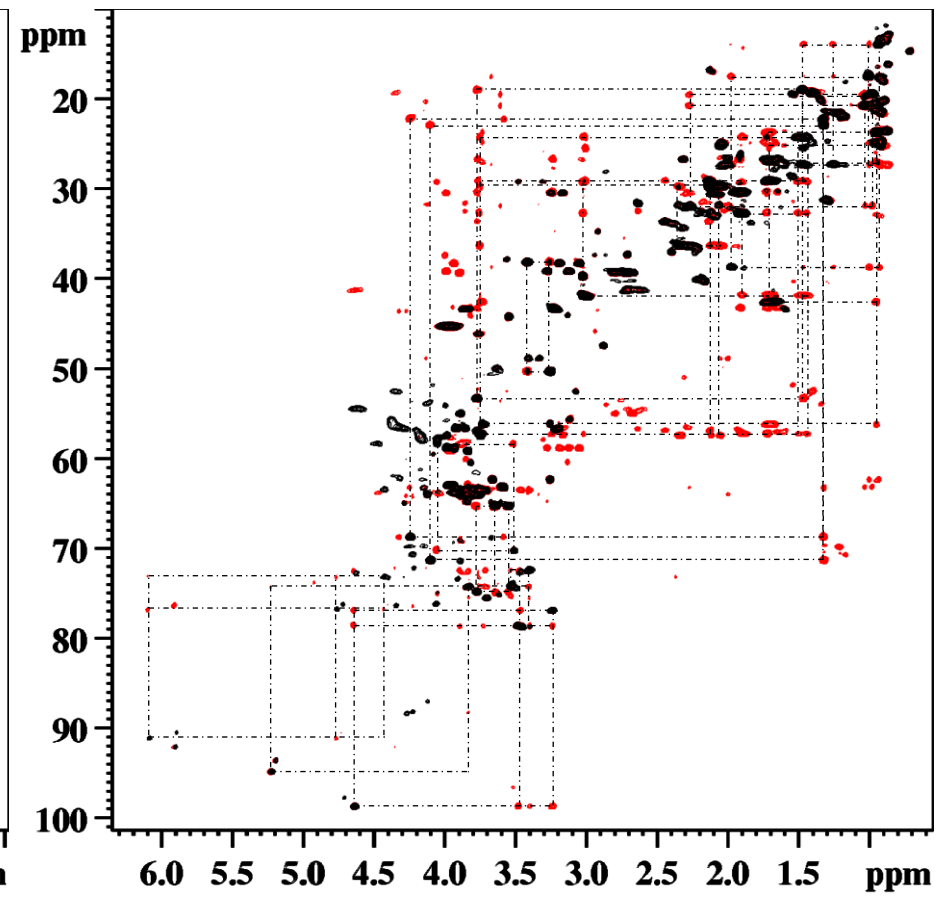
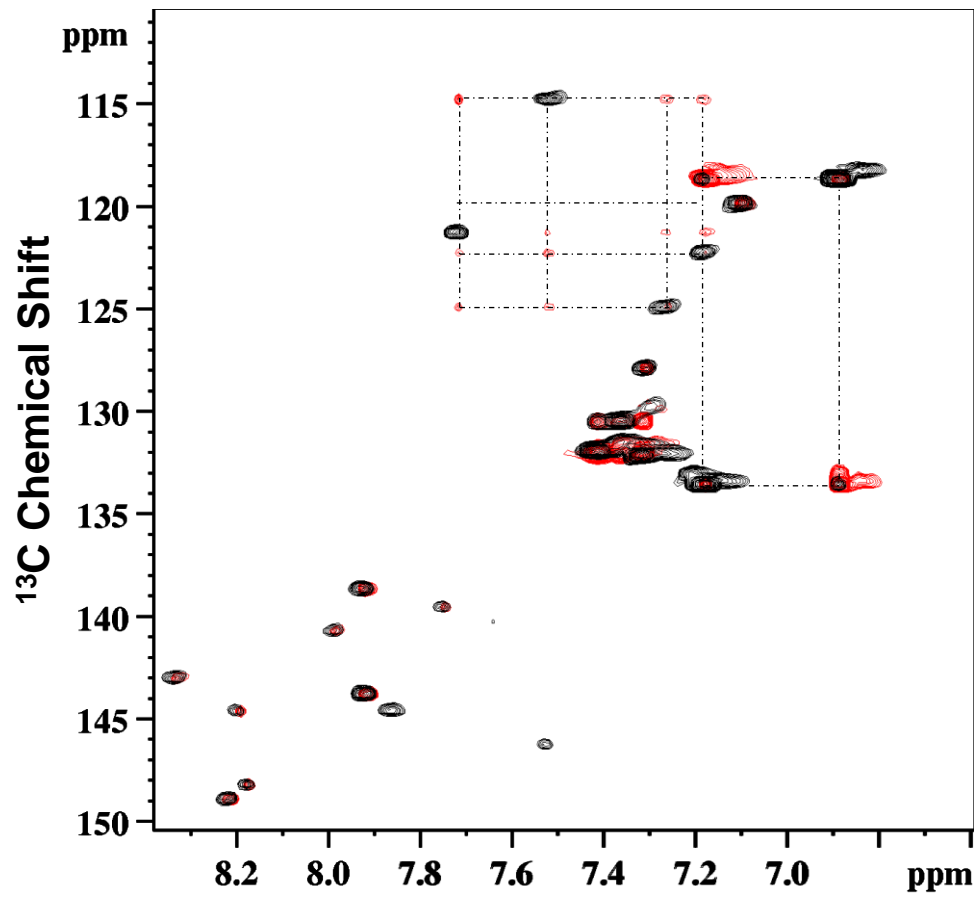
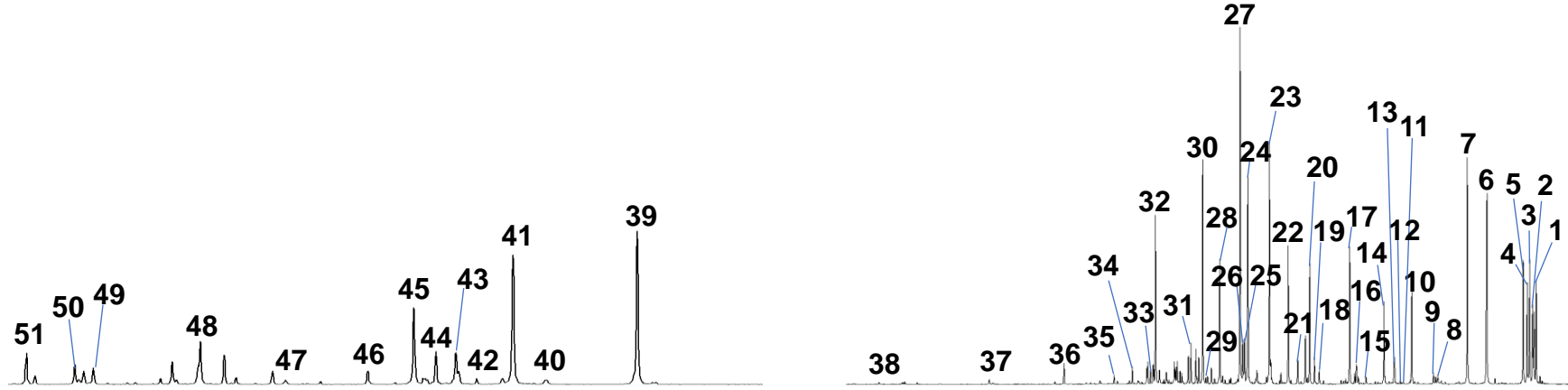


