chem-bla-ics

The Open Science Notebook 10 years ago

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So, with all these people blogging about the Open Science Notebook (yes, each word is one distinct blog) it is worth looking back in time. To make clear what I put under the OSN: a notebook in which experimental details and outcome are written down. So, what did the OSN look like almost ten years ago?

It looked like the early open source chemoinformatics projects, such as CompChem and JMDraw set up by Christoph (the SourceForge projects have, unfortunately, been deleted; so I cannot link to the original project pages). JChemPaint and Jmol also originate from those years.

These projects were OSNs *avant le lettre*: an experiment in chemoinformatics is the definition of a new (or reformulation of an old) algorithm, writing down the experiment (source code in this code), uploaded into a repository (Open Science!) for everyone to comment on, possible sent around an announcement for discussion to mailing list, and reporting the outcome (preferable in a peer-reviewed journal). While I am ranting^Wtalking about the issues, chemoinformatics is in the luxurious situation that reproducibility of a procedure is **much** easier, except for the missing data part .

Just wanted to say that OSN is really nothing new, not to chemistry anyway. Maybe for lab chemists. Jean-Claude has shown to be very successful in promoting these open science ideas among lab chemists, and congratulate him with the exposure in all those magazine interviews lately. Cheers!

Open Science versus Open Source

Oh, and let me make the distinction between open source in general and open science. Many of the current open source software in chemistry(/chemoinformatics) are **not** open science. Open science means that every step in the development process is open, where is many chemoinformatics programs are *dumped* into the open source sphere at the end. That is not the way it should be.

For the lab chemists: *^W is a shortcut for 'delete the previous word'*.