
Subject: Chemaxon PKA (java exception occuring)
Posted by [jeffchem](#) on Wed, 28 May 2025 11:24:42 GMT
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Hi DataWarrior folks.

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

I'm trying to calculate the highest 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. DataWarrior.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?
