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In Silico Evaluation of Potential Anti-malarial Plant Metabolites

Mani Jain[1] and Indira P. Sarethy[2]

[1,2]Department of Biotechnology, Jaypee Institute of Information Technology, A-10, Sector-62, Noida-201307, India

Abstract—*Malaria, caused by the protozoan Plasmodium falciparum, is the cause for fatalities in many tropical and subtropical countries, despite antimalarial drugs being available. Increasing resistance to existing antimalarial drugs has necessitated the need to develop new classes of medicines for treatment of malaria. Natural products and their derivatives have been the base for the majority of currently available anti-malarial drugs. This fact substantiates that new leads can emerge from plant metabolites. This study focuses on the in silico prediction of selected plant metabolites for their antimalarial activity as well as any associated cytotoxic and other physiological effects. Based on literature, seventy six plant metabolites documented to have in vitro and in vivo antimalarial activities ranging from excellent to moderate, based on their IC50 values were selected (IC50 value<1μM, excellent/potent ; IC50 of 1-20μM, good ; and IC50 of 20-100 μM, moderate). These compounds were analysed for anti-malarial/anti-plasmodial activity using the software Prediction of Activity Spectra for Substances (PASS). Further, those compounds showing potent in vivo anti-malarial activity were analysed for possible toxic and physiological effects. Results of the analysis show that while broadly, anti-malarial/anti-plasmodial activity is predicted by PASS, the Pa<Pi (probable activity-to-probable inactivity) ratio varies as compared to in vivo studies. The results show the utility of the tool in predicting activity of compounds in a broad-based manner.*