

Send for the Software Specialists

Matt Segall of **BioFocus DPI** argues that using drug discovery software provided by specialist developers will free up time, money and resources for the process of drug discovery itself.

With the cost of developing a new drug continuing to spiral, dramatic restructuring has taken place in many of the largest pharma companies in an effort to control costs and improve flexibility.¹ Only recently, GlaxoSmithKline announced that it plans to cut a further 350 jobs in research and development and that it is “seeking to substantially increase collaboration with external R&D partners.” In-house resources are increasingly focused on the core competencies of drug design and development, while activities that do not directly provide a competitive advantage are being outsourced to specialist providers. Examples of these activities include synthetic chemistry, high-throughput screening and compound management.

In this context, it is interesting to note that when it comes to the software that supports drug discovery, in-house platforms often still dominate. Almost unique among high-tech industries, pharma still devotes a significant effort to in-house software development. For example, the automotive, aerospace and microelectronics industries all rely on specialist developers to provide computational tools.²

In the past, it may have been necessary to develop drug discovery software in-house, because commercial software in this field was immature. However, this is no longer the case, and the principal explanation for this practice is that the costs of in-house development are often hidden and perceived as lower than the upfront costs of investing in commercial software. However, the real cost of developing, maintaining and supporting in-house software may be surprising. A software platform can take several full time equivalent (FTE) years to develop, and, as such, could run into millions. Furthermore, ongoing maintenance, evolution and support of the resulting platform may cost hundreds of thousands of dollars more. This easily exceeds the cost of many commercial software platforms.

The hidden costs are not only monetary. Specialist software developers benefit from working with many different drug discovery organisations and gain experience in developing a wide range of applications. Furthermore, developing user-friendly, intuitive software is a specialist skill. Unless all the scientists involved in drug discovery — many of whom are not computational experts — find software easy to work with, it will not be used to its full potential. Thus, intuitive commercial platforms can perform better and achieve wider adoption and impact.

Focus your efforts

In addition to the aforementioned expense of building in-house software platforms, companies developing in-house solutions risk missing out on third-party innovations. Externally developed platforms provide a widely applicable, intuitive and interactive environment that goes beyond the organisation and visualisation of data to help to guide decisions and maximise the chance of success against a project’s specific goals.

The key objective of such a platform is to focus synthetic and experimental resources on chemistries most likely to yield an optimal balance of biological and physicochemical properties, reducing wasted effort and improving the likelihood of success in development and on the market. This requires integration of data from multiple sources, including *in silico* predictions, *in vitro* assays and *in vivo* experiments. All of these data must be rigorously assessed against the success criteria for a project, taking into account both the relative importance of different criteria and the uncertainty present in data from all sources. Many organisations and drug discovery projects have benefited from this approach, as demonstrated in a number of case studies.³

Using a desktop interface that provides bench scientists and project leaders easy access to powerful computational tools can enhance the value of in-house computational scientists, as they will focus their efforts on areas that add a competitive advantage, such as modelling proprietary chemistry or targets. With the results of this work being deployed efficiently to key decision makers, the impact on the direction and success of a project is maximised.

Ultimately, better software will lead to better decisions, which in turn will generate better outcomes in terms of higher quality drug candidates, reduced late-stage attrition and improved ROI in drug discovery.

References

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