Classification of essential oil composition in *Rosa damascena* Mill. Genotypes using an Electronic Nose

Abstract

One of the major problems in the industry of medicinal and aromatic plants (MAPs) is the absence of a quick, easy and inexpensive method for controlling the quality of these plants. *Rosa damascena* Mill., is an aromatic plant which is cultivated for its high-value essential oil in Iran, Bulgaria and Turkey. In this study, essential oils were extracted from nine genotypes of *Rosa*, and their components were identified by gas chromatography and mass spectrometry analysis (GC-MS). Then, the samples from different genotypes were grouped in three classes (C1, C2, C3) based on their total percentage of the six most important constituents, which have a major role in the quality of essential oil (i.e., *phenyl ethyl alcohol, trans rose oxide, citronellol, nerol, geraniol, geranial*). An electronic nose (EN) system was designed based on metal oxide semiconductor (MOS) sensors, and trained to identify the categories to which samples of essential oils could be classified. The response patterns of the sensors were recorded and further analyzed by chemometrics methods. Based on the results, principal components analysis (PCA) and linear discrimination analysis (LDA) showed that 85% and 99% of sample variance could be explained by the first two principal components (PC1, PC2) and two linear discrimination axis (LD1, LD2), respectively. LDA was performed on sensor response variables by cross- validated dataset (5- fold) and the classification accuracy was 95%. Finally, an error-correcting output codes (ECOC) classifier as a multiclass model for support vector machines (SVM) was considered and the classification accuracy was increased to 99%. These results reveal that an EN can be used as a quick, easy, accurate and inexpensive system for the classification of essential oil composition in *Rosa damascena* Mill.

Keywords:

Rosa damascena, Electronic Nose, Aromatic plants, Essential oil, Chemometrics, Classification

1. Introduction

In the last decades, the use of the medicinal and aromatic plants (MAPs) in food, cosmetic and medicine industrials has been increased considerably (Baby et al., 2005). The world market of MAPs has systematically increased its value from 355 million dollars in 1976 to 5.51 billion dollars in 2002. Predictions state that this market can reach a value of 5000 billion dollars in 2050 (Mohammadi, 2015). Essential oils are highly concentrated, volatile, hydrophobic mixtures of chemicals extracted from MAPs. About 90% of global essential oil production is consumed by the flavor and fragrance industries (Lubbe and Verpoorte, 2011). As a rational consequence, the recognition of genotypes and the classification of essential oils according to their quality can be highly crucial for the processing and production of products with higher quality.

The most aromatic species of rose, scientifically named as *Rosa damascena* Mill., known as "*Gol-e-Mohammadi*" in Persian (Naquvi et al., 2014). It is a furry shrub (deciduous) and one of the most important fragrant types of *Rosaceae* family, which is cultivated extensively in Iran, Turkey and Bulgaria (Kaul et al., 2009). Rose products consist of rose oil, rose water, rose concrete, rose absolute, petal and dry bud that rose oil is the most important product (Baydar and Baydar, 2005; Tabaei-Aghdaei et al., 2007; Kumar et al., 2013). The essential oil of *Rosa damascena* is the most valuable essential oil in the world market, and this is why it is nicknamed 'liquid gold' (Pal et al., 2014). This essential oil is vastly employed in perfumery, hygienic and cosmetic industries to produce creams, shampoos, soaps and lotions; in foodstuffs as food additive, pudding and jelly and in the pharmaceutical industry for its anti-HIV, anti-bacterial, anti-oxidation and sedation properties (Naquvi et al., 2014; Shohayeb et al., 2014; Ozkan, 2004). According to the literature, the maximum value of qualification and quantitation of essential oil having a minimum value of wax compounds (which reduce quality) is obtained from rose petals

(Ahmadi et al., 2007). Currently, there are some methods for the classification of aromatic materials such as sensory analysis performed by test panels formed by several experts that are provided with a list of features and a few samples to score. For example, the evaluated features are aroma, weight, size, color and veins in the case of ginseng (Cui et al., 2015) and aroma, color and flavor are the main features evaluated for tea (Bhattacharyya et al., 2008). This method may turn out to be fast in the first vision but it is limited in stability, measurement standardization, reproducibility, sample throughput and, furthermore, it is rather expensive (Guohua et al., 2015). An alternative is the use of instrumental methods such as gas chromatography (GC), GC coupled with mass spectrometry (GC/MS), high performance liquid chromatography (HPLC) and thin layer chromatography (TLC), which are objective and precise but are expensive, destructive, time-consuming and need to be performed by well-trained operators (Baby et al., 2005; Xiao et al., 2014). These methods are only suitable for quality examination in laboratory condition (Guohua et al., 2015). Therefore, the development of easy, low cost, accurate and high throughput methods for the quality assessment and classification of essential oils is highly demanded and the electronic nose technique could be a good approach.

The electronic nose is an instrument that comprises an array of electronic gas sensors with partial specificity and an appropriate pattern recognition system, capable of recognizing simple or complex odors (El Barbri et al., 2008; Ghasemi-Varnamkhasti et al., 2011). In the electronic noses, the fingerprints or patterns resulting from the volatile compounds present in the headspace of the samples under analysis are recognized and classified (Ghasemi-Varnamkhasti and Aghbashlo, 2014). Electronic noses are relatively fast, inexpensive, easy to use, reliable and non-destructive instruments (Loutfi et al., 2015). ENs have found many applications in the food industry such as product classification (Bhattacharyya et al., 2008; Qiu et al., 2015;

Trirongjitmoah et al., 2015), quality and shelf life recognition (Ghasemi-Varnamkhasti et al., 2011; Gomez et al., 2007) (Benedetti et al., 2008), fruits ripeness recognition (Asikin et al., 2015; Brezmes et al., 2005; Zakaria et al., 2012) and assessment of adulterated products (Subari et al., 2012; Yu et al., 2007; Mildner-Szkudlarz and Jeleń, 2008; Marina et al., 2010). Also more recently, the electronic nose has been used in medical applications for diagnosing some diseases such as cancer via breath analysis (Westenbrink et al., 2014; Adiguzel and Kulah, 2015; Alfatni et al., 2013).

