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RESEARCH ARTICLE

In-Silico Enactment of *Musa paradisiaca (L.)* Exudate Against the Urotlithiatic Disease by Docking Study

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Abstract

Objectives: Urolithiasis is a condition that occurs when the stones exit the renal pelvis and move onto the remainder of the urinary collecting system. *Musa paradisiaca (L.)* is a plant with high nutritive value and has been used for the treatment of various diseases including urolithiasis. The objective of the present study was designed to detect the receptor-ligand binding energy and interaction through a molecular docking from the bio-active compounds in an exudates of *M. paradisiaca pseudo* stem on urolithiatic causative protein named as glycolate oxidase receptor (PDB ID: 2RDU). **Methods:** In silico study especially molecular docking was performed using AutodockVina and the best confirmation between ligand and protein were selected using Lamarkaina Genetic Algorithm (LGA) and ligand protein interaction was visualized using PyMol viewer. **Novelty:** Totally three various bio-active compounds are elucidated named as Olean-12-ene-3 beta, 28-diol, Tricyclo[8.4.1.1(3,8)] hexadeca- 3,5,7,10,12,14-hexaene- 2,9-dione, anti and 2H-Pyran,2-(7-heptadecynyloxy)tetrahydro- from the exudate of experimental sample. Three phyto active compounds or secondary metabolites were used for the present prediction by docking. The present result of molecular docking clearly revealed that olean 12 -ene-3 beta, 28 diol is the best biologically effective ligand observed through a highest docking score (-7.2 k cal/mol) on glycolate oxidase receptor than other two ligand compounds. In conclusion the compound olean 12 -ene-3 beta, 28 diol could be act as a potential lead molecule for urolithiasis.

Keywords: Musa paradisiaca; Exudate; GCMS; Urolithiasis; AutoDock; PyMol Viewer

1 Introduction

Musa paradisiaca (L.), is a crop indigenous to the tropical and subtropical regions of the world[(1)], has been reported to promote healthy digestion, improve affective state and serve as a good source of electrolytes for the body[(2)]. Traditionally it has also

been shown to be more useful in the management of independent of diabetes[3] and nephritis and kidney stone related diseases[4]. *Musa paradisiaca* has been used in the treatment of urolithiasis by the rural people in South India[5]. The remote people of South India had been using the juice of *M. paradisiaca* pseudostem for kidney stone *M. paradisiaca* is a commonly available plant in India[6]. The pseudostem exudate contains the rich source of bioactive compounds[7] and the aqueous juice of pseudostem had been used traditionally by the rural people of South India against nephritis, uremia, and urolithiasise disease as indigenous folk remedies. Urolithiasis or formation of urinary stone causes a major impact on public health and economy globally since last two decades[8].Modern diagnostic and therapeutic aids such as extra corporeal shock wave lithotripsy, ureteroscopy, and percutaneous nephrolithotomy had revolutionized the urological practices but cannot altered the recurrence of stone formation and also have adverse side effects[9]. Insilico study through computational prediction especially molecular docking supports the identification of lead compound within a short duration. In this context receptor-ligand binding affinity and energy value estimation is a suitable technique for structure based drug designing and exact phytocompound or combination of few phytochemicals can easily be predicted[10]. Still, no one work has been done the similar kind of research. Hence, the present study was framed this objective such as insilico study was to detect suitable receptor ligand binding energy and interaction through molecular docking and drug ability potential of three biologically active phytocompounds from the pseudostem exudate in *M. paradisiaca* on kidneystone disease causative protein of Glycolate Oxidase (PDB ID:2RDU)

2 Methodology

2.1 Ligand preparation

The three dimensional structure of the Tricyclo[8.4.1.1(3,8)]hexadeca-3,5,7,10,12,14-hexaene-2,9-dione, anti- and 2H-Pyran, 2-(7-heptadecynyloxy)tetrahydro- was obtained from the Pubchem database. The compounds in .sdf format were converted into the pdb format using Openbabel software. The compound Olean-12-ene-3beta,28-diol is available in 2D structure. The 3D coordinates of the compound was generated using Open babel software and saved in the pdb format[11].

