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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

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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.html>

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

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