

Table S2 Quantitative comparison of volatile compounds (expressed in $\mu\text{g kg}^{-1}$) in Yangfan *Douchi* during the fermentation process.

No.	Volatile compound	Content ($\mu\text{g kg}^{-1}$)					RI	LRI	Identification
		D0	D3	D5	D20	D35			
Alcohols									
1	Ethanol	ND	226.37 \pm 31.42a	ND	13.78 \pm 2.74b	ND	427	812	MS, RI, LRI
2	1-Butanol	8.09 \pm 1.18a	ND	ND	6.25 \pm 10.82a	ND	659	1062	MS, RI, LRI
3	1-Butanol, 3-methyl-	ND	152.97 \pm 68.48a	25.01 \pm 1.9b	84.01 \pm 14.34b	77.49 \pm 22.38b	736	1137	MS, RI, LRI
4	Levomenthol	3.1 \pm 1.03	ND	ND	ND	ND	1175	1140	MS, RI, LRI
5	1-Butanol, 2-methyl-	20.08 \pm 1.94	ND	ND	ND	ND	739	1127	MS, RI, LRI
6	1-Pentanol	4.71 \pm 2.73	ND	ND	ND	ND	765	1172	MS, RI, LRI
7	Cyclohexanol, 2,4-dimethyl-	ND	ND	ND	4.46 \pm 3.35	ND	1032	1192	MS, RI, LRI
8	1-Octen-3-ol	84.46 \pm 22.9c	170.62 \pm 42.54b	90.57 \pm 14.39c	188.99 \pm 18.09b	251.96 \pm 34.35a	980	1386	MS, RI, LRI
9	Cyclohexanol, 2,3-dimethyl-	0.77 \pm 0.53	ND	ND	ND	ND	-	1418	MS, RI, LRI
10	4-Ethylcyclohexanol	ND	ND	ND	ND	0.55 \pm 0.4	1003	1440	MS, RI, LRI
11	1-Hexanol, 2-ethyl-	ND	15.95 \pm 4.49	ND	ND	ND	1030	1454	MS, RI, LRI
12	1-Octyn-3-ol	ND	ND	ND	ND	8.93 \pm 0.54	-	1216	MS, RI, LRI
13	1-Hexanol	118.11 \pm 32.38a	14.44 \pm 2.23b	3.41 \pm 1.1b	5.46 \pm 0.93b	4.5 \pm 0.58b	868	1289	MS, RI, LRI
14	2-Hexen-1-ol, (Z)-	0.06 \pm 0.06	ND	ND	ND	ND	868	1561	MS, RI, LRI
15	2,3-Butanediol	ND	4.12 \pm 1.94	ND	ND	ND	788	1560	MS, RI, LRI
16	3-Octanol	7.4 \pm 1.29c	21.43 \pm 3.64b	10.91 \pm 1.95c	35.26 \pm 2.54a	31.78 \pm 4.4a	994	1339	MS, RI, LRI
17	1-Nonanol	3.57 \pm 1.1a	ND	ND	0.97 \pm 1.68b	3.59 \pm 0.93a	1173	1539	MS, RI, LRI
18	Benzyl alcohol	3.46 \pm 1.52a	1.3 \pm 1.14b	0.36 \pm 0.63b	ND	ND	1036	1970	MS, RI, LRI

