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ORIGINAL RESEARCH

In-silico Screening of Anticancer Potential of P*ongamia pinnata* and R*ubia cordifolia* Phytoconstituents: A Molecular Docking Approach

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ABSTRACT

Pongamia pinnata Linn belongs to Fabaceae and *Rubia cordifolia* belongs to Rubiaceae families, holds a significant place in herbal medicine. The present study aims to determine the anticancer properties of the *R. cordifolia* and *P. pinnata.* Both plants are rich in active constituents, responsible for the treatment of various diseases. Since in-silico methods are promising and useful for drug design through natural plants, the present research includes the in-silico evaluation to elucidate the anticancer potential of *P. pinnata* and *R. cordifolia* against ERα (PDB ID: 1R5K) and BRCA1 (PDB ID: 1JNX), targets associated with breast cancer. Docking results showed strong binding affinities between active constituents of *R. cordifolia* and *P. pinnata* with BRCA1, ranging from (−6.2 to -6.8 kcal/mol), and with another target Erαconstituents of *R. cordifolia* exhibited strong interactions, ranging from (−5.4 to -8.8 kcal/mol), while *P. pinnata* constituent from (-6.2 to -8.1kcal/mol). Both the plants displayed the highest binding affinities with stable hydrogen bonds. These findings suggest a promising potential of *R. cordifolia* and *P. Pinnata* against breast cancer.

Keywords: Breast Cancer, Erα, BRCA1, Molecular docking

INTRODUCTION

Medicinal plants have been the basis of many traditional medicines throughout the world for thousands of years and continue to provide new remedies to mankind with less or no side effects (Mishra, B. *et al.*, 2013). *Pongamia pinnata* (Linn.) Pierre is a medium-sized, glabrous tree commonly known as Karanja in Hindi, Indian Beech in English, and Pongam in Tamil (Arote *et al.*, 2010). *P. pinnata*, an important species from the Fabaceae family, is the sole species in the genus Pongamia. The chemical properties of *P. pinnata* have led to the isolation of karanjin, a furanoflavone, which has become a trademark compound of this species. The pharmacological effects of its various extracts and chemical constituents include antioxidant, antimicrobial, anti-parasite, anti-convulsant, anti-inflammatory, anti-diabetic, anti-hyperammonemic, cytotoxic, insecticidal, anthelminthic, and immunomodulatory activities. (Al Muqarrabun *et al.*, 2013; Navyatha Karamala *et al.*, 2025)

Rubia cordifolia Linn. (Rubiaceae) is characterized by its very long, cylindrical, and flexuose roots, which are covered with a thin red bark. This plant is also known as Indian Madder or Manjistha and is widely recognized for its medicinal properties (Mishra *et al*., 2024; Patil *et al.*, 2009).

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Cancer is a major health problem in individuals, and it is the prime cause of death worldwide. Every year approx. 18 million people are diagnosed with cancer (Mishra, B. *et al.*, 2025; Tiwari *et al.*, 2024). Among all cancers, breast cancer, characterised by unregulated growth of cells, resistance to apoptosis, and metastatic spread fuelled by hormonal, genetic, and epigenetic changes, continues to rank among the top causes of cancer-related death for women globally. Although targeted therapies, radiation, and chemotherapy have advanced, multidrug resistance and serious side effects have made it necessary to look for safer and more effective natural alternatives (Cohen *et al.*, 2002). In this regard, medicinal plants having promising anticancer properties against breast carcinoma, like *P. pinnata* and *R. cordifolia*, have drawn a lot of interest. By modifying the expression of Bcl-2 family proteins and blocking NF-κB signalling pathways, *R. cordifolia*, which is abundant in anthraquinones like alizarin, purpurin, and rubiadin, has strong cytotoxic and pro-apoptotic effects on breast cancer cells, thereby reducing tumour growth and metastasis (El-Banna *et al.*, 2025).

