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Non-destructive characterisation of lip cosmetics using attenuated total reflectance fourier-transform infrared spectroscopy with chemometrics

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ABSTRACT

Lip cosmetics present a challenging identification and differentiation of lip cosmetics in forensics, given their similar chemical compositions, particularly within the same colour category. The authors utilised attenuated total reflection spectroscopy and chemometrics to analyse 30 brown lip cosmetic samples across five categories: lip crayons, lip glosses, liquid lipsticks, lip pencils, and solid lipsticks. The major findings observed in the analysis of lip cosmetics included weak intensity spectra for key functional groups such as hydroxy, aliphatic, carbonyl-containing species, and ether. In addition, the hierarchical cluster analysis grouped most samples into two main clusters: lip crayons and most solid lipsticks in one, and most lip glosses, liquid lipsticks, and lip pencils. Principal component analysis revealed clear clusters of lip glosses, liquid lipsticks, and lip pencils, with scattered lip crayons and solid lipsticks. Furthermore, trace analyses yielded limited results, with only one trace (TR3T) showing similarity to the lip gloss (LG2) spectrum. This study sheds light on the complexities surrounding the differentiation of lip cosmetics. Further studies should study several types of lip cosmetics with varying shades and analyse their traces on different substrates to produce accurate, reliable, and generalised outcomes. These findings emphasise the need for more comprehensive investigations to enhance forensic analytical approaches.

Keywords: *Forensic science; lip cosmetics; infrared spectroscopy; attenuated total reflectance spectroscopy, chemometrics*

INTRODUCTION

Evidence at a crime scene consists of various materials, some of which are present in minute traces, such as lip cosmetics. Lip cosmetics, such as lipsticks, are crucial in forensic investigations because of their prevalence and transferability. Lipstick smears often encountered on surfaces such as drinking cups, tissue paper, clothing, bedding, and cigarette butts (Gładysz et al., 2021) can establish links between suspects at crime scenes and victims, providing investigative leads in cases of sexual assault, robbery, and homicide. Although there

is no direct evidence, cosmetic traces play a significant role in crime reconstruction and offer invaluable insights into the sequence of crime events (Asrul Fahmi, 2019; Ezegbogu & Osadolor, 2019; Gładysz et al., 2020).

Understanding the chemical composition and transfer of lip cosmetic traces is essential for their effective utilisation in forensic casework. Thus, meticulous collection and analysis of trace materials in forensic investigations provide essential information about samples and their sources. Various techniques have been employed for trace analysis, including non-destructive methods such as Fourier-transform infrared (FTIR) spectroscopy. FTIR spectroscopy, particularly attenuated total reflectance (ATR) FTIR spectroscopy, is an effective analytical technique that enables the identification and analysis of the chemical composition of various materials. Chemometrics involves the application of mathematical and statistical methods to chemical data and the extraction of meaningful information from complex spectral datasets in the context of spectroscopic analyses. ATR FTIR spectroscopy is combined with chemometric tools, such as principal component analysis (PCA), linear discriminant analysis (LDA), and hierarchical cluster analysis (HCA), to identify patterns, classify samples, and make predictions based on spectral information. This method offers rapid and accurate identification and differentiation of various brands and shades of lip products, including those found in trace quantities on various substrates (Chophi et al., 2020; Mohamed Ghazali & Ismail, 2018; Sharma et al., 2019).

The choice of ATR FTIR spectroscopy over other techniques is justified by its non-destructive nature, minimal sample preparation, cost-effectiveness, and repeatable results that are generated quickly. Unlike Raman spectroscopy, ATR FTIR spectroscopy does not display limitations such as strong interfering fluorescence and highly priced lasers (Ezegbogu & Osadolor, 2019; Gładysz et al., 2021). Previous studies have used ATR FTIR spectroscopy to analyse lipstick smears and have produced successful results. Kaur et al. (2020) used ATR FTIR and chemometric techniques (principal component analysis, PCA, and linear discriminant analysis, LDA) to classify red, pink, and brown lipstick samples according to their brands. Chophi et al. (2020) differentiated red shades of lipstick samples using PCA and PCA-LDA with a high discriminating power. Sharma et al. (2019) performed ATR FTIR analysis on lipstick samples and calculated discrimination power by factor analysis, hierarchical cluster analysis (HCA), and k-mean cluster analysis. The most recent works include Yadav et al. (2023) analysis of lip balms using PCA and LDA, and Ka Khei et al. (2023) analysis of red lipsticks using partial least square-discriminant analysis (PLS-DA). However, research on lip cosmetics is limited to solid lipsticks of primarily red shades, leaving a gap in the analysis of other lip cosmetics, such as liquid lipsticks, lip pencils, and other lip products. For instance, darker or brown shades trend globally during the fall and winter months and represent a significant portion of the market. Thus, it is necessary to conduct similar studies on other lip cosmetic types with various colour shades.

This study aimed to fill this research gap by applying chemometrics to ATR FTIR spectra of various lip cosmetic types to enhance their characterisation and identification in forensic investigations. By understanding the chemical characteristics of lip cosmetics through ATR FTIR spectroscopy and chemometrics, this study sought to shed light on the forensic significance of these cosmetics as trace evidence in real-world investigations. Additionally, it enhances its potential as an emerging forensic science standard for trace evidence analysis.

METHODOLOGY

Sample collection

Thirty lip cosmetics samples with similar brown shades were procured from various brands in Selangor, Malaysia, encompassing both popular and lesser-known brands. The selection was based on the product type, including lip crayons, lip glosses, liquid lipsticks, lip pencils, and solid lipsticks, and with the rationale that similar shades require spectral and chemometrics analyses to distinguish them. Each sample was uniquely de-identified for analysis, focusing on brown colour shades and specific lip cosmetic types intended for investigation, ensuring a representative sample set for analysis. Reference codes were assigned for each type using the first letters and consequent numbering, as follows: lip crayon LC1 to LC5 for five samples; lip gloss LG1 to LG6 for six samples; liquid lipstick LL1 to LL7 for seven samples; lip pencil LP1 to LP5 for five samples; and lipstick LS1 to LS7 for seven samples.

Experimental analysis

Sample preparation

Lip cosmetics were sparingly applied to commonly encountered substrates – cloth, paper, tissue, and wet wipes (Table 1). Lip cosmetics were applied to the forearm and wiped off after five minutes of drying time using substrates cut into squares (3 cm × 3 cm) to standardise the experimental conditions for accurate analysis. The substrate samples were air-dried further and stored in labelled envelopes to minimise contamination until FTIR analysis.

Spectrophotometric analysis of lip cosmetic samples

Spectra were obtained using an IRAffinity-1 FTIR spectrophotometer (Shimadzu, Japan) with a MIRacle™

Single Reflection ATR sampling accessory (PIKE Technologies, USA). Data were recorded as absorbance between 4000 and 400 cm^{-1} using a LabSolutions IR analytical data system (Shimadzu, Japan) with 45 scans accumulated per sample at a resolution of 8.0, which is in the recommended range for balancing spectral detail and potential peak broadening in solid or liquid samples (Resolution and Aperture, n.d.). The wavelength range (4000 to 400 cm^{-1}) was chosen for its effectiveness in analysing lip cosmetic functional groups. Pure samples were placed directly on the crystal plate with a spatula without a substrate. Spectral readings were taken in ten replicates before trace samples were prepared. The ATR crystal plate was cleaned with acetone (Bendosen) to prevent contamination and erroneous readings. Basic pre-treatment steps such as background scans of the clean crystal and blank substrates were conducted.

Table 1

Specifications of substrates used in the present study

Substrate	Specifications
Cloth	95% cotton blouse, black
Paper	80gsm printer paper
Tissue	4ply pocket tissue, fragrance-free
Wet Wipe	Spunlace nonwoven material infused with Aloe vera and vitamin E, fragrance-free

Chemometric analysis

Data from the FTIR spectral analysis were processed in Microsoft Excel and analysed using Minitab statistical software. The conventional interpretation of patterns in the spectrum is time-consuming and challenging, particularly when dealing with samples that share similar spectra and chemical structures. To address this, chemometric techniques such as hierarchical cluster analysis (HCA) and principal component analysis (PCA) were applied. HCA, which employs complete linkage techniques and Euclidean distance as a proximity measure, was used to link the clusters in the dataset, aiding the assignment of lip cosmetic samples to their source of origin. PCA was used to simplify the data into variables for better visualisation of the spectral pattern. The results were displayed using scree and score plots for the first two components, facilitating the observation of compositional variations among lip crayons, lip glosses, liquid lipsticks, lip pencils, and lipsticks.

