Macedonian Pharmaceutical Bulletin, 72 (Suppl 1) 415 - 416 (2026)
Online ISSN: 1857-8969
DOI: 10.33320/maced.pharm.bull.2026.72.03.200
Short communication

Vibrational spectroscopy and spectral imaging for rapid analysis of natural products: opportunities and challenges

Olga Gigopulu[1*], Nikola Geskovski[1], Gjoshe Stefkov[1], Petre Makreski[2]

[1] *Ss. Cyril and Methodius University in Skopje, Faculty of Pharmacy, 1000 Skopje, N. Macedonia*
[2]*Ss. Cyril and Methodius University in Skopje, Faculty of Natural Sciences and Mathematics, Institute of Chemistry, 1000 Skopje, N. Macedonia*

Introduction

Natural products derived from medicinal plants, foods, fungi, and forest resources are complex matrices containing a wide range of primary and secondary metabolites. Their qualitative and quantitative characterization is essential for quality control, authentication, and the assessment of biological activity. High-performance liquid chromatography (HPLC), gas chromatography coupled with mass spectrometry (GC-MS), and liquid chromatography–mass spectrometry (LC-MS) remain the reference methods for detailed compositional analysis. However, these methods often involve destructive sample preparation, long analysis times, and significant operational costs (Balekundri and Mannur, 2020).

Vibrational spectroscopy has emerged as an attractive complementary approach because it enables rapid, non-invasive, and reagent-free analysis. The spectral information obtained reflects the molecular vibrations of chemical bonds, providing a unique molecular fingerprint of the sample. Combined with advanced chemometric, vibrational spectroscopy can be used for classification, authentication, adulteration detection, and quantitative prediction of target analytes (Huck, 2015).

Vibrational spectroscopy in natural product analysis

Among vibrational techniques, NIR spectroscopy has gained particular popularity due to its minimal sample preparation requirements and the ability to analyze solids, powders, liquids, and intact plant materials. NIR spectroscopy has been successfully applied to determine moisture, essential oil content, cannabinoids, polyphenols, alkaloids, and other bioactive compounds in medicinal and aromatic plants (Huck, 2015).

FTIR spectroscopy, especially when coupled with attenuated total reflectance (ATR), provides detailed information on functional groups and has become an efficient tool for authenticity testing and quality control of herbal medicines (Huck, 2015). In recent years, our research group has contributed to the development and application of FTIR spectroscopy combined with chemometric analysis for the rapid characterization and quality assessment of *Cannabis sativa* inflorescences and extracts, enabling their discrimination and supporting quality control and authentication.

Raman spectroscopy offers complementary information and is particularly useful for aqueous samples because water exhibits weak Raman

*olga.gigopulu@ff.ukim.edu.mk

scattering. Recent developments in portable and handheld Raman and NIR devices have expanded the application of these techniques beyond the laboratory, allowing in-field analysis and on-site quality assessment (Huang, 2016).

The effectiveness of vibrational spectroscopy strongly depends on the application of multivariate statistical methods. Principal component analysis (PCA), partial least squares regression (PLSR), and support vector machines (SVM) are commonly employed to extract meaningful information from complex spectral datasets. These chemometric approaches transform spectroscopic measurements into robust predictive models capable of rapidly estimating the concentration of key constituents and detecting deviations from expected quality attributes (Huck, 2015).

Spectral imaging and remote sensing applications

The integration of spectroscopy with digital imaging has enabled the development of multispectral and hyperspectral imaging systems that simultaneously acquire spatial and spectral information. Unlike conventional spectroscopy, spectral imaging provides a spectrum for each pixel, allowing visualization of the spatial distribution of chemical constituents within a sample (Sandasi et al., 2017).

Hyperspectral imaging is widely applied in food science, pharmaceutical quality control, medicinal plant authentication, and crop phenotyping. It enables detection of adulterants, assessment of product uniformity, identification of fungal contamination, and monitoring of changes during drying, storage, and processing, as well as estimation of chlorophyll, water content, and secondary metabolites with high accuracy (Sandasi et al., 2017).

The recent availability of lightweight hyperspectral and multispectral sensors mounted on unmanned aerial vehicles (UAVs) has further expanded the analytical capabilities of these methods. Aerial spectral imaging enables rapid, non-destructive monitoring of large agricultural and forested areas, facilitating the assessment of plant health, disease detection, stress monitoring, biomass estimation, and evaluation of phytochemical variability. Such approaches are increasingly important for precision agriculture, sustainable harvesting of medicinal plants, and the management of forest resources (Sandasi et al., 2017).

Opportunities and current challenges

Vibrational spectroscopy and spectral imaging offer rapid, non-destructive, and reagent-free analysis with minimal sample preparation, aligning with green analytical chemistry principles. Portable instruments further enable in-field and real-time quality assessment (Huck, 2015). However, spectral complexity, including overlapping bands and indirect structure–signal relationships, requires robust chemometric models based on large, well-characterized datasets. Model performance can be affected by instrument variability, environmental conditions, and matrix effects, limiting transferability and accuracy (Huck, 2015). Hyperspectral imaging additionally generates large datasets that pose computational challenges, although advances in machine learning, cloud computing, and sensor miniaturization are expected to enhance future applications in natural product analysis (Sandasi et al., 2017).

References

Balekundri, A., Mannur, V., 2020. Quality control of the traditional herbs and herbal products: a review. Future Journal of Pharmaceutical Sciences 6, 67. https://doi.org/10.1186/s43094-020-00091-5

Huang, C.-C., 2016. Applications of Raman spectroscopy in herbal medicine. Applied Spectroscopy Reviews 51, 1–11. https://doi.org/10.1080/05704928.2015.1092154

Huc,k C.W., 2015. Infrared spectroscopic technologies for the quality control of herbal medicines. In Evidence-Based Validation of Herbal Medicine, 477–493. https://doi.org/10.1016/B978-0-12-800874-4.00022-2

Geskovski, N. et al., 2021. Mid-infrared spectroscopy as process analytical technology tool for estimation of THC and CBD content in Cannabis flowers and extracts. Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy 251, 119422. https://doi.org/10.1016/j.saa.2020.119422

Sandasi, M. et al., 2017. Application of hyperspectral imaging in the quality control of medicinal plants and products. Journal of International Medical Research 28(7), 1127–1138. https://doi.org/10.1177/0960336017736247