# The Effects of Different Extraction Methods on The Aroma Fingerprint, Recombination And Visualization of Clam Soup

## Sensory assessment

The 32 sensory evaluation panelists were selected from 80 members of the laboratory (students and teachers) via sensitivity test of odor and taste (zhao, Deng, & Liu, 2015), include basic flavor test, olfactory match test, three-point test, and ranking order test. Sensory evaluation was performed with clam soup and odorants solution. The odor and taste were evaluated by Quantitative Descriptive Analysis (QDA) method (Silva, Estévez, Ferreira, Silva, Lemos, Ida, et al., 2018). The development of descriptive terminology, final selection of judges and final evaluation of the samples were done before evaluation. At the end, 13 assessors (age ranging from 23 to 35) from both genders were selected. The amplitude of attributes was rated in four kinds of non-structured linear scales according to different factors contributed to the final production, with terms of descriptor anchored at the extremes. Evaluations took place in individual booths under white fluorescence light. The samples were labeled with three-digit random numbers, presented in a monadic sequential way in a balanced complete block design. Two samples were presented to the panelists in each session, with the serving order of the samples randomized according to the Latin Square design.

Table S1 Questionnaire

| Name： | Sex：male and female | Age range：23-35 | |
|---|---|---|---|
| Question | | Tick the choice | |
| Whether sensory analysis is necessary? | | Yes □ (80) | No □ (0) |
| Are you interested in sensory analysis? | | Yes □ (52) | No □ (28) |
| Experience in sensory analysis? | | Yes □ (48) | No □ (32) |
| Are there any foods you don't eat? | | Yes □ (31) | No □ (49) |
| Are you familiar with sensory evaluation methods? | | Yes □ (48) | No □ (32) |
| Have you had any allergies? | | Yes □ (80) | No □ (0) |
| Whether there is any nasal disease? | | No nasal disease (68)<br>Have nasal disease (12) | |
| Food preferences (sour, sweet, bitter, spicy, etc.) | | Sweet (45), Spicy (35) | |
| Favorite and least favorite foods | | Favorite foods (apple, chocolate, strawberry, biscuits, cake, cherry, etc.)<br>Dislike foods (coriander, garlic, onion, preserved egg, durian, Spirrali piain, etc) | |
| Describe your favorite foods. (at least 3 feature) | | sweet, succulent, fragrant, savoury, tasty, etc. | |
| The appropriate words to describe the flavor of carp meat (at least 2) | | umami, fishy, meaty, earthy, fatty, etc. | |
| Which odor words are associated with seafood? (at least 2) | | umami, fishy, meaty | |
| Which odor are associated with “fresh” and “clean”? (at least 2) | | umami, meaty | |
| Describe the flavor and texture of apples. (at least 3) | | sweet, sour, crisp, hard | |
| Qualification evaluation results | | | |

Table S2-1 Preparation of substance for the paired comparison test

| | Descriptor | Compounds | Concentration |
|---|---|---|---|
| Taste | Sweet | sugar | 16 g/L |
| | Sour | citric acid | 1 g/L |
| | Bitter | caffeine | 0.5 g/L |
| | Salty | sodium chloride | 5 g/L |
| | Astringent | aluminium potassium sulfate | 0.5 g/L |
| | Metallic | ferrous sulfate | 0.01 g/L |
| Odor | Citric Odor | citral | 0.001M/L |
| | Vanilla Odor | vanillina | 0.001M/L |
| | Thymic Odor | thymol | 0.001M/L |
| | Jasmine Odor | benzyl acetate | 0.001M/L |

Table S2-2 Answer sheet of the paired comparison test

No.: Name: Date:

| | Taste | | | | | | Odor | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| References | 187 | 265 | 557 | 147 | 248 | 352 | 631 | 982 | 741 | 659 |
| Samples | | | | | | | | | | |
| Descriptor | | | | | | | | | | |

**Note：** Remember the characteristics of references firstly, and then matching the samples to the references. Write down the descriptor.

