Supplementary Information

Reanalysis of Public Metabolomics Data Reveals Class-Specific Dysregulation of *N*-Acyl Lipids and Related Molecules in Atopic Dermatitis

Natâna S. Cunha,[a,b] Anthony R. Moreira,[a,c] Tainara C. Vieira,[a,d] Sandro D. Souza,[a,e] José Diogo E. Reis[a,b] and Paulo Wender P. Gomes*[*,a,b,c,e]

[a]Central Integrada em Metabolômica da Amazônia, Instituto de Ciências Exatas e Naturais, Universidade Federal do Pará, 66075-110 Belém-PA, Brazil

[b]Programa de Pós-Graduação em Química, Instituto de Ciências Exatas e Naturais, Universidade Federal do Pará, 66075-110 Belém-PA, Brazil

[c]Faculdade de Química, Instituto de Ciências Exatas e Naturais, Universidade Federal do Pará, 66075-110 Belém-PA, Brazil

[d]Faculdade de Farmácia, Instituto de Ciências da Saúde, Universidade Federal do Pará, 66075-110 Belém-PA, Brazil

[e]Programa de Pós-Graduação em Biodiversidade e Biotecnologia (BIONORTE), Universidade Federal do Pará, 66075-110 Belém-PA, Brazil

*e-mail: wendergomes@ufpa.br

ORCID ID:
Natâna: https://orcid.org/0009-0002-2063-5989
Anthony: https://orcid.org/0009-0001-0816-5104
Tainara: https://orcid.org/0009-0009-8452-1009
Sandro: https://orcid.org/0009-0005-6969-9045
José: https://orcid.org/0000-0002-4709-4521
Paulo: https://orcid.org/0000-0001-5478-2448

Table S1. Universal spectrum identifiers (USIs) used in the mass spectrometry search tool (MASST) batch search. This table lists the USIs for all filtered and annotated molecules. Each USI corresponds to the MS/MS spectrum submitted to MASST, enabling reproducible lookup and comparison across public datasets

Compound	USI
MS3671	mzspec:GNPS2:TASK-8f30422fd9cd42e3bad550c8688e239f-nf_output/clustering/spectra_reformatted.mgf:scan:3671
MS4733	mzspec:GNPS2:TASK-8f30422fd9cd42e3bad550c8688e239f-nf_output/clustering/spectra_reformatted.mgf:scan:4733
MS7693	mzspec:GNPS2:TASK-8f30422fd9cd42e3bad550c8688e239f-nf_output/clustering/spectra_reformatted.mgf:scan:7693
MS7781	mzspec:GNPS2:TASK-8f30422fd9cd42e3bad550c8688e239f-nf_output/clustering/spectra_reformatted.mgf:scan:7781
MS3772	mzspec:GNPS2:TASK-8f30422fd9cd42e3bad550c8688e239f-nf_output/clustering/spectra_reformatted.mgf:scan:3772
MS4221	mzspec:GNPS2:TASK-8f30422fd9cd42e3bad550c8688e239f-nf_output/clustering/spectra_reformatted.mgf:scan:4221
MS3931	mzspec:GNPS2:TASK-8f30422fd9cd42e3bad550c8688e239f-nf_output/clustering/spectra_reformatted.mgf:scan:3931
MS3918	mzspec:GNPS2:TASK-8f30422fd9cd42e3bad550c8688e239f-nf_output/clustering/spectra_reformatted.mgf:scan:3918
MS195	mzspec:GNPS2:TASK-8f30422fd9cd42e3bad550c8688e239f-nf_output/clustering/spectra_reformatted.mgf:scan:195
MS401	mzspec:GNPS2:TASK-8f30422fd9cd42e3bad550c8688e239f-nf_output/clustering/spectra_reformatted.mgf:scan:401
MS208	mzspec:GNPS2:TASK-8f30422fd9cd42e3bad550c8688e239f-nf_output/clustering/spectra_reformatted.mgf:scan:208
MS387	mzspec:GNPS2:TASK-8f30422fd9cd42e3bad550c8688e239f-nf_output/clustering/spectra_reformatted.mgf:scan:387

