Research on of the Sausage Flavour by GC-MS and Electronic Nose

Xin Yang¹, Limin Zheng¹,²* and Lu Yang¹,²

¹College of Information and Electrical Engineering, China Agricultural University, Beijing, 100083, China
²Beijing Laboratory of Food Quality and Safety, China Agricultural University, Beijing, 100083, China

*Corresponding author’s e-mail: zhenglimin@cau.edu.cn

Abstract. To rapidly and objectively evaluate the flavour of sausages using an electronic nose, the experiment extracted the volatile components of 6 different kinds of sausages of a certain sausages brand manufacturer and identified them using gas chromatography-mass spectrometry (GC-MS). Sensory evaluation and an electronic nose were used to evaluate the flavour attributes of sausages. Partial least squares discrimination analysis (PLS-DA) was used to identify and classify the electronic nose data of different varieties of sausages samples; The volatile components were identified by the method of variable important in the projection (VIP); The correlation between critical flavour components and the sensory attribute was established by partial least squares regression (PLSR). According to the PLS-DA results, the electronic nose has good distinguishing ability for different kinds of sausages and different production batches of the same kind of sausages; A total of 118 volatile flavour compounds were identified in sausages; Through the method of VIP, 44 kinds of differential characteristic substances were obtained and classified by PLS-DA discriminant analysis, which was consistent with the electronic nose classification result mapping relationship; The PLSR shows that sensory attribute has a good correlation with the differential flavour components. Therefore GC-MS, electronic nose and sensory analysis can comprehensively evaluate the flavour differences of the sausages.

1. Introduction
Sausage is a popular smoked enema food. Its flavour is an indicator that both manufacturers and consumers pay attention to. However, due to its complex flavour, it has rarely been clearly analyzed so far.

In the detection of volatile flavour substances in sausages, gas chromatography-mass spectrometry (GC-MS) can detect the type and content of flavour substances in the samples, but can not analyze the contribution of these substances to the overall flavour of the sample[1][2], sensory evaluation is simple and practical but subjective[3], while the electronic nose can compare the overall flavour characteristics of the sample, and there is no subjective factor influencing in the artificial sensory evaluation, those technologies were beneficial to comprehensively study the flavour of the food[4]. Wang[5] obtained the mapping relationship between electronic nose data and GC-MS data, indicating that it is feasible to use an electronic nose to detect and identify the difference between volatile flavours of different pork. Tian[6] used electronic nose and GC-MS to identify the aroma components of chicken essence, combined with the sensory evaluation to analyze the effect of...
processing and storage on chicken flavour, indicating that GC-MS and electronic nose combined with stoichiometry can comprehensive evaluation of the olfactory flavour of chicken seasonings.

On the basis of the electronic nose can effectively distinguish different samples of sausages, the volatile components of different sausages were identified by GC-MS technique, and the different characteristic flavours of different sausages were obtained by variable important in the projection (VIP) method. The partial least squares discrimination analysis (PLS-DA) was used to obtain the mapping relationship between the electronic nose detection data and the volatile components of the sausages, which indicated the feasibility of using the electronic nose to detect and identify the differences in volatile flavours between different sausages. Partial least squares regression (PLSR) analysis of the correlation between the characteristic flavour and the sensory attributes, in order to comprehensively evaluate the difference in the flavour of the sausages by GC-MS, electronic nose combined with sensory evaluation.

2. Materials and methods

2.1 Material
Six varieties of sausages which consist of Pure sausage, Children sausage, Red sausage, Exquisite sausage, Big sausage, and Flavoured sausage (Give them numbers A–F) were collected from a certain sausages brand manufacturer. After the material was retrieved, it was stored at 4°C.

2.2 Instruments and equipment
Trace1310-TSQ8000 GC-MS combined instrument(Thermo Fisher Scientific, USA); Fiber 75 μm Manual Solid Phase Microextraction Sampler, divinylbenzene/carboxen/polydimethysiloxane extraction head (Supelco, USA).

