

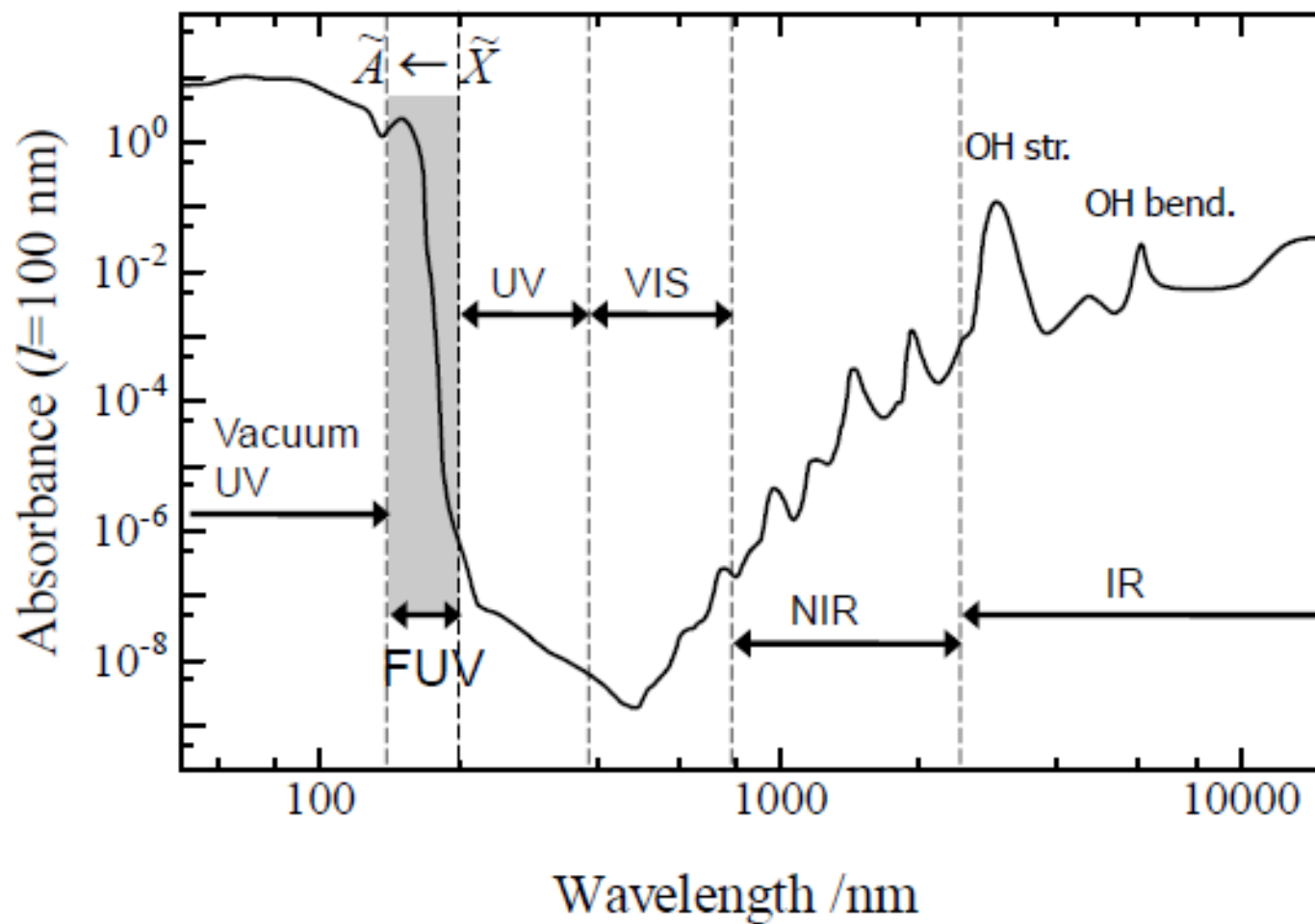
# Water Structure Studied by NIR Spectroscopy with the Aid of Difference Spectra, 2DCOS, and PCA



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# Water Research in the Ozaki Group



- Water, aqueous solutions, water-solvent interaction, water-polymer interaction, water diffusion,,,
  - **IR, Raman, NIR, and FUV**
  - **NIR**—Vibrational Spectroscopy
  - **FUV**—Electronic Spectroscopy
- T. Goto et al.

# NIR Spectra of Water

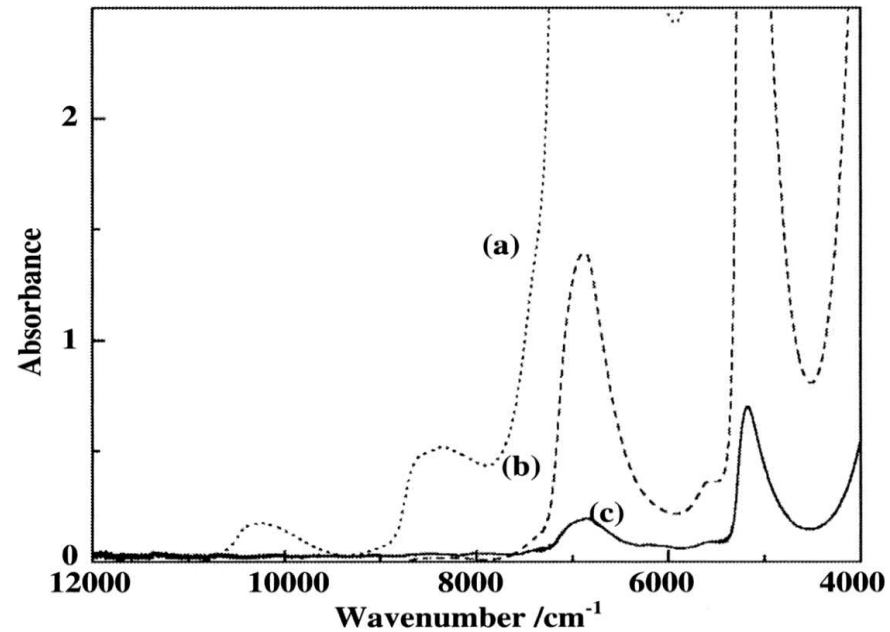


Fig. 9.1 NIR spectra of water in the 900–2500 nm (11 100–4000 cm<sup>-1</sup>) region

