Dr Marcus Gastreich, BioSolveIT, gave this presentation at the "Streamlining Drug Discovery" symposia held in Shanghai, China on 31 May 2018 and Tokyo, Japan on 5 June 2018.

Abstract

Abou-Gharbia and Childers's 2014 J. Med Chem paper highlighted that the field of therapeutic drug discovery is rapidly changing. According to them, for example more than 1,300 mergers and acquisitions have led to enormous restructurings and widespread job losses. Additional factors such as block buster drug patent expirations, changing educational priorities, and a younger generation of researchers that have grown up with smartphones, have transformed the discipline. This new era exerts an enormous pressure on research and the necessity to adapt software. Such changes, however, must not happen at the expense of the depth of understanding and quality of our tools.

 Using an interplay of modern graphics card possibilities and novel algorithms — that exploit for example indexing, tree-based methods, or artificial intelligence (AI) methods — we can today support visual, instant hypothesis generation. Embedded in user interfaces that are intuitive and easy to learn, there is now a new generation of computational tools available to non-specialists that can cover selected tasks that previously had to be conducted by specially trained computational experts. In contrast to mere numbers, an appropriate visualization enhances the user's ability to accept or decline a computer-generated result. Overall, this change in focus leads to much faster and more informed decisions, at the same time freeing time for the specialist computational researchers to pursue those problems that require the specialist's proficiency, more efficiently.

We will give examples from (a) hit finding where synthetically accessible compounds are mined from giant chemical spaces [2], through (b) indexed rescaffolding and fragment-based ligand design (FBLD, [3]), to (c) lead optimization cases where molecular design is visually assisted in a "gamified" software environment [4].

[1] Abou-Gharbia, M and Childers, WE J. Med. Chem. 57, 13, 5525-5553, 2014.
[2] www.biosolveit.de/REALSpaceNavigator, BioSolveIT, Germany, 2018.
[3] Maass et al., J. Chem. Inf. Model., 47, 390-399, 2007.
[4] www.biosolveit.de/SeeSAR, BioSolveIT, Germany, 2018.

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