

Additional file 1: Table S1

Compound	Ions	Exact ion	dwell time (ms)	Sum formula	RT (min)
Pyruvic acid 1MeOX 1TBDMS	174–180	0	15	C ₆ H ₁₂ O ₃ NSi	6.62
Lactic acid 2TBDMS	261–267	0.1	15	C ₁₁ H ₂₅ O ₃ Si ₂	8.35
Alanine 2TBDMS	260–266	0.1	15	C ₁₁ H ₂₆ NO ₂ Si ₂	8.89
Glycine 2TBDMS	246–252	0.1	15	C ₁₀ H ₂₄ NO ₂ Si ₂	9.4
γ-Aminobutyric acid 2TBDMS	274–281	0.2	15	C ₁₂ H ₂₈ NO ₂ Si ₂	11.74
Succinic acid 2TBDMS	289–296	0.1	15	C ₁₂ H ₂₅ O ₄ Si ₂	12.04
Fumaric acid 2TBDMS	287–294	0.1	15	C ₁₂ H ₂₃ O ₄ Si ₂	12.18
Serine 2TBDMS	390–396	0.2	15	C ₁₇ H ₄₀ NO ₃ Si ₃	13.54
Methionine 2TBDMS	320–328	0.2	10	C ₁₃ H ₃₀ NO ₂ SSi ₂	14.17
2-Oxoglutaric 1MeOX 2TBDMS	346–354	0.2	10	C ₁₄ H ₂₈ NO ₅ Si ₂	14.86
Malic acid 3TBDMS	419–426	0.2	15	C ₁₈ H ₃₉ O ₅ Si ₃	15.06
Aspartic acid 3TBDMS	418–425	0.2	15	C ₁₈ H ₄₀ NO ₄ Si ₃	15.48
Glutamic acid 3TBDMS	432–440	0.3	10	C ₁₉ H ₄₂ NO ₄ Si ₃	16.56
Glutamine 3TBDMS	431–439	0.3	10	C ₁₉ H ₄₃ N ₂ O ₃ Si ₃	18.22
Citric acid 4TBDMS	591–600	0.3	10	C ₂₆ H ₅₅ O ₇ Si ₄	19.17