

Conflict of Interest. Or why I am stepping down as Editor-in-Chief of the *Journal of Cheminformatics*.

In this open letter, I will explain why I intend to step down as Editor-in-Chief of the *Journal of Cheminformatics*, which also happens to be a Springer Nature journal. It took me two years to come to this decision, and it cannot be claimed that I did not carefully evaluate the various aspects of it. However, I have now come to the conclusion that the opportunity it gives me to implement my ambition to shape open science chemistry now conflicts with the interests of Springer Nature. I will here outline some of the things I have taken into consideration.

The *Journal of Cheminformatics* has done and is doing important work to enable Open Science in the field of cheminformatics. This started with [being a CC-BY Open Access journal](#), for more than 10 years already. But the founders of the journal, David Wild and Christoph Steinbeck also set out to promote Open Science, and particularly for the science described in the articles. Over the years, the details about open grew and now the journal's expectations are high: full access to open source and open data where these are needed to reproduce the claims in the article. And being operated by BioMed Central (now BMC), the journal benefitted from their early innovation, like the policy that all data in the article is CC0, the XML download button, etc.

When I [became](#) Editor-in-Chief of the journal in 2016, it was because of the ambition of the journal and the platform it gave me to further Open Science in cheminformatics and in chemistry in general. Rajarshi Guha and I have been discussing and exploring options on how to make the journal articles more powerful and more supportive of Open Science. We set up a Twitter account, a GitHub organization, we started forking git repositories cited in the publications, we proposed ORCID identifiers for all authors (to put research better in their context), etc. In this role I am expected to attract new and old authors to submit their research. And I honestly believe the journal has unique features to offer. I am proud of the Citation Typing Ontology working our journal started.

BMC as part of Springer was merged into Springer Nature [in 2015](#). The *Journal of Cheminformatics* became just another journal under the same publisher as *Springer Nature*. And this merger is where the story of the *Conflict of Interest* starts (see Figure 1).

After the merger, I observed a number of changes. First, merging of platforms. That makes sense and can benefit the various original publishing groups. Indeed, an example is that the *Journal of Cheminformatics* now uses the same website platform as the Nature Research journals. This caused problems. Not all of our articles showed up properly. And at least one author saw essential research get misrepresented in the new layout of the article. But we have seen many smaller issues too, some of these that took months to get solved. This really hurts the quality of the journal and is one that I find hard to defend with a journal with an article processing charge (APC).

