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NATURAL ALKALOIDS AS POTENTIAL ANTIMALARIAL DRUGS FROM *BAUHINIA PURPUREA* LEAVES -AN *IN-SILICO* APPROACH

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Bauhinia purpurea alkaloids compounds, Antimalarial receptor protein, ADMET, Molecular Docking, Antimalarial

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ABSTRACT: Malaria is the most important parasitic disease in humans, with transmission occurring in over 100 countries with a population of three billion people. Protozoan parasites of the genus Plasmodium cause it. These parasites are transmitted from one person to another by the female anopheles mosquito. Medicinal plants possess many phytochemicals of great therapeutic value, and many effectively kill malaria parasites. These compounds working by variety of mechanisms and in most of the cases they exhibit their antimalarial potentiality by inhibiting many proteins involved in cell growth and division. Molecular docking is a computational approach which facilitates the finding of the best molecule from a group which may bind with the highest affinity with the intended target by providing a virtual biological system. This process works on the basis of specific algorithm and involves scoring function to rank the molecules that fit with the target. The present study has been designed to investigate the antimalarial potential of seven alkaloid compounds from the leaves of *Bauhinia purpurea.* Three standard antimalarial drugs have been selected and docked against antimalarial receptor protein 6KP2. The results are compared with the alkaloid compounds of *Bauhinia purpurea*. Among them Ombuin a chief molecule from *Bauhinia purpurea* alkaloids derived from leaves shows least binding energies with best docking score among all the chosen compounds and the value was found to be -8.16 Kcal/mol of binding pose energy against antimalarial receptor protein 6KP2 which is more than that of the standard drug. The results supports that *Bauhinia purpurea* leaves exhibits good antimalarial potential because of the presence of Ombuin like alkaloids. Further from ADMET properties of the Analogs is also showing the better result than available drug.

INTRODUCTION: Malaria is considered one of the top three killer mosquito-borne communicable diseases [1]. It affects 400–500 million people leading to approximately 2.5 million deaths annually [2]. It is caused by protozoan parasites of the genus plasmodium. These parasites are transmitted from one person to another by the female anopheles mosquito.

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Plasmodium develops in the mosquito's gut and is passed on in the saliva of an infected insect each time it takes a new blood meal. When an infected mosquito bites a human, the parasite rapidly goes to the liver within 30 min. There the parasite starts reproducing rapidly in the liver. The parasites then enter into red blood cells and reproduce after that bursting; the parasites release and spread in the host's blood.

It is injected by another mosquito and the life cycle continues like this [3]. The malarial parasite depends on humans and mosquitoes to carry out its deadly life cycle. Malaria is complex, but it is a curable and preventable disease [4]. Lives can be saved if the disease is detected early and adequately treated.

It is known what action is necessary to prevent the disease and to avoid or contain epidemics and other critical situations. In view of the overwhelming generation and quick spread of drug-resistant parasites, there is a need to develop new safe and affordable antimalarial agents to overcome the growing malarial resistance against drugs. The rapid spread of resistance to current quinoline antimalarial has made malaria a major global problem [5, 6]. Because a vaccine for malaria is not available, it is essential to find new antimalarial drugs and understand their antimalarial mechanism for treating patients [7, 8]. The drug resistance development against antimalarial medicines such as amodioquine, chloroquine, artemisinin, and anti-folates is turn out to be a severe health issue that stimulates the researcher to synthesize novel antimalarial compounds [9, 10].

Plants are a tremendous source for the discovery of new products of medicinal value for drug development. Today several distinct chemicals derived from plants are more important drugs used in one or more countries worldwide. Many of the drugs used today are simple synthetic modifications or copies of the naturally obtained plant-based extracts and chemicals [11]. Medicinal plants are a very beneficial and important aspect of the indigenous healthcare system in India [12]. In recent years, ayurvedic systems of medicine with special emphasis on bioactive compounds have been of global importance.

