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Hierarchical Identification of Sulfur-Fumigated Yam Slices Using NIRS with Ensemble Learning and 1D-CNN

Leiming Yuan[1], Yuiman Chan[2], Baojun Xu[3,*], Jun Xu[2,*], Furong Zhu[1,*]

1. Department of Physics, Faculty of Science, Hong Kong Baptist University, Hong Kong, China
2. School of Chinese Medicine, Hong Kong Baptist University, Hong Kong, China
3. Food Science and Technology Program, Department of Life Sciences, Beijing Normal-Hong Kong Baptist University, Zhuhai, China

Corresponding authors: baojunxu@bnbu.edu.cn (B. Xu); davidxujun@hkbu.edu.hk (J. Xu); frzhu@hkbu.edu.hk (F. Zhu)

Highlights

1) Fresh yam slices were sulfur-fumigated and desulfurized to create samples with varying sulfur dioxide residues.
2) Neighborhood component analys and 1D-CNN dimensionality reduction were used to process spectral information.
3) Hierarchical classification was employed for quality-focused categorization of yam slices.
4) Ensemble learning integrated multiple classifiers, significantly improving hierarchical classification performance.
5) The proposed method achieved 96.84% multi-class accuracy, an 8% increase over the baseline of 88.88%.

Background

Yam slices are a key traditional Chinese medicinal material (CMM), but sulfur fumigation, widely used for preservation, induces chemical changes that are invisible to the eye and may endanger health. The Chinese Pharmacopoeia (2025 Edition) limits SO_2 residues (≤150 mg/kg for most herbs, ≤400 mg/kg for yam). Conventional detection methods like acid-base titration are slow and labor-intensive, often requiring more than two hours per sample.

Near-infrared spectroscopy (NIRS) has improved CMM quality evaluation by allowing rapid, non-destructive analysis. However, the multicomponent complexity of CMM makes multi-class classification with NIRS challenging, especially for distinguishing compliant from non-compliant sulfur-fumigated yam slices. To overcome this, a hierarchical classification strategy was introduced, applying a divide-and-conquer approach to break complex tasks into a series of sequential, refined classifications.

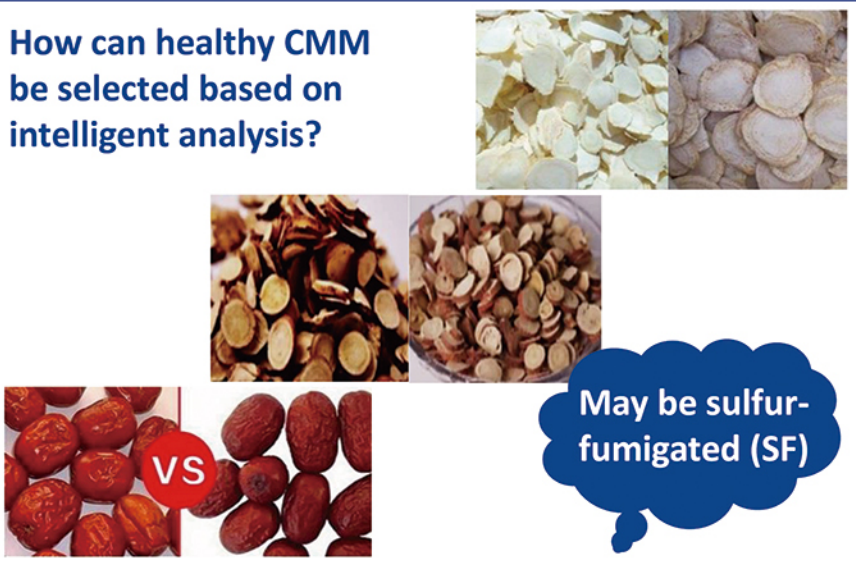

Fig.1 Visual inspection alone cannot reliably distinguish sulfur-fumigated CMMs from non-fumigated ones.

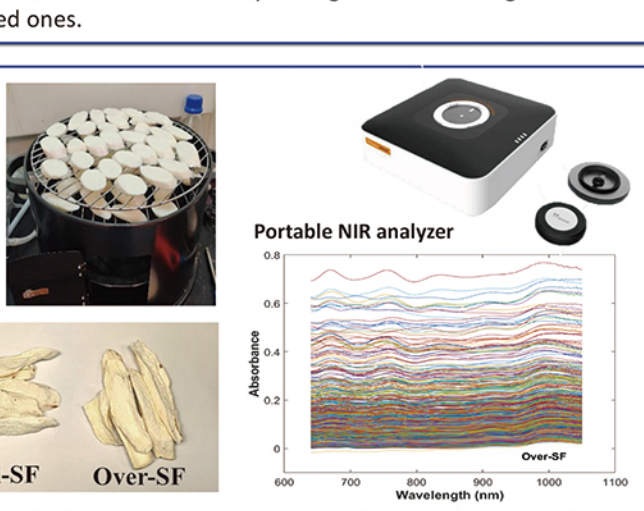

Fig.2 Preparation of sulfur-fumigated yam slices and collection of their spectral data.

