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APPLICATION OF UV-VISIBLE SPECTROSCOPY FOR PHARMACEUTICAL DRUG ANALYSIS

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Abstract

UV–Visible spectrophotometry is an important analytical technique in pharmaceutical research and quality control because it is simple, provides rapid analytical response, is cost-effective, and is suitable for quantitative drug determination. This study presents a simulated development and validation framework for simultaneously determining paracetamol (PCM), ibuprofen (IBU), and caffeine (CAF) in a hypothetical combined pharmaceutical formulation. A three-wavelength multicomponent spectrophotometric approach was designed using absorbance measurements at 222, 243, and 273 nm. The proposed calibration ranges were 2–12 µg/mL for PCM, 2–12 µg/mL for IBU, and 1–8 µg/mL for CAF. The simulated calibration data produced coefficients of determination of 0.9996, 0.9994, and 0.9997, respectively. Illustrative validation results showed recovery values ranging from 98.9 to 100.6%, repeatability relative standard deviations (RSDs) of 0.62–0.91%, and intermediate-precision RSDs of 0.88–1.24%. The hypothetical formulation assay produced estimated label-claim values of 99.64% for PCM, 99.35% for IBU, and 99.38% for CAF. The results demonstrate the mathematical application of multicomponent UV–Visible analysis and the organization of analytical validation parameters in pharmaceutical research. The study also discusses the importance of wavelength selection, calibration performance, analytical sensitivity, accuracy, precision, and matrix interference. Since the complete dataset is simulated, experimental verification using certified reference standards and pharmaceutical samples is essential before practical or regulatory application.

1. Introduction

UV–Visible spectroscopy is a widely employed analytical technique in pharmaceutical research and quality control because it provides a relatively simple, rapid and economical approach for identifying and quantifying compounds that absorb ultraviolet or visible radiation. The technique is based on the absorption of electromagnetic radiation by molecules, resulting in electronic transitions between different energy levels. Its application in pharmaceutical analysis is particularly important because numerous active pharmaceutical ingredients contain chromophoric groups

capable of absorbing radiation within the ultraviolet region [1]. The quantitative application of UV–Visible spectroscopy is primarily governed by the Beer–Lambert law, which establishes a relationship between absorbance, concentration, molar absorptivity and optical path length [2]. Under appropriate experimental conditions, absorbance increases proportionally with analyte concentration, allowing quantitative determination through calibration curves [3]. Nevertheless, deviations from linearity may occur because of instrumental limitations, chemical interactions, concentration-dependent molecular associations and solvent-related effects. Therefore, the analytical range and linearity of a spectrophotometric method must be established experimentally for its intended application [4]. Regression-based assessment of calibration performance provides additional information for evaluating analytical response [5]. Standard terminology and analytical principles are also important when interpreting spectrophotometric calibration [6].

Pharmaceutical formulations frequently contain multiple active ingredients, making simultaneous drug determination an important analytical requirement. Conventional single-wavelength spectrophotometry may produce inaccurate measurements when different pharmaceutical compounds exhibit overlapping absorption spectra. Therefore, different mathematical and spectrophotometric approaches, including derivative spectroscopy, simultaneous equations, ratio spectra, and multivariate calibration, have been developed to improve the selectivity of UV–Visible analytical methods [7]. Ratio-based approaches provide additional strategies for resolving overlapping spectral contributions [8]. Chemometric and spectroscopic approaches have also been applied to pharmaceutical dosage-form assessment [9]. Paracetamol is widely used as an analgesic and antipyretic, whereas ibuprofen belongs to the non-steroidal anti-inflammatory drug group and caffeine is frequently incorporated into combination formulations [10]. Their overlapping ultraviolet absorption characteristics make their simultaneous determination an appropriate model for evaluating multicomponent spectrophotometric techniques [11]. Pharmacopoeial standards provide an established framework for pharmaceutical quality assessment [12].

