

# Differences in the Stool Metabolome between Vegans and Omnivores: Analyzing the NIST Stool Reference Material

Raquel Cumeras <sup>1,2</sup>, Tong Shen <sup>1</sup>, Luis Valdiviez <sup>1</sup>, Zakery Tippins <sup>1</sup>, Bennett D. Haffner <sup>1</sup> and Oliver Fiehn <sup>1,\*</sup>

<sup>1</sup> West Coast Metabolomics Center, University of California Davis, Davis, CA 95616, USA;

raquel.cumeras@ucdavis.edu (R.C.); tsshenn@ucdavis.edu (T.S.);

lvaldiviez@ucdavis.edu (L.V.);

ztippins@ucdavis.edu (Z.T.); bdlikes3.14159@gmail.com (B.D.H.)

<sup>2</sup> Oncology Department, Nutrition and Metabolism Department, Institut d'Investigació Sanitària Pere Virgili (IISPV), Universitat Rovira i Virgili (URV), 43204 Reus, Spain

\* Correspondence: ofiehn@ucdavis.edu

**Supplementary Figure S1.** Fold-changes (FC) distribution by assay per vegan versus omnivore analysis.

**Supplementary Figure S2.** Fold-changes (FC) distribution by assay per vegan versus omnivore analysis.

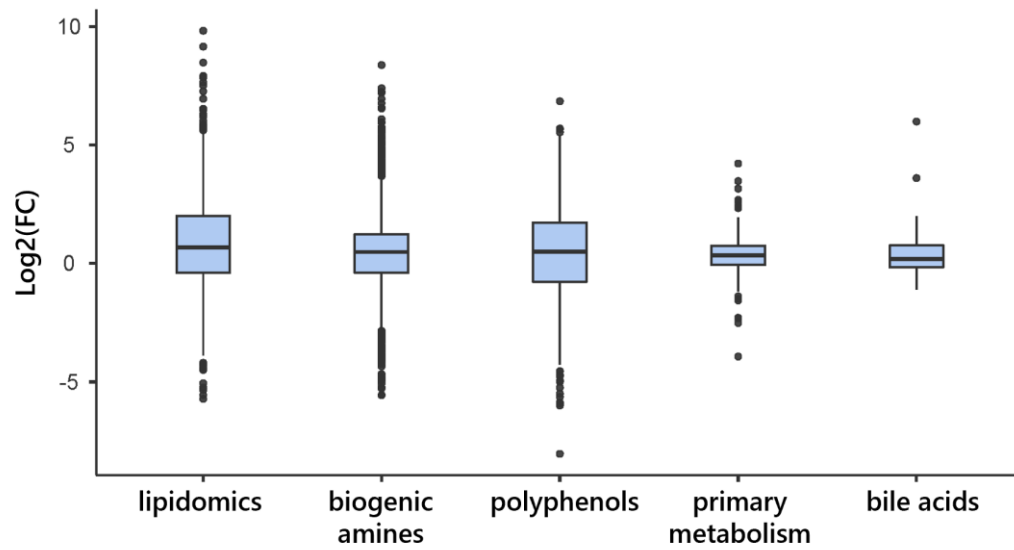
**Supplementary Figure S3.** Distribution and cumulative percentage of technical variation of annotated metabolites in QC samples.

**Supplementary Figure S4.** PLS-DA with the z-score scale of the 4RGTM (top left) with the loadings plot (middle) and some of the compound's boxplots showing the differences in z-score from the different regions of the loadings plot. Data considered: CSH, HILIC, PFP, and GC.

