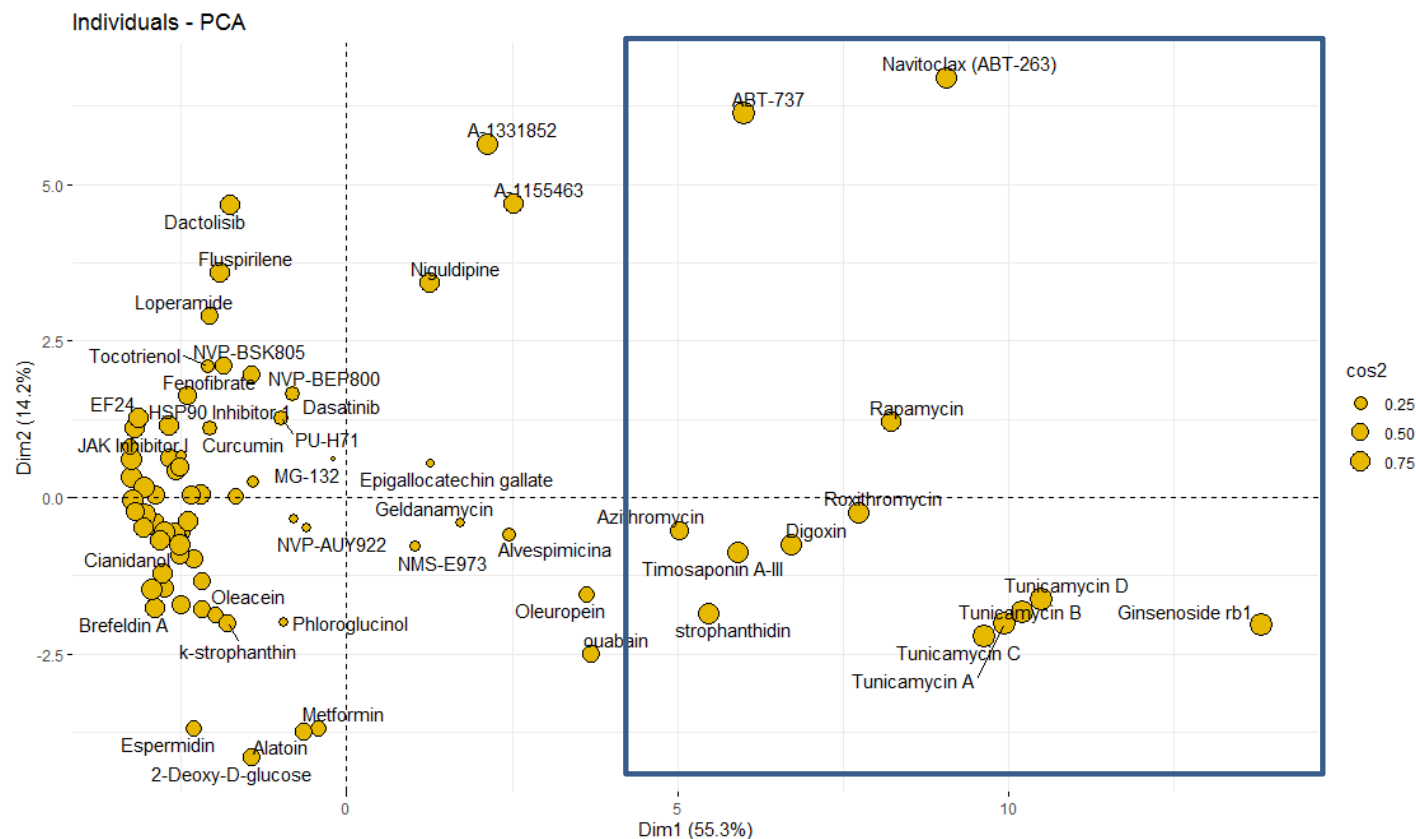


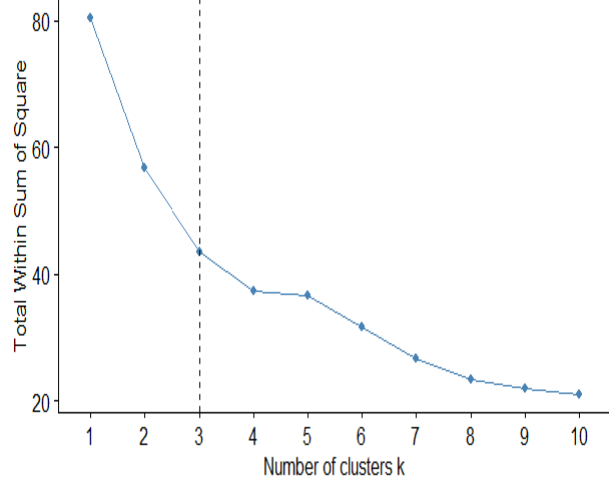
# Supplementary figures



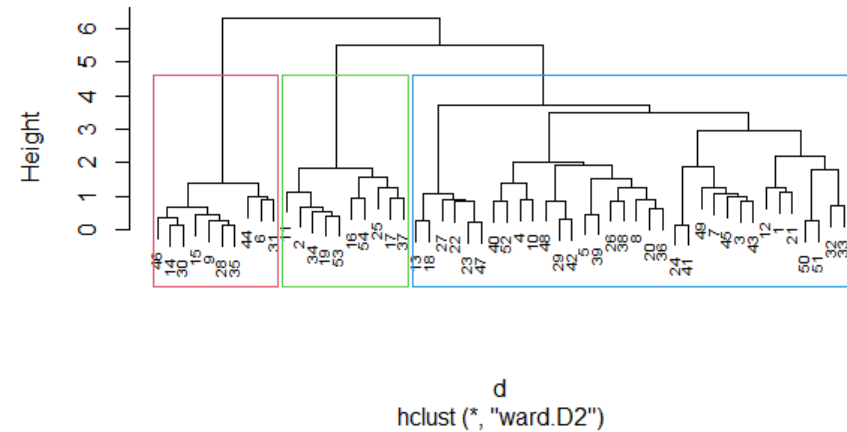
**Figure-1.** Principal component analysis (PCA) score plot of the analyzed senolytic compounds with respect to their molecular descriptors. GPCR.ligand, Ion.channel.modulator, Kinase.inhibitor, Nuclear.receptor.ligand, Protease.inhibitor, Enzyme.inhibitor, nviolations, natoms, log.Kp.cm.s., Lipinski.violations, Ghose.violations, Veber.violations, Egan.violations, Muegge.violations, Bioavailability.Score, Molweight, cLogP, cLogS, H.Acceptors, H.Donors, Total.Surface.Area, Polar.Surface.Area, Druglikeness, Shape.Index, Molecular.Flexibility, Electronegative.Atoms, Rotatable.Bonds, Aromatic.Rings, Aromatic.Atoms, sp3.Atoms, and Symmetric.atoms.

