

Table S1: Pathways hit by Mouse BioCyc Database

BioCyc_ID	Pathway total	Hits.total	Hits.sig	Expected	p.value
<i>anandamide degradation</i>	6	6	6	3.7763	<0.001
<i>bile acid biosynthesis, neutral pathway</i>	44	44	23	27.693	0.002
<i>glycerol-3-phosphate shuttle</i>	7	7	6	4.4057	0.004
<i>triacylglycerol biosynthesis</i>	6	6	5	3.7763	0.012
<i>CDP-diacylglycerol biosynthesis I</i>	8	8	6	5.035	0.013
<i>CDP-diacylglycerol biosynthesis II</i>	8	8	6	5.035	0.013
<i>glycerol degradation IV</i>	8	8	6	5.035	0.013
<i>biosynthesis of estrogens</i>	20	20	11	12.588	0.020
<i>cardiolipin biosynthesis II</i>	7	7	5	4.4057	0.032
<i>cardiolipin biosynthesis I</i>	7	7	5	4.4057	0.032
<i>biosynthesis of serotonin and melatonin</i>	19	19	10	11.958	0.038
<i>serotonin and melatonin biosynthesis</i>	19	19	10	11.958	0.038
<i>aerobic respiration -- electron donors reaction list</i>	11	11	6	6.9232	0.087
<i>sphingomyelin metabolism</i>	4	4	3	2.5175	0.089
<i>nonaprenyl diphosphate biosynthesis I</i>	2	2	2	1.2588	0.095
<i>pyridine nucleotide cycling</i>	25	25	11	15.735	0.113
<i>phospholipases</i>	5	5	3	3.1469	0.174
<i>palmitate biosynthesis I (animals)</i>	13	13	6	8.1819	0.182
<i>2-amino-3-carboxymuconate semialdehyde degradation to glutaryl-CoA</i>	19	19	8	11.958	0.203
<i>trans, trans-farnesyl diphosphate biosynthesis</i>	3	3	2	1.8881	0.226
<i>urate degradation to allantoin</i>	3	3	2	1.8881	0.226
<i>biosynthesis of androgens</i>	11	11	5	6.9232	0.228
<i>biosynthesis of prostaglandins</i>	17	17	7	10.699	0.247
<i>catecholamine biosynthesis</i>	26	26	10	16.364	0.257
<i>choline biosynthesis III</i>	6	6	3	3.7763	0.271
<i>L-dopachrome biosynthesis</i>	12	12	5	7.5526	0.298
<i>ubiquinol-6 biosynthesis (eukaryotic)</i>	27	27	10	16.993	0.304
<i>oleate biosynthesis II (animals)</i>	4	4	2	2.5175	0.363
<i>arginine degradation III (arginine decarboxylase/agmatinase pathway)</i>	4	4	2	2.5175	0.363
<i>putrescine biosynthesis I</i>	4	4	2	2.5175	0.363
<i>mevalonate pathway I</i>	7	7	3	4.4057	0.372
<i>phosphatidylcholine biosynthesis I</i>	7	7	3	4.4057	0.372
<i>arsenate detoxification I (glutaredoxin)</i>	7	7	3	4.4057	0.371
<i>histidine degradation III</i>	29	29	10	18.252	0.401
<i>TCA cycle variation III (eukaryotic)</i>	11	11	4	6.9232	0.455
<i>TCA cycle</i>	11	11	4	6.9232	0.455
<i>histamine biosynthesis</i>	8	8	3	5.035	0.469
<i>tetrahydrobiopterin biosynthesis I</i>	5	5	2	3.1469	0.489
<i>tetrahydrobiopterin biosynthesis II</i>	5	5	2	3.1469	0.489
<i>spermine biosynthesis</i>	5	5	2	3.1469	0.489
<i>spermidine biosynthesis I</i>	5	5	2	3.1469	0.489
<i>branched-chain alpha-keto acid dehydrogenase complex</i>	5	5	2	3.1469	0.489
<i>(deoxy)ribose phosphate degradation</i>	5	5	2	3.1469	0.489
<i>histamine degradation</i>	18	18	6	11.329	0.497

<i>Rapoport-Luebering glycolytic shunt</i>	2	2	1	1.2588	0.522
<i>creatine-phosphate energy transfer</i>	2	2	1	1.2588	0.522
<i>acetyl-CoA biosynthesis (from citrate)</i>	2	2	1	1.2588	0.522
<i>pyrimidine deoxyribonucleosides degradation</i>	2	2	1	1.2588	0.522
<i>adenosine nucleotides degradation II</i>	9	9	3	5.6644	0.559
<i>nicotine degradation II</i>	56	56	17	35.245	0.582
<i>eumelanin biosynthesis</i>	6	6	2	3.7763	0.598
<i>urate biosynthesis/inosine 5'-phosphate degradation</i>	6	6	2	3.7763	0.598
<i>NAD biosynthesis from 2-amino-3-carboxymuconate semialdehyde</i>	13	13	4	8.1819	0.605
<i>L-glutamine biosynthesis II (tRNA-dependent)</i>	10	10	3	6.2938	0.640
<i>proline degradation III</i>	10	10	3	6.2938	0.640
<i>proline degradation II</i>	10	10	3	6.2938	0.640
<i>ubiquinol-8 biosynthesis (eukaryotic)</i>	17	17	5	10.699	0.641
<i>citrulline-nitric oxide cycle</i>	21	21	6	13.217	0.669
<i>1,25-dihydroxyvitamin D3 biosynthesis</i>	3	3	1	1.8881	0.669
<i>xanthine and xanthosine salvage</i>	3	3	1	1.8881	0.669
<i>glutamate removal from folates</i>	3	3	1	1.8881	0.669
<i>glutathione-mediated detoxification</i>	3	3	1	1.8881	0.669
<i>purine ribonucleosides degradation to ribose-1-phosphate</i>	3	3	1	1.8881	0.669
<i>nicotine degradation III</i>	52	52	15	32.728	0.674
<i>adenine and adenosine salvage I</i>	7	7	2	4.4057	0.688
<i>xylitol degradation</i>	7	7	2	4.4057	0.688
<i>glutamine degradation I</i>	7	7	2	4.4057	0.688
<i>guanosine nucleotides degradation III</i>	7	7	2	4.4057	0.688
<i>lysine degradation II</i>	18	18	5	11.329	0.696
<i>tyrosine biosynthesis II</i>	11	11	3	6.9232	0.709
<i>ceramide biosynthesis</i>	11	11	3	6.9232	0.709
<i>UDP-N-acetyl-D-glucosamine biosynthesis II</i>	11	11	3	6.9232	0.709
<i>phenylalanine degradation I (aerobic)</i>	11	11	3	6.9232	0.709
<i>creatine biosynthesis</i>	15	15	4	9.4407	0.728
<i>tryptophan degradation I (via anthranilate)</i>	15	15	4	9.4407	0.728
<i>proline biosynthesis II</i>	19	19	5	11.958	0.745
<i>citrulline biosynthesis</i>	37	37	10	23.287	0.750
<i>glutamine biosynthesis II</i>	8	8	2	5.035	0.761
<i>PRPP biosynthesis I</i>	8	8	2	5.035	0.761
<i>gamma-linolenate biosynthesis II (animals)</i>	8	8	2	5.035	0.761
<i>heme degradation</i>	8	8	2	5.035	0.761
<i>heme biosynthesis from uroporphyrinogen-III I</i>	12	12	3	7.5526	0.768
<i>adenine and adenosine salvage III</i>	4	4	1	2.5175	0.771
<i>gluconeogenesis I</i>	13	13	3	8.1819	0.816
<i>glycine degradation (creatine biosynthesis)</i>	13	13	3	8.1819	0.816
<i>glycolysis I</i>	13	13	3	8.1819	0.816
<i>pyrimidine ribonucleotides interconversion</i>	9	9	2	5.6644	0.819
<i>pyrimidine deoxyribonucleotides de novo biosynthesis I</i>	9	9	2	5.6644	0.819
<i>5-aminoimidazole ribonucleotide biosynthesis II</i>	9	9	2	5.6644	0.819
<i>pentose phosphate pathway (non-oxidative branch)</i>	9	9	2	5.6644	0.819
<i>D-glucuronate degradation I</i>	9	9	2	5.6644	0.819
<i>4-hydroxyproline degradation I</i>	9	9	2	5.6644	0.819

<i>glutamate biosynthesis II</i>	5	5	1	3.1469	0.842
<i>alanine biosynthesis II</i>	5	5	1	3.1469	0.842
<i>adenine and adenosine salvage VI</i>	5	5	1	3.1469	0.842
<i>tRNA splicing</i>	5	5	1	3.1469	0.842
<i>NAD salvage pathway III</i>	5	5	1	3.1469	0.842
<i>tetrapyrrole biosynthesis II</i>	5	5	1	3.1469	0.842
<i>biotin-carboxyl carrier protein assembly</i>	5	5	1	3.1469	0.842
<i>fatty acid activation</i>	5	5	1	3.1469	0.842
<i>ethanol degradation II (cytosol)</i>	5	5	1	3.1469	0.842
<i>formaldehyde oxidation II (glutathione-dependent)</i>	5	5	1	3.1469	0.842
<i>glutamate degradation X</i>	5	5	1	3.1469	0.842
<i>beta-alanine degradation I</i>	5	5	1	3.1469	0.842
<i>alanine degradation III</i>	5	5	1	3.1469	0.842
<i>L-arabinose degradation II</i>	5	5	1	3.1469	0.842
<i>lactose degradation III</i>	5	5	1	3.1469	0.842
<i>acetate conversion to acetyl-CoA</i>	5	5	1	3.1469	0.842
<i>fatty acid &beta;-oxidation I</i>	5	5	1	3.1469	0.842
<i>fatty acid &beta;-oxidation II (core pathway)</i>	5	5	1	3.1469	0.842
<i>Targeted protein degradation</i>	5	5	1	3.1469	0.842
<i>proline biosynthesis II (from arginine)</i>	33	33	8	20.77	0.846
<i>purine and pyrimidine metabolism</i>	18	18	4	11.329	0.855
<i>citrulline degradation</i>	14	14	3	8.8113	0.856
<i>dopamine degradation</i>	34	34	8	21.399	0.870
<i>sphingosine and sphingosine-1-phosphate metabolism</i>	23	23	5	14.476	0.884
<i>phenylalanine degradation III</i>	19	19	4	11.958	0.884
<i>urea cycle</i>	27	27	6	16.993	0.885
<i>glycolysis V (Pyrococcus)</i>	15	15	3	9.4407	0.888
<i>UDP-N-acetyl-D-galactosamine biosynthesis II</i>	6	6	1	3.7763	0.891
<i>lipoate salvage and modification</i>	6	6	1	3.7763	0.891
<i>pyridoxal 5'-phosphate salvage pathway</i>	6	6	1	3.7763	0.891
<i>N-acetylglucosamine degradation I</i>	6	6	1	3.7763	0.891
<i>ribose degradation</i>	6	6	1	3.7763	0.891
<i>epoxysqualene biosynthesis</i>	11	11	2	6.9232	0.898
<i>phosphatidylethanolamine biosynthesis II</i>	11	11	2	6.9232	0.898
<i>spermine biosynthesis II</i>	11	11	2	6.9232	0.898
<i>glutamine degradation II</i>	11	11	2	6.9232	0.898
<i>lipoate biosynthesis and incorporation II</i>	20	20	4	12.588	0.908
<i>arginine biosynthesis IV</i>	37	37	8	23.287	0.924
<i>S-adenosyl-L-methionine cycle II</i>	12	12	2	7.5526	0.925
<i>5-aminoimidazole ribonucleotide biosynthesis I</i>	12	12	2	7.5526	0.925
<i>glutathione biosynthesis</i>	12	12	2	7.5526	0.925
<i>glycolysis III</i>	12	12	2	7.5526	0.925
<i>putrescine degradation III</i>	12	12	2	7.5526	0.925
<i>methionine degradation I (to homocysteine)</i>	12	12	2	7.5526	0.925
<i>salvage pathways of pyrimidine ribonucleotides</i>	7	7	1	4.4057	0.925
<i>valine degradation</i>	21	21	4	13.217	0.927
<i>asparagine biosynthesis I</i>	17	17	3	10.699	0.933
<i>isoleucine degradation</i>	17	17	3	10.699	0.933

