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Prediction of microbial dynamics during grape pomace composting using NIR spectroscopy and ANN modeling

Tea Sokač Cvetnić, Korina Krog, Maja Benković, Tamara Jurina, Davor Valinger, Jasenka Gajdoš Kljusurić, Ivana Radojčić Redovniković, Ana Jurinjak Tušek
University of Zagreb Faculty of Food Technology and Biotechnology, Pierottijeva 6, 10000 Zagreb, Croatia

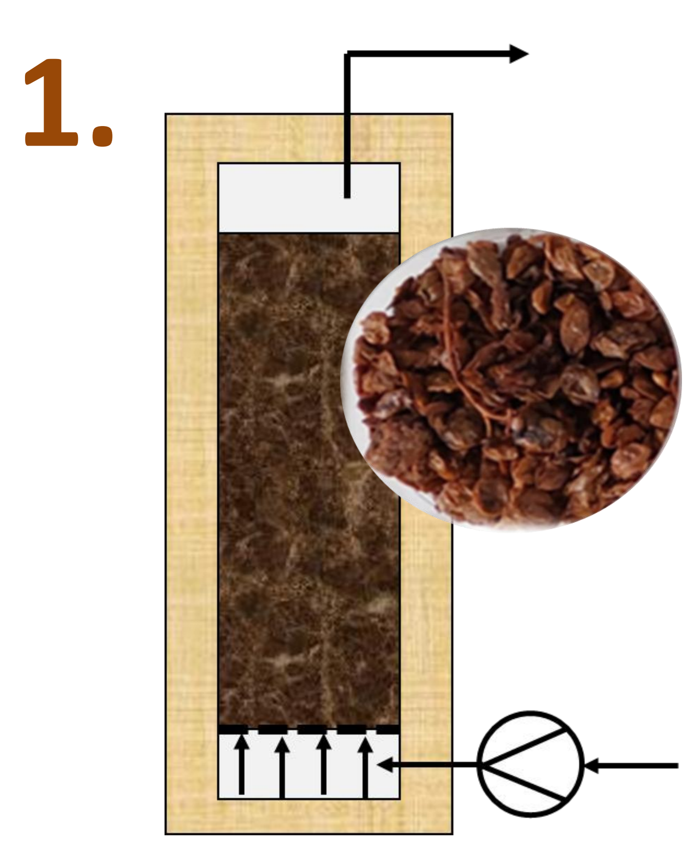
INTRODUCTION & AIM

Introduction The management of agro-industrial residues such as grape pomace poses both environmental and economic challenges for the wine industry. As a byproduct rich in organic matter, grape pomace can be effectively transformed into nutrient-rich compost through biological decomposition, offering a sustainable pathway for waste valorization and soil enrichment. However, monitoring the microbial dynamics that drive composting remains complex and time-consuming when relying on conventional microbiological methods. Recent advances in analytical technologies have introduced near-infrared (NIR) spectroscopy as a rapid, non-destructive alternative for real-time process monitoring. When combined with machine learning approaches such as Artificial Neural Networks (ANNs), NIR spectroscopy holds promise for accurately predicting microbial activity and optimizing composting conditions.

Aim of the Research This study aimed to develop and evaluate predictive models for monitoring microbial population dynamics during composting of grape pomace using NIR spectroscopy integrated with ANN modeling. The objective was to establish a fast, reliable, and non-invasive method to predict bacterial, fungal, and total microorganism counts, thereby improving process control and promoting sustainable composting practices.

METHODS

1.



Grape skin composting in thermally insulted laboratory reactors (V = 5L) with constant aeration for 30 days.

