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INVESTIGATION THE STORAGE STABILITY OF YOGURT USING PARAFAC (PARALLEL FACTOR ANALYSIS)

Ahammed Basheer P K M[1], Dr. Shrikant Sharma[2]

Department of Biotechnology

[1,2]Shri Venkateshwara University, Gajraula (Uttar Pradesh)

Abstract

Yogurt's storage stability was assessed using PARAFAC (parallel factor analysis) and fluorescence spectroscopy. 5-week storage studies at 4^0C yielded fluorescence maps and direct front face fluorescence measurements on yoghurt samples with excitation and emission wavelengths ranging from 270–550 nm. For the yoghurt, PARAFAC detected three fluorophores that were linked to the storage conditions, which they analysed using fluorescence landscapes. Lumichrom, tryptophan, and riboflavin have been identified as the most likely fluorescent chemicals. Yogurt's ability to withstand oxidation and maintain its quality can be swiftly assessed using fluorescence spectroscopy and chemical measurements. Using standard chemical analysis to measure riboflavin concentration yielded regression models with an error of 0.09% PPM, or 7% of the yoghurt samples' mean riboflavin level. Many fluorescence data matrices, particularly those with lower emission wavelengths, have missing values (below excitation). The solution and computation times skyrocketed when zeros were used to fill in some of the model's gaps.

Keywords: Fluorescence spectroscopy; parallel factor analysis; yogurt

1. Introduction

Fluorescence spectroscopy is one of the fastest and most sensitive tools for examining molecular environments. All kinds of biological samples can benefit from this non-destructive analytical method for detecting fluorescent molecules and their surrounding environment. Fluorophores such as aromatic amino acids and vitamins such as cofactors can be very helpful in food analysis. [1] Initially proposed the use of chemometrics for food analysis in 1982, which has led to an increase in the use of autofluorescence. Fluorescence spectroscopy has been employed in dairy

research for chemometric investigation of structural reformation in milk proteins and their physicochemical nature during heating, coagulation and cheese manufacturing and the analysis of oxidative changes in processed cheese during storage [2]. An entirely new approach for quickly determining the quantity of vitamin A and B has been developed using fluorescence spectroscopy [3].

Using front-face fluorescence spectroscopy, the oxidative stability and chemical alterations in yoghurt samples were examined in this study. There were a number of conditions in which yoghurt samples were stored. PARAFAC was used to examine fluorescence landscapes for structure.

Real-world applications for PARAFAC modelling of fluorescence data have recently gained attention [4]. In addition, because emission below the excitation wavelength has no practical importance, PARAFAC modelling may be impeded by light scattering effects and the large number of fluorescence landscapes with missing values. In order to keep the decomposition stable, [5] proposes inserting zeros in the places with missing values.

2. Methodology

2.1. Storage of yogurt with other packaging materials

Arla Foods amba provided plain yoghurt with a 3.5 percent fat content (Viby, Denmark). Polylactate (PLA) and polystyrene (PS) were used to make hard cups for the yoghurt, and the PS cups had the better oxygen permeability and light transmission. There is a 35 cc headspace volume in each package with 180 g of yoghurt and 155 g for PLA. The cups were sealed with a colourless and transparent laminate. For five weeks, the samples were kept at 4 8C under a radiant flux of about 3500 lx fluorescent light "(Philips fluotone, TLD 18W/830)." The container containing the samples was lighted from the top and sides. Temperature and light fluctuations might have an impact on the results if the samples weren't switched out frequently enough. More information about packaging materials may be found at [6].

2.2. Experimental design

Two similar storage experiments were conducted on two batches of yogurt. There were a total of 21 samples taken from each batch after 0, 7, 14, 21, 28 and 35 days of storage (five days, two light conditions, two packaging materials and one starting sample). In total, 42 separate samples were analysed. For each batch, three cups from the same circumstances were picked and considered triplicates. In order to ensure accuracy, each analysis was performed twice. It was combined with the cup of yoghurt before to taking the measurements.

2.3. Fluorescence spectroscopy

For the fluorescence landscapes, the yoghurt was filled with 15 grams and a measuring probe was dipped 1 mm into the yoghurt sample to record fluorescence..

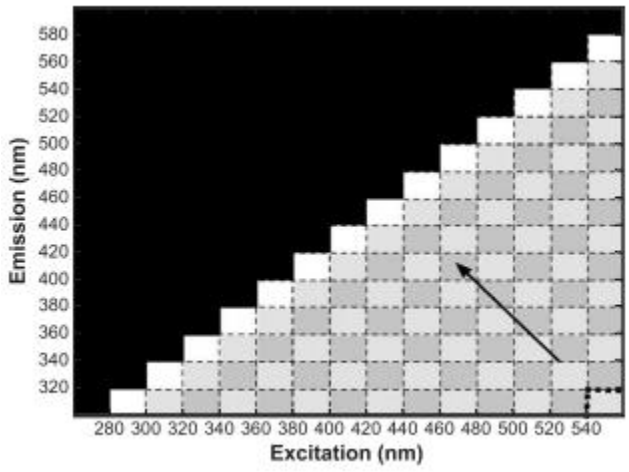

Fig. 1Schematic representation of the recorded data matrices for fluorescence;the fluorescence signal is captured within the dark region. As a result of this measurement, all of the other data points are left blank.

