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Research Article

A Structure Based Molecular Docking of Acacia Catechu Against Contractile Protein *Plasmodium falciparum* – A Malarial Disease

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ABSTRACT

The bioactive compounds of *Acacia catechu* using gas chromatography-mass spectroscopy and the inhibitory activity against contractile protein *Plasmodium falciparum* against the protozoan disease were studied. This research mainly focuses on finding novel drug screening against the malarial enzyme. The compounds of *Acacia catechu* are screened using Lipinski rule of five with absorption distribution metabolism excretion (ADMET) properties in which the character, as well as behavior of the drug compound, is known. The compounds were checked for its dosage level in human and rat as well as distribution properties in the blood-brain barrier and central neuro system. The compounds 9,12,15-Octadecatrienoic acid has a higher affinity with -7.95 Kcal/mol followed by Phthalic acid, butyl 2- pentyl ester -7.35 Kcal/mol and Furo[2,3-d] Pyrimidine-4,6 [5H,7H]-dion -6.24 Kcal/mol were docked using Autodock software. The compound 9,12,15- Octadecatrienoic acid, Phthalic acid butyl 2- pentyl ester, Furo[2,3-d] Pyrimidine-4,6 [5H,7H]-dion has higher affinity such as -7.95 Kcal/mol, -7.35 Kcal/mol and -6.24 Kcal/mol, respectively. Thus this research proves that the drug compounds of *Acacia catechu* have novel therapeutic drug activity against virulent enzymes.

INTRODUCTION

Actin is the favorable macromolecule of microfilaments that mainly possess essential roles in central processes within the cell system, as well as transport, cellular division, and motility. The first biological activity of simple protein is its chemical process to create filaments that may generate force at cell membranes or act as staging structures or tracks for motor proteins.^[1,2] These filaments area unit on a timer supported the reaction of tightly certain nucleotide, the formation of intermediate ADP that is an inorganic phosphate (Pi) simple protein, and at last, the discharge of Pi. The physiological tightly certain power ion coordinating the certain ester in simple protein is Mg^{2+} . However, simple protein is sometimes pure within the calcium-bound category that features a higher crucial concentration of chemical process.^[3,4] The actins present in plasmodium have short filaments that contain a

noncanonical link between nucleotide molecules; however, some microfilaments that constrain structural factors are unknown. The situation of this supermolecule contains metallic ions throughout the reaction by exploiting the phosphate cluster that correlates with three-letter amino acids like essential amino acid, lysine, and amino alkanic acid and essential amino acid.^[5] The loops of the tertiary supermolecule square measure are mainly connected with the simple protein protomer that links the inner and outer domain. Sarcomeres square measure divided into units that square measure derived by I bands and also the unit of measurement bisected by Z discs and A bands with a dark M in the middle. I bands accommodate skinny protein filaments, tropomyosin, and troponin. Thick filaments unit of measurement created from simple protein.^[6] The A band consists of overlapping skinny with thick filaments and various proteins. *Acacia catechu* (Wild or

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Khair) belongs to a family Mimosaceae, this plant contains herbal remedies and is used as ayurvedic medicine. The medicinal character in plant helps to cure stomach and gastrointestinal diseases. Antioxidant properties are also reported from both extract (Wild and Khair) rather than an anti-cognitive disorder, anti-acetylcholinesterase, and anti-schizophrenic reports were not available.^[7]

Phytochemical screening

The biochemical studies show the presence of phytochemicals like resins, saponins, flavonoids, alkaloids, steroids, glycosides, protein, and carbohydrate.^[8,9] The physiochemical parameters like ash content, soluble acid ash, water-soluble ash, water-soluble extractives, volatile oil, fiber content, and total sugar were analyzed in which various factors like CO_3^{2-} , PO_4^{3-} , SO_4^{2-} , AL^{3+} , Ca^{2+} , Mg^{2+} , and K^+ were found to be positive.^[10] The flavonoids and the tannins present in the plant plays a major role as an inhibitory factor against virulent enzymes. This plant has fluorescence behavior of different extracts of *Acacia catechu* with extractives like petroleum ether, benzene, acetone, etc.^[11]