Table S2-3 Results of the paired comparison test

| The case of correctly | Number of panelists | |
|---|---|---|
| | Taste | Odor |
| Absolutely right | 42 | 38 |
| accuracy rate between 90%-100% | 9 | 11 |
| accuracy rate between 80%-90% | 12 | 8 |
| accuracy rate between 70%-80% | 5 | 7 |
| accuracy rate between 60%-70% | 9 | 11 |
| Accuracy rate less 60% | 3 | 5 |

Table S3-1 Preparation of substance for the triangle test

| compounds | Concentration |
|---|---|
| citric acid | 1 g/L |
| sugar | 16 g/L |
| benzyl acetate | 0.001M/L |

Table S3-2 Answer sheet of the triangle test

| No.: | Name: | | Date: |
|---|---|---|---|
| | 1 | 2 | 3 |
| Sample | 768 □ | 126 □ | 213 □ |
| | 328 □ | 356 □ | 653 □ |
| | 578 □ | 986 □ | 553 □ |

**Note:** Feel samples successively according to the serial number. Two samples are the same and one is different. Select different samples and mark "×" in the corresponding box and descript the sample.

Table S3-3 Results of the triangle test

| The case of correctly | Number of panelists |
|---|---|
| Absolutely right | 72 |
| accuracy rate between 90%-100% | 8 |
| accuracy rate between 80%-90% | 0 |
| accuracy rate between 70%-80% | 0 |
| accuracy rate between 60%-70% | 0 |
| Accuracy rate less 60% | 0 |

Table S4-1 Preparation of substance for the ranking test

| | Compounds | Concentration |
|---|---|---|
| Taste | citric acid (g/L) | 0.1, 0.15, 0.22, 0.34 |
| Odor | benzyl acetate (mg/kg) | 5, 10, 20, 40 |

Table S4-2 Answer sheet of the ranking test

| No.: | Name: | Date: |
|---|---|---|
| | compounds | Sequence (from weak to strong) |
| Taste | citric acid | |
| Odor | benzyl acetate | |

Table S4-3 Results of the ranking test

| The case of correctly | Number of panelists | |
|---|---|---|
| | Taste | Odor |
| Absolutely right | 35 | 38 |
| accuracy rate between 90%-100% | 13 | 7 |
| accuracy rate between 80%-90% | 14 | 11 |
| accuracy rate between 70%-80% | 9 | 12 |
| accuracy rate between 60%-70% | 5 | 6 |
| Accuracy rate less 60% | 4 | 6 |

Table S5-1 Preparation of substance for the descriptive ability test

| Compounds | Descriptor |
|---|---|
| benzaldehyde | bitter almonds, cherries |
| 1-Octen-3-ol | mushroom |
| ionone | Violets, raspberries |
| menthol | mint |
| vanillina | vanilla |
| benzyl acetate | jasmine |

Table S5-2 Answer sheet of the descriptive ability test

No.: Name: Date:

| Compounds | Odor |
|---|---|
| A | |
| B | |
| C | |
| D | |
| E | |
| F | |

Table S5-3 Results of the triangle test

| The case of correctly | Number of panelists |
|---|---|
| Absolutely right | 54 |
| accuracy rate between 90%-100% | 10 |
| accuracy rate between 80%-90% | 11 |
| accuracy rate between 70%-80% | 5 |
| accuracy rate between 60%-70% | 0 |
| Accuracy rate less 60% | 0 |

## Odorants information

Table S6 Results of volatile compounds in clam soup identified by different extraction methods.

| No. | compounds | RI | Identification | SPME | SDE | LL-SAFE | SAFE-LL | SAFE-P&T | P&T |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 2H-Pyran, 3,4-dihydro- | 716 | MS,RI. | | | + | + | | |
| 2 | Toluene | 754 | MS,RI,Std. | | | + | + | + | + |
| 3 | 1-Pentene, 3-methyl- | 758 | MS,RI. | | | | + | | |
| 4 | 1-Pentanol (CAS) | 771 | MS,RI,Std. | | | + | + | + | + |
| 5 | 3-Hexanone | 783 | MS,RI. | | | | + | | |
| 6 | 2-Hexanone | 789 | MS,RI. | | | | + | | |
| 7 | Hexanal | 802 | MS,RIStd. | | | + | + | + | + |
| 8 | Pyrazine, methyl- | 822 | MS,RI,Std. | | | + | + | | |
| 9 | Acetic acid, butyl ester | 824 | MS,RI,Std. | | | | | + | + |
| 10 | Furfural | 834 | MS,RI,Std. | | | + | + | | + |
| 11 | 2-Hexenal, (E)- | 854 | MS,RI,Std. | | | + | + | | + |
| 12 | Benzene, ethyl- | 860 | MS,RI,Std. | | + | + | + | + | + |
| 13 | Benzene, 1,3-dimethyl- | 862 | MS,RI,Std. | | + | + | + | + | + |
| 14 | p-Xylene | 868 | MS,RI,Std. | | + | + | + | + | + |
| 15 | 1-Hexanol (CAS) | 871 | MS,RI,Std. | | | + | + | + | + |
| 16 | Cyclohexanol | 883 | MS,RI,Std. | | | + | + | + | + |
| 17 | Styrene | 890 | MS,RI,Std. | | | + | + | + | + |
| 18 | Heptanal | 903 | MS,RI,Std. | | | + | + | + | + |
| 19 | Methional | 907 | MS,RI,Std. | | | + | + | | |
| 20 | Butyrolactone | 913 | MS,RI,Std. | | | + | + | | |
| 21 | 2,4-Hexadienal | 914 | MS,RI,Std. | | | | | | + |

