

---

Subject: Protonation state of cmpds

Posted by [shwang](#) on Fri, 11 Nov 2022 01:08:57 GMT

[View Forum Message](#) <> [Reply to Message](#)

---

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

[View Forum Message](#) <> [Reply to Message](#)

---

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.

---