<i>arginine degradation VI (arginase 2 pathway)</i>	26	26	5	16.364	0.940
<i>tRNA charging pathway</i>	73	73	17	45.945	0.944
<i>serine biosynthesis</i>	13	13	2	8.1819	0.944
<i>uridine-5'-phosphate biosynthesis</i>	13	13	2	8.1819	0.944
<i>cyclic AMP biosynthesis</i>	8	8	1	5.035	0.948
<i>riboflavin, FMN and FAD transformations</i>	8	8	1	5.035	0.948
<i>tryptophan degradation to 2-amino-3-carboxymuconate semialdehyde</i>	18	18	3	11.329	0.949
<i>arginine degradation I (arginase pathway)</i>	23	23	4	14.476	0.956
<i>valine degradation I</i>	23	23	4	14.476	0.956
<i>tyrosine degradation I</i>	28	28	5	17.623	0.962
<i>biosynthesis of corticosteroids</i>	9	9	1	5.6644	0.964
<i>pentose phosphate pathway (oxidative branch)</i>	9	9	1	5.6644	0.964
<i>dermatan sulfate degradation (metazoa)</i>	9	9	1	5.6644	0.964
<i>N-acetylneuraminic acid and N-acetylmannosamine degradation</i>	9	9	1	5.6644	0.964
<i>formaldehyde oxidation I</i>	9	9	1	5.6644	0.964
<i>aspartate degradation II</i>	9	9	1	5.6644	0.964
<i>L-cysteine degradation I</i>	9	9	1	5.6644	0.964
<i>glutamate degradation VII</i>	15	15	2	9.4407	0.970
<i>aspartate biosynthesis</i>	10	10	1	6.2938	0.975
<i>selenocysteine biosynthesis II (archaea and eukaryotes)</i>	10	10	1	6.2938	0.975
<i>lipoate biosynthesis and incorporation I</i>	10	10	1	6.2938	0.975
<i>L-cysteine degradation III</i>	10	10	1	6.2938	0.975
<i>sucrose degradation V (mammalian)</i>	10	10	1	6.2938	0.975
<i>adenosine nucleotides de novo biosynthesis</i>	11	11	1	6.9232	0.983
<i>L-carnitine biosynthesis</i>	11	11	1	6.9232	0.983
<i>starch degradation</i>	11	11	1	6.9232	0.983
<i>coenzyme A biosynthesis</i>	11	11	1	6.9232	0.983
<i>Leucine Catabolism</i>	22	22	3	13.846	0.984
<i>leucine degradation I</i>	22	22	3	13.846	0.984
<i>L-ascorbate biosynthesis VI</i>	12	12	1	7.5526	0.988
<i>bupropion degradation</i>	12	12	1	7.5526	0.988
<i>CMP-N-acetylneuraminic acid biosynthesis I (eukaryotes)</i>	13	13	1	8.1819	0.992
<i>glucose and glucose-1-phosphate degradation</i>	13	13	1	8.1819	0.992
<i>folate polyglutamylation</i>	14	14	1	8.8113	0.994
<i>4-aminobutyrate degradation I</i>	16	16	1	10.07	0.997
<i>glutamate degradation III (via 4-aminobutyrate)</i>	16	16	1	10.07	0.997
<i>glutamate degradation IV</i>	17	17	1	10.699	0.998
<i>folate transformations II (plants)</i>	29	29	2	18.252	1.000

Table S2: Pathways hit by Mouse KEGG Database

KEGG_Pathway	Pathway total	Hits.total	Hits.sig	Expected	p.value
<i>Primary bile acid biosynthesis</i>	57	57	34	17.49	<0.001
<i>Steroid hormone biosynthesis</i>	137	137	60	42.037	<0.001
<i>Glycerolipid metabolism</i>	9	9	7	2.7615	0.005
<i>Steroid biosynthesis</i>	68	68	30	20.865	0.012
<i>Biosynthesis of unsaturated fatty acids</i>	37	37	18	11.353	0.016
<i>Glycosaminoglycan degradation</i>	17	17	9	5.2162	0.045
<i>Tryptophan metabolism</i>	125	125	47	38.355	0.052
<i>Retinol metabolism</i>	32	32	14	9.8188	0.080
<i>Glycosaminoglycan biosynthesis - heparan sulfate / heparin</i>	2	2	2	0.61368	0.094
<i>Arachidonic acid metabolism</i>	30	30	13	9.2051	0.096
<i>Glycerophospholipid metabolism</i>	31	31	13	9.512	0.121
<i>Fatty acid degradation</i>	10	10	5	3.0684	0.161
<i>Ubiquinone and other terpenoid-quinone biosynthesis</i>	28	28	11	8.5915	0.212
<i>Drug metabolism - other enzymes</i>	34	34	13	10.432	0.215
<i>Histidine metabolism</i>	50	50	18	15.342	0.247
<i>Nicotinate and nicotinamide metabolism</i>	29	29	11	8.8983	0.253
<i>Linoleic acid metabolism</i>	6	6	3	1.841	0.268
<i>Folate biosynthesis</i>	27	27	10	8.2846	0.297
<i>Terpenoid backbone biosynthesis</i>	19	19	7	5.8299	0.358
<i>Glycosaminoglycan biosynthesis - chondroitin sulfate / dermatan sulfate</i>	13	13	5	3.9889	0.366
<i>Porphyrin and chlorophyll metabolism</i>	45	45	15	13.808	0.402
<i>Glyoxylate and dicarboxylate metabolism</i>	20	20	7	6.1368	0.417
<i>Fatty acid elongation</i>	8	8	3	2.4547	0.465
<i>Biotin metabolism</i>	5	5	2	1.5342	0.486
<i>Nitrogen metabolism</i>	5	5	2	1.5342	0.486
<i>Sphingolipid metabolism</i>	38	38	12	11.66	0.513
<i>alpha-Linolenic acid metabolism</i>	6	6	2	1.841	0.594
<i>Citrate cycle (TCA cycle)</i>	13	13	4	3.9889	0.601
<i>Fatty acid biosynthesis</i>	34	34	10	10.432	0.628
<i>D-Glutamine and D-glutamate metabolism</i>	10	10	3	3.0684	0.635
<i>Mucin type O-glycan biosynthesis</i>	10	10	3	3.0684	0.635
<i>Glycosphingolipid biosynthesis - lacto and neolacto series</i>	3	3	1	0.92051	0.667
<i>Glycosphingolipid biosynthesis - ganglio series</i>	3	3	1	0.92051	0.667
<i>Sulfur metabolism</i>	3	3	1	0.92051	0.667
<i>Lysine degradation</i>	35	35	10	10.739	0.669
<i>Phosphonate and phosphinate metabolism</i>	8	8	2	2.4547	0.758
<i>Mannose type O-glycan biosynthesis</i>	8	8	2	2.4547	0.758
<i>Glycosphingolipid biosynthesis - globo and isoglobo series</i>	4	4	1	1.2274	0.769

<i>Phenylalanine, tyrosine and tryptophan biosynthesis</i>	20	20	5	6.1368	0.783
<i>Taurine and hypotaurine metabolism</i>	17	17	4	5.2162	0.816
<i>Phenylalanine metabolism</i>	47	47	12	14.421	0.824
<i>Vitamin B6 metabolism</i>	25	25	6	7.671	0.827
<i>Arginine biosynthesis</i>	37	37	9	11.353	0.848
<i>Drug metabolism - cytochrome P450</i>	98	98	26	30.07	0.848
<i>Arginine and proline metabolism</i>	71	71	18	21.786	0.870
<i>Pentose phosphate pathway</i>	23	23	5	7.0573	0.880
<i>D-Arginine and D-ornithine metabolism</i>	19	19	4	5.8299	0.881
<i>Glycosylphosphatidylinositol (GPI)-anchor biosynthesis</i>	15	15	3	4.6026	0.885
<i>beta-Alanine metabolism</i>	43	43	10	13.194	0.894
<i>Cysteine and methionine metabolism</i>	58	58	14	17.797	0.895
<i>Ascorbate and aldarate metabolism</i>	11	11	2	3.3752	0.896
<i>Tyrosine metabolism</i>	129	129	33	39.582	0.921
<i>Glycolysis / Gluconeogenesis</i>	12	12	2	3.6821	0.923
<i>Starch and sucrose metabolism</i>	12	12	2	3.6821	0.923
<i>Inositol phosphate metabolism</i>	13	13	2	3.9889	0.943
<i>Thiamine metabolism</i>	13	13	2	3.9889	0.943
<i>Pyrimidine metabolism</i>	43	43	9	13.194	0.946
<i>N-Glycan biosynthesis</i>	18	18	3	5.5231	0.948
<i>Valine, leucine and isoleucine biosynthesis</i>	27	27	5	8.2846	0.950
<i>Aminoacyl-tRNA biosynthesis</i>	71	71	16	21.786	0.954
<i>Galactose metabolism</i>	21	21	3	6.4436	0.977
<i>Caffeine metabolism</i>	21	21	3	6.4436	0.977
<i>Metabolism of xenobiotics by cytochrome P450</i>	110	110	25	33.752	0.978
<i>Pantothenate and CoA biosynthesis</i>	44	44	8	13.501	0.981
<i>One carbon pool by folate</i>	17	17	2	5.2162	0.984
<i>Pentose and glucuronate interconversions</i>	23	23	3	7.0573	0.987
<i>Fructose and mannose metabolism</i>	28	28	4	8.5915	0.988
<i>Valine, leucine and isoleucine degradation</i>	34	34	5	10.432	0.991
<i>Purine metabolism</i>	77	77	15	23.627	0.992
<i>Alanine, aspartate and glutamate metabolism</i>	45	45	6	13.808	0.998
<i>Amino sugar and nucleotide sugar metabolism</i>	38	38	4	11.66	0.999
<i>Glutathione metabolism</i>	44	44	5	13.501	0.999
<i>Butanoate metabolism</i>	21	21	1	6.4436	1.000
<i>Glycine, serine and threonine metabolism</i>	42	42	3	12.887	1.000

Table S3: Pathways analysis with significant KEGG metabolites by mouse KEGG Database

