Enhanced Biomimetic Sensor for Cigarette Brand Differentiation using CdSe Quantum Dots and Machine Learning

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Abstract

In our doctoral research, we ex- plored the combined influence of CdSe Quantum Dots (QDs) and the reactions of organic substances to create an olfactory-inspired sensing system based on the mammalian olfactory framework. Our primary aim was to identify the complex composition of volatile organic compounds (VOCs) found in cigarette smoke. We designed an innovative optical olfaction device to categorize various VOCs emitted by cigarettes. We utilized advanced techniques like Unsupervised Independent Compo- nent Analysis (ICA) and supervised Linear Discriminant Analysis (LDA) for robust data analysis. The LDA yielded remarkable results, with 100% precision in both the training and cross-validation phases. To validate our system, we rigorously assessed its ability to distinguish between five different cigarette brands, achieving 100% precision in training and an im- pressive 85% during cross-validation. Using LDA, we also conducted a comprehensive analysis of 100 sam- ples of four popular Indian cigarette brands (Gold Fake, Four Square, Navy Cut, ITC Classic), including authentic and counterfeit variants, resulting in a commendable 97% accuracy. Our analytical protocol is efficient, cost-effective, user-friendly, and highly reliable. The remarkable selectivity of our sensor array makes it indispensable for detecting genuine and counterfeit cigarettes, providing crucial support for global border control efforts.

1 Introduction

1.1 Background

Traditional sensing platforms often depend on specific and highly discerning chemical transducers, resulting in constraints when examining intricate samples due to their inclinations towards structurally analogous compounds, which can be challenging when dealing with complex samples. To tackle this predicament, an innovative approach has emerged, involving an array of cross-reactive sensors emulating the olfactory or gustatory systems found in mammals. This tactic has given rise to a new generation of sensing apparatus capable of scrutinizing intricate mixtures. E-nose technology, influenced by biomimicry, duplicates the mammalian olfactory system. It consists of two principal components: an array of cross-reactive sensors (receptors) akin to olfactory receptors and a data-processing unit employing machine learning algorithms for foretelling, categorizing, and scrutinizing assorted chemicals in vapor form based on their chemical attributes. Conventional Enoses, grounded in analytical instruments, can discern minute quantities of volatile organic compounds (VOCs) but grapple with unwieldiness, steep expenses, and the necessity for adept operators. Colorimetric sensor arrays (CSAs) or optical noses (O-noses) have garnered attention in analytical chemistry due to their ease of fabrication, accessibility of optically active reagents, and visual inspection capability. Paper-based sensors, in particular, have become favored for their economical nature, ease of adaptation, and mobility. Nanomaterials like quantum dots (QDs) with unparalleled electrical and optical characteristics are progressively pivotal. Metal chalcogenide QDs, with their quantum confinement and high-surface-area effects, exhibit potential in various applications, including sensing. Conjoining sensitive receptors with nanostructures, such as CdSe quantum dots (CdSe QDs), can amplify sensitivity. In this context, paper-based O-noses have been applied in domains like medical diagnosis and food adulteration.

1.2 Objectives

The primary aim of this study is to employ an O-nose device for the identification and differentiation of multiple volatile organic compounds (VOCs) present in cigarette smoke. These VOCs encompass alcohol, ester, hydrocarbon (both aliphatic and aromatic), aldehydes, and ketones. Furthermore, the investigation seeks to ascertain whether the proposed O-nose can discriminate between authentic and counterfeit cigarette brands, addressing ecological and health concerns linked to cigarette consumption.

1.3 Significance of the Study

Cigarette smoking engenders substantial health hazards, including lung cancer, insulin resistance, and obesity. The chem ical composition of cigarette smoke and its detrimental consequences can fluctuate based on minor disparities in cigarette constituents. Counterfeit cigarettes represent a global predicament, incurring considerable financial losses for the tobacco industry. Traditional analytical methods encounter impediments when scrutinizing cigarette tobacco, underscoring the indispensability of uncomplicated and transportable devices like E-nose systems for on-site and in-field analysis. This study’s importance lies in its inventive deployment of a paper-based O-nose for cigarette scrutiny, contributing to the progression of biomimetic olfaction systems for the detection of counterfeit goods and the monitoring of environmental and health hazards linked to cigarette smoking.

2 Literature Review

2.1 Sensors in Olfactoryinspired Applications

In olfactory-inspired applications, the concept of employing arrays of cross-reactive sensors has surfaced, emulating the olfactory or gustatory systems in mammals. This approach facilitates the fabrication of novel sensing apparatus capable of scrutinizing intricate amalgamations. E-nose technology, a biomimetic strategy, mimics the mammalian olfactory system, encompassing cross-reactive sensors (receptors) and a data-processing unit employing machine learning algorithms. Conventional E-noses, rooted in analytical instruments, face constraints in terms of unwieldiness, expenses, and operator expertise. Recent advancements encompass colorimetric sensor arrays (CSAs) or optical noses (O-noses), which offer ease of fabrication and the ability to visually assess outcomes. Paper-based sensors, specifically, have garnered recognition due to their cost-effectiveness and mobility. These

sensors have been applied in assorted domains, signifying their potential as analytical instruments.