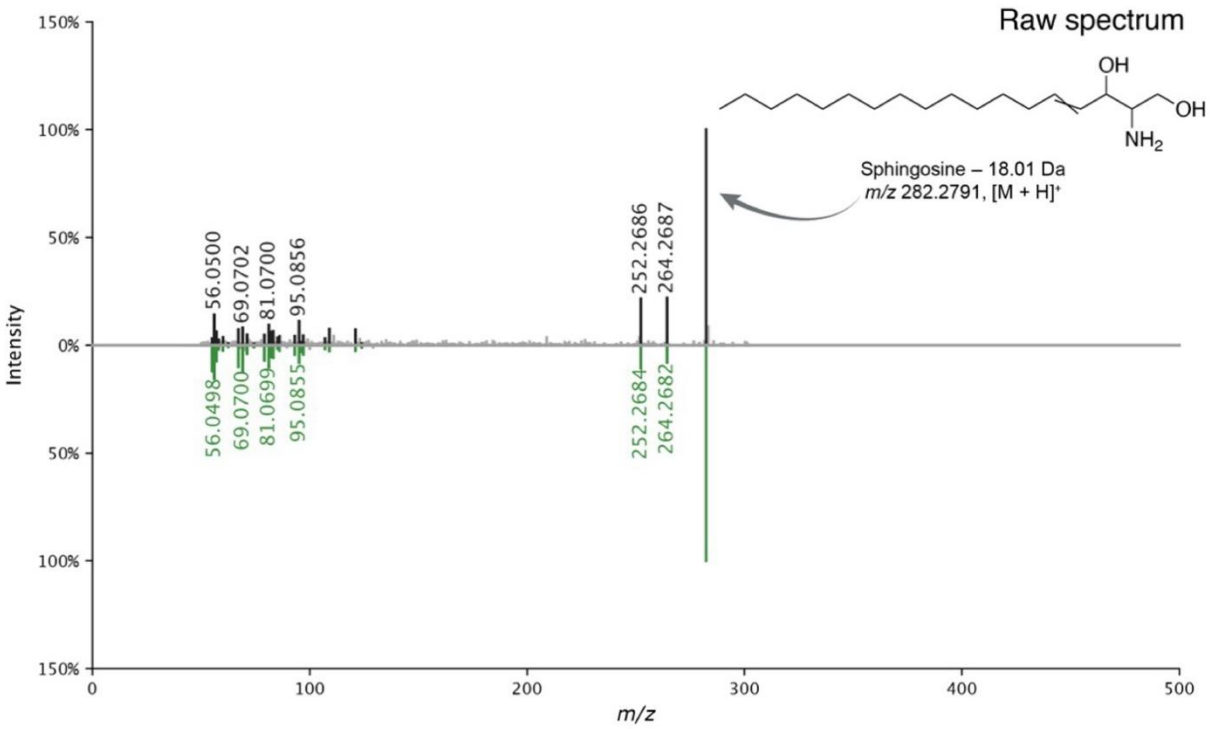

Figure S1. Mirror plot between the experimental and reference spectra of sphingosine - 18.01 Da *m/z* 282.2791, $[M + H]^+$ (ID 3671).

