

# Understanding causes of photooxidation in dairy products by fluorescence spectroscopy and multivariate curve resolution

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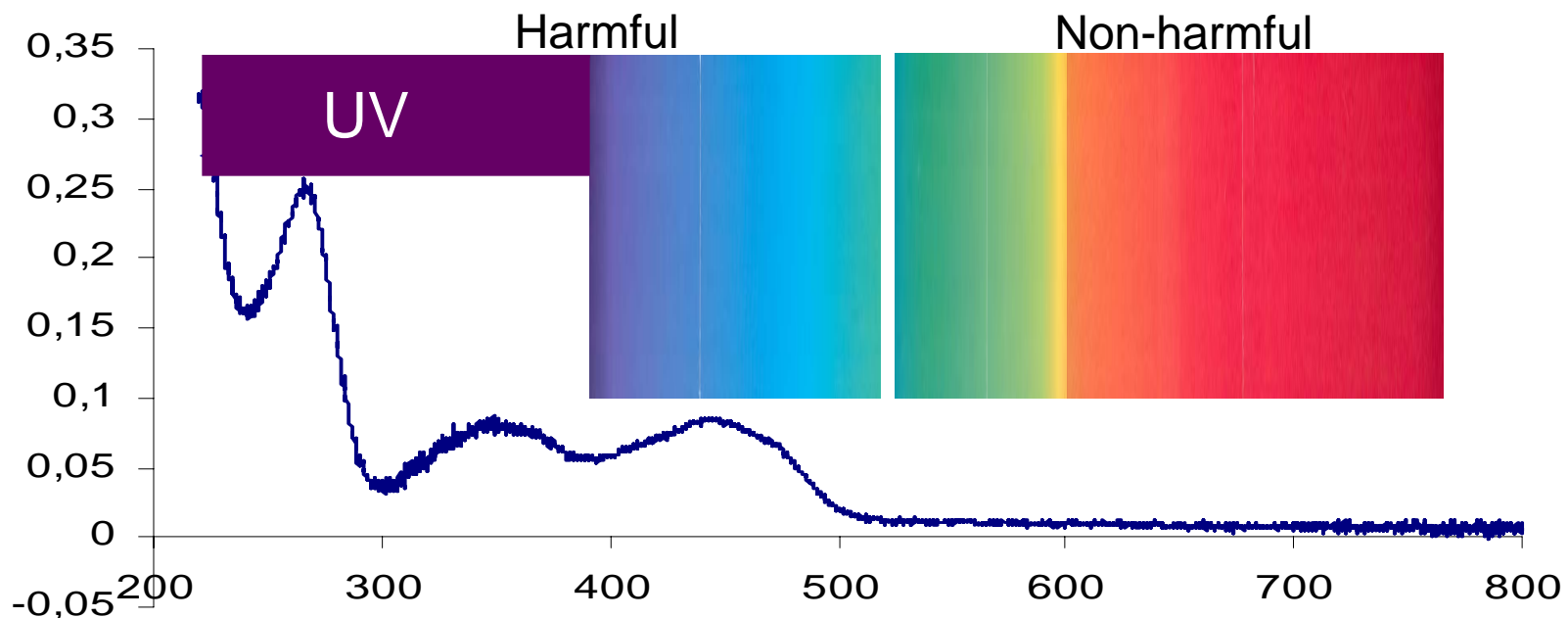
*Johan Moan, Norwegian Radium Hospital  
Rasmus Bro, KVL*

# Dairy products get oxidised when exposed to light

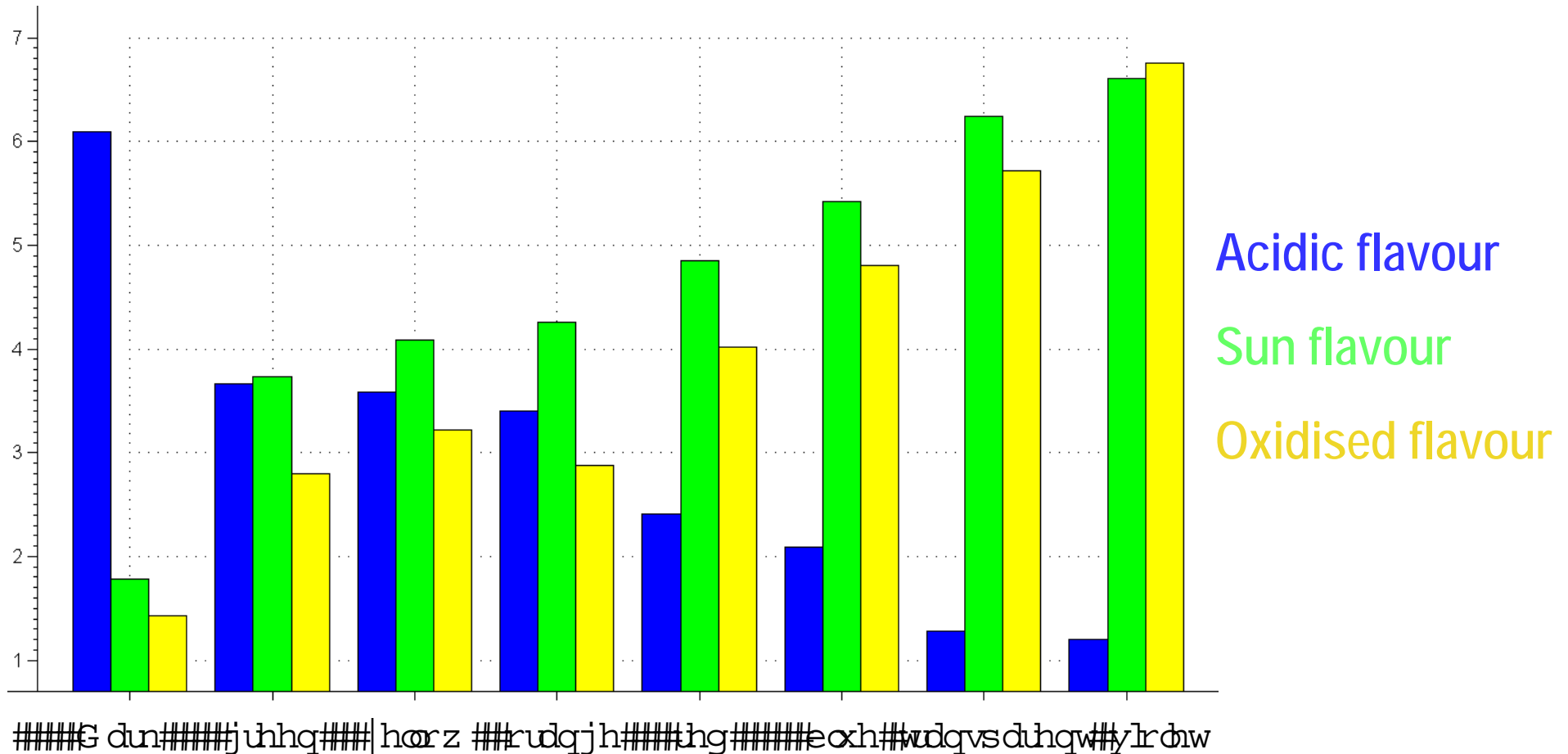


# Why?

- Because they contain light-sensitizers
- Riboflavin has been regarded to be the **only** natural light sensitizer in dairy products.

