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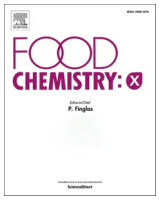

Rapid screening of fumonisins in maize using near-infrared spectroscopy (NIRS) and machine learning algorithms

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ABSTRACT

Fumonisins occurrence in maize represents a significant global challenge, impacting economic stability and food safety. This study evaluates the potential of near-infrared (NIR) spectroscopy combined with chemometric algorithms to detect fumonisins in maize. For fumonisin B1 (FB1) and B2 (FB2) levels were developed predictive NIR models using partial least squares (PLS) and artificial neural networks (ANN). PLS models demonstrated strong correlation coefficient (R^2) values of 0.90 (FB1), 0.98 (FB2), and 0.91 (FB1 + FB2) for calibration, with ratio of prediction to deviation (RPD) values ranging 2.8–3.6. Similarly, ANN models showed good predictive performance, particularly for FB1 + FB2, with $R = 0.99$, and the root means square error (RMSE) of 131 μg/kg for calibration; and $R = 0.95$, RMSE = 656 μg/kg for validation.

These findings underscore the efficacy of NIR spectroscopy as a rapid, non-destructive tool for fumonisin screening in maize, with chemometric algorithms enhancing model accuracy, offering a valuable method for ensuring food safety.

1. Introduction

Maize (*Zea mays* L.) is a globally significant cereal crop, but its high susceptibility to fungal infections—caused by *Penicillium* spp., *Fusarium* spp., *Aspergillus* spp., and *Alternaria* spp.—throughout growth, harvest, storage, and processing stages being significant challenges (Nada et al., 2022; Price et al., 2024). These infections often lead to the production of mycotoxins, secondary metabolites that are harmful to human and animal health (Shi et al., 2023). Among the most prevalent mycotoxins in maize are aflatoxins (AFB1, AFB2, AFG1, and AFG2), fumonisins (FB1, FB2, and FB3), zearalenone (ZEN), deoxynivalenol (DON), T-2 toxin (T-2 and HT-2), and ochratoxins (OTA) (Udomkun et al., 2017).

The Food and Agriculture Organization (FAO) estimates that 25 % of the global food supply is contaminated with mycotoxins (Guan et al., 2022), with cereals accounting for over 10 % of global aflatoxin exposure (Eskola et al., 2020). Aflatoxins, produced primarily by *Aspergillus flavus* and *A. parasiticus*, are highly toxic and carcinogenic and AFB1 is the most prevalent aflatoxin in maize crops (Udomkun et al., 2017). In a study of maize samples from Tanzania, aflatoxins were detected in 69 % of the 52 maize samples analyzed, with 33 % of these samples exceeding the permitted limit (> 10 μg/kg). The mean concentrations of aflatoxins in the maize samples ranged from 1.6 to 86.6 μg/kg (Kibwana et al., 2023). Fumonisins, with maize contamination rates reported to approach nearly 70–80 % in some studies (Li et al., 2024) are primarily produced by *Fusarium verticillioides* and *F. proliferatum*, with FB1 being the predominant toxin, accounting for up to 70 % of the total fumonisin contamination in maize flour (Damiani et al., 2019). Between 2012 and 2019, approximately 20 % of the 98 maize samples tested in Spain

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exhibited FB1 + FB2 levels exceeding the permitted limit (> 4000 μg/kg) (Tarazona et al., 2020). In Brazil, 12 % of the 148 samples showed FB1 + FB2 concentrations above the limit (> 5000 μg/kg) (Oliveira et al., 2015), while in South Korea, the occurrence of FB1 + FB2 was below the established limits (Woo et al., 2024). DON, a trichothecene mycotoxin produced by *Fusarium graminearum* and *F. culmorum* (Kos et al., 2017), contaminates 10–86 % of maize, often co-occurring with derivatives such as DON-3-glucoside (Nathanail et al., 2015), varying 13.43–123.15 μg/kg in maize (Woo et al., 2024). T-2 toxin is primarily produced by *Fusarium tricinctum*, *Fusarium sporotrichioides*, and *Fusarium poae*. It is widely detected in 28 % of maize samples, with concentrations ranging from 0.51 to 56.61 μg/kg (Guo et al., 2024). ZEN and OTA, produced by *Fusarium* and *Aspergillus* species respectively, are also frequently detected, with contamination rates of 50 % and 60 % reported in maize (Mazaheri, 2023). In Kenya, 18 % of the 480 maize samples tested between 2018 and 2020 displayed ZEN levels exceeding 1000 μg/kg (Kagot et al., 2022). The mean levels of OTA in maize samples ranged from not detected (nd) to 318 μg/kg (Kos et al., 2020).