Some reports can be found in the literature about the use of electronic noses for the quality evaluation of medicinal plants include the quality control of *valerians* by electronic nose and HPLC (Baby et al., 2005), the discrimination and characterization of three cultivars of *perilla frutescens* by means of sensory descriptors, electronic nose and tongue analysis (Laureati et al., 2010), a quality control method for *musk* by electronic nose coupled with chemometrics (Ye et al., 2011). This approach has also been envisaged for other plants such as *eurycoma longifolia* (Shafiqul Islam et al., 2006), *cymbidium ensifolium* (Huang et al., 2011; Zhang et al., 2014), *ginseng* (Lee et al., 2005; Li et al., 2012; Cui et al., 2015), *asari radix* (Li et al., 2013), *apiaceae* (Lin et al., 2013), *lonicera japonica* (Xiong et al., 2014), *glycyrrhiza glabra* L. (Russo et al., 2014) and *zizyphus jujube* Mill. (Guohua et al., 2015).

To date, no study has been reported on the application of electronic nose for the classification of essential oil of *Rosa damascena* and this is the main novelty of this research. Considering the importance of classification and related issues in the industry of MAPs, the adoption of electronic nose technology seems to be helpful. Therefore the major aim of this paper is to evaluate an electronic nose based on metal oxide semiconductor (MOS) gas sensors and suitable chemometrics techniques for the classification of essential oil of *Rosa damascena*. Gas

chromatography–mass spectrometry (GC-MS) has been employed as an objective method to establish quality categories among the samples available, based on the identification of the volatile compounds present in their headspace.

2. Material and Methods

2.1. Samples preparation

As a first phase of the experiment, the petals of nine different genotypes of *Rosa damascena* were collected from farm (51º longitude and 35º latitude at 1320 m above sea level) located in Research Institute of Forests and Rangelands (RIFR) during the blooming season (early May to late June, 2014). The petals were separated early morning and immediately transferred to laboratory for extraction.

2.2. Essential oil extraction

In the next step, 400 g of petals of each genotype were weighed and then their essential oil was extracted by hydrodistillation using Clevenger apparatus for 2 hours. The extracted oil samples were dehydrated by anhydrous sodium sulfate and stored in dark glass bottles at 4ºC until analyzed by GC and GC-MS.

2.3. Gas chromatography (GC)

Essential oils were analyzed by GC, using a Thermo-UFM ultra-fast gas chromatograph equipped with a Ph-5 fused silica column (10 m length × 0.1 mm i.d., film thickness 0.4 μm). Oven temperature was held at 60 ºC for 5 min and then programmed to 285 ºC at a rate of 5 $^{o}Cmin^{-1}$;flame ionization detector (FID) and injector temperatures both were 280 ºC; Helium (99.999% purity) was used as a carrier gas with flow rate of 1.1 $mLmin^{-1}$.

2.4. Gas Chromatography–Mass Spectrometry (GC-MS)

GC–MS analysis was carried out by Varian 3400 GC–MS system equipped with AOC-5000 Auto injector and DB-5 fused silica capillary column (30 m length × 0.25 mm i.d., film thicknesses 0.25 μm). Temperature was programmed to 60 ^{o}C for 4 min and then increased at the rate of 5 ^{o}Cmin^{-1} to 285 ^{o}C and held for 5 min; injector and interface temperatures were 240 ^{o}C and 250 ^{o}C, respectively; ionization voltage was 70 eV; sample injection volume 2 μL (dilution: 1 μL oil in 2 mL dichloromethane); Helium (99.999% purity) was used as a carrier gas with flow rate of 1.1 mLmin^{-1}.

2.5. Identification of components

The percentages of compounds were calculated by area normalization method, regardless of response factors. The retention indices were calculated for all volatile constituents, using a homologous series of n-alkanes (C_8-C_{24}). The essential oil components were then identified by comparison of their mass spectra with those of a computer library or with authentic compounds and confirmed by comparison of their retention indices, either with those of authentic compounds or with data published in the literature (Adams, 2007; Davies, 1990).

2.6. Electronic nose

To analyze odor patterns, an electronic nose system was designed based on metal oxide semiconductor (MOS) sensors. A schematic representation of the electronic nose and the measurement system components is shown in Fig. 1. Seven tin oxide-based gas sensors purchased from Figaro Engineering (Osaka, Japan) and MQ (Henan, China) were used in the sensor array. The numbers, names and related specifications of the sensors are given in Table. A 12 V power supply was used for micropumps (P_1 and P_2) and solenoid valves (V_1 and V_2). A 5 V heating voltage was used to supply the operating temperature according to the Figaro

Engineering and MQ data sheets.

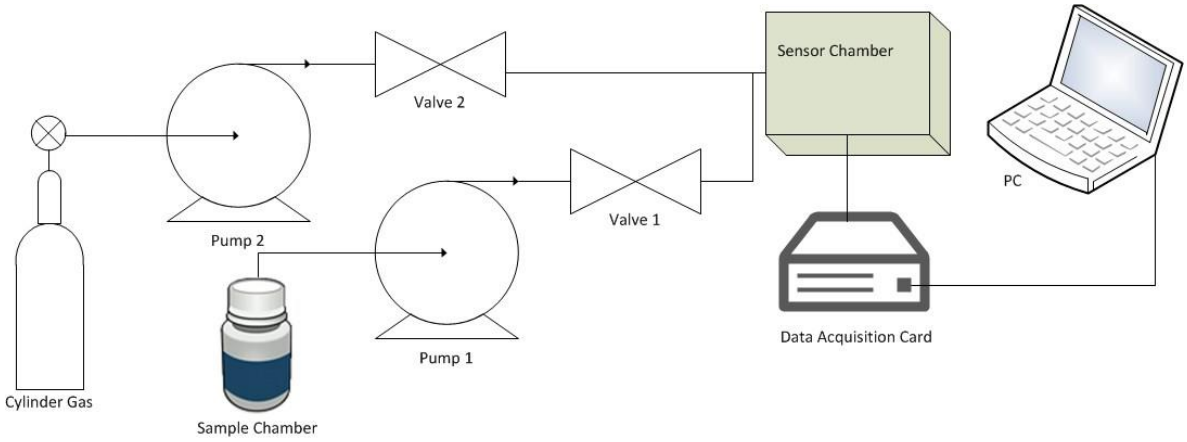

Fig. 1. Schematic representation of the electronic nose system

Table 1

Sensor array used in the electronic nose system.

Sensor Number	Sensor Name	Target Gas
S1	MQ-135	NH3, NOx, Alcohol, Benzene, Smoke,CO2
S2	MQ-5	LPG, Natural gas , Town gas
S3	MQ-136	H_2S
S4	MQ-138	n-Hexane, Benzene, NH3, Alcohol, ,Smoke, CO
S5	MQ-3	Alcohol
S6	TGS-832	Chlorofluorocarbons
S7	TGS-822	Organic Solvent Vapors

2.7. Electronic nose measurements

The processing was divided in three time phases including *baseline*, *injection* and *purging*

and sensors response was recorded as a voltage change versus time graph (Fig. 2). A description of the phases is follows:

1- *Baseline*: to obtain a stable sensor response dry air enters to the sensor chamber by passing through P_2 and V_2 at a 0.8 mL/min flow rate. This step takes 60 s.