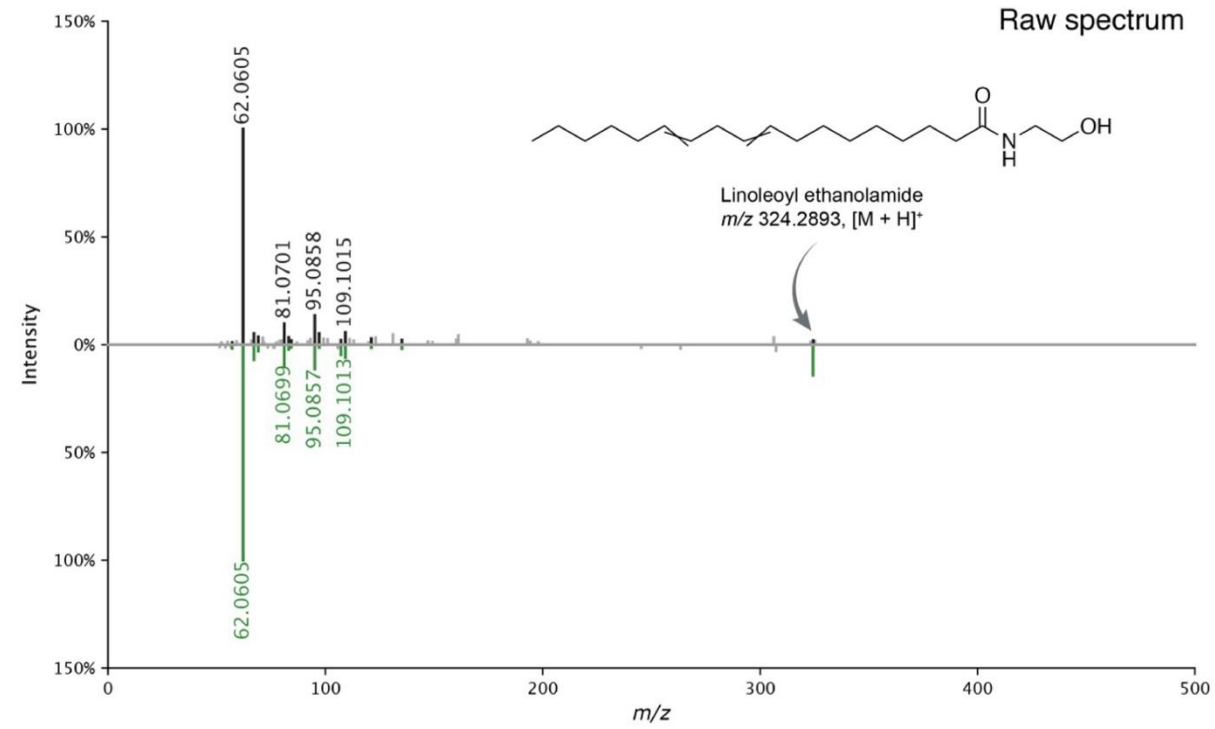

Figure S2. Mirror plot between the experimental and reference spectra of linoleoyl ethanolamide *m/z* 324.2893, $[M + H]^+$ (ID 4733).

