A Mechanistic Study of Analgesic and Anticancer Activity of unexplored plant Strobilanthes Kunthiana Phytocosntituents using Molecular Docking Studies.

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Research Article

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Abstract

Background: Cancer is one of the leading causes of death worldwide, and the pain associated with it is very intense. Plants are a significant source of medications, particularly anticancer and analgesic medicines. One significant plant, Strobilanthes Kunthiana, is well-known for its assortment of medical applications. As a result, additional studies were carried out using these two Phytocosntituents, lupeol and betulin, to examine their analgesic and anticancer characteristics using PDB IDs 2MUB and 4XI3. The examination on the basis of molecular docking and ADME profiles served as the foundation for this study.

Objective: Based on molecular docking investigations, to suggest a mechanism of Strobilanthes Kunthiana Phytocosntituents for anticancer and analgesic activity.

Method: Molecular docking studies of Phytoconstituents of Strobilanthes Kunthiana were performed using the PyRx Virtual Screening software.

Results: According to the results of molecular docking, numerous ingredients, such as lupeol and betulin exhibit higher dock scores better than standard medications against analgesic and anticancer targets.

Conclusion: Based on molecular docking studies. Various chemical constituents may act as effective inhibitors of various proteins 2MUB, 4XI3. This information can be used to design new anticancer medicines**.**

1.0. Introduction

India is the leading country worldwide as a rich source of medicinal plants with Ayurvedic, Unani, and Siddha medicine. Among them, many plants are unexplored pharmacologically and chemically for medicinal use [1]. Natural substances produced by plants are utilized as complementary treatments and have a significant impact on global health. Plants have given the human race a variety of incredible medical agents and natural chemicals that are the source of all pharmaceuticals. Even if many plants are studied for their potential as medicines, more understudied plants need to be investigated for the same goal [2]. It is commonly known that neelakurinji has both decorative and therapeutic qualities. This plant produces beautiful blue blooms that bloom in a cluster on numerous branches, creating a fantastic visual feast. When the blossom reaches maturity, it turns from light blue to purple-blue. The Western Ghats valleys, where this unusual plant was found, are a popular destination for tourists [3]. S. kunthiana leaf callus extract in vitro provides a crucial component for pharmacological activity [4]. Acute respiratory inflammation, gastrointestinal disorders, rheumatism, anxiolytic, anti-diabetic, laxative, anti-cancer, diuretic, anti-arthritic, and anti-inflammatory activities [5]. This review aims to highlight the biology, pharmacological properties, and conservation status of Neelakurinji. We intend to investigate Neelakurinji's activity by performing virtual docking on cancerous protein for cancer.

1.1. Taxonomy of Neelakurinji

Botanical name: *Strobilanthes Kunthiana, Strobilanthes anamallaica, Strobilanthes heyneanus, Strobilanthes Pulriyensis.*

Kingdom: Plantae, Sub-kingdom: Phanerogamia, Division: Angiospermia, Class: Eudicots

Sub-class: Asterids, Family: Acanthaceae, Genus: Strobilanthe

1.2. Origin

Asia is where this species originated. It is mostly endemic to tropical Asia and Madagascar, although it may also be found in north temperate Asia [5]. The entire plant of S. kunthianus was harvested in Tamilnadu, India's Thalaikuntha area, close to Udhagamandalam. The plant was recognized and verified at the Coimbatore, Tamil Nadu, India location of the Botanical Survey of India (Figure.1).

1.3. Morphology

S. kunthiana is a tiny undershrub that may grow to a height of 30 to 60 cm; occasionally, under congenial conditions, it can reach 2 m or more. An essential part of the understory in tropical evergreen forests is neelakurinji [6]. The farinose indumentum on the bottom leaf surface easily distinguishes Strobilanthes kunthiana from other members of the group. It is arguably the most well-known species of Strobilanthes, and since 1838, 12 mass flowering occurrences every year have been observed [7].

2.0. Plant Biology

The *Strobilanthes* shrubby species are either semelparous, monocarpic, or hapaxanth [8]. Because they only have one chance to reproduce, these Strobilanthes species invest all of their power and energy in huge blooming and fruiting near the end of their lifespan [9]. The several shrubby species of Strobilanthes reach heights of 1 to 7 m and grow vegetative for 3 to 15 years. At the end of their lifespan, they reach the reproductive stage in between 4 and 16 years, burst into synchronized blooming, and cover the completely hill range or the region where they are found [10]. To discuss the evolutionary significance of Strobilanthes kunthiana' synchronized masting and flowering displayed three theories and flower growing shrub has been shown in (Figure. 2) [11]. **(I)** According to the outcrossing theory, simultaneous flowering and a strong visual display improve cross-pollination. Cross-pollination helps to increase species diversity. As a result, the parent plants generate vigorous seedlings and high-quality seeds. **(II)** According to the predator satiation hypothesis, synchronous production causes perennial species to produce more seeds. Predators of seeds can eat seeds during the years when they are being sown, but this will not greatly damage the subsequent generation. They will then perish during the years when no seeds are being sown. Satisfaction of predators is a type of anti-predator adaptation. Due to masting, individual plant species may readily elude seed predators. (III) A third theory contends that interspecific conflict causes monocarpic organisms to exhibit reproductive synchronization.

2.1. Phytoconstituents:

The phytochemical screening of S. *kunthiana* reported the presence of alkaloids, glycosides, saponins, flavonoids, tannins, terpenoids, steroids and phenols. Other varieties of *Strobilanthes Strobilanthes crispus, S. neilgherrensis, Strobilanthes callosus, Strobilanthes ixocephala, Strobilanthes auriculatus, Strobilanthes discolor, Strobilanthes cusia, Strobilanthes cuspidatus, Strobilanthes foliosus, Strobilanthes consanguineus, Strobilanthes gossypinus, Strobilanthes pulneyensis, Strobilanthes perrottetianus, Strobilanthes papillous* [12].

The GC-MS analysis of methanolic extract of callus of S. *kunthiana* identified the 10 bioactive phytoconstituents. The principle compounds were lupeol, Betulin, 9,12-octadecadienoic acid, hexadecenoic acid, methyl ester, 9-octadecenoic acid, methyl ester, alpha-amyrin, β-sitosterol, 4-amino-tetrahydro-2H-pyran-3,5-diol,

Decahydro-1,1,4a,8-tetramethyl phenanthren-2 (1H,3H,4Bh)-one, (Dheptadecanoic acid, 16-methyl-methyl ester, 2,6-bis (1,1-dimethylethyl0-4-methylphenol, 3-methyl-2-ketobutyric acid, 2,2,3,4-tetramethyl-5-hexen-3-ol, N-(tertbutoxycarbonyl)-2(-methoxyphenyl) allylamine, cyclotrisiloxane, hexamethyl, benzene sulfonamide (Fig. 3) [4]. Whereas, phytoconstitiutents lupeol and Botulin were found in larger concentration, Hence, this research approaches to target cancer because cancer is one of the leading causes of death worldwide, and the pain associated with it is very intense. Consequently, more research was conducted employing these two Phytocosntituents lupeol, Betulin to investigate their analgesic and anticancer properties using PDB IDs 2MUB and 4XI3. The 3D structure of PDB IDs 2MUB and 4XI3 has been shown in (Figure. 4). This research was based on the analysis of molecular docking and ADME (Absorption, Distribution, Metabolism and Excretion profiles.

2.2. Pharmacological Properties:

Strobilanthes kunthiana is a rich source of medicinally important Phytocosntituents and produces various pharmacological properties includes antifungal, antibacterial, antiviral, antifungal, anxiolytics, acute respiratory inflammatory, anti-diabetic, stomach ailments, diuretics, laxative, anticancer, anti-arthritic [5], analgesic [13], anti-biofilm [14], enzyme inhibitor, antidepressants [15], anti-giardial activity [16], antiseptic, hypocholesterolemia 5-alpha reductase inhibitor, cytotoxic and protect skin against UV rays [17].

3.0. Materials And Methods

3.1. Chemical constituents utilized in study of molecular docking:

The chemical components of Strobilanthes kunthiana used in molecular docking investigations listed in Table 1.

3.2. The Molecular Targets for the Molecular Docking Studies:

The constituents of Strobilanthes kunthiana were subjected to molecular docking investigations against the various targets protein listed in Figure. 5.

3.3. Molecular Docking of Constituents:

Study were out computationally utilizing PyRx Virtual Screening software for docking studies, the following processes were used.

3.3.1. Protein Molecule Preparation:

The 3D structures of human proteins such as (Analgesic protein PDB ID: 2MUB) and (anticancer PDB ID: 4XI3) protein were obtained from the protein database (PDB) and the proteins were prepared by eliminating extra water content, ligand molecules, and het-atoms. Hydrogen atoms have been introduced, zero-order bonds were established, charges were stabilized, and any deficient disulfide bonds have been fixed using BIOVIA-discovery studio 2021 software. which was then imported PyRx software includes Autodock-vina wizard Python and Open Babel, while Open Babel is used to perform energy minimization on effective ligand molecules, while Vina wizard is used to execute docking on chosen prepared molecules.

3.3.2. Ligand molecule selection:

Study were out computationally utilizing PyRx Virtual Screening software, which has been used to screen libraries of different active chemicals against potential therapeutic targets. From the PubChem database, the active ligand's 3D structure was obtained. While utilizing the molecular programmed PyRx-Python, ligand molecule energy reduction was carried out using PyRx In-builded open Babel tools, while Vina wizard is used to execute docking on chosen prepared molecules

3.3.3. Receptor Grip generation.

Glide molecular docking used the ligand-bounding of the protein's, X ray crystal structure to identify the active site receptor grids and to bind components in multiple potential conformations.

3.3.4 Molecular Docking

Docking was carried out utilizing PyRx Virtual Screening software includes Autodock-vina wizard Python and Open Babel, while Open Babel is used to perform energy minimization of ligand molecules. Whereas, Vina wizard is used to execute docking on chosen prepared molecules. The binding score were calculated in kcal/mol. Various interaction like hydrogen bonding, hydrophilic interaction, hydrophobic, pi-pi stacking and Vander wall interaction were examined.

3.3.5. Assessment of the Docking Study

Based on dock scores and findings from ligand-protein interactions, docking studies were assessed. The components with higher docking scores than the norm interact well with the target protein. Pymol was used to depict the molecular docking study, and BIOVIA-discovery studio 2021 was utilized to investigate the 2D and 3D interaction [18].

3.3.6. Assessment of Constituents' ADME Properties

The constituents' ADME (Absorption, Distribution, Metabolism, and Excretion) properties were assessed using the SwissADME toll. Numerous parameters have been calculated during the ADME study, including molecular mass, hydrogen bond donor and acceptor, solubility, percentage of human oral absorption, the octanol/water partition coefficient (Q logPo/w), the blood brain barrier (BBB) permeability, skin permeability, GI absorption, drug likeness etc.

3.1. Analgesic Activities of Strobilanthes kunthiana:

Phospholipases A2 (PLA2s) are members of an enzyme superfamily that hydrolyzes the sn-2 fatty acids in membrane phospholipids. It is known that these enzymes have wide number of roles in the generation of various lipid mediators as well as the preservation of membrane phospholipid homeostasis. Phospholipase A2 Inhibitors are medications used to treat disorders like peripheral vascular disease that are linked to increased platelet production and platelet aggregation. These medications function by blocking the PLA2 enzyme, which hydrolyzes membrane phospholipids into lysophospholipids and then into platelet-activating factor. The phospholipase A2 enzyme, PDE3, can be inhibited by all of the phytochemicals in Strobilanthes kunthiana. In several physiological functions, including phospholipid digestion and metabolism, host defense, and signal transduction phospholipase A2 is an essential enzyme. Further the COX and LOX enzymes used to convert arachidonic acid into eicosanoids. These eicosanoids from arachidonic acid are essential for triggering immunological responses, inflammation, and the remission of inflammation (Figure. 5) [19].

