Table S3 The correlation analysis between L-ZS9-producing metabolites, microbiota diversity and immune factors at the positive ion mode.

Var 1	Interraction	Var 2	Cor	*P* value
IgG	Positive	*Bifidobacterium adolescentis*	0.8328	0.0028
MDA	Positive	*Clostridium clostridioforme*	0.7128	0.0207
sIgA	Positive	*Gemmiger formicilis*	0.7333	0.0158
IgG	Positive	*Enterococcus cecorum*	0.6687	0.0345
MDA	Negative	*Enterococcus cecorum*	-0.6848	0.0289
sIgA	Positive	*Eubacterium biforme*	0.6970	0.0251
sIgA	Positive	*Ruminococcus torques*	0.6606	0.0376
sIgA	Positive	*Blautia producta*	0.7697	0.0092
T-SOD	Positive	*Cetobacterium somerae*	0.6727	0.0330
sIgA	Positive	*Collinsella stercoris*	0.6485	0.0425
sIgA	Positive	*Faecalibacterium prausnitzii*	0.8424	0.0022
sIgA	Negative	*Prevotella copri*	-0.6606	0.0376
sIgA	Positive	*Coprococcus*	0.6606	0.0376
TNF-α	Positive	*Peptococcus*	0.6485	0.0425
sIgA	Positive	*Slackia*	0.6970	0.0251
T-SOD	Positive	*Anaerobiospirillum*	0.6727	0.0330
MDA	Negative	*Oscillospira*	-0.7091	0.0217
T-SOD	Positive	*Catenibacterium*	0.8283	0.0031
sIgA	Positive	*Gemmiger*	0.7576	0.0111
IgG	Positive	*Enterococcus*	0.6322	0.0498
sIgA	Positive	*Enterococcus*	0.6485	0.0425
MDA	Negative	*Enterococcus*	-0.7697	0.0092
sIgA	Positive	*Dialister*	0.6364	0.0479
sIgA	Positive	*Eubacterium*	0.7697	0.0092
IgG	Positive	*Veillonella*	0.7599	0.0108
sIgA	Positive	*Adlercreutzia*	0.6970	0.0251
MDA	Negative	*Streptococcus*	-0.6485	0.0425
MDA	Negative	*Escherichia*	-0.6485	0.0425
sIgA	Positive	*Blautia*	0.7333	0.0158
sIgA	Positive	*Faecalibacterium*	0.8424	0.0022
sIgA	Positive	*Collinsella*	0.7212	0.0186
sIgA	Positive	*Lactobacillus*	0.8424	0.0022
MDA	Negative	*Prevotella*	-0.6485	0.0425
sIgA	Positive	*Allobaculum*	0.7212	0.0186
Lactobacillus	Negative	3-Phospho-D-glycerate	-0.9152	0.0002
Lactobacillus	Negative	N-Acetylcadaverine	-0.9030	0.0003
Lactobacillus	Negative	Stearidonic Acid	-0.8909	0.0005
Lactobacillus	Negative	Phosphoenolpyruvate	-0.8788	0.0008
Lactobacillus	Positive	L-Tyrosine	0.8667	0.0012
Lactobacillus	Positive	Acetylcarnitine	0.8667	0.0012
Lactobacillus	Positive	trans-2-Hydroxycinnamic acid	0.8545	0.0016

Faecalibacterium prausnitzii	Positive	Choline	0.8424	0.0022
Faecalibacterium	Positive	Choline	0.8424	0.0022
Lactobacillus	Negative	Deoxyadenosine	-0.8424	0.0022
Lactobacillus	Positive	D-Alanyl-D-alanine (D-Ala-D-Ala)	0.8424	0.0022
Ruminococcus torques	Negative	2'-Deoxyadenosine 5'-monophosphate (dAMP)	-0.8424	0.0022
Prevotella copri	Positive	2'-Deoxyadenosine 5'-monophosphate (dAMP)	0.8424	0.0022
Lactobacillus	Positive	gamma-L-Glutamyl-L-glutamic acid	0.8303	0.0029
Lactobacillus	Negative	Diaminopimelic acid	-0.8303	0.0029
Blautia producta	Negative	N-Acetylcadaverine	-0.8303	0.0029
Allobaculum	Negative	2'-Deoxyadenosine 5'-monophosphate (dAMP)	-0.8303	0.0029
Prevotella copri	Negative	Diacetyl	-0.8182	0.0038
Lactobacillus	Negative	D-Proline	-0.8182	0.0038
Lactobacillus	Negative	2'-Deoxyadenosine 5'-monophosphate (dAMP)	-0.8182	0.0038
Lactobacillus	Positive	3-Aminobutanoic acid	0.8182	0.0038
Ruminococcus torques	Positive	L-Citrulline	0.8061	0.0049
Lactobacillus	Positive	Glutaraldehyde	0.8061	0.0049
Prevotella copri	Negative	L-Glutamate	-0.8061	0.0049
Blautia producta	Negative	2'-Deoxyadenosine 5'-monophosphate (dAMP)	-0.8061	0.0049
Eubacterium	Negative	2'-Deoxyadenosine 5'-monophosphate (dAMP)	-0.8061	0.0049
Lactobacillus	Negative	L-Carnosine	-0.8061	0.0049
Lactobacillus	Positive	Cytosine	0.8061	0.0049
Lactobacillus	Negative	Daidzein	-0.8061	0.0049
Eubacterium biforme	Positive	Glutaraldehyde	0.7939	0.0061
Ruminococcus torques	Positive	L-Glutamate	0.7939	0.0061
Allobaculum	Positive	L-Glutamate	0.7939	0.0061
Ruminococcus torques	Positive	Acetylcholine	0.7939	0.0061
Faecalibacterium prausnitzii	Negative	Phosphoenolpyruvate	-0.7939	0.0061
Faecalibacterium	Negative	Phosphoenolpyruvate	-0.7939	0.0061
Lactobacillus	Positive	Dopamine	0.7939	0.0061
Lactobacillus	Negative	Flavin adenine dinucleotide (FAD)	-0.7939	0.0061
