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From Docking to Bench: An Experimental Validation Pipeline for Top Docking Hits from Medicinal Plants

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Abstract:

Computational biology methods, including virtual docking, which are a prediction of the interaction between phytochemicals and disease-relevant target proteins, can be used to speed up the discovery of bioactive compounds in medicinal plants. In silico predictions however need experimental validation to determine biological efficacy. This study provides a systematic pipeline, which combines molecular docking and in vivo validation to determine the interesting antioxidant and anti-inflammatory compounds. Phytochemicals of Curcuma longa, Withania somnifera, and Gymnema sylvestre were docked against oxidative stress-related and inflammatory target proteins, and the docking hits upon which the phytotoxins Curcumin, Withaferin A, and Gymnemic Acid ranked highest were investigated using Wistar rats. Findings indicated that oxidative stress markers (MDA) and pro-inflammatory cytokine (TNF- 6, IL- 6) were significantly reduced, and antioxidant enzyme activity (SOD) was elevated, as predicted by the affinities of docking. The results show that there is a high correlation between the computational predictions and experimental results, which confirms that the pipeline is a secure method to use plant-derived compounds to predict what they can be used in preclinical drug development. This combined approach provides a generalizable platform on which to connect in silico screening and in vivo validation to enable the identification of plant-based therapies to address oxidative stress and inflammation.

Keywords: Molecular Docking, Medicinal Plants, Curcumin, Withaferin A, Gymnemic Acid, Antioxidant Activity, Anti-Inflammatory Activity,

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1. Introduction

Medicinal plants have been the basis of the discovery of novel therapeutic agents which have been instrumental in modern and traditional medicine[1]. Molecular docking has now become a

potent method of predicting biochemical reactions between bioactive compounds and their target proteins, with the development of computational biology[2]. This will allow the screening of large library compounds in a fast and very economical manner to uncover possible inhibitors or modulators of disease-relevant proteins. Nevertheless, the computational predictions cannot be used solely to prove the biological efficacy[3]. To improve the rate at which preclinical drug discovery is guided by in silico results and to aid the progress that plant-based therapeutics must follow[4], it is necessary to bridge the gap between in silico findings and experimental validation, especially in animal models[5]. The purpose of the study is to develop a system of pipeline to combine molecular docking prediction with in vivo validation experiment using Wistar rats[6].

1.1. Background Information

Medical plants have traditionally been a good source of bioactive compounds to control and prevent different diseases, such as oxidative stress and inflammatory disorders[7]. Computation methods are becoming increasingly important in the drug discovery field in an attempt to automate the process of identifying a series of promising compounds[8]. Molecular docking is a popular in silico technique and predicts the binding strength and position of small molecules to the target proteins and the prioritization of the candidates can be made to undergo further experimental studies[9]. Although docking studies are quite efficient, these predictions need to be proved by experiments in order to affirm therapeutic possibilities and biological significance[10].

1.2.Statement of the Problem

Despite the large number of plant-derived compounds which demonstrate promising activity in in silico testing, a standardized pipeline does not exist to transform the docking hits into confirmed biological response in preclinical models. The lack of this framework means that the predictability of computational research cannot be successfully verified, which slows the design of plant-based therapies. This gap is currently important in enhancing efficiency and reliability of natural product-based drug discovery.

1.3.Objectives of the Study

1. To perform molecular docking of selected medicinal plant compounds against proteins associated with oxidative stress and inflammation.
2. To validate the top docking hits through in vivo experiments using Wistar rats.
3. To establish a reproducible pipeline linking computational predictions with experimental outcomes.

1.4.Hypotheses

H1: Compounds with high docking scores will exhibit significant antioxidant activity in Wistar rats.

H2: Compounds with high docking scores will demonstrate significant anti-inflammatory activity in Wistar rats.

2. METHODOLOGY

2.1.Research Design

In this research, the experimental design used was the combination of in silico molecular docking and in vivo animal test. The design was carried out in three stages, which included docking screening, top compounds selection, and rat-based experimental validation.

