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Virtual Screening Approach as a Potent Technology in Drug Design Campaigns. Methods, Applications and Computational Perspectives.

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In recent years the Virtual Screening (VS) has become increasingly popular, as a alternative approach to HTS in the pharmaceutical and academic researches, especially in hit discovery and lead optimization [1,2].
VS is a technology using high-performance computing to analyze large database of chemical compounds to identify possible drug candidates (top-ranked hits) for biological evaluation [3]. Virtual screening methods could be divided into structure-based and those using active compounds as templates (ligand-based VS). The type of methods used in VS are strongly dependent on information available as an input. Hence, a lot of different approaches to VS are known, combining one or more methods in one protocol. A broad range of computational techniques (e.g. 2D fingerprints, 1D molecular descriptors, docking and scoring, pharmacophore similarity search, clustering), machine learning (e.g. ANN, RF, SVM, NBC, SOM, BKD, etc.) and statistical (e.g. PCA, DPD, ROC) methods can be applied [4].
Here, we show our implementation of multistep approach to virtual screening (mVS) of commercially available compound libraries. The databases of the largest vendors such as Enamine, ChemBridge and ChemDiv have been analyzed, adopted and used as a molecular screening space (approx. 3M compounds). Some examples are provided to further demonstrate the effectiveness of this technology in hit discovery [5].
In order to increase the overall efficiency, the mVS is still extensively expanded and great efforts are being made to develop and validate new tools, methodology and infrastructure.

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