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Molecular Docking Analysis of Bioactive Compounds of *Acacia Concinna* against Fungal Protein

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Abstract

Objective: The bioactive compounds of *Acacia concinna* and inhibition potential were studied against antifungal activity. In this research, the protein responsible for fungal disease causes skin infection and oral infection which was docked against the active compounds.

Materials and Methods: The protein responsible for this disease was studied and retrieved from PDB. The active compounds were screened by using Lipinski rule of five and ADMET (Absorption Distribution Metabolism Excretion and Toxicity) properties. The molecular docking analysis was done against the virulent protein by using Autodock 4.2.6 software and was visualized by using Discovery studio 3.1.

Result: Geranyl acetone has the highest binding energy of -4.25 Kcal/mol against the candidapepsin-1 followed by *Trans*-linalool oxide -4.22 Kcal/mol, Methyl salicylate -4.18 Kcal/mol, *Cis*-Linalool oxide, -4.16 Kcal/mol and 5-Methyl-2-furfural -3.75 Kcal/mol. The Hydrogen bond interaction, vanderwaals interaction of molecules was studied. This research work mainly focuses on targeting the potential drug against virulent enzymes that reduces the cost spent on clinical trials and for the development of novel therapeutic products.

Keywords: *Acacia concinna*, Lipinski rule of five, ADMET, Autodock, Geranyl acetone

INTRODUCTION

Acacia concinna commonly known as Shikakai or Chikaikkai is a well-known plant for its shampoo-like property. This plant is common in the warm plain regions of south and central India. It's a thorny plant that is broad-based and flattened whose leaves have caducousstipules. Flower of *Acacia concinna* are pink with reduced subtending bracts. It's famous in India for its usage for hair care since the ancient times. Furthermore, *Acacia concinna* has various applications in medical and other fields. Ayurvedic texts states *Acacia concinna* usage as a shampoo with antidandruff property. This shampoo effectively cleans dirt and grease from hair without altering its structure. This herb improves hair volume and texture. It cures leprosy and skin related diseases such as oedema. Folklore medicines states Shikakai's analgesic, anti-bacterial, and insect repellent and wound healing property are very efficiently utilised. Its leaves are used in malarial fever and the decoctions of the pods are used to relieve biliousness and acts as a purgative. Traditionally Shikakai is employed as an oral rinse to cure halitosis, dental caries, and mouth ulcers and gum bleeding. It relives leg, hip and joint pain when applied to affected regions after a hot castor oil massage. This herb has cleansing and inflammation properties used as a tincture or infusion in bath and washes skin infections such as accumulated pus and exudates such as skin rash. *Acacia concinna* has various medicinal usages such as for pain, constipation, jaundice, dandruff, age spots, gum diseases, leprosy and psoriasis [1]. These plant medications can be commercially available or prepared at home individually. The leaves, barks and pods have been used as a herbal medicine for emetic, purgative and expectorant treatments. It pharmacological properties are antioxidant, anti-coagulant, anti-platelet, anti-thrombotic, antidermatophytic and immune adjuvant [2-3].

Phytochemical analysis

Phytochemical composition of extracts differs based on the polarity of the solvent being used. This is due to the solubility of different compounds in various solvents. Aqueous extracts contains hydrophilic compounds, whereas ethanol extract contains both hydrophobic and hydrophilic phytochemical constituent. Alkaloids, Flavanoids, Phytosterols, Saponins and Phenolic compounds are found in all extracts of aqueous, benzene, chloroform, petroleum ether, butanol and methanol. Tannins, gums and mucilage are present in all extracts except in petroleum ether and butanol [4-5]. The powder characters include crystals of calcium oxalate and oil globules, cells containing saponins. The bark contains high level of saponins which are foam forming agents. These pods contain the saponin with trihydroxymonocarboxylic acid that exhibits acidic activity and surfactant property [6-8]. Methanolic fraction extracts of pods of *Acacia concinna* enhances activity of Th1 and Th2 helper T cells [9].

