Tentative Outline

Special Issue for Current Medicinal Chemistry

Guest Editor: Kerly Fernanda Mesquita Pasqualoto

Computer-aided approaches and innovation: how to accelerate drug development

Aims & Scope:

The use of computer-aided drug design (CADD) strategies and methods in the early stage of drug development can avoid the synthesis of thousands of compounds, driving the efforts to more promising compounds, having more suitable pharmacodynamic and pharmacokinetic features and low toxicity, as well. Because of that, the number of biological assays to be performed would also be reduced decreasing the use of animal experimentation. Therefore, the radical innovation workflow would be less time-consuming and less expensive, increasing significantly the chances of success to reach the final product. Many promising molecules have failed into the clinical trials, though, mostly because they show unfavorable pharmacokinetic properties or cause adverse reactions in humans. In this regard, there is an urgent need to identify successful treatments for many diseases, such as cancer, neurodegenerative, inflammatory, orphan and neglected diseases, in innovative ways that could overcome those drawbacks. Drug repositioning, or repurposing, is the process of finding new uses outside the scope of the original medical indications for existing drugs or compounds. It represents a novel and promising direction to accelerate drug development, because the safety profiles of the candidates for repositioning. The clinical trials for alternative indications are cheaper, potentially faster and carry less risk than de novo drug development. In this Special Issue, computer-aided approaches, strategies, challenges and perspectives are highlighted in order to provide an overview regarding the potentialities of the in silico tools to effectively drive the drug repositioning offering innovative and alternative treatments.

Keywords: computer-aided drug design strategies; drug discovery; drug repositioning or repurposing; molecular modeling; virtual screening; network based methods; QSAR/QSPR approaches; SAR approaches; molecular docking; target based strategies; ligand based strategies; polypharmacology; machine learning algorithms; topological graph theory; protein-protein interactions; enrichment analysis; connectivity map; microarray data analysis; chemoinformatics; computational biology; bioinformatics.

Sub topics:

1. Drug repurposing: changing the landscape of academic drug discovery
2. In silico drug repositioning with a purpose: strategies and challenges
3. Web-based tools to drive drug discovery: successful examples of collaborative research
4. Advances in computational biology and systematic drug repositioning: network-based methods
5. Effective strategy for drug repositioning: identification of new drugs against cancer cell signaling pathways
6. Technologies and repurposing drug strategies for orphan diseases

Tentative Publication Date: May 2018