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.

Subject: Re: HBD/HBA
Posted by thomas on Fri, 13 May 2022 16:06:49 GMT
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The HBA and HBD counts in DataWarrior are very simple.
Every oxygen and nitrogen is considered an acceptor and every oxygen and nitrogen with at least an attached hydrogen is considered a donor.

Subject: Re: HBD/HBA
Posted by P_Fitz on Mon, 06 Mar 2023 19:59:59 GMT
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Is this an accurate way to do HBA/HBD? I wouldn't consider an amide -N an H bond acceptor.

Subject: Re: HBD/HBA
Posted by nbehrnd on Mon, 06 Mar 2023 22:28:01 GMT
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Initially for curiosity, I submitted a few simple molecules to the assignment to H-bond donors, and acceptors

DW assigns last entry 6, diacetamide, 3 acceptors and 1 donor. This contrasts to Etter's paper[1] with two accptors and one donor only.

Do follow medicinal chemistry and solid state chemistry/crystallography different conventions here?

With regards,

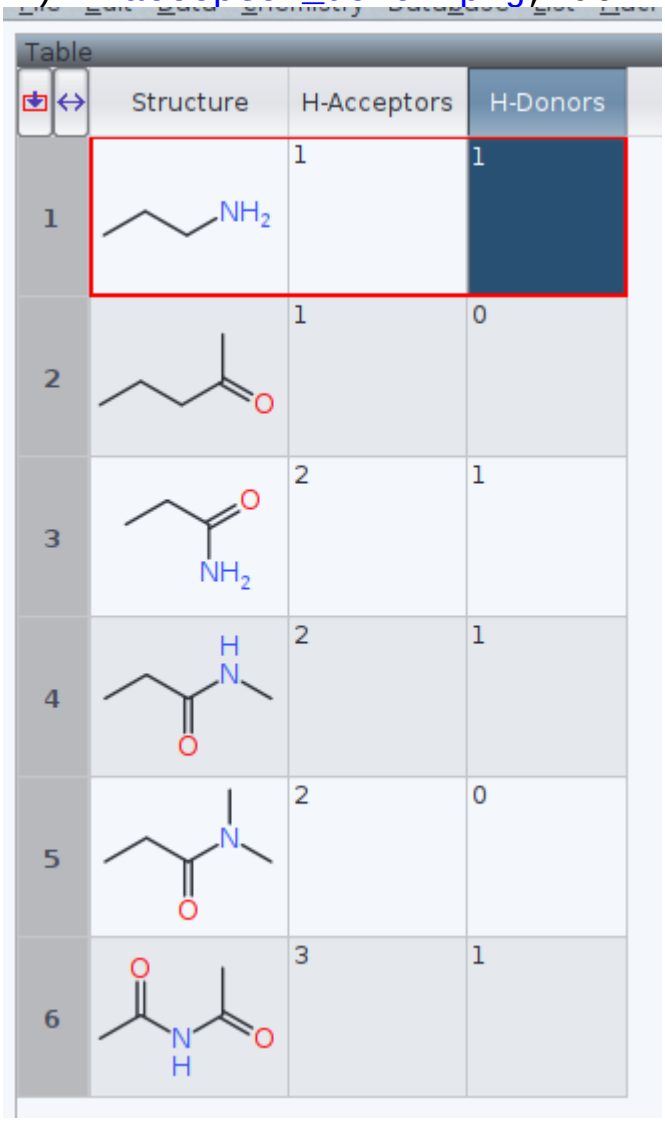
Norwid

[1] Etter, M. C. Encoding and decoding hydrogen-bond patterns of organic compounds. Acc. Chem. Res. 1990, 23, 120-126 (DOI https://doi.org/10.1021/ar00172a005).