2.2 Protein preparation

The crystal structure of the target protein was obtained from the Protein Data Bank Table 1. The target proteins were downloaded in pdb format. For docking, all water molecules and the ligands attached to the complex proteins were removed and polar hydrogen atoms were added to the refined model using Auto Dock tools[12]. The protein was prepared and saved in the PDBQT format.

Table 1. List of biologically effective compounds from the experimental sample of *M. paradisiaca* exudate

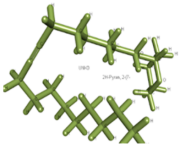
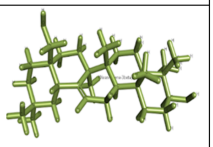
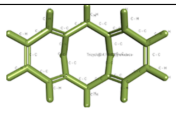
Sl. No	Bioactive Compounds	Structure
1	Olean-12-ene-3beta,28-diol	
2	Tricyclo [8.4.1.1(3,8)] hexadeca-3,5,7,10,12,14-hexaene-2,9-dione, anti-	
3	2H-Pyran, 2-(7-heptadecynyloxy)tetrahydro-	

Table 1. Selected Experimental Urolithiatic Disease, Receptor and its protein ID

Disease	Receptor	Protein ID
Urolithiasis (Calcium oxalate, hyper oxaluria)	Glycolate Oxidase	2RDU

3 Results and Discussion

3.1 Retrieval of glycolateoxidase(PDB ID:2RDU protein sequence

GlycolateOxidase(PDB.ID:2RDU);>SMB89252.1 glycolate oxidase(PDB.ID:2RDU) accessory protein

MLDKDTLKELIRIVGRENVLTSEVSLATYMYDATLLYGKPDVVVFVENAQQIASILKLANSKGIPVTPRGAGMGLSGGT VPHRGGIVIVMTRMNRILEIDPQNRVAVVEPGVTNMELQKAVAPYGLMYVPDPASQKVSTMGGNFGENAGGMRG IKYGVTKDHILGVELVLPTGDIVRIGGKWEPIVPELNLLALLIGSEGTLGIATQIIVRLLPLPRAVKTLLAVYNTLEEAGN SVSQIVAQGIIPTTLELMDNKVIQAVEEWLHIGLPLEAGAVLLIEVDGWGPELERQAEKIKEICQANGATQVQLARDAA ERDNLWLARRSAIGAMARLRPSYDLEDATVPRSRLPEMLRRVEAIAEKYRIPIGMLAHAGDGNLHPLVLFDERDQE EMERVHRTREEIFRAALELGGTLSGEHGIGLGKLDFMPLAFTPAELDFMRRERRAFDPNGILNPGKFIPESPQGI

3.2 Screening of Best homologous

The BLAST results were analyzed and the best protein hits were selected based on the percentage of identity, similarity and query coverage. The identity range was 29- 69%, similarity range was 47-76% and E- value range was 7e-24.

3.3 MSA and phylogenetic characterization

The multiple sequence analysis was performed with CLUSTAL W and the conservation present in the target protein was interpreted. The phylogram represents that query is closely related to templates 3SF5-B and 1POT-A. However, template 3SF5-B was selected due to its better quality. Hence the best template for homology modeling was identified to be 3SF5-B chain B, X-ray crystal structure of glycolate oxidase accessory protein complex. The Resolution factor of the structure is 2.49 Å and R value is 0.175.

3.4 Proteogenomic analysis

The molecular weight was found to be 31008.8 Daltons and theoretical isoelectric point was 6.31. Leucine was the predominant amino acid identified in Urease protein which constitutes 10.9% of the total content. The secondary structure of Urease was predicted by CFSSP. It was predicted that 70.0% were α helices, 77.7 % were extended strand and 10.6% were random coils similar report has been opined by various authors[13,14]. The predicted structure was submitted in CASTP server for the identification of possible catalytic residues available in the model. The selected pocket volume is 1.4 Å and the surface area 68.4.

