International Research Journal of Innovations in Engineering and Technology (IRJIET)

ISSN (online): 2581-3048

Volume 8, Issue 7, pp 43-52, July-2024

https://doi.org/10.47001/IRJIET/2024.807004

Insilico Approach to Find Bioactive Compound against Fruit Rot Disease (FRD) in *Areca Catechu*

[1]Sharada S B, [2]Ajay A Shettigar, [3]Bhuvaneshwari, [4]Shailashree C Ganiger

[1]Associate Professor, Department of Biotechnology, Basaveshwar Engineering College, Bagalkote, Karnataka, India
[2,3,4]Student of Biotechnology Engineering, Basaveshwar Engineering College, Bagalkote, Karnataka, India

***Abstract* - *Phytophthora meadii* is a fungal species which causes Fruit Rot Disease (FRD) in *Areca catechu* affects the quality and yield which is main threat for agricultural economy. Traditional methods include chemical fungicides like bordeaux mixture, Fosetyl-al, metalaxyl, mancozeb, copper oxychloride, cymoxalin, copper sulfate, etc in treatment of FRD, which can lead to environmental and health issues. In this study, an in silico approach was employed to identify potential bioactive compounds that could serve as effective agents against the pathogens responsible for FRD in *Areca catechu.* Utilizing a combination of molecular docking and virtual screening, we screened a comprehensive library of natural compounds for their ability to inhibit key enzymes and proteins associated with FRD pathogens. The molecular docking analysis focused on identifying compounds with high binding affinities to target proteins, suggesting their potential efficacy in disrupting pathogen activity. Among the screened compounds, several compounds have shown strong binding affinities indicating their potential as bioactive agents against FRD pathogens. These findings provide a promising foundation for the development of natural, environmentally-friendly treatments for FRD in *Areca catechu*.**

Keywords: *Areca catechu*, Fruit Rot Disease, FRD, Molecular docking, bioactive compounds.

I. INTRODUCTION

Areca catechu is commonly known as betel nut or areca nut belongs to the family Arecaceae (palm family). It is grown in tropical regions of Asia and Pacific. In India, it is seen in coastal areas of Karnataka, Kerala, Tamil Nadu, West Bengal, Assam etc. Karnataka is the largest producer of *Areca catechu*. India's annual production is about 14 lakh tonnes and it is cultivated on around 7.7 lakh hectares area. Arecanut is chewed along with lime and betel leaves which acts as stimulant. *Areca catechu* is medium sized tree which grows straight 20 m (66 ft) in height with trunk size of 10-15cm (4-6 in) in diameter [11].

Taxonomy

Kingdom- Plantae
Phylum- Angiosperms
Class- Monocots
Order- *Arecales*
Family- *Arecaceae*
Genes- *Areca*
Species- *A. catechu*[11]

Fruit rot disease is commonly called as koleroga in karnataka. It is caused by a fungal species *Phytopthora meadii*. Due to heavy rain in monsoon season, humidity increases on the surface of the nut which provides suitable environment for the growth of pathogen. The fungus invades and disrupts the cell wall of the fruit that leads to rotting of nuts results in yield loss.

Fungus adheres to the surface of fruit then releases the zoospores. These zoospores combine together to form an encysted zoospores. Encysted zoospores produces germ tube, through germ tube spores enter plant body and infect the plant. The mycelium grows on infected plant body results in yellowing and browning of leaves. It under goes two types of reproduction namely asexual and sexual reproduction. Mycelium produces the sporangium which rapidly spread and infects the host and restarting the asexual reproduction. In sexual reproduction, oogonium and antheridium fuse together to form oospore results in the formation of multinucleate sporangium, this cycle continues.

Figure 1: Fruit Rot Disease (FRD)

International Research Journal of Innovations in Engineering and Technology (IRJIET)

ISSN (online): 2581-3048

Volume 8, Issue 7, pp 43-52, July-2024

https://doi.org/10.47001/IRJIET/2024.807004

Conventional methods are used to treat fruit rot disease by spraying some chemicals namely Bordeaux mixture, Metalaxyl, mancozeb, aliette, etc. However, this method is not much effective and precise to target site instead insilico approach is more efficient with fewer side effects. Below softwares helps us to screen the chemical compounds virtually to identify potential candidates in inhibiting the pathogen in fruit rot diseases.

List of softwares used for docking

Autodock comprises of automated docking tools. These tools are designed to predict the size of molecules that involves substrates or drug (target) molecules, bind to a receptor of known 3D structure. Current distributions of AutoDock consist of two generations of software: AutoDock 4 and AutoDock Vina. More recently, we developed AutoDock-GPU, an accelerated version of AutoDock4 that is hundreds of times faster than the original single-CPU docking code. AutoDock 4 actually consists of two main programs: Autodock performs the docking of the ligand to a set of grids describing the target protein; autogrid pre-calculates these grids. AutoDock Vina does not require choosing atom types and pre-calculating grid maps for them. Instead, it calculates the grids internally, for the atom types that are needed, and it does this virtually instantly.

Open babel GUI is a chemical tool box which is designed to understand the many languages of chemical data. This is an open source helps to search, analyse and convert one file format to another file format.

PyMOL is one of the few mostly open-source model visualization tools available for use in structural biology. The Py part of the software's name refers to the program having been written in the programming language Python.

