Supplementary Table 1 Interaction strength of correlation-based microbiota-metabolite functional modules

Metabolites	Target microbiome	Weight	Correlation
Omeprazole sulphone	Fusicatenibacter	0.122123412	positive
5-Hydroxyomeprazole	Fusicatenibacter	0.288071891	positive
DL-Tryptophan	Fusicatenibacter	0.231961135	positive
Indole-3-acrylic acid	Fusicatenibacter	0.222059236	positive
L-Phenylalanine	Fusicatenibacter	-0.066740012	negative
L-Tyrosine	Fusicatenibacter	-0.084166135	negative
Mycophenolic acid	Fusicatenibacter	0.272093894	positive
Stercobilin	Fusicatenibacter	0.439350892	positive
PE (14: 0e/22: 2)	Fusicatenibacter	0.104877161	positive
Homoarginine	Fusicatenibacter	0.285504733	positive
Phenylglyoxylic acid	Fusicatenibacter	0.279636941	positive

Methyl-2-aminobenzoate	Fusicatenibacter	0.55468967	positive
3-Methoxytyramine	Fusicatenibacter	0.494178069	positive
3-[(3-chloro-4-hydroxy-5-methylanilino)methylidene]pentane-2,4-dione	Fusicatenibacter	0.271568728	positive
Feruloyl Putrescine	Fusicatenibacter	0.030622537	positive
1-benzyl-4-(4-nitrophenyl)piperazine	Fusicatenibacter	0.147048048	positive
EMH	Fusicatenibacter	0.390172377	positive
2-Hydroxycinnamic acid	Fusicatenibacter	-0.083799398	negative
Methyl nicotinate	Fusicatenibacter	0.559090513	positive
Lysopa 16: 0	Fusicatenibacter	0.066006605	positive
Omeprazole sulphone	Ruminococcus2	0.196516957	positive
5-Hydroxyomeprazole	Ruminococcus2	0.297525206	positive
DL-Tryptophan	Ruminococcus2	0.142071494	positive
Indole-3-acrylic acid	Ruminococcus2	0.140238313	positive

L-Phenylalanine	Ruminococcus2	-0.221061315	negative
L-Tyrosine	Ruminococcus2	-0.319706691	negative
Mycophenolic acid	Ruminococcus2	0.076986528	positive
Stercobilin	Ruminococcus2	-0.112373969	negative
PE (14: 0e/22: 2)	Ruminococcus2	0.24214096	positive
Homoarginine	Ruminococcus2	-0.387167736	negative
Phenylglyoxylic acid	Ruminococcus2	0.003483043	positive
Methyl-2-aminobenzoate	Ruminococcus2	-0.038863428	negative
3-Methoxytyramine	Ruminococcus2	0.066361137	positive
3-[(3-chloro-4-hydroxy-5-methylanilino)methylidene]pentane-2,4-dione	Ruminococcus2	0.105774519	positive

Feruloyl Putrescine	Ruminococcus2	-0.035563703	negative
1-benzyl-4-(4-nitrophenyl)piperazine	Ruminococcus2	0.410594814	positive
EMH	Ruminococcus2	0.25533865	positive
2-Hydroxycinnamic acid	Ruminococcus2	-0.324289643	negative
Methyl nicotinate	Ruminococcus2	0.037580202	positive
Lysopa 16: 0	Ruminococcus2	-0.098066172	negative
Omeprazole sulphone	Enterococcus	-0.140142809	negative
5-Hydroxyomeprazole	Enterococcus	-0.318206613	negative
DL-Tryptophan	Enterococcus	-0.127365082	negative
Indole-3-acrylic acid	Enterococcus	-0.124479789	negative

L-Phenylalanine	Enterococcus	-0.10427318	negative
L-Tyrosine	Enterococcus	-0.016899574	negative
Mycophenolic acid	Enterococcus	-0.404316164	negative
Stercobilin	Enterococcus	0.114175171	positive
PE (14: 0e/22: 2)	Enterococcus	0.044099724	positive
Homoarginine	Enterococcus	-0.105519291	negative
Phenylglyoxylic acid	Enterococcus	-0.174766326	negative
Methyl-2-aminobenzoate	Enterococcus	-0.264622598	negative
3-Methoxytyramine	Enterococcus	-0.350769206	negative
3-[(3-chloro-4-hydroxy-5-methylanilino)methylidene]pentane-2,4-dione	Enterococcus	-0.223816309	negative

Feruloyl Putrescine	Enterococcus	-0.209389844	negative
1-benzyl-4-(4-nitrophenyl)piperazine	Enterococcus	-0.147136463	negative
EMH	Enterococcus	-0.376290171	negative
2-Hydroxycinnamic acid	Enterococcus	-0.020609237	negative
Methyl nicotinate	Enterococcus	-0.270393184	negative
Lysopa 16: 0	Enterococcus	-0.240693822	negative
Omeprazole sulphone	Butyricicoccus	0.147190909	positive
5-Hydroxyomeprazole	Butyricicoccus	0.027128586	positive
DL-Tryptophan	Butyricicoccus	-0.053890569	negative
Indole-3-acrylic acid	Butyricicoccus	-0.055356979	negative

