Asian Journal of Physical and Chemical Sciences

Volume 13, Issue 4, Page 51-64, 2025; Article no.AJOPACS.144328
ISSN: 2456-7779

Forensic Authentication of Paracetamol Using FTIR and UV–Vis Spectroscopy Coupled with Similarity Metrics

Kipronoh Theophilus Korir [a*], Jared O. Gwaro [a] and Duke Oeba [b]

[a] Department of Mathematics and Physical Science, Maasai Mara University, P.O. Box 861 – 20500, Narok, Kenya.
[b] Department of Physics, Faculty of Science, Egerton University, P.O Box 536-20115, Egerton, Kenya.

Authors' contributions

This work was carried out in collaboration among all authors. All authors read and approved the final manuscript.

Article Information

DOI: https://doi.org/10.9734/ajopacs/2025/v13i4263

Open Peer Review History:
This journal follows the Advanced Open Peer Review policy. Identity of the Reviewers, Editor(s) and additional Reviewers, peer review comments, different versions of the manuscript, comments of the editors, etc are available here: https://pr.sdiarticle5.com/review-history/144328

Original Research Article

Received: 25/07/2025
Published: 06/10/2025

ABSTRACT

The global circulation of counterfeit and substandard medicines poses a serious threat to public health and challenges forensic science in generating reliable evidence. Paracetamol, a widely used analgesic and antipyretic, is among the most frequently falsified drugs in low- and middle-income countries. This study employed Ultraviolet-Visible (UV-Vis) and Fourier Transform Infrared (FTIR) spectrophotometry to authenticate paracetamol (PAR). The specific objectives were to examine

**Corresponding author: E-mail: kipronotheophilus19@gmail.com;*

Cite as: *Kipronoh Theophilus Korir, Jared O. Gwaro, and Duke Oeba. 2025. "Forensic Authentication of Paracetamol Using FTIR and UV–Vis Spectroscopy Coupled With Similarity Metrics". Asian Journal of Physical and Chemical Sciences 13 (4):51–64. https://doi.org/10.9734/ajopacs/2025/v13i4263.*

active pharmaceutical ingredients, and to identify unknown components in paracetamol PAR1–PAR4 samples were analyzed against a certified reference standard. FTIR spectra were obtained using potassium bromide pelletization, while UV–Vis spectra were recorded by dissolving the sample in methanol and phosphate buffer, followed by dilution with distilled water. The data obtained were evaluated by Pearson correlation coefficients (r) and Euclidean distance (ED). Results showed that PAR1 ($r \geq 0.99$, ED = 0.051) and PAR3 ($r = 0.9983$, ED = 0.0389) matched the standard and were classified as authentic. In contrast, PAR2 ($r = 0.992$, ED = 0.084) exhibited a shifted amide band with reduced absorbance, while PAR4 ($r = 0.991$, ED = 0.089) showed weakened O–H bands confirming suspect and counterfeit status, respectively. This work addresses a key forensic gap by introducing quantitative, pharmacopeia-compliant thresholds for paracetamol authentication. The novelty lies in combining FTIR and UV–Vis spectra with similarity metrics to deliver objective and legally defensible authentication of paracetamol. The protocol strengthens scientific reliability while offering a scalable, low-cost tool for surveillance and regulatory enforcement in regions most affected by counterfeit medicines.

Keywords: Forensic drug analysis; spectrophotometry; counterfeit drugs; paracetamol.

1. INTRODUCTION

The authentication of pharmaceuticals is one of the most urgent challenges in forensic science today, as counterfeit medicines continue to undermine public health and regulatory systems worldwide (Cáceres-Pérez, 2025, Ehsan et al., 2025). The World Health Organization (WHO) estimates that up to 10% of pharmaceuticals in circulation in low and middle-income countries are falsified, with consequences that include therapeutic failure, drug resistance, and in some cases fatalities (Bakker et al., 2021). Paracetamol (acetaminophen), one of the most widely used analgesics and antipyretics, has been repeatedly identified as a common counterfeit target (Bakker et al., 2021, Raj, 2025). Its accessibility, high demand, and low production cost make it a strategic model compound for forensic validation of authentication methods (Bunn, 2019; Jadhav et al., 2021). Traditional analytical techniques such as chromatography and mass spectrometry provide high sensitivity and specificity but are limited by high cost, lengthy procedures, sample destruction, and dependence on sophisticated laboratory infrastructure (Bakker et al., 2021, Siddique, 2023; Kammrath et al., 2023). These constraints make them unsuitable for rapid screening in the very environments where counterfeit circulation is most prevalent. Spectroscopic methods, by contrast, are rapid, non-destructive, cost-effective, and require minimal sample preparation (Dirito, 2025; Mullani et al., 2022). Four different brands of paracetamols were randomly collected from licensed pharmacies and Narok County referral hospital. This sampling strategy was intended to ensure an unbiased representation of commonly dispensed paracetamol products, thereby enhancing the reliability and generalizability of the forensic analysis. Narok County was selected as the study site to reflect the real-world constraints of low-resource rural settings, where drug quality testing infrastructure is often limited or absent. Fourier Transform Infrared (FTIR) spectroscopy generates molecular fingerprints by probing vibrational transitions of chemical bonds (Enders et al., 2021), while Ultraviolet–Visible (UV–Vis) spectrophotometry detects electronic transitions through absorption maxima (λ_{max}), providing insights into adulteration (Alaboodi et al., 2025). Both techniques are grounded in the interaction of electromagnetic radiation with matter (Sliddique, 2024). FTIR records characteristic vibrational signatures in the infrared region that reveal structural features of the active pharmaceutical ingredient (API), while UV–Vis monitors reproducible absorption patterns in the ultraviolet–visible spectrum that indicate formulation consistency or deviation (Akash, 2025). Counterfeit medicines are fake drugs made to look genuine and sold for profit. They are a growing public health and forensic concern, particularly in low- and middle-income countries where regulatory oversight is limited. According to the World Health Organization (WHO), counterfeit and substandard medicines account for approximately 10–50% of the pharmaceutical market in Sub-Saharan regions. These products endanger patients by failing to provide the intended therapeutic effect and by exposing them to toxic or ineffective substitutes. Beyond health risks, counterfeits undermine confidence in healthcare systems and complicate law enforcement and judicial processes. It is essential to distinguish counterfeits from contaminants or adulterated medicines.