II. OBJECTIVES

- To identify the existing bioactive compounds for fruit rot disease in *Areca catechu.*
- To perform molecular docking using Autodock Vina and to get the binding affinity scores.
- To filter and analyse the best interaction between the target and the bioactive compoundfrom docking results for fruit rot disease in *Areca catechu.*

III. METHODOLOGY

3.1 Selection and listing of bioactive active compounds for Docking studies

Selection and listing of bioactive compounds was performed using the tools namely PDB (Protein Data Bank), Chembl and Pubchem. For protein go to the Protein Data Bank website: www.rcsb.org.Search for the Protein: In the search bar, enter the name, keyword, or PDB ID of the protein of interest. Select the Protein Entry Browse through the search results and select the entry that best matches your query. Each entry will have a PDB ID and a brief description. Download the Protein Structure File. On the protein's detailed page, look for the "Download Files" section. There we find options to download the structure file in different formats. The most common format is the PDB format (.pdb file). Click on "PDB Format" to download the .pdb file. Save the File. Similarly the process goes with the Chembl and Pubchem. Open babel GUI is a tool which is used to convert one file format to required file format. Convert chemical file formats easily using a graphical interface. Supports over 110 different chemical file formats, allowing conversion between various formats (e.g., SMILES, InChI, MOL, XYZ).

Table 1: List of receptor molecules

Name of receptor	Order
Chitin molecule	2-26
Calcium binding protein	27-54

Link for protein:
https://docs.google.com/spreadsheets/d/1uyYVfoPeuZOGmD9lWBPEJFf7CFI8qc_e9SAzlAWoVr0/edit#gid=0

Table 2: List of ligands

Name of ligand	2d	3d
Fosetyl-al	2	219
Metalaxyl	3-28	220-239
Mancozeb	29-48	240-247
Copper oxichloride	49-51	248
Cymoxanil	52-64	249-256
Cupric sulfate	65	
Lime	66-68	257
Dithane M45	69	258
Dithane M46	70	
Dithane M47	71	
Isothiazolinone	71-82	259-268
Chlorothalonil	83-97	269-280
Dimethomorph	98-104	281-287
Fenamidone	105-109	288-291
Carbendazin	110-111	292

International Research Journal of Innovations in Engineering and Technology (IRJIET)

ISSN (online): 2581-3048

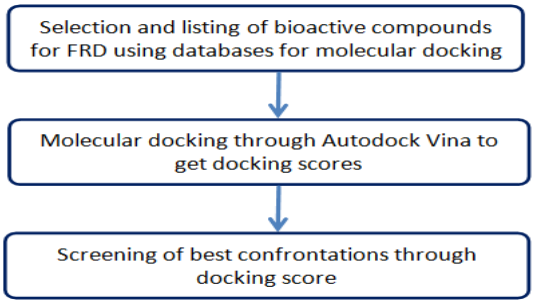
Volume 8, Issue 7, pp 43-52, July-2024

https://doi.org/10.47001/IRJIET/2024.807004

Mandipropamid	112-122	293-302
Iprovalicarb	123-129	303-309
Benthiavalicarb	130-140	310-319
Cyazofamid	141-146	320-325
Cycocel	147	326
Famoxadone	148-151	327-329
Propineb	152-157	330-333
Carboxylic acid amide	158-172	334-348
Cyanoimidazole	173-179	349-355
Potassium phosphonate	180-217	356-381
Fosetyl-aluminium D15	218	

Link for 2D /3D ligand molecule:
https://docs.google.com/spreadsheets/d/1BILEAlI_HUSLKVsmJ6xVarsKO_Dz8C5mwsJYroRd7bI/edit#gid=0

Flowchart



3.2 Docking through Autodock Vina

Open Auto dock Vina and set a path to carryout the docking process, then click on file option and choose the downloaded PDB structure file which will appears on the screen. PDB structure consists of water molecule and other chains. In Auto dock Vina, consider only one chain and remove water molecules and other hetero atoms from the protein structure which are not required, then repair the missing atoms (edit → misc → repair missing atoms) it will take around 4 minutes to complete the process based on number of amino acids present in protein structure. Add polar hydrogens and kolmn charges to it. Check for equal charge distribution (edit → charge →check charge distribution).

From the file, download the ligand structure. The ligand structure binds to the protein structure. Automatically Auto dock will add the hydrogen atoms and charges and also show how many rotatetable bonds, aromatic carbons are present. Go to ligand option, then torsion free detect option it will show the route of ligand. Now, check for the active torsion sites. Then click on turn so that ligand molecule will be added. Create grid (grid → macromolecules → choose) and save as 'receptor. PDB file'. Grid → Set map types → Choose ligand → Grid box. Since we don't know the active site of the protein, blind docking is done. For blind docking, the grid box is added to whole protein structure. In some cases, active sites of protien can be obtained from their web page that can be directly used for docking. Then find the XYZ coordinates of crystal structure. Using active site value of protein and choose the last atoms values of amino acids based on number of active sites that are known and sum up the number of coordinates and divide it by number of amino acids. The exact values of XYZ coordinates are obtained. Put these values in grid box. Then we found the exact location of active site of amino acid.

