chem-bla-ics

Open Source, Open Data at the European Bioinformatics Institute

Egon Willighagen

Published December 7, 2007

Citation

Willighagen, E. (2007, December 7). Open Source, Open Data at the European Bioinformatics Institute. *Chem-bla-ics*. https://doi.org/10.59350/dw744-0sa70

Keywords

Bioinfo, Jchempaint, Jmol, Bioclipse

chem-bla-ics

I was pleased to hear that Christoph will move to the EBI early next year. Christoph has been working on Open Source and Open Data chemoinformatics since at least 1997. I first got in contact with Christoph when I wrote code for JChemPaint (which Christoph developed) to be able to read Chemical Markup Languages (CML). This also got me into contact with Dan Gezelter who is the original author of Jmol, to which I also added CML support. And, of course, with Henry and Peter, who first developed CML. This was **before** XML was an official recommendation, and I have worked with CML files which you would no longer recognize. It was in Dan's office that the CDK was founded, where Christoph, Dan and I designed data classes to replace the JChemPaint and Jmol data classes. Both JChemPaint and Jmol were rewritten afterwards, but for Jmol it was later decided that more tuned classes were needed to achieve to required performance for the live rendering of tens of thousands of atoms.

Well, Christoph has done many other Open Source and Open Data stuff, including the NMRShiftDB, Bioclipse, and Seneca, a tool for computer-aided structure elucidation (CASE). The scientific impact for Christoph's work is considerable. When I realize that much of his past work was setting out foundations, and that these foundations have found the be solid, I am happy to hear that he can now start to apply his work to life science problems, where current methods are failing.

Christoph, cheers!