3.5 Comparative modeling

The Swiss Modeller program was executed and a series of files were generated and the final modeled protein. The superimposition was performed to analyze the structural alignment, backbone threading and fold recognition of modeled protein. Almost 273 residues are aligned between the target and template with a Z score of 66.9. It has noticed that RMSD value of threaded structure to be 0.5 which indicate the backbone configuration of the protein is good. The modeled protein was visualized in PyMOL[15]. It has observed that the random coils were predominant in the modeled protein and beta sheets were present in small proportion (Figure 1). The percentage of alpha helix was found to be 70 % accounting 191 residues of the sequence. The extended strand is 77.7% and random coil 10.6%.

3.6 Validation of the modeled protein

The modeled protein is further validated by Ramachandran Plot generated by PROCHECK. The plot value was found to be 84.8% with 164 residues in the favored region. 18.35% of the residues lie in additional allowed region and 7.6% in the generously allowed region. Only about 0.9% of the residues were located in the disallowed region. The number of glycine residues are 22 and proline residues are 18.

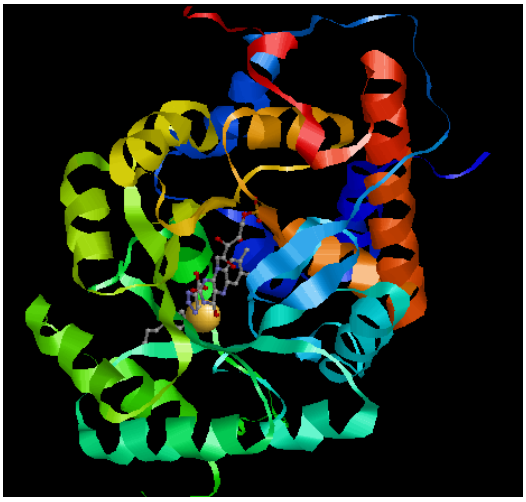


Fig 1. Modeled view of experimental receptor protein of Glycolate Oxidase

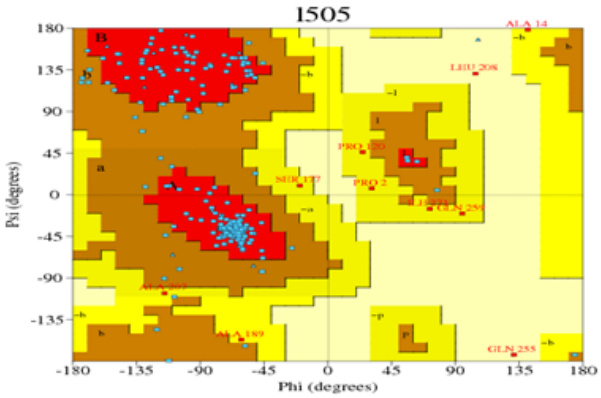


Fig 2. Ramachandran plot for check the validation of an experimental receptor protein of GlycolateOxidase(PDB.ID:2RDU)

3.7 Docking of glycolateOxidase(PDB ID:2RDU protein with three ligand molecules

The modeled protein was docked against the three various compounds from the *M. paradisiaca* exudate sample are used to treat kidney stone. The selected compounds are Olean-12-ene-3beta,28-diol,Tricyclo[8.4.1.1(3,8)]hexadeca-3,5,7,10,12,14-hexaene-2,9-dione, anti- and 2H-Pyran, 2-(7-heptadecynyloxy) tetrahydro.

3.8 Drug likeness evaluation

The Lipinski rule of five for the compounds was predicted via Lipinski drug filter.