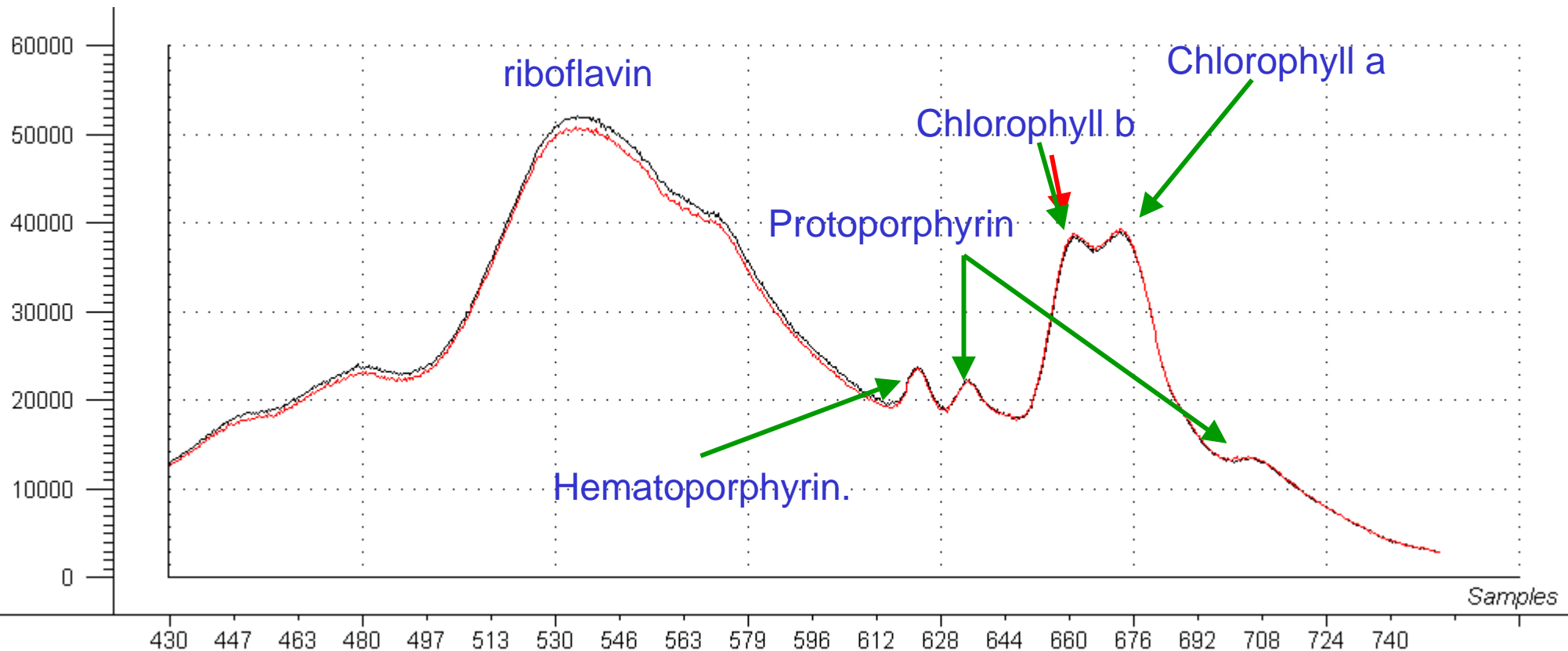


# Actual sensory effect on cheese after light exposure



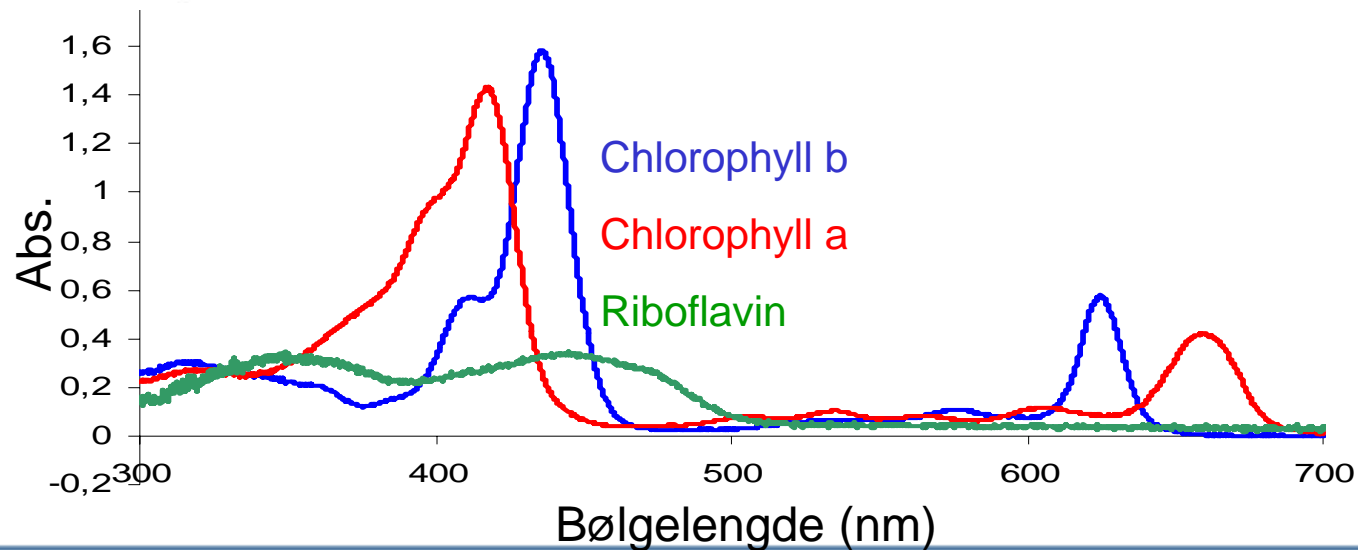
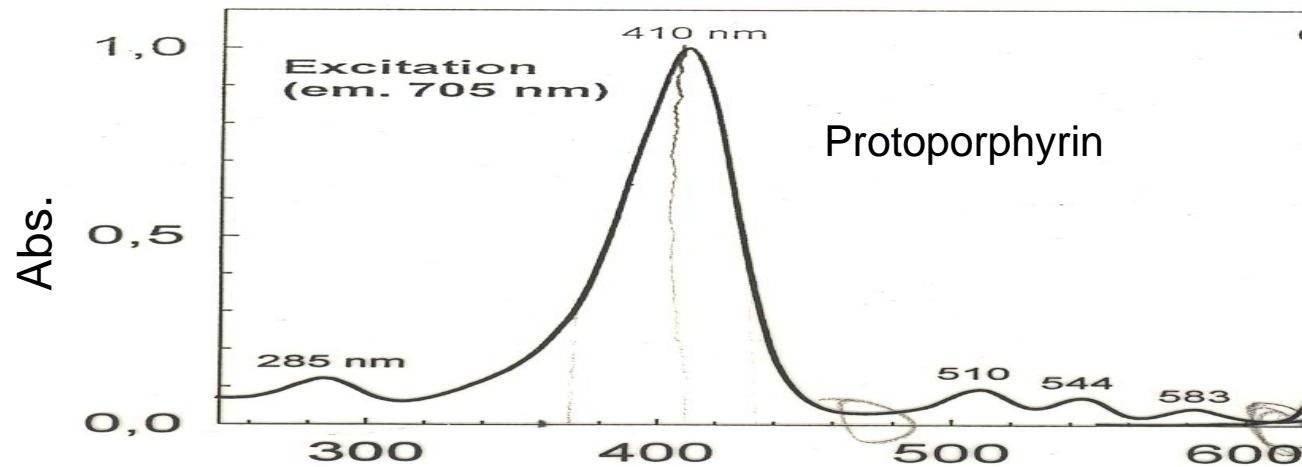
Acidic flavour  
 Sun flavour  
 Oxidised flavour

# Fluorescence from cheese: possible components...



smor\_mo1 smor\_mo2

# Absorption spectra



Which chemical components are in the butter?

