

## Editorial

Dear Readers,

The present copy of the journal Current Computer-Aided Drug Design (CCADD) is the inaugural issue of the journal. CCADD is a review journal which has been started to provide the scientific community involved in the drug design and drug discovery with a comprehensive and cohesive coverage on different topics of fast developing computer-aided drug design that may be related to the methodologies, their applications, and the end results. Since the pioneering work of Corwin Hansch in 1962-64 that laid the foundations of QSAR (quantitative structure-activity relationships) by three important contributions: the combination of several physicochemical parameters in one equation, the definition of lipophilicity parameter  $\pi$ , and the formulation of the parabolic model for nonlinear lipophilicity-activity relationships, the area of computer-aided drug design with the development of computer technology went through a revolutionary change from two-dimensional to three-dimensional and now to four-dimensional QSAR. The development became so fast that many journals were started to publish exclusively the work on QSAR with the self-indicative names such as Journal of Computational Chemistry, Quantitative Structure-Activity Relationships, Journal of Computer-Aided Molecular Design, Journal of Chemical Information and Computer Science, SAR and QSAR in Environmental Research, and so on, and various other journals related to chemistry, pharmaceutical chemistry, or medicinal chemistry, allocated ample space to publish the work on QSAR and molecular modeling. The area of CCADD now covers a large number of topics such as 2-D QSAR methodologies, its applications, 3-D QSARs and their applications, 3-D QSAR and docking, virtual high-throughput screening, structure-based drug design, scoring functions, pharmacophore analyses and 3D searches, fragment-based combinatorial library design, diversity assessment, predictive toxicology, ADME/Tox models, new descriptors, etc. However, so far no such journal has been available that may provide a comprehensive coverage with critical assessment of the day-to-day developments in these topics. The Bentham Science has now taken this step, starting a review journal Current Computer-Aided Drug Design, wherein the leading scientists from all over the world are invited to contribute the review articles on the topics in which they have expertise. Each issue would aim to publish a series of timely in-depth reviews written by leaders in the fields on certain important topics. The present issue contains ten articles covering a variety of interesting topics.

The issue starts with an article of Zhu *et al.* on the calculation log P, a molecular parameter that describes the lipophilicity of the molecules and that has been the most fundamental molecular descriptor used in the QSAR study. Various approaches have been described in the literature for the evaluation of log P, but Zhu *et al.* present in this article a new group contribution approach to the calculation of log P. While lipophilicity has been found to be a very important factor for drugs to cross the cell membrane, in article 2 Degim has discussed the skin penetration, showing that lipophilicity plays an important role in skin penetration, too. Degim's article, however, presents a detailed account of the mechanism of skin penetration. It presents a review of some of the mathematical models and techniques that have used some molecular descriptors and properties which have been constructed to predict and understand percutaneous penetration and transdermal delivery.

Next to lipophilicity, the most important descriptors of drug actions have been the electronic parameters. In article 3, Cherkasov gives an account of inductive parameters developed in the last 10 years. A number of methods derived from the original approach have been reviewed and discussed including those for 'inductive' electronegativity, 'inductive' hardness-softness and 'inductive' partial charges. Wang *et al.* then discuss in article 4 the importance of Proteomics in Computer-Aided Drug Design. Proteomics has great promise in identification of protein targets and biochemical pathways involved in disease

processes. Proteomics as a whole increasingly plays an important role in the multi-step drug-development process. In article 5, Canduri and de Azevedo Jr. discuss the relevant structural features that may guide the structure based-design of a new generation of CDK (cyclin-dependent kinase 2) inhibitors. Following Canduri's article, there are 2 excellent articles, one by Shoji (article 6) and one by Vračko (article 7), that discuss the application of artificial neural network in the drug design. While the article by Shoji surveys the applications of neural network methodologies to the field of Quantitative Structure-Toxicity Relationships (QSTRs) in environment to predict specifically ecotoxicity, the article by Vračko reviews its application not only to QSTRs but, in a broader sense, to all QSARs. In article 8, Mizushina *et al.* report the three-dimensional structural analysis of binding sites of two inhibitors (nervonic acid, NA, and lithocholic acid, LCA) of polymerase  $\beta$  (pol  $\beta$ ) and topoisomerase II (topo II), suggesting that the NA and LCA-binding domains of pol  $\beta$  and topo II are three-dimensionally very similar. In article 9, Krovat *et al.* present recent advances in docking and scoring. Parameters that influence docking results, combination of different docking algorithms and scoring functions, performance of scoring functions, docking using homology models, and ligand and protein flexibility have been beautifully examined to give an overview of the state-of-the-art methods. Besides, a survey of innovative approaches in molecular docking and scoring has been presented. Lastly, Anderson and Wright describe in article 10 the design and docking of virtual compound libraries to structures of drug targets. This review provides a detailed analysis of the use of virtual library screening (VLS) in the drug discovery process. I thank all the authors of this issue for their excellent stimulating contributions and hope that readers will greatly enjoy reading these articles as I did and that these contributions will be of great value to those involved in the area of drug design.

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