Subject: Re: Cluster t-SNE plot
Posted by thomas on Wed, 20 Mar 2019 22:29:19 GMT
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Hi Angus,

this is currently not possible. I would suggest to always cluster compounds on a chemical descriptor, because that would reflect compound similarity much better than the reduced 2 or three dimensions after t-SNE. Of course, clusters based on the t-SNE positions would look perfectly nice in the t-SNE view, but would be far from perfect groups of similar compounds.

Thomas