

Table S3. Peak information, relative intensity and <i>p</i> -value of volatile compounds by HS sampling										
Compound name	RI ^a	Quantitative e <i>m/z</i>	Relative peak height (mean ± SD) ^b					Reliability ^c	<i>p</i> -value ^d	
			0 week	18 weeks					Control vs. LAB + EtOH	Control vs. Acid + Yeast
				Control	LAB + EtOH	Acid + Yeast	Acid + EtOH			
Acetaldehyde		44	0.353±0.02	2.515±0.275	1.270±0.292	2.239±0.222	0.712±0.020	A, B	0.012 *	0.33
Methanethiol		48	0.034±0.00	0.035±0.002	0.043±0.003	0.036±0.003	0.032±0.002	A, B	0.032	0.827
2-Propanone (Acetone)		43	0.112±0.02	1.182±0.063	1.222±0.163	1.580±0.029	1.490±0.096	B	0.76	< 0.01 *
2-Propanol		45	0.102±0.010	0.101±0.012	0.118±0.022	0.099±0.006	0.078±0.013	A, B	0.404	0.844
Furan		68	0.002±0.00	0.040±0.008	0.044±0.003	0.047±0.003	0.031±0.001	A, B	0.566	0.308
Ethyl formate	501.72	45	N.D.	0.093±0.006	0.243±0.024	0.105±0.001	0.102±0.013	A, B	< 0.01 *	0.042
2-Methyl-2-propanol	510.20	59	0.001±0.00	0.056±0.032	0.011±0.005	0.006±0.003	0.009±0.003	A, B	0.183	0.156
Methyl acetate	512.43	43	N.D.	0.058±0.012	0.08±0.017	0.072±0.002	0.071±0.006	A, B	0.222	0.245
2-Methyl-propanal (Isobutyraldehyde)	535.67	43	0.056±0.00	1.605±0.093	1.706±0.291	2.161±0.061	1.659±0.078	B	0.665	< 0.01 *
2,3-Butanedione (Diacetyl)	562.23	43	0.007±0.00	0.740±0.060	0.021±0.005	0.898±0.039	0.013±0.001	A, B	< 0.01 *	0.035
2-Butanone	572.36	43	0.095±0.02	0.516±0.025	0.435±0.068	0.490±0.017	0.354±0.014	A, B	0.191	0.299
2-Methyl-furan	592.73	82	0.001±0.00	0.007±0.001	0.012±0.001	0.012±0.002	0.016±0.004	A, B	0.014 *	0.023
2-Ethoxy-2-methyl-propane	617.63	59	0.002±0.00	0.011±0.004	0.009±0.004	0.004±0.003	0.008±0.002	A, B	0.547	0.103
2-Butenal	624.46	39	0.001±0.00	0.009±0.001	0.003±0.001	0.016±0.002	0.007±0.002	B	< 0.01 *	0.018
3-Methyl-butanal (Isovaleraldehyde)	634.48	44	0.108±0.01	1.549±0.127	1.165±0.085	1.775±0.068	0.961±0.049	A, B	0.024 *	0.09
3-Methyl-2-butanone	639.92	43	0.002±0.00	0.040±0.007	0.052±0.012	0.041±0.006	0.044±0.002	B	0.297	0.903
2-Methyl-butanal (Valeraldehyde)	645.17	57	0.081±0.01	1.493±0.054	1.590±0.139	2.095±0.073	1.677±0.114	B	0.41	< 0.01 *
2-Pentanone	666.55	43	0.005±0.00	0.018±0.003	0.009±0.005	0.020±0.002	0.007±0.001	A, B	0.08	0.564
2,3-Pentanedione	671.32	43	0.006±0.00	0.026±0.004	0.011±0.002	0.017±0.005	0.006±0.002	A, B	0.013 *	0.157
Ethyl propionate	693.64	57	N.D.	0.185±0.030	0.142±0.028	0.191±0.008	0.082±0.006	A, B	0.208	0.816
<i>n</i> -Propyl acetate	695.99	43	0.001±0.00	0.021±0.005	0.008±0.000	0.015±0.005	0.005±0.001	A, B	0.062	0.287
2-Methyl-1-butanol (Active amyl alcohol)	722.58	57	0.044±0.00	0.580±0.007	0.111±0.026	0.514±0.027	0.064±0.005	A, B	< 0.01 *	0.028
Dimethyl disulfide	730.63	94	0.004±0.00	0.019±0.003	0.014±0.004	0.024±0.003	0.013±0.004	A, B	0.242	0.173
Ethyl 2-methylpropanoate (Ethyl isobutyrate)	744.68	43	N.D.	0.144±0.035	0.228±0.046	0.158±0.012	0.121±0.024	A, B	0.109	0.611
