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MOLECULAR DOCKING AND ADMET STUDIES OF BIOACTIVE COMPOUNDS OF *RHIZOPORA MUCORNATA* AGAINST BACTERIAL ENZYME PROTEIN TYROSINE PHOSPHATASE

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Keywords:

Rhizopora mucornata, Protein tyrosine phosphatase, Molecular docking, ADMET, 3-methyl-2-(2-oxopropyl) furan

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ABSTRACT: Objective: The bioactive compounds of *Rhizopora mucornata* were docked against the bacterial enzyme protein tyrosine phosphatase to determine the potential inhibition. In this research the molecular docking analysis of drug compounds with virulent protein was studied. **Material and Methods:** Protein Tyrosine phosphatase is an enzyme that is being present in staphylococcus infection that plays an important role in cellular localization, enzyme stability. The target enzyme for S*taphylococcus aureus* was studied and retrieved from PDB. The bioactive compounds from the leaf extract of *Rhizopora mucornata* was screened for Lipinski rule of Five and ADMET properties. Autodock 4.2.3 software was used for molecular docking, and the visualization was done by using discovery studio 3.1. **Result:** The compound 3-methyl-2-(2-oxopropyl) furan shows better binding energy with -1.14 Kcal/mol against the enzyme protein tyrosine phosphatase followed by 3-cyclopentylpropionic acid, 4-methoxyphenyl ester +35.14 Kcal/mol. The hydrogen interactions and Vander Waals interactions, along with total residues of amino acids were studied. This research mainly focuses on targeting the virulent enzyme by using potential drugs to discover a novel therapeutic product.

INTRODUCTION: The *Rhizophora mucornata* is a plant species that is found in the coasts and rivers banks of East-Africa through Madagascar, island of Indian Ocean, southeastern mainland of Asia, Indonesia, Philippines to northeastern Australia and south pacific region. *Rhizophora* is the genus name which is derived from Greek language, where "*Rhizo*" means roots "*phora*" means bearing that is root bearing.

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This species is commonly called loop-root mangrove, red mangrove or Asiatic mangrove [1]. The trees are either small or medium-sized trees of about 10 to 15 meters and 20 to 25 meters respectively. These small and medium-sized plants are found in banks of the rivers and the fringes of the sea.

The leaves are elliptical of approximately 12 cm long and 6 cm wide and have large number of stilt roots. The seeds are viviparous, and the fruit is single-seeded and germinates on the trunk [2]. The pollen grains are pollinated through wind or insects. The flowers are bisexual and self-compatible. The edible part of the plant is the fruit which baked and eaten. The shoot of this plant is consumed as vegetable.

According to Malesian archipelago the important source of tannin is the barks. The timber is used for the construction of buildings, in making the fish traps and as firewood. The uses of the plants also include in manufacturing adhesives plywood. This plant is used as medicine in curing haematuria, other diseases and disorders [3]. The use of this wood is very limited because of its lightweight, poor durability and small size of the trunk.

Phytochemical Analysis: The *Rhizophora mucornata* is subjected to phytochemical analysis and is found to have compounds such as steroids, alkaloids, flavonoids, glycosides, saponins, phenols [6]. The phytochemical analysis is one of the basic methods used in the field of plant technology. It is an analytical method in which we can find out the compounds present in the plant. Many phytochemical analyses have been done based on this particular species. Using the leaf extract obtained from the plant, different tests are taken place to find out the compounds present in the plant and the following results are obtained are alkaloids, terpenoids, steroids, tannins, quinones, saponins, flavonoids, cardiac glycosides and phenols [4, 5]. The root extract consists of saponins, alkaloids, flavonoids, and triterpenes. Then bark contains alkaloids, tannin, saponin, phenolic, flavonoid, terpenoid and glycosides, the fruit and flower of this plant also shows same result as bark but the amount present in some particular components have some variations from the above results taken from the five-different parts present in the *Rhizophora mucornata* leaf contain a greater number of compound than other four parts [6].