The cut off values include:

Molecular mass less than 500Da

Less than 5 hydrogen bond donors

Less than 10 hydrogen bond acceptors

High lipophilicity (expressed as Log P less than 5)

The results show that the compounds obey Lipinski rule of five and they can be strongly recommended as a drug.

Table 2. Drug likeness evaluation of ligand molecules from the experimental exudate

S. No	Compound Name	Properties
1.	Olean-12-ene-3beta,28-diol	Molecular Weight = 177.19984 Hydrogen bond acceptor = 2 Hydrogen bond donar = 1 Log p = 2.1 Molar Refractivity = 34.28
2.	Tricyclo[8.4.1.1(3,8)]hexadeca-3,5,7,10,12,14-hexaene-2,9-dione, anti-	Molecular Weight = 176.21508 Hydrogen bond acceptor = 2 Hydrogen bond donar = 3 Log p = 0.2 Molar Refractivity = 54.677
3.	2H-Pyran, 2-(7-heptadecynyloxy)tetrahydro	Molecular Weight = 165.14608 Hydrogen bond acceptor = 3 Hydrogen bond donar = 1 Log p = 1.1 Molar Refractivity = 55.174

3.9 Molecular docking

Molecular docking approach can be used to study the interaction between a ligands and the target proteins at the atomic level. In the present study molecular docking studies were performed using AutoDockVina[16]. Docking studies were performed for the three compounds in order to evaluate their binding affinity to the three different target proteins. After docking, the three proteins were ranked according to their binding energy. The least binding energy of the ligands were selected as the best pose. The best confirmation between the ligand and protein were selected using Lamarkaina Genetic Algorithm (LGA). The hydrogen bond interaction between the compounds and proteins are visualized using PyMOLviewer[17].The target protein was selected for the docking studies. Glycolate oxidase protein was docked against three different compounds. Similar findings were agreed with other part of juice extract in the same experimental plant[18]. Docking scores and intermolecular interactions of the protein with the compounds were listed below.

Table 3. Molecularinteractionand binding affinity of the target protein Glycolyte oxidase(PDB ID:2RDU) with three different compounds

PDB ID	Compound name	Docking score (Kcal/mol)	Number of hydrogen bond interaction	Interacting residues
2RDU	Olean-12-ene-3beta,28-diol	-7.2	1	GLU338
	Tricyclo[8.4.1.1(3,8)]hexadeca-3,5,7,10,12,14-hexaene-2,9-dione, anti-	-7.0	2	VAL286, GLY284
	2H-Pyran, 2-(7-heptadecynyloxy)tetrahydro-	-5.4	3	ASP160, GLN264, TYR163

The binding affinity of the selected compounds with the target proteins were analysed using molecular docking studies. The interaction between the protein and ligands were studied using Pymol viewer. The binding mode of the selected compounds with the target protein were analysed using AutodockVina.

From theTable 3 showed the docking results of the selected compounds with the target protein Glycolate Oxidase (PDB ID: 2RDU). The compound Olean-12-ene-3beta,28-diol showed the least binding energy and selected as a best pose with the binding affinity -7.2 Kcal/mol with a single hydrogen bond interaction at the residue GLU338. The compound Tricyclo[8.4.1.1(3,8)]hexadeca-3,5,7,10,12,14-hexaene-2,9-dione, anti- showed the similar binding energy with -7.0 Kcal/mol with two hydrogen bond interactions at the interacting residues of VAL286 and GLY284. 2H-Pyran, 2-(7-heptadecynyloxy) tetrahydro- compound exhibited the docking results with three hydrogen bond interactions with the binding affinity of -5.4 Kcal/mol.

