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Integrated Transcriptome Guided Identification and in Silico Validation of Venom Nerve Growth Factor NGF from Naja Naja as a Structure based Anti-Venom Target

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ABSTRACT: Snakebite continues to pose a major challenge across many tropical regions [1-3], Causing thousands of mortality and morbidity annually. Antivenom that saves life do not detect all the toxin but sometimes trigger bad immune responses [4-6]. With the help of advanced technology like transcriptomics and computational biology [7-9] Researchers can now zoom in various venom protein in the complex venom cocktail and study them down to their molecular detail for better treatment and targets you see structure-based method.

In this study, a transcriptome guided bioinformatics workflow was used to identify and validate a reliable venom Target from Naja Naja. Venom gland RNA-seq data Were assembled De novo. Followed by protein prediction and functional annotation. Among the detected toxin families Venom nav growth factor was identified as structurally complete and computationally tractable candidate for structure-based analysis. Structure based virtual screening of selected phytochemicals was performed using molecular docking and the top ranked complexes were analysed through 100 ns molecular dynamic simulations under NPT conditions. Stability analysis including RMSD, RMSF, interaction persistence and secondary structure evaluation confirmed sustained ligand binding during the simulation. Both Leg Binded to the targets attacker site Where diosmin settled faster while Hesperidin showed fluctuations towards the end of the simulation. The ADMET prediction for the selected candidates Showed promising pharmacokinetic and safety results. This study shows that combining transcriptomics with structure-based modelling is a solid way to pinpoint venom target and spot new helper molecules It's a smart move to push antivenom therapy forward.

1. INTRODUCTION

Snake bite envenomation is a neglect Tropical disease That cause many mortality and morbidity [10] Countries in South and South West Asia Carry a significant proportion of this global Problem, With India reporting one of the highest numbers of snake bite related deaths [11-13] Annually. Among the medically important species the spectacled Cobra Naja Naja its main cause for many envenomation cases and is associated with civil neurotoxicity and inflammatory effects.

Conventional antivirum therapy remains the primary treatment [14-16] for the snake bite envelation and is typically produced through the immunisation of animals such as horses with crude vinam mixtures. Although Anti Venom have saved countless lives, they have often exhibited several limitations stop These include incomplete neutralisation of specific venom components, Variability in effectiveness against geographically diverse venom composition and the risk of adverse immunological reactions

such as serum sickness and anaphylaxis [17-19]. Considering the drawback in the existing treatment complementary therapeutic strategies developed had Increased that can target specific venom protein involved in the pathophysiology of environment.

Advances in high throughput sequencing technologies [20-23] have enabled the comprehensive characterizations of Venom Grand Transcriptomes. The detailed identification of the toxin encoding genes expressed in venomous species. Venom gland transcriptomics provides direct inside [24-27] into toxin gene expression, isoform diversity and sequence completeness Making it a powerful tool for venom profiling. Compared with traditional proteomic approaches transcriptome analysis allows researchers to explore the complete venom related transcripts Including low abundance toxin variance that may play important biological roles.

When combined with structure based computational techniques Transfer from drive and talks in discovery can significantly accelerate the identification of proteins that are suitable for structure-based inhibitor design. Computational methods such as molecular docking [28-31] and molecular dynamic stimulations enables the evaluation of protein ligand interaction providing valuable insights into potential inhibitory compounds that may modulate venom protein activity.

Previous studies Investigating Naja Naja Venom composition have primarily focused on toxin diversity, geographical variations and relative abundance of major toxins family among these three finger toxins represents the most abundant components [32-35] which are responsible for many of the neurotoxic effects associated with cobra envenomation. Even though they are small in size and highly constrained structure of these toxins can limit their suitability for small molecule inhibition development using conventional docking strategies

Venom nerve growth factor NGF [36- 39] represents a biologically active venom component with a well characterised structural architecture. Venom derived NGF has been implicated in several physiological responses associated with envenomation including Pain, Sensation inflammation and modulation of Local tissue responses. Due to its relatively larger molecular surface and defined tertiary structure, NGF provides a structurally tractable target for structure based computational studies.

In this study we employed a transcriptome guided computational pipeline to discover and prioritise venom protein from Naja Naja Venom Gland RNA-seq data. The workflow includes De novo transcript assembly, protein coding sequence prediction and functional annotation to identify the potential venom toxins. Based on the transcript completeness, annotation confidence and structural Suitability venom nerve growth factor was selected as the primary target for structure-based analysis

With the identification of ngf, Molecular docking and molecular dynamic simulation were performed to evaluate the binding interaction between the mgf and the selected phytochemical compounds. Through this integrated computational strategy, the present study aims to Demonstrate how transruptomics drive and target identification combined with structure-based modelling can facilitate the discovery of potential urgent molecules to Next generation anti venom development.

