Subject: Protonation state of cmpds
Posted by shwang on Fri, 11 Nov 2022 01:08:57 GMT
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Hi,
I am new to DataWarrior, and I was wondering if there is any way that it can predict the total charge of the compound or display protonated state?
Thank you.

Subject: Re: Protonation state of cmpds
Posted by thomas on Fri, 11 Nov 2022 09:00:40 GMT
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You could count the number of basic and acidic atoms, which uses a simple rule base algorithm. If you need more, you would need the capka.jar plugin (and a license for it) from ChemAxon, which DataWarrior can use to calculate pKa-values. With that you could create protonation states for any given pH value.