

Article

Detection of 2,4,6-Trichloroanisole in Sparkling Wines Using a Portable E-Nose and Chemometric Tools

Ramiro Sánchez ^{1,*} , Jesús Lozano ² , Patricia Arroyo ²  and Félix Meléndez ² 

¹ Centro de Investigaciones Científicas y Tecnológicas de Extremadura (CICYTEX), Instituto Tecnológico Agroalimentario de Extremadura, Avda. Adolfo Suárez s/n, 06007 Badajoz, Spain

² Industrial Engineering School, University of Extremadura, 06006 Badajoz, Spain

* Correspondence: ramiro.sanchez@juntaex.es; Tel.: +34-924-012-656

Abstract: This study addresses the contamination of sparkling wines by 2,4,6-trichloroanisole (TCA), a compound responsible for the “cork taint” or musty aroma in wines. Currently, its detection requires complex and expensive techniques such as chromatography and sensory panels. An innovative method is proposed using an electronic nose (e-nose) prototype, offering objective, non-destructive, and cost-effective analysis. The e-nose’s ability to detect TCA at various concentrations was evaluated in sparkling wines from different batches and a spiked wine sample. The results analyzed using Principal Component Analysis (PCA) successfully differentiated the samples. An Artificial Neural Network Discriminant Analysis (ANNDA) classified wines based on whether their TCA concentration exceeded 2 ng/L, achieving 88% accuracy. A quantitative predictive model using Partial Least Squares (PLS) analysis yielded an R^2 of 0.84 across wines and 0.95 in a single sample. These advances highlight the potential of the e-nose to improve quality control in the wine industry.

Keywords: chromatographic analysis; electronic nose; olfactory contamination; cork taint detection; sensor array; wine quality assessment



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1. Introduction

Sparkling wines are renowned for their characteristic effervescence and are in high demand globally due to their association with celebrations. Notable examples of sparkling wines include cava and champagne [1]. However, the presence of 2,4,6-trichloroanisole (TCA) in these wines represents a significant quality and economic challenge for the wine industry.

TCA was first identified in 1982 as the cause of musty odors in wine, leading to the characterization of this defect as “cork taint”. Since then, it has been recognized that TCA and other related haloanisoles can become airborne and settle on surfaces within wineries, making their removal particularly difficult. These compounds have a devastating impact on the aroma and overall quality of wine [2]. In addition to negatively affecting the sensory perception of sparkling wine, TCA contamination results in significant economic losses for producers due to product returns and damage to brand reputation [3]. Detecting and eliminating TCA is complex and costly, posing additional challenges to maintaining the quality and reputation of sparkling wines on a global scale [4,5].

To address the issue of TCA, the industry has implemented measures such as banning chlorine-based agents in cork processing, replacing hypochlorite with hydrogen peroxide, which does not lead to haloanisole problems, and enhancing analytical controls. Despite

these measures, the average cork contamination has been reduced, but the problem of TCA has not been fully resolved [2].

The olfactory threshold is determined by assessing the minimum concentration of a volatile compound detectable by at least 50% of the members of a sensory panel. In a previous study, TCA was identified as the primary compound responsible for the cork taint defect [6], characterized by a low sensory threshold and an off-putting odor of cork, wet cardboard, and mold. A panel of 12 specialists conducted duo-trio tests, with at least 50% of the evaluators clearly identifying the unpleasant TCA odor at concentration thresholds in water, white wine, and red wine of 3.2, 4.3, and 7.6 ng/L, respectively.

TCA interferes with olfactory receptors and can quickly cause sensory fatigue, reducing the ability to perceive its presence and potentially suppressing wine aromas even at concentrations below established sensory thresholds [7]. This masking effect can occur at sub-threshold levels as low as 0.1–1 ng/L. White wines typically have lower TCA detection thresholds compared to red wines, a difference attributed to the less complex phenolic composition of white wines, which makes off-flavors like TCA more perceptible in the matrix [6].

Detectable concentrations of TCA that impact product quality are extremely low, making their detection and quantification essential. Traditional techniques for TCA detection include chromatographic methods. An effective and rapid microextraction technique, based on ultrasound-assisted emulsification microextraction, was proposed for the pre-concentration of TCA from wine samples prior to analysis by gas chromatography coupled with tandem mass spectrometry (GC-MS/MS), calibrated for white and red wines within the range of 5–1000 ng/L, achieving coefficients of determination (R^2) ≥ 0.9995 [8]. This approach uses ultrasonic energy to disperse a small volume of organic solvent into the aqueous sample, enhancing analyte transfer without the need for solid-phase supports. The method offers advantages such as low solvent consumption, short extraction times, and simplicity, making it suitable for routine analysis. While the validated range effectively covers most expected contamination levels, expanding sensitivity below 5 ng/L could be of interest in contexts where the early detection of sub-threshold TCA concentrations is critical.

Although GC-MS remains the reference method for the quantification of TCA due to its high analytical sensitivity—often capable of detecting concentrations well below sensory thresholds—it also has practical limitations for rapid or on-site application. Sample preparation often requires solvent extraction and skilled personnel, and the instrumentation itself carries significant costs and maintenance requirements [2]. In contrast, electronic noses provide a nondestructive, solvent-free, and faster alternative that can be deployed directly in production environments. Although their sensitivity is generally lower than that of GC-MS, recent reviews suggest that electronic nose systems are well suited to detect TCA concentrations in the low ng/L range, which are relevant for quality control purposes in winemaking [9]. Their speed, portability, and ease of use make them particularly effective for preliminary screening, allowing quick decisions to be made and helping to prioritize samples for confirmatory GC-MS analysis when necessary.

In this context, electronic nose (e-nose) technology, a device that tries to simulate human olfactory capabilities using gas sensors and pattern recognition algorithms, emerges as a promising technology for aroma evaluation in the wine industry. An electronic nose generally integrates a set of functional modules. These include a sampling unit to capture volatile compounds, a sensor array that reacts to the chemical profile, electronics for signal acquisition, and software algorithms for data interpretation. The captured sensor patterns are processed to differentiate samples based on previously learned characteristics [10]. Electronic nose technology can detect and quantify aromatic compounds in wine [11].

Electronic noses can be classified according to the type of sensors employed, including conducting polymer sensors (CPs), metal oxide semiconductor sensors (MOs), metal oxide semiconductor field-effect transistors (MOSFETs), and mass-sensitive sensors such as quartz crystal microbalance (QMB) and surface acoustic wave (SAW) devices [9]. Each technology offers specific advantages in terms of sensitivity, selectivity, stability, and cost, depending on the application requirements [9]. In the wine industry, electronic noses equipped with these sensors have been successfully used for detecting wine aging, identifying spoilage-related volatile compounds, and discriminating among different wine varieties [9].

This technology has been successfully used to detect TCA in cork. E-nose systems with metal oxide sensors have successfully classified cork stoppers with varying levels of TCA contamination at ng/L levels [12,13]. The hypothesis is that the electronic nose can effectively discriminate between different levels of TCA in sparkling white wine samples. The objective of this study was to classify sparkling wine samples according to their TCA content and establish the efficacy of the electronic nose in identifying and quantifying TCA in sparkling wines, thereby contributing to improved quality control practices in the wine industry. The main innovation of this work lies in applying the e-nose directly to liquid sparkling wine, as opposed to previous studies that focused on the detection of TCA in cork stoppers or the winery environment.

