

SUPPLEMENTARY DATA

Analytical methodology for a metabolome atlas of goat's plasma, milk and feces using ¹H-NMR and UHPLC-HRMS

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SAMPLE PREPARATION

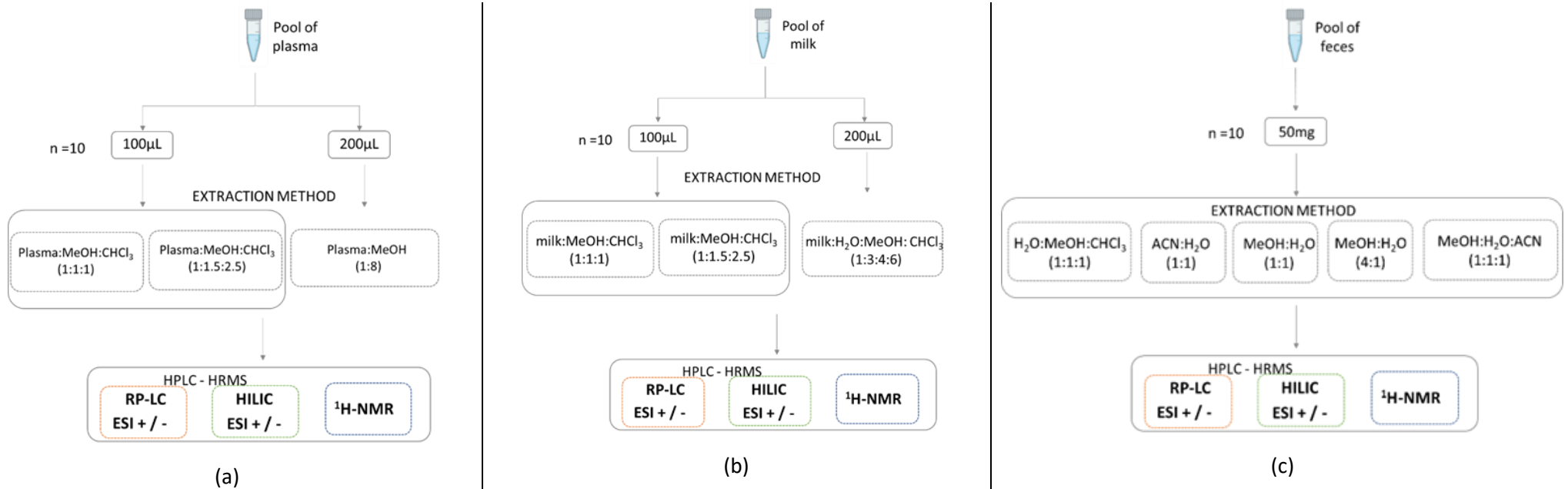


Figure S1. Schematic presentation of the preparation procedures applied on the pool of plasma (a), milk (b) and feces (c) for the selection of the optimum protocol for the maximum metabolome coverage by UHPLC-MS and ¹H-NMR.

PLASMA

		RP-LC	HILIC	NMR	Total
Plasma:MeOH :CHCl ₃ (1 :1 :1) (n=10)	Number of metabolites :	137	131	39	229
	CV<30%	108	97	39	198
	CV<20%	81	73	39	161
	CV<10%	32	31	29	78
	CV % mean (min-max)	22% (4%-93%)	27% (3%-135%)	8% (4%-15%)	18% (3%-93%)
Plasma:MeOH :CHCl ₃ (1 :2.5 :1) (n=10)	Number of metabolites :	145	129	36	230
	CV<30%	123	84	36	184
	CV<20%	103	65	35	160
	CV<10%	40	21	24	69
	CV % mean (min-max)	18% (4%-92%)	26% (3%-135%)	8% (3%-20%)	19% (3%-92%)
Plasma:MeOH (1 :8) (n=10)	Number of metabolites :	136	153	38	237
	CV<30%	120	61	38	169
	CV<20%	98	33	38	140
	CV<10%	41	15	30	78
	CV % mean (min-max)	16% (1%-50%)	41% (2%-120%)	6% (1%-19%)	24% (1%-120%)

Table S1: Number of extracted metabolites and coefficient of validation in blood for the different extraction methods using ¹H-NMR and UHPLC-MS

MILK

		RP-LC	HILIC	NMR	Total
Milk:MeOH :CHCl ₃ (1 :1 :1) (n=10)	Number of metabolites :	142	131	35	234
	CV<30%	126	97	35	200
	CV<20%	111	58	35	166
	CV<10%	68	13	28	95
	CV % mean (min-max)	14% (1%-102%)	25% (1%-107%)	7% (3%-17%)	17% (1%-84%)
Milk:MeOH :CHCl ₃ (1 :2.5 :2.5) (n=10)	Number of metabolites :	144	131	35	237
	CV<30%	95	90	35	172
	CV<20%	69	49	34	125
	CV<10%	19	8	23	45
	CV % mean (min-max)	30% (4%-175%)	27% (1%-110%)	9% (7%-20%)	25% (1%-122%)
Milk:H ₂ O:MeOH :CHCl ₃ (1 :3 :4 :6) (n=10)	Number of metabolites :	139	151	33	263
	CV<30%	121	109	33	221
	CV<20%	107	107	32	187
	CV<10%	65	35	21	100
	CV % mean (min-max)	15% (2%-78%)	20% (2%-84%)	8% (2%-22%)	17% (2%-84%)

Table S2: Number of extracted metabolites and coefficient of validation in milk for the different extraction methods using ¹H-NMR and UHPLC-MS

FECES

		RP-LC	HILIC	NMR	Total
H ₂ O:MeOH :CHCl ₃ (1 :1 :1) (n=10)	Number of metabolites :	236	250	28	347
	CV<30%	194	199	21	286
	CV<20%	175	143	17	241
	CV<10%	141	109	7	192
	CV % mean (min-max)	15% (2%-92%)	21% (3%-168%)	21% (5%-53%)	17% (2%-168%)
ACN:H ₂ O 1 :1 (n=10)	Number of metabolites :	236	256	28	348
	CV<30%	195	220	28	306
	CV<20%	169	196	28	280
	CV<10%	111	124	8	186
	CV % mean (min-max)	17% (2%-103%)	17% (3%-149%)	11% (6%-17%)	14% (2%-97%)
MeOH:H ₂ O 1 :1 (n=10)	Number of metabolites :	238	262	28	355
	CV<30%	198	222	28	313
	CV<20%	187	191	26	289
	CV<10%	137	132	13	215
	CV % mean (min-max)	15% (2%-98%)	16% (2%-157%)	11% (5%-24%)	14% (2%-157%)
MeOH:H ₂ O 4:1 (n=10)	Number of metabolites :	240	261	28	353
	CV<30%	201	221	25	313
	CV<20%	188	204	22	291
	CV<10%	138	140	19	222
	CV % mean (min-max)	15% (2%-99%)	16% (3%-119%)	13% (4%-54%)	13% (2%-119%)
MeOH:H ₂ O:ACN 1:1: (n=10)	Number of metabolites :	236	254	28	348
	CV<30%	201	219	28	310
	CV<20%	185	203	28	296
	CV<10%	149	138	16	225
	CV % mean (min-max)	14% (2%-95%)	15% (1%-119%)	9% (5%-15%)	13% (1%-119%)

Table S3: Number of extracted metabolites and coefficient of validation in fecal for the different extraction methods using ¹H-NMR and UHPLC-MS

List of metabolites found in each biological matrix or shared between two or three matrices

Table S4: Metabolites extracted from each biological matrix according to the best preparation procedure, with a CV<30%.

Only in plasma				
Metabolite	Chemical class	HMDB	PubChem	KEGG
Dihydroxyacetone phosphate	Acides phosphoriques	HMDB0001473	668	C00111
Acetone	Aliphatic compounds cyclic and acyclic	HMDB0001659	180	C00207
Dimethylglycine	Amino acids-Peptides-Derivatives	HMDB0000092	673	C01026
L-Cystine	Amino acids-Peptides-Derivatives	HMDB0000192	67678	C00491
Thyroxine	Amino acids-Peptides-Derivatives	HMDB0000248	5819	C01829
1-Hydroxy-2-naphthoate	Aromatic compounds-Vitamins-Amines	METPA0374		C03203
4-Hydroxycinnamic acid	Aromatic compounds-Vitamins-Amines	HMDB0002035	637542	C00811
Bilirubin	Aromatic compounds-Vitamins-Amines	HMDB0000054	21252250	C00486
Phenylacetic acid	Aromatic compounds-Vitamins-Amines	HMDB0000209	999	C07086
Phenylpyruvic acid	Aromatic compounds-Vitamins-Amines	HMDB0000205	997	C00166
(S)-3-Hydroxyisobutyric acid	Lipids: Fatty acids-Steroids-Hormones-Vitamins	HMDB0000023	87	C06001
Methyl jasmonate	Lipids: Fatty acids-Steroids-Hormones-Vitamins	HMDB0036583	5367719	C11512
Guanosine monophosphate	Nucleotides-Nucleosides-Derivatives	HMDB0001397	6804	C00144
Xanthosine	Nucleotides-Nucleosides-Derivatives	HMDB0000299	64959	C01762
Pyruvic acid	Organic acids	HMDB0000243	1060	C00022

