

Supplementary Table 1 – Metabolic standard suppliers and relevant solvent and concentrations of stock solution. Suppliers catalogue and lot numbers are included where applicable.

Metabolite	Supplier	Cas#	Solvent	Concentration of Stock Solution (mg mL <sup>-1</sup> )
Alpha-Tocopherol	Sigma T1350 / SLBR3897V	58-95-7	*Arrives pre-dissolved	10
Coenzyme A <sub>neg</sub>	Sigma C4282	85-61-0	Water	10
Indole-3-lactic acid	Sigma I6608/BCBV7835	832-97-3	Water	10
Kynurenic acid	Sigma K3375/SLBN5154V	492-27-3	ACN/Water 50:50	10
L-Kynurenine	Sigma K8625/BCBQ6256 V	2922-83-0	ACN/Water 50:50	10
Pyruvic acid	Sigma I07360	127-17-3	Water	10
Tryptophan methyl ester	Sigma 364517/STBD2377 V	7524-52-9	Water	10
Uracil	Sigma U1128 / SLBS7452	66-22-8	ACN/Water 50:50	10
2-Hydroxybutyric acid	Sigma 20116	300-85-6	Water	10
Inosine	Sigma I4125-1g	58-63-9	Water	10
D-Xylose	Sigma X3877/SLBN4994V	58-86-6	ACN/Water 50:50	10
Hippuric acid	Sigma 112003-5g	495-69-2	ACN/Water 50:50	10
Cholic acid	Sigma C1254/81H0777	73163-53-8	Water	10
Picolinic acid	Sigma P42800/WXBC172 6V	98-98-6	Water	10
Choline	Sigma C7017/BCBW8074	67-48-1	Water	10
Deoxycholic acid	Sigma D2510	83-44-3	Water	10
Melatonin	Sigma M5250/SLBO9501 V	71-31-4	100% ACN	10
Palmitic acid	Sigma P0500/SLBM2076V	57-10-3	Ethanol	10
Biotin	Sigma B4639 / SLBQ9710V	58-85-5	ACN/Water 50:50	1
Cortisol	Sigma H4001	50-23-7	ACN/Water 50:50	2.5
cis-Aconitic acid	Sigma A3412/SLBK8456V	585-84-2	Water	10

4-Hydroxyphenylpyruvic acid	Sigma 114286-1g	156-39-8	100% ACN	10
Hydroxyisocaproic acid	Sigma 219819/02211HP	498-36-2	Water	10
NAD+	Sigma N0632/SLBN3457V	20111-18-6	Water	10
Succinate	Sigma 224731/MKBX8466 V	150-90-3	Water	10
Pyridoxine	Sigma P6280 / SLBQ9706V	65-23-6	Water	10
L-Methionine sulfoximine	Sigma M5379/SLBB7453 V	15985-39-4	Water	10
a-ketoglutarate	FLUKA 75890/32605191	328-50-7	Water	10
Thymidine	Sigma T1895 / SLBS3925	50-89-5	Water	10
Glucose 6-phosphate	Sigma G7250/052K7043	3671-99-8	Water	10
Fructose 1,6-bisphosphate	Sigma F6803/087K1434V	9024-52-6...	Water	10
Phosphoenolpyruvate	ALDRICH 860077/03204DD	4265-07-0	Water	10
Niacinamide	Sigma N0636 / SLBR8359V	98-92-0	Water	10
Glyoxylate	Sigma G4502/SLBP7443V	918149-31-2	Water	10
Spermidine	Sigma 49761/BCBS0158V	124-20-9	Water	10
Pantothenic acid	Sigma P5155 / 031M1718V	79-83-4	Water	10
D-Xylitol	Sigma X3375/MKBQ8024 V	87-99-0	Water	10
3-Hydroxyanthranilic acid	Sigma 148776/05316BH	548-93-6	ACN/Water 50:50	0.5
I3S: Indoxyl sulfate	Sigma I3875/BCBW7910	2642-37-7	Water	10
Methylcysteine	Sigma M6626-5g	1187-84-4	Water	10
3-Phosphoglycerate	FLUKA 79472/41705288	80731-10-8	Water	10
Myoinositol	Sigma I5125	87-89-8	Water	10
Fumarate	Sigma 240745/079188C	110-17-8	ACN/Water 50:50	5
Adenine	Sigma A9126 / SLBD8719V	73-24-5	ACN/Water 50:50	1

NADH_neg	Sigma N8129/SLBK2717V	606-68-8	Water	10
Guanine	Sigma 51030 / BCBQ2038V	73-40-5	HCl	10
Thiamine	Sigma T1270 / SLBS0838V	59-43-8	Water	10
Adenosine triphosphate	Sigma a2383/slbj8105v	34369-07-8	Water	10
Folic acid	Sigma F8758 / SLBN1618V	59-30-3	DMSO	10
NADPH	Roche 1010782000/115383 32	53-57-6	Water	10
2-Ketobutyric acid	Sigma K401-5g	600-18-0	Water	10
p-Aminobenzoic acid	Sigma A9878 / 036K1339	150-13-0	100% ACN	10
Phenyllactic acid	Sigma 113069/bgbb6474v	20312-36-1	100% ACN	10
Glucose 1-phosphate	Sigma G7018-1g	56401-20-8	Water	10
Lactate	Sigma 7022/BCBN5986V	867-56-1	Water	10
Thymine	Sigma T0376 / BCBJ1826V	65-71-4	ACN/Water 50:50	5
Lipoic acid	Sigma T1395 / SLBD0109V	1200-22-2	100% ACN	10
Quinolinic acid	Internal	89-00-9	ACN/Water 50:50	10
Indole-3-propionic acid	Sigma 57400/1113061	830-96-6	DMSO	10
Indole-3-carboxylic acid	OLCHEM/0031721	771-50-6	95% Ethanol	5
Cyanocobalamin	Sigma V6629 / SLBR2523V	68-19-9	Water	10
S-Adenosylhomocysteine	Sigma C1231 / SCOL 129-1	57-88-5	ACN/Water 50:50	2.5
DL-Homocysteine	Sigma H4628	454-29-5	Water	2.5
IND: Indole	Sigma I3408/MCKD9719	120-72-9	Water	10
Indole-3-acetamide	Sigma 286281	879-37-8	Water	10
Indole-3-acetic acid	Sigma I2886	87-51-4	Ethanol	10
Indole-3-aldehyde	Sigma 129445	487-98-8	DMSO	10
Indole-oxy sulfate	Internal	487-94-5	Water	10
Ammonium Formate	Sigma F0507	64-18-6	Water	10
L-Cystathionine	Sigma C7505	56-88-2	ACN/Water 50:50	10
Methylglyoxal	Sigma IM0252	78-98-8	*Arrives pre- dissolved	10
GMP sodium salt	Sigma G8377	85-32-5	Acetic Acid	10

