

Supplementary document S2. Molecular mass, chemical formula, retention time (RT), ionization mode, and analytical parameters.

Compounds	Molecular weight (g/mol)	Chemical formula	Retention time (min)	Ionization Mode (ESI)	Parent ion (<i>m/z</i>)	Fragment ion (<i>m/z</i>)	Collision Energy (V)
TMAO	75.1	C ₃ H ₉ NO	0.60	+	76.4	58.2 59.2	19 12
Tyrosine	181.1	C ₉ H ₁₁ NO ₃	0.78	+	182.1	136.1 165.0	30 20
Phenylalanine	165.1	C ₉ H ₁₁ NO ₂	1.57	+	166.2	120.1 103.0	14 27
Kynurenine	208.1	C ₁₀ H ₁₂ N ₂ O ₃	1.87	+	213.1	98.2 146.4	15 19
Tryptophan	204.1	C ₁₁ H ₁₂ N ₂ O ₂	4.75	+	205.1	188.1 146.0	10 17
Hippuric acid	179.1	C ₉ H ₉ NO ₃	4.75	-	178.1	77.1 131.8	17 21
Phenylacetyl-glutamine	264.1	C ₁₃ H ₁₆ N ₂ O ₄	4.82	+	270.1	130.1 136.1	15 15
p-cresyl glucuronide	284.1	C ₁₃ H ₁₆ O ₇	5.08	-	283.1	107.1 113.1	31 12
Kynurenic acid	189.0	C ₁₀ H ₇ NO ₃	5.63	+	190.1	116.0 190.1	31 19
Indoxyl sulfate	213.0	C ₈ H ₇ NO ₄ S	5.75	-	212.1	80.0 81.0	23 17
Indole-3-acetic acid	175.1	C ₁₀ H ₉ NO ₂	6.00	+	176	130.1 103.1	16 31
p-cresyl sulfate	188.0	C ₇ H ₈ O ₄ S	6.18	-	187.1	107.1 105.1	21 34
CMPF	240.1	C ₁₂ H ₁₆ O ₅	7.05	-	239.1	195.1 151.1	12 16