Subject: Skelspheres descriptor
Posted by ECG93 on Fri, 04 Mar 2022 13:23:37 GMT
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It is reported that Skelspheres considers stereochemistry, but how much is the threedimensionality considered? For example when dealing with a library of molecules with high sp3 fraction.

Probably flexophore descriptor would be more appropriate for "Analyse similarity cliffs", but for PCA Skelspheres can't be used as it is not a vector.