ADP_neg	Sigma A27541/SLBD2826 V	20398-34-9	Water	10
acetyl-CoA_neg	Sigma A2056/SLBC4098V	102029-73-2	Water	10
L-2-Hydroxyglutaric acid	Sigma 90790	63512-50-5	Water	10
Glutathione	Sigma G6013 / SLBH9664V	70-18-8	Water	10
Nicotinic acid	Sigma N0761 / SLBR6825V	59-67-6	Water	10
Citrate	Sigma 251275	77-92-9	Water	10
GTP	Sigma G5884/076K7014	86-01-1	Water	10
D-Sorbitol	Sigma S1876/BCBT4918	50-70-4	Water	10
Xanthine	Sigma H9377/SLBH5921V	68-94-0	ACN/Water 50:50	10
Methionine sulfoxide	Sigma 64430-5g F	62697-73-8	Water	10
Phenylpyruvic acid	Sigma 286958/BCBL5546 V	156-06-9	100% ACN	10
NADP	Roche 10128031001/14935 762	53-59-8	Water	10
Fructose 6-phosphate	Sigma F3627/094K7024	26177-86-6	Water	10
Oxaloacetate	Sigma O4126/095K1110V	328-42-7	Water	10
L-Carnitine	Sigma C0283-1g	6645-46-1	Water	10
2-phosphoglycerate	Sigma	9014-08-8..	Water	10
Isocitrate	Sigma I1252/103K3855	1637-73-6	Water	10
Adenosine monophosphate	Sigma A1752 / SLBD5188V	61-19-8	Water	10
Succinyl-CoA	Sigma S1129/SLBJ4795V	108347-97-3	Water	2
Malate	Sigma 240176/14602LB	6915-15-7	Water	10
L-Ascorbic acid	Sigma A4544 / SLBN3833V	50-81-7	Water	10
2-KEtOHexanoic acid	Sigma/K6625- 250mg	13022-85-0	Water	10
Serotonin	Sigma H9623/SLBP9361V	153-98-0	Water	10
Allantoin	Sigma 93791/BCBV3695	97-59-6	ACN/Water 50:50	2.5
Cholesteryl sulfate	Sigma C9523/SLBH9227V	2864-50-8	ACN/Water 50:50	10

Adenosine	Sigma D5011/MKBR0885 V	2457-80-9	ACN/Water 50:50	10
Putresine	Sigma 51799/BCBR7255V (AS)	110-60-1	Water	10
5 Hydroxy Tryptophan	Sigma H9772/BCBW4403	4350-09-8...	Water	10
Pipecolic Acid	Sigma 237752/09814LEV	3105-95-1	Water	10
Hydroxyl kynurenine	Sigma 1771/088M4066V	2147-61-7	Ethanol	3
Linoleic Acid	Sigma L1376/SLCC7896	60-33-3	Ethanol	10
Citrulline	Internal	372-75-8	Water	10
Pyridoxal	Sigma P9130/SLBH8026V	65-22-5	Water	10
3- Indole Acrylic Acid	Sigma I2273/MKCJ6570	1204-06-4	DMSO	5
16:0 Lyso PC	Avanti 855675P/ 25mg-A-081	17364-16-8	Chloroform	10
18:0 Lyso PC	Avanti 855775C/25mg-A- 083	19420-57-6	Chloroform	10
L-Alanine	Sigma Standard Set AAS18- 5ml/slbf8136v	N/A for Set	*Arrives pre- dissolved	270ng/ul
L-Arginine				270ng/ul
L-Asparagine				270ng/ul
L-Aspartic acid				270ng/ul
L-Cystine				135 ng/ul
L-Leucine				270ng/ul
L-Glutamic acid				270ng/ul
L-Glutamine				270ng/ul
Glycine				270ng/ul
L-Histidine				270ng/ul
L-Lysine				270ng/ul
L-Methionine				270ng/ul
L-Phenylalanine				270ng/ul
L-Proline				270ng/ul
L-Serine				270ng/ul
L-Threonine				270ng/ul
L-Tryptophan	270ng/ul			
L-Tyrosine	270ng/ul			
L-Valine	270ng/ul			
1-Methyladenosine	Cayman 16937	15763-06-1	Water	10
Asymmetric dimethylarginine	Cayman 80230	220805-2201	DMSO/Water 50:50	3.5
Glycerophosphocholine	Cayman 20736	28319-77-9	Water	10

Isovalerate	Sigma 129542-100ml	503-74-2	liquid	10ul into 1ml
Muramic acid	Sigma M2503-5mg	1114-41-6	Water	10
Taurocholic acid	Sigma T4009-250mg	81-24-3	Water	10
Glutathione oxidized disodium	Sigma G4626-100mg	103239-24-3	Water	10
Indole-3-acetaldehyde	I1000-25mg	20095-27-6	40% Ethanol/Water	10
Tryptamine	Fisher - A03001G (TCI)	343-94-2	Water	10
$\gamma$ -aminobutyric acid	Sigma A2129-25g, BCBX6886	56-12-2	Water	10
Putresine	Sigma D13208-25g, BCCB0170	110-60-1	Water	10
Spermine	Sigma 55513-100mg, BCCB2495	71-44-3	Water	10
Riboflavin	Sigma R9504 / WXBC1765V	83-88-5	10% DMSO/Water	0.23
Hypoxanthine	Sigma H9636 / SLBD4750V	68-94-0	70% EtOH/Water	1
cAMP	Sigma A9501-1G	60-92-4	50:50 EtOH/Water	2.5
Isopentyl pyrophosphate	Sigma I0503-1VL	116057-53-5	Ethanol	1
Mevalonic Acid	Sigma 43987-10mg	32451-23-3 free acid	Ethanol	5
Lanosterol-95	Sigma 700099P-5mg	79-63-0	DMF	2
Squalene	Sigma S3626-10ml	111-02-4	*Arrives pre-dissolved	0.01
Geranyl pyrophosphate	Sigma G6772-1VL	763-10-0	Ethanol	100%
Farnesyl pyrophosphate	Sigma F6892-1VL	13058-04-3	Ethanol	0.01
24S-hydroxycholesterol	Sigma SML 1648-1mg	474-73-7	Ethanol	200%
25-hydroxycholesterol	Sigma H1015-10mg	2140-46-7	Ethanol	2.5
Histamine	Sigma H7125-1G	51-45-6	Ethanol	10
Cholecalciferol (Vit D3)	Sigma C9756-1G	67-97-0	Ethanol	10
Coenzyme Q10	Sigma C9538-100mg	303-98-0	Ethanol	0.3
5-Hydroxyindole-3 acetic acid	Sigma H8876-100mg	54-16-0	DMSO	10
5- Methoxytryptamine	Sigma 286583-100mg	608-07-1	DMSH	17
2-Aminobenzoic acid	A89855-25G/ anthranilic acid	118-92-3	DMSO	10

