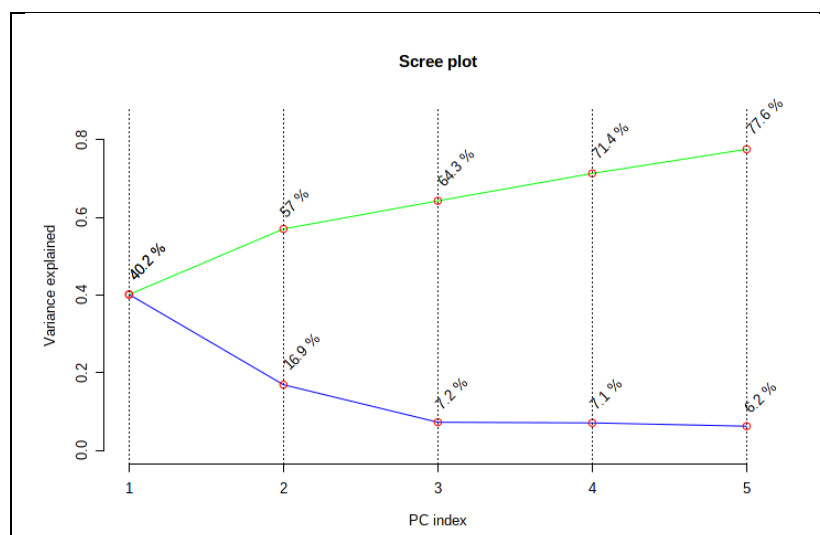


**Supplementary Figure S1.** Data transformation and normalization prior to clustering and PCA analysis. Box plots and kernel density plots before and after normalization. The density plots are based on all samples. Selected methods: Row-wise normalization: N/A; Data transformation: Log Normalization; Data scaling: Autoscaling.



**Supplementary Figure S2.** Principal components (PCs) derived from the amino acids variables. Scree plot showing the variance explained by PCs. The green line on top shows the accumulated variance explained; the blue line underneath shows the variance explained by individual PC.