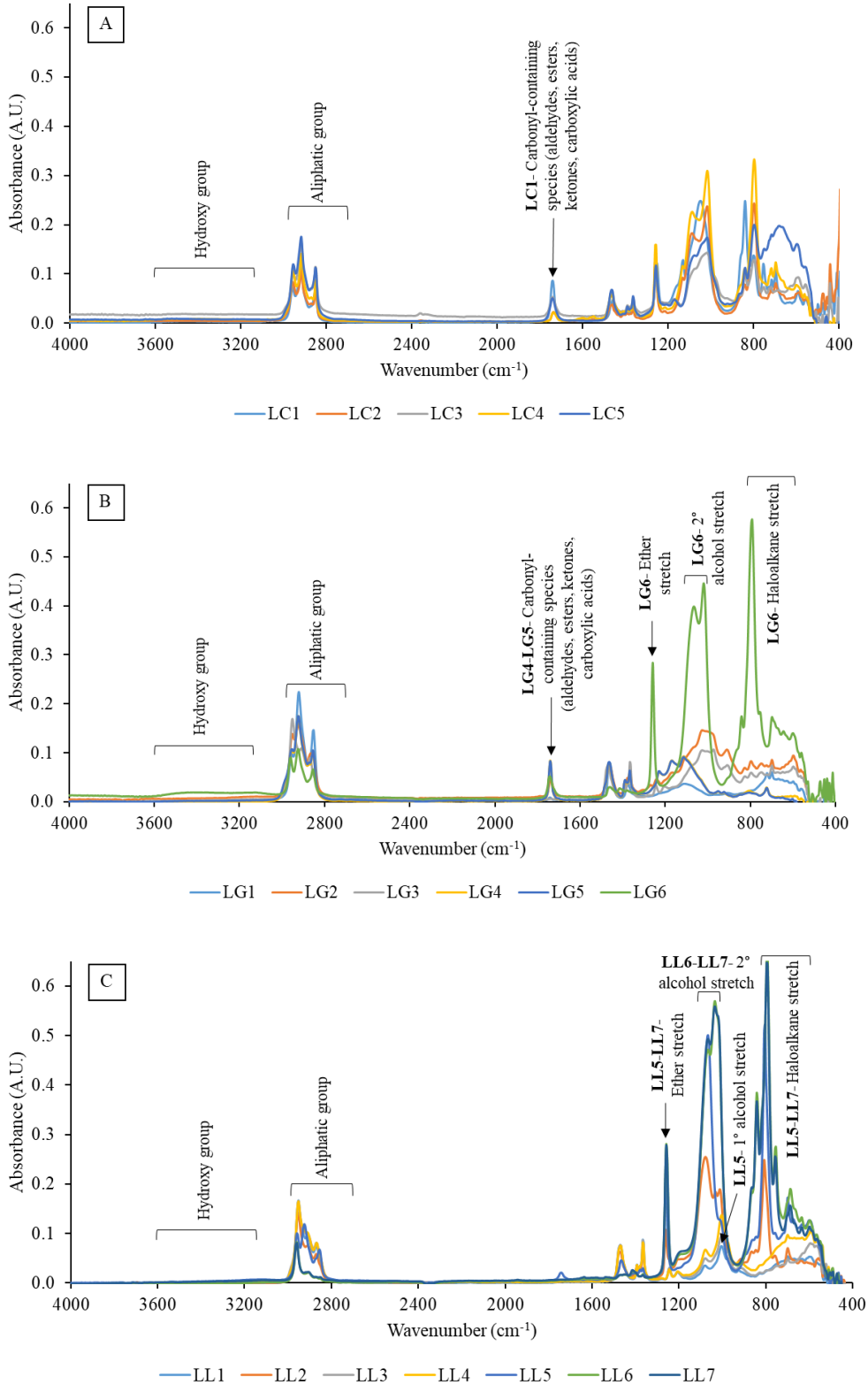
RESULTS

Spectral examination of source samples

Spectra for qualitative and quantitative analyses were collected using an IRAffinity-1 FTIR spectrophotometer with a MIRacle™ Single Reflection ATR sampling accessory. Because samples of similar compositions were being evaluated, the entirety of the ATR FTIR spectra was assessed to determine the functional groups in this study's lip cosmetic source/pure samples. At wavenumbers of 3600-3100 cm^{-1}, broad bands of weaker intensity were observed for all samples across the five lip cosmetic types (Figures 1A – 1E), indicating the presence of O-H vibrations from compounds such as alcohol and water. At 3000-2700 cm^{-1}, weak bands were noted for all samples, where aliphatic groups (C-H sp^3) were ordinarily detected as having moderately strong to strong intensities. A similar observation was made for peaks in most samples that would have otherwise been recognised for C=O carbonyl-containing species such as aldehydes, esters, ketones, and carboxylic acids that are seen in the 1750-1700 cm^{-1} region. Samples LG6 (lip gloss) and LL5-LL7 (liquid lipsticks) showed a weak band of ether (aryl C-O) stretching vibrations near 1250 cm^{-1} and moderate to strong intensity bands of haloalkane stretches with chlorine groups (C-Cl_x) in the 860-505 cm^{-1} region. These samples also showed moderate peaks for secondary alcohol stretching at 1150-1000 cm^{-1}, except for LL5, which showed moderate peaks for primary alcohol stretching at 1075-1025 cm^{-1} (Larkin, 2011; Thompson, 2018). Ultimately, the results of the visual examination concluded that the spectra displayed weak intensity where there should have been strong or moderate bands for functional groups such as hydroxy group (3600-3100 cm^{-1}), aliphatic groups (3000-2700 cm^{-1}), carbonyl-containing species (1750-1700 cm^{-1}), and ether (near 1250 cm^{-1}). These bands/peaks are tabulated in Table 2.