L-Phenylalanine	Butyricicoccus	-0.222140762	negative
L-Tyrosine	Butyricicoccus	-0.116946202	negative
Mycophenolic acid	Butyricicoccus	0.174853372	positive
Stercobilin	Butyricicoccus	-0.122445239	negative
PE (14: 0e/22: 2)	Butyricicoccus	0.05755132	positive
Homoarginine	Butyricicoccus	-0.042709193	negative
Phenylglyoxylic acid	Butyricicoccus	0.259004675	positive
Methyl-2-aminobenzoate	Butyricicoccus	0.160021997	positive
3-Methoxytyramine	Butyricicoccus	0.21592888	positive
3-[(3-chloro-4-hydroxy-5-methylanilino)methylidene]pentane-2,4-dione	Butyricicoccus	0.157272478	positive
Feruloyl Putrescine	Butyricicoccus	-0.028594996	negative

1-benzyl-4-(4-nitrophenyl)piperazine	Butyricicoccus	0.161656891	positive
EMH	Butyricicoccus	0.214442815	positive
2-Hydroxycinnamic acid	Butyricicoccus	-0.131976905	negative
Methyl nicotinate	Butyricicoccus	0.256071855	positive
Lysopa 16: 0	Butyricicoccus	0.351906158	positive
Omeprazole sulphone	Parabacteroides	-0.168515639	negative
5-Hydroxyomeprazole	Parabacteroides	-0.070413499	negative
DL-Tryptophan	Parabacteroides	0.217108287	positive
Indole-3-acrylic acid	Parabacteroides	0.220775657	positive
L-Phenylalanine	Parabacteroides	0.281261478	positive
L-Tyrosine	Parabacteroides	0.078481712	positive
Mycophenolic acid	Parabacteroides	-0.064539792	negative

Stercobilin	Parabacteroides	0.02548822	positive
PE (14: 0e/22: 2)	Parabacteroides	-0.021268795	negative
Homoarginine	Parabacteroides	0.227560291	positive
Phenylglyoxylic acid	Parabacteroides	-0.036490329	negative
Methyl-2-aminobenzoate	Parabacteroides	0.098468877	positive
3-Methoxytyramine	Parabacteroides	-0.090950769	negative
3-[(3-chloro-4-hydroxy-5-methylanilino)methylidene]pentane-2,4-dione	Parabacteroides	-0.165765111	negative
Feruloyl Putrescine	Parabacteroides	0.266984515	positive
1-benzyl-4-(4-nitrophenyl)piperazine	Parabacteroides	-0.199486629	negative
EMH	Parabacteroides	-0.074074079	negative
2-Hydroxycinnamic acid	Parabacteroides	0.068946551	positive

Methyl nicotinate	Parabacteroides	0.070963604	positive
Lysopa 16: 0	Parabacteroides	0.22148883	positive
Omeprazole sulphone	Lactobacillus	-0.281539428	negative
5-Hydroxyomeprazole	Lactobacillus	-0.27340245	negative
DL-Tryptophan	Lactobacillus	-0.134978101	negative
Indole-3-acrylic acid	Lactobacillus	-0.140338933	negative
L-Phenylalanine	Lactobacillus	-0.043457051	negative
L-Tyrosine	Lactobacillus	-0.024315204	negative
Mycophenolic acid	Lactobacillus	-0.277014768	negative
Stercobilin	Lactobacillus	0.07428582	positive

PE (14: 0e/22: 2)	Lactobacillus	-0.045371458	negative
Lactobacillus	Homoarginine	0.105014877	positive
Phenylglyoxylic acid	Lactobacillus	-0.017326976	negative
Methyl-2-aminobenzoate	Lactobacillus	-0.240758811	negative
3-Methoxytyramine	Lactobacillus	-0.347113895	negative
3-[(3-chloro-4-hydroxy-5-methylanilino)methylidene]pentane-2,4-dione	Lactobacillus	-0.021443329	negative
Feruloyl Putrescine	Lactobacillus	-0.199882464	negative
1-benzyl-4-(4-nitrophenyl)piperazine	Lactobacillus	-0.185697533	negative
EMH	Lactobacillus	-0.214605083	negative

2-Hydroxycinnamic acid	Lactobacillus	-0.022592079	negative
Methyl nicotinate	Lactobacillus	-0.35218754	negative
Lysopa 16: 0	Lactobacillus	-0.185506089	negative
Omeprazole sulphone	Eubacterium	-0.094815207	negative
5-Hydroxyomeprazole	Eubacterium	0.035797578	positive
DL-Tryptophan	Eubacterium	0.271674593	positive
Indole-3-acrylic acid	Eubacterium	0.275157601	positive
L-Phenylalanine	Eubacterium	-0.058044807	negative
L-Tyrosine	Eubacterium	-0.002128505	negative
Mycophenolic acid	Eubacterium	-0.114541752	negative

Stercobilin	Eubacterium	0.283091118	positive
PE (14: 0e/22: 2)	Eubacterium	-0.142403259	negative
Homoarginine	Eubacterium	0.171247874	positive
Phenylglyoxylic acid	Eubacterium	0.071982157	positive
Methyl-2-aminobenzoate	Eubacterium	0.513163121	positive
3-Methoxytyramine	Eubacterium	0.391064354	positive
3-[(3-chloro-4-hydroxy-5-methylanilino)methylidene]pentane-2,4-dione	Eubacterium	0.128677781	positive
Feruloyl Putrescine	Eubacterium	-0.081463678	negative
1-benzyl-4-(4-nitrophenyl)piperazine	Eubacterium	-0.011608961	negative
EMH	Eubacterium	0.088615072	positive
2-Hydroxycinnamic acid	Eubacterium	-0.002515505	negative