2. MATERIALS AND METHODS

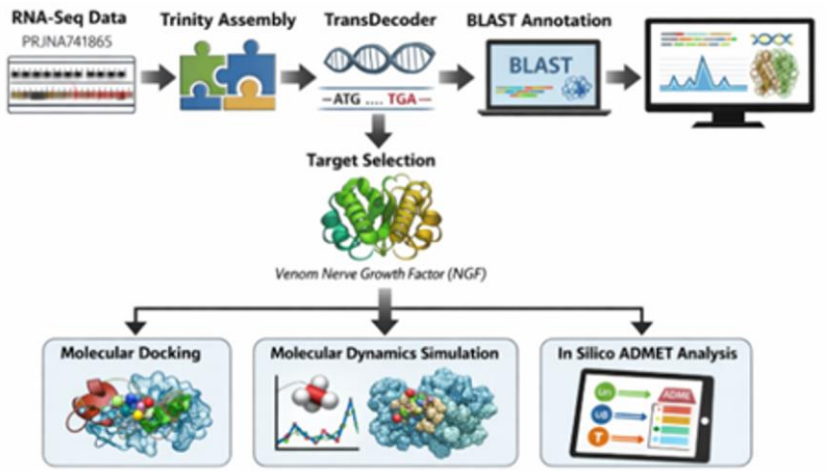

Figure 1: Overview of the transcriptome-guided computational workflow used for venom protein identification, target selection, molecular docking and molecular dynamic simulation.

2.1 Venom Gland RNA Seq Data

Venom gland transcriptome raw sequence data of Naja Naja (Sri Lankan Spectacled Cobra) was retrieved from NCBI database PRJNA741865 [40] was processed using the galaxy bioinformatics platform for quality control, denovo transcriptome assembly and downstream venom gene identification.

2.2 Denovo Transcrptiome Assembly

Draw sequencing reads were subjected to quality assessment and assembled denovo using the Trinity assembly implemented in Galaxy [40]. The resulting transcriptome represents a comprehensive set of expressed venom gland transcripts.

2.3 Prediction Of Protein Coding Sequences

Protein coding regions were predicted from the assembled transcripts using TRANSDECODER [41]. Both the complete and partial open reading frames (ORF) where retained for functional annotation to maximise the venom gene recovery.

2.4 Functional Annotation And Toxin Identification

Director protein sequences were functionally annotated using BLASTp and BLASTx [42] Searches against the Unipot KB databases, with emphasis on curated venom entries A stringent E value cutoff of 1×10^{-5} Was applied to identify high confidence talks in matches.

2.5 Target Validation And Selection Strategy

Identified venom protein were evaluated based on sequence identity, alignment length, query coverage, E value significance, transcript redundancy and structural completeness. Proteins represented by fragmented or partial sequences were excluded from structure-based analysis Venom nerve growth factor (NGF) was selected by primary target based on full length sequence recovery Hai annotation confidence and structural tractability.

2.6 Molecular Docking

Molecular dock Was performed using Pyrex 0.8 which integrates the Orthodox Vena Docking engine for structure based virtual screening. The 3D structure of the ngf dimer is prepared by removing water molecules and heteroatom and radiation of polar hydrogen and conversion of pdbqt format. Begin structures were retrieved from PubChem databases and an energy minimization using the open babel Platform within the PyRx Was run successfully. Ligand were Converted into pdbqt format with assignment of Gasteiger partial charges return to docking [52].

The binding pockets on the NGF protein were predicted using P-2 rank V2 .5 .1. ligand docking was focused on the top ranked pocket interface region. The docking grid box was generated and automatically optimised using PyRx Vinaa Wizard Auto grid box adjustment options to ensure full coverage of the predicted binding region. The Vinaa search space was centred at X = 3.1048, y =50.231 and Z = 2 2122 with the grid box dimensions of 25 X 25 X 25 Å. Docking was performed using an exhaustiveness value of 8 and best rank to post was selected by the lowest binding affinity score and favourable interaction geometry. Protein ligand interactions were analysed and visualisations were performed using Discovery Studio Visualizer.

2.7 Molecular Dynamics Simulation

The top ranked ngf ligand complexes were subjected to molecular dynamic simulations using the dismount simulation package under NPT ensemble condition at 300 K. each system was simulated for 100 ns in an explicit solvent environment With the appropriate Ionic neutralisation. Trajectory analysis including route means square deviation, root means square fluctuation, secondary structure evaluation, protein ligand contact analysis and ligand torsional behaviour providing dynamic validation beyond the static docking force.