Amongst them is *Bauhinia purpurea* (*B. purpurea)* which is a well known plant with versatile therapeutic potential. *Bauhinia purpurea* is one of the plants that has gained interest among researchers as a potential new source of medicinal agents [13]. Orchid tree, *Bauhinia purpurea*, is a tropical evergreen small tree or shrub up to 4-10 m tall and 2m across. It has an erect and slender stem, crooked branches, green leaves and large, purple and orchid-like flowers. It is native to south China and Southeast Asia. The orchid tree exhibits medicinal properties. Its root is carminative, flowers are laxative and the bark, roots and flowers, when mixed with rice water, are used in poultice form as a maturant. It is also a foodplant. The leaves, buds, and young seedpods are cooked and eaten as vegetables. The flower buds can also be pickled and used in curries. Aside from the above mentioned uses of the plant, it also yields a gum. The bark is a source of tannins and fiber used for dyeing. The fine wood is durable and used in carpentry and fuel. Orchid tree is also cultivated as an ornamental tree. Common names are Orchid Tree, Purple butterfly tree, Mountain Ebony, Geranium Tree, and Purple *Bauhinia*. The plant *Bauhinia purpurea* is a moderate evergreen tree used by tribes of India as cattle feed. Various biological activities are ascribed to bauhinia species. *Bauhinia purpurea*a most important species used to treat several ailments in the traditional system of medicine. *Bauhinia purpurea* was reported for its antidiarrhoeal, antimalarial, antidiabetic, anticancer, thyroidgl, and stimulating properties [14].

Bauhinia purpurea was reported for the presence of various phytochemical constituents. It contain glycosides, saponin, phenolic compounds, tannins, flavonoids, fixed oils, fats, proteins, flavones glycoside, fatty acid, tocopherols, cardiac glycosides, carbohydrates, alkaloids, sterol, steroids, flavanones, lutein, beta-sitosterol *etc*., [15-18].

At recent times molecular modeling and computational based studies is the pleasant tool to identify the potent drug. So, we tried our best to find the effective probable agents to treat malaria from the natural alkaloids of *Bauhinia purpurea.* Remarkably, there have been no reports of any antimalarial activity from *Bauhinia purpurea* until now. Therefore, this study aims to identify compounds from the natural alkaloids of *Bauhinia purpurea* as they contain

- 1, 2 - Benzene Dicarboxylicacid Dibutylester,
- 5,6-dihydro-1,7-dihydroxy-3,4-dimethoxy-2-methyldibenzoxepoin,
- 2, 7- dimethoxy – 3 – methyl - 9, 10-dihydrophenanthrene -1, 4dione,
- (2S) - 5, 7 – dimethoxy - 3, 4 – dimethoxy - 2-methyldibenzoxepin,
- Ombuin,
- Quercetin,
- Kaempferol-7,4-dimethylether-3-O-b-D-glucopyranoside,
- Chloroquine,
- Mefloquine,
- Primaquine.

The antimalarial activity of the above alkaloids of *Bauhinia purpurea* leaves is compared with the standard antimalarial drugs. These alkaloids and drugs were docked against the antimalarial receptor protein (PDB ID: 6KP2)

MATERIALS AND METHODS: In molecular modeling, docking is a method that predicts the preferred orientation of one molecule to a second when bound to each other to form a stable complex. This plays a vital role in signal transduction. Schrodinger suit-2019 Maestro 12.2 version is used for molecular docking.

Ligand preparation, Grid generation, Glide docking and 2D and 3D representation of ligand-receptor interaction were obtained using Schrodinger suit-2019 Maestro 12.2 version and the chemical structures of ligands were refined using Chemdraw. Discovery Studio Visualizer was used for the visualization of the structures.

Protein Preparation: The crystal structure of protein PDB ID: 6KP2 obtained from the Protein Data Bank (PDB) and was used in this study.

In general, the protein structures are refined for their bond orders, formal charges and missing hydrogen atoms, topologies, incomplete and terminal amide groups.

