



Fig. S2. (a) Score plot of the supervised partial least squares discriminant analysis (PLS-DA) in control and BC samples of cohort 1. x- and y-axes indicate the first and the second PLS-DA component. Each plot corresponds to one sample after averaging the concentration of each lipid in repeated measurements. (b) Partial least squares discriminant analysis (PLS-DA) classification using different numbers of components. The red star indicates the best classifier by 10-fold cross-validation. (c) Partial least squares discriminant analysis (PLS-DA) model validation by permutation tests of prediction accuracy showed that it was not overfitting. The p-value based on permutation is $p < 0.01$ (0/100).