2. Materials and Methods

In this study, an e-nose system was employed to analyze the potential presence of TCA in sparkling white wine samples. Two main experiments were conducted: one focused on the discrimination of samples based on their TCA content, and the other aimed at predicting TCA concentrations using the e-nose.

Additionally, chromatographic analyses were performed to characterize the volatile profile of the sparkling wines and quantitatively determine TCA concentrations. The experimental design, sample selection, and methods employed for the analysis are described in detail below.

2.1. Experimental Design

Ten bottles of sparkling white wine, predominantly made from Macabeo and Parrellada grape varieties, were selected from different production batches of a local winery. Each bottle was chosen based on preliminary organoleptic characteristics suggesting possible TCA contamination, such as cork taint odor. The samples were stored at 4 °C until analysis to preserve their volatile composition. The samples were analyzed using gas chromatography–mass spectrometry (GC/MS) prior to solid-phase microextraction (SPME) for volatile profile characterization and TCA concentration determination. Simultaneously, the samples were also analyzed using the e-nose. Due to confidentiality agreements with the winery, detailed information about the identity and specific parameters of the wine samples cannot be disclosed.

Two main experiments were conducted to assess the e-nose's discriminatory ability regarding TCA contamination in sparkling wines.

2.1.1. Discrimination of Sparkling Wines Based on TCA Content

The e-nose's ability to discriminate between ten sparkling wine samples was evaluated by measuring the headspace of the samples. Principal Component Analysis (PCA) was performed on the entire set of ten wines, as well as a separate PCA to distinguish wines with TCA content above or below 2 ng/L. The actual TCA concentration in the samples was determined in triplicate using GC/MS. The headspace of the samples was analyzed with the e-nose in a thermostatic bath at 25 °C. In this study, a TCA threshold of 2 ng/L was used

to classify the wines using Artificial Neural Network Discriminant Analysis (ANNDA). This threshold is supported by existing literature, which indicates that consumer rejection occurs at TCA levels of 10 ng/L, while experts can detect the defect at levels as low as 5 ng/L and even at 2 ng/L when compared to an uncontaminated control wine [14].

2.1.2. Quantitative TCA Prediction Using the E-Nose

A Partial Least Squares (PLS) model was developed to assess the correlation between experimental values obtained by chromatography and those predicted by the e-nose for the ten wines. Additionally, a single wine, initially free of TCA, was spiked with increasing concentrations of a TCA solution. The control wine selected for the spiking experiments was a sparkling wine whose TCA content was confirmed as 'not detected' by chromatographic analysis prior to the addition of external TCA solutions. The TCA was supplied by Sigma-Aldrich Chemie (Steinheim, Germany), and five concentration levels were obtained: C1 = 0.0 ng/L, C2 = 2.0 ng/L, C3 = 10.0 ng/L, C4 = 50.0 ng/L, and C5 = 100 ng/L. The headspace of these samples was analyzed with the e-nose in a thermostatic bath at 25 °C. This approach allowed the determination of different concentrations in the same wine and assessed the influence of TCA concentration versus wine variability.

2.2. Chromatographic Analysis

Two different chromatographic analyses were performed: one for the characterization of the volatile organic compound profile in sparkling wine and another for the determination of TCA. The analyses, conducted in triplicate, included ten different wines labeled V1 to V10.

The extraction of volatile profiles in sparkling wines was carried out using GC-MS following conditions similar to those used previously [15]. A 2 mL sample of each sparkling wine was placed in 20 mL vials, which were then sealed with a PTFE septum cap. Each sample was maintained at 35 °C for 30 min, after which a Solid-Phase Microextraction (SPME) fiber was inserted into the headspace for an additional 30 min, followed by desorption in the GC injection port for 5 min at 260 °C. A 1 cm long fiber with a 65 µm polydimethylsiloxane/divinylbenzene (PDMS/DVD) film with Stable Flex (Supelco, Bellefonte, PA, USA) was used. Wine samples were analyzed using a Bruker Scion 456-GC gas chromatograph with a triple quadrupole mass spectrometer (Bruker, Falkenried, Hamburg, Germany). The GC system was equipped with a Supelcowax 10 capillary column (Supelco, Bellefonte, PA, USA) with a 20M polyethylene glycol stationary phase (30 m × 0.25 mm × 0.25 µm). The temperature program was as follows: 40 °C for 10 min, then 40 °C to 200 °C at 2 °C/min, holding for 1 min at 200 °C, then 200 °C to 250 °C at 2 °C/min, and finally holding at 250 °C for 10 min. The spectra were compared with the NIST 20.L library search program.

For the determination of TCA, the operational conditions were adjusted following standardized OIV-MA-AS315-16 protocols. Ten milliliters of wine were transferred to a 20 mL vial, and 3 g of sodium chloride plus 50 µL of an internal standard (2,4,6-trichloroanisole, ≥99% purity, Sigma-Aldrich, St. Louis, MO, USA; Cat. No. 235393-1G) was added to each vial. The vial was sealed with a PTFE septum cap, homogenized for 10 min, and incubated at 35 °C ± 2 °C for at least 15 min using the same thermostatic heating block described above. Headspace extraction was performed using SPME after incubation. The SPME fiber was desorbed at 260 °C for at least 2 min in the GC injector in splitless mode. For TCA quantification, a GC/MS 6890/5973N system (Agilent Technologies, Santa Clara, CA, USA) was used with a 100 µm PDMS fiber (Supelco, Bellefonte, PA, USA). Separation was performed using a DB5 capillary column, J&W, 30 m × 0.25 mm, with a 0.25 µm film thickness (Agilent Technologies, Santa Clara, CA, USA). The temperature program was 50 °C for 2 min, increased to 130 °C at 25 °C/min, increased to 200 °C at 5 °C/min,

held at 200 °C for 5 min, and finally increased to 280 °C at 25 °C/min with a final 5 min isotherm [6].

Detection was performed using mass spectrometry with specific ion monitoring for 2,4,6-trichloroanisole (ions m/z 195, 210, 212), quantified at m/z 195, and the internal standard 2,4,6-trichloroanisole (TCA)-d5, with 98% purity (ions m/z 199, 215, 217), quantified at m/z 215. The results were expressed in ng/L of TCA present in the sample, rounded to the nearest tenth according to the OIV-MA-AS315-16 protocol.

2.3. E-Nose System

The e-nose device used in this study is an in-house-developed prototype at the University of Extremadura, which communicates via Bluetooth through a mobile application. It is a portable, compact, and low-power device utilizing five metal oxide semiconductor (MOS) gas sensors capable of detecting a wide range of volatile organic compounds (VOCs). These sensors, sourced from various manufacturers, offer broad-spectrum VOC sensitivity and are characterized by the integration of digital electronics combined with a micro hotplate and detectors on a single chip. These sensors incorporate internal processing algorithms and directly provide estimated values of eCO_2 (ppm), TVOC (ppb), and resistance (Ω) through proprietary internal processing, including factory calibration and compensation for temperature and humidity. Because of this and the complex olfactory matrix that wines present, it is difficult to perform traditional calibration curves. Other environmental parameters such as temperature, relative humidity, and atmospheric pressure can also be detected with these sensors. The specific configuration of the sensors and their signals is detailed in Table 1.

Table 1. Sensors included in the electronic nose prototype.

