APLIKASI SPEKTROSKOPI INFRAMERAH DAN KEMOMETRIKA DALAM ANALISIS KEHALALAN PRODUK

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OUTLINE PRESENTASI

- Pendahuluan Analisis Halal
- Spektroskopi Inframerah
- Kemometrika
- Aplikasi Spektroskopi IR-kemometrika untuk analisis kehalalan produk
  - Sediaan Farmasi
  - Makanan

International Journal of
Molecular Sciences

MDPI

Review

The Application of Molecular Spectroscopy in Combination with Chemometrics for Halal Authentication Analysis: A Review

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check for updates

Abstract: Halal is an Arabic term used to describe any components allowed to be used in any products by Muslim communities. Halal food and halal pharmaceuticals are any food and pharmaceuticals which are safe and allowed to be consumed according to Islamic law (Shariah). Currently, in line

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Review on analytical methods for analysis of porcine gelatine in food and pharmaceutical products for halal authentication

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ARTICLE INFO

Keywords:
Porcine gelatine
Bovine gelatine
Halal authentication
Pharmaceutical
Peptide marker

ABSTRACT

Background: Gelatine is one of the components commonly used in food, cosmetics and pharmaceutical products due to its gelling properties. The most commonly used gelatines in those products are porcine and bovine gelatines. Unclear labelling and information regarding the actual sources of gelatines in products have become the main concern among societies in terms of religion and health aspects. Porcine gelatine (PG) is prohibited to be consumed by Muslim and Jewish and considered non-halal (and non-kosher) following some scholars of thought. While bovine gelatine (BG) is associated with certain diseases of bovine spongiform encephalopathy, as a consequence, there is a need to develop reliable methods for identifying gelatine sources in the products.
Scope and approach: This review highlighted some analytical methods including physico-chemical methods as

Locally Rooted, Globally Respected

www.ugm.ac.id

Review:

The Chemometrics Techniques in Combination with Instrumental Analytical Methods Applied in Halal Authentication Analysis

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Abstract: *Halal food is taken into account as any food permitted to be consumed by Muslim according to Syariah law. Due to the development of science and technology in which some new food components such as food additives have been synthesized and produced, some industries used non-halal components such as pig derivatives in food products to reduce the production cost. Non-halal components added in food products are difficult to detect visually due to the close similarity between non-halal ingredients and components present in food. As a consequence, some scientists developed and proposed some instrumental techniques like spectroscopy, chromatography and molecular biology-based methods for identification of non-halal components. Food matrix is very complex to be analyzed. Therefore, the signals obtained during chemical and biological analyses are very complex which are difficult to interpret. Fortunately, a statistical technique called with chemometrics can be used an alternative method to handle the complex data met during analysis of non-halal components. Chemometrics has been widely used in many aspects of analysis in many types of the sector. In this review, some chemometrics techniques used to treat responses obtained from instrumental measurements intended for analysis of non-halal components in food matrix were highlighted.*

Keywords: *chemometrics; non-halal component; authentication; classification; multivariate calibration*

INTRODUCTION TO HALAL ANALYSIS

- Halal authentication analysis is intended to confirm that the products (food, cosmetics, pharmaceuticals) are free-non halal-components
- The advanced technology in the industries has led to the use of non-halal components in the product.
  - *Pork*
  - *Lard*
  - *Porcine gelatines*
- Montowska and Pospiech (2010) reported that some food and pharmaceutical products available in the market may be labelled with incorrect or missing information related to ingredients sources.

Montowska, M., & Pospiech, E. (2010). Authenticity determination of meat and meat products on the protein and DNA basis. *Food Reviews International*, *27*(1), 84–100.

ANALYSIS OF NON-HALAL COMPONENT

Food Reviews International
Publication details, including instructions for authors and subscription information:
http://www.tandfonline.com/loi/lfri20

Analysis of Pig Derivatives for Halal Authentication Studies

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Non-halal components commonly found in food, cosmetics and pharmaceutical products are pig derivatives (lard, pork, porcine gelatin) and alcohol

- To comply with halal requirement, more stringent auditing/monitoring system is needed by Halal Authorities or Certification Bodies
- Reliable state-of-the-art scientific methods are required for analysis of non-halal components (e.g porcine origin, alcohol) in halal food
- Analytical techniques become major challenge for authentication of halal products

METHODS FOR HALAL AUTHENTICATION

- **Lard**
  - FTIR spectroscopy, especially combined with chemometrics (Lard, lipid based food)
  - GC-MS (certain fatty acids in lard)
  - Differential scanning calorimetry (Lard, lipid based food)
  - Electronic nose or fast gas chromatography (analysis aroma profile)
- **Pork**
  - Real-time PCR
  - Enzyme immunosorbent assay
- **Porcine Gelatin**
  - RT-PCR (DNA-based methods for analysis of porcine DNA and non-allowed meat DNA)
  - LC-MS (peptide profile)

METHODS FOR HALAL AUTHENTICATION

- *Screening/exploratory*
  - Differential scanning calorimetry (Lard, lipid based food)
  - Electronic nose or fast gas chromatography (analysis aroma profile)
  - FTIR spectroscopy
- *Confirmatory*
  - RT-PCR (DNA-based methods for analysis of porcine DNA and non-allowed meat DNA)
  - LC-MS-MS (peptide profile)
  - GC-MS (certain fatty acids as markers in lard)

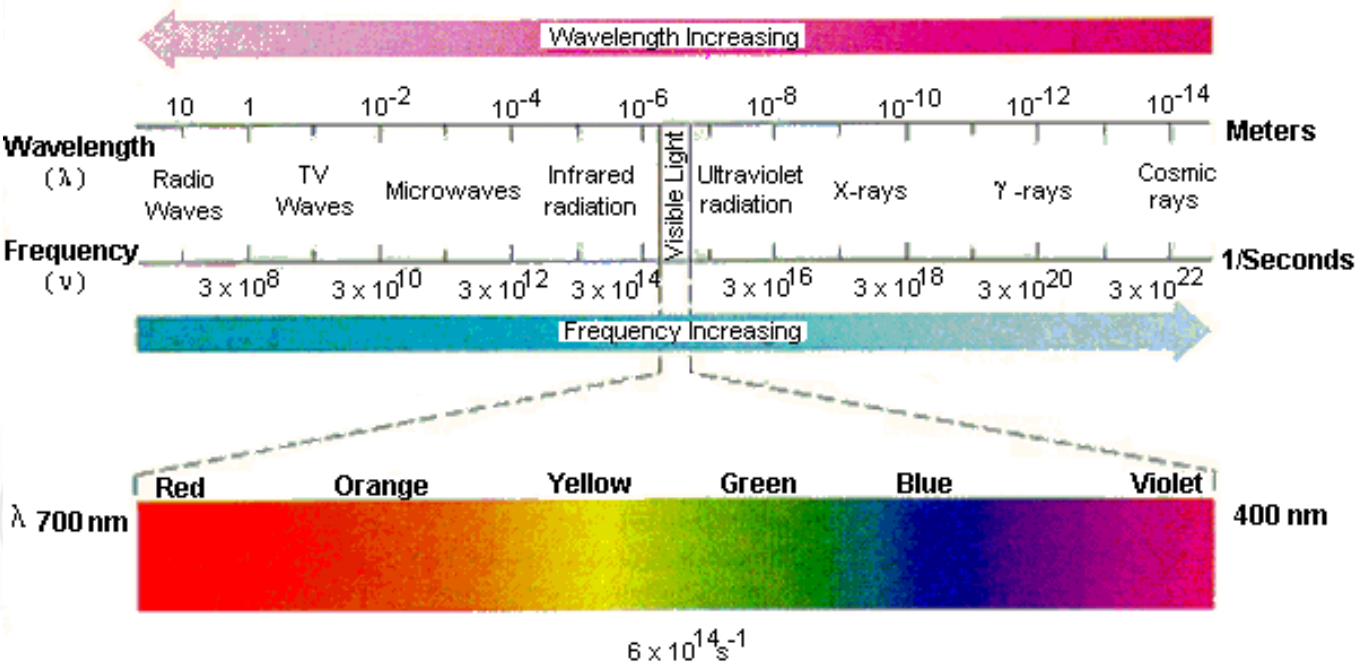
STANDARD METHODS

- Candidate of standard method
  - Lard: GC-MS
  - Pork: DNA based method
  - Gelatin: LC-MS/MS and PCR based methods
- To be standard methods, analytical techniques used must be:
  - Specific
  - Accurate
  - Precise
  - Sensitive
  - Robust

SPEKTROSKOPI INFRAMERAH

- Spektroskopi mempelajari interaksi antara radiasi elektromagnetik (EMR) dengan bahan (sampel)
- Jenis Spektroskopi
  - Spektroskopi sinar X
  - Spektroskopi UV-vis
  - Spektroskopi inframerah
  - Spektroskopi NMR
  - Spktrometri massa

RADIASI ELEKTROMAGNETIK

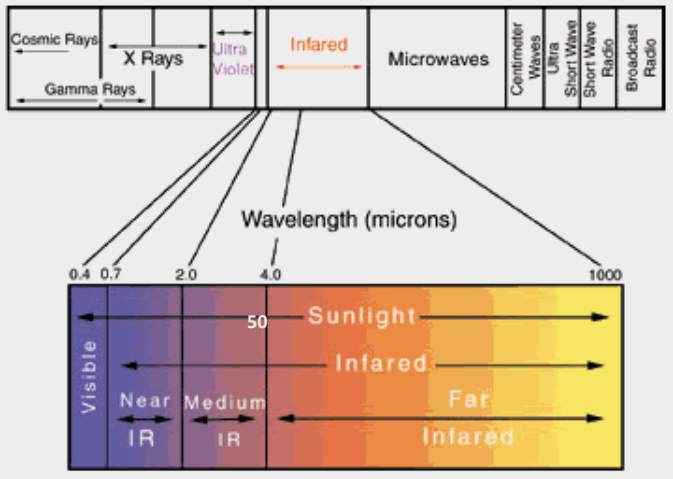


Infrared Spectroscopy

- **Infrared spectroscopy** (**IR spectroscopy** or Vibrational **Spectroscopy**) is the **spectroscopy** that deals with the **infrared** region of the electromagnetic spectrum, that is light with a longer wavelength and lower frequency than visible light.
- It covers a range of techniques, mostly based on absorption **spectroscopy**.

