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Considerations and future perspectives for the vibrational spectroscopic analysis of forensic cosmetic evidence

Katy A. Bruce[1] | Donna C. Arnold[1] | Georgina Sauzier[2] |
Simon W. Lewis[2]

[1]School of Chemistry and Forensic Science, Division of Natural Sciences, University of Kent, Kent, UK

[2]School of Molecular and Life Sciences, Curtin University, Perth, Western Australia, Australia

Correspondence
Katy A. Bruce and Donna C. Arnold, School of Chemistry and Forensic Science, Division of Natural Sciences, University of Kent, Canterbury, Kent CT2 7NH, UK.
Email: k.a.bruce@kent.ac.uk, and d.c.arnold@kent.ac.uk

Abstract

Cosmetics such as makeup or other personal products are widely used and easily transferred upon physical contact. As such, they may be used as trace evidence to link people to each other or to places in criminal investigations. To maximize their probative value, it is important to understand the variability among representative market products and the way in which they transfer to, or persist on various surfaces. Additionally, it is required that analysis techniques be nondestructive, readily available and relatively inexpensive. Raman spectroscopy and attenuated total reflectance—Fourier transform infrared (ATR-FTIR) are powerful tools for probing the chemistry of trace cosmetics. As well as fitting the criteria above, they offer the capability of studying a wide range of sample types with minimal prior preparation. The complementary information derived from these techniques can help analysts to understand and visualize spectral variability, potentially enabling discrimination between samples. However, the move from academic research toward forensic casework is not without challenges. In this article, we provide a focused exploration of the current state-of-the-art in forensic cosmetic research; providing context for how we may begin to address these challenges to more effectively exploit cosmetic traces for criminal investigation.

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Forensic Chemistry and Trace Evidence > Emerging Technologies and Methods

Forensic Chemistry and Trace Evidence > Trace Evidence

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1 | INTRODUCTION

Cosmetic products are used by a wide cross-section of society for skin care and beautification. As a result, the global cosmetic market was worth an estimated US \$676 billion in 2023 and continues to grow (statista.com). The use of

cosmetics is independent of age, gender, ethnicity, or socioeconomic status; thus, it is not unreasonable to expect that cosmetic traces of some description may be encountered during criminal investigations.

Makeup, also known as decorative cosmetics, encompasses a broad range of products (shown in Figure 1) intended to beautify the wearer's appearance or to conceal real or perceived skin imperfections such as blemishes, scars, hyperpigmentation, or tattoos. Many of these products are easily transferred from one surface or one person to another, making them useful in linking individuals or locations involved in criminal activity. Makeup products of any single type can also be purchased in a wide array of formulations, leading to the possibility of source discrimination. Furthermore, consumer trends reveal that facial makeup (in particular, foundation, concealer, bronzer, highlighter, blush, and finishing powder) is typically applied in a layered sequence, with the resulting product mixing likely to give distinctive residues. As such, these cosmetics have significant probative potential as transfer evidence.

Unsurprisingly, this has led to a large number of studies related to the differentiation, identification, persistence, and transference of cosmetic products, as summarized in Table 1. Figure 2 provides a graphical representation of the proportion of this research focused on specific categories of makeup or study purpose—to identify market variability among cosmetic formulations; or to examine the transference and persistence of cosmetic traces within a forensic context. Previous review articles have discussed the forensic analysis of cosmetics, placing heavy emphasis on chromatographic analysis and heavy metal detection or focusing on a narrow range of cosmetic products (Chophi et al., 2019; Gładysz et al., 2021). By contrast, this review seeks to cover a range of decorative cosmetics, reflecting consumer usage trends and concentrating on vibrational spectroscopic analyses. A recent review by Evangeline et al. (2024) discusses the use of Raman spectroscopy for dermatological applications including cosmetic analysis; however, the focus was on the cosmetic components and their relevance within the dermatological sector rather than within a forensic context.

A graphical summary of analytical techniques applied to cosmetic samples in previous research is given in Figure 3. It should be noted, however, that many of these techniques are limited by their destructive nature and/or the requirement for specialist instrumentation and user knowledge that may not be readily available in all forensic science laboratories. For that reason, there has been significant interest in vibrational spectroscopy modalities such as attenuated total reflectance Fourier transform infrared (ATR-FTIR) and Raman spectroscopy as powerful, non-destructive (samples can be analyzed in situ after application to a substrate) and accessible methods for the analysis of cosmetic traces. These techniques provide complementary information on the rotational and vibrational modes present in a material with minimal sample preparation and are suited to samples in both solid and liquid forms. Nonetheless, challenges remain with respect to high fluorescence contributions, background effects, and spectral variability, which are discussed further in Section 3.

In this article, we discuss the current literature landscape related to Raman and FTIR spectroscopic analyses of decorative cosmetic products within a forensic context. We place emphasis on providing insight into current limitations related to both technology and experimental design, and provide perspective which may inform future developments and improvements for these types of analyses.