Sensor	Manufacturer	Signals
BME680	Bosch Sensortech GmbH, Reutlingen, Germany	Temperature, Relative Humidity, Pressure, Resistance value (Ω)
SGP30	Sensirion AG, Stäfa, Switzerland	CO_2 , TVOCs ¹ , H_2 (raw signal ²), Ethanol (raw signal)
ZMOD4410	Renesas Electronic Corporation, Tokyo, Japan	Ethanol (raw signal), Resistance value (Ω), CO_2 , TVOCs, IAQ ³
CCS811	ScioSense B.V., Eindhoven, The Netherlands	CO_2 , TVOCs, Resistance value
iAQ-Core	ScioSense B.V., Eindhoven, The Netherlands	CO_2 (ppm), TVOCs (ppb) y Resistance value (Ω)

¹ Total Volatile Organic Compounds. ² Signal derived from the sensor resistance. ³ Air Quality Index.

This E-nose is an improvement over the previous manual version [16] as it includes an additional sensor (ZMOD4410) and the inclusion of a solenoid valve and pump for automatic sampling. The e-nose is driven by the PIC32MM0256GPM048 microcontroller from Microchip (Chandler, AZ, USA), which has sufficient memory and computing power for this application, as well as several I²C and UART buses to communicate with the other components. For external communication, the e-nose has the Bluetooth Low-Energy module RN4871, also from Microchip, which enables data exchange via transparent UART with a smartphone.

On the pneumatic side, the e-nose has a solenoid valve with two inputs and one output, which allows automatic switching between clean filtered reference air and sample gas. The output of the solenoid valve is connected to the inlet of a pneumatic diaphragm pump, which pushes the sample into the inlet of the cell containing the sensors. These gases finally exit the cell outlet.

This electronic and pneumatic system is encapsulated in a housing measuring $118 \times 82 \times 22.5$ mm. Inside is also a rechargeable +3.7 VDC lithium battery that powers the entire system. The e-nose has a micro-USB port that allows this battery to be recharged with a smartphone charger. The power consumption is 684 mW with a sensor response time of two seconds. The block diagram and an image of the e-nose prototype showing the printed circuit board (PCB), solenoid valves, pump, battery, and interconnected tubing for sample flow control are shown in Figure 1.

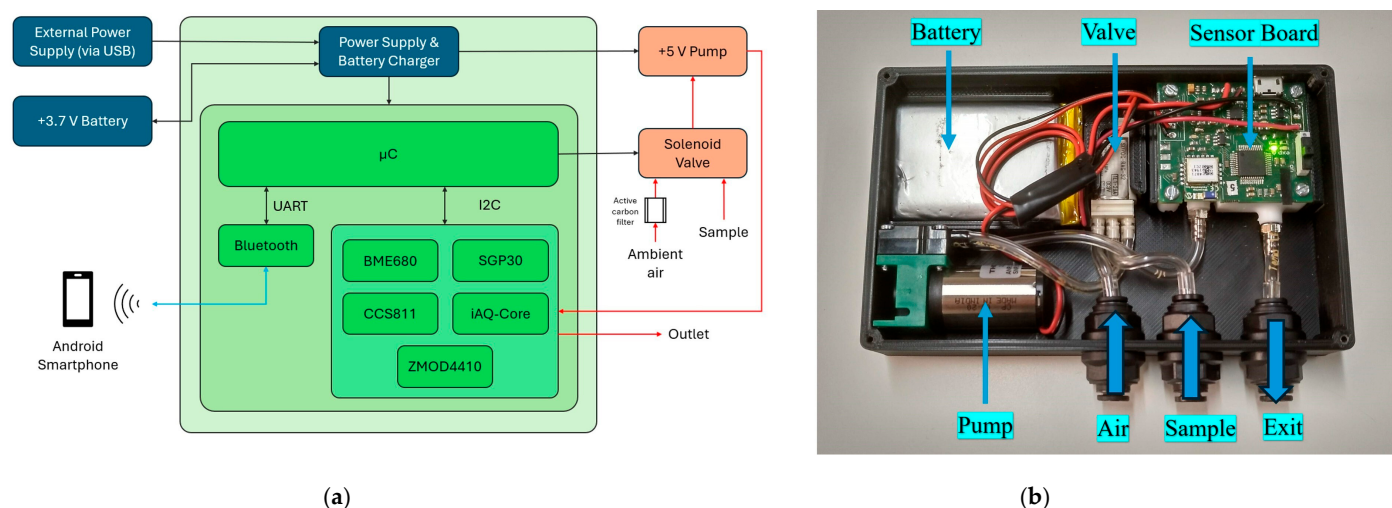


Figure 1. (a) Block diagram of the electronic nose and (b) internal view of the portable e-nose prototype. The main components are labeled, including the battery, pump, valve, sensor board, and the flow direction. The sensor board integrates five gas sensors: BME680, SGP30, CCS811, iAQ-Core, and ZMOD4410.

For measurement, 10 mL of the wine sample was placed in a beaker sealed with a lid containing two holes: one for sample headspace suction and the other for the intake of ambient air previously filtered through an inline activated carbon filter (granular activated carbon, $\varnothing 26 \times 82$ mm; Ref. MXCRB-0422, Laboratoriumdiscounter, IJmuiden, The Netherlands), to eliminate background VOCs and ensure a clean baseline before sample introduction. E-nose measurements were conducted in 60 s sampling and cleaning cycles at a controlled temperature of 25 °C. Five replicates were measured for each wine sample.

Data collected by the e-nose were analyzed using multivariate analysis techniques to classify the samples and predict TCA concentration.

2.4. Multivariate Data Analysis

To assess statistical differences in chromatographic analyses among the different wines, a one-way analysis of variance (ANOVA) was employed. Tukey post hoc tests were performed to identify specific pairs of groups with significant differences. The results were considered statistically significant when $p < 0.05$. All statistical analyses were performed using IBM SPSS Statistics 20 (SPSS Inc., Chicago, IL, USA). Data were expressed as mean $\pm$ standard deviation (SD).

For pattern identification and classification in the e-nose data from TCA-contaminated wines, multivariate analysis methods were applied using the PLS_Toolbox 9.1 (Eigenvector Research Inc., Wenatchee, WA, USA) within the Matlab R2023a 9.14.0.2206163 environment (The Mathworks Inc., Natick, MA, USA). An unsupervised exploratory PCA was used [17] to reduce the dimensionality of the input variables, resulting in two principal components as linear combinations of the original response vectors. This analysis showed how the wine samples containing TCA clustered according to their levels.

From the original data obtained by the sensors, characteristic data are derived from the difference between the maximum value ($X_{\max}$), which represents the average of the last five values during exposure to the reference gas (clean air), and the minimum value ($X_{\min}$), which represents the average of the last five values during exposure to the sample headspace. Subsequently, before proceeding with more complex analyses, the collected data are autoscaled using MATLAB R2024b (The MathWorks, Inc., Natick, MA, USA) and PLS_Toolbox 9.5 (Eigenvector Research Inc., Wenatchee, WA, USA). This process involves centering and scaling each variable to a unit standard deviation by subtracting the mean and dividing each value by its standard deviation. This approach not only facilitates effective comparison of responses from different sensors but also ensures that all variables carry equal weight in subsequent analyses.

Additionally, hierarchical clustering analysis (HCA) was applied using the K-Nearest Neighbor Distance. This type of analysis is commonly used in statistics to classify a dataset into groups based on its characteristics. Subsequently, a supervised classification ANNDA was performed, consisting of an input layer with a number of neurons equal to the number of input variables and an output layer with the classes. A confusion matrix was derived from cross-validation predictions generated using “random subsets” with 5 splits and 10 iterations. This approach was strategically chosen to address the limited data available, as the multiple splits and iterations help to mitigate biases and reduce overfitting, ultimately leading to more robust and generalizable predictions. This setup provided a robust assessment of the ANNDA model with a dataset of 50 observations and 2 final classes. The proportion of correct predictions was calculated from the sum of the diagonal elements found in the confusion matrices. In addition, the following metrics were used to study the network performance:

TPR (True-Positive Rate or Recall): Measures the model’s ability to correctly identify all positive samples. It is calculated as the number of true positives divided by the total actual positives ($TP + FN$).