2- *Injection*: the headspace of the sample chamber is injected into the sensor chamber during 200 s by passing through P_1 and V_1 at a 0.8 mL/min flow rate. This step lasts until the response of sensors reach a stable voltage.

3- *Purging*: P_2 and V_2 path are opened again and dry air is injected again into the sensor chamber for 500 s so sensors regain their baseline values.

The measurements were carried out in 21 replicates for every genotype while data were recorded and transferred to computer by data acquisition during measurements.

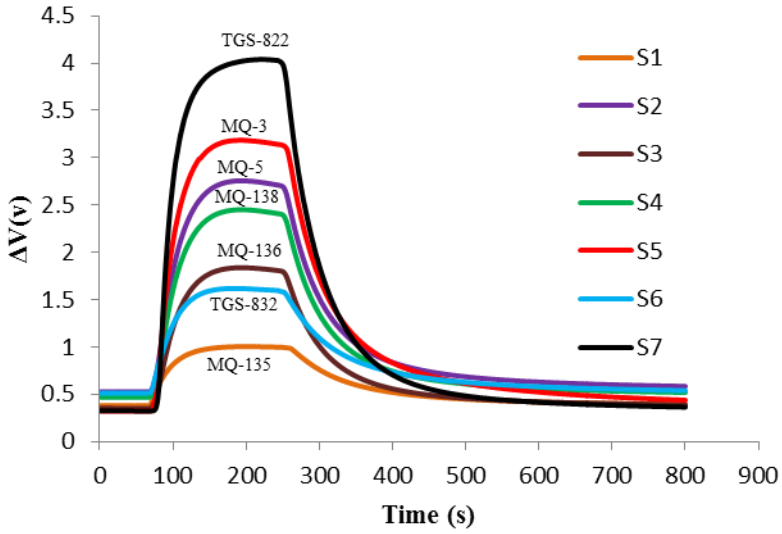

Fig. 2. One of the sensors response recorded using seven sensors of the e-nose.

2.8. Statistical processing and data analysis

After data collection, the features related to individual sensors were extracted by data

preprocessing. The goal of signal preprocessing is to extract relevant information from the sensors response and prepare the data for multivariate pattern analysis. The preprocessing is described in three stages: *baseline manipulation*, *compression*, and *normalization* (Pearce et al., 2006). In the first stage the sensor responses were manipulated with respect to their baseline for the purposes of drift compensation, contrast enhancement and scaling by fractional method. In this method, the baseline is subtracted and then divided from the sensor response according to Eq. (1).

$$Y_s(t) = \frac{X_s(t) - X_s(0)}{X_s(0)} \tag{1}$$

where $Y_s(t)$ is the resulting response, $X_s(t)$ is the sensor response and $X_s(0)$ is the baseline.

The second stage was performed by feature extraction of sensors response in the injection phase (Pearce et al., 2006). The compression of sensor response results in improved selectivity, reduced acquisition time and increased sensor lifetime (Gutierrez-Osuna, 2002). The normalization is generally used to remove the scaling effect caused by concentration changes on the patterns of the sensors (Scott et al., 2006). Auto scaling is the most frequently used scaling technique and is often used when responses are on different magnitude scales (Ghasemi-Varnamkhasti et al., 2015). This method standardizes a variable according to Eq. (2):

$$Z_j = \frac{(x_j - \bar{x}_l)}{st_l} \tag{2}$$

where Z_j is the value of x_j after auto scaling, x_j is the value for the variable before scaling, $\bar{x}_l$ is defined as the variable mean and st_l as the standard deviation of the variable. As a consequence, the mean and standard deviation of sensor responses are set at zero and one, respectively. Finally, a data matrix was created in which rows stood for samples or individuals and columns consisted variables or predictors (sensors). For data analyzing, several chemometrics tools

including principal component analysis (PCA), linear discriminant analysis (LDA) and support vector machines (SVM) were considered as multivariate statistics methods. PCA is a linear, unsupervised and pattern recognition technique used for analyzing, classifying, and reducing the dimensionality of numerical datasets in a multivariate problem (Costache et al., 2009). This technique has been widely used by researchers to display the response of an electronic nose to simple and complex odors and it provides qualitative information for electronic nose pattern recognition (Ye et al., 2011; Ghasemi-Varnamkhasti et al., 2015). LDA is a linear and supervised learning classifier that maximizes the variance among categories and minimizes the variance within categories by discriminant functions (Lin et al., 2013). SVM is a classification (and regression) technique which has been proposed on the basis of statistical learning theory (SLT) by (Cortes and Vapnik, 1995). The main idea of SVM is to separate the classes with the particular hyperplane, which maximizes a quantity called margin. The margin is the distance from a hyperplane separating the classes to the nearest point in the dataset (Pardo and Sberveglieri, 2005). The SVM classifier originally is a binary classifier but an error-correcting output codes (ECOC) model transform multi class problems (more than two class) to binary by output coding methods such as one- versus- one (OVO) and one- versus- all (OVA). Therefore, SVM classifier can be used by Classification Partitioned ECOC that is a set of error-correcting output codes (ECOC) models trained on cross-validated folds (k- fold) for SVMs or other classifiers. In k-fold cross-validation, the original sample is randomly partitioned into *k* equal sized subsamples. Of the *k* subsamples, a single subsample is retained as the validation data for testing the model, and the remaining $k - 1$ subsamples are used as training data. The cross-validation process is then repeated k times (the folds), with each of the k subsamples used exactly once as the validation data. The *k* results from the folds can then be averaged (or otherwise combined) to produce a single estimation. The advantage of this method over repeated random sub-sampling is that all observations are used for both training and validation, and each observation is used for validation exactly once. There exists an extensive research on pattern recognition and classification of electronic nose data by this methods (Acevedo et al., 2007; Brerton, 2007; Li et al., 2009; Papadopoulou et al., 2013).

In this paper, data dimensional reduction (number of variables) and variables selection with an optimized classification was done by PCA technique. The classification accuracy was then calculated by use of the classification techniques of LDA, and SVM on cross- validated data.

