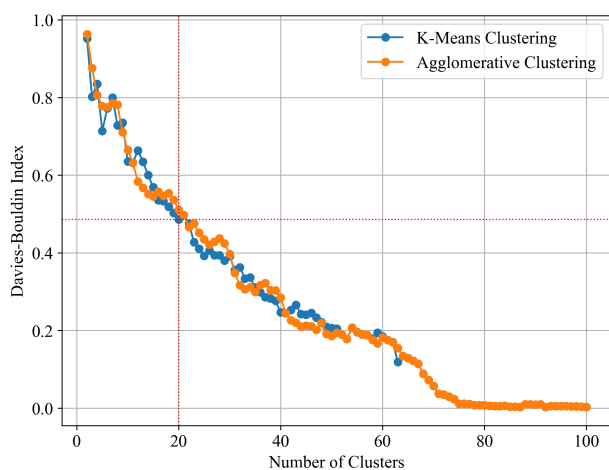


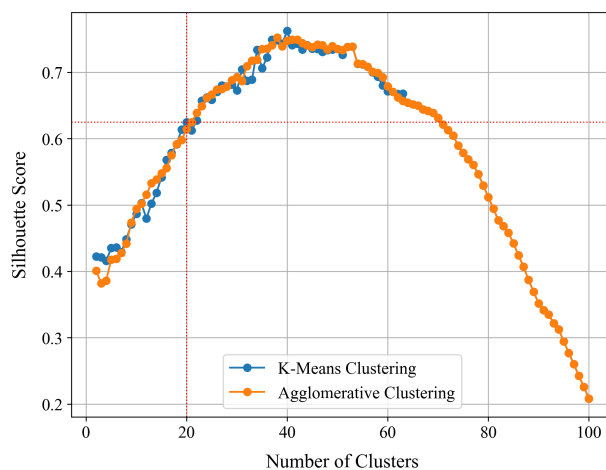
# SUPPLEMENTARY INFORMATION

## Probing Curcumin Reactive Conformers in Keto-enol Tautomerization Enhanced by Clustering with t-SNE

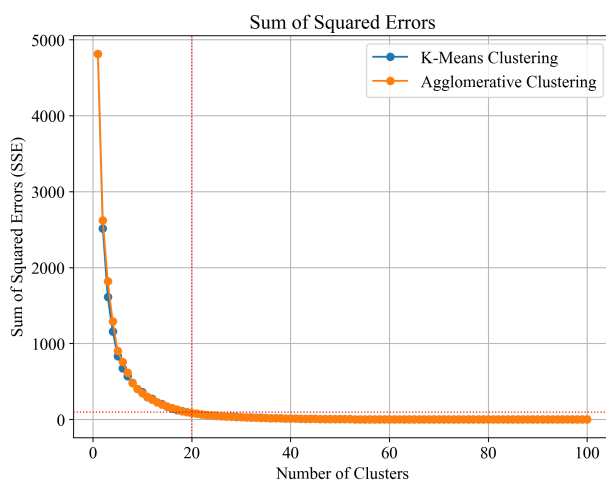
Febdian Rusydi, Etika Dessi Susanti, Ira Puspitasari, Rizka Nur Fadilla, Roichatul Madinah, and  
Mark Lee Wun Fui



