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EXPLORING THE PHYTOCHEMICALS OF ASPARAGUS RACEMOSUS USING INSILICO AND INVITRO APPROACHES

Vishnudas D and Danie Kingsley J
Department of Integrative Biology, School of Bio Sciences & Technology (SBST),
Vellore Institute of Technology (VIT), Vellore
Email: daniekingsley@gmail.com

Abstract

Asparagus racemosus plant fresh root sample was screened for phytochemical constituents that were found to be effective against E.coli, Pseudomonas aeruginosa, and Staphylococcus aureus with zone of inhibition of 16mm, 15mm, and 14mm. The Green synthesized nanoparticles were characterized using UV (Peak at 445nm confirmed the presence of silver nanoparticles), FTIR (The N-H and C-O stretching of the aromatic amine groups with the peak at 1631.78cm-1, 1400.32cm-1, 1080. 14cm-1 indicated the presence of silver nanoparticles), XRD (confirmed the crystal structure of the silver nanoparticles),HR-SEM (Spherical shaped nanoparticles ranging from 32.6nm to 150nm). Molecular docking analysis using iGEMDOCK of phytoligands against target glycoprotein for anti-cancer (30WJ), anti-inflammatory (4COX),the anti-bacterial (3UX) and antiviral (GP120) activities were performed and bioactive compound Shatavarin exhibited best antibacterial (-107.944), anti-cancer (-118.366), antiviral (-107.169), anti-inflammatory (-172.98) activities. ADME screening was performed for drug worthiness of the phytoligands of Asparagus racemosus which also confirms to Lipinski rule 5. The phyto ligand Shatavarin is a notable drug candidate for further analysis.

Keywords: Asparagus racemosus, iGEMDOCK, PyMOL, QSAR, ADMET.

Introduction

The sample plant species named Asparagus racemosus known as Satawar, Satamuli, Satavari have wide spread applications in Ayurveda as a versatile female tonic (Kolmar Sharma & Maheep Bhatnagar ,2011). Traditionally Shatavarin roots were experimented due to its wide spread medicinal activity upon dyspepsia, diarrhoea, dysentery and nervous disorders. Besides many studies reveals that the plant also has antioxidant, immune stimulant, anti-dyspepsia and antitussive effects (Ravishankar et al.,2012).The Asparagus racemosus wild is a perennial shrub and the pharmacological activity of the root extracts were used for antiulcer, anti-oxidant (Mandal SC et al.,2000;Kamat JP et al.,2000), anti-bacterial activities (Venkatesan N et al.,2005).Satawar, Shatavari or Shatamull were the other names of Asparagus species and broadly seen in Sri Lankan and Indian Himalayas. The echo friendly biological target drug design also mentioned as rational drug designs were the inventive process of finding new medications for various diseases in current era (Baran A et al., 2021). Computer Aided Drug Design (CADD) focused and utilized technologies under computational chemistry were useful for studying drug related biological molecules. Computational method is most versatile and preferably accurate technique to lead unique speed on drug design and applicability (Becker OM et al., 2006). Drug designing using the computers includes different levels. The Level one

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indicates hit identification using virtual screening (structure or ligand-based design),level two dictates hit-to-lead optimization of affinity and selectivity (structure-based design, QSAR etc.) (Shide Liang et al., 2009). High enrichment and mining potential were used for improving protein ligand interaction and structural based drug design contains mostly consensus scoring, (Akifumi Oda et al., 2006) geometric and cluster analysis (Yang X et al., 2021; Ashwini Naganthran et al., 2022).

Phytochemical analysis of the plant part under investigations changed with different variable parameters which uniquely depends on plant parts, different solvent and extraction methods utilized (Ncube NS et al, 2008). The different methods of extractions focused and depend on length of the extraction periods, solvents used, pH of the solvent, temperature, particle sizes etc (Das K et al., 2010). The Phytoconstituents named Sarsasapogenin and Shatavarin I-IV were commonly present in roots, leaves and fruits of Asparagus racemosus. The main habitat exists in immunity is to create a defending behaviour for protection against the foreign particles approaching the host cell (Bere A W et al., 2021; Khan M S et al., 2021). The foreign or non-self-particle mostly includes different criteria of microorganisms which may rarely more harmful to the immunity (Citi V et al., 2021; Rahuman MBH et al., 2021). The specific and nonspecific host receptors identifies antigens and antibodies were created for boosting auto immunity (Shahenur Alam Sakib et al., 2021;(Alhag SK et al., 2021). The Bio mimetic delivery strategy were highly different from others by mimicking the novel structures, functions, biological systems and its biosynthetic pathways(Shanmugapriya Karuppusamy et al., 2021;Sapozhnikov SV et al.,2021) .High Bio compatibility and low immunogenicity , long systematic circulation and lesion targeting were the considerable advantages which makes a complete novel strategies for nano systems (Chong Li et al.,2019).The highly developed molecules shows healthy way of penetration through Blood Brain Barriers. Subsequently minimized drug molecules were developed by attaining perfect structure and function relationship through the replacement of the toxic site by substituent modification of by cyclic structure, and replacement of disulfide bond by lactam band in Ligand modified targeted drug strategy (Ranit Kedmi et al., 2018; Qingpo LI et al., 2018).

