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Phytochemical and In Silico Evaluation of the Antimalarial Potential of Tecomella undulata through Molecular Docking and ADMET Analysis

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"Phytochemical and *In Silico* Evaluation of the Antimalarial Potential of *Tecomella undulata* through Molecular Docking and ADMET Analysis

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Authors' Contributions

Madhu Verma : she was responsible for the foundational research and experimental phases of the study. This included conducting comprehensive literature reviews to gather essential background information, acquiring and processing the *Tecomella undulata* plant material, and executing the hands-on laboratory procedures required for the successful extraction and profiling of the targeted phytochemicals**.**

Himanshu : he led the computational research and manuscript preparation. This involved designing and performing the *in silico* molecular docking studies to evaluate the binding affinities of the extracted compounds against malarial targets. Additionally, he was responsible for interpreting the computational data, drafting the original manuscript, and typing the final paper.

All authors reviewed and approved the final version of the manuscript and agreed to be accountable for all aspects of the work.

Abstract

Plasmodium is the most prevalent infectious disease and a significant worldwide public health problem, particularly in tropical and subtropical regions. Most of the clinical drugs are plant-originated products. Traditionally, therapeutic shrubs have been utilized to treat a wide range of illnesses and are regarded as important sources of therapeutic chemicals. That's why medicinal plants *Tecomella undulata* were chosen for this study because of their historic usage in folk medicine and their therapeutic significance. Firstly, plant compounds were extracted from the PubChem database, and their ADMET and drug-likeness pharmaceutics were analyzed with the help of the Swiss ADME (https://www.swissadme.ch/) tool. Compounds that met Lipinski's rules were shortlisted for further molecular docking examination. Molecular docking of selected compounds was performed against three important *Plasmodium falciparum* proteins, FP-2, FP-3, and Plm-2. 2D and 3D conformations of best binding interactions were prepared with the help of the Discovery Studio visualizer. Among all the selected compounds, Dehydrotectol showed the best binding energy score of -10.3 kcal/mol with both the target proteins and could be a promising bioagent for the treatment of malaria.

Key terms: *Tecomella undulata*, *Plasmodium falciparum*, Falcipain-2, Falcipain-3, Plasmepsin-2, and Malaria

Introduction

Malaria is a most prevalent and infectious disease, despite many efforts taken to control it by different international organizations and the scientific community. According to a WHO report (1)2024, *Plasmodium* infected 282 million people worldwide with approximately 610000 mortalities, mainly in Africa (94%), followed by the Eastern Mediterranean and Southeast Asia (1,2). The worldwide incidence of malaria decreased to 37% from 2000 to 2015 (3). The overall reduction in rates of malaria can be credited to the use of artemisinin-based combination therapies (4). Malaria is known to cause severe types of illness in immunocompromised people, pregnant women, and children below the age group of 5 years. The diseases are spread to humans by the bites of an infected female Anopheles mosquito. Several mosquito species can transmit the deadly illness malaria to humans. Five *Plasmodium* species—Plasmodium *falciparum*, *Plasmodium vivax*, *Plasmodium ovale*, *Plasmodium malariae*, and *Plasmodium*

knowlesi—are responsible for causing this illness in humans (5). The most fatal type of malaria is observed from infection of *P. falciparum*, as other species of *Plasmodium* typically cause milder symptoms. Infection with *P. falciparum* is especially dangerous for infants and pregnant mothers, leading to respiratory distress and severe anemia (6). Due to the non-availability of any successful malaria vaccines, drug therapy as well as vector management techniques are only preventive measures to control the number of illnesses. Drug development primarily targets the parasite's blood infection stages, which is easier to study in laboratories. To keep pregnant women safe from malaria, it is recommended that they use insecticide-treated nets (ITNs), intermittent preventive treatment during pregnancy (IPTp), and antenatal care (ANC) (7,8).

Malaria remains a significant cause of sickness and fatality in many low-and middle-income nations, despite decades of study and a worldwide malaria campaign. A variety of natural, semi-synthetic, and synthetic medicines are used to treat malaria. Quinoline derivatives, antifolates, and artemisinin derivatives are the most prescribed antimalarial drugs in recent years (9).

A crucial metabolic mechanism for the internal growth within erythrocytes of the plasmodium parasite is hemoglobin degradation, which takes place in an acidic feeding vacuole where the parasite uses several proteases to break down all of the host hemoglobin in order to obtain amino acids (10, 11). Aspartic proteases, such as plasmin-2, start the degradation process by cleaving and disrupting the molecule's original structure, exposing it to further proteolysis (12, 13). Later the breakdown of hemoglobin is advanced by another aspartic protease called plasmin-2 (14, 15). The 3rd essential ingredient is cysteine protease Falcipain, which works in concert with aspartic protease to ensure full hemoglobin breaking while effectively breaking down denatured globulin protein (16, 17). The unique characteristics of proteases, their sequence, & combined interactions render the pathway a great target for malaria treatment. The proteases within the digestive vacuole are also susceptible to antimalarial agents such as chloroquine (18). Consequently, the development of medicines that precisely target these proteases may function as significant antimalarial agents.

As per our traditional literature and books, we have been utilizing the plants as medicines since ancient times. This is because a wide variety of secondary metabolites of the plants have the potential to treat many ailments (19). Numerous plant families like Asteraceae, Fabaceae, Liliaceae, and several more are reported to have different therapeutic qualities (9, 20). According to Qayum et al. (2016), different plant parts such as leaves, branches, stems, flowers,

fruits, and roots offer excellent therapeutic qualities. Therefore, the current work has been aimed at identifying a novel antimalarial molecule.

The current study involved the phytochemicals of the ***Tecomella undulata*** against the main target protein of the *Plasmodium falciparum* via the utilized molecular docking and ADMET analysis. And we hypothesize that the phytochemicals will halve the growth of Plasmodium by inhibiting the different phases of its life cycle.

MATERIALS AND METHODS

To determine the bioactive substances found in *Tecomella undulata, a* thorough analysis of scientific literature was conducted. For the investigation, only substances with well-defined chemical structures and information accessible in the PubChem (http://pubchem.ncbi.nlm.nih.gov/) database were taken into account. After 17 substances of *Tecomella undulata* were chosen for further studies, their pharmacokinetic characteristics—such as absorption, distribution, metabolism, excretion, and toxicity (ADMET)—were assessed by using software Swiss ADME (SwissADME) (21,22).

ADMET screening and drug resemblance of the substances

Phytocompounds of the plant *Tecomella undulata* is extracted from PubChem to check pharmacokinetic properties such as absorption, distribution, metabolism, excretion, and toxicity (ADMET). Then we use the Swiss ADME website to calculate compound drug likeness. The physiological parameters that were used to investigate include number of hydrogen bond acceptors and donors, molecular weight, topological surface area, skin permeation, blood-brain barrier permeability, gastrointestinal absorption, solubility, topological surface area, and molar refractivity (Oduselu et al., 2019). For toxicity calculation we use ProTox 2.0 (ProTox-3.0 - Prediction of TOXicity of chemicals). We use SMILES files of all compounds for ADMET analysis (23).

Preparation of ligand and receptor

17 *Tecomella undulata* compounds' 3D structure was obtained from the PubChem database in SDF format. Open Babel was then used to translate the compounds' SDF structure into PDB format. The energy of the ligand was minimized and thereafter turned into. PyRx-related Pdbqt format at AutoDock. Protein crystal structures, the RCSB protein data bank provided FP-2 (3BPF), FP-3 (3BPM), and Plm (4z22) in legacy PDB format: Falcipain-2 (PDB id: 3BPF, resolution 2.90A°), Falcipain-3 (PDB id: 3BPM, resolution 2.50A°), and Plasmepsin-2 (PDB ID: 4Z22, resolution 2.62A°) (https://www.rcsb.org/). After obtaining the target protein's crystal structure, it was cleaned using a series of sequential procedures, such as removing water molecules, heteroatoms, and unnecessary chains and adding polar hydrogens. Discovery Studio

Visualizer is stored in PDB format, and the ligand is also saved in PDB format using the Visualizer in Discovery Studio. After being cleaned, the structure was put into PyRx and transferred into macromolecules in Pdbqt format (24, 25).

Target proteins

Falcipain-2 (3BPF), Falcipain-3 (3BPM), and Plasmepsin-2 (4Z22)

Falcipain-2

Plasmodium falciparum's falcipain-2 is an essential player in the digestive vacuole haemoglobin breakdown process. It is a cysteine protease belonging to the papain family. Antimalarial medications may be developed with it since blocking it interrupts the supply of amino acids, hinders the growth of the parasite, and ultimately causes the parasite to die (26, 27).

Falcipain-3

Plasmodium falciparum produces falcipain-3, a cysteine protease that resembles papain; it is active in the late trophozoite and schizont stages, when it continues to break down hemoglobin-derived peptides. It is a significant target for antimalarial drugs since blocking it hinders parasite growth and, in conjunction with blocking Falcipain-2, effectively limits haemoglobin digestion (28).

Plasmepsin-2

Plasmepsin-2, a pepsin-like aspartic protease found in *Plasmodium falciparum*'s digestive vacuole, starts the breakdown of haemoglobin. It produces substrates for downstream processes by catalyzing the initial stage of haemoglobin cleavage. It is a desirable target for the creation of antimalarial medications because its blockage interferes with the uptake of nutrients and the survival of parasites (29).

Figure 1: *Plasmodium Falciparum* protein chains **(A)** Falcipain-2 (3BPF) **(B)** Falcipain-3 (3BPM) and **(C)** Plasmepsin-2 (4Z22)

Molecular docking method

Within the standard protocol of using AutoDock 4.2, we determine whether one of the chosen chemicals may be an inhibitor, primarily focusing on the active region of Falcipain-2, Falcipain-3, and Plasmepsin-2. We kept all amino acids as rigid while all ligands were treated as flexible during the whole process of docking. We use a grid box such as to encompass the entire area of targeted protein, such as Plasmepsin-2, Falcipain-2, and Falcipain-3, where the grid dimension is 60.0×60.0×60.0 dots spaced 0.375 Å apart in a grid. The grid box of each

protein was centered on the active-site region in which the native ligand was bound. The grid-center coordinates used for docking were -45.5095, -14.5344, -10.4623 for Falcipain-2; -2.3375, 27.9996, -27.4042 for Falcipain-3; and -5.2772, 2.3395, -16.3476 for Plasmepsin-2. We selected the Lamarckian Genetic Algorithm as the docking engine with 100 dockings per ligand, then ranked the results on the basis of binding energy, and the lowest energy poses for each protein-ligand were selected for the further analysis. Discovery Studio Visualizer was used for visualizations of binding interactions (24). Binding free energy was used as the main measure for assessing how strongly a ligand binds and for choosing the most suitable ligand conformation.

