nature portfolio

https://doi.org/10.1038/s41596-020-00475-0

Supplementary information

The maternal serum metabolome by multisegment injection-capillary electrophoresis-mass spectrometry: a high-throughput platform and standardized data workflow for large-scale epidemiological studies

In the format provided by the authors and unedited

Supplementary Information for:

The Maternal Serum Metabolome by Multisegment Injection-Capillary Electrophoresis-Mass Spectrometry: A High Throughput Platform and Standardized Data Workflow for Large-scale Epidemiological Studies

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Supplementary Table 1| Summary of 66 authenticated serum metabolites consistently detected in a majority (> 75%) of samples with adequate precision (QCs with CV < 30%) in pregnant women across 3 of 4 birth cohort studies by MSI-CE-MS.

						START		FAMILY		ABC		CHILD		
Metabolite ID	***m/z*:RMT:mode**	**HMDB ID or Molecular Formula/Mass Error**	**Level of ID**	**% CV QC[(i)]**	**ICC[(iii)]**	**% CV QC[(ii)]**	**ICC[(iv)]**	**% CV QC[(ii)]**	**ICC[(iv)]**	**% CV QC[(ii)]**	**ICC[(iv)]**	**% CV QC[(ii)]**	**ICC[(iv)]**	***p*-value[(v)]**
Glycine	76.039:0.710:p	HMDB0000123	1	9.7	0.86	13.4	0.69	8.1	0.85	4.8	0.96	8.3	0.92	2.38E-14
Trimethylamine *N*-oxide	76.077:0.555:p	HMDB0000925	1	23.8	0.93	30.9	0.90	14.8	0.97	22.0	0.86	23.5	0.94	7.44E-05
Alanine	90.056:0.762:p	HMDB0000161	1	9.5	0.83	11.7	0.72	8.6	0.81	7.1	0.87	8.7	0.87	2.11E-16
Dimethylglycine	104.071:0.808:p	HMDB0000092	1	18.0	0.76	20.9	0.60	13.8	0.79	10.3	0.86	20.7	0.80	3.15E-02
Choline	104.108:0.578:p	HMDB0000097	1	20.2	0.88	25.3	0.80	12.1	0.76	14.4	0.98	22.6	0.82	4.48E-10
Serine	106.050:0.846:p	HMDB0000187	1	8.4	0.89	8.8	0.88	6.1	0.88	8.2	0.92	10.0	0.86	1.25E-13
Creatinine	114.066:0.621:p	HMDB0000562	1	10.1	0.81	13.9	0.63	7.4	0.88	8.1	0.78	8.4	0.89	1.06E-15
Proline	116.070:0.907:p	HMDB0000162	1	7.5	0.92	9.0	0.86	5.4	0.95	6.9	0.90	8.3	0.89	4.63E-38
Guanidinoacetic acid	118.053:0.701:p	HMDB0000128	2	19.6	0.74	25.3	0.53	18.9	0.57	9.4	0.83	16.3	0.91	4.20E-05
Valine	118.086:0.835:p	HMDB0000883	1	13.9	0.64	18.3	0.34	13.1	0.53	8.3	0.82	10.7	0.83	3.95E-06
Theronine	120.065:0.887:p	HMDB0000167	1	8.5	0.87	8.6	0.86	7.7	0.88	6.4	0.88	9.8	0.84	3.92E-18
Unknown 1	129.066:0.739:p	$C_5H_8N_2O_2$/7.7 ppm	3	17.6	0.85	17.7	0.78	13.0	0.90	18.0	0.82	21.5	0.86	5.46E-01
Pipecolic acid	130.086:0.588:p	HMDB0000070	2	14.9	0.66	22.3	0.24	11.5	0.76	19.5	0.50	10.9	0.83	1.32E-02
Creatine	132.077:0.748:p	HMDB0000064	1	10.3	0.91	11.9	0.87	7.2	0.95	7.5	0.94	12.1	0.90	1.59E-03
Isoleucine	132.102:0.846:p	HMDB0000172	1	12.1	0.91	30.0	0.32	8.5	0.80	12.2	0.91	12.1	0.95	2.85E-01
Leucine	132.102:0.856:p	HMDB0000687	1	11.4	0.89	14.5	0.82	7.3	0.83	12.0	0.84	11.2	0.95	4.19E-02
Asparagine	133.057:0.887:p	HMDB0000168	1	12.8	0.74	15.1	0.58	9.1	0.71	8.5	0.85	15.0	0.71	5.45E-26

