

Documents

Fadzillah, N.A.^a, Elgharbawy, A.^a, Jamaluddin, M.A.^a, Tukiran, N.A.^a, Windarsih, A.^b, Rohman, A.^{c d}, Sukri, S.J.M.^e, Muhammad, N.W.F.^f, Hamid, A.H.^g

Authentication analysis of animal fats adulteration in nail polish simulation using Raman spectroscopy coupled with chemometrics

(2025) *Vibrational Spectroscopy*, 138, art. no. 103785, .

DOI: 10.1016/j.vibspec.2025.103785

^a International Institute for Halal Research and Training (INHART), International Islamic University Malaysia, Kuala Lumpur, 50728, Malaysia

^b Research Center for Food Technology and Processing (PRTPP), National Research and Innovation Agency (BRIN), Yogyakarta, 55861, Indonesia

^c Department of Pharmaceutical Chemistry, Faculty of Pharmacy, Universitas Gadjah Mada, Yogyakarta, 55281, Indonesia

^d Center of Excellence, Institute for Halal Industry and Systems (PUIPT-IHIS), Universitas Gadjah Mada, Yogyakarta, 55281, Indonesia

^e Department of Islamic Management, Faculty of Tehnology, Design and Management UCYP University, Pahang, Kuantan, Malaysia

^f Faculty of Contemporary Islamic Studies, Sultan Ismail Petra International Islamic University College, Kelantan, Kota Bharu, Malaysia

^g Academy of Islamic Contemporary Studies, Universiti Teknologi MARA, Selangor, Shah Alam, Malaysia

Abstract

Cosmetics are being used daily by many people, and their consumption is on the rise every year. These products are adulterated with cheaper alternatives to increase their profit. As more cosmetics are available in the market, the authenticity of halal cosmetics has raised much concern among Muslim consumers throughout the world. Therefore, authentication analysis of cosmetic products is urgently needed. This study was conducted to detect beef tallow (BT), chicken fat (CF), lard (LD), and mutton fat (MF) in nail polish using Raman spectrometry combined with chemometrics. Partial least square-discriminant analysis (PLS-DA) and hierarchical cluster analysis (HCA) were successfully used to differentiate animal fats into four subclasses. In addition, partial least square (PLS) and orthogonal PLS (OPLS) regression were adequate to detect and predict the levels of BT, CF, LD, and MF in nail polish with $R^2 > 0.990$ both in calibration and validation models. The best prediction model for BT was from OPLS at the wavenumber range of 100–3200 cm⁻¹ with $R^2 > 0.990$ and RMSEC as well as RMSEP lower than 2.0 %. Meanwhile PLS model demonstrated the best model to predict CF, LD, and MF was the PLS with $R^2 > 0.990$ and RMSEC as well as RMSEP around 1–2.40 %. This study revealed the potential application of Raman spectroscopy in combination with chemometrics as an effective and efficient technique for authenticating nail polish base formulation adulterated with animal fats. © 2025 Elsevier B.V.

Author Keywords

Animal fats; Chemometrics; Cosmetic; Nail polish; Raman spectroscopy

Index Keywords

Hierarchical clustering; Animal fat, Authentication analysis, Beef tallow, Chemometrices, Cosmetic products, Fat adulterations, Nail polish, Partial least squares discriminant analyses (PLSDA), Partial least-squares, Raman spectrometries; Raman spectroscopy

References

- Faria-Silva, C., Ascenso, A., Costa, A.M., Marto, J., Carvalheiro, M., Ribeiro, H.M., Simões, S.

Feeding the skin: a new trend in food and cosmetics convergence

(2020) *Trends Food Sci. Technol.*, 95, pp. 21-32.

- Celeiro, M., Garcia-Jares, C., Llompart, M., Lores, M.

Recent advances in sample preparation for cosmetics and personal care products analysis

(2021) *Molecules*, 26, p. 4900.

2021, Vol. 26, Page 4900

- Rahman, F., Khan, S., Talukder, S.