RESULTS AND DISCUSSION

After examination of molecular docking analysis of phytocompounds with the targeted proteins, the binding energy score of *Tecomella undulata* varied from -6.2 to -10.3 kcal/mol. The ligand-protein interaction that has the minimum binding energy is considered the best docking complex and chosen for further analysis. Lower binding energy of the complexes shows the strong connections and increased ligand-protein complex stability in molecular docking (30). From the docking results of *Tecomella undulata,* Dehydrotectol showed the best binding energies: -9.8, -10.0, and -10.3 kcal/mol for Falcipain-2, Falcipain-3, and Plasmepsin-2. The 2D and 3D molecular docking conformation of the highest binding score exhibited compounds of the plant.

The present molecular docking study showed that the selected phytochemicals of *Tecomella undulata* have different binding affinities toward Falipain-2, Falcipain-3, and Plasmpsin-2. Amongst the four compounds, dehydrotectol exhibited the strongest and most consistent binding with docking scores of -9.8 kcal/mol, -10.0 kcal/mol, and -10.3 kcal/mol against Falipain-2, Falcipain-3, and Plasmpsin-2, respectively. Dehydrotectol showed the highest affinity against Plasmodium falciparum (Plasmepsin-2, -10.3 kcal/mol), indicative of favorable interactions of dehydrotectol with this malaria-associated protease. 2-methylanthraquinone also showed good binding, particularly against plasmepsin-2 (-8.8 kcal/mol). Crisilineol, however, showed moderate binding between -7.1 and -7.5 kcal/mol. The glycoside-like compound (CID 162935416) exhibited comparatively weak binding with a range of -6.2 to -6.5 kcal/mol. Docking scores are only computational predictions and should be treated as relative indicators of binding potential, rather than direct evidence of biological activity (31, 25).

Previous biological research on *T. undulata* supports these conclusions. According to Sachdeva et al. (2023), *T. undulata* leaf extract exhibited good in vitro anti-plasmodial activity against

both the resistant INDO strain (IC_{50} = 15.3 µg/mL) and the chloroquine-sensitive P. falciparum 3D7 (IC50 = 15 µg/mL), with cytotoxicity against HEK293 cells exceeding 200 µg/mL and a selective index greater than 13.3. Although the previous work assessed a crude extract rather than specific chemicals, this experimental data reinforces the significance of the current docking results. Therefore, the high binding seen for 2-methylanthraquinone and dehydrotectol may aid in identifying substances that merit more investigation as potential contributions to *T. undulata's* anti-plasmodial action. However, without isolation and biological confirmation, the activity of a crude extract should not be attributed to a single ingredient because it may be the consequence of additive or synergistic effects among several elements.

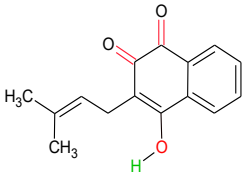
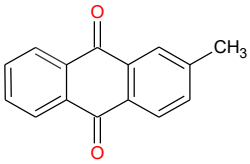
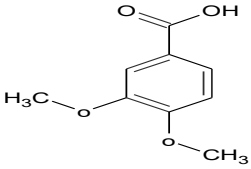
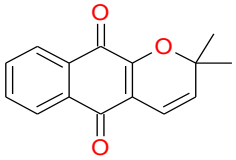
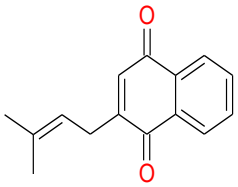
The computational potential of *T. undulata* metabolites has also been shown by earlier molecular-docking studies. Several *T. undulata* compounds, such as betulinic acid, ursolic acid, lapachone, sitosterol, stigmasterol, and quercitrin, were found to interact favorably with cancer-related protein targets by Riaz et al. (2022). In a similar vein, Khandelwal et al. (2002) identified a number of quinone-type molecules from T. undulata and discovered that 2-methylquinizarin had an interaction with Met94 and a docking score of -7.70 kcal/mol against CDK7. The dehydrotectol scores in the current study, especially -10.3 kcal/mol against Plasmepsin-2, suggest a positive computational interaction with the chosen malaria target when compared to these published results. However, because docking systems, scoring functions, protein structures, ligand synthesis techniques, and search settings may vary, direct comparison of docking scores between research should be done with caution.

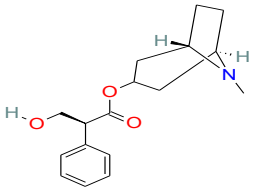
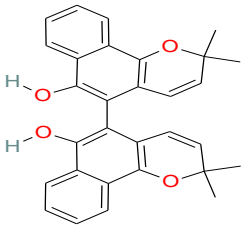
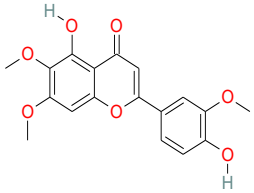
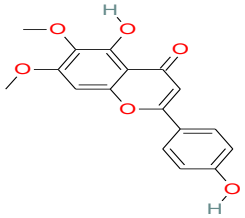
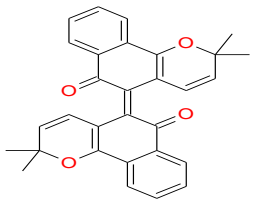
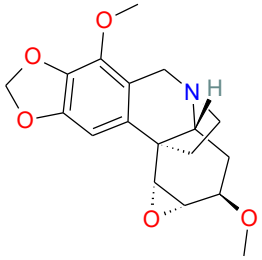
The current study is further supported by the biological significance of the chosen targets. While Plasmepsin-2 is an aspartic protease linked to haemoglobin digestion in P. falciparum, Falipain-2 and Falcipain-3 are important cysteine proteases involved in haemoglobin degradation and parasite growth (32-34). Parasite survival and nutrition uptake may be hampered by inhibition of these proteolytic enzymes. Thus, the anticipated binding of 2-methylanthraquinone and dehydrotectol to these targets offers a tenable molecular explanation for their potential anti-plasmodial actions. Studies on parasite development and enzyme-inhibition tests are needed to validate this theory.

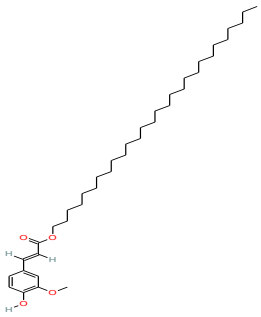
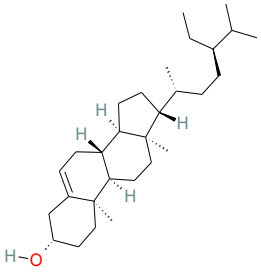
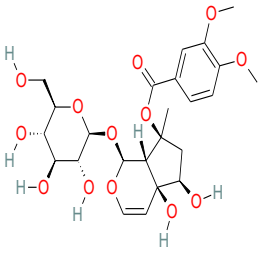
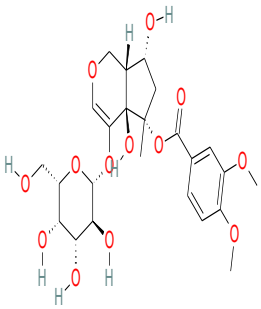
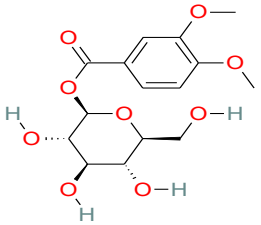
Overall, the current results, in addition to the previously described experimental evidence, indicate that T. undulata possesses phytochemicals that may have antimalarial activity. Dehydrotectol seems to be the most promising lead. Followed by 2-methylantraquinone. Nevertheless, the docking scores represent predicted binding affinity and cannot alone confirm antimalarial efficacy. Further studies involving the analysis of binding site interactions, molecular dynamics, inhibition of enzymes, parasite-based assays, and in vivo validation are

necessary to establish the therapeutic potential of these compounds. Moreover, evaluations of pharmacokinetic properties, cytotoxicity, metabolic stability, and selectivity against parasite enzymes will be required before these compounds can be considered as potential antimalarial leads.

Table 1: Phytoconstituents of plant *Tecomella undulata* with CID, molecular formula, molecular weight, and their structure

S. No.	Compound Name	CID	Structure	Molecular weight	Formula
1.	Lapachol	3884		242.27 g/mol	$C_{15}H_{10}O_3$
2.	2-Methylanthraquinone	6773		222.24 g/mol	$C_{15}H_{10}O_2$
3.	3,4-Dimethoxybenzoic acid	7121		182.17 g/mol	$C_9H_{10}O_4$
4.	1-Triacontanol	68972		438.8 g/mol	$C_{30}H_{62}O$
5.	Xyloidone	72734		240.25 g/mol	$C_{15}H_{12}O_3$
6.	Deoxylapachol	97448		226.27 g/mol	$C_{15}H_{14}O_2$

7.	Hyoscyamine (Benzeneacetic acid)	154417		289.4 g/mol	$C_{17}H_{23}NO_3$
8.	Tectol	161453		450.5 g/mol	$C_{30}H_{26}O_4$
9.	Cirsilineol	162464		344.3 g/mol	$C_{18}H_{16}O_7$
10.	Cirsimaritin	188323		314.29 g/mol	$C_{17}H_{14}O_6$
11.	Dehydrotectol	3037329		448.5 g/mol	$C_{30}H_{24}O_4$
12.	Undulatine	3083985		331.4 g/mol	$C_{18}H_{21}NO_5$

13.	Octacosyl ferulate	5743442		586.9 g/mol	$C_{38}H_{66}O_4$
14.	B-sitosterol	11870456		414.7 g/mol	$C_{29}H_{50}O$
15.	Tecoside	101277358		528.5 g/mol	$C_{24}H_{32}O_{13}$
16.	Harpagide 8-(3,4-dimethoxybenzoate)	162871330		528.5 g/mol	$C_{24}H_{32}O_{13}$
17.	veratroyl glucoside	162935416		344.31 g/mol	$C_{15}H_{20}O_9$

ADMET Analysis

Tecomella undulata metabolites were subjected to an ADMET analysis to use their pharmacoeutical characteristics and drug-likeness properties (Lipinski's rule) by using bioinformatics software SwissADME and protox 2.0 (35). Lipinski's rule of five suggests that a drug-like molecule should have three out of the following parameters: the molecular weight

must be under 500k Da, the number of intermolecular hydrogen attraction donor should be 5 or less than 5 and should contain maximum 10 or below 10 H-bonding acceptor groups. Three or more of these requirements had to be met for a compound to be considered for further analysis (35). Toxicity profiles and ADMET for every phytocompound of the plant *Tecomella undulata* are listed in table. During ADMET analysis, compounds that met Lipinski's parameters were shortlisted, four compounds were selected from the plant which is enlisted in table. Further, interaction of selected compounds with the target proteins was then evaluated by in silico docking to examine their molecular binding strength against important biocatalysts including in the breakdown of Hb pathway.

