Subject: Compound properties
Posted by xhubei08 on Thu, 15 Sep 2016 18:41:09 GMT
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Compound properties such as "Aromatic Atoms count" and "sp3-Atoms count" are calculated via the "Add Compound Properties" entry in DataWarrior. Is there a document in which all the compound properties are defined? For example, I would like to know if hydrogen atoms are included in "Aromatic Atoms Count".

Thanks,
Xiche Hu

Subject: Re: Compound properties
Posted by thomas on Fri, 23 Sep 2016 21:04:34 GMT
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you are right that DataWarrior lacks a more detailled explanation of the properties. I will try to add that soon. On the other hand the counts are rather simple and often self explanatory. Hydrogen atoms are never considered, neither implicit nor explicit ones.

Hope that this quick answer helps a little,

Thomas