

Supplemental Data Table 1 UNNM-01-12VW		Fold of Change			Statistical Values						Mean Values			Standard Deviation		
		CKD3 CKD2	CKD4 CKD2	CKD4 CKD3	CKD3 CKD2		CKD4 CKD2		CKD4 CKD3		CKD2	CKD3	CKD4	CKD2	CKD3	CKD4
					p-value	q-value	p-value	q-value	p-value	q-value						
Biochemical Name	Platform															
glycine	GC/MS	1.3	1.36	1.04	0.08	0.08	0.04	0.03	0.73	0.98	0.845	1.100	1.147	0.341	0.344	0.333
N-acetylglycine	GC/MS	1.45	1.21	0.84	0.02	0.04	0.30	0.14	0.24	0.88	0.641	0.929	0.777	0.125	0.320	0.336
serine	GC/MS	1.31	1.31	1	0.02	0.04	0.01	0.01	0.96	0.99	0.812	1.063	1.063	0.239	0.180	0.154
threonine	GC/MS	1.15	1.21	1.06	0.41	0.20	0.10	0.06	0.58	0.92	0.898	1.028	1.088	0.194	0.327	0.264
betaine	LC/MS pos	0.82	0.54	0.66	0.15	0.12	0.00	0.00	0.13	0.88	1.478	1.209	0.793	0.410	0.802	0.402
aspartate	GC/MS	1.15	1.22	1.06	0.33	0.18	0.28	0.13	0.83	0.98	0.869	0.998	1.057	0.387	0.331	0.434
asparagine	GC/MS	1.36	1.58	1.16	0.09	0.09	0.01	0.01	0.29	0.88	0.798	1.087	1.261	0.302	0.435	0.475
alanine	GC/MS	1.31	1.42	1.09	0.02	0.04	0.01	0.01	0.32	0.88	0.803	1.051	1.144	0.253	0.175	0.216
N-acetylalanine	LC/MS neg	1.38	1.54	1.12	0.13	0.11	0.06	0.05	0.68	0.98	0.815	1.127	1.258	0.314	0.594	0.833
glutamate	GC/MS	0.8	1.07	1.34	0.43	0.21	0.79	0.29	0.32	0.88	1.188	0.950	1.276	0.746	0.245	0.676
glutamine	LC/MS pos	0.98	0.92	0.94	0.69	0.26	0.22	0.11	0.53	0.92	1.043	1.024	0.963	0.127	0.212	0.178
pyroglutamine*	LC/MS pos	2.03	1.33	0.65	0.11	0.10	0.58	0.22	0.30	0.88	0.825	1.677	1.095	0.462	1.325	0.813
histidine	LC/MS neg	1.09	1.09	1	0.16	0.12	0.16	0.09	0.98	0.99	0.918	1.004	1.003	0.132	0.128	0.134
3-methylhistidine	LC/MS neg	1.65	2.66	1.61	0.46	0.21	0.44	0.18	0.88	0.98	1.013	1.674	2.693	0.886	1.952	4.134
lysine	LC/MS pos	0.66	0.59	0.9	0.02	0.04	0.00	0.00	0.79	0.98	1.270	0.834	0.751	0.286	0.454	0.342
pipecolate	LC/MS pos	1.1	0.96	0.87	0.96	0.31	0.84	0.29	0.82	0.98	1.395	1.538	1.337	1.149	1.344	1.133
N6-acetyllysine	LC/MS pos	1.47	1.56	1.06	0.03	0.04	0.13	0.07	0.86	0.98	0.902	1.328	1.406	0.266	0.541	0.967
glutaroyl carnitine	LC/MS pos	1.57	1.63	1.04	0.04	0.06	0.30	0.14	0.59	0.92	0.813	1.275	1.329	0.429	0.585	1.199
phenylalanine	LC/MS pos	1.3	1.21	0.92	0.02	0.04	0.01	0.01	0.55	0.92	0.853	1.112	1.029	0.124	0.320	0.140
phenylacetate	LC/MS neg	1.39	1	0.72	0.07	0.07			0.07	0.88	0.507	0.707	0.507	0.000	0.311	0.000
p-cresol sulfate	LC/MS neg	1.91	1.61	0.84	0.22	0.15	0.31	0.14	0.82	0.98	0.945	1.802	1.521	0.860	1.939	1.288
tyrosine	LC/MS pos	1.26	0.91	0.72	0.52	0.23	0.34	0.15	0.27	0.88	1.049	1.327	0.956	0.212	0.776	0.175
3-(4-hydroxyphenyl)lactate	GC/MS	1.5	0.99	0.66	0.51	0.22	0.79	0.29	0.41	0.90	0.901	1.353	0.892	0.373	1.261	0.574
3-methoxytyrosine	LC/MS pos	1.42	1.43	1.01	0.00	0.01	0.01	0.01	0.97	0.99	0.697	0.987	0.995	0.144	0.212	0.279
phenylacetylglutamine	LC/MS pos	2.31	1.62	0.7	0.28	0.17	0.39	0.16	0.69	0.98	0.817	1.885	1.322	0.608	2.027	1.724
phenol sulfate	LC/MS neg	1.32	1.78	1.35	0.83	0.28	0.12	0.07	0.24	0.88	1.040	1.370	1.847	0.709	1.566	1.393
kynurenine	LC/MS pos	1.16	1.24	1.07	0.37	0.19	0.10	0.06	0.55	0.92	0.944	1.093	1.171	0.234	0.391	0.337
tryptophan	LC/MS pos	1	0.88	0.88	0.70	0.26	0.29	0.14	0.78	0.98	1.064	1.060	0.933	0.254	0.426	0.186
indolelactate	LC/MS pos	0.98	1.28	1.3	0.69	0.26	0.46	0.19	0.33	0.88	1.017	0.998	1.300	0.357	0.538	0.800
indoleacetate	LC/MS pos	0.65	0.55	0.85	0.03	0.04	0.01	0.01	0.25	0.88	1.572	1.015	0.859	0.731	0.384	0.428
tryptophan betaine	LC/MS pos	1.36	1.34	0.98	0.63	0.25	0.59	0.22	0.95	0.99	1.215	1.656	1.631	1.434	1.751	1.439
serotonin (5HT)	LC/MS pos	1.48	1.8	1.21	0.01	0.04	0.00	0.01	0.35	0.88	0.592	0.877	1.065	0.001	0.318	0.482
C-glycosyltryptophan*	LC/MS pos	1.78	2.31	1.3	0.04	0.06	0.01	0.01	0.44	0.91	0.734	1.306	1.694	0.314	1.076	1.771

