# Targeted Clinical Metabolomics Platform for the Stratification of Diabetic Patients

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## *Supplemental Material*

## Supplemental Methods

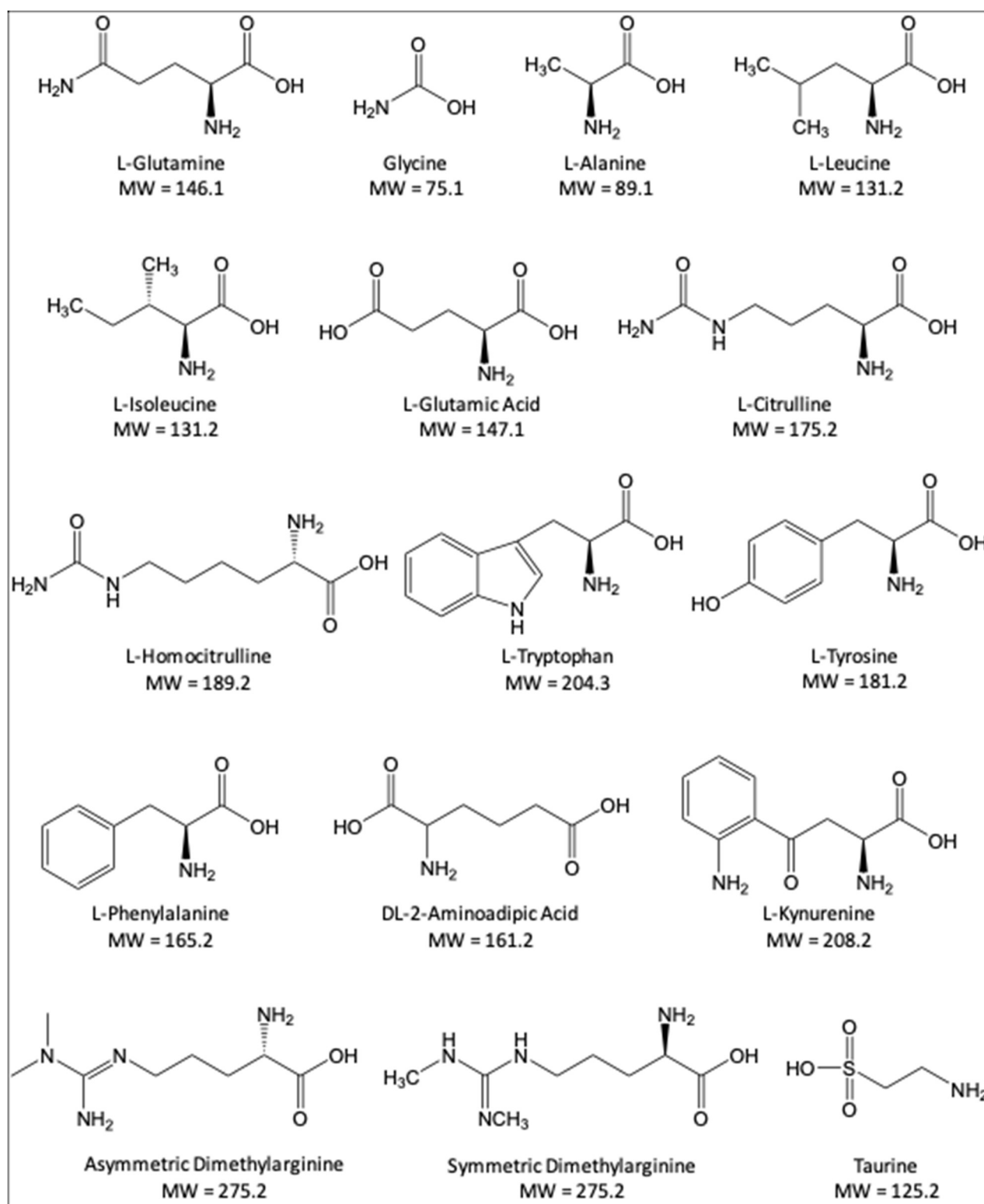**Figure S1A.** Structures of compounds of interest, amino acids and amino acid related compounds.



