# Detection and classification of pesticide residues in dandelion (*Taraxacum officinale* L.) by electronic nose combined with chemometric approaches

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**Abstract:** In this study, for the first time a suitable pesticide residue detection system for dandelion (*Taraxacum officinale* L.) was established based on electronic nose to determine and study the concentration of pesticide residue in dandelion. Dandelions were sprayed with different concentrations of pesticides (avermectin, trichlorfon, deltamethrin, and acetamiprid), respectively. Data collection was performed by application of an electronic nose equipped with 12 metal oxide semiconductor (MOS) sensors. Data analysis was conducted using different methods including BP neural network and random forest (RF) as well as the support vector machine (SVM). The results showed the superior effectiveness of SVM in discrimination and classification of non-exceeding maximum residue limits (MRLs) and exceeding MRLs standards. Moreover, the model trained by SVM has the best performance for the classification of pesticide categories in dandelion, and the classification accuracy was 91.7%. The results of this study can provide reference for further development and construction of efficient detection technology of pesticide residues based on electronic nose for agricultural products.

**Keywords:** electronic nose, dandelion, *Taraxacum officinale* L., pesticide residue, classification
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## 1 Introduction

Dandelion (*Taraxacum officinale* L.) is a herbaceous perennial belonging to the Asteraceae family. Dandelion is a dual-use plant with both botanical medicine and food applications, drawing increasing attention[1]. In the field of traditional Chinese medicine, dandelion is used for the treatment of internal and external heat poisoning, sore carbuncles, damp and hot jaundice, hot tingling pain, etc.[2] Dandelion contains terpenoids, polysaccharides, flavones, coumarins, organic acids, and other active components, some examples of which are coumarins, which demonstrate antitumor, anti-inflammatory, antimicrobial, and anticoagulant properties[3]. In addition to being a medicinal material, dandelion contains rich nutritional value such as protein, fat carbohydrate, etc.[4] Dandelion is also used in compost to prevent infestation by pests[5] and as a mosquito repellent[6]. Meanwhile, dandelion is abundant in resources, long-term edible safety, and low in price, preliminary results have been achieved in the development of functional foods, beverages, health products, cosmetics, and other fields in recent years[7-9]. Accordingly, the increasing market demand for dandelion has resulted in its extensive cultivation.

Producers often adopt the planting mode of interplanting dandelion between fruit trees. The growth cycle of fruit trees is long after planting, and it usually takes many years to form a crown. During this period, the dandelion is interplanted reasonably by employing the characteristics of low shade and sufficient lighting under young trees. It can not only effectively prevent the growth of weeds, but also improve soil fertility. Thus, the dandelion interplanting can achieve a double harvest effect[10]. When spraying pesticides on fruit trees, pesticides, and their residues are easily dispersed to areas other than those intended due to spray drift from pesticide applications. Cumulative evidence suggests that chronic exposure to pesticides is linked with the development of numerous diseases, including cancers, asthma, diabetes, Parkinson’s disease,

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hormone disruption, allergies, hypersensitivity, and a decrease in human reproduction[11,12]. Due to fresh dandelion is often eaten as raw food, the measurement of the level of contaminants is significant to verify dandelion quality and security and public concern concerning pesticide residue contamination in dandelion has grown. The problem of pesticide residue seriously affects people's food safety, so efficient and rapid pesticide residue detection technology is extremely important.

At present, many analytical techniques have been developed to detect pesticides in food, such as improved surface Raman spectroscopy[13], high-performance liquid chromatography[14], electrophoresis[15], enzyme-linked immunosorbent assay[16], and electrochemical techniques[17]. Compared with traditional gas analytical equipment including, GC-MS, high-performance liquid chromatography (HPLC) and Fourier transform infrared (FT-IR) spectrometry, electronic nose is a relatively inexpensive and less time-consuming approach. Although these methods show high accuracy, selectivity, and reproducibility, they have some major limitations in their practical application. For instance, they can involve complex sample preparation procedures, time-consuming detection processes, and skilled personnel, which make them inappropriate for real-time applicability and high-throughput monitoring of samples, thus resulting in inconvenience for in-situ detection. Recognition of the limitations and advantages of various methods could be helpful to appropriately employ other ways. Therefore, there is a high demand for the development of simple, high-speed, economical but highly precise and reliable analytical systems for the trace monitoring of pesticide residue in dandelion. Electronic nose (E-nose) as a "e-sensing" technology, can imitate human olfaction function to recognize volatile (often aroma) compounds[18,19]. Electronic nose is another promising non-destructive system that has been popularly applied to detect and quantify food quality in the last decade[20-23]. The e-nose has been revealed to be a practical technique for quality inspection and grading of vegetables[24]. Chen et al[25] proposed the utilization of e-nose sensors to identify the freshness of the bell pepper samples and high prediction values ($R^2$ = 0.9783) for the prediction models were achieved. Similarly, in conjunction with the selected chemometrics, Long et al[26] used an e-nose to distinguish the odor composition of two varieties of galangal. As a new type of artificial olfactory system, the arrival of the e-nose has provided a new option for non-destructive quality assessment of agricultural and food products.

In recent years, although electronic nose has been applied in the field of food detection continuously, there is little research on pesticide residue detection in fruits and vegetables. Therefore, there are no studies concerning the occurrence of insecticides in dandelion. Reviews on the potential health hazards associated with the consumption of contaminated dandelion samples are not available. Therefore, it is of certain theoretical and practical significance to study the pesticide residue detection technology of dandelion. This study, based on an electronic nose combined with chemometric approaches established a suitable pesticide residue detection system for dandelion to determine and study the concentration of pesticide residue in dandelion. It will be quite valuable for monitoring the quality and safety of fresh food products.

