Application of Computational Techniques in Drug prediction research

Aim &Scope:

Humans have used small molecule drugs to treat diseases for many years, while many protein relation research techniques have been developed to study the interaction between small molecule compounds and protein molecules, particularly they are helpful to find targets and develop new drugs in the medical areas. Apart from these, drug studies also can help researchers explore the link between biomolecules in the biological field, for example, drug-target interaction, association of medicinal molecules and non-coding RNAs, drug-drug interaction, drug-pathway interaction drug-side effect association. Especially, drug-target interactions can help researchers find drug-target mechanisms of function and have a more particular knowledge of the physiological activity of the living body. Due to the fact that the researches of drugs in the biological field and medical field are costly and time-consuming in particularly, many computational techniques are proposed to learn drug function mechanism, which could save lots of time and money. Computational models generally rely on various data information, but biological data have been gradually enriched in recent years which are limited to material conditions. These computational methods not only provide new directions for experimental scientists but also narrow the scope of candidates to accelerate drug discovery. Therefore, it is necessary to develop effective computational methods to uncover potential drug-target interaction prediction, small molecules and non-coding RNAs interaction prediction. Then, biological experiments could be implemented for validation based on the prediction results with higher predicted scores.

We will invite investigators to contribute reviews describing recent findings which use computational techniques for the research of drug prediction. The manuscript submitted to our special issue should discuss some analysis of the results by comparison with some published experimental studies.

Potential topics include: (1) Drug–target interactions prediction; (2) Drug combinations prediction; (3) Drug-drug interaction prediction; (4) Anticancer drug response prediction; (5) Drug-pathway interaction prediction; (6) Small molecule-non-coding RNA interaction prediction; (7) Drug-side effect association prediction; (8) Computational models for drug repurposing

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