2.8 Insilio Admet Analysis

Shortlisted phytochemicals were evaluated for absorption, distribution, metabolism, Excretion and toxicity properties using online production platform to assess drug likeness and safety profiles [46- 48].

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3. RESULTS AND DISCUSSION

3.1 Transcriptome Assembly And ORF Prediction

Trinity De novo Assembly generated comprehensive Naja Naja venom gland transcriptome protein coding regions were predicted using transdecoder, resulting in multiple putative toxins and Venom Associated Protein sequence for further downstream of functional annotation.

3.1.1 Transfer From Assembly Quality

The Trinity Dinovo Assembly of Naja Naja venom gland transcriptome generated 80,752 transcripts with total assembled length 53,314,975 bp. The assembly showed an N50 of 986 bp with the mean transcript length of 660 bp Maximum transcript length of 13,734 bp Overall GC content of the assembly transcript from 44.58 %. Transcriptome completeness assessment using BUSCO V 5.8 .0 against the vertebra_ODP 10 data set Reported 42.3% complete BUSCO (31.7% single copy and 10.6% duplicated), 23.0% fragmented and 34.7% missing. The observed BUSCO profile is consistent with tissue specific venom gland transcriptome assemblies where toxin enrich expression reduces the recover of universal housekeeping orthologs.

3.2 Identification Of Venom Protein Families

BLAST analysis identified several venom components including three finger toxin, cytotoxins, venom serine protease and venom nerve growth factor. Many classes were represented by short peptide fragments.

Table 1. Selection of Venom nerve growth factor NGF

Trinity Transcript ID	Toxin Family	UniProt Reference	Query Length (aa)	% Identity
TRINITY_DN597_c1_g3_i8.p1	Nerve Growth Factor (NGF)	P01140 (NGFV_NAJNA)	116	96.55
TRINITY_DN7_c0_g3_i2.p1	Venom Serine Protease (VSP)	P86545 (VSP_NAJNA)	36	97.22
TRINITY_DN1174_c1_g1_i1.p1	Three-finger toxin (3FTx)	P86538 (3SA2A_NAJNA)	59	98.31
TRINITY_DN202_c0_g1_i16.p2	Three-finger toxin (3FTx)	C0HM08 (3S12_NAJNA)	62	87.10

3.3 Selection Of Venom Nerve Growth Factor NGF

Venom nerve growth factor demonstrated the strongest validation matrices among all the identified venom proteins including full length sequence recovery (116 amino acids), high sequence identity greater than 96% extremely significant E-value ($<1 \times 10^{-80}$) and multiple independent transcript support. In contrast other toxin families such as three finger toxin and venom serine protease were predominantly represented by the short mature peptides, limiting their suitability for structure based docking and molecular dynamic simulation. This evidence-based selection strategy ensures that NGF was not only chosen based on expression abundance but on combined transcriptomic reliability and structural tractability thereby maximizing the robotness of downstream computational analysis.

3.4 Homology Modelling And Structural Validation Of NGF

Since a complete experimental structure corresponding to the recovered venom NGF transcript was not directly available for docking analysis a three-dimensional structural model was generated using Swiss model, an automated homology modelling platform. The full length NGF amino acid sequence obtained from the transcriptome assembly 116 amino acids were submitted to the SWISS MODEL cover for the template-based structure prediction

The template identification was performed automatically by SWISS MODEL pipeline using sequence similarity and search against the protein databases (PDB). Experimentally resolved nerve growth factor structures where high sequence similarity

was selected as modelling templates, enabling accurate reconstruction of NGF tertiary structure. The resulting homology model preserves the characteristic NGF fold consisting the beta strand rich structural elements connected by the flexible loop regions.

The generated NGF model was further submitted to Structural Equality Assessment to ensure the suitability for downstream structure-based analysis. Model validation matrices indicating good structural stability the Molprobity score was 2.41 suggesting acceptable stereochemical quality of the predicted structure in addition Ramachandran plot analysis showed 95.28% of the residue located in the favourable regions confirming proper backbone geometry and minimal stearic clashes. The validated NGF model was used for molecular docking and molecular dynamic simulations [43- 45]. Structural visualization and figure preparation of the model NGF protein where perform do using PyMOL, enabling geographical representation of the predicted three-dimensional structure.