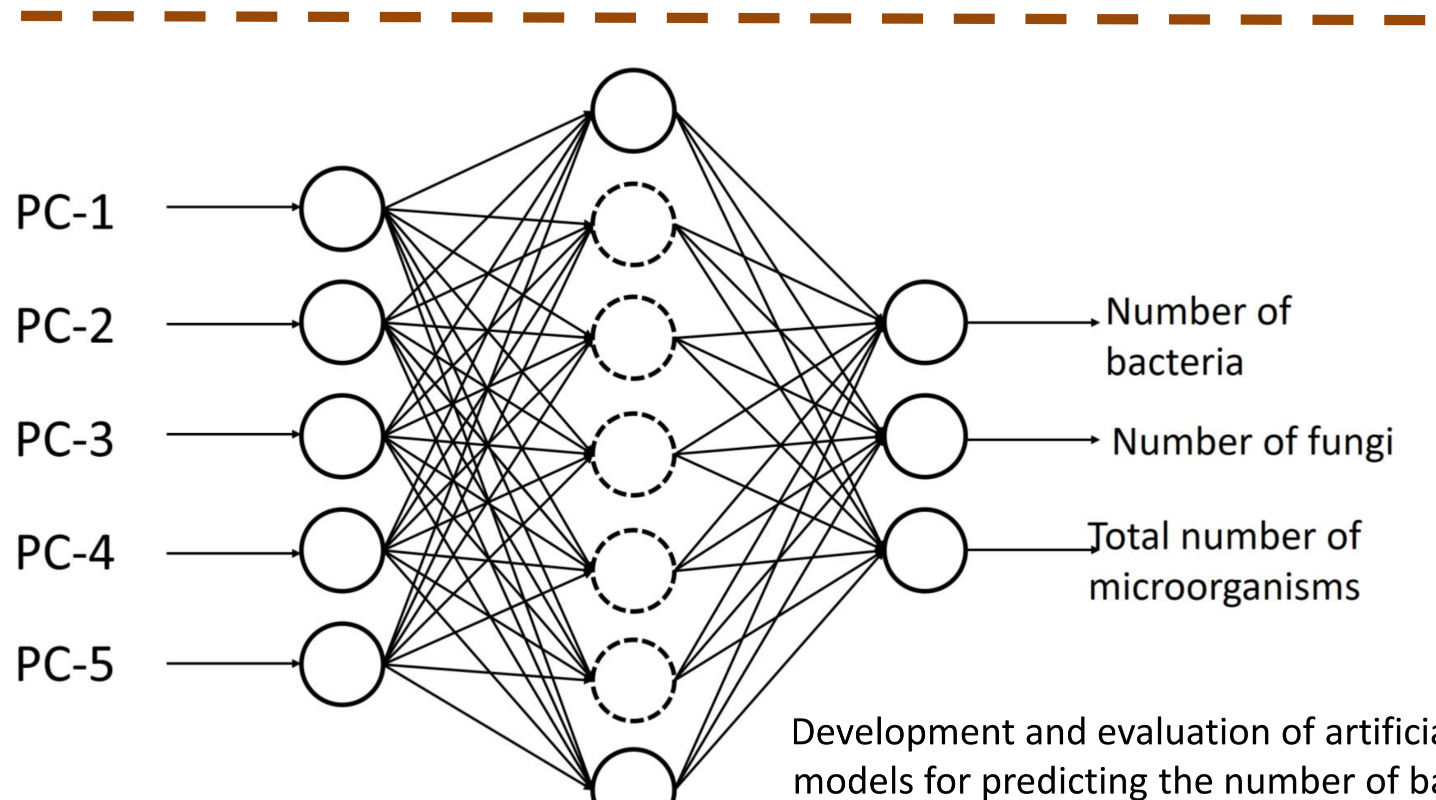
2.

Microbiological analyses on samples taken every 72 h and NIR spectroscopy of compost samples using a semi-process NIR spectrometer (NIR-128-1.7-USB/6.25/50 µm, Control Development inc., USA).

3. Preprocessing of NIR spectra in the program Unscrambler X 10.1. (CAMO AS, Norway) and analysis of basic components in the program Statistica 14.0. (TIBCO® Statistica, Palo Alto, USA) .

(i) Raw NIR spectra
(ii) Smoothing (S)
(iii) First order derivative (SG1D)
(iv) Second order derivative (SG2D)
(v) Standard Normal Variate (SNV)
(vi) Multiplicative Scatter Correction (MSC)
(viii) S + MSC
(ix) SG1D +SNV
(x) SG1D + MSC
(xi) SG2D + SNV
(xii) SG2D + MSC

4.



Development and evaluation of artificial neural network models for predicting the number of bacteria, fungi and the total number of microorganisms in compost based on the first 5 factors of PCA analysis .