Blautia	Negative	2'-Deoxyadenosine 5'-monophosphate (dAMP)	-0.7939	0.0061
Prevotella copri	Negative	Adenine	-0.7939	0.0061
Other(<0.0005)	Negative	3-Aminobutanoic acid	-0.7939	0.0061
Clostridium spiroforme	Positive	Dopamine	0.7903	0.0065
Lactobacillus	Negative	D-Fructose 1,6-bisphosphate	-0.7818	0.0075
Lactobacillus	Positive	L-Glutamate	0.7818	0.0075
Lactobacillus	Positive	D-Glucose 6-phosphate	0.7818	0.0075
Ruminococcus torques	Positive	Diacetyl	0.7818	0.0075
Gemmiger formicilis	Negative	N-Acetylcadaverine	-0.7818	0.0075
Eubacterium biforme	Negative	N-Acetylcadaverine	-0.7818	0.0075
Other(<0.0005)	Positive	Flavin adenine dinucleotide (FAD)	0.7818	0.0075
Bacteroides plebeius	Negative	Adenine	-0.7818	0.0075
Lactobacillus helveticus	Negative	2-Hydroxyadenine	-0.7818	0.0075
Blautia producta	Positive	L-Citrulline	0.7697	0.0092

Lactobacillus	Negative	3.alpha.-Mannobiose	-0.7697	0.0092
Gemmiger formicilis	Positive	Glutaraldehyde	0.7697	0.0092
Ruminococcus torques	Positive	Creatine	0.7697	0.0092
Faecalibacterium prausnitzii	Positive	Ile-Asp	0.7697	0.0092
Faecalibacterium	Positive	Ile-Asp	0.7697	0.0092
Bacteroides plebeius	Negative	Acetylcholine	-0.7697	0.0092
Lactobacillus	Positive	Acetylcholine	0.7697	0.0092
Lactobacillus	Positive	Diacetyl	0.7697	0.0092
Eubacterium	Negative	3-Phospho-D-glycerate	-0.7697	0.0092
Eubacterium biforme	Negative	2'-Deoxyadenosine 5'-monophosphate (dAMP)	-0.7697	0.0092
Ruminococcus	Negative	2'-Deoxyadenosine 5'-monophosphate (dAMP)	-0.7697	0.0092
Bacteroides	Negative	Adenine	-0.7697	0.0092
Faecalibacterium prausnitzii	Positive	Cytosine	0.7697	0.0092
Faecalibacterium	Positive	Cytosine	0.7697	0.0092
Bacteroides plebeius	Positive	2-Hydroxyadenine	0.7697	0.0092
Adlercreutzia	Positive	Choline	0.7576	0.0111
Gemmiger	Positive	Glutaraldehyde	0.7576	0.0111
Bacteroides plebeius	Negative	Thr-Glu	-0.7576	0.0111
Lactobacillus	Positive	Ile-Asp	0.7576	0.0111
Blautia producta	Positive	L-Glutamate	0.7576	0.0111
Ruminococcus	Positive	L-Glutamate	0.7576	0.0111
Blautia	Positive	L-Glutamate	0.7576	0.0111
Blautia producta	Positive	Acetylcholine	0.7576	0.0111
Prevotella copri	Negative	Acetylcholine	-0.7576	0.0111
Prevotella copri	Negative	4-Aminobutyric acid	-0.7576	0.0111
Lactobacillus helveticus	Negative	N-Acetylcadaverine	-0.7576	0.0111
Eubacterium biforme	Negative	3-Phospho-D-glycerate	-0.7576	0.0111
Blautia producta	Negative	3-Phospho-D-glycerate	-0.7576	0.0111
Faecalibacterium prausnitzii	Negative	3-Phospho-D-glycerate	-0.7576	0.0111
Faecalibacterium	Negative	3-Phospho-D-glycerate	-0.7576	0.0111
Blautia producta	Negative	Phosphoenolpyruvate	-0.7576	0.0111
Lactobacillus	Positive	4-Hydroxybutanoic acid lactone	0.7576	0.0111
Ruminococcus torques	Positive	Adenine	0.7576	0.0111
Lactobacillus	Positive	Nicotinamide	0.7576	0.0111
Lactobacillus	Positive	L-Histidine	0.7576	0.0111
Prevotella copri	Negative	L-Citrulline	-0.7455	0.0133
Other(<0.0005)	Positive	3.alpha.-Mannobiose	0.7455	0.0133
Eubacterium	Positive	Glutaraldehyde	0.7455	0.0133
Bacteroides	Negative	Thr-Glu	-0.7455	0.0133
Faecalibacterium prausnitzii	Positive	gamma-L-Glutamyl-L-glutamic acid	0.7455	0.0133
Faecalibacterium	Positive	gamma-L-Glutamyl-L-glutamic acid	0.7455	0.0133
Lactobacillus	Positive	L-Pipecolic acid	0.7455	0.0133
Gemmiger	Positive	L-Glutamate	0.7455	0.0133
Eubacterium	Positive	L-Glutamate	0.7455	0.0133

Gemmiger	Negative	N-Acetylcadaverine	-0.7455	0.0133
Bacteroides	Positive	N-Acetylcadaverine	0.7455	0.0133
Gemmiger	Negative	2'-Deoxyadenosine 5'-monophosphate (dAMP)	-0.7455	0.0133
Blautia producta	Positive	Glycerophosphocholine	0.7455	0.0133
Slackia	Positive	Glycerophosphocholine	0.7455	0.0133
Other(<0.0005)	Negative	Acetylcarnitine	-0.7455	0.0133
Clostridium spiroforme	Positive	L-Proline	0.7416	0.0141
Bulleidia p-1630-c5	Positive	L-Citrulline	0.7333	0.0158
Faecalibacterium prausnitzii	Positive	L-Citrulline	0.7333	0.0158
Faecalibacterium	Positive	L-Citrulline	0.7333	0.0158
Lactobacillus	Positive	Cyclohexylamine	0.7333	0.0158
Blautia producta	Positive	Choline	0.7333	0.0158