| No. | compounds | RI | Identification | SPME | SDE | LL-SAFE | SAFE-LL | SAFE-P&T | P&T |
|---|---|---|---|---|---|---|---|---|---|
| 22 | Oxime-, methoxy-phenyl-_ | 928 | MS,RI. | + | | | | | |
| 23 | 2-Cyclohexen-1-one | 934 | MS,RI,Std. | | | | | + | + |
| 24 | Butanoic acid, 3-hydroxy-, ethyl ester | 936 | MS,RI,Std. | | | + | + | | |
| 25 | Hexanal, 2-ethyl- | 958 | MS,RI,Std. | | | | | + | + |
| 26 | Benzaldehyde | 959 | MS,RI,Std. | | | + | + | + | + |
| 27 | Nonane, 4-methyl- | 964 | MS,RI. | | | | | | + |
| 28 | Nonane, 2-methyl- | 967 | MS,RI. | | | | | | + |
| 29 | 1-Heptanol | 971 | MS,RI,Std. | | | + | + | | |
| 30 | Octane, 3-ethyl- | 974 | MS,RI. | | + | | | | |
| 31 | Benzene, 1,2,4-trimethyl- | 976 | MS,RI. | | + | | | | |
| 32 | 1-Octen-3-ol | 982 | MS,RI,Std. | | | + | + | + | + |
| 33 | Phenol | 983 | MS,RI,Std. | | | + | + | | |
| 34 | 5-Hepten-2-one, 6-methyl- | 990 | MS,RI,Std. | | | | | + | + |
| 35 | Furan, 2-pentyl- | 994 | MS,RI,Std. | | | + | + | | |
| 36 | Decane | 1000 | MS,RI. | | + | + | + | + | + |
| 37 | Octanal | 1005 | MS,RI,Std. | + | | + | + | + | + |
| 38 | Nonane, 2,5-dimethyl- | 1015 | MS,RI. | | | + | + | | + |
| 39 | Nonane, 2,6-dimethyl- | 1023 | MS,RI. | | | + | + | | |
| 40 | 1-Hexanol, 2-ethyl- | 1030 | MS,RI,Std. | | | + | + | + | + |
| 41 | Benzenemethanol | 1033 | MS,RI,Std. | | | + | + | | |
| 42 | Decane, 4-methyl- | 1059 | MS,RI. | | | + | + | | |
| 43 | 1-Octanol | 1071 | MS,RI,Std. | | | + | + | | + |
| 44 | Benzenemethanol, .alpha.,.alpha.-dimethyl- | 1085 | MS,RI,Std. | | | + | + | | |

