



Title: Computational studies of Herbal Nano Particles.

1. Mosquitoes

1A. *Aedes aegypti*

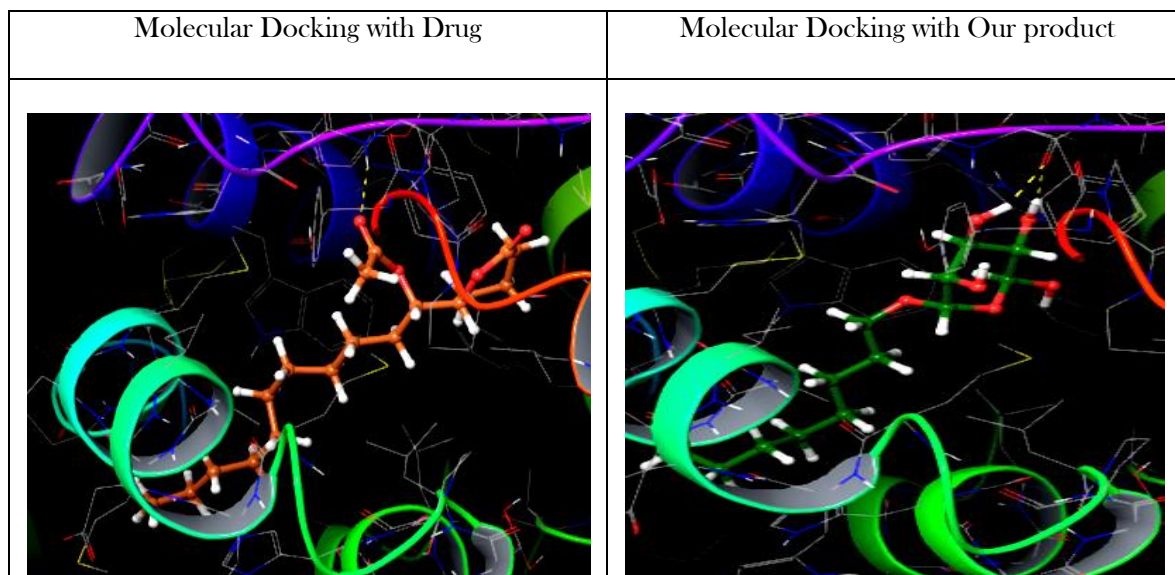
1B. *Aenopheles gambiae* & *Aenopheles stephensi*


2C. *Culex Sp.*

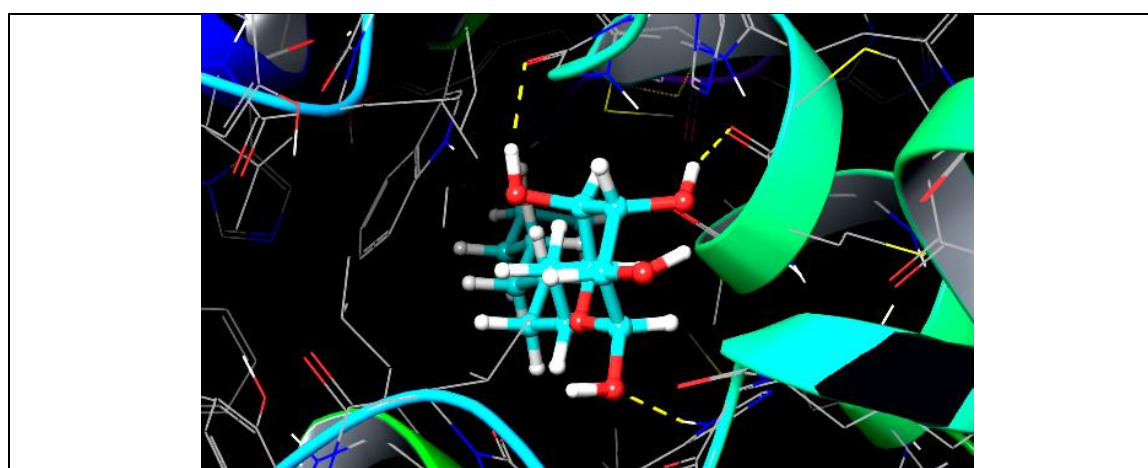
Experiments:

1. Homology Modeling
2. Target Site Mapping
3. Molecular docking
4. Induced Fit Docking
5. Molecular Dynamic Simulation
 - ❑ Scrodinger software was used for all above experiments
 - ❑ Validation of all the experiments was done based on Pose, Score, Types of molecular interaction, RMSD values and counter experiments
 - ❑ Comparative studies performed with best available drug in the market for respective target

