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Isolation of compound and molecular docking studies of *Wedelia calendulacea* extract fractions against dengue vector, *Aedes aegypti*

Abstract

Mosquito, *Aedes aegypti* is a most critical public health problem in a lot of countries, and controlling of mosquito is a biggest challenge in the control programme. There is a need for decision biological active molecules to control mosquito in order to prevent dengue virus transmission. To assess is isolation of major phyto-compound (MPC) Phenol, 2-methyl-5-(1-methylethyl) and molecular docking of plant, *Wedelia calendulacea* (*W. calendulacea*) against *Ae. aegypti*. In the ovicidal activity, 100% mortality was extracted by fraction 6 tested at 10 ppm against *Ae. aegypti*. In mass spectra analysis, a total of nineteen compounds was identified in the methanolic extract composition, the main component was Phenol, 2-methyl-5-(1-methylethyl). Molecular docking studies performed with the mosquito juvenile hormone-binding protein (MJHP) demonstrated that the Phenol, 2-methyl-5-(1-methylethyl) compound towards the one enzyme. The findings thus reveal that the medicinal plant compound can be a better possible to accessible chemicals to control mosquitoes.

Keywords: major phyto-compound, methanolic extract, *aedes aegypti*, *wedelia calendulacea,* molecular docking, mosquito juvenile hormone-binding protein

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Introduction

The World Health Organization is highlighting a collection of diseases spread by insects and other vectors, as well as the significant health and economic costs they impose, and what may be done to alleviate these costs. Diseases like dengue and yellow fever often lead to large-scale outbreaks, overwhelming healthcare systems and causing considerable economic and social disruption.[1] Today, there is a revived interest in traditional medicine and an increasing demand for more drugs from very important medicinal plant sources. Moreover, these challenges have underscored the need for developing innovative strategies for targeted mosquito control. As noted by Brooks (1976), the effectiveness of insecticides largely depends on their ability to penetrate semi-permeable membranes. Conversely, metabolic resistance to insecticides involves enzymatic modifications that transform highly toxic insecticides into less harmful compounds. Enzymes such as oxidases, glutathione S-transferases (GST), and esterases play a key role in metabolic resistance in pathogens. Furthermore, resistance to pyrethroids and pyrethrins has been linked to metabolic processes and oxidative enzyme systems.[2] Though resistance is an evolutionary phenomenon, it may be effectively addressed by using suitable and thorough resistance monitoring and management measures as part of an integrated vector management strategy.[3–6] Due to the problems encountered during the detection of biological properties and the economic costs of the experimental methods, computational methods such as molecular docking are desired for predicting the binding of the protein and ligand, and their affinities.[7,8] Computer apparatus such as molecular docking techniques contribute to understanding the interaction of phyto-chemical compounds and receptors. It predicts the binding of the target protein to the ligand with orientation in the targeted binding site. These techniques make the discovery of effective bioactive compounds with mosquitocidal activities easier.[9–11]

Wedelia calendulaceae is a small, much-branched herb from the Asteraceae family, commonly known as "Bhringraj" in Hindi and "Wedelia" in Chinese. Traditionally used in Ayurveda, Siddha, and Unani medicine, *W. calendulaceae* is valued for its hepatoprotective, anti-inflammatory, and wound-healing properties. It contains wedelolactone and demethylwedelolactone, which aid liver health and reduce inflammation. Its extracts treat skin diseases, dermatitis, eczema, and acne. The leaves are applied to wounds, while the juice is used for hair growth and dyeing grey hair. Studies show that W. chinensis has analgesic effects comparable to those of aspirin and morphine. It has been used to treat rheumatic fever, arthritis, multiple sclerosis, and osteoporosis. The ethanolic extract has shown promising results in liver protection, prostate cancer suppression, and neuropharmacological applications. Due to habitat destruction and unsustainable harvesting, conservation efforts are needed. The plant is propagated via seeds and stem cuttings, though in vitro methods offer alternatives for preservation and large-scale cultivation. This study aims to investigate the essential phytochemical compounds and explore the mechanisms by which bioactive compounds interact with the active site of the mosquito juvenile hormone protein (MJHP).

