Supplementary Table S2: Urinary concentration values for NICU newborns and reference values found in HMDB (www.hmdb.ca, accessed on May 30, 2023) and Pubmed **(**https://pubmed.ncbi.nlm.nih.gov**,** accessed on May 30, 2023 **)**

Metabolite	**HMDB CODE**	**This study** **µmol/mmol Cr**	**Normal values (HMDB)** **µmol/mmol Cr**	**Abnormal values (HMDB)** **µmol/mmol Cr**	**Values reported in other studies searched in Pubmed**
1-Methylnicotinamide	HMDB0000699	61.37 (40.64-92.98)	0.82 (0.26-2.3)[11]	-	
3-Methoxytyramine	HMDB0000022	0.09 (0.07-0.14)	-	-	
5-Hydroxylysine	HMDB0000450	5.91 (4.13-8.16)	4.97 - 116.9[12]	-	37(13-114) µM/g Cr[13]
7-Methylguanine	HMDB0000897	10.79 +/- 0.86	-	-	
α-Aminobutyric acid	HMDB0000650, HMDB0000452	0.48 (0.14-1.22)	1.13 +/- 4.52[14]	-	15.2(8-26) µM/g Cr[13]
Asymmetric dimethylarginine	HMDB0001539	5.76 (4.47-7.58)	0.98-4.87[6]	-	14.8 (10.3–21.7) mmol/mmol Cr [15] 12.2 +/- 4.6[16]
Alanine	HMDB0000161	75.45 (53.05-122.77)	32.25-147.8[6]	427.6-681.4[17]	1161(630-2227) µM/g Cr [13]
Allantoin	HMDB0000462	16.48 (12.33-22.54)	-	-	19.1 +/-18.5[18]
Arginine	HMDB0000517	13.50 (9.47-21.18)	6.82-30.52[6]	-	424(288-731) µM/g Cr[13]
Asparagine	HMDB0000168	12.77 (7.96-24.28)	0.42-10.5[6]	20.7-447[19]	528(264-1033) µM/g Cr[13]
Aspartic acid	HMDB0000191	14.27 (9.19-21.64)	5.57-34.61[6]	-	2.6(0-16.5) µM/g Cr[13]
β-Alanine	HMDB0000056	7.24 (5.07-11.33)	10.18 +/- 10.18[14]	-	1154(627-2224) µM/g Cr[13]
Betaine	HMDB0000043	398.69 (286.91-503.31)	74.09-410.3[6]	-	13.62 ± 3.71[20]

Carnosine	HMDB0000033	21.55 (8.70-83.05)	0.47-35.49[6]	-	1.45 ± 0.61µmol/mmol Cr [20] 84(29-269) µM/g Cr[13]
Choline	HMDB0000097	8.08 (5.14-11.09)	3.99-50.7[6]	-	
Citrulline	HMDB0000904	1.81 (1.26-3.21)	0 - 10.97[12]	63.8-549.4[19]	33(14-73) µM/g Cr[13]
Creatine	HMDB0000064	21.86 (7.18-123.08)	4.66-455.3[6]	-	
Cystathionine	HMDB0000099	10.73 (6.39-17.60)	32.79 +/- 27.13[14]	-	349(153-703) µM/g Cr[13]
Cytidine	HMDB0000630	0.27 (0.21-0.42)	1.1-10.7[21]	-	
Diacetylspermine	HMDB0002172	2.29 (1.16-3.10)	0.37-3.11[6]	-	
Dimethylamine	HMDB0000087	71.95 (44.20-116.10)	20-60[21]	-	282 +/- 44 µmol/mmol Cr [16]
Dopamine	HMDB0000073	0.29 +/- 0.02	0.13-2.63[6]	0.49 +/- 0.06[22]	
Ethanolamine	HMDB0000149	296.05 +/- 25.65	31.89-427.74 [6]	204-1600[23]	3243(1345-5142) µM/g Cr[13]
Glutamine	HMDB0000641	64.71 (51.53-108.46)	16.16-134.4[6]	0-8[24]	1144(647-2152) µM/g Cr[13]
Glutamic acid	HMDB0000148	6.31 (4.56-16.08)	1.96-35.26[6]	-	96(48-178) µM/g Cr[13]
Glycine	HMDB0000123	419.12 (254.10-781.58)	102.6-853.6[6]	-	7408(3343-14352) µM/g Cr[13]
Guanine	HMDB0000132	0.28 (0.17-0.41)	-	-	
Histidine	HMDB0000177	63.73 (36.37-98.87)	21.09-188.1[6]	246.7-642.7[19]	1601(858-3265) µM/g Cr[13]