Ornithine	133.097:0.586:p	HMDB0000214	1	14.9	0.90	21.9	0.58	9.6	0.86	10.8	0.88	11.1	0.94	3.60E-50
Aspartic acid	134.044:0.974:p	HMDB0000191	1	9.2	0.92	10.3	0.85	6.4	0.92	8.9	0.95	10.4	0.93	2.82E-13
Hypoxanthine	137.046:1.077:p	HMDB0000157	1	13.0	0.97	18.5	0.83	5.8	0.97	13.0	0.85	11.2	0.99	7.52E-12
Proline betaine	144.099:0.962:p	HMDB0004827	1	18.0	0.99	19.7	0.96	11.7	0.98	11.2	0.98	22.6	0.97	1.15E-09
γ-Butyrobetaine	146.118:0.690:p	HMDB0001161	1	26.7	0.87	31.0	0.89	23.0	0.87	23.7	0.27	n/a	n/a	n/a
Glutamine	147.076:0.911:p	HMDB0000641	1	8.7	0.80	11.6	0.69	5.2	0.91	6.8	0.86	8.9	0.80	2.53E-04
Lysine	147.113:0.588:p	HMDB0000182	1	14.8	0.67	24.1	0.43	7.6	0.89	12.5	0.82	10.3	0.83	2.60E-04
Glutamic acid	148.060:0.925:p	HMDB0000148	1	7.8	0.97	8.3	0.93	5.9	0.96	7.2	0.97	9.5	0.97	1.27E-07
Methionine	150.058:0.897:p	HMDB0000696	1	10.8	0.76	14.7	0.50	6.1	0.85	9.7	0.80	10.6	0.86	7.63E-03
Histidine	156.077:0.628:p	HMDB0000177	1	10.0	0.77	12.1	0.72	8.7	0.76	9.2	0.75	9.5	0.84	4.23E-08
2-Aminooctanoic acid	160.133:0.714:p	HMDB0000991	2	20.0	0.79	25.4	0.57	18.6	0.80	13.2	0.84	17.0	0.89	1.14E-20
Aminoadipic acid	162.076:0.918:p	HMDB0000510	1	22.9	0.76	26.2	0.83	17.8	0.69	26.3	0.37	n/a	n/a	n/a
Carnitine	162.112:0.723:p	HMDB0000062	1	11.8	0.76	15.2	0.61	8.3	0.87	9.3	0.84	20.0	0.80	2.13E-09
Phenylalanine	166.086:0.925:p	HMDB0000159	1	6.8	0.94	9.1	0.85	4.5	0.94	6.1	0.97	6.8	0.94	5.59E-23
3-Methylhistidine	170.092:0.643:p	HMDB0000479	1	14.6	0.97	17.1	0.96	12.8	0.97	13.5	0.94	14.4	0.98	1.42E-31
Arginine	175.119:0.609:p	HMDB0000517	1	11.7	0.91	15.3	0.82	8.1	0.90	12.2	0.90	10.6	0.90	1.03E-45
Citrulline	176.102:0.936:p	HMDB0000904	1	9.9	0.84	10.1	0.80	6.7	0.92	7.8	0.88	12.9	0.83	1.23E-02
Tyrosine	182.081:0.956:p	HMDB0000158	1	7.9	0.87	10.5	0.71	5.4	0.90	6.0	0.92	7.9	0.91	2.80E-13
Monomethylarginine	189.134:0.613:p	HMDB0029416	1	15.0	0.88	16.8	0.81	9.3	0.95	19.4	0.69	16.4	0.89	1.86E-02
Asymmetric-Dimethylarginine	203.150:0.645:p	HMDB0001539	1	18.1	0.83	21.2	0.87	13.5	0.81	20.2	0.32	n/a	n/a	n/a
Symmetric-Dimethylarginine	203.1450:0.657:p	HMDB0003334	1	20.6	0.64	24.1	0.59	16.5	0.75	20.6	0.31	n/a	n/a	n/a
Acetylcarnitine	204.123:0.765:p	HMDB0000201	1	14.2	0.84	16.4	0.68	8.5	0.93	12.7	0.85	16.7	0.85	2.63E-17

