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Lead identification of newer polyphenol derivatives of *Punica granatum peel* against polycystic ovary syndrome: Molecular docking approaches

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Abstract
Background: Polycystic ovarian syndrome (PCOS) is a complex endocrine and metabolic disorder, often characterised by anovulation, infertility, obesity, insulin resistance, and the presence of polycystic ovaries. Lifestyle, diet, environmental pollutants, genetics, intestinal dysbiosis, neuroendocrine alterations, and obesity contribute to the susceptibility of females to PCOS. These factors may aggravate metabolic syndrome by causing hyperinsulinemia, oxidative stress, hyperandrogenism, impaired folliculogenesis, and irregular menstrual cycles. Pomegranate extract may aid in the regulation of hormonal imbalances and the facilitation of regular menstrual cycles. The extract's rich nutritional profile promotes placental development and foetal growth, perhaps reducing the risk of preterm delivery. Pomegranate extract may improve insulin sensitivity and reduce inflammation and oxidative damage in PCOS. Computational techniques are often utilised to expedite drug development through the screening of potential lead compounds.
Purpose: Current work was designed to check efficacy of *P.granatum* peel polyphenol against PCOS disorder**.**
Methodology: Scientific validation of the current investigation was done by computational based molecular docking study of newer lead molecules of *P.granatum* peel against CYP11A1 genes.
Result: The polyphenol found in *P. granatum* has been identified as an effective against PCOS and their lead molecules delphinidin and pelargonidin demonstrating effective binding to the target protein CYP11A1 with binding energies of -7 and -7.43 kcal/mol, respectively.
Conclusion: The findings indicated that each selected lead chemical for additional investigation shown significant inhibitory activity against CYP11A1, hence revealing its effectiveness against PCOS.

Keywords: *P.granatum*, molecular docking, CYP11A1, delphinidin & pelargonidin

Introduction
Polycystic ovarian syndrome (PCOS) is a diverse endocrine condition affecting numerous women of reproductive age globally. This condition is frequently linked to enlarged and dysfunctional ovaries, elevated testosterone levels, and insulin resistance, among other factors. Approximately 10% of women are expected to experience PCOS before to menopause and contend with its implications [1]. Despite the established association between elevated luteinizing hormone (LH) to follicle-stimulating hormone (FSH) ratios and increased gonadotropin-releasing hormone (GnRH) frequency as contributing factors to PCOS, the precise aetiology and pathophysiology remain inadequately understood [2-3]. Evidence indicates the influence of several external and internal elements, including insulin resistance (IR), hyperandrogenism (HA), environmental influences, genetics, and epigenetics. Moreover, it is important to note that PCOS elevates the risk of other issues such as cardiovascular illnesses, type 2 diabetes mellitus, metabolic syndrome, depression, and anxiety. To address this problem, the paramount action is to reduce body weight by at least 5%; hence, a consistent exercise regimen and diets devoid of fats and sugars are advised for all women with PCOS. Moreover, in certain instances, the adoption of complementary and alternative medical approaches, with or without additional therapies, is favoured owing to preexisting beliefs, reduced expenses, and other factors [4-5].

