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