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Inhibitory potential of erectile dysfunction - PDE5 enzyme by *Carissa carandas* fruit derived bioactive: Molecular docking

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Abstract
Background: Male sexual dysfunction encompasses a range of illnesses that impair sexual function, including erectile dysfunction (ED), Peyronie's disease (PD), and premature ejaculation (PE). Over 50% of men aged 40 to 70 report experiencing some degree of erectile dysfunction, indicating a significant prevalence that increases with age. Age, diabetes mellitus, cancer, stroke, hypertension, penile trauma, depression, anxiety, and disruptions in central serotonin neurotransmission and 5-HT postsynaptic receptor functionality are risk factors for male sexual dysfunction. The International Index of Erectile Dysfunction, the Sexual Health Inventory for Men, and the Premature Ejaculation Diagnostic Tool are three questionnaires utilised for screening these conditions. The fruits of C. carandas are acknowledged for their efficacy in alleviating haemorrhoids, appetite loss, nerve disorders, oedema, colic, splenomegaly, hepatomegaly, amenorrhoea, cardiovascular illnesses, cerebral anorexia in humans, and for treating fever. It is employed in the management of epilepsy, diarrhoea, canine bites, myopathic spasms, coughs and colds, leprosy, itch, inflammation, malaria, and dermal infections.
Method: The purpose of the current study was to assess the efficiency of bioactive found in *C. carandas* for their inhibitory influence on PDE-5 enzyme to elicit the aphrodisiac potency. The Auto Dock software used a grid-based docking algorithm to determine the bond.
Result: *C. carandas* fruit found to be effective aphrodisiac agent and effectively binds to be target protein PDE-5 with binding energy of -10.92 & -8.55 kcal/mol for β-sitosterol and lupeol respectively.
Conclusion: The outcome of findings revealed that phytosterol and triterpenoid showed potent inhibitory effect on *PDE-5* enzyme which reflects the efficacy of *C. carandas* fruit as potent aphrodisiac agent.

Keywords: *C. carandas* molecular docking**,** β-sitosterol**,** lupeol**,** pde5 enzyme

Introduction
Sexual dysfunction can affect both men and women, with prevalence increasing with age. Alongside the desire, arousal, and orgasmic stages of the typical sexual response cycle, pain may also induce dysfunction [1]. Human sexual function is complex, encompassing both physiological and psychological components. As the diagnosis relies on clinical symptoms, a comprehensive sexual history and focused physical examination are important. Men's sexual dysfunction may arise from several reasons, each associated with distinct risk factors and treatments. A disinterest in contemplating or participating in sexual activities, either solo or with a partner, indicates diminished sexual drive [2]. Erectile dysfunction (ED) is the chronic or recurring inability to attain or maintain a penile erection sufficient for sexual enjoyment. Erectile dysfunction is a rather common problem. As several men fail to self-report their erectile dysfunction symptoms, physicians must probe into sexual function and health to establish a diagnosis [3].

Pathophysiology and Risk Factors
Reduced sexual interest or desire, along with numerous sexual dysfunctions such as erectile dysfunction and premature ejaculation, is likely associated with compromised health. Age has been recognised as a significant risk factor for male sexual dysfunction, independent of health considerations [4-5]. This study concluded that, irrespective of health status or previous erectile function, there is a tenfold disparity in the relative risk of erectile

dysfunction associated with advancing age. The incidence of erectile dysfunction was minimal among men who had a healthy lifestyle and were free from chronic diseases. Five In contrast, physical exercise, low body fat, moderate alcohol use, and absence of a smoking history were associated with a reduced risk. Comorbid conditions, including diabetes mellitus (DM), cancer, stroke, and hypertension, were linked to an elevated risk for erectile dysfunction (ED). Both vascular and neural pathways are essential for erectile dysfunction [6]. *Carissa carandas Linn. (Family: Apocynaceae),* referred to as Karonda in northern India [7].

***Carissa carandas* Fruit**

Carissa carandas has been utilised from ancient times to customarily address several human illnesses. *C. carandas* is the most recognised member of its genus, having been utilised as a traditional medicinal plant for millennia under the Ayurvedic system of medicine practiced on the Indian subcontinent. Consequently, the conventional applications of C. carandas are well established. The root is recognised for its bitter, stomachic, antidiarrheal, and antihelminthic qualities. The mature fruits are employed in curries, tarts, puddings, and chutney. When somewhat under-ripe, they are transformed into jelly. In India, green, acidic fruits are transformed into pickles. Devoid of skin and seeds, and flavoured with sugar and cloves, they have gained popularity as an alternative to apples in tarts. The immature fruit is utilised medically as an astringent. The mature fruit is utilised as an antiscorbutic and a treatment for nausea. The fruits have been utilised as agents in tanning and dyeing; British settlers in India clearly preferred the karanda for its resemblance to gooseberries. Karanda leaves have provided sustenance for the tussar silkworm. The leaf decoction is esteemed for its efficacy in treating intermittent fever, diarrhoea, oral irritation, antibacterial activity, and earache. A paste made from pulverised roots functions as a fly repellent [8-11]. In current studies, PDE5 was chosen as a target molecule involved in the erectile dysfunction".