Infrared Radiation

- Frequencies - 12800 to 10 cm^{-1}
  - (cm^{-1} = wavenumbers)
- Divided into three Regions
  - Near : 12800 to 4000 cm^{-1}
  - Middle: 4000 to 400 cm^{-1}
  - Far: 400 to 10 cm^{-1}



INFRARED SPECTROSCOPY

IR spectroscopy is based on the interaction between EMR and matters (samples) in IR regions

FTIR spectroscopy

Rapid and sensitive
Non destructive
Ease in sample presentation
used for qualitative
quantitative analyses

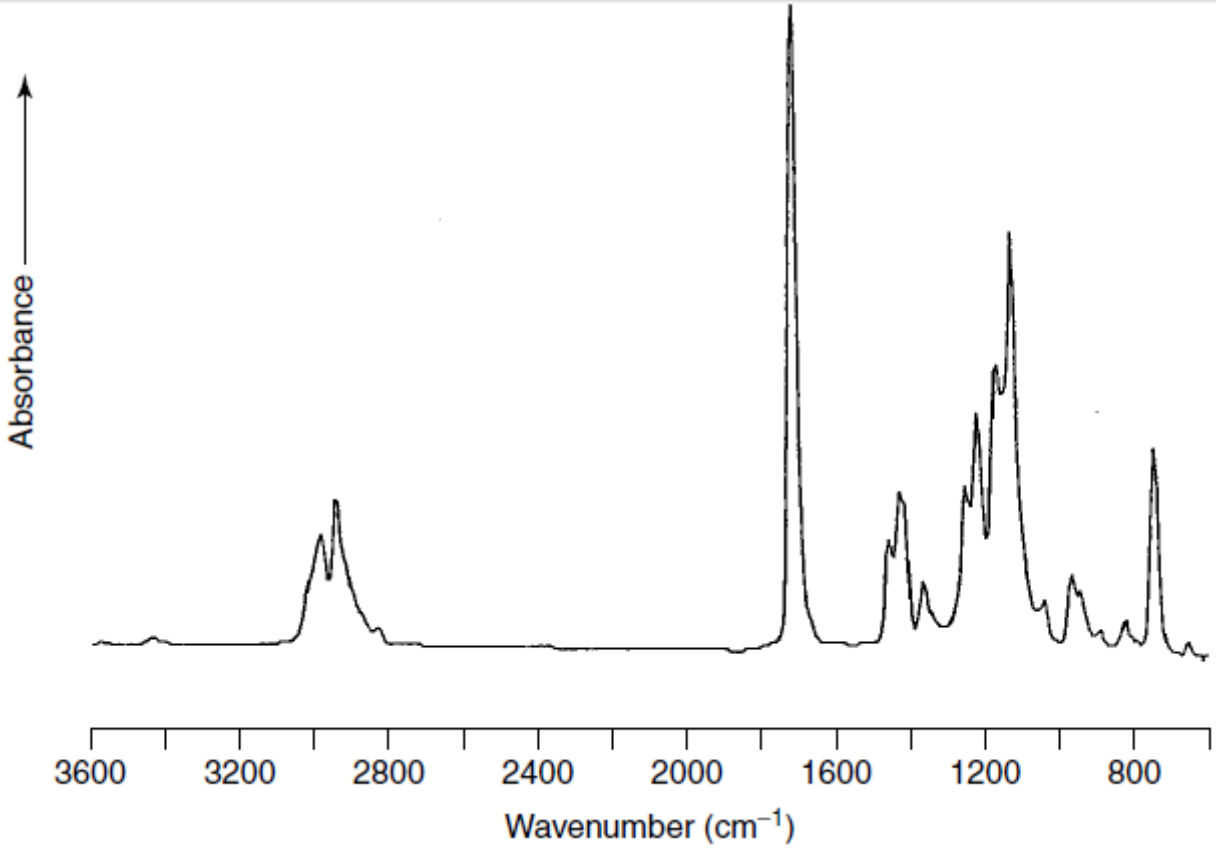
FINGER PRINT TECHNIQUE

Scanning Spektra IR

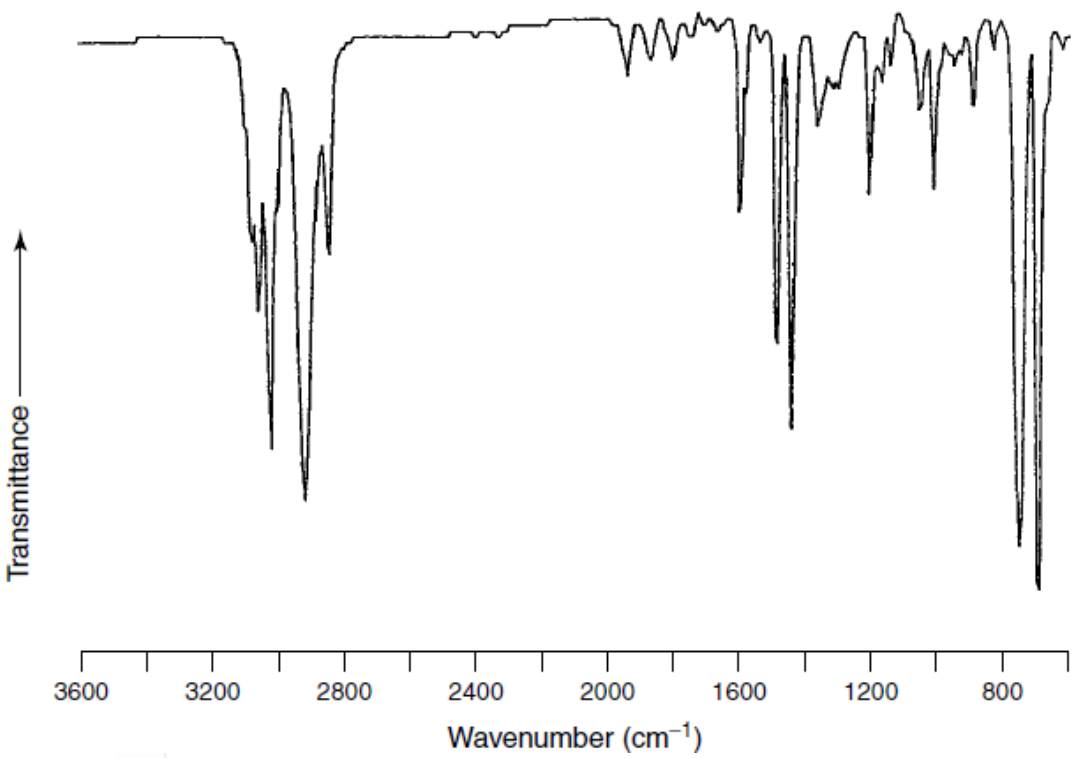
Absorbansi = Analisis kualitatif dan kuantitatif

Transmitans = Analisis kualitatif

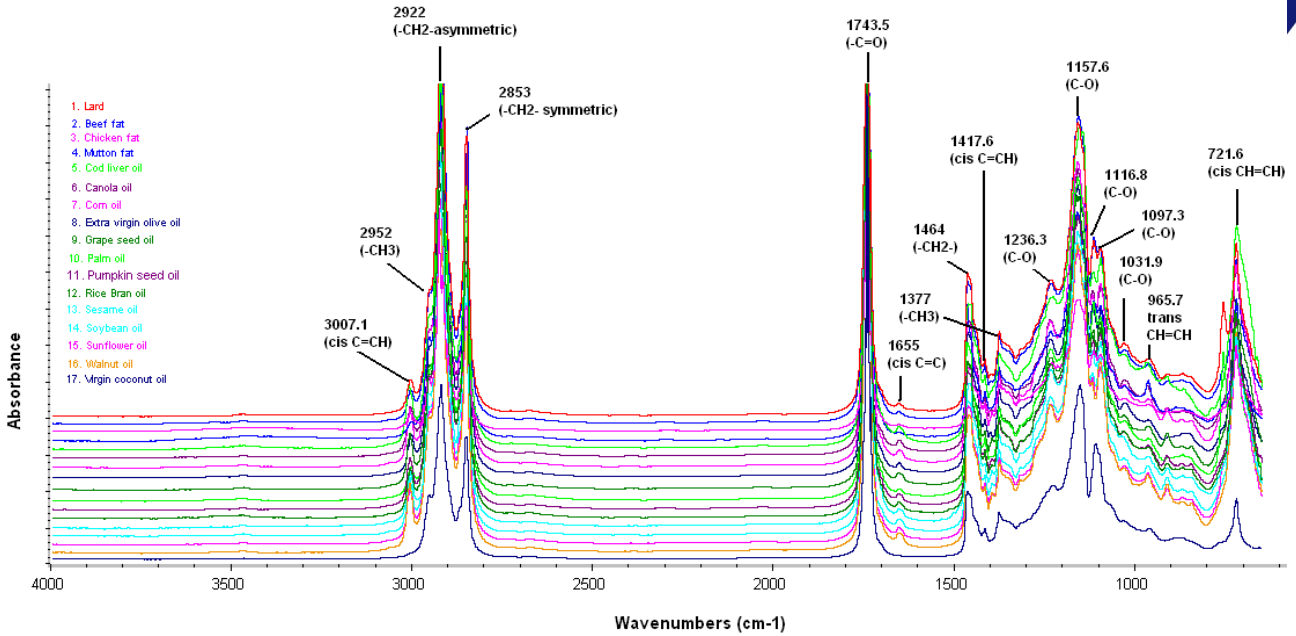
PEMINDAIAN SPEKTRA INFRAMERAH: ABSORBANSI



PEMINDAIAN SPEKTRA INFRAMERAH: TRANSMITANS



FTIR SPECTRA OF LARD AND OTHERS



Rohman et al. (2011): JAOCS

Jumlah Puncak (peak) /Bahu (shoulder)
Intensitas (absorbansi atau transmitans) puncak/bahu
Frekuensi eksak tiap puncak/bahu

