



**Supplement Figure 2** Permutation test performed with 200 random permutations in an OPLS-DA model showing  $R^2$  (green dot) and  $Q^2$  (blue square) values from the permuted analysis (bottom left), which were lower than that of the corresponding original values (top right). “a” and “b” represent the permutation of metabolomic data generated in positive and negative ion modes, respectively.