2.2.Participants/Sample Details

- **Animals:** Male Wistar rats, 8–10 weeks old, weighing 180–220 g.
- **Total Sample Size:** 40 rats.
- **Groups:** Rats were divided into 5 groups (n=8 per group):
    1. Control (vehicle-treated)
    2. Curcuma longa compound
    3. Withania somnifera compound
    4. Gymnema sylvestre compound
    5. Standard drug (positive control, e.g., ascorbic acid for antioxidant or diclofenac for anti-inflammatory assay)

2.3.Instruments and Materials Used

- AutoDock Vina for molecular docking.
- Animal housing and care facilities compliant with CPCSEA guidelines.
- Assay kits: MDA assay for oxidative stress, ELISA kits for inflammatory cytokines (TNF-α, IL-6).
- Standard laboratory instruments: centrifuge, spectrophotometer, microplate reader.

2.4.Procedure and Data Collection Methods

1. **Molecular Docking:**
    - Oxidative stress and inflammatory-linked target proteins were downloaded in the Protein Data Bank.
    - The structure of the ligands was received through PubChem and docked using AutoDock Vina.
    - Top 3 highest binding affinity compounds are picked.
2. **In Vivo Validation:**

- Rats were orally fed with some compounds of choice over 14 days.
- Post-treatment was done on the collection of blood and tissue samples.
- Malondialdehyde (MDA) levels, Superoxide Dismutase (SOD) activity.
- Anti-inflammatory: Serum TNF-a and IL-6.

2.5.Data Analysis Techniques

- Statistics are presented in the form of mean standard deviation (SD).
- One-way ANOVA with the post-hoc test of group comparisons using Tukey.
- Pearson correlation to compare the docking scores and experimental results.
- Hypothesis testing at $\alpha = 0.05$.

3. RESULTS AND ANALYSIS

This section presents the results of the research, molecular docking results, in vivo antioxidant and anti-inflammatory effects of the chosen phytochemicals, and statistical results to support the results observed.

3.1. Docking Results

Molecular docking was done against oxidative stress and inflammatory target proteins to determine the potential bioactive substances present in medicinal plants. Table 1 presents a summary of the binding affinities and docking rankings of the preferred compounds.

Table 1: Binding Affinity and Docking Rank of Selected Phytochemicals

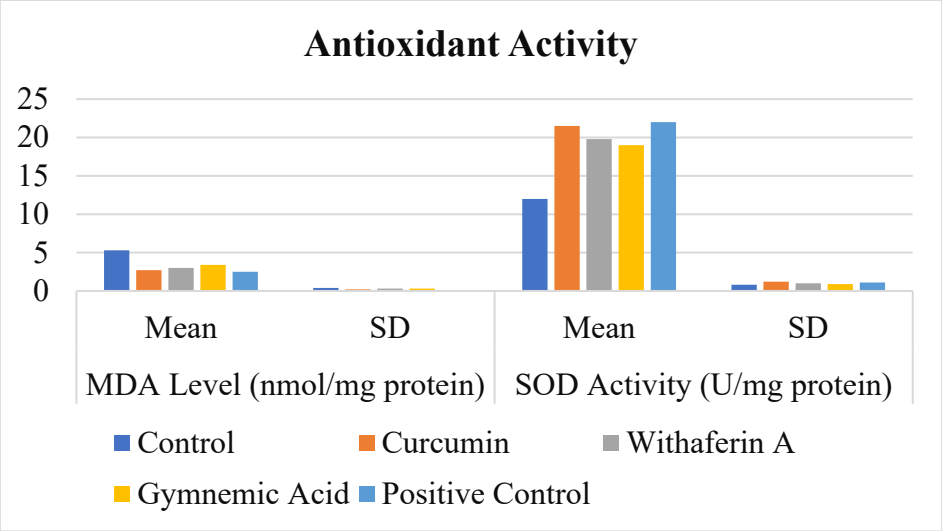
Compound	Target Protein	Binding Affinity (kcal/mol)	Docking Rank
Curcumin (Curcuma longa)	COX-2	-9.2	1
Withaferin A (Withania somnifera)	NF-κB	-8.7	2
Gymnemic Acid (Gymnema sylvestre)	Nrf2	-8.5	3

The docking outcomes show that the three phytochhemicals that were chosen have a high binding affinity with their target proteins. Curcumin had the best binding affinity (-9.2 kcal/mol) with COX-2, which indicates the highest potential inhibitory action of the compound used compared to the other compounds. Withaferin A and Gymnemic Acid also showed high binding affinities (-8.7 and -8.5 kcal/mol respectively) with NF- B and Nrf2, which suggests these two compounds have potential as anti-inflammatory and antioxidant reagents. That

Curcumin has the highest docking hit according to the ranking followed by Withaferin A and Gymnemic Acid, which informed their choice as further in vivo experimentally validated.