Only in Milk				
Metabolite	Chemical class	HMDB	PubChem	KEGG
4-Methylcatechol	Aromatic compounds-Vitamins-Amines	HMDB0000873	9958	C06730
Adenosine monophosphate	Nucleotides-Nucleosides-Derivatives	HMDB0000045	6083	C00020
ADP-glucose	Nucleotides-Nucleosides-Derivatives	HMDB0006557	16500	C00498
Butanal	Aliphatic compounds cyclic and acyclic	HMDB0003543	261	C01412
Cellobiose	Sugars	HMDB000055	10712	C00185
D-Fructose	Sugars	HMDB00660	5984	C00095
D-Tagatose	Sugars	HMDB03418	439312	C00795
D-Xylitol	Sugars	HMDB02917	6912	C00379
Dethiobiotin	Lipids: Fatty acids-Steroids-Hormones-Vitamins	HMDB0003581	445027	C01909
Dimethyl sulfone	Organic acids	HMDB0004983	6213	C11142
Galactaric acid	Sugars	HMDB0000639	3037582	C00879
Galactose 1-phosphate	Sugars	HMDB0000645	123912	C00446
Glucaric acid	Sugars	HMDB0000663	33037	C00818
Glycerol 3-phosphate	Lipids: Fatty acids-Steroids-Hormones-Vitamins	HMDB0000126	439162	C00093
Heptanoic acid	Lipids: Fatty acids-Steroids-Hormones-Vitamins	HMDB0000666	8094	C17714
Hypotaurine	Organic acids	HMDB0000965	107812	C00519
L-Fucose	Sugars	HMDB0000174	3034656	C01019
L(-)-Nicotine	Aromatic compounds-Vitamins-Amines	HMDB0001934	89594	C00745
Melatonin	Aromatic compounds-Vitamins-Amines	HMDB0001389	896	C01598
N-Methylhydantoin	Aliphatic compounds cyclic and acyclic	HMDB03646	69217	C02565

Oxoglutaric acid	Lipids: Fatty acids-Steroids-Hormones-Vitamins	HMDB0000208	51	C00026
Palatinose	Sugars	HMDB0256083	52994241	C01742
Phenylacetylglycine	Amino acids-Peptides-Derivatives	HMDB00821	68144	C05598
Phosphocreatine	Amino acids-Peptides-Derivatives	HMDB0001511	587	C02305
Phosphocreatine	Amino acids-Peptides-Derivatives	HMDB0001511	587	C02305
Sorbitol	Sugars	HMDB00247	5780	C00794
Sucrose	Sugars	HMDB0000258	5988	C00089
Theophylline	Aromatic compounds-Vitamins-Amines	HMDB0001889	2153	C07130
Uridine-5-diphospho-n-acetylglucosamine	Nucleotides-Nucleosides-Derivatives	HMDB00290	445675	C00043
Uridine diphosphate-N-acetylgalactosamine	Nucleotides-Nucleosides-Derivatives	HMDB0000304	1167	C00203
Uridine diphosphate glucose	Sugars	HMDB0000286	53477679	C00029
Uridine diphosphategalactose	Sugars	HMDB0000302	18068	C00052

Milk Plasma				
Metabolite	Chemical class	HMDB	PubChem	KEGG
Glycolaldehyde dimer	Aliphatic compounds cyclic and acyclic		186078	
Gamma-Aminobutyric acid	Amino acids-Peptides-Derivatives	HMDB0000112	223130	C00334
Dimethylamine	Aromatic compounds-Vitamins-Amines	HMDB0000087	674	C00543
Theobromine	Aromatic compounds-Vitamins-Amines	HMDB0002825	5429	C07480
3-Hydroxybutyric acid	Lipids: Fatty acids-Steroids-Hormones-Vitamins	HMDB0000357	441	C01089
Lithocholytaurine	Lipids: Fatty acids-Steroids-Hormones-Vitamins	HMDB0000722	53477716	C02592
3-Hydroxymethylglutaric acid	Organic acids	HMDB0000355	1662	C03761
Acetoacetic acid	Organic acids	HMDB0000060	96	C00164
Citric acid	Organic acids	HMDB0000094	311	C00158
Methylmalonic acid	Organic acids	HMDB0000202	487	C02170
Allose	Sugars	HMDB0001151	12285879	C01487
Alpha-Lactose	Sugars	HMDB0000186	84571	C00243
D-Galactose	Sugars	HMDB0000143	439357	C00984
L-Sorbose	Sugars	HMDB0001266	441484	C08356

Milk Feces				
Metabolite	Chemical class	HMDB	PubChem	KEGG
1-Aminocyclopropanecarboxylic acid	Amino acids-Peptides-Derivatives	HMDB0036458	535	C01234
2-Hydroxypyridine	Aromatic compounds-Vitamins-Amines	HMDB0013751	8871	C02502
3-Aminoisobutanoic acid	Amino acids-Peptides-Derivatives	HMDB0003911	64956	C05145
3-Methyladenine	Aromatic compounds-Vitamins-Amines	HMDB0011600	1673	C00913
4-Hydroxybenzaldehyde	Aromatic compounds-Vitamins-Amines	HMDB0011718	126	C00633
5-Hydroxylysine	Amino acids-Peptides-Derivatives	HMDB0000450	4433	C16741
Acetamide	Aromatic compounds-Vitamins-Amines	HMDB0031645	178	C06244
Anserine	Amino acids-Peptides-Derivatives	HMDB0000194	112072	C01262
Cholic acid	Lipids: Fatty acids-Steroids-Hormones-Vitamins	HMDB0000619	221493	C00695
Citraconic acid	Lipids: Fatty acids-Steroids-Hormones-Vitamins	HMDB0000634	643798	C02226
Corticosterone	Lipids: Fatty acids-Steroids-Hormones-Vitamins	HMDB0001547	5753	C02140
Cortisol	Lipids: Fatty acids-Steroids-Hormones-Vitamins	HMDB0000063	657311	C00735
Cortisol-21-acetate	Lipids: Fatty acids-Steroids-Hormones-Vitamins		5744	C02821
Cyclic AMP	Nucleotides-Nucleosides-Derivatives	HMDB0000058	6076	C00575
Diacetyl	Aliphatic compounds cyclic and acyclic	HMDB0003407	650	C00741

Epinephrine	Aromatic compounds-Vitamins-Amines	HMDB0000068	5816	C00788
Ethanolamine	Aliphatic compounds cyclic and acyclic	HMDB0000149	700	C00189
Fumaric acid	Lipids: Fatty acids-Steroids-Hormones-Vitamins	HMDB0000134	444972	C00122
Glucosamine 6-phosphate	Sugars	HMDB0001254	439217	C00352
Glucose 6-phosphate	Sugars	HMDB0001401	5958	C00092
Glyceraldehyde-3-phosphatediethylacetal	Aliphatic compounds cyclic and acyclic		3334922	
Imidazoleacetic acid	Aromatic compounds-Vitamins-Amines	HMDB0002024	96215	C02835
Indolepyruvate	Aromatic compounds-Vitamins-Amines	HMDB0060484	803	C00331
Kynurenic acid	Amino acids-Peptides-Derivatives	HMDB0000715	3845	C01717
L-Acetylcarnitine	Lipids: Fatty acids-Steroids-Hormones-Vitamins	HMDB0000201	7045767	C02571
L-Allothreonine	Amino acids-Peptides-Derivatives	HMDB0004041	99289	C05519
L-Dihydroorotic acid	Aliphatic compounds cyclic and acyclic	HMDB0003349	439216	C00337
Mannitol	Sugars	HMDB0000765	6251	C00392
N-Acetyl-D-glucosamine	Sugars	HMDB0000215	439174	C00140
N-Acetylgalactosamine	Sugars	HMDB0000212	84265	C01074
N-Acetyl-L-methionine	Amino acids-Peptides-Derivatives	HMDB0011745	6180	C02712
N-Acetylmannosamine	Sugars	HMDB0001129	11096158	C00645
Niacinamide	Aromatic compounds-Vitamins-Amines	HMDB0001406	936	C00153
Nicotinic acid	Aromatic compounds-Vitamins-Amines	HMDB0001488	938	C00253

N-Methyltryptamine	Aromatic compounds-Vitamins-Amines	HMDB0004370	6088	C06213
N-Trimethyllysine	Amino acids-Peptides-Derivatives		440121	C03793
Oxfenicine	Amino acids-Peptides-Derivatives	HMDB0246152	36143	D05292
Pantolactone	Aliphatic compounds cyclic and acyclic	HMDB0059876	439368	C01012
Pterin	Aromatic compounds-Vitamins-Amines	HMDB0000802	73000	C00715
Pyrrole-2-carboxylic acid	Amino acids-Peptides-Derivatives	HMDB0004230	12473	C05942
Riboflavin	Aromatic compounds-Vitamins-Amines	HMDB0000244	493570	C00255
Salicyluric acid	Aromatic compounds-Vitamins-Amines	HMDB0000840	10253	C07588
Thymine	Aromatic compounds-Vitamins-Amines	HMDB0000262	1135	C00178
trans-Aconitic acid	Organic acids	HMDB0000958	444212	C02341
trans-Ferulic acid	Aromatic compounds-Vitamins-Amines	HMDB0000954	445858	C01494
Tryptophanol	Aromatic compounds-Vitamins-Amines	HMDB0003447	10685	C00955

