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.