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In Silico Study of Diuretic by Using the Flower of Aerva Lanata L

Haseena Parveen.N, and Dr.C.A.Annapoorani*

Avinashilingam Institute for Home Science and Higher Education for Women, Coimbatore, India

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ABSTRACT

Diuretics are medications commonly used to treat conditions characterized by fluid retention, such as edema and hypertension. Diuretics promote increased urine production, which can help flush out toxins and potentially prevent the formation of kidney stones.This increased urine output can potentially help in flushing out small stones or reducing the concentration of stone-forming substances in the urine. The flower of *Aerva lanata*L has been studied for its potential therapeutic effects in the context of kidney stones and diuretic properties. It may possess anti-urolithic properties, which could be beneficial in preventing or treating kidney stones. *Aervalanata* flowers are known for their diuretic effects, meaning they can increase urine production. This property has been traditionally used to treat conditions associated with fluid retention and urinary problems. It exhibits anti-inflammatory properties, which can help reduce inflammation and associated symptoms in various conditions. *Aervalanata* has been investigated for its potential to prevent the formation of urinary stones (urolithiasis) due to its diuretic and urinary alkalizing propertiesand it also have antineoplastic activity.

Keywords: Kidney stone, Diuretics, *Aerva lanata* flower, Osteopontin, Biological activity, Antineoplastic, Anti-inflammatory.

INTRODUCTION

Nature has been a vast reservoir of remedies in the form of medicinal herbs for the treatment of numerous ailments since ancient times. Plants have been a part of the therapeutic practice both in traditional and modern era. Herbs contain many phytoconstituents that contribute to their vast array of pharmacological activities leading to the production of beneficial effects. 80% of people throughout the world depend on herbal medicines for some fraction of their primary health care according to latest reports by World Health Organization. Herbal medicines have gained popularity over conventional medicines owing to their reduced risk of side effects, effectiveness with chronic conditions, lower cost and widespread availability (Bitasta& Madan2016)

Microbial diseases and metabolic disorders are gradually spreading among the human race as a result of the dense population and malnutrition. Allopathy medicines are more effective and provide fast recovery for variety of microbial infections, and metabolic disorders. Plant-based therapy has the potential to cure the microbial infections while also boosting immune mechanisms and providing humans with extended resistance to infectious microbial agents (Narayanan, *et al*2021).

Kidney stones, one of the most painful of the urologic disorders, are not a product of modern life. Unfortunately, kidney stones are one of the most common disorders of the urinary tract. A large number of people are suffering from urinary stone problem all over the globe. Kidney stones, which are solid crystals that form from dissolved minerals in urine, can be caused by both environmental and metabolic problems. Calcium oxalate or phosphate stones account for almost 70% of all renal stones observed in economically developed countries. Higher consumption of fructose has been tied to kidney stone risk. A less energy dense diet may decrease the incidence of stones. This fact has been documented during far years when diets containing minimal fat and protein resulted in a decreased incidence of urinary stones. Those afflicted with recurrent urinary stone disease are encouraged to maintain a diet restricted in sodium and protein intake.

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Postmenopausal women with low estrogen levels have an increased risk for kidney stones. Women who have had their ovaries removed are also at increased risk(Sofia*et al* 2016).

Globally, kidney stone disease prevalence and recurrence rates are increasing, with limited options of effective drugs. Urolithiasis affects about 12% of the world population at some stage in their lifetime. It affects all ages, sexes, and races but occurs more frequently in men than in women within the age of 20–49 years. If patients do not apply meta phylaxis, the relapsing rate of secondary stone formations is estimated to be 10–23% per year, 50% in 5–10 years, and 75% in 20 years of the patient. Recent studies have reported that the prevalence of urolithiasis has been increasing in the past decades in both developed and developing countries (Alelign& Petros, 2018).

Pashanabheda (stone breaking) plants are a group of medicinal plants which are used in Indian traditional medicinal system by Ayurvedic practitioners as antiurolithiatic drugs. Traditionally *Aervalanata* (L) also known as *Pashanabheda*, used for various medicinal uses including both antiurolithiatic and diuretic. The reported phytochemical constituents present in *A.lanataL* are responsible for various biological activities. These constituents include alkaloids, flavanoids, methyl grevillate, lupeol, lupeol acetate benzoic acid, β-sitosteryl acetate and tannic acid (Dinnimath, *et al*2017).

*Aervalanata*L is also known as knot grass and it is a perennial shrub. These plants are branching shrub, roots are like woody, and flowers are like soft spikes. The flowers bloom in the first year of cultivation. Leaves are oval in shape, they are 0.5-1.5 in length, are alternately arranged. The leaves are present in the main stem. The whitish flowers have two lobes and red bases, grown in leaf axils have 0.1in long, the pink, green, white flowers are also seen. These plants are self-pollinated, bisexual and are cultivated in 90 meters above these level, and are grown only in tropical climate. The whole plant is useful for many diseases (Athira, Nair,2017).