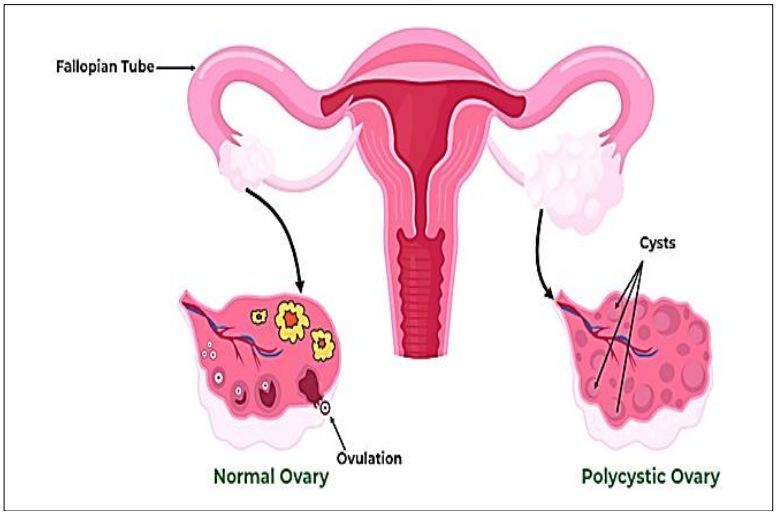


Fig 1: PCOS

Medicinal plants have garnered significant interest throughout antiquity, and contemporary research has revealed several valuable and helpful species. The identification and side effects of these medications are of considerable significance, prompting several investigations, including randomised controlled trials, case studies, and animal research, into herbal pharmaceuticals. Women with PCOS have around double the testosterone levels compared to typical women and frequently experience insulin resistance [6]. Pomegranates (*Punica granatum* L.; Family: Punicaceae) are spherical, crimson, succulent, and tasty fruits containing arils (edible seeds). Pomegranates are among the oldest known fruit plants, dating back to 4000-3000 BCE [7].

***Punica granatum* Peel**

Clinical study indicates that pomegranates may enhance cardiac blood flow, reduce blood viscosity, inhibit arterial plaque formation, and lower cholesterol levels, so serving as a significant aid in the prevention of cardiovascular illnesses, myocardial infarctions, and strokes. Pomegranates are recognised for their antioxidant and anti-inflammatory properties. They are also an excellent source of fibre. Pomegranates primarily consist of flavonoids, ellagitannins, punicalagin, ellagic acid, vitamins, and minerals. Ellagitannin and punicalagin are the primary components of pomegranate. Punicalagins have anti-inflammatory and antioxidant qualities that provide preventive benefits for cardiovascular issues, cancer, urinary functions, and the health of the brain and prostate. The fruits, skins, and seeds of pomegranates possess various medicinal properties. Pomegranate juice is utilised in the treatment of diarrhoea and jaundice [8-9].

Description of lead molecule [11-14]

Experiment Works

Selection of Lead molecule

The literature analysis indicates that Pomegranate peel (PoP), a byproduct of juice production typically seen as trash, constitutes around 30-40% of the fruit. Phenolic compounds, a category of bioactive phytochemicals, are predominantly located in the peel of pomegranate fruit. The primary phenolic compounds identified in the literature regarding PoP encompass flavonoids (including anthocyanins such as pelargonidin, delphinidin, cyanidin, along with their derivatives, and anthoxanthins such as catechin, epicatechin, and quercetin), tannins (specifically ellagitannins and ellagic acid derivatives such as punicalagin, punicalin, and pedunculagin), and phenolic acids (including chlorogenic, caffeic, syringic, sinapic, p-coumaric, ferulic, ellagic, gallic, and cinnamic acid) [10]. Consequently, newer phenolic derivatives, namely pelargonidin and delphinidin, were selected as lead molecules for the current work.

Table 1: Comparative description of pelargonidin and delphinidin

Description	Pelargonidin	Delphinidin
Molecular formula	$C_{15}H_{11}O_5$	$C_{15}H_{11}O_7$
Synonym	2-(4-hydroxyphenyl)chromenylium-3, 5, 7-triol	Flavylium, 3, 3', 4', 5, 5', 7-hexahydroxy
Molecular weight	271.24 g/mol	303.24 g/mol
Pharmacology	Antioxidant status, thereby reducing oxidative DNA damage, cellular proliferation, differentiation, apoptosis, angiogenesis, and reverse drug resistance of metastatic cells, and potentially induces cell cycle arrest, thereby interfering in colorectal carcinogenesis.	Antioxidant, antimutagenesis, anti-inflammatory anti-angiogenic properties.

Selection of target receptors

Polycystic ovarian syndrome is a multifaceted illness linked to reproductive and endocrine systems, potentially leading to infertility and metabolic disorders in individuals of childbearing age. Polycystic Ovary Syndrome (PCOS) appears to be a complex condition arising from the interplay of several genetic and environmental influences. Limited study has been undertaken thus far regarding the influence of polymorphisms on infertility. Numerous research highlights the significance of the steroidogenesis pathway and genetic variations in the development of PCOS [15]. The main genes implicated in the aetiology of PCOS are CYP11A1, CYP17A1, and CYP19A1. "In current studies, CYP11A1 was chosen as a target molecule as it is key genes involved in the ovarian dysfunctions in PCOS".