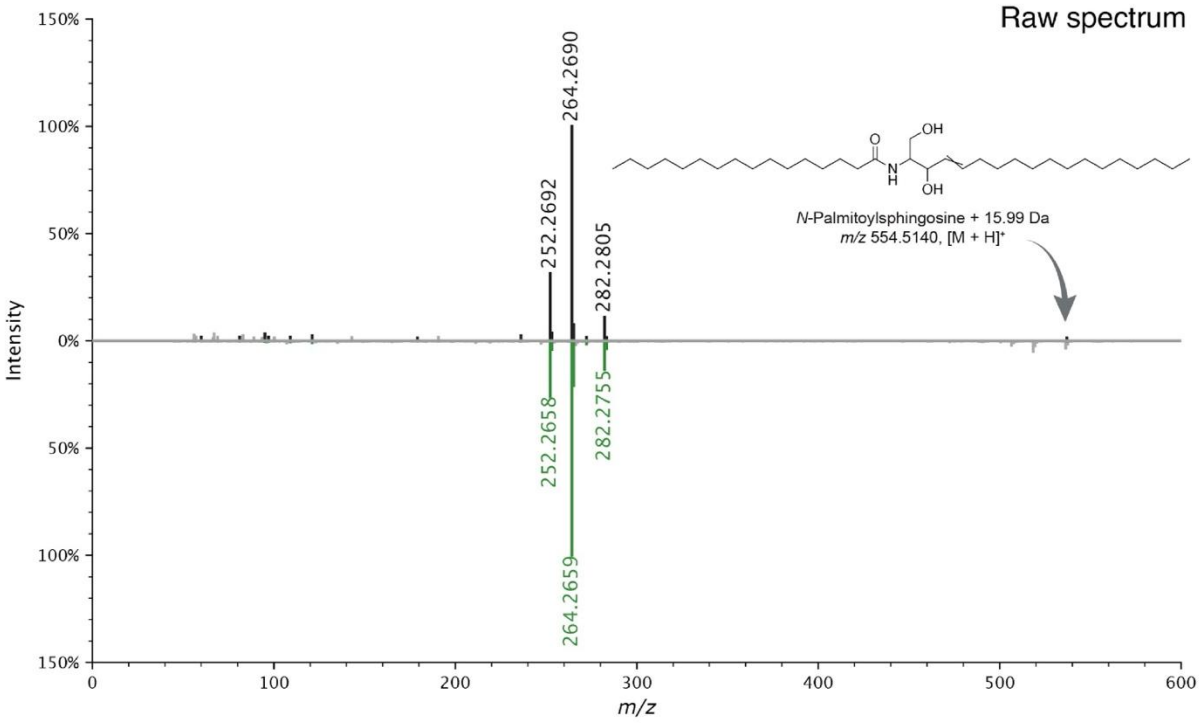

Figure S3. Mirror plot between the experimental and reference spectra of *N*-palmitoylsphingosine + 15.99 Da *m/z* 554.5140, $[M + H]^+$ (ID 7693). The observed +15.99 Da mass shift corresponds to an oxidized analog, most likely reflecting hydroxylation, and was annotated using the suspect library.

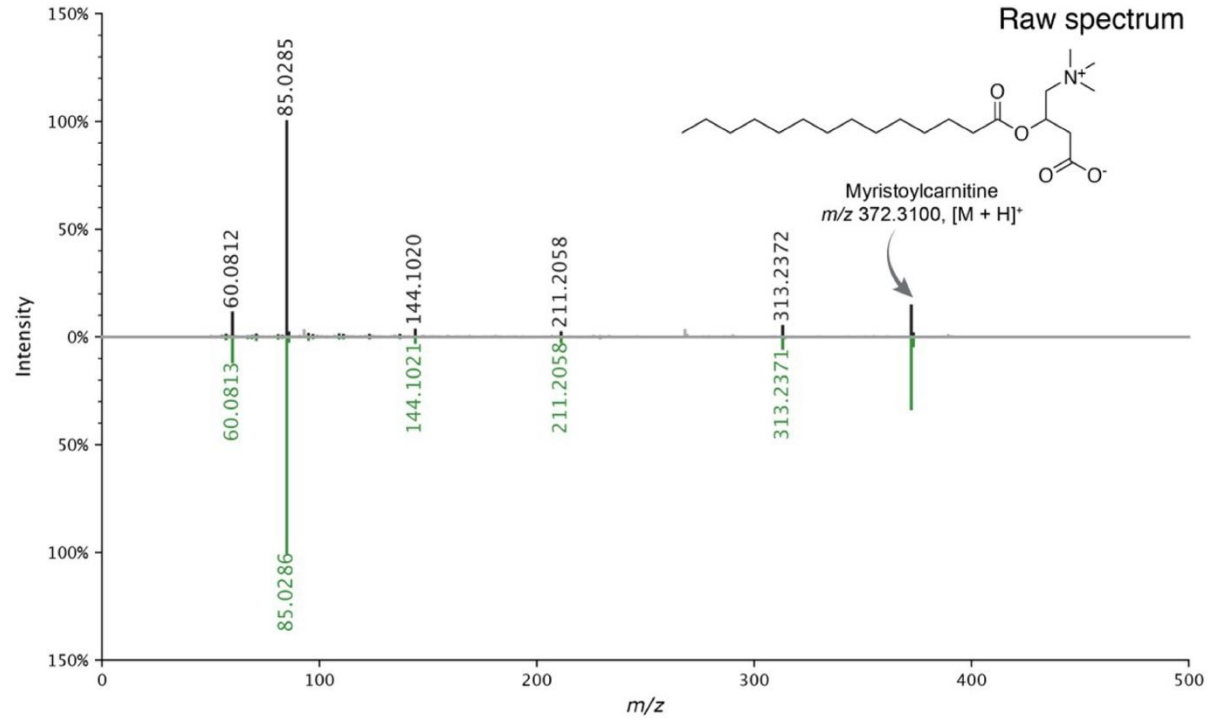

Figure S4. Mirror plot between the experimental and reference spectra of myristoylcarnitine *m/z* 372.3100, $[M + H]^+$ (ID 3772).

