Research and Reviews: Drug Delivery

Computer-Assisted Drug Design Future Challenges and Perspectives

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Commentary

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DESCRIPTION

Computational drug design is a rapidly growing field which is now a very important component in the discipline of medicinal chemistry. At the same time many medicinal chemists lack significant formal training in this field and may not have a clear understanding of some of the terminology used but need to grasp concepts, follow research results, define problems for, and utilize findings of, computational drug design.

In this context the IUPAC Medicinal Chemistry Section Committee felt it would be useful to develop a glossary of terms in computational drug design for easy reference purposes. Also there is the possibility that in different countries certain terms may not have the same meaning and in such a case there would be value in trying to establish an international definition standard. Accordingly a Working Party of seven experts in the field was assembled who constructed a glossary of some 100 terms. Concise but sufficiently explanatory definitions have been formulated based on a variety of literature sources and selected key references provided.

CADD is an exciting and continually evolving area that leverages new data and methods to provide approaches that tackle the ever-changing needs of drug discovery. The scope continues to grow, and applications now span the whole drug discovery process. The availability of experimental data for model building for multiple endpoints or selectivity targets enables CADD to tackle the needed multidimensional optimization challenge, and a combination of models for the different endpoints can be used, together with a variety of methods. This creates the need for

improved methods to achieve such optimization using predictive models, with both a prediction and confidence level in the value being important. Models that alone may be of less perceived value as the user has a good understanding of the structure activity can be used simultaneously in a multidimensional way to search exhaustively large numbers of possible structures and structural changes to identify more optimal solutions (e.g., potency with selectivity and desired properties). The methods and approaches used have expanded enormously, and now include areas such as data mining; the amount of data that is now electronically available, such as structure activity data, is ever increasing, with the addition now of records from published journals and patents, as well as commercial databases and in-house data from HTS. Probabilistic modeling approaches like Bayesian statistical models that can be rapidly used to analyze large and noisy data sets, to give predictive models that can be applied to the next iteration of experimental work enable CADD to further impact areas such as HTS analysis, library design, and virtual screening.

Protein structures continue to become more available, and the methods and force fields are also developing for SBDD, with one goal to be able to predict accurately ligand-binding energies/affinities. SBDD will thus continue to be an increasingly applicable enabling approach in drug discovery, considering both the target and off-/anti-targets. The existence and importance of poly-pharmacology for many drugs, affecting potentially the efficacy and the adverse effects, have been highlighted by the systematic analyses of drugs against multiple. Such data, that show how very similar compounds, that could be considered the same ‘chemotype’ as there are only relatively small changes to substituents, can have very different broad biological profiles, offer new challenges to CADD to explain and predict such differences, with the realization that ‘selectivity targets’ may be in quite different target classes.