Corticosterone	Sigma C2505-500MG	50-22-6	DMSH	10
Adenosyl homocysteine	Sigma A9384-25mg	979-92-0	DMSO	3
Methoxyindole-3-acetic acid	Sigma m14935-1G	3471-31-6	EtOH	2.6
Pyroglutamic acid	Sigma 83160-25G	98-79-3	Water	20
2-phospho-d- glyceric acid	Sigma 79470-50mg	83418-48-8	Water	10
2,3-Diphospho-d- glyceric acid	Sigma D5764-25mg	102783-53-9	Water	10
Glutamyl-l-alanine	Sigma 483834-500mg	5875-41-2	Water	10
Uridine 5' triphosphate	Sigma 94370-250mg	91183-98-1	Water	10
Uridine 5' diphosphate	Sigma U4375-25mg	116295-90-0	Water	10
N-Acetyl-glucosamine	Sigma A8625-5g	7512-17-6	Water	10
Cysteine	Sigma W326305-100g	52-90-4	Water	10
Guanosine diphosphate	Sigma G7127-25mg	43139-22-6	Water	10
Glucosamine	Sigma G4875-25G	3416-24-8	Water	10
Gluconolactone	Sigma G4750-100g	90-80-2	Water	10
D-sedoheptulose 7 phosphate	Sigma 78832-1mg	2646-35-7	Water	4
D-glyceraldehyde-3- phosphate	Sigma G5251-25mg	591-59-3	Water	10
2'-deoxyribose 5' phosphate	Sigma D3126-25mg	207671-46-3	Water	10
3,7 d-hydroxy 12 oxocholan 24-oic acid	Sigma T154083-5mg	8/4/2458	DMSO	5
Hyocholic acid	Sigma 700159P-1mg	547-75-1	DMSO	10
Tauro-beta-muricholic acid	Sigma 700244-1mg	145022-92-0	EtOH/DMSO 50:50	5
Beta muricholic acid	Sigma 700233P-1mg	2393-59-1	EtOH/DMSO 50:50	5
Alpha muricholic acid	Sigma 700232P-1mg	2393-58-0	EtOH/DMSO 50:50	5
Dehydrolithocholic acid	Cayman 29544	1553-56-6	DMSO	10
Glycohyodeoxycholic Acid	Cayman 22643	13042-33-6	DMSO	10
Murideoxycholic acid	Cayman 20290	668-49-5	DMSO	5
Myristoyl-L-carnitine	Sigma 61367	25597-07-3	DMSO	10
Isovaleryl-L-carnitine	Sigma 51371-10mg	31023-24-2	DMSO	10
Stearoyl-L-carnitine	Sigma 61229	25597-09-5	DMSO	10
Hyodeoxycholic acid	Sigma H3878-5g	83-49-8	DMSO	10
5a-cholest-7-en-3b-ol	Sigma C3652-25mg	80-99-9	DMSO	0.5
Dehydrocholic acid	Sigma 116650-200mg	81-23-2	DMSO	10

3-(2-hydroxyethyl)indole	Sigma T90301-5g	526-55-6	20 mg/ml	20
Ne-acetyl-L-Lysine	Sigma A4021-1g	682-04-6	Water	10
$\alpha$ -methyl-DL-tryptophan	Sigma M8377-100mg	153-91-3	DMSO	20
N-Acetylserotonin	Sigma A1824-100mg	1210-83-9	Ethanol	10
3-amino isobutyric acid	Sigma 217794-1G	144-90-1	Water	5
Tryptophol	Sigma T90301-5g	526-55-6	Ethanol	10
Cortisone	Sigma C2755-250mg	53-06-05	Ethanol	10
5-Cholesten-3 $\beta$ -ol-7-one	Sigma C2394 -100mg	566-28-9	Ethanol	10
5 $\alpha$ -Cholestane	Sigma C8003-100mg	481-21-0	Ethanol	10
Cholesterol 5 $\alpha$ ,6 $\alpha$ -epoxide	Sigma C2773-50mg	1250-95-9	Ethanol	10
Methyl-S-cystein	Sigma, M6626-5G	1187-84-4	Water	10
3-(4hydroxyphenyl)propionic	Sigma H52406-5G	501-97-3	Water	10
Deoxyribose 5-phosphate	Sigma, D3126-25mg	102916-66-5	Water	10
Uridine 5'-diphosphate	Sigma, 94330-100mg	58-98-0/27821-45-0	Water	7
S-Lactoylglutathione	Sigma, L7140-25MG	25138-66-3/54398-03-7	Water	7
S-(methyl)glutathione	Sigma, M4139-100mg	2922-56-7	Water	2.5
S-Adenosylmethionine	Sigma, A7007-25MG	485-80-3/86867-01-8	Water	5
Thiamine pyrophosphate	Sigma, C8754-1G	154-87-0	MeOH/Water 50:50	1
Dihydroxyacetone phosphate	Sigma, 51269-100mg	57-04-5	Water	10
D-Ribulose 5-phosphate	Sigma, R9875-5mg	4151-19-3/93-87-8	Water	10
D-Lactaldehyde	Sigma, 42418-1ml	747536	Water	10
D-Ribose	Sigma, R7500-10mg	613-83-2/50-69-1	Water	10
D-Ribose 5-phosphate	83875-250mg	4300-28-1/207671-46-3	Water	10
FAD	Sigma, F6625-10mg	146-14-5/84366-81-4	Water	5
Acetoacetyl-CoA	Sigma, A2181-5mg	1420-36-6	Water	10
Cholesteryl oleate : CE(18:1(9Z))	Sigma C9253-100mg	303-43-5	Chloroform	10

Cholesteryl palmitate : CE(16:0)	Sigma C6072-1g	601-34-3	Chloroform	10
Cholesteryl stearate : CE(18:0)	Sigma C79409-5g	35602-69-8	Chloroform	10
Ergosterol	Sigma PHR1512- 200mg	57-87-4	Chloroform	10
Diosgenin	Sigma D1634-5g	512-04-9	Chloroform	10
Stigmasterol	Sigma 47132 10mg/1ml	83-48-7	Chloroform	10
gamma- Glutamylcysteine	Sigma, G0903- 25mg	636-58-8	Water	10
Guanosine diphosphate	Sigma, G7127- 10mg	146-91- 8/43139-22-6	Water	10
Uridine triphosphate	Sigma, U6625- 25mg	63-39- 8/19817-92-6	Water	10
Cysteinylglycine	Sigma, C0166- 25mg	19246-18-5	Water	5
Cytidine monophosphate N- acetylneuraminic acid	Sigma, C8271-1mg	3063-71-6	Water	10
D-Fructose	Sigma, F2793- 500mg	53188-23-1	Water	1
Glucosamine 6- phosphate	Sigma, G5509- 10mg	3616-42-0	Water	10
N-Acetylmannosamine	Sigma, A8625- 10MG	7772-94- 3/7512-17-6	Water	10
L-3- Hydroxykynurenine	Sigma, H1771- 25mg	606-14-4/484- 78-6	Ethanol	10
Propylene glycol	Sigma, PHR1051- 1.5G	57-55-6	Water	10

Supplementary Table 2 – Percent carryover for analytical standards in HILIC and RP.