Methyl nicotinate	Eubacterium	0.53560917	positive
Lysopa 16: 0	Eubacterium	0.139307536	positive
Omeprazole sulphone	Megasphaera	0.032576427	positive
5-Hydroxyomeprazole	Megasphaera	-0.024385245	negative
DL-Tryptophan	Megasphaera	-0.069013067	negative
Indole-3-acrylic acid	Megasphaera	-0.068259855	negative
L-Phenylalanine	Megasphaera	-0.064582026	negative
L-Tyrosine	Megasphaera	-0.026268275	negative
Mycophenolic acid	Megasphaera	-0.199206367	negative
Stercobilin	Megasphaera	0.052442399	positive

PE (14: 0e/22: 2)	Megasphaera	-0.084163749	negative
Megasphaera	Homoarginine	-0.202519929	negative
Phenylglyoxylic acid	Megasphaera	-0.163541198	negative
Methyl-2-aminobenzoate	Megasphaera	-0.319079516	negative
3-Methoxytyramine	Megasphaera	-0.236037871	negative
3-[(3-chloro-4-hydroxy-5-methylanilino)methylidene]pentane-2,4-dione	Megasphaera	0.015911608	positive
Feruloyl Putrescine	Megasphaera	0.054513733	positive
1-benzyl-4-(4-nitrophenyl)piperazine	Megasphaera	0.176800358	positive
EMH	Megasphaera	-0.022217723	negative
2-Hydroxycinnamic acid	Megasphaera	-0.036624943	negative

Methyl nicotinate	Megasphaera	-0.195929322	negative
Lysopa 16: 0	Megasphaera	-0.205043227	negative
Omeprazole sulphone	Roseburia	-0.175558067	negative
5-Hydroxyomeprazole	Roseburia	0.088513586	positive
DL-Tryptophan	Roseburia	0.139932267	positive
Indole-3-acrylic acid	Roseburia	0.132219465	positive
L-Phenylalanine	Roseburia	0.038193234	positive
L-Tyrosine	Roseburia	-0.074924363	negative
Mycophenolic acid	Roseburia	-0.017627646	negative
Stercobilin	Roseburia	0.248095135	positive
PE (14: 0e/22: 2)	Roseburia	-0.075284739	negative

Homoarginine	Roseburia	0.184556336	positive
Phenylglyoxylic acid	Roseburia	-0.075475278	negative
Methyl-2-aminobenzoate	Roseburia	0.280782725	positive
3-Methoxytyramine	Roseburia	0.205674723	positive
3-[(3-chloro-4-hydroxy-5-methylanilino)methylidene]pentane-2,4-dione	Roseburia	-0.053255062	negative
Feruloyl Putrescine	Roseburia	-0.056927825	negative
1-benzyl-4-(4-nitrophenyl)piperazine	Roseburia	0.012853492	positive
EMH	Roseburia	0.104296907	positive
2-Hydroxycinnamic acid	Roseburia	-0.074189811	negative
Methyl nicotinate	Roseburia	0.230465873	positive
Lysopa 16: 0	Roseburia	0.070143343	positive

Omeprazole sulphone	Ruminococcus	-0.095439966	negative
5-Hydroxyomeprazole	Ruminococcus	0.209453028	positive
DL-Tryptophan	Ruminococcus	0.088452069	positive
Indole-3-acrylic acid	Ruminococcus	0.084590336	positive
L-Phenylalanine	Ruminococcus	-0.081824456	negative
L-Tyrosine	Ruminococcus	0.029054942	positive
Mycophenolic acid	Ruminococcus	-0.07594045	negative
Stercobilin	Ruminococcus	0.257448849	positive
PE (14: 0e/22: 2)	Ruminococcus	-0.080169579	negative
Homoarginine	Ruminococcus	0.105186244	positive
Phenylglyoxylic acid	Ruminococcus	0.058661559	positive
Methyl-2-aminobenzoate	Ruminococcus	0.359876713	positive

3-Methoxytyramine	Ruminococcus	0.225819419	positive
3-[(3-chloro-4-hydroxy-5-methylanilino)methylidene]pentane-2,4-dione	Ruminococcus	0.111070789	positive
Feruloyl Putrescine	Ruminococcus	-0.185363171	negative
1-benzyl-4-(4-nitrophenyl)piperazine	Ruminococcus	0.064540189	positive
EMH	Ruminococcus	0.214214587	positive
2-Hydroxycinnamic acid	Ruminococcus	0.034571703	positive
Methyl nicotinate	Ruminococcus	0.321259385	positive
Lysopa 16: 0	Ruminococcus	0.252460625	positive
Omeprazole sulphone	Blautia	-0.002566218	negative
5-Hydroxyomeprazole	Blautia	0.195215838	positive
DL-Tryptophan	Blautia	0.115479792	positive
Indole-3-acrylic acid	Blautia	0.108514344	positive

