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Forensic Analysis of Nail Polish Using ATR-FTIR Spectroscopy with Chemometric Method

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Structured Abstract

Background: Nail polishes are cosmetic paints that can be found at a crime scene and provide information to reconstruct the crime when analyzed using a non-destructive technique like ATR-FTIR spectroscopy. The objective of this research is to characterize different brands of nail polish based on their chemical constituent, to discriminate respective nail polishes using the chemometric method as well as to study the impact of glass and cotton substrates on nail polish spectra.

Methods: Ten different brands of nail polish were smeared on the ATR crystal to obtain FTIR spectra. The respective nail polishes were also smeared on glass and cotton substrates and then analyzed using ATR-FTIR spectroscopy. Principal component analysis (PCA) and Hierarchical clustering analysis (HCA) were applied to distinguish the spectra using Unscrambler X software.

Results: All spectra of nail polish samples provide different organic compounds (hydroxyl group, aliphatic amine, aliphatic compounds, talc or mica, aromatic compounds, nitrocellulose, nitro group, acid, and ester) based on the characterization of nail polish samples. The chemometric method provides high discriminating power, with a 98.16% and 97.70% success rate for manual comparison and PCA, respectively. A plot of all PCs in a scree plot offered better discrimination of samples as it accounted for 98.75% variance in a dataset. Based on the scatter plot between the loading values of the PCs, the first fourth PCs were enough to explain the maximum variance from the dataset, which is 96%; PC1 = 71%, PC2 = 17%, PC3 = 6%, and PC4 = 2%. HCA clustering was discovered, and all of the nail polish samples were divided into 10 distinct clusters based on the respective agglomerative distances.

Conclusion: In conclusion, the application of the ATR-FTIR technique with the chemometric method effectively discriminated almost all the samples and it has the potential to give accurate discrimination of nail polish exhibits obtained in forensic laboratories. The chemometric method is feasible in discriminating the respective nail polishes. The presence of glass and cotton as substrate gives some effect on the spectrum of nail polish.

Keywords: Nail polish, ATR-FTIR, PCA, HCA, Discrimination

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