METHODOLOGY

Plant collection and extract preparation

The healthy, disease free *Aervalanata* L. was collected from natural habitats, A. Kalayam Puthur, Palani Taluk, Dindigul district, Tamil Nadu, India. The flowers were then shade dried and sieved into fine powder, extracted using double boiling method and evaporated stored in a sterile container for potential use.

Gas chromatography-mass spectrometer (GC-MS) analysis

The Phytocompounds present in the extract of the flower of *A.lanata* L was identified using GC-MS analysis. The GC-MS system was equipped with a flame ionization detector and capillary column of HP-5 (5 per cent phenyl methyl siloxane, film thickness 0.25mm). At a flow rate of 2.5 ml/min, nitrogen was employed as the carrier gas, with a split injector (split ratio 50:1) and a split flow of 60 ml/min. The oven temperature was programmed from 90°C

Kingdom:	Plantae
Phylum:	Tracheophyta
Class:	Magnoliopsida
Order:	Caryophyllales
Family:	Amaranthaceae
Genus:	Aerva

Figure.1 Taxonomical Classification of Mountain knotgrass or *Aerva Lanata* L

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for 2 min, increased to 90°C - 200°C at the rate of 8°C per min and additionally with an increase of 200°C-250°C at the rate of 3°C per min. Temperatures for the injector and detector were set to 280°C and 250°C, respectively. The methanolic extract (0.1mL) was injected into the GC-MS instrument for its analysis. Ion source temperatures were maintained at 200°C and the mass spectra were taken at 70eV with a total run time of 32.4 min (Hossain *et al*., 2014). The GCMS mass spectrum data were analyzed using the database of the National Institute of Standard and Technology (NIST) to interpret the results.

Ligand generation

The data of the entire ligand is obtained from a website namely the PubChem database (http://pubchem.ncbi.nlm.nih.gov). The 2D structure of a ligand molecule is converted into a 3D structure by using the Biovia discovery studio application. The 2D file should be converted into .pdb format to obtain a 3D structure. Later, the smiles of the ligand molecule are taken and given for further process.

Biological Activity Prediction

Way2Drug is a computational platform designed for predicting the biological activities of chemical compounds. Way2Drug offers a versatile toolkit for drug discovery and development processes. By analyzing molecular structures and their interactions with biological targets. Way2Drug can forecast various pharmacological properties such as toxicity, potency, and mechanism of action. PASS Online predicts over 4000 kinds of biological activity, including pharmacological effects, mechanisms of action, toxic and adverse effects, interaction with metabolic enzymes and transporters, influence on gene expression.

Receptor preparation and molecular docking

The cytotoxic activity of phytocompounds identified from *A.lanata*L, the crystal structures of four apoptosis regulator protein molecule Osteopontin (PDB ID: 3CXD),which shows an essential role, especially we have taken the effective protein of kidney stone and their three - dimensional structures were retrieved from Protein Data Bank (PDB www.rcsb.org) (Berman et al., 2000).

The grid map and grid size were calculated using an auto grid to represent the protein binding size for docking. The spacing of 0.375A was fixed between the grid points by Maestro

Schrodinger and included the effective protein. Schrodinger**'s** software is used by pharmaceutical companies, biotech firms, and academic researchers to simulate and model the behavior of molecules at the atomic level. This accelerates the design and develops new drugs and materials more efficiently, reducing the time and cost of bringing them to market.The docking pose with the better binding affinity score (kcal/mol) is ranked as the top orientation for each ligand against each receptor and the binding interaction studies were analyzed. The docking interactions were analyzed using receptor-ligand interaction options.

RESULTS AND DISCUSSION

Flowers of *A.lanata* L were submitted for identification in Botanical Survey of India, Tamil Nadu Agricultural University, Coimbatore, Tamil Nadu, India. The specimen was identified and authenticated as *Aerva lanata* L. The identification has been officially confirmed by the Botanical Survey of India. The authentication number assigned to this specimen is BSI/SRC/5/23/2023-24/TECH/39

GC-MS analysis of the flower of *Aerva lanata* L

The outbreak of cause of kidney stones in kidney is predictable through the results of GC-MS analysis (Mushtaq *et al*., 2018). Table 1 depicts the phyto compounds analyzed in the extract of the flower of *A. lanata* L

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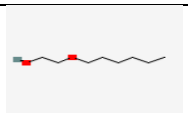
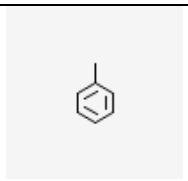
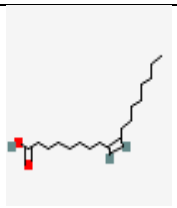
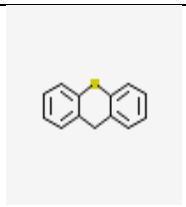
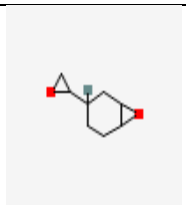
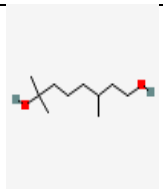
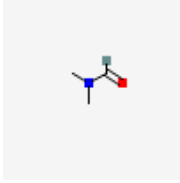
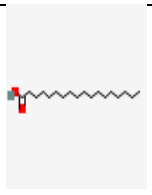
Table 1GC-MS analysis of the compounds in the flower of *A.lanata* L

