

Identification of Cosmetics Using Near-Infrared Spectroscopy

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Abstract— Non-destructive identification of cosmetics is essential to confirm their identity and purity. Near-infrared (NIR) spectroscopy provides a fast and non-destructive method for cosmetic identification. For this study, 99 raw materials and 30 products were measured using a palm sized NIR spectrometer. Spectral pre-treatment and analysis involved techniques such as multiplicative scatter correction-first derivative (MSC-D1), correlation in wavelength space (CWS), and Principal Component Analysis (PCA) respectively. Among the raw materials, 66 exhibited strong NIR activity, 25 showed medium NIR activity, and eight had weak NIR activity, while all 30 samples were found to be NIR active.

The CWS method revealed a high frequency of Type II errors, with 81 out of 99 raw materials mismatching. All 30 of the products also resulted in mismatches. PCA proved to be the more accurate of the data analysis techniques with creams 97% of variance was accounted for in PC1, and PC scores demonstrating strong differentiation among seven of the eight cream products. In contrast, the perfume products displayed 84% variance in PC1 and 13% in PC2, with two of the seven products showing significant discrimination from the others.

This study confirmed that NIR spectroscopy is well-suited for this application as it provides a quick analysis time, no sample preparation and allows for sample preservation.

Keywords—near-infrared spectroscopy, cosmetics, correlation in wavenumber space, principal component analysis

INTRODUCTION

Cosmetic products refer to any substance or mixture designed to come into contact with external parts of the human body (such as the skin, hair, and nails) or with the teeth and mucous membranes of the mouth. Their purpose is to clean, fragrance, alter appearance, mask body odours, or maintain the body in good condition[1]. Counterfeit cosmetics could be encountered anywhere whether online, in-store or at beauty salons. Counterfeit cosmetics are defined as products that are intentionally and illegally designed to imitate authentic ones, often misleading consumers into thinking they are buying the genuine item [2]. Lower-cost alternatives to more expensive original products, such as perfumes or cosmetic foundations, are widely available; however, these more affordable items are

also susceptible to counterfeiting, a fact that the public often does not realise.[2] The UK Intellectual Property Office launched the ‘Choose Safe not Fake’ campaign in 2024 which targets beauty and hygiene counterfeit products, which the consumers have often purchased assuming they are produce in the same or similar conditions as the genuine products which is not often the case leading to health issues and possibly even death [3].

Previous methods used for looking at cosmetic samples include high pressure liquid chromatography (HPLC)[4], [5], [6] gas chromatography-mass spectrometry (GC-MS) [2],[7],[8],[9] and Fourier-transform infrared spectroscopy (FTIR)[10],[11],[12].

NIR is a non-destructive analytical technique that offers a fast method for detecting and comparing suspected counterfeit products without requiring any sample preparation. It works by measuring the absorption of electromagnetic radiation in the NIR region, typically between 800 nm and 2500 nm [13]. Absorption in this range is primarily due to molecular vibrations, particularly the overtones and combination bands of fundamental vibrational modes, generating a spectrum. This technique provides insights into both the chemical composition and physical properties of the samples, making it ideal for real-time monitoring [14]. Given the complexity of raw NIR spectra, statistical data analysis, known as chemometrics, is employed to extract meaningful chemical information from the non-specific and poorly resolved data [15].

Previous studies related to NIR spectroscopic applications of cosmetics products include the classification of cosmetic foundations in crime scenes [16], quality control of cosmetic mixtures[17], predicting the viscosity of shampoos [18], determining the shelf life of products[19] and evaluation of cosmetic moisturising properties [20].

This study expands upon earlier research by including a comparative analysis of raw materials and cosmetic products, which may uncover how small variations in the formulation can influence the results. By establishing the connection between raw materials and cosmetic formulations, the research improves the accuracy and applicability of the palm-sized portable NIR instrument for rapid, on-site analysis in

industrial settings. Additionally, it offers a more cost-effective and sustainable solution by eliminating the need for sample preparation and laboratory testing, while facilitating a high-throughput analysis method.

METHOD

A. Materials

A total of 99 raw materials and 30 cosmetic products were used in this study (Table 1). The raw materials included pure substances and mixtures yet were all ingredients used in cosmetic products. The formulations of these products included solutions, suspensions, emulsions, powder, creams and ointments. Raw materials and products were of different colours including transparent, light and dark colours. All products were stored in 2 mL glass vials prior to measurement in order to ensure protection from humidity and temperature.