Counterfeit drugs are deliberately manufactured to mimic genuine products for economic gain, often with falsified packaging and labelling. In contrast, contaminants or adulterants arise from poor handling, accidental impurities, or the substitution of active ingredients with cheaper alternatives (Kaur et al., 2025). While both categories pose serious health risks, counterfeits involve deliberate deception, making them a primary focus of forensic authentication and regulatory enforcement (Hauk et al., 2021). This research aims to develop and evaluate practical forensic methods to authenticate paracetamols samples and detect substandard or falsified formulations. This dual optical approach offers a comprehensive perspective, combining structural fingerprinting with quantitative assessment, making it highly suitable for forensic authentication (Kumar et al., 2025, Sumalatha, 2024). Previous research has shown the potential of FTIR to detect counterfeit formulations through altered O–H, amide C=O, and aromatic C–H bands (Hawas, 2023), and of UV–Vis to confirm authenticity through stable λ_{max} values while identifying adulteration via spectral shifts (Sen et al., 2021, Dirito, 2025). Yet most studies have applied these methods in isolation and focused on pharmaceutical quality control rather than forensic decision-making (Akash, 2025, Singhal et al., 2024). A systematic, comparative application of FTIR and UV–Vis within a unified framework tailored for counterfeit detection remains largely unexplored, especially in resource-limited forensic laboratories (Kaur et al., 2025). To address this gap, the present study evaluates the forensic applicability of FTIR and UV–Vis in paracetamol authentication using a pharmacopoeia reference and four commercial formulations (Alaboodi et al., 2025, Dugaje, 2025). A quantitative framework is adopted in which FTIR results are assessed by spectral correlation coefficient (r), error deviation (ED), and spectral similarity index (SSI), while UV–Vis results are evaluated through λ_{max}, absorbance at λ_{max}, and relative standard deviation (RSD) across replicates (Alshehri et al., 2025). Classification thresholds such as FTIR $r \geq 0.98$ and $ED \leq 0.05$; UV–Vis λ_{max} 243–245 nm with $RSD \leq 2\%$) provide reproducible criteria for distinguishing authentic from falsified samples (Watson, 2025, Kadhem, 2021, Theodore & Vongsutilers, 2024). To our knowledge, this is the first systematic study to apply such a unified, quantitative framework combining FTIR and UV–Vis to the forensic authentication of paracetamol. By integrating complementary spectroscopic measurements with explicit decision metrics, this work establishes a rapid, low-cost, and reliable workflow for authenticating paracetamol. The approach is directly applicable to forensic and regulatory laboratories in low-resource environments where counterfeit medicines are most prevalent, while its broader relevance extends to global pharmaceutical enforcement. The following sections describe the experimental design, analytical workflow, and comparative evaluation of FTIR and UV–Vis applied to authentic and suspect paracetamol formulations (Ehsan et al., 2025). As summarized in Table 1, few studies address these issues in real-world, informal Sub-Sahara markets**,** highlighting the gap in applying these techniques to authentic drug samples from rural settings. This literature gap underscores the novelty and urgency of the current study (Rusmalina et al., 2025, Pazhayattil & Sharma, 2025, Song et al., 2020).

Table 1 highlights the fragmented nature of prior counterfeit-drug detection studies. Song (2020) focused only on identifying paracetamol functional groups, but the lack of counterfeit validation limited its forensic relevance. Hawas (2023) compared original and counterfeit drugs but relied on FTIR alone, overlooking the confirmatory strength of UV–Vis, making results vulnerable to single-technique bias. Lapo (2024) emphasized quantitative active pharmaceutical ingredient (API) analysis but without molecular fingerprinting, restricting its utility for forensic authentication. In contrast, the present study integrates both FTIR and UV–Vis within a single framework. This dual approach strengthens accuracy by combining structural fingerprinting with quantitative reproducibility, thereby overcoming the limitations of earlier studies. The forensic strength of Table 1 lies in showing that no prior work has unified these two complementary tools within a regulatory-compliant workflow, making this research the first to establish a replicable, field-ready model for counterfeit drug authentication in Sub-Saharan markets.

The novelty of this research lies in the integrated forensic application of FTIR and UV-Vis spectroscopy to evaluate real-world Over the counter (OTC) analgesic samples from a rural African market. Unlike earlier works that focused on individual methods in controlled laboratory settings, this study demonstrates the practicality of combining two non-invasive techniques to detect counterfeit pharmaceuticals under actual market conditions (Alaboodi et al., 2025, Cáceres-Pérez, 2025). The inclusion of

Table 1. Comparative review of studies using FTIR and UV-Vis spectroscopy for forensic drug

Study	Key Findings	Limitations
Song (2020)	Identified API functional groups	No detection of counterfeits
Hawas (2023)	Compared original and counterfeit samples using FTIR.	No validation with UV-Vis to real world
MJP Lapo (2024)	Quantified APIs using UV-Vis.	No comparison
This study (2025)	Employs both FTIR + UV-Vis	Complement each other and coupled with similarity metrics.

anonymized samples from Narok also adds originality and contextual relevance, offering insight into the challenges of pharmaceutical fraud in underserved regions. This study has the potential to influence both scientific practice and public health policy. It provides a replicable, low-cost analytical model for screening pharmaceuticals in resource-limited areas. It also contributes to forensic chemistry, pharmaceutical regulation, and counterfeit drug detection (Peltier-Rivest, 2019). Regulatory bodies and local health officials can adopt the methods tested here for wider surveillance campaigns, thereby improving consumer safety and pharmaceutical supply chain integrity (Osei, 2020, Mallah et al., 2015, Ugwu et al., 2025, Patil & Patil, 2024).

2. METHODLOGY

2.1 Experimental Details

2.1.1 Sample collection and ethical compliance

Paracetamol samples were investigated: one pharmacopoeia standard reference and four commercial formulations coded PAR1–PAR4. The reference was obtained from an accredited supplier and served as the authentic control. The commercial formulations were collected from both licensed pharmacies and informal markets, ensuring representation of both authentic and potentially falsified drugs. A purposive stratified sampling strategy was used, dividing the outskirts of Narok town into four clusters based on administrative boundaries and distance from the town centre. This ensured diversity in pharmaceutical sources and enhanced the reliability of the subsequent forensic analysis using FTIR and UV-Visible spectrophotometry (Singhal et al., 2024). Drug samples were sorted and anonymized based on manufacturer and batch numbers to ensure objectivity during analysis. A research permit was first obtained from the National Commission for Science, Technology and Innovation (NACOSTI) under license number NACOSTI/P/25/4176274. All procedures adhered to current ethical standards for non-human subject research in the physical sciences and followed the updated OECD Guidelines on Good Laboratory Practice (GLP**)** for chemical and forensic analysis (Kaurov, 2025, Alshehri et al., 2026, Abd El-Hamid et al., 2024).

