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Research Article

Molecular Docking Studies on Polyphenols of *Moringa oleifera* for its Enhanced Production of Heamoglobin and Impact of its Extracts on *Drosophila melanogaster*

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ABSTRACT

The work that I have chosen is to treat anaemia, a disorder that affects mostly children and women which is prominently because of the iron deficiency in the nutrition. Deficiency of iron at this phase of life affects development of brain and might have uncontrolled results on cognitive development. Iron deficiency anemia was evaluated to predict that 40%-60% of brain impairment, predominantly 6-24 months from under developed countries. *Drosophila melanogaster* also called common fruit fly is a well-studied, considered and highly monitored model organism for genetics for comprehending molecular mechanisms of human illness. Many fundamental physiological, biological and neurological characteristics are preserved between mammals and fruit fly and about 75% of human pathogenic genes are predicted to contain functioning homologin the fly. *Moringa oleifera*'s methanolic extraction of leaf has high value of free radical scavenging property. *M. oleifera* leaf supplementation enhances mortality, locomotion and capacity of reproduction in fruit fly. Hence *Moringa oleifera* leaf is considered to be safe and may be considered in the management of impact that predisposes to free radical insults. Our main goal is to develop a drug to find a remedy for this disease using polyphenols which are found abundantly in *Moringa oleifera*. Polyphenols prevent anaemic disorder that cause iron deficiency and also provides other nutritional benefits.

Keywords: Anemia; Haemoglobin; *Moringa oleifera*; Iron deficiency; Astragalin; Oxygen; RBC

INTRODUCTION

Haemoglobin, a protein present in red blood cells helps to carry oxygen all over the body. Oxygen produces energy and charges the cells. When haemoglobin levels are low it may be a symptom for several health illness which includes different sorts of cancer and anaemia. Haemoglobin levels drop down when the body is unable to produce required amount of red blood cells due to any type of disease or condition. When our body doesn't meet the demand of oxygen supply due to low haemoglobin level, it makes one feel very weak and tired. Normal range of haemoglobin levels differs for women and men. The normal level is estimated around 14.0-17.5 grams per deciliter (gm/dL) for men. The normal level is estimated around 12.3-15.3 grams per deciliter (gm/dL). A serious low level of haemoglobin is 13.5 gm/dL and below for men. For women it is considered to be 12 gm/dL [1].

Moringa oleifera is a plant commonly called as the drumstick tree. It has many other names such as horseradish, ben oil tree and miracle tree. It has been used for its abundant medicinal properties to cure health problems and for nutritional benefits over centuries. It also has multiple anti properties which are remarkable like antibacterial, anti-inflammatory, antiviral, antidepressant and many more [2].

Molecular docking is a tool used in computer aided drug design and structural molecular biology. The result of ligand-protein docking is to predict the three-dimensional structure between the binding of the ligand with the protein. Thriving docking process search increased-dimensional gaps effectively and utilize a scoring program that rectifies ranks candidate dockings. Utilization of docking can be to execute virtual screening on huge study of compounds, result the scores and predict the purpose of how the ligands resist the target, which is not valuable in lead growth. The execution of the input structures for the docking very essential like the docking itself, and

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examine the results of stochastic finding methods can at times not be clear [3].

The common fruit fly, scientifically known as *Drosophila melanogaster* has been studied in many investigations in the field of biology as an invertebrate replacement to mammals for its huge betterment compared to many alternate model organisms, reasons behind this are short life cycle, high prolificacy, easy to handle, great availability of genetic information. Its behavior can be associated to its development, which can be speculate the physiological circumstance. We have enhanced easy and vigorous observable assays for evaluating survival of the larvae, climbing ability of the adult, behavior of reproduction and the life cycle and life span of the fruit fly [4].

MATERIALS AND METHODS

The protein selection and retrieval from protein data bank

The protein haemoglobin 3D structure was retrieved from the protein data bank. The protein is prepared by Autodock software where the bonds were assigned, fixation of charges, addition of hydrogen atoms and incorporating the orientation of the group. On binding to the low-density Lipoprotein Receptor-related Protein (LRP)/CD91 which is a receptor related protein through which haemoglobin can regulate various signaling pathways and haemoglobins with increased oxygen affinity have substitutions affecting the α1β2 contact of the tetramer. The PDB coordinates are optimized target protein with minimum energy and a more stable conformation. Haemoglobin with the receptor protein CD91 was chosen with therapeutic potential for treating anaemia [5].

Construction and retrieval of ligand structures

The bioactive compound is being chosen from *Moringa oleifera* leaf extracts for this study. The different ligands were retrieved from the PubChem compound database.

Preparation of target protein

The enzymes were studied and retrieved from PDB. The protein was selected based on regulating various signaling pathways. The protein is responsible for inducing anti-inflammatory properties against liver cirrhosis. The hydrophobic molecules were eliminated along with heteroatomic molecules. Single chain was determined for the docking analysis and was visualized using Pymol software [6].