Pharmacological and medicinal activities of Acacia concinna

Acacia concinna fruits are used for washing hair, promoting hair growth, an expectorant, emetic and purgative. Methanol extract of the plant bark showed anti-bacterial activity against gram positive bacteria *staphylococcus aureus, Streptococcus mutans, Lactobacillus casei, Lactobacillus acidophilus,* and *Bacillus megaterium. Acacia concinna* treats infectious organ related diseases. It's a stimulant of diuretic and liver stimulant used to treat chronic cough, asthmatic obstruction, jaundice and vomiting, liver disease, lump formation in abdomen, lice and dandruff. This plant is implemented as a home remedy to cure various diseases such as skin itching, psoriasis, pimple, constipation, hyper pigmentation, jaundice and gum infection [10]. The fruit from this plant produces saponins which are of low pH and

possess detergent action. These properties give *Acacia concinna* antibacterial cleansing properties. This harwash paste acts as a remedy for Pityirasiscapitis. Decoction of the leaves acts as a purgative and is used to relieve malaria. Pods of *Acacia concinna* are grounded to prepare and ointment used as a skin cream. Leaves of *Acacia concinna* are made into paste to make hair cleanser, prevent diabetes and skin diseases. The leaf extract is used for treating malaria. Studies have proven pod extracts have antidermatophytic properties against Trichophytonrubrum, T. mentagrophytes, T. violaceum, Microsporumnanum and Epidermophytonfloccosum. Methanolic extracts show immunological adjuvant activity, ethanolic extracat show hepatoprotctive activity, antifungal, antibacterial and acts as a contraceptive. Studies evaluate insecticidal activity of the seed and leaves extract of *A. concinna*. The plant possesses surfactant type catalyst, antioxidant, Anthelmintic and inhibits Heinz Body Induction [11-15].

MATERIALS AND METHOD

Bioactive compounds of Gas Chromatography- Mass Spectrometry (GC-MS) analysis from Acacia concinia

A. concinia volatile organic compounds extract through distillation process. GC-MS is carried out using Shimadzu QP 2000 A equipment. The bioactive compounds obtained from *Acacia concinna* are Furfural, 5-Methyl-2-furfural, Phenyl acetaldehyde, *cis*-Linslool oxide, *trans*-Linalool oxide, Methyl salicylate, ∝-Terpinolene (tentative), Geranyl acetone, Tetradecanoic acid, 6,10,14-Trimethyl-2-pentadecannone, Methyl palmitate, Palmitic acid, Isopropyl palmitate, Methyl linoleate and Linoleic acid (tentative). These bioactive compounds were reported by [16]. The major group of compounds found are long chain fatty acid with esters and five members oxygenated heterocyclic compounds. Furfural, 5-methyl-2-furfural, Linalool oxides, phenyl acetaldehyde and methyl salicylate heterocyclic compounds which originate form pyrolysis reaction, oxidation of linalool, identified in many essential oil and in foodstuffs with a sweet green odour reminiscent of hyacinth and present in ointment preparation respectively. Fatty acids and esters present in the pods aroma are limited in their contribution towards fragrance or aroma substance. No report is available of *Acacia concinia* against the virulence of fungal and bacterial enzyme Candidapepsin-1. These compounds are docked at their molecular level against the enzymes considered, Candidapepsin-1. The molecular level docking will elucidate the interaction between the ligand and the active sites of the enzymes leading to novel medicinal discovery in the field of drug discovery and development. The Lipinski's rule of five assesses the durability of a drug molecule. The bioactive compound analysis satisfies the Lipinski's rule of five. The rule comprises of five criteria namely molecular weight (< 500), log P (<+5.6), Number of hydrogen donors (<5), Number of hydrogen acceptors (<10), and Molar refractivity (40-130). It evaluates the drug-likeliness of a compound to be consumed orally acting as a potent factor to be satisfied for further drug synthesis.