Experimental Works

Selection of Lead molecule

As per literature survey *C.carandas* fruit contained β-sitosterol, carindone, steroids, terpenes, lupeol, cardenolides, carissone, flavonoids, tannins, benzenoids, lignans, phenylpropanoid, coumarins and sesquiterpenes [12-13].

Numerous *in-vitro* and *in-vivo* investigations have shown that β-sitosterol exhibit several biological properties such as calming and anxiolytic effects; narcotic and immune-stimulating effects; antibacterial, antineoplastic, inflammation-causing, lipid-lowering, and hepatoprotective effects; and antioxidant, anti-diabetic, and wound-healing effects in contrast to respiratory and non-alcoholic fatty liver disease illnesses. β-sitosterol is a promising natural substance for the management of cholesterol and inflammation [14].

Lupeol is a pentacyclic triterpenoid commonly distributed in the plant kingdom and is found in edible fruits and vegetables. It is a naturally occurring triterpene that is used to reduce the inflammatory responses and also have immunomodulating properties. Lupeol and its derivative have a great potential to act as an anti- inflammatory, anti-microbial, anti-proliferative, anti-invasive, anti-angiogenic, antiprotozoal, and cholesterol-lowering agent. Various studies have shown that anti-inflammatory activity of lupeol through the modulation of p-38 pathways inhibits neuroinflammation in the cerebellum and induces neuroprotection [15].

Erectile dysfunction (ED) is a prevalent condition affecting male sexual health, characterized by the inability to achieve or maintain satisfactory erections. ED has a multifactorial pathogenesis in which psychological, hormonal, neurologic, cardiovascular, and lifestyle factors all contribute to a progressive decline of erectile function. A critical underlying mechanism involves oxidative stress (OS), an imbalance between reactive oxygen species (ROS) production and antioxidant defences, which disrupts endothelial function, reduces nitric oxide (NO) bioavailability, and contributes to vascular dysfunction [16]. The release of nitric oxide (NO) in blood vessel walls triggers the relaxing and opening of vessels, for enhanced blood flow. Research studies of male pelvic tissue levels of nitric oxide reveal that the effect of nitric oxide on smooth muscle relaxation is a key factor in mediating the erection process. Ascorbic acid augments NO production and increases its bioactivity in the vascular system in a variety of body processes [17-18].

Description of lead molecule [19-22].

Table 1: Comparative description of β-sitosterol and lupeol

Description	β-sitosterol	Lupeol
Molecular formula	$C_{29}H_{50}O$	$C_{30}H_{50}O$
Synonym	22,23-Dihydrostigmasterol	lup-20(29)-en-3-ol
Molecular weight	414.7 g/mol	426.7 g/mol
Pharmacology	They exhibit several biological properties such as calming and anxiolytic effects; narcotic and immune-stimulating effects;antibacterial, antineoplastic, inflammation-causing, lipid-lowering, and hepatoprotective effects; and antioxidant, anti-diabetic, and wound-healing effects in contrast to respiratory and non-alcoholic fatty liver disease illnesses.	Lupeol has shown promising benefits in the management of cancer and many other human diseases such as diabetes, obesity, cardiovascular diseases, kidney and liver problems, skin diseases, and neurological disorders. The pharmacological effects of lupeol primarily rely on its capacity to revitalize the cellular antioxidant, anti-inflammatory and anti-apoptotic mechanisms.

Selection of target receptors

PDE5 is an enzyme found primarily in the smooth muscle of the corpus cavernosum that selectively cleaves and degrades cGMP to 5′-GMP. *PDE5* inhibitors are similar in structure to cGMP; they competitively bind to PDE5 and inhibit cGMP hydrolysis, thus enhancing the effects of NO. This increase in cGMP in the smooth muscle cells is responsible for prolonging an erection. *PDE-5* inhibitors lack a direct effect on corpus cavernosum smooth-muscle relaxation. Therefore, after administration, adequate sexual stimulation is necessary for an erection to occur [23].

Molecular docking studies of β-sitosterol and lupeol against PDE5

Ligand Preparation

2D Structure of β-sitosterol and lupeol were drawn using ChemSketch [24], the two-dimensional structure of the prepared ligand was converted into their 3-D structures optimized with 3D geometry. The optimized structure was saved in PDB format for AutoDock compatibility. The basic structures of the prepared ligand were given below:

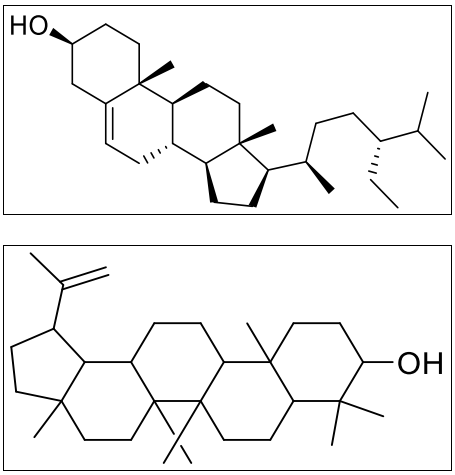


Fig 1: 2D structure of β-sitosterol and lupeol

Preparation of the grid file

The regions of interest used by Autodock were defined by considering grid area by making a grid box around the active sites. Grid box plays a central role in process of docking as it is made to cover all the amino acids present in active sites necessary for binding other than those present in receptor. Grid box has 3 thumbwheel widgets which let us change the number of points in the x, y and z dimensions. The spacing and grid points for all the considered receptors in the current study are given in table 1 [25-27].

