

Table S1. Spearman's correlation analysis between compounds and lung functions.

Compound	FEV1%		FVC%		FEV1/FVC	
	Spearman's coefficient	<i>p</i> -value	Spearman's coefficient	<i>p</i> -value	Spearman's coefficient	<i>p</i> -value
L-alanine	-0.320	ns	-0.575	< 0.001	0.073	ns
L-aspartate	-0.215	ns	-0.421	0.009	0.085	ns
L-glutamate	-0.265	ns	-0.439	0.007	0.101	ns
L-glutamine	-0.233	ns	-0.424	0.009	0.083	ns
glycine	-0.159	ns	-0.406	0.013	0.146	ns
L-histidine	-0.346	0.036	-0.558	< 0.001	0.043	ns
L-leucine	-0.248	ns	-0.359	0.029	0.054	ns
L-lysine	-0.298	ns	-0.469	0.003	0.067	ns
L-phenylalanine	-0.209	ns	-0.499	0.002	0.157	ns
L-proline	-0.336	0.042	-0.423	0.009	-0.013	ns
L-serine	-0.203	ns	-0.421	0.010	0.038	ns
L-tyrosine	-0.155	ns	-0.432	0.008	0.193	ns
L-valine	-0.067	ns	-0.335	0.043	0.242	ns
AMP	-0.097	ns	-0.331	0.046	0.149	ns
Thymidine	0.026	ns	-0.461	0.004	0.446	0.006
IMP	-0.378	0.021	-0.370	0.024	-0.087	ns
Inosine	-0.029	ns	-0.437	0.007	0.267	ns

Allantoate	-0.299	ns	-0.471	0.003	0.051	ns
(S)(+)-Allantoin	-0.248	ns	-0.336	0.042	-0.007	ns
Urate	-0.226	ns	-0.338	0.041	0.031	ns
5-6-Dihydrothymine	-0.269	ns	-0.402	0.014	0.068	ns
4-Pyridoxate	-0.158	ns	0.069	ns	-0.358	0.030
Phosphate	0.163	ns	0.444	0.006	-0.135	ns
Diphosphate	0.120	ns	0.453	0.005	-0.200	ns
D-Glyceraldehyde 3-phosphate/Glycerone phosphate	0.378	0.021	0.238	ns	0.265	ns
Pyruvate	-0.136	ns	-0.511	0.001	0.232	ns
Lactate	-0.107	ns	-0.407	0.012	0.140	ns
Maltotriose	-0.086	ns	-0.500	0.002	0.240	ns
Mannitol	-0.316	ns	-0.468	0.003	0.055	ns
D-Ribose	-0.009	ns	-0.392	0.016	0.273	ns
D-Rhamnose	-0.267	ns	-0.523	<0.001	0.121	ns
D-Arabitol	-0.276	ns	-0.407	0.012	-0.045	ns
Citrate	-0.257	ns	-0.512	0.001	0.132	ns
2-Oxoglutarate	-0.028	ns	-0.311	ns	0.328	0.047
Succinate	-0.053	ns	-0.357	0.030	0.203	ns

Fumarate	0.055	ns	-0.314	ns	0.356	0.031
2-Hydroxyglutarate/Citramalate	-0.216	ns	-0.507	0.001	0.180	ns
alpha-D-Ribose 1-phosphate	0.295	ns	-0.029	ns	0.352	0.033
Glutathione disulfide	-0.006	ns	0.378	0.021	-0.265	ns
5-Oxoproline	-0.231	ns	-0.455	0.005	0.028	ns
S-Glutathionyl-L-cysteine	-0.128	ns	0.326	0.049	-0.279	ns
Ascorbate	-0.088	ns	-0.473	0.003	0.274	ns
gamma-Glutamyl-Se-methylselenocysteine	-0.301	ns	-0.422	0.009	-0.028	ns
gamma-L-Glutamyl-D-alanine	-0.245	ns	-0.432	0.008	-0.013	ns
(5-L-Glutamyl)-L-glutamine	-0.015	ns	-0.466	0.004	0.283	ns
Dimethylglycine	-0.226	ns	-0.449	0.005	0.126	ns
Phosphoserine	-0.130	ns	-0.396	0.015	0.087	ns
Ornithine	-0.328	0.048	-0.552	<0.001	0.061	ns
L-Citrulline	-0.341	0.039	-0.531	<0.001	0.008	ns
N-Acetylneuraminate	-0.127	ns	-0.378	0.021	0.166	ns
alpha-D-Glucosamine 1-phosphate	-0.213	ns	-0.350	0.033	0.024	ns
Homocarnosine	-0.456	0.005	-0.426	0.009	-0.217	ns
Carnosine	-0.262	ns	-0.512	0.001	0.036	ns