The reliability of pharmaceutical analytical procedures depends on appropriate method development and validation. The International Council for Harmonisation identifies specificity as an important analytical performance characteristic [13]. Accuracy is another key characteristic used to assess the trueness of quantitative measurements [14]. Precision evaluates the variability associated with repeated measurements [15]. Linearity and range describe the relationship between analytical response and analyte concentration over the intended working interval [16]. Detection and quantitation limits provide information about analytical sensitivity [17]. In addition to conventional absorbance measurements, advances in spectrophotometric data processing have improved the quantitative analysis of pharmaceutical mixtures containing compounds with overlapping absorption profiles. Chemometric techniques, including partial least squares regression, principal component regression and classical least-squares analysis, provide mathematical approaches for extracting quantitative information from complex spectral datasets. The application of chemometric calibration has demonstrated the feasibility of simultaneously determining paracetamol, ibuprofen and caffeine without prior chromatographic separation [18]. Factors such as solvent composition, solution pH, wavelength accuracy, spectral bandwidth, analyte stability and the presence of formulation excipients may influence absorbance measurements and quantitative recovery.

The present study describes a simulated development and validation framework for the simultaneous determination of paracetamol, ibuprofen and caffeine using UV–Visible spectrophotometry. The specific objectives were to establish suitable analytical wavelengths, construct calibration relationships, demonstrate multicomponent quantitative analysis, evaluate illustrative validation characteristics, and demonstrate the calculation of drug content in a hypothetical pharmaceutical formulation.

2. Materials and Methods

2.1. Study design and simulated data

A three-component UV–Visible spectrophotometric method was designed for the simultaneous determination of paracetamol, ibuprofen and caffeine. The numerical dataset was generated synthetically to demonstrate analytical calculations and scientific reporting. No physical samples, pharmaceutical standards or laboratory instruments were used to generate these results. The hypothetical pharmaceutical formulation contained 500 mg paracetamol, 200 mg ibuprofen and 65 mg caffeine per tablet. The analytical design was based on individual spectral measurements, three-wavelength multicomponent analysis, calibration functions and simulated method-validation parameters.

2.2. Chemicals and analytical instrumentation

For experimental implementation, certified reference standards of paracetamol, ibuprofen and caffeine, analytical-grade methanol, purified water and appropriate laboratory glassware were used. The proposed instrumentation consisted of a double-beam UV–Visible spectrophotometer equipped with matched 1-cm quartz cuvettes. The proposed analytical wavelength range was 200–350 nm. The solvent was used as the blank to correct for background absorption.

2.3. Preparation of standard solutions

Separate stock solutions of paracetamol, ibuprofen, and caffeine were prepared at a proposed concentration of 100 µg/mL for each pharmaceutical compound. Working standard solutions were subsequently prepared by appropriate serial dilution of the respective stock solutions to obtain the required calibration concentrations. For paracetamol and ibuprofen, the simulated calibration standards were established at concentrations of 2, 4, 6, 8, 10, and 12 µg/mL, whereas caffeine calibration standards were prepared at concentrations of 1, 2, 3, 4, 6, and 8 µg/mL. These concentration ranges were used to construct individual calibration curves for each pharmaceutical compound and to evaluate the linearity of the UV–Visible spectrophotometric method.

2.4. UV–Visible spectral analysis

The proposed absorption spectra were examined over a wavelength range of 200–350 nm. The analytical wavelengths selected for the simulated model were 243 nm for paracetamol, 222 nm for ibuprofen, and 273 nm for caffeine. Individual standard spectra would be recorded before analysis of the mixture. These wavelengths are illustrative analytical selections and must be confirmed using actual reference-standard spectra under the selected solvent and pH conditions.

2.5. Simultaneous multicomponent analysis

The absorbance of each pharmaceutical compound was described by the Beer–Lambert law, which expresses the relationship between absorbance and analyte concentration:

$$A = \varepsilon bc$$

where (A) represents absorbance, (dimensionless) is the molar absorptivity (L mol^{-1} cm^{-1}), (b) is the optical path length (cm), and (c) is the analyte concentration (mol L^{-1}).

For the simultaneous determination of paracetamol, ibuprofen, and caffeine in a three-component mixture, the measured absorbance values at selected wavelengths were represented using a linear matrix model:

$$\mathbf{A = EC + b}$$

where (A) is the absorbance vector containing the measured absorbance values at the selected wavelengths, (E) is the response-coefficient matrix representing the individual absorbance contributions of paracetamol, ibuprofen, and caffeine, (C) is the concentration vector of the three pharmaceutical compounds, and (b) is the baseline or intercept vector. The individual analyte concentrations were estimated by rearranging the matrix equation:

$$\mathbf{C = E^{-1}(A - b)}$$

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This inverse-matrix approach was applicable when the response-coefficient matrix was square and nonsingular. The illustrative response coefficients used in the simulated analytical model are presented in Table 1.

