Subject: Cluster t-SNE plot
Posted by amorrison on Sat, 16 Mar 2019 06:28:38 GMT
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Hi,

I'm really liking the t-SNE visualisation. If I wanted to bin the compounds based on their t-SNE positions is this possible and how would I go about it? So similar to the cluster compounds but using t-SNE to a certain distance.

Thanks,

Angus

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