Table 2: Grid parameters used in current docking analysis of PDE5

S. No.	Receptor	x-axis	y-axis	z-axis	Spacing	x center	y center	z center
1	PDE5	50	50	50	0.442	17.544	-8.204	13.099

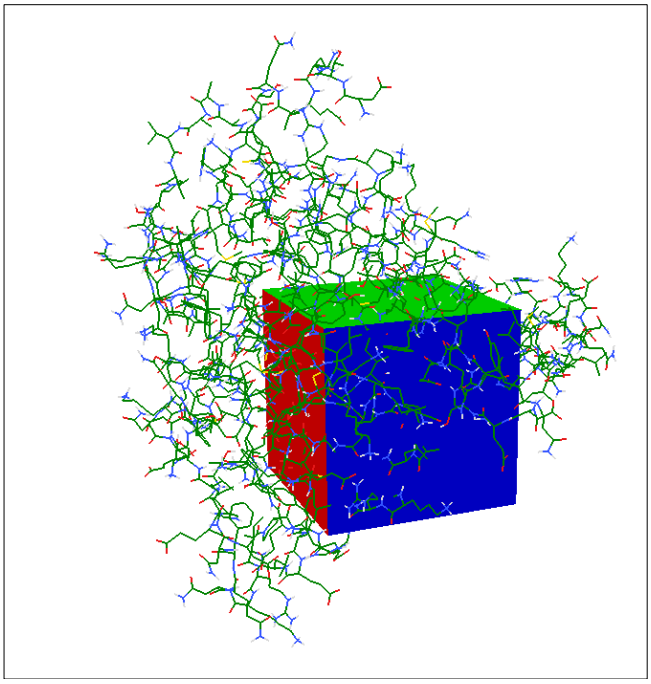


Fig 2: Grid box covering all active sites in PDE5 receptor

Preparation of the docking file

All the calculations were carried out by using Autodock 4.2 as docking tool. The visualization and other programs necessary for docking studies were performed out by means of Pymol, Chimera, DS visualizer, MMP Plus [28-29].

Docking Study

Crystal structure

The crystal structure of the protein consisting of PDE5 receptor is downloaded from the Protein Data Bank portal. All the primary information regarding all the receptor's structure was registered in the Protein data bank [29-31]. The complex ligand was separated by using Chimera software for all the target receptors.

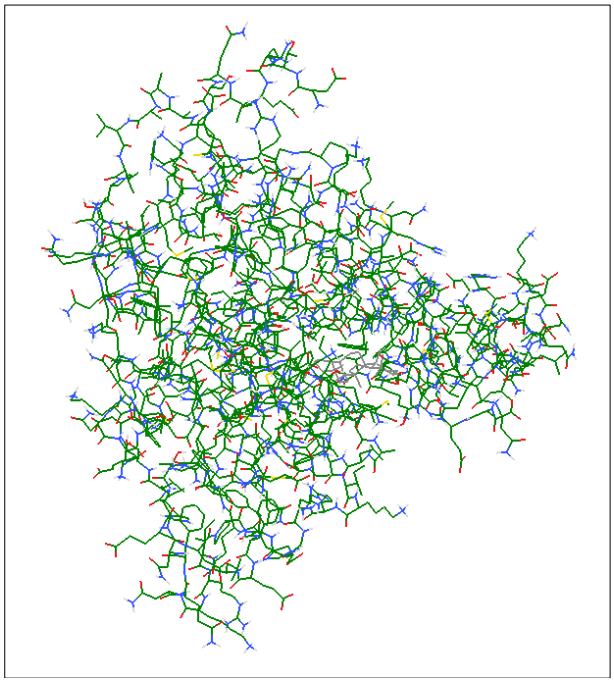


Fig 3: Crystal structure of PDE5 receptor (PDB ID-3tgg)

Processing of Protein

All the downloaded receptor proteins are having only one chains, i.e. chain A, which has been selected for experimental purpose and complex ligand was removed from it. The bound ligand was separated from the macromolecular complex by using software Chimera [30-34].

Molecular Docking Simulation Studies

Docking of ligands like βsitosterol and lupeol against PDE5 receptor was performed by Autodock. All the bonds of each ligand were kept flexible, while no residues in receptor were made flexible [35-38].

