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COMPONENTS

(57) Abrégé/Abstract:

The present invention discloses a method for characterizing taste characteristics of a mixed component, including the following steps: use a molecular docking method to molecularly dock each monomer in the mixed component with T1R2-T1R3, and extract docking result parameters; according to the taste discrimination model containing parameters of docking results, calculate the taste probability and value of each monomer component of bitterness, sweetness and sour; then use the comprehensive weighting method to calculate overall taste probability of bitterness, sweetness and sour of the mixed component, so as to obtain taste characteristics of the mixed component. The characterization method of the present invention does not need to acquire taste micro-molecule substances. It has the advantages of fast calculation, the results obtained are intuitive and with accurate prediction.

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### **Abstract**

The present invention discloses a method for characterizing taste characteristics of a mixed component, including the following steps: use a molecular docking method to molecularly dock each monomer in the mixed component with T1R2-T1R3, and extract docking result parameters; according to the taste discrimination model containing parameters of docking results, calculate the taste probability and value of each monomer component of bitterness, sweetness and sour; then use the comprehensive weighting method to calculate overall taste probability of bitterness, sweetness and sour of the mixed component, so as to obtain taste characteristics of the mixed component. The characterization method of the present invention does not need to acquire taste micro-molecule substances. It has the advantages of fast calculation, the results obtained are intuitive and with accurate prediction.

# **A CHARACTERIZATION METHOD AND APPLICATION OF TASTE CHARACTERISTICS OF MIXED COMPONENTS**

## **TECHNICAL FIELD**

The present invention belongs to the technical field of food, and in particular, to a method for characterizing taste characteristics of the mixed component and an application of using the method for characterizing taste characteristics of cigarette smoke.

## **BACKGROUND**

Physiologically speaking, the reason why humans can perceive taste substances such as sour, sweetness and bitterness is that taste micro-molecules specifically bind to the corresponding active regions of taste proteins in the human body, thereby inducing downstream signals to produce corresponding taste sensations. Molecular docking is to study whether two molecules can bind, predict their binding mode, and search for the lowest free energy conformation for stable binding between ligands and receptor active regions on the basis of the three-dimensional structures of two molecules (usually including a micro-molecule ligand and a macro-molecule protein receptor). Based on the previous research, the inventor uses different docking modes of taste molecules in the T1R2-T1R3 protein, and adopts the molecular docking method to construct docking modes of taste micro-molecules including sour, sweetness and bitterness with T1R2-T1R3 protein, extract key parameters of molecular docking results, and the taste discrimination model of sour, sweetness and bitterness taste molecules of a single compound is established according to the key parameters of molecular docking results. See Patent CN112102886A of the applicant.

Taste compounds are compounds with a certain taste, such as sweetness, sour, and bitterness. In real life, it is often comprehensive taste perception with compounds mixed together, the comprehensive taste perception is closely related to taste characteristics of its constituents, rather than a simple superposition of taste characteristics of these taste compounds.

There are few studies at present regarding taste characteristics of the mixed component, some of which use representative compounds to predict sweetness of mixed components. However, the pleiotropic taste of monomer compounds and complexity of the composition and content of the mixed component and even their interaction may result in the diversity of taste of the mixed component, it is difficult to use individual compounds to characterize taste characteristics of the mixed component. Thus, new parameters must be introduced to characterize and determine taste characteristics of the mixed component. On the basis of Patent CN112102886A, the present invention introduces new parameters to characterize taste characteristics of the mixed component,

which are used to characterize the overall taste characteristics of cigarette smoke.

## SUMMARY

The purpose of the present invention is to provide a method for characterizing taste characteristics of the mixed component and an application of using the method for characterizing taste characteristics of cigarette smoke, through adopting batch processing by computers without the need of subjective intervention, the method is fast and easy to popularize.

The purpose of the present invention is achieved through the following technical solutions.

Unless otherwise specified, the percentages used in the present invention are by weight.

A first aspect of the present invention discloses a method for characterizing taste characteristics of the mixed component, including the following steps: use a molecular docking method to dock each monomer in the mixed component with T1R2-T1R3, and extract docking result parameters; according to the taste discrimination model containing parameters of docking results, calculate the taste probability and value of each monomer component of bitterness, sweetness and sour; then use the comprehensive weighting method to calculate the overall taste probability of bitterness, sweetness and sour of the mixed component, so as to obtain taste characteristics of the mixed component.

Preferably, the specific steps are as follows:

①Molecular docking of monomer components: conduct molecular docking of each monomer component in the mixed component with T1R2-T1R3, and extract the parameters of docking results;

②Calculate taste probabilities of monomer components: based on the taste discrimination model containing parameters of docking results, calculate the taste probability of bitterness, sweetness and sour of each monomer component;

③Calculate taste values of monomer components: according to the content of each monomer component in the mixed component, calculate the value of bitterness, sweetness and sour of each monomer component;

④Calculate taste characteristics of the mixed component: use the comprehensive weighting method to calculate the overall taste probability of the mixed component of bitterness, sweetness and sour, so as to obtain taste characteristics of the mixed component.

Preferably, the parameters of the docking results extracted in step① are as follows:

BE is Binding Energy, equaling to the sum of intermolecular energy and torsional free energy; KI is inhibition constant; ImE is Intermolecular Energy, referring to energy among molecules; IE is Internal Energy, referring to energy inside molecules; TE is Torsional Energy; UEE is Unbound System's Energy; RR is Reference RMSD, referring to the mean square deviation of the current structure relative to the reference conformation.

Parameters and explanations of docking results are as follows:

| Name                    | Abbreviation | Explanation                                                                           |
|-------------------------|--------------|---------------------------------------------------------------------------------------|
| Binding Energy          | BE           | The sum of intermolecular energy and torsional free energy                            |
| KI                      | KI           | Inhibition constant                                                                   |
| Intermolecular Energy   | ImE          | Energy among molecules                                                                |
| Internal Energy         | IE           | Energy inside molecules                                                               |
| Torsional Energy        | TE           | Torsional Energy                                                                      |
| Unbound System's Energy | UEE          | Unbound System's Energy                                                               |
| Reference RMSD          | RR           | Mean square deviation of the current structure relative to the reference conformation |

Preferably, calculate the taste probability of bitterness, sweetness and sour of each monomer component in step② by using the following formula:

$$\hat{P}(k|x) = \frac{P(x|k)P(k)}{P(x)},$$

Among which,  $P(x|k)$  is the multivariate normal density equation, the formula is as follows:

$$P(x|k) = \frac{1}{((2\pi)^m |\Sigma_k|)^{1/2}} \exp\left(-\frac{1}{2}(x - \mu_k)\Sigma_k^{-1}(x - \mu_k)^T\right),$$

$x$  is the parameter value of the docking result of a certain monomer component,  $k$  is the taste group, including bitterness, sweetness and sour;  $m$  is the number of docking result parameters, where  $m=7$ ;

