Near infrared spectroscopy to detect toxic contaminants in cereals

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Introduction

Since decades, near infrared (NIR) spectroscopy is widely used in the food and feed sectors to implement rapidly, inexpensive and efficient control tools for the quality of products. NIR spectra can be considered as fingerprint of a product which can be modified by factors as the presence of undesirable substances. The aim of this work is to demonstrate, through two case studies, the performance of NIR spectroscopy to detect undesirable and toxic contaminants in cereals intended for the food and feed sectors.

Reference method

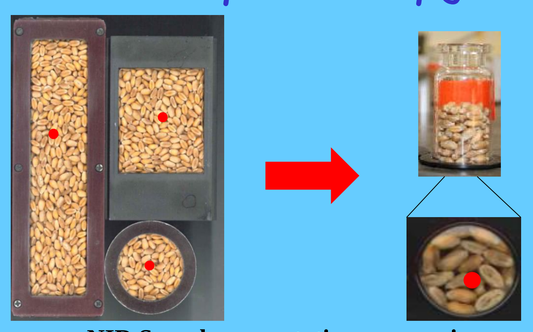
Sorting by visual observation

Confirmation by microscope

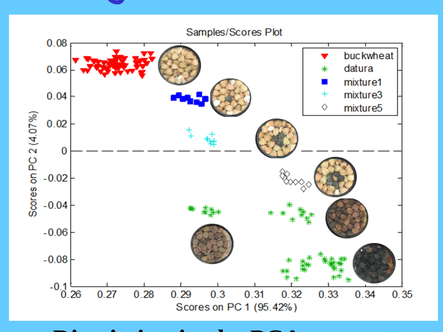
Contaminants in cereals concern, among others, impurities such as straw, grains coming from other botanical origins or insects but also undesirable toxic substances such as sclerotium of ergot (*Claviceps purpurea)* and datura seeds (*Datura stramonium)* known for their high probability of content in alkaloids. The method used in food/feed companies is based on visual observations and on confirmation by optical microscopy.

IAG-Method A4: Method for the determination of ergot (claviceps purpurea) in animal feedingstuff
Commission Regulation EU n° 742/201, EN 15587

NIR spectroscopy at laboratory level



NIR Sample presentation accessories for quantitative and qualitative analysis



Discrimination by PCA on spectra between Datura seeds and buckwheat kernels

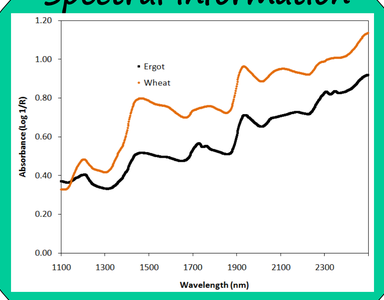
With the recent high throughput sample presentation accessories, classical NIR spectrometers allow analysing a large number of small fractions per unit of time. Moreover, chemometric tools such as Principal Component Analysis (PCA), applied to the NIR spectra allow discriminating between pure Datura seeds, buckwheat kernels and mixture of both.

Vermeulen P. , Fernández Pierna J.A. , Dardenne P. & Baeten V. (2013). Detection of datura seeds containing alkaloids in buckwheat production by NIRS and NIR hyperspectral imaging. Poster in: 16th ICNIRS, 3-7 June 2013, Montpellier - France

Light Microscopy

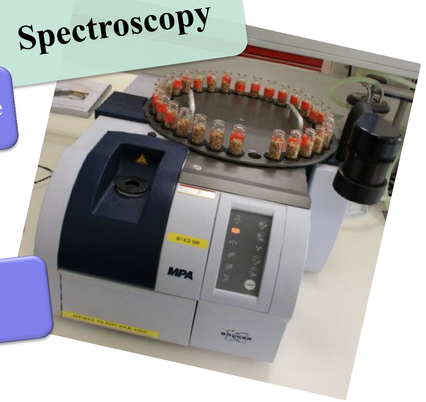
- High skilled personal
- Size sample 250g
- Morphological markers distroyed in silage

Spectral information



NIR Spectroscopy

- Non Destructive
- 1 spectrum/ subsample
- Screening method
- Rapid method



From the visual observation ...

to the NIR Spectroscopy ...

and NIR hyperspectral imaging system

A screening method for detection of contaminants in cereals

At the lab level ...