B. Instrumentation

For this study the JDSU palm sized MicroNIR 1700 Pro Spectrometer (now known as Viavi MicroNIR 1700EC) with a linear variable filter (LVF) dispersing element and 128-pixel uncooled InGaAs photodiode array was used. Samples were obtained from Hampshire Cosmetics Ltd based on their popularity with the public and included 99 raw materials including waxes, creams, perfumes, and oils, along with 30 cosmetic products including hair and skin products with a range of colours and consistencies from various brands. Each sample was measured three times to obtain an average reading, with the measurements taken directly through their glass vials; this eliminated the need for sample preparation or instrumentation cleaning during the analysis. Prior to sample readings the instrument was calibrated by taking light and dark background readings to ensure optimal performance.

C. Data Analysis

For spectral quality the interpretation of NIR activity considered the number of peaks, absorption range, maximum peak intensity and signal to noise (S/N) ratio. The number of peaks present indicate the substance that is being analysed; having more peaks present allows for higher differentiation between substances as there are more data points for comparison. The absorbance range refers to the highest and lowest wavenumbers examined by the method to assess the absorption spectrum. A broader wavenumber range introduces more variables, which increases the potential for distinguishing between substances, however this largely

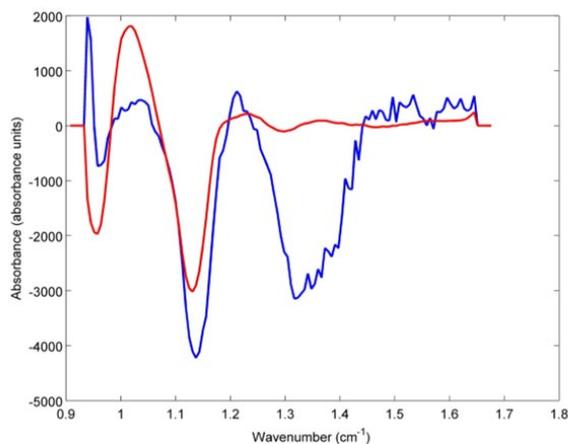


Fig 1. MSCD1 treated NIR spectra of BUH087 (blue) and BUH091 (red) measured using the JDSU palm sized micro-NIR spectrometer

depends on the quality of the peaks present in the spectrum. Maximum peak intensity refers to the strength of the spectrum signal, indicating the NIR activity of the substance and shows the effectiveness of the technique. The S/N ratio measures the level of the desired signal relative to background noise. It is calculated by dividing the mean spectrum by the standard deviation of its replicates, using the maximum intensity spectral peak. A higher S/N ratio indicates a higher quality spectrum, as it shows the signal is less impacted by background interference.

Correlation in wavelength space (CWS) compared spectral similarity of raw materials and products and is calculated as a numerical value between 0-1. The threshold used was 0.95 with a value of >0.95 considered a match[13]. All raw materials and products were expected to give r values of >0.95 when tested against their own spectra, and r values of <0.95 when tested against other raw materials/products. A Type I error, or false positive, occurs when a raw material/product produces an r value of less than 0.95 for its own spectrum. A Type II error, or mismatch (false negative), happens when a raw material/product generates an r value greater than 0.95 for the spectrum of a different sample. Obtaining an r value of 1 is unlikely due to spectral noise[21]

Principal component analysis (PCA) is based on reducing dimensions of data into 2D or 3D based on variances. PCA is interpreted using scores, loadings, and variance. Scores evaluate how closely samples are clustered, determining whether they are similar, identical, or different, and identifying the significant wavenumbers. Loadings signify the dimensions, where the first dimension (PC1) accounts for the highest variance in the data, the second (PC2) explains the second highest variance, unrelated to the first, and the third (PC3) identifies variance not related to the previous components. Variance indicates the contribution to each principal component. For this dataset, products were grouped based on two formulation types (creams and perfumes) due to their similar components.

