

Table S2. Fold Changes of Metabolites in Refined Profile

Fold Change: Cases of WTC-LI/Control	
	<1
	>1

Super Pathway	Sub Pathway	Metabolite	Comp ID	KEGG	HMDB	PubChem	WTC-LI Control	CAS	Retention Index	Mass	
Amino Acid	Alanine and Aspartate Metabolism	N-acetylaspargine	33942		HMDB06028	99715		4033-40-3	785	175.07	
	Glutamate Metabolism	N-acetylglutamine	33943	C02716	HMDB06029	182230		2490-97-3	2140	187.07	
	Glycine, Serine and Threonine Metabolism	Dimethylglycine	5086	C01026	HMDB00092	673		1118-68-9	1104	104.07	
	Leucine, Isoleucine and Valine Metabolism		Methylsuccinate	15745		HMDB01844	10349		498-21-5	2800	131.03
			Isobutyrylcarnitine	33441		HMDB00736	168379		25518-49-4	2810	232.15
	Lysine Metabolism		N2-acetyllysine	36751	C12989	HMDB00446	92907		1946-82-3	3372.6	187.11
	Methionine, Cysteine, SAM and Taurine Metabolism		Lanthionine	42002			0		8/2/83	1730	209.06
	Phenylalanine and Tyrosine Metabolism		Vanillylmandelate (VMA)	1567	C05584	HMDB00291	1245		55-10-7	941	197.05
Tryptophan Metabolism		Serotonin	2342	C00780	HMDB00259	5202		153-98-0	2550	177.1	
Urea cycle; Arginine and Proline Metabolism		Proline	1898	C00148	HMDB00162	145742		147-85-3	1603	116.07	
Carbohydrate	Pentose Metabolism	Arabonate/xylonate	48255						2664.6	165.04	
Cofactors and Vitamins	Ascorbate and Aldarate Metabolism	Gulonate	46957		HMDB03290	9794176		20246-53-1	2750	195.05	
		Threonate	27738	C01620	HMDB00943	151152		70753-61-6	2384	135.03	
Lipid	Fatty Acid Metabolism (also BCAA Metabolism)	Propionylcarnitine	32452	C03017	HMDB00824	107738		17298-37-2	2590	218.14	
	Fatty Acid, Dicarboxylate	Azelate (nonanedioate)	18362	C08261	HMDB00784	2266		123-99-9	1276	187.1	
	Fatty Acid, Monohydroxy		2-hydroxypalmitate	35675		HMDB31057	92836		764-67-0	5511.2	271.23
			2-hydroxystearate	17945	C03045		69417		629-22-1	5695	299.26
	Lysolipid		1-arachidonoyl-GPE (20:4n6)	35186		HMDB11517	42607465			1450	502.29
	Phospholipid Metabolism		1-palmitoyl-2-arachidonoyl-GPC (16:0/20:4n6)	52462			10747814		35418-58-7	2091	782.57
			1-stearoyl-2-arachidonoyl-GPC (18:0/20:4)	42450			16219824		35418-59-8	2300	810.6
			Docosahexaenoylcholine	53263						1378	414.34
	Polyunsaturated Fatty Acid (n3 and n6)		Arachidonate (20:4n6)	1110	C00219	HMDB01043	444899		506-32-1	5535	303.23
	Sphingolipid Metabolism		Sphingosine	17747	C00319	HMDB00252	5353955		123-78-4	1393	300.29
Sphinganine			17769	C00836	HMDB00269	3126		3102-56-5	1413	302.31	
Lignoceroyl sphingomyelin (d18:1/24:0)			57330						60037-60-7	3437	815.7
Sphingosine 1-phosphate			34445	C06124	HMDB00277	5283560			26993-30-6	1850	378.24
Nucleotide	Pyrimidine Metabolism, Uracil containing	Uridine	606	C00299	HMDB00296	6029		58-96-8	1457.6	243.06	
Peptide	Dipeptide	Prolylglycine	40703			0		2578-57-6	2136	173.09	
Xenobiotics	Benzoate Metabolism	4-methylcatechol sulfate	46146						2665	203	