Subject: Globularity
Posted by P_Fitz on Wed, 24 Mar 2021 01:53:23 GMT
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I'm dabbling a bit in chemoinformatics and was wondering how a globularity score (specifically as referred to by eNTRy rules https://www.nature.com/articles/nature22308.pdf) compares to the Shape Index that is calculated in data warrior.

Thanks so much for developing and supporting such a great tool for free. I've found it very useful in my research.

Patrick Fitzgerald