RESULTS AND DISCUSSION

Overall, the raw materials were mostly NIR active with 66 showing strong NIR activity, 25 demonstrating medium NIR activity and 8 displaying weak NIR activity. Raw materials with weak NIR activity were fairly similar with number of

TABLE I. SUMMARY OF PRODUCTS AND CHARACTERISTICS

Product type	Number of products	Colours
Liquid	12	Transparent and coloured
Gel	2	Colourless
Emulsion	14	White and coloured
Suspension	2	White

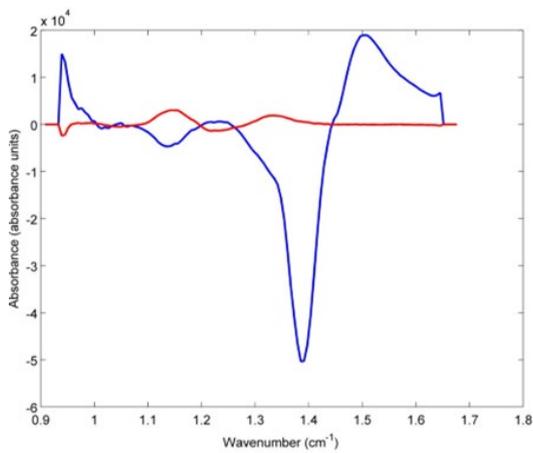


Fig 2. MSCD1 treated NIR spectra of BUH114 (blue) and BUH117 (red) measured using the JDSU palm sized micro-NIR spectrometer

peaks ranging from 2-5 and spectral ranges between 0.932-1.651cm⁻¹ which is due to the limited range of the palm sized instrument. The absorbance intensities ranged from 0.0043-0.0077 absorbance units, however there were two outliers (BUH087 and BUH091, shown in Figure 1) with absorbance units of 4301.28 and 3348.45 respectively. The lowest S/N ratio was 7.0 for BUH083 and the highest was 15.5 for BUH091. Raw materials with medium NIR activity had between 2-6 peaks observed in comparison to the strong NIR activity samples which had between 4-11 peaks. The spectral ranges for these raw materials were found to be 0.932-1.651cm⁻¹ with absorbance intensities ranging from 1159.24 absorbance units for BUH061 to 537578.4 absorbance units for BUH074. Two of the raw materials BUH073 and BUH079 were outliers with very low absorbance intensities of 0.008 and 0.007 absorbance units respectively. A large range of S/N ratios were observed values ranging from 5-32.

All measured products were NIR active which was expected as the majority of materials were additives/excipients which were more NIR active due to the H-bonds present. No weak NIR activity products were observed and only two products showed medium NIR activity which were BUH114 and BUH117 (shown in Figure 2). The aforementioned products showed 3 and 4 peaks respectively, with a spectral range of 0.932-1.651cm⁻¹ and absorbance intensities of 54745.4 for BUH114 and 2723.072 for BUH117. The S/N ratios were 36 and 12 respectively. There were 28 products with strong NIR

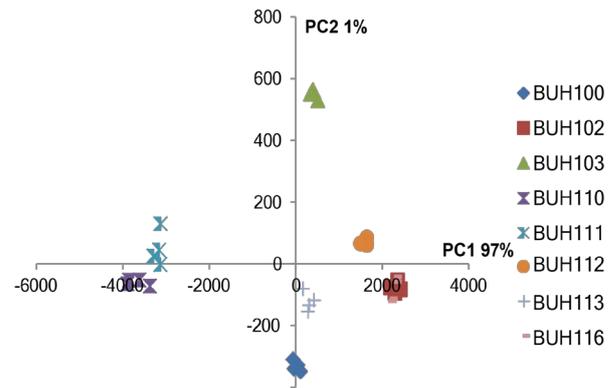


Fig 4. PCA showing the cream products including: BUH100, BUH102, BUH103, BUH110, BUH111, BUH112, BUH113, and BUH116, measured using the JDSU palm sized micro-NIR spectrometer

activity which showed peak numbers ranging from 5-7, a spectral range of 0.932-1.651cm⁻¹ and absorbance intensities ranging from 2619.315 for BUH123 to 1148000 absorbance units for BUH107. The S/N ratio range was between 12-38. CWS showed a high frequency of Type II errors, with mismatches occurring in 81 out of 99 raw materials and in all 30 of the products (shown in Figure 3). Only 18 raw materials showed no mismatches. The range of mismatches per sample varied from 1 to 33, with the fewest mismatches recorded for BUH002 and BUH094, which had 1 and 2 mismatches, respectively. BUH002 mismatched with BUH094 with a correlation of 0.97; the samples were of the same material and molecular formula/structure, but they differed in particle size. The spectra of both samples showed a slight difference at 1143nm (CH group) and 1400nm (water peak). The largest mismatch was observed was for BUH062 against BUH011 with a correlation of 0.99, this match was expected as both samples are expected to be the same. 22 samples had 20-30 mismatches, 65 samples had between 10-20 mismatches and 21 samples had less than 10 mismatches. With regards to PCA the cream products showed that PC1 contributed to 97% of the variance amongst the spectra, when the PC scores were plotted there was a strong discrimination between cream products with 7 of the 8 samples clustered separately (shown in Figure 4). Samples BUH102 and BUH116 showed the strongest similarity with overlapping points, but all other cream products did not show any similarities with each other.