Medicinal Values: This kind of plant basically used in most of Asian countries as medicine and also as a remedy for some particular diseases like diarrhea, hemorrhage, dysentery, diabetes, angina [Ischemic chest pain] and haematuria. Old leaves and roots are used by Malayans during childbirth, barks of this plant are used for bloody urine by Burmese [7], leaves of these plants are used for fish injuries [11,] but the honey which is taken from these flowers are said to be poisonous [8]. *Rhizophora mucornata* is used for diabetes due to the presence of flavonoids. Therefore the current study aimed to determine the potential of the drug compound against protein tyrosine phosphatase by molecular docking analysis [9].

MATERIALS AND METHODS:

Compounds Retrieved from *Rhizopora mucornata* by Gas Chromatography-Mass Spectroscopy: *Rhizopora mucornata* contains organic compounds by distillation process. GCMS is carried out using Shimadzu QP 2000. The bioactive compounds obtained from *Rhizopora mucornata* are l-(+)-ascorbic acid 2,6-di-hexadecanoate, 2R-acetoxymethyl-1,3,3-trimethyl-4t- (3- methyl- 2buten- 1- yl)- 1 t- cyclohexanol, 3-methyl- 2- (2- oxopropyl)furan, n-propyl 11- octa-decenoate, Phytol, 3-cyclopentylpropionic acid, 4-methoxyphenyl ester, 1,3,3-trimethyl-2-hydroxy-methyl-3,3-dimethyl-4(3-methylbut-2-enyl)-cyclo-hexene, 2, 6, 10, 14, 18, 22-tetracosahexaene, 2, 6, 10, 15, 19, 23 hexamethyl, Beta-Amyrin, Clianosterol, (4α-trans)-decahydro-4α-methyl-1-methylene- 7- (1methylethylidene)- naphthalene, Olean-18-ene, 1-Pentatriacontanol, Stigmasterol compounds were reported by saranya *et al*. [10] The group of compounds present are alcoholic compounds, fatty acid and secondary metabolites. No reports were available in performing molecular docking analysis against *Staphylococcus aureus* in the leaf extract of *Rhizopora mucornata*. The bioactive compounds obtained from the leaf extract were docked against protein tyrosine phosphatase which is responsible for inducing staph infection [11]. The drug compounds were screened for Lipinski rule of five based on the following standard parameters with molecular weight < 500, logP <5.6, Number of hydrogen donors <5, Number of hydrogen acceptor <10 and Molar Refractivity 40-130. This study mainly screens the drug-likeness against target protein for drug discovery.

Enzyme Target Preparation: Enzyme protein tyrosine phosphatase with PDB Id: 3rof is the drug target against the bioactive compounds. The targeted protein was searched in Protein Data Bank by downloading it in pdb format. The hydrophobic molecules and the hetero-atoms were removed by using pymol viewer.

Protein Tyrosine Phosphatase Enzyme: It follows the signal transduction pathway, followed by an enzyme for cell cycle and MAP kinase pathway. The enzyme tyrosine phosphatase contains two low molecular weight proteins like PtpA and PtpB that produce pathogenic staphylococcus infection. Most strains are resistant

to penicillin and MRSA that are common in the hospitals and are emerging in the community. The staphylococcus infection mostly infects the skin and can be spread. The virulent infection had caused severe damage is Methicillin-Resistant *Staphylococcus aureus* (MRSA) that has high pathogenicity causing infection that interchanging the nature from a drug to toxin character. Along with strain some coagulase-negative bacteria are being produced like *Staphylococcus aureus* and *Staphylococcus endocarditis* that interferes with the immune defences [11]. There are 30 different types of infection caused by staph infection through both coagulase-positive and negative strains, by which the staphylococcus have the ability to synthesize or secrete many factors that allow the bacteria to survive in host of bacterial cell. By characterizing the *Staphylococcus aureus* only three tyrosine phosphatase is known [12].

An infected patient should be treated with methicillin, if he/she is resistant to methicillin, vancomycin will be introduced into the patient, rather than that ampicillin is also used to the staph infection. Some methods like surgical and oral treatment are being processed on the prospective conditions. The key characteristics of (LMW-PTP) is that it binds at the active site fold with the members of classical tyrosine and dual-specificity phosphatases families. At certain stage the LMW-PTP fold is conserved in *Staphylococcus aureus* by synthesizing and cloning in expression vector. The unique features Of PtpA are that the loops are on the peripheral of the molecule while loop 2 is close to active site that causes difference in substrate recognition. The diagnosis of staph infection begins with attempting to culture the bacteria from an infected site in any area with pus or blisters should be cultured [13].