3.2. Result and Discussion.

Table.1: Docking result and interaction of ligand molecules against target site.

Molecule Name	Target site	PDB ID	Dock score (kcal/mol)	Interacting amino acids residues
Botulin	Analgesic activity	2MUB	-5.8	PHE33, LEU34, TYR32, SER5,ARG31, CYS30
Lupeol	Analgesic activity	2MUB	-6.5	PHE33, TYR32, LEU34, ARG31
Ibuprofen	Analgesic activity	2MUB	-5.1	PHE15, GLY1, TRP14, ILE12, TYR13, ARG17, TYR16
Dexamethasone	Analgesic activity	2MUB	-5.5	PHE33, TYR32, SER5, ARG31, CYS30.
Paracetamol	Analgesic activity	2MUB	-4.1	ILE12, PHE15, THR:2, GLY11.

1) The molecular docking of Botulin against analgesic protein was performed by using PDB ID: 2MUB and dock score − 5.8 kcal/mol was obtained. The active ligand Botulin contain Cyclopentane ring shown Pi-alkyl interaction PHE33 amino acid residue. Whereas, cyclohexane ring enhances hydrophobic interaction by interacting through Vander wall interaction with LEU34, TYR32, SER5, ARG31, CYS30 amino acid residues. 2D, 3D structure of ligand Botulin with receptor site interaction has been shown in (Table. 2) and (Figure no.6).

2) Using PDB ID: 2MUB, the molecular docking of lupeol to an analgesic protein was carried out, and a dock score of -6.5 kcal/mol was achieved. The cyclopentane ring of the active ligand Lupeol forms a Pi-sigma connection with the PHE33 amino acid residue, and the cyclopentane rings contain electron-donating group interacts with the TRY32 and LEU34 amino acids, which are involved in a hydrophobic interaction. In contrast, the cyclohexane ring has a hydroxyl group that forms a hydrogen connection with the amino acid residue ARG31. The receptor site interaction and 2D and 3D structures of the ligand Lupeol have been shown in (Table .2) and (Figure no.7). The standard compound dexamethasone and Ibuprofen shows docking score − 5.5 And − 5.1 kcal/mol lesser than the ligand Botulin and lupeol, are assessed for analgesic activity. Dexamethasone contain cyclopentane ring exhibit hydrophobic Pi-alkyl interaction with PHE33 amino acid reside and Ibuprofen contain hydroxyl group shows hydrogen bonding with PHE15 amino acid, whereas, substituted phenyl ring shows Pi-cation interaction with GLY11 (glycine) and hydrophobic interaction Pi-alkyl, alkyl, Pi-Pi stacked interaction with TRP14, ILE12. The receptor site interaction and 2D and 3D structures of the ligand Lupeol, Dexamethasone and Ibuprofen have been shown in (Table. 2) and (Figure. 7, 8, 9).

4.0. Anticancer Activity

The second most common cause of mortality for women is breast cancer. The FDA has authorized a number of medications for the treatment of BC. The development of drug resistance, toxicity, and selectivity issues are the main limitations of currently available medications. Other treatments, such as hormone therapy, surgery, radiation, and immunological therapy, are also in use, but they have adverse reactions, including bioavailability

difficulties, non-selectivity, and pharmacokinetic-pharmacodynamics complications. Therefore, it is necessary to promote new molecules that are less harmful and more successful at treating cancer. Due to their ability to treat cancer with the fewest adverse effects, the Strobilanthes Kunthianus plant recently came in the picture and our effort to evaluate the receptor binding through docking studies (Figure. 10) [20].

Cancer is the sixth leading cause of death worldwide. According to the WHO, there were 18.2 million cancer cases reported globally in 2018–2019, and there were 9.7 million cancer deaths overall. Nearly 2,680 instances are identified in men, and there are an estimated 268.700 cases of invasive breast cancer and 48200 cases of ductal carcinoma in women. Due to breast cancer, around 41,760 women and 500 men died [21]. Androgen is converted into oestrogen by the enzyme known as aromatase. Breast tissue expresses more cytochrome-450 aromatase enzymes. Breast cancer may occur as a consequence of oestrogen production that is too high [22]. The second most prevalent cause of death for women is breast cancer. The main sources of oestrogen release in premenopausal women are the ovaries and breast, while in postmenopausal women the main sources are the liver and adipose tissue [23, 24]. Antagonizing oestrogen production and release is the greatest therapy, since breast cancer needs oestrogen to continue developing and progressing [25]. As a consequence, Strobilanthes Kunthiana, which has Lupeol and Botulin as its main constituents and has steroid moiety, can inhibit the aromatase enzyme, which prevents breast cancer from progressing.

4.1. Result and Discussion against cancer protein.

Table 3
Docking result and interaction of ligand molecules against cancer target site.

Molecule Name	Target site	PDB ID	Dock score (kcal/mol)	Interacting amino acids residues
Botulin	Breast Cancer protein	4XI3	-6.5	PHE33, LEU34, TYR32, SER5,ARG31, CYS30
Lupeol	Breast Cancer protein	4XI3	-7.1	PHE33, TYR32, LEU34, ARG31
Azathioprine	Breast Cancer protein	4XI3	-7.0	THR347, LEU346, PHE404, LEU349, ALA350, GLU353, ARG394, LEU387.

1) Botulin was molecularly docked against a cancer protein using PDB ID: 4XI3, and a dock score of -6.5 kcal/mol was achieved. In addition to other rings involved in vander wall interaction, the active ligand Botulin has a cyclohexane ring with a hydroxyl group that forms hydrogen bond with ASP321 amino acid residue. ligand Botulin's 2D and 3D structures and interactions with receptor sites have been shown in (Table. 4) and (Figure.11).

Lupeol was molecularly docked against a cancer protein using PDB ID: 4XI3, and a docking score of -7.1 kcal/mol was achieved. The active ligand Lupeol has cyclohexane ring forms hydrogen bond with GLN441 amino acid residue, in addition to other rings involved in vander wall interaction. Ligand Lupeol 2D and 3D structures and interactions with receptor sites have been shown in (Table. 4) and (Figure.12). The docking score of Lupeol and Botulin was compared against standard anticancer agents Azathioprine and dock score was 7.0 kcal/mol. It exhibits that Lupeol has higher docking score then the Azathioprine. Hence further biological, clinical

and micro label study still required to assessed the activity of active ligand molecules. Whereas, 2D, 3D structure of Azathioprine has been shown in (Table 4) and (Fig. 13).

5.0. Adme Properties Of The Constituents

The Constituents with Better Docking Scores Than the Respective Standard had Their ADME Properties examined, and the Results are Summarized in (Table 5–9). The Constituents of strobilanthes kunthiana with Better Docking Scores Than the Respective Standard had their ADME Propertiesevaluated. During ADME measurement, an even more refined set of parameters is used that provides greater understanding of the evaluation of drug action in silico, such as the molecular mass lower than 500 Daltons [26]. partition coefficient QPlog Po/w), permissible limits is (-2 to 6.5) [27]. Number of heavy atoms, hydrogen bond donor (Permeable limit less than 5) and hydrogen bond acceptor (Permeable limit less than 10. Log *S* (ESOL) water solubility range, insoluble <-10 < poorly < -6 < moderately < -4 < soluble < -2 < very soluble < 0 < highly. Gastrointestinal absorption, blood-brain barrier (QPlogBB) gives permeability. Drugs with a value of > 0.3 easily penetrate the blood-brain barrier, while those with a value of 1.0 are poorly dispersed to the brain, Its normal range is from − 2.00 to + 1.00 [28]. Pharmacokinetic Log K_p to (skin permeation). Drug-likeness according to Lipinski, Ghose, veber, egan rule. The boiled egg structure, yellow colour represhant (BBB) blood brain barrier permeability, and white colour HIA represent absorption capability from intestine Hence the various constituents can absorb from intestine as well permeable from blood brain barrier (Figure. 14–19). Whereas, ADME studies of all constituent has been shown in Table 5–9. In silico ADME studies revealed that the majority of compounds' various properties, including QPlog Po/w, GI absorption, Log *S* (ESOL) and QPlogKp, were within an acceptable range.

Table 5
Smile form, molecular weight of all dock compounds.

Compound	Canonical SMILES	Formula	Molecular Weight
Lupeol	CC(= C) [CH]1CC[C]2([CH]1[CH]1CC[CH]3[C]([C]1(C)CC2) (C)CC[CH]1[C]3(C)CC[CH](C1(C)C) O) C	C30H500	426.72
Botulin	OC[C]12CC[CH]([CH]2[CH]2[C](CC1) (C)[C]1(C)CC[CH]3[C] ([CH]1CC2) (C)CC[CH](C3(C)C) O) C(= C) C)	C30H5002	442.72
Ibuprofen	CC(Cc1ccc(cc1) C(C(= O) O) C) C	C13H18O2	206.28
Dexamethasone	OCC(= O) [C]1(O)[CH](C)C[CH]2[C]1(C)C[CH](O) [C]1([CH]2CCC2 = CC(= O) C = C[C]12C) F	C22H29FO5	392.46
Paracetamol	CC(= O) Nc1 ccc (cc1) O	C8H9NO2	151.16
Azathioprine	NSc1nc2c([NH]1) cncn2	C5H5N5S	167.19

Table 6
Various variability parameter of all docked compounds.

Molecule Number	Heavy atoms Num.	Aromatic heavy atoms	Fraction Csp3	Rotatable bonds Number	H-bond acceptors Num.	H-bond donors	Molar refractivity
Lupeol	31	0	0.93	1	1	1	135.14
Botulin	32	0	0.93	2	2	2	136.30
Ibuprofen	15	6	0.46	4	2	1	62.18
Dexamethasone	28	0	0.73	2	6	3	101.96
Paracetamol	11	6	0.12	2	2	2	42.78
Azathioprine	11	9	0.00	1	4	2	41.31

Table 7
Lipophilicity study all docked compounds.

Molecular Number	Lipophilicity iLOGP	Lipophilicity XLOGP3	Lipophilicity WLOGP	Lipophilicity MLOGP	Lipophilicity SILICOS-IT	Consensus Log P o/w
Lupeol	4.72	9.87	8.02	6.92	6.82	7.27
Botulin	4.47	8.28	7.00	6.00	6.21	6.39
Ibuprofen	2.17	3.50	3.07	3.13	3.15	3.00
Dexamethasone	2.29	1.94	2.32	1.62	2.58	2.15
Paracetamol	1.21	0.46	1.16	0.91	0.89	0.93
Azathioprine	0.30	-0.20	0.32	-1.63	0.55	-0.13

Table 8
Pharmacokinetic, water solubility study of all docked compounds.

Molecule Number	Water solubility Log *S* (ESOL)	Pharma cokinetic GI absorption	Pharma cokinetic BBB permeant	Pharma cokinetic P-gp substrate	Pharma cokinetic CYP1A2 inhibitor	Pharma cokinetic CYP2C19 inhibitor	Pharma cokinetic CYP2C19 inhibitor
Lupeol	-8.64	Low	No	No	No	No	No
Botulin	-7.67	Low	No	No	No	No	No
Ibuprofen	-3.36	High	Yes	No	No	No	No
Dexamethasone	-3.36	High	No	Yes	No	No	No
Paracetamol	-1.34	High	Yes	No	No	No	No
Azathioprine	-1.29	High	No	No	No	No	No

Table 9
ADME studies of all docked compounds.