Go to file and save in current. Create grid parameter file and save. Click on 'run→Click on autogrid →browse →launch', the gridlock is created. Next go for 'docking→ macromolecule→ set rigid docking (receptor file)'. Again go for docking→ ligand →choose ligand (click on accept). Now go for 'docking →search parameter→ genetic algorithm (change the parameters)→ click on accept'. Then docking→ output→ lamarckian GA(4.2)[save this file]. Then all set for docking, go to run→ run autodock(browse docking file and docking parameter). After few minutes based on number of runs docking process has been done. Some major files has been generated namely GLG file and many grid log file and DLG file. DLG file gives information about about binding energies of protein. Go to analyse → docking→open (DLG format file). next analyse → macromolecules→ open. Go to analyse → conformation →play. Go to open pannel option, build hydrogen bond and show information.

For multiple ligand docking, create a new folder, using mgltools create pdbqt files for receptor and copy the configuration of the receptor file from mgltools. Configuration receptor file includes center X,Y,Z and size X,Y,Z. Using bash script, different pdbqt files from folder can be identifed. It creates the multiple folders and directories based on the ligand name. The output will be out.pdbqt and also creates log files using log.text. Go to terminal, navigate to the directory and for multiple ligand docking execute the script, add vina executable and press enter. Output ligand file is created in the folder and a log file is also created which consists of binding affinity or binding energy.

3.3 Screening of compounds through docking scores

Screening is done through docking scores obtained where each ligand receives a docking score for its best pose. Lower (or more negative) scores typically indicate better binding affinity. The ligands are ranked based on their docking scores.

International Research Journal of Innovations in Engineering and Technology (IRJIET)

ISSN (online): 2581-3048

Volume 8, Issue 7, pp 43-52, July-2024

https://doi.org/10.47001/IRJIET/2024.807004

The top-ranked ligands are considered the most promising candidates for further study. To facilitate the analysis, ligands are often grouped and color-coded. Different chemical families or classes of ligands can be assigned different colors.

The best confrontations (poses) of the top-ranked ligands are analyzed in detail to understand their binding modes. Key interactions with the protein, such as hydrogen bonds, hydrophobic interactions, and salt bridges, are examined. Based on the docking scores and binding mode analysis, the most promising ligands are selected for further experimental validation and optimization.

IV. RESULTS AND DISCUSSION

Docking for both groups of receptor molecules has been performed, and top hits for each ligand are filtered based on the RMSD value and binding affinity. All these tophits' results were combined into a single file, and a scatter plot was obtained for each receptor molecule under a similar category.

Two categories were grouped as Chitin molecules and Calcium-binding proteins, respectively. For each group, 12 binding score scatter plots were obtained. These scatter plots are combined on a single page for easy analysis of the performance of ligands in each category.

Linux terminal is used to filter all the output results and identify the tophits based on the RMSD values.

Table 1: Image of top_score.txt files obtained after filtering the results

Output will be druglig_out.pdbqt			
1	-5.0	0.000	0.000
Output will be druglig1_out.pdbqt			
1	-6.0	0.000	0.000
Output will be druglig10_out.pdbqt			
1	-6.3	0.000	0.000
Output will be druglig100_out.pdbqt			
1	-6.0	0.000	0.000
Output will be druglig101_out.pdbqt			
1	-6.0	0.000	0.000
Output will be druglig109_out.pdbqt			
1	-5.0	0.000	0.000
Output will be druglig111_out.pdbqt			
1	-3.5	0.000	0.000
Output will be druglig112_out.pdbqt			
1	-3.6	0.000	0.000
Output will be druglig113_out.pdbqt			
1	-5.0	0.000	0.000
Output will be druglig114_out.pdbqt			
1	-3.4	0.000	0.000
Output will be druglig116_out.pdbqt			
1	-6.5	0.000	0.000
Output will be druglig120_out.pdbqt			
1	-8.0	0.000	0.000
Output will be druglig124_out.pdbqt			
1	-4.4	0.000	0.000
Output will be druglig125_out.pdbqt			
1	-4.9	0.000	0.000
Output will be druglig126_out.pdbqt			
1	-5.0	0.000	0.000
Output will be druglig127_out.pdbqt			
1	-5.9	0.000	0.000
Output will be druglig128_out.pdbqt			
1	-6.0	0.000	0.000
Output will be druglig129_out.pdbqt			
1	-4.3	0.000	0.000

Output will be druglig_out.pdbqt			
1	-4.9	0.000	0.000
Output will be druglig1_out.pdbqt			
1	-6.0	0.000	0.000
Output will be druglig10_out.pdbqt			
1	-7.0	0.000	0.000
Output will be druglig100_out.pdbqt			
1	-6.2	0.000	0.000
Output will be druglig101_out.pdbqt			
1	-6.7	0.000	0.000
Output will be druglig109_out.pdbqt			
1	-4.5	0.000	0.000
Output will be druglig111_out.pdbqt			
1	-3.4	0.000	0.000
Output will be druglig112_out.pdbqt			
1	-3.4	0.000	0.000
Output will be druglig113_out.pdbqt			
1	-5.8	0.000	0.000
Output will be druglig114_out.pdbqt			
1	-3.7	0.000	0.000
Output will be druglig116_out.pdbqt			
1	-7.5	0.000	0.000
Output will be druglig120_out.pdbqt			
1	-8.3	0.000	0.000
Output will be druglig124_out.pdbqt			
1	-4.2	0.000	0.000
Output will be druglig125_out.pdbqt			
1	-5.3	0.000	0.000
Output will be druglig126_out.pdbqt			
1	-5.9	0.000	0.000
Output will be druglig127_out.pdbqt			
1	-6.1	0.000	0.000
Output will be druglig128_out.pdbqt			
1	-6.7	0.000	0.000
Output will be druglig129_out.pdbqt			
1	-4.4	0.000	0.000
Output will be druglig13_out.pdbqt			

