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# A BIOINFORMATICS APPROACH IN INSECTICIDAL PROPERTY OF PHENOLIC COMPOUNDS AGAINST MOSQUITO JUVENILE HORMONE-BINDING PROTEIN (mJHBP)

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## ABSTRACT

Molecular docking study wildly used for pharmacologist and academic researches, they are different algorithm based program was used. Phenolic acids are plant secondary metabolites widely spread throughout the plant, phenolic acids naturally bioactive properties like antioxidant, anti-inflammatory, anti-diabetic and etc., Mosquitoes can transmit diverse infectious pathogens and parasites that cause diseases such as several viral infection and etc., Therefore mosquitoes also called disease vectors. In the aim of present study were computational approach on insecticidal activity using phenolic acid sub-derivatives against mosquitoe species Juvenile hormone (JH) protein (PDB ID: 5V13). To find out on molecular docking study using program of Autodock vina through new generation of Autodock, Autodock as Lamarckian Genetic Algorithm, Autodock vina output score evaluate on Caffeic acid -7.30, Ellagic acid -7.90, Gallic acid -7.10, Syringic acid -6.70 and Vanillic acid -6.80 Binding affinity (Kcal/mol) were reported on 5V13 protein (JH) binding scores. Overall phenolic acid sub-derivatives were binding with insect Juvenile hormone (JH), to be conclude by phenolic acids were mosquitoe larvae species suggests that the effects of JH on development of insect.

**Keywords:** Insecticidal activity, *In silico*, Phenolic acid, Mosquito juvenile hormone-binding protein, PDB: 5V13 (mJHBP).

## INTRODUCTION

Mosquitoes can transmit diverse infectious pathogens and parasites that cause diseases such as several viral infection, vectors for living organisms that can transmit infectious pathogens between animals to humans. The vectors are bloodsucking insects (mosquito) transmit it into a new host, after the pathogen has replicated. Mosquito more than 3,400 species have been recorded worldwide (Baranitharan et al., 2018). Mosquito-borne viral infections are responsible for a significant degree of mortality across the globe due to the severe infections cause continually and they increase every year. The viruses are dependent on the mosquito vector as the primary transmission to new vertebrate hosts (avian, livestock, and human populations) by Trammell and Goodman, (2021). Mosquito Juvenile hormone (JH) is a key regulator of development and reproduction in mosquitoes. (Zhu and Noriega, 2016). Present investigate the mosquito juvenile hormone-binding protein (mJHBP) was inhibited the natural phenolic acids

Phenolic acids are plant aromatic secondary metabolites, widely throughout the plants. Phenolic acids were biological roles as secondary metabolites and potential protective role, against oxidative damage diseases (Rebecca, 2003). Plant biologically active compounds are search of new promising substances and for the further development of new drugs (Prokopenko et al., 2019). In the aim of our study computational approach on insecticidal activity using phenolic acid sub-derivatives against Mosquito juvenile hormone-binding protein – Molecular docking, phenolic acids were natural plant secondary metabolites, they are eco-friendly substance.

## METHODOLOGY

### *In silico* molecular docking

Computational drug discovery technique in the recent day of Pharmaceutical research has been successful in molecular modeling with different algorithm based programing software's been used. The ligand and protein binding scores according to algorithm based program thereby may use any software for protein and ligand interactions for best results (Velavan *et al.*, 2020).

The ligand as phenolic acid like Caffeic acid, Ellagic acid, Gallic acid, Syringic acid and Vanillic acid were obtained from Pubchem database, ligands were converted in to PDB format using Open bable software. 5V13 Mosquito juvenile hormone-binding protein by Kim *et al.* (2017) was obtained from PDB database and generally removed, all water molecules and any other Ligand molecules prior to docking, using Pymol software prepared protein was saved as PDB formed. Molecular docking software used in PyRx 0.8, virtual screening tool (Autodock vina program) software for grid dimension prepared (Center x = 252.44, center y = 5.60 and center z = 362.47 for chain A) (Trott and Olson, 2010).

## RESULTS AND DISCUSSION

In the present study carried out computational approach on insecticidal activity against mosquitoe species Juvenile hormone (JH) protein using phenolic acid sub-derivatives. Juvenile hormone (JH) is a key regulator of insect development and reproduction, given the name mosquito juvenile hormone-binding protein (mJHBP) by Kim *et al.*, 2017. They are Autodock vina was new generation of Autodock, Autodock as Lamarckian Genetic Algorithm, Autodock vina output score evaluate on Caffeic acid -7.30, Ellagic acid -7.90, Gallic acid -7.10, Syringic acid -6.70 and Vanillic acid -6.80 Binding affinity (Kcal/mol) were reported on 5V13 protein binding scores (Table 1).

Phenolic acids are a subclass of a larger category of secondary metabolites in plant kingdom, they are natural bioactive properties. Ellagic acid was high active properties while Syringic acid was low active properties compare with in between the ligand. They are following active properties order as Ellagic acid > Caffeic acid > Gallic acid > Vanillic acid > Syringic acid were present study reported (Figure 1).