Detecting mycotoxins across various stages of the maize supply chain is essential for ensuring food safety, reducing economic losses, and mitigating public health risks (Nada et al., 2022). Therefore, there is an urgent requirement for fast, non-destructive and accurate methods for detection and quantification of mycotoxins occurrence in maize grains (Camardo Leggieri, Mazzoni, Fodil, et al., 2021).

Conventional analytical techniques such as high-performance liquid chromatography (HPLC) (Hoppe et al., 2024), high-performance liquid chromatography–tandem mass spectrometry (HPLC-MS/MS) (Guan et al., 2022), ultra-high-performance liquid chromatography-tandem mass spectrometry (UHPLC−MS/MS) (Guo et al., 2024), ultra-high-performance liquid chromatography-tandem time-of-flight mass spectrometry (UHPLC−ToF-MS) (Silva et al., 2019), enzyme-linked immunosorbent assay (ELISA) (Tong et al., 2021) and immunoassays (Freitas et al., 2019) offer high sensitivity and accuracy but are expensive, time-consuming, and require skilled operators and complex sample preparation.

Recent advancements in non-destructive methods have shown promise for faster, cost-effective detection of mycotoxins (Zhao et al., 2024). Techniques such as hyperspectral imaging (Kim et al., 2023), aptamer sensors (Nirala et al., 2025; Y. Wang et al., 2025), immunoassays based on inner filter (Hu Jiang et al., 2023), immunochromatography assay (Chen et al., 2023), and artificial olfactory sensors (Qu et al., 2024) provide innovative alternatives. Among these, near-infrared (NIR) spectroscopy stands out for its rapid, non-destructive nature, eco-friendly, and reagent-free analysis of chemical properties (Chavez et al., 2022; Shen et al., 2022). NIR operates in the 12,000–4000 cm^{-1} range, utilizing the absorption of specific wavelengths by chemical bonds (e.g., C—H, O—H, N—H) to reveal the molecular composition of samples (Shen et al., 2022) and this technique has been evaluated for its potential in detecting mycotoxins (Bailly et al., 2024). The complexity of NIR spectra, resulting from overlapping peaks, necessitates the use of advanced chemometric tools to extract meaningful data.

Partial least squares (PLS), a widely used linear regression method, has been applied for detecting aflatoxins (Bailly et al., 2024), ZEA (Tyska et al., 2021), fumonisins (Shen et al., 2022) and DON (Smeesters et al., 2016) in maize. In two studies, PLS algorithm was applied for development of predictive models for FB1 + FB2 quantification in maize, with R^2 ranging 0.80–0.90 and RPD 3.0–3.3 (Shen et al., 2022). Artificial neural networks (ANNs), which excel at modelling complex nonlinear relationships, are increasingly recognized as a powerful tool for predictive modelling of mycotoxin contamination (Acquarelli et al., 2017). Although ANN has been considered highly effective for extracting insights from nonlinear and imprecise data, its application in developing predictive models for mycotoxin occurrence in maize remains limited.

This study aims to evaluate the application of NIR spectroscopy as a rapid, non-destructive method for detecting and quantifying individual fumonisin B1, fumonisin B2, and their sum (B1 + B2). By developing multivariate models using both PLS and ANN algorithms for the first time, this research seeks to enhance the efficiency and accuracy of fumonisin detection, contributing to improved food safety monitoring within maize supply chains.

2. Material and methods

2.1. Sampling

One hundred and fifty maize samples were collected from various farms in the Tagus Valley region between 2018 and 2020 to monitor mycotoxin levels. The entire maize field was harvested at maturity (17–19 % moisture), and sampling was carried out directly in the field from the harvester tank using a vertical segmented probe with seven chambers. This method allowed maize to be collected from different depths, ensuring a representative sample. Approximately 3 kg of maize was harvested from each field variety, and 1 kg was fully milled to guarantee homogeneity. All maize grains were dried until 11–13 % of moisture content in an oven (Memmert UFB 400, Germany). The grinding of each sample was standardized and performed in a Retsch rotor mill (SK300), with a particle size of approximately 1.00 mm in diameter. Each maize flour sample was stored in polypropylene bag at −20 °C until fumonisins extraction.

2.2. Mycotoxin analysis

2.2.1. Extraction

The extraction's maize sample were done as described by Silva et al. (2019), using 80 % (*v*/v) acetonitrile for 1 h at 110 rpm on an orbital shaker (Uetze/Hänigsen, Germany). After two centrifugations at 3000 rpm for 10 min, the supernatants were combined. The supernatant was diluted with ultra-pure water (1,1 ratio) and then filtered.