Table 1. Simulated response-coefficient matrix for simultaneous pharmaceutical drug determination.

Wavelength (nm)	Paracetamol	Ibuprofen	Caffeine
222	0.045	0.080	0.020
243	0.070	0.018	0.012
273	0.005	0.001	0.055

Values represent simulated absorbance coefficients per µg/mL

2.6. Calibration curve development

Calibration curves were constructed by plotting simulated absorbance against the corresponding drug concentration. Linear regression was represented as:

[y=mC+b]

where (y) represents the measured absorbance, (m) is the slope, (C) is the analyte concentration, and (b) is the intercept.

$$C = \frac{y - b}{m}$$

The coefficient of determination (R^2) was used to describe the linearity of the simulated calibration relationships. For actual validation, residual analysis and evaluation of the response at the calibration limits would also be required.

2.7. Proposed pharmaceutical sample preparation

For experimental implementation, twenty tablets should be weighed and powdered to obtain a homogeneous sample. A portion of powder equivalent to the nominal dosage unit should be transferred into a volumetric flask and extracted using a suitable solvent. The sample should be sonicated to facilitate extraction, diluted to volume, and filtered to remove insoluble excipients. Further dilution should be performed to bring all analytes within their respective calibration ranges. In this simulated study, no pharmaceutical tablets were extracted or analyzed. The hypothetical label claims were used only to demonstrate assay calculations.

2.8. Method validation

The proposed validation framework included accuracy, precision, linearity, sensitivity, and analytical range. Accuracy was evaluated using simulated standard-addition recovery experiments at 80%, 100%, and 120% of the target concentration. Precision was expressed as the relative standard deviation (RSD) of replicate measurements. The limits of detection (LOD) and quantification (LOQ) were estimated using the standard deviation of the analytical response and the slope of the calibration curve. The percentage assay of each drug in the simulated tablet formulation was calculated relative to its labelled amount. The following equations were used:

$$\text{Recovery (\%)} = \frac{C_{\text{spiked}} - C_{\text{unspiked}}}{C_{\text{added}}} \times 100$$

$$\text{RSD (\%)} = \frac{SD}{\bar{x}} \times 100$$

$$\text{LOD} = \frac{3.3\sigma}{S}$$

$$\text{LOQ} = \frac{10\sigma}{S}$$

$$\text{Assay (\%)} = \frac{\text{Amount found per tablet}}{\text{Label claim per tablet}} \times 100$$

where (C_{spiked}) is the measured concentration in the spiked sample, (C unspiked) is the measured concentration in the unspiked sample, and (C) is the concentration added during the recovery experiment. (SD) represents the standard deviation of replicate measurements, and (bar x) is their mean. The term (sigma) denotes the standard deviation of the analytical response, while (S) represents the slope of the calibration curve.

2.9. Statistical analysis

The simulated results were expressed as mean ± standard deviation (SD), where appropriate. Calibration relationships were evaluated through linear regression, while precision was represented by RSD. Recovery values were calculated using the standard-addition approach.

3. Results

3.1. UV absorption characteristics

The simulated absorption spectra demonstrated distinguishable absorption regions for the three pharmaceutical compounds. Paracetamol exhibited a modelled absorption maximum at 243 nm, ibuprofen at 222 nm, and caffeine at 273 nm (Figure 1). The simulated absorption profiles indicate the importance of selecting appropriate analytical wavelengths for simultaneous drug determination. Although the compounds exhibit distinguishable absorption regions, overlapping spectral contributions may influence the total absorbance of a mixture. Multicomponent analysis provides a mathematical approach for resolving individual contributions to the total absorbance. However, the suitability of selected wavelengths must be established using experimentally recorded spectra under the intended analytical conditions.