	Total Compd	Hits	Raw p	$-\log(p)$	FDR	Impact
<i>Tyrosine Metabolism</i>	55	28	3.35E-06	5.4748	0.000261	0.5889
<i>Androgen and Estrogen Metabolism</i>	29	11	1.31E-05	4.8835	0.00051	0.39114
<i>Pterine Biosynthesis</i>	18	6	4.58E-05	4.3387	0.000615	0.19622
<i>Sphingolipid Metabolism</i>	36	7	4.99E-05	4.302	0.000615	0.18008
<i>Vitamin B6 Metabolism</i>	15	5	5.64E-05	4.2487	0.000615	0.12736
<i>Purine Metabolism</i>	63	14	6.31E-05	4.1999	0.000615	0.15079
<i>Pyrimidine Metabolism</i>	54	9	0.000145	3.8386	0.000946	0.10901
<i>Catecholamine Biosynthesis</i>	14	7	0.000146	3.8368	0.000946	1
<i>Plasmalogen Synthesis</i>	16	2	0.000146	3.8368	0.000946	0
<i>Phospholipid Biosynthesis</i>	25	4	0.000176	3.7546	0.000946	0.22297
<i>Porphyryn Metabolism</i>	36	7	0.000177	3.7523	0.000946	0.41621
<i>Steroidogenesis</i>	42	29	0.000182	3.7403	0.000946	0.12416
<i>Methionine Metabolism</i>	39	6	0.000233	3.6318	0.001138	0.15864
<i>Amino Sugar Metabolism</i>	31	5	0.000277	3.5572	0.001272	0.21875
<i>Androstenedione Metabolism</i>	23	11	0.000366	3.436	0.001587	0.3866
<i>Bile Acid Biosynthesis</i>	60	25	0.000387	3.4127	0.001587	0.21067
<i>Arachidonic Acid Metabolism</i>	65	31	0.000453	3.3441	0.001766	0.61779
<i>Retinol Metabolism</i>	30	11	0.000498	3.303	0.001793	0.34729
<i>Spermidine and Spermine Biosynthesis</i>	14	2	0.000506	3.2961	0.001793	0.42857
<i>Pentose Phosphate Pathway</i>	27	6	0.000547	3.2619	0.001833	0.49071
<i>Histidine Metabolism</i>	35	10	0.000589	3.2301	0.001837	0.63914
<i>Arginine and Proline Metabolism</i>	48	13	0.00071	3.1489	0.002129	0.40217
<i>Caffeine Metabolism</i>	20	4	0.001083	2.9655	0.003128	0
<i>Urea Cycle</i>	23	5	0.001151	2.9388	0.003208	0.5722
<i>Steroid Biosynthesis</i>	43	18	0.001308	2.8835	0.003515	0.19549
<i>Alpha Linolenic Acid and Linoleic Acid Metabolism</i>	17	7	0.001363	2.8654	0.003515	0.46429
<i>Selenoamino Acid Metabolism</i>	28	1	0.001438	2.8421	0.003515	0
<i>Nicotinate and Nicotinamide Metabolism</i>	32	7	0.001454	2.8374	0.003515	0.010436
<i>Glycine and Serine Metabolism</i>	50	3	0.001487	2.8277	0.003515	0
<i>Valine, Leucine and Isoleucine Degradation</i>	51	4	0.002099	2.6779	0.004816	0.008926
<i>Thiamine Metabolism</i>	9	1	0.002262	2.6455	0.005041	0
<i>Glycerolipid Metabolism</i>	23	3	0.002589	2.5869	0.005609	0.27322
<i>Vitamin K Metabolism</i>	9	2	0.002874	2.5416	0.006058	1
<i>Estrone Metabolism</i>	20	5	0.003011	2.5213	0.00618	0.73973
<i>Citric Acid Cycle</i>	25	2	0.003181	2.4975	0.006361	0.13043
<i>Aspartate Metabolism</i>	34	6	0.003308	2.4805	0.006374	0.095833
<i>Fatty Acid Biosynthesis</i>	33	4	0.003356	2.4742	0.006374	0.12432
<i>Glycolysis</i>	20	3	0.003514	2.4542	0.006374	0.17788
<i>Gluconeogenesis</i>	30	3	0.003514	2.4542	0.006374	0.15462
<i>Biotin Metabolism</i>	7	2	0.003689	2.4332	0.006521	0.25
<i>Carnitine Synthesis</i>	16	4	0.003762	2.4246	0.006521	0.54118
<i>Cardiolipin Biosynthesis</i>	11	2	0.004146	2.3824	0.00688	0.2987
<i>De Novo Triacylglycerol Biosynthesis</i>	9	2	0.004146	2.3824	0.00688	0.2
<i>Glycerol Phosphate Shuttle</i>	8	3	0.004435	2.3531	0.007053	0.57143
<i>Mitochondrial Electron Transport Chain</i>	15	3	0.004435	2.3531	0.007053	0.30519
<i>Galactose Metabolism</i>	31	5	0.004789	2.3197	0.007284	0.15652

<i>Betaine Metabolism</i>	18	3	0.004856	2.3138	0.007284	0.3053
<i>Phosphatidylcholine Biosynthesis</i>	18	3	0.005471	2.262	0.007818	0.39024
<i>Pantothenate and CoA Biosynthesis</i>	19	4	0.005513	2.2586	0.007818	0.24427
<i>Glutamate Metabolism</i>	45	3	0.005876	2.2309	0.008184	0.48631
<i>Phenylacetate Metabolism</i>	8	2	0.006601	2.1804	0.009032	0
<i>Phosphatidylethanolamine Biosynthesis</i>	13	1	0.006772	2.1693	0.009107	0.5
<i>Fatty Acid Metabolism</i>	40	2	0.007946	2.0998	0.010505	0
<i>Starch and Sucrose Metabolism</i>	26	3	0.008383	2.0766	0.010897	0.01083
<i>Folate Metabolism</i>	24	2	0.008785	2.0563	0.011233	0.10565
<i>Fructose and Mannose Degradation</i>	28	3	0.011009	1.9583	0.013744	0.01676
<i>Beta-Alanine Metabolism</i>	26	6	0.011101	1.9546	0.013744	0
<i>Mitochondrial Beta-Oxidation of Long Chain Saturated Fatty Acids</i>	24	1	0.016801	1.7747	0.020476	0
<i>Taurine and Hypotaurine Metabolism</i>	9	1	0.019381	1.7126	0.023257	0.14286
<i>Lactose Degradation</i>	9	1	0.02273	1.6434	0.026072	0
<i>Lactose Synthesis</i>	14	1	0.02273	1.6434	0.026072	0
<i>Trehalose Degradation</i>	11	1	0.02273	1.6434	0.026072	0
<i>Ubiquinone Biosynthesis</i>	18	1	0.023134	1.6358	0.026151	0
<i>Fatty Acid Elongation In Mitochondria</i>	33	1	0.027812	1.5558	0.030991	0
<i>Transfer of Acetyl Groups into Mitochondria</i>	18	1	0.033243	1.4783	0.036521	0.065327
<i>Ammonia Recycling</i>	25	3	0.042519	1.3714	0.046063	0.30729
<i>Cysteine Metabolism</i>	24	2	0.068197	1.1662	0.069083	0.37
<i>Glutathione Metabolism</i>	19	2	0.068197	1.1662	0.069083	0.051537
<i>Glucose-Alanine Cycle</i>	9	1	0.068197	1.1662	0.069083	0.4375
<i>Malate-Aspartate Shuttle</i>	7	1	0.068197	1.1662	0.069083	0.28571
<i>Alanine Metabolism</i>	14	1	0.068197	1.1662	0.069083	0
<i>Sulfate/Sulfite Metabolism</i>	19	1	0.076334	1.1173	0.076334	0

Table S4. Top 25 pathways with significant KEGG metabolites by mouse KEGG Database.

Pathways	Total Cmpd	Hits	Raw p	-log(p)	FDR	Impact
<i>Tyrosine Metabolism</i>	55	28	3.35E-06	5.4748	0.000261	0.5889
<i>Androgen and Estrogen Metabolism</i>	29	11	1.31E-05	4.8835	0.00051	0.39114
<i>Pterine Biosynthesis</i>	18	6	4.58E-05	4.3387	0.000615	0.19622
<i>Sphingolipid Metabolism</i>	36	7	4.99E-05	4.302	0.000615	0.18008
<i>Vitamin B6 Metabolism</i>	15	5	5.64E-05	4.2487	0.000615	0.12736
<i>Purine Metabolism</i>	63	14	6.31E-05	4.1999	0.000615	0.15079
<i>Pyrimidine Metabolism</i>	54	9	0.000145	3.8386	0.000946	0.10901
<i>Catecholamine Biosynthesis</i>	14	7	0.000146	3.8368	0.000946	1
<i>Plasmalogen Synthesis</i>	16	2	0.000146	3.8368	0.000946	0
<i>Phospholipid Biosynthesis</i>	25	4	0.000176	3.7546	0.000946	0.22297
<i>Porphyrin Metabolism</i>	36	7	0.000177	3.7523	0.000946	0.41621
<i>Steroidogenesis</i>	42	29	0.000182	3.7403	0.000946	0.12416
<i>Methionine Metabolism</i>	39	6	0.000233	3.6318	0.001138	0.15864
<i>Amino Sugar Metabolism</i>	31	5	0.000277	3.5572	0.001272	0.21875
<i>Androstenedione Metabolism</i>	23	11	0.000366	3.436	0.001587	0.3866
<i>Bile Acid Biosynthesis</i>	60	25	0.000387	3.4127	0.001587	0.21067
<i>Arachidonic Acid Metabolism</i>	65	31	0.000453	3.3441	0.001766	0.61779
<i>Retinol Metabolism</i>	30	11	0.000498	3.303	0.001793	0.34729
<i>Spermidine and Spermine Biosynthesis</i>	14	2	0.000506	3.2961	0.001793	0.42857
<i>Pentose Phosphate Pathway</i>	27	6	0.000547	3.2619	0.001833	0.49071
<i>Histidine Metabolism</i>	35	10	0.000589	3.2301	0.001837	0.63914
<i>Arginine and Proline Metabolism</i>	48	13	0.00071	3.1489	0.002129	0.40217
<i>Caffeine Metabolism</i>	20	4	0.001083	2.9655	0.003128	0
<i>Urea Cycle</i>	23	5	0.001151	2.9388	0.003208	0.5722
<i>Steroid Biosynthesis</i>	43	18	0.001308	2.8835	0.003515	0.19549

Table S5: Metabolites involved in steroid associated pathways.

