

## **SUPPLEMENTAL MATERIAL**

<b>Table S1. Targeted panel of metabolites</b>	
MDC ID	Compound name
0125_Ribulose 5-phosphate	Ribulose 5-phosphate sodium salt
0108_ADP / 0273_3,5-ADP	Adenosine diphosphate
0243_IDP	Inosine 5-diphosphate
0132_IMP	2-Inosine-5-monophosphate / Inosinic acid
0154_O-Phosphoethanolamine	O-Phosphoethanolamine
0179_Glucosamine 6-phosphate	D-GLUCOSAMINE 6-PHOSPHATE
0147_Gluconic acid	GLUCONATE
0246_Nicotinamide hypoxanthine dinucleotide	NICOTINAMIDE HYPOXANTHINE DINUCLEOTIDE
0192_Ciliatine	(2-AMINOETHYL)PHOSPHONATE
0159_Tartaric acid	Tartaric acid
0367_Sn-Glycero-3-phosphocholine	SN-GLYCERO-3-PHOSPHOCHOLINE
0191_Glucuronolactone	D-GLUCURONOLACTONE
0200_Galactitol	GALACTITOL
0020_Citicoline	Cytidine 5-Diphosphocholine / Citicoline / Choline 5-cytidine diphosphate
0312_Glucosaminic acid	GLUCOSAMINATE
0341_Methionine sulfoximine	METHIONINE SULFOXIMINE
0048_4-Hydroxyproline	4-Hydroxy-L-Proline
0149_Dihydroorotic acid	Dihydroorotic acid
0028_Cystine	Cystine
0013_Aspartic acid	Aspartic acid
0223_N-Methylaspartic acid	N-METHYL-D-ASPARTIC ACID
0017_2,3-cyclic CMP	Cytidine 2,3-Cyclic Monophosphate / 2,3-Cyclic CMP
0168_Thiourea	Thiourea
0092_Orotic acid	Orotic acid
0012_Aspargine	L-Asparagine
0068_Serine	Serine
0038_Glutamine	Glutamine
0160_Nicotinamide mononucleotide	Nicotinamide mononucleotide
0234_Nalpha-Acetylasparagine	N-ALPHA-ACETYL-L-ASPARAGINE
0026_Cystathionine	Cystathionine
0098_Homoserine	Homoserine
0057_Methionine Sulfoxide	Methionine sulfoxide
0070_Threonine / 0359_Allothreonine	Threonine/Allothreonine

0322_S-Carboxymethylcysteine	S-CARBOXYMETHYL-L-CYSTEINE
0183_Betaine	BETAINE
0226_N-methylglutamic Acid	N-METHYL-L-GLUTAMATE
0378_N-Acetylserine	N-ACETYL-DL-SERINE
0039_Glutamic acid	Glutamic acid
0073_TMP	Thymidine 5'-monophosphate / 5-Thymidylic acid
0021_Citrulline	Citrulline
0158_dCMP	2-Deoxycytidine 5-monophosphate
0064_Proline	Proline
0336_3-Ureidopropionic acid	3-UREIDOPROPIONATE
0008_Alanine	Alanine
0146_Sarcosine	Sarcosine
0302_C6_sugar_amine	C6 sugar amine
0076_Uracil	Uracil
0370_Trigonelline	TRIGONELLINE
0242_N-Acetylaspartic acid	N-AMIDINO-L-ASPARTATE
0369_2,3-Diaminopropionic acid	DL-2,3-Diaminopropionic acid monohydrochloride
0091_NAD	Nicotinamide adenine dinucleotide
0358_5-Hydroxylysine	DL-5-HYDROXYLYSINE
0321_Orthanilic acid	ANILINE-2-SULFONIC ACID
0143_Beta-Alanine	Beta-Alanine
0201_5-Oxoproline	5-OXO-D-PROLINE
0164_dAMP	Deoxyadenosine monophosphate
0023_Creatine	Creatine
0364_Citramalic acid	CITRAMALATE
0097_Xanthine	Xanthine
0061_Ornithine	Ornithine
0044_Histidine	Histidine
0371_3,4-Dihydroxyphenylglycol	3,4-DIHYDROXYPHENYL GLYCOL
0085_Fumaric acid	Fumaric acid
0055_Lysine	Lysine
0049_Hypoxanthine	Hypoxanthine / 6-Hydroxypurine
0325_N-Acetylglutamic acid	N-ACETYL-DL-GLUTAMIC ACID
0059_Nicotinic acid	Nicotinic acid
0077_Uridine	Uridine
0373_2-Hydroxybutyric acid	2-HYDROXYBUTYRIC ACID
0036_Gamma-aminobutyric acid	Gamma-aminobutyric acid / 4-aminobutanoic acid
0140_Pipecolic acid	Pipecolic acid