International Research Journal of Innovations in Engineering and Technology (IRJIET)

ISSN (online): 2581-3048

Volume 8, Issue 7, pp 43-52, July-2024

https://doi.org/10.47001/IRJIET/2024.807004

Output will be druglig13_out.pdbqt			
1	-5.7	0.000	0.000
Output will be druglig131_out.pdbqt			
1	-4.0	0.000	0.000
Output will be druglig132_out.pdbqt			
1	-3.0	0.000	0.000
Output will be druglig133_out.pdbqt			
1	-5.2	0.000	0.000
Output will be druglig134_out.pdbqt			
1	-4.7	0.000	0.000
Output will be druglig135_out.pdbqt			
1	-5.8	0.000	0.000
Output will be druglig144_out.pdbqt			
1	-8.3	0.000	0.000

1	-6.0	0.000	0.000
Output will be druglig131_out.pdbqt			
1	-3.7	0.000	0.000
Output will be druglig132_out.pdbqt			
1	-3.6	0.000	0.000
Output will be druglig133_out.pdbqt			
1	-5.6	0.000	0.000
Output will be druglig134_out.pdbqt			
1	-5.1	0.000	0.000
Output will be druglig135_out.pdbqt			
1	-5.7	0.000	0.000
Output will be druglig144_out.pdbqt			
1	-9.0	0.000	0.000

Table 2: Image of ligand entries and their docking scores for plotting the scatter plots

0	-3.3
1	-5
10	-6.2
100	-4.3
101	-4.5
109	-3.3
111	-2.5
112	-2.2
113	-4.4
114	-3.4
116	-6.6
120	-6.7
124	-2.9
125	-4
126	-4.9
127	-4.1
128	-4.3
129	-3.3
13	-4.7
131	-2.5
132	-2.2
133	-3.8
134	-3.9
135	-4.2
144	-6.3
145	-4.3
146	-4.2
15	-3.6
150	-4.6
151	-2.7
152	-5.1
153	-2.6
155	-3.2
159	-5.1
163	-4.4
169	-5.1
172	-3.4
173	-1.8
174	-6.8

0	0
1	-3.5
3	-3.6
4	-5.4
10	-3
13	0
15	-5.4
18	0
21	0
22	-3.1
23	0
24	0
25	0
26	-1.4
29	-1.9
30	0
31	-5.2
32	0
33	-4.7
34	0
36	-3.5
37	0
38	-6.2
39	-4.3
41	-4.1
42	0
44	-3.4
45	-6.4
47	-6
48	0
100	-2.3
101	-3.2
109	-2
111	-2.8
112	0
113	0
114	0
116	0
120	0

0	-4.4
1	-5.2
3	-4.5
4	-5.3
5	-5.1
7	-4.4
8	-5.4
10	-6.9
13	-4.5
15	-5.4
18	-6
21	-7.3
22	-4.1
23	-4.6
24	-4.5
25	-4.9
26	-3.2
29	-3.1
30	-3.4
31	-4.3
32	-2.8
33	-5.8
34	-3.8
36	-3.8
37	-4.7
38	-6.4
39	-5.2
41	-5.1
42	-4.6
44	-4.1
45	-5.9
47	-6.6
48	-4.8
49	-7.1
50	-5.8
52	-6
53	-2.3
56	-6.6
57	-5.8

0	-4.9
1	-6
3	-5.7
10	-7
13	-6
15	-5.7
18	-7.2
21	-7.9
22	-5.8
23	-5.1
24	-5.7
25	-5.7
26	-3.7
29	-3.5
30	-4
31	-4.9
32	-3.7
33	-5.8
100	-6.2
101	-6.7
109	-4.5
111	-3.4
112	-3.4
113	-5.8
114	-3.7
116	-7.5
120	-8.3
124	-4.2
125	-5.3
126	-5.9
127	-6.1
128	-6.7
129	-4.4
131	-3.7
132	-3.6
133	-5.6
134	-5.1
135	-5.7
144	-9

International Research Journal of Innovations in Engineering and Technology (IRJIET)
ISSN (online): 2581-3048
Volume 8, Issue 7, pp 43-52, July-2024
https://doi.org/10.47001/IRJIET/2024.807004

175	-3.6	124	-3.1	60	-5.6	145	-5.4
176	-6.7	125	-3.7	62	-6.1	146	-4.2
178	-4.1	126	-0.4	63	-4.4	150	-5.5
179	-3.7	127	0	65	-4.6	151	-3.9
18	-6.2	128	0	68	-4.7	152	-8.1
182	-6.2	129	-2.5	69	-5.7	153	-3.7
183	-4.8	131	-2	70	-7.2	155	-6.3
184	-5.5	132	-3.9	71	-4.4	159	-7.9
186	-2.8	133	0	76	-5	163	-5.8
187	-4.9	134	0	79	-7.7	169	-6.6
188	-2.9	135	-3.6	80	-6.3	172	-4.9

4.1 Inference for Chitin molecules:

All the ligands that are docked against the chitin molecules have an average binding score ranging from -2 to -7. Among them, the ligands ranging from 0-100 & 200-300have performed well with a higher average docking score of less than-7 in 7 out of the 12 chitin molecule receptor structures. The ligands ranging from 100-200 have performed well with a higher average docking score of less than -7 in 9 out of the 12chitinmolecule receptor structures. The scatter plot is given in the Figure 2.

