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