The optional parameters including radial basis function (RBF) as a kernel function, OVO method for output coding and 5-fold cross validation were implemented in analyses. Matlab v8.5 (The Mathworks, Natick, MA, USA) and R v3.2.1 were used for data analysis.

3. Results and discussion

3.1. *Rosa damascena* compounds

Rose compounds were identified by the results of chemical analysis (Fig. 3). According to the literature, six original constituents are determinant factors for quality and value of essential oil (Rusanov et al., 2011; Naquvi et al., 2014). The specification of these compounds and their percentage for each genotype are detailed in Table 2. According to the results, the genotypes were classified in three classes (C1, C2 and C3) of increasing quality, based on the total percent of these compounds in their essential oil. As a consequence, genotypes belonged to class C1 if their total percentage of the constituents was below 5%. Therefore, genotypes g1, g2 and g3 belong to class C1. Genotypes for which the total percentage of the compounds laid in the 10% to 40% range, were in class C2 (g4, g5 and g6). Finally, when this percentage exceeded 50%, the genotypes were assigned to class C3 (g7, g8 and g9). As shown in Table 2, some genotypes did not include all the compounds. As an instance, *phenyl ethyl alcohol* and *nerol* were not detected in the first three genotypes (g1- g3). Given the increasing presence of the six constituents that are determinant for its quality, it can be inferred that the quality and economic value of essential oil increases from genotypes g1 to g9.

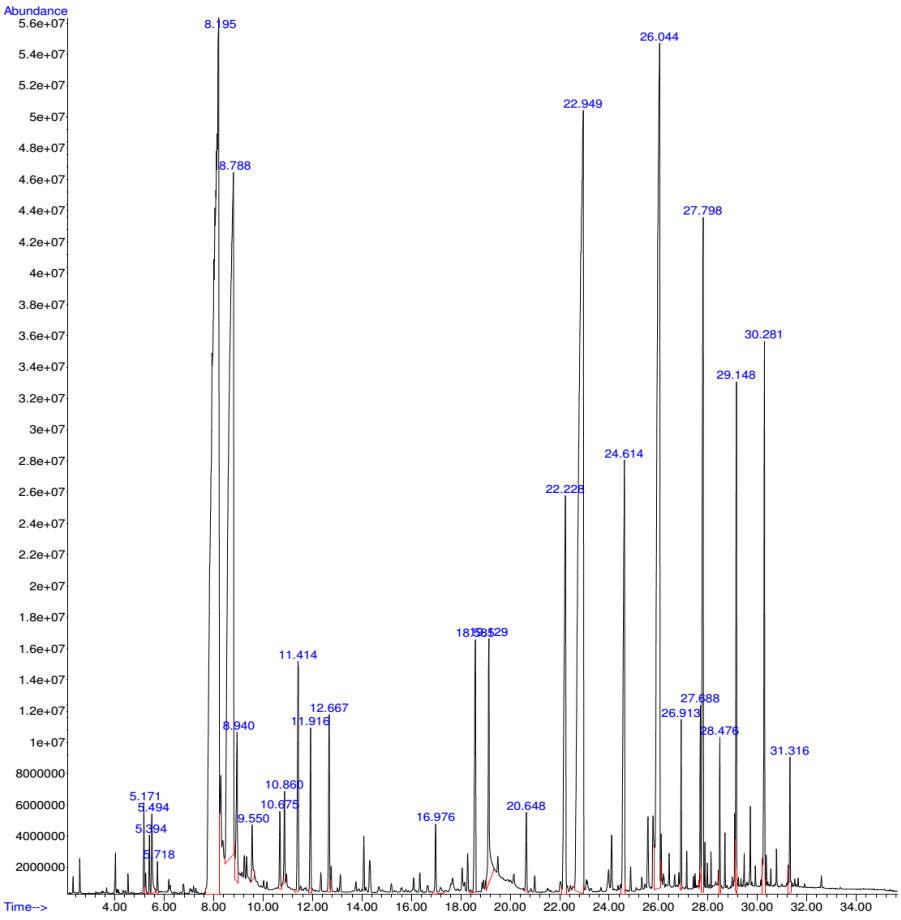

Fig. 3. Instance graph from GC-MS results for class C1.

Table 2

Specification of six original constituents and their percentage for each genotype.

Comp.No	Comp.Name	Formula	Volatile oil components in Genotypes (%)								
			g1	**g2**	**g3**	**g4**	**g5**	**g6**	**g7**	**g8**	**g9**
1	Phenyl ethyl alcohol	$C_8H_{10}O$	ND*	ND	ND	ND	0.2	0.47	0.62	0.16	0.74
2	Trans rose oxide	$C_{10}H_{18}O$	0.2	0.12	0.32	0.23	0.4	0.83	0.51	0.51	1.05
3	Citronellol	$C_{10}H_{20}O$	0.14	0.4	0.54	6.28	2.35	9.0	35.7	54.1	23.38
4	Nerol	$C_{10}H_{18}O$	ND	ND	ND	0.6	ND	ND	7.26	2.61	18.2
5	Geraniol	$C_{10}H_{18}O$	0.8	2.12	2.66	3.5	8.05	28.1	24.25	11.16	34.02
6	Geranial	$C_{10}H_{16}O$	ND	ND	0.14	ND	0.21	ND	0.28	0.28	0.38
Total Percent			**1.14**	**2.64**	**3.66**	**10.61**	**11.21**	**38.4**	**68.62**	**68.82**	**77.77**

***: ND= Not Detected**

3.2. Classification by chemometrics tools

A PCA was performed. The variance from the database that is explained by each principal component is shown in Fig. 4. The first two components (PC1, PC2) explain nearly 85% of total variance, so it seems accurate enough to analyze the dataset by using these two components only. The loadings plot shown in Fig. 5 shows that sensors S2, S4, S5 and S7 are better than sensors S6, S3 and S1 for classification. According to the loadings plot, the importance of a variable (i.e., a sensor) on the PCA classification model, increases with the distance between this variables and the origin. In other words, the closer to the unit circle drawn in the loadings plot that a variable is located, the more important is this variable for the model (e.g. sensor S1 has minimum effect on classification). Therefore, the information from the loadings plot can be used to remove sensors (variables), which do not contribute significantly to the PCA model, which helps to reduce the fabrication costs of the sensor array of the electronic nose system (Ghasemi-Varnamkhasti et al., 2012). Score plots for the first two principal components (PC1 and PC2) and linear discriminant

