

Food Chemistry Advances 2025

Untargeted metabolomics profiling for the geographical

by shanti lestari

Submission date: 15-Jul-2025 07:06PM (UTC+0700)

Submission ID: 2715108329

File name: Food_Chemistry_Advance_2025.pdf (3.57M)

Word count: 5480

Character count: 32052



Untargeted metabolomics profiling for the geographical authentication of traditional pempek using high-resolution orbitrap mass spectrometry

Agus Supriadi^{a,*}, Sherly Ridhowati^a, Daniel Saputra^b, Wulandari^c, Shanti Dwita Lestari^a

^a Department of Fisheries Product Technology, Faculty of Agriculture, Sriwijaya University, Indonesia

^b Department of Agricultural Engineering, Faculty of Agriculture, Sriwijaya University, Indonesia

^c Department of Fisheries Product Technology, Faculty of Animal Science, Jambi University, Indonesia

ARTICLE INFO

Keywords:

Chemometric analysis
Geographical authentication
Orbitrap HRMS
Pempek
Untargeted metabolomics

ABSTRACT

The geographical authentication of traditional foods, such as Pempek, is increasingly important due to globalisation and rising consumer demand for product authenticity. Pempek, a traditional Indonesian dish, varies by region due to differences in fish species and local preparation methods. This study utilised untargeted metabolomics with High-Resolution Orbitrap Mass Spectrometry (HRMS) to identify metabolite markers associated with the geographical origin of Pempek. Samples from Palembang, Jambi, and other regions were analysed using chemometric techniques, revealing significant variations in metabolic profiles between these areas. The HRMS-based approach successfully detected region-specific markers and demonstrated its potential as a reliable method for geographical authentication, fostering confidence for the future of food authenticity. These findings contribute to preserving the cultural and economic significance of traditional foods like Pempek and highlight the broader application of metabolomics in food authentication.

1. Introduction

The geographical authentication of traditional foods has gained significant importance in the context of globalisation and increasing consumer awareness regarding product authenticity. Pempek, a typical fish cake served with a spicy sweet and sour sauce, originating from South Sumatera, Indonesia, and is renowned for its cultural and culinary importance. As an intangible cultural heritage (Surya et al., 2023; Wargadale et al., 2023), the composition of Pempek, determined by the type and proportions of fish and starch, differs regionally due to variations in local fish availability and preparation methods. White-fleshed fish are predominantly chosen for the production of high-quality Pempek. The most expensive Pempek is prepared from bronze knifefish (*Chitala* sp.), a freshwater fish, endemic to Sumatera Island, due to its white flesh colour, excellent gelation properties, and delectable flavour. Due to the decreased population of bronze knifefish and its status as fully protected species, Narrow-barred Spanish mackerel and snakehead fish have been more frequently used as they offer a delectable flavour and white flesh at a more reasonable price. Mackerel is a sea species that is not exclusive to the South Sumatra Sea and can be captured in any ocean. While snakehead fish are freshwater fish that are frequently observed in wetland waters, including those in southern

Sumatera. Pempek generally has an open formulation, it can be produced in any region from other fish varieties that have low economic value or even surimi; however, the quality and type of fish used will determine the quality of Pempek such as taste, aroma, and textures.

Additionally, the physical, chemical, and organoleptic properties of Pempek are distinctive due to the variability of its processing methods, which are influenced by the culinary traditions of various regions. Pempek, as a traditional dish, demonstrates a diversity of artisanal methods that vary by location and individual producing it, notably in the kneading process and ingredient combining order. The regularity and characteristics of the dough are determined by the unique intuition and technique of each Pempek artisan. As a result, Pempek's quality varies among areas, even when created by individuals utilizing the same basic ingredients. The flexibility of raw material selection, the ease of processing adaptation, and the competition from comparable gel-based products all contribute to concerns about the preservation of Pempek's geographical authenticity (Supriadi et al., 2018).

The growing demand for authentic products has increased the importance of food origin in consumer choices, linking product quality and safety to geographical indicators (Principal et al., 2022). Safeguarding the geographical authenticity of Pempek is thus vital for cultural preservation and economic protection. Conventional methods for

* Corresponding author.

E-mail address: agussupriadi_thi@unsri.ac.id (A. Supriadi).

 <https://doi.org/10.1016/j.focha.2025.100914>

Received 27 September 2024; Received in revised form 29 January 2025; Accepted 3 February 2025

Available online 4 February 2025

2772-753X/© 2025 The Author(s). Published by Elsevier Ltd. This is an open access article under the CC BY-NC license (<http://creativecommons.org/licenses/by-nc/4.0/>).

authenticating food products, such as sensory and chemical analyses (Supriadi et al., 2020), have limited accuracy and reliability in determining specific geographical origins. In contrast, advanced techniques like High-Resolution Mass Spectrometry (HRMS), particularly Orbitrap technology, offer improved precision by allowing detailed analysis of chemical compositions (Cajka, 2024; Mihailova et al., 2021; Pan et al., 2022). Mass spectrometry (MS) yields both qualitative and quantitative data on compounds, which are ionised and categorised according to their mass-to-charge ratio. For untargeted metabolomic profiling, this technique enables the comprehensive chemical analysis without prior knowledge of the food's metabolite composition (Bozza et al., 2024; Anjar Windarsih et al., 2022; Yong et al., 2022). HRMS has been successfully applied to authenticate various single-ingredient food products by identifying chemical markers linked to their geographical origins, such as rice (Ratnasekhar et al., 2021), red wine (Pan et al., 2022), and tea (Ren et al., 2022a). However, the application of HRMS for the identification of chemical markers in processed foods with complex ingredients, like Pempek, has not been previously explored. This study offers valuable insights into the application of HRMS and chemometric analysis for the detection of chemical markers, addressing the challenges posed by the complexity and heterogeneity of compounds found in food matrices as well as the interaction of various metabolites derived from various raw materials and preparation methods. The utilization of this method for characterizing Pempek produced in a specific geographical region has yet to be thoroughly investigated.