Are they all active, or are some of them predominant?

If we knew, we could optimise transmission properties of the packing materials to minimise photooxidation

Example from butter:

## Strategy:

- Design light exposure experiment which induces the necessary spectral variation and sensory variation
- Measure fluorescence excitation-emission landscapes and perform sensory measurements on the butter samples
- Estimate pure chemical components and their scores from the fluorescence landscapes by MCR (PARAFAC)
- By regression: Find which of the pure components that explain variation in sensory attributes

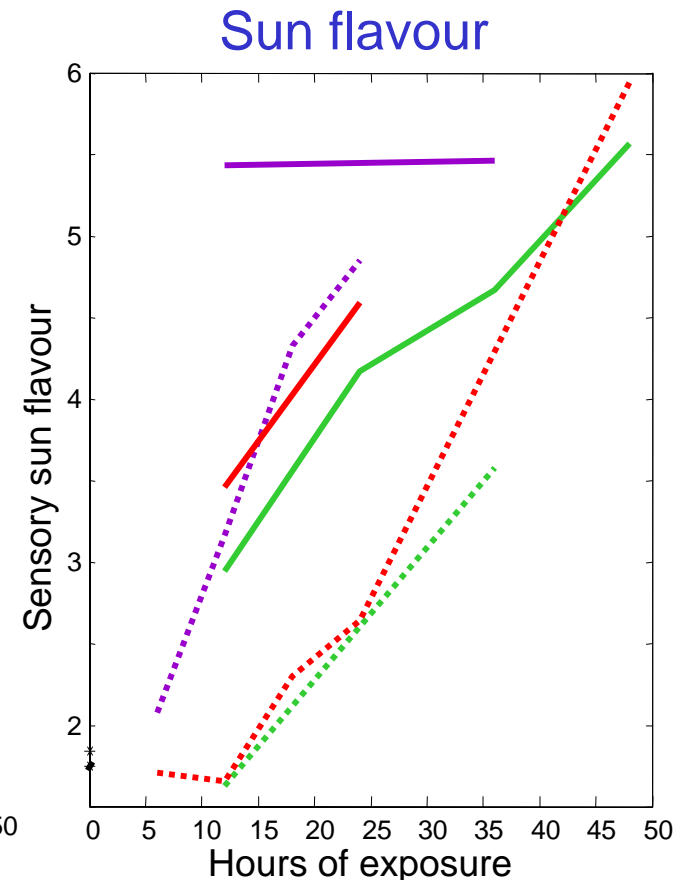
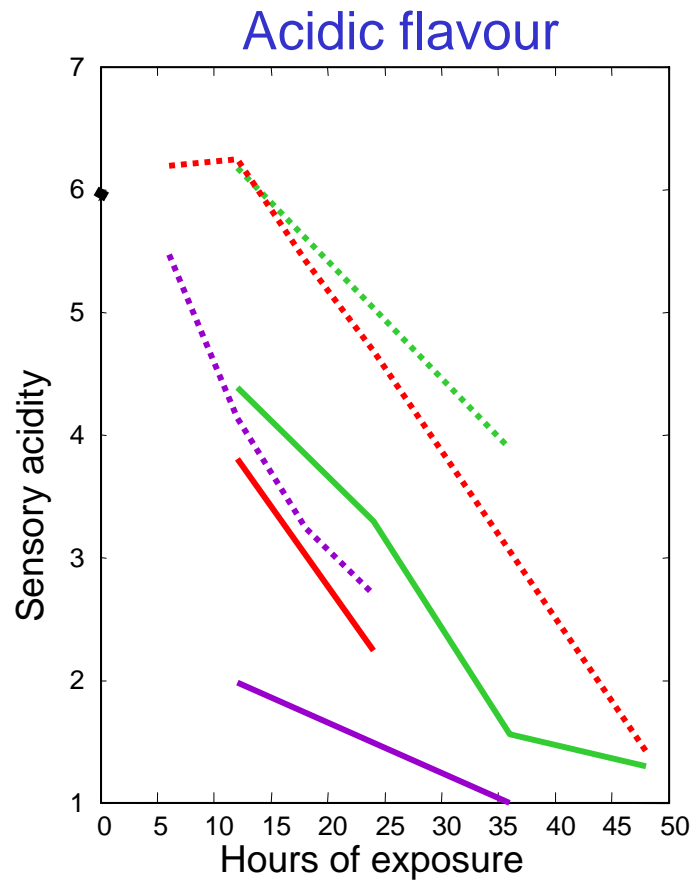
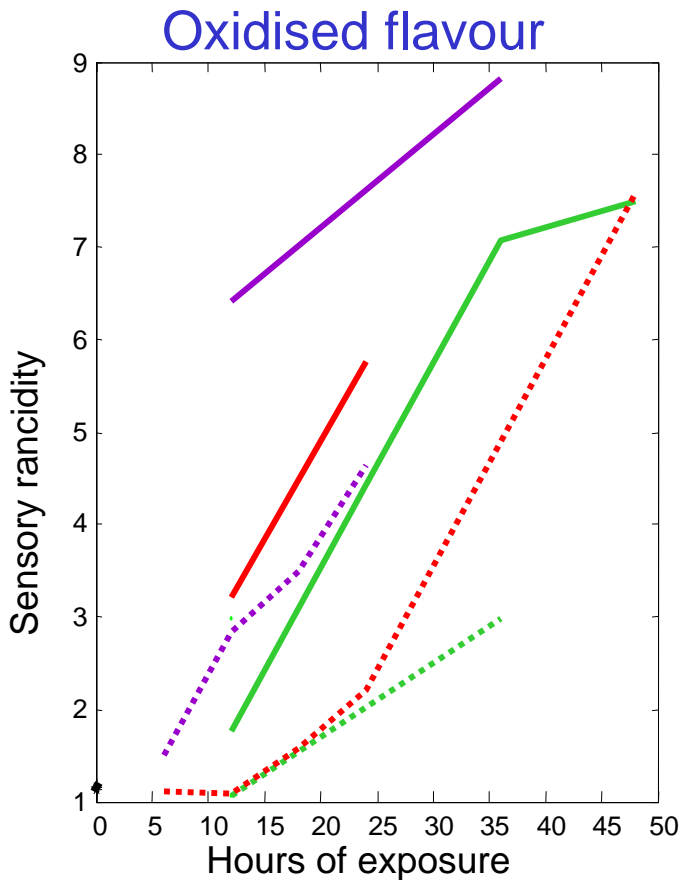
# Light exposure design

- Violet, green or red light (or in dark)
- Low oxygen (close to vacuum), high oxygen (air access)
- F: fluorescence landscape, S: sensory analysis

