

**Supplementary Table 1.** Altered metabolism in plasma and tumor associated with withaferin A (WA)

treatment in mouse mammary tumor virus-*neu* (MMTV-*neu*) mice

Pathway	Plasma (Scaled intensity) (Mean ± 95% CI)			Tumor (Scaled intensity) (Mean ± 95% CI)		
	Control*	WA*	<i>P</i> †	Control*	WA*	<i>P</i> †
<b><i>Carbohydrate_Aminosugars metabolism</i></b>						
<i>N</i> -Acetylglucosamine				.96 ± .21	1.07 ± .31	.51
<i>N</i> -Acetylglucosamine 6-phosphate				1.00 ± .16	.83 ± .27	.24
<i>N</i> -Acetylneuraminate				1.04 ± .22	.88 ± .41	.42
Erythronate	.84 ± .15	.99 ± .18	.14	1.30 ± .56	.89 ± .23	.13
Fucose	1.03 ± .25	.96 ± .19	.60	.93 ± .18	1.01 ± .23	.52
<b><i>Carbohydrate_Fructose, mannose, galactose, starch, and sucrose metabolism</i></b>						
Fructose	1.13 ± .37	.91 ± .24	.26	1.14 ± .47	.90 ± .32	.34
Galactose				.93 ± .32	1.07 ± .46	.56
Lactose				1.32 ± .81	1.17 ± 1.03	.78
Maltose				1.37 ± .94	.91 ± .72	.38
Mannitol				1.13 ± .37	1.00 ± .35	.54
Mannose	1.08 ± .31	1.06 ± .27	.91	.91 ± .22	1.03 ± .26	.42
Mannose-6-phosphate				1.08 ± .18	.90 ± .22	.16
3-Sialyllactose				1.04 ± .55	.97 ± .62	.85
Sorbitol	1.55 ± .50	.79 ± .21	.01	1.21 ± .25	.92 ± .52	.24
Sucrose	2.58 ± 1.56	.89 ± .44	.03			
<b><i>Carbohydrate_Glycolysis, gluconeogenesis, pyruvate metabolism</i></b>						
1,5-Anhydroglucitol (1,5-AG)	1.12 ± .12	.91 ± .08	.01	1.16 ± .26	.88 ± .29	.11
1,3-Dihydroxyacetone	1.59 ± .57	.95 ± .14	.02	.95 ± .35	1.02 ± .21	.69
3-Phosphoglycerate	1.43 ± .87	1.12 ± .60	.50	1.31 ± .28	.89 ± .24	.02
Glucose	1.09 ± .13	.91 ± .10	.02	1.12 ± .60	.90 ± .34	.47
Glycerate	1.14 ± .28	.99 ± .10	.24	.91 ± .19	1.15 ± .25	.09
Lactate	1.17 ± .19	.86 ± .21	.02	1.42 ± .30	.84 ± .18	.002
Phosphoenolpyruvate (PEP)	1.19 ± .75	.80 ± .39	.30	1.39 ± .28	.87 ± .22	.004
Pyruvate	1.19 ± .35	1.03 ± .23	.39			
Fructose-6-phosphate				1.04 ± .17	.96 ± .25	.53

Glucose-6-phosphate (G6P)				1.09 ± .18	.90 ± .21	.12
Glucuronate				.90 ± .26	1.26 ± .42	.11
Isobar: fructose 1,6-diphosphate, glucose 1,6-diphosphate, myo-inositol 1,4 or 1,3-diphosphate				1.32 ± .50	.59 ± .37	.01
<b><i>Carbohydrate_Nucleotide sugars, pentose metabolism</i></b>						
Arabinose	.82 ± .60	.53 ± .37	.35			
Arabitol	.99 ± .18	1.20 ± .56	.40	.91 ± .19	1.06 ± .29	.34
Isobar: ribulose 5-phosphate, xylulose 5-phosphate	1.30 ± .91	.70 ± .40	.17	1.13 ± .15	.81 ± .21	.01
6-Phosphogluconate				.96 ± .43	.91 ± .30	.83
Ribitol	1.31 ± .29	.86 ± .12	.004			
Ribose	1.23 ± .27	.92 ± .17	.04	.83 ± .25	.91 ± .24	.59
Ribulose	1.17 ± .33	.88 ± .13	.08	.90 ± .23	.93 ± .25	.85
Sedoheptulose-7-phosphate				.99 ± .19	1.02 ± .30	.82
Threitol	1.01 ± .31	.97 ± .26	.84			
Xylitol	1.58 ± .58	.87 ± .13	.01	1.22 ± .32	.91 ± .27	.10
Xylonate	1.04 ± .23	.95 ± .24	.56	.96 ± .19	1.19 ± .40	.25
Xylulose				.78 ± .26	.99 ± .27	.20
<b><i>Energy_Krebs cycle</i></b>						
cis-Aconitate	1.07 ± .19	1.06 ± .25	.99			
Citrate	1.19 ± .32	.87 ± .11	.0496	1.14 ± .28	.82 ± .44	.16
Fumarate	1.22 ± .27	.95 ± .32	.15	1.12 ± .11	.81 ± .23	.01
alpha-Ketoglutarate	.95 ± .47	1.29 ± .61	.31			
Malate	1.28 ± .39	.95 ± .38	.18	1.32 ± .69	.76 ± .24	.09
Succinate	1.35 ± .62	.74 ± .33	.06	1.14 ± .21	1.09 ± .24	.74
Succinylcarnitine	1.18 ± .23	.96 ± .17	.09	1.08 ± .25	.97 ± .23	.48
<b><i>Energy_Oxidative phosphorylation</i></b>						
Phosphate	1.12 ± .22	.99 ± .16	.29	.98 ± .08	.96 ± .13	.81
<b><i>Lipid_Bile acid metabolism</i></b>						
Cholate	1.89 ± 2.59	1.65 ± 2.59	.88			
Deoxycholate	1.19 ± .51	1.08 ± .50	.73			
Taurochenodeoxycholate	.93 ± .27	6.47 ± 12.69	.32			
Taurocholate	.98 ± .29	4.15 ± 7.46	.33	1.21 ± .45	1.46 ± 1.23	.65
Taurodeoxycholate	.98 ± .35	2.15 ± 2.63	.31			
Tauro-beta-muricholate				.78 ± .35	1.55 ± 1.59	.28

