*Supporting Information for*

# Development of Pretreatment Approaches for Authentic Representation of Tea Infusion Aroma

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**Table S1**. List of the 129 compounds information identified in tea infusion.

| No | Compounds | CAS | RI | | Relative content（ug/L） | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | cal | ref | D 30+30 | I 30+30 | D 30+45 | I 30+45 | dI 30+45 | D 60+60 | I 60+60 | dI 60+60 |
| 1 | Dimethyl ether | 115-10-6 | 654 | / | 1.432±0.052 | 1.395±0.153 | 1.219±0.075 | 0.988±0.308 | 0.465±0.363 | 0.263±0.082 | 0.247±0.042 | 0.628±0.391 |
| 2 | Propanal, 2-methyl- | 78-84-2 | 660 | 662 | 0.007±0.001 | 0.009±0.012 | 0.089±0.003 | 0.088±0.004 | 0.041±0.005 | 0.014±0.003 | 0.015±0.007 | 0.014±0.002 |
| 3 | Furan, 3-methyl- | 930-27-8 | 670 | 646 | 0.052±0.003 | 0.022±0.004 | 0.065±0.001 | 0.026±0.004 | 0.146±0.039 | 0.013±0.003 | 0.004±0.002 | 0.004±0.001 |
| 4 | Butanal, 3-methyl- | 590-86-3 | 682 | 669 | 0.411±0.027 | 0.25±0.023 | 0.674±0.018 | 0.461±0.188 | 0.416±0.114 | 0.034±0.003 | 0.049±0.014 | 0.018±0.002 |
| 5 | Benzene | 71-43-2 | 684 | 667 | 1.865±0.3 | 1.336±0.021 | 3.085±0.048 | 3.616±0.242 | 2.998±0.704 | 0.279±0.068 | 0.32±0.096 | 0.076±0.016 |
| 6 | Butanal, 2-methyl- | 96-17-3 | 684 | 681 | 0.134±0.01 | 0.072±0.014 | 0.217±0.009 | 0.117±0.018 | 0.626±0.103 | 0.013±0.002 | 0.036±0.009 | 0.01±0.004 |
| 7 | Pentanal | 110-62-3 | 699 | 690 | 0.884±0.053 | 0.724±0.097 | 0.17±0.001 | 0.149±0.028 | 0.265±0.021 | 0.059±0.012 | 0.15±0.064 | 0.208±0.086 |
| 8 | Furan, 2-ethyl- | 3208-16-0 | 699 | 702 | 0.819±0.134 | 0.188±0.006 | 0.472±0.027 | 0.536±0.047 | 0.639±0.034 | 0.08±0.009 | 0.196±0.089 | 0.145±0.048 |
| 9 | 2,4-Dimethylfuran | 3710-43-8 | 706 | 708 | 0.344±0.044 | 0.087±0.007 | 0.045±0.003 | 0.108±0.137 | 0.061±0.008 | 0.023±0.001 | 0.022±0.003 | 0.007±0.004 |
| 10 | 2-Butenal, 2-methyl- | 1115-11-3 | 724 | 744 | 0.018±0.009 | 0.011±0.002 | 0.016±0.006 | 0.015±0.001 | 0.012±0.004 | 0.03±0.006 | 0.03±0.006 | 0.021±0.003 |
| 11 | Toluene | 108-88-3 | 743 | 760 | 0.509±0.013 | 0.271±0.198 | 0.53±0.013 | 0.594±0.04 | 0.776±0.039 | 0.428±0.311 | 0.59±0.028 | 0.147±0.009 |
| 12 | 3-Hexanone, 2-methyl- | 7379-12-6 | 762 | 784 | 0.275±0.039 | 0.027±0.014 | 0.004±0.001 | 0.004±0.001 | 0.151±0.009 | 0.116±0.087 | 0.013±0.003 | 0.006±0.001 |
| 13 | Furan, 2-methoxy- | 25414-22-6 | 771 | / | 0.804±0.143 | 0.629±0.029 | 1.378±0.084 | 1.484±0.156 | 0.913±0.03 | 1.781±0.264 | 1.112±0.052 | 1.094±0.181 |
| 14 | Furan, 2-ethyl-5-methyl- | 1703-52-2 | 773 | 789 | 0.029±0.004 | 0.017±0.002 | 0.036±0.006 | 0.041±0.004 | 0.044±0.003 | 0.034±0.007 | 0.025±0.005 | 0.034±0.008 |
| 15 | Hexanal | 66-25-1 | 775 | 799 | 2.06±0.293 | 0.294±0.036 | 0.03±0.003 | 0.032±0.004 | 1.087±0.064 | 1.636±0.3 | 0.808±0.113 | 0.412±0.457 |
| 16 | 1H-Pyrrole, 3-ethyl- | 1551-16-2 | 784 | / | 0.361±0.164 | 0.157±0.01 | 0.459±0.038 | 0.459±0.031 | 0.324±0.023 | 0.31±0.234 | 0.232±0.027 | 0.258±0.113 |
| 17 | 2-Pentenal, 2-methyl- | 623-36-9 | 805 | 826 | 0.958±0.854 | 0.778±0.902 | 0.028±0.002 | 0.026±0.005 | 0.015±0.001 | 0.036±0.004 | 0.041±0.009 | 0.018±0.002 |