Metabolite	HILIC		RP	
	Carryover (%)	Passed Filters?	Carryover (%)	Passed Filters?
(R)-lipoic acid	<1	Yes	<1	Yes
1-Methyladenosine	13.81	Yes	<1	Yes
1H-Indole-3-carboxaldehyde	1.61	Yes	<1	Yes
2-Aminobenzoic acid	37.31	Yes	<1	Yes
2-Hydroxyglutarate	<1	Yes	99.89	No
2-Ketobutyric acid	15.40	Yes	8.86	Yes
2-Ketohexanoic acid	1.62	Yes	6.38	Yes
2,3-Diphosphoglyceric acid	66.06	No	41.37	No
3-Aminoisobutanoic acid	4.11	Yes	43.21	No
3-Hydroxyanthranilic acid	1.65	Yes	208.15	Yes
3-Phosphoglyceric acid	41.04	Yes	<1	Yes
4-Hydroxyphenylpyruvic acid	10.91	Yes	257.35	No
5-Hydroxy-L-tryptophan	<1	Yes	<1	Yes
5-Hydroxyindoleacetic acid	<1	Yes	<1	Yes
5-Methoxytryptamine	<1	Yes	<1	No
7-Ketocholesterol	<1	Yes	14.30	Yes
Acetyl-CoA	5.39	Yes	39.93	No
Adenine	<1	Yes	<1	Yes
Adenosine	2.30	Yes	9.15	No
Adenosine monophosphate	3.34	Yes	2.37	Yes
Adenosine triphosphate	N/A	Yes	15.22	Yes
ADP	N/A	No	2.76	Yes
Allantoin	<1	Yes	120.24	No
alpha-Methyl-DL-tryptophan	<1	Yes	896.12	No
Alpha-Tocopherol	6.52	Yes	100.00	No
Asymmetric dimethylarginine	5.72	Yes	<1	Yes
Biotin	<1	Yes	<1	Yes
Cholesterol	<1	Yes	2.60	No
Cholesterol sulfate	<1	Yes	19.09	No
Cholic acid	<1	Yes	<1	Yes
Choline	3.23	Yes	<1	Yes
cis-Aconitic acid	<1	Yes	<1	Yes
Citric acid	3.08	Yes	<1	Yes
Citrulline	<1	Yes	13.60	Yes
Coenzyme Q10	NA	Yes	28600.00	No

Corticosterone	3.67	Yes	<1	Yes
Cortisone	661.64	No	<1	Yes
Cyanocobalamin	2.49	Yes	<1	Yes
Cyclic AMP	<1	Yes	298.63	No
D-Fructose	82.80	Yes	N/A	No
D-Glyceraldehyde 3-phosphate	9.55	Yes	212.82	No
D-Ribose	9.57	Yes	N/A	No
D-Ribose 5-phosphate	1.95	Yes	111.39	No
D-Ribulose 5-phosphate	1.96	Yes	540800.00	No
D-Sedoheptulose 7-phosphate	4.17	Yes	<1	Yes
D-Xylose	<1	Yes	297.86	No
Deoxycholic acid	NA	Yes	<1	Yes
Deoxyribose 5-phosphate	5.37	No	<1	Yes
Desaminotyrosine	1.53	Yes	21.48	Yes
Dihydroxyacetone phosphate	9.82	Yes	149.76	No
Diosgenin	2.54	Yes	1.35	Yes
DL-Homocystine	40.01	No	NA	No
Epoxycholesterol	5.84	Yes	102.50	No
Ergosterol	92.64	Yes	1.66	Yes
FAD	1.35	Yes	<1	No
Farnesyl pyrophosphate	19.29	Yes	<1	Yes
Folic acid	<1	Yes	<1	Yes
Fructose 1,6-bisphosphate	4.14	Yes	<1	Yes
Fructose 6-phosphate	3.20	Yes	1.51	Yes
Fumaric acid	<1	Yes	2.79	Yes
gamma-Glutamylcysteine	6.12	Yes	<1	Yes
Gluconolactone	<1	Yes	149.45	No
Glucosamine	1.54	Yes	2.13	Yes
Glucosamine 6-phosphate	35.33	Yes	NA	No
Glucose 1-phosphate	11.65	Yes	3.30	Yes
Glucose 6-phosphate	119.01	No	<1	Yes
Glutathione	NA	No	3.89	No
Glycerophosphocholine	1.12	Yes	<1	Yes
Glycine	3.00	Yes	<1	Yes
Glyoxylic acid	4.36	No	583.33	No
Guanine	3.67	Yes	1.35	Yes
Guanosine	1.85	Yes	7.90	No
Guanosine diphosphate	2.65	Yes	15.96	Yes
Guanosine triphosphate	1.28	No	<1	Yes
Hippuric acid	<1	Yes	<1	Yes
Histamine	<1	Yes	<1	Yes