Molecular docking studies

Ligand Preparation

2D Structure of delphinidin and pelargonidin were drawn using ChemSketch [16], 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:

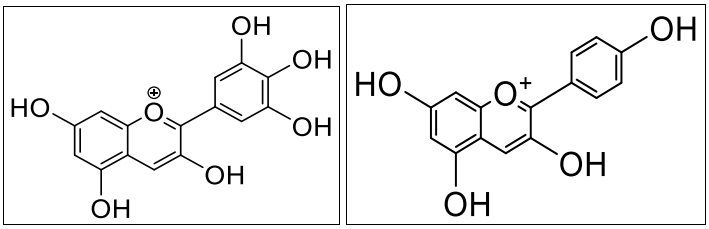


Fig 2: 2D structure of delphinidin and pelargonidin

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 the considered receptor in the current study are given in table 1[17-22].

Table 2: Grid parameters used in current docking analysis

S. No.	Receptor	x-axis	y-axis	z-axis	Spacing	x center	y center	z center
1	CYP11A1	50	50	50	0.5403	15428	-6.983	17.418

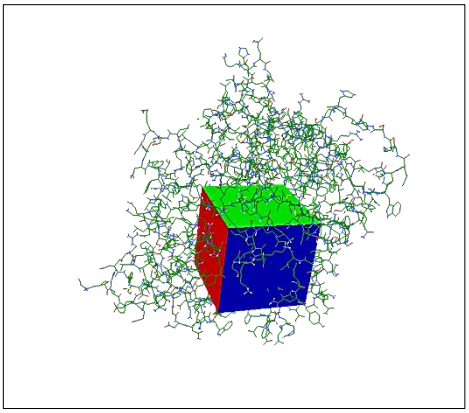


Fig 3: Grid box covering all active sites in CYP11A1 receptor

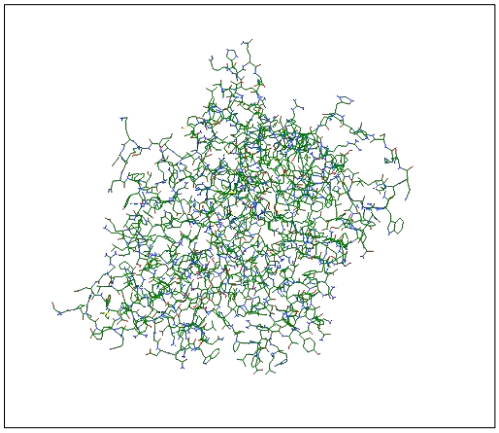


Fig 4: Crystal structure of CYP11A1 receptor (PDB ID-3n9y)

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 [23].

Docking Study

Crystal Structure

The crystal structure of the protein consisting of CYP11A1 receptor was downloaded from the Protein Data Bank portal. All the primary information regarding all the receptor's structure was registered in the Protein data bank [24-25]. The complex ligand was separated by using Chimera software for all the target receptors.

Processing of Protein

The downloaded receptor protein is having two chains, i.e. chain A and B, out of which has chain A 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 [26].

Molecular Docking Simulation Studies

Docking of ligand delphinidin and pelargonidin against CYP11A1 receptor was performed by Autodock. All the bonds of each ligand were kept flexible, while no residues in receptor were made flexible [27-29].