| 18 | 3-Hexen-1-ol, (E)- | 928-97-2 | 834 | 855 | 0.055±0.019 | 0.005±0.005 | 0.156±0.013 | 0.17±0.019 | 0.262±0.019 | 1.017±0.176 | 0.635±0.04 | 0.553±0.057 |
| 19 | Ethylbenzene | 100-41-4 | 837 | 860 | 0.213±0.004 | 0.351±0.028 | 0.141±0.004 | 0.164±0.015 | 0.063±0.003 | 0.081±0.016 | 0.05±0.005 | 0.051±0.007 |

| No | Compounds | CAS | RI | | Relative content（ug/L） | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | cal | ref | D 30+30 | I 30+30 | D 30+45 | I 30+45 | dI 30+45 | D 60+60 | I 60+60 | dI 60+60 |
| 20 | Benzene, 1,3-dimethyl- | 108-38-3 | 847 | 867 | 0.106±0.026 | 0.16±0.011 | 0.414±0.012 | 0.481±0.065 | 0.148±0.001 | 0.139±0.008 | 0.149±0.017 | 0.137±0.008 |
| 21 | (S)-(+)-3-Methyl-1-pentanol | 42072-39-9 | 851 | / | 0.005±0.002 | 0.004±0.002 | 0.046±0.004 | 0.047±0.002 | 0.057±0.008 | 0.223±0.007 | 0.119±0.021 | 0.112±0.021 |
| 22 | n-Butyl ether | 142-96-1 | 865 | 873 | 0.182±0.026 | 0.149±0.004 | 0.207±0.018 | 0.171±0.019 | 0.141±0.015 | 0.071±0.01 | 0.1±0.01 | 0.06±0.002 |
| 23 | 2-Heptanone | 110-43-0 | 873 | 892 | 0.02±0.002 | 0.022±0.001 | 0.05±0.004 | 0.054±0.002 | 0.064±0.004 | 0.156±0.018 | 0.136±0.023 | 0.09±0.005 |
| 24 | 2-n-Butyl furan | 4466-24-4 | 873 | 897 | 0.124±0.017 | 0.116±0.004 | 0.023±0.003 | 0.023±0.002 | 0.043±0.003 | 0.057±0.001 | 0.044±0.004 | 0.048±0.003 |
| 25 | 2-Propenoic acid, butyl ester | 141-32-2 | 882 | 892 | 0.22±0.028 | 0.195±0.009 | 0.262±0.012 | 0.217±0.023 | 0.164±0.01 | 0.26±0.033 | 0.215±0.018 | 0.16±0.002 |
| 26 | Heptanal | 111-71-7 | 888 | 903 | 0.384±0.046 | 0.349±0.003 | 0.504±0.024 | 0.415±0.036 | 0.725±0.053 | 1.665±0.129 | 0.932±0.055 | 0.984±0.018 |
| 27 | Propanoic acid, butyl ester | 590-01-2 | 896 | 900 | 0.001±0.001 | 0.002±0.001 | 0.222±0.01 | 0.183±0.018 | 0.068±0.003 | 0.085±0.023 | 0.064±0.004 | 0.053±0.008 |
| 28 | 2,3,4-Trimethylpyrrole | 3855-78-5 | 908 | / | 0.031±0.001 | 0.015±0.002 | 0.085±0.009 | 0.08±0.006 | 0.048±0.009 | 0.116±0.03 | 0.101±0.013 | 0.087±0.005 |
| 29 | Hexanoic acid, methyl ester | 106-70-7 | 914 | 929 | 0.001±0.001 | 0.001±0.001 | 0.091±0.008 | 0.091±0.003 | 0.015±0.002 | 0.024±0.004 | 0.025±0.004 | 0.016±0.001 |
| 30 | Hexanal, 3,3-dimethyl- | 55320-57-5 | 939 | / | 0.002±0.001 | 0.001±0.002 | 0.01±0.001 | 0.009±0.001 | 0.012±0.002 | 0.013±0.002 | 0.014±0.002 | 0.009±0.001 |
| 31 | Benzene, propyl- | 103-65-1 | 945 | 950 | 0.005±0.001 | 0.005±0.002 | 0.011±0.002 | 0.015±0.001 | 0.008±0.002 | 0.033±0.005 | 0.039±0.012 | 0.015±0.006 |
| 32 | 2-Heptanone, 6-methyl- | 928-68-7 | 948 | 954 | 0.005±0.001 | 0.004±0.002 | 0.01±0.001 | 0.01±0.001 | 0.011±0.002 | 0.023±0.002 | 0.023±0.003 | 0.018±0.002 |
| 33 | Benzaldehyde | 100-52-7 | 955 | 960 | 0.026±0.023 | 0.031±0.006 | 0.169±0.016 | 0.173±0.001 | 0.13±0.013 | 0.773±0.094 | 0.503±0.014 | 0.694±0.071 |
| 34 | Benzene, 1,2,4-trimethyl- | 95-63-6 | 955 | 968 | 0.048±0.001 | 0.031±0.006 | 0.013±0.002 | 0.017±0.005 | 0.01±0.002 | 0.898±0.161 | 0.489±0.036 | 0.621±0.061 |