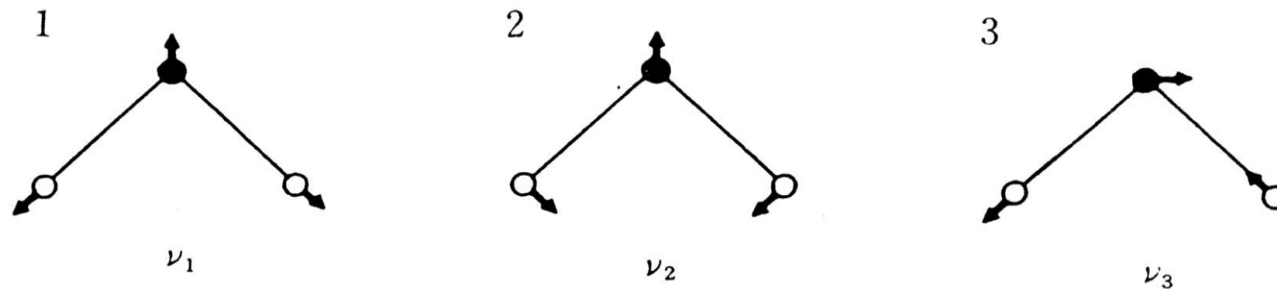
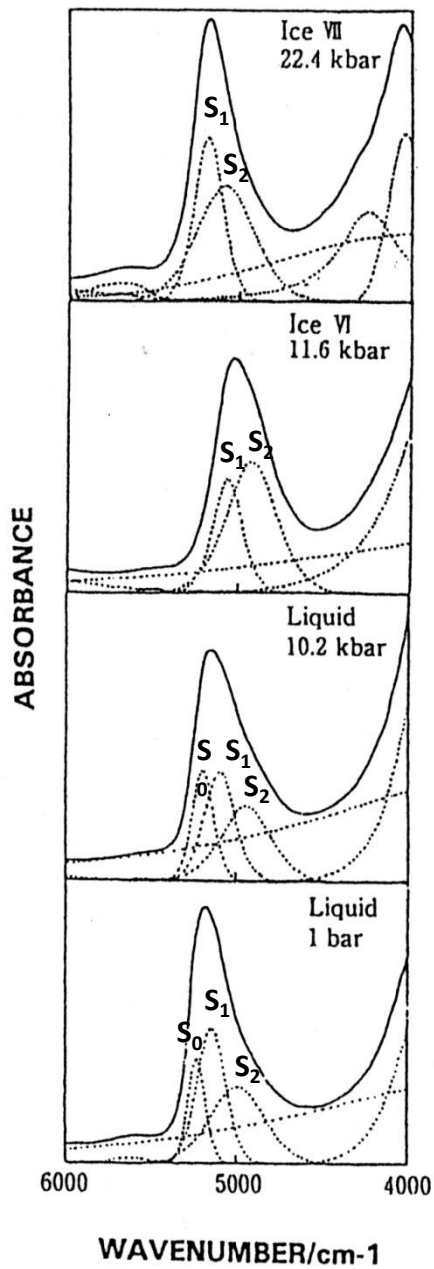


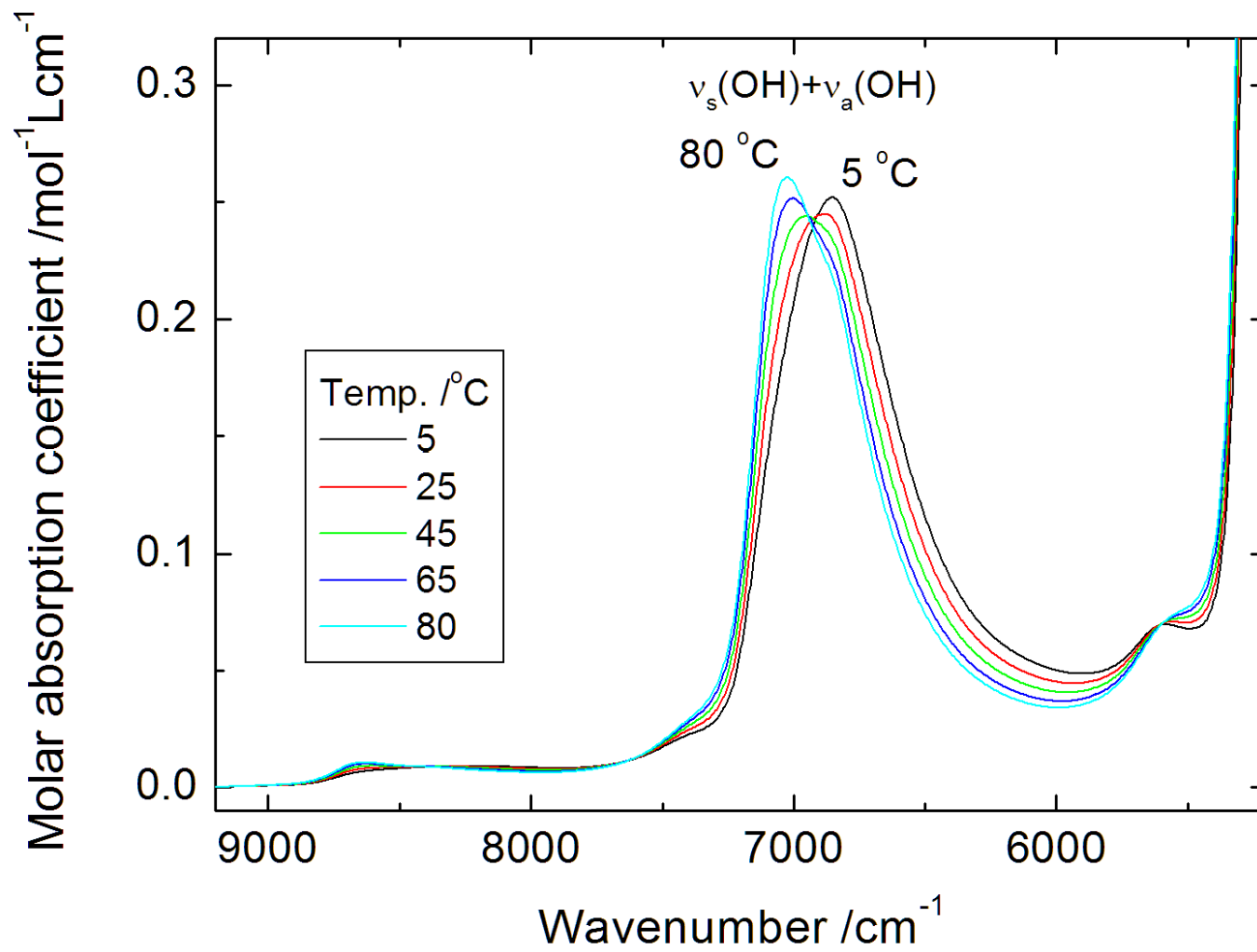
Fig. 9.2 Vibrational modes of water:  $\nu_1$  symmetric OH stretching mode,  $\nu_2$  OH bending mode,  $\nu_3$  antisymmetric OH stretching mode