## 2 Materials and methods

### 2.1 Materials

The insecticides commonly used at present mainly include pyrethroids, organophosphates, neonicotinoids and biological insecticides, to name a few[27]. Deltamethrin, trichlorfon, acetamiprid and avermectin are pyrethroids, organophosphates, neonicotinoids and biological insecticides, respectively. They are widely used on fruit trees during planting. Therefore, the above four pesticides were selected as the research objects. The specific components of the 4 pesticides are listed in Table 1.

**Table 1 Brand and active ingredient concentration of pesticides**

| Pesticide | Brand | Active component concentration | Formulation types |
|---|---|---|---|
| Avermectin | Jianjue | 1.8% | Wettable powder |
| Trichlorfon | Anama | 90% | Granular |
| Deltamethrin | Zeren | 10% | Soluble powder |
| Acetamiprid | Bayer | 2.5% | Emulsifiable concentrate |

### 2.2 Sample preparation

In this study, the non-pesticide contaminated dandelion samples were collected under the fruit trees. The dandelion used in the experiment was picked at the teaching practice base of the Horticultural College of Jilin Agricultural University on the same day. The dandelion paste respectively with avermectin, trichlorfon, deltamethrin, and acetamiprid mixed, according to the national food safety standards maximum residue limits of pesticide in food GB2763-2016[28], respectively made into maximum residue limits (MRLs) 0.5 times, 1 time, 2 times, 3 times and 5 times, a total of five concentrations of 20 samples, as listed in Table 2. The samples were analyzed without pesticide treatment, generating a control check for each analyte.

**Table 2 Preparation of four pesticides**

| Pesticide | The concentration | | | | |
|---|---|---|---|---|---|
| Avermectin | 0.5 times (0.5A) | 1 time (1A) | 2 times (2A) | 3 times (3A) | 5 times (5A) |
| Trichlorfon | 0.5 times (0.5B) | 1 time (1B) | 2 times (2B) | 3 times (3B) | 5 times (5B) |
| Deltamethrin | 0.5 times (0.5C) | 1 time (1C) | 2 times (2C) | 3 times (3C) | 5 times (5C) |
| Acetamiprid | 0.5 times (0.5D) | 1 time (1D) | 2 times (2D) | 3 times (3D) | 5 times (5D) |

Note: A, B, C, and D in the table are the maximum residues of avermectin, trichlorfon, deltamethrin, and acetamiprid in the leaf vegetables defined by the National Standard for Food Safety GB2763-2016.

For data collection with the electronic nose, 20 g of the sample was used for each pesticide with 50 replicates. The evaluated samples included 20 types of pesticides (0.025 mg/kg avermectin, 0.05 mg/kg avermectin, 0.10 mg/kg avermectin, 0.15 mg/kg avermectin, 0.25 mg/kg avermectin, 0.10 mg/kg trichlorfon, 0.20 mg/kg trichlorfon, 0.40 mg/kg trichlorfon, 0.80 mg/kg trichlorfon, 1.00 mg/kg trichlorfon, 1.00 mg/kg deltamethrin, 2.00 mg/kg deltamethrin, 4.00 mg/kg deltamethrin, 6.00 mg/kg deltamethrin, 10.00 mg/kg deltamethrin, 0.75 mg/kg acetamiprid, 1.50 mg/kg acetamiprid, 3.00 mg/kg acetamiprid, 4.50 mg/kg acetamiprid, 7.50 mg/kg acetamiprid). Therefore, 1000 tests (20 samples with 50 replicas) were employed for sampling.

### 2.3 Gas sensors

The features of the metal oxide semiconductor (MOS) sensors are listed in Table 3. These sensors are classified as MOS sensors which have high chemical stability, long life, low response to humidity, proper cost, sensitivity and applicability for a wide range of chemicals and foods[29].

### 2.4 Fabrication of the electronic nose detection system

The electronic nose used in the research included sensors, electronic section, pumps, ventilation unit, and software required for data processing and statistical analysis, as shown in Figure 1. The bionic electronic nose system is designed by the Key Laboratory of Bionic Engineering, Ministry of Education, Jilin University[30].

**Table 3 Features of the sensors used in the electronic nose system**

| Number | Sensor name | Main applications(gas detector) | Manufacturer and country |
|---|---|---|---|
| S1 | TGS2612 | Methane, liquid petroleum gas | Figaro, Japan |
| S2 | GSBT11 | VOCs (e.g. acetone) | Ogam, Korea |
| S3 | WSP2110 | Benzene, Toluene, Formaldehyde | Winsen, China |
| S4 | MP135 | Ethanol, Cigarette smoke, Air pollutants | Winsen, China |
| S5 | MS1100 | Toluene, Benzene, Formaldehyde, VOCs | Ogam, Korea |
| S6 | MP901 | Alcohol, Cigarette smoke, Formaldehyde,Toluene, Benzene, Acetone | Winsen, China |
| S7 | TGS2611 | Natural gas, Methane | Figaro, Japan |
| S8 | TGS2620 | Alcohol, Organic solvents steam | Figaro, Japan |
| S9 | TGS2602 | Ammonia, Hydrogen sulfide (high sensitivity to VOC and odorous gases) | Figaro, Japan |
| S10 | TGS2610 | Butane, Liquid Petroleum Gas, Propane | Figaro, Japan |
| S11 | TGS2600 | Hydrogen, Ethanol, Hydrocarbons, etc. | Figaro, Japan |
| S12 | TGS2603 | Trimethyl amine, Methyl mercaptan, Hydrogen sulfide, etc. | Figaro, Japan |

