Paroxetine administration affects microbiota and bile acid levels in mice

Supplementary Material

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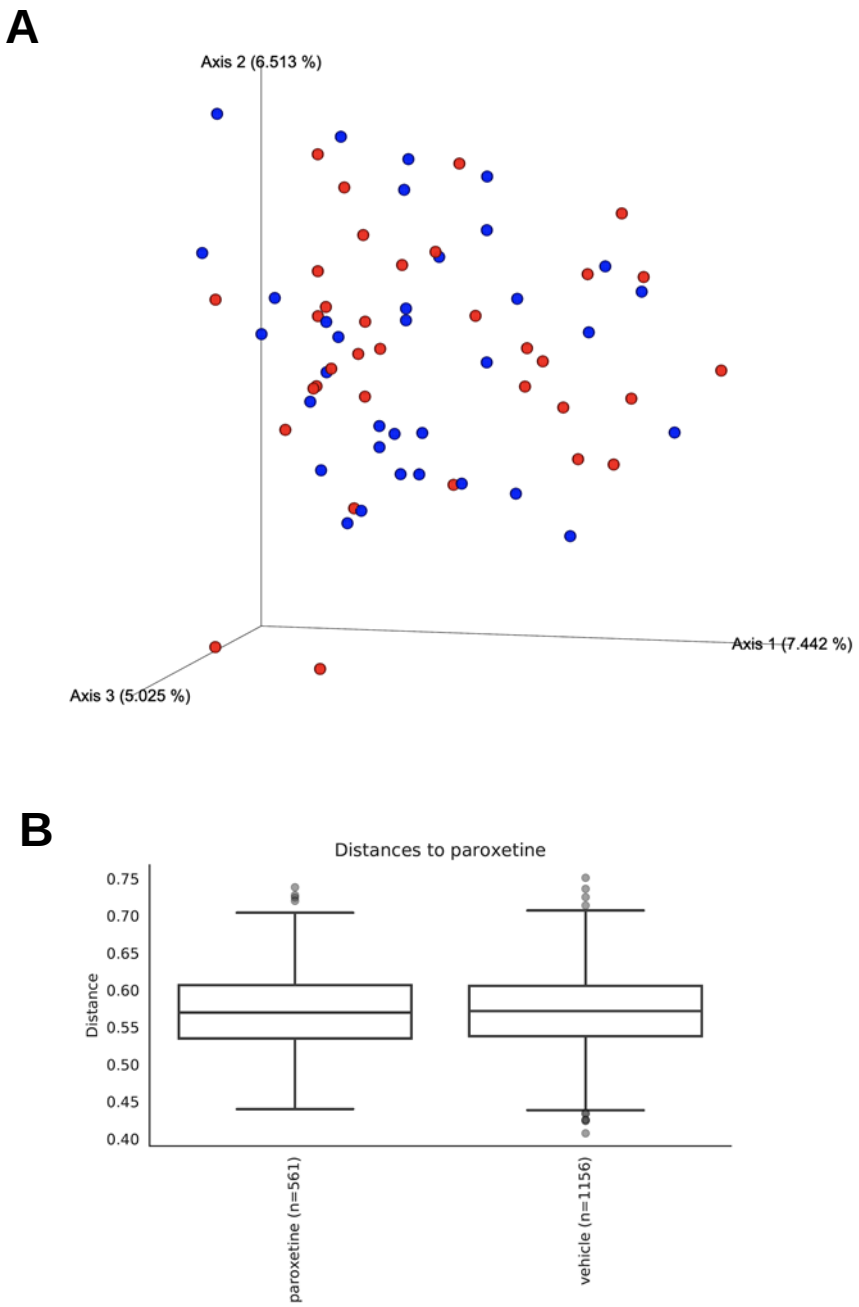
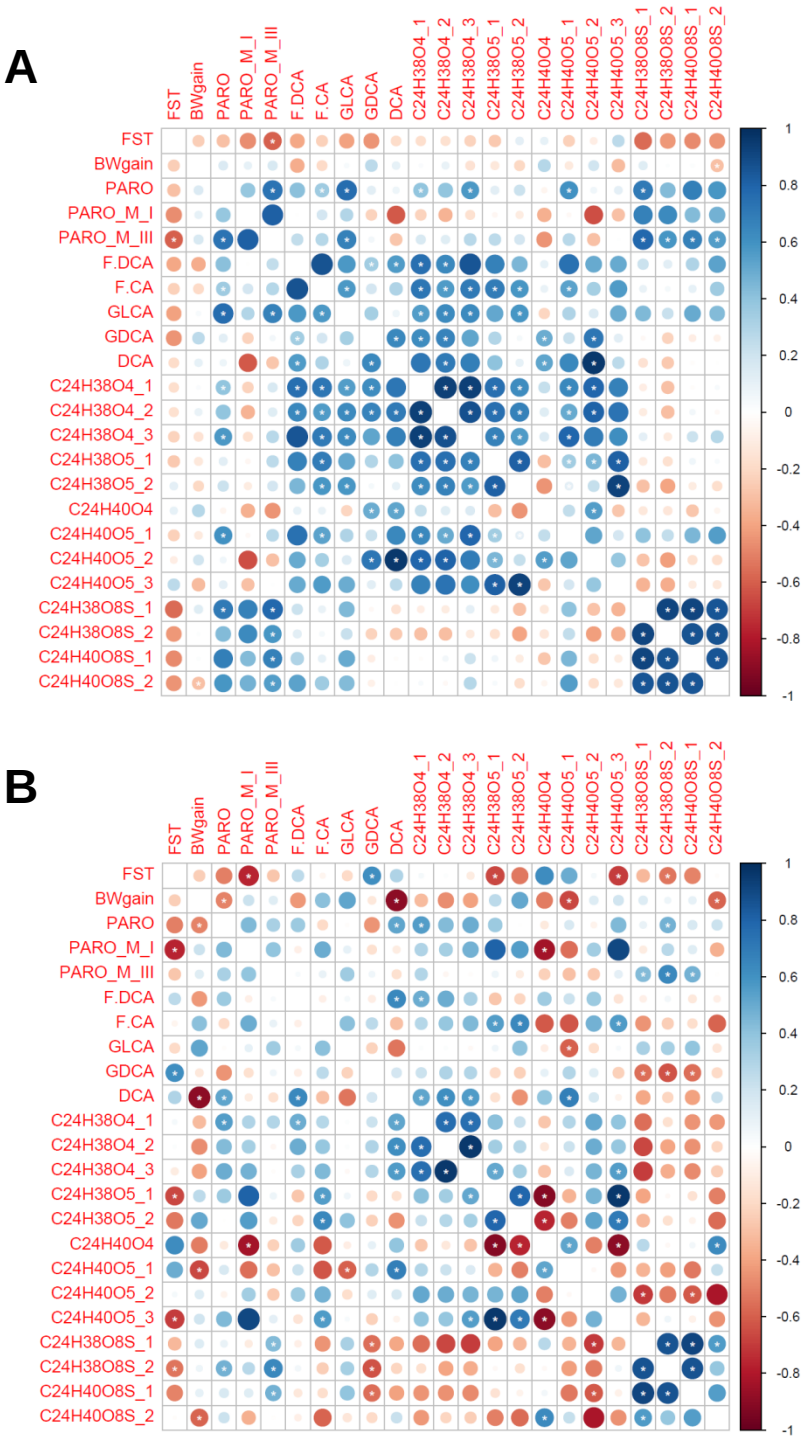
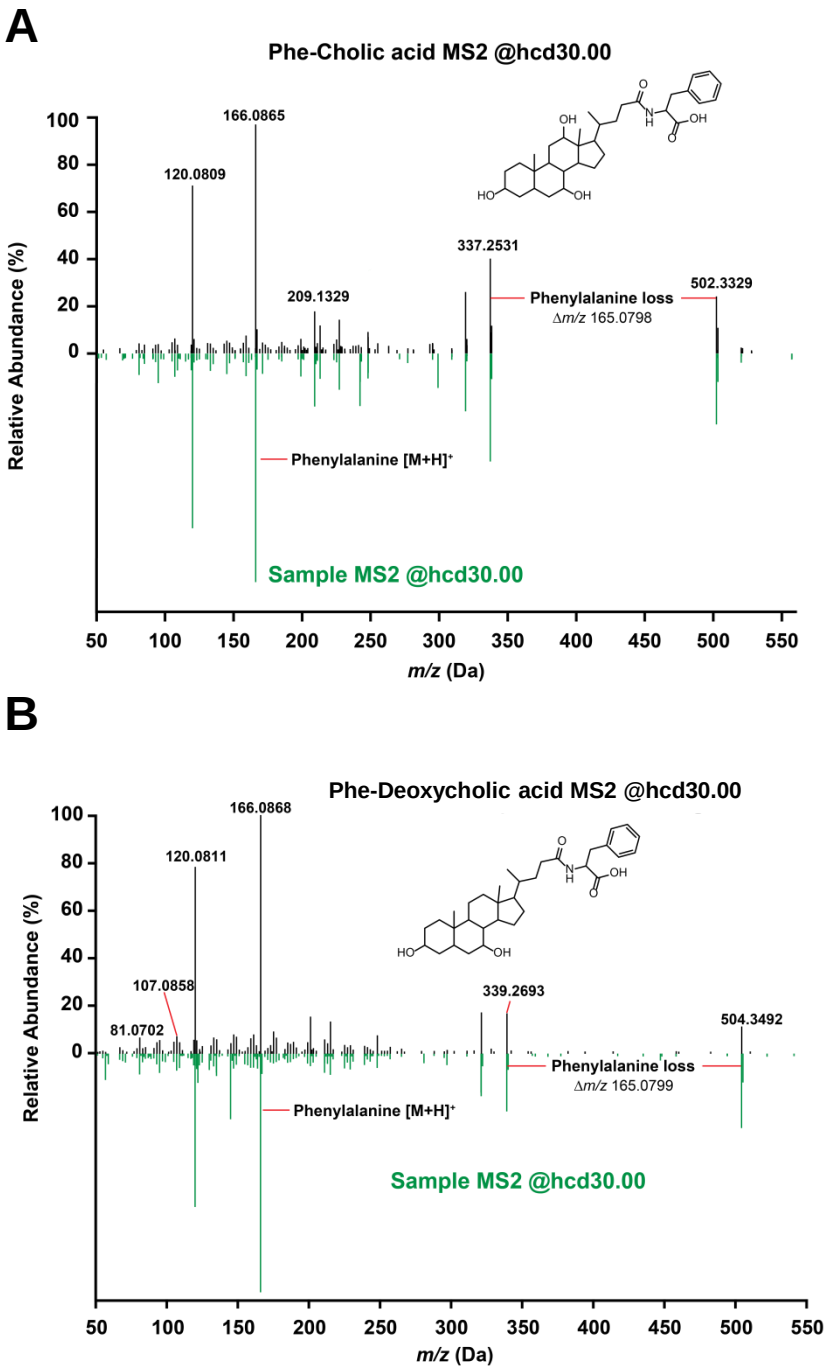