ADMET Properties: The compounds retrieved from *Rhizopora mucornata* were screened by using ADMET properties which mainly concentrates on the Absorption Distribution Metabolism Excretion and Toxicity of the compounds. These properties show the proportional activity of compounds in water solubility, gastrointestinal absorption, plasma protein binding, cytochrome P450. The toxicity of the drug compound was tested by knowing the dosage of humans, rat and the toxic substance of drugs against liver and skin. The drug screening was done by using Swiss ADME tool of Swiss Institute of Bioinformatics (http://www. sib.swiss) to calculate the compound behavior. The canonical smiles were retrieved from PubChem and NIST library. The Swiss ADME is mainly based on the principle of vector algorithm knowing as inhibitor as well as substrate [14].

Discover Studio 3.1- Visualizer: The software Discovery studio 3.1 was developed by Accelrys that shows the ligand interactions with 3 letters and ID and insertion code. The program is free of cost which plays a major role in showing the interactions of protein with ligand. This software mainly deals with macromolecule engineering, ligand-receptor interaction, pharmacophore modeling [15].

RESULTS AND DISCUSSION: The docking analysis will only be carried out if the bioactive compounds of *Rhizopora mucornata* satisfies the Lipinski rule of five. Based on the standard profile the bioactive compounds must possess molecular mass 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. The compounds that satisfies the Lipinski rule of software are 2R-acetoxymethyl- 1, 3, 3- trimethyl-4t-(3-methyl-2 buten- 1- yl)- 1t- cyclohexanol, 3-methyl-2-(2-oxo-propyl)furan, n-propyl 11-octadecenoate, Phytol, 3-cyclopentylpropionic acid, 4-methoxyphenyl ester, 1,3,3-trimethyl-2-hydroxymethyl-3,3-dimethyl-4(3-methylbut- 2- enyl)- cyclohexene and (4α-trans)-decahydro- 4α- methyl- 1- methylene- 7- (1methyl-ethylidene)-naphthalene as shown in **Table 1**. The satisfied compounds were further screened for ADMET properties and molecular docking was done for the determination of protein ligand interactions.

ADMET Properties: The satisfied compounds were screened for ADMET properties by using Swiss model. The absorption properties of the compounds were analyzed, the compound n-propyl 11-octadecenoate, Phytol, and (4α-trans)-deca-hydro- 4α- methyl- 1- methylene-7-(1methylethyli-dene)-naphthalene ranges from -7.544 to -6.496 log mol/L. The calcium carbonate permeability shows a better permeability in n-propyl 11-octadecenoate. The gastrointestinal absorption shows 97% of

absorption in 3-methyl-2-(2-oxopropyl) furan compound. The glycoprotein substrate and the inhibitor shows no result in all the compounds as shown in **Table 2.**

TABLE 1: SCREENING OF LIPINSKI RULE OF FIVE AGAINST BIOACTIVE COMPOUNDS OF *RHIZOPORA MUCORNATA*

Compound name	Molecular weight (Less than 500D)	Hydrogen bond donor (Less than 5)	Hydrogen bond acceptor (Less than 10)	LOGp (Less than 5)	Molar refractivity (Between 40-130)
l-(+)-ascorbic acid 2,6-dihexadecanoate	652	8	2	10.2	183.2
2R-acetoxymethyl-1,3,3-trimethyl-4t-(3-methyl-2buten-1-yl)-1t-cyclohexanol	282	1	3	3.7	81.29
3-methyl-2-(2-oxopropyl)furan	138	0	2	1.7	37.82
n-propyl 11-octadecenoate	324	0	2	4.2	100.6
Phytol	296	1	1	3.3	95.56
3-cyclopentylpropionic acid, 4-methoxyphenyl ester	248	0	3	3.5	69.82
1,3,3-trimethyl-2-hydroxymethyl-3,3-dimethyl-4(3-methylbut-2-enyl)-cyclohexene	222	1	1	4.0	70.33
2,6,10,14,18,22-tetracosahexaene, 2,6,10,15,19,23hexamethyl	410	0	0	10.3	140.0
Beta-Amyrin	426	1	1	8.16	130.71
Clianosterol	414	1	1	8.02	128.2
(4α-trans)-decahydro-4α-methyl-1-methylene-7-(1methylethylidene)-naphthalene	204	0	0	4.86	66.81
Olean-18-ene	424	0	1	8.37	123.7
1-Pentatriacontanol	508	1	1	12.87	165.1
Stigmasterol	412	1	1	7.8	128.1