Lactobacillus	Positive	Choline	0.7333	0.0158
Lactobacillus	Positive	Ala-Asp	0.7333	0.0158
Coprococcus	Negative	Diaminopimelic acid	-0.7333	0.0158
Blautia producta	Positive	D-Glucose 6-phosphate	0.7333	0.0158
Allobaculum	Positive	Diacetyl	0.7333	0.0158
Collinsella stercoris	Negative	N-Acetylcadaverine	-0.7333	0.0158
Faecalibacterium prausnitzii	Negative	N-Acetylcadaverine	-0.7333	0.0158
Eubacterium	Negative	N-Acetylcadaverine	-0.7333	0.0158
Blautia	Negative	N-Acetylcadaverine	-0.7333	0.0158
Faecalibacterium	Negative	N-Acetylcadaverine	-0.7333	0.0158
Eubacterium	Negative	Phosphoenolpyruvate	-0.7333	0.0158
Other(<0.0005)	Negative	trans-2-Hydroxycinnamic acid	-0.7333	0.0158
Gemmiger formicilis	Negative	2'-Deoxyadenosine 5'-monophosphate (dAMP)	-0.7333	0.0158
Slackia	Negative	2'-Deoxyadenosine 5'-monophosphate (dAMP)	-0.7333	0.0158
Lactobacillus	Positive	S-Methyl-5'-thioadenosine	0.7333	0.0158
Lactobacillus	Positive	Glycerophosphocholine	0.7333	0.0158
Lactobacillus	Positive	L-Proline	0.7333	0.0158
Clostridium spiroforme	Positive	S-Adenosylmethionine	0.7234	0.0180
Blautia	Positive	L-Citrulline	0.7212	0.0186
Lactobacillus	Positive	L-Citrulline	0.7212	0.0186
Blautia producta	Positive	Glutaraldehyde	0.7212	0.0186
Slackia	Positive	Glutaraldehyde	0.7212	0.0186
Lactobacillus	Positive	Ile-Glu	0.7212	0.0186
Coprococcus	Negative	D-Fructose 1,6-bisphosphate	-0.7212	0.0186
Faecalibacterium prausnitzii	Positive	Uridine 5'-diphosphate (UDP)	0.7212	0.0186
Faecalibacterium	Positive	Uridine 5'-diphosphate (UDP)	0.7212	0.0186
Lactobacillus	Positive	Uridine 5'-diphosphate (UDP)	0.7212	0.0186
Faecalibacterium prausnitzii	Negative	Deoxyadenosine	-0.7212	0.0186
Faecalibacterium	Negative	Deoxyadenosine	-0.7212	0.0186
Adlercreutzia	Positive	gamma-L-Glutamyl-L-glutamic acid	0.7212	0.0186
Faecalibacterium prausnitzii	Positive	Creatine	0.7212	0.0186
Faecalibacterium	Positive	Creatine	0.7212	0.0186

Gemmiger formicilis	Positive	L-Glutamate	0.7212	0.0186
Faecalibacterium prausnitzii	Positive	L-Glutamate	0.7212	0.0186
Faecalibacterium	Positive	L-Glutamate	0.7212	0.0186
Lactobacillus	Positive	N6,N6,N6-Trimethyl-L-lysine	0.7212	0.0186
Turicibacter	Positive	D-Glucose 6-phosphate	0.7212	0.0186
Blautia producta	Positive	Diacetyl	0.7212	0.0186
Blautia	Positive	Diacetyl	0.7212	0.0186
Coprococcus	Negative	N-Acetylcadaverine	-0.7212	0.0186
Enterococcus	Negative	3-Phospho-D-glycerate	-0.7212	0.0186
Adlercreutzia	Negative	3-Phospho-D-glycerate	-0.7212	0.0186
Eubacterium biforme	Positive	Glycerophosphocholine	0.7212	0.0186
Bacteroides	Positive	2-Hydroxyadenine	0.7212	0.0186
Anaerobiospirillum	Negative	Betaine	-0.7212	0.0186
Clostridium spiroforme	Positive	Phosphorylcholine	0.7173	0.0195
Clostridium spiroforme	Positive	3-Aminobutanoic acid	0.7112	0.0211
Gemmiger formicilis	Positive	L-Citrulline	0.7091	0.0217
Slackia	Positive	L-Citrulline	0.7091	0.0217
Bulleidia	Positive	L-Citrulline	0.7091	0.0217
Lactobacillus	Positive	P-Fluorophenylalanine	0.7091	0.0217
Bacteroides	Negative	Glycerol 3-phosphate	-0.7091	0.0217
Lactobacillus	Positive	Glycerol 3-phosphate	0.7091	0.0217
Coprococcus	Positive	Glutaraldehyde	0.7091	0.0217
Bacteroides	Negative	Glutaraldehyde	-0.7091	0.0217
Allobaculum	Positive	Glutaraldehyde	0.7091	0.0217
Bacteroides plebeius	Negative	Guanosine 5'-diphosphate (GDP)	-0.7091	0.0217
Lactobacillus	Positive	Ala-Glu	0.7091	0.0217
Bulleidia p-1630-c5	Positive	Uridine 5'-diphosphate (UDP)	0.7091	0.0217
Lactobacillus	Positive	alpha-D-Glucose 1-phosphate	0.7091	0.0217
Coprococcus	Negative	Deoxyadenosine	-0.7091	0.0217
Blautia producta	Positive	Creatine	0.7091	0.0217
Ruminococcus	Positive	Creatine	0.7091	0.0217
Lactobacillus	Positive	Creatine	0.7091	0.0217
Gemmiger	Negative	Diaminopimelic acid	-0.7091	0.0217
Blautia	Positive	Acetylcholine	0.7091	0.0217
Lactobacillus	Positive	4-Aminobutyric acid	0.7091	0.0217
Slackia	Negative	N-Acetylcadaverine	-0.7091	0.0217
Adlercreutzia	Negative	N-Acetylcadaverine	-0.7091	0.0217
Gemmiger formicilis	Negative	3-Phospho-D-glycerate	-0.7091	0.0217