L-Glutamine
MW = 146.1

Glycine
MW = 75.1

L-Alanine
MW = 89.1

L-Leucine
MW = 131.2

L-Isoleucine
MW = 131.2

L-Glutamic Acid
MW = 147.1

L-Citrulline
MW = 175.2

L-Homocitrulline
MW = 189.2

L-Tryptophan
MW = 204.3

L-Tyrosine
MW = 181.2

L-Phenylalanine
MW = 165.2

DL-2-Aminoadipic Acid
MW = 161.2

L-Kynurenine
MW = 208.2

Asymmetric Dimethylarginine
MW = 275.2

Symmetric Dimethylarginine
MW = 275.2

Taurine
MW = 125.2

**Figure S2.** Structures of compounds of interest, bile acids.



Cholic Acid
MW = 408.6

Deoxycholic Acid
MW = 392.6

Glycocholic Acid
MW = 465.6

Taurocholic Acid
MW = 515.7

Deoxychenocholic Acid
MW = 392.6

Tauroursoeoxycholic Acid
MW = 499.7

Glycodeoxycholic Acid
MW = 449.6

Taurodeoxycholic Acid
MW = 498.7

Ursodeoxycholic Acid
MW = 392.6

Glycoursodeoxycholic Acid
MW = 449.6

Glycochenodeoxycholic Acid
MW = 499.6

Taurochenodeoxycholic Acid
MW = 498.7

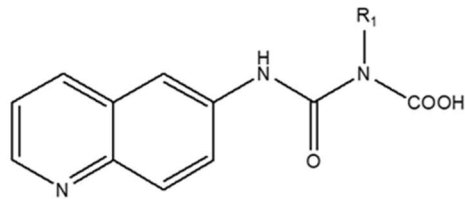**Figure S3.** Structures of compounds of interest, small organic acids and other metabolites of interest.



Azelaic Acid
MW = 188.2

L-3-Hydroxybutyric Acid
MW = 104.1

Gammabutyrobetaine
MW = 145.2

Creatinine
MW = 113.1

Indoxyl sulfate
MW = 213.1

N-methyl-nicotinamide
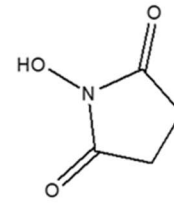MW = 136.2
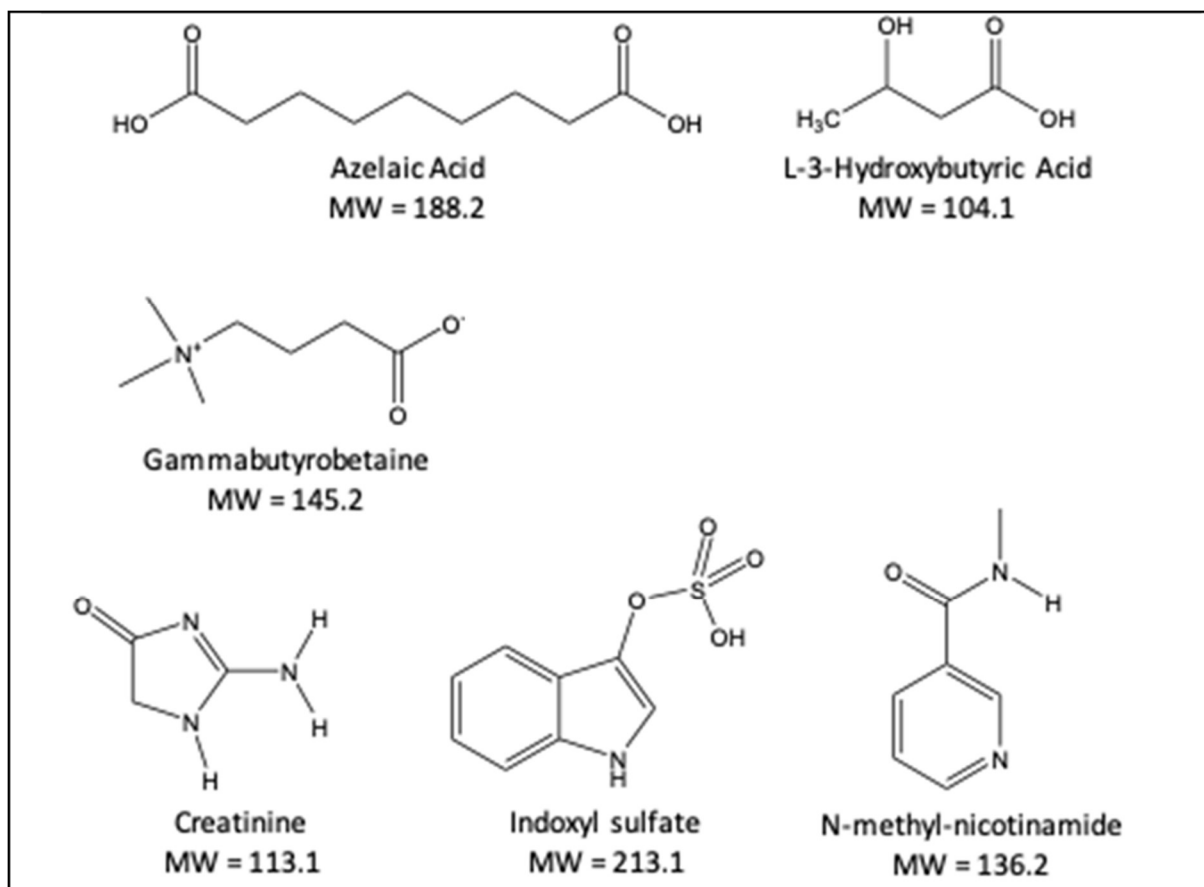
**Figure S4.** Derivatization reaction.
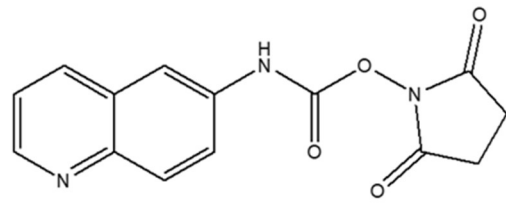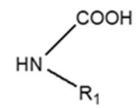
AQC reagent            Amino acid

