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Structural Analysis and Docking of Stilbene Synthase Protein from Chinese Grape Vine *Vitis pseudoreticulata*

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Authors' contributions

This work was carried out in collaboration between all authors. All authors have contributed equally for the manuscript. All authors read and approved the final manuscript.

Original Research Article

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ABSTRACT

Aims: The present work aims to perform the molecular modeling of stilbene synthase protein from Chinese grape vine *Vitis pseudoreticulata.*
Place and Duration of Study: The study has been performed in the Department of Biotechnology, GITAM Institute of Technology, GITAM University, Visakhapatnam, India for a period of 8 months.
Methodology: The sequence of *Vitis* STS protein was obtained by BLAST search from DFCI web server using Arabidopsis Stilbene synthase sequence. To read the amino acid pattern among these sequences, Multiple Sequence alignment have been performed using clustal W. The secondary and 3D structures were predicted for the protein and the stability of the structures was determined through Ramachandran plot and PROSA analysis. 3D structure obtained using Swiss model workspace was utilized for docking studies.
Results: In the multiple sequence alignment except Gossypium and Ipomea remaining sequences were aligning well. The secondary structure of the protein is possessing helices, coils and sheets respectively and most of the protein structure is coiled. The predicted model was subjected to evaluation by PROSA with a Z score of -10.1. Ramachandran plot revealed that the predicted that 96.6% residues were in favoured region, 2.6% were in allowed region and 0.8% were in outlier region proving that the predicted model is acceptable. Docking STS protein with secondary metabolite ligands

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elucidated that anethole, ascorbic acid and arbutin have good binding affinity.
Conclusion: The structural model of *Vitis pseudoreticulata* stilbene synthase has been determined, and *in silico* docking studies have elucidated that this protein has docked with some of the essential secondary metabolites like anethole, ascorbic acid and arbutin which might enhance the performance when they enter into a biological system.

Keywords: Stilbene synthase; Vitis pesudoreticulata; molecular modeling; docking.

1. INTRODUCTION

Stilbenes are one of the important members in the phytoalexin group of secondary metabolites, produced in grapevines, which has numerous remarkable biological properties [1]. Resveratrol (3,5,4'-trihydroxystilbene) is the main representative of this group located in the skin of grape berries, involved in the inhibition of the cellular events associated with carcinogenesis, neurodegenerative disorders, inflammation, reported to possess antioxidant properties, cardio protective properties and is capable of inhibiting the LDL oxidation, during the initial stages pathogenesis and atheroscelrosis [2]. Resveratrol shows potent antiviral activity against various families of DNA and RNA viruses by inhibiting the growth of vaccinia virus [3]. Oxyresveratrol shows inhibitory activity in HSV-1 and in VZV infections [4].

Resveratrol is synthesized *via* the well-characterized phenylalanine/polymalonate pathway, the key step of which is catalyzed by the enzyme stilbene synthase (STS). Stilbene synthase belongs to the type III group of the polyketide synthase enzyme super family which converts one molecule of p-coumaroyl-CoA and three molecules of malonyl-CoA into 3,4',5-trihydroxystilbene or resveratrol. This enzyme is a dimer with a molecular weight 90 kDa having an iso-electric point (pI) of 4.8. A conserved cysteine residue, located in the central section of the protein has been shown to be essential for the catalytic activity of STS enzyme and represents the binding site for the p-coumaroyl-CoA starting substrate [5].

The first grapevine STS gene was cloned from *Vitis vinifera* cv. Optima, and functional characterization has been studied in *Escherichia coli* [6]. Till date, 43 genes encoding STS in grapevine have been identified among which 20 of these genes were found to be expressed in response to a pathogen attack [7]. Chinese native *Vitis pseudoreticulata* represent a valuable genetic resource for grapevine disease resistance breeding and is a valuable resource of STS genes. The structure of the STS protein has not been solved in the *vitis* species. In the present study, we report the molecular structure of the stibene synthase protein from *Vitis pseudoreticulata* and its docking studies to determine the binding abilities of this protein, which has also been performed *in Silico* for identifying the co-factors which are interacting with this protein.

2. MATERIALS AND METHODS

2.1 Sequence Information

The sequences of the stilbene synthase gene for *Vitis pseudoreticulata* (ABF06886.1) were obtained from genebank by BLAST search with Stilbene synthase of Arabidopsis STS sequence (AT1G02050.1) obtained from Arabidopsis.org as source. Among these sequences *Vitis psuedoreticulata* sequence with accession TC146050 is the full length cDNA sequence of VpSTS6 and has been deposited in GenBank with Acc. No. DQ445490

[8]. These sequences were translated into the amino acid sequences and their ORFs were determined.

2.2 Secondary Structure Prediction

The secondary structure prediction of the *Vitis pseudoreticulata* STS protein was carried out using protein structure prediction server PSIPRED to identify the similarities among their protein structures [9].

2.3 Ramachandran Plot

The core of the predicted protein structure or allowed areas in the plot showing the preferred regions for psi/phi angle pairs for residues in *Vitis pseudoreticulata* stibene synthase protein was determined through Ramachandran plot using RAMPAGE server [10].

2.4 3D Structure Prediction

Swiss model work space was used in the prediction of 3D Structure of STS Protein based on sequence to profile search using an adapted HH Search protocol for protein structure prediction. Query sequence was submitted in alignment mode [11].

2.5 3D Structure Validation

3D structure obtained through Swiss model was crosschecked for the validity using PDBsum, which summarizes the data regarding the experimentally determined structural model in PDB [12]. This database will provide a comprehensive over view of all the contents of each structure deposited in Protein data Bank.

2.6 Docking Studies of *Vitis pseudoreticulata* Protein

The prediction of ligand interactions with *Vitis pseudoreticulata* stilbene synthase protein was performed through Molegro Virtual Docker, which handles all aspects of the docking process from preparation of the molecules to determination of the potential binding sites of the target protein and prediction of the binding modes of the ligands [13].

3. RESULTS AND DISCUSSION

3.1 Multiple Sequence Alignment

Clustal W was conducted with the result of the protein sequences after BLAST search with 9 plant species and no major gaps were found after aligning the mentioned sequences (Annex 1). Except Gossypium TC260016 and Ipomea TC4048 remaining sequences exhibited good alignment pattern. Ipomea TC 4048 is the only sequence that have major gaps and variations in the pattern of alignment indicating it is a sequence with minor similarity among the considered sequences. When comparative studies on different STS *Vitis* species was conducted deletions, single nucleotide changes and insertions were observed between the base pairs of 780 and 960. However, the rest of the sequence is conserved [14]. Variations among the considered sequences are limited to the first 10 amino acids except for *Ipomea* TC4048 and *Gossypium* TC260016. Gossypium showed a great dissimilarity in the first

80AA and latter aligned well with the remaining part of the sequences, where as *Ipomea* TC4048 exhibited such variations throughout the alignment except in the amino acids from 161 to 240. Rest of the alignment is highly conserved showing their unique origin. The protein of other six STS genes considered fo this study were exhibiting 94% to 99% homology illustrating their similarity in function [5].

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3.2 Secondary Structure of STS Protein

Proteins are the most complex chemical entities in nature comprising of a large number of atoms, variable composition, convoluted topology and complex surface features, which make simple descriptions of protein structures almost impossible [15]. Secondary structure of a protein will play primordial role in bioinformatics for the drug research and development. But the secondary structures of all proteins were not yet predicted. The reason is some proteins may be novel proteins or there are no experimentally determined structures for the existing sequences to substantiate the requirements and to eliminate this dearth in the knowledge. Several databases are providing tools to model the secondary structures basing on their Fasta sequences. In the present study, the secondary structure of *Vitis pseudoreticulata* protein was predicted using PSIPRED, which gave clear information regarding its protein structure. First helix is from 4 to 10 and the second helix is from 33-44 in the protein similarly in 3,4,8,9,11,12,13 helixes also exhibit subtle differences either in inception or culmination of the helixes. Remaining helixes are in same position for both structures. In coils 4,5,6,9,12,13,14,16,18,19,22,23,24 and in strands at 2,3,4,6,8,11,12 have a one amino acid residue difference either in inception or culmination (Fig. 1 and Table 1).

