INTERNATIONAL JOURNAL OF PHARMACEUTICAL SCIENCES
[ISSN: 0975-4725; CODEN(USA): IJPS00]
Journal Homepage: https://www.ijpsjournal.com

OPEN ACCESS

Research Paper

Computational Docking Study of Phytochemicals Isolated from Barleria Albostellata C.B Clarke

Dr. M. Srinivasa Murthy*[1], Dr. Saritha Kodithala[2], Dr. Mohammad Mansoor [3], Ch. Sampath Kumar[4], Dr. Ashok Kumar Uppuluru[5], Dr. SajidMiya[6]

[1]. Principal & Professor,Vignan Institute of Pharmaceutical Sciences, Deshmukhi,Yadadri Bhuvanagiri
[2]. Associate professor, HOD, Department of Pharmacognosy, Vignan Institute of Pharmaceutical Sciences, Near Ramoji filmcity ,Yadadri Bhuvanagiri Dist, Telangana.
[3]. Associate professor, Dept of Pharmacology, Devaki Amma Memorial College of Pharmacy, Chelembra, Pulliparamba, Mallapuram Kerala.
[4]. Assistant Professor, Dept of Pharmacology, jyotismathi institute of pharmaceutical sciences, Karimnagar.Telangana.
[5]. Professor & HOD,Department of Pharmacognosy, Max Institute of Pharmaceutical Sciences, Khammam, Telangana.
[6]. Associate Professor, Dept of Pharmacology, Mesco College of Pharmacy,Mustaid Pura Karwan Road Hyderabad..

ARTICLE INFO

Published: 13 Apr 2026
Keywords:
Barleria albostellata, Molecular docking, Phytoconstituents,Heptafluorobutyric acid,Alzheimer disease.
DOI:
10.5281/zenodo.19549285

ABSTRACT

Alzheimer disease (AD) is a progressive neurodegenerative disease results in death of brain cells. It causes memory loss and cognitive decline. The symptoms are mild at first and become more severe overtime. Many phytochemicals have been isolated from medicinal plants with anti- alzheimer activity.To perform molecular docking studies of the isolated compound on Alzheimer target protein using Autodock® software Version1.5.6. Evaluation of molecular docking analysis of isolated phytoconstituents from methanolic extracts of Barleria albostellata whole plant phytoconstituents such as Carbamic Acid, Eicosanoic Acid, 9 Oxononanoic Acid, Heptafluorobutyric Acid, Pentadecanoic Acid, Sulphurous Acid were docked with anti-alzhemier drug target proteins such acetylcholinesterase using Autodock 4.2 software. Heptafluorobutyric acid (-6.58 Kcal/mol) has significant bind energy with acetylcholinesterase when compared with standard.Remaining phytoconstituents such as carbamic acid, eicosanoic acid, 9 oxononanoic acid, pentadecanoic acid, sulphurous acid showed moderate to less binding affinity with target proteins

***Corresponding Author:** Dr. M. Srinivasa Murthy
Address: *Principal & Professor,Vignan Institute of Pharmaceutical Sciences, Deshmukhi,Yadadri Bhuvanagiri.*
Email ✉: sarithagubba1984@gmail.com

Relevant conflicts of interest/financial disclosures: The authors declare that the research was conducted in the absence of any commercial or financial relationships that could be construed as a potential conflict of interest.

INTRODUCTION

Molecular docking is a crucial aspect of computer-aided drug design (CADD) technique to study how a small molecule (ligand/drug) interacts with a macromolecule (protein/enzyme, DNA, etc.). Molecular docking basically addresses three key goals - virtual screening, pose prediction, and binding affinity estimation.[1] Docking is performed using free or licensed molecular docking software such as Autodockvina, PyRx, CCDC GOLD, Schrodinger, MOE, GLIDE, among others provide varied approaches to simulate these interactions.By retrieving protein structures from the PDB, researchers can analyze how different compounds interact with specific enzymes, aiming to find the most energetically favorable configuration for a ligand-enzyme complex.[2] This process helps in understanding potential interactions between molecules, aiding drug design and discovery.Docking serves as a crucial tool in rational drug design by predicting how small molecule candidates bind to protein targets. A statistical scoring function translates interacting energy into numerical docking scores, offering insights into the strength of molecular interactions. This process aids in assessing the affinity and activity of potential drugs within the body.