L-Phenylalanine	Blautia	-0.066715543	negative
L-Tyrosine	Blautia	0.022912657	positive
Mycophenolic acid	Blautia	-0.055351906	negative
Stercobilin	Blautia	0.153789754	positive
PE (14: 0e/22: 2)	Blautia	-0.111436955	negative
Homoarginine	Blautia	0.007332055	positive
Phenylglyoxylic acid	Blautia	0.029511502	positive
Methyl-2-aminobenzoate	Blautia	0.139858859	positive
3-Methoxytyramine	Blautia	0.190083403	positive
3-[(3-chloro-4-hydroxy-5-methylanilino)methylidene]pentane-2,4-dione	Blautia	0.159288792	positive
Feruloyl Putrescine	Blautia	0.165154432	positive
1-benzyl-4-(4-nitrophenyl)piperazine	Blautia	0.106671554	positive

EMH	Blautia	0.122067449	positive
2-Hydroxycinnamic acid	Blautia	0.018146824	positive
Methyl nicotinate	Blautia	0.236641922	positive
Lysopa 16: 0	Blautia	0.166788856	positive
Omeprazole sulphone	Akkermansia	-0.116310494	negative
5-Hydroxyomeprazole	Akkermansia	0.06470127	positive
DL-Tryptophan	Akkermansia	0.173801651	positive
Indole-3-acrylic acid	Akkermansia	0.168488937	positive
L-Phenylalanine	Akkermansia	0.302417514	positive
L-Tyrosine	Akkermansia	0.146289381	positive
Mycophenolic acid	Akkermansia	0.033770588	positive
Stercobilin	Akkermansia	0.097526254	positive
PE (14: 0e/22: 2)	Akkermansia	-0.078924521	negative

Homoarginine	Akkermansia	0.023907214	positive
Phenylglyoxylic acid	Akkermansia	-0.060147515	negative
Methyl-2-aminobenzoate	Akkermansia	-0.0734293	negative
3-Methoxytyramine	Akkermansia	-0.115172055	negative
3-[(3-chloro-4-hydroxy-5-methylanilino)methylidene]pentane-2,4-dione	Akkermansia	-0.007399852	negative
Feruloyl Putrescine	Akkermansia	0.406232899	positive
1-benzyl-4-(4-nitrophenyl)piperazine	Akkermansia	0.039841705	positive
EMH	Akkermansia	0.169991275	positive
2-Hydroxycinnamic acid	Akkermansia	0.144012504	positive
Methyl nicotinate	Akkermansia	-0.034722382	negative
Lysopa 16: 0	Akkermansia	0.197690746	positive
Omeprazole sulphone	Citrobacter	0.176695036	positive

5-Hydroxyomeprazole	Citrobacter	0.018056427	positive
DL-Tryptophan	Citrobacter	-0.062276248	negative
Indole-3-acrylic acid	Citrobacter	-0.06190775	negative
L-Phenylalanine	Citrobacter	0.016949378	positive
L-Tyrosine	Citrobacter	0.136344449	positive
Mycophenolic acid	Citrobacter	0.016212449	positive
Stercobilin	Citrobacter	-0.101337091	negative
PE (14: 0e/22: 2)	Citrobacter	-0.123067223	negative
Homoarginine	Citrobacter	-0.123078503	negative
Phenylglyoxylic acid	Citrobacter	-0.221099107	negative

Methyl-2-aminobenzoate	Citrobacter	-0.173562799	negative
3-Methoxytyramine	Citrobacter	0.00257949	positive
3-[(3-chloro-4-hydroxy-5-methylanilino)methylidene]pentane-2,4-dione	Citrobacter	0.244314513	positive
Feruloyl Putrescine	Citrobacter	-0.110181055	negative
1-benzyl-4-(4-nitrophenyl)piperazine	Citrobacter	0.154018261	positive
EMH	Citrobacter	-0.057112035	negative
2-Hydroxycinnamic acid	Citrobacter	0.144082918	positive
Methyl nicotinate	Citrobacter	-0.099494598	negative
Lysopa 16: 0	Citrobacter	0.053058923	positive
	Dialister	0.138279524	positive
5-Hydroxyomeprazole	Dialister	0.122303005	positive

DL-Tryptophan	Dialister	0.092186349	positive
Indole-3-acrylic acid	Dialister	0.089248139	positive
L-Phenylalanine	Dialister	0	positive
L-Tyrosine	Dialister	0.066477009	positive
Mycophenolic acid	Dialister	0.434080791	positive
Stercobilin	Dialister	-0.025342064	negative
PE (14: 0e/22: 2)	Dialister	-0.012853492	negative
Homoarginine	Dialister	-0.039298563	negative
Phenylglyoxylic acid	Dialister	0.019465643	positive
Methyl-2-aminobenzoate	Dialister	0.267744416	positive
3-Methoxytyramine	Dialister	0.246075115	positive
3-[(3-chloro-4-hydroxy-5-methylanilino)methylidene]pentane-2,4-dione	Dialister	0.254889746	positive

Feruloyl Putrescine	Dialister	-0.024974788	negative
1-benzyl-4-(4-nitrophenyl)piperazine	Dialister	0.210062785	positive
EMH	Dialister	0.127065951	positive
2-Hydroxycinnamic acid	Dialister	0.063171522	positive
Methyl nicotinate	Dialister	0.227711301	positive
Lysopa 16: 0	Dialister	-0.026441469	negative
Omeprazole sulphone	Streptococcus	-0.151590139	negative
5-Hydroxyomeprazole	Streptococcus	-0.359270463	negative
DL-Tryptophan	Streptococcus	0.023095958	positive
Indole-3-acrylic acid	Streptococcus	0.022729356	positive
L-Phenylalanine	Streptococcus	0.050953079	positive
L-Tyrosine	Streptococcus	0.113280176	positive

