Computational Drug Repositioning: A Review on Databases and Approaches

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Abstract: Data in the biological, chemical, and clinical domains are accumulating at ever- increasing rates and have the potential to accelerate and inform drug develop- ment in new ways [3]. Challenges and opportunities now lie in developing analytic tools to transform these often complex and heterogeneous data into testable hypotheses and actionable insights. This is the aim of computational pharmacology, which uses *in silico* techniques to better understand and predict how drugs affect biological systems, which can in turn improve clinical use, avoid unwanted side effects, and guide selection and development of better treatments [1][2]. One exciting application of computational pharmacology is drug repurposing finding new uses for existing drugs. Repositioning of previously approved drugs is a promising methodology because it reduces the cost and duration of the drug development pipeline. Computational repositioning is especially appealing because of the ability to rapidly screen candidates in silico and to reduce the number of possible repositioning candidates [4]. What is unclear, however, is how useful such methods are in producing clinically efficacious repositioning hypotheses. Furthermore, there is no agreement in the field over the proper way to perform validation of in silico predictions, and in fact no systematic review of repositioning validation methodologies.we review the computational repositioning literature and capture studies in which authors claimed to have validated their work. Our analysis reveals widespread variation in the types of strategies, predictions made and databases used as 'gold standards'. We highlight a key weakness of the most commonly used strategy and propose a path forward for the consistent analytic validation of repositioning techniques.

Keywords: drug repositioning [1], network [2], computational method[3], drug-disease[4]

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