Name of the compound	Molecular weight (g/mol)	Formula	Area (%)	Structure
1-Butanol, 4-butoxy	146.23	C8H18O2	1.72	
Bicyclo [3.2.0] hepta-2,6-diene	92 .14	C7H8	6.27	
9- Octadecenoic acid (Z)	282.5	C18H34O2	1.18	
6H-Dibenzo [b, d] thiopyran	198.29	C13H10S	4.02	
5-t-Butyl-2-(5H)-furanone	140 .18	C8H12O2	1.22	
1,10-Decanediol	174.29	C10H22O2	2.07	
Propanal, oxime	73.09	C3H7NO	1.38	
Hepta decanoic acid, methyl ester	284.5	C18H36O2	1.86	

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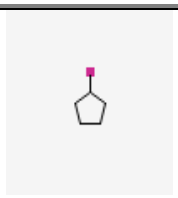
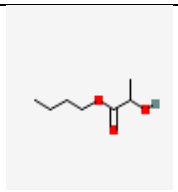
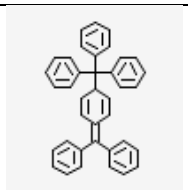
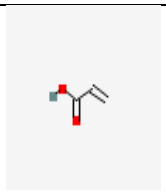
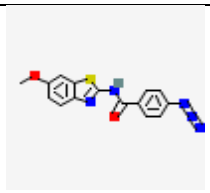
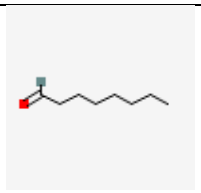
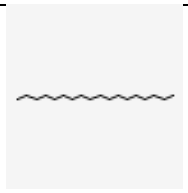
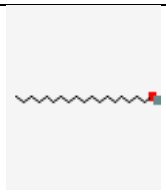
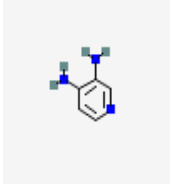
1-Cyclopropyl2-fluoro ethane	88.12	C5H9F	3.01	
1,3-Dioxane-2-propanol	146.18	C7H14O3	1.00	
3- benzhydryl dene 6-trithycycloh	544	C38H30	1.00	
2-Oxetanone	72.06	C3H4O2	2.25	
4-azido-n-benzamine	325.3	C15H11N5 O2S	1.70	
Oxirane, hexyl	128.21	C8H16O	2.36	
Pentadecane,2,6,10-trimethyl	254.5	C18H38	1.0	
Bis-(3,5,5-trimethylhexyl) ether	270.5	C18H38O	6.69	
2-(Azidomethyl)-1,3-butadiene	109.13	C5H7N3	1.84	

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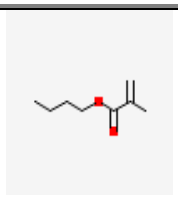
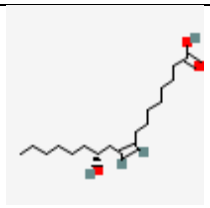
Buthy methacrylate	142.2	C8H14O2	2.22	
Ricinoleic acid	298.5	C18H34O3	8.25	

MS chromatogram analysis of the extract of flower of *A. lanata* L revealed 19 distinct peaks in that area percentage was high in 11 peaks were as follows Bicyclo [3.2.0] hepta-2,6-diene (6.27), 6H-Dibenzo [b, d] thiopyran (4.02), 1,10-Decanediol (2.07), 1-Cyclopropyl2-fluoro ethane (3.01), 2-Oxetanone (2.25), Oxirane, hexyl (2.36), Bis-(3,5,5-trimethylhexyl) ether (6.69), Buthy methacrylate(2.22) and Ricinoleic acid (8.25)