Lactobacillus	Positive	D-Pipecolinic acid	0.7091	0.0217
Eubacterium biforme	Negative	Phosphoenolpyruvate	-0.7091	0.0217
Enterococcus	Negative	Phosphoenolpyruvate	-0.7091	0.0217
Bacteroides plebeius	Positive	2'-Deoxyadenosine 5'-monophosphate (dAMP)	0.7091	0.0217
Bulleidia p-1630-c5	Negative	2'-Deoxyadenosine 5'-monophosphate (dAMP)	-0.7091	0.0217
Allobaculum	Positive	Adenine	0.7091	0.0217

Blautia producta	Positive	Cytosine	0.7091	0.0217
Faecalibacterium prausnitzii	Negative	Daidzein	-0.7091	0.0217
Faecalibacterium	Negative	Daidzein	-0.7091	0.0217
Adlercreutzia	Positive	Glycerophosphocholine	0.7091	0.0217
Faecalibacterium prausnitzii	Positive	Betaine	0.7091	0.0217
Megamonas	Positive	Betaine	0.7091	0.0217
Faecalibacterium	Positive	Betaine	0.7091	0.0217
Clostridium spiroforme	Positive	N6,N6,N6-Trimethyl-L-lysine	0.6991	0.0245
Bacteroides plebeius	Negative	L-Citrulline	-0.6970	0.0251
Collinsella	Positive	Choline	0.6970	0.0251
Lactobacillus helveticus	Positive	Glutaraldehyde	0.6970	0.0251
Lactobacillus	Negative	Isomaltose	-0.6970	0.0251
Cetobacterium	Negative	D-Fructose 1,6-bisphosphate	-0.6970	0.0251
Lactobacillus	Positive	Thr-Glu	0.6970	0.0251
Ruminococcus torques	Positive	Uridine 5'-diphosphate (UDP)	0.6970	0.0251
Bulleidia	Positive	Uridine 5'-diphosphate (UDP)	0.6970	0.0251
Bulleidia p-1630-c5	Positive	Creatine	0.6970	0.0251
Prevotella copri	Negative	Creatine	-0.6970	0.0251
Enterococcus	Positive	D-Alanyl-D-alanine (D-Ala-D-Ala)	0.6970	0.0251
Bulleidia p-1630-c5	Positive	L-Glutamate	0.6970	0.0251
Slackia	Positive	L-Glutamate	0.6970	0.0251
Slackia	Negative	Diaminopimelic acid	-0.6970	0.0251
Adlercreutzia	Positive	N6,N6,N6-Trimethyl-L-lysine	0.6970	0.0251
Adlercreutzia	Positive	Acetylcholine	0.6970	0.0251
Dialister	Positive	D-Glucose 6-phosphate	0.6970	0.0251
Adlercreutzia	Positive	D-Glucose 6-phosphate	0.6970	0.0251
Bacteroides	Negative	D-Glucose 6-phosphate	-0.6970	0.0251
Blautia	Positive	D-Glucose 6-phosphate	0.6970	0.0251
Bacteroides plebeius	Negative	Diacetyl	-0.6970	0.0251
Ruminococcus	Positive	Diacetyl	0.6970	0.0251
Bacteroides plebeius	Positive	N-Acetylcadaverine	0.6970	0.0251
Collinsella	Negative	N-Acetylcadaverine	-0.6970	0.0251
Allobaculum	Negative	N-Acetylcadaverine	-0.6970	0.0251
Gemmiger	Negative	3-Phospho-D-glycerate	-0.6970	0.0251
Bifidobacterium adolescentis	Positive	4-Hydroxybutanoic acid lactone	0.6970	0.0251
Coprococcus	Negative	L-Carnosine	-0.6970	0.0251
Adlercreutzia	Positive	Nicotinamide	0.6970	0.0251
Eubacterium biforme	Positive	L-Citrulline	0.6848	0.0289
Gemmiger	Positive	L-Citrulline	0.6848	0.0289
Adlercreutzia	Positive	L-Citrulline	0.6848	0.0289
Ruminococcus	Positive	L-Citrulline	0.6848	0.0289
Bacteroides plebeius	Negative	Glycerol 3-phosphate	-0.6848	0.0289
Lactobacillus	Positive	Phosphorylcholine	0.6848	0.0289
Butyricicoccus pullicaecorum	Positive	Glutaraldehyde	0.6848	0.0289

Lactobacillus	Positive	DL-Indole-3-lactic acid	0.6848	0.0289
Bulleidia	Positive	Creatine	0.6848	0.0289
Eubacterium biforme	Positive	L-Glutamate	0.6848	0.0289
Bacteroides	Negative	L-Glutamate	-0.6848	0.0289
Bulleidia p-1630-c5	Positive	Diacetyl	0.6848	0.0289
Bifidobacterium adolescentis	Negative	3-Phospho-D-glycerate	-0.6848	0.0289
Collinsella stercoris	Negative	3-Phospho-D-glycerate	-0.6848	0.0289
Lactobacillus	Positive	(3-Carboxypropyl)trimethylammonium cation	0.6848	0.0289
Gemmiger formicilis	Negative	Phosphoenolpyruvate	-0.6848	0.0289
Adlercreutzia	Negative	Phosphoenolpyruvate	-0.6848	0.0289
Other(<0.0005)	Negative	Dopamine	-0.6848	0.0289
Faecalibacterium prausnitzii	Negative	2'-Deoxyadenosine 5'-monophosphate (dAMP)	-0.6848	0.0289
Bacteroides	Positive	2'-Deoxyadenosine 5'-monophosphate (dAMP)	0.6848	0.0289
Faecalibacterium	Negative	2'-Deoxyadenosine 5'-monophosphate (dAMP)	-0.6848	0.0289
Escherichia	Negative	L-Carnosine	-0.6848	0.0289
Blautia producta	Positive	Adenine	0.6848	0.0289
Blautia	Positive	Adenine	0.6848	0.0289
Lactobacillus	Positive	Adenine	0.6848	0.0289
Bacteroides plebeius	Negative	Glycerophosphocholine	-0.6848	0.0289
