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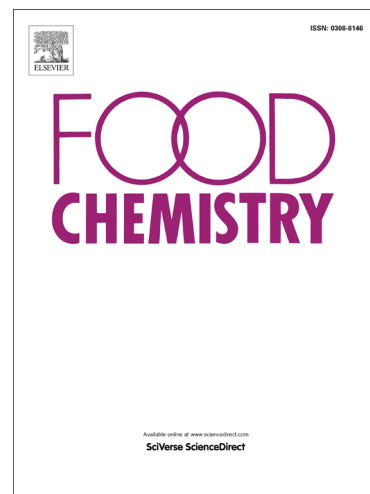
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## Detection of adulterants in grape nectars by attenuated total reflectance Fourier-transform mid-infrared spectroscopy and multivariate classification strategies

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### Abstract

There is no any doubt about the importance of food fraud control, as it has implications in food safety and in consumer health. Focusing on fruit beverages, some types of adulterations have been detected more frequently, such as substitution with less expensive fruits. A methodology based on attenuated total reflectance Fourier-transform mid-infrared spectroscopy (ATR-FTIR) and multivariate classification was applied to detect whether grape nectars were adulterated by substitution with apple juice or cashew juice. A total of 126 samples were obtained and analyzed. Two strategies were proposed: one-class and multiclass approaches. Soft independent modeling of class analogy (SIMCA), partial least squares discriminant analysis (PLS-DA) and partial least squares density modeling (PLS-DM) were used to build the models. Among them, PLS-DA presented the best performance with a sensitivity and specificity of nearly 100%. The multiclass strategy was preferred if the adulterants to be studied are known because it provides additional information.

### Highlights

- The detection of grape nectar adulteration with cashew or apple was studied.
- One-class and multiclass approaches were implemented.
- The multivariate classification methods SIMCA, PLS-DA and PLS-DM were compared.
- PLS-DA provided better performance to detect grape nectar adulterations.

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