| No. | compounds | RI | Identification | SPME | SDE | LL-SAFE | SAFE-LL | SAFE-P&T | P&T |
|---|---|---|---|---|---|---|---|---|---|
| 45 | Benzoic acid, methyl ester | 1095 | MS,RI,Std. | | | + | + | | + |
| 46 | Undecane | 1100 | MS,RI. | | | + | + | | |
| 47 | Decane, 2,4-dimethyl- | 1103 | MS,RI. | | | + | + | | |
| 48 | Nonanal | 1105 | MS,RI,Std. | + | | + | + | + | + |
| 49 | Benzaldehyde dimethyl acetal | 1111 | MS,RI,Std. | | | + | + | | |
| 50 | Benzene, 1,2,3,5-tetramethyl- | 1115 | MS,RI,Std. | | | + | + | | |
| 51 | Benzene, 1,2,4,5-tetramethyl- | 1120 | MS,RI,Std. | | | + | + | | |
| 52 | Benzene, 1-ethyl-3,5-dimethyl- | 1123 | MS,RI. | | + | | | | |
| 53 | triethyl phosphate | 1126 | MS,RI,Std. | | | + | + | | |
| 54 | Benzene, 1,2,3,4-tetramethyl- | 1152 | MS,RI. | | + | + | + | | |
| 55 | Benzene, 4-ethyl-1,2-dimethyl- | 1160 | MS,RI. | | + | | | | |
| 56 | Undecane, 2-methyl- | 1165 | MS,RI. | | | + | + | | |
| 57 | Naphthalene | 1183 | MS,RI,Std. | + | | + | + | + | + |
| 58 | 3-Dodecene, (Z)- | 1193 | MS,RI. | | + | | | | |
| 59 | Dodecane | 1200 | MS,RI. | | + | + | + | | + |
| 60 | Decanal | 1206 | MS,RI,Std. | + | | + | + | + | + |
| 61 | Undecane, 2,4-dimethyl- | 1211 | MS,RI. | | | + | + | | |
| 62 | Undecane, 2,6-dimethyl- | 1215 | MS,RI. | | | + | + | | |
| 63 | Benzothiazole | 1223 | MS,RI,Std. | | | + | + | | |
| 64 | Undecane, 4-ethyl- | 1245 | MS,RI. | | | + | + | | |
| 65 | Dodecane, 5-methyl- | 1251 | MS,RI. | | | + | + | | |
| 66 | Benzene, 1,3-bis(1,1-dimethylethyl)- | 1256 | MS,RI,Std. | | | | | | + |
| 67 | Dodecane, 2,6,11-trimethyl- | 1257 | MS,RI. | | + | | | | |
| 68 | Dodecane, 4-methyl- | 1260 | MS,RI. | | | + | + | | |

| No. | compounds | RI | Identification | SPME | SDE | LL-SAFE | SAFE-LL | SAFE-P&T | P&T |
|---|---|---|---|---|---|---|---|---|---|
| 69 | Dodecane, 2-methyl- | 1265 | MS,RI. | | | + | + | | |
| 70 | Dodecane, 2,6,11-trimethyl- | 1281 | MS,RI. | + | + | + | + | | |
| 71 | Tridecane | 1300 | MS,RI. | + | + | + | + | | |
| 72 | Naphthalene, 1-methyl- | 1313 | MS,RI. | | + | | | | |
| 73 | Naphthalene, 2-methyl- | 1332 | MS,RI. | | + | | | | |
| 74 | Dodecane, 4,6-methyl- | 1327 | MS,RI. | | | + | + | | |
| 75 | Phenol, 2-(1,1-dimethylethyl)-4-methyl- | 1354 | MS,RI,Std. | | | + | + | | |
| 76 | Eugenol | 1359 | MS,RI,Std. | | | + | + | | |
| 77 | Tridecane, 2-methyl- | 1364 | MS,RI. | | | | + | | |
| 78 | Tridecane, 3-methyl- | 1371 | MS,RI. | | | | + | | |
| 79 | Tetradecane | 1400 | MS,RI. | + | + | + | + | + | |
| 80 | Naphthalene, 2,7-dimethyl- | 1404 | MS,RI,Std. | | | + | + | | |
| 81 | Naphthalene, 1,3-dimethyl- | 1420 | MS,RI,Std. | | | + | + | | |
| 82 | Naphthalene, 2,6-dimethyl- | 1427 | MS,RI. | | + | | | | |
| 83 | Naphthalene, 1,6-dimethyl- | 1444 | MS,RI. | | + | | | | |
| 84 | Tetradecane, 4,11-dimethyl- | 1463 | MS,RI. | | | + | + | | |
| 85 | 1-Dodecanol | 1474 | MS,RI,Std. | | | + | + | | |
| 86 | Naphthalene, 1,5-dimethyl- | 1484 | MS,RI. | | + | | | | |
| 87 | Pentadecane | 1500 | MS,RI. | + | | + | + | | |
| 88 | Phenol, 2,5-bis(1,1-dimethylethyl)- | 1513 | MS,RI. | | | + | + | | |
| 89 | Butylated Hydroxytoluene | 1516 | MS,RI,Std. | + | | + | + | | |
| 90 | Phenol,2,4-bis(1,1-imethylethyl)- | 1523 | MS,RI. | | + | | | | |
| 91 | Phenol, 3,5-bis(1,1-imethylethyl)- | 1526 | MS,RI. | | + | | | | |

