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 1063 times