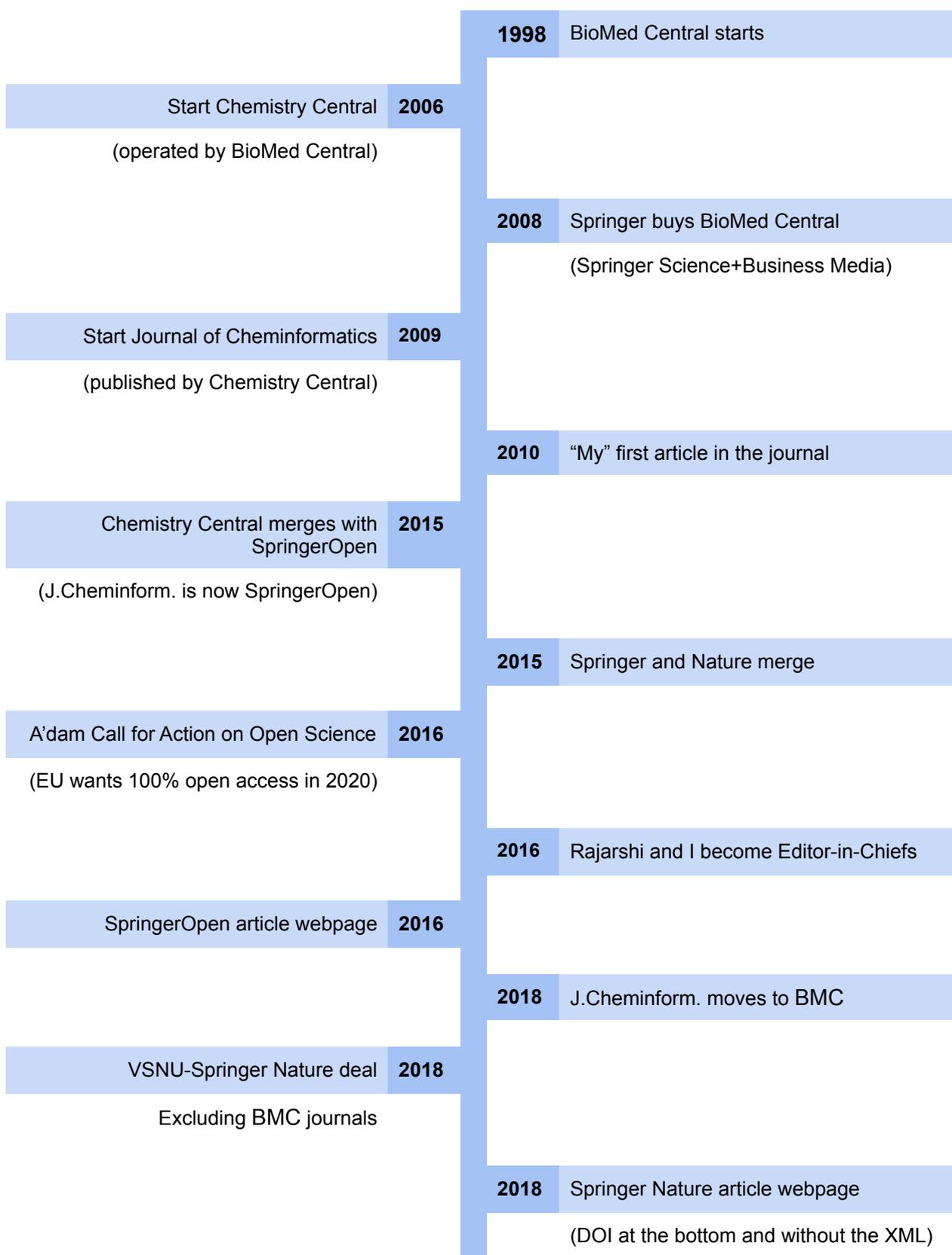


Figure 1: A sketch of the timeline looks like this (several years are clickable for a reference).

Another BMC feature that was lost in the migration is the ability to download the source code of the article, the underlying XML (see Figure 2). This XML simplifies text mining, and if Open Science is about making reuse and collaborations easier, then providing source code to things is just an essential aspect. The same pattern we see with the ReadCube functionality in the new web interface. ReadCube is a format that makes text mining impossible: earlier versions allowed me to extract text, but this was lost in later versions. We already have PDFs to make articles look alike, and am still unsure what benefit ReadCube has to the scholarly community.

The screenshot shows the article page for "The Spectral Game: leveraging Open Data and crowdsourcing for education" in the Journal of Cheminformatics, Volume 1. The page is marked as "Open Access". The authors listed are Jean-Claude Bradley, Robert J Lancashire, Andrew SID Lang, and Antony J Williams. The abstract states: "We report on the implementation of the Spectral Game, a web-based game where players try to match molecules to various forms of interactive spectra including 1D/2D NMR, Mass Spectrometry and Infrared spectra. Each correct selection earns the player one point and play continues until the player supplies an incorrect answer. The game is usually played using a web browser interface, although a version has been developed in the virtual 3D environment of Second Life. Spectra uploaded as Open Data to ChemSpider in JCAMP-DX format are used for the problem sets together with structures extracted from the website. The spectra are displayed using JSpectView, an..."

Figure 2: The 2009 article webpage allowed readers to download the article in the “source” XML format, perfectly fitting the open science approach.

In my opinion, these things conflict with the interest of the journal. It conflicts with the principles of Open Science. That makes my job as Editor-in-Chief feel really awkward. If we decide to reject articles that do not comply with our journal standards, I feel uneasy when the journal website starts to stop caring about Open Science ideas. For example, what if the CC-BY license is no longer enough to get access to the source of the article or to even see the article because one must accept cookies first? The journal requires research to be available without the need to log in somewhere, to ensure the science to be readily available. Hiding half of the journal front page by default is in stark contrast with that standard (see Figure 3).