# Navitoclax clustering

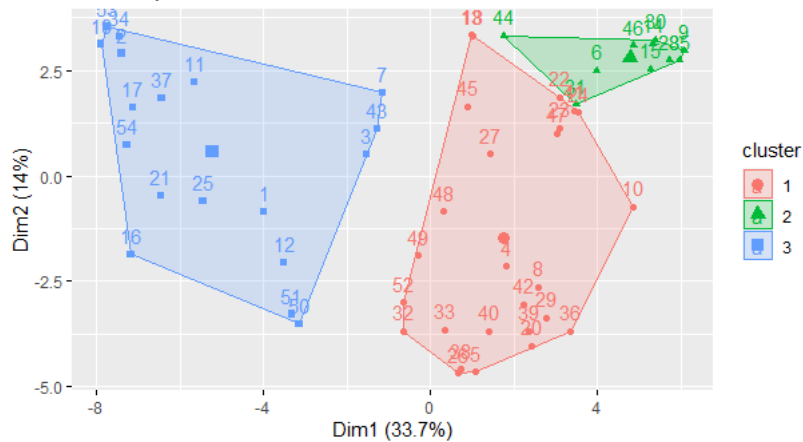
Optimal number of clusters



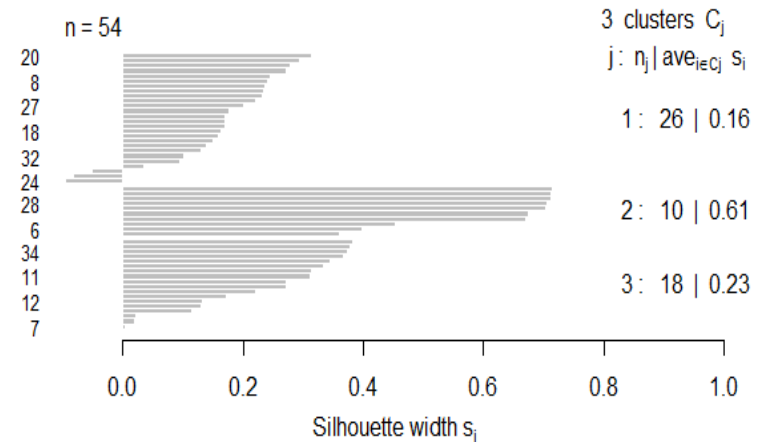
Cluster Dendrogram



Cluster plot

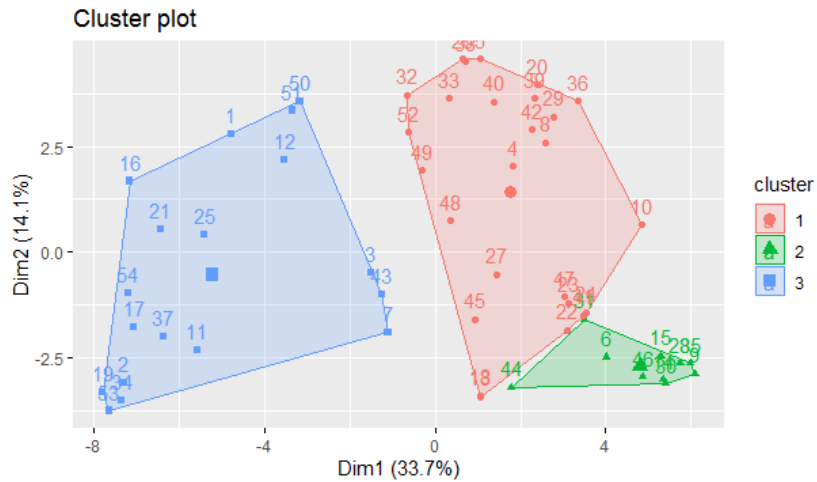
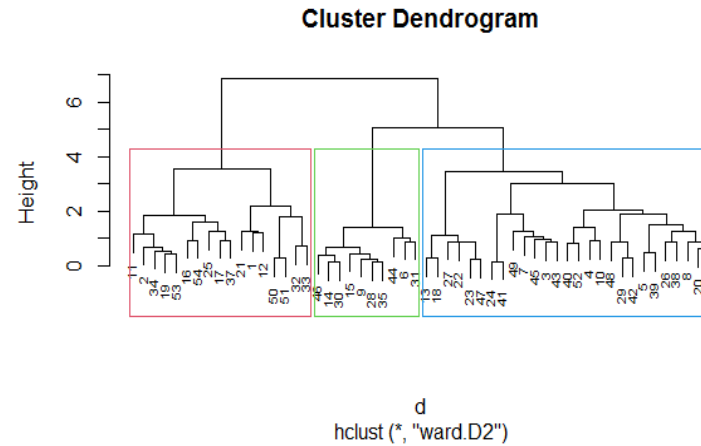
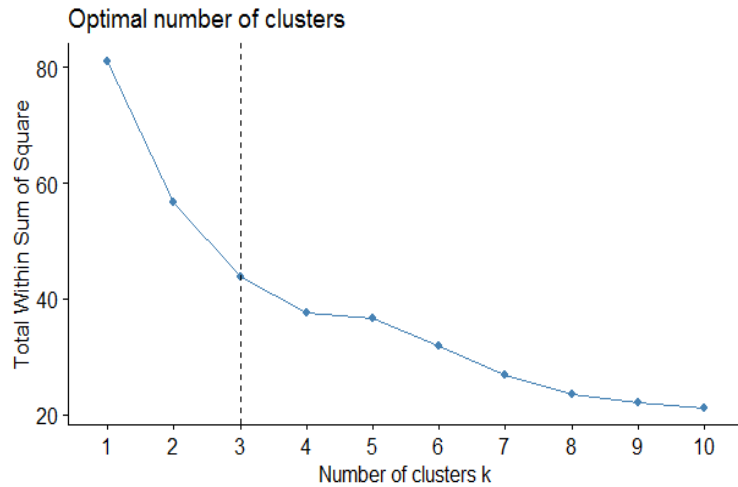