MATERIALS AND METHODS

Biologically Active Compounds of *Acacia Catechu* by Using Gas Chromatography–Mass Spectrometry (GCMS)

The biologically active compounds of the *Acacia catechu* were analyzed using GCMS, and the peaks were compared using WILEY and NIST libraries. The major components found in the hydroethanolic leaf extract were Benzenamine, 3 ethoxy, 2Methyl-1,2,3,4-tetrahydro betacarboline, 1-Methoxy-4-(4-Methoxy benzene), 2-naphthalenamine, phthalic acid, 6-ethyl-3-octyl butyl ester, phthalic acid, butyl 2-pentyl ester, hexadecanoic acid, ethyl ester, 12-methoxy19-norpo docarpa, furo[2,3-d] pyrimidine-4,6

[5H,7H]-dion, Phytol 9,12,15-octadecatrienoic acid, butylphosphoric acid, di(4-methoxy benzene) and 2-pyridine carbonitrile, 1,2,5,6.^[12] The phytochemicals have better antioxidant activities against several diseases due to the presence of various phytochemicals. The compounds were analyzed using the Lipinski rule of five in which various parameters were checked like hydrogen bond acceptor and donor, molecular weight, lipophilicity and molar refractivity.

Preparation of Contractile Protein

The three-dimensional (3-D) structure of the contractile protein were taken from the protein data bank ID is 6I4L as shown in Fig. 1 with active site presentation. The protein, along with actin, is responsible for causing disease like *Plasmodium falciparum* that consists of virulent malarial strain. This disease plays an important role in suppressing the immunity system by interfering with phagocytic functions of macrophage. The contractile protein gets precipitated at pH 5 in which the malaria strain gets activated in smooth muscles. The protein stored in the database is at a resolution of 1.83 Å at X-ray diffraction method. The protein mainly consists of A chain comprises of 378 amino acids. The three-letter coding active sites of amino acids in *Plasmodium falciparum* are shown in Fig. 1. The sequence of amino acid in protein is mainly responsible for stabilizing the macromolecules of the mutant protein to induce the protozoan enzyme.^[13,14]

Absorption Distribution Metabolism Excretion ADMET Properties

The physiochemical properties like ADMRT were screened with the bioactive compounds of *Acacia catechu* determined from GCMS. These property plays a major role to analyze the behavior and characteristic of drug materials like water absorption level, gastrointestinal

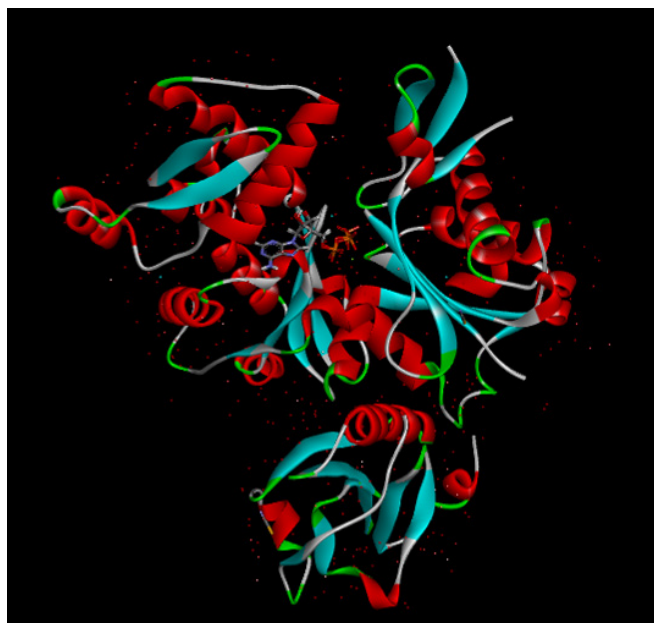
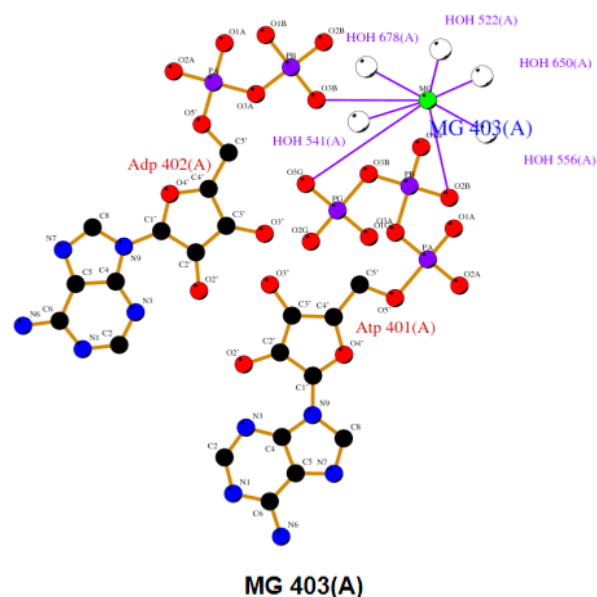