2.2.2. Detection and quantification

Ultra-High Performance Liquid Chromatography combined with Time-of-Flight Mass Spectrometry (UHPLC-ToF-MS) (Shimadzu, Japan) equipped with an electrospray ion source, in positive ionization mode (ESI+) was used to perform the fumonisins analysis. The method and gradient program used was described and validated previously by the authors Silva et al., 2019, with a mobile phase of formic acid and acetonitrile. The flow rate of 0.5 mL/min, and a Zorbax Eclipse Plus C18 column. Fumonisins showed a limit of detection (LOD) 62.5 μg/kg and the limit of quantification (LOQ) of 125 μg/kg, respectively.

2.3. Near infrared spectroscopy

Near infrared spectra (NIR) of maize flours were collected using a transflection MPA apparatus (Bruker Optics, Ettlingen Germany), trough the diffuse reflectance integrating sphere. Approximately 5 g of maize flour was placed into the specific NIR container and compacted to achieve a consistent packing density, after which the spectrum was measured. NIR spectra of samples were recorded within the range of 12,000–4000 cm^{-1}, using a spectral resolution of 16 cm^{-1} and averaging 16 scans. The wavenumber range was divided into 1154 data points, with each interval corresponding to 6.93 cm^{-1}.

2.4. Multivariate analysis

2.4.1. Partial least squares

The preprocessed spectra were correlated with analytical values to develop calibration models for fumonisin B1 (FB1), fumonisin B2 (FB2), and their sum (FB1 + FB2) in maize using partial least squares (PLS) regression. The PLS method, based on latent variables (LVs) (Wold et al., 2001), reduces the original spectral data into a smaller set of factors through linear combinations, which are then used in regression analysis to generate a predictive equation. To improve model accuracy, various

techniques were applied to eliminate irrelevant spectral variables, ensuring that only the most relevant contribute to the calibration process. This multivariate calibration approach establishes a predictive model linking spectral features (wavenumbers) to target properties (parameter values). However, spectral noise and other interfering factors can negatively impact the model, leading to calibration and prediction errors (Wold et al., 2001).

A total of 150 samples were divided into calibration (75 %) and validation (25 %) datasets to develop and assess the models. The performance of the final PLS calibration and validation models was evaluated using the root mean square error of calibration (RMSEC), root mean square error of prediction (RMSEP), and the correlation coefficient (R). The optimal combination of spectral regions and second-derivative preprocessing was selected based on the model with the lowest RMSEC and RMSEP, the highest R, and the minimal number of latent variables (LVs) while still capturing sufficient data variance. The predictive ability of the model was further assessed using the ratio of prediction to deviation (RPD), where RPD $\geq$ 2.5 indicates suitability for quantitative prediction, and RPD $\geq$ 3 signifies excellent predictive accuracy (Hui Jiang et al., 2021).

2.4.2. Artificial neural network (ANN)

The input, hidden, and output layers are components of the ANN. The factors assessed are represented by the number of nodes in the input layer, whereas the classes are associated with the number of neurons in the output layer. Each neuron in the hidden and output layer was linked to every node in the layer above it via a corresponding numerical weight. Initial information is received by the input layer, processed by the hidden layer, and connected to the model's outcomes by the output layer (Inglis et al., 2024).

Multilayer perceptron (MLP) is a neural network architecture used for regression models, namely for backpropagation learning algorithms, being usually used for prediction and classification. A hyperbolic tangent sigmoid transfer function was used at the input layer and the hidden layer, and a pure line transfer function was used at the output layer. A total of 61 spectra out of 133 spectra were used for training, and the rest were equally divided for validation and testing (20 spectra). Multilayer feed-forward has been trained with the Broyden-Fletcher-Goldfarb-Shanno (BFGS) learning algorithm (200 epoch). The number of neurons in the hidden layer was optimized in an early stop learning procedure. The best topology of the ANNs was searched using the training, validation, and testing data sets. According to the correlation coefficient determination (R^2) and root mean square error (RMSE) values, the best ANNs models were developed.

For backpropagation algorithm implementation, the hyperbolic tangent function was used (tansig). During the ANN development, the Levenberg-Marquardt algorithm, derived from Newton's method, was designed for minimizing functions that are sums of nonlinear functions. The Broyden-Fletcher-Goldfarb-Shann (BFGS) algorithm, usually used for nonlinear least squares, creates a training multilayer perceptron algorithm (BFGS/AG).

2.5. Statistical analysis

The fumonisins levels were measured in triplicate, for processing of results was using the PeakView™ and MultiQuant™ (SCIEX, Foster City, CA, USA) software. The PLS and ANN models were developed and evaluated using MATLAB® software (R2023a) (MathWorks, Inc., Massachusetts, USA).

3. Results and discussion

3.1. Mycotoxins occurrence in maize samples

The levels of fumonisins detected in 150 maize samples are summarized in Table 1. Only fumonisins (B1 and B2) contamination were observed in tested maize samples, inducing the development of predictive models only for fumonisins.