The water molecules beyond $5A^{o}$ were removed. The possible ionization states were generated in the protein structure and the most stable state was chosen. The hydrogen bonds were assigned, and orientations of the retained water molecules were corrected [19].

The crystal structure of the prepared protein which was used for the receptor grid construction. The binding box dimensions (within which the centroid of a docked posies confined) of the protein were setto$14A^{o}$ x$14A^{o}$x$14A^{o}$.

Ligand Preparation: The ligand structures were generated in the CDX format using Chem Draw ultra version 12.0. These ligands were then converted to the mol 2 format and the ligands were prepared by Lig Prep module of Maestro in the Schrodinger suite 2019.

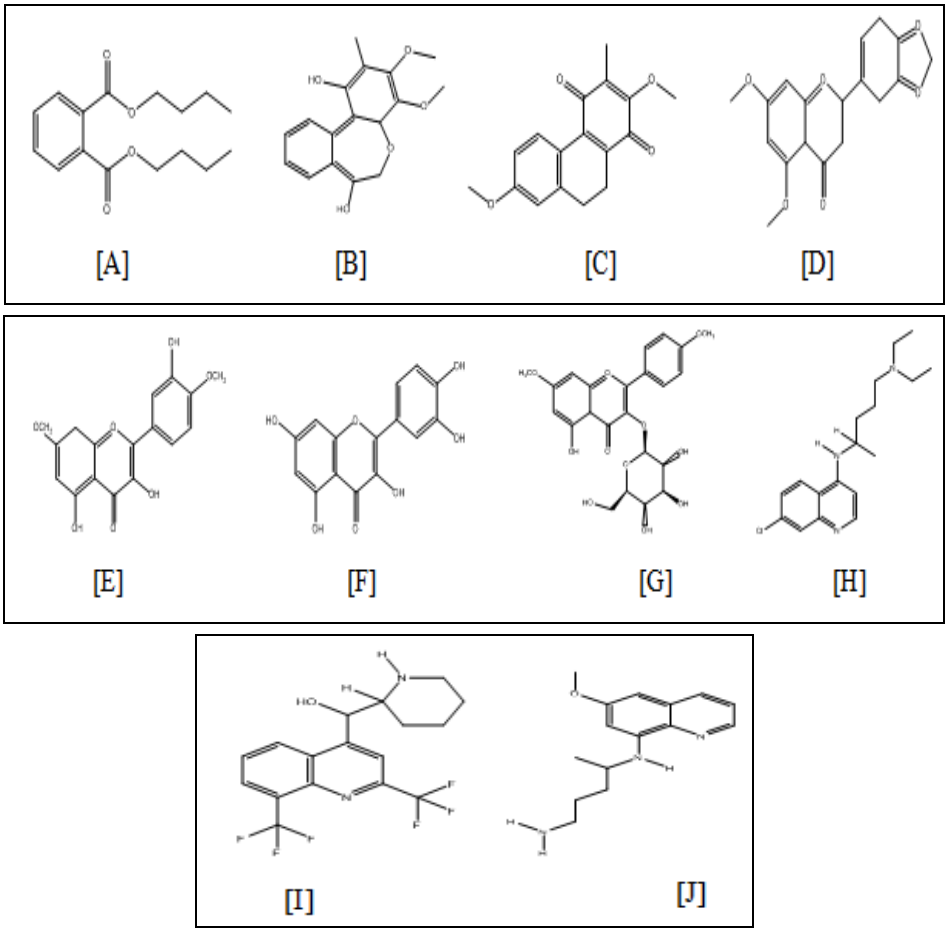


FIG. 1: CHEMICAL STRUCTURES OF THE LIGANDS AND DRUGS

They were converted from 2D to 3D structures by including stereochemical, ionization, tautomeric variations, as well as energy minimization and optimized for their geometry, desalted and corrected for their chiralities and missing hydrogen atoms [20, 21].

