Subject: Re: Globularity
Posted by thomas on Tue, 30 Mar 2021 15:10:58 GMT
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I made another update with another method to calculate globularity based on the volume and area of the solvent excluded surface (Van der Waals surface). The globularity is the surface of a perfect sphere, whose volume exactly matches the molecule's volume, divided by the real surface of the molecule. In my opinion this is the most reasonable globularity calculation. I also added some documentation and explanation.

Thomas