Table 1
Descriptive statistics of fumonisins levels in maize samples.

	Mean	Min.	Max.	SD
FB1 (μg/kg)	899	62.5	4000	996
FB2 (μg/kg)	426	62.5	2861	598
FB1 + FB2 (μg/kg)	1275	62.5	5915	1198

SD- standard deviation

FB1 levels ranged from 62.5 μg/kg to 4000 μg/kg, with a mean value of 899 μg/kg. FB2 concentrations varied between 62.5 μg/kg levels and 2861 μg/kg, with a mean of 426 μg/kg. In comparison, lower levels of FB1 (75.8–499.6 μg/kg) and FB2 (14.2–98.1 μg/kg) were reported in maize collected in South Korea (Woo et al., 2024). Higher levels were found in Spain, with FB1 ranging from nd to 5903 μg/kg and FB2 from nd to 740.1 μg/kg (García-Díaz et al., 2020). Similar mean values were observed for FB1 (765 μg/kg) and FB2 (562 μg/kg) at harvest in Nigeria (Liverpool-Tasie et al., 2019), while in Serbia, FB1 levels ranged from 192 to 4253 μg/kg and FB2 from 72 to 3118 μg/kg in 2015 (Kos et al., 2020). The combined FB1 + FB2 levels averaged 1275 μg/kg, with a maximum of 5915 μg/kg, which is lower than the levels found in maize harvested from various regions of Brazil, where FB1 + FB2 ranged from 62.4 to 10,080 μg/kg, with a mean of 2204 μg/kg (Oliveira et al., 2017). These variations in mycotoxin levels have been linked to factors such as climate conditions, agronomic practices, fungal activity, crop variety selection, and genetic factors. Approximately 5 % of our tested samples exceeded the European Union maximum tolerable limit for FB1 + B2 (< 4000 μg/kg), while about 10 % of the samples showed fumonisin levels at the limit of detection (62.5 μg/kg).

3.2. Spectral analysis of maize samples

Representative NIR spectra from fumonisin-contaminated and non-contaminated maize samples are shown in Fig. 1. The full raw NIR spectra (12,000–4000 cm^{-1}) are displayed in Fig. 1a, while a selected region (4100–8600 cm^{-1}) highlighting key spectral differences is shown in Fig. 1b.

The spectral differences likely reflect compositional and property variations due to fungal presence, metabolic activities, and associated changes in maize (Bailly et al., 2024). Fungal infestation in maize grains leads to a reduction in essential nutrients such as proteins, fats, and vitamins, resulting in spectral modifications, which can be detected by NIR using mathematical techniques to enhance relevant information. As a result of the investigation, the most significant spectral ranges for fumonisins are between 4000 and 8000 cm^{-1} (Tyska et al., 2021). Major absorption peaks were observed at 8333 cm^{-1}, 6803 cm^{-1}, and 5263 cm^{-1}, corresponding to the combination and overtone vibrations of C—H, O—H, and N—H bonds, which indicate maize chemical composition. The spectral bands around 10,000 cm^{-1} are linked to the second overtone of O—H stretching, primarily associated with starch (Tao et al., 2019).

The absorbance peaks at 6803 cm^{-1} are attributed to the first overtone of O—H stretching in carbohydrates and N—H stretching in proteins in maize (Liu, Deng, et al., 2022). Peaks near 8333 cm^{-1} correspond to the overtone of C groups or the second overtone of C—H stretching in C—H groups, associated with fatty acids, fats, and chitin—an essential component of fungal cell walls (Shen et al., 2022). Additionally, the feature at 6803 cm^{-1} represents the first overtone of O—H functional groups, along with C—H stretching and deformation. These functional groups are present in various biologically significant molecules, such as carbohydrates and proteins, and are associated with mycotoxins (Liu, He, et al., 2022). The absorption peak at 5263 cm^{-1} arises from O—H combinational vibrations, which are traditionally used to assess moisture content in biological samples. This peak also carries

