

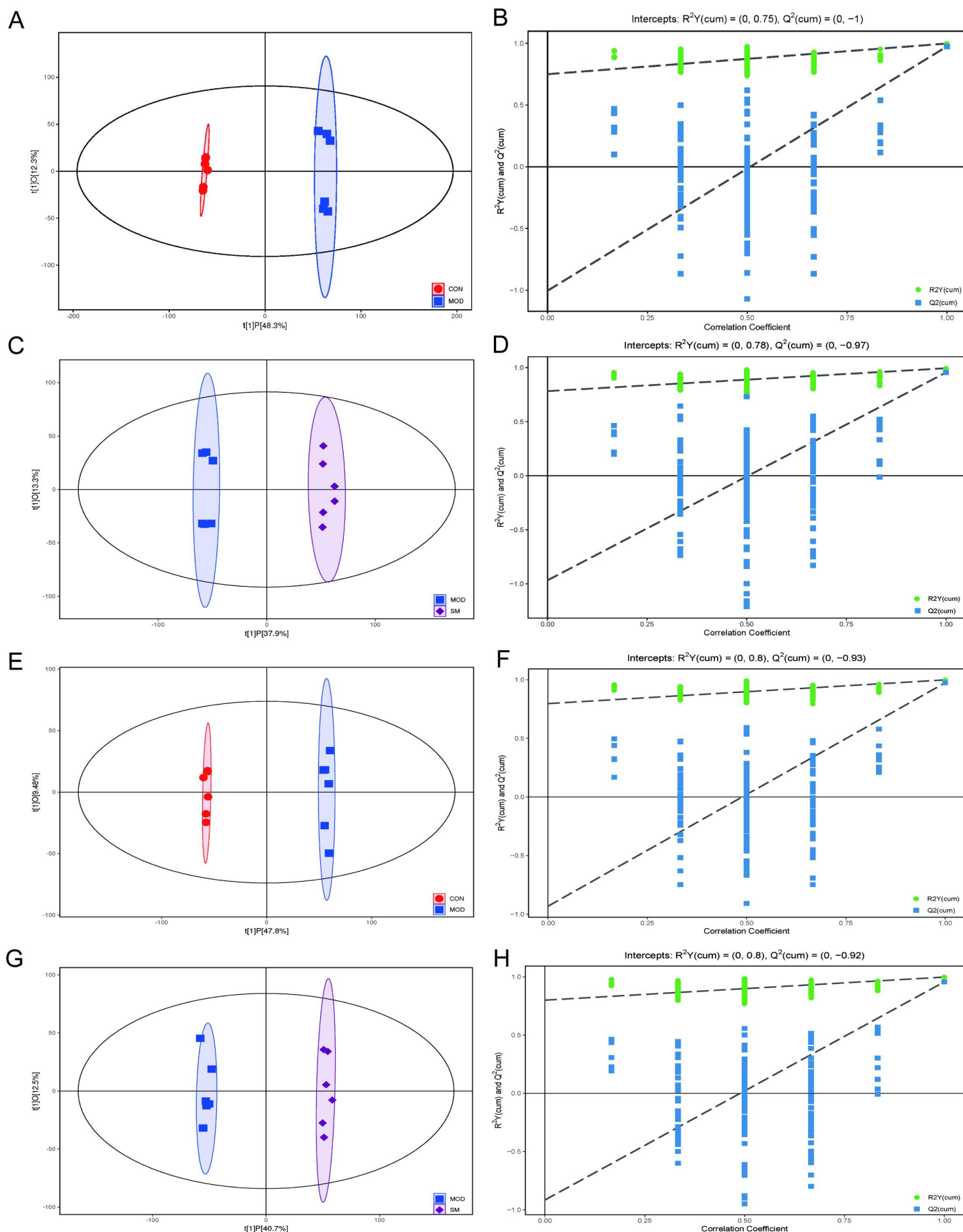


Figure S5. OPLS-DA analysis of metabolites profile. (A) Comparison plots in positive-ion mode for CON and MOD groups ($R^2X=0.606$, $R^2Y=0.998$, $Q^2=0.974$). (B) Permutation test for comparison between CON and MOD groups in positive-ion mode ($n=200$). (C) Comparison between CON and MOD groups in negative-ion mode ($R^2X=0.573$, $R^2Y=0.999$, $Q^2=0.974$). (D) Permutation test for comparison between CON

and MOD groups in positive-ion mode (n= 200). (E) Comparison between CON and MOD groups in positive-ion mode ($R^2X=0.513$, $R^2Y=0.995$, $Q^2=0.954$). (F) Permutation test for comparison between CON and MOD groups in positive-ion mode (n= 200). (G) Comparison between MOD and SM group in negative-ion mode ($R^2X=0.532$, $R^2Y=0.997$, $Q^2=0.956$). (H) Permutation test for comparison between MOD and SM groups in positive-ion mode (n= 200).