Histamine	HMDB0000870	0.012 +/- 0.001	0.01-0.04[6]	-	
Homocitrulline	HMDB0000679	3.14 (2.45-4.68)	0 - 10.18[12]	-	
Hypoxanthine	HMDB0000157	17.09 (10.51-28.19)	<5.2[25]	88[26]	17 +/- 38 μM/μM Cr[18]
Isoleucine	HMDB0000172	2.35 (1.32-4.29)	0.29-7.30[6]	-	
Inosine	HMDB0000195	0.59 (0.38-1.00)	0-25[21]	-	
Kynurenine	HMDB0000684	0.18 (0.08-0.70)	0.02-0.71[6]	-	
Leucine	HMDB0000687	6.47 (4.23-15.05)	0.33-13.41[6]	53.9-17.7[19]	
Lysine	HMDB0000182	119.52 (38.07-209.52)	10.5-140.5[6]	268.3-365.2[19]	2878(1304-7527) μM/g Cr[13]
Methionine	HMDB0000696	3.68 (2.76-5.71)	0.54-4.81[6]	-	34(14-69) μM/g Cr[13]
Methionine Sulfoxide	HMDB0002005	0.52 (0.21-0.99)	0.6-3.59[6]	-	
Methylhistidine	HMDB0000479	42.71 (31.68-56.08)	32.79 +/- 20.35[14]	-	197(141-277) μM/g Cr[13]
N1-Acetylspermidine	HMDB0001276	2.06 (1.74-3.53)	-	-	
N-Acetylputrescine	HMDB0002064	20.14 (11.77-28.46)	-	-	
Nudifloramide	HMDB0004193	17.23 (12.63-22.96)	0.71 (0.13-2.88)[11]	-	

Ornithine	HMDB0000214	7.11 (2.36-19.71)	1.44-24.36[6]	92.57-123.8[19]	259(84-1051) μM/g Cr[13]
Phenylalanine	HMDB0000159	9.18 (7.09-15.78)	4.14-14.15[6]	414.7[27]	122(74-207) μM/g Cr[13]
Proline	HMDB0000162	47.98 (34.13-109.22)	9.5-78.2[6]	-	1145(334-3459) μM/g Cr[13]
Putrescine	HMDB0001414	0.29 (0.17-0.46)	0.03-3.42[6]	-	
Sarcosine	HMDB0000271	3.69 (2.01-5.49)	0.55-9.98[6]	2703 [28]	192(113-514) μM/g Cr[13]
Serine	HMDB0000187	106.75 (74.87-156.83)	32.19-145.5[6]	341.6-735[19]	1640(805-3327) μM/g Cr[13]
Serotonin	HMDB0000259	0.12 (0.10-0.15)	0.1-0.35[6]	0.22[29]	
Taurine	HMDB0000251	1107.39 (537.18-1691.0)	74.64-284[6]	1261[26]	2939(289-10577) μM/g Cr[13]
Threonine	HMDB0000167	56.31 (24.51-119.66)	9.24-96.17[6]	226.2-1060[19]	833(354-1810) μM/g Cr[13]
Trimethylamine N-oxide	HMDB0000925	5.62 (0.36-10.44)	0.30-43.08[6]	-	
Total Dimethylarginine	HMDB0003334 + HMDB0001539	30.46 (22.86-37.28)	5.33-18.11[6] 0.98-4.87[6]	-	31.0 (21.7– 65.9) mmol/mmol Cr 26.1 +/- 4.5[16]
trans-4-Hydroxyproline	HMDB0000725	67.94 (43.53-132.88)	8.12-92.19[6]	1957[30]	744(304-1397) μM/g Cr[13]
Tryptophan	HMDB0000929	3.82 (2.59-6.49)	1.86-6.03[6]	-	50(27-99) μM/g Cr[13]
Tryptamine	HMDB0000303	0.06 (0.04-0.08)	-	-	
Tyrosine	HMDB0000158	5.03 (2.60-7.72)	2.1-14.81[6]	35.15-369[19]	112(62-238) μM/g Cr[13]