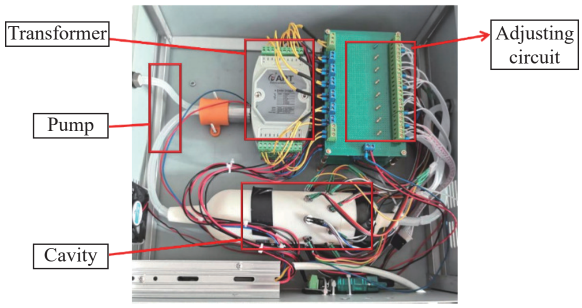


Figure 1 Electronic nose system diagram

By analyzing the structural characteristics and flow field distribution inside the nasal passage of the dog's nasal chamber, an optimized bionic electronic nasal chamber simulating the nasal chamber of the dog was proposed, which effectively solved the problems of bloated and inflexible operation of the detection device.

### 2.5 Experiment process

For data collection with the electronic nose, 20 g of the sample was used for each composition with 50 replicates. Therefore, 1000 tests were employed for the data collection of the self-designed sensor array. The process of collecting the experimental data was as follows (Figure 2).

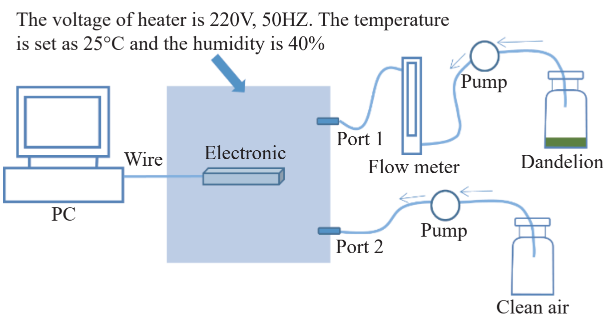


Figure 2 Electronic nose system

1) Preheating

Before the electronic nose system is used, it should be preheated for about 2 hours so that the sensor can reach the working temperature at 200°C. Then, the response value of each sensor to the surrounding environment is collected, and the sensor's response value in the environment atmosphere is no longer changed as a benchmark to judge whether the sensor is restored.

2) Cleaning

Before each electronic nose test, clean air should be used to clean the air chamber and airway of the electronic nose. During cleaning, an air pump is inserted into the clean air to blow the clean air into the air chamber at a high rate to blow away the gas molecules attached to the surface of the metal oxide sensor. After analysis of each sample, the e-nose performed a sensor self-cleaning step of 300 s duration by flowing ambient air, to return the sensor response to the zero-gas condition.

3) Test

Put 20 g sample to be tested into a beaker, and seal it with plastic wrap for 10min, Subsequently, a needle was used to perforate the flask septum containing the sample, and the headspace air was sucked into the detection chamber (1 L/min) for 90 s. When the sample gas passes through the gas chamber, it interacts with the sensor surface to change the resistance value, thus causing the change of sensor signal. Use the data acquisition card to collect sensors' electrical signal changes of 0-5 V, then upload it to the computer through the USB data cable save it to the Excel file, and then preprocess the original data.

### 2.6 Pre-processed

In all the stages, the output voltage of the sensors changed due to exposure to different smells, and their voltage response was collected by data collection cards. The signals of sensors were transferred to the computer at 1 s intervals using a USB port. To remove the noise, the data were pre-processed by fractional method. In this method, the obtained response will be normalized in addition to being dimensionless[31].

$$x' = (x - \bar{x})/\sigma$$

where, $\bar{x}$ is the average response; while $x$ and $x'$ are the sensor response in the smell pulse stage, and its pre-processed response, respectively; $\sigma$ is the standard deviation.

For obtaining a fusion signals matrix, the E-nose features were firstly pretreated by setting the mean value at the origin of each variable and then dividing them by their standard deviation in order to eliminate the effect of index dimension.

### 2.7 Features extraction

In this study, the data sampling time of the electronic nose was set at 90 s and the frequency parameter was set at 50 Hz, so 4500 data were obtained from each sensor in each group of experiments. This results in a large amount of data, and not all of the data is needed for classification recognition. Feature extraction is to extract the information that can represent the whole response signal from the sensor response signal, so as to achieve the purpose of simplifying the data. Finding a suitable feature pattern extraction method can improve the efficiency of pattern recognition and play a very important role in the process of data analysis. According to reports, at home and abroad the method of feature extraction can be divided into three categories: a feature extraction method based on the original response curve (maximum response, the response curve integral value, etc.)[32], a feature extraction method based on space transform (Fourier transform, discrete wavelet transform, etc.), a feature extraction method based on curve fitting model (lorentz model, a polynomial model, gaussian model, etc.). Although there are many methods to extract characteristic values, the method based on the original response curve is still the most used and the most effective one in sensor data preprocessing.

From the data obtained from the test, it can be seen that the maximum response value of the sensor is also a steady-state value during the whole process of the sensor response, which can not only reflect the stable response of the sensor to the sample gas but also reflect the maximum degree of its change. The integral value can be expressed as the area of the response curve and time axis in the response interval, reflecting the overall response of the sensor to the volatile components of the tested sample. Therefore, the maximum value (MAX) and integral value (IV) of the response curve of the electronic nose were selected as the characteristic values in this experiment.