Table 2: ADMET properties of *Tecomella undulata*

Sr. No.	Compound	CID	NHBA	NHBD	MR (Molar Refractivity)	TPSA (A^2)	Water Solubility Class (ESOL)	GIA	BBB-P	P-gp substrate	Log Kp (Skin permeasurement)	LD_{50} (mg/kg)	Predicted toxicity class	Log P
1	**Lapachol**	3884	1	18	69.95	54.37	-3.455	92.865	0.539	No	-2.655	680	4	3.08
2	**2-Methylanthraquinone**	6773	2	0	64.72	34.14	-3.779	99.436	0.398	Yes.	-2.145	2795	5	2.77
3	**3,4-Dimethoxybenzoic acid**	7121	4	1	46.39	55.76	-1.778	100	-0.249	No	-2.728	2000	4	1.4

4	**1-Triacontanol**	68972	1	1	147.49	20.23	-6.271	84.993	1.063	No	-2.738	1000	4	10.92
5	**Xyloidone**	72734	3	0	66.81	43.37	-3.425	97.665	0.648	No	-2.677	2000	4	2.68
6	**Deoxylapachol**	97448	2	0	67.8	34.14	-4.099	95.867	0.361	No	-2.213	500	4	3.35
7	**Hyoscyamine (Benzeneacetic acid)**	154417	4	1	84.51	49.77	-1.943	94.508	0.234	Yes.	-4.488	380	4	1.87
8	**Tectol**	161453	4	2	139.18	58.92	-4.592	92.229	-0.195	Yes	-2.735	500	4	7.44
9	**Cirsilineol**	162464	6	2	91.44	98.36	-3.326	100	-0.738	Yes	-2.754	5000	5	2.9

10	**Cirsimaritin**	188323	2	0	119.72	12.47	-3.481	93.987	-0.59	Yes	-2.745	1190	4	2.89
11	**Dehydrotectol**	3037329	4	0	131.78	52.6	-5.78	98.146	-0.205	No	-2.673	8000	6	6.23
12	**Undulatine**	3083985	6	0	87.29	52.69	-2.806	96.754	0.007	No	-3.186	450	4	1.54
13	**Octacosyl ferulate**	5743442	4	1	185.74	55.76	-4.036	84.135	-1.041	No	-2.735	9600	6	12.12
14	**β-sitosterol**	11870451 6		1	133.23	20.23	-6.773	94.464	0.781	No	-2.783	890	4	8.02

15	**Tecoside**	10127731358	6	121.49	193.83	-2.869	33.669	-1.647	Yes	-2.735	2000	4	-1.58
16	**[(4aS,5S,7R,7aR)-4a,7-dihydroxy-5-methyl-4[(2R,3S,4R,5S,6S)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy-1,6,7,7a-tetrahydrocyclopenta[c]pyran-5yl]3,4-dimethoxybenzoate**	16287131330	6	121.49	193.83	-2.951	49.091	-1.626	Yes	-2.735	2260	5	-1.58
17	**3,4-Dimethoxybenzoic acid β-D-glucopyranosyl ester**	16293549116	4	78.36	134.91	-2.161	60.403	-1.205	Yes	-2.791	2260	5	-1.34

Abbreviations: NHBA = Number H-bond acceptor, NHBD = Number H-bond donors, TPSA = Topological Polar Surface Area, GIA = Gastro-intestinal absorption, BBB-P = Blood Brain barrier Permeability, MR = Molar Refractivity

Docking Interactions

After examination of molecular docking analysis of phytocompounds with the targeted proteins, the binding energy score of *Tecomella undulata* varied from -6.2 to -10.3 kcal/mol. The ligand-protein interaction that has the minimum binding energy is considered the best docking complex and chosen for further analysis. Lower binding energy of the complexes shows the strong connections and increased ligand-protein complex stability in molecular docking (30). From the docking results, *Tecomella undulata* Dehydrotectol showed the best binding energies. In the case of protein Falcipain-2 binding energy, Dehydrotectol showed a binding energy of -9.8 kcal/mol, which is better when compared with standard chloroquine (-6.2 kcal/mol). While in Falcipain-3, Dehydrotectol showed the best binding energy of -10.0 kcal/mol, which is better than chloroquine (-6.06 kcal/mol). At last, in Plasmepsin-2, again, Dehydrotectol showed the best binding energy of 10.3 kcal/mol, which was better than chloroquine (-7.32 kcal/mol). The second best result in Falcipain-2, Falcipain-3, and Plasmepsin-2 is shown by 2-Methylanthraquinone with binding energies of -7.3, -7.7, and -8.8 kcal/mol, respectively.

Figure 2: Molecular docking interaction of phytochemicals of *Tecomella undulata* against falcipain-2 protein (PDB ID: 3BPF) (A) 3D structure of 2-methylanthraquinone (B) 3D structure of cirsilineol (C) 3D structure of dehydrotectol (D) 3D structure of 3,4-dimethoxybenzoic acid β-D-glucopyranosyl ester.

Figure 3: Molecular docking interaction of phytochemical of *Tecomella undulata* against falcipain-2 protein PDB ID: 3BPF (A) 3D structure of 2-Methylanthraquinone (B) 3D structure of Cirsilineol (C) 3D structure of Dehydrotectol (D) 3D structure of 3,4-Dimethoxybenzoic acid β-D-glucopyranosyl ester

Figure 4: Molecular docking interaction of phytochemical of *Tecomella undulata* against Plasmepsin-2 protein PDB ID: 4Z22 (A) 3D structure of 2-Methylanthraquinone (B) 3D structure of Cirsilineol (C) 3D structure of Dehydrotectol (D) 3D structure of 3,4-Dimethoxybenzoic acid β-D-glucopyranosyl ester

Table 3: Binding energy with ligands (Tecomella *undulata*) protein Falcipain-2, Falcipain-3, and Plasmepsin-2

S. No.	Compound Name	CID	Binding energy of Falcipain-2	Binding energy of Falcipain-3	Binding energy Plasmepain-2
1.	2-Methylanthraquinone	6773	-7.3	-7.7	-8.8
2.	Cirsilineol	162464	-7.1	-7.5	-7.2
3.	Dehydrotectol	3037329	-9.8	-10.0	-10.3
4.	3,4-Dimethoxybenzoic acid β-D-glucopyranosyl ester	162935416	-6.5	-6.5	-6.2

Conclusion

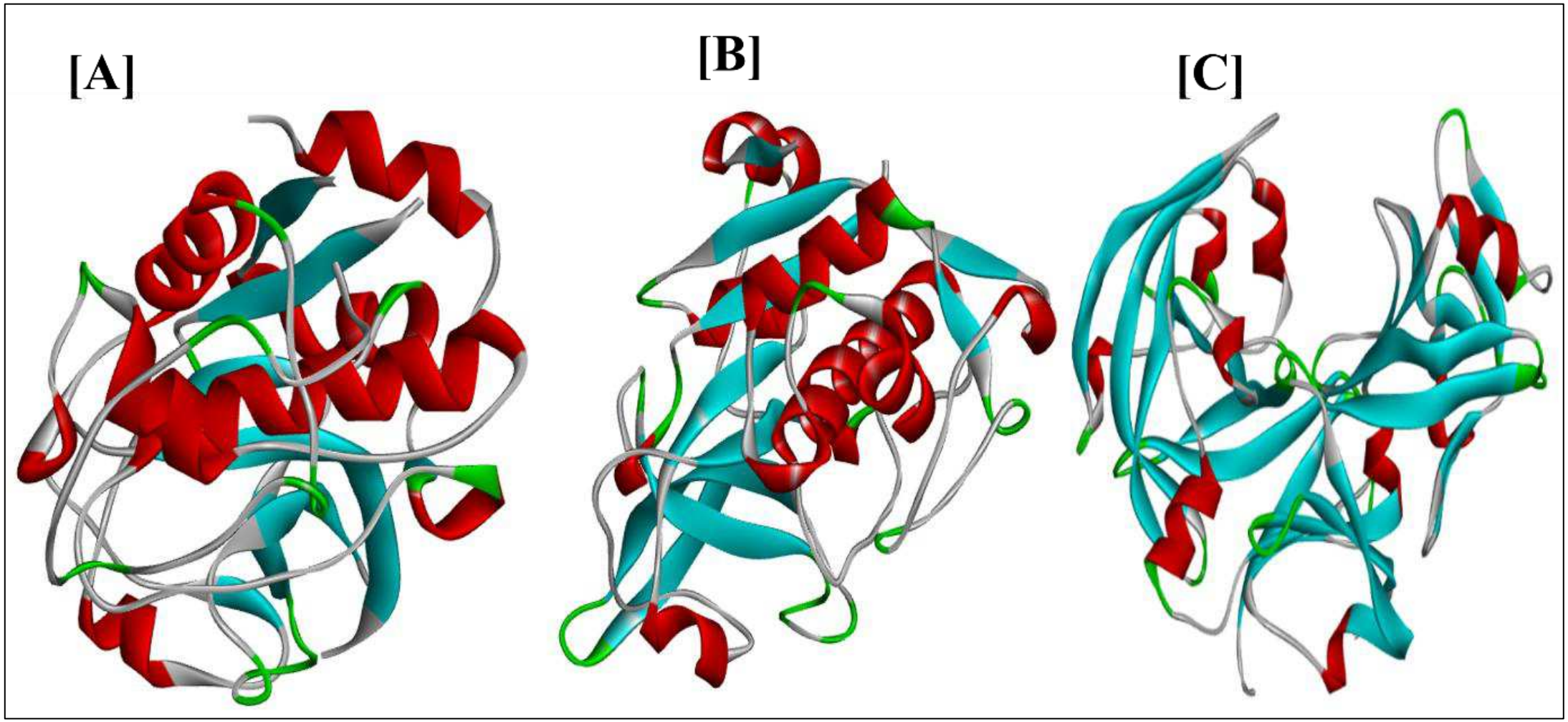
As drug resistance in malaria becomes an increasingly urgent concern, new treatment approaches are essential. Plant-derived chemicals offer a wide range of therapeutic benefits. This study emphasizes the potential of bioactive compounds extracted from *Tecomella undulata.* The result revealed that friedelin exhibited the strongest binding affinity across all three target proteins. Overall, these findings suggest that such bioactive molecules could contribute to the development of new, more effective drug candidates with potentially fewer adverse effects.