Figure S1. Heatmap of correlate bacterial variances and nuclear magnetic resonance (NMR) signals. Green bar and red bar indicates data from bacterial analysis or NMR measurements, respectively. Axis of ordinate and abscissas are same order. This figure shows low correlation with bacterial data to NMR.



^1H Chemical Shift

Figure S2. Annotation of metabolites in gut contents extract using Kpi/D₂O.

2D *j*-res projection spectra(top panel), HSQC spectra(black) and HSQC-TOCSY spectra(red).
The peak IDs are consistent with those in Table S2.

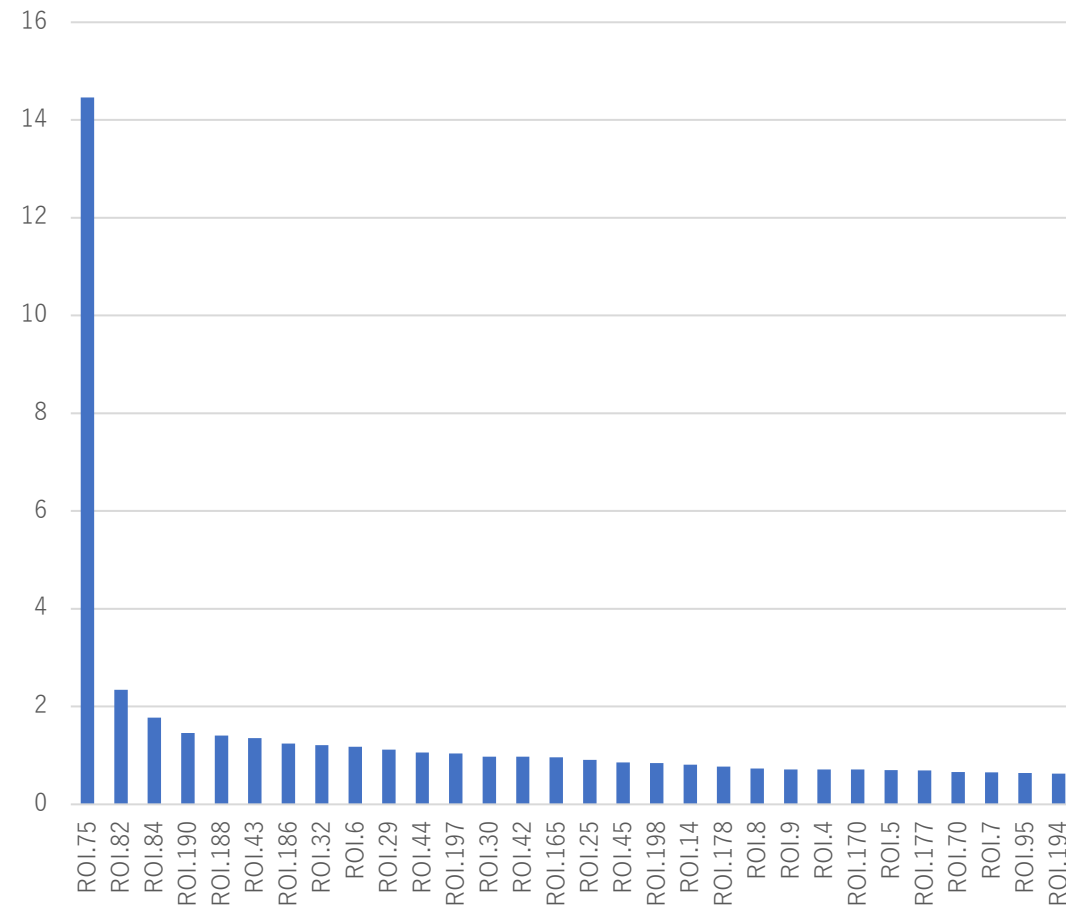
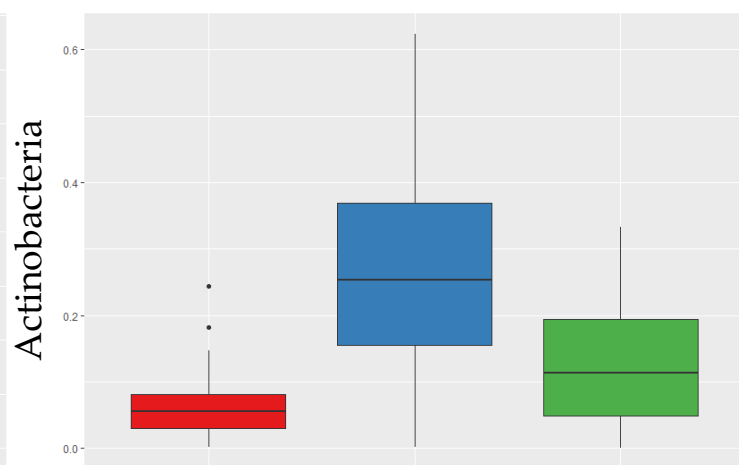
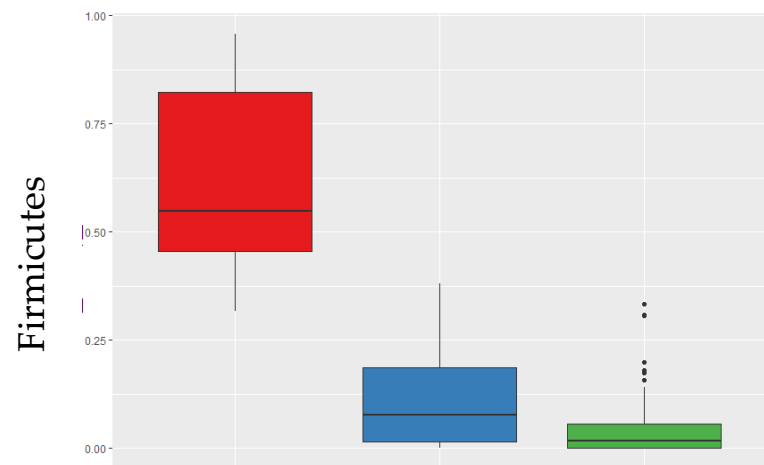
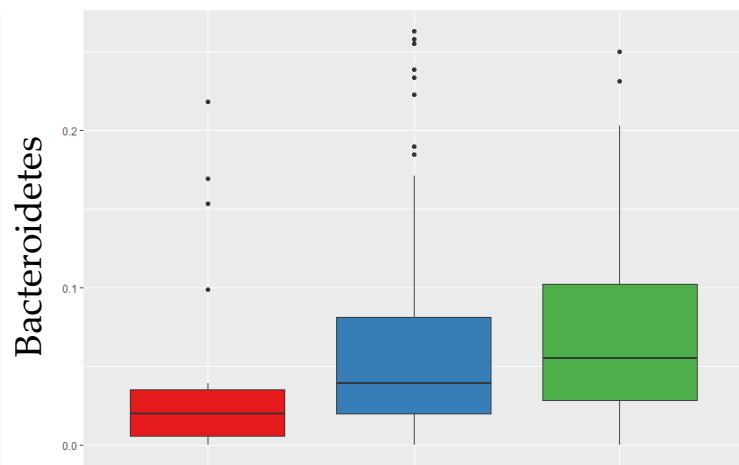
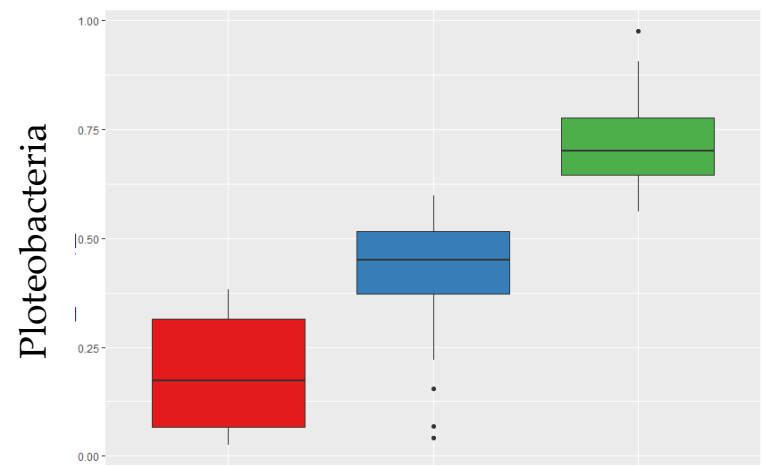
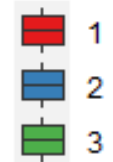