Measurements of each sample's fluorescence were made possible thanks to the Bio-View spectrofluorometer pulsed xenon lamp, light conductor, and measurement probe (Delta Light & Optics, Den brand). The fluorescence landscapes were generated using 15 different excitation and emission wavelengths, each separated by 20 nm intervals and bandwidths. Only emission wavelengths above the excitation wavelength were recorded, resulting in 120 data points (black in Fig. 1) for each experiment.

"The fluorescence landscapes are broken down into several trilinear components or factors by PARAFAC. Decomposition via PARAFAC aims to reduce residual e_{ijk} to a minimum by minimising its sum of squares

$$x_{ijk} = \sum_{f=1}^{F} a_{if} b_{if} c_{kf} + e_{ijk} \, (i = 1, \dots, I$$
$$j = 1, \dots, J; k = 1, \dots, K; f = 1, \dots, F) \dots \dots \dots (1)$$

Where,sample i

Excitationwavelength$j$,

Emission wavelength k

Elementx_{ijk}

Sample scores a

Excitation loadings b

Emission loadings c_{kf}

Residuale_{ijk} ."

A PARAFAC model was derived for each batch separately, and then the results were checked to make sure that the excitation and emission loadings were within acceptable limits. With the use of PARAFAC modelling, we looked at each of the 42 samples three times to ensure completeness. After excluding an outlier, there were only 125 yoghurt samples in the model. As a result, a 125x15x15 three-way data array was analysed.

3.1. Managingmisplaced values

Figure 1 shows that 47 percent of fluorescence data matrices are blank, while the remaining data points have missing values. Filling up the gaps with zeros was tried out. PARAFAC models for this set of fluorescence data were constructed using a combination of zeros added to replace missing values and zeros inserted until the emission wavelength equalled the excitation wavelength. If you look at Figure 1, you'll see that there are 15 unique solutions to the problem of identifying all intermediate data sets with zeroed cells added up to the diagonal line. Instead of missing data, a gradient from 0% to 100% of zeros was employed. Non-negativity was applied to all PARAFAC models across all computation methods.

3.2. Riboflavin chemical analysis

Yogurt's riboflavin content was measured using an Aminco Bowman series 2 luminescence spectrofotometer using the fluorometric technique developed by AOAC (1990). "(SLM-Aminco, Urbana, IL, USA)" Before performing the fluorometric measurement, a chemical extraction and cleaning of the riboflavin is necessary, this takes time and necessitates the use of organic solvents. Both the excitation and emission spectra were in the range of 446/525 nm.

3.3. Calibrationof Riboflavin

The conventional riboflavin content of 42 averaged samples was linked to the fluorescence landscapes. Cross-validation with one variable omitted was employed. It is possible to quantify how well a model can predict results by looking at its Root Mean Square Error of Cross Validation (RMSECV). PARAFAC scores were calculated using the partial least squares (PLS) and multiple linear regression (MLR) models (MLR). N-PLS regression was used to calibrate the three-way fluorescence landscape array, and PLS regression was used to calibrate the unfolded fluorescence emission spectra.

3.4. Data analysis Software

The N-way Toolbox and the PLS Toolbox 2.0 (MatLab 6.5, Math Works) Expectation maximisation is used to manage missing values in PARAFAC modelling in the N-Way Toolbox. MatLab may be used to download the spectral data and the reference riboflavin values.

4. Results

4.1. Fluorescence spectroscopy

Two yogurt samples are depicted in Figure 2's fluorescence landscape. The two polar opposites of the experiment's scope are fresh yoghurt (a) and yoghurt maintained in the most extreme conditions (b). Excitation wavelengths between 300 nm and roughly 370 nm show the largest fluorescence peaks, with excitation wavelengths between 370 and 490 nm and emission wavelengths between 500 and 550 nm for the fresh sample. According to fluorescence peak excitation and emission characteristics, tryptophan and riboflavin are the principal fluorescence providers. When tested in pure solutions, riboflavin and tryptophan were found to have the highest maximal excitation and emission wavelengths of 285/365 nm and 520 nm in pure solutions, respectively; It appears that the 270-nm excitation of riboflavin has been absorbed by

other molecules in this circumstance. Tryptophan fluorescence is still visible after 35 days of storage, as shown in figure 2b, but the riboflavin signal appears to have dropped dramatically. The excitation/emission maxima of lumichrome, a photochemical breakdown product of riboflavin, appear to be increasing, with the excitation/emission maxima recorded at about 360/450 nm in a model system, in the fluorescence profile, with an apparent increase. These findings were investigated further using PARAFAC.