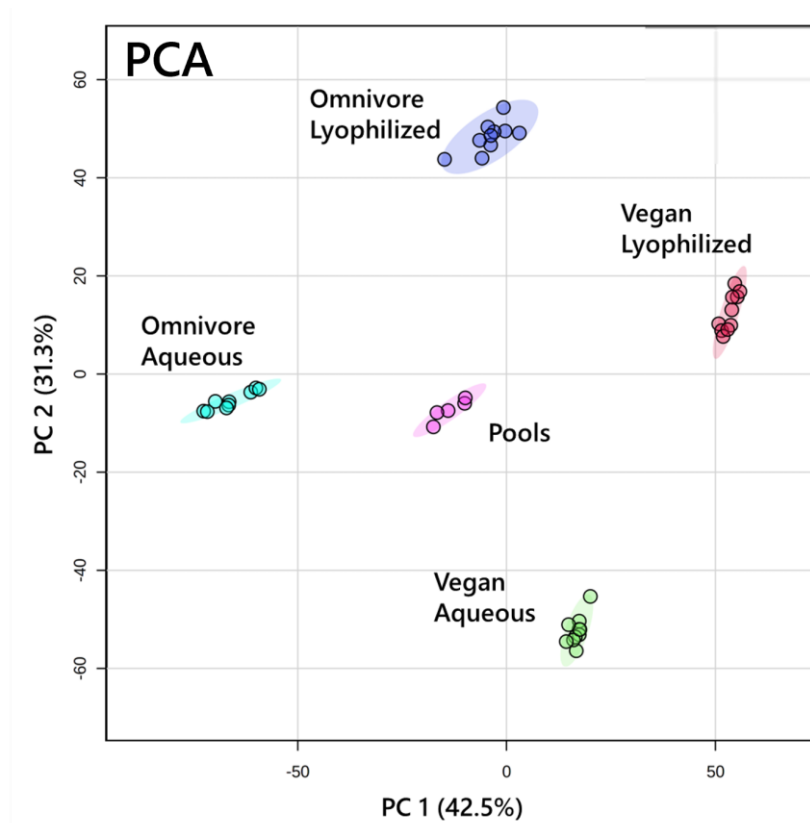
**Supplementary Figure S5.** Heatmap of the 4RGTM, with hierarchical clustering groups lyophilized and aqueous RGTMs.

**Supplementary Figure S6.** Reconstruction of the Purine metabolism pathway.

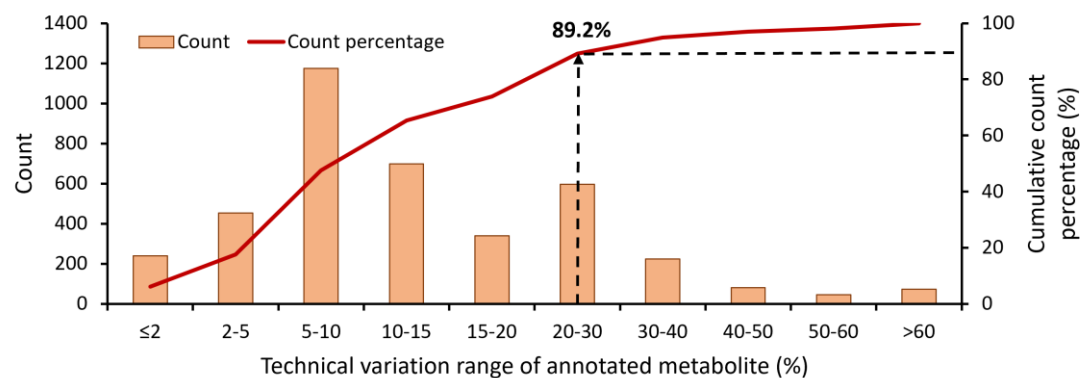
**Supplementary Figure S7.** Distribution of AAHFAs per type of diet, and MSMS identification.