(a) Davies-Bouldin Index

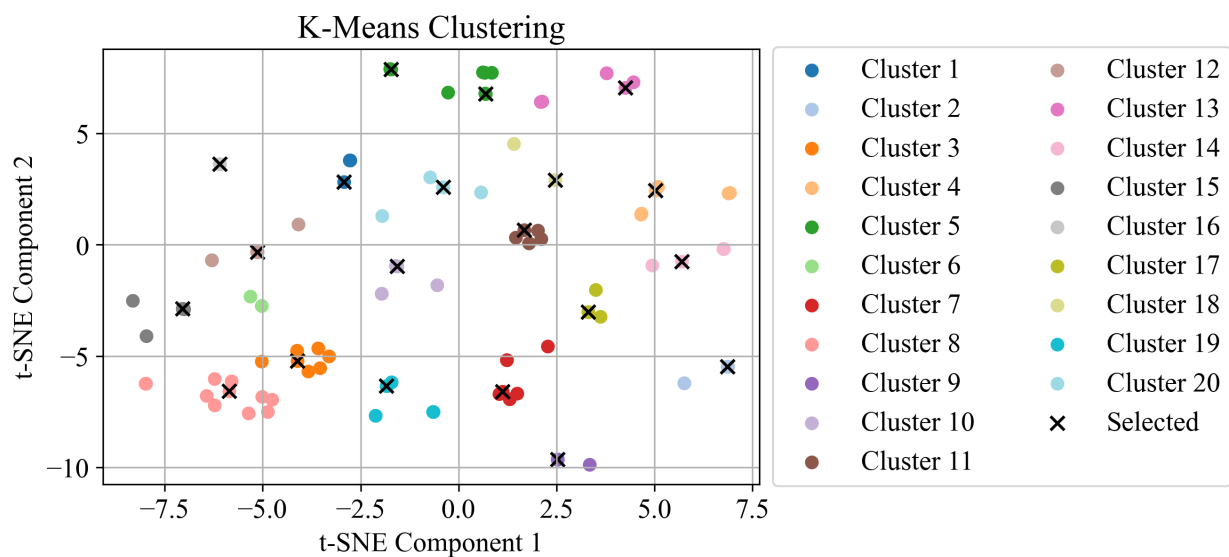


(b) Silhouette score

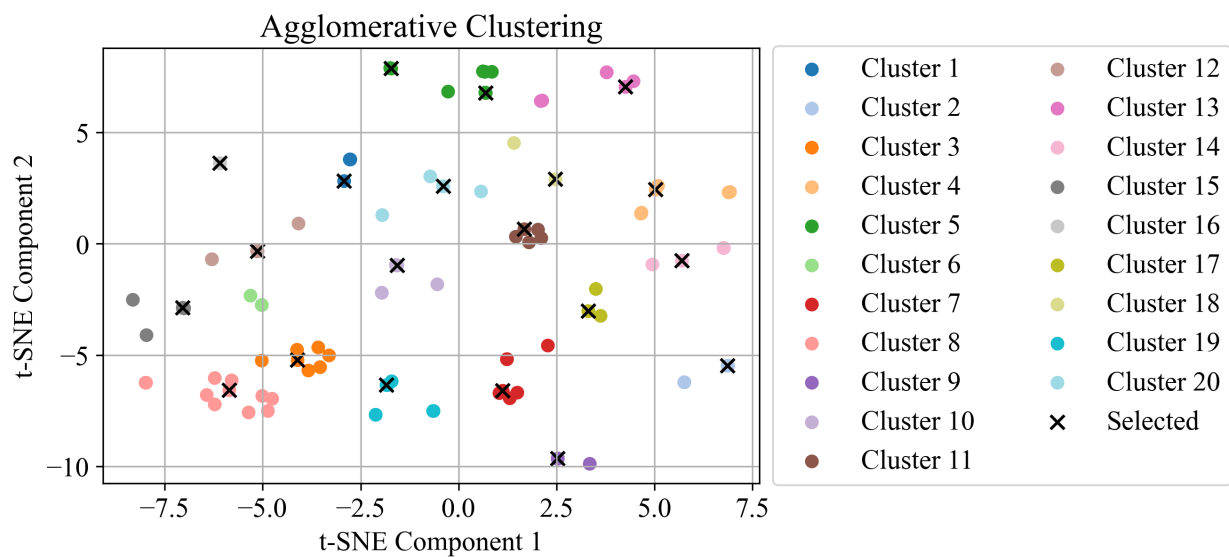


(c) Inertia

Figure SI1: Evaluation metrics for clustering algorithms for optimizing the number of representative enol conformers. The optimal number is indicated by the red-dotted lines.



(a) K-Means Clustering



(b) Agglomerative Clustering

Figure SI2: The twenty enol clusters along with the selected representative conformers in the conformational space.