axis (LD1, LD2) are shown in Fig. 6. These results show that LDA can explain 99% of the between groups variance (Fig. 6b) and PCA explains 85% of the total data variance (Fig. 6a). Classification results by using LDA (employing a 5-Fold cross-validation strategy) reached a classification accuracy of 95%. The confusion matrix is shown in Table 3. Since LDA is a linear classifier, it did not perform an appropriate separation between the classes C1- C2 and C2- C3, especially for data overlapping at the classes' borders. Subsequently, classification was attempted with a SVM classifier employing a Classification Partitioned ECOC model. The classification accuracy increased to 99% according to the confusion matrix shown in Table 3. Once more, a 5-Fold cross-validation strategy was implemented. Classification results based on maximum posterior probabilities for S5 (MQ-3) and S7 (TGS-822) variables are illustrated in Fig. 7. These sensors were selected since they showed better responses (higher intensity and, therefore, less affected by noise) based on results shown in Fig. 2 and Fig. 5. The results show that samples with higher posterior probabilities have been attributed to their class correctly. There is some overlapping between C2 and C3, which may attributed to the existence of some response drift, caused by small changes in the environmental conditions such as temperature and humidity, during the time lapse needed for collecting the large number of replicate measurements (Pearce et al., 2006).

According to these results, the electronic nose system can be employed as a useful tool for classification of rose essential oils. Although some authors have shown results on the use of electronic nose systems in the field of medicinal plants (Guohua et al., 2015; Cui et al., 2015; Russo et al., 2014), as far as we know this is the first time that an e-nose is applied for screening the quality of rose essential oils, showing its usefulness for further developing the rose processing industry.

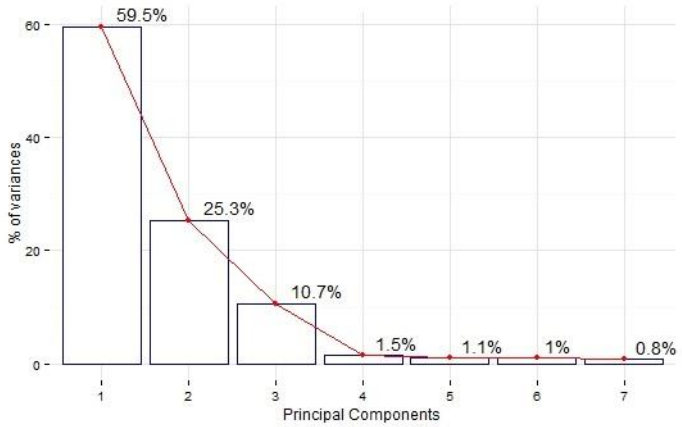

Fig. 4. Explained variance by principal components.

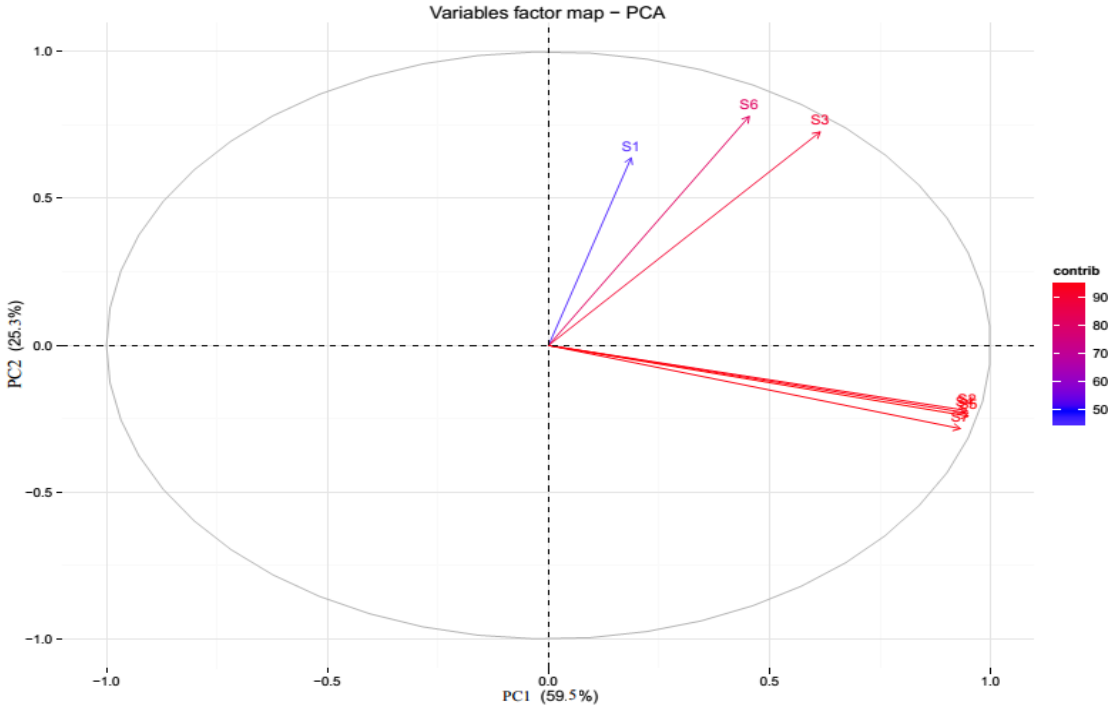

Fig. 5. Loading plot of PC1 and PC2.