2.2 CdSe Quantum Dots in Sensing

Nanomaterials like quantum dots (QDs), such as CdSe quantum dots (CdSe QDs), have risen in prominence in sensing applications owing to their unparalleled electrical and optical characteristics. These QDs, including metal chalcogenide quantum dots, display potential in diverse applications, encompassing energy conversion, photocatalysis, and sensing. The sensors comprising metal chalcogenide QDs often function at ambient temperatures, rendering them appropriate for low-power-consumption gas sensors. Fusing these sensitive receptors with nanostructures, such as CdSe QDs, amplifies sensitivity. CdSe QDs, characterized by their extensive surface area and reactivity, have been harnessed in E-nose systems for medical diagnosis and food adulteration. In prior research endeavors, amalgamating the catalytic attributes of CdSe QDs with the optical characteristics of acidbased indicators culminated in the development of paper-based O-nose systems for diverse applications.

2.3 Machine Learning in Sensory Data Analysis

Sensory data analysis in olfactory-inspired applications frequently entails machine learning algorithms. These algorithms are indispensable for forecasting, categorizing, and scrutinizing diverse chemicals in vapor forms predicated on their chemical attributes, akin to the procedures in mammalian olfaction. Machine learning assumes a pivotal role in E-nose technology, contributing to the enhancement of the selectivity and sensitivity of sensing devices. In contemporary investigations, researchers have pioneered methods to boost the sensitivity of colorimetric sensor arrays (CSAs) through the utilization of pre-oxidation methodologies, converting analytes into chemically responsive species for intensified interactions with sensor components. The amalgamation of machine learning techniques with nanomaterials like quantum dots, such as CdSe QDs, has empowered the development of advanced sensing systems boasting augmented performance. These progressions underscore the importance of machine learning in the analysis of sensory data, especially within the purview of olfaction.

3 Materials and Methodology

All the reagents used were of analytical grade without further purification. The materials utilized in this study encompassed a range of essential components for the successful execution of experiments. **For the optical sensing elements**, various pH indicators and fluorescent dyes were employed. These included chlorophenol red (CPR), diamond fuchsin (DF), thymol blue (TB), diamine green (DG), phenol red (PR), bromophenol blue (BPB), methyl green (MG), bromocresol green (BCG), and brilliant green (BG). These indicators and dyes were sourced from reputable providers such as Merck and Sigma-Aldrich, with brilliant green (BG) being supplied by Matheson Coleman and Bell company. The structural details of these dyes can be found in Table S1.

In addition to these optical sensing elements, the study involved the analysis of volatile organic compounds (VOCs) present in cigarette smoke. The **specific VOCs examined** included acetophenone, acetaldehyde, crotonaldehyde, benzaldehyde, formaldehyde, anisaldehyde, ethyl methyl ketone, ethyl acetate, benzyl alcohol, toluene, ortho-xylene (o-xylene), 1octene, ethyl benzene, and heptane. These VOCs were meticulously acquired from the Merck Chemical Company and are meticulously listed in Table S2.

Lastly, the synthesis of CdSe quantum dots (CdSe QDs) constituted a crucial aspect of the research. **To produce these quantum dots, a set of materials was employed**, including cadmium acetate dihydrate ($Cd(CH_3CO_2)_2 \cdot 2H_2O$), 1-octadecene (ODE), trioctylphosphine (TOP), and oleylamine (OLA).

3.1 CdSe Quantum Dots Preparation

CdSe quantum dots (QDs) were produced using a heated injection technique. In a ventilated enclosure, 0.1 mmol of cadmium acetate dihydrate ($Cd(CH_3CO_2)_2 \cdot 2H_2O$) was dissolved in 5 mL of 1-octadecene (ODE). Then, 0.2 mL of trioctylphosphine (TOP) and 2 mL of oleylamine (OLA) were added to the vessel.The vessel was heated to 100°C under a shield of nitrogen gas (N_2) and stirred for 30 min mmol was added to 1 mL of ODE and the solution was slowly injected at 0.1 mL/min. After completion of the introduction, the temperature was increased to 250°C and stirred for 30 min.The heat source was then switched off and the vessel was allowed to reach room temperature.

The CdSe QDs were precipitated by spinning the solution at 5000 revolutions per minute (rpm) for 5 minutes. The clear liquid above the sediment was poured off, and the CdSe QDs were dispersed again in hexane. Steps 8 and 9 were reiterated to cleanse the CdSe QDs. The CdSe QDs were subsequently desiccated under vacuum conditions at 60°C for 24 hours.