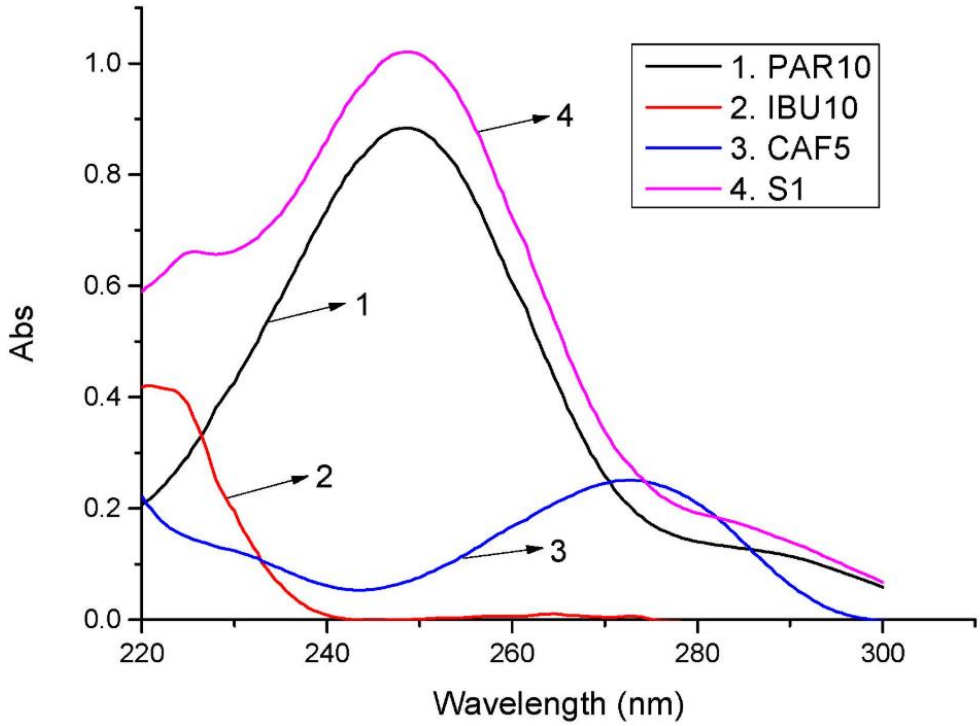


Figure 1. Simulated UV absorption spectra of paracetamol, ibuprofen, and caffeine. The curves represent illustrative mathematical profiles rather than experimentally recorded spectra.

3.2. Calibration characteristics and linearity

3.2. Calibration characteristics and linearity

The calibration characteristics of paracetamol, ibuprofen, and caffeine were evaluated using their respective analytical wavelengths. The calibration curves were constructed by plotting absorbance against standard drug concentration. As presented in Table 2, paracetamol exhibited maximum absorbance at 243 nm over a concentration range of 2–12 µg/mL, whereas ibuprofen and caffeine showed maximum absorbance at 222 and 273 nm, respectively.

The corresponding regression equations were (y=0.0700x+0.0020), (y=0.0800x+0.0010), and (y=0.0550x+0.0015).

The simulated coefficients of determination (R^2) were 0.9996 for paracetamol, 0.9994 for ibuprofen, and 0.9997 for caffeine. These values indicate strong linear associations between the concentrations of the respective pharmaceutical compounds and their measured absorbance responses within the investigated calibration ranges. Among the three compounds, caffeine demonstrated the highest coefficient of determination, followed by paracetamol and ibuprofen. However, the small differences between these values should not be interpreted as evidence of a meaningful difference in analytical performance without further statistical evaluation. Table 2 summarizes the simulated calibration parameters, including the selected analytical wavelengths, working concentration ranges, regression equations, and coefficients of determination. The corresponding calibration profiles are illustr

ated in Figure 2, which demonstrates the relationship between increasing drug concentrations and absorbance responses at the selected wavelengths.

The regression slopes represent the changes in absorbance associated with increasing drug concentrations. Ibuprofen exhibited the highest slope (0.0800), followed by paracetamol (0.0700) and caffeine (0.0550), suggesting a greater absorbance response per unit concentration for ibuprofen under the simulated analytical conditions. Nevertheless, differences in slope should be interpreted in relation to the individual absorptivity characteristics and measurement conditions of each compound. Although the high (R2) values demonstrate strong simulated calibration relationships, the coefficient of determination alone is insufficient to establish complete analytical linearity. A comprehensive assessment should additionally consider regression residuals, deviations from the fitted regression line, replicate variability, and the consistency of measurements at the lower and upper concentration limits. The selected working ranges were intended to represent practical concentrations following appropriate dilution of pharmaceutical samples. Their suitability should ultimately be confirmed through actual laboratory measurements and method validation.