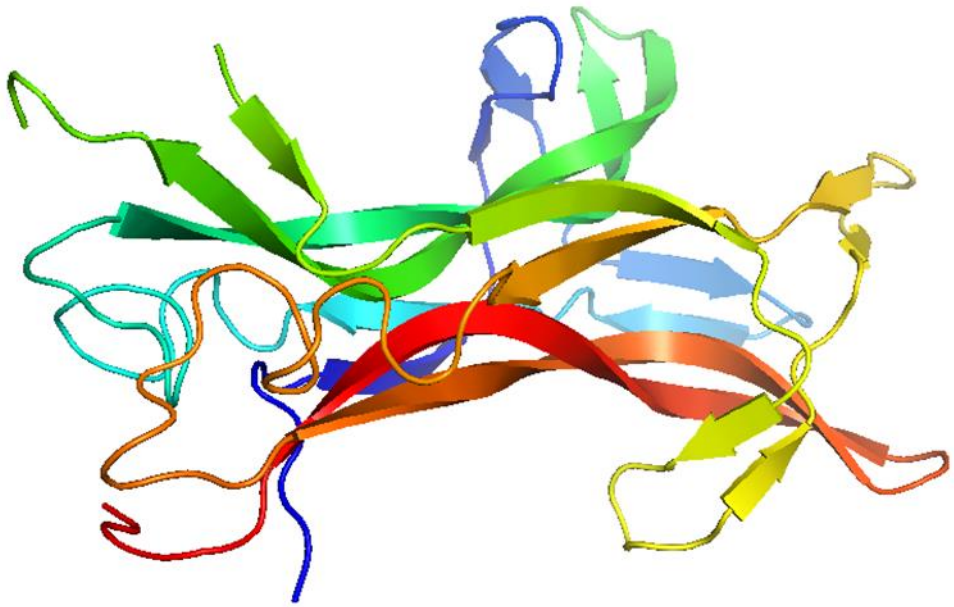

Figure 1. Homology model 3 D structure of Venom nerve growth factor NGF generated using Swiss model server the ribbon representation highlights the B stand rich architecture of NGF suitable for downstream structure-based analysis

3.5 Molecular Docking Analysis

Docking analysis revealed a favourable binding affinity between NGF and selected phytochemicals including flavonoids and glycosylated phenols. compounds the Diosmin and Hesperidin exhibit stronger binding energies compared to another ligand. This is because due to increased hydrogen bonding and surface complementarity. These results are consistent with previous NGF targeting computational studies and support the feasibility of small molecular modulation of venom nerve growth factor.

3.5.1 Binding Site Interpretation And Interaction Analysis

Docking intersection analysis demonstrated that the top ranked phytochemical diosmin and Hesperidin consistently occupied a surface accessible binding pocket on ngf dimer. The docked complexes were stabilised by multiple conventional hydrogen bonds carbon hydrogen bonds and π-interactions with residue located near the ngf functional surface. Notably Both Ligand exhibit overlapping interaction patterns with key residues such as Cys106, Ser12, Glu10, Val107, and Phe84, Indicating a conserved binding region rather than a random surface association. The localization of docking process near the predicted ngf receptor recognition Slash interface Regions suggest that these compounds may exhibit competitive Allosteric modulation of ngf mediated receptor interactions including potential disruption of NGF–TrkA association. Overall, the interaction profile supports the structural feasibility of targeting venom ngf using flavonoid glycosides for antivenom-oriented inhibitor discovery.

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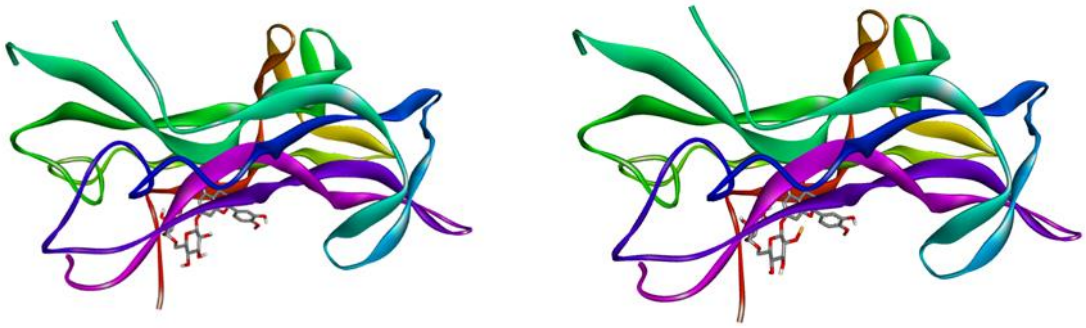


Figure2. Three-dimensional structure of venom nerve growth factor showing rocking binding doses of top ranked phytochemicals Hesperidin and Diosmin.