The electronic nose device adopts the E-nose electronic nose system of China Agricultural University, which was mainly composed of 16 TGS series gas sensors (9 TGS8 series sensors and 7 TGS2000 series sensors), signal acquisition system and pattern recognition system.

2.3 Method
2.3.1 Sensory evaluation. The sausages samples were placed in an official evaluation cup, and 10 sensory appraisal professionals were selected to score the sausages according to sensory indexes such as sausages, garlic, pepper, smoky, sweet, and greasy feelings. Each sensory appraiser repeatedly evaluated each sample of the sausages three times. At the end of each evaluation, the sensory index of the sausages was scored. The score was 5 points, 0 points, almost none; 1 point, weaker; 2 points, more obvious; 3 points, obvious; 4 points, rich.

2.3.2 Electronic nose detection. Accurately weigh 10g of the sausages samples and place them in a Petri dish in an electronic nose-tight chamber. The volatile matter was measured by headspace inhalation. The measurement temperature was kept at 40 °C, and each sample was sampled for 300 s. The sensor was cleaned for 60 s before the test and the cleaning flow rate was 3 L/min.

2.3.3 Detecting flavour substances. The sample was minced and mixed. Accurately weigh 5g of the sample into the solid phase micro-extraction vial and screw the lid. The solid phase micro-extraction bottle was placed in a 55°C water bath for 10 mins, and then the solid phase micro-extraction needle was placed. Inserted into the bottle, the fiber head was in the headspace state and adsorbed the aroma compound for 30 mins. GC conditions: DB-Wax polar column (30m×0.25mm, 0.25μm) for gas chromatography; high purity helium (purity>99.99%) as carrier gas; flow rate 1.0 mL/min (constant); no split. Temperature programmed for gas chromatography: inlet temperature 230 °C, column temperature 40 °C for 3 mins, 4 °C / min to 200 °C for 1 min, then 10 °C / min to 230 °C 5 mins. MS
conditions: Electron ionization mode; interface temperature 230°C; electron energy 70 eV; ion source temperature 260°C; mass spectrometry masses to scan range was set to 40 ~ 600u.

2.3.4 Data analysis method. Electronic nose and GC-MS analysis: The obtained data of the sausages electronic nose and the selected 44 flavour substances were classified by PLS-DA using SIMCA 14.1 statistical software.

Qualitative volatile flavours: Compounds were identified by NIST, Willey library search, and compounds with a matching degree greater than 700 were selected.

Volatile Flavour Material Quantification: The percent content of each compound was calculated using the area normalization method.

Screening for differential flavours between groups: In the PLS-DA model with supervised pattern recognition, the most commonly used method for evaluating variable contributions was the VIP method. Using VIP to screen for differential compounds between groups, the variable with VIP>1.0 was statistically significant[7].

Sensory evaluation analysis: Sensory datas were analyzed using the letter labeling method[8] in multiple comparisons.

Correlation analysis between GC-MS and sensory evaluation: The relationship between the characteristic flavour substance and the sensory attribute was analyzed by PLSR in SIMCA 14.1, and then drew a PLSR load map.

3. Results and analysis

3.1 PLS-DA analysis results from sausages electronic nose

Figure 1. Effect of partial least squares model.

The electronic nose test obtained 6 samples of sausages samples, 15 samples per sample, a total of 90 samples, and the different varieties of sausages data set consisted of all 90 data. The data set of the electronic nose was classified by PLS-DA, and the classification effect of the model was shown in figure 1. From the distribution of the sample, the 15 replicate of the same sample can contribute to a mass, and the 6 samples do not overlap each other, and the difference was obvious, indicating that the stability and repeatability of the electronic nose data were good. The results show that the results of electronic nose analysis can distinguish the different flavours of sausages.
3.2 GC–MS analysis

3.2.1 Analysis of test results. A total of 118 different volatile substances were detected by GC-MS. The contents of volatile substances in each of the sausages samples were shown in table 1. The results showed that there were differences in volatile substances in different types of sausages samples.