The preliminary phytochemical extraction helps to confirm the different phytochemicals present in the sample materials (Sivakumar T &Gajalekshmi D ,2014) through basic quantitative aspects .Different parameters used for extraction includes water, acetone, ether, chloroform and alcohol and extraction methods of the sample plant under study contains plant tissue homogenization, serial exhaustive extraction (Qingpo Li et al.,2018), Soxhlet extraction, maceration ,decoction ,Infusion, digestion, percolation and sonication. The variable parameters which affects screening of the phytochemicals depends upon particle size, nature and origin of the plant material and degree of processing and particle size (Nikhal SB et al., 2010). Based on the crystal structures of the target proteins and high-throughput molecular docking methods, four phases of Gem dock methods were used. These phases include target protein structure analysis, chemical compound optimization, molecular docking and post-docking analysis (Keskin C et al., 2021).

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Materials and Methods

Collection of Asparagus racemosus fresh root and leaf samples

The plant root and leaf samples were collected from VIT University. The collected samples were washed with double distilled water and dried under room temperature. The fine crushed pieces of samples were kept under sterilized conditions. Crude extract of sample fresh root and fresh leaf were kept in hot water bath for a few hours and filtered three times with the help of Whatman filter paper.

Preliminary phytochemical screening analysis

Different phytochemicals present in the samples were confirmed by preliminary phytochemical analysis. The extract of core sample plant's root and leaf at three different conditions under investigations were treated with the different tests for preliminary phytochemical verifications (Berman HM et al, 2000; Prasanth Tiwari et al., 2011). The phytochemicals present in the crude extract were confirmed with the help of preliminary phytochemical analysis (Nagamani et al., 2012). Asparagus racemosus contains four different steroidal Saponins and Shatavarin (I-IV) major glycoside residue with 3-glucose and rhaminose moieties attached to saraspogenin moieties. Many studies conducted in medicinal and scientific research fields reveals that steroidal Saponins were the source of huge variety of phytochemical constituents (Immunoside, polycyclic alkaloids, isoflavonons ,dihydrophenantherene, racemofuran, carbohydrates, flavonoids, Sterols, trace minerals, miscellaneous essential fatty acids and quercetin 3-glucourbnides etc).

Data sets for Insilco study

In this study, the coordinates of three cancer target proteins were selected and obtained from Protein Data Bank (PDB) (Berman HM, et al., 2000). The PDB entry GP120 (antiviral), 4COX (anti-inflammatory), 30WJ (anticancer) and 3UX (anti-bacterial) were selected for structural analysis according to its high-resolution crystallographic structure. For computational studies the PDB coordinates of obtained target proteins were refined by eliminating the co-crystallized ligand molecule. The crystallographic water molecules were removed from the atomic coordinate file and the polar hydrogen atoms and kollman-united charges were added to the each target protein. The structure obtained and its energy minimized and refined by using Swiss Protein Data Bank Viewer. The chemical structure of Shatavarin, Saraspogin and Asparagamine were sketched with the help of Chemsketch and 3-Dimensional conversion and geometry optimization of all the three compounds were performed by using chimera (Eric F Pettersen et al., 2004) for flexible conformations of the compounds during the docking analysis.

Docking analysis between target proteins and Shatavarin, Saraspogin and Asparagamine molecules by iGEMDOCK.