| No. | compounds | RI | Identification | SPME | SDE | LL-SAFE | SAFE-LL | SAFE-P&T | P&T |
|---|---|---|---|---|---|---|---|---|---|
| 92 | Tetradecane, 2,6,10-trimethyl- | 1533 | MS,RI. | | + | + | + | | |
| 93 | Naphthalene, 1,6,7-trimethyl- | 1558 | MS,RI. | | + | | | | |
| 94 | Pentadecane, 2-methyl- | 1564 | MS,RI. | | | + | | | |
| 95 | Pentadecane, 3-methyl- | 1571 | MS,RI. | | | + | | | |
| 96 | Naphthalene, 1,4,5-trimethyl- | 1575 | MS,RI. | | + | | | | |
| 97 | Hexadecane | 1600 | MS,RI. | + | + | + | + | | |
| 98 | 1H-Benzocyclohepten-7-ol, 2,3,4,4a,5,6,7,8-octahydro-1,1,4a,7-tetramethyl-, cis- | 1608 | MS,RI. | | | + | + | | |
| 99 | Heptadecane | 1700 | MS,RI. | | + | + | + | | |
| 100 | Heptadecane, 2-methyl- | 1714 | MS,RI. | | + | | | | |
| 101 | Hexadecane, 2,6,10,14-tetramethyl- | 1758 | MS,RI. | | + | | | | |
| 102 | Octadecane | 1800 | MS,RI. | | + | + | + | | |
| 103 | Octadecane, 2-methyl- | 1822 | MS,RI. | | + | | | | |
| 104 | 1,2-Benzenedicarboxylic acid, bis(2-methylpropyl) ester | 1871 | MS,RI. | | | + | + | | |
| 105 | Nonadecane | 1900 | MS,RI. | | | + | + | | |
| 106 | Dibutyl phthalate | 1965 | MS,RI,Std. | | | + | + | | |
| 107 | Eicosane | 2000 | MS,RI. | | + | + | + | | |
| 108 | Heneicosane | 2100 | MS,RI. | | + | + | + | | |
| 109 | Docosane | 2200 | MS,RI. | | | + | + | | |
| 110 | Acetic acid n-octadecyl ester | 2210 | MS,RI,Std. | | | + | + | | |
| 111 | Tricosane | 2300 | MS,RI. | | | + | + | | |
| 112 | Hexanedioic acid, bis(2- | 2302 | MS,RI,Std. | | | + | + | | |

| No. | compounds | RI | Identification | SPME | SDE | LL-SAFE | SAFE-LL | SAFE-P&T | P&T |
|---|---|---|---|---|---|---|---|---|---|
| | ethylhexyl) ester | | | | | | | | |
| 113 | Phenol, 2,2'-methylenebis[6-(1,1-dimethylethyl)-4-methyl- | 2328 | MS,RI,Std. | | | + | + | | |
| 114 | Pentacosane | 2500 | MS,RI. | | | + | + | | |
| 115 | Hexacosane | 2600 | MS,RI. | | | + | + | | |
| 116 | Heptacosane | 2700 | MS,RI. | | | + | + | | |
| 117 | Octacosane | 2800 | MS,RI. | | | + | + | | |
| 118 | Nonacocane | 2900 | MS,RI | | | + | + | | |
| 119 | Triacontane | 3000 | MS,RI. | | | + | + | | |

MS, identified by mass spectral data.

RI, identified by retention indices.

Std., identified by standards.

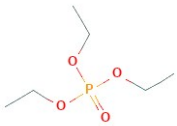
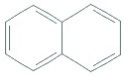
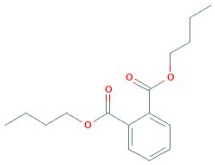
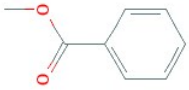
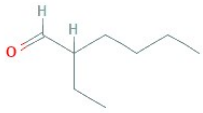
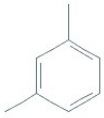
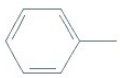
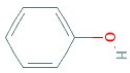
Table S7 Quantification of 49 volatile compounds in clam soup via different extraction methods.