| Compound species | Number of compounds | A(%) | B(%) | C(%) | D(%) | E(%) | F(%) |
|------------------|---------------------|------|------|------|------|------|------|
| Aldehyde         | 10                  | 6.15 | 4.79 | 2.95 | 18.22| 5.09 | 2.41 |
| Alcohol          | 16                  | 11.83| 13.68| 8.05 | 5.05 | 17.15| 5.78 |
| Ketones          | 14                  | 2.90 | 5.42 | 2.89 | 6.34 | 4.30 | 1.61 |
| Ester            | 7                   | 1.41 | 1.05 | 0.54 | 0.50 | 2.45 | 1.00 |
| Ether            | 6                   | 45.70| 2.05 | 33.67| 20.23| 0.79 | 13.61|
| Phenols          | 18                  | 20.28| 35.38| 25.34| 20.75| 33.45| 24.08|
| Olefins          | 24                  | 9.60 | 28.61| 24.26| 19.59| 31.40| 47.57|
| Alkane           | 3                   | 0.01 | 2.73 | 0.22 | 0.12 | 0.08 | 0.30 |
| Acid             | 6                   | 0.157| 0.83 | 0.38 | 0.21 | 0.10 | 0.15 |
| Benzene          | 8                   | 0.433| 2.87 | 0.68 | 6.32 | 2.3  | 1.18 |
| Other            | 6                   | 1.50 | 1.76 | 0.92 | 1.82 | 1.63 | 1.98 |

The VIP value obtained by PLS-DA can be found to distinguish the characteristic substances of the sausages sample. The higher the VIP value, the greater the difference weight in different sausages samples, the more the difference between different varieties of sausages can be reflected\(^9\).

3.2.2 Screening for differential flavours between groups. The VIP value obtained by PLS-DA can be found to distinguish the characteristic substances of the sausages sample. The higher the VIP value, the greater the difference weight in different sausages samples, the more the difference between different varieties of sausages can be reflected\(^9\).

The flavour substances which contributed to the separation of different varieties of the sausages were screened by VIP>1.0 as the standard. The 44 flavour substances and their percentages were as showed in table A1. The selected 44 flavour substances were classified by PLS-DA, and the results were shown in figure 2.

Figure 2. Sorting flavours with PLS-DA.
There was a clear classification of the volatile components in the sausages, and there was a consistent mapping relationship between the classification pattern and the electronic nose detection data\cite{5}.

The flavour substances and VIP values of the selected sausages of different varieties and other varieties of the sausages were shown in table 2.