TABLE 2: ABSORPTION PROPERTIES OF BIOACTIVE COMPOUNDS

Compound	Water solubility (log mol/L)	$CaCo_2$ permeability (Log P in 10^{-6} cm/Sec)	GI absorption (%)	Skin permeability (Log Kp)	P-glycoprotein substrate	P-glycoprotein I inhibitor
2R-acetoxymethyl-1,3,3-trimethyl-4t-(3-methyl-2buten-1-yl)-1t-cyclohexanol	-3.774	1.395	93.39	-2.985	No	No
3-methyl-2-(2-oxopropyl)furan	-1.023	1.634	97.08	-2.331	No	No
n-propyl 11-octadecenoate	-7.138	1.193	91.64	-2.731	No	No
Phytol	-7.544	1.515	90.71	-2.576	No	No
3-cyclopentylpropionic acid, 4-methoxyphenyl ester	-1.231	1.361	96.01	-2.937	No	No
1,3,3-trimethyl-2-hydroxymethyl-3,3-dimethyl-4(3-methylbut-2-enyl)-cyclohexene	-4.555	1.508	92.35	-1.596	No	No
(4α-trans)-decahydro-4α-methyl-1-methylene-7-(1methylethylidene)-naphthalene	-6.496	1.424	95.06	-1.763	No	No

The distribution of the bioactive compounds mainly shows the value of Blood-Brain Barrier permeability and Central Nervous System permeability. All the compounds in **Table 3** show that the drug compounds have less than 0.9 log BB in the Blood-Brain Barrier permeability, and the Central Nervous System permeability is less than -1.000, which results that the drug is safe while they are entered in the body.

TABLE 3: DISTRIBUTION PROPERTIES OF BIOACTIVE COMPOUNDS

Compound	VDss (human) (Log L/kg)	Fraction unbound (human) (Fu)	BBB permeability (Log BB)	CNS permeability (Log PS)
2R-acetoxymethyl-1,3,3-trimethyl-4t-(3-methyl-2buten-1-yl)-1t-cyclohexanol	0.148	0.354	0.275	-2.766
3-methyl-2-(2-oxopropyl)furan	-0.06	0.554	0.055	-2.266
n-propyl 11-octadecenoate	0.025	0	0.799	-1.123
Phytol	0.468	0	0.806	-1.563
3-cyclopentylpropionic acid, 4-methoxyphenyl ester	0.457	0	0.207	-1.721
1,3,3-trimethyl-2-hydroxymethyl-3,3-dimethyl-4(3-methylbut-2-enyl)-cyclohexene	0.404	0.278	0.602	-2.298
(4α-trans)-decahydro-4α-methyl-1-methylene-7-(1methylethylidene)-naphthalene	0.612	0.084	0.778	-1.404

The metabolism properties of the bioactive compounds mainly deal with cytochrome P450 that contains heme as a cofactor, which is also known as hemeproteins. The substrate and the inhibitor of cytochrome were screened as shown in **Table 4**.

TABLE 4: METABOLISM PROPERTIES OF BIOACTIVE COMPOUNDS

Compound	CYP2D6 substrate	CYP3A4 substrate	CYP1A2 inhibitor	CYP2C19 inhibitor	CYP2C9 inhibitor	CYP2D6 inhibitor	CYP3A4 inhibitor
2R-acetoxymethyl-1,3,3-trimethyl-4t-(3-methyl-2buten-1-yl)-1t-cyclohexanol	No	No	No	Yes	No	No	No
3-methyl-2-(2-oxopropyl)furan	No	No	No	No	No	No	No
n-propyl 11-octadecenoate	No	Yes	Yes	No	No	No	No
Phytol	No	Yes	Yes	No	No	No	No
3-cyclopentylpropionic acid, 4-methoxyphenyl ester	No	No	No	No	No	No	No
1,3,3-trimethyl-2-hydroxymethyl-3,3-dimethyl-4(3-methylbut-2-enyl)-cyclohexene	No	No	No	Yes	Yes	No	No
(4α-trans)-decahydro-4α-methyl-1-methylene-7-(1methylethylidene)-naphthalene	No	Yes	Yes	No	No	No	No