Creatine	-0.177	ns	-0.355	0.031	-0.011	ns
Creatinine	-0.169	ns	-0.410	0.012	0.057	ns
trans-4-Hydroxy-L-proline	-0.241	ns	-0.380	0.020	0.018	ns
Quinolinic acid	-0.332	0.044	-0.505	0.001	0.021	ns
Anthranilate	-0.033	ns	-0.352	0.033	0.228	ns
L-Adrenaline	-0.235	ns	-0.415	0.011	0.060	ns
Ethanolamine phosphate	0.012	ns	-0.329	0.047	0.281	ns
N-Methylethanolamine phosphate	0.198	ns	0.377	0.021	0.001	ns
Acetylcholine	-0.084	ns	-0.325	0.050	0.231	ns
acyl-C20:4	0.303	ns	0.416	0.011	-0.052	ns
Butanoic/Butyric acid	-0.146	ns	-0.395	0.015	0.208	ns
Hexanoic acid (caproate)	0.444	0.006	0.227	ns	0.349	0.034
Dodecanoic acid (lauric acid)	0.340	0.039	0.095	ns	0.273	ns
Tetradecanoic acid (myristic acid)	0.344	0.037	0.300	ns	0.137	ns
Hexadecanoic acid (palmitic acid)	0.411	0.011	0.357	0.030	0.126	ns
Dodecanedioic acid	0.158	ns	0.464	0.004	-0.242	ns
DG(16:0;16:0)	-0.206	ns	0.043	ns	-0.439	0.007
DG(16:0;18:0)	-0.026	ns	0.357	0.030	-0.272	ns

DG(P-8:0;18:4)	0.201	ns	-0.155	ns	0.376	0.022
FA(14:0)	0.315	ns	0.342	0.038	0.039	ns
FA(19:0)	-0.142	ns	0.167	ns	-0.337	0.042
FA(20:0)	0.358	0.029	0.325	0.050	0.065	ns
FA(16:0)	0.423	0.009	0.271	ns	0.113	ns
FA(18:0)	0.413	0.011	0.287	ns	0.126	ns
Hex2Cer(d18:1;24:1)	-0.238	ns	0.144	ns	-0.377	0.021
LPC(20:4)	-0.013	ns	0.337	0.041	-0.345	0.036
LPC(P-24:1)	-0.347	0.036	-0.184	ns	-0.309	ns
LPC(18:3)	0.195	ns	0.534	<0.001	-0.178	ns
LPC(18:2)	0.114	ns	0.347	0.035	-0.197	ns
LPC(19:2)	0.144	ns	0.401	0.014	-0.202	ns
LPE(20:3)	-0.037	ns	0.424	0.009	-0.371	0.024
LPE(18:2)	0.029	ns	0.363	0.027	-0.280	ns
LPE(22:4)	0.026	ns	0.351	0.033	-0.221	ns
LPE(22:5)	0.022	ns	0.413	0.011	-0.268	ns
LPI(O-23:7)	-0.055	ns	-0.341	0.039	0.039	ns
LSM(d18:0)	0.219	ns	-0.264	ns	0.432	0.008

PC(36:4)	0.123	ns	0.349	0.034	-0.145	ns
PC(33:1)	0.095	ns	0.326	0.049	-0.187	ns
PC(O-38:3)	-0.293	ns	0.120	ns	-0.394	0.016
PE(36:1)	0.129	ns	0.335	0.043	-0.154	ns
PG(32:0)	0.370	0.024	0.316	ns	0.159	ns
PG(36:1)	0.101	ns	0.334	0.044	-0.181	ns
PG(16:0;18:1)	0.159	ns	0.325	0.049	-0.105	ns
TG(18:0;18:0;18:0)	-0.032	ns	0.359	0.029	-0.269	ns
TG(29:0;16:1)	-0.427	0.008	-0.054	ns	-0.368	0.025
TG(27:0;19:2)	0.232	ns	0.363	0.027	0.028	ns
TG(14:0;16:0;16:0)	0.197	ns	-0.281	ns	0.373	0.023
TG(15:0;16:0;16:0)	0.297	ns	-0.095	ns	0.394	0.016
TG(16:0;16:0;18:0)	-0.360	0.029	-0.106	ns	-0.294	ns
TG(24:0;16:0;16:0)	0.158	ns	-0.139	ns	0.329	0.047
TG(12:0;12:0;12:0)	-0.015	ns	-0.293	ns	0.329	0.046
TG(14:0;16:0;18:0)	0.271	ns	-0.261	ns	0.461	0.004

ns, not significant; FEV1, Forced Expiratory Volume in 1 s percentage predicted; FVC, Forced Vital Capacity percentage predicted; DG, diacylglycerol; FA, fatty acid; LPC, Lysophosphatidylcholine; LPE, Lysophosphatidylethanolamine; LPI, Lysophosphatidylinositol; LSM, Lysosphingomyelin; PC, Phosphatidylcholine; PE, Phosphatidylethanolamine; PG, phosphatidylglycerol; TG, triglyceride.