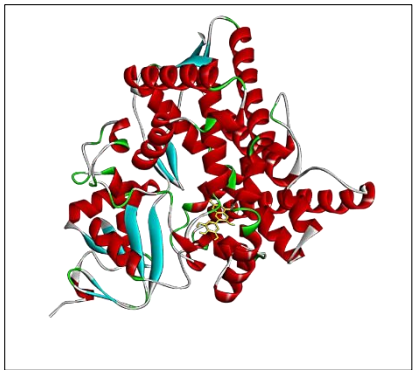


Fig 5: Binding mode of delphinidin within the active site of CYP11A1 receptor

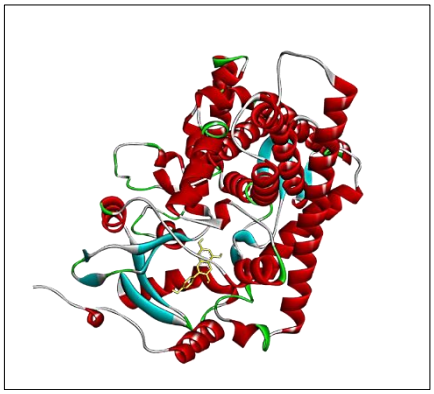


Fig 6: Binding mode of pelargonidin within the active site of CYP11A1 receptor

Toxicity & ADME-T Studies

The ligand molecules viz. delphinidin and pelargonidin was 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 [30].

Result and Discussion

Historically, natural supplements such as herbal and plant-based substances were employed to address ailments including hormonal imbalances and mitigate their significant negative effects. The acceptability of natural supplements has increased due to their lack of side effects or harm to the human body. The market for natural supplements has increased by 15% for the purpose of regulating oestrogen and progesterone levels in the human body. Hormones are chemical messengers secreted by endocrine glands essential for sustaining human reproductive and metabolic health. An alteration in hormone secretion levels results in hormonal imbalance. Approximately 59.6% of women in India are experiencing hormone imbalances due to lifestyle factors. Natural supplements such as maca, liquorice, omega-3 fatty acids, vitamins B and D, ashwagandha, probiotics, turmeric, DIM, and DHEA are employed to effectively address hormonal imbalances, as pharmaceutical interventions may result in significant side effects, including PCOS/PCOD, infertility, irregular menstruation, hypogonadism, and acromegaly. Polycystic ovarian syndrome (PCOS) is an endocrine and gynaecological condition that impacts numerous women of reproductive age. The prevalence of PCOS fluctuates considerably, between 2.2% and 26%. The early identification of PCOS is essential owing to its related consequences. Modifications in lifestyle are crucial for management; yet, several persons remain uninformed regarding this ailment. Enhanced public information is essential, especially for reproductive-age adults with obesity, who face elevated risks. The increasing incidence is probably associated with lifestyle variables. To enable early diagnosis and avert future problems, including metabolic syndrome, diabetes, endometrial cancer, cardiovascular disease, and nonalcoholic fatty liver disease, research questionnaires should be administered to young women in the population. Obese patients with PCOS should prioritise knowing BMI and the significance of weight loss. Patients with PCOS frequently encounter monthly abnormalities, hirsutism, sleeplessness, and mental health challenges, adversely affecting their quality of life.

Flavonoids are currently recognised as the preferred therapeutic agents for their efficacy in treating hyperlipidaemia, hyperglycemia, oxidative stress, and hyperandrogenism associated with PCOS. Flavonoids are intricate compounds with several advantageous features, including antibacterial, antiviral, antiulcerogenic, cytotoxic, antineoplastic, anti-inflammatory, antioxidant, antihypertensive, hepatoprotective, hypolipidemic, and anti-platelet actions. Pomegranate peel is a substantial source of antioxidants, polyphenols, dietary fibre, and vitamins, which enhance its notable bioactivity. Research has shown that pomegranate peel possesses anti-inflammatory, cardioprotective, wound healing, anticancer, and antibacterial activities due to the presence of phytochemicals, including gallic acid, ellagic acid, and punicalagin.

Previous studies have shown that Pelargonidin (PG) has several health advantages, including anti-cancer properties, enhancement of neurological conditions, anti-inflammatory effects, antioxidant capabilities, anti-diabetic actions, and bacteriostatic activities. The PG has significant anti-inflammatory properties primarily affecting Mitogen-Activated Protein Kinases (MAPK) and nuclear transcription factors NF-κB and AP-1.