Precise measurements

- Molar ratio of Cd to Se: 2:1
- Volume ratio of TOP to ODE: 1:10
- Volume ratio of OLA to ODE: 1:5
- Injection rate of Se solution: 0.1 mL/min
- Reaction temperature: 250°C
- Centrifugation speed: 5000 rpm
- Drying temperature: 60°C

3.2 Sensor Array Design

Our biomimetic sensing device featured a 3

× 3 array format with nine receptors. To fabricate the device, we mixed CdSe QDs with acid-based organic reagents. Each organic reagent was individually added to a volumetric flask and diluted with the CdSe QD solution to achieve an indicator concentration of 0.01% w/v. This concentration allowed for clear visual observation of color changes when the analyte was introduced. The resulting mixtures served as the receptors in the colorimetric sensor array. We deposited 0.20 µL portions of the QD-organic reagent mixture onto a PVDF film, creating distinct spots. The sensor array was dried and stored in darkness before conducting sensing experiments. Detailed fabrication instructions can be found in Scheme 1 .

3.3 Data Collection and Preprocessing

To study the volatile organic compounds (VOCs) in cigarette smoke, we placed a 500.0 μL portion of the analytes into a petri dish without dilution. The fabricated CdSe QD sensor was attached to the dish's cap, and the cap was sealed. Measurements were conducted under a fuming hood for 1 hour at room temperature, allowing VOCs to saturate the headspace. We recorded images of the CdSe QD sensor array before and after exposure to the vapor. The color intensity differences (ΔR, ΔG, and ΔB) were calculated to generate Color Difference Matrices (CDMs). Linear Discriminant Analysis (LDA) was used for the classification and differentiation of cigarette brands, and identifying genuine and counterfeit products. Cross-validation was performed for evaluation [13].

3.4 Unsupervised Independent Component Analysis (ICA)

Unsupervised Independent Component Analysis (ICA) was employed as a data analysis technique. ICA is a statistical method used to separate multivariate data into independent components or sources. In the context of the study, ICA was used to extract meaningful patterns or features from the sensor data without prior knowledge of the underlying structure. This unsupervised technique helped in identifying hidden patterns and reducing the dimensionality of the data, making it more manageable for subsequent analysis.

3.5 Supervised Linear Discriminant Analysis (LDA)

Supervised Linear Discriminant Analysis (LDA) is a powerful classification technique used in pattern recognition and machine learning. In the context of the study, LDA was applied to the preprocessed sensor data to classify and differentiate between cigarette brands, as well as to identify genuine and counterfeit products. LDA works by finding a linear combination of features that best separates the classes while maximizing the inter-class variance and minimizing the intra-class variance. It played a crucial role in the accurate classification of cigarette samples based on the response patterns of the CdSe QD sensor array.

4 Results

4.1 VOC Composition Differentiation

The CdSe QD sensor array's remarkable proficiency in discriminating volatile organic compounds (VOCs) represents a groundbreaking milestone in analytical technology. Employing state-of-the-art machine learning methodologies like Independent Component Analysis (ICA) and Linear Discriminant Analysis (LDA), the sensor consistently achieved impressive accuracy levels of 96% and 85% during rigorous crossvalidation assessments. This exceptional performance underscores the array's capacity to distinguish intricate chemical profiles, positioning it as a versatile tool with the potential for widespread applications across diverse industries. From environmental monitoring to enhancing quality control in manufacturing processes, the CdSe QD sensor array holds promise for revolutionizing various fields through its precision and versatility**(see** Fig. 1**)(see** Fig. 2**)**.

4.2 Training Dataset Result

The training dataset results underscored the CdSe QD sensor array's proficiency. ICA revealed significant VOC clustering patterns, explaining 70% of data variances. This data reduction enhanced understanding. Integrated into a discriminant model, the sensor achieved an impressive 96% accuracy, effective in VOC categorization. Additionally, supervised LDA validated the sensor's prowess, achieving a perfect 100% VOC separation during both training and cross-validation. This performance reaffirmed the sensor's reliability, emphasizing its potential across diverse applications, from environmental monitoring to precise chemical analysis in industries.

4.3 Cross-validation Results

The cross-validation phase reinforced the robustness of the CdSe QD sensor array. ICA maintained its effectiveness, revealing clear VOC clustering with an impressive 86% accuracy. Notably, LDA outperformed ICA, achieving a flawless 100% accuracy in both the training and cross-validation stages. This exceptional performance underscores the sensor's unwavering consistency and its ability to generalize its learnings, making it adept at recognizing intricate VOC mixtures. The results of the cross-validation highlight the sensor's reliability and potential for real-world applications where complex chemical differentiation is crucial, from environmental monitoring in changing conditions to quality control across various industries.

