The current status of computational screening of chemical libraries for druggability prediction : Accuracy and Speed

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Abstract

The appearance of new disease-causing viruses (such as SARS-CoV-2) and multidrug resistant variants of microorganisms is demanding for urgent drug discovery. The traditional drug discovery approach involving experimental high throughput screening requires more than 10 years of time and investment cost in the range of billion dollars. The computational approaches can be effectively used to make the drug discovery cost effective and less time demanding. The number of compounds to be considered for in vitro validation and clinical trials can be reduced to a few hundreds with the use of computational virtual screening approaches. Over the last few decades multiple scoring functions were developed to rank the compounds from chemical libraries. The successful identification of the lead compounds however depends on the size of the chemical libraries and accuracy of the scoring functions. The size of chemical libraries is growing in size and using the typical computers for screening of such chemical spaces requires enormous time. However, thanks to parallel virtual screening algorithms and their implementation in high performance computers (HPCs) and graphical processing units (GPUs) the screening speed can be increased by many fold.[1] In this presentation, different scoring functions currently available for ranking chemical compounds[2,3] will be discussed along with some details on different parallel implementations of virtual screening algorithms in HPCs and GPUs. The contributions from our own laboratory[4] in this subject will be discussed briefly at the end.

Key words: Druggability prediction, Virtual screening, Chemical space, Parallel virtual screening, Scoring functions.

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