Milk Feces Plasma				
Metabolite	Chemical class	HMDB	PubChem	KEGG
Acetylcholine	Aliphatic compounds cyclic and acyclic	HMDB0000895	6060	C01996
Allantoin	Aliphatic compounds cyclic and acyclic	HMDB0000462	204	C01551
Biotin	Aliphatic compounds cyclic and acyclic	HMDB0000030	171548	C00120
Choline	Aliphatic compounds cyclic and acyclic	HMDB0000097	305	C00114
Creatinine	Aliphatic compounds cyclic and acyclic	HMDB0000562	588	C00791
Cyclohexane-1,2-Diol	Aliphatic compounds cyclic and acyclic		13601	C03739
L-Carnitine	Aliphatic compounds cyclic and acyclic	HMDB0000062	2724480	C00318
Methylguanidine	Aliphatic compounds cyclic and acyclic	HMDB0001522	10111	C02294
O-Phosphoethanolamine	Aliphatic compounds cyclic and acyclic	HMDB0000224	1015	C00346
Pantothenic acid	Aliphatic compounds cyclic and acyclic	HMDB0000210	6613	C00864
Phosphorylcholine	Aliphatic compounds cyclic and acyclic	HMDB0001565	8691	C00588
Propanal	Aliphatic compounds cyclic and acyclic	HMDB0003366	527	C00479
Trimethylamine	Aliphatic compounds cyclic and acyclic	HMDB0000906	1146	C00565
Ureidopropionic acid	Aliphatic compounds cyclic and acyclic	HMDB0000026	111	C02642
2,4-Dihydroxypyrimidine-5-carboxylic acid	Amino acids-Peptides-Derivatives		90301	C03030
3-Methylhistidine	Amino acids-Peptides-Derivatives	HMDB0000479	64969	C01152
4-Hydroxy-L-proline	Amino acids-Peptides-Derivatives	HMDB0006055	69248	C01015
5-Aminolevulinic acid	Amino acids-Peptides-Derivatives	HMDB0001149	137	C00430

Acetylglycine	Amino acids-Peptides-Derivatives	HMDB0000532	10972	
Beta-Alanine	Amino acids-Peptides-Derivatives	HMDB0000056	239	C00099
Betaine	Amino acids-Peptides-Derivatives	HMDB0000043	247	C00719
Citrulline	Amino acids-Peptides-Derivatives	HMDB0000904	9750	C00327
Creatine	Amino acids-Peptides-Derivatives	HMDB0000064	586	C00300
Formyl-L-methionylpeptide	Amino acids-Peptides-Derivatives		13611	C11439
Glycine	Amino acids-Peptides-Derivatives	HMDB0000123	750	C00037
Guanidoacetic acid	Amino acids-Peptides-Derivatives	HMDB0000128	763	C00581
Hippuric acid	Amino acids-Peptides-Derivatives	HMDB0000714	464	C01586
L-Arginine	Amino acids-Peptides-Derivatives	HMDB0000517	6322	C00062
L-Asparagine	Amino acids-Peptides-Derivatives	HMDB0000168	6267	C00152
L-Aspartic acid	Amino acids-Peptides-Derivatives	HMDB0000191	5960	C00049
L-Glutamic acid	Amino acids-Peptides-Derivatives	HMDB0000148	33032	C00025
L-Glutamine	Amino acids-Peptides-Derivatives	HMDB0000641	5961	C00064
L-Histidine	Amino acids-Peptides-Derivatives	HMDB0000177	6274	C00135
L-Homoserine	Amino acids-Peptides-Derivatives	HMDB0000719	12647	C00263
L-Isoleucine	Amino acids-Peptides-Derivatives	HMDB0000172	6306	C00407
L-Kynurenine	Amino acids-Peptides-Derivatives	HMDB0000684	161166	C00328
L-Leucine	Amino acids-Peptides-Derivatives	HMDB0000687	6106	C00123
L-Lysine	Amino acids-Peptides-Derivatives	HMDB0000182	5962	C00047
L-Methionine	Amino acids-Peptides-Derivatives	HMDB0000696	6137	C00073

L-Norleucine	Amino acids-Peptides-Derivatives	HMDB0001645	21236	C01933
L-Phenylalanine	Amino acids-Peptides-Derivatives	HMDB0000159	6140	C00079
L-Proline	Amino acids-Peptides-Derivatives	HMDB0000162	145742	C00148
L-Serine	Amino acids-Peptides-Derivatives	HMDB0000187	5951	C00065
L-Threonine	Amino acids-Peptides-Derivatives	HMDB0000167	6288	C00188
L-Tryptophan	Amino acids-Peptides-Derivatives	HMDB0000929	6305	C00078
L-Tyrosine	Amino acids-Peptides-Derivatives	HMDB0000158	6057	C00082
L-Valine	Amino acids-Peptides-Derivatives	HMDB0000883	6287	C00183
N-Acetyl-L-alanine	Amino acids-Peptides-Derivatives	HMDB0000766	88064	
N-Acetyl-L-phenylalanine	Amino acids-Peptides-Derivatives	HMDB0000512	74839	C03519
N-Acetyl-leucine	Amino acids-Peptides-Derivatives	HMDB0011756	70912	C02710
N-Acetylserine	Amino acids-Peptides-Derivatives	HMDB0002931	65249	
N-acetyltryptophan	Amino acids-Peptides-Derivatives	HMDB0013713	700653	
Ornithine	Amino acids-Peptides-Derivatives	HMDB0000214	6262	C00077
Orotic acid	Amino acids-Peptides-Derivatives	HMDB0000226	967	C00295
Pipecolic acid	Amino acids-Peptides-Derivatives	HMDB0000070	849	C00408
Pyroglutamic acid	Amino acids-Peptides-Derivatives	HMDB0000267	7405	C01879
Sarcosine	Amino acids-Peptides-Derivatives	HMDB0000271	1088	C00213
2-Aminophenol	Aromatic compounds-Vitamins-Amines	METPA0236		C01987
3-(2-Hydroxyphenyl)propanoic acid	Aromatic compounds-Vitamins-Amines	HMDB0033752	873	C01198
3-Hydroxyphenylacetic acid	Aromatic compounds-Vitamins-Amines	HMDB0000440	12122	C05593

3-Methyldioxyindole	Aromatic compounds-Vitamins-Amines	HMDB0004186	151066	C05834
3,4-Dihydroxybenzeneacetic acid	Aromatic compounds-Vitamins-Amines	HMDB0001336	547	C01161
5-Hydroxyindoleacetic acid	Aromatic compounds-Vitamins-Amines	HMDB0000763	1826	C05635
Adenine	Aromatic compounds-Vitamins-Amines	HMDB0000034	190	C00147
Benzyl alcohol	Aromatic compounds-Vitamins-Amines	HMDB0003119	244	C03485
Cytosine	Aromatic compounds-Vitamins-Amines	HMDB0000630	597	C00380
Gentisic acid	Aromatic compounds-Vitamins-Amines	HMDB0000152	3469	C00628
Guanine	Aromatic compounds-Vitamins-Amines	HMDB0000132	764	C00242
Homogentisic acid	Aromatic compounds-Vitamins-Amines	HMDB0000130	780	C00544
Homovanillic acid	Aromatic compounds-Vitamins-Amines	HMDB0000118	1738	C05582
Hypoxanthine	Aromatic compounds-Vitamins-Amines	HMDB0000157	790	C00262
Indoleacetic acid	Aromatic compounds-Vitamins-Amines	HMDB0000197	802	C00954
Indoxyl sulfate	Aromatic compounds-Vitamins-Amines	HMDB0000682	10258	
Lumichrome	Aromatic compounds-Vitamins-Amines	METPA0216		C01727
N-Acetylserotonin	Aromatic compounds-Vitamins-Amines	HMDB0001238	903	C00978
N,N-Dimethylphenethylamine	Aromatic compounds-Vitamins-Amines	HMDB0032243	86536	
Ortho-Hydroxyphenylacetic acid	Aromatic compounds-Vitamins-Amines	HMDB0000669	11970	C05852
p-Hydroxyphenylacetic acid	Aromatic compounds-Vitamins-Amines	HMDB0000020	127	C00642
Paraxanthine	Aromatic compounds-Vitamins-Amines	HMDB0001860	4687	C13747
Protocatechuic acid	Aromatic compounds-Vitamins-Amines	HMDB0001856	72	C00230
Pyrocatechol	Aromatic compounds-Vitamins-Amines	HMDB0000957	3390	C15571

trans-Cinnamic acid	Aromatic compounds-Vitamins-Amines	HMDB0000930	444539	C10438
Trigonelline	Aromatic compounds-Vitamins-Amines	HMDB0000875	5570	C01004
Uracil	Aromatic compounds-Vitamins-Amines	HMDB0000300	1174	C00106
Uric acid	Aromatic compounds-Vitamins-Amines	HMDB0000289	1175	C00366
Urocanic acid	Aromatic compounds-Vitamins-Amines	HMDB0000301	736715	C00785
Xanthine	Aromatic compounds-Vitamins-Amines	HMDB0000292	1188	C00385
Thymine	Aromatic compounds-Vitamins-Amines	HMDB0000262	1135	C00178
12-Hydroxydodecanoic acid	Lipids: Fatty acids-Steroids-Hormones-Vitamins	HMDB0002059	79034	C08317
2-Hydroxybutyric acid	Lipids: Fatty acids-Steroids-Hormones-Vitamins	HMDB0000008	11266	C05984
4-Trimethylammoniobutanoic acid	Lipids: Fatty acids-Steroids-Hormones-Vitamins	HMDB0001161	134	C01181
Caproic acid	Lipids: Fatty acids-Steroids-Hormones-Vitamins	HMDB0000535	8892	C01585
Ethylmalonic acid	Lipids: Fatty acids-Steroids-Hormones-Vitamins	HMDB0000622	11756	
Galactitol	Lipids: Fatty acids-Steroids-Hormones-Vitamins	HMDB0000107	11850	C01697
Glycerophosphocholine	Lipids: Fatty acids-Steroids-Hormones-Vitamins	HMDB0000086	71920	C00670
Glycocholic acid	Lipids: Fatty acids-Steroids-Hormones-Vitamins	HMDB0000138	23617285	C01921
Ketoleucine	Lipids: Fatty acids-Steroids-Hormones-	HMDB0000695	70	C00233