2.2 Reagents and Apparatus

Four batches of paracetamol tablets (coded PAR1–PAR4) were purchased from pharmacies in Narok County, Kenya, and analysed against a certified reference standard. FTIR spectra were collected from KBr pellets (1:200 w/w, sample) between 4000–400 cm^{-1} at a resolution of 2 cm^{-1} with baseline correction (Alaboodi et al., 2025). The Ultra-violet spectra were recorded in the range of 200–400 nm. Paracetamol tablets were first finely crushed into powder to ensure uniformity, after which an accurate 100 mg was weighed. The drug sample was first dissolved in methanol and phosphate buffer (Ph 6.8), followed by dilution with distilled water.(Bunn, 2019). Each spectrum was acquired in triplicate.

2.3 Samples Characterization

Table 2 summarizes the general properties of paracetamol. Acetaminophen, chemically known as N-(4-hydroxyphenyl) acetamide, has the molecular formula $C_8H_9NO_2$ and molecular weight 151.16 g/mol (Evans-Nguyen, 2021, Chen et al., 2024). Its structure contains a benzene ring substituted with a hydroxyl group (-OH) and an acetamide (-$NHCOCH_3$) moiety, giving the molecule phenolic and amide functional features (Singhal et al., 2025). Physically, paracetamol is a white to off-white crystalline solid, odourless, with a slightly bitter taste. It melts at 168–172 °C and is sparingly soluble in cold water (14 mg/mL at 25 °C), more soluble in boiling water, and moderately soluble in ethanol and acetone. It may degrade under heat, moisture, or prolonged light exposure (Chen et al., 2024, Singhal et al.,

2025). FTIR bands: O–H stretching at 3320–3360 cm^{-1}, amide C=O stretching near 1650 cm^{-1}, aromatic C=C stretching at 1500–1600 cm^{-1}, and a fingerprint region rich in peaks between 1500–500 cm^{-1}. UV–Vis absorption: λ_{max} at 243–245 nm in aqueous solution due to $\pi \rightarrow \pi^*$ electronic transitions (Hauk et al., 2021). Preliminary forensic inspection revealed PAR1 and PAR3 to be uniform in appearance and packaging. PAR2 tablets were irregular in size with faded imprints, while PAR4 showed surface roughness, discoloration, and poorly aligned blister packs. These macroscopic traits suggested potential counterfeit or poor-quality manufacturing (Wayland et al., 2022, Torres Vargas, 2025).

Certified pharmaceutical reference standards for each paracetamol sample, obtained were subjected to identical characterization protocols (Gupta et al., 2025, Bunn, 2019). Their inclusion provided a validated spectral baseline for comparison, enabling detection of chemical or structural deviations in test samples (Ehsan et al., 2025). The chemical structure of the paracetamol drug sample is as shown in Fig. 1 (Cáceres-Pérez, 2025).

2.3.1 Fourier transform infrared analysis

FTIR spectrophotometer was used to characterize the molecular structure and identify diagnostic functional groups of the active pharmaceutical ingredients (APIs) in paracetamol with the aim of supporting forensic differentiation between authentic and potentially counterfeit samples (Mishra et al., 2025, Azeez & Azeez, 2022). The spectra of the analysed samples were recorded over 4000–400 cm^{-1}, with 10 scans per run to allow rapid data acquisition suitable for forensic workflows samples (Mishra et al., 2025, Azeez & Azeez, 2022). For FTIR analysis, each drug sample was finely ground using a clean porcelain mortar and pestle, then mixed with infrared-grade potassium bromide (KBr) in a 1:200 (w/w) ratio. The mixture was further homogenized and compressed into transparent discs using a hydraulic pellet press at approximately 10 tons of pressure (Enders et al., 2021). Pellets were stored in desiccators to prevent moisture interference in the mid-infrared region. This protocol, aligned with USP <854> and ASTM E1252 standards, enabled the acquisition of reproducible fingerprint spectra essential for forensic comparison and detection of structural anomalies associated with counterfeit formulations (Dirito, 2025, Kaur et al., 2025, Pazhayattil & Sharma, 2025). Each sample was analysed in triplicate, and the raw spectra were exported to MATLAB (R2023a, MathWorks, USA) for baseline correction, smoothing, and normalization. Spectral analysis emphasized the O–H, amide C=O, aromatic C=C, and fingerprint regions, which are diagnostic of paracetamol. Spectral analysis emphasized the O–H, amide C=O, aromatic C=C functional groups, and fingerprint regions, which are diagnostic of paracetamol (Dugaje, 2025, Yan, 2025).

Table 2. General properties of paracetamol

Property	Description
Chemical name	N-(4-hydroxyphenyl) acetamide
Molecular formula	$C_8H_9NO_2$
Molecular weight	151.16 g/mol
Melting point	168–172 °C
Physical appearance	White to off-white crystalline solid
Key FTIR peaks	O–H (3320–3360 cm^{-1}); C=O (1650 cm^{-1}); C=C (1500–1600 cm^{-1})
UV–Vis λ_{max}	243 nm (aqueous solution)

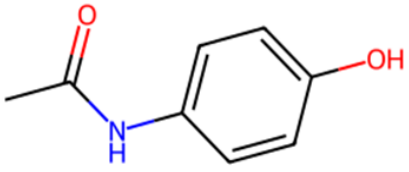

Fig. 1. Chemical structures of paracetamol. This structure was used to interpret key FTIR and UV-Vis spectral features during sample characterization (Kaur et al., 2025)

2.3.2 Ultraviolet-visible analysis

UV–Vis spectra were measured using a Shimadzu UV-1800 double-beam spectrophotometer (Velevska et al., 2025). Paracetamol samples were prepared by dissolving 100 mg of powdered tablet in methanol to ensue efficient solubilisation of the analyte, subsequently diluted with phosphate buffer (pH6.8) to maintain spectral consistency. It was subsequently topped with 100 mL distilled water to achieve target concentration while minimizing ionic interference. The solution was then transferred into 1 cm quartz cuvettes ready for scanning. The scanning range was 200–400 nm at 1 nm intervals. Distilled water served as the blank, and the pharmacopoeia standard solution acted as the control. Each solution was scanned in triplicate, with each scan requiring <60 seconds, ensuring methodological rigor while maintaining rapid screening. Solvent blanks were used for baseline correction during instrument calibration to eliminate matrix interference and enhance result fidelity (Abd El-Hamid et al., 2025). For UV-Visible analysis, drug-specific solubilisation strategies were applied. Paracetamol (100 mg) was dissolved in methanol, sonicated, filtered, and diluted with phosphate buffer (pH 6.8) prior to measurement at maximum wavelength (Hauk et al., 2021). Absorbance data were exported into MATLAB for spectral smoothing, and λ_{max} determination (Bunn, 2019, Xu et al., 2025).