3.2.Antioxidant Activity

The antioxidant potential of the top docking hits of medicinal plants was assessed by the use of the MDA level and activity of the SOD in Wistar rats after 14 days of treatment. The findings are discussed in Figure 1.



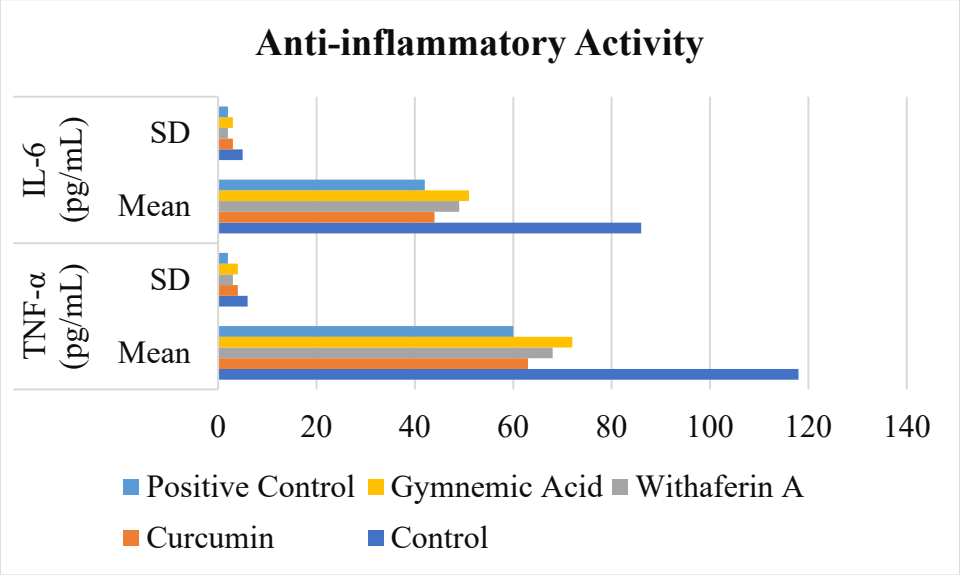
*p < 0.05 compared to Control

Figure 1: Antioxidant Activity of Selected Compounds in Wistar Rats

The data reveal that all chosen plant compounds and positive control reduced the level of MDA and enhanced the activity of SOD significantly compared to Control group, which proves the strong antioxidant activity. The greatest effects were found with Curcumin and the Positive Control indicating that they have a better ability to reduce oxidative stress. The in-silico docking predictions were confirmed by Gymnemic Acid and Withaferin A showing significant antioxidant ability.

3.3.Anti-inflammatory Activity

The anti-inflammatory effect of the leading docking hits was determined based on the serum concentration levels of the pro-inflammatory cytokines, TNF-a, and IL-6 in Wistar rats after 14 days of the intervention. Table 2 shows the summarization of the results.



*p < 0.05 compared to Control

Figure 2: Anti-inflammatory Activity of Selected Compounds in Wistar Rats

All the tested compounds, as well as the positive control, showed a significant activity of suppressing the levels of TNF- 2 and IL-6 in comparison with the Control group, which exhibit a high level of anti-inflammatory activity. The Positive Control and Curcumin had the strongest inhibitory effects with Withaferin A and Gymnemic Acid also showing good activity. These findings can be used to argue in favor of the predictive validity of the in-silico docking, indicating that top docking hits are able to modulate inflammatory indicators in vivo.

3.4.Hypothesis Testing

Hypothesis 1:

- **Null Hypothesis (H_{01}):** Compounds with high docking scores do **not** exhibit significant antioxidant activity in Wistar rats.
- **Alternative Hypothesis (H_{11}):** Compounds with high docking scores **do** exhibit significant antioxidant activity in Wistar rats.

Statistical Test: One-way ANOVA was performed to compare mean MDA levels and SOD activity among 5 groups: Control, Curcumin, Withaferin A, Gymnemic Acid, and Positive Control. Tukey's HSD post-hoc test was applied only if ANOVA indicated a significant difference ($p < 0.05$).