Mycophenolic acid	Streptococcus	-0.181085044	negative
Stercobilin	Streptococcus	0.103381909	positive
PE (14: 0e/22: 2)	Streptococcus	-0.100073314	negative
Homoarginine	Streptococcus	0.02327926	positive
Phenylglyoxylic acid	Streptococcus	0.085601687	positive
Methyl-2-aminobenzoate	Streptococcus	-0.197782056	negative
3-Methoxytyramine	Streptococcus	-0.248189901	negative
3-[(3-chloro-4-hydroxy-5-methylanilino)methylidene]pentane-2,4-dione	Streptococcus	-0.174136194	negative
Feruloyl Putrescine	Streptococcus	-0.018696728	negative
1-benzyl-4-(4-nitrophenyl)piperazine	Streptococcus	-0.170087977	negative

EMH	Streptococcus	-0.090175953	negative
2-Hydroxycinnamic acid	Streptococcus	0.109614151	positive
Methyl nicotinate	Streptococcus	-0.244707177	negative
Lysopa 16: 0	Streptococcus	0.037756598	positive
Omeprazole sulphone	Bifidobacterium	-0.008065255	negative
5-Hydroxyomeprazole	Bifidobacterium	0.329575659	positive
DL-Tryptophan	Bifidobacterium	-0.049857942	negative
Indole-3-acrylic acid	Bifidobacterium	-0.054623774	negative
L-Phenylalanine	Bifidobacterium	-0.248167155	negative
L-Tyrosine	Bifidobacterium	-0.269452847	negative

Mycophenolic acid	Bifidobacterium	0.070014663	positive
Stercobilin	Bifidobacterium	-0.019613234	negative
PE (14: 0e/22: 2)	Bifidobacterium	0.170454545	positive
Homoarginine	Bifidobacterium	-0.095133352	negative
Phenylglyoxylic acid	Bifidobacterium	-0.136926039	negative
Methyl-2-aminobenzoate	Bifidobacterium	-0.000916506	negative
3-Methoxytyramine	Bifidobacterium	0.113646779	positive
3-[(3-chloro-4-hydroxy-5-methylanilino)methylidene]pentane-2,4-dione	Bifidobacterium	0.118046009	positive
Feruloyl Putrescine	Bifidobacterium	0.104848319	positive
1-benzyl-4-(4-nitrophenyl)piperazine	Bifidobacterium	-0.012463343	negative
EMH	Bifidobacterium	0.048020528	positive

2-Hydroxycinnamic acid	Bifidobacterium	-0.268719642	negative
Methyl nicotinate	Bifidobacterium	0.022912657	positive
Lysopa 16: 0	Bifidobacterium	-0.066715543	negative
Omeprazole sulphone	Phascolarctobacterium	-0.034621564	negative
5-Hydroxyomeprazole	Phascolarctobacterium	-0.053235308	negative
DL-Tryptophan	Phascolarctobacterium	0.013588033	positive
Indole-3-acrylic acid	Phascolarctobacterium	0.018799882	positive
L-Phenylalanine	Phascolarctobacterium	0.081334608	positive
L-Tyrosine	Phascolarctobacterium	-0.055096683	negative
Mycophenolic acid	Phascolarctobacterium	-0.199521051	negative

Stercobilin	Phascolarctobacterium	-0.004467299	negative
PE (14: 0e/22: 2)	Phascolarctobacterium	0.215899645	positive
Homoarginine	Phascolarctobacterium	0.132715996	positive
Phascolarctobacterium	Phascolarctobacterium	0.073710427	positive
Methyl-2-aminobenzoate	Phascolarctobacterium	0.071104503	positive
3-Methoxytyramine	Phascolarctobacterium	0.03276019	positive
3-[(3-chloro-4-hydroxy-5-methylanilino)methylidene]pentane-2,4-dione	Phascolarctobacterium	-0.003350474	negative
Feruloyl Putrescine	Phascolarctobacterium	0.158589101	positive
1-benzyl-4-(4-nitrophenyl)piperazine	Phascolarctobacterium	0.035548993	positive
EMH	Phascolarctobacterium	0.162296974	positive
2-Hydroxycinnamic acid	Phascolarctobacterium	-0.063100593	negative
Methyl nicotinate	Phascolarctobacterium	0.065706517	positive

Lysopa 16: 0	Phascolarctobacterium	0.209385431	positive
Omeprazole sulphone	Clostridium_XlVa	0.02621208	positive
5-Hydroxyomeprazole	Clostridium_XlVa	0.001099808	positive
DL-Tryptophan	Clostridium_XlVa	-0.089084411	negative
Indole-3-acrylic acid	Clostridium_XlVa	-0.092750436	negative
L-Phenylalanine	Clostridium_XlVa	-0.115469208	negative
L-Tyrosine	Clostridium_XlVa	-0.110713959	negative
Mycophenolic acid	Clostridium_XlVa	0.034090909	positive
Stercobilin	Clostridium_XlVa	-0.195399139	negative
PE (14: 0e/22: 2)	Clostridium_XlVa	0.262829912	positive
Homoarginine	Clostridium_XlVa	-0.153606453	negative