Types of cosmetics

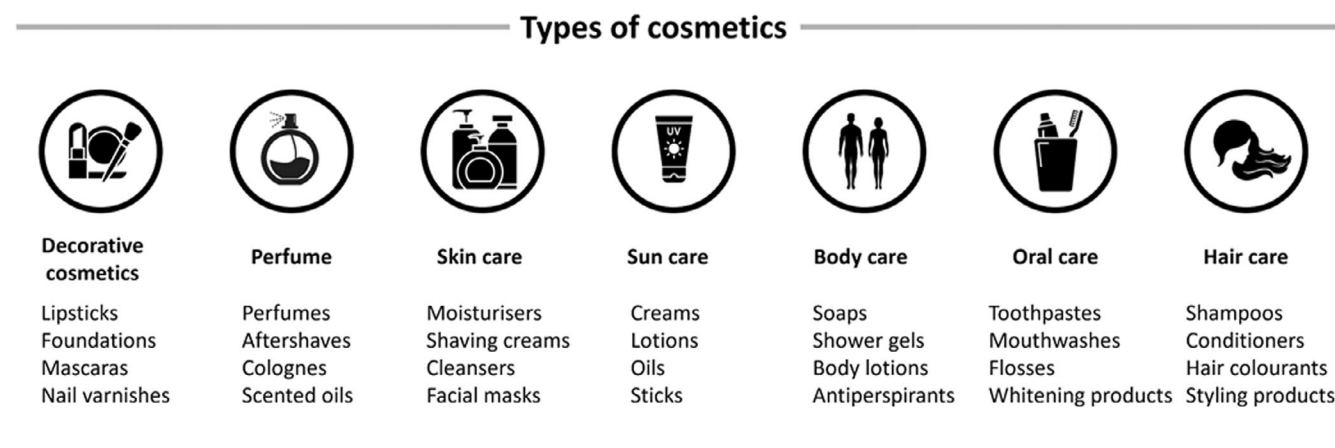| Decorative cosmetics	Perfume	Skin care	Sun care	Body care	Oral care	Hair care
Lipsticks	Perfumes	Moisturisers	Creams	Soaps	Toothpastes	Shampoos
Foundations	Aftershaves	Shaving creams	Lotions	Shower gels	Mouthwashes	Conditioners
Mascaras	Colognes	Cleansers	Oils	Body lotions	Flosses	Hair colourants
Nail varnishes	Scented oils	Facial masks	Sticks	Antiperspirants	Whitening products	Styling products

FIGURE 1 Schematic representation of the primary types of cosmetics with example products.

TABLE 1 Summary of all studies on cosmetics by type and analysis technique.

Analytical technique	Cosmetic type	References
ATR-FTIR/FTIR/FTIR-microscopy	Lipstick	Alblooshi et al. (2024), Chophi et al. (2020b), Gładysz et al. (2017, 2020), Ka Khei, Verma, Tan, et al. (2023a), Kaur et al. (2020), Pasieczna-Patkowska and Olejnik (2014), Sharma, Bharti, and Kumar (2019), Wong et al. (2019)
	Lip balm	Yadav et al. (2023)
	Lip gloss	Sharma et al. (2016)
	Glitter	Najjar and Bridge (2018), Vernoud et al. (2011)
	Eyeshadow	Chophi, Sharma, Jossan, and Singh (2021), Pasieczna-Patkowska and Olejnik (2014)
	Eyeliner/kohl/kajal	Arora et al. (2021), Asri, Verma, Ibrahim, Sharma, and Nor (2021), Chophi, Sharma, Jossan, and Singh (2021), Pasieczna-Patkowska and Olejnik (2014), Sharma, Chophi, et al. (2019), Sharma, Bharti, and Kumar (2019)
	Mascara	Arora et al., 2021
	Nail varnish	Chophi et al. (2020a), Gupta and Kaur (2023), Ka Khei, Verma, Tan, et al. (2023b), Koçak and Kang (2022), Cho and Lee (2020)
	Depigmenting cream	Pasieczna-Patkowska and Olejnik (2014)
	Face cream	Sharma et al. (2021)
	Sunscreen	Angrish et al. (2020)
	Foundation	Sharma, Chophi, et al. (2020), Gordon and Coulson (2004)
	Hair colorant	Boll et al. (2017)
	Hairspray/gel/wax	Liechti and Lory (2024)
	Vermilion	Chophi, Sharma, Jossan, and Singh (2021), Singh et al. (2022)
DRIFTS	Lipstick	Lennard and Mazzella (1991), Pasieczna-Patkowska and Olejnik (2014)
	Eyeshadow	Pasieczna-Patkowska and Olejnik (2014)
	Eyeliner	Pasieczna-Patkowska and Olejnik (2014)
	Depigmenting cream	Pasieczna-Patkowska and Olejnik (2014)
EDXRF	Lipstick	Melquiades et al. (2015)
	Lip gloss	Melquiades et al. (2015)
	Nail varnish	Melquiades et al. (2015), Misra et al. (1992)
	Eyeshadow	Melquiades et al. (2015)
Fluorescence observation	Lipstick	Ehara and Marumo (1998)
GC	Lipstick	Russell and Welch (1984), Ehara and Marumo (1998)
GC-FID	Foundation	Gordon and Coulson (2004)
GC–MS (Including HS-SPME. Py-GC–MS and UAE-GC–MS)	Lipstick	Gładysz et al. (2018, 2020, 2022), Griffin et al. (1996), Keagy (1983), Lim Bin Abdullah et al. (2011)
	Lip balm	Griffin et al. (1996)
	Lip gloss	Zellner and Quarino (2009)
	Eyeshadow	Griffin et al. (1996)
	Mascara	Griffin et al. (1996)
	Perfume	Gherghel et al. (2016, 2018, 2019, 2020)
	Moisturizing lotion	Raynor et al. (2021)
HPLC	Lipstick	Andrasko (1981), Reuland and Trinler (1984)
	Nail varnish	Tebbett et al. (1987)
	Face cream	Chourasiya et al. (2023)

