Journal of Computer-Aided Molecular Design, **16:** 767–768, 2002.
KLUWER/ESCOM

Current perspective of information technologies in drug discovery

Ferran Sanz[1] & Federico Gago[2]
[1]*Research Group on Biomedical Informatics (GRIB), IMIM. Universitat Pompeu Fabra, C/ Dr. Aiguader 80, E-08003 Barcelona, Spain;* [2]*Departamento de Farmacología, Universidad de Alcalá, E-28871 Madrid, Spain*

This special issue of the *Journal of Computer-Aided Molecular Design* aims to provide a representative sample of research activities in the area of applications of information technologies and computational tools in Medicinal Chemistry research. The published reports are based on lectures and oral communications presented at the 17th International Symposium on Medicinal Chemistry (ISMC) held in Barcelona from September 1st to 5th, 2002. The ISMC constitutes a prestigious series of scientific events organised biennially under the auspices of the European Federation for Medicinal Chemistry. The last edition of the ISMC gathered together more than one thousand scientists from fifty countries belonging to both industry and academia in approximately the same proportion.

It is well known that the discovery and development of a new drug currently requires a huge effort, about 10-12 years and 800 million Euro, and the trend towards a permanent growth of such an effort has not been reversed up to now. The intensive and relevant use of new information technologies has been postulated as a way to accelerate and optimise the drug discovery process [1]. To a large extent, information drives the development of new drugs, and the the power of computers can be harnessed to sieve vast numbers of molecules with potential medicinal value. Computational procedures include the "in silico" creation, characterization, and filtering of molecular libraries. Computer-based "virtual screening" experiments can automatically assess the fulfillment of drug-likeness criteria or pharmacophoric patterns, as well as perform the simulated docking of large series of compounds to 3D models of their potential targets. A recent extension of the virtual screening strategy is the chemogenomics approach, which aims to link both chemical and biological spaces by a joint analysis of libraries of selected ligands and related targets. It is noteworthy that early virtual screening of ADMET properties is an additional computational task that is becoming crucial for optimising the flow along the drug discovery pipeline.

The artificial confrontation between combinatorial chemistry and rational drug design is being overcome. On one hand, combinatorial chemistry is a powerful strategy that has incorporated computational tools for the rational planning and exploration of molecular diversity. On the other hand, the acceleration of pace of structural determination of protein structures in both unbound and ligand-bound forms, as well as ongoing improvements in methods for the prediction and refinement of such structures, has allowed the consolidation of structure-based methods in lead discovery and optimisation enterprises.

If we consider the technological platforms on which computer-assisted drug discovery is taking place, the emerging Grid technology offers interesting possibilities for massive computation and data sharing [2]. A phenomenon not independent of the previous one is the way in which clusters of commodity-priced computers are replacing supercomputers at a fraction of the price.

We are also becoming aware of the increasing need for collaborative tools and applications for the e-workplace, with the objective of enhancing and accelerating the sharing of knowledge in drug discovery and development projects, since they imply the participation of numerous scientists, often belonging to different organisations and almost always located in distant places.

Last but not least, it has to be pointed out that the present genomics and proteomics revolution, through the concourse of bioinformatics, is generating interesting and powerful possibilities for seminal aspects of future therapeutics such as the discovery of new potential drug targets or the pharmacogenomics-based individualization of treatment and dosage selection. In this respect, the integration of health and genomic information collected from large samples of subjects

and the subsequent data mining is a promising way to generate useful knowledge for the drug discovery and development processes.

We expect that the present collection of articles, written by some of the experts in the field, will be useful to a majority of readers and encourage further work in this exciting area of research.

References

1. Bjerrum OJ. New Safe Medicines Faster: a proposition for a pan-European research effort. Nature Rev. Drug Discov. 1 (2002) 395–8.
2. Richards WG. Virtual screening using grid computing: the screensaver project. Nature Rev. Drug Discov. 1 (2002) 551–5.