Table 1. The amino acid distribution of *Vitis pseudoreticulata* secondary structure

Structure	Aminoacids						
Coil	1-3	11-16	26-32	45-49	62 -73	79-90	117-125
	133-139	148-155	160-164	181-184	196- 205	215-219	225-237
	241-244	248-253	260-262	268-270	288-299	303-306	317-320
	334-338	354-366	374	386- 392			
Helix	4-10	33-44	50-61	74-78	91-116	140-147	165 -180
	206 -214	271-287	307-316	321-333	339 - 353	375 - 385	
Strand	17-25	126-132	156-159	185-195	220-224	238-240	245-247
	254-259	263-267	300-302	367-373			

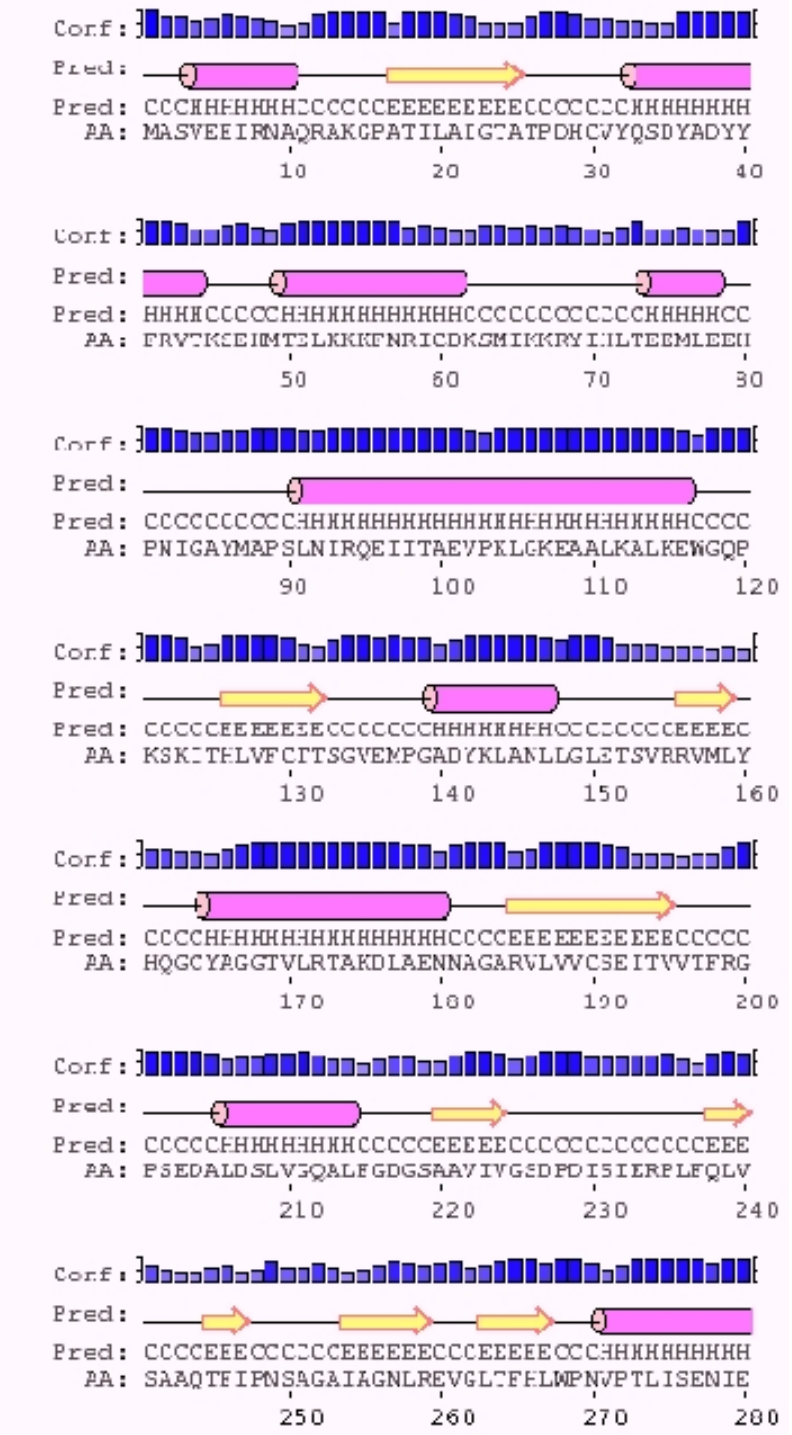
Conf:
Pred:
Pred: CCCHHHHHHHCCCCCCEEEEEEEECCCCCCHHHHHHHH
AA: MASVEEIRNAQRAKGPATILAIGTATPDHCVYQSDYADYY
10 20 30 40
Conf:
Pred:
Pred: HHHHCCCCCHHHHHHHHHHHHCCCCCCCCCCHHHHHCC
AA: FRVTKSEIMTELKKKFNRICDKSMIKKRYIHLTEEMLEEI
50 60 70 80
Conf:
Pred:
Pred: CCCCCCCCCHHHHHHHHHHHHHHHHHHHHHHHHCCCC
AA: PNIGAYMAPSLNIRQEIITAEVPKLGKEAALKALKEWGQP
90 100 110 120
Conf:
Pred:
Pred: CCCCCEEEEEECCCCCCCHHHHHHHHCCCCCCCCEEEEC
AA: KSKITFLVFCITSGVEMPGADYKLANLLGLETSVRRVMLY
130 140 150 160
Conf:
Pred:
Pred: CCCCHHHHHHHHHHHHHHHHCCCCEEEEEEEEEEEECCCCC
AA: HQGCYAGGTVLRTAKDLAENNAGARVLVVCSEITVVTFRG
170 180 190 200
Conf:
Pred:
Pred: CCCCCHHHHHHHHHCCCCCEEEEECCCCCCCCCCCCCEEE
AA: PSEDALDSLVSQALFGDGSAAVIVGSDPDISIERPLFQLV
210 220 230 240
Conf:
Pred:
Pred: CCCCEEECCCCCCEEEEEECCCEEEEECCCHHHHHHHHH
AA: SAAQTFIPNSAGAIAGNLREVGLCFHLWPNVPTLISENIE
250 260 270 280

Fig. 1. Secondary structure prediction of *Vitis pseudoreticulata* STS protein

The secondary structure indicates whether a given amino acid lies in a helix, strand or coil [16,17]. In the proposed structure most of the amino acid residues reside in the coil which indicates random coils are dominant rather than helix or strand. Helical structures are more prominent next to coils in the structure among which most of them are in αR region.

3.3 3D Structure

3D structure is highly essential for docking the protein with other ligands so that the affinity of a structure towards other structures could be deduced, which is needed in understanding the function of the protein during its interaction with other compounds. *Vitis psuedo reticulata* model based on the template 3tsyA was the result generated by the Swissmodel workspace. This template was found to be 4-coumaroyl-CoA ligase Stilbene synthase fusion protein of *Arabidopsis thaliana* and *Vitis vinifera* (Fig. 2).

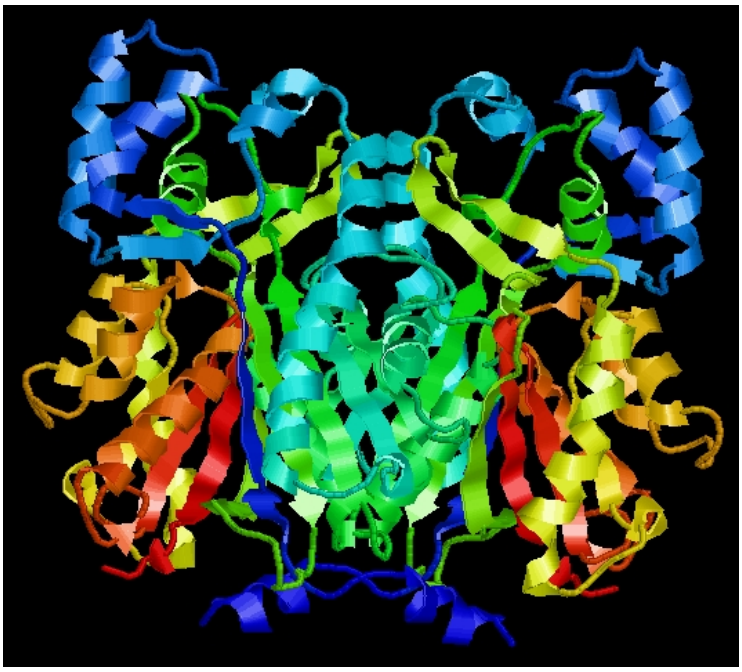

Fig. 2. The 3D Structure model of *Vitis psuedoreticulata* STS protein

3.4 Model Validation

The predicted model has been subjected to the model validation using PDB sum. 3tsyA is the PDB code of proposed Xray diffraction model with a name 4-coumaroyl-coa-ligase stilbene synthase fusion protein with an identity with the sequence around 97.7%, which validates that the proposed template is correlating with the data (Table 2).