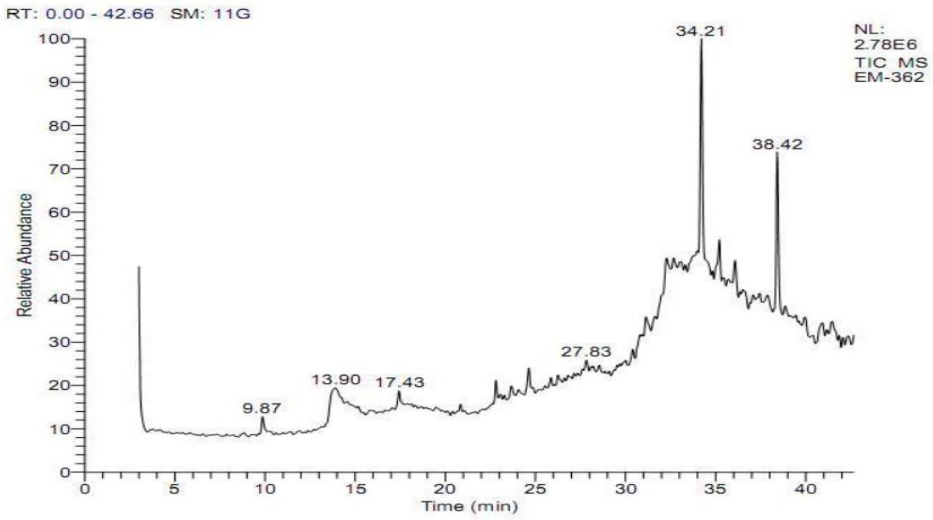


Fig. 2. GC- MS of the flower of *A.lanata*L

The gas chromatogram showed the presence of distinctive compounds which were clearly depicted as peaks (Fig. 2).

Biological activity prediction

Biological activity has been predicted using PASS server. If Pa>0.7, the substance is very likely to exhibit the activity in experiment, but the chance of the substance being the analogue of a known pharmaceutical agent is also high. If 0.5 < Pa < 0.7, the substance is likely to exhibit the activity in experiment, but the probability is less.

Table 2 Activities of 1-Butanol, 4-butoxy C8H18O2

Pa	Pi	Activity
0,950	0,002	Fucasterol-epoxide lyase inhibitor
0,950	0,002	Sugar-phosphatase inhibitor
0,942	0,003	Alkenyl glycerol phosphocholine hydrolase inhibitor

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0,934	0,002	Alkanal monooxygenase (FMN-linked) inhibitor
0,922	0,002	Carboxypeptidase Taq inhibitor
0,920	0,001	Glucan 1,4-alpha-maltotriohydrolase inhibitor
0,921	0,003	Alkylacetyl glycerol phosphatase inhibitor
0,918	0,003	Dextranase inhibitor
0,919	0,004	Phobic disorders treatment
0,917	0,004	Ubiquinol-cytochrome-c reductase inhibitor
0,911	0,003	Pullulans inhibitor
0,906	0,002	Peptide-N4-(N-acetyl-beta-glucosaminyl)asparagine amidase inhibitor
0,906	0,002	Alkylglycerone-phosphate synthase inhibitor
0,908	0,005	Polypepsin inhibitor
0,903	0,002	Gluconate 5-dehydrogenase inhibitor
0,905	0,005	Sphinganine kinase inhibitor
0,900	0,003	Exoribonuclease II inhibitor
0,899	0,003	Glyceryl-ether monooxygenase inhibitor
0,898	0,003	Levanase inhibitor
0,899	0,005	Saccharopepsin inhibitor
0,899	0,005	Acrocylindropepsin inhibitor
0,899	0,005	Chymosin inhibitor
0,894	0,001	Sclerosant
0,890	0,002	Leukopoiesis stimulant
0,891	0,003	Eye irritation, inactive
0,896	0,009	Aspulvinonedimethylallyltransferase inhibitor
0,887	0,002	Coccolysin inhibitor
0,896	0,012	Membrane integrity agonist
0,884	0,003	Poly(alpha-L-guluronate) lyase inhibitor
0,886	0,005	Mannotetraose 2-alpha-N-acetylglucosaminyltransferase inhibitor
0,882	0,003	Xylan endo-1,3-beta-xylosidase inhibitor
0,880	0,002	Diuretic inhibitor
0,881	0,003	IgA-specific serine endopeptidase inhibitor
0,878	0,003	Macrophage colony stimulating factor agonist

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0,879	0,003	Sarcosine oxidase inhibitor
0,875	0,002	Poly lyase inhibitor
0,877	0,006	Acylcarnitine hydrolase inhibitor
0,874	0,002	Anthranilate-CoA ligase inhibitor
0,877	0,007	Benzoate-CoA ligase inhibitor
0,870	0,001	Oryzin inhibitor
0,872	0,004	Cardiovascular analeptic
0,870	0,003	IgA-specific metalendopeptidase inhibitor
0,868	0,002	Hydroxylamine reductase (NADH) inhibitor
0,869	0,004	Phosphatidylcholine-retinol O-acyltransferase inhibitor
0,871	0,006	G-protein-coupled receptor kinase inhibitor
0,871	0,006	Beta-adrenergic receptor kinase inhibitor
0,863	0,003	Phosphatidyl glycerol phosphatase inhibitor
0,862	0,002	Prenyl-diphosphatase inhibitor
0,861	0,004	Lysine 2,3-aminomutase inhibitor
0,858	0,002	Steroid N-acetylglucosaminyltransferase inhibitor
0,858	0,002	Protein-tyrosine sulfotransferase inhibitor
0,858	0,004	Acetylesterase inhibitor
0,872	0,018	CYP2C12 substrate
0,853	0,003	Trimethylamine-oxide aldolase inhibitor
0,853	0,003	Beta-mannosidase inhibitor
0,854	0,004	Skin irritation, inactive
0,853	0,004	Lipoprotein lipase inhibitor
0,853	0,004	N-acetylneuraminate 7-O(or 9-O)-acetyltransferase inhibitor
0,852	0,004	5-O-(4-coumaroyl)-D-quinate 3'-monooxygenase inhibitor
0,849	0,006	Glycosylphosphatidylinositol phospholipase D inhibitor
0,843	0,004	Cutinase inhibitor
0,841	0,002	Phenylacetate-CoA ligase inhibitor
0,847	0,011	CYP2J substrate
0,837	0,003	Phenol O-methyltransferase inhibitor
0,835	0,003	Laccase inhibitor