Enzyme targets

Enzymes Candidapepsin-1 (PDB Id: 2qzw) is drug targets implemented in this research. Details and structure of the proteins were retrieved from the Protein Data Bank database. Water molecules were removed by using pymol viewer. After the removal of water molecules the structure was visualized by using Discovery studio visualize 3.1.

Candidapepsin-1 enzyme structure

Candidapepsin-1 is an apoenzyme that mainly takes place in aspartic proteinase (Sap) family. SAP-1 is mainly situated on the chromosome 6 of Sap family creature adds to this proteinase enzymatic property. Candidapepsin-1 is a proteolytic harmful compound that causes parasitic types of Candida albicans. This chemical causes oral and skin contaminations that remain steady and dynamic at pH 5.0. Candidapepsin-1 is comparably similar in structure and capacity to that of isoenzyme Candipepsin-5. A sum of 10 subclasses of acidic hydrolases is available in the Sap family from Candipepsin-1 to 10. Candidapepsin-1, Candidapepsin-2 and Candidapepsin-3 show different contrast from Candidapepsin-5 that depends on its electrostatic charge and basic structure along with the enzyme active site.

Amino acid covering the aspartic albican protein of the catalyst comprises of A and B chain and comprises of 391 amino acids with a negative electrostatic charge. This dynamic site is available in the range of Asp82 and Asp267 of the catalyst. The most inhibitory of the protein is Pepstatin A. Thus, atomic docking of the catalyst with bioactive plant metabolites makes upgrades in the current medication advancement process [17].

ADMET properties

The bioactive compounds were subjected to perform different types of properties like Absorption, Distribution, Metabolism, Excretion and Toxicology (ADMET). These properties include several parameters like aqueous solubility, Blood Brain Barrier (BBB), plasma protein binding, cytochrome inhibition, intestinal absorption and hepatotoxicity were evaluated. The drug likeness of the bioactive compounds were performed by using SwissADME tool of Swiss Institute of Bioinformatics (http://www.sib.swiss) was used to calculate the behaviour of each compounds. The canonical smiles were retrieved from pubchem and evaluvated by using Swiss ADME tool. The Swiss ADME tool is based on the principle of vector machine algorithim that can easily analyse data sets of known inhibitor/non-inhibitor as well as substrate/non substrate [18].

Discovery studio 3.1- Visualizer

Discovery studio 3.1 is the software developed by Accelrys that provides necessary information about interactions of small and large molecules taking part in an interaction. This is a free of cost programme providing comprehensive information for the scientific community to view and analyse ligand-receptor interactions. This software deals with macromolecule engineering, ligand-receptor interaction, pharmacophore modelling, antibody modelling and optimization stimulations, and macromolecule design and protein-protein interactions.

RESULTS AND DISCUSSION

The molecular docking analysis differentiates the binding energy of each compound and it drug likeness against bacterial or fungal diseases. These active compounds are screened using Lipinski rule of five as shown in Table 1. The standard criteria for drug likeness of each compounds were molecular mass should be less than 500 dalton, Hydrogen bond donor less than 5, hydrogen bond acceptors less than 10, high lipophilicity less than 5 (LOGp) and molar refractivity between 40-130. Based on this criteria the compound that are satisfied for Lipinski rule of five are 5-Methyl-2-furfural, *Cis*-Linalool oxide, Furfural, Geranyl acetone, Methyl salicylate, Phenyl acetaldehyde, Tetradecanoic acid and *Trans*-linalool oxide.

ADMET properties

The satisfied compounds are then evaluated by using Absorption, Distribution, Metabolism, Excretion and Toxicity (ADMET) tool. Swiss ADME tool was used to evaluate several parameters of the compound as drug molecule. The ADMET properties of every compound were listed in Table 2-5.

