
Subject: issue with permeability
Posted by [vamsi9k](#) on Mon, 13 Mar 2017 11:57:12 GMT
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Dear Thomas,

First of all datawarrior is a one of best integrated tool i ever used. Changes in latest version are really interesting like fuzzy score, permeability property . i am not able to calculate permeability score as it is complaining issue with marvin plugin. please suggest me work around for this problem.

please provide me if you have any working example with Fuzzy score calculation.

OS : Linux and Windows 64 bit

Thank you and your help will be highly appreciated.

with best regards,
vamsi

Subject: Re: issue with permeability
Posted by [thomas](#) on Tue, 21 Mar 2017 20:50:25 GMT
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Dear Vamsi,

the permeability calculation requires the ChemAxon pKa plugin to be in the class path, because it considers the charged fraction of the molecule at $pK_a=7.4$. I missed to disable the 'permeability' checkbox in the calculate properties dialog, if the chemaxon classes are not available, which usually is the case in the open-source version. If you have a license to the ChemAxon plugin you may put it into the class path (at least on Mac and Linux). But this still requires some effort and is described somewhere else in this Forum.

For the fuzzy score please refer to the manual that you find when you open the 'Fuzzy Score' dialog and press the Help button.

Hope this helps, Thomas

Subject: Re: issue with permeability
Posted by [pc419714@ohio.edu](#) on Thu, 11 Apr 2019 17:31:10 GMT
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How do you install the ChemAxon pka plugin? Permeability would be something we would like to

calculate. Thanks

Subject: Re: issue with permeability

Posted by [thomas](#) on Sun, 14 Apr 2019 19:55:39 GMT

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you need to have a license of ChemAxon's pKa plugin, install the software on you computer and add all jar files to the DataWarrior classpath. For Linux this is easy, because you just have to adapt the /opt/datawarrior/datwarrior batch file. On MacOS it probably would work to put all jar files into /Applications/DataWarrior/Contents/Java/, which I have never tried. For Windows it is a little more complicated, because for technical reasons you cannot change the class path and add more jar file references. But the Windows class path contains a reference to a file 'capka.jar', which is not part of the standard Windows installation, but if you unpack all ChemAxon jars and repackage them into a 'capka.jar', which you put into the DataWarrior installation folder alongside the other jar files, then this should work.

In mid term, we plan to provide our own pKa prediction algorithm, which would be then build into DataWarrior and would ungray all property claculation options that depends on pKa values.

Thomas
