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Anti-malarial discovery from plant sources: Chemo-informatics approach

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Background and Aims: There is an urgent need to identify new anti-malarial drug targets for both prophylaxis and chemotherapy, due to the increasing problem of drug resistance to malaria parasites. In the present study, the aim was to discover novel, effective plant-based extracts for the activity against malaria using chemo-informatics and traditional medicine.
Methods: Herbs 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: 200 unrelated plant species belong to 65 family from 50 original and review articles was obtained. The IC_{50} range was considered as active between 0.05 - 50 µg/ml. Candidate compounds further investigated for their mechanism of action by in silico methods.
Conclusions: 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; Traditional Medicine; Chemo-informatics