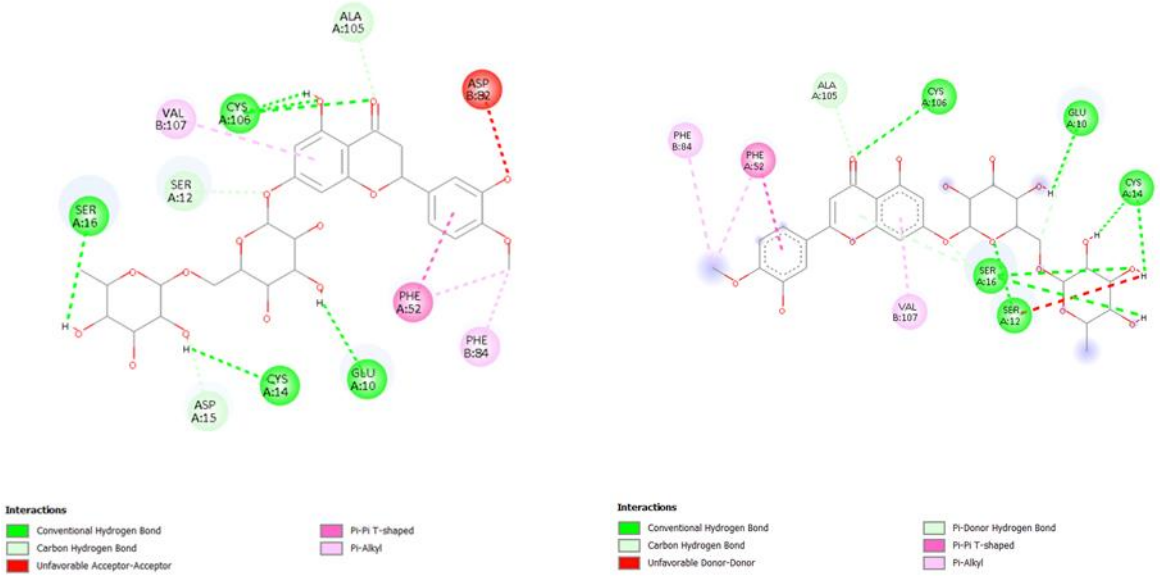


figure 3: Two-dimensional Interaction diagrams of NGF hesperidin and NGF diosmin complexes illustrating hydrogen bonding and hydrophobic interactions.

3.6 Molecular Dynamic Simulation

The Docking results were validated and evaluated for dynamic stability and ligand binding in 100 ns molecular dynamic Simulation which was performed for NGF protein and the selected ligand diosmin and Hesperidin complexes using NPT ensemble conditions at 300K in Desmond Simulation package. Trajectory analysis Has root mean square deviation, root mean square fluctuation, radius of gyration and protein ligand interaction analysis providing comprehensive insights into structural stability and binding behaviour of complexes during the simulation.

3.6.1 Root Mean Square Deviation Analysis

A root means square deviation analysis was performed to evaluate the structural stability of ngf protein backbone and the positional stability of the ligands throughout the 100 ns molecular dynamics trajectory. During the evaluation NGF Diosmin complex Show the protein backbone fluctuated between 2.4 to 3.0 Å that indicates sustainable structural behaviour during the entire simulation. The ligand MST reminder relatively consistent throughout the trajectory that shows diosmin maintained Stable interactions within the predicted binding region of the NGF protein. Complex reached equilibrium earlier in the simulation indicating rapid stabilisation of the protein ligand system.

In contrast, The NGF Hesperiden Complex exhibited protein RMSD values stabilising around 2.2 to 2.8 Å. The Ligand RMSD showed moderate fluctuations during the initial phase of the simulation indicating conformational adjustments of Hesperiden within the binding pockets. After approximately 60 ns. The ligand stabilised and maintained consistent RMSD values for the reminder of the simulation suggested stable binding within NGF interaction regions.

These initial fluctuations likely represent ligand reorientation within the binding pocket before achieving an energetically favourable confirmation. Once stabilised, the Hesperidin complex displayed rmsd values comparable to the Dioxin System. Overall, Both the complexes maintained RMSD Values within the acceptable stability range 1-3 Å for protein ligand simulations, indicating that ligand binding did not significantly disrupt the structural integrity of NGF.

