

Table S1. Peak information, relative intensity and *p*-value of Hydrophilic compounds

Compound name	RI ^a	Quantitative <i>m/z</i>	Relative peak height (mean \pm SD) ^b						<i>p</i> -value ^c	
			0 week	18 weeks				Control vs. LAB +	Control vs. Acid +	
				Control	LAB + EtO	Acid +	Yea Acid + EtOH			
Lactic acid	1050.89	87	0.004 \pm 0.00	0.075 \pm 0.00	0.078 \pm 0.00	0.065 \pm 0.00	0.061 \pm 0.006	0.489	0.141	
Alanine	1094.65	116	0.404 \pm 0.07	1.760 \pm 0.22	1.449 \pm 0.13	1.416 \pm 0.08	1.092 \pm 0.072	0.174	0.120	
Valine	1207.39	144	0.295 \pm 0.03	1.105 \pm 0.10	0.943 \pm 0.07	1.224 \pm 0.07	1.029 \pm 0.024	0.151	0.269	
Glycerol	1260.98	147	0.676 \pm 0.03	2.461 \pm 0.08	0.732 \pm 0.01	2.447 \pm 0.15	0.784 \pm 0.017	< 0.01 *	0.920	
Phosphate	1261.06	299	0.273 \pm 0.02	0.999 \pm 0.02	0.970 \pm 0.03	1.042 \pm 0.00	0.997 \pm 0.009	0.430	0.084	
Leucine	1263.10	158	0.409 \pm 0.04	1.645 \pm 0.08	1.460 \pm 0.11	1.825 \pm 0.08	1.596 \pm 0.009	0.137	0.109	
Isoleucine	1284.84	158	0.228 \pm 0.02	0.926 \pm 0.05	0.787 \pm 0.04	1.006 \pm 0.05	0.870 \pm 0.025	0.049	0.221	
Proline	1293.33	142	0.346 \pm 0.06	1.307 \pm 0.19	1.039 \pm 0.11	1.582 \pm 0.09	1.296 \pm 0.039	0.166	0.142	
Glycine	1299.05	174	0.367 \pm 0.02	1.022 \pm 0.05	0.976 \pm 0.04	1.186 \pm 0.04	1.060 \pm 0.007	0.365	0.025	
Succinic acid (or aldehyde)	1306.40	147	0.066 \pm 0.00	0.164 \pm 0.01	0.062 \pm 0.00	0.160 \pm 0.00	0.066 \pm 0.002	< 0.01 *	0.695	
Serine	1348.11	204	0.192 \pm 0.02	0.563 \pm 0.03	0.486 \pm 0.02	0.785 \pm 0.03	0.657 \pm 0.021	0.064	< 0.01 *	
Threonine	1373.21	218	0.062 \pm 0.00	0.200 \pm 0.01	0.175 \pm 0.00	0.224 \pm 0.00	0.184 \pm 0.004	0.065	0.060	
Malic acid	1474.32	147	0.155 \pm 0.01	0.162 \pm 0.02	0.148 \pm 0.01	0.183 \pm 0.00	0.166 \pm 0.009	0.481	0.295	
<i>meso</i> -Erythritol	1488.33	147	0.477 \pm 0.03	0.454 \pm 0.02	0.407 \pm 0.03	0.487 \pm 0.01	0.424 \pm 0.005	0.135	0.157	
Aspartic acid	1507.17	232	0.272 \pm 0.02	0.673 \pm 0.05	0.563 \pm 0.06	1.107 \pm 0.02	0.984 \pm 0.004	0.154	< 0.01 *	
Methionine	1513.65	176	0.035 \pm 0.00	0.128 \pm 0.01	0.112 \pm 0.01	0.134 \pm 0.00	0.120 \pm 0.004	0.193	0.533	
Pyroglutamic acid	1519.72	156	0.164 \pm 0.05	0.404 \pm 0.08	0.579 \pm 0.00	0.288 \pm 0.07	0.445 \pm 0.136	0.104	0.214	
Glutamic acid	1606.99	246	0.708 \pm 0.07	1.619 \pm 0.09	1.388 \pm 0.06	1.826 \pm 0.09	1.479 \pm 0.046	0.052	0.096	