Table 1 Classification process for NIR spectral data of sulfur-fumigated yam slices.

Preprocess	Machine learnings	Calibration set F1-score (%)	Prediction set weighted F1-Score (%)
Full spectra	LDA	92.66	88.88
z-score + Full spectra	LDA	93.39	88.52
z-score + NCA spectral selection	LDA	95.4	91.12
	SVM	90.6	91.09
	ANN	89.39	88.98
	KNN	77.78	71.75
	NB	55.53	58.38

Note: NCA: neighborhood component analysis; LDA: linear discriminant analysis; SVM: support vector machine; ANN: artificial neural network; KNN: k-nearest neighbors; NB: naïve bayes;

Results

The results indicate that direct three-class classification yielded suboptimal performance, with a maximum accuracy of 91.12%. LDA achieved the highest accuracy among tested models. Z-score preprocessing improved training accuracy of LDA by 0.7% but did not affect prediction accuracy. Applying NCA for dimensionality reduction further increased training accuracy of LDA to 95.4%, with a slight improvement in prediction accuracy to 91.12%.

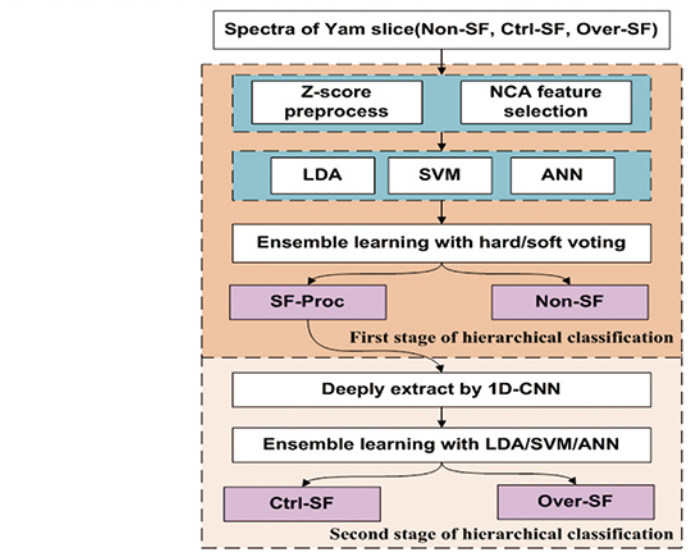

Fig.3 Schematic of the hierarchical classification process for yam slices using NIR spectral data.

Table 2 Binary classification of yam slices in the first stage of HCC.

Labels	Algorithms	Prediction set weighted F1-Score (%)
Non-SF and SF-Proc	LDA	98.94
	SVM	99.06
	ANN	95.9
	KNN	86.64
	Bayes	82.65
	LDA+SVM+ANN	99.65
	Hard voting ensemble	150,2.1,700
	LDA+SVM+ANN	97.84
	Soft voting ensemble	152,0;21,680

Table 3 Binary classification of yam slices in the second stage of HCC.

labels	Algorithms	Prediction set Weight F1-Score
Over-SF and Ctrl-SF	1D-CNN+softmax	97.11
	1D-CNN++LDA	95.14
	1D-CNN++SVM	95.01
	1D-CNN++ANN	97.11
	LDA+SVM+ANN	96.57
	Hard voting Ensemble	[330,2; 22,346]
	LDA+SVM+ANN	96.57
	Soft voting Ensemble	[331,1; 23,345]

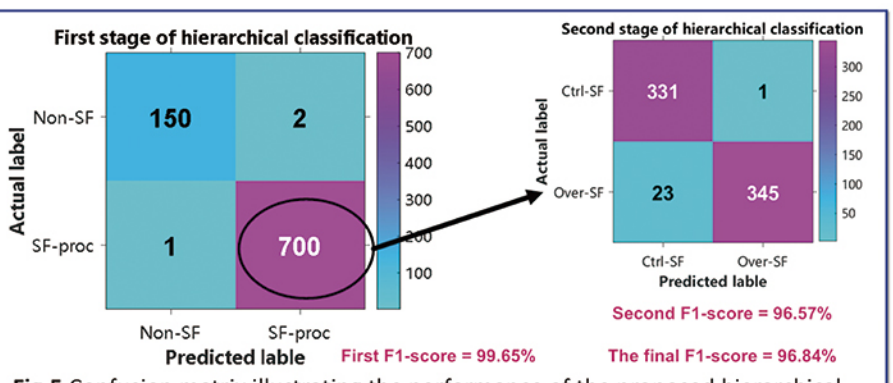

Fig.5 Confusion matrix illustrating the performance of the proposed hierarchical classification model.

Conclusion

A hierarchical chemometric classification (HCC) framework, integrating portable NIRS, NCA variable selection, ensemble learning, and 1D-CNN feature extraction, was developed for non-destructive identification of sulfur-fumigated yam slices. By decomposing the three-class problem into sequential binary classifications, the approach effectively addressed spectral overlaps, achieving 96.84% accuracy, an 8% improvement over conventional multi-class models, with the best SVM model achieving only 88.88%.