Figure 1

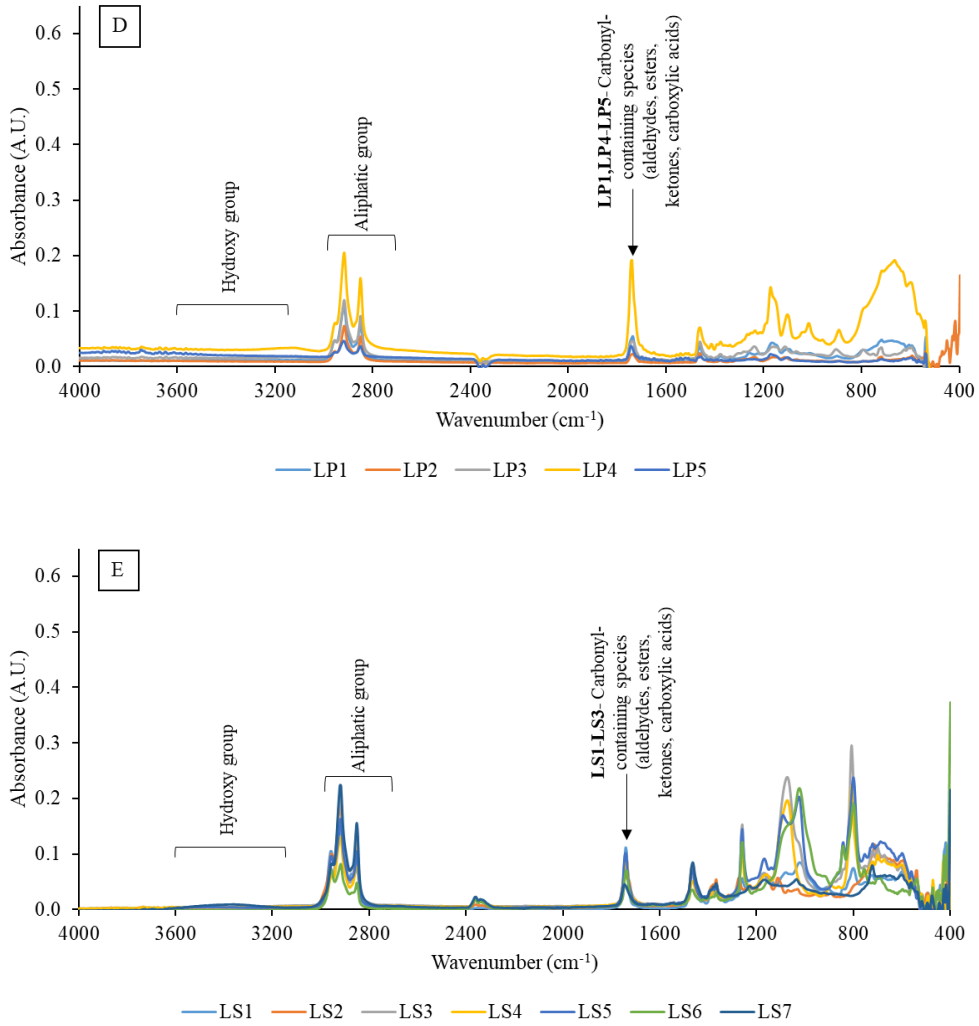
ATR FTIR spectra



Notes: ATR FTIR spectra obtained from (A) five lip crayons (LC1-LC5), (B) six lip glosses (LG1-LG6), (C) seven liquid lipsticks (LL1-LL7), (D) five lip pencils (LP1-LP5), and (E) seven solid lipsticks (LS1-LS7).

Figure 1 (continued)

ATR FTIR spectra



Notes: ATR FTIR spectra obtained from (A) five lip crayons (LC1-LC5), (B) six lip glosses (LG1-LG6), (C) seven liquid lipsticks (LL1-LL7), (D) five lip pencils (LP1-LP5), and (E) seven solid lipsticks (LS1-LS7).

Table 2

ATR FTIR band/peak assignment in lip cosmetic samples.

Sample(s)	Spectral Band/Peak (cm^{-1})	Band/Peak Assignments	References
All	3600-3100	Hydroxy group (O-H) vibrations	(Larkin, 2011; Thompson, 2018)
All	3000-2700	Aliphatic groups (C-H sp^3)	(Larkin, 2011; Thompson, 2018)
Most	1750-1700	Carbonyl-containing (C=O) species	(Larkin, 2011; Thompson, 2018)
LG6, LL5-LL7	Near 1250	Ether (aryl C-O) stretching vibrations	(Larkin, 2011; Thompson, 2018)
LG6, LL5-LL7	1150-1000	Secondary alcohol stretching	(Larkin, 2011; Thompson, 2018)
LL5	1075-1025	Primary alcohol stretching	(Larkin, 2011; Thompson, 2018)
LG6, LL5-LL7	860-505	Haloalkane stretching with chlorine groups (C-Cl_x)	(Larkin, 2011; Thompson, 2018)

Multivariate statistical analyses on source samples

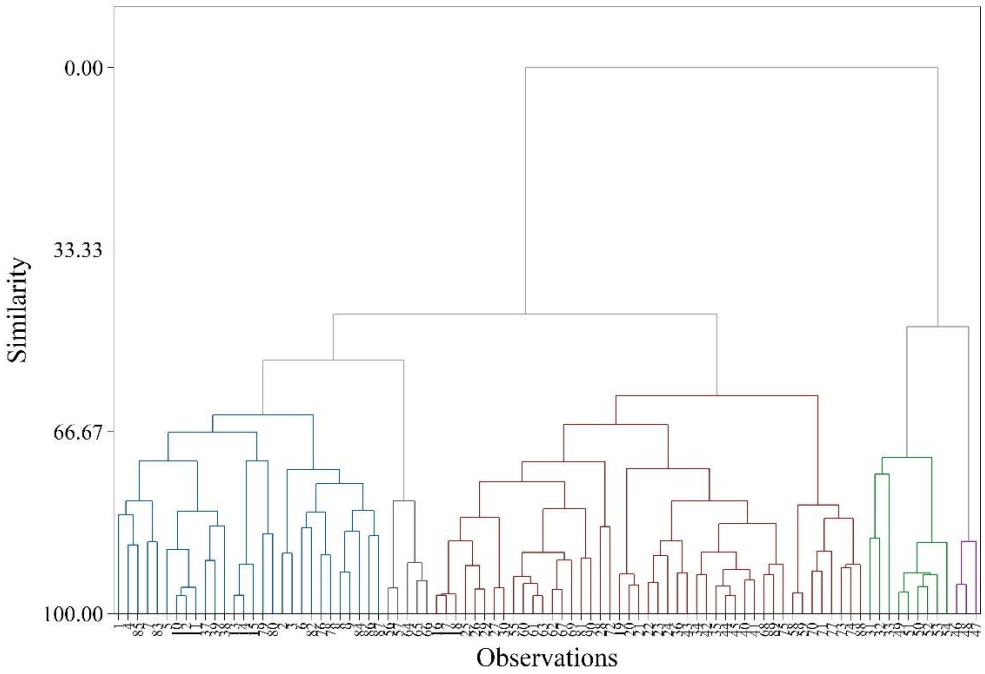
Hierarchical cluster analysis

The lip cosmetic samples in this study have similar chemical structures and absorptions in most spectral regions. Therefore, trial and error runs of HCA were performed for several regions in the spectra. It was found that the fingerprint region, 1500-400 cm^{-1}, gave better results than other regions. Additionally, unique absorption bands and the highest differences between samples were observed in the fingerprint region. Using complete linkage as the linkage strategy and Euclidean distance to measure the proximity or dissimilarity of observations, a dendrogram was created using a final partition of five clusters, occurring at a similarity level of approximately 60, and identified by colour coding the clusters (Figure 2). These chosen parameters were utilised to measure the differences between observations, providing a robust method for identifying distinct groupings or clusters within the data.

All lip crayons and most solid lipsticks shared cluster 1 (blue), while most lip glosses, liquid lipsticks, and lip pencils shared cluster 2 (red). Few exceptions were noted; for instance, LS1, LS2, and LS7 were seen in cluster 2 (red). Cluster 3 (green) contained LG6 and LL6, cluster 4 (purple) had LL5, and cluster 5 (grey) had LP1 and LP4.

Figure 2

A dendrogram showing partial discrimination of lip cosmetics was constructed using complete linkage and Euclidean distance



Notes: Clusters were colour-coded using the Minitab software. Blue: Cluster 1, red: Cluster 2, green: Cluster 3, purple: Cluster 4, and grey: Cluster 5.

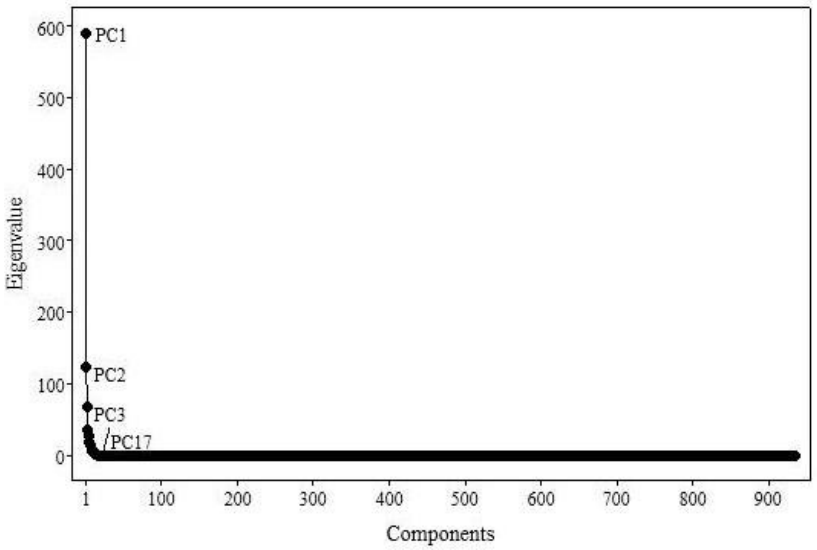
Principal component analysis

PCA was carried out on the entire ATR FTIR spectrum from 4000 to 400 cm^{-1}. Analysis using Minitab software identified 17 principal components with eigenvalues greater than 1 according to the Kaiser criterion. An ideal scree plot would show a steep curve and a straight line separated by an elbow bend. The principal components can be identified at this junction between the curve and the line. However, components were abundant in this analysis's scree plot (Figure 3) to discern the number from visual observations alone. The first principal component (PC1) accounted for 63.1% of the total variance, and the first four principal components explained 87.7% of the variation in the data. Typically, the first two components are used because they explain much of the variance in the data, offering a condensed representation of the dataset while retaining essential information for effective sample differentiation. A score plot (Figure 4) was constructed to display the cluster outcomes of the samples based on their scores in these two components. The unanimity of PCA is that samples situated adjacently share similar characteristics. Notably, clear clusters with few outliers were observed for lip glosses, liquid lipsticks, and lip pencils, whereas clusters of lip crayons and solid lipsticks were dispersed among the other three.

