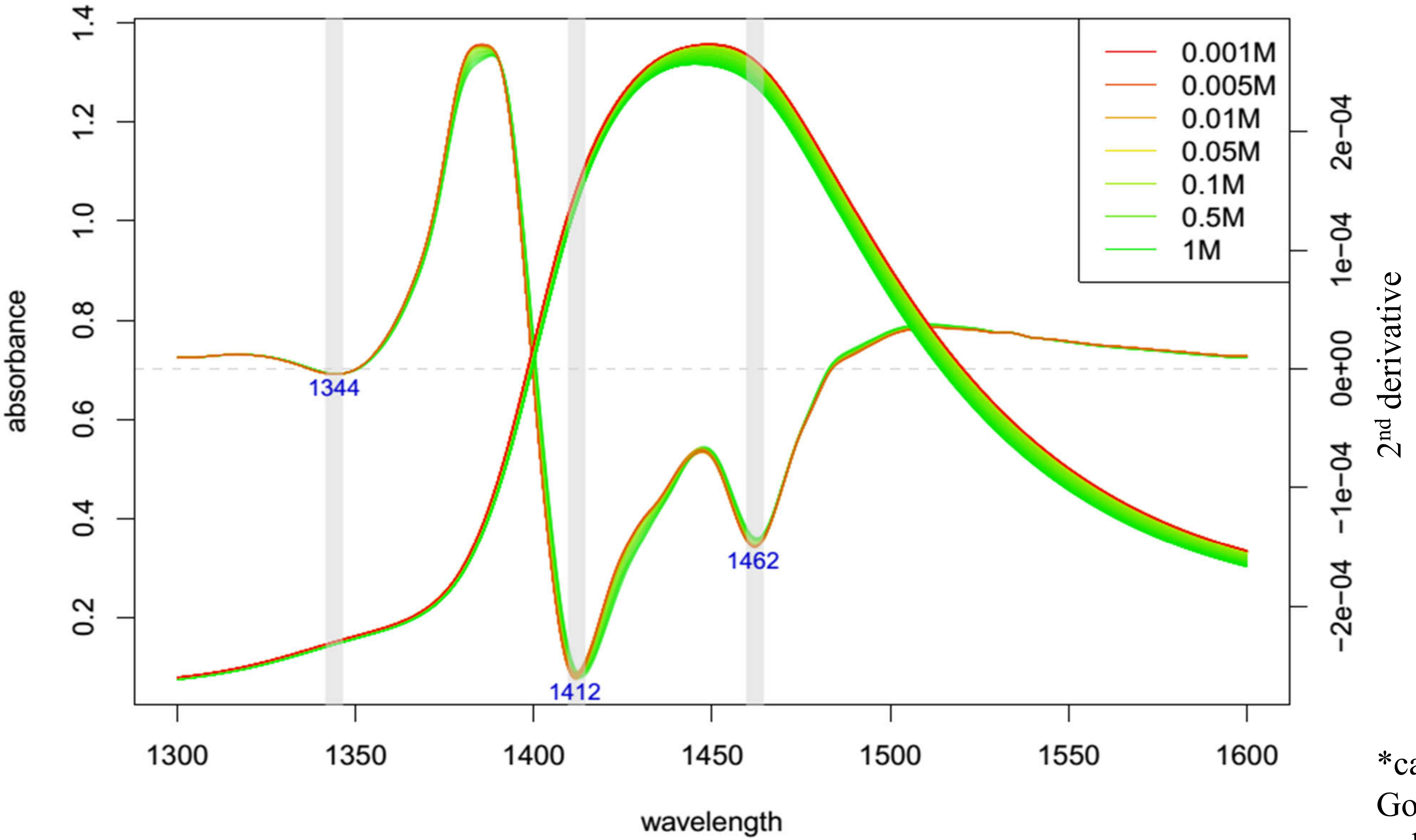
Aquagrams (AUC) of Milli-Q water in the temperature range of 20-70°C





