
Subject: Chemaxon pKa plugin

Posted by [matthewk](#) on Thu, 23 Feb 2023 18:29:59 GMT

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I have been trying to enable Datawarrior's cLogD, permeability, and ionization property calculations, but have run into some errors along the way.

I found the required capka.jar file from a previous thread, which was very helpful. I also have the most recent version of chemaxon marvin suite installed and am using a free license for it.

When I placed the capka.jar file into the DW directory, that did allow me to select the cLogD, permeability and ionization properties in the calculate properties window. Which at first made me think that I had done everything correctly. However, when running the calculation I see this error:

"uncaught exception:org.json.JSONArray.<init>(Ljava/lang/String;)V"

And if I try again I see another error:

"uncaught exception: could not initialize class chemaxon.license.licensehandler\$singletonholder"

Could anyone offer any insight or suggestions for resolving these issues? Do I need a different license, or does it need to be in a different location? Do I need to do anything else to the capka.jar file?

Thank you so much!
