

Unraveling the antibacterial mechanism of Plasma-activated lactic acid against *Pseudomonas ludensis* by untargeted metabolomics

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Table S1. Differential metabolites of PALA treated *P. ludensis* identified through untargeted metabolomics

Serial number	Name	Log2 (T/CK)	P-value	VIP
1	3-[4-(3,5-dichloro-4-pyridinyl) piperazino]-1,1,1-trifluoro-2-propanol	-3.08	1.45E-05	1.0053
2	Maltopentaose	-6	5.00E-09	1.9066
3	γ-Glutamylcysteine	-8.06	9.58E-08	2.5691
4	Adenosine	-3.53	8.65E-06	1.1434
5	L-Homocitrulline	-5.91	2.47E-07	1.8878
6	Xanthosine	-6.54	9.26E-06	2.1513
7	Reduced nicotinamide adenine dinucleotide	-5.56	1.36E-06	1.7552
8	D-α-Hydroxyglutaric acid	-7.76	2.53E-07	2.4907
9	Gamma-Glu-Leu	-5.7	1.41E-06	1.8345
10	D-Ribose	-3.84	5.28E-08	1.2234
11	S-Adenosylhomocysteine	-7.52	5.44E-05	2.4119
12	N-Acetylaspartic acid	-8.23	1.33E-09	2.6149
13	Ranolazine	-5.94	1.43E-06	1.9073
14	D-(-)-Fructose	-4.74	4.52E-09	1.5041
15	2-Methylbutyric acid	2.2	0.013751	1.0636
16	Inosine	-3.49	6.19E-06	1.1224
17	N6-Succinyl Adenosine	-5.87	6.85E-09	1.8689
18	Nicotinamide adenine dinucleotide (NAD+)	-5.02	4.14E-06	1.6248
19	Nitrofurantoin	-6.12	2.14E-06	1.956
20	DL-Glyceraldehyde3-phosphate	-3.56	5.67E-07	1.134
21	Retrorsine	-5.03	8.21E-07	1.5988
22	L (+)-Ornithine	-4.91	1.05E-06	1.5739
23	Uridine	-5.12	1.68E-05	1.6898
24	N6-Acetyl-L-lysine	-8.77	1.51E-08	2.7963
25	Pantothenic acid	-6.67	3.07E-07	2.1411
26	(R)-3-Hydroxy myristic acid	-3.87	0.000631	1.3559
27	DL-Norvaline DL	-3.09	9.76E-05	1.0253
28	2'-Deoxycytidine	-4.72	4.98E-06	1.5255
29	2-(acetylamino)-3-(1H-indol-3-yl) propanoic acid	-7.79	1.31E-10	2.474

