Subject: Re: Similarity Analysis query
Posted by thomas on Thu, 29 Aug 2024 18:37:55 GMT
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Hi Sansun,

1) The cutoff similarity limit for connection lines is at least 80%, but it is dynamically increased depending on the number of highly similar pairs. If most molecules are considered similar to most of the others, the algorithm cannot work.

2) It is true that molecules not connected to any other molecules tend to be more often close to the edge, because they are not drawn to the center. Since the center density is much higher at the end of the attraction phase, a correction is applied that moves all molecules towards the edge to achieve a similar density at all areas.

Hope this explains it...

Thomas