Potential of NIR and ATR-FT/MIR spectroscopy for the analysis of mycotoxins in naturally contaminated barley

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Globally, mycotoxins in food and feed are serious threats to the health of human and animals. Ergot alkaloids (EAs) are mycotoxins formed by *Claviceps* fungal species and have been frequently detected in barley as well as other cereals. The purpose of this study was to examine the potential of applying NIR and ATR-FT/MIR spectroscopy for the quantitative determination of six major EAs in naturally contaminated barley samples. Sixty-seven barley samples were collected from Western Canada and analyzed for six major EAs by liquid chromatography–tandem mass spectrometry technique. Forty-nine barley samples were positive for EAs. The mean concentrations of ergocornine, ergocristine, ergocryptine, ergometrine, ergosine, ergotamine and the sum-total EAs in positive barley samples were 120.91, 554.81, 235.64, 411.03, 127.36, 351.18, and 1150.50 μg/kg, respectively. Most of the samples contained low levels of EAs and the ranges of EAs content were very large. 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.

Results showed that most of the constructed models obtained poor calibration and cross-validation parameters and none of the models was able to predict external samples. The relatively low levels of EAs in the contaminated barley samples might be lower than the detection limit of the conventional NIR and ATR-FT/MIR spectroscopy. More efforts are needed to investigate the determination limit of infrared spectroscopic techniques in detecting EAs in feed. EAs can harm the health and productivity of livestock (beef, dairy, swine, sheep, poultry), such as cow lactation performance, growth, reproductive performance, pregnancy rates, etc. The establishment of rapid method based on infrared spectroscopy for screening major mycotoxins in feed ingredients will help the dairy farmers to minimize the mycotoxin hazards.