Phenylglyoxylic acid	Clostridium_XlVa	-0.228759968	negative
Methyl-2-aminobenzoate	Clostridium_XlVa	-0.13417652	negative
3-Methoxytyramine	Clostridium_XlVa	-0.083585373	negative
3-[(3-chloro-4-hydroxy-5-methylanilino)methylidene]pentane-2,4-dione	Clostridium_XlVa	0.127211072	positive
Feruloyl Putrescine	Clostridium_XlVa	0.248556504	positive
1-benzyl-4-(4-nitrophenyl)piperazine	Clostridium_XlVa	0.0271261	positive
EMH	Clostridium_XlVa	-0.093475073	negative
2-Hydroxycinnamic acid	Clostridium_XlVa	-0.109247549	negative
Methyl nicotinate	Clostridium_XlVa	0.046925122	positive
Lysopa 16: 0	Clostridium_XlVa	0.198313783	positive

Omeprazole sulphone	Lachnospiracea_incertae_sedis	-0.157455779	negative
5-Hydroxyomeprazole	Lachnospiracea_incertae_sedis	-0.131610302	negative
DL-Tryptophan	Lachnospiracea_incertae_sedis	-0.074053708	negative
Indole-3-acrylic acid	Lachnospiracea_incertae_sedis	-0.079552745	negative
L-Phenylalanine	Lachnospiracea_incertae_sedis	-0.286656891	negative
L-Tyrosine	Lachnospiracea_incertae_sedis	-0.335074697	negative
Mycophenolic acid	Lachnospiracea_incertae_sedis	-0.017961877	negative
Stercobilin	Lachnospiracea_incertae_sedis	0.068188067	positive
PE (14: 0e/22: 2)	Lachnospiracea_incertae_sedis	0.03042522	positive
Homoarginine	Lachnospiracea_incertae_sedis	-0.041609385	negative

Phenylglyoxylic acid	Lachnospiracea_incertae_sedis	0.092200532	positive
Methyl-2-aminobenzoate	Lachnospiracea_incertae_sedis	-0.053340666	negative
3-Methoxytyramine	Lachnospiracea_incertae_sedis	0.01026487	positive
3-[(3-chloro-4-hydroxy-5-methylanilino)methylidene]pentane-2,4-dione	Lachnospiracea_incertae_sedis	-0.076253323	negative
Feruloyl Putrescine	Lachnospiracea_incertae_sedis	0.079186143	positive
1-benzyl-4-(4-nitrophenyl)piperazine	Lachnospiracea_incertae_sedis	-0.15872434	negative
EMH	Lachnospiracea_incertae_sedis	0.126099707	positive
2-Hydroxycinnamic acid	Lachnospiracea_incertae_sedis	-0.336541107	negative
Methyl nicotinate	Lachnospiracea_incertae_sedis	0.163688022	positive
Lysopa 16: 0	Lachnospiracea_incertae_sedis	-0.055718475	negative
Omeprazole sulphone	Veillonella	-0.235078399	negative

5-Hydroxyomeprazole	Veillonella	-0.411112145	negative
DL-Tryptophan	Veillonella	-0.099018982	negative
Indole-3-acrylic acid	Veillonella	-0.097552034	negative
L-Phenylalanine	Veillonella	-0.120278703	negative
L-Tyrosine	Veillonella	-0.115155409	negative
Mycophenolic acid	Veillonella	-0.289695656	negative
Stercobilin	Veillonella	0.167048691	positive
PE (14: 0e/22: 2)	Veillonella	-0.08617529	negative
Homoarginine	Veillonella	-0.006968002	negative
Phenylglyoxylic acid	Veillonella	0.002200422	positive

Methyl-2-aminobenzoate	Veillonella	-0.127624466	negative
3-Methoxytyramine	Veillonella	-0.234711662	negative
3-[(3-chloro-4-hydroxy-5-methylanilino)methylidene]pentane-2,4-dione	Veillonella	-0.291555893	negative
Feruloyl Putrescine	Veillonella	-0.262216935	negative
1-benzyl-4-(4-nitrophenyl)piperazine	Veillonella	-0.267693454	negative
EMH	Veillonella	-0.35020171	negative
2-Hydroxycinnamic acid	Veillonella	-0.115888883	negative
Methyl nicotinate	Veillonella	-0.141560471	negative
Lysopa 16: 0	Veillonella	-0.337733796	negative

Omeprazole sulphone	Megamonas	0.134515598	positive
5-Hydroxyomeprazole	Megamonas	0.084388073	positive
DL-Tryptophan	Megamonas	0.038303089	positive
Indole-3-acrylic acid	Megamonas	0.039111598	positive
L-Phenylalanine	Megamonas	-0.237275491	negative
L-Tyrosine	Megamonas	-0.249728057	negative
Mycophenolic acid	Megamonas	0.072152769	positive
Stercobilin	Megamonas	0.086409344	positive
PE (14: 0e/22: 2)	Megamonas	0.315289409	positive
Megamonas	Megamonas	-0.058616865	negative
Phenylglyoxylic acid	Megamonas	-0.040021117	negative
Methyl-2-aminobenzoate	Megamonas	0.292882197	positive