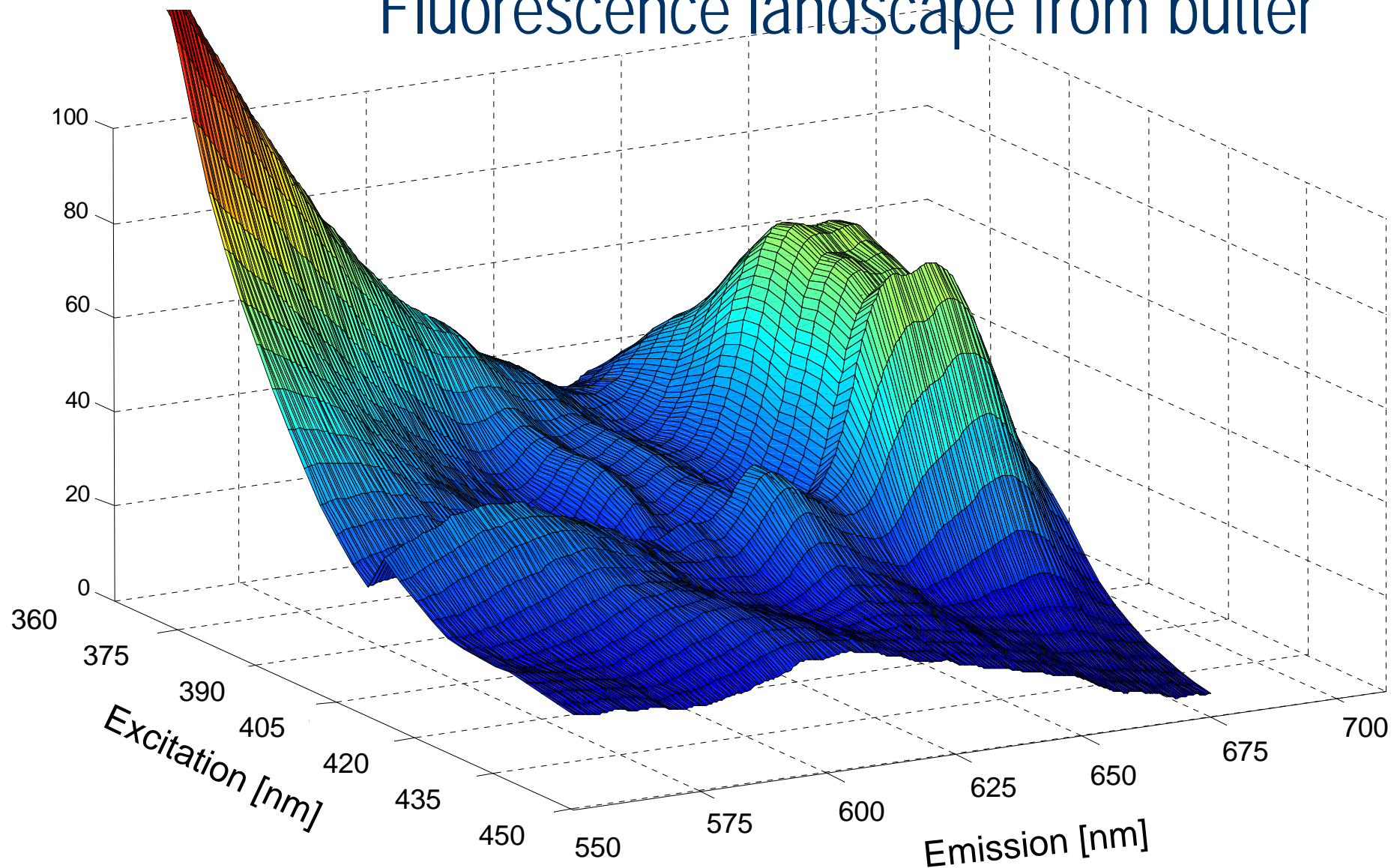
Exposure time (h)	High oxygen				Low oxygen			
	Violet	Green	Red	Dark	Violet	Green	Red	Dark
6								
12								
18								
24								
30								
36								
42								
48								