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					p-value	q-value	p-value	q-value	p-value	q-value						
Biochemical Name	Platform															
3-indoxyl sulfate	LC/MS neg	1.35	1.35	1	0.56	0.23	0.29	0.14	0.67	0.98	1.186	1.595	1.600	0.914	1.499	1.414
indolepropionate	LC/MS pos	1.44	0.78	0.54	0.57	0.23	0.40	0.17	0.18	0.88	1.179	1.703	0.920	0.620	1.802	0.603
3-methyl-2-oxobutyrate	LC/MS neg	1.07	1.08	1.02	0.91	0.29	0.65	0.24	0.81	0.98	0.954	1.018	1.033	0.207	0.349	0.296
3-methyl-2-oxovalerate	LC/MS neg	0.97	1.1	1.13	0.87	0.28	0.42	0.17	0.33	0.88	0.961	0.933	1.058	0.305	0.302	0.284
beta-hydroxyisovalerate	LC/MS neg	0.97	0.96	1	0.82	0.28	0.81	0.29	0.99	0.99	0.779	0.752	0.751	0.283	0.281	0.280
alpha-hydroxyisocaproate	LC/MS neg	1.1	1.24	1.13	0.72	0.26	0.60	0.23	0.83	0.98	0.580	0.635	0.718	0.148	0.321	0.585
isoleucine	LC/MS pos	0.95	1.08	1.15	0.79	0.27	0.32	0.14	0.07	0.88	1.004	0.950	1.088	0.279	0.185	0.161
leucine	LC/MS pos	0.96	0.98	1.02	0.64	0.25	0.92	0.31	0.66	0.98	1.029	0.989	1.009	0.212	0.280	0.150
valine	LC/MS pos	0.98	1.02	1.04	0.84	0.28	0.68	0.25	0.51	0.92	0.991	0.970	1.011	0.222	0.210	0.128
3-hydroxyisobutyrate	GC/MS	1.37	1.16	0.85	0.21	0.14	0.56	0.22	0.51	0.92	0.792	1.087	0.920	0.251	0.569	0.418
4-methyl-2-oxopentanoate	LC/MS neg	0.99	1.07	1.09	0.71	0.26	0.58	0.22	0.44	0.91	0.974	0.961	1.045	0.269	0.395	0.277
alpha-hydroxyisovalerate	LC/MS neg	1.05	0.85	0.81	0.27	0.17	0.12	0.07	0.77	0.98	2.256	2.360	1.920	1.314	3.850	3.316
isobutyrylcarnitine	LC/MS pos	1.44	1.59	1.1	0.32	0.18	0.14	0.08	0.66	0.98	1.066	1.534	1.693	1.030	1.283	1.554
2-methylbutyrylcarnitine	LC/MS pos	1.31	1.12	0.86	0.52	0.23	0.85	0.29	0.46	0.91	0.843	1.103	0.946	0.438	0.733	0.950
isovalerylcarnitine	LC/MS pos	1.07	1.16	1.09	0.77	0.27	0.60	0.23	0.80	0.98	1.039	1.109	1.206	0.438	0.479	0.570
cysteine	GC/MS	1.03	0.85	0.82	0.99	0.31	0.27	0.13	0.31	0.88	1.052	1.078	0.890	0.297	0.408	0.322
methionine	LC/MS neg	1.36	1.09	0.8	0.15	0.12	0.13	0.07	0.35	0.88	0.943	1.285	1.025	0.128	0.660	0.101
2-hydroxybutyrate (AHB)	GC/MS	1.4	1.37	0.98	0.25	0.17	0.28	0.13	0.94	0.99	0.832	1.164	1.136	0.454	0.732	0.689
dimethylarginine (SDMA + ADMA)	LC/MS pos	8.06	4.84	0.6	0.00	0.00	0.01	0.01	0.17	0.88	0.497	4.006	2.403	0.133	2.273	1.774
arginine	LC/MS neg	1.51	1.53	1.01	0.06	0.07	0.10	0.06	0.93	0.99	0.675	1.020	1.032	0.238	0.480	0.559
ornithine	LC/MS pos	0.28	0.16	0.57	0.00	0.00	0.00	0.00	0.34	0.88	4.327	1.195	0.683	1.387	1.316	0.334
urea	GC/MS	1.32	1.51	1.14	0.17	0.13	0.09	0.06	0.67	0.98	0.803	1.062	1.210	0.351	0.474	0.772
proline	LC/MS pos	1.28	0.97	0.76	0.21	0.14	0.84	0.29	0.15	0.88	0.966	1.239	0.936	0.260	0.518	0.246
citrulline	LC/MS pos	1.58	1.31	0.83	0.03	0.05	0.08	0.05	0.42	0.90	0.825	1.304	1.082	0.194	0.586	0.362
N-acetylorithine	LC/MS pos	1.66	1.39	0.84	0.09	0.09	0.07	0.05	0.87	0.98	0.905	1.501	1.257	0.762	0.999	0.400
trans-4-hydroxyproline	GC/MS	1.23	1.4	1.14	0.44	0.21	0.25	0.12	0.71	0.98	0.973	1.199	1.361	0.362	0.581	0.937
creatine	LC/MS pos	0.97	1.22	1.25	0.64	0.25	0.85	0.29	0.58	0.92	0.978	0.952	1.192	0.460	0.752	0.694
creatinine	LC/MS pos	1.16	1.23	1.06	0.75	0.26	0.98	0.33	0.82	0.98	1.085	1.264	1.337	0.296	0.655	1.344
2-aminobutyrate	LC/MS pos	1.14	1.28	1.13	0.59	0.24	0.05	0.04	0.28	0.88	0.889	1.010	1.140	0.262	0.401	0.237
4-acetamidobutanoate	LC/MS pos	2.17	1.71	0.79	0.17	0.13	0.15	0.08	0.85	0.98	0.866	1.876	1.483	0.232	2.613	1.542
5-oxoproline	LC/MS pos	1.46	1.42	0.97	0.03	0.04	0.09	0.06	0.74	0.98	0.806	1.180	1.140	0.309	0.388	0.391
aspartylphenylalanine	LC/MS pos	2	3.56	1.78	0.02	0.04	0.00	0.00	0.07	0.88	0.354	0.710	1.261	0.000	0.496	0.798
pro-hydroxy-pro	LC/MS pos	2.49	4.46	1.79	0.03	0.05	0.00	0.00	0.05	0.88	0.466	1.162	2.079	0.251	1.268	1.677

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					p-value	q-value	p-value	q-value	p-value	q-value						
