Algorithm and Software Development Analysis of various softwares and their authenticity, using docking techniques for inhibition of the enzyme G6PD to prevent the growth of malarial parasite, *Plasmodium Falciparum*

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Of the four species of Plasmodium, mortality in human is caused by *Plasmodium falciparum*. This parasite is killed by the oxidative stress produced in the erythrocytes due to the inhibition of enzyme G6PD (Glucose 6-phophate Dehydrogenase). During normal detoxification, H_2O_2 is converted to H_2O, which is catalysed by the enzyme glutathione peroxidase. This Conversion requires NADPH produced during the G6PD catalysed reaction. The mechanism of action of the antimalarial drugs, like primaquine, is to inhibit the G6PD enzyme, thereby,

increasing the toxic H_2O_2 concentration in the RBCs which is toxic for Malarial parasite. In this work, we perform the docking of various compounds on G6PD using some of the widely used docking softwares. These dry lab results are then compared to the wet lab results. We can observe that the dry lab results show deviation from the wet lab results. The deviations of results, obtained with different softwares, are statistically analysed. Upon analysis, the software which shows results closest to the wet lab experiments is designated to be the most authentic of the other softwares.