FPR (False-Positive Rate): Indicates the percentage of negative results incorrectly classified as positive. It is calculated as the number of false positives divided by the total true negatives ($TN + FP$).

TNR (True-Negative Rate): Demonstrates the model’s ability to accurately identify negative samples. It is calculated as the number of true negatives divided by the total actual negatives ($TN + FP$).

FNR (False-Negative Rate): Reflects the percentage of positive results that were incorrectly classified as negative. It is calculated as the number of false negatives divided by the total true positives ($TP + FN$).

N: Total number of samples tested in each category.

Error (Err): Proportion of incorrect predictions (sum of false positives and false negatives) compared to the total number of samples.

Precision (P): Proportion of true positives in relation to all positive predictions ($TP + FP$), indicating the accuracy of the model’s positive predictions.

F1 Score: Harmonic mean of precision and recall, providing a comprehensive measure of accuracy considering both precision and recall.

Furthermore, supervised quantitative PLS analysis was used to build quantification models correlating chromatography and e-nose results. A total of 50 observations corresponding to the 10 wines were divided into 2 sets: a calibration set containing 70% of the samples, used for calibration and cross-validation, and a validation set containing the remaining 30%, used only to test the robustness and accuracy of the developed models. The parameters used to evaluate model accuracy were the root mean square error of calibration (RMSEC), cross-validation (RMSECV), and the coefficients of determination

for cross-validation (R^2_{CV}) and prediction (R^2_{Pred}). The samples were randomly divided between the two sets.

3. Results

The following section presents the results obtained from the chromatographic analysis of volatile compound profiles, TCA quantification, and e-nose analysis.

3.1. Chromatographic Analysis:

Chromatographic analysis was performed to characterize the volatile compound profile of ten sparkling wine samples and to quantify the presence of TCA, the compound responsible for cork taint. These results contribute to understanding the aromatic complexity of each sample and offer insight into how TCA may affect the sensory perception of volatile compounds—serving as a basis for evaluating the performance of the electronic nose (e-nose).

Table 2 presents the relative peak areas ($\times 10^7 \pm SD$) of 17 volatile compounds identified in the headspace. These include esters, alcohols, acids, and aldehydes, all of which showed statistically significant differences across samples ($p < 0.05$). Their associated odor descriptors range from fruity and floral to rancid or herbaceous, reflecting the potential sensory differentiation among the wines.

Ethanol showed the highest variability among samples, with relative peak areas ranging from 76.58×10^7 in V6 to 238.76×10^7 in V9. Esters such as ethyl octanoate ranged from 29.82 (V9) to 61.86 (V10), ethyl hexanoate from 24.11 (V9) to 38.44 (V1), and ethyl 3-methylbutanoate from 0.34 (V9) to 0.56 (V6), indicating substantial variability in aroma-contributing compounds. Fatty acids also varied considerably: hexanoic acid ranged from 0.59 (V10) to 3.78 (V2), while octanoic acid ranged from 12.10 (V9) to 21.66 (V8). 2-Phenylethanol, a major floral compound, varied from 2.88 (V6) to 8.65 (V1). These differences in the volatile composition provide a foundation for the multivariate discrimination observed.

Beyond VOCs analysis, Figure 2 presents the TCA concentrations quantified by GC-MS. The dashed red line at 2 ng/L represents the sensory threshold used in this study to classify wines based on perceptible contamination.

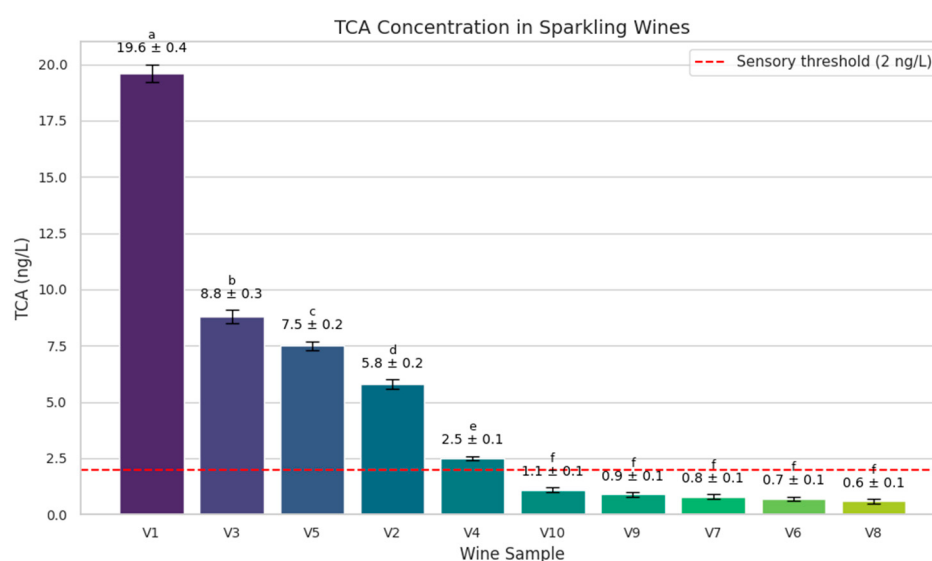


Figure 2. Concentration of TCA in sparkling wine samples as determined by GC-MS. Letters above the bars indicate statistically significant differences between samples according to Tukey's HSD test ($p < 0.05$); samples sharing the same letter do not differ significantly.

Table 2. Volatile compounds found in the headspace of sparkling wine determined by GC-MS expressed as mean area value $\pm$ standard deviation.