| 35 | 1-Heptanol | 111-70-6 | 969 | 970 | 0.004±0.002 | 0.003±0.001 | 0.005±0.002 | 0.004±0.001 | 0.008±0.002 | 0.054±0.008 | 0.051±0.009 | 0.056±0.005 |
| 36 | 1-Octen-3-ol | 3391-86-4 | 980 | 978 | 0.036±0.033 | 0.002±0.001 | 0.047±0.007 | 0.041±0.005 | 0.059±0.01 | 0.587±0.103 | 0.42±0.052 | 0.381±0.055 |
| 37 | Tetraethyl silicate | 78-10-4 | 984 | / | 0.001±0.001 | 0.001±0.001 | 0.084±0.007 | 0.086±0.006 | 0.025±0.005 | 1.679±0.146 | 0.045±0.008 | 0.039±0.002 |

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|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | cal | ref | D 30+30 | I 30+30 | D 30+45 | I 30+45 | dI 30+45 | D 60+60 | I 60+60 | dI 60+60 |
| 38 | Butanoic acid, butyl ester | 109-21-7 | 998 | 994 | 0.001±0.001 | 0.001±0.001 | 0.004±0.001 | 0.003±0.001 | 0.046±0.005 | 0.084±0.012 | 0.072±0.007 | 0.083±0.008 |
| 39 | Hexanoic acid, ethyl ester | 123-66-0 | 1002 | 1001 | 0.001±0.001 | 0.001±0.001 | 0.03±0.004 | 0.029±0.003 | 0.042±0.01 | 0.085±0.013 | 0.109±0.066 | 0.092±0.01 |
| 40 | Octanal | 124-13-0 | 1006 | 1004 | 0.001±0.001 | 0.001±0.001 | 0.07±0.006 | 0.054±0.011 | 0.14±0.009 | 0.55±0.009 | 0.32±0.019 | 0.357±0.041 |
| 41 | 2,4-Heptadienal, (E,E)- | 4313-03-5 | 1014 | 1022 | 0.002±0.001 | 0.001±0.001 | 0.072±0.003 | 0.086±0.01 | 0.025±0.003 | 0.294±0.042 | 0.176±0.018 | 0.275±0.015 |
| 42 | Acetic acid, hexyl ester | 142-92-7 | 1017 | 1018 | 0.001±0.001 | 0.002±0.001 | 0.008±0.001 | 0.008±0.001 | 0.011±0.002 | 0.047±0.011 | 0.026±0.004 | 0.023±0.003 |
| 43 | 1,3-Cyclohexadiene, 1-methyl-4-(1-methylethyl)- | 99-86-5 | 1019 | 1018 | 0.006±0.001 | 0.003±0.001 | 0.009±0.001 | 0.008±0.001 | 0.008±0.002 | 0.043±0.007 | 0.04±0.003 | 0.021±0.001 |
| 44 | 2-Hexen-1-ol, acetate, (E)- | 2497-18-9 | 1009 | 1010 | 0.008±0.002 | 0.003±0.001 | 0.806±0.026 | 0.962±0.105 | 2.053±0.22 | 6.599±0.697 | 4.642±0.375 | 5.486±0.286 |
| 45 | D-Limonene | 5989-27-5 | 1033 | 1025 | 0.006±0.001 | 0.005±0.001 | 0.074±0.007 | 0.078±0.009 | 0.088±0.019 | 0.565±0.022 | 0.216±0.023 | 0.379±0.098 |
| 46 | 1-Hexanol, 2-ethyl- | 104-76-7 | 1035 | 1031 | 0.005±0.002 | 0.005±0.004 | 0.011±0.003 | 0.03±0.007 | 0.012±0.003 | 0.147±0.016 | 0.13±0.027 | 0.067±0.003 |
| 47 | Benzeneethanol, .beta.-ethenyl- | 6052-63-7 | 1036 | / | 0.001±0.001 | 0.001±0.001 | 0.005±0.002 | 0.006±0.002 | 0.009±0.002 | 0.017±0.002 | 0.015±0.004 | 0.021±0.002 |
| 48 | Benzene, iodo- | 591-50-4 | 1037 | 1033 | 0.001±0.001 | 0.001±0.001 | 0.013±0.001 | 0.004±0.002 | 0.002±0.001 | 0.003±0.002 | 0.006±0.002 | 0.004±0.001 |
| 49 | Cyclohexanone, 2,2,6-trimethyl- | 2408-37-9 | 1039 | 1035 | 0.027±0.005 | 0.008±0.001 | 0.05±0.004 | 0.05±0.002 | 0.037±0.004 | 0.083±0.017 | 0.094±0.013 | 0.091±0.008 |
| 50 | 2,4,6-Trimethyl-1,3,6-heptatriene | 24648-33-7 | 1042 | / | 0.006±0.002 | 0.005±0.001 | 0.013±0.002 | 0.013±0.001 | 0.015±0.003 | 0.059±0.009 | 0.119±0.011 | 0.05±0.005 |
| 51 | 3-Octen-2-one | 1669-44-9 | 1044 | 1036 | 0.004±0.001 | 0.003±0.002 | 0.005±0.001 | 0.005±0.001 | 0.004±0.002 | 0.033±0.013 | 0.037±0.01 | 0.029±0.006 |
| 52 | Benzeneacetaldehyde | 122-78-1 | 1049 | 1042 | 0.007±0.001 | 0.004±0.002 | 0.253±0.031 | 0.191±0.01 | 0.052±0.015 | 1.138±0.158 | 1.389±0.246 | 1.089±0.12 |