4.2 Inference for Calcium-binding proteins:

All the ligands that are docked against the calcium-binding proteins have an average binding score ranging from -2 to -7. Among them, the ligands ranging from100-150 & 150-200 have performed well with a higher average docking score of less than -7 in 9 out of the 12 calcium-binding protein receptor structures. The scatter plot is given in the Figure 3.

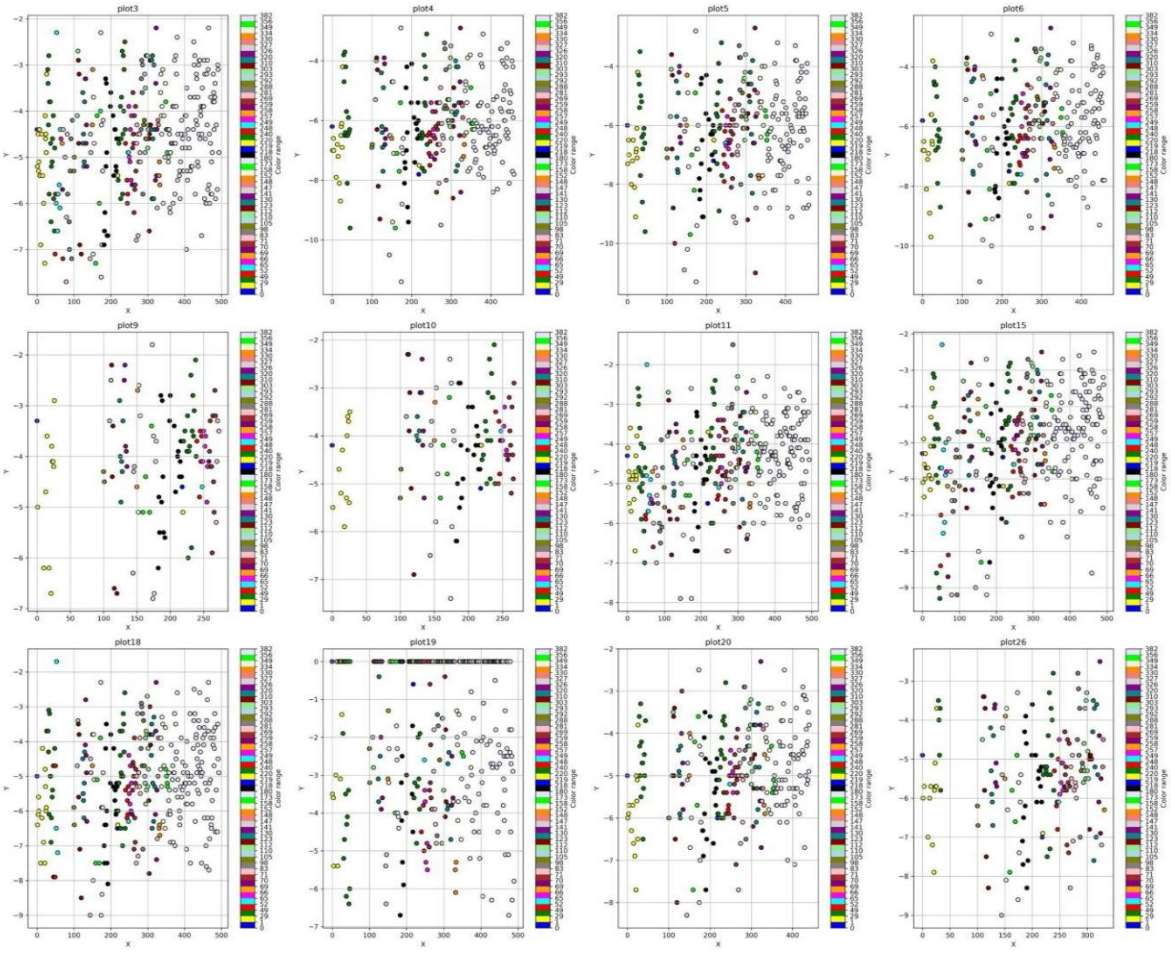


Figure 2: Chitin molecule and ligand interaction

International Research Journal of Innovations in Engineering and Technology (IRJIET)

