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Molecular docking-based screening of Liquiritin from Glycyrrhiza Glabra as a potential anti-Alzheimer's agent

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Abstract
Alzheimer's disease (AD) remains a major challenge in neurodegenerative disorder management, with limited treatment options available. This study investigates Liquiritin, a bioactive compound from Glycyrrhiza glabra, for its potential as an anti-Alzheimer's agent. Molecular docking simulations were conducted with the amyloid beta-protein precursor (PDB ID: 1AAP), comparing Liquiritin with Donepezil. Liquiritin exhibited a MolDock score of -103.59, indicating comparable or stronger binding affinity than Donepezil, with a higher Rerank score and stronger hydrogen bond interactions. The results suggest that Liquiritin could offer a promising alternative for Alzheimer's treatment. These findings support the need for further experimental validation of Liquiritin's neuroprotective effects.

Keywords: Alzheimer's disease, Liquiritin, Glycyrrhiza glabra, molecular docking, amyloid beta-protein precursor

Introduction
Alzheimer disease (AD) is a progressive neurodegenerative condition that is associated with memory impairment, deterioration in cognitive functions as well as changes in behavior. It ranks among the most common causes of dementia and millions of individuals in the world have this crippling disorder [1, 2]. Though great efforts have been made in understanding the disease, the therapeutic interventions of the Alzheimer disease have not yet been sufficient, with most of the interventions only offering symptomatic treatment to patients instead of treating or preventing the disease [3, 4]. The existing pharmacological therapies, which are mainly aimed at the issue of neurotransmitter imbalance, e.g. acetylcholine, do not resolve the causes of the illness e.g. the accretion of beta-amyloid plaques, tau protein tangles and neuroinflammation. These problems emphasize the critical necessity of the creation of new and efficient therapeutic agents capable of addressing a variety of pathways that are engaged in AD development [3, 5-7].
The therapeutic potential of natural products has been well established over time and the natural products present a source of bioactive compounds with a wide range of pharmacological properties. One of them, Glycyrrhiza glabra or licorice, has been promising due to its diverse medicinal properties, such as antioxidant, anti-inflammatory, anti-cancer and neuroprotective [8-11]. Licorice is traditionally used in many cultures to treat respiratory conditions, digestive conditions and skin conditions. Recently, however, its use in the treatment of neurodegenerative diseases, such as Alzheimer, has been starting to show itself [10, 12, 13]. Glycyrrhizin, liquiritin And is liquiritigenin are key bioactive compounds in Glycyrrhiza glabra with promising neuroprotective effects which include the potential to alleviate oxidative stress, prevent inflammation and modulate several important neurosurvivance and neuroregeneration molecular pathways [14-16].
Computational approaches such as molecular docking have over the past years turned out to be invaluable assets in drug discovery especially in the field of identifying potential inhibitors to certain proteins that are part of the disease progression [17, 18]. 0 Molecular docking mimics the process of interaction between small molecules (ligands) and target proteins and one can predict both binding affinities and the mode of interaction.

The method is useful in the process of narrowing down extensive lists of natural compounds to those that are worthy of further experimental confirmations [19-21]. Docking studies have been extensively applied in the context of the Alzheimer disease to determine compounds, which are capable of inhibiting beta-amyloid peptide aggregation, preventing tau protein phosphorylation or regulating neuroinflammatory responses [22-25].

This research intends to use docking-based screening to investigate the prospects of bioactive compounds of Glycyrrhiza glabra as anti-Alzheimer agents. Through assessing the interactions of these compounds with some major Alzheimer-related proteins, the research aims at creating viable leads that could be used in the generation of more effective Alzheimer therapeutic options. By this in silico strategy, we will have the chance of speeding up the process of discovering novel, multi-target anti-Alzheimer agents based on this popular medicinal plant.

Materials and Methods

Protein Preparation

The docking experiment commenced with the set up of the target protein structures in Molegro Virtual Docker (MVD). Protein Data Bank (PDB) was searched to obtain the 3D crystal structure of protease inhibitor domain of an amyloid beta-protein precursor of Alzheimer (PDB ID: 1AAP). The selection of this structure was due to high-resolution data (less than 2.5 A) which guaranteed accuracy and integrity of the structure. The structure of the protein was imported into the MVD workspace with the help of the "File Import Molecule Protein" functionality and optimized and refined [26-28].