Fig. 1: Three letter coding active sites of amino acids

absorption, the penetration level of drug molecules in the central nervous system, and blood-brain barrier. The hepatoprotective and skin permeability measures were also analyzed for both humans and rats. The ADMET properties were analyzed using the software <http://www.sib.swiss> for calculating the behavior of drug compounds that directly based on the principle of the vector-based algorithm.^[15,16]

Molecular Docking Using Autodock 4.2.6

The software Autodock 4.2.6 is mainly used for protein-ligand docking in which compounds will be rigid like structure. The parameters utilized for the process of docking will be a genetic algorithm in which the output file format will be of the Lamarckian genetic algorithm. The software can able to perform protein-protein interactions and ligand-protein interactions for showing better potential activity against virulent enzymes. The grid points for the total map were 64,000, with grid spacing 0.375 Å (default). The grid size set as default was 20 Å. The center grid box sizes in the protein sequence were centered as x center: -16.302, y center: -23.34, and -16.245, respectively.

RESULTS AND DISCUSSION

The biologically active compounds of *Acacia catechu* were confirmed using Lipinski rule of five to determine the drug properties. The bioactive compound that satisfies

the lipinski rule of five are benzenamine, 3-ethoxy, 12-methoxy19-norpo docarpa, furo[2,3-d] pyrimidine-4,6 [5h,7h]-dion, 2methyl-1,2,3,4-tetrahydro beta-carboline, 1-methoxy-4-(4-methoxy benzene), phthalic acid, butyl 2-pentyl ester, 9,12,15-octadecatrienoic acid, butylphosphoric acid, di(4-methoxy benzene) and 2-pyridine carbonitrile, 1,2,5,6 are listed in Table 1.

Absorption Distribution Metabolism Excretion (ADMET) Properties

The compounds that mainly satisfy the Lipinski rule of five were screened for ADMET for better identification of potential activity. The absorption properties of the drug were analyzed in which the water solubility of the drug molecule, glycoprotein inhibitor and substrate, gastrointestinal absorption, and skin permeability was shown in Table 2. The distribution properties that include the permeability level of the blood-brain barrier (BBB) and central nervous system (CNS) were shown in Table 3. The metabolism properties of the drug compounds have better-promising parameters under cytochrome p450 which, as shown in Table 4. The excretion and toxicity level was analyzed in which the dosage level of the drug compound was tabulated in Tables 5 and 6 along with hepatotoxicity test and skin sensation.^[15-17]

Molecular Docking Studies

The docking analysis was done against virulent enzyme *Plasmodium falciparum*, which was compared with the