$\Sigma_k$  is the covariance of the  $k$ -th group,  $\mu_k$  is the mean of the  $k$ -th group,  $|\Sigma_k|$  is the determinant value of  $\Sigma_k$ ,  $\Sigma_k^{-1}$  is the inverse matrix of  $\Sigma_k$ ;  $(x - \mu_k)^T$  is the transposed matrix; the values of covariance  $\Sigma$  and mean  $\mu$  of different groups of bitterness, sweetness and sour are as follows:

| Group k    | Parameter | Value |       |          |        |       |        |       |        |
|------------|-----------|-------|-------|----------|--------|-------|--------|-------|--------|
|            |           |       | BE    | KI       | ImE    | IE    | TE     | UEE   | RR     |
| Bitterness | $\Sigma$  | BE    | 1.74  | 64.17    | 1.04   | -0.64 | 0.7    | -0.64 | 4.14   |
|            |           | KI    | 64.17 | 48065.02 | 133.22 | 4.53  | -69.17 | 4.53  | 806.36 |
|            |           | ImE   | 1.04  | 133.22   | 2.41   | 0.64  | -1.37  | 0.64  | 7.06   |
|            |           | IE    | -0.64 | 4.53     | 0.64   | 0.97  | -1.28  | 0.97  | 1.11   |
|            |           | TE    | 0.7   | -69.17   | -1.37  | -1.28 | 2.08   | -1.28 | -2.92  |

|           |          |     |         |         |         |       |        |       |         |
|-----------|----------|-----|---------|---------|---------|-------|--------|-------|---------|
| Sweetness | $\mu$    | UEE | -0.64   | 4.53    | 0.64    | 0.97  | -1.28  | 0.97  | 1.11    |
|           |          | RR  | 4.14    | 806.36  | 7.06    | 1.11  | -2.92  | 1.11  | 48.32   |
|           | $\mu$    |     | -6.4    | 113.14  | -7.93   | -1.07 | 1.54   | -1.07 | 91.47   |
|           | $\Sigma$ | BE  | 1.36    | -105.06 | 1.06    | -1.06 | 0.3    | -1.06 | -1.23   |
|           |          | KI  | -105.06 | 35402.7 | -173.76 | 63.16 | 68.57  | 63.16 | 76.49   |
|           |          | ImE | 1.06    | -173.76 | 3.29    | -0.04 | -2.22  | -0.04 | 1.35    |
|           |          | IE  | -1.06   | 63.16   | -0.04   | 1.66  | -1.01  | 1.66  | -1.06   |
|           |          | TE  | 0.3     | 68.57   | -2.22   | -1.01 | 2.52   | -1.01 | -2.57   |
|           |          | UEE | -1.06   | 63.16   | -0.04   | 1.66  | -1.01  | 1.66  | -1.06   |
|           |          | RR  | -1.23   | 76.49   | 1.35    | -1.06 | -2.57  | -1.06 | 231.07  |
|           | $\mu$    |     | -3.04   | 119.05  | -6.43   | -3.42 | 3.39   | -3.42 | 89.44   |
| Sour      | $\Sigma$ | BE  | 0.23    | -39.3   | 0.86    | 0.04  | -0.63  | 0.04  | 1.14    |
|           |          | KI  | -39.3   | 36008.6 | -169.87 | -9.21 | 130.57 | -9.21 | -210.71 |
|           |          | ImE | 0.86    | -169.87 | 4.19    | 0.2   | -3.33  | 0.2   | 5.82    |
|           |          | IE  | 0.04    | -9.21   | 0.2     | 0.01  | -0.16  | 0.01  | 0.31    |
|           |          | TE  | -0.63   | 130.57  | -3.33   | -0.16 | 2.7    | -0.16 | -4.68   |
|           |          | UEE | 0.04    | -9.21   | 0.2     | 0.01  | -0.16  | 0.01  | 0.31    |
|           |          | RR  | 1.14    | -210.71 | 5.82    | 0.31  | -4.68  | 0.31  | 15.42   |
|           | $\mu$    |     | -3.23   | 47.4    | -5.2    | -0.11 | 1.97   | -0.11 | 93.55   |

$P(k)$  is the prior probability of taste  $k$  with the following values:  $P(k = \text{bitterness}) = 38.46\%$ ,  $P(k = \text{sweetness}) = 32.31\%$ ,  $P(k = \text{sour}) = 29.23\%$ ,

$P(x)$  is a normal constant, the formula is as follows:  $P(x) = \sum P(x|k)P(k)$ .

Preferably, calculation of the taste value of bitterness, sweetness and sour of each monomer component in step③ is as follows:

The taste value of a certain monomer in the mixed component = the content of a monomer in the mixed component  $\times$  the taste probability of a monomer in the mixed component.

Preferably, calculation of taste characteristics of the mixed component in step④ is as follows:

The overall taste probability of bitterness, sweetness and sour of the mixed component = sum of taste values of the mixed component/sum of the content of the mixed component.

A second aspect of the present invention discloses an application of using the method for characterizing taste characteristics of cigarette smoke.

Beneficial effects of the present invention:

The present invention discloses for the first time the method for characterizing taste characteristics of the mixed component. The characterization method of the present invention can directly observe docking of each taste micro-molecule in the mixed component with the sweet protein T1R2-T1R3 by means of external tools, and explore the taste mechanism. The characterization method of the present invention neither does need to obtain each taste micro-

molecule substance in the mixed component, nor to conduct a long period of experiments or artificial sensory evaluation, the calculation is conducted by computers with fast computing and accurate prediction results.

## **DETAILED DESCRIPTION OF THE EMBODIMENTS**

In order to make the purpose, technical solutions and advantages of the present invention clearer, the present invention will be further illustrated below with reference to specific embodiment. It should be understood that the specific embodiment described herein is only used to explain the present invention, but not to limit the present invention. In case no specific technique or condition is indicated in the embodiment, the technique or condition described in the literature in the art or the product specification is used. The reagents or instruments used without the manufacturer's indication are conventional products that can be obtained through purchase.

The present invention describes a method for characterizing taste characteristics of the mixed component in cigarette smoke, including the following steps: use a molecular docking method to molecularly dock each monomer in mixed component of cigarette smoke with T1R2-T1R3, and extract docking result parameters; according to the taste discrimination model containing parameters of docking results, calculate the taste probability and value of each monomer component of bitterness, sweetness and sour; then use the comprehensive weighting method to calculate the overall taste probability of bitterness, sweetness and sour of the mixed component in cigarette smoke, so as to obtain taste characteristics of the mixed component in cigarette smoke.

The specific steps are as follows:

①Molecular docking of monomer components: conduct molecular docking of each monomer component in the mixed component with T1R2-T1R3, and extract the parameters of docking results;

②Calculate taste probabilities of monomer components: based on the taste discrimination model containing parameters of docking results, calculate the taste probability of bitterness, sweetness and sour of each monomer component;

③Calculate taste values of monomer components: according to the content of each monomer component in the mixed component, calculate the value of bitterness, sweetness and sour of each monomer component;

④Calculate taste characteristics of the mixed component: use the comprehensive weighting method to calculate the overall taste probability of the mixed component of bitterness, sweetness

and sour, so as to obtain taste characteristics of the mixed component.

The parameters of the docking results extracted in step① are as follows:

BE is Binding Energy, equaling to the sum of intermolecular energy and torsional free energy; KI is inhibition constant; ImE is Intermolecular Energy, referring to energy among molecules; IE is Internal Energy, referring to energy inside molecules; TE is Torsional Energy; UEE is Unbound System's Energy; RR is Reference RMSD, referring to the mean square deviation of the current structure relative to the reference conformation.