### 2.8 Data analysis

Artificial neural network is a common method in various data analysis algorithms. Based on different network structures, excitation functions, and learning strategies, artificial neural networks can be divided into many categories, such as radial basis function network, feedback neural network, and self-organizing neural network[33]. In so many artificial neural networks, researchers pay more and more attention to the Back Propagation Artificial neural network (BP-ANN)[34]. At present, BP neural network has become the most widely used artificial neural network.

BP neural network, jointly proposed by Rumelhart and Mcclelland, is a multi-layer feedforward artificial neural network with continuous transfer function, mainly including input layer, hidden layer, and output layer[35]. The typical BP neural network structure is shown in Figure 3 BP neural network is based on sample learning to error back propagation algorithm as a way of training, and into the target of minimizing the root mean square error, in turn, the network weights and threshold to adjust, so that the BP neural network prediction output end goal, the looming belong to the nonlinear supervised learning algorithm. Therefore, the learning process of the BP neural network is essentially to make constant adjustments in the connection weight and threshold between the layers to make the mapping of the output and input into the ideal state.

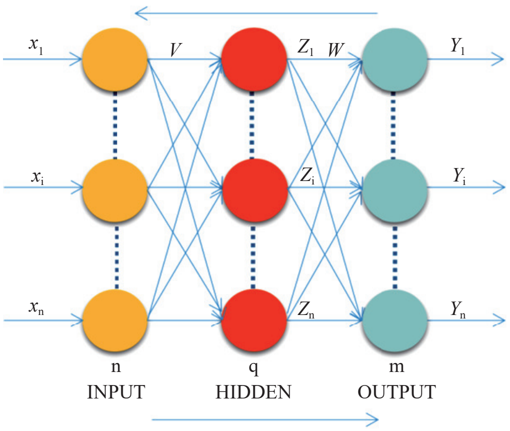


Figure 3 Basic structure of BP neural network

Random forest (RF) is a collection of multiple trained decision trees, and when a sample is to be classified, each decision tree will "vote" for the class of the sample. The sample is then assigned based on the majority vote[36]. Due to the relatively large number of decision trees, the attributes for training the decision trees can be randomly selected from all the attributes without necessarily choosing the one with the most information gain. The training of an RF can be achieved by many different approaches. For example, m random samples are selected from the training sample pool with replacement to train the decision trees (bootstrap RF). Alternatively, training can be conducted by maintaining a set of weights over the original training set S and adjusting these weights based on successful classification. The weights of examples that are misclassified are increased, and the weights of examples that are correctly classified are reduced[37].

Support vector machine (SVM) is one of the supervised training methods used for regression and classification. The SVM algorithm is categorized as the pattern detection algorithm. It can be used for pattern detection or classification of objects. This method is relatively new and has shown proper efficiency in classification compared to the previous methods such as perceptron neural networks. SVM classifier works on the basis of linear classification of the data. In the linear division of the data, it is tried to choose the line with the higher confidence margin[38,39]. Ten-fold cross-validation was used to detect the accuracy of classification and compare the effects of different feature extraction methods on classification results.

After data pre-processing, BP-ANN, RF, and SVM methods were employed to analyze the data obtained from the electronic nose system and implement the pattern detection algorithm or classify them. Feature extraction and model construction were implemented on MATLAB R2016b.

## 3 Results and discussion

### 3.1 Sensors response

The E-nose was sensitive to changes in the aroma of samples. Yang et al.[40] reported that the slightest change in the concentration of volatile organic compounds could alter the response of the sensor array. To better understand the nature of changes in the sensor array responses to the aroma of dandelion samples that are affected by different pesticides, it is necessary to have a comprehension knowledge of changes in tissue structure and volatile compounds generated by the mentioned treatments. The aroma characterization of dandelion samples was analyzed using an E-nose equipped with 12 MOS sensors, which were not sensitive to the involved molecules. After the beginning of the headspace injection step, the sensors reacted to the presence of volatiles. For instance, typical responses of the sensors toward the aroma of dandelion samples are presented in Figure 4.

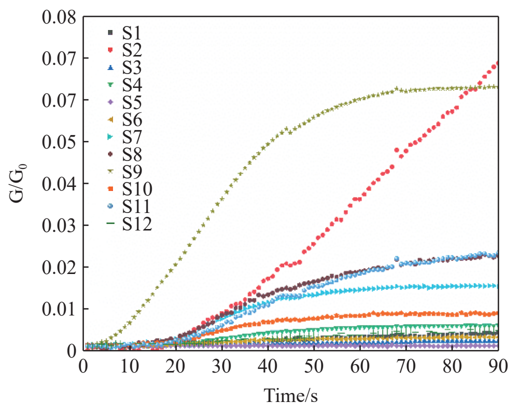


Figure 4 Response of sensor array related to dandelion samples

In Figure 4, the $x$-axis represents the duration of the test step in the third process, and the $y$-axis represents the relative changes in the sensors' response. The response changes of each sensor to different treatments were not the same. This suggests that the aroma profiles of different treatments were not similar, and the E-nose technique could distinguish the aroma of samples by different pesticide treatments. The results showed that sensors S2(GSBT11) and S9(TGS2602) had the highest range of changes, while sensors

S5(MS1100) had the lowest reaction ranges. It can be stated that the interaction of sensors S2(GSBT11) and S9(TGS2602) could play a significant role in the differentiation of aroma profiles of samples.