Derivatized amino acid      N-hydroxysuccinimide

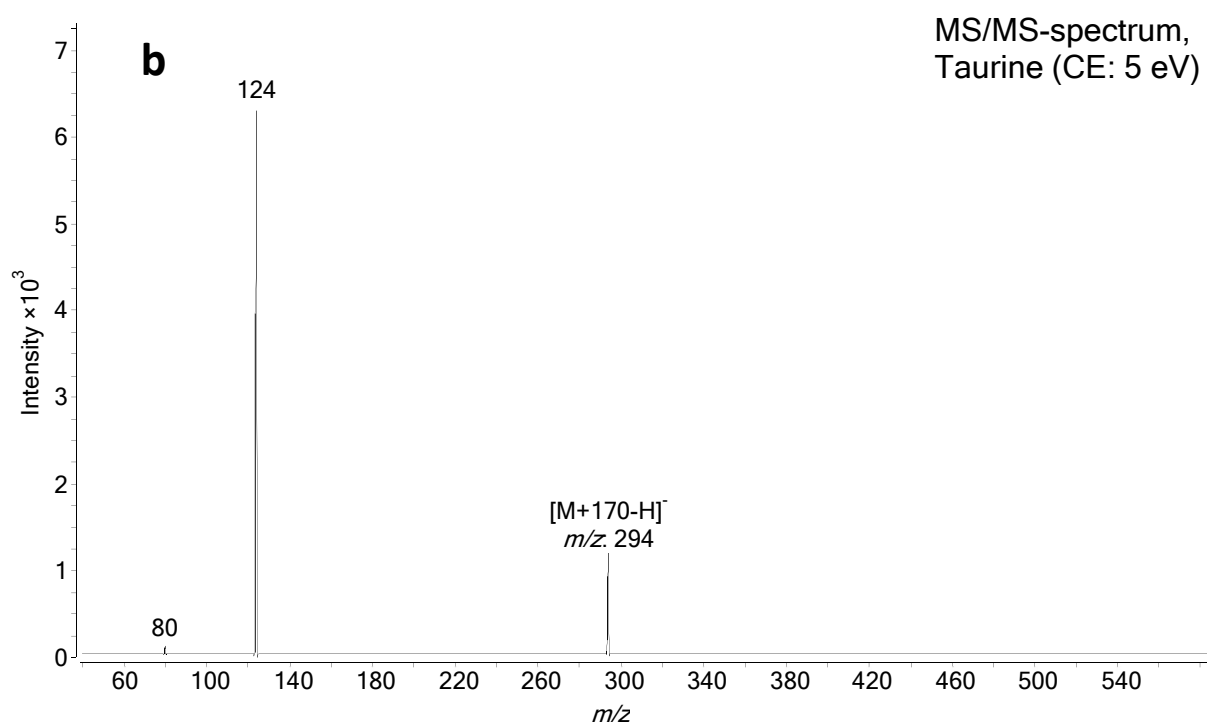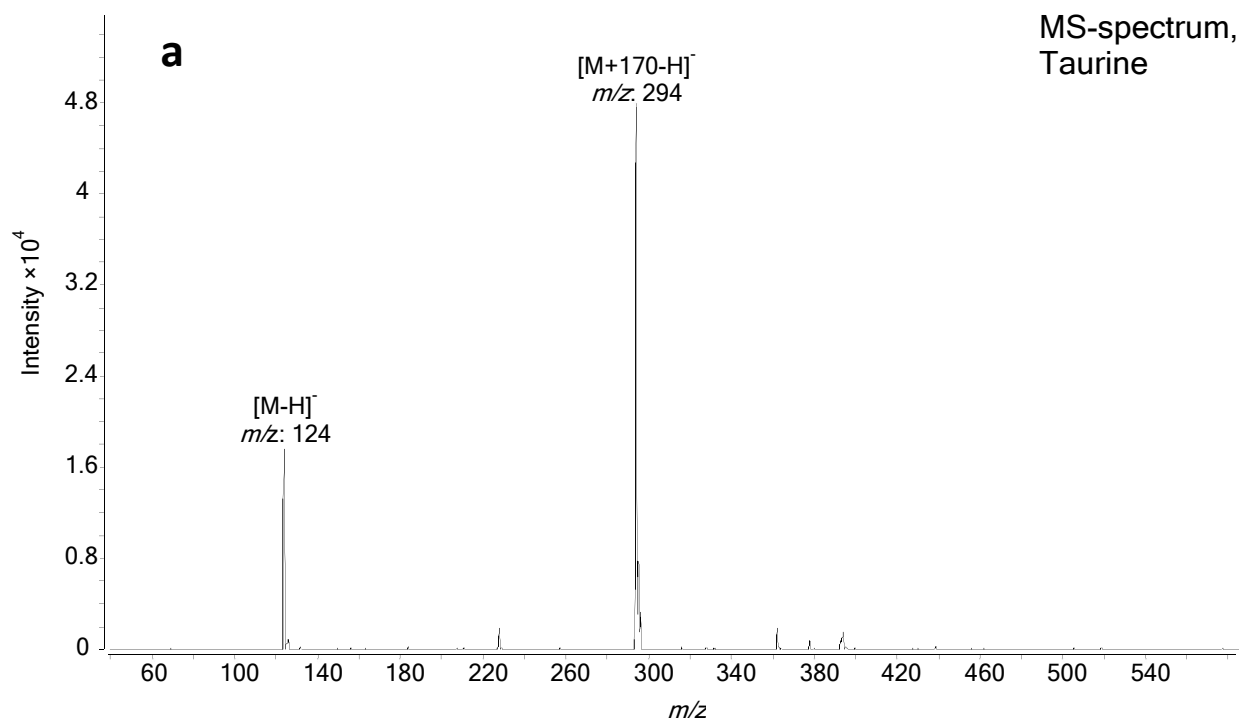**Figure S5. a)** MS-spectrum and **b)** MS/MS-spectrum of Taurine.