Name	RT (min)	CAS N°	Odor Descriptor	Area $\times 10^7$									
				V1	V2	V3	V4	V5	V6	V7	V8	V9	V10
Ethanol	1.68	64-17-5	sharp and alcoholic smell	217.78 $\pm$ 3.80 _{bc}	213.26 $\pm$ 5.65 _{bc}	217.01 $\pm$ 3.61 _{bc}	197.72 $\pm$ 5.02 _d	224.84 $\pm$ 5.52 _{ab}	76.58 $\pm$ 2.35 _e	221.21 $\pm$ 6.99 _b	214.46 $\pm$ 3.76 _{bc}	238.76 $\pm$ 5.79 _a	205.74 $\pm$ 4.91 _{cd}
1-Butanol, 3-methyl-	4.27	123-51-3	alcoholic, pungent, cognac, fruity, banana	50.25 $\pm$ 1.04 _e	53.38 $\pm$ 1.53 _{de}	60.83 $\pm$ 2.64 _{ab}	55.20 $\pm$ 2.24 _{cde}	57.43 $\pm$ 0.64 _{abcd}	62.41 $\pm$ 2.06 _a	61.89 $\pm$ 1.44 _a	59.22 $\pm$ 2.60 _{abc}	57.76 $\pm$ 2.15 _{abcd}	56.55 $\pm$ 0.22 _{bcd}
Ethyl 2-hydroxypropanoate	6.95	687-47-8	rum, with fruity and creamy notes	12.21 $\pm$ 0.34 _d	13.05 $\pm$ 0.16 _{cd}	14.63 $\pm$ 0.55 _{ab}	14.08 $\pm$ 0.30 _{bc}	14.30 $\pm$ 0.22 _{ab}	14.86 $\pm$ 0.26 _{ab}	14.81 $\pm$ 0.62 _{ab}	15.34 $\pm$ 0.36 _a	15.27 $\pm$ 0.46 _a	14.38 $\pm$ 0.06 _{ab}
2,2-Dimethyl-1-butanol	8.36	1185-33-7	soft, sweet and slightly fruity or floral smell	0.40 $\pm$ 0.02	0.13 $\pm$ 0.00	nd	nd	0.26 $\pm$ 0.01	nd	0.25 $\pm$ 0.00	nd	0.32 $\pm$ 0.01	nd
Ethyl 2-methylbutanoate	8.53	7452-79-1	strong and unpleasant smell, similar to cheese	0.27 $\pm$ 0.01 _c	0.21 $\pm$ 0.01 _d	0.27 $\pm$ 0.01 _c	0.21 $\pm$ 0.01 _d	0.23 $\pm$ 0.01 _d	0.70 $\pm$ 0.02 _a	0.27 $\pm$ 0.00 _{bc}	0.23 $\pm$ 0.00 _d	0.15 $\pm$ 0.01 _e	0.29 $\pm$ 0.01 _b
Ethyl 3-methylbutanoate	8.69	108-64-5	fruity, apple, pineapple	0.43 $\pm$ 0.01 _c	0.37 $\pm$ 0.01 _d	0.53 $\pm$ 0.02 _{ab}	0.41 $\pm$ 0.01 _c	0.42 $\pm$ 0.01 _c	0.56 $\pm$ 0.01 _a	0.50 $\pm$ 0.01 _b	0.43 $\pm$ 0.02 _c	0.34 $\pm$ 0.01 _d	0.55 $\pm$ 0.02 _a
1-Hexanol	9.68	111-27-3	fresh, herbaceous smell	0.73 $\pm$ 0.02 _a	0.67 $\pm$ 0.02 _{ab}	0.69 $\pm$ 0.02 _{ab}	0.72 $\pm$ 0.02 _a	0.70 $\pm$ 0.02 _{ab}	0.71 $\pm$ 0.02 _{ab}	0.70 $\pm$ 0.02 _a	0.72 $\pm$ 0.01 _{ab}	0.67 $\pm$ 0.02 _{ab}	0.65 $\pm$ 0.02 _a
3-Methylbutyl acetate	9.83	123-92-2	pleasant, fruity, and sweet smell	0.73 $\pm$ 0.02 _d	0.80 $\pm$ 0.03 _{cd}	0.92 $\pm$ 0.01 _b	0.80 $\pm$ 0.02 _c	0.91 $\pm$ 0.02 _b	0.97 $\pm$ 0.02 _{ab}	0.94 $\pm$ 0.02 _{ab}	0.94 $\pm$ 0.03 _{ab}	0.83 $\pm$ 0.03 _c	0.99 $\pm$ 0.04 _a
Ethyl hexanoate	16.18	123-66-0	tropical fruit/pineapple	38.44 $\pm$ 0.75 _a	30.47 $\pm$ 0.59 _{de}	35.16 $\pm$ 0.92 _{bc}	32.78 $\pm$ 0.44 _{cd}	30.86 $\pm$ 0.77 _{de}	38.03 $\pm$ 0.76 _a	28.11 $\pm$ 0.89 _e	34.03 $\pm$ 1.14 _{bc}	24.11 $\pm$ 0.35 _f	35.94 $\pm$ 1.60 _{ab}
Hexanoic acid	17.96	142-62-1	strong and unpleasant smell of rancid fat	2.21 $\pm$ 0.07 _e	3.78 $\pm$ 0.04 _a	3.26 $\pm$ 0.10 _c	3.43 $\pm$ 0.07 _{bc}	3.74 $\pm$ 0.06 _a	2.95 $\pm$ 0.04 _d	1.41 $\pm$ 0.04 _f	3.66 $\pm$ 0.16 _{ab}	3.39 $\pm$ 0.08 _c	0.59 $\pm$ 0.02 _g
Nonanal	21.49	124-19-6	fresh and citrusy smell, with floral nuances	0.51 $\pm$ 0.02 _d	0.62 $\pm$ 0.02 _b	0.40 $\pm$ 0.01 _e	0.67 $\pm$ 0.01 _a	0.65 $\pm$ 0.01 _{ab}	0.66 $\pm$ 0.01 _{ab}	0.55 $\pm$ 0.01 _{cd}	0.69 $\pm$ 0.03 _a	0.57 $\pm$ 0.02 _c	0.45 $\pm$ 0.01 _e
2-Phenylethanol	22.07	60-12-8	sweet and floral scent of roses	8.65 $\pm$ 0.24 _a	6.14 $\pm$ 0.20 _b	4.50 $\pm$ 0.12 _{de}	4.81 $\pm$ 0.06 _d	5.33 $\pm$ 0.14 _c	2.88 $\pm$ 0.10 _h	4.01 $\pm$ 0.14 _f	4.30 $\pm$ 0.02 _{ef}	3.37 $\pm$ 0.13 _g	3.16 $\pm$ 0.07 _{gh}
Diethyl succinate	25.40	123-25-1	fruity, reminiscent of apples or grapes	14.84 $\pm$ 0.58 _a	14.64 $\pm$ 0.32 _{ab}	14.14 $\pm$ 0.08 _{ab}	14.28 $\pm$ 0.41 _{ab}	14.01 $\pm$ 0.30 _{ab}	13.84 $\pm$ 0.44 _{ab}	13.71 $\pm$ 0.54 _{ab}	14.46 $\pm$ 0.47 _{ab}	13.88 $\pm$ 0.27 _{ab}	13.45 $\pm$ 0.57 _b

Table 2. Cont.

Name	RT (min)	CAS N°	Odor Descriptor	Area ×10 ⁷									
				V1	V2	V3	V4	V5	V6	V7	V8	V9	V10
Ethyl octanoate	26.15	106-32-1	sweet fruity, brandy-, apple and banana-like	54.44 ± 1.91 ^{bcd}	52.32 ± 0.31 ^{cd}	50.45 ± 0.92 ^d	50.04 ± 1.89 ^d	41.99 ± 1.38 ^e	58.28 ± 2.57 ^{ab}	36.13 ± 1.52 ^f	56.43 ± 0.70 ^{bc}	29.82 ± 0.89 ^g	61.86 ± 2.94 ^a
Decanal	26.46	112-31-2	aldehydic type odor	0.39 ± 0.01	0.26 ± 0.01	0.59 ± 0.01	nd	0.46 ± 0.01	nd	0.83 ± 0.02	nd	nd	nd
Octanoic Acid	27.12	124-07-2	slightly unpleasant rancid-like smell	14.95 ± 0.37 ^d	19.39 ± 0.74 ^b	16.49 ± 0.43 ^{cd}	18.82 ± 0.73 ^b	18.36 ± 0.52 ^b	14.85 ± 0.37 ^d	19.30 ± 0.45 ^b	21.66 ± 0.78 ^a	12.10 ± 0.46 ^e	18.15 ± 0.81 ^{bc}
Ethyl decanoate	35.03	110-38-3	waxy, fruity, sweet-apple, nut-like, winey	2.41 ± 0.07 ^a	2.48 ± 0.06 ^a	1.70 ± 0.04 ^{de}	1.83 ± 0.07 ^{cd}	1.59 ± 0.03 ^{ef}	1.87 ± 0.06 ^{cd}	1.44 ± 0.04 ^{fg}	0.19 ± 0.01 ^h	1.35 ± 0.04 ^g	2.17 ± 0.06 ^b

a, b, c, d, e, f, g, h. Letters indicate significant differences between samples (*p* < 0.05). Samples sharing the same letter do not differ significantly from each other according to the Tukey HSD test. RT: retention time. Odor descriptors from the PubChem (<https://pubchem.ncbi.nlm.nih.gov/>, accessed on 21 March 2025).