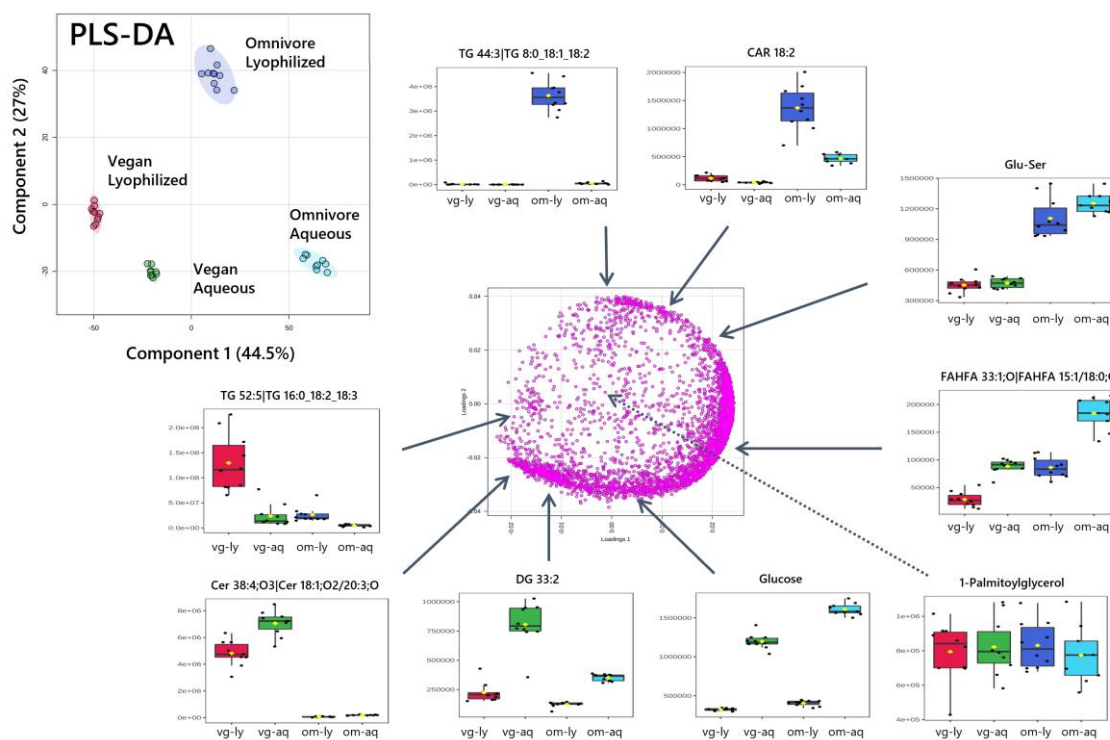
**Figure S1.** Fold-changes (FC) distribution by assay per vegan versus omnivore analysis.



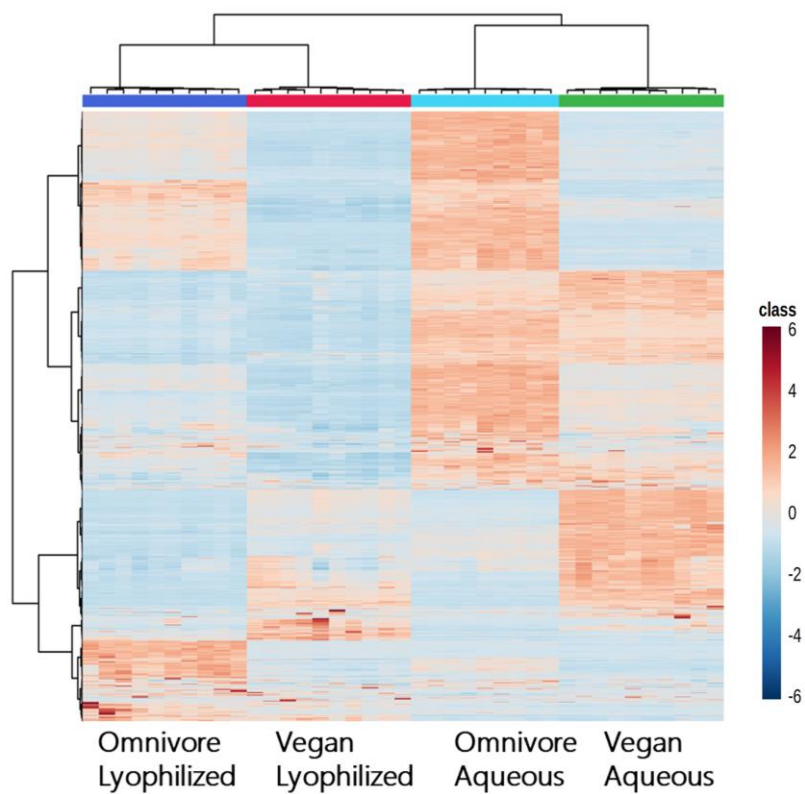
**Figure S2.** Fold-changes (FC) distribution by assay per vegan versus omnivore analysis.



