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Future Challenges Involved in Computer Assisted Drug Design and its Optimization

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Commentary

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DESCRIPTION

CADD is a fascinating and constantly developing field that uses fresh data and techniques to offer solutions to the ever changing needs of drug discovery. Applications now cover the entire drug development process, including the utilisation of biological fingerprints, attrition prediction, and the modelling of *in vitro* data to predict *in vivo* effects. CADD can handle the necessary multidimensional optimisation challenge since experimental data for model construction for many endpoints or selectivity objectives is available. A combination of models for the various endpoints can be used, as well as a range of techniques.

As a result, there is a need for better strategies to use predictive models for such optimisation, where both the accuracy of the prediction and the degree of confidence in the value are crucial. When a user has a solid understanding of the structure activity relationship, models that alone might not be as valuable can be utilised in tandem to exhaustively search through a huge number of potential structures and structural alterations to find more effective solutions (e.g., potency with selectivity and desired properties).

With the addition of records from published journals and patents, as well as records from commercial databases and internal data from HTS, the methods and approaches used have greatly expanded and now cover areas like data mining. The amount of data that is now electronically available, such as structure activity data, is also constantly growing. CADD can have a greater impact on areas like HTS analysis, library design, and virtual screening thanks to probabilistic modelling techniques like Bayesian statistical models, which can quickly analyses large and noisy data sets and produce predictive models that can be used in the subsequent iteration of experimental work.

With the aim of being able to precisely forecast ligand binding energies/affinities, protein structures are becoming more readily available, and methodologies and force fields for SBDD are also evolving. As a result, SBDD will continue to be a useful enabling strategy in the drug development process, taking into account both the target and off/antitargets.

The comprehensive assessments of medications against many targets have brought attention to the existence and significance of polypharmacology for many drugs, potentially impacting efficacy and side effects.

These data present new challenges for CADD to explain and predict these differences given the realisation that "selectivity targets" may be in very different target classes and that very similar compounds, which could be considered the same "chemotype," can have very different broad biological profiles.

The reader is urged to take into consideration all of the methodologies discussed in this volume, both the more established and the relatively new ones, in order to address the unique requirements of each medicinal chemistry project.

The very wide range of CADD related approaches is still expanding, and fresh new ways are constantly being introduced. The effects on drug development should increase as CADD develops to incorporate the new techniques and data available, spanning the entire process from the identification of appropriate targets and hits through the differentiation and attrition of clinical candidates.