The detailed study on intermolecular interactions between the target proteins and sample ligand (Shatavarin, Saraspogin and Asparagamine) molecules, the automated docking program iGEMDOCK software were used (Jinn-Moon Yang et al., 2004). The selected GP120 (antiviral), 4COX (anti-inflammatory), 30WJ (anti-cancer) and 3UX (anti-bacterial) as target proteins to perform the docking analysis of chemical compounds Shatavarin, Saraspogin and Asparagamine. The 3D coordinates of each therapeutic target proteins were implemented

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through the GEMDOCK Graphical User Environment Interface. Before docking the output path was set and GEMDOCK default parameters includes the population size (n=200), generation (g=70) and number of solutions (s=10) to elucidate the probable binding conformation of three compounds. The individual binding conformation of each compound were observed and their binding affinity with the target proteins were analyzed (Bednarz-Misa I et al.2021; Willmore ZN et al., 2021). The best binding conformations and the binding energy of each compound were selected for further application studies. In the post docking analysis, binding energy value and the details of interacted residues were saved in output folder (Daniel Seeliger et al., 2010) and Protein-ligand binding conformation was analyzed and visualized by using PyMOL (VanGoolMMJetal., 2021; MaitiAetal., 2021)

Results and Discussions

Results

Preliminary Phytochemical Screening Analysis

The result obtained mainly varied due to the presence various variable parameters such as change in the climate, pH concentrations, different solvent quantity and conditions, and finally variety of minerals uptakes from the soil. Fresh and healthy Asparagus racemosus root and leaf sample out of contamination showed perfect phytochemical drugs very useful for treating various diseases. The overall experiment showed aqueous root extract at three different conditions had more phytochemicals. Gas Chromatography commonly used as an analytical method that unifies techniques of Gas Chromatography and Mass spectroscopy to identify different components through GC fractions of the A.racemosus root metabolic extract under study. There exist huge areas of applied areas like detection of the drug, fire investigation, environmental analysis etc in the case of Gas chromatography (Sivakumar.T &Gajalakshmi, 2014). The tick mark in the (Table 1) depicts the presence of phytochemicals present and cross mark represents the absence of phytochemicals. Comparatively aqueous fresh root extract contains more phytochemicals as compared to fresh leaf extract.

Table 1
Phytochemicals present of A.racemosus fresh root and leaf samples at three different conditions.

Phytochemicals present	Leaf extracts			Root extracts		
	Fresh	Sundry	Hot air oven	Fresh	Sundry	Hot air oven
Alkaloids	√	√	√	√	√	√
Carbohydrates	√	√	√	√	√	×
Tannins	×	√	×	√	√	√
Flavonoids	×	√	×	√	√	√

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Saponins	√	×	√	√	√	√
Steroids	√	×	×	√	×	√
Glycosides	√	√	√	√	√	√

Green-synthesis of silver nanoparticles

The dark brown Color variation upon the mixed solution of silver nitrate (0.1mM AgNO3) and the root extract after 24hrs of incubation dictates the visual identification of the presence of silver nanoparticles.

Characterization of silver nano particles

UV-Visible spectroscopy

The preliminary characterizations of silver nanoparticles were done by UV-Spectrophotometer and wavelength ranges between (200-600) nm. The conformation and presence of nanoparticles were confirmed by SPR broad peak obtained at 445nm which represented in (Figure1).

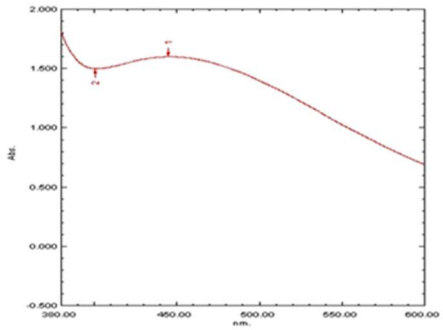

Figure 1.UV-Visble spectroscopy analyzed datum recorded at known concentration of A.racemosus sample root fresh extract.

FTIR Analysis

The N-H and C-O stretching of the aromatic amine groups were shown as peak value obtained at (1631.78cm-1, 1400.32cm-1, 1080. 14cm-1). The N-H and C-O stretching of the aromatic amine groups were shown as peak value obtained indicated the presence of silver nano particles in (Figure 2.1) The C-H , O-H and phenol stretching vibration of protein were clearly shown as maximum peak values(3487 cm-1,2013.68 cm-1,1631.78 cm-1,10 82.07cm-1,713.66 cm-1) in (Figure 2.2). The strong binding capabilities C-O forms different amino acid residues and stability of the medium was increased due to the presence of the nano particles. FTIR analysis of sample fresh freeze dried reductant root sample and fresh aqueous root samples were clearly showed in (Figure.2).

