## Subject: Re: issue with permeability
Posted by thomas on Tue, 21 Mar 2017 20:50:25 GMT

Dear Vamsi,

the permeability calculation requires the ChemAxon pKa plugin to be in the class path, because it considers the charged fraction of the molecule at pKa=7.4. I missed to disable the 'permeability' checkbox in the calculate properties dialog, if the chemaxon classes are not available, which usually is the case in the open-source version. If you have a license to the ChemAxon plugin you may put it into the class path (at least on Mac and Linux). But this still requires some effort and is described somewhere else in this Forum.

For the fuzzy score please refer to the manual that you find when you open the 'Fuzzy Score' dialog and press the Help button.

Hope this helps, Thomas