**3.2 Classification and analysis of dandelion pesticide concentrations exceeding MRLs by BP-ANN, RF, and SVM using E-nose**

In order to explore the rapid detection technology of whether the pesticide residues in dandelion exceed the standard, according to MRLs amount of different pesticide residues defined by the national food safety standards, for avermectin, trichlorfon, deltamethrin and acetamiprid 4 pesticides. Accordingly, the dandelions were classified into two groups (Figure 5): group 1 contains concentrations that did not exceed MRLs, including control check (no pesticide treatment), MRLs 0.5 times and 1 time samples (MRLs); group 2 contains pesticides exceeded MRLs in dandelion samples, including MRLs 2 times, 3 times and 5 times samples. The electronic nose was used to classify four kinds of pesticides in dandelion and whether the pesticide residues in dandelion exceeded the standard. With the integral value (IV) and maximum value (MAX) as the characteristic values, BP neural network, random forest (RF), and support vector machine (SVM) analysis were carried out respectively to explore the distinguishing ability of electronic nose and compare the classification effects of different algorithms. Repeat 50 times for each sample.

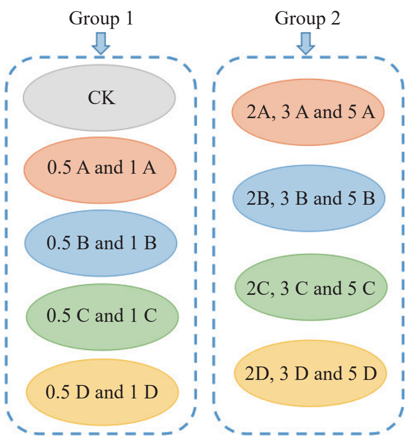


Figure 5 Design scheme of an electronic nose to distinguish different types of pesticides: the acronyms are presented in Table 2

Through the above analysis, it can be seen that it is feasible to apply electronic nose technology to the rapid classification of excessive pesticide residue in dandelion. According to the odor pattern characteristics of pesticide residues in dandelion, the integral value (IV) and maximum value (MAX) of the response curve of the electronic nose were extracted as the characteristic values. At the same time, BP-ANN, RF, and SVM three pattern recognition algorithms are used to discuss the influence of different characteristic values (maximum and integral values). By comparing the accuracy of classification results of different methods of selecting characteristic values, it can be seen that the classification effect of characteristic values based on the maximum value is better than the integral value. It may be because the maximum response value can not only reflect the stable response of the sensor to the sample gas but also reflect the maximum degree of its change, which is more suitable for the study of such problems, so the classification result is better. As shown in Figure 6, the recognition accuracies of BP-ANN, RF, and SVM using the characteristic value of maximum are 82.7%, 83.0%, and 94.5%, respectively.

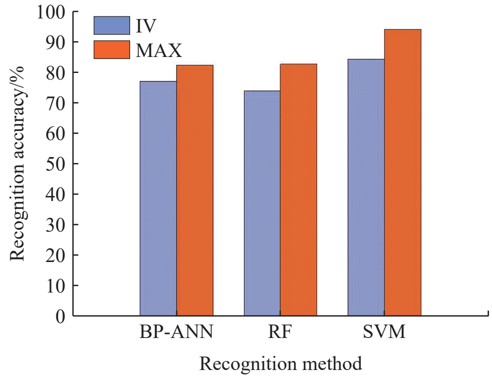


Figure 6 Classification results of using different characteristic values based on BP-ANN, RF and SVM

**3.3 Classification of pesticide concentrations in dandelion by BP-ANN, RF, and SVM using E-nose**

When the pesticide concentration of dandelion does not exceed the standard, it can be eaten. Therefore, in a study, the identification and classification of various types of pesticides were investigated based on BP-ANN, RF, and SVM methods according to E-nose under the condition of excessive residue. Accordingly, group 2 was classified into four groups (Figure 7): group A contains pesticides that exceeded MRLs of avermectin in dandelion samples, including MRLs 2, 3, and 5 times samples; group B contains pesticides that exceeded MRLs of trichlorfon in dandelion samples, including MRLs 2 times, 3 times and 5 times samples; group C contains pesticides exceeded MRLs of deltamethrin in dandelion samples, including MRLs 2 times, 3 times and 5 times samples; group D contains pesticides exceeded MRLs of acetamiprid in dandelion samples, including MRLs 2 times, 3 times and 5 times samples. Each sample was repeated 50 times so that 600 sets of exceeding sample data were obtained.

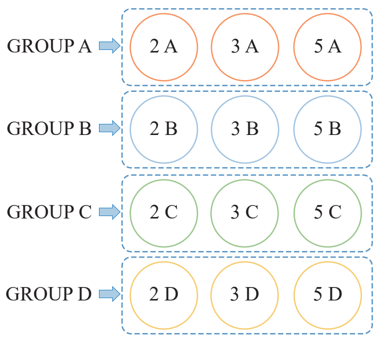


Figure 7 Design scheme of E-nose to differentiate pesticide categories: the acronyms are presented in Table 2

The recognition results of the classification model for pesticide residue detection based on BP-ANN, RF, and SVM are listed in Table 4. It can be seen from the table that, among the three classification methods, the SVM classification accuracy rate reaches 91.7%, and the classification effect is the best. The classification accuracy of RF is 89.0%. The classification accuracy of BP-ANN is

**Table 4 Classification results of pesticide categories based on BP-ANN, RF and SVM**

| Index | BP-ANN | RF | SVM |
|---|---|---|---|
| Recognition rate | 74.30% | 89.00% | 91.70% |
| Sensitivity | 82.00% | 89.50% | 94.25% |
| Precision | 82.20% | 89.67% | 94.25% |
| Specifity | 94.00% | 96.50% | 98.08% |
| F1 score | 82.03% | 89.50% | 94.24% |

74.3%, and the classification effect is the worst. It can be seen from the above analysis that it is feasible to apply electronic nose technology to the classification of pesticide categories in dandelion under the condition of exceeding the standard of MLRs.