(Continues)

TABLE 1 (Continued)

Analytical technique	Cosmetic type	References
LDMS	Nail varnish	O'Neill et al. (2009)
Magnetic levitation	Glitter	Lockett et al. (2013)
MEKCC	Lipstick	Gładysz et al. (2019, 2020, 2022), Król et al. (2020)
Microscopy (optical)	Glitter	Aardahl et al. (2005), Grieve (1987)
MSP	Lipstick	Choudhry (1991)
	Hair colourant	Barrett et al. (2011)
NAA	Lipstick	Misra and Mittal (2004)
NIR	Foundation	Skobeeva et al. (2022)
PAS	Lipstick	Pasieczna-Patkowska and Olejnik (2014)
	Eyeshadow	Pasieczna-Patkowska and Olejnik (2014)
	Eyeliner	Pasieczna-Patkowska and Olejnik (2014)
Raman	Lipstick	Gardner et al. (2013), Gładysz et al. (2022), López-López et al. (2014), Salahioglu et al. (2013), Salahioglu and Went (2012)
	Lip gloss	Gardner et al. (2015)
	Lip balm	Gardner et al. (2015)
	Nail varnish	López-López et al. (2015)
	Face cream	Asri, Verma, Ibrahim, Nor, et al. (2021)
SALDI-MS	Face serum	AlSaeed et al. (2022), Al-Sayed et al. (2022)
	Moisturising cream	AlSaeed et al. (2022), Al-Sayed et al. (2022)
SEM-EDS	Lipstick	Andrasko (1981), Choudhry (1991), Kumar Singh et al. (2023)
	Foundation	Gordon and Coulson (2004)
	Glitter	Najjar and Bridge (2020)
	Shimmer	Najjar and Bridge (2020)
	Vermilion	Kumar Singh et al. (2023)
SERDS	Lipstick	Zhang et al. (2020)
SERRS	Lipstick	Rodger et al. (1998), White (2000)
SIMS	Nail varnish	Gresham et al. (2000)
Spectroradiometry	Blush	Curtis et al. (2023)
STE-LDI-MSI	Lipstick	De Oliveira et al. (2013)
TEM	Blush	Curtis et al. (2023)
TLC	Lipstick	Andrasko (1981), Barker et al., 1972; Joshi et al. (2013), Lim Bin Abdullah et al. (2011), Russell and Welch (1984), Saran and Mishra (2015), Srivastava et al. (2013)
	Lip gloss	Sharma et al. (2016)
	Hairspray	Kaur et al. (2015)
	Face cream	Chourasiya et al. (2023)
	Vermilion	Chandel et al. (2013)
TOF-SIMS	Lipstick	Lee and Lee (2021), Terlier et al. (2020)
	Foundation	Terlier et al. (2020)
	Nail varnish	Terlier et al. (2020)
	Sunscreen	Terlier et al. (2020)
	Hand cream	Terlier et al. (2020)
XRD	Blush	Curtis et al. (2023)
XRF	Foundation	Kulikov et al. (2012)

FIGURE 2 Schematic representation of the number of publications as a function of population variability; contact transfer; and/or persistence. Categories from left to right: Lip cosmetics, face (cheek) cosmetics, eye cosmetics, nail cosmetics, skin care products, hair care products, glitters, and perfumes.

Spectroscopy	Mass spectrometry	Chromatography	Other
ATR-FTIR*	SALDI-MS	HPLC	Electron microscopy
Raman*	TOF-SIMS	GC	Reflectivity
		TLC	XRD

FIGURE 3 Schematic representation of the primary analysis methodologies used in the analysis of cosmetic trace evidence. * denotes non-destructive techniques.

2 | CURRENT LITERATURE REPORTED FOR VIBRATIONAL SPECTROSCOPIES IN COSMETIC ANALYSIS

Considerable literature exists on the forensic examination of "*point*" cosmetics, where these are defined as products designed for use on a specific facial area (e.g., lip, cheek, and eye makeup) rather than for general all-over use, with fewer reports on cosmetics such as foundation. These studies have typically focused on examining market variability, although recent years have seen a shift toward factors impacting transfer and persistence at the activity level. This article is not intended to be an exhaustive review of research in forensic cosmetic analysis but is rather intended to highlight key studies illustrating the current scope of the field.

