



Figure S7: Dendrograms resulting from hierarchical clustering analysis of the molecular dynamics trajectories of the apo-E6 system. Each dendrogram was generated using Ward's method and euclidean distance metric over the subspace of the three first principal components obtained in each apo-E6 assay. **a)** Assay 1, three groups chosen. **b)** Assay 2, two groups chosen. **c)** Assay 3, one group chosen.