Tauroursodeoxycholate	.84 ± .19	12.53 ± 26.72	.32			
<b><i>Lipid_Carnitine metabolism</i></b>						
Acetylcarnitine	.95 ± .12	.98 ± .11	.68	1.13 ± .24	.94 ± .20	.17
Carnitine	1.09 ± .14	.96 ± .16	.17	1.02 ± .20	1.02 ± .22	.97
3-Dehydrocarnitine	1.01 ± .10	1.05 ± .15	.62	.99 ± .25	1.05 ± .33	.72
Deoxycarnitine	1.13 ± .20	.95 ± .30	.25	1.10 ± .16	.89 ± .23	.09
Hexanoylcarnitine	1.79 ± 1.36	1.31 ± .91	.50			
Octanoylcarnitine	1.23 ± .66	1.09 ± .30	.66			
Oleoylcarnitine				1.37 ± .60	.95 ± .50	.22
Palmitoylcarnitine	.87 ± .37	1.38 ± .68	.15	1.56 ± .55	.82 ± .50	.03
Stearoylcarnitine	.86 ± .35	1.06 ± .32	.32	1.43 ± .60	.60 ± .44	.02
<b><i>Lipid_Diacylglycerol</i></b>						
1,2-Dipalmitoylglycerol	1.18 ± .33	1.00 ± .36	.39	1.10 ± .35	1.07 ± .28	.90
1,3-Dipalmitoylglycerol	1.35 ± .41	.88 ± .32	.0491	1.06 ± .26	1.09 ± .31	.89
<b><i>Lipid_Endocannabinoid</i></b>						
Palmitoyl ethanolamide	.87 ± .25	1.13 ± .28	.13	1.32 ± .53	1.14 ± .40	.55
<b><i>Lipid_Eicosanoid</i></b>						
12-HETE	1.68 ± .79	.76 ± .44	.03	1.54 ± .66	.83 ± .32	.04
6-Keto prostaglandin F1alpha				1.41 ± .87	1.03 ± .37	.36
<b><i>Lipid_Essential fatty acid</i></b>						
Dihomo-linolenate (20:3n3 or n6)	1.10 ± .28	1.05 ± .13	.68	1.55 ± .64	.80 ± .58	.06
Docosahexaenoate (DHA; 22:6n3)	1.01 ± .14	1.04 ± .13	.68	1.29 ± .49	.93 ± .63	.31
Docosapentaenoate (n3 DPA; 22:5n3)	1.03 ± .22	1.06 ± .16	.74	1.46 ± .65	.93 ± .73	.22
Docosapentaenoate (n6 DPA; 22:5n6)	1.01 ± .11	.90 ± .18	.25	1.32 ± .63	.94 ± .63	.33
Linoleate (18:2n6)	.90 ± .16	1.21 ± .19	.01	1.06 ± .51	1.15 ± .54	.77
Linolenate [alpha or gamma; (18:3n3 or 6)]	.94 ± .26	1.16 ± .23	.15	1.12 ± .62	1.19 ± .54	.83
<b><i>Lipid_Fatty acid, branched</i></b>						
Isopalmitic acid				.73 ± .42	1.08 ± .37	.16
13-Methylmyristic acid	.99 ± .15	1.02 ± .06	.69			
15-Methylpalmitate (isobar with 2-methylpalmitate)	1.01 ± .07	1.07 ± .11	.26			
17-Methylstearate	.92 ± .20	1.17 ± .26	.09	1.10 ± .48	1.01 ± .65	.81
<b><i>Lipid_Fatty acid, dicarboxylate</i></b>						
Azelate (nonanedioate)	5.49 ± 4.50	.75 ± .17	.03			

Docosadioate	1.28 ± .70	1.00 ± .43	.44			
Eicosanodioate	.93 ± .28	1.01 ± .21	.64			
Hexadecanedioate	1.10 ± .46	1.12 ± .38	.92			
2-Hydroxyglutarate	1.10 ± .32	1.02 ± .20	.64			
Sebacate (decanedioate)	1.91 ± 1.06	.90 ± .21	.04			
Suberate (octanedioate)	1.77 ± 1.10	.75 ± .38	.06			
Tetradecanedioate	1.13 ± .29	.97 ± .21	.29			
Undecanedioate	1.22 ± .27	.91 ± .13	.03			
<b><i>Lipid_Fatty acid, monohydroxy</i></b>						
13-HODE + 9-HODE	1.29 ± .62	.96 ± .29	.26	.87 ± .53	1.40 ± .72	.19
2-Hydroxyoctanoate	.93 ± .28	.90 ± .39	.89			
2-Hydroxypalmitate	.92 ± .14	1.05 ± .14	.14	.96 ± .33	1.07 ± .33	.58
2-Hydroxystearate	.98 ± .33	1.26 ± .33	.19			
3-Hydroxyoctanoate	1.02 ± .18	1.15 ± .29	.38			
3-Hydroxydecanoate				1.74 ± 2.07	2.49 ± 2.92	.63
4-Hydroxybutyrate (GHB)	1.22 ± .71	1.14 ± .42	.83	1.10 ± .32	.91 ± .20	.23
<b><i>Lipid_Fatty acid metabolism (also BCAA metabolism)</i></b>						
Butyrylcarnitine	1.38 ± .65	1.11 ± .49	.45	.97 ± .32	.92 ± .27	.74
Butyrylglycine	1.12 ± .60	1.07 ± .47	.87			
Propionylcarnitine	1.29 ± .49	.90 ± .19	.10	1.12 ± .22	.78 ± .18	.01
<b><i>Lipid_Fatty acid metabolism</i></b>						
Hexanoylglycine	.88 ± .39	1.06 ± .26	.40			
Isovalerate	1.11 ± .39	1.03 ± .26	.68			
Valerylcarnitine	1.84 ± 1.06	.89 ± .35	.06			
Valerylglycine	1.24 ± .78	.90 ± .26	.34			
<b><i>Lipid_Glycerolipid metabolism</i></b>						
Choline	1.08 ± .17	1.02 ± .09	.51	.94 ± .12	1.11 ± .09	.02
Choline phosphate				1.17 ± .61	1.16 ± .39	.98
Ethanolamine				.74 ± .26	1.21 ± .35	.02
Glycerol	.95 ± .11	1.06 ± .23	.33	1.02 ± .22	1.27 ± .28	.12
Glycerol 3-phosphate (G3P)	1.21 ± .29	.83 ± .15	.02	.95 ± .34	1.12 ± .33	.42
Glycerophosphoethanolamine				1.07 ± .64	1.08 ± .45	.97
Glycerophosphorylcholine (GPC)	1.02 ± .30	.99 ± .24	.86	.86 ± .25	1.01 ± .15	.23