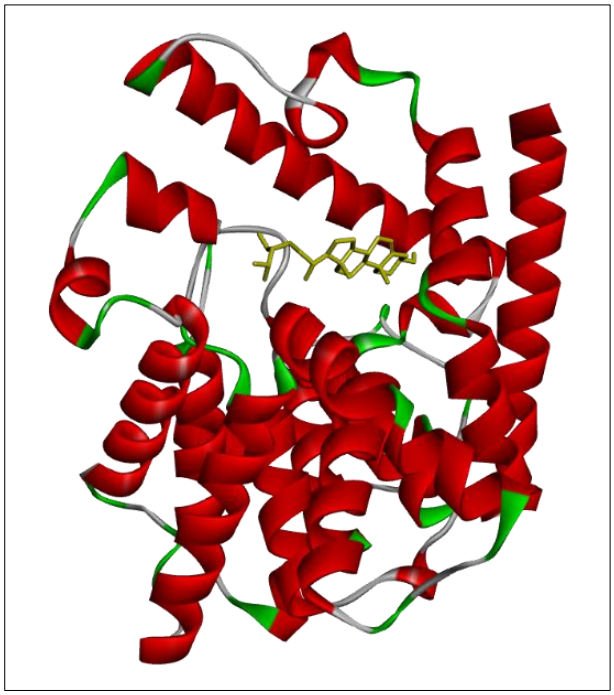


Fig 4: Binding mode of β-sitosterol within the active site of PDE5 receptor

Fig 5: Binding mode of lupeol within the active site of PDE5 receptor

Toxicity & ADME-T Studies

The ligand molecules *viz*. βsitosterol and lupeol were studied by online program OSIRIS, for prediction of presence of any toxic group as well as presence of any toxic group and ADME- T properties [39].

Result and Discussion

Sexual dysfunction impacts 10–52% of men and 25–63% of women, becoming a significant medical and social issue. Given the substantial incidence of erectile dysfunction among men, which is the principal cause of male impotence, it is considered one of the most critical public health concerns. Erectile dysfunction (ED) is the persistent inability to achieve or sustain an erection sufficient for satisfactory sexual activity. It is estimated that 20 to 30 million men have some type of sexual dysfunction. It predominantly affects middle-aged and older guys. Fifty percent of men with diabetes mellitus encounter erectile dysfunction. Atherosclerosis accounts for around 40% of erectile dysfunction instances in individuals over 50. Herbal formulations in the Ayurvedic system of medicine consistently exhibit a distinctive array of good benefits due to their remarkable therapeutic effectiveness, without inducing undesirable consequences. The fruit of the plant C. carandas was scientifically proven for its aphrodisiac capabilities. The active ingredients present in the fruit were utilised as lead molecules for a computational molecular docking investigation targeting the PDE-5 enzyme. Traditionally, it is claimed to remedy gastrointestinal distress, neurological disorders, serve as a cardiotonic, possess anthelmintic properties, and exhibit anti-hypertensive effects. The fruits of C. carandas are recognised for their ability to alleviate piles, appetite loss, nerve disorders (as a nervine), oedema, colic, splenomegaly, hepatomegaly, amenorrhoea, cardiovascular diseases, cerebral anorexia in humans, and to cure fever. It is utilised for the treatment of epilepsy, diarrhoea, canine bites, myopathic spasms, coughs and colds, leprosy, pruritus, inflammation, malaria, and cutaneous infections. It is recognised for its ability to enhance female libido, combat microbial infections and intestinal parasites, restore liver function, and mitigate blood putrefaction and rheumatoid arthritis. In recent years, beta sitosterol, a plant sterol prevalent in several fruits, vegetables, and nuts, has surfaced as a viable natural treatment for erectile dysfunction. Beta sitosterol has been investigated for its impact on prostate health and cholesterol levels, both of which are intricately associated with sexual function. Studies indicate that beta sitosterol may enhance blood circulation, diminish inflammation, and promote hormonal equilibrium, all of which can facilitate improved erectile performance. Terpenoids have anticancer, anti-inflammatory, antibacterial, antiviral, and antimalarial properties, enhance transdermal absorption, prevent and cure cardiovascular disorders, and demonstrate hypoglycemic effects. Moreover, prior research has identified several potential uses of terpenoids, including insect resistance, immunoregulation, antioxidation, anti-aging, and neuroprotection. This study aimed to assess the efficacy of bioactive compounds in *C. carandas* fruits in inhibiting PDE-5 enzymes to determine their aphrodisiac potential. A docking-based computer analysis of the PDE-5 enzyme has been conducted to provide the most probable mechanism of action for the selected lead phytoconstituent.

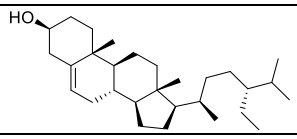
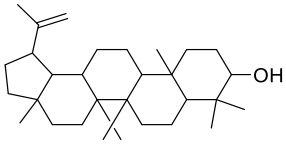
PDE5 is an enzyme mostly located in the smooth muscle of the corpus cavernosum, which specifically hydrolyses and degrades cGMP to 5′-GMP. PDE5 inhibitors possess a structural resemblance to cGMP; they competitively associate with PDE5 and obstruct cGMP breakdown, hence amplifying the effects of nitric oxide (NO). The elevation of cGMP in smooth muscle cells is accountable for extending the duration of an erection. PDE-5 inhibitors do not directly induce relaxation of the corpus cavernosum smooth muscle. Consequently, following medication, sufficient sexual excitement is essential for an erection to manifest. The results of the current investigation indicated that the selected lead molecules serve as effective in treating and preventing ED, binding to the target protein of PDE5 with binding energies of -10.92 & -8.55 kcal/mol for β-sitosterol and lupeol respectively. The outcome was recorded in Table 2. The binding mechanism of the selected lead compounds is illustrated in Figures 4 -5. The two-dimensional and three-dimensional interactions of the selected chemical are illustrated in Figures 6-9. The affinity of lead compounds for the receptor was determined to be relatively comparable. The interaction of β-sitosterol & lupeol with the active site of PDE5 is illustrated as follows:

Table 3: Molecular interactions of β-sitosterol and lupeol with target protein residues

Compound	Conventional Hydrogen bounding	π-alkyl	Alkyl	Week Vander's interaction
β-sitosterol	Glu775	Leu765,Ala767, ILE778,Phe820, Phe786	Val782,Tyr612 His657,His613	Glu785,Ser661 Val660,ASN662 Leu681,GLN817 Leu725,Leu804
Lupeol	ASN662	Phe820,ILE768 Leu765,Tyr612 His613,Leu725 Leu681	ASN662	Asp724,Glu682 Ser661,Asp764

The interaction results indicated that lead molecules attach at comparable positions by typical hydrogen, alkyl, π-alkyl and vander waal's interactions, demonstrating a synergistic effect of both compounds from *C. carandas fruit* in exerting protective action on ED. The pharmacokinetic profile indicates a favourable pharmacokinetic profile; however, it also presents significant hazardous consequences, including mutagenicity, tumorigenicity, and reproductive toxicity. The pharmacokinetic and toxicity profiling data of ligands such as β-sitosterol & lupeol are presented in Figures 10-11 and Tables 3-5. All ligand compounds have demonstrated promising docking scores theoretically.

Table 4: Results of docking of ligands like β-sitosterol and lupeol against PDE5 receptor

S. No.	Compound Name	Structure	PDE5
1	β-sitosterol		-10.92
2	Lupeol		-8.55

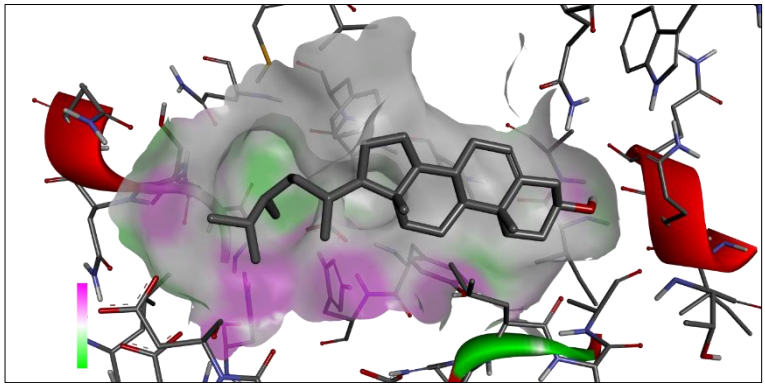


Fig 6: Three-dimensional binding mode of βsitosterol within the active site of PDE5 receptor

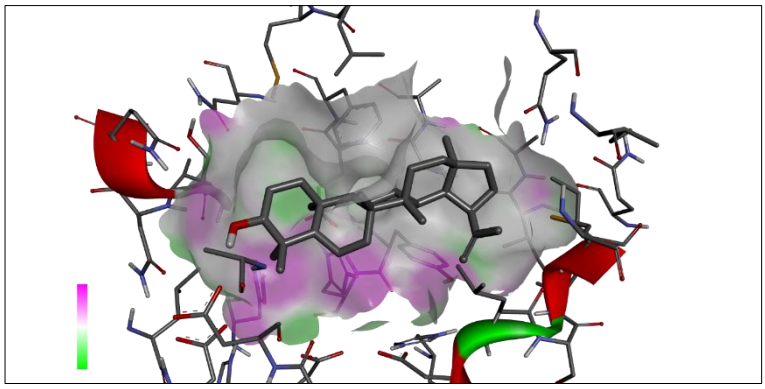


Fig 7: Three-dimensional binding mode of lupeol within the active site of PDE5 receptor

