

## Antiitch Efficacy of Henna Bioactive Components by Inhibition of Kappa-Opioid Receptors

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In recent times, focus on plant research has increased all over the world and a large body of evidence has been collected to show the immense potential of medicinal plants used in various traditional systems. Nowadays, we are seeing a great deal of public interest in the use of herbal remedies. One of these plants, *Lawsonia Inermis* Linn (Family: Lythraceae) which is commonly known as henna, is mainly present in subtropical and tropical areas and is used all over the world. Henna attracts the care of scientists for its therapeutic activities ranging from antiinflammatory to anticancer activities [1]. Phytochemical studies in the henna plant have indicated the presence of several bioactive molecules like isoplumpagin, lupeol, 30-norlupan-3-ol-20-one, betuhennan, betuhennanic acid, and n-tridecanoate phenolic glycosides, lawsoniaside,  $\beta$ -sitosterol and stigmasterol in leaves and roots. Lawsone (2-hydroxy-1,4-naphthoquinone), the red-orange dye present in the henna leaf paste, is being used in modern pharmacopeia as a starting molecule for the synthesis of clinically important anticancer drugs such as atovaquone, lapachol, and dichloroallyl lawsone [2].

This study is an in-silico approach to investigate the antiitch activity of some bioactive molecules of Henna. Isoplumpagin, lawsaritol, lawsone, lupeol, and stigmasterol were docked against the kappa-opioid receptor (PDB ID: 4DJH), and the results were compared with the antiitch-approved drug, gabapentin. All the selected ligands revealed better efficacy than gabapentin. The results showed that the best binding affinity is in the sequence stigmasterol > lawsaritol > lupeol > isoplumpagin > lawsone > gabapentin, with lots of convergence points. Stigmasterol, with a docking score of -11.54 kcal/mol and an inhibition constant of 3.46 nM exhibited the best antiitch activity and can be considered an effective frame to design new antiitch drugs.

**Keywords:** Antiitch, Henna, Kappa-opioid receptor, Molecular docking

### References

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