1.6 Structural Bio-informatics study of inhibitory role of secondary metabolites of *Calotropis procera* on Sterol carrier protein (AeSCP-2) of *Aedes aegypti*

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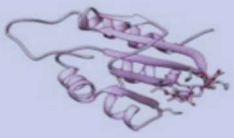
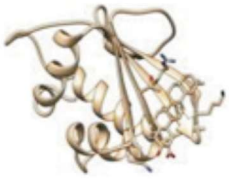
OBJECTIVES

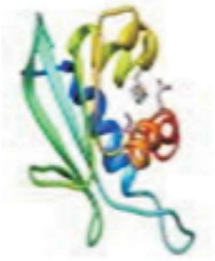
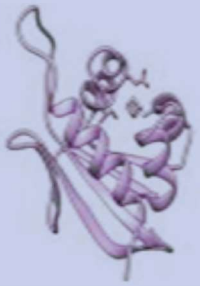
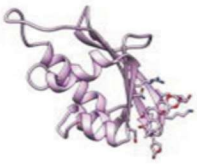
1. To derive structure and orientation of AeSCP-2 protein and latex compounds of *C. procera* for its possible interaction.
2. Identification, implication and isolation of larvicidal compounds inhibiting AeSCP-2 Protein and establishment of its role as new larvicidal compound.

PROGRESS

The study was undertaken to study inhibitory role of chemical compounds of *C.procera* by determining their ability to interact with Aedes sterol carriear protein. Inhibitors of Aedes sterol carriear protein will determine effective larvicide against dengue vectors. The knowledge derived from this research will aid for rational design of new insecticide for control of mosquito population.In continuation of our earliar work virtual screening of chemical compound of C.procera such as Ucharidin, Cymarin ,Beta amyrin, Uscharin, Calotropin ,erysinomide , Boivinidae, calotoxin, Calactin and Asclepin with 3D structure of AeSCP-2 (PDB ID 2KSH) was carried out using Patch dock online server and refinement was done by using fire dock server. The docked pose, structure of interaction of ligands and protein was svisualised by the Chimera software. After refinement 10 models were created for each interaction. On the basis of Binding energy best model was selected. Lowest binding energy of interaction showed highest stability. Binding energy shown in increasing order (table 1) . Uscharin, Cymarin shown highest level of stability and Calactin Asclepin shown lowest level of stabilty. In silico analysis of secondary metabolites of *C.procera* play important role in control of in Aedes larvae. Further molecular diagnosis simulations and wet laboratory experiments will be performed to assess the larvicidal effect of constituent metabolites present in *Calotropis* extract against dengue vectors.

Table 1. Binding enery of docked pose by docking software

Ligand	binding energy kcal/mole	Docked pose (Ligand + Aedes sterol carrier protein)
Uscharidin	-40.73	
Cymarin	-39.29	
Beta amyrin	-38.00	

Uscharin	-37.06	
Calotropin	-31.35	
Erysinomide	-30.54	
Boivinidae	-22.79	
calotoxin	-22.79	
Calactin	-14.15	
Asclepin	-13.34