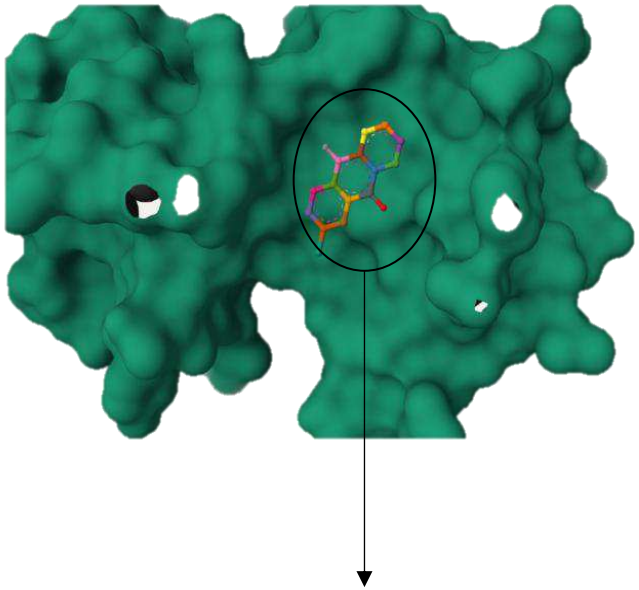
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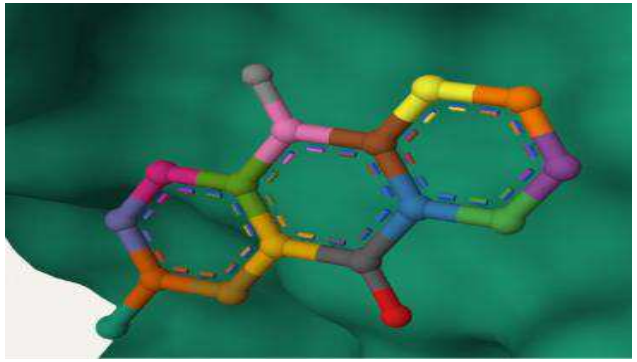
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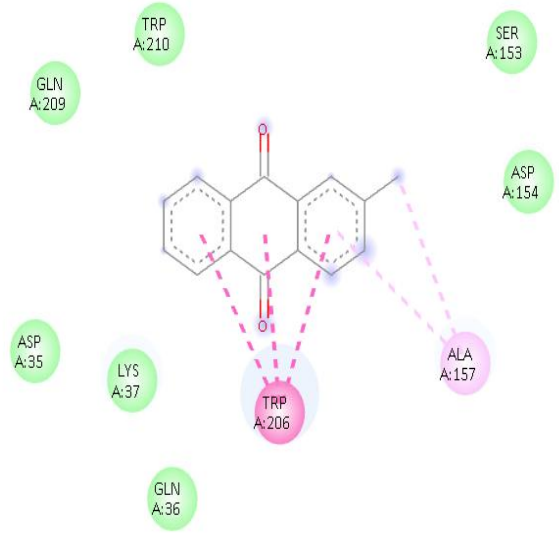
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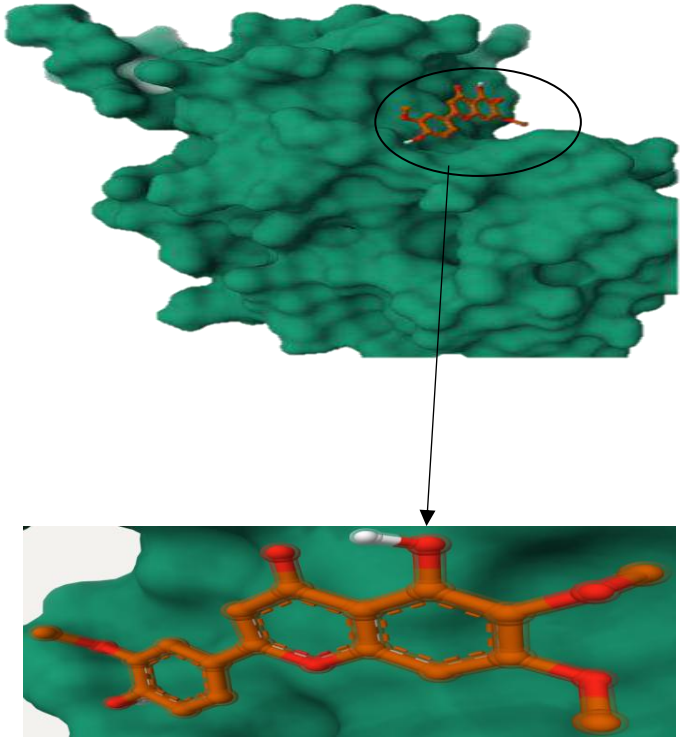