| No | Compounds | CAS | RI | | Relative content（ug/L） | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | cal | ref | D 30+30 | I 30+30 | D 30+45 | I 30+45 | dI 30+45 | D 60+60 | I 60+60 | dI 60+60 |
| 53 | 3-Formyl-4,5-dimethyl-pyrrole | 1000145-89-7 | 1053 | / | 0.002±0.002 | 0.001±0.001 | 0.158±0.017 | 0.148±0.01 | 0.135±0.018 | 1.182±0.266 | 0.669±0.018 | 0.971±0.009 |
| 54 | β-Ocimene | 13877-91-3 | 1054 | 1031 | 0.007±0.002 | 0.005±0.001 | 0.047±0.003 | 0.046±0.003 | 0.124±0.011 | 0.268±0.024 | 0.264±0.019 | 0.236±0.01 |
| 55 | 4-Undecene, 3-methyl-, (Z)- | 74645-87-7 | 1066 | / | 0.058±0.054 | 0.092±0.02 | 0.004±0.002 | 0.003±0.001 | 0.008±0.001 | 0.083±0.013 | 0.044±0.002 | 0.055±0.002 |
| 56 | Decane, 4-methyl- | 2847-72-5 | 1069 | 1060 | 0.064±0.014 | 0.042±0.007 | 0.003±0.001 | 0.002±0.001 | 0.005±0.001 | 0.012±0.001 | 0.013±0.004 | 0.011±0.003 |
| 57 | Formic acid, octyl ester | 112-32-3 | 1082 | 1109 | 0.115±0.022 | 0.126±0.008 | 0.021±0.007 | 0.016±0.003 | 0.048±0.006 | 0.866±0.077 | 0.361±0.283 | 0.627±0.041 |
| 58 | Benzene, 2-ethyl-1,4-dimethyl- | 1758-88-9 | 1083 | 1072 | 0.006±0.001 | 0.004±0.001 | 0.006±0.001 | 0.007±0.001 | 0.008±0.002 | 0.022±0.006 | 0.02±0.008 | 0.018±0.001 |
| 59 | Pyrazine, 2,6-diethyl- | 13067-27-1 | 1086 | 1078 | 0.012±0.011 | 0.001±0.001 | 0.025±0.002 | 0.024±0.002 | 0.011±0.002 | 0.216±0.042 | 0.245±0.048 | 0.236±0.017 |
| 60 | Linalool | 78-70-6 | 1114 | 1104 | 0.001±0.001 | 0.001±0.001 | 0.32±0.029 | 0.337±0.033 | 0.439±0.019 | 5.621±0.686 | 4.634±0.51 | 4.499±0.122 |
| 61 | Nonanal | 124-19-6 | 1119 | 1109 | 0.003±0.001 | 0.001±0.001 | 0.264±0.042 | 0.206±0.043 | 0.425±0.014 | 1.986±0.075 | 1.321±0.064 | 1.573±0.027 |
| 62 | (E)-4,8-Dimethylnona-1,3,7-triene | 19945-61-0 | 1126 | 1116 | 0.003±0.001 | 0.001±0.001 | 0.037±0.002 | 0.037±0.002 | 0.129±0.014 | 0.14±0.012 | 0.167±0.014 | 0.178±0.01 |
| 63 | Benzene, 1,2,3,5-tetramethyl- | 527-53-7 | 1130 | 1123 | 0.001±0.001 | 0.001±0.001 | 0.014±0.001 | 0.017±0.002 | 0.017±0.001 | 0.033±0.005 | 0.035±0.002 | 0.034±0.002 |
| 64 | Benzene, 1,2-dichloro-4-methyl- | 95-75-0 | 1131 | 1125 | 0.001±0.001 | 0.001±0.001 | 0.004±0.001 | 0.006±0.002 | 0.005±0.001 | 0.011±0.001 | 0.011±0.002 | 0.011±0.001 |
| 65 | 2,4,6-Octatriene, 2,6-dimethyl- | 673-84-7 | 1141 | 1119 | 0.006±0.001 | 0.003±0.003 | 0.005±0.001 | 0.005±0.001 | 0.006±0.001 | 0.033±0.004 | 0.04±0.004 | 0.017±0.001 |
| 66 | 1,3,8-p-Menthatriene | 18368-95-1 | 1143 | 1118 | 0.001±0.001 | 0.001±0.001 | 0.004±0.001 | 0.004±0.001 | 0.008±0.001 | 0.038±0.003 | 0.038±0.003 | 0.032±0.005 |
| 67 | (R,S)-5-Ethyl-6-methyl-3E-hepten-2-one | 57283-79-1 | 1155 | 1143 | 0.001±0.001 | 0.001±0.001 | 0.01±0.002 | 0.009±0.001 | 0.009±0.001 | 0.07±0.008 | 0.059±0.004 | 0.067±0.002 |

| No | Compounds | CAS | RI | | Relative content（ug/L） | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | cal | ref | D 30+30 | I 30+30 | D 30+45 | I 30+45 | dI 30+45 | D 60+60 | I 60+60 | dI 60+60 |
