

**Title Of The Manuscript In ‘Title Case’ Written In ‘Times New Roman’ Font  
Size 14 & Bold**

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## **Preparation of Manuscript**

### **Main Text:**

Entire document has be typed in **1.5 spacing** and ‘Times New Roman’ style and font size 12.  
Entire document should have a margin of 2.54cm on all 4 sides.

### **Main Headings:**

Should be in ‘Times New Roman’ font style, font size 14, Bold and Title Case.

### **Sub Headings:**

Should be in ‘Times New Roman’ font style, font size 12, Bold and Title Case.

### **Referencing Style:**

‘**Vancouver**’ referencing style is to be followed for all references. In Text references should be mentioned in Arabic Numerals in first-come-first-serve basis and the numbers should be entered in superscripted square brackets at the end of sentences like <sup>[1,2]</sup>. The references in the bibliography at the end of the document should be represented in the following format ‘Vancouver’

#### **Journal Article:**

1. Kumar S. Computational identification and binding analysis of orphan human cytochrome P450 4X1 enzyme with substrates. BMC Res Notes. 2015;8(1):1–10.
2. Stalin K, Ravi L, Raghavan V. Extraction, purification and structural elucidation of environmentally benign antifouling metabolite from *Streptomyces thermolineatus* VITKV6A. Environmental Technology & Innovation. 2022;25:102096.

### **Figures & Tables**

All figures and tables should be numbered sequentially, and should appear in the main text where they are discussed. Figures should be of high quality (minimum 300dpi). All figures and tables should have a self-explanatory legend. Figure’s legend should be below the figure, while table’s legend should be above the table.

### **Plagiarism Report**

**Manuscripts will be accepted only if the plagiarism content is less than 12%.**

## **Abstract**

Abstract should be written in 'Times New Roman' with font size 12 and should contain word count of 150 to 250 words. Highlight the key findings and significance of this study. What are the key methods incorporated in this study. What does the study conclude and what are its future prospects.

**Keywords:** *Erysiphe necator*, Homology modeling, Protein drug targets, PMDB, AutoDock.

*(Separate each key word with coma)*

## **Introduction**

Grape is one of the most important economical and commercial fruit for the world and it is a major contribution to the country's GDP (Gross domestic product) and it is a wide adaptability crop <sup>[1,2]</sup>. *Vitis vinifera* is a dicotyledonous and annual crop plant species that is a member of the Vitaceae family, commonly called "grape" and "draksha"<sup>[3]</sup>, it's cultivated in temperate, sub-tropical, tropical regions, all over the world <sup>[1,3,4]</sup>. Global production of grape is estimated to 67 million metric tons per annum at present. China is one of the leading country in the production of grape with 8,651.83 thousand tons, followed by Italy (7,787.83 thousand tons), the united states of America (6,777.73 thousand tons), Spain (6,107.20 thousand tons), France, Turkey, Argentina, chile, and south Africa<sup>[1]</sup>. India occupies the eighteenth position in world for production of grape and it's cultivated in an area of 111.4 thousand hectares with a production of 1,234.9 thousand tons <sup>[1]</sup>. Almost 71% of global grape production is used for wine, 27% fresh fruit, 2% dried fruit <sup>[3]</sup>.

## **Materials & Methods**

### **Isolation Of Bacteria**

The soil sample is serially diluted upto  $10^{-4}$  dilutions and the diluted sample is loaded on to a freshly prepared nutrient agar plate. The cultured plates are then incubated at 37°C for 24hrs and then observed for colony growth <sup>[4]</sup>.