RESULTS & DISCUSSION

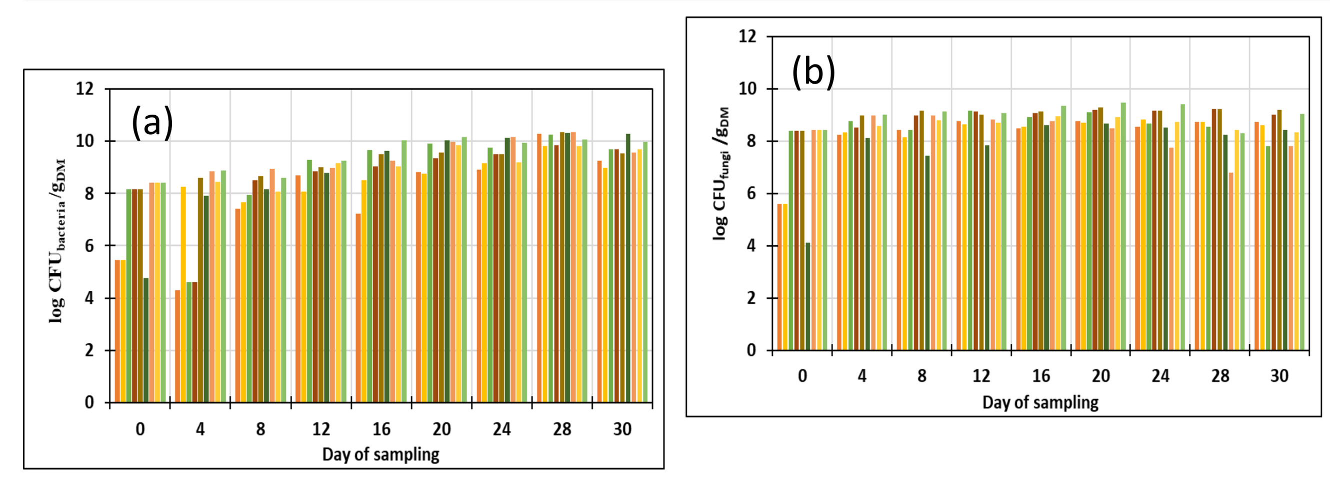


Figure 1. Change in the number of (a) bacteria and (b) fungi during composting

Figure 1 shows the growth of microorganisms during the composting. The growth is related to the pH value. In the first days, due to the acidic environment, fungi and molds predominate in all reactors (Figure 1b), and later, when the pH is in the neutral or alkaline range, bacteria predominate (Figure 1a).

NIR spectra for compost samples recorded with an NIR spectrometer in the wavelength range from 904 to 1699 nm are shown in Figure 2. The spectra of compost samples for all reactors have the same trend, and the differences between the spectra are in the wavelength range of 1350–1550 nm, which indicates O–H bonds, i.e., the differences in this spectral range can be associated with the water content in the samples.

