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Review Article

SPECTROSCOPY IN BIOMEDICAL DIAGNOSTICS: A COMPREHENSIVE SYSTEMATIC REVIEW

[1]Aiswarya R, [2*]Subha C, [3]Swathi T, [4]Monish Raj R and [5]B Nazreen

[1] PERI Institute of Technology, Chennai- 48, Tamil Nadu, India
[2*]PERI College of Arts and Science, Chennai - 48, Tamil Nadu, India
[3]PERI College of Physiotherapy, Chennai - 48, Tamil Nadu, India
[4]PERI College of Pharmacy, Chennai - 48, Tamil Nadu, India
[5] PERI College of Nursing, Chennai - 48, Tamil Nadu, India

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ABSTRACT

Spectroscopy has emerged as a powerful analytical and diagnostic tool in biomedical science, offering non-invasive, rapid, and label-free detection of biomolecular changes associated with disease. This comprehensive systematic review examines the applications of ultraviolet-visible (UV–Vis) and Fourier Transform Infrared (FTIR) spectroscopy in biomedical diagnostics. A literature survey spanning 1987 to 2024 was conducted across databases including Scopus, Web of Science, ScienceDirect, and Google Scholar. The review identifies spectroscopy's role in disease detection, biofluid analysis, drug quality assessment, and biomolecular fingerprinting. FTIR spectroscopy demonstrates high specificity in molecular vibration analysis, while UV–Vis spectroscopy provides sensitivity in quantifying biochemical transitions. Together, these modalities support advancements in clinical chemistry, oncology, and metabolomics. Despite their diagnostic promise, challenges such as data standardization, spectral overlap, and interpretation bias remain. Future work should integrate artificial intelligence and nanotechnology to enhance diagnostic precision and clinical applicability.

Keywords: Spectroscopy, UV–Vis, FTIR, Biomedical Diagnostics, Biofluids, Molecular Fingerprinting.

INTRODUCTION

Spectroscopy has evolved into a cornerstone of modern biomedical diagnostics due to its ability to provide real-time, non-invasive insights into biochemical and structural alterations at the molecular level. Techniques such as Ultraviolet–Visible (UV–Vis) and Fourier Transform Infrared (FTIR) spectroscopy enable rapid biochemical fingerprinting of biofluids and tissues, allowing clinicians to detect diseases at early stages. Despite the widespread adoption of spectroscopic techniques in materials and chemical sciences, their translation into clinical diagnostics remains in its developmental phase. Previous studies have demonstrated potential in cancer screening, metabolic disorder monitoring, and pathogen detection; however, comparative analyses and standardized methodologies are still lacking. This review systematically consolidates existing research on spectroscopic diagnostic applications, highlighting technological advancements, methodological challenges, and future prospects for clinical implementation. Sala *et al*. (2020) provide a comprehensive account of FTIR biofluid analysis as a translational diagnostic platform, arguing that serum/plasma FTIR fingerprints can enable rapid screening with minimal sample preparation. Naseer *et al*. (2021) reviewed ATR-FTIR biofluid studies and emphasized spectral fingerprinting for disease classification while highlighting the need for standardized protocols. Tiernan *et al*. (2020) examined ATR-FTIR instrumentation and spectroscopic imaging specifically for biopharmaceuticals, underscoring how imaging and mapping improve molecular specificity in complex fluids. Collectively, these works position FTIR as a practical, label-free technique with strong translational potential, provided pre-analytical and analytical variability are controlled (Sala *et al*., 2020; Naseer *et al*., 2021; Tiernan *et al*., 2020). Naseer *et al*. (2021) synthesized evidence across ATR-FTIR biofluid studies and

*Corresponding Author: Subha C, PERI College of Arts and Science, Chennai -48, Tamil Nadu, India Email: publications@peri.ac.in.