The bond orders of these ligands were fixed and the charged groups were neutralized. The ionization and tautomeric states were generated between pH of 6.8 to 7.2 using Epik module. A single low-energy ring confirmation per ligand was generated and the optimized ligands were used for docking analysis.

Glidelig and Docking: The glide docking of the designed molecules was carried out using the receptor grid and the ligand molecules. The favourable interactions between ligand molecules and the receptor were scored using Glide module of ligand docking program. All the docking calculations were performed using extra precision (XP) mode. The docking process was run in a flexible docking mode which automatically generates conformations for each input ligand.

The ligand poses generated were passed through a series of hierarchal filters that evaluate the ligand's interaction with the receptor. The spatial fit of the ligand to the defined active site and examines the complementarily of the ligand-receptor interactions using grid-based method by the empirical Chem Score function. This algorithm recognizes favourable hydrogen bonding, hydrophobic, and metal-ligation interactions and penalizes steric clashes. Poses that pass these initial screens enter the final stage of the algorithm, which involves valuation and minimization of grid approximation OPLS non-bonded ligand-receptor interaction energy [22].

Finally, the minimized poses were re-scored using Glide Score scoring function. The XP-Glidescore of active compounds were summarized and the fitness scores for each ligand are compared.

ADMET Property Analysis: The *in-silico* ADME properties of the proposed compounds were determined by quikprop of Schrodingers of twaremaestro 12.2 version. The quikprop module of Schrodinger is a quick, accurate, easy-to-use absorption, distribution, metabolism and excretion (ADME) prediction program design to produce certain descriptors related to ADME [23]. It predicts both significant physicochemical descriptors and pharmacokinetic ally relevant properties. ADME properties determine the drug-like activity of ligand molecules based on Lipinski's rule of five.

RESULTS AND DISCUSSION: The phytoconstituents of *Bauhinia purpurea* taken for the comparative computational docking studies are the seven alkaloids compounds [A to G] and to compare their activity with the three standard antimalarial drugs such as [H to J]. These alkaloids and drugs were docked against the antimalarial receptor proteins (PDB ID: 6KP2) and analyzed for antimalarial potential.

TABLE 1: GLIDE SCORE USING SCHRODINGER SOFTWARE

Antimalarial receptor							
PDB ID: 6KP2							
Compound code	**Compound Name**	**GSore**	**DockScore**	**Lipophilic EvdW**	**PhobEn**	**HBond**	**Electro**
[A]	1,2-BenzeneDicarboxylicacidDibutylester	-4.17	-4.17	-4.26	0	-0.7	-0.1
[B]	5,6-dihydro-1,7-dihydroxy-3,4-dimethoxy-2-methyldibenzoxepoin	-3.65	-3.05	-0.55	0	-1.64	-0.64
[C]	2,7-dimethoxy-3-methyl-9,10-dihydrophenanthrene-1,4dione	-1.44	-1.44	-1.24	0	-1.02	-1.02
[D]	(2S)-5,7-dimethoxy-3,4-dimethoxy-2-methyldibenzoxepin	-4.52	-4.52	-3.5	0	-0.64	0.01
[E]	Ombuin	-8.16	-8.15	-2.38	0	-4.29	-1.16
[F]	Quercetin	-6.16	-6.12	-2.55	0	-2.41	-0.78
[G]	Kaempferol-7,4-dimethylether-3-O-B-D-glucopyranoside	-4.31	-4.31	-1.14	0	-3.11	-1.06
[H]	Chloroquine	-3.14	-1.47	-4.53	0	-0.02	-0.09
[I]	Mefloquine	-1.17	-1.17	-0.58	0	-0.7	-0.41
[J]	Primaquine	-5.57	-5.57	-2.69	0	-1.94	-0.89

The best-simulated results among all the compounds were evaluated based upon the glide score given in **Table 1,** which were docked using the module Maestro 12.2 version of the Schrodinger Software.