Biochemical Name	Platform															
cyclo(leu-pro)	LC/MS pos	0.55	0.36	0.65	0.42	0.21	0.11	0.07	0.33	0.88	1.971	1.093	0.716	2.732	1.073	0.516
phenylalanyltryptophan	LC/MS pos	1.11	2.39	2.16	0.74	0.26	0.02	0.02	0.04	0.88	0.736	0.817	1.762	0.543	0.570	1.150
gamma-glutamylvaline	LC/MS pos	1.17	1.22	1.04	0.27	0.17	0.07	0.05	0.62	0.95	0.912	1.065	1.108	0.236	0.311	0.250
gamma-glutamylleucine	LC/MS pos	1.12	1.3	1.16	0.51	0.22	0.03	0.02	0.15	0.88	0.821	0.921	1.070	0.283	0.310	0.161
gamma-glutamylisoleucine*	LC/MS pos	1.61	1.7	1.06	0.01	0.03	0.01	0.01	0.78	0.98	0.695	1.117	1.184	0.196	0.440	0.510
gamma-glutamylmethionine	LC/MS pos	1.09	0.85	0.78	0.70	0.26	0.37	0.16	0.21	0.88	1.044	1.138	0.887	0.387	0.474	0.291
gamma-glutamylglutamine	LC/MS pos	3.83	4.78	1.25	0.00	0.00	0.00	0.00	0.13	0.88	0.275	1.053	1.313	0.166	0.417	0.349
gamma-glutamylphenylalanine	LC/MS pos	1.45	1.29	0.89	0.03	0.04	0.01	0.01	0.59	0.92	0.903	1.311	1.165	0.240	0.480	0.181
gamma-glutamyltyrosine	LC/MS pos	1.19	0.97	0.82	0.55	0.23	0.95	0.32	0.53	0.92	0.993	1.179	0.966	0.366	0.631	0.193
bradykinin, des-arg(9)	LC/MS pos	4.95	1.42	0.29	0.26	0.17	0.17	0.09	0.60	0.92	0.764	3.779	1.083	0.306	7.550	0.651
ADSGEGDFXAEGGGVR*	LC/MS pos	2.06	2.82	1.37	0.01	0.03	0.00	0.00	0.24	0.88	0.465	0.957	1.311	0.000	0.516	0.761
DSGEGDFXAEGGGVR*	LC/MS pos	689.13	826.73	1.2	0.00	0.00	0.00	0.00	0.21	0.88	0.002	1.034	1.240	0.001	0.765	0.795
ADpSGEGDFXAEGGGVR*	LC/MS pos	18.01	45.27	2.51	0.00	0.01	0.00	0.00	0.04	0.88	0.045	0.818	2.055	0.017	0.683	2.624
erythronate*	GC/MS	1.61	1.45	0.9	0.31	0.18	0.28	0.13	0.95	0.99	0.992	1.597	1.438	0.393	1.737	1.299
fructose	GC/MS	2.83	1.76	0.62	0.03	0.04	0.00	0.01	0.50	0.92	0.763	2.157	1.343	0.346	1.695	0.534
mannitol	GC/MS	6.94	3.8	0.55	0.08	0.09	0.02	0.02	0.98	0.99	0.216	1.495	0.819	0.059	2.326	0.745
mannose	GC/MS	0.67	0.68	1.02	0.19	0.14	0.24	0.12	0.78	0.98	1.572	1.046	1.070	1.004	0.444	0.365
1,5-anhydroglucitol (1,5-AG)	LC/MS neg	0.76	0.62	0.82	0.54	0.23	0.26	0.13	0.53	0.92	1.291	0.978	0.801	0.711	0.487	0.295
glycerate	GC/MS	0.69	0.51	0.74	0.04	0.05	0.00	0.00	0.02	0.88	1.185	0.823	0.608	0.378	0.225	0.163
glucose	GC/MS	0.69	0.71	1.02	0.09	0.09	0.11	0.06	0.83	0.98	1.422	0.984	1.003	0.697	0.307	0.293
1,6-anhydroglucose	GC/MS	0.55	0.49	0.89	0.33	0.18	0.29	0.14	0.96	0.99	1.391	0.759	0.675	1.891	0.751	0.510
pyruvate	GC/MS	0.48	0.39	0.8	0.01	0.03	0.00	0.00	0.33	0.88	1.921	0.925	0.744	1.014	0.526	0.453
lactate	GC/MS	0.91	0.93	1.02	0.63	0.25	0.58	0.22	0.86	0.98	1.210	1.100	1.127	0.434	0.310	0.558
arabitol	GC/MS	1.3	1.75	1.35	0.24	0.16	0.01	0.01	0.19	0.88	0.826	1.073	1.450	0.206	0.557	0.904
gluconate	GC/MS	1.43	1.01	0.7	0.99	0.31	0.69	0.25	0.73	0.98	0.859	1.232	0.866	0.663	2.085	0.462
arabinose	GC/MS	0.8	0.68	0.84	0.61	0.24	0.32	0.14	0.56	0.92	0.787	0.631	0.531	0.656	0.421	0.165
xylonate	GC/MS	1.8	2.35	1.3	0.13	0.11	0.05	0.04	0.56	0.92	0.636	1.145	1.493	0.025	1.131	1.648
citrate	GC/MS	0.76	0.51	0.67	0.08	0.08	0.00	0.00	0.04	0.88	1.506	1.147	0.773	0.499	0.501	0.218
alpha-ketoglutarate	GC/MS	1.34	0.95	0.71	0.51	0.22	0.84	0.29	0.41	0.90	0.625	0.839	0.593	0.253	0.755	0.172
succinate	GC/MS	1.15	1.23	1.07	0.31	0.18	0.04	0.03	0.45	0.91	0.824	0.951	1.015	0.170	0.314	0.209
malate	GC/MS	0.68	0.51	0.75	0.06	0.07	0.00	0.00	0.23	0.88	1.344	0.918	0.690	0.471	0.486	0.162
acetylphosphate	GC/MS	1.7	1.92	1.13	0.00	0.00	0.00	0.00	0.40	0.90	0.630	1.073	1.213	0.169	0.280	0.332
phosphate	GC/MS	0.44	0.3	0.69	0.00	0.00	0.00	0.00	0.41	0.90	2.679	1.167	0.804	0.452	0.910	0.190

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					p-value	q-value	p-value	q-value	p-value	q-value						
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linoleate (18:2n6)	LC/MS neg	1.42	1.63	1.15	0.38	0.19	0.00	0.00	0.30	0.88	0.740	1.050	1.210	0.195	0.485	0.364