ISSN (online): 2581-3048

Volume 8, Issue 7, pp 43-52, July-2024

https://doi.org/10.47001/IRJIET/2024.807004

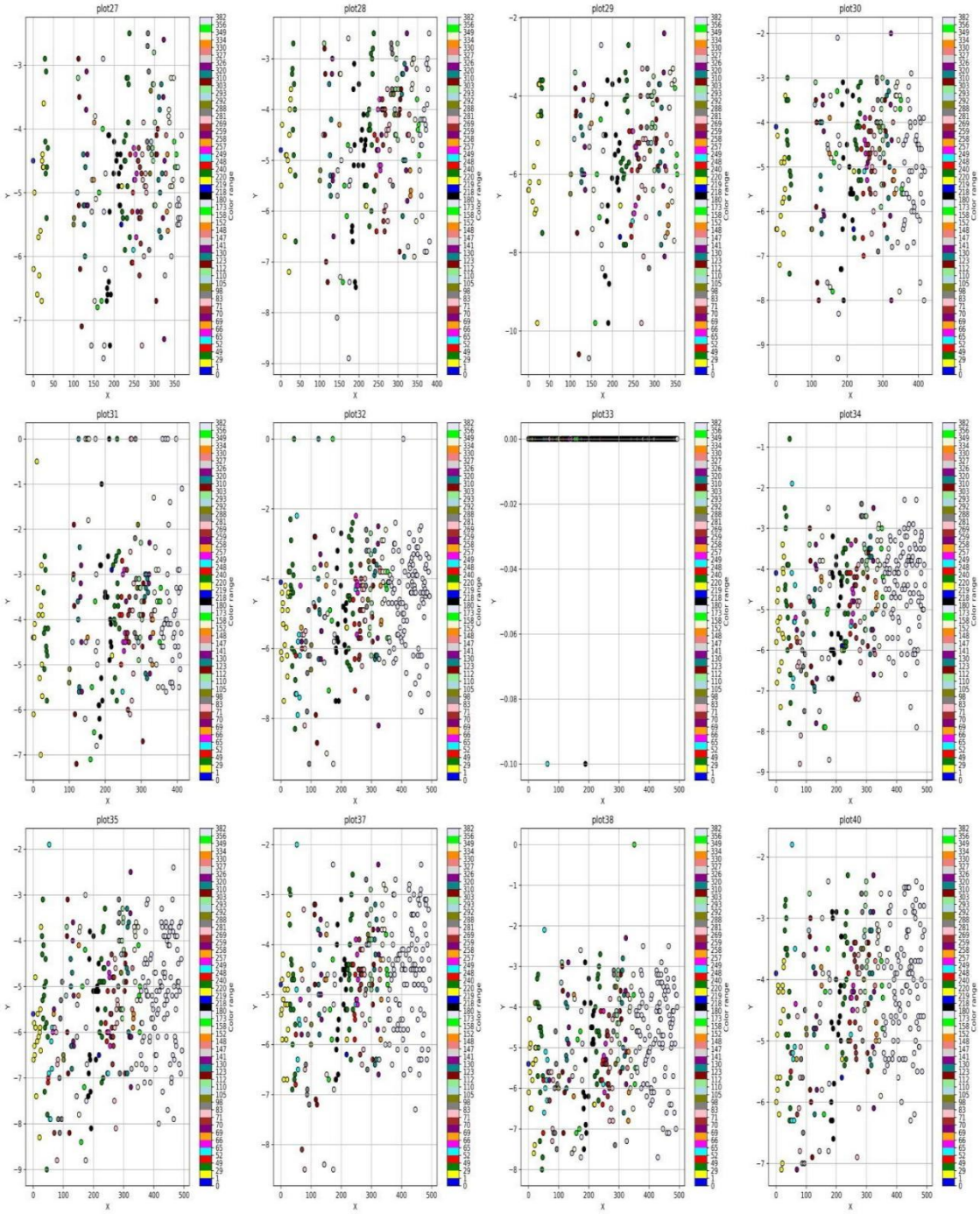


Figure 3: Calcium binding protein and ligand interaction

4.3 Best performing ligand:

Among all the ligands, there are a few ligands that have performed extremely well with far higher docking scores. Among them, cyazofamid, cyanoimidazole, propeneb, and mandipropamid are the ligands with binding scores below -10. Cyanoimidazole has the highest binding score of -11.4 with the chitin molecule receptor structure (1DQC). Also, cyazofamid has docking scores of -10.5, -10.9, -11.2, and -10.7 with three chitin receptor structures (1DQC, 7WJL, 7WJO) and one calcium-binding protein receptor structure (1A03), respectively.

V. DISCUSSION

Insilico methods, such as molecular docking, are essential in modern research for predicting interactions between molecules and biological targets. AutoDock Vina, a widely used molecular docking tool, has been successful in similar projects due to its accuracy and efficiency in identifying high-affinity compounds. In our study, we employed AutoDock

ISSN (online): 2581-3048
Volume 8, Issue 7, pp 43-52, July-2024
https://doi.org/10.47001/IRJIET/2024.807004

Vina to find potential solutions for fruit rot disease in Areca catechu (betel nut), a significant threat to cultivation causing substantial economic losses. AutoDock Vina has proven to be an effective software for addressing problems related to plant species. Its advanced algorithms and high accuracy in predicting molecular interactions make it a valuable tool for agricultural research (Trott & Olson, 2010). Numerous studies have utilized AutoDock Vina to identify compounds that can combat plant diseases and improve crop protection. For instance, it has been successfully applied to find potential inhibitors for various plant pathogens, leading to sustainable and environmentally friendly solutions. The software's ability to handle large datasets efficiently makes it ideal for screening numerous ligands against multiple plant receptor targets. Overall, AutoDock Vina's success in similar projects underscores its importance in developing effective treatments for plant diseases. We gathered two groups of receptor structures and multiple ligand categories from the literature, performing docking studies for each receptor against each ligand to identify high-affinity compounds. The docking studies identified several promising ligands, including cyazofamid, cyanoimidazole, propeneb, and mandipropamid, with binding scores below -10. Cyanoimidazole had the highest binding score (-11.4) with the chitin molecule receptor (1DQC), and cyazofamid showed high scores with multiple receptors, including chitin and calcium-binding proteins. Traditional chemical treatments for fruit rot can have adverse environmental and health effects, highlighting the need for sustainable alternatives. The high-affinity ligands identified offer a promising basis for further research and experimental validation, demonstrating the value of computational methods like AutoDock Vina in developing sustainable agricultural solutions.