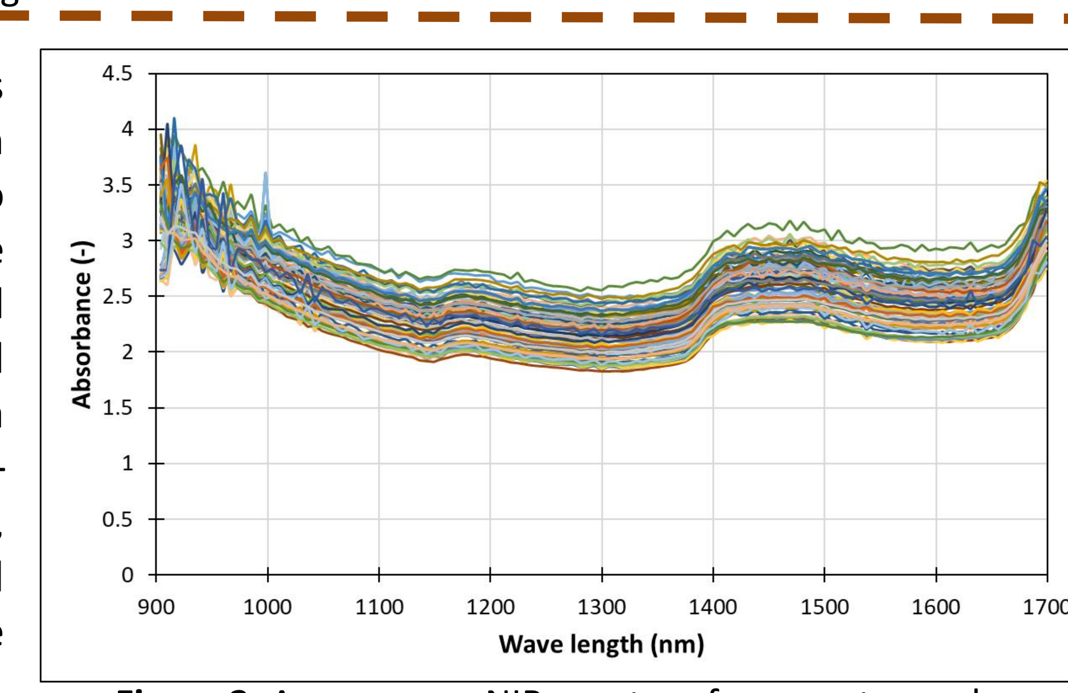


Figure 2. Average raw NIR spectra of compost samples

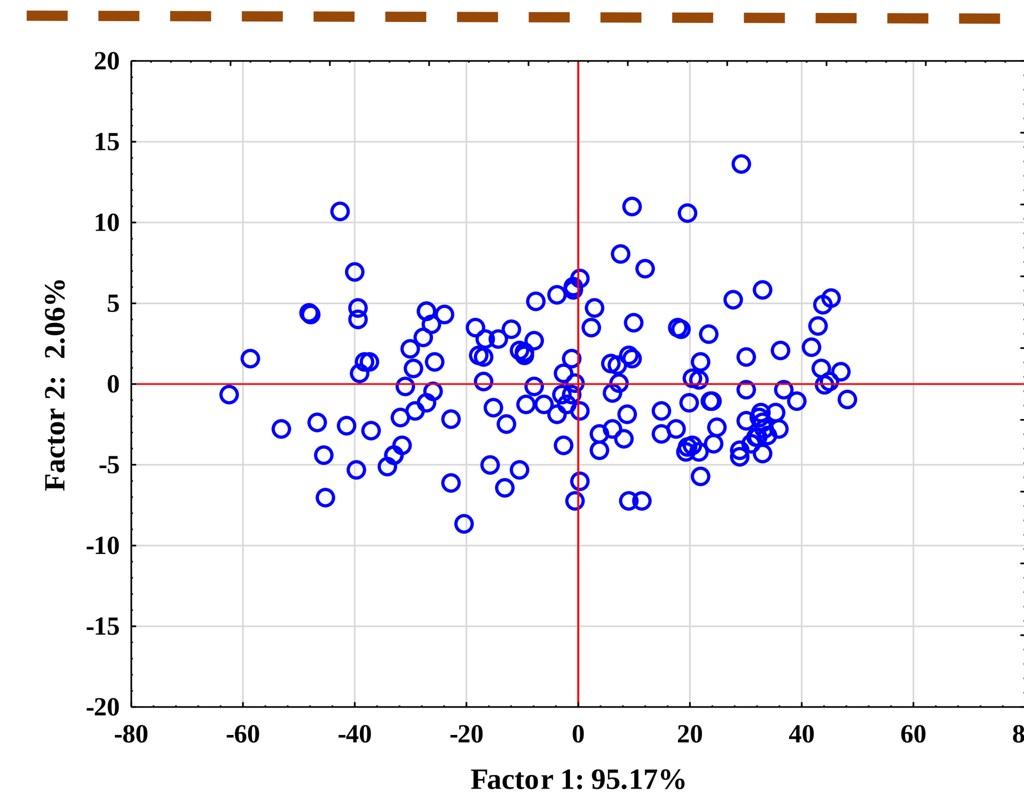


Figure 3. PCA analysis of raw NIR spectra of compost samples

The results of the principal component analysis (PCA) of the raw spectra are shown in Figure 4. It can be seen that the first two factors describe more than 95% of the variability in the data for the compost samples. Also, overlapping data was observed, indicating similarities between the samples and also the need for preprocessing of the spectra to extract specific information.

ANN models for prediction of microbial dynamics in compost were developed using the first 5 factors from the PCA as inputs to the models. With regard to predicting the number of fungi and total microorganisms in compost, the acceptable preprocessing method was SG2D+MSC which resulted in the model with the highest error range ratio values of 15.075 and 12.040, respectively. For predicting the number of bacteria, the smoothing method resulted in the model with the highest RER value of 10.084 (Table 1).

Table 1. ANN models for prediction of microbial dynamics during the composting process based on the NIR spectra gathered (R_{pred}^2=coefficient of determination for prediction; $R_{pred,adj}^2$=adjusted coefficient of determination for prediction; RMSEP=root mean square of prediction; SEP=standard error of prediction; RPD=ratio of prediction to deviation; RER=ratio of the error range).

Model output	Preprocessing	ANN	Prediction					
			R_{pred}^2	$R_{pred,adj}^2$	RMSEP	SEP	RPD	RER
$\log CFU_{bacteria}$	smoothing	MLP 5-6-1	0.841	0.8078	0.597	0.127	2.496	10.084
$\log CFU_{fungi}$	SG2D+MSC	MLP 5-9-1	0.884	0.859	0.349	0.074	2.885	15.075
$\log CFU_{total\ number\ of\ m.o.}$	SG2D+MSC	MLP 5-9-1	0.823	0.786	0.875	0.186	2.341	12.040

CONCLUSION/ FUTURE PERSPECTIVE

This study demonstrated that integrating NIR spectroscopy with ANN modeling **provides a fast, non-destructive method for monitoring microbial dynamics during grape pomace composting**. Smoothing was most effective for predicting bacterial counts, while SG2D+MSC best modeled fungal and total microorganisms. **The approach enables real-time, accurate compost monitoring**, enhancing process efficiency and sustainability. **Future research should validate these models at larger scales** and explore integration with IoT and automated control systems to enable smart composting. **Applying this framework to other agro-industrial wastes could further support circular economy and sustainable resource management initiatives.**