This study mainly discusses the classification effect of electronic nose detection technology on the pesticide concentration in dandelion under the condition of excessive residue. As shown in Figure 8, different concentrations of avermectin, trichlorfon, deltamethrin, and acetamiprid were designed for treatment, which were 2 times, 3 times, and 5 times the maximum residue defined by national standards, respectively. Each process was repeated 50 times. Thus, a total of 150 sets of data were collected for each pesticide, and the maximum signal response curve was taken as the characteristic value. BP-ANN, RF, and SVM pattern recognition methods were used to explore the recognition ability of the electronic nose, and the recognition effect of different algorithms was compared.

The recognition results of BP-ANN, RF and SVM methods for different concentrations of 4 kinds of pesticides are shown in Figure 9. To the avermectin, trichlorfon, deltamethrin and acetamiprid, both the recognition methods of RF and SVM exhibited higher accuracy than BP-ANN. However, to the

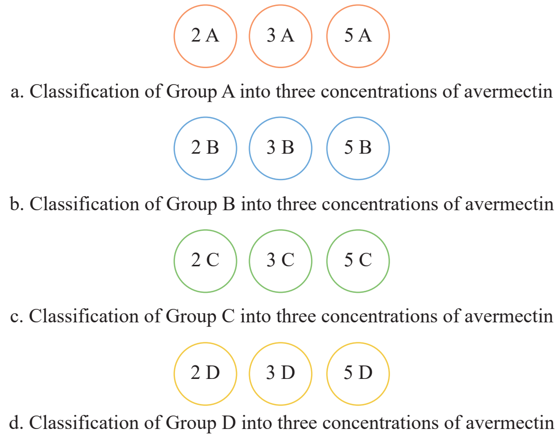


Figure 8 Design scheme of E-nose to differentiate pesticide concentrations: the acronyms are presented in Table 2

acetamiprid, the recognition accuracy of SVM is much higher than RF. The comprehensive analysis results indicate that the recognition method of SVM has good stability, which is more feasible to identify the concentration of different pesticides in the case of excessive residues in dandelion by electronic nose detection technology.

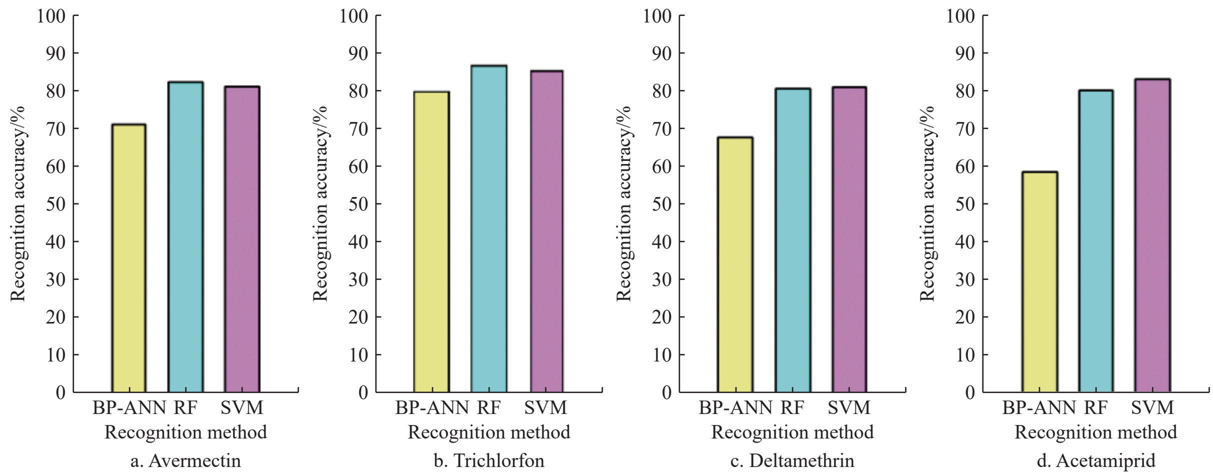


Figure 9 Recognition results of BP-ANN, RF and SVM method for different concentrations of 4 kinds of pesticides

## 4 Conclusions

A gas sensor array that contained 12 MOS sensors was prepared, and the detection and classification of pesticide residues in dandelion under the fruit trees was achieved with the help of chemometric methods. In this research, dandelion samples were treated with different pesticides of avermectin, trichlorfon, deltamethrin, and acetamiprid. According to the maximum residue limits (MRLs) of different pesticides defined by national food safety standards, dandelions were mixed with different MRLs times (0.5, 1.0, 2.0, 3.0, and 5.0) of pesticide. The results showed the superior effectiveness and precision of the SVM method in the discrimination and classification of non-exceeding MRLs and exceeding MRLs standards when compared with BP-ANN and RF methods. The total classification precision was 82.7%, 83.0%, and 94.5% for the BP-ANN, RF and SVM methods, respectively. In all methods, the classification of avermectin, trichlorfon, deltamethrin, and acetamiprid, SVM method was better and more precise than BP-ANN and RF methods. The classification precision was 74.3%, 89.0%, and 91.7% for the BP-ANN, RF and SVM methods, respectively. What's more, in order to verify the classification accuracy of the detection system, each pesticide was divided into four concentrations and adopted BP-ANN, RF, and SVM methods to establish models. The results prove that the model trained by SVM has the best performance for four concentrations in exceeding MRLs standard.