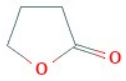
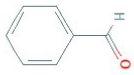
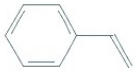
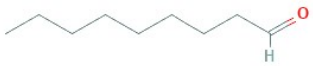
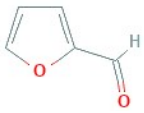
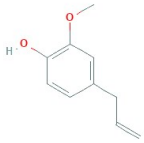
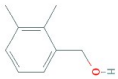
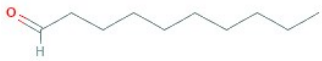
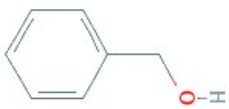
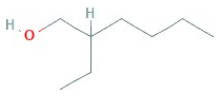
| No. | Compounds | LL-SAFE (ng/mL) | SAFE-LL (ng/mL) | SAFE-P&T (ng/mL) | P&T (ng/mL) |
|---|---|---|---|---|---|
| 1 | triethyl phosphate | 91.05±1.85 | 70.13±1.66 | n/a | n/a |
| 2 | p-xylene | 7.65±0.99 | 4.26±0.95 | 6.37±0.89 | 8.29±0.35 |
| 3 | naphthalene | 2.31±0.92 | 1.34±0.22 | 3.08±0.08 | 2.64±0.61 |
| 4 | dibutyl phthalate | 15.97±0.30 | 10.81±0.84 | n/a | n/a |
| 5 | benzoic acid, methyl ester | 15.28±0.68 | 14.98±0.83 | n/a | 36.28±1.23 |
| 6 | 2-ethyl-hexanal | n/a | n/a | 2.75±0.41 | 5.71±0.19 |
| 7 | 1-heptanol | 4.83±0.27 | 4.66±0.55 | n/a | n/a |
| 8 | 1,3-dimethyl-benzene | 5.63±0.41 | 1.19±0.06 | 6.95±0.18 | 2.48±0.64 |
| 9 | toluene | 4.51±0.79 | 2.58±0.14 | 4.16±0.30 | 5.65±0.07 |
| 10 | phenol | 7.84±0.12 | 7.31±0.23 | n/a | n/a |
| 11 | butyrolactone | 9.21±0.74 | 10.73±0.22 | n/a | n/a |
| 12 | benzaldehyde | 7.34±0.58 | 8.22±0.43 | 25.63±1.20 | 28.74±1.57 |
| 13 | 1-dodecanol | 41.79±1.97 | 12.63±0.86 | n/a | n/a |
| 14 | styrene | 1.74±0.09 | 0.82±0.28 | 2.32±0.63 | 9.30±0.41 |
| 15 | nonanal | 19.19±0.94 | 11.84±0.49 | 16.85±0.25 | 12.23±0.68 |
| 16 | furfural | 2.71±0.46 | 2.85±0.16 | n/a | 2.59±0.33 |
| 17 | eugenol | 8.21±0.39 | 7.61±0.37 | n/a | n/a |
| 18 | dimethyl-benzenemethanol | 8.03±0.18 | 6.57±0.49 | n/a | n/a |
| 19 | decanal | 14.38±0.44 | 11.33±0.32 | 7.73±0.87 | 11.46±0.97 |
| 20 | benzenemethanol | 18.19±1.25 | 20.30±0.86 | n/a | n/a |
| 21 | 2-ethyl-1-hexanol | 38.97±1.06 | 33.72±0.76 | 27.73±1.24 | 156.42±2.77 |
| 22 | 1-octanol | 9.65±0.80 | 9.37±0.86 | n/a | 23.94±1.07 |
| 23 | 1,2,4,5-tetramethyl-benzene | 0.75±0.03 | 0.60±0.05 | n/a | n/a |
| 24 | octanal | 11.11±0.66 | 7.61±0.65 | 24.56±1.00 | 36.89±0.98 |

