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Lead compounds for the development of new anti-malarial form marine source: Computational approach

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Background and Aims: Malaria is a major public health problem mainly due to the development of resistance by the most lethal causative parasitic species, Plasmodium falciparum to the mainstay drugs like chloroquine. Historically, compounds containing novel structure from natural origin represent a major source for the discovery and development of new drugs for several diseases. In the present study, the aim was to discover novel, effective compounds for the activity against malaria using chemo-informatics from marine source.
Methods: marine organisms containing anti-malarial compounds were searched in sources like www.google.com, www.scirus.com, www.sciencedirect.com and www.ncbi.nlm.nih.gov. Two chemo-informatics servers (http://pubchem.ncbi.nlm.nih.gov/ search/search.cgi) and (http://cactus.nci.nih.gov/ncidb2) were used to perform similarity search with best anti-malarial compounds.
Results: More than 65 compounds was obtained from more than 40 marine organisms (22 compounds from sponges, 11 compounds from Cyanobacteria, 5 compounds from aglae, 5 from Streptomyces and 6 from marine fungus). The IC_{50} ranges of compounds were between 0.07 nM - 48 µM. Candidate compounds with more potent anti-malarial activity were selected for further investigation on their mechanism of action by in silico methods.
Conclusions: These findings underline the potential of secondary metabolites, derived from marine microorganisms, to inhibit Plasmodium growth. Chemical and bioinformatics methods can be used for discovery and design novel candidate compounds for efficient malaria chemo- therapy. In silico results must be confirmed by *in vitro* and *in vivo* anti-plasmodial activity assays for further developments.

Keywords: Malaria; Marine organisms; Chemo-informatics