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MINI REVIEW

The employment of Fourier transform infrared spectroscopy coupled with chemometrics techniques for traceability and authentication of meat and meat products

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ABSTRACT

Meat-based food such as meatball and sausages are important sources of protein needed for the human body. Due to different prices, some unethical producers try to adulterate high-price meat such as beef with lower priced meat like pork and rat meat to gain economical profits, therefore, reliable and fast analytical techniques should be developed, validated, and applied for meat traceability and authenticity. Some instrumental techniques have been applied for the detection of meat adulteration, mainly relied on DNA and protein using polymerase chain reaction and chromatographic methods, respectively. But, this method is time-consuming, needs a sophisticated instrument, involves complex sample preparation which make the method is not suitable for routine analysis. As a consequence, a simpler method based on spectroscopic principles should be continuously developed. Food samples are sometimes complex which resulted in complex chemical responses. Fortunately,

ARTICLE HISTORY

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KEYWORDS

FTIR spectroscopy; authentication analysis; chemometrics; meat; meat products

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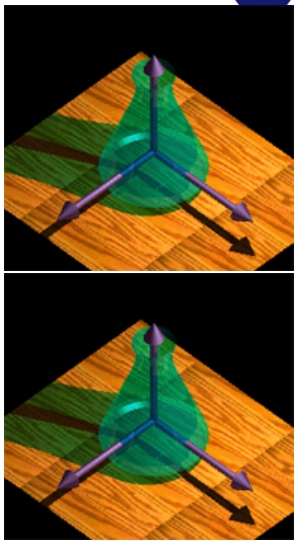
KEMOMETRIKA

- Kemometrika = Kimia + metrik
- Secara definisi: kemometrika adalah penggunaan ilmu statistika dan matematika untuk pengolahan data kimia
- Data kimia dapat berasal dari:
  - Kromatogram
  - Spektrum UV, IR, NMR dan sebagainya

CHEMOMETRICS

Chemometrics is the application of mathematical or statistical methods to chemical data.

The International Chemometrics Society (ICS): *Chemometrics is the science of relating measurements made on a chemical system or process to the state of the system via application of mathematical or statistical methods.*



Chemometrics research spans a wide area of different methods which can be applied in chemistry.
Chemometrics tries to build a bridge between the methods and their application in chemistry.

TEKNIK KEMOMETRIKA YANG UMUM DIGUNAKAN UNTUK ANALISIS HERBAL

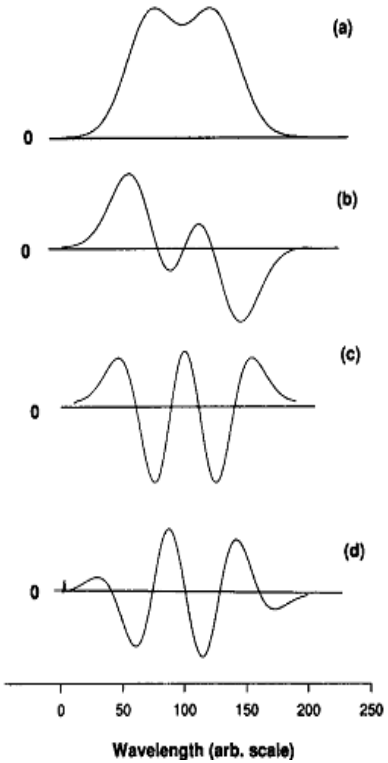
- Pengolahan data
  - Derivatisasi
- Pengelompokkan
  - Exploratory data analysis
  - Pengenalan pola tersupervisi (*Discriminant analysis*)
  - Pengenalan pola tidak tersupervisi (Cluster Analysis)
- Analisis Kuantitatif
  - Kalibrasi multivariat (Classical least square, SMLR, PCR dan PLS)

Pengolahan data: Derivatisasi

- Derivatisasi ini kebanyakan digunakan untuk mentransformasikan data Spektra (UV, IR)
- Tujuan: untuk lebih memisahkan puncak-puncak yang overlapping
- Beberapa *software* menyediakan fasilitas ini.

DERIVATIVE SPECTRA

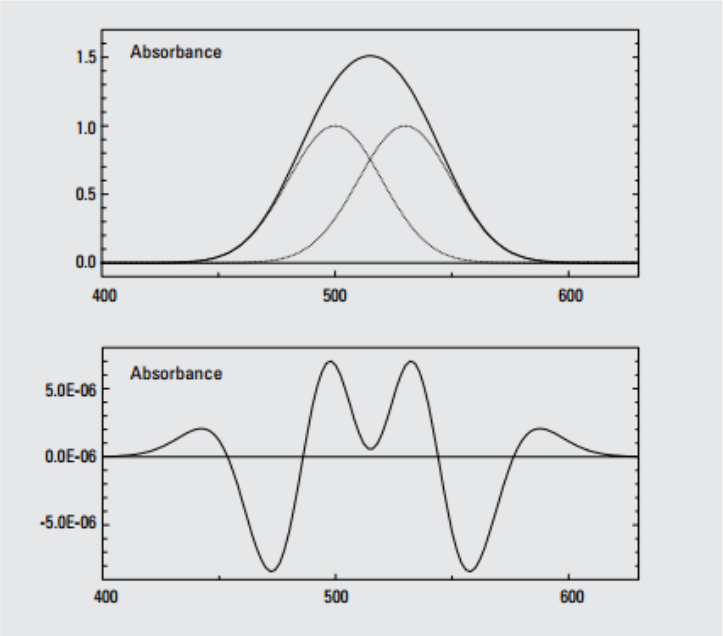
- A pair of overlapping Gaussian peaks (a), and the first- (b), second- (c), and third-order (d) derivative spectra.
- Derivative spectra can resolve the overlapping peaks.
- Sensitivity of derivative spectra was reduced



PROCESSING DATA: DERIVATIZATION

Advantage:
Derivative spectra will enhance the resolution among peaks, especially for overlapping peak → Quantitative analysis is more accurate.

Disadvantage:
Resulting spectra are difficult to interpret
sensitivity is sometimes lowered



EXAMPLE OF DERIVATIVE SPECTRA

Food Research International 43 (2010) 886–892

Contents lists available at ScienceDirect

Food Research International

journal homepage: www.elsevier.com/locate/foodres

Fourier transform infrared (FTIR) spectroscopy for analysis of extra virgin olive oil adulterated with palm oil

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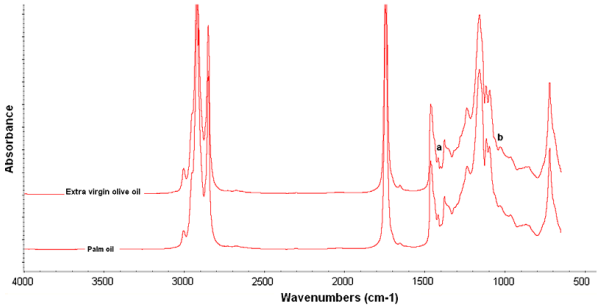
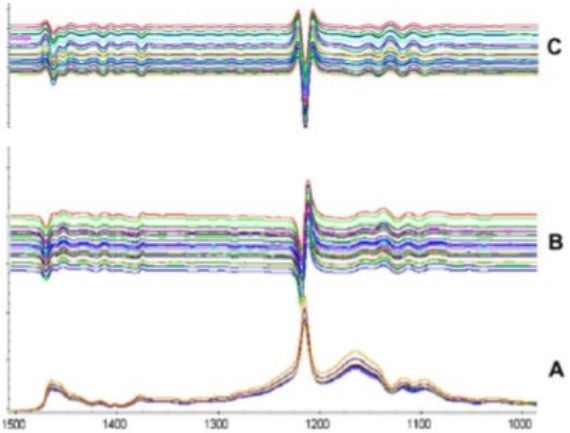


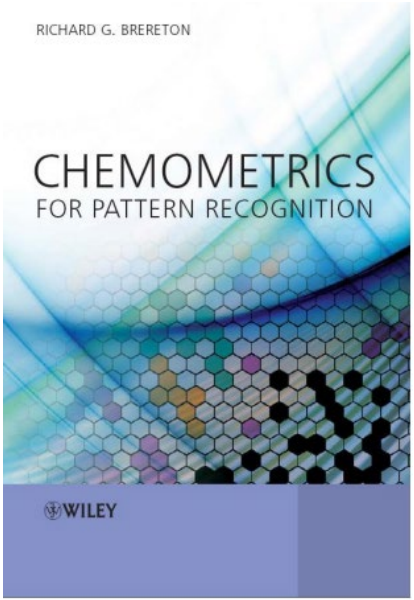
Fig. 1. FTIR spectra of extra virgin olive oil and palm oil at frequency of 4000–650 cm^{-1}.