VI. CONCLUSION

The Insilico approach has proven to be a valuable and efficient method for identifying potential bioactive compounds to combat fruit rot disease in Areca catechu. Insilico methods significantly reduce the time and cost associated with traditional drug discovery and development processes. Virtual screening and molecular docking allow for the rapid evaluation of numerous compounds for their potential biological activity against specific targets associated with fruit rot disease. This high-throughput capability enables the identification of promising candidates from large datasets. In silico tools facilitate the identification of compounds that specifically interact with molecular targets known to play a crucial role in the pathology of fruit rot disease. This targeted approach increases the likelihood of discovering effective bioactive compounds. While in silico methods are powerful, they are most effective when integrated with experimental validation, ultimately contributing to sustainable agricultural practices and the protection of this economically important crop.

REFERENCES

[1] Alessio Del Conte, Alexander Miguel Monzon, Damiano Clementel, Giorgia F. Camagni, Giovanni Minervini, Silvio C. E. Tosatto and Damiano Piovesan. (2023), 'RING-PyMOL: residue interaction networks of structural ensembles and molecular dynamics', *Bioinformatics*, Volume 39, Issue: 5.

[2] Amith Abraham, Sunil Kumar Puthenpurackal Narayanan, Shaji Philip, Divya Gopalakrishnan Nair, Aparna Chandrashekaran and Jayachandran Kochupurackal. (2013), 'In silico characterization of a noval β-1, 3-gluanase gene from bacillusamyloliquefaciens-a bacterial endophyte of Hevea brasiliensis antagonistic to *phytophthora meadii', J Mol Model*, Volume19, Issue:3, pages: 999-1007.

[3] Balanagouda Patil, Vinayaka Hegde, Shankarappa Sridhar, Hanumappa Narayanaswamy, Munjunatha K. Naik , Kiran Kumar R. Patil, Hosahatti Rajashekara and Ajay Kumar Mishra. (2022), 'Exploring the Impact of Climatic Variables on Arecanut Fruit Rot Epidemic by Understanding the Disease Dynamics in Relation to Space and Time', *Journal of Fungi* Volume 8, Issue: 7, page: 745.

[4] Balanagouda Patil, Vinayaka Hegde, Shankarappa Sridhar, R.Thava Prakasa Pandian, Shivaji H.Thube, Gangaraj Karyath Palliath, Sunil S. Gangurde and Prakash Kumar Jha. (2022), 'Multigene phylogeny and haplotype analysis reveals predominance of oomycetous fungus, *Phytophthora meadii* (McRae) associated with fruit rot disease of arecanut in India', *Saudi Journal of Biological Sciences*, Volume 29, Issue: 8.

[5] Balanagouda Patil, Vinayaka Hegde, Shankarappa Sridhar, R.Thava Prakasa Pandian, Shivaji H.Thube and Hanumappa Narayanaswamy. (2023), 'Development and evaluation of fungicide-amended urea briquettes (FAUB's) to combat fruit rot disease of arecanut: A farmers-friendly approach', *International Association for the Plant Protection Sciences*, Volume 165.

[6] Basil N. Ziogas, Anastasios N. Markoglou, Dimitrios I. Theodosiou, Ageliki Anagnostou and Stavroula Boutopoulou. (2006), ' A High Multi-drug Resistance to Chemically Unrelated Oomycete Fungicides in Phytophthora infestans', *European Journal of Plant Pathology*, Volume 115, pages 283-292.

[7] C. Kannan and C. T. Jose. (2009), 'Activation of defense enzymes in arecanut (Areca catechu L.)

ISSN (online): 2581-3048
Volume 8, Issue 7, pp 43-52, July-2024
https://doi.org/10.47001/IRJIET/2024.807004

seedlings upon inoculation with biocontrol agents', *Journal of Plantation Crops*, Volume 37(2), pages: 134-137.

[8] Celia Maya. (2023), 'Using PyMOL to Understand Why COVID-19 Vaccines Save Lives', *ACS publication*, Volume 100(3).

[9] G. M. Hegde. (2015), 'Bio-efficacy of potassium phosphonate against nut rot disease ofareca nut (Areca catechu L.) in the northern Karnataka of India', *Sri Lanka Journal of Food and Agriculture* Volume 1(2), pages: 9-14.

[10] George Andrew S. Inglis. (2021), 'BABEL: using deep learning to translate between single-cell datasets', *Communication Biology*, Volume 4', Issue:1, pages 591-591.

[11] George W. Staples and Robert F.Bevacqua. (2006), 'Areca catechu (Betel nut palm)', *Species Profiles for Pacific Island Agroforestry*, ver .I.3.

[12] Hao Ding, Guangzhen Zhou, Long Zhao, Xinyu Li, Yicheng Wang, Chengcai Xia, Zhiqiang Xia and Yinglang Wan (2023), 'Genome-Wide Association Analysis of Fruit Shaped-Related traits in Areca catechu', *Int. J. Mol. Sci.*, Volume 24.

[13] I.Thanseem, A. Joseph and A.Thulaseedharan. (2005), 'Induction and differential expression of β-1,3-gluanase mRNAs in tolerant and susceptible Hevea clones in response to infection by phytophthora meadii', *Tree Physiology*, Volume25, Pages:1361-1368.

[14] Jerome Eberhardt, Diogo Santos-Martins, Andreas F Tillack, Stefano Forli. (2021), 'AutoDock Vina 1.2.0: New Docking Methods, Expanded Force Field, and Python Binding', *J. Chem. Inf. Model.*, Volume 61(8), Pages: 3891-3898.