linolenate [alpha or gamma; (18:3n3 or 6)]	LC/MS neg	1.64	2.11	1.29	0.33	0.18	0.00	0.00	0.22	0.88	0.661	1.085	1.398	0.238	0.525	0.559
dihomo-linolenate (20:3n3 or n6)	LC/MS neg	1.3	1.48	1.14	0.42	0.21	0.01	0.01	0.29	0.88	0.870	1.128	1.290	0.284	0.545	0.359
eicosapentaenoate (EPA; 20:5n3)	LC/MS neg	2.37	3.73	1.57	0.16	0.13	0.00	0.00	0.12	0.88	0.607	1.438	2.262	0.365	1.432	1.490
docosapentaenoate (n3 DPA; 22:5n3)	LC/MS neg	1.84	2.55	1.39	0.13	0.11	0.00	0.00	0.11	0.88	0.623	1.143	1.590	0.288	0.641	0.552
docosahexaenoate (DHA; 22:6n3)	LC/MS neg	2.08	2.3	1.1	0.10	0.09	0.00	0.00	0.46	0.91	0.671	1.399	1.542	0.229	0.847	0.705
caproate (6:0)	LC/MS neg	1.67	2.11	1.26	0.06	0.07	0.00	0.00	0.17	0.88	0.562	0.940	1.186	0.374	0.435	0.383
heptanoate (7:0)	LC/MS neg	1.39	1.72	1.23	0.07	0.08	0.00	0.00	0.10	0.88	0.598	0.834	1.027	0.258	0.313	0.201
caprylate (8:0)	LC/MS neg	1.41	1.31	0.93	0.11	0.10	0.05	0.04	0.95	0.99	0.751	1.058	0.980	0.372	0.381	0.178
pelargonate (9:0)	LC/MS neg	1.3	1.5	1.15	0.04	0.05	0.00	0.00	0.10	0.88	0.744	0.970	1.112	0.172	0.217	0.114
caprate (10:0)	LC/MS neg	1.14	1.04	0.91	0.45	0.21	0.52	0.21	0.73	0.98	1.002	1.147	1.046	0.256	0.463	0.150
undecanoate (11:0)	LC/MS neg	1.44	1.57	1.09	0.01	0.03	0.00	0.00	0.48	0.92	0.818	1.178	1.283	0.194	0.356	0.371
laurate (12:0)	LC/MS neg	1.03	1.01	0.98	0.82	0.28	0.82	0.29	0.98	0.99	1.049	1.079	1.055	0.353	0.343	0.214
5-dodecenoate (12:1n7)	LC/MS neg	2.46	0.71	0.29	0.09	0.09	0.16	0.09	0.01	0.88	1.084	2.663	0.767	0.629	2.585	0.309
myristate (14:0)	LC/MS neg	1.09	1.13	1.04	0.94	0.30	0.32	0.14	0.48	0.92	1.038	1.127	1.174	0.425	0.670	0.343
myristoleate (14:1n5)	LC/MS neg	1.2	0.91	0.76	0.62	0.25	0.63	0.23	0.89	0.98	1.463	1.756	1.331	1.409	1.773	0.544
palmitate (16:0)	LC/MS neg	1.2	1.25	1.04	0.64	0.25	0.08	0.05	0.50	0.92	0.920	1.104	1.150	0.315	0.528	0.313
palmitoleate (16:1n7)	LC/MS neg	1.14	1.07	0.94	0.87	0.28	0.36	0.16	0.40	0.90	1.263	1.440	1.357	1.006	1.394	0.555
margarate (17:0)	LC/MS neg	1.54	1.49	0.97	0.25	0.17	0.03	0.03	0.70	0.98	0.804	1.237	1.194	0.375	0.633	0.414
10-heptadecenoate (17:1n7)	LC/MS neg	1.21	1.28	1.05	0.83	0.28	0.10	0.06	0.36	0.89	0.898	1.090	1.145	0.509	0.738	0.342
stearate (18:0)	LC/MS neg	1.2	1.25	1.04	0.53	0.23	0.11	0.06	0.59	0.92	0.938	1.123	1.171	0.294	0.441	0.367
oleate (18:1n9)	LC/MS neg	1.34	1.39	1.04	0.48	0.22	0.03	0.03	0.45	0.91	0.871	1.164	1.212	0.399	0.685	0.355
cis-vaccenate (18:1n7)	GC/MS	0.23	0.64	2.73	0.09	0.09	0.62	0.23	0.19	0.88	1.181	0.277	0.757	1.524	0.187	0.839
stearidonate (18:4n3)	LC/MS neg	2.42	2.38	0.98	0.07	0.07	0.01	0.01	0.57	0.92	0.511	1.237	1.215	0.511	1.221	0.599
nonadecanoate (19:0)	LC/MS neg	1.58	1.59	1.01	0.11	0.10	0.01	0.01	0.59	0.92	0.705	1.115	1.124	0.263	0.668	0.345
10-nonadecenoate (19:1n9)	LC/MS neg	1.61	1.37	0.85	0.50	0.22	0.05	0.04	0.57	0.92	0.909	1.461	1.248	0.712	1.338	0.419
eicosenoate (20:1n9 or 11)	LC/MS neg	1.72	1.39	0.81	0.45	0.21	0.08	0.05	0.70	0.98	0.980	1.686	1.365	0.655	1.755	0.575
dihomo-linoleate (20:2n6)	LC/MS neg	1.66	1.39	0.83	0.32	0.18	0.07	0.05	0.88	0.98	0.783	1.303	1.086	0.444	0.965	0.422
dihomo-alpha-linolenate (20:3n3)	LC/MS neg	1.3	1.48	1.14	0.42	0.21	0.01	0.01	0.29	0.88	0.870	1.128	1.290	0.284	0.545	0.359
arachidonate (20:4n6)	LC/MS neg	1.86	2.2	1.18	0.01	0.03	0.00	0.00	0.19	0.88	0.631	1.176	1.386	0.180	0.501	0.304
adrenate (22:4n6)	LC/MS neg	1.39	1.41	1.01	0.34	0.18	0.02	0.02	0.52	0.92	0.869	1.210	1.221	0.403	0.625	0.291
3-hydroxydecanoate	LC/MS neg	1.18	0.72	0.61	0.83	0.28	0.39	0.16	0.34	0.88	1.193	1.407	0.857	0.931	1.349	0.261
16-hydroxypalmitate	LC/MS neg	0.95	0.63	0.67	0.73	0.26	0.07	0.05	0.20	0.88	1.491	1.422	0.946	0.859	0.935	0.229

Supplemental Data Table 1 UNNM-01-12VW		Fold of Change			Statistical Values						Mean Values			Standard Deviation		
