

Supplementary Table 2. Metabolites previously reported in newborns and infants

Metabolite	HMDB ID	Mean \pm SD μ M	Mean \pm SD (μ M/mM creatinine)	2.5% - 97.5% Percentile (μ M/mM creatinine)	Literature values (μ M/mM creatinine)
Glycine	HMDB0000123	1581 \pm 957.3	362.1 \pm 185.5	102.6-853.6	113-1427 ^a [1]
Alanine	HMDB0000161	353.5 \pm 261.1	76.6 \pm 28.6	32.2-147.8	10.5-340.1 ^a [2]
Serine	HMDB0000187	354.9 \pm 207.8	78.3 \pm 27.4	32.2-145.5	180 (25.3-334.7) ^c [3]
Proline	HMDB0000162	126.9 \pm 86.4	28.5 \pm 15.4	9.5-78.2	8-260 ^a [1]
Valine	HMDB0000883	31.2 \pm 25.6	6.75 \pm 3.40	1.0-18.4	1.2-23.9 ^a [2]
Threonine	HMDB0000167	151.4 \pm 110.4	34.0 \pm 19.5	9.24-96.2	2.83-137.6 ^a [2]
Taurine	HMDB0000251	5526 \pm 5919	1067 \pm 649.5	74.6-2841	250-910 ^a [4]
4-Hydroxyproline	HMDB0000725	136.1 \pm 63.6	34.3 \pm 18.3	8.12-92.2	4-230 ^a [1]
Leucine	HMDB0000687	27.9 \pm 24.1	5.95 \pm 2.87	0.33-13.4	6.67 (0-13.33) ^c [3]
Isoleucine	HMDB0000172	13.3 \pm 11.1	2.86 \pm 1.44	0.29-7.30	3.75 \pm 2.75 ^b [5]
Asparagine	HMDB0000168	14.07 \pm 9.35	3.72 \pm 2.5	0.42-10.5	0.0-5.0 ^a [6]
Aspartic acid	HMDB0000191	78.9 \pm 47.7	17.6 \pm 7.2	5.57-34.6	25.1 (20-30.2) ^c [3]
Glutamine	HMDB0000641	269.5 \pm 203.4	57.2 \pm 26.6	16.2-134.4	15.7-337.6 ^a [2]
Glutamic acid	HMDB0000148	61 \pm 69.6	12.5 \pm 8.21	1.96-35.3	37.8 (8.89-66.7) ^c [3]
Methionine	HMDB0000696	11.0 \pm 9.3	2.24 \pm 0.89	0.54-4.81	4.45 (0-8.89) ^c [3]
Histidine	HMDB0000177	373.4 \pm 364.6	71.4 \pm 41.2	21.1-188.1	16.4-433.5 ^a [2]
a-Aminoadipic acid	HMDB0000510	33.3 \pm 27.9	6.95 \pm 3.91	1.23-15.5	1.1-31.1 ^a [2]
Phenylalanine	HMDB0000159	37.8 \pm 32.1	7.58 \pm 2.50	4.14-14.2	14.7 (5.33-24) ^c [3]
Arginine	HMDB0000517	73.5 \pm 54.2	15.3 \pm 5.47	6.82-30.5	1.1-63.3 ^a [2]
Tyrosine	HMDB0000158	26.9 \pm 18.7	5.91 \pm 3.05	2.10-14.8	4.41-77.5 ^a [2]
Tryptophan	HMDB0000929	15.7 \pm 10.5	3.36 \pm 0.98	1.90-6.03	1.6-35.6 ^a [2]
Carnosine	HMDB0000033	31.1 \pm 49.7	5.81 \pm 7.60	0.47-35.5	3.05-115.4 ^a [2]
Ornithine	HMDB0000214	29.3 \pm 20.4	7.07 \pm 4.93	1.44-24.4	0-29.9 ^a [2]
Lysine	HMDB0000182	190.2 \pm 103.3	46.9 \pm 29.1	10.5-140.5	3-170 ^a [1]
Sarcosine	HMDB0000271	10.93 \pm 9.57	2.43 \pm 1.72	0.55-9.98	0-8.48 ^a [2]
Tyramine	HMDB0000306	4.32 \pm 2.67	0.95 \pm 0.49	0.30-2.54	0.0 ^a [4]
