Subject: ChemAxon plugin
Posted by Christophe on Thu, 03 Feb 2022 11:19:41 GMT
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Hello,

I've just get a ChemAxon licence and I'd like to activate the "clogD at pH 7.4" as well as all options included into the "Ionization" table from the "Calculate Compound Properties" Menu.

Can somebody please explain the procedure to use the ChemAxon capabilities into DataWarrior?
Thanks
Christophe

Subject: Re: ChemAxon plugin
Posted by thomas on Thu, 10 Feb 2022 09:08:03 GMT
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Hello Christophe,

you can search this forum for 'capka' and find some posts. I did it myself about 15 years ago and suspect that the same procedure should work also with the current ChemAxon pKa plugin, but since I don't have the current plugin, I cannot confirm this. Basically, you have to unpack all jar files into one directory and then repack everything from that directory into a new 'capka.jar' file. You also have to put the license file where the license code can find it.

If you want, you can contact me offline to work together on creating a reproducible procedure, e.g. a bash script doing the entire conversion, which we could publish afterwards on this forum for others to re-use.

Thomas

Subject: Re: ChemAxon plugin
Posted by timritchie on Mon, 21 Feb 2022 12:16:10 GMT
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Hi,
I would also like to activate the ChemAxon pKa functionality in DataWarrior (Windows 10), and would be happy to help working out a script or procedure to enable this.
Regards,
Tim Ritchie.

Subject: Re: ChemAxon plugin
Posted by timritchie on Mon, 21 Feb 2022 12:19:05 GMT

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By the way, when DataWarrior calculates a logD value, is it using the logP value from DataWarrior or from ChemAxon...

Subject: Re: ChemAxon plugin
Posted by nbehrnd on Tue, 22 Feb 2022 21:03:20 GMT
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Dear Tim,

re your second question, as outlined by the documentation,[1] clogD requires /both/ input by clogP (DataWarrior) .and. pKa (ChemAxxon). A subsequent page[2] briefly describes 5k+ experimentally recorded data were used to train the model used for clogP, as well as showing the correlation plot for 5k+ of other (non training) data.

Norwid

[1] https://openmolecules.org/help/chemistry.html#MolecularPrope rties
[2] https://openmolecules.org/properties/properties.html

Subject: Re: ChemAxon plugin
Posted by Christophe on Tue, 01 Mar 2022 12:00:24 GMT
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Hello everyone,

I tried to apply the procedure kindly given by Thomas, but when I try to generate .jar file I have a problem:
According this procedure I should "Unpack the chosen jar files first (rename to zip and unzip). Then merge all the files and directories found into one directory."

I cannot merge them because they share common file names. How can I keep their content in one file sharing the same name? I don't know if I make myself clear.
Furthermore the generated file would be huge

All the best

Subject: Re: ChemAxon plugin
Posted by thomas on Fri, 04 Mar 2022 18:49:48 GMT
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Hi Christophe,

if there are files with the same name in the same folder hierarchy, then this is most likely, because the originally separated ChemAxon jar files contained the same external dependencies, which are redundant, if merged. You should be able to just overwrite these files that they are contained just once. Indeed the merged file would be huge, but it should work.

When I did this 15 years ago, I removed all files, which were not needed for the pKa calculation, which reduced the file size by more than a factor of 1000. After trying various other methods for this, I turned to a brute force method: Running a bash script, which was removing one file after another. After every file removal I calculated pKa with the remaining files and checked, if the procedure still worked. If not, then the files was added again and the script continued with removing the next file. Finally, I had to add a few removed files, when I discovered that different structure classes required different Java classes for the pKa calculation, which were invoked with ClassForName.

Subject: Re: ChemAxon plugin
Posted by timritchie on Thu, 17 Mar 2022 10:41:39 GMT
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Hi,
Many thanks for the clarification.
Regards, Tim.

Subject: Re: ChemAxon plugin
Posted by timritchie on Fri, 18 Mar 2022 15:56:39 GMT
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Hi, I am still struggling with getting the ChemAxon pKa function to work in DataWarrior (Windows 10 64-bit). I have added the capka.jar file to the DW folder, but the pKa-related options are still greyed out.
When the ChemAxon.jar files are extracted, should they be put into one single folder with no subfolders, before zipping, or does that not matter?
Thanks,
Tim.

Subject: Re: ChemAxon plugin
Posted by timritchie on Sat, 19 Mar 2022 08:57:48 GMT
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An update: I obtained a capka.jar file from ChemAxon, which enables the pKa-related calculations in DataWarrior if you hold a licence for the protonation plugin (Windows 10 OS).

Subject: Re: ChemAxon plugin
Posted by mlmiranda on Mon, 28 Mar 2022 16:14:11 GMT
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Hi Tim,
Could you please share more info about the capka.jar file from ChemAxon? How can I get it? I have a ChemAxon license and I've also been struggling with making the ChemAxon pKa function "active" to work in DataWarrior.

Thanks in advance for your response.
Lily

Subject: Re: ChemAxon plugin
Posted by Christophe on Wed, 30 Mar 2022 08:23:00 GMT
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Hello Tim,

This is great news.
Could you please post the methodology you applied to get this positive result?

In my case, I get a capka.jar file that put in the root file of DW but when I launched DW I get an error message related to the java version of chemaxon I used (JRE11 or more) which according, Thomas, is not compatible with JRE8 that is still currently in used with DW.

So I was waiting for an update of DW with JRE11 to continue, and I hope, to activate the ChemAxon pka functions.
Regards
Christophe

Subject: Re: ChemAxon plugin
Posted by thomas on Mon, 27 Jun 2022 10:02:52 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

Subject: Re: ChemAxon plugin
Posted by Flammable on Thu, 01 Dec 2022 15:01:00 GMT
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Hi thomas, that link is giving a 404 error. I've tried compiling my own capka.jar and thought it would work except I got this error:

Uncaught Exception:chemaxon/marvin/calculations/pKaPlugin has been compiled by a more recent version of Java Runtime (class file version 55.0), this version of Java Runtime only recognizes class file versions up to 52.0

Any way around this?

Subject: Re: ChemAxon plugin
Posted by thomas on Thu, 01 Dec 2022 19:06:04 GMT
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DataWarrior is using a JRE 1.8. Thus any jar files accessed by it must not have newer bytecode version than that. If you compile yourself with javac, then use "-target 1.8". That should do it...