2.1 | Lip cosmetics

Lipsticks (including both wax-based and liquid lipsticks as well as glosses, balms, and tints) are by far the most widely studied form of cosmetic trace evidence. Initial studies focused largely on the visual comparison of spectral data

collected by ATR-FTIR and/or Raman spectroscopy. Gardner et al. (2013) reported the Raman spectroscopic analysis of 80 red, pink, brown, and purple-brown lipsticks, from 23 different manufacturers, across 40 different product lines. They utilized laser wavelengths of both 532 and 780 nm, noting the latter was more effective for fluorescent samples. Similarly, López-López et al. (2014) used confocal Raman microscopy to study 49 lipsticks encompassing different brands and product lines, in different colors (red, pink, brown, and purple). They did not report high discriminatory rates but rather that the data could be assembled into 30 different groups, which showed no relationship between brand or color. Five of the red lipsticks were further "*kissed*" onto 12 different substrates including fabric, glass, paper (cigarettes), metal and plastic household objects to simulate natural contact transfer. The authors found that the substrates did contribute to the spectrum, but that the cosmetic remained identifiable (by comparison with the original spectral data) within the composite spectrum. A substrate spectral subtraction was trialed, importantly noting that this approach could introduce both new and negative bands in the resultant spectrum. This finding is significant as it shows that spectral subtraction techniques may yield a spectrum that is not representative of the original sample (López-López et al., 2014).

Salahioglu and Went (2012) investigated 69 brown, pink, and red lipsticks across ten different brands using Raman spectroscopy. The authors found that while 15 of the lipsticks gave distinct spectra, the remaining 54 could only be grouped into seven families based on their peak profiles (chemical composition). These groupings did not always follow those expected for either color or brand in line with the observations of López-López et al. (2014). They also noted that red lipsticks were the most difficult to distinguish, with all the red lipsticks analyzed falling into a single group (Salahioglu & Went, 2012). A caveat to this study was that a large proportion of the lipsticks analyzed were also obtained via donation in the form of store testers, introducing doubt as to the origin of spectral variability (due to potential contamination) and thus, the reliability of the results.

The authors later extended this study to look at lipstick traces on forensically relevant substrates such as glass, tissues and cigarette filters, alongside aging studies (Salahioglu et al., 2013). They demonstrated that while the spectra for some lipsticks remained unchanged over long periods of time (up to 2 years), others saw changes related to individual spectral peaks. The authors made no assertion as to the likely origin of this phenomenon, but one can assume it may relate to either the material's consistency, the loss of water content, or chemical degradation of components. A subset of lipsticks were also analyzed in situ on different substrates. The authors found that fluorescence arising from the various substrates could largely be mitigated using different laser wavelengths, concluding that a 473-nm laser was best suited for these analyses. This contrasts with the Gardner et al. (2013) study, which found that a 780 nm laser was most effective. A *k*-nearest neighbors classifier applied to a test set of these lipsticks resulted in a 100% correct classification (Salahioglu et al., 2013).

Improvement of the visual discriminatory power by Raman spectroscopy has also been investigated for a small number of red wax-based lipsticks using surface enhanced resonance Raman spectroscopy (SERRS) (Rodger et al., 1998). SERRS involved the addition of surfactants containing silver nanoparticles to a lipstick smear on either glass or cotton. The authors investigated the best surfactants for providing reduced fluorescence and high discrimination and concluded that poly(L-lysine) was the most favorable, considerably quenching the background fluorescence. However, the effectiveness of this protocol on more contemporary formulations such as liquid lipsticks, glosses or balms remains untested.

Red- and nude-shaded lipsticks (including wax, liquid and gloss formulations) were studied using ATR-FTIR by Wong et al. (2019). The authors noted distinct changes in the spectra of liquid lipsticks in the ten mins immediately following application, presumably due to drying. They noted the significance for sampling within a forensic context, as traces recovered at a scene are likely to be days to weeks old rather than freshly deposited. Principal component analysis (PCA) determined that although many products exhibited similar formulations, certain products had distinct chemical components. Linear discriminant analysis (LDA) models produced classification accuracies between 93% and 100% depending on colour. These models were validated using a test set deliberately selected to reflect a range of similar and dissimilar samples, retaining a 93% classification for red-shaded lipsticks but a reduced classification (when compared to the original LDA classification) of 73% for nude-shaded samples (Wong et al., 2019).

Gładysz et al. (2017, 2022) have performed multiple studies using ATR-FTIR and other techniques for the analysis of lipsticks. Initially, they studied 38 red wax-based lipsticks across several brands, using ATR-FTIR coupled to PCA and cluster analysis. They demonstrated that whilst lipsticks could be grouped, they showed no clear trends by shade or manufacturer, similar to previous studies (López-López et al., 2014; Salahioglu et al., 2013). They later studied seven red lipsticks by ATR-FTIR alongside GC–MS and capillary electrophoresis (Gładysz et al., 2020). All traces were analyzed by smearing lipstick onto substrates such as paper, cotton and glass and storing under different conditions.