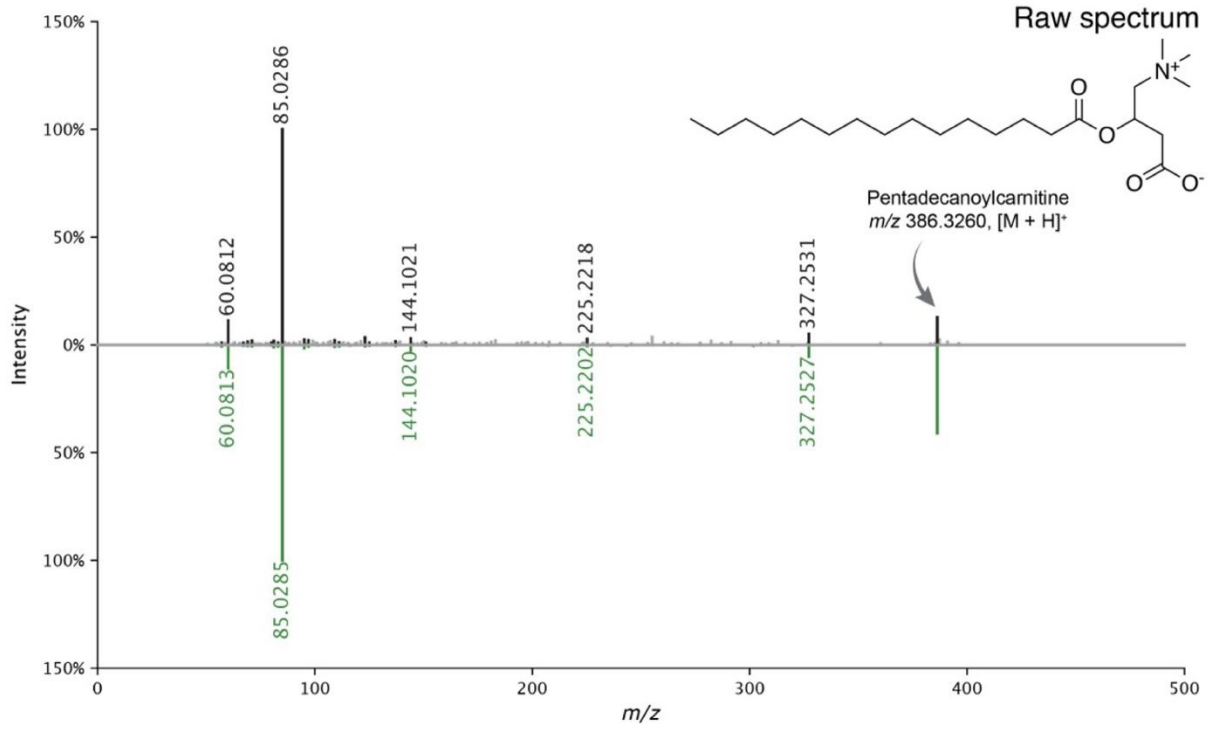

Figure S5. Mirror plot between the experimental and reference spectra of pentadecanoylcarnitine *m/z* 386.3260, $[M + H]^+$ (ID 3931).