Table 1: Compounds analyzed in lipinski rule of five

Compound	Mass of compounds	Hydrogen bond donor	Hydrogen bond acceptor	LOGp	Molar refractivity
Benzenamine, 3 ethoxy	193	0	2	2.93	61.17
12-Methoxy19-norpo docarpa	244	1	1	5.18	73.96
Furo[2,3-d] pyrimidine-4,6 [5h,7h]-dion	196	0	5	0.50	43.55
2Methyl-1,2,3,4-tetrahydro betacarboline	186	1	1	2.15	58.33
2-Naphthalenamine	297	2	3	5.99	96.48
Phthalic acid, 6-ethyl-3-octyl butyl ester	362	0	4	5.79	104.4
1-Methoxy-4-(4-methoxy benzene)	212	0	4	1.74	55.69
Phthalic acid, butyl 2-pentyl ester	292	0	4	3.99	81.43
Hexadecanoic acid, ethyl ester	284	0	2	6.03	86.94
Phytol	296	1	1	6.3	95.56
9,12,15-Octadecatrienoic acid	278	1	2	5	86.89
Butylphosphoric acid, di(4-methoxy benzene)	172	4	5	-0.149	36.25
2-Pyridine carbonitrile, 1,2,5,6	104	0	2	0.95	28.95

Table 2: Absorption properties of compounds

Compound	Water solubility (log mol/L)	CaCo ₂ permeability (Log P _{abb} in 10 ⁻⁶ cm/Sec)	GI absorption (%)	Skin permeability (Log Kp)	P-glycoprotein substrate	P-glycoprotein I inhibitor
Benzenamine, 3-ethoxy	-1.643	1.453	93.28	-2.969	No	No
Furo[2,3-d] pyrimidine-4,6 [5h,7h]-dion	-1.429	0.797	98.14	-2.683	No	No
2Methyl-1,2,3,4-tetrahydro betacarboline	-2.64	1.276	93.76	-2.617	Yes	No
1-Methoxy-4-(4-methoxy benzene)	-1.766	1.633	95.91	-1.397	No	No
Phthalic acid, butyl 2-pentyl ester	-4.594	1.639	94.19	-2.649	No	No
9,12,15-Octadecatrienoic acid	-5.787	1.577	92.83	-2.722	No	No
Butylphosphoric acid, di(4-methoxy benzene)	-0.11	-0.61	54.01	-3.504	No	No
2-Pyridine carbonitrile, 1,2,5,6	-2.208	1.635	97.06	-2.817	No	No



Table 3: Distribution properties of compounds

Compounds	VDss (human) (Log L/kg)	Fraction unbound (human) (Fu)	BBB permeability (Log BB)	CNS permeability (Log PS)
Benzenamine, 3-ethoxy	0.322	0.463	0.324	-2.139
Furo[2,3-d] pyrimidine-4,6 [5h,7h]-dion	-0.343	0.614	-0.638	-2.92
2Methyl-1,2,3,4-tetrahydro betacarboline	0.914	0.375	0.356	-1.491
1- Methoxy-4-(4-methoxy benzene)	0.166	0.382	0.469	-1.814
Phthalic acid, butyl 2- pentyl ester	0.053	0.107	-0.066	-2.406
9,12,15- Octadecatrienoic acid	-0.617	0.056	-0.115	-1.547
Butylphosphoric acid, di(4-methoxy benzene)	-0.708	0.746	-1.135	-3.941
2-Pyridine carbonitrile, 1,2,5,6	-0.207	0.638	-0.277	-2.746

Table 4: Metabolism properties of compounds

Compound	CYP2D6 substrate	CYP3A4 substrate	CYP1A2 inhibitor	CYP2C19 inhibitor	CYP2C9 inhibitor	CYP2D6 inhibitor	CYP3A4 inhibitor
Benzenamine, 3-ethoxy	No	No	No	No	No	No	No
Furo[2,3-d] pyrimidine-4,6 [5h,7h]-dion	No	No	No	No	No	No	No
2Methyl-1,2,3,4-tetrahydro betacarboline	Yes	Yes	Yes	No	No	Yes	Yes
1-Methoxy-4-(4-methoxy benzene)	No	No	No	No	No	No	No
Phthalic acid, butyl 2-pentyl ester	No	Yes	Yes	Yes	No	No	No
9,12,15-Octadecatrienoic acid	No	Yes	Yes	No	No	No	Yes
Butylphosphoric acid, di(4-methoxy benzene)	No	No	No	No	No	No	No
2-Pyridine carbonitrile, 1,2,5,6	No	No	No	No	No	No	No

