Subject: t-SNE
Posted by sansun on Fri, 15 Jul 2022 07:48:38 GMT
View Forum Message <> Reply to Message

Hi

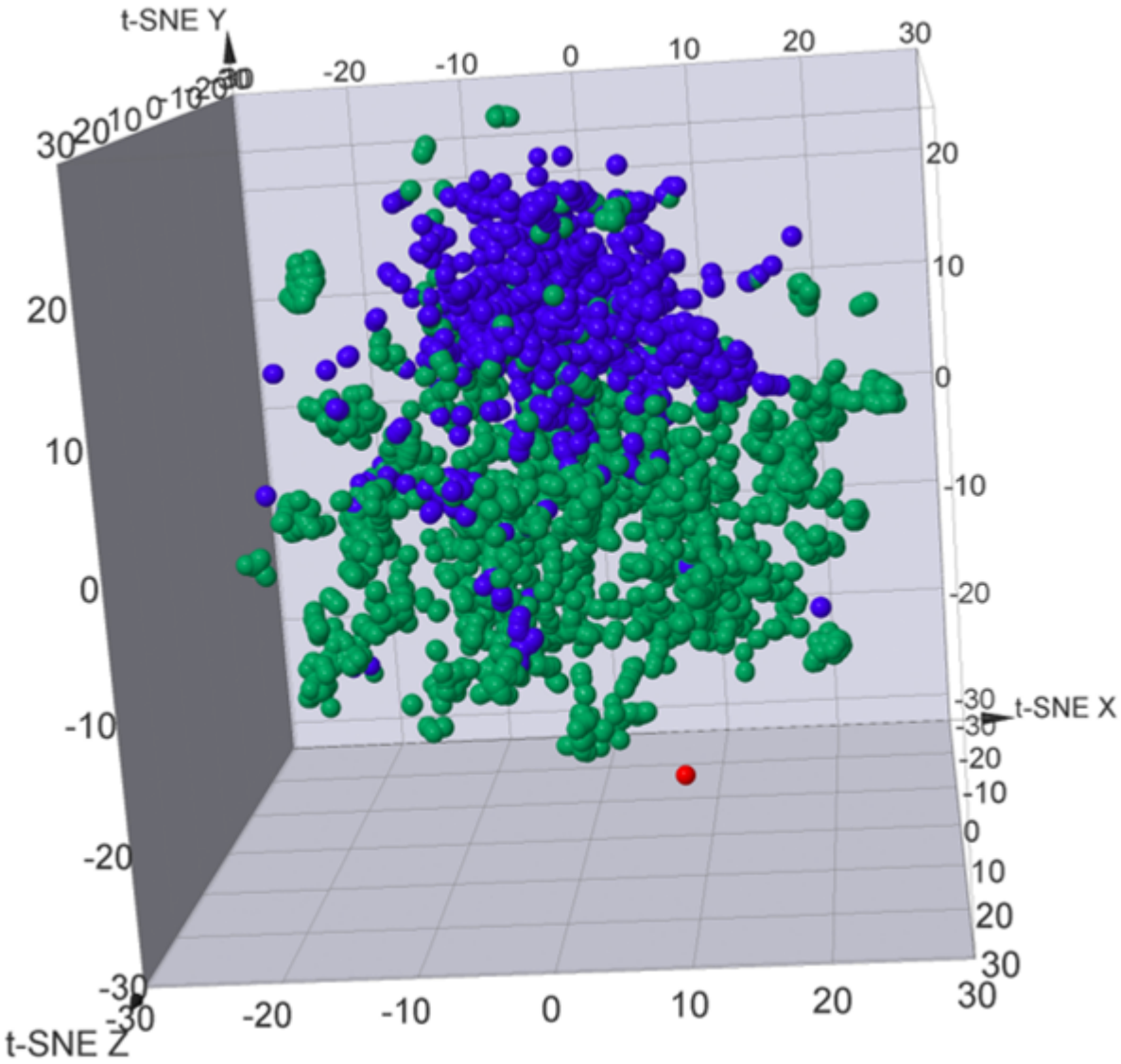
I have generated t-SNE 3D plot to compare two libraries (green and blue) using SkelSphere descriptor.
The molecules in the two libraries are kind of making separate clusters. Can we say the chemical space of the two libraries do not overlap considerably or they contain different type of structures?

If yes, how can we represent this conclusion quantitatively using t-SNE?

Thanks
SS

File Attachments

1) tSNE.png, downloaded 1802 times


t-SNE Y
t-SNE X
t-SNE Z