Hydroxyisocaproic acid	<1	Yes	<1	Yes
Hydroxykynurenine	2.01	Yes	<1	Yes
Hypoxanthine	<1	Yes	<1	Yes
Indole	<1	Yes	<1	Yes
Indole-3-carboxylic acid	<1	Yes	3.98	Yes
Indole-3-propionic acid	1.79	Yes	<1	Yes
Indoleacetic acid	<1	Yes	<1	Yes
Indoleacrylic acid	31.15	Yes	<1	Yes
Indolelactic acid	<1	Yes	<1	Yes
Indoxyl sulfate	<1	Yes	<1	Yes
Inosine	<1	Yes	<1	Yes
Isocitric acid	3.47	Yes	<1	Yes
Isovalerylcarnitine	17.55	Yes	<1	Yes
Kynurenic acid	<1	Yes	<1	Yes
L-3-Hydroxykynurenine	<1	Yes	47.65	Yes
L-3-Phenyllactic acid	<1	Yes	<1	Yes
L-Alanine	2.78	Yes	<1	Yes
L-Arginine	1.77	Yes	<1	Yes
L-Asparagine	58.32	No	176.98	No
L-Aspartic acid	<1	Yes	1.29	Yes
L-Carnitine	12.95	Yes	<1	Yes
L-Cystathionine	1.29	Yes	<1	Yes
L-Cysteine	100.00	No	8.83	Yes
L-Cystine	NA	No	<1	Yes
L-Glutamic acid	2.55	Yes	<1	Yes
L-Glutamine	2.39	Yes	<1	Yes
L-Histidine	17.46	Yes	<1	Yes
L-Kynurenine	<1	Yes	<1	Yes
L-Lactic acid	10.61	Yes	16.52	Yes
L-Leucine	2.75	Yes	<1	Yes
L-Lysine	2.26	Yes	<1	Yes
L-Malic acid	<1	Yes	<1	Yes
L-Methionine	<1	Yes	<1	Yes
L-Phenylalanine	1.79	Yes	<1	Yes
L-Proline	<1	Yes	<1	Yes
L-Serine	4.05	Yes	4.60	Yes
L-Threonine	<1	Yes	10.67	Yes
L-Tryptophan	<1	Yes	<1	Yes
L-Tyrosine	<1	Yes	<1	Yes
L-Valine	<1	Yes	<1	Yes
Lanosterin	97.95	Yes	100.00	No

Lathosterol	NA	No	199.03	No
Linoleic acid	1.25	Yes	120.20	No
LysoPC(16:0)	<1	Yes	2.53	Yes
LysoPC(18:0)	<1	Yes	6.70	No
Melatonin	2.54	Yes	<1	Yes
Methionine sulfoxide	<1	Yes	<1	Yes
Mevalonic acid	<1	Yes	1066.10	Yes
myo-Inositol	<1	Yes	15.05	No
N-Acetyl-D-glucosamine	<1	Yes	<1	Yes
N-Acetylmannosamine	<1	Yes	NA	No
N-Acetylserotonin	<1	Yes	71.46	No
N6-Acetyl-L-lysine	2.14	Yes	<1	Yes
NAD	<1	Yes	<1	Yes
NADP	NA	No	<1	Yes
Niacinamide	1.13	Yes	<1	Yes
Nicotinic acid	<1	Yes	<1	Yes
Oxalacetic acid	2.29	Yes	110.42	Yes
Oxidized glutathione	NA	No	<1	Yes
Oxoglutaric acid	<1	Yes	44.17	Yes
p-Aminobenzoic acid	2.39	Yes	<1	Yes
Pantothenic acid	<1	Yes	<1	Yes
Phenylpyruvic acid	<1	Yes	<1	Yes
Phosphoenolpyruvic acid	<1	Yes	<1	Yes
Picolinic acid	<1	Yes	<1	Yes
Pipecolic acid	7.63	Yes	<1	Yes
Putrescine	480.71	No	3.02	Yes
Pyridoxal	<1	Yes	<1	Yes
Pyridoxine	<1	Yes	<1	Yes
Pyroglutamic acid	1.26	Yes	4.85	Yes
Pyruvic acid	3.48	Yes	6.21	Yes
Quinolinic acid	<1	Yes	<1	Yes
Riboflavin	<1	Yes	1.05	Yes
S-Adenosylhomocysteine	<1	Yes	<1	Yes
S-Adenosylmethionine	N/A	No	<1	Yes
S-Lactoylglutathione	<1	Yes	1.11	No
S-Methyl-L-cysteine	2.33	Yes	<1	Yes
Serotonin	<1	Yes	<1	Yes
Spermidine	N/A	No	<1	Yes
Spermine	<1	Yes	<1	Yes
Stearoylcarnitine	<1	Yes	2.22	Yes
Stigmasterol	71.94	Yes	272.73	No

Succinic acid	5.62	Yes	2.03	Yes
Taurocholic acid	N/A	Yes	<1	Yes
Tetradecanoylcarnitine	6.33	Yes	<1	Yes
Thiamine	<1	Yes	<1	Yes
Thymidine	2.05	Yes	<1	Yes
Thymine	2.14	Yes	<1	Yes
Tryptamine	<1	Yes	66.94	No
Tryptophanol	2.51	Yes	<1	Yes
Uracil	2.98	Yes	<1	Yes
Uridine 5'-diphosphate	9.47	No	105.74	No
Xanthine	<1	Yes	7.64	Yes
Xylitol	1.03	Yes	5.15	No

Supplementary Table 3 – Figures of merit for analytical standards in HILIC and RP where a suitable calibration curve was calculated

Metabolite	HILIC			RP		
	R <sup>2</sup>	LLOQ (ng $\mu\text{L}^{-1}$ )	ULOQ (ng $\mu\text{L}^{-1}$ )	R <sup>2</sup>	LLOQ (ng $\mu\text{L}^{-1}$ )	ULOQ (ng $\mu\text{L}^{-1}$ )
(R)-lipoic acid	0.973	0.005	0.500	0.973	0.010	1.000
1H-Indole-3-acetamide	N/A	N/A	N/A	0.935	0.005	0.100
1H-Indole-3-carboxaldehyde	0.990	0.050	1.000	0.965	0.005	0.500
2-Aminobenzoic acid	N/A	N/A	N/A	0.964	0.005	0.100
5-Hydroxyindoleacetic acid	N/A	N/A	N/A	0.978	0.005	1.000
3-Aminoisobutanoic acid	0.982	0.050	1.000	N/A	N/A	N/A
7-Ketocholesterol	0.935	0.005	0.050	0.978	1.000	0.500
Adenosine monophosphate	N/A	N/A	N/A	0.880	0.050	0.500
Allantoin	0.898	0.010	1.000	N/A	N/A	N/A
Asymmetric dimethylarginine	N/A	N/A	N/A	0.914	0.010	1.000
Biotin	0.981	0.005	0.500	0.997	0.005	1.000
Cholesterol sulfate	0.914	0.005	0.100	N/A	N/A	N/A
Cholic acid	0.885	0.005	0.050	N/A	N/A	N/A
Choline	0.849	0.005	1.000	0.958	0.005	0.050
Corticosterone	0.943	0.050	1.000	0.988	0.010	1.000
Cyclic AMP	0.671	0.005	0.500	N/A	N/A	N/A
D-Sedoheptulose 7-phosphate	N/A	N/A	N/A	0.986	0.005	0.100
D-Xylose	0.726	0.005	0.100	N/A	N/A	N/A
Deoxycholic acid	0.634	0.005	0.050	N/A	N/A	N/A
Deoxyribose 5-phosphate	N/A	N/A	N/A	0.975	0.005	0.100
Epoxycholesterol	0.918	0.005	0.050	N/A	N/A	N/A
Folic acid	0.789	0.005	0.100	0.982	0.005	0.500

