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Prediction of Adulteration Levels in *Anoectochilus roxburghii* Powder Using Multispectral Derivative Fusion

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Abstract: *Objective:* To determine the extent to which fusion of raw multispectral data with derivative spectra improves prediction of adulteration levels in *Anoectochilus roxburghii* powder. *Methods:* Eleven adulteration levels from 0% to 100% were prepared, with 10 independent replicates per level, yielding 110 records. Eight channels were used to derive three representations - raw, first-derivative, and second-derivative spectra - and partial least squares regression was used to compare single-representation and fused inputs. *Results:* On the test set, the fusion model achieved a coefficient of determination of 0.9965, a root mean square error of 1.859, and a mean absolute error of 1.424. Overall performance exceeded that of the single-representation models, although errors were relatively larger at intermediate adulteration levels. *Conclusion:* Joint representation of raw intensity, local slope, and curvature may improve prediction accuracy for continuous adulterant proportions while reducing overall bias.

Keywords: *Anoectochilus roxburghii*; Multispectral spectroscopy; Derivative spectra; Adulteration level; Quantitative prediction

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1. Introduction

Once *Anoectochilus roxburghii* is processed into powder, conventional identification cues such as external appearance and tissue morphology are markedly diminished. If a visually similar powder is then added as an adulterant, rapid sensory discrimination becomes impractical. Near-infrared spectroscopy combined with chemometrics has long been used for authenticity assessment and estimation of adulteration proportions in traditional Chinese medicinal materials [1]. Portable near-infrared detection has also shown that powdered medicinal materials can be screened rapidly for adulteration on the basis of spectral patterns [2]. The documented occurrence of adulterated Ziziphi Spinosae Semen in a compound preparation further indicates that adulteration is not an isolated event but a persistent quality-control concern [3]. A spectroscopic method

that can rapidly return a continuous adulterant mass fraction would therefore be directly relevant to acceptance testing of powdered raw materials and in-process spot checks.

Raw spectra, Savitzky-Golay first-derivative spectra, and second-derivative spectra have previously been used for quantitative analysis of adulteration in *Anoectochilus roxburghii* powder, with multi-channel joint representation showing greater predictive capability [4]. In studies of other medicinal materials, work on Ganoderma lucidum extracts has shown that spectral preprocessing combined with partial least squares regression can establish a relatively stable mapping between spectra and adulteration proportion [5]. Detection of different adulterants in Ziziphi Spinosae Semen likewise suggests that both adulterant composition and mass fraction affect the spectral response [6]. Under discrete multispectral conditions, however, the way in which raw intensity, local slope, and curvature complement one another remains unclear, as does the error range in which fusion provides the greatest benefit. Accordingly, the present analysis compares four input schemes in terms of accuracy, bias, and robustness across concentration intervals.

2. Materials and sample design

2.1. *Anoectochilus roxburghii* and adulteration levels

The study period extended from January 5 to March 31, 2026. The samples consisted of *Anoectochilus roxburghii* powder and a representative adulterant powder. Eleven levels were set at 10% increments from 0% to 100% by mass fraction, with 10 independent replicates at each level, for a total of 110 records. Within each level, 7 records were assigned to training, 1 to validation, and 2 to testing. Thus, all three subsets covered the full concentration range, and correspondence among samples was maintained using fixed identifiers. The configuration of adulteration levels and spectral processing is shown in **Table 1**. Replicate counts were identical across levels, and the same samples were used for all three spectral representations. The stratified 7:1:2 split reduced, to some extent, performance shifts caused by an uneven distribution of adulteration levels.