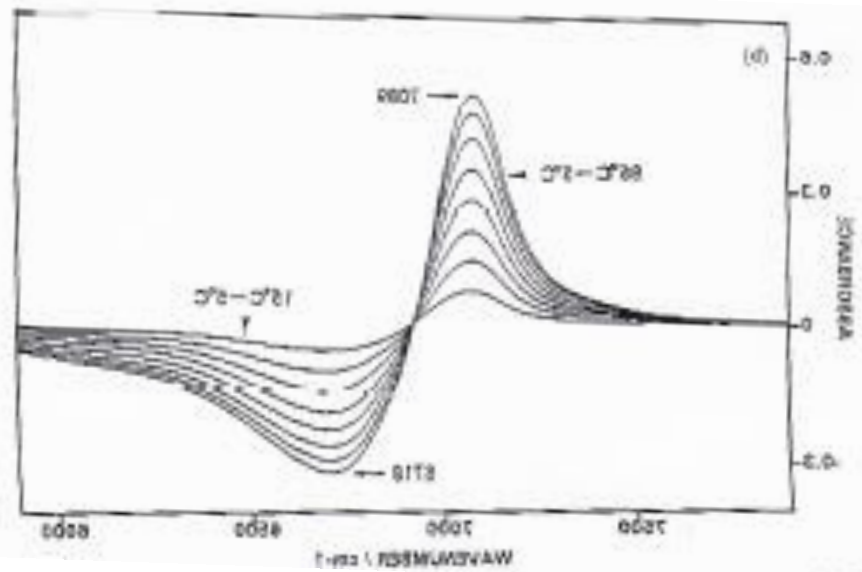
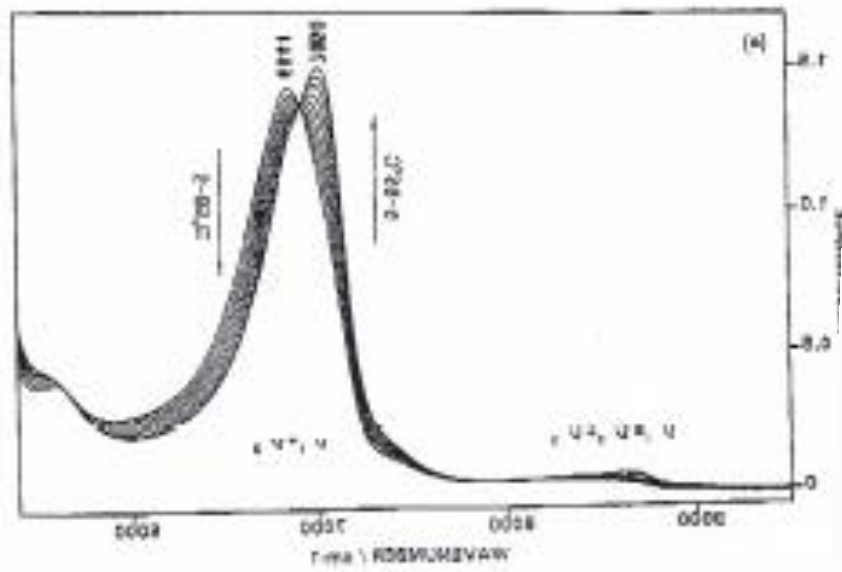


# Spectral Analysis Methods

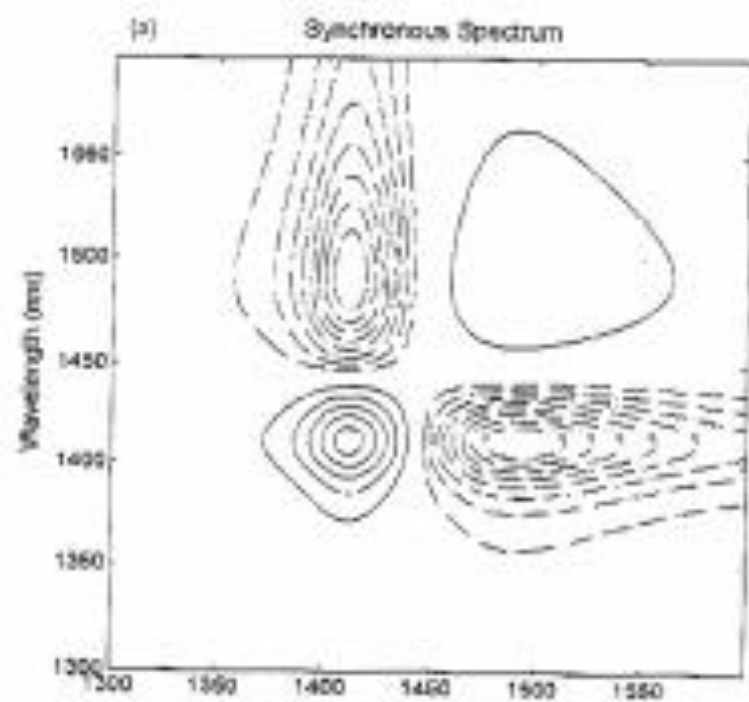
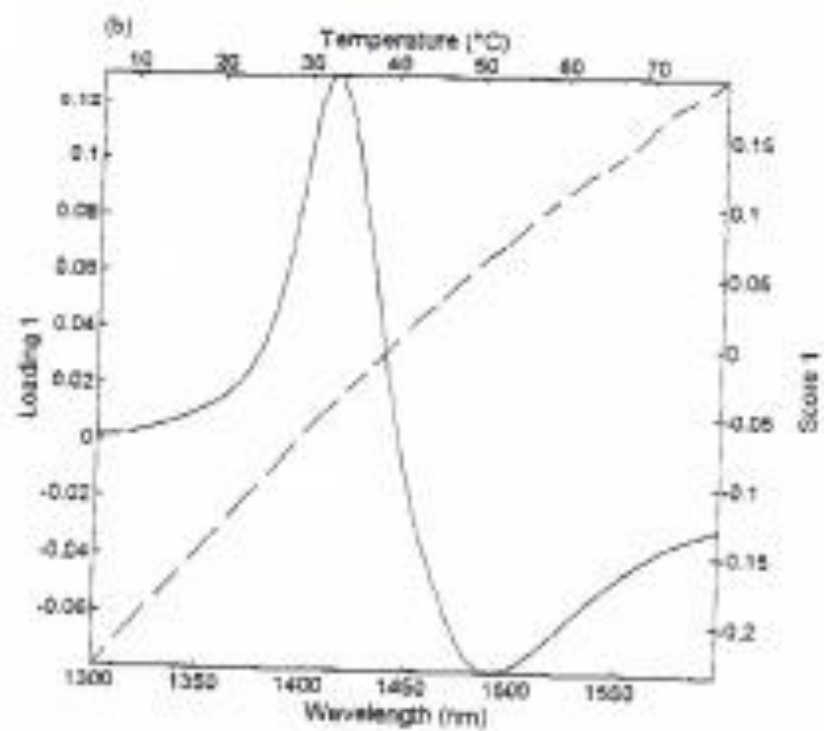
- **Difference Spectra**
- **Two-dimensional Correlation Spectroscopy**
- **Principal Component Analysis**
- **Self- Modeling Curve Resolution.**
  