Docking is most used in the field of drug design and docking is applied to:

- Hit identification: Docking with a scoring function efficiently screens drug databases *in silico*to identify molecules likely to bind to a specific protein target.
- Lead optimization: Docking predicts the ligand's binding orientation to a protein, aiding in the design of more potent and selective analogs based on this information.
- Bioremediation: Protein-ligand docking predicts enzyme interactions degrading pollutants, aiding in identifying potential biodegradation pathways for environmental cleanup efforts.[3]

The primary aim of this study was to determine the optimal positions and orientations for ligands within the enzyme or receptor's binding center. It also aimed to assess the impact of isolated phytoconstituents from *Barleria albostellata* on their antialzhemier properties.Material and Methods

1. Docking software

Among the different types of software's available for docking, it used the Autodock4.2 software for the molecular docking investigation of proteins involved in anti-alzheimer Activity.[4-9]

2. Phytoconstituents / Ligands

The Ligands were collected from an article published by Manohar Reddy and his co- workers (2022). Phytoconstituents or ligands like Carbamic Acid, Pentadecanoic Acid, Eicosanoic Acid, 9 Oxononanoic Acid, Heptafluorobutyric Acid and Sulphurous Acid were used for molecular docking studies.[10]

3. Potential targets and binding sites

The 3D structures of antialzhemier drug targets such as acetylcholinesterase are obtained from protein database bank. Based on these ligands in crystallized structures the active sites in receptors were determined.[4-9]

4. Docking

Docking was executed to acquire probable conformations and positions for the ligand-receptor complexes at the binding site. Binding site was determined using the previous knowledge of the original ligand's interaction site. For the stimulation runs, each ligand was kept flexible, but

the amino acid residues of active site were kept rigid and default parameters values were taken. Alzheimer targets for various proteins were selected based on the literature survey. The structures of all the receptors were obtained from PDB format. Docking studies were performed against acetylcholinesterase using Autodock 4.2 software with isolated phytoconstituents and standard Rivastigmine as ligands. The results obtained in the form of binding energy and amino acids interactions by hydrogen bonding.[10-11]

RESULTS AND DISCUSSION

In silico methods are computer-based methods widely used in the pharmacological field of science to help discover inhibitors with high binding capabilities with a protein target. *In silico* methods have been used to create various inhibitors for a spectrum of diseases. Molecular Docking is an important method in molecular biology and computeraided drug design. Ligand-protein docking helps predict the binding mode of a Ligand and Protein of known 3-dimensional structures. Evaluation of molecular docking analysis of isolated phytoconstituents from methanolic extracts of *Barleria albostellata* whole plant phytoconstituents such as Carbamic Acid, Eicosanoic Acid, 9 Oxononanoic Acid,Heptafluorobutyric Acid, Pentadecanoic Acid, Sulphurous Acid were docked with antialzhemier drug target proteins such acetyl choline esterase using Autodock 4.2 software. The binding energy of phytoconstituents from methanolic extracts of *Barleria albostellata* whole plant such as Carbamic Acid, Pentadecanoic Acid, Eicosanoic Acid, 9 Oxononanoic Acid, Heptafluorobutyric Acid and Sulphurous Acid with acetyl choline esterase was found to be -4.65, -4.89, -4.92, -4.21,6.58 and -5.48 Kcal/mol. Heptafluorobutyric acid was interaction with 10 amino acids. Heptafluorobutyric acid (-6.58 Kcal/mol) has significant bind energy with acetylcholine esterase when compared with standard Rivastigmine (-10.56Kcal/mol) **(Table.1&2 and Figure.1&2).** Methanolic extracts of *Barleria albostellata* whole plant phytoconstituent such Heptafluorobutyric acid has highly bind with acetyl choline esterase and inhibited it to possess the antialzheimer activity.

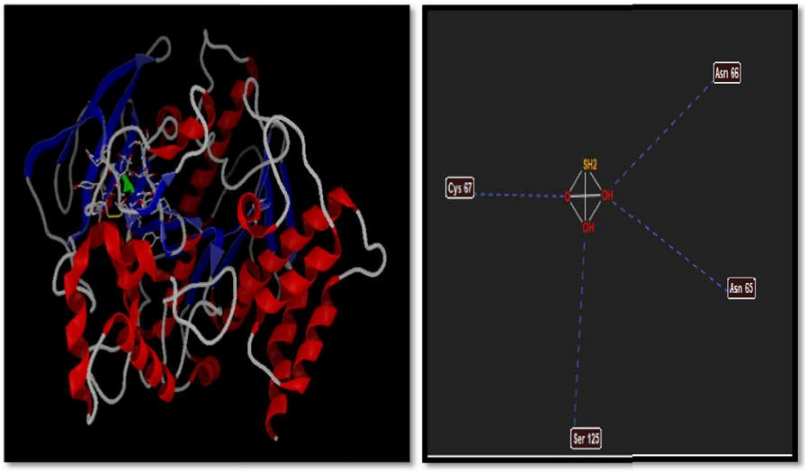
Table.1: Phytoconstituents of Barleria albostellata docking with acetyl cholinesterase

S.No	Phytoconstituents	Docking binding Energy (Kcal/mol)	Amino acid interaction
1	Carbamic acid	-4.65	Phe 155 Val 236 Val 293 Ser 291
2	Pentadecanoic acid	4.89	Val 293 Val 236 Phe 155
3	Eicosanoic acid	-4.92	Asn 65 Ser 125 Asn 66
			Phe 155

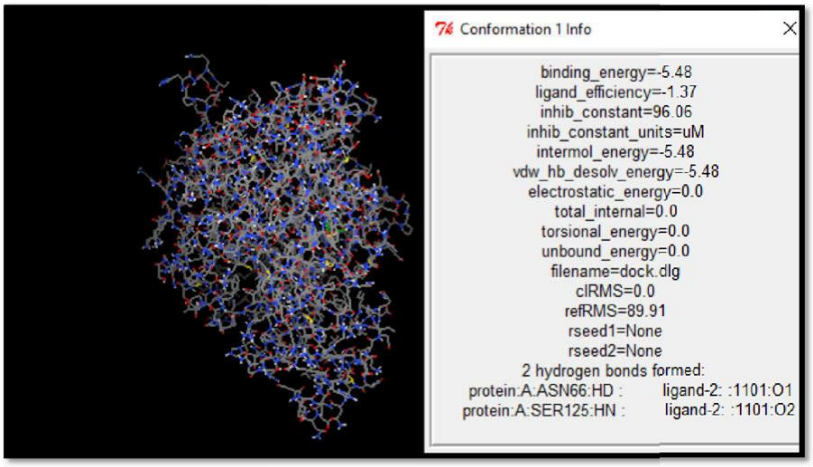
4	9 Oxononanoic acid	-4.21	Ser 291 Val 236 Val 293
5	Heptafluorobutyric acid	-6.58	Asn 65 Asn 66 Cys 67 Pro 64 Cys 94 Tyr 116 Gly 123 Ser 124 Ser 125 Ser 147
6	Sulphurous acid	-5.48	Asn 65 Asn 66 Cys 67 Ser 125

1. Sulphurous acid

3D Structure **2D Structure**

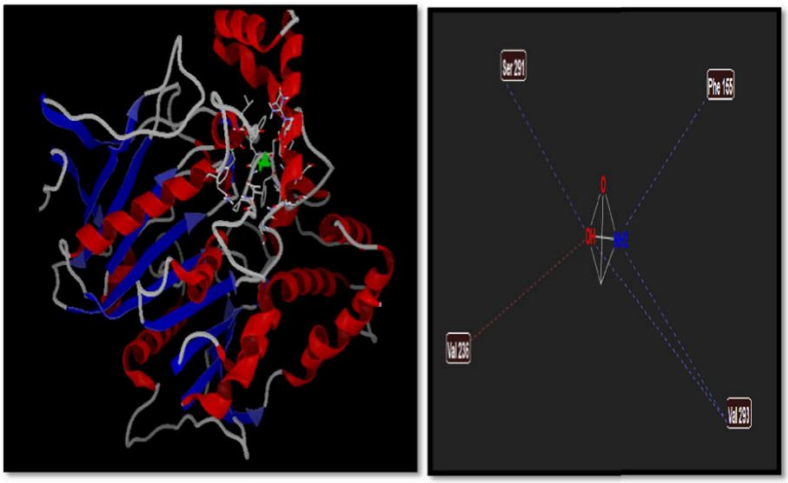


Docking binding Energy (Kcal/mol)

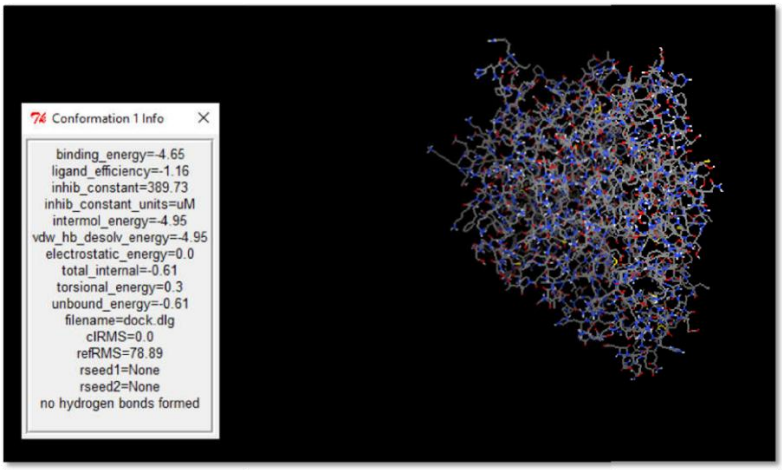


2. Carbamic acid

3D Structure **2D Structure**

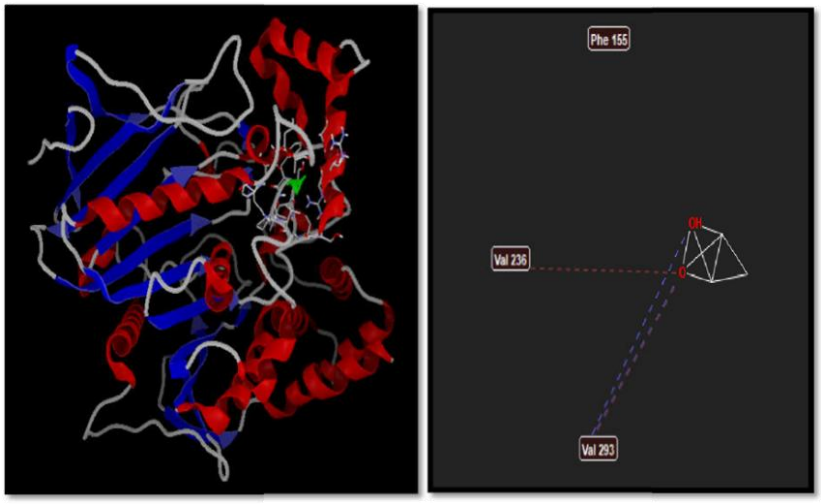


Docking binding Energy (Kcal/mol)

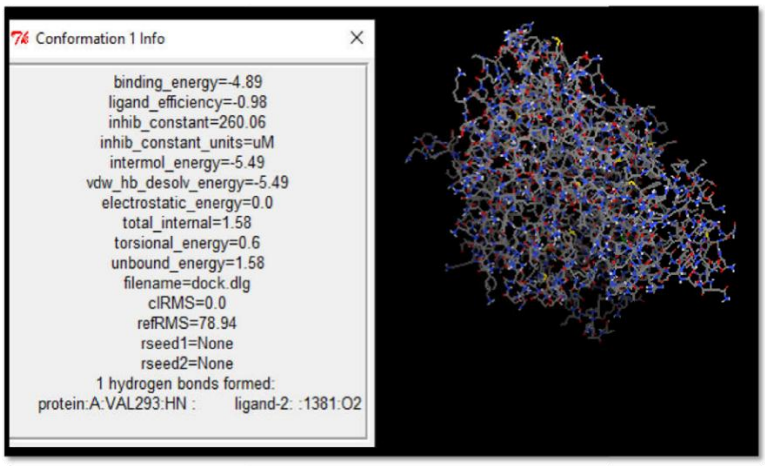


3. Pentadecanoic acid

3D Structure **2D Structure**

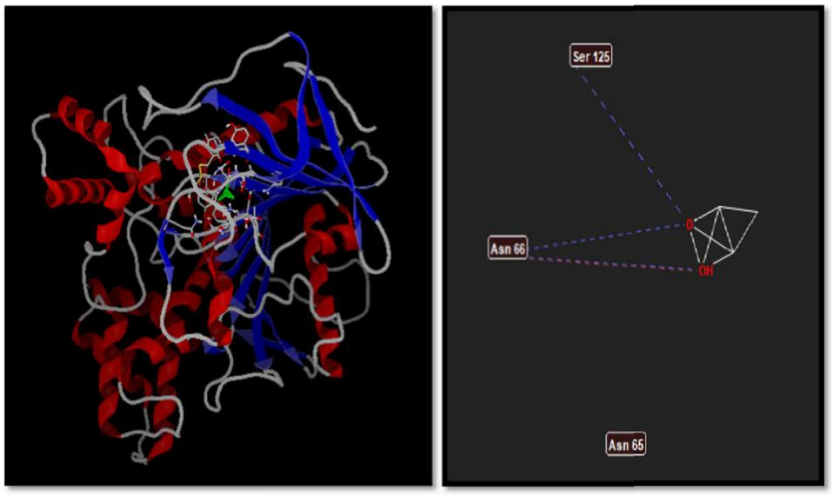


Docking binding Energy (Kcal/mol)

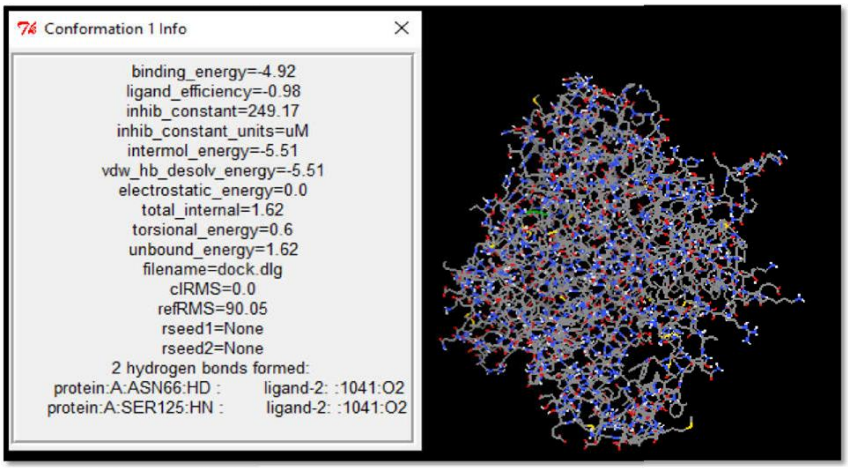


4. Eicosanoic acid

3DStructure **2D Structure**

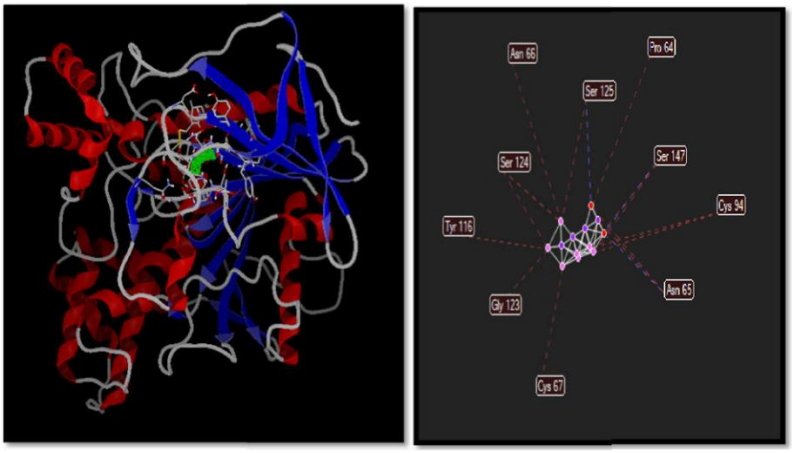


Docking binding Energy (Kcal/mol)

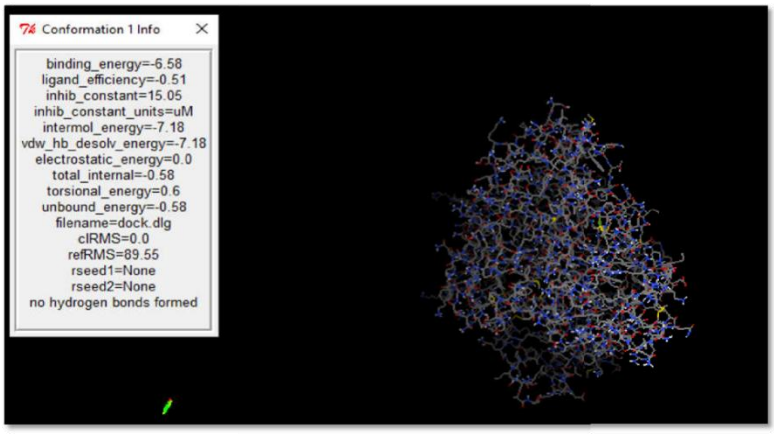


5. Heptafluorobutyric acid

3D Structure 2D Structure

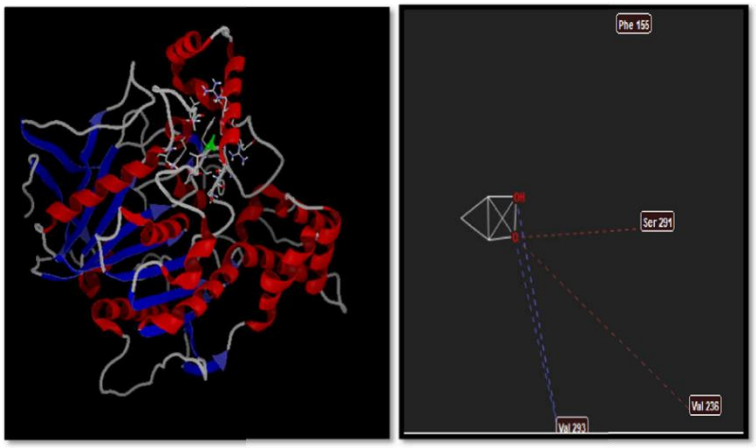


Docking binding Energy (Kcal/mol)



6. 9 Oxononanoic acid

3D Structure 2D Structure



Docking binding Energy (Kcal/mol)

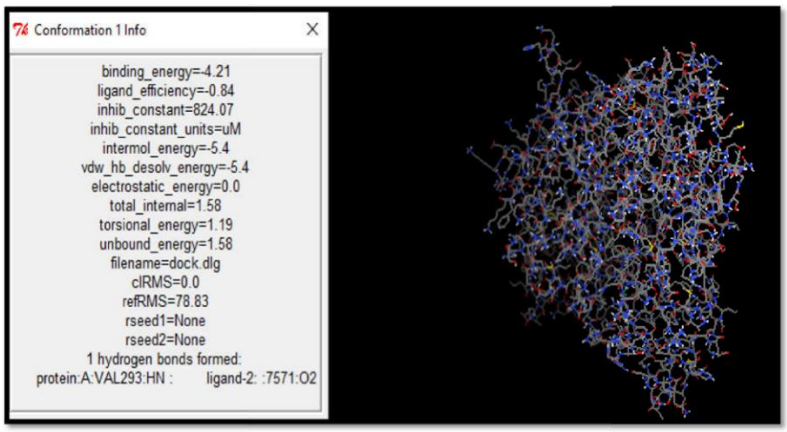
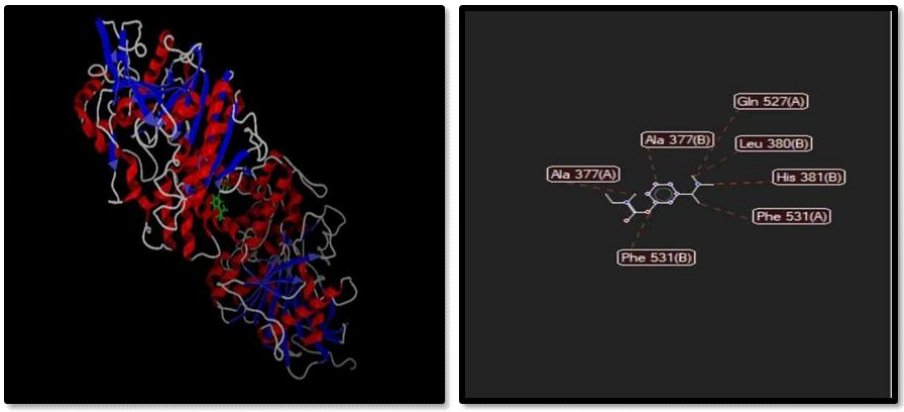


Table.2: Standard drug Rivastigmine docking with acetyl cholinesterase

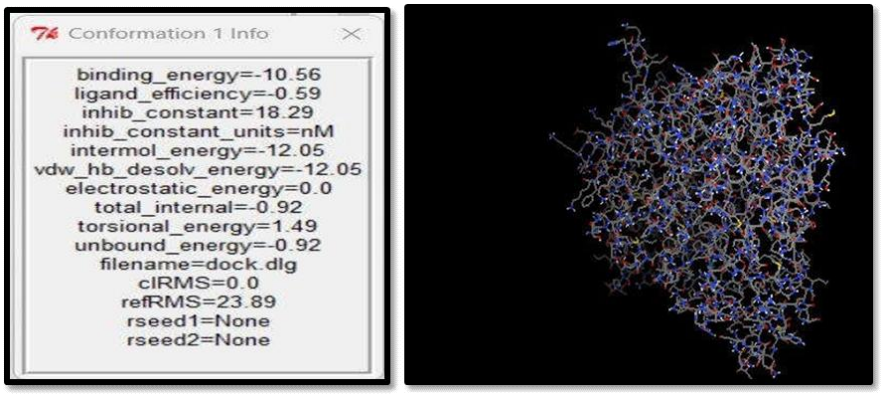
S.No	Ligand	Docking binding Energy (Kcal/mol)	Aminoacid interaction
1	Rivastigmine	-10.56	Ala377 Gln527 Leu380 His381 Phe531

Fig.2 3D,2D structure and binding energy of Rivastigmine docking with acetyl cholinesterase

3D Structure 2D Structure



Docking binding Energy (Kcal/mol)



CONCLUSION

Among the in-silico docking study for isolated phytoconstituents from methanolic extracts *of Barleria albostellata* whole plant phytoconstituents such as Carbamic Acid, Eicosanoic Acid, 9 Oxononanoic Acid, Heptafluorobutyric Acid, Pentadecanoic Acid, Sulphurous Acid were docked with antialzhemier drug target proteins such acetyl choline esterase using Autodock4.2 software. HeptafluorobutyricAcid (-6.58 Kcal/mol) has significant bind energy with acetyl choline esterase when compared with standard Rivastigmine (-10.56Kcal/mol). This efferts will choose for further study and chemical synthesis as anti-alzheimer drugs for the management of Alzheimer. In future it may lead to the development of Heptafluorobutyric acid agonists for anti- alzheimer activity

REFERENCES

1. Ajay N.Jain.Anthony Nicholls. Recommendations for evaluation of computational methods.Journal of computer aided molecular design.2008;22:133–139.
2. Michael Berry, BurtramC. Fielding and Junaid Gamieldien.Potential Broad-Spectrum Inhibitors of the Coronavirus 3CLpro: A Virtual Screening and Structure-Based Drug Design Study. Bioinformatics and Computational Biology of Viruses.2015;7(12):6642– 6660.
3. Suresh, P., S., Kumar, A., Kumar, R., Singh, V., P., An Insilco approach to bioremediation: Laccase as a case study. Journal of Molecular Graphics and Modelling. 2008; 26:845-849.
4. Ramu B, Sathish Kumar M, Ramakrishna M (2015) Current Regulatory Scenario for Conducting Clinical Trials in India. Pharmaceut Reg Affairs. 4:137. doi: 10.4172/2167-7689.1000140
5. B.Ramu et al, Formulation of Lamotrigine Orodispersible Tablets by Using New Generation Superdisintegrants World Journal of Pharmacy and Pharmaceutical Sciences Volume 4,2015, Issue 06, 631- 643.
6. Rithvik Ganesh, IyanarKannan. Molecular Docking study of certain Plant Alkaloids as Inhibitors of Various Drug Targets of Alzheimer Disease. Biomedical and Pharmacology Jounal 2017; 10(3):1489-1494. and D. M. Barton, “Drug discovery in the era of the genome,” *Pharmacol. Ther.*, vol. 92, pp. 57–66, 2001
7. SARITHA K, MURALI R, SRINIVASAN N, M. SRINIVASA MURTHY Isolation of Stigmasterol from Artabotrys Odoratissimus: Synthesis, Characterization, Molecular Docking Studies of its analogues against Estrogen Receptor, Korean Journal of Physiology and Pharmacology, Volume 28, Issue 1, 2024, ISSN:1226-4512.
8. RamuB. Method Development and Validation for the Determination of Citalopram Hbr by HPLC method in bulk drug and pharmaceutical dosage form.Pharm. Anal. Acta201785362.
9. Ramu B. Formulation of Lamotrigine Orodispersible Tablets By Using New Generation Superdisintegrants Generation Superdisintegrants World Journal Of Pharmacy And Pharmaceutical Sciences. 2015; 4:631- 43.
10. Ramu B, Saibaba SV. Role of community pharmacist in management of anaemia. Pharm Pharmacol Int J. 2018;6(3):216–220. DOI: 10.15406/ppij.2018.06.00178..
11. Somarouthu Venkata Saibaba, Bandameedi Ramu. Role of Community Pharmacist in Management of Anaemia. Open Science

Journal of Clinical Medicine. Vol. 6, No. 2, 2018, pp. 5-9.

12. Gopikrishna, A.; Ramu, B.; Srikanth, G.; Rajkamal, B. Formulation of isoniazide sustained release formulation by using carbopol 934 P. Int. J. Appl. Pharm. Sci. Res. 2016, 1, 60–69.
13. RAMESH, C., RAMU, B., RAJKAMAL, B. (2016) .Formulation of Colon Specific Didanosine Enteric Coated Matrix Tablets Using Sensitive Polymer. The Pharmaceutical and Chemical Journal, 3(2), 1-14.
14. P.P. Deepika et al. Formulation and evaluation of doxorubicin nanopsonges for targeted drug delivery African J. Biol. Sci. (South Africa) (2024)

HOW TO CITE: Dr. M. Srinivasa Murthy, Dr. Saritha Kodithala, Dr. Mohammad Mansoor, Ch. Sampath Kumar, Dr. Ashok Kumar Uppuluru, Dr. SajidMiya, Computational Docking Study of Phytochemicals Isolated from Barleria Albostellata C.B Clarke, Int. J. of Pharm. Sci., 2026, Vol 4, Issue 4, 1970-1979 https://doi.org/10.5281/zenodo.19549285