Molecule Number	Pharmacokinetic CYP2D6 inhibitor	Pharmacokinetic CYP3A4 inhibitor	Pharmacokinetic Log K_p (skin permeation)	Drug likeness Lipinski	Drug likeness Ghose	Drug likeness Veber	Drug likeness Egan
Lupeol	No	No	-1.90 cm/s	Yes; 1 violation: MLOGP > 4.15	No; 3 violations: WLOGP > 5.6, MR > 130, atoms > 70	Yes	No; 1 violation: WLOGP > 5.88
Botulin	No	No	-3.12 cm/s	Yes; 1 violation: MLOGP > 4.15	No; 3 violations: WLOGP > 5.6, MR > 130, atoms > 70	Yes	No; 1 violation: WLOGP > 5.88
Ibuprofen	No	No	-5.07 cm/s	Yes; 0 violation	Yes	Yes	Yes
Dexamethasone	No	No	-7.32 cm/s	Yes; 0 violation	Yes	Yes	Yes
Paracetamol	No	No	-6.90 cm/s	Yes; 0 violation	No; 1 violation: MW < 160	Yes	Yes
Azathioprine	No	No	-7.46 cm/s	Yes; 0 violation	No; 1 violation: atoms < 20	Yes	Yes

Conclusion

Numerous Strobilanthes kunthiana chemical components were docked against the proteins with the PDB IDs 2MUB, 4XI3. This research over its constituents demonstrated that many Phytocosntituents, such as lupeol and Botulin, had better docking scores than standard medications against various bacterial targets (As shown in Table 1,2,3,4), indicating that they may act by inhibiting such proteins and that may be used as a strike or lead for the development of novel anticancer agents against corresponding biological targets.

Declarations

Ethical Approval: Not applicable

Competing interests: Not applicable

Authors' contributions: Girish Chandra Arya has completed all docking studies, Vikash Jakhmola did mechanistic portion, Shefali Mehla compiled pharmacological Properties, Neeraj Bainsal prepared

Pharmacognostic studies of Strobilanthes kunthiana.

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Tables

Table 2 and 4 are available in the Supplementary Files section

Figures

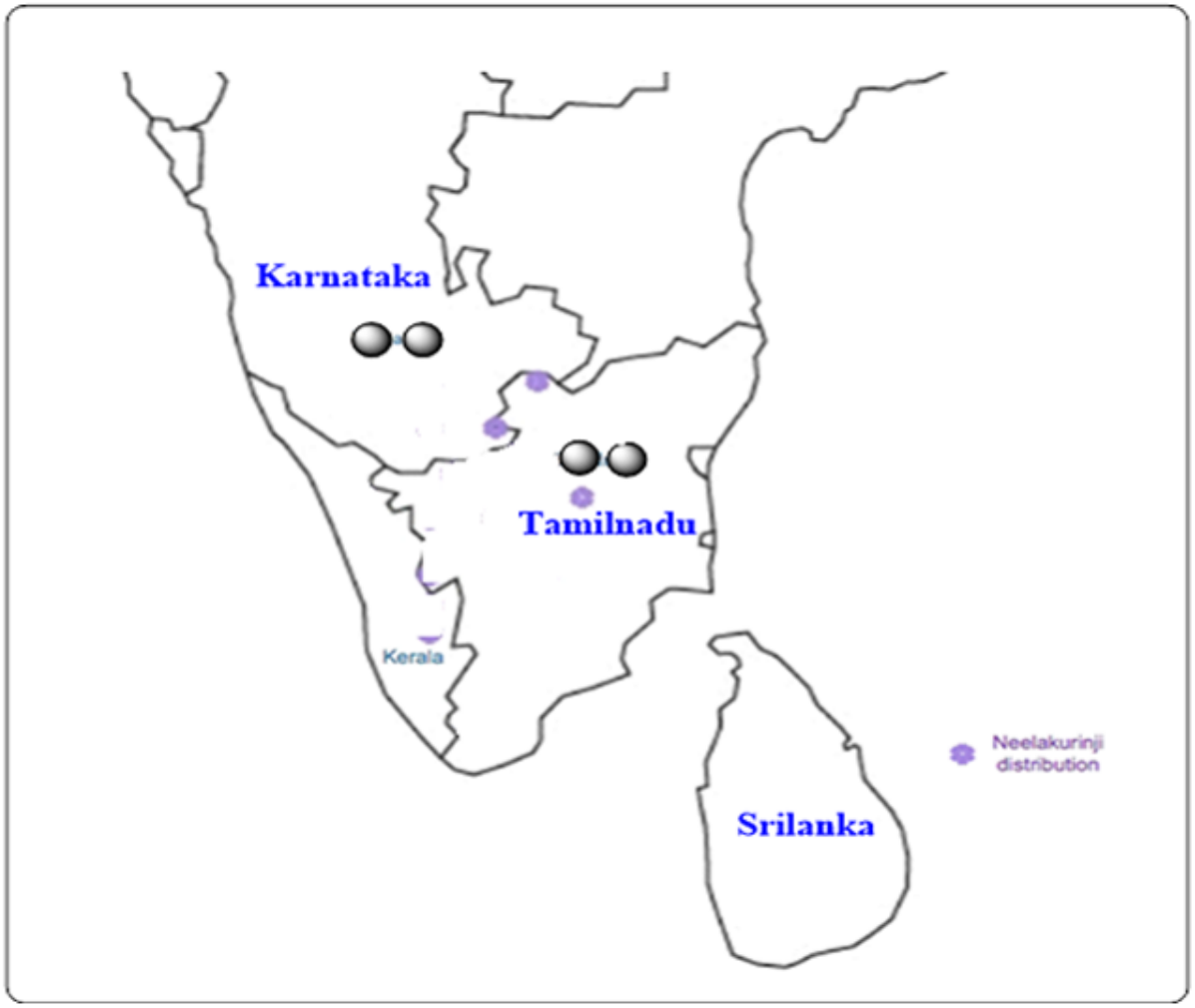

Figure 1

Distribution of Strobilanthes Kunthianus in Indian origin.

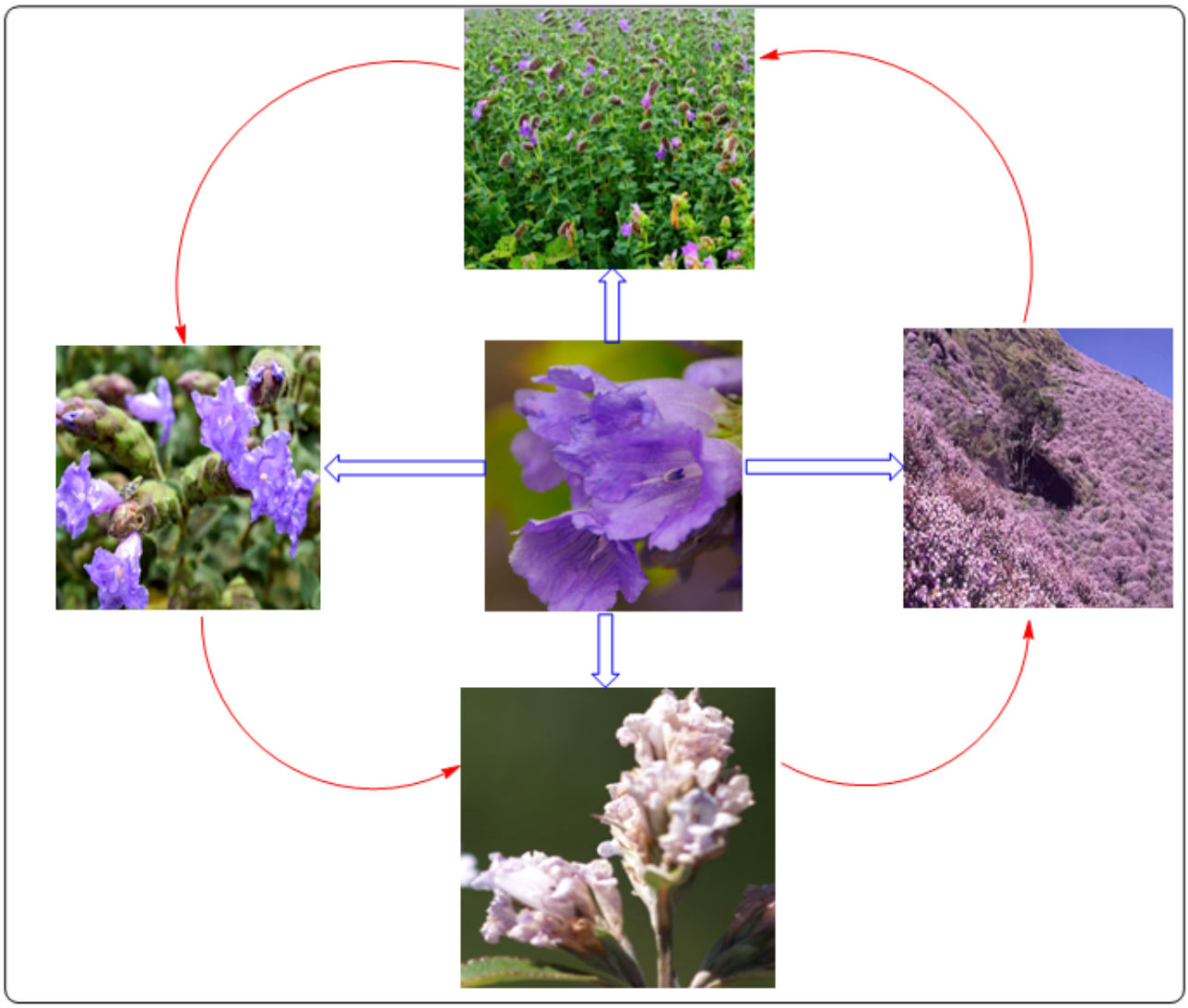

Figure 2

Flower growing shrub of *Strobilanthes Kunthiana*.

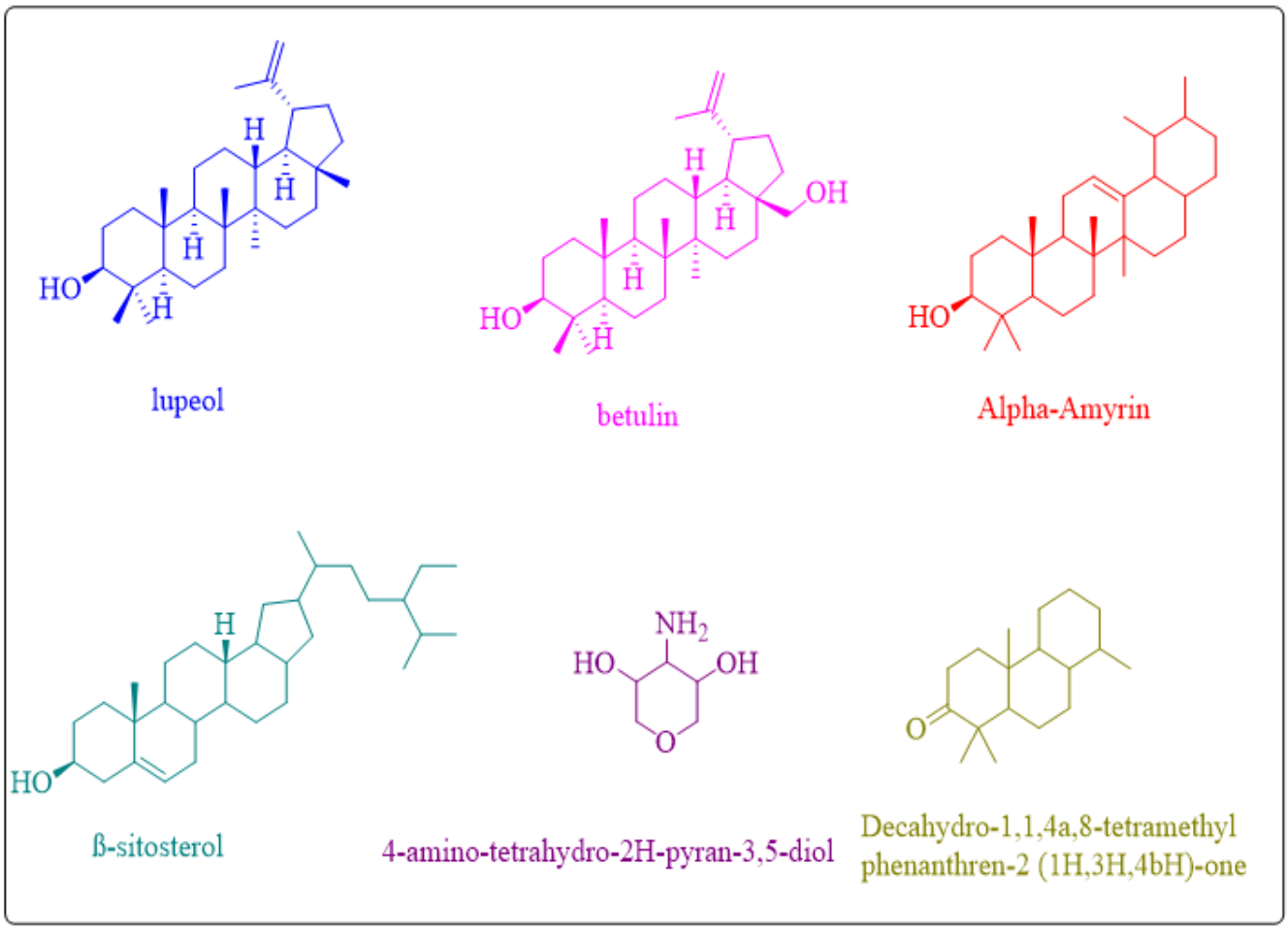

Figure 3

Chemical structure of *S. kunthianus* compounds that have been identified.

