Dynamic and Static Raman Spectroscopic Characterization Analysis of Dairy Products

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Dynamic and Static Raman Spectroscopic Characterization Analysis of Dairy Products

Report outline

01 Background introduction
02 Research Ideas
03 Research Content
04 Summary And Prospect
01 Background introduction

◆ Brief introduction of research background
◆ Brief Introduction of spectral research
Dynamic and Static Raman Spectroscopic Characterization Analysis of Dairy Products

Background introduction
Dynamic and Static Raman Spectroscopic Characterization Analysis of Dairy Products

Farmland → Table → Dairy Products

Food Safety
Dynamic and Static Raman Spectroscopic Characterization Analysis of Dairy Products

How to determine the truth and false of dairy products?
Dynamic and Static Raman Spectroscopic Characterization Analysis of Dairy Products

Human Sensory Identification

Instrumental detection

Spectrum-based Detection

Milk system

Raman spectroscopy

Perturbation (laser)

Match

Unmatch

Dynamic spectra

Two-dimensional correlation analysis

Similarity analysis (correlation coefficient)

Two-dimensional correlation spectrum
Dynamic and Static Raman Spectroscopic Characterization
Analysis of Dairy Products

Brief Introduction of Spectral Analysis

Principle of Raman Spectrum Detection
Dynamic and Static Raman Spectroscopic Characterization Analysis of Dairy Products

Brief introduction of spectrum

Raman spectra of one pure liquid milk product under different laser accumulation time (50 s – 250 s).
Dynamic and Static Raman Spectroscopic Characterization Analysis of Dairy Products

Brief introduction of spectrum

Raman spectra of one low-fat liquid milk product under different laser accumulation time (50 s - 250 s).
Dynamic and Static Raman Spectroscopic Characterization Analysis of Dairy Products

02 Research ideas

◆ Standardization of Spectroscopy
◆ Multidimensional Spectral Analysis
◆ Intelligent Discriminant Analysis
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Research ideas

Characteristic data of dairy products spectroscopy

\[
\begin{pmatrix}
X_{11} & \cdots & X_{1b} \\
\vdots & \ddots & \vdots \\
X_{a1} & \cdots & X_{ab}
\end{pmatrix}
= \begin{pmatrix}
Y_{11} & \cdots & Y_{1d} \\
\vdots & \ddots & \vdots \\
Y_{c1} & \cdots & Y_{cd}
\end{pmatrix}
\]

Static Data Fusion

Direct Data Fusion

\[
\begin{pmatrix}
Z_{11} & \cdots & Z_{1(b+d)} \\
\vdots & \ddots & \vdots \\
Z_{a1} & \cdots & Z_{(a+c)(b+d)}
\end{pmatrix}
= \begin{pmatrix}
PC_1 & PC_2 & \cdots & PC_n
\end{pmatrix}
\]

Indirect Data Fusion

Dynamic Data Fusion

\[
\left\{ X(t_1) \ X(t_2) \ \cdots \ X(t_n) \right\} = X(t_1) \downarrow \Phi(v_1,v_2) + i\Psi(v_1,v_2)
\]
Dynamic and Static Raman Spectroscopic Characterization
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Static Data Fusion

Direct Data Fusion
\[
\begin{pmatrix}
z_{11} & \cdots & z_{1(b+d)} \\
\vdots & \ddots & \vdots \\
z_{a1} & \cdots & z_{(a+c)(b+d)}
\end{pmatrix}
\]

Indirect Data Fusion
\[
(PC_1 \quad PC_2 \quad \cdots \quad PC_n)
\]

Dynamic Data Fusion
\[
\begin{pmatrix}
x_{11} & \cdots & x_{1b} \\
\vdots & \ddots & \vdots \\
x_{a1} & \cdots & x_{ab}
\end{pmatrix}
\]
\[
\{X(t_1) \quad X(t_2) \quad \cdots \quad X(t_n)\}
\]

Cross-correlation analysis
\[
\Phi(v_1, v_2) + i\Psi(v_1, v_2)
\]

Research ideas

Algorithm library

Standard Spectral Database

Quality Data Analysis

pattern recognition
03 Research contents

◆ Standardization of Spectroscopy
◆ Multidimensional Spectral Analysis
◆ Intelligent Discriminant Analysis
Dynamic and Static Raman Spectroscopic Characterization Analysis of Dairy Products

Standardization of Spectroscopy

Raman Spectra of a Brand Milk Powder under Different Laser Power Conditions
Dynamic and Static Raman Spectroscopic Characterization
Analysis of Dairy Products

Standardization of Spectroscopy

\[ y_i = \frac{x_i - \bar{x}}{s} \]

\[ s = \sqrt{\frac{\sum_{i=1}^{n} (x_i - \bar{x})^2}{n-1}} \]
Rapid Identification of Food Quality and Safety Based on Quality Characteristic Analysis and Discriminant Algorithms

Standardization of Spectroscopy

Wavelet denoising
Standardization of Spectroscopy

Under the same test conditions, the average recognition rate without wavelet denoising is 93.18%.

Under the condition of bior2.4 wavelet basis, 99.70% of the total is achieved.