| Numbering | A&Other | B&Other | C&Other | D&Other | E&Other | F&Other |
|-----------|---------|---------|---------|---------|---------|---------|
| A1        | 1.81    | -       | -       | 1.08    | -       | 1.13    |
| A2        | 1.87    | 1.11    | -       | -       | 1.08    | 1.12    |
| A3        | -       | -       | 1.30    | -       | 1.16    | -       |
| A4        | -       | -       | 1.41    | 1.90    | -       | -       |
| B1        | 2.01    | 1.15    | -       | -       | 1.13    | 1.01    |
| B2        | 1.10    | 1.74    | 1.26    | 1.04    | 1.43    | 1.09    |
| B3        | 2.17    | -       | 1.01    | -       | -       | -       |
| B4        | -       | 1.10    | 1.08    | -       | 1.78    | -       |
| B5        | -       | 1.21    | 1.06    | -       | 1.12    | 1.28    |
| B6        | -       | 1.05    | 1.13    | -       | 1.94    | -       |
| B7        | -       | 1.60    | -       | -       | -       | 1.18    |
| B8        | -       | 1.29    | 1.21    | 1.17    | 1.76    | 1.26    |
| B9        | 1.32    | -       | -       | 1.17    | 1.57    | -       |
| C1        | 2.09    | -       | 1.01    | -       | -       | -       |
| C2        | -       | 1.37    | 1.33    | 1.04    | -       | 1.29    |
| C3        | 1.08    | 1.91    | 1.31    | -       | 1.26    | 1.13    |
| C4        | -       | 1.08    | -       | -       | -       | 1.17    |
| C5        | -       | 1.03    | -       | 1.33    | -       | 1.62    |
| D1        | -       | -       | 1.27    | -       | 1.51    | 1.09    |
| D2        | -       | -       | 1.14    | 1.24    | 1.20    | -       |
| E1        | 2.10    | -       | 1.05    | -       | -       | -       |
| E2        | 1.39    | 1.38    | 1.62    | -       | 1.35    | -       |
| F1        | 1.20    | -       | -       | -       | 1.09    | 1.03    |
| F2        | 1.01    | -       | -       | -       | 1.09    | -       |
| F3        | 1.07    | -       | 1.11    | -       | 1.97    | -       |
| F4        | 1.05    | 1.05    | 1.04    | 1.12    | 1.54    | 1.12    |
| F5        | -       | 1.47    | -       | 1.34    | 1.13    | 1.08    |
| F6        | 1.35    | 1.25    | -       | -       | -       | -       |
| G1        | -       | 1.39    | 1.08    | -       | -       | -       |
| G2        | 1.28    | -       | -       | -       | -       | 1.39    |
| G3        | 1.02    | 1.81    | 1.23    | -       | 1.21    | 1.06    |
| G4        | 1.06    | -       | 2.27    | 1.10    | 1.01    | 1.04    |
| G5        | 1.07    | -       | 1.21    | -       | -       | 2.03    |
There were Bicyclo[3.1.0]hexan-2-ol, 2-methyl-5-(1-methylethyl), (1R,2R,5S)-rel-, Phenol, 2,6-dimethoxy-Guaiacol, and 1,4-Cyclohexadiene,1-methyl-4-(1-methylethyl)- that have important contributions to the differentiation of various varieties of sausages from other varieties of sausages. 2,6-dimethoxy-Guaiacol was a woody aroma substance volatilized by lignin of broad-leaved tree, 1,4-Cyclohexadiene,1-methyl-4-(1-methylethyl)- was a substance with a sweet lemon flavour in star anise\textsuperscript{[10]}. The most contributing flavour substance that distinguishes the Pure sausage from other varieties of sausages was 1-Octen-3-ol, which exhibits the characteristics of mushroom flavour, and gives a certain kind of woody green gas to the sausages when it was separated for a long time\textsuperscript{[11]}. The most different flavour substance between Children sausage and other varieties of sausages was 2-Cyclopenten-1-one, 3,4-dimethyl-, which has a sweet fragrance and was a commonly used food additive\textsuperscript{[12]}. The sausages with the most different flavour substances from other varieties of sausages was Red sausage. The most important difference flavours substance that distinguishes the Red sausage from other varieties of sausages was Ocimene, which has grassy fragrance and was the main aroma component of dried chili\textsuperscript{[13]}. 2-Furancarboxaldehyde, 5-methyl- was the flavour substance that makes the greatest contribution to distinguish Exquisite sausage from other varieties of sausages, and gives the aroma of the sausages oil\textsuperscript{[14]}. The most important flavour substance that makes Big sausage differ from other varieties of sausages was Phenol, 3,4-dimethyl-, which was the main functional smoke component of liquid smokers\textsuperscript{[15]}. The most important of the different flavours that distinguish Flavoured sausage from other varieties of sausages was Caryophyllene, which was an oil-like aroma brought by cinnamon\textsuperscript{[16]}.