# Sensory responses

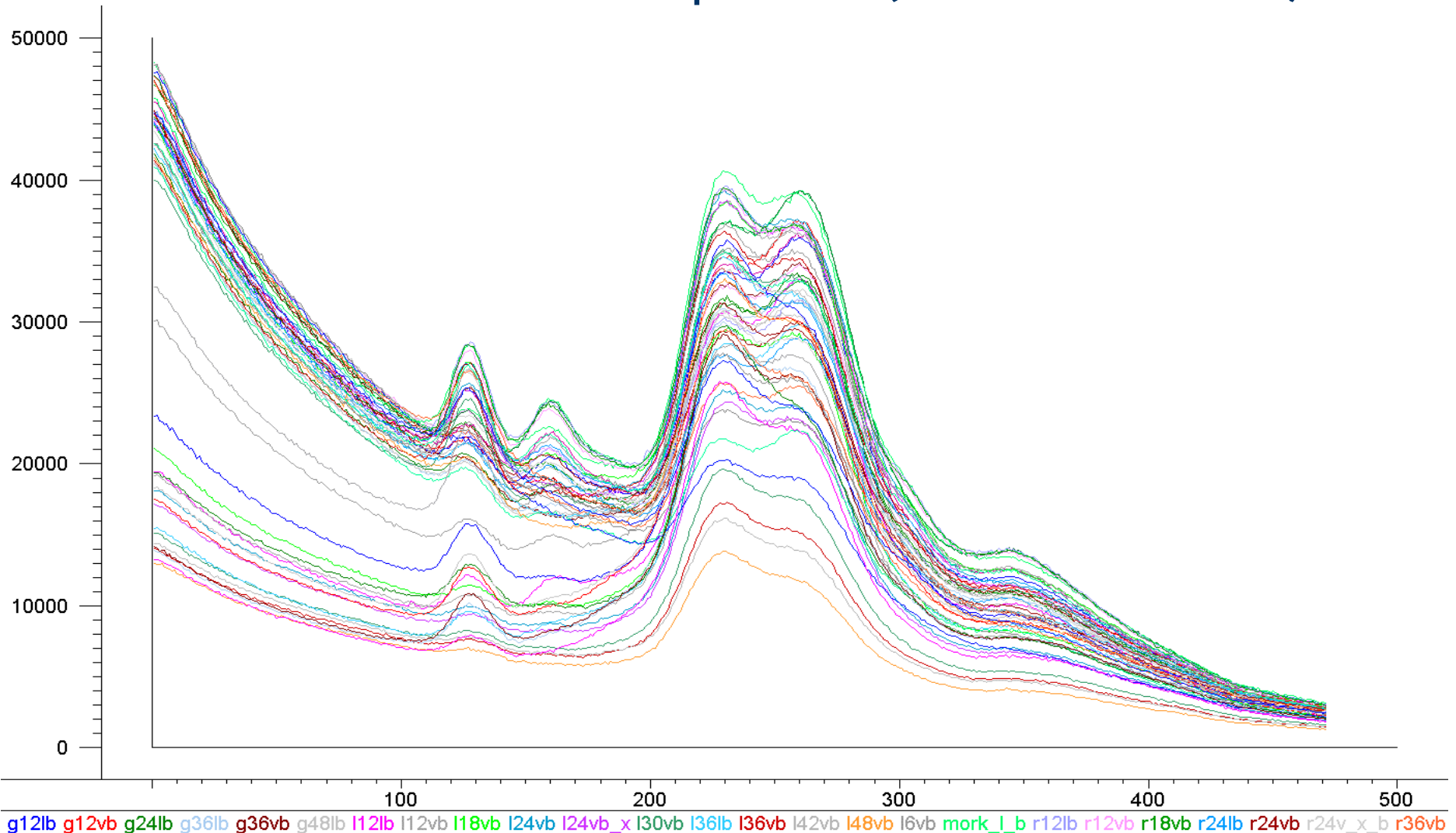
———— High oxygen  
 ..... Low oxygen



# Fluorescence landscape from butter



# Fluorescence emission spectra (for ex. 380 nm)



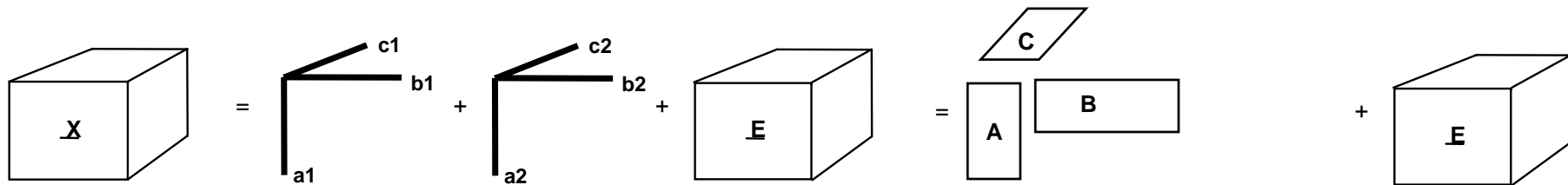
# PARallel FACtor analysis - PARAFAC

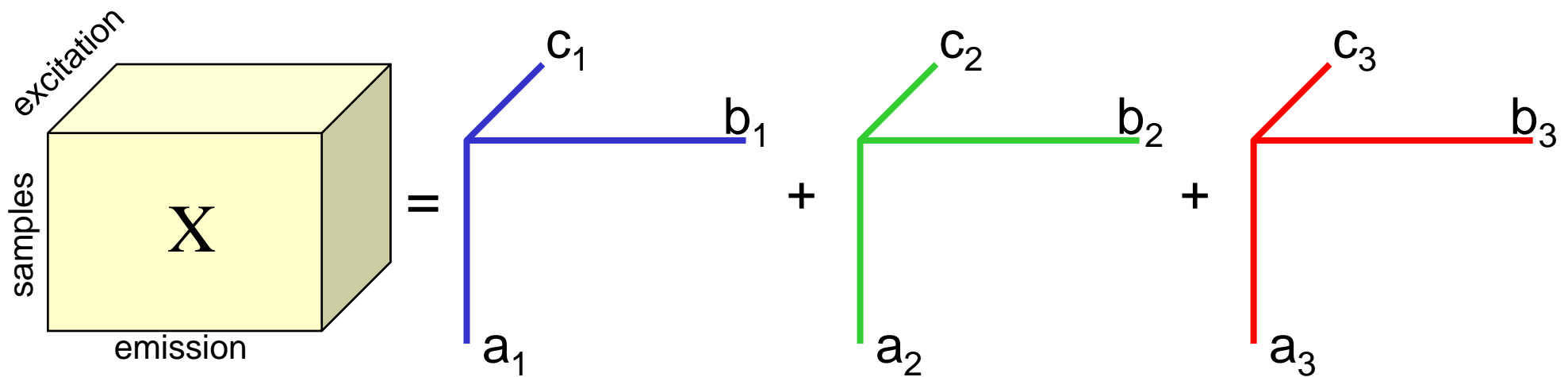
- PCA - bilinear model,

$$x_{ij} = \sum_{f=1}^F t_{if} p_{jf} + e_{ij}$$

- PARAFAC - trilinear model,

$$x_{ijk} = \sum_{f=1}^F a_{if} b_{jf} c_{kf} + e_{ijk}$$

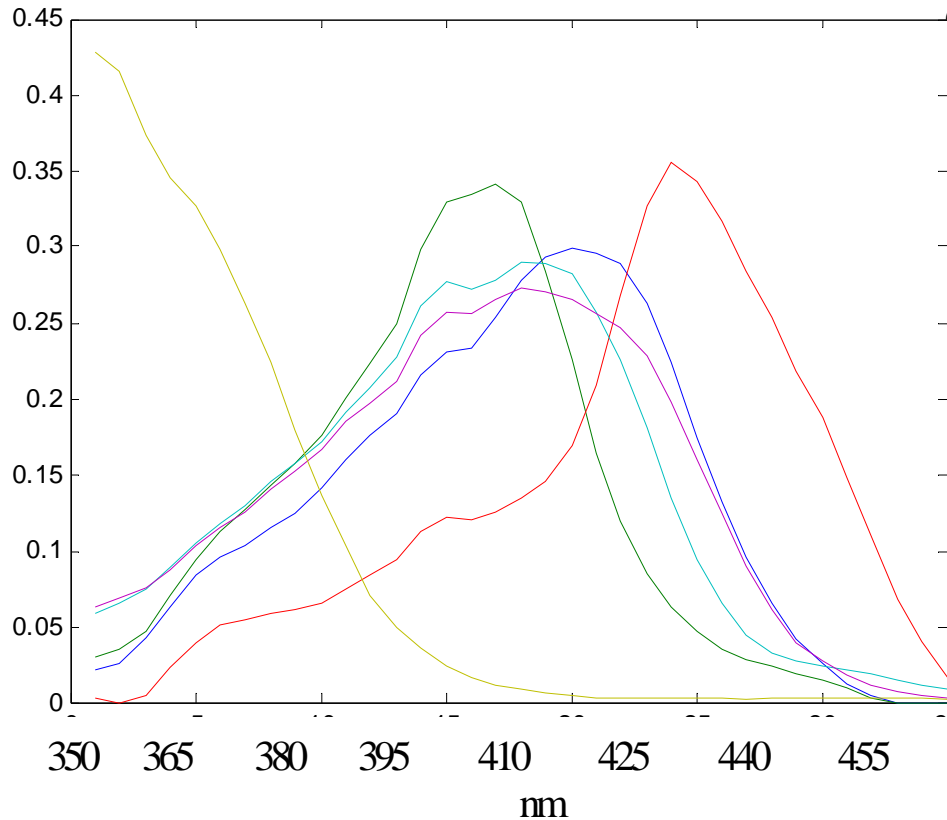




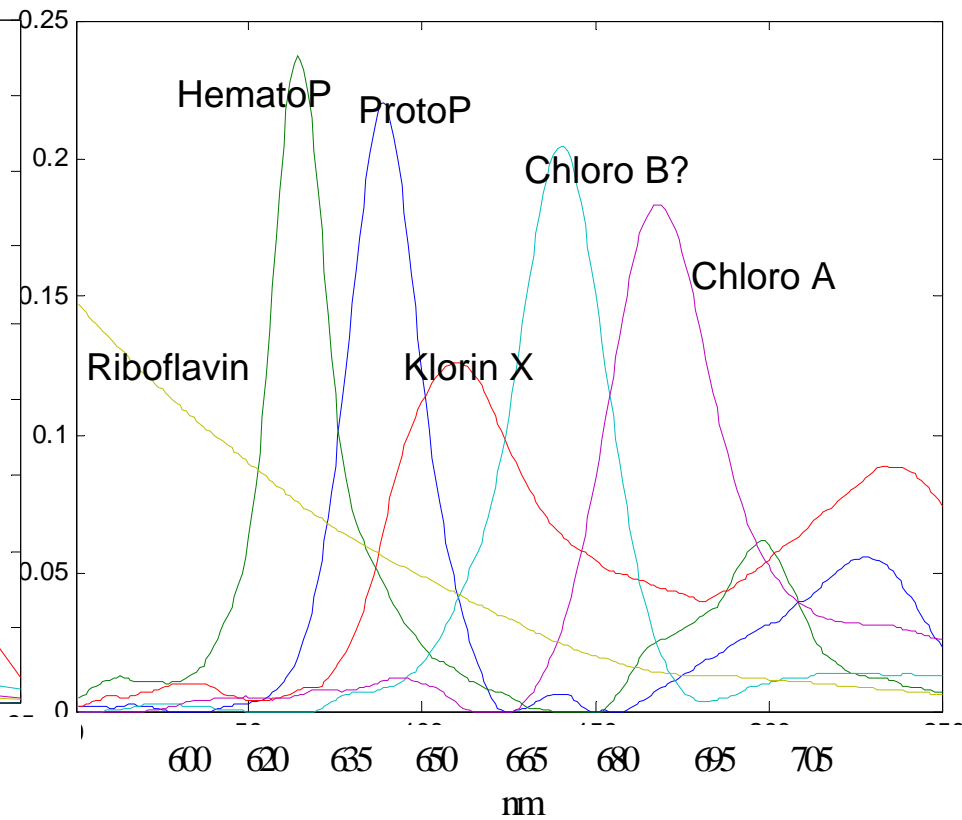
- Mixtures can be resolved
- Concentrations can be estimated
- Pure spectral profiles can be estimated
- For fluorescence landscapes: pure excitation and emission spectra can be estimated