For further discrimination, a three-dimensional scatterplot (Figure 5) was constructed to confirm the groupings in PC1, PC2, and PC3, which explained 83.8% of the total variation. It reaffirmed the clusters observed for lip glosses, liquid lipsticks, and lip pencils, but it also showed the dispersion of lip crayons and solid lipsticks.

Figure 3

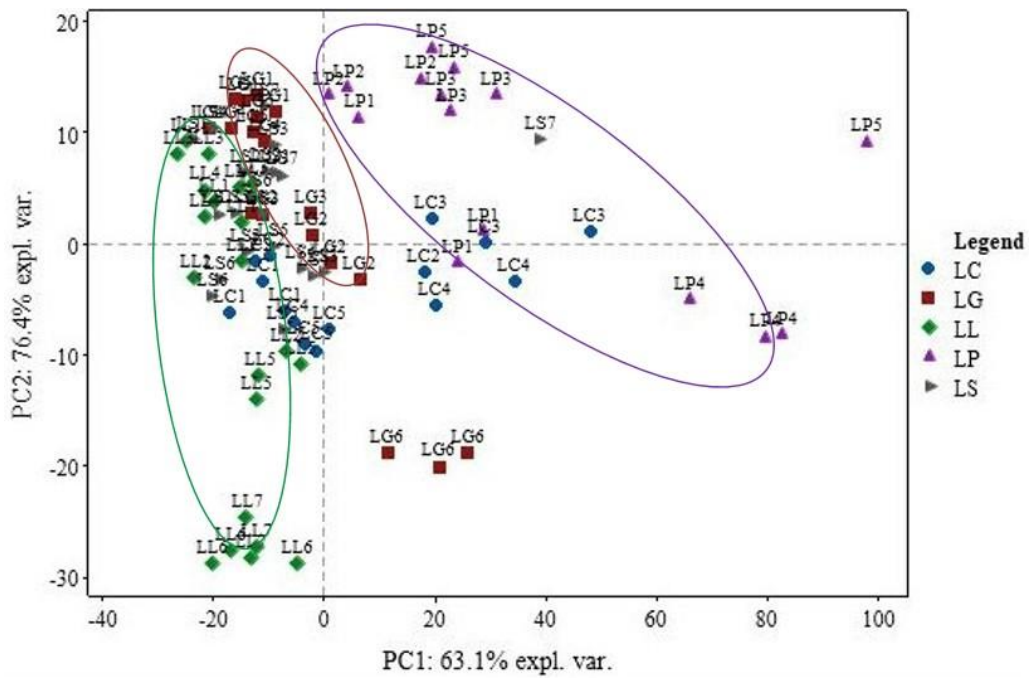
Scree plot for lip cosmetics showing the number of principal components versus their corresponding eigenvalue



Notes: Minitab software identified 17 principal components (labelled) according to the Kaiser criterion.

Figure 4

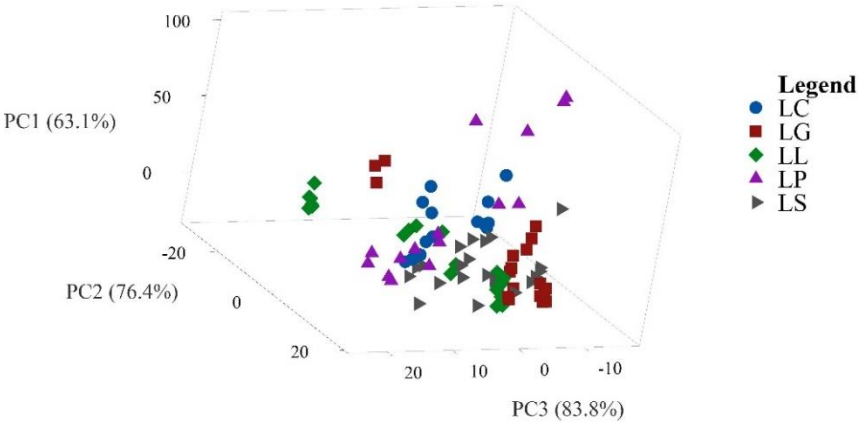
PCA score plot for lip cosmetics



Notes: PCA score plot for lip cosmetics showing three distinct clusters of LG, LL, and LP (circled in red, green, and purple), with exceptions of scattered plots of LC, LS, and a few LG, LL, and LP.

Figure 5

3D scatter plot of PC1, PC2, and PC3 for lip cosmetics



Notes: Percentages in brackets indicate the total variance.

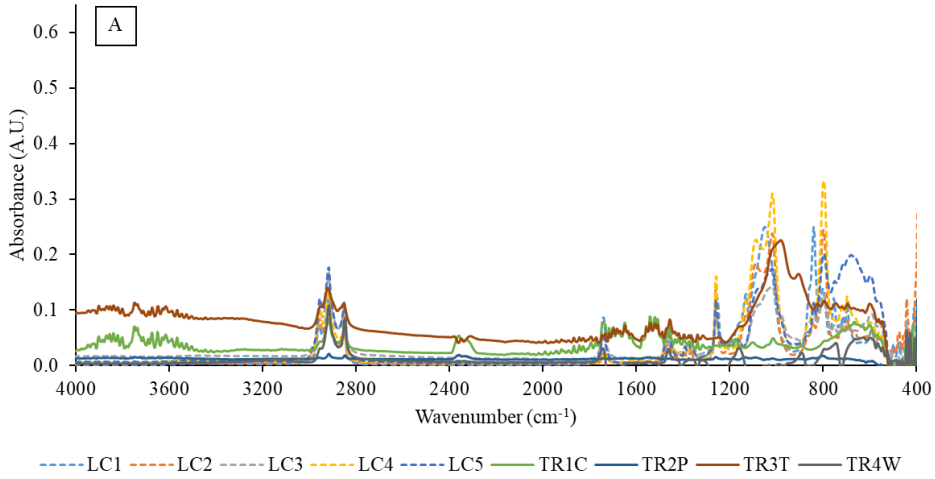
Trace analyses on unknown samples

The lip cosmetics were transferred to cloth, paper, tissue, and wet wipe substrates to stimulate traces left at a crime scene, chosen for their ability to mimic real-world scenarios and unique interactions with lip cosmetics, and their potential to carry trace evidence. Instances of these scenarios include accidental transfers to clothing, messages on paper, and using tissues and wet wipes to wipe off makeup.

Each of the four trace samples was randomly selected from the investigated substrates and assigned as an unknown sample: TR1C (trace #1 from cloth), TR2P (trace #2 from paper), TR3T (trace #3 from tissue), and TR4W (trace #4 from wipe). The absorbance of the blank substrates was measured and subtracted from the absorbance of the traces to account for substrate interference. The ATR FTIR spectra of all trace samples displayed weaker bands across the spectra, thus making it harder to distinguish and compare against the source (pure) samples (Figures 6A - 6E). Notably, TR3T closely resembled the lip gloss sample LG2 spectra, particularly in the 3000-2700 cm^{-1} and 1200-500 cm^{-1} regions (Figure 7), thus suggesting a potential link between the two. It is essential, however, to acknowledge the limitation of the observation of weaker bands in the spectra of all trace samples, which emphasises the need for additional research and confirmation to establish a definite link between TR3T and LG2.

Figure 6

Comparison of ATR FTIR spectra of trace samples



Notes: Comparison of ATR FTIR spectra of trace samples TR1C, TR2P, TR3T, and TR4W against source category of (A) lip crayons (LC1-LC5), (B) lip glosses (LG1-LG6), (C) liquid lipsticks (LL1-LL7), (D) lip pencils (LP1-LP5), and (E) solid lipsticks (LS1-LS7).

