

Table S6. Factor loading of principal component analysis

Compound name	PC1	PC2
Alanine	0.07095	0.116696
Arabinose	0.029039	-0.17644
Arabitol	0.122079	0.006097
Aspartic acid	0.049664	-0.16405
Citric acid + Isocitric acid	0.01807	-0.1785
Fructose	-0.04323	-0.15621
Galactose	0.0919	-0.08576
Glucose	-0.07981	-0.05768
Glutamic acid	0.112563	-0.06442
Glutamine	0.03524	0.095115
Glycerol	0.12379	0.022147
Glycine	0.080938	-0.12545
Histidine	0.099062	-0.06601
Inositol	0.106726	-0.05256
Isoleucine	0.108293	-0.07078
Lactic acid	-0.01034	0.140239
Leucine	0.100745	-0.08091
Lysine	0.101688	-0.03637
Malic acid	0.073435	-0.0903
Mannitol	0.048255	-0.14792
<i>meso</i> -Erythritol	0.107965	-0.04788
Methionine	0.097478	-0.04591
Ornithine	0.012709	0.174268
Phenylalanine	0.118549	-0.02674
Phosphate	0.084847	-0.07686
Proline	0.09384	-0.09916
Pyroglutamic acid	-0.08805	0.076659
Ribose	0.021316	-0.17748
Serine	0.07328	-0.14834
Succinic acid (or aldehyde)	0.124761	0.022929
Threonine	0.114305	-0.05709
Tryptophan	-0.12217	0.014092
Tyrosine	-0.05621	-0.15367
Valine	0.10395	-0.06726
Xylitol	0.073697	0.144908
Xylose	0.043191	-0.15142
( <i>R</i> )-Dihydro-3-hydroxy-4,4-dimethyl-2(3H)-furanone	0.047258	-0.14961
( <i>Z,Z</i> )-9,12-Octadecadienoic acid (Linoleic acid)	0.044974	-0.07467
1,2,3-Benzenetriol (Pyrogallol)	-0.01388	0.06685
1,4-Benzenediol	-0.03284	0.161787
1-Butanol	0.124785	0.01858
1-Hydroxy-2-butanone	0.124344	0.014419
1-Hydroxy-2-propanone (Acetol)	0.013415	-0.16943
1-Propanol	0.120242	0.041909
2-(4-Hydroxyphenyl)ethanol	0.121897	0.041195
2(5 <i>H</i> )-furanone	0.007597	-0.15296
2,3-Butanediol	0.12295	0.024854
2,5-Dimethyl-4-hydroxy-3(2 <i>H</i> )-furanone (HDMF)	-0.06712	0.142812
2-Acetylpyrrole	-0.10846	-0.0274
2-Butenoic acid	0.114162	0.005812
2-Furancarboxaldehyde (Furfural)	0.119887	-0.0044
2-Furanmethanol (Furfuryl alcohol)	0.106203	0.044028
2-Hydroxy-3-methyl-2-cyclopenten-1-one (Cyclotene)	0.051394	0.165339
2-Methoxy-4-vinylphenol (4-Vinylguaiacol)	-0.01403	0.137674
2-Methoxy-6-methyl-4-pyran-4-one	0.119139	0.044629
2-Methyl-1-propanol (Isobutyl alcohol)	0.11891	0.051572
2-Methyl-2-butenic acid	-0.10118	0.039553