Category A: Mosquito Repellent (PDB : 3OGN) Odorant-binding Protein



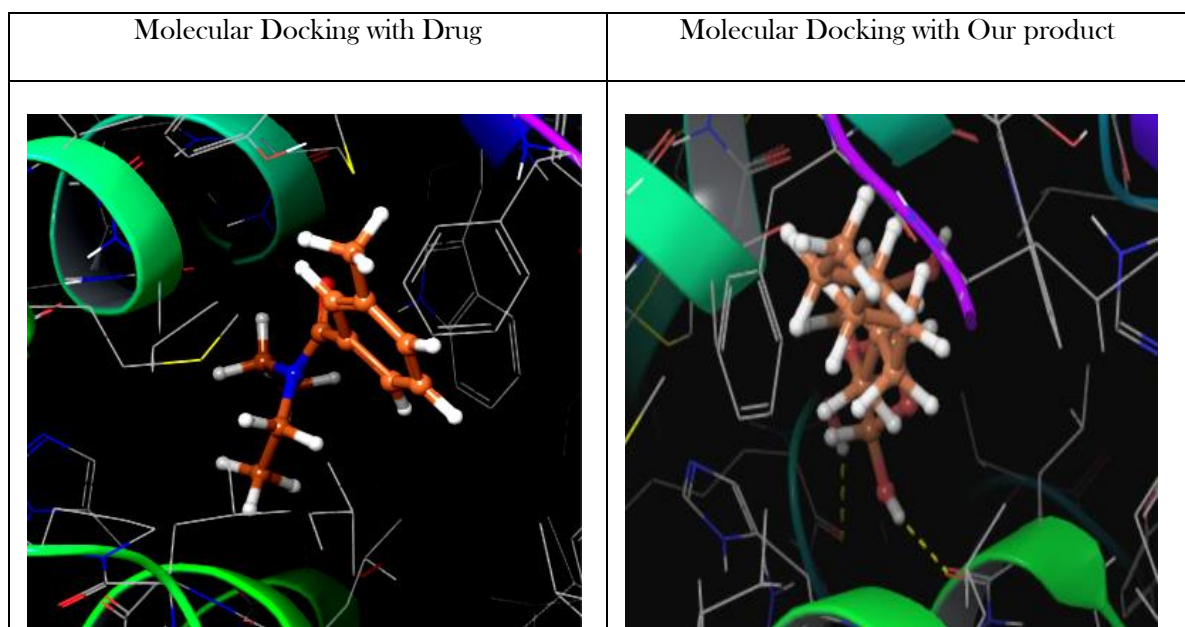
 Induced Fit Docking:




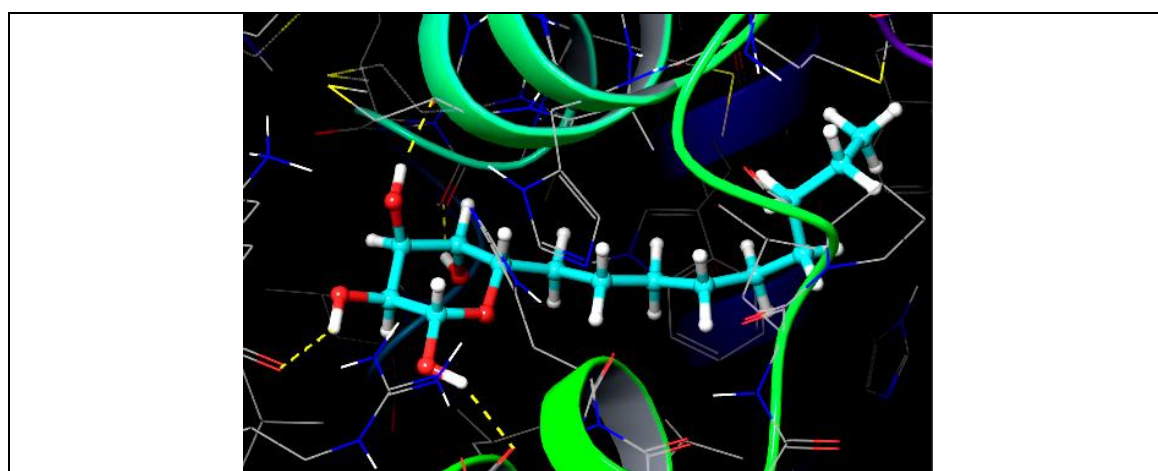
Docking Table	Drug Docking Score	Herbal Nano particle Docking Score	Drug Interaction Energy Value	Herbal Nano particle Interaction Energy Value
	-10.761	-10.253	-56.357	-58.818

Induced Fit Table	Ligand	IFD Score for the best pose	Total No. of poses generated
	Drug	-7.419	
	Herbal Nano Particle	-9.723	