Figure 6 (continued)

Comparison of ATR FTIR spectra of trace samples

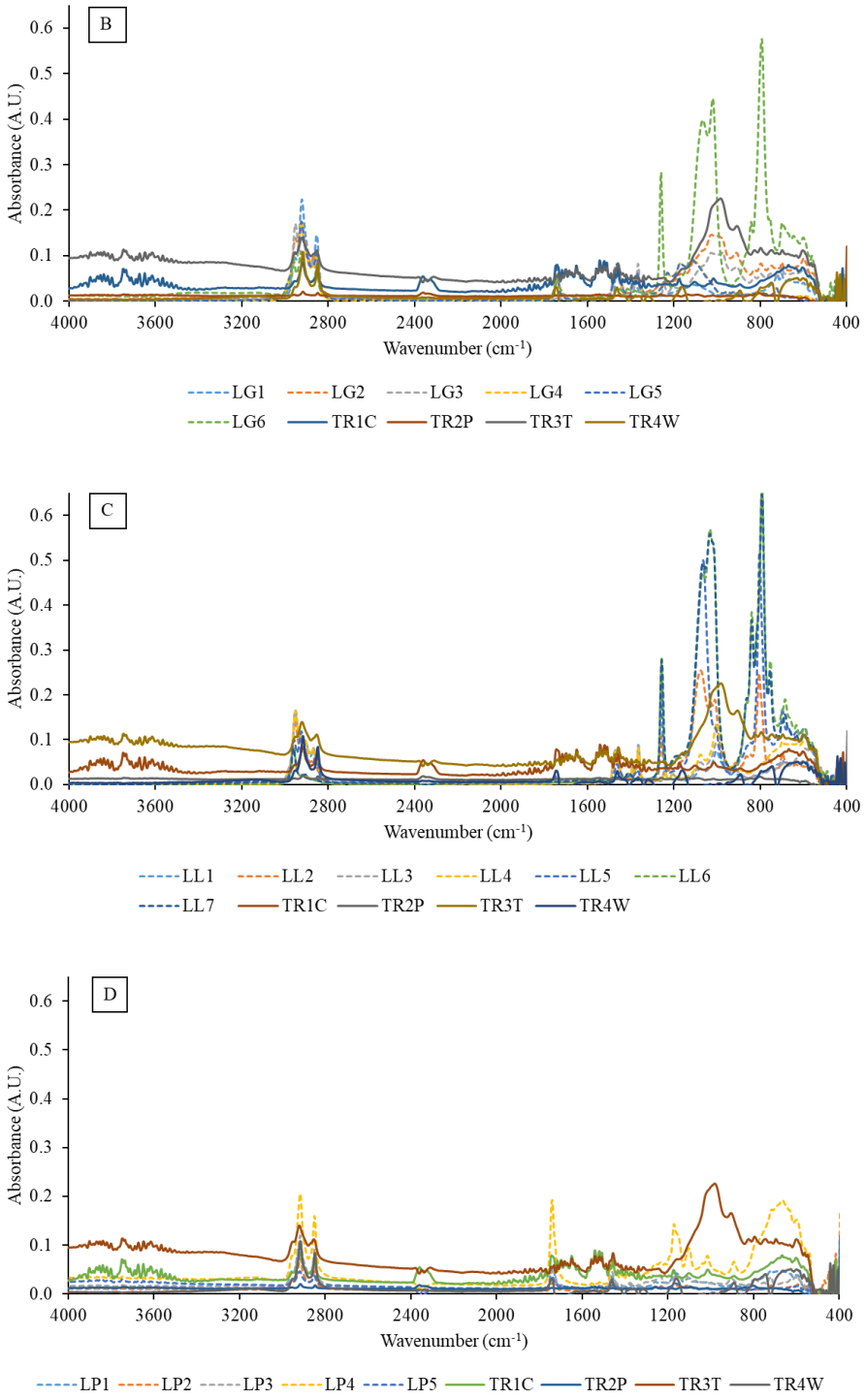


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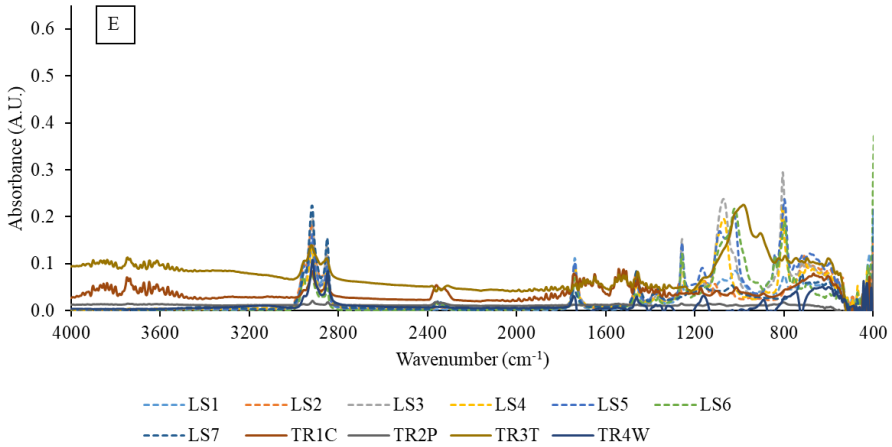
Figure 6 (continued)

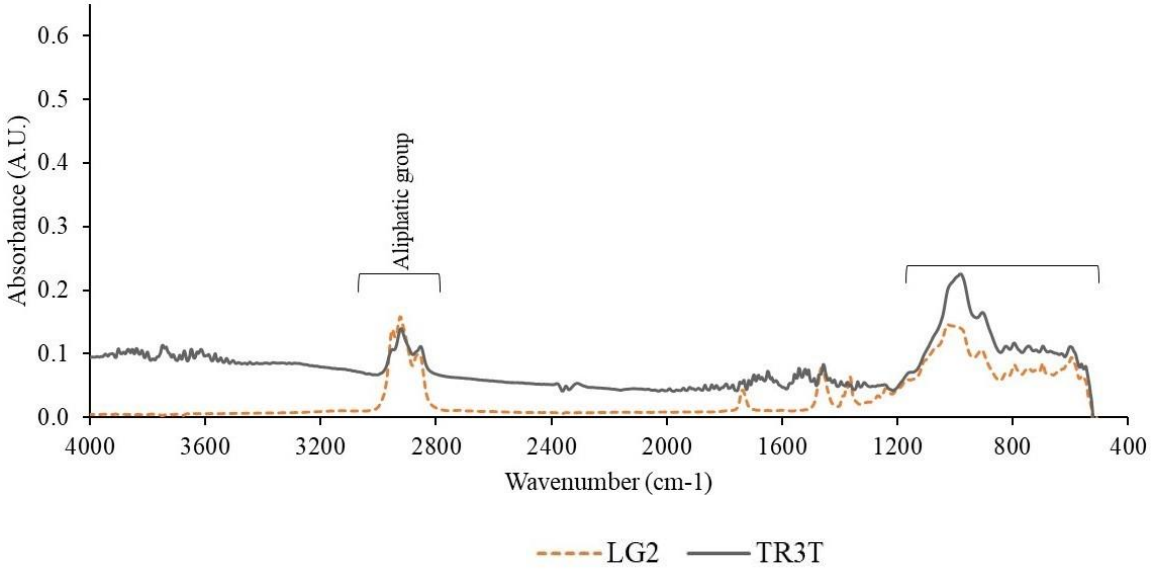
Comparison of ATR FTIR spectra of trace samples



Notes: Comparison of ATR FTIR spectra of trace samples TR1C, TR2P, TR3T, and TR4W against source category of (A) lip crayons (LC1-LC5), (B) lip glosses (LG1-LG6), (C) liquid lipsticks (LL1-LL7), (D) lip pencils (LP1-LP5), and (E) solid lipsticks (LS1-LS7).