Spectra	Equation	
	Calibration	Validation
Normal	$y = 1.000x - 0.089$	$y = 0.995x + 0.165$
1st derivative	$y = 1.001x - 0.146$	$y = 0.998x + 0.001$
2nd derivative	$y = 0.998x - 0.268$	$y = 0.971x + 0.635$
Normal	$y = 1.000x - 0.115$	$y = 0.993x + 0.211$
1st derivative	$y = 1.001x - 0.166$	$y = 0.999x - 0.057$
2nd derivative	$y = 1.004x - 0.518$	$y = 0.982x + 0.004$



PENGELOMPOKKAN (*CLASSIFICATION TECHNIQUE*)

- Untuk teknik pengelompokkan, ada 2 kelompok yaitu:
- Exploratory data analysis
- Unsupervised pattern recognition
  - Cluster analysis
- Supervised pattern recognition
  - Discriminant analysis



International Journal of Molecular Sciences

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The Application of Molecular Spectroscopy in Combination with Chemometrics for Halal Authentication Analysis: A Review

Abdul Rohman [1,2,*] and Anjar Windarsih [3]

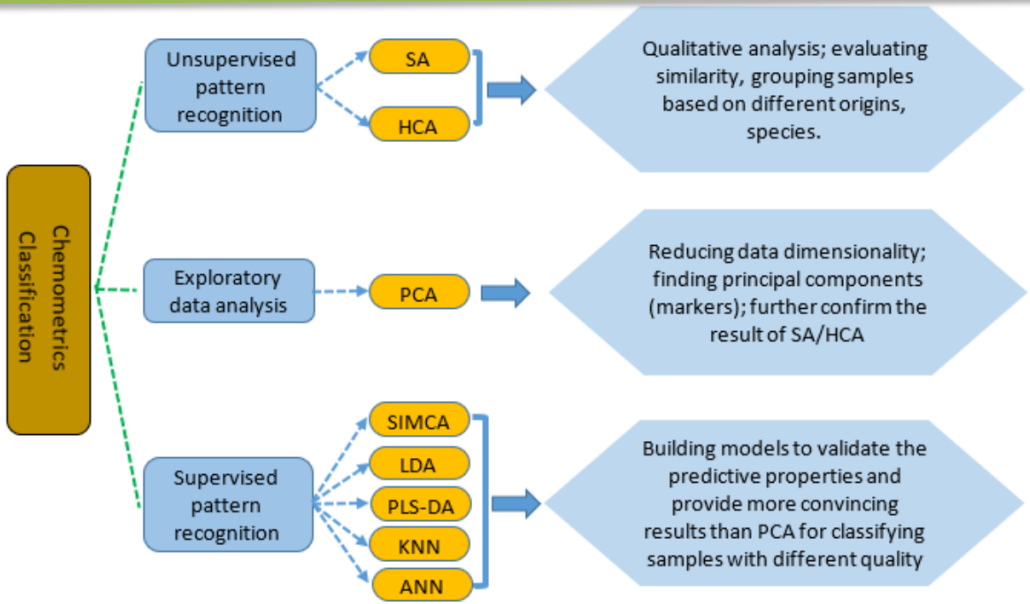

Figure 1. The chemometrics techniques widely applied for the classification of objects. SA = similarity analysis, HCA = hierarchical clustering analysis, PCA = principal component analysis, SIMCA = soft independent modeling of class analogy, LDA = linear discriminant analysis, PLS-DA = partial least squares discriminant analysis, KNN = k-nearest neighbors, and ANN = artificial neural networks [30].

PENGELOMPOKKAN DENGAN PCA

- *Principal Component analysis* (PCA) sebenarnya adalah suatu teknik pengurangan jumlah data (*data reduction*)
- Output PCA adalah mencari komponen utama (*principle component*) dari serangkaian data
- PC juga disebut dengan variabel tersembunyi (latent variables) karena sampel-sampel yang sama/mirip akan mempunyai nilai PC1 dan PC2, ..., PCn yang sama
- **Apa yang dimaksud dengan PC?**

PCA UNTUK PENGELOMPOKAN

J Am Oil Chem Soc (2011) 88:187–192
DOI 10.1007/s11746-010-1659-x

ORIGINAL PAPER

Differentiation of Lard From Other Edible Fats and Oils by Means of Fourier Transform Infrared Spectroscopy and Chemometrics

Yaakob B. Che Man · A. Rohman · T. S. T. Mansor

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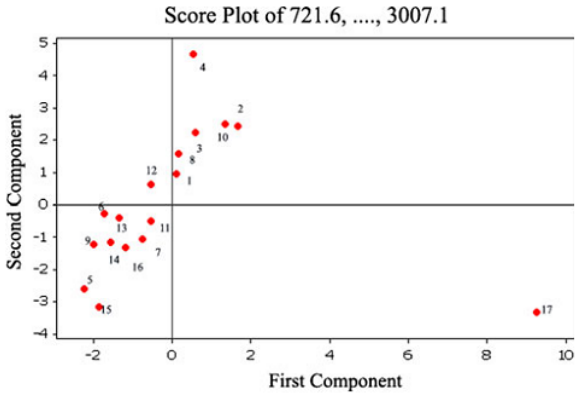
Abstract Fourier transform infrared (FTIR) spectra at mid infrared regions (4,000–650 cm^{-1}) of lard and 16 edible fats and oils were compared and differentiated. The economical point of views. The food industry prefers to blend lard with some vegetable oils to minimize production costs because lard or industrially modified lard can be



Principal component analysis (PCA)

A technique for reducing the amount of data when there is correlation present.

It is worth stressing that it is not a useful technique if the variables are uncorrelated.

The idea behind PCA is to find **principal components *Z1, Z2, . . . , Zn which are linear*** combinations of the original variables describing each specimen, *X1, X2, . . . , Xn, i.e.*

$$Z_1 = a_{11}X_1 + a_{12}X_2 + a_{13}X_3 + \cdots a_{1n}X_n$$
$$Z_2 = a_{21}X_1 + a_{22}X_2 + a_{23}X_3 + \cdots a_{2n}X_n$$
etc.

Principle components

- Creating a new set of variables in this way may seem a pointless exercise, since we obtain *n new variables in place of the n original ones, and hence* no reduction in the amount of data.

- However, the principal components are also chosen so that the PC1 (Z_1), *accounts for most of the variation* in the data set, the second (PC2), Z_2, *accounts for the next largest variation* and so on.
- Hence, when significant correlation occurs, the number of useful PCs is much less than the number of original variables.

LOADING PLOT: SUATU CATATAN

- Sudut antar vector menunjukkan bagaimana variabel-variabel ini berkorelasi satu sama lain.
  - Jika dua vector dekat satu dengan yang lain yang membentuk sudut sempit maka hal tersebut menunjukkan adanya korelasi yang positif antar dua variabel.
  - Jika antar variabel membentuk sudut mendekati 90^o, maka keduanya tidak berkorelasi
  - Jika antar vector variabel berpencar dan membentuk sudut yang dekat dengan 180^o maka menunjukkan keduanya berkorelasi negatif.

PCA BI-PLOT

- PCA bi-plot simply merge an usual PCA plot with a plot of loadings. The arrangement is like this:
  - Bottom axis: PC1 score.
  - Left axis: PC2 score.
  - Top axis: loadings on PC1.
  - Right axis: loadings on PC2.
- In other words, the left and bottom axes are of the PCA plot — use them to read PCA scores of the samples (dots). The top and right axes belong to the loading plot — use them to read how strongly each characteristic (vector) influence the principal components.

Aplikasi PCA untuk pengelompokan lemak babi

J Am Oil Chem Soc (2011) 88:187–192
DOI 10.1007/s11746-010-1659-x

ORIGINAL PAPER

Differentiation of Lard From Other Edible Fats and Oils by Means of Fourier Transform Infrared Spectroscopy and Chemometrics

Yaakob B. Che Man · A. Rohman · T. S. T. Mansor

Di artikel ini digunakan dua kemometrika:
PCA
Cluster Analysis

Received: 3 May 2010 / Accepted: 20 July 2010 / Published online: 13 August 2010
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Abstract Fourier transform infrared (FTIR) spectra at mid infrared regions (4,000–650 cm^{-1}) of lard and 16 edible fats and oils were compared and differentiated. The chemometrics of principal component analysis and cluster analysis (CA) was used for such differentiation using FTIR spectra intensities of evaluated fats and oils. With PCA, an "eigenvalue" of about 90% was achieved using four principal components (PCs) of variables (FTIR spectra absorbances at the selected frequency regions). PC1 economical point of views. The food industry prefers to blend lard with some vegetable oils to minimize production costs because lard or industrially modified lard can be mixed efficiently with vegetable oils to produce cost-effective margarines, shortenings, and other oil-based foods. From a religious perspective, the presence of lard in any food products precludes consumption by Muslims [1, 2]. Therefore, there is a great demand for rapid and reliable techniques for lard differentiation and classifica-

PCA pengelompokkan lemak Babi

Karena unit variabel sama, gunakan matriks covariance

Table 2 Peak intensities (absorbances) for each frequency in lard and other edible fats and oils