30	7-methylpyrimido[4,5-d] pyrimidin-4-amine	-4.83	4.38E-06	1.5551
31	L-(+)-Citrulline	-4.48	7.65E-06	1.4475
32	2'-Deoxyinosine	-8.86	9.98E-07	2.8932
33	4-Butylresorcinol	-6.82	5.73E-07	2.1732
34	Cyclic ADP-ribose	-4.88	8.48E-08	1.5576
35	N-Acetylglycine	-5.09	1.38E-05	1.6626
36	2-Isopropylmalic acid	-6.8	1.01E-09	2.1624
37	N-Acetylornithine	-7.67	5.72E-07	2.4661
38	Asp-glu	-4.74	7.36E-07	1.4946
39	Citric acid	-6.04	3.15E-09	1.9228
40	L-Glutathione oxidized	-6.04	4.44E-06	1.9646
41	L-Hydroxyproline	-3.81	3.25E-07	1.2094
42	mesaconic acid	-4.75	1.22E-08	1.5114
43	(2E)-1-(2-hydroxy-3,4,5,6-tetramethoxy-phenyl)-3-phenylprop-2-en-1-one	5.26	3.40E-05	1.7199
44	6-Methylquinoline	-3.88	6.66E-05	1.2836
45	L-Glutathione (reduced)	-8.77	3.67E-07	2.8232
46	N-{6-[(7-chloro-4-quinazoliny) oxy]-3-pyridinyl}-4-methoxybenzamide	-3.7	2.19E-05	1.1619
47	UMP	-5.19	9.72E-07	1.6665
48	Cytidine 5'-monophosphate (hydrate)	-5.18	3.67E-06	1.673
49	N-Acetyl-L-tyrosine	-5.25	2.86E-10	1.669
50	2-mercapto-4-(2-thienyl)-5,6,7,8-tetrahydro-quinoline-3-carbonitrile	-4.51	1.22E-05	1.4531
51	D-glutamine	-3.65	2.46E-06	1.1675
52	Neopterin	-5.5	4.72E-07	1.7624
53	Adenosine diphosphate (ADP)	-4.11	2.85E-06	1.3052
54	4-morpholino-3-nitrobenzene-1-sulfonamide	-4.94	2.56E-05	1.5952
55	N-[2-(1,5-dimethyl-4-nitro-1H-pyrazol-3-yl) vinyl] -N,N-dimethylamine	-5.58	1.67E-06	1.7998
56	Epinephrine	-4.4	1.01E-06	1.3889
57	D-2-Aminoadipic acid	-5.19	1.21E-09	1.6471
58	5'-S-Methyl-5'-thioadenosine	-4.57	7.93E-08	1.4557
59	NAD+	-4.23	4.92E-05	1.3695
60	4-cyclopropyl-6-methoxy-1,3,5-triazin-2-amine	-4.44	1.96E-05	1.4491
61	RLH	2.93	0.003268	1.1264
62	Epigallocatechin	-5.35	1.52E-06	1.7208
63	Gedunin	-5.59	1.79E-06	1.779
64	gamma-Glutamylcysteine	-5.43	6.02E-06	1.752
65	2,4-Dihydroxybenzoic acid	-8.43	5.61E-10	2.6771
66	N1-(1H-1,2,3-benzotriazol-5-yl)-3,4,5-trimethoxybenzamide	3.51	3.17E-05	1.1014
67	4-chloro-5-morpholino-2-quinoxalin-2-ylpyridazin-3(2H)-one	-3.68	2.44E-05	1.1823
68	Guanosine	-3.39	1.23E-06	1.0827
69	13,14-Dihydro-15-keto-tetranor prostaglandin F1 α	-3.02	0.000786	1.0617
70	Adenylocuccinic Acid	-4.85	3.26E-07	1.5371