**Table 1: Molecular docking with Mosquito juvenile hormone-binding protein (PDB: 5V13 protein chain A)**

| Ligand | Molecular formula | M. weight (g/mol) | Binding affinity (Kcal/mol) | 5V13 (chain A) Amino acids binding |
|---|---|---|---|---|
| **Caffeic acid** | $C_9H_8O_4$ | 180.16 | -7.30 | TYR 64, VAL 65, SER 69, LEU 74, PHE 87, TYR 129, LEU 72, VAL 68, TRP 53, TYR 33, TRP 50, VAL 51. |
| **Ellagic acid** | $C_{14}H_6O_8$ | 302.19 | -7.90 | GLU 208, LYS 78, ASP 76, ARG 86, ARG 83, ARG 73, TYR 75, GLU 70, PRO 77, GLU 206. |
| **Gallic acid** | $C_7H_6O_5$ | 170.12 | -7.10 | GLY 199, ARG 198, ILE 203, THR 204, ARG 73, GLN 28, GLU 205, ARG 201, GLU 71, LEU 72. |
| **Syringic acid** | $C_9H_{10}O_5$ | 198.17 | -6.70 | TYR 33, TRP 50, TRP 53, PHE 284, GLY 146, ALA 285, TYR 148, LEU 30, ALA 281, VAL 51, PHE 269, VAL 34, TRP 278, LEU 37, TYR 64. |
| **Vanillic acid** | $C_8H_8O_4$ | 168.15 | -6.80 | ILE 203, ARG 198, THR 204, GLU 71, GLU 205, ARG 73, ARG 201, LEU 72, ARG 24, GLN 28. |

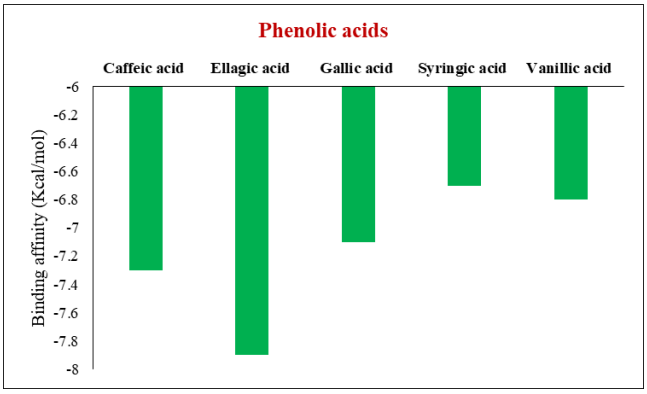


**Figure 1: Molecular docking score graphically represented**

Insect growth and development (metamorphosis, reproduction) of under control of juvenile hormones (JH) (Noriega *et al.*, 2006). In the present study the crystal structure of the mosquito juvenile hormone binding protein (mJHB), binding with phenolic acid they are strong interaction with JH active site (Figure 2 to 6). Similarly Ramos *et al.* (2019) evaluate on interaction with the juvenile hormone was −11.4 kcal/mol for the molecule ZINC00001021 and Araújo *et al.* (2021) 5V13 complex (*Ae. aegypti*), the *Aspergillol B* and (+)-N-deoxymilitarinone showed a higher binding affinity value compared to JHIII (control) used with a value of -9.4 and -9.7 Kcal/mol.

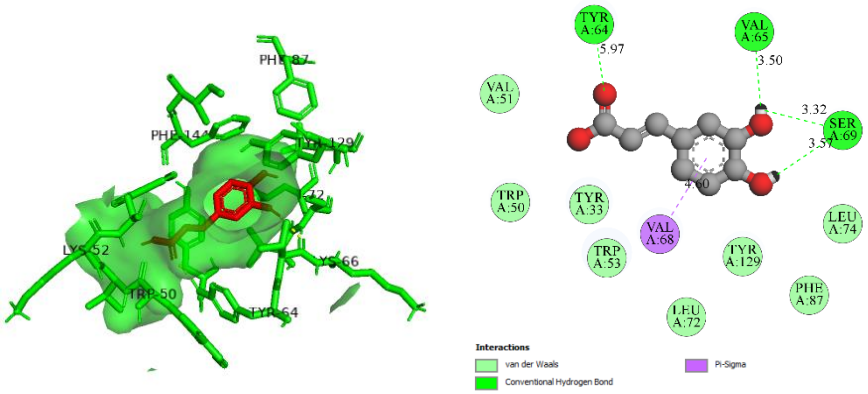


**Figure 2: 3D and 2D view of Caffeic acid ligand binding/interaction with mosquitoe Juvenile hormone (JH) protein (5V13 chain A)**

