

---

Subject: Re: HBD/HBA

Posted by [zhentg](#) on Tue, 07 Mar 2023 08:25:04 GMT

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

---

Great that this topic is discussed.

We also found the HBA/HBD counts are different from those provided by PubChem(calculated by CACTVS).

Interestingly, RDkit HBA/HBD counts seems to be similar to DW.

It will be great if the CACTVS HBA/HBD count algorithm be adapted in DW.

---