Phosphoethanolamine				1.00 ± .08	1.01 ± .20	.86
<b><i>Lipid_Inositol metabolism</i></b>						
Chiro-inositol				1.29 ± .97	.65 ± .21	.15
Inositol 1-phosphate (IIP)	.87 ± .16	1.12 ± .19	.03	.96 ± .14	1.19 ± .29	.12
Myo-inositol	1.17 ± .34	.74 ± .22	.02	1.33 ± .51	.91 ± .23	.10
Scyllo-inositol				1.34 ± .74	1.16 ± .54	.65
<b><i>Lipid_Ketone bodies</i></b>						
3-Hydroxybutyrate (BHBA)	.84 ± .58	1.18 ± .58	.35	1.13 ± .68	1.10 ± .39	.94
<b><i>Lipid_Long chain fatty acid</i></b>						
Adrenate (22:4n6)	1.09 ± .28	1.03 ± .15	.70	1.24 ± .41	.87 ± .53	.23
Arachidonate (20:4n6)	1.07 ± .13	.95 ± .14	.18	1.04 ± .26	.75 ± .33	.13
Dihomo-linoleate (20:2n6)	.92 ± .23	1.13 ± .19	.11	1.36 ± .43	.88 ± .69	.18
Docosadienoate (22:2n6)	.96 ± .10	1.10 ± .21	.18	1.55 ± .67	.92 ± .83	.19
Docosatrienoate (22:3n3)				1.71 ± .71	.82 ± .67	.0488
Eicosenoate (20:1n9 or 11)	.86 ± .18	1.32 ± .30	.01	1.16 ± .34	.83 ± .44	.18
10-Heptadecenoate (17:1n7)	.94 ± .29	1.25 ± .26	.09	1.13 ± .53	1.07 ± .54	.85
Margarate (17:0)	.92 ± .16	1.05 ± .13	.16	1.16 ± .41	1.07 ± .49	.74
Mead acid (20:3n9)	1.02 ± .18	1.02 ± .33	.98			
Myristate (14:0)	.88 ± .19	1.24 ± .20	.01	1.24 ± .47	1.27 ± .57	.92
Myristoleate (14:1n5)	.75 ± .28	1.17 ± .25	.02	.96 ± .42	1.14 ± .48	.50
Nonadecanoate (19:0)	.96 ± .16	1.10 ± .17	.16	1.04 ± .38	1.07 ± .50	.92
10-Nonadecenoate (19:1n9)	.90 ± .29	1.35 ± .36	.04	1.23 ± .53	1.20 ± .72	.95
Oleate (18:1n9)	.81 ± .34	1.27 ± .28	.03	.97 ± .44	1.38 ± .57	.20
Palmitate (16:0)	.88 ± .13	1.04 ± .08	.03	1.04 ± .33	1.10 ± .41	.80
Palmitoleate (16:1n7)	.75 ± .29	1.24 ± .27	.01	1.18 ± .63	1.23 ± .62	.90
Pentadecanoate (15:0)	.99 ± .14	1.02 ± .14	.76			
Stearate (18:0)	.89 ± .11	1.07 ± .09	.01	1.03 ± .18	1.02 ± .31	.96
Stearidonate (18:4n3)	.96 ± .35	1.22 ± .44	.30			
<i>cis</i> -Vaccenate (18:1n7)	1.00 ± .12	1.17 ± .37	.34	1.03 ± .28	1.03 ± .34	1.00
<b><i>Lipid_Medium chain fatty acid</i></b>						
Caprate (10:0)	.73 ± .25	1.56 ± .54	.01	.98 ± .09	.98 ± .24	.99
Caproate (6:0)	.83 ± .16	1.20 ± .23	.01	.71 ± .32	1.19 ± .54	.09
Caprylate (8:0)	.71 ± .23	1.57 ± .58	.01	.94 ± .22	1.05 ± .34	.54

5-Dodecenoate (12:1n7)	.76 ± .24	1.35 ± .29	.003			
Heptanoate (7:0)	.77 ± .12	1.49 ± .51	.01	1.90 ± 2.16	1.80 ± 1.59	.93
Laurate (12:0)	.74 ± .19	1.17 ± .18	.002	1.04 ± .11	1.00 ± .24	.75
Pelargonate (9:0)	.69 ± .23	1.59 ± .60	.01	.96 ± .12	.98 ± .26	.93
Undecanoate (11:0)	.73 ± .21	1.34 ± .35	.003	1.00 ± .23	1.05 ± .22	.74
10-Undecenoate (11:1n1)	.78 ± .33	1.05 ± .47	.29			
<b><i>Lipid_Short chain fatty acid</i></b>						
Valerate	.86 ± .29	.94 ± .37	.72			
<b><i>Lipid_Lysolipid</i></b>						
1-Arachidonoylglycerophosphocholine	1.11 ± .26	1.07 ± .35	.85	.98 ± .48	.74 ± .43	.40
2-Arachidonoylglycerophosphocholine	1.38 ± .93	1.44 ± .99	.91	1.17 ± .58	.72 ± .43	.17
1-Arachidonoylglycerophosphoethanolamine	1.01 ± .31	1.03 ± .19	.86	1.09 ± .35	1.19 ± .42	.66
2-Arachidonoylglycerophosphoethanolamine	1.23 ± .49	1.16 ± .30	.77	1.15 ± .41	1.07 ± .43	.75
1-Arachidonoylglycerophosphoinositol	1.06 ± .28	1.07 ± .20	.93	1.18 ± .33	.94 ± .57	.41
1-Arachidoylglycerophosphocholine	1.30 ± 1.12	1.02 ± .37	.57			
1-Docosahexaenoylglycerophosphocholine	1.08 ± .42	1.17 ± .62	.78	1.44 ± .77	.67 ± .33	.0462
2-Docosahexaenoylglycerophosphocholine	1.63 ± 1.37	1.73 ± 1.42	.90	1.56 ± .87	.87 ± .80	.19
2-Docosahexaenoylglycerophosphoethanolamine	1.34 ± .93	1.47 ± 1.08	.84	1.10 ± .40	.88 ± .53	.45
1-Docosapentaenoylglycerophosphocholine	1.42 ± 1.10	1.16 ± .62	.62			
2-Docosapentaenoylglycerophosphoethanolamine				1.15 ± .51	.84 ± .52	.34
1-Eicosadienoylglycerophosphocholine	1.47 ± 1.37	1.15 ± .59	.62	1.52 ± .87	.78 ± .52	.11
1-Eicosatrienoylglycerophosphocholine	1.35 ± .94	1.37 ± .83	.97	1.82 ± 1.31	.77 ± .37	.09
2-Eicosatrienoylglycerophosphocholine				1.65 ± .98	.66 ± .27	.04
1-Heptadecanoylglycerophosphocholine	1.45 ± 1.21	1.21 ± .82	.70	1.13 ± .55	.81 ± .28	.25
1-Linoleoylglycerophosphocholine	1.01 ± .25	1.00 ± .28	1.00	1.19 ± .52	.72 ± .48	.14
2-Linoleoylglycerophosphocholine	1.04 ± .42	1.04 ± .32	.98	1.16 ± .52	.73 ± .55	.20
1-Linoleoylglycerophosphoethanolamine	1.03 ± .30	1.01 ± .34	.93	.93 ± .38	1.05 ± .60	.71
2-Linoleoylglycerophosphoethanolamine	1.05 ± .40	1.01 ± .35	.86	1.11 ± .62	1.26 ± .61	.70
1-Myristoylglycerophosphocholine	2.41 ± 2.17	1.25 ± .61	.25	1.57 ± 1.15	.91 ± .55	.24
2-Myristoylglycerophosphocholine	1.69 ± 1.40	1.15 ± .51	.41	1.14 ± .33	.66 ± .29	.02
1-Oleoylglycerophosphocholine	1.65 ± 1.75	1.75 ± 1.64	.92	1.55 ± 1.20	1.05 ± .67	.41
2-Oleoylglycerophosphocholine	1.66 ± 1.48	1.73 ± 1.25	.93	1.49 ± .95	.88 ± .50	.20
1-Oleoylglycerophosphoethanolamine	1.01 ± .23	1.00 ± .27	.94	1.10 ± .45	1.00 ± .44	.73
2-Oleoylglycerophosphoethanolamine	.97 ± .22	.92 ± .27	.70	1.22 ± .50	1.04 ± .41	.52
1-Oleoylglycerophosphoinositol				.83 ± .28	.74 ± .35	.64