Table 2. Validation of STS protein structure using PDB sum

PDB Code	Model	Identity (%)	Name of the protein
3tsyA	X ray Crystallography	97.7%	4-coumaroyl-coa-ligase stilbene synthase fusion protein

3.5 Model Evaluation by PROSA

ProSA-web *z*-scores of all protein chains in PDB were determined by X-ray crystallography (light blue) or NMR spectroscopy (dark blue) with respect to their length. The plot shows only chains with less than 1000 residues and a *z*-score ≤ 10. The *z*-score of *Vitis pseudoreticulata* was highlighted as large black dots in the light blue region representing that the structures are X-ray crystallography structures with a Z score value of -10.1 (Fig. 3). Z score plots elucidated that structure of *Vitis pseudoreticulata* possess model quality [18].

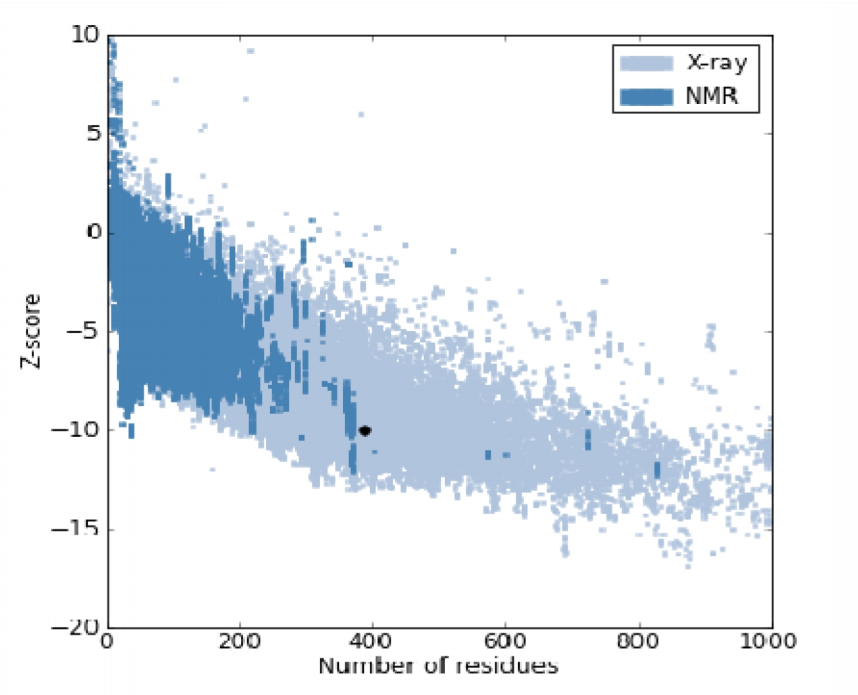

Fig. 3. PROSA (Protein Structure Analysis)-Z Plot of *Vitis pseudoreticulata* stilbene synthase protein structure

3.6 Ramachandran Plot Analysis

Using RAMPAGE the modeled 3D structure was evaluated [19]. RAMPAGE facilitates new mode of picturising the Ramachandran plot where a single plot can be classified into four different plots based on the amino acid base pair in the structure. General, Glycine, Pre pro and Proline are the four different plots which clearly elucidates the position of general amino acids, glycine and proline residues respectively. All these four plots comprehensively viewed as a single complete Ramachandran plot. The Ramachandran plot shows the phi-psi torsion angles for all residues in the structure except those at the chain termini. Glycine residues are separately identified by triangles as these are not restricted to the regions of the plot appropriate to the other side chain types. The colouring/shading on the plot represents the different regions were as described by [20]. The darkest areas correspond to the "core" regions representing the most favourable combinations of phi-psi values. The percentage of residues in the "core" regions is one of the better guides to the stereochemical quality. The Ramachandran plot for *Vitis pseudoreticulata* using RAMPAGE, revealed that among the 386 residues, 373 (96.6%) were in favoured region, 10 (2.6%) were in allowed region and 3 (0.8%) were in outlier region proving again that the predicted model is acceptable (Fig. 4). Ramachandran plot for general, glycine, pre-proline and proline were also performed and it showed the glycine, pre-Pro and proline of *Vitis pseudoreticulata* falling under allowed regions and also those glycine residues falling in disallowed region (Fig. 4). The overall results provided in the study confirm that the predicted 3-Dimenrsional structure of *Vitis pseudoreticulata* is acceptable and of good quality.

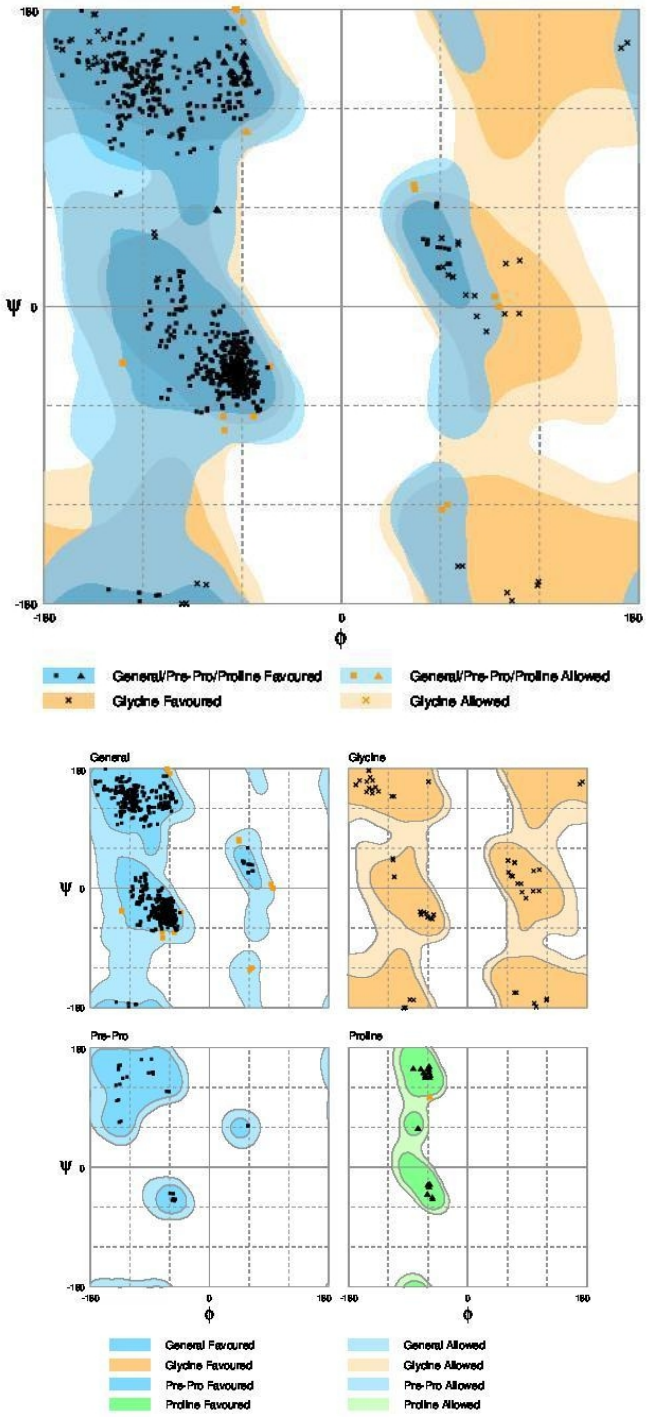

Fig. 4. Ramachandran Plot of *Vitis pseudoreticulata* stilbene synthase protein secondary structure

3.7 Docking of *Vitis pseudoreticulata* STS Protein

Protein docking is molecular modeling technique, which predicts the position and orientation of ligand when it is bound to the specific protein or its receptor, which has a wide amount of applications in the pharmacy for identification of specific target [21]. In the present study, the stilbene synthase protein of *Vitis pseudoreticulata* was docked with the 19 different ligands (Fig. 5). The docking of protein was set up with 19 ligands for 5 runs and by the completion of docking we obtained 95 different poses (Fig. 5). For all the poses of 19 ligands, MolDock score, Rerank score, Interaction, H bond and Docking score were calculated which was tabulated and mentioned in Annexure 1. Among the 95 poses best poses depending on the Moldock score were selected and tabulated in Table 3.

