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Molecular Docking Study of Phytochemicals of Gymnema Sylvestre and Their Effects on the Complex of SARS-CoV2 Spike Protein and Human ACE2

Akshay R. Yadav*

Assistant Professor, Department of Pharmaceutical Chemistry, Rajarambapu College of Pharmacy, Kasegaon, Dist-Sangli, Maharashtra, India-415404

*Corresponding author E-mail: akshayyadav24197@gmail.com

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ABSTRACT

Gymnema is known as "mesasrngi" in Ayurvedic medicine, and both the dried leaf (mesasrngi leaf) and dried root (mesasrngi root) are used therapeutically. The plant's leaves are used to treat diabetes, obesity, and dental caries as a digestive, antiviral, diuretic, antiallergic, hypoglycemic, hypolipidemic, and antiobesity agent. Gymnema's dried leaf and root, depending on dosage type and composition, are also used to treat svasa (bronchial asthma), kasa (cough), kustha (leprosy and other skin diseases), and vrana (wounds), among other conditions, according to the Ayurvedic Pharmacopoeia of India. Human ACE2 receptor (PDB ID-1R42) is considered as receptor protein for molecular docking study of spike protein fragment with its receptor in human host. To identify the hypothetical binding motif of the title compounds using VLifeMDS software by *in-silico* (molecular docking studies). These findings showed that the binding energy in all active compounds ranged from -25.48 to -68.26 kcal/mol. If compared to the standard -80.12 kcal/mol. The phytocompounds Gymnemasin C and Gymnamine minimum dock score were found to be potent, with a docking score of -68.26 and -52.90 respectively. As a result, the study provides experimental support for traditional antidotes, and these phytocompounds may be promoted as potential lead molecules in the future.

Keywords : *Gymnema sylvestre, In-silico* docking, Phytoconstituents, SARS-CoV2, Human ACE2.

I. INTRODUCTION

While experimental research results have since confirmed the use of gymnema for some of these conditions, the main active constituents of the plant are still unknown. Gymnemic acid, a combination of at least 17 different saponins, is considered to be the main constituent of gymnema[1]. This acid is widely used as a standardisation and quality control marker in most commercial gymnema preparations. G, on the other hand, has a variety of other chemical constituents that have been identified. Gymnema

saponins, for example, are a major component of gymnema, and there are at least seven different forms of them[2-3]. These compounds, as well as the polypeptide Gurmarin, the alkaloid conduritol, gymnamine, gypenoside, and the dammarane-type saponins gymnemasides and gymnemasin B, C, and D, are thought to be responsible for the plant's hypoglycemic and antisaccharide effects[4]. As a result, it's difficult to say the markers are likely to be the best measures of consistency and effectiveness without further research into Gymnema's chemistry and the effects of each constituent.

Figure 1: *Gymnema sylvestre*

Diabetes mellitus is becoming more popular and widespread around the world. This upward trend, along with the dramatic increase in associated morbidity and mortality, is expected to have a significant effect on households, populations, health-care services, and financing[5]. As a result, new cost-effective interventions for disease management are required. Given that G. sylvestre targets a number of diabetes-related etiological factors. Considering that more than 800 plants have been commonly used to treat diabetes, and that most plants have a wide range of clinical effects, it's possible that phytomedicine may provide a revolutionary approach to this chronic disease. However, few plants were found to be validated by rigorous clinical evidence in an earlier study of herbs and nutrient supplements that claimed to improve glycemic control[6]. In addition to six well-known strains of human-infectious coronaviruses. Two other particularly pathogenic SARS-CoV and MERS-CoV-viruses, SARS-CoV-2 also causes major respiratory failure and death. Furthermore, the population has become vulnerable to highly pathogenic coronaviruses and have grown into events of public health, there by increasing the need to prepare a possible reappearance or to produce new viruses[7]. COVID-19 is hard to foresee before the end of the pandemic; high-death coronavirus. Seven different coronaviruses are currently known to cause human breathing disorders. The latest SARS-CoV-2 coronavirus outbreak in December 2019 is in the coronavirus 2B type, which is 80 % identical to the SARS-CoV genome[8]. In the future too, continuous mutation is likely. A variety of CoV therapies, such as immunomodulations, vaccines, antivirals specific to CoV and host-specific antivirals are being developed. Many people with COVID-19 have severe breathing problems[9-10]. The molecular docking approach can be used to model the interaction between a small molecule and a protein at the atomic level, which allow us to characterize the behavior of small molecules in the binding site of target proteins as well as to elucidate fundamental biochemical processes[11]. The docking process involves two basic steps: prediction of the ligand conformation as well as its position and orientation within these sites (usually referred to as *pose*) and assessment of the binding affinity[12-18]. These two steps are related to sampling methods and scoring schemes, respectively, which will be discussed in the theory section. The purpose of the scoring function is to delineate the correct poses from incorrect poses, or binders from inactive compounds in a reasonable computation time[19-22]. However, scoring functions involve estimating, rather than calculating the binding affinity between the protein and ligand and through these functions, adopting various assumptions and simplifications. Scoring functions can be divided in force-field-based, empirical and knowledge-based scoring functions. Classical force-field-based scoring functions assess the binding energy by calculating the sum of the non-bonded (electrostatics and van der Waals)