- S. SASIC et al.

# Temperature different NIR spectra of liquid water

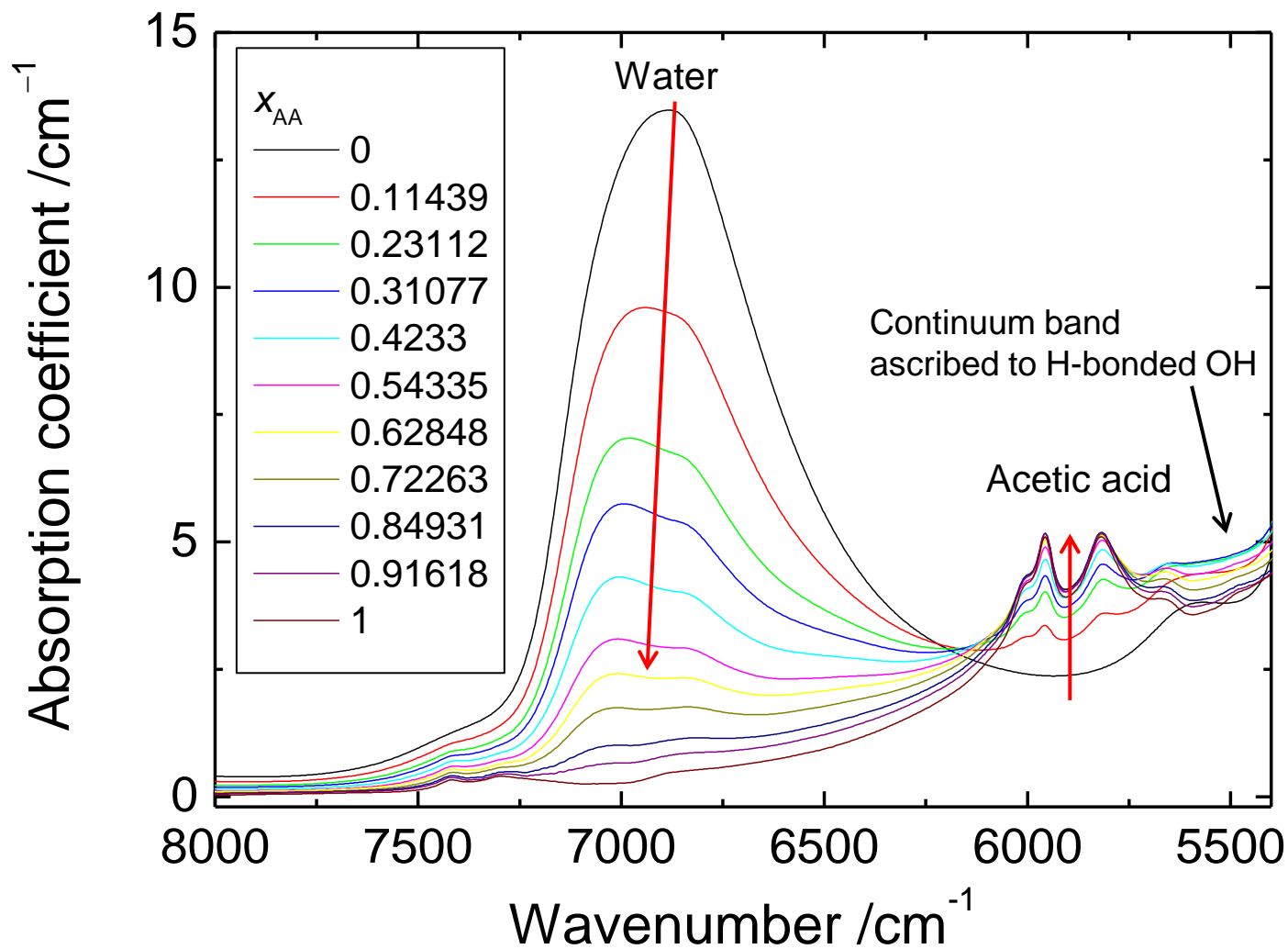








# NIR spectra of acetic acid-water binary solutions

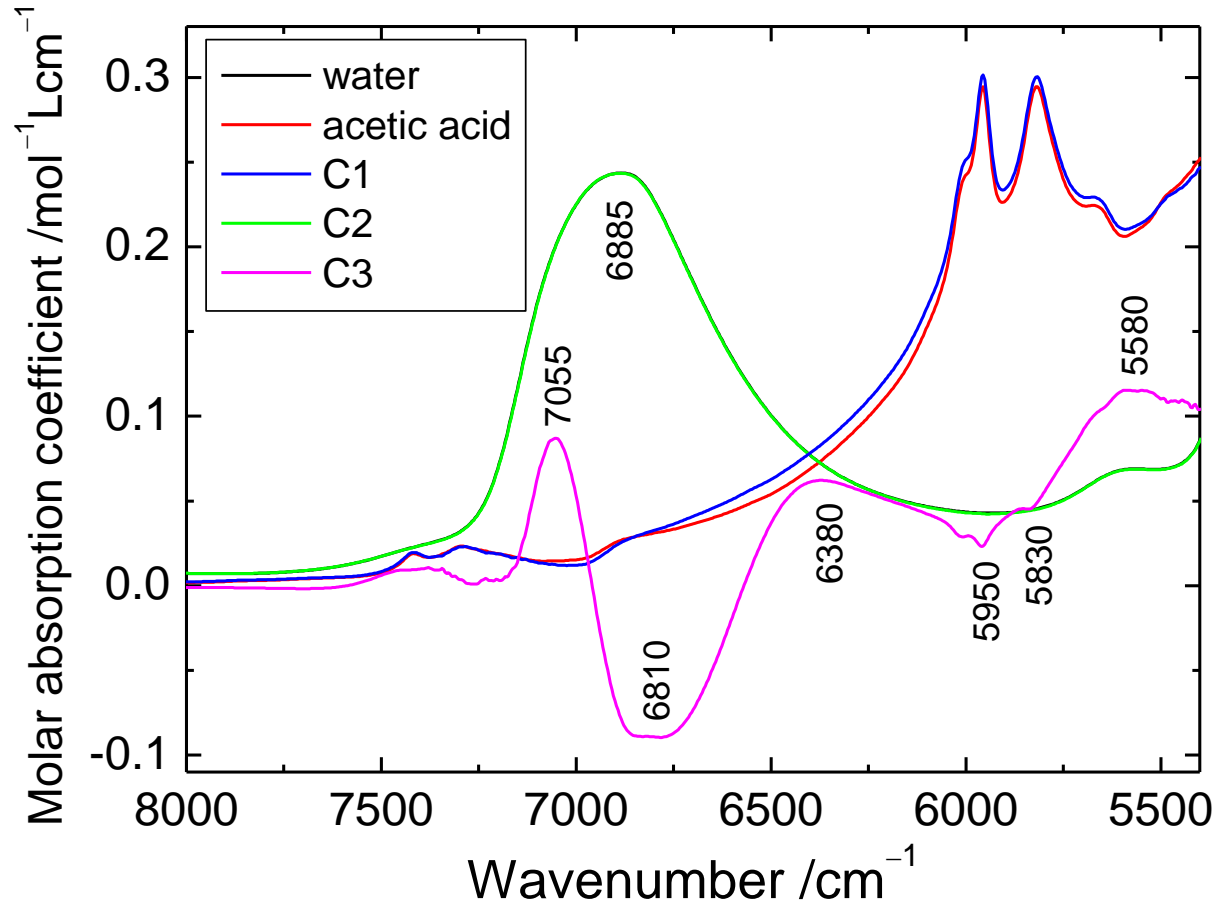


As the acetic acid concentration rises, the O-H bands get more structured.

# Multivariate analysis of the binary solution spectra

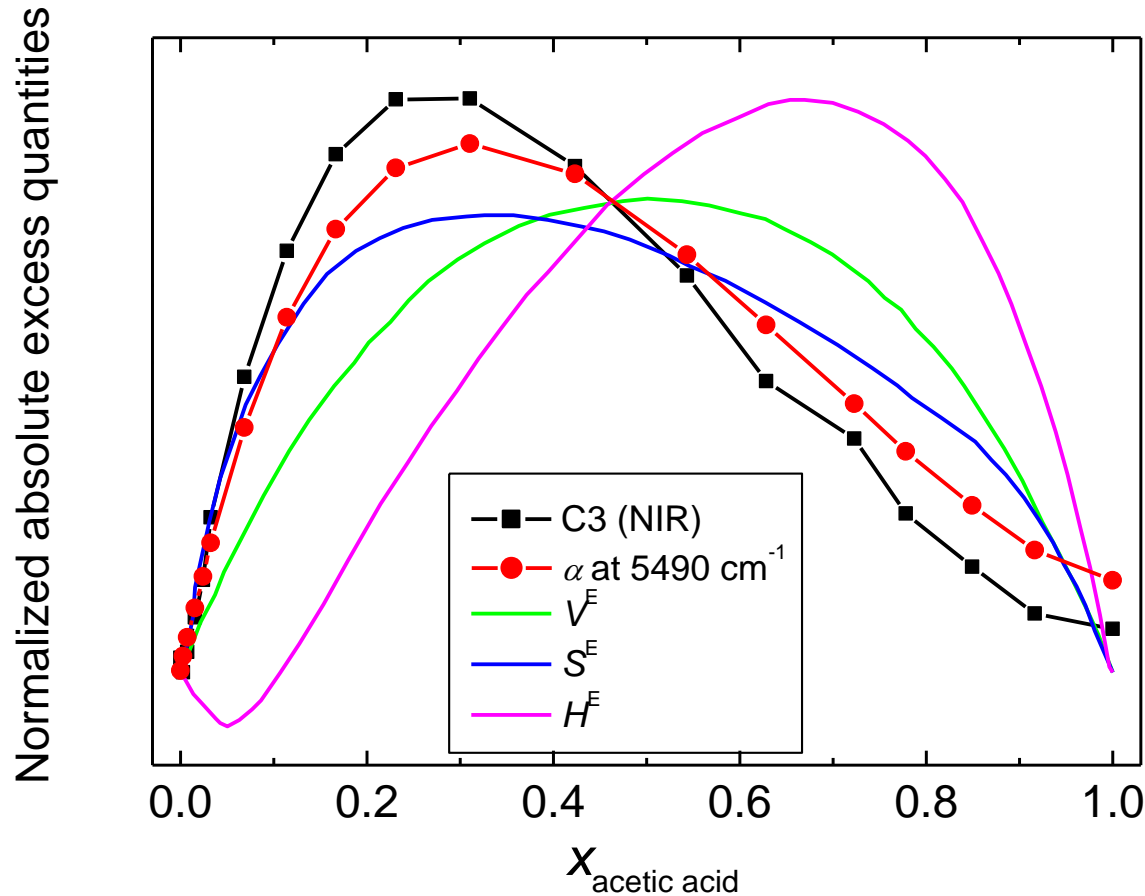
- The molecular interaction between acetic acid and water is shown as a **third component (C3)**.

$$\left(\frac{Abs}{l}\right)_{real} = \epsilon_{pure1} * c_1 + \epsilon_{pure2} * c_2 + \epsilon_{N.I.} * c_{N.I.}$$



- The C3 spectrum shows the increase in the weaker H-bonded water and decrease in the stronger H-bonded species.