No	Oils	Frequency							
		721.6	868.3	965.7	1,031.9	1,097.3	1,116.8	1,157.6	1,236.3
1	Lard	0.986 ± 0.02	0.246 ± 0.09	0.334 ± 0.00	0.413 ± 0.00	0.966 ± 0.01	0.973 ± 0.01	1.654 ± 0.03	0.755 ± 0.02
2	Beef	0.987 ± 0.11	0.236 ± 0.10	0.397 ± 0.01	0.387 ± 0.16	0.928 ± 0.03	0.969 ± 0.02	1.583 ± 0.44	0.753 ± 0.15
3	Chicken	0.946 ± 0.02	0.244 ± 0.00	0.325 ± 0.13	0.406 ± 0.00	0.932 ± 0.01	0.990 ± 0.01	1.649 ± 0.85	0.762 ± 0.02
4	Mutton	0.683 ± 0.14	0.211 ± 0.11	0.389 ± 0.01	0.374 ± 0.00	0.869 ± 0.36	0.943 ± 0.12	1.470 ± 0.06	0.685 ± 0.29
5	CLO	1.134 ± 0.01	0.365 ± 0.00	0.437 ± 0.00	0.000 ± 0.00	0.967 ± 0.01	0.896 ± 0.00	1.630 ± 0.89	0.809 ± 0.00
6	Canola	1.068 ± 0.02	0.261 ± 0.12	0.401 ± 0.00	0.428 ± 0.00	0.963 ± 0.00	0.933 ± 0.01	1.609 ± 0.01	0.763 ± 0.00
7	Corn	1.076 ± 0.01	0.255 ± 0.11	0.375 ± 0.22	0.437 ± 0.00	0.990 ± 0.01	0.922 ± 0.11	1.661 ± 0.02	0.789 ± 0.00
8	EVOO	0.981 ± 0.18	0.247 ± 0.03	0.316 ± 0.17	0.415 ± 0.05	0.930 ± 0.16	0.964 ± 0.18	1.604 ± 0.38	0.764 ± 0.15
9	Grape seed	1.091 ± 0.02	0.260 ± 0.16	0.382 ± 0.25	0.441 ± 0.00	0.993 ± 0.03	0.918 ± 0.29	1.652 ± 0.35	0.787 ± 0.12
10	Palm	0.929 ± 0.01	0.237 ± 0.00	0.310 ± 0.08	0.397 ± 0.00	0.946 ± 0.00	1.012 ± 0.00	1.665 ± 0.02	0.769 ± 0.00
11	Pumpkin seed	1.085 ± 0.02	0.255 ± 0.28	0.358 ± 0.19	0.432 ± 0.00	0.986 ± 0.01	0.939 ± 0.01	1.612 ± 0.02	0.777 ± 0.01
12	Rice Bran	0.975 ± 0.02	0.247 ± 0.13	0.348 ± 0.21	0.429 ± 0.22	0.923 ± 0.02	0.923 ± 0.02	1.575 ± 0.05	0.767 ± 0.31
13	Sesame	1.012 ± 0.04	0.256 ± 0.09	0.359 ± 0.20	0.454 ± 0.16	0.953 ± 0.02	0.906 ± 0.02	1.589 ± 0.08	0.783 ± 0.01
14	Soybean	1.111 ± 0.01	0.266 ± 0.15	0.397 ± 0.00	0.430 ± 0.09	1.009 ± 0.45	0.919 ± 0.01	1.641 ± 0.73	0.772 ± 0.42
15	Walnut	1.166 ± 0.02	0.277 ± 0.15	0.418 ± 0.00	0.451 ± 0.15	1.026 ± 0.00	0.907 ± 0.07	1.618 ± 0.02	0.791 ± 0.01
16	Sunflower	1.116 ± 0.01	0.260 ± 0.14	0.374 ± 0.02	0.431 ± 0.21	1.002 ± 0.07	0.911 ± 0.06	1.598 ± 0.12	0.773 ± 0.05
17	VCO	0.767 ± 0.01	0.268 ± 0.13	0.375 ± 0.00	0.460 ± 0.18	1.429 ± 0.01	0.000 ± 0.00	2.187 ± 1.25	0.000 ± 0.00

Lanjutan data absorbansi

No	Oils	Frequency							
		1,377.2	1,417.6	1,464.7	1,654.7	1,743.5	2,852.8	2,922	3,007.1
1	Lard	0.471 ± 0.02	0.328 ± 0.01	0.796 ± 0.01	0.076 ± 0.00	2.633 ± 1.18	1.555 ± 0.04	2.015 ± 1.89	0.217 ± 0.00
2	Beef	0.51 ± 0.11	0.342 ± 0.33	0.916 ± 0.89	0.069 ± 0.01	2.529 ± 2.21	2.069 ± 0.52	2.554 ± 1.21	0.152 ± 0.01
3	Chicken	0.465 ± 0.03	0.319 ± 0.01	0.770 ± 0.01	0.076 ± 0.01	2.698 ± 1.91	1.543 ± 0.02	2.214 ± 1.71	0.192 ± 0.01
4	Mutton	0.382 ± 0.05	0.267 ± 0.03	0.706 ± 0.29	0.061 ± 0.00	2.199 ± 1.49	1.544 ± 0.35	2.275 ± 0.03	0.106 ± 0.06
5	CLO	0.483 ± 0.00	0.367 ± 0.00	0.736 ± 0.00	0.112 ± 0.00	2.435 ± 0.10	1.300 ± 0.01	1.875 ± 0.23	0.291 ± 0.00
6	Canola	0.472 ± 0.01	0.333 ± 0.00	0.768 ± 0.01	0.099 ± 0.00	2.204 ± 0.25	1.371 ± 0.02	1.973 ± 0.03	0.283 ± 0.00
7	Corn	0.499 ± 0.00	0.347 ± 0.00	0.775 ± 0.00	0.092 ± 0.00	2.492 ± 0.13	1.352 ± 0.01	1.960 ± 0.02	0.310 ± 0.00
8	EVOO	0.489 ± 0.11	0.324 ± 0.20	0.815 ± 0.30	0.078 ± 0.03	2.497 ± 0.74	1.545 ± 0.35	2.170 ± 0.83	0.235 ± 0.09
9	Grapeseed	0.493 ± 0.08	0.348 ± 0.17	0.763 ± 0.27	0.096 ± 1.02	2.479 ± 0.18	1.305 ± 0.01	1.835 ± 0.04	0.338 ± 0.00
10	Palm	0.488 ± 0.00	0.330 ± 0.00	0.818 ± 0.00	0.062 ± 0.01	2.576 ± 0.25	1.674 ± 0.02	2.476 ± 0.10	0.174 ± 0.00
11	Pumpkin seed	0.486 ± 0.00	0.339 ± 0.00	0.773 ± 0.01	0.088 ± 0.00	2.686 ± 0.11	1.409 ± 0.02	2.085 ± 0.08	0.287 ± 0.00
12	Rice Bran	0.486 ± 0.05	0.325 ± 0.02	0.777 ± 0.03	0.080 ± 0.00	2.459 ± 0.44	1.412 ± 0.06	2.084 ± 0.13	0.248 ± 0.01
13	Sesame	0.463 ± 0.01	0.330 ± 0.15	0.746 ± 0.02	0.088 ± 0.01	2.427 ± 0.11	1.326 ± 0.05	2.007 ± 0.10	0.282 ± 0.00
14	Soybean	0.466 ± 0.05	0.341 ± 0.01	0.760 ± 0.01	0.094 ± 0.00	2.463 ± 0.31	1.326 ± 0.03	1.931 ± 0.85	0.323 ± 0.14
15	Walnut	0.485 ± 0.02	0.359 ± 0.00	0.744 ± 0.01	0.105 ± 0.00	2.750 ± 0.15	1.222 ± 0.02	1.718 ± 0.07	0.378 ± 0.01
16	Sunflower	0.486 ± 0.03	0.341 ± 0.02	0.757 ± 0.04	0.094 ± 0.00	2.674 ± 0.32	1.307 ± 0.08	1.863 ± 0.15	0.328 ± 0.02
17	VCO	0.577 ± 0.00	0.375 ± 0.00	0.836 ± 0.00	0.000 ± 0.00	3.021 ± 1.52	1.560 ± 0.02	2.303 ± 0.06	0.000 ± 0.00

Hasil PCA dengan Minitab

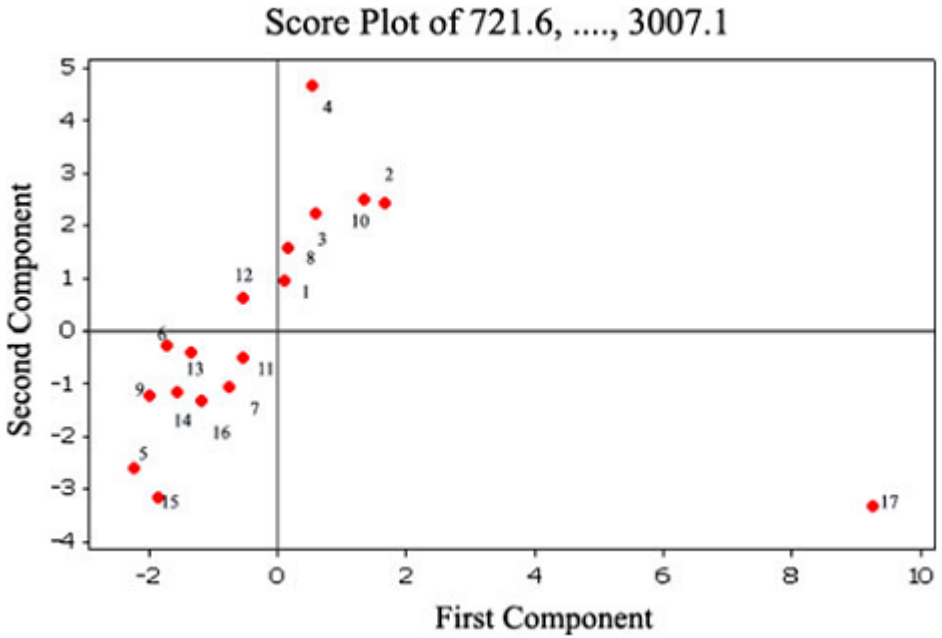


Fig. 2 The score plot for the first two principal components (PC) for 17 studied edible fats and oils: *1* Lard, *2* beef fat, *3* chicken fat, *4* mutton fat, *5* cod liver oil, *6* canola oil, *7* corn oil, *8* extra virgin olive oil, *9* grape seed oil, *10* palm oil, *11* pumpkin seed oil, *12* rice bran oil, *13* sesame oil, *14* soybean oil, *15* walnut oil, *16* sunflower oil, *17* virgin coconut oil

Cluster Analysis

- Cluster analysis (CA) meupakan teknik pengelompokkan sampel
- Sebagaimana dengan PCA, cluster analysis termasuk unsupervised pattern recognition
- CA membagi kelompok obyek, sehingga obyek yang sama akan masuk pada kelas/kelompok yang sama
- Parameter yang digunakan adalah Jarak Euclidean