The excretion and toxicity of the compounds were analyzed in which the human dosage of the drug will be examined along with the rat at chronic and acute toxicity. The liver toxicity also been examined in which all the compound are safe against liver toxicity and compound like 2R-acetoxymethyl- 1, 3, 3- trimethyl- 4t- (3- methyl- 2 buten-1-yl)-1t-cyclohexanol are safe against skin sensitisation and remaining compounds have skin sensitisation as shown in **Table 5**.

The molecular docking analysis was done against protein tyrosine phosphatase for staph infection. The control docking was done against vancomycin a standard drug used for curing S*taphylococcus aureus* which results in the binding energy of +125.63 with grid size 20 Å. The algorithm used in docking is a genetic algorithm with rigid structure file.

The compound 3- methyl- 2- (2-oxopropyl)furan shown better binding energy at -1.14 Kcal/mol followed by 1, 3, 3-trimethyl-2-hydroxymethyl-3,3-dimethyl- 4(3- methylbut- 2- enyl)- cyclohexene at +46.16 Kcal/mol. This states that the *Rhizopora mucornata* does not have activity against

antibacterial strains. The highest binding energy of -1.14 Kcal/mol consists of one hydrogen atom with amino acid residue CYS 138. The pictorial representation of 2D and 3D interaction of protein and ligand interaction are shown in **Fig. 1-4**. The binding energy and the interactions of each molecular docking were shown in **Table 6**.

TABLE 5: EXCRETION AND TOXICITY OF BIOACTIVE COMPOUNDS

Compound	Renal OCT2 substrate	AMES toxicity	Max. tolerated dose (human) (Log mg/kg/day)	hERG I inhibitor	Oral Rat Acute Toxicity (LD_{50}) (mol/kg)	Oral Rat Chronic Toxicity (LOAEL) (Log mg/kg)	Liver Toxicity	Skin sensitization
2R-acetoxymethyl-1,3,3-trimethyl-4t-(3-methyl-2buten-1-yl)-1t-cyclohexanol	No	No	0.29	No	1.807	1.985	No	No
3-methyl-2-(2-oxopropyl)furan	No	No	0.901	No	2.261	1.751	No	Yes
n-propyl 11-octadecenoate	No	No	0.064	No	1.532	3.771	No	Yes
Phytol	No	No	0.05	No	1.607	1.043	No	Yes
3-cyclopentylpropionic acid, 4-methoxyphenyl ester	No	No	0.29	No	1.825	1.977	No	Yes
1,3,3-trimethyl-2-hydroxymethyl-3,3-dimethyl-4(3-methylbut-2-enyl)-cyclohexene	No	No	0.305	No	1.696	1.209	No	Yes
(4α-trans)-decahydro-4α-methyl-1-methylene-7-(1methylethylidene)-naphthalene	No	No	0.202	No	1.572	1.557	No	Yes

