

Additional file 13: Relevant parameters of detected compounds

Compound	Sum Formula	Exact Mass [g/mol]	Monitored Ion(s)	BPC m/z	Ret. Time [min]
2-aminobenzimidazole (ISTD)	C ₇ H ₇ N ₃	133.0640	[M+H] ⁺	134.0713	5.4
<i>N</i> -acetylglutamate	C ₇ H ₁₁ NO ₅	189.1659	[M+H] ⁺	190.1729	1.5
<i>N</i> -acetylglutamyl phosphate	C ₇ H ₁₂ NO ₈ P	269.0301	[M+H] ⁺	270.0373	n.d.
<i>N</i> -acetylglutamate semialdehyde	C ₇ H ₁₁ NO ₄	173.0688	[M+H] ⁺	174.0761	1.6
<i>N</i> -acetylornithine	C ₇ H ₁₄ N ₂ O ₃	174.1004	[M+H] ⁺	175.1074	6.4
L-ornithine	C ₅ H ₁₂ N ₂ O ₂	132.0899	[M+H] ⁺	133.0972	8.0
L-citrulline	C ₆ H ₁₃ N ₃ O ₃	175.0957	[M+H] ⁺	176.1027	6.2
[U- ¹³ C]-L-citrulline	¹³ C ₆ H ₁₃ N ₃ O ₃	181.1160	[M+H] ⁺	182.1230	6.2
L-argininosuccinate	C ₁₀ H ₁₈ N ₄ O ₆	290.1226	[M+H] ⁺	291.1296	7.3
L-arginine	C ₆ H ₁₄ N ₄ O ₂	174.1117	[M+H] ⁺	175.1190	8.0
[U- ¹³ C]-L-arginine	¹³ C ₆ H ₁₄ N ₄ O ₂	180.1349	[M+H] ⁺	181.1393	8.0
<i>N</i> -acetylglutamine	C ₇ H ₁₂ N ₃ O ₄	188.0797	[M+H] ⁺	189.087	2.3
[U- ¹³ C]- <i>N</i> -acetylglutamine	¹³ C ₇ H ₁₂ N ₃ O ₄	195.1032	[M+H] ⁺	196.116	2.3
L-lysine	C ₆ H ₁₄ N ₂ O ₂	146.1055	[M+H] ⁺	147.1128	8.1
[U- ¹³ C]-L-lysine	¹³ C ₆ H ₁₄ N ₂ O ₂	152.1258	[M+H] ⁺	153.1331	8.1
<i>N</i> -acetylglutamate (MRM mode)	C ₇ H ₁₁ NO ₅	189.1659	Fragments	84.044 +102.056 +130.048 +148.050	1.5
[U- ¹³ C]- <i>N</i> -acetylglutamate (MRM mode)	¹³ C ₇ H ₁₁ NO ₅	196.1894	Fragments	88.055 +106.068 +135.065 +153.073	1.5

BPC: Base Peak Chromatogram; n.d.: not determined