(2022),

R. Ranjan Kumar, Article in The Indian veterinary journal. (accessed August 17, 2024).

- Kunik, O., Saribekova, D., Lazzara, G., Cavallaro, G.
Emulsions based on fatty acid from vegetable oils for cosmetics
(2022) *Ind. Crops Prod.*, 189.
- Manin, L.P., Pizzo, J.S., Rydlewski, A.A., Santos, P.D.S., Galuch, M.B., Zappielo, C.D., Santos, O.O., Visentainer, J.V.
Evaluation of the adulteration of edible and cosmetic sunflower oils by GC-FID and ESI-MS
(2021) *J. Braz. Chem. Soc.*, 32, pp. 2086-2094.
- Aziz, A.A., Nordin, F.N.M., Zakaria, Z., Abu Bakar, N.K.
A systematic literature review on the current detection tools for authentication analysis of cosmetic ingredients
(2022) *J. Cosmet. Dermatol.*, 21, pp. 71-84.
- Haleem, A., Khan, M.I., Khan, S., Jami, A.R.
Research status in Halal: a review and bibliometric analysis
(2020) *Mod. Supply Chain Res. Appl.*, 2, pp. 23-41.
- Farman, Q., Pakeeza, D.S.
An analysis of shariah law and legal perspectives on cosmetic product regulations
(2024) *Islam. Res. J. {الندوة}*, 2, pp. 53-77.
- Cristiano, L., Guagni, M.
Zoaceuticals and cosmetic ingredients derived from animals
(2022) *Cosmetics*, 9, p. 13.
2022, Vol. 9, Page 13
- Kurniawati, D.A., Cakravastia, A.
A review of halal supply chain research: Sustainability and operations research perspective
(2023) *Clean. Logist. Supply Chain*, 6.
- Yadav, S.
Edible oil adulterations: current issues, detection techniques, and health hazards
(2018) *Int J. Chem. Stud.*, 6, pp. 1393-1397.
- Owolabi, I.O., Olayinka, J.A.
Incidence of fraud and adulterations in ASEAN food / feed exports: a 20-year analysis of RASFF 's notifications
(2021) *PLoS One*, 16.
- Jian, L., Yuan, X., Han, J., Zheng, R., Peng, X., Wang, K.
Screening for illegal addition of glucocorticoids in adulterated cosmetic products using ultra-performance liquid chromatography/tandem mass spectrometry with precursor ion scanning
(2021) *Rapid Commun. Mass Spectrom.*, 35.
- Jairoun, A.A., Al-Hemyari, S.S., Shahwan, M., Jamshed, S., Bisgwa, J.
Development and validation of a novel cosmetics safety assessment scale (CSAS): factual understanding of cosmetic safety and fostering international awareness
(2022) *PLoS One*, 17.
- Aziz, A.A., Abdullah Sani, M.S., Zakaria, Z., Abu Bakar, N.K.
Discrimination and authentication of lard blending with palm oil in cosmetic soap formulations
(2023) *Int J. Cosmet. Sci.*, 45, pp. 444-457.