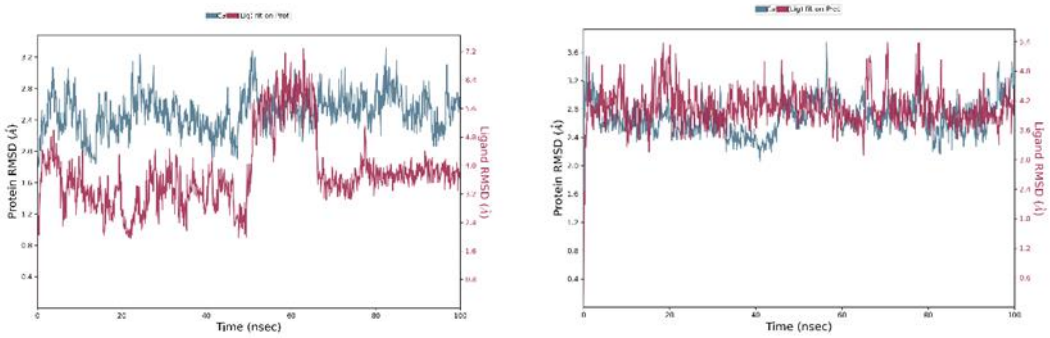


Figure 4. Protein ligand RMSD profile obtained from 100 ns molecular dynamic simulations for NGF phytochemical complexes

3.6.2 Root Mean Square Fluctuations Analysis

Residue level flexibility of Ngf during molecular dynamic simulations were evaluated using root mean square fluctuation RMSF. The NGF diosmin complex exhibited RMSF value mostly within 1-2.5 Å Armstrong indicating moderate flexibility typical of surface loop and terminal regions. Higher fluctuations where primarily observed in flexible loop regions Which is expected in protein structures. Importantly, the residues located near the predicted ligand binding regions showed relatively low fluctuations, suggesting stable ligand interactions with the NGF surface. The Ngf Hesperidin complex kept its RMSF (root mean square fluctuation) Values mostly below two Armstrong which means the protein structures stayed stable during the ligand binding. There were only small fluctuations in the loop region the residue actually interacting with the Hesperidin did not fluctuate much showing ligand binded well within the NGF binding site. This are a massive analysis shows that binding the ligand does not throw NGF's flexibility out of balance both the complex state study over the course of the simulation process.

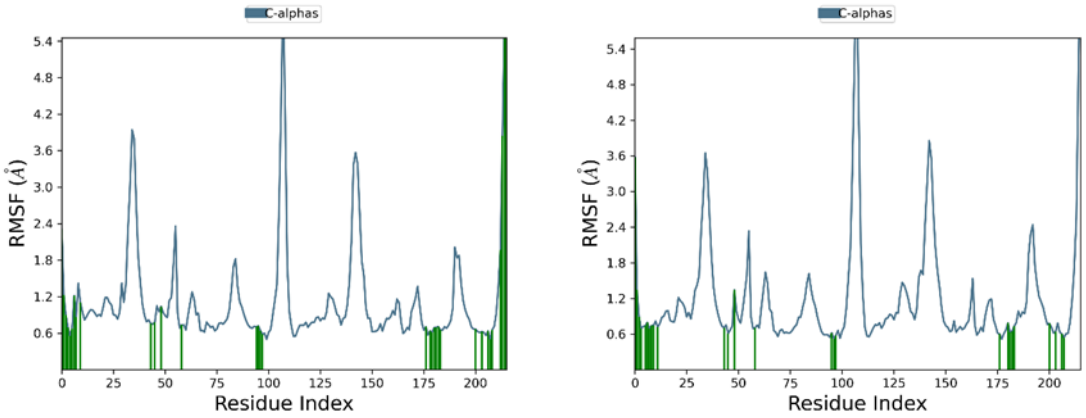


figure 5 Residue level RMSF profiles of Ngf during 100 ns molecular dynamic simulations for the NGF deosmin and ngf hesperidin complexes.

3.6.3 Radius Of Gyration (Rg) Analysis

Analysis Of radius of gyration Is to cheque the compactness and the folding of the protein during the molecular dynamic simulations. For the NGF diosmin complex. The radius of gyration stayed flat for all the 100 ns only showing minor ups and downs. That are considered normal in protein dynamics. This tells us the diosmin binding did not make the protein expand or destabilise It kept its usual shape. When NGF was bound to Hesperidin There were slightly more radius of gyration fluctuation but nothing out of the ordinary for simulation like this. Even with Fluctuation the overall radius of gyration remained solid, Ngf structure did not fall apart during the ligand binding in short both the binding led ngf kept its original compact shape throughout the Molecular dynamic simulation process.