Delphinidin suppressed proliferation, obstructed anchorage-independent growth, and caused apoptosis in ER-positive, triple-negative, and HER2-overexpressing breast cancer cell lines. Delphinidin, extracted from Punica granatum L, selectively reduced the histone acetyltransferase (HAT) activities of p300/CBP. It also suppressed p65 acetylation in MH7A cells, a human synovial cell line associated with rheumatoid arthritis. The impact of delphinidin on human Glyoxalase I (GLO I) was examined, demonstrating a significant inhibitory effect on GLO I and indicating its potential for the development of new GLO I inhibitory anticancer agents.

The literature analysis indicates that *P. granatum* peel is a rich source of polyphenols. The scientific confirmation of the polyphenol presents in P. granatum peel, demonstrating efficacy against PCOS, was examined by *in-silico* molecular docking. As a result, the phenolic derivatives pelargonidin and delphinidin were chosen as lead compounds for this study.

The results of the current investigation indicated that the selected lead molecules serve as effective in treating and preventing PCOS, binding to the target protein of CYP11A1 with binding energies of -7 & -7.43 kcal/mol for delphinidine and pelargonidine respectively. The Ki values were determined to be 7.34 and 3.61 µM for delphinidine and pelargonidine respectively. The outcome was recorded in Table 2. The binding mechanism of the selected lead compounds is illustrated in Figures 5 and 6. The two-dimensional and three-dimensional interactions of the selected chemical are illustrated in Figures 7-10. The affinity of lead compounds for the receptor was determined to be relatively comparable. The interaction of delphinidine and pelargonidine with the active site of CYP11A1 is illustrated as follows:

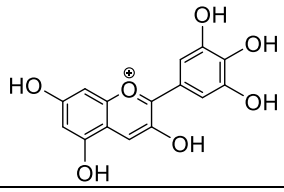
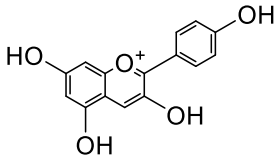
Table 3: Molecular interactions of delphinidin and pelargonidin with the target protein

Compound	Conventional Hydrogen bounding	π-alkyl	π-π stacked	Week Vander's interaction	π -cation	π -donar H bond	π -σ
Delphinidine	Glu 283 Arg112 GlN422 Arg421	Leu101	-	Ala286 Gly287 Phe202 Trp87 Cys423 Trp108	Arg81	Leu424	-
Pelargonidine	GLN356 Thr354 Ser352 Leu460	Val57 Leu209	Phe82	Leu54 Tyr61 ASN56 Glu58 Ser59 Leu375 Phe458 ILE84	-	GLN377	Val353

The interaction results indicated that both lead molecules attach at comparable positions by typical hydrogen, pi-alkyl, and pi-pi interactions, demonstrating a synergistic effect of both compounds from *P. granatum* in exerting protective action on PCOS.

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 delphinidine and pelargonidine are presented in Figures 11-12 and Tables 3-5. All ligand compounds have demonstrated promising docking scores theoretically.

Table 4: Results of docking of ligands like delphinidin and pelargonidin against CYP11A1 receptor

