



**Supplemental Figure 1.** Association between HMO and fecal microbiota of BF infants as determined by PLS regression analysis. Data were log transformed and mean centered before the PLS regression. The predictive performance was evaluated by tenfold cross-validation. The influential HMO were identified by VIP scores. The direction of correlation (positive: red; negative: blue) was determined by PLS regression coefficients. Only bacterial genus presented in > 50% BF infants were analyzed. 2'FL, 2'-fucosyllactose; BF, Breast-fed; DFLNHa, difucosyllacto-N-hexaose a; DSLNT, disialyllacto-N-tetraose; HMO, human milk oligosaccharides; LDFT, lactodifucotetraose; LNFP I, lacto-N-fucopentaose I; LNFP II, lacto-N-fucopentaose II; LSTb, sialyllacto-N-tetraose b; MFLNH III, monofucosyllacto-N-hexaose III. MSE, mean-squared errors for PLS model; PLS, partial least square; VIP, variable importance in the projection.