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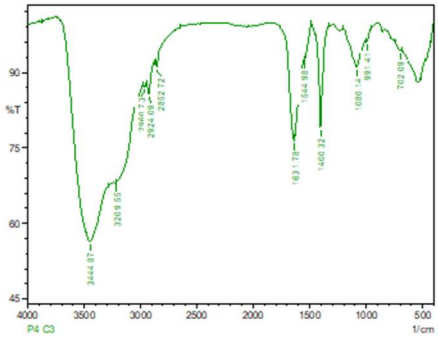

Figure2.1.N-H and C-O stretching of the aromatic amine groups of the freeze dried **Lyophilized sample mixed with Kbr pellet**

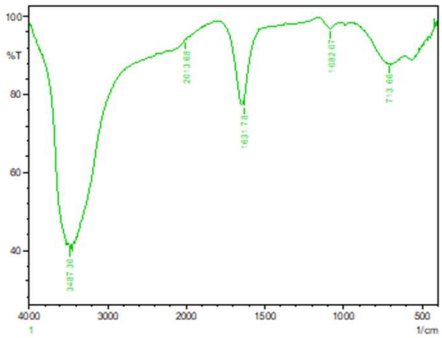

Figure2.2.C-H, O-H and phenol stretching vibration of protein fresh sample extract
Figure2.FTIR analysis of aqueous root samples at reductant and fresh extract condition

XRD Analysis

XRD pattern revealed the structure of the synthesized silver NPs in (Figure3).The XRD pattern results showed the 2ø Scale 27.808º, 2ø scale value 27.849º and 2ø scale value 27.905 corresponding to (111) representing the Face Centred Cubic structure of silver and obtained results were clearly located. Size of the silver nano particles were determined by laser diffraction method and highest peak obtained by plotting Braggs peak in (x=1, y=1, z=1) at 2ø Scale.

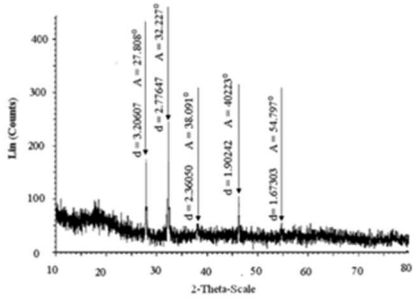

Figure3. XRD-Datum of reductant A.racemosus root extract

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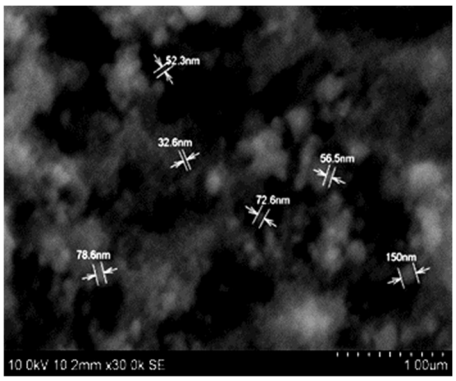

Figure4.HR-SEM analysis of root sample after reduction

HR-SEM Analysis

The HR-SEM image showed formation of spherical and elliptical shaped nano particles. The Particle size ranges from 32.6nm, 150nm, 78.6nm, 72.6nm, 56.5nmin (Figure4.) dictates the different bright elliptical and the spherical shape (nm) after HR-SEM analysis shows the presence of silver nitrate after reductions.

Antibacterial activity

Bacterial cultures were streaked and wells were punctured in Mueller Hinton Agar (MHA). Subsequently the extract with concentrations of 10 µl, 50µl, 100µl and 150µl were loaded in the wells. The zone of inhibitions were noted and documented after overnight showed in Table2.

Table2

A.racemosus sample root antibacterial activity study analysis

Micro organisms	***A.racemosus* fresh root sample**			
	10µl/well	50µl/well	100µl/well	150µl/well
	Zone of inhibitions (mm)			
E.coli	10	11	12	16
Staphylococcus aureus	10	12	11	14
Bacillus cereus	9	10	11	13
Pseudomonas aeruginosa	10	11	12	15
Salmonella typhimurium	10	11	13	12

Docking analysis using iGEMDOCK

The 3D structures of glycoprotein GP120 (antiviral), cycoloxygenase (4COX-anti-inflamatory), 30WJ (anticancer) and 3UX (anti-bacterial) were analyzed and Shatavarin,

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Saraspogin and Asparagamine were optimized to have minimal potential energy using chimera. After energy minimization, three compounds were docked into the each target protein to study the molecular basis of atomic interaction and binding affinity of Shatavarin, Saraspogin and Asparagamine. From the docking analysis, listed best binding conformation based on total binding energy for each compound in (Table3, Table4, Table5, Table6).

