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Establishing time stability for multivariate qualitative methods. Case study: Sudan I and IV adulteration in food spices

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ABSTRACT

A multivariate qualitative method using UV-visible spectroscopic data and a PLS-DA chemometric treatment was proposed to identify whether paprika samples were adulterated with Sudan I and Sudan IV dyes, or their mixtures. The method was validated by calculating the main performance parameters (sensitivity and specificity) and determining the stability over time.

Three classes were defined: unadulterated samples (class 1), samples adulterated with Sudan I (class 2) and samples adulterated with Sudan IV (class 3). A total of 81 samples belonging to these classes were analyzed. There was also an additional data set consisting of 54 samples adulterated with a mixture of two dyes at two different concentration levels, which were analyzed and predicted with the established models. In addition, all 135 samples were analyzed at different times over a 6-month period to study the model's stability over time.

In general, the main performance parameters were very satisfactory. As far as training samples is concerned, sensitivity was 100% for the three classes studied. And specificity was 100% for the unadulterated class and for the adulterated with Sudan IV class, and slightly lower (96%) for the adulterated with Sudan I class. Regarding samples from the additional set, excellent specificities were obtained because no samples were assigned to the unadulterated class. In addition, sensitivity was close to 100% for the Sudan IV class and around 75% for the Sudan I class. All the main performance parameters were maintained throughout the 6 months of the study.

Keywords: multivariate classification, PLS-DA, time stability, food adulteration, individual and blends adulterants, Sudan dyes

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