Subject: ChemAxon calculated properties
Posted by drc007 on Fri, 25 Jul 2014 19:16:48 GMT
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I'm having a look at DataWarrior and I'd like to calculate most basic pKa using the ChemAxon tools which I have installed. When I open an sdf file with DataWarrior and select Add calculated properties I find the ChemAxon tools are greyed out.

Subject: Re: ChemAxon calculated properties
Posted by ffadmin on Sat, 02 Aug 2014 10:37:32 GMT
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the pKa and logD calculation are not available in the free DataWarrior version,
because they require commercial software from ChemAxon, the pKa plugin, which
Actelion has licensed for internal usage, but cannot provide to the public.

However, if you have a license to the necessary subset of the ChemAxon software,
you may put all ChemAxon files needed for pKa calculation into a new .jar file
(this is a zip file with extention 'jar' instead of 'zip') call it 'capka.jar'
and copy it into the datawarrior installation directory that includes all
other jar files. DataWarrior would recognize the file and would enable the options
for pKa and logD. Since finding the needed files is a little tricky, you may
unpack all ChemAxon jar-files into one directory, zip them again and rename
to 'capka.jar'.

I realize that this is a little cumbersome, but currently there is no other
solution.

Hope this helps,

Thomas

Subject: Re: ChemAxon calculated properties
Posted by MussaQ on Thu, 04 Dec 2014 16:46:39 GMT
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Quote:if you have a license to the necessary subset of the ChemAxon software,
you may put all ChemAxon files needed for pKa calculation into a new .jar file

I have an academic license for chemaxon (for the entire Marvin and JChem suites) through my institute, I was wondering if you knew the location of these files required for the LogD calculations? I have had no luck on Mac or windows in trying to locate them.

Much appreciated.

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

Subject: Re: ChemAxon calculated properties

Posted by MussaQ on Fri, 05 Dec 2014 19:15:34 GMT
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Thank you very much for your detailed reply, but I am still cannot access the pKa option.

I tried 2 options, in both cases the files were placed in the same directory as datawarrior.jar

1) Easy method; I searched all .jar files in the chemaxon folder under the applications folder on a Mac OSX, extracted them all and then re-zipped them and called it capka.jar (167MB file!)

2)Option 3, pasted all the .jar files i found and added their names to the Info.plist accordingly, datawarrior took longer than usual to load but no luck.

I am not familiar (brave) enough with scripting to attempt the second (difficult) option. However, would it be possible if you could provide the list of files that did work for you? so that I can cross reference with the files I found.

Subject: Re: ChemAxon calculated properties
Posted by thomas on Mon, 08 Dec 2014 19:52:58 GMT
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I checked the issue and must appologize, because the capka.jar is not recognized on Windows. This only works on Linux and MacOSX. The mechanism to locate the installation directory that DataWarrior uses seems not reliable on Windows, e.g. because of an interference with the caching
mechanism. I will change the mechanism in the upcoming update. If you like and if you tell me which
OS you use (win32 or win64) I can send you a link to a 4.0 beta version with this issue solved.

Thomas

Subject: Re: ChemAxon calculated properties
Posted by MussaQ on Wed, 10 Dec 2014 11:49:20 GMT
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Thanks for your time on the matter,

I primarily use Mac OSX and attempted the 2 options previously mentioned on that OS, however I do have access to a Windows machine and it is a 64-bit type. I could try it on that OS.

Mussa

Subject: Re: ChemAxon calculated properties
Posted by thomas on Wed, 10 Dec 2014 20:07:30 GMT
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Another thing came to my mind. One needs to make sure that the ChemAxon license file is at the proper location. More information can be found on the ChemAxon web site:

https://docs.chemaxon.com/display/licensing/Installing+licen ses

"The default location is .chemaxon/license.cxl (Unix) or chemaxon\license.cxl (Windows) under the user's home directory. From the 5.3.2 version license files can also be located at (.)chemaxon/licenses/*.cxl, the name of the license files can arbitrarily be changed."

MacOSX is not mentioned, but I assume that the ChemAxon software works with the license file being
located at /Users/<username>/.chemaxon/license.cxl.

Can you check, whether your Info.plist file contains the capka.jar file in the classpath?

Anyway I will send you a link to a fresh beta 4.0 version for MacOSX till Thursday. Please let me know, if that solves the issue.

Kind regards,

Thomas

Subject: Re: ChemAxon calculated properties
Posted by thomas on Thu, 11 Dec 2014 19:50:59 GMT
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here is the promised upload link for DataWarrior Macintosh version 4.0.0 beta

https://www.dropbox.com/sh/9v64ckfy1mxcayu/AACO3mmc_ha4m5iO7 tmIffy0a?dl=1

The capka.jar finding mechanism is changed and should now work on any platform.
Many small other issues were fixed, but the biggest change is macro support:
Workflows can be recorded as a macro. Individual tasks of macros can be edited,
if they need a configuration and macros can be executed. Macros can be part of
a DataWarrior data file or they can be exported into separate files. Macro files
in a special folder show up in a new macro menu and can be executed on any data file.

Macros are not fully tested and most certainly there are many small bugs left.
This is a beta version and the macro file format may even change in a few tiny aspects.

If you encounter problems, please let me know. Otherwise have fun...

Thomas

Subject: Re: ChemAxon calculated properties
Posted by chemist on Tue, 17 Jan 2017 09:45:31 GMT
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Thanks for creating really great software!

I have been struggling with Chemaxon calculated properties. I also have this free academic lisence but enabling these chemaxon properties seems quite difficult.

What I have tried:

1. Go to chemaxon directory
2. Searh .jar
3. copy all of them to new folder
4. extract all .jars by ticking [x]"Extract archives to subfolders"
5. zip all to capka.zip
6. rename -> capka.jar
7. move to datawarrior.exe location

I have also lisence file in correct location.

I just started to think if in the academic version there is some limitation to batch calculation of pKa values.

I have lisence for following products:
Marvin Applets
Marvin Beans
Instant JChem
JChem Base
Standardizer
Screen
Reactor
JKlustor
Metabolizer
Markush Search
Protonation Plugin Group
Partitioning Plugin Group
Isomers Plugin Group
Markush Enumeration Plugin
Structure to Name Plugin
Name to Structure
JChem for Excel
Structure Search
IUPAC naming plugin
Web Services Server

Structure Checker
Predictor Plugin
MCES
3D Screen
Molecular Descriptors
Instant JChem VIZ
ECFP/FCFP
Document to Structure
NMR Predictor
JChem for Office
Markush Editor
Solubility Plugin
Structural Calculations

Subject: Re: ChemAxon calculated properties
Posted by thomas on Sun, 05 Feb 2017 22:02:59 GMT
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your procedure seems correct. I need to verify that, but I can only try with an old version, because we didn't update since quite a while.

Can you start DataWarrior from the command line? Do you get any error message then?
Are your checkboxes for pKa and LogD in the property prediction dialog enabled?
If not, then you either have a problem with the class path or you miss the file /chemaxon/marvin/calculations/pKaPlugin.class in your capka.jar?
It is part of the ChemAxon pKa-Plugin. Can you check for that class file?

Regards, Thomas