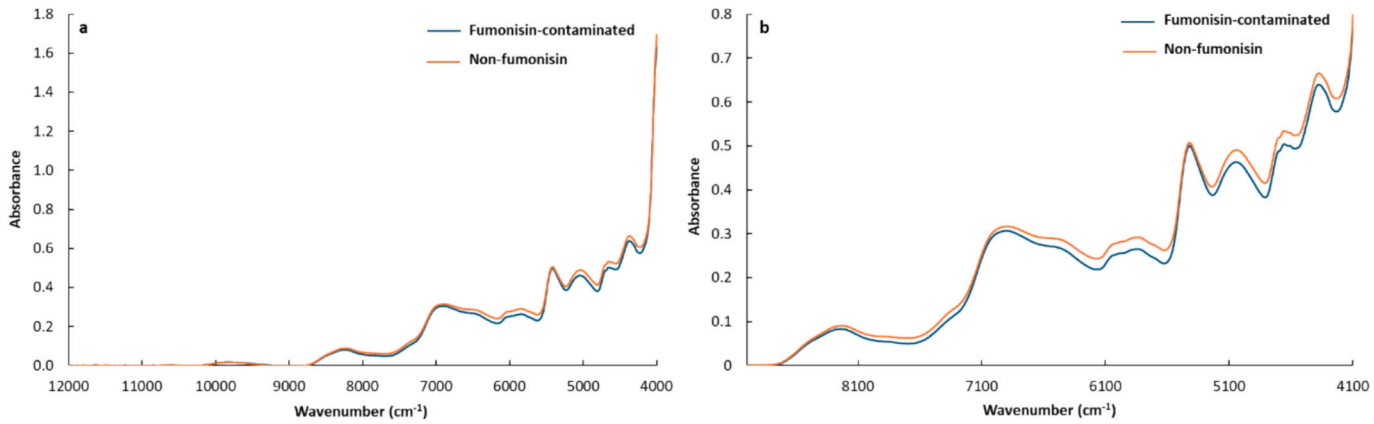

Fig. 1. NIR spectra from fumonisin-contaminated and non-contaminated maize samples: (a) full spectral interval (4000–12,000 cm^{-1}) and (b) selected spectral interval (4100–8600 cm^{-1}).