Materials and methods

I. Plant material and extraction

Fully matured leaves of *W. calendulacea* were collected during the growing season (March–May) of 2023 from various locations in Yercaud (11°77'48" N and 78°20'97" E), Salem District, Tamil Nadu, India. The freshly harvested leaves were thoroughly washed multiple times with water to remove any impurities. They were then shade-dried at room temperature and subsequently preserved in a hot air oven at 50ºC for 30 minutes. The dried material was finely ground using an electric blender. A total of 500 g of powdered plant material was placed in a Soxhlet apparatus, and successive extraction was performed using methanol as the solvent for 72 hours. The solvent was then evaporated under vacuum using a rotary evaporator (Heidolph, Germany), and the dried extract was stored at 4ºC until further bioassay.[12]

II. Ovicidal activity

Ovicidal activity was assessed using the specified method.[13] The eggs from each concentration were individually transferred to cups

containing distilled water for hatching evaluation after being counted under a photomicroscope (Leica, Germany). Further, each treatment was repeated five times (n=100 per replicate) along with controls, and the hatch rates were assessed 48h post-treatment by following formula.

$$\%\ \text{of egg mortality} = \frac{\text{Number of hatched larvae}}{\text{Total no. of eggs}} \times 100$$

III. Gas chromatography–Mass spectrometry analysis

Gas chromatography-mass spectrometry (GC-MS) was performed using a Turbo Mass Gold mass detector (Perkin Elmer) with an Elite-5MS column (5% Diphenyl/95% Dimethylpolysiloxane, 30 × 0.25 mm × 0.25 mm df). The oven temperature was programmed to increase from 50ºC to 280ºC at a rate of 5ºC per minute and was held at this temperature for 36 minutes. The delta and interface temperatures were set at 200ºC and 280ºC, respectively. Helium was used as the carrier gas at a constant flow rate of 1.0 ml per minute. A 2 µl sample was injected with a split ratio of 10:1. Electron impact mass spectrometry (EIMS) was carried out at 70 eV, with the ion source and quadrupole temperatures maintained at 250ºC and 200ºC, respectively.[14]

IV. In silico docking studies

A molecular docking study was conducted to assess the binding efficiency of Phenol, 2-methyl-5-(1-methylethyl) within the active site of the selected drug targets. The Lamarckian genetic algorithm method, integrated into the AutoDock 4.2 program, was utilized for this purpose.[15] The ligand compound, Phenol, 2-methyl-5-(1-methylethyl), was obtained from the PDB Sum database with the PDB ID: 5V13. The ligand compound is derived from *Aedes aegypti* juvenile hormone-binding protein, sourced from the Protein Data Bank. Prior to molecular docking, the energy-minimized 3D atomic coordinates of the juvenile hormone-binding protein were generated using the ACD/ChemSketch server (Schüttelkopf and Van, 2004). Subsequently, Gasteiger-Marsili partial charges were assigned to Phenol, 2-methyl-5-(1-methylethyl), and non-polar hydrogen atoms were merged. All torsions were set to rotate during docking. The Lamarckian Genetic Algorithm (LGA) was employed for molecular docking, with a maximum of 21 compounds analyzed for each case. The docking algorithm was executed using PyMOL and compiled under the ACD/ChemSketch software.

V. Selection of target protein

In order to carry out protein modeling investigates, 3D structure of sterol shipper juvenile hormone-binding protein of *Ae. aegypti* larvae were retrieved from Protein Data Bank (PDB) and through ACD/ChemSketch software.

VI. Molecular docking analysis

Finally docking studies for the target protein juvenile hormone-binding protein and Phenol, 2-methyl-5-(1-methylethyl) compound (ligands) of *W. calendulacea* were performed using PDB ID is 5V13.[16,17]

VII. Data analysis

Ovicidal data were examined using a two-way ANOVA (factors: the tested fraction and the tested dose), followed by Tukey's HSD test. The significance level was established at $P<0.05$.