Tyramine	HMDB0000306	0.38 (0.27-0.52)	0.30-2.54[6]	-	
Uracil	HMDB0000300	3.05 (1.76-4.24)	8-110[21]	-	
Uridine	HMDB0000296	1.35 (0.71-2.90)	0-15[21]	-	
Valine	HMDB0000883	8.60 (5.47-18.58)	0.99-18.44[6]	-	135(67-284) μM/g Cr[13]
Glucose	HMDB0000122	683.75 (382.16-1119.80)	106.3-1193[6]	-	30.67 ± 4.81μmol/mmol Cr [20]
C0	HMDB0000062	2.87 (1.76-6.00)	0.79-5.66[6]	-	
C2	HMDB0000201	0.67 (0.40-1.58)	0.38-1.86[6]	-	
C4:1	HMDB0013126	0.02 (0.01-0.03)	0.01-0.04[6]	-	
C4	HMDB0002013	0.21 (0.10-0.37)	0.05-0.33[6]	-	
C3OH	HMDB0013125	0.02 (0.01-0.05)	0.01-0.06[6]	-	
C5:1	HMDB0002366	0.07 (0.05-0.10)	0.03-0.16[6]	-	
C5	HMDB0013128	0.10 (0.05-0.25)	0.02-0.29[6]	-	
C4OH	HMDB0013127	0.05 (0.03-0.09)	-	-	
C6:1	HMDB0013161	0.04 (0.03-0.06)	0.01-0.02[6]	-	

C5OH	HMDB0013132	0.14 (0.10-0.21)	0.04-0.29[6]	-	
C5:1DC	HMDB0013129	0.04 (0.02-0.05)	0.0-0.03[6]	-	
C5DC	HMDB0013130	0.06 (0.05-0.08)	0.02-0.1[6]	-	
C8	HMDB0000791	0.05 (0.04-0.09)	0.02-0.31[6]	-	
C5MDC	HMDB0000552	0.08 (0.06-0.10)	0.03-0.13[6]	-	
C9	HMDB0006320	0.07 (0.06-0.09)	-	-	
C7DC	HMDB0013328	0.04 (0.03-0.05)	0.02-0.09[6]	-	
C10:1	HMDB0013205	0.08 (0.02-0.15)	0.03-0.2[6]	-	
C12:1	HMDB0013326	0.06 (0.02-0.08)	0.02-0.14[6]	-	
C12DC	HMDB0013327	0.02 (0.01-0.03)	0.01-0.29[6]	-	
C16:1	HMDB0013207	0.03 (0.02-0.05)	0.0-0.03[6]	-	
2-Hydroxy-3-methylvaleric acid	HMDB0000317	0.04 (0.02-0.06)	-	-	
2-Hydroxybutyric acid	HMDB0000008	2.53 (1.56-6.08)	5.0 (0.0-10.0)[11]	-	
2-hydroxyglutaric acid	HMDB0059655	18.25+/- 1.50	51.9 (13.7-97.3)[31]	62[32]	21.1 +/-5.5 µmol/mmol Cr [33]

