Achieving a robust Vis/NIR model for microbial contamination detection of Persian leek by spectral analysis based on genetic, iPLS algorithms and VIP scores

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Abstract

Microbial contamination of vegetables is always known as a major food safety challenge. Persian leek is one of the most widely used herbs. Detection of *Escherichia coli* (*E. coli* ATCC 8739) in vegetables is very important issue for post-harvest management. Non-destructive assessment of *E. coli* ATCC 8739 contamination of leek as a main aim of this study were investigated using visibe/near-infrared spectroscopy combined with three variable selection approaches and partial least squares discriminant analysis as a promising chemometrics tool: Genetic Algorithm-PLSDA, interval PLS algorithm-DA and variable influence on projection scores-PLSDA. Reflectance spectra in interactance mode were measured on different treatments of *E. coli* ATCC 8739 solution (0.1, 0.2 and 0.3 mL) on leek samples in the spectral range of 350–1100 nm. The spectra (R) were captured at three different positions of sample by random in triplicate. The calibration and internal validation sets were created with 150 (75 %) and 50 (25 %) leek samples, respectively. In order to prevent incorrect results due to over-fitting, the final developed model has been deeply validated with external validation set of 50 samples. Five key features selected by genetic algorithm showed high performance of *E. coli* ATCC 8739 detection with 100 %, 98 % and 0.8 of sensitivity, specificity and classification error, respectively. Besides, a high prediction ability (>95 % correct classification in internal validation set and >89 % in external validation set) were achieved between 490, 500, 570, 740, and 970 nm spectral distances and the presence of *E. coli* ATCC 8739 contamination. In general, The Vis/NIR spectroscopy method for non-destructive detection of *E. coli* ATCC 8739 contamination on Persian leek in food safety application is feasible and practical. We further demonstrate the capability of genetic algorithm to detect the bacterial cells in the samples at the early growth stage.