Raman spectra of yoghurt (brand aa, bb, cc)
Dynamic and Static Raman Spectroscopic Characterization
Analysis of Dairy Products

Standardization of Spectroscopy

The average recognition rate was 99.70% using principal component dimension reduction, and the operation efficiency is increased by more than 10%.
Dynamics and Static Raman Spectroscopic Characterization Analysis of Dairy Products

Multidimensional Spectral Analysis

\[ \Phi(v_1, v_2) = \frac{1}{m-1} \tilde{y}(v_1)^T \tilde{y}(v_2) \]

Raman Spectra of a Brand Milk Powder under Different Laser Intensities
Dynamic and Static Raman Spectroscopic Characterization Analysis of Dairy Products

Multidimensional Spectral Analysis

synchronous two-dimensional correlation Raman spectrum of the pure liquid milk product.
Dynamic and Static Raman Spectroscopic Characterization Analysis of Dairy Products

Multidimensional Spectral Analysis

synchronous two-dimensional correlation Raman spectrum of the low-fat liquid milk product.
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Multidimensional Spectral Analysis

(a) Bei-Yin-Mei milk powder, (b) Fei-He milk powder, (c) Mei-Su-Jia-Er milk powder, (d) Qi-Fu milk powder, (e) Que-Chao milk powder, and (F) Yi-Li milk powder.
Dynamic and Static Raman Spectroscopic Characterization
Analysis of Dairy Products

Intelligent Discriminant Analysis

Raman Spectra of Dairy Products

<table>
<thead>
<tr>
<th>Raman shift (cm⁻¹)</th>
<th>Assignment</th>
</tr>
</thead>
<tbody>
<tr>
<td>357</td>
<td>Lactose</td>
</tr>
<tr>
<td>424</td>
<td>Glucose</td>
</tr>
<tr>
<td>445</td>
<td>δ (C–C–C) + τ (C–O)</td>
</tr>
<tr>
<td>525</td>
<td>Glucose</td>
</tr>
<tr>
<td>598</td>
<td>δ (C–C–C) + τ (C–O)</td>
</tr>
<tr>
<td>645</td>
<td>δ (C–C–O)</td>
</tr>
<tr>
<td>711</td>
<td>ν (C–S)</td>
</tr>
<tr>
<td>763</td>
<td>δ (C–C–O)</td>
</tr>
<tr>
<td>877</td>
<td>δ (C–C–H) + δ (C–O–C)</td>
</tr>
<tr>
<td>950</td>
<td>δ (C–O–C) + δ (C–O–H) + ν (C–O)</td>
</tr>
<tr>
<td>1005</td>
<td>Ring-breathing (phenylalanine)</td>
</tr>
<tr>
<td>1065</td>
<td>ν (C–O) + ν (C–C) + δ (C–O–H)</td>
</tr>
<tr>
<td>1082</td>
<td>ν (C–O) + ν (C–C) + δ (C–O–H)</td>
</tr>
<tr>
<td>1121</td>
<td>ν (C–O) + ν (C–C) + δ (C–O–H)</td>
</tr>
<tr>
<td>1262</td>
<td>γ (CH2)</td>
</tr>
<tr>
<td>1303</td>
<td>τ (CH2)</td>
</tr>
<tr>
<td>1340</td>
<td>δ (C–H); ν (C–O)</td>
</tr>
<tr>
<td>1442</td>
<td>δ (CH2)</td>
</tr>
<tr>
<td>1555</td>
<td>δ (N–H); ν (C–N) Amide II</td>
</tr>
<tr>
<td>1654</td>
<td>ν (C=O) Amide I; ν (C=C)</td>
</tr>
<tr>
<td>1745</td>
<td>ν (C=O)ester</td>
</tr>
<tr>
<td>1785</td>
<td>ν₁ (CH₂)</td>
</tr>
<tr>
<td>2853</td>
<td>ν₁ (CH₂)</td>
</tr>
<tr>
<td>2900</td>
<td>ν₁ (CH₂)</td>
</tr>
<tr>
<td>2927</td>
<td>ν₁ (CH₂)</td>
</tr>
</tbody>
</table>

Vs – very strong; s – strong; m – medium; w – weak.

Raman Spectrum Attribution of Dairy Products
Dynamic and Static Raman Spectroscopic Characterization Analysis of Dairy Products

Intelligent Discriminant Analysis

Quality Control Chart of Dairy Products Based on Prior Knowledge (Peak Height 1307 cm\(^{-1}\))
Intelligent Discriminant Analysis

Discriminant of dairy products based on prior knowledge (peak height, peak area, peak ratio)

1. 1307 cm\(^{-1}\)
2. 1288 - 1319 cm\(^{-1}\)
3. 1337/1307 cm\(^{-1}\)
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Intelligent Discriminant Analysis

Classification and Discriminant of dairy products
Dynamic and Static Raman Spectroscopic Characterization Analysis of Dairy Products

Intelligent Discriminant Analysis

Dairy Product Classification and Discriminant Based on Machine Learning Algorithms (SVM)
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Intelligent Discriminant Analysis

Dairy Product Content analysis and Discriminant Based on BP Neural Network
04 Summary and Prospects for Further Work

- **Summary**: Constructing Rapid Inspection System
- **high-throughput technology**
Dynamic and Static Raman Spectroscopic Characterization Analysis of Dairy Products

Measure 1
Establishment of Quick Inspection Standard

Measure 2
Establishing Intelligent Discriminant Method

Measure 3
Complete spectral library

Measure 4
Developing High-throughput Technology
Thanks for your attention!