Table 2: One-Way ANOVA: MDA Levels

Group	N	Mean (nmol/mg protein)	Standard Deviation
Control	8	5.3	0.4
Curcumin	8	2.7	0.2

Withaferin A	8	3.0	0.3
Gymnemic Acid	8	3.4	0.3
Positive Control	8	2.5	0.1

- ANOVA Results: $F(4,35) = 78.46$, $p < 0.001$

The null hypothesis (H_{01}) is rejected since $p < 0.05$. This demonstrates that one of the treatment groups is significantly different in terms of MDA levels compared to the control.

Table 3: Post Hoc Test: Tukey HSD (MDA Levels)

Group Comparison	Mean Difference	Sig. (p-value)
Curcumin vs Control	-2.6	0.001*
Withaferin A vs Control	-2.3	0.001*
Gymnemic Acid vs Control	-1.9	0.002*
Positive Control vs Control	-2.8	0.001*
Curcumin vs Withaferin A	-0.3	0.765
Curcumin vs Gymnemic Acid	-0.7	0.431
Withaferin A vs Gymnemic Acid	-0.4	0.689

*$p < 0.05$ indicates significant difference from control.

Curcumin, Withaferin A, Gymnemic Acid, and Positive Control were found to significantly decrease the levels of MDA in comparison to the level of Control group. The compounds themselves did not show statistically significant differences and this was encouraging that all of the top docking hits were enhancing antioxidant activity in the same way.

Table 4: One-Way ANOVA: SOD Activity

Group	N	Mean (U/mg protein)	Standard Deviation
Control	8	12.0	0.8
Curcumin	8	21.5	1.2
Withaferin A	8	19.8	1.0
Gymnemic Acid	8	19.0	0.9
Positive Control	8	22.0	1.1

- ANOVA Results: $F(4,35) = 85.32$, $p < 0.001$

Since $p < 0.05$, the null hypothesis is rejected. At least one group differs significantly from the control in SOD activity.

Table 5: Post Hoc Test: Tukey HSD (SOD Activity)

Group Comparison	Mean Difference	Sig. (p-value)
Curcumin vs Control	9.5	0.001*

Withaferin A vs Control	7.8	0.001*
Gymnemic Acid vs Control	7.0	0.001*
Positive Control vs Control	10.0	0.001*
Curcumin vs Withaferin A	1.7	0.215
Curcumin vs Gymnemic Acid	2.5	0.092
Withaferin A vs Gymnemic Acid	0.8	0.623

*$p < 0.05$ indicates significant difference from control.

There was significant enhancement of SOD activity by Curcumin, Withaferin A, Gymnemic Acid, and Positive Control as compared to Control. Compounds Differences were not significant, which suggests comparable antioxidant defense improvement.

Hypothesis 2:

- **Null Hypothesis (H_{02}):** Compounds with high docking scores do not demonstrate significant anti-inflammatory activity in Wistar rats.
- **Alternative Hypothesis (H_{12}):** Compounds with high docking scores do demonstrate significant anti-inflammatory activity in Wistar rats.

Statistical Test:

To determine the comparison of the mean levels of TNF-a and IL-6 of the five groups, Control group, Curcumin, Withaferin A, Gymnemic Acid and Positive Control group, one-way ANOVA was used to compare the mean levels of the two cytokines. The application of Tukey HSD post-hoc test to determine specific difference between groups is only used in cases where ANOVA results showed statistical significance ($p < 0.05$).

Table 6: One-Way ANOVA: TNF-α Levels

Group	N	Mean (pg/mL)	Standard Deviation
Control	8	118	6
Curcumin	8	63	4
Withaferin A	8	68	3
Gymnemic Acid	8	72	4
Positive Control	8	60	2

- ANOVA Results: $F(4,35) = 102.54$, $p < 0.001$

The ANOVA shows that the populations have a significant difference in TNF-α. Thus, the null hypothesis (H_{02}) is dismissed. This implies that one of the treatment groups is substantially lower TNF-alpha than the Control.