Compound name	PC1	PC2
2-Methylbutanoic acid	-0.08563	0.06836
2-Methylpropanoic acid (Isobutyric acid)	-0.05589	0.102082
2-Phenylethyl alcohol	0.120988	0.042569
3-(Methylthio)-1-propanal (Methional)	-0.05857	-0.01292
3-(Methylthio)-1-propanol (Methionol)	0.121031	0.045426
3,5-Dihydroxy-6-methyl-2,3-dihydro-4H-pyran-4-one	-0.02822	-0.04624
3,5-Dimethyl-4-heptanone	0.122048	0.0307
3-Hydroxy-2-butanone (Acetoin)	0.122737	-0.01423
3-Hydroxy-2-methyl-4H-pyran-4-one (Maltol)	-0.0789	-0.00385
3-Methyl-1-butanol	0.119594	0.047177
3-Methyl-2(5H)-Furanone	0.124137	1.46E-02
3-Methylbutanoic acid (Isovaleric acid)	-0.09889	0.059962
4-Ethyl-2,6-dimethoxyphenol	-0.10645	0.039452
4-Hydroxy-5-methyl-furanone	-0.12263	-0.00169
4-Oxopentanoic acid (Levulinic acid)	-0.07004	-0.13794
5(or 2)-Ethyl-4-hydroxy-2(or 5)-methyl-3(2H)-furanone (HEMF)	0.122639	0.028782
5-Ethyl-2(3H)-furanone	0.124216	0.019749
5-Ethyldihydro-2(3H)-furanone ( <i>gamma</i> -hexalactone)	0.108717	0.069712
Acetic acid	0.000743	0.081498
Benzoic acid	-0.03399	0.023457
Butanoic acid (Butyric acid)	0.099416	0.078903
Caprolactam	0.024498	-0.07437
Dihydro-2(3H)-Furanone ( <i>gamma</i> -Butyrolactone)	0.076335	0.137946
Dihydro-5-methyl-2(3H)-furanone ( <i>gamma</i> -Valerolactone)	0.124144	0.005334
Ethyl hexadecanoate (Ethyl Palmitate)	0.10953	-0.03014
Ethyl lactate	0.049464	-0.07243
Hexanoic acid (Caproic acid)	-0.07261	0.104453
mono-Ethyl succinate	0.124635	0.007293
n-Hexadecanoic acid (Palmitic acid)	0.109079	0.04464
Phenylacetaldehyde	0.106924	0.014845
Phenylacetic acid	-0.04704	0.096495
(Z)-1,5-Octadien-3-ol	-0.02164	0.077065
(Z)-3,7-Dimethyl-2-octene	0.102428	0.012915
1-Octen-3-ol	-0.01147	0.033148
2,3-Butanedione (Diacetyl)	0.123014	0.008848
2,3-Pentanedione	0.085862	0.101063
2,6-Dimethyl-pyrazine	0.029803	0.090015
2-Butanone	0.092378	0.087972
2-Butenal	0.106234	-0.06947
2-Ethoxy-2-methyl-propane	-0.0061	0.064172
2-Methyl-1-butanol (Active amyl alcohol)	0.121634	0.047278
2-Methyl-2-propanol	0.042914	0.091648
2-Methyl-butanal (Valeraldehyde)	0.05729	-0.12194
2-Methylbutyl acetate	0.114534	0.057977
2-Methyl-furan	-0.06467	-0.11421
2-Methyl-propanal (Isobutyraldehyde)	0.062248	-0.07391
2-Methylpropyl acetate (Isobutyl acetate)	0.122567	0.038998
2-Pentanone	0.115203	0.020961
2-Propanol	0.006367	0.104228
2-Propanone (Acetone)	0.023809	-0.14477
3,4-Hexanedione	0.118863	0.053549
3-Methyl-2-butanone	-0.0483	0.022365
3-Methyl-butanal (Isovaleraldehyde)	0.113252	0.020986
3-Methylbutyl acetate (Isoamyl acetate)	0.118597	0.051922
3-Octanol	0.02099	0.120937
3-Octanone	0.107809	0.049073
Acetaldehyde	0.108228	0.078694
Benzaldehyde	0.057083	0.127513

Compound name	PC1	PC2
Butyl acetate	0.123668	0.003007
Dimethyl disulfide	0.094479	-0.01966
Ethyl 2-methylbutanoate	-0.09199	0.037996
Ethyl 2-methylpropanoate (Ethyl isobutyrate)	-0.02392	0.072501
Ethyl 3-methylbutanoate (Ethyl isovalerate)	-0.04547	0.061951
Ethyl benzoate	-0.00359	0.095967
Ethyl butanoate	0.024505	0.093588
Ethyl dodecanoate (Ethyl laurate)	0.057666	0.091387
Ethyl formate	-0.07608	0.073225
Ethyl heptanoate	0.034339	0.144364
Ethyl hexanoate (Ethyl caproate)	-0.0421	0.090202
Ethyl propionate	0.102052	0.066645
Furan	0.041983	0.041584
Methanethiol	-0.0407	0.10385
Methyl acetate	-0.03715	-0.02557
<i>n</i> -Propyl acetate	0.102561	0.064709