1-Oleoylglycerophosphoserine				1.27 ± .67	1.24 ± .72	.94
1-Palmitoleoylglycerophosphocholine	1.31 ± .74	1.17 ± .60	.73	1.14 ± .59	.80 ± .42	.29
2-Palmitoleoylglycerophosphocholine	1.40 ± .99	1.82 ± 1.21	.54	1.25 ± .54	.76 ± .44	.12
1-Palmitoleoylglycerophosphoethanolamine				1.08 ± .50	1.14 ± .34	.81
2-Palmitoleoylglycerophosphoethanolamine				1.23 ± .57	.93 ± .66	.42
1-Palmitoylglycerophosphocholine	1.31 ± .86	1.43 ± .96	.83	1.25 ± .68	.88 ± .52	.33
2-Palmitoylglycerophosphocholine	1.12 ± .57	1.06 ± .46	.85	1.14 ± .38	.72 ± .43	.11
1-Palmitoylglycerophosphoethanolamine	1.01 ± .22	.94 ± .23	.61	.98 ± .31	.93 ± .39	.85
2-Palmitoylglycerophosphoethanolamine	1.23 ± .54	1.03 ± .35	.48	1.05 ± .31	.83 ± .56	.43
1-Palmitoylglycerophosphoinositol	1.03 ± .17	.92 ± .20	.33	1.11 ± .29	1.24 ± .69	.68
1-Palmitoylplasménylethanolamine	1.11 ± .19	.95 ± .14	.12	1.04 ± .28	.87 ± .37	.38
1-Pentadecanoylglycerophosphocholine	1.21 ± .35	1.04 ± .39	.47			
1-Stearoylglycerophosphocholine	1.25 ± .74	1.28 ± .61	.94	1.13 ± .48	.83 ± .44	.29
2-Stearoylglycerophosphocholine	1.47 ± 1.59	1.58 ± 1.29	.91	1.41 ± .75	.92 ± .49	.22
1-Stearoylglycerophosphoethanolamine	.94 ± .14	1.04 ± .22	.41	1.03 ± .33	1.07 ± .46	.89
1-Stearoylglycerophosphoinositol	.77 ± .20	1.14 ± .23	.01	1.22 ± .52	1.37 ± .85	.71
<b><i>Lipid_Monoacylglycerol</i></b>						
1-Linoleoylglycerol (1-monolinolein)	.95 ± .26	1.31 ± .71	.27	1.36 ± 1.66	1.41 ± 1.11	.96
2-Linoleoylglycerol (2-monolinolein)				.82 ± .32	.89 ± .32	.71
1-Oleoylglycerol (1-monoolein)	.97 ± .25	1.15 ± .44	.43			
2-Oleoylglycerol (2-monoolein)				.81 ± .24	.88 ± .28	.65
1-Palmitoylglycerol (1-monopalmitin)				1.07 ± .37	1.09 ± .40	.94
2-Palmitoylglycerol (2-monopalmitin)				1.33 ± .57	.99 ± .33	.25
<b><i>Lipid_Sphingolipid</i></b>						
Palmitoyl sphingomyelin	1.08 ± .18	1.05 ± .19	.84	1.01 ± .18	.98 ± .24	.84
Sphinganine				1.05 ± .28	.68 ± .33	.07
Sphingosine	1.08 ± .25	.84 ± .24	.13	1.04 ± .30	.75 ± .41	.20
Stearoyl sphingomyelin	1.09 ± .36	1.35 ± .56	.37	1.00 ± .33	1.12 ± .31	.56
<b><i>Lipid_Sterol/Steroid</i></b>						
Campesterol	1.00 ± .22	1.03 ± .31	.85	1.13 ± .18	.92 ± .40	.27
Cholesterol	1.05 ± .12	1.01 ± .14	.64	1.08 ± .11	.88 ± .16	.03
Corticosterone	1.38 ± .89	1.63 ± .95	.67			
7-alpha-Hydroxycholesterol				.78 ± .60	2.20 ± 1.93	.12