Table 1. Configuration of adulteration levels and spectral processing

Adulteration design		Spectral representation			Data split		
Adulterant fraction/%	Replicates	Raw	First derivative	Second derivative	Train.	Valid.	Test
0	10	8	8	8	7	1	2
10	10	8	8	8	7	1	2
20	10	8	8	8	7	1	2
30	10	8	8	8	7	1	2
40	10	8	8	8	7	1	2
50	10	8	8	8	7	1	2
60	10	8	8	8	7	1	2
70	10	8	8	8	7	1	2
80	10	8	8	8	7	1	2
90	10	8	8	8	7	1	2
100	10	8	8	8	7	1	2

2.2. Multispectral acquisition and correction

All multispectral records were standardized to eight discrete channels, with the channel order kept fixed

throughout. The acquisition workflow followed a white-reference and dark-reference correction scheme so that background illumination, dark current, and overall scale differences were handled within a common framework. Each record underwent completeness checks and outlier quality control before derivative transformation and modeling. Previous work on near-infrared quality evaluation of traditional Chinese medicinal materials has identified consistent acquisition conditions, reproducible preprocessing, and separation of training from prediction as important prerequisites for stable quantitative results [7]. In addition, every input scheme used the same samples and the same data split, and channel order remained unchanged. Differences in performance therefore primarily reflect the spectral representation itself and associated scaling effects.

3. Multispectral derivative fusion method

3.1. Raw and derivative spectra

The raw multispectral representation retained the relative response of each of the eight channels. Along the same ordered channel sequence, smoothing was performed using a Savitzky-Golay second-order polynomial with a five-point window, after which the first and second derivatives were calculated. Functionally, the first derivative emphasizes changes in local slope and helps suppress slowly varying baseline drift, whereas the second derivative highlights local curvature and turning points, adding structural differences that may be less apparent in the raw intensities. Research on visible-near-infrared detection of powder adulteration has shown that combining spectral preprocessing with chemometric regression can estimate adulterant content with high accuracy [8]. All three representations were derived from the same records, with processing parameters fixed before modeling and applied consistently to every data subset.

3.2. Multi-channel feature fusion

Feature fusion aligned the eight raw channels, eight first-derivative channels, and eight second-derivative channels by sample to form a 24-dimensional joint input; each single-representation scheme used its corresponding eight-dimensional feature vector. Before modeling, standardization parameters were estimated from the training data only and then applied to the validation and test sets, preventing scale differences from altering the relative weighting of channels. Applications of hyperspectral techniques to rapid testing of traditional Chinese medicinal materials indicate that multi-channel features combined with chemometric models can exploit information complementarity while compressing variables [9]. Under the common regression framework, all input schemes used the same target variable and evaluation procedure so that any fusion gain can be interpreted directly as the complementary contribution of spectral information at different derivative orders.

4. Construction of the adulteration-level prediction model

4.1. Data partitioning and evaluation

At each adulteration level, 7 records were assigned to training, 1 to validation, and 2 to testing, yielding 77 training records, 11 validation records, and 22 independent test records. Partial least squares regression (PLSR) was used to establish a latent-variable mapping between adulterant mass fraction and spectral features. The number of candidate latent variables was not fixed a priori but selected according to validation-

set error; the raw, first-derivative, second-derivative, and fused inputs used 6, 4, 2, and 3 latent variables, respectively. After parameter selection, the training and validation sets were combined for model fitting, while the test set was reserved for final evaluation. This arrangement helps distinguish fitting performance from predictive performance on independent data [10].

Performance was evaluated using the coefficient of determination (R^2), root mean square error (RMSE), mean absolute error (MAE), residual prediction deviation (RPD), and mean bias (Bias). RPD was calculated as the ratio of the standard deviation of the test-set target values to RMSE, whereas Bias indicates the direction of overall prediction error. Research on spectroscopic identification of traditional Chinese medicinal materials has consistently emphasized that performance should not be judged from a single metric; goodness of fit, prediction error, and validation design should be considered jointly [11]. Accordingly, all models were evaluated using the same test-set metrics together with residuals stratified by adulteration interval.