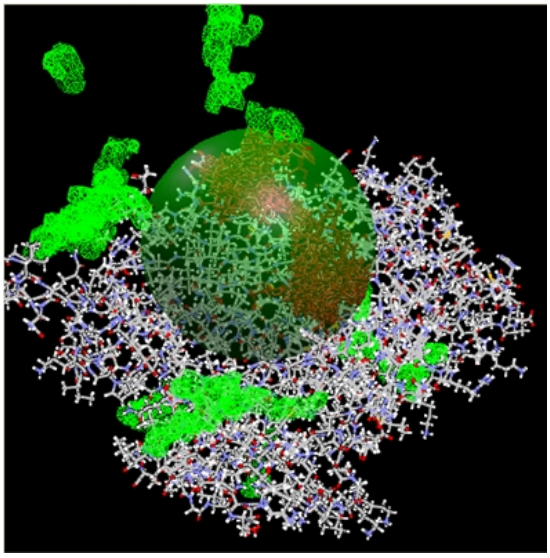

Fig. 5. Structural view of *Vitis pseudoreticulata* stilbene synthase docking

Moldock score was the energy score and Rerank score is amalgamation of several factors such as Van der Waals forces, electrostatic interactions etc. Interaction in the table infers to the interaction energy between receptor and the ligand. H bond refers to Hydrogen bonding energy and the docking score was the score assigned to the ligand pose during docking. Only Lowest energy predictions were considered while refining the initial docking and accessing the docking result [22], since the protein complex stability will be high. Hence the poses extracted from the table of ligands from annexure have lowest energy scoring in the form of Moldock and Docking score rendering stable complex. In the selected poses anethole, ascorbic acid and arbutin found to have lowest energy scoring with good binding affinity with the receptor, which can be deduced by their Docking scores -73.0593, -69.0895 and -67.2462 along with caffeic acid, carvacrol, d'alpha terpineol , alpha terpinene and alpha phellandrene, which produced good docking affinity with the Vitis STS protein. Orientin, ethyl palmitate and betacarotene metabolites were not found to be in good poses since their moldock score and Docking scores are high in contrast to remaining poses (Table 3).

Table 3. The ligand poses illustrating MolDock scores and interactions after Docking

S.No	Ligand	MolDock Score	Rerank score	Interaction	Hbond	Docking score
1.	alpha cadinene	-11.2268	264.947	-22.7842	0	-8.25899
2.	alpha hellandrene	-59.7907	-34.1215	-66.9869	0	-58.0402
3.	alpha humulene	-13.7914	576.985	0.664821	0	-11.1331
4.	alpha terpinene	-61.0945	-22.8404	-66.7354	0	-59.1912
5.	anethole	-72.4321	-32.6314	-77.611	-0.0905799	-73.0953
6.	arbutin	-48.8852	336.656	-45.9135	-8.26634	-67.2462
7.	ascorbic acid	-53.6854	-21.614	-43.7066	-1.2405	-69.0895
8.	betacarotene	156.307	2292.75	141.028	0	162.449
9.	beta pinene	-7.7379	271.872	-18.457	0	-6.25486
10.	bicyclogermacrene	-4.43039	414.676	-3.2389	0	-2.42886
11.	caffeic acid	-63.5549	-51.9764	- 66.6725	-1.37625	- 66.3742
12.	carvacrol	-61.9916	33.0288	-70.3386	-3.5096	-60.2448
13.	chlorogenic acid	-4.86094	385.073	-21.4736	5.53634	-36.3123
14.	d'alpha terpineol	-57.513	69.7978	-65.5694	-4.44911	-56.4451
15.	ethylmyristate	8.04373	556.462	-16.0593	-0.16131	2.47012
16.	ethylpalmitate	11.4685	728.373	-9.16122	-2.31852	14.4594
17.	limonene	-61.3746	-10.6364	-67.1619	0	-59.314
18.	orientin	147.944	1575.04	143.189	16.8457	113.27
19.	terpynilacetate	-28.3059	195.79	-47.1153	-0.535413	-35.3939

4. CONCLUSION

The structural analysis of proteins is important for understanding its function based on their positioning of specific amino acids at target sites. In the present study, the structural model of *Vitis pseudoreticulata* stilbene synthase has been determined, which provides an insight of its molecular function towards the understanding of its importance in the prevention of cardiovascular diseases and carcinogenesis. Further studies are in progress for comparative analysis and homology modeling of STS protein from medicinal plants.

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REFERENCES

1. Alessandro V, Ian BD, Marianna F, Sara Z, Margherita L. Genome-wide analysis of the grapevine stilbene synthase multigenic family: genomic organization and expression profiles upon biotic and abiotic stresses. BMC Plant Biology. 2012;12(8):130-151.
2. Marques FZ, Markus MA, Morris BJ. Resveratrol: cellular actions of a potent natural chemical that confers a diversity of health benefits. International journal of Biochemistry and Cell Biology. 2009;41(11):2125-2128.

3. Cheltsov AV, Aoyagi M, Aleshin A, Yu EC, Gilliland T, Zhai D, Bobkov AA, Reed JC, Liddington RC, Abagyan R. Vaccinia virus virulence factor N1L is a novel promising target for antiviral therapeutic intervention. Journal of Medicinal Chemistry. 2010;53(10):3899–3906
4. Sasivimolphan P, Lipipun V, Likhitwitayawuid K, Takemoto M, ,Pramyothin P, Hattori M, Shiraki K. Inhibitory activity of oxyresveratrol on wild-type and drug-resistant varicella-zoster virus replication in vitro. Antiviral Research. 2009;84(1):95–97.
5. Weirong X, Yihe Y, Qi Z, Jiahua D, Lingmin D, Xiaoqing X, Yan X, Chaohong, Z, Yuejin W. Expression pattern, genomic structure, and promoter analysis of the gene encoding stilbene synthase from Chinese wild Vitis pseudoreticulata. Journal of Experimental Botany. 2011;62(8):2745–2761.
6. Melchior F, Kindl H. Grapevine stilbene synthase cDNA only slightly differing from chalcone synthase cDNA is expressed in *Escherichia coli* into a catalytically active enzyme. FEBS Letters. 1990;268(1):17–20.
7. Jaillon O, Aury JM, Noel B, et al. The grapevine genome sequence suggests ancestral hexaploidization in major angiosperm phyla. Nature; 2007;449(7161):463-467.
8. Xiping W, Yuejin W, Chaohong Z and Junke Z, Isolation and characterization of cDNA encoding stilbene synthases. Vitis. 2007;46(3):104–109.
9. Altschul SF, Madden TL, Schäffer AA, Zhang J, Zhang Z, Miller W, Lipman DJ. Gapped BLAST and PSI-BLAST: a new generation of protein database search programs. Nucleic Acids Research. 1997;25(17):3389-3402.
10. Ramachandran GN, Ramakrishnan C, Sasisekharan V. Stereochemistry of polypeptide chain configurations. Journal of Molecular Biology. 1963;7(1):95-99.
11. Bordoli L, Kiefer F, Arnold K, Benkert P, Battey J and Schwede T. Protein structure homology modelling using SWISS-MODEL Workspace. Nature Protocols. 2009;4(1):1-13.
12. Laskowski RA. PDBsum new things. Nucleic Acids Research.2009;37(Database issue): D355–D359.
13. Thomsen R, Christensen MH. MolDock: A new technique for high-accuracy molecular docking. Journal of Medical Chemistry. 2006;49(11):3315-3321.
14. Huang H, Lu J, Hunter W, Litz RE, Scorza R. Comparative Analysis of Stilbene Synthase Genes among Vitis Species. 2007;738(1):755-758.
15. Ingale AG, Chikhale NJ. (2010) Prediction of 3D structure of paralytic insecticidal toxin (ITX-1) of *Tegenaria agrestis* (Hobo Spider). Journal of Data Mining, Genomics and Proteomics. 2010;1(1):102-104.
16. Jyotsna C, Ashish P, Shailendra G, Verma MK. Homology modelling and binding site identification of 1 deoxyd- xylulose 5 phosphate reductoisomerase of *Plasmodium falciparum*: new drug target for *Plasmodium falciparum.* International Journal of Engineering Science and Technology. 2010;2(8):3468-3472.
17. Ojeiru FE, Kazuya T, Yuki H, Mohammed SM and Shunsuke M. Circular Dichroism Studies on C-terminal Zinc Finger Domain of Transcription Factor GATA-2. Yonago Acta medica. 2010;53(1):25–28.
18. Wiederstein M, Sippl MJ. ProSA-web: interactive web service for the recognition of errors in three-dimensional structures of proteins. Nucleic Acids Research. 2007;35. (web server issue): W407-W410.
19. Lovell SC, Davis IW, Arendall WB et al. Structure validation by C Cαgeometry:φ,$\psi$and C β deviation. Proteins: Structure, Function, and Genetics. 2003;50(3):437–450.
20. Morris AL, MacArthur MW, Hutchinson EG, Thornton JM. Stereochemical quality of protein structure coordinates. Proteins. 1992;12(1):345–364.