7-beta-Hydroxycholesterol	.80 ± .22	.95 ± .35	.39	1.02 ± .52	2.07 ± 1.36	.11
7-alpha-Hydroxy-3-oxo-4-cholestenoate (7-Hoca)	.95 ± .22	1.15 ± .30	.22			
beta-Sitosterol	.85 ± .27	1.05 ± .42	.35	1.00 ± .15	.92 ± .32	.58
<b><i>Nucleotide_Purine metabolism, adenine containing</i></b>						
Adenine				1.21 ± .27	.91 ± .27	.08
Adenosine				1.38 ± .57	1.11 ± .59	.46
Adenosine 2'-monophosphate (2'-AMP)				1.54 ± .79	.67 ± .53	.0465
Adenosine 3'-monophosphate (3'-AMP)				1.40 ± .88	.87 ± .45	.22
Adenosine 5'-monophosphate (AMP)	1.35 ± 1.04	.13 ± .01	.02	1.65 ± 1.27	3.86 ± 6.32	.43
2'-Deoxyadenosine 3'-monophosphate				1.19 ± .47	1.70 ± .97	.28
N1-Methyladenosine	1.01 ± .16	1.02 ± .21	.88	.98 ± .15	.92 ± .22	.62
<b><i>Nucleotide_Purine metabolism, guanine containing</i></b>						
N6-Carbamoylthreonyladenosine	.99 ± .21	.90 ± .26	.55	.84 ± .26	1.02 ± .25	.26
2'-Deoxyguanosine				.78 ± .30	1.53 ± .83	.07
Guanosine				.96 ± .48	1.01 ± .36	.85
Guanosine 5'- monophosphate (5'-GMP)				1.22 ± .97	2.10 ± 2.48	.45
7-Methylguanine	1.12 ± .43	1.07 ± .34	.84			
N1-Methylguanosine	1.05 ± .13	.94 ± .13	.15	.92 ± .16	.92 ± .18	.93
<b><i>Nucleotide_Pyrimidine metabolism, cytidine containing</i></b>						
N4-Acetylcytidine	1.03 ± .11	.99 ± .15	.65			
Cytidine	1.04 ± .13	.95 ± .07	.20	1.12 ± .23	.97 ± .36	.44
Cytidine-3'-monophosphate (3'-CMP)				1.97 ± 1.61	.83 ± .21	.12
Cytidine 5'-monophosphate (5'-CMP)				.99 ± .26	.95 ± .25	.80
2'-Deoxycytidine	.98 ± .13	1.00 ± .18	.86	1.08 ± .21	1.12 ± .35	.82
2'-Deoxycytidine 5'-monophosphate				1.07 ± .29	.97 ± .30	.57
5-Methyl-2'-deoxycytidine	1.19 ± .19	.92 ± .06	.01			
<b><i>Nucleotide_Pyrimidine metabolism, orotate containing</i></b>						
Orotate	1.48 ± .44	.91 ± .11	.01	1.05 ± .12	.82 ± .28	.10
<b><i>Nucleotide_Pyrimidine metabolism, thymine containing</i></b>						
Thymidine	1.12 ± .22	.98 ± .11	.20	1.04 ± .24	1.13 ± .31	.60
Thymine				1.31 ± .60	.99 ± .34	.28
<b><i>Nucleotide_Purine metabolism, (hypo)xanthine/inosine containing</i></b>						
2'-Deoxyinosine				.90 ± .32	1.61 ± .92	.11



Hypoxanthine	1.43 ± .43	.86 ± .15	.01	.98 ± .42	.87 ± .42	.67
Inosine	1.93 ± 1.76	.89 ± .27	.19	.90 ± .38	.90 ± .39	1.00
Inosine 5'-monophosphate (IMP)				.99 ± 1.34	1.94 ± 2.46	.44
Xanthine	6.13 ± 9.62	.94 ± .20	.22	1.07 ± .16	.95 ± .15	.21
Xanthosine	1.78 ± 1.62	.90 ± .55	.25	1.11 ± .38	.99 ± .36	.61
<b><i>Nucleotide_Pyrimidine metabolism, uracil containing</i></b>						
2'-Deoxyuridine	1.03 ± .21	1.00 ± .24	.82			
5,6-Dihydrouracil	1.43 ± .48	.98 ± .17	.05	1.33 ± .87	1.10 ± .68	.62
5-Methyluridine (ribothymidine)				1.28 ± .67	.99 ± .14	.33
Pseudouridine	.90 ± .17	.97 ± .21	.56	.94 ± .13	.90 ± .28	.76
Uracil	1.43 ± .48	.85 ± .17	.02	1.18 ± .25	.96 ± .26	.17
Uridine	1.27 ± .40	.91 ± .18	.07	1.11 ± .28	1.05 ± .30	.73
Uridine monophosphate (5' or 3')				.81 ± .73	1.62 ± 1.91	.37
<b><i>Nucleotide_Purine metabolism, urate metabolism</i></b>						
Allantoin	1.08 ± .30	.84 ± .28	.19	1.20 ± .32	.83 ± .31	.07
Urate	1.07 ± .30	.88 ± .22	.25	1.01 ± .31	1.01 ± .33	1.00
<b><i>Nucleotide_Purine and pyrimidine metabolism</i></b>						
Methylphosphate				1.04 ± .25	1.27 ± .44	.32
<b><i>Amino acid_Alanine and aspartate metabolism</i></b>						
N-Acetylalanine	1.06 ± .16	.98 ± .19	.49	1.08 ± .25	.97 ± .20	.41
N-Acetyl-beta-alanine	1.12 ± .22	1.00 ± .18	.32			
N-Acetylaspartate (NAA)	1.23 ± .31	.93 ± .16	.07	.90 ± .32	.99 ± .23	.59
Alanine	1.42 ± .40	.94 ± .16	.02	1.06 ± .20	.96 ± .18	.41
beta-Alanine				1.04 ± .24	1.01 ± .23	.88
Asparagine	1.12 ± .26	.92 ± .11	.12	.98 ± .21	.93 ± .25	.71
Aspartate	1.27 ± .30	.94 ± .15	.04	1.03 ± .37	1.00 ± .22	.89
3-Ureidopropionate	1.42 ± .50	1.06 ± .44	.23	1.29 ± .37	1.17 ± .73	.72
<b><i>Amino acid_Butanoate metabolism</i></b>						
2-Aminobutyrate	1.06 ± .21	.98 ± .15	.46	1.01 ± .39	.91 ± .38	.70
<b><i>Amino acid_Creatine metabolism</i></b>						
Creatine	1.21 ± .30	1.12 ± .33	.61	1.14 ± .37	.95 ± .23	.33
Creatinine	1.07 ± .29	.94 ± .31	.48	1.31 ± .49	1.11 ± .39	.46
<b><i>Amino acid_Cysteine, methionine, SAM, taurine metabolism</i></b>						

