

## Research Article



## Multi-Targetted Molecular Docking Analysis of Selected Phytoconstituents of *Bauhinia acuminata*

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### ABSTRACT

Traditional medicine is often considered to be a kind of complementary or alternative medicine (CAM) nowadays. Therefore, documenting and identifying the herbs that are effective in treating various diseases is vital for future disease control programs. The study aims to perform Molecular docking analysis of the phytoconstituents of the *Bauhinia acuminata* named Quercetin, Bauhinone, Beta-sitosterol, and Kaempferol 3-glycoside with the target proteins with PDB IDs namely 2ITY, 1A52, 3L4U, IT02, 5COX, 6VYO involved in Lung cancer, breast cancer, anti-diabetes, anti-obesity, anti-inflammatory, and SARS COV-2. Chemscketch software, the study of the in-silico docking was done using Autodock.4.2 software and the binding interactions are visualized using Discovery studio 3.1. The docking scores and analysis of the interactions of the phytoconstituents with target proteins suggests that all the selected 5 phytoconstituents showed excellent binding to 2ITY and 5-COX as opposed to the standard drugs Erlotinib and Aspirin. In this study, it was concluded that the investigated phytoconstituents showed potent inhibiting activity, and the dock scores as opposed to standard as in Table 6, directly represent possible binding to the target proteins indicating their good biological activity as in lung cancer and anti-inflammatory action.

**Keywords:** Autodock 4.2, *Bauhinia acuminata*, Discovery studio 3.1, Molecular docking, Phytoconstituents.

### QUICK RESPONSE CODE →

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### INTRODUCTION

Traditional medicine defines by the World Health Organization (WHO) as: “the summation of total knowledge, practices, and skills based on the historical theories, beliefs, and experiences to maintain the human or animal health and to prevent, diagnose, improve, or treat physical/mental illnesses” in indigenous to various cultures<sup>1</sup>.

Herbal remedies are widely used in both developing and developed world countries to treat various illnesses indispensable<sup>2</sup>. The WHO reported, to treat their illnesses about 80% of the world's population are depending primarily on traditional medicines. Traditional medicine is often considered a kind of complementary or alternative medicine (CAM)<sup>3</sup> nowadays. Herbal medicines include herbal preparations, raw herbs, and finished herbal products, as well as additives derived from different kinds of plant parts/herbs. Many advantages are shown by the active components of these herbs, like lower toxicity and allergenicity than when compared to some commercial medications, regulating immunological responses, and causing viral destruction<sup>4</sup>. In the research trials<sup>5</sup>, to prevent viral infections various common herbs have been

utilized, and their effectiveness has been established. Therefore, documenting and identifying the herbs that are effective in treating various contagious diseases is vital for future disease control programs.

*Bauhinia acuminata* is an evergreen shrub belonging to the family of Fabaceae grown in the areas of Southeast Asia such as Malaysia, Indonesia, or the Philippines. For conventional drugs, bark, leaves, stem, blooms, and roots have been utilized. In India, it is a traditional plant, and its extract in studies have shown that *Bauhinia acuminata* have significant biological activities such as in the treatment of lung cancer<sup>6</sup>, breast cancer<sup>7</sup>, anti-diabetic<sup>8</sup>, anti-obesity<sup>9</sup>, anti-inflammatory<sup>10</sup>. Based on the reported anti-lung cancer, anti-breast, anti-diabetic, anti-obesity activities, molecular docking studies have been planned to establish the contribution of the activity by the phytoconstituents.

*Bauhinia acuminata* has been chemically studied and reported wherein the important chemical constituents isolated from *Bauhinia acuminata* are around 13 but 4 among them are chosen for our studies such as Quercetin, Bauhinone, Beta-sitosterol, and Kaempferol-3-glycoside. Therefore, these 4 phytoconstituents will be evaluated in this study on the docking behavior of EGFR<sup>11</sup>, ESTROGEN ALPHA RECEPTOR<sup>12</sup>, ALPHA GLUCOSIDASE<sup>13</sup>, HMG COA<sup>14</sup>, 5COX<sup>15</sup>, SAR COV-2<sup>16</sup> using an Insilco molecular docking analysis with Autodock.4.2 software and also an investigation on the enzymes binding sites using Discovery Studio Version 3.1.