**Figure S3.** Distribution and cumulative percentage of technical variation of annotated metabolites in QC samples.



**Figure S4.** PLS-DA with the z-score scale of the 4RGTM (top left) with the loadings plot (middle) and some of the compound's boxplots showing the differences in z-score from the different regions of the loadings plot. Data considered: CSH, HILIC, PFP, and GC.



**Figure S5.** Heatmap of the 4RGTM, with hierarchical clustering groups lyophilized and aqueous RGTMs.

# Purine metabolism

Primary metabolism  
Biogenic amines

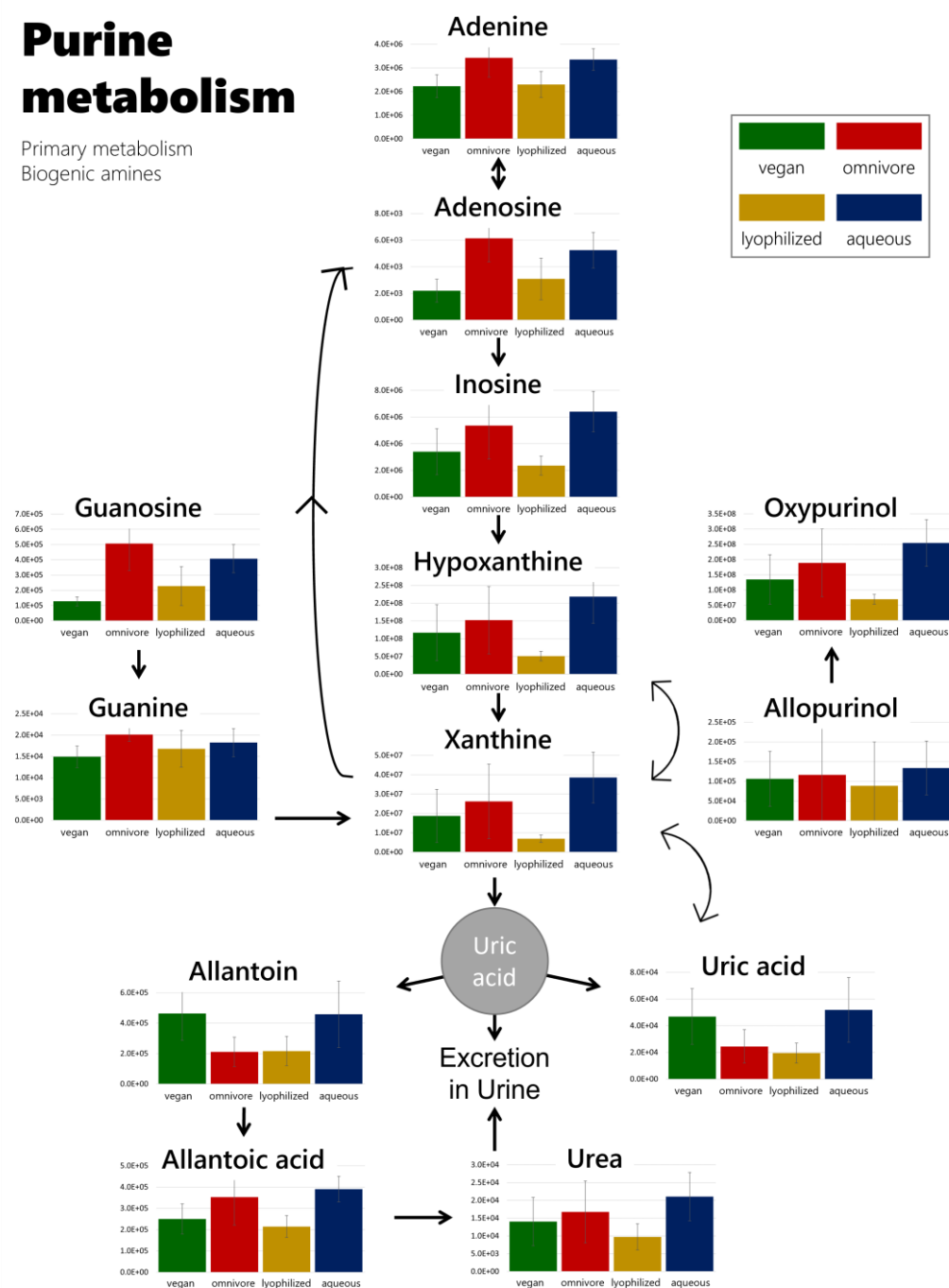
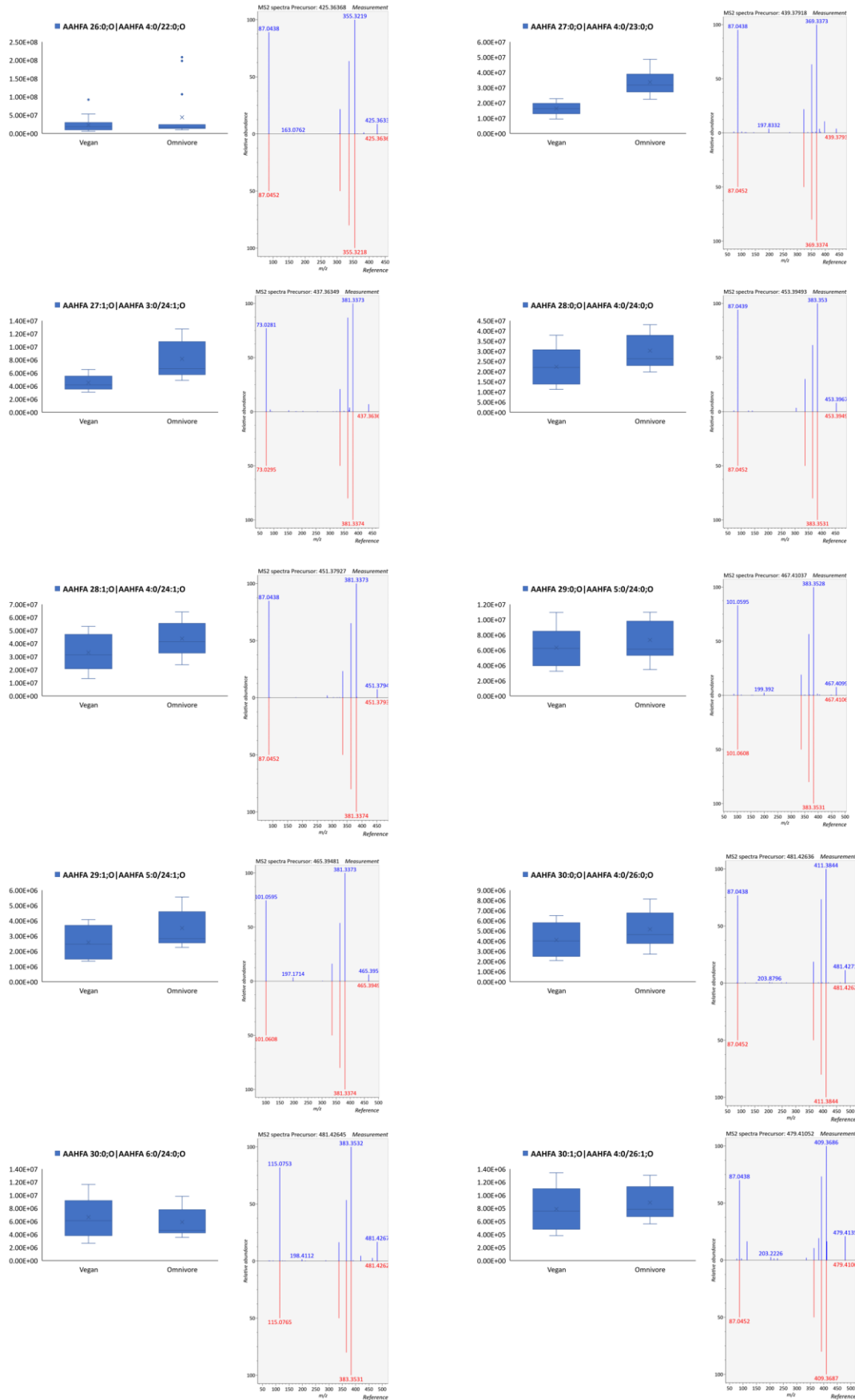
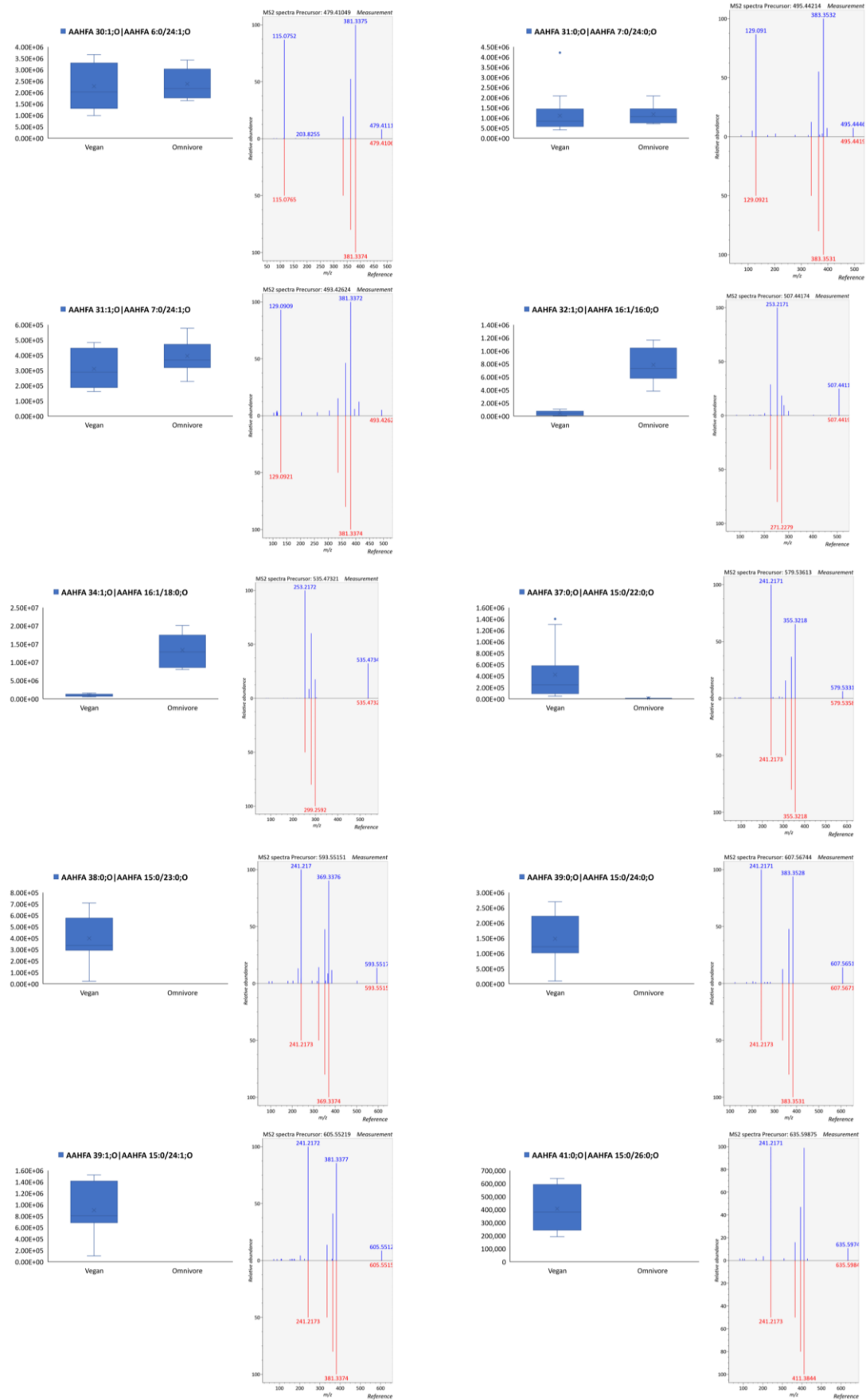


Figure S6. Reconstruction of the Purine metabolism pathway.



# metabolites





**Figure S7.** Distribution of AAHFAs per type of diet, and MSMS identification.