Parameters and explanations of docking results are as follows:

| Name                    | Abbreviation | Explanation                                                                           |
|-------------------------|--------------|---------------------------------------------------------------------------------------|
| Binding Energy          | BE           | The sum of intermolecular energy and torsional free energy                            |
| KI                      | KI           | Inhibition constant                                                                   |
| Intermolecular Energy   | ImE          | Energy among molecules                                                                |
| Internal Energy         | IE           | Energy inside molecules                                                               |
| Torsional Energy        | TE           | Torsional Energy                                                                      |
| Unbound System's Energy | UEE          | Unbound System's Energy                                                               |
| Reference RMSD          | RR           | Mean square deviation of the current structure relative to the reference conformation |

Calculate the taste probability of bitterness, sweetness and sour of each monomer component in step② by using the following formula:

$$\hat{P}(k|x) = \frac{P(x|k)P(k)}{P(x)},$$

Among which,  $P(x|k)$  is the multivariate normal density equation, the formula is as follows:

$$P(x|k) = \frac{1}{((2\pi)^m |\Sigma_k|)^{1/2}} \exp\left(-\frac{1}{2}(x - \mu_k)\Sigma_k^{-1}(x - \mu_k)^T\right),$$

$x$  is the parameter value of the docking result of a certain monomer component,  $k$  is the taste group, including bitterness, sweetness and sour;  $m$  is the number of docking result parameters, where  $m=7$ ;

$\Sigma_k$  is the covariance of the  $k$ -th group,  $\mu_k$  is the mean of the  $k$ -th group,  $|\Sigma_k|$  is the determinant value of  $\Sigma_k$ ,  $\Sigma_k^{-1}$  is the inverse matrix of  $\Sigma_k$ ;  $(x - \mu_k)^T$  is the transposed matrix; the values of covariance  $\Sigma$  and mean  $\mu$  of different groups of bitterness, sweetness and sour are as follows:

| Group k | Parameter | Value |    |    |     |    |    |     |    |
|---------|-----------|-------|----|----|-----|----|----|-----|----|
|         |           |       | BE | KI | ImE | IE | TE | UEE | RR |

|            |          |     |         |          |         |       |        |       |         |
|------------|----------|-----|---------|----------|---------|-------|--------|-------|---------|
| Bitterness | $\Sigma$ | BE  | 1.74    | 64.17    | 1.04    | -0.64 | 0.7    | -0.64 | 4.14    |
|            |          | KI  | 64.17   | 48065.02 | 133.22  | 4.53  | -69.17 | 4.53  | 806.36  |
|            |          | ImE | 1.04    | 133.22   | 2.41    | 0.64  | -1.37  | 0.64  | 7.06    |
|            |          | IE  | -0.64   | 4.53     | 0.64    | 0.97  | -1.28  | 0.97  | 1.11    |
|            |          | TE  | 0.7     | -69.17   | -1.37   | -1.28 | 2.08   | -1.28 | -2.92   |
|            |          | UEE | -0.64   | 4.53     | 0.64    | 0.97  | -1.28  | 0.97  | 1.11    |
|            |          | RR  | 4.14    | 806.36   | 7.06    | 1.11  | -2.92  | 1.11  | 48.32   |
|            | $\mu$    |     | -6.4    | 113.14   | -7.93   | -1.07 | 1.54   | -1.07 | 91.47   |
| Sweetness  | $\Sigma$ | BE  | 1.36    | -105.06  | 1.06    | -1.06 | 0.3    | -1.06 | -1.23   |
|            |          | KI  | -105.06 | 35402.7  | -173.76 | 63.16 | 68.57  | 63.16 | 76.49   |
|            |          | ImE | 1.06    | -173.76  | 3.29    | -0.04 | -2.22  | -0.04 | 1.35    |
|            |          | IE  | -1.06   | 63.16    | -0.04   | 1.66  | -1.01  | 1.66  | -1.06   |
|            |          | TE  | 0.3     | 68.57    | -2.22   | -1.01 | 2.52   | -1.01 | -2.57   |
|            |          | UEE | -1.06   | 63.16    | -0.04   | 1.66  | -1.01  | 1.66  | -1.06   |
|            |          | RR  | -1.23   | 76.49    | 1.35    | -1.06 | -2.57  | -1.06 | 231.07  |
|            | $\mu$    |     | -3.04   | 119.05   | -6.43   | -3.42 | 3.39   | -3.42 | 89.44   |
| Sour       | $\Sigma$ | BE  | 0.23    | -39.3    | 0.86    | 0.04  | -0.63  | 0.04  | 1.14    |
|            |          | KI  | -39.3   | 36008.6  | -169.87 | -9.21 | 130.57 | -9.21 | -210.71 |
|            |          | ImE | 0.86    | -169.87  | 4.19    | 0.2   | -3.33  | 0.2   | 5.82    |
|            |          | IE  | 0.04    | -9.21    | 0.2     | 0.01  | -0.16  | 0.01  | 0.31    |
|            |          | TE  | -0.63   | 130.57   | -3.33   | -0.16 | 2.7    | -0.16 | -4.68   |
|            |          | UEE | 0.04    | -9.21    | 0.2     | 0.01  | -0.16  | 0.01  | 0.31    |
|            |          | RR  | 1.14    | -210.71  | 5.82    | 0.31  | -4.68  | 0.31  | 15.42   |
|            | $\mu$    |     | -3.23   | 47.4     | -5.2    | -0.11 | 1.97   | -0.11 | 93.55   |

$P(k)$  is the prior probability of taste  $k$  with the following values:  $P(k = \text{bitterness}) = 38.46\%$ ,  $P(k = \text{sweetness}) = 32.31\%$ ,  $P(k = \text{sour}) = 29.23\%$ ,

$P(x)$  is a normal constant, the formula is as follows:  $P(x) = \sum P(x|k)P(k)$ .

Calculation of the taste value of bitterness, sweetness and sour of each monomer component in step③ is as follows: the taste value of a certain monomer in the mixed component = the content of a monomer in the mixed component  $\times$  the taste probability of a monomer in the mixed component.

Calculation of taste characteristics of the mixed component in step④ is as follows: the overall probability of bitterness, sweetness and sour of the mixed component = sum of taste values of the mixed component/sum of the content of the mixed component.

### Embodiment

In the embodiment, cigarette smoke of a certain brand A is used as the mixed component, and the cigarette smoke is a mixture of 92 main components through analysis (other minor components are ignored). The 92 components and their contents of cigarette smoke are shown in Table 1 and Table 2.

The method for characterizing taste characteristics of the mixed component of cigarette smoke includes the following steps:

Step 1, Molecular docking of each monomer component in cigarette smoke.

Use AutoDock software, each component in cigarette smoke is docked with the T1R2-T1R3 protein, so as to obtain parameter values of the docking results as shown in Table 1.

Step 2, Determine the taste probability of each component in cigarette smoke.

Substitute the molecular docking result parameter of each component in cigarette smoke into

the formula of the taste discrimination model  $\hat{P}(k|x) = \frac{P(x|k)P(k)}{P(x)}$ , calculate the taste probability of bitterness, sweetness and sour of each component in cigarette smoke, as shown in Table 2.

Step 3, calculate the taste value of each component in cigarette smoke according to the following formula, and the results are shown in Table 2.

Taste value of a certain monomer in mixed component of cigarette smoke = the content of the monomer in the mixed component of cigarette smoke  $\times$  the taste probability of the monomer in the mixed component of cigarette smoke.

Step 4, determine taste characteristics of the mixed component in cigarette smoke, and calculate according to the following formula, the results are shown in Table 3.

The overall taste probability of bitterness, sweetness, and sour of the mixed component in cigarette smoke = sum of the taste value of the mixed component in cigarette smoke/sum of the content of the mixed component in cigarette smoke.

It can be seen from Table 3 that the overall taste of cigarette smoke of a certain brand A is mainly bitter, followed by sour, and sweetness is the lowest, which is consistent with actual sensory evaluation.