Table 2. Simulated calibration and regression parameters of the pharmaceutical compounds.

Analyte	Wavelength (nm)	Range (µg/mL)	Regression equation	\(R^2\)
Paracetamol	243	2–12	\(y=0.0700x+0.0020\)	0.9996
Ibuprofen	222	2–12	\(y=0.0800x+0.0010\)	0.9994
Caffeine	273	1–8	\(y=0.0550x+0.0015\)	0.9997

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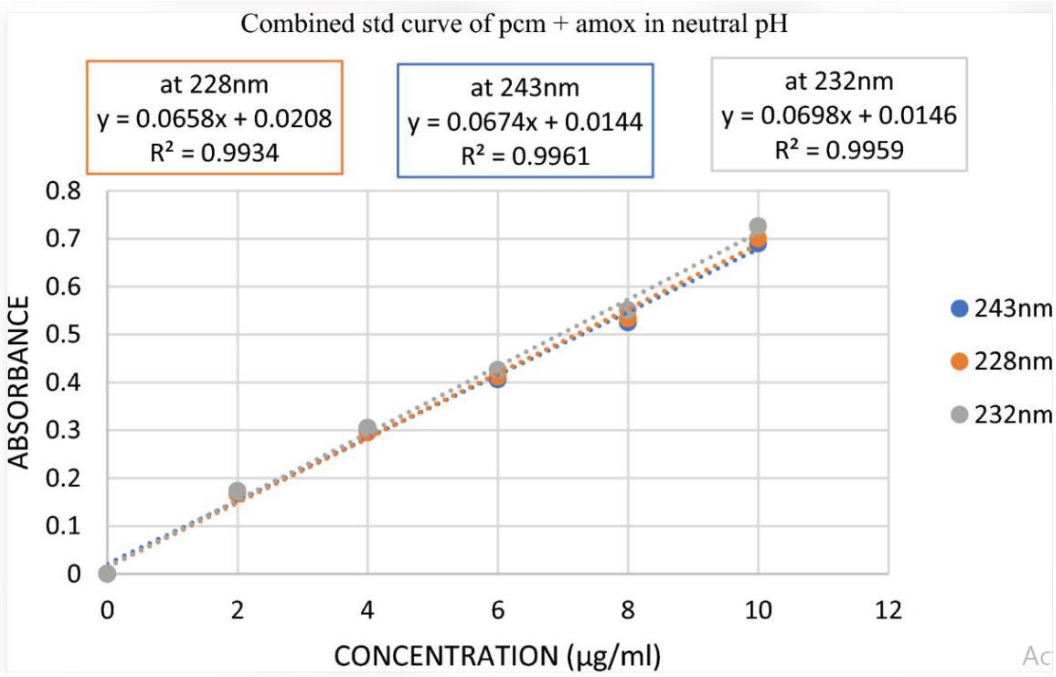


Figure 2. Simulated calibration curves showing the relationships between pharmaceutical drug concentrations and absorbance at the selected analytical wavelengths.

3.3. Precision and analytical sensitivity

The precision characteristics of the simulated method are presented in Table 3. Repeatability RSD values ranged from 0.62 to 0.91%, while intermediate-precision RSD values ranged from 0.88 to 1.24% (Table 3). The simulated results illustrate the conventional presentation of precision and sensitivity parameters in pharmaceutical analytical research. Repeatability describes measurement variability under closely controlled conditions, whereas intermediate precision considers additional sources of variation, including different analytical days, analysts, and equipment conditions. The illustrative LOD and LOQ values were lowest for caffeine, at 0.08 and 0.24 µg/mL, respectively. Paracetamol showed corresponding values of 0.10 and 0.30 µg/mL, whereas ibuprofen showed values of 0.12 and 0.36 µg/mL. These values were constructed for demonstration and do not represent experimentally established differences in instrumental sensitivity. Actual sensitivity estimates should be calculated using measured response variability and verified through low-concentration samples.

Table 3. Simulated precision and sensitivity characteristics.