Phenylalanine	1624.37	218	0.112 \pm 0.00	0.409 \pm 0.01	0.367 \pm 0.01	0.430 \pm 0.00	0.374 \pm 0.007	0.041	0.135	
Xylose	1634.02	103	0.488 \pm 0.05	0.286 \pm 0.02	0.260 \pm 0.02	0.358 \pm 0.02	0.346 \pm 0.014	0.382	0.037	
Arabinose	1641.31	103	0.484 \pm 0.05	0.183 \pm 0.02	0.151 \pm 0.01	0.503 \pm 0.02	0.471 \pm 0.044	0.200	< 0.01 *	
Ribose	1655.47	147	0.022 \pm 0.00	0.008 \pm 0.00	0.008 \pm 0.00	0.012 \pm 0.00	0.012 \pm 0.000	0.975	< 0.01 *	
Xylitol	1682.93	217	0.015 \pm 0.00	0.041 \pm 0.00	0.031 \pm 0.00	0.030 \pm 0.00	0.018 \pm 0.001	< 0.01 *	< 0.01 *	
Arabitol	1696.87	217	0.969 \pm 0.04	1.214 \pm 0.06	0.980 \pm 0.02	1.255 \pm 0.06	0.978 \pm 0.022	< 0.01 *	0.526	
Glutamine	1763.13	156	0.004 \pm 0.00	0.005 \pm 0.00	0.005 \pm 0.00	0.004 \pm 0.00	0.004 \pm 0.001	0.599	0.165	
Citric acid + Isocitric acid	1800.10	147	0.029 \pm 0.00	0.003 \pm 0.00	0.004 \pm 0.00	0.043 \pm 0.00	0.040 \pm 0.003	0.361	< 0.01 *	
Ornithine	1803.90	142	0.138 \pm 0.01	1.007 \pm 0.09	0.810 \pm 0.07	0.303 \pm 0.02	0.242 \pm 0.014	0.085	< 0.01 *	
Fructose	1847.48	103	0.018 \pm 0.00	0.005 \pm 0.00	0.007 \pm 0.00	0.016 \pm 0.00	0.036 \pm 0.002	0.036	< 0.01 *	
Galactose	1868.19	205	0.149 \pm 0.01	0.281 \pm 0.01	0.264 \pm 0.00	0.301 \pm 0.01	0.278 \pm 0.002	0.152	0.171	
Glucose	1875.81	147	1.638 \pm 0.16	1.044 \pm 0.04	1.719 \pm 0.09	1.479 \pm 0.10	1.500 \pm 0.106	< 0.01 *	< 0.01 *	
Mannitol	1905.36	205	0.193 \pm 0.00	0.175 \pm 0.00	0.174 \pm 0.00	0.219 \pm 0.00	0.198 \pm 0.012	0.865	< 0.01 *	

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				Control	LAB + EtO	Acid + Yea	Acid + EtOH			
Lysine	1908.12	174	0.186 \pm 0.01	0.508 \pm 0.04	0.465 \pm 0.01	0.531 \pm 0.01	0.474 \pm 0.005	0.261	0.524	
Histidine	1912.76	154	0.039 \pm 0.00	0.129 \pm 0.02	0.102 \pm 0.01	0.157 \pm 0.01	0.116 \pm 0.014	0.217	0.209	
Tyrosine	1929.67	218	0.139 \pm 0.01	0.169 \pm 0.00	0.186 \pm 0.00	0.189 \pm 0.00	0.201 \pm 0.005	< 0.01 *	0.012	
Inositol	2072.92	217	0.024 \pm 0.00	0.168 \pm 0.00	0.158 \pm 0.00	0.173 \pm 0.00	0.162 \pm 0.003	0.091	0.301	
Tryptophan	2214.31	202	0.018 \pm 0.00	0.005 \pm 0.00	0.046 \pm 0.00	0.003 \pm 0.00	0.033 \pm 0.003	< 0.01 *	0.225	

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

b: Relative intensity of compounds are displayed as mean \pm 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.