



# Docking studies to elucidate the therapeutic potential of phytochemicals derived from *Piper nigrum* for the treatment of vitiligo.

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## INTRODUCTION

Vitiligo, affecting 0.1%-2% globally, results from a complex interplay of 20% environmental and 80% genetic factors. Emerging in childhood or young adults, it indiscriminately impacts individuals of any age, sex, or race.

Vitiligo, an autoimmune disorder, presents as depigmented macules causing melanocyte loss. Two forms exist: segmental (one-sided) and non-segmental (both sides), with complex origins and variable responses to therapy. [1] *Piper nigrum*, or black pepper (Fig. 1), a key spice, is vital in global production of 80,000 metric tons/year, dominated by India, Sarawak, Indonesia, and emerging producer Brazil. Renowned for its medicinal applications, *Piperine*, a pungent alkaloid, imparts various pharmacological benefits. [2]



Fig. 1 -- *Piper Nigrum* Spice (Black Pepper)

Protein JAK1 (Fig. 2) belongs to *Janus Kinase* Family and binds cytokine receptor through amino terminal FERM domains and link them to molecules of the STAT family. [3] CDK1 (Fig. 3), in complex with *cyclin B*, regulates mitosis. The serine/threonine kinase CDK1 forms a heterodimer with cyclin B1 called CDK1/CyclinB1. [4]

Scientific literature supports exploring *Piper nigrum* and JAK1, CDK1 as promising avenues for vitiligo therapy. The interaction of JAK1 and CDK1 with Guaiacol and (E)-Piperolein-A respectively is shown in Fig.- 4 and Fig.-5



Fig. 2-- 3D mol of JAK1

Fig. 3 -- 3D mol of CDK1

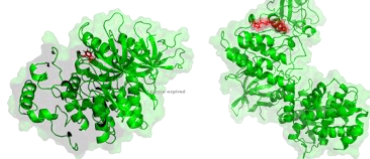


Fig. 4

Fig. 5

Fig. 4 - Ligand interaction of JAK1 with GUA  
Fig. 5 - Ligand interaction of CDK1 with PIP

## METHODOLOGY

The workflow of ligand Docking is shown below (Fig.6).

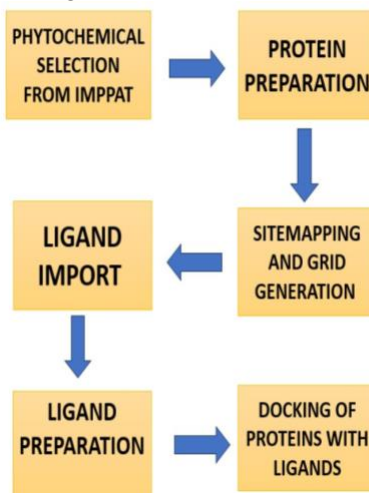


Fig. 6 - Workflow of Ligand Docking

## RESULT

The phytochemicals from *Piper nigrum* exhibited promising results in their interaction with JAK1 and CDK1 (Fig.-8) with the docking score falling within the range of (-6.00 to -6.60). Among the phytochemicals tested from both proteins, *Guaiacol*, *Benzyl Alcohol*, *Carvacrol*, *(E)-Piperolein A*, *Benzyl benzoate*, and *4-Carvomenthenol* emerged standout ligands with strong potential for interaction with JAK1 and CDK1, demonstrating their eligibility for further investigation. The Graph represents Docking Scores (Fig.-7).

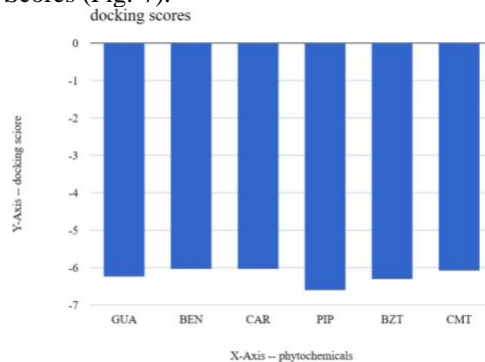


Fig.7 - Bar Graph representing docking scores of phytochemicals.

GUA	BEN	CAR	PIP	BZT	CMT
-6.256	-6.054	-6.036	-6.610	-6.315	-6.082

Fig. 8 - Precise Docking Scores of Phytochemicals

## CONCLUSION

This research highlights the potential of *Piper nigrum* derived phytochemicals as novel therapeutics for Vitiligo. The identified compound exhibit promises for further research. These findings contribute to the exploration of alternative treatments for vitiligo, emphasizing the potential of natural compounds in addressing this autoimmune disorder.

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## ABBREVIATIONS

- GUA – GUAIACOL  
 BEN --- BENZYL ALCOHOL  
 CAR --- CARVACROL  
 PIP -- (E)-PIPEROLEIN A  
 BZT --- BENZYL BENZOATE  
 CMT --- 4-CARVOMENTHENOL