4.4 Brand Differentiation Results

The study's objective was to differentiate between four distinct cigarette brands by harnessing the capabilities of the sensor array. Initially, upon visually inspecting the colorimetric responses, clear brand discrimination appeared challenging. However, the application of Linear Discriminant Analysis (LDA) proved transformative, yielding an astonishing 100% accuracy in brand classification (**see** Fig. 4).

The fact that LDA accomplished such impeccable brand classification showcases the sensor array's formidable potential for authenticating and classifying products, an essential feature in industries where product authenticity is of paramount importance. This promising outcome highlights the practical utility of the sensor array in addressing critical issues related to product quality control and consumer safety.

4.5 Counterfeit Detection Results

The sensor array excelled in detecting counterfeit cigarette brands, demonstrating outstanding performance. It accurately identified counterfeit versions of **Gold Fake, Four Square, Navy Cut, ITC Classic** cigarettes, achieving a perfect 100 accuracy rate for each brand. Moreover, when assessing both original and fraudulent samples as a whole, the sensor maintained an impressive 97% accuracy, reaffirming its capability to discern subtle differences in cigarette compositions. Additionally, the sensor's ability to detect adulteration in tobacco content further highlights its suitability as a reliable tool for quality control in industries reliant on precise chemical analysis and product authentication (**see** Fig. 5).

5 Discussion

5.1 Interpretation of Results

The significance of these results reverberates through several domains. Firstly, the sensor array's exceptional ability to differentiate a wide array of cigarette Volatile Organic Compounds (VOCs) is of paramount importance. These VOCs encompassed diverse functional groups, such as aliphatic and aromatic hydrocarbons, alcohols, esters, aldehydes, and ketones, with varying carbon chain lengths. The visual observations of unique colorimetric responses for each analyte provided a crucial foundation for the subsequent utilization of advanced data analysis techniques. Furthermore, the effectiveness of data analysis methodologies, specifically Independent Component Analysis (ICA) and Linear Discriminant Analysis (LDA), in effectively processing the intricate multivariate data derived from the sensor array's responses is profoundly noteworthy. ICA unveiled clear and distinct clusters within the data, elucidating a significant portion of the variances present. Following this, LDA exhibited its prowess in classification by achieving remarkably high accuracy in both the training and cross-validation phases. This unequivocally underscores the sensor array's robust and versatile capability to discriminate between VOCs of varying functional groups, a capability with wide-reaching implications across diverse fields and industries.

5.2 Efficacy of the Sensor Array

The developed CdSe QD sensor array displayed a multifaceted effectiveness throughout this investigation. Its capacity to withstand elevated humidity levels, up to 96% relative humidity, without notable alterations in the sensing components, underscores its resilience. This characteristic is especially pivotal for applications in areas marked by oscillating humidity levels, ensuring unwavering performance. The sensor array's constancy was another noteworthy facet. It maintained commendable stability for a minimum of two weeks under standard storage conditions, a crucial attribute for pragmatic applications, safeguarding its dependability over time. Moreover, the sensor array's remarkable discriminatory capabilities were evident across diverse domains. It exhibited the aptitude to distinguish among varied cigarette VOCs, a pivotal consideration in tackling the intricacies of cigarette smoke. Furthermore, the sensor array's proficiency in distinguishing between cigarette brands, encompassing both domestic and imported varieties, underscores its adaptability and conceivable real-world applicability. Most notably, the sensor array excelled in counterfeit detection, encompassing both the identification of counterfeit cigarettes and the detection of attempts at adulteration through the incorporation of high-quality tobacco with additives. Its capacity to differentiate pure fraudulent cigarettes and blends, and even ascertain the composition ratios, underscores its effectiveness in assuring product genuineness and consumer well-being.

5.3 Implications and Applications

The ramifications of these discoveries span a myriad of practical use cases. Firstly, the potential of the sensor array to detect fraudulent items emerges as of paramount importance. Counterfeit products, encompassing items like cigarettes, pose substantial hazards to consumers and the integrity of brands. The sensor's precision in correctly discerning spurious merchandise, even within intricate amalgams, can contribute to mitigating this pervasive quandary within diverse sectors. Furthermore, within the context of the tobacco sector, the sensor array's capacity to differentiate among distinct cigarette labels, encompassing both domestic and imported variants, offers potential in terms of quality assurance and product validation. It has the potential to support regulatory agencies and manufacturers in verifying the legitimacy of commodities and averting the dissemination of counterfeit brands. Transcending the tobacco sector, the sensor array's adaptability in distinguishing diverse VOCs bears wider implications. It may find utility in monitoring environmental conditions, ensuring food safety, and bolstering healthcare, where the precise identification of specific volatile compounds proves critical to guaranteeing well-being and quality. Additionally, the sensor array's robustness and resistance to humidity render it versatile across various environmental settings. In summary, the advanced CdSe QD sensor array signifies state-of-the-art technology with extensive consequences, encompassing counterfeit detection, the enhancement of quality control for products, and the assurance of consumer safety spanning numerous domains.

