Subject: Re: ChemAxon calculated properties
Posted by thomas on Thu, 04 Dec 2014 21:55:35 GMT
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DataWarrior is looking for a file name 'capka.jar' in the same directory, where datawarrior.jar is located.
If it finds this file and if it contains the needed Java classes, it will work.

If you want to do that, there are two options:

The easy one: Unpack all ChemAxon jar files into one directory and zip them again into one big jar that you rename to 'capka.jar'. This should work, but the disadvantage is that the file will be more than 100Mbyte in size.

The difficult one: Unpack all ChemAxon jar files into one directory, remove the file that are not needed and zip the rest into one jar that you rename to 'capka.jar'. This works and results in a file that is less than 1Mbyte. The problem: Locating the unneeded files is rather cumbersome. I tried with two obfuscators to track dependencies and purge the rest. This didn't work for various reasons. The approach that worked, is the following:
I wrote a java program that used the ChemAxon API to create a ChemAxon Molecule object from a molfile, to predict the pKa values, then checked the values and wrote an empty text file 'OK.txt' to indicate that the ChemAxon API worked correctly. Then, I set the Java classpath to access the ChemAxon API from the unpacked folder with all ChemAxon class and data files. Then I used a linux script to stepwise delete one file after another from the ChemAxon directory with checking whether OK.txt was written. If not I undeleted the evidently necessary file and went to the next. That gave me the core set of needed files. The I noticed that different molfile/molecule features required additional classes to work, which I added manually when the ClassNotFoundException was raised. Evidently, ChemAxon software uses heavily Class.forName() calls, whenever a molfile contains a specific feature. If you are brave enough to go through this, I can send you the Linux scripts I used to create the file.

If you are running Linux or OSX, you have a third option. Put all the ChemAxon jar files in the directory that contains datawarrior.jar and add all ChemAxon jar file names to the class path. On linux this is in the file 'datawarrior'. On OSX it is in Info.plist. You can access that file if you click right mouse on the DataWarrior icon, select 'Show Package Content' and open the 'Contents' folder.

I am sorry for the cumbersome stuff, but for obvious reasons I cannot send you a copy of the capka.jar file.

Good luck,

Thomas