Table 5: Toxicity and excretion properties of compounds

Compound	Renal OCT2 substrate	AMES toxicity	Max. tolerated dose (human) (Log mg/kg/day)	hERG 1 inhibitor	Oral rat acute toxicity (LD50) (mol/kg)	Oral rat chronic toxicity (LOAEL) (Log mg/kg)	Liver Toxicity	Skin sensitization
Benzenamine, 3 ethoxy	No	No	0.548	No	2.201	1.735	No	Yes
Furo[2,3-d] pyrimidine-4,6 [5h,7h]-dion	No	No	1.361	No	2.765	2.111	Yes	No
2Methyl-1,2,3,4-tetrahydro beta-carboline	Yes	Yes	-0.018	No	2.76	1.603	No	Yes
1- Methoxy-4-(4-methoxy benzene)	No	No	0.905	No	1.822	2.007	No	Yes
Phthalic acid, butyl 2- pentyl ester	No	No	1.531	No	1.748	2.384	No	No
9,12,15- Octadecatrienoic acid	No	No	-0.84	No	1.441	3.115	Yes	Yes
Butylphosphoric acid, di(4-methoxy benzene)	No	No	1.555	No	1.943	2.25	No	No
2-Pyridine carbonitrile, 1,2,5,6	No	No	1.092	No	2.336	1.603	No	Yes

standard drug as control. When compared with standard drug the bioactive compounds have a high affinity towards the virulent enzymes. The binding energy of each ligand molecule is listed along with the types of interactions like hydrogen and vander Waals interaction. The active site of the enzymes was docked in which the compound 9, 12, 15-octadecatrienoic acid has higher affinity with -7.95 Kcal/mol followed by Phthalic acid, butyl 2-pentyl ester -7.35 Kcal/mol and Furo [2,3-d] pyrimidine-4,6 [5H,7H]-dion -6.24 Kcal/mol. The total number of residues interacted between ligand and virulent protein are LYS 19, ASN 17, GLY 16, ASP 158, GLY 303, GLY 302, VAL 340, ASP 155, GLY 14, SER 15, GLY 159, TYR 338, GLY 157, VAL 31, GLN 138, LYS 337, GLY 308, LYS 19, SER 15, ASP 158, ASN 17, GLY 14, GLY 16, ARG 336, SER 142, SER 301, SER 339,

LYS 337, TYR 338, ASP 12, ASP 155, VAL 340, HIS 162, GLY 157, SER 161, VAL 160, GLY 75, GLY 302, SER 136, GLY 129, HIS 162, GLN 138, SER 15, ASP 158, ASN 13, ALA 109, GLY 75, PRO 110, ASP 155, ALA 139, SER 161, VAL 160, SER 156, GLY 157, GLY 16, GLY 159, ASN 13. *Acacia catechu* has greater inhibitory activity against malaria disease by interfering with a normal habitat of the human body. These compounds do not have any toxic factors which have been evaluated using Lipinski rule of five and ADMET properties. The Table 6 and Figs. 2 to 4 shows detailed information about the active amino acids involved in structure-based drug design with pictorial representation. The structure-based drug design strategy plays a major role in designing the potential drug against the virulent protein.