<i>N</i> -Acetylmethionine	1.15 ± .45	.80 ± .26	.14	1.11 ± .31	1.10 ± .26	.97
<i>S</i> -Adenosylhomocysteine	3.33 ± 2.29	1.02 ± .41	.03	.92 ± .25	1.03 ± .27	.50
Cysteine				1.19 ± .47	.86 ± .24	.16
Cystine				.94 ± .43	1.28 ± .53	.25
<i>N</i> -Formylmethionine	1.18 ± .21	.96 ± .11	.05	1.03 ± .21	.94 ± .37	.63
Homocysteine				1.70 ± .93	.88 ± .27	.07
2-Hydroxybutyrate (AHB)	1.12 ± .44	.87 ± .33	.31	1.19 ± .36	.96 ± .51	.38
Hypotaurine				1.01 ± .26	1.00 ± .30	.94
Methionine	1.27 ± .50	.89 ± .31	.15	1.12 ± .22	.95 ± .16	.17
Methionine sulfoxide				1.18 ± .31	1.03 ± .33	.44
Taurine	1.26 ± .35	.93 ± .34	.13	1.30 ± .49	1.01 ± .48	.33
<b><i>Amino acid_Glutamate metabolism</i></b>						
<i>N</i> -Acetyl-aspartyl-glutamate (NAAG)				.93 ± .42	1.00 ± .46	.81
<i>N</i> -Acetylglutamate				.89 ± .19	1.01 ± .25	.40
gamma-Aminobutyrate (GABA)				3.14 ± 3.69	1.00 ± .28	.19
Glutamate	1.20 ± .27	.88 ± .18	.04	.95 ± .16	1.13 ± .15	.08
Glutamate, gamma-methyl ester				1.33 ± .53	1.14 ± .55	.57
Glutamine	1.04 ± .07	.93 ± .10	.06	.98 ± .19	1.05 ± .11	.51
<b><i>Amino acid_Glutathione metabolism</i></b>						
Cysteine-glutathione disulfide				1.55 ± .91	.74 ± .39	.07
Glutathione, oxidized (GSSG)	3.92 ± 3.61	.67 ± .48	.05	5.47 ± 6.43	.69 ± .43	.10
Glutathione, reduced (GSH)				1.44 ± .90	.70 ± .24	.08
<i>S</i> -Methylglutathione	1.59 ± .81	.84 ± .44	.08			
Ophthalmate	1.31 ± .53	.97 ± .37	.24			
5-Oxoproline	1.03 ± .14	.95 ± .10	.29	.84 ± .26	1.07 ± .28	.18
<b><i>Amino acid_Glycine, serine and threonine metabolism</i></b>						
<i>N</i> -Acetylglycine	.98 ± .29	1.06 ± .30	.65	1.00 ± .25	1.04 ± .18	.76
<i>N</i> -Acetylserine	1.19 ± .31	.96 ± .17	.15	1.22 ± .64	.95 ± .17	.35
<i>N</i> -Acetylthreonine				1.02 ± .18	.92 ± .28	.53
Betaine	.94 ± .17	.96 ± .20	.83	.97 ± .25	.98 ± .17	.97
Dimethylglycine	1.16 ± .31	.82 ± .25	.07			
Glycine	1.06 ± .17	1.02 ± .13	.62	.95 ± .20	1.03 ± .28	.58
Homoserine	1.58 ± .69	.71 ± .24	.01	1.03 ± .25	.92 ± .31	.51

beta-Hydroxypyruvate	1.17 ± .18	.88 ± .12	.01	.73 ± .11	.80 ± .15	.34
Serine	1.12 ± .27	.94 ± .17	.21	.95 ± .18	.93 ± .22	.87
Threonine	1.11 ± .38	.94 ± .15	.34	1.02 ± .11	1.01 ± .13	.96
<b><i>Amino acid_Guanidino and acetamido metabolism</i></b>						
4-Acetamidobutanoate	.98 ± .22	1.01 ± .17	.82			
<b><i>Amino acid_Histidine metabolism</i></b>						
3-Methylhistidine	1.14 ± .31	1.02 ± .12	.39			
1-Methylimidazoleacetate	1.07 ± .26	1.12 ± .22	.71			
Histamine				.72 ± .54	1.45 ± .96	.14
Histidine	1.10 ± .18	.97 ± .17	.23	1.03 ± .20	1.01 ± .24	.85
Imidazole propionate	1.26 ± .34	.95 ± .26	.12			
<i>cis</i> -Urocanate	1.11 ± .25	.95 ± .21	.28			
<i>trans</i> -Urocanate	1.20 ± .24	.90 ± .26	.06			
<b><i>Amino acid_Lysine metabolism</i></b>						
N6-Acetyllysine	1.06 ± .12	.92 ± .11	.06			
2-Amino adipate				1.07 ± .28	.89 ± .27	.28
Glutarate (pentanedioate)	2.02 ± 1.50	.82 ± .43	.09	.92 ± .21	1.74 ± .92	.06
Glutaroyl carnitine	1.37 ± .36	.90 ± .12	.01			
Lysine	1.22 ± .45	.86 ± .29	.13	.98 ± .18	.92 ± .18	.58
Pipecolate	1.00 ± .20	1.17 ± .22	.21	1.10 ± .46	1.13 ± .40	.91
<b><i>Amino acid_Phenylalanine &amp; tyrosine metabolism</i></b>						
N-Acetylphenylalanine	1.31 ± .32	.93 ± .08	.02			
N-Acetyltyrosine	1.18 ± .29	.79 ± .27	.04			
<i>p</i> -Cresol sulfate	1.19 ± .39	.81 ± .42	.14	1.25 ± .41	.65 ± .40	.03
Epinephrine	2.15 ± 1.50	.68 ± .26	.04			
4-Hydroxyphenylacetate	1.11 ± .36	.93 ± .20	.32			
3-(4-Hydroxyphenyl)lactate	1.17 ± .24	.81 ± .21	.02	1.93 ± 1.04	.90 ± .59	.06
4-Hydroxyphenylpyruvate	1.94 ± 1.03	.75 ± .28	.02			
Phenol sulfate	.91 ± .28	.90 ± .31	.96	1.35 ± .70	1.14 ± .53	.58
Phenylacetyl glycine	1.06 ± .18	.96 ± .30	.51	1.11 ± .24	.99 ± .27	.42
Phenylalanine	1.20 ± .14	1.00 ± .09	.01	.98 ± .12	.94 ± .18	.66
Phenyllactate (PLA)	1.09 ± .25	.73 ± .19	.02	.86 ± .40	.64 ± .00	
3-Phenylpropionate (hydrocinnamate)	.95 ± .17	1.07 ± .39	.53			

