

Table S8. Heat map of statistically significant biochemicals profiled in serum. Shaded cells indicate $p \leq 0.05$ (red indicates that the mean values are significantly higher for that comparison; green values significantly lower). Blue-bolded text indicates $0.05 < p < 0.10$.			Fold of Change		
			Welch's Two Sample t-Tests		
PATHWAY SORT	BIOCHEMICAL NAME	SUPER PATHWAY	<u>MR</u> CF	<u>MR + CYS</u> CF	<u>MR</u> MR + CYS
1	glycine	Amino acid	0.82	0.69	1.2
3	dimethylglycine	Amino acid	1.37	0.82	1.66
4	N-acetyl glycine	Amino acid	1.17	1.00	1.17
7	serine	Amino acid	2.70	0.86	3.14
16	threonine	Amino acid	2.52	0.75	3.39
17	N-acetylthreonine	Amino acid	2.84	0.96	2.97
21	betaine	Amino acid	0.71	0.88	0.81
23	alanine	Amino acid	0.69	0.72	0.95
27	N-acetyl-beta-alanine	Amino acid	1.26	1.09	1.16
29	aspartate	Amino acid	2.12	0.67	3.18
33	asparagine	Amino acid	0.82	0.88	0.94
36	3-ureidopropionate	Amino acid	0.86	2.68	0.32
38	glutamate	Amino acid	0.77	0.68	1.13
42	glutamine	Amino acid	1.47	1.18	1.25
43	pyroglutamine*	Amino acid	0.83	0.91	0.91
48	histidine	Amino acid	1.55	0.74	2.1
51	3-methylhistidine	Amino acid	0.61	1.09	0.56
66	lysine	Amino acid	1.16	0.93	1.25
69	pipecolate	Amino acid	0.98	1.16	0.84
77	phenyllactate (PLA)	Amino acid	0.07	0.29	0.24
78	phenylalanine	Amino acid	0.94	0.93	1.01
80	phenylacetate	Amino acid	0.51	0.69	0.75
82	p-cresol sulfate	Amino acid	0.73	5.29	0.14
90	tyrosine	Amino acid	0.41	0.96	0.43
91	3-(4-hydroxyphenyl)lactate	Amino acid	0.37	1.00	0.37
97	4-hydroxyphenylpyruvate	Amino acid	2.15	0.59	3.66
111	N-acetylphenylalanine	Amino acid	0.69	0.69	1.01
112	N-acetyltyrosine	Amino acid	0.40	0.84	0.48
114	phenylacetyl glycine	Amino acid	0.21	0.78	0.27
119	3-phenylpropionate (hydrocinnamate)	Amino acid	1.21	0.67	1.79
121	phenol sulfate	Amino acid	0.21	0.73	0.29
125	kynurenine	Amino acid	0.45	1.06	0.42
126	tryptophan	Amino acid	0.71	1.00	0.7
127	indolelactate	Amino acid	0.25	0.45	0.56
129	indoleacetate	Amino acid	0.52	0.58	0.89
138	serotonin (5HT)	Amino acid	1.59	0.76	2.1
139	N-acetyltryptophan	Amino acid	1.03	0.95	1.08
141	C-glycosyltryptophan*	Amino acid	0.81	1.15	0.7
147	3-indoxyl sulfate	Amino acid	0.17	0.85	0.2
148	indolepropionate	Amino acid	0.54	0.44	1.23
149	3-methyl-2-oxobutyrate	Amino acid	1.25	0.87	1.44
150	3-methyl-2-oxovalerate	Amino acid	0.86	0.86	1
155	beta-hydroxyisovalerate	Amino acid	0.90	0.66	1.36
157	isoleucine	Amino acid	0.95	0.93	1.03
158	leucine	Amino acid	1.05	0.92	1.14