# 1. Estimation of PARAFAC loadings

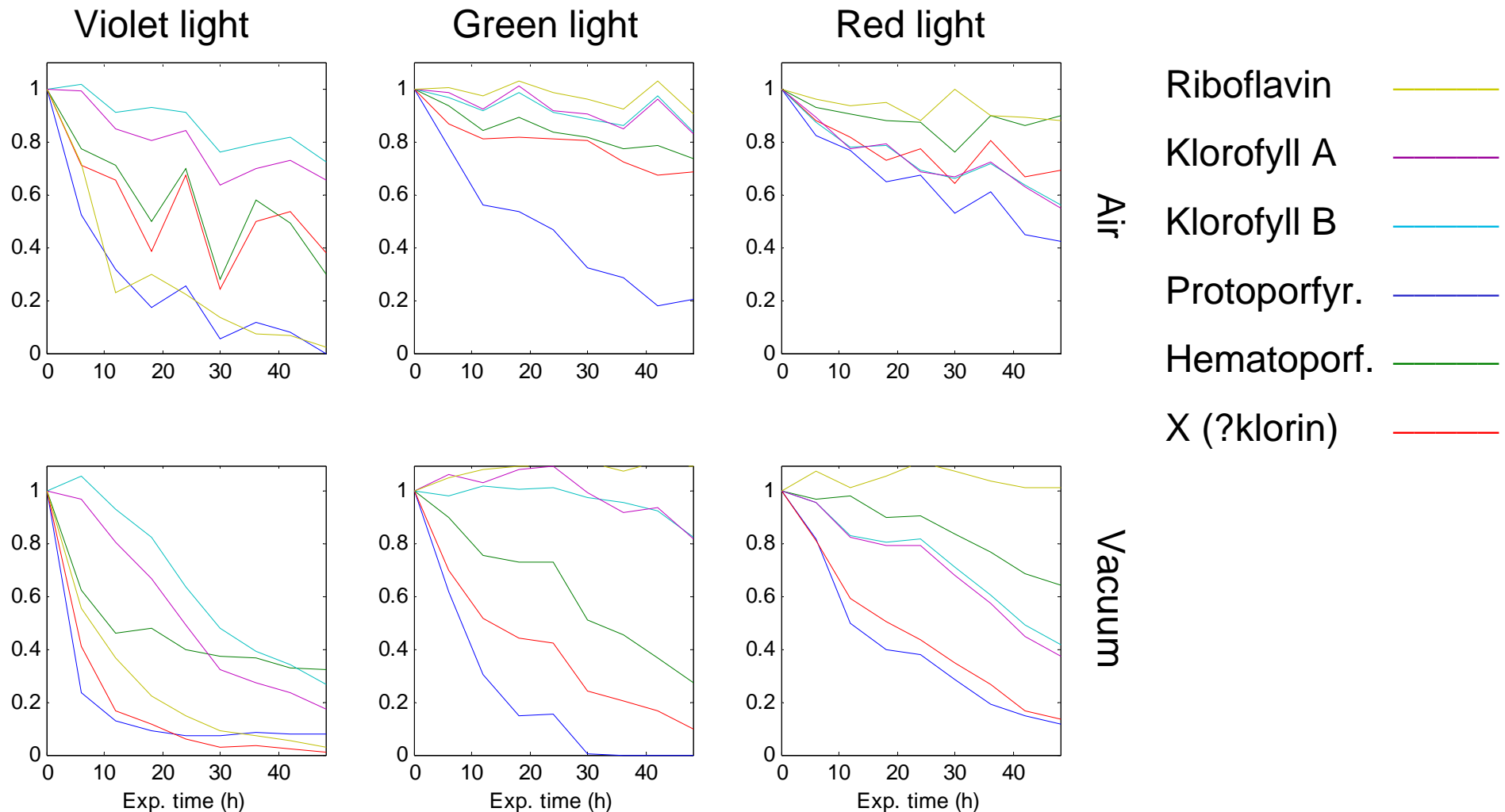
Excitation



Emission

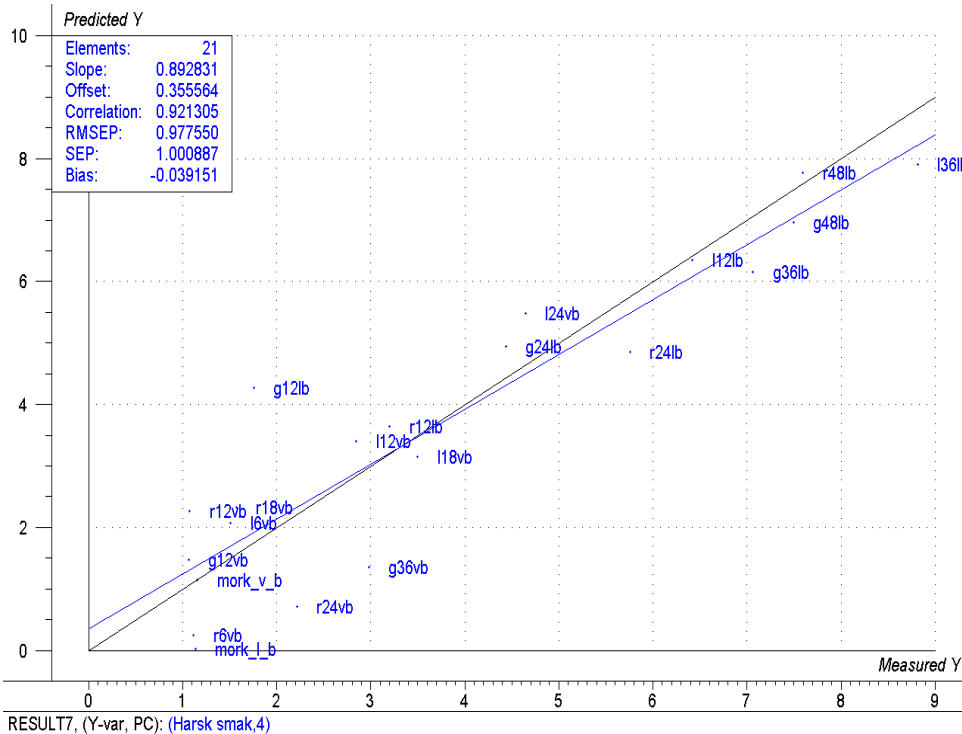


## 2. Relative concentrations (scores) are estimated

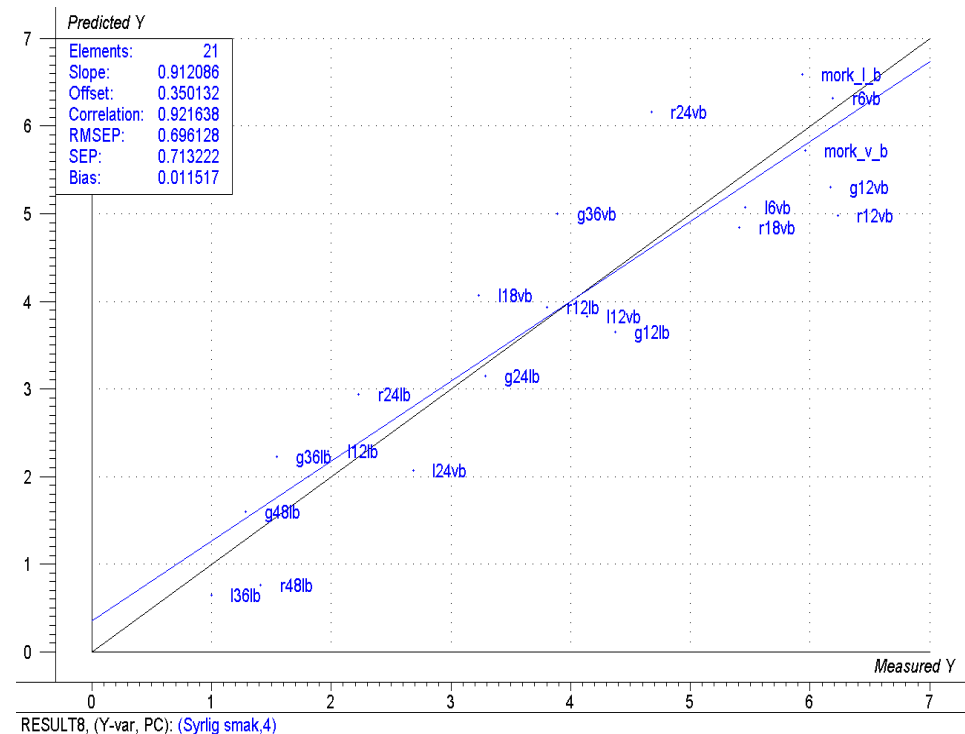


# 3a) Connection between PARAFAC scores and sensory analysis

## Oxidised flavour

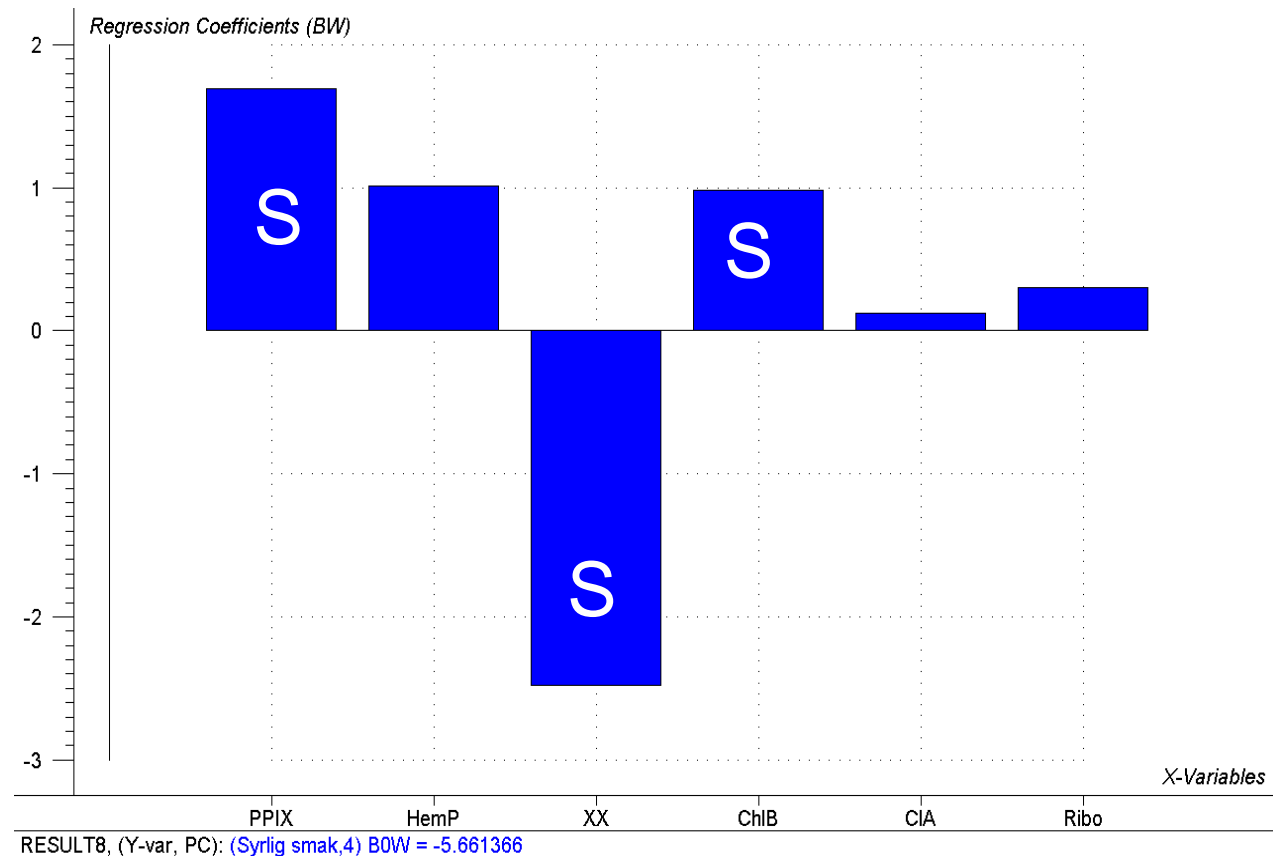


## Acidic flavour

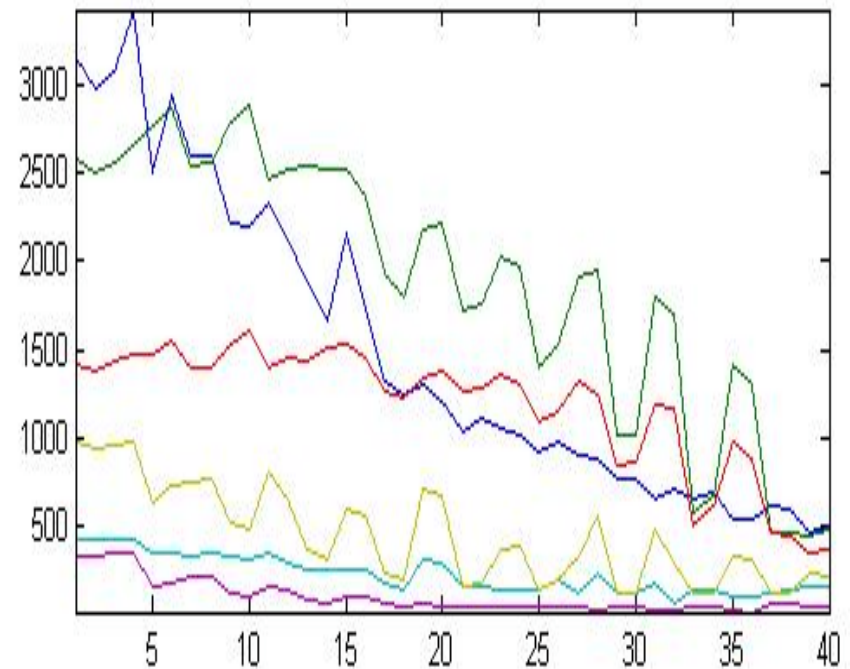
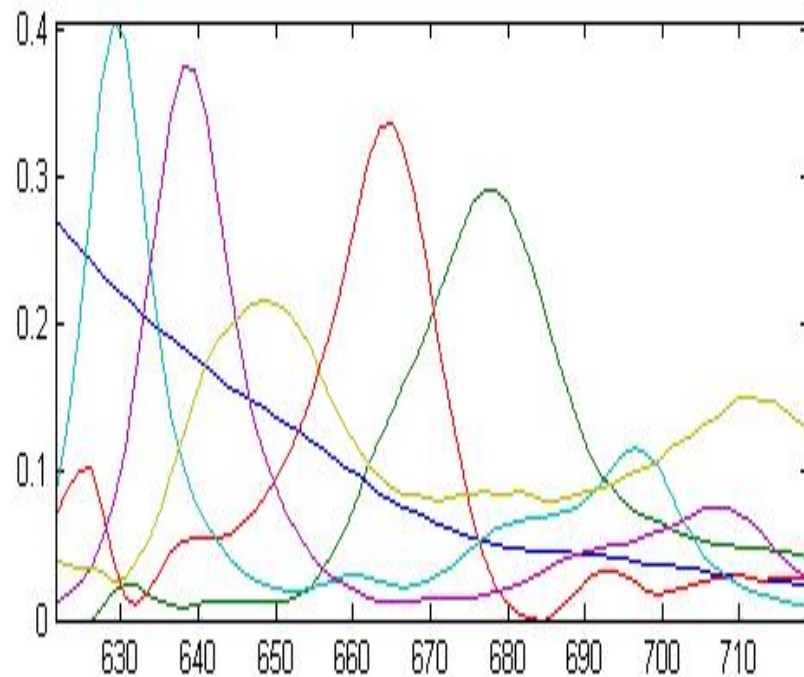