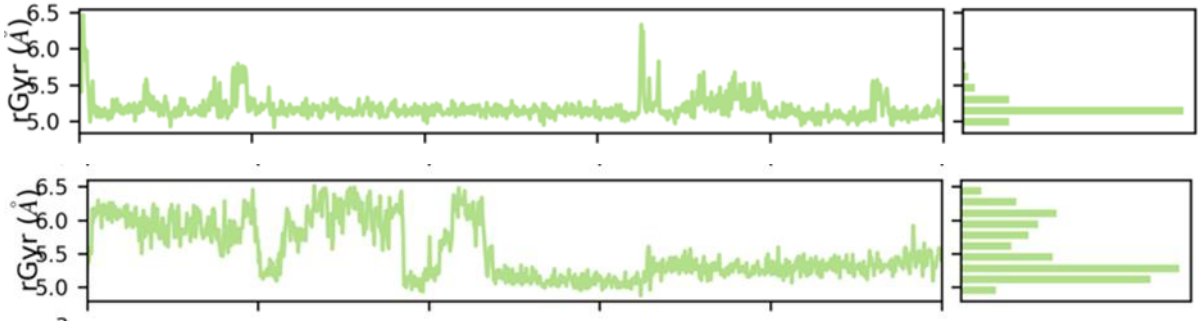
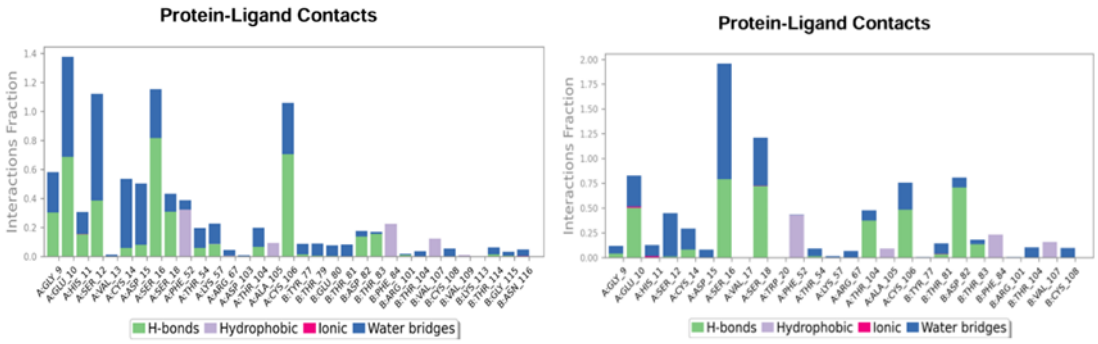


Figure 6. Radius of gyration (Rg) profiles of NGF during the 100 ns molecular dynamics simuation of NGF diosmin and NGF hesperidin complexes.

3.6.4 Protein Ligand Interaction Stability

To check how well the ligand hung on the protein during the simulation, we dug into their contacts both the diosmin and hesperidin kept strong interactions with NGF come on hydrogen contacts and some π stacking. The most important residues for their bindings were scr 12, glu 10, phe 84, Val 107 and cys 106, most of them hung out near NGF's receptor interface. The ligands might actually modulate what NGF does by sticking to their regions that matter most of its activity. Hesperidin made slightly long-lasting contacts but the diosmin settled in earlier during the simulation. Overall, both the ligands clung on throughout, showing stable protein ligand complexes.



3.6.5 Overall MD Simulation Conclusion

Both diosmin and hesperidin kept steady complexes with NGF that's a big take away from our simulation results. The diosmin found its groove and stabilized earlier, while Hesperidine needed a short adjustment phase but stuck after about 60 ns. When you look closer ligand binding barely changed NGF structure or its flexibility. Radius of gyration and root mean square fluctuation analysis Back that up. These Flavoredoid glycosides are stable binders for NGF making them strong candidates for further structure based anti-venom research.

3.7 In Silico ADMET Profiling

To evaluate the drug likeliness and safety of the top ranked phytochemicals identified in this study former in silico absorption, distribution, metabolism, excretion and toxicity Adm ET Profiling was performed. Oral toxicity prediction analysis indicated

that Diosmin belongs to toxicity class 5 with predicted median lethal dose of approximately 500 mg kg suggesting low acute oral toxicity These findings support the favourable safety profile of potential therapeutic applications

Phytochemical property analysis revealed that Diosmin possess multiple hydrogen bond donors and acceptors A high topological polar surface area and a low predicted octanol water partition coefficient consistent with its hydrophilic nature Although the molecular weight of molecular weight exceeds The conventional threshold defined by Lipinski rule of five such as deviations Are commonly observed in bio active flavonoids Glycosides and do not necessarily Preclude Biological activity particularly for non-oral or adjacent therapeutic strategies.

Overall, The ADMET Results suggest that Diosmin exhibits Acceptable safety characteristics and drug likely properties Supporting its further evaluation as a potential ngf modulating scaffold in anti-venom research.