# Concentration profile of C3 with the molar excess quantities (volume, entropy, and enthalpy)



- The C3 profile along acetic acid mole fraction is similar to  $\alpha_{5490\text{cm}^{-1}}$  and  $S^E$  rather than  $V^E$  and  $H^E$ .

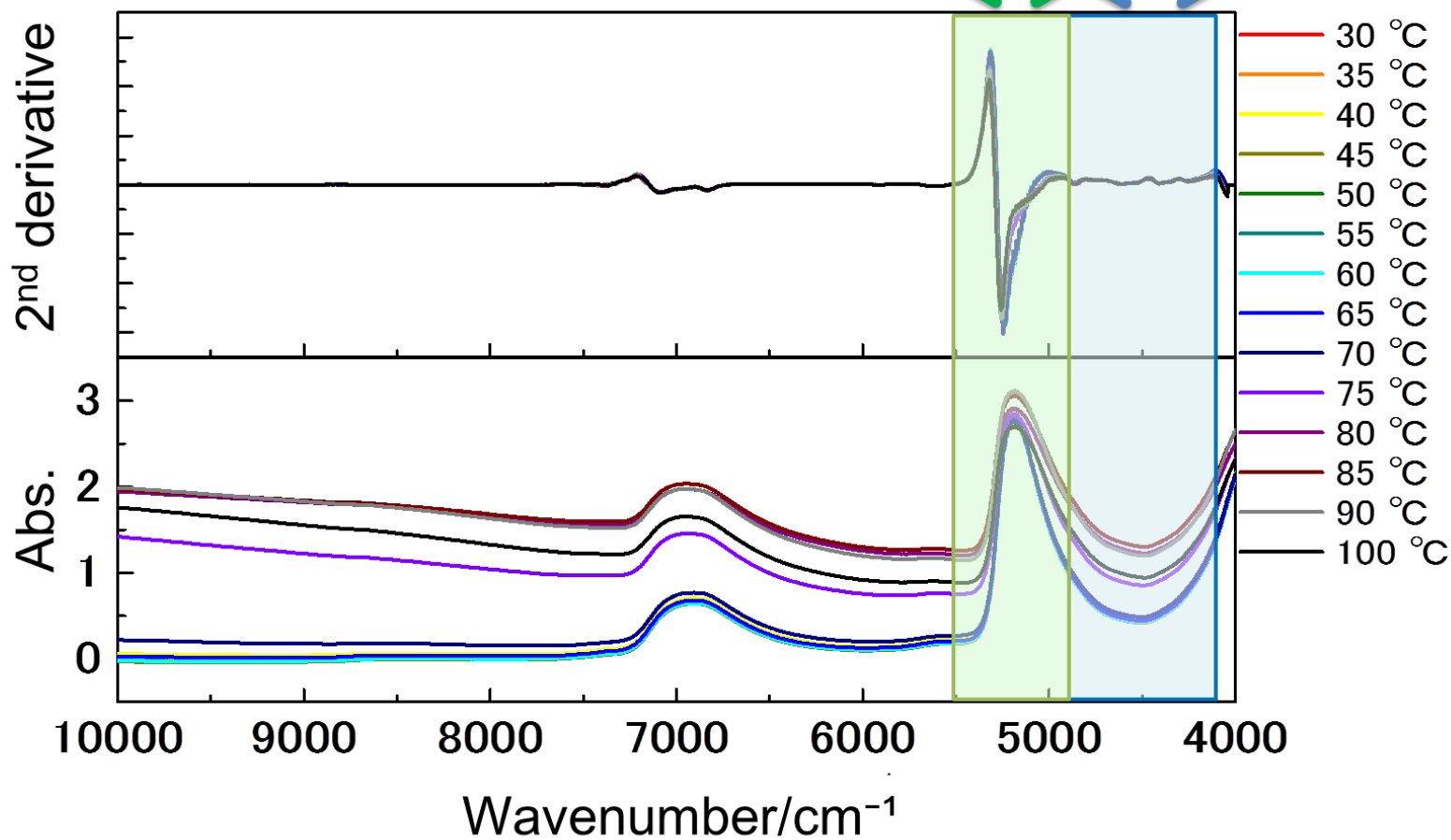
>> **The entropic effect governs the molecular interaction between acetic acid and water.**

>> This is also confirmed from the absorptivity ( $\alpha$ ) profile at  $5490 \text{ cm}^{-1}$  showing that the H-bond variety between acetic acid and water is maximized at  $x_{\text{acetic acid}} \approx 0.3$ .