### 3b) The pure components contributing to explain sensory changes are:

- Protoporphyrin
- Chlorofyll B
- X (Chlorin?)



## 4. The model can be used to estimate concentrations for new samples from new experiments



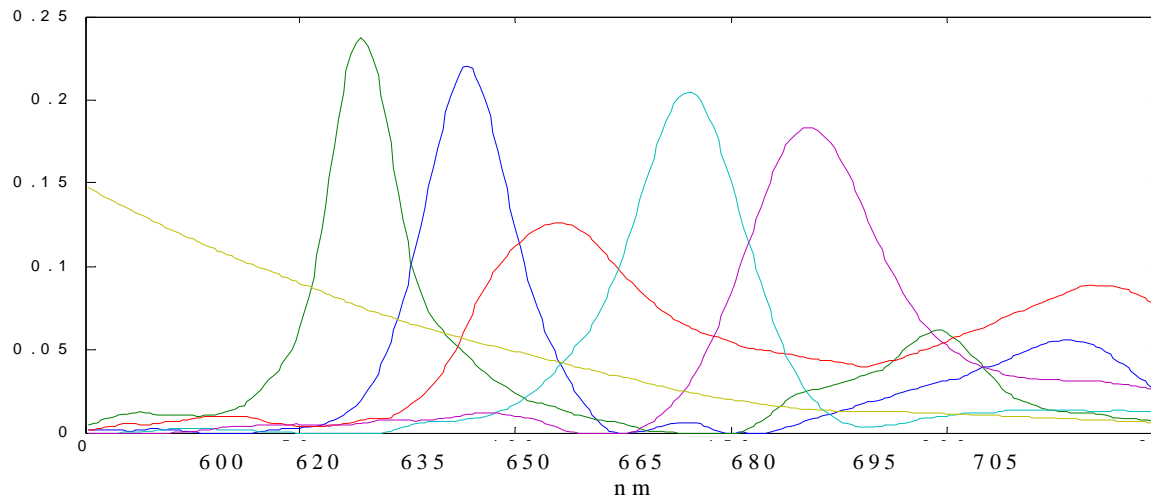
## 5. Same model will also work for cheese, milk, sour cream, youghurt...??

- Because of its trilinear structure: Theoretically Yes.

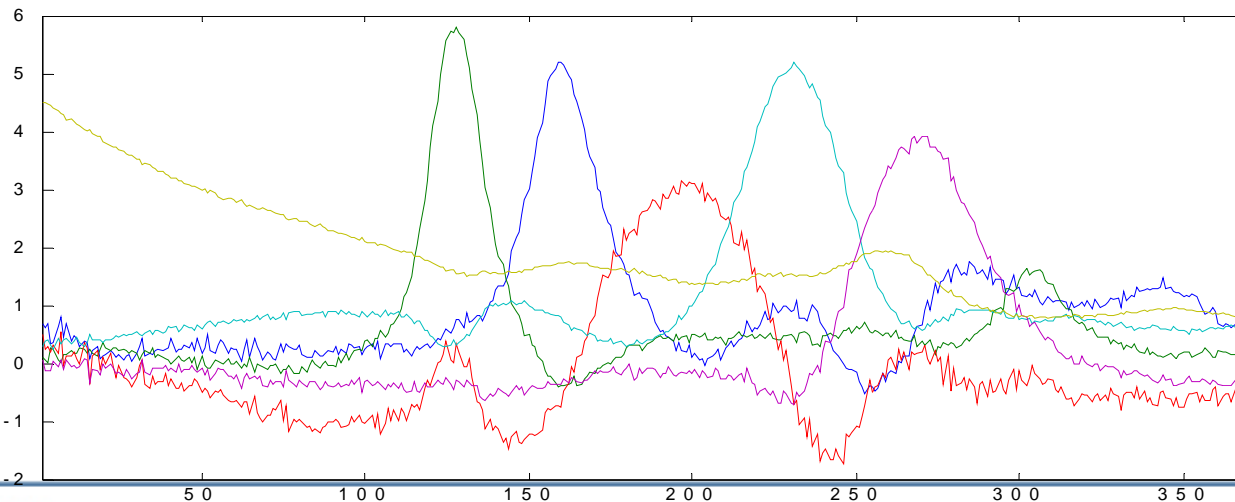
## Conclusions:

- Experimental design, fluorescence spectroscopy and multivariate curve resolution make it possible to separate the light sensitizers in dairy products.
- The approach is relatively simple and makes research in the field much more effective, informative and fun.
- The process of obtaining a good calibration data set requires careful consideration and time.

# ICA compared to PARAFAC



PARAFAC



ICA



Use the model to estimate degradation of each component in new samples, different experimental design