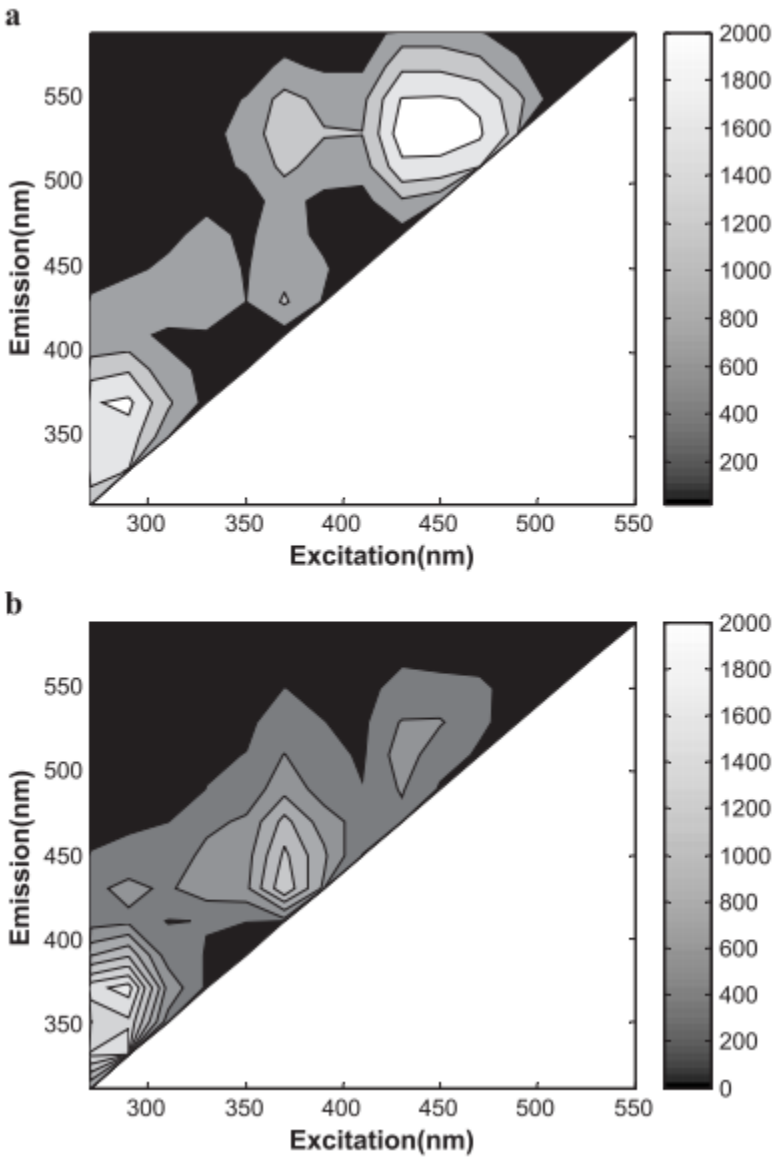

Fig. 2. The fluorescence landscape of a yoghurt sample is seen in this contour map. Fresh yoghurt samples (a) and 35-day-old yoghurt samples (b) in polystyrene

4.2. PARAFAC

One to four components were used to estimate PARAFAC models of fluorescence landscapes. Three fluorescence phenomena were found in the yoghurts during split-half trials and an evaluation of residual systematic, leading researchers to conclude that a PARAFAC model with three components was most suited for this experiment.

Because of fluorescence constraints, 47% of the data in the measured excitation–emission matrix (landscape) are missing. The PARAFAC decomposition may be erroneous based on the significant number of missing data points. To expedite the decomposition, zeros were used to fill in any missing values. If we use a different amount of zeroes to replace missing data, we can see how PARAFAC models break down depicted in Figure 5. As can be seen utilising the last three models, the fluorescence patterns that are compatible with riboflavin's fluorescence properties are only present in the last three models. Figure 1 depicts three alternative fluorescence loading patterns with zeros added to a band with four missing values and a band with two missing values.

4.3. Riboflavin

Riboflavin and fluorescence signals have been linked in numerous regression models. Researchers believe that the comparison of PARAFAC component 1 to traditional riboflavin concentration may be due to the fluorescence of riboflavin. Based on PARAFAC score and riboflavin content, an R^2 of 94% has been established. The amount of riboflavin in samples can be calculated using a regression model enhanced by fluorescence landscapes and the additional PARAFAC scores.

5. Conclusions

A food sample was examined for its oxidative quality using fluorescence spectroscopy and PARAFAC. Riboflavin, tryptophan, and lumichrom (a byproduct of riboflavin) fluorescence spectra were employed to monitor the yoghurt's storage status. This supplied data on the yogurt's molecular evolution. In this work, fluorescence landscapes were shown to have issues with PARAFAC modelling, which resulted in a model solution that was both inaccurate physically and erroneous chemically. When a specific number of the missing values were substituted with zeros, an appropriate decomposition was obtained. Only 43% of the original data could be used in viable PARAFAC models because of the missing variables. Analysis of fluorescence

landscapes and yoghurt riboflavin concentrations showed that the approach may be used to quickly determine riboflavin levels in yogurts.

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