The current research results showed that In-silico approach for critical drug progression in pharmacological enforcement particularly urolithiatic disease on both infective kidney stone causative diseases. According to the docking assessment study, Lipinski's standard is a major key factor for drug design in clinical research field. Because it's a unique phenomenon for determination of lead structure along with its step- wise extended activity and selectivity. Moreover, as prescription like properties, Lipinski's standard assay stands for, it has near 5 hydrogen bond donor's not more than 10 hydrogen bond acceptors, nuclear band under 350- 500 Dalton. Apart from the present study selected the biologically active compounds (Photoactive compounds) from the *M. paradisiaca* exudate expressed the following compounds named as Tricyclo[8.4.1.1(3,8)]hexadeca-3,5,7,10,12,14-hexaene-2,9-dione, 2H-Pyran, 2-(7-heptadecynyloxy) tetrahydro and Olean-12-ene-3beta,28-diol[19]. All the three biocompounds are subjected with chemsketch 12.0 programming for determine whether they possessed 3-D structure for drug docking program. Fortunately all the three biocompounds were possessed and assessed 3-Dimensional plans and besides evaluated the Lipinski's properties, it was represented in Table 1.

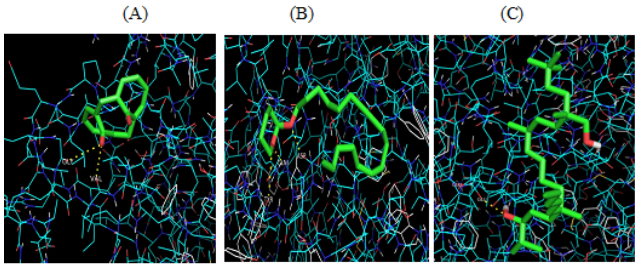


Fig 3. Interactions between (A) Tricyclo[8.4.1.1(3,8)]hexadeca-3,5,7,10,12,14-hexaene-2,9-dione,anti , (B) 2H-Pyran, 2-(7-heptadecynyloxy)tetrahydro (C), Olean-12-ene-3beta,28-diol and Glycolate Oxidase (PDB ID:2RDU)

More over the examination of this current research work recently referenced traditional medicinal samples, the experimental exudate was contains satisfiably five standards of Lipinski's properties, Hence, antiurolithiatic medicinal. Similarly considers as an obvious undertaking to appreciate the food as well as medicinal substance properties. So it can definitely that can make a spoon of medicinal particles either productive (or) maybe cheaply available (or) expensive clinical disillusionments, previously this kind agreeable opinion has been made by several researchers [20,21]. Though the receptor of glycolate oxidase perceived for the singular ailments in the present in-silico examination have been given in the Tables 2 and 3. Apart from the drug interaction Table 3 denoted results that to discover the dynamic test in the design and it was observed that the dynamic potential site contains the following typical amino acids like GLO, VAL, GLY, ASP, GLN, TYR.

In this current assessment, among the three compounds (Ligand molecules) docked with IUBP, usually the amino acids are attracted with the receptor and ligand co-ordinated effort were noticed on the following special amino acids GLO, VAL, GLY, ASP, GLN, TYR, (Table 2). However, the relationship between 2-H-Pyran 2-(7-heptadecynyloxy) tetrahydro and glycolate oxidase ligand shows more vibrant harbour ranking score -5.4 (Kcal/mol) followed by close to the another ligand molecule of Tricyclo 8.4.1.1(3,8) hexadeca-3,5,7,10,12,14-hexane – 2,9-dione, showed most critical dock score (-7.0 kcal/mol) finally the third compound olean-12-ene-3beta, 28-diol depicted that lowest dock scoring actually -7.2(kcal/mol) with the respective receptor molecule [22]. It was considering as weak relationship with the receptor molecule glycolate oxidase (PDB ID 2RDU). From the present study was clearly indicated that among the three ligand molecule 2-H-Pyran 2-(7-heptadecynyloxy) tetrahydro represent as a potential drug likeliness compound against the receptor molecule of glycolate oxidase (PDB ID: 2RDU) because it possessed significant docking score remarkable hydrogen bond interaction collaboration with glycogen oxidase receptor. The present study also been opined the accepted findings are depicted by Venkatesan et al., [3] Computational advances played a significant influence in the drug development process. Virtual screening approaches are frequently and widely utilized to minimize the cost and time of drug development. Molecular docking is a technique that is used to discover novel ligands for protein structure and plays a significant role in structure based drug design. Molecular docking approaches are routinely used in modern drug design to help understand drug receptor interaction. It has been shown in the literatures that these computation techniques can strongly support and help the design of novel, more potent inhibitors by revealing the mechanism of drug receptor interaction [23]. Computer aided drug design (CADD) helps in identifying small molecules by orienting and scoring them in the active binding site a protein. By using Lipinski's rule of five which was derived empirically from the world drug index is used to filter the drug for its capability of drug for human use. In the present study, all the compound satisfied Lipinski rules are expected to be active in humans after oral administration. The molecular properties which influence ADMET are recognized a long side therapeutic potency as key determinants of whether a molecule can be successfully developed as a drug. The novel ligands biology activity was helpful to predict by scoring function. These results revealed that Benzoxazolinone has the ability to bind towards the active site of Urease protein and prevents the self-association of protein to form a toxic aggregate.