The ADMET properties of each compounds predicts that the majority of the compounds are drug likeness based on the gastro intestinal absorption in which the percentage of every compounds satisfies the maximum absorption rate along with the glycoprotein will not be inhibited. The Distribution rate of bioactive compounds are so less to penetrate across the Blood Brain Barrier (BBB) and Central Nervous System (CNS). The cytochrome metabolism in the majority of the bioactive compounds was not inhibited and non substrate form. The excretion and toxicity parameters show the level of dosage in human and rat in which especially the furfural shows the good ingestion rate.

Table 1: compounds analysed in Lipinski rule of five

Compound Name	Compound Structure	Mass	Hydrogen bond donor	Hydrogen bond acceptor	LOGp	Molar Refractivity
5-Methyl-2-furfural		110	0	2	1.4005	28.83
Cis-Linalool oxide		170	1	2	1.881	49.01
Furfural		96	0	2	1.092	24.09
Geranyl acetone		194	0	1	4.04	62.34
Isopropyl palmitate		298	0	2	6.42	91.53
Linolenic acid		278	1	2	5.6	86.89
Methyl linoleate		294	0	2	5.97	91.37
Methyl palmitate		270	0	2	5.64	82.32
Methyl salicylate		152	1	3	1.17	39.44
Palmitic acid		256	1	2	5.55	77.94
Phenyl acetaldehyde		120	0	1	1.42	36.20
Tetradecanoic acid		228	1	2	4.77	68.71
Trans-linalool oxide		170	1	2	1.88	49.00

Table 2: Absorption properties of compounds

Compound	Water solubility (log mol/L)	Caco2 permeability (Log Pabb in 10^{-6} cm/Sec)	GI absorption (%)	Skin permeability (Log Kp)	P-glycoprotein substrate	P-glycoprotein I inhibitor
5-Methyl-2-furfural	-0.358	1.624	97.42	-2.61	Yes	No
Cis-Linalool oxide	-1.223	1.403	94.87	-2.68	No	No
Furfural	-0.118	1.609	100	-2.69	Yes	No
Geranyl acetone	-4.98	1.505	94.24	-1.273	No	No
Methyl salicylate	-1.881	1.202	89.45	-2.716	No	No
Phenyl acetaldehyde	-1.508	1.636	95.89	-1.524	No	No
Tetradecanoic acid	-4.952	1.560	92.69	-2.705	No	No
Trans-linalool oxide	-1.233	1.403	94.87	-2.684	No	No

Table 3: Distribution properties of compounds

Compound	VDss (human) (Log L/kg)	Fraction unbound (human) (Fu)	BBB permeability (Log BB)	CNS permeability (Log PS)
5-Methyl-2-furfural	-0.141	0.647	-0.032	-2.801
Cis-Linalool oxide	0.084	0.63	0.217	-3.030
Furfural	-0.155	0.633	-0.038	-2.756
Geranyl acetone	0.307	0.276	0.653	-1.922
Methyl salicylate	-0.009	0.49	-0.222	-2.185
Phenyl acetaldehyde	0.145	0.384	0.158	-1.684
Tetradecanoic acid	-0.578	0.171	-0.027	-1.925
Trans-linalool oxide	0.084	0.63	0.217	-3.030

Table 4: Metabolism properties of compounds

Compound	CYP2D6 substrate	CYP3A4 substrate	CYP1A2 inhibitor	CYP2C19 inhibitor	CYP2C9 inhibitor	CYP2D6 inhibitor	CYP3A4 inhibitor
5-Methyl-2-furfural	No	No	No	No	No	No	No
Cis-Linalool oxide	No	No	No	No	No	No	No
Furfural	No	No	No	No	No	No	No
Geranyl acetone	No	No	No	No	No	No	No
Methyl salicylate	No	No	No	No	No	No	No
Phenyl acetaldehyde	No	No	Yes	No	No	No	No
Tetradecanoic acid	No	No	No	No	No	No	No
Trans-linalool oxide	No	No	No	No	No	No	No