Fructose 1,6-bisphosphate	0.957	0.010	0.500	N/A	N/A	N/A
Fructose 6-phosphate	N/A	N/A	N/A	0.871	0.005	0.500
Gluconolactone	0.656	0.005	0.050	N/A	N/A	N/A
Glucose 1-phosphate	N/A	N/A	N/A	0.872	0.005	0.050
Glucose 6-phosphate	N/A	N/A	N/A	0.952	0.010	0.100
Glycerophosphocholine	0.966	0.010	1.000	0.967	0.005	1.000
Guanosine	0.965	0.050	1.000	N/A	N/A	N/A
Guanosine triphosphate	N/A	N/A	N/A	0.968	0.005	0.500
Hippuric acid	0.784	0.005	1.000	0.994	0.005	1.000
Histamine	N/A	N/A	N/A	0.924	0.005	1.000
Hydroxyisocaproic acid	0.994	0.005	1.000	0.972	0.005	0.050
Hydroxykynurenine	N/A	N/A	N/A	0.911	0.005	0.050
Indole	N/A	N/A	N/A	0.965	0.005	0.050
Indole-3-carboxylic acid	N/A	N/A	N/A	0.973	0.050	1.000
Indole-3-propionic acid	0.925	0.050	1.000	0.977	0.005	0.500
Indoleacetic acid	N/A	N/A	N/A	0.956	0.005	0.500
Indolelactic acid	0.987	0.005	0.100	0.977	0.005	1.000
Indoxyl sulfate	0.924	0.005	0.100	0.995	0.005	1.000
Isocitric acid	N/A	N/A	N/A	0.984	0.005	0.500
Inosine	0.996	0.005	0.050	N/A	N/A	N/A
Isovalerylcarnitine	0.717	0.005	0.100	0.971	0.005	0.050
Kynurenic acid	0.802	0.005	0.100	0.983	0.005	0.050
L-3-Phenyllactic acid	0.980	0.005	1.000	N/A	N/A	N/A
L-Alanine	0.973	0.100	1.000	N/A	N/A	N/A
L-Arginine	N/A	N/A	N/A	0.969	0.005	0.050
L-Aspartic acid	0.956	0.050	0.500	0.877	0.005	1.000
L-Carnitine	0.953	0.010	0.100	0.944	0.005	0.050
L-Cystine	N/A	N/A	N/A	0.978	0.005	0.100
L-Glutamic acid	0.973	0.050	1.000	N/A	N/A	N/A
L-Glutamine	N/A	N/A	N/A	0.953	0.005	0.100
L-Histidine	0.497	0.010	0.500	0.945	0.010	1.000
L-Kynurenine	N/A	N/A	N/A	0.997	0.005	1.000
L-Leucine	N/A	N/A	N/A	0.938	0.005	0.500
L-Lysine	N/A	N/A	N/A	0.927	0.005	0.050
L-Malic acid	N/A	N/A	N/A	0.988	0.005	0.500
L-Methionine	N/A	N/A	N/A	0.982	0.010	0.500
L-Phenylalanine	0.966	0.010	0.500	0.989	0.005	1.000
L-Proline	0.846	0.010	0.500	0.937	0.005	0.500
L-Threonine	0.882	0.050	1.000	N/A	N/A	N/A
L-Tryptophan	0.897	0.005	0.050	0.992	0.010	1.000
L-Valine	N/A	N/A	N/A	0.991	0.005	0.500

Linoleic acid	0.936	0.005	0.050	N/A	N/A	N/A
LysoPC(18:0)	0.865	0.010	1.000	N/A	N/A	N/A
Melatonin	0.836	0.005	0.100	0.963	0.005	0.050
Methionine sulfoxide	0.893	0.005	0.100	N/A	N/A	N/A
Mevalonic acid	0.996	0.005	1.000	N/A	N/A	N/A
N-Acetyl-D-glucosamine	0.930	0.005	1.000	0.946	0.010	1.000
N-Acetylmannosamine	0.953	0.005	0.500	N/A	N/A	N/A
N-Acetylserotonin	0.496	0.005	0.500	N/A	N/A	N/A
N6-Acetyl-L-lysine	0.991	0.005	0.500	N/A	N/A	N/A
Nicotinic acid	0.943	0.005	0.100	0.973	0.005	1.000
Oxalacetic acid	0.953	0.005	1.000	N/A	N/A	N/A
Oxoglutaric acid	0.938	0.010	0.100	N/A	N/A	N/A
Pantothenic acid	0.975	0.005	0.500	0.934	0.005	0.500
Phenylpyruvic acid	0.952	0.010	0.500	N/A	N/A	N/A
Phosphoenolpyruvic acid	N/A	N/A	N/A	0.972	0.010	1.000
Pipecolic acid	0.956	0.005	0.100	0.964	0.005	0.500
Pyridoxal	0.941	0.005	0.100	N/A	N/A	N/A
Pyridoxine	0.974	0.005	0.050	N/A	N/A	N/A
Quinolinic acid	0.331	0.005	0.500	N/A	N/A	N/A
Riboflavin	0.775	0.010	1.000	N/A	N/A	N/A
S-Adenosylhomocysteine	N/A	N/A	N/A	0.912	0.005	0.500
S-Adenosylmethionine	N/A	N/A	N/A	0.930	0.010	1.000
S-Methyl-L-cysteine	N/A	N/A	N/A	0.960	0.005	0.500
Serotonin	0.972	0.005	0.500	0.867	0.005	0.050
Stearoylcarnitine	0.806	0.005	0.500	N/A	N/A	N/A
Succinic acid	0.926	0.050	1.000	N/A	N/A	N/A
Taurocholic acid	0.995	0.005	0.500	N/A	N/A	N/A
Thiamine	0.844	0.005	1.000	0.996	0.005	0.500
Tryptophanol	0.959	0.010	0.100	0.578	0.005	0.500
Uracil	0.983	0.005	0.100	0.581	0.010	0.500
Xanthine	0.994	0.005	0.050	N/A	N/A	N/A
Xylitol	0.943	0.005	0.100	N/A	N/A	N/A
p-Aminobenzoic acid	N/A	N/A	N/A	0.983	0.010	1.000

Supplementary Table 4 – Calculated percent recovery (%) for analytical standards where suitable calibration curves were established in RP. \* indicates that the signal of the recovery sample or analytical standard at the spiked concentration was below the limit of linearity while \*\* indicates the signal fell above the limit of linearity