Steroid Biosynthesis (25/42)	
Compound Common Name	Relative to EcN
<i>Vitamin D3</i>	=
<i>Calcidiol</i>	Down
<i>Calcitriol</i>	Up
<i>5-Dehydroavenasterol</i>	Up
<i>Isofucosterol</i>	Down
<i>Presqualene diphosphate</i>	Down
<i>Squalene</i>	Down
<i>(S)-2,3-Epoxysqualene</i>	=
<i>Lanosterol</i>	=
<i>24,25-Dihydrolanosterol</i>	Up
<i>14-Demethyl lanosterol</i>	Down
<i>3-Keto-4-methylzymosterol</i>	Down
<i>4alpha-Methylzymosterol</i>	Down
<i>4alpha-Carboxy-5alpha-cholesta-8,24-dien-3beta-ol</i>	Down
<i>Zymosterol</i>	=
<i>5alpha-Cholest-8-en-3beta-ol</i>	Up
<i>Lathosterol</i>	Up
<i>7-Dehydrodesmosterol</i>	Down
<i>Cholesterol</i>	Up
<i>Demosterol</i>	=
<i>24-Methylenecholesterol</i>	Down
<i>Campesterol</i>	Down
<i>Obtusifoliol</i>	=
<i>4alpha-Methylfecosterol</i>	Down
<i>24-Methylenelophenol</i>	Down
Terpenoid backbone biosynthesis (6/18)	
Compound Common Name	Relative to EcN
<i>5-phosphomevalonate</i>	Up
<i>(R)-5-Diphosphomevalonate</i>	Down
<i>Isopentenyl diphosphate</i>	Up
<i>Dimethylallyl diphosphate</i>	Up
<i>trans,trans-Farnesyl PP</i>	=
<i>Geranylgeranyl PP</i>	Down
Steroid hormone biosynthesis (21/77)	
Compound Common Name	Relative to EcN
<i>Androsterone</i>	Down
<i>Pregnenolone</i>	=
<i>Progesterone</i>	Up
<i>11-Deoxycorticosterone</i>	Down
<i>Corticosterone</i>	Down
<i>18-Hydroxycorticosterone</i>	Down
<i>Aldosterone</i>	Down
<i>Testosterone</i>	Down
<i>Estradiol-17beta</i>	Up
<i>Cholesterol</i>	Up
<i>17alpha-hydroxypregnenolone</i>	Down
<i>17alpha-Hydroxyprogesterone</i>	Down
<i>Androstenedione</i>	Up
<i>5alpha-Androstane-3,17-dione</i>	Up
<i>4-Methylpentanal</i>	Up
<i>Dehydroepiandrosterone</i>	Down
<i>Dehydroepiandrosterone sulfate</i>	Up

<i>Cortisone</i>	Down
<i>17alpha,21-Dihydroxy-5beta-pregnane-3,11,20-trione</i>	Down
<i>19-Oxoandrost-r-ene-3,17-dione</i>	Down
<i>Estrone</i>	=
Bile acid biosynthesis (15/46)	
Compound Common Name	Relative to EcN
<i>Cholesterol</i>	Up
<i>7a-hydroxycholesterol</i>	Down
<i>7a-hydroxycholest-4-en-3-one</i>	Down
<i>3alpha,7alpha,12alpha,26-Tetrahydroxy-5beta-cholestane</i>	Down
<i>7alpha,27-Dihydroxycholesterol</i>	Down
<i>7alpha-Hydroxycholesterol</i>	Down
<i>Cerebrosterol</i>	Down
<i>3alpha,7alpha,26-Trihydroxy-5beta-cholestane</i>	Down
<i>7alpha,12alpha-Dihydroxy-5beta-cholestan-3-one</i>	Down
<i>7alpha-Hydroxy-5beta-cholestan-3-one</i>	Down
<i>Glycochenodeoxycholate</i>	Down
<i>Taurochenodeoxycholate</i>	Down
<i>Glycocholate</i>	Down
<i>Cholic acid</i>	Down
<i>Taurine</i>	Up
<i>Taurocholate</i>	Up

Table S6: Significant pathways hit by full peak list.

KEGG pathway	Total	Hits	Hits.sig	p value
<i>Steroid hormone biosynthesis</i>	134	134	98	<0.001
<i>Porphyrin and chlorophyll metabolism</i>	45	45	36	0.006
<i>Arachidonic acid metabolism</i>	29	29	24	0.017
<i>Primary bile acid biosynthesis</i>	55	55	40	0.042

Table S7: Filtered KEGG metabolites of mice treated with BioColoniz and BioPersist

Query.Mass	Matched.Compound	Matched.Form	Retention.Time
529.9841	C00002	M+Na[1+]	1.149558
405.0099	C00015	M+H[1+]	1.782646
786.1643	C00016	M+H[1+]	5.214057
248.0321	C00018	M+H[1+]	1.76339
400.1512	C00019	M+H[1+]	8.001902
348.0699	C00020	M+H[1+]	1.313763
148.0606	C00025	M+H[1+]	33.72424
147.113	C00047	M+H[1+]	33.72356
134.0447	C00049	M+H[1+]	14.56968
308.0906	C00051	M+H[1+]	17.58262
324.0587	C00055	M+H[1+]	5.693146
457.1122	C00061	M+H[1+]	6.283572
175.119	C00062	M+H[1+]	33.73277
483.9909	C00063	M+H[1+]	1.165404
147.0766	C00064	M+H[1+]	33.76097
106.0496	C00065	M+H[1+]	18.68196
150.0583	C00073	M+H[1+]	23.83392
133.0975	C00077	M+H[1+]	1.12571
205.097	C00078	M+H[1+]	24.55321
166.0859	C00079	M+H[1+]	23.83925
182.0811	C00082	M+H[1+]	12.61815
261.0367	C00085	M+H[1+]	12.95701
343.124	C00089	M+H[1+]	1.295607
261.0367	C00092	M+H[1+]	12.95701
173.0209	C00093	M+H[1+]	30.10224
122.0272	C00097	M+H[1+]	14.08137
446.1762	C00101	M+H[1+]	1.191109
261.0367	C00103	M+H[1+]	12.95701
113.0348	C00106	M+H[1+]	33.00292
138.0549	C00108	M+H[1+]	20.74401
103.0393	C00109	M+H[1+]	21.61245
171.0058	C00111	M+H[1+]	30.30602
231.0272	C00117	M+H[1+]	23.27942
171.0058	C00118	M+H[1+]	30.30602
245.0958	C00120	M+H[1+]	6.009464
132.102	C00123	M+H[1+]	6.730754
615.1536	C00128	M+H[1+]	1.314913
247.0127	C00129	M+H[1+]	1.697023
349.0534	C00130	M+H[1+]	1.293901
156.0765	C00135	M+H[1+]	8.492633
222.0972	C00140	M+H[1+]	26.82375
117.0548	C00141	M+H[1+]	24.45544
458.1779	C00143	M+H[1+]	8.776238
364.0654	C00144	M+H[1+]	11.69558
136.0618	C00147	M+H[1+]	25.43827
116.0709	C00148	M+H[1+]	5.24558

133.0608	C00152	M+H[1+]	1.348017
123.0554	C00153	M+H[1+]	15.61794
136.0426	C00155	M+H[1+]	16.51873
103.0393	C00164	M+H[1+]	21.61245
165.0543	C00166	M+H[1+]	13.63665
298.0964	C00170	M+H[1+]	14.55133
127.0503	C00178	M+H[1+]	33.00906
131.1294	C00179	M+H[1+]	1.136909
118.0865	C00183	M+H[1+]	6.409756
387.3614	C00187	M+H[1+]	27.54422
120.0657	C00188	M+H[1+]	33.73069
195.0495	C00191	M+H[1+]	6.709652
179.0551	C00198	M+H[1+]	18.96367
231.0272	C00199	M+H[1+]	23.27942
343.124	C00208	M+H[1+]	1.295607
268.1027	C00212	M+H[1+]	5.002028
243.0978	C00214	M+H[1+]	1.636238
148.0606	C00217	M+H[1+]	33.72424
305.2469	C00219	M+H[1+]	17.73756
231.0272	C00231	M+H[1+]	23.27942
103.0393	C00232	M+H[1+]	21.61245
474.1731	C00234	M+H[1+]	4.799718
247.0127	C00235	M+H[1+]	1.697023
308.0635	C00239	M+H[1+]	9.74828
152.0565	C00242	M+H[1+]	14.44934
343.124	C00243	M+H[1+]	1.295607
126.0221	C00245	M+H[1+]	11.9606
257.2472	C00249	M+H[1+]	23.28472
168.0654	C00250	M+H[1+]	20.74727
343.124	C00252	M+H[1+]	1.295607
124.0394	C00253	M+H[1+]	8.502337
377.1455	C00255	M+H[1+]	5.150964
137.0457	C00262	M+H[1+]	9.01555
240.109	C00268	M+H[1+]	1.310345
310.1134	C00270	M+H[1+]	1.593417
261.0367	C00275	M+H[1+]	12.95701
287.1998	C00280	M+H[1+]	12.35711
269.0881	C00294	M+H[1+]	33.70708
245.0769	C00299	M+H[1+]	33.716
132.0769	C00300	M+H[1+]	11.50266
489.1146	C00307	M+H[1+]	14.54103
170.0804	C00314	M+H[1+]	6.425848
146.1653	C00315	M+H[1+]	32.93224
300.2891	C00319	M+H[1+]	27.09294
176.1032	C00327	M+H[1+]	1.482687
209.0921	C00328	M+H[1+]	33.73034
268.1027	C00330	M+H[1+]	5.002028
204.0652	C00331	M+H[1+]	13.74618

104.0707	C00334	M+H[1+]	8.8291
159.0401	C00337	M+H[1+]	19.27693
315.0755	C00341	M+H[1+]	21.38
142.0263	C00346	M+H[1+]	12.59673
103.0393	C00349	M+H[1+]	21.61245
260.0535	C00352	M+H[1+]	1.282515
198.0761	C00355	M+H[1+]	17.94759
302.0638	C00357	M+H[1+]	6.963005
332.0744	C00360	M+H[1+]	1.807355
348.0699	C00362	M+H[1+]	1.313763
169.0357	C00366	M+H[1+]	33.70574
285.2208	C00376	M+H[1+]	23.84408
266.1205	C00378	M+H[1+]	8.528942
153.0408	C00385	M+H[1+]	33.71561
227.1136	C00386	M+H[1+]	11.63568
284.0991	C00387	M+H[1+]	33.70708
112.0871	C00388	M+H[1+]	26.66853
161.1074	C00398	M+H[1+]	11.38709
380.1206	C00401	M+H[1+]	14.97616
134.0447	C00402	M+H[1+]	14.56968
132.102	C00407	M+H[1+]	6.730754
130.0864	C00408	M+H[1+]	6.413186
315.2311	C00410	M+H[1+]	12.3596
444.1614	C00415	M+H[1+]	30.60505
175.023	C00417	M+H[1+]	1.423596
353.2306	C00427	M+H[1+]	15.51013
115.0505	C00429	M+H[1+]	33.02094
132.0657	C00430	M+H[1+]	22.69676
175.1079	C00437	M+H[1+]	33.73638
177.0501	C00438	M+H[1+]	6.421992
175.0715	C00439	M+H[1+]	33.7211
460.1941	C00440	M+H[1+]	3.186331
261.0367	C00446	M+H[1+]	12.95701
277.1396	C00449	M+H[1+]	2.11092
128.0707	C00450	M+H[1+]	26.02041
271.1688	C00468	M+H[1+]	18.58317
287.2366	C00473	M+H[1+]	21.00566
244.0927	C00475	M+H[1+]	33.7211
138.0912	C00483	M+H[1+]	14.67751
585.2684	C00486	M+H[1+]	12.73338
162.1126	C00487	M+H[1+]	33.72967
177.0614	C00499	M+H[1+]	1.184174
583.2532	C00500	M+H[1+]	25.62905
442.1476	C00504	M+H[1+]	5.031572
133.0975	C00515	M+H[1+]	1.12571
291.2309	C00523	M+H[1+]	21.86768
229.0811	C00526	M+H[1+]	6.001648
169.0973	C00534	M+H[1+]	1.575012

