Identifying a Potential Novel Obesity Drug Candidate Using Bioinformatics

Abstract

The application of bioinformatics to drug discovery and repurposing is becoming increasingly prevalent. Using applications based on the L1000 database, a resource containing gene expression changes observed in human cell-lines perturbed with small molecules, the time and resources required to search for potential novel or repurposable drug candidates for a wide range of diseases has significantly decreased. In this work, potential drug candidates for the treatment of obesity were screened using the L1000 Characteristic Direction Signature Search engine ($L1000CDS_2$) and the Connectivity Map (CMap) method. A commercially available compound, currently in preclinical trials for cancer treatment, was found to be a high-ranking perturbagen in both of the aforementioned screenings. After performing functional enrichment analysis using Enrichr and Touchstone applications, it was revealed that this compound is strongly connected to mechanisms of action relating to the treatment of obesity. Various biological pathways possibly relating to obesity were also identified. The results of this study provide promising future research for this potential novel anti-obesity drug. As a step further, a theoretically more potent compound was also proposed. This paper also provides insight and guidance into different *in silico* methods of screening for potential drug candidates, a base for future AI-driven drug discovery.