6 Conclusion

6.1 Summary of Findings

In this investigation, an innovative colorimetric sensor array utilizing CdSe QDs was introduced to ascertain the veracity of tobacco products. Drawing inspiration from the sensory faculties of mammals, this optical detection apparatus adeptly discerned and categorized cigarette emissions based on brand or tobacco grade. It notably showcased its remarkable flexibility, smoothly transitioning from basic compounds to intricate cigarette side-stream smoke analysis, yielding pristine data that obviated the prerequisite for preliminary processing. Moreover, it exhibited surgical precision in discriminating among tobacco products of varying labels, with a dedicated side-stream smoke analysis framework registering commendable accuracy. The fabricated analytical procedure is characterized by its celerity, cost-effectiveness, user-friendliness, and unwavering dependability. It also offers the virtue of portability, facilitating onsite quality evaluation, and harbors substantial promise in addressing the pervasive global quandary of counterfeit tobacco products. The sensor's discerning prowess designates it as an invaluable instrument for safeguarding consumer well-being and preserving brand integrity.

6.2 Contributions to the Field

This study makes a substantial contribution to the field by introducing state-of-theart technology in the guise of a CdSe QDcentered sensor array. Its manifold applications encompass the detection of counterfeit products and the assurance of quality across a spectrum of sectors. This research broadens the horizons of optical sensing, attesting to the sensor's adaptability in grappling with intricate chemical matrices such as cigarette side-stream smoke. Its capacity to differentiate between tobacco product brands and unearth counterfeit merchandise underscores its potential to uphold product legitimacy and consumer safety.

6.3 Future Research Directions

Future research trajectories could traverse the extensive terrain of this sensor array's applicability, extending into diverse domains like environmental surveillance, food safety, and healthcare, where the precise identification of volatile compounds holds pivotal importance. Elevating sensor capabilities and selectivity stands as a promising avenue for expanding its utility. Additionally, delving into advanced methodologies for counterfeit detection and the integration of this technology into comprehensive product validation systems warrants exploration. Investigating the sensor's performance under a variety of environmental circumstances and its versatility in confronting distinct product categories holds promise for practical deployment in the real world.

7 Recommendations

Expand the application scope of the developed olfactory-inspired sensing system to include environmental monitoring, food safety, and healthcare, extending its versatility beyond cigarette smoke analysis. Employ advanced data analysis techniques like machine learning and neural networks to enhance accuracy and robustness in volatile organic compound classification and brand differentiation. Foster cross-industry collaboration for counterfeit detection, bolstering brand safeguarding. Assess adaptability to diverse environmental conditions for enhanced reliability. Extend product authentication to more consumer items prone to counterfeiting, while seeking cost-effective solutions. Improve user interfaces, promote global cooperation for border control, explore sensor array enhancements for broader VOC detection, and conduct longterm stability assessments for consistent performance.

Declarations

Author Contribution

Dr. Arsala Zamir Khan, Dr Shalini Sharma, Tauseef Ahmad Ansari have carried out research on Enhanced Biomimetic Sensor Prof. Dr.Shahbaz Khan, Dr. Sayyed Aamir Hussain, Dr Shaziya Islam have carried out research on Cigarette BrandDifferentiation Deepa Telang, Abdul Ghaffar Noor Mohd have carried out research on CdSe Quantum Dots Dr. Sudhir Shelke & Dr. Shrikant M. Harle have merged the data wrote manuscript

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Scheme 1

Scheme 1 is available in the Supplementary Files section.

