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Subject: Clustering by similarity of structure

Posted by [Rasajna](#) on Mon, 21 Apr 2025 18:55:23 GMT

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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 measure of similarity, is it tanimoto's coefficient?

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