

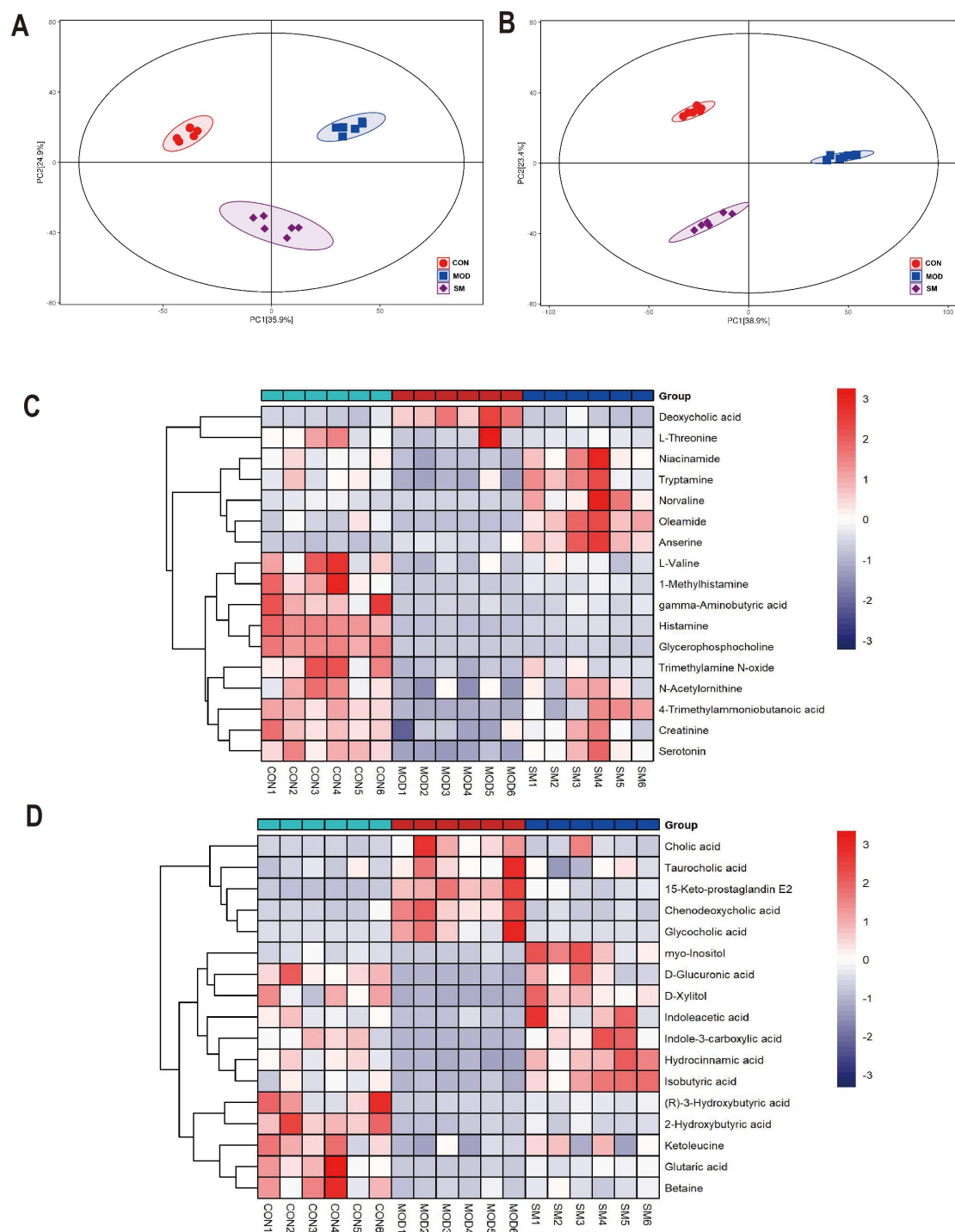


Figure S4. PCA analysis of metabolites profile. CON: turquoise; MOD: red; SM: dark blue. (A) PCA score plots for positive-ion mode ($R^2X = 0.680$). (B) PCA score plots for negative-ion mode ($R^2X = 0.674$). (C) Heat map of the differential metabolites in positive-ion mode. (D) Heat map of the differential metabolites in negative-ion mode.