Silhouette plot - K-means

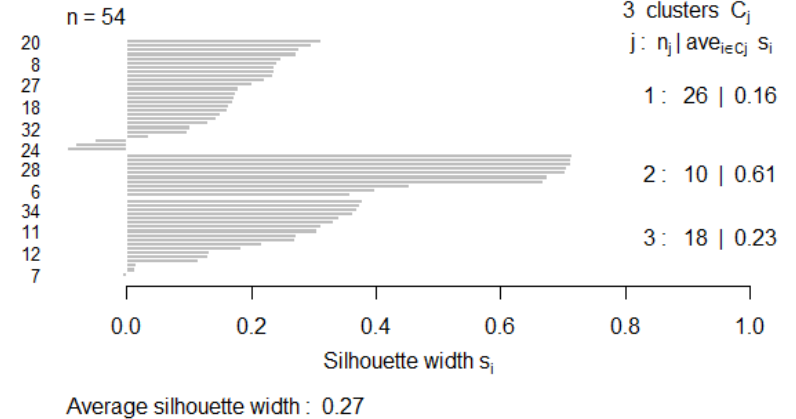


Average silhouette width : 0.27

# ABT737 clustering

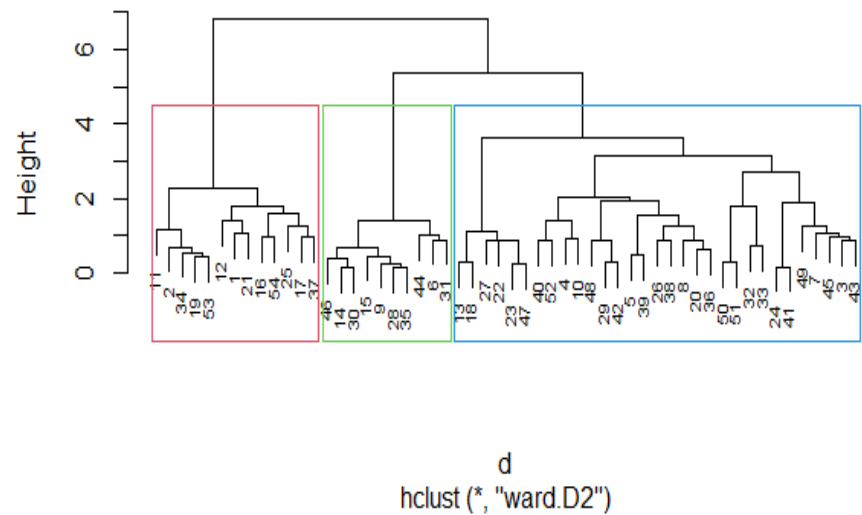


## Silhouette plot - K-means

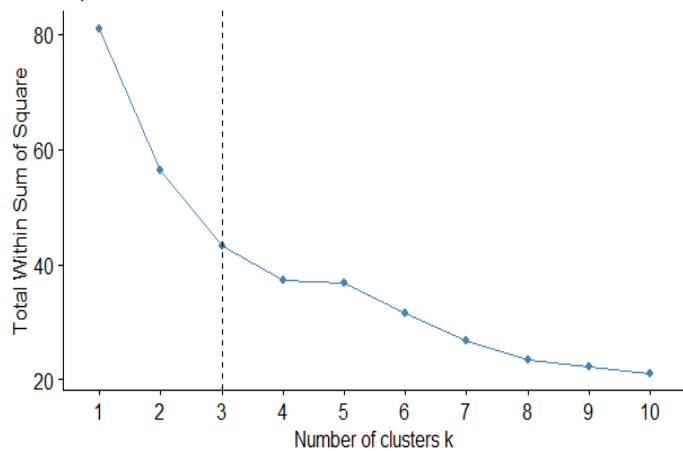


# Tunicamycin A clustering

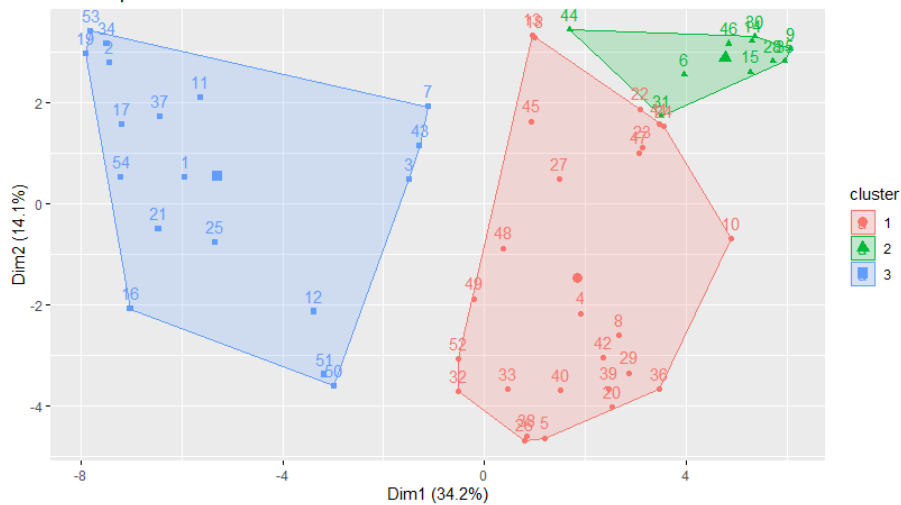
## Cluster Dendrogram



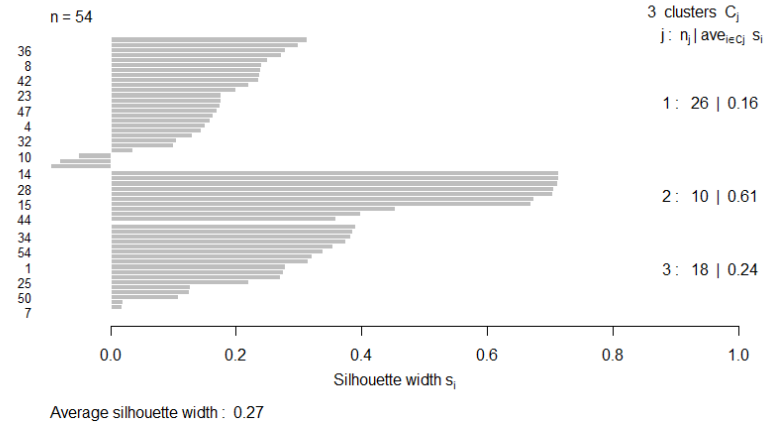
## Optimal number of clusters



## Cluster plot

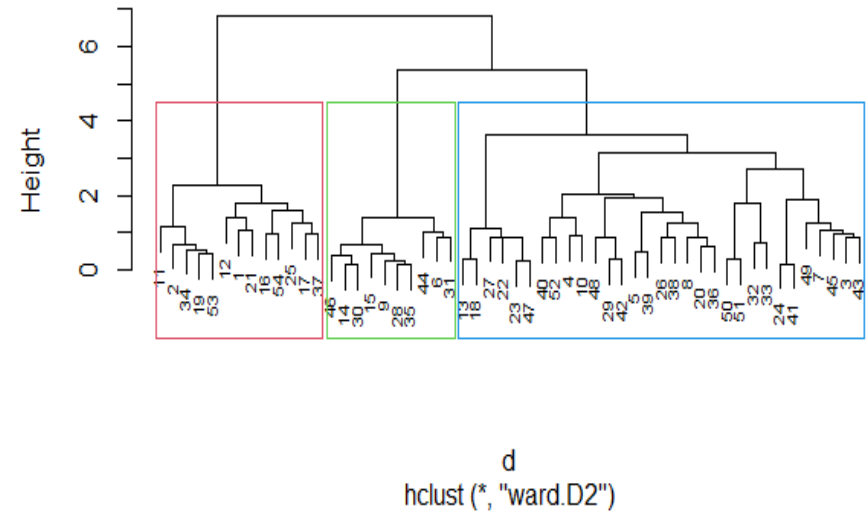