recommended harmonized sample handling and spectral preprocessing to improve cross-study comparability. Shrivastava *et al*. (2023) and Shrivastava & Verma (2023) performed systematic/meta-analytic assessments of vibrational spectroscopy in oral and head-and-neck cancers respectively, reporting promising pooled sensitivities but also noting heterogeneity driven by small sample sizes and inconsistent chemometric approaches. Anderson *et al*. (2020) offered a systematic review on vibrational spectroscopy as a liquid-biopsy tool, mapping methodological gaps and translational obstacles. Together, these reviews quantify the promise of spectroscopy while stressing methodological standardization before large-scale clinical deployment. Yang *et al*. (2022) demonstrated ATR-FTIR plus chemometrics for lung cancer diagnosis using patient samples, showing discriminative spectral markers and robust classification metrics in pilot cohorts. Sala *et al*. (2019) reported a serum-based FTIR pilot study for brain cancer screening, suggesting FTIR's feasibility as a non-invasive pre-screening tool. Wang, Li and Zhang (2021) reviewed infrared spectroscopy methods in early cancer detection and highlighted chemometric pipelines that consistently improved diagnostic performance in oncology studies. These studies collectively show FTIR/UV workflows can detect cancer-related biochemical shifts in biofluids, but larger validation cohorts are still needed. Anderson & Walsh (2020) reviewed vibrational spectroscopy of human blood, detailing spectral regions linked to proteins, lipids and nucleic acids and discussing clinical challenges such as biological variability and water absorption. Monteiro *et al*. (2024) explored high-wavenumber IR spectroscopy of plasma and reported diagnostic value in specific high-frequency bands. Q. Wang *et al*. (2017) combined UV–Vis and ATR-FTIR to study postmortem interval changes in rabbit plasma, illustrating how multi-modal spectroscopy can track biochemical time-courses. These contributions map how different spectral windows and modalities capture complementary biochemical information in biofluids.

Pandey *et al*. (2022) summarized UV–Vis approaches for clinical biomarker quantification, emphasizing UV–Vis's strength for targeted, quantitative assays (e.g., enzyme or chromophore measurements). Q. Wang *et al*. (2017) provided an applied example where UV–Vis complemented ATR-FTIR for postmortem biochemical monitoring. Hashem *et al*. (2020), though focused on food authentication, demonstrate UV–Vis + FTIR combined workflows that are translatable to diagnostic contexts where both sensitivity (UV–Vis) and molecular fingerprinting (FTIR) are required. Anderson, Young & Gardner (2022) present spectral data fusion of Raman and FTIR for cancer detection, illustrating how combining orthogonal spectral information increases classification robustness. Anderson & Smith (2022) review machine-learning pipelines for FTIR classification in oncology, discussing feature-selection, cross-validation, and model generalizability. Wang *et al*. (2021) and other methodological reviews stress chemometric rigor e.g., avoiding overfitting and using independent test sets — as essential for moving spectroscopy from pilot studies to clinical assays. These works collectively argue that ML + careful data fusion are key enablers of clinically useful spectroscopic diagnostics. Kazarian & Byrne (2020) provide an authoritative treatment of ATR-FTIR instrumentation and biomedical uses, describing sampling accessories, spatial resolution trade-offs and strategies to mitigate water absorption. Tiernan *et al*. (2020) discuss spectroscopic imaging for biopharmaceuticals, emphasizing spatially resolved FTIR to study heterogeneity in biological samples. Theakstone & Davies (2021) review clinical perspectives for FTIR of biofluids, noting how improved ATR hardware and detector sensitivity are unlocking new diagnostic niches. Sala, Jones & Martin-Hirsch (2020) and Naseer (2021) both highlight pre-analytical factors—sample collection, storage, drying, and substrate effects—as major sources of inter-study variability. Sala *et al*. propose SOPs for sample handling to increase reproducibility, while Naseer emphasizes that protocol harmonization is a prerequisite for multi-center validation studies. These papers are widely cited as foundational for establishing rigorous spectral diagnostic pipelines. Bunaciu, Aboul-Enein & Ivan (2021) discuss FTIR spectral markers as disease indicators and the analytical pitfalls in assigning molecular origins to spectral bands. Ricci *et al*. (2015) and Petit & Puskar (2018) illustrate how material-specific fingerprinting (e.g., tannins or nanodiamonds) can be generalized to complex biological matrices, but interpretation requires careful reference spectra and controls. These works underscore both the interpretative power and the caution needed when linking spectral features to specific biomolecules. Petit & Puskar (2018) review FTIR analysis of nanodiamonds and their surface chemistry — useful background for sensor surface functionalization and nanotechnology-enhanced spectroscopy in diagnostics. Maleki & Mashinchian (2011) show combined UV and FTIR analyses for microbial characterization, indicating how spectroscopy helps in pathogen identification in biomedical contexts. These niche applications point to opportunities where spectroscopy is paired with nanomaterials or microbiological assays.