Vitamins					
1-Methyladenosine	Nucleotides-Nucleosides-Derivatives	HMDB0003331	27476	C02494	
5'-Methylthioadenosine	Nucleotides-Nucleosides-Derivatives	HMDB0001173	439176	C00170	
Adenosine	Nucleotides-Nucleosides-Derivatives	HMDB0000050	60961	C00212	
Deoxycytidine	Nucleotides-Nucleosides-Derivatives	HMDB0000014	13711	C00881	
Deoxyguanosine	Nucleotides-Nucleosides-Derivatives	HMDB0000085	187790	C00330	
Guanosine	Nucleotides-Nucleosides-Derivatives	HMDB0000133	6802	C00387	
Inosine	Nucleotides-Nucleosides-Derivatives	HMDB0000195	6021	C00294	
N6-(delta2-Isopentenyl)-adenine	Nucleotides-Nucleosides-Derivatives	METPA1684		C04083	
Thymidine	Nucleotides-Nucleosides-Derivatives	HMDB0000273	5789	C00214	
Uridine	Nucleotides-Nucleosides-Derivatives	HMDB0000296	6029	C00299	
3-Hydroxycapric acid	Organic acids	HMDB0002203	26612		
4-Acetamidobutanoic acid	Organic acids	HMDB0003681	18189	C02946	
Acetic acid	Organic acids	HMDB0000042	176	C00033	
Azelaic acid	Organic acids	HMDB0000784	2266	C08261	
Citramalic acid	Organic acids	HMDB0000426	441696	C00815	
Formic acid	Organic acids	HMDB0000142	284	C00058	
L-Lactic acid	Organic acids	HMDB0000190	61503	C00186	
L-Malic acid	Organic acids	HMDB0000156	222656	C00149	
N-Acetylputrescine	Organic acids	HMDB0002064	122356	C02714	
Suberic acid	Organic acids	HMDB0000893	10457	C08278	

Succinic acid	Organic acids	HMDB0000254	1110	C00042
Taurine	Organic acids	HMDB0000251	1123	C00245
2-Deoxy-D-Glucose	Sugars		3865	C00586
Alpha-D-Glucose	Sugars	HMDB0003345	79025	C00267
D-Galactosamine	Sugars	METPA0263		C02262
D-Mannose	Sugars	HMDB0000169	18950	C00936
Gluconic acid	Sugars	HMDB0000625	10690	C00257
Glyceric acid	Sugars	HMDB0000139	439194	C00258
L-Arabitol	Sugars	HMDB0001851	94154	C00532
Methyl beta-D-glucopyranoside	Sugars	HMDB0029965	94214	
myo-Inositol	Sugars	HMDB0000211		C00137
N-Acetylneuraminate	Sugars		3568	C00270
Ribitol	Sugars	HMDB0000508		C00474

Feces				
Metabolite	Chemical class	HMDB	PubChem	KEGG
Ciliatine	Acides phosphoriques	HMDB0011747	339	C03557
3-Dehydroshikimate	Aliphatic compounds cyclic and acyclic	METPA0312		C02637
Acetoin	Aliphatic compounds cyclic and acyclic	HMDB0003243	4068	C00466
Agmatine	Aliphatic compounds cyclic and acyclic	HMDB0001432	199	C00179
Cadaverine	Aliphatic compounds cyclic and acyclic	HMDB0002322	273	C01672
Quinic acid	Aliphatic compounds cyclic and acyclic	HMDB0003072	6508	C00296
Valerolactone	Aliphatic compounds cyclic and acyclic	NA	10953	C02240
Shikimic acid	Aliphatic compounds cyclic and acyclic	HMDB0003070	8742	C00493
Spermidine	Aliphatic compounds cyclic and acyclic	HMDB0001257	1102	C00315
3-Sulfinioalanine	Amino acids-Peptides-Derivatives	HMDB0000996	439270	C00606
L-Alanine	Amino acids-Peptides-Derivatives	HMDB0000161	5950	C00041
L-Cystathionine	Amino acids-Peptides-Derivatives	HMDB0000099	439258	C02291
N-Formylglycine	Amino acids-Peptides-Derivatives		75606	
Picolinic acid	Amino acids-Peptides-Derivatives	HMDB0002243	1018	C10164
Quinaldic acid	Amino acids-Peptides-Derivatives	HMDB0000842	7124	C06325
5-Hydroxy-L-tryptophan	Amino acids-Peptides-Derivatives	HMDB0000472	144	C00643
L-Dopa	Amino acids-Peptides-Derivatives	HMDB0000181	6047	C00355
DL-O-Phosphoserine	Amino acids-Peptides-Derivatives	HMDB0001721	106	C01005

Homocysteine	Amino acids-Peptides-Derivatives	HMDB0000742	778	C00155
S-Adenosylhomocysteine	Amino acids-Peptides-Derivatives	HMDB0000939	439155	C00021
2-Aminoisobutyric acid	Amino acids-Peptides-Derivatives	HMDB0001906	6119	C03665
3-Methoxytyrosine	Amino acids-Peptides-Derivatives	HMDB0001434	1670	
Diaminopimelic acid	Amino acids-Peptides-Derivatives	HMDB0001370	99290	C00666
3-Nitrotyrosine	Amino acids-Peptides-Derivatives	HMDB0001904	65124	
Cysteic acid	Amino acids-Peptides-Derivatives	HMDB0002757	25701	C00506
Hydroxykynurenine	Amino acids-Peptides-Derivatives	HMDB0000732	89	C02794
2-Hydroxyphenethylamine	Aromatic compounds-Vitamins-Amines	HMDB0001065	1000	C02735
3-Methoxytyramine	Aromatic compounds-Vitamins-Amines	HMDB0000022	1669	C05587
4-Hydroxyphenylpyruvic acid	Aromatic compounds-Vitamins-Amines	HMDB0000707	979	C01179
Dihydrouracil	Aromatic compounds-Vitamins-Amines	HMDB0000076	649	C00429
Isovaleric acid	Aromatic compounds-Vitamins-Amines	HMDB0000718	10430	C08262
L-Histidinol	Aromatic compounds-Vitamins-Amines	HMDB0003431	165271	C00860
p-Aminobenzoic acid	Aromatic compounds-Vitamins-Amines	HMDB0001392	978	C00568
Purine	Aromatic compounds-Vitamins-Amines	HMDB0001366	1044	C15587
Pyridoxine	Aromatic compounds-Vitamins-Amines	HMDB0000239	1054	C00314
Resorcinol monoacetate	Aromatic compounds-Vitamins-Amines		5055	D02393
Tyramine	Aromatic compounds-Vitamins-Amines	HMDB0000306	5610	C00483
Uracil-5-carboxylic acid	Aromatic compounds-Vitamins-Amines		90301	C03030
Vanillylmandelic acid	Aromatic compounds-Vitamins-Amines	HMDB0000291	736172	C05584

2,6-Dihydroxypyridine	Aromatic compounds-Vitamins-Amines	METPA0354		C03056
3-Hydroxybenzaldehyde	Aromatic compounds-Vitamins-Amines		101	C03067
5-Methylcytosine	Aromatic compounds-Vitamins-Amines	HMDB0002894	65040	C02376
Biliverdin	Aromatic compounds-Vitamins-Amines	HMDB0001008	5353439	C00500
Norepinephrine	Aromatic compounds-Vitamins-Amines	HMDB0000216	439260	C00547
4-Hydroxybenzoic acid	Aromatic compounds-Vitamins-Amines	HMDB0000500	135	C00156
Benzoic acid	Aromatic compounds-Vitamins-Amines	HMDB0001870	243	C00539
3-Amino-4-hydroxybenzoic acid	Aromatic compounds-Vitamins-Amines		65083	C12115
3-Amino-5-hydroxybenzoic acid	Aromatic compounds-Vitamins-Amines		127115	C12107
3-Hydroxyanthranilic acid	Aromatic compounds-Vitamins-Amines	HMDB0001476	86	C00632
3,4-Dihydroxymandelic acid	Aromatic compounds-Vitamins-Amines		85782	C05580
Ethyl-3-indole acetate	Aromatic compounds-Vitamins-Amines			C00954
Hydroquinone	Aromatic compounds-Vitamins-Amines	HMDB0002434	785	C00530
Vanylglycol	Aromatic compounds-Vitamins-Amines	HMDB0001490	10805	C05594
1H-Indole-3-acetamide	Aromatic compounds-Vitamins-Amines	HMDB0029739	397	C02693
Dimethylbenzimidazole	Aromatic compounds-Vitamins-Amines	HMDB0003701	675	C03114
Indoleacetaldehyde	Aromatic compounds-Vitamins-Amines	HMDB0001190	800	C00637
1-Naphthylamine	Aromatic compounds-Vitamins-Amines	METPA1135		C14790
5-Hydroxymethyluracil	Aromatic compounds-Vitamins-Amines	HMDB0000469	78168	C03088
Serotonin	Aromatic compounds-Vitamins-Amines	HMDB0000259	5202	C00780
Caprylic acid	Lipids: Fatty acids-Steroids-Hormones-Vitamins	HMDB0000482	379	C06423