The **Table 1** shows the G-score, number of hydrogen bonds, interacting residues, H-bond distance and glide or binding energy of all the molecules. The results we obtained from the docking studies revealed that the compounds from leaves of *Bauhunia purpureaie* the natural products have very low binding pose energies when compared to the standard antimalarial drugs. Especially, [E] Ombuin a versatile molecule from *Bauhinia purpurea* alkaloids shows best score among all the chosen compounds and it was found to be -8.16 Kcal/mol of binding pose energy against antimalarial receptor protein 6KP2.

The other six *Bauhinia purpurea* alkaloids compounds also have better binding pose energies with the antimalarial receptor protein than the three standard drugs [H-J].

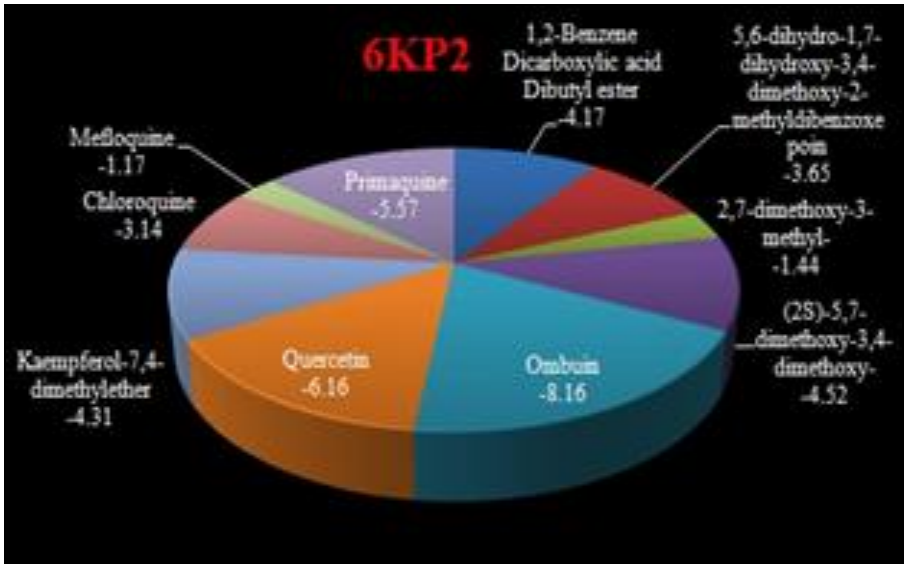


FIG. 2: GRAPHICAL REPRESENTATION OF COMPARATIVE GLIDE SCORE OF LIGAND & PROTEIN BINDING

ADMET Properties: For preliminary identification, docking studies were done to predict the physiochemical drug absorption and drug-likeness using a program ADMET (Adsorption, Distribution, Metabolism, Excretion and Toxicity). Drug likeness test was carried out using Lipinski rule of five and Jorgensen's rule of three.

Quikprop tools of Schrödinger software suit were used to predict the ADMET properties of eight alkaloids compounds from leaves of *Bauhinia purpurea* natural products and two anticancer drugs. The output of Quikprop gave several principal descriptors and ADMET properties as shown in **Table 2**.