Raw and 2nd derivative* absorbance spectra of 0.001-1M KCl solutions

n = 180



blue shift with increasing KCl concentration

*calculated with Savitzky-Golay filter using 2nd order polynomial and 21 points

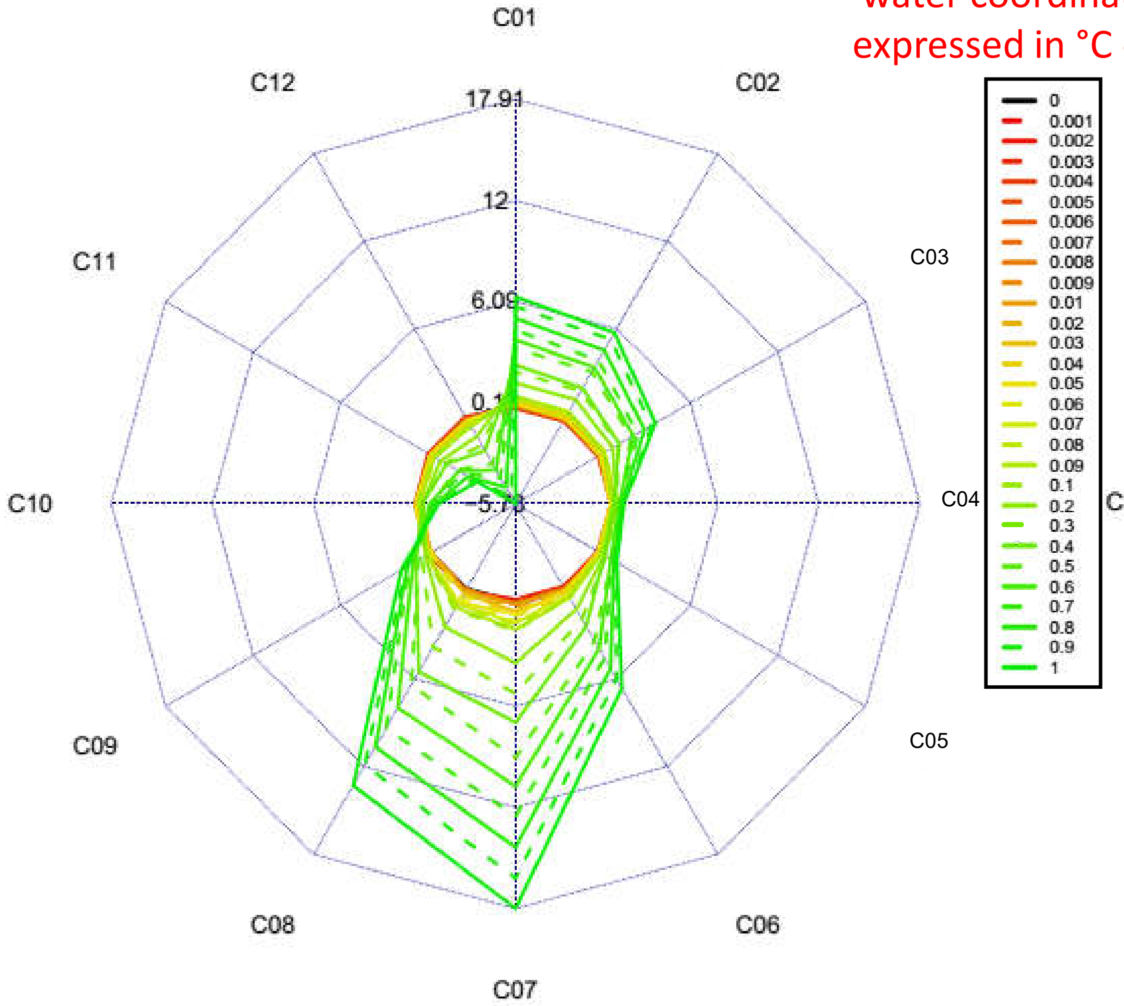
Aquagrams (AUC) of aqueous solution of KCl and MQ