		CKD3 CKD2	CKD4 CKD2	CKD4 CKD3	CKD3 CKD2		CKD4 CKD2		CKD4 CKD3		CKD2	CKD3	CKD4	CKD2	CKD3	CKD4
					p-value	q-value	p-value	q-value	p-value	q-value						
Biochemical Name	Platform															
2-hydroxystearate	LC/MS neg	1.57	1.29	0.82	0.28	0.18	0.01	0.01	0.96	0.99	0.791	1.245	1.020	0.226	0.661	0.130
2-hydroxypalmitate	LC/MS neg	1.35	1.18	0.87	0.75	0.26	0.08	0.05	0.69	0.98	0.920	1.240	1.082	0.253	1.000	0.160
sebacate (decanedioate)	LC/MS pos	4.87	8.13	1.67	0.00	0.02	0.00	0.00	0.03	0.88	0.155	0.756	1.263	0.019	0.570	0.445
azelate (nonanedioate)	LC/MS neg	8.58	17.95	2.09	0.01	0.03	0.00	0.00	0.02	0.88	0.127	1.087	2.272	0.021	0.972	1.286
octadecanedioate	LC/MS neg	0.98	0.67	0.69	0.14	0.12	0.05	0.04	0.87	0.98	1.215	1.195	0.819	0.532	1.897	0.703
3-carboxy-4-methyl-5-propyl-2-furanpropanoate (CMPE)	LC/MS neg	18.28	23.58	1.29	0.06	0.07	0.00	0.00	0.17	0.88	0.307	5.608	7.234	0.279	11.864	7.195
oleamide	LC/MS pos	1.03	1.28	1.24	0.73	0.26	0.87	0.30	0.64	0.96	1.029	1.061	1.313	0.727	1.201	1.174
propionylcarnitine	LC/MS pos	0.86	0.81	0.95	0.36	0.19	0.21	0.11	0.72	0.98	1.126	0.968	0.917	0.418	0.336	0.376
butyrylcarnitine	LC/MS pos	0.49	0.38	0.76	0.02	0.04	0.00	0.00	0.86	0.98	2.492	1.229	0.936	1.803	1.319	0.774
isovalerate	LC/MS neg	2.03	2.43	1.2	0.01	0.03	0.00	0.00	0.16	0.88	0.481	0.975	1.168	0.148	0.421	0.211
carnitine	LC/MS pos	0.62	0.61	0.97	0.00	0.01	0.00	0.00	0.87	0.98	1.390	0.867	0.844	0.185	0.372	0.207
3-dehydrocarnitine*	LC/MS pos	1.08	1.53	1.41	0.52	0.23	0.13	0.07	0.26	0.88	1.023	1.105	1.563	0.469	0.409	1.167
acetylcarnitine	LC/MS pos	0.95	0.88	0.92	0.61	0.24	0.37	0.16	0.73	0.98	1.219	1.156	1.069	0.428	0.581	0.487
hexanoylcarnitine	LC/MS pos	0.88	0.97	1.1	0.58	0.24	0.95	0.32	0.52	0.92	1.234	1.085	1.194	0.791	0.549	0.507
octanoylcarnitine	LC/MS pos	0.88	0.84	0.96	0.91	0.29	0.97	0.32	0.85	0.98	1.369	1.201	1.151	1.279	0.769	0.663
decanoylcarnitine	LC/MS pos	0.71	0.62	0.87	0.54	0.23	0.30	0.14	0.63	0.96	1.712	1.216	1.056	1.794	0.696	0.583
laurylcarnitine	LC/MS pos	0.82	0.56	0.68	0.75	0.26	0.35	0.15	0.58	0.92	2.043	1.683	1.143	2.256	1.323	0.675
palmitoylcarnitine	LC/MS pos	0.93	0.55	0.59	0.50	0.22	0.02	0.02	0.19	0.88	1.511	1.412	0.837	0.746	1.112	0.386
oleoylcarnitine	LC/MS pos	0.87	0.66	0.76	0.33	0.18	0.11	0.07	0.76	0.98	1.749	1.514	1.147	1.334	1.525	0.959
cholate	LC/MS neg	0.55	1.4	2.54	0.62	0.25	0.89	0.30	0.55	0.92	2.633	1.454	3.696	4.482	2.108	6.210
glycocholate	LC/MS pos	1.96	0.13	0.07	0.45	0.21	0.01	0.01	0.14	0.88	4.207	8.244	0.549	4.058	20.881	0.310
taurocholate	LC/MS neg	14.75	0.36	0.02	0.58	0.24	0.05	0.04	0.15	0.88	1.346	19.863	0.491	1.163	44.588	0.189
taurochenodeoxycholate	LC/MS neg	12.48	0.19	0.01	0.83	0.28	0.04	0.03	0.29	0.88	2.078	25.940	0.386	2.057	62.115	0.351
ursodeoxycholate	LC/MS neg	1.23	1.12	0.91	0.68	0.26	0.83	0.29	0.85	0.98	1.016	1.250	1.138	0.452	1.606	1.089
hyodeoxycholate	LC/MS neg	0.24	0.36	1.51	0.00	0.00	0.00	0.00	0.07	0.88	2.681	0.641	0.967	1.772	0.549	0.596
glycochenodeoxycholate	LC/MS neg	2.92	0.11	0.04	0.20	0.14	0.00	0.00	0.21	0.88	12.067	35.263	1.339	12.006	99.211	1.991
glycolithocholate sulfate*	LC/MS neg	0.64	0.7	1.1	0.48	0.22	0.41	0.17	0.80	0.98	1.459	0.933	1.022	1.220	0.533	0.803
tauroolithocholate 3-sulfate	LC/MS neg	1.68	0.89	0.53	0.53	0.23	0.88	0.30	0.44	0.91	1.002	1.684	0.896	0.741	1.675	0.604
glycochenolate sulfate*	LC/MS neg	0.76	1.05	1.38	0.28	0.17	0.77	0.28	0.16	0.88	1.091	0.832	1.147	0.524	0.436	0.538
taurochenolate sulfate*	LC/MS neg	2.68	1.76	0.66	0.02	0.04	0.03	0.03	0.42	0.90	0.678	1.816	1.193	0.376	1.586	0.755
glycerol	GC/MS	0.74	0.79	1.06	0.03	0.05	0.08	0.05	0.83	0.98	1.153	0.856	0.906	0.290	0.331	0.375
choline	LC/MS pos	1.38	1.32	0.95	0.05	0.06	0.08	0.05	0.73	0.98	0.836	1.157	1.100	0.334	0.344	0.376