162	N-acetyl leucine	Amino acid	1.72	0.90	1.91
164	N-acetyl isoleucine	Amino acid	1.68	0.78	2.14

167	valine	Amino acid	1.06	0.89	1.19
168	2-hydroxyisobutyrate	Amino acid	1.73	1.16	1.49
170	4-methyl-2-oxopentanoate	Amino acid	1.20	0.90	1.32
175	alpha-hydroxyisovalerate	Amino acid	2.55	0.75	3.38
176	isovalerylglycine	Amino acid	0.64	0.48	1.34
177	isobutyrylcarnitine	Amino acid	0.79	0.78	1.02
179	2-methylbutyroylcarnitine	Amino acid	0.46	0.99	0.46
181	isovalerylcarnitine	Amino acid	0.69	0.74	0.93
188	cysteine	Amino acid	0.77	0.95	0.81
191	cystine	Amino acid	0.80	1.28	0.63
199	methionine	Amino acid	0.26	0.37	0.7
201	N-acetylmethionine	Amino acid	0.39	0.28	1.4
203	2-hydroxybutyrate (AHB)	Amino acid	1.31	0.51	2.56
212	dimethylarginine (SDMA + ADMA)	Amino acid	1.50	1.59	0.95
213	arginine	Amino acid	1.06	0.86	1.24
216	ornithine	Amino acid	2.15	0.87	2.48
217	urea	Amino acid	1.39	1.07	1.29
218	proline	Amino acid	1.13	1.00	1.13
220	citrulline	Amino acid	0.87	0.86	1.01
224	trans-4-hydroxyproline	Amino acid	0.50	1.01	0.5
232	creatine	Amino acid	1.38	1.07	1.29
233	creatinine	Amino acid	0.89	1.04	0.85
235	2-aminobutyrate	Amino acid	1.27	0.61	2.07
246	4-guanidinobutanoate	Amino acid	1.12	0.71	1.58
253	5-oxoproline	Amino acid	8.12	1.10	7.4
254	glutathione, oxidized (GSSG)	Amino acid	0.73	0.67	1.09
255	cysteine-glutathione disulfide	Amino acid	0.67	0.93	0.72
256	ophthalmate	Amino acid	13.38	0.82	16.26
272	alanylalanine	Peptide	0.58	0.88	0.66
298	pro-hydroxy-pro	Peptide	0.88	1.24	0.71
321	gamma-glutamylvaline	Peptide	1.65	0.96	1.72
323	gamma-glutamylleucine	Peptide	1.38	1.03	1.34
324	gamma-glutamylisoleucine*	Peptide	1.25	1.01	1.24
327	gamma-glutamylmethionine	Peptide	0.25	0.47	0.53
329	gamma-glutamylglutamine	Peptide	1.18	1.23	0.96
331	gamma-glutamylphenylalanine	Peptide	0.82	0.92	0.89
332	gamma-glutamyltyrosine	Peptide	0.45	1.17	0.39
333	gamma-glutamylthreonine*	Peptide	4.24	0.81	5.22
336	gamma-glutamylalanine	Peptide	0.90	1.05	0.86
352	ADTGTTSEFXEAGGDXR*	Peptide	0.50	0.89	0.57
359	TDSDKVDXSXAR*	Peptide	0.79	0.94	0.84
360	TTSDKVDXSXAR*	Peptide	0.65	1.11	0.58
361	ATTSDKVDXSXA*	Peptide	0.57	0.83	0.69
362	TTSDKVDXSXA*	Peptide	1.24	0.90	1.38
363	ATTSDKVDXSXAR*	Peptide	0.28	0.82	0.34
365	SDKVDXSXA*	Peptide	0.79	0.93	0.85
372	erythronate*	Carbohydrate	1.33	0.92	1.45
389	fructose	Carbohydrate	1.16	0.89	1.31
402	mannose	Carbohydrate	0.91	1.13	0.8
410	sorbitol	Carbohydrate	1.24	1.03	1.2
414	sucrose	Carbohydrate	0.84	0.81	1.03
