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Subject: Re: cLogD

Posted by [thomas](#) on Tue, 16 Jun 2020 20:15:51 GMT

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cLogD requires a pKa prediction, which DataWarrior cannot do itself yet. However, DataWarrior may use the commercial ChemAxon pKa-plugin to do the prediction. If the DataWarrior installation folder contains a capka.jar file, which contains the needed ChemAxon software, then cLogD and pKa prediction are enabled.

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