| 68 | cis-3-Hexenyl iso-butyrate | 41519-23-7 | 1157 | 1142 | 0.06±0.004 | 0.044±0.012 | 0.012±0.002 | 0.013±0.002 | 0.035±0.004 | 0.136±0.01 | 0.112±0.011 | 0.123±0.002 |
| 69 | Pyrazine, 3,5-diethyl-2-methyl- | 18138-05-1 | 1168 | 1148 | 0.001±0.001 | 0.001±0.001 | 0.006±0.001 | 0.005±0.001 | 0.002±0.001 | 0.044±0.003 | 0.07±0.012 | 0.071±0.003 |
| 70 | 2-Nonenal, (E)- | 18829-56-6 | 1175 | 1165 | 0.001±0.001 | 0.001±0.001 | 0.002±0.001 | 0.002±0.001 | 0.004±0.002 | 0.101±0.008 | 0.047±0.005 | 0.068±0.003 |
| 71 | 1-Nonanol | 143-08-8 | 1187 | 1174 | 0.001±0.001 | 0.001±0.001 | 0.008±0.003 | 0.006±0.004 | 0.003±0.001 | 0.193±0.03 | 0.149±0.043 | 0.169±0.008 |
| 72 | 1,4-Benzenedicarboxaldehyde | 623-27-8 | 1188 | 1166 | 0.001±0.001 | 0.001±0.001 | 0.002±0.001 | 0.002±0.001 | 0.003±0.001 | 0.044±0.004 | 0.036±0.007 | 0.054±0.003 |
| 73 | (3R,6S)-2,2,6-Trimethyl-6-vinyltetrahydro-2H-pyran-3-ol | 39028-58-5 | 1190 | 1173 | 0.004±0.001 | 0.001±0.001 | 0.005±0.001 | 0.006±0.002 | 0.009±0.001 | 0.739±0.061 | 0.433±0.042 | 0.601±0.072 |
| 74 | Terpinen-4-ol | 562-74-3 | 1195 | 1185 | 0.001±0.001 | 0.001±0.001 | 0.002±0.001 | 0.002±0.001 | 0.001±0.001 | 0.034±0.006 | 0.019±0.001 | 0.023±0.002 |
| 75 | Naphthalene | 91-20-3 | 1196 | 1183 | 0.001±0.001 | 0.001±0.001 | 0.027±0.004 | 0.027±0.002 | 0.055±0.01 | 0.382±0.026 | 0.453±0.04 | 0.549±0.043 |
| 76 | Isophthalaldehyde | 626-19-7 | 1197 | / | 0.001±0.001 | 0.001±0.001 | 0.004±0.001 | 0.003±0.001 | 0.003±0.002 | 0.026±0.003 | 0.022±0.001 | 0.034±0.006 |
| 77 | Butanoic acid, 3-hexenyl ester, (E)- | 53398-84-8 | 1202 | 1185 | 0.06±0.016 | 0.021±0.008 | 0.75±0.108 | 0.846±0.164 | 2.367±0.141 | 9.832±0.332 | 9.107±0.911 | 9.623±0.211 |
| 78 | Methyl salicylate | 119-36-8 | 1205 | 1206 | 0.001±0.001 | 0.001±0.001 | 0.068±0.018 | 0.07±0.017 | 0.128±0.015 | 2.525±0.496 | 1.591±0.362 | 2.412±0.133 |
| 79 | α-Terpineol | 98-55-5 | 1210 | 1193 | 0.001±0.001 | 0.001±0.001 | 0.003±0.001 | 0.003±0.001 | 0.003±0.001 | 0.081±0.014 | 0.057±0.007 | 0.076±0.003 |
| 80 | Octanoic acid, ethyl ester | 106-32-1 | 1212 | 1197 | 0.006±0.006 | 0.002±0.003 | 0.008±0.003 | 0.011±0.007 | 0.008±0.001 | 0.064±0.009 | 0.178±0.021 | 0.04±0.006 |

| No | Compounds | CAS | RI | | Relative content（ug/L） | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | cal | ref | D 30+30 | I 30+30 | D 30+45 | I 30+45 | dI 30+45 | D 60+60 | I 60+60 | dI 60+60 |
| 81 | 1,3-Cyclohexadiene-1-carboxaldehyde, 2,6,6-trimethyl- | 116-26-7 | 1213 | 1198 | 0.006±0.001 | 0.004±0.001 | 0.041±0.005 | 0.041±0.003 | 0.027±0.004 | 0.282±0.045 | 0.213±0.014 | 0.245±0.005 |
| 82 | Dodecane | 112-40-3 | 1216 | 1200 | 0.031±0.011 | 0.037±0.006 | 0.009±0.004 | 0.065±0.057 | 0.043±0.062 | 1.66±0.544 | 1.061±0.101 | 0.069±0.018 |
| 83 | Decanal | 112-31-2 | 1222 | 1208 | 0.058±0.017 | 0.01±0.004 | 0.084±0.007 | 0.329±0.447 | 2.237±0.327 | 0.835±0.133 | 0.871±0.055 | 8.747±0.703 |
| 84 | 1-Cyclohexene-1-carboxaldehyde, 2,6,6-trimethyl- | 432-25-7 | 1233 | 1224 | 0.001±0.001 | 0.001±0.001 | 0.029±0.004 | 0.027±0.001 | 0.025±0.004 | 0.238±0.026 | 0.192±0.008 | 0.23±0.002 |