Analysis was then performed at varying time intervals over the course of 12 months. Additional variables such as transfer by different individuals, the length of time lipstick had been worn prior to deposition, and the impact of smoking or beverage consumption on the resultant transfer were investigated in an attempt to model likely crime scene traces. They saw significant spectral changes among products with oily or liquid formulations while "*drier*" samples remained unchanged. Additionally, they reported that light appeared to accelerate changes in chemical composition, independent of substrate (Głądysz et al., 2020).

A combination of ATR-FTIR and Raman spectroscopy was used to investigate 20 pink "*MAC*" brand lipsticks by Alblooshi et al. (2024). These authors found that a 780 nm laser was best suited for Raman analysis of these lipsticks. However, it is not clear whether this relates to enhanced spectral information or removal of fluorescence. With the exception of eight pairings, the majority of these samples could be visually differentiated from each other. It was also reported that Raman was more effective than ATR-FTIR at differentiating between lipsticks, presumably as a result of differences in inorganic components that are more readily probed using Raman spectroscopy. Nonetheless, this study only considered "*MAC*" lipsticks so the conclusions drawn are only applicable to a specific sample set and thus may not be representative of wider lipstick populations (Alblooshi et al., 2024).

Lastly, high discrimination between lipsticks has been reported by Sharma, Bharti, and Kumar (2019) using ATR-FTIR, and by Zhang et al. (2020) using Raman spectroscopy. Sharma, Bharti, and Kumar (2019) studied 25 non-branded, unregulated marketplace lipsticks which were "*kissed*" onto paper substrates. They reported 100% discrimination between spectra using factor analysis and 99% using hierarchical cluster analysis (HCA)/k means clustering techniques, using an average spectrum generated from five replicates for each sample. Given many of the samples are closely arranged in the reported scores plot, this may suggest that use of the original unaveraged spectra could have resulted in some sample overlap, lowering the discrimination rate. It is also worth mentioning that due to the unregulated nature of these samples, there is less control of ingredients and/or manufacturing processes; this may result in the high sample differentiation seen (Sharma, Bharti, & Kumar, 2019).

Zhang et al. (2020) performed shifted excitation Raman difference spectroscopy (SERDS) at a wavelength of 785 nm for 70 lipstick samples, deconvoluting the spectra using a back-propagated neural network. k-means clustering combined with PCA gave a reported 99.88% discrimination. However, only 34% of the total variance was accounted for in the first three principal components, suggesting a high level of sample variability that may pose challenges in applying this model to expanded sample sets.

2.2 | Foundations

Foundations have been studied far less than lipsticks, with only three papers detailing the use of vibrational spectroscopic methods. For example, 31 cosmetic foundations from 23 brands were investigated using ATR-FTIR, with samples deposited onto wet and dry cotton substrates (Sharma et al. 2020). Visual comparison of the spectra gave a 98% discrimination accuracy, which was increased to 100% using PCA and LDA with averaged spectra as reported in their lipstick studies and discussed above (Sharma, Bhardwaj, & Kumar, 2019; Sharma et al. 2020).

Similarly, liquid foundations across three different brands on four different fabrics (including cotton blend and acrylic) have been analyzed using NIR spectroscopy by Skobeeva et al. (2022). Despite optical effects arising from darker pigments, resulting in almost featureless spectra, and standard normal variate (SNV) pretreatment failing to improve models, the authors still reported 93% discrimination rates from PCA-LDA using a test set. It appears that this was largely based on differences in background position rather the resolvable spectral features.

Gordon and Coulson (2004) investigated and compared the effectiveness of FTIR, gas chromatography coupled with a flame ionization detector (GC-FID) and scanning electron microscopy—energy dispersive x-ray spectroscopy (SEM–EDX) for the forensic analysis of 53 foundation samples. These samples represented a cross spread of the New Zealand cosmetic foundation market and were analyzed straight from the source as well as deposited onto cotton substrates. FTIR was found to be the best single technique with 98.3% discriminating power, although challenges were encountered when analyzing samples containing talc as this dominated the spectrum. Interestingly, there was no apparent trend between pairs of indistinguishable products and the manufacturer or formulation, consistent with what has been reported for lipstick samples (López-López et al., 2014; Salahioglu et al., 2013). A small number of foundations were also unable to be distinguished from the cotton substrate due to absorption of the product into the fabric on application (Gordon & Coulson, 2004).

2.3 | Eye cosmetics

A limited range of studies have examined decorative eye cosmetics such as kohl (Sharma, Bhardwaj, & Kumar, 2019), and eyeshadows (Chophi, Sharma, Jossan, & Singh, 2021). Notably, Asri, Verma, Ibrahim, Sharma, and Nor (2021) used a combination of ATR-FTIR and Raman spectroscopy to study 45 kajal (kohl) samples across seven brands on substrates including dry tissue, wet tissue, cotton, nylon, polyester and plastic. Interestingly, PLS-DA modeling allowed for 100% discrimination of the samples analyzed via Raman, but only 86.7% for the ATR-FTIR analyses. This may indicate greater variability associated with inorganic ingredients such as mica or oxide pigments. Eyeliner and mascara traces have also been studied by ATR-FTIR on paper (Arora et al., 2021). PCA and PLS-DA were performed on data acquired from 102 cosmetic samples (62 eyeliners from 37 brands and 40 mascaras from 24 brands), developing a classifier capable of distinguishing between the two categories with 95% accuracy. However, individual product identification was not examined. A subset of samples was also analyzed on cotton fabric and wet versus dry tissue paper. Minor contributions from the substrate were observed, which could be adequately removed through background subtraction, although it is noted that this resulted in the loss of some minor peaks associated with the cosmetic, which may need to be considered when taking discrimination into account (Arora et al., 2021).