Phenylpyruvate	1.20 ± .45	.87 ± .31	.17			
Tyrosine	1.23 ± .30	.92 ± .13	.04	1.00 ± .14	.90 ± .19	.32
<b><i>Amino acid_Polyamine metabolism</i></b>						
5-Methylthioadenosine (MTA)	1.27 ± .46	.70 ± .35	.04	1.20 ± .23	.90 ± .29	.08
Putrescine				1.28 ± .35	.97 ± .62	.33
Spermidine				1.13 ± .16	.91 ± .29	.15
<b><i>Amino acid_Tryptophan metabolism</i></b>						
N-Acetyltryptophan	.97 ± .13	1.13 ± .21	.15			
C-Glycosyltryptophan	1.23 ± .27	.92 ± .09	.02	1.18 ± .34	.85 ± .18	.07
Indoleacetate	1.04 ± .36	.97 ± .17	.69			
Indolelactate	1.55 ± .45	.90 ± .16	.01	4.14 ± 4.75	1.12 ± 1.12	.17
Indolepropionate	.88 ± .22	1.03 ± .37	.43			
3-Indoxyl sulfate	.99 ± .18	1.01 ± .12	.79	1.33 ± .47	.79 ± .31	.04
Kynurenate	1.11 ± .42	.99 ± .41	.63			
Kynurenine	1.12 ± .21	1.15 ± .45	.88	1.17 ± .36	.99 ± .31	.39
Serotonin (5HT)	2.23 ± 1.24	.78 ± .29	.02			
Tryptophan	1.02 ± .16	.92 ± .13	.28	.99 ± .20	.89 ± .21	.44
<b><i>Amino acid_Urea cycle; arginine-, proline-, metabolism</i></b>						
5-Aminovalerate				.87 ± .26	1.33 ± .52	.09
Arginine	1.20 ± .18	.93 ± .15	.02	1.02 ± .32	.88 ± .32	.49
Assymetric dimethylarginine (ADMA)	1.06 ± .21	.87 ± .13	.09	.94 ± .19	1.03 ± .24	.53
Citrulline	.96 ± .07	1.10 ± .10	.02	.92 ± .18	1.08 ± .27	.27
Homocitrulline	1.00 ± .26	.94 ± .16	.63			
<i>trans</i> -4-Hydroxyproline	.91 ± .21	.97 ± .25	.68	1.02 ± .29	.94 ± .17	.58
Ornithine	2.48 ± 2.07	.73 ± .71	.08	.90 ± .25	.96 ± .21	.65
Proline	1.54 ± .55	.92 ± .27	.03	1.05 ± .21	1.02 ± .21	.83
Urea	1.12 ± .21	.99 ± .17	.25	1.13 ± .35	.87 ± .26	.18
<b><i>Amino acid_Valine, leucine and isoleucine metabolism</i></b>						
N-Acetylisoleucine	.91 ± .24	1.11 ± .37	.29			
N-Acetylleucine	1.04 ± .23	.83 ± .26	.17			
N-Acetylvaline				.80 ± .18	.72 ± .16	.46
2-Hydroxyisobutyrate	.94 ± .20	1.10 ± .18	.18			
3-Hydroxyisobutyrate	1.34 ± .44	.99 ± .32	.15			

alpha-Hydroxyisovalerate	1.68 ± .64	.97 ± .45	.0483	1.47 ± .60	.69 ± .31	.02
beta-Hydroxyisovalerate	.94 ± .14	1.11 ± .29	.22			
Hydroxyisovaleroyl carnitine	.70 ± .31	1.31 ± .65	.06	.88 ± .67	.99 ± .36	.74
Isobutyrylcarnitine	1.37 ± .49	.95 ± .22	.08	1.79 ± 1.07	.75 ± .41	.05
Isoleucine	1.04 ± .15	.96 ± .12	.33	.98 ± .16	.98 ± .16	.98
Isovalerylcarnitine	1.51 ± .71	1.24 ± 1.11	.64	2.69 ± 2.27	1.01 ± .74	.12
Isovalerylglycine	1.19 ± .39	1.10 ± .58	.77			
Leucine	1.09 ± .20	.94 ± .11	.14	.98 ± .12	.96 ± .18	.84
Levulinate (4-oxovalerate)	.95 ± .21	1.10 ± .23	.27			
2-Methylbutyrylcarnitine	1.33 ± .56	.89 ± .28	.12	1.97 ± 1.44	.75 ± .31	.07
Methylglutaroylcarnitine	1.27 ± .39	.90 ± .32	.12			
3-Methyl-2-oxobutyrate	1.13 ± .33	1.04 ± .11	.53			
4-Methyl-2-oxopentanoate	1.14 ± .38	1.02 ± .14	.48	1.73 ± 1.40	2.24 ± 2.34	.67
3-Methyl-2-oxovalerate	1.16 ± .40	1.02 ± .06	.45	.77 ± .43	1.10 ± .77	.38
Valine	1.11 ± .21	.98 ± .16	.26	1.01 ± .14	.93 ± .16	.40
<b><i>Peptide_Dipeptide</i></b>						
Alanylalanine	.92 ± .13	1.08 ± .28	.24	1.19 ± .32	1.00 ± .29	.31
Aspartylleucine				.92 ± .31	1.24 ± .41	.17
Aspartylphenylalanine				.98 ± .19	.99 ± .27	.94
Glycylglycine				1.15 ± .39	.93 ± .25	.28
Glycylleucine				1.24 ± .38	1.19 ± .54	.88
Glycylphenylalanine				1.08 ± .25	1.01 ± .36	.71
Glycylproline				1.04 ± .19	.93 ± .19	.37
Isoleucylglutamate				.72 ± .25	.98 ± .39	.20
Isoleucylglycine				1.11 ± .23	1.09 ± .50	.95
Prolylalanine				1.67 ± 1.46	.87 ± .39	.23
Pro-hydroxy-pro	1.01 ± .30	.99 ± .21	.93	1.26 ± .45	.98 ± .23	.21
Serylleucine				.93 ± .17	1.15 ± .20	.06
<b><i>Peptide_Dipeptide derivative</i></b>						
Anserine	1.33 ± .50	1.03 ± .34	.26	1.42 ± 1.09	1.99 ± 1.20	.42
Carnosine				1.14 ± .41	.93 ± .30	.34
<b><i>Peptide_Fibrinogen cleavage peptide</i></b>						
SPVPDXVPGSFK	.99 ± .41	1.61 ± 1.02	.20			

