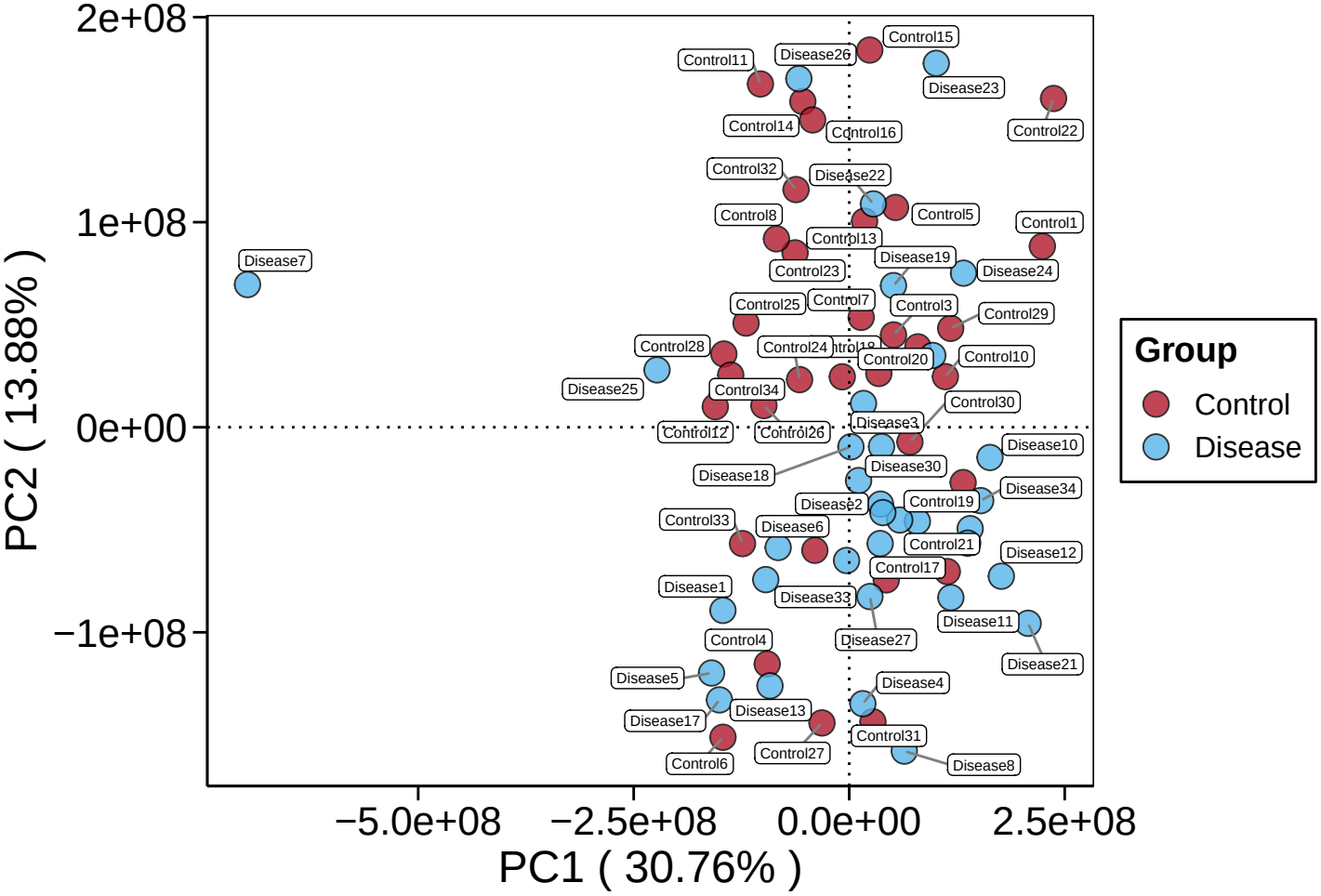PCA – Metabolites