In the contemporary era, there have been significant changes in the medical treatment of urolithiasis. Currently, urolithiasis care comprises not only stone removal but also recurrence prevention. ROS, which causes oxidative stress, is one of the key components in the pathogenesis of kidney stone disease. Oxalate causes a rise in the free radical generation that can cause cell death, crystal deposition in the renal tubules, and the development of calcium oxalate stones [24]. As a result, therapy with natural antioxidants may be an appropriate strategy for reducing the oxidative stress and kidney damage brought on by hyperoxaluria.In recent years, use of natural antioxidant obtained from food and other biomaterial has been increasing due to their safety, and nutritional and therapeutic value. Plants are rich source of bioactive chemicals which are beneficial without any side-effects there by an increased interest to identify natural compounds with antioxidant activity [24] Biomedical research

on the health benefits of these compounds are of great interest. Natural compounds with antioxidant activity can act as an anti-kidney stone drug by inhibiting the ammonia production. Urease protein and thereby hindering stone formation, also simulate the theoretical binding of the ligands (plant compounds) to the active site of Urease protein and its ability to inhibit Stone formation. Ramachandran plot revealed that the protein structure is suitable for docking studies. Hence Benzoxazolinone can be further developed as a potential drug for Kidney stone.

4 Conclusion

Docking technique is a very important tool in the rational design of drugs which helps to predict the interactions between a ligand molecule from the sample of pseudostem exudate and a receptor molecule from the urolithiatic disease causative protein in order to predict the affinity and the activity of the small molecules assured the potential characteristic particularly act as a medicine. Urinary calculi, commonly known as kidney stones, are solid particles developed within the urinary system. *M.paradisiaca* stem juice includes three bioactive components, affording to the GC-MS study. The revealed compounds were described and working in molecular docking experiments against object proteins using the GC-MS data of *M. paradisiaca* stem juice. The compound Olean-12-ene-3beta, 28-diol showed the maximum binding affinity with the target protein, 2RDU. Therefore, from the results it is identified that the compound Olean-12-ene-3beta,28-diol could be exploited as a lead molecule. In the present study, an attempt was made to investigate the protective effect of *M. paradisiaca* against urolithiasis by means of molecular docking study. Therefore, the current study concludes that these three compounds such as Olean-12-ene-3beta,28-diol, Tricyclo[8.4.1.1(3,8)]hexadeca-3,5,7,10,12,14-hexaene-2,9-dione, anti- and 2H-Pyran, 2-(7-heptadecynyloxy)tetrahydro- extracted from the exudate of *M. paradisiac*a act as a possible better drug against the urolithiatic diseases. Hence the present study concluded, amoung the three docked bioactive compounds, olean 12 -ene-3 beta, 28 diolmight be enacted as a potential drug molecule for urolithiatic diseases.

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