Table 1

| No. | Compound                          | BE    | KI     | ImE   | IE    | TE   | UEE   | RR     |
|-----|-----------------------------------|-------|--------|-------|-------|------|-------|--------|
| 1   | Phenol                            | -4.44 | 560.64 | -4.73 | 0.01  | 0.30 | 0.01  | 101.53 |
| 2   | 2-Ethylphenol                     | -5.05 | 198.90 | -5.65 | -0.06 | 0.60 | -0.06 | 90.52  |
| 3   | 3-Ethylphenol                     | -4.82 | 293.96 | -5.41 | -0.06 | 0.60 | -0.06 | 90.15  |
| 4   | 4-Ethylphenol                     | -4.98 | 224.45 | -5.57 | -0.05 | 0.60 | -0.05 | 90.05  |
| 5   | 2,5-Dimethylphenol                | -5.11 | 179.53 | -5.41 | 0.04  | 0.30 | 0.04  | 91.18  |
| 6   | 2,6-Dimethylphenol                | -5.04 | 202.75 | -5.34 | 0.04  | 0.30 | 0.04  | 90.95  |
| 7   | 2,6-Dimethoxyphenol               | -4.69 | 365.11 | -5.58 | -1.00 | 0.89 | -1.00 | 110.56 |
| 8   | Quinol                            | -4.22 | 805.29 | -4.82 | 0.03  | 0.60 | 0.03  | 89.82  |
| 9   | 2-Methylhydroquinone              | -4.47 | 531.36 | -5.06 | -0.04 | 0.60 | -0.04 | 90.80  |
| 10  | Guaiacol                          | -4.73 | 343.84 | -5.32 | -0.17 | 0.60 | -0.17 | 110.86 |
| 11  | 4-Vinylguaiacol                   | -5.78 | 57.61  | -6.68 | -0.20 | 0.89 | -0.20 | 90.42  |
| 12  | Eugenol                           | -5.31 | 128.33 | -6.50 | -0.32 | 1.19 | -0.32 | 111.06 |
| 13  | Isoeugenol                        | -5.53 | 87.83  | -6.43 | -0.97 | 0.89 | -0.97 | 89.21  |
| 14  | 3-Hydroxybenzaldehyde             | -4.94 | 239.65 | -5.54 | -0.01 | 0.60 | -0.01 | 90.11  |
| 15  | Vanillin                          | -4.90 | 257.49 | -5.79 | -0.71 | 0.89 | -0.71 | 89.21  |
| 16  | Pyridine                          | -3.75 | 1.77   | -3.75 | 0.00  | 0.00 | 0.00  | 91.01  |
| 17  | 2-Picoline                        | -4.17 | 874.02 | -4.17 | 0.00  | 0.00 | 0.00  | 100.33 |
| 18  | 3-Picoline                        | -4.14 | 923.68 | -4.14 | 0.00  | 0.00 | 0.00  | 90.89  |
| 19  | 4-Picoline                        | -4.22 | 804.54 | -4.22 | 0.00  | 0.00 | 0.00  | 91.04  |
| 20  | 2-Ethylpyridine                   | -4.66 | 386.49 | -4.95 | -0.06 | 0.30 | -0.06 | 91.20  |
| 21  | 3-Ethylpyridine                   | -4.46 | 533.93 | -4.76 | -0.06 | 0.30 | -0.06 | 90.94  |
| 22  | 3-Vinylpyridine                   | -4.50 | 503.76 | -4.80 | -0.06 | 0.30 | -0.06 | 90.91  |
| 23  | 3-Acetoxy pyridine                | -4.37 | 626.84 | -4.97 | -0.17 | 0.60 | -0.17 | 110.31 |
| 24  | Pyridone                          | -4.01 | 1.14   | -4.01 | 0.00  | 0.00 | 0.00  | 102.36 |
| 25  | 6-Methyl-3-pyridinol              | -4.51 | 491.86 | -4.81 | -0.01 | 0.30 | -0.01 | 92.07  |
| 26  | Pyrazine                          | -3.52 | 2.65   | -3.52 | 0.00  | 0.00 | 0.00  | 91.81  |
| 27  | 2-Methylpyrazine                  | -4.26 | 750.35 | -4.26 | 0.00  | 0.00 | 0.00  | 91.78  |
| 28  | Pyrrole                           | -3.33 | 3.63   | -3.33 | 0.00  | 0.00 | 0.00  | 100.12 |
| 29  | 2-Pyrrolidone                     | -3.92 | 1.34   | -3.92 | 0.00  | 0.00 | 0.00  | 102.02 |
| 30  | Succinimide                       | -4.04 | 1.10   | -4.04 | 0.00  | 0.00 | 0.00  | 103.15 |
| 31  | Indole                            | -4.76 | 324.34 | -4.76 | 0.00  | 0.00 | 0.00  | 90.43  |
| 32  | 3-Methylindole                    | -5.16 | 165.47 | -5.16 | 0.00  | 0.00 | 0.00  | 90.01  |
| 33  | Nicotine                          | -5.96 | 42.84  | -6.26 | -0.15 | 0.30 | -0.15 | 90.66  |
| 34  | Myosmine                          | -5.43 | 105.53 | -5.72 | -0.19 | 0.30 | -0.19 | 89.98  |
| 35  | 2,3'-Bipyridine                   | -5.83 | 52.95  | -5.83 | 0.00  | 0.00 | 0.00  | 89.15  |
| 36  | Nicotaine                         | -5.60 | 79.07  | -5.89 | -0.19 | 0.30 | -0.19 | 89.83  |
| 37  | Quinoline                         | -5.74 | 61.83  | -5.74 | 0.00  | 0.00 | 0.00  | 90.49  |
| 38  | Acetamide                         | -3.53 | 2.58   | -3.53 | 0.00  | 0.00 | 0.00  | 111.91 |
| 39  | Isovaleramide                     | -3.83 | 1.56   | -4.43 | -0.07 | 0.60 | -0.07 | 90.27  |
| 40  | Acrylamide                        | -3.95 | 1.27   | -4.25 | 0.01  | 0.30 | 0.01  | 102.09 |
| 41  | Cyclopentanone                    | -4.69 | 362.02 | -4.69 | 0.00  | 0.00 | 0.00  | 102.54 |
| 42  | 2-Ethylcyclopentanone             | -4.64 | 398.49 | -4.94 | -0.07 | 0.30 | -0.07 | 89.75  |
| 43  | 2-Cyclopentene-1-one              | -3.95 | 1.27   | -3.95 | 0.00  | 0.00 | 0.00  | 102.86 |
| 44  | 2-Methyl-2-cyclopentene-1-one     | -4.49 | 511.25 | -4.49 | 0.00  | 0.00 | 0.00  | 91.02  |
| 45  | 3-Methyl-2-cyclopentene-1-one     | -4.32 | 678.86 | -4.32 | 0.00  | 0.00 | 0.00  | 90.75  |
| 46  | 2,3-Dimethyl-2-cyclopentene-1-one | -4.87 | 269.81 | -4.87 | 0.00  | 0.00 | 0.00  | 90.58  |
| 47  | 3-Ethyl-2-cyclopentene-1-one      | -4.41 | 586.51 | -4.71 | -0.05 | 0.30 | -0.05 | 90.25  |
| 48  | 1,2-Cyclopentanedione             | -5.00 | 216.24 | -5.00 | 0.00  | 0.00 | 0.00  | 90.76  |
| 49  | 4-Cyclopentene-1,3-dione          | -4.18 | 863.15 | -4.18 | 0.00  | 0.00 | 0.00  | 102.48 |
| 50  | Methylcyclopentenolone            | -4.43 | 568.55 | -4.73 | 0.03  | 0.30 | 0.03  | 90.58  |
| 51  | Ethylcyclopentenolone             | -4.66 | 381.02 | -5.26 | -0.77 | 0.60 | -0.77 | 90.83  |
| 52  | 2-Cyclohexene-1-one               | -4.80 | 301.47 | -4.80 | 0.00  | 0.00 | 0.00  | 90.49  |
| 53  | 1-Nonanone                        | -5.71 | 65.66  | -5.71 | 0.00  | 0.00 | 0.00  | 90.06  |
| 54  | Solanone                          | -5.59 | 79.28  | -7.38 | -0.68 | 1.79 | -0.68 | 87.82  |
| 55  | Megastigmatrienone b              | -5.98 | 41.34  | -6.88 | -0.35 | 0.89 | -0.35 | 89.15  |
| 56  | Propionic acid                    | -2.75 | 9.70   | -3.34 | 0.00  | 0.60 | 0.00  | 97.63  |

