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