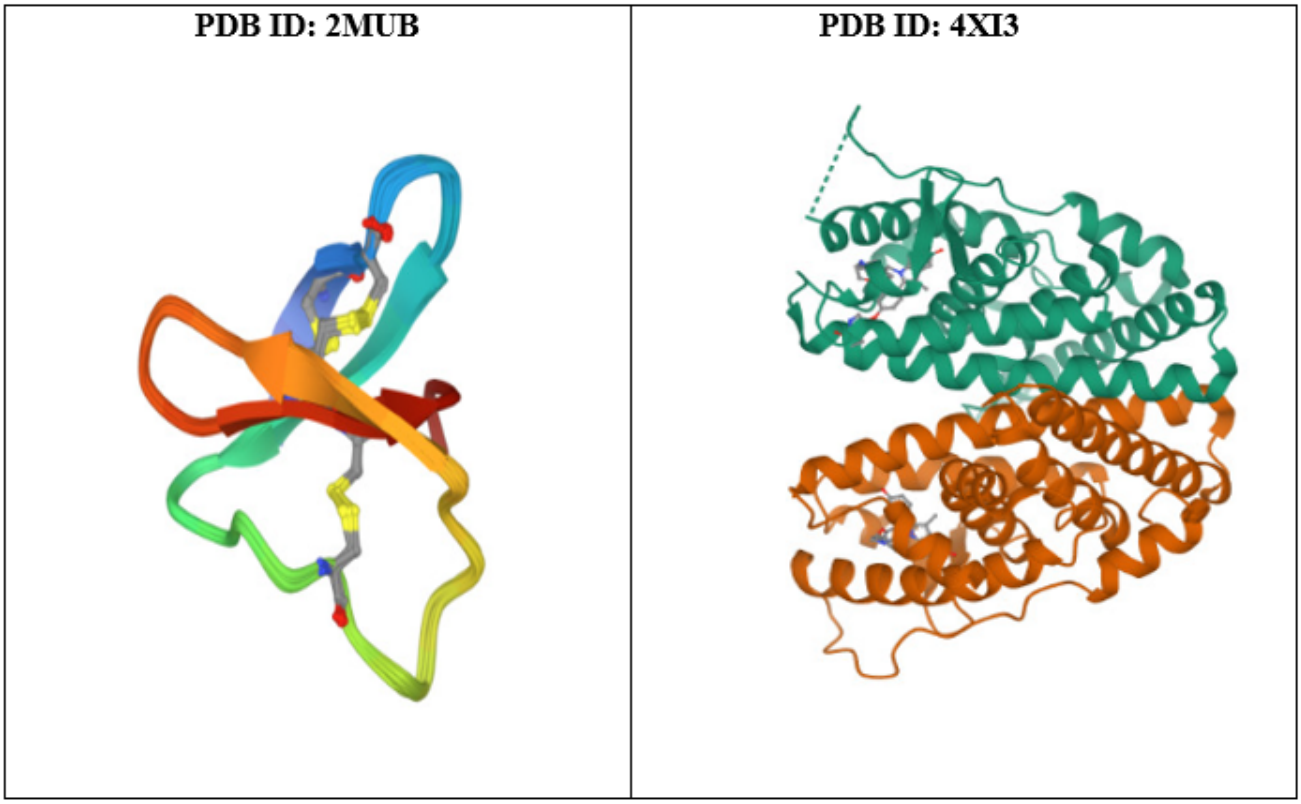

Figure 4

3D structure of Protein 2MUB and 4XI3.

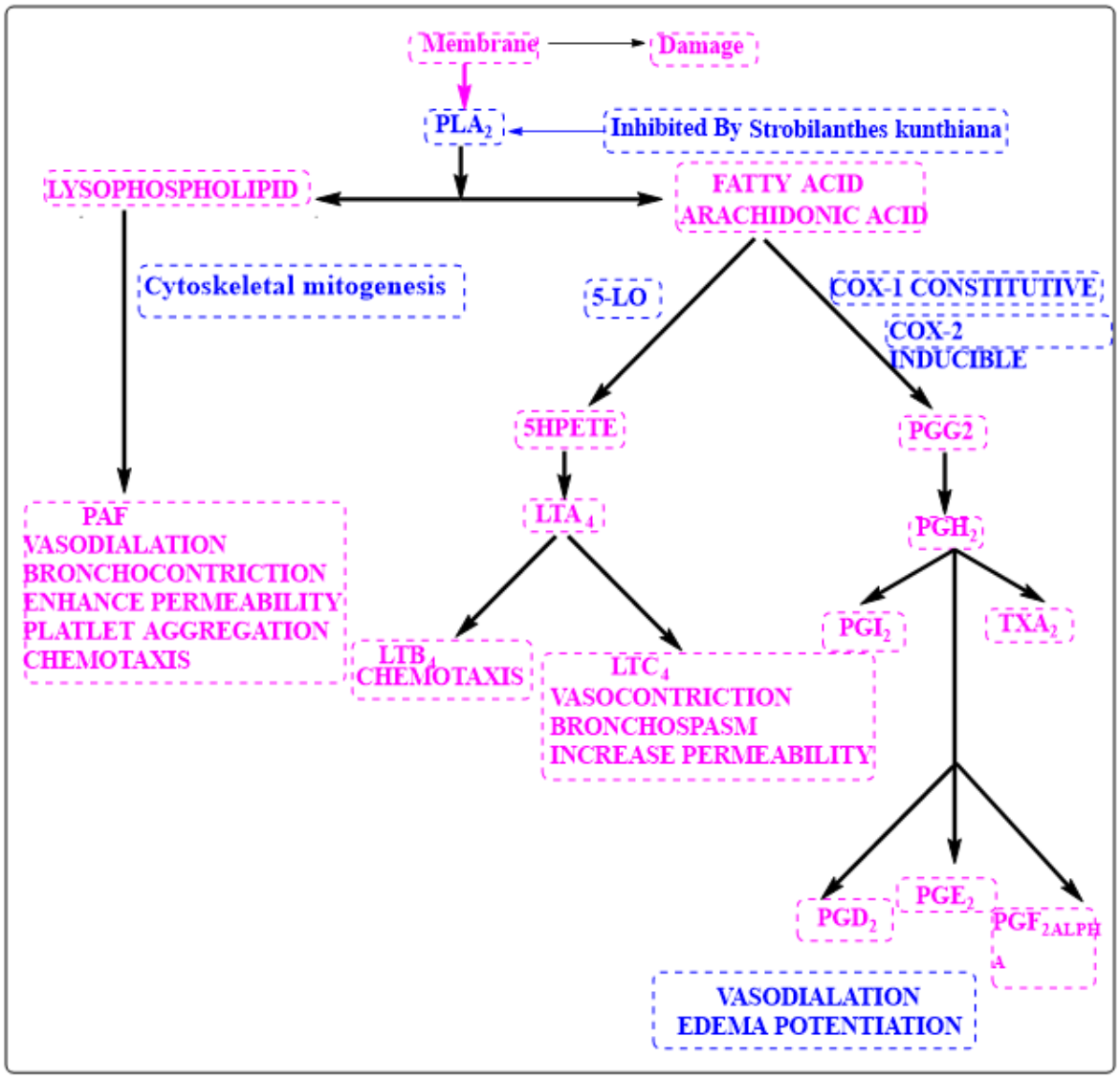

Figure 5

Mechanism of action involved in phospholipase A2 inhibition.

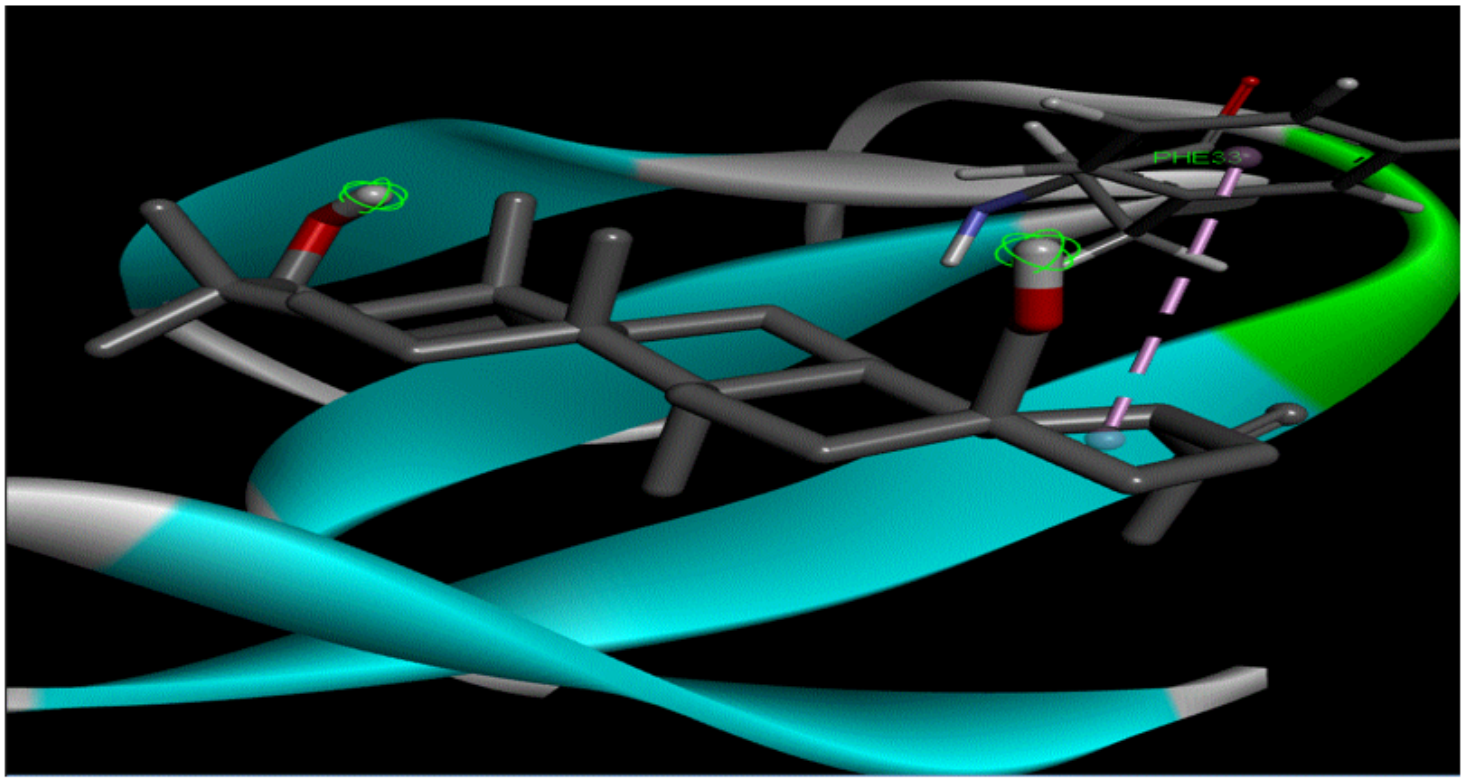

Figure 6

3D structure of Botulin against Analgesic receptor using PDB ID: 2MUB.