Table 5: Excretion and Toxicity properties of compounds

Compound	Renal OCT2 substrate	AMES toxicity	Max. tolerated dose (human) (Log mg/kg/day)	hERG I inhibitor	Oral Rat Acute Toxicity (LD50) (mol/kg)	Oral Rat Chronic Toxicity (LOAEL) (Log mg/kg)	Liver Toxicity	Skin Sensitisation
5-Methyl-2-furfural	No	Yes	1.009	No	2.445	1.763	No	Yes
Cis-Linalool oxide	No	No	0.891	No	1.917	2.221	No	Yes
Furfural	No	Yes	1.063	No	2.429	1.730	No	Yes
Geranyl acetone	No	No	0.266	No	1.559	1.284	No	yes
Methyl salicylate	No	Yes	0.769	No	1.764	2.305	No	No
Phenyl acetaldehyde	No	No	0.892	No	1.695	1.801	No	Yes
Tetradecanoic acid	No	No	-0.559	No	1.477	3.034	No	Yes
Trans-linalool oxide	No	No	0.891	No	1.917	2.221	No	Yes

Table 6: Interactions of various bioactive compounds

Compound	Binding energy	Vanderwaals Interaction	No. Of hydrogen bonds	Hydrogen interactions	Total no of residues
5-Methyl-2-furfural	-3.75	ASP86, GLY220, SER13, VAL12, THR221	3	THR222, TYR225, ILE223	ASP86, GLY220, SER13, VAL12, THR221, THR222, TYR225, ILE223
Cis-Linalool oxide	-4.16	ASP86, VAL12, SER13, GLY220, THR221, ILE223	2	THR222, TYR225	ASP86, VAL12, SER13, GLY220, THR221, ILE223, THR222, TYR225
Furfural	-3.28	ASP86, GLY220, THR221	3	THR222, TYR225, ILE223	ASP86, GLY220, THR221, THR222, TYR225, ILE223
Geranyl acetone	-4.25	ASP86, THR221, GLY220, VAL12, ASP218, GLY34, ASP32, ILE123, ILE30, ILE119, SER13	1	THR222	ASP86, THR221, GLY220, VAL12, ASP218, GLY34, ASP32, ILE123, ILE30, ILE119, SER13, THR222
Methyl salicylate	-4.18	ASP86, ILE305, THR221	4	GLY220, THR 222, ILE223, TYR225	ASP86, ILE305, THR221, GLY220, THR 222, ILE223, TYR225
Phenyl acetaldehyde	-3.32	GLY220, ASP86, ILE305, GLY85, THR221	3	ILE223, TYR225, THR222	GLY220, ASP86, ILE305, GLY85, THR221, ILE223, TYR225, THR222
Tetradecanoic acid	-2.34	ASP218, ASP86, ILE123, THR221, TYR84, ASP32, ILE30, SER35, SER13, VAL12, TYR225	2	THR222, GLY220	ASP218, ASP86, ILE123, THR221, TYR84, ASP32, ILE30, SER35, SER13, VAL12, TYR225, THR222, GLY220
Trans-linalool oxide	-4.22	ASP86, VAL12, SER13, GLY220, ILE223, THR221	2	THR222, TYR225	ASP86, VAL12, SER13, GLY220, ILE223, THR221, THR222, TYR225

In the current study, the target protein was analysed by docking analysis with various bioactive compounds. The bioactive compounds are screened by using Lipinski rule of five and ADMET properties that shows the property of each compound. Throughout the docking analysis the lowest the binding energy shows the greater active site interactions. The control docking has been done with pepstatin A that shows the binding energy of +1.4 Kcal/mol. Geranyl acetone with highest binding energy of -4.25 Kcal/mol and followed by *Trans*-linalool oxide -4.22 Kcal/mol, Methyl salicylate -4.18 Kcal/mol, *Cis*-Linalool oxide -4.16 Kcal/mol and 5-Methyl-2-furfural -3.75 Kcal/mol also have good binding interactions. The vanderwaals interactions energy and the hydrogen interactions were listed in Table 6. Throughout the analysis, the amino acid THR222 (Threonine) shows better bondage with hydrogen atoms for all bioactive compounds. Geranyl acetone isolated from *Acacia concinna* has immense antifungal activity against candidapepsin. *Acacia concinna* extract shows good result against antifungal activities as reported in [19] . This study proves that essential bioactive compounds of *Acacia concinna* have a good antifungal activity in In-vitro as well as In-silico and these compounds can also be used for various activities. As a result, the binding interactions of amino acid along with bio active compounds are shown in Figure 2-7.