2.4 Data Analysis

Quantitative interpretation was performed using integrated instrument software (LabSolutions IR for FTIR and UV–Vis) with MATLAB-based processing (Akash, 2025). For FTIR analysis, the correlation coefficient (r) was calculated relative to the standard, Euclidean distance (ED) quantified peak shifts, and a spectral similarity index (SSI) summarized full-spectrum matching. For UV–Vis analysis, the maximum absorbance was observed at wavelength corresponding to the λ_{max}, and relative standard deviation (RSD) were computed across replicates (Kumar et al., 2025)). For FTIR, the correlation coefficient (r) was calculated relative to the standard, error deviation (ED) quantified peak shifts, and a spectral similarity index (SSI) summarized full-spectrum matching. For UV–Vis, $\lambda_{max,}$ absorbance at λ_{max}, and relative standard deviation (RSD) were computed across replicates (Kumar et al., 2025). The λmax range of 243–245 nm is directly adopted from pharmacopeia monographs (USP, BP, WHO), all of which consistently report paracetamol absorbance maxima within this window. The correlation coefficient threshold ($r \geq 0.98$) and Euclidean distance cut-off ($ED \leq 0.05$) are not pharmacopeia specifications but are adapted from established spectroscopic similarity studies where such limits reliably distinguished authentic from falsified formulations (Kumar et al., 2025). To strengthen traceability, we validated these thresholds against the certified paracetamol reference spectrum and confirmed consistency across replicate analyses. Thus, while pharmacopeia guidance was followed wherever available, author-defined thresholds were only introduced where official standards are absent, and these were benchmarked against literature and empirical data to ensure clarity, objectivity, and external validation (Sumalatha, 2024, Nakitare et al., 2025). MATLAB was used for spectral overlays, baseline correction, error propagation, and graphical visualizations. Authentic FTIR spectra: $r \geq 0.98$ and $ED \leq 0.05$. Authentic UV–Vis spectra: $\lambda_{, max}$ within 243–245 nm. Values outside these ranges ($\Delta \lambda_{max,} \geq 2$ nm or RSD > 5%) indicated possible adulteration, poor formulation, or counterfeit (Alaboodi et al., 2025, Sah & Sah, 2024, Theodore & Vongsutilers, 2024).

3. RESULTS AND DISCUSSION

3.1 Forensic Drug Analysis using Fourier Transform Infrared spectrophotometer

3.1.1 Paracetamol

Table 3 shows FTIR reference spectrum of paracetamol showed characteristic absorption bands corresponding to O–H stretching (3315 cm^{-1}), amide C=O stretching (1662 cm^{-1}), aromatic C–H stretching (3030 cm^{-1}), and C–N stretching (1275 cm^{-1}) (Hauk et al., 2021).

Table 4 shows the quantitative FTIR similarity metrics that classify the authenticity of the paracetamol samples. PAR1 and PAR3 recorded the highest similarity indices (SSI >0.97, r ≥0.98, ED ≤0.05), confirming them as authentic formulations with strong agreement to the reference spectrum (Kumar et al., 2025). PAR2, despite a high correlation coefficient (r = 0.992), showed a larger error deviation (ED = 0.084) and lower SSI, placing it in the suspect or substandard category due to structural shifts. PAR2 shows a high similarity index (SSI = 0.9542) and strong correlation coefficient (r =

0.992), confirming the presence of genuine paracetamol. However, its Euclidean distance (ED = 0.084) and higher absorbance deviation (Δ Abs = 0.0112 ± 0.0198) suggest under-dosing relative to pharmacopeia standards. This quantitative pattern supports classification as substandard, since the active ingredient is authentic but below the required strength. In contrast, PAR4 presents both lower similarity (SSI = 0.9478) and higher deviations (ED = 0.0895; Δ Abs = 0.0127 ± 0.0216), consistent with deliberate substitution or falsification, thus warranting classification as *counterfeit.* PAR4 had the lowest similarity score and highest error deviation, indicating multiple spectral anomalies consistent with counterfeiting. These results demonstrate that quantitative thresholds provide objective and reproducible classification, distinguishing authentic drugs from falsified or poorly manufactured ones.

Table 5 clearly distinguishes authenticity from falsified paracetamol samples based on FTIR deviations. PAR1 and PAR3 showed all diagnostic peaks with only minor variations, confirming authenticity (Kumar et al., 2025). PAR2 exhibited a shifted amide C=O band and reduced absorbance, consistent with a substandard formulation rather than deliberate falsification. In contrast, PAR4 lacked key peaks and showed anomalous bands, providing strong evidence of counterfeiting. This classification highlights FTIR's ability to translate spectral anomalies into clear forensic outcomes, separating genuine, substandard, and counterfeit drugs in a legally defensible manner (Alaboodi et al., 2025).

Fig. 2 shows FTIR spectroscopic analysis of paracetamol samples (PAR1–PAR4) revealed variable conformity to the certified reference spectrum, aligned with USP <854> and British Pharmacopeia specifications (Lawson et al., 2018, Chen et al., 2024). Samples PAR2 and PAR4 displayed significant deviations, particularly within the functional group and fingerprint regions. Notably, PAR4 exhibited a broadened O–H stretch 3200–3500 cm^{-1}, absence of aromatic C=C vibrations (1600 cm^{-1}), and emergence of anomalous peaks within 800–1200 cm^{-1}, indicative of possible excipient contamination (Enders et al., 2021).

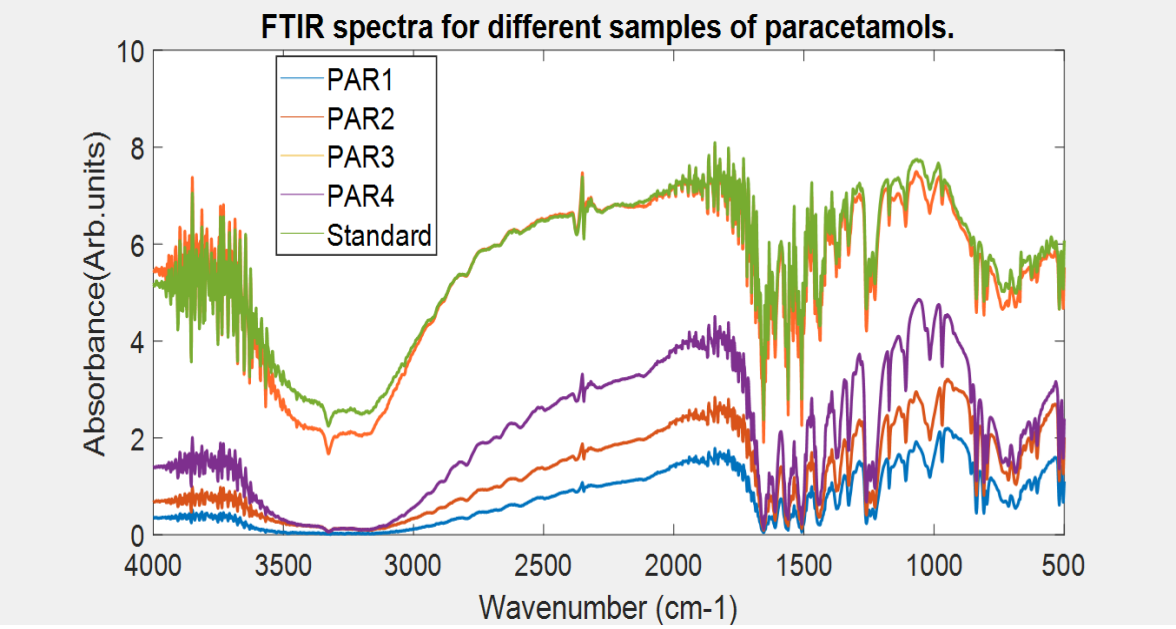

Fig. 2. FTIR spectra for different samples of paracetamol

Table 3. FTIR Functional Group Assignments for Paracetamol Samples (4000–400 cm^{-1})