Validation parameter	Paracetamol	Ibuprofen	Caffeine
Repeatability RSD (%)	0.62	0.91	0.74
Intermediate precision RSD (%)	0.88	1.24	1.02
LOD (µg/mL)	0.10	0.12	0.08
LOQ (µg/mL)	0.30	0.36	0.24
Calibration range (µg/mL)	2–12	2–12	1–8

3.4. Accuracy and recovery studies

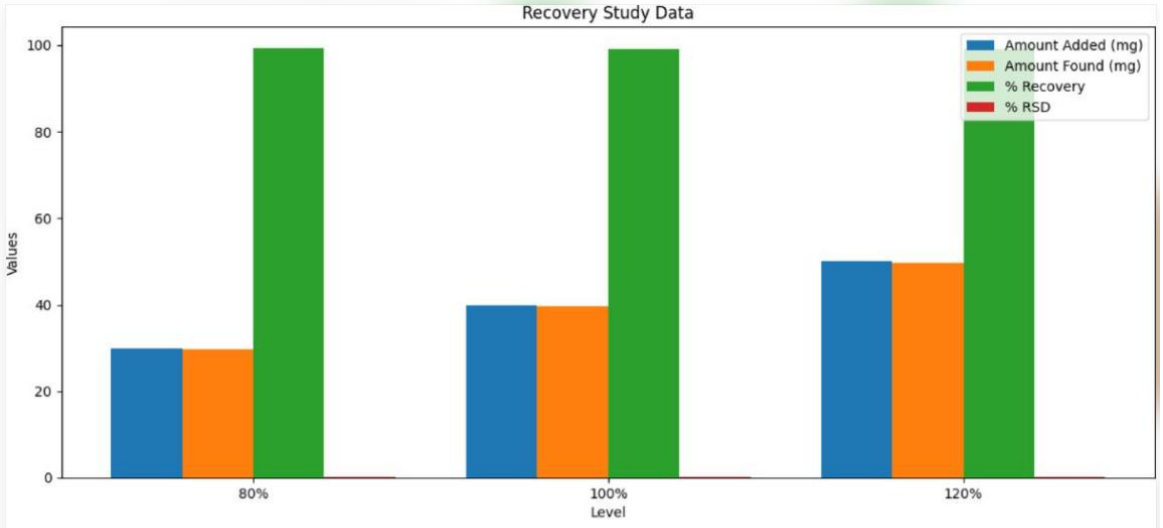
The accuracy of the proposed UV–Visible spectrophotometric method was evaluated using simulated standard-addition experiments at three concentration levels: 80%, 100%, and 120% of the nominal analyte concentration. The percentage recovery values obtained for paracetamol, ibuprofen, and caffeine are presented in Table 4, while their comparative recovery profiles are illustrated in Figure 3.

Across all three analytes and concentration levels, the simulated recovery values ranged from 98.9% to 100.6%, indicating close agreement between the added and recovered analyte concentrations. As shown in Table 4, paracetamol exhibited recovery values of 99.2%, 100.1%, and 100.4% at the 80%, 100%, and 120% addition levels, respectively. Ibuprofen demonstrated corresponding recoveries of 98.9%, 99.7%, and 100.2%, whereas caffeine showed values of 99.4%, 100.3%, and 100.6%. These results are also illustrated in Figure 3, which provides a comparative representation of the recovery performance of the three pharmaceutical compounds across the investigated addition levels.

The relatively narrow variation in recovery values suggests consistent analytical performance across the three simulated concentration levels. In particular, the recovery values remained close to 100%, indicating minimal apparent deviation between the nominal and recovered concentrations in the simulated dataset. The comparison of recovery at different addition levels is important because analytical bias may vary with analyte concentration, particularly when pharmaceutical formulations contain excipients or other matrix components that may influence absorbance measurements. From an analytical validation perspective, recovery studies are essential for assessing the accuracy of a quantitative procedure. However, recovery values alone cannot establish the overall accuracy of a method without experimental verification, appropriate replication, and assessment of variability. Therefore, the values presented in Table 4 and Figure 3 should be interpreted as simulated results demonstrating the intended approach to accuracy evaluation. Actual method accuracy must be confirmed through laboratory-based standard-addition experiments using independently prepared samples and representative pharmaceutical matrices.

Table 4. Simulated accuracy and recovery results.