Supplementary Figure 1. (A) Unweighted UniFrac microbiome distances projected using principle coordinate analysis for analysis of beta-diversity of the microbiome data. Blue spheres are fecal samples from vehicle-treated mice (n=34), red spheres are samples from paroxetine-treated mice (n=34). (B) Boxplots of unweighted UniFrac distances of samples in PCoA plot above used to calculate PERMANOVA testing. p-value from the PERMANOVA test is 0.982.



Supplementary Figure 2: Fecal pellet bile acid levels are associated with body weight gain, behavior, and other bile acid levels. Correlation matrix is based on Spearman correlation. Significance is indicated by white asterisk ($p < 0.1$). (A) One week treatment and (B) two weeks treatment. Correlations are based on the paroxetine (PARO)-treated mouse group (n=10).



Supplementary Figure 3: (A) MS2 spectrum of the newly found phenylalanocholic acid (Phe-Cholic acid) molecule in the sample mirrored against the Phe-Cholic acid molecule found in the GNPS database. (B) MS2 spectrum of the newly found phenylalanodeoxycholic acid (Phe-Deoxycholic acid) molecule in the sample mirrored against the Phe-Deoxycholic acid molecule found in the GNPS database. Second best hit was to phenylchenodeoxycholic acid spectrum.

Supplementary Table 1: Parameters used for MZmine feature detection

Crop filtering

- Retention time: 0 – 5.6 min
- m/z: 50 – 5990

Mass detection

- MS1 mass detector: 2.0 E5
- MS2 mass detector: 1.0 E2

ADAP Chromatogram builder

- Min group size in # scans 5
- Group intensity threshold 2.0E5
- Min time span (min): 0.05
- Min highest intensity: 6.0 E5
- m/z tolerance: 0.005 m/z or 10 ppm

Chromatogram deconvolution

- Local min search
  - Chromatogram threshold: 0.01%
  - Search minimum in RT range (min): 0.40
  - Min relative height: 0.01%
  - Min absolute height: 6.0 E5
  - Min ration of peak top/edge: 3
  - Peak duration range (min): 0.05 – 0.40
- m/z range for MS2 scan pairing (Da): 0.05
- RT range for MS2 scan pairing (min): 0.2

Isotope peak grouper:

- m/z tolerance: 0.01 m/z or 10 ppm
- Retention time tolerance (min): 0.1
- Maximum charge: 4

Join Alignment

- m/z tolerance: 0.005 m/z or 10 ppm
- Weight for m/z: 90
- Retention time tolerance (min): 0.3
- Weight for RT: 10

Peak list row filter

- Minimum peaks in a row: 2
- Reset the peak number ID

Gap fill

- Intensity tolerance: 20%
- m/z tolerance: 0.01 m/z or 10 ppm
- Retention time tolerance (min): 0.2

Supplementary Table 2: Metabolite and meta data from mouse behavior experiments (Supplementary Table 2.xlsx).