Subject: Basic Nitrogen
Posted by sansun on Fri, 07 Aug 2020 10:43:36 GMT
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How does DW calculates 'Basic Nitrogen' atom?

How does it estimates pKa?

Is there any citation/literature for this?

Subject: Re: Basic Nitrogen
Posted by nbehrnd on Fri, 07 Aug 2020 15:14:46 GMT
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«Basic Nitrogen», as available under Chemistry -> From Chemical Structure -> Calculate Properties and then index card «Functional Groups» reads that the threshold applied is a pKa above 7. DW explicitly states that this a rough estimate.

The pKa estimation in the next tab, «Ionization» refers to the ChemAxon method. It is very likely that this refers to the documentation at

https://docs.chemaxon.com/display/docs/pKa_calculation.html

which include worked examples as well as literature references, too.

Subject: Re: Basic Nitrogen
Posted by thomas on Fri, 07 Aug 2020 16:18:00 GMT
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Unless you have the ChemAxon pKa plugin licensed and installed properly for DataWarrior to recognize it, DataWarrior does not calculate pKa values. Therefore, those properties that need a pKa prediction are greyed out in the dialog.

The basic nitrogen count, however, is using a rule based approach and does not need a pKa prediction. It checks the local atom environment for every nitrogen. For instance uncharged aliphatic nitrogens without an attached carbony group (or vinylogous carbony) are considered basic, unless they are part of an imine, etc. For aromatic nitrogens it is checked, whether there are other nitrogens in the same ring that reduce basicity or amino groups in ortho or para position which increase basicity. Some rules of thumb decide. For this there is no literature, but you can check the source code. This part is easy to understand, if you have some basic programming knowledge. It is in package com.actelion.research.chem, class AtomFunctionAnalyzer, method isBasicNitrogen(StereoMolecule mol, int atom):

https://github.com/Actelion/openchemlib/blob/master/src/main/java/com/actelion/research/chem/AtomFunctionAnalyzer.java