The flavours and their VIP values of the different varieties of the sausages group that was screened out were as showed in table 3.

| Numbering | A&B | A&C | A&D | A&E | A&F | B&C | B&D | B&E | B&F | C&D | C&E | C&F | D&E | D&F | E&F |
|-----------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| A1        | -   | -   | 1.39 | -   | 1.26 | -   | -   | -   | -   | -   | -   | -   | -   | -   | -   |
| A2        | 1.16 | -   | -   | 1.22 | 1.26 | -   | -   | -   | -   | -   | -   | -   | -   | -   | -   |
| A3        | -   | -   | -   | -   | -   | -   | -   | -   | 1.21 | -   | -   | -   | -   | -   | -   |
| A4        | -   | -   | -   | -   | -   | -   | -   | -   | -   | 1.69 | -   | -   | -   | -   | -   |
| B1        | 1.13 | -   | -   | 1.19 | 1.21 | -   | -   | -   | 1.10 | -   | -   | -   | -   | -   | 1.21 |
| B2        | 1.21 | 1.36 | 1.04 | 1.17 | 1.19 | 1.22 | 1.33 | -   | 1.26 | -   | 1.14 | -   | 1.14 | 1.07 | 1.24 |
There were 4~18 kinds of different flavour substances between different varieties of sausages. The difference in flavour between Pure sausage and Exquisite sausage was the least, and the difference between Red sausage and Big sausage was the most. 2-Cyclopenten-1-one, 3,4-dimethyl- was the most different flavour substance between Pure sausage and Children sausage, and it was also the most different flavour substance between Children sausage and other varieties. 1-Octen-3-ol was the most
different flavour substance between Pure sausage and Red sausage. It was also the most different flavour substance between Pure sausage and other varieties. The most important difference between Pure sausage and Exquisite sausage was Hexanal, which was raw oil and woody\cite{17}. It was the highest content of aldehydes in dry ham\cite{11} volatile aldehydes\cite{18}. Phenol, 3,4-dimethyl- was the most different flavour substance between Pure sausage and Big sausage, and it was the most different flavour substance between Big sausage and other varieties. The most distinguishing flavour substance between Pure sausage and Flavoured sausage was 3-Carene which was derived from black pepper with a spicy odor\cite{19}. The most important differential flavours substance that distinguishes Children sausage from Red sausage was Benzene, 1,2-(methyleneoxy)-4-propenyl-, (E)-. The main substance in oil, Alpha-Terpineol\cite{20}, was the most important flavour substance between Children sausage and Exquisite sausage and Flavoured sausage. It was also the most different flavour between Exquisite sausage and Big sausage. The most different flavour substance between Children sausage and Big sausage was 2-Cyclohexen-1-ol, 1-methyl-4-(1-methylethyl)-, trans-. Branched alcohol was a flavour component not found in fresh meat and has strong volatility\cite{21}. 2-Furancarboxaldehyde, 5-methyl- was the most different flavour substance between Red sausage and Exquisite sausage, and it was also the most different flavour between Exquisite sausage and other varieties. Ocimene was the most important flavour substance between Red sausage and Big sausage and Flavoured sausage. It was also the most different flavour between Red sausage and other varieties. The most different substance between Exquisite sausage and Flavoured sausage was 2-Cyclopenten-1-one, 2,3-dimethyl-, which was a sweet food additive. 1,4-Cyclohexadiene, 1-methyl-4-(1-methylethyl)- was the most important difference flavour substance that distinguishes Big sausage from Flavoured sausage. It was also a different flavour substance that has important contributions to distinguish each kind of sausages from other varieties.