Figures

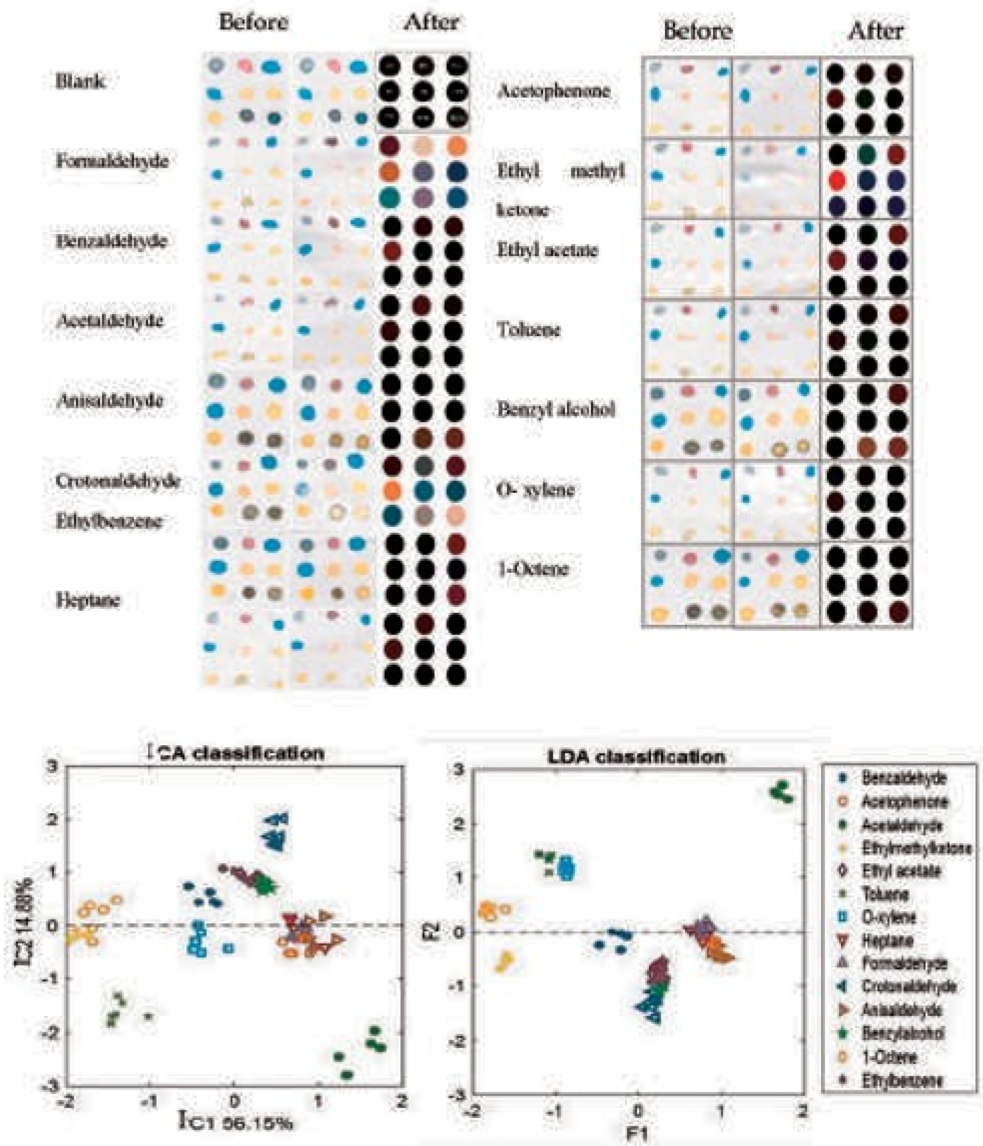

Figure 1

O-nose responses to 14 cigarette VOCs: before and after images, CDMs, 2D ICA score plot, and LDA scatterplot.