This research aimed at highlighting the detection and classification of pesticide residues in dandelions by electronic nose combined with chemometric approaches. In this study, e-nose is used for practical applications. As a new non-destructive method, rapid identification of pesticide residues in dandelion using e-nose. Classification and analysis of dandelion pesticide concentrations exceeding MRLs using E-nose. Classification of pesticide categories in dandelion. Classification of pesticide concentrations in dandelion using E-nose. By analyzing the recognition results, it was found that SVM has a high recognition accuracy and good application prospects. Moreover, the limitation of this study is that few countries have published results on pesticide residues and dandelion and/or using E-nose to distinguish pesticide residues. Nonetheless, the main point of the study is that pesticide residues in this study can be a representative sample of all vegetables, as well as the fact that many pesticide residues were similarly found in some vegetables. In conclusion, this research fills the gap in knowledge on pesticide residues in dandelion. As well as the electronic nose is a new type of method for the detection and classification of pesticide residues, and the research results can lay a foundation for further establishing an accurate detection model of pesticide residues in dandelion based on electronic nose technology. It will be quite valuable for monitoring the quality and safety of agricultural products.

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## [References]

[1] González-Castejón M, Visioli F, Rodriguez-Casado A. Diverse biological activities of dandelion. Nutrition Reviews, 2012; 70(9): 534–547.

[2] Ovadje P, Chatterjee S, Griffin C, Hamm C, Pandey S. Selective induction of apoptosis through activation of caspase-8 in human leukemia cells (Jurkat) and CMML cells by Dandelion extract. Free Radical Biology and Medicine, 2010; 49: S67.

[3] Jędrejek D, Kontek B, Lis B, Stochmal A, Olas B. Evaluation of antioxidant activity of phenolic fractions from the leaves and petals of dandelion in human plasma treated with $H_2O_2$ and $H_2O_2$/Fe. Chemico-Biological Interactions, 2017; 262: 29–37.

[4] Tang H X, Zhao T W, Sheng Y J, Zheng T, Fu L Z, Zhang Y S. *Dendrobium officinale* Kimura et Migo: A review on its Ethnopharmacology, Phytochemistry, Pharmacology, and Industrialization. Evidence-Based Complementary and Alternative Medicine, 2017; 2017: 7436259.

[5] Huber M, Triebwasser-Freese D, Reichelt M, Heiling S, Paetz C, Chandran J N, et al. Identification, quantification, spatiotemporal distribution and genetic variation of major latex secondary metabolites in the common dandelion (*Taraxacum officinale* agg. ). Phytochemistry, 2015; 115: 89–98.

[6] Chen K, Zhang M, Bhandari B, Mujumdar A S. Edible flower essential oils: a review of chemical compositions, bioactivities, safety and applications in food preservation. Food Research International, 2021; 139: 109809.

[7] Dariusz J, Bernadetta L, Agata R, Anna S, Beata O. Comparative phytochemical, cytotoxicity, antioxidant and haemostatic studies of *Taraxacum officinale* root preparations. Food Chemical Toxicology, 2019; 126: 233–247.

[8] Xue Y S, Zhang S M, Du M, Zhu M J. Dandelion extract suppresses reactive oxidative species and inflammasome in intestinal epithelial cells. Journal of Functional Foods, 2017; 29: 10–18.

[9] You Y, Yoo S, Yoon H G, Park J, Lee Y H, Kim S, et al. *In vitro* and *in vivo* hepatoprotective effects of the aqueous extract from *Taraxacum officinale* (dandelion) root against alcohol-induced oxidative stress. Food and Chemical Toxicology, 2010; 48(6): 1632–1637.

[10] Cen Y, Li L J, Guo L Y, Li C H, Jiang G M. Organic management enhances both ecological and economic profitability of apple orchard: A case study in Shandong Peninsula. Scientia Horticulturae, 2020; 265: 109201.

[11] Betarbet R, Sherer T B, MacKenzie G, Garcia-Osuna M, Panov A V, Greenamyre J T. Chronic systemic pesticide exposure reproduces features of Parkinson's disease. Nature Neuroscience, 2000; 3: 1301–1306.

[12] Casals-Casas C, Desvergne B. Endocrine disruptors: From endocrine to metabolic disruption. Annual Review of Physiology, 2011; 73: 135–162.

[13] Wang P, Wu L, Lu Z C, Li Q, Yin W M, Ding F, et al. Gecko-inspired nanotentacle surface-enhanced raman spectroscopy substrate for sampling and reliable detection of pesticide residues in fruits and vegetables. Analytical Chemistry, 2017; 89(4): 2424–2431.

[14] Watanabe E, Baba K. Highly sensitive quantification of pyrethroid insecticide etofenprox in vegetables with high-performance liquid chromatography and fluorescence detection. Journal of Chromatography A, 2015; 1385: 35–41.

[15] Bol'shakova D S, Amelin V G. Determination of pesticides in environmental materials and food products by capillary electrophoresis. Journal of Analytical Chemistry, 2016; 71: 965–1013.

[16] Songa E A, Okonkwo J O. Recent approaches to improving selectivity and sensitivity of enzyme-based biosensors for organophosphorus pesticides: A review. Talanta, 2016; 155: 289–304.