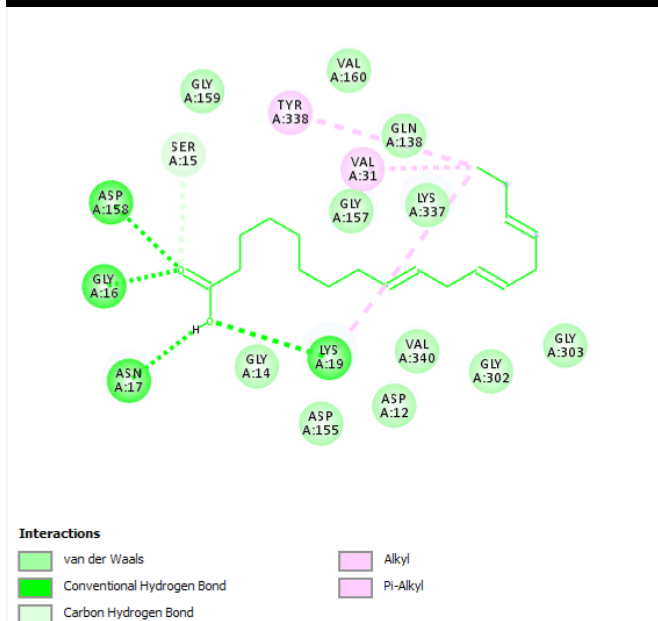
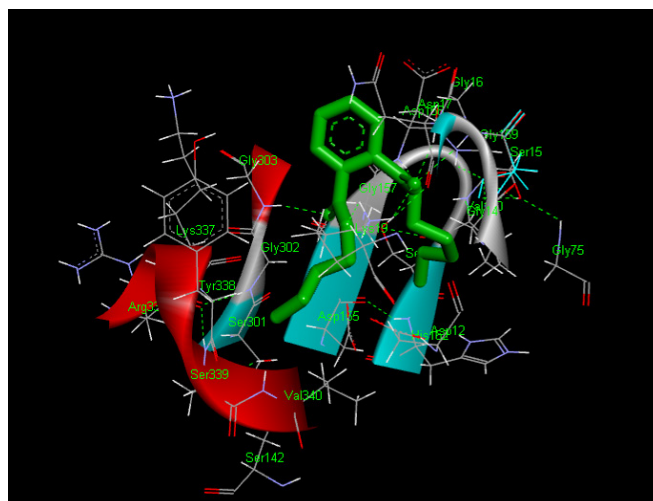
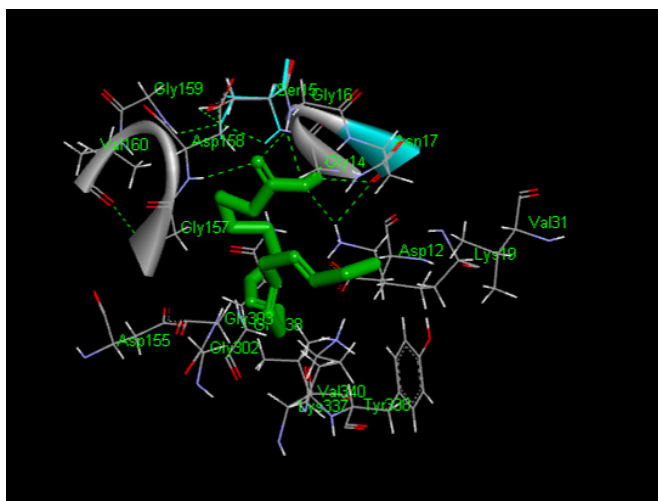


