Subject: publication for druglikeness score?
Posted by chemtv on Mon, 19 Feb 2018 15:04:46 GMT
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Hi,
I am looking at the description for the drug score and druglikeness scores in Datawarrior and wondered if there is a publication with more detail and analysis?
Thanks,
Greg

Subject: Re: publication for druglikeness score?
Posted by thomas on Thu, 01 Mar 2018 21:28:54 GMT
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Hi Greg,

at that time we didn't have the time to publish. Thus, the only public explanation is what you can find
via this URL: http://www.openmolecules.org/propertyexplorer/druglikeness.h tml
The fragments and their contributions to the score are part of the DataWarrior source code and could be
easily transformed into chemical structures, if that is of interest.

Thomas