Molecular docking analysis

The best match between a receptor molecule and ligand can be determined using docking. It involves various steps like:

- Protein preparation
- Ligand preparation
- Binding site preparation
- Scoring energy evaluation

Docking studies was performed to determine the inhibition potential of drug molecule against liver cirrhosis with polyphenolic compounds of *Punica granatum* extracts using Autodock vina software. Autodock vina software is an automated docking tool that functions by Lamarckian genetic algorithm. The ligand molecule which binds to the receptor with known 2D or 3D structure can be predicted. The bases of drug development process can be formed by the interaction of the molecules with the receptor [7].

To perform docking the protein needs to be converted from PDB format to PDBQT format using Autodock software. The ligand conversion from SDF to PDBQT can be done using Open Babel software.

Methodology of *Drosophila melanogaster* activity on *Moringa oleifera* leaf extract

Sample collection and preparation: The plant substance was collected at Lalbagh botanical garden Bangalore. The collected plant substance was identified and authenticated. Collection of fresh leaves, cleansing with tap water, cleaning with distilled water was followed. The leaves were shade dried for 11-16 days to make sure that the nutrients and phytocomponents are conserved. The dries leaves were crushed using a motor and pestle. The sample was now soaked using ethanol 99.9%.

Preparation of the extract: Using Soxhlet apparatus the leaves which were extracted by hot continuous extraction. Around 200 ml of both socked leaf and ethanol were extracted for 9 hours until the extraction of the leaves was complete using Soxhlet apparatus. Further evaporation was done for concentration of the extraction [8].

Media preparation: Media preparation for 500 ml of standardized media, distilled water about 500 ml was taken, jaggery of about 50 grams was taken in a container and was boiled to dissolve it completely. Sooji around 50 grams was cooked for 15 minutes and for media solidification 5 grams of agar was added. Constant stirring was done to avoid lumps and to dissolve completely. The *Moringa oleifera* leaves extract was added to the media and allowed to cool down to 50 degrees. Preservative was added as propionic acid of about 3.7 ml. The prepared media was transferred into bottles immediately to avoid further solidifying. About 50 ml of sample was poured and allowed to solidify for about 5 hours and later cotton plugged.

Methodology: The experiment contained various assays such a locomotion, wet starvation test, dry starvation test, reproductivity and life span. The tests were performed on 15 day and the extraction were fed at various concentration such as 20 mg, 40 mg, 60 mg, 80 mg and 100 mg. The control was kept in two bottles. The deaths of the flies were noted periodically [9].

For each test 5 bottles were allotted and each contained 6 flies (3 males and 3 females).

Considering small number of flies will give clear and aid in better evaluation and determination of their activity.

- Test for life span

- Test for wet starvation
- Test for dry starvation
- Test for reproduction
- Test for locomotion

RESULTS AND DISCUSSION

Molecular docking of all the five bioactive compounds from *Moringa oleifera* leaf extract was carried out against the protein hemoglobin using Autodock vina software. The best compound with lowest glide (binding) energy produced by the hydrogen bond formation are being selected. From the docking approach we can determine that Astragalin was the compound with the better protein target interaction. Based on the binding energy of the molecules that were screened and investigated for interaction through Autodock vina, the pictures depict that the ligands interact appropriately with the target protein hemoglobin.

There are two ligands (astragalin and Isoquercetin) with highest binding energy score of -6.8 as shown in the Table 1. The interaction with the protein is being suited the best for the prevention of the anemic condition by increasing the protein hemoglobin. The other ligands also show high affinity and binding scores towards the target protein such as Nicotiflavin, Rutin and vitexin with high scores of -6.6, -6.4 and -6.5 respectively. The 3D images of the ligand with the protein, along with the corresponding amino acids, hydrogen bonds and hydrophobic interaction can be visualized.

Table 1: Binding affinity of bioactive compounds.

Serial no.	Compound	Binding affinity
1	Astragalin	-6.8
2	Isoquercetin	-6.8
3	Nicotiflavin	-6.6
4	Rutin	-6.4
5	vitexin	-6.5

CONCLUSION

Computational methods are being considered as one of the most effective ways in developing a potential drug. The results obtained indicate the receptor-based pharmacophore anticipation of the hemoglobin protein was effective in the determination of the amino acids which are essential in target drug interaction. PLIP (Protein Ligand Interaction Profiler) is a software which detects automation and visualization for the analysis of protein ligand interaction with 3D structures and also provides comprehensive analysis.

The results from this study helped us to find that Astragalin and Isoquercetin were the good compounds responsible in the increasing the iron and vitamin c content by from the *Moringa oleifera* leaf extract with highest binding energy of -6.8 and exhibits prevention of anemia and prevents damage of red blood cells.

We conclude that the leaves of *Moringa oleifera* aids in medicinal uses and therapeutics its phytochemicals. We have examined that the extract of the leaves has positive effect on many factors of development in *Drosophila*. It is administered that male population increased with the exposure of increase in concentration. Over generations the number of offspring's have increased by 3 times from the initial generation.

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