289.2156	C00535	M+H[1+]	12.35726
169.0494	C00544	M+H[1+]	16.82075
170.0804	C00547	M+H[1+]	6.425848
252.109	C00559	M+H[1+]	33.73613
330.0588	C00575	M+H[1+]	1.340781
353.2306	C00584	M+H[1+]	15.51013
185.0808	C00588	M+H[1+]	20.16098
121.0647	C00601	M+H[1+]	10.82235
195.0495	C00618	M+H[1+]	6.709652
231.0272	C00620	M+H[1+]	23.27942
190.0712	C00624	M+H[1+]	33.71532
155.0338	C00628	M+H[1+]	13.5503
154.0498	C00632	M+H[1+]	33.71209
261.0367	C00636	M+H[1+]	12.95701
160.0758	C00637	M+H[1+]	4.921535
355.2462	C00639	M+H[1+]	14.45946
153.0544	C00642	M+H[1+]	12.32861
221.0919	C00643	M+H[1+]	3.743194
222.0972	C00645	M+H[1+]	26.82375
473.1893	C00664	M+H[1+]	5.673936
261.0367	C00668	M+H[1+]	12.95701
251.0701	C00669	M+H[1+]	34.90124
258.1097	C00670	M+H[1+]	18.19958
215.0316	C00672	M+H[1+]	30.11827
215.0316	C00673	M+H[1+]	30.11827
289.2156	C00674	M+H[1+]	12.35726
409.2939	C00695	M+H[1+]	12.35965
353.2306	C00696	M+H[1+]	15.51013
283.2627	C00712	M+H[1+]	27.5121
118.0865	C00719	M+H[1+]	6.409756
363.215	C00735	M+H[1+]	18.00106
106.0496	C00740	M+H[1+]	18.68196
203.2232	C00750	M+H[1+]	4.911067
361.1995	C00762	M+H[1+]	18.99294
116.0709	C00763	M+H[1+]	5.24558
301.2157	C00777	M+H[1+]	24.47838
177.1024	C00780	M+H[1+]	5.023704
139.0502	C00785	M+H[1+]	18.87505
184.0965	C00788	M+H[1+]	14.68544
175.119	C00792	M+H[1+]	33.73277
183.0864	C00794	M+H[1+]	15.02273
147.0766	C00819	M+H[1+]	33.76097
196.0605	C00822	M+H[1+]	33.72093
445.3089	C00828	M+H[1+]	23.72783
129.0697	C00829	M+H[1+]	12.36223
279.1382	C00831	M+H[1+]	1.091527
238.094	C00835	M+H[1+]	8.613163
302.3048	C00836	M+H[1+]	15.54152

184.0602	C00847	M+H[1+]	18.65224
220.118	C00864	M+H[1+]	1.68117
228.0978	C00881	M+H[1+]	33.7211
241.1293	C00884	M+H[1+]	14.6058
287.2366	C00899	M+H[1+]	21.00566
319.2256	C00909	M+H[1+]	18.72885
315.1185	C00921	M+H[1+]	17.78326
227.1024	C00931	M+H[1+]	33.72666
346.0549	C00942	M+H[1+]	1.975309
273.1843	C00951	M+H[1+]	12.6392
176.0706	C00954	M+H[1+]	17.75711
162.076	C00956	M+H[1+]	21.53216
120.9955	C00957	M+H[1+]	20.22927
219.1127	C00978	M+H[1+]	16.61243
186.0165	C01005	M+H[1+]	1.249509
349.1127	C01007	M+H[1+]	14.29653
165.0758	C01019	M+H[1+]	15.22104
104.0707	C01026	M+H[1+]	8.8291
146.0924	C01035	M+H[1+]	33.75716
179.0551	C01040	M+H[1+]	18.96367
176.0557	C01042	M+H[1+]	1.638406
162.0402	C01044	M+H[1+]	19.9008
427.3926	C01054	M+H[1+]	20.31499
199.0247	C01061	M+H[1+]	16.79161
233.0428	C01068	M+H[1+]	1.282053
569.3106	C01079	M+H[1+]	11.13015
345.0792	C01081	M+H[1+]	1.398319
343.124	C01083	M+H[1+]	1.295607
261.0367	C01094	M+H[1+]	12.95701
261.0367	C01097	M+H[1+]	12.95701
229.0472	C01107	M+H[1+]	25.02646
132.0657	C01110	M+H[1+]	22.69676
382.2708	C01120	M+H[1+]	15.99046
363.215	C01124	M+H[1+]	18.00106
163.0241	C01127	M+H[1+]	1.081079
359.1036	C01134	M+H[1+]	4.120554
356.1607	C01137	M+H[1+]	8.807321
309.0143	C01143	M+H[1+]	1.731586
170.0924	C01152	M+H[1+]	1.925291
132.0657	C01157	M+H[1+]	22.69676
169.0494	C01161	M+H[1+]	16.82075
385.3459	C01164	M+H[1+]	19.95375
132.0657	C01165	M+H[1+]	22.69676
261.0367	C01172	M+H[1+]	12.95701
331.2262	C01176	M+H[1+]	12.32344
261.0367	C01177	M+H[1+]	12.95701
181.0493	C01179	M+H[1+]	14.97796
338.0639	C01185	M+H[1+]	1.246182

387.3614	C01189	M+H[1+]	27.54422
104.0707	C01205	M+H[1+]	8.8291
289.2156	C01227	M+H[1+]	12.35726
216.0629	C01233	M+H[1+]	17.53549
343.124	C01235	M+H[1+]	1.295607
420.9677	C01243	M+H[1+]	1.174124
420.9677	C01245	M+H[1+]	1.174124
467.2397	C01246	M+H[1+]	18.46372
208.0602	C01252	M+H[1+]	14.7447
206.1618	C01259	M+H[1+]	23.8475
837.055	C01260	M+H[1+]	12.35965
241.1293	C01262	M+H[1+]	14.6058
435.3459	C01301	M+H[1+]	25.66851
353.2306	C01312	M+H[1+]	15.51013
179.0483	C01419	M+H[1+]	15.48939
285.2785	C01530	M+H[1+]	27.10463
401.3408	C01561	M+H[1+]	23.85975
173.1532	C01571	M+H[1+]	0.109861
180.0655	C01586	M+H[1+]	20.47065
281.2471	C01595	M+H[1+]	18.22158
233.1284	C01598	M+H[1+]	14.1054
417.3353	C01673	M+H[1+]	20.46908
183.0864	C01697	M+H[1+]	15.02273
427.3926	C01724	M+H[1+]	20.31499
415.3928	C01753	M+H[1+]	23.33585
285.0831	C01762	M+H[1+]	33.70574
361.1995	C01780	M+H[1+]	18.99294
401.3771	C01789	M+H[1+]	27.67883
385.3459	C01802	M+H[1+]	19.95375
777.6926	C01829	M+H[1+]	11.71408
130.05	C01879	M+H[1+]	24.13728
466.3143	C01921	M+H[1+]	21.82105
443.3877	C01943	M+H[1+]	19.28927
317.2467	C01953	M+H[1+]	21.59278
153.9984	C01962	M+H[1+]	33.76837
451.3552	C02059	M+H[1+]	27.29169
537.4459	C02094	M+H[1+]	7.215161
285.2208	C02110	M+H[1+]	23.84408
347.2203	C02140	M+H[1+]	17.98446
337.2357	C02165	M+H[1+]	15.49291
563.2646	C02191	M+H[1+]	20.63196
353.2306	C02198	M+H[1+]	15.51013
158.0448	C02220	M+H[1+]	17.50901
130.05	C02237	M+H[1+]	24.13728
149.0448	C02266	M+H[1+]	20.10221
223.0753	C02291	M+H[1+]	0.992649
104.0707	C02356	M+H[1+]	8.8291
101.0965	C02373	M+H[1+]	19.95229

651.7966	C02465	M+H[1+]	10.65377
393.2981	C02528	M+H[1+]	20.94821
351.1244	C02538	M+H[1+]	10.10222
149.0448	C02630	M+H[1+]	20.10221
133.0608	C02642	M+H[1+]	1.348017
201.1846	C02679	M+H[1+]	0.190386
237.0872	C02700	M+H[1+]	1.802107
131.1181	C02714	M+H[1+]	33.73634
165.0543	C02763	M+H[1+]	13.63665
127.0503	C02835	M+H[1+]	33.00906
300.2891	C02934	M+H[1+]	27.09294
146.0812	C02946	M+H[1+]	13.87389
240.109	C02953	M+H[1+]	1.310345
400.3408	C02990	M+H[1+]	25.69708
161.0595	C03012	M+H[1+]	8.503156
506.0187	C03028	M+H[1+]	26.19554
230.0425	C03090	M+H[1+]	5.243353
256.1064	C03150	M+H[1+]	1.210592
331.2262	C03205	M+H[1+]	12.32344
225.0866	C03227	M+H[1+]	1.337853
307.2623	C03242	M+H[1+]	12.39067
661.3201	C03263	M+H[1+]	12.11962
104.0707	C03284	M+H[1+]	8.8291
228.0273	C03287	M+H[1+]	1.362302
453.3705	C03313	M+H[1+]	29.59781
296.0636	C03373	M+H[1+]	10.43633
326.1082	C03410	M+H[1+]	1.641652
132.0657	C03440	M+H[1+]	22.69676
380.1118	C03451	M+H[1+]	21.08421
221.1898	C03461	M+H[1+]	21.01087
474.1731	C03479	M+H[1+]	4.799718
118.0502	C03508	M+H[1+]	33.73341
261.0367	C03546	M+H[1+]	12.95701
114.0553	C03564	M+H[1+]	8.833755
403.3564	C03594	M+H[1+]	21.61666
157.0609	C03680	M+H[1+]	33.71151
317.2467	C03681	M+H[1+]	21.59278
238.094	C03684	M+H[1+]	8.613163
168.0294	C03722	M+H[1+]	1.683894
154.0863	C03758	M+H[1+]	5.425553
137.0595	C03765	M+H[1+]	19.4312
289.2156	C03772	M+H[1+]	12.35726
189.1601	C03793	M+H[1+]	1.285928
142.0499	C03824	M+H[1+]	15.87889
287.0635	C03838	M+H[1+]	5.154103
387.3614	C03845	M+H[1+]	27.54422
261.0367	C03862	M+H[1+]	12.95701
291.2309	C03917	M+H[1+]	21.86768

261.0367	C04006	M+H[1+]	12.95701
317.2467	C04042	M+H[1+]	21.59278
153.0544	C04043	M+H[1+]	12.32861
146.0812	C04076	M+H[1+]	13.87389
323.1273	C04079	M+H[1+]	16.92621
240.109	C04244	M+H[1+]	1.310345
302.0638	C04257	M+H[1+]	6.963005
130.05	C04281	M+H[1+]	24.13728
130.05	C04282	M+H[1+]	24.13728
291.2309	C04295	M+H[1+]	21.86768
291.2309	C04373	M+H[1+]	21.86768
186.0399	C04409	M+H[1+]	3.174905
302.0638	C04501	M+H[1+]	6.963005
333.2418	C04518	M+H[1+]	20.71312
435.3459	C04554	M+H[1+]	25.66851
369.1717	C04555	M+H[1+]	16.16782
314.0741	C04640	M+H[1+]	12.84688
313.2364	C04717	M+H[1+]	8.529103
450.333	C04722	M+H[1+]	18.29037
367.0637	C04734	M+H[1+]	1.240443
321.2408	C04742	M+H[1+]	19.3696
321.2408	C04805	M+H[1+]	19.3696
455.0823	C04823	M+H[1+]	7.089664
353.2306	C04853	M+H[1+]	15.51013
399.3614	C05103	M+H[1+]	21.11973
383.3289	C05107	M+H[1+]	19.5447
413.3773	C05108	M+H[1+]	15.10156
429.4081	C05109	M+H[1+]	28.8709
516.2982	C05122	M+H[1+]	11.52467
126.1026	C05127	M+H[1+]	27.10999
111.0556	C05130	M+H[1+]	33.74204
333.2418	C05138	M+H[1+]	20.71312
305.2106	C05139	M+H[1+]	12.29049
303.1943	C05140	M+H[1+]	24.47082
289.1793	C05141	M+H[1+]	14.20466
132.0657	C05147	M+H[1+]	22.69676
910.2231	C05266	M+H[1+]	17.20519
303.1943	C05284	M+H[1+]	24.47082
301.1792	C05285	M+H[1+]	18.58563
303.1943	C05290	M+H[1+]	24.47082
291.2309	C05293	M+H[1+]	21.86768
305.2106	C05294	M+H[1+]	12.29049
303.1943	C05295	M+H[1+]	24.47082
301.1792	C05297	M+H[1+]	18.58563
287.1635	C05298	M+H[1+]	12.32651
301.1792	C05299	M+H[1+]	18.58563
287.1635	C05300	M+H[1+]	12.32651
289.1793	C05301	M+H[1+]	14.20466