Wavenumber (cm^{-1})	Functional groups	Forensic Note
3315	O–H stretching	Weak in PAR4
3160–3030	Aromatic C–H stretching	Shifted in PAR4
1662	Amide C=O stretching	Shifted in PAR2

Wavenumber (cm^{-1})	Functional groups	Forensic Note
1610–1500	Aromatic C=C stretching	Reduced in PAR4
1275	Amide C–N stretching	Absent in PAR4
855	Aromatic C–H bending	Extra peak in PAR4

Table 4. Quantitative FTIR Similarity Metrics for Paracetamol Samples

Samples	SSI	r	ED	ΔAbs ± SD	Classification
PAR1	0.9786	0.9980	0.0510	0.0064 ± 0.00141	Authentic
PAR2	0.9542	0.9920	0.0840	0.0112 ± 0.0198	Substandard
PAR3	0.9865	0.9983	0.0389	0.00048 ± 0.0116	Authentic
PAR4	0.9478	0.9914	0.0895	0.0127 ± 0.0216	Counterfeit

Table 5. Forensic Interpretation of Spectral Deviations in Paracetamol Samples

Sample	Observed Deviations	Forensic description	Interpretations
PAR1	All diagnostic peaks present	High similarity	Authentic
PAR2	Shifted amide C=O band, reduced absorbance	Reduced absorbance	Substandard
PAR3	Strong match to reference; minor deviations	Minor deviations	Authentic
PAR4	Weakened O–H, missing fingerprint peaks	Large deviations	Counterfeit

3.2 Forensic Drug Analysis using Ultra-violet Visible Spectrophotometer

3.2.1 Paracetamol

Ultraviolet-Visible (UV-Vis) spectroscopic analysis was employed to evaluate the authenticity and chemical integrity of four paracetamol tablet samples (PAR1–PAR4), using standard sample as reference (Alaboodi et al., 2025, Mengesha et al., 2024). All measurements were conducted in methanol using a 1 cm quartz cuvette, and spectra were recorded in the 200–400 nm range under validated analytical conditions, including repeatability (%RSD <2%) in accordance with USP <857> guidelines (Nwokedi et al., 2025, Nwokedi et al., 2025).

Fig 3 shows UV spectral data for different samples of paracetamols. The reference standard displayed two well-resolved absorption maxima at approximately 243 nm, with peak absorbance reaching 0.5 (Alaboodi et al., 2025). These spectral features are consistent with documented profiles of pure paracetamol in methanol solution and meet pharmacopeia criteria for identity testing. Samples PAR1 and PAR3 exhibited near-identical spectral profiles to the reference, with matching peak positions and comparable absorbance intensities (>95% spectral congruence) (Osei, 2020, Patriarca et al., 2024). This close alignment indicates the presence of the correct active pharmaceutical ingredient (API) at appropriate concentrations. Based on these findings and predefined acceptance criteria, PAR1 and PAR3 were classified as authentic (Nwokedi et al., 2025, Velevska et al., 2025). Sample PAR2, however, displayed a significant reduction in absorbance at 243 nm. These deviations suggest either API under-dosing, formulation inconsistencies, or degradation. The attenuated spectral response places PAR2 in the category of suspect possible counterfeit, raising concerns over substandard manufacturing or poor storage practices (Khalid, 2024). The most anomalous results were observed in sample PAR4, which presented a broadened and poorly defined peak between 250–270 nm, with a reduced absorbance of ~0.14. Notably, PAR4 also exhibited an additional absorbance peak at 310 nm, absent in the reference and other samples (Rosendo et al., 2023). This secondary peak corresponds to p-aminophenol, a toxic degradation product of paracetamol formed via hydrolytic or oxidative pathways.

The presence of p-aminophenol above pharmacopeia impurity limits (typically <0.05%) signals chemical instability and suggests improper formulation, contamination, or degradation due to heat or moisture. Accordingly, PAR4 was designated as likely counterfeit and may pose a public health risk (Bakker et al., 2021, Cáceres-Pérez, 2025).

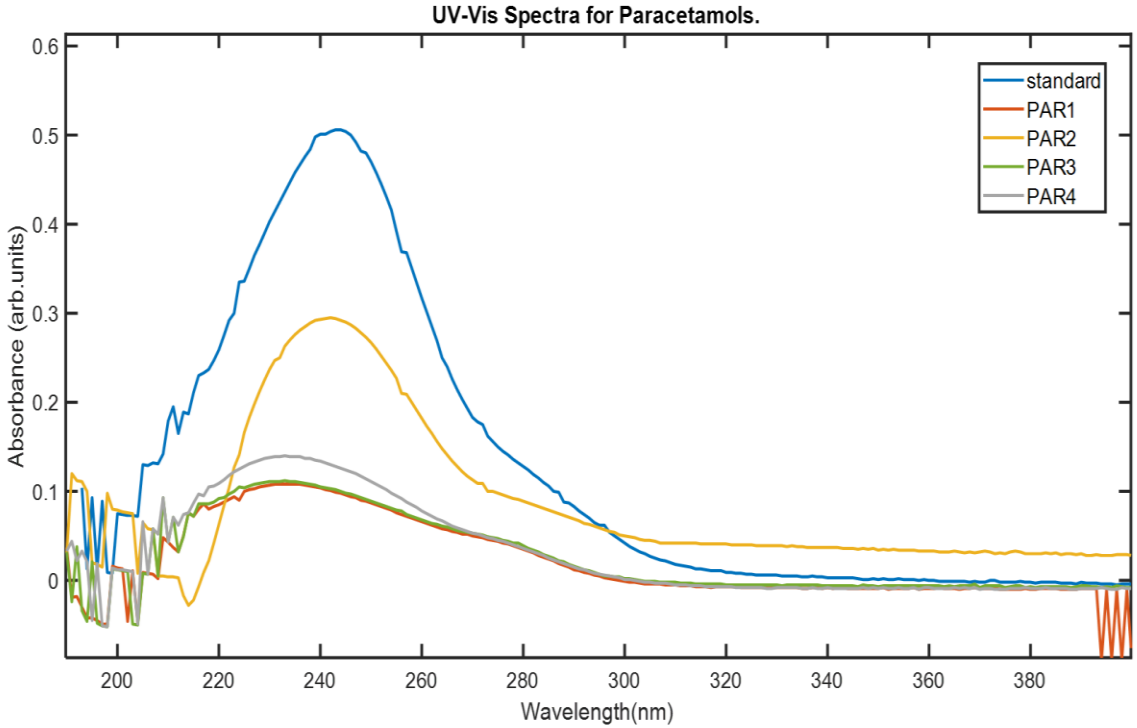

Fig. 3. UV-Vis spectra for different samples of paracetamols

Table 6. Regulatory Comparison of Pharmacopeial Specifications for Paracetamol (USP, WHO vs Study Results)