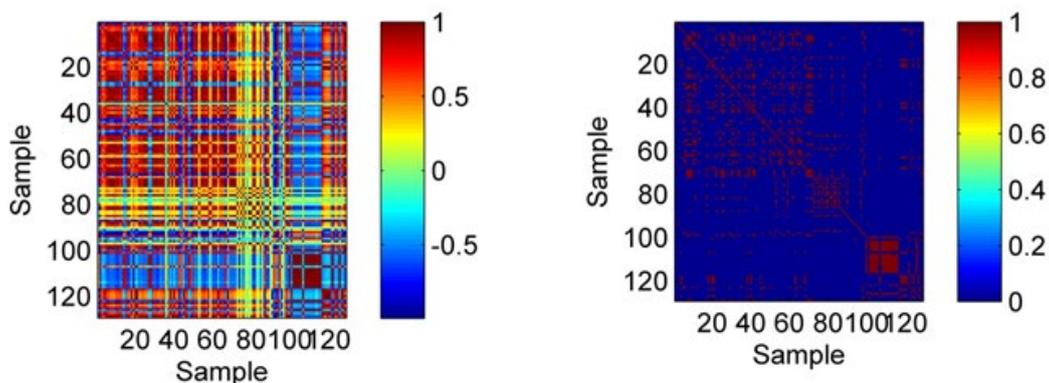


Fig 3. Correlation map of the MSCD1 treated NIR spectra of (a) raw materials (1-99) and (b) products (100:129) measured using the JDSU palm sized micro-NIR spectrometer.

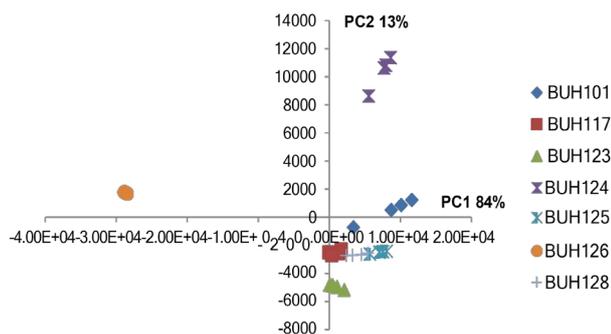


Fig 5. PCA showing the perfume products including: BUH101, BUH117, BUH123, BUH124, BUH125, BUH126, and BUH128, measured using the JDSU palm sized micro-NIR spectrometer

The perfume products showed that PC1 contributed to 84% variance amongst the spectra, and PC2 13% of the variance. PC scores showed a large range of discrimination with regards to sample BUH124 and BUH126 in comparison to the other samples (shown in Figure 5). A lack of accuracy was observed for samples BUH101 and BUH124, in comparison to BUH117, BUH125 and BUH128 which were found to be similar.

CONCLUSION

This study explored the use of palm-sized Near-Infrared (NIR) spectroscopy for the rapid detection of contamination in cosmetic ingredients as they entered the production line. The primary goal was to assess whether the technique could reliably identify contaminants with minimal impact on the samples being tested. The results confirmed that the palm sized NIR is well-suited for this purpose due to several key advantages. Its compact size and portability allow for easy, on-site use, making it highly convenient in a fast-paced production setting. The device also provides quick analysis times, allowing for direct monitoring of ingredients, which is critical in fast-paced manufacturing settings. Additionally, the technique does not require any complex sample preparation, which saves both time and resources, and it does not destroy or alter the samples during testing, ensuring that they remain intact for further use or processing. Although it is compact in size, the palm-sized NIR device successfully generated high-quality spectral data for the cosmetic samples, delivering reliable and accurate results even with the instrument's limited NIR wavelength range. This capability is essential for detecting contamination and ensuring product quality without compromising efficiency.

Overall, the study demonstrated that this method is not only practical but also effective in maintaining quality control standards in the cosmetics industry, making it a valuable tool for manufacturers to include on the production line for initial sample testing purposes. Further analysis on any suspicious cosmetic samples could be undertaken within a laboratory environment using techniques which could be complementary to the NIR results obtained, such as FTIR which could provide more insight into the molecular information of the samples, HPLC which could detect trace amounts of substances within

complex samples or GC-MS which could look at volatile and low molecular weight compounds such as fragrances.

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