Subject: Chemaxon PKA (java exception occuring)
Posted by jeffchem on Wed, 28 May 2025 11:24:42 GMT
View Forum Message <> Reply to Message

Hi DataWarrior folks.

I'm having an issue with the Chemaxon PKA calculation.

I'm trying to calculate the higest basic pKa; ChemAxon method under the Ionization section.
a) I have chemaxon license.
b) I am using the capka.jar (downloaded from Chemaxon site)
c) cLogD at ph=7.4; via logP and ChemAxon pKa works fine.

When I run DataWarrior from the command line and print to a log file. DataWarior.exe > out.txt
I can see that there is an exception occuring in the java code.
Unexpected ChemAxon Exception:java.lang.NoSuchMethodError: 'void chemaxon.marvin.calculations.pKaPlugin.setMolecule(chemaxon. struc.Molecule)'

Has anyone else encountered this issue? Any work arounds?

Subject: Re: Chemaxon PKA (java exception occuring)
Posted by thomas on Fri, 30 May 2025 12:38:42 GMT
View Forum Message <> Reply to Message

it looks like DataWarrior doesn't find the capka.jar when you start from the command line. If you launch datawarrior_xxx.jar from the command line on any platform, then you could add the capka.jar to the class path. If you just start DataWarrior.exe on Windows, you should make sure that the working directory for DataWarrior is the installation directory...

Subject: Re: Chemaxon PKA (java exception occuring)
Posted by jeffchem on Mon, 02 Jun 2025 21:02:10 GMT
View Forum Message <> Reply to Message

Hi Thomas,

I respectfully disagree.
It appears to me running Datawarrior via the command line is picking up the capka.jar correctly.
When I'm running from the command line, I'm execute from within the installation directory:
c:\Program Files\DataWarrior

If I rename my capka.jar to xx_capka.jar then all of the chemaxon options are all greyed as one would expect. So to me that suggests DataWarrior is recognizing the capka.jar via the command line.

I only attempted to run from the command line to find some hint as to why the acidic pka & basic pka under the ionization section are not working. Neither of these calculations work regardless of normal or via command line.

It seems the capka.jar that is downloaded from Chemaxon isn't compatible with these two calculations.