Possibility of using NIR and ATR-FT/MIR) spectroscopy for the quantification of major ergot alkaloids in wheat

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Ergot alkaloids (EAs) are mycotoxins produced by fungi species of the Claviceps genus and are frequent contaminants of cereal grains. EAs could be found in cereals even when ergot sclerotia are removed from them by hand-cleaning procedure. However, conventional detection techniques based on wet chemistry usually are expensive and time-consuming and reply on complex extraction and cleanup procedures. Infrared spectroscopy has shown great potential in non-destructive contaminants detection area. This study aims to examine the possibility of using NIR and ATR-FT/MIR spectroscopy as a non-destructive and rapid method for the quantitative determination of six major EAs in wheat. Totally, 107 wheat samples were collected in western Canada and analyzed for the six major EAs by liquid chromatography–tandem mass spectrometry method. Seventy-five wheat samples were contaminated with EAs levels above the limit of quantification (1.25 µg/kg). The mean concentrations of ergocornine, ergocristine, ergocryptine, ergometrine, ergosine, ergotamine and the sum-total EAs in positive wheat samples were 97.48, 743.31, 142.07, 150.59, 56.88, 337.48 and 1099.32 µg/kg, respectively. The NIR (680-2500 nm) and MIR (4000-700 cm^{-1}) spectra of wheat samples were collected and calibrated with EAs reference values using PLS regression technique based on different spectral preprocessing methods and selected wavelength ranges.

In general, the PLS models developed for EAs in wheat samples showed poor cross-validation performance and none of them was capable of predicting external samples. The relatively low concentration of EAs in most of the collected barley samples might be below the detection limit of the two spectroscopy techniques employed. More efforts are required to explore the direct detection limit of the NIR and ATR-FT/MIR techniques for the quantification of mycotoxins in different sample matrix. The development of fast screening methods for mycotoxin detection based on infrared spectroscopy will contribute to the prevention and control of mycotoxins in dairy industry.