Figure 7

Comparison of ATR FTIR spectra of trace sample TR3T with source lip gloss LG2

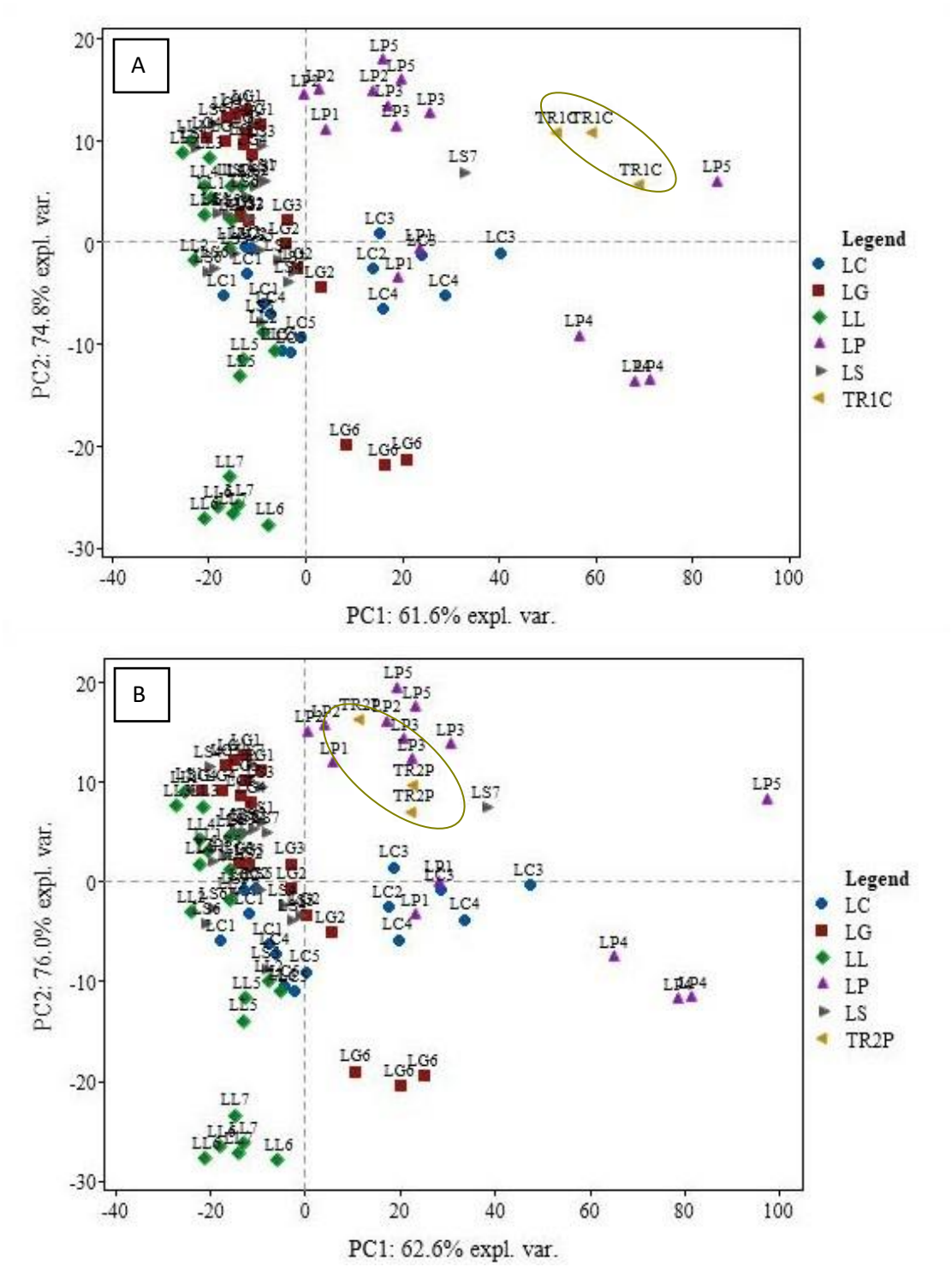


Notes: The source sample is represented by a dashed line, while the trace sample is represented by a solid line.

To assess trace classification, PCA was conducted using the ATR FTIR spectral data of the trace samples. Score plots (Figures 8A – 8D) and three-dimensional scatterplots (Figures 9A – 9D) were used to distinguish and confirm the source of the traces. However, these observations suggest an inconclusive outcome. PCA could not correctly classify lip cosmetic traces according to the categories. All four trace samples seemed to either be part of or lie beyond the lip pencil cluster in all score plots and scatterplots. In conclusion, the results of trace analyses were inadequate, as only one trace (TR3T) out of four samples showed similarity with the pure/original sample LG2 in the visual spectral examination, but none in traces' PCA.

Figure 8

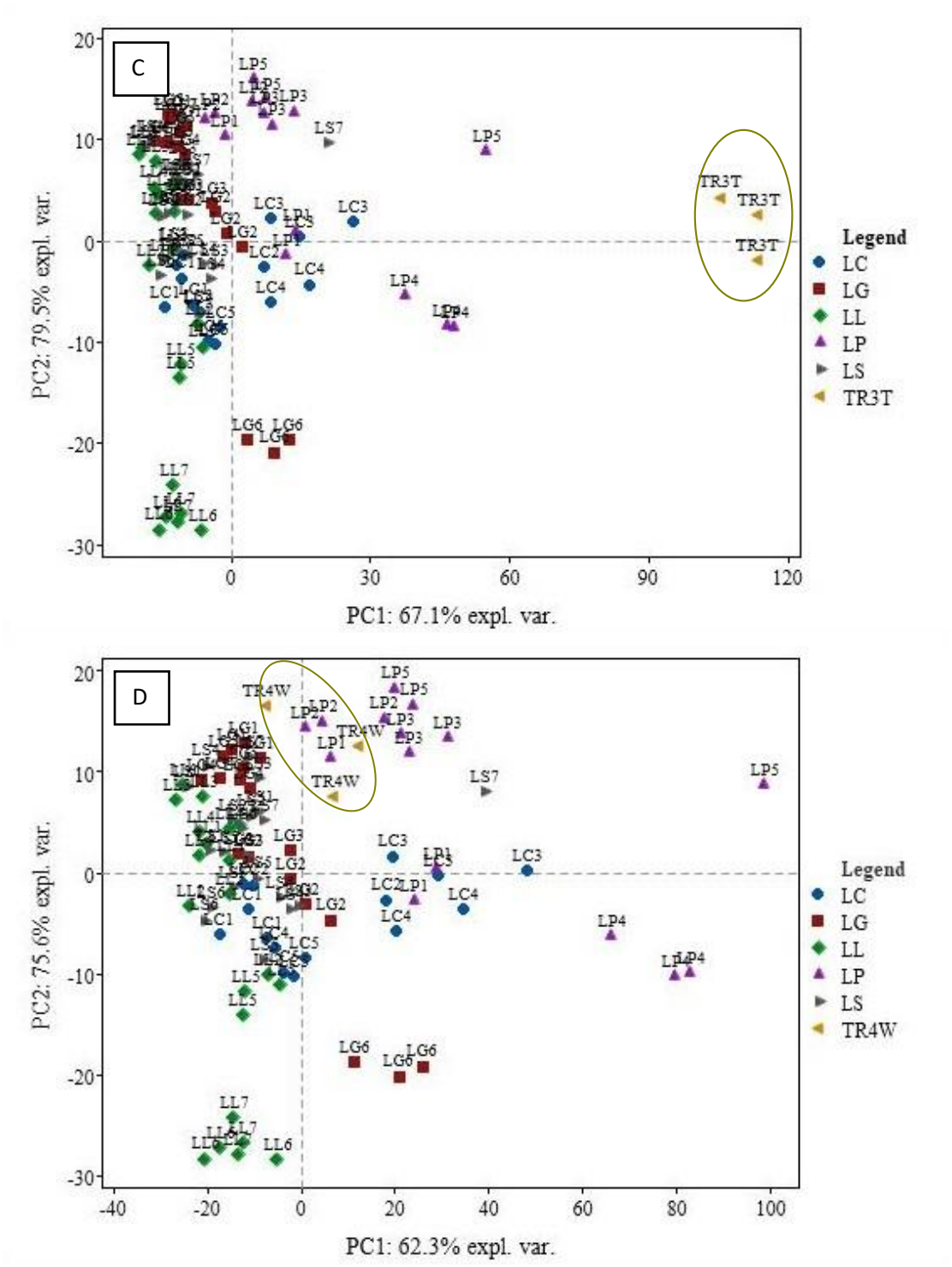
PCA score plots for selected trace samples