Results and discussion

I. Ovicidal activity

Wedelia calendulacea leaf methonalic extract fractions (LMEFs) were showed for the presence of major phytochemical groups accountable of ovicidal activity. These six MEFs of *W. calendulacea* were tested for their biological activity against the selected vector mosquito species, which have been checked for their ovicidal activity on *An. stephensi*. Fraction 6 was screened EH (Eggs Hatchability)/ ENH (Eggs No Hatchability)% of 14.6/36.2% at 5 ppm and 100% mortality at 10, 15, 20, 25, 30ppm, respectively. Moreover, fraction 5 was focused EH/ENH% values of 10.3/53.4%, 22.6/4.1% at 5, 10 ppm and 100% mortality at 15, 20, 25, 30 ppm, respectively. Fraction 4 was noticed EH/ENH% values of 8.4/61%, 16.1/30.1%, 23.7/0.7% at 5, 10, 15 ppm and 100% mortality at 20, 25, 30 ppm, respectively. Fraction 3 were screened EH/ENH% values of 6.2/69.7%, 12.3/46.5%, 17.3/25.3%, 22.4/5% at 5, 10, 15, 20 ppm and 100% mortality at 25, 30 ppm, respectively. Fraction 2 were noticed EH/ENH% values of 4.1/78.2%, 8.3/61.3%, 12.6/44.4%, 16.4/29%, 21.2/9.7% at 5, 10, 15, 20, 25 ppm and 100% mortality at 30 ppm, respectively. Fraction 1 was focused EH/ENH% values of 2.7/83.7%, 6.3/70.2%, 9.7/55.7%, 13.3/42.1%, 16.5/28.5%, 20.6/12.4% at 5, 10, 15, 20, 25 and 30 ppm, respectively, has been shown in Table 1.

Table 1 Ovicidal activity of *A. adenophora* selected compounds tested against eggs (0-6h old) of *An. stephensi.*

Fractions	EH/ENH % (48 hrs)						
	control	5 ppm	10 ppm	15 ppm	20 ppm	25 ppm	30 ppm
Fraction 6	25/0	14.6/36.2%	0/ENH	0/ENH	0/ENH	0/ENH	0/ENH
Fraction 5	25/0	10.3/53.4%	22.6/4.1%	0/ENH	0/ENH	0/ENH	0/ENH
Fraction 4	25/0	8.4/61%	16.1/30.1%	23.7/0.7%	0/ENH	0/ENH	0/ENH
Fraction 3	25/0	6.2/69.7%	12.3/46.5%	17.3/25.3%	22.4/5%	0/ENH	0/ENH
Fraction 2	25/0	4.1/78.2%	8.3/61.3%	12.6/44.4%	16.4/29%	21.2/9.7%	0/ENH
Fraction 1	25/0	2.7/83.7%	6.3/70.2%	9.7/55.7%	13.3/42.1%	16.5/28.5%	20.6/12.4%

EH- Eggs hatchability, ENH %- Eggs no hatchability

Similarly, a higher concentration of 3.0 mg/cm² ensured complete protection for up to 120 minutes, while lower concentrations of 2.0 and 1.0 mg/cm² provided full protection for 80 and 40 minutes, respectively. Reports indicate that an even higher concentration of 4.0 mg/cm² offered 100% protection for 120, 160, and 200 minutes.[18,19] Complete mortality was observed at three different deterrent feeding concentrations ranging from 75 to 125 ppm. Furthermore, the ovicidal activity of *Pisonia alba* resulted in 100% mortality at 240, 300, and 360 × 10^6.[20] Of the *Punica granatum* methanol extract tested for100% (no hatchability) ovicidal activity against *An. stephensi* at 210 ppm, 280ppm and 350ppm, respectively.[2] The ovicidal activity of a citronellal compound of 45 mg/L screened at 0.75 concentrations of 1.50 mg/cm² against *An. stephensi*.[21,22]