**Figure S6. a)** MS-spectrum and **b)** MS/MS-spectrum of Azelaic Acid.

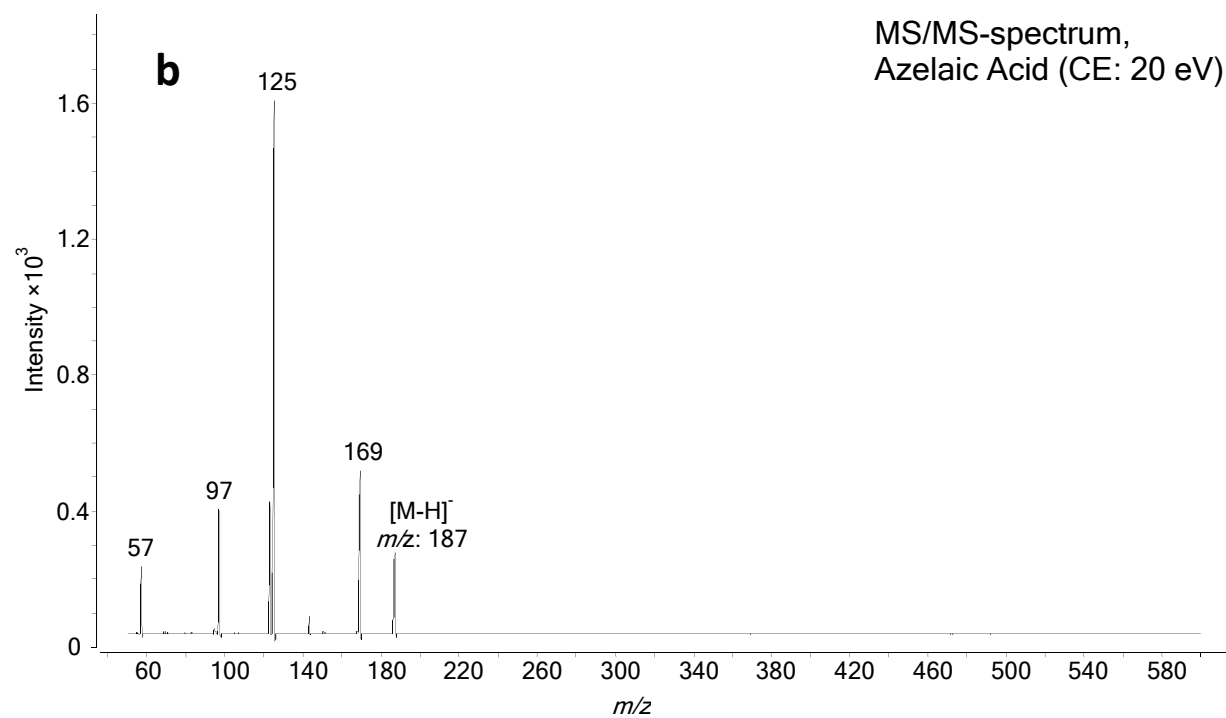