21. Cerqueira NM, Fernandes PA, Eriksson LA, Ramos MJ. MADAMM: A multistaged docking with an automated molecular modeling protocol. Proteins: Structure, Function and Bioinformatics. 2009;74(1):192–206.
22. Vijayalakshmi C, Tom LB, Juan F-R. Efficient restraints for protein-protein docking by comparison of observed amino acid substitution patterns with those predicted from local environment. Journal of Molecular Biology. 2006;357(5):1669–1682.

ANNEXURE

Multiple Sequence Alignment

CLUSTAL 2.1 multiple sequence alignment

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pseudoreticulata_TC146050  ------MASVEEIRNAQRAKGPATILAIGTATPDHCVYQSDYADYYFRVT
Vitis_TC144127             ------MASVEEIRNAQRAKGPATILAIGTATPDHCVYQSDYADFYFRVT
Vitis_TC152941             ------MASVEEFRNAQRAKGPATILAIGTATPDHCVYQSDYADYYFRVT
Medicago_TC177640          ------MAYLEGIRESQRARGPATILAIGTATPVNCIYQSDFTDYYFRVT
Lycopersicon_TC217840      ------MVTVEEVRRAQRAKGPATIMAIGTATPSNCVDQSTYPDYYFRIT
Lycopersicon_TC217706      ------MVTVEEYRKAQRAEGPATILAIGTSTPSNCVDQSTYPDYYFRIT
Ipomoea_TC623              ------MVTVEEVRKAQRAQGPATIMAIGTSTPQNCVDQSTYPDYYFRIT
Gossypium_TC229867         ------MVTVEEVRKAQRAQGPATVLAIGTSTPPNCVDQSTYPDYYFRIT
Glycine_TC434240           ------MVSVAEIRQAQRAEGPATILAIGTANPPNRVDQSTYPDYYFRIT
Medicago_TC200217          ------MVSVSEIRNAQRAEGPATILAIGTANPANCVEQSTYPDFYFKIT
Glycine_TC425486           ------MVSVEEIRKAQRAEGPATVMAIGTATPPNCVDQSTYPDYYFRIT
Arabidopsis_TC373951       -MVMGDTPSLDEIRKAQRADGPAGILAIGTANPANHVIQAEYPDYYFRIT
Arabidopsis_TC372306       -----MAPSLEEIRKAQRADGPAGILGIGTANPPNHVLQAEYPDYYFRIT
Gossypium_TC260016         --------------------------------------------------
Helianthus_TC40680         MASSLTGVDVGTFRKAQRAEGPATILAIGTATPSHCVYQADYPDYYFRIT
Oryza_TC488917             ---MAAAVTVEEVRRAQRAEGPATVLAIGTATPANCVYQADYPDYYFRIT
Oryza_TC494384             --MVTSTVKLEEVRRMQRAEGMAAVLAIGTATPANCVYQTDYPDYYFRVT
Helianthus_TC39714         ------MLSIQEFRKAQRAEGPANILAIGTATPPNCVLQTTYPDYYFRIT
Ipomoea_TC4048             -------------------MNKTHALDMFPYSLNTCRVARSFSGFSP---

pseudoreticulata_TC146050  KSEHMTELKKKFNRICDKSMIKKRYIHLTEEMLEEHPNIGAYMAPSLNIR
Vitis_TC144127             KSEHMTALKKKFNRICDKSMIKKRYIHLTEEMLEEHPNIGAYMAPSLNIR
Vitis_TC152941             KSEHMTELKKKFNRICDKSMIKKRYIHLTEEMLEEHPNIGAYMAPSLNIR
Medicago_TC177640          KSEHMTQLKAKLKRICEKSMIKKRYIHLTEEILKEHPNISTYEEPSLNVR
Lycopersicon_TC217840      NSEHMTELKEKFKRMCDKSMINKRYMHLTEEILKENPNICEYMAPSLDAR
Lycopersicon_TC217706      NSEHKTELKEKFKRMCDKSMIKKRYMHLTEEILKENPNMCAYMAPSLDAR
Ipomoea_TC623              NSEHLVELKEKFKRMCEKSMIKKRYMYLTEEILKENPNICAYMAPSLDAR
Gossypium_TC229867         NSEHKTELKEKFKRMCEKSMIKKRYMYLTEEILNENPNVCEYMAPSLDAR
Glycine_TC434240           NSDHMTELKEKFQRMCDKSMIKTRYMYLNEEILKENPNMCAYMAPSLDAR
Medicago_TC200217          NSEHKTELKEKFQRMCDKSMIKRRYMYLTEEILKENPSVCEYMAPSLDAR
Glycine_TC425486           NSEHMTELKEKFKRMCDKSMIKKRYMYLNEEILKENPSVCAYMAPSLDAR
Arabidopsis_TC373951       NSEHMTDLKEKFKRMCDKSTIRKRHMHLTEEFLKENPNMCAYMAPSLDAR
Arabidopsis_TC372306       NSDHMTDLKEKFKRMCDKSMIRKRHMHLTEEFLKENPKMCAYMAPSLDTR
Gossypium_TC260016         MTDLKHKFKRMCDKSMIKKRHMYLTEEILKENPNMCAYMASSLDAR
Helianthus_TC40680         KSDHMVDLKQKFQRMCDNSMIRKRYMHVTEEFLKQNPNMCEYMAPSLDAR
Oryza_TC488917             KSEHMVELKEKFKRMCDKSQIRKRYMHLTEEILQENPNMCAYMAPSLDAR
Oryza_TC494384             NSEHLTNLKERFQRMCESSQIRKRYTHLTEEILQENPSMCVFTAPSLDAR
Helianthus_TC39714         KSEHKKDLKEKFTRMCEKSMIKKRYMYLTEEILNEKPNMCAYNAPSLDDR
Ipomoea_TC4048             ------NLSSTWSRIAGPPGWAIQKMEFQSEMPRG------LNASDKHFS
                                 *.    *:.  .    :   . .*: .          .. .