S. No	Compound Name	Structure	Binding Energy
1	Delphinidin		-7.0 (ki: 7.34 µM)
2	Pelargonidin		-7.43 (ki: 3.61 µM)

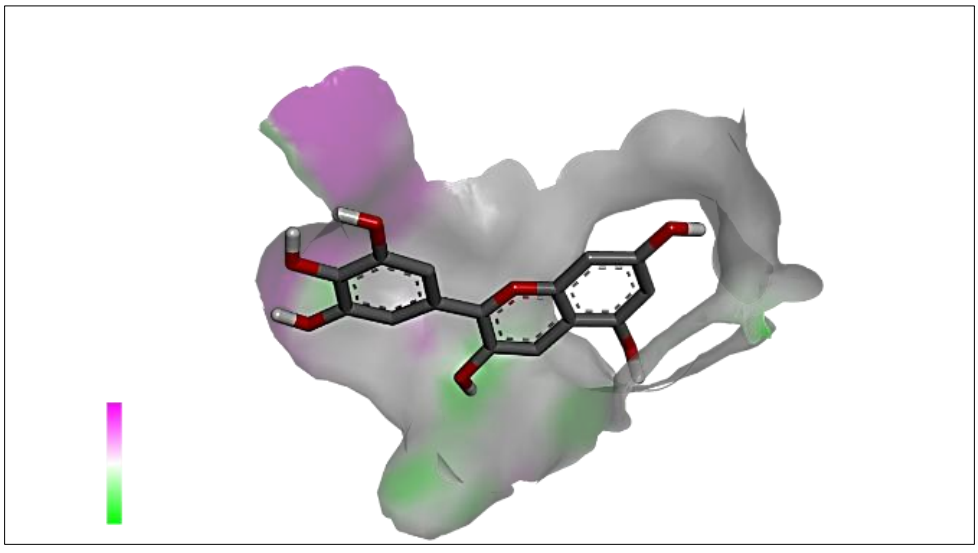


Fig 7: Three-dimensional binding mode of delphinidin within the active site of CYP11A1 receptor

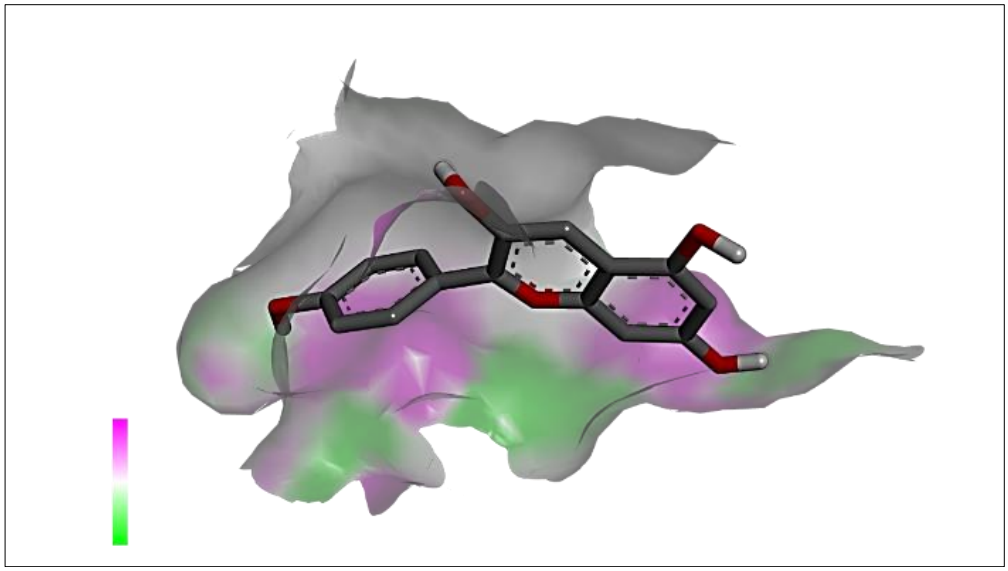


Fig 8: Three-dimensional binding mode of pelargonidin within the active site of CYP11A1 receptor