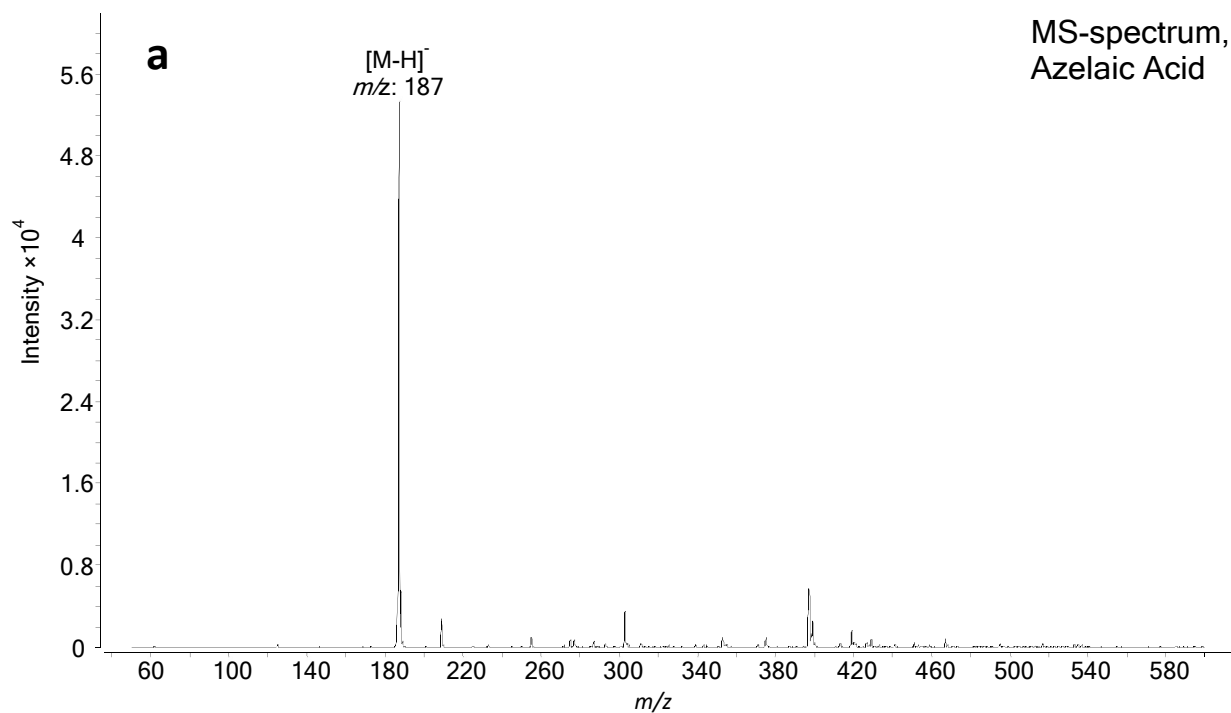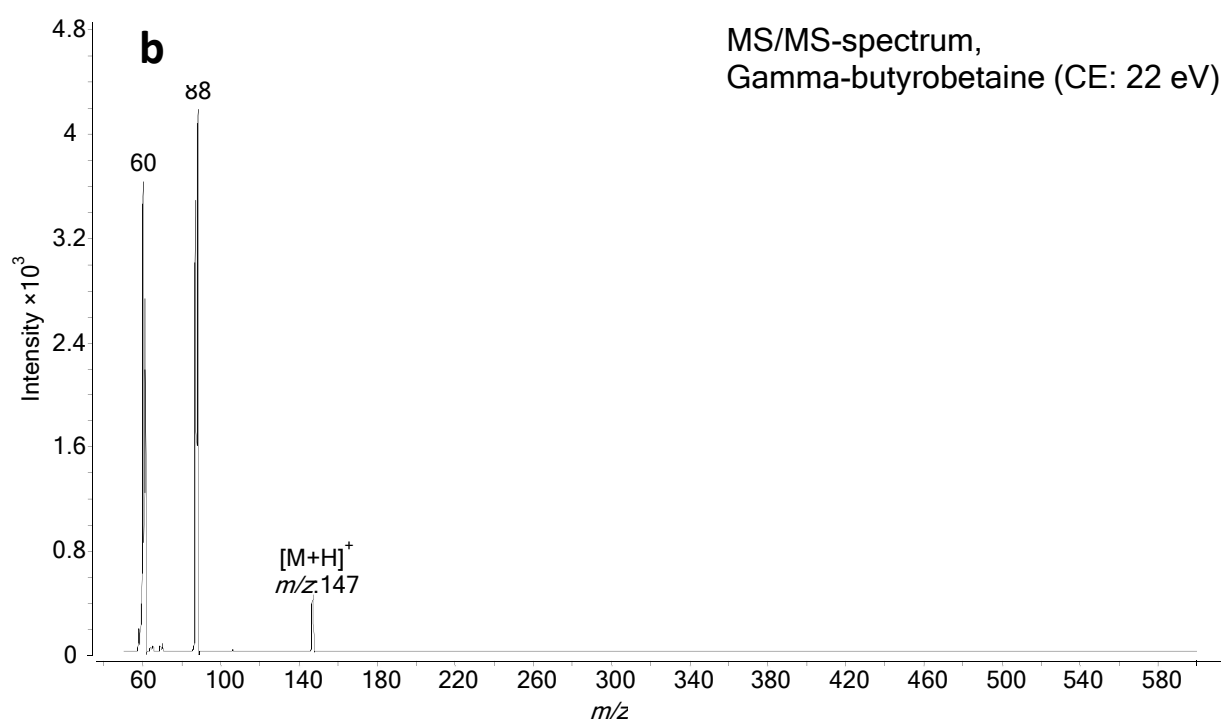