Notes: Percentages indicate total variance. PCA score plots for selected trace samples (with repeatability): (A) TR1C on cloth substrate, (B) TR2P on paper substrate, (C) TR3T on tissue substrate, and (D) TR4W on wipe substrate

Figure 8 (continued)

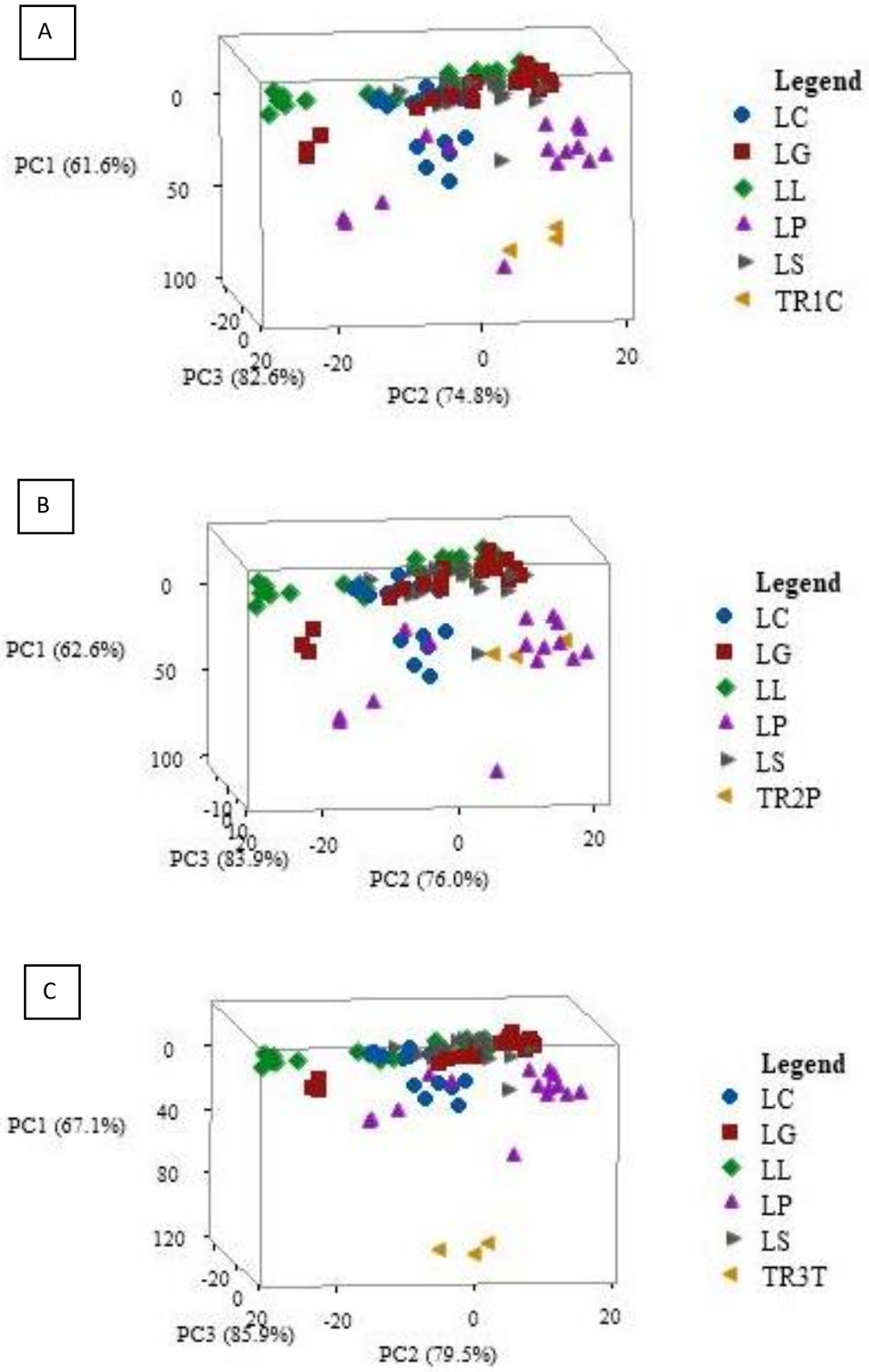
PCA score plots for selected trace samples



Notes: Percentages indicate total variance. PCA score plots for selected trace samples (with repeatability): (A) TR1C on cloth substrate, (B) TR2P on paper substrate, (C) TR3T on tissue substrate, and (D) TR4W on wipe substrate

Figure 9

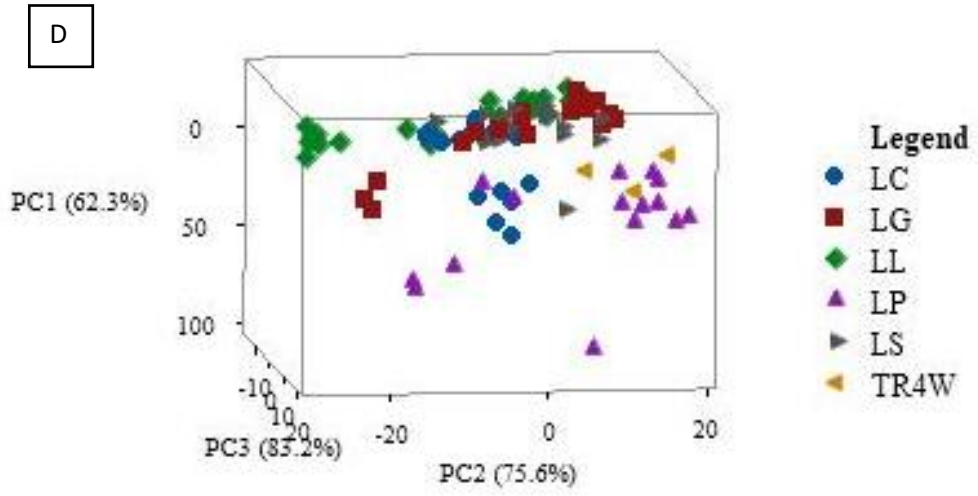
3D scatter plots of PC1, PC2, and PC3 for trace samples



Notes: Percentages in brackets indicate total variance. 3D scatter plots of PC1, PC2, and PC3 for trace samples (with repeatability): (A) TR1C on cloth substrate, (B) TR2P on paper substrate, (C) TR3T on tissue substrate, and (D) TR4W on wipe substrate

Figure 9 (continued)

3D scatter plots of PC1, PC2, and PC3 for trace samples



Notes: Percentages in brackets indicate total variance. 3D scatter plots of PC1, PC2, and PC3 for trace samples (with repeatability): (A) TR1C on cloth substrate, (B) TR2P on paper substrate, (C) TR3T on tissue substrate, and (D) TR4W on wipe substrate

DISCUSSION

The weak intensity bands observed in the spectra could indicate subtle differences in the chemical compositions of the samples, highlighting the importance of considering even minor variations for accurate differentiation. The weak intensities of bands such as those observed for hydroxy groups (3600-3100 cm^{-1}), aliphatic groups (3000-2700 cm^{-1}), carbonyl-containing species (1750-1700 cm^{-1}), and ether groups (near 1250 cm^{-1}) suggest challenges in sample differentiation, especially for lip cosmetics with overlapping or similar functional group contributions.

A typical lipstick spectrum has a single broad band attributed to water and hydroxyl groups between 3740-3100 cm^{-1}, C-H and CH_3 stretching vibrations between 3050-2775 cm^{-1}, and several peaks below 1800 cm^{-1}, including C=O stretching vibrations around 1730 cm^{-1}, CH_2 scissor deformation at 1465 cm^{-1}, and C=O stretching and C-H bending vibrations at 1172 cm^{-1} (Gładysz et al., 2017). S. Sharma et al. (2016) conducted their study on lip glosses and noted C-H stretching vibrations at 3026 cm^{-1} and 2920 cm^{-1} and C-H bending vibrations at 1493 cm^{-1}, as well as 1603 cm^{-1} and 1105 cm^{-1} bands for carboxylic/fatty acids and esters. Further research is required to collect more data on the compositions of multiple lip cosmetic types, specifically lip crayons, lip pencils, and liquid lipsticks, for comparison with the results obtained in this study.

