
Subject: Drug score

Posted by [plonacyrdwan](#) on Wed, 14 Jan 2015 23:14:52 GMT

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How can I calculate overall drug score in DataWarrior? In OSIRIS it is not a problem, but there I can not find anywhere this option.

Best regards

Subject: Re: Drug score

Posted by [thomas](#) on Thu, 29 Jan 2015 20:10:07 GMT

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DataWarrior does not directly calculate the drugscore as the Property Explorer did. You can calculate the drugscore with a formula after calculating the properties that the drugscore is composed of.

I have created a macro file that does everything for you and attached it to this message. I suggest that you download and save it in your 'Macro' folder of your DataWarrior installation, which usually would be on Windows here:

c:\Program Files (x86)\DataWarrior\Macro\

If there is no Macro folder, you have to create one. If you work on Linux or the Macintosh, then it works analogously. Once the dwam file is in the Macro-folder and after starting DataWarrior you find in its Macro-menu under Run-Macro 'Calculate Properties'. When you select that, DataWarrior calculates all needed properties and afterwards from them the DrugScore.

For that to work, you need the current version 4.1.0.

Kind regards,

Thomas

File Attachments

1) [Calculate Properties.dwam](#), downloaded 2580 times

Subject: Re: Drug score

Posted by [dalafave](#) on Fri, 17 Jun 2016 00:07:28 GMT

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Hi Thomas,

Thank you for creating the macro for DataWarrior, Calculate Properties. It helped me a great deal. I'd like to cite it in my paper. What would the proper citation be? Thanks!

Subject: Re: Drug score
Posted by [thomas](#) on Sun, 19 Jun 2016 19:18:31 GMT
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since the macro is not described anywhere except on this website I suggest to cite this URL and/or the DataWarrior paper available at <http://pubs.acs.org/doi/abs/10.1021/ci500588j>. I will soon release a DataWarrior update and the macro will be part of it.

Kind regards, Thomas

Subject: Re: Drug score
Posted by [Sifontes](#) on Thu, 29 Oct 2020 13:56:11 GMT
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Dear Thomas,
I installed the macro successfully and performed some test calculations. It worked fantastically. So far, I had run the calculations in a dedicated excel spreadsheet. Thanks for that new contribution!!! However, I have a doubt. In the formula for the calculation of the drug score, the coefficients for drugability are 1 and 0. That results in an inversely proportional contribution of druglikeness to the drug score, ie. the higher the druglikeness, the lower the drug score. Please, correct me if I'm wrong.
Best wishes,
Sergio

Subject: Re: Drug score
Posted by [thomas](#) on Thu, 05 Nov 2020 12:29:38 GMT
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Dear Sergio,

the contribution factor for the druglikeness part is: $*(1-0.5/(1+\exp(\text{Druglikeness})))$.
Thus, if druglikeness increases, then the sum $(1+...)$ grows, $0.5/\text{sum}$ gets smaller and $1-0.5/\text{sum}$ grows towards 1.
Currently, I don't see a problem here. Do you refer to a different formula?

Best wishes, Thomas