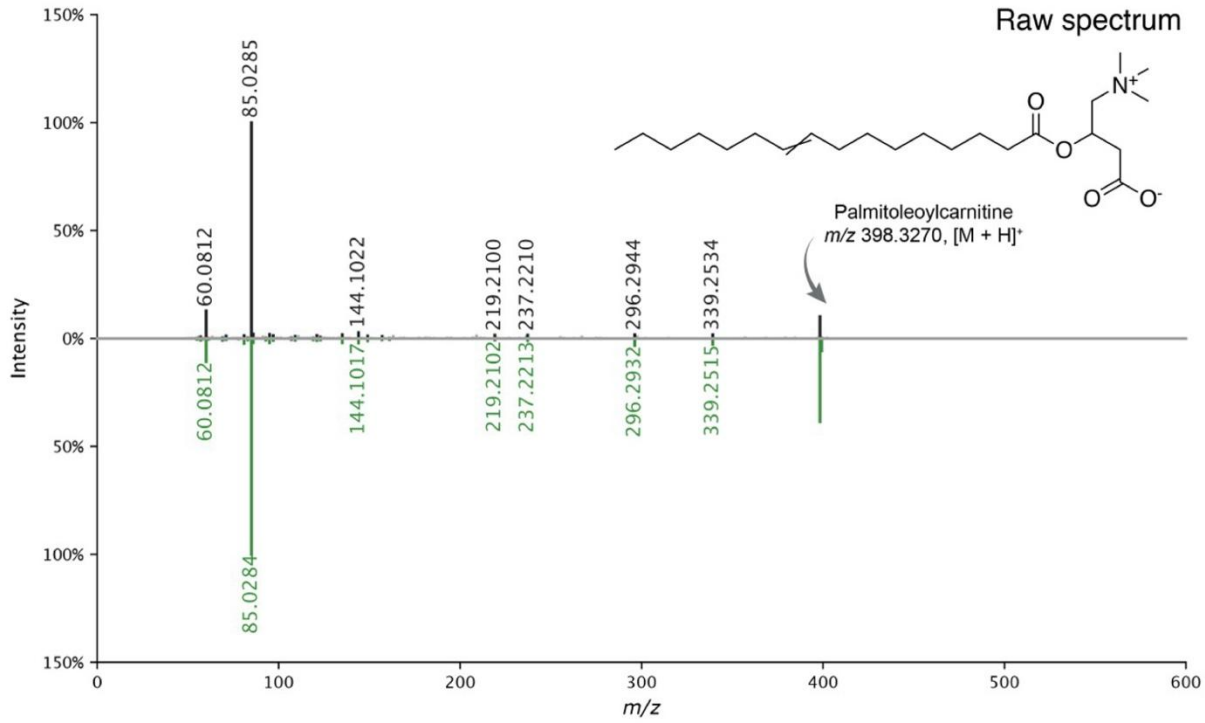

Figure S6. Mirror plot between the experimental and reference spectra of palmitoleoylcarnitine *m/z* 398.3270, $[M + H]^+$ (ID 3918).