Among the flavours with significant differences among different varieties of sausages, Phenol, 2-methoxy-4-(1-propenyl)- was only an important marker for distinguishing the difference between Red sausage and Children sausage, and it was a characteristic smoke constituent of beech trees\cite{22}. 2,3-Octanedione and Diallyl sulfide were only important markers for distinguishing the difference between Pure sausage and Red sausage, 2,3-Octanedione with sweet milk fragrance has a higher content in the sausages with longer processing time\cite{23}. Cyclobutene, 2-propenylidene- has an aroma of garlic and was an essential substance that affects the overall flavour of the sausages\cite{24}. Phenol, 4-ethyl-2-methoxy- was only an important marker for distinguishing the difference between Pure sausage and Big sausage, and it was a substance with a sweet smell and smoke fragrance in smoked tobacco\cite{25}. Beta-Pinene and Caryophyllene were only important markers for distinguishing the difference between Pure sausage and Flavoured sausage. Beta-Pinene derived from nutmeg has resin scent\cite{26}. Cyclobutene, 2-propenylidene- and 1,3-Cyclohexadiene, 1-methyl-4-(1-methylethyl)- with sweet aroma were only important markers for distinguishing the difference between Children sausage and Red sausage. Ethanone, 1-(2-furanyl)- was only an important marker for distinguishing the difference between Children sausage and Exquisite sausage. It was widely found in natural and processed food aroma components\cite{27}. It was a smoky-flavoured meat flavoured spice with meat flavour\cite{22}. 2-Furanmethanol was only an important marker for distinguishing the difference between Children sausage and Flavoured sausage. It was naturally found in black tea and has sweet barbecue flavour\cite{28}. 2-Furancarboxaldehyde, 5-methyl- and 2-Methylphenylacetylene were only important markers for distinguishing the difference between Red sausage and Exquisite sausage. Azulene with tea aroma was only an important marker to distinguish the difference between Red sausage and Flavoured sausage.

Qualitative and quantitative research on these substances can support the differentiation of different varieties of sausages, and can also add corresponding characteristic compound control indicators in the production of sausages, highlighting the differences in the characteristics of each species of sausages, and further study the characteristic flavour substances in production. The formation and change process was of great significance to the study of the sausages.
3.3 Sensory evaluation analysis

Sensory evaluation of the sensory attributes (meat, garlic, pepper, smoky, sweet, and greasy) of the six kinds of sausages. Sensory evaluation results were analyzed by analysis of variance, and the mean and standard deviation from sensory attributes were found in table 4.

Table 4. Sensory evaluation score.

| Sausages number | Meat    | Garlic  | Pepper  | Smoky   | Sweet   | Greasy  |
|-----------------|---------|---------|---------|---------|---------|---------|
| A               | 2.49±0.97a | 1.93±0.84a | 1.64±0.86b | 1.94±0.62b | 0.69±0.76b | 1.54±0.83a |
| B               | 1.97±0.82bc | 1.60±0.89bc | 1.56±0.88bc | 2.33±0.82a  | 1.28±0.96a  | 1.22±0.79bc |
| C               | 2.18±0.81b  | 1.88±0.87ab | 1.71±0.86ab | 1.86±0.69b  | 0.78±0.82b  | 1.76±0.89a  |
| D               | 2.54±0.94a  | 1.88±0.97ab | 1.82±0.89ab | 2.06±0.68b  | 0.88±0.91b  | 1.28±0.67b  |
| E               | 1.76±0.84c  | 1.38±0.84c  | 1.35±0.82c  | 2.39±0.94a  | 1.39±0.91a  | 1.04±0.68c  |
| F               | 2.24±0.91ab | 1.72±0.99ab | 1.99±0.84a  | 2.01±0.75b  | 1.33±0.97a  | 1.19±0.68bc |

a The values in the table were mean ± standard deviation, abc represents the significant difference in the value of each column, and the difference in the same column was not significant, and the difference was significant (P < 0.05).

It can be seen from table 4 that there was a significant difference (P<0.05) between the sensory attributes of different varieties of sausages, meat, garlic, pepper, smoky, sweet, and greasy. Chira[29] believes that sensory attributes can well explain the flavour differences in different varieties of sausages. The garlic flavour of sample Pure sausage was significantly stronger than other varieties, probably due to the high content of diallyl sulfide in Pure sausage. The pepper flavours score of sample Flavoured sausage far exceeded that of other samples, probably because this sample contained more olefinic substances with pepper scent.

3.4 PLSR with differential feature flavour material and sensory evaluation

Figure 3. PLS regression plots showing the correlation between GC-MS and sensory evaluation.