Parameter	USP Spec	WHO Spec	Study Std	PAR1	PAR2	PAR3	PAR4
UV λ_{max}	243 ± 2 nm	243 ± 2 nm	243 nm	243 nm	246 nm	243 nm	249 nm
O–H	3310–3320 cm^{-1}	3310–3320 cm^{-1}	3315 cm^{-1}	3320 cm^{-1}	3315 cm^{-1}	3310 cm^{-1}	3325 cm^{-1}
C=O	1660 cm^{-1}	1660 cm^{-1}	1662 cm^{-1}	1665 cm^{-1}	1660 cm^{-1}	1658 cm^{-1}	Absent
C–N	1275 cm^{-1}	1275 cm^{-1}	1275 cm^{-1}	1275 cm^{-1}	Absent	1275 cm^{-1}	Absent

Table 6 elevates the forensic relevance of this work by aligning experimental findings with globally recognized USP and WHO specifications. Authentic samples (PAR1, PAR3) demonstrated complete compliance, confirming that the analytical framework can reliably distinguish genuine formulations (Pathak et al., 2023, Velevska et al., 2025). PAR2, with a λ_{max} shift to 246 nm and attenuated absorbance, sits in a forensic "grey zone" as a substandard but not outright falsified drug, a distinction critical for regulatory response. PAR4, however, violated multiple pharmacopeial thresholds shifted $\lambda_{max,}$ absent amide C=O, and anomalous UV peaks consistent with toxic degradation products providing irrefutable evidence of counterfeiting (Bakker et al., 2021). This direct benchmarking against pharmacopeial standards strengthens the evidentiary chain, allowing findings from this study to transition seamlessly from laboratory analysis into forensic testimony and regulatory enforcement (Akash, 2025).

4. CONCLUSION

This study applied Fourier Transform Infrared (FTIR) and Ultraviolet–Visible (UV–Vis) spectroscopy with two objectives: to examine active pharmaceutical ingredients and to identify unknown components in paracetamol. The analysis confirmed the integrity of the active pharmaceutical ingredient in authentic samples (PAR1 and PAR3), which showed the expected O–H, amide C=O, aromatic C=C, and C–N bands. In contrast, PAR2 presented a shifted amide C=O absorption, while PAR4 lacked key diagnostic peaks, demonstrating compromised molecular structure and reduced API quality. The investigation also revealed unknown or degraded components in suspect and counterfeit samples. PAR2 displayed reduced absorbance at λ_{max} (246 nm), suggesting under-dosing or poor formulation. PAR4 exhibited an additional UV peak at 310 nm, consistent with p-aminophenol, a toxic degradation product, confirming the presence of harmful impurities. Among the four samples tested, two were authentic (50%), one was substandard/suspect (25%), and one was counterfeit (25%). Quantitative thresholds (FTIR: $r \geq 0.98$, ED ≤ 0.05; UV–Vis: λ_{max} = 243–245 nm, RSD ≤ 2%) enabled objective and reproducible classification. The findings demonstrate that spectroscopic authentication of pharmaceuticals can generate legally defensible evidence while exposing the risks counterfeit and substandard drugs pose to public health.

ETHICAL APPROVAL

A research permit was obtained from National Commission for Science, Technology and Innovation (NACOSTI) under license number NACOSTI/P/25/4176274. Ethical approval was not required because the study did not involve human or animal subjects.

DISCLAIMER (ARTIFICIAL INTELLIGENCE)

Author(s) hereby declare that NO generative AI technologies such as Large Language Models (ChatGPT, COPILOT, etc.) and text-to-image generators have been used during the writing or editing of this manuscript.

ACKNOWLEDGEMENT

The author gratefully acknowledges the Higher Education Loans Board (HELB) Postgraduate Scholarship for providing the financial support that made this study possible. Special appreciation is extended to Maasai Mara Universitys, particularly the School of Pure and Applied Sciences and the Department of Mathematics and Physical Sciences, for providing the research infrastructure, technical resources, and an enabling academic environment.

COMPETING INTERESTS

Authors have declared that no competing interests exist.

REFERENCES

Abd El-Hamid, S. M., Aziz, S. W., Mohamed, A. A., El-Gedamy, M. S., Salem, A. E., Mohammed, S. F., & Elshafie, H. S. (2025). Structural, spectroscopic, and docking analysis of N, O-donor ligand metal complex nanoparticles with hypolipidemic effects via lipoprotein lipase activation in high-fat diet mice. *Chemistry & Biodiversity, 22*, e202403003.

Abd El-Hamid, S. M., Aziz, S. W., Sadeek, S. A., Sabry, M. A., & El-Gedamy, M. S. (2024). Synthesis, spectral analysis, XRD, molecular docking simulation of dithranol and glycine mixed ligand complexes and their potential role in suppressing breast cancer cells via down-regulating the expression of protein metalloproteinase-9. *Applied Organometallic Chemistry*, e7650.

Akash, M. S. H., & Khan, R. (2025). Comprehensive insights into infrared spectroscopy. In *Essentials of pharmaceutical analysis* (pp. 161–208). Springer Nature Singapore.

Alaboodi, A. S., Kadhim, S. A., & Hussein, A. S. (2025). Ultraviolet-visible spectroscopy, importance, principle, structure and most important applications: A study review. *International Journal of Novel Research in Physics Chemistry & Mathematics, 12*, 53–60.

Alshehri, A., Alqahtani, A., Alsayari, A., & Almrasy, A. A. (2025). An eco-friendly chemometrics-assisted UV spectrophotometric method for simultaneous determination of sofosbuvir, simeprevir, and ledipasvir in pharmaceuticals. *BMC Chemistry, 19*(1), 156. https://doi.org/10.1186/s13065-025-00923-z

Alshehri, B. M., Salem, A. E., El-Gedamy, M. S., Aziz, S. W., Sadeek, S. A., Mohammed, S. F., Alzahrani, D., & Abd El-Hamid, S. M. (2026). Molecular structure characterization of some new pregabalin-2,2'-bipyridine mixed ligand metal complexes and possible insights on alleviation of its testicular-enhanced apoptosis side effect. *Journal of Molecular Structure, 1349*, 143765.