Ergocalciferol	Lipids: Fatty acids-Steroids-Hormones-Vitamins	HMDB0000900	5280793	C05441
Lithocholic Acid	Lipids: Fatty acids-Steroids-Hormones-Vitamins	HMDB0000761	11740284	C03990
Maleic acid	Lipids: Fatty acids-Steroids-Hormones-Vitamins	HMDB0000176	444972	C01384
Mono-methylglutarate	Lipids: Fatty acids-Steroids-Hormones-Vitamins		6993194	
Oleic acid	Lipids: Fatty acids-Steroids-Hormones-Vitamins	HMDB0000207	445639	C00712
Rosmarinic acid	Lipids: Fatty acids-Steroids-Hormones-Vitamins	HMDB0003572	5281792	C01850
Sphinganine	Lipids: Fatty acids-Steroids-Hormones-Vitamins	HMDB0000269	91486	C00836
Vitamin A	Lipids: Fatty acids-Steroids-Hormones-Vitamins	HMDB0000305	445354	C17276
Petroselinic acid	Lipids: Fatty acids-Steroids-Hormones-Vitamins	HMDB0002080	5461010	C08363
All-trans-retinoic acid	Lipids: Fatty acids-Steroids-Hormones-Vitamins	HMDB0001852	444795	C00777
Chenodeoxycholic acid	Lipids: Fatty acids-Steroids-Hormones-Vitamins	HMDB0000518	10133	C02528
Cholesteryl acetate	Lipids: Fatty acids-Steroids-Hormones-Vitamins	HMDB0003822	6427285	C02530
2-Methylglutaric acid	Lipids: Fatty acids-Steroids-Hormones-Vitamins	HMDB0000422	12046	
7-Dehydrocholesterol	Lipids: Fatty acids-Steroids-Hormones-Vitamins	HMDB0000032	439423	C01164
Glycerol	Lipids: Fatty acids-Steroids-Hormones-Vitamins	HMDB0000131	753	C00116
Alpha-Tocopherol	Lipids: Fatty acids-Steroids-Hormones-Vitamins	HMDB0001893	14985	C02477
Elaidic acid	Lipids: Fatty acids-Steroids-Hormones-Vitamins	HMDB0000573	637517	C01712
Cortexolone	Lipids: Fatty acids-Steroids-Hormones-Vitamins	HMDB0000015	53477676	C05488
Deoxycorticosterone acetate	Lipids: Fatty acids-Steroids-Hormones-Vitamins		5952	C14554
Valeric acid	Lipids: Fatty acids-Steroids-Hormones-Vitamins	HMDB0000892	7991	C00803
5'-Deoxyadenosine	Nucleotides-Nucleosides-Derivatives	HMDB0001983	439182	C05198

dCMP	Nucleotides-Nucleosides-Derivatives	HMDB0001202	13945	C00239
Cytidine2',3'-cyclicphosphate	Nucleotides-Nucleosides-Derivatives		5401	C02354
5'UMP	Nucleotides-Nucleosides-Derivatives		3405	C00105
Cytidine	Nucleotides-Nucleosides-Derivatives	HMDB0000089	6253	C00475
Cyclic GMP	Nucleotides-Nucleosides-Derivatives	HMDB0001314	24316	C00942
Deoxyuridine	Nucleotides-Nucleosides-Derivatives	HMDB0000012	13712	C00526
Dimethylsulfone	Organic acids	HMDB0004983	6213	C11142
Malonic acid	Organic acids	HMDB0000691	867	C04025
Pimelic acid	Organic acids	HMDB0000857	385	C02656
4-Heptenal diethyl acetal	Organic acids	HMDB0032306	97750	C04067
Isobutyric acid	Organic acids	HMDB0001873	6590	C02632
D-Maltose	Sugars	HMDB0000163	10991489	C00208
Rhamnose	Sugars	HMDB0000849	25310	C00507
D-Lyxose	Sugars		3759	C00476
2-Acetamido-2-deoxy-beta-glucosylamine	Sugars			
Glucosamine	Sugars	HMDB0001514	439213	C00329
D-Ribose	Sugars	HMDB0000283	5779	C00121
2-Amino-2-deoxy-D-gluconate	Sugars	METPA0433		C03752

Feces Plasma				
Metabolite	Chemical Class	HMDB	PubChem	KEGG
Diethanolamine	Aliphatic compounds cyclic and acyclic	HMDB0004437	8113	C06772
Putrescine	Aliphatic compounds cyclic and acyclic	HMDB0001414	1045	C00134
4-Guanidinobutanoic acid	Amino acids-Peptides-Derivatives	HMDB0003464	500	C01035
5-Aminopentanoic acid	Amino acids-Peptides-Derivatives	HMDB0003355	138	C00431
Aminoadipic acid	Amino acids-Peptides-Derivatives	HMDB0000510	469	C00956
Carnosine	Amino acids-Peptides-Derivatives	HMDB0000033	439224	C00386
L-Norvaline	Amino acids-Peptides-Derivatives		4949	C01826
N-Acetyl-L-aspartic acid	Amino acids-Peptides-Derivatives	HMDB0000812	65065	C01042
N-Acetylglutamic acid	Amino acids-Peptides-Derivatives	HMDB0001138	185	C00624
N-Alpha-acetyllysine	Amino acids-Peptides-Derivatives	HMDB0000446	192590	C12989
2',4'-Dihydroxyacetophenone	Aromatic compounds-Vitamins-Amines	HMDB0029659	6990	C03663
2-Aminobenzoic acid	Aromatic compounds-Vitamins-Amines	HMDB0001123	227	C00108
3-Hydroxybenzoic acid	Aromatic compounds-Vitamins-Amines	HMDB0002466	7420	C00587
Caffeic acid	Aromatic compounds-Vitamins-Amines	HMDB0001964	1549111	C01481
Histamine	Aromatic compounds-Vitamins-Amines	HMDB0000870	774	C00388
Hydroxyphenyllactic acid	Aromatic compounds-Vitamins-Amines	HMDB0000755	9378	C03672
Indole-3-methyl acetate	Aromatic compounds-Vitamins-Amines	HMDB0029738	74706	

Phenylacetaldehyde	Aromatic compounds-Vitamins-Amines	HMDB0006236	998	C00601
Pyridoxamine	Aromatic compounds-Vitamins-Amines	HMDB0001431	1052	C00534
Salicylamide	Aromatic compounds-Vitamins-Amines	HMDB0015687	5147	NA
Tryptamine	Aromatic compounds-Vitamins-Amines	HMDB0000303	1150	C00398
17a-Estradiol	Lipids: Fatty acids-Steroids-Hormones-Vitamins	HMDB0000429	68570	C02537
2,3-Dihydroxypropyl tetradecanoate	Lipids: Fatty acids-Steroids-Hormones-Vitamins		79050	
21-Tetrahydroxy-5-alpha-pregnan-20-one	Lipids: Fatty acids-Steroids-Hormones-Vitamins		5864	
3-Methylglutaric acid	Lipids: Fatty acids-Steroids-Hormones-Vitamins	HMDB0000752	12284	
Butyric acid	Lipids: Fatty acids-Steroids-Hormones-Vitamins	HMDB0000039	264	C00246
Cortisone	Lipids: Fatty acids-Steroids-Hormones-Vitamins	HMDB0002802	225609	C00762
Deoxycholic acid	Lipids: Fatty acids-Steroids-Hormones-Vitamins	HMDB0000626	222528	C04483
Dihydroxy-beta-cholanate	Lipids: Fatty acids-Steroids-Hormones-Vitamins			
Gamma-Linolenic acid	Lipids: Fatty acids-Steroids-Hormones-Vitamins	HMDB0003073	5280933	C06426
Glycerol monoacetate	Lipids: Fatty acids-Steroids-Hormones-Vitamins		33510	
Leukotriene B4	Lipids: Fatty acids-Steroids-Hormones-Vitamins	HMDB0001085	5283128	C02165
Deoxyadenosine	Nucleotides-Nucleosides-Derivatives	HMDB0000101	13730	C00559
Adipic acid	Organic acids	HMDB0000448	196	C06104
Isocitric acid	Organic acids	HMDB0000193	1198	C00311
Propionic acid	Organic acids	HMDB0000237	1032	C00163
D-Glucuronic acid	Sugars	HMDB0000127	94715	C00191

List of metabolites according to the platform

Table S5: Metabolites detected by platform in plasma, milk and feces. In bold the platform where the metabolite was annotated with the lowest CV (best reproducibility)

Plasma (Blood :MeOH : CHCl ₃ 1 :1 :1)	
Metabolite	Analytical platform
3-Hydroxycapric acid	RP+
1-hydroxy-2-naphthoate	HILIC-
1-Methyladenosine	RP- HILIC+
Glycerol monoacetate	HILIC+
2',4'-Dihydroxyacetophenone	RP+
2,4-Dihydroxypyrimidine-5-carboxylic acid	HILIC-
Gentisic acid	HILIC-
2-Aminophenol	HILIC+
Deoxyadenosine	NMR
2-Deoxy-D-Glucose	RP+
Deoxyguanosine	HILIC-
2-Hydroxybutyric acid	RP- NMR
Ortho-Hydroxyphenylacetic acid	HILIC-
Ketoleucine	RP- NMR

Protocatechuic acid	HILIC-
3,4-Dihydroxybenzeneacetic acid	HILIC-
3-(2-Hydroxyphenyl)propanoic acid	RP- HILIC-
Hydroxyphenyllactic acid	HILIC-
21-Tetrahydroxy-5-alpha-pregnan-20-one	HILIC-
Dihydroxy-beta-cholante	HILIC-
3-Hydroxymethylglutaric acid	HILIC-
3-Hydroxybenzoic acid	HILIC-
3-Hydroxybutyric acid	NMR
(S)-3-Hydroxyisobutyric acid	HILIC- NMR
3-Hydroxyphenylacetic acid	HILIC-
3-Methylglutaric acid	RP-
3-Methyldioxyindole	RP-
Ureidopropionic acid	RP-
4-Acetamidobutanoic acid	RP-
Gamma-Aminobutyric acid	RP+
4-Hydroxycinnamic acid	HILIC+
4-Guanidinobutanoic acid	RP+
4-Hydroxy-L-proline	RP+
p-Hydroxyphenylacetic acid	HILIC-
5-Aminolevulinic acid	RP+
5-Aminopentanoic acid	RP+