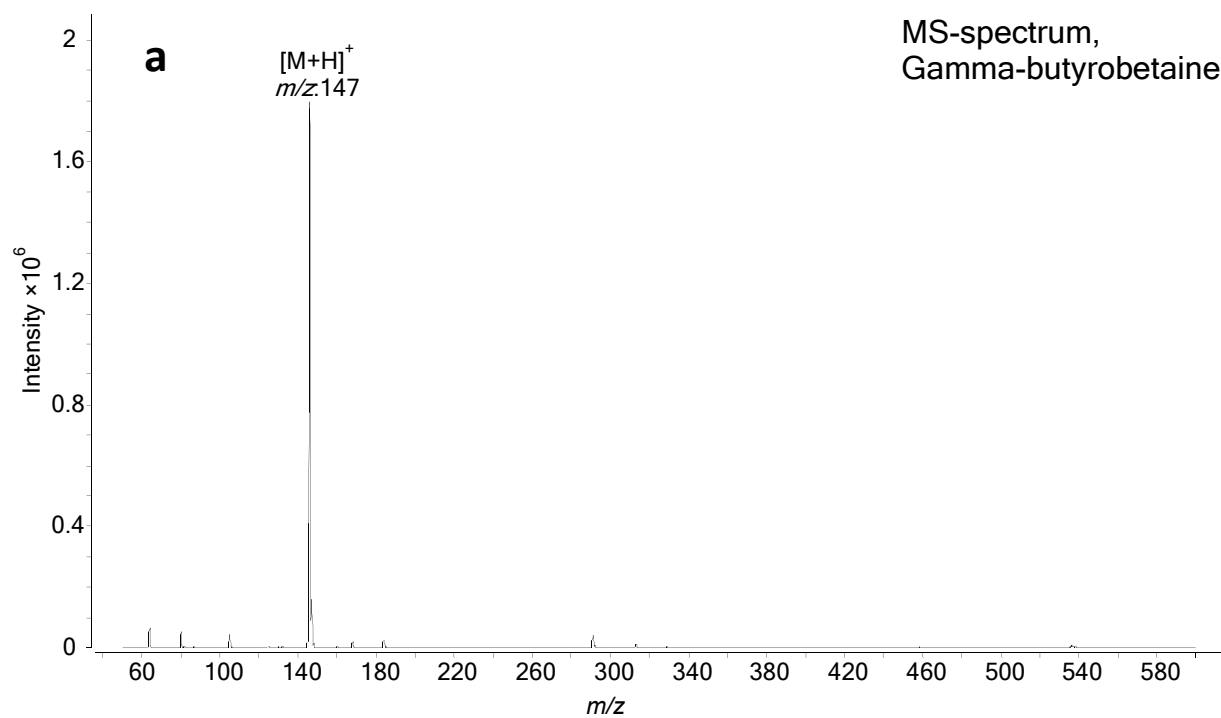**Figure S7. a)** MS-spectrum and **b)** MS/MS-spectrum of Gamma-butyrobetaine.