TCA levels ranged from 0.6 ng/L (V8) to 19.6 ng/L (V1), indicating heterogeneous contamination. These values are critical to understanding the potential for cork taint. Samples such as V1—well above the sensory threshold range of 1.5–4 ng/L [3]—are highly likely to present noticeable sensory defects. In contrast, V6 to V10, all below 1.1 ng/L, are considered free from perceptible TCA-related aromas. Intermediate samples (V2 to V5) show variable risk, with V3 (8.8 ng/L) and V5 (7.5 ng/L) nearing or exceeding the detection threshold.

Although no direct correlation was observed between TCA concentration and the levels of individual volatile compounds, the data suggest that high TCA levels may suppress fruity and floral notes through sensory masking or receptor interference. For example, despite high levels of 2-phenylethanol in V1, its floral perception may be compromised due to TCA presence.

In summary, both VOC composition and TCA levels should be interpreted independently to assess sparkling wine quality. While TCA does not appear to influence the formation of volatile compounds, it has a profound effect on their sensory expression. This dual-layer chromatographic analysis also provides an essential reference for validating the e-nose's capacity to detect and classify samples based on olfactory deviations caused by TCA.

3.2. E-Nose Analysis

The effectiveness of an e-nose in differentiating between wines depends on detecting these complex volatile profiles and how they may be affected by TCA contamination levels.

To illustrate the raw sensor responses obtained by the e-nose, Figure 3 presents examples of the time-resolved signals for two representative wines: V3 (8.8 ng/L TCA) and V7 (0.8 ng/L TCA), selected to reflect contrasting contamination levels.

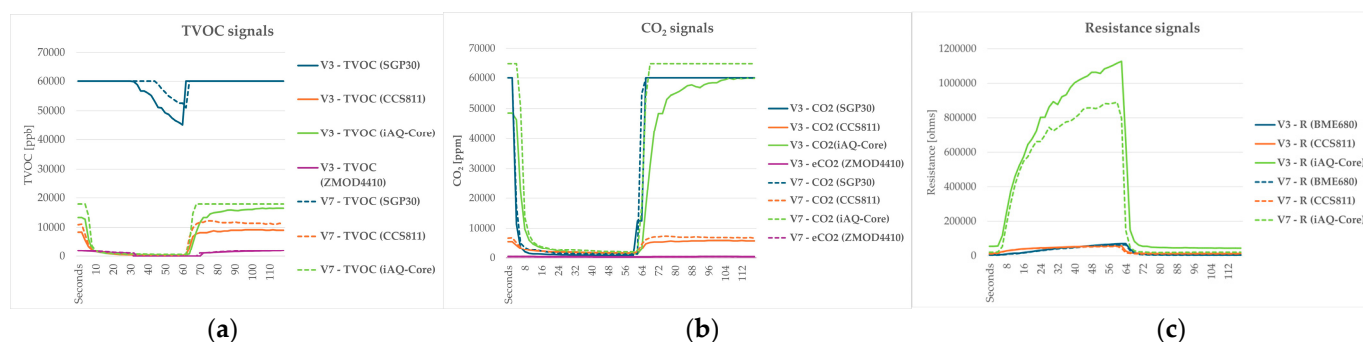


Figure 3. Raw sensor signals obtained for wines V3 (8.8 ng/L TCA) and V7 (0.8 ng/L TCA) during e-nose analysis. The plots show time-resolved signals related to (a) TVOC, (b) CO₂, and (c) resistance from selected sensors. Measurements illustrate the response kinetics to different headspace compositions and are used for subsequent feature extraction.

The figure displays sensor outputs related to TVOCs, CO₂ concentration, and resistance across the five gas sensors. These signals capture the dynamic behavior of the sensor array during exposure to wine headspace and clean air, showing distinct response magnitudes associated with each sample. Differences in response intensity and recovery profiles highlight the influence of volatile composition, supporting the feasibility of multivariate pattern analysis.

Multivariate statistical analysis could provide deeper insights into these relationships and verify the discrimination of wines through techniques such as PCA, clustering, ANNDA, or PLS.

The data obtained from the e-nose analysis of the headspace of the ten TCA-contaminated wines are represented in Figure 4.

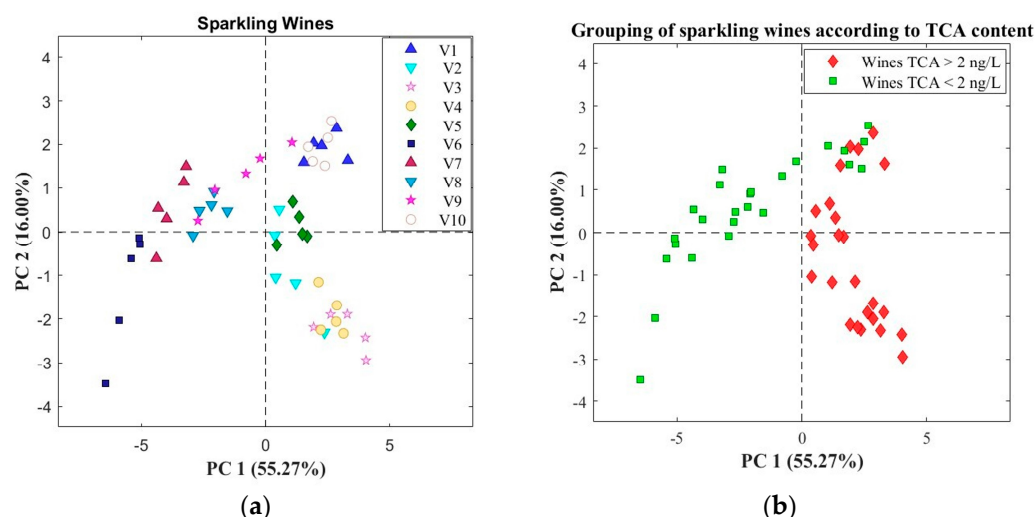


Figure 4. (a) PCA score plot showing the clustering of e-nose measurements for each wine sample. Each point represents one replicate measurement. (b) PCA grouping of wine samples based on TCA levels: wines with < 2 ng/L and ≥ 2 ng/L. The red dashed line represents the sensory detection threshold for TCA (2 ng/L). The plot illustrates the distribution of e-nose responses in the PCA space and the separation trend based on contamination level.

The graphs in Figure 4 show a PCA analysis for the ten TCA-contaminated wines. This type of analysis is used to reduce the dimensionality of the data and visualize the relationships between samples (in this case, the different wines) based on their volatile compound profiles.

Figure 4a represents the projection of the observations for the ten wines onto the first two principal components (PC1 and PC2), which explain 55.27% and 16.00% of the total data variability, respectively. Each point on the graph corresponds to an e-nose measurement for a specific wine, with different colors and symbols representing the various wines (V1 to V10). The points representing each wine tend to cluster, suggesting that the e-nose can differentiate the volatile profiles of the various wines. For example, wine V1 clusters in the upper right corner of the graph, while wine V6 is more dispersed in the lower left corner. However, there is some overlap between the values of V1 and V10, as well as little differentiation between V3 and V4, and significant overlap between V5 and V2, and between V9 and V8. This overlap may indicate that these wines have similar volatile profiles or that the e-nose is not effectively distinguishing them using the first two principal components.

