

Table S1: The numbers in the loading graphs of PCA represent the specific information of the compounds

number	compounds	number	compounds
1	ethyl caproate	58	2,6,10-trimethyldodecane
2	ethanol	59	methyl 2-(propanoylamino)benzoate
3	phenethyl alcohol	60	7,9-dimethyl-hexadecane
4	benzyl alcohol	61	1,3,5,7-cyclooctatetraene
5	decane	62	1-methyl-2-(3-methylpentyl)- cyclopropane
6	ethyl acetate	63	dihydroaplotaxene
7	ethyl pentadecanoate	64	decene
8	(R,R)-2,3-butanediol	65	ethyl butyrate
9	ethyl octadecanoate	66	eicosane
10	2,3-butanediol	67	2-furanmethanol
11	9,12-octadecadienoic acid ethyl ester	68	methallyl alcohol
12	ethyl myristate	69	crotonyl alcohol
13	2-phenyl-2-butenal	70	2-methylhexadecanoic acid
14	1,2-dimethoxybenzene	71	11,14-eicosadienoic acid
15	acetaldehyde	72	methacrolein
16	crotonaldehyde	73	2-vinyl-2-butenal
17	2-acetyl pyrrole	74	(E,E)-2,4-hexadienal
18	2,5-dimethyl-pyrazine	75	2-ethyl-5-methyl-pyridine
19	ethyl oleate	76	ethyl 5-amino-1,2,3-thiadiazole-4- carboxylate
20	styrene	77	3,5-dimethylpyrazole
21	phenol	78	methyl anthranilate
22	4,6-dimethyl-undecane	79	3,8-dimethyl-undecane
23	dibutyl terephthalate	80	2-ethyl-furan
24	methanethiol	81	ethyl lactate
25	ethyl isovalerate	82	isoamyl acetate
26	4-methylnonane	83	isobutyraldehyde
27	4,6-dimethyldodecane	84	isobutyl alcohol
28	isobutyric acid	85	2-pentylfuran
29	diethyl phthalate	86	furfural
30	2-pyrrolecarbaldehyde	87	isopentyl alcohol
31	ethyl isobutyrate	88	dodecane
32	2-methyl-pyrazine	89	ethyl (9E)-9-octadecenoate
33	4,6-dimethyl-pyrimidine	90	isopentyl formate
34	2,3-dimethyl-pyrazine	91	2,8-dimethylundecanoic acid methyl ester
35	trimethyl-pyrazine	92	11,14,17-eicosatrienoic acid
36	1,2-dimethyl-hydrazine	93	2,6-dimethyl-pyrazine
37	2,2,4,6,6-pentamethyl-heptane	94	2,6-dimethyl-heptadecane
38	2,2,11,11-tetramethyl-dodecane	95	2,5-dihydrofuran

39	pentadecane	96	caryophyllene
40	2,3,3-trimethyl-pentane	97	methyl hexadecanoate
41	2,3,4-trimethyl-hexane	98	diethyl succinate
42	( <i>E</i> )-2,3-epoxydecane	99	ethyl valerate
43	acetic acid	100	ethyl heptanoate
44	ethyl palmitate	101	1,1-dimethylcyclopropane
45	ethyl heptadecanoate	102	mequinol
46	2-butenal	103	hexyl formate
47	benzaldehyde	104	ethyl nonanoate
48	hexahydrofarnesylacetone	105	butyl isobutyl phthalate
49	ethyl linolenate	106	Linoleic alcohol
50	ethyl caprylate	107	phenylacetaldehyde
51	acetoin	108	3-methyl-2-(2-methyl-2-butenyl)-furan
52	isovaleraldehyde	109	dipentene
53	2-methyl-2,4-hexadiene	110	nonanoic acid
54	3-furanmethanol	111	dibutyl phthalate
55	ethyl laurate	112	octanoic acid
56	ethyl pentadec-9-enoate	113	4-hydroxy-2-butanone
57	2-butyloctanol	114	2,5-di-tert-butylphenol
		115	1-methyl-5-(1-methylethenyl)-cyclohexene

Table S2: Compounds represented by abscissa numbers and their VIP values in VIP plot