| 85 | 1-Phenyl-2-butanone | 1007-32-5 | 1237 | / | 0.001±0.001 | 0.001±0.001 | 0.012±0.001 | 0.005±0.005 | 0.002±0.001 | 0.336±0.036 | 0.139±0.019 | 0.302±0.076 |
| 86 | cis-3-Hexenyl-.alpha.-methylbutyrate | 53398-85-9 | 1245 | 1233 | 0.001±0.001 | 0.001±0.001 | 0.281±0.122 | 0.294±0.111 | 1.076±0.062 | 3.95±0.059 | 3.024±0.1 | 3.932±0.054 |
| 87 | 6-Undecanone | 927-49-1 | 1253 | 1249 | 0.001±0.001 | 0.001±0.001 | 0.007±0.002 | 0.006±0.002 | 0.01±0.002 | 0.51±0.077 | 0.377±0.02 | 0.514±0.029 |
| 88 | Benzene, 1,3-bis(1,1-dimethylethyl)- | 1014-60-4 | 1261 | 1249 | 0.001±0.001 | 0.001±0.001 | 0.001±0.001 | 0.002±0.001 | 0.001±0.001 | 0.003±0.001 | 0.024±0.004 | 0.003±0.001 |
| 89 | 2,6-Octadien-1-ol, 3,7-dimethyl-, (Z)- | 106-25-2 | 1265 | 1255 | 0.001±0.001 | 0.001±0.001 | 0.003±0.001 | 0.012±0.013 | 0.06±0.005 | 6.15±0.141 | 4.369±0.527 | 4.525±0.339 |
| 90 | 1-Cyclohexene-1-acetaldehyde, 2,6,6-trimethyl- | 472-66-2 | 1268 | 1253 | 0.001±0.001 | 0.001±0.001 | 0.008±0.002 | 0.008±0.001 | 0.007±0.001 | 0.046±0.002 | 0.046±0.005 | 0.052±0.005 |
| 91 | 2-Decenal, (E)- | 3913-81-3 | 1275 | 1268 | 0.001±0.001 | 0.001±0.001 | 0.001±0.001 | 0.001±0.001 | 0.002±0.001 | 0.048±0.003 | 0.025±0.002 | 0.035±0.003 |
| 92 | Citral | 5392-40-5 | 1265 | 1272 | 0.001±0.001 | 0.001±0.001 | 0.005±0.004 | 0.007±0.012 | 0.06±0.005 | 2.941±0.765 | 3.857±0.56 | 4.53±0.333 |
| 93 | 1-Decanol | 112-30-1 | 1285 | 1269 | 0.001±0.001 | 0.001±0.001 | 0.001±0.001 | 0.001±0.001 | 0.001±0.001 | 0.056±0.003 | 0.041±0.005 | 0.045±0.005 |

| No | Compounds | CAS | RI | | Relative content（ug/L） | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | cal | ref | D 30+30 | I 30+30 | D 30+45 | I 30+45 | dI 30+45 | D 60+60 | I 60+60 | dI 60+60 |
| 94 | n-Valeric acid cis-3-hexenyl ester | 35852-46-1 | 1295 | 1270 | 0.01±0.004 | 0.001±0.001 | 0.002±0.001 | 0.002±0.001 | 0.004±0.001 | 0.04±0.002 | 0.044±0.002 | 0.038±0.002 |
| 95 | Tridecane | 629-50-5 | 1309 | 1300 | 0.003±0.001 | 0.002±0.001 | 0.003±0.003 | 0.001±0.001 | 0.002±0.001 | 0.071±0.097 | 0.013±0.003 | 0.017±0.004 |
| 96 | Undecanal | 112-44-7 | 1315 | 1305 | 0.001±0.001 | 0.001±0.001 | 0.003±0.002 | 0.004±0.002 | 0.004±0.002 | 0.048±0.002 | 0.075±0.01 | 0.045±0.017 |
| 97 | (Z)-Hex-3-enyl (E)-2-methylbut-2-enoate | 1000373-73-0 | 1325 | / | 0.069±0.001 | 0.02±0.003 | 0.006±0.004 | 0.006±0.003 | 0.007±0.002 | 0.16±0.015 | 0.184±0.008 | 0.167±0.009 |
| 98 | 1, 1, 5-Trimethyl-1, 2-dihydronaphthalene | 1000357-25-8 | 1345 | / | 0.001±0.001 | 0.001±0.001 | 0.028±0.007 | 0.026±0.005 | 0.011±0.004 | 0.072±0.006 | 0.062±0.003 | 0.067±0.006 |
| 99 | Hexanoic acid, 3-hexenyl ester, (Z)- | 31501-11-8 | 1362 | 1369 | 0.071±0.001 | 0.026±0.002 | 0.05±0.043 | 0.151±0.019 | 1.597±0.073 | 7.643±0.256 | 6.009±0.317 | 7.772±1.084 |
| 100 | cis-3-Hexenyl cis-3-hexenoate | 61444-38-0 | 1363 | 1388 | 0.071±0.001 | 0.025±0.002 | 0.05±0.043 | 0.151±0.019 | 0.088±0.016 | 0.994±0.087 | 0.673±0.008 | 0.991±0.114 |
| 101 | 2-Cyclopenten-1-one, 3-methyl-2-(2-pentenyl)-, (Z)- | 488-10-8 | 1369 | 1389 | 0.001±0.001 | 0.001±0.001 | 0.005±0.002 | 0.005±0.001 | 0.022±0.006 | 1.415±0.182 | 1.736±0.284 | 2.045±0.29 |