Lactobacillus helveticus	Positive	Glycerophosphocholine	0.6848	0.0289
Blautia	Positive	Glycerophosphocholine	0.6848	0.0289
Clostridium spiroforme	Negative	Flavin adenine dinucleotide (FAD)	-0.6748	0.0323
Eubacterium	Positive	L-Citrulline	0.6727	0.0330
Blautia	Positive	Choline	0.6727	0.0330
Lactobacillus	Positive	Ser-Asp	0.6727	0.0330
Bacteroides	Positive	D-Fructose 1,6-bisphosphate	0.6727	0.0330
Prevotella copri	Negative	Uridine 5'-diphosphate (UDP)	-0.6727	0.0330
Adlercreutzia	Positive	Uridine 5'-diphosphate (UDP)	0.6727	0.0330
Adlercreutzia	Negative	Deoxyadenosine	-0.6727	0.0330
Bacteroides plebeius	Negative	Creatine	-0.6727	0.0330
Lactobacillus	Positive	Uridine 5'-monophosphate (UMP)	0.6727	0.0330
Adlercreutzia	Positive	L-Pipecolic acid	0.6727	0.0330
Bacteroides plebeius	Negative	L-Glutamate	-0.6727	0.0330
Dialister	Positive	L-Glutamate	0.6727	0.0330
Bacteroides plebeius	Negative	D-Glucose 6-phosphate	-0.6727	0.0330
Ruminococcus torques	Positive	4-Aminobutyric acid	0.6727	0.0330
Bulleidia	Positive	Diacetyl	0.6727	0.0330
Eubacterium	Positive	Diacetyl	0.6727	0.0330
Adlercreutzia	Positive	Diacetyl	0.6727	0.0330
Dialister	Negative	N-Acetylcadaverine	-0.6727	0.0330
Bacteroides plebeius	Negative	N6-Acetyl-L-lysine	-0.6727	0.0330
Cetobacterium	Positive	N-Acetyl-L-Histidine	0.6727	0.0330
Slackia	Positive	D-Pipecolinic acid	0.6727	0.0330
Gemmiger	Negative	Phosphoenolpyruvate	-0.6727	0.0330

Blautia	Negative	Phosphoenolpyruvate	-0.6727	0.0330
Collinsella	Negative	Phosphoenolpyruvate	-0.6727	0.0330
Other(<0.0005)	Negative	L-Tyrosine	-0.6727	0.0330
Veillonella	Positive	trans-2-Hydroxycinnamic acid	0.6727	0.0330
Bulleidia	Negative	2'-Deoxyadenosine 5'-monophosphate (dAMP)	-0.6727	0.0330
Dialister	Negative	2'-Deoxyadenosine 5'-monophosphate (dAMP)	-0.6727	0.0330
Adlercreutzia	Negative	2'-Deoxyadenosine 5'-monophosphate (dAMP)	-0.6727	0.0330
Butyricicoccus	Negative	2'-Deoxyadenosine 5'-monophosphate (dAMP)	-0.6727	0.0330
Collinsella	Negative	2'-Deoxyadenosine 5'-monophosphate (dAMP)	-0.6727	0.0330
Adlercreutzia	Positive	Cytosine	0.6727	0.0330
Allobaculum	Negative	Daidzein	-0.6727	0.0330
Gemmiger formicilis	Positive	Glycerophosphocholine	0.6727	0.0330
Prevotella copri	Negative	Glycerophosphocholine	-0.6727	0.0330
Eubacterium	Positive	Glycerophosphocholine	0.6727	0.0330
Lactobacillus	Positive	L-Arginine	0.6727	0.0330
Lactobacillus	Positive	gamma-L-Glutamyl-L-phenylalanine	0.6606	0.0376
Ruminococcus torques	Positive	Choline	0.6606	0.0376
Ruminococcus	Positive	Uridine 5'-diphosphate (UDP)	0.6606	0.0376
Bacteroides	Negative	Dihydroxyfumarate	-0.6606	0.0376
Blautia	Positive	Creatine	0.6606	0.0376
Prevotella copri	Negative	L-Pipecolic acid	-0.6606	0.0376
Bulleidia	Positive	L-Glutamate	0.6606	0.0376
Collinsella	Positive	L-Glutamate	0.6606	0.0376
Lactobacillus	Positive	ADP-ribose	0.6606	0.0376
Gemmiger formicilis	Negative	Diaminopimelic acid	-0.6606	0.0376
Eubacterium	Negative	Diaminopimelic acid	-0.6606	0.0376
Bulleidia	Positive	Acetylcholine	0.6606	0.0376
Bacteroides	Negative	Acetylcholine	-0.6606	0.0376
Allobaculum	Positive	Acetylcholine	0.6606	0.0376
Prevotella copri	Negative	D-Glucose 6-phosphate	-0.6606	0.0376
Allobaculum	Positive	D-Glucose 6-phosphate	0.6606	0.0376
Blautia	Positive	4-Aminobutyric acid	0.6606	0.0376
Allobaculum	Positive	4-Aminobutyric acid	0.6606	0.0376
Other(<0.0005)	Positive	Stearidonic Acid	0.6606	0.0376
Ruminococcus torques	Positive	N6-Acetyl-L-lysine	0.6606	0.0376
Lactobacillus	Positive	N6-Acetyl-L-lysine	0.6606	0.0376
Slackia	Negative	3-Phospho-D-glycerate	-0.6606	0.0376
Blautia	Negative	3-Phospho-D-glycerate	-0.6606	0.0376
Prevotella copri	Negative	N-Acetyl-L-Histidine	-0.6606	0.0376
Faecalibacterium prausnitzii	Positive	D-Pipecolinic acid	0.6606	0.0376
Faecalibacterium	Positive	D-Pipecolinic acid	0.6606	0.0376
Collinsella stercoris	Negative	Phosphoenolpyruvate	-0.6606	0.0376
Allobaculum	Negative	Phosphoenolpyruvate	-0.6606	0.0376
Bifidobacterium adolescentis	Positive	L-Tyrosine	0.6606	0.0376