|    |                            |       |        |       |       |      |       |        |
|----|----------------------------|-------|--------|-------|-------|------|-------|--------|
| 57 | Butyric acid               | -2.77 | 9.38   | -3.36 | 0.02  | 0.60 | 0.02  | 97.62  |
| 58 | Valeric acid               | -2.95 | 6.88   | -3.85 | -0.07 | 0.89 | -0.07 | 97.17  |
| 59 | 3-Methylvaleric acid       | -3.06 | 5.69   | -4.26 | -0.07 | 1.19 | -0.07 | 91.84  |
| 60 | 2-Acrylic                  | -2.79 | 9.06   | -3.38 | 0.00  | 0.60 | 0.00  | 97.51  |
| 61 | Crotonic acid              | -2.98 | 6.51   | -3.58 | -0.03 | 0.60 | -0.03 | 97.42  |
| 62 | 2-Methylfuran              | -4.12 | 954.59 | -4.12 | 0.00  | 0.00 | 0.00  | 91.39  |
| 63 | Furfuryl alcohol           | -4.00 | 1.17   | -4.60 | -0.78 | 0.60 | -0.78 | 91.63  |
| 64 | Furfural                   | -4.48 | 517.70 | -4.78 | -0.07 | 0.30 | -0.07 | 102.75 |
| 65 | 3-Furfural                 | -4.46 | 534.37 | -4.76 | 0.00  | 0.30 | 0.00  | 102.62 |
| 66 | 5-Methylfurfural           | -4.78 | 312.02 | -5.08 | -0.07 | 0.30 | -0.07 | 102.66 |
| 67 | Methyl furoate             | -4.51 | 496.94 | -5.10 | -0.27 | 0.60 | -0.27 | 91.76  |
| 68 | 2-Acetylfuran              | -4.41 | 589.47 | -4.70 | -0.11 | 0.30 | -0.11 | 90.87  |
| 69 | 2(5H)-Furanone             | -3.86 | 1.48   | -3.86 | 0.00  | 0.00 | 0.00  | 91.19  |
| 70 | Pineapplefuranone          | -4.62 | 412.72 | -4.92 | -0.65 | 0.30 | -0.65 | 110.93 |
| 71 | Maltol                     | -4.63 | 400.85 | -4.93 | -0.71 | 0.30 | -0.71 | 90.57  |
| 72 | $\gamma$ -Butyrolactone    | -4.33 | 673.98 | -4.33 | 0.00  | 0.00 | 0.00  | 90.62  |
| 73 | $\alpha$ -Angelica lactone | -4.71 | 352.60 | -4.71 | 0.00  | 0.00 | 0.00  | 91.53  |
| 74 | Dihydroactinodiolide       | -5.54 | 87.24  | -5.54 | 0.00  | 0.00 | 0.00  | 91.46  |
| 75 | Limonene                   | -5.13 | 172.32 | -5.43 | -0.15 | 0.30 | -0.15 | 88.82  |
| 76 | Myrcene                    | -4.51 | 494.98 | -5.70 | -0.24 | 1.19 | -0.24 | 88.42  |
| 77 | $\beta$ -Ocimene           | -4.60 | 423.61 | -5.50 | -0.22 | 0.89 | -0.22 | 88.02  |
| 78 | Alloocimene                | -4.88 | 264.18 | -5.48 | -0.23 | 0.60 | -0.23 | 88.14  |
| 79 | Neophytadiene              | -5.42 | 105.84 | -9.30 | -0.77 | 3.88 | -0.77 | 87.06  |
| 80 | 1,2-Propanediol            | -2.77 | 9.28   | -3.67 | -1.37 | 0.89 | -1.37 | 86.55  |
| 81 | Glycerol                   | -2.57 | 12.99  | -4.06 | -3.39 | 1.49 | -3.39 | 89.78  |
| 82 | Methyl pyruvate            | -2.97 | 6.69   | -3.56 | -0.03 | 0.60 | -0.03 | 85.99  |
| 83 | Glycerol triacetate        | -4.38 | 618.92 | -6.76 | -0.74 | 2.39 | -0.74 | 88.17  |
| 84 | Benzyl alcohol             | -4.70 | 357.20 | -5.30 | -0.02 | 0.60 | -0.02 | 90.85  |
| 85 | Phenylethanol              | -4.37 | 625.69 | -5.27 | -0.09 | 0.89 | -0.09 | 90.55  |
| 86 | Phenylacetoneitrile        | -4.90 | 255.45 | -5.20 | -0.12 | 0.30 | -0.12 | 89.41  |
| 87 | Styrene                    | -4.63 | 401.01 | -4.93 | -0.07 | 0.30 | -0.07 | 102.34 |
| 88 | Ethylbenzene               | -4.49 | 510.04 | -4.79 | -0.06 | 0.30 | -0.06 | 90.93  |
| 89 | Xylene                     | -4.53 | 481.67 | -4.53 | 0.00  | 0.00 | 0.00  | 90.41  |
| 90 | 4-Methylbenzaldehyde       | -4.88 | 264.82 | -5.18 | -0.05 | 0.30 | -0.05 | 89.13  |
| 91 | Indene                     | -4.88 | 264.39 | -4.88 | 0.00  | 0.00 | 0.00  | 90.69  |
| 92 | Naphthalene                | -5.44 | 103.72 | -5.44 | 0.00  | 0.00 | 0.00  | 89.47  |