3-Methoxytyramine	Megamonas	0.289547099	positive
3-[(3-chloro-4-hydroxy-5-methylanilino)methylidene]pentane-2,4-dione	Megamonas	0.235377031	positive
Feruloyl Putrescine	Megamonas	-0.261047175	negative
1-benzyl-4-(4-nitrophenyl)piperazine	Megamonas	0.176845021	positive
EMH	Megamonas	0.043857565	positive
2-Hydroxycinnamic acid	Megamonas	-0.235174904	negative
Methyl nicotinate	Megamonas	0.295914104	positive
Lysopa 16: 0	Megamonas	-0.160272116	negative
Omeprazole sulphone	Prevotella	-0.009448678	negative
5-Hydroxyomeprazole	Prevotella	-0.329786371	negative

DL-Tryptophan	Prevotella	-0.021282458	negative
Indole-3-acrylic acid	Prevotella	-0.016879191	negative
L-Phenylalanine	Prevotella	-0.050632933	negative
L-Tyrosine	Prevotella	0.043757468	positive
Mycophenolic acid	Prevotella	0.013758949	positive
Stercobilin	Prevotella	-0.150261495	negative
PE (14: 0e/22: 2)	Prevotella	0.152082251	positive
Homoarginine	Prevotella	0.079900954	positive
Phenylglyoxylic acid	Prevotella	-0.119805563	negative
Methyl-2-aminobenzoate	Prevotella	-0.106045353	negative

3-Methoxytyramine	Prevotella	-0.009265208	negative
3-[(3-chloro-4-hydroxy-5-methylanilino)methylidene]pentane-2,4-dione	Prevotella	-0.034033587	negative
Feruloyl Putrescine	Prevotella	0.116044439	positive
1-benzyl-4-(4-nitrophenyl)piperazine	Prevotella	0.005687032	positive
EMH	Prevotella	-0.002384885	negative
2-Hydroxycinnamic acid	Prevotella	0.039170732	positive
Methyl nicotinate	Prevotella	0.008623065	positive
Lysopa 16: 0	Prevotella	-0.149880819	negative
Omeprazole sulphone	Klebsiella	0.245023476	positive
5-Hydroxyomeprazole	Klebsiella	0.236950819	positive
DL-Tryptophan	Klebsiella	0.087606671	positive
Indole-3-acrylic acid	Klebsiella	0.08797361	positive

L-Phenylalanine	Klebsiella	0.111172309	positive
L-Tyrosine	Klebsiella	0.130538527	positive
Mycophenolic acid	Klebsiella	0.017611455	positive
Stercobilin	Klebsiella	0.025135317	positive
PE (14: 0e/22: 2)	Klebsiella	0.029535877	positive
Homoarginine	Klebsiella	-0.005504084	negative
Phenylglyoxylic acid	Klebsiella	-0.166039869	negative
Methyl-2-aminobenzoate	Klebsiella	-0.000550408	negative
3-Methoxytyramine	Klebsiella	0.181909979	positive
3-[(3-chloro-4-hydroxy-5-methylanilino)methylidene]pentane-2,4-dione	Klebsiella	0.261352259	positive
Feruloyl Putrescine	Klebsiella	-0.199706517	negative

1-benzyl-4-(4-nitrophenyl)piperazine	Klebsiella	0.429279212	positive
EMH	Klebsiella	0.237571188	positive
2-Hydroxycinnamic acid	Klebsiella	0.14007894	positive
Methyl nicotinate	Klebsiella	0.103293311	positive
Lysopa 16: 0	Klebsiella	0.069895461	positive
Omeprazole sulphone	Gemmiger	-0.007148749	negative
5-Hydroxyomeprazole	Gemmiger	0.293648613	positive
DL-Tryptophan	Gemmiger	0.149023921	positive
Indole-3-acrylic acid	Gemmiger	0.150490331	positive
L-Phenylalanine	Gemmiger	-0.082111437	negative
L-Tyrosine	Gemmiger	-0.087984603	negative
Mycophenolic acid	Gemmiger	0.016129032	positive

Stercobilin	Gemmiger	0.231509487	positive
PE (14: 0e/22: 2)	Gemmiger	0.019061584	positive
Homoarginine	Gemmiger	0.052240858	positive
Phenylglyoxylic acid	Gemmiger	0.060856017	positive
Methyl-2-aminobenzoate	Gemmiger	0.197232152	positive
3-Methoxytyramine	Gemmiger	0.185867474	positive
3-[(3-chloro-4-hydroxy-5-methylanilino)methylidene]pentane-2,4-dione	Gemmiger	0.061222622	positive
Feruloyl Putrescine	Gemmiger	0.123545047	positive
1-benzyl-4-(4-nitrophenyl)piperazine	Gemmiger	0.214442815	positive
EMH	Gemmiger	0.380865103	positive
2-Hydroxycinnamic acid	Gemmiger	-0.103381909	negative
Methyl nicotinate	Gemmiger	0.233525801	positive

Lysopa 16: 0	Gemmiger	-0.08101173	negative
Omeprazole sulphone	Faecalibacterium	-0.050591147	negative
5-Hydroxyomeprazole	Faecalibacterium	0.388781965	positive
DL-Tryptophan	Faecalibacterium	0.159472093	positive
Indole-3-acrylic acid	Faecalibacterium	0.161671708	positive
L-Phenylalanine	Faecalibacterium	-0.034090909	negative
L-Tyrosine	Faecalibacterium	0.034643937	positive
Mycophenolic acid	Faecalibacterium	-0.058284457	negative
Stercobilin	Faecalibacterium	0.491797271	positive
PE (14: 0e/22: 2)	Faecalibacterium	-0.166788856	negative
Homoarginine	Faecalibacterium	0.020346439	positive