Azeez, A. M., & Fathalla, N. A. (2022). Determination of ketoprofen in tablet dosage forms by derivative IR spectroscopy. *Egyptian Journal of Chemistry, 65*(1), 215–219.

Bakker, I. M., Ohana, D., & Venhuis, B. J. (2021). Current challenges in the detection and analysis of falsified medicines. *Journal of Pharmaceutical and Biomedical Analysis, 197*, 113948. https://doi.org/10.1016/j.jpba.2021.113948

Bunn, G. P. (2019). Status and applicability of US regulations: CGMP. In *Good manufacturing practices for pharmaceuticals* (7th ed., pp. 1–17). CRC Press.

Cáceres-Pérez, J. B., Sánchez-Gómez, A. R., Sánchez-Escudero, J., Martínez, A. M., & Fernández-Escudero, F. (2025). The current situation of medicines quality in low-and middle-income countries: New challenges to be addressed.

Chen, C. J., Lokesh, B. V., & Akowuah, G. A. (2024). Quantitative applications of ATR-FTIR spectroscopy with chemometrics for the estimation of amikacin in amikacin sulphate injections. *Current Analytical Chemistry, 20*(3), 201–208.

Dirito, P. (2025). Development of spectroscopic and chromatographic techniques for the determination of drugs and other materials in the fight against illicit trafficking and commercial fraud.

Dugaje, T. A. B. (n.d.). *World Journal Medical & Pharmaceutical Research, World*, 1.

Ehsan, H., Wardak, F. R., Karimi, H., Kamal, F., Aminpoor, H., Salam, A., & Mehrpoor, A. J. (2025). Comprehensive narrative analysis of antimicrobial resistance in Afghanistan: Key drivers, challenges, and strategic interventions. *Journal of Health, Population and Nutrition, 44*, 265.

Enders, A. H. C., Narváez-Neira, A. A., Franco-Cisneros, M. F., Vega-Álvarez, J. C. M., & Carranza, A. H. (2021). Functional group identification for FTIR spectra using image-based machine learning models. *Analytical Chemistry, 93*(28), 9711–9718. https://doi.org/10.1021/acs.analchem.1c01234

Evans-Nguyen, K. C. (Ed.). (2021). *Forensic Chemistry* (Vol. 22). American Chemical Society.

Gupta, N. N., & M. K. B. V. T. A. D. A. A. &. N. N. P. (2025). The importance of labeling and certification: Ensuring quality and transparency. In *Unleashing the Power of Functional Foods and Novel Bioactives* (pp. 449–465). Academic Press.

Hauk, C., Hagen, N., & Heide, L. (2021). Identification of substandard and falsified medicines: Influence of different tolerance limits and use of authenticity inquiries. *The American Journal of Tropical Medicine and Hygiene, 104*(5), 1936. https://doi.org/10.4269/ajtmh.20-1276

Hawas, H. R. (2023). *Forensic examination of original and counterfeit medications using FTIR analysis* (Doctoral dissertation).

Jadhav, R. S. M. K. R. A. M. E. D., & S. M. V. N. (2021). *Pharmaceutical product development: e-Book for B. Pharm 8th semester as per PCI syllabus*. Thakur Publication Private Limited.

Kadhem, A. J. (2021). *Molecularly imprinting polymer sensor for the detection of testosterone and endocrine disrupting chemicals in environmental and biomedical applications* (Doctoral dissertation, University of Missouri--Columbia).

Kammrath, B. W., Leary, P. E., & Crocombe, R. A. (2023). Detection and analysis of

counterfeit drugs. In *Trends in Counterfeit Drugs* (pp. 87–144).

Kaur, B. M., & 34. A. R. H. M. M. V. K. K. G. K. M. O. M. K. &. B. M. (2025). Aspirin vs. ibuprofen: Unveiling the distinct cyclooxygenase-1/2 behaviour and dual efficacy of their synthesized analogues via molecular modeling and in vitro biological assessment. *RSC Medicinal Chemistry, 16*(5), 2027–2048.

Kaur, R., Choudhary, T., Kaur, R., Garg, M., Chauhan, N. S., Jain, A., & Baldi, A. (2025). Adulteration in herbal medicines: A comprehensive review on types, detection, and health impacts. *Pharmacognosy Research, 17*(4).

Kaurov, A. A., & Orlov, N. (2025). The afterlife of a ghost-written paper: How corporate authorship shaped two decades of glyphosate safety discourse. *Environmental Science & Policy, 171*, 104160.

Khalid, K. I. (2024). UV-Vis spectroscopy in non-destructive testing. In *Non-destructive characterization method* (pp. 391–416). Elsevier.

Kumar, R., Salwan, S., Kumar, P., Bansal, N., & Kumar, B. (2025). Electroanalysis advances in pharmaceutical sciences: Applications and challenges ahead. *Analytica, 6*(2), 12.

Lawson, G., Ogwu, J., & Tanna, S. (2018). Quantitative screening of the pharmaceutical ingredient for the rapid identification of substandard and falsified medicines using reflectance infrared spectroscopy. *PLoS ONE, 13*(8), e0202059.

M. B. N. C. A. H. S. R. A. &. T. J. Patriarca, “Atomic spectrometry update: review of advances in the analysis of clinical and biological materials, foods and beverages.,” Journal of Analytical Atomic Spectrometry, pp. 39(3), 624, 2024.

Mallah, M. A., Sherazi, S. T. H., Bhanger, M. I., Mahesar, S. A., & Bajeer, M. A. (2015). A rapid Fourier-transform infrared (FTIR) spectroscopic method for direct quantification of paracetamol content in solid pharmaceutical formulations. *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy, 141*, 64–70.

Mengesha, D. R., & 43. A. B. H. R. R. G. L. &. D. R. (2024). Substandard and falsified medicines in African pharmaceutical markets: A case study from Ethiopia. *Social Science & Medicine, 349*, 116882.

Mishra, A., Aghaee, M., Tamer, I. M., & Budman, H. (2025). Spectroscopic advances in real-time monitoring: A review of vibrational and fluorescence techniques. *Spectroscopy Journal, 3*(2), 12.

Mullani, A. K., Shinde, A. S., Mote, G. D., Sutar, G. V., Sajne, S. J., Saralaya, M. G., ... & Jangade, N. M. (2022). Impurity profile study of aspirin in bulk and tablet dosage forms. *Journal of Pharmaceutical Negative Results, 13*.