0018_3,5-cyclic GMP	Guanosine 3,5-Cyclic Monophosphate / 3,5-Cyclic GMP
0253_2,3-cyclic AMP	ADENOSINE 2,3-CYCLIC MONOPHOSPHATE
0030_Cytosine	Cytosine
0006_Adenylsuccinic acid	Adenylosuccinic acid / Adenylsuccinic acid
0204_Methylguanidine	METHYLGUANIDINE
0221_3-Hydroxymethylglutaric acid	3-HYDROXY-3-METHYLGLUTARATE
0346_4-Imidazoleacetic acid	4-IMIDAZOLEACETIC ACID
0047_Homocystine	Homocystine
0404_Maleic acid	MALEIC ACID
0438_2-Hydroxypyridine	2-HYDROXYPYRIDINE
0305_Thiamine monophosphate	THIAMINE MONOPHOSPHATE
0010_Arginine	Arginine
0170_3-Aminoisobutanoic acid	3-Aminoisobutanoic acid
0060_Ophthalmic acid	Ophthalmic acid
0211_4-Acetamidobutanoic acid	4-ACETAMIDOBUTANOATE
0014_3,5-cyclic AMP	Adenosine 3,5-Cyclic Monophosphate / 3,5-Cyclic AMP
0058_Nicotinamide	Nicotinamide
0461_Pterin	PTERIN
0051_Inosine	Inosine
0133_Purine	Purine
0056_Methionine	Methionine
0267_N-Alpha-acetyllysine	NALPHA-ACETYL-L-LYSINE
0024_Creatinine	Creatinine
0015_Carnitine	Carnitine
0189_O-Succinylhomoserine	O-SUCCINY-L-L-HOMOSERINE
0327_6-Hydroxynicotinic acid	6-HYDROXYNICOTINATE
0491_Itaconic acid	ITACONATE
0086_Glutathione oxidized	Glutathione oxidized / Glutathione disulfide
0512_Vanillylmandelic acid	3-METHOXY-4-HYDROXYMANDELATE
0043_Guanosine	Guanosine
0259_5-Methylcytosine	5-METHYLCYTOSINE HYDROCHLORIDE
0283_2-Deoxyguanosine	2-DEOXYGUANOSINE
0029_Cytidine	Cytidine
0071_Thymidine	Thymidine
0323_N-Acetylputrescine	N-ACETYLPUTRESCINE
0337_5-Aminopentanoic acid	5-AMINOPENTANOATE
0514_4-Quinolinecarboxylic acid	4-QUINOLINECARBOXYLIC ACID

0062_Pantothenic acid	Pantothenic acid
0202_4-Pyridoxic acid	4-PYRIDOXATE
0293_Indoxyl sulfate	INDOXYL SULFATE
0462_Ethylmalonic acid	ETHYLMALONIC ACID
0193_Selenomethionine	SELENOMETHIONINE
0278_Pyridoxamine	PYRIDOXAMINE
0351_Theobromine	THEOBROMINE
0426_Desmeninol	2-HYDROXY-4-(METHYLTHIO)BUTYRIC ACID
0178_2-Deoxycytidine	DEOXYCYTIDINE
0266_Octopamine	OCTOPAMINE
0004_Adenine	Adenine
0005_Adenosine	Adenosine
0205_1-Methyladenosine	1-METHYLADENOSINE
0442_Protocatechuic acid	3,4-DIHYDROXYBENZOATE
0194_Paraxanthine	PARAXANTHINE
0532_Hydroxyphenyllactic acid	3-(4-HYDROXYPHENYL)LACTATE
0075_Tyrosine	Tyrosine
0209_Urocanic acid	UROCANATE
0381_3-Hydroxykynurenine	3-HYDROXYKYNURENINE
0286_N-Acetylmethionine	N-ACETYL-DL-METHIONINE
0469_4-Aminobenzoic acid	4-AMINOBENZOATE
0531_3-Methyladenine	3-METHYLADENINE
0516_Pyridoxal	PYRIDOXAL
0034_Epinephrine	Epinephrine / Adrenaline
0536_Pyrrole-2-carboxylic acid	PYRROLE-2-CARBOXYLATE
0460_2-Quinolinecarboxylic acid	2-QUINOLINECARBOXYLIC ACID
0343_3-Methoxytyrosine	3-METHOXY-L-TYROSINE
0412_Pimelic acid	6-CARBOXYHEXANOATE
0533_Biotin	BIOTIN
0425_Thiopurine S-methylether	THIOPURINE S-METHYLETHER
0195_Caffeine	CAFFEINE
0421_Caffeic acid	CAFFEATE
0537_5-Hydroxyindoleacetic acid	5-HYDROXYINDOLEACETATE
0050_Isoleucine	Isoleucine
0459_Hippuric acid	HIPPURATE
0489_N-Acetylserotonin	N-ACETYLSEROTONIN
0481_Gentisic acid	2,5-DIHYDROXYBENZOATE