Molecular docking offers a rational and cost-effective *in silico* strategy to evaluate the anticancer potential of *P. pinnata* and *R. cordifolia*. A computational approach predicts the binding affinities and interaction bonds between target proteins and plant-derived phytoconstituents, including flavonoids, furano-flavonoids, and anthraquinones. Through molecular docking, the identification of promising phytochemicals is achieved by simulating their binding conformations and energetics. It also aids in optimizing lead molecules by elucidating their probable mechanism of action at the molecular and atomic levels. Consequently, this method provides a targeted, hypothesis-driven framework that accelerates anticancer drug discovery and supports the scientific validation of traditional medicinal uses of these plants (Karamala *et al.*, 2025).

The current research is focused on discovering the possible anticancer phytoconstituents of *P. pinnata* and *R. cordifolia* through molecular docking. Molecular docking helps to predict the binding affinities between phytoconstituents and cancer targets.

MATERIALS AND METHODS

Selection of Plant constituents

The pharmacological activities of *R. cordifolia* roots and *P. pinnata* leaves are attributed to their diverse phytochemical constituents with reported anticancer properties. The roots of *R. cordifolia* are rich in anthraquinones and naphthoquinones such as alizarin, purpurin, manjistin, rubiadin, and mollugin, which exhibit cytotoxic, pro-apoptotic, and antiproliferative effects against various cancer cell lines (Wen *et al.*, 2022). Likewise, *P. pinnata* leaves contain bioactive flavonoids and furanoflavonoids, including karanjin, pongamol, glabrin, and pinnatin, known for their ability to induce apoptosis, inhibit angiogenesis, and suppress tumor cell growth. Specifically, karanjin has demonstrated estrogen receptor modulation and cytotoxic effects in breast cancer cell lines, making it a suitable candidate for docking analysis. The diverse phytochemical profile of both plants justifies their selection for computational exploration of anticancer potential (Devidas *et al.*, 2024).

TARGET PROTEIN SELECTION

The human estrogen receptor alpha (ERα), retrieved from the Protein Data Bank (PDB ID: 1JNX), was selected as the primary molecular target for this docking study. ERα is a ligand-activated transcription factor that plays a pivotal role in breast cancer development by promoting estrogen-dependent gene expression and cell proliferation (Farcas *et al.*, 2021). Inhibiting ERα's ligand-binding domain has proven effective in controlling tumor progression and improving therapeutic outcomes. Thus, screening of *P. pinnata* and *R. cordifolia* compounds against ERα offers a rational strategy for identifying novel natural inhibitors with therapeutic potential against estrogen-dependent breast cancer (Dobrzycka *et al.*, 2003; Saha Roy *et al.*, 2012).

MOLECULAR DOCKING

Molecular docking was performed to investigate the binding interactions between the selected phytoconstituents and the target protein ERα (1JNX). The ligands alizarin and purpurin (from *R. cordifolia*) and karanjin and pongamol (from *P. pinnata*) were selected based on literature reports of anticancer activity. Ligand structures were retrieved from PubChem, energy-minimized, and converted to PDBQT format using Open Babel and Auto Dock Tools (Pavan *et al.*, 2025).

The 3D crystal structure of ERα (1JNX) was prepared using BIOVIA Discovery Studio, which involved removal of water molecules, addition of polar hydrogen atoms, and deletion of co-crystallized ligands. The receptor was then saved in PDBQT format for docking. Auto Dock Vina was used for docking. More negative binding energies indicated stronger and more stable ligand–protein interactions (Yadav *et al.*, 2025).

The docking analysis aimed to identify potent phytoconstituents capable of binding to the ligand-binding domain of ERα, thereby potentially modulating its activity and exerting anticancer effects. The study establishes a computational foundation for future biochemical validation and structure-based drug design using phytochemicals from *P. pinnata* and *R. cordifolia*.

Table 1: Molecular docking analysis of active constituents from r. Cordifolia roots and p. Pinnata leaves against brca1 (pdb id: 1jnx) a potential anticancer agent.

Plants	Active constituents	Hydrogen bonds	Binding affinity	Figures
R. cordifolia **[Roots]**	Alizarin	LEUX:1657, VALX:1654	-6.3kcal/mol	a.
	Purpurin	ARGX:1835	-6.2kcal/mol	b.
	Munjistin	GLYX:1656, LEUX:1657	-6.8kcal/mol	c.
P. pinnata **[Leaves]**	Karanjin	GLYX:1656,	-6.1kcal/mol	d.
	Pongamol	LEUX:1701, LYSX:1702	-6.2kcal/mol	e.