Lactobacillus	Positive	Ser-Glu	0.6606	0.0376
Lactobacillus	Positive	L-Phenylalanine	0.6606	0.0376
Faecalibacterium prausnitzii	Negative	L-Carnosine	-0.6606	0.0376
Faecalibacterium	Negative	L-Carnosine	-0.6606	0.0376
Dialister	Positive	Adenine	0.6606	0.0376
Ruminococcus	Positive	Adenine	0.6606	0.0376
Lactobacillus	Positive	Triethanolamine	0.6606	0.0376
Ruminococcus torques	Positive	Glycerophosphocholine	0.6606	0.0376
Gemmiger	Positive	Glycerophosphocholine	0.6606	0.0376
Veillonella	Positive	Acetylcarnitine	0.6606	0.0376
Coprococcus	Negative	2-Hydroxyadenine	-0.6606	0.0376
Cetobacterium	Negative	2-Hydroxyadenine	-0.6606	0.0376
Clostridium spiroforme	Positive	Acetylcarnitine	0.6565	0.0392
Catenibacterium	Negative	2-Hydroxyadenine	-0.6565	0.0392
Clostridium spiroforme	Negative	3.alpha.-Mannobiose	-0.6505	0.0417
Bacteroides_coprophilus	Negative	Betaine	-0.6505	0.0417
Collinsella	Positive	L-Citrulline	0.6485	0.0425
Allobaculum	Positive	L-Citrulline	0.6485	0.0425
Blautia producta	Positive	P-Fluorophenylalanine	0.6485	0.0425
Collinsella stercoris	Positive	Choline	0.6485	0.0425
Slackia	Positive	Choline	0.6485	0.0425
Butyricicoccus	Positive	Glutaraldehyde	0.6485	0.0425
Blautia	Positive	Glutaraldehyde	0.6485	0.0425
Bacteroides	Negative	Guanosine 5'-diphosphate (GDP)	-0.6485	0.0425
Gemmiger	Negative	D-Fructose 1,6-bisphosphate	-0.6485	0.0425
Bacteroides	Negative	L-Carnitine	-0.6485	0.0425
Bacteroides	Negative	Ala-Glu	-0.6485	0.0425
Faecalibacterium prausnitzii	Positive	L-Tryptophan	0.6485	0.0425
Faecalibacterium	Positive	L-Tryptophan	0.6485	0.0425
Anaerobiospirillum	Negative	Ile-Asp	-0.6485	0.0425
Coprococcus	Positive	L-Glutamate	0.6485	0.0425
Bulleidia p-1630-c5	Positive	Acetylcholine	0.6485	0.0425
Eubacterium biforme	Positive	Acetylcholine	0.6485	0.0425
Ruminococcus	Positive	Acetylcholine	0.6485	0.0425
Eubacterium biforme	Positive	D-Glucose 6-phosphate	0.6485	0.0425
Faecalibacterium prausnitzii	Positive	D-Glucose 6-phosphate	0.6485	0.0425
Eubacterium	Positive	D-Glucose 6-phosphate	0.6485	0.0425
Faecalibacterium	Positive	D-Glucose 6-phosphate	0.6485	0.0425
Blautia producta	Positive	4-Aminobutyric acid	0.6485	0.0425
Slackia	Positive	4-Aminobutyric acid	0.6485	0.0425
Adlercreutzia	Positive	4-Aminobutyric acid	0.6485	0.0425
Ruminococcus torques	Negative	N-Acetylcadaverine	-0.6485	0.0425
Coprococcus	Negative	3-Phospho-D-glycerate	-0.6485	0.0425
Collinsella	Negative	3-Phospho-D-glycerate	-0.6485	0.0425

Allobaculum	Negative	3-Phospho-D-glycerate	-0.6485	0.0425
Lactobacillus	Positive	N-Acetyl-L-Histidine	0.6485	0.0425
Gemmiger	Positive	D-Pipecolinic acid	0.6485	0.0425
Veillonella	Positive	L-Tyrosine	0.6485	0.0425
Butyricicoccus pullicaecorum	Negative	2'-Deoxyadenosine 5'-monophosphate (dAMP)	-0.6485	0.0425
Coprococcus	Negative	2'-Deoxyadenosine 5'-monophosphate (dAMP)	-0.6485	0.0425
Gemmiger	Negative	L-Carnosine	-0.6485	0.0425
Bulleidia p-1630-c5	Positive	Adenine	0.6485	0.0425
Lactobacillus	Positive	L-Fucose-1-phosphate	0.6485	0.0425
Anaerobiospirillum	Negative	Cytosine	-0.6485	0.0425
Collinsella	Positive	Cytosine	0.6485	0.0425
Lactobacillus	Positive	Cytidine 5'-monophosphate (CMP)	0.6485	0.0425
Turicibacter	Positive	Glycerophosphocholine	0.6485	0.0425
Bacteroides	Negative	Glycerophosphocholine	-0.6485	0.0425
Bifidobacterium adolescentis	Positive	Acetylcarnitine	0.6485	0.0425
Prevotella copri	Positive	2-Hydroxyadenine	0.6485	0.0425
Dialister	Negative	2-Hydroxyadenine	-0.6485	0.0425
Clostridium	Negative	2-Hydroxyadenine	-0.6485	0.0425
Clostridium spiroforme	Positive	trans-2-Hydroxycinnamic acid	0.6444	0.0443
Faecalibacterium prausnitzii	Positive	Cyclohexylamine	0.6364	0.0479
Faecalibacterium	Positive	Cyclohexylamine	0.6364	0.0479
Bacteroides plebeius	Negative	Glutaraldehyde	-0.6364	0.0479
Dialister	Positive	Glutaraldehyde	0.6364	0.0479
Lactobacillus	Positive	Guanosine 5'-diphosphate (GDP)	0.6364	0.0479
Gemmiger formicilis	Negative	D-Fructose 1,6-bisphosphate	-0.6364	0.0479
Lactobacillus	Positive	L-Carnitine	0.6364	0.0479
Bacteroides plebeius	Negative	Ala-Glu	-0.6364	0.0479
