Subject: Re: Chemaxon PKA (java exception occuring)
Posted by jeffchem on Mon, 02 Jun 2025 21:02:10 GMT
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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.