The clustering results of HCA indicated shared compositions between the studied lip cosmetic types, likely due to the presence of common ingredients such as oils, waxes, and colourants (Gładysz et al., 2021; Wong et al., 2019). Since multiple lip cosmetics can belong to the same cluster, clustering may not always make it easier to identify individual lipsticks in forensic applications. However, clustering may be useful for ruling out or identifying potential suspects or evidence sources.

Despite capturing a significant amount of variance (87.7%) in the first four principal components, PCA also faced challenges in clearly differentiating all lip cosmetic types. While clear clusters were observed for some categories, the inconclusive outcome in classifying all categories may be attributed to shared or similar chemical compositions among lip crayons, solid lipsticks, and the other three categories (lip glosses, liquid lipsticks, and lip pencils) due to the commonality of components such as waxes, oils, and colourants (Gładysz et al., 2021; Wong et al., 2019). Although PCA generally offers valuable insights into sample clustering, incorporating techniques such as LDA may complement the PCA data, thereby providing further discrimination and enhancing the classification accuracy of lip cosmetic categories. Additionally, exploring other multivariate tools or refining the spectral preprocessing methods may enhance the discrimination power for forensic lip cosmetic analysis.

Weaker ATR FTIR bands in trace samples were likely influenced by the porous or fibrous nature of the substrates, which may have hindered the proper deposition and absorption of the lip cosmetics. The challenges faced in detecting clear spectral patterns in trace samples align with findings from previous studies, like those from the lipstick study of Gładysz et al. (2020) which faced similar challenges with cotton substrates, referring to substantial interference in the ATR FTIR spectra with overlapping bands of traces and the material, and limited sample availability due to cotton's porous nature and trace drying on the surface. The PCA results were

inconclusive for categorizing trace samples as none of them could be distinctly classified as belonging to a specific lip cosmetic category.

Overall, the trace analysis was only partially successful, as TR3T was the only sample showing any resemblance to its corresponding source sample in spectral examination, and none of the traces showed alignment in PCA. The poor outcomes may be attributed to several factors. One probable explanation is the quality and quantity of the traces. The results may be unreliable if the sample has a low quantity or is contaminated. Another possibility is the presence of interfering variables that cannot be foreseen or accounted for in trace analyses. Furthermore, the nature of the substrates used, such as porosity and fibrous textures, likely influences trace transfer, adhesion, and spectral intensity, leading to significantly impacting the sensitivity and specificity of forensic analysis using ATR FTIR spectroscopy (Gładysz et al., 2020).

To the best of the authors' knowledge, there are no reported studies using chemometrics for the discrimination of lip cosmetics and identification of their traces on various substrates using type classification, that is, the type they are marketed as. Other studies in this field using ATR FTIR spectroscopy to aid forensic lip cosmetic investigations have produced successful results. It is worth mentioning that most of these studies were conducted on red-shaded lipsticks and focused on their brand-wise grouping or discrimination.

For instance, Yadav et al. (2023) analysed 20 brands of lip balms using PCA and LDA and reported a high PCA-LDA training accuracy of 92.5% but a validation accuracy of 83.33%. Ka Khei et al. (2023) analysed 90 lipstick samples according to their brands using the partial least squares - discriminant analysis (PLS-DA) model and reported a high area under the curve (AUC) figure of 0.99 for all brands but one that had an AUC of 0.94. They also reported 100% accuracy in linking trace samples with their source. Kaur et al. (2020) analysed 55 red, 57 pink, and 47 brown lipstick samples according to their brands using PCA and LDA and reported high accuracy in classification (87.27% red lipsticks, 80.7% pink lipsticks, 93.61% brown lipsticks by PCA; 100% by LDA). Chophi et al. (2020) analysed 38 red lipstick samples using PCA and PCA-LDA with 100% discriminating power and 81.48% correct classification. Wong et al. (2019) analysed 22 red and 18 nude lipstick samples using PCA and LDA with 100% accuracy in red lipsticks and misclassification reported in nude lipsticks. V. Sharma et al. (2019) analysed 25 red and maroon lipstick samples using factor analysis and cluster analysis and discriminated all samples, 98.67% and 100% for each analysis, respectively. Mohamed Ghazali & Ismail (2018) analysed 12 red lipstick samples using PCA and HCA and successfully discriminated into six distinctive clusters according to their brands. Gładysz et al. (2017) analysed 38 red lipstick samples using PCA, cluster analysis, and correlation coefficient, and the discriminating power for each statistical tool was reported to be 29%, 51%, and 93%, respectively. In contrast to the above research, the present study included multiple lip cosmetic types and focused on the discrimination by lip cosmetic type.

Limitations of this study include inadequate sampling of traces on the substrates and weaker spectra generated from ATR FTIR spectroscopy. This can affect forensic applications by potentially reducing the accuracy of sample classification and source attribution, emphasising the need for robust analytical methods to overcome such challenges (Gładysz et al., 2021). Additionally, this research was limited to brown shades of lip cosmetics from five categories; thus, the results may not be generalisable to other colours or types of lip cosmetics.

The present study highlights the need for further research on the trace analysis of lip cosmetics in forensic science to improve the accuracy of the results. Several recommendations can be considered to address these limitations. First, increasing the number of samples would provide more robust data and increase the chances of accurately identifying and grouping the samples. Combining ATR-FTIR spectroscopy with other analytical techniques such as Raman spectroscopy can provide complementary information and improve the accuracy of the analysis. Using high-quality substrates for sample collection increases the chances of capturing a complete range of spectra, providing more information for identification and grouping. Implementing advanced data pre-processing techniques, such as noise reduction, baseline correction, and multivariate analysis, can help improve the accuracy and reliability of the results. Expanding this study to include several types of lip cosmetics, such as lip balms, lip tints, and lip stains, can provide a more comprehensive understanding of the trace analysis of lip cosmetics in forensic science.

CONCLUSION

In the current study, trace analysis of lip cosmetics using ATR FTIR spectroscopy and chemometrics was conducted on 30 samples of brown shade-lip cosmetics from five categories: lip crayons, lip glosses, liquid lipsticks, lip pencils, and solid lipsticks. Despite the use of chemometric techniques such as hierarchical cluster analysis (HCA) and principal component analysis (PCA), it was challenging to achieve a definitive conclusion about the grouping of the lip cosmetic samples concerning their types and the identification of traces with their source of origin. Observations from HCA showed a grouping pattern where lip crayons and most solid lipsticks formed the first cluster, while most lip glosses, liquid lipsticks, and lip pencils shared the second cluster. Similarly, the PCA results exhibited distinct clusters with some outliers for lip glosses, liquid lipsticks, and lip pencils, whereas lip crayons and solid lipsticks showed scattered clusters. Thus, the PCA results were in conformance with the HCA results. The trace analysis results were inconclusive, with only trace (TR3T) showing partial similarity to the lip gloss (LG2) spectrum. However, it is important to note that despite these analytical methods, limitations exist in

achieving a comprehensive understanding of sample grouping and source identification. Further elaboration of the outcomes of HCA and PCA analyses, including detailed discussions on score plots and their limitations, would provide a more nuanced interpretation of the study's results.

AUTHOR CONTRIBUTIONS

Hajera Thakur led the conceptualisation, formal analysis, investigation, and resource management, and authored the original draft, while also contributing to visualisation. Nurul Ain Abu Bakar contributed to the reviewing, editing, and supervision of the project. Muhammad Naeim Mohamad Asri guided the conceptualisation and supervised the work. All authors have read and approved the final manuscript.

ETHICS APPROVAL

Not applicable.

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Not applicable.

CONFLICTS OF INTEREST

The authors declare no conflict of interest in this work.

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Abbreviations: ATR: Attenuated total reflectance. FTIR: Fourier-transform infrared. GC: Gas chromatography. GC-MS: Gas chromatography-mass spectrometry. HCA: Hierarchical cluster analysis. HPLC: High-performance liquid chromatography. LC: Lip crayon. LDA: Linear discriminant analysis. LG: Lip gloss. LL: Liquid lipstick. LP: Lip pencil. LS: Lipstick/solid lipstick. MS: Mass spectrometry. PC: Principal component. PCA: Principal component analysis. TLC: Thin-layer chromatography. TR1C: Trace #1 from cloth. TR2P: Trace #2 from paper. TR3T: Trace #3 from tissue. TR4W: Trace #4 from wipe. UV-vis: Ultraviolet-visible.

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