This study aims to fill this gap by implementing an untargeted metabolomics approach to identify metabolite markers that indicate the geographical origin of Pempek as a multicomponent traditional food. The integration of metabolomic data with multivariate statistical analysis enhances the accuracy of regional classification of Pempek, while also setting up a practical method for traceability and preventing counterfeiting. This approach offers a reliable method for geographical authentication and plays a significant role in establishing quality standards for traditional foods.

2. Material and methods

2.1. Sample collection

Pempek samples were collected from four geographically distinct regions influenced by the historical culinary practices of the Sriwijaya Kingdom: Palembang (PP) in South Sumatera, Jambi (PJ) in Jambi Province, Bengkulu (PB) in Bengkulu Province, and Bandar Lampung (PL) in Lampung Province. A total of 96 samples were bought from 48 vendors in PP, 13 in PJ, 20 in PB, and 15 in PL. Direct interviews conducted with the producers revealed that only 4 out of 13 PJ samples and 4 out of 48 PP samples used snakehead fish (*Channa striata*) as the raw material for Pempek. The PL samples were exclusively derived from narrow-barred Spanish mackerel (*Scomberomorus* sp.), while the PB samples were derived from mackerel and cobia (*Rachycentron* sp.) due to the province's proximity to the Indian Ocean. The Pempek samples made from mackerel and cobia fish were omitted from this study due to the primary focus on the geographical indication of Pempek as a traditional Palembang dish. These types of marine fish are widely distributed and are not restricted to a specific geographical area. In contrast, the snakehead fish, which is commonly found in rivers and swamps in Sumatra, was classified as having distinctive geographical characteristics and was more representative in the authentication of Palembang's Pempek. Consequently, 4 PPS (Pempek Palembang Snakehead) and 4 PJS (Pempek Jambi Snakehead) were chosen as samples, with the addition of 4 PPM (Pempek Palembang Mackerel) as a comparison element to enhance the authentication analysis. The sample size was statistically adequate according to the Slovin's formula. Each sample was vacuum-packed, frozen at -18°C , and thawed at 4°C before analysis.

2.2. Sample preparation

For metabolomics analysis, 100 mg of each Pempek sample was weighed and homogenised in 1 mL of HPLC-grade methanol. Samples were vortexed for 2 min and sonicated for 30 min at 25°C to facilitate metabolite extraction. Following sonication, the samples were centrifuged at $5000 \times g$ for 10 min, and the supernatant was filtered through a $0.20\text{ }\mu\text{m}$ nylon filter. The filtrates were used for further analysis in the metabolomics workflow, ensuring consistency and reproducibility across all experimental replicates.

2.3. Metabolomics analysis

Untargeted metabolomics profiling was performed using a Thermo Scientific™ Vanquish™ Horizon UHPLC system coupled with an Orbitrap™ Exploris 240 High-Resolution Mass Spectrometer (HRMS). Chromatographic separation was achieved using a Thermo Scientific™ Accucore™ 2.8 column ($100\text{ mm} \times 2.1\text{ mm}$, $2.6\text{ }\mu\text{m}$ particle size) maintained at 40°C . The mobile phase consisted of MS-grade water with 0.1% formic acid (A) and MS-grade acetonitrile with 0.1% formic acid (B), with a flow rate of 0.3 mL/min . The gradient started at 5% B, increased to 90% over 16 min, and was held for 4 min before returning to 5% by 25 min. The injection volume was $5\text{ }\mu\text{L}$.

The HRMS operated in full MS/dd-MS2 mode with polarity switching, capturing spectra at a resolution of 60,000 FWHM across the mass range of $70\text{--}800\text{ m/z}$. Data-dependent fragmentation (dd-MS2) was conducted at 30,000 FWHM using normalised collision energies of 30, 50, and 70. The ion source was set to 3500 V for positive mode and 2500 V for negative mode, with other parameters optimised for metabolite detection.

2.4. Data processing and statistical analysis

Mass spectrometry data were processed using Compound Discoverer 3.3 software (Thermo Fisher Scientific). Features were detected with a 5-ppm mass tolerance and grouped by retention time with a tolerance of 0.2 min. Compounds were annotated using the ChemSpider database, including FooDB and LipidMaps Structure Database. MS2 spectra were matched to the mzCloud database for further compound annotation.

Chemometric analysis was performed using MetaboAnalyst 6.0. Data normalisation was conducted using the sum method, followed by logarithmic transformation and autoscaling. Partial Least Squares Discriminant Analysis (PLS-DA) and Orthogonal Partial Least Squares Discriminant Analysis (OPLS-DA) were used to distinguish between Pempek samples from different regions. Model quality was evaluated based on $R^2(\text{cum})$ and $Q^2(\text{cum})$ values, with thresholds of >0.5 indicating good fit and predictive accuracy. The analysis of Variable Importance in Projection (VIP) was performed alongside the Total Ion Chromatogram (TIC) to adequately identify key metabolite compounds. The VIP scores greater than 2 were considered significant for identifying discriminatory metabolites. Identification and analysis of differential metabolites were performed using <https://bioinformatics.psb.ugent.be/webtools/Venn/> software (UGent Bioinformatics & Evolutionary Genomics).