[15] K.S. Muralikrishna, K.M. Sharadraj, K. P. Gangaraj, N.R. Nagaraja, Anitha Karun, M.K. Rajesh and P. Chowdappa. (2018), 'In vitro assay for screening of Areca spp. for Phytophthora resistance', *International Journal of Innovative Horticulture*, Volume 7(2), Pages: 139-142.

[16] Maja Brus-Szkalej, Christian B. Andersen, Ramesh R. Vetukuri and Laura Grenville-Briggs Didymus's. (2021), 'A family of cell wall transglutaminases is essential for appressorium development pathogenicity in Phytophthora infestans', *Swedish University of Agricultural Sciences*.

[17] Naruki Yoshikawa and Geoffrey R. Hutchison. (2019), 'Fast, efficient fragment- based coordinate generation for Open Babel,' *Journal of Chemiformatics*, Volume 11, Article number: 49.

[18] Neol M. O'Boyle, Michael Bank, Craig A. James, Chris Morley, Tim Vandermeersch and Geoffrey R. Hutchison. (2011), 'Open Babel: An open chemical toolbox', 3:33.

[19] Oleg Trott1and Arthur J Olson. (2010), 'AutoDock Vina: Improving the speed and accuracy of docking with a new scoring function, efficient optimization, and multithreading', Vol.31(2):455-61.

[20] Olivia Alford and David Toth. (2017), 'Energy-Efficient Virtual Screening with ARM-CPU-Based Computers', Vol 8, Issue 2.

[21] Ram Bahadur Khadka, Bhim Chaulagain, Surendra Subedi, Madan Marasini, Rajana Rawal, Narayan Pathak,Ishwori Prasad Goutam, Tika Ram Chapagain, Bhim Bahadur Khatri and Dipak Sharma-Poudyal. (2020), 'Evaluation of fungicides to control potato late blight (Phytophthora infestans) in the plains of Nepal', *Journal of Phytopathology* Volume 168, Issue 5.

[22] Ramaswamy Manimekalai, Smita Nair, A. Naganeeswaran, Anitha Karun, Suresh Malhotra and V. Hubbali. (2018), 'Transcriptome sequencing and de nova assembly in arecanut, Areca catechu L elucidates the secondary metabolite pathway genes', *Biotechnology reports* 63-69.

[23] Richard W. Jones and Manuel Ospina-Giraldo. (2011), 'Novel cellulose-binding-domain protein in Phytophthora is cell wall localized', 6(8):e23555.

[24] Sandro Cosconati, Stefano Forli, Alex L. Perryman, Rodney Harris, David S. Goodsell and Arthur J. Olson. (2010), 'Virtual Screening with AutoDock: Theory and Practice', *Exper Opin Drug Discov*., Volume 5(6), Pages:597-607.

[25] Serena Rosignoli and Alessandro Paiardini. (2022), 'Boosting the Full Potential of PyMOL with Structural Biology Plugins', Volume 12 (12), Pages: 1764.

[26] Shuguang Yuan, H. C. Stephen Chan, Zhenquan Hu. (2017), 'Using PyMOL as a platform for computational drug design', Pages: 7-28.

[27] Tim Skern. (2018), 'An Archive and a Tool: PDB and PyMOL', *Exploring Protein Structure: Principles and Practice*, Pages: 7-28.

[28] Yigal Cohen and Ulrich Gisi. (2007), 'Differential Activity of Carboxylic Acid Amide Fungicides Against Various Developmental Stages of Phytophthora infestans', *Phytopathology*, Volume 97(10), Pages: 1274-83.

[29] Zhiyuan Yin, Nan Wang, Weiwei Duan, Lei Pi, Danyu Shen, Daolong Dou. (2021), 'Phytophthora capsici CBM1- containing protien CBP3 is an apoplastic effector with plant immunity inducing activity', *Molecular Plant Pathology*, Volume 22(11), Pages: 1358-1369.

ISSN (online): 2581-3048
Volume 8, Issue 7, pp 43-52, July-2024
https://doi.org/10.47001/IRJIET/2024.807004

AUTHORS BIOGRAPHY

Dr. Sharada S B is an Associate Professor Department of Biotechnology Basaveshwar Engineering College, Bagalkote, which comes under the Visvesvaraya technological University, Karnataka, India.

Ajay A Shettigar is a final year student pursuing a B.E. in Biotechnology from Basaveshwar Engineering College, Bagalkote, which comes under the Visvesvaraya technological University, Karnataka, India.

Bhuvaneshwari is a final year student pursuing B.E. in Biotechnology from Basaveshwar Engineering College, Bagalkote, which comes under the Visvesvaraya technological University, Karnataka, India.

Shailashree C Ganiger is a final year student pursuing B.E. in Biotechnology from Basaveshwar Engineering College, Bagalkote, which comes under the Visvesvaraya technological University, Karnataka, India.

Citation of this Article:

Sharada S B, Ajay A Shettigar, Bhuvaneshwari, & Shailashree C Ganiger. (2024). Insilico Approach to Find Bioactive Compound against Fruit Rot Disease (FRD) in *Areca Catechu*. *International Research Journal of Innovations in Engineering and Technology - IRJIET*, 8(7), 43-52, Article DOI https://doi.org/10.47001/IRJIET/2024.807004

****

