Subject: cLogD
Posted by thurow.sam@gmail.com on Tue, 16 Jun 2020 13:46:09 GMT
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Hi everybody!

the option that calculate logD is unclickcable, is there a way to activate that button?

thanks

Sam

Subject: Re: cLogD
Posted by thomas on Tue, 16 Jun 2020 20:15:51 GMT
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cLogD requires a pKa prediction, which DataWarrior cannot do itself yet. However, DataWarrior may use the commercial ChemAxon pKa-plugin to do the prediction. If the DataWarrior installation folder contains a capka.jar file, which contains the needed ChemAxon software, then cLogD and pKa prediction are enabled.

Subject: Re: cLogD
Posted by bruce on Tue, 02 Feb 2021 21:15:27 GMT
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I am about to purchase the chemaxon cLogD plugin for datawarrior-

are there any procedures written up so i can install this functionality into the program?

thanks!

Subject: Re: cLogD
Posted by thomas on Tue, 02 Feb 2021 21:47:17 GMT
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No, unfortunately, there is no easily reproducible procedure described. DataWarrior checks for a file called 'capka.jar' among its jar files. If it finds it and if the accessed classes and their dependencies are inside it in the proper folder hierarchy representing the package names, then it should work. You should also place the license file where the ChemAxon documentation expects it to be. I did it only once many years ago. At that time it was a cumbersome procedure, because the original pKa-plugin contained many jar files with altogether more than 100MB content. To add this to a DataWarrior installation was prohibitive, even though it was an in-house Actelion installation. Therefore, I unpacked all jar files into one root directory and intended to remove everything that was not needed for the pKa-calculation. I tried various Java obfuscators, because

they have a mode to not obfuscate Java bytecode, but just remove unused dependencies. None of them could handle this amount of Java stuff. Finally I ended up removing one file after another with a script and checking after every step that the pKa calculation still works. Problematic was that the code often uses the reflection API and that required classes depend on certain features of the molecule (really a mess). Different molecules needed different classes added via classForName()!!! My procedure finally reduced the size from >100MB to 0.72MB.

Of course, if you unpack all jars into one root directory and pack everything again into one large capka.jar, it should work. However, I didn't try this with the current pKa-plugin.

The classes required by DataWarrior are:
chemaxon.formats.MolFormatException;
chemaxon.formats.MolImporter;
chemaxon.marvin.calculations.pKaPlugin;
chemaxon.marvin.plugin.PluginException;

I also attach a list of all files that I have added and that seems to be complete...

If your are successful with the current ChemAxon plugin, then please let other users know.

Thomas

File Attachments
1) capka.txt, downloaded 837 times

Subject: Re: cLogD
Posted by bruce on Wed, 03 Feb 2021 17:29:53 GMT
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thanks Thomas. Very much appreciate all of the work you have done on this program

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Subject: Re: cLogD
Posted by jdion on Tue, 21 Sep 2021 16:56:56 GMT
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Has anyone made progress on this issue recently?

I've followed the steps with the most recent Chemaxon releases and haven't been successful.

Does Datawarrior have a log that describes it's attempts to use the Chemaxon classes and any errors?

Thanks!

Subject: Re: cLogD
Posted by thomas on Mon, 27 Jun 2022 16:27:33 GMT
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If you have a ChemAxon license, you can now download an official capka.jar file from the ChemAxon website, which was built for DataWarrior using just the classes needed and being compatible with Java 8 that DataWarrior uses. Of course, you also need to have the proper license file at the right location in your file system. The download link is:
https://chemaxon.com/download?dl=%2Fdata%2Fdownload%2Fcalcul
ators%2F.datawarrior%2Fcapka.jar