3. Result and discussion

3.1. LC–HRMS untargeted metabolomic profiling analysis of Pempek

The metabolic profiles of Pempek samples from three groups (PPS, PPM, and PJS) demonstrate differing retention times, spanning from 0 to 25 mins, as indicated by the total ion chromatograms (TIC) (Fig. 1). TIC shows the intensity of all ions identified in a sample. Fragmentation spectra, which are commonly produced by tandem mass spectrometry (MS/MS), can be utilised to identify particular ions that contribute to the TIC peaks. Because each signal represents a different ion or metabolite, a

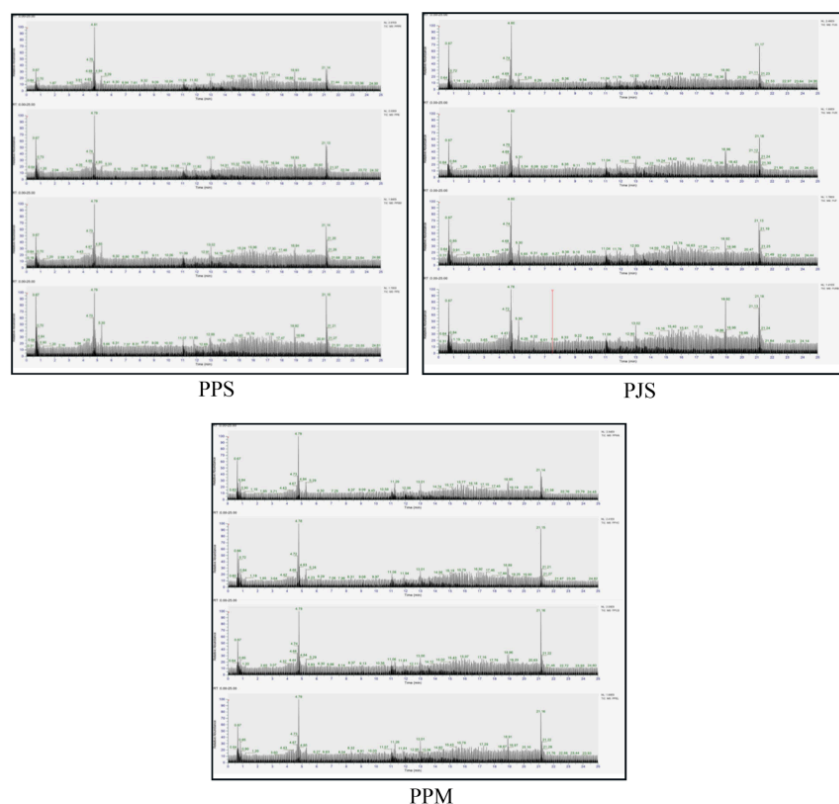


Fig. 1. The total ion chromatograms (TIC) of Pempek groups (PPS, PJS and PPM). A high-resolution image of TIC is provided in the supplementary data.

fragmentation analysis can reveal the structural properties of these molecules. In this work, fragmentation data for a [Figure 2](#) ions are utilised to confirm the identity of the discovered metabolites. After peak alignment and filtration using Compound Discoverer 3.3, the TIC derived from the identified matrix data of 12 samples exhibited 1323 peaks at m/z /rt values. The data filtering procedure integrated in the MetaboAnalyst program was applied to improve the modelling process of untargeted metabolomics datasets. The standard deviation (SD) and interquartile range (IQR) were used to identify significant variables, while excluding constant data that does not contribute meaningful information for analysis and may adversely affect statistical outcomes. A total of 504 metabolites were removed due to their consistent presence in all samples, resulting in the identification and validation of 819 metabolite data points. The resulting TIC indicated the most prominent peaks at retention times of 0.6, 4.8, and 21.0 (minute) indicating key metabolites unique to each group. Volatile organic compounds (VOCs) and light fatty acids are commonly detectable after 0.6 mins of retention. At 4.8 mins, molecules with bigger structures and stronger polarity, such as amino acids, are often detected. Meanwhile, by 21 mins, bigger, more polar, or complex metabolites, such as lipids, are usually found. The

discovery of these three categories of chemicals is consistent with the marker metabolites for each category.

This TIC analysis is essential for assessing food quality, as it identifies metabolites unique to particular food categories and establishes a basis for an extensive metabolomic examination. The hypothesis that the chemical composition of Pempek is determined by its geographical origin is supported by the differences in intensity and retention time observed among the peaks. Differences in TIC profiles can be used to identify differences in food metabolomic profiles based on geographic origin. Previous studies based on TIC successfully identified significant regional differences in the metabolomic profiles of rice from 5 provinces in China, Vietnam and India (Ratnasekhar et al., 2021). Different TIC patterns in *Poria cocos* were observed in samples and affected by environmental conditions in different regions (Liu et al., 2023). The variations in the TIC spectrum of red wine samples were able to identify differences in key metabolites that were in line with environmental and processing factors (Pan et al., 2022). Additional studies have documented similar effects in tea (Ren et al., 2022a; Tan & Zhou, 2024), kimchi (Hye Hur et al., 2023), and salami (Sgroi, 2021). These results indicate that TIC analysis has the potential to offer more profound

insights into the quality and chemical composition of food products. The uniqueness of Pempek's metabolites could stem from variations in raw materials and processing methods across different regions, highlighting the significance of untargeted metabolomics for geographical authentication.