pseudoreticulata_TC146050  QEIITAEVPKLGKEAALKALKEWGQPKSKITHLVFCTTSGVEMPGADYKL
Vitis_TC144127             QEIITAEVPKLGKEAALKALKEWGQPKSKITHLVFCTTSGVEMPGADYKL
Vitis_TC152941             QEIITAEVPRLGRDAALKALKEWGQPKSKITHLVFCTTSGVEMPGADYKL
Medicago_TC177640          QDILVEEVPKLGEKAALKAIKEWGRPKSEITHLIFCSTSGVDMPGADYQL
Lycopersicon_TC217840      QDIVVVEVPKLGKEAAQKAIKEWGQPKSKITHVVFCTTSGVDMPGADYQL
Lycopersicon_TC217706      QDIVVVEVPKLGKEAAQKAIKEWGQPKSKITHLVFCTTSGVDMPGCDYQL
Ipomoea_TC623              QDIVVVEVPKLGKEAAQKAIKEWGQPKSKITHLVFCTTSGVDMPGADYQL
Gossypium_TC229867         QDMVVVEVPKLGKEAATKAIKEWGQPKSKITHLVFCTTSGVDMPGADYQL
Glycine_TC434240           QDMVVVEVPKLGKEAAVKAIKEWGQPKSKITHLIFCTTSGVDMPGADYQL
Medicago_TC200217          QDMVVVEVPRLGKEAAVKAIKEWGQPKSKITHLIVCTTSGVDMPGADYQL
Glycine_TC425486           QDMVVVEVPKLGKEAATKAIKEWGQPKSKITHLIFCTTSGVDMPGADYQL
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Arabidopsis_TC373951        QDIVVVEVPKLGKEAAVKAIKEWGQPKSKITHLVFCTTSGVDMPGADYQL
Arabidopsis_TC372306        QDIVVVEVPKLGKEAAVKAIKEWGQPKSKITHVVFCTTSGVDMPGADYQL
Gossypium_TC260016          QDIVVVEVPKLGKEAATKAIKEWGHPKSKITHLVFCTTSGVDMPGADYQL
Helianthus_TC40680          QDVVVVEVPKLGKEAAIKAIKEWGYPKSKITHLVFCTTSGVDMPGADYQL
Oryza_TC488917              QDIVVVEVPKLGKAAAQKAIKEWGQPRSRITHLVFCTTSGVDMPGADYQL
Oryza_TC494384              QDMVVAEVPKLGKAAAEEAIKEWGQPMSRITHLVFCTTNGVDMPGADYQV
Helianthus_TC39714          QDIVVVEVPKLGKEAATRAIKEWGQPKSKITHLVFCTTSGVDMPGADYQL
Ipomoea_TC4048              MLFETMEGTSLSKWNVRPTSRRWPSMAPQLSGASVCAAETS---------
                                   . . * . *..  .  : :.*    ..::   .*::.

pseudoreticulata_TC146050   ANLLGLETSVRRVMLYHQGCYAGGSVLRTAKDLAENNAGARVLVVCSEIT
Vitis_TC144127              ANLLGLEPSVRRVMLYHQGCYAGGTVLRTAKDLAENNAGARVLVVCSEIT
Vitis_TC152941              ANLLGLETSVRRVMLYHQGCYAGGTVLRTAKDLAENNAGARVLVVCSEIT
Medicago_TC177640           IKLLNLNPSTKRFMLYHQGCYAGGTVLRLAKDLAENNIGARVLVVCSEIT
Lycopersicon_TC217840       TKLLGLRPSVKRLMMYQQGCFAGGTVIRLAKDLAENNKGARVLVVCSEIT
Lycopersicon_TC217706       AKLLGLRPSVKRLMMYQQGCFAGGTVLRLAKDLAENNKGARVLVVCSEIT
Ipomoea_TC623               TKLLGLQPSVKRFMMYQQGCFAGGTVIRLAKDLAENNKGARVLVVCSEIT
Gossypium_TC229867          TKLLGLRPSVKRLMMYQQGCFAGGTVLRVAKDLAENNKGARVLVVCSEIT
Glycine_TC434240            TKQLGLRPYVKRYMMYQQGCFAGGTVLRLAKDLAENNKGARVLVVCSEIT
Medicago_TC200217           TKLLGLRPYVKRYMMYQQGCFAGGTVLRLAKDLAENNKGARVLVVCSEVT
Glycine_TC425486            TKLLGLRPSVKRYMMYQQGCFAGGTVLRLAKDLAENNKGARVLVVCSEIT
Arabidopsis_TC373951        TKLLGLRPSVKRLMMYQQGCYAGGTVLRLAKDLAENNRGARVLVVCSEIT
Arabidopsis_TC372306        TKLLGLRPSVKRLMMYQQGCFAGGTVLRLAKDLAENNRGARVLVVCSEIT
Gossypium_TC260016          TKLLGLRPSVKRIMMYQQGCFAGGTVLRLAKDLAENNKDARVLVVCSEIT
Helianthus_TC40680          TKLLGLRPSVQRFMLYQQGCFAGGTVLRLAKDLAENNKGARVLVVCSEIT
Oryza_TC488917              AKMLGLRPNVNRLMMYQQGCFAGGTVLRVAKDLAENNRGARVLAVCSEIT
Oryza_TC494384              AKMLGLPTSVKRLMMYQQGCFAGGTVLRVAKDLAENNRGARVLVVCSEIM
Helianthus_TC39714          TKLLGLRSSVKRFMMYQQGCFAGGTVLRMAKDLAENNKGARVLVVCSEIT
Ipomoea_TC4048              ---------------WNSGFSAGGGVG------ADDDRGG---------S
                                           ::.*  *** *       *::: ..

pseudoreticulata_TC146050   VVTFRGPSEDALDSLVGQALFGDGSAAVIVGSDP-DISIERPLFQLVSAA
Vitis_TC144127              VVTFRGPSEDALDSLVGQALFGDGSAAVIVGSDP-DISIERPLFQLVSAA
Vitis_TC152941              VVTFRGPSEDALDSLVGQALFGDGSAAVIVGSDP-DVSIERPLFQLVSAA
Medicago_TC177640           VVTFRGPNETHLDSLVGQALFGDGASSVIVGSNP-NTTLERPLFHLVSAS
Lycopersicon_TC217840       AVTFRGPSDTHLDSMVGQALFGDGAAAMIIGSDP-LPEVERPLFELVSAA
Lycopersicon_TC217706       AVTFRGPSESHLDSLVGQALFGDGAAAIIIGSDP-IIGVERPLFELVSAA
Ipomoea_TC623               AVTFRGPSDAHLDSLVGQALFGDGAAALIIGSDP-DPDLERPLFQLVSAA
Gossypium_TC229867          AVTFRGPSDTHLDSLVGQALFGDGAAAVIIGADP-VPEIEKPMFELVSAA
Glycine_TC434240            AVTFRGPSDTHLDSLVGQALFGDGAAAVIVGSDP-IPQVEKPLYELVWTA
Medicago_TC200217           AVTFRGPSDTHLDSLVGQALFGDGAAALIVGSDP-VPEIEKPIFEMVWTA
Glycine_TC425486            AVTFRGPTDTHLDSLVGQALFGDGAAAVIVGSDP-LP-VEKPLFQLVWTA
Arabidopsis_TC373951        AVTFRGPSDTHLDSLVGQALFSDGAAALIVGSDPDTSVGEKPIFEMVSAA
Arabidopsis_TC372306        AVTFRGPSDTHLDSLVGQALFSDGAAALIVGSDPDTSVGEKPIFEMVSAA
Gossypium_TC260016          AVTFRGPSDTHLDSLVGQALFADGAGAVIIGADPDSKT-ERPLYQFVSAA
Helianthus_TC40680          AVTFRGPSESHLDSLVGQALFGDGAAAIVVGSDP-DLDVERPLFEMVSAA
Oryza_TC488917              AVTFRGPSESHLDSMVGQALFGDGAAAVIVGSDPDEAV-ERPLFQMVSAS
Oryza_TC494384              AMAFRGPSESHLDSLVGHALFGDGAAAVIVGSDPDEAADERPLFQIVSAS
Helianthus_TC39714          AVTFRGPDDSHLDSLVGQALFGDGAAAIIVGSDP-LPDIEKPLFEIISAA
Ipomoea_TC4048              VAEQRLADEAVEVGLVGAAESDDG----DLGADD------EDAGGFVVLG
                             .   * . :    .:** *   **     :*::       .    ::  .

