Subject: Re: Globularity
Posted by thomas on Wed, 24 Mar 2021 16:13:09 GMT
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Hi Patrick,

the shape index is based on the 2D-graph of the molecule and looks at the those two atoms that have the longest distance in terms of bonds between them. This length and the atom count of the molecule are used to calculate the shape index.

The globularity is calculated from atoms coordinates in conformers. It is basically doing a singular value decomposition to rotate the molecule in the coordinate system such that its width (size in x-direction) is maximized. Then it is rotated around the x-axis until its height is maximized. After that globularity is calculated as the molecule size in z-direction devided by the size in x-direction.

Shape index and globularity have a slight negative correlation, but one can hardly used as substitute for the other. I have just added a globularity calculation to DataWarrior (dev version). The results correlate (0.83) with the Nature paper's glob value. This is not a perfect correlation. I use up to 128 non-energy minimized conformers and average the result. If I minimize conformers with MMFF94s+ or reduce their number and therefore overpopulate low energy conformers, then the correlation gets worse. Probably, the conformers used in the paper were random conformers with no bias on low energy and most likely not forcefield minimized.

Hope this helps,

Thomas