Subject: what parameters shall be used to create t-SNE or PCA visualization in Data Warrior
Posted by yi02@hotmail.com on Thu, 03 Mar 2022 23:15:40 GMT
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Hi, there:

I am new to chemoinformatics, and I tried to create t-SNE visualization with Data Warrior for a group of compounds that I tried to see if any patterns or classes formed amongst them. I did Data->Create t-SNE Visualization, and then choose Structure [FragFp] amongst a list of potential parameters offered from the dropdown list. I saw other options such as cLogP,cLogS, H-Acceptors etc, are those potential or good parameters to be used for t-SNE or PCA visualization? Shall I try each of them? Or, Is there other features or structure descriptors we can used to create t-SNE and/or PCA? and is there a way for us to create such structure descriptors or parameters in Data Warrior?

Thanks so much in advance!
Best
Mike

Subject: Re: what parameters shall be used to create t-SNE or PCA visualization in Data Warrior
Posted by thomas on Sat, 02 Apr 2022 15:28:07 GMT
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Hi Mike,

t-SNE or PCA are usually done with lots of parameters, which is either one chemical descriptor (if it is a vector) or many numerical criteria. For instance, these could be inhibition values on many targets. Among the descriptors the SkelSpheres should be the best option, because is represents chemical structure similarity better the the simpler and faster binary descriptors. Descriptors can be added to a file with 'Chemistry->From Chemical Structure->Calculate Descriptor->...

Thomas