Antiviral activity study

The best docking poses for each compound in to each target protein were determined and the one having lowest binding energy among the 30 different poses generated. The lower energy scores represent the better protein-ligand molecule binding affinity compared to higher binding energy scores. Shatavarin shows best binding conformation with GP120 (Total energy = -107.169 Kcal/Mol). The best binding conformation of Shatavarin at the gap binding sites and the binding residues involved in the interaction, corresponding 2D interaction models, hydrogen bonds and bond distances for antiviral target enzymes were clearly shown inTable3, (Figure5).

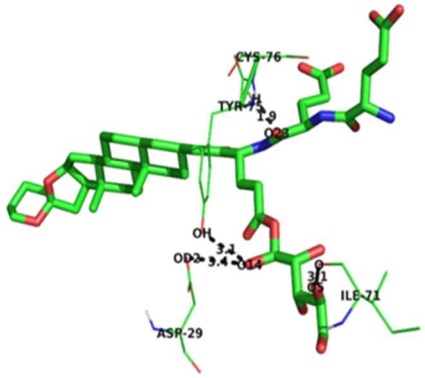

Figure5.Antiviral drug docking analysis

Table3 Antiviral drugs hydrogen bonds and interaction residues

No	Compound Name	Number of Hydrogen Bonds	Interaction Residues and Gap binding site	Hydrogen bond and bond distance
1	Shatavarin	4	ILE -71 (0 - 05) TYR-75 (OH - 014) ASP-29 (OD2-014) CYS-76 (OH - 023)	3.1 3.1 3.4 1.9
2	Saraspogin	Nil	Nil	Nil

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3	Asparagamine	Nil	Nil	Nil

Anti cancer activity study

Docking analysis of Shatavarin, Saraspogin and Asparagamine with cancer target enzyme 30WJ, Shatavarin has best binding affinity with the 30WJ. Docking of Shatavarin results in the formation of more than 8 hydrogen bonds with amino acid residues LYS158, LYS49, ASP120, TYR50, and SER51 etc were shown in Table4. Binding of Shatavarin in the binding site of 30WJ and corresponding 2D interaction models, hydrogen bonds and bond distance are depicted in (Figure6).

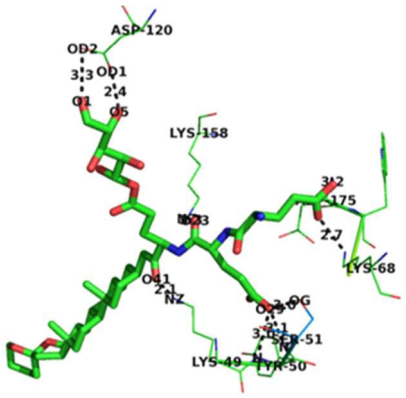

Figure6. Anticancer drug docking analysis

Table4 Anticancer drugs hydrogen bonds and interaction residues

No	Compound Name	No of H:Bond	Interaction residues and Gap binding site	Hydrogen bond and bond distance
1	Shatavarin	9	LYS-158 (NZ - 0.23) LYS-049 (NZ - 0.41) ASP-120 (OD1- 05) ASP-120 (OD2 - 01) TYR-050 (N - 0.29) LYS-068 (N - 0.34) SER-051 (OG - 0.20) ASP-120 (OD2 - 0.1) SER-051 (OG - 0.29)	3.3 2.1 2.4 3.3 3.1 2.7 3.1 3.3 3
2	Saraspogin	Nil	Nil	Nil
3	Asparagamine	Nil	Nil	Nil

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Anti-inflammatory activity study

The post docking analysis of Shatavarin has shown higher affinity with 4COX which has key role in inflammatory pathway (Total energy = -172.98 Kcal/Mol). Shatavarin binds to the 4COX and forms five H-bond and its binding residues are ARG44, GLN42, TYR 122, LYS473 and ARG44 the best binding pose of Shatavarin in the binding site of cycoloxygenase and corresponding 2D interaction models, hydrogen bonds and bond distance are depicted in (Figure7), Table5.