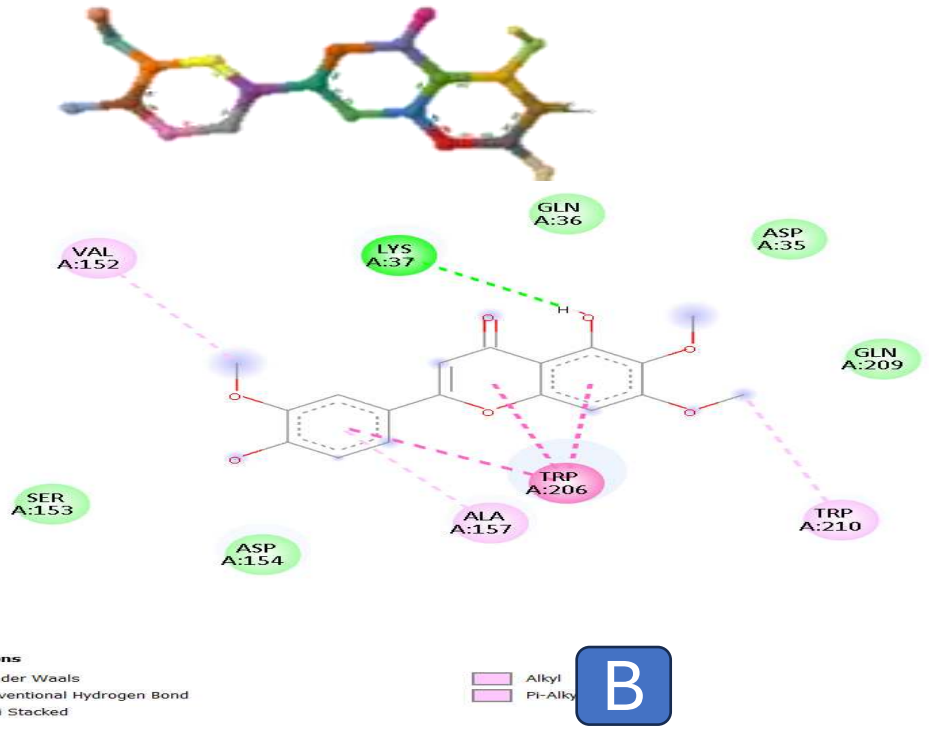


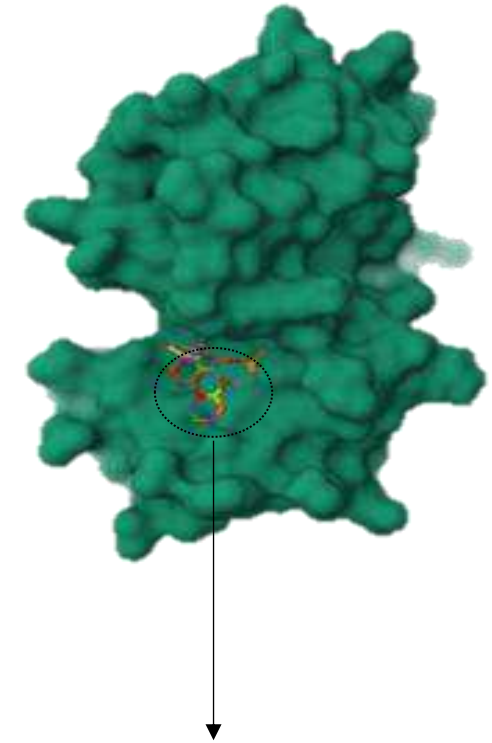
3BPF with 2-Methylanthraquinone

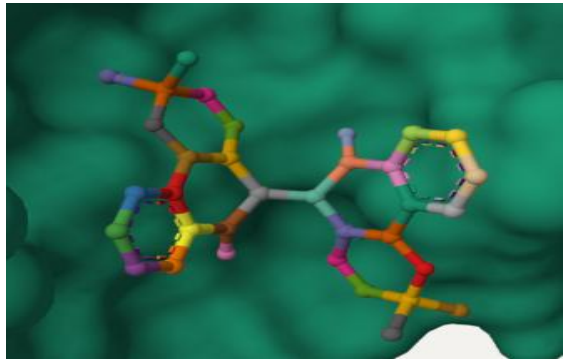




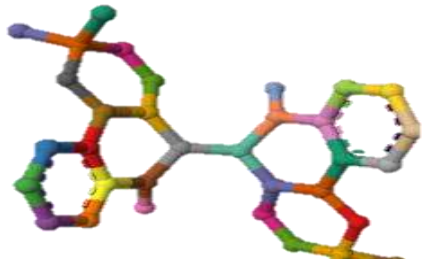
3BPF with Cirsilineol

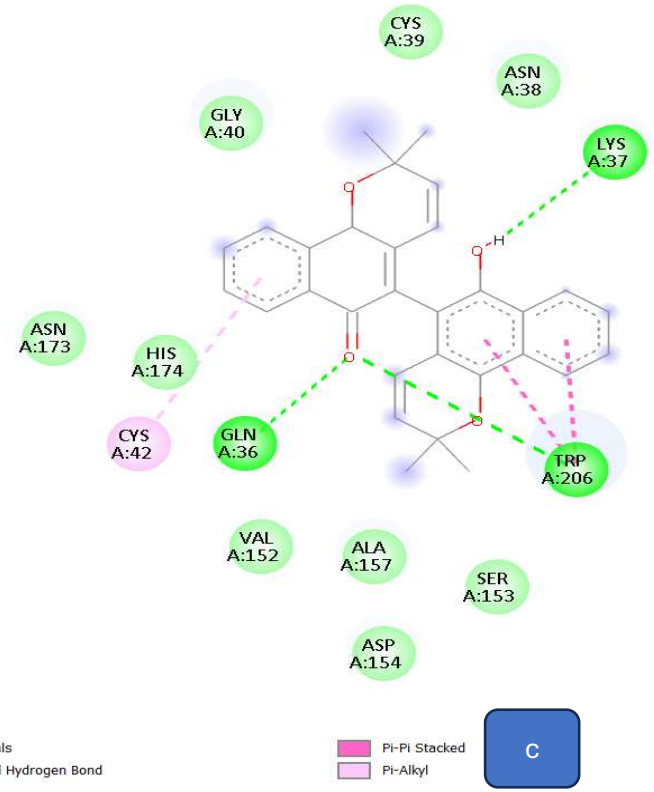


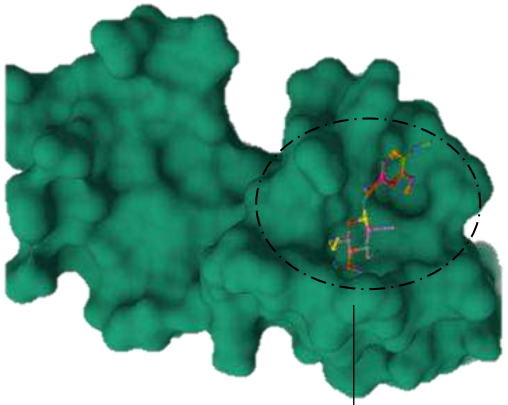


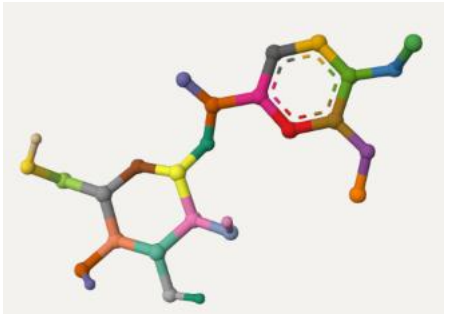


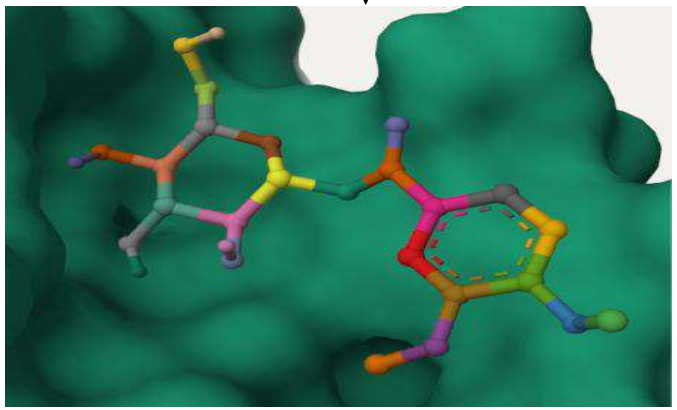
3BPF with Dehydrotectol



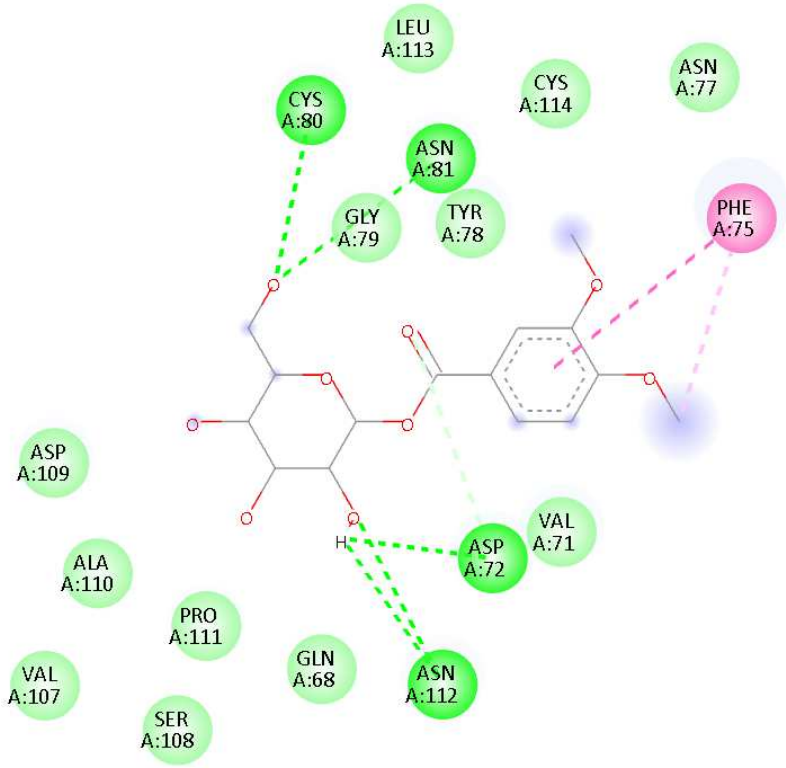


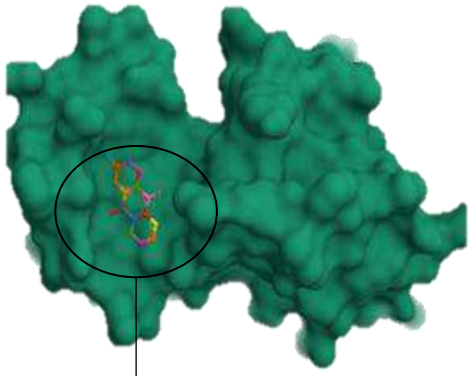




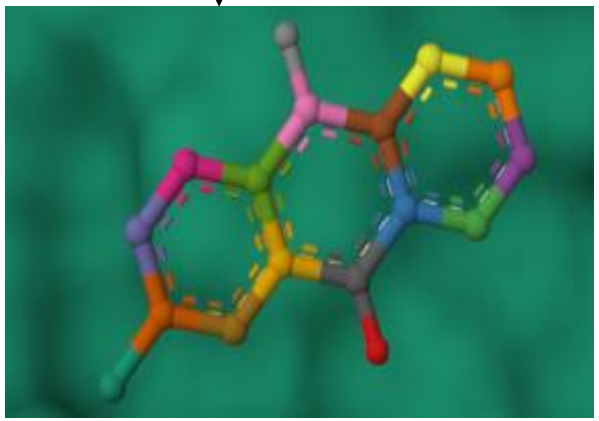