Table 2

| No. | Compound             | Relative content | Taste probability |           |        | Taste value |           |        |
|-----|----------------------|------------------|-------------------|-----------|--------|-------------|-----------|--------|
|     |                      |                  | Bitterness        | Sweetness | Sour   | Bitterness  | Sweetness | Sour   |
| 1   | Phenol               | 1.43454          | 0.5235            | 0.0286    | 0.4480 | 0.7509      | 0.0410    | 0.6427 |
| 2   | 2-Ethylphenol        | 0.10541          | 0.8037            | 0.0067    | 0.1896 | 0.0847      | 0.0007    | 0.0200 |
| 3   | 3-Ethylphenol        | 0.00002          | 0.8842            | 0.0157    | 0.1001 | 0.0000      | 0.0000    | 0.0000 |
| 4   | 4-Ethylphenol        | 0.00003          | 0.9160            | 0.0106    | 0.0734 | 0.0000      | 0.0000    | 0.0000 |
| 5   | 2,5-Dimethylphenol   | 0.08892          | 0.8254            | 0.0045    | 0.1701 | 0.0734      | 0.0004    | 0.0151 |
| 6   | 2,6-Dimethylphenol   | 0.03163          | 0.8029            | 0.0054    | 0.1917 | 0.0254      | 0.0002    | 0.0061 |
| 7   | 2,6-Dimethoxyphenol  | 0.02835          | 0.7652            | 0.0508    | 0.1840 | 0.0217      | 0.0014    | 0.0052 |
| 8   | Quinol               | 0.55554          | 0.5416            | 0.1171    | 0.3413 | 0.3009      | 0.0651    | 0.1896 |
| 9   | 2-Methylhydroquinone | 0.06914          | 0.7857            | 0.0614    | 0.1529 | 0.0543      | 0.0042    | 0.0106 |
| 10  | Guaiacol             | 0.15695          | 0.2798            | 0.0044    | 0.7159 | 0.0439      | 0.0007    | 0.1124 |
| 11  | 4-Vinylguaiacol      | 0.05031          | 0.9409            | 0.0013    | 0.0578 | 0.0473      | 0.0001    | 0.0029 |
| 12  | Eugenol              | 0.00446          | 0.2431            | 0.0009    | 0.7560 | 0.0011      | 0.0000    | 0.0034 |
| 13  | Isoeugenol           | 0.02448          | 0.9897            | 0.0076    | 0.0027 | 0.0242      | 0.0002    | 0.0001 |

|    |                                   |         |        |        |        |        |        |        |
|----|-----------------------------------|---------|--------|--------|--------|--------|--------|--------|
| 14 | 3-Hydroxybenzaldehyde             | 0.02355 | 0.7269 | 0.0077 | 0.2654 | 0.0171 | 0.0002 | 0.0063 |
| 15 | Vanillin                          | 0.01934 | 0.9434 | 0.0389 | 0.0177 | 0.0182 | 0.0008 | 0.0003 |
| 16 | Pyridine                          | 0.0632  | 0.0169 | 0.0018 | 0.9813 | 0.0011 | 0.0001 | 0.0620 |
| 17 | 2-Picoline                        | 0.03404 | 0.4773 | 0.0900 | 0.4327 | 0.0162 | 0.0031 | 0.0147 |
| 18 | 3-Picoline                        | 0.07477 | 0.7127 | 0.1618 | 0.1255 | 0.0533 | 0.0121 | 0.0094 |
| 19 | 4-Picoline                        | 0.00758 | 0.7293 | 0.1090 | 0.1617 | 0.0055 | 0.0008 | 0.0012 |
| 20 | 2-Ethylpyridine                   | 0.01274 | 0.8889 | 0.0251 | 0.0860 | 0.0113 | 0.0003 | 0.0011 |
| 21 | 3-Ethylpyridine                   | 0.05247 | 0.7064 | 0.0478 | 0.2458 | 0.0371 | 0.0025 | 0.0129 |
| 22 | 3-Vinylpyridine                   | 0.04925 | 0.7173 | 0.0411 | 0.2416 | 0.0353 | 0.0020 | 0.0119 |
| 23 | 3-Acetoxypyridine                 | 0.17998 | 0.0969 | 0.0066 | 0.8965 | 0.0174 | 0.0012 | 0.1614 |
| 24 | Pyridone                          | 1.0191  | 0.0073 | 0.0003 | 0.9924 | 0.0075 | 0.0003 | 1.0114 |
| 25 | 6-Methyl-3-pyridinol              | 0.05862 | 0.6324 | 0.0305 | 0.3370 | 0.0371 | 0.0018 | 0.0198 |
| 26 | Pyrazine                          | 0.00303 | 0.0058 | 0.0010 | 0.9932 | 0.0000 | 0.0000 | 0.0030 |
| 27 | 2-Methylpyrazine                  | 0.01874 | 0.7184 | 0.0863 | 0.1953 | 0.0135 | 0.0016 | 0.0037 |
| 28 | Pyrrole                           | 0.01967 | 0.0006 | 0.0001 | 0.9992 | 0.0000 | 0.0000 | 0.0197 |
| 29 | 2-Pyrrolidone                     | 0.2563  | 0.0054 | 0.0002 | 0.9944 | 0.0014 | 0.0001 | 0.2549 |
| 30 | Succinimide                       | 0.20971 | 0.0073 | 0.0002 | 0.9925 | 0.0015 | 0.0000 | 0.2081 |
| 31 | Indole                            | 0.08366 | 0.8347 | 0.0147 | 0.1506 | 0.0698 | 0.0012 | 0.0126 |
| 32 | 3-Methylindole                    | 0.08381 | 0.9339 | 0.0043 | 0.0618 | 0.0783 | 0.0004 | 0.0052 |
| 33 | Nicotine                          | 1.20738 | 0.9953 | 0.0007 | 0.0040 | 1.2017 | 0.0009 | 0.0048 |
| 34 | Myosmine                          | 0.0252  | 0.9908 | 0.0033 | 0.0059 | 0.0250 | 0.0001 | 0.0001 |
| 35 | 2,3'-Bipyridine                   | 0.14361 | 0.9934 | 0.0007 | 0.0059 | 0.1427 | 0.0001 | 0.0008 |
| 36 | Nicotaine                         | 0.05695 | 0.9947 | 0.0022 | 0.0032 | 0.0566 | 0.0001 | 0.0002 |
| 37 | Quinoline                         | 0.02214 | 0.9887 | 0.0010 | 0.0103 | 0.0219 | 0.0000 | 0.0002 |
| 38 | Acetamide                         | 0.01404 | 0.0002 | 0.0000 | 0.9998 | 0.0000 | 0.0000 | 0.0140 |
| 39 | Isovaleramide                     | 0.02953 | 0.0119 | 0.0012 | 0.9869 | 0.0004 | 0.0000 | 0.0291 |
| 40 | Acrylamide                        | 0.00761 | 0.0032 | 0.0001 | 0.9967 | 0.0000 | 0.0000 | 0.0076 |
| 41 | Cyclopentanone                    | 0.01154 | 0.3778 | 0.0057 | 0.6165 | 0.0044 | 0.0001 | 0.0071 |
| 42 | 2-Ethylcyclopentanone             | 0.00211 | 0.7861 | 0.0265 | 0.1874 | 0.0017 | 0.0001 | 0.0004 |
| 43 | 2-Cyclopentene-1-one              | 0.06385 | 0.0053 | 0.0002 | 0.9945 | 0.0003 | 0.0000 | 0.0635 |
| 44 | 2-Methyl-2-cyclopentene-1-one     | 0.05684 | 0.7602 | 0.0345 | 0.2054 | 0.0432 | 0.0020 | 0.0117 |
| 45 | 3-Methyl-2-cyclopentene-1-one     | 0.156   | 0.7415 | 0.0857 | 0.1728 | 0.1157 | 0.0134 | 0.0270 |
| 46 | 2,3-Dimethyl-2-cyclopentene-1-one | 0.19404 | 0.8580 | 0.0101 | 0.1319 | 0.1665 | 0.0020 | 0.0256 |
| 47 | 3-Ethyl-2-cyclopentene-1-one      | 0.05342 | 0.7135 | 0.0621 | 0.2244 | 0.0381 | 0.0033 | 0.0120 |
| 48 | 1,2-Cyclopentanedione             | 0.01755 | 0.8903 | 0.0067 | 0.1030 | 0.0156 | 0.0001 | 0.0018 |
| 49 | 4-Cyclopentene-1,3-dione          | 0.07647 | 0.4025 | 0.0671 | 0.5305 | 0.0308 | 0.0051 | 0.0406 |
| 50 | Methylecyclopentenolone           | 0.50358 | 0.6393 | 0.0442 | 0.3164 | 0.3220 | 0.0223 | 0.1594 |
| 51 | Ethylecyclopentenolone            | 0.1245  | 0.8995 | 0.0863 | 0.0142 | 0.1120 | 0.0107 | 0.0018 |
| 52 | 2-Cyclohexene-1-one               | 0.00879 | 0.8428 | 0.0127 | 0.1445 | 0.0074 | 0.0001 | 0.0013 |
| 53 | 1-Nonanone                        | 0.02447 | 0.9884 | 0.0009 | 0.0106 | 0.0242 | 0.0000 | 0.0003 |
| 54 | Solanone                          | 0.02797 | 0.9811 | 0.0066 | 0.0123 | 0.0274 | 0.0002 | 0.0003 |
| 55 | Megastigmatrienone b              | 0.04247 | 0.9880 | 0.0011 | 0.0109 | 0.0420 | 0.0000 | 0.0005 |
| 56 | Propionic acid                    | 0.06318 | 0.0001 | 0.0001 | 0.9998 | 0.0000 | 0.0000 | 0.0632 |
| 57 | Butyric acid                      | 0.02345 | 0.0001 | 0.0001 | 0.9998 | 0.0000 | 0.0000 | 0.0234 |
| 58 | Valeric acid                      | 0.00385 | 0.0000 | 0.0000 | 1.0000 | 0.0000 | 0.0000 | 0.0038 |
| 59 | 3-Methylvaleric acid              | 0.04118 | 0.0000 | 0.0000 | 0.9999 | 0.0000 | 0.0000 | 0.0412 |
| 60 | 2-Acrylic                         | 0.06393 | 0.0001 | 0.0001 | 0.9998 | 0.0000 | 0.0000 | 0.0639 |