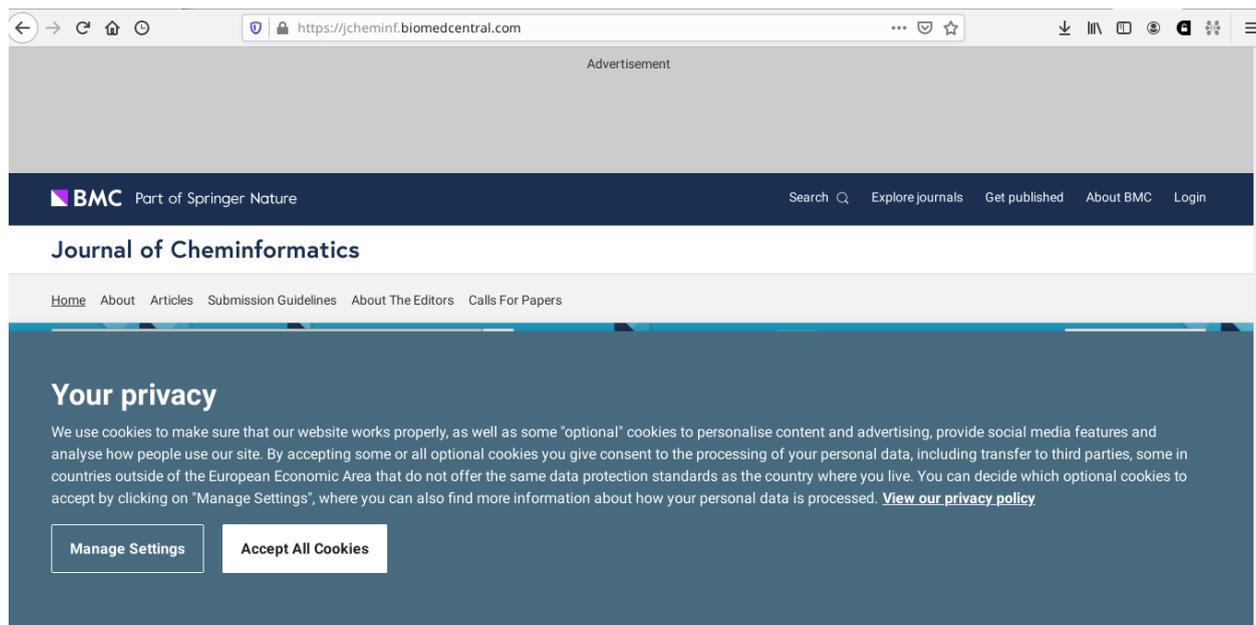


Figure 3: Half of the *Journal of Cheminformatics* website is hidden without “logging in”.

But besides these more technical aspects, there is a significant conflict of interest at a higher level. Repeatedly, Springer Nature is cherishing the idea that some journals have to be better than other journals, often associated with the impact factor. Indeed, Springer Nature still favors the more expensive journals over the most cost-efficient journals. I observe that there is a *Nature Chemistry* and *BMC Chemistry* journal. The second has a lower APC, is 100% CC-BY, and both demand high quality research (what else). And what I believe the scholarly community needs is fewer journals, not more. The impression I get is that Springer Nature does not have an interest in moving to the Open Science world sketched by BMC. Instead, it feels that more and more, BMC journals have to be like a back-up brand for the Nature Publishing Group journals. I strongly feel that science does not benefit from propagating a two-class community: one for the rich scholars and one for the rest.

This pattern seems harsh, but became reality for me with the [2018-2021 big deal](#) Springer Nature made with the Dutch universities, where the BMC journals are bluntly excluded from the deal ([since 2015](#)). The deal financially urges me to publish in a semi-paywalled journal, with lower open science standards, at a cost higher than in the BMC journal. How am I not to conclude that Springer Nature does not think the *Nature* journals are indeed more important than BMC journals. I am hopeful the new deal with the VSNU will correct this, but this should not have happened in the first place.

Why does this matter to me and my role as Editor-in-Chief? First, where I am supposed to attract authors to the journal, Springer Nature shows they do not want authors to publish in the *Journal of Cheminformatics*. Second, Dutch scholars, like me, are paying money via the overhead model for a deal where I only get something in return if I do not publish in a full Open Access journal. Again, a clear conflict of interest.

This led me to a conclusion. I can no longer have a role as Editor-in-Chief. The conflicting interests of Springer Nature and I are just too exhausting and having to explain to past, current, and future authors of the *Journal of Cheminformatics* how the Springer Nature interests make

sense is just too stressful. I am tired of seeing our efforts to promote Open Science countered by continuous support for the temporary hybrid business model: the 2016 [Amsterdam Call for Action on Open Science](#) was a call for action, because the big publishers were not moving much in the past 15 years. The *Call for Action* set a goal of 100% Open Access in 2020, which the big publishers were unable to reach in 5 years. While Springer Nature has [now joined the cOAlition S ideas](#), this is still decades away from what Open Science aims for. Meanwhile, the associated APCs for some Springer Nature journals are so high, I can fund a researcher for two months for the price (not cost) of one article. And I have not seen any plans on attempting to lower the price or even cost.

I cannot be part of this conflict of interest which touches directly on my integrity as an independent scholar. I no longer have the energy to defend an APC that I cannot justify, the website that prefers looks over quality, to explain problems with our website. And at the same time demand high Open Science standards.

We have a long way to go for FAIR research output, and not the least in chemistry, a central science. The current pandemic showed the need and advantages of Open Science. What would have happened if publishers were not “kind enough” to give access to coronavirus literature. We must speed up our efforts to live up to our responsibilities to society and to our human rights.

Therefore, I will be stepping down as Editor-in-Chief of the journal on December 31 2021. In the coming months I will work with the rest of the team and I expect to serve in this role until the end of the year. I am looking forward to continuing working on promoting Open Science and on the dissemination of cheminformatics research output. I do not currently know what shape this will take. Where possible, I would be delighted if this will improve the knowledge dissemination of the journal with innovative technologies.

Egon Willighagen