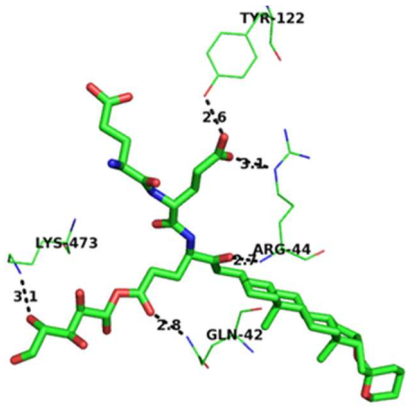

Figure7. Anti-inflammatory drug docking analysis

Table 5 Anti inflammatory drugs hydrogen bonds and interaction residues

No	Compound Name	No of H:Bond	Interaction Residues and Gap binding site	Hydrogen bond and bond distance
1	Shatavarin	5	ARG-044 (N - 04) GLN-042 (NE2-017) TYR-122 (OH -029) LYS-473 (NZ - 05) ARG-044 (NE -028)	2.7 2.8 2.6 3.1 3.1
2	Saraspogin	Nil	Nil	Nil
3	Asparagamine	Nil	Nil	Nil

Anti-bacterial activity study

Docking analysis of Shatavarin has shown best conformation with 3UX (total energy = -

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107.944 Kcal/Mol). The binding affinity of Shatavarin towards 3UX was investigated .The detailed on analysis of the interaction and position of Shatavarin in the 3UX catalytic site noted that 4 H-bonds are found and the amino acid residues VAL222 and GLU224 were involved in the H-bond formation. Acidic amino acid GLU224 is crucial residue because it formed more number of H-bonds with Shatavarin. The surface of 3UX with a Shatavarin along with the binding residues of 3UX is labelled and hydrogen bond distances are shown in (Figure 8), Table6.

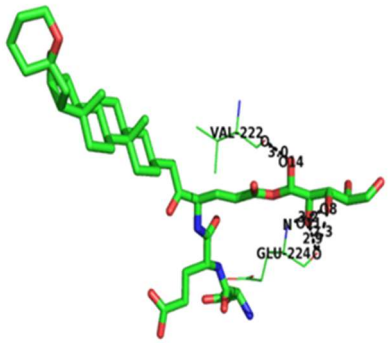

Figure8.Antibacterial drugs docking analysis

Table6Antibacterial drugs hydrogen bonds and interaction residues

N0	Compound Name	Number of H:Bond	Interaction Residues and Gap binding site	Hydrogen bond and bond distance
1	Shatavarin	4	VAL-222 (O - 014) GLU-224 (N - 08) GLU-224 (O - 08) GLU-224 (O - 01)	3.0 3.2 2.3 2.9
2	Saraspogin	Nil	Nil	Nil
3	Asparagamine	Nil	Nil	Nil

Table7 Binding energy of known drugs

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N0	Name	Binding Energy			
		3UX (antibacterial)	30WJ (anticancer)	4COX (anti - inflammatory)	GP120 (antiviral)
1	Shatavarin	-107.94	-118.37	-172.98	-107.17
2	Saraspogin	-74.018	-70.931	-99.944	-82.798
3	Asparagamine	-83.139	-89.281	-106.46	-80.616

The overall binding energy of different drugs and its known antimicrobial activity were shown in Table7. The binding energy and affinity towards different drugs varies depending upon the variation of different environmental parameters. Computing physico chemical descriptions and Predicting ADME parameters, pharmacokinetic properties drug like nature and medicinal chemistry friendliness of one or multiple small molecules to support drug discovery of the root fresh sample of A.racemosus were showed in Table8.

Table 8 ADME Analysis of Phytoligands and drug likeness

Compounds	MW(g/mol)	Number of Rotatable Bonds	H-bond Acceptor	H-bond donor	LogP o/w (iLOGP)	Lipinski Violation
Shatavarin I (C51H86O23)	1067.21	15	23	14	4.17	3
Asparanin B Shatavarin IV	887.1	8	17	9	4.87	3

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(C45H74O17)						
Schidigerasaponin D5 (C39H64O13)	740	6	13	7	5.43	3
Asarinin (C20H18O6)	354	2	6	0	3.46	0
Saponins Beta-Aescin Beta-Escin (C55H86O24)	1131.26	16	24	13	4.01	3
SAPONIN (C58H94O27)	1223.3	14	27	15	3.10	3