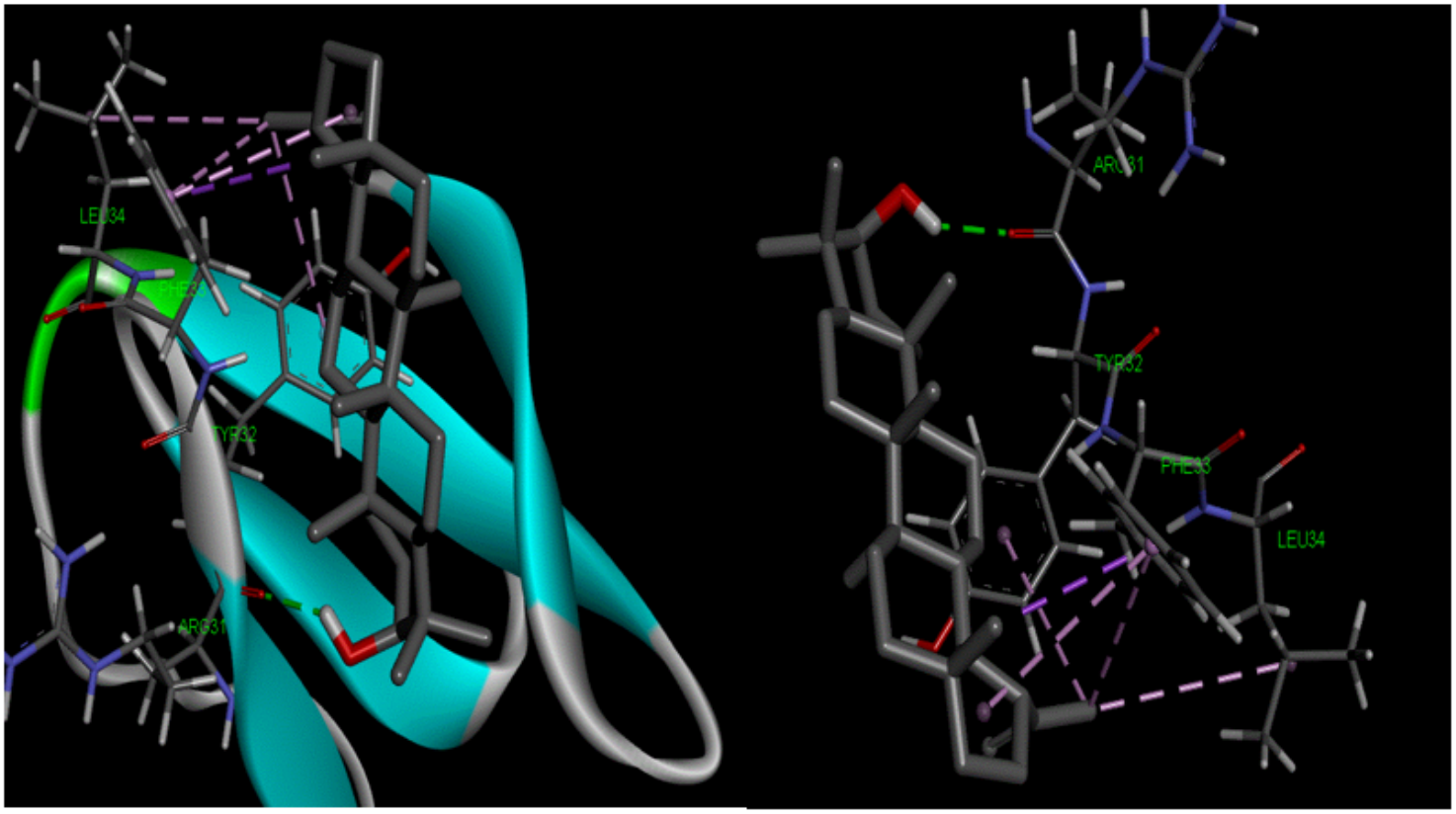

Figure 7

3D structure of Lupeol against Analgesic receptor using PDB ID: 2MUB.

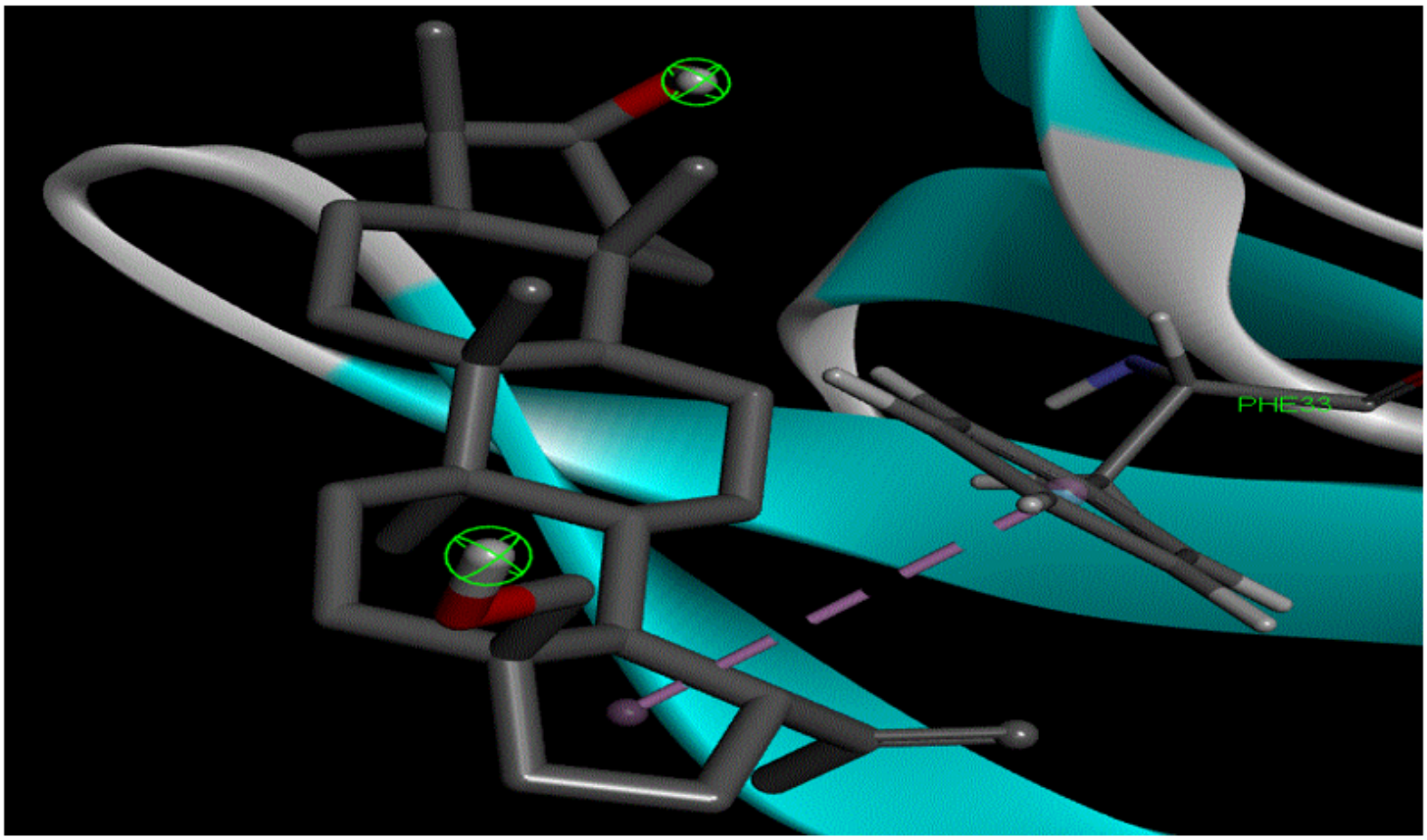

Figure 8

3D structure of Standard Dexamethasone against Analgesic receptor using PDB ID: 2MUB.

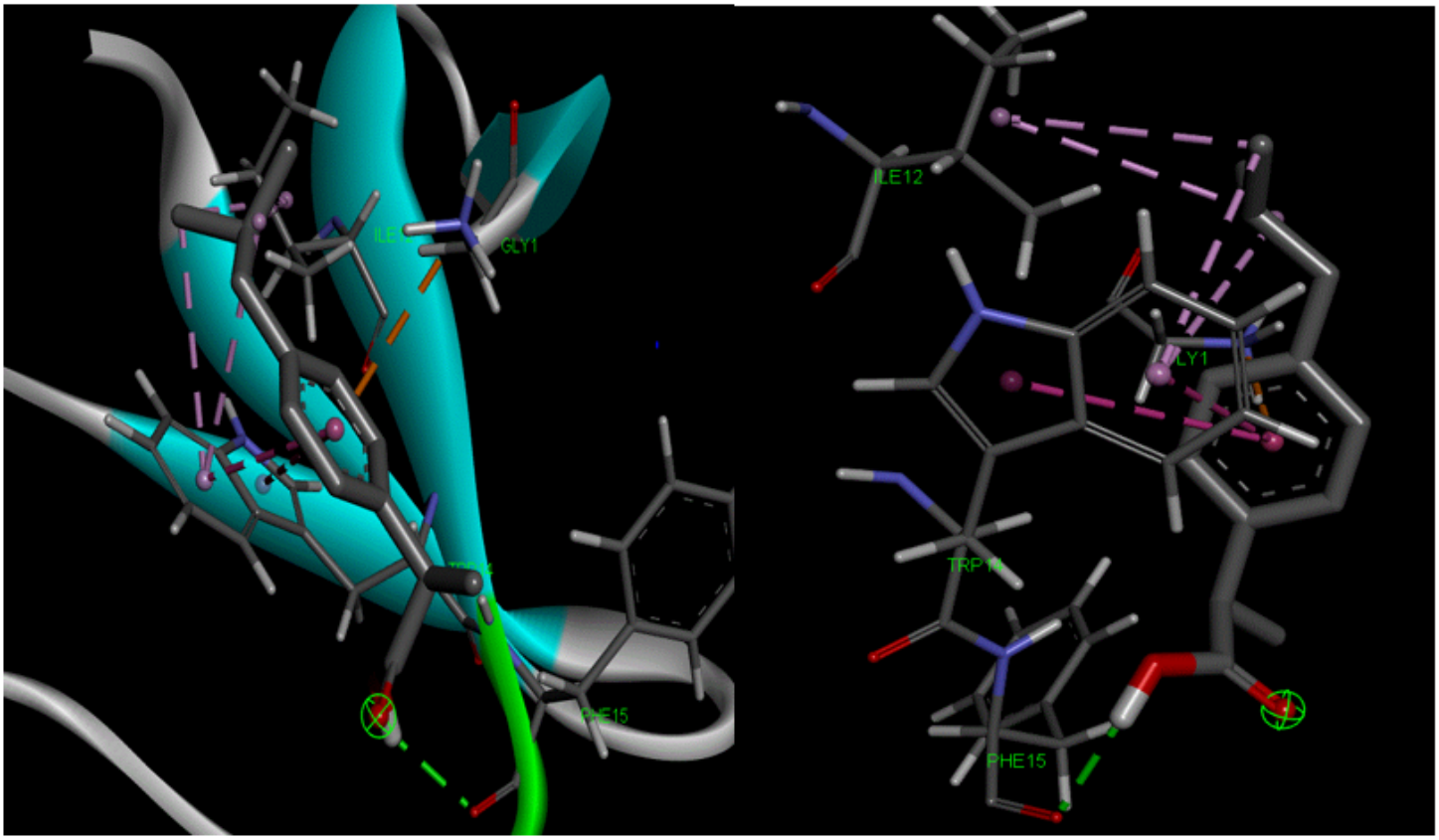

Figure 9

3D structure of Standard Ibuprofen against Analgesic receptor using PDB ID: 2MUB.

