Supplemental Table 2. Targeted metabolomics analysis on the serum from MKO and Flox mice

Metabolites (ng/mL)	flox_s1224	flox_s1281	flox_s1282	flox_s1285	k0_s1221	k0_s1223	k0_s1225	k0_s1283
L_Histidine	22129	18337	19833	19520	23411	21778	36063	17812
Dimethylglycine	1601	1752	1970	1488	1438	1589	1702	1200
Gamma_Aminobutyric acid	287	244	332	270	302	189	242	167
L_Serine	18495	18978	22294	18105	19153	18116	32284	11564
L_threonine	14191	14535	12371	11429	16886	14860	24241	11340
L_Homoserine	332	1071	132	45	45	1068	45	777
Creatine	77454	68304	91520	51660	69829	54181	114075	84053
N_Acetylserotonin	57	30	106	96	88	79	59	75
Hydroxypropionic acid	947	869	973	892	1111	1522	1245	1583
Aminocaproic acid	166	17	185	101	172	99	237	200
Glycylproline	897	1071	1463	830	1093	751	5898	810
Adenosine monophosphate	567	559	568	542	536	654	869	10220
3_Methylindole	3443	5168	7355	9652	6997	10843	8174	5855
L_Lactic acid	794713	866848	837058	605858	578697	618427	779233	719780
Methylcysteine	286	383	395	534	233	258	266	333
L_Tyrosine	46288	43481	38334	39090	47035	51083	80709	34996
5_Hydroxy_L_tryptophan	761	675	525	921	417	356	896	2269
L_Asparagine	79012	86550	79712	69071	96059	82421	170214	64833
L_Phenylalanine	27612	23007	26151	23423	26628	24350	47275	30760
Hydroxyphenyllactic acid	309	465	395	337	512	338	695	420
L_Kynurenine	597	625	1151	562	60	813	917	924
L_Aspartic acid	4908	3430	8743	2141	2655	1750	19626	887
5_L_Glutamyl_L_alanine	741	783	980	713	654	1128	1342	531
But_2_enoic acid	99	0	88	48	80	100	0	0
Pyrrole_2_carboxylic acid	61	66	55	67	61	54	60	85
2_Hydroxy_3_methylbutyric acid	3492	3901	3993	4582	3781	4621	3478	4642
Picolinic acid	190	177	187	196	187	190	190	203
4_Hydroxybenzoic acid	25	0	40	8	0	41	16	19
Ortho_Hydroxyphenylacetic acid	61	67	80	64	70	78	54	61
Hippuric acid	173	162	546	130	185	799	477	182
L_Malic acid	13434	20625	14012	7706	17081	14184	28014	29140
N_Acetyl_L_aspartic acid	895	719	1863	1281	505	749	1236	758
Ethylmethylacetic acid	471	511	571	566	527	564	537	646
2_Methyl_4_pentenoic acid	19	24	17	17	20	28	35	19
Benzoic acid	576	545	569	515	513	485	542	558
2_Hydroxycaproic acid	127	124	90	112	138	123	124	139
Phenylacetic acid	201	172	186	199	185	263	271	366
Indoleacetic acid	68	61	61	51	64	88	78	74
Glutaric acid	321	313	298	244	323	326	536	538
trans_Aconitic acid	159968	138459	216595	134553	131648	180274	157302	182705

2_Phenylpropionate	28	25	25	24	28	41	64	25
Hydrocinnamic acid	17	6	7	2	19	50	117	4
Benzenebutanoic acid	789	709	748	777	773	768	751	809
Indoleacrylic acid	8	4	10	19	11	14	7	6
3_Indolepropionic acid	230	386	347	351	676	491	506	221
4_Hydroxyphenylpyruvic acid	6555	4755	3639	2103	4708	7264	8038	5258
Azelaic acid	1269	888	2567	992	428	1352	1424	1494
Sebacic acid	1433	1272	1983	1412	1240	1447	1490	1672
Benzamide	2622	2819	2670	3113	2487	2972	2747	2889