Discussions

Phytochemical constituents and pharmaceutically relevant properties, such as molecular weight, H-bond donors, H-bond acceptors, logP (octanol/water), and their position according to Lipinski's rule of 5 in Table7(Keskin C et al.,2021). The drug molecule shows poor absorption and permeation when they have more than 5 hydrogen bond donors, molecular weight over 500, logP is over 5 and more than 10 hydrogen bond acceptors. In this study, out of 19 ligand 16 structures showed possible values for the properties analyzed and exhibited drug-like characteristics based on Lipinski's rule of 5. Methicillin has more than 7 rotatable bonds. Rotatable bond more than 10 and molecular weight more than 500 can lead to decreased permeability and oral bioavailability. But ceftobiprole and ceftaroline shows molecular weights more than 500. Hence to improve the action of these two drugs we have highlighted the non-essential regions. This may possibly be spliced to reduce the molecular mass. However, the effectiveness of these low molecular mass compounds has to be tested in both in-vivo and in-vitro (Rachel E.Rigsby et al., 2016; Liangjiang et al., 2010).

The bio-reduction of aqueous Ag+ ions by the root extracts shows good UV result ranging

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between 400-600nm at known mixing ratio. The reduction of the metal ions through fresh root extracts leading to the formation of silver nano particles of fairly well-defined dimensions. The green chemistry approaches towards the synthesis of silver nano particles have many advantages (Mohammad Asif, 2021).The positive outcomes upon applied areas of such eco-friendly nanoparticles in bactericidal, wound healing and other medical applications makes this method potentially exciting for the large-scale synthesis of other inorganic materials (Nano materials)(Jayasree G.V. et al.,2013).The N-H and C-O stretching of the aromatic amine groups and stretching aromatic amine groups peak values of FTIR analysis indicates presence of silver nanoparticles at three different processed sample conditions. The strong binding capabilities C-O forms different amino acid residues and stability of the medium was increased due to the presence of the nano particles. The different bright elliptical and the spherical shape (nm) after HR-SEM analysis results shows the presence of silver nitrate after reductions. Comparatively aqueous fresh root extract contains more phytochemicals as compared to fresh leaf extract and the result obtained mainly varied due to the presence various variable parameters such as change in the climate, pH concentration, and different solvent quantity used, different conditions, and different minerals uptakes from the soil (Shabaaz J.P. Begum et al., 2022). Fresh and healthy Asparagus racemosus root and leaf sample out of contamination showed perfect phytochemical drugs useful for treating various diseases (Sapana Jadoun et al., 2021).The quantitative phytochemical screening analysis with highly stable variable parametric situations were selected for drug formulation and designing purpose by docking and post docking analysis(Nagamani et.al.,2012;Prasanth Tiwari et.al.,2011). The phytochemical constituent Shatavarin shows best and strong interaction for drug formulation and drug design method using iGEMDOCK analysis. The overall binding energy of drugs having antiviral GP120 (-107.169), anticancer 30WJ (-118.366), anti-inflammatory 4COX (-172.98) and anti bacterial 3UX (-107.944) effects with unique docking scores (Fengxu Wu et al., 2020; Fan Yi et al., 2018).

Conclusions

The green synthesis of fresh sample root reveals better nanoparticles characterization and phytochemical analysis result. The binding energy and affinity towards different drugs varies depending upon the variation of different environmental parameters. Shatavarin the phytochemical constituent of A.racemosus root shows better antibacterial result of the selected gram positive and gram negative microorganisms against E.coli, Pseudomonas aeruginosa, and Staphylococcus aureus with maximum zone of inhibition of 16mm, 15mm, and 14mm. The Small molecules and its drug likeness habitat, pharmacokinetic behaviours, medicinal chemistry friendliness were smoothly done and analyzed through Swiss ADME tool. The main advantage of the tool is high echo friendly nature and accuracy .All the components of the sample material understudy were analyzed and drug likeness habitat were investigated .The best drug likeness habitat helps for drug formulation and drug designing upon the A.racemosus root sample .The different small compounds named Shatavarin I, Shatavarin B (AsparaninB), SchidigerasaponinD5 and Saponins were executed and drug likeness of the sample plant under study were clearly investigated. Finally concluded that fresh root sample shows better

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application studies of silver nanoparticles, anti-microbial, anti-cancer, anti-inflammatory studies etc. Drug formulation and active areas of drugs can be designed by PyMOL, GUI and CADD.

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