Metabolite	Spiked Concentration (ng uL <sup>-1</sup> )					
	0.005	0.01	0.05	0.1	0.5	1.0
(R)-lipoic acid	*	121.2 ± 51	86.1 ± 18	56.2 ± 9	37.9 ± 3	39.4 ± 4
1H-Indole-3-acetamide	167.4 ± 64	181.8 ± 24	111.1 ± 12	80.8 ± 25	**	**
1H-Indole-3-carboxaldehyde	224.2 ± 21	218.6 ± 20	177.7 ± 7	193.5 ± 16	110.9 ± 6	**
2-Aminobenzoic acid	139.2 ± 1	110.7 ± 13	93.6 ± 2	91.8 ± 7	**	**
5-Hydroxyindoleacetic acid	181.3 ± 16	190.6 ± 8	179.2 ± 2	138.1 ± 30	118.2 ± 13	106.1 ± 5
Adenosine monophosphate	< LOD	< LOD	205.5 ± 5	114.1 ± 19	104.5 ± 17	138.2 ± 12
Asymmetric dimethyl arginine	*	*	193.8 ± 19	131.2 ± 7	63.9 ± 10	61.7 ± 9
Biotin	< LOD	195.4 ± 64	151.9 ± 28	153.7 ± 23	157.0 ± 10	131.0 ± 9
Choline	220.3 ± 66	215.3 ± 11	95.0 ± 13	**	**	**
Corticosterone	*	141.4 ± 25	141.4 ± 39	112.1 ± 6	96.5 ± 4	126.9 ± 14
Deoxyribose 5-phosphate	75.9 ± 5	44.3 ± 7	20.9 ± 2	19.5 ± 3	**	**
Folic acid	119.1 ± 0.5	102.1 ± 35	76.8 ± 17	88.6 ± 26	43.5 ± 7	**
Glycerophosphocholine	269.7 ± 42	195.1 ± 58	56.6 ± 9	56.5 ± 16	43.4 ± 12	35.5 ± 2
Guanosine triphosphate	*	*	*	41.9 ± 15	31.2 ± 9	**
Hippuric acid	388.6 ± 46	251.0 ± 15	144.5 ± 7	131.0 ± 8	99.8 ± 1	104.3 ± 14
Histamine	23.1 ± 3	22.4 ± 1	17.9 ± 7	14.0 ± 2	10.1 ± 1	7.5 ± 2
Hydroxyisocaproic acid	128.4 ± 56	83.9 ± 18	88.2 ± 28	**	**	**
Hydroxykynurenine	68.4 ± 12	93.4 ± 52	92.7 ± 16	**	**	**
Indole	290 ± 156	255.6 ± 135	228.1 ± 33	**	**	**
Indole-3-carboxylic acid	< LOD	< LOD	< LOD	161.2 ± 35	125.7 ± 14	106.3 ± 9
Indole-3-propionic acid	298.1 ± 18	244.1 ± 21	173.4 ± 28	194.9 ± 26	123.3 ± 10	**
Indoleacetic acid	*	434.3 ± 96	166.2 ± 2	153.2 ± 3	83.6 ± 2	**
Indolelactic acid	171.5 ± 13	143.6 ± 25	109.5 ± 13	98.4 ± 14	71.1 ± 6	64.0 ± 7
Indoxyl sulfate	*	209.1 ± 14	117.0 ± 5	110.8 ± 8	99.6 ± 2	101.7 ± 6

Isovalerylcarnitine	147.7 ± 16	119.0 ± 16	82.4 ± 2	**	**	**
Kynurenic acid	131.4 ± 5	127.2 ± 17	108.5 ± 9	**	**	**
L-Aspartic acid	*	*	63.2 ± 4	45.7 ± 3	30.9 ± 2	30.4 ± 2
L-Cystine	225.1 ± 15	153.1 ± 18	45.7 ± 2	25.6 ± 4	**	**
L-Histidine	*	*	167.0 ± 21	86.3 ± 0.8	38.6 ± 2	38.1 ± 1
L-Kynurenine	180.4 ± 6	162.0 ± 7	120.2 ± 16	86.4 ± 11	89.1 ± 7	94.0 ± 10
L-Leucine	< LOD	193.3 ± 199	99.2 ± 66	71.1 ± 14	73.1 ± 8	**
L-Lysine	< LOD	49.79 ± 16	30.7 ± 8	**	**	**
L-Malic acid	< LOD	198.8 ± 35	103.0 ± 4	86.2 ± 10	59.3 ± 6	**
L-Methionine	*	576.6 ± 75	176.6 ± 20	193.5 ± 28	115.2 ± 9	**
L-Phenylalanine	297.9 ± 83	159.4 ± 182	131.1 ± 41	140.1 ± 23	113.6 ± 5	123.6 ± 11
L-Threonine	*	*	144.5 ± 46	54.1 ± 22	81.1 ± 12	104.4 ± 19
L-Valine	< LOD	< LOD	< LOD	12.0 ± 15	23.2 ± 5	**
Melatonin	256.1 ± 76	253.0 ± 89	140.0 ± 22	**	**	**
N-Acetyl-D-glucosamine	< LOD	< LOD	< LOD	< LOD	13.5 ± 2	10.9 ± 4
Nicotinic acid	< LOD	< LOD	< LOD	< LOD	13.1 ± 2	19.4 ± 5
p-Aminobenzoic acid	< LOD	*	71.2 ± 23	113.2 ± 21	80.5 ± 30	87.2 ± 19
Pantothenic acid	< LOD	*	24.1 ± 19	65.3 ± 46	107.4 ± 12	89.3 ± 13
Phosphoenolpyruvic acid	*	59.9 ± 2	42.9 ± 4	90.8 ± 27	48.5 ± 3	39.2 ± 10
Pipecolic acid	469.6 ± 48	379.5 ± 48	173.2 ± 24	262.5 ± 31	123.8 ± 2	**
S-Adenosylhomocysteine	68.4 ± 2	80.1 ± 18	74.7 ± 7	133.0 ± 7	46.4 ± 7	**
S-Adenosylmethionine	< LOD	< LOD	212.1 ± 98	227.0 ± 47	151.7 ± 49	**
S-Methyl-L-cysteine	112.9 ± 12	108.5 ± 24	70.1 ± 9	49.1 ± 4	39.4 ± 1	**
Serotonin	132.5 ± 29	125.1 ± 35	99.3 ± 16	**	**	**
Thymidine	116.9 ± 2	90.6 ± 9	78.8 ± 3	115.8 ± 3	68.8 ± 5	**
Tryptophanol	< LOD	282.0 ± 101	278.7 ± 21	160.0 ± 30	35.8 ± 1	**
Uracil	*	114.1 ± 22	84.4 ± 15	57.6 ± 2	35.9 ± 5	**

Supplementary Table 5 – Calculated percent recovery (%) for analytical standards where suitable calibration curves were established using HILIC. \* indicates that the signal of the recovery sample or analytical standard at the spiked concentration was below the limit of linearity while \*\* indicates the signal fell above the limit of linearity