## MATERIALS AND METHODS

### Molecular docking

Molecular docking studies are being carried out for 4 phytoconstituents of *Bauhinia acuminata* which have been reported already in the previous works. Six different target proteins are used for docking studies, namely 2ITY, 1A52, 3L4U, IT02, 5COX, 6VYO involved in Lung cancer, breast cancer, anti-diabetes, anti-obesity, anti-inflammatory, and SAR COV-2. The software used are Chemscketch, Autodock.4.2, and Discovery studio version 3.1.

### Ligand preparation

The 2D structures of the 4 phytoconstituents of *Bauhinia acuminata* were drawn in Chemscketch which is an openly accessible tool. The structures were then saved into Mol format with the assistance of Chemscketch software itself.

### Target receptor selection and preparation

Data on the 3D crystal structures of EGFR, ESTROGEN ALPHA RECEPTOR, ALPHA GLUCOSIDASE, HMGCOA, 5COX, and SARS COV-2 were recovered from RCSB in PDB format. The water molecules were deleted in the crystal structures it is well known that the PDB format often has poor or missing assignments of explicit hydrogens, so the optimized target receptors are included with hydrogen bonds and then saved as a pdbqt file and used for docking simulation.

### Protocol of Docking

The topological investigation of the protein structures including dynamic binding site/pocket was controlled by utilizing PHARMIT, before moving to molecular docking<sup>17</sup>. Ligand restricting sites in the protein residues are reasonable for anticipated for some the ligand that can be bind reversibly. Anyway, the right direction for other amino acid residues of the protein affirm was given. Docking studies were performed by AutoDock To decide the coupling mode and cooperation of the selected phytoconstituents and targets 4.2<sup>18,19</sup>. The pdbqt files of

the receptor protein and *Bauhinia acuminata* phytoconstituents alongside the grid box getting at the dynamic site of the receptor for compound interaction was done through Auto Dock GUI program. To permit appropriate binding adaptability at the docked site the framework size limits along X, Y, and Z hub was scaled at 40 Å with a network dividing of 1 Å. The ligands were kept adaptable and the receptor was dealt with unbending elements to achieve the best fitting compliance regarding the receptor complex. The created arrangements of docking were grouped and those with root mean square deviation (RMSD) esteem <1.0 Å were viewed as just referred in the given reference. The coupling adaptation of ligands is the one with the least binding affinity was portrayed as the steadiest compliance of the ligands as for the receptor.

### Interaction of Protein-ligand studies

The interaction investigations of the protein-ligand complexed files perception were finished by Autodock.4.2. Autodock.4.2 can create large 3D pictures of small atoms and proteins. The polar (hydrogen bond) and non-polar connections among receptor and little ligand(s) were pictured by Autodock4.2 programming. For visualizing the protein-ligand interactions, Discovery Studio 2019 (BIOVIA)<sup>20</sup> was utilized.

## RESULTS AND DISCUSSION

The computational approach is a Bioactivity score, which known drugs in their structural features and molecular properties can be used to determine whether a particular molecule is similar. According to the bioactivity score, if >0 is active; if (-5.0 to - 0.0) is moderately active, and if <-5.0 is inactive. In the present study, all of the 4 *Bauhinia acuminata* constituents showed active scores (>0) toward enzyme inhibitors descriptors. However, for other descriptors, these compounds exhibited active to moderate active scores with none showing inactive score (<-5.0), as shown in Table no 1 which is already reported is considered for our present work.

**Table 1:** 4 ligands using Molinspiration online software tool for the Bioactivity scores.

PHYTO-CONSTITUENT	GPCR LIGAND	MODULATION OF ION CHANNEL	INHIBITION OF KINASE	LIGAND OF NUCLEAR RECEPTOR	INHIBITION OF PROTEASE	INHIBITION OF ENZYME
Quercetin	-0.06	-0.19	0.28	0.36	-0.25	0.28
Bauhinione	-0.13	-0.18	0.1	0.06	-0.29	0.34
Beta-sitosterol	0.14	0.04	-0.51	0.73	0.07	0.51
Kaempferol-3-glucoside	0.06	-0.05	0.1	0.2	-0.05	0.41

**GPCR ligand:** G protein-coupled receptor ligand.

### Interaction of Protein-ligand Complex

the protein-ligand complex file analyzing the interacting protein binding sites (amino acid), After docking analysis, the *Bauhinia acuminata* herb of the phytoconstituents

constituents against EGFR, ESTROGEN ALPHA RECEPTOR ALPHA, ALPHA GLUCOSIDASE, HMG-COA, 5COX, SARS COV-2 reveals, active pockets of the proteins occupy all the ligands binding active sites (means amino acid residues) (Figure 1, 2,3, 4, and 5). Ligand-receptor interactions depict in these studies, almost all the target proteins are having



the highest interaction that is shown in (Table 2, 3, 4, 5, 6, and Table 7 for standards). The important residues that are importantly involved in protein conformation modification

are substantial for protein stabilization and otherwise for which residues ligand-receptor complex resolves the important conundrum.

