

---

Subject: Re: Cluster t-SNE plot  
Posted by [thomas](#) on Wed, 20 Mar 2019 22:29:19 GMT  
[View Forum Message](#) <> [Reply to Message](#)

---

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

---