2-Hydroxyisobutyric acid	HMDB0000729	0.60 (0.35-0.97)	0.1 (0.1-3.8)[31]	-	
2-oxoadipic acid	HMDB0000225	12.41 (6.29-19.87)	-	135[34]	
2-oxoisocaproic acid	HMDB0000695	0.58 (0.39-0.87)	0-0.2[21]	-	
3,4-Dihydroxybutyric acid	HMDB0000337	5.26 (4.24-6.80)	73.0 +/- 24.0 [11]	-	
3-Deoxyglucosone	HMDB0005876	7.12 (5.01-8.52)	-	-	
3-Hydroxybutyric acid	HMDB0000011	1.62 (0.90-5.40)	0.72-23.3[6]	51.04-56.47[35]	16.28 +/- 3.50[33]
3-Hydroxyisobutyric acid	HMDB0000336	12.33 (5.09-23.56)	-	-	
3-Hydroxyisovaleric acid	HMDB0000754	7.21 (4.65-11.74)	12.2 (0.1-43.2)[31]	1154.8 [36]	
3-Hydroxyphenylacetic acid	HMDB0000440	0.63 +/- 0.04	-	0.67 +/- 2.9[37]	
3-Methyladipic acid	HMDB0000555	0.48 +/- 0.04	-	-	
4-Hydroxyphenylacetic acid	HMDB0000020	7.96(4.70-14.16)	24.2 (8.6-73.2)[31]	428.0 +/- 164.0[38]	
4-Hydroxyphenylpyruvic acid	HMDB0000707	150.31(60.04-507.20)	4.6 (0.1-21.3)[31]	24.00 +/- 30.5[37]	
5-Hydroxyindoleacetic acid	HMDB0000763	8.69 +/- 0.38	11.0 (4.0-18.0)[39]	0.9 +/- 0.0[39]	
5-Oxoproline	HMDB0000267	22.99 (19.74-38.23)	7.3 (0.1-29.3)[31]	1980 – 6040[40]	
alpha-Ketoglutaric acid	HMDB0000208	162.32 (71.28-284.43)	30.79-398.2[6]	385.200-1367.300 [41]	

alpha-Ketoisovaleric acid	HMDB0000019	1.81 (0.52-5.32)	0.16 +/- 0.48 [42]	-	
Argininic acid	HMDB0003148	8.21 (3.83-13.95)	-	-	
Benzoic acid	HMDB0001870	0.52 (0.30-0.85)	-	-	
Butyric acid + Isobutyric acid	HMDB0000039 + HMDB0001873	3.49 (1.36-5.61)	0.06-0.86[6]	-	
Caproic acid	HMDB0000535	0.46 (0.14-0.75)	0.91 +/- 1.05[42]	-	
Caprylic acid	HMDB0000482	0.15 (0.04-0.22)	0.39 +/- 0.37[42]	-	
cis-Aconitic acid	HMDB0000072	45.72 +/- 2.82	67.9 (14.3-100.7)[31]	6.4-293.5[17]	
Citric acid	HMDB0000094	379.57 (228.21-614.87)	39.6-893[6]	998[32]	
Dimethylglycine	HMDB0000092	15.04 (11.87-21.42)	15-220[21]	-	
Ethylmalonic acid	HMDB0000622	4.14 (3.10-5.81)	0.012 +/- 0.00[33]	2.56-10.26[43]	
2,5-Furandicarboxylic acid	HMDB0004812	1.39 (0.64-3.43)	2.7 (0.1-9.1)[31]	-	
Fumaric acid	HMDB0000134	10.34 (6.40-21.12)	2.09-37.66[6]	17-124[44]	
Glutaric acid	HMDB0000661	1.51 (0.74-3.15)	1.896 +/- 0.862 [33]	3.3-44.0[45]	7.623 +/-3.321µmol/mmol Cr [33]
Glyceric acid	HMDB0000139	3.18 (1.06-7.97)	21.6 (0.5-91.1) [31]	-	
Guanidinopropionic acid	HMDB0013222	13.71 (6.38-69.84)	-	-	
Guanidoacetic acid	HMDB0000128	11.30 (7.28-20.30)	93-190 [21]	-	