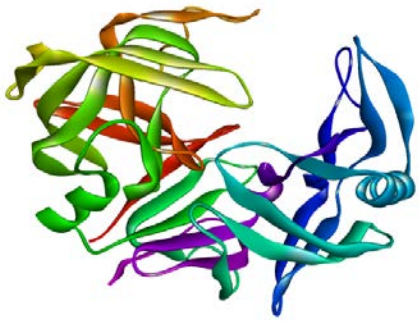

Figure 1: A chain amino acid of candidapepsin 1

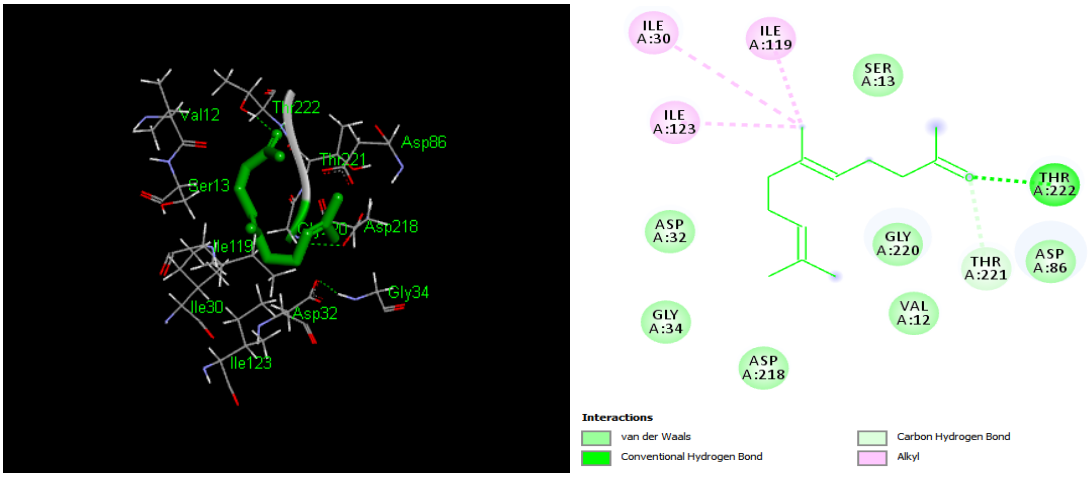

Figure 2: 3D and 2D confirmation interactions of Geranyl acetone against candidapepsin-1

