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Subject: Re: What do I do with the entries assigned to multiple categories?

Posted by [Nastasia](#) on Fri, 24 Jul 2015 12:42:10 GMT

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I have a number of molecules, some of which are the same. However, they were retrieved from different sources (source is important, so it is a descriptor as well), when I merge them by structure, my descriptors are merged as well, so I have some sort of multiple categories case. And when I build polts I still have some individual cases and all the other entries are assigned to multiple category, and I need my descriptors to be treated separately. Same will happen if I try to merge common scaffolds.

What I need in the end: to be able to order my molecules by similarity, to plot them, and it will be super awesome if I could use common scaffold as markers' label, but not showing all the labels at the same time, more like one label for a group of similar markers.

All in all, I am trying to merge/group structures, but not to loose/merge any descriptors. How can I group them to have them in some categories like: all having the same scaffold1...scaffold100, but not merging them?

I hope I explained it) And thank you.

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