Figure 4b shows the same data projection onto the first two principal components, but this time the points are color-coded according to TCA contamination levels: green for wines with $\text{TCA} > 2$ ng/L and red for wines with $\text{TCA} < 2$ ng/L. A partial separation was observed between wines with different TCA contamination levels, although with considerable overlaps, particularly between samples V1 and V10. This suggests that the e-nose response is influenced by the overall volatile matrix and not exclusively by TCA concentration. Wines with $\text{TCA} > 2$ ng/L primarily cluster on the right side of the graph, while wines with $\text{TCA} < 2$ ng/L are located on the left side. The first two principal components captured relevant information associated with TCA concentration, contributing to the partial separation observed between contaminated and uncontaminated wines. However, the overlap between V1 (with the highest TCA concentration) and V10 (with undetectable levels) highlights the complexity of the sample matrix and suggests that the e-nose response is influenced not only by TCA but also by the broader volatile profile.

The clustering observed in the graphs reinforces the e-nose's discriminative capability, although the overlap between some wines suggests that additional techniques or a greater number of components may be needed to improve accuracy in certain cases.

A cluster analysis model was applied to help evaluate the predictive capacity of the e-nose. The cluster graph is shown in Figure 5.

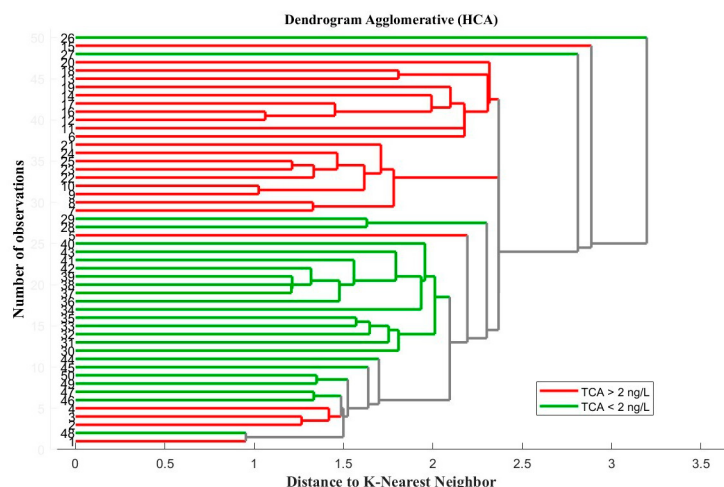


Figure 5. Cluster graph showing two main clusters.

In the dendrogram of Figure 5, two main clusters are observed, grouping the wines based on their TCA concentrations. The red cluster, located at the top, groups the wines with concentrations higher than 2 ng/L TCA, while the green cluster, at the bottom, includes wines with concentrations lower than 2 ng/L. The 50 observations correspond to five for each wine analyzed in order from V1 to V10. However, some samples, such as observations 26 and 27 from wine V6 in green within the red cluster, and observations 1, 2, 3, 4, and 5 from wine V1 in red within the green cluster, do not follow the expected pattern, indicating that other factors, besides TCA, influence the similarity between wines. This reinforces the idea that TCA concentration is not the sole determinant in cluster formation, and other volatile compounds could significantly influence the outcome. The consistency observed between these clusters and the results of the PCA analysis validates the findings, highlighting the importance of TCA presence at low concentrations for the sensory characterization of wines.

Next, an ANNDA classification model was applied using the most probable prediction rule to evaluate the e-nose's ability to classify sparkling wines according to their TCA concentrations, categorized as greater or less than 2 ng/L (Table 3).

Table 3. Confusion matrix corresponding to the 50 observations of the ten analyzed wines.

Predicted Class	Actual Class	
	>2 ng/L TCA	<2 ng/L TCA
>2 ng/L TCA	23	4
<2 ng/L TCA	2	21

In the analysis of 50 observations from the ten wines evaluated, a high level of accuracy was achieved in classifying samples with concentrations above and below 2 ng/L of TCA. Specifically, 23 samples with concentrations above 2 ng/L and 21 samples with concentrations below this threshold were correctly identified. Misclassifications were minimal, with four false positives and two false negatives. These results demonstrate the effectiveness of the model in distinguishing between the two analyzed categories.

The classification success rate of the ANNDA model is 88%. Table 4 summarizes the key performance metrics of this model for classifying samples based on their TCA content.

Table 4. Performance metrics for the classification of samples by TCA content.

Class	TPR (Recall)	FPR	TNR	FNR	N	Err	P (Precision)	F1 (F1 Score)
>2 ng/L TCA	0.92	0.16	0.84	0.08	25	0.12	0.85	0.88
<2 ng/L TCA	0.84	0.08	0.92	0.16	25	0.12	0.91	0.87
Matthew's Correlation Coefficient (MCC) = 0.76								

Analysis of Results: Precision, recall, and the F1 Score are crucial for assessing the model's efficacy. Precision ranges from 0.85 for the ">2 ng/L TCA" category to 0.91 for "<2 ng/L TCA", indicating high accuracy in the model's positive predictions. Recall rates of 0.92 for ">2 ng/L TCA" and 0.84 for "<2 ng/L TCA" demonstrate the model's effective capability to identify positive samples at both TCA levels. The F1 Score exceeding 0.87 for both categories indicates a well-maintained balance between precision and recall.

The MCC of 0.76 confirms a strong overall performance of the model, evidencing its effectiveness in accurately classifying both positive and negative samples. These results underscore the robustness and reliability of the ANNDA model, highlighting the potential of electronic noses and advanced classification models to enhance quality control in the wine industry by facilitating early detection of contaminants like TCA and the production of higher-quality wines.

Finally, quantitative PLS models were applied. In the first case, the TCA concentrations of the ten wines correlated with the data obtained from the e-nose, as shown in Figure 6.

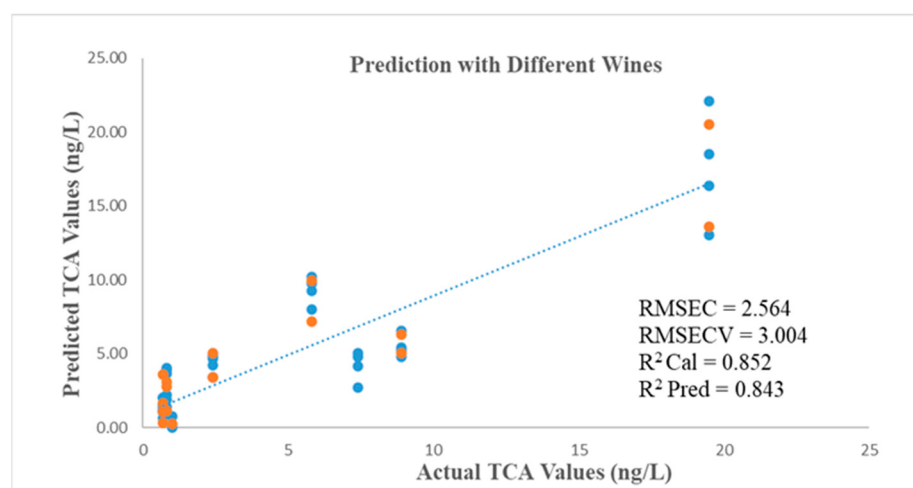


Figure 6. Correlation between TCA concentrations measured by GC-MS and those predicted by the e-nose using a PLS model. Blue points represent the calibration dataset, while orange points correspond to the validation dataset.