- Kua, J.M., Azizi, M.M.F. (2022), pp. 1906-1932.
M.A. Abdul Talib, H.Y. Lau, Adoption of analytical technologies for verification of authenticity of halal foods – a review, 39
- Hashim, P., Hashim, D.M.
A review of cosmetic and personal care products: Halal perspective and detection of ingredient
(2013) *Pertanika J. Sci. Technol.*, 21, pp. 281-292.
- Nurani, L.H., Riswanto, F.D.O., Windarsih, A., Edityaningrum, C.A., Guntarti, A., Rohman, A.
Use of chromatographic-based techniques and chemometrics for halal authentication of food products: A review
(2022) *Int J. Food Prop.*, 25, pp. 1399-1416.
- Zhu, X., Gu, S., Guo, D., Huang, X., Chen, N., Niu, B., Deng, X.
Determination of porcine derived components in gelatin and gelatin-containing foods by high performance liquid chromatography-tandem mass spectrometry
(2023) *Food Hydrocoll.*, 134.
- Ghazali, H.H., Tukiran, N.A.
Analysis of pork adulteration In recycled frying oils using Raman spectroscopy
(2021) *Malays. J. Halal Res.*, 4, pp. 14-17.
- Windarsih, A., Arsanti Lestari, L., Erwanto, Y., Rosiana Putri, A., Irnawati, Ahmad Fadzillah, N., Rahmawati, N., Rohman, A.
Application of raman spectroscopy and chemometrics for quality controls of fats and oils: a review
(2021) *Food Rev. Int.*, pp. 1-20.
- Qu, C., Li, Y., Du, S., Geng, Y., Su, M., Liu, H.
Raman spectroscopy for rapid fingerprint analysis of meat quality and security: principles, progress and prospects
(2022) *Food Res. Int.*, 161.
- Ahmmed, F., Fuller, I.D., Killeen, D.P., Fraser-Miller, S.J., Gordon, K.C.
Raman and infrared spectroscopic data fusion strategies for rapid, multicomponent quantitation of krill oil compositions
(2021) *ACS Food Sci. Technol.*, 1, pp. 570-578.
- Senger, R.S., Scherr, D.
Resolving complex phenotypes with Raman spectroscopy and chemometrics
(2020) *Curr. Opin. Biotechnol.*, 66, pp. 277-282.
- Diz, E.L., Portela, R., Barton, B., Thomson, J.
(2022), 76 (9), pp. 1021-1041.
(accessed August 17, 2024). 2022, Chemometrics for Raman Spectroscopy Harmonization, Applied Spectroscopy
- Yazgan Karacaglar, N.N., Bulat, T., Boyaci, I.H., Topcu, A.
Raman spectroscopy coupled with chemometric methods for the discrimination of foreign fats and oils in cream and yogurt
(2019) *J. Food Drug Anal.*, 27, pp. 101-110.
- Covaci, F.D., Berghian-Grosan, C., Feher, I., Magdas, D.A.
Edible oils differentiation based on the determination of fatty acids profile and raman spectroscopy-a case study
(2020) *Appl. Sci.*, 10, p. 8347.
2020, Vol. 10, Page 8347

- Taylan, O., Cebi, N., Tahsin Yilmaz, M., Sagdic, O., Bakhsh, A.A.
Detection of lard in butter using Raman spectroscopy combined with chemometrics
(2020) *Food Chem.*, 332.
- Farooqui, S., Mishra, A.
Preparation and invitro characterization of nail polish prepared by using natural dye
(2019) *Int. J. Pharm. Sci. Nutr. Sci. Res. Rev.*, 2, pp. 1-4.
(accessed December 2, 2024).
- Rohman, A., Windarsih, A., Lukitaningsih, E., Rafi, M., Betania, K., Fadzillah, N.A.
The use of FTIR and Raman spectroscopy in combination with chemometrics for analysis of biomolecules in biomedical fluids: A review
(2019) *Biomed. Spectrosc. Imaging*, 8, pp. 55-71.
- Gao, F., Ben-Amotz, D., Zhou, S., Yang, Z., Han, L., Liu, X.
Comparison and chemical structure-related basis of species discrimination of animal fats by Raman spectroscopy using near-infrared and visible excitation lasers
(2020) *LWT*, 134.
- Saleem, M., Amin, A., Irfan, M.
Raman spectroscopy based characterization of cow, goat and buffalo fats
(2021) *J. Food Sci. Technol.*, 58, pp. 234-243.
- Jiménez-Carvelo, A.M., Martín-Torres, S., Ortega-Gavilán, F., Camacho, J.
PLS-DA vs sparse PLS-DA in food traceability. A case study: authentication of avocado samples
(2021) *Talanta*, 224.
- Rohman, A., Che Man, Y.B.
The optimization of FTIR spectroscopy combined with partial least square for analysis of animal fats in quartenary mixtures
(2011) *Spectroscopy*, 25, pp. 169-176.
- Worley, B., Halouska, S., Powers, R.
Utilities for quantifying separation in PCA/PLS-DA scores plots
(2013) *Anal. Biochem*, 433, pp. 102-104.
- dos, E.V., Pereira, S., Fernandes, D.D.D.S., de Araújo, M.C.U., Diniz, P.H.G.D., Maciel, M.I.S.
Simultaneous determination of goat milk adulteration with cow milk and their fat and protein contents using NIR spectroscopy and PLS algorithms
(2020) *Lwt*, 127.
- Li, F., Zhang, J., Wang, Y.
(2022), Vibrational Spectroscopy Combined with Chemometrics in Authentication of Functional Foods.
- Xu, Y., Zhong, P., Jiang, A., Shen, X., Li, X., Xu, Z., Shen, Y., Lei, H.
Raman spectroscopy coupled with chemometrics for food authentication: a review
(2020) *TrAC - Trends Anal. Chem.*, 131.
Article#116017
- Fakayode, S.O., Baker, G.A., Bwambok, D.K., Bhawawet, N., Elzey, B., Siraj, N., Macchi, S., Warner, I.M.
Molecular (Raman, NIR, and FTIR) spectroscopy and multivariate analysis in consumable products analysis1
(2020) *Appl. Spectrosc. Rev.*, 55, pp. 647-723.
- Filzmoser, P., Nordhausen, K.
Robust linear regression for high-dimensional data: An overview
(2021) *Wiley Inter. Rev. Comput. Stat.*, 13.