pseudoreticulata_TC146050   QTFIPNSAGAIAGNLREVGLTFHLWPNVPTLISENIEKCLTQAFDPLGIS
Vitis_TC144127              QTFIPNSAGAIAGNLREVGLTFHLWPNVPTLISENIEKCLTQAFDPLGIS
Vitis_TC152941              QTFIPNSAGAIAGNLREVGLTFHLWPNVPTLISENIEKCLTQAFDPLGIS
Medicago_TC177640           ETILPNSEGAIEGHLREVGLTFHLKDNVPSLIGENIEKSLEETFHPLGIT
Lycopersicon_TC217840       QTLLPDSEGAIDGHLREVGLTFHLLKDVPGLISKNIEKSLIEAFQPLGIS
Lycopersicon_TC217706       QTLVPDSEGAIDGHLREVGLTFHLLKDVPGLISKNIEKSLLEAFQPLGIS
Ipomoea_TC623               QTILPDSGGAIDGHLREVGLTFHLLKDVPGLISKHIEKSLNEAFQPLGIH
Gossypium_TC229867          QTILPDSDGAIDGHLREVGLTFHLLKDVPGLISKNIEKSLVEAFQPLGIS
Glycine_TC434240            QTIAPDSEGAIDGHLREVGLTFHLLKDVPGIVSKNIDKALFEAFNPLNIS
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Medicago_TC200217          QTIAPDSEGAIDGHLREAGLTFHLLKDVPGIVSKNINKALVEAFEPLGIS
Glycine_TC425486           QTILPDSEGAIDGHLREVGLTFHLLKDVPGLISKNIEKALVEAFQPLGIS
Arabidopsis_TC373951       QTILPDSDGAIDGHLREVGLTFHLLKDVPGLISKNIEKSLDEAFKPLGIS
Arabidopsis_TC372306       QTILPDSDGAIDGHLREVGLTFHLLKDVPGLISKNIEKSLDEAFKPLGIS
Gossypium_TC260016         QTILPDSDGAIDGHLREVGLNFHLLKDVPGLISKNIEKSLVEAFSPIGIW
Helianthus_TC40680         QTILPESEGAIDGHLREAGLTFHLLKDVPGLIANNIEKALAHAFSPLGID
Oryza_TC488917             QTILPDSEGAIDGHLREVGLTFHLLKDVPGLISKNIERALGDAFTPLGIS
Oryza_TC494384             QTILPGTEDAIVGHLREVGLTFHLPKDVPEFISDSVEGALTDAFMPLGVH
Helianthus_TC39714         QTILPDSRGAIDGHLREVGLTFHLLKDVPGLISKHIEESLVEAFQPLGID
Ipomoea_TC4048             EILGDAEDGAAG----EAALLVHHEALDGGAEAEELGELVVGAGH-----
                           : :     .*      *..* .*         .. :   :  :

pseudoreticulata_TC146050  DWKSLFWIAHPGGPAILDAVEAKLK-DKKKLEATRHVLSEYGNMSSACVL
Vitis_TC144127             DWNSLFWIAHPGGPAILDAVEAKLNLDKKKLEATRHVLSEYGNMSSACVL
Vitis_TC152941             DWNSLFWIAHPGGPAILDAVEAKLNLEKKKLEATRHVLSEYGNMSSACVL
Medicago_TC177640          DWNSLFWVTHPGGPAIIKRIEETVGLNSDKLNATKHVLSEYGNMSSACVI
Lycopersicon_TC217840      DWNSIFWIAHPGGPAILDQVELKLSLKPEKLRATRQVLSDYGNMSSACVL
Lycopersicon_TC217706      DWNSLFWIAHPGGPAILDQVELKLGLKPEKLRATREVLSNYGNMSSACVL
Ipomoea_TC623              DWNSLFWIAHPGGPAILDQVEEKLELKPEKLRATRHVLSEYGNMSSACVL
Gossypium_TC229867         DWNSLFWIAHPGGPAILDQVEAKLALKPEKLRATRHVLSEYGNMSSACVL
Glycine_TC434240           DYNSIFWIAHPGGPAILDQVEQKLGLKPEKMKATRDVLSEYGNMSSACVL
Medicago_TC200217          DYNSIFWIAHPGGPAILDQVEQKLALKPEKMKATREVLSEYGNMSSACVL
Glycine_TC425486           DYNSIFWIAHPGGPAILDQVEAKLGLKPEKMEATRHVLSEYGNMSSACVL
Arabidopsis_TC373951       DWNSLFWIAHPGGPAILDQVEIKLGLKEEKMRATRHVLSEYGNMSSACVL
Arabidopsis_TC372306       DWNSLFWIAHPGGPAILDQVEIKLGLKAEKMRATRHVLSEYGNMSSACVL
Gossypium_TC260016         DWNSIFWIAHPGGPAILDQIEAKLCLKEDKLRATRHVLSEFGNMSSACVL
Helianthus_TC40680         DWNTIFWIAHPGGPAILDQVELKLGLEEQKMRATRHVLSEYGNMSSACVL
Oryza_TC488917             DWNSIFWVAHPGGPAILDQVEAKVGLDKERMRATRHVLSEYGNMSSACVL
Oryza_TC494384             DWNSIFWVVHPGGPAILDQVEEKVALHKARMRASRNVLSEYGNMASATVL
Helianthus_TC39714         DWNSLFWIAHPGGPAILDQVEEKLALTPDKLRATRHVLSEYGNMSSACVL
Ipomoea_TC4048             --------VDAAGGAEDDVGDLGLWLAPLLDGALGGFFPKFGDFHHHNVL
                           ....* *  .  :  :        *   .:..:*::    *:

pseudoreticulata_TC146050  FILDEMRKKSLKGE-----RATTG---EGLDWGVLFGFGPGLTIET---V
Vitis_TC144127             FILDEMRKKSLKGE-----RATTG---EGLDWGVLFGFGPGLTIET---V
Vitis_TC152941             FILDEMRKKSLKGE-----KATTG---EGLDWGVLFGFGPGLTIET---V
Medicago_TC177640          FILDEMRRRSMEEG-----KTTTG---EGLKWGVLFGFGPGLTMET---I
Lycopersicon_TC217840      FILDEMRKASSKEG-----LSTTG---EGLDWGVLFGFGPGLTVET---V
Lycopersicon_TC217706      FILDEMRKASTKEG-----LGTTG---EGLEWGVLFGFGPGLTVET---V
Ipomoea_TC623              FILDEMRKASSKEG-----LNTTG---EGLEWGVLFGFGPGLTVET---V
Gossypium_TC229867         FILDEMRKKSREDG-----LQTTG---EGLEWGVLFGFGPGLTVET---V
Glycine_TC434240           FILDEMRRKSAENG-----HKTTG---EGLEWGVLFGFGPGLTIET---V
Medicago_TC200217          FILDEMRKKSAQDG-----LKTTG---EGLEFGVLFGFGPGLTIET---V
Glycine_TC425486           FILDQMRKKSIENG-----LGTTG---EGLDWGVLFGFGPGLTVET---V
Arabidopsis_TC373951       FILDEMRKKSAKDG-----VATTG---EGLEWGVLFGFGPGLTDET---V
Arabidopsis_TC372306       FILDEMRKKSAKDG-----AATTG---EGLEWGVLFGFGPGLTVET---V
Gossypium_TC260016         FIMDEMRKKSLDQG-----MPTTG---EGYEWGVLFGFGPGLTVET---V
Helianthus_TC40680         FILDEMRKKSTEEG-----KTTTG---EGLDWGVLFGFGPGLTVET---V
Oryza_TC488917             FILDEMRKRSAEDG-----HATTG---EGMDWGVLFGFGPGLTVET---V
Oryza_TC494384             FVLDEMRKLSADDG-----HATTG---EGMDWGVLFGFGPGLTVET---I
Helianthus_TC39714         FILNEMRHASATEASVPPERASSGACCSALDRGLLLKPWSSIVCPSSRWI
Ipomoea_TC4048             PGIQRRRHVFTKAW-------------------VFLQYFLG---------
                           ::. *:                        :::    .

pseudoreticulata_TC146050      VLHSIPMVTN------
Vitis_TC144127                 VLHSIPMVTN------
Vitis_TC152941                 VLHSIPMVTN------
Medicago_TC177640              ALHSANIDHGY-----
Lycopersicon_TC217840          VLHNVST---------
Lycopersicon_TC217706          VLHSVAA---------
Ipomoea_TC623                  VLHSVSA---------
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Gossypium_TC229867          VLHSVAA---------
Glycine_TC434240            VLHSVAI---------
Medicago_TC200217           VLRSIAI---------
Glycine_TC425486            VLRSVTL---------
Arabidopsis_TC373951        VLHSVPL---------
Arabidopsis_TC372306        VLHSVPL---------
Gossypium_TC260016          VLHSIPTRAN------
Helianthus_TC40680          VLHSLPTTVPTSTT--
Oryza_TC488917              VLHSVPITAGAAA---
Oryza_TC494384              VLHSVPITAAAPLIMQ
Helianthus_TC39714          VVLSSNVC--------
Ipomoea_TC4048              ----------------
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Table of Poses obtained after docking