3BPF with 3,4-Dimethoxybenzoic acid β-D-glucopyranosyl ester

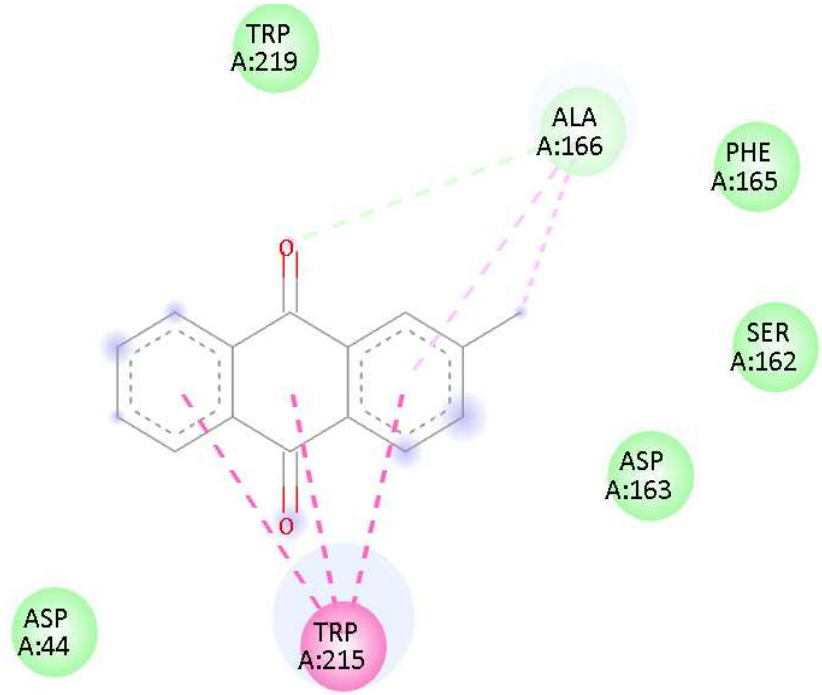




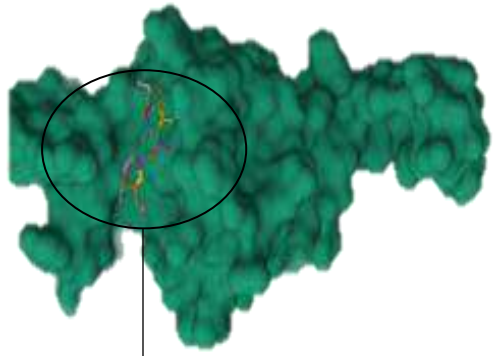


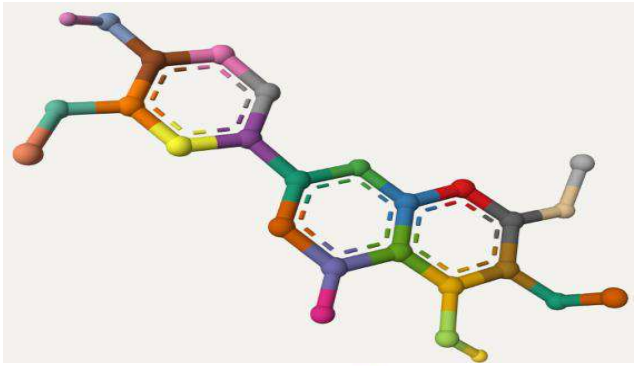


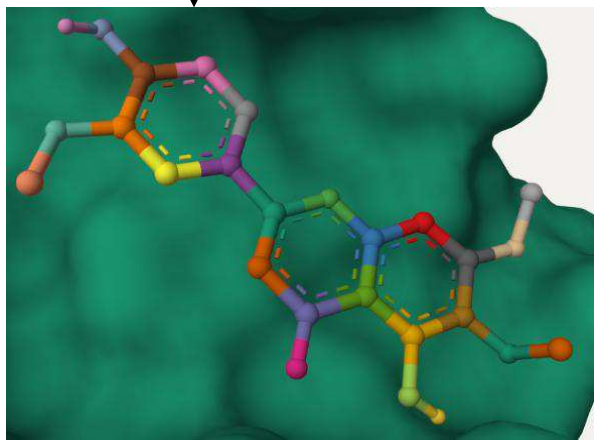
3BPM with 2-Methylanthraquinone



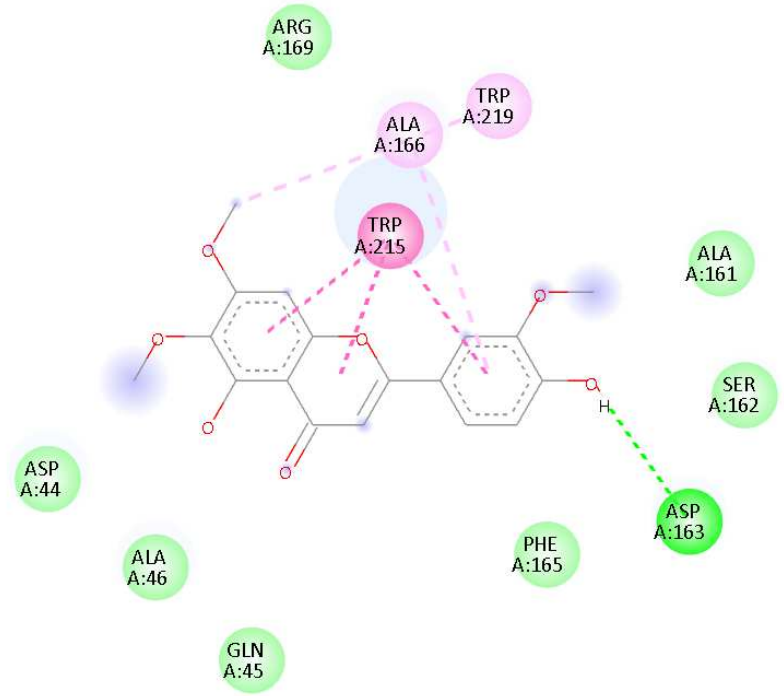






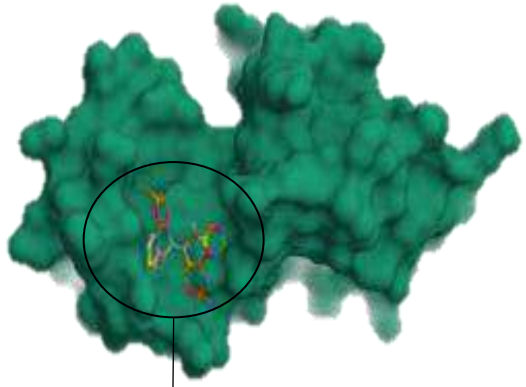


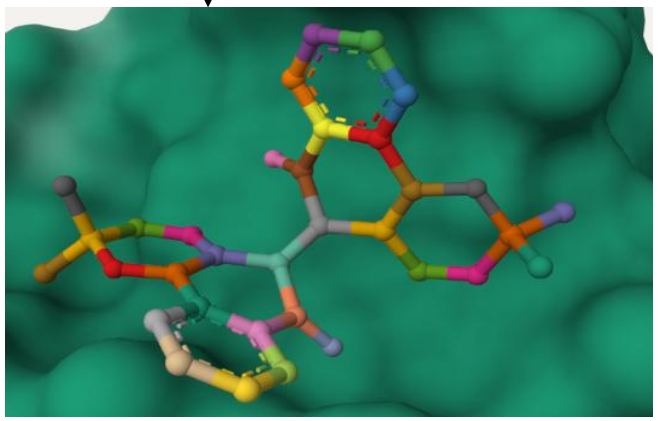
3BPM with Cirsilineol



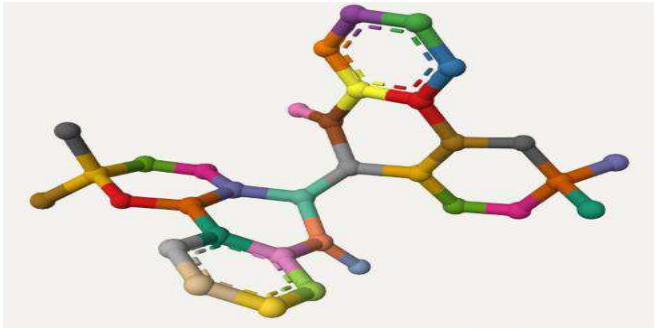


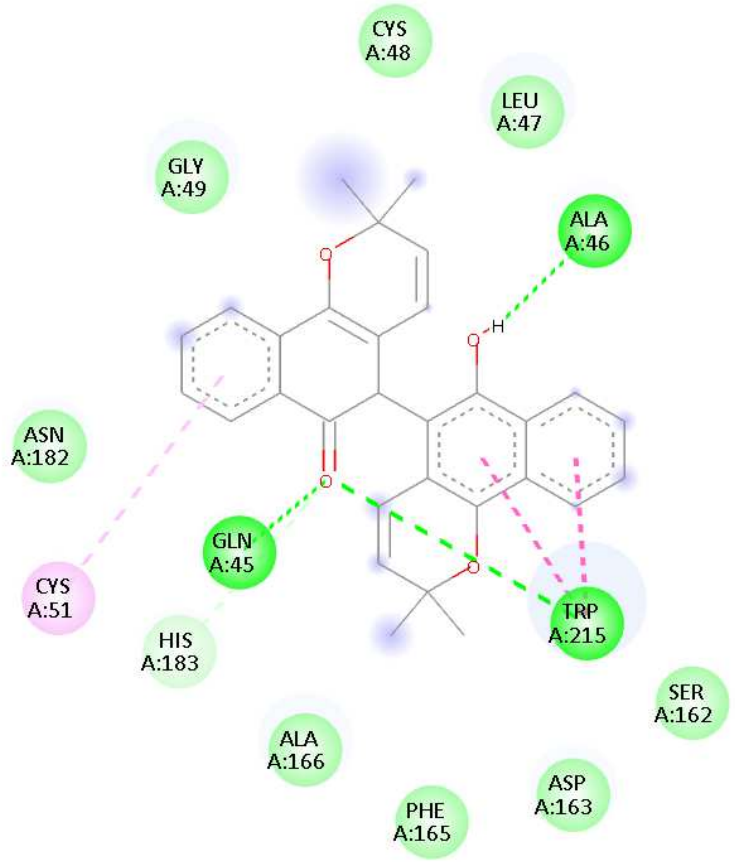
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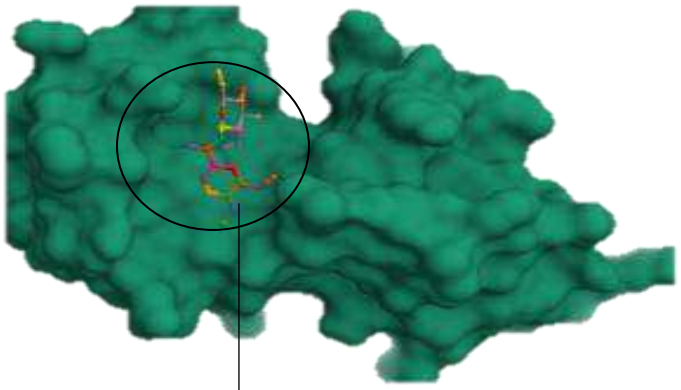