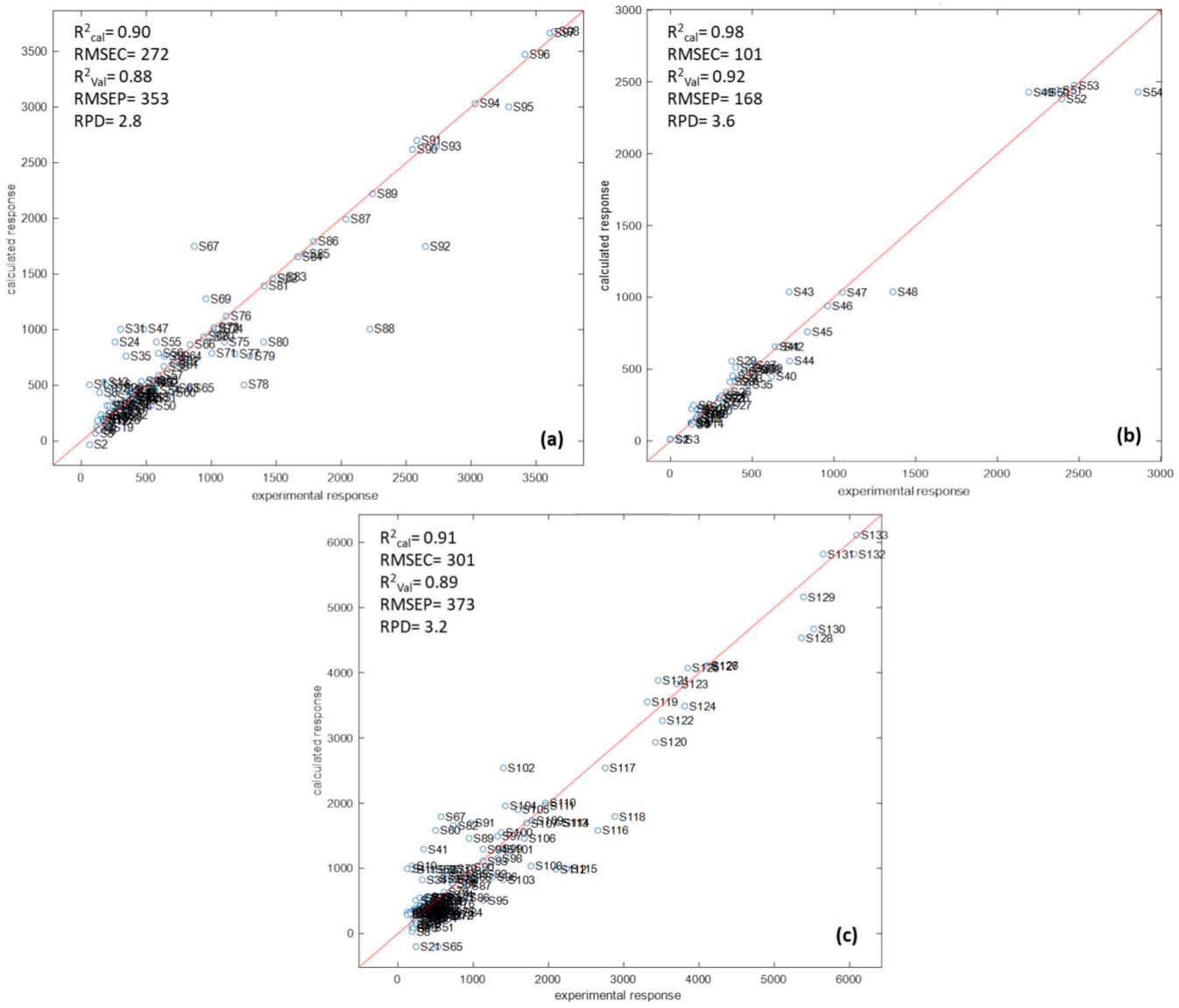

Fig. 2. Predictive PLS model parameters and linear regression plots for the calibration data set using second derivative pre-processed treatment, for: (a) FB1, (b) FB2, and (c) FB1 + FB2 concentrations in maize samples.

N—H combinational vibrations linked to polysaccharides and proteins (Shen et al., 2022).

Absorbance intensity was lower in fumonisin-contaminated samples compared to non-contaminated samples (Fig. 1), emphasizing the potential of raw NIR spectral data for detecting contamination. Similar phenomena have been reported for FB1 + FB2 contamination in maize (Borràs-Vallverdú et al., 2024; Shen et al., 2022) and DON contamination in wheat (Zhang et al., 2021), where fungal activity was shown to alter carbohydrate and protein levels, leading to physical grain deterioration. This deterioration likely increased grain porosity, resulting in light scattering effects and reducing the absorption of NIR radiation (Tao et al., 2019).

Physical and chemical changes in samples became increasingly significant due to.

fungal infection, and thus the spectra exhibited certain regular changes in response.

3.3. Partial least square (PLS) models

The parameters of the developed PLS models and linear regression plots for predicted versus measured FB1, FB2, and FB1 + FB2 concentrations are shown in Fig. 2.

The optimal PLS models for FB1, FB2, and FB1 + FB2 used 10 principal components (PCs) and 2nd derivative preprocessing. These models exhibited strong predictive performance with R^2 values of 0.90 (calibration) and 0.88 (validation) for FB1, and RMSEC and RMSEP values of 272 μg/kg and 403 μg/kg, respectively. FB2 models showed higher accuracy with R^2 values of 0.98 for both calibration and validation, and SEC and SEP values of 101 μg/kg and 336 μg/kg, respectively. FB1 + FB2 models achieved R^2 values of 0.91 (calibration) and 0.89 (validation), with RMSEC and RMSEP values of 260 μg/kg and 373 μg/kg, respectively.

RPD values ranged from 2.8 to 3.6, with determination coefficients exceeding 0.88, indicating strong predictive ability for fumonisins (Hui Jiang et al., 2021). Previous studies reported by cross-validation R^2cal = 0.99, RMSEC = 588 μg/kg and RPD = 2.0 for FB1; while for FB2 R^2cal = 0.98, RMSEC = 258 μg/kg and RPD = 2.0 for FB2 (Tyska et al., 2021). Borràs-Vallverdú et al. (2024) presented R^2 = 0.76, RMSEC = 3.7 mg/kg and RPD = 2.0 for FB1, and R^2 = 0.81, RMSEC = 2.1 mg/kg and RPD = 2.3 for FB2, using near-infrared hyperspectral imaging (NIR-HSI). For FB1 + FB2 in maize, similar model parameters were reported with R^2 = 0.98, RMSEP = 659 μg/kg and RPD = 3.3 (Tyska et al., 2021). In another study, Shen et al. (2022) observed lower values, with R^2 = 0.78 and RMSEC = 20.15 mg/kg during calibration, and R^2 = 0.80, RMSEP = 18.77 mg/kg, and RPD = 3.0 in validation. This model utilized MSC (multiplicative scatter correction), first Savitzky-Golay (SG) derivative preprocessing, and 11 PCs.

A screening model for contaminated maize developed by Giacomo and Stefania (2013) achieved high calibration accuracy (R^2cal = 0.99, R^2val = 0.91, RMSEC = 0.144 mg/kg, and RMSEP = 0.893 mg/kg). However, overfitting was evident due to the use of 21 PCs. Additionally, Ghilardelli et al. (2022) developed a NIR calibration model using random forest classification for the sum of fumonisin concentrations, achieving an accuracy of 88.3 % and an average precision of 92.4 %.

Table 2
Calibration, validation, and testing artificial neural networks (ANN) models parameters for FB1, FB2, and FB1 + FB2 levels.