0525_3-Hydroxyphenylacetic acid	3-HYDROXYPHENYLACETATE
0349_5-Hydroxytryptophan	5-HYDROXY-L-TRYPTOPHAN
0229_Thyrotropin releasing hormone	THYROTROPIN RELEASING HORMONE
0163_Pyridoxine	Pyridoxine
0487_Dethiobiotin	DETHIOBIOTIN
0007_ADMA / 0067_SDMA Dimethylarginine	Dimethylarginine
0416_Mandelic acid	MANDELIC ACID
0053_Leucine	Leucine
0318_5-Deoxyadenosine	5-DEOXYADENOSINE
0295_Normetanephrine	DL-NORMETANEPHRINE
0503_N-Acetylleucine	N-ACETYL-L-LEUCINE
0338_Norleucine	NORLEUCINE
0493_Suberic acid	SUBERIC ACID
0430_2-Pyrocatechuic acid	2,3-DIHYDROXYBENZOATE
0410_Kynurenic acid	4-HYDROXY-2-QUINOLINECARBOXYLIC ACID
0033_Dopamine	Hydroxytyramine / Dopamine
0388_Xanthurenic acid	XANTHURENIC ACID
0473_2-Aminophenol	2-AMINOPHENOL
0450_3-Indoleacetamide	INDOLE-3-ACETAMIDE
0274_3-Nitrotyrosine	3-NITRO-L-TYROSINE
0506_Salicylamide	SALICYLAMIDE
0413_N-Acetylphenylalanine	N-ACETYL-L-PHENYLALANINE
0063_Phenylalanine	Phenylalanine
0466_Melilotic acid	3-(2-HYDROXYPHENYL)PROPANOATE
0479_Anthranilic acid	ANTHRANILATE
0433_Ferulic acid	FERULATE
0422_Lumichrome	LUMICHROME
0505_Salsolinol	1-METHYL-6,7-DIHYDROXY-1,2,3,4-TETRAHYDROISOQUINOLINE
0173_N-acetyltryptophan	N-acetyl-D-tryptophan
0052_Kynurenine	Kynurenine
0482_Azelaic acid	AZELAIC ACID
0420_Indoleacetic acid	N-ACETYL-L-ASPARTIC ACID
0395_Tyramine	TYRAMINE
0403_Melatonin	MELATONIN
0356_Guanidinosuccinic acid	INDOLE-3-ACETATE
0432_Indole-3-ethanol	INDOLE-3-ETHANOL
0436_10-Hydroxydecanoic acid C10:0(OH)	10-HYDROXYDECANOATE

0396_Cortisol	CORTISOL
0467_3-Methoxytyramine	3-METHOXYTYRAMINE
0069_Serotonin	Serotonin
0454_Lipoamide	LIPOAMIDE
0415_3,5-Diiodotyrosine	3,5-DIIODO-L-TYROSINE
0074_Tryptophan	Tryptophan
0434_Glycocholic acid	GLYCOCHOLATE
0423_Tryptophanamide	L-TRYPTOPHANAMIDE
0307_S-Hexylglutathione	S-HEXYL-GLUTATHIONE
0449_Hydrocortisone 21-acetate	CORTISOL 21-ACETATE
0463_3,5-Diiodothyronine	3,5-DIIODO-L-THYRONINE
MDC= Molecular Determinants Core	