The water molecules were eliminated unless essential to stabilize the ligand and heteroatoms that would not be essential were eliminated so that they would not cause interference during docking. Repair Add Missing Hydrogens tool was used to add polar hydrogens to provide correct distribution of charges and geometry. The correct atom types and bond orders were automatically determined by MVD to be consistent in the molecular structure. In detection of potential binding sites in the amyloid beta-protein precursor, the "Detect Cavities" functionality was applied. The active binding pocket adopted as the most biologically relevant cavity with the optimal volume and minimum energy was chosen to be utilized in the further simulations [29-31].

Ligand Preparation

Another important thing about molecular docking is how the ligand should be prepared in order to predict its interaction with the target protein. In this investigation, Liquiritin, a bioactive substance of Glycyrrhiza glabra (licorice) was used as the ligand. Also, Donepezil, a conventional treatment medication used in the treatment of Alzheimer disease was also utilized as a comparison treatment. Liquiritin chemical structure was retrieved in PubChem database in either 2D or 3D format and stored in standard file formats (.molor.sdf) [32-34].

The minimization of energy of the ligands was done with the help of Chem3D software in which the MM2 force field or the MMFF94 force field was used to attain a geometrically stable and energetically preferred conformation. Such a procedure reduced steric strain, maximized the bond anglesand made the ligands take up their lowest energy conformation. The 3D minimized structures were then exported in the form of .mol2 or .sdf to be compatible with MVD. Importation of the ligands into MVD was done through the option of File Import Molecule Ligandand the hydrogen atoms that were missing were added to meet the requirement of valence. MVD automatically checked and fixed the atom types and bond orders in order to prepare the ligands to undergo docking simulations [33, 35-37].

Preparation and Import of Molecules

The target protein (Alzheimer amyloid beta-protein precursor, PDB ID: 1AAP) and the ligands (Liquiritin and Donepezil) were all loaded into the MVD workspace to be simulated in docking. The protein and the ligands were kept in their protonated forms at a physiological pH (7.4). This was used to guarantee adequate electrostatic potential and hydrogen-bonding patterns, that are important in ensuring reliable docking results [32, 38-40].

The binding site was defined with Docking Wizard tool of MVD. The active binding pocket was chosen manually and the coordinates (X, Y, Z) and radius (812 A) of the binding pocket were given to make sure that the docking algorithm was binding to the biologically active parts of the protein [41-43].

Docking Setup

With MVD a new docking project was created through the Docking → Start Docking Wizard → Create New Docking Job menu. MolDock SE (Simplex Evolution) algorithm was selected because it is very effective in the exploration of the ligand conformational space. The binding affinity was defined using the scoring functions, MolDock Score or Re-Rank Score, which is based on non-bonded interactions and steric complementarity [44-46].

They were adjusted to the following parameters of the docking simulation: number of runs = 1030, maximum iterations = 15002000 and population size = 50100. The Constrain Docking was activated to facilitate particular interactions amongst the residues of the amyloid beta-protein precursor with the ligands. Energy threshold was set at 100 and 1020 poses per ligand was saved to be analyzed. After the parameters were set, then the docking simulation was triggered and the software ran conformational searches repeatedly until the best binding poses surpassing minimum energy scores were found [47-49].

Docking Analysis

After docking simulation was completed, MVD produced a priority list of ligand-protein binding poses of the ligand-protein interaction, ranked by MolDock Scores (predicted binding energies). The lowest (most negative) score pose was the most stable and energetically favorable complex, which suggests a high affinity of the ligand and the protein active site [50-52].

In order to visualize the molecular interactions, MVD View Ligand Interactions function was utilized. This gave specific graphic images of hydrogen bonds, hydrophobic contacts and electrostatic interactions between Liquiritin or Donepezil and the amyloid beta-protein preceptor residues. The bond lengths (in AA) and interactant amino acids were measured to determine the stability of the interaction and the specificity of the interactions. The docking was checked by the binding poses against the co-crystallized ligands [53, 54].