Fig. 2: 2D and 3D interactions of 9,12,15-octadecatrienoic acid

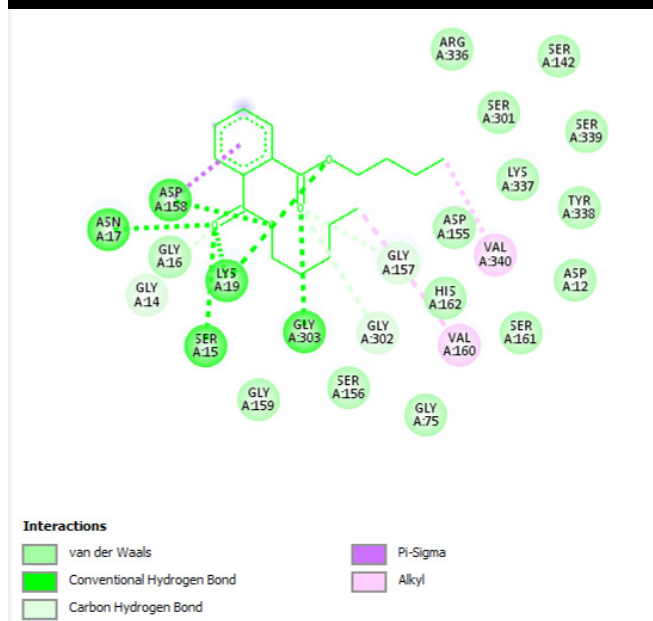


Fig. 3: 2D and 3D interactions of phthalic acid, butyl 2-pentyl ester

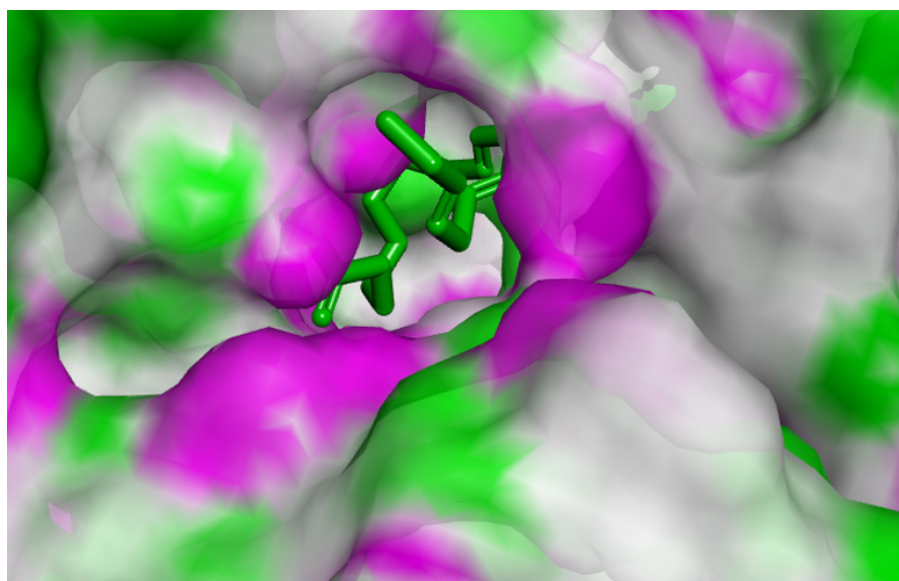


Fig. 4: Surface image of 9,12,15-octadecatrienoic acid



Table 6: Interactions of various bioactive compounds

Compound	Binding energy Kcal/mol	Vanderwaals interaction	No. of hydrogen bonds	Hydrogen interactions	Total no. of residues
Benzenamine, 3-ethoxy	-5.17	ASP 155, LYS 19, ASN 17, ASP 158, GLY 16, GLY 14, GLY 157, GLY 159, GLY 75, ASN 13, GLN 138, SER 161, HIS 162, VAL 160	1	SER 15	SER 15, ASP 155, LYS 19, ASN 17, ASP 158, GLY 16, GLY 14, GLY 157, GLY 159, GLY 75, ASN 13, GLN 138, SER 161, HIS 162, VAL 160
Furo[2,3-d] Pyrimidine-4,6 [5H,7H]-dion	-6.24	ASN 13, ALA 109, GLY 75, PRO 110, ASP 155, ALA 139, SER 161, VAL 160, SER 156, GLY 157, GLY 16, GLY 159, ASN 13	4	HIS 162, GLN 138, SER 15, ASP 158	HIS 162, GLN 138, SER 15, ASP 158, ASN 13, ALA 109, GLY 75, PRO 110, ASP 155, ALA 139, SER 161, VAL 160, SER 156, GLY 157, GLY 16, GLY 159, ASN 13
2Methyl-1,2,3,4-tetrahydro betacarboline	-6.23	TYR 338, GLY 302, GLY 157, VAL 160, ASP 158, SER 15, GLY 75, GLY 14, LYS 19, ASN 133, GLN 138, THR 107, VAL 340, LYS 337	1	ASP 12	ASP 12, TYR 338, GLY 302, GLY 157, VAL 160, ASP 158, SER 15, GLY 75, GLY 14, LYS 19, ASN 133, GLN 138, THR 107, VAL 340, LYS 337
1-methoxy-4-(4-Methoxy benzene)	-5.41	GLY 157, ASN 13, GLN 138, GLY 75, VAL 160, GLY 159, GLY 14, ASP 158, GLY 16, ASN 17, TYR 338, GLY 303, THR 304, GLY 302	2	SER 15, LYS 19	SER 15, LYS 19, GLY 157, ASN 13, GLN 138, GLY 75, VAL 160, GLY 159, GLY 14, ASP 158, GLY 16, ASN 17, TYR 338, GLY 303, THR 304, GLY 302
Pthalic acid, butyl 2-pentyl ester	-7.39	GLY 14, GLY 16, ARG 336, SER 142, SER 301, SER 339, LYS 337, TYR 338, ASP 12, ASP 155, VAL 340, HIS 162, GLY 157, SER 161, VAL 160, GLY 75, GLY 302, SER 136, GLY 129	5	GLY 308, LYS 19, SER 15, ASP 158, ASN 17	GLY 308, LYS 19, SER 15, ASP 158, ASN 17, GLY 14, GLY 16, ARG 336, SER 142, SER 301, SER 339, LYS 337, TYR 338, ASP 12, ASP 155, VAL 340, HIS 162, GLY 157, SER 161, VAL 160, GLY 75, GLY 302, SER 136, GLY 129