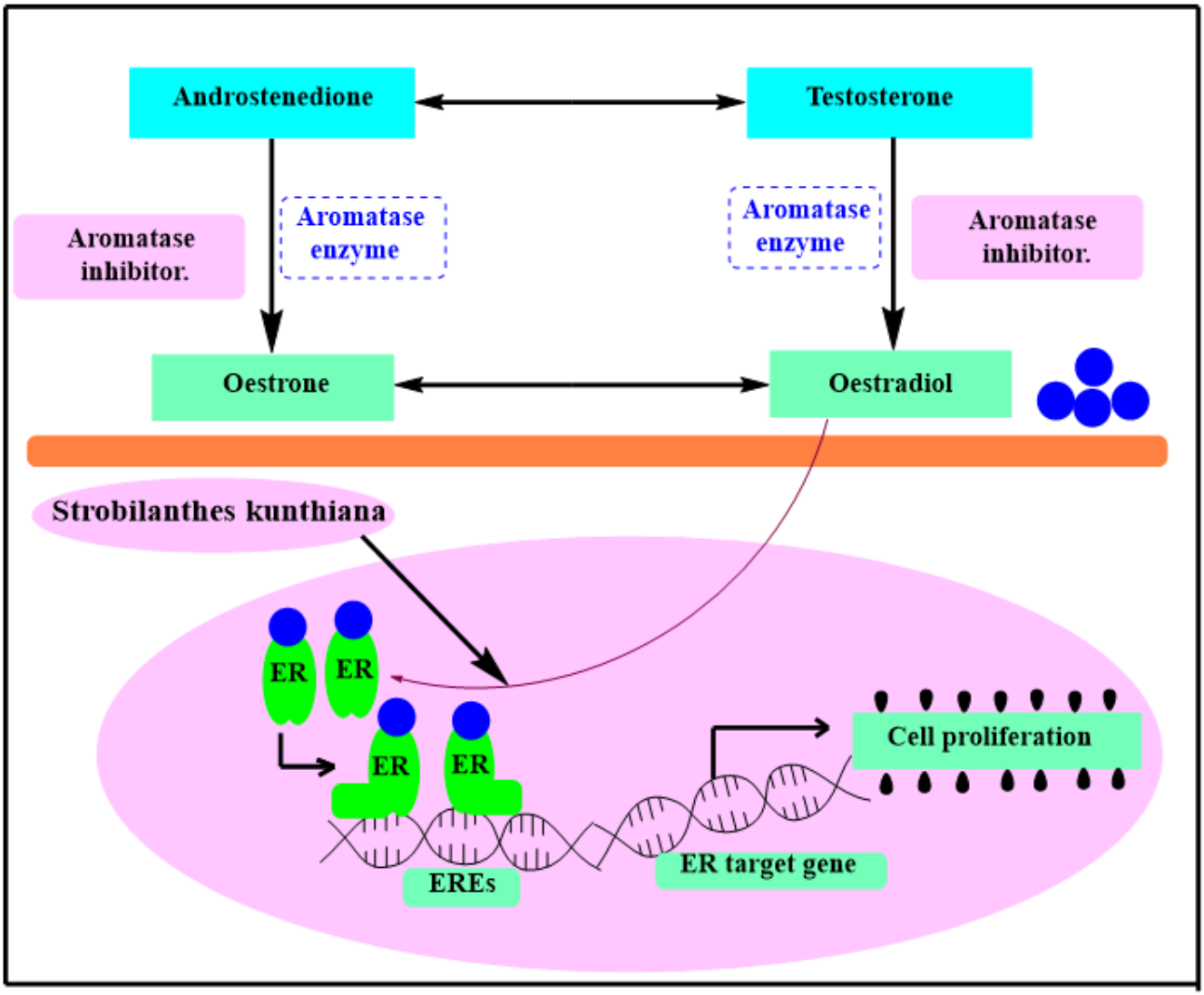

Figure 10

Mechanism of Aromatase enzyme inhibition

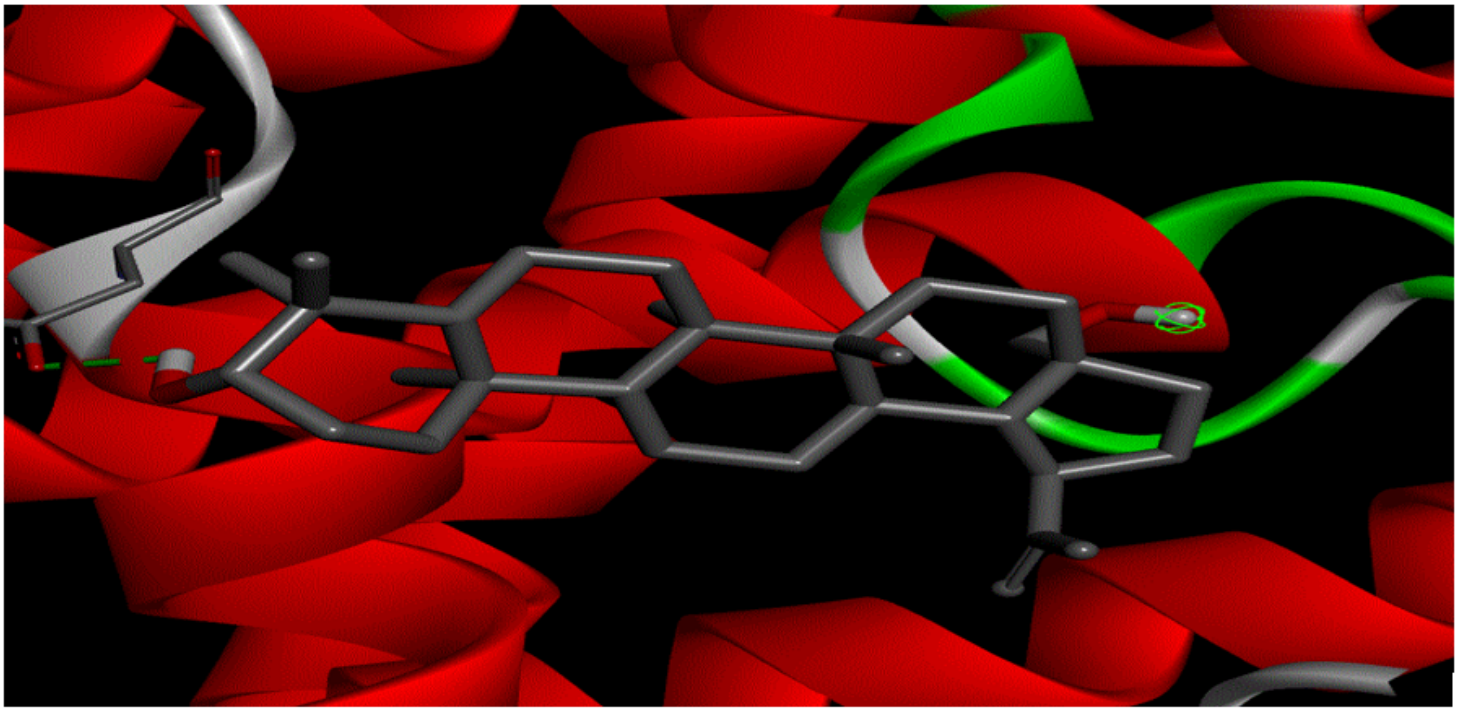

Figure 11

3D structure of Botulin against cancer protein using PDB ID: 4XI3.

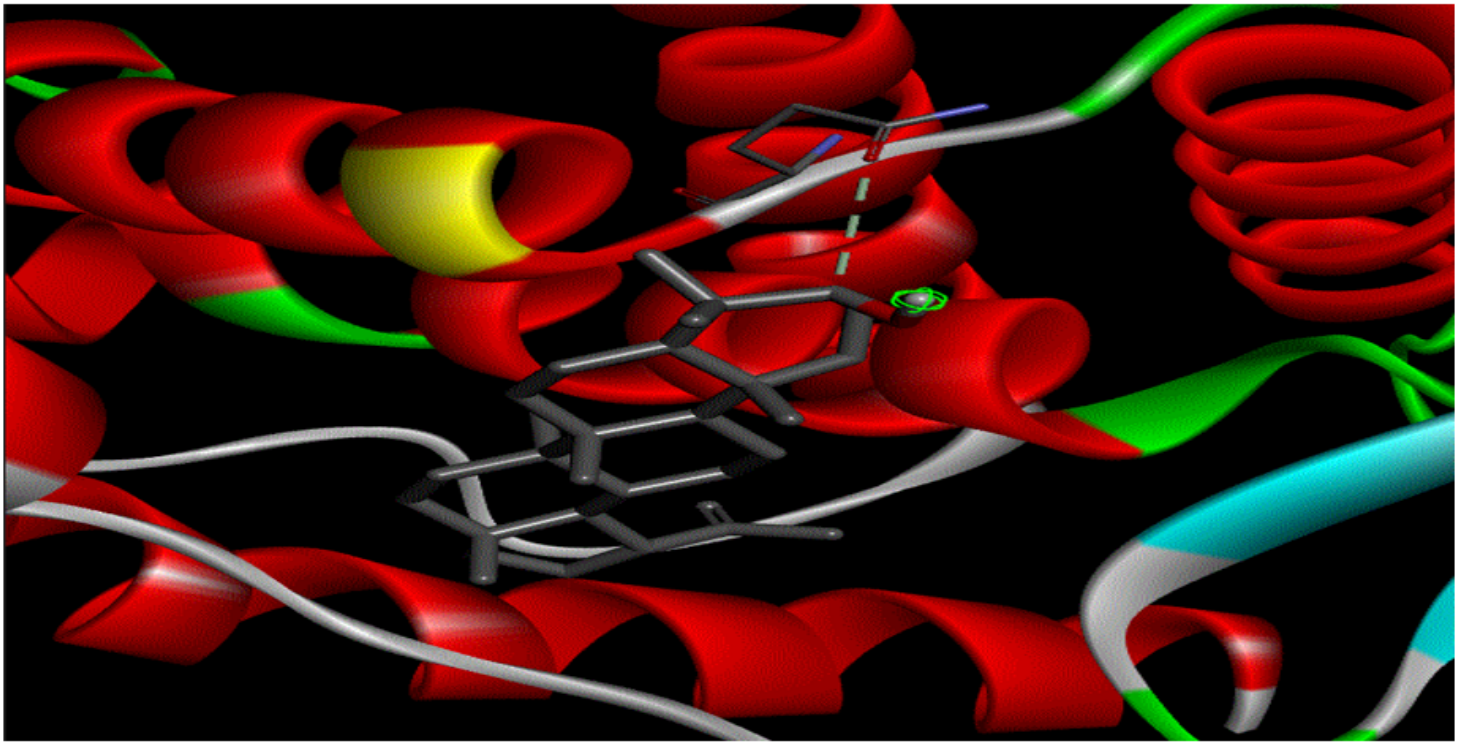

Figure 12

3D structure of Lupeol against cancer protein using PDB ID: 4XI3.