Figure 6 shows the relationship between experimental TCA values obtained by chromatography for ten different wines and the predictions made by the e-nose using a PLS regression model. The results indicate a significant correlation ($R^2 = 0.843$), suggesting that the e-nose has a good capacity to predict TCA concentrations despite the intrinsic variability among wine samples. However, this variability among wines may limit the model's maximum precision, reflected in the dispersion of some points around the regression line.

On the other hand, Figure 7 presents the results of TCA prediction in a single wine spiked with increasing TCA concentrations.

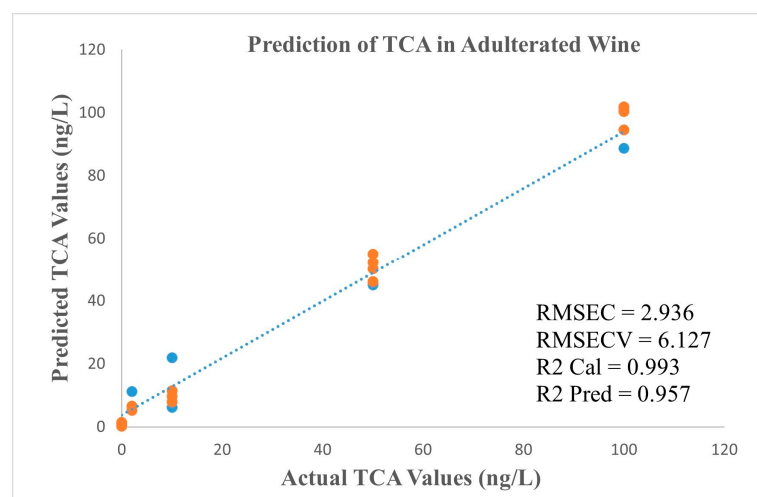


Figure 7. Actual TCA values determined by GC-MS in spiked wine sample versus predicted values with e-nose. Orange points represent the calibration dataset, while blue points correspond to the validation dataset.

In this case, the correlation between theoretical values and those predicted by the e-nose is remarkably high ($R^2 = 0.957$), indicating that when wine matrix variability is minimized, the PLS model can predict TCA concentration with great accuracy. This excellent fit suggests that the matrix's consistency allows the e-nose to identify and quantify TCA more accurately, as the only changing factor is the TCA concentration.

Comparing the results of both figures, the e-nose shows more consistent and precise performance when used with a homogeneous matrix, as in the case of the spiked wine. This implies that variability between different wines introduces complexity that may affect the precision of predictions. These findings underscore the importance of considering matrix composition in the quantitative analysis of specific compounds such as TCA. In summary, while the e-nose is effective in predicting TCA in different wines, its precision significantly increases when wine variability is controlled, highlighting its potential in quality control applications where conditions are more uniform.

4. Discussion

The e-nose analysis demonstrated a remarkable ability to capture differences in the volatile profiles of wines, aligning with chromatographic results in discriminating samples with varying levels of TCA, as suggested by other authors [18]. These findings corroborate previous studies indicating that electronic noses can be effective tools for detecting contaminants in complex matrices like wine [19].

The use of PCA and cluster analysis provided a clear visualization of how wine samples are grouped according to their volatile profile and TCA concentration. The results highlight the potential of using a portable e-nose to detect differences in volatile profiles of sparkling wines with varying levels of TCA. However, the observed overlaps between certain samples, along with the influence of the broader aromatic matrix, indicate that further validation with more diverse wine sets is needed before the technique can be applied reliably in real-world scenarios. These findings are consistent with those obtained by other authors [18]. Moreover, the PLS regression models applied to wine samples with varying TCA content and to a spiked wine sample demonstrated that the e-nose's accuracy significantly improves under controlled conditions. The high correlation obtained in the spiked wine confirms that when matrix variability is minimized, the e-nose can accurately predict TCA concentrations, as previously reported [20]. Despite the promising results, the study faced challenges related to the inherent variability of sparkling wine samples and

the e-nose's sensitivity to environmental factors during measurement. Sample variability can significantly impact the device's classification ability, underscoring the importance of continuous calibration and sensor adjustment to adapt to different production contexts. Additionally, the influence of factors such as humidity and temperature on sensor sensitivity highlights the need to maintain standardized conditions during analysis, which is crucial for ensuring the reliability and reproducibility of the results [18].

The results obtained open several avenues for future research. Additionally, the relatively small number of wine samples ($n = 10$) and total observations ($n = 50$) increases the risk of overfitting in multivariate models such as ANNDA and PLS, despite the use of random subset cross-validation. This limitation should be taken into account when interpreting the predictive performance of the models. Future work will include larger and more diverse wine sample sets to validate and generalize the findings of this study, as well as improve model robustness for broader industrial applications. The limitations of MOS sensors, such as drift, LOD, and the reproducibility of measurements, must also be taken into account. A primary focus could be on optimizing sensor selection and improving data analysis algorithms to enhance the specificity and sensitivity of the electronic nose system, minimizing the effect of matrix variability. Another promising area of research is the application of the e-nose for in situ and real-time detection of TCA and other volatile contaminants directly on production lines. This would involve developing portable and robust devices capable of operating under industrial conditions, providing effective tools for quality control and food safety.

The application of the electronic nose for TCA detection in champagne has the potential to revolutionize quality control practices in enology, offering a rapid, non-destructive, and cost-effective alternative to traditional analytical methods. Implementing this technology could significantly improve the efficiency of contaminant detection, contributing to the production of high-quality wines and sparkling wines, ensuring consumer satisfaction. Given its compact design and rapid response time, the portable e-nose developed in this study could be integrated into the quality control processes of wineries for preliminary screening of TCA contamination in sparkling wines prior to bottling or shipment.

5. Conclusions

This study highlights the significant potential of the e-nose as a complementary tool to gas chromatography for the detection and quantification of TCA in sparkling wines. The results demonstrate the potential of a portable e-nose device to detect aroma differences in sparkling wines with similar volatile profiles and varying TCA contamination levels under controlled conditions. However, further validation with a broader variety of wine samples is necessary to confirm its applicability to more complex real-world matrices. The correlation with GC-MS results confirms its sensitivity to detecting TCA, though further optimization is needed to enhance its ability to discriminate other volatile compounds present in wines.

To maximize its effectiveness, it is crucial to continue developing models that account for the complexity of the wine's volatile profile. With the ongoing optimization of sensors, algorithms, and the development of portable devices, as well as the study of a larger number of samples, the e-nose could become a standard in quality control and food safety within enology, ensuring the quality and consistency of the final product.

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R.S.; funding acquisition, R.S. and J.L. All authors have read and agreed to the published version of the manuscript.

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Abbreviations

The following abbreviations are used in this manuscript:

ANND	Artificial Neural Network Discriminant Analysis
GC-MS	Gas Chromatography–Mass Spectrometry
GC-MS/MS	Gas Chromatography–Tandem Mass Spectrometry
MOS	Metal Oxide Semiconductor
PCA	Principal Component Analysis
PLS	Partial Least Squares
PLS-R	Partial Least Squares Regression
R ²	Coefficient of Determination
RT	Retention Time
SPME	Solid-Phase Microextraction
TCA	2,4,6-Trichloroanisole
TVOC	Total Volatile Organic Compounds
VOCs	Volatile Organic Compounds

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