430	1,5-anhydroglucitol (1,5-AG)	Carbohydrate	1.88	0.87	2.15
432	glycerate	Carbohydrate	0.65	1.01	0.65
436	glucose	Carbohydrate	0.79	1.00	0.79
450	pyruvate	Carbohydrate	0.24	0.57	0.41

451	lactate	Carbohydrate	0.89	0.68	1.29
468	ribose	Carbohydrate	1.42	0.88	1.61
479	xylitol	Carbohydrate	1.94	0.87	2.23
491	citrate	Energy	1.26	0.82	1.53
500	alpha-ketoglutarate	Energy	0.53	0.44	1.19
501	succinate	Energy	0.90	0.53	1.68
504	fumarate	Energy	0.78	0.58	1.34
507	malate	Energy	0.96	0.44	2.16
510	acetylphosphate	Energy	0.74	0.72	1.04
511	phosphate	Energy	0.70	0.76	0.93
512	pyrophosphate (PPi)	Energy	0.69	0.57	1.2
512.5	linoleate (18:2n6)	Lipid	1.29	1.61	0.8
516	linolenate [alpha or gamma; (18:3n3 or 6)]	Lipid	1.52	1.32	1.15
517	dihomo-linolenate (20:3n3 or n6)	Lipid	0.58	0.93	0.62
519	docosapentaenoate (n3 DPA; 22:5n3)	Lipid	1.68	2.35	0.72
520	docosapentaenoate (n6 DPA; 22:5n6)	Lipid	0.82	0.33	2.46
521	docosahexaenoate (DHA; 22:6n3)	Lipid	1.13	0.68	1.65
525	caproate (6:0)	Lipid	0.87	1.08	0.81
526	heptanoate (7:0)	Lipid	0.77	0.97	0.8
527	caprylate (8:0)	Lipid	0.66	1.16	0.57
528	pelargonate (9:0)	Lipid	0.70	1.03	0.68
529	caprate (10:0)	Lipid	0.64	1.08	0.59
532	laurate (12:0)	Lipid	0.70	0.93	0.75
535	myristate (14:0)	Lipid	1.03	1.06	0.98
536	myristoleate (14:1n5)	Lipid	1.02	1.04	0.98
538	palmitate (16:0)	Lipid	1.19	1.18	1
539	palmitoleate (16:1n7)	Lipid	1.46	1.20	1.22
541	margarate (17:0)	Lipid	0.87	0.91	0.95
542	10-heptadecenoate (17:1n7)	Lipid	0.94	1.10	0.85
543	stearate (18:0)	Lipid	1.10	1.01	1.09
545	oleate (18:1n9)	Lipid	1.17	1.27	0.92
554	10-nonadecenoate (19:1n9)	Lipid	1.05	1.39	0.75
559	eicosenoate (20:1n9 or 11)	Lipid	0.77	1.18	0.65
561	dihomo-linoleate (20:2n6)	Lipid	0.85	1.19	0.72
565	arachidonate (20:4n6)	Lipid	0.97	0.71	1.37
571	adrenate (22:4n6)	Lipid	0.92	0.97	0.95
580	palmitate, methyl ester	Lipid	0.44	1.31	0.34
604	2-hydroxypalmitate	Lipid	1.11	1.28	0.87
610	2-hydroxyglutarate	Lipid	0.94	0.98	0.96
615	sebacate (decanedioate)	Lipid	1.61	1.02	1.57
616	azelate (nonanedioate)	Lipid	1.56	0.97	1.6
617	dodecanedioate	Lipid	1.29	1.08	1.2
618	tetradecanedioate	Lipid	1.63	1.20	1.36
619	hexadecanedioate	Lipid	1.54	0.91	1.7
620	octadecanedioate	Lipid	1.84	0.96	1.92
621	undecanedioate	Lipid	1.53	1.02	1.5
632.65	methyl palmitate (15 or 2)	Lipid	0.98	1.08	0.91
632.7	17-methylstearate	Lipid	0.80	1.28	0.63
672	12-HETE	Lipid	1.54	0.63	2.43
683	propionylcarnitine	Lipid	0.74	0.89	0.83
685	butyrylcarnitine	Lipid	0.24	0.94	0.26