- Lee, G., Lee, K.
Feature selection using distributions of orthogonal PLS regression vectors in spectral data
(2021) *BioData Min.*, 14, pp. 1-16.
- Zhao, M., Downey, G., Odonnell, C.P.
Dispersive RAMAN spectroscopy and multivariate data analysis to detect offal adulteration of thawed beefburgers
(2015) *J. Agric. Food Chem.*, 63, pp. 1433-1441.
- Lee, J.Y., Park, J.H., Mun, H., Shim, W.B., Lim, S.H., Kim, M.G.
Quantitative analysis of lard in animal fat mixture using visible Raman spectroscopy
(2018) *Food Chem.*, 254, pp. 109-114.
- Elderderi, S., Bonnier, F., Perse, X., Byrne, H.J., Yvergnaux, F., Chourpa, I., Elbashir, A.A., Munnier, E.
Label-free quantification of nanoencapsulated piperonyl esters in cosmetic hydrogels using raman spectroscopy
(2023) *Pharmaceutics*, 15, p. 1571.
2023, Vol. 15, Page 1571
- Ali, E.M.A., Edwards, H.G.M., Hargreaves, M.D., Scowen, I.J.
Raman spectroscopic investigation of cocaine hydrochloride on human nail in a forensic context
(2008) *Anal. Bioanal. Chem.*, 390, pp. 1159-1166.
- Jentzsch, P.V., Ramos, L.A., Ciobotă, V.
Handheld Raman spectroscopy for the distinction of essential oils used in the cosmetics industry
(2015) *Cosmetics*, 2, pp. 162-176.
2015, Vol. 2, Pages 162-176
- Üçüncüoğlu, D., İláslan, K., Boyacı, İ.H., Özay, D.S.
Rapid detection of fat adulteration in bakery products using Raman and near-infrared spectroscopies
(2013) *Eur. Food Res. Technol.*, 237, pp. 703-710.
- Chen, J., Liu, W., Cao, X., Zhang, Q., Zou, X.
Rapid identification of milk powder adulteration based on surface-enhanced Raman spectroscopy
(2024) *AIP Adv.*, 14.

Correspondence Address

Fadzillah N.A.; International Institute for Halal Research and Training (INHART), Malaysia; email: nurrulhidayah@iium.edu.my

Publisher: Elsevier B.V.

ISSN: 09242031

CODEN: VISPE

Language of Original Document: English

Abbreviated Source Title: Vib. Spectrosc.

2-s2.0-86000323137

Document Type: Article

Publication Stage: Final

Source: Scopus