Category A: Mosquito Repellent (PDB : 3N7H) Odorant - Binding Protein



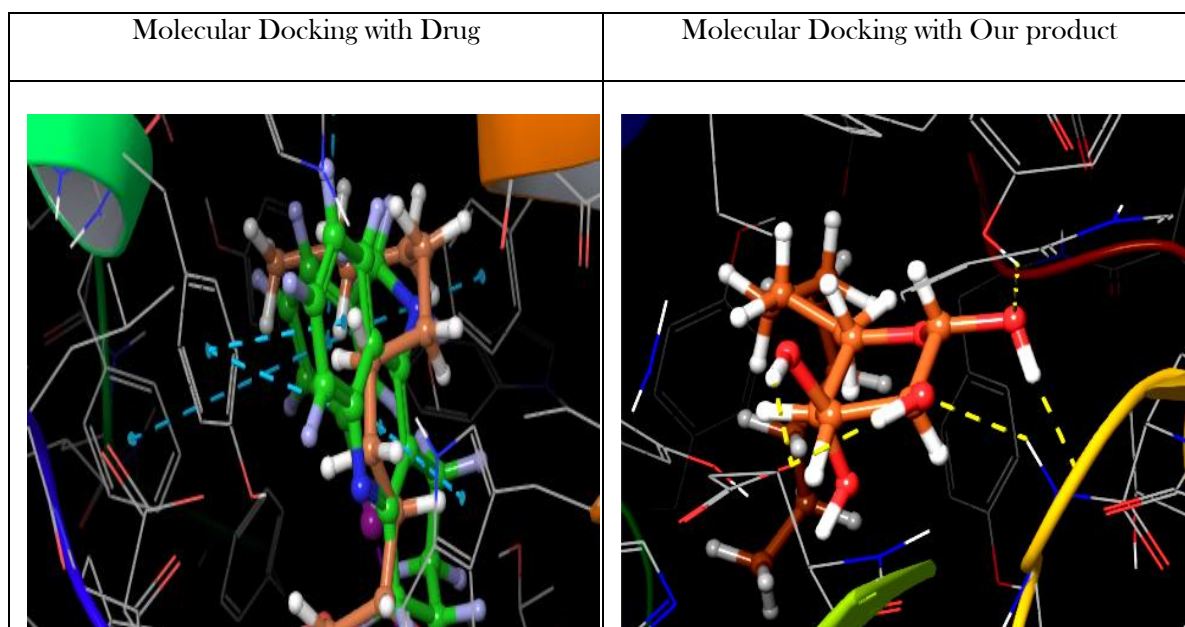
 Induced Fit Docking:



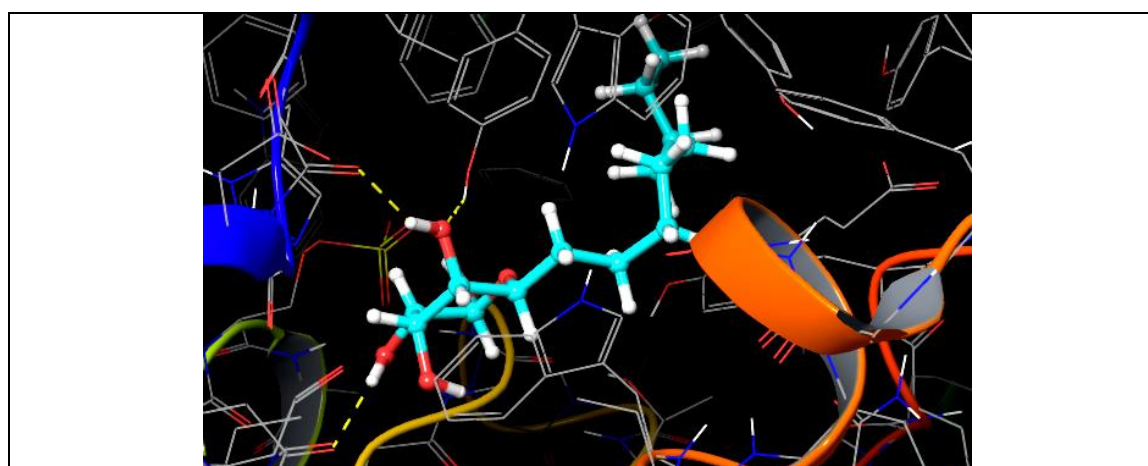
Docking Table	Drug Docking Score	Herbal Nano particle Docking Score	Drug Interaction Energy Value	Herbal Nano particle Interaction Energy Value
	-6.915	-9.592	-38.423	-59.224

Induced Fit Table	Ligand	IFD Score for the best pose	Total No. of poses generated
	Drug	-7.550	24
	Herbal Nano Particle	-11.704	

Category B: Mosquitocide (Acetyl Choline Esterase: Homology Modeling)



■ Induced Fit Docking:



Docking Table	Drug Docking Score	Herbal Nano particle Docking Score	Drug Interaction Energy Value	Herbal Nano particle Interaction Energy Value
	-6.915	-9.592	-38.423	-59.224

Induced Fit Table	Ligand	IFD Score for the best pose	Total No. of poses generated
	Drug	-7.550	24
	Herbal Nano Particle	-11.704	

Conclusion:

1. Herbal Nano particle based computational docking and simulation studies against mosquito proteins showed it can work as Repellent and Mosquitocidal both.
2. Docking studies were also performed against **Sodium Ion Channel** (standard biological target) of all 3 species of mosquito, that showed wonderful interaction profile, proving the powerful mosquitocidal activity of the herbal nano particles compared to standard.
3. DEET has been the best Mosquito Repellent so far. But, this data shows that this herbal based nano molecules shows better molecular interactions profile compared to DEET at each of the mosquito developmental stages.
4. In addition to that, being herbal by nature, these molecules won't be harmful or environmental pollutant, showing its potentiality to work in the market.