

Supplementary Table 1 Identification of the urine metabolites of healthy pregnant women involved in panel regression analysis

Marker	Ionization mode	tR (min)	m/z	Chemical identity	Mass error (ppm)	Related features	Major MS/MS fragment ions (m/z)
1	ES ⁺	4.09	347.168	[2M+H] ⁺ of 2-oxoarginine (HMDB04225)	0.26	m/z 174.088 ([M+H] ⁺), m/z 196.0696 ([M+Na] ⁺)	132, 105
2	ES ⁺	2.09	157.077	[M+H] ⁺ of 3-Indoleacetonitrile (HMDB06524)	2.72	m/z 201.07 ([M+HCOO] ⁻), m/z 179.0587 ([M+Na] ⁺)	140, 130
3	ES ⁺	0.51	156.021	[M+K] ⁺ of Indole (HMDB00738)	3.62	m/z 118.0666 ([M+H] ⁺), m/z 140.05 ([M+Na] ⁺), m/z 116.05 ([M-H] ⁻), m/z 162.05 ([M+HCOO] ⁻)	118, 91
4	ES ⁺	0.88	148.040	[M+H] ⁺ of Indole-5,6-quinone (HMDB06779)	0.93	m/z 165.07 ([M+NH ₄] ⁺), m/z 146.02 ([M-H] ⁻)	119
5	ES ⁺	5.02	463.157	[2M+H] ⁺ of n2-succinyl-l-glutamic acid 5-semialdehyde (HMDB01180)	1.32	m/z 232.0825 ([M+H] ⁺), m/z 270.1727 ([M+K] ⁺)	214, 196
6	ES ⁺	0.54	227.126	[2M+H] ⁺ of creatinine (HMDB00562)	1.55	m/z 114.0665 ([M+H] ⁺), m/z 136.0484 ([M+Na] ⁺)	86

7	ES ⁺	3.04	175.124	[M+H] ⁺ of n-methyltryptamine (HMDB04370)	2.70	m/z 173.1075 ([M-H] ⁻), m/z 197.1053 ([M+Na] ⁺)	144, 132
8	ES ⁺	6.16	291.121	[M+H] ⁺ of n-succinyl-1,1-2,6-diaminopimelate (HMDB12267)	6.08	m/z 313.1013 ([M+Na] ⁺), m/z 329.2098 ([M+K] ⁺)	273, 227

tR, retention time; ppm, parts per million; M, intact molecule (e.g., [M+H]⁺ stands for the positive ion formed by the intact molecule adding a proton); “Related features” refers to the features generated from identical molecules including features of quasi or adduct molecular ions, diametric ions and so on which possess the similar retention time and chromatographic shape. 3-indoleacetonitrile, n-methyltryptamine and n-succinyl-1,1-2,6-diaminopimelate were identified by comparison of retention time with standards.