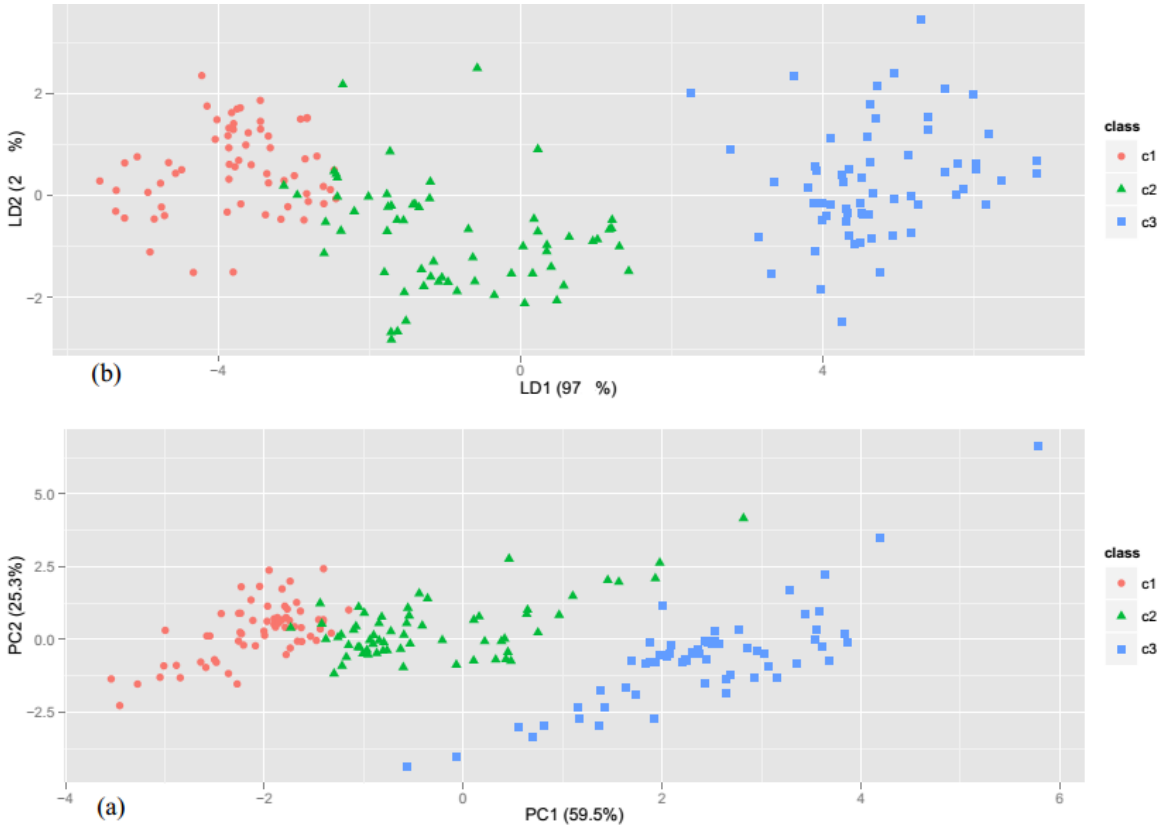

Fig. 6. Score plots on PC1& PC2 (a) and LD1 & LD2 (b).

Table 0

Confusion Matrix for LDA and ECOC model

Analysis	Real/Predicted	C1	C2	C3	Success rate
	C1	62	1	0	
LDA	**C2**	6	57	0	0.95
	C3	0	1	62	
	C1	63	0	0	
ECOC	**C2**	0	63	0	0.99
	C3	0	1	62	

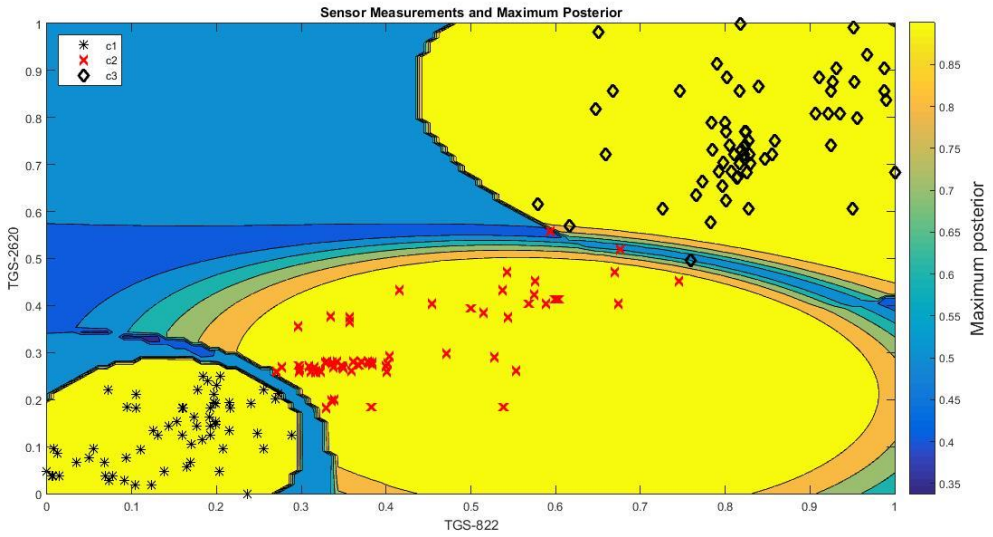

Fig. 7. Classification based on maximum posterior probabilities on S5- S7 variables.

4. Conclusions

Considering the increasing application of medicinal and aromatic plants in the world and their considerable economic value, there is a growing concern about tracing their quality. Being accurate, easy-to-use, rapid, inexpensive and adaptable to real-time, laboratory or in the field operation, the electronic nose shows the potential to become a powerful tool in the industry. In this research the rose genotypes were classified in three classes by using GC-MS analysis and then, an electronic nose based on MOS sensors was designed and trained employing chemometrics tools to sort samples according to the GC-MS-identified classes. A principal component analysis was used to identify which sensors among the array could give important information. Linear discriminant analysis and support vector machines were explored to build classification models, which reached a success rate of 95% and 99%, respectively in the classification of essential oil samples. A fold validation approach was implemented to estimate these success rates. Finally, the results show that the electronic nose can be a useful tool for quality authentication of *Rosa damascena* essential oil.

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References

Acevedo, F.J., Maldonado, S., Domínguez, E., Narváez, A., López, F., 2007. Probabilistic support vector machines for multi-class alcohol identification. Sensors Actuators, B Chem. 122, 227–235.

Adams, R.P., 2007. Identification of Essential Oil Components by Gas Chromatography/Mass Spectrometry, 4th ed. ed. Allured Publishing Corporation.

Adiguzel, Y., Kulah, H., 2015. Biosensors and Bioelectronics Breath sensors for lung cancer diagnosis 65, 121–138.

Ahmadi, K., Sefidkon, F., Asareh, M.., 2007. Comparison of quantity and quality of the essential oils of different parts of rose flower (petals, sepals and other parts) in two genotypes of Rosa damascena. Pajouhesh and Sazandegi 79, 62–71.

Alfatni, M.S.M., Shariff, A.R.M., Abdullah, M.Z., Marhaban, M.H.B., Saaed, O.M. Ben, 2013. The application of internal grading system technologies for agricultural products - Review. J. Food Eng. 116, 703–725.

Asikin, Y., Maeda, G., Tamaki, H., Mizu, M., Oku, H., Wada, K., 2015. Cultivation line and fruit ripening discriminations of Shiikuwasha (Citrus depressa Hayata) peel oils using aroma compositional , electronic nose , and antioxidant analyses. Food Res. Int. J. 67, 102–110.

Baby, R., Cabezas, M., Castro, E., Filip, R., De Reca, N.E.W., 2005. Quality control of medicinal plants with an electronic nose. Sensors Actuators, B Chem. 106, 24–28.