Phenylpyruvic acid	1733	1496	1365	1535	1632	2444	2257	1106
Methylmalonic acid	8904	11862	6245	4107	6609	4896	19654	20594
D_2_Hydroxyglutaric acid	2235	2256	2664	1757	1687	2062	2542	3469
Galactonic acid	41	41	41	251	166	244	394	376
D_Gluconolactone	466	527	921	546	525	492	433	756
Glycolic acid	5783	5484	5772	5721	6388	5750	5127	7279
L_Alpha_aminobutyric acid	246	249	303	319	271	264	256	306
Glyceric acid	2059	1541	1576	1377	1301	1351	1848	1495
Acetylglycine	2135	1750	2434	1670	1960	2381	2106	3102
L_Pipecolic acid	1132	880	1272	1121	1308	1642	1094	1482
Erythronic acid	3314	2299	7601	1493	1963	1791	2618	3173
N_Acetylserine	241	249	327	229	209	215	198	273
Ribonolactone	69	48	48	48	52	48	48	53
Ribonic acid	97	103	152	122	109	90	91	92
N_Acetylglutamine	436	470	1063	304	518	405	389	313
L_Acetylcarnitine	22980	15997	19894	18658	16813	15424	19417	27934
N_Acetylneuraminic acid	6056	4566	9272	5663	4817	5294	6874	6170
Melibiose	357	758	736	685	520	666	976	1080
C1 0	40662	36176	45079	37749	40459	42902	40164	40245
p_Cresol sulfate	3046	5476	4679	1660	2487	5303	1496	3459
C2 0	1646	1258	4760	2516	1841	3889	2177	2200
L_Valine	44299	42105	32591	36827	56931	52540	63868	48850
Pyroglutamic acid	12296	10721	17202	8187	8665	7315	27021	13418
5_Aminolevulinic acid	211	202	285	151	209	154	495	189
D_Glucose	1446119	2088568	1858874	2152065	1336389	1412316	1321639	1841259
3,4_Dihydroxymandelic acid	72	13	39	92	39	13	61	70
Lactulose	94	156	143	215	388	225	242	65
D_Maltose and Alpha_Lactose	733	1127	1005	755	1331	692	720	892
3_Hydroxybutyric acid	50053	50012	53775	67801	53527	38906	47665	157324
alpha_Hydroxyisobutyric acid	3491	3042	3677	2827	3387	3969	2243	2698
2_Hydroxybutyric acid	4295	4539	4334	5019	4017	4152	5612	10900
3_Hydroxyisovaleric acid	648	600	581	650	636	630	652	655
Glutaconic acid	12828	10377	15384	11241	12965	12981	12205	14762
L_Isoleucine and L_Leucine	66161	65692	71387	54097	84530	74538	158163	72738
D_Xylose	2721	2115	1580	2854	1761	1171	1241	1671

D_Ribulose	370	276	367	401	222	341	287	439
Beta_D_Fucose	672	1280	1645	1021	1802	979	593	1476
p_Hydroxymandelic acid	100	72	129	78	92	98	80	81
D_Fructose	3228	6945	2543	2748	19521	19554	11331	22660
C3 0	761	582	729	731	572	641	764	704
Glyceraldehyde	317	143	358	72	161	195	325	319
L_Norleucine	119	68	77	171	243	9	9	254
3_ 3_Hydroxyphenyl _3_hydroxypropanoic acid	249	244	207	154	294	214	376	303
2_Furoic acid	27	17	33	13	15	12	41	28
3_Hydroxyanthranilic acid	404	338	28	511	416	328	356	396
L_Tryptophan	43824	35477	39417	43818	35210	42248	54060	40583
C4 0	301	263	276	286	263	292	320	307
Isobutyric acid	598	419	412	517	486	395	412	488
Mandelic acid	41	29	37	38	45	66	32	35
Malonic acid	146	141	189	110	133	120	172	195
Alpha_N_Phenylacetyl_L_glutamine	76	81	79	81	77	220	91	79
Tartaric acid	1300	2072	3852	388	2858	7845	3381	3284