Supplemental Data Table 1 UNNM-01-12VW		Fold of Change			Statistical Values						Mean Values			Standard Deviation		
		CKD3 CKD2	CKD4 CKD2	CKD4 CKD3	CKD3 CKD2		CKD4 CKD2		CKD4 CKD3		CKD2	CKD3	CKD4	CKD2	CKD3	CKD4
					p-value	q-value	p-value	q-value	p-value	q-value						
Biochemical Name	Platform															
glycerol 3-phosphate (G3P)	GC/MS	1.36	1.76	1.29	0.06	0.07	0.00	0.00	0.04	0.88	0.791	1.080	1.395	0.221	0.385	0.297
glycerophosphorylcholine (GPC)	LC/MS pos	1.72	2.54	1.48	0.32	0.18	0.00	0.00	0.08	0.88	0.557	0.959	1.416	0.254	0.974	0.835
myo-inositol	GC/MS	2.27	2.01	0.89	0.03	0.05	0.01	0.01	0.98	0.99	0.810	1.841	1.631	0.340	1.671	1.157
scyllo-inositol	GC/MS	1.97	1.27	0.64	0.15	0.12	0.34	0.15	0.45	0.91	0.586	1.156	0.742	0.335	1.214	0.467
3-hydroxybutyrate (BHBA)	GC/MS	1.56	1.3	0.84	0.36	0.19	0.34	0.15	0.96	0.99	1.258	1.958	1.641	1.174	2.082	1.290
1-oleoylglycerophosphoethanolamine	LC/MS neg	0.69	0.46	0.66	0.09	0.09	0.01	0.01	0.40	0.90	1.702	1.172	0.779	0.943	1.106	0.422
1-linoleoylglycerophosphoethanolamine*	LC/MS neg	0.66	0.61	0.93	0.04	0.05	0.02	0.02	0.82	0.98	1.534	1.012	0.940	0.742	0.560	0.397
1-arachidonoylglycerophosphoethanolamine*	LC/MS neg	0.83	0.93	1.12	0.15	0.12	0.49	0.20	0.40	0.90	1.104	0.912	1.025	0.288	0.294	0.302
2-arachidonoylglycerophosphoethanolamine*	LC/MS neg	0.74	0.95	1.29	0.06	0.07	0.55	0.21	0.36	0.89	1.061	0.783	1.008	0.367	0.277	0.528
1-myristoylglycerophosphocholine	LC/MS pos	0.53	0.46	0.86	0.03	0.05	0.01	0.01	0.89	0.98	1.741	0.931	0.805	0.785	0.651	0.492
1-palmitoylglycerophosphocholine	LC/MS pos	0.73	0.69	0.94	0.01	0.03	0.00	0.00	0.78	0.98	1.266	0.923	0.870	0.241	0.287	0.194
2-palmitoylglycerophosphocholine*	LC/MS pos	0.56	0.53	0.95	0.00	0.01	0.00	0.00	0.82	0.98	1.519	0.843	0.802	0.378	0.431	0.428
1-palmitoleoylglycerophosphocholine*	LC/MS pos	0.33	0.36	1.11	0.01	0.03	0.04	0.03	0.51	0.92	2.690	0.882	0.976	1.815	1.057	0.668
1-heptadecanoylglycerophosphocholine	LC/MS pos	0.87	0.55	0.63	0.52	0.23	0.01	0.01	0.02	0.88	1.349	1.173	0.741	0.536	0.545	0.255
1-stearoylglycerophosphocholine	LC/MS pos	0.88	0.75	0.85	0.29	0.18	0.05	0.04	0.58	0.92	1.243	1.096	0.928	0.328	0.544	0.359
2-stearoylglycerophosphocholine*	LC/MS pos	0.67	0.61	0.91	0.11	0.10	0.05	0.04	0.71	0.98	1.426	0.956	0.869	0.703	0.609	0.591
1-oleoylglycerophosphocholine	LC/MS pos	0.6	0.57	0.95	0.03	0.04	0.02	0.02	0.84	0.98	1.591	0.962	0.911	0.635	0.440	0.351
2-oleoylglycerophosphocholine*	LC/MS pos	0.58	0.43	0.73	0.01	0.03	0.00	0.00	0.33	0.88	1.764	1.030	0.756	0.714	0.628	0.269
1-linoleoylglycerophosphocholine	LC/MS pos	0.75	0.68	0.91	0.03	0.04	0.00	0.01	0.52	0.92	1.270	0.948	0.866	0.323	0.259	0.232
1-eicosatrienoylglycerophosphocholine*	LC/MS pos	0.69	0.75	1.1	0.18	0.13	0.35	0.15	0.50	0.92	1.457	1.004	1.100	0.768	0.474	0.422
1-arachidonoylglycerophosphocholine*	LC/MS pos	1.26	1.47	1.17	0.68	0.26	0.01	0.01	0.23	0.88	0.905	1.139	1.333	0.227	0.613	0.394
1-docosahexaenoylglycerophosphocholine*	LC/MS pos	1.18	1.46	1.23	0.21	0.14	0.00	0.01	0.11	0.88	0.863	1.019	1.256	0.163	0.284	0.341
1-palmitoylglycerol (1-monopalmitin)	GC/MS	0.67	0.43	0.64	0.21	0.15	0.01	0.01	0.09	0.88	1.287	0.866	0.556	0.793	0.532	0.188
1-linoleoylglycerol (1-monolinolein)	LC/MS neg	4.79	6.73	1.41	0.00	0.00	0.00	0.00	0.09	0.88	0.310	1.481	2.084	0.193	0.923	0.762
stearoyl sphingomyelin	GC/MS	2.14	2.07	0.96	0.34	0.18	0.29	0.14	0.97	0.99	0.574	1.232	1.187	0.416	1.097	1.034
lathosterol	GC/MS	1.14	0.82	0.72	0.65	0.25	0.53	0.21	0.28	0.88	0.524	0.596	0.428	0.386	0.409	0.201
cholesterol	GC/MS	1.03	1.01	0.97	1.00	0.31	0.98	0.32	0.99	0.99	1.017	1.051	1.022	0.160	0.328	0.210
dehydroisoandrosterone sulfate (DHEA-S)	LC/MS neg	0.87	0.55	0.64	0.32	0.18	0.04	0.03	0.52	0.92	1.478	1.280	0.819	0.878	0.933	0.685
epiandrosterone sulfate	LC/MS neg	0.51	0.77	1.5	0.06	0.07	0.15	0.08	0.94	0.99	1.594	0.819	1.232	1.022	0.481	1.267