Baydar, H., Baydar, N.G., 2005. The effects of harvest date, fermentation duration and Tween 20 treatment on essential oil content and composition of industrial oil rose (Rosa damascena Mill.). Ind. Crops Prod. 21, 251–255.

Benedetti, S., Buratti, S., Spinardi, A., Mannino, S., Mignani, I., 2008. Electronic nose as a non-destructive tool to characterise peach cultivars and to monitor their ripening stage during shelf-life. Postharvest Biol. Technol. 47, 181–188.

Bhattacharyya, N., Bandyopadhyay, R., Bhuyan, M., Tudu, B., Ghosh, D., Jana, A., 2008. Electronic Nose for Black Tea Classification and Correlation of Measurements With "Tea Taster" Marks. IEEE Trans. Instrum. Meas. 57, 1313–1321.

Brereton, R.G., 2007. Applied Chemometrics for Scientists, Applied Chemometrics for Scientists.

Brezmes, J., Fructuoso, M.L.L., Llobet, E., Vilanova, X., Recasens, I., Orts, J., Saiz, G., Correig, X., 2005. Evaluation of an electronic nose to assess fruit ripeness. IEEE Sens. J. 5, 97–108.

Cortes, C., Vapnik, V., 1995. Support-vector networks. Mach. Learn. 20, 273–297.

Costache, G.N., Corcoran, P., Puslecki, P., 2009. Combining PCA-based datasets without retraining of the basis vector set. Pattern Recognit. Lett. 30, 1441–1447.

Cui, S., Wang, J., Yang, L., Wu, J., Wang, X., 2015. Qualitative and quantitative analysis on aroma characteristics of ginseng at different ages using E-nose and GC – MS combined with chemometrics. J. Pharm. Biomed. Anal. 102, 64–77.

Davies, N.W., 1990. Gas chromatographic retention indices of monoterpenes and sesquiterpenes on methyl silicone and Carbowax 20M phases. J. Chromatogr.

El Barbri, N., Llobet, E., El Bari, N., Correig, X., Bouchikhi, B., 2008. Electronic Nose Based on Metal Oxide Semiconductor Sensors as an Alternative Technique for the Spoilage Classification of Red Meat. Sensors 8, 142–156.

Ghasemi- Varnamkhasti, M., Aghbashlo, M., 2014. Electronic nose and electronic mucosa as innovative instruments for real- time monitoring of food dryers. Trends Food Sci. Technol. 38, 158–166.

Ghasemi-Varnamkhasti, M., Mohtasebi, S.S., Siadat, M., Ahmadi, H., Razavi, S.H., 2015. From simple classification methods to machine learning for the binary discrimination of beers using electronic nose data. Eng. Agric. Environ. Food 8, 44–51.

Ghasemi-Varnamkhasti, M., Mohtasebi, S.S., Siadat, M., Lozano, J., Ahmadi, H., Razavi, S.H., Dicko, A., 2011. Aging fingerprint characterization of beer using electronic nose. Sensors Actuators, B Chem. 159, 51–59.

Ghasemi-Varnamkhasti, M., Mohtasebi, S.S., Siadat, M., Razavi, S.H., Ahmadi, H., Dicko, A., 2012. Discriminatory power assessment of the sensor array of an electronic nose system for the detection of non alcoholic beer aging. Czech J. Food Sci. 30, 236–240.

Gomez, A.., Wang, J., Pereira, A.G., 2007. Mandarian Ripeness Monitoring And Quality Attribute Evalution Using An Electronic Nose Technique. Am. Soc. Agric. Biol. Eng. 50, 2137–2142.

Guohua, H., Jiaojiao, J., Deng, S., Xiao, Y., Mengtian, Z., Minmin, W., Dandan, Y., 2015. Winter jujube (Zizyphus jujuba Mill .) quality forecasting method based on electronic nose. Food Chem. 170, 484–491.

Gutierrez-Osuna, R., 2002. Pattern analysis for machine olfaction: A review. IEEE Sens. J. 2, 189–202.

Huang, Y., Li, F., Xia, Y., Chen, K., 2011. Scent profiling of Cymbidium ensifolium by electronic nose. Sci. Hortic. (Amsterdam). 128, 306–310.

Kaul, K., Karthigeyan, S., Dhyani, D., Kaur, N., Sharma, R.K., Ahuja, P.S., 2009. Morphological and molecular analyses of Rosa damascena × R. bourboniana interspecific hybrids. Sci. Hortic. (Amsterdam). 122, 258–263.

Kumar, R., Sharma, S., Sood, S., Agnihotri, V.K., 2013. Agronomic interventions for the improvement of essential oil content and composition of damask rose (Rosa damascena Mill.) under western Himalayas. Ind. Crops Prod. 48, 171–177.

Laureati, M., Buratti, S., Bassoli, A., Borgonovo, G., Pagliarini, E., 2010. Discrimination and characterisation of three cultivars of Perilla frutescens by means of sensory descriptors and electronic nose and tongue analysis. Food Res. Int. 43, 959–964.

Lee, S.K., Kim, J.H., Sohn, H.J., Yang, J.W., 2005. Changes in aroma characteristics during the preparation of red ginseng estimated by electronic nose, sensory evaluation and gas chromatography/mass spectrometry. Sensors Actuators, B Chem. 106, 7–12.

Li, C., Xu, F., Cao, C., Shang, M.Y., Zhang, C.Y., Yu, J., Liu, G.X., Wang, X., Cai, S.Q., 2013. Comparative analysis of two species of Asari Radix et Rhizoma by electronic nose, headspace GC-MS and chemometrics. J. Pharm. Biomed. Anal. 85, 231–238.

Li, H., Liang, Y., Xu, Q., 2009. Support vector machines and its applications in chemistry. Chemom. Intell. Lab. Syst. 95, 188–198.

Li, S., Li, X.R., Wang, G.L., Nie, L.X., Yang, Y.J., Wu, H.Z., Wei, F., Zhang, J., Tian, J.G., Lin, R.C., 2012. Rapid discrimination of Chinese red ginseng and Korean ginseng using an electronic nose coupled with chemometrics. J. Pharm. Biomed. Anal. 70, 605–608.

Lin, H., Yan, Y., Zhao, T., Peng, L., Zou, H., Li, J., Yang, X., Xiong, Y., Wang, M., Wu, H., 2013. Rapid discrimination of Apiaceae plants by electronic nose coupled with multivariate statistical analyses. J. Pharm. Biomed. Anal. 84, 1–4.