TDTEDKGEFLSEGGGV	1.78 ± 1.72	1.06 ± .81	.38			
TDTEDKGEFLSEGGGVR	1.90 ± 1.41	.75 ± .59	.10			
<b><i>Peptide_gamma-Glutamyl</i></b>						
gamma-Glutamylalanine	1.22 ± .38	.84 ± .20	.06	.97 ± .28	.98 ± .23	.92
gamma-Glutamylcysteine				1.11 ± .52	1.27 ± .60	.65
gamma-Glutamylglutamate				1.05 ± .54	.94 ± .35	.69
gamma-Glutamylglutamine	1.10 ± .21	1.04 ± .24	.64	.89 ± .36	1.07 ± .28	.37
gamma-Glutamylglycine				.82 ± .30	1.07 ± .30	.20
gamma-Glutamylisoleucine	1.12 ± .26	.91 ± .16	.12	.96 ± .23	1.14 ± .33	.32
gamma-Glutamylleucine	1.15 ± .34	.88 ± .16	.11	.89 ± .27	1.04 ± .28	.37
gamma-Glutamylmethionine	1.22 ± .63	.96 ± .40	.41	.96 ± .28	.98 ± .21	.90
gamma-Glutamylphenylalanine	1.32 ± .38	.89 ± .14	.03	.90 ± .25	1.12 ± .32	.22
gamma-Glutamylthreonine	1.34 ± .42	1.02 ± .26	.15	.95 ± .34	1.09 ± .27	.48
gamma-Glutamyltryptophan	.95 ± .24	.89 ± .23	.68	1.02 ± .27	1.08 ± .28	.69
gamma-Glutamyltyrosine	1.34 ± .48	.89 ± .25	.07	.98 ± .30	1.09 ± .31	.55
gamma-Glutamylvaline	1.22 ± .37	.96 ± .24	.19	.98 ± .34	1.01 ± .29	.88
<b><i>Cofactors and vitamins_Ascorbate and aldarate metabolism</i></b>						
Ascorbate (Vitamin C)				1.18 ± .56	.90 ± .37	.34
Dehydroascorbate				1.11 ± .30	.96 ± .40	.50
Gulono-1,4-lactone	1.35 ± .44	.87 ± .23	.04			
Threonate	1.07 ± .21	1.01 ± .17	.66			
<b><i>Cofactors and vitamins_Folate metabolism</i></b>						
Dihydrobiopterin	1.35 ± .43	.85 ± .18	.02			
5-Methyltetrahydrofolate (5MeTHF)				.82 ± .40	1.10 ± .33	.22
<b><i>Cofactors and vitamins_Hemoglobin and porphyrin metabolism</i></b>						
Bilirubin (E,E)	1.51 ± .94	.87 ± .17	.13			
Biliverdin	1.09 ± .46	.89 ± .35	.43	1.39 ± .50	.65 ± .39	.02
Heme	1.03 ± .35	1.15 ± .51	.66	1.26 ± .75	.43 ± .36	.03
<b><i>Cofactors and vitamins_Nicotinate and nicotinamide metabolism</i></b>						
Nicotinamide	.99 ± .10	.91 ± .30	.52	1.02 ± .19	1.00 ± .16	.89
Nicotinamide adenine dinucleotide (NAD+)				1.03 ± .23	.90 ± .25	.38
Nicotinamide riboside				.86 ± .44	1.52 ± 1.10	.21
<b><i>Cofactors and vitamins_Pantothenate and CoA metabolism</i></b>						

Pantothenate	1.07 ± .20	.94 ± .13	.21	1.09 ± .72	1.07 ± .27	.96
<b><i>Cofactors and vitamins_Pyridoxal metabolism</i></b>						
Pyridoxal	1.20 ± .27	.81 ± .18	.01	.89 ± .20	.93 ± .24	.79
<b><i>Cofactors and vitamins_Riboflavin metabolism</i></b>						
Flavin adenine dinucleotide (FAD)				1.02 ± .28	1.00 ± .34	.89
Flavin mononucleotide (FMN)				1.09 ± .49	1.04 ± .42	.86
Riboflavin (Vitamin B2)				1.12 ± .22	1.09 ± .22	.80
<b><i>Cofactors and vitamins_Tocopherol metabolism</i></b>						
alpha-Tocopherol	1.02 ± .17	.98 ± .14	.70	1.19 ± .51	.88 ± .37	.27
<b><i>Cofactors and vitamins_Vitamin B6 metabolism</i></b>						
Pyridoxate	1.25 ± .32	.96 ± .14	.07			
<b><i>Xenobiotics_Benzoate metabolism</i></b>						
Benzoate	.63 ± .24	1.87 ± .78	.003	1.07 ± .09	.97 ± .35	.53
Catechol sulfate	1.10 ± .30	1.08 ± .44	.93	.95 ± .42	.82 ± .32	.57
Hippurate	.98 ± .16	1.00 ± .33	.90	1.02 ± .29	1.08 ± .44	.82
4-Hydroxyhippurate	1.02 ± .16	1.10 ± .36	.67			
Methyl-4-hydroxybenzoate	.80 ± .17	1.23 ± .25	.004			
<b><i>Xenobiotics_Chemical</i></b>						
Dexpanthenol				1.00 ± 0.00	1.00 ± 0.00	
2-Ethylhexanoate	.72 ± .18	1.65 ± .55	.002			
2-Ethylhexanoate (isobar with 2-propylpentanoate)				1.04 ± .12	1.08 ± .26	.73
Glycerol 2-phosphate	1.06 ± .14	.89 ± .15	.07	.91 ± .38	1.01 ± .29	.64
Glycolate (hydroxyacetate)	1.41 ± .89	1.25 ± .69	.74	1.98 ± 1.88	3.78 ± 4.30	.38
Oxamate				1.10 ± .29	1.17 ± .31	.68
Trizma acetate	2.51 ± 2.90	2.13 ± 2.17	.81	1.22 ± .96	1.42 ± 2.56	.87
<b><i>Xenobiotics_Drug</i></b>						
Penicillin G				.79 ± .62	.52 ± .34	.39
<b><i>Xenobiotics_Food component/Plant</i></b>						
N-Glycolylneuraminate				1.23 ± .56	.88 ± .23	.19
5-Hydroxymethylfurfural				1.02 ± .25	1.23 ± .52	.39
Stachydrine	1.02 ± .32	1.76 ± 1.47	.27	.83 ± .37	1.29 ± 1.08	.36
Tartarate	3.09 ± 2.08	1.11 ± .67	.0496			

Vanillin	.83 ± .16	1.09 ± .18	.02			
<b><i>Xenobiotics_Sugar, sugar substitute, starch</i></b>						
Erythritol	1.23 ± .31	.95 ± .25	.11	1.46 ± .84	1.01 ± .35	.26

\* Plasma and tumor specimens were used from MMTV-*neu* mice administered control or WA (n = 8 mice per group).

† All *P* values were calculated by a two-sided Student's *t* test.