Tryptophan	205.097:0.925:p	HMDB0030396	1	11.9	0.90	13.4	0.87	7.1	0.96	11.2	0.92	14.6	0.86	7.05E-10
Propionylcarnitine	218.114:0.790:p	HMDB0000824	1	24.4	0.92	28.1	0.92	16.1	0.96	31.3	0.46	n/a	n/a	n/a
Cystine	241.030:0.934:p	HMDB0000192	1	22.7	0.89	21.9	0.96	8.3	0.89	36.2	0.95	27.3	0.41	4.91E-145
Tryptophan betaine	247.144:1.153:p	HMDB0061115	1	n/a	n/a	16.1	0.95	17.2	0.97	n/a	n/a	n/a	n/a	n/a
Cysteinylglycine disulfide	298.053:0.808;p	HMDB0000709	2	n/a	n/a	12.1	0.98	11.8	0.80	n/a	n/a	19.7	0.70	n/a
Unknown 2	334.688:0.805:p	$C_{20}H_{47}N_{18}O_6S$/3.6 ppm	3	n/a	n/a	27.3	0.96	n/a	n/a	19.5	0.97	n/a	n/a	n/a
Unknown 3	471.738:0.888:p	$C_{30}H_{55}N_{25}O_{11}$/9.6 ppm	4	20.5	0.96	23.3	0.91	12.4	0.98	28.4	0.81	n/a	n/a	n/a
Pyruvic acid	87.009:1.629:n	HMDB0000243	1	11.2	0.92	12.1	0.93	10.5	0.91	11.5	0.91	n/a	n/a	n/a
Lactic acid	89.025:1.412:n	HMDB0000190	1	17.6	0.90	9.5	0.90	9.4	0.87	11.0	0.77	28.2	0.81	4.45E-54
3-Hydroxybutyric acid	103.040:0.950:n	HMDB0000357	1	12.7	0.96	16.7	0.91	8.5	0.98	9.8	0.98	n/a	n/a	n/a
2-Hydroxybutyric acid	103.040:1.295:n	HMDB0000008	1	12.5	0.89	13.6	0.85	12.1	0.90	10.9	0.92	n/a	n/a	n/a
α-Ketoisovaleric acid	115.040:1.340:n	HMDB0000019	1	13.7	0.73	16.5	0.70	12.3	0.73	8.4	0.87	n/a	n/a	n/a
Unknown 4	117.056:1.244:n	$C_5H_{10}O_3$/0 ppm	3	18.8	0.77	19.0	0.81	19.3	0.78	18.1	0.77	n/a	n/a	n/a
Taurine	124.007:0.990:n	HMDB0000251	2	16.0	0.85	14.0	0.91	19.5	0.58	9.6	0.92	n/a	n/a	n/a
Oxo-proline	128.035:1.262:n	HMDB0000267	1	17.0	0.95	16.3	0.88	11.2	0.77	11.0	0.89	23.4	0.93	2.07E-14
3-Methyl-2-oxovaleric acid	129.056:1.268:n	HMDB0000491	1	12.4	0.88	9.8	0.89	10.0	0.87	10.0	0.82	21.5	0.81	9.99E-12
Malic acid	133.014:2.293:n	HMDB0000744	1	17.3	0.84	18.2	0.86	17.9	0.74	13.4	0.74	n/a	n/a	n/a
Unknown 5	145.014:0.866:n	$C_5H_{10}N_2O_3$/3.5 ppm	4	13.6	0.67	14.9	0.74	11.5	0.69	13.3	0.67	15.5	0.44	6.89E-08
Xanthine	151.026:1.192:n	HMDB0000292	2	18.0	0.77	18.1	0.83	18.5	0.63	17.5	0.72	n/a	n/a	n/a
Uric acid	167.021:1.198:n	HMDB0000289	1	15.6	0.69	11.7	0.79	9.5	0.84	9.7	0.86	23.3	0.50	4.93E-10
Hippuric acid	178.051:1.134:n	HMDB0000714	1	20.4	0.97	12.8	0.98	15.4	0.96	14.0	0.99	30.0	0.95	2.28E-04
Glucose	179.056:0.999:n	HMDB0000122	1	6.9	0.95	4.3	0.95	6.4	0.93	5.2	0.92	12.4	0.93	5.71E-22

Unknown 6	180.952:2.075:n	$C_3H_4NO_4S_2$/9.8 ppm	4	22.4	0.77	31.8	0.44	12.4	0.91	10.9	0.52	25.8	0.81	6.98E-11
Citric acid	191.020:2.519:n	HMDB0000094	1	12.0	0.92	12.1	0.94	11.0	0.93	14.7	0.73	n/a	n/a	n/a
Gluconic acid	195.052:1.160:n	HMDB0000625	1	15.8	0.74	16.5	0.81	12.7	0.77	19.3	0.24	n/a	n/a	n/a
Unknown 7	248.071:0.766:n	$C_{16}H_{11}NO_2$/3.8 ppm	4	17.2	0.83	22.6	0.79	10.5	0.92	14.5	0.39	n/a	n/a	n/a
Phenylacetylglutamine	263.104:1.087:n	HMDB0006344	1	16.6	0.92	18.2	0.97	14.3	0.92	18.1	0.83	n/a	n/a	n/a

[(i)] CV of QC when using inter-batch corrected data, [(ii)] CV of QC when using within cohort intra-batch corrected data, [(iii)] ICC value for metabolites across all cohorts and [(iv)] ICC for metabolites within each cohort. The Shapiro–Wilk test was used for normality test. [(v)] p-value determined for 46 serum metabolites with different responses measured across all 4 birth cohorts using a Kurskal Wallis test. A Shapiro–Wilk test was used for normality.