Figure S3. The results of mining the characteristic variance of the groups that were determined using i-means. Axis of ordinate indicates gini impurity (importance). The graph shows importance ranking of NMR. NMR importance has one (ROI.75. is TMAO) and others are not much different.

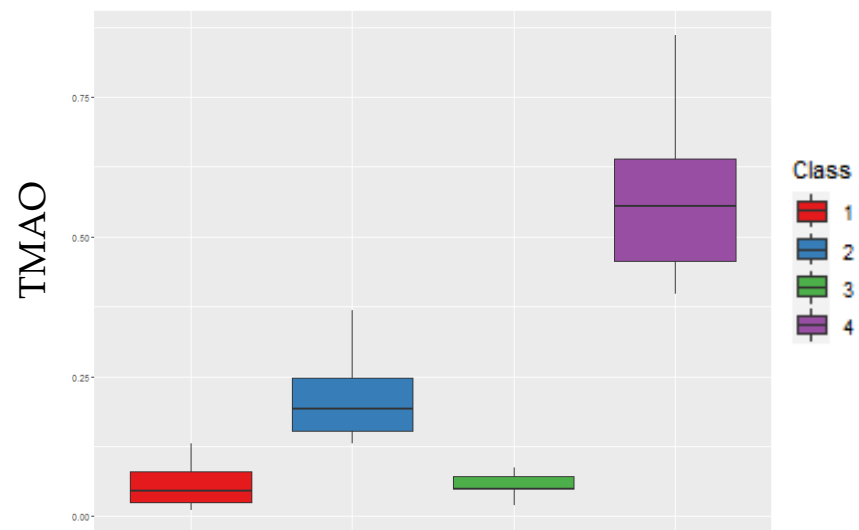
A



Class



B



Class



Figure S4. Box plots of the group result using i-means importance and classification. A: Four of highest importance phyla depicted separation by i-means classification. B: TMAO ratio to sum of each sample NMR intensity depicted by i-means classification. Axis of ordinate express ratio to sum. Firmicutes, Actinobacteria and Ploteobacteria characteristically belong to group by i-means classification. Highest TMAO group is 4 but others are not much different.

