J Comput Aided Mol Des (2012) 26:27–28
DOI 10.1007/s10822-011-9491-4

PERSPECTIVE

# Democratization of computational chemistry and Chem(o)informatics

**Frank K. Brown**

Received: 6 October 2011 / Accepted: 8 November 2011 / Published online: 29 December 2011


It was the mid 1980s that saw the dawn of real growth in computational chemist. There was the convergence in theory, computational power and growth in funding, both pharmaceutical and government, that paved the way for fast improvements in methods, descriptors, expert software and employment opportunities. Over the next decade most pharmaceutical and biotech companies established computational chemistry group and the industry stated to better understand the role of these groups in the overall drug discovery process. Computational chemistry was paired with crystallography and other analytical methods which allowed the experts to predict and rationalize results. This could well be the golden years for computational chemistry. However, like most technologies, the methods reach a point where they matured with slow improvements. Most of the improvements came in software ease of use or computational efficiencies.

In the mid 1990s there was real growth in chem(o)-informatics[1] due to an explosion in data brought about by combinatorial chemistry and high throughput screening. Many computational chemists expanded their skill into handling and modeling large datasets. These models proved useful in guiding projects along the lines of team based or global models. The ability to aggregate and model data was followed by various ways to deploy the models to the desktop of the non-experts. This practice of deploying individual models to the desktop was followed by workflow tools that made automating the practice much more efficient. Now it is routine to build 100 or 1000 s of models [2] and make these models available to the enterprise via any number of ways; i.e. web apps, Excel, and SharePoint.

So, over the years discussed above software has progressive become easier to use which in turn broadened the reach and impact of the science, but where does this go from here? If you see the funding sources of both pharmaceutical companies and government agencies decreasing the way I do, then you will understand there must be a new approach to sustain this craft. The approach hinges' on the concept that was sought for years, the ability to mix and match the best of breed methods on a single platform. There will be many app store(s) for computational methods in the near future that provides a new market place of methods and models. This market place will fill the gap in funding cause by the economic downturn by providing a way to sell information, methods, workflows and models. However, this market place will not only be to sell methods and services to experts, but rather the democratization of computational science to the non-expert experimentalist. The expert consulting approach of computational chemistry will give way to a broad adaption of more routine calculations guided by rigorous processes [2] and delivered via cloud based platforms. There are several starts to this already. In addition to these more academic approaches, there are also the commercial offerings. It is after all, commercial platforms, which lead the way in app stores, Apple, Google, etc.

This more scientific app store will need to able to integrate both methods and data and then deliver this globally to a new generation of scientist that will participate in open innovation for solving complex problems. This is already underway in neglected diseases programs [3]. Cloud based software already enables these enterprises to manage projects. The next request will be for more public data related to the targets of interest to be added to

F. K. Brown (✉)
Accelrys, Inc, 10188, Telesis Court, Suite 100, San Diego, CA 92121, USA
e-mail: frank.brown@accelrys.com

the sites. This is followed by request for computational models to help rationalize the results. This will be followed by the need to provide a platform to integrated newly developed methods and models for persons from outside the original network. This will progress to create a market place for methods, data, and possibly, licensing of IP. Overall, this move to an open innovation cloud based solutions changes the power of the global science equation. Now, good ideas and recognition for those ideas will not be limited to scientist in rich and powerful companies and countries. Now, through the access offer by these new open innovation platforms, the democratization of computational science will take place. This will in turn increase the value of computational chemistry and chem(o)informatics in the global market place. This will attract more clever persons to these fields, thereby, drive the next step in innovation by accessing a global talent pool interested in advancing these fields.

## References

1. Brown FK (1998) Chapter 35. Chemoinformatics: what is it and how does it impact drug discovery. In: Bristol JA (ed) Annual reports in medicinal chemistry, vol 33, pp 375
2. Rodgers SL, Davis AM, Tomkinson NP, van de Waterbeemd Han (2011) Predictivity of simulated ADME AutoQSAR models over time. Mol Inform 30(2–3):256–266
3. Bost F, Jacobs RT, Kowalczyk P (2010) Informatics for neglected diseases collaborations. Curr Opin Drug Discov Devel 13:286–296