Ligand	MolDockScore	Rerank Score	Interaction	Hbond	Docking Score
alpha cadinene	-11.2268	264.947	-22.7842	0	-8.25899
alpha cadinene	21.5689	316.263	14.3156	0	23.0894
alpha cadinene	32.404	353.492	25.2117	0	33.1717
alpha cadinene	18.6566	394.63	11.4037	0	19.2029
alpha cadinene	31.2986	436.445	20.9394	0	33.2932
alpha phellandrene	-59.7907	-34.1215	-66.9869	0	-58.0402
alpha phellandrene	-21.9202	18.8228	-29.0443	0	-20.5082
alpha phellandrene	-21.4612	19.88	-28.0854	0	-20.6486
alpha phellandrene	-64.5717	21.0947	-70.4924	0	61.6797
alphaphellandrene	-17.8454	37.7754	-23.9967	0	-17.2052
alpha humulene	-3.02398	404.301	11.4322	0	-1.16495
alpha humulene	29.5181	536.239	43.9743	0	30.8845
alpha humulene	-13.7914	576.985	0.664821	0	-11.1331
alpha humulene	24.5409	580.895	38.9971	0	26.2801
alpha humulene	34.4531	648.484	48.9093	0	36.0553
alphaterpinene	-61.0945	-22.8404	-66.7354	0	-59.1912
alphaterpinene	-59.7004	-17.126	-64.4997	0	-58.5231
alphaterpinene	-56.9559	27.1105	-63.0194	0	-55.17
alphaterpinene	-57.0669	30.5307	-63.1236	0	-55.4954
alphaterpinene	-55.9766	35.3109	-62.5088	0	-54.4323
anethole	-72.4321	-32.6314	-77.611	-0.0905799	-73.0953
anethole	-71.9113	-32.0382	-77.104	0.00258462	-72.2648
anethole	-40.2859	-27.7284	-46.5912	-0.401479	-40.1367
anethole	-41.8438	-25.3587	-48.7095	0	-41.3916
anethole	-41.6753	39.2466	-47.3848	0.396859	-43.7133
arbutin	-38.268	159.004	-41.2065	-11.7685	-36.6202
arbutin	-22.8787	196.619	-25.6626	-7.70146	-26.7309
arbutin	-40.6953	259.128	-45.5431	-5.67511	-62.8637
arbutin	-24.8708	284.87	-31.2483	-12.9577	-29.4392
arbutin	-48.8852	336.656	-45.9135	-8.26634	-67.2462
ascorbic acid	-63.7698	-42.8544	-52.376	-5.08547	-65.3316

ascorbic acid	-58.7286	-36.6686	-55.5644	-8.38655	-64.0753
ascorbic acid	-56.4209	-27.9544	-43.8425	-5.50833	-64.0385
ascorbic acid	-53.6854	-21.614	-43.7066	-1.2405	-69.0895
ascorbic acid	-50.9529	-16.5463	-40.25	-0.754188	-63.2417
betacarotene	158.779	2000.69	123.129	0	164.539
betacarotene	177.29	2137.46	151.595	0	183.191
betacarotene	156.307	2292.75	141.028	0	162.449
betacarotene	179.051	2322.52	156.739	0	185.989
betacarotene	164.189	2353.96	154.824	0	169.063
beta pinene	-5.19113	114.62	-15.9102	0	-4.21634
beta pinene	-3.67268	118.818	-14.3917	0	-2.18652
beta pinene	-7.98036	172.117	-18.6995	0	-6.14916
beta pinene	-3.24276	184.58	-13.9618	0	-1.51545
beta pinene	-7.7379	271.872	-18.457	0	-6.25486
bicyclogermacrene	-4.43039	414.676	-3.2389	0	-2.42886
bicyclogermacrene	-4.54698	421.511	-3.35567	0	-2.04765
bicyclogermacrene	27.3694	476.221	28.5608	0	29.2057
bicyclogermacrene	31.8987	485.693	33.0902	0	33.0539
bicyclogermacrene	35.1938	505.996	36.3852	0	37.3957
caffeic acid	-63.5549	-51.9764	-66.6725	-1.37625	-66.3742
caffeic acid	-61.4301	-51.0554	-64.2921	-2.60288	-61.1802
caffeic acid	-57.4554	-48.0685	-60.5466	0.643993	-62.8849
caffeic acid	-61.6687	-42.3902	-65.1907	-5.49293	-64.6174
caffeic acid	-57.668	-30.5368	-61.1678	-5.45955	-60.3379
carvacrol	-61.9916	33.0288	-70.3386	-3.5096	-60.2448
carvacrol	-61.7967	33.5164	-70.2047	-3.06541	-59.8901
carvacrol	-19.4639	50.9128	-28.2203	0	-18.5757
carvacrol	-18.3207	78.2381	-27.2395	0.350208	-20.8352
carvacrol	-13.8491	78.9676	-26.0203	-0.056982	-18.2035
chlorogenic acid	-4.50592	381.698	-22.3335	-2.59451	-22.1117
chlorogenic acid	-4.86094	385.073	-21.4736	5.53634	-36.3123
chlorogenic acid	-9.61088	407.399	-24.011	4.06447	-19.0279
chlorogenic acid	24.8361	486.728	9.28545	4.1239	-14.5795
chlorogenic acid	-8.64264	487.148	-21.5209	-14.529	-18.9769
d'alpha terpineol	-57.513	69.7978	-65.5694	-4.44911	-56.4451
d'alpha terpineol	-12.5656	88.8803	-20.6436	0	-11.2343
d'alpha terpineol	-12.3261	93.4992	-20.4268	0	-11.0453
d'alpha terpineol	-12.769	93.5904	-24.111	0	-10.4276
d'alpha terpineol	-7.3349	167.117	-15.4219	-2.86162	-8.42239
ethylmyristate	4.39444	424.288	-21.9055	-0.616917	2.62466
ethylmyristate	10.6395	441.226	-18.9254	-5.98156	11.9135
ethylmyristate	6.87721	551.026	-19.1775	-2.82233	6.3102
ethylmyristate	8.04373	556.462	-16.0593	-0.16131	2.47012
ethylmyristate	12.823	665.495	5.90702	-1.22442	13.2683
ethylpalmitate	22.985	623.994	3.29794	-4.27697	28.0885
ethylpalmitate	11.4685	728.373	-9.16122	-2.31852	14.4594

ethylpalmitate	26.3948	856.83	-4.30561	-3.50024	27.1261
ethylpalmitate	29.0976	882.55	2.48862	-5.59091	31.4594
ethylpalmitate	32.9553	963.378	14.1442	-2.70155	36.3208
limonene	-61.3746	-10.6364	-67.1619	0	-59.314
limonene	-57.1523	-8.60453	-63.302	0	-55.6239
limonene	-20.2753	15.8401	-27.5934	0	-19.4456
limonene	-21.4833	55.5801	-27.2036	0	-20.0412
limonene	-22.9033	60.0609	-28.9222	0	-22.0364
orientin	147.944	1575.04	143.189	16.8457	113.27
orientin	209.811	1881.15	211.064	26.4186	170.198
orientin	210.556	1881.52	210.286	24.3259	170.225
orientin	219.321	2144.78	225.849	13.4998	169.958
orientin	249.385	2146.59	239.546	7.32234	210.817
terpynilacetate	3.44946	135.162	-15.6107	-2.87821	4.17333
terpynilacetate	-28.3059	195.79	-47.1153	-0.535413	-35.3939
terpynilacetate	-41.1743	204.658	-56.6756	-3.80523	-41.2484
terpynilacetate	-17.7066	234.416	-38.4689	5.37924	-28.3947
terpynilacetate	20.831	246.529	8.03735	4.03673	12.8456

Peer-review history:
The peer review history for this paper can be accessed here:
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