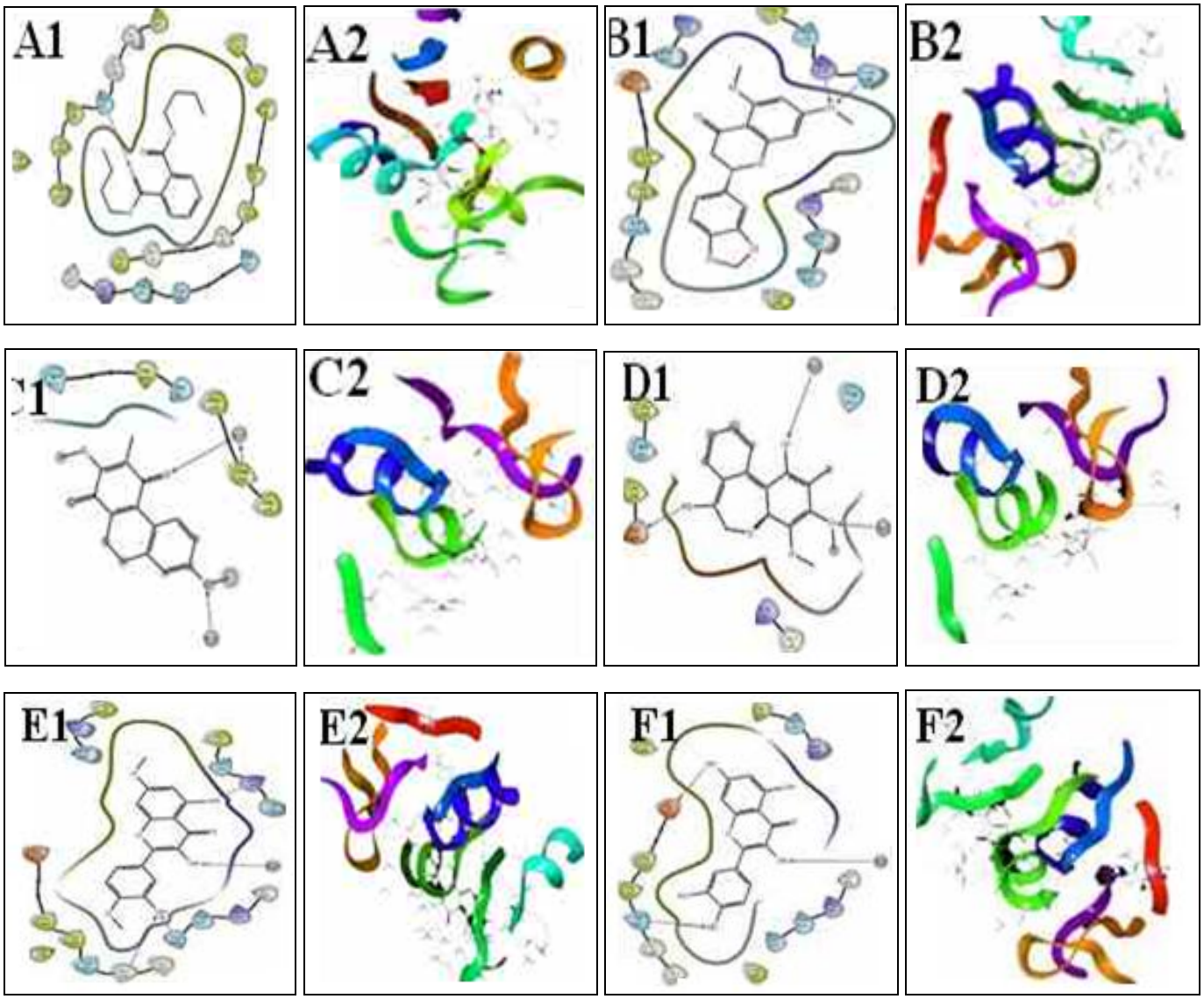
Various other physicochemical properties such as molecular weight, nonpolar and polar surface area, water solubility, logP, which are represented by different descriptors were calculated. Molecular lipophilicity is usually quantified as logP and aqueous solubility is usually defined as logS. SASA (Total solvent accessible surface area) for eight alkaloids compounds from leaves of *Bauhunia purpurea* natural products and two anticancer drugs gave the value in the range between 513.596 to 694.98 which came under the standard range (300-1000).

FASA, (Hydrophobic Component of SASA), FISA (Hydrophliic Component of SASA), PISA (π component of SASA), QP Polrz (Predicted polarizability), QPlogPoct (Predicted octane/gas partition coefficient, QPlogPo/w (Predicted octane/water partition coefficient) and QlogS (Predicted aqueous solubility) [24] are the other descriptors which were studied. Ideal ranges of various descriptors were calculated with reference to 95% of the drug presented in **Table 2,** and various descriptors of compound [E] are found to be in the ideal range.