TABLE 6: BINDING ENERGY AND INTERACTION OF DOCKED COMPOUNDS

Compound name	Binding energy Kcal/mol	Vanderwaals Interaction	No. of hydrogen bonds	Hydrogen interactions	Total no. of residues
2R-acetoxymethyl-1,3,3-trimethyl-4t-(3-methyl-2buten-1-yl)-1t-cyclohexanol	+67.04	MET 17, ADA 18, ILE 21, ARG 25, VAL 134, MET 22, MET 85, LEU 107, PHA 6, SER 137, LEU 141, PHE 110, VAL 83, CYS 138	0	-	MET 17, ADA 18, ILE 21, ARG 25, VAL 134, MET 22, MET 85, LEU 107, PHA 6, SER 137, LEU 141, PHE 110, VAL 83, CYS 138
3-methyl-2-(2-oxopropyl)furan	-1.14	MET 85, ALA 18, PHE 6, VAL 134, MET 22, LEU 141, VAL 83, PHE 110, SER 137, ILE 21, LEU 107	1	CYS 138	CYS 138, MET 85, ALA 18, PHE 6, VAL 134, MET 22, LEU 141, VAL 83, PHE 110, SER 137, ILE 21, LEU 107
n-propyl 11-octadecenoate	+66.83	MET 17, ARG 14, VAL 130, VAL 118, ALA 18, ILE 21, VAL 134, LEU 107, PHE 6, UNK 0, LEU 141, LYS 106, PHE 105, VAL 83, SER 137, PHE 110, CYS 138, MET 22, MET 85	0	-	MET 17, ARG 14, VAL 130, VAL 118, ALA 18, ILE 21, VAL 134, LEU 107, PHE 6, UNK 0, LEU 141, LYS 106, PHE 105, VAL 83, SER 137, PHE 110, CYS 138, MET 22, MET 85
Phytol	+61.82	TYR 131, MET 17, VAL 118, ILE 21,	0		TYR 131, MET 17, VAL 118, ILE 21,

		VAL 130, PHE 6, VAL 134, MET 22, SER 38, VAL 83, PHE 110, PHE 105, LYS 106, LEU 141, CYS 138, GLU 19, ALA 18, MET 85, SER 15, ARG 14			VAL 130, PHE 6, VAL 134, MET 22, SER 38, VAL 83, PHE 110, PHE 105, LYS 106, LEU 141, CYS 138, GLU 19, ALA 18, MET 85, SER 15, ARG 14
3-cyclopentylpropionic acid, 4-methoxyphenyl ester	+35.14	PHE 110, VAL 83, SER 137, LEU 141, CYS 138, MET 22, ILE 21, VAL 134, ALA 18, MET 17, ARG 14, MET 85, VAL 118, VAL 130, PHE 105, LYS 106			PHE 110, VAL 83, SER 137, LEU 141, CYS 138, MET 22, ILE 21, VAL 134, ALA 18, MET 17, ARG 14, MET 85, VAL 118, VAL 130, PHE 105, LYS 106
1,3,3-trimethyl-2-hydroxymethyl-3,3-dimethyl-4(3-methylbut-2-enyl)-cyclohexene	+46.16	MET 22, ILE 21, VAL 134, LEU 135, C0YS 138, SER 137, LEU 141, LEU 107, PHE 110, VAL 83, PHE 6, GLU 19, ALA 20	2	ALA 18, MET 17	ALA 18, MET 17, MET 22, ILE 21, VAL 134, LEU 135, CYS 138, SER 137, LEU 141, LEU 107, PHE 110, VAL 83, PHE 6, GLU 19, ALA 20
(4α-trans)-decahydro-4α-methyl-1-methylene-7-(1methylethylidene)-naphthalene	+61.05	MET 17, ILE 21, MET 22, CYS 138, SER 137, LEU 141, PHE 110, LEU 107, PHE 6, ALA 18, VAL 83, VAL 134	0		MET 17, ILE 21, MET 22, CYS 138, SER 137, LEU 141, PHE 110, LEU 107, PHE 6, ALA 18, VAL 83, VAL 134

