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