chem-bla-ics

Opensource Chemistry and Opensource Chemoinformatics

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The Blue Obelisk mailing list has seen an interesting discussion on ambiguity in the term 'open source', triggered by a study by Beth Ritter Guth. For example, Jean-Claude Bradley performs 'open source' science (see his Useful Chemistry blog) who is not opposed to using closed source software, while the Blue Obelisk is about 'open source' software. It seemed that this was contradicting, and Peter Murray-Rust [wp:en] wrote up a lengthy overview of the use of the term 'open'.

Now, I have been giving the 'open source' ambiguity some thinking (well, about a month or so...), and came to the following conclusions:

1. open source has the exact same meaning in both Bradley-like open source chemistry, and BO-like open source chemoinformatics
2. both have the same goal
3. it's just the research topic that is different

Ad 1: same meaning of ‘open source’

I think ‘open source’ just means that every has the right to reproduce (and distribute and the same or modified shape) products created from the source.

In ‘open source chemistry’ (Bradley-like, sorry for the term :) the source is are the details about the chemical reactions to perform, the product being being able to run the whole reaction pathway.

In ‘open source chemoinformatics’ (Blue Obelisk-like) the source is the procedure that described how to get from one set of bits to another, really quite like getting from one molecule to another. Chemoinformatics, being IT science, just makes it a lot easier to distribute the algorithm to do that. (Sure, CMLReact is getting along quite nicely.)

The analogy even goes further, both science do not only depend on open source. Like Bradley-like open source science allows embedding proprietary stuff (glass-ware, closed-source software, chemical both from Acros (now Fisher), …), so does BO-like open source science, which uses tons of proprietary stuff too (computers, Sun’s JVM, MS-Windows).

Ad 2: same goal

I can be short on this one. For both ‘open source’ initiatives the goal is to share knowledge and make science reproducible.

Ad 3: different topic

So, the confusion was just coming from the fact to what extend ‘open source’ tools are being used. Can you do open source science without using open source chemoinformatics? Sure. In a utopic situation, all tools and small bits are ‘open source’ (though some are agnostic to this). But fact is, that many Blue Obelisk members use ‘closed source’ tools all the time, even if they do not have too. At least everyone is doing ‘open source’ on their specialisms, both in open source chemistry and in open source chemoinformatics.

I guess we should just be stop being short on ‘open source software’ to remove any ambiguity of the term ‘open source’. As a spin-off, this would make Bradley’s work fit in nicely with ODOSOS: open data, open source, open standards.