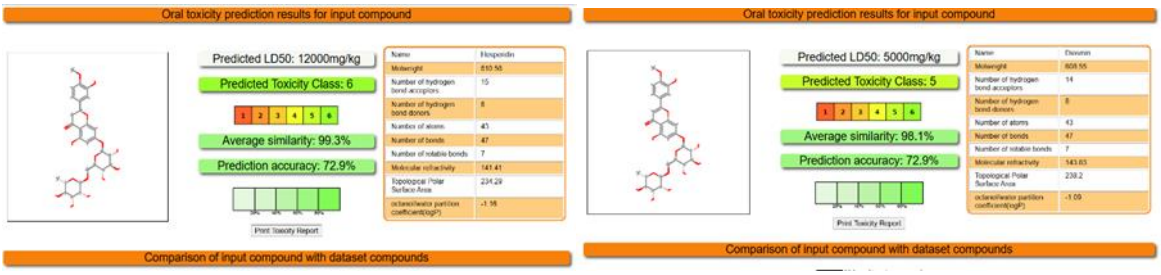


Figure 7. In silico ADMET profiling of the top ranked phytochemical indicating acceptible pharmacokinetic and toxicity properties

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3.4 Discussion

Snakebite envenomation reminds a major health problem in tropical regions and conventional anti venom often fails to neutralise all the venom components. Transcriptomic and computational approaches are now allowing the identification of venom protein that may serve as urgent therapy for this problem.

Although three finger toxins are most abundant neurotoxin components of Naja Naja Venom They are small size and rigid disulfide drift structure makes them unsuitable for small molecular inhibition design First Venom growth factor Has a well-defined structure making it more suitable for docking and molecular dynamic studies. NGF contributes to paying Inflammation and local tissue damage during the invention. Using a transcript tone guided pipeline ngf was selected based on complete sequence information strong annotation and structural suitability. Structure based virtual screening identified the flavonoid glycosides diosmin and hesperidin as a promising NGF binding compounds instal both showed stable hydrogen bonding and hydrophobic interactions near the functional interface of NGF

Molecular dynamic simulation over 100 ns confirmed that both NGF ligand complexes remained stable. D Osman stabilised rapidly while Hesperidin required more time before reaching a stable orientation. Rmsf and radius of gyration analysis further showed that ligand winding did not significantly alter NGF structure. ADMET analysis suggested the deosome has acceptable safety and pharmacokinetic properties. Although this flavonoid glycoside exceeds some Lipinski limits Such as deviations are common among the natural compounds. This study demonstrates that the combining Transcriptomics with structured based computational approaches can identify venom targets and potential inhibitors supporting the development of complementary therapies to enhance the antivenom treatment.

4. CONCLUSION

This study demonstrates the effectiveness of integrating venom gland transcriptomics with structure based computational approaches for the identification of potential therapeutic targets in snake venom. Using RNA-seq data from Naja Naja venom glands, a transcriptome-guided workflow enabled the identification and prioritization of venom proteins based on sequence completeness, annotation confidence, and structural suitability. Among the identified toxin families, venom nerve growth factor (NGF) emerged as a structurally reliable and computationally tractable target for further analysis [50].

Structure based virtual screening and molecular docking revealed favourable interactions between NGF and selected ligand, particularly diosmin and hesperidin. Molecular dynamics simulations provided dynamic validation of these interactions demonstrating stable protein ligand complexes throughout the 100 ns simulation period [51]. The NGF and Diosmin complex achieved equilibrium earlier in the simulation, while hesperidin required a short conformational adjustment before stabilizing, indicating comparable but slightly different binding dynamics. Importantly, additional analyses including RMSF and radius of gyration confirmed that ligand binding did not significantly disrupt the structural stability of the NGF protein.

Overall, these findings highlight the potential of transcriptomics driven target discovery combined with molecular modelling to identify candidate molecules that may modulate venom proteins. Such computational strategies provide a valuable framework for the discovery of adjunct therapeutic compounds that could complement existing antivenom treatments and contribute to the development of next generation antivenom strategies [53].

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AUTHOR CONTRIBUTIONS

Mohana S J: Conceptualization, Investigation, Methodology, Laboratory Analysis.

Shanmugapriya M: Data Curation, Formal Analysis, Supervision, Writing—Review & Editing.

CONFLICT OF INTEREST

The authors declare that there is no conflict of interest.

ETHICS STATEMENT

Ethical approval was not required for this study.

DATA AVAILABILITY STATEMENT

Data supporting the findings of this study are available from the corresponding author upon reasonable request.

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