Subject: Re: Globularity
Posted by thomas on Fri, 26 Mar 2021 16:13:16 GMT
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Hi Patrick again,

I just deployed an update, because the recent version was based on the singular values and created too small globularity values. Strangely, the Nature dataset's globularity values also seem too small. Now my calculation uses a singular value decomposition to determine the three orthogonal axes through the molecule that represent largest, second largest and smallest variance of the atom coordinates. Then, I determine along the axes the size of the molecule and divide the smallest by the largest size resulting in a reasonable globularity value. I average individual values of up to 32 random conformers, which were not minimized, but produced with a bias for low energy. The correlation with the 'glob' values of the Nature dataset is smaller than before, but if you explore conformers, create surfaces and visually inspect the molecules, it makes much more sense. One more thing to mention is that the conformers contain all hydrogen atoms, which gives on average slightly larger values than without hydrogens.

Thomas