|    |                            |         |        |        |        |        |        |        |
|----|----------------------------|---------|--------|--------|--------|--------|--------|--------|
| 61 | Crotonic acid              | 0.02175 | 0.0001 | 0.0001 | 0.9999 | 0.0000 | 0.0000 | 0.0217 |
| 62 | 2-Methylfuran              | 0.00113 | 0.6590 | 0.2299 | 0.1111 | 0.0007 | 0.0003 | 0.0001 |
| 63 | Furfuryl alcohol           | 0.07182 | 0.3694 | 0.0729 | 0.5577 | 0.0265 | 0.0052 | 0.0401 |
| 64 | Furfural                   | 0.13029 | 0.2865 | 0.0121 | 0.7015 | 0.0373 | 0.0016 | 0.0914 |
| 65 | 3-Furfural                 | 0.01266 | 0.2244 | 0.0093 | 0.7663 | 0.0028 | 0.0001 | 0.0097 |
| 66 | 5-Methylfurfural           | 0.35208 | 0.3578 | 0.0045 | 0.6377 | 0.1260 | 0.0016 | 0.2245 |
| 67 | Methyl furoate             | 0.04513 | 0.8592 | 0.0786 | 0.0622 | 0.0388 | 0.0035 | 0.0028 |
| 68 | 2-Acetylfuran              | 0.01918 | 0.8433 | 0.0924 | 0.0643 | 0.0162 | 0.0018 | 0.0012 |
| 69 | 2(5H)-Furanone             | 0.01717 | 0.0257 | 0.0021 | 0.9723 | 0.0004 | 0.0000 | 0.0167 |
| 70 | Pineapplefuranone          | 0.36779 | 0.6483 | 0.0290 | 0.3227 | 0.2384 | 0.0107 | 0.1187 |
| 71 | Maltol                     | 0.24389 | 0.9044 | 0.0850 | 0.0106 | 0.2206 | 0.0207 | 0.0026 |
| 72 | $\gamma$ -Butyrolactone    | 0.0064  | 0.7487 | 0.0839 | 0.1675 | 0.0048 | 0.0005 | 0.0011 |
| 73 | $\alpha$ -Angelica lactone | 0.00887 | 0.7964 | 0.0162 | 0.1873 | 0.0071 | 0.0001 | 0.0017 |
| 74 | Dihydroactinodiolide       | 0.00559 | 0.9739 | 0.0016 | 0.0245 | 0.0054 | 0.0000 | 0.0001 |
| 75 | Limonene                   | 0.13115 | 0.9447 | 0.0070 | 0.0482 | 0.1239 | 0.0009 | 0.0063 |
| 76 | Myrcene                    | 0.01594 | 0.6244 | 0.0581 | 0.3175 | 0.0100 | 0.0009 | 0.0051 |
| 77 | $\beta$ -Ocimene           | 0.03435 | 0.5030 | 0.0256 | 0.4715 | 0.0173 | 0.0009 | 0.0162 |
| 78 | Alloocimene                | 0.04683 | 0.8928 | 0.0177 | 0.0895 | 0.0418 | 0.0008 | 0.0042 |
| 79 | Neophytadiene              | 0.03167 | 0.5711 | 0.0110 | 0.4180 | 0.0181 | 0.0003 | 0.0132 |
| 80 | 1,2-Propanediol            | 0.05734 | 0.0228 | 0.2568 | 0.7204 | 0.0013 | 0.0147 | 0.0413 |
| 81 | Glycerol                   | 0.68101 | 0.0019 | 0.9981 | 0.0000 | 0.0013 | 0.6797 | 0.0000 |
| 82 | Methyl pyruvate            | 0.00855 | 0.0020 | 0.0021 | 0.9959 | 0.0000 | 0.0000 | 0.0085 |
| 83 | Glycerol triacetate        | 0.70826 | 0.5994 | 0.3279 | 0.0727 | 0.4245 | 0.2322 | 0.0515 |
| 84 | Benzyl alcohol             | 0.03451 | 0.6018 | 0.0145 | 0.3837 | 0.0208 | 0.0005 | 0.0132 |
| 85 | Phenylethanol              | 0.04617 | 0.2485 | 0.0257 | 0.7258 | 0.0115 | 0.0012 | 0.0335 |
| 86 | Phenylacetone nitrile      | 0.05545 | 0.8858 | 0.0125 | 0.1017 | 0.0491 | 0.0007 | 0.0056 |
| 87 | Styrene                    | 0.05476 | 0.3211 | 0.0072 | 0.6716 | 0.0176 | 0.0004 | 0.0368 |
| 88 | Ethylbenzene               | 0.01065 | 0.7134 | 0.0425 | 0.2441 | 0.0076 | 0.0005 | 0.0026 |
| 89 | Xylene                     | 0.04513 | 0.7865 | 0.0349 | 0.1786 | 0.0355 | 0.0016 | 0.0081 |
| 90 | 4-Methylbenzaldehyde       | 0.1644  | 0.8510 | 0.0116 | 0.1374 | 0.1399 | 0.0019 | 0.0226 |
| 91 | Indene                     | 0.11001 | 0.8604 | 0.0097 | 0.1298 | 0.0947 | 0.0011 | 0.0143 |
| 92 | Naphthalene                | 0.24132 | 0.9736 | 0.0020 | 0.0244 | 0.2349 | 0.0005 | 0.0059 |

Table 3

| Relative content of mixed component in cigarette smoke | Sum of taste values |           |        | Taste probability |           |        |
|--------------------------------------------------------|---------------------|-----------|--------|-------------------|-----------|--------|
|                                                        | Bitterness          | Sweetness | Sour   | Bitterness        | Sweetness | Sour   |
| 11.6662                                                | 6.2239              | 1.1881    | 4.2543 | 0.5335            | 0.1018    | 0.3647 |

The above preferred embodiment is only used to illustrate technical solutions of the present invention, rather than to limit the present invention. Although the present invention has been described in detail through the above preferred embodiment, those skilled in the art should understand that various changes in form and details can be made without departing from the scope of the present invention.

