A Novel Approach on G6PD Enzyme Deficiency Treatment: Drug Repurposing

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Around the globe, G6PD enzyme deficiency is one of the widely-encountered diseases. There are more than 140 variants but the Mediterranean variant is commonly seen in the world. Therefore, there is no adequate treatment for this enzyme deficiency. Based on researches, G6PD enzyme deficiency patients might have hemolytic crisis by taking some substances into the body. Hence, the intake of substances leads to serious disorders in body. Avoidance of these substances as a treatment method can reduce the risk of hemolysis on a large scale. In this project, we aimed to increase the quality of patients' lives, showing drug repurposing as a treatment method without limiting the intake of those substances. To achieve this purpose, we used free and available bioinformatics databases. We have downloaded molecular structures of G6PD enzyme and modeled Mediterranean variant mutation. Additionally, we have analyzed molecular interactions between the mutant enzyme and selected molecules. Using AutoDockTools has enabled us to observe a lot of interactions. After determining the molecules with the highest scores, structurally similar compounds are detected from ChemMineTools. New molecules are simulated on these databases and the final affinity scores are compared. According to results, folic acid has the highest score in the first molecules group. Also, methylene blue has the highest score as a negative molecule. Based on the last data, structurally folic acid similar molecule CID 123321736 has the highest affinity scores of all the molecules. In this project, CID 123321736, which is a molecule with patent for ophthalmological diseases, is suggested for treatment of enzyme deficiency based on its affinity scores. This shows drug repurposing as a treatment as it is aimed.

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