Phenylglyoxylic acid	Faecalibacterium	0.094950051	positive
Methyl-2-aminobenzoate	Faecalibacterium	0.371734948	positive
3-Methoxytyramine	Faecalibacterium	0.311428835	positive
3-[(3-chloro-4-hydroxy-5-methylanilino)methylidene]pentane-2,4-dione	Faecalibacterium	0.069104574	positive
Feruloyl Putrescine	Faecalibacterium	0.146824306	positive
1-benzyl-4-(4-nitrophenyl)piperazine	Faecalibacterium	0.027859238	positive
EMH	Faecalibacterium	0.116202346	positive
2-Hydroxycinnamic acid	Faecalibacterium	0.049308038	positive
Methyl nicotinate	Faecalibacterium	0.272752269	positive
Lysopa 16: 0	Faecalibacterium	-0.105571848	negative
Omeprazole sulphone	Escherichia	-0.152195843	negative
5-Hydroxyomeprazole	Escherichia	-0.299440737	negative

DL-Tryptophan	Escherichia	-0.400293405	negative
Indole-3-acrylic acid	Escherichia	-0.40212709	negative
L-Phenylalanine	Escherichia	-0.004033737	negative
L-Tyrosine	Escherichia	0.10653709	positive
Mycophenolic acid	Escherichia	0.146314641	positive
Stercobilin	Escherichia	-0.349500334	negative
PE (14: 0e/22: 2)	Escherichia	-0.083241663	negative
Homoarginine	Escherichia	-0.096451824	negative
Phenylglyoxylic acid	Escherichia	0.186302382	positive
Methyl-2-aminobenzoate	Escherichia	-0.25671588	negative

3-Methoxytyramine	Escherichia	-0.411662251	negative
3-[(3-chloro-4-hydroxy-5-methylanilino)methylidene]pentane-2,4-dione	Escherichia	-0.128908046	negative
Feruloyl Putrescine	Escherichia	-0.012652426	negative
1-benzyl-4-(4-nitrophenyl)piperazine	Escherichia	-0.328932915	negative
EMH	Escherichia	-0.241657515	negative
2-Hydroxycinnamic acid	Escherichia	0.100302562	positive
Methyl nicotinate	Escherichia	-0.144861104	negative
Lysopa 16: 0	Escherichia	0.261459497	positive
Omeprazole sulphone	Bacteroides	-0.041792686	negative
5-Hydroxyomeprazole	Bacteroides	0.157272478	positive

DL-Tryptophan	Bacteroides	-0.064888645	negative
Indole-3-acrylic acid	Bacteroides	-0.065988452	negative
L-Phenylalanine	Bacteroides	0.033357771	positive
L-Tyrosine	Bacteroides	-0.063422235	negative
Mycophenolic acid	Bacteroides	-0.037756598	negative
Stercobilin	Bacteroides	0.125378059	positive
PE (14: 0e/22: 2)	Bacteroides	-0.023460411	negative
Homoarginine	Bacteroides	-0.074237009	negative
Phenylglyoxylic acid	Bacteroides	0.25093942	positive
Methyl-2-aminobenzoate	Bacteroides	0.010814774	positive

3-Methoxytyramine	Bacteroides	-0.130143892	negative
3-[(3-chloro-4-hydroxy-5-methylanilino)methylidene]pentane-2,4-dione	Bacteroides	0.009531665	positive
Feruloyl Putrescine	Bacteroides	0.070754285	positive
1-benzyl-4-(4-nitrophenyl)piperazine	Bacteroides	-0.04068915	negative
EMH	Bacteroides	-0.152492669	negative
2-Hydroxycinnamic acid	Bacteroides	-0.0582898	negative
Methyl nicotinate	Bacteroides	-0.111630465	negative
Lysopa 16: 0	Bacteroides	-0.117668622	negative
Omeprazole sulphone	Others	-0.014847402	negative
5-Hydroxyomeprazole	Others	0.150123729	positive
DL-Tryptophan	Others	0.079919348	positive

Indole-3-acrylic acid	Others	0.07442031	positive
L-Phenylalanine	Others	-0.256964809	negative
L-Tyrosine	Others	-0.122628541	negative
Mycophenolic acid	Others	0.097507331	positive
Stercobilin	Others	0.416277153	positive
PE (14: 0e/22: 2)	Others	-0.093108504	negative
Homoarginine	Others	0.127394373	positive
Phenylglyoxylic acid	Others	0.174502796	positive
Methyl-2-aminobenzoate	Others	0.28448355	positive
3-Methoxytyramine	Others	0.215378976	positive
3-[(3-chloro-4-hydroxy-5-methylanilino)methylidene]pentane-2,4-dione	Others	0.285033454	positive
Feruloyl Putrescine	Others	0.127760976	positive

1-benzyl-4-(4-nitrophenyl)piperazine	Others	0.063782991	positive
EMH	Others	0.234604106	positive
2-Hydroxycinnamic acid	Others	-0.130327193	negative
Methyl nicotinate	Others	0.35597104	positive
Lysopa 16: 0	Others	-0.052419355	negative