Subject: Molecules representative within a cluster
Posted by jfsanchezs on Sat, 09 Jan 2021 16:34:44 GMT
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Greetings.

I have read that the molecules marked as the representative is the most similar to all others in the cluster. However, I don't understand how this molecule is defined. Under which parameters the "representative molecule" is calculated?

Thank you for your attention and support.

PD. Congrats on this amazing software, BTW.

Subject: Re: Molecules representative within a cluster
Posted by thomas on Wed, 13 Jan 2021 19:58:26 GMT
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For any molecule in any cluster all similarity values to all other molecules within the same cluster are added. Within a cluster all molecules have the same number of other cluster members. Therefore, that molecule with the highest similarity sum within one cluster is the one that on average is most similar to all other cluster members and therefore is the one that is most central in a cluster. Does this explain it?