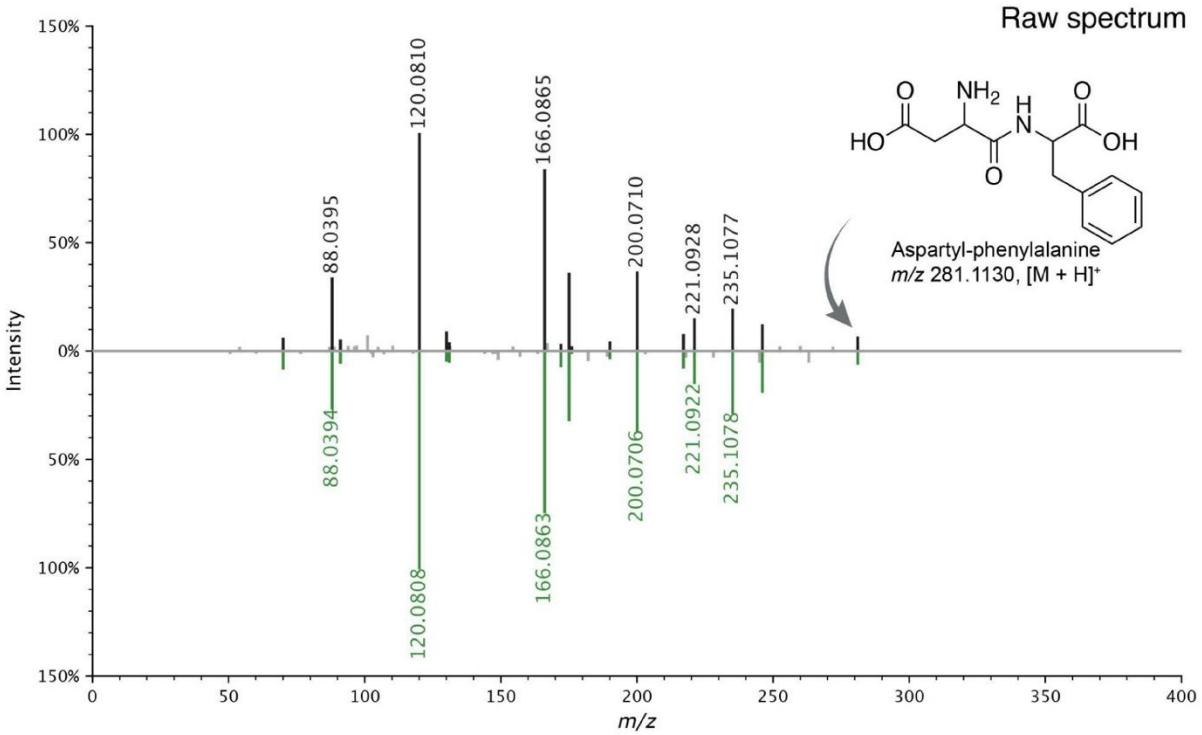

Figure S7. Mirror plot between the experimental and reference spectra of aspartyl-phenylalanine *m/z* 281.1130, $[M + H]^+$ (ID 195).