**Table 2:** Binding affinities, inhibition constants of Quercetin with all the 6 protein targets, and the amino acids involved in the interactions using Autodock.4.2.

PHYTO CONSTITUENT	PDB ID	BINDING OF ENERGY (Kcal/mol)	CONSTANT INHIBITION (Ki) $\mu$ M	INVOLVEMENT AMINO ACIDS IN INTERACTIONS
QUERCETIN	2ITY	-6.601	14.47	1H-bond interaction with ASP 855, 1H-bond interaction with LYS 745, 1H-bond interaction with THR 790, 1H-bond interaction with MET 793.
	1A52	-10.78	0.0126	1 H-bond interaction with LEU 387, 1H-bond with LEU346, 1H-bond with LEU 391, 1H-bond with HIS 524, 1H-bond with ARG 394, $1\pi$ - $\pi$ T-shaped interaction with Phe 404.
	3L4U	-9.09	0.2189	2H-bond interactions with His600 1H-bond interaction with Asp327 1H-bond interaction with MET444, 1H-bond with Arg526, $1\pi$ -Cationic with ASP 42, $1\pi$ -Sigma with TRP 406.
	1T02	-7.82	1.87	1H-bond interaction with GLU 288, 1H-bond interaction with ASN 282, $1\pi$ -Cationic interaction with ARG 285.
	5COX	-11.06	0.0078	1H-bond interaction with His386 1H-bond interaction with His214 2H-bond interaction with Gln289 1H-bond interaction with Lys215, 1H-bond interaction with PHE 210, 1H-bond interaction with ASN 382.
	6VYO	-9.39	0.1316	2H-bonds with HIS 145, 1H bond Interaction with ILE 146, 1H-bond with SER 79, 1H-bond with Asn-75, $1\pi$ - $\pi$ T shaped interaction with TRP 52.

**Table 3:** The Binding affinities, inhibition constants of Bauhinione with all the 6 protein targets, and the amino acids involved in the interactions using autodock.4.2.

PHYTO -CONSTITUENT	PDB ID	BINDING OF ENERGY (Kcal/mol)	CONSTANT INHIBITION (Ki) $\mu$ M	INVOLVEMENT AMINO ACIDS IN INTERACTIONS
BAUHINONE	2ITY	-7.86	1.74	2H-bonds with Lys745
	1A52	-10.09	0.0436	No H-bond interactions. $3\pi$ - $\pi$ T shaped interactions with PHE 404, with Leu391, $1\pi$ - $\pi$ T shaped interaction with Phe 404, $1\pi$ -Sigma bond with LEU 391.
	3L4U	-7.65	2.53	1H-bond with ARG 526, SH-with Met444, $3\pi$ -Cationic interactions with ASP 542.
	1T02	-6.39	21.32	2H-bonds with LYS 745, 1H-bond with Asn271, 2SH bonds with MET766, $2\pi$ -Sigma bonds with THR 790.
	5COX	-9.09	0.2166	1H-bond with HIS 207, 1H-bonds with GLN 289, 1H-bond with THR 212, 1H-bond with HIS 386. $1\pi$ -Sigma bond with LYS 211
	6VYO	-7.2	5.26	1H-bond with HIS 207, 1H-bond with GLN 289.

**Table 4:** Binding affinities, inhibition constants of Kaempferol-3 glycoside with all the 6 protein targets and the amino acids involved in the interactions using Autodock.4.2.