Blautia producta	Positive	Uridine 5'-diphosphate (UDP)	0.6364	0.0479
Blautia producta	Positive	gamma-L-Glutamyl-L-glutamic acid	0.6364	0.0479
Bacteroides plebeius	Negative	Dihydroxyfumarate	-0.6364	0.0479
Slackia	Positive	D-Glucose 6-phosphate	0.6364	0.0479
Collinsella	Positive	D-Glucose 6-phosphate	0.6364	0.0479
Eubacterium	Positive	4-Aminobutyric acid	0.6364	0.0479
Eubacterium biforme	Positive	Diacetyl	0.6364	0.0479
Blautia producta	Positive	N6-Acetyl-L-lysine	0.6364	0.0479
Adlercreutzia	Positive	D-Pipecolinic acid	0.6364	0.0479
Adlercreutzia	Positive	Dopamine	0.6364	0.0479
Lactobacillus	Positive	N6-Methyl-L-lysine	0.6364	0.0479
Collinsella stercoris	Negative	2'-Deoxyadenosine 5'-monophosphate (dAMP)	-0.6364	0.0479
Bulleidia	Positive	Adenine	0.6364	0.0479
Gemmiger	Negative	Daidzein	-0.6364	0.0479
Eubacterium	Negative	Daidzein	-0.6364	0.0479
Dialister	Positive	Glycerophosphocholine	0.6364	0.0479
Eubacterium biforme	Positive	Nicotinamide	0.6364	0.0479

Turicibacter	Positive	Nicotinamide	0.6364	0.0479
Prevotella	Negative	Uracil	-0.6364	0.0479
Ruminococcus torques	Negative	2-Hydroxyadenine	-0.6364	0.0479
Bulleidia	Negative	2-Hydroxyadenine	-0.6364	0.0479
Daidzein	Negative	sIgA	-0.9636	0.0000
L-Glutamate	Positive	sIgA	0.9515	0.0000
Phosphoenolpyruvate	Negative	sIgA	-0.9273	0.0001
2'-Deoxyadenosine 5'-monophosphate (dAMP)	Negative	sIgA	-0.9030	0.0003
1-Aminocyclopropanecarboxylic acid	Negative	IL-6	-0.8788	0.0008
3-Phospho-D-glycerate	Negative	sIgA	-0.8788	0.0008
Choline	Positive	sIgA	0.8667	0.0012
Glyceraldehyde 3-phosphate	Negative	IL-6	-0.8667	0.0012
Creatine	Positive	sIgA	0.8667	0.0012
Ile-Asp	Positive	sIgA	0.8667	0.0012
His-Ile	Negative	IL-6	-0.8667	0.0012
L-Citrulline	Positive	sIgA	0.8545	0.0016
DL-Indole-3-lactic acid	Positive	sIgA	0.8424	0.0022
Uridine 5'-diphosphate (UDP)	Positive	sIgA	0.8424	0.0022
L-Tryptophan	Negative	IL-6	-0.8424	0.0022
D-Alanyl-D-alanine (D-Ala-D-Ala)	Positive	sIgA	0.8424	0.0022
N-Acetylcadaverine	Negative	sIgA	-0.8424	0.0022
L-Carnosine	Negative	sIgA	-0.8424	0.0022
Dimethylaminopurine	Positive	IL-6	0.8424	0.0022
Adenosine 5'-diphosphate (ADP)	Negative	IL-6	-0.8424	0.0022
gamma-L-Glutamyl-L-glutamic acid	Positive	sIgA	0.8303	0.0029
4-Aminobutyric acid	Positive	sIgA	0.8303	0.0029
N6-Acetyl-L-lysine	Negative	IL-6	-0.8303	0.0029
D-Pipecolinic acid	Positive	sIgA	0.8303	0.0029
Cytosine	Positive	sIgA	0.8303	0.0029
Dihydroxyfumarate	Negative	IL-6	-0.8182	0.0038
Norharmane	Negative	IL-6	-0.8182	0.0038
D-Glucose 6-phosphate	Positive	sIgA	0.8182	0.0038
Adenosine monophosphate (AMP)	Positive	sIgA	0.8182	0.0038
Adenine	Positive	sIgA	0.8182	0.0038
S-Methyl-5'-thioadenosine	Positive	sIgA	0.8182	0.0038
His-Pro	Negative	IL-6	-0.8182	0.0038
Phe-Gln	Negative	IL-6	-0.8182	0.0038
P-Fluorophenylalanine	Positive	sIgA	0.8061	0.0049
Glutaraldehyde	Positive	sIgA	0.8061	0.0049
L-Tryptophan	Positive	sIgA	0.8061	0.0049
Diacetyl	Positive	sIgA	0.8061	0.0049
N-Acetyl-L-Histidine	Positive	sIgA	0.8061	0.0049
L-Fucose-1-phosphate	Positive	sIgA	0.8061	0.0049

2'-O-methylcytidine	Negative	IL-6	-0.7939	0.0061
Creatine	Negative	IL-6	-0.7939	0.0061
Diaminopimelic acid	Negative	sIgA	-0.7939	0.0061
Dimethylaminopurine	Negative	sIgA	-0.7939	0.0061
L-Histidine	Positive	sIgA	0.7939	0.0061
L-Carnitine	Positive	sIgA	0.7818	0.0075
Deoxyadenosine	Negative	sIgA	-0.7818	0.0075
Nicotinamide adenine dinucleotide (NAD)	Negative	IL-6	-0.7818	0.0075
Arg-Glu	Negative	IL-6	-0.7818	0.0075
Tyramine	Negative	IL-6	-0.7818	0.0075
Phe-Gln	Positive	sIgA	0.7818	0.0075
Adenosine 5'-diphosphate (ADP)	Positive	sIgA	0.7818	0.0075
L-Citrulline	Negative	IL-6	-0.7697	0.0092
L-Carnitine	Negative	IL-6	-0.7697	0.0092
Creatinine	Negative	IL-6	-0.7697	0.0092
gamma-L-Glutamyl-L-phenylalanine	Negative	IL-6	-0.7576	0.0111
Choline	Negative	IL-6	-0.7576	0.0111
Dihydroxyfumarate	Positive	sIgA	0.7576	0.0111
N6-Acetyl-L-lysine	Positive	sIgA	0.7576	0.0111
His-Pro	Positive	sIgA	0.7576	0.0111
Glycerophosphocholine	Positive	sIgA	0.7576	0.0111
L-Arginine	Positive	sIgA	0.7576	0.0111