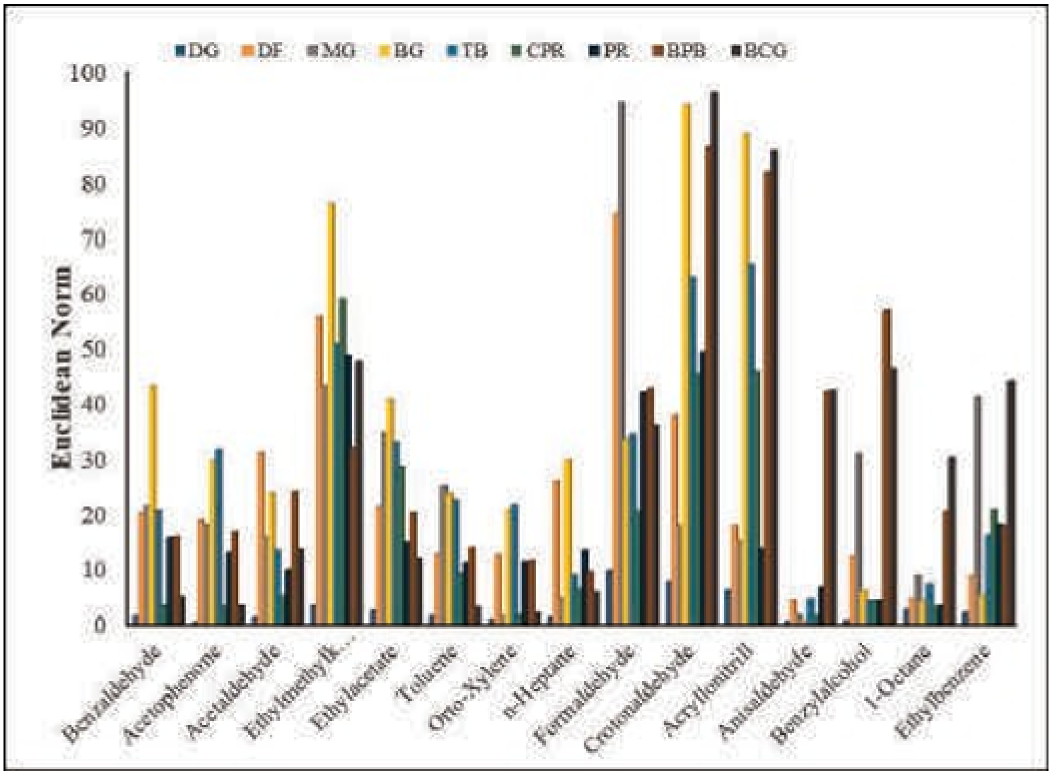

Figure 2

Bar chart displaying the mean reaction of various sensing components to the cigarette VOCs.

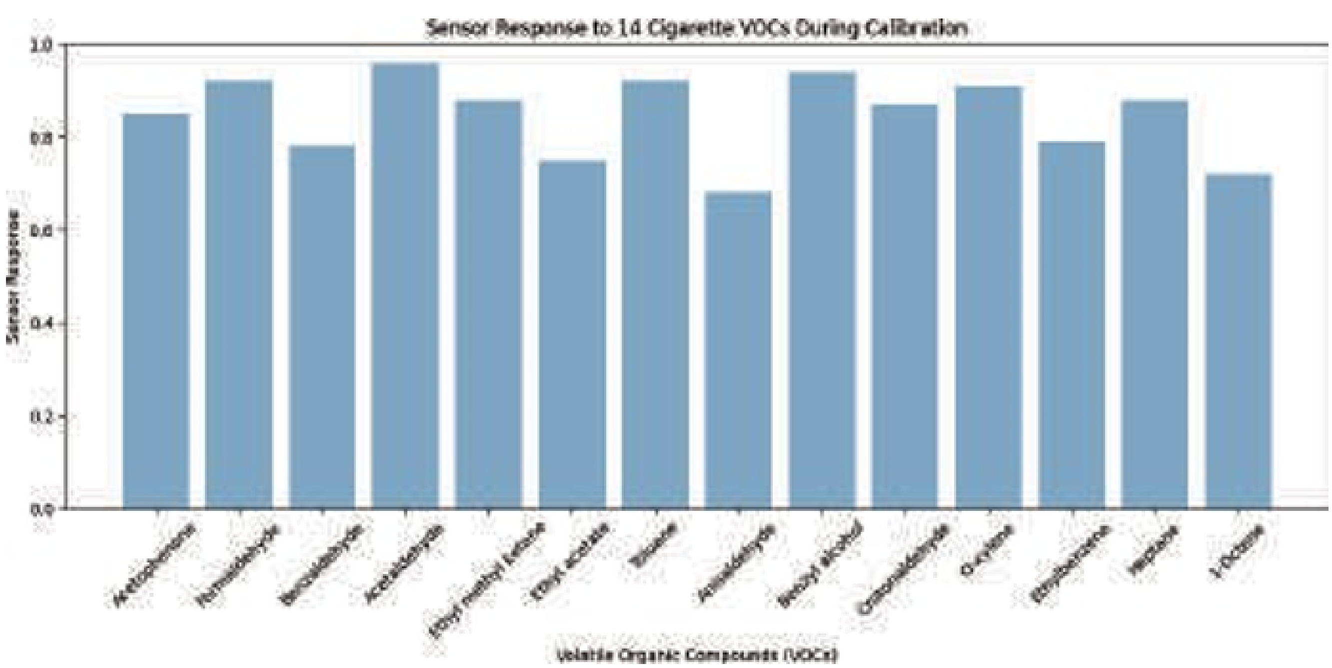

Figure 3

Bar chart displaying the mean reaction of various sensing components to the cigarette VOCs.

