
Subject: Re: ChemAxon plugin
Posted by [nbehrnd](#) on Tue, 22 Feb 2022 21:03:20 GMT
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Dear Tim,

re your second question, as outlined by the documentation,[1] clogD requires /both/ input by clogP (DataWarrior) .and. pKa (ChemAxxon). A subsequent page[2] briefly describes 5k+ experimentally recorded data were used to train the model used for clogP, as well as showing the correlation plot for 5k+ of other (non training) data.

Norwid

[1] <https://openmolecules.org/help/chemistry.html#MolecularProperties>

[2] <https://openmolecules.org/properties/properties.html>