303.1943	C05302	M+H[1+]	24.47082
122.0965	C05332	M+H[1+]	11.06176
246.1559	C05340	M+H[1+]	33.74784
218.15	C05341	M+H[1+]	33.74199
261.0367	C05345	M+H[1+]	12.95701
181.0493	C05350	M+H[1+]	14.97796
337.2357	C05356	M+H[1+]	15.49291
343.124	C05400	M+H[1+]	1.295607
255.1066	C05401	M+H[1+]	6.682354
343.124	C05402	M+H[1+]	1.295607
385.3459	C05437	M+H[1+]	19.95375
385.3459	C05439	M+H[1+]	19.95375
385.3459	C05443	M+H[1+]	19.95375
421.3671	C05444	M+H[1+]	22.39116
419.3514	C05445	M+H[1+]	17.78244
437.361	C05446	M+H[1+]	29.20153
403.3564	C05451	M+H[1+]	21.61666
405.3715	C05452	M+H[1+]	22.51145
419.3514	C05453	M+H[1+]	17.78244
421.3671	C05454	M+H[1+]	22.39116
401.3408	C05455	M+H[1+]	23.85975
500.3028	C05465	M+H[1+]	23.57811
450.3194	C05466	M+H[1+]	27.26142
363.215	C05469	M+H[1+]	18.00106
365.2319	C05471	M+H[1+]	17.7429
365.2319	C05473	M+H[1+]	17.7429
351.2526	C05476	M+H[1+]	20.42797
349.237	C05478	M+H[1+]	15.43913
317.2467	C05479	M+H[1+]	21.59278
333.2418	C05485	M+H[1+]	20.71312
349.237	C05487	M+H[1+]	15.43913
347.2203	C05488	M+H[1+]	17.98446
365.2319	C05489	M+H[1+]	17.7429
345.2046	C05490	M+H[1+]	27.52813
347.2203	C05497	M+H[1+]	17.98446
333.2044	C05498	M+H[1+]	18.88938
419.3514	C05499	M+H[1+]	17.78244
403.3564	C05500	M+H[1+]	21.61666
419.3514	C05501	M+H[1+]	17.78244
403.3564	C05502	M+H[1+]	21.61666
449.2179	C05503	M+H[1+]	14.44121
465.2134	C05504	M+H[1+]	11.93727
253.0931	C05512	M+H[1+]	1.961663
120.0657	C05519	M+H[1+]	33.73069
373.1897	C05552	M+H[1+]	18.19007
171.0651	C05576	M+H[1+]	15.04394
169.0494	C05577	M+H[1+]	16.82075
150.0551	C05578	M+H[1+]	9.624975

148.039	C05579	M+H[1+]	1.254768
185.0446	C05580	M+H[1+]	5.406827
167.07	C05581	M+H[1+]	9.038739
183.0652	C05582	M+H[1+]	16.32428
183.0652	C05583	M+H[1+]	16.32428
199.0604	C05584	M+H[1+]	2.419662
139.039	C05585	M+H[1+]	16.28647
168.1016	C05587	M+H[1+]	12.30781
198.1123	C05588	M+H[1+]	11.05948
184.0965	C05589	M+H[1+]	14.68544
185.0808	C05594	M+H[1+]	20.16098
194.0812	C05598	M+H[1+]	9.136829
176.0706	C05634	M+H[1+]	17.75711
192.0654	C05635	M+H[1+]	15.60469
181.0973	C05636	M+H[1+]	1.816415
162.0548	C05637	M+H[1+]	16.81222
181.0973	C05638	M+H[1+]	1.816415
162.0548	C05639	M+H[1+]	16.81222
265.1185	C05642	M+H[1+]	1.840134
249.1224	C05643	M+H[1+]	16.5605
224.0551	C05645	M+H[1+]	5.245861
209.0921	C05647	M+H[1+]	33.73034
253.0819	C05648	M+H[1+]	1.352068
225.0866	C05651	M+H[1+]	1.337853
166.0498	C05653	M+H[1+]	24.56138
206.0811	C05660	M+H[1+]	18.54532
271.0196	C05699	M+H[1+]	1.255103
661.3201	C05768	M+H[1+]	12.11962
655.2741	C05770	M+H[1+]	14.40792
591.3162	C05791	M+H[1+]	18.49761
311.2001	C05819	M+H[1+]	12.4711
125.0709	C05827	M+H[1+]	12.16529
141.0658	C05828	M+H[1+]	2.270081
257.0899	C05841	M+H[1+]	7.27995
255.0648	C05844	M+H[1+]	14.39166
467.3497	C05849	M+H[1+]	23.62965
153.0544	C05852	M+H[1+]	12.32861
130.0864	C05936	M+H[1+]	6.413186
148.0606	C05938	M+H[1+]	33.72424
163.0241	C05946	M+H[1+]	1.081079
497.2675	C05951	M+H[1+]	20.03326
369.2254	C05956	M+H[1+]	9.240941
337.2357	C05965	M+H[1+]	15.49291
337.2357	C05966	M+H[1+]	15.49291
404.0956	C05983	M+H[1+]	1.328876
390.0799	C05993	M+H[1+]	1.28154
103.0393	C06002	M+H[1+]	21.61245
223.2053	C06081	M+H[1+]	14.756

380.2555	C06124	M+H[1+]	17.24451
333.0591	C06196	M+H[1+]	1.303049
163.0749	C06205	M+H[1+]	10.84308
191.1177	C06212	M+H[1+]	11.32035
390.0799	C06241	M+H[1+]	1.28154
419.3514	C06341	M+H[1+]	17.78244
145.1224	C06423	M+H[1+]	0.304563
229.216	C06424	M+H[1+]	18.7667
313.3094	C06425	M+H[1+]	19.67684
279.2312	C06426	M+H[1+]	21.83646
279.2312	C06427	M+H[1+]	21.83646
303.231	C06428	M+H[1+]	12.34661
329.2469	C06429	M+H[1+]	14.83467
169.0858	C06459	M+H[1+]	15.29531
313.0704	C06800	M+H[1+]	9.164868
137.0595	C07086	M+H[1+]	19.4312
124.0394	C07446	M+H[1+]	8.502337
195.0877	C07481	M+H[1+]	33.01451
180.0771	C07585	M+H[1+]	5.860138
277.0257	C07645	M+H[1+]	1.087314
417.3353	C07712	M+H[1+]	20.46908
413.3773	C08821	M+H[1+]	15.10156
477.2473	C11061	M+H[1+]	10.78074
479.2264	C11131	M+H[1+]	11.37959
477.2109	C11132	M+H[1+]	9.501037
447.2011	C11133	M+H[1+]	14.39221
465.2469	C11134	M+H[1+]	3.920707
467.2626	C11135	M+H[1+]	13.66023
467.2626	C11136	M+H[1+]	13.66023
569.1743	C11376	M+H[1+]	29.75524
411.3614	C11455	M+H[1+]	15.5464
411.3614	C11508	M+H[1+]	15.5464
413.3773	C11522	M+H[1+]	15.10156
318.2998	C12144	M+H[1+]	20.72656
403.3564	C13550	M+H[1+]	21.61666
319.2627	C13712	M+H[1+]	20.1356
174.0549	C14040	M+H[1+]	18.10554
269.0956	C14556	M+H[1+]	5.088776
321.2408	C14748	M+H[1+]	19.3696
321.2408	C14749	M+H[1+]	19.3696
321.2408	C14768	M+H[1+]	19.3696
321.2408	C14769	M+H[1+]	19.3696
321.2408	C14770	M+H[1+]	19.3696
321.2408	C14771	M+H[1+]	19.3696
339.2513	C14772	M+H[1+]	15.19597
339.2513	C14773	M+H[1+]	15.19597
339.2513	C14774	M+H[1+]	15.19597
339.2513	C14775	M+H[1+]	15.19597

321.2408	C14778	M+H[1+]	19.3696
337.2357	C14781	M+H[1+]	15.49291
355.2462	C14782	M+H[1+]	14.45946
145.0647	C14786	M+H[1+]	8.495488
145.0647	C14787	M+H[1+]	8.495488
190.0496	C14800	M+H[1+]	14.74731
208.0602	C14801	M+H[1+]	14.7447
190.0496	C14802	M+H[1+]	14.74731
337.2357	C14812	M+H[1+]	15.49291
337.2357	C14813	M+H[1+]	15.49291
355.2462	C14814	M+H[1+]	14.45946
337.2357	C14823	M+H[1+]	15.49291
297.2416	C14825	M+H[1+]	21.31646
297.2416	C14826	M+H[1+]	21.31646
269.0956	C14849	M+H[1+]	5.088776
269.0956	C14850	M+H[1+]	5.088776
269.0956	C14851	M+H[1+]	5.088776
287.1055	C14852	M+H[1+]	14.79938
285.0912	C14854	M+H[1+]	5.717135
112.9561	C14857	M+H[1+]	30.37492
112.9561	C14858	M+H[1+]	30.37492
112.9561	C14859	M+H[1+]	30.37492
420.0391	C14861	M+H[1+]	1.149721
350.1013	C14871	M+H[1+]	20.01481
289.2517	C15492	M+H[1+]	21.85209
301.2157	C15493	M+H[1+]	24.47838
419.3514	C15518	M+H[1+]	17.78244
403.3564	C15519	M+H[1+]	21.61666
419.3514	C15520	M+H[1+]	17.78244
163.0426	C15606	M+H[1+]	4.557357
403.3564	C15610	M+H[1+]	21.61666
413.3773	C15776	M+H[1+]	15.10156
399.3614	C15777	M+H[1+]	21.11973
397.3458	C15778	M+H[1+]	24.47878
397.3458	C15780	M+H[1+]	24.47878
399.3614	C15781	M+H[1+]	21.11973
413.3773	C15782	M+H[1+]	15.10156
411.3614	C15783	M+H[1+]	15.5464
443.3512	C15808	M+H[1+]	20.46768
397.3458	C15816	M+H[1+]	24.47878
415.3928	C15915	M+H[1+]	23.33585
512.1266	C15974	M+H[1+]	12.20502
498.1107	C15976	M+H[1+]	12.65418
512.1266	C15978	M+H[1+]	12.20502
207.051	C16241	M+H[1+]	1.184738
277.2158	C16300	M+H[1+]	12.39841
167.0555	C16353	M+H[1+]	22.74126
183.0514	C16355	M+H[1+]	33.71889

