

# I don't blame Individuals in Commercial Chemoinformatics



Published December 13, 2007

## Citation

Willighagen, E. (2007, December 13). I don't blame Individuals in Commercial Chemoinformatics. *Chem-bla-ics*. <https://doi.org/10.59350/c2vv2-thb23>

## Keywords

Openscience

## Abstract

The comment I left in the ChemSpider blog, was probably a bit blunt. ChemSpider announced having licensed software from OpenEye. I have seen such announcements more often, but am intrigued about the nature of such announcements. Is it bad that ChemSpider is using OpenEye software? Certainly not.

## Copyright

Copyright © None 2007. Distributed under the terms of the [Creative Commons Attribution 4.0 International License](#), which permits unrestricted use, distribution, and reproduction in any medium, provided the original author and source are credited.

The [comment I left](#) in the [ChemSpider](#) blog, was probably a bit blunt. ChemSpider announced having licensed software from [OpenEye](#). I have seen such announcements more often, but am intrigued about the nature of such announcements. Is it bad that ChemSpider is using OpenEye software? Certainly not. But it is surprising that they “*announced today they had entered into an agreement that will **allow** the incorporation of a number of OpenEye’s products into ChemZoo’s online chemistry database and property prediction service, ChemSpider*” (emphasis mine).

Is it really special that you buy software and then use it? Maybe, it increasingly is, with a number of good software products freely available. Even many proprietary products are freely available, sometimes to a selected group only, though. Or, is there some license behind this that restricts you in what you may and may not do with it?

Anyway, I made the somewhat inconsiderate comment: “*Amazing! (Forgive me that I [have] not read every bit...) But, amazing! A press release for the fact that one may use software ;)*”.

Anthony replied with these lines: “*Yes, I think it is amazing that companies of this caliber are willing to provide their tools at no cost to systems like ChemSpider*”. He read my sarcasm correctly. I find it absurd that the future of chemoinformatics is left to the goodwill of benevolent companies. Chemoinformatics is way too important, and in way to crappy state, to be kept as proprietary toy to industry; that’s [something I argued before](#) .

Let me try to explain where my sarcasm is coming from.

## I do not blame Individuals in Commercial Chemoinformatics

There is nothing wrong with getting payed for what you do. I get payed for the software I develop too, though most of my contributions to the [CDK](#), [Jmol](#) or even some of my contributions to [Bioclipse](#) I have made as a hobby, in my spare time, unpaid. Nothing wrong with a good hobby, I would say.

But I do not blame people for not doing the same. Neither do I blame myself for making a reasonable living in The Netherlands, unlike all those poor bastards who struggle to make it to the next month, like [many in the United States](#). But I do not like the situation. Neither do I blame people for being religious, though I really dislike several of the things the *Church* is trying to make people believe (such as that [the HIV virus can get through condoms](#)). I hate the situation.

## I do not dislike the Commercial Model

People have to make a living. I do; anyone does. I do feel, however, there is a difference between making a living because you work, and getting money because you happen to be at the right side of the money flow. There is a difference between a baker getting up at 5am every morning to feed a village, and someone selling a thin slice of bread via eBay to a poor African

soul who just received his/her OPLC laptop. Not that I think this really applies to the ChemSpider/OpenEye deal; just to make a statement about commercialism.

The Bill Gates foundation spending a lot of money on scientific research is what Dutch would call **een sigaar uit eigen doos**. This translates to something like getting a present you paid yourself. Literally, 'to get a cigar from one's own box'. But that's another story.

## I hate the situation

I hate the situation that research for new drugs is so expensive, and medicine likewise. I hate it that the pharmaceutical industry cannot sell these drugs cheaply to development countries, because they will be sold expensively in western markets. But I do not blame the scientists working in the pharma industry.

I hate the situation that scientific results cannot be reproduced independently, because software is being used as a black box. But I do not blame the guy who wrote the code.

I hate the situation that I cannot contribute the excellent products around, because they disallow me to discuss my work with others. But I do not blame the guy who sold me the license.

I hate the situation that many very qualified scientists have to find a post-doc after post-doc before they give up and do to industry. I hate the situation that the better scientist you are, the less science you actually do, because all time is spent on getting further funds. But I do not blame those who pay for those temporary post-doc positions.

I hate the situation that people have to use commercial models for their scientific contributions, just to make a living, even though they would have loved to contribute that to mankind. But I do not blame them for wanting to be able to fulfill their primary living requirements (and those of their families).

I hate the situation I review papers for free for commercial publishers, just to help science progress. I do blame myself for not having stopped doing that yet.

But I do not blame ChemSpider for buying or using commercial products. I do not blame the people working at OpenEye for making a living. But I do find it absurd that we have to be amazed that scientific software is put to work.

I apologize for being blunt, but I cannot apologize for disliking the current situation chemoinformatics is in.