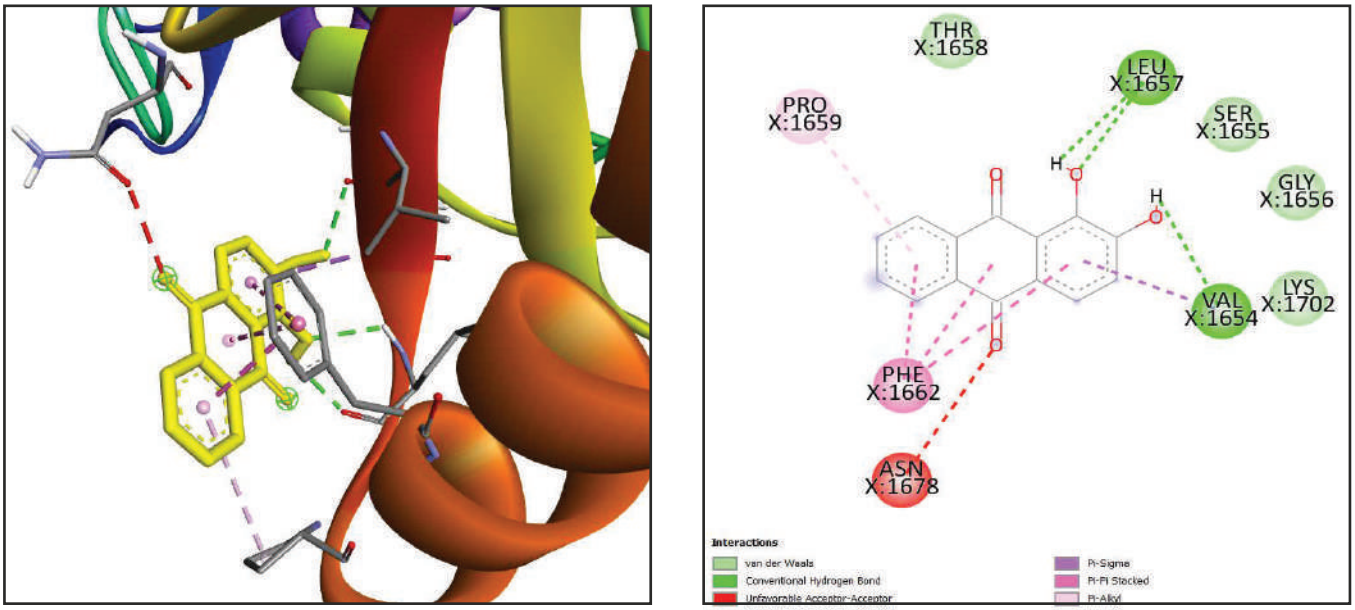

Figure A: Alizarin

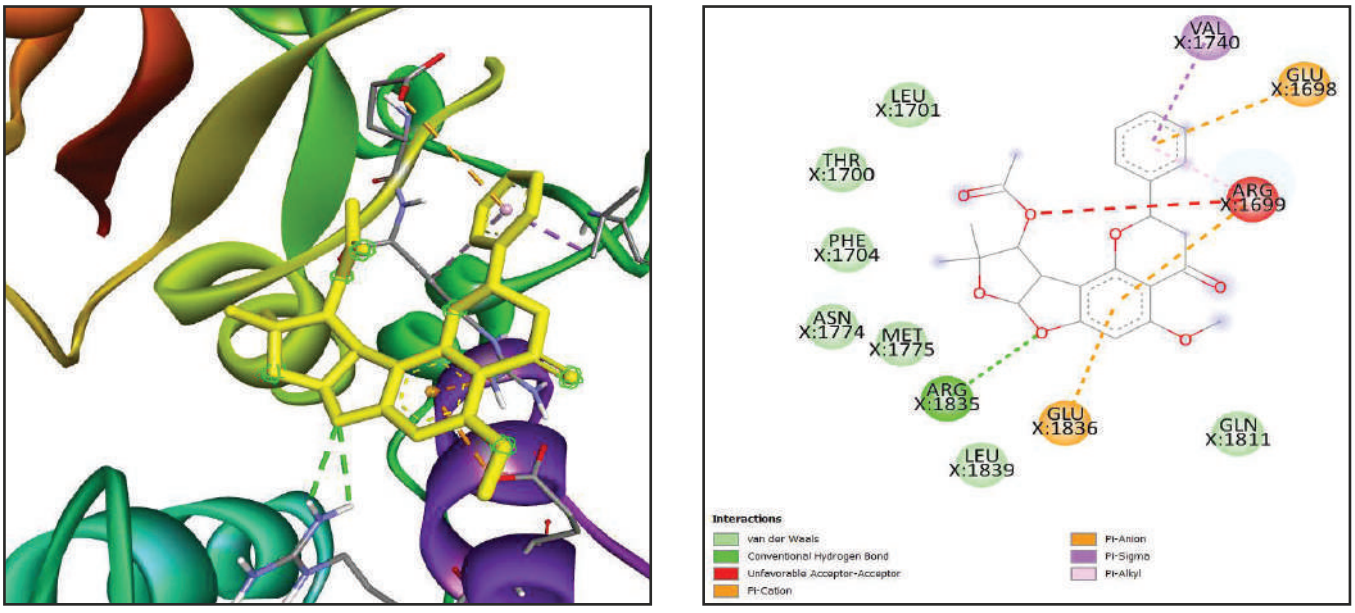

Figure B: Purpurin

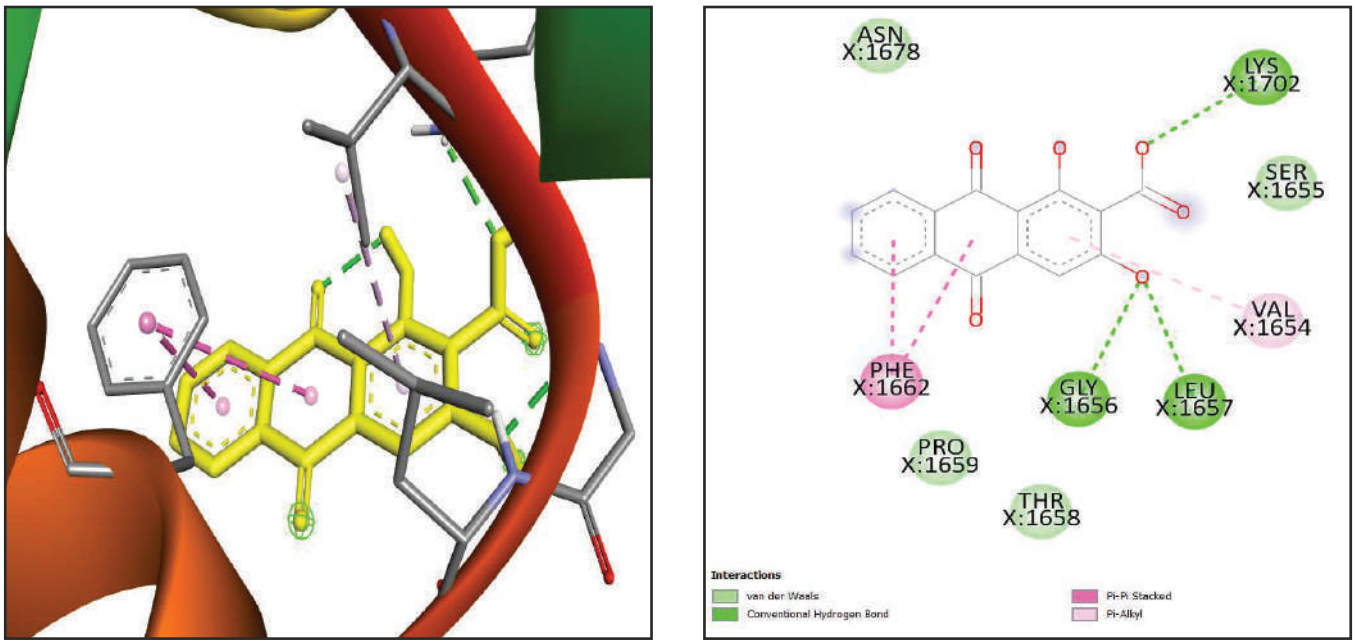

Figure c: Munjistin

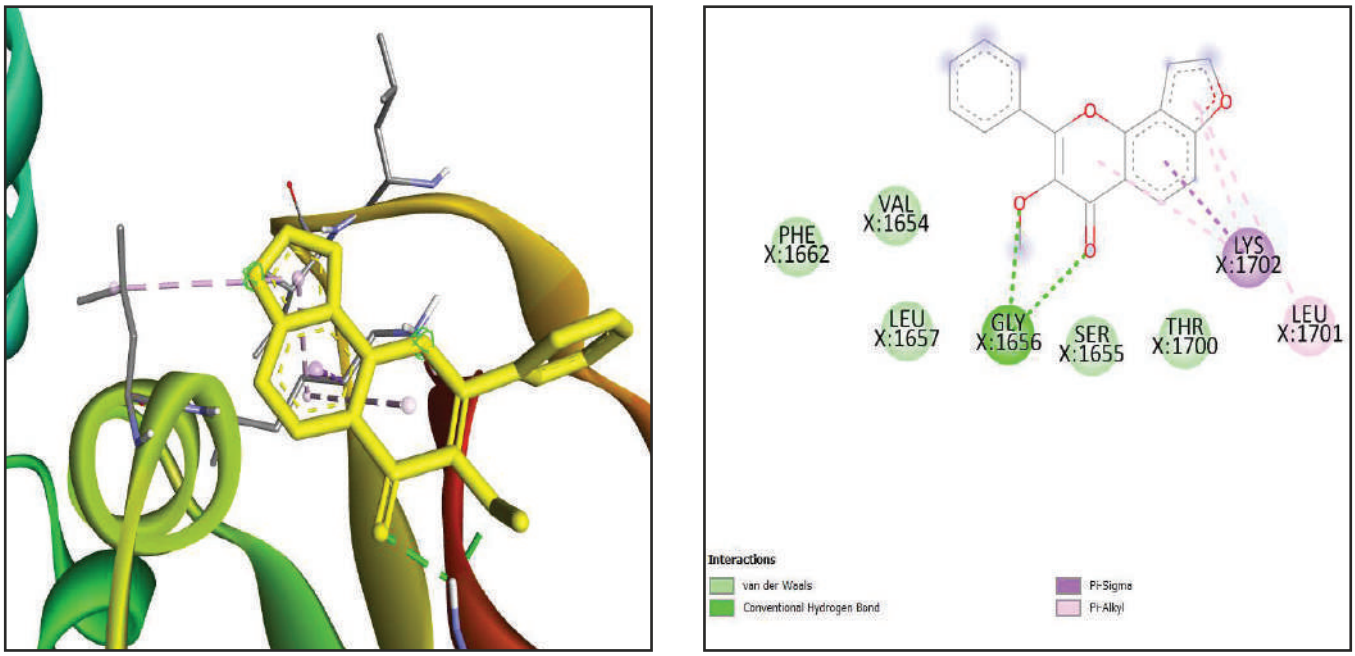

Figure d: Karanjin