3.2. Chemometric analysis

Chemometric analysis, employing Partial Least Squares Discriminant Analysis (PLS-DA) and Orthogonal Partial Least Squares Discriminant Analysis (OPLS-DA), provided crucial insights into the metabolomic differences between Pempek samples from the two geographical groups: Palembang (PPS and PPM) and Jambi (PJS). The clear separation of samples in the PLS-DA score plots (Fig. 2A-D) highlights distinct clustering based on geographical origin, indicating significant regional variations in the metabolomic profiles of Pempek. Fig. 2 illustrates that Component 1 distinctly differentiates between the groups, highlighting

the impact of geographical factors on their metabolite composition.

The superiority of the OPLS-DA models over PLS-DA in this study is reflected in their improved predictive accuracy and stronger model fit, with R^2 of Y values approaching 1, particularly in comparisons to PPS vs PPM (Fig. 3). Additionally, the Q^2 values, which measure predictive capability, were consistently higher for OPLS-DA models, demonstrating robust performance distinguishing between the three groups. This improvement is attributed to OPLS-DA's ability to enhance model interpretability by separating correlated and uncorrelated variation, thus providing a more refined classification of Pempek samples based on their metabolic signatures.

The application of high-resolution Orbitrap mass spectrometry (HRMS) combined with chemometric methods has proven effective for food authentication. Previous studies have similarly utilised HRMS and chemometric techniques to authenticate foods such as olive oil and wine by identifying metabolomic signatures linked to geographical origin Dou *et al.* (2022). The clustering observed in the PLS-DA and OPLS-DA

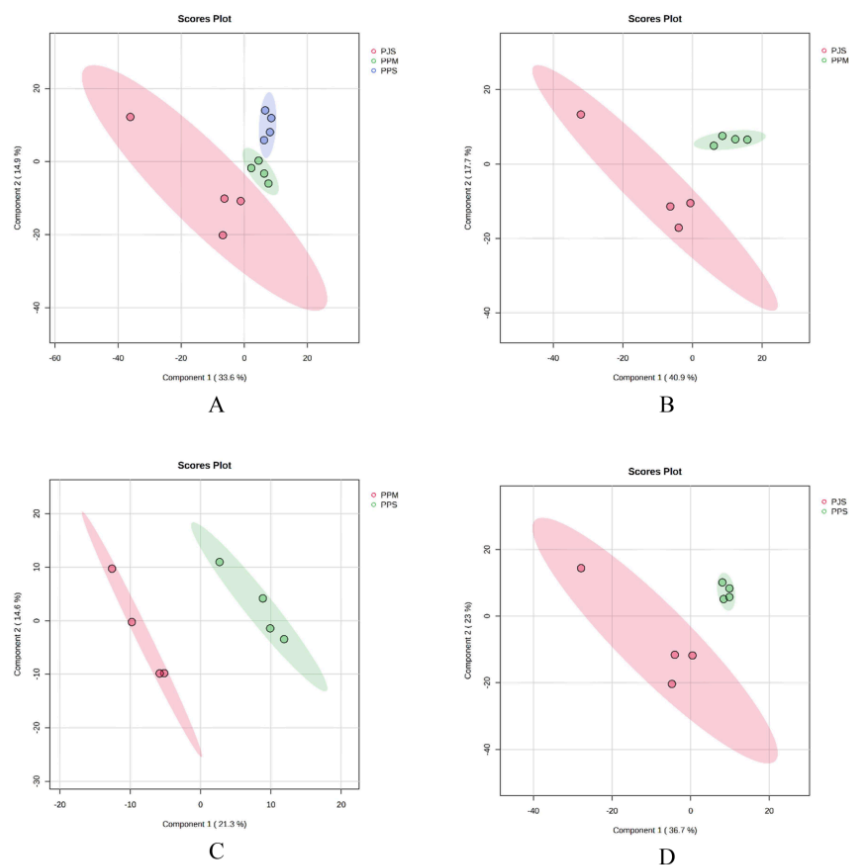


Fig. 2. The Partial least-squares discriminant analysis (PLS-DA) score plots: PJS vs PPM vs PPS (A), PPM vs PPS (B), PJS vs PPS (C) and PJS vs PPM (D).