Phenyllactic acid	42	28	47	30	60	75	90	43
Selenomethionine	13614	11769	12713	14569	17320	16228	11529	12322
Oxalic acid	1106	1022	1384	1121	1114	1300	898	1467
Maleic acid	2829	3889	2638	1685	2862	2549	5031	5870
Methylsuccinic acid	225	220	216	188	221	236	356	335
Adipic acid	723	709	641	518	564	737	808	900
Methylglutaric acid	41	52	56	44	50	67	53	52
Phthalic acid	17	14	20	17	14	18	16	25
cis_Aconitic acid	137844	111890	189875	113357	105741	149092	141660	159068
TwMCA	9	330	318	1241	161	671	493	1319
Pimelic acid	184	48	407	48	60	142	159	183
C6 0	1149	520	715	546	468	512	831	789
Fructose 1,6_bisphosphate	11364	10145	9892	9819	11944	9072	9392	10959
Phosphoribosyl pyrophosphate	8144	9151	6008	6461	10222	7729	6125	7065
Isocitric acid	475	433	837	535	371	646	551	622
2_Methylhexanoic acid	17	17	20	21	15	20	18	15
C7 0	136	76	147	91	65	96	98	101
Pyruvate	479762	313070	359320	297065	228142	368716	283991	190067
12_DHCA	442	753	385	464	389	669	413	797
wMCA	714	779	694	753	693	779	778	946
Oxoglutaric acid	32324	51739	34385	37992	45264	49833	64029	79830
C8 0	2585	2470	1672	1803	3001	1970	2031	3491
CA	158	194	127	181	164	260	194	392
GCA	116	118	210	444	78	357	297	226
C9 0	774	609	765	656	587	627	627	733
C10 0	5551	5265	2372	4009	7155	3054	3409	8271
C11 1 cis_10	1475	1594	1570	1679	1559	1534	1555	1608

Trehalose	14694	14828	14589	15164	15521	14685	16614	16061
CDCA	646	575	445	593	670	596	578	1281
C11 0	1706	1790	1727	1756	1687	1712	1681	1856
C12 1 cis_11	3733	2570	3269	4165	2955	2150	2240	3621
C12 0	164863	128009	61451	138643	206384	53223	68993	234814
C13 1 cis_12	2298	2252	2373	2417	2344	2340	2253	2374
C14 1 cis_9	15202	9598	12442	17311	12991	6947	7118	12178
C14 1 trans_9	41543	39834	41520	45413	41654	42038	41268	45429
C18 1 cis_9 12_OH	813	577	1403	668	450	671	824	990
C18 1 trans_9 12_OH	881	458	1567	443	350	718	894	1088
LCA	192	259	221	279	148	253	239	237
DCA	1125	1092	1050	1176	985	910	1010	1019
C14 0	81861	73482	65708	77966	82862	54812	60798	86516
C15 1	2431	2488	2546	2606	2464	2475	2481	2804
C15 0	6770	6558	6579	7301	6189	6460	6005	7973
C17 1 cis_10	4524	3985	4582	4921	3596	3405	3339	5323
C18 2 trans_9 12	5382	5619	5941	6700	5493	5059	4807	6203
C20 5 cis_5 8 11 14 17	2343	2268	2248	2363	1912	1587	1876	2615
C22 5 cis_7 10 13 16 19	9825	8988	9731	11540	8592	6737	6738	11691
Succinic acid	7985	10310	5651	3736	6031	4399	17105	17813
Citramalic acid	151	138	457	161	136	451	240	113
C16 0	345846	323464	337616	418633	343082	241927	280221	408764
C17 0	12688	12486	11794	11627	10843	11134	10293	16516
C18 1 cis_9	181180	286985	296064	163944	245662	220588	222452	304445
C19 0	7460	11346	6267	9988	11126	3593	5320	13315
C22 2 cis_13 16	2658	3150	4080	3002	2040	2036	3323	4497
L_Lysine	26767	24922	38553	25270	34479	27356	115213	28861
L_Alanine	802	835	921	697	706	976	956	974