19	Phenylethyl Alcohol	ND	48.39±10.12a	ND	44.16±1.93a	43.66±3.57a	1116	2024	MS, RI, LRI
20	β-Ethylphenethyl alcohol	ND	ND	ND	3.47±2.7	ND	1261	2123	MS, RI, LRI
Aldehydes									
21	Octanal	ND	ND	ND	ND	5.49±2.91	1003	1199	MS, RI, LRI
22	2-Heptenal, (Z)-	ND	ND	2.82±0.12 ^b	ND	7.98±0.57 ^a	958	1236	MS, RI, LRI
23	Hexanal	22.14±3.13 ^a	7.53±7.12 ^{bc}	15.44±3.83 ^{ab}	4.7±0.54 ^c	12.4±5.4 ^{bc}	800	927	MS, RI, LRI
24	Decanal	3.12±3.11 ^a	ND	2.44±0.41 ^a	7.47±4.35 ^a	2.99±2.64 ^a	1206	1453	MS, RI, LRI
25	Nonanal	15.12±5.14 ^a	4.31±3.41 ^c	10.5±1.38 ^{ab}	7.39±1.91 ^{bc}	9.96±2.25 ^{abc}	1104	1323	MS, RI, LRI
26	Benzaldehyde	7.44±6.16 ^b	39.38±13.56 ^a	14.76±1.23 ^b	49.52±1.99 ^a	41.16±6.4 ^a	962	1465	MS, RI, LRI
27	2-Nonenal, (E)-	2.26±2.01 ^a	ND	0.12±0.21 ^a	0.96±1.66 ^a	1.87±3.25 ^a	1162	1493	MS, RI, LRI
28	2-Octenal, (E)-	ND	ND	2.9±0.51	ND	ND	1060	1358	MS, RI, LRI
29	Benzeneacetaldehyde	ND	30.76±5.45 ^{ab}	15.97±2.44 ^c	28.08±6.18 ^b	37.85±2.76 ^a	1045	1619	MS, RI, LRI
30	Benzeneacetaldehyde, α-ethyl-	ND	ND	ND	12.01±1.87	ND	-	1693	MS, RI, LRI
31	Benzaldehyde, 4-methoxy-	0.12±0.11 ^a	ND	0.43±0.38 ^a	0.88±0.48 ^a	3.19±3.84 ^a	1250	2164	MS, RI, LRI
32	Benzeneacetaldehyde, α-ethylidene-	ND	ND	ND	32.61±6.47 ^a	12.55±1.33 ^b	1279	2035	MS, RI, LRI
Ketones									
33	3-Heptanone, 4-methyl-	3.14±1.67	ND	ND	ND	ND	-	827	MS, RI, LRI
34	3-Octanone	ND	ND	11.02±0.03 ^c	50.88±0.53 ^b	59.04±5.99 ^a	986	1156	MS, RI, LRI
35	2-Octanone	6.17±0.59	ND	ND	ND	ND	990	1201	MS, RI, LRI
36	1-Octen-3-one	ND	ND	5.02±0.36 ^a	5.11±3.28 ^a	ND	979	1220	MS, RI, LRI
37	2,3-Octanedione	ND	ND	ND	7.04±1.8	ND	984	1240	MS, RI, LRI
38	3-Octanone, 2-methyl-	ND	ND	6.55±1.25 ^{ab}	ND	7.82±7.7 ^a	985	1243	MS, RI, LRI
39	Ethanone, 1-(2-hydroxy-5-methylphenyl)-	ND	ND	ND	80.63±7.07 ^b	109.58±14.59 ^a	1316	2390	MS, RI, LRI
40	4-Hydroxy-2-methylacetophenone	ND	4.88±1.45	ND	ND	ND	-	2395	MS, RI, LRI

Alkenes									
41	Undecane	16.58±1.24 ^a	10.81±6.74 ^a	8.97±0.85 ^a	15.67±12.74 ^a	23.73±9.51 ^a	1100	1001	MS, RI, LRI
42	Dodecane	2.27±2.07	ND	ND	ND	ND	1200	1112	MS, RI, LRI
43	Hexadecane	9.54±5.88	ND	ND	ND	ND	1600	1163	MS, RI, LRI
44	Decane, 3,7-dimethyl-	3.56±2.89	ND	ND	ND	ND	1125	1220	MS, RI, LRI
45	Dodecane, 2,6,10-trimethyl-	0.46±0.19	ND	ND	ND	ND	1366	1385	MS, RI, LRI
46	Nonadecane	1.87±1.97	ND	ND	ND	ND	1900	1393	MS, RI, LRI
47	Pentadecane	ND	ND	ND	ND	13.14±2.38	1500	1459	MS, RI, LRI
Olefin									
48	Styrene	ND	ND	ND	21.65±0.9 ^b	43.3±2.83 ^a	893	1150	MS, RI, LRI
49	Caryophyllene	ND	ND	11.55±6.37 ^a	8.68±0.39 ^a	10.94±3.71 ^a	1419	1556	MS, RI, LRI
Esters									
50	Butanoic acid, 2-methyl-, ethyl ester	ND	ND	ND	ND	17.59±3.16	849	882	MS, RI, LRI
51	Carbonic acid, decyl propyl ester	0.46±0.66	ND	ND	ND	ND	-	1244	MS, RI, LRI
52	Sulfurous acid, hexyl undecyl ester	0.11±0.17	ND	ND	ND	ND	-	1314	MS, RI, LRI
53	Benzoic acid, methyl ester	ND	ND	ND	ND	2.45±1.84	1171	1599	MS, RI, LRI
54	Tetradecanoic acid, ethyl ester	ND	6.74±7.44 ^c	ND	13.3±1.57 ^b	44.7±0.59 ^a	1794	2229	MS, RI, LRI
55	Pentadecanoic acid, ethyl ester	ND	ND	ND	ND	5.17±1.92	1894	2364	MS, RI, LRI
56	Sulfurous acid, 2-propyl undecyl ester	0.18±0.25	ND	ND	ND	ND	-	1648	MS, RI, LRI
57	Benzoic acid, ethyl ester	ND	31.08±23.01 ^b	ND	43.47±6.4 ^b	93.18±14.96 ^a	1171	1656	MS, RI, LRI
58	Benzeneacetic acid, ethyl	ND	ND	ND	2.34±0.75 ^b	10.38±1.83 ^a	1246	1822	MS, RI, LRI