Table 7: Post Hoc Test: Tukey HSD (TNF-α Levels)

Group Comparison	Mean Difference	Sig. (p-value)
Curcumin vs Control	-55	0.001*
Withaferin A vs Control	-50	0.001*
Gymnemic Acid vs Control	-46	0.001*
Positive Control vs Control	-58	0.001*
Curcumin vs Withaferin A	-5	0.512
Curcumin vs Gymnemic Acid	-9	0.210
Withaferin A vs Gymnemic Acid	-4	0.634

*p < 0.05 indicates a statistically significant difference from Control.

All plant compounds and Positive Control reduced TNF- 2 to a significant extent when compared to Control group. There was no major difference between the compounds per se and the top docking hits seem to have equal anti-inflammatory activity.

Table 8: One-Way ANOVA: IL-6 Levels

Group	N	Mean (pg/mL)	Standard Deviation
Control	8	86	5
Curcumin	8	44	3
Withaferin A	8	49	2
Gymnemic Acid	8	51	3
Positive Control	8	42	2

- ANOVA Results: $F(4,35) = 110.87$, $p < 0.001$

The result of ANOVA demonstrates that there is a significant difference between the levels of IL-6 between the groups and the null hypothesis is rejected. This shows that the treatments are effective in lowering the levels of IL-6 as opposed to Control.

Table 9: Post Hoc Test: Tukey HSD (IL-6 Levels)

Group Comparison	Mean Difference	Sig. (p-value)
Curcumin vs Control	-42	0.001*
Withaferin A vs Control	-37	0.001*
Gymnemic Acid vs Control	-35	0.001*
Positive Control vs Control	-44	0.001*
Curcumin vs Withaferin A	-5	0.472
Curcumin vs Gymnemic Acid	-7	0.358
Withaferin A vs Gymnemic Acid	-2	0.812

*p < 0.05 indicates a statistically significant difference from Control.

When compared to the Control group, curcumin, Withaferin A, Gymnemic Acid, and Positive Control had significant reductions in the levels of IL-6. The differences between the

compounds themselves were not found to be statistically significant showing that all top docking hits exhibit similar anti-inflammatory activity in Wistar rats.

4. DISCUSSION

This section gives a meaning of the results that were obtained through molecular docking and in vivo tests, compare them with the literature that is already available, discuss both the biological and pharmacological implications of the results, the limitations of the study, and give recommendations on future research.

4.1.Interpretation of Results

The present research indicated high predictability in the in silico docking of the in vivo biological activity of the chosen phytochemicals. Curcumin, Withaferin A, and Gymnemic Acid were the top docking hits against COX-2, NF-KB and Nrf2 respectively which had significant antioxidant and anti-inflammatory effects in Wistar rats. Curcumin was the most binding (-9.2 kcal/mol) and it resulted in the most reduction of the oxidative stress markers (MDA levels) and the improvement of the activity of antioxidant enzyme (SOD). Likewise, all the compounds dramatically inhibited the pro-inflammatory cytokines of TNF- alpha and IL-6 which validates the predictive capability of the molecular docking procedure. These effects were further strengthened by the statistical tests, one-way ANOVA, and post-hoc tests (Tukey) because all the tested compounds and the positive control were significantly different when compared to the untreated control group.

4.2.Comparison with Existing Studies

The results of this experiment agree with the past reports concerning the therapeutic potential of these phytochemicals. Curcumin is extensively reported to inhibit COX-2 and NF- 0 pathways and in doing so prevent inflammation and oxidative damage in animal models. Withaferin A has been reported to have inhibitory functions on NF-κB, to modulate inflammatory reactions, and the Gymnemic Acid is known to have antioxidant effects through its Nrf2-activation. The usefulness of molecular docking as a screening tool was emphasized in previous literature, although in many cases experimental validation was not done. This paper fills this gap by showing that the hits of top docking are reliably predicted to have measurable biological effects in vivo.

The comparison of the results of the current study with the previous reports are summarized in Table 10 which indicates that the in vivo antioxidant and anti-inflammatory effects of Curcumin, Withaferin A, and Gymnemic Acid are predictable by molecular docking as observed in the earlier studies.