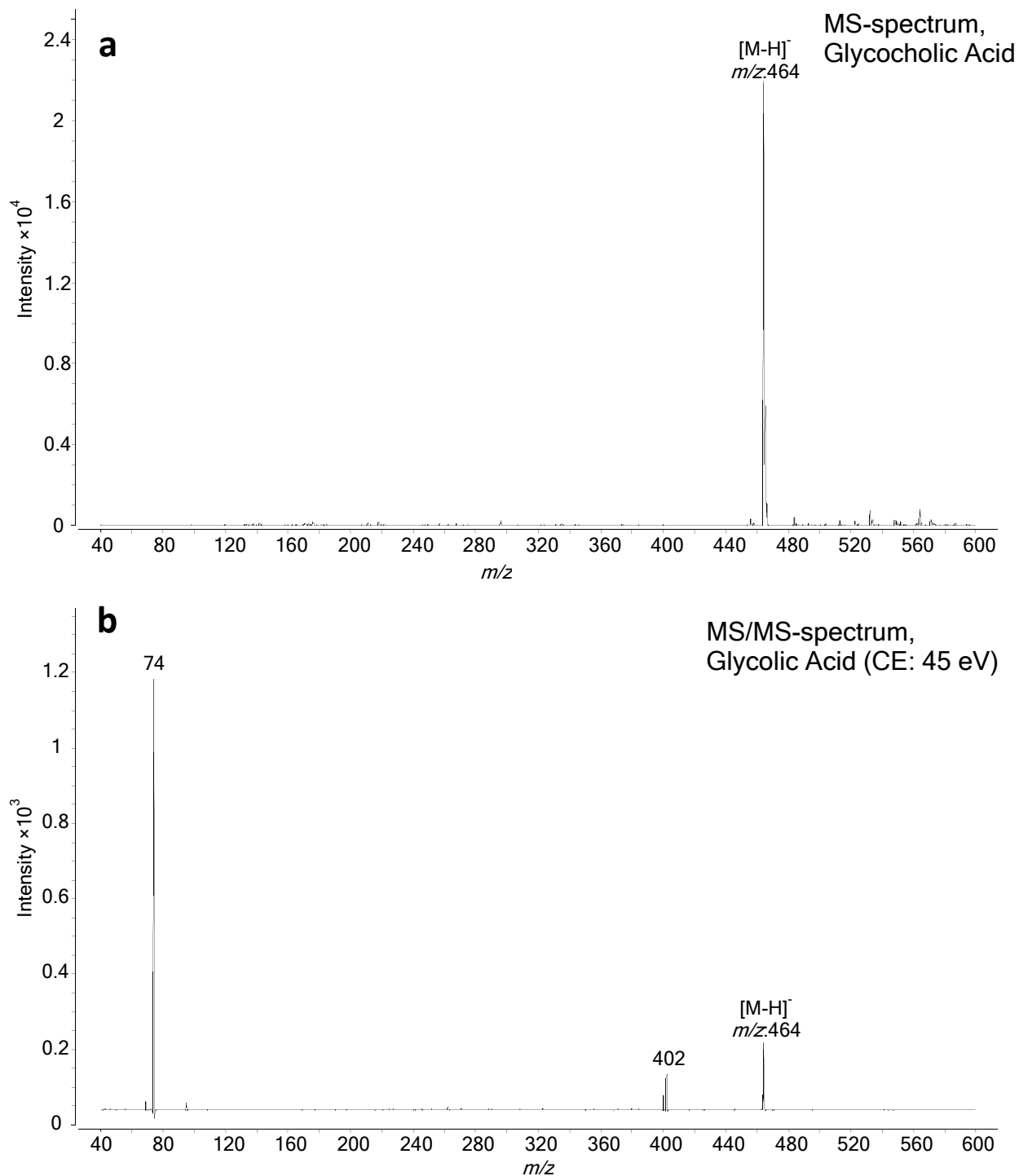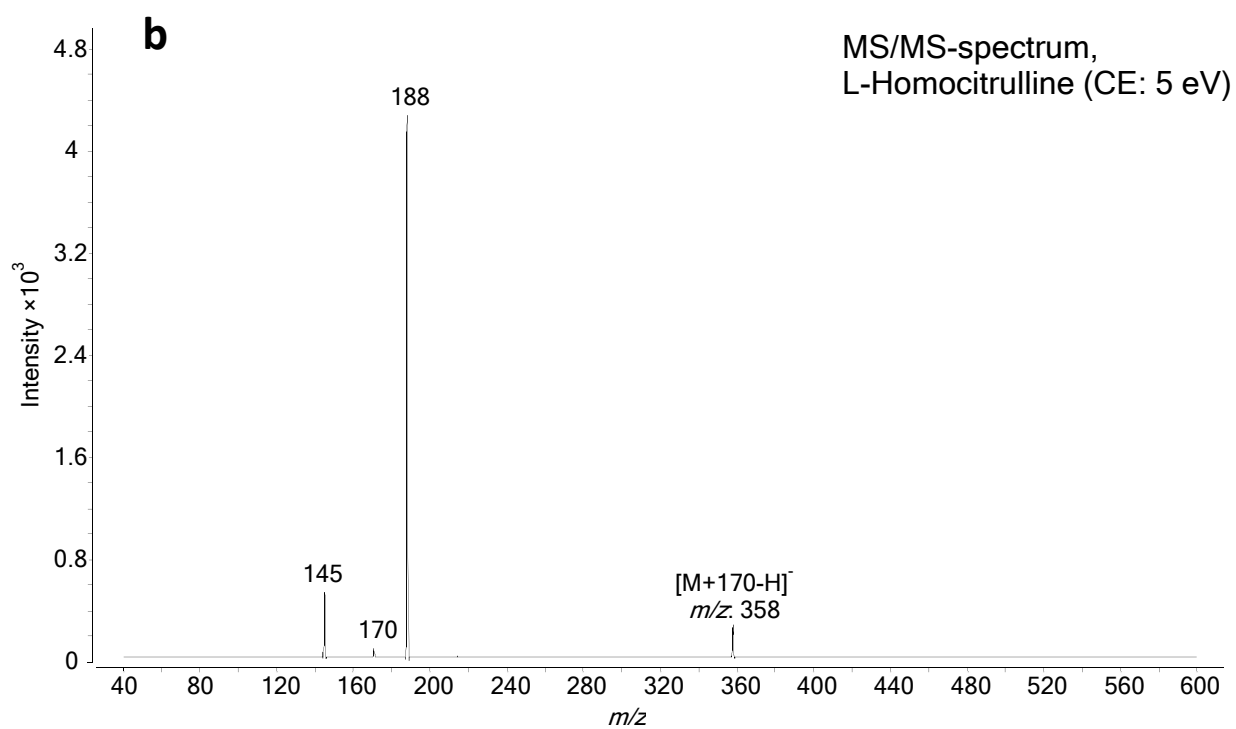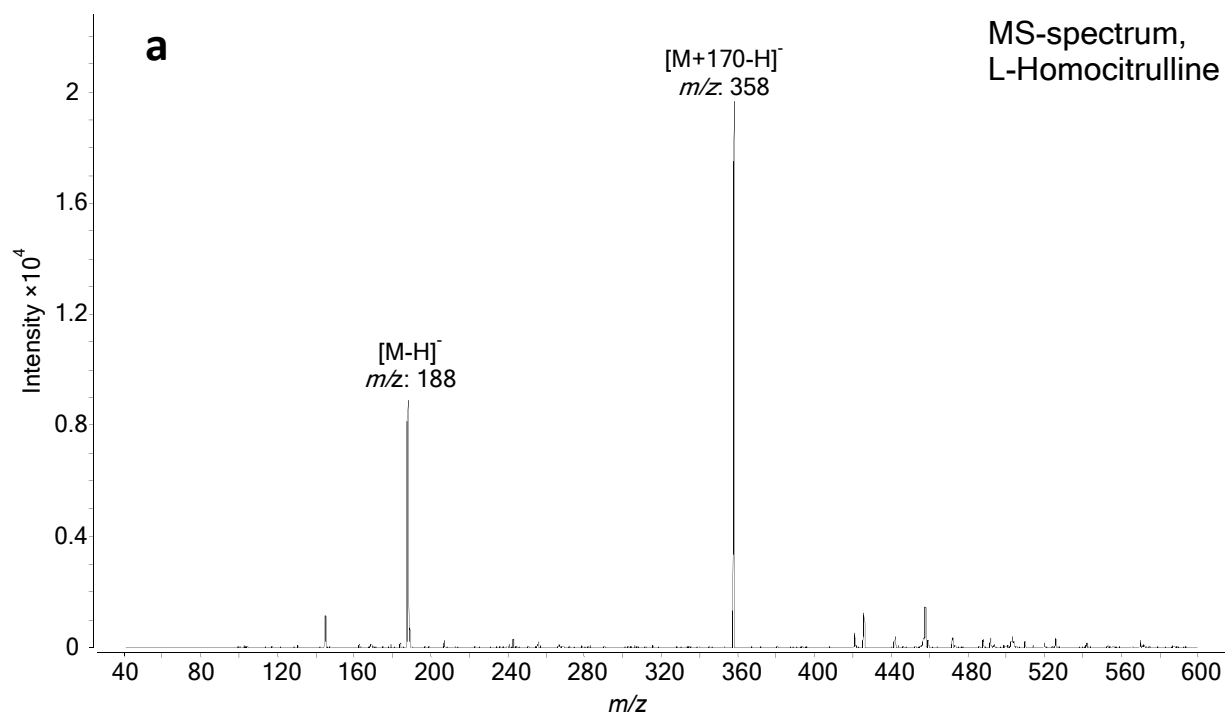**Figure S8. a)** MS-spectrum and **b)** MS/MS-spectrum of Glycolic Acid.

**Figure S9. a)** MS-spectrum and **b)** MS/MS-spectrum of L-Homocitrulline.

# References

1. MacLean B, Tomazela DM, Shulman N, Chambers M, Finney GL, Frewen B, et al. Skyline: An open source document editor for creating and analyzing targeted proteomics experiments. Bioinformatics (Oxford, England) 2010;26:966-8.

2. Team RC. R: A language and environment for statistical computing, r foundation for statistical computing. Vienna, Austria 2017.