Euclidian Distance

- Jarak Euclidean dirumuskan dengan:

$$d = \sqrt{(x_1 - y_1)^2 + (x_2 - y_2)^2 + \cdots + (x_n - y_n)^2}$$

- Dua buah sampel yang mempunyai jarak Euclidean yang dekat menunjukkan kemiripan
- Semakin kecil jaraknya → semakin mirip → masuk dalam kelompok yang sama

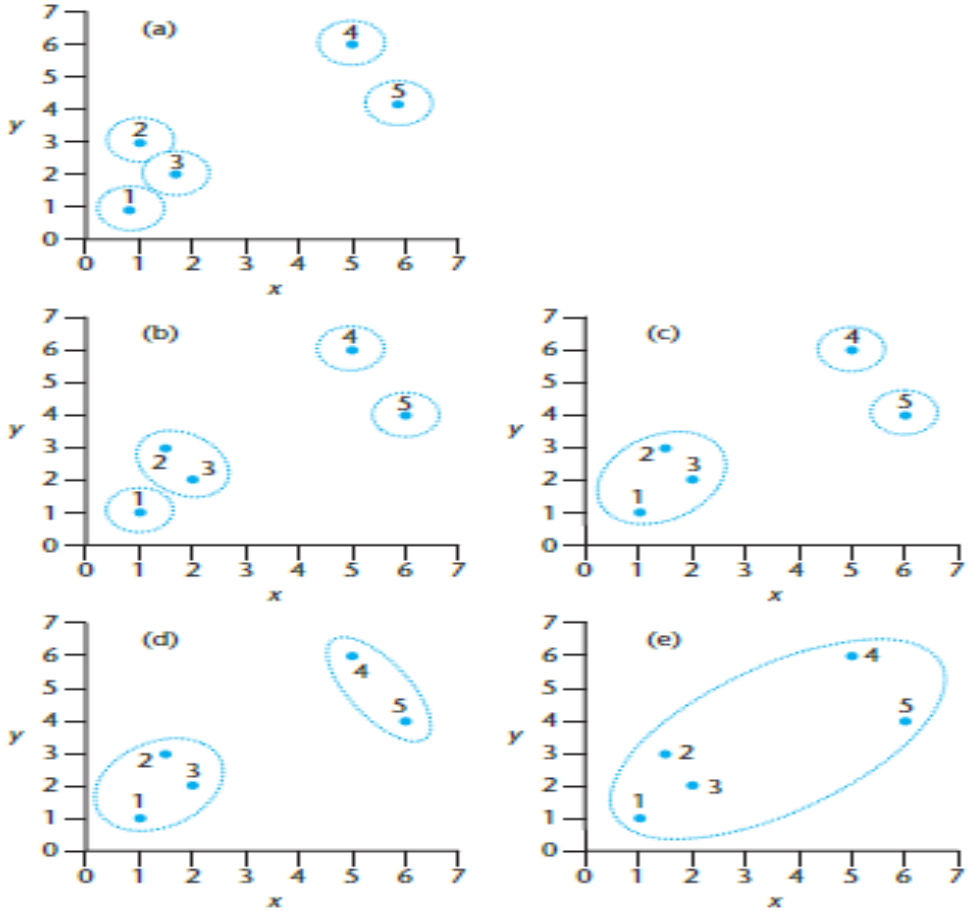
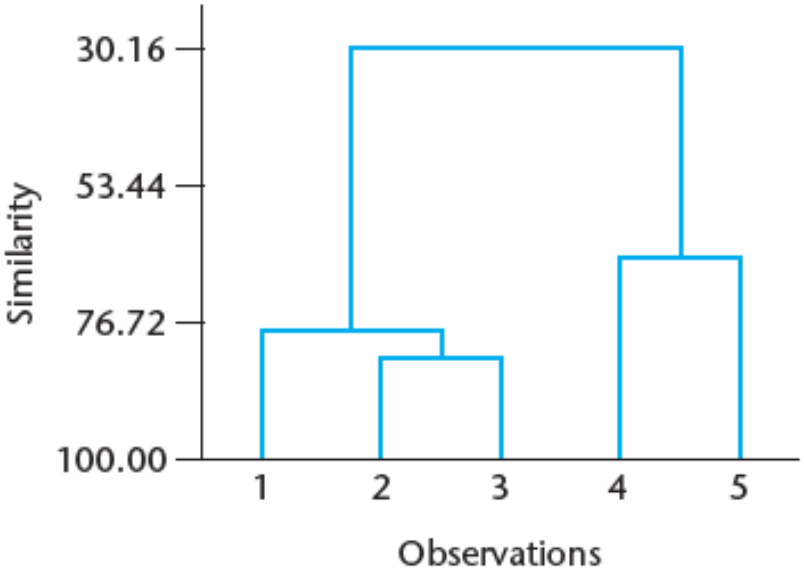


Figure 8.6 Stages in clustering: the dotted lines enclose clusters.

Dendrogram illustrating the stages of clustering



DISCRIMINANT ANALYSIS

- PCA dan Cluster analysis → Unsupervised pattern recognition
- Discriminant Analysis → Supervised pattern recognition
  - Tujuan metode *supervised pattern recognition* adalah untuk menggunakan objek-objek ini untuk menemukan suatu aturan meletakkan suatu objek baru yang kelompoknya tidak diketahui ke dalam kelompok yang benar (diketahui dengan pasti).

DISCRIMINANT ANALYSIS

- The starting point of linear discriminant analysis (LDA) is to find a linear discriminant function (LDF), *Y*, which is a linear combination of the original measured variables:

$$Y = a1X1 + a2X2 + \ldots\ldots + anXn$$

  - The original *n* measurements for each object are combined into a single value of *Y (similar to linear regression)*.
  - The coefficients are chosen in such a way that *Y* reflects the difference between groups as much as possible: objects in the same group will have similar values of *Y* and objects in different groups will have very different values of *Y*.
  - Thus the LDF provides a means of discriminating between the two groups

Aplikasi Spektroskopi IR-kemometrika untuk analisis kehalalan produk

- Kombinasi kemometrika dengan menggunakan variable nilai absorbansi pada bilangan gelombang tertentu
- Optimasi bilangan gelombang, jenis spektra dan kemometrika yang digunakan
- Aplikasi Spektroskopi IR-kemometrika untuk analisis kehalalan produk
  - Sediaan Farmasi
  - Makanan

OPTIMASI FTIR SPEKTRA-KEMOMETRIKA UNTUK ANALISIS KUANTITATIF

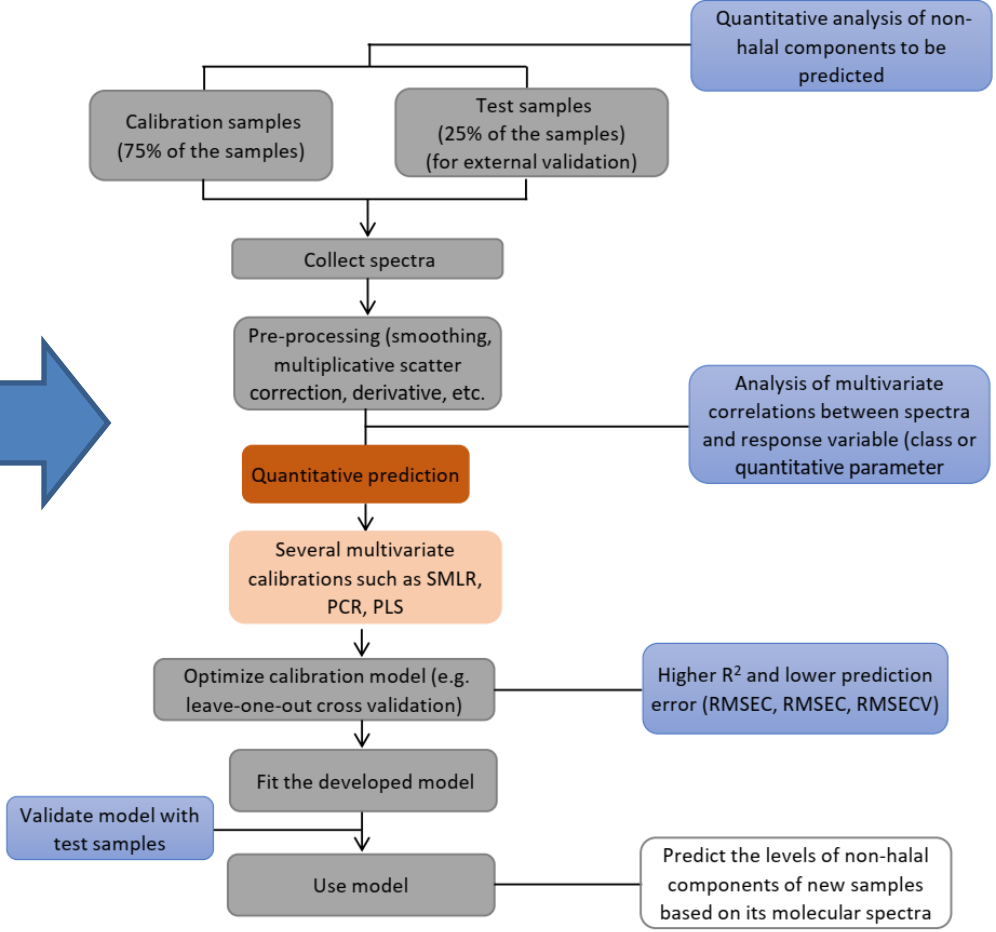


Figure 2. Scheme of quantitative analysis of non-halal components in food and pharmaceutical products assisted by multivariate calibration [42].