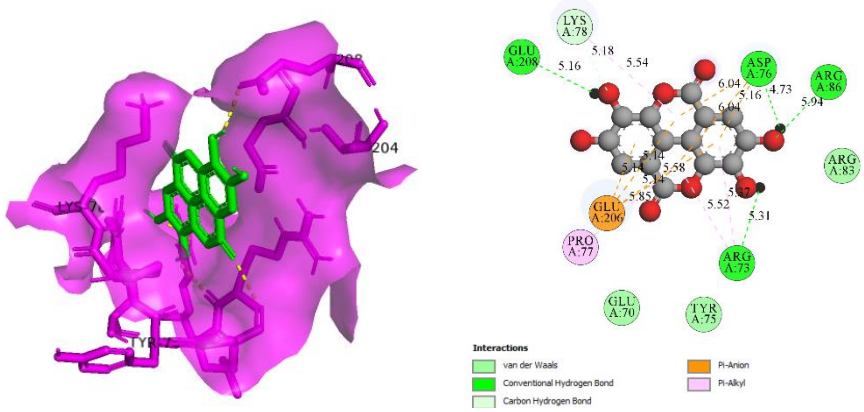


**Figure 3: 3D and 2D view of Ellagic acid ligand binding/interaction with mosquitoe Juvenile hormone (JH) protein (5V13 chain A)**

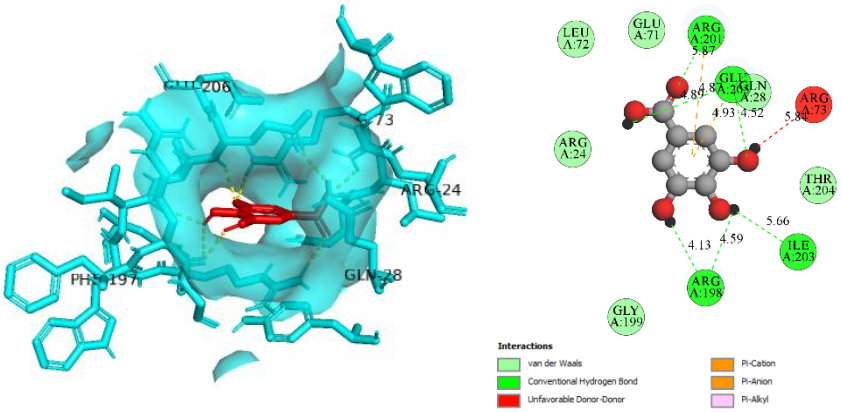


**Figure 4: 3D and 2D view of Gallic acid ligand binding/interaction with mosquitoe Juvenile hormone (JH) protein (5V13 chain A)**

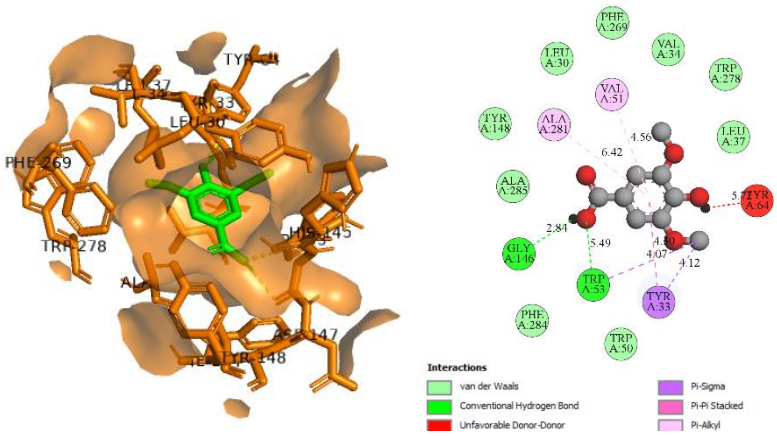


**Figure 5: 3D and 2D view of Syringic acid ligand binding/interaction with mosquitoe Juvenile hormone (JH) protein (5V13 chain A)**

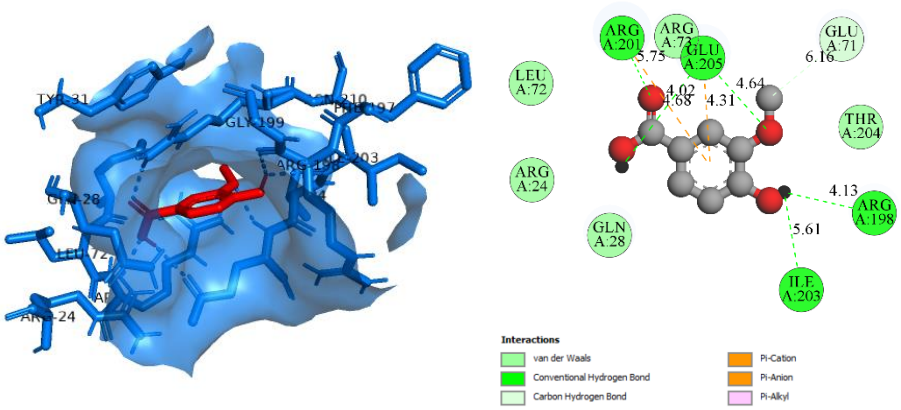


**Figure 6: 3D and 2D view of Vanillic acid binding/ligand interaction with mosquitoe Juvenile hormone (JH) protein (5V13 chain A)**

## CONCLUSION

Phenolic acid sub-derivatives are best insecticidal active properties were concluded against mJHBP. Phenolic acid against the mosquitoe larvae species suggests that the effects of JH on development of insect.

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