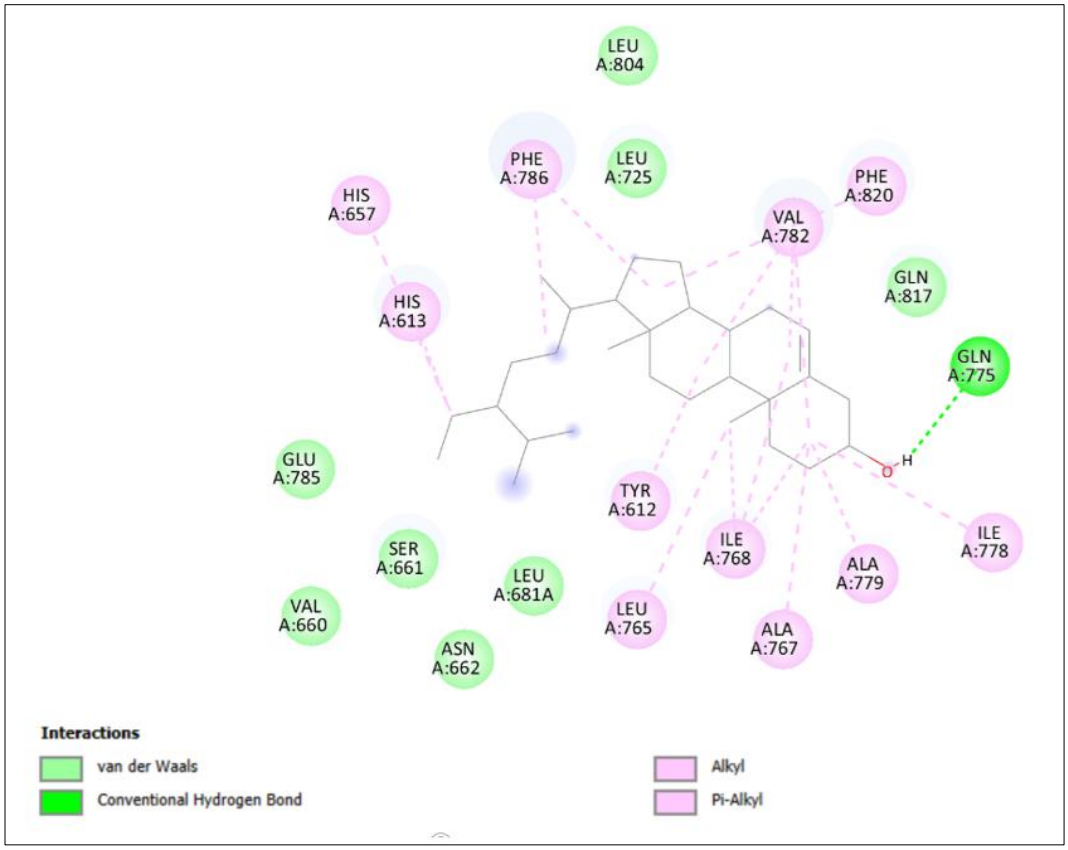


Fig 8: Two-dimensional binding mode of βsitosterol within the active site of PDE5 receptor

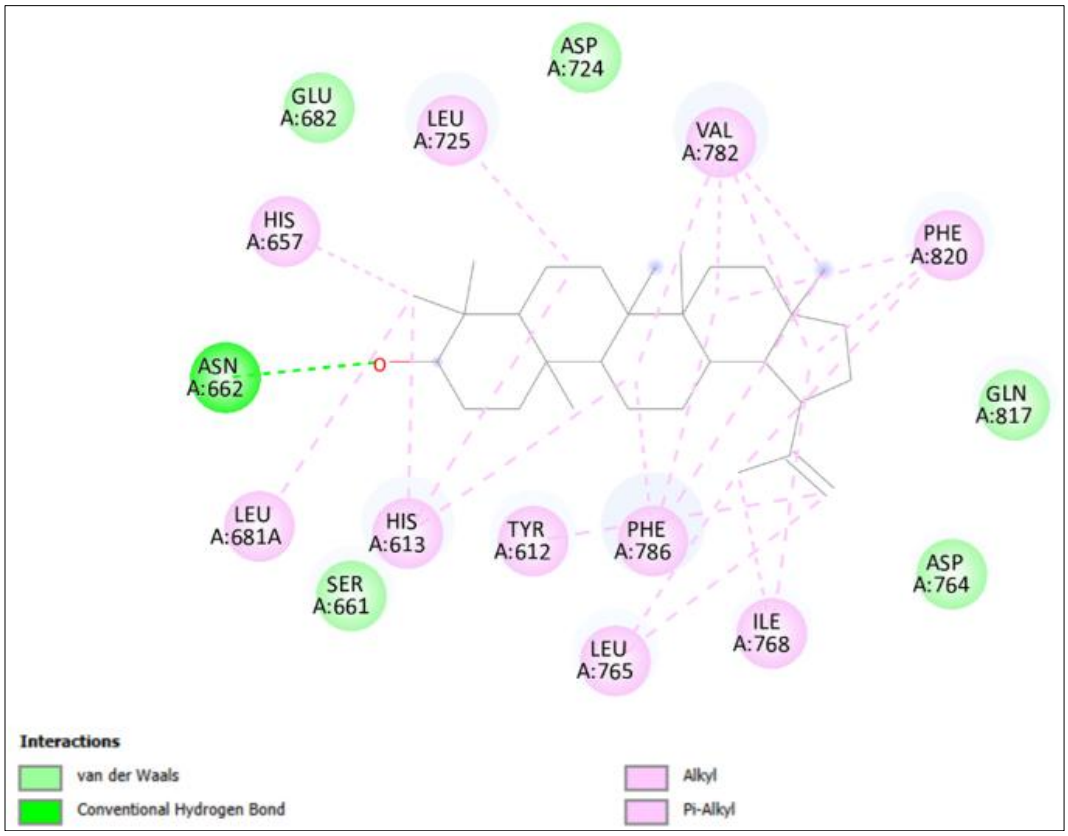


Fig 9: Two-dimensional binding mode of lupeol within the active site of PDE5 receptor