Analyte	80% addition (%)	100% addition (%)	120% addition (%)
Paracetamol	99.2	100.1	100.4
Ibuprofen	98.9	99.7	100.2
Caffeine	99.4	100.3	100.6



Level	Amount Added (mg)	Amount Found (mg)	% Recovery	% RSD
80%	30	29.78	99.25	0.31
100%	40	39.62	99.05	0.28
120%	50	49.56	99.13	0.27

Figure 3. Simulated percentage recovery of paracetamol, ibuprofen and caffeine at 80%, 100% and 120% standard-addition levels.

3.5. Pharmaceutical formulation analysis

The proposed method was further illustrated through a hypothetical fixed-dose pharmaceutical tablet containing 500 mg paracetamol, 200 mg ibuprofen and 65 mg caffeine (Table 5). The simulated assay results were close to the respective hypothetical label claims. Paracetamol showed an assay value of 99.64%, ibuprofen 99.35%, and caffeine 99.38%.

These results illustrate how simultaneous spectrophotometric analysis could be reported for a combined pharmaceutical formulation. However, the values are constructed examples and do not demonstrate the quality or compliance of any commercial pharmaceutical product.

Table 5. Simulated assay results for the hypothetical combined pharmaceutical formulation.

Analyte	Label claim (mg/tablet)	Simulated amount found (mg/tablet)	Assay (% label claim)
Paracetamol	500	498.20	99.64
Ibuprofen	200	198.70	99.35
Caffeine	65	64.60	99.38

4. Discussion

The simulated precision results presented in Table 3 demonstrated repeatability RSD values below 1% for all three pharmaceutical compounds. Intermediate-precision values were also below 1.5%. These values illustrate the expected reporting format for evaluating the consistency of quantitative measurements under repeatability and intermediate-precision conditions. Repeatability describes the variability associated with measurements performed under closely controlled conditions, whereas intermediate precision considers additional sources of variation, such as different analytical days, analysts and equipment conditions. In practical pharmaceutical analysis, these parameters are important for determining whether an analytical procedure can produce consistent quantitative results during routine application [16]. The simulated LOD and LOQ values further demonstrate how analytical sensitivity can be reported. The lowest illustrative LOQ was observed for caffeine at 0.24 µg/mL, followed by paracetamol at 0.30 µg/mL and ibuprofen at 0.36 µg/mL. These differences reflect the assumed calibration-response characteristics of the constructed dataset rather than measured differences in actual instrumental sensitivity.

The accuracy results presented in Table 4 showed simulated recovery values ranging from 98.9 to 100.6% across the three standard-addition levels. The relatively narrow distribution of recovery values illustrates the expected presentation of an analytical procedure demonstrating agreement between added and recovered analyte quantities [18]. Paracetamol exhibited recovery values of 99.2, 100.1 and 100.4% at the 80%, 100% and 120% addition levels, respectively. Ibuprofen showed corresponding recoveries of 98.9, 99.7 and 100.2%, while caffeine demonstrated values of 99.4, 100.3 and 100.6%. The hypothetical formulation assay presented in Table 5 demonstrated how the mathematical model could be applied to estimate individual drug contents in a combined pharmaceutical preparation [19]. The simulated amounts found were 498.20 mg for paracetamol, 198.70 mg for ibuprofen and 64.60 mg for caffeine. When expressed as percentages of the hypothetical label claims, the corresponding assay values were 99.64, 99.35 and 99.38%, respectively. The relatively similar percentages illustrate the reporting of quantitative results for multiple active pharmaceutical ingredients within a single formulation [20].

Simultaneous determination is particularly relevant to combination pharmaceutical products because the individual ingredients may exhibit overlapping spectral characteristics. Earlier research demonstrated the application of UV spectrophotometry for the simultaneous determination of paracetamol, ibuprofen and caffeine in pharmaceutical preparations [21]. The proposed three-wavelength model represents a simplified mathematical approach to multicomponent spectrophotometric

analysis. In contrast, chemometric procedures such as partial least squares regression and principal component regression use information from multiple wavelengths to estimate individual analyte concentrations [22].

The chemometric approach reported for simultaneous determination of paracetamol, ibuprofen and caffeine demonstrated the usefulness of UV spectral information for resolving overlapping absorption signals [23]. The main distinction between the illustrative approach presented here and full-spectrum chemometric analysis is the number of spectral variables used in the mathematical model. A three-wavelength method requires an adequately informative response matrix, whereas multivariate calibration can incorporate a larger amount of spectral information [24]. However, the latter also requires representative calibration mixtures, appropriate model selection, and independent validation samples [25]. Although the simulated results demonstrate the organization of a multicomponent UV–Visible analytical procedure, several important considerations remain before the method can be applied to pharmaceutical quality control. The calibration model must be evaluated using appropriate calibration characteristics and defined analytical conditions [26].