5. Validation and analysis of results

5.1. Spectral response across adulteration levels

Most channels showed a continuous response across adulteration levels, but the locations of greatest sensitivity differed among the three spectral representations. For the raw spectra, the correlation coefficient with adulteration level was approximately 0.984 for channel 08, 0.945 for channel 07, and -0.858 for channel 05. For the first derivative, the absolute correlation coefficients of channels 07, 08, and 06 all exceeded 0.99, while the second-derivative channel 05 had a correlation coefficient of approximately 0.991. These patterns indicate that local slope and curvature contribute additional information on adulteration level. Hyperspectral-image authentication of Ziziphi Spinosae Semen has likewise shown that a small number of key bands can concentrate discriminatory information on medicinal materials [12]. The fused input therefore spans three complementary levels of information: intensity, slope, and curvature.

5.2. Predictive performance of the fusion model

Table 2 summarizes adulteration-level prediction performance for the different spectral inputs. On the test set, the three-representation fusion model achieved $R^2 = 0.9965$, RMSE = 1.859, MAE = 1.424, RPD = 17.410, and Bias = -0.237, outperforming the three single-representation schemes overall. Relative to the raw-spectrum model, R^2 increased by 0.0007, RMSE decreased by 9.1%, MAE decreased by 15.9%, and absolute Bias decreased by 26.7%. The combined use of derivative information and raw intensity therefore captured complementary local variation, improving continuous-level regression while maintaining low overall bias.

Table 2. Adulteration-level prediction performance for different spectral inputs

Input scheme	R^2	RMSE	MAE	RPD	Bias
Raw spectra	0.9958	2.044	1.694	15.832	-0.323
First derivative	0.9952	2.189	1.810	14.783	-0.607
Second derivative	0.9934	2.565	2.102	12.619	-1.102
Three-representation fusion	0.9965	1.859	1.424	17.410	-0.237

In quantitative adulteration research on traditional Chinese medicinal materials, a dual-branch network also yielded a high coefficient of determination on independent test data, indicating that joint use of multi-

source features can enhance quantitative discrimination of complex powders [13]. A stable fusion gain was still observed here within a latent-variable regression framework, suggesting that the improvement is not specific to a particular deep architecture. Because the studies differ in adulterant type, spectral range, target scale, and sample complexity, comparisons are most appropriately focused on methodological trends and validation design. The high RPD obtained in the present analysis is also related to the test set spanning the full 0%-100% adulteration range and to the broad dispersion of target values, which supports an interpretable comparison among relatively simple models.

5.3. Error distribution and robustness boundaries

When evaluated by interval, the fusion model yielded MAE = 0.494, Bias = -0.443, and a maximum absolute error of 1.398 over 0%-30%; MAE = 2.177, Bias = -0.688, and a maximum absolute error of 3.365 over 40%-70%; and MAE = 1.662, Bias = 0.638, and a maximum absolute error of 3.459 over 80%-100%. Errors were therefore more concentrated at intermediate adulteration levels, whereas the two end ranges did not show a persistent drift in the same direction. Research on nondestructive detection of Poria adulteration has similarly indicated that near-infrared methods are suitable for rapid screening, while model boundaries can be affected by the medicinal material, adulterant type, and acquisition conditions [14]. Within the current adulteration-level and processing framework, the results support the stated methodological interpretation.

6. Conclusions

Overall, the three-representation fusion model produced R^2 = 0.9965, RMSE = 1.859, MAE = 1.424, RPD = 17.410, and Bias = -0.237 on the 22 test records. Relative to the raw-spectrum model, RMSE and MAE decreased by 9.1% and 15.9%, respectively. Spectral-response analysis showed that raw intensity, local slope, and curvature had different sensitive channels, so their joint representation exploited complementary information. Interval-stratified residuals further showed larger errors at intermediate adulteration levels, without clear instability at either end of the range. Under the current multispectral channel configuration and adulteration-level design, derivative fusion improved the accuracy of continuous adulterant-proportion prediction for *Anoectochilus roxburghii* powder.

Disclosure statement

The author declares no conflict of interest.

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