

---

Subject: Re: HBD/HBA

Posted by [thomas](#) on Sat, 18 Mar 2023 16:25:59 GMT

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

---

Admittedly, DataWarrior's (or RDkit's) simple approach of calculating HBA/HBD do not really reflect the reality in some cases. They just use the method applied in Lipinsky's 'rule of five' paper. This way DataWarrior's calculated HBA/HBD values can directly be used in the 'rule of five' context.

---