PHYTO-CONSTITUENT	PDB ID	BINDING OF ENERGY (Kcal/mol)	CONSTANT INHIBITION (Ki) $\mu$ M	INVOLVEMENT AMINO ACIDS IN INTERACTIONS
KAEMPFEROL-3-GLYCOSIDE	2ITY	-9.46	0.1264	1H-bond with ASP 855,1H-bond with MET 793, 1H-bond with LYS 745, 1H-bond with PHE 856, 1 $\pi$ -Cationic interaction with MET 766, 1 $\pi$ -Sigma bond with THR 854, 1 $\pi$ -Sigma bond with VAL 726.
	1A52	2.9	Unavailable	1H-bond interaction with ARG 394, 1H-bond interaction with LEU 391.
	3L4U	-9.50	0.1083	1H-bond with HIS 600,2H-bonds with GLN 603,2H-bonds with TYR 605,1H-bond with SER 448, 1H-bond with ASP 283, 1 $\pi$ - $\pi$ T shaped interaction with TRP 406, 1 $\pi$ - $\pi$ T shaped interaction with TYR 299,2 $\pi$ -Cationic interactions with ASP 542, 3 $\pi$ -Cationic interactions with MET 444.
	1T02	-8.74	0.6061	2H-bonds with ARG 261, 1H-bond interaction with PRO 84, 1H-bond interaction with GLN 364, 1 $\pi$ -Sigma-bond interaction with ALA 368, 1 $\pi$ -Cationic interaction with LYS 267.
	5COX	-10.89	0.0106	1H-bond with TYR 385,2H-bonds with ASN 382,1H-bond with HIS 386,1H-bond with GLN 454, 1H-bond with THR 206, 1 $\pi$ -Cationic interaction with HIS 207, 1 $\pi$ -Cationic interaction with HIS 388.
	6VYO	-9.23	0.176	1H-bond with ILE 146,1H-bond with ASN 75, 1 $\pi$ -Cationic interaction with ASP 82, 1 $\pi$ - $\pi$ T shaped interaction with TRP 52.

**Table 5:** Binding affinities, inhibition constants of  $\beta$ - Sitosterol with all the 6 protein targets and the amino acids involved in the interactions using Autodock.4.2.

PHYTO CONSTITUENT	PDB ID	BINDING OF ENERGY (Kcal/mol)	CONSTANT INHIBITION (Ki) $\mu$ M	INVOLVEMENT AMINO ACIDS IN INTERACTIONS
$\beta$ - SITOSEROL	2ITY	-7.36	4.04	1H-bond with HIS 805,1H-bond with HIS 988.
	1A52	-4.31	2170	1 $\pi$ -alkyl interaction with LEU 346, 1 $\pi$ -alkyl interaction with MET 357, 1 $\pi$ -alkyl interaction with PRO 324, 2 $\pi$ -alkyl interactions with LEU 391, 4 $\pi$ -alkyl interactions with LEU 387, 2 $\pi$ -alkyl interactions with PHE 404, 2 $\pi$ -alkyl interactions with ALA 350.
	3L4U	-8.91	0.2956	1H-bond with LYS 480,2 $\pi$ -Sigma interactions with PHE 575, 3 $\pi$ -Sigma interactions with TYR 299, 2 $\pi$ -Sigma interactions with TRP 406, 1 $\pi$ -Sigma interaction with MET 444, 1 $\pi$ -Sigma interaction with TRP 441, 1 $\pi$ -Sigma interaction with HIS 600.
	1T02	-7.09	6.43	5 $\pi$ -alkyl interactions with LYS 267, 1 $\pi$ -alkyl interaction with ALA 368, 1 $\pi$ -alkyl interaction with ALA 263.
	5COX	-10.77	0.0127	1H-bond with GLN 289,1 $\pi$ -alkyl interaction with LYS 211, 1 $\pi$ -alkyl interaction with HIS 207, 1 $\pi$ -alkyl interactions with HIS 214, 2 $\pi$ -alkyl interactions with HIS 386,2 $\pi$ -alkyl interactions with MET 458.
	6VYO	-7.07	10.22	3 $\pi$ -sigma interactions with TRP 52, 1 $\pi$ -sigma interaction with HIS 145, 2 $\pi$ -sigma interactions with ILE 146.



**Table 6:** Binding affinities, inhibition constants of standards with all the 6 protein targets, and the amino acids involved in the interactions using Autodock.4.2.