2.4 | Other cosmetics

The forensic analysis of nail varnishes has received moderate attention, with four studies using ATR-FTIR (Chophi et al., 2020a; Gupta & Kaur, 2023; Ka Khei, Verma, Tan, et al., 2023b; Koçak & Kang, 2022), one using FTIR microspectroscopy (Cho & Lee, 2020) and one using confocal Raman spectroscopy (López-López et al., 2015). López-López et al. (2015) used confocal Raman spectroscopy to examine 56 regular and 21 gel-based nail polishes. In keeping with other Raman studies discussed herein, they found that the 780 nm laser was superlative to the 532 nm laser due to sample burning and fluorescence effects (Alblooshi et al., 2024; Gardner et al., 2013). In addition to analyzing the nail polishes on aluminum foil, they also investigated nail polish transfer smears on white paper, flakes of polish, and polish removed from a volunteer's nails using acetone-soaked cotton swabs. All methods yielded spectra where the sample could be identified but substrate interference remained an issue. Most importantly, this study highlighted the problem of sample heterogeneity, with nearly 20% of the nail polishes exhibiting distinct spectral variations across replicates (López-López et al., 2015).

Vermilion, in the form of Sindoor, has also been investigated as a type of cosmetic evidence. Sindoor is used as a cosmetic powder in some religious and cultural practices. Chophi, Sharma, and Singh (2021) analyzed 42 vermilion samples using ATR-FTIR and performed PCA-LDA on the data set, achieving a 95% calibration accuracy (Chophi, Sharma, & Singh, 2021). However, this level of accuracy could only be reported for PCA-LDA models that were generated using a truncated spectral range. When the model was generated using the entire spectral range, the accuracy fell to 78%. This indicates that the initial models were based on highly variable spectral regions. This opens debate around sampling ranges and the consideration of data which should be incorporated into models to enable forensically valid conclusions to be reached. We discuss this further in Section 3.

Lastly, ATR-FTIR and synchrotron FTIR microscopy have been used to investigate cosmetic glitters. Najjar and Bridge (2018) studied 36 cosmetic glitters purchased from a single manufacturer covering a wide color palette. HCA and subsequent PCA suggested that the data could be organised into six groupings. Validation of this model was investigated using LDA, kNN and support vector machine (SVM) methodologies. LDA resulted in a 99.2% correct classification rate, with 11 misclassifications due to the spectral similarities between some of the groupings. In contrast, both kNN and SVM gave higher classification rates of 100% and 99.3%, respectively, with the latter only misclassifying one pair. However, it is not clear from these data if the groupings relate to any specific colors and thus dyes (Najjar & Bridge, 2018).

Vernoud et al. (2011) studied four multilayered glitter samples from a single manufacturer using synchrotron FTIR. The use of synchrotron facilities provides data with increased resolution and intensity, enabling cross-sectional studies to be performed at the micro-level. Within a single cross-section, seven spectrally distinct layers were able to be readily resolved. Layer thicknesses and composition then allowed for samples to be discriminated. However, from a forensic perspective, access to synchrotron facilities can be limited and expensive, restricting their applicability to casework, except perhaps in high-profile cases.

3 | DISCUSSION OF LIMITATIONS AND CRITICAL FACTORS

3.1 | Instrument and data analysis

Despite their obvious advantages, both ATR-FTIR and Raman spectroscopies have limitations associated with their measurement capabilities. Raman spectroscopy can suffer from low discriminatory power due to high fluorescence contributions, although there have been instances in which better classification of cosmetics was achieved using Raman spectroscopy coupled to chemometric techniques (Asri, Verma, Ibrahim, Sharma, & Nor, 2021). With respect to sample fluorescence, few authors have looked at the role that laser wavelength may play. Gardner et al. (2013) demonstrated that fluorescence could be effectively removed when moving from a laser wavelength of 532 to 785 nm. In contrast, Salahioglu and Went (2012) and Salahioglu et al. (2013) remarked that the 473 nm laser performed best in their studies. However, these studies will have inevitably drawn comparison from the laser wavelengths available in their own laboratories, making direct comparisons between the literature cautionary. From a fluorescence perspective, it is generally accepted within Raman communities that higher wavelength lasers typically lead to a reduction in fluorescent spectral features (although they may not be completely removed). Nonetheless, it is also important to recognize that forensic laboratories may not have access to multiple laser sources, limiting the ability to resolve fluorescence through these means. In order to overcome materials fluorescence, manufacturers are incorporating algorithms into their software packages which allow for the effective treatment of fluorescent spectra. This also opens up artificial intelligence (AI) and machine learning routes for deconvoluting spectral information from fluorescent backgrounds, but the validity of these approaches when applied to real forensic case evidence warrants further dialogue.