## Silhouette plot - K-means

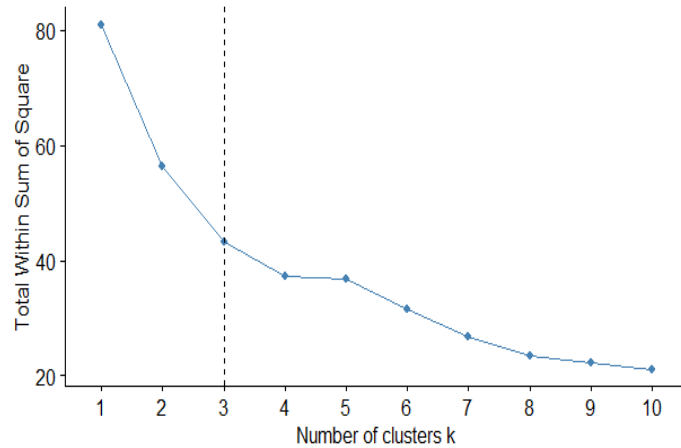


# Tunicamycin B clustering

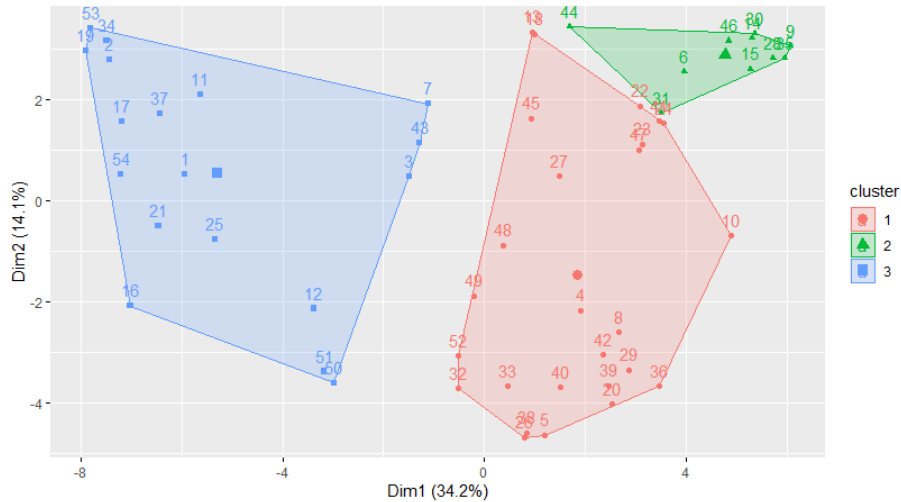
## Cluster Dendrogram



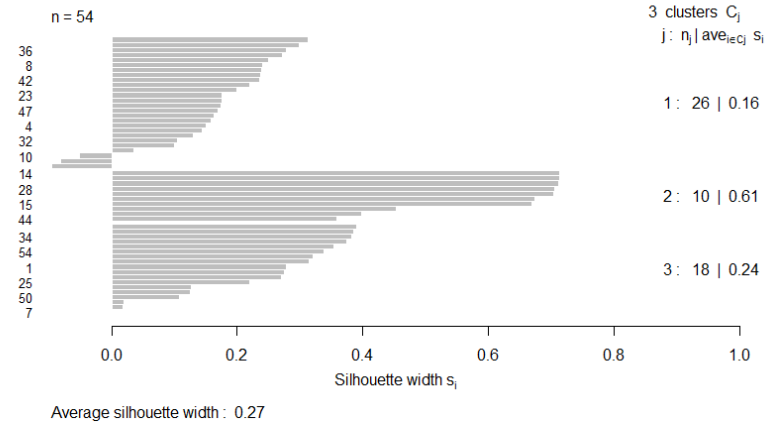
## Optimal number of clusters



## Cluster plot

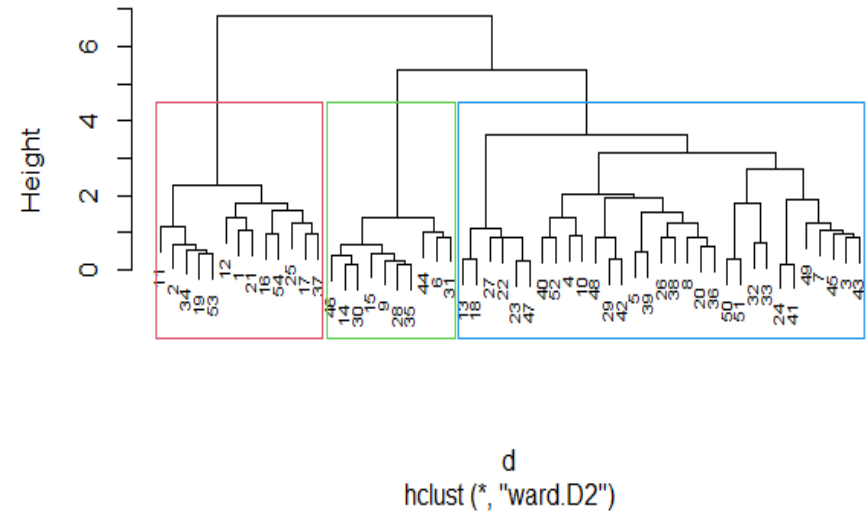


## Silhouette plot - K-means

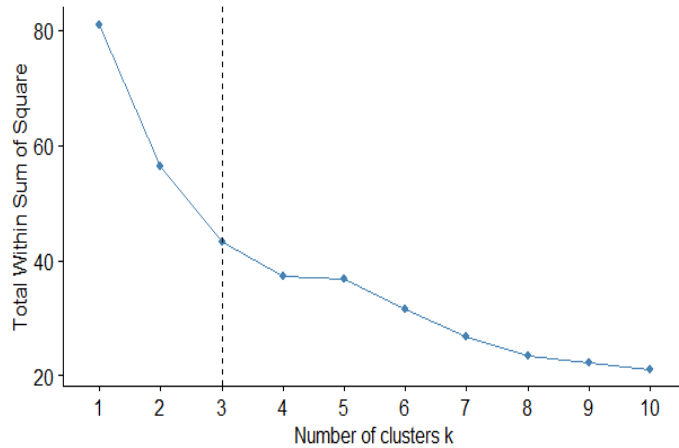


# Tunicamycin C clustering

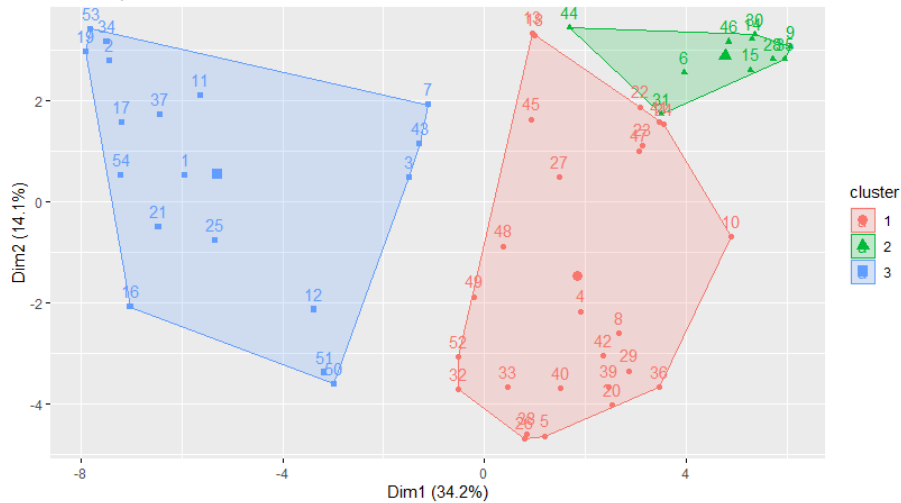
Cluster Dendrogram



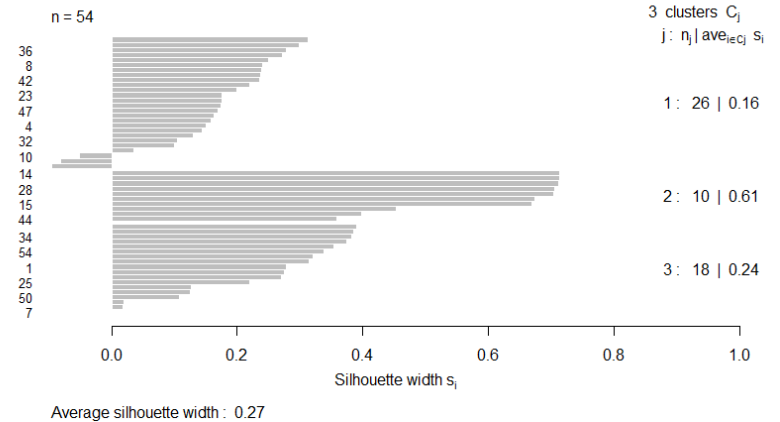