Differentiation of Lard From Other Edible Fats and Oils by Means of Fourier Transform Infrared Spectroscopy and Chemometrics

Yaakob B. Che Man · A. Rohman · T. S. T. Mansor

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Abstract Fourier transform infrared (FTIR) spectra at mid infrared regions (4,000–650 cm^{-1}) of lard and 16 edible fats and oils were compared and differentiated. The chemometrics of principal component analysis and cluster analysis (CA) was used for such differentiation using FTIR economical point of views. The food industry prefers to blend lard with some vegetable oils to minimize production costs because lard or industrially modified lard can be mixed efficiently with vegetable oils to produce cost-effective margarines, shortenings, and other oil-based

ANALYSIS OF LARD IN COSMETICS

J Am Oil Chem Soc (2012) 89:1537–1543
DOI 10.1007/s11746-012-2052-8

ORIGINAL PAPER

Quantitative Analysis of Lard in Cosmetic Lotion Formulation Using FTIR Spectroscopy and Partial Least Square Calibration

Endang Lukitaningsih · Miftahus Sa'adah · Purwanto · Abdul Rohman

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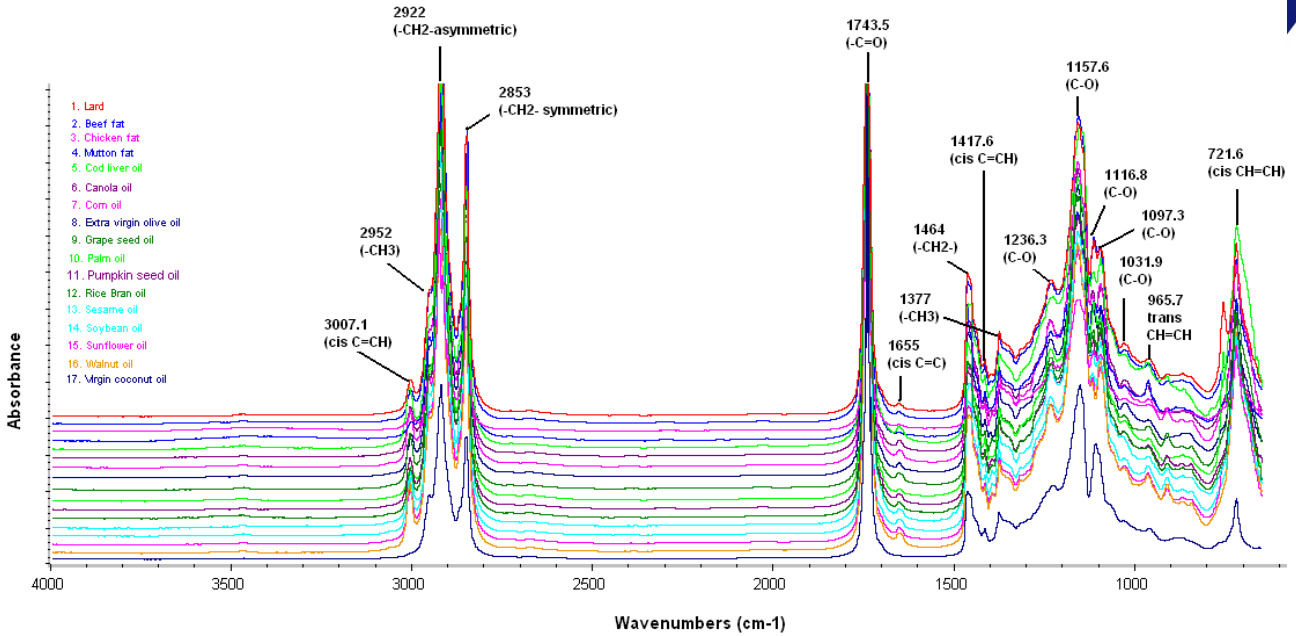
© AOCS 2012

Abstract Fourier transform infrared (FTIR) spectroscopy in combination with chemometrics of partial least squares (PLS) has been optimized for rapid determination of lard in a binary mixture with palm oil in a cosmetic lotion formulation. Lard, palm oil, and a binary mixture were

Introduction

In recent years, the use of personal care products in the form of cream and lotion cosmetic products has increased tremendously [1]. Human exposure to cosmetic formula-

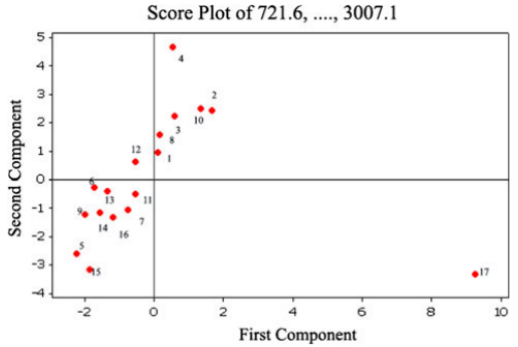
FTIR SPECTRA OF LARD AND OTHERS

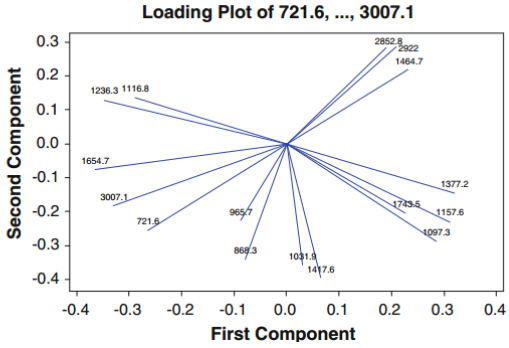


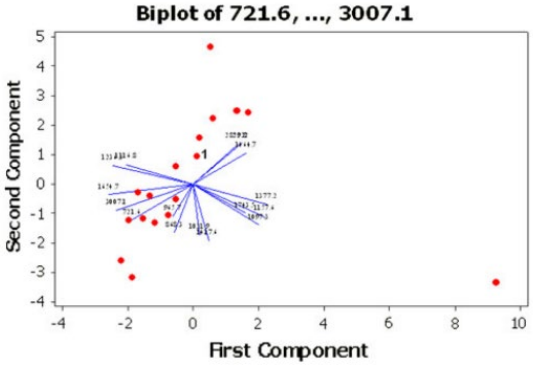
Rohman et al. (2011): JAOCS

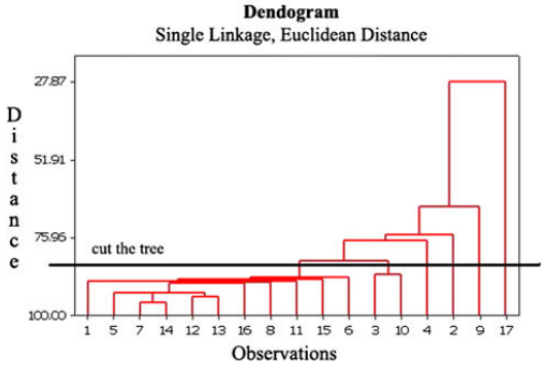
Jumlah Puncak (peak) /Bahu (shoulder)
Intensitas (absorbansi atau transmitans) puncak/bahu
Frekuensi eksak tiap puncak/bahu

CLASSIFICATION OF LARD AND OTHERS









1 Lard, 2 beef fat, 3 chicken fat, 4 mutton fat, 5 cod liver oil, 6 canola oil, 7 corn oil, 8 extra virgin olive oil, 9 grape seed oil, 10 palm oil, 11 pumpkin seed oil, 12 rice bran oil, 13 sesame oil, 14 soybean oil, 15 walnut oil, 16 sunflower oil, 17 virgin coconut oil

AUTHENTICATION OF HALAL MEAT USING FTIR SPECTROSCOPY

Meat adulterant	Meat adulterated	Meat-based products	Chemometrics	Wavenumbers (cm^{-1})	Results	References
Pork	Beef	Beef jerkys (dendeng)	LDA	Whole mid IR region (4,000–650)	LDA model could classify and predict the adulteration of Beef jerkys with pork, allowing 100% accuracy of the sample tested.	[39]
Pork offal (PO)	Beef offal (BO)	Fresh meat	SIMCA, LDA	1,002–1,240, 1,700–1,714, and 1,764–1,795 (BO) and 1,105–1,182 (PO).	SIMCA with mean-centered data could provide best model for the identification of BO, while LDA using non-scaled spectra offered best performance in classifying of PO	[40]
Pork	Beef	The mixture of beef-pork	PLS-Kernel calibration	Absorbance ratios of $A_{1,654\ cm^{-1}}/A_{1,745\ cm^{-1}}$, $A_{1,540\ cm^{-1}}/A_{1,745\ cm^{-1}}$, and $(A_{1,395\ cm^{-1}} + A_{1,450\ cm^{-1}})/ A_{1,175\ cm^{-1}}$	PLS-kernel calibration could predict the levels of pork in the mixture of pork-beef	[41]
Pork	Minced beef	Pork-beef fillet	PLSR	3,200–800 cm^{-1}	PLSR could predict the levels of pork with RMSEC of 4.88%, RMSEP of 9.45% and RMSECV of 10.30%	[42]
Pork	Beef	Ham sausages	PLSDA	Whole mid IR region (4,000–650)	PLSDA with standard normal variate treatment could classify halal (beef) sausage with sensitivity and specificity of 0.913 and 0.929.	[43]
Pork	Beef	Beef Meatballs	PLSR	1,200–1,000 cm^{-1},	PLSR could predict pork in beef meatballs with R^2 for	

AUTHENTICATION OF HALAL MEAT USING FTIR SPECTROSCOPY

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MINI REVIEW

The employment of Fourier transform infrared spectroscopy coupled with chemometrics techniques for traceability and authentication of meat and meat products