5-Hydroxyindoleacetic acid	RP+ HILIC-
5'-Methylthioadenosine	RP+ HILIC+
Pyroglutamic acid	RP+
Acetic acid	NMR
Acetoacetic acid	HILIC-
Acetone	NMR
N-Acetyl-L-alanine	RP+
N-Acetyl-L-aspartic acid	HILIC+
N-Acetylglutamic acid	RP+
Acetylglycine	RP-
N-Acetylleucine	RP+
N-Acetylneuraminate	RP-
N-Acetyl-L-phenylalanine	RP- HILIC-
N-Acetylputrescine	HILIC+
N-Acetylserine	RP-
N-Acetylserotonin	HILIC+
N-acetyltryptophan	RP-
Adenine	RP+
Adenosine	HILIC-
Adipic acid	RP+
Allantoin	RP- HILIC+ NMR
Allose	HILIC-

Alpha-D-Glucose	RP- HILIC- NMR
Aminoadipic acid	RP-
2-Aminobenzoic acid	HILIC+
L-Arabitol	HILIC-
L-Arginine	RP-
L-Asparagine	RP- HILIC+
L-Aspartic acid	RP-
Azelaic acid	RP-
Benzyl alcohol	RP- HILIC-
Beta-Alanine	RP+ NMR
Betaine	RP+
Bilirubin	HILIC+
Biotin	RP+
Butyric acid	NMR
Caffeic acid	HILIC-
L-Carnitine	RP+
Carnosine	RP- NMR
Pyrocatechol	RP-
Choline	NMR
trans-Cinnamic acid	RP+ HILIC-
Citramalic acid	RP-
Citric acid	NMR

Citrulline	RP-
Cortisone	HILIC-
Creatine	RP- NMR
Creatinine	NMR
Cyclohexane-1,2-Diol	HILIC+
L-Cystine	RP-
Cytosine	RP+
4-Trimethylammoniobutanoic acid	RP+
Deoxycholic acid	HILIC-
Deoxycytidine	HILIC-
Diethanolamine	HILIC+
Dihydroxyacetone phosphate	HILIC-
N,N-Dimethylphenethylamine	HILIC+
Dimethylamine	NMR
Dimethylglycine	NMR
17a-Estradiol	HILIC+
O-Phosphoethanolamine	RP-
Ethylmalonic acid	RP-
Formic acid	NMR
Formyl-L-methionylpeptide	RP-
Galactitol	HILIC-
D-Galactosamine	RP+

D-Galactose	HILIC-
D-Glucuronic acid	RP-
L-Glutamic acid	RP-
L-Glutamine	RP+
Glyceric acid	RP-
Glycerophosphocholine	RP+
Glycine	RP+ NMR
Glycocholic acid	RP-
Glycolaldehyde dimer	HILIC+
Guanidoacetic acid	RP+ HILIC+
Guanine	HILIC-
Guanosine	HILIC+
Guanosine monophosphate	RP+
Caproic acid	HILIC+
Hippuric acid	RP- HILIC- NMR
Histamine	HILIC+
L-Histidine	RP- NMR
Homogentisic acid	HILIC-
L-Homoserine	RP-
Homovanillic acid	HILIC-
Hypoxanthine	RP-
Indoleacetic acid	RP+ HILIC-

Indoxyl sulfate	RP- HILIC-
Inosine	RP+ HILIC+
Isocitric acid	RP-
L-Isoleucine	NMR
N6-(delta2-Isopentenyl)-adenine	RP-
L-Kynurenine	RP+
L-Lactic acid	RP- NMR
Alpha-Lactose	NMR
L-Leucine	NMR
L-Norleucine	RP+
Leukotriene B4	RP+
Gamma-Linolenic acid	HILIC+
Lumichrome	RP+ HILIC+
L-Lysine	RP+ NMR
L-Malic acid	RP-
D-Mannose	HILIC+ NMR
L-Methionine	RP- NMR
Methyl beta-D-glucopyranoside	HILIC-
Indole-3-methyl acetate	RP+ HILIC+
Methyl jasmonate	HILIC+
Methylguanidine	HILIC+
3-Methylhistidine	NMR

Methylmalonic acid	HILIC-
myo-Inositol	HILIC-
N-Alpha-acetyllysine	RP+
L-Norvaline	RP+
Acetylcholine	NMR
12-Hydroxydodecanoic acid	RP- HILIC-
Ornithine	RP+
Orotic acid	HILIC-
Pantothenic acid	HILIC+
Paraxanthine	RP+ HILIC+
Phenylacetaldehyde	HILIC-
Phenylacetic acid	HILIC-
L-Phenylalanine	RP+ HILIC+
Phenylpyruvic acid	HILIC+
Phosphorylcholine	NMR
Pipecolic acid	RP- HILIC+
L-Proline	RP+
Propanal	HILIC+
Propionic acid	NMR
Putrescine	RP+
Pyridoxamine	RP+
Pyruvic acid	NMR

2,3-Dihydroxypropyl tetradecanoate	RP+ HILIC+
Ribitol	HILIC-
Salicylamide	HILIC+
Sarcosine	NMR
L-Serine	RP+
Sorbose	HILIC-
Suberic acid	RP-
Succinic acid	RP-
Taurine	RP-
Lithocholytaurine	HILIC-
Theobromine	HILIC+
L-Threonine	RP+ NMR
Thymidine	HILIC+ HILIC-
Thyroxine	RP-
Trigonelline	HILIC+
Trimethylamine	HILIC+
Tryptamine	RP+
L-Tryptophan	RP- HILIC+ NMR
L-Tyrosine	RP- HILIC+ NMR
Uracil	RP+ HILIC+
Uric acid	RP+ HILIC-
Uridine	RP- HILIC+

Urocanic acid	RP+
L-Valine	RP+ HILIC+ NMR
Xanthine	RP+ HILIC-
Xanthosine	HILIC-

Milk	
(Milk :H ₂ O :MeOH :CHCl ₃ 1 :3 :4 :6)	
Metabolites	Analytical platform
3-Hydroxycapric acid	RP- HILIC+
1-Aminocyclopropanecarboxylic acid	RP+
1-Methyladenosine	HILIC+
2,4-Dihydroxypyrimidine-5-carboxylic acid	HILIC-
Gentisic acid	HILIC-
2-Aminophenol	HILIC+
2-Deoxy-D-Glucose	RP+ HILIC-
Deoxyguanosine	HILIC-
2-Hydroxybutyric acid	RP-
Ortho-Hydroxyphenylacetic acid	HILIC-
2-Hydroxypyridine	HILIC+
Citraconic acid	HILIC-
Oxoglutaric acid	NMR
Protocatechuic acid	HILIC-

3,4-Dihydroxybenzeneacetic acid	HILIC-
Cyclic AMP	HILIC+
3-(2-Hydroxyphenyl)propanoic acid	RP- HILIC-
3-Aminoisobutanoic acid	HILIC-
3-Hydroxymethylglutaric acid	HILIC-
3-Hydroxybutyric acid	NMR
3-Hydroxyphenylacetic acid	HILIC-
3-Methyldioxyindole	RP+
3-Methyladenine	RP+ HILIC-
Ureidopropionic acid	RP-
4-Acetamidobutanoic acid	RP- HILIC+
Gamma-Aminobutyric acid	RP+ HILIC+
Kynurenic acid	RP+
4-Hydroxybenzaldehyde	HILIC-
Oxfenicine	RP+
4-Hydroxy-L-proline	RP+ HILIC+
p-Hydroxyphenylacetic acid	RP- HILIC-
Imidazoleacetic acid	HILIC-
Ketoleucine	RP- HILIC-
4-Methylcatechol	RP-
5-Aminolevulinic acid	RP+ HILIC+
5-Hydroxyindoleacetic acid	HILIC+

5-Hydroxylysine	RP+
5'-Methylthioadenosine	RP+ HILIC+
Pyroglutamic acid	RP-
L-Fucose	HILIC-
Acetamide	NMR
Acetic acid	NMR
Acetoacetic acid	HILIC- NMR
N-Acetyl-L-alanine	RP+
L-Acetylcarnitine	HILIC+ NMR
N-Acetylgalactosamine	HILIC-
N-Acetyl-D-glucosamine	HILIC+
Acetylglycine	RP+
N-Acetylleucine	HILIC-
N-Acetylmannosamine	RP+ HILIC-
N-Acetyl-L-methionine	RP-
N-Acetylneuraminate	RP-
N-Acetyl-L-phenylalanine	RP- HILIC-
N-Acetylputrescine	HILIC+
N-Acetylserine	RP-
N-Acetylserotonin	HILIC+
N-acetyltryptophan	RP-
Adenine	HILIC+