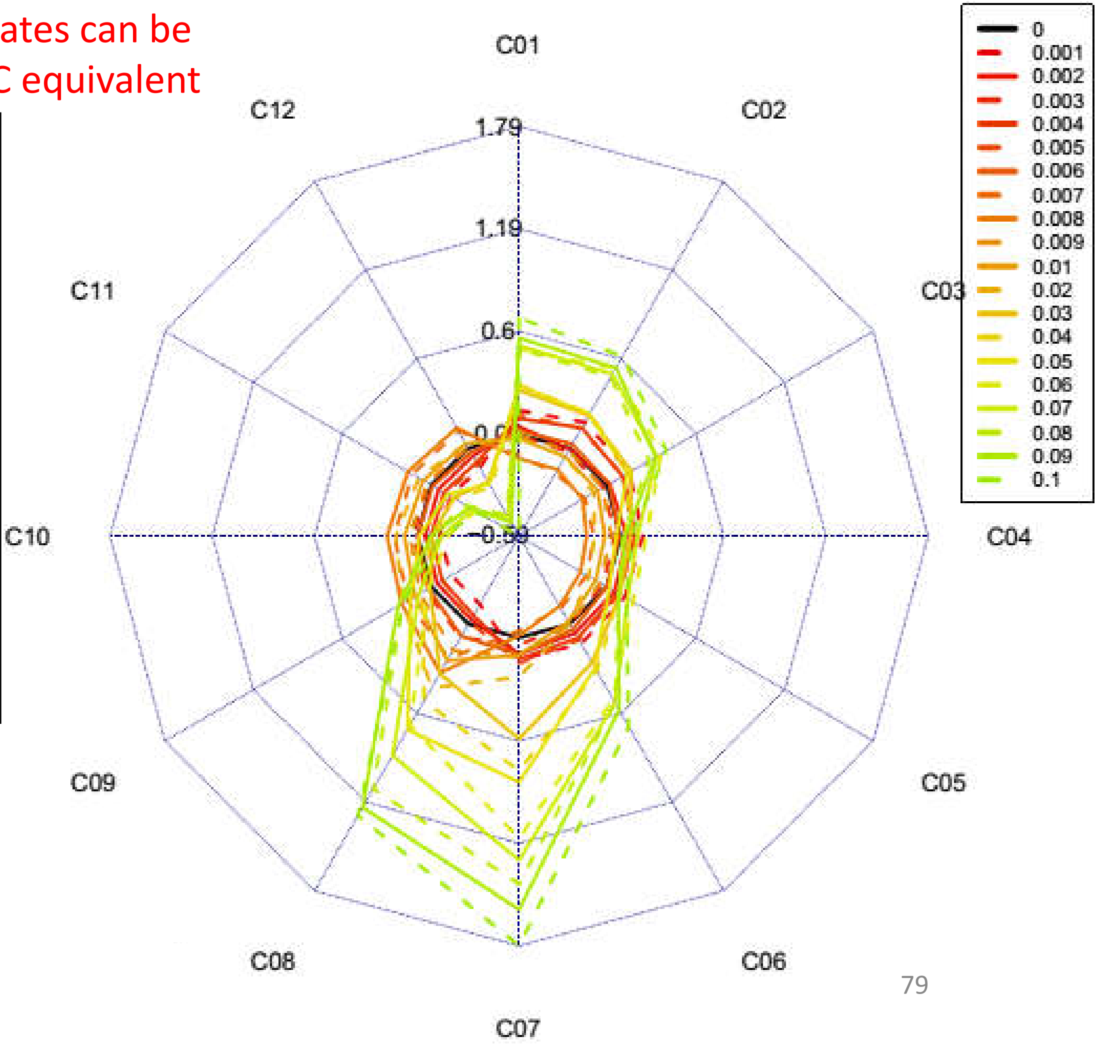
($n_{MQ} = 150$)
($n_{KCl} = 180$)

KCl concentration: 0.001-1M

Temperature: 25.0°C !!!

Effect of salt (KCl) on the different water coordinates can be expressed in °C equivalent





Conclusion

- The newly developed Aquagram provide information about the ratio of the water species:
    - in an absolute scale
    - with **expressive unit** on the **scale**
- The **results** acquired with the new applications, tools and measurement protocols **can further extend** the range of possible **applications of Aquaphotomics** and to understand more about the rules of water

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