Subject: openchemlib-js
Posted by Dennis on Wed, 02 May 2018 06:06:52 GMT

The source code of Datawarrior shows that Thomas Sander wrote (almost) the entire program. Thanks for that, it's a very nice piece of work.

On 'github.com/Actelion/openchemlib' a part of the source code of datawarrior is hosted and on github.com/cheminfo/openchemlib-js', this is converted into javascript. Could you tell me how all is correlated and how Datawarrior is part of this?

Subject: Re: openchemlib-js
Posted by thomas on Sat, 05 May 2018 12:34:51 GMT

Hi Dennis,

openchemlib is basically the chemistry informatics engine behind DataWarrior. It contains classes to handle molecules, to perceive rings and stereochemistry, to canonicalize molecules, to interconvert to smiles and molfiles, to calculate similarities, to do substucture matching, to to visualize and edit 2D-molecules, etc. It has a BSD open source license, which means that anybody can use the source code for any purpose.

DataWarrior as an end-user application brings the functionality (and more) to the the user. DataWarrior is practically a superset of OpenChemLib. Its source code has a more restrictive license (GPL3), which requires derived software to publish any additional code also under the GPL3 license. This way it is difficult to make a commercial product out of DataWarrior and to charge large sums of money just because somebody added a tiny feature. Those files, which are part of OpenChemLib, of cause, can still be used under the BSD license.

openchemlib-js is a derived JavaScript based version of OpenChemLib. It is maintained by people at EPFL und also BSD licensed.

Hope this clarifies it,

Thomas