[17] Xu F, Cui Z M, Li H, Luo Y L. Electrochemical determination of trace pesticide residues based on multiwalled carbon nanotube grafted acryloyloxy ferrocene carboxylates with different spacers. RSC Advances, 2017; 7(12): 7431–7441.

[18] Chen P, Li Y B, Cui T H, Ruan R. Nanoparticles based sensors for rapid detection of foodborne pathogens. International Journal of Agricultural & Biological Engineering, 2013; 6(1): 28–35.

[19] Liu W, Fan Y, Liu Q, Xu F, Zhang L, Hu H. Identification of the flavor profiles of Chinese pancakes from various areas using smart instruments combined with E-noses and E-tongues. International Journal of Agricultural & Biological Engineering, 2023; 16: 283–290.

[20] Makarichian A, Chayjan R A, Ahmadi E, Zafariet D. Early detection and classification of fungal infection in garlic (A. sativum) using electronic nose. Computers and Electronics in Agriculture, 2022; 192: 106575.

[21] Grassi S, Benedetti S, Magnani L, Pianezzola A, Buratti S. Seafood freshness: e-nose data for classification purposes. Food Control, 2022; 138: 108994.

[22] Jr S LS, Siqueira H V, Menegotto B A, Schroeder L C, Pessenti I L, Ayub R A. Discrimination analysis of wines made from four species of blueberry through their olfactory signatures using an E-nose. LWT, 2023; 187: 115320.

[23] Zeng H, Han H Y, Huang Y D, Wang B. Rapid prediction of the aroma type of plain yogurts via electronic nose combined with machine learning approaches. Food Bioscience, 2023; 56: 103269.

[24] Mohd Ali M, Hashim N, Abd Aziz S, Lasekan O. Principles and recent advances in electronic nose for quality inspection of agricultural and food products. Trends in Food Science & Technology, 2020; 99: 1–10.

[25] Chen L Y, Wu C C, Chou T I, Chiu S W, Tang K T. Development of a dual MOS electronic nose/camera system for improving fruit ripeness classification. Sensors, 2018; 18: 3256.

[26] Long Q, Li Z, Han B, Hosseini H G, Zhou H Y, Wang S M, et al. Discrimination of two cultivars of *Alpinia officinarum* hance using an electronic nose and gas chromatography-mass spectrometry coupled with chemometrics. Sensors, 2019; 19: 572.

[27] Al-Nasir F M, Jiries A G, Al-Rabadi G J, Alu'datt M H, Tranchant C C, Al-Dalain S A, et al. Determination of pesticide residues in selected citrus fruits and vegetables cultivated in the Jordan Valley. LWT, 2020; 123: 109005.

[28] Hrynko I, Lozowicka B, Kaczynski P. Comprehensive analysis of insecticides in melliferous weeds and agricultural crops using a modified QuEChERS/LC-MS/MS protocol and of their potential risk to honey bees (*Apis mellifera* L. ). Science of The Total Environment, 2019; 657: 16–27.

[29] Fardin A, Esmaeil M G, Hekmat R, Heidarbeigi K. Using an E‐nose machine for detection the adulteration of margarine in cow ghee. Journal of Food Engineering, 2018; 41(6): 12806.

[30] Chang Z Y, Sun Y H, Zhang Y C, Gao Y L, Weng X H, Cheng D H, et al. Bionic optimization design of electronic nose chamber for oil and gas detection. Journal of Bionic Engineering, 2018; 15: 533–544.

[31] Arshak K, Moore E, Lyons G M, Harris S C. A review of gas sensors employed in electronic nose applications. Sensor Review, 2013; 24(2): 181–198.

[32] Burlachenko J, Kruglenko I, Snopok B, Persaud K. Sample handling for electronic nose technology: state of the art and future trends. TrAC Trends in Analytical Chemistry, 2016; 82: 222–236.

[33] Yan J, Guo X Z, Duan S K, Jia P F, Wang L D, Peng C, et al. Electronic nose feature extraction methods: A review. Sensors, 2015; 15(11): 27804–27831.

[34] Bhagya Raj G V S, Dash K K. Comprehensive study on applications of artificial neural network in food process modeling. Critical Reviews in Food Science and Nutrition, 2022; 62(10): 2756–2783.

[35] Heidarbeigi K, Mohtasebi S S, Foroughirad A, Ghasemi-Varnamkhasti M, Rafiee S, Rezaei K. Detection of adulteration in saffron samples using

electronic nose. International Journal of Food Properties, 2015; 18(7): 1391–1401.

[36] Wiederoder M S, Nallon E C, Weiss M. Graphene nanoplatelet-polymer chemiresistive sensor arrays for the detection and discrimination of chemical warfare agent simulants. ACS Sens., 2017; 2(11): 1669–1678.

[37] Elith J, Leathwick J R, Hastie T. A working guide to boosted regression trees. Journal of Animal Ecology, 2008; 77(4): 802–813.

[38] Pardo M, Sberveglieri G. Classification of electronic nose data with support vector machines. Sensors and Actuators B:Chemical, 2015; 107(2): 730–737.

[39] Mahmodi K, Mostafaei M, Mirzaee-Ghaleh E. Detection and classification of diesel-biodiesel blends by LDA, QDA and SVM approaches using an electronic nose. Fuel, 2019; 258: 116114.

[40] Yang W J, Yu J, Pei F, Mariga A M, Ma N, Fang Y, et al. Effect of hot air drying on volatile compounds of *Flammulina velutipes* detected by HS-SPME-GC-MS and electronic nose. Food Chemistry, 2015; 196: 860–866.