Optimal number of clusters



Cluster plot

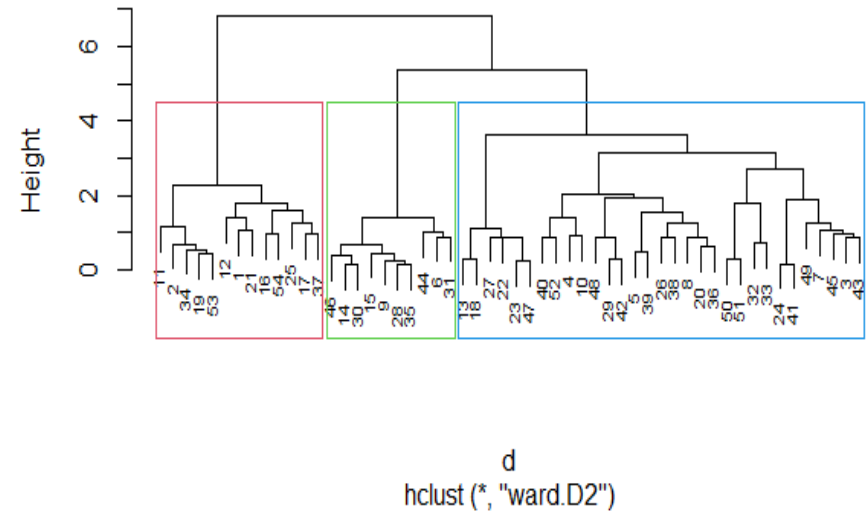


Silhouette plot - K-means

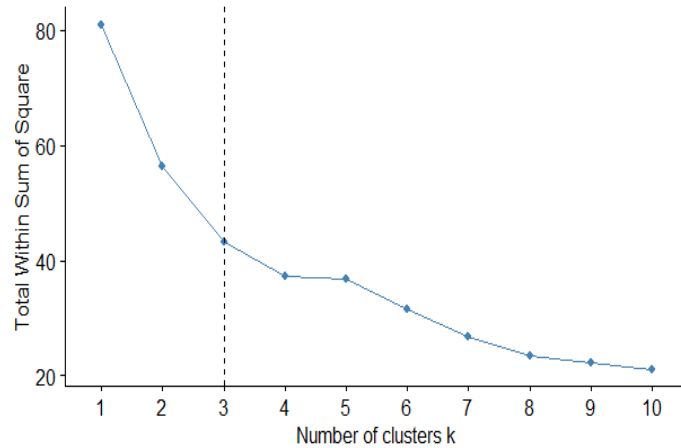


# Tunicamycin D clustering

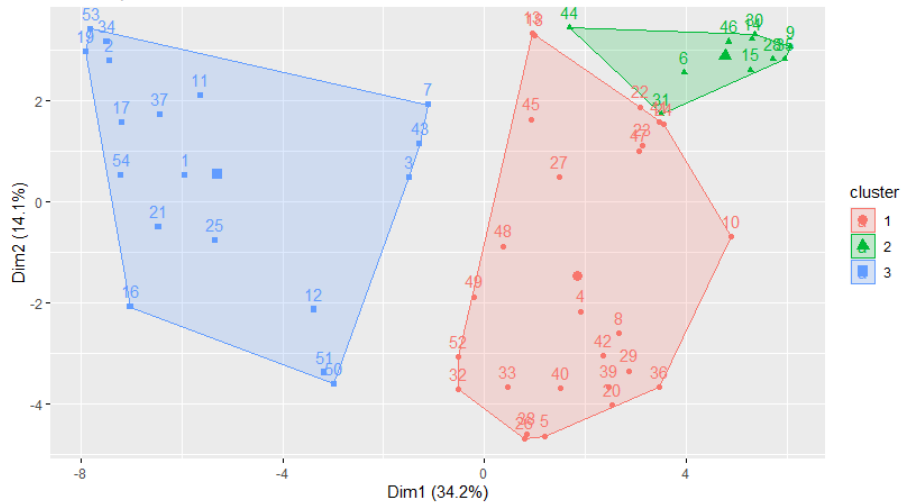
## Cluster Dendrogram



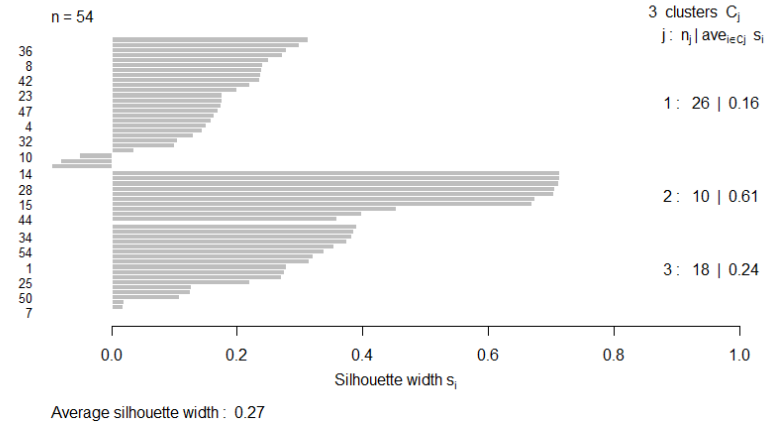
## Optimal number of clusters



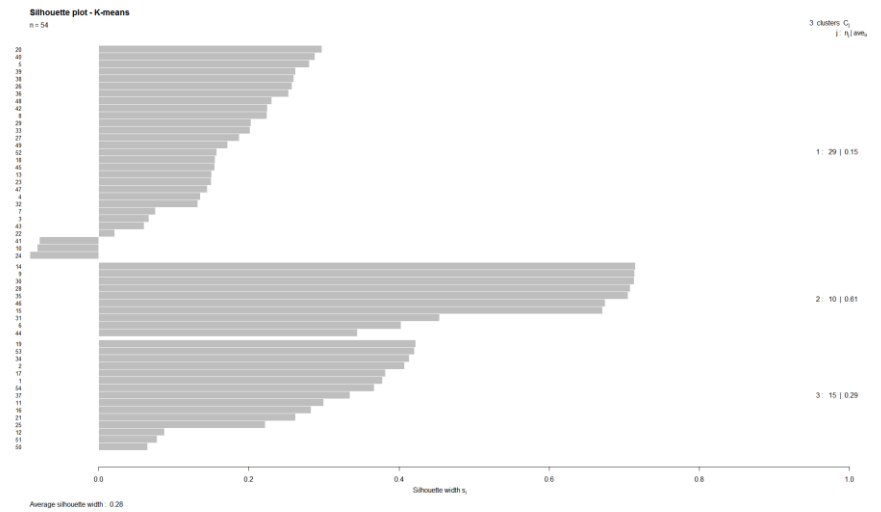
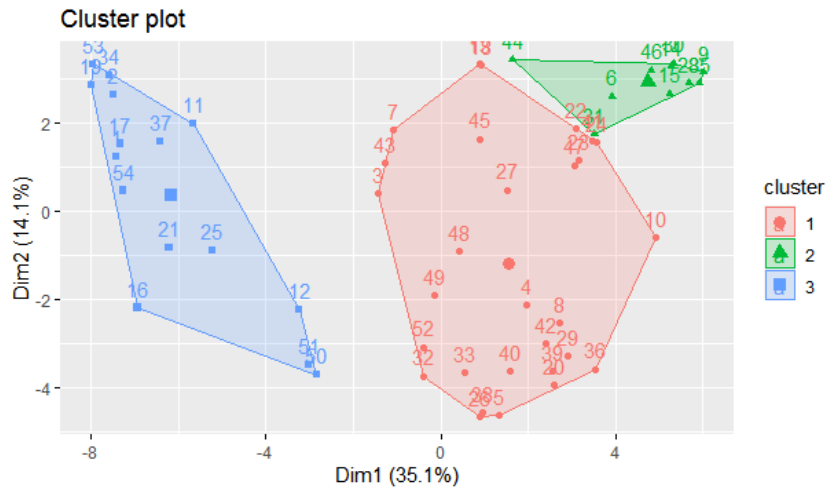
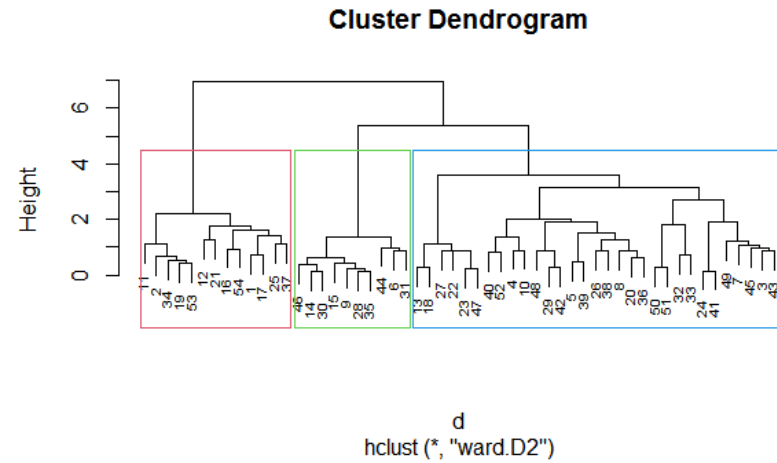
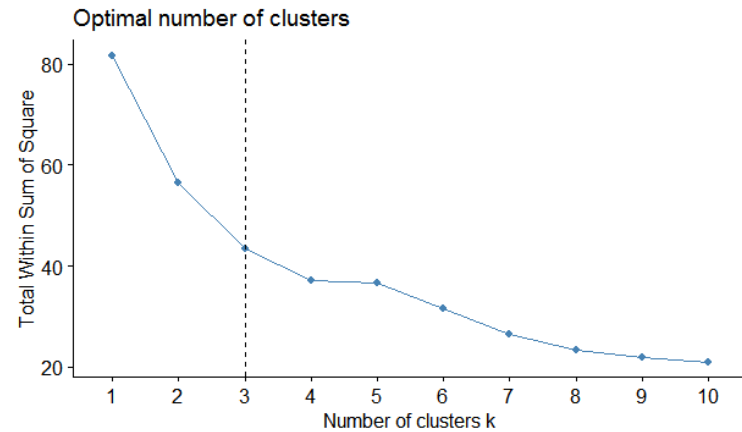
## Cluster plot