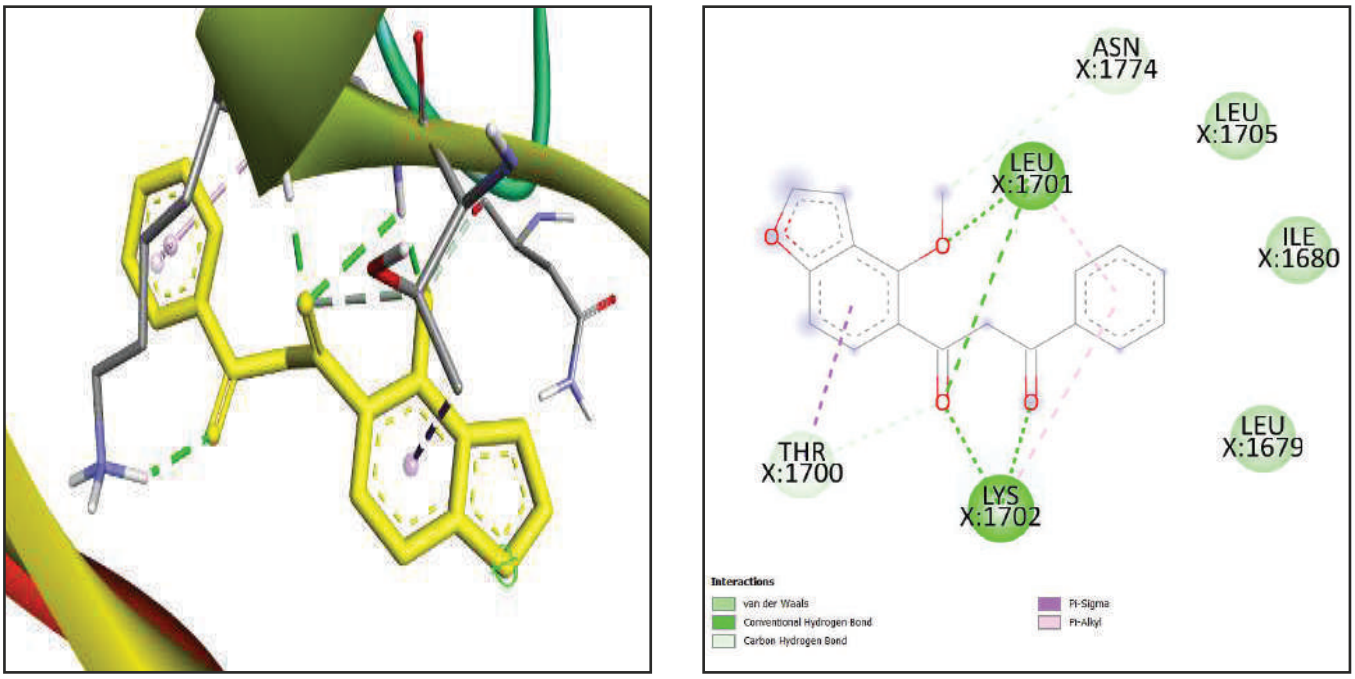

Figure e: Pongamol

Table 2: Molecular docking analysis of active constituents from r. Cordifolia roots and p. Pinnata leaves against erα (pdb id: 1r5k) as a potential anticancer agent.

Plants	Active constituents	Hydrogen bonds	Binding affinity	Figure
R. cordifolia **[Roots]**	Alizarin	LEUA:536, ASNC:348	-8.3 kcal/mol	a.
	Glabrin	LYSA:449, ARGA:394	-5.4 kcal/mol	b.
	Purpurin	ASNA:519	-7.2 kcal/mol	c.
	Munjistin	ARGA:394, LEUA:387	-8.8 kcal/mol	d.
	Rubiadin	TYRA:331	-8.1 kcal/mol	e.
P. pinnata **[Leaves]**	Pinnatin	ASNC:348	-7.8 kcal/mol	f.
	Mollugin	THRA:347, LEUA:346	-7.6 kcal/mol	g.
	Karanjin	LEUA:536	-8.1 kcal/mol	h.
	Pongamol	THRA:347	-6.2 kcal/mol	i.