II. Gas Chromatography–Mass Spectrometry analysis

Mass spectra analyses of twenty one compounds of *W. calendulacea* LME were detected representing 100%, with concentration of percentage (%) and molecular formula has been shown in Table 2. The major phytocompounds in LME of *W. calendulacea* are Phenol, 2-methyl-5-(1-methylethyl)- (32.32% and $C_{10}H_{14}O$), n-Hexadecanoic acid (11.32% and $C_{16}H_{32}O_2$), Hancolupenone (7.81% and $C_{30}H_{48}O$), Urs-12-en-24-oic acid, 3-oxo-, methyl ester, (+)- (6.33% and $C_{31}H_{48}O_3$), 3,7,11,15-Tetramethyl-2-hexadecen-1-o1 (5.92% and $C_{20}H_{40}O$), á-Amyrin (5.69% and $C_{30}H_{50}O$), Phytol (4.92% and $C_{20}H_{40}O$), Cholest-4-en-3-one (4.21% and $C_{27}H_{44}O$) and Ar-tumerone (3.81% and $C_{15}H_{20}O$) (Figure 1). The findings of this study align with the GC-MS analysis of the LE, which identified twenty compounds, with Limonene dioxide, Neophytadiene, and Palmitic acid as the primary constituents.[23] Additionally, the mass spectral analysis validated these compounds, revealing that the molecules comprise eight carbon atoms, fifteen hydrogen atoms, and four oxygen atoms, which were represented in different colors.[3] The medicinal plant *Erythrina variegata* LME was found to contain 12-octadecenoic acid methyl ester, which exhibited significant toxicity against HVMs.[4] *Petalonema alatum* LME was identified to have various major phytocompounds (MPCs), including 5-thio-D-glucose, 5-allylsulfanyl-1-(4-methoxy-phenyl)-1H-tetrazole, (E)-10-heptadecen-8-ynoic acid methyl ester, and Z-11-hexadecenoic acid.[24] GC-MS analysis of *Loranthus pentandrus* LME was conducted to determine its primary phytocompounds, revealing a total of 20 chemical constituents in the methanol extract, accounting for 100% of the composition.[25]

Table 2 Components identified in *A. adenophora* by GC-MS

MF	Name of compound	RT (min)*	PA (%)	MW	MI
$C_{10}H_{14}O$	Z-8-Methyl-9-tetradecanoic acid	4.23	1.54	150	*RI-MS*
$C_{15}H_{24}$	Bicyclo[7.2.0]undec-4-ene, 4,11,11-trimethyl-8-methylene,[1R-(1R*,4Z,9S*)]-	8.32	2.59	204	*RI-MS*
$C_{15}H_{24}$	Trans-á-Bergamotene	9.44	0.49	204	*RI-MS*
$C_{15}H_{24}O$	Caryophyllene oxide	11.71	0.36	220	*RI-MS*
$C_{15}H_{20}O$	Ar-tumerone	12.43	5.46	216	*RI-MS*
$C_{20}H_{40}O$	3,7,11,15-Tetramethyl-2-hexadecen-1-o1	13.67	2.02	296	*RI-MS*
$C_{16}H_{32}O_2$	n-Hexadecanoic acid	14.66	6.87	256	*RI-MS*
$C_{20}H_{40}O$	Phytol	19.96	17.64	296	*RI-MS*
$C_{18}H_{32}O_2$	9,12-Octadecadienoic acid (Z,Z)-	21.31	18.23	280	*RI-MS*
$C_{15}H_{28}O_2$	Phenol, 2-methyl-5-(1-methylethyl)-	21.42	21.90	240	*RI-MS*
$C_{16}H_{32}O_3$	Methoxyacetic acid, 4-tridecyl ester	22.86	7.25	272	*RI-MS*
$C_{30}H_{50}$	Squalene	24.36	3.71	410	*RI-MS*
$C_{15}H_{18}O_3$	à-Santonin	25.23	4.58	402	*RI-MS*
$C_{28}H_{48}O_2$	Ç-Tocopherol	26.62	14.49	416	*RI-MS*
$C_{29}H_{50}O_2$	Vitamin E	27.42	0.57	430	*RI-MS*
$C_{28}H_{48}O_2$	Cholestan-3-ol, 2-methylene-, (3á,5á)-	27.93	3.27	400	*RI-MS*
$C_{29}H_{48}O_2$	Cholesta-22,24-dien-5-ol, 4,4-dimethyl-	29.18	1.48	412	*RI-MS*
$C_{30}H_{48}O$	Hancolupenone	30.84	1.47	424	*RI-MS*
$C_{31}H_{48}O_3$	Urs-12-en-24-oic acid, 3-oxo-, methyl ester, (+)-	32.42	3.11	468	*RI-MS*

MF, molecular formula; RT, retention time (min); PA, peak area; MW, molecular weight; MI, mode of identification