**Table S2. Top 20 metabolites (or features) contributing to the first 6 dimensions of PC analysis**

<b>PC1</b>	<b>PC2</b>	<b>PC3</b>
t1 Phenylalanine	t2 Serine	t3 Leucine
t1 Proline	r32 4-Hydroxyproline	t3 Serine
cum Histidine	t2 Phenylalanine	t3 Phenylalanine
t1 Histidine	r32 Serine	t3 Lysine
t1 Isoleucine	r32 Histidine	t3 Histidine
t1 Serine	r32 Alanine	t3 Isoleucine
t1 Lysine	r32 Glutamine	t3 Proline
t1 Leucine	r32 Tyrosine	t3 Tyrosine
t1 Methionine Sulfoxide	r32 N-Acetylserine	t3 Methionine Sulfoxide
cum Methionine	t2 Histidine	t3 Glutamine
t1 Arginine	t2 Lysine	r31 Proline
cum Lysine	r32 Proline	t3 Alanine
t1 Alanine	r32 Cystine	t3 Methionine
t1 Methionine	t2 Tyrosine	r31 Alanine
cum Methionine Sulfoxide	r32_ Tryptophan	t3 4-Hydroxyproline
t1 5-Oxoproline	r32 Phenylalanine	r31 Phenylalanine
t1 Tyrosine	t2 Glutamine	t3 5-Oxoproline
t1 Tryptophan	t2 Alanine	r31 Isoleucine
cum Alanine	r32 Sn-Glycero-3-phosph	r31 Methionine



cum Phenylalanine

r32 Ornithine

r31 Glutamine

**PC4**

**PC5**

**PC6**

r21 Lysine

r32 Paraxanthine

Cum 3-Methoxytyrosine

r31 Lysine

r32 Isoleucine

t1 Asparagine

r31 Ornithine

r32 Leucine

t2 3-Methoxytyrosine

r21 5-Oxoproline

r32 Methionine

r31 Galactitol

r31 Histidine

r32 Phenylalanine

Cum Glutamic acid

r21 Histidine

r32 Tryptophan

Cum Cystine

r21 Ornithine

r32 2,3-Diaminopropioni

Cum Glutamine

r31 5-Oxoproline

r325-Oxoproline

Cum Asparagine

r31 Arginine

r32 Glutamic acid

t3 3-Methoxytyrosine

r21 Arginine

r32 Hippuric acid

t1 3-Methoxytyrosine

r31 Creatinine

r32 Sn-Glycero-3-phosph

r21 Gluconic acid

r21 Carnitine

r32 Proline

r21 Galactitol

r21 Creatinine

r32 Tyrosine

Cum 4-Hydroxyproline

t2 Caffeine

r32 Histidine

r31 Gluconic acid

t2 Paraxanthine

r32 Indoxyl sulfate

t2 Glutamic acid

Cum Paraxanthine

t3 Serine

t1 Ornithine

r31 Carnitine

t3 Glutamine

t1 4-Hydroxyproline

Cum Caffeine

t2 Sn-Glycero-3-phosphocho

t1 Cystine

t3 Caffeine

r32 Galactitol

t2 Cystine

t1 Paraxanthine

Cum Sn-Glycero-3-phosph

t1 Leucine

*Abbreviations: t1 – time point one, immediate pre-op; t2 – time point 2, immediate post-op; t3 – time point 3, 12 hours post op; r21 – ratio of t2 to t1; r31 – ratio of t3 to t1; r32 – ratio of t3 to t2; cum – cumulative values from t1, t2, t3.*