Antimalarial receptors are overexpressed in about 70% of all Malaria diseases. The seven alkaloid compounds of *Bauhinia purpurea* [A to G] interfering with the binding of Antimalarial receptor and to compare their activity with the three standard antimalarial drugs such as [H to J] [25-28]. These alkaloids and drugs were docked against the antimalarial receptor proteins (PDB ID: 6KP2).

TABLE 2: ADMET TEST RESULTS

Properties	A	B	C	D	E	F	G	H	I	J	Standard Value
Mol_MW	278.347	302.326	284.311	328.321	330.293	302.24	476.436	319.876	378.317	259.35	130-725
Dipole	5.447	2.299	3.4	3,437	5.471	5.375	8.783	6.186	6.832	1.714	1.0-12.5
SASA	627.838	513.596	516.004	548.582	567.473	517.335	694.98	666.03	583.958	544.536	300-1000
FOSA	387.578	277.152	330.143	301.732	185.414	0	270.933	374.546	190.617	276.381	0-750
FISA	83.226	70.849	74.359	45.909	180.561	285.844	238.001	23.084	53.523	74.135	7-330
PISA	157.033	165.596	111.502	200.942	201.498	231.491	186.046	196.801	120.156	194.021	0-450
QPlogKp	-1.732	-1.858	-2.305	-1.466	-3.657	-5.492	-4.29	-2.546	-3.857	-3.593	-8-1.0
QPpolrz	32.57	29.198	29.702	33.202	31.48	27.516	41.616	36.491	34.118	28.435	13-70
QPlogPC16	9.691	8.881	7.963	8.976	10.344	10.739	14.263	11.161	7.986	9.383	4-18
QPlogPoct	12.502	14.631	12.398	13.735	16.511	18.657	27.724	15.524	17.497	15.125	8-35
QPlogPw	5.04	9.24	7.201	7.941	10.681	14.41	20.733	6.483	8.787	9.397	4-45
QPlogPo/w	3.859	2.629	2.114	2.725	2.05	0.384	0.539	4.613	3.874	2.206	-2-6.5
QPlogS	-4.594	-3.328	-2.983	-3.277	-3.913	-2.88	-3.085	-4.733	-4.547	-2.433	-6.5-0.5
CIQPlogS	-3.488	-4.03	-3.269	-4.323	-4.751	-4.043	-4.671	-3.663	-4.719	-2.389	-6.5-0.5
DonorHB	0	2	0	0	2	4	4	1	2	3	0-6
AcceptanceH B	4	4.7	5.5	5.75	5.25	5.25	13	4	4.2	3.75	2-20
Rule of Five	0	0	0	0	0	0	1	0	0	0	max 4