androsterone sulfate	LC/MS neg	0.45	0.53	1.18	0.05	0.07	0.06	0.05	0.95	0.99	2.135	0.956	1.124	1.846	0.709	1.180
cortisol	LC/MS pos	0.68	0.62	0.9	0.10	0.09	0.03	0.03	0.79	0.98	1.449	0.992	0.894	0.718	0.469	0.379
cortisone	LC/MS pos	0.86	0.59	0.69	0.20	0.14	0.00	0.01	0.08	0.88	1.059	0.907	0.628	0.203	0.320	0.276
7-alpha-hydroxy-3-oxo-4-cholestenoate (7-Hoca)	LC/MS neg	0.78	0.86	1.09	0.30	0.18	0.43	0.18	0.86	0.98	1.550	1.214	1.326	1.084	1.102	1.122

Supplemental Data Table 1 UNNM-01-12VW		Fold of Change			Statistical Values						Mean Values			Standard Deviation		
		CKD3 CKD2	CKD4 CKD2	CKD4 CKD3	CKD3 CKD2		CKD4 CKD2		CKD4 CKD3		CKD2	CKD3	CKD4	CKD2	CKD3	CKD4
					p-value	q-value	p-value	q-value	p-value	q-value						
Biochemical Name	Platform															
4-androsten-3beta,17beta-diol disulfate 1*	LC/MS neg	0.55	0.26	0.47	0.09	0.09	0.01	0.01	0.54	0.92	3.909	2.164	1.020	3.756	3.462	0.958
4-androsten-3beta,17beta-diol disulfate 2*	LC/MS neg	0.97	0.54	0.55	0.52	0.23	0.01	0.01	0.11	0.88	1.254	1.219	0.675	0.535	0.802	0.452
5alpha-androstan-3beta,17beta-diol disulfate	LC/MS neg	0.39	0.27	0.7	0.02	0.04	0.00	0.00	0.42	0.90	2.602	1.008	0.710	1.989	1.040	0.848
pregnen-diol disulfate*	LC/MS neg	0.67	0.34	0.5	0.17	0.13	0.00	0.00	0.13	0.88	2.035	1.360	0.682	1.725	1.112	0.483
xanthine	LC/MS pos	2.37	4.27	1.8	0.04	0.06	0.00	0.01	0.18	0.88	0.502	1.189	2.146	0.118	1.196	2.334
hypoxanthine	LC/MS neg	1.01	1.03	1.02	0.34	0.18	0.26	0.13	0.48	0.92	0.938	0.947	0.964	0.000	0.026	0.068
inosine	LC/MS neg	2.91	4.72	1.62	0.02	0.04	0.00	0.00	0.14	0.88	0.300	0.873	1.416	0.000	0.817	0.931
N1-methyladenosine	LC/MS pos	0.93	0.78	0.84	0.38	0.19	0.02	0.02	0.39	0.90	1.087	1.013	0.851	0.202	0.422	0.216
adenosine 5'-monophosphate (AMP)	LC/MS pos	0.55	0.54	0.98	0.02	0.04	0.02	0.02	0.34	0.88	1.350	0.742	0.729	0.964	0.039	0.000
guanosine	LC/MS neg	1.52	2	1.32	0.06	0.07	0.01	0.01	0.22	0.88	0.505	0.765	1.007	0.000	0.436	0.492
urate	LC/MS neg	1.11	1.06	0.95	0.28	0.17	0.44	0.18	0.64	0.96	0.978	1.085	1.034	0.191	0.221	0.161
uridine	LC/MS neg	1.05	1.31	1.25	0.75	0.26	0.04	0.03	0.07	0.88	0.906	0.948	1.184	0.289	0.258	0.238
pseudouridine	LC/MS neg	1.48	1.64	1.11	0.11	0.10	0.07	0.05	0.76	0.98	0.946	1.403	1.554	0.256	0.993	1.274
ascorbate (Vitamin C)	GC/MS	7.15	11.46	1.6	0.00	0.01	0.00	0.00	0.19	0.88	0.114	0.811	1.301	0.000	0.668	0.999
threonate	GC/MS	2.65	3.27	1.23	0.03	0.04	0.00	0.00	0.18	0.88	0.453	1.203	1.483	0.296	0.711	0.439
heme	LC/MS pos	0.34	0.1	0.3	0.01	0.03	0.00	0.00	0.23	0.88	5.139	1.747	0.529	4.173	2.381	0.492
bilirubin (Z,Z)	LC/MS neg	2.01	1.43	0.71	0.33	0.18	0.08	0.05	0.97	0.99	0.901	1.814	1.291	0.312	1.979	0.521
bilirubin (E,E)*	LC/MS neg	1.29	1.07	0.83	0.72	0.26	0.57	0.22	0.97	0.99	1.058	1.368	1.129	0.428	0.848	0.353
bilirubin (E,Z or Z,E)*	LC/MS pos	1.02	0.74	0.73	0.44	0.21	0.25	0.12	0.87	0.98	1.288	1.319	0.958	0.862	1.312	0.458
biliverdin	LC/MS pos	0.92	0.33	0.36	0.14	0.12	0.00	0.00	0.62	0.95	1.729	1.595	0.568	1.245	1.879	0.295
nicotinamide	LC/MS pos	0.86	0.65	0.76	0.37	0.19	0.04	0.03	0.35	0.88	1.240	1.064	0.810	0.539	0.594	0.408
pantothenate	LC/MS pos	0.95	1.44	1.52	0.73	0.26	0.47	0.19	0.34	0.88	0.847	0.804	1.220	0.407	0.472	1.031
alpha-tocopherol	GC/MS	1.31	1.79	1.36	0.16	0.12	0.03	0.03	0.03	0.88	0.782	1.026	1.397	0.428	0.331	0.472
gamma-tocopherol	GC/MS	1.02	1.81	1.77	0.82	0.28	0.04	0.03	0.05	0.88	0.502	0.512	0.908	0.059	0.089	0.552
pyridoxate	LC/MS neg	1.55	1.81	1.17	0.59	0.24	0.01	0.01	0.14	0.88	0.818	1.270	1.485	0.525	1.797	0.753
hippurate	LC/MS neg	2.88	1.62	0.56	0.34	0.18	0.92	0.31	0.42	0.90	1.092	3.145	1.765	0.936	5.985	3.096
2-hydroxyhippurate (salicylurate)	LC/MS neg	1.11	4.34	3.92	0.84	0.28	0.34	0.15	0.42	0.90	0.524	0.581	2.275	0.437	0.508	5.448