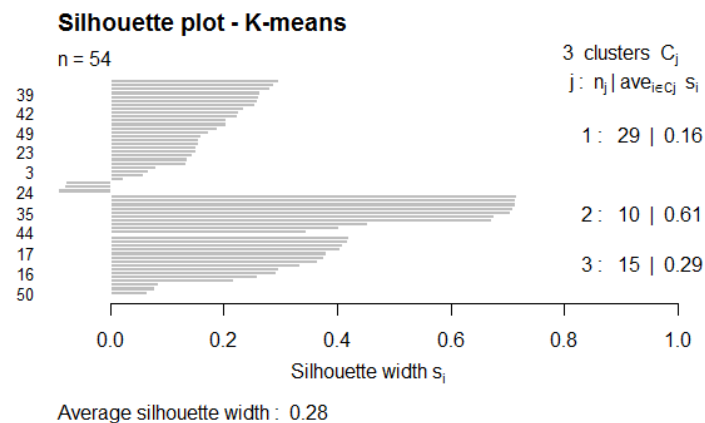
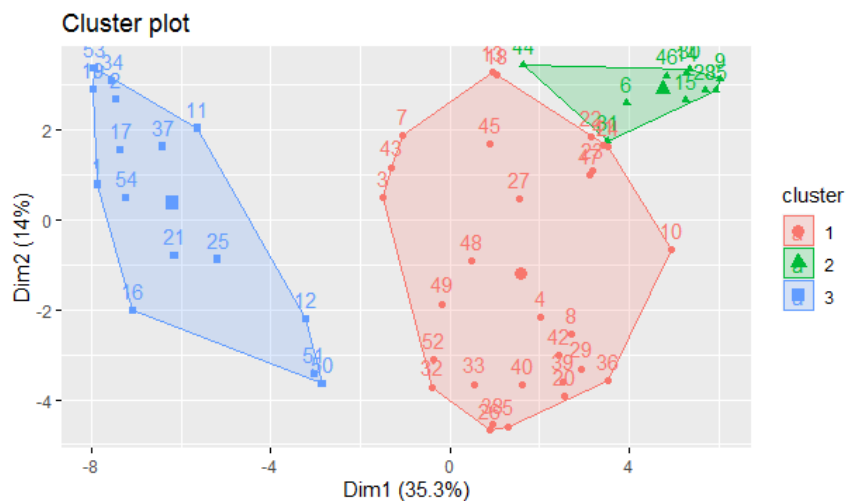
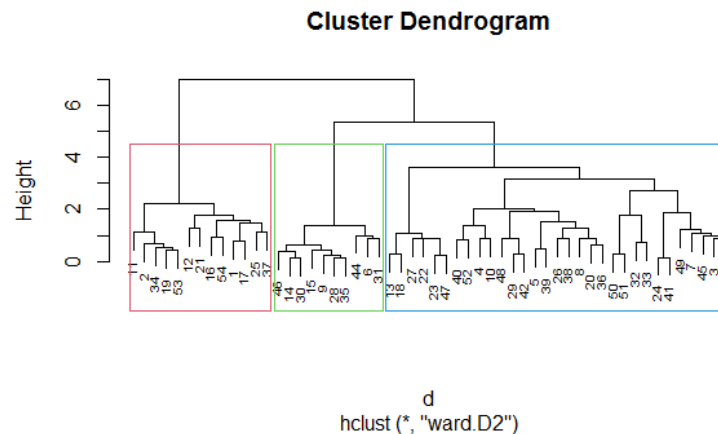
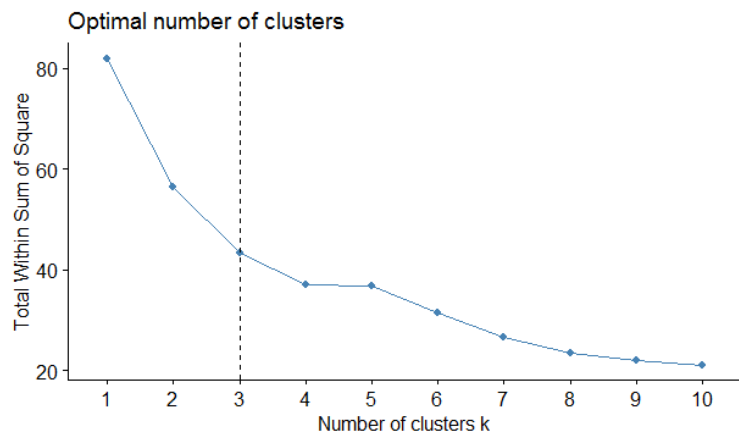
## Silhouette plot - K-means



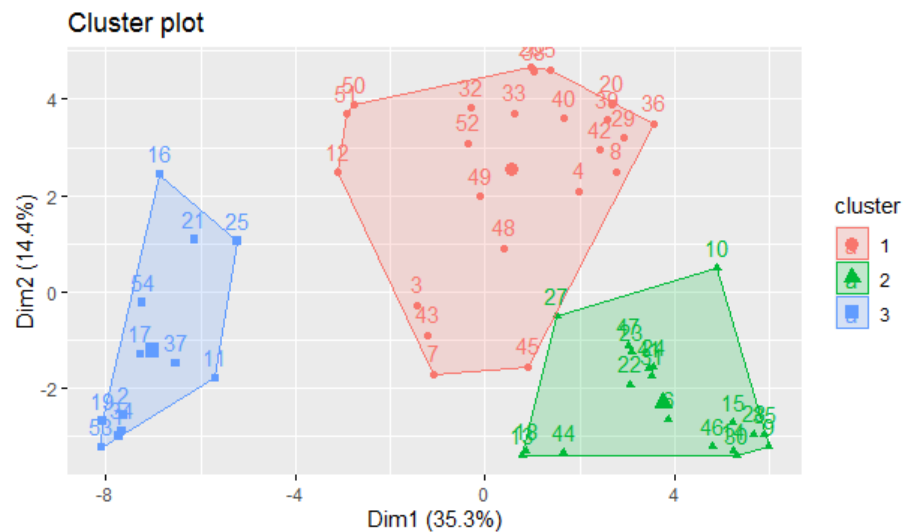
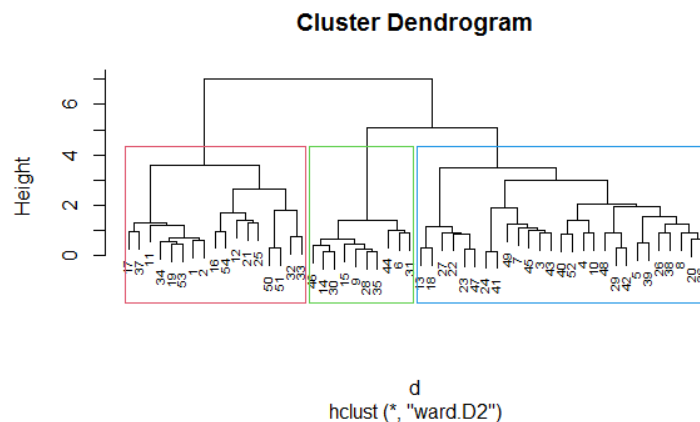
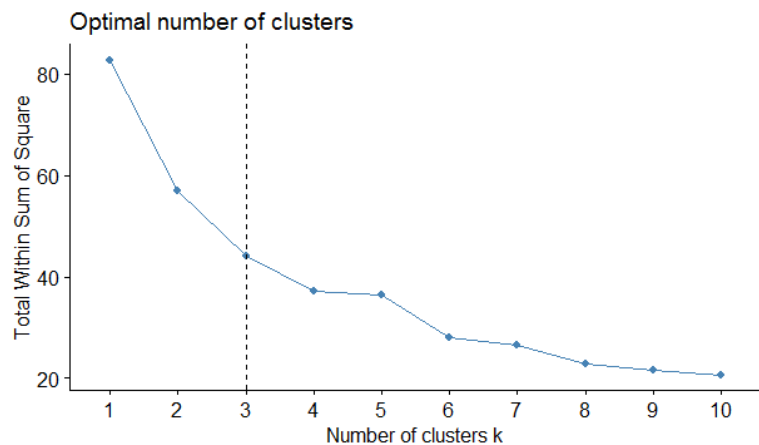
# Gingenoside Rb1 clustering