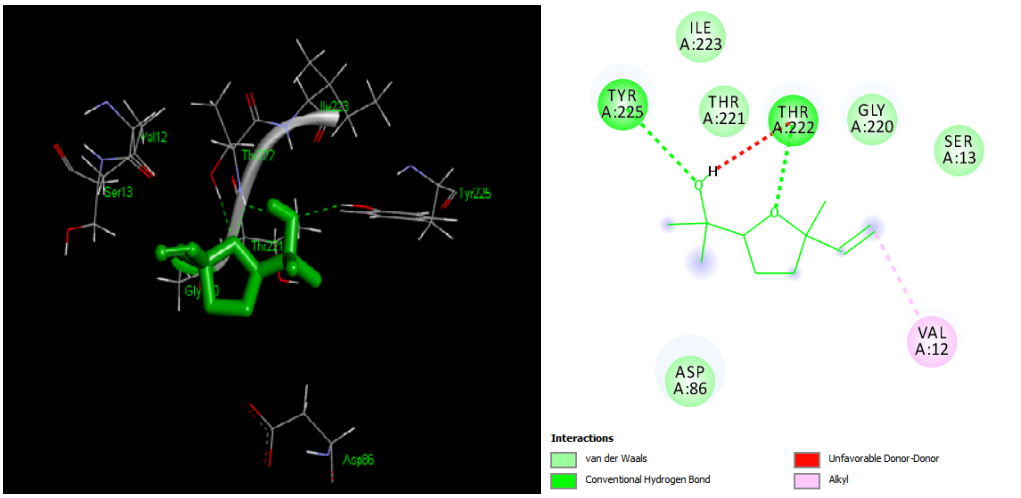

Figure 3: 3D and 2D confirmation interactions of Trans-linalool oxide against candidapepsin-1

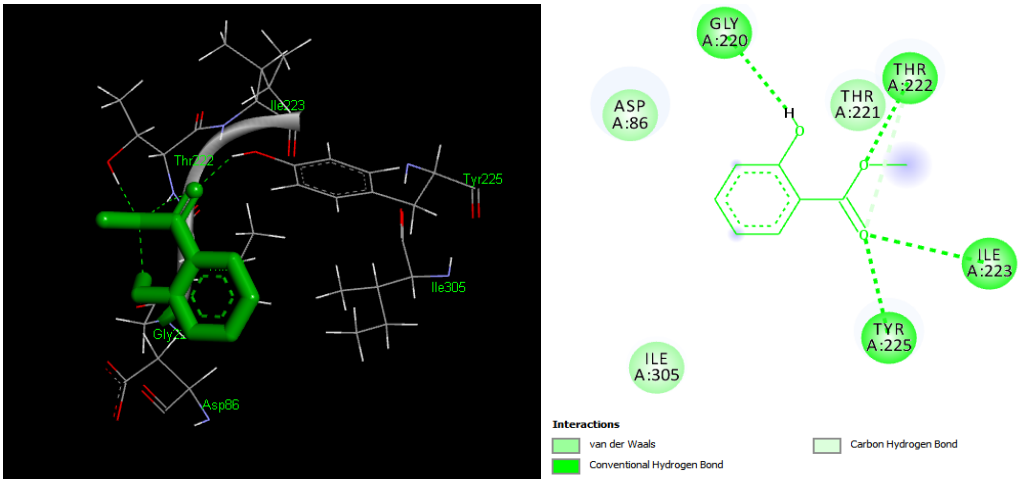

Figure 4: 3D and 2D confirmation interactions of Methyl salicylate oxide against candidapepsin-1

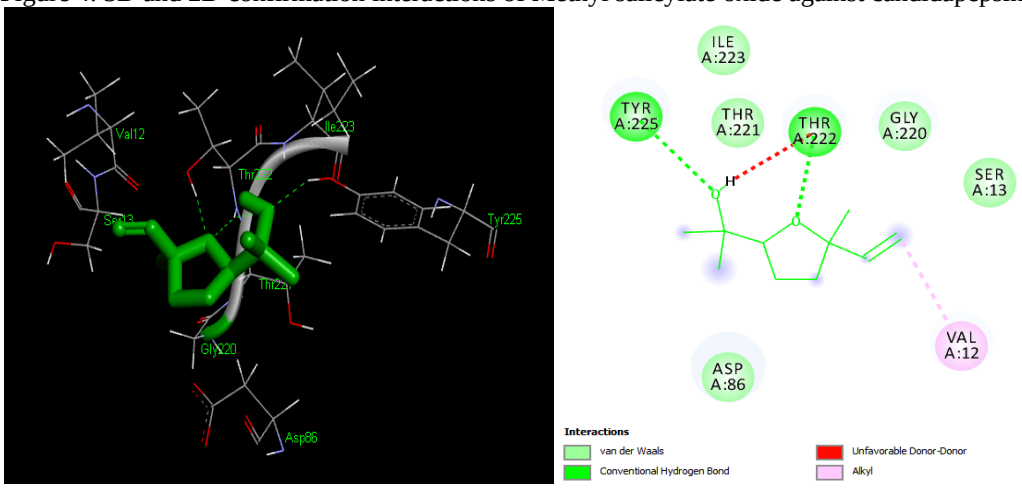

Figure 5: 3D and 2D confirmation interactions of *Cis*-Linalool oxide against candidapepsin-1

