Supplementary Material

# Evaluation of the Chemosensoric Properties of Commercially Available Dog Foods using Electronic Sensors and GC-MS/O Analysis

**Hyangyeon Jeong[1†], Moon Yeon Youn[2†], Sojeong Yoon[1], Seong Jun Hong[1], Seong Min Jo[1], Kyeong Soo Kim[3], Eun Ju Jeong[4], Hyun-Wook Kim[5], Eui-Cheol Shin[1,2,6*]**

## 1. Supplementary Tables

**Supplementary Table S1** Volatile compounds of 10 dog foods using E-nose.

(Peak area x $10^3$)

| Compounds | RT[1)](RI[2)]) | Sensory description | ASC | AS | AP | AF | AC | IS | ITS | IS2 | IS3 | IS4 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| **Acids and esters(21)** | | | | | | | | | | | | |
| Methyl formate | 17.58(380) | Fruity | 10.16±0.82 | 12.98±0.60 | 0.28±0.03 | 8.15±1.12 | ND[3)] | ND | ND | ND | ND | ND |
| Methyl acetate | 27.21(533) | Fruity | ND[3)] | ND | 2.78±0.34 | ND | ND | ND | ND | ND | ND | ND |
| Formic acid | 29.78(574) | - | ND | 0.53±0.04 | ND | ND | ND | ND | ND | ND | ND | ND |
| Acetic acid | 33.29(616) | Sour | ND | ND | 0.13±0.03 | ND | ND | ND | ND | ND | ND | ND |
| Isopropyl acetate | 36.31(641) | Sweet | ND | ND | 0.05±0.09 | ND | ND | ND | ND | ND | ND | ND |
| Propyl acetate | 45.21(718) | Sweet | ND | ND | ND | ND | ND | ND | ND | ND | 0.25±0.06 | ND |
| Methyl butanoate | 45.24(719) | Sweet | 0.14±0.03 | ND | ND | ND | 0.06±0.01 | ND | ND | ND | ND | ND |
| Butyl acetate | 54.13(804) | - | ND | ND | ND | ND | ND | ND | ND | ND | ND | 0.21±0.02 |
| Propyl propanoate | 54.25(806) | Fruity, Sweet | ND | ND | ND | ND | ND | ND | 0.18±0.05 | ND | ND | ND |
| Propylacrylate | 55.73(823) | - | ND | ND | ND | 0.10±0.01 | ND | ND | ND | ND | ND | ND |

| | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Methyl pentanoate | 55.81(824) | Fruity, Nutty | ND | ND | ND | ND | ND | ND | 0.08±0.01 | ND | ND | ND |
| Ethyl 2-methylbutyrate | 57.87(848) | Sweet | ND | ND | ND | ND | ND | ND | ND | ND | ND | 0.16±0.01 |
| Isoamyl acetate | 59.29(865) | Fruity, Fresh | ND | ND | ND | ND | ND | ND | ND | 0.02±0.03 | ND | 0.09±0.03 |
| Pentanoic acid | 61.95(897) | Beefy. Sweet | ND | ND | ND | 1.05±0.41 | 1.32±0.06 | ND | ND | ND | ND | ND |
| Heptanoic acid | 71.69(1,142) | Cheese, Oily | ND | ND | ND | ND | ND | ND | ND | 0.07±0.02 | ND | ND |
| Benzoic acid | 71.80(1,143) | - | ND | 0.06±0.05 | ND | ND | ND | ND | ND | ND | ND | ND |
| Benzyl acetate | 73.13(1,166) | Burnt, Sweet | ND | 0.11±0.10 | ND | ND | ND | ND | 0.10±0.06 | ND | ND | ND |
| Methyl cinnamate | 85.44(1,399) | Fruity, Sweet | 0.19±0.04 | 0.21±0.01 | 0.17±0.02 | ND | ND | ND | ND | ND | ND | ND |
| Methyl dodecanoate | 91.40(1,531) | Coconut, Oily | 0.64±0.04 | ND | ND | ND | 0.11±0.01 | ND | ND | ND | ND | ND |
| Octyl caprylate | 101.51(1,761) | Oily | ND | ND | ND | 0.09±0.01 | ND | 0.09±0.02 | 0.09±0.01 | ND | ND | ND |
| Dodecyl butyrate | 101.66(1,765) | Oily, Fruity | 0.10±0.03 | ND | ND | ND | 1.69±0.09 | ND | ND | ND | ND | ND |
| **Alcohols(24)** | | | | | | | | | | | | |
| Methanol | 20.33(423) | - | ND | 4.17±0.44 | ND | 3.20±0.18 | 2.15±0.14 | 3.33±0.41 | 4.89±0.19 | 2.00±0.18 | ND | ND |
| Ethanol | 21.21(437) | Ethanol, Sweet | ND | 1.09±0.04 | ND | ND | 0.28±0.05 | 0.89±0.05 | 1.86±0.01 | ND | ND | ND |
| 2-Methyl-2-propanaol | 23.67(476) | - | ND | ND | ND | ND | ND | 0.14±0.09 | 0.56±0.04 | 0.29±0.06 | 0.06±0.10 | ND |
| 2-Propanol | 25.17(500) | Etheral, Acetone | ND | ND | 2.74±0.74 | ND | ND | ND | ND | ND | ND | ND |
| 1-Propanol | 27.27(534) | Ethanol, Fruity | 1.74±0.24 | ND | ND | ND | ND | ND | 2.16±0.21 | 1.60±0.18 | 6.30±0.68 | 1.92±0.29 |
| 2-Mercaptoethanol | 29.63(571) | Sulfurous | ND | ND | ND | ND | ND | ND | ND | 0.64±0.21 | ND | ND |
| 2-Butanol | 29.87(575) | Oily | 0.42±0.17 | ND | ND | ND | 2.66±0.07 | ND | ND | ND | ND | ND |
| 2-Methyl-1-propanol | 33.19(615) | Bitter, Oily | ND | ND | ND | ND | ND | 0.14±0.02 | ND | ND | ND | ND |

| | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Butanol | 39.81(671) | Oily, Sweet | 0.12±0.11 | ND | 0.76±0.14 | ND | ND | ND | ND | ND | ND | ND |
| 1-Methoxy-2-propanol | 40.39(675) | - | ND | ND | ND | ND | ND | ND | 1.75±0.21 | ND | 1.39±0.24 | ND |
| 1-Penten-3-ol | 40.42(676) | Burnt, Butter | ND | 7.26±0.35 | ND | ND | ND | ND | ND | ND | 0.10±0.17 | ND |
| Trometamol | 41.43(684) | Burnt, Butter | ND | ND | ND | ND | ND | ND | ND | 0.07±0.06 | ND | ND |
| 3-Pentanol | 43.56(702) | Nutty, Oily | 3.83±0.27 | ND | 12.18±1.46 | 1.35±0.07 | 2.01±0.13 | 0.07±0.01 | ND | ND | ND | ND |
| 3-Methyl-1-butanol | 47.63(741) | Bitter, Butter | ND | 0.16±0.01 | ND | 0.29±0.08 | ND | ND | ND | ND | ND | ND |
| 1,2-Butanediol | 49.66(761) | Butter | 0.57±0.03 | ND | 0.10±0.01 | ND | 0.09±0.01 | ND | ND | ND | 0.03±0.04 | ND |
| Pentanol | 49.70(761) | Fruity, Oily | ND | 0.09±0.05 | ND | ND | ND | ND | ND | ND | ND | ND |
| 1-Hexen-3-ol | 50.94(773) | Green | 0.47±0.09 | ND | ND | ND | 0.24±0.02 | ND | ND | ND | ND | ND |
| 2,3-Butanediol | 53.12(794) | Fruity | 0.14±0.03 | 0.13±0.00 | ND | 0.28±0.03 | ND | ND | ND | ND | ND | ND |
| 2-Hexanol | 54.20(805) | Fruity | 0.59±0.05 | 0.56±0.01 | 0.54±0.04 | ND | 0.20±0.02 | 0.24±0.06 | ND | 0.20±0.03 | ND | ND |
| 2,3-Dimethyl-1-pentanol | 55.73(823) | - | ND | ND | ND | ND | ND | 0.16±0.01 | ND | 0.14±0.01 | 0.25±0.01 | ND |
| 1-Hexanol | 59.45(867) | Oily, Sweet | ND | ND | ND | ND | ND | ND | 0.11±0.01 | ND | ND | ND |
| 2-Cresol | 67.73(1,062) | Sweet | ND | ND | ND | ND | ND | ND | ND | ND | 0.78±0.13 | ND |
| *α*-Terpineol | 74.85(1,194) | Citrus, Oily | ND | ND | ND | ND | ND | ND | 0.09±0.01 | ND | ND | ND |
| 2-Butyloctanol | 79.90(1,288) | - | ND | 0.28±0.07 | ND | ND | ND | ND | ND | ND | ND | ND |
| | | | | | | | | | | | | |
| **Aldehydes(16)** | | | | | | | | | | | | |
| Propenal | 22.58(459) | Almond | ND | 2.83±0.13 | ND | ND | ND | ND | ND | ND | ND | ND |
| Propanal | 24.81(495) | Cocoa, Nutty | ND | ND | ND | ND | ND | ND | 0.23±0.05 | ND | ND | ND |
| Butanal | 30.15(579) | Cocoa, Musty | ND | ND | ND | 5.45±0.23 | ND | 1.18±0.05 | 1.80±0.02 | ND | 3.29±0.19 | 2.15±0.09 |
| 2-Butenal | 35.98(638) | Green | 2.28±0.04 | 0.16±0.12 | 0.10±0.06 | 0.09±0.01 | ND | 0.15±0.02 | ND | 0.23±0.05 | ND | ND |
| 2-Methylbutanal | 38.63(661) | Almond, Coffee | ND | ND | ND | ND | ND | ND | ND | ND | 0.62±0.00 | ND |

| | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Pentanal | 42.43(693) | Almond, Green | ND | ND | 0.51±0.16 | ND | ND | ND | ND | ND | ND | ND |
| 2-Pentenal | 47.70(742) | Oily, Green | 0.35±0.04 | ND | ND | ND | ND | ND | ND | ND | ND | ND |
| 2-Methylpentanal | 49.53(760) | Cheese, Fruity | ND | ND | ND | ND | 0.06±0.00 | ND | ND | ND | ND | 0.06±0.01 |
| 2-Hexenal | 57.98(850) | Almond, Oily | ND | 0.07±0.01 | ND | ND | ND | ND | ND | ND | ND | ND |
| 2-Nonenal | 71.71(1,142) | Citrus, Oily | ND | ND | ND | ND | 0.04±0.03 | ND | ND | ND | ND | ND |
| 6-Decenal | 75.26(1,201) | Green | ND | 0.09±0.04 | ND | ND | ND | ND | ND | ND | ND | ND |
| 2-Decenal | 78.75(1,266) | Green | ND | ND | ND | ND | ND | ND | ND | ND | ND | 0.03±0.03 |
| *α*-Terpinen-7-al | 78.79(1,267) | Oily | ND | ND | 0.02±0.03 | 0.04±0.04 | ND | 0.02±0.03 | ND | ND | 0.02±0.03 | ND |
| 2,4-Decadienal | 79.89(1,287) | Oily, Green | ND | ND | 0.27±0.05 | 0.31±0.02 | ND | 0.28±0.05 | ND | ND | 0.29±0.07 | ND |
| Undecanal | 80.68(1,302) | Citrus, Oily | 0.34±0.04 | ND | ND | ND | ND | ND | ND | ND | ND | 0.27±0.07 |
| Dodecanal | 85.81(1,407) | Citrus, Oily | ND | ND | ND | 0.17±0.01 | ND | ND | ND | ND | ND | ND |
| | | | | | | | | | | | | |
| **Hydrocarbons(28)** | | | | | | | | | | | | |
| Butane | 17.61(380) | - | 0.51±0.37 | ND | 29.92±3.81 | ND | ND | ND | ND | ND | ND | ND |
| 2-Methylbutane | 22.55(459) | - | ND | ND | ND | 3.45±0.48 | ND | ND | ND | 10.06±1.61 | ND | ND |
| Dichloromethane | 24.77(494) | Sweet | ND | 0.26±0.06 | ND | ND | 5.16±0.46 | ND | ND | ND | 0.36±0.33 | ND |
| Acetonitrile | 27.27(534) | Sweet | 4.05±0.38 | 6.80±0.13 | ND | 2.44±0.24 | ND | ND | ND | ND | ND | ND |
| 3-Methylpentane | 29.82(574) | - | ND | ND | 0.30±0.11 | ND | 1.55±0.02 | ND | ND | ND | ND | ND |
| Hexane | 31.49(600) | Alkane | 1.59±0.24 | ND | ND | ND | 0.02±0.03 | 1.02±0.10 | 1.59±0.01 | ND | 1.65±0.09 | 2.21±0.15 |
| 1,2-Dichloroethene | 32.91(612) | Sweet | ND | ND | ND | ND | ND | ND | ND | ND | ND | ND |
| Benzene | 37.98(655) | - | 0.43±0.03 | ND | ND | ND | ND | ND | ND | ND | ND | ND |
| Trichloroethylene | 42.36(692) | Sweet | ND | 0.18±0.05 | ND | ND | ND | ND | ND | ND | ND | ND |
| Heptane | 42.41(692) | Alkane | ND | ND | ND | ND | ND | ND | 0.37±0.13 | ND | ND | ND |

| | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1,2-Dichloropropane | 43.55(702) | Sweet | ND | ND | ND | ND | ND | ND | 2.47±0.14 | ND | 1.09±0.04 | ND |
| Dibromomethane | 43.65(703) | - | ND | ND | ND | ND | ND | 1.00±0.12 | ND | ND | ND | ND |
| Ethylcyclopentane | 46.81(734) | - | ND | ND | ND | ND | ND | ND | ND | ND | 0.32±0.24 | ND |
| Methylcyclohexane | 47.35(739) | Sweet | ND | ND | ND | ND | ND | 0.08±0.08 | ND | ND | ND | ND |
| 4-Octene | 53.11(794) | - | ND | ND | 0.09±0.00 | ND | ND | 0.06±0.01 | 0.06±0.05 | ND | 0.24±0.03 | ND |
| 2,4-Octadiene | 55.83(824) | - | ND | ND | 0.13±0.01 | ND | 0.06±0.01 | ND | ND | ND | ND | ND |
| Chlorobenzene | 57.95(849) | Almond | ND | ND | 0.06±0.01 | ND | ND | 0.14±0.02 | ND | ND | ND | ND |
| Nonane | 61.95(897) | Alkane | ND | 1.57±0.17 | 1.36±0.12 | ND | 2.64±1.20 | 0.52±0.10 | ND | 0.80±0.25 | ND | 1.35±0.42 |
| Decane | 65.25(998) | Sweet, Fruity | 3.90±3.13 | 3.51±2.54 | 3.15±1.66 | 3.00±1.33 | ND | 2.34±1.16 | 2.52±0.94 | 2.06±0.82 | 2.26±0.73 | 2.17±0.72 |
| Limonene | 67.23(1,050) | Citrus | 1.13±0.51 | 1.01±0.40 | 1.16±0.37 | 1.33±0.64 | ND | ND | ND | ND | ND | ND |
| $\gamma$-Terpinene | 67.33(1,052) | Citrus, Oily | ND | ND | ND | ND | ND | 0.29±0.23 | 1.08±0.29 | ND | ND | 0.94±0.29 |
| 1,2-Dihydrobenzene | 67.35(1.053) | - | ND | ND | ND | ND | ND | ND | ND | 0.72±0.40 | ND | ND |
| 5-Ethyldecane | 71.68(1,141) | - | 0.04±0.03 | ND | ND | 0.08±0.03 | 0.06±0.06 | ND | ND | ND | ND | ND |
| Diterpene | 73.36(1,169) | - | 0.10±0.02 | ND | ND | ND | 0.16±0.00 | ND | ND | ND | ND | ND |
| Tetradecane | 85.71(1,405) | Alkane | ND | ND | ND | ND | 0.60±0.03 | 0.16±0.01 | ND | 0.16±0.03 | 0.18±0.01 | ND |
| 2,4-Dinitrotoluene | 91.28(1,529) | - | ND | 0.68±0.03 | 0.66±0.04 | ND | ND | ND | ND | ND | ND | ND |
| 2-Methylheptadecane | 101.65(1,764) | - | ND | ND | ND | ND | ND | ND | ND | 0.10±0.01 | 0.11±0.01 | ND |
| **Heterocyclic compounds(18)** | | | | | | | | | | | | |
| Trimethylamine | 20.28(423) | Amine, Fishy | 9.58±0.58 | ND | 2.71±0.34 | 0.80±0.07 | ND | ND | ND | 1.46±0.23 | 3.57±0.23 | ND |
| Diethyl ether | 23.72(477) | Etheral | 2.87±0.48 | ND | ND | 1.40±0.35 | ND | ND | ND | 2.59±0.30 | ND | ND |
| Acetonitrile | 26.04(514) | Sweet | ND | ND | ND | ND | ND | 8.97±1.71 | 2.47±0.18 | 5.28±0.33 | 0.03±0.06 | 5.40±0.51 |

| | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| *tert*-Butyl methyl ether | 28.15(548) | Fruity, Ethanol | ND | 2.94±0.04 | 1.30±0.21 | ND | ND | ND | ND | ND | 3.94±0.49 | ND |
| Diisopropyl ether | 33.01(613) | Etheral | ND | ND | ND | ND | ND | ND | ND | ND | 0.11±0.02 | ND |
| 1-Butanamine | 36.61(644) | Fishy | ND | ND | ND | ND | ND | 0.17±0.05 | 0.06±0.05 | ND | ND | ND |
| Pyrazine | 45.17(718) | Bitter, Nutty | 0.19±0.07 | ND | 0.11±0.03 | 0.09±0.03 | ND | ND | 0.13±0.02 | 0.25±0.08 | ND | ND |
| Pyrrole | 47.65(742) | Coffee, Nutty | ND | ND | ND | ND | ND | ND | 0.17±0.09 | 0.29±0.04 | ND | ND |
| Dimethylformamide | 50.95(773) | Amine | ND | ND | ND | ND | ND | ND | ND | 0.37±0.03 | 0.23±0.11 | 0.14±0.07 |
| Dibutyl ether | 59.38(866) | - | ND | ND | ND | ND | ND | ND | ND | ND | 0.02±0.04 | ND |
| Pentyl-benzene | 73.03(1,164) | Oily | ND | ND | ND | ND | ND | ND | ND | 0.10±0.01 | 0.12±0.02 | ND |
| 2-Methoxy-3-sec-butylpyrazine | 73.19(1,167) | Carrot, Musty | ND | ND | ND | ND | ND | 0.13±0.01 | ND | ND | ND | ND |
| Indole | 78.71(1,265) | Burnt, Sweet | ND | ND | ND | ND | ND | ND | 0.04±0.03 | 0.02±0.03 | ND | ND |
| Anethole | 81.07(1,310) | Oily, Sweet | ND | ND | ND | ND | ND | ND | 0.32±0.05 | ND | ND | ND |
| Methyl eugenol | 85.71(1,405) | Fresh, Sweet | ND | ND | ND | ND | ND | ND | 0.18±0.01 | ND | ND | 0.18±0.02 |
| Myristicin | 91.25(1,528) | Balsamic | ND | ND | ND | ND | ND | 0.61±0.02 | 0.61±0.06 | 0.67±0.11 | ND | 0.57±0.03 |
| Propazine | 101.45(1,760) | - | ND | ND | ND | ND | ND | ND | ND | ND | ND | 0.11±0.02 |
| Ambroxide | 104.69(1,833) | Dry, Sweet | 2.02±0.08 | ND | 1.77±0.12 | 1.92±0.21 | ND | 1.90±0.09 | 1.94±0.15 | 1.83±0.07 | 1.95±0.11 | 1.87±0.12 |
| **Ketones(11)** | | | | | | | | | | | | |
| Propan-2-one | 24.82(495) | Fruity, Sweet | 1.05±0.47 | ND | ND | ND | ND | ND | ND | ND | ND | ND |
| 2-Butanone | 31.29(600) | Butter, Sweet | ND | 3.21±0.08 | 4.21±0.80 | 1.46±0.16 | 0.38±0.01 | ND | ND | 1.49±0.08 | ND | ND |
| 1-Hydroxy-2-propanone | 37.11(648) | Sweet | ND | 0.22±0.01 | ND | ND | ND | ND | 0.20±0.05 | ND | 0.45±0.01 | 0.21±0.03 |
| 2-Pentanone | 40.37(675) | Fruity, Sweet | 0.47±0.07 | ND | ND | ND | 0.09±0.02 | ND | ND | 0.18±0.08 | 0.22±0.04 | ND |

| | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 3-Penten-2-one | 45.11(717) | - | ND | ND | ND | ND | ND | ND | ND | ND | ND | 0.10±0.13 |
| 2-Hexanone | 53.03(793) | Acetone, Fruity | ND | ND | ND | 0.04±0.04 | 1.06±0.62 | ND | ND | ND | ND | ND |
| 3-Hexen-2-one | 57.93(849) | - | ND | ND | ND | ND | ND | ND | 0.21±0.02 | ND | 0.33±0.01 | ND |
| δ-Hexalactone | 68.59(1,085) | Coconut, Creamy | ND | ND | ND | ND | ND | ND | ND | ND | ND | ND |
| 3-Nonen-2-one | 71.59(1,140) | Fruity | ND | ND | ND | ND | ND | 0.08±0.00 | 0.07±0.00 | ND | 0.09±0.01 | 0.06±0.01 |
| 2-Decanone | 75.28(1,201) | Citrus | 0.06±0.06 | ND | ND | ND | 0.26±0.09 | ND | ND | ND | ND | ND |
| δ-Octalactone | 79.91(1,288) | Coconut, Sweet | ND | ND | ND | ND | ND | ND | ND | 0.29±0.07 | ND | ND |
| **Furans(5)** | | | | | | | | | | | | |
| Furan | 24.71(493) | Etheral | ND | ND | ND | 0.27±0.18 | ND | ND | ND | ND | ND | 0.08±0.13 |
| 3-Methylfuran | 33.06(614) | - | 0.48±0.08 | 0.14±0.02 | ND | ND | ND | ND | ND | ND | ND | ND |
| 2-Ethylfuran | 42.45(693) | Burnt, Sweet | ND | 8.48±0.46 | 0.23±0.04 | ND | ND | 0.06±0.05 | ND | 2.98±0.33 | ND | 2.10±0.13 |
| Furfural | 55.82(824) | Almond, Sweet | 0.15±0.01 | 0.15±0.01 | ND | ND | ND | ND | ND | ND | ND | ND |
| 2-Butylfuran | 62.02(898) | Sweet | 1.32±0.19 | ND | ND | ND | ND | ND | ND | ND | ND | ND |
| **Sulfur-containing compounds(5)** | | | | | | | | | | | | |
| Methanethiol | 23.77(478) | Fishy | ND | ND | 0.08 | ND | 0.75 | ND | ND | ND | ND | ND |
| Thiophene | 40.41(676) | Sulfurous | ND | ND | 0.31±0.27 | 6.80±0.55 | ND | 0.77±0.09 | ND | 2.03±0.33 | ND | 1.60±0.18 |
| Butanethiol | 45.13(717) | Sulfurous | ND | ND | ND | ND | ND | ND | 0.19 | ND | ND | ND |
| 2-Methylthiophene | 50.84(772) | Sulfurous | ND | 0.45 | ND | 0.49 | ND | ND | ND | ND | ND | ND |

| | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Methional | 62.03(898) | Vegetable | ND | ND | ND | ND | ND | ND | 1.42 | ND | 1.11 | ND |

ASC:Asian_salmon and chicken, AS: Asian_salmon, AP: Asian_poultry, AF: Asian_fish, AC: Asian_chicken, IS:International_salmon, ITS:International_turkey and salmon, IS2:International_salmon, IS3:International_salmon, IS4: :International_salmon. Data represent the mean ± SD in triplicate. 1)RT: retention time 2)RI: retention indices 3)ND: not detected

**Supplementary Table S2** Volatile compounds of 10 dog foods using GC/MS

(ug/ g)

| **Volatile compounds** | **RT[1)] (min)** | **RI[2)]** | **I.D.[3)]** | **ASC** | **AS** | **AP** | **AF** | **AC** | **IS** | **ITS** | **IS2** | **IS3** | **IS4** |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| **Acids and esters(29)** | | | | | | | | | | | | | |
| Ethyl 3-hydroxydodecanoate | 6.79 | <800 | MS | ND[4)] | ND | ND | ND | ND | 0.06±0.01 | ND | ND | ND | ND |
| 2-Ethylhexyl acrylate | 7.02 | <800 | MS | ND | ND | 0.19±0.01 | ND | ND | ND | ND | ND | ND | ND |
| Heptanoic acid, 1-methylethyl ester | 7.55 | <800 | MS | ND | ND | ND | ND | ND | 0.84±0.01 | ND | ND | ND | ND |
| Hexanoic acid | 7.65 | <800 | MS | 0.41±0.01 | ND | ND | ND | ND | ND | 0.31±0.01 | 0.25±0.01 | ND | ND |
| Butanoic acid | 8.14 | 815 | MS | 2.32±0.01 | 0.57±0.01 | ND | 0.62±0.19 | ND | 1.18±0.20 | 1.17±0.36 | 1.34±0.76 | 0.90±0.57 | 0.97±0.88 |
| 3-Methylbutanoic acid | 9.59 | 860 | MS | ND | 0.22±0.01 | ND | 0.93±0.36 | ND | 0.25±0.01 | 0.36±0.02 | ND | 0.80±0.37 | 0.21±0.13 |
| Isovaleric acid | 9.77 | 865 | MS | ND | ND | ND | ND | ND | ND | ND | ND | ND | 0.51±0.01 |
| 2-Methyl octanoic acid | 10.07 | 873 | MS | ND | 0.29±0.18 | ND | ND | ND | ND | 0.52±0.01 | ND | ND | 1.52±0.01 |
| 2-Methyl butanoic acid | 10.09 | 874 | MS | ND | 0.26±0.01 | 0.31±0.09 | ND | ND | 0.85±0.01 | ND | ND | 1.30±0.31 | 0.60±0.01 |
| Pentanoic acid | 11.01 | 911 | MS/RI | ND | 0.55±0.01 | ND | 2.15±1.45 | ND | ND | 1.01±0.19 | 1.12±1.01 | ND | ND |

| | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Propyl-propanedioic acid | 11.11 | 901 | MS | ND | ND | ND | ND | ND | 1.03±0.01 | ND | ND | ND | ND |
| 2-Amino-4-methylbenzoic acid | 11.41 | 911 | MS | ND | ND | ND | ND | ND | ND | ND | ND | 0.41±0.01 | 1.08±0.01 |
| 4-Methyl-pentanoic acid | 12.87 | 956 | MS | 0.09±0.01 | ND | 0.29±0.01 | ND | ND | ND | ND | ND | ND | 0.175±0.01 |
| Octyl chloroformate | 13.53 | 975 | MS | ND | ND | 1.07±0.01 | ND | ND | ND | ND | ND | ND | ND |
| Heptanoic acid | 14.08 | 991 | MS | 1.14±0.01 | 0.32±0.01 | 0.28±0.01 | 0.26±0.01 | ND | 1.51±1.15 | ND | 0.83±0.18 | ND | 0.17±0.01 |
| Sobutyl octyl carbonate | 15.26 | 1028 | MS | ND | ND | ND | ND | ND | ND | ND | 1.66±0.01 | ND | ND |
| Oxalic acid, 2-ethylhexyl isobutyl ester | 15.63 | 1040 | MS | ND | ND | 3.46±0.01 | ND | ND | ND | ND | ND | ND | ND |
| Decan-2-yl 2-methylbutanoate | 16.2 | 1058 | MS | ND | ND | ND | ND | ND | 0.30±0.01 | ND | ND | ND | ND |
| 2,4-Hexadienedioic acid | 16.81 | 1077 | MS | ND | ND | 1.17±0.92 | ND | ND | ND | ND | ND | ND | ND |
| Sorbic acid | 16.86 | 1079 | MS | ND | ND | 1.36±0.01 | ND | ND | ND | ND | ND | ND | ND |
| Heptanoic acid, ethyl ester | 17.55 | 1099 | MS | 0.33±0.05 | ND | ND | ND | ND | ND | ND | ND | ND | ND |
| Pentadecyl chloroacetate | 17.84 | 1110 | MS | ND | 0.25±0.01 | ND | ND | ND | ND | ND | ND | ND | ND |
| Octanoic acid | 19.69 | 1173 | MS | 0.22±0.01 | ND | ND | ND | ND | ND | 0.15±0.01 | 0.27±0.01 | ND | ND |
| Octanoic acid, ethyl ester | 20.41 | 1197 | MS | 1.17±0.01 | 0.58±0.29 | ND | ND | 0.13±0.01 | ND | ND | ND | ND | ND |

| | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Hexyl-2-methylbutyrate | 21.52 | 1238 | MS | ND | ND | ND | ND | ND | ND | 0.07±0.01 | ND | ND | ND |
| Hexanedioic acid, dimethyl ester | 21.73 | 1246 | MS | ND | ND | ND | ND | ND | ND | ND | 0.26±0.01 | ND | ND |
| Nonanoic acid | 22.3 | 1266 | MS | ND | ND | ND | ND | ND | ND | 0.08±0.01 | ND | ND | ND |
| Decanoic acid, ethyl ester | 25.68 | 1393 | MS | ND | 1.04±0.59 | 0.09±0.01 | 0.12±0.02 | 0.29±0.01 | ND | ND | 0.11±0.01 | ND | ND |
| Sulfurous acid, 2-propyl tridecyl ester | 25.77 | 1396 | MS | ND | ND | 0.07±0.01 | ND | ND | ND | ND | ND | ND | ND |
| **Alcohols(19)** | | | | | | | | | | | | | |
| Isoamyl alcohol | 6.09 | <800 | MS | 1.00±0.01 | ND | ND | ND | ND | ND | ND | ND | ND | ND |
| 1-Pentanol | 6.12 | <800 | MS | 0.81±0.64 | ND | 0.83±0.07 | ND | ND | ND | ND | ND | ND | ND |
| 1-Butoxy-2-propanol | 12.61 | 949 | MS | ND | ND | ND | ND | ND | ND | ND | ND | 0.65±0.05 | ND |
| Heptanol | 13.52 | 975 | MS | ND | ND | 1.17±0.01 | ND | ND | ND | ND | ND | ND | ND |
| 1-Octen-3-ol | 13.84 | 984 | MS | ND | 5.06±0.01 | 3.69±0.01 | ND | ND | ND | ND | ND | ND | ND |
| 1-Ethynylcyclopentanol | 15.52 | 1037 | MS | ND | 0.72±0.01 | ND | ND | ND | ND | ND | ND | ND | ND |
| 3,5-Octadien-2-ol | 15.74 | 1044 | MS | 0.50±0.01 | 1.23±0.01 | ND | ND | ND | ND | ND | ND | ND | ND |
| Cyclohexanol | 16.21 | 1059 | MS | 0.69±0.01 | ND | ND | ND | ND | ND | ND | ND | ND | ND |
| 1-Octanol | 16.7 | 1074 | MS | ND | 0.75±0.01 | ND | ND | ND | ND | ND | ND | ND | ND |
| 4-Cresol | 16.82 | 1077 | MS | ND | ND | ND | ND | ND | 0.34±0.05 | ND | ND | ND | ND |
| 9-Octadecen-1-ol | 18.72 | 1141 | MS | ND | ND | ND | ND | 0.05±0.01 | ND | ND | ND | ND | ND |

| | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 4-Terpineol | 19.94 | 1181 | MS | ND | ND | ND | ND | ND | ND | 0.23±0.01 | ND | ND | ND |
| 1-Dodecanethiol | 20.25 | 1191 | MS | ND | ND | ND | ND | ND | ND | 0.19±0.01 | ND | ND | ND |
| 1-Tetradecanol | 20.26 | 1192 | MS | ND | ND | ND | ND | ND | ND | ND | 0.04±0.01 | ND | ND |
| 2-Hexyl-1-octanol | 23.62 | 1314 | MS | 0.07±0.01 | ND | ND | ND | ND | ND | ND | ND | ND | ND |
| 2-Vinylguaiacol | 23.67 | 1316 | MS | ND | ND | ND | ND | ND | ND | ND | 0.23±0.16 | ND | ND |
| 2-Butyl-2,7-octadien-1-ol | 25.17 | 1374 | MS | ND | 0.11±0.09 | 0.08±0.01 | ND | ND | ND | ND | ND | ND | ND |
| 4-Benzene-1,2-diol | 25.93 | 1403 | MS | 0.04±0.01 | ND | ND | ND | ND | ND | ND | ND | ND | ND |
| *p*-Guaiacol | 27.97 | 1486 | MS | 0.03±0.01 | ND | ND | ND | ND | ND | ND | ND | ND | ND |
| 2,6-bis-*p*-Cresol | 27.59 | 1471 | MS | 0.03±0.01 | 0.29±0.18 | 0.18±0.03 | ND | ND | 0.11±0.02 | 0.18±0.01 | ND | ND | ND |
| **Aldehydes(17)** | | | | | | | | | | | | | |
| 3-Methyl-butanal | 4.41 | <800 | MS | 0.03±0.01 | 0.75±0.01 | 0.04±0.01 | ND | 0.29±0.01 | ND | ND | ND | ND | ND |
| Pentanal | 4.61 | <800 | MS | ND | 0.26±0.01 | ND | ND | ND | ND | ND | ND | ND | ND |
| 2-Pentenal | 6.57 | <800 | MS | ND | ND | ND | ND | ND | ND | ND | ND | ND | 0.07±0.01 |
| 3-Methoxy-propanal | 7.72 | <800 | MS | ND | ND | ND | ND | ND | ND | ND | 0.22±0.01 | ND | ND |
| Hexanal | 7.95 | 808 | MS/RI | ND | 18.26±16.62 | 46.21±1.76 | 3.42±0.01 | 4.60±0.94 | ND | ND | ND | ND | 4.71±1.61 |
| 3-Furaldehyde | 9.02 | 843 | MS | ND | ND | ND | ND | ND | ND | ND | 0.09±0.01 | ND | ND |
| 4-Hexenal | 9.78 | 865 | MS | 2.73±0.01 | ND | ND | ND | ND | ND | ND | ND | ND | ND |
| Heptanal | 11.27 | 906 | MS/RI | ND | 1.61±0.01 | ND | ND | ND | 0.77±0.01 | ND | ND | 0.66±0.01 | 0.85±0.60 |
| Benzaldehyde | 13.22 | 966 | MS/RI | 2.15±0.01 | 2.59±1.83 | 2.35±0.08 | 1.52±0.33 | 0.71±0.37 | ND | ND | 2.86±1.06 | 2.66±0.42 | 1.85±0.55 |

| | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Octanal | 14.59 | 1005 | MS/RI | 2.80±0.21 | 3.26±1.02 | 3.64±1.19 | ND | ND | ND | ND | ND | ND | ND |
| 2,4-Heptadienal | 14.83 | 1014 | MS | ND | ND | ND | ND | 1.87±0.04 | ND | ND | ND | ND | ND |
| Benzeneacetaldehyde | 15.9 | 1049 | MS | ND | 0.78±0.01 | ND | ND | ND | 0.35±0.01 | ND | 0.89±0.01 | ND | ND |
| Nonanal | 17.72 | 1105 | MS/RI | 1.98±0.28 | 2.47±1.11 | 3.65±1.13 | 1.00±0.20 | 1.25±0.01 | 0.73±0.18 | 0.80±0.02 | 1.44±0.49 | 0.71±0.24 | 9.49±11.61 |
| 2,5-bis-benzaldehyde | 17.99 | 1115 | MS | ND | ND | ND | ND | ND | ND | ND | ND | ND | 1.00±0.01 |
| Decanal | 20.67 | 1206 | MS/RI | 0.07±0.01 | ND | 0.10±0.01 | ND | ND | ND | ND | ND | ND | ND |
| *β*-Cyclocitral | 21.17 | 1225 | MS | 0.07±0.01 | ND | ND | ND | ND | 0.03±0.01 | 0.07±0.01 | ND | ND | ND |
| 2-Butyl-2-octenal | 25.17 | 1374 | MS | ND | ND | 0.07±0.01 | ND | ND | ND | ND | 0.09±0.01 | ND | ND |
| **Hydrocabons(67)** | | | | | | | | | | | | | |
| Methylbenzene | 6.99 | <800 | MS | ND | 12.44±6.65 | ND | 2.85±0.01 | ND | ND | 0.71±0.23 | ND | ND | 2.12±0.06 |
| 1,3,5-Cycloheptatriene | 7.15 | <800 | MS | ND | ND | ND | ND | ND | ND | 0.51±0.01 | 0.19±0.01 | ND | ND |
| Ethylbenzene | 9.93 | 870 | MS | ND | ND | ND | ND | 0.14±0.01 | ND | ND | ND | ND | ND |
| 4-Methyl-octane | 9.99 | 871 | MS | 1.95±0.83 | ND | ND | ND | ND | ND | ND | 0.22±0.01 | ND | ND |
| 1,4-Dimethylbenzene | 10.18 | 876 | MS | ND | ND | ND | 2.00±1.07 | ND | ND | ND | ND | ND | ND |
| 1,3-Dimethylbenzene | 10.26 | 879 | MS | ND | 1.47±0.01 | ND | 1.48±0.01 | ND | ND | ND | ND | ND | ND |
| Pulegone | 11.64 | 918 | MS | ND | ND | 0.76±0.01 | ND | ND | ND | ND | ND | ND | ND |
| Sulfonylbis-methane | 11.81 | 924 | MS | ND | ND | ND | ND | 0.83±0.01 | ND | ND | ND | ND | ND |

| | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| *trans*-Ocimene | 12.34 | 940 | MS | ND | ND | ND | ND | 0.03±0.01 | ND | ND | ND | ND | ND |
| $\alpha$-Pinene | 12.33 | 941 | MS | ND | ND | ND | ND | ND | 0.40±0.09 | 0.35±0.19 | ND | 0.57±0.06 | 0.37±0.01 |
| 1,2,3-Trimethylcyclopentane | 13.54 | 976 | MS | ND | 2.42±0.92 | ND | ND | ND | ND | ND | ND | ND | ND |
| 2-Decene | 13.65 | 979 | MS | ND | ND | ND | 0.46±0.01 | ND | ND | ND | ND | ND | ND |
| Fucose | 14.01 | 989 | MS | ND | ND | 0.76±0.01 | ND | ND | ND | ND | ND | ND | ND |
| 2,2,4,6,6-Pentamethylheptan | 14.18 | 993 | MS | ND | ND | ND | ND | ND | ND | ND | ND | 4.60±0.01 | 5.83±0.01 |
| 2,2-Dimethyltetradecane | 15.23 | 1027 | MS | ND | ND | ND | ND | ND | ND | 1.40±0.07 | ND | ND | 1.96±0.69 |
| 1-Ethyl-2,4-dimethylbenzene | 15.31 | 1030 | MS | ND | 0.35±0.01 | ND | ND | ND | ND | ND | ND | ND | ND |
| 3-Methyloctane | 15.38 | 1032 | MS | ND | ND | ND | 0.93±0.01 | ND | ND | ND | ND | ND | ND |
| 2,5-Dimethylheptane | 15.4 | 1033 | MS | ND | ND | 1.53±0.01 | ND | ND | ND | ND | ND | ND | ND |
| Limonene | 15.44 | 1034 | MS/RI | ND | ND | ND | ND | ND | 0.53±0.13 | ND | ND | ND | ND |
| 2,2,8-Trimethyldecane | 15.47 | 1035 | MS | ND | ND | ND | ND | ND | ND | ND | 1.38±0.01 | ND | ND |
| 3-Ethyl-2-methyl-1,3-hexadiene | 15.5 | 1036 | MS | 0.69±0.01 | 1.10±0.01 | 0.75±0.01 | ND | ND | ND | ND | ND | ND | ND |
| 3,3-Dimethylhexane | 15.56 | 1038 | MS | ND | ND | ND | ND | ND | ND | ND | ND | ND | 3.48±0.01 |
| 2,6,10-Trimethyldodecane | 15.63 | 1040 | MS | ND | ND | 2.90±0.01 | ND | ND | ND | ND | ND | ND | ND |

| | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 5-Methyl-octadecane, | 15.9 | 1049 | MS | ND | ND | ND | 0.52±0.16 | ND | ND | ND | ND | ND | ND |
| Propyl-cyclopentane | 15.97 | 1051 | MS | ND | ND | ND | 0.06±0.01 | ND | ND | ND | ND | ND | ND |
| 6-Methyl-tridecane | 16.03 | 1053 | MS | ND | ND | ND | ND | ND | ND | ND | ND | ND | 0.24±0.01 |
| 2,6,8-Trimethyl-decane | 16.06 | 1054 | MS | ND | ND | 1.72±0.01 | ND | ND | ND | ND | ND | ND | ND |
| 5-Butylnonane | 16.09 | 1055 | MS | 0.49±0.01 | ND | ND | ND | ND | ND | ND | ND | ND | ND |
| 7,9-Dimethylhexadecane | 16.1 | 1055 | MS | ND | ND | ND | ND | ND | ND | ND | 0.52±0.01 | ND | ND |
| 2-Methyldecane | 16.19 | 1058 | MS | ND | ND | ND | 2.08±0.15 | ND | ND | 1.45±0.01 | 1.94±0.01 | ND | 1.90±0.01 |
| 2,3-Epoxyheptane | 16.21 | 1059 | MS | 0.68±0.01 | ND | ND | ND | ND | ND | ND | ND | ND | ND |
| 2,2,3,4-Tetramethylpentane | 16.27 | 1061 | MS | ND | ND | 0.58±0.01 | ND | ND | ND | ND | ND | ND | ND |
| 2,3,6-Trimethyldecane | 16.32 | 1062 | MS | ND | ND | ND | ND | ND | ND | ND | 3.56±0.01 | ND | ND |
| 3-Methylhexadecane | 16.48 | 1067 | MS | ND | ND | 0.49±0.01 | ND | ND | ND | ND | ND | ND | ND |
| 3,8-Dimethyldecane | 16.49 | 1068 | MS | ND | ND | ND | ND | ND | ND | ND | 2.96±0.01 | ND | ND |
| 5-Methyltridecane | 16.69 | 1074 | MS | ND | 1.41±0.01 | ND | 1.68±0.01 | ND | ND | ND | ND | ND | ND |
| 4,8-Dimethylundecane | 16.85 | 1078 | MS | ND | ND | ND | 1.86±0.01 | ND | ND | ND | ND | ND | ND |

| | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 2,8-Dimethyl-undecane | 16.87 | 1079 | MS | ND | ND | ND | ND | ND | ND | 1.44±0.03 | ND | ND | 2.88±1.49 |
| 7-Methylhexadecane | 17.04 | 1084 | MS | ND | ND | ND | 0.56±0.01 | ND | ND | ND | ND | ND | ND |
| 2,3,6,7-Tetramethyloctane | 17.11 | 1086 | MS | ND | ND | ND | ND | 0.90±0.01 | ND | ND | 2.00±0.01 | 2.08±0.01 | ND |
| 3-Ethyltetracosane | 17.17 | 1088 | MS | ND | ND | ND | ND | ND | ND | ND | ND | ND | 0.49±0.01 |
| 3,3-Dimethylhexane | 17.27 | 1091 | MS | ND | ND | ND | ND | 0.47±0.01 | ND | ND | 1.53±0.01 | ND | ND |
| 2-Methyldodecane | 17.56 | 1099 | MS | ND | ND | ND | 0.32±0.01 | ND | ND | ND | ND | ND | ND |
| 4-Methylundecane | 17.67 | 1103 | MS | ND | ND | ND | ND | ND | ND | ND | 4.46±0.90 | ND | ND |
| Dimethyl-4-aniline | 18 | 1115 | MS | ND | ND | ND | ND | ND | ND | ND | ND | 2.81±0.01 | ND |
| 1-Ethyl-3,5-dimethylbenzene | 18.24 | 1124 | MS | ND | ND | ND | 0.19±0.08 | ND | ND | ND | ND | ND | ND |
| 2,2,6-Trimethyldecane | 18.32 | 1127 | MS | ND | ND | ND | ND | ND | ND | ND | 0.47±0.01 | ND | ND |
| Tridecane | 18.41 | 1129 | MS | ND | ND | ND | ND | 0.30±0.01 | ND | ND | ND | 0.16±0.01 | ND |
| 2,3,5-Trimethyldecane | 18.88 | 1146 | MS | ND | ND | ND | ND | ND | ND | ND | ND | ND | 0.19±0.01 |
| 6,6-Diethylhoctadecane | 18.9 | 1147 | MS | ND | 0.03±0.01 | ND | ND | ND | ND | ND | ND | ND | ND |

| | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 2-Butyl-1-decene | 19.55 | 1169 | MS | ND | ND | ND | ND | ND | ND | ND | ND | ND | 0.14±0.01 |
| 3-Methyl-undecane | 19.65 | 1172 | MS | ND | 0.52±0.01 | ND | ND | ND | ND | ND | ND | ND | ND |
| 1-Tridecene | 20.25 | 1130 | MS | ND | ND | ND | ND | ND | ND | 0.20±0.01 | ND | ND | 0.29±0.01 |
| Dodecane | 20.47 | 1198 | MS/RI | ND | 0.49±0.23 | 0.49±0.04 | 0.12±0.03 | 0.45±0.01 | ND | ND | ND | 0.28±0.10 | 0.77±0.45 |
| 8-Methyl-heptadecane | 22.7 | 1280 | MS | 1.76±0.01 | ND | ND | ND | ND | ND | ND | ND | ND | ND |
| 1-Methyl-4-cyclohexane | 23.13 | 1295 | MS | ND | ND | ND | ND | ND | ND | 0.56±0.01 | ND | ND | ND |
| 2,4-Dimethyldecane | 23.21 | 1298 | MS | ND | ND | ND | ND | ND | ND | ND | 0.04±0.01 | ND | ND |
| 2-Methyldodecane | 23.28 | 1300 | MS | 0.34±0.01 | ND | ND | ND | ND | ND | ND | ND | ND | ND |
| 3,3-Dimethylhexane | 24.15 | 1335 | MS | 0.59±0.01 | ND | ND | ND | ND | ND | ND | ND | ND | ND |
| 2-Isopropenyl-*p*-cymene | 24.85 | 1362 | MS | 0.04±0.01 | ND | ND | ND | ND | ND | ND | ND | ND | ND |
| 3-Methylheneicosane | 25.04 | 1369 | MS | ND | 0.04±0.01 | ND | ND | ND | ND | ND | ND | ND | ND |
| Tetradecane | 25.77 | 1397 | MS/RI | ND | ND | ND | ND | 0.08±0.01 | ND | ND | 0.13±0.01 | ND | 0.16±0.01 |
| *trans*-Caryophyllene | 26.49 | 1426 | MS | ND | ND | ND | ND | ND | ND | 0.09±0.01 | ND | ND | ND |
| Tritetracontane | 28.02 | 1488 | MS | 0.05±0.01 | ND | ND | ND | ND | ND | ND | ND | ND | ND |
| 2,6,10-Trimethylpentadecane | 29.09 | 1533 | MS | ND | ND | ND | ND | ND | ND | ND | 0.03±0.01 | ND | ND |

| | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Hentriacontane | 29.18 | 1537 | MS | 0.14±0.01 | ND | ND | ND | ND | ND | ND | ND | ND | ND |
| Tetracosane | 29.41 | 1547 | MS | ND | ND | ND | ND | ND | ND | ND | 0.06±0.01 | ND | ND |
| **Heterocyclic compounds(21)** | | | | | | | | | | | | | |
| Trimethylamine | 2.16 | <800 | MS | ND | ND | ND | ND | ND | ND | ND | ND | 0.46±0.01 | ND |
| 1,2-Dimethylhydrazine | 3.72 | <800 | MS | ND | ND | ND | ND | ND | ND | ND | 0.23±0.15 | ND | ND |
| Ethyl-1,3-dithioisoindoline | 8.45 | 825 | MS | ND | 0.38±0.01 | ND | ND | ND | 4.87±0.01 | ND | ND | ND | ND |
| 3,5-Dimethylpyrazole | 9.1 | 845 | MS | 1.74±0.01 | ND | ND | ND | ND | ND | ND | ND | ND | ND |
| Methoxy-phenyl-oxime | 11.34 | 909 | MS | ND | ND | ND | ND | 4.07±0.01 | ND | ND | ND | ND | ND |
| 2,5-Dimethylpyrazine | 11.57 | 916 | MS | ND | ND | ND | ND | ND | 0.74±0.01 | ND | ND | ND | ND |
| 2,6-Dimethylpyrazine | 11.6 | 917 | MS | 0.70±0.01 | 1.27±0.84 | 0.57±0.01 | ND | ND | 0.17±0.01 | ND | ND | ND | ND |
| 1-Nonyne | 15.23 | 1027 | MS | ND | ND | ND | ND | ND | 0.34±0.01 | ND | ND | ND | ND |
| Phytane | 15.72 | 1043 | MS | ND | ND | ND | 0.89±00.01 | ND | ND | ND | ND | ND | 2.09±0.01 |
| 2-Acetylpyrrole | 16.4 | 1065 | MS | ND | ND | ND | ND | ND | 0.09±0.01 | ND | ND | 0.37±0.10 | ND |
| 2,6-Diethylpyrazine | 16.95 | 1081 | MS | ND | ND | ND | ND | ND | ND | ND | ND | 0.91±0.14 | ND |

| | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 2-Ethyl-3,5-dimethyl-pyrazine | 16.97 | 1082 | MS | 1.16±0.08 | 0.89±0.28 | 1.03±0.01 | 1.22±0.31 | 0.65±0.01 | 0.49±0.08 | ND | ND | ND | ND |
| Tetramethyl-pyrazine | 17.21 | 1089 | MS | ND | 1.38±0.44 | ND | ND | ND | ND | ND | ND | ND | ND |
| 3-Methyl-1H-indazole | 17.58 | 1100 | MS | ND | ND | ND | ND | ND | 0.16±0.01 | ND | ND | ND | ND |
| 2-Droxybenzylpyrrole | 17.9 | 1112 | MS | 2.83±0.01 | ND | 1.31±0.01 | ND | ND | ND | ND | 0.67±0.01 | ND | ND |
| Maltol | 17.94 | 1113 | MS | ND | ND | ND | ND | ND | ND | ND | ND | 0.35±0.01 | ND |
| 2-3-Indole | 19 | 1151 | MS | 0.14±0.01 | 0.25±0.01 | ND | ND | ND | 0.23±0.01 | ND | 0.39±0.01 | 0.26±0.01 | ND |
| Hexadecylene oxide | 20.66 | 1205 | MS | ND | 0.06±0.01 | ND | ND | ND | ND | ND | ND | ND | ND |
| 1-2-Pyrrolidon | 20.86 | 1213 | MS | ND | ND | ND | ND | ND | ND | ND | ND | ND | 0.12±0.01 |
| Butylhydroxyanisole | 27.96 | 1486 | MS | ND | 0.07±0.05 | ND | 0.42±0.01 | ND | ND | ND | 0.72±0.58 | ND | 0.11±0.01 |
| Dihydroactinidiolide | 29.13 | 1535 | MS | ND | ND | ND | ND | ND | 0.04±0.01 | ND | ND | ND | ND |
| **Ketones(18)** | | | | | | | | | | | | | |
| 2-Heptanone | 10.95 | 897 | MS | ND | ND | 0.03±0.03 | ND | 0.80±0.32 | ND | ND | ND | ND | ND |
| Dimethyl sulfone | 11.83 | 924 | MS/RI | ND | ND | ND | ND | 0.73±0.01 | ND | ND | ND | ND | ND |
| 4,4-Dimethylcyclohexan-1-one | 13.54 | 976 | MS | 0.86±0.01 | ND | ND | ND | ND | ND | ND | ND | ND | ND |
| 2,3-Octanedione | 14.01 | 988 | MS | ND | 1.81±0.01 | ND | ND | ND | ND | ND | ND | ND | ND |
| 6-Methyl-5-hepten-2-one | 14.06 | 990 | MS | ND | ND | ND | ND | ND | ND | ND | ND | ND | 2.03±0.01 |
| 3-Octen-2-one | 15.72 | 1043 | MS/RI | 0.54±0.01 | 0.80±0.01 | 1.24±0.01 | ND | ND | ND | ND | ND | ND | ND |

| | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| $\gamma$-Hexalactone | 16.22 | 1059 | MS | ND | 0.82±0.22 | ND | ND | ND | ND | ND | ND | ND | ND |
| 1-Phenylethanone | 16.6 | 1071 | MS | ND | ND | ND | ND | 0.62±0.01 | ND | ND | ND | ND | ND |
| 3,5-Octadiene-2-one | 16.71 | 1074 | MS | ND | ND | ND | ND | 5.83±2.17 | 0.86±0.21 | 3.14±0.12 | ND | ND | ND |
| 2-Nonanone | 17.36 | 1094 | MS | 0.62±0.05 | 1.22±0.77 | ND | ND | ND | ND | ND | ND | ND | ND |
| 5-Methyl-2-cyclohexanone | 19.57 | 1169 | MS | ND | ND | ND | ND | ND | ND | 2.08±0.01 | ND | ND | ND |
| 2-Piperidinone | 19.81 | 1177 | MS | ND | 0.24±0.01 | ND | 0.17±0.07 | ND | ND | ND | ND | 1.46±0.44 | 0.29±0.20 |
| 2-Decanone | 20.3 | 1193 | MS | 0.34±0.08 | ND | ND | 0.10±0.01 | ND | ND | ND | 0.25±0.15 | ND | ND |
| *tert*-Butyl-*p*-benzoquinone | 20.6 | 1203 | MS | ND | ND | ND | ND | ND | 0.84±0.01 | ND | ND | ND | ND |
| Chrysanthenone | 20.88 | 1214 | MS | ND | 0.30±0.01 | ND | ND | ND | ND | ND | ND | ND | ND |
| Carvone | 21.8 | 1248 | MS | ND | ND | ND | ND | ND | ND | 0.28±0.01 | ND | ND | ND |
| 3-Butyl-2-cyclohexen-1-one | 22.41 | 1270 | MS | 0.07±0.01 | ND | ND | ND | ND | ND | ND | ND | ND | ND |
| 2,5-Dimethyl-crotonophenone | 24.83 | 1361 | MS | ND | ND | 0.03±0.01 | ND | ND | ND | ND | ND | ND | ND |
| **Furans(7)** | | | | | | | | | | | | | |
| 2,5-Dimethylfuran | 9.06 | 844 | MS | 1.18±0.01 | ND | ND | ND | ND | ND | ND | 0.92±0.01 | ND | ND |
| 2-Furancarboxaldehyde | 9.08 | 845 | MS | 0.97±0.01 | ND | ND | 0.44±0.01 | ND | ND | ND | 0.31±0.08 | ND | ND |
| Furfural | 9.15 | 847 | MS | 1.30±0.01 | ND | ND | ND | ND | ND | ND | 0.20±0.01 | ND | ND |

| | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 2-Furanmethanol | 9.76 | 865 | MS | 5.18±0.23 | ND | ND | ND | ND | ND | ND | ND | ND | ND |
| 2-Pentylfuran | 14.22 | 994 | MS | 8.50±0.70 | 13.14±3.29 | 14.37±0.25 | 3.97±0.58 | 6.54±0.62 | 1.55±0.32 | 5.92±0.25 | 8.29±2.02 | ND | ND |
| 3-Methylbenzofuran | 17.58 | 1100 | MS | ND | ND | ND | ND | ND | 0.25±0.01 | ND | ND | ND | ND |
| 5-Heptyldihydro-2-furanone | 24.92 | 1365 | MS | 0.07±0.01 | ND | ND | ND | ND | ND | ND | ND | ND | ND |
| **Sulfur-containing compounds(2)** | | | | | | | | | | | | | |
| 1-Dodecanethiol | 20.25 | 1191 | MS | ND | ND | ND | ND | ND | ND | 0.19±0.01 | ND | ND | ND |
| 2-Formyl-3-methylthiophene | 18.27 | 1125 | MS | ND | ND | ND | ND | ND | ND | ND | ND | 0.41±0.01 | ND |

ASC: Asian_salmon and chicken, AS: Asian_salmon, AP: Asian_poultry, AF: Asian_fish, AC: Asian_chicken, IS: International_salmon, IST: International_turkey and salmon, IS2: International_salmon, IS3: International_salmon, IS4: International_salmon. Data represent the mean ± SD in triplicate.
1)RT: retention time 2)RI: retention indices 3)I.D.: identification 4)ND: not detected