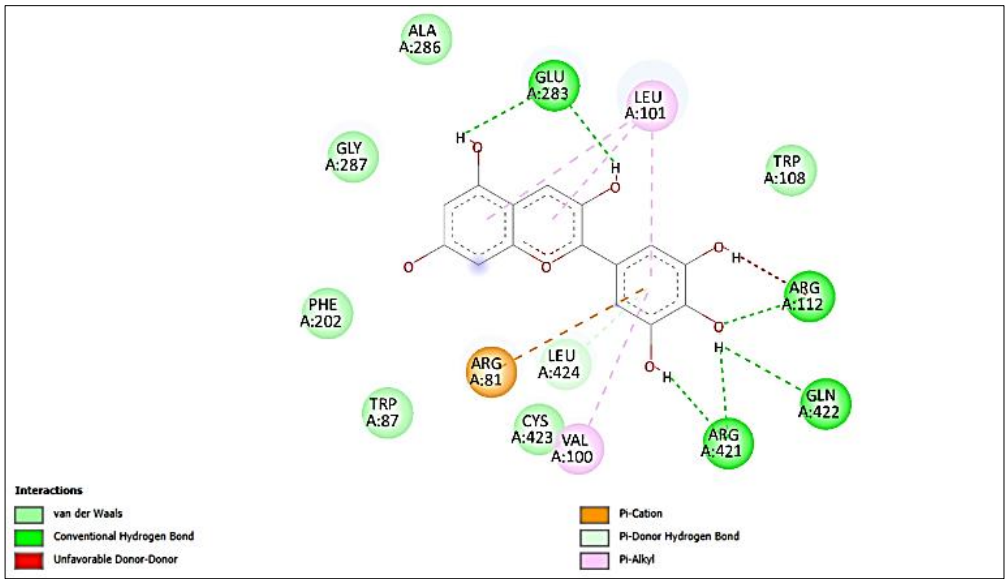


Fig 9: Two-dimensional binding mode of delphinidin within the active site of CYP11A1 receptor

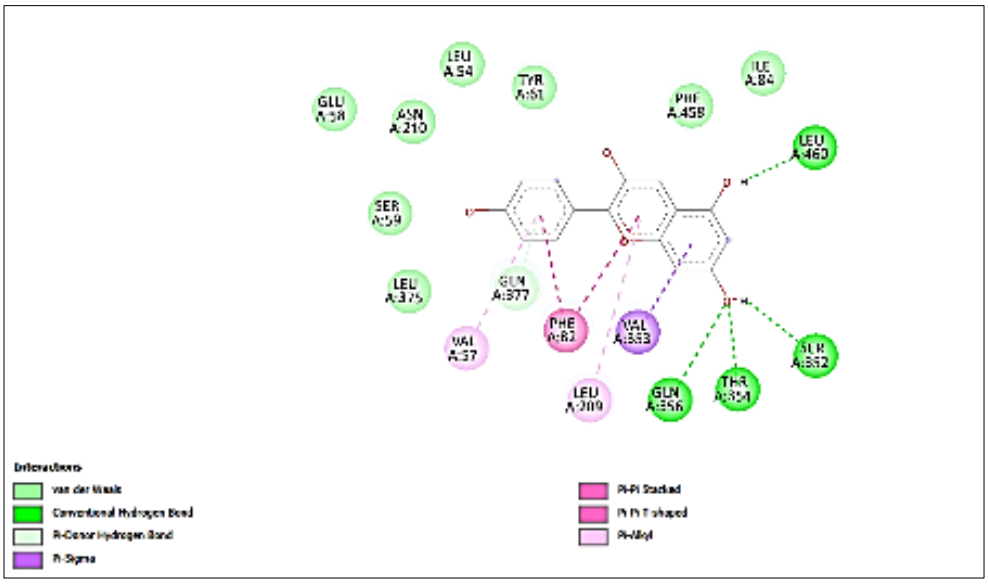


Fig 10: Two-dimensional binding mode of pelargonidin within the active site of CYP11A1 receptor

