**FIGURE S1** The OPLS-DA score plots, S-plots and 100-permutation test generated from the OPLS-DA data of the normal, model and PF groups in the ESI- mode. A: The pair-wise comparisons between the normal and model groups; B: The S-plots of the OPLS-DA model for the normal and model groups; C: The 100-permutation test for the normal and model groups; D: The pair-wise comparisons between model and PF groups. E: The S-plots of the OPLS-DA model for the model and PF groups. F: The 100-permutation test for the model and PF groups.