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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.

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