689	isovalerate	Lipid	0.65	1.08	0.61
691	deoxycarnitine	Lipid	1.45	1.10	1.32
692	carnitine	Lipid	0.86	1.20	0.72
693	3-dehydrocarnitine*	Lipid	1.78	0.90	1.98

694	acetylcarnitine	Lipid	1.14	0.98	1.17
696	hexanoylcarnitine	Lipid	1.21	1.18	1.02
709	cholate	Lipid	1.34	1.20	1.12
710	12-dehydrocholate	Lipid	0.76	0.49	1.56
712	glycocholate	Lipid	7.87	2.03	3.87
713	taurocholate	Lipid	0.06	1.83	0.03
718	3-dehydrocholate	Lipid	2.32	1.47	1.58
719	deoxycholate	Lipid	1.46	0.68	2.16
720	taurodeoxycholate	Lipid	0.13	0.91	0.15
721	glycodeoxycholate	Lipid	9.28	1.41	6.59
734	6-beta-hydroxylithocholate	Lipid	2.47	0.59	4.19
736	beta-muricholate	Lipid	0.87	0.49	1.77
740	alpha-muricholate	Lipid	1.04	0.55	1.88
750	glycerol	Lipid	1.03	1.14	0.91
751	choline	Lipid	0.97	0.81	1.19
752	glycerol 3-phosphate (G3P)	Lipid	0.27	0.87	0.31
753	glycerophosphorylcholine (GPC)	Lipid	0.81	1.06	0.76
760	myo-inositol	Lipid	0.83	0.77	1.07
763	inositol 1-phosphate (I1P)	Lipid	0.48	0.72	0.67
769	3-hydroxybutyrate (BHBA)	Lipid	2.44	1.12	2.17
771	1,2-propanediol	Lipid	1.27	0.89	1.43
775	1-palmitoylglycerophosphoethanolamine	Lipid	0.86	1.69	0.51
780	1-stearoylglycerophosphoethanolamine	Lipid	0.99	1.47	0.68
781	1-oleoylglycerophosphoethanolamine	Lipid	0.47	0.99	0.48
782	2-oleoylglycerophosphoethanolamine*	Lipid	0.54	1.08	0.5
783	1-linoleoylglycerophosphoethanolamine*	Lipid	0.56	1.19	0.47
784	2-linoleoylglycerophosphoethanolamine*	Lipid	0.59	1.34	0.44
785	1-arachidonoylglycerophosphoethanolamine*	Lipid	0.91	1.43	0.64
786	2-arachidonoylglycerophosphoethanolamine*	Lipid	1.07	1.70	0.63
791	1-myristoylglycerophosphocholine	Lipid	1.04	1.73	0.6
793	1-pentadecanoylglycerophosphocholine*	Lipid	1.00	1.31	0.77
794	1-palmitoylglycerophosphocholine	Lipid	1.02	1.08	0.94
795	2-palmitoylglycerophosphocholine*	Lipid	1.25	1.29	0.96
796	1-palmitoleoylglycerophosphocholine*	Lipid	0.57	1.51	0.38
798	1-heptadecanoylglycerophosphocholine	Lipid	0.86	0.96	0.89
799	1-stearoylglycerophosphocholine	Lipid	0.77	0.49	1.58
800	2-stearoylglycerophosphocholine*	Lipid	1.11	0.65	1.71
801	1-oleoylglycerophosphocholine	Lipid	0.83	1.07	0.78
802	2-oleoylglycerophosphocholine*	Lipid	1.14	1.93	0.59
803	1-linoleoylglycerophosphocholine	Lipid	1.02	1.24	0.82
804	2-linoleoylglycerophosphocholine*	Lipid	1.12	1.32	0.85
805	1-arachidoylglycerophosphocholine	Lipid	1.62	0.85	1.89
806	1-eicosadienoylglycerophosphocholine*	Lipid	1.08	1.22	0.88
807	1-eicosatrienoylglycerophosphocholine*	Lipid	0.54	1.90	0.28