Adenosine	RP+ HILIC-
ADP-glucose	RP-
Adenosine monophosphate	RP-
Allantoin	RP- HILIC+
Allose	HILIC-
L-Allothreonine	HILIC+
Galactose 1-phosphate	HILIC+
Alpha-D-Glucose	RP- HILIC- NMR
Anserine	RP+
L-Arabitol	RP- HILIC-
L-Arginine	RP+ HILIC-
L-Asparagine	RP+ HILIC-
L-Aspartic acid	RP-
Azelaic acid	RP-
Benzyl alcohol	HILIC-
Beta-Alanine	RP+ HILIC+ NMR
Betaine	RP+ HILIC+
Biotin	RP- HILIC+
Butanal	HILIC+
L-Carnitine	RP+ HILIC+
Pyrocatechol	RP-
Cellobiose	HILIC-

Cholic acid	HILIC-
Choline	RP+ NMR
trans-Cinnamic acid	RP+
Citramalic acid	HILIC+
Citric acid	NMR
Citrulline	RP- HILIC-
Corticosterone	RP+
Cortisol	RP+
Cortisol-21-acetate	RP+
Creatine	RP+ HILIC+ NMR
Phosphocreatine	NMR
Creatinine	RP- HILIC+
Cyclohexane-1,2-Diol	HILIC+
Cytosine	RP+ HILIC+
4-Trimethylammoniobutanoic acid	RP+ HILIC+
Deoxycytidine	HILIC+
Dethiobiotin	RP+
Diacetyl	HILIC+
L-Dihydroorotic acid	RP+
Dimethyl sulfone	NMR
N,N-Dimethylphenethylamine	HILIC+
Dimethylamine	NMR

Epinephrine	RP+
Ethanolamine	HILIC+
O-Phosphoethanolamine	RP-
Ethylmalonic acid	HILIC-
trans-Ferulic acid	RP- HILIC+
Formic acid	NMR
Formyl-L-methionylpeptide	RP-
D-Fructose	HILIC-
Fumaric acid	NMR
Galactaric acid	RP-
Galactitol	HILIC-
D-Galactosamine	RP+
D-Galactose	HILIC-
Gluconic acid	RP-
Glucosamine 6-phosphate	RP-
Glucose 6-phosphate	RP-
L-Glutamic acid	RP+ HILIC-
L-Glutamine	RP+ HILIC+
Glyceraldehyde-3-phosphatediethylacetal	RP+
Glyceric acid	RP-
Glycerol 3-phosphate	HILIC+
Glycerophosphocholine	RP+ HILIC+

Glycine	RP+ HILIC+
Glycocholic acid	RP-
Glycolaldehyde dimer	HILIC+
Guanidoacetic acid	RP+ HILIC+
Guanine	HILIC+
Guanosine	RP+ HILIC+
Heptanoic acid	HILIC+
Caproic acid	HILIC+
Hippuric acid	RP- HILIC+ NMR
L-Histidine	RP-
Homogentisic acid	HILIC+
L-Homoserine	RP- HILIC-
Homovanillic acid	HILIC-
Hypotaurine	HILIC-
Hypoxanthine	RP- HILIC+
Indoleacetic acid	RP+
Tryptophanol	RP+ HILIC-
Indolepyruvate	HILIC+
Indoxyl sulfate	RP- HILIC-
Inosine	RP- HILIC+ NMR
L-Isoleucine	HILIC+
N6-(delta2-Isopentenyl)-adenine	RP-

L-Kynurenine	RP+
L-Lactic acid	RP- HILIC- NMR
Alpha-Lactose	NMR
L-Leucine	HILIC+
Lumichrome	RP+ HILIC-
L-Lysine	RP+
L-Malic acid	RP-
Mannitol	RP- HILIC-
D-Mannose	HILIC+
Melatonin	HILIC+
L-Methionine	RP-
Methyl beta-D-glucopyranoside	HILIC-
Methylguanidine	HILIC+
3-Methylhistidine	RP+
Methylmalonic acid	RP+
N-Methyltryptamine	RP+ HILIC+
myo-Inositol	RP+ HILIC- NMR
N-Trimethyllysine	RP+ HILIC+
Niacinamide	RP+ HILIC+
Nicotinic acid	RP-
L(-)-Nicotine	HILIC+
N-Methylhydantoin	NMR

L-Norleucine	HILIC+
Phenylacetyl glycine	NMR
Acetylcholine	NMR
12-Hydroxydodecanoic acid	RP-
Ornithine	RP+ HILIC-
Orotic acid	HILIC- NMR
Palatinose	HILIC-
Pantolactone	HILIC-
Pantothenic acid	RP- HILIC+
Paraxanthine	HILIC+
L-Phenylalanine	RP- HILIC+
Phosphorylcholine	RP+ NMR
Pipecolic acid	HILIC+
L-Proline	RP+ HILIC+
Propanal	HILIC+
Pterin	RP+
Pyrrole-2-carboxylic acid	HILIC+
Ribitol	HILIC-
Riboflavin	HILIC+
Glucaric acid	RP-
Salicyluric acid	HILIC+
Sarcosine	HILIC+

L-Serine	RP- HILIC+
Sorbitol	HILIC-
L-Sorbose	HILIC-
Suberic acid	RP-
Succinic acid	RP- HILIC+ NMR
Sucrose	HILIC-
D-Tagatose	HILIC-
Taurine	RP- HILIC+ NMR
Lithocholytaurine	HILIC-
Theobromine	HILIC+
Theophylline	HILIC+
L-Threonine	RP+ HILIC-
Thymidine	HILIC-
Thymine	RP+ HILIC+
trans-Aconitic acid	RP- HILIC- NMR
Trigonelline	RP+ HILIC+
Trimethylamine	HILIC+
L-Tryptophan	RP- HILIC+
L-Tyrosine	RP+ HILIC+
Uracil	RP- HILIC+
Uric acid	RP+ HILIC-
Uridine	RP- NMR

Uridine diphosphategalactose	HILIC- NMR
Uridine diphosphate glucose	HILIC- NMR
Uridine diphosphate-N-acetylgalactosamine	HILIC-
Uridine-5-diphospho-n-acetylglucosamine	HILIC- NMR
Urocanic acid	RP+ HILIC-
L-Valine	RP+
Xanthine	RP- HILIC-
D-Xylitol	HILIC-

FECS (MeOH : H ₂ O 4 :1)	
Metabolites	Analytical platform
3-Hydroxycapric acid	RP+
1-Aminocyclopropanecarboxylic acid	RP+ HILIC +
1-Methyladenosine	RP+ HILIC +
1-Naphthylamine	HILIC+
Glyceryl monoacetate	HILIC+
2',4'-Dihydroxyacetophenone	HILIC-
2,4-Dihydroxypyrimidine-5-carboxylic acid	HILIC-
Gentisic acid	RP- HILIC-
Diaminopimelic acid	RP+

2,6-Dihydroxypyridine	HILIC+
2-Acetamido-2-deoxy-beta-glucosylamine	RP+ HILIC-
2-Aminoisobutyric acid	HILIC+
Ciliatine	RP-
2-Aminophenol	RP+ HILIC-
Deoxyadenosine	RP- HILIC+
dCMP	RP-
2-Deoxy-D-Glucose	RP+ HILIC-
Deoxyguanosine	HILIC-
2-Hydroxybutyric acid	RP-
Ortho-Hydroxyphenylacetic acid	HILIC- NMR
2-Hydroxypyridine	HILIC+
2-Methylglutaric acid	HILIC-
Citraconic acid	HILIC-
Quinaldic acid	HILIC-
Protocatechuic acid	HILIC-
3,4-Dihydroxybenzeneacetic acid	HILIC-
L-Dopa	RP+ HILIC+
3-(2-Hydroxyphenyl)propanoic acid	RP- HILIC-
Hydroxyphenyllactic acid	RP-
4-Hydroxyphenylpyruvic acid	RP+

21-Tetrahydroxy-5-alpha-pregnan-20-one	RP+ HILIC-
Dihydroxy-beta-cholanate	HILIC-
Lithocholic Acid	RP-
3-Amino-4-hydroxybenzoic acid	HILIC+
3-Amino-5-hydroxybenzoic acid	RP+
3-Aminoisobutanoic acid	HILIC-
3-Dehydroshikimate	RP-
3-Hydroxyanthranilic acid	RP+ HILIC+
3-Hydroxybenzaldehyde	HILIC-
3-Hydroxybenzoic acid	RP- HILIC-
Hydroxykynurenine	RP+
3-Hydroxyphenylacetic acid	RP- HILIC-
Vanillylmandelic acid	RP- HILIC+
3-Methoxytyrosine	HILIC+
3-Methoxytyramine	RP+ HILIC-
3-Methylglutaric acid	RP- HILIC-
3-Methyldioxyindole	RP- HILIC+
3-Methyladenine	RP+ HILIC+
3-Nitrotyrosine	RP-
3-Sulfinioalanine	RP-
Ureidopropionic acid	RP+ HILIC+

4-Acetamidobutanoic acid	HILIC-
p-Aminobenzoic acid	HILIC-
4-Guanidinobutanoic acid	RP+ HILIC+
Kynurenic acid	RP+ HILIC+
Vanylglycol	HILIC+
4-Hydroxybenzaldehyde	HILIC-
4-Hydroxybenzoic acid	HILIC-
Oxfenicine	RP+
4-Hydroxy-L-proline	RP+ HILIC+
p-Hydroxyphenylacetic acid	RP+ HILIC-
Imidazoleacetic acid	RP+ HILIC+
Ketoleucine	RP- HILIC-
Dihydrouracil	RP+ HILIC+
5-Aminolevulinic acid	RP+
5-Aminopentanoic acid	RP+ HILIC+
5'-Deoxyadenosine	HILIC+
5-Hydroxyindoleacetic acid	RP+ HILIC-
5-Hydroxylysine	RP+
5-Hydroxymethyluracil	RP-
5-Hydroxy-L-tryptophan	RP-
5-Methylcytosine	RP+ HILIC+