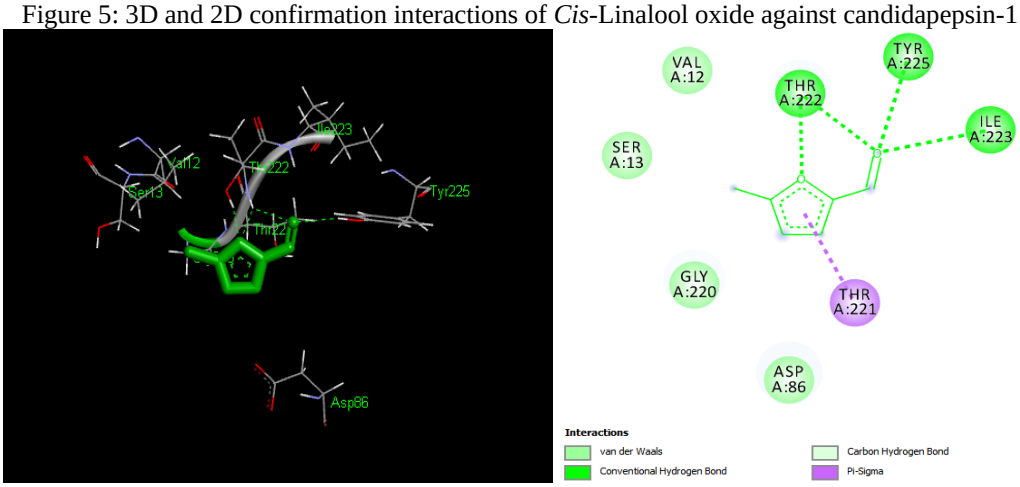

Figure 6: 3D and 2D confirmation interactions of 5-Methyl-2-furfural against candidapepsin-1

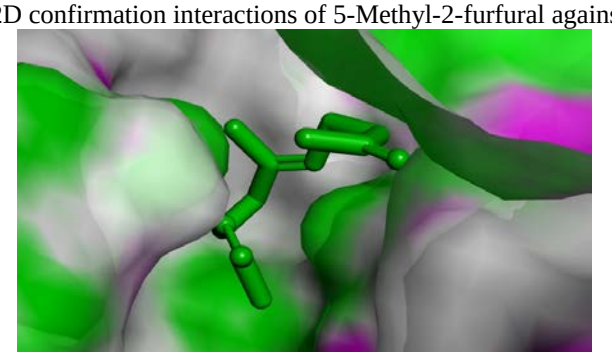

Figure 7: Docking confirmation of Geranyl acetone with surface image

CONCLUSION

Acacia concinna is traditionally used in ayurvedic medicine in ancient against several pathogenic diseases like anti bacterial, antifungal, antipyrogenic and anti-inflammatory. This study reveals the potential activity of bioactive compounds from *Acacia concinna* against candida species. Geranyl acetone showed better drug reliable properties in Lipinski rule of five and ADMET properties. The active compounds of *Acacia concinna* have the ability to use a drug molecule with proper dosage for human as well as rat as shown in ADMET properties. The geranyl acetone with binding energy -4.25 Kcal/mol showed better results than the control docking of pepstatin A with binding energy of +1.4 Kcal/mol. Thus the active compounds of *Acacia concinna* inhibits the virulent enzymes that leads to anti fungal activity with novel discovery of plant based therapeutic product. The molecular docking analysis provides comprehensive details for clinical trials on animals and also plays a major role in drug discovery modules.

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