Nakitare, J., Mathangani, S., & Kamau, G. (2025). Research data management in universities in Kenya: Critical analysis of the legal and policy frameworks. *The Journal of Academic Librarianship, 51*(6), 103139.

Nwokedi, V. U. O. C. O. A. B. I. I. J. K. F. J. C. E. E. O., & S. P. E. (2025). A review on safety and public health implications of use of over-the-counter pain medication. *Journal of Pharma Insights and Research, 3*(2), 194–202.

Osei, M. A., & Boadu, A. A. (2020). Evaluation of the authenticity of analgesic tablets sold in Ghana using FTIR spectroscopy. *Scientific African, 8*, e00432.

Pathak, R., Gaur, V., Sankrityayan, H., & Gogtay, J. (2023). Tackling counterfeit drugs: The challenges and possibilities. *Pharmaceutical Medicine, 37*(4), 281–290.

Patil, S. D., & C. S. S. (2024, March). A brief review on application of design of experiment for the analysis of pharmaceuticals using HPLC. *Annales Pharmaceutiques Françaises, 82*(2), 203–228. Elsevier Masson.

Patriarca, M. B. N. C. A. H. S. R. A., & T. J. (2024). Atomic spectrometry update: Review of advances in the analysis of clinical and biological materials, foods and beverages. *Journal of Analytical Atomic Spectrometry, 39*(3), 624.

Pazhayattil, A. B., & Sharma, S. (2025). Analytical tools for investigation and generation of supporting evidence. In *Pharmaceutical Manufacturing Deviation and Failure Investigations: Principles, Practices, and Case Studies* (pp. 33–52). Springer Nature Switzerland.

Pazhayattil, A. B., & Sharma, S. (2025). Analytical tools for investigation and generation of supporting evidence. In *Pharmaceutical Manufacturing Deviation and Failure Investigations: Principles,*

Practices, and Case Studies (pp. 33–52). Cham: Springer Nature Switzerland.

Peltier-Rivest, D. P. C. (2019). Detecting counterfeit pharmaceutical drugs: A multi-stakeholder forensic accounting strategy. *Journal of Financial Crime, 26*(4), 1027–1047.

Raj, N. P., Ayyanar, Y., Thangavelu, P., Senthilkumar, S., Kumaran, A., Sivakumar, S., & Selvakumar, N. (2025). Counterfeit medicine: A major public health concern and effective remedies for combatting the crisis. *Discover Pharmaceutical Sciences, 1*(1), 1–22.

Rosendo, L. M. A. M. S. A. Y. B. A. T. C. G. P. R., & G. E. (2023). Sensors in the detection of abused substances in forensic contexts: A comprehensive review. *Micromachines, 14*(12), 2249.

Rusmalina, S. N. B. Z. S. J. L. C. N. J. C., & O. A. D. (2025). Review on application of spectrophotometry UV-Vis for identifying BKO in Jamu. *BIS Health and Environmental Science, 2*, V225012.

Sah, M., & M. K. M. L. H. P. &. M. H. S.. (2024). Physical analysis of aspirin in different phases and states using density functional theory. *Heliyon, 10*(11).

Sen, S., Dundar, Z., Uncu, O., & Ozen, B. (2021). Potential of Fourier-transform infrared spectroscopy in adulteration detection and quality assessment in buffalo and goat milks. *Microchemical Journal, 166*, 106207.

Siddique, I. (2023). High-performance liquid chromatography: Comprehensive techniques and cutting-edge innovations. *European Journal of Advances in Engineering and Technology, 10*(9), 66–70.

Siddique, I. (2024). Exploring functional groups and molecular structures: A comprehensive analysis using FTIR spectroscopic development, 1–2.

Singhal, A., Saini, U., Chopra, B., Dhingra, A. K., Jain, A., & Chaudhary, J. (2024). UV-visible spectroscopy: A review on its pharmaceutical and bio-allied sciences applications. *Current Pharmaceutical Analysis, 20*(3), 161–177.

Singhal, M., Sorjonen, J., Wikström, H., Upadhyay, P., Alhusban, F., Murphy, D., ... & Tajarobi, P. (2025). Exploring the impact of formulation and tablet shape on tablet integrity: A comprehensive investigation using mechanical and imaging techniques. *Journal of Pharmaceutical Sciences*, Article 103832.

Song, Y., Cong, Y., Wang, B., & Zhang, N. (2020). Applications of Fourier transform infrared spectroscopy to pharmaceutical preparations. *Expert Opinion on Drug Delivery, 17*(4), 551–571.

Sumalatha, C., Kumar, U. P., Kumar, K. P. S., & Venkateswara Rao, N. (2024). A comprehensive review of unimodal and multimodal fingerprint biometric authentication systems: Fusion, attacks, and template protection. *IEEE Access, 12*, 64300–64334.

Theodore, M., & Vongsutilers, V. (2024). Development of Attenuated Total Reflectance Fourier Transform Infrared spectroscopy coupled with multivariate classification chemometric model for routine screening of paracetamol, ibuprofen, and aspirin adulteration in herbal plants. *Current Pharmaceutical Analysis, 20*(4), 283–297.

Torres Vargas, D. G. (2025). Comparison of Near Infrared Spectra of three lichen substances and several common synthetic organic sunscreens. *Journal of Cosmetic Dermatology, 24*(7), e70288.

Ugwu, C. N., Ugwu, O. P. C., Alum, E. U., Eze, V. H. U., Basajja, M., Ugwu, J. N., ... & Uti, D. E. (2025). Sustainable development goals (SDGs) and resilient healthcare systems: Addressing medicine and public health challenges in conflict zones. *Medicine, 104*(7), e41535.

Velevska, N., Deconinck, E., Rebiere, H., Nakov, N., Brezovska, K., Atanasova, A., ... & Acevska, J. (2025). Simultaneous quantification of ibuprofen and paracetamol in combined tablet formulations by UV-VIS spectrophotometry and chemometric modelling. *Next Research*, Article 100559.

Watson, M. (2025). *Identification of substandard and falsified vaccines using spectroscopic techniques and machine learning algorithms* (Doctoral dissertation, Liverpool John Moores University).

Wayland, E., Richomme, J., & Kew, R. B. G. (2022). *Kew-Plant Words: A book of 250 curious words for plant lovers*. Hachette UK.

Xu, L. X. Y. Y. K. P. H. X. J. G. Y., & W. H. (2025). Machine learning-assisted chemical tongues based on dual-

channel inclusion complexes for rapid identification of nonsteroidal anti-inflammatory drugs in food. *ACS Sensors, 10*(3).

Yan, C. (2025). A review on spectral data preprocessing techniques for machine learning and quantitative analysis. *iScience*.

Peer-review history:
The peer review history for this paper can be accessed here:
https://pr.sdiarticle5.com/review-history/144328