Creatine	HMDB0000064	209.2 \pm 325.1	56.0 \pm 105.1	4.66-455.3	25-776 ^a [7]
Betaine	HMDB0000043	780.5 \pm 311.8	189.6 \pm 69.8	74.1-410.3	44-1200 ^a [4]
Choline	HMDB0000097	92.39 \pm 103.2	18.32 \pm 11.05	3.99-50.7	0-94 ^a [8]
1-Methylhistidine	HMDB0000001	299.4 \pm 287.8	54.9 \pm 28.4	18.6-145.2	1.92-47.4 ^a
3-Methylhistidine	HMDB0000479				9.95-39.6 ^a [2]
Lactic acid	HMDB0000190	741.5 \pm 779.5	166.9 \pm 171.8	47-774.2	0-540 ^a [9]
3-Hydroxybutyric acid	HMDB0000357	27.8 \pm 29.5	5.52 \pm 5.15	0.72-23.3	2.0 (0.5-9.8) ^c [10]
alpha-Ketoglutaric acid	HMDB0000208	494.6 \pm 214.9	135.0 \pm 5.01	30.8-398.2	150.5 (10.0-836.3)[10]
Citric acid	HMDB0000094	1833 \pm 1666	396.6 \pm 221	39.6-893.5	46-1400 ^a [4]
Succinic acid	HMDB0000254	91.3 \pm 69.2	21.8 \pm 15.4	4.35-81.2	9-360 ^a [4]
Fumaric acid	HMDB0000134	59.6 \pm 42.2	14.2 \pm 9.01	2.09-37.7	10.4 (2.8-53.7) ^c [10]
Pyruvic acid	HMDB0000243	163.5 \pm 96.3	36.9 \pm 15.1	19.6-89.1	21.2 (8.8-59.3) ^c [10]
Hippuric acid	HMDB0000714	261.5 \pm 285.7	64.1 \pm 63.2	1.51-213.0	49-150 ^a [4]
Methylmalonic acid	HMDB0000202	12.3 \pm 17.0	2.79 \pm 3.60	0.42-19.7	10-20 ^a [4]
Homovanillic acid	HMDB0000118	2.08 \pm 1.76	0.64 \pm 0.54	0.04-1.99	0-25 ^a [11]
Indoleacetic acid	HMDB0000197	1.68 \pm 1.46	0.41 \pm 0.41	0.03-1.95	5.2 (0.1-31.0) ^c [10]
Dopamine	HMDB0000073	7.86 \pm 9.00	1.17 \pm 0.72	0.13-2.63	0.03-2.28 ^a [12]
Kynurenine	HMDB0000684	0.81 \pm 0.94	0.16 \pm 0.17	0.02-0.71	0.56 \pm 0.91 ^{ab} [5]
Butyric acid	HMDB0000039	1.05 \pm 0.12	0.31 \pm 0.19	0.06-0.86	3.2 (0.0-6.4) ^{ac} [3]
HPHPA	HMDB0002643	2.83 \pm 4.50	0.58 \pm 0.83	0.01-3.37	0.3-12.7 ^a [13]

Isobutyric acid	HMDB0001873	1.34±0.28	0.11±0.20	0.02-1.05	15.0 (12.0-27.0) ^{*c} [3]
Uric acid	HMDB0000289	6421±2585	1780±1057	218.8-4202	2000-4000 ^{*a} [14]
Valerylcarnitine (C5)	HMDB0013128	0.26±0.27	0.06±0.05	0.02-0.29	0-3.0 ^{*a} [15]

^{*}Infant (0-1-year-old), ^aData expressed as interquartile range ^bData expressed as mean ± SD ^cData expressed as median (range)

Supplementary Table 3: Creatinine urinary concentration in newborns

Metabolite	HMDB ID	Mean ± SD μM	2.5% - 97.5% Percentile μM	Literature values (μM)
Creatinine	HMDB0000562	4952.0±3381.0	1083.0-16760.0	2300.0 (980.0-10520.0)[3]

References for Supplementary Tables 2 and 3

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