**Table S3. Association between principal components loads and outcomes**

<b>Composite- mortality/morbidity</b>						
<b>Parameter</b>	<b>Estimate</b>	<b>SE</b>	<b>OR</b>	<b>LCL</b>	<b>UCL</b>	<b>p-value</b>
Site = 2	2.5713	0.5524	13.0828	4.4186	38.7359	<.001
PGE ever = 0	-2.3215	0.6667	0.0981	0.0265	0.3637	0.001
STAT category	0.7071	0.2868	2.0281	1.1544	3.5632	0.01
Pre-surgery lactate	0.8811	0.5812	2.4136	0.7703	7.5622	0.13
Gestational age birth	-0.2656	0.209	0.7667	0.5085	1.1561	0.20
PC1	0.194	0.0489	1.2141	1.1029	1.3365	<.001
<b>Composite - cardiac</b>						
<b>Parameter</b>	<b>Estimate</b>	<b>SE</b>	<b>OR</b>	<b>LCL</b>	<b>UCL</b>	<b>p-value</b>
Site = 2	1.7387	0.5087	5.6899	2.0941	15.4606	0.001
PGE ever = 0	-1.1979	0.6765	0.3018	0.0799	1.1404	0.08
STAT category	0.7343	0.3098	2.084	1.1338	3.8307	0.02
Pre-surgery lactate	1.3524	0.5839	3.8667	1.2276	12.1796	0.02
Gestational age birth	-0.1182	0.2149	0.8885	0.5825	1.3554	0.58
PC1	0.1429	0.0448	1.1536	1.0564	1.2598	0.001
<b>Hepatic</b>						
<b>Parameter</b>	<b>Estimate</b>	<b>SE</b>	<b>OR</b>	<b>LCL</b>	<b>UCL</b>	<b>p-value</b>
Site = 2	1.7943	0.5538	6.0153	2.026	17.8592	0.001
PGE ever = 0	-2.5462	0.6967	0.0784	0.0199	0.3081	<.001
STAT category	0.9034	0.331	2.468	1.2879	4.7295	0.006
Pre-surgery lactate	-0.0927	0.6245	0.9115	0.2672	3.1094	0.88
Gestational age birth	-0.3044	0.2312	0.7376	0.4683	1.1617	0.19
PC1	0.2454	0.0556	1.2781	1.1458	1.4257	<.001
<b>Lactate</b>						

Parameter	Estimate	SE	OR	LCL	UCL	p-value
Site = 2	1.5581	0.5362	4.7498	1.6561	13.6226	0.004
PGE ever = 0	-1.2537	0.733	0.2854	0.0676	1.2052	0.09
STAT category	1.0129	0.3706	2.7536	1.3293	5.7038	0.006
Pre-surgery lactate	1.4959	0.6119	4.4634	1.3411	14.8542	0.01
Gestational age birth	-0.1564	0.238	0.8552	0.5358	1.3652	0.51
PC1	0.124	0.045	1.132	1.0362	1.2367	0.006

### AKI

Parameter	Estimate	SE	OR	LCL	UCL	p-value
Site = 2	-0.0911	0.4223	0.9129	0.3982	2.0933	0.83
PGE ever = 0	0.3593	0.5544	1.4323	0.4819	4.2576	0.52
RACHS class	0.2391	0.2391	1.2701	0.794	2.0318	0.32
Pre-surgery lactate	-0.4263	0.4719	0.6529	0.2583	1.6503	0.37
Gestational age birth	0.1899	0.1599	1.2091	0.8831	1.6555	0.24
PC1	0.0655	0.0289	1.0677	1.0087	1.1301	0.02
PC3	0.0799	0.0358	1.0832	1.0096	1.1621	0.03

Abbreviations: AIC - Akaike Information Criterion, Estimate – regression parameter estimate, LCL – lower 95% confidence limit, OR – odds ratio, PC - principal component, PGE – prostaglandins, REL – Reliability score, SE – standard error, UCL – upper 95% confidence limit

**Table S4. Final multivariable analysis between principal components loads, top metabolic hits and outcomes**

**Composite**

**morbidity/mortality**

Parameter	Rel	Estimate	SE	OR	LCL	UCL	p-value
Site = 2	.	3.6594	0.9285	38.838	6.2645	240.7845	<.001
PGE ever = 0	.	-2.9055	1.0386	0.0547	0.0071	0.4212	0.005
STAT category	.	0.214	0.4158	1.2386	0.5471	2.804	0.61
Pre-surgery lactate	.	2.4624	0.9957	11.7329	1.6584	83.0091	0.01
Gestational age birth	.	-0.1315	0.3241	0.8768	0.4638	1.6576	0.68
T3 Cystine	100.0%	-0.0664	0.0216	0.9358	0.8969	0.9763	0.002
T3 4-Hydroxyproline	100.0%	0.0799	0.0213	1.0832	1.0388	1.1295	<.001
T3 3-Methoxytyrosine	95.6%	-3.7156	1.1672	0.0243	0.0025	0.2412	0.002
r21 Homoserine	93.4%	-1.3991	0.6561	0.2468	0.068	0.896	0.03
t1 Ornithine	98.2%	-0.0075	0.003	0.9925	0.9867	0.9984	0.01
t1 Phenylalanine	75.0%	0.0032	0.0012	1.0032	1.0009	1.0055	0.007
t1 Methionine	91.4%	0.0122	0.006	1.0123	1.0004	1.0243	0.04