interactions[26-29]. The electrostatic terms are calculated by a Coulombic formulation. Since such point charge calculations have problems in modeling the protein's real environment a distance-dependent dielectric function is generally used to modulate the contribution of charge–charge interactions[30-34]. The van der Waals terms are described by a Lennard-Jones potential function. Adopting different parameter sets for the Lennard-Jones potential can vary the "hardness" of the potential which controls how close a contact between protein and ligand atoms can be acceptable[35-39]. Force-field-based scoring functions also have the problem of slow computational speed. Thus cut-off distance is used to handle the non-bonded interactions. This also results in decreasing the accuracy of long-range effects involved in binding. Extensions of force-field-based scoring functions consider the hydrogen bonds, salvations and entropy contributions. Software programs, such as DOCK, GOLD and AutoDock, offer users such functions[40-45]. They have some differences in the treatment of hydrogen bonds, the form of the energy function etc.. Furthermore, the results of docking with force-field-based functions can be further refined with other techniques, such as linear interaction energy and free-energy perturbation methods (FEP) to improve the accuracy in predicting binding energies. In empirical scoring functions, binding energy decomposes into several energy components, such as hydrogen bond, ionic interaction, hydrophobic effect and binding entropy[46-49]. Each component is multiplied by a coefficient and then summed up to give a final score. Coefficients are obtained from regression analysis fitted to a test set of ligand-protein complexes with known binding affinities. Empirical scoring functions have relatively simple energy terms to evaluate. However, it is unclear as to how well they are suited for ligand-protein complexes beyond the training set[50-52]. Additionally, each term in empirical scoring functions may be treated in a different manner by different software, and the numbers of the terms included are also different. LUDI, PLP, ChemScore are examples derived from empirical scoring functions Knowledge-based scoring functions use statistical analysis of ligand-protein complexes crystal structures to obtain the interatomic contact frequencies and/or distances between the ligand and protein. They are based on the assumption that the more favorable an interaction is, the greater the frequency of occurrence will be. These frequency distributions are further converted into pairwise atom-type potentials[53-54]. The score is calculated by favoring preferred contacts and penalizing repulsive interactions between each atom in the ligand and protein within a given cutoff. The appeal of knowledge-based functions is computational simplicity, which can be exploited to screen large compound databases. They can also model some uncommon interactions like sulphur-aromatic or cation-π, which are often poorly handled in empirical approaches. However, they are still faced with the problem that some interactions are underrepresented in the limited training sets of crystal structures as well as by the bias inherent in the selection of proteins for successful structure determination thus the obtained parameters may not be suitable for widespread use, especially with interactions involving metals or halogens. PMF, DrugScore, SMoG and Bleep are examples of knowledge-based functions which differ mainly in the size of training sets, the form of the energy function, the definition of atom types, distance cutoff or other parameters[63-64]. Consensus scoring is a recent strategy that combines several different scores to assess the docking conformation[55-56]. A pose of ligand or a potential binder could be accepted when it scores well under a number of different scoring schemes. Like ADME analysis, molecular docking study, microwave extraction of plant extract proved to be time consuming process as Microwave-assisted extraction (MAE) is a method for extracting solutes from a solid matrix and transferring them to a solvent. The mechanism is complicated by phenomena such as electromagnetic transfer, heat transfer, mass transfer, and momentum transfer[57-58].

The characteristics of heat and mass transfer are extremely important when designing process engineering. Microwave radiation's ability to penetrate and combine with a substrate allows for precise and regulated heat. As a result, the microwave technique can be adapted to deliver high-power electromagnetic energy to the compounds of interest in the substrate. When compared to other extraction methods, the energy-saving factors and short processing times result in lower production costs and improved product uniformity and yields, resulting in high-quality products. Since the extraction occurs as a result of changes in the cell structure induced by electromagnetic waves, the microwave extraction (MAE) process differs from traditional methods (solid–liquid or simply extraction)[59-62]. Molecular docking is an appealing scaffold for understanding medicinal biomolecular interactions in rational drug design as well as in the mechanical analysis in order, primarily noncovalently, to insert the molecule (ligand) into the favorite binders of the particular target area of the DNA/protein (receptor)[64]. The information gathered from the docking method can be used to demonstrate the binding energy, free energy and complex stability. Furthermore, in Ayurvedic literature, the routine use of coriander seed decoction is considered to be effective in reducing the amount of blood lipids[65-66].