		Calibration		Validation		Testing	
	LVs	Rcal	RMSE	Rval	RMSE	Rtest	RMSE
FB1	12	0.98	200	0.71	794	0.91	457
FB2	12	0.99	109	0.87	344	0.93	271
FB1 + FB2	12	0.99	131	0.95	656	0.91	128

LVs- Latent variables; RMSE- Root mean square error.

3.4. Artificial neural network (ANN) models

Statistical parameters for calibration, validation, and testing ANN models predicting FB1, FB2, and FB1 + FB2 concentrations in maize are summarized in Table 2.

The ANN model for FB1 achieved correlation coefficients of 0.98, 0.71, and 0.91 for calibration, validation, and testing datasets, respectively. For FB2, the corresponding coefficients were 0.99, 0.87, and 0.93. The combined FB1 + FB2 model yielded coefficients of 0.99, 0.95, and 0.91. RMSE values ranged from 200 to 794 μg/kg for FB1, 109–344 μg/kg for FB2, and 131–656 μg/kg for FB1 + FB2. The ANN predictive models for FB1, FB2, and FB1 + FB2 demonstrated strong calibration performance, though their validation results were slightly weaker (Table 2), suggesting the calibration overfitting and challenges in adapting the new data for model. This may be due to sample variability or small spectral differences not fully accounted for during calibration. Additionally, the limited size of the calibration set may constrain ANN effectiveness, as these models typically perform best with more than five hundred samples (Bailly et al., 2024).

Comparable results have been reported for AFB1 with R ranging 0.90–0.99 and RMSE of 1.35–6.62 μg/kg for predictive model (B. Wang et al., 2022; Liu, He et al., 2022) and for ZEN (R = 0.95 and RMSE = 3.66 μg/kg) in predictive dataset (Liu, Deng et al., 2022). However, no prior studies applied ANN models specifically to NIR-based fumonisin detection. Good predictive performance was achieved for aflatoxins content in maize using Standard Normal Variate + First derivative (SNV + D1) preprocessing with Rcal = 0.99, RMSE = 0.91 μg/kg, and Rtest = 0.74, RMSE = 4.9 μg/kg as reported by (Bailly et al. (2024).

Consistent with findings from other studies (Bailly et al., 2024) artificial neural network (ANN) models outperformed PLS models, particularly for detecting FB1 + FB2, underscoring their potential in handling complex data modelling. Additionally, ANN predictive models employing machine learning approaches for fumonisin contamination in harvested maize achieved accuracy levels exceeding 75 % (Camardo Leggieri, Mazzoni, & Battilani, 2021).

Our results indicate that the best calibration and validation models for predicting FB1 + FB2 occurrence in maize samples were achieved using the ANN method, may be due their capability to capture model complex and non-linear relationships (Bailly et al., 2024). However, for individual FB1 and FB2, the PLS algorithm demonstrated slightly better performance in calibration and validation. These findings highlight the importance of developing predictive models that leverage both PLS and ANN features to fully explore the potential of NIR spectroscopy for fumonisin prediction in maize samples.

The Fig. 3 illustrates the distribution of 60 representative maize samples used to construct the ANN models, categorized by three levels of FB1 + FB2 concentrations: 30 % of the samples fall within the range of 125–300 μg/kg, 40 % within 300–3500 μg/kg, and 30 % exceed 3500 μg/kg, with the goal to evaluate the performance of NIR for fumonisin screening.

The quantitative analytical model for FB1 + FB2 concentration was constructed using 10 latent variables and second derivative preprocessed data. The results indicate that artificial neural networks (ANN) are an ideal algorithm for modelling complex matrices, as they can identify and interpret associations while generating generalized outcomes from specific data models (Sampaio et al., 2023). This nonlinear modelling approach proved effective for quantifying FB1 + FB2 contamination intervals, achieving correlation coefficients of 0.99, 0.79 and 0.86, for calibration, validation, and testing, respectively. The categorized ANN model exhibited exceptional calibration performance, demonstrating its ability to capture nearly all of the variance within the training data. While performance on the test set remained strong, it was slightly lower than on the training set, as predicted (Bailly et al., 2024). This suggests that the model is relatively robust but could still be improved through additional data or methods aimed at improving generalization. In literature was found a study, that ANN model