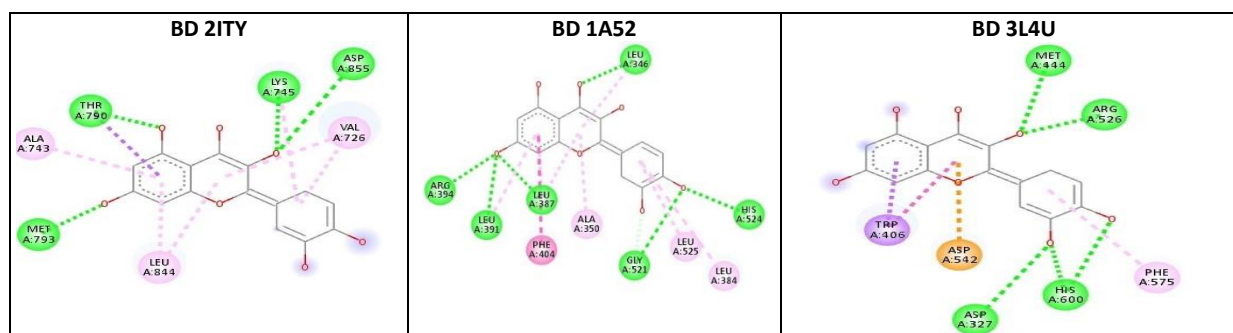
STANDARDS	PDB ID	BINDING OF ENERGY (Kcal/mol)	CONSTANT INHIBITION (Ki) $\mu$ M	INVOLVEMENT AMINO ACIDS IN INTERACTIONS
ERLOTINIB	2ITY	-6.1	33.83	No H-bond interactions, $1\pi$ -Sigma interaction with VAL 726, $1\pi$ -Sigma interaction with LEU 844.
TAMOXIFEN	1A52	-8.82	0.339	1H-bond interaction with ARG 194.
ACARBOSE	3L4U	-9.85	0.061	2H-bonds with LYS 480, 2H-bonds with PHE 450, 1H-bond with ASP203, 1H-bond with MET 444, 2H-bonds with ARG 256, 1H-bond with ASP 443, 1H-bond with TRP 539, 1H-bond with ARG 598, 2H-bonds with HIS 600.
SIMVASTATIN	1T02	-7.42	3.64	1H-bond with ASN 365, 1H-bond with HIS 265, 1H-bond with ARG 261, $1\pi$ -Sigma interaction with ALA 368.
ASPRIN	5COX	-5.38	114.77	1H-bond with SER 451, 1H-bond with ALA 450.
N3 INHIBITOR OF 6LU7	6VYO	-8.08	1.19	2H-bond interactions with HIS 145, 1H-bond with ASP 144, $1\pi$ -sigma interactions with GLY 147, $2\pi$ -T shaped interaction with TRP 52.

**Table 7:** Table showing docking scores (Binding energy) of phytoconstituents and the Standards with different target Proteins.

PDB ID	QUERCETIN	BAUHINONE	KAEMPFEROL-3-GLYCOSIDE	$\beta$ -SITOSTEROL	ERLOTINIB	TAMOXIFEN	ACARBOSE	SIMVASTATIN	ASPRIN	N3 INHIBITOR OF 6LU7
	BINDING ENERGY (Kcal/mol)									
2ITY	-6.601	-7.86	-9.46	-7.36	-6.1	-	-	-	-	-
1A52	-10.78	-10.09	2.9	-4.31	-	-8.82	-	-	-	-
3L4U	-9.09	-7.65	-9.5	-8.91	-	-	-9.85	-	-	-
1T02	-7.82	-6.39	-8.74	-7.09	-	-	-	-7.42	-	-
5COX	-11.06	-9.09	-10.89	-10.77	-	-	-	-	-5.38	-
6VYO	-9.39	-7.2	-9.23	-7.07	-	-	-	-	-	-8.08