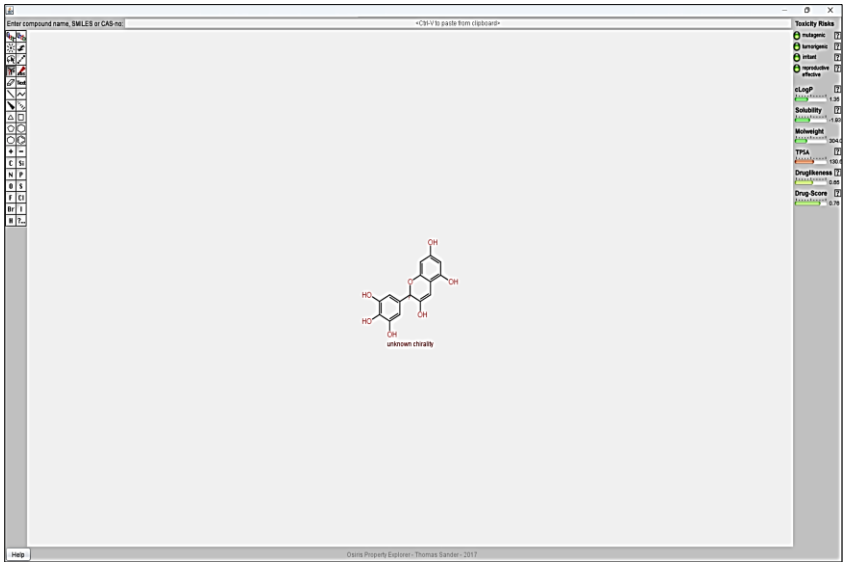


Fig 11: Pharmacokinetic and toxicity profiling of delphinidin

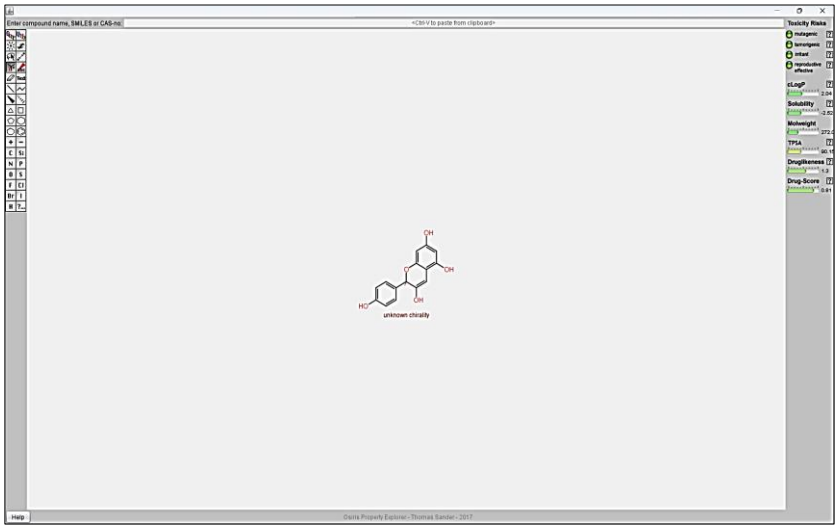


Fig 12: Pharmacokinetic and toxicity profiling of pelargonidin

Table 3: Pharmacokinetic Profiling of lead molecules

Compound	ADMET			
	Mutagenic	Tumorigenic	Irritant	Reproductive effectivity
Delphinidin	NO	NO	NO	No
Pelargonidin	NO	NO	NO	No

Table 4: Lipinski Properties of lead molecules

Compound	*cLogP*	Solubility	Mol.wt.	TPSA	Drug likeness	Drug score
Delphinidin	1.36	-1.90	303	130	0.56	0.70
Pelargonidin	2.84	-2.52	272	90.05	1.3	0.91

Table 5: Drug likeness of lead molecules

Compound	Lipinski rule of five	H bond donar	H bond acceptor (<10)
Delphinidin	Yes	6	4
Pelargonidin	Yes	6	4

Conclusion

This study conducted a theoretical assessment of the binding affinities (kcal/mol) of selected polyphenols with CYP11A1 (Cytochrome P450 Family 11 Subfamily A Member 1), a protein-coding gene associated with PCOS, to evaluate their efficacy and identify potential lead compounds from *P. granatum* peel. The molecular docking analyses revealed a favourable docking score. Computational screening for new herbal inhibitors (phytochemicals) may facilitate the development of commercial formulations for enhanced Polycystic Ovary Syndrome (POS) treatment.

Divulgence of Investigation

The daily use of P. granatum peel powder may offer prophylactic and preventive benefits against PCOS. The findings indicated that the lead compounds had an inhibitory impact on CYP11A1. Delphinidin and Pelargonidin present in P. granatum peel extract bind to CYP11A1 through

hydrogen, π-alkyl and π -σ interactions, resulting in the inhibition of CYP11A1, which plays a crucial role in steroidogenesis. This inhibition minimises the excessive synthesis of androgens and mitigates the danger of hyperandrogenism. The antioxidant activity of P. granatum peel has shown favourable results due to its capacity to combat oxidative stress. Antioxidants can enhance the ovarian environment, facilitate follicular maturation, and increase oocyte quantities, while also regulating lipid and glucose metabolism and vascular endothelial cell function in patients with PCOS. This results in reduced adiposity and a lower incidence of chronic complications, ensuring long-term benefits for patients.

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