71	Cytidine 5'-Monophosphate-N-Acetylneuraminic Acid	-4.9	8.21E-06	1.559
72	FKK	-4.79	7.97E-06	1.5097
73	Glycyl-L-leucine	-5.05	9.48E-07	1.6217
74	α -Lapachone	-5.12	2.49E-06	1.638
75	1-(4-methylphenyl)-3-(2-pyridylthio) pyrrolidine-2,5-dione	-4.39	1.16E-07	1.3933
76	S-Adenosyl-L-methionine	-3.78	7.33E-08	1.1988
77	γ -L-Glutamyl-L-glutamic acid	-4.58	6.81E-07	1.4647
78	2-[[methyl(2,3,4,5,6-pentahydroxyhexyl)amino] methylidene] malononitrile	-4.52	1.90E-06	1.4438
79	HKK	-3.87	8.55E-08	1.2272
80	S-Lactoylglutathione	-3.42	0.000129	1.1203
81	5-Hydroxytryptophan	-4.34	1.78E-06	1.3935
82	N8-Acetylspermidine	-4.77	3.63E-06	1.533
83	[4-(1H-indol-4-yl)piperazino](2-thienyl)methanone	-6.48	2.14E-10	2.0592
84	Uridine monophosphate (UMP)	-5.73	8.31E-08	1.814
85	L-Glutamic acid	-4.37	2.34E-06	1.3952
86	Kynurenic acid O-hexside	-3.96	3.73E-07	1.2516
87	S-(Methyl)Glutathione	-7.51	1.51E-06	2.4253
88	Hypoxanthine	-7.72	2.23E-09	2.4503
89	N,N-dimethyl-5-nitro-6-[3-(trifluoromethyl)phenoxy]pyrimidin-4-amine	4.85	3.78E-05	1.493
90	N-Acetyl-DL-glutamic acid	-5.64	2.76E-06	1.8091
91	5-Methyluridine	-3.4	8.07E-07	1.0869
92	L-arginine	-4.05	4.42E-07	1.2794
93	3-hydroxy-N-(1-hydroxy-4-methylpentan-2-yl)-5-oxo-6-phenylhexanamide	4.7	9.53E-06	1.5178
94	Tiglic acid	-3.71	3.35E-05	1.2001
95	2'-Deoxyadenosine 5'-monophosphate	-3.66	2.92E-06	1.1691
96	L-Cysteine-glutathione gisulfide	-3.59	9.21E-06	1.1598
97	2'-Deoxyadenosine 5'-monophosphate (dAMP)	-5.65	5.51E-09	1.7961
98	2-(Formylamino)Benzoic Acid	-4.54	1.40E-05	1.4761
99	3-(5-phenyl-1,3-oxazol-2-yl)-4-(trifluoromethyl)pyridine	-4.52	1.59E-06	1.4441
100	3-Methyladipic acid	-3.19	0.000116	1.053
101	nor-6 β -Oxycodol	-4.49	7.60E-08	1.4331
102	Ala-Gln	-5.35	1.42E-06	1.7093
103	Ethylmalonate	-7.57	8.77E-10	2.4063
104	Xanthine	-4.37	0.00028	1.5461
105	Thymidine	-8.14	1.54E-06	2.6583
106	8-Bromoguanosine	-4.81	3.24E-06	1.519
107	Isophorone	-3.3	3.17E-06	1.0419
108	DL-Tryptophan	-4.38	3.72E-05	1.4448
109	Cytosine	-6.94	7.71E-08	2.2138
110	Maltotetraose	-7.12	8.78E-08	2.2668
111	2'-Deoxyadenosine	-4.77	1.02E-07	1.5077
112	L-Tyrosine	-3.79	8.31E-05	1.2667

113	gamma-Glutamylleucine	-4.84	7.24E-05	1.5964
114	N-Acetyl-aspartic acid	-5.78	5.71E-07	1.8523
115	2,6-Dihydroxypurine	-6.34	7.69E-07	2.0227
116	2-Hydroxycinnamic acid	-3.79	3.79E-06	1.223
117	Adenosine 5'-monophosphate	-5.8	2.68E-06	1.8729
118	N-Acetyl-L-leucine	-5.35	6.34E-05	1.6743
119	2-Furoic acid	-4.27	5.63E-07	1.3476
120	Guanosine monophosphate	-4.67	8.94E-06	1.5159
121	D-Raffinose	-5.12	0.000112	1.752
122	N-Acetylvaline	-5.13	6.84E-09	1.6306
123	2-Aminoadipic acid	-6.46	1.88E-08	2.0549
124	Cys-Gly	-7.05	1.49E-07	2.2527
125	4-(trifluoromethyl)nicotinic acid	-5.48	5.16E-06	1.755
126	D - (+)-Maltose	-6.41	8.05E-06	2.1003
127	Spermidine	-4.31	0.000136	1.4722
128	4-hydroxy-1-methyl-3-(phenylthio)-1,2-dihydroquinolin-2-one	-6.07	1.66E-08	1.9343
129	Pantetheine	-8.58	8.84E-09	2.7184
130	2'-Deoxyadenosine-5'-monophosphate	-5.02	2.27E-06	1.6129
131	Nicotinamide adenine dinucleotide	-5.12	7.33E-08	1.6314

Note: Name, name of metabolites; Log2 (T/CK), Log2 values of the ratio of average intensities of 4 replicates of treatment and control; *P*-value, statistical differences of two groups through t-test. VIP: Variable Importance in the Projection by the use of PLS-DA model.

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