**Interactions**

	Conventional Hydrogen Bond		Pi-Pi T-shaped
	Pi-Anion		Pi-Alkyl
	Pi-Sigma		

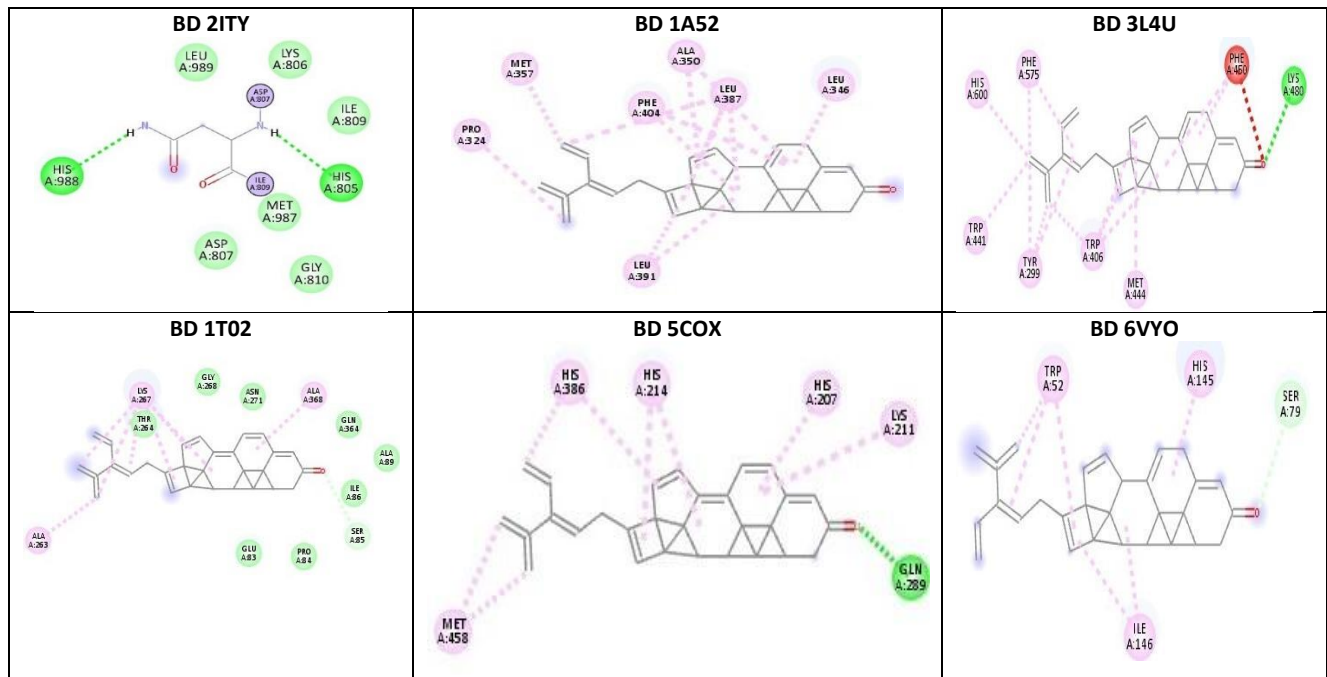






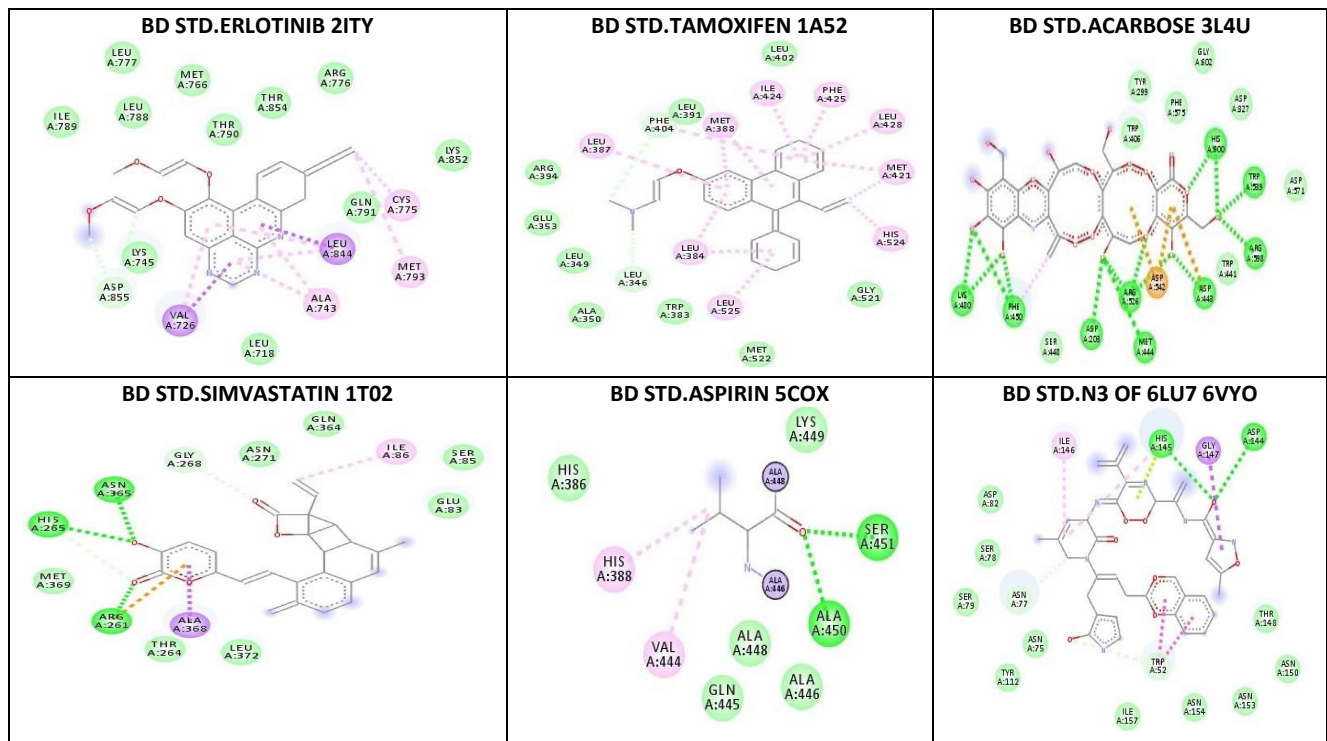
BD is the best docking confirmation

**Figure 3.** Bauhinia-Kaempferol binding interactions with different target proteins



BD is the best docking confirmation

**Figure 4:** Bauhinia-Beta-sitosterol binding interactions with different target proteins



BD is the best docking confirmation

**Figure 5.** Binding interactions of standards drugs with different target proteins

In this in-silico study, the phytoconstituents of Bauhinia acuminata exhibited the most negative value of docking score toward 2ITY, 1A52, 3L4U, IT02, 5COX, and 6VYO and the best affinity have seen and was formed.

The binding energies obtained by the 4 phytoconstituents with the six target proteins 2ITY, 1A52, 3L4U, IT02, 5COX, 6VYO are listed in (Table 2, 3, 4,5, 6, and Table 7 for standards) and the binding interactions with the amino acids of the six target proteins are given in (Figures 1,2, 3,

4 and 5. If the affinity of the active compound to bind to the target protein was more exceptional or the binding energy value of the phytoconstituents with the six target proteins was more negative than the ability. This shows that active compounds and target proteins between more robust and more stable interactions have occurred.

Among all the data depicted in (Table 2, 3,4,5, 6, and Table 7 for standards) it appears that all the phytoconstituents bond to all target proteins and have lower binding energy compared and showing the best bond with all the six target proteins. Quercetin, Bauhinione, Beta-sitosterol, and Kaempferol all showed the potentials in binding with all of the six-targeted proteins with the docking and good binding energies and affinity constants to establish the respective biological activities showing activity against lung cancer, breast cancer, in obesity, in inflammation, and in minimizing Covid-19 complications treatments.