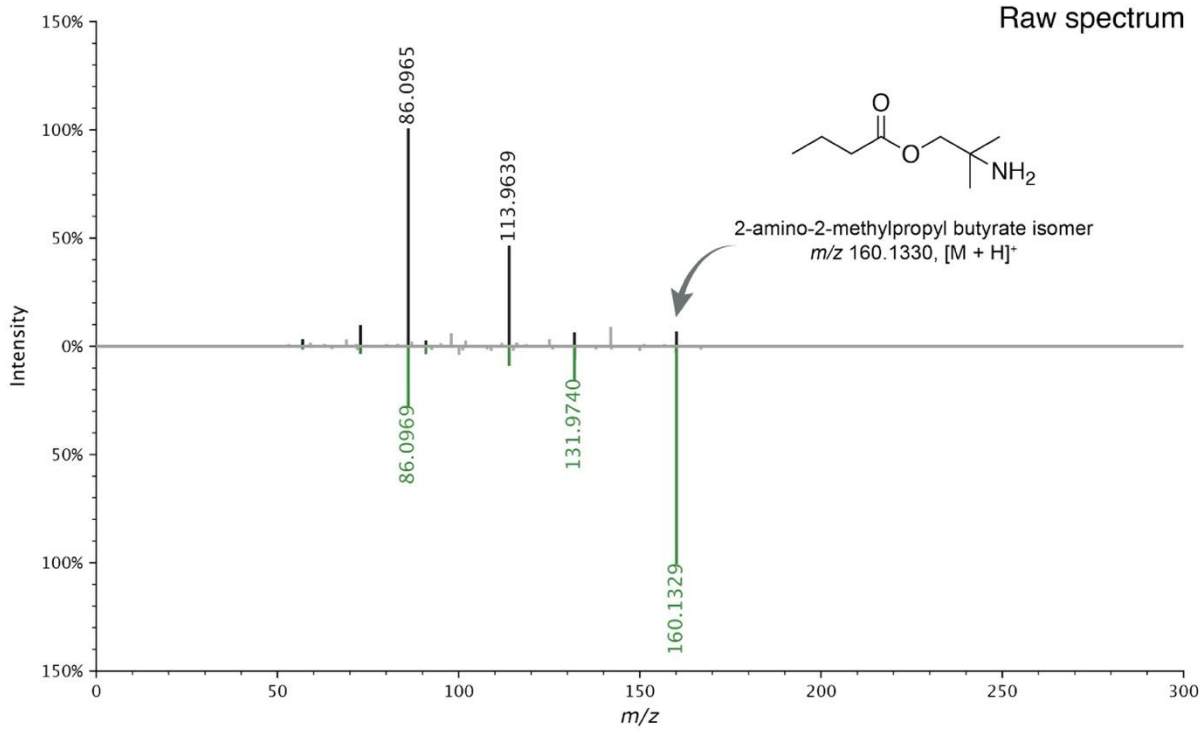

Figure S8. Mirror plot between the experimental and reference spectra of 2-amino-2-methylpropyl butyrate isomer *m/z* 160.1330, $[M + H]^+$ (ID 401).

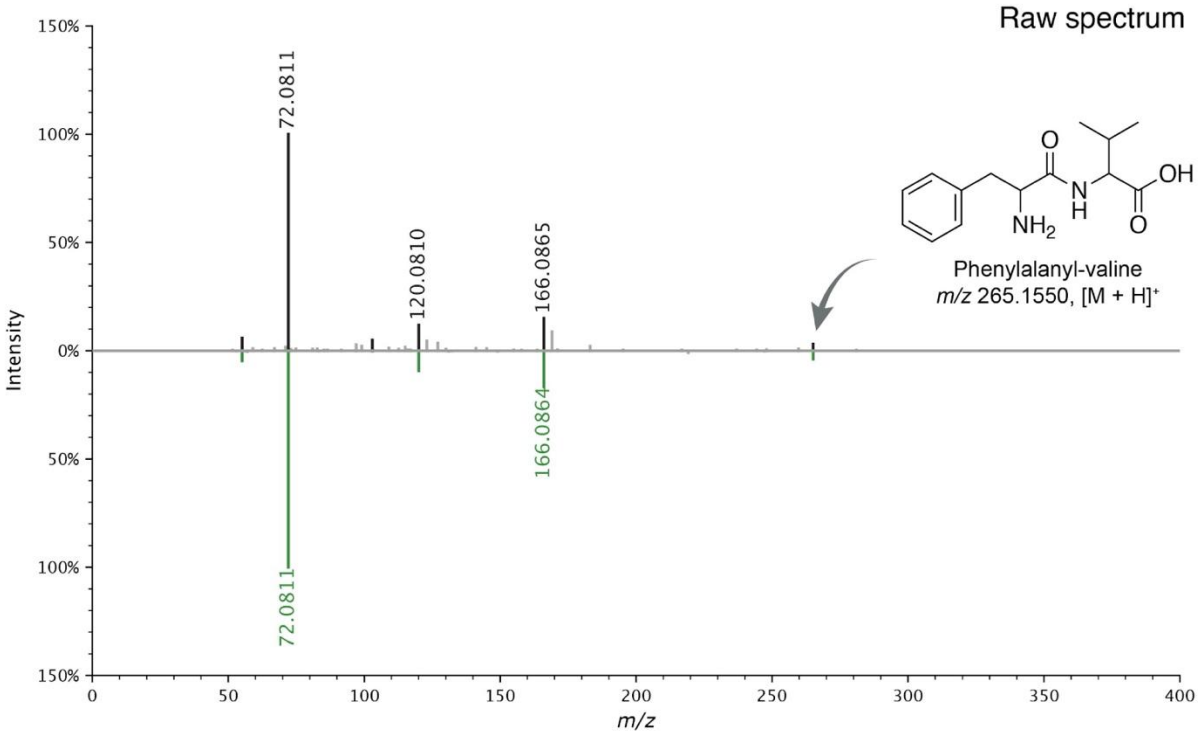

Figure S9. Mirror plot between the experimental and reference spectra of phenylalanyl-valine *m/z* 265.1550, $[M + H]^+$ (ID 387).