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Novel Substance Identification via Normalized Spectral Similarity Scoring in Near-Infrared Imaging

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ABSTRACT

In the Engineering Biology frontier, Near-infrared (NIR) imaging offers a rapid, non-destructive approach for substance identification, leveraging the unique spectral fingerprints of materials. However, traditional spectral similarity metrics often suffer from sensitivity to variations in illumination intensity, instrument drift, and sample heterogeneity, leading to inaccurate identification. This abstract presents a novel methodology that enhances the robustness and accuracy of NIR-based substance identification by employing normalized spectral similarity scoring.

The core innovation lies in the pre-processing of NIR spectral data through normalization. Specifically, each spectral signature is normalized to a unit vector, effectively eliminating the influence of magnitude variations while preserving the intrinsic spectral shape. This normalization step ensures that subsequent similarity comparisons are based solely on the spectral profile, rather than absolute intensity values. This approach significantly mitigates the impact of environmental and instrumental fluctuations, enabling more reliable comparisons across diverse datasets.

Following normalization, a refined similarity score is calculated using the cosine similarity metric. This metric, which measures the cosine of the angle between two normalized spectral vectors, provides a robust measure of spectral correlation. A higher cosine similarity score indicates a greater degree of spectral matching and thus a higher likelihood of identical substance composition.

The method further incorporates a statistical framework to establish a threshold for significant similarity, accounting for potential noise and spectral variations within a given substance class.

This normalized spectral similarity scoring method offers several key advantages. Firstly, it enhances the consistency and reliability of substance identification by minimizing the impact of extraneous variables. Secondly, it enables the comparison of spectra acquired under varying conditions, facilitating the creation of robust spectral libraries. Thirdly, the statistical framework provides a quantitative measure of confidence in the identification,

improving the overall accuracy and interpretability of results.

Experimental validation on a diverse dataset of pharmaceutical, polymer, and food samples demonstrates the superior performance of the proposed method compared to traditional spectral similarity metrics. The normalized approach achieves significantly higher identification accuracy and reduced false positive rates, particularly in challenging scenarios involving low signal-to-noise ratios and significant intensity variations. This methodology represents a significant advancement in NIR-based substance identification, offering a more robust and reliable tool for a wide range of applications, including quality control, process monitoring, and forensic analysis.

KEY WORDS

Engineering Biology, Near-infrared (NIR) imaging, Substance identification, Spectral fingerprints, Normalized spectral similarity, Cosine similarity metric, Spectral normalization, Statistical framework, Robust spectral libraries, Identification accuracy, Non-destructive analysis

BIOGRAPHY

Michael K. Akindeju *(Ph. D, FIChemE, FRACI, CEng, RPEQ)* is a certified business architect and adjunct associate professor at the Institute of Science, Innovation, and Sustainability at Federation University, Australia. He is the principal process engineering consultant and director at MKPro Group, where he brings expertise in research, development and engineering to the advanced manufacturing and processing of minerals and nanoparticles. He is the current chair of IChemE Mining & Minerals SIG.

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