Cyclohexylamine	Positive	sIgA	0.7455	0.0133
alpha-D-Glucose 1-phosphate	Positive	sIgA	0.7455	0.0133
Ile-Asp	Negative	IL-6	-0.7455	0.0133
Adenosine monophosphate (AMP)	Negative	IL-6	-0.7455	0.0133
Betaine	Negative	T-SOD	-0.7455	0.0133
Isomaltose	Negative	sIgA	-0.7333	0.0158
Ile-Glu	Positive	sIgA	0.7333	0.0158
Acetylcholine	Positive	sIgA	0.7333	0.0158
Stearidonic Acid	Negative	sIgA	-0.7333	0.0158
Adenine	Negative	IL-6	-0.7333	0.0158
S-Methyl-5'-thioadenosine	Negative	IL-6	-0.7333	0.0158
Nicotinamide	Positive	sIgA	0.7333	0.0158
P-Fluorophenylalanine	Negative	IL-6	-0.7212	0.0186
D-Fructose 1,6-bisphosphate	Negative	sIgA	-0.7212	0.0186
1-Aminocyclopropanecarboxylic acid	Positive	sIgA	0.7212	0.0186
Norharmane	Positive	sIgA	0.7212	0.0186
4-Hydroxybutanoic acid lactone	Positive	sIgA	0.7212	0.0186
L-Phenylalanine	Positive	sIgA	0.7212	0.0186
Betaine	Positive	sIgA	0.7212	0.0186
3-Phospho-D-glycerate	Negative	IgG	-0.7112	0.0211
Cyclohexylamine	Negative	IL-6	-0.7091	0.0217
Ser-Asp	Negative	IL-6	-0.7091	0.0217

Guanosine 5'-diphosphate (GDP)	Negative	IL-6	-0.7091	0.0217
Glyceraldehyde 3-phosphate	Positive	sIgA	0.7091	0.0217
alpha-D-Glucose 1-phosphate	Negative	IL-6	-0.7091	0.0217
D-Proline	Negative	sIgA	-0.7091	0.0217
Ser-Glu	Positive	sIgA	0.7091	0.0217
L-Arginine	Negative	IL-6	-0.7091	0.0217
gamma-L-Glutamyl-L-phenylalanine	Positive	sIgA	0.6970	0.0251
Creatinine	Positive	sIgA	0.6970	0.0251
Ala-Glu	Positive	sIgA	0.6970	0.0251
Nicotinamide adenine dinucleotide (NAD)	Positive	sIgA	0.6970	0.0251
Arg-Glu	Positive	sIgA	0.6970	0.0251
L-Phenylalanine	Negative	IL-6	-0.6970	0.0251
N6-Methyl-L-lysine	Negative	IL-6	-0.6970	0.0251
Acetylcarnitine	Positive	sIgA	0.6970	0.0251
Phosphoenolpyruvate	Negative	IgG	-0.6869	0.0282
Glycerol 3-phosphate	Positive	sIgA	0.6848	0.0289
Ser-Asp	Positive	sIgA	0.6848	0.0289
Ala-Asp	Positive	sIgA	0.6848	0.0289
Vanillin	Positive	sIgA	0.6848	0.0289
DL-Indole-3-lactic acid	Negative	IL-6	-0.6848	0.0289
2'-O-methylcytidine	Positive	sIgA	0.6848	0.0289
Uridine 5'-monophosphate (UMP)	Positive	sIgA	0.6848	0.0289
Uridine 5'-monophosphate (UMP)	Negative	IL-6	-0.6848	0.0289
L-Pipecolic acid	Positive	sIgA	0.6848	0.0289
(3-Carboxypropyl)trimethylammonium cation	Positive	sIgA	0.6848	0.0289
L-Tyrosine	Positive	sIgA	0.6848	0.0289
Cytosine	Negative	IL-6	-0.6848	0.0289
L-.alpha.-Amino-.gamma.-butyrolactone	Negative	IL-6	-0.6848	0.0289
Cytidine 5'-monophosphate (CMP)	Negative	IL-6	-0.6848	0.0289
4-Hydroxybutanoic acid lactone	Positive	IgG	0.6809	0.0302
gamma-L-Glutamyl-L-glutamic acid	Positive	IgG	0.6748	0.0323
Thr-Glu	Positive	sIgA	0.6727	0.0330
L-Glutamate	Negative	IL-6	-0.6727	0.0330
ADP-ribose	Positive	sIgA	0.6727	0.0330
N-Acetyl-L-Histidine	Negative	IL-6	-0.6727	0.0330
L-Fucose-1-phosphate	Negative	IL-6	-0.6727	0.0330
Glycerophosphocholine	Negative	IL-6	-0.6727	0.0330
L-Tyrosine	Positive	IgG	0.6687	0.0345
Thr-Glu	Negative	IL-6	-0.6606	0.0376
Vanillin	Negative	IL-6	-0.6606	0.0376
L-Aspartate	Negative	IL-6	-0.6606	0.0376
Tyramine	Positive	sIgA	0.6606	0.0376
N6-Methyl-L-lysine	Positive	sIgA	0.6606	0.0376

trans-2-Hydroxycinnamic acid	Positive	sIgA	0.6606	0.0376
L-.alpha.-Amino-.gamma.-butyrolactone	Positive	sIgA	0.6606	0.0376
Glycerol 3-phosphate	Negative	IL-6	-0.6485	0.0425
Isomaltose	Positive	IL-6	0.6485	0.0425
Ile-Glu	Negative	IL-6	-0.6485	0.0425
Guanosine 5'-diphosphate (GDP)	Positive	sIgA	0.6485	0.0425
gamma-L-Glutamyl-L-valine	Negative	IL-6	-0.6485	0.0425
Uridine 5'-diphosphate (UDP)	Negative	IL-6	-0.6485	0.0425
N6,N6,N6-Trimethyl-L-lysine	Positive	sIgA	0.6485	0.0425
(3-Carboxypropyl)trimethylammonium cation	Negative	IL-6	-0.6485	0.0425
L-Methionine	Positive	sIgA	0.6485	0.0425
L-Methionine	Negative	IL-6	-0.6485	0.0425
Acetylcarnitine	Positive	IgG	0.6444	0.0443
Ala-Asp	Negative	IL-6	-0.6364	0.0479
Ile-Asp	Negative	T-SOD	-0.6364	0.0479
D-Pipecolinic acid	Negative	IL-6	-0.6364	0.0479
Dopamine	Positive	sIgA	0.6364	0.0479
Flavin adenine dinucleotide (FAD)	Negative	sIgA	-0.6364	0.0479
L-Proline	Positive	sIgA	0.6364	0.0479