II. MATERIALS AND METHODS

Molecular Docking Study:

The VLifeMDS 4.1 software was used to perform the molecular docking study. VLifeMDS 4.1 software has provided both rigid (no torsional flexibility for both a protein and a ligand) and flexible (torsional flexibility for a rigid protein ligand) molecular docking. Either experimentally known or theoretically developed through knowledge-based protein modeling or homology modeling was the target or receptor. The molecular docking tool was designed to obtain a preferred interaction geometry of ligand-receptor complexes with minimum interaction energy assisted by various scoring functions. Electrostatics only, the steric and electrostatic sum (force-field parameters), and the dock score. For lead optimization, this utility allowed us to screen a collection of compounds. The interaction energy between the ligand and the receptor protein is minimized using VLifeMDS.

Protein Preparation:

Human ACE2 receptor (PDB ID-1R42) is considered as receptor protein for molecular docking study of spike protein fragment with its receptor in human host. Only high atoms, water, cofactors and metal ions can be used in a standard PDB structure, and multimerical structures can be used. These entities are not familiar with bond instructions, topologies or formal atomic costs. The raw PDB structure should therefore be prepared for docking in a suitable way.

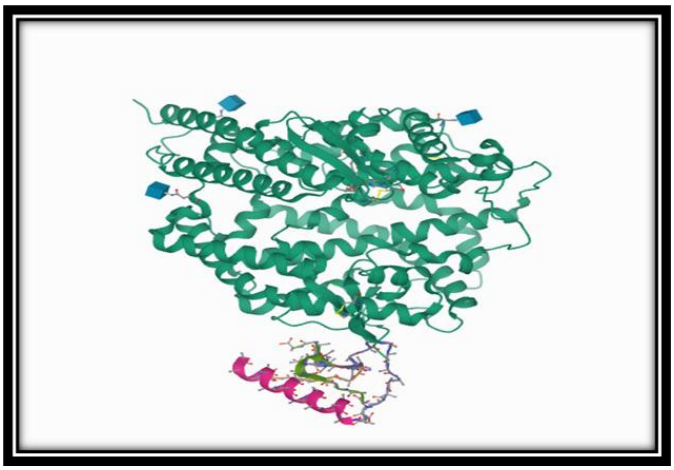

Figure 2: 3D View of Human ACE2 receptor (PDB ID-1R42)

Ligand preparation

The 2D structures of the compounds were built and then converted into 3D. Then, using MMFF, the 3D structures were energetically minimized to the rms gradient of 0.01.

Identification of cavities

Enzyme cavities were calculated by using the software's cavity determination option. To assign an appropriate active site, the cavities in the receptor were mapped. The basic function used to map the cavities was the receptor's surface mapping and the geometric voids were defined and the void was scaled for its hydrophobic characteristics. Therefore, based

on their size and hydrophobic surface area, all the cavities that are present in the receptor are classified and ranked. Considering the dimensions and the hydrophobic surface area, as an active site, the cavity is considered to be the best void.

Scoring function

The distinction is based on the scoring or fitness feature of good or bad docked conformation. Only electrostatic and both steric and electrostatic interactions between receptor ligand and dock score scoring function are used by MDS fitness functions. The dock score measures binding affinity with a recognized 3D structure of a given protein-ligand complex[67-68].

Table 1: Phytoconstituents used in study

Sr. no	Name of Phytoconstituents
1	Gymnamine
2	Gypenoside
3	Gymnemasin B
4	Gymnemasin C
5	Gymnemasin D
6	Conduritol

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III. RESUTLS AND DISCUSSION

Molecular docking study were subjected on Human ACE2 receptor (PDB ID-1R42) is considered as receptor protein for molecular docking study of spike protein fragment with its receptor in human host. The phytocompounds Gymnemasin C and Gymnamine minimum dock score were found to be potent, with a docking score of -68.26 and -52.90 respectively. Where the main interaction between ligand and receptor can be observed, the best pose obtained by docking results is reported. phytocompound 4 had a high binding affinity with ACE2 protein and it made hydrogen bond interaction with Asp 757, Glu 663. Standard drug Hydroxychloroquine showed a high binding affinity with ACE2, and it made hydrogen bond interaction with Gly 625, Met 695, Arg 743, Asp 757 and Lys 646 The standard dock score was found to be -72.89.

Table 1: Docking score of Phytoconstituents of *Gymnema sylvestre*

Sr. no	Phytochemical constituents	Mol dock score (Kcal/mol)
1	Gymnamine	-52.90
2	Gypenoside	-30.21
3	Gymnemasin B	-29.82
4	Gymnemasin C	-68.26
5	Gymnemasin D	-25.48
6	Conduritol	-47.91
7	Hydroxychloroquine	-72.89

IV. CONCLUSION

The attraction of the ligand's binding affinity towards protein is determined by the force between the S-protein fragment, ACE2 and Gymnemasin C. Protein-ligand binding strength is known as binding affinity. This affinity specifies whether a ligand can eventually bind or separate from the surface of the protein and return to its unbound state. Docking servers calculate the binding affinity of various docking structures in the absence and presence of spike protein for non-competitive modulators.

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