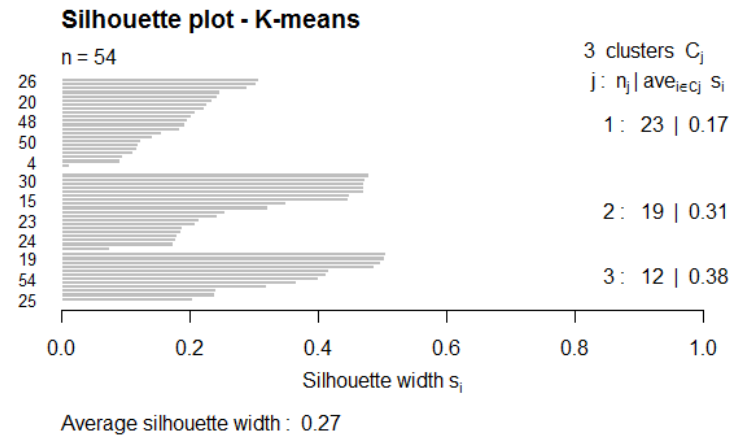
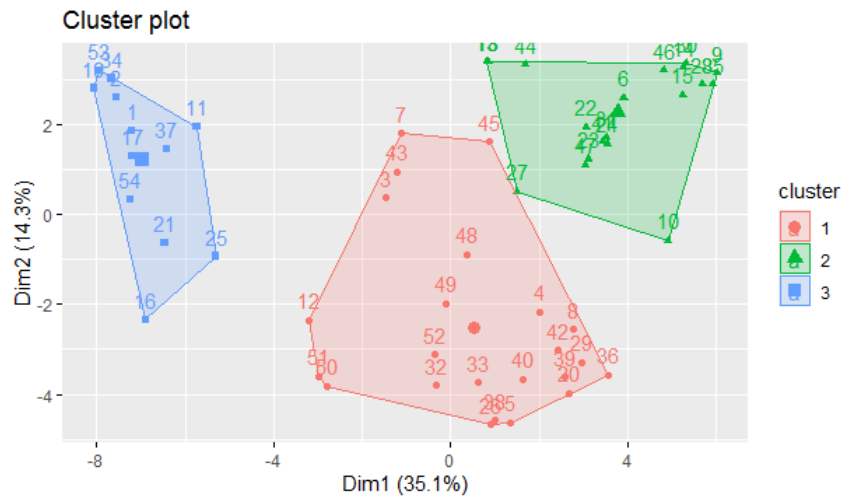
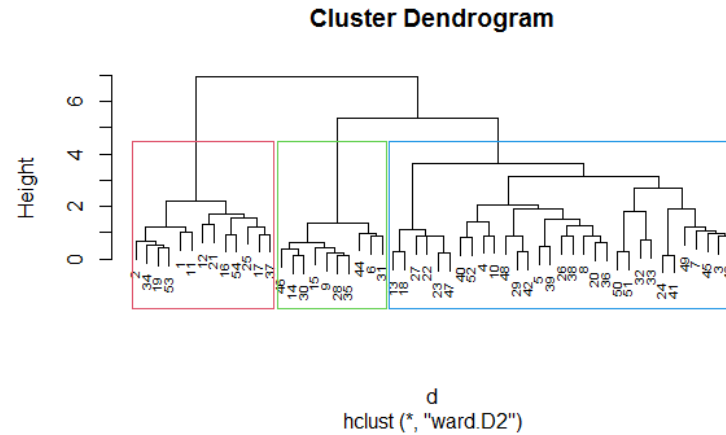
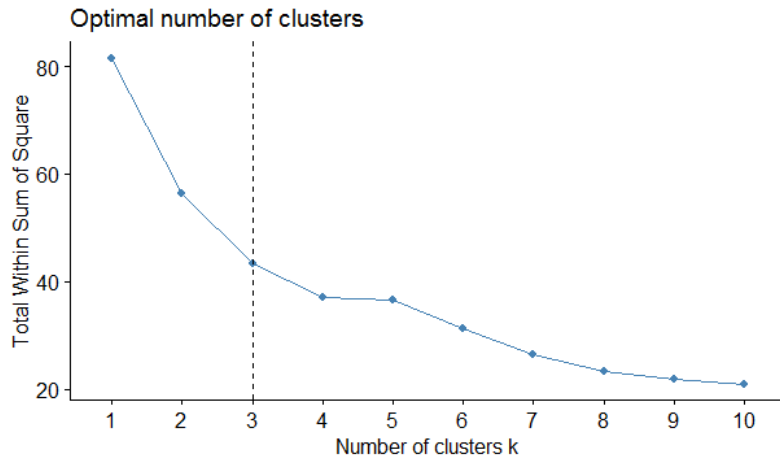
# Timosaponin aIII clustering



