
Subject: Molecules clustering, few questions

Posted by [pocin](#) on Wed, 04 Feb 2015 14:58:22 GMT

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Hi, I have three questions. I looked up the manual and also the publication without any luck.

I have clustered my library of 325 molecules into fixed number of clusters (50) without specifying the minimal co value using Flexophore descriptor.

In the manual, there is something about weighted mean similarities of cluster members. How do I find out this value? I would like to know how similar are molecules in my cluster and also how different are each clusters between each other.

Second - What is meant by "Is cluster representative"? Is it the most similar molecule to all others in the cluster?

Also is there any native way how to display cluster size or do I have to do it externally in a spreadsheet?

Thanks in advance and have nice rest of the day,
Robin

PS: Thank you for developing such an amazing software!