9,12,15-octadecatrienoic acid	-7.95	GLY 303, GLY 302, VAL 340, ASP 155, GLY 14, SER 15, GLY 159, TYR 338, GLY 157, VAL 31, GLN 138, LYS 337	4	LYS 19, ASN 17, GLY 16, ASP 158	LYS 19, ASN 17, GLY 16, ASP 158, GLY 303, GLY 302, VAL 340, ASP 155, GLY 14, SER 15, GLY 159, TYR 338, GLY 157, VAL 31, GLN 138, LYS 337
2-pyridine carbonitrile, 1,2,5,6	-5.06	TYR 338, LYS 337, SER 142, SER 301, ARG 336, GLY 302, ASP 155, ASP 12, LYS 19	3	TRP 341, SER 339, VAL 340	TRP 341, SER 339, VAL 340, TYR 338, LYS 337, SER 142, SER 301, ARG 336, GLY 302, ASP 155

CONCLUSION

This research work concludes that the structure-based drug designing of molecules against virulent enzymes shows better inhibitory activity. The ligand compounds of *Acacia catechu* were docked against malarial enzyme *Plasmodium falciparum*. They were screened using the Lipinski rule of five and ADMET properties in which the compounds show various properties. The drugs were checked for activities, whether it breaches the blood-brain barrier as well as the central neuro system. Then the satisfied compounds were docked using Autodock software, in which the compounds like 9,12,15-octadecatrienoic acid has a higher affinity with -7.95 Kcal/mol followed by phthalic acid, butyl 2-pentyl ester -7.35 Kcal/mol and Furo[2,3-d] pyrimidine-4,6 [5H,7H]-dion -6.24 Kcal/mol. The inhibition of virulent enzyme leads to the discovery of novel drugs that can be used as a therapeutic agent after several trials. The comprehensive docking provides high accuracy studies. Hence, this research concludes that *Acacia catechu* has better inhibitor potential activity against malarial disease, and the bioactive compounds from *Acacia catechu* have better drug liking properties.

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