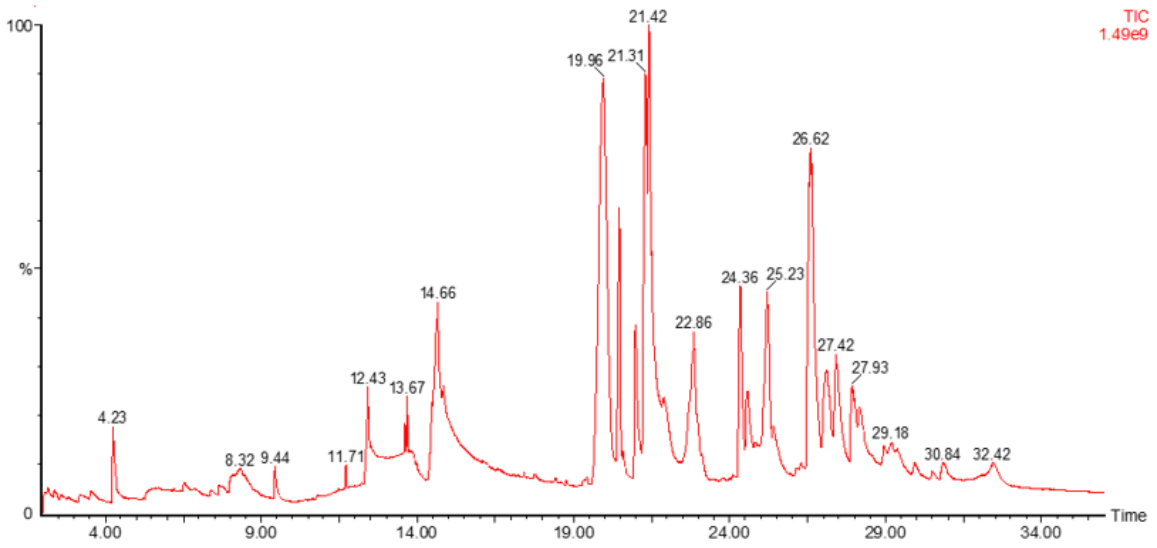

Figure 1 Chemical constituents of LME of *W. calendulacea* (GC-MS Chromatogram).

III. In silico docking

For molecular docking studies, the ligand Phenol, 2-methyl-5-(1-methylethyl) was docked against MJHP. The protein structure was obtained from the Swiss-Prot database, while the 3D structure of MJHP was retrieved from the PDB database (Figure 2). The ligand, Phenol, 2-methyl-5-(1-methylethyl), was drawn using ACD/ChemSketch software after downloading its 2D structure (Figure 3). In silico molecular docking was utilized to calculate the binding affinity and binding energy (in kcal/mol) between the ligand and MJHP. This study confirmed the presence of a binding site between the protein and ligand. The formation of hydrogen bonds further validated the docking process. The 3D structure of Phenol, 2-methyl-5-(1-methylethyl) docked against MJHP was analyzed using the Argus Lab tool, and the docking reports were visualized and examined through the PyMol visualization tool (Figure 4). The docking interaction between Phenol, 2-methyl-5-(1-methylethyl) and MJHP resulted in a docking score of -8.2151 kcal/mol, forming two hydrogen bonds. These findings indicate the presence of a binding site involving three proteins and seven ligands. The docking process was further validated by hydrogen bond formation. According to Lipinski's rule, the analyzed compound qualifies as a promising therapeutic drug. The in silico docking studies highlight the potential of Phenol, 2-methyl-5-(1-methylethyl) as a natural mosquitocidal agent for mosquito control. Notably, this study is the first recorded report on the molecular docking of Phenol, 2-methyl-5-(1-methylethyl) against MJHP. The visualization of the docked complex between Phenol, 2-methyl-5-(1-methylethyl) and MJHP was performed using the PyMol tool. Similar molecular docking studies have been conducted by Rajesh et al.,[26] Flora et al.,[27] Jayameena et al.,[28], Jayaprakash et al.,[29] Karthika et al.,[30] Rajini Selvaraj et al.,[31] Hemalatha et al.,[32] Mohamad et al.,[33] Manimekalai et al.,[34] Padmavathy et al.,[35] and Angalammal et al.[36] This study demonstrated improved docking binding energy in the selected compounds. The findings further confirm that three compounds from *Momordica tuberosa* serve as ideal candidates for designing and developing effective mosquito control agents.[24] Ten compounds were chosen for molecular docking studies, among which the phytocompounds Pectolinaringenin, Naphthalene decahydro-2,2-dimethyl, and Gamma-linolenic acid were identified as potential mosquito control agents.[37]