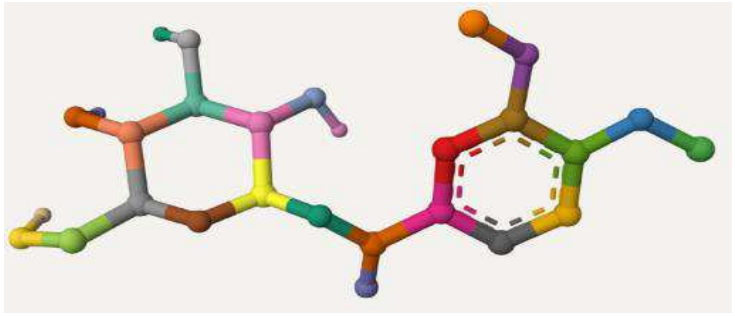


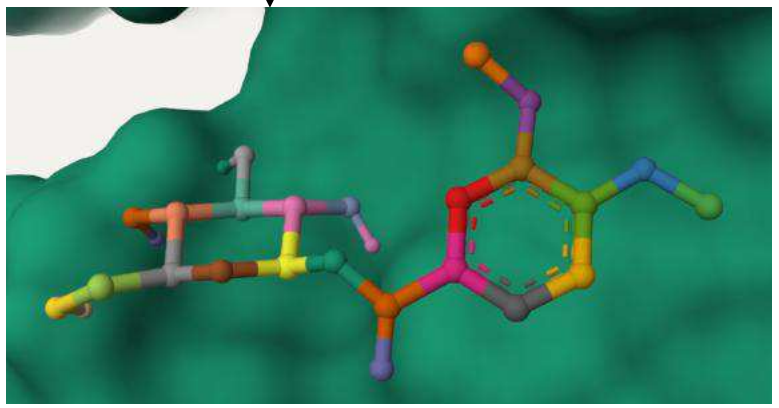
3BPM with Dehydrotectol

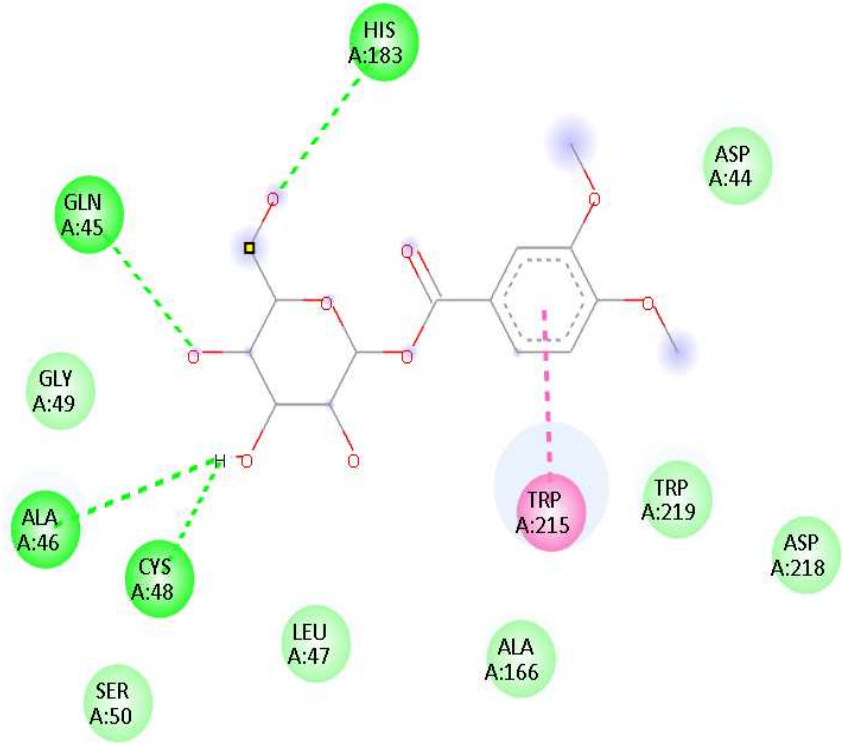






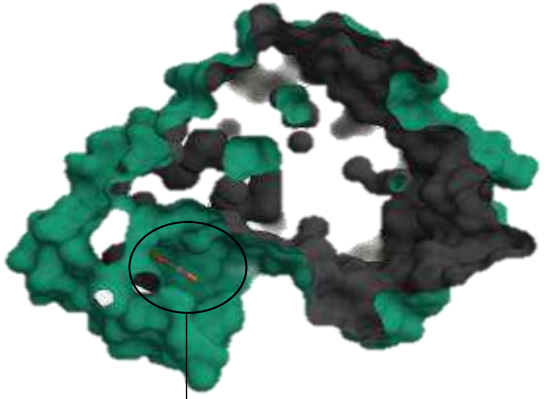




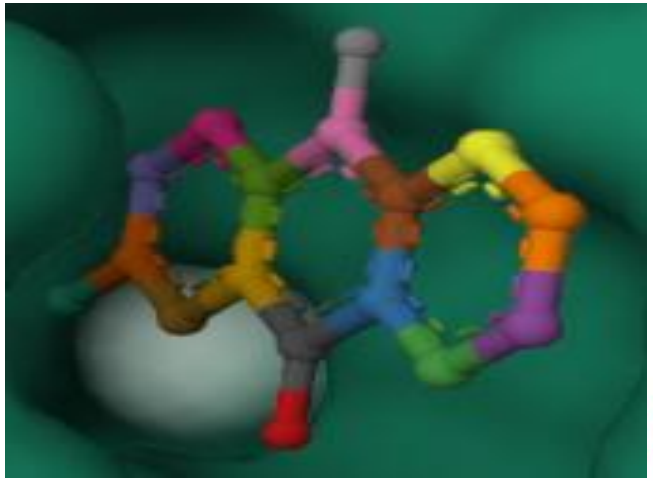


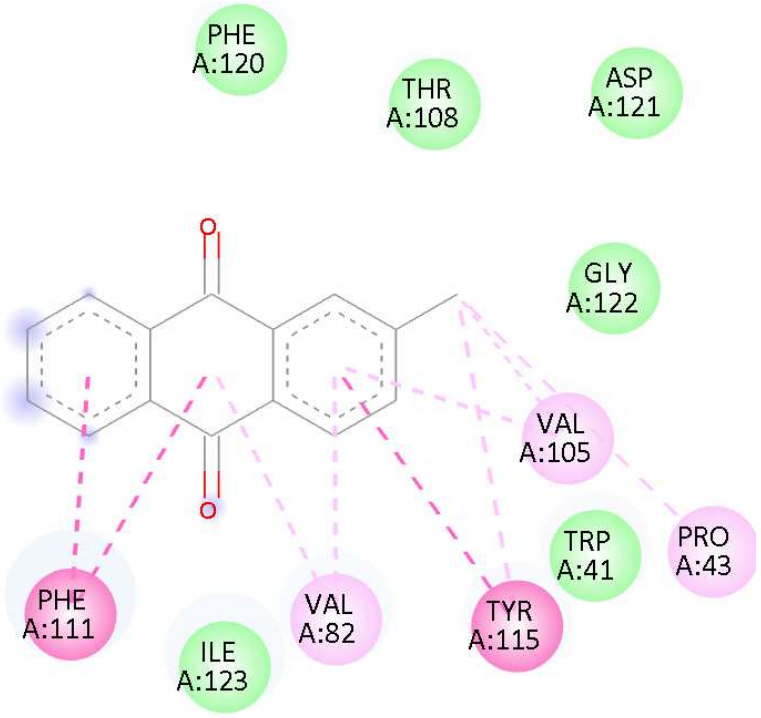
3BPM with 3,4-Dimethoxybenzoic acid β-D-glucopyranosyl ester