Volatile flavours were correlated with sensory attributes[30] to facilitate the identification of substances that affect sensory attributes. Flavouring substances that have a greater contribution to distinguishing different varieties of sausages have a good correlation with various sensory attributes. The smoky flavour score has a significant positive correlation with most phenolic substances, and the sweetness and pepper flavour scores also have their own The flavour of the sweet and aroma was positively correlated, and the garlic score was also significantly positively correlated with the sulfur-containing substances.
4. Conclusions
The electronic nose technique, SPME-GC-MS method, and sensory evaluation were used to analyze the differential characteristics of the sausages samples. The electronic nose classification showed that it can effectively distinguish different kinds of sausages. GC-MS detected 118 kinds of flavour substances in 6 sausages samples, and 44 kinds of flavour substances which contributed to the separation of different colors of the sausages were obtained according to the VIP. The PLS-DA classification results were consistent with the electronic nose classification results. Sensory evaluation analysis showed that there were differences in different taste flavours of different varieties of sausages. The correlation analysis between flavour characteristics and sensory evaluation showed that flavour substances were the factors affecting sensory attributes. Studies have shown that GC-MS, electronic nose combined with sensory evaluation can comprehensively evaluate the differential volatile flavour substances in the sausages, and more comprehensively evaluate the aroma of the sausages.

5. Appendices

Table A1. Flavour substances useful for classification.