number	Var ID (Primary)	M2.VIP [5]	number	Var ID (Primary)	M2.VIP [5]
1	methacrolein	3.5692	58	methallyl alcohol	0.456093
2	ethyl palmitate	3.40473	59	isovaleraldehyde	0.449327
3	acetic acid	3.01936	60	2-pyrrolicarbaldehyde	0.448799
4	methyl hexadecanoate	2.86248	61	acetoin	0.444318
5	9,12-octadecadienoic acid ethyl ester	2.75584	62	butyl isobutyl phthalate	0.435967
6	2-butenal	2.69231	63	ethyl pentadecanoate	0.430486
7	ethanol	2.46809	64	ethyl nonanoate	0.428012
8	ethyl oleate	2.10399	65	2,5-ditertbutylphenol	0.418902
9	ethyl acetate	1.90072	66	ethyl octadecanoate	0.418039
10	phenethyl alcohol	1.88767	67	crotonyl alcohol	0.417726
11	2-ethyl-furan	1.66646	68	1,2- dimethoxybenzene	0.405447
12	acetaldehyde	1.63239	69	2-pentylfuran	0.391383
13	trimethyl-pyrazine	1.38892	70	2-ethyl-5-methyl- pyridine	0.384293
14	ethyl (9E)-9-octadecenoate	1.38705	71	ethyl linolenate	0.377197
15	(R,R)-2,3-butanediol	1.37848	72	hexyl formate	0.374109
16	ethyl caproate	1.33368	73	4,6-dimethyldodecane	0.367797

17	4-hydroxy-2-butanone	1.23432	74	ethyl isovalerate	0.366347
18	2,3-butanediol	1.18601	75	dipentene	0.362084
19	crotonaldehyde	1.09161	76	diethyl phthalate	0.341839
20	2-methyl-pyrazine	1.06549	77	4,6-dimethyl-undecane	0.332404
21	2-methyl-2,4-hexadiene	1.0309	78	ethyl heptanoate	0.322822
22	2-furanmethanol	1.02483	79	3-methyl-2-(2-methyl-2-butenyl)-furan	0.317123
23	2,2,4,6,6-pentamethyl-heptane	1.02267	80	7,9-dimethyl-hexadecane	0.303638
24	isobutyric acid	1.00276	81	isobutyl alcohol	0.282685
25	2-phenyl-2-butenal	0.965845	82	2,3,3-trimethyl-pentane	0.279388
26	dibutyl terephthalate	0.963231	83	1-methyl-5-(1-methylethenyl)-cyclohexene	0.275691
27	1,1-dimethylcyclopropane	0.962852	84	11,14-eicosadienoicacid	0.272222
28	ethyl caprylate	0.961584	85	phenol	0.266546
29	benzaldehyde	0.933607	86	decane	0.266515
30	dibutyl phthalate	0.903617	87	ethyl pentadec-9-enoate	0.261686
31	isopentyl formate	0.899145	88	2,6,10-trimethyldodecane	0.254341
32	2-vinyl-2-butenal	0.873774	89	caryophyllene	0.241697
33	ethyl myristate	0.869219	90	ethyl heptadecanoate	0.239037
34	furfural	0.790308	91	octanoic acid	0.238003
35	ethyl lactate	0.773015	92	ethyl butyrate	0.233453
36	2-butyloctanol	0.741799	93	11,14,17-eicosatrienoicacid	0.230276
37	hexahydrofarnesylacetone	0.728119	94	Linoleic alcohol	0.221346
38	2,3-dimethyl-pyrazine	0.714096	95	4-methylnonane	0.217782
39	pentadecane	0.711463	96	decene	0.213525
40	3,5-dimethylpyrazole	0.690514	97	2,2,11,11-tetramethyl-dodecane	0.210898
41	1,2-dimethyl-hydrazine	0.680933	98	ethyl valerate	0.204145
42	styrene	0.65732	99	1-methyl-2-(3-methylpentyl)-cyclopropane	0.196417
43	ethyl laurate	0.656969	100	eicosane	0.188898
44	2,5-dimethyl-pyrazine	0.653073	101	2,3,4-trimethyl-hexane	0.181269
45	3-furanmethanol	0.641658	102	mequinol	0.177185

46	1,3,5,7-cyclooctatetraene	0.639318	103	methyl anthranilate	0.175919
47	ethyl isobutyrate	0.626934	104	2-acetyl pyrrole	0.172074
48	benzyl alcohol	0.604273	105	ethyl 5-amino-1,2,3-thiadiazole-4-carboxylate	0.15786
49	phenylacetaldehyde	0.5822	106	dodecane	0.1568
50	4,6-dimethyl-pyrimidine	0.575103	107	isobutyraldehyde	0.150123
51	diethyl succinate	0.538253	108	(E)-2,3-epoxydecane	0.146915
52	methyl 2-(propanoylamino)benzoate	0.493848	109	2,8-dimethylundecanoic acid methyl ester	0.130016
53	isopentyl alcohol	0.493784	110	2,5-dihydrofuran	0.126053
54	isoamyl acetate	0.490105	111	methanethiol	0.0935
55	dihydroaplotaxene	0.48715	112	2,6-dimethyl-pyrazine	0.0913453
56	nonanoic acid	0.46522	113	3,8-dimethyl-undecane	0.0885825
57	(E,E)-2,4-hexadienal	0.463235	114	2,6-dimethyl-heptadecane	0.087334
			115	2-methylhexadecanoic acid	0.0800639