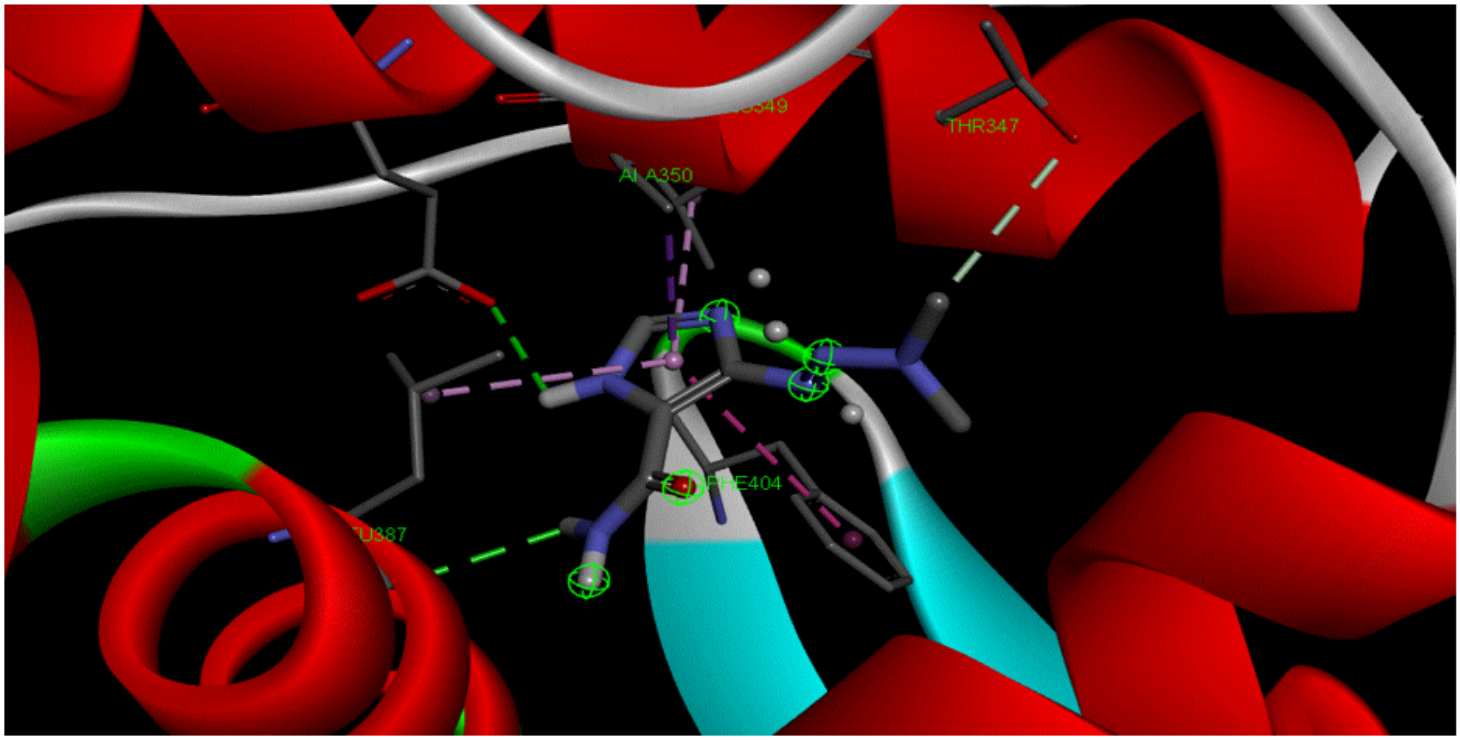

Figure 13

3D structure of standard Azathioprine against cancer protein using PDB ID: 4XI3.

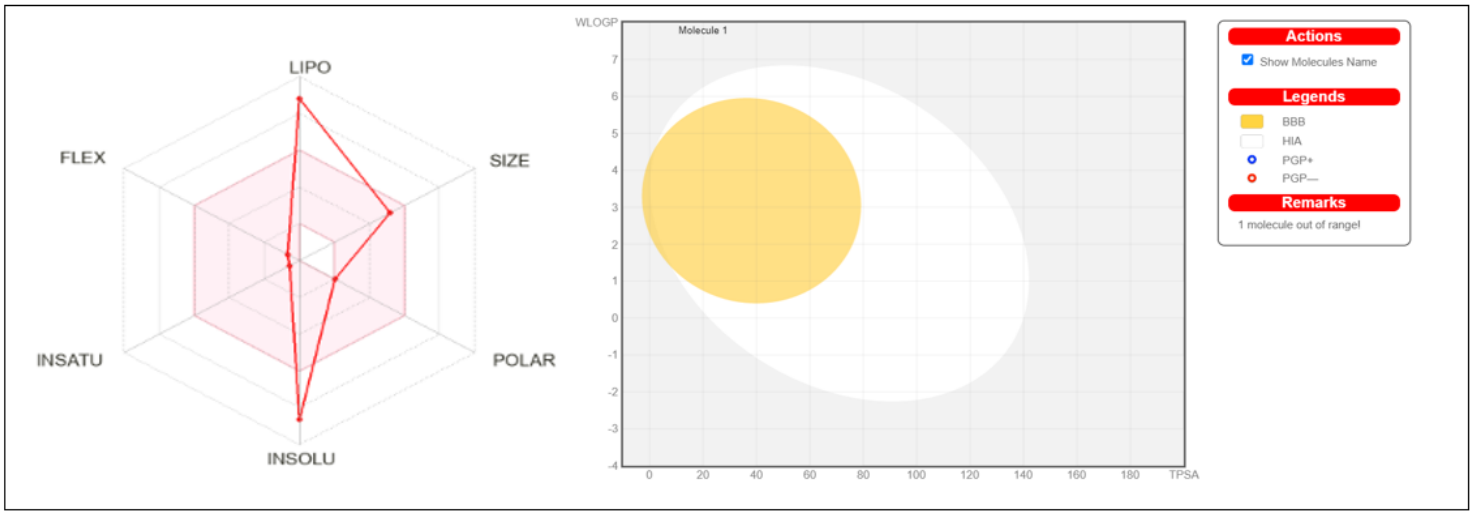

Figure 14

Diagrammatic illustration of the perception of chemicals in the WLOGP-versus-TPSA utilizing BOILED-Egg to assess oral absorption, gastrointestinal absorption (HIA), and brain penetration (BBB) of Lupeol.

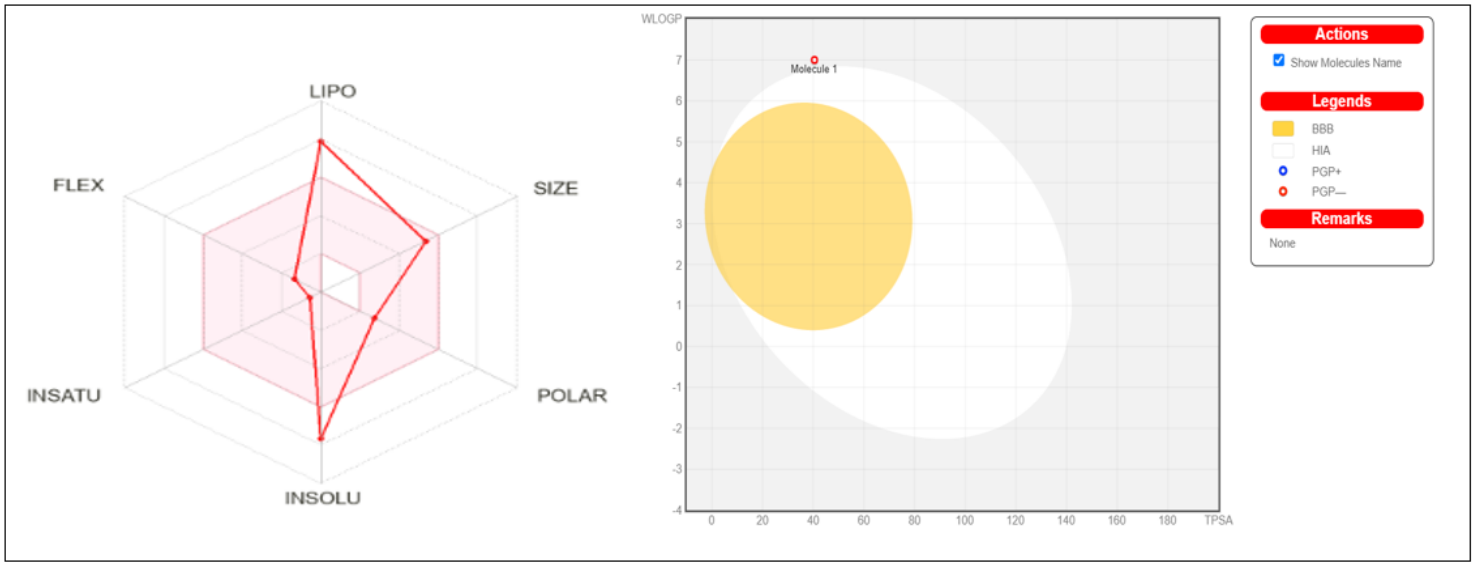

Figure 15

Diagrammatic illustration of the perception of chemicals in the WLOGP-versus-TPSA utilizing BOILED-Egg to assess oral absorption, gastrointestinal absorption (HIA), and brain penetration (BBB) of Botulin.

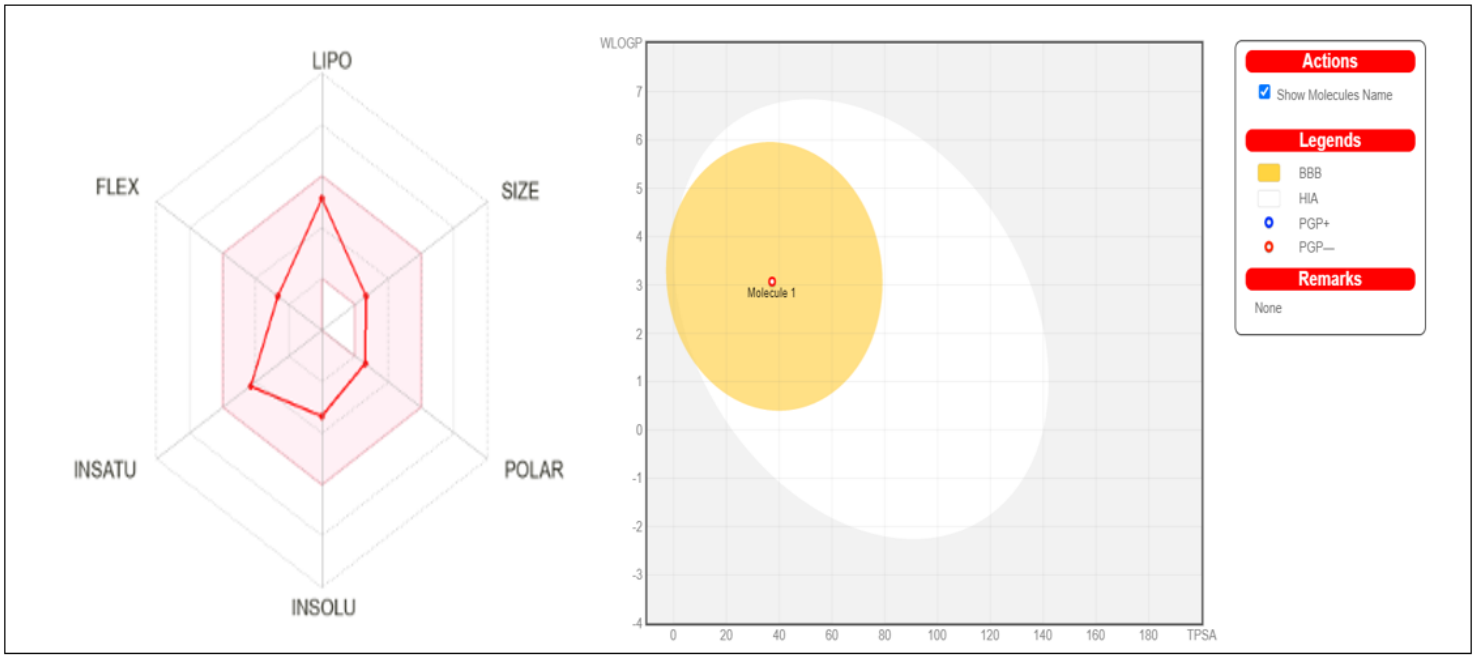

Figure 16

Diagrammatic illustration of the perception of chemicals in the WLOGP-versus-TPSA utilizing BOILED-Egg to assess oral absorption, gastrointestinal absorption (HIA), and brain penetration (BBB) of Ibuprofen.