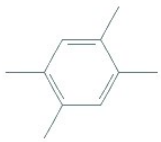
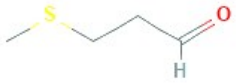
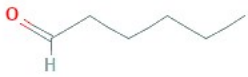
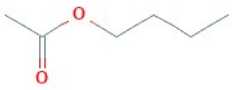
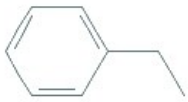
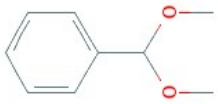
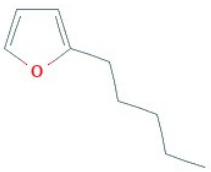
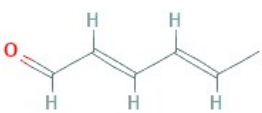
| No. | Compounds | LL-SAFE (ng/mL) | SAFE-LL (ng/mL) | SAFE-P&T (ng/mL) | P&T (ng/mL) |
|---|---|---|---|---|---|
| 25 | methional | 20.46±1.17 | 10.61±0.44 | n/a | n/a |
| 26 | hexanal | 8.49±0.30 | 3.46±0.80 | 52.50±1.15 | 29.16±0.79 |
| 27 | heptanal | 4.86±0.72 | 2.70±0.31 | 15.61±0.77 | 13.65±0.80 |
| 28 | acetic acid, butyl ester | 0.39±0.39 | n/a | 2.68±0.15 | 1.16±0.12 |
| 29 | 1-pentanol | 2.48±0.45 | 2.61±0.31 | 5.68±0.24 | 5.11±0.81 |
| 30 | ethyl-benzene | 1.85±0.11 | n/a | 1.10±0.64 | 0.90±0.68 |
| 31 | benzaldehyde dimethyl acetal | 10.86±0.32 | 6.51±0.71 | n/a | n/a |
| 32 | 2-pentyl-furan | 0.05±0.01 | 2.28±0.02 | n/a | n/a |
| 33 | 2,4-hexadienal | n/a | n/a | n/a | 31.14±1.44 |
| 34 | 1-octen-3-ol | 4.22±0.20 | 4.17±0.57 | 4.18±0.57 | 11.55±0.33 |
| 35 | 1-hexanol | 10.08±0.60 | 9.72±0.28 | 9.46±0.74 | 20.18±1.12 |
| 36 | 1,3-dimethyl-naphthalene | 1.97±0.09 | 1.79±0.10 | n/a | n/a |
| 37 | 6-methyl-5-hepten-2-one | n/a | n/a | 6.44±0.61 | 10.35±0.62 |
| 38 | butylated hydroxytoluene | 19.87±1.19 | 12.01±0.51 | n/a | n/a |
| 39 | methyl-pyrazine | 4.61±0.32 | 4.72±0.18 | n/a | n/a |
| 40 | benzothiazole | 4.33±0.81 | 5.37±0.16 | n/a | n/a |
| 41 | 3-hydroxy-butanoic acid, ethyl ester | 11.29±0.82 | 11.81±0.14 | n/a | n/a |
| 42 | 2-cyclohexen-1-one | n/a | n/a | 4.73±0.10 | 8.69±0.18 |
| 43 | (e)-2-hexenal | 9.74±0.86 | 6.03±0.58 | n/a | 17.80±0.27 |
| 44 | cyclohexanol | 41.79±2.30 | 44.36±1.72 | 3.78±0.73 | 16.64±0.47 |
| 45 | acetic acid n-octadecyl ester | 94.43±4.23 | 184.89±2.47 | n/a | n/a |
| 46 | 2,7-dimethyl-naphthalene | 2.32±0.06 | 2.19±0.03 | n/a | n/a |

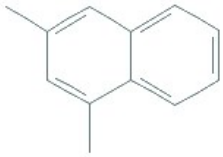
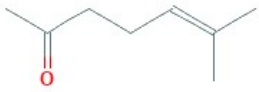
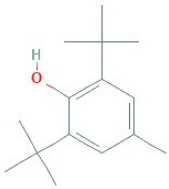
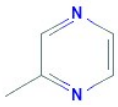
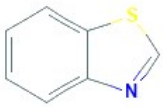
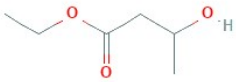
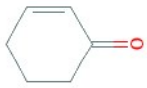
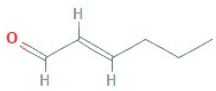
| No. | Compounds | LL-SAFE (ng/mL) | SAFE-LL (ng/mL) | SAFE-P&T (ng/mL) | P&T (ng/mL) |
|---|---|---|---|---|---|
| 47 | 2-(1,1-dimethylethyl)-4-methyl-phenol | 5.87±0.12 | 5.37±0.85 | n/a | n/a |
| 48 | 1,3-bis(1,1-dimethylethyl)-benzene | n/a | n/a | n/a | 2.48±0.03 |
| 49 | 1,2,3,5-tetramethyl-benzene | 4.08±0.18 | 3.82±0.11 | n/a | n/a |