All the selected 5 phytoconstituents showed excellent binding to 2ITY and 5COX as opposed to the standard drugs Erlotinib and Aspirin.

Quercetin and Bauhinone showed potent inhibiting activity on 1A52 indicating their good biological activity as opposed to the standard drug of Tamoxifen for breast cancer.

Quercetin and Kaempferol exhibited potent inhibiting activity on IT02 indicating their good biological activity as opposed to the standard drug of Simvastatin for anti-obesity.

Quercetin and Kaempferol showed potent inhibiting activity on 6VYO indicating their good biological activity as opposed to the standard drug of N3 inhibitor of 6LU& for SARS COV-2.

Quercetin is the Phyto-constituent that is showing good binding with 5 of 6 selected protein targets with good docking scores compared to the standards.

## CONCLUSION

The enzyme targets namely 2ITY, 1A52, 3L4U, IT02, 5-COX, and 6VYO have paved a new insight into the understanding of phytoconstituents against *Bauhinia acuminata* as potential inhibitors.

Recently, the study showed the potential to dock and bind with all the mentioned target enzymes as the selected ligands from *Bauhinia acuminata*. Hence, it is suggested that the results of this study have paved as a potential 2ITY, 1A52, 3L4U, IT02, 5-COX, and 6VYO inhibitors with the prevention of associated disorders of Lung cancer, breast cancer, anti-diabetic, anti-obesity, anti-inflammatory and also in minimizing Covid-19 complications for better understanding of these 4ligands of *Bauhinia acuminata*.

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