| 102 | Tetradecane | 629-59-4 | 1373 | 1400 | 0.001±0.001 | 0.001±0.001 | 0.003±0.003 | 0.002±0.001 | 0.002±0.001 | 0.019±0.003 | 0.015±0.004 | 0.025±0.002 |
| 103 | 1H-3a,7-Methanoazulene, 2,3,4,7,8,8a-hexahydro-3,6,8,8-tetramethyl-, [3R-(3.alpha.,3a.beta.,7.beta.,8a.alpha.)]- | 469-61-4 | 1388 | 1416 | 0.001±0.001 | 0.001±0.001 | 0.001±0.001 | 0.002±0.001 | 0.001±0.001 | 0.03±0.009 | 0.049±0.014 | 0.03±0.008 |

| No | Compounds | CAS | RI | | Relative content（ug/L） | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | cal | ref | D 30+30 | I 30+30 | D 30+45 | I 30+45 | dI 30+45 | D 60+60 | I 60+60 | dI 60+60 |
| 104 | α-Ionone | 127-41-3 | 1394 | 1424 | 0.001±0.001 | 0.001±0.001 | 0.002±0.001 | 0.002±0.001 | 0.001±0.001 | 0.057±0.009 | 0.055±0.005 | 0.059±0.004 |
| 105 | 1H-3a,7-Methanoazulene, octahydro-3,8,8-trimethyl-6-methylene-, [3R-(3.alpha.,3a.beta.,7.beta.,8a.alpha.)]- | 546-28-1 | 1401 | 1428 | 0.001±0.001 | 0.001±0.001 | 0.001±0.001 | 0.001±0.001 | 0.001±0.001 | 0.137±0.168 | 0.043±0.011 | 0.032±0.014 |
| 106 | 5,9-Undecadien-2-one, 6,10-dimethyl-, (Z)- | 3879-26-3 | 1431 | 1427 | 0.001±0.001 | 0.001±0.001 | 0.001±0.001 | 0.001±0.001 | 0.001±0.001 | 0.213±0.021 | 0.097±0.01 | 0.152±0.034 |
| 107 | 2,5-Cyclohexadiene-1,4-dione, 2,6-bis(1,1-dimethylethyl)- | 719-22-2 | 1451 | 1472 | 0.001±0.001 | 0.001±0.001 | 0.001±0.001 | 0.005±0.003 | 0.001±0.001 | 0.002±0.002 | 0.046±0.019 | 0.001±0.001 |
| 108 | 1-Dodecanol | 112-53-8 | 1469 | 1471 | 0.001±0.001 | 0.001±0.001 | 0.001±0.001 | 0.001±0.001 | 0.001±0.001 | 0.042±0.014 | 0.055±0.04 | 0.03±0.004 |
| 109 | 3-Buten-2-one, 4-(2,6,6-trimethyl-1-cyclohexen-1-yl)- | 14901-07-6 | 1476 | 1491 | 0.001±0.001 | 0.001±0.001 | 0.007±0.003 | 0.007±0.003 | 0.007±0.001 | 0.604±0.07 | 0.525±0.014 | 0.633±0.024 |
| 110 | 2,4-Di-tert-butylphenol | 96-76-4 | 1511 | 1502 | 0.001±0.001 | 0.001±0.001 | 0.002±0.001 | 0.004±0.004 | 0.004±0.001 | 0.234±0.026 | 0.165±0.023 | 0.142±0.019 |
| 111 | Tridecanal | 10486-19-8 | 1517 | 1517 | 0.001±0.001 | 0.001±0.001 | 0.001±0.001 | 0.001±0.001 | 0.001±0.001 | 0.028±0.028 | 0.028±0.015 | 0.178±0.008 |
| 112 | Naphthalene, 1,2,4a,5,8,8a-hexahydro-4,7-dimethyl-1-(1- | 523-47-7 | 1529 | 1519 | 0.001±0.001 | 0.001±0.001 | 0.04±0.013 | 0.026±0.002 | 0.079±0.005 | 4.677±0.81 | 1.708±0.253 | 2.746±0.132 |

| No | Compounds | CAS | RI | | Relative content（ug/L） | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | cal | ref | D 30+30 | I 30+30 | D 30+45 | I 30+45 | dI 30+45 | D 60+60 | I 60+60 | dI 60+60 |
| | methylethyl)-, [1S-(1.alpha.,4a.beta.,8a.alpha.)]- | | | | | | | | | | | |
| 113 | Naphthalene, 1,2,3,4-tetrahydro-1,6-dimethyl-4-(1-methylethyl)-, (1S-cis)- | 483-77-2 | 1534 | 1519 | 0.001±0.001 | 0.001±0.001 | 0.06±0.014 | 0.057±0.005 | 0.128±0.047 | 5.659±0.548 | 2.267±0.067 | 3.582±0.624 |
| 114 | Naphthalene, 1,2,3,4,4a,7-hexahydro-1,6-dimethyl-4-(1-methylethyl)- | 16728-99-7 | 1547 | 1533 | 0.001±0.001 | 0.001±0.001 | 0.003±0.003 | 0.003±0.002 | 0.008±0.003 | 0.558±0.067 | 0.22±0.02 | 0.319±0.041 |
