Subject: Clustering by similarity of srtucture
Posted by Rasajna on Mon, 21 Apr 2025 18:55:23 GMT
View Forum Message <> Reply to Message

Hello, I was using data warrior for clustering molecules from a database based on the structure. I wanted to know more about the parameters and the algorithm being used so I can explain it while presenting my work and just better understand the results. I saw an answer on the forum that said DW uses agglomerative hierarchical clustering but what is the the measure of similarity, is it tanimoto's coeffiecient?