| Kind | Number | Numbering | Name                                           | A(%) | B(%) | C(%) | D(%) | E(%) | F(%) |
|------|--------|-----------|------------------------------------------------|------|------|------|------|------|------|
| Aldehyde 4 | A1 | | Hexanal | 2.07 | 0.89 | 0.58 | 0.27 | 0.84 | 0.33 |
|       | A2 | | Heptanal | 0.40 | - | 0.11 | 0.15 | - | - |
|       | A3 | | Furfural | 1.49 | 1.45 | 0.58 | 1.38 | 2.16 | 0.62 |
|       | A4 | | 2-Furancarboxaldehyde, 5-methyl- | 0.99 | 1.28 | 0.74 | 2.76 | 1.35 | 1.05 |
|       | B1 | | Allyl mercaptan | 7.07 | 0.12 | 1.66 | 2.08 | 0.07 | 0.81 |
|       | B2 | | Bicyclo[3.1.0]hexan-2-ol, 2-methyl-5-(1-methylethyl), (1R,2R,5S)-rel- | 0.01 | 2.21 | 0.07 | 0.05 | 1.92 | 0.10 |
|       | B3 | | 1-Octen-3-ol | 0.36 | - | - | - | - | - |
|       | B4 | | Cyclohexanol, 1-methyl-4-(1-methylethenyl), cis- | 0.01 | 1.21 | 0.01 | - | 2.14 | - |
| Alcohol 9 | B5 | | 2-Cyclohexen-1-ol, 1-methyl-4-(1-methylethenyl), trans- | 1.23 | 1.50 | 1.34 | 0.68 | 0.11 | - |
|       | B6 | | 3-Cyclohexen-1-ol, 4-methyl-1-(1-methylethenyl)- | - | 3.03 | - | - | - | 6.39 | 0.04 |
|       | B7 | | 2-Furanmethanol | 2.16 | 3.37 | 2.33 | 1.70 | 2.13 | 1.46 |
|       | B8 | | Alpha-Terpineol | 0.33 | 0.70 | 0.10 | - | 0.95 | - |
|       | B9 | | 2-Cyclopenten-1-one, 2-hydroxy-3-methyl- | 0.26 | 1.19 | 1.04 | 0.36 | 1.70 | 0.81 |
| Ketones 5 | C1 | | 2,3-Octanedione | 0.10 | - | - | - | - | - |
|       | C2 | | 2-Cyclopenten-1-one, 2-methyl- | 0.72 | 1.36 | 0.53 | 1.16 | 1.00 | 0.47 |
|       | C3 | | 2-Cyclopenten-1-one, 3,4-dimethyl- | - | 0.29 | - | - | 0.02 | 0.20 |
|       | C4 | | 2-Butanone, 1-(acetyloxy)- | 0.07 | 0.18 | 0.06 | 0.08 | 0.16 | - |
|       | C5 | | 2-Cyclopenten-1-one, 2,3-dimethyl- | 0.92 | 1.49 | 0.92 | 1.60 | 1.24 | 0.49 |
| Ester 2 | D1 | | Acetic acid, butyl ester | 0.89 | 0.75 | - | - | 1.35 | - |
|       | D2 | | 2,5-Octadecadiynoic acid, methyl ester | - | 0.02 | - | 0.07 | 0.06 | - |
| Ether 2 | E1 | | Diallyl sulfide | 9.25 | 1.27 | - | - | - | - |
|       | E2 | | Diallyl disulfide | 35.01 | 0.71 | 32.74 | 19.50 | 0.74 | 13.27 |
| Phenols 6 | F1 | | Phenol, 2-methoxy-4-methyl- | 2.64 | 6.58 | 4.89 | 4.45 | 6.26 | 2.99 |
|                  |                     | 0.79  | 1.86  | 1.30  | 0.92  | 1.91  | 1.22  |
|------------------|---------------------|-------|-------|-------|-------|-------|-------|
| Phenol, 4-ethyl-2-methoxy- | F2                   |       |       |       |       |       |       |
| Phenol, 3,4-dimethyl- | F3                   | 0.06  | 0.46  | 0.15  | 0.23  | 1.12  | 0.23  |
| Phenol, 2,6-dimethoxy- | F4                   | 0.91  | 2.02  | 1.86  | 0.72  | 2.71  | 0.82  |
| Guaiacol         | F5                   | 5.71  | 12.50 | 8.65  | 2.74  | 10.59 | 4.78  |
| Phenol, 2-methoxy-4-(1-propenyl)- | F6                  | -     | 0.13  | 0.10  | 0.04  | 0.09  | 0.07  |
| Cyclobutene, 2-propenylidene- | G1                  | 0.03  | 0.16  | -     | 0.07  | 0.04  | 0.03  |
| Beta-Pinene      | G2                   | 0.18  | 1.46  | 1.27  | 0.80  | 1.69  | 2.36  |
| Phellandrene     | G3                   | -     | 4.18  | -     | 0.26  | 3.00  | 0.03  |
| Ocimene          | G4                   | -     | -     | 9.27  | 6.82  | -     | -     |
| 3-Carene         | G5                   | -     | 3.09  | -     | -     | 4.73  | 9.94  |
| 1,3-Cyclohexadiene, 1-methyl-4-(1-methylbutyl)- | G6                  | -     | 1.11  | -     | -     | 1.45  | 0.18  |
| D-Limonene       | G7                   | 2.65  | 4.93  | 7.46  | 3.04  | 6.41  | 15.00 |
| 1,4-Cyclohexadiene, 1-methyl-4-(1-methylbutyl)- | G8                  | 0.20  | 4.06  | 0.20  | 0.35  | 3.60  | 0.37  |
| Cyclohexene, 1-methyl-4-(1-methylbutylidene)- | G9                  | 3.96  | 1.72  | 0.04  | 0.05  | 1.65  | 0.56  |
| Caryophyllene    | G10                  | 1.02  | 2.33  | 3.82  | 2.76  | 2.40  | 12.50 |
| Benzene, 1,2-(methylenedioxy)-4-propenyl-, (E)- | G11                 | -     | 0.79  | -     | 0.10  | 1.22  | -     |
| Benzene, 1-methyl-2-(1-methylbutyl)- | H1                  | 0.31  | 2.45  | 0.53  | 0.25  | 2.09  | 1.05  |
| 2-Methylphenylacetylene | H2                  | 0.05  | -     | -     | 0.52  | -     | -     |
| Furan, 2-pentyl- | I1                   | 0.10  | 0.25  | 0.11  | 0.13  | 0.42  | 0.05  |
| Ethanone, 1-(2-furanyl)- | I2                  | 1.16  | 1.51  | 0.81  | 0.05  | 1.10  | 0.94  |
| Azulene          | I3                   | 0.25  | -     | -     | 0.91  | 0.07  | 0.82  |

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