809	1-arachidonoylglycerophosphocholine*	Lipid	0.84	0.89	0.95
810	2-arachidonoylglycerophosphocholine*	Lipid	0.80	1.18	0.67
811	1-docosapentaenoylglycerophosphocholine*	Lipid	0.64	0.24	2.65
813	1-docosaheptaenoylglycerophosphocholine*	Lipid	0.72	0.68	1.06
816	1-palmitoylglycerophosphoinositol*	Lipid	0.63	1.01	0.62
818	1-stearoylglycerophosphoinositol	Lipid	0.43	0.85	0.51
821	1-arachidonoylglycerophosphoinositol*	Lipid	0.43	0.75	0.58
825.5	1-palmitoylplasmaenylethanolamine*	Lipid	1.03	0.84	1.23
831	1-palmitoylglycerol (1-monopalmitin)	Lipid	0.44	1.37	0.32
833	1-stearoylglycerol (1-monostearin)	Lipid	0.65	0.69	0.94
864	palmitoyl sphingomyelin	Lipid	0.78	0.71	1.1

865	stearoyl sphingomyelin	Lipid	0.86	0.51	1.67
881	cholesterol	Lipid	0.71	0.70	1.01
913	corticosterone	Lipid	1.40	0.51	2.75
916	beta-sitosterol	Lipid	0.56	0.83	0.67
918	campesterol	Lipid	0.69	1.00	0.69
919	fucosterol	Lipid	0.85	1.03	0.83
934	7-alpha-hydroxy-3-oxo-4-cholestenoate (7-Hoca)	Lipid	5.89	1.04	5.64
951	inosine	Nucleotide	3.37	1.00	3.37
958	N1-methyladenosine	Nucleotide	0.95	1.14	0.83
994	urate	Nucleotide	1.31	0.85	1.55
995	allantoin	Nucleotide	1.15	0.94	1.22
997	cytidine	Nucleotide	1.06	1.08	0.98
999	5-methylcytidine	Nucleotide	1.17	1.00	1.18
1000	N4-acetylcytidine	Nucleotide	2.57	1.48	1.74
1006	2'-deoxycytidine	Nucleotide	0.72	1.07	0.68
1011.5	5-methyl-2'-deoxycytidine	Nucleotide	1.07	1.27	0.84
1017	thymidine	Nucleotide	1.16	0.84	1.38
1022	uracil	Nucleotide	1.14	1.12	1.02
1023	5,6-dihydrouracil	Nucleotide	1.06	0.86	1.24
1024	uridine	Nucleotide	1.07	0.87	1.23
1025	pseudouridine	Nucleotide	1.19	1.01	1.19
1039	gulono-1,4-lactone	Cofactors and vitamins	1.74	1.61	1.08
1042	threonate	Cofactors and vitamins	0.42	1.07	0.4
1055	heme*	Cofactors and vitamins	0.87	2.30	0.38
1063	nicotinamide	Cofactors and vitamins	3.32	1.12	2.96
1085	pantothenate	Cofactors and vitamins	1.11	0.99	1.12
1105	alpha-tocopherol	Cofactors and vitamins	0.42	0.64	0.66
1123	hippurate	Xenobiotics	1.10	0.82	1.35
1135	benzoate	Xenobiotics	0.63	0.84	0.76
1151	glycolate (hydroxyacetate)	Xenobiotics	0.83	0.81	1.03
1157	glycerol 2-phosphate	Xenobiotics	0.36	0.79	0.46
1191	2-ethylhexanoate	Xenobiotics	0.33	0.89	0.37
1272	tartarate	Xenobiotics	0.59	0.78	0.75
1275	indoleacrylate	Xenobiotics	1.18	0.77	1.53
1360	erythritol	Xenobiotics	0.89	0.87	1.02
	X - 01497	N/A	0.60	0.95	0.64
	X - 02029	N/A	0.05	0.60	0.08
	X - 02973	N/A	0.92	0.98	0.94