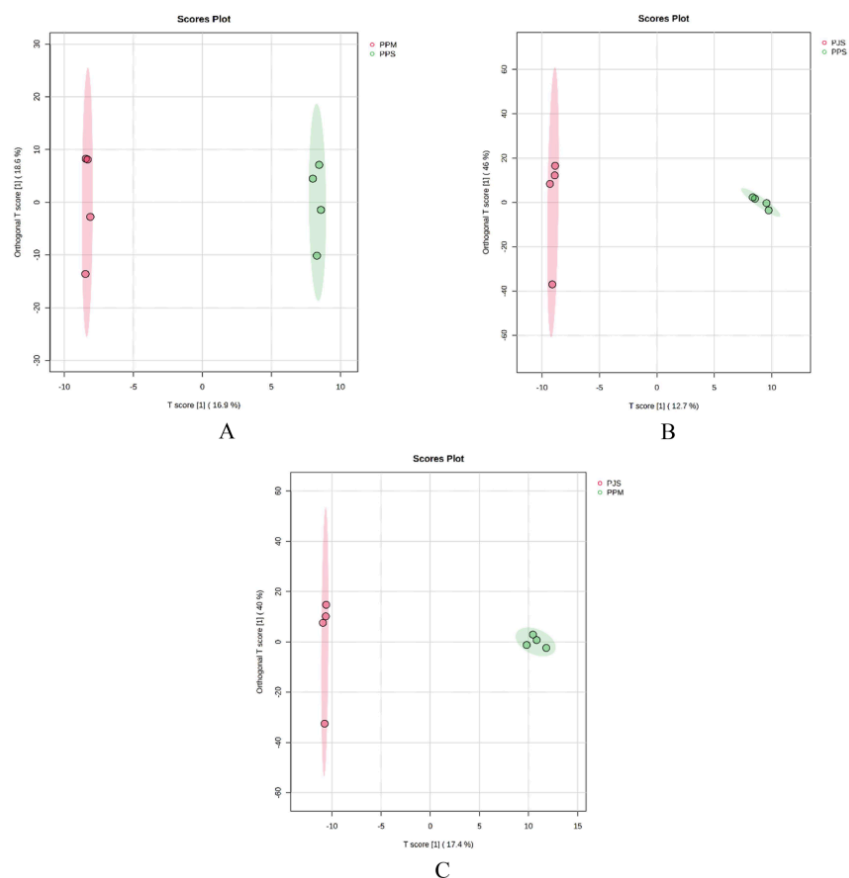


Fig. 3. The orthogonal partial least-squares discriminant analysis (OPLS-DA) score plots: PPM vs PPS (A), PJS vs PPS (B) and PJS vs PPM (C).

score plots in this study confirms that the metabolomic profiles of Pempek can vary significantly based on regional factors. These results align with findings in other traditional foods, such as rice (Ratnasekhar et al., 2021) and tea (Ren et al., 2022b), where metabolomic markers were successfully used for geographical differentiation.

Table 1
The evaluation parameters of the PLS-DA and OPLS-DA model of pempek groups.

Model	Group	R ² _Y	R ² _X	Q ²	Accuracy
PLS-DA	PJS vs PPM	–	0,951	0,107	0,7
	PJS vs PPS	–	0,953	–0,522	0,5
	PPS vs PPM	–	0,988	–0,051	0,5
	PPS vs PJS vs PPM	–	0,927	–0,502	0,5
OPLS-DA	PJS vs PPM	0,998	–	0,537	–
	PJS vs PPS	0,998	–	0,441	–
	PPS vs PPM	1	–	0,574	–

The performance metrics of the chemometric models, presented in Table 1, underscore the reliability of OPLS-DA for classification tasks in food authentication. While PLS-DA demonstrated strong explanatory power, its predictive ability was less reliable, as indicated by relatively lower Q² values, particularly in comparisons like PJS vs PPS. In contrast, the OPLS-DA models exhibited consistently higher Q² values, with better classification accuracy, making them the preferred method for distinguishing between the Pempek samples. This distinction is crucial for ensuring reliable geographical authentication, especially when the accuracy of predictions is essential.

The combination of chemometric analysis, specifically OPLS-DA, with HRMS data has established a strong framework for verifying the geographical origin of Pempek. The clear differentiation of samples according to their metabolomic profiles illustrates the efficacy of this method in identifying regional variations. This approach enhances food traceability while aiding in the fight against food fraud and ensuring the

authenticity of traditional foods, thereby safeguarding cultural heritage and bolstering consumer confidence.

3.4. Identification and analysis of candidate differential metabolites

The Variable Importance in Projection (VIP) is a metric quantifies the contribution of each metabolite to the classification or prediction model. This metric is crucial in metabolomics studies employing multivariate data analysis to identify metabolites with significant predictive capabilities, facilitating the selection of biomarkers for diverse applications, including food quality assessment and authenticity verification. The regression coefficients of metabolites in the model are utilised to calculate the VIP score in metabolomics research. A VIP score exceeding 1 signifies that a metabolite effectively differentiates between sample groups, and this methodology has been employed to identify adulteration in beef (A Windarsih et al., 2023). VIP rankings can also serve to evaluate the metabolic profiles of various foods, alongside food quality. The classification of coffee based on metabolites with elevated VIP scores correlates with quality markers and sensory attributes (Vezzulli et al., 2022). The compounds that improve the flavour and aroma of fermented foods can be identified through VIP ratings, contributing to a deeper understanding of the fermentation process (Adebo et al., 2021).

The metabolite compounds present in Pempek arise from natural substances as well as derivatives resulting from various materials and processing methods. The VIP score serves to highlight the importance of key metabolites in differentiating between Pempek groups. Metabolites with a VIP score exceeding 2 are regarded as significant characteristics, which include Tucupentol ($C_{35}H_{64}O_8$), (9R,10R)-9,10-dihydroxyoctadecanoic acid ($C_{18}H_{36}O_4$), and 2-(ethylamino) acetic acid ($C_4H_9NO_2$). Tucupentol is a novel metabolite compound known as mono-tetrahydrofuran-pentahydroxy-acetogenin, classified as a derivative of fatty acids. The (9R,10R)-9,10-dihydroxyoctadecanoic acid is a fatty acid derivative compound containing two hydroxyl groups (-OH) at positions 9 and 10 in the carbon chain of stearic acid. This compound plays a significant role in fatty acid metabolism and serves as a structural element in lipids or as an intermediary in various lipid biosynthesis pathways. In lipidomic research, this compound serves as a tool to delineate metabolites generated from the metabolism of fatty acids.