Metabolite	Spiked Concentration (ng uL <sup>-1</sup> )					
	0.005	0.01	0.05	0.1	0.5	1.0
(R)-lipoic acid	< LOD	< LOD	< LOD	83.3 ± 11	33.1 ± 2	22.7 ± 2
1H-Indole-3-carboxyaldehyde	*	*	36.9 ± 2	30.1 ± 3	49.6 ± 6	61.4 ± 5
3-Aminoisobutanoic acid	*	*	137.5 ± 9	145.5 ± 18	129.7 ± 5	128.5 ± 12
7-Ketocholesterol	394.3 ± 169	273.5 ± 50	239.7 ± 99	**	**	**
Allantoin	*	305.2 ± 31	169.1 ± 17	138.0 ± 12	123.9 ± 6	119.8 ± 10
Biotin	7.0 ± 3	7.6 ± 1	12.0 ± 3	13.2 ± 10	10.7 ± 3	**
Cholesterol sulfate	433.2 ± 14	250.5 ± 8	109.7 ± 4	84.5 ± 3	**	**
Cholic acid	58.6 ± 35	22.9 ± 7	21.1 ± 12	**	**	**
Choline	514.7 ± 135	403.6 ± 51	191.1 ± 37	157.8 ± 35	91.6 ± 27	70.3 ± 8
Corticosterone	*	*	605.2 ± 56	451.7 ± 111	184.7 ± 34	97.1 ± 12
Cyclic AMP	47.7 ± 2	51.7 ± 3	50.3 ± 3	56.3 ± 2	40.3 ± 1	**
D-Xylose	368.1 ± 182	96.4 ± 25	42.6 ± 23	30.1 ± 9	**	**
Folic acid	645.6 ± 421	131.8 ± 80	106.2 ± 43	207.7 ± 110	**	**
Gluconolactone	243.7 ± 61	241.9 ± 58	160.4 ± 15	**	**	**
Guanosine	*	*	67.6 ± 14	66.2 ± 11	37.8 ± 11	26.3 ± 1
Hippuric acid	201.9 ± 11	157.1 ± 37	134.1 ± 20	91.0 ± 30	72.1 ± 12	82.5 ± 5
Hydroxyisocaproic acid	49.6 ± 37	43.3 ± 5	45.5 ± 6	45.1 ± 2	67.4 ± 5	74.4 ± 3
Indole-3-propionic acid	*	*	281.0 ± 99	262.4 ± 51	250.8 ± 36	200.2 ± 20
Indolelactic acid	179.3 ± 21	146.0 ± 34	105.8 ± 13	97.6 ± 6	**	**
Inosine	54.2 ± 7	53.7 ± 10	53.8 ± 5	**	**	**
Kynurenic acid	12.7 ± 3	10.8 ± 2	6.9 ± 6	5.0 ± 4	**	**
L-3-Phenyllactic acid	93.6 ± 14	94.7 ± 10	79.1 ± 13	85.7 ± 7	105.2 ± 8	110.6 ± 6
L-Aspartic acid	*	*	66.7 ± 2	71.6 ± 5	92.3 ± 3	**
L-Glutamic acid	*	*	423.0 ± 120	253.2 ± 8	155.6 ± 33	130.7 ± 3
L-Histidine	*	*	5.7 ± 2	8.2 ± 4	10.1 ± 2	9.7 ± 2
L-Phenylalanine	*	*	240.1 ± 21	135.8 ± 1	53.1 ± 1	**

L-Proline	*		893.5 ± 64	481.7 ± 22	99.2 ± 2	**
Linoleic acid	33.4 ± 9	23.0 ± 18	15.1 ± 2	**	**	**
Melatonin	120.6 ± 9	106.3 ± 6	71.8 ± 6	56.9 ± 14	**	**
Methionine sulfoxide	< LOD	619.8 ± 140	442.1 ± 20	455.9 ± 48	**	**
Mevalonic acid	203.3 ± 27	182.8 ± 45	151.9 ± 3	134.5 ± 39	143.6 ± 15	131.0 ± 7
N-Acetyl-D-glucosamine	150.6 ± 21	150.7 ± 8	114.8 ± 18	81.4 ± 42	50.5 ± 20	27.5 ± 7
N-Acetylmannosamine	196.3 ± 48	125.3 ± 109	103.5 ± 10	64.4 ± 39	42.2 ± 22	**
N6-Acetyl-L-lysine	298.8 ± 73	234.1 ± 9	173.0 ± 15	165.3 ± 33	114.1 ± 18	**
Nicotinic acid	12.7 ± 4	14.7 ± 2	17.1 ± 4	14.0 ± 2	**	**
Oxalacetic acid	629.3 ± 187	556.4 ± 110	679.9 ± 96	682.2 ± 77	311.1 ± 32	231.1 ± 14
Pantothenic acid	110.3 ± 30	95.3 ± 12	107.6 ± 21	79.7 ± 22	72.6 ± 9	**
Phenylpyruvic acid	*	302.9 ± 67	91.6 ± 9	49.6 ± 28	37.8 ± 9	**
Pipecolic acid	350.7 ± 36	263.7 ± 69	159.0 ± 10	120.9 ± 8	**	**
Pyridoxal	101.0 ± 25	85.0 ± 39	49.9 ± 4	45.9 ± 6	**	**
Pyridoxine	35.0 ± 5	26.7 ± 6	23.8 ± 4	**	**	**
Quinolinic acid	5.7 ± 15	16.6 ± 3	22.4 ± 5	24.9 ± 11	28.6 ± 5	**
Riboflavin	*	117.9 ± 26	54.3 ± 29	52.9 ± 39	19.4 ± 4	10.2 ± 3
Serotonin	*	356.2 ± 37	178.9 ± 16	168.7 ± 31	202.5 ± 27	**
Stearoylcarnitine	339.0 ± 7	324.8 ± 28	245.3 ± 23	248.2 ± 12	88.5 ± 6	**
Succinic acid	*	*	68.3 ± 60	82.9 ± 3	53.0 ± 2	16.3 ± 13
Taurocholic acid	18.2 ± 4	16.8 ± 2	11.6 ± 2	14.6 ± 1	6.2 ± 10	**
Thiamine	159.1 ± 47	202.4 ± 57	184.8 ± 26	166.1 ± 52	91.2 ± 22	64.2 ± 14
Tryptophanol	*	287.9 ± 151	212.7 ± 35	116.4 ± 36	**	**
Uracil	94.4 ± 11	94.2 ± 10	72.5 ± 4	58.0 ± 2	**	**
Xylitol	24.0 ± 11	27.3 ± 0.9	9.7 ± 6	7.3 ± 2	**	**