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0,832	0,001	Undecaprenyl-diphosphatase inhibitor
0,836	0,005	Linoleate diol synthase inhibitor
0,833	0,005	Membrane integrity antagonist
0,838	0,014	Chlordecone reductase inhibitor
0,830	0,008	NADPH peroxidase inhibitor
0,825	0,003	Shikimate O-hydroxycinnamoyltransferase inhibitor
0,824	0,003	Ecdysone 20-monooxygenase inhibitor
0,837	0,017	Testosterone 17beta-dehydrogenase (NADP+) inhibitor
0,829	0,009	CYP2J2 substrate
0,825	0,007	GST A substrate
0,823	0,007	Arginine 2-monooxygenase inhibitor
0,818	0,003	Alkenyl glycerol phosphor ethanolamine hydrolase inhibitor
0,811	0,001	Deoxyribose-phosphate aldolase inhibitor
0,819	0,010	Feruloyl esterase inhibitor
0,810	0,003	Long-chain-aldehyde dehydrogenase inhibitor
0,810	0,003	Procollagen N-endopeptidase inhibitor
0,816	0,010	Glucose oxidase inhibitor
0,809	0,005	Venombin AB inhibitor

(Pa – probability of Active, Pi – probability of inactive)

Table 3 Activities of Dethiobiotin$C_{10}H_{18}N_2O_3$

Pa	Pi	Activity
0,861	0,012	Testosterone 17beta-dehydrogenase (NADP+) inhibitor
0,843	0,009	Acylcarnitine hydrolase inhibitor
0,826	0,003	Leukopoiesis stimulant
0,829	0,014	CYP2J substrate
0,814	0,004	Insulin promoter
0,821	0,016	Polypepsin inhibitor
0,816	0,015	Anti-eczematic
0,811	0,011	CYP2J2 substrate

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0,810	0,016	Mucomembranous protector
0,791	0,022	Saccharopepsin inhibitor
0,791	0,022	Chymosin inhibitor
0,761	0,003	Erythropoiesis stimulant
0,761	0,004	Diuretic inhibitor
0,758	0,013	Protein-disulfide reductase (glutathione) inhibitor
0,774	0,044	Phobic disorders treatment
0,729	0,009	Methylamine-glutamate N-methyltransferase inhibitor
0,715	0,010	Pterin deaminase inhibitor
0,717	0,018	Alkylacetyl glycerol phosphatase inhibitor

(Pa – probability of Active, Pi – probability of inactive)

Table 4 Activities of Ricinoleic acid $C_{18}H_{34}O_3$

Pa	Pi	Activity
0,955	0,002	CYP2J substrate
0,954	0,002	CYP2J2 substrate
0,946	0,002	Alkyl acetyl glycerol phosphatase inhibitor
0,940	0,003	Acylcarnitine hydrolase inhibitor
0,937	0,002	GST A substrate
0,936	0,001	CYP4A11 substrate
0,937	0,003	Diuretic inhibitor
0,937	0,003	Saccharopepsin inhibitor
0,937	0,003	Chymosin inhibitor
0,933	0,001	CYP4A substrate
0,932	0,001	Leukotriene-B4 20-monooxygenase inhibitor
0,929	0,001	Macrophage colony stimulating factor agonist
0,926	0,004	Prostaglandin-E2 9-reductase inhibitor
0,922	0,001	Prostaglandin-A1 DELTA-isomerase inhibitor
0,917	0,002	Phosphatidlglycerophosphatase inhibitor

