chem-bla-ics

Be in my Advisory Board #1: being a good Open Science citizen

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Abstract

I recently saw that blogger.com blogs gained a poll feature. From now on, I will try to be a bit more Open Science, in addition to Open Source. From now on, you can be in my Advisory Board. To do so, vote on my next chemblaics (aka Open Source Chemoinformatics) project. The poll can be found on the left side of this blog.

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Finishing the new JChemPaint code

Goal of this option is to use the code written by Niels in his ProgrammeerZomer project to implement a new JChemPaint based on Java2D and independent of the widget set used (Swing/AWT/SWT/...).

CML-roundtripping of the CDK data model

The goal of this project is to ensure that all information the CDK data model can hold can be roundtripped in CML.

##Integrating InChI-NestedVM in Bioclipse Rich is, besides an excellent blogger, also someone who is not afraid to try new things. Recently, he experimented with compiling the InChI library into a Java executable . Bioclipse already is able to generate InChIs, using the code written by Sam Adams for the CDK, but a InChI/NestedVM plugin for Bioclipse could make a nice show case.

Writing CDK News articles

On the other hand, you might find that I should focus on getting a new CDK News issue out, for which we are stilling lacking (finished) contributions.

It's up to you. Deadline in about two weeks; still got some other things to finish :)