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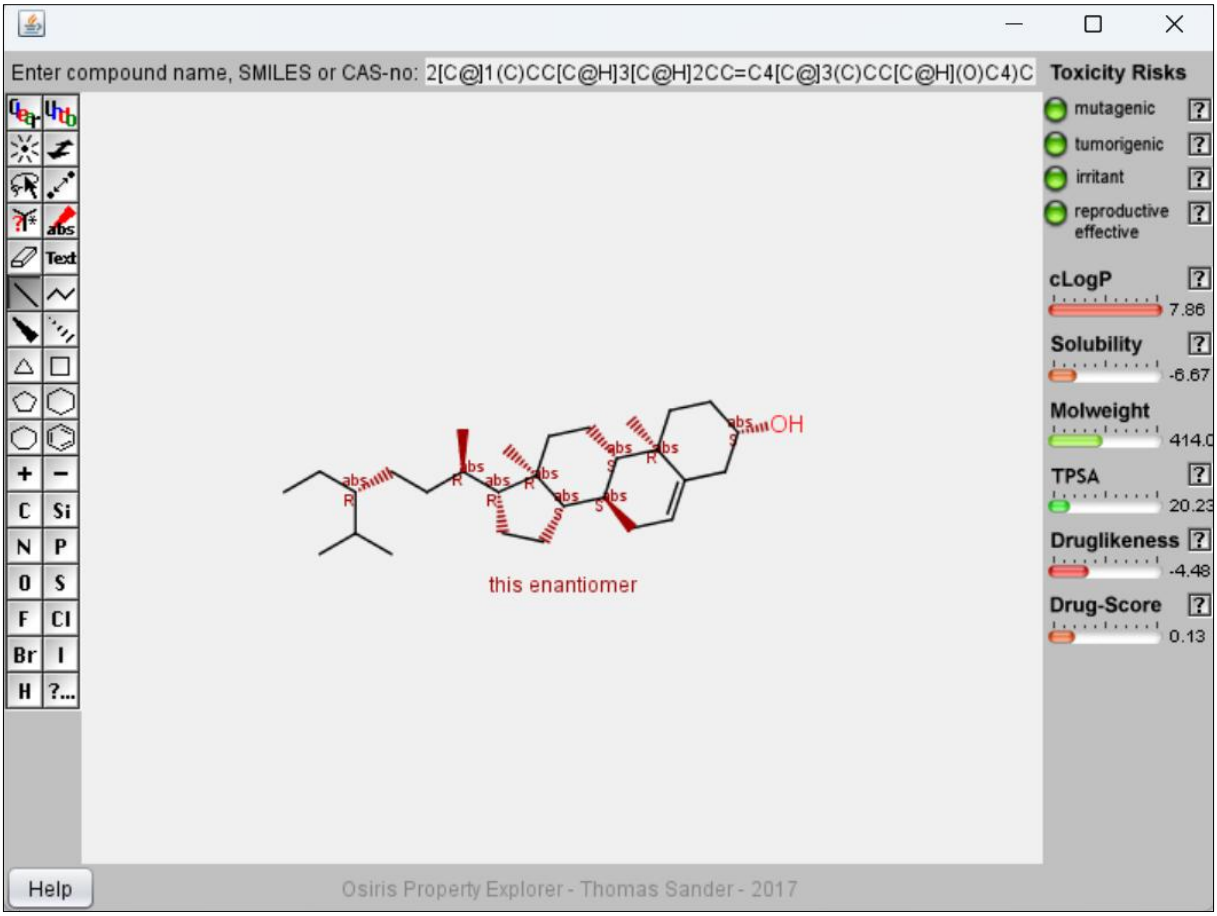