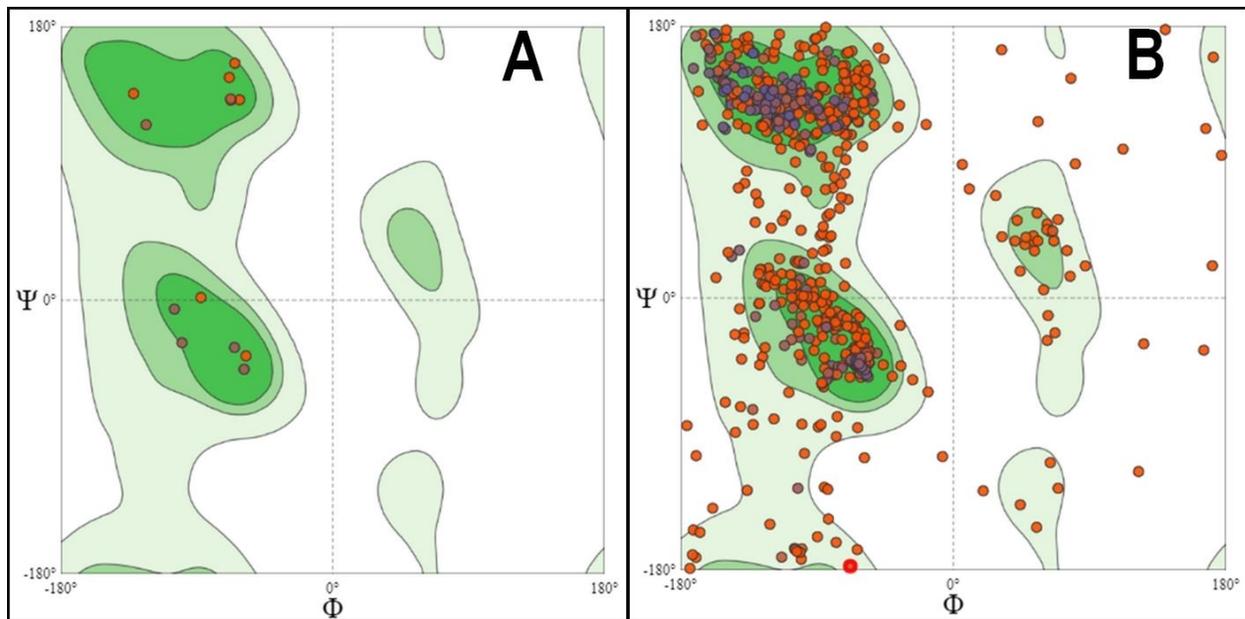
### **Extraction Of Phytochemicals**

Dried plant leaf samples are grounded well using mortar and pestle and the phytochemicals are extracted using maceration technique for 48hrs. The mixture of solvents and plant sample are mixed in magnetic stirrer for 48hrs and then the solvent is separated using filtration via Whatmann No.1 filter paper. The filtered solvents are then dried to obtain crude extract of the phytochemicals <sup>[5]</sup>.

## Results And Discussion

### Ramachandran Plot Analysis

The ramachandran plot analysis was performed for all protein model structures constructed in SWISSModel tool. The protein models that demonstrated more than 90% of residues in the favored regions of the ramachandran plot were considered to be reliable for structural applications. All 66 proteins demonstrated above 90% of the residues within the favored regions in the ramachandran plot and hence were considered for further processing. Graphical representation of ramachandran plot analysis of a preferred protein model with 100% of residues in favored region and a least preferred model with 82% of residues within the favored region are shown in Figure.1.



**Figure.1:** Ramchandran plot protein analysis of constructed protein models. A: Preferred model with 100% residues in favored region; B: Least preferred model with 82% residues in the favored region.

## PMDB ID submission

All 66 protein model structures that were verified using ramachandran plot were then submitted to PMDB (Protein Model Data Base: [srv00.recas.ba.infn.it](http://srv00.recas.ba.infn.it) > PMDB) website. The protein model structures were submitted to public database for easy access to researchers to further applications of the same. The list of constructed protein models that were submitted to PMDB is tabulated in Table.1.

**Table.1:** Modeled protein structure submissions to PMDB

Sl.No.	Drug target name	UniProt ID	PMDB ID
1	ATP-dependent DNA helicase PIF1	A0A0B1PEI0	PM0082721
2	Adenylyltransferase and sulfurtransferase uba4	A0A0B1P610	PM0082722
3	Phosphatidylserine decarboxylase proenzyme 2	A0A0B1P526	PM0082728
4	Putative myosin class v myosin	A0A0B1P6S1	PM0082816
5	ATP-dependent 6-phosphofructokinase	A0A0B1PDE5	PM0082731
6	NADPH--cytochrome P450 reductase	A0A0B1P387	PM0082732
7	Proliferating cell nuclear antigen	A0A0B1NZA1	PM0082733
8	Adenylate kinase	A0A0B1P0M5	PM0082735
9	GTP:AMP Phosphotransferase	A0A0B1PEI1	PM0082736
10	Glutathione reductase	A0A0B1P915	PM0082738

## **Conclusion**

The current study aimed at construction of 3D computational protein model structures of a un explored fungal pathogen *Erysiphe necator* that causes powdery mildew disease, which causes a great economical impact in grapewine crop cultivation. Further to demonstrate the SBCADD application of the constructed protein models, protein-ligand docking analysis was carried between two known antifungal drugs and their drug targets. Among the two test antifungal agents, tebuconazole was found to be a better effective antibiotic that could possibly help control the infection of this pathogen in grape cultivation. However, further in-silico validation and in-vitro studies are required for confirmation.

## **Acknowledgement:**

The authors thank the institution for supporting this research work.

## **Conflict Of Interest**

No known conflict of interest.

## **Funding Source**

No funding was availed for this work.

## References:

1. Shinde PV. An Economics of Grapes under Horticulture in India. *Int J Res Sci Innov.* 2016;3(2):69–71.
2. Sharma D, Rani R, Chaturvedi M, Yadav JP. Antibacterial Capacity and Identification of Bioactive Compounds By Gcms of Allium Cepa. *Int J Pharm Pharm Sci.* 2018;10(2):116.
3. Kumar S, Sandhir R, Ojha S. Evaluation of antioxidant activity and total phenol in different varieties of Lantana camara leaves. *BMC Res Notes.* 2014;7(1):1–9.