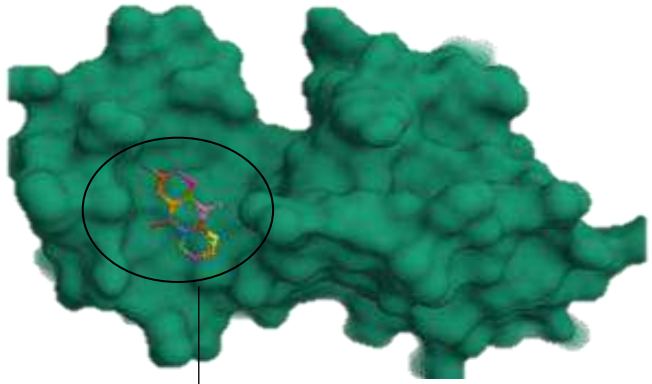


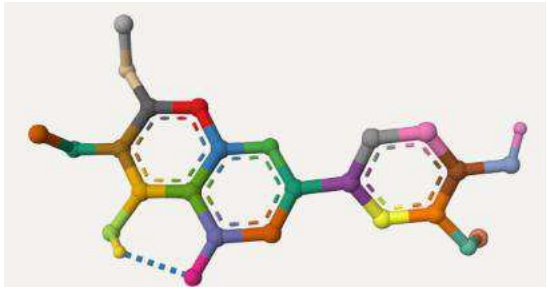


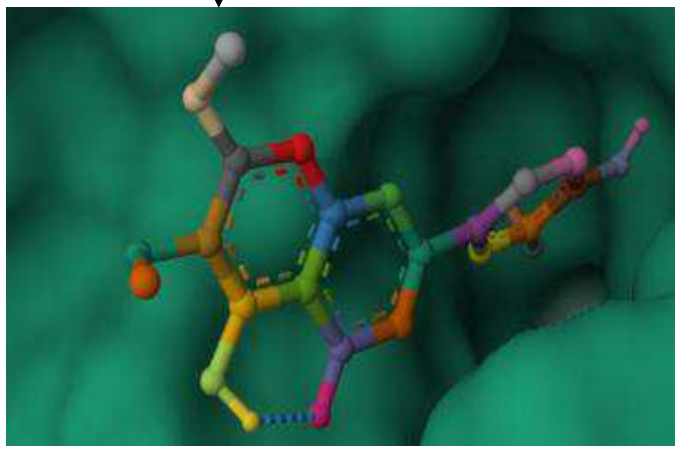




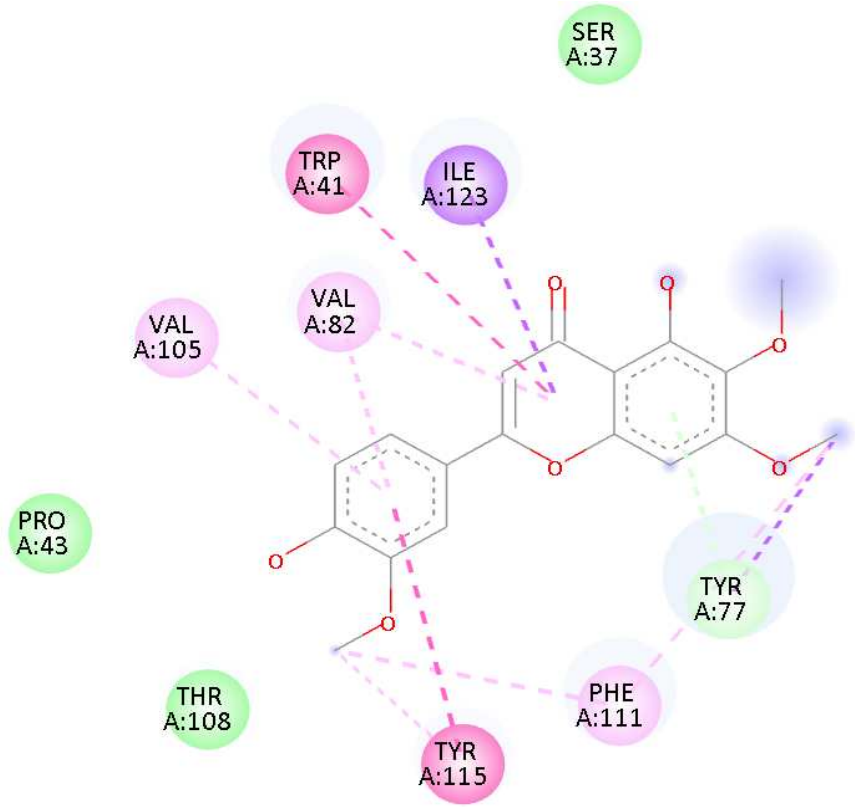
4Z22 with 2-Methylanthraquinone

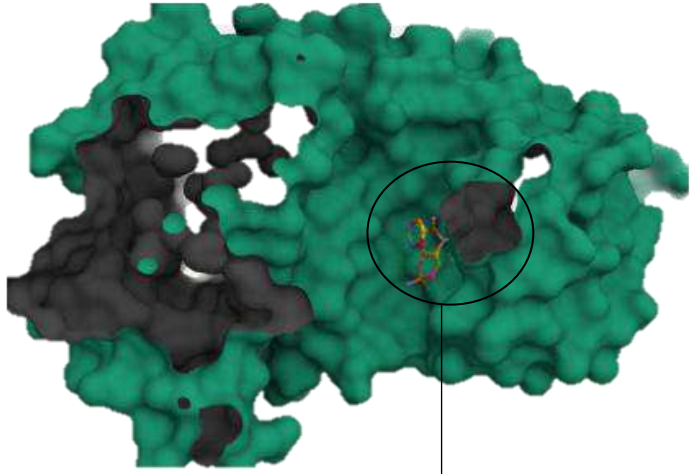


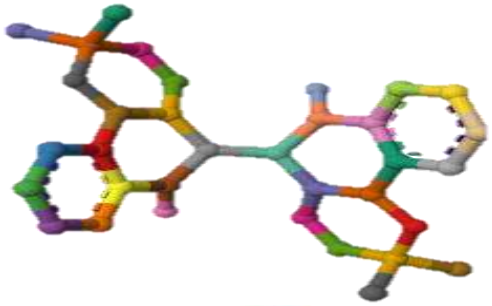


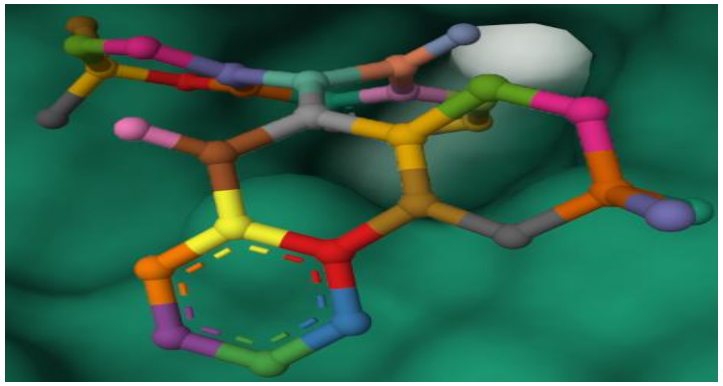


4Z22 with Cirsilineol

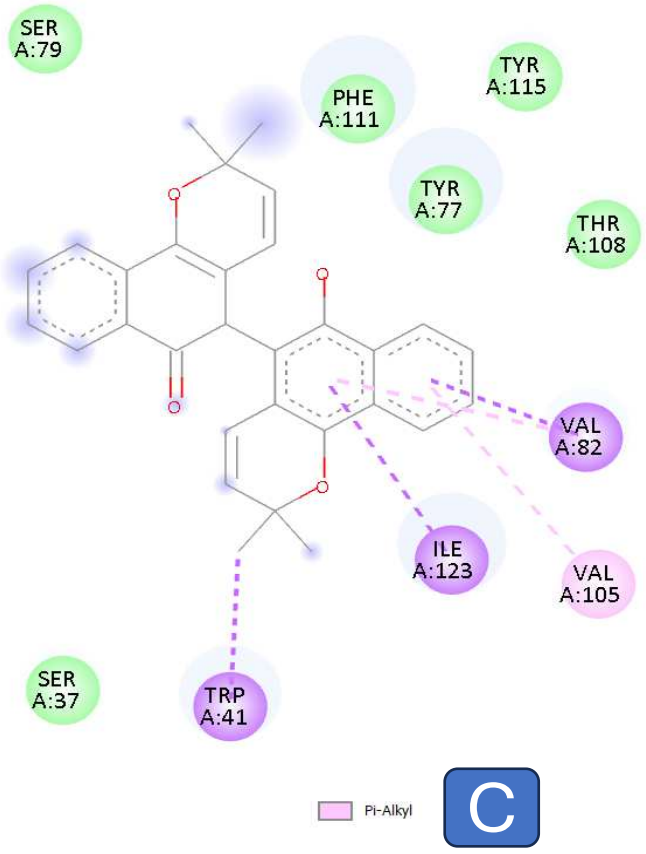


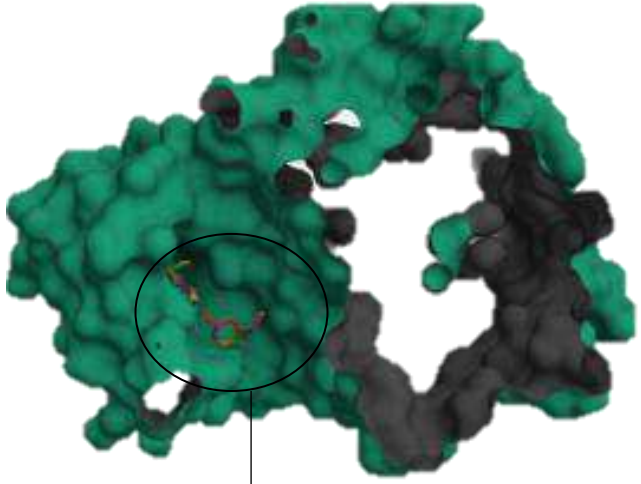


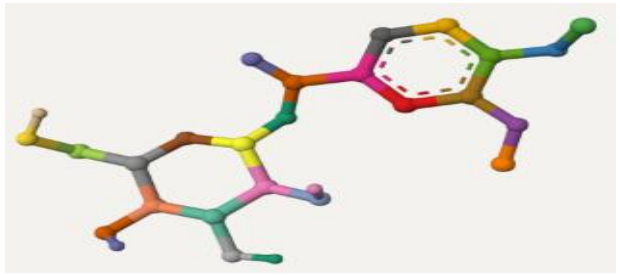


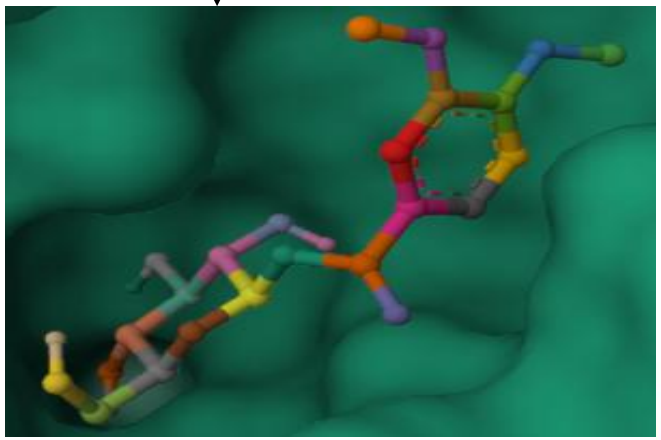


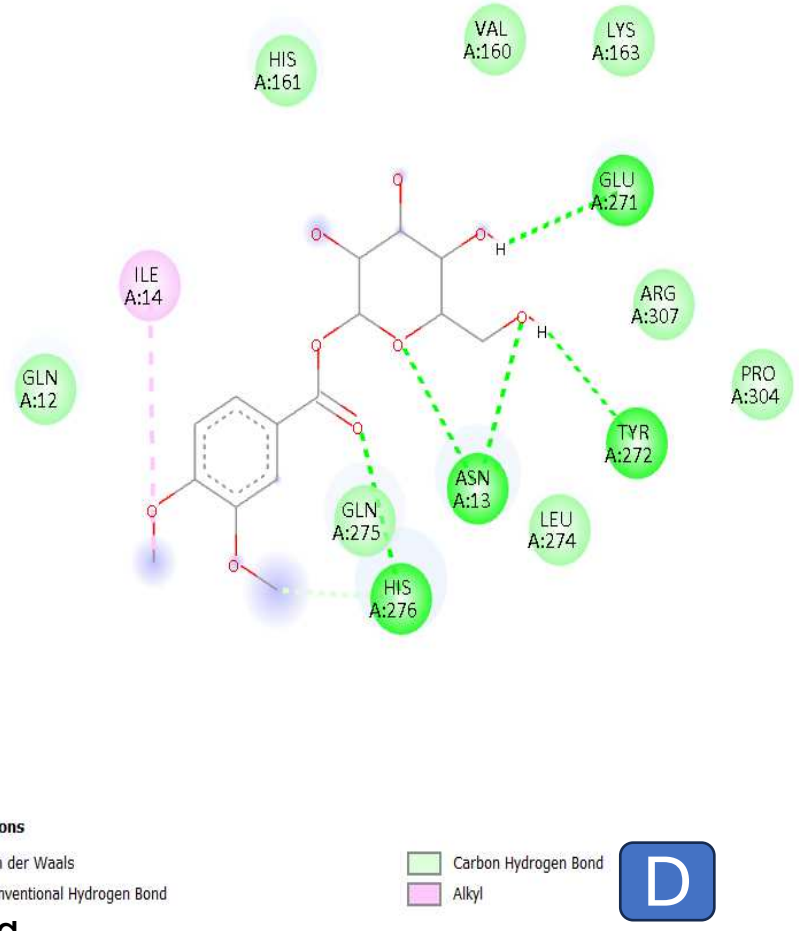
4Z22 with Dehydrotectol











4Z22 with 3,4-Dimethoxybenzoic acıd β-D-glucopyranosyl ester