The highest VIP score of metabolite markers is [(2R)-2-[(5Z,8Z,11Z,14Z,17Z)-icosa-5,8,11,14,17-pentaenoyl]oxy-3-pentadecanoyloxypropyl] 2-(trimethylazaniumyl)ethyl phosphate ($C_{43}H_{76}NO_8P$)

in PJS, 2-(ethylamino)acetic acid ($C_4H_9NO_2$), commonly known as N-Ethylglycine in PPM, and (2S)-4-[(2S)-2,6-dihydroxy-9-[(2S,5R)-5-[(1R,4S,5S)-1,4,5-trihydroxyheptadecyl]oxolan-2-yl]nonyl]-2-methyl-2H-furan-5-one ($C_{35}H_{64}O_9$), commonly referred to as Tucupentol, in PPS. The $C_{43}H_{76}NO_8P$ is a phosphatidylcholine while the $C_4H_9NO_2$ is a metabolite classified within the category of structurally modified amino acids. N-Ethylglycine is an ethyl amide of glycine, synthesised through the addition of an ethyl group ($-CH_2CH_3$) to the amine nitrogen of glycine.

The analysis of differential metabolites between the three Pempek groups (PPS, PPM, and PJS) using Venn diagrams (Fig. 4A and 4B) highlighted distinct and shared metabolic profiles. Fig. 4A illustrates that 46 metabolites were shared among all three groups, however each group had distinct metabolites: 17 exclusives to PPM, 6 unique to PPS, and 20 distinctive to PJS. These findings reinforce the idea that geographical factors contribute significantly to the variation in metabolomic profiles.

Volcano plots illustrating fold changes and statistical significance (Fig. 5) identified key metabolites which showed significant differential expression between the groups.

Compounds identified as N-(2-hydroxyethyl) icosanamide ($C_{26}H_{41}NO$), [(2R)-2-[(5Z,8Z,11Z,14Z,17Z)-icosa-5,8,11,14,17-pentaenoyl]oxy-3-pentadecanoyloxypropyl] 2-(trimethylazaniumyl) ethyl phosphate ($C_{43}H_{76}NO_8P$) and (2S,3R)-2-aminotetradecan-3-ol were significantly high in PJS, but found in low concentration in PPS. On the contrary, the [(2S)-1-tetradecanoyloxy-3-[(2R,3R,4S,5R,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxypropan-2-yl] (Z)-hexadec-9-enoate ($C_{39}H_{72}O_{10}$), (11Z,13E)-15-oxoicosa-11,13-dienoic acid ($C_{20}H_{34}O_3$), 18-(2-methylprop-2-enyloxy)octadecyl 2-methylprop-2-enoate ($C_{26}H_{46}O_4$), 2-[(Z)-hexadec-7-enyl]-3-methylidenebutanedioic acid ($C_{21}H_{36}O_4$), (2S)-4-[(2S)-2,6-dihydroxy-9-[(2S,5R)-5-[(1R,4S,5S)-1,4,5-trihydroxyheptadecyl]oxolan-2-yl]nonyl]-2-methyl-2H-furan-5-one ($C_{35}H_{64}O_9$), (9R,10R)-9,10-dihydroxyoctadecanoic acid ($C_{18}H_{36}O_4$), and 2-(ethylamino)acetic acid ($C_4H_9NO_2$) were prevalent in PPS but sparse in PJS. As for the PMS, 2-(ethylamino) acetic acid was the most predominant, succeeded by (9R,10R)-9,10-dihydroxyoctadecanoic acid. In contrast to the PPS, the PMS exhibited a low abundance of $C_{20}H_{34}O_3$ and $C_{39}H_{72}O_{10}$, both classified as lipid compounds. All of these identified metabolites could serve as potential biomarkers for geographical authentication of Pempek. Their elevated concentrations in specific groups solidify their role

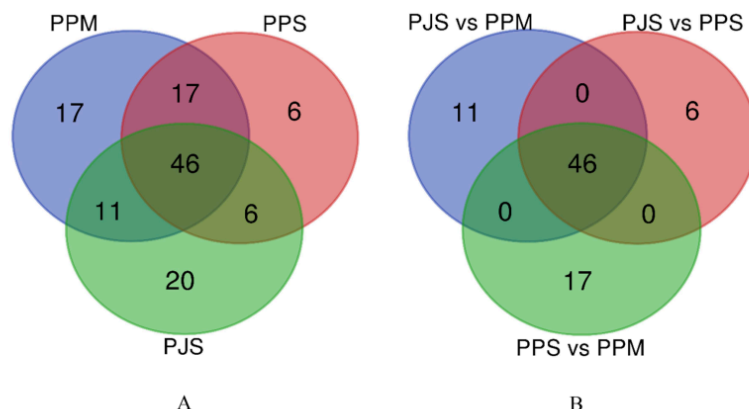
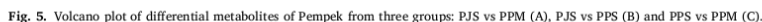


Fig. 4. The number of differential metabolites Venn diagram analysis in PPS vs PJS vs PPM (A) and PJS vs PPS: PJS vs PPS: PPS vs PPM (B).



This research elucidates the chemical composition of Pempek as influenced by regional variations stemming from diverse raw materials (fish and starch types, such as sago or tapioca), their ratios, and processing methods. Pempek, originating from the same location, exhibited distinct metabolites when produced from different fish species, particularly to snakehead and mackerel.

Chemometric approaches integrated with metabolomic analysis could properly determine geographical markers in food products (Zhou et al., 2020), and their application has been successfully employed in the geographical authenticity of Pempek in the present study. Identifying distinctive metabolite markers indicative of geographical origins, such as N-(2-hydroxyethyl)icosanamide, [(2R)-2-(5Z,8Z,11Z,14Z,17Z)-icos-5,8,11,14,17-pentaenyl]oxy-3-pentadecanoyloxypropyl], tri-(methylazaniumyl)ethyl 5-sphosphate and (2S,3R)-2-aminotetradecan-3-ol (Jambi's Pempek); [(2S)-1-tetradecanoyloxy-3-[(2R,3R,4S,5R,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxypropan-2-yl]-2-hexadec-9-enoate, (11Z,13E)-15-oxoicosa-11,13-dienoic acid (Palembang's Pempek) as well as 2-(ethylamino)acetic acid sometimes referred to as N-ethylglycine, serve as biomarkers for mackerel Pempek has emphasised the relevance of HR Orbitrap MS in food authentication. Extending this method to other traditional Indonesian foods could further enhance food traceability and protect regional culinary identities. Future research should explore applying these techniques to other food products, contributing to broader food authenticity and cultural preservation strategies. The findings of this study affirm the value of

4. Conclusion

Ethical statement

This article does not contain any studies that would require an ethical statement.