Loutfi, A., Coradeschi, S., Mani, G.K., Shankar, P., Rayappan, J.B.B., 2015. Electronic noses for food quality: A review. J. Food Eng. 144, 103–111.

Lubbe, A., Verpoorte, R., 2011. Cultivation of medicinal and aromatic plants for specialty industrial materials. Ind. Crops Prod. 34, 785–801.

Marina, a. M., Man, Y.B.C., Amin, I., 2010. Use of the SAW sensor electronic nose for detecting the adulteration of virgin coconut oil with RBD palm kernel olein. JAOCS, J. Am. Oil Chem. Soc. 87, 263–270.

Mildner-Szkudlarz, S., Jeleń, H.H., 2008. The potential of different techniques for volatile compounds analysis coupled with PCA for the detection of the adulteration of olive oil with hazelnut oil. Food Chem. 110, 751–761.

Mohammadi, A., 2015. A Review of Medicinal plants of Kohgiluyeh-va-Boyerahmad province from Iran due to employment creation and permanent development. Biol. Forum 7, 749–751.

Naquvi, K.J., Ansari, S.H., Ali, M., Najmi, a K., 2014. Volatile oil composition of Rosa damascena. J. Pharmacogn. Phytochem. 2, 130–134.

Ozkan, G., 2004. Note: Antioxidant and Antibacterial Activities of Rosa Damascena Flower Extracts. Food Sci. Technol. Int. 10, 277–281.

Pal, P.K., Agnihotri, V.K., Gopichand, Deosharan Singh, R., 2014. Impact of level and timing of pruning on flower yield and secondary metabolites profile of Rosa damascena under western Himalayan region. Ind. Crops Prod. 52, 219–227.

Papadopoulou, O.S., Panagou, E.Z., Mohareb, F.R., Nychas, G.J.E., 2013. Sensory and microbiological quality assessment of beef fillets using a portable electronic nose in tandem with support vector machine analysis. Food Res. Int. 50, 241–249.

Pardo, M., Sberveglieri, G., 2005. Classification of electronic nose data with support vector machines. Sensors Actuators, B Chem. 107, 730–737.

Pearce, T.C., Schifman, S.S., Nagle, H.T., Gardner J.W., 2006. Handbook of Machine Olfaction. Wiley.

Qiu, S., Gao, L., Wang, J., 2015. Classification and regression of ELM , LVQ and SVM for E-nose data of strawberry juice. J. Food Eng. 144, 77–85.

Rusanov, K., Kovacheva, N., Rusanova, M., Atanassov, I., 2011. Traditional Rosa damascena flower harvesting practices evaluated through GC/MS metabolite profiling of flower volatiles. Food Chem. 129, 1851–1859.

Russo, M., Serra, D., Suraci, F., Di Sanzo, R., Fuda, S., Postorino, S., 2014. The potential of e-nose aroma profiling for identifying the geographical origin of licorice (Glycyrrhiza glabra L.) roots. Food Chem. 165, 467–474.

Scott, S.M., James, D., Ali, Z., 2006. Data analysis for electronic nose systems. Microchim. Acta 156, 183–207.

Shafiqul Islam, a. K.M., Ismail, Z., Saad, B., Othman, A.R., Ahmad, M.N., Shakaff, A.Y.M., 2006. Correlation studies between electronic nose response and headspace volatiles of Eurycoma longifolia extracts. Sensors Actuators B Chem. 120, 245–251.

Shohayeb, M., Abdel-Hameed, E.S.S., Bazaid, S. a., Maghrabi, I., 2014. Antibacterial and antifungal activity of Rosa damascena MILL. essential oil, different extracts of rose petals. Glob. J. Pharmacol. 8, 1–7.

Subari, N., Mohamad Saleh, J., Md Shakaff, A., Zakaria, A., 2012. A Hybrid Sensing Approach for Pure and Adulterated Honey Classification. Sensors 12, 14022–14040.

Tabaei-Aghdaei, S.R., Babaei, A., Khosh-Khui, M., Jaimand, K., Rezaee, M.B., Assareh, M.H., Naghavi, M.R., 2007. Morphological and oil content variations amongst Damask rose (Rosa damascena Mill.) landraces from different regions of Iran. Sci. Hortic. (Amsterdam). 113, 44–48.

Trirongjitmoah, S., Juengmunkong, Z., Srikulnath, K., Somboon, P., 2015. Classification of garlic cultivars using an electronic nose. Comput. Electron. Agric. 113, 148–153.

Westenbrink, E., Arasaradnam, R.P., O'Connell, N., Bailey, C., Nwokolo, C., Bardhan, K.D., Covington, J. a., 2015. Development and application of a new electronic nose instrument for the detection of colorectal cancer. Biosens. Bioelectron. 67, 733–738.

Xiao, Z., Yu, D., Niu, Y., Chen, F., Song, S., Zhu, J., Zhu, G., 2014. Characterization of aroma compounds of Chinese famous liquors by gas chromatography-mass spectrometry and flash GC electronic-nose. J. Chromatogr. B Anal. Technol. Biomed. Life Sci. 945-946, 92–100.

Xiong, Y., Xiao, X., Yang, X., Yan, D., Zhang, C., Zou, H., Lin, H., Peng, L., Xiao, X., Yan, Y., 2014. Quality control of Lonicera japonica stored for different months by electronic nose. J. Pharm. Biomed. Anal. 91, 68–72.

Ye, T., Jin, C., Zhou, J., Li, X., Wang, H., Deng, P., Yang, Y., Wu, Y., Xiao, X., 2011. Can odors of TCM be captured by electronic nose? The novel quality control method for musk by electronic nose coupled with chemometrics. J. Pharm. Biomed. Anal. 55, 1239–1244.

Yu, H., Wang, J., Xu, Y., 2007. Identification of adulterated milk using electronic nose. Sensors Mater. 19, 275–285.

Zakaria, A., Md Shakaff, A.Y., Masnan, M.J., Saad, F.S.A., Adom, A.H., Ahmad, M.N., Jaafar, M.N., Abdullah, A.H., Kamarudin, L.M., 2012. Improved maturity and ripeness classifications of Magnifera Indica cv. harumanis mangoes through sensor fusion of an electronic nose and acoustic sensor. Sensors (Switzerland) 12, 6023–6048.

Zhang, B., Huang, Y., Zhang, Q., Liu, X., Li, F., Chen, K., 2014. Scientia Horticulturae Fragrance discrimination of Chinese Cymbidium species and cultivars using an electronic nose 172, 271–277.