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ABSTRACT

Meat-based food such as meatball and sausages are important sources of protein needed for the human body. Due to different prices, some unethical producers try to adulterate high-price meat such as beef with lower priced meat like pork and rat meat to gain economical profits, therefore, reliable and fast analytical techniques should be developed, validated, and applied for meat traceability and authenticity. Some instrumental techniques have been applied for the detection of meat adulteration, mainly relied on DNA and protein using polymerase chain reaction and chromatographic methods, respectively. But, this method is time-consuming, needs a sophisticated instrument, involves complex sample preparation which make the method is not suitable for routine analysis. As a consequence, a simpler method based on spectroscopic principles should be continuously developed. Food samples are sometimes complex which resulted in complex chemical responses. Fortunately,

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KEYWORDS

FTIR spectroscopy; authentication analysis; chemometrics; meat; meat products

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ANALYSIS OF NON-HALAL MEAT

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Analysis of lard in meatball broth using Fourier transform infrared spectroscopy and chemometrics

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ABSTRACT

Meatball is one of the favorite foods in Indonesia. For the economic reason (due to the price difference), the substitution of beef meat with pork can occur. In this study, FTIR spectroscopy in combination with chemometrics of partial least square (PLS) and principal component analysis (PCA) was used for analysis of pork fat (lard) in meatball broth. Lard in meatball broth was quantitatively determined at wavenumber region of 1018–1284 cm^{-1}. The coefficient of determination (R^2) and root mean square error of calibration (RMSEC) values obtained were 0.9975 and 1.34% (v/v), respectively. Furthermore, the classification of lard and beef fat in meatball broth as well as in commercial samples was performed at wavenumber region of 1200–1000 cm^{-1}. The results showed that FTIR spectroscopy coupled with chemometrics can be used for quantitative analysis and classification of lard in meatball broth for Halal verification studies. The developed method is simple in operation, rapid and not involving extensive sample preparation.

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Analysis of pork adulteration in beef meatball using Fourier transform infrared (FTIR) spectroscopy

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Beef meatball
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Partial least square (PLS)

ABSTRACT

Meatball is one of the favorite foods in Indonesia. The adulteration of pork in beef meatball is frequently occurring. This study was aimed to develop a fast and non destructive technique for the detection and quantification of pork in beef meatball using Fourier transform infrared (FTIR) spectroscopy and partial least square (PLS) calibration. The spectral bands associated with pork fat (PF), beef fat (BF), and their mixtures in meatball formulation were scanned, interpreted, and identified by relating them to those spectroscopically representative to pure PF and BF. For quantitative analysis, PLS regression was used to develop a calibration model at the selected fingerprint regions of 1200–1000 cm^{-1}. The equation obtained for the relationship between actual PF value and FTIR predicted values in PLS calibration model was $y = 0.990x + 0.004$, with coefficient of determination (R^2) and root mean square error of calibration are 0.999 and 0.442, respectively. The PLS calibration model was subsequently used for the prediction of independent samples using laboratory made meatball samples containing the mixtures of BF and PF. Using 4 principal components, root mean square error of prediction is 0.742. The results showed that FTIR spectroscopy can be used for the detection and quantification of pork in beef meatball formulation for Halal verification purposes.

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The employment of FTIR spectroscopy in combination with chemometrics for analysis of rat meat in meatball formulation

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Partial least square
Principal component analysis
Rat meat

ABSTRACT

For Indonesian community, meatball is one of the favorite meat food products. In order to gain economical benefits, the substitution of beef meat with rat meat can happen due to the different prices between rat meat and beef. In this present research, the feasibility of FTIR spectroscopy in combination with multivariate calibration of partial least square (PLS) was used for the quantitative analysis of rat meat in the binary mixture of beef in meatball formulation. Meanwhile, the chemometrics of principal component analysis (PCA) was used for the classification between rat meat and beef meatballs. Some frequency regions in mid infrared region were optimized, and finally, the frequency region of 750–1000 cm^{-1} was selected during PLS and PCA modeling. For quantitative analysis, the relationship between actual values (x-axis) and FTIR predicted values (y-axis) of rat meat is described by the equation of $y = 0.9417x + 2.8410$ with coefficient of determination (R^2) of 0.993, and root mean square error of calibration (RMSEC) of 1.79%. Furthermore, PCA was successfully used for the classification of rat meat meatball and beef meatball.

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Original Article

The potential use of infrared spectroscopy and multivariate analysis for differentiation of beef meatball from dog meat for Halal authentication analysis

W.S. Rahayu[1,2], S. Martono[1], Sudjadi[1] and Abdul Rohman[1,3,#]

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ABSTRACT

Objective: The objective of this research was to assess the suitability of FTIR spectroscopy coupled with multivariate analysis of partial least square regression (PLSR) along with pattern recognition technique of principal component analysis (PCA) for rapid quantitative and qualitative (identification) analysis of dog meat in beef meatball formulation.

Materials and Methods: The lipid fraction of meatball was obtained by employing two different extraction techniques, namely Bligh-Dyer and Folch method. FTIR spectral bands correlated with beef fat, pork fat, chicken fat and rat fat were measured, interpreted, and qualitatively analyzed. The small variations among spectra were exploited as a basis tools to differentiate between dog fat and

The use of FTIR spectra for porcine gelatin

- Porcine gelatin is frequently used in capsule shell (pharmaceutical products) or candies (food products).
- FTIR spectra could be applied as screening method
- Need further confirmation using real-time PVR or LC-MS/MS

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A rapid ATR-FTIR spectroscopic method for classification of gelatin gummy candies in relation to the gelatin source

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Gelatin
Chemometrics
Source determination
Gummy candy
Halal food

ABSTRACT

Gelatin is widely used in gummy candies because of its unique functional properties. Generally, porcine and bovine gelatins are used in the food industry. FTIR-ATR combined with chemometrics analysis such as hierarchical cluster analysis (HCA) (OPUS Version 7.2 software), principal component analysis (PCA) (OPUS Version 7.2 software) and partial least squares-discriminant analysis (PLS-DA) (Matlab R2017b) were used for classification and discrimination of gelatin gummy candies related to their gelatin source. The spectral region between 1734 and 1528 cm^{-1} was selected for chemometric analysis. The potential of FTIR spectroscopy for determination of bovine and porcine source in gummy candies was examined and validated by a real-time polymerase chain reaction (PCR) method. Twenty commercial samples were tested by developed ATR-FTIR methodology and RT-PCR technique, mutually confirming and supporting results were obtained. Gummy candies were classified and discriminated in relation to the bovine or porcine source of gelatin with 100% success without any sample preparation using FTIR-ATR technique.

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Analytical Methods

An evaluation of Fourier transforms infrared spectroscopy method for the classification and discrimination of bovine, porcine and fish gelatins

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ABSTRACT

The objective of this research was to develop a rapid spectroscopic technique as an alternative method for the differentiation and authentication of gelatin sources in food products by using attenuated total reflectance Fourier transform infrared (ATR–FTIR) spectra combined with chemometrics. Clear discrimination and classification of all the studied gelatin sources (bovine, porcine, and fish) were achieved by hierarchical cluster and principle component analysis (PCA). Amide-I (1700–1600 cm^{-1}) and Amide-II (1565–1520 cm^{-1}) spectral bands were used in a chemometric method. Moreover, ATR–FTIR spectral data successfully discriminated pure bovine gelatin from mixture of bovine and porcine gelatins, which is very important for the food industry. The method that we adopted could be beneficial for rapid, simple and economic determination of both gelatin presence and its origin from food products such as yogurt, ice cream, milk dessert or other gelatin containing products such as pharmaceuticals and cosmetics.

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Differentiation of gelatin sources

- Suitable for analysis of gelatin sources
  - Porcine
  - Bovine
  - Porcine
- Need classification chemometrics
  - PCA
  - Cluster analysis

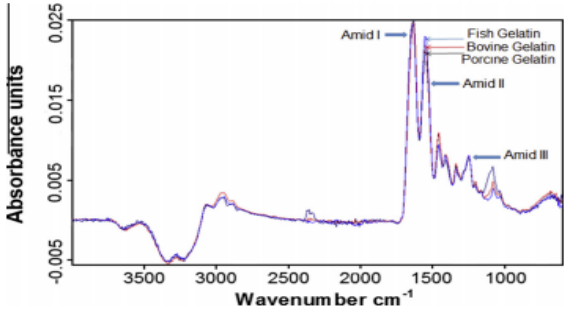

Fig. 1. FTIR spectrum of the fish gelatin, bovine gelatin and porcine gelatin.

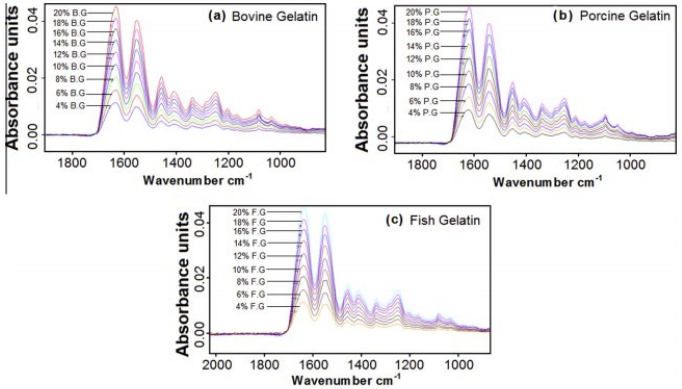

Fig. 2. Concentration-dependent FTIR spectra of bovine gelatin (B.G) (a), porcine gelatin (P.G) (b) and fish gelatin (F.G) (c).

Advantages and Disadvantages of FTIR

- Advantages
  - Simple and some cases without any sample preparation
  - Specific because FTIR spectra are fingerprint in nature

- Disadvantages
  - The developed method can only be used for formulations of samples consistent with those tested
  - If the composition of the sample to be analyzed is different, FTIR spectra of the analyte in the mixture will also be different.
  - the presence of non-halal components in the different food samples is quantified using different spectral regions.