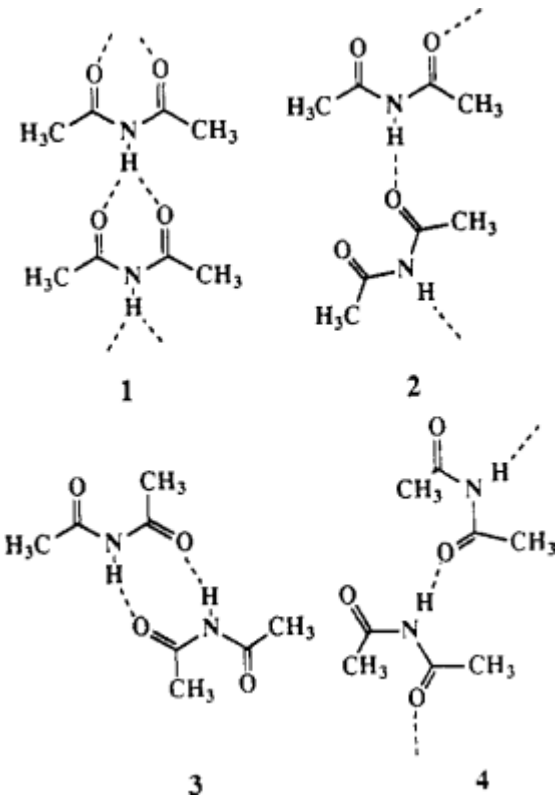
[2] Etter, M. C.; MacDonald, J. C.; Bernstein, J. Graph Set Analysis of Hydrogen-Bond Patterns in Organic Crystals. Acta Cryst. B 1990, 46, 256-262 (DOI https://doi.org/10.1107/S0108768189012929)

File Attachments

1) H-acceptor_donor.png, downloaded 1785 times



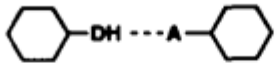
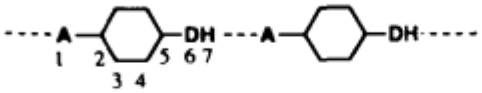
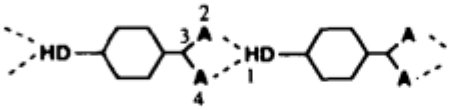
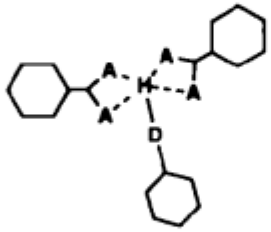
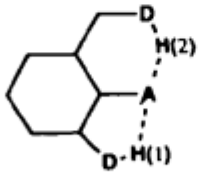
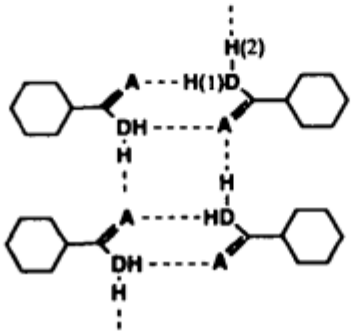
2) Etter_graphs_diacetamide.png, downloaded 1754 times



3) Etter_graphs_2.png, downloaded 1839 times

Table 1. *Examples of graph-set assignments*

The hexagons are meant to represent any organic ligand. This specific form is given so the degrees of the patterns can be assigned in this table. If the organic ligands were other kinds of groups, then the degrees of some of the patterns would change.

(I)		$N_1 = D$
(II)		$N_1 = C(7)$
(III)		$N_1 = C_1^2(8)[R_1^2(4)]$
(IV)		$N_1 = 2R_1^2(4)$
(V)		$N_1 = S(6)S(5)$ $N_2 = S_2^1(9)$
(VI)		$N_1 = C(4)R_2^2(8)$ $N_2 = R_4^2(8)$

Subject: Re: HBD/HBA
Posted by zhentg on Tue, 07 Mar 2023 08:25:04 GMT
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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 algrithm be adapted in DW.

Subject: Re: HBD/HBA
Posted by thomas on Sat, 18 Mar 2023 16:25:59 GMT
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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.