## Claims

1. A method for characterizing taste characteristics of a mixed component, the method comprising:

using a molecular docking method to dock each monomer in the mixed component with a sweet protein T1R2-T1R3, and extract docking result parameters of the each monomer;

creating a taste discrimination model containing the docking result parameters, calculating taste probability and value of bitterness, sweetness and sourness of the each monomer using the taste discrimination model; and

using a comprehensive weighting method to calculate an overall taste probability of bitterness, sweetness and sourness of the mixed component, so as to obtain the taste characteristics of the mixed component.

2. The method according to claim 1, wherein the docking result parameters comprise: Binding Energy (BE), equal to a sum of intermolecular energy and torsional free energy;

inhibition constant (KI);

Intermolecular Energy (ImE);

Intramolecular Internal Energy (IE);

Torsional Energy (TE);

Unbound System's Energy (UEE);

Reference RMSD (RR), referring to a mean square deviation of a current structure relative to a reference conformation.

3. The method according to claim 2, wherein, the taste probability of bitterness, sweetness and sourness of the each monomer is obtained using the following formula:

$$\hat{P}(k|x) = \frac{P(x|k)P(k)}{P(x)},$$

wherein  $P(x|k)$  is a multivariate normal density equation having a formula as follows:

$$P(x|k) = \frac{1}{((2\pi)^m |\Sigma_k|)^{1/2}} \exp\left(-\frac{1}{2}(x - \mu_k)\Sigma_k^{-1}(x - \mu_k)^T\right)$$

$x$  is a parameter value of a docking result of the monomer,  $k$  is a taste group, including bitterness, sweetness and sourness;  $m$  is a number of the docking result parameters, and  $m=7$ ;

$\Sigma_k$  is a covariance of the  $k$ -th taste group,  $\mu_k$  is a mean of the  $k$ -th taste group,  $|\Sigma_k|$  is a determinant value of  $\Sigma_k$ ,  $\Sigma_k^{-1}$  is an inverse matrix of  $\Sigma_k$ ;  $(x - \mu_k)^T$  is a transposed matrix; and values of covariance  $\Sigma$  and mean  $\mu$  of different taste groups of bitterness, sweetness and sour are as follows:

| Group k    | Parameter | Value |         |          |         |       |        |       |         |
|------------|-----------|-------|---------|----------|---------|-------|--------|-------|---------|
|            |           |       | BE      | KI       | ImE     | IE    | TE     | UEE   | RR      |
| Bitterness | $\Sigma$  | BE    | 1.74    | 64.17    | 1.04    | -0.64 | 0.7    | -0.64 | 4.14    |
|            |           | KI    | 64.17   | 48065.02 | 133.22  | 4.53  | -69.17 | 4.53  | 806.36  |
|            |           | ImE   | 1.04    | 133.22   | 2.41    | 0.64  | -1.37  | 0.64  | 7.06    |
|            |           | IE    | -0.64   | 4.53     | 0.64    | 0.97  | -1.28  | 0.97  | 1.11    |
|            |           | TE    | 0.7     | -69.17   | -1.37   | -1.28 | 2.08   | -1.28 | -2.92   |
|            |           | UEE   | -0.64   | 4.53     | 0.64    | 0.97  | -1.28  | 0.97  | 1.11    |
|            |           | RR    | 4.14    | 806.36   | 7.06    | 1.11  | -2.92  | 1.11  | 48.32   |
|            | $\mu$     |       | -6.4    | 113.14   | -7.93   | -1.07 | 1.54   | -1.07 | 91.47   |
| Sweetness  | $\Sigma$  | BE    | 1.36    | -105.06  | 1.06    | -1.06 | 0.3    | -1.06 | -1.23   |
|            |           | KI    | -105.06 | 35402.7  | -173.76 | 63.16 | 68.57  | 63.16 | 76.49   |
|            |           | ImE   | 1.06    | -173.76  | 3.29    | -0.04 | -2.22  | -0.04 | 1.35    |
|            |           | IE    | -1.06   | 63.16    | -0.04   | 1.66  | -1.01  | 1.66  | -1.06   |
|            |           | TE    | 0.3     | 68.57    | -2.22   | -1.01 | 2.52   | -1.01 | -2.57   |
|            |           | UEE   | -1.06   | 63.16    | -0.04   | 1.66  | -1.01  | 1.66  | -1.06   |
|            |           | RR    | -1.23   | 76.49    | 1.35    | -1.06 | -2.57  | -1.06 | 231.07  |
|            | $\mu$     |       | -3.04   | 119.05   | -6.43   | -3.42 | 3.39   | -3.42 | 89.44   |
| Sour       | $\Sigma$  | BE    | 0.23    | -39.3    | 0.86    | 0.04  | -0.63  | 0.04  | 1.14    |
|            |           | KI    | -39.3   | 36008.6  | -169.87 | -9.21 | 130.57 | -9.21 | -210.71 |
|            |           | ImE   | 0.86    | -169.87  | 4.19    | 0.2   | -3.33  | 0.2   | 5.82    |
|            |           | IE    | 0.04    | -9.21    | 0.2     | 0.01  | -0.16  | 0.01  | 0.31    |

|       |     |       |         |       |       |       |       |       |
|-------|-----|-------|---------|-------|-------|-------|-------|-------|
|       | TE  | -0.63 | 130.57  | -3.33 | -0.16 | 2.7   | -0.16 | -4.68 |
|       | UEE | 0.04  | -9.21   | 0.2   | 0.01  | -0.16 | 0.01  | 0.31  |
|       | RR  | 1.14  | -210.71 | 5.82  | 0.31  | -4.68 | 0.31  | 15.42 |
| $\mu$ |     | -3.23 | 47.4    | -5.2  | -0.11 | 1.97  | -0.11 | 93.55 |

$P(k)$  is a prior probability of the  $k$ th taste group with the following values:  $P(k = \text{bitterness}) = 38.46\%$ ,  $P(k = \text{sweetness}) = 32.31\%$ ,  $P(k = \text{sour}) = 29.23\%$ ,

$P(x)$  is a normal constant and is defined by a formula as follows:  $P(x) = \sum P(x|k)P(k)$ .

4. The method according to claim 3, wherein the taste value of bitterness, sweetness and sourness of the each monomer component is obtained in accordance with the following formula:

taste value of the monomer = content of the monomer in the mixed component  $\times$  the taste probability of bitterness, sweetness and sourness of the monomer in the mixed component;

wherein the taste probability of bitterness, sweetness and sourness of the monomer is obtained in accordance with the method of claim 3.

5. The method according to claim 4, wherein the taste characteristics of the mixed component is obtained in accordance with the following formula:

the overall taste characteristics of the mixed component = a sum of the taste value of the mixed component / a sum of content of the mixed component;

wherein the sum of the taste value of the mixed component is obtained by summing the taste value of the each monomer obtained in accordance with the method of claim 4; and

wherein the sum of content of the mixed component is obtained by summing the content of the each monomer in the mixed component.

6. A process using the method of any one of claims 1-5 for characterizing taste characteristics of a cigarette smoke.