	ester								
59	Acetic acid, 2-phenylethyl ester	ND	9.08±2.44	ND	ND	ND	1258	1870	MS, RI, LRI
60	Phenol, 3-methyl-5-(1-methylethyl)-, methylcarbamate	0.58±0.53 ^b	ND	5.66±1.68 ^a	ND	ND	1687	2393	MS, RI, LRI
61	Hexadecanoic acid, methyl ester	ND	18.19±7.16 ^c	3.38±0.95 ^d	28.99±7.84 ^b	50.46±1.29 ^a	1926	2439	MS, RI, LRI
62	Hexadecanoic acid, ethyl ester	ND	98.56±5.33 ^c	3.74±1.07 ^d	152.58±5.34 ^b	595.47±63.39 ^a	1993	2493	MS, RI, LRI
63	Linoleic acid ethyl ester	ND	66.05±1.2 ^b	ND	102.73±1.41 ^b	345.39±49.75 ^a	2162	2860	MS, RI, LRI
64	Ethyl Oleate	ND	26.42±2.31 ^b	ND	34.09±6.87 ^b	189.39±24.39 ^a	2173	2780	MS, RI, LRI
Benzene derivative									
65	Ethylbenzene	2.44±0.67 ^b	ND	ND	ND	29.04±3.03 ^a	855	1024	MS, RI, LRI
66	p-Xylene	ND	42.45±13.19 ^b	23.27±1.08 ^c	39.41±14.82 ^{bc}	63.59±8.41 ^a	865	1033	MS, RI, LRI
67	Benzene, 1,3-dimethyl-	35.08±10.97 ^a	ND	ND	23.01±39.86 ^a	ND	866	1038	MS, RI, LRI
68	Benzene, 1-ethyl-2-methyl-	ND	ND	ND	8.14±1.67 ^b	12.79±3.11 ^a	970	1105	MS, RI, LRI
69	Mesitylene	ND	ND	9.33±0.42 ^a	5.69±2.79 ^b	ND	972	1175	MS, RI, LRI
70	Benzene, 1,2,3-trimethyl-	4.9±1.65 ^b	ND	ND	ND	24.18±8.48 ^a	1013	1185	MS, RI, LRI
71	Benzene, 1,3-bis(1,1-dimethylethyl)-	2.25±0.77 ^c	5.39±0.39 ^c	2.18±0.36 ^c	73.33±5.35 ^a	16.82±6.72 ^b	1247	1361	MS, RI, LRI
72	Benzene, propyl-	ND	15.58±8.01	ND	ND	2.13±3.68	953	1633	MS, RI, LRI
Acids									
73	Acetic acid	ND	ND	1.64±2.83 ^b	2.72±4.71 ^b	15.61±1.27 ^a	610	1392	MS, RI, LRI
Phenols									
74	Phenol, 2-methoxy-	ND	ND	ND	429.98±126.67 ^a	324.66±25.75 ^b	1090	1935	MS, RI, LRI
75	Phenol, 4-ethyl-	ND	5.4±2.61 ^c	1.41±0.31 ^c	177.16±19.55 ^a	98.96±8.04 ^b	1169	2370	MS, RI, LRI
76	Phenol	ND	ND	ND	55.19±13.23 ^a	62.93±2.49 ^a	980	2150	MS, RI, LRI

77	Phenol, 4-ethyl-2-methoxy-	ND	ND	ND	49.96±5.49 ^a	24.79±2.29 ^b	1282	2181	MS, RI, LRI	
78	2,4-Di-tert-butylphenol	11.07±3.75 ^{bc}	40.12±9.91 ^a	3.74±0.72 ^c	30.63±22.03 ^{ab}	17.39±4.81 ^{bc}	1519	2546	MS, RI, LRI	
79	Maltol	10.32±4.18 ^a	5.53±6.38 ^{ab}	ND	ND	ND	1110	2096	MS, RI, LRI	
Furan(one)s										
80	2(3H)-Furanone, dihydro-5-pentyl-	1.42±1.3	ND	ND	ND	ND	1363	2178	MS, RI, LRI	
81	Benzofuran, 2,3-dihydro-	ND	6.19±3.24 ^c	11.48±3.56 ^c	94.51±1.79 ^b	112.54±4.26 ^a	1224	2629	MS, RI, LRI	
Others										
82	Heptanamide, 4-ethyl-5-methyl-	0.16±0.15	ND	ND	ND	ND	-	1824	MS, RI, LRI	
83	12-Crown-4	0.43±0.43	ND	ND	ND	ND	-	2787	MS, RI, LRI	

ND: not detected.

Calculated retention index (RI) on DB-WAX column.

Identification methods: MS, mass spectrometry; RI, retention indices; LRI, linear retention indices.