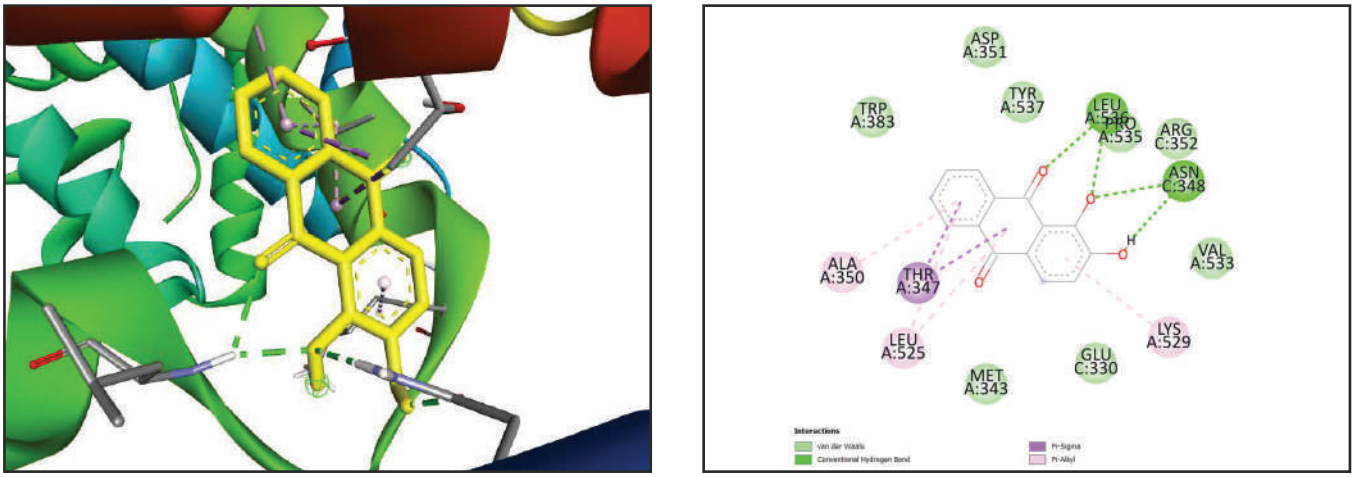

Figure a: Alizarin

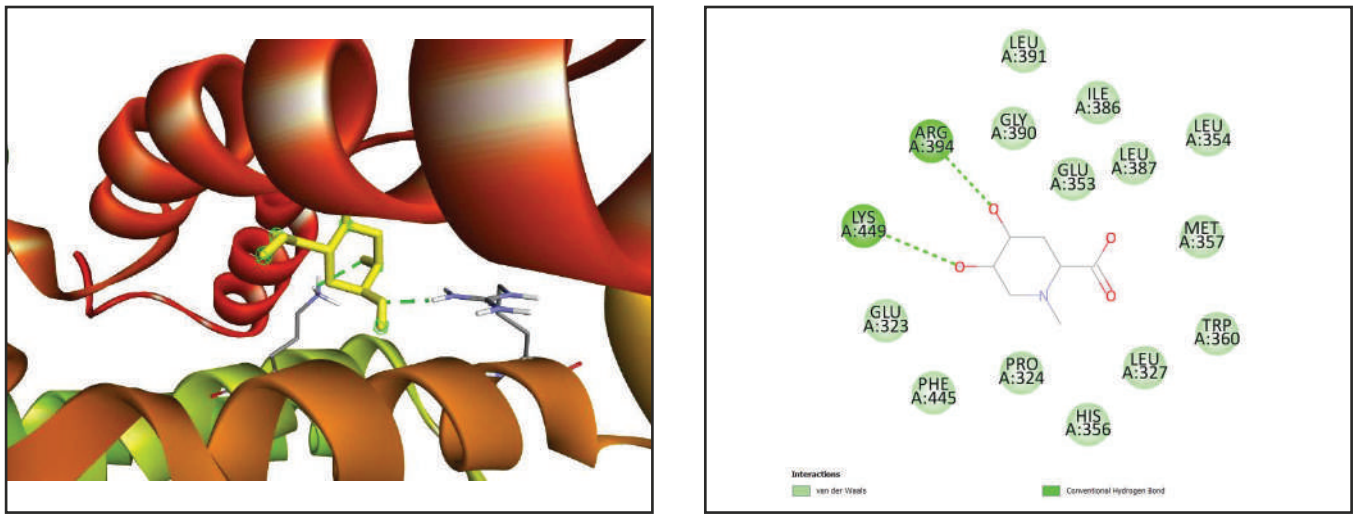

Figure b: Glabrin