Glycyl_L_leucine	16	4	15	12	23	0	112	0
Alpha_ketoisovaleric acid	2291	2193	2007	2303	2565	1737	2901	2183
Ketoleucine	5918	5994	5212	5298	5430	4613	7512	5345
3_Methyl_2_oxovaleric acid	3886	3739	3392	3844	3972	3530	4502	3891
Glycine	3877	3374	5085	3571	3242	3547	4361	2138
Guanidoacetic acid	90	125	366	172	107	152	132	144
N_Acetylornithine	60565	55943	59865	34235	33705	58340	55537	60814
Citrulline	11996	12948	13015	11611	10788	11234	14253	7988
L_Proline	65087	70248	52660	41647	94691	71895	103335	45692
L_Methionine	21904	19334	16257	18674	23567	24912	41736	11362
L_Alloisoleucine	15141	15338	12024	13158	20337	17900	23173	17850
D_Xylulose	426	358	510	617	177	389	197	686
p_Hydroxyphenylacetic acid	177	173	21	21	392	252	46	21
N_Methylnicotinamide	176	122	167	176	111	211	232	415
Acetoacetic acid	18012	9352	11856	19104	17793	11093	6393	8474
Suberic acid	358	385	1319	643	245	489	1021	832

TUDCA	257	231	174	419	286	409	251	525
THDCA	211	295	210	611	147	235	259	316
TCA	1700	3686	1713	11305	858	3122	4395	2850
Citric acid	28563	27366	40093	21128	20631	29489	28562	31568
TDCA	351	680	360	2890	277	440	559	385
TCDCA	198	182	95	526	126	208	294	296
bMCA	2084	2274	1900	2062	2280	2559	2219	3073
Acetaminophen	282	248	749	303	222	333	218	486
bUDCA	29	38	33	38	38	38	33	39
UDCA	404	408	399	414	423	438	413	537
Oxoadipic acid	1758	992	1837	697	1124	1175	2431	1752
GCDCA	34	59	57	47	58	63	29	51
C13 0	2243	2303	2309	2469	2326	2241	2319	2485
C18 0 12_OH	1680	1626	1811	1625	1617	1641	1809	1748
C16 1 cis_9	82976	61707	66741	90855	60076	28450	35220	83029
C16 1 trans_9	9161	8153	8303	9099	7975	6283	6571	8678
C17 1 trans_10	3765	4141	4659	4492	4159	4320	4080	5067
C18 3 cis_9 12 15	4545	4027	3242	4881	4790	2511	2423	6430
C18 3 cis_6 9 12	988	1009	668	1118	729	388	524	1266
C18 2 cis_9 12	68792	59929	46603	72387	55406	37541	40377	85093
C19 2 cis_10 13	3293	3458	3782	3521	3585	3821	3516	4019
C20 4 cis_5 8 11 14	36485	31051	22065	39456	29068	15953	27408	24891
C20 3 cis_8 11 14	3439	4057	3375	3987	3037	2418	2777	4314
C22 6 cis_4 7 10 13 16 19	33751	33391	26913	41264	28947	20827	24039	30768
C22 5 cis_4 7 10 13 16	10255	8915	8319	11541	8965	7837	8261	9580
C22 4 cis_7 10 13 16	16427	11768	11435	17610	11370	9337	9877	12274
C18 1 trans_11	2982	2732	4525	3579	2423	3106	2957	3293
C18 0	418619	415486	374809	508769	467173	273272	371502	497461
C19 1 cis_10	20037	19984	22170	23549	19501	19486	18718	27203
C19 1 cis_7	2017	2157	2302	2178	2156	2242	2043	2456
C20 2 cis_11 14	6040	5979	4646	6830	4246	3633	3507	5909
C20 1 cis_11	70493	93333	47331	81478	42278	28693	29959	74997
C20 1 cis_5	500	524	426	658	225	311	307	663
C21 2 cis_12 15	1121	1392	1538	1471	1551	1498	1353	1744
C21 1 cis_12	3197	1862	1498	2302	1999	1437	1050	3163
C22 3 cis_13 16 19	1763	1879	1818	2412	1893	1816	1513	2757