CRediT authorship contribution statement

Agus Supriadi: Writing – original draft, Methodology, Funding acquisition, Conceptualization. **Sherly Ridhowati:** Formal analysis, Data curation. **Daniel Saputra:** Writing – review & editing, Supervision, Conceptualization. **Wulandari:** Resources. **Shanti Dwita Lestari:** Writing – review & editing.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Acknowledgement

The authors would like to acknowledge the financial support from The Ministry of Education and Culture, Republic Indonesia (Fundamental Grand No. 090/E5/PG.02.00.PL/2024)

Supplementary materials

Supplementary material associated with this article can be found, in the online version, at [doi:10.1016/j.focha.2025.100914](https://doi.org/10.1016/j.focha.2025.100914).

Data availability

The data that has been used is confidential.

References

- Adebo, O. A., Oyeiyinka, S. A., Adebiyi, J. A., Feng, X., Wilkin, J. D., Kewuyemi, Y. O., Abrahams, A. M., & Tugizimana, F. (2021). Application of gas chromatography–mass spectrometry (GC-MS)-based metabolomics for the study of fermented cereal and legume foods: A review. *International Journal of Food Science & Technology*, 56(4), 1514–1534. <https://doi.org/10.1111/ijfs.14794>
- Bozza, D., Barboni, D., Spadafora, N. D., Felletti, S., De Luca, C., Nosengo, C., Compagnin, G., Cavazzini, A., & Catani, M. (2024). Untargeted metabolomics approaches for the characterization of cereals and their derived products by means of liquid chromatography coupled to high resolution mass spectrometry. *Journal of Chromatography Open*, 6. <https://doi.org/10.1016/j.jcoa.2024.100168>. Elsevier B.V.
- Cajka, T. (2024). Liquid chromatography–mass spectrometry–based metabolomics approaches for foodomics research. *Current opinion in food science*. Elsevier Ltd. <https://doi.org/10.1016/j.cofs.2024.101201>. Vol. 58.
- Creydt, M., & Fischer, M. (2018). Omics approaches for food authentication. *Electrophoresis* (pp. 1569–1581). Wiley-VCH Verlag. <https://doi.org/10.1002/elps.201800004>. Vol. 39, Issue 13.
- Dou, X., Zhang, L., Yang, R., Wang, X., Yu, L., Yue, X., Ma, F., Mao, J., Wang, X., Zhang, W., & Li, P. (2022). Mass spectrometry in food authentication and origin traceability. *Mass Spectrometry Reviews*, e21779. <https://aplscholar.org/CompusID248569989>.
- Hye Hur, S., Kim, H., Kim, Y. K., An, J. M., Hye Lee, J., & Jin Kim, H. (2023). Discrimination between Korean and Chinese Kimchi using inductively coupled plasma-optical emission spectroscopy and mass spectrometry: A multivariate analysis of Kimchi. *Food Chemistry*, 423(April), Article 136235. <https://doi.org/10.1016/j.foodchem.2023.136235>
- Liu, X., Zhong, C., Xie, J., Liu, H., Xie, Z., Zhang, S., & Jin, J. (2023). Geographical region traceability of Poria cocos and correlation between environmental factors and biomarkers based on a metabolomic approach. *Food Chemistry*, 417. <https://doi.org/10.1016/j.foodchem.2023.135817>
- Mihailova, A., Kelly, S. D., Chevallier, O. P., Elliott, C. T., Maestroni, B. M., & Cannavan, A. (2021). High-resolution mass spectrometry-based metabolomics for the discrimination between organic and conventional crops: A review. In *Trends in Food Science and Technology*, 110 pp. 142–154). Elsevier Ltd. <https://doi.org/10.1016/j.tifs.2021.01.071>
- Pan, Y., Gu, H. W., Lv, Y., Yin, X. L., Chen, Y., Long, W., Fu, H., & She, Y. (2022). Untargeted metabolomic analysis of Chinese red wines for geographical origin traceability by UPLC-QTOF-MS coupled with chemometrics. *Food Chemistry*, 394. <https://doi.org/10.1016/j.foodchem.2022.133473>
- Principal, A., Glogovetan, A. I., Sedik, P., & Pocol, C. B. (2022). The importance of certification with PDO and PGI quality schemes: A critical analysis of the romanian beekeeping sector. *Bulletin of University of Agricultural Sciences and Veterinary Medicine Cluj-Napoca. Food Science and Technology*, 78(2). <https://doi.org/10.15835/buasvmcn-fst.2021.0024>
- Ratnashekar, C., Chevallier, O., McCarron, P., McGrath, T. F., Wu, D., Nguyen Doan Duy, L., Kapil, A. P., McBride, M., & Elliott, C. T. (2021). Metabolomic fingerprinting of volatile organic compounds for the geographical discrimination of rice samples from China, Vietnam and India. *Food Chemistry*, 334. <https://doi.org/10.1016/j.foodchem.2020.127553>
- Ren, Y.feng, Feng, C., Ye, Z.hao, Zhu, H.yan, Hou, R.yan, Granato, D., Cai, H.mei, & Peng, C.yi (2022a). Keemun black tea: Tracing its narrow-geographic origins using comprehensive elemental fingerprinting and chemometrics. *Food Control*, 133(PB), Article 108614. <https://doi.org/10.1016/j.foodcont.2021.108614>
