5

SUMMARY AND CONCLUSION

- The study **"*In silico* studies to screen ovicidal and repellent activity of selected plant extracts against the filarial vector, *Culex quinquefasciatus* (Diptera: Culicidae)"** included the leaves and flowers of selected five plants namely *C. gigantea, T. peruviana, T. erecta, L. camara* and *B. acuminata* on the eggs of *C. quinquefasciatus*. The efficacy of different plants varied from one another on the basis of their toxic effects
- Observations were made at 48, 72 and 96 h of the study period to record the percentage of egg hatchability
- Among the leaf extracts, maximum ovicidal activity (100% egg mortality) was noted at the concentration of 250 and 300 ppm in chloroform extract of *T. peruviana* followed by ethanol extract of *C. gigantea* at 300 ppm
- Among the flower extracts, zero percentage egg hatchability was noted in chloroform extract of *T. erecta* which possessed very high ovicidal activity at 150, 200, 250 and 300 ppm concentration followed by ethanolic extract of *C. gigantea* at concentrations ranging from 200-300 ppm
- Repellent activity of the selected plant extracts were tested against the adults of *C. quinquefasciatus* and the observations were made at 30,60,90,120,150 and 180 min of the study period to record the percentage of repellent activity
- Among the flower extracts, at the higher concentration of 5.0mg/cm^2 highest repellent activity (100% protection from mosquito bites) was observed in chloroform extract of *T. erecta* flower followed by ethanol extract of *C. gigantea* flower upto 150 min
- Among the leaf extracts maximum repellency was observed in ethanol extract of *C. gigantea* leaf followed by chloroform extract of *T. peruviana* leaf

providing 100% protection from mosquito bites upto 120 and 90 min at the concentration of 5.0mg/cm^2 respectively

- Phytochemical screening was carried out for ethanol extract of *C. gigantea* leaf and flower, chloroform extract of *T. peruviana* leaf and chloroform extract of *T. erecta* flower
- The phytochemical analysis showed the presence of alkaloids, tannins, phenols, flavonoids, sterols, terpenoids, saponins, antraquinones, proteins and quinones in the leaf and flower extracts
- GC-MS analysis was carried out for ethanol extract of *C. gigantea* leaf and flower, chloroform extract of *T. peruviana* leaf and chloroform extract of *T. erecta* flower
- The GC-MS analysis of ethanol extract of *C. gigantea* leaf and chloroform extract of *T. peruviana* leaf revealed 16 and 17 major peaks in the mass spectrum respectively, whereas GC-MS analysis of ethanol extract of *C. gigantea* flower and chloroform extract of *T. erecta* flower showed 13 and 14 major peaks in the mass spectrum respectively,
- The presence of characteristic peaks M-13, M-14, M-15, M-18, M-19, M-27, M-28, M-44, M-45 in the mass spectrum confirmed the presence of hydrocarbon, methyl, hydroxyl, nitrogen, carbonyl and carboxylic acid functional groups in the extracts analyzed
- *In silico* studies were carried out to analyse the biological activity of the ligands structures retrieved from PubChem using PASS
- The three dimensional structure of *C. quinquefasciatus* Odorant Binding Protein (OBP) (PDB id 2L2C) was retrieved from Protein Data Bank
- Totally fourteen secondary metabolites of *C. gigantea*, *T. peruviana* and *T. erecta* were docked against the respective site of *C. quinquefasciatus* odorant binding protein (PDB id 2L2C), of which ten were highly binding with the target protein

- Among the ten ligands, peruvianoside I, beta amyrin, cis-ocimene and linalool recorded good glide scores
- Molecular dynamic simulation experiments were performed to check the stability of the best docked complexes

CONCLUSION

Mosquitoes are a serious threat to public health through which several dangerous diseases are transmitted in both animals and human beings. The protein-ligand interaction plays a significant role in structural based drug designing against many diseases. The plants used in the present study are easily available in most of the agricultural and non-agricultural fields and the usage of these plants for medicinal purposes were reported by several researchers. Although, these plants were used as famous traditional folk medicine by many cultures, and also has been subjected to extensive phytochemical and bioactive investigations, the computational prediction of potential drugs from it by the process of drug docking have not been completely investigated yet. In the present work, the four phytochemicals peruvianoside I, beta amyrin, cis-ocimene and linalool were highly binding with the odorant binding protein (2L2C) of *C. quinquefasciatus* by producing good glide scores and the bonds showed good structural stability in molecular dynamics simulation experiments and therefore, it may have an ability to suppress human seeking behaviour of mosquitoes. From these results, it can be concluded that the integration of computational and experimental approaches proposed in this study exemplifies a genuine computer-aided discovery of mosquito ovicides and repellents that may be a better option against the mosquitoes than the existing harmful synthetic ones.

Scope of further research

- Many plants can be probed to identify the compounds responsible for mosquito ovicidal and repellent activities as an alternate source
- Several compounds from the plants can be extracted using various solvents and its characterization can be studied

- Many chemical components of plants can be tested *in silico* for drug designing, that may give new effective drug against top most killer mosquito borne diseases
- The future insight would be to search for other possible modifications in the proposed molecules, to get a better drug with high binding efficiency
- The drugs can be studied experimentally to identify their efficiency in binding and inhibition
- Further research is needed for refinement and for enriching the activity of the ligands attacking the odorant binding protein, to determine the dosages of safety levels, to explore this promising avenue for mosquito control and to ensure the healthy state of humans

Recommendations

India is one of the largest consumers of chemical pesticides, which destroy the natural enemies of non-target pests. Insect pests have developed resistance to several insecticides. Moreover, most of the pesticides are toxic and non biodegradable and have adverse effects on the environment by polluting soil and water and affecting health. Recently, bio-pesticides of plant origin are used against several insect species, especially disease transmitting vectors, based on the fact that compounds of plant origin are safer to use, without phototoxic properties and leave no scum in the environment. Therefore, the modern society can be recommended to shift towards biological control methods or use of plant resources in controlling insects and pests that has been practiced for centuries by local people to prevent arthropod bites to control the mosquito borne diseases.