catechol sulfate	LC/MS neg	1.44	1.24	0.86	0.78	0.27	0.29	0.14	0.48	0.92	1.089	1.573	1.352	1.007	2.604	0.806
4-vinylphenol sulfate	LC/MS neg	1.32	2.18	1.65	0.92	0.29	0.25	0.12	0.34	0.88	1.059	1.403	2.310	0.788	1.524	2.576
glycolate (hydroxyacetate)	GC/MS	0.85	0.83	0.98	0.18	0.13	0.12	0.07	0.81	0.98	0.850	0.721	0.706	0.247	0.139	0.096
iminodiacetate (IDA)	GC/MS	0.32	0.15	0.45	0.00	0.00	0.00	0.00	0.20	0.88	4.452	1.439	0.655	2.340	1.630	0.266
salicylate	LC/MS neg	0.46	0.63	1.38	0.70	0.26	0.61	0.23	0.28	0.88	1.509	0.692	0.958	3.378	0.873	0.736
salicyluric glucuronide*	LC/MS neg	1.72	4.67	2.71	0.33	0.18	0.18	0.09	0.49	0.92	0.397	0.684	1.855	0.248	0.890	3.931

Supplemental Data Table 1 UNNM-01-12VW		Fold of Change			Statistical Values						Mean Values			Standard Deviation		
		CKD3 CKD2	CKD4 CKD2	CKD4 CKD3	CKD3 CKD2		CKD4 CKD2		CKD4 CKD3		CKD2	CKD3	CKD4	CKD2	CKD3	CKD4
					p-value	q-value	p-value	q-value	p-value	q-value						
Biochemical Name	Platform															
4-acetamidophenol	LC/MS pos	1.37	1.24	0.91	0.69	0.26	0.85	0.29	0.84	0.98	0.414	0.568	0.514	0.281	0.607	0.605
p-acetamidophenylglucuronide	LC/MS neg	1.61	1.32	0.82	0.40	0.20	0.37	0.16	0.91	0.99	0.387	0.624	0.510	0.192	0.733	0.363
2-propylpentanoate (valproate)	LC/MS neg	2.32	2.29	0.98	0.00	0.00	0.00	0.00	0.91	0.99	0.541	1.257	1.238	0.251	0.561	0.394
pioglitazone*	LC/MS pos	1	1	1							1.000	1.000	1.000	0.000	0.000	0.000
hydroxypioglitazone*	LC/MS pos	1	1	1							1.000	1.000	1.000	0.000	0.000	0.000
naproxen	GC/MS	1	1	1							1.000	1.000	1.000	0.000	0.000	0.000
metformin	LC/MS pos	1	1	1							1.000	1.000	1.000	0.000	0.000	0.000
metoprolol	LC/MS pos	1	2.04	2.04			0.17	0.09	0.17	0.88	0.190	0.190	0.388	0.000	0.000	0.427
metoprolol acid metabolite*	LC/MS pos	9.28	64.82	6.98	0.29	0.18	0.16	0.09	0.48	0.92	0.454	4.216	29.440	0.046	11.746	75.934
hydrochlorothiazide	LC/MS neg	1	1	1							1.000	1.000	1.000	0.000	0.000	0.000
EDTA	LC/MS neg	0.67	0.55	0.83	0.00	0.02	0.00	0.00	0.17	0.88	0.933	0.621	0.514	0.232	0.227	0.000
quininate	GC/MS	1.25	3.03	2.42	0.74	0.26	0.12	0.07	0.21	0.88	0.451	0.564	1.368	0.267	0.517	2.202
piperine	LC/MS pos	2.65	3.61	1.36	0.04	0.06	0.01	0.01	0.43	0.91	0.460	1.217	1.658	0.459	0.830	1.495
thymol sulfate	LC/MS neg	1.03	2.46	2.38	0.75	0.26	0.51	0.20	0.37	0.90	0.925	0.957	2.278	0.981	1.295	3.941
N-(2-furoyl)glycine	LC/MS neg	0.76	0.75	0.98	0.59	0.24	0.55	0.21	0.92	0.99	0.770	0.585	0.576	0.746	0.163	0.132
stachydrine	LC/MS pos	2.07	0.58	0.28	0.36	0.19	0.95	0.32	0.26	0.88	2.383	4.932	1.384	3.495	8.117	1.796
homostachydrine*	LC/MS pos	0.86	0.72	0.83	0.45	0.21	0.08	0.05	0.27	0.88	1.206	1.043	0.867	0.463	0.380	0.299
caffeine	LC/MS pos	0.92	0.17	0.19	0.17	0.13	0.00	0.00	0.29	0.88	3.474	3.202	0.606	2.179	4.686	0.319
paraxanthine	LC/MS pos	0.78	0.37	0.48	0.29	0.18	0.03	0.03	0.38	0.90	1.693	1.318	0.626	1.165	1.723	0.341
theobromine	LC/MS pos	0.45	0.36	0.81	0.21	0.14	0.14	0.08	0.82	0.98	2.499	1.125	0.908	2.701	0.962	0.473
theophylline	LC/MS pos	0.85	0.54	0.63	0.56	0.23	0.07	0.05	0.24	0.88	1.348	1.150	0.727	0.816	0.859	0.255
1-methylurate	LC/MS pos	2.05	0.94	0.46	0.50	0.22	0.74	0.27	0.38	0.90	0.652	1.336	0.613	0.321	2.258	0.342
1,7-dimethylurate	LC/MS pos	1.51	0.79	0.52	0.70	0.26	0.10	0.06	0.24	0.88	0.701	1.059	0.553	0.264	1.442	0.000
1-methylxanthine	LC/MS pos	1.03	1	0.97	0.86	0.28	0.89	0.30	0.95	0.99	0.749	0.774	0.749	0.163	0.418	0.237
3-methylxanthine	LC/MS pos	0.87	0.7	0.8	0.40	0.20	0.38	0.16	0.87	0.98	0.836	0.729	0.586	0.652	0.931	0.218
5-acetylamino-6-amino-3-methyluracil	LC/MS neg	1.8	1	0.55	0.34	0.18			0.34	0.88	0.199	0.360	0.199	0.000	0.506	0.000
cotinine	LC/MS pos	1	1.05	1.05			0.34	0.15	0.34	0.88	0.785	0.785	0.828	0.000	0.000	0.136
erythritol	GC/MS	1.53	1.55	1.02	0.29	0.18	0.15	0.08	0.80	0.98	0.986	1.508	1.533	0.376	1.390	1.228