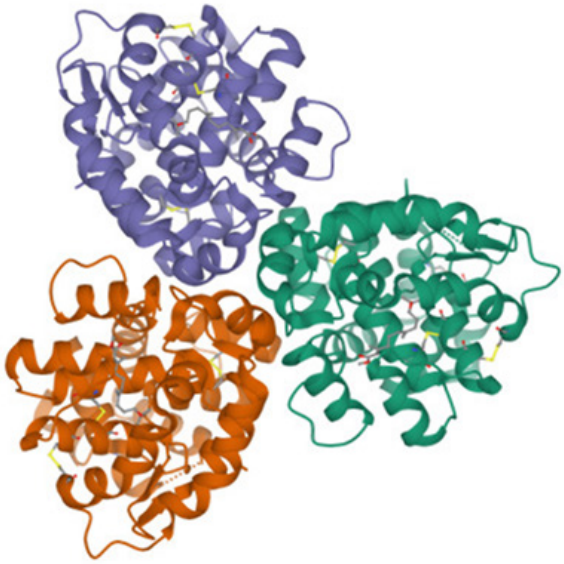

Figure 2 3-D structure of Mosquito juvenile hormone-binding protein.

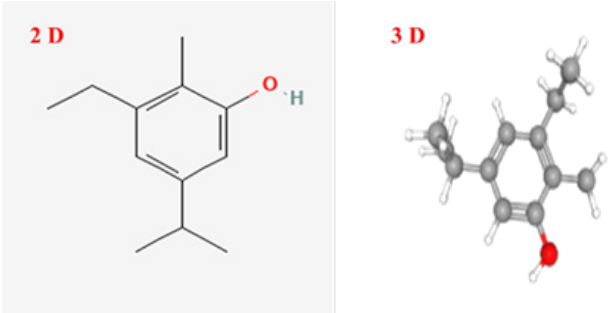

Figure 3 Structure of Phenol, 2-methyl-5-(1-methylethyl).

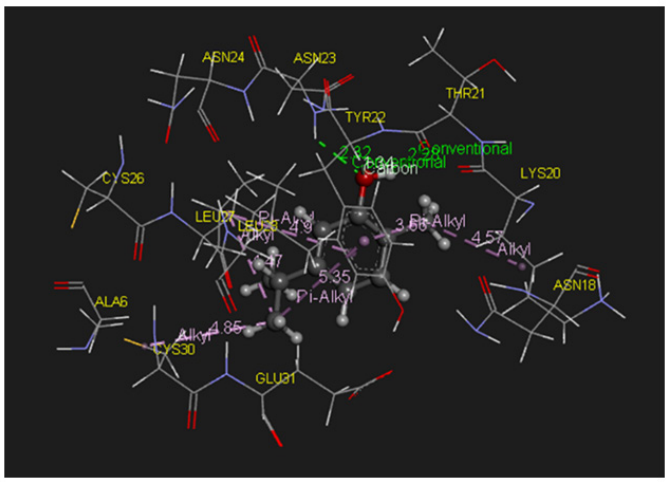

Figure 4 Visualization of docked complex with PyMol tool Phenol, 2-methyl-5-(1-methylethyl) docked with MJHP

Conclusion

The results of this study identified twenty-one compounds from the LME of *W. calendulacea*. One compound was selected for molecular docking analysis, and the MPC exhibited a strong interaction with MJHP. These findings clearly demonstrate that the *W. calendulacea* compound has the potential to inhibit MJHP activity against *Ae. aegypti* by binding to amino acid residues at its active site. The compound Phenol, 2-methyl-5-(1-methylethyl) displayed a stronger binding affinity compared to MJHP. Additionally, further in-vitro studies are necessary to evaluate the effectiveness of these potential inhibitors in molecular docking research and assess their practical applications in real-world settings.

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Conflicts of interest

The authors declare that there was no conflict of interest.

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