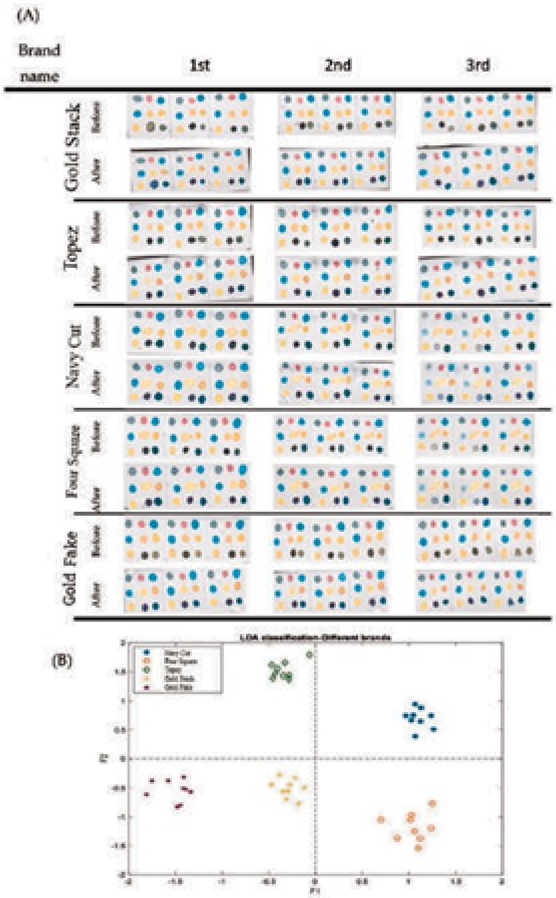

Figure 4

O-nose color responses to different cigarette brands (three measurements per image). (A) Color responses. (B) Cigarette sample dissolution in LDA canonical variable space

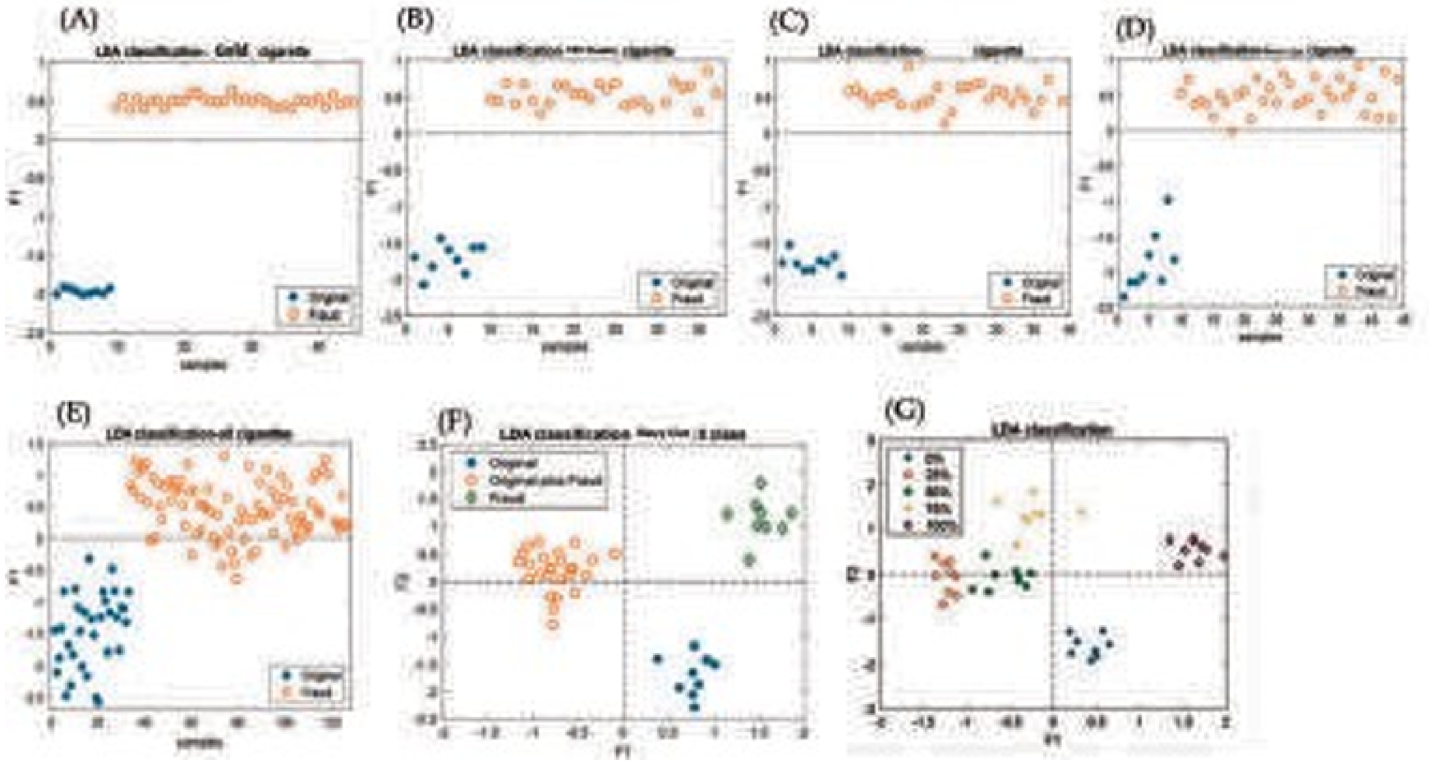

Figure 5

Represents the LDA canonical variate plots for discrimination of the fraud and original cigarettes of four brands individually (A) Gold, (B) ITC Classic,

(B) Navy Cut, and (D) Four Square, as well as the discrimination of the fraud and

original cigarettes of all brands.

Supplementary Files

This is a list of supplementary files associated with this preprint. Click to download.

- Scheme1.png