

Supplementary information

## GC-MS metabolomics and antifungal characteristics of autochthonous *Lactobacillus* strains

Scano et al.

Table S1 - Carbohydrates fermentation profiles of *Lactobacillus* strains.

Acid produced from	<i>L. plantarum</i>			<i>L. brevis</i>		<i>L. sakei</i>			
	4/16898	1/14537	C1/15	M8/1	DSM 32516	S3/1	S4	S5	S3
Amygdalin	+	+	+	-	-	-	-	-	-
Arabinose	+	+	+	+	-	-	-	+	+
Cellobiose	+	+	+	-	-	+	-	-	-
Galactose	+	+	+	+	+	+	+	+	+
Lactose	+	+	+	-	-	+	-	-	-
Inulin	-	+	-	-	-	-	-	-	-
Maltose	+	+	+	+	+	-	-	+	-
Mannitolo	+	+	+	-	-	-	-	-	-
Mannose	+	+	+	-	-	+	+	+	+
Melezitose	+	+	+	-	-	-	-	-	-
Melibiose	+	-	+	-	-	+	+	+	+
Raffinose	-	-	+	-	-	-	-	-	-
Ribose	+	+	+	+	-	+	+	+	+
Sorbitol	+	+	+	-	-	-	-	-	-
Sucrose	+	+	+	-	+	+	+	+	+
Trehalose	+	+	+	-	+	+	+	+	+
Xylose	-	-	-	-	-	-	-	-	-
CO <sub>2</sub> from glucose	-	-	-	+	+	-	-	-	-
Esculin hydrolysis	+	+	+	-	-	-	-	-	-
Ammonia from arginine	-	-	-	+	-	+	+	+	-

Table S2. List of metabolites and GC-MS characteristics.

Metabolite	Abbreviation	Class	Rt <sup>a</sup>	m/z <sup>b</sup>	
Lactic acid	LacA	OA <sup>c</sup>	15.80	147	
Glyceric acid	GlycA	OA	16.71	147	Broth <sup>d</sup>
Valine	Val	AA	16.22	72	Broth
Unknown			17.05	258	

Oxalic acid	OxalicA	OA	17.32	147	
Leucine	Leu	AA	17.54	86	Broth
3-Hydroxy butyric acid	BHBA	OA	17.68	147	
2-Hydroxy isovaleric acid	AHVA	OA	17.78	145	
Isoleucine	Ile	AA	17.90	86	Broth
Unknown			18.10	281	
2-Hydroxy isocaproic acid	AHCA	OA	18.96	159	
Phosphate	Pho		19.24	147	Broth
Unknown			19.61	299	
Threonine	Thr	AA	19.87	117	Broth
Glycine	Gly	AA	20.05	174	Broth
Succinic acid	SuccA	OA	20.10	147	
Propanoic acid	PropA	OA	20.28	219	
2,3-butandiol	2,3-butandiol		21.11	117	
Unknown			21.17	58	
Malic acid	MalA	OA	22.28	281	
Unknown			22.53	147	
Pyroglutamic acid	PyroGA	AA	22.65	84	
Erithriol	Erithriol	S	22.84	217	
Unknown			22.94	156	
4-aminobutanoic acid	GABA	OA	23.01	174	
Unknown			23.37	147	
3-phenyllactic acid	3-phen-LacA	OA	23.69	193	
Erythrose	Erythrose	S	24.9	147	
Unknown			25.17	147	
Arabitol	Arabitol	S	25.38	217	
Unknown			25.71	231	
Citric acid	CitrA	OA	25.89	147	Broth
Unknown			26.64	204	
Unknown			26.72	217	
Unknown			26.81	157	
Fructose	Fructose	S	27.05	103	Broth
Glucose	Glucose	S	27.22	204	Broth
Mannose	Mannose	S	27.33	319	Broth
Galactose	Galactose	S	27.66	319	Broth
Xylose	Xylose	S	27.78	204	
Unknown			27.89	241	
Talose	Talose	S	28.09	204	Broth
Unknown			28.55	204	
Myo-inositol	Myo-inos	S	29.16	305	Broth
Unknown			29.50	59	

Octadecenamide	Oleamide	FA	31.27	59	
Unknown			31.64	147	
Unknown			32.27	117	
Unknown			32.74	103	
Unknown			32.85	371	
Palmitic acid	PalmA	FA	33.03	371	
Sucrose	Sucrose	S	33.51	361	Broth
Unknown			33.77	117	
Stearic acid	StearA	FA	34.43	399	
Threulose	Threulose		34.57	361	Broth
Unknown			35.46	217	
Maltose	Maltose	S	35.51	361	Broth
Unknown			36.55	217	

a) retention time (min); b)  $m/z$  of ion fragment used for semiquantitative purpose; c) OA = organic acids, AA = amino acids and analogues, S = saccharides and polyols, FA = fatty acids and analogues; d) annotated in broth samples.

Figure S1. PLS-DA coefficients Overview Plot. The plot displays the X-variable coefficients, together with their SE in cross validation, for the three Y-class for those annotated metabolites having VIP values > 1 (LacA, BHBA, AHVA, AHCA, SuccA, MalA, PyroGA, Erythriol, GABA, 3-phen-LacA, Erythrose, Arabinol, Fructose, Glucose, Mannose, Mono-sacch, Sucrose, StearA, Maltose, metabolites abbreviated as in Table S2).