	X - 03002	N/A	0.78	1.09	0.72
	X - 03003	N/A	1.25	1.05	1.19
	X - 03088	N/A	0.45	0.75	0.6
	X - 03094	N/A	0.66	0.66	1
	X - 03249	N/A	0.21	0.35	0.58
	X - 04357	N/A	0.95	0.48	2
	X - 04495	N/A	2.17	0.62	3.51
	X - 04498	N/A	1.24	0.72	1.73
	X - 04499	N/A	1.12	0.47	2.4
	X - 04807	N/A	1.49	0.81	1.85
	X - 04874	N/A	0.34	0.79	0.43
	X - 04987	N/A	0.67	0.69	0.97
	X - 06267	N/A	0.75	0.71	1.06
	X - 06306	N/A	0.24	0.22	1.12
	X - 09069	N/A	0.63	0.98	0.65
	X - 09706	N/A	0.87	1.18	0.74
	X - 10500	N/A	0.85	0.96	0.88

	X - 10503	N/A	0.64	1.04	0.61
	X - 10505	N/A	0.74	1.31	0.56
	X - 10634	N/A	0.17	0.18	0.93
	X - 10964	N/A	3.57	0.93	3.86
	X - 11175	N/A	1.51	1.47	1.03
	X - 11204	N/A	1.14	0.98	1.16
	X - 11315	N/A	0.88	0.79	1.11
	X - 11327	N/A	1.22	1.20	1.01
	X - 11333	N/A	1.09	1.49	0.73
	X - 11334	N/A	1.15	0.70	1.64
	X - 11412	N/A	0.47	0.92	0.51
	X - 11533	N/A	0.78	0.90	0.87
	X - 11538	N/A	1.07	0.80	1.33
	X - 11542	N/A	1.02	1.00	1.02
	X - 11550	N/A	0.50	0.93	0.54
	X - 11593	N/A	0.39	0.54	0.73
	X - 11662	N/A	0.32	1.05	0.31
	X - 11687	N/A	0.80	0.86	0.93
	X - 11861	N/A	0.79	0.89	0.9
	X - 12051	N/A	0.85	1.33	0.64
	X - 12100	N/A	0.62	1.01	0.62
	X - 12110	N/A	0.85	1.23	0.69
	X - 12156	N/A	0.51	0.67	0.77
	X - 12205	N/A	0.93	0.85	1.09
	X - 12206	N/A	0.55	1.34	0.41
	X - 12216	N/A	0.61	0.76	0.8
	X - 12435	N/A	1.02	1.19	0.86
	X - 12439	N/A	0.43	0.77	0.56
	X - 12442	N/A	1.58	1.18	1.33
	X - 12478	N/A	2.37	0.44	5.38
	X - 12556	N/A	3.38	0.76	4.48
	X - 12627	N/A	0.82	0.58	1.42
	X - 12771	N/A	2.66	0.76	3.48
	X - 12776	N/A	1.32	1.05	1.26
	X - 12786	N/A	0.76	0.53	1.43
	X - 12801	N/A	1.47	1.28	1.15
	X - 13429	N/A	3.84	1.00	3.84
	X - 13452	N/A	1.61	0.92	1.74
	X - 13496	N/A	0.86	1.08	0.79
	X - 13505	N/A	1.65	1.00	1.65
	X - 13708	N/A	0.89	0.93	0.96
	X - 14567	N/A	0.42	0.77	0.54
	X - 14603	N/A	0.87	0.84	1.04
	X - 15011	N/A	0.47	0.71	0.66
	X - 15483	N/A	1.49	1.06	1.41
	X - 15624	N/A	0.86	1.04	0.83
	X - 15646	N/A	0.87	0.63	1.39
	X - 15649	N/A	2.22	0.80	2.78
	X - 15667	N/A	0.63	1.14	0.55
	X - 16206	N/A	0.99	1.03	0.96
	X - 16234	N/A	1.31	0.77	1.69
	X - 16243	N/A	1.08	0.54	1.99
	X - 16245	N/A	0.34	0.74	0.46
	X - 16480	N/A	0.81	0.72	1.12
	X - 16557	N/A	1.03	0.90	1.15

	X - 16578	N/A	0.51	0.81	0.62
	X - 16595	N/A	0.75	1.10	0.68
	X - 16803	N/A	12.84	0.72	17.78
	X - 16819	N/A	1.83	0.35	5.24
	X - 16831	N/A	1.51	0.78	1.93
	X - 17010	N/A	0.97	0.91	1.07
	X - 17024	N/A	1.96	0.30	6.5
	X - 17160	N/A	0.83	0.94	0.88
	X - 17254	N/A	2.13	2.32	0.92
	X - 17269	N/A	0.63	0.90	0.7