197.0673	C16356	M+H[1+]	7.685183
167.0555	C16358	M+H[1+]	22.74126
183.0514	C16359	M+H[1+]	33.71889
197.0673	C16360	M+H[1+]	7.685183
201.0985	C16362	M+H[1+]	1.3059
519.2234	C16543	M+H[1+]	14.60854
251.1751	C16560	M+H[1+]	5.410648
207.1496	C16561	M+H[1+]	4.59939
160.1808	C16565	M+H[1+]	33.82031
476.1937	C16577	M+H[1+]	18.70788
255.0976	C16582	M+H[1+]	1.307288
255.0976	C16584	M+H[1+]	1.307288
196.0967	C16586	M+H[1+]	12.60761
194.0812	C16587	M+H[1+]	9.136829
210.0761	C16591	M+H[1+]	26.59274
194.0812	C16595	M+H[1+]	9.136829
192.0654	C16596	M+H[1+]	15.60469
167.0378	C16614	M+H[1+]	8.70012
151.0518	C16631	M+H[1+]	6.610805
263.0665	C16633	M+H[1+]	3.701584
246.0882	C16635	M+H[1+]	1.355685
317.2105	C16677	M+H[1+]	12.41908
317.2105	C16679	M+H[1+]	12.41908
317.2105	C16680	M+H[1+]	12.41908
285.2208	C16681	M+H[1+]	23.84408
287.2366	C16682	M+H[1+]	21.00566
329.064	C16756	M+H[1+]	1.376888
340.0625	C17267	M+H[1+]	1.21792
417.3353	C17331	M+H[1+]	20.46908
417.3353	C17332	M+H[1+]	20.46908
417.3353	C17333	M+H[1+]	20.46908
433.33	C17335	M+H[1+]	25.22764
417.3353	C17336	M+H[1+]	20.46908
431.314	C17337	M+H[1+]	19.44933
417.3353	C17339	M+H[1+]	20.46908
333.2418	C18038	M+H[1+]	20.71312
333.2418	C18040	M+H[1+]	20.71312
319.2627	C18041	M+H[1+]	20.1356
321.2785	C18042	M+H[1+]	19.01897
397.2029	C18044	M+H[1+]	22.29297
305.2106	C18045	M+H[1+]	12.29049
305.2106	C18075	M+H[1+]	12.29049
433.33	C18231	M+H[1+]	25.22764
364.0654	C18239	M+H[1+]	11.69558
257.1321	C19488	M+H[1+]	7.625285
291.1369	C19490	M+H[1+]	25.53118
307.1322	C19559	M+H[1+]	30.24849
353.0846	C19562	M+H[1+]	1.262819

224.1034	C19563	M+H[1+]	1.332115
224.1034	C19566	M+H[1+]	1.332115
210.124	C19574	M+H[1+]	1.341994
329.064	C19586	M+H[1+]	1.376888
347.077	C19588	M+H[1+]	8.38876
329.064	C19595	M+H[1+]	1.376888
291.1369	C19607	M+H[1+]	25.53118
326.2143	C19691	M+H[1+]	17.4272
322.0772	C20775	M+H[1+]	26.97987
233.1121	C21015	M+H[1+]	6.407136
290.1346	C21016	M+H[1+]	33.71719
129.0661	C21028	M+H[1+]	1.35344
147.0766	C21029	M+H[1+]	33.76097
401.3771	C21106	M+H[1+]	27.67883
240.109	C21640	M+H[1+]	1.310345
429.3358	C22112	M+H[1+]	15.54659
383.3301	C22136	M+H[1+]	16.61558
204.2075	G00001	M+H[1+]	1.187793
204.2075	G00023	M+H[1+]	1.187793
366.3085	G00024	M+H[1+]	21.30292
528.509	G00036	M+H[1+]	13.01982
528.509	G00123	M+H[1+]	13.01982
204.2075	G00143	M+H[1+]	1.187793
342.3076	G00146	M+H[1+]	19.64655
566.4045	G00148	M+H[1+]	10.68556
457.4073	G00156	M+H[1+]	29.46419
633.5066	G00157	M+H[1+]	29.72207
777.7079	G00526	M+H[1+]	8.297493
478.4086	G00872	M+H[1+]	11.18833
464.4094	G01391	M+H[1+]	26.11165
398.3092	G02632	M+H[1+]	10.96982
478.4086	G09660	M+H[1+]	11.18833
366.3085	G13026	M+H[1+]	21.30292
734.6099	G13039	M+H[1+]	29.39394
654.5077	G13040	M+H[1+]	19.35429
366.3085	G13087	M+H[1+]	21.30292
193.0683	C00021	M+2H[2+]	18.81894
129.0182	C00026	M-H ₂ O+H[1+]	20.16351
203.0526	C00031	M+Na[1+]	33.72074
309.097	C00032	M+2H[2+]	17.35862
101.0237	C00042	M-H ₂ O+H[1+]	22.80984
466.9638	C00075	M-H ₂ O+H[1+]	1.182177
203.0526	C00095	M+Na[1+]	33.72074
115.0371	C00116	M+Na[1+]	1.286308
133.0498	C00121	M-H ₂ O+H[1+]	2.112768
203.0526	C00124	M+Na[1+]	33.72074
203.0526	C00137	M+Na[1+]	33.72074
276.9968	C00158	M+HCOOK[1+]	1.196

203.0526	C00159	M+Na[1+]	33.72074
189.0162	C00181	M+K[1+]	1.275531
519.0422	C00190	M-H ₂ O+H[1+]	26.108
270.9621	C00197	M+HCOOK[1+]	1.241367
449.9965	C00206	M+K[1+]	19.26041
203.0526	C00221	M+Na[1+]	33.72074
113.0594	C00233	M-H ₂ O+H[1+]	10.843
248.9562	C00236	M-H ₂ O+H[1+]	1.241964
179.0551	C00257	M-H ₂ O+H[1+]	18.96367
189.0162	C00259	M+K[1+]	1.275531
203.0526	C00267	M+Na[1+]	33.72074
241.1181	C00272	M[1+]	33.71282
545.9582	C00286	M+K[1+]	1.161711
189.0162	C00310	M+K[1+]	1.275531
276.9968	C00311	M+HCOOK[1+]	1.196
189.0162	C00312	M+K[1+]	1.275531
135.9263	C00320	M+Na[1+]	31.07175
183.0268	C00322	M+Na[1+]	1.308019
264.0481	C00329	M+HCOOK[1+]	1.572462
279.0295	C00345	M(Cl ₃ 7)+H[1+]	1.834299
433.1888	C00353	M-H ₂ O+H[1+]	16.83027
175.0579	C00379	M+Na[1+]	1.268478
167.0912	C00418	M+H ₂ O+H[1+]	1.290062
365.1292	C00448	M-H ₂ O+H[1+]	17.87426
162.0049	C00459	M(C ₁₃)+3H[3+]	1.095293
610.2473	C00461	M-H ₂ O+H[1+]	9.695953
264.0819	C00492	M+H+Na[2+]	3.102378
191.9944	C00506	M+Na[1+]	6.409815
175.0579	C00532	M+Na[1+]	1.268478
429.0568	C00570	M-H ₂ O+H[1+]	12.7549
140.0425	C00581	M+Na[1+]	9.54429
268.0584	C00627	M+H ₂ O+H[1+]	1.390548
270.9621	C00631	M+HCOOK[1+]	1.241367
271.0458	C00647	M+Na[1+]	7.020133
264.0819	C00721	M+H+Na[2+]	3.102378
217.1948	C00751	M+H+Na[2+]	14.44367
179.0551	C00800	M-H ₂ O+H[1+]	18.96367
203.0526	C00984	M+Na[1+]	33.72074
224.9759	C00988	M+HCOONa[1+]	1.244777
368.0274	C01103	M[1+]	1.167728
248.9562	C01159	M-H ₂ O+H[1+]	1.241964
562.8931	C01284	M-H ₂ O+H[1+]	1.173286
705.1843	C01613	M+K[1+]	1.270474
214.0824	C01674	M+2H[2+]	1.441264
176.0345	C01693	M-H ₂ O+H[1+]	6.19492
137.0623	C01801	M(Cl ₃ 7)+H[1+]	1.741327
598.3131	C02166	M-CO+H[1+]	9.456751
101.0237	C02170	M-H ₂ O+H[1+]	22.80984

214.0392	C02305	M(S34)+H[1+]	1.166254
203.0526	C02336	M+Na[1+]	33.72074
199.0215	C02670	M+Na[1+]	1.539744
160.0606	C02918	M+Na[1+]	33.72491
199.0215	C03289	M+Na[1+]	1.539744
242.0662	C03366	M[1+]	1.665004
290.1238	C03406	M[1+]	1.356165
589.319	C03428	M(S34)+H[1+]	5.113352
527.4657	C03455	M(Cl37)+H[1+]	29.54057
176.0831	C03771	M(S34)+H[1+]	12.26102
446.0692	C03794	M-H2O+H[1+]	6.873296
176.0345	C04185	M-H2O+H[1+]	6.19492
338.0639	C04677	M[1+]	1.246182
255.0976	C04874	M[1+]	1.307288
219.9847	C05335	M+Na[1+]	1.09731
213.0011	C05379	M+Na[1+]	30.19706
327.127	C05399	M-H2O+H[1+]	18.76844
264.0819	C05404	M+H+Na[2+]	3.102378
323.0289	C05640	M+Na[1+]	1.165792
105.0008	C05823	M-H2O+H[1+]	17.42665
520.2671	C05859	M(C13)+H[1+]	19.92242
193.1112	C05933	M(Cl37)+H[1+]	1.31294
233.0062	C06054	M+H2O+H[1+]	1.291653
180.0655	C07480	M[1+]	1.734409
170.9142	C07490	M+Na[1+]	1.713307
315.0047	C07646	M+Na[1+]	17.53625
557.2102	C09332	M-H2O+H[1+]	7.214856
205.0379	C12248	M(Cl37)+H[1+]	1.224797
277.1039	C12270	M-CO+H[1+]	1.387287
180.0655	C13747	M[1+]	1.734409
194.9409	C14453	M+Na[1+]	1.080712
194.9409	C14839	M+Na[1+]	1.080712
194.9409	C14840	M+Na[1+]	1.080712
371.0902	C14853	M+HCOONa[1+]	5.368328
532.1903	C14855	M-CO2+H[1+]	13.50651
532.1903	C14856	M-CO2+H[1+]	13.50651
337.113	C14874	M(Cl37)+H[1+]	15.15381
130.0651	C15522	M(C13)+2H[2+]	10.02794
249.0375	C16361	M+K[1+]	1.261755
207.1014	C16453	M[1+]	16.90589
389.2288	C16545	M(C13)+H[1+]	6.411318
461.168	C16578	M[1+]	9.960549
313.1515	C16608	M(Cl37)+H[1+]	14.59779
313.1074	C16610	M(C13)+H[1+]	7.053735
378.0408	C16615	M[1+]	1.224044
336.0528	C16619	M-CO2+H[1+]	1.243079
461.168	C16643	M[1+]	9.960549
145.0973	C16741	M-H2O+H[1+]	33.78954

