Special Issue

Computational Drug Repurposing

Message from the Guest Editors

Computational drug repurposing, i.e., finding new treatments for diseases using FDA approved drugs via computational methods, is one alternative method for increasing the efficacy of pharmaceutical research. Using modern computational tools to narrow the search for efficacious drugs from a pool of drugs greatly decreases cost. Furthermore, since all of the drugs being considered are FDA-approved, their toxicity and side effects profile are known, and the time from bench-to-bedside for a new indication is reduced as they have already been subjected to clinical trials. Though many different approaches are being taken for drug repurposing, there has been no effort to assemble a comprehensive collection of knowledge of this field, specifically focused on computational methods, to have as a reference for novices and experts alike. In this Special Issue of Pharmaceutics, an understanding of how state-of-the-art computational drug repurposing methods make the drug-discovery process more efficient, as well as the juxtaposition of drug repurposing and drug-design methods, will be comprehensively explored.

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