Subject: HBD/HBA
Posted by chemsandra on Fri, 08 Apr 2022 13:13:31 GMT
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I have a question about hydrogen bond donors (HBD) and hydrogen bond acceptors (HBA). I was wondering how DataWarrior software defines HBD and HBA. Is there any literature reference about this?

I used KNIME and DataWarrior to calculate the number of HBA and HBA. However, the result of using both software is different.

I would be grateful for the help with this.