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Discrimination of Sunscreen Formulations using Non-destructive Infrared Spectroscopy Coupled with Chemometrics

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Structured Abstract

Background: Sunscreens are widely used to protect the skin from ultraviolet (UV) radiation and are generally classified into three types which are physical sunscreens containing inorganic components, chemical sunscreens containing organic UV filters and hybrid sunscreens that combine both. In forensic investigations sunscreen can serve as trace evidence when transferred onto different surfaces at a crime scene. However, due to its invisible and sometimes colourless nature, analytical techniques that are non-destructive, rapid and require minimal sample preparation are required.

Methods: Attenuated Total Reflectance Fourier Transform Infrared (ATR-FTIR) spectroscopy was employed as a suitable analytical technique for sunscreen analysis because samples can be analysed directly on the ATR crystal without extensive preparation. Due to sunscreen comprise of complex chemical composition, the chemometric techniques including Principal Component Analysis (PCA), PCA coupled with Linear Discriminant Analysis (PCA-LDA) and Hierarchical Cluster Analysis (HCA) were applied to assist in the interpretation of complex ATR-FTIR spectra obtained from ten sunscreen samples analysed on different substrates and by brand.

Results: The fingerprint region was identified as the most significant spectral region as it contains characteristic absorption bands of UV filters, while the O–H region indicated the presence of moisture components in the formulations. PCA reduced spectral complexity but showed limited ability to discriminate samples with subtle spectral differences due to its unsupervised nature, PCA-LDA improved discrimination by incorporating known class information and achieved higher classification accuracy for substrate type (96.67%) compared to sunscreen brand discrimination (12.22%). HCA further supported the PCA-LDA results by clustering samples based on similarity, with glass substrates forming the most distinct cluster due to reduced contact between the smooth glass surface and the ATR crystal resulting in lower absorbance intensity, while cloth samples exhibited slightly lower intensities than no-substrate samples due to absorption of sunscreen residues into the cloth.

Conclusion: In conclusion, this study shows that ATR-FTIR spectroscopy combined with chemometric analysis is a promising non-destructive method for identifying sunscreen residues, particularly based on substrate type, with potential applications in forensic trace evidence analysis.

Keywords: Sunscreen residues, Forensic trace evidence, ATR-FTIR spectroscopy, Chemometrics, PCA-LDA

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