- Ren, Y.feng, Feng, C., Ye, Z.hao, Zhu, H.yan, Hou, R.yan, Granato, D., Cai, H.mei, & Peng, C.yi (2022b). Keemun black tea: Tracing its narrow-geographic origins using comprehensive elemental fingerprinting and chemometrics. *Food Control*, 133(PB), Article 108614. <https://doi.org/10.1016/j.foodcont.2021.108614>
- Sgroi, F. (2021). Food traditions and consumer preferences for cured meats: Role of information in geographical indications. *International Journal of Gastronomy and Food Science*, 25(May), Article 100386. <https://doi.org/10.1016/j.ijgfs.2021.100386>
- Supriadi, A., Saputra, D., Priyanto, G., Baahaki, A., & Pambayun, R. (2020). The profile of pempek as a determining factor of quality, originality and ethnicity. *Journal of Physics: Conference Series*, 1485, Article 012032. <https://doi.org/10.1088/1742-6596/1485/1/012032>
- Supriadi, Agus, Saputra, D., Priyanto, G., Pambayun, R., & Oswari, L. D. (2018). Mapping and development strategy of Pempek - A specialty traditional food of South Sumatra, Indonesia. *Potravinarsko Slovak Journal of Food Sciences*, 12(1), 707–715. <https://doi.org/10.5219/975>
- Surya, R., Destifen, W., & Stephanie, S. (2023). Review on pempek, a traditional fishcake from South Sumatra, Indonesia: History, nutritional aspects, current development, and innovation. *International Journal of Gastronomy and Food Science*, 34. <https://doi.org/10.1016/j.ijgfs.2023.100828>. AZTI-Tecnalia.
- Tan, H. R., & Zhou, W. (2024). Metabolomics for tea authentication and fraud detection: Recent applications and future directions. *Trends in Food Science and Technology*. Elsevier Ltd. <https://doi.org/10.1016/j.tifs.2024.104558>. Vol. 149.
- Vezzulli, F., Rocchetti, G., Lambri, M., & Lucini, L. (2022). Metabolomics combined with sensory analysis reveals the impact of different extraction methods on coffee beverages from coffea arabica and coffea canephora var. Robusta. *Foods*, (6), 11. <https://doi.org/10.3390/foods11060807>
- Wargadalem, F. R., Wasino, & Yulifar, I. (2023). Pempek Palembang: history, food making tradition, and ethnic identity. *Journal of Ethnic Foods*, 10(1). <https://doi.org/10.1186/s42779-023-00209-z>
- Windarsih, A., Bakar, N. K. A., Rohman, A., Riswanto, F. D. O., & Erwanto, Y. (2023). Untargeted lipidomics approach using LC-orbitrap HRMS to discriminate lard from beef tallow and chicken fat for the authentication of halal. *Grasas Y Aceites*, 74(3), e512. <https://doi.org/10.3989/gya.0980221>
- Windarsih, Anjar, Suratno, Warmiko, H. D., Indrianiingsih, A. W., Rohman, A., & Uluamuddin, Y. I. (2022). Untargeted metabolomics and proteomics approach using liquid chromatography-Orbitrap high resolution mass spectrometry to detect pork adulteration in Pangasius hypophthalmus meat. *Food Chemistry*, 386. <https://doi.org/10.1016/j.foodchem.2022.132856>
- Yong, C. H., Muhammad, S. A., Aziz, F. A., Nasir, F. I., Mustafa, M. Z., Ibrahim, B., Kelly, S. D., Cannavan, A., & Seow, E. K. (2022). Detecting adulteration of stingless bee honey using untargeted 1H NMR metabolomics with chemometrics. *Food Chemistry*, 368. <https://doi.org/10.1016/j.foodchem.2021.130808>
- Zhong, P., Wei, X., Li, X., Wei, X., Wu, S., Huang, W., Koidis, T., Xu, Z., & Lei, H. (2022). Untargeted metabolomics by liquid chromatography-mass spectrometry for food authentication: A review. *Comprehensive Reviews in Food Science and Food Safety*, 21. <https://doi.org/10.1111/1541-4337.12938>

Food Chemistry Advances 2025 Untargeted metabolomics profiling for the geographical

ORIGINALITY REPORT

8%

SIMILARITY INDEX

8%

INTERNET SOURCES

5%

PUBLICATIONS

5%

STUDENT PAPERS

PRIMARY SOURCES

1

nrc-publications.canada.ca

Internet Source

1%

2

hdl.handle.net

Internet Source

1%

3

plantaedb.com

Internet Source

1%

4

eprints.whiterose.ac.uk

Internet Source

1%

5

patents.google.com

Internet Source

1%

6

zfin.org

Internet Source

1%

7

Goldy Bhowmick, Dilip K. Rai, Oyenike Olatunji, Kieran Kilcawley et al. "Inhibitors of methane (CH₄) producing bacteria: Development of hydrolysates and fermentates from brown seaweeds and identification of biomolecules with enteric CH₄ abatement potential", Springer Science and Business Media LLC, 2024

Publication

1%

8

Submitted to Sriwijaya University

Student Paper

1%

9

www.mdpi.com

Internet Source

1%

Exclude quotes	On	Exclude matches	< 1%
Exclude bibliography	On		