When compared to Raman, ATR-FTIR gives limited information on inorganic components. This can pose a significant problem for analyzing mineral makeup that exclusively comprises metal oxides and micas, such as the BareMinerals Original Foundation range. Raman can generally measure both organic and inorganic components, but the different requirements for a vibrational mode to be Raman active or infrared active mean that the two techniques are complementary in nature. Vibrational modes detected in ATR-FTIR are often not the same as those detected in Raman spectroscopy, or there can be a variation in peak sensitivity and intensity between the two techniques, meaning using them in tandem could be expected to give better sample discrimination. Only a few studies have applied this technique combination to cosmetic analysis thus far (Alblooshi et al., 2024; Asri, Verma, Ibrahim, Sharma, & Nor, 2021).

Care also needs to be taken in decisions about how we treat background-related effects in spectral data. It is not an easy task to determine if background variation is linked to sample variability, small changes in measurement conditions (e.g., focusing in Raman spectroscopy), or matrix (substrate) effects. It is essential that we do not remove true chemical variability, but more important that we do not introduce variability where there is none. Background treatment has largely focused on the use of SNV treatments aimed at background smoothing and minimizing the effects of background slopes (Arora et al., 2021; Sharma, Bharti, & Kumar, 2019). More recently, Liu et al. have demonstrated that machine learning and in particular, convolutional neural networks, are capable of identifying substances from noisy spectra without the need for preprocessing (Liu et al., 2019). However, all types of spectral pre-processing must be carried out conservatively to avoid overfitting of the data; overzealous processing could result in spectra that bear little resemblance to their original version, invalidating variability or similarity conclusions drawn.

To overcome substrate effects, authors have looked at collecting spectral data for blank substrates and then simply subtracting this from the spectral data of interest (Sharma, Bhardwaj, & Kumar, 2019). Generally, this approach has been successful, but there are instances where this either results in negative peaks or removes sample peaks of interest that happen to overlap with those of the underlying substrate (López-López et al., 2014). Few studies consider substrate variability and the effects that these may have on the resultant spectral variability. We can take this a step further in that few studies consider anything other than white substrates, free from pigments and other additives, which may complicate spectral analysis of the trace. It has been noted previously that the ability to discriminate between samples is also dependent on color of substrate and thickness of smear (Gardner et al., 2013). It is clear that further research is required in this area to understand the complexities that are added through choice of substrate. When discussing substrates, it is also important to mention the growing use of SERRS and other enhancement methodologies such as those reported by Rodger in their analysis of lipsticks (Rodger et al., 1998). These methodologies are typically dependent on resonance effects between substrates (or nanoparticles) and the material of interest. The resonance effects enhance spectral features at wavelengths related to the resonance. With complex mixtures, such as those expected for cosmetics, understanding both the chemistry and the physics behind spectral behavior becomes critical as variation may not be inherent to sample differentiation but rather the underlying chemistry and physics of using such enhancement

methods. Thus, the benefits and necessity of using Raman spectral enhancement methodologies need to be carefully considered with respect to their applicability to forensic casework.

3.2 | Statistical analysis and interpretation

Many authors have reported a discriminatory power (DP) based on the visual variability of spectral information (Angrish et al., 2020; Sharma, Chophi, et al., 2020). However, it remains unclear in much of the literature what level of visual variability constitutes discrimination between two samples. Additionally, statistical calculations are hugely dependent on the number of samples being analyzed, and it is well known that increasing sample numbers decreases our likelihood of discriminating all possible pairs. For this reason, we need to be careful with the weighting given to DP values.

Multivariate analysis (or chemometrics) is gaining popularity as a powerful approach for the detection and modeling of variability within a spectral data set, while removing some of the bias associated with visual comparisons of spectra. Chemometrics applies well-established mathematical algorithms to simplify complex datasets and identify latent patterns that may enable discrimination by source, which in some instances may be extended to developing classification models for questioned samples. Review articles on chemometrics in forensic science have been published by Sauzier et al. (2021) and Kumar and Sharma (2018).

An important aspect, however, is to consider the quality of the data that we are trying to model. We have all heard the adage "*rubbish in, rubbish out*" and this is never truer than when trying to provide models in a forensic science environment. We can report a 100% ability to tell samples apart, but we need to think about this in terms of the reliability of the data put in. It is also important to note here that chemical variability within a sample can also be visualized using microscopy. For example, shimmery or pearlescent products often have metal oxide-coated mica or borosilicate glass particles added to the cosmetic formulation to give the "*glitter-like*" appearance. These particles are then randomly distributed throughout the cosmetic matrix leading to heterogeneity in the sample. Without understanding the visual complexities of the sample it can be difficult to fully appreciate spectral variation across a sample; in other words, *where* you analyze is just as important as *how* you analyze. The application of various chemometric methods to cosmetic samples of forensic interest is discussed in more detail by Burnier and Bruce (2023).