Hippuric acid	HMDB0000714	27.57 (16.64-44.00)	1.51-213[6]	-	189.79 ± 5.24 µmol/mmol Cr[20]
Indolelactic acid	HMDB0000671	0.11 (0.07-0.22)	-	-	
Indoxyl sulfate	HMDB0000682	2.57 (1.67-4.03)	-	-	
Isocitric acid	HMDB0000193	45.72 +/- 2.77	19.0 (5.0-34.0)[11]	-	
Kynurenic acid	HMDB0000715	4.94 (3.81-7.06)	-	-	
Lactic acid	HMDB0000190	165.77 (85.81-350.52)	46.99-774.2[6]	352[32]	
Maleic acid	HMDB0000176	1.14 (0.73-1.78)	10.4 [31]	-	
Malic acid	HMDB0000156	64.79 (32.94-109.83)	36.1(12.4-121.6[31]	110 [32]	
Malonic acid	HMDB0000691	0.92 +/- 0.07	-	2170.7-5438.1 [46]	
Methylmalonic acid	HMDB0000202	0.87 (0.36-1.23)	0.42-19.74[6]	-	32.192+/-6.937µmol/mmol Cr [33]
Orotic acid	HMDB0000226	2.05 +/- 0.15	0.061 +/- 0.003[33]	>20 [47]	1.129 +/- 0.874µmol/mmol Cr [33]
Phenylacetic acid	HMDB0000209	0.12 (0.08-0.19)	-	55.6 +/- 87.3[37]	
Phenylacetylglutamine	HMDB0006344	22.67 (17.32-33.98)	-	-	
p-Hydroxyhippuric acid	HMDB0013678	4.55 (3.40-7.47)	4.2-19.59[6]	-	
Pipecolic acid	HMDB0000070	0.15 (0.14-0.24)	0 - 25.33 [12]	-	

Propionic acid	HMDB0000237	8.40 (3.04-13.01)	0-76[21]	-	
Pyruvic acid	HMDB0000243	7.17 (5.60-13.41)	9.55-89.06[6]	-	
Quinaldic acid	HMDB0000842	0.01 (0.01-0.02)	-	-	
Quinolinic acid	HMDB0000232	18.29 (14.14-24.02)	0.67 +/- 1.34 [42]	-	
Shikimic acid	HMDB0003070	0.68 +/- 0.04	-	-	
Succinic acid	HMDB0000254	111.02 (31.39-241.29)	4.35-81.2[6]	75-185 [44]	
Tartaric acid	HMDB0000956	1.47 (0.95-2.88)	0-60[21]	-	
Threonic acid	HMDB0000943	89.49 (69.00-103.31)	63.0 +/- 21.0 [11]	-	
Uric acid	HMDB0000289	927.36 +/- 78.40	218.8-4202[6]	20 [26]	
Tiglylglycine	HMDB0000959	0.79 (0.55-0.97)	0-3.8[48]	87[49]	
Xanthine	HMDB0000292	12.90 (7.06-23.41)	<40 [50]	991[26]	
Xanthosine	HMDB0000299	2.14 (1.63-3.42)	-	-	
N1-Acetyl-Lysine	HMDB0000446	0.67 (0.48-1.15)	-	-	
N6-Acetyl-Lysine	HMDB0000206	1.14 (0.90-1.49)	-	-	
N-Acetyl-Alanine	HMDB0000766	4.00 (1.75-8.27)	-	-	

N-Acetyl-Arginine	HMDB0004620	1.84 (1.07-2.66)	-	-	
N-Acetyl-Asparagine	HMDB0006028	2.69 (2.05-4.40)	-	-	
N-Acetyl-Aspartic acid	HMDB0000812	26.26 (18.78-40.70)	33.2 (4.9-65.5) [31]	-	
N-Acetyl-Glutamine	HMDB0006029	4.12 +/- 0.22	-	-	
N-Acetyl-Glutamic acid	HMDB0001138	3.47 (2.78-4.83)	0-42[21]	-	
N-Acetyl-Glycine	HMDB0000532	4.16 (3.28-5.36)	0 [51]	170 +/- 18[51]	
N-Acetyl-Histidine	HMDB0032055	8.13 (3.72-9.89)	-	-	
N-Acetyl-Isoleucine	HMDB0061684	0.47 (0.32-0.74)	-	-	
N-Acetyl-Leucine	HMDB0011756	0.54 (0.34-1.12)	-	-	
N-Acetyl-Methionine	HMDB0011745	1.22 (0.91-1.40)	-	-	
N-Acetyl-Proline	HMDB0094701	0.43 (0.25-0.60)	-	-	
N-Acetyl-Serine	HMDB0002931	5.02 (2.63-8.14)	-	-	
N-Acetyl-Tyrosine	HMDB0000866	0.22 (0.1-0.55)	1.6 (0-6.4) [52]	75 (0-781)[52]	
N-Acetyl-Valine	HMDB0011757	0.73 (0.53-0.83)	-	-	