



QSAR-Based Studies for Drug Repurposing

10

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Abstract

The search for new therapeutic agents is a constant endeavor. The synthetic drug pipelines are drying out, and now the clinically established agents are being evaluated for other ailments. Drug repurposing, drug reprofiling, drug repositioning, or therapeutic switching is a method in which drug development for a new indication starts with an already known drug. Repurposing could reduce the 10–17 years' process to 3–12 years. This facilitates the circumvention of several pre-approval assessments necessary for a newly developed medication. Inclusion of novel informatics approaches and systems biology to reveal unknown targets or mechanisms of approved drugs improves drug repurposing methods. A combination of both, computational and experimental, assays is desirable to repurpose drugs for new indications. A computational platform and algorithm, a comprehensive database and toolset, resource for protein sequence and functional information are the essentials for drug repurposing. Various approaches in computer-aided drug design processes are proving effective in the design of new molecules, virtual screening, and lead optimization. The approach could be furthered by sequence alignment, molecular docking, and molecular dynamics simulations. Thus, computational screening for repurposing of drugs has become a vital approach in the development of new therapeutic agents, offering significant reduction in time, investment, and an improved success rate.

Keywords

Drug repurposing · Computational screening · Ligand-based · Target-based · Quantitative structure activity relationship—QSAR

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257