**Composite - cardiac**

Parameter	Rel	Estimate	SE	OR	LCL	UCL	p-value
Site = 2	.	2.1294	0.6018	8.4098	2.5776	27.4382	<.001
PGE ever = 0	.	-1.1273	0.7525	0.3239	0.0738	1.421	0.13
STAT category	.	0.7338	0.3276	2.083	1.0942	3.9651	0.03
Pre-surgery lactate	.	1.4609	0.6842	4.3098	1.1235	16.5329	0.03
Gestational age birth	.	-0.0094	0.252	0.9907	0.6038	1.6255	0.97
Cum Proline	90.8%	0.0014	0.0005	1.0014	1.0005	1.0023	0.003
T3 Proline	73.0%	0.0032	0.0013	1.0032	1.0006	1.0058	0.02
T3 Leucine	62.0%	-0.0202	0.0075	0.98	0.9657	0.9945	0.007

### Hepatic

Parameter	Rel	Estimate	SE	OR	LCL	UCL	p-value
Site = 2	.	1.1931	0.6519	3.2973	0.9159	11.8708	0.07
PGE ever = 0	.	-2.898	0.8879	0.0551	0.0096	0.3156	0.001
STAT category	.	1.3183	0.444	3.7371	1.5618	8.942	0.003
Pre-surgery lactate	.	0.5358	0.7452	1.7088	0.3951	7.3899	0.47
Gestational age birth	.	-0.5332	0.3063	0.5867	0.3214	1.0711	0.08
t1 Carnitine	76.2%	0.0104	0.0025	1.0105	1.0054	1.0155	<.001
T3 Tyrosine	99.0%	0.0058	0.0018	1.0058	1.0022	1.0095	0.002
t1 Aspartic acid	93.2%	0.1012	0.0462	1.1065	1.0105	1.2116	0.03
r21 Caffeine	99.6%	-0.2577	0.107	0.7728	0.6263	0.9537	0.02

### Lactate

Parameter	Rel	Estimate	SE	OR	LCL	UCL	p-value
Site = 2	.	0.6703	0.7341	1.9548	0.462	8.2714	0.36
PGE ever = 0	.	-0.8979	0.9172	0.4074	0.0672	2.4704	0.33
STAT category	.	0.9303	0.3016	2.5353	1.4017	4.5857	0.002
Pre-surgery lactate	.	1.3468	0.8898	3.8451	0.6692	22.0929	0.13
Gestational age birth	.	-0.2032	0.3036	0.8161	0.4494	1.482	0.50
R31 Galactitol	98.2%	0.0056	0.0021	1.0056	1.0016	1.0097	0.007
T3 Proline	98.8%	0.005	0.0016	1.005	1.0019	1.008	0.001
t1 Methionine	98.4%	0.007	0.0028	1.0071	1.0015	1.0126	0.01
T3 Leucine	74.6%	-0.0201	0.0086	0.9801	0.9637	0.9968	0.02

### AKI

Parameter	Rel	Estimate	SE	OR	LCL	UCL	p-value
Site = 2	.	-0.3546	0.4885	0.7015	0.2686	1.8318	0.47
PGE ever = 0	.	0.3374	0.6385	1.4013	0.3996	4.9138	0.60

STAT category	.	0.1128	0.1818	1.1194	0.7831	1.6001	0.54
Pre-surgery lactate	.	-0.1401	0.5091	0.8693	0.3197	2.3638	0.78
Gestational age birth	.	0.2503	0.1766	1.2844	0.9078	1.8172	0.16
T3 Alanine	69.2%	0.0809	0.0439	1.0843	0.9947	1.1819	0.07
T3 Glutamic acid	76.4%	0.0086	0.0037	1.0087	1.0013	1.016	0.02
T3 4-Hydroxyproline	70.4%	0.0238	0.0093	1.0241	1.0055	1.043	0.01
T3 Serine	72.6%	-0.022	0.0082	0.9782	0.9627	0.9941	0.007
t1 Ornithine	80.6%	0.0024	0.0009	1.0024	1.0005	1.0042	0.01

*Abbreviations: AIC - Akaike Information Criterion, Estimate – regression parameter estimate, LCL – lower 95% confidence limit, OR – odds ratio, PC - principal component, PGE – prostaglandins, REL – Reliability score, SE – standard error, UCL – upper 95% confidence limit*