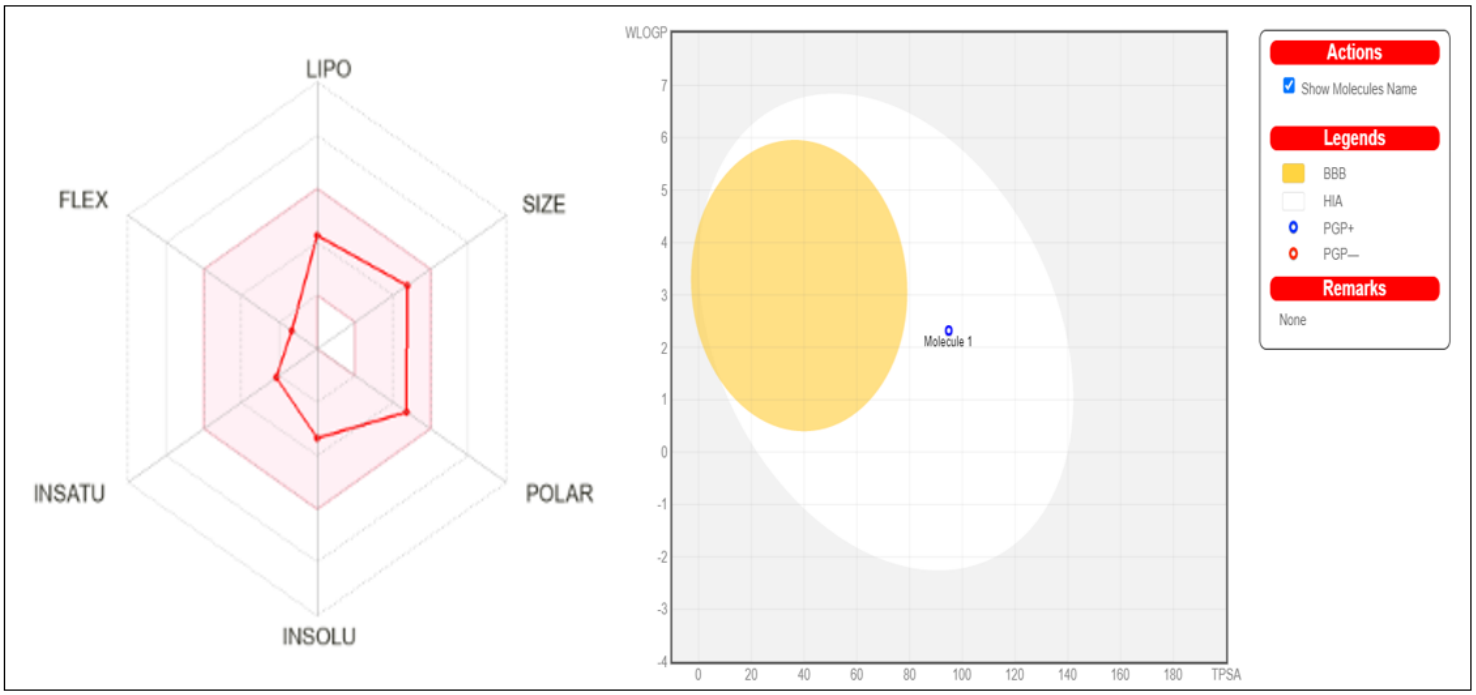

Figure 17

Diagrammatic illustration of the perception of chemicals in the WLOGP-versus-TPSA utilizing BOILED-Egg to assess oral absorption, gastrointestinal absorption (HIA), and brain penetration (BBB) of Dexamethasone.

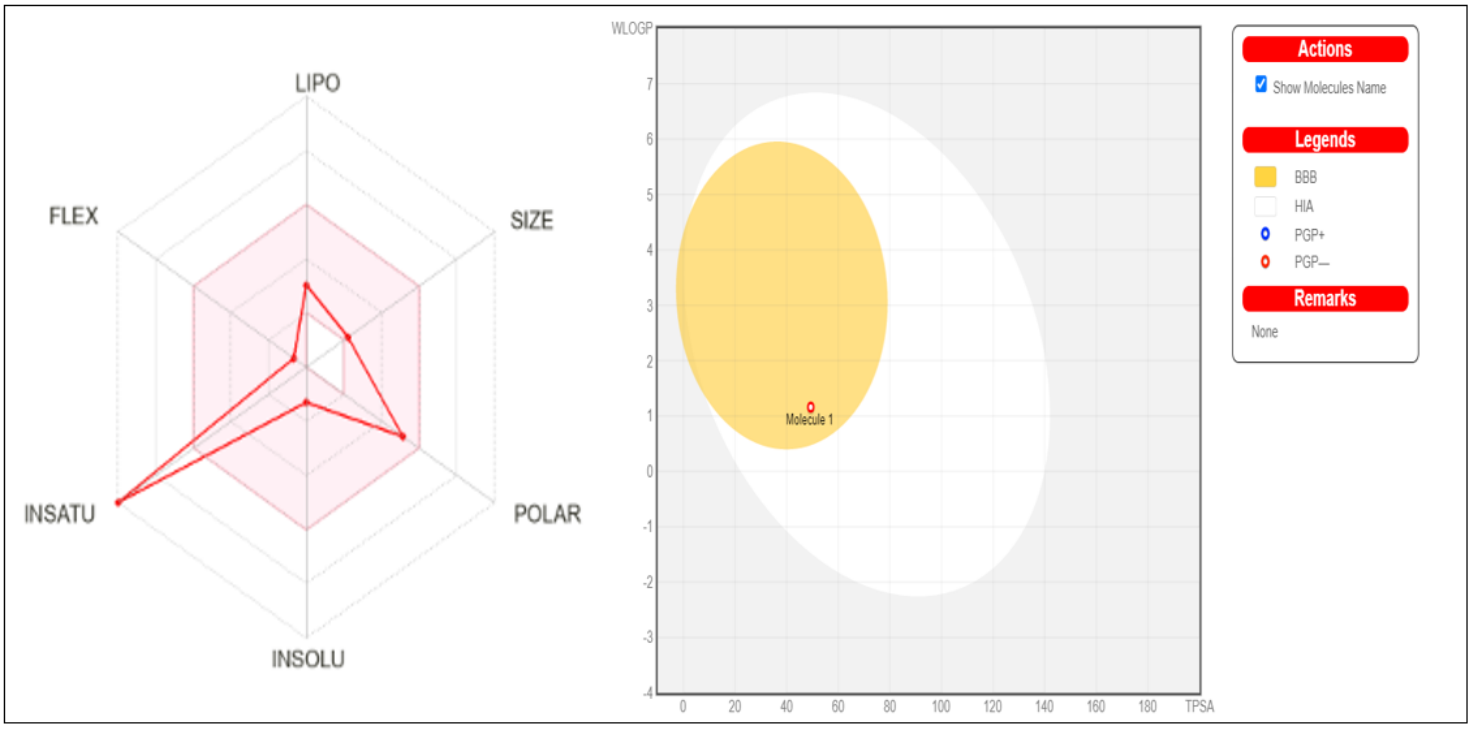

Figure 18

Diagrammatic illustration of the perception of chemicals in the WLOGP-versus-TPSA utilizing BOILED-Egg to assess oral absorption, gastrointestinal absorption (HIA), and brain penetration (BBB) of Azathioprine.

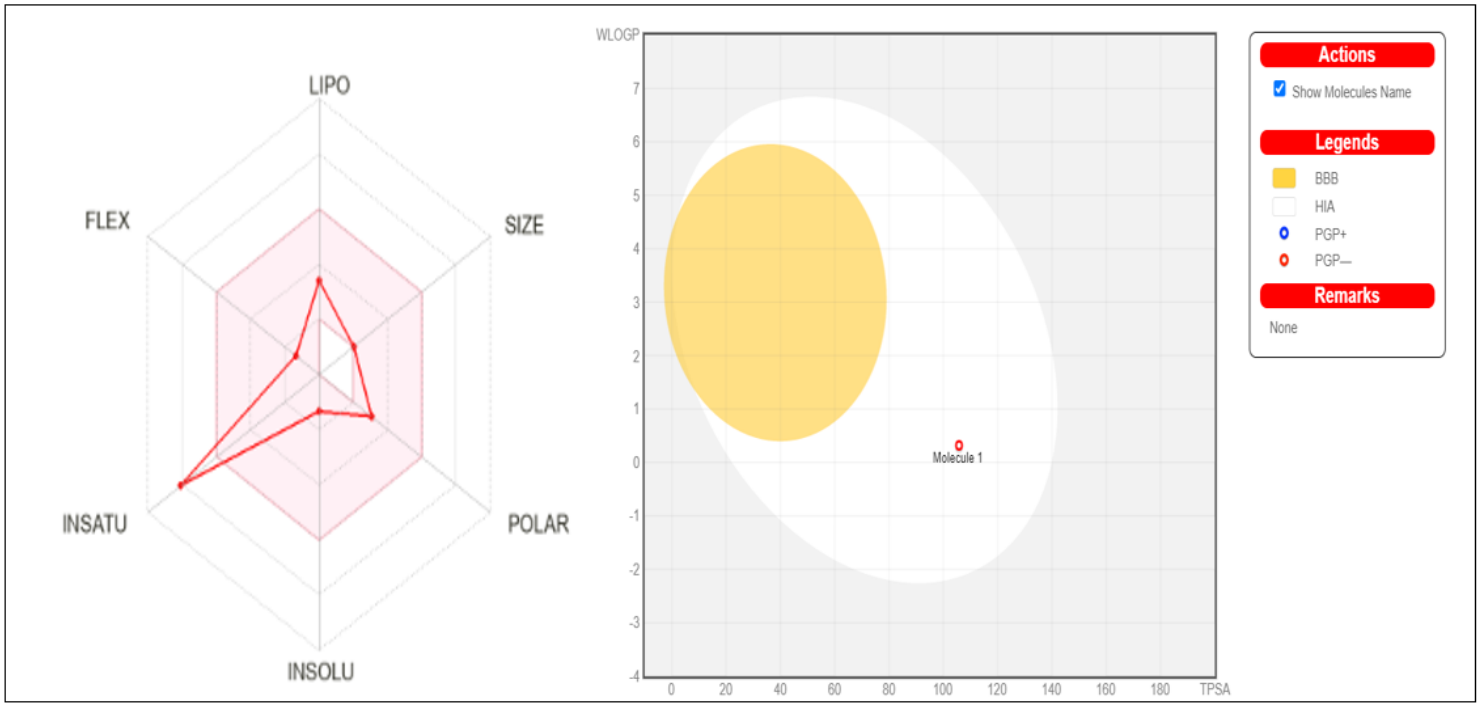

Figure 19

Diagrammatic illustration of the perception of chemicals in the WLOGP-versus-TPSA utilizing BOILED-Egg to assess oral absorption, gastrointestinal absorption (HIA), and brain penetration (BBB) of PCM.

Supplementary Files

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- GraphicalAbstracts.png