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0,916	0,003	Lipoprotein lipase inhibitor
0,916	0,003	Linoleate diol synthase inhibitor
0,916	0,003	Lipid metabolism regulator
0,916	0,004	Sphinganine kinase inhibitor
0,915	0,004	Anti-eczematic
0,908	0,005	Polyporopepsin inhibitor
0,906	0,004	Beta-adrenergic receptor kinase inhibitor
0,906	0,004	G-protein-coupled receptor kinase inhibitor
0,906	0,005	Alkenyl glycerol phosphocholine hydrolase inhibitor
0,903	0,002	All-trans-retinyl-palmitate hydrolase inhibitor
0,897	0,005	Pro-opiomelanocortin converting enzyme inhibitor
0,891	0,002	Xylan endo-1,3-beta-xylosidase inhibitor
0,891	0,003	Sarcosine oxidase inhibitor
0,889	0,001	BRAF expression inhibitor
0,886	0,003	Phosphatidate phosphatase inhibitor
0,877	0,003	Vaso-protector
0,872	0,003	D-lactaldehyde dehydrogenase inhibitor
0,870	0,007	Mucomembranous protector
0,866	0,004	Dextranase inhibitor
0,861	0,004	Carboxypeptidase Taq inhibitor
0,863	0,008	Sugar-phosphatase inhibitor
0,856	0,005	Fucosterol-epoxide lyase inhibitor
0,851	0,001	Platelet aggregation stimulant
0,741	0,004	Biotinidase inhibitor
0,742	0,005	Anti-infective
0,738	0,002	Uroporphyrinogen decarboxylase inhibitor
0,742	0,006	Glucan 1,4-alpha-maltotriohydrolase inhibitor
0,740	0,005	Endopeptidase So inhibitor

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0,740	0,005	Alkenyl glycerol phosphor ethanolamine hydrolase inhibitor
0,737	0,003	Protein-Npi-phosphohistidine-sugar phosphotransferase inhibitor
0,733	0,001	Leukotriene-C4 synthase inhibitor
0,740	0,008	Cutinase inhibitor
0,743	0,011	UDP-glucuronosyltransferase substrate
0,747	0,018	Protein-glutamate methylesterase inhibitor
0,731	0,002	Sclerosant
0,727	0,001	Cyclooxygenase substrate
0,729	0,003	1-Alkylglycerophosphocholine O-acetyltransferase inhibitor
0,729	0,004	CYP2E1 inhibitor
0,730	0,005	Reductant
0,727	0,004	Gastrin inhibitor
0,725	0,003	4-Hydroxybenzoate nonprenyltransferase inhibitor
0,733	0,011	Hypolipemic
0,726	0,005	Shikimate O-hydroxycinnamoyl transferase inhibitor
0,723	0,002	Platelet adhesion inhibitor
0,757	0,037	Testosterone 17beta-dehydrogenase (NADP+) inhibitor
0,722	0,004	GST P substrate
0,722	0,003	2-Oxoglutarate decarboxylase inhibitor
0,725	0,007	Anti-hypercholesterolemic
0,726	0,009	N-benzyloxycarbonylglycine hydrolase inhibitor
0,720	0,003	Phosphoenolpyruvate-protein phosphotransferase inhibitor
0,727	0,011	IgA-specific serine endopeptidase inhibitor
0,718	0,004	Vitamin-K-epoxide reductase (warfarin-insensitive) inhibitor
0,720	0,006	3-Phytase inhibitor
0,717	0,004	Galactolipase inhibitor
0,715	0,004	CYP2C8 inhibitor
0,716	0,005	MMP9 expression inhibitor

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0,714	0,004	Phosphatidylcholine-sterol O-acyltransferase inhibitor
0,713	0,004	Aspergillopepsin I inhibitor
0,722	0,014	Venombin AB inhibitor
0,710	0,002	Oxidizing agent
0,711	0,003	Catalase inhibitor
0,709	0,002	15-Hydroxyprostaglandin-D dehydrogenase (NADP+) inhibitor
0,710	0,003	Anti-inflammatory, intestinal
0,703	0,003	Acyl-CoA hydrolase inhibitor
0,703	0,003	Palmitoyl-CoA hydrolase inhibitor
0,704	0,004	GST M substrate
0,702	0,003	Carnosine synthase inhibitor
0,702	0,003	Dolichyl-phosphatase inhibitor
0,704	0,006	TNF expression inhibitor
0,701	0,004	GST P1-1 substrate
0,702	0,005	Cytoprotectant
0,742	0,049	CYP2C12 substrate
0,702	0,010	CYP2C8 substrate
0,704	0,016	Peptidyl-dipeptidase inhibitor
0,707	0,053	Gluconate 2-dehydrogenase (acceptor) inhibitor

(Pa – probability of Active, Pi – probability of inactive)

Table 5 Activities of (1R,2R)-2-(2-Benzenesulfonylethyl)-1-(tert-butyldimethylsilyloxy) cyclopropane C17H28O3SSi

Pa	Pi	Activity
0,700	0,015	Apoptosis agonist
0,618	0,005	Antiprotozoal
0,608	0,002	HIV-1 reverse transcriptase inhibitor
0,614	0,010	Anti-ulcerative
0,575	0,004	Transcription factor NF kappa B inhibitor