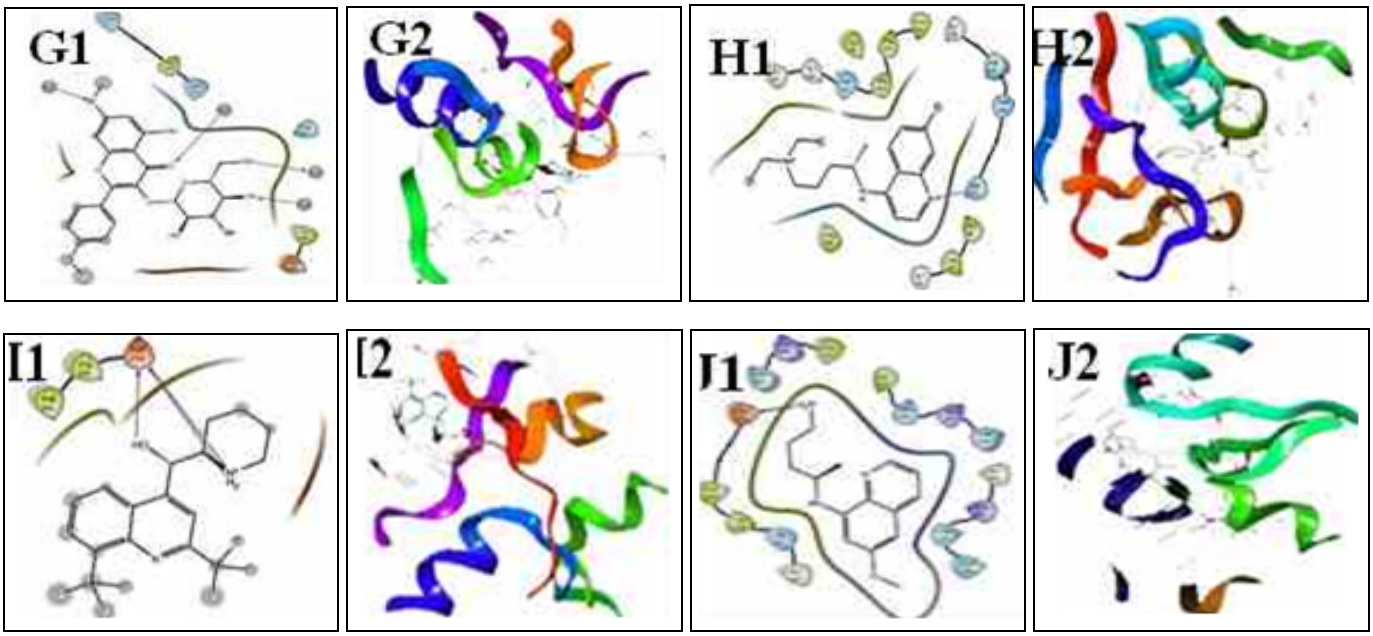


FIG. 3: LIGAND INTERACTION OF *BAUHINIA PURPUREA* LEAVES ALKALOIDS [A1-G1], STANDARD ANTIMALARIAL DRUGS, [H1-J1] AND BINDING MODEL OF *BAUHINIA PURPUREA* LEAVES ALKALOIDS [A2-G2], STANDARD ANTIMALARIAL DRUGS [H2-J2] AGAINST 6KP2

CONCLUSION: The Protein-Ligand interaction plays a significant role to identity structural-based drug designing. The present study from natural alkaloids of *Bauhinia purpurea* leaves were chosen compounds [A to G]*ie.*, [A] 1,2-Benzene Dicarboxylicacid Dibutylester, [B] 5,6-dihydro-1,7-dihydroxy-3,4-dimethoxy-2-methyldibenzoxepoin, [C] 2, 7 – dimethoxy – 3 – methyl - 9, 10-dihydrophenanthrene-14dione, [D](2S)-5,7-dimethoxy-3,4-dimethoxy-2- methyldibenzoxepin, [E] Ombuin, [F] Quercetin, [G] Kaempferol-7,4-dimethylether-3-O-b-D-glucopyranoside. The antimalarial potential were analysed by molecular modelling tool in *Bauhinia purpurea* leaves and the results were compared with the standard antimalarial drugs such as [H] Chloroquine, [I] Mefloquine and [J] Primaquine. These alkaloids and drugs were docked against the antimalarial receptor proteins (PDB ID: 6KP2). The results suggest that compound [E] is a highly potential compound responsible for the antimalarial activity of *Bauhinia purpurea* leaves against the protein 6KP2, an antimalarial receptor. It shows the least binding energies with the best docking score among all the chosen compounds, and the value was found to be -8.16 Kcal/mol of binding pose energy against antimalarial receptor protein 6KP2, which is more than that of the standard drug and appears to be an attractive compound for the development of new antimalarial agents. These findings provide more evidence to support the traditional use of *Bauhinia purpurea* leaves extract for malaria treatment. Structural models of its interactions at the 6KP2 active site are plausibly useful for the future design of antimalarial drugs.

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CONFLICTS OF INTEREST: The authors declared that they have no conflict of interest.

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