5'-Methylthioadenosine	RP+ HILIC+
Pyroglutamic acid	RP- HILIC-
Valerolactone	HILIC+
Pimelic acid	HILIC-
Acetamide	NMR
Acetic acid	NMR
Acetoin	HILIC-
N-Acetyl-L-alanine	RP+
N-Acetyl-L-aspartic acid	RP-
L-Acetylcarnitine	HILIC+ NMR
N-Acetylgalactosamine	HILIC-
N-Acetyl-D-glucosamine	RP- HILIC+
N-Acetylglutamic acid	RP+
Acetylglycine	RP-
N-Acetylleucine	RP+
N-Acetylmannosamine	RP+ HILIC+
N-Acetyl-L-methionine	RP- HILIC+
N-Acetylneuraminate	RP+
N-Acetyl-L-phenylalanine	RP+ HILIC+
N-Acetylputrescine	RP+ HILIC+
N-Acetyserine	RP+

N-Acetylserotonin	RP- HILIC+
N-acetyltryptophan	RP+
Adenine	RP+ HILIC+
Adenosine	RP+ HILIC+
Cyclic AMP	HILIC-
S-Adenosylhomocysteine	HILIC+
Adipic acid	RP- HILIC-
Agmatine	RP+
L-Alanine	HILIC+
Allantoin	RP-
L-Allothreonine	HILIC+
Alpha-D-Glucose	HILIC-
Alpha-Tocopherol	HILIC+
Aminoadipic acid	RP+ HILIC+
Anserine	HILIC+
2-Aminobenzoic acid	HILIC-
L-Arabitol	RP-
L-Arginine	RP+ HILIC+
L-Asparagine	RP+ HILIC-
L-Aspartic acid	RP+
Azelaic acid	RP- HILIC-

Benzoic acid	HILIC-
Benzyl alcohol	HILIC-
Beta-Alanine	RP+ HILIC+ NMR
Betaine	RP+ HILIC+ NMR
Biliverdin	HILIC+
Biotin	RP+ HILIC+
Butyric acid	HILIC- NMR
Cadaverine	RP+ HILIC+
Caffeic acid	RP-
Caprylic acid	HILIC-
L-Carnitine	RP+ HILIC+
Carnosine	RP+ HILIC+
Pyrocatechol	RP- HILIC-
Chenodeoxycholic acid	HILIC-
Cholic acid	RP+
7-Dehydrocholesterol	HILIC+
Cholesteryl acetate	HILIC+
Choline	RP+ NMR
trans-Cinnamic acid	RP+ HILIC-
Citramalic acid	RP- HILIC+
Citrulline	RP+ HILIC+

Corticosterone	HILIC+
Cortisol	RP+
Cortisol-21-acetate	RP-
Cortisone	HILIC-
Creatine	RP+
Creatinine	RP+ HILIC+
Cyclohexane-1,2-Diol	HILIC-
L-Cystathionine	RP-
Cysteic acid	RP- HILIC-
Cytidine	RP+ HILIC+
Cytidine2',3'-cyclicphosphate	RP-
Cytosine	RP+ HILIC+
4-Trimethylammonibutanoic acid	RP+ HILIC+
Deoxycholic acid	HILIC-
Deoxycorticosterone acetate	RP+
Deoxycytidine	RP- HILIC+
Deoxyuridine	HILIC+
Diacetyl	HILIC+
Diethanolamine	RP+ HILIC+
4-Heptenal diethyl acetal	HILIC-
L-Dihydroorotic acid	RP-

3,4-Dihydroxymandelicacid	RP-
N,N-Dimethylphenethylamine	HILIC - NMR
Dimethylbenzimidazole	RP+
Elaidic acid	HILIC-
Epinephrine	RP+
17a-Estradiol	HILIC+
Ethanolamine	HILIC+
O-Phosphoethanolamine	RP+
Ethyl-3-indole acetate	HILIC-
Ethylmalonic acid	RP- HILIC-
trans-Ferulic acid	HILIC-
Formic acid	NMR
N-Formylglycine	RP+
Formyl-L-methionylpeptide	RP+
Fumaric acid	RP-
Galactitol	RP+
D-Galactosamine	RP+
Gluconic acid	RP-
2-Amino-2-deoxy-D-gluconate	RP-
Glucosamine	RP- HILIC+
Glucosamine 6-phosphate	RP-

Glucose 6-phosphate	RP-
D-Glucuronic acid	RP-
L-Glutamic acid	RP+ HILIC+
L-Glutamine	RP+ HILIC-
Glyceraldehyde-3-phosphatediethylacetal	RP-
Glyceric acid	RP-
Glycerol	NMR
Glycerophosphocholine	RP+ HILIC+
Glycine	RP+ HILIC+ NMR
Glycocholic acid	RP-
Guanidoacetic acid	HILIC+
Guanine	RP- HILIC+
Guanosine	RP+ HILIC+
Cyclic GMP	RP-
Caproic acid	HILIC-
Hippuric acid	RP- HILIC+
Histamine	RP+ HILIC+
L-Histidine	RP+ HILIC+
L-Histidinol	HILIC+
Homocysteine	RP+
Homogentisic acid	RP+

L-Homoserine	RP-
Homovanillic acid	HILIC-
Hydroquinone	HILIC-
Hypoxanthine	RP+ HILIC+
Indoleacetaldehyde	HILIC+
1H-Indole-3-acetamide	RP+ HILIC+
Indoleacetic acid	RP+ HILIC-
Tryptophanol	HILIC+
Indolepyruvate	HILIC-
Indoxyl sulfate	HILIC-
Inosine	RP- HILIC-
Isobutyric acid	HILIC- NMR
Isocitric acid	RP-
L-Isoleucine	HILIC+ NMR
N6-(delta2-Isopentenyl)-adenine	RP- HILIC+
Isovaleric acid	NMR
L-Kynurenine	RP-
L-Lactic acid	RP- HILIC- NMR
L-Leucine	HILIC+
L-Norleucine	RP+
Leukotriene B4	RP+ HILIC-

Gamma-Linolenic acid	HILIC+
Lumichrome	RP+ HILIC+
L-Lysine	RP+ HILIC+
D-Lyxose	RP+ HILIC-
L-Malic acid	RP-
Maleic acid	HILIC-
Malonic acid	RP-
D-Maltose	RP-
Mannitol	RP-
D-Mannose	HILIC+
L-Methionine	RP+ HILIC+
Methyl beta-D-glucopyranoside	HILIC-
Methylguanidine	HILIC+
3-Methylhistidine	RP+
Indole-3-methyl acetate	RP+ HILIC+
N-Methyltryptamine	RP+ HILIC+
Mono-methylglutarate	HILIC-
myo-Inositol	HILIC-
N-Alpha-acetyllysine	RP- HILIC+
N-Trimethyllysine	RP+ HILIC+
Niacinamide	RP+ HILIC+

Nicotinic acid	RP+ HILIC+
Norepinephrine	RP+
L-Norvaline	RP+ HILIC+
Acetylcholine	NMR
Oleic acid	RP+ HILIC+
12-Hydroxydodecanoic acid	RP+ HILIC-
Ornithine	RP+ HILIC+
Orotic acid	RP+ HILIC-
Pantolactone	HILIC-
Pantothenic acid	RP+ HILIC+
Paraxanthine	HILIC+
Valeric acid	NMR
Petroselinic acid	HILIC-
Phenylacetaldehyde	HILIC-
L-Phenylalanine	RP+ HILIC+ NMR
2-Hydroxyphenethylamine	HILIC+
Phosphorylcholine	NMR
DL-O-Phosphoserine	RP-
Picolinic acid	HILIC+
Pipecolic acid	RP+
L-Proline	RP+ HILIC+

Propanal	HILIC+
Propionic acid	NMR
Pterin	RP+ HILIC+
Purine	RP+ HILIC+
Putrescine	RP+
Pyridoxamine	RP+
Pyridoxine	RP+
Pyrrole-2-carboxylic acid	RP+ HILIC-
Quinic acid	RP-
2,3-Dihydroxypropyl tetradecanoate	RP+
Cortexolone	HILIC+
Resorcinol monoacetate	HILIC-
All-trans-retinoic acid	RP+ HILIC+
Vitamin A	HILIC+
Rhamnose	HILIC-
Ribitol	HILIC-
Riboflavin	RP+ HILIC+
D-Ribose	HILIC-
Rosmarinic acid	HILIC-
Salicylamide	RP- HILIC-
Salicyluric acid	HILIC+

Sarcosine	HILIC-
L-Serine	RP- HILIC+
Serotonin	RP+ HILIC+
Shikimic acid	HILIC+
Spermidine	RP+ HILIC+
Sphinganine	RP+
Suberic acid	RP- HILIC-
Succinic acid	RP- HILIC+ NMR
Taurine	RP- HILIC-
L-Threonine	RP+ HILIC+ NMR
Thymidine	RP- HILIC-
Thymine	RP+ HILIC-
trans-Aconitic acid	RP-
Trigonelline	RP+ HILIC+
Trimethylamine	HILIC+
Tryptamine	HILIC+
L-Tryptophan	RP+ HILIC+
Tyramine	HILIC+
L-Tyrosine	RP+ HILIC- NMR
Uracil	RP+ HILIC-
Uracil-5-carboxylic acid	RP+

Uric acid	RP+
Uridine	RP+ HILIC+
5'UMP	HILIC+
Urocanic acid	RP+ HILIC+
L-Valine	RP+ HILIC+ NMR
Ergocalciferol	HILIC+
Xanthine	RP+ HILIC-