Subject: Re: ChemAxon calculated properties
Posted by ffadmin on Sat, 02 Aug 2014 10:37:32 GMT
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the pKa and logD calculation are not available in the free DataWarrior version, because they require commercial software from ChemAxon, the pKa plugin, which Actelion has licensed for internal usage, but cannot provide to the public.

However, if you have a license to the necessary subset of the ChemAxon software, you may put all ChemAxon files needed for pKa calculation into a new .jar file (this is a zip file with extention 'jar' instead of 'zip') call it 'capka.jar' and copy it into the datawarrior installation directory that includes all other jar files. DataWarrior would recognize the file and would enable the options for pKa and logD. Since finding the needed files is a little tricky, you may unpack all ChemAxon jar-files into one directory, zip them again and rename to 'capka.jar'.

I realize that this is a little cumbersome, but currently there is no other solution.

Hope this helps,

Thomas