| 115 | 1,6,10-Dodecatrien-3-ol, 3,7,11-trimethyl- | 7212-44-4 | 1578 | 1558 | 0.001±0.001 | 0.001±0.001 | 0.001±0.001 | 0.001±0.001 | 0.002±0.002 | 0.183±0.02 | 0.268±0.084 | 0.142±0.038 |
| 116 | 4-Isopropyl-6-methyl-1-methylene-1,2,3,4-tetrahydronaphthalene | 50277-34-4 | 1583 | 1566 | 0.001±0.001 | 0.001±0.001 | 0.001±0.001 | 0.001±0.001 | 0.003±0.001 | 0.146±0.023 | 0.054±0.009 | 0.148±0.028 |
| 117 | 2,2,4-Trimethyl-1,3-pentanediol diisobutyrate | 6846-50-0 | 1608 | 1587 | 0.001±0.001 | 0.001±0.001 | 0.002±0.002 | 0.009±0.008 | 0.001±0.001 | 0.024±0.007 | 0.25±0.22 | 0.036±0.014 |
| 118 | Phenol, 2,4,6-tri-tert-butyl- | 732-26-3 | 1611 | / | 0.001±0.001 | 0.001±0.001 | 0.001±0.001 | 0.001±0.001 | 0.001±0.001 | 0.001±0.001 | 0.008±0.001 | 0.001±0.001 |
| 119 | Tetradecanal | 124-25-4 | 1641 | 1617 | 0.001±0.001 | 0.001±0.001 | 0.001±0.001 | 0.001±0.001 | 0.005±0.004 | 0.012±0.002 | 0.01±0.002 | 0.011±0.001 |
| 120 | Cedrol | 77-53-2 | 1641 | 1611 | 0.001±0.001 | 0.001±0.001 | 0.001±0.001 | 0.001±0.001 | 0.001±0.001 | 0.088±0.004 | 0.06±0.004 | 0.055±0.014 |

| No | Compounds | CAS | RI | | Relative content（ug/L） | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | cal | ref | D 30+30 | I 30+30 | D 30+45 | I 30+45 | dI 30+45 | D 60+60 | I 60+60 | dI 60+60 |
| 121 | α-Corocalene | 20129-39-9 | 1644 | 1623 | 0.001±0.001 | 0.001±0.001 | 0.001±0.001 | 0.001±0.001 | 0.002±0.001 | 0.211±0.038 | 0.077±0.014 | 0.125±0.016 |
| 122 | 2,6-Bis(1,1-dimethylethyl)-4-(1-oxopropyl)phenol | 14035-34-8 | 1647 | 1635 | 0.001±0.001 | 0.001±0.001 | 0.002±0.001 | 0.004±0.003 | 0.003±0.002 | 0.011±0.003 | 0.018±0.01 | 0.008±0.003 |
| 123 | Ylangenal | 41610-68-8 | 1666 | 1674 | 0.001±0.001 | 0.001±0.001 | 0.001±0.001 | 0.001±0.001 | 0.001±0 | 0.057±0.005 | 0.062±0.011 | 0.064±0.006 |
| 124 | Tetradecanoic acid, ethyl ester | 124-06-1 | 1813 | 1794 | | | 0.001±0.001 | 0.001±0.001 | 0.001±0.001 | 0.003±0.002 | 0.004±0.004 | 0.002±0.002 |
| 125 | Cyclopenta[g]-2-benzopyran, 1,3,4,6,7,8-hexahydro-4,6,6,7,8,8-hexamethyl- | 1222-05-5 | 1865 | 1850 | | | 0.001±0.001 | 0.001±0.001 | 0.001±0 | 0.017±0.005 | 0.014±0.002 | 0.016±0.003 |
| 126 | Phthalic acid, hept-4-yl isobutyl ester | 1000356-78-3 | 1875 | / | | | 0.003±0.004 | 0.009±0.007 | 0.002±0.001 | 0.708±0.046 | 0.664±0.009 | 0.5±0.012 |
| 127 | Nonadecane | 629-92-5 | 1908 | 1900 | | | 0.001±0.001 | 0.001±0.001 | 0.001±0.001 | 0.001±0.001 | 0.003±0.001 | 0.019±0.002 |
| 128 | Dibutyl phthalate | 84-74-2 | 1956 | 1970 | | | 0.001±0.001 | 0.003±0.002 | 0.003±0.001 | 0.353±0.406 | 0.406±0.06 | 0.201±0.146 |
| 129 | Hexadecanoic acid, ethyl ester | 628-97-7 | 1984 | 1994 | | | 0.001±0.001 | 0.001±0.001 | 0.001±0.001 | 0.009±0.001 | 0.002±0.001 | 0.002±0.001 |

Note: Retention index referred to the literature value was founded in the website: https://webbook.nist.gov/chemistry/. '/', the RI was not founded. blank, the compound was not detected in the sample. D = pure water; I = ionized water; dI = diluted ionized water. Numeric codes indicate: temperature + time. e.g., D 60+60= pure water, extraction at 60°C for 60 min. All extraction conditions employed a consistent tea-to-water ratio of 1g:10 mL.