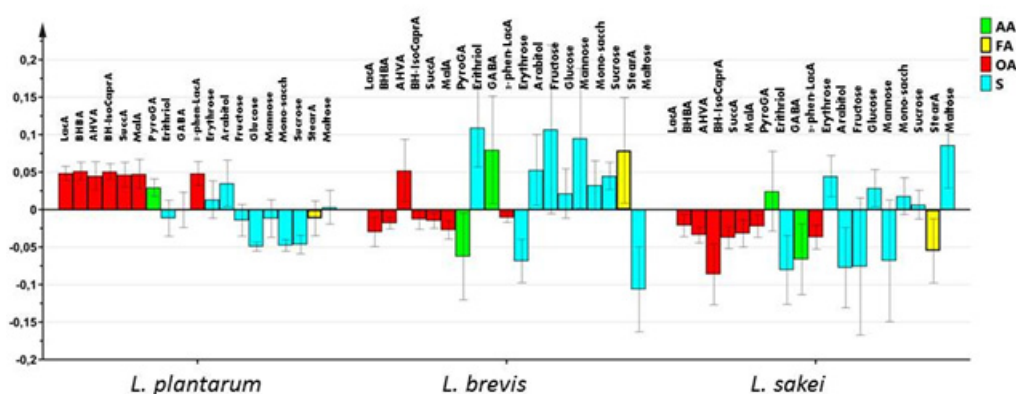


Figure S2. Heat map of  $r$  Pearson correlation values of GC-MS data matrix.  $r$  values are colored from red ( $r = +1$ ) to blue ( $r = -1$ ) scale.

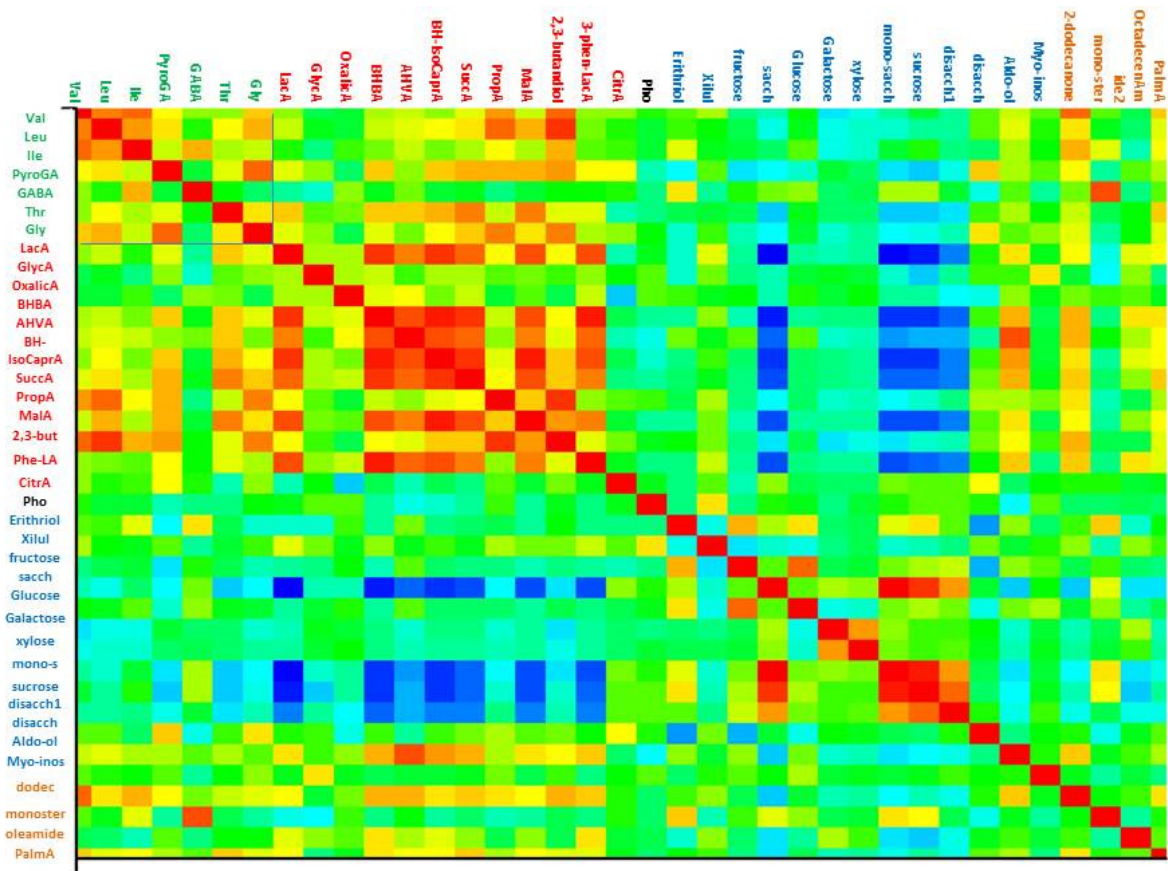


Figure S3. Correlation plot of lactic acid ( $x$ -axis) *vs.* glucose ( $y$ -axis) levels. Lb, Lp, and Ls = *L. brevis*, *L. plantarum* and *L. sakei*.

