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