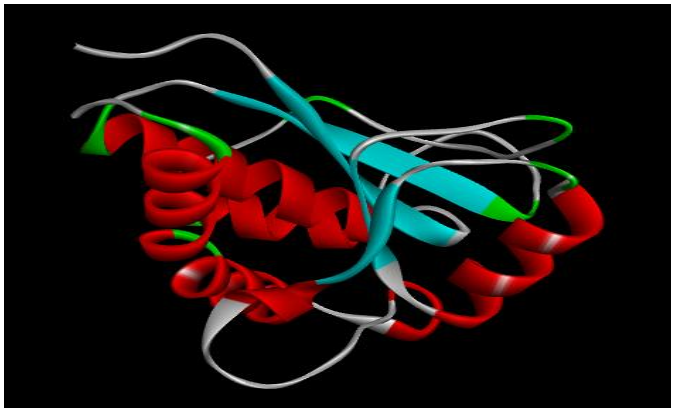

FIG. 1: A SIDE CHAIN AMINO ACID FOR PROTEIN TYROSINE PHOSPHATASE

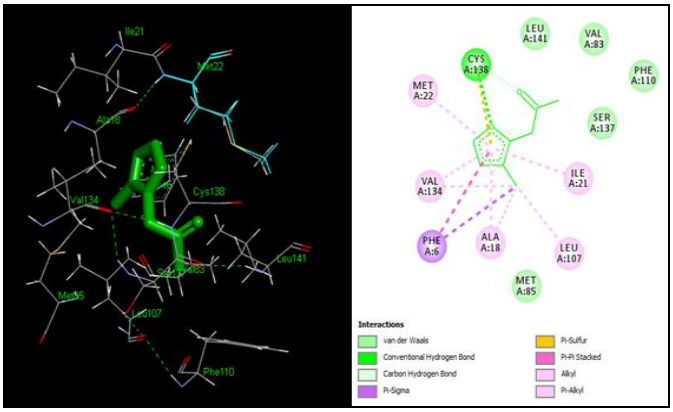

FIG. 2: 3D AND 2D INTERACTIONS OF DOCKED CONFIRMATION IN 3-METHYL-2-(2-OXOPROPYL)FURAN

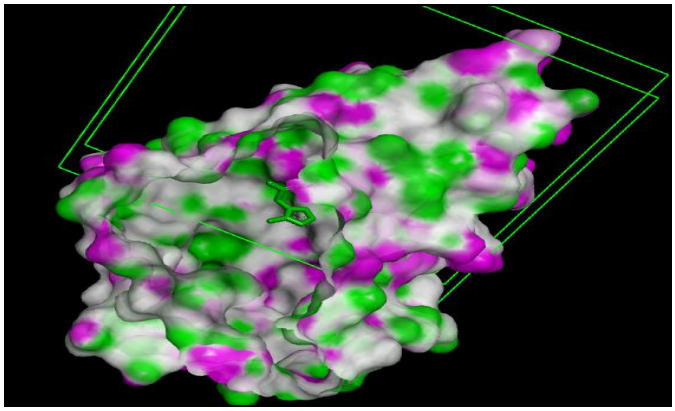

FIG. 3: SURFACE INTERACTIONS OF DOCKED CONFIRMATION IN 3-METHYL-2-(2-OXOPROPYL) FURAN

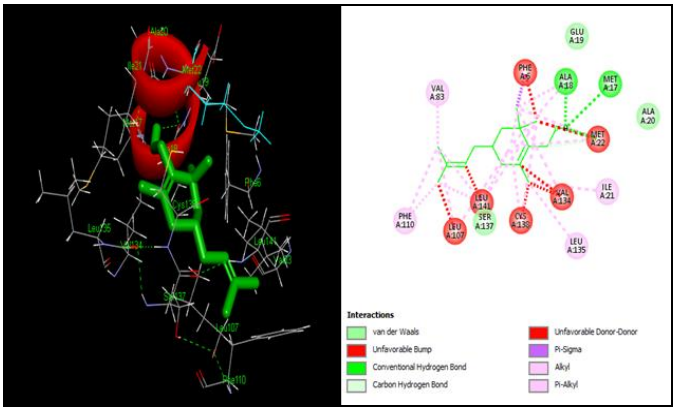

FIG. 4: 2D AND 3D DOCKED CONFIRMATION OF 1,3,3-TRIMETHYL-2-HYDROXYMETHYL-3,3-DIMETHYL-4(3-METHYLBUT-2-ENYL)-CYCLOHEXENE

CONCLUSION: *Rhizopora mucornata* is traditionally used against diabetes, anti-inflammatory and anti pyrogenic. The bioactive compound 3-methyl-2-(2-oxopropyl) furan shows better binding energy with hydrogen binding atoms. The bioactive compounds were screened for Lipinski rule of five and ADMET properties. Thus the bioactive compounds partially inhibit the virulent enzymes that lead to novel discovery of plants against drug compounds. The docking analysis determines the novel drug discovery and also discovery of modules.

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CONFLICTS OF INTEREST: Nil

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