2-Methylpropyl acetate (Isobutyl acetate)	757.38	43	N.D.	0.066±0.009	0.006±0.001	0.058±0.001	0.004±0.002	A, B	0.01 *	0.352
3,4-Hexanedione	775.64	57	0.002±0.00	0.015±0.001	0.002±0.000	0.013±0.001	N.D.	A, B	< 0.01 *	0.064
Hexanal	778.87	43	0.005±0.00	N.D.	N.D.	N.D.	N.D.	A, B	-	-
Ethyl butanoate	782.75	71	N.D.	0.022±0.005	0.022±0.005	0.018±0.002	0.015±0.003	A, B	0.982	0.387
Butyl acetate	793.96	43	N.D.	0.133±0.009	0.019±0.006	0.172±0.005	0.015±0.006	A, B	< 0.01 *	< 0.01 *
Ethyl 2-methylbutanoate	835.74	57	N.D.	0.051±0.011	0.119±0.02	0.053±0.004	0.077±0.012	A, B	0.014 *	0.856
Ethyl 3-methylbutanoate (Ethyl isovalerate)	837.28	88	N.D.	0.054±0.013	0.084±0.018	0.052±0.006	0.054±0.013	A, B	0.133	0.838
3-Methylbutyl acetate (Isoamyl acetate)	858.39	43	N.D.	0.042±0.008	0.007±0.002	0.033±0.002	0.006±0.002	A, B	< 0.01 *	0.184
2-Methylbutyl acetate	861.32	43	N.D.	0.018±0.004	0.006±0.003	0.016±0.001	0.003±0.000	A, B	0.019 *	0.434
2,6-Dimethyl-pyrazine	890.79	108	0.004±0.00	0.006±0.000	0.006±0.002	0.006±0.001	0.005±0.001	B	0.982	0.267
(<i>Z</i>)-3,7-Dimethyl-2-octene	893.43	70	N.D.	0.002±0.000	0.001±0.000	0.003±0.001	0.001±0.000	B	< 0.01 *	0.454
Benzaldehyde	942.12	106	0.004±0.00	0.013±0.002	0.011±0.002	0.011±0.001	0.006±0.001	A, B	0.415	0.317
(<i>Z</i>)-1,5-Octadien-3-ol	958.45	57	0.010±0.00	0.002±0.001	0.002±0.001	0.002±0.001	0.001±0.001	B	0.418	0.963
1-Octen-3-ol	964.02	57	0.180±0.07	0.002±0.001	0.058±0.017	0.051±0.002	0.049±0.003	A, B	0.514	0.722
3-Octanone	968.48	43	N.D.	0.009±0.002	0.004±0.001	0.008±0.002	0.001±0.001	A, B	0.037 *	0.66
Ethyl hexanoate (Ethyl caproate)	978.96	88	N.D.	0.010±0.002	0.012±0.003	0.008±0.000	0.009±0.001	A, B	0.326	0.155
3-Octanol	981.38	59	0.01±0.00	0.004±0.000	0.004±0.001	0.003±0.000	0.003±0.000	A, B	0.782	0.086
2-Octenal	1038.39	41	0.012±0.00	N.D.	N.D.	N.D.	N.D.	A, B	-	-
Ethyl heptanoate	1078.22	88	N.D.	0.002±0.000	0.001±0.000	0.001±0.000	0.001±0.000	A, B	0.251	0.11
Ethyl benzoate	1158.33	105	N.D.	0.013±0.001	0.016±0.003	0.014±0.001	0.011±0.002	A, B	0.261	0.712
Ethyl dodecanoate (Ethyl laurate)	1177.38	88	N.D.	0.006±0.002	0.004±0.000	0.005±0.001	0.004±0.001	A, B	0.106	0.284

a: Retention indices (RI) were determined using n-alkanes C11–C32

b: Relative intensity of compounds are displayed as mean ± standard deviation for three independent experiments. Control: control samples inoculated with *Zygosaccharomyces rouxii* and *Tetragenococcus halophilus*. LAB + EtOH: Samples inoculated with *T. halophilus* and added ethanol.

Acid + Yeast: Samples added lactic acid and acetic acid and inoculated with *Z. rouxii*. Acid + EtOH: Sample added lactic acid, acetic acid and ethanol.

c: *p*-value are calculated by Aloutout 2 software. Significant constituents were marked.

d: Reliability of volatile annotation was shown as follows: A, mass spectrum and retention index were consistent with those of an authentic compound;

B, mass spectrum and retention index were consistent with those of the literature (12, 44-46);