3.3 | Research design for operational relevance

It is becoming increasingly recognized that the focus of trace evidence research needs to move beyond simple discrimination and toward determining activity-level propositions, which necessitates studies involving transfer and persistence of cosmetics under operational conditions. There has been an increasing volume of contemporary cosmetic research making use of forensically applicable substrates and simulated transfer of samples that may represent more of a real-world scenario, for example "*kissing*" of lipstick traces (López-López et al., 2014; Sharma, Bharti, & Kumar, 2019). However, we would argue that more needs to be done. Laboratory-based simulations are certainly an important endeavor, however, in order to truly understand cosmetic trace dynamics, we need to move towards the analysis of genuine casework samples. Analytical workflows—akin to the American Society of Trace Evidence Examiners best practice guidelines—also need to be established to identify best practices in our cosmetic trace examination approach.

The contradicting results reported across different studies may link back to the choice and number of samples, as researchers may naturally gravitate to availability within a price bracket rather than considering samples which might represent a true market survey. In that vein, we need to be mindful of the global market and account for jurisdictional differences in cosmetic manufacture and/or regulation. For example, an ingredient that is permitted for use in cosmetic products in one country, may be prohibited in another. Furthermore, given the increase in globalization it is also pertinent to consider that international cosmetic products may be of relevance in investigations beyond country of origin. With regards to the choice of cosmetic, relatively few researchers have chosen to analyze eye, cheek, and facial makeup when compared to lip products. It is assumed that this apparent cosmetic selection bias relates to people's perception of product use, and therefore its value in a forensic context.

Lastly, it is important to consider that no makeup product is designed for use in complete isolation from other skin care and cosmetic products. This is particularly true of complexion products such as primer, foundation, bronzer, highlighter, and setting powder that are designed to be used together in a sequence. During wear, these products will

combine with eccrine secretions and sebum on the skin and cause the layered products to mix; hence any cosmetic traces may comprise a variety of different products in varying proportions. As a result, further work is needed to ascertain how we analyze these complex traces and interpret the resultant spectra; meaningful information must be extracted so that these methodologies may be incorporated into forensic practice and judicial processes.

4 | CONCLUSION

The published literature clearly demonstrates the power of both ATR-FTIR and Raman spectroscopies for non-destructive (in situ), cheap and effective analysis of makeup samples, particularly in combination with emerging methods of statistical data analysis. Despite this, there are several challenges to be addressed in future research that are not limited to data collection and treatment. It is also clear that we need to develop a greater depth of understanding of market, manufacturing, and chemical and substrate variability to inform interpretation of results. Reporting high discriminatory rates, whilst perhaps attractive from a publishing perspective, does not necessarily reflect the true measure of performance for a given analytical approach.

It is now time to widen the scope of this research to include more types of makeup and broader cosmetic types that may be encountered in mixed samples, alongside moving toward combining analytical techniques for increased sample discrimination. Analytical frameworks and methodologies for cosmetic analysis would allow for easier comparison between studies, enabling the sharing of results for a common goal. This would hasten the initial cosmetic market survey and chemical variability studies so that more complex scenarios could be researched.

However, it is important that we consider technology limitations as we further develop methodologies for their potential integration into case work. The United Nations Sustainable Development Goals (SDGs) call for not only reduced inequality (SDG 10) but also equitable access to peace, justice and strong institutions (SDG 17), energy and sustainability (SDGs 7 and 11) and industry, innovation and infrastructure (SDG 9). Development of robust, accessible methodologies that provide consistency across the work being published throughout the Global North and Global South, but that also recognizes regional-specific judicial needs and capabilities is challenging. While doing so will ultimately lead to a comprehensive forensic science research framework, it needs to be sensitive to regional capability and drive toward multilevel solutions. Furthermore, technique homogenization (e.g., a one size fits all approach) is most likely not the best way to standardize forensic trace evidence research.

This review thus highlights the need for consistent and robust data treatment and analysis methodologies to enable comparison and shared understanding. Alongside this we need to expand studies to include a variety of transfers and substrates, persistence intervals, simulations for activity level propositions, and eventually, real casework samples.

AUTHOR CONTRIBUTIONS
Katy A. Bruce: Conceptualization (lead); funding acquisition (supporting); writing – original draft (equal); writing – review and editing (equal). **Georgina Sauzier:** Conceptualization (supporting); funding acquisition (supporting); writing – original draft (equal); writing – review and editing (equal). **Simon W. Lewis:** Conceptualization (supporting); funding acquisition (supporting); writing – original draft (equal); writing – review and editing (equal). **Donna C. Arnold:** Conceptualization (supporting); funding acquisition (lead); project administration (lead); supervision (lead); writing – original draft (equal); writing – review and editing (equal).

CONFLICT OF INTEREST STATEMENT
The authors declare no conflicts of interest.

DATA AVAILABILITY STATEMENT

Data sharing is not applicable to this article as no new data were created or analyzed in this study.

ORCID

Katy A. Bruce https://orcid.org/0000-0003-4321-1564
Donna C. Arnold https://orcid.org/0000-0003-0239-5790
Georgina Sauzier https://orcid.org/0000-0002-9908-7956
Simon W. Lewis https://orcid.org/0000-0002-2049-1586

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