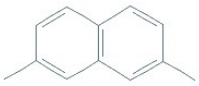
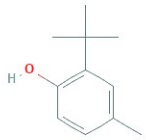
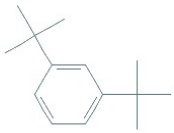
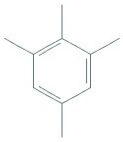
Table S8 List of 49 volatiles compounds selected.

| No. | Key odorants | CAS no. | structure |
|---|---|---|---|
| 1 | triethyl phosphate | 78-40-0 |  |
| 2 | p-xylene | 106-42-3 |  |
| 3 | naphthalene | 91-20-3 |  |
| 4 | dibutyl phthalate | 84-74-2 |  |
| 5 | benzoic acid, methyl ester | 93-58-3 |  |
| 6 | 2-ethyl-hexanal | 123-05-7 |  |
| 7 | 1-heptanol | 111-70-6 |  |
| 8 | 1,3-dimethyl-benzene | 108-38-3 |  |
| 9 | toluene | 108-88-3 |  |
| 10 | phenol | 108-95-2 |  |

| | | | |
|---|---|---|---|
| 11 | butyrolactone | 96-48-0 |  |
| 12 | benzaldehyde | 100-52-7 |  |
| 13 | 1-dodecanol | 112-53-8 |  |
| 14 | styrene | 100-42-5 |  |
| 15 | nonanal | 124-19-6 |  |
| 16 | furfural | 98-01-1 |  |
| 17 | eugenol | 97-53-0 |  |
| 18 | α,α-dimethyl-benzenemethanol | 13651-14-4 |  |
| 19 | decanal | 112-31-2 |  |
| 20 | benzenemethanol | 100-51-6 |  |
| 21 | 2-ethyl-1-hexanol | 104-76-7 |  |
| 22 | 1-octanol | 111-87-5 |  |

| | | | |
|---|---|---|---|
| 23 | 1,2,4,5-tetramethyl-benzene | 95-93-2 |  |
| 24 | octanal | 124-13-0 |  |
| 25 | methional | 3268-49-3 |  |
| 26 | hexanal | 66-25-1 |  |
| 27 | heptanal | 111-71-7 |  |
| 28 | acetic acid, butyl ester | 123-86-4 |  |
| 29 | 1-pentanol | 71-41-0 |  |
| 30 | ethyl-benzene | 100-41-4 |  |
| 31 | benzaldehyde dimethyl acetal | 1125-88-8 |  |
| 32 | 2-pentyl-furan | 3777-69-3 |  |
| 33 | 2,4-hexadienal | 142-83-6 |  |

| | | | |
|---|---|---|---|
| 34 | 1-octen-3-ol | 3391-86-4 |  |
| 35 | 1-hexanol | 111-27-3 |  |
| 36 | 1,3-dimethyl-naphthalene | 575-41-7 |  |
| 37 | 6-methyl-5-hepten-2-one | 110-93-0 |  |
| 38 | butylated hydroxytoluene | 128-37-0 |  |
| 39 | methyl-pyrazine | 109-08-0 |  |
| 40 | benzothiazole | 95-16-9 |  |
| 41 | 3-hydroxy-butanoic acid, ethyl ester | 5405-41-4 |  |
| 42 | 2-cyclohexen-1-one | 930-68-7 |  |
| 43 | (E)-2-hexenal | 6728-26-3 |  |
| 44 | cyclohexanol | 108-93-0 |  |
| 45 | acetic acid n-octadecyl ester | 822-23-1 |  |

| | | | |
|---|---|---|---|
| 46 | 2,7-dimethyl-naphthalene | 582-16-1 |  |
| 47 | 2-(1,1-dimethylethyl)-4-methyl-phenol | 2409-55-4 |  |
| 48 | 1,3-bis(1,1-dimethylethyl)-benzene | 1014-60-4 |  |
| 49 | 1,2,3,5-tetramethyl-benzene | 527-53-7 |  |

**Reference**

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