- On-line analysis
- Thousands spectra/ subsample
- Spatial information
- Large samples analysis
- Detection of multiple contaminants

NIR Hyperspectral Imaging

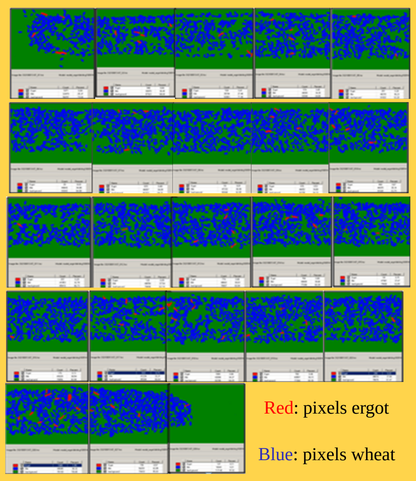
up to the field level

- In field analysis
- Early detection
- Precision farming

http://www.lethist.lautre.net

Ground-based systems

NIR hyperspectral imaging in lab.



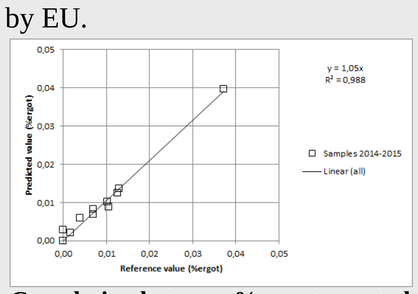
Ergot quantification in cereals

NIR hyperspectral imaging system (NIR-HIS) combines spectral and spatial dimension information and allows to acquire several thousand spectra per sample. NIR-HIS and chemometric tools, together with image analysis can be used as control method to assess the presence and the quantity of contaminants such as ergot bodies in cereals. Using such technology, up to 50 kg of cereals can be analysed in 1 hour with a limit of ergot detection far below the limit of 500 mg/kg fixed by the European Commission for food. This methodology allows multi contaminants detection and can be easily integrated in an automatic cereal control scheme.

Vermeulen P. , Fernández Pierna J.A. , van Egmond H.P. , Zegers J. , Dardenne P. & Baeten V. (2013). Validation and transferability study of a method based on near-infrared hyperspectral imaging for the detection and quantification of ergot bodies in cereals. *Analytical and Bioanalytical Chemistry,* 405: (24), 7765-7772

Control lab. samples

A correlation of 0.99 was obtained between the % of ergot determined by reference method and NIR-HIS analyses of 16 samples from control laboratory collected during one year period (2014-2015). The figure shows that all the cereal samples contained a level of ergot lower than the 0.05 % limit fixed by EU.

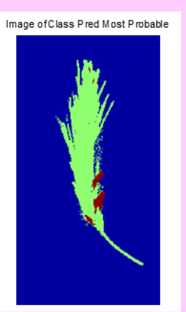


Correlation between % ergot counted visually and predicted by NIR-HIS

Follow up in the field

For crop management on field scale, ground based systems are advantageous against satellite and airborne. The information provided by the sensor installed on i.e. the tractor could be applied on-line for precision disease control independently of the weather conditions (clouds) and with the spatial resolution required. Together with the reduction of weight, size and price, the implementation of these sensors on platforms such as tractors could play an important role in the framework of the implementation of precision agriculture.

Sclerotia of ergot on rye in field at CRA-W



Discrimination by NIR and chemometrics between healthy and infected rye head

Conclusions

NIR instrument combined with adequate sample presentation accessories or with hyperspectral imaging system could be the perfect tools for the detection and quantification of contaminants in cereals. It allows scanning rapidly a large number of small sample fractions and analysing a representative portion of the sample in order to lower the limit of the detection and to match the official control requirement. This approach could be used as a control tool at the reception of grains, at the entrance of the factory or in a near future at the field level for an early detection.

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