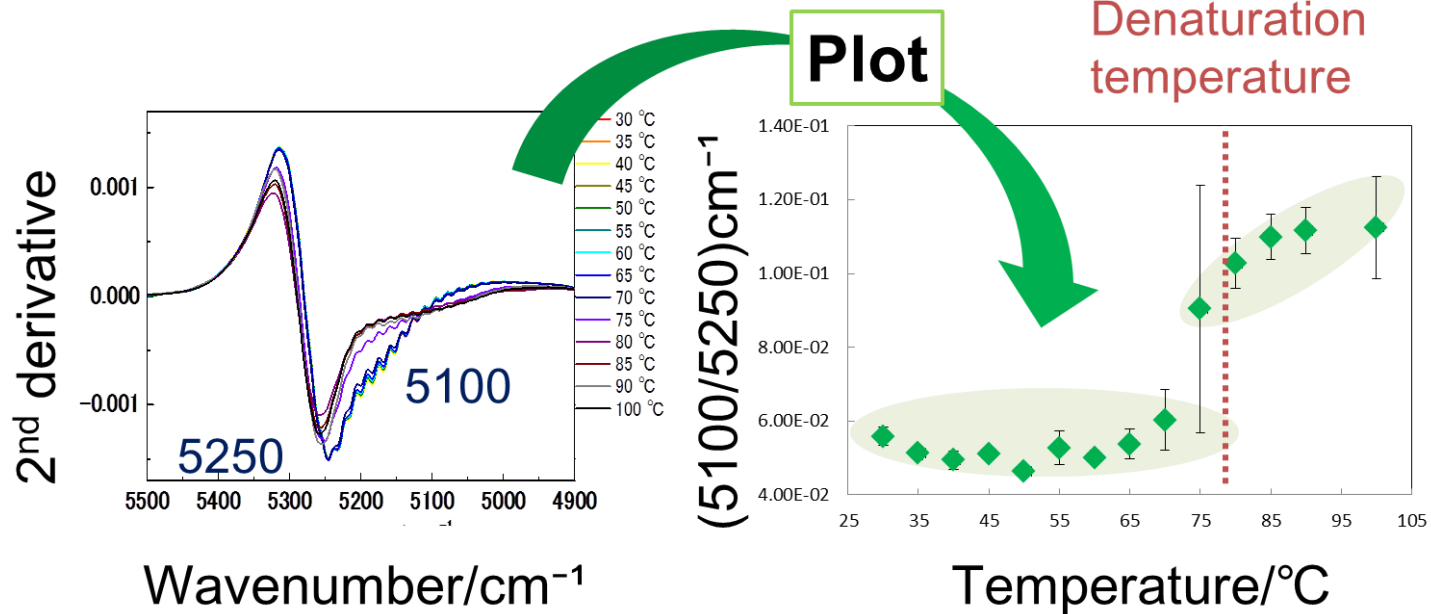
# Heating Ovalbumin

Water-related  
band region

Combination  
region



## ~ Water ~



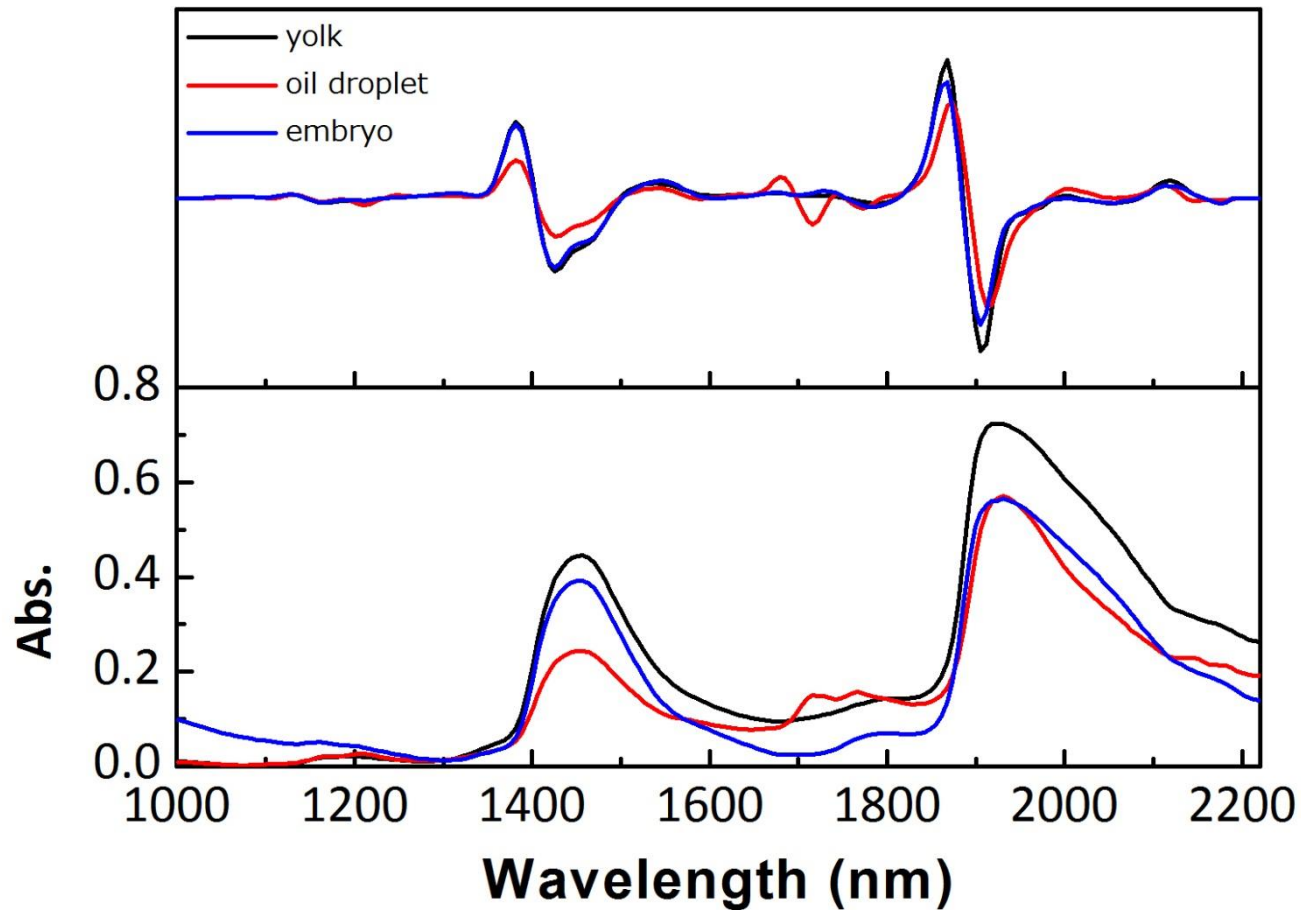
Intensity ratio; (5100/5250)cm<sup>-1</sup>