Fig 10: Pharmacokinetic and toxicity profiling of beta- sitosterol

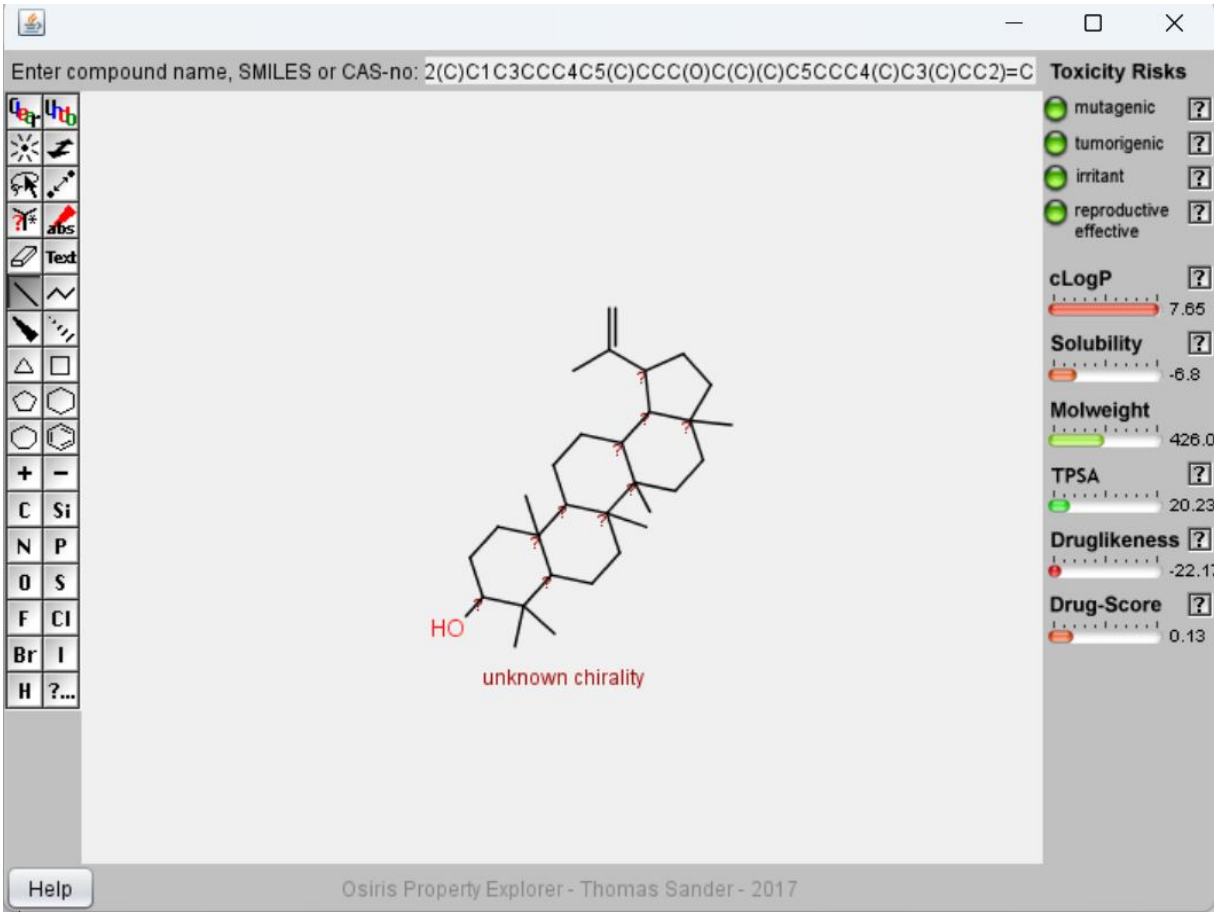


Fig 11: Pharmacokinetic and toxicity profiling of Lupeol

Table 5: Pharmacokinetic Profiling of lead molecules

Compound	ADMET			
	Mutagenic	Tumorigenic	Irritant	Reproductive effectivity
β-sitosterol	NO	NO	NO	No
Lupeol	NO	NO	NO	No

Table 6: Lipinski Properties of lead molecules

Compound	*cLogP*	Solubility	Mol.wt.	TPSA	Drug likeness	Drug score
β-sitosterol	7.86	-6.67	414	20.23	-4.48	0.13
Lupeol	7.65	-6.8	426	20.23	-22.13	0.13

Table 7: Drug likeness of lead molecules

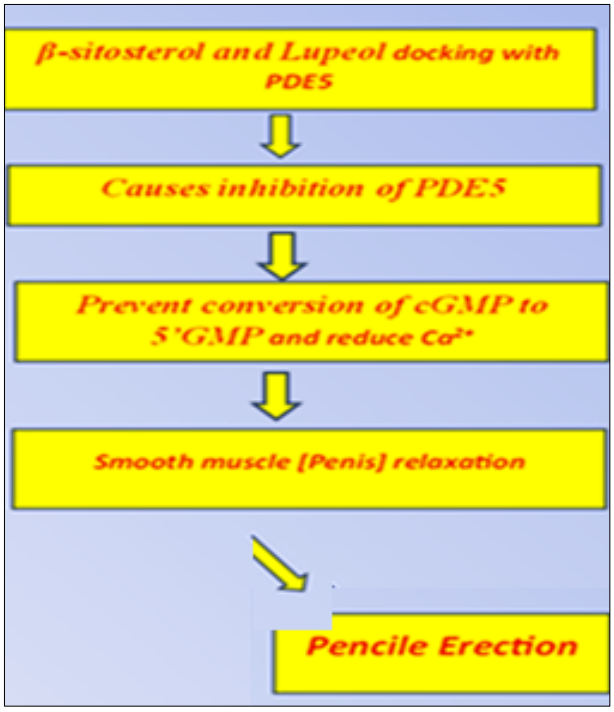
Compound	Lipinski rule of five	H bond donar (<5)	H bond acceptor (<10)
β-sitosterol	Yes	1	1
Lupeol	Yes	1	1

Concluding Remarking

Herbal formulations in the Ayurvedic system of medicine consistently exhibit a distinctive array of good benefits due to their remarkable therapeutic effectiveness, without inducing undesirable consequences. The fruit of the plant *C. carandas* was scientifically proven for its aphrodisiac capabilities. The active ingredients present in the fruit were utilised as lead molecules for a computational molecular docking investigation targeting the PDE-5 enzyme**.** The finding suggested that selected lead bioactive showed potent inhibitory potential against PDE-5 and possess aphrodisiac efficacy.

Divulgence of Investigation

The mechanism of action of above selected lead molecule showed pictorially as follows:



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