841.5684	C17432	M-H ₂ O+H[1+]	12.35459
468.3204	C18043	M(C13)+H[1+]	23.32683
275.1238	C19489	M(Cl37)+H[1+]	1.624462
275.1238	C19561	M(Cl37)+H[1+]	1.624462
275.1238	C19604	M(Cl37)+H[1+]	1.624462
250.0324	C20239	M+K[1+]	1.400762
343.19	C20265	M+H ₂ O+H[1+]	21.88868
388.9928	C21750	M-H ₂ O+H[1+]	30.67969
508.9511	C21751	M+Na[1+]	7.63579
129.0182	C21943	M+Na[1+]	20.16351
970.8853	G00027	M+Na[1+]	1.177844
383.2656	G00092	M+NaCl[1+]	5.365113
218.1617	G00145	M+K[1+]	13.64446
750.5867	G00149	M+Na[1+]	14.22563
155.0892	G00154	M+Na[1+]	8.266845
379.2667	G00155	M+HCOOK[1+]	14.7427
685.4682	G00711	M+HCOOK[1+]	27.00005
145.0973	G10617	M-H ₂ O+H[1+]	33.78954
145.0973	G10618	M-H ₂ O+H[1+]	33.78954
185.0886	G13027	M+Na[1+]	12.26406
917.6851	G13037	M+Na[1+]	19.69927
959.7885	G13038	M+Na[1+]	29.74691
959.7885	G13042	M+Na[1+]	29.74691
663.596	G13043	M-H ₂ O+H[1+]	26.13058
885.5905	G13093	M+Na[1+]	29.76853
1059.694	G13094	M-H ₂ O+H[1+]	16.15494
526.4904	G13128	M+Na[1+]	26.67383

Table S8: KEGG pathways of mice treated with BioPersist and BioColoniz

KEGG pathway	Total Cmpd	Hits	Raw p	FDR	Impact
<i>Valine, leucine and isoleucine degradation</i>	40	14	7.07E-07	5.59E-05	0.17531
<i>Tryptophan metabolism</i>	41	35	6.60E-06	0.000261	0.99103
<i>Drug metabolism - other enzymes</i>	38	12	1.97E-05	0.000487	0.17648
<i>beta-Alanine metabolism</i>	21	11	2.88E-05	0.000487	0.27239
<i>Purine metabolism</i>	66	35	3.08E-05	0.000487	0.75027
<i>Arginine and proline metabolism</i>	38	29	5.37E-05	0.000707	0.70799
<i>Mucin type O-glycan biosynthesis</i>	12	3	8.51E-05	0.00087	0.70874
<i>Histidine metabolism</i>	16	16	8.81E-05	0.00087	0.99998
<i>Aminoacyl-tRNA biosynthesis</i>	48	20	0.000117	0.001031	0.25001
<i>Pentose phosphate pathway</i>	22	14	0.000154	0.001049	0.73159
<i>Alanine, aspartate and glutamate metabolism</i>	28	18	0.000155	0.001049	0.89504
<i>Pantothenate and CoA biosynthesis</i>	19	11	0.000159	0.001049	0.33571
<i>Tyrosine metabolism</i>	42	35	0.000209	0.001273	0.84602
<i>Folate biosynthesis</i>	27	16	0.000228	0.001284	0.28633
<i>Phosphatidylinositol signaling system</i>	28	7	0.00029	0.001526	0.37115
<i>Primary bile acid biosynthesis</i>	46	31	0.000317	0.001555	0.45774
<i>Glycine, serine and threonine metabolism</i>	34	17	0.000335	0.001555	0.42701
<i>Porphyrin and chlorophyll metabolism</i>	30	12	0.000402	0.001764	0.68741
<i>Glutathione metabolism</i>	28	10	0.000425	0.001769	0.37473
<i>Metabolism of xenobiotics by cytochrome P450</i>	64	44	0.000615	0.002389	0.69501
<i>Pyrimidine metabolism</i>	39	23	0.000635	0.002389	0.58278
<i>Lysine degradation</i>	25	12	0.000679	0.002393	0.52583
<i>Fatty acid degradation</i>	39	3	0.000707	0.002393	0.00436
<i>Arginine biosynthesis</i>	14	10	0.000727	0.002393	0.59898
<i>Valine, leucine and isoleucine biosynthesis</i>	8	7	0.000846	0.002672	0
<i>Ether lipid metabolism</i>	20	2	0.001013	0.003078	0
<i>Ubiquinone and other terpenoid-quinone biosynthesis</i>	9	8	0.001246	0.003647	1
<i>Inositol phosphate metabolism</i>	30	11	0.00138	0.003893	0.49975
<i>Glycosaminoglycan degradation</i>	23	9	0.001505	0.004101	0.33333
<i>Pentose and glucuronate interconversions</i>	18	13	0.001829	0.004816	0.65624
<i>Phenylalanine metabolism</i>	12	10	0.001992	0.005077	1
<i>Drug metabolism - cytochrome P450</i>	27	17	0.002378	0.005871	0.30769
<i>One carbon pool by folate</i>	9	8	0.002457	0.005883	0.87936
<i>Nicotinate and nicotinamide metabolism</i>	15	8	0.002562	0.005952	0.52325
<i>Terpenoid backbone biosynthesis</i>	18	12	0.002787	0.00628	0.79047
<i>Glycolysis / Gluconeogenesis</i>	26	11	0.002862	0.00628	0.44178
<i>Ascorbate and aldarate metabolism</i>	10	6	0.003621	0.007731	0.75
<i>Glycosylphosphatidylinositol (GPI)-anchor biosynthesis</i>	14	5	0.004039	0.008396	0.64435
<i>Biotin metabolism</i>	10	3	0.004646	0.009411	0.35
<i>Glycerolipid metabolism</i>	16	4	0.007884	0.01557	0.28037
<i>alpha-Linolenic acid metabolism</i>	13	2	0.00809	0.015586	0.33333
<i>Cysteine and methionine metabolism</i>	33	20	0.008286	0.015586	0.87465
<i>Retinol metabolism</i>	16	15	0.010553	0.019389	0.83832
<i>Steroid biosynthesis</i>	42	39	0.011385	0.020441	1
<i>D-Arginine and D-ornithine metabolism</i>	4	4	0.012032	0.021122	0

<i>Taurine and hypotaurine metabolism</i>	8	5	0.01372	0.0233	0.42857
<i>Amino sugar and nucleotide sugar metabolism</i>	37	23	0.013862	0.0233	0.62599
<i>Vitamin B6 metabolism</i>	9	8	0.016537	0.027218	1
<i>Steroid hormone biosynthesis</i>	77	74	0.016975	0.027368	0.94489
<i>N-Glycan biosynthesis</i>	41	4	0.019829	0.031111	0.00676
<i>Arachidonic acid metabolism</i>	36	27	0.020085	0.031111	0.72633
<i>Thiamine metabolism</i>	7	4	0.021563	0.032759	0
<i>Biosynthesis of unsaturated fatty acids</i>	36	12	0.024622	0.036701	0
<i>Sphingolipid metabolism</i>	21	8	0.027631	0.040422	0.34077
<i>Glycerophospholipid metabolism</i>	36	8	0.032118	0.046134	0.27094
<i>Fatty acid elongation</i>	39	2	0.033014	0.046573	0.01148
<i>Mannose type O-glycan biosynthesis</i>	17	2	0.060182	0.083411	0
<i>Fructose and mannose metabolism</i>	18	10	0.063239	0.086137	0.65563
<i>Caffeine metabolism</i>	12	11	0.070437	0.094314	1
<i>Glyoxylate and dicarboxylate metabolism</i>	32	9	0.088443	0.11645	0.17726
<i>Neomycin, kanamycin and gentamicin biosynthesis</i>	2	1	0.129	0.16706	0
<i>Pyruvate metabolism</i>	22	2	0.13482	0.17179	0.0591
<i>Phenylalanine, tyrosine and tryptophan biosynthesis</i>	4	4	0.14846	0.18616	1
<i>Selenocompound metabolism</i>	20	2	0.15466	0.19091	0.15909
<i>Galactose metabolism</i>	27	20	0.21285	0.25787	0.8676
<i>Starch and sucrose metabolism</i>	15	9	0.21543	0.25787	0.48365
<i>Propanoate metabolism</i>	23	4	0.22208	0.26185	0.08122
<i>Linoleic acid metabolism</i>	5	2	0.27628	0.32097	1
<i>Butanoate metabolism</i>	15	7	0.29185	0.33373	0.17461
<i>Nitrogen metabolism</i>	6	2	0.29571	0.33373	0
<i>Lipoic acid metabolism</i>	8	1	0.34038	0.37874	0
<i>Riboflavin metabolism</i>	4	4	0.36734	0.40306	1
<i>D-Glutamine and D-glutamate metabolism</i>	6	6	0.40093	0.43389	1
<i>Glycosaminoglycan biosynthesis - chondroitin sulfate / dermatan sulfate</i>	10	5	0.43073	0.45983	0.71429
<i>Synthesis and degradation of ketone bodies</i>	5	1	0.43956	0.463	0.6
<i>Sulfur metabolism</i>	8	2	0.59031	0.61362	0.21277
<i>Citrate cycle (TCA cycle)</i>	20	6	0.75827	0.7714	0.27668
<i>Glycosaminoglycan biosynthesis - heparan sulfate / heparin</i>	4	1	0.76163	0.7714	0
<i>Fatty acid biosynthesis</i>	47	5	0.88033	0.88033	0.01473

Table S9: Metabolites annotated in tryptophan degradation pathways

Common Name	KEGG ID	Significance	Relative to BioColoniz
<i>L-Tryptophan</i>	C00078	ns	N/A
<i>N-Acetylserotonin</i>	C00978	ns	N/A
<i>Melatonin</i>	C01598	ns	N/A
<i>5-Hydroxykynurenamine</i>	C05638	ns	N/A
<i>5-Hydroxykynurenine</i>	C05651	ns	N/A
<i>5-Hydroxy-L-tryptophan</i>	C00643	ns	N/A
<i>L-Formylkynurenine</i>	C02700	ns	N/A
<i>2-Oxoadipate</i>	C00322	ns	N/A
<i>2-Amino-3-carboxymuconate semialdehyde</i>	C04409	ns	N/A
<i>3-Hydroxyanthranilate</i>	C00632	ns	N/A
<i>L-Kynurenine</i>	C00328	ns	N/A
<i>3-Hydroxy-L-kynurenine</i>	C03327	ns	N/A
<i>3-Hydroxykynurenamine</i>	C05636	ns	N/A
<i>2-Aminomuconate semialdehyde</i>	C03824	ns	N/A
<i>5-Hydroxy-N-formylkynurenine</i>	C05648	ns	N/A
<i>5-Hydroxyindoleacetaldehyde</i>	C05634	ns	N/A
<i>Formyl-5-hydroxykynurenamine</i>	C05642	ns	N/A
<i>5-Methoxyindoleacetate</i>	C05660	ns	N/A
<i>Formyl-N-acetyl-5-methoxykynurenamine</i>	C05642	ns	N/A
<i>2-Aminomuconate</i>	C02220	ns	N/A
<i>Cinnavalinate</i>	C05640	ns	N/A
<i>4-(2-Amino-3-hydroxyphenyl)-2,4-dioxobutanoate</i>	C05645	ns	N/A
<i>Indole-3-acetate</i>	C00954	ns	N/A
<i>N-Methylserotonin</i>	C06212	ns	N/A
<i>Serotonin</i>	C00780	0.0036	Up
<i>6-Hydroxymelatonin</i>	C05643	0.0211	Up
<i>Anthranilate</i>	C00108	0.055	down
<i>4,6-Dihydroxyquinoline</i>	C05639	0.02	down
<i>4-(2-Aminophenyl)-2,4-dioxobutanoate</i>	C01252	0.0048	DOWN
<i>4,8-Dihydroxyquinoline</i>	C05637	0.02	Down
<i>Tryptamine</i>	C00398	0.0382	Down
<i>Indolepyruvate</i>	C00331	0.0325	Up
<i>Indole-3-acetaldehyde</i>	C00637	0.037	Up
<i>5-Hydroxyindoleacetate</i>	C05635	0.0012	Down