5100 cm<sup>-1</sup>; Strongly hydrogen bonding

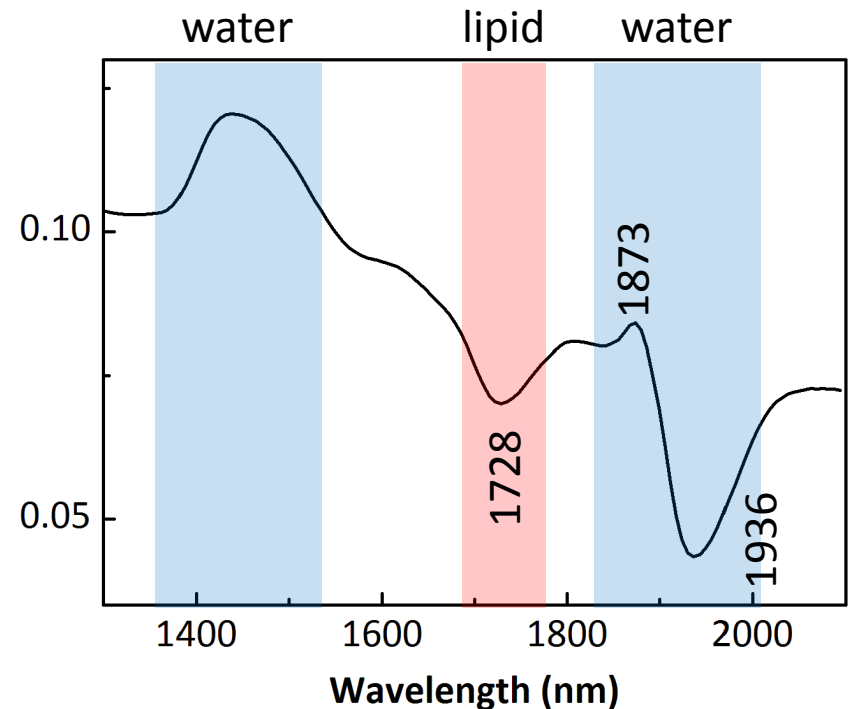
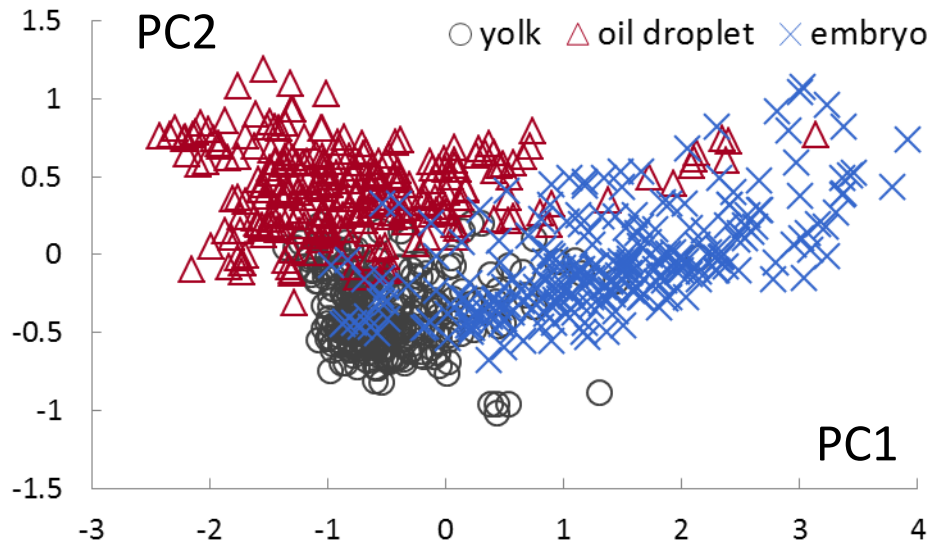
5250 cm<sup>-1</sup>; Weakly hydrogen bonding

- ▶ Along with heat denaturation, a change in the value of the intensity ratio was observed
- ...It is considered that **water molecules** around the  $\beta$ -sheet behave differently.

# NIR spectrum of fertilized eggs measured on 5<sup>th</sup> day



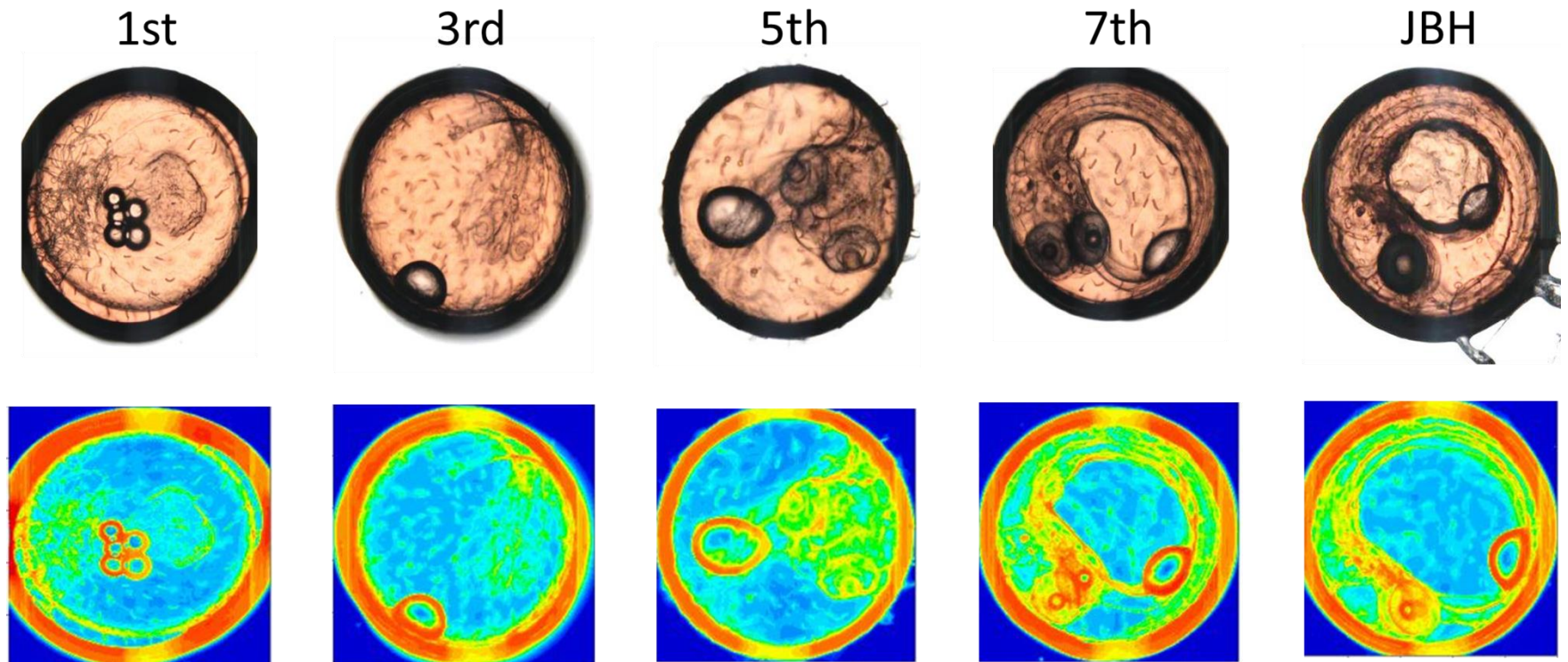
# PCA in 3parts



- Clearly separated 3parts.
- It is indicated that weakly and strongly hydrogen bonded in 3parts mainly were different.



# NIR images projected by PC1 Loading spectrum of PCA in 3parts



- It could visualized not only yolk, oil droplet and embryo also bloodstream in clear.

# *World Research Center for Molecular Spectroscopy*

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