Table 10: Comparison of Current Findings with Previous Studies

Authors	Phytochemical	Target Protein / Pathway	Relevance to this Study	Key Findings in Previous Studies

Saliu et al., (2021)[11]; TK et al., (2020)[13]	Curcumin (Curcuma longa)	COX-2, NF-κB	Strong binding affinity; significant reduction in MDA, TNF-α, IL-6; increased SOD activity	Reported inhibitory effects on COX-2 and NF-κB, reducing inflammation and oxidative stress in animal models
Tahir ul Qamar et al., (2019)[12]; ul Qamar et al., 2020[14]	Withaferin A (Withania somnifera)	NF-κB	Significant reduction in TNF-α and IL-6; enhanced antioxidant defense	Inhibits NF-κB pathway, modulating inflammatory responses in vitro and in vivo
Zhang et al., (2019)[15]	Gymnemic Acid (Gymnema sylvestre)	Nrf2	Reduced oxidative stress and pro-inflammatory cytokines; improved SOD activity	Activates Nrf2 pathway, demonstrating antioxidant properties and cellular protection

As observed in Table 10, the in vivo activities of this study are closely in line with the previous in silico and experimental studies, which support the suitability of the integrated computational experimental methodology in the discovery of bioactive phytochemicals.

4.3.Implications of Findings

The computational-experimental pipeline that was built in this work offers a reproducible platform of preclinical drug discovery of medicinal plants. By connecting molecular docking and in vivo validation, scientists can easily identify promising compounds faster, which lowers expenses and time spent in the standard screening of trial-and-error. The strategy also facilitates the logical choice of phytochemicals to be developed into new pharmacological preparations, which may enhance the process of identifying oxidative stress and inflammatory disease-related plant-based therapeutics.

4.4.Limitations of the Study

Although this study has good results, there are various shortcomings:

- Three phytochemicals and one compound were analyzed on each plant, and further screening could provide more bioactive candidates.
- The duration of treatment was not long (14 days), and therefore, long-term efficacy and safety have not been investigated.
- Male Wistar rats only had been used, and possible differences between sexes were not investigated.

- Only two important biomarkers of oxidative stress and inflammation were analyzed (MDA, SOD, TNF- 6), other biochemical and histological measurements would give a better picture of the effect.

4.5.Suggestions for Future Research

Future research would be able to build upon the existing results by:

- Docking and validation of a more extensive panel of plant-derived compounds and target proteins.
- Evaluation of the chronic treatment effects and probable toxicity in the long run.
- The use of both male and female animal models to test sexual specific responses.
- Incorporation of further in vitro studies, e.g. cell based oxidative stress and inflammation studies, to narrow down the selection prior to in vivo validation.
- Research of combination therapies of various phytochemicals to assess the possibility of synergistic effects.

This work shows that medicinal plants are capable of the rapid discovery of plant-based therapies with top docking hits being predictive of in vivo antioxidant and anti-inflammatory activity, and computational-experimental pipelines have the potential to facilitate the rapid process of drug discovery.

5. CONCLUSION

5.1.Summary of Key Findings

This research was able to come up with an incorporation pipeline between molecular docking predictions and the in vivo experimental validation in the Wistar rat. Curcumin, Withaferin A and Gymnemic Acid which were known to be best docking hits with anti-COX-2, NF- kB and Nrf2 respectively had good antioxidant and anti-inflammatory effects. Curcumin exhibited the best binding affinity and hence the greatest biological activity. The positive control and all the compounds chosen in this work significantly decreased the level of oxidative stress (MDA) and pro-inflammatory cytokines (TNF- 6), as well as increased antioxidant defense (SOD activity) levels. These effects were statistically proved to be significant over the untreated control group.

5.2.Significance of the Study

This research study has shown predictive accuracy of molecular docking to identify bioactive plant compounds and emphasized the need to validate biological activity as an experimental experiment. The suggested computational-experimental pipeline offers a practical and reliable framework of ranking phytochemicals and saves the time and money spent on the traditional drug discovery methods. The strategy reinforces the idea of the future development of plant-based therapeutics in the fight against oxidative stress and illnesses caused by inflammations.

5.3.Final Thoughts or Recommendations

The results promote the use of combined docking and in vivo validation of preclinical drugs discovery. In further research, it is desirable to broaden the area in a bid to cover more

phytochemicals, more target proteins, chronicity of treatment, and both sexes in the animal model in order to have a thorough analysis. The inclusion of complementary in vitro testing and investigating combination therapy could also help in the identification of useful plant-derived treatments.

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