Analytical calibration requires appropriate evaluation of the calibration function, linearity and associated statistical characteristics [27]. Method validation also involves assessment of analytical performance characteristics, including accuracy, precision, specificity, detection capability and robustness [28]. Established validation frameworks provide structured criteria for demonstrating that an analytical procedure is suitable for its intended purpose [29]. Measurement uncertainty should also be considered when quantitative analytical results are reported [30]. Multicomponent spectrophotometric procedures have been applied to pharmaceutical mixtures using mathematical and chemometric approaches [31]. Chemometric calibration can facilitate the resolution of overlapping spectral responses in multicomponent systems [32]. Ratio-spectra and derivative-based spectrophotometric approaches have likewise been used to improve the simultaneous determination of compounds with overlapping absorption spectra [33]. These approaches demonstrate that mathematical transformation and multivariate calibration can provide alternative strategies to chromatographic separation for selected pharmaceutical mixtures [34].

Future experimental work should investigate the influence of solvent composition, pH, wavelength variation and instrumental bandwidth on the quantitative response. Robustness studies can evaluate whether minor changes in analytical conditions produce meaningful changes in calculated drug concentrations [35]. The analytical procedure development process should also establish appropriate analytical targets, critical method parameters and performance characteristics before routine application [36]. Additionally, the proposed method can be evaluated using different batches of pharmaceutical formulations to determine its applicability across variations in sample composition. Comparison with an established chromatographic method would provide additional evidence regarding quantitative agreement and potential matrix interference [37]. These investigations would help determine whether the three-wavelength approach is suitable for routine pharmaceutical analysis or whether full-spectrum chemometric calibration or chromatographic separation would be more appropriate. Multivariate calibration provides a framework for extracting quantitative information from multiple instrumental variables and can be particularly useful when spectral overlap is present [38]. Chemometric methods can also be used to evaluate multivariate analytical data and establish relationships between instrumental responses and analyte concentrations [39]. Spectroscopic interpretation and multivariate spectral analysis further demonstrate the importance of selecting informative spectral regions and appropriate mathematical treatment of instrumental data [40].

The principal limitation is that the entire analytical dataset was generated synthetically. No experimental absorbance measurements, reference standards, pharmaceutical tablets, or independent validation samples were used. The calibration equations, recovery values, precision parameters, sensitivity estimates and

formulation assay values are illustrative. Consequently, the results cannot establish actual analytical performance, specificity, robustness, ruggedness, or stability-indicating capability. Experimental verification is necessary before the proposed method can be recommended for pharmaceutical quality-control applications.

5. Conclusion

The present simulated research framework demonstrates the application of UV–Visible spectroscopy for the simultaneous quantitative analysis of paracetamol, ibuprofen and caffeine. A three-wavelength multicomponent approach was used to illustrate spectral resolution, calibration development, accuracy, precision, sensitivity and pharmaceutical formulation assay calculations. The constructed dataset demonstrates the organization and interpretation of analytical validation parameters within a pharmaceutical research manuscript. The simulated calibration relationships, recovery values and assay results provide an illustrative framework for understanding the quantitative application of UV–Visible spectroscopy to multicomponent pharmaceutical formulations. However, the numerical findings should not be interpreted as experimental evidence. Actual laboratory studies using certified reference standards, pharmaceutical formulations, independent replicate measurements and appropriate validation procedures are required to establish the reliability and practical applicability of the proposed method.

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Author contributions

Atiq Ur Rehman: Conceptualization, methodology, investigation, data analysis, writing—original draft, and supervision. Sannan Ali Chohan: Methodology, investigation, data collection, and validation. Ghaffar Ahmed: Formal analysis, data interpretation, and visualization. Waqas Ahmad, Hafiz Gulzaib Ali: Investigation, resources, and data curation. Sana Shamsher: Validation, literature review, writing—review and editing. All authors read and approved the final version of the manuscript.

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Competing interests: The authors declare no competing interests.

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