
Subject: t-SNE

Posted by [sansun](#) on Fri, 15 Jul 2022 07:48:38 GMT

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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 1387 times