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0,540	0,009	Transcription factor inhibitor
0,529	0,006	Antiviral
0,520	0,010	Thiol protease inhibitor
0,512	0,004	Antiviral (HIV)
0,504	0,022	Anti-infective
0,404	0,017	RNA directed DNA polymerase inhibitor
0,455	0,085	Antineoplastic
0,371	0,003	Falcipain inhibitor
0,371	0,003	Falcipain 2 inhibitor
0,371	0,004	Catalase stimulant
0,439	0,073	Phosphatidylcholine-retinol O-acyltransferase inhibitor
0,363	0,001	Diuretic inhibitor
0,454	0,101	Sugar-phosphatase inhibitor
0,359	0,011	Prostaglandin E1 antagonist
0,439	0,103	Gastrin inhibitor
0,479	0,147	Aspulvinonedimethylalltransferase inhibitor
0,387	0,077	Alcohol O-acetyltransferase inhibitor
0,363	0,053	Antiviral (Herpes)
0,312	0,016	DNA directed RNA polymerase inhibitor
0,353	0,065	All-trans-retinyl-palmitate hydrolase inhibitor
0,350	0,091	Lactase inhibitor
0,372	0,142	Macrophage colony stimulating factor agonist
0,309	0,079	Glucan 1,4-alpha-maltotriohydrolase inhibitor
0,403	0,176	Polypepsin inhibitor
0,318	0,092	Gluconate 5-dehydrogenase inhibitor
0,328	0,137	Anti-inflammatory
0,312	0,125	GST A substrate
0,348	0,162	Antiviral (Rhinovirus)

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0,340	0,196	Platelet aggregation stimulant
0,314	0,202	Complement factor D inhibitor

(Pa – probability of Active, Pi – probability of inactive)

Table 6 Activities of 1,3-Dioxane-2-propanol$C_{13}H_{26}O_3$

Pa	Pi	Activity
0,816	0,015	CYP2H substrate
0,757	0,040	CDP-glycerol glycerol phosphotransferase inhibitor
0,708	0,014	CYP3A5 substrate
0,713	0,031	Sugar-phosphatase inhibitor
0,725	0,059	Ubiquinol-cytochrome-c reductase inhibitor
0,708	0,042	Saccharopepsin inhibitor
0,708	0,042	Diuretic inhibitor
0,708	0,042	Acrocylindropepsin inhibitor

(Pa – probability of Active, Pi – probability of inactive)

The results indicated that all the compounds exhibit Diuretic inhibitor, phosphotransferase inhibitor, Antiviral, Anti-infective, Insulin promoter, Anti-inflammatory and anti-urolithiatic activities given in table 2 to table 6. The findings suggest that the plant has the potential to exhibit multiple biological activities and could be a promising candidate for further in vivo studies.

Molecular docking

Totally 19 compounds have been selected for docking studies, out of 19 compounds 17 compounds have binding affinity with the selected protein which causes kidney stones. Out of 17 of the compounds only 5 ligands have much higher docking scores. The glide score, number of H- bonds, Distance of H- Bonds, interacted residues and ligand atom.

Table 7Docking score of inhibitory molecules against complex epitope binding protein (PDB id: 3CXD) with the flower of*Aervalanata*

S No	**Compound**	**G score**	**No of H bonds**	**Distance**	**Protein Residues**
1.	7211 1-Butanol, 4-butoxy	-5.40	5	1.74	GLY H: 130
				1.91	GLY H: 132
				1.94	SER L: 116
				2.62	THR H: 140
				2.74	LYS L: 207

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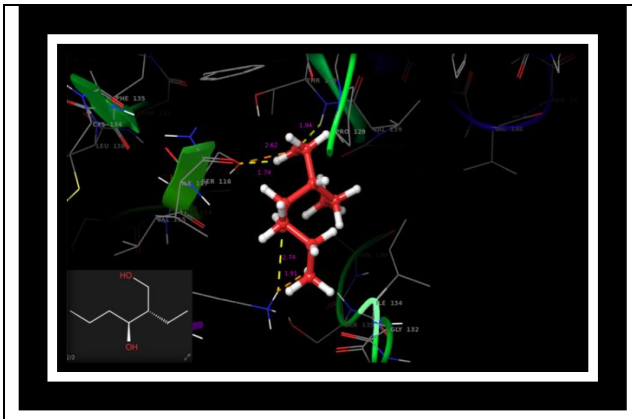
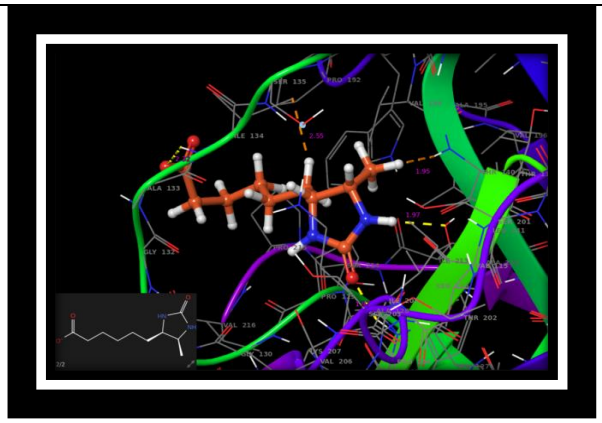
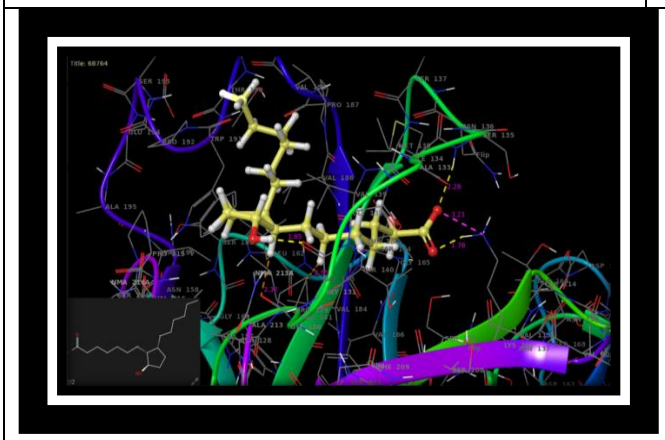
2.	445027 Dethiobiotin	-4.45	4	1.95	ILE L: 134
				1.97	LYS L: 207
				1.97	ILE H: 117
				2.32	SER L: 116
3.	68764 Ricinoleic acid	-4.43	3	1.76	GLY H: 131
				1.85	SER H: 135
				2.28	LYS L: 207
4.	162405619 (1R,2R)-2-(2-Benzenesulfonylethyl)-1-(tert-butyldimethylsilyloxy)cyclopropane	-4.20	1	3.21	LYS L: 207
5.	7833 1,3-Dioxane-2-propanol	-3.09	2	2.14	THR H: 140
				2.53	ILE L: 117