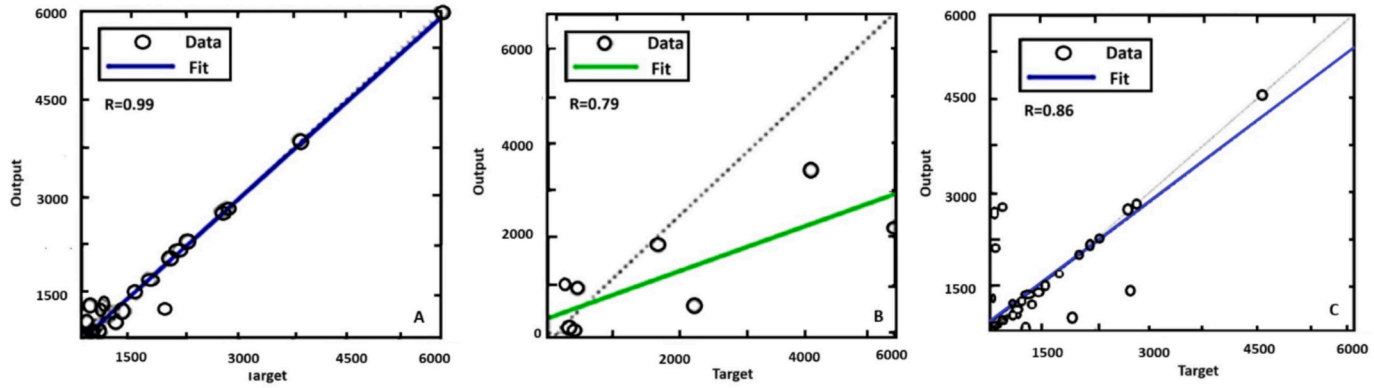

Fig. 3. ANN models for categorized by three levels of FB1 + FB2 (30 % of the samples fall within the range of 125–300 μg/kg, 40 % within 300–3500 μg/kg, and 30 % exceed 3500 μg/kg): (A) calibration, (B) testing, and (C) validation datasets.

demonstrated the efficiency of an electronic nose (e-nose) in distinguishing contaminated maize samples at levels above or below the legal limits, reaching an accuracy of 77 % for aflatoxin B1 and 78 % for fumonisins (Camardo Leggieri, Mazzoni, Fodil, et al., 2021). Another study demonstrated that neural network models, integrating multiple data sources— daily weather conditions, satellite imagery and soil data, achieved high class-specific accuracy in predicting mycotoxin levels over a one-year period. The results highlighted this dynamic geospatial models' effectiveness in monitoring annual mycotoxin levels in maize, with predictive validations of 73 % for aflatoxin and 85 % for fumonisin. The authors also categorized two levels groups (high and low) for aflatoxins (high >20 μg/kg; low ≤20 μg/kg) and fumonisins (high >5000 μg/kg; low ≤5000 μg/kg), obtained for aflatoxins the testing data set of 0.98 and for fumonisins was 0.96, developed by ANN approach, showing for high contamination level of aflatoxins and fumonisins a balanced accuracy of 73 % and 85 %, respectively (Castano-Duque et al., 2023). These findings underscore the efficacy of ANN models in enhancing the predictive accuracy of NIR spectroscopy for fumonisin detection in maize.

4. Conclusion

This study evaluated the performance of NIR spectroscopy as a rapid and efficient methodology for detecting fumonisin occurrence in maize samples using PLS and ANN algorithms. For the first time, two distinct statistical approaches were applied to assess NIR performance for FB1 and FB2 detection in maize.

The results emphasise the potential of raw NIR spectra to distinguish similarities and differences between fumonisin-contaminated and uncontaminated samples, as reflected in the positions and intensities of the characteristic spectral peaks. The coefficients of determination for fumonisin content calibration ranged from 0.90 to 0.98, and for validation, from 0.71 to 0.95, using both PLS and ANN methods. Predictive models demonstrated high performance, with the PLS method being more effective for FB2 detection, while the ANN approach was proficient in modelling combined FB1 + FB2 concentrations.

These findings suggest that NIR spectroscopy, combined with PLS and ANN algorithms, is a fast and reliable tool for assessing fumonisin levels in maize samples. However, further studies are necessary to enhance model accuracy and enable its direct application in harvested maize. To improve food safety, predictive NIR models could be instrumental in restricting the processing of contaminated samples and facilitating the early identification of cereal lots exceeding European legal limits for fumonisin levels (>4000 μg/kg) within the agricultural food supply chain.

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CRediT authorship contribution statement

Bruna Carbas: Writing – original draft, Visualization, Validation, Software, Methodology, Investigation, Formal analysis, Data curation, Conceptualization. **Pedro Sampaio:** Writing – original draft, Validation, Software, Methodology, Investigation. **Sílvia Cruz Barros:** Writing – review & editing, Formal analysis. **Andreia Freitas:** Writing – review & editing, Methodology, Formal analysis. **Ana Sanches Silva:** Writing – review & editing, Validation, Supervision, Resources, Methodology. **Carla Brites:** Writing – review & editing, Supervision, Project administration, Methodology, Funding acquisition, Conceptualization.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper. The authors are an Editorial Board Member/Editor-in-Chief/Associate Editor/Guest Editor for this journal and was not involved in the editorial review or the decision to publish this article.

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Data availability

Data will be made available on request.

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