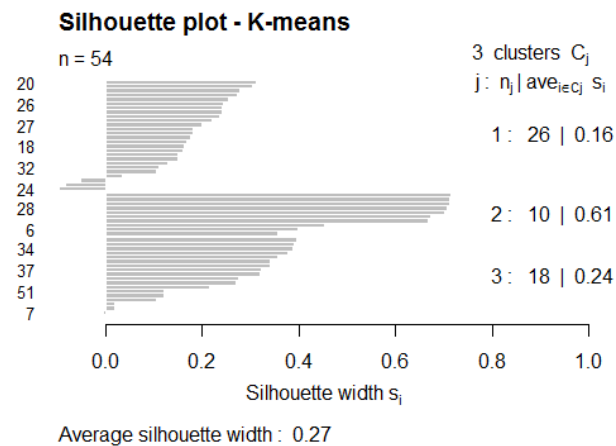
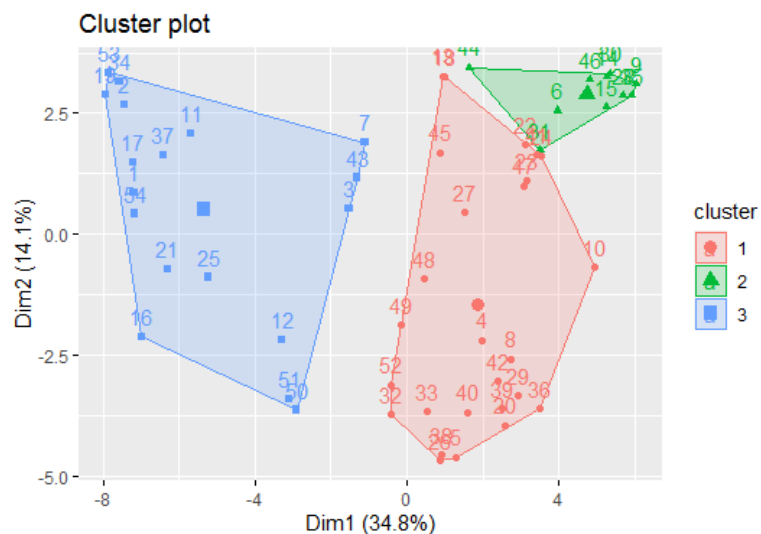
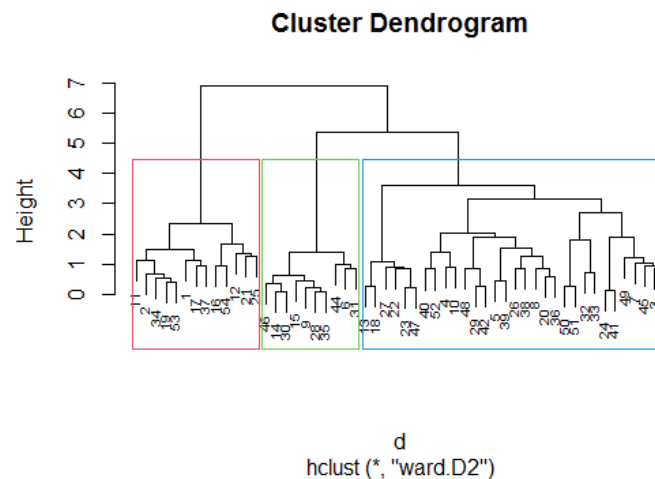
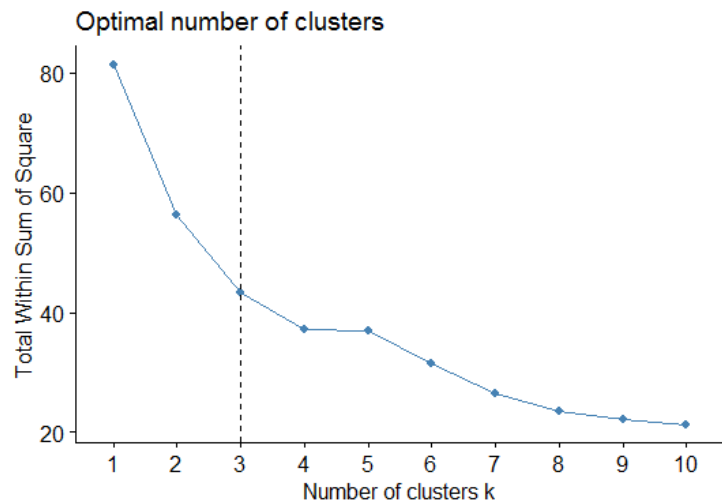
# Digoxin clustering



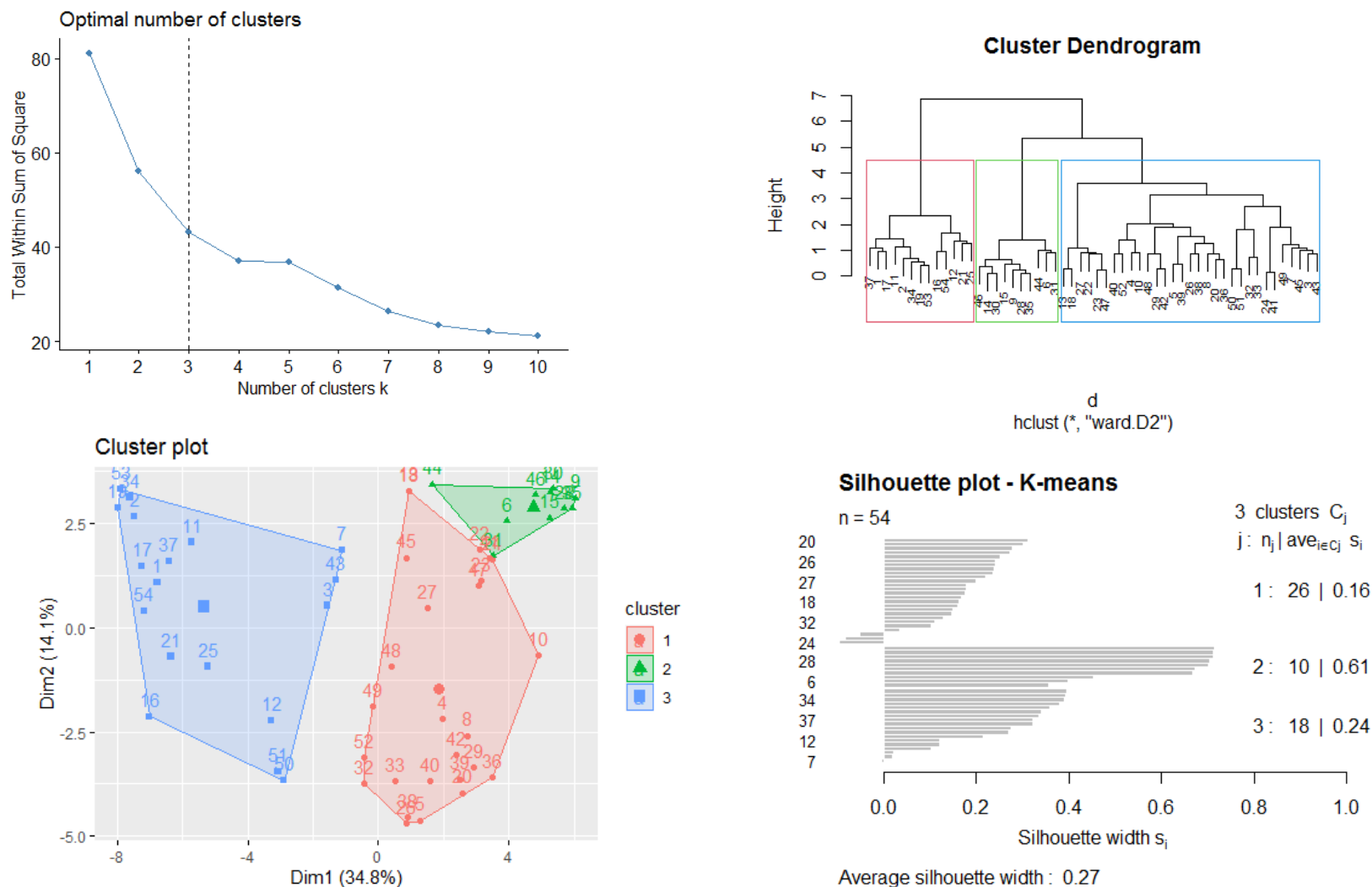
# Rapamycin clustering



# Roxithromycin clustering



## Azithromycin clustering



**Figure-2.** Representative results of the comparison among NPs and senolytic leads by fingerprints. The following steps were carried out for the selection of putative senolytics employing the comparison among 53 NPs with the senolytic lead (n=54): A) The suitable number of clusters was determined by Elbow method. B) Clusterization of Ward's method, the senolytic cluster are marked in red and senolytic molecule as 1. C) Cluster plot using Kmeans showing the same molecules in the senolytic cluster marked in blue. D) Silhouette cluster representation to corroborate the first clusterization methods.