

Title Application of vapour-phase Fourier transform infrared spectroscopy (FTIR) and statistical feature selection methods for identifying *Salmonella enterica typhimurium* contamination in beef

Author Jayendra K. Amamcharla, Suranjan Panigrahi, Catherine M. Logue, Martin Marchello and Julie S. Sherwood

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Abstract

This paper describes the application of gas-phase Fourier transform infrared (FTIR) spectroscopy for its ability to discriminate between *Salmonella enterica typhimurium* (*Salmonella typhimurium*) contaminated packaged beef samples and uncontaminated samples. A suitable headspace sampling system was used to deliver the headspace volatiles from the packaged meat to the FTIR gas cell. FTIR spectral signatures collected on headspace volatiles of meat packages were used to classify the meat samples based on their *S. typhimurium* populations. The most informative wavenumbers (features) were selected using three univariate and one multivariate feature selection algorithms. The selected wavenumbers were then used to develop the statistical discriminant models and validated using bootstrapping. It was found that sequential forward selection provided the highest estimated classification accuracy of 99% and mean estimated classification accuracy of 95% (validated using linear discriminant analysis and bootstrapping technique). The results support the use of gas phase FTIR to discriminate *S. typhimurium* contaminated beef samples.