Subject: Re: Lilly Medchem Rules
Posted by mvamos on Mon, 27 Apr 2020 22:25:13 GMT
View Forum Message <> Reply to Message

I do wonder what the druglikeness (pi) in the "drug score" actually measures, or how it's measured. My feeling is this Lilly calc might be less about solubility/polarity like the "drug score" and more related to functional groups.

The authors of the 2012 paper do have a paper from 2018 (https://doi.org/10.1021/acsmedchemlett.8b00097 on a related topic, but it seems to be a distinct set of PAINS rules. So perhaps the 2012 paper is the best guide.