a) 7211 (1-Butanol, 4-butoxy)



b) 445027 (Dethiobiotin)



c) 68764 (Ricinoleic acid)

Figure3 Compounds docked against complex epitope binding protein (PDB id 3CXD) with flower of *A.lanata*L

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The compound 1-Butanol, 4-butoxy(7211) has a good glide score of -5.40$A^0$and 5H- bonds with high interaction against target protein followed by compound Dethiobiotin (445027) with glide score about -4.45 A^0 and 4H bond and compound 12-Hydroxy-9-octadecenoic acid (68764) with glide score -4.43 A^0 and 3H bond binding against diuretic inhibitor. But the glide score is lesser than1-Butanol, 4-butoxy. Hence, the compound 1-Butanol, 4-butoxy (7211) has been chosen for further analysis and the complex structure –binding protein is taken for maestro docking approach.

Kidney stones remain a significant health concern in modern times due to several contributing factors. Changes in diet and lifestyle, including increased consumption of processed foods high in sodium and animal proteins, as well as decreased water intake, have contributed to a rise in kidney stone prevalence. Additionally, obesity rates have increased, which is linked to a higher risk of developing kidney stones due to altered metabolic factors and increased urinary excretion of calcium oxalate. Environmental factors such as climate change and rising temperatures can lead to dehydration, promoting the formation of kidney stones. Furthermore, certain medical conditions and medications that affect urinary tract function or calcium metabolism can predispose individuals to kidney stone formation. The impact of kidney stones is not only limited to the acute pain they cause but can also lead to complications such as urinary tract infections, kidney damage, and recurrent stone formation. As a result, kidney stones represent a considerable burden on healthcare systems globally. The flower of *A.lanata*L has been studied for its potential therapeutic effects in the context of kidney stones and diuretic properties. Diuretics promote increased urine production, which can help flush out toxins and potentially prevent the formation of kidney stones. Research suggests that *A. lanata*L may contain bioactive compounds that contribute to its diuretic activity.*A. lanata*L may possess anti-urolithic properties, which could be beneficial in preventing or treating kidney stones. Molecular docking is a computational technique used to predict the binding interactions between small molecules (ligands) and target proteins (receptors). In the context of kidney diuretic activity, researchers can use molecular docking to simulate how specific compounds from *A.lanata*L interact with proteins involved in regulating fluid balance and urine production in the kidneys. Overall, the integration of GC-MS analysis with molecular docking techniques provides valuable insights into the pharmacological properties of natural products like *A.lanata*L and contributes to the discovery of novel drug candidates for kidney diuretic and related therapeutic applications.

CONCLUSION

In this research project, an insilico study was conducted to explore the diuretic and anti-urolithiatic potential of compounds derived from the flower of *Aerva lanata* L. Gas chromatography-mass spectrometry (GC-MS) analysis was employed to identify the chemical constituents of the flower extract. Subsequently, molecular docking studies using the Maestro Schrödinger platform were carried out to predict the binding affinity of these compounds with relevant target proteins associated with diuretic and anti-urolithiatic activities. The molecular docking results revealed promising interactions, with docking scores reaching -5.4, suggesting strong potential for these compounds as therapeutic agents in the treatment of conditions related to kidney stone formation, fluid retention and antineoplastic. This study underscores the utility of computational methods in drug discovery and natural product research.

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