MATERIALS AND METHODS

This systematic review adopted the PRISMA (Preferred Reporting Items for Systematic Reviews and Meta-Analyses) framework to maintain methodological transparency and reproducibility. The primary objective was to identify, evaluate, and synthesize peer-reviewed research applying UV–Visible (UV–Vis) and Fourier Transform Infrared (FTIR) spectroscopy to biomedical diagnostics, including disease detection, biofluid screening, and molecular characterization of pathological conditions. This methodology ensured that every included paper directly addressed how spectroscopy supports biomedical diagnostics—for example, FTIR detecting biochemical fingerprints of cancer in serum, or UV–Vis quantifying hemoglobin and enzyme transitions for disease monitoring. Data synthesis emphasized diagnostic performance, reproducibility, and translational readiness rather than purely physical or chemical characterization.

RESULTS AND DISCUSSION

The literature demonstrates a rapid growth of spectroscopy-based biomedical studies over the past decade. Most publications concentrate on oncology, metabolic disorders, and infectious disease detection, emphasizing non-invasive biofluid analysis such as serum, plasma, urine, and saliva. FTIR spectroscopy especially Attenuated Total Reflectance (ATR-FTIR) has become the most frequently used technique because of minimal sample preparation and strong molecular fingerprinting capacity. UV- Vis spectroscopy complements FTIR by providing quantitative concentration analysis and enzyme or chromophore assays.

Table 1. Comparison between two methodologies.

Technique	Strengths	Limitations	Diagnostic Use
UV–Vis	High sensitivity for quantifying analytes, rapid measurement, low cost	Requires transparent samples, limited molecular specificity	Enzyme kinetics, chromophore and hemoglobin analysis
FTIR	Distinguishes functional groups, high specificity, minimal reagents	Sensitive to water absorption, needs baseline correction	Cancer, diabetes, metabolic & infectious disease detection

Recent studies (Sala *et al*., 2020; Naseer *et al*., 2021; Shrivastava *et al*., 2023) confirm diagnostic accuracies ranging from 85 – 95 % for distinguishing healthy and diseased spectra using chemometric classifiers such as PCA-LDA, SVM, and Random Forest**.** Machine-learning integration has further improved reproducibility and minimized operator bias (Anderson and Smith, 2022). Persistent barriers include biological variability**,** water interference**,** and limited inter-laboratory reproducibility**.** Lack of centralized spectral databases also restricts cross-validation between studies. Addressing these limitations through larger cohort validation and standardized spectral repositories remains a top priority.

CONCLUSION

This systematic review confirms that UV–Vis and FTIR spectroscopy are promising analytical platforms for biomedical diagnostics due to their sensitivity, speed, and non-destructive nature. FTIR provides detailed biochemical fingerprinting, whereas UV–Vis offers rapid quantitative measurements. The synergy of these two modalities supported by chemometrics and AI—enables early disease detection and personalized diagnostic strategies. Nevertheless, successful clinical translation depends on standardizing spectral acquisition, preprocessing algorithms, and diagnostic thresholds. When combined with portable instrumentation and intelligent data analytics, spectroscopic diagnostics can revolutionize point-of-care testing and complement existing laboratory assays. Future investigations should Develop large, open-access spectral databases with standardized metadata for biofluids and tissues. Integrate artificial intelligence and deep-learning architectures to automate spectral interpretation and reduce human bias. Design portable, miniaturized FTIR/UV–Vis sensors for bedside or remote clinical use. Conduct multi-center clinical trials comparing spectroscopy-based diagnostics with established biochemical and imaging methods. Explore hybrid modalities, combining spectroscopy with microfluidics, nanotechnology, and biosensors for multiplexed real-time diagnostics. These will bridge the gap between laboratory proof-of-concepts and full-scale clinical implementation, advancing spectroscopy from an analytical tool to a mainstream diagnostic technology.

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CONFLICT OF INTERESTS

The authors declare no conflict of interest

ETHICS APPROVAL

Not applicable

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AI TOOL DECLARATION

The authors declares that no AI and related tools are used to write the scientific content of this manuscript.

DATA AVAILABILITY

Data will be available on request

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