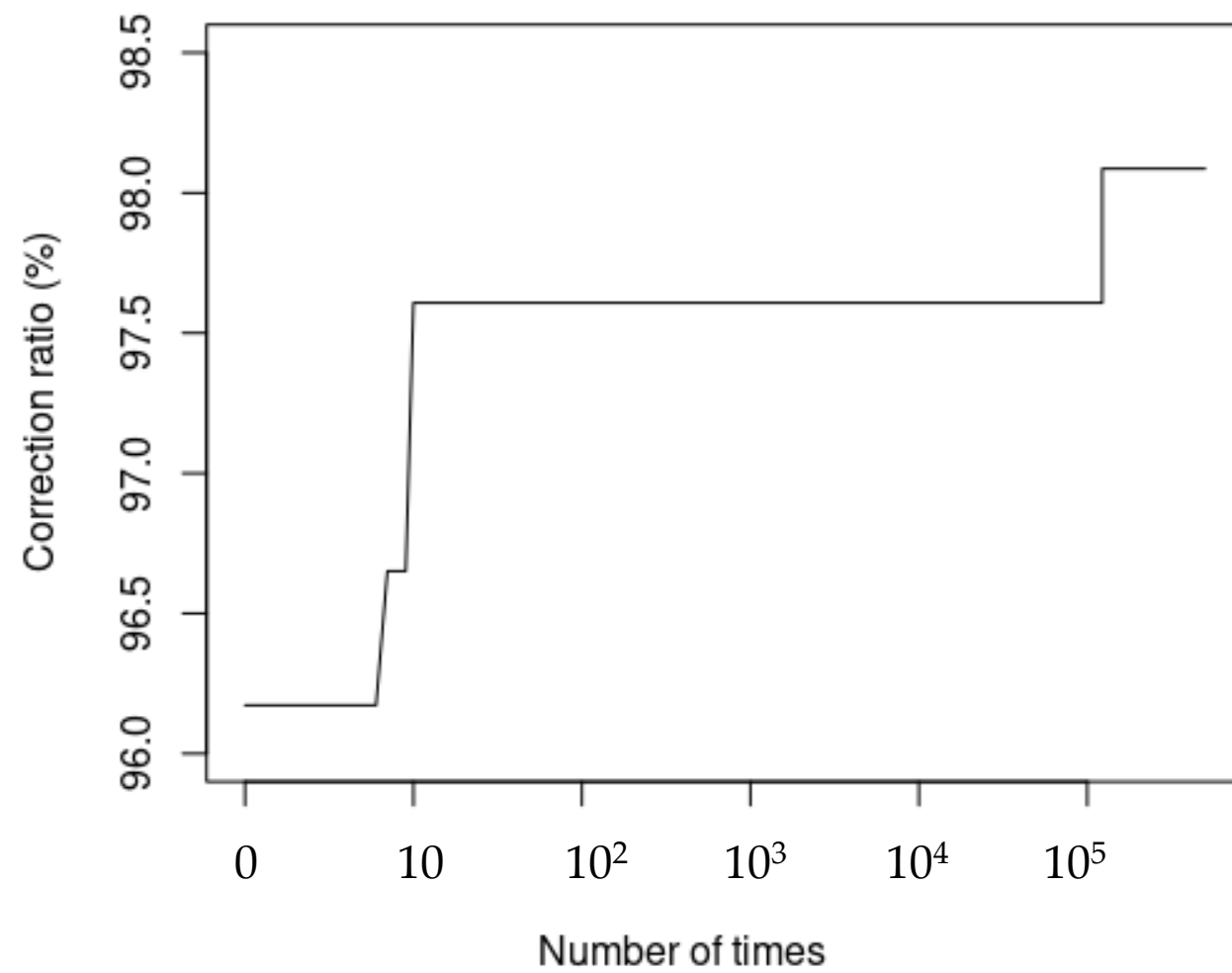


Figure S5. Line graph of $1 - \text{error rate}$ (correction ratio) using i-means. Axis of ordinate indicates correction ratio. Abscissa axis is number of i-means calculations in logarithmic scale. The value is representative results using phyla data in this study repeated 500 000. In this case, error rate is rapidly improved in 100 times and about 100 000 repeating led to convergence to plateau.