Also, the energy components such as hydrogen bonding, van der Waals forces, steric interaction, electrostatics and torsional penalties were also studied in an effort to expound on the binding mechanisms. The resulting products were exported as either .mol2, .pdb, or image file to be further analyzed and displayed, such as the generation of 2D, 3Dand secondary interaction maps that were employed in publication figures [55, 56]. Docking analysis of a bioactive compound of Glycyrrhiza glabra (licorice) Liquiritin and Donepezil, a conventional Alzheimer drug, to the protease inhibitor domain of the Alzheimer amyloid beta-protein precursor (PDB ID: 1AAP) had showed promising results. Liquiritin displayed a MolDock score of -103.59 as indicated in Table 1, slightly lower than the -99.98 that was registered by Donepezil indicating that Liquiritin has a similar, but not better binding affinity. Liquiritin had a Rerank score of -51.52 that is much better than the -76.14 of Donepezil indicating that Liquiritin could be more specific and effective with the protein. Besides that, the hydrogen bond analysis revealed that Liquiritin interacted stronger with the protein with a bond value - 9.63 as opposed to that of Donepezil at -2.04. This is an indication that Liquiritin can be more stable in its interaction and this is a reason why it has a greater potential as an effective anti-Alzheimer agent. The binding modes and interactions of each of the two compounds with the amyloid beta-protein precursor are visually represented in the 2D, 3D and secondary interaction figures (Figures 1-6). The formation of numerous and strong hydrogen bonds and hydrophobic interactions was found to increase the stability of Liquiritin and its specificity with the target protein. These findings indicate that Liquiritin may provide a good alternative to Donepezil in the treatment of Alzheimer and requires more experimental research to support the interest.

Table 1: Ranking of Ligands and Poses against Crystal Structure of the Protease Inhibitor Domain of Alzheimer's Amyloid Beta-Protein Precursor Protein Based On Moldock Score Protein: 1AAP

Ligand	Species Name	MolDock	Rerank	H Bond
503737	Liquiritin	-103.59	-51.52	-9.63
3152	Donepezil (Standard Drug)	-99.98	-76.14	-2.04

Fig 1-6: Interactions of Ligands with Protein

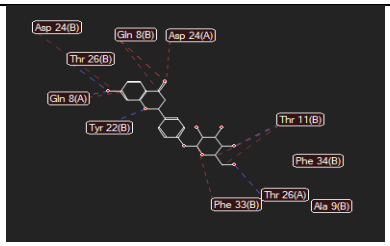

Fig 1: 2D Interaction of Liquiritin with 1AAP

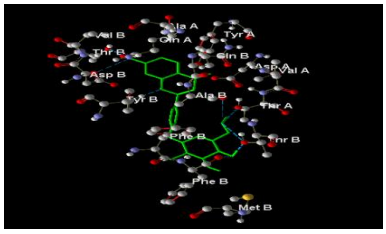

Fig 2: Secondary Interaction of Liquiritin with 1AAP

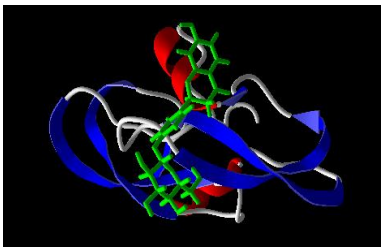

Fig 3: 3D Interaction of Liquiritin with 1AAP

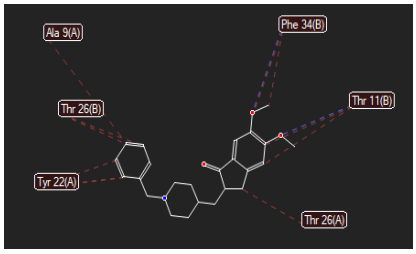

Fig 4: 2D Interaction of Donepezil with 1AAP

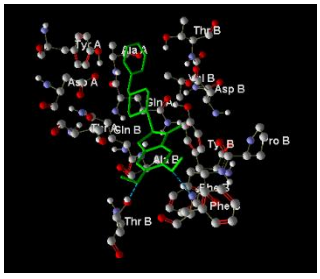

Fig 5: 3D Interaction of Donepezil with 1AAP

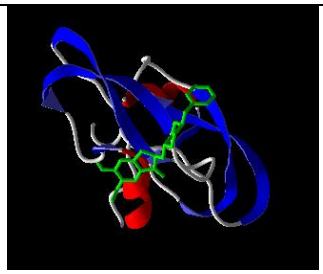

Fig 6: Secondary Interaction of Donepezil with 1AAP

Results and Discussion

Alzheimer disease (AD) is a major cause of dementia, which is characterized by the presence of beta-amyloid plaques, tau protein tangles and neuro inflammation. Although there are improvements in the understanding of the disease, the management approaches are largely only providing symptomatic relief as opposed to preventing the disease, so novel therapeutic agents are necessary [57, 58]. This paper has examined the bioactive constituent of Liquiritin of Glycyrrhiza glabra (licorice) as a possible anti-Alzheimer agent, with molecular docking to understand the mechanism of action of this compound with the protease inhibitor domain of the amyloid beta-protein precursor of Alzheimer (PDB ID: 1AAP). The data shows that Liquiritin has an equivalent, albeit slightly higher binding affinity than that of Donepezil, which is a conventional Alzheimer drug [11, 59].

Table 1 indicates that Liquiritin had a MolDock score of -103.59 which is a little lower than the score of Donepezil which was -99.98. This notwithstanding, Liquiritin had an Rerank score of -51.52 which was much higher than that of Donepezil at -76.14 indicating that Liquiritin may interact with the protein specifically and in a more stable fashion. This is also reinforced by the hydrogen bond analysis which depicted Liquiritin bond value to be -9.63, which is much stronger than that of Donepezil of -2.04 and so, Liquiritin might have more stable binding properties, which contributes to its potential as a good anti-Alzheimer agent. The neuroprotective effect of Glycyrrhiza glabra and its bioactive constituents, including glycyrrhizin and liquiritin has been investigated as a therapeutic option in previous studies. Indeed, research has demonstrated that liquiritin has the ability to alleviate oxidative stress which is a significant

cause of neurodegeneration in AD. [13, 60] The potential of natural compounds in preventing tau protein phosphorylation and inhibiting the aggregation of beta-amyloid has been also proved by the molecular docking studies, including those by Zhang *et al*. (2024). These results are congruent with the outcome of this research where Liquiritin demonstrated good interaction with the amyloid beta-protein precursor, indicating that it may serve as a good substitute or supplement to existing therapies such as Donepezil [61, 62].

The ligand-protein interactions (Figures 1-6) indicate the stability and selectivity of the binding of Liquiritin, as these interactions are characterised by strong hydrogen bonds and hydrophobic interactions with major residues of the target protein. These results indicate that Liquiritin may be a key ingredient in dealing with various pathological processes of Alzheimer disease and therefore it is the most promising to be subjected to further experimental support and clinical development [63, 64].

The in silico results of this research indicate that the Liquiritin of Glycyrrhiza glabra would be a good lead compound in the development of new therapies to treat Alzheimer. There is a need to further validate it through experimental experiments such as *in vivo* and *in vitro* experiments to establish its potential as an effective form of treatment to AD.

Conclusion

This study explores the potential of Liquiritin, a bioactive compound from Glycyrrhiza glabra, as an anti-Alzheimer's agent through molecular docking against the amyloid beta-protein precursor (PDB ID: 1AAP). The results show that Liquiritin has a comparable or slightly superior binding affinity compared to Donepezil, the standard Alzheimer's drug. With a MolDock score of -103.59 and stronger hydrogen bond interactions (bond value -9.63), Liquiritin demonstrates greater stability and specificity in its interaction with the target protein. These findings suggest that Liquiritin could be a promising alternative to Donepezil in Alzheimer's treatment. Further experimental studies, including *in vitro* and *in vivo* validation, are needed to confirm its efficacy as a therapeutic agent for Alzheimer's disease.

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