Subject: Re: Clustering by similarity of srtucture
Posted by thomas on Mon, 21 Apr 2025 19:11:41 GMT
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that depends on the descriptor you use. FOr the simple binary fingerprints (FragFp, PathFp, and SphereFp) it is Tanimoto. SkeletonSpheres similarioty is also a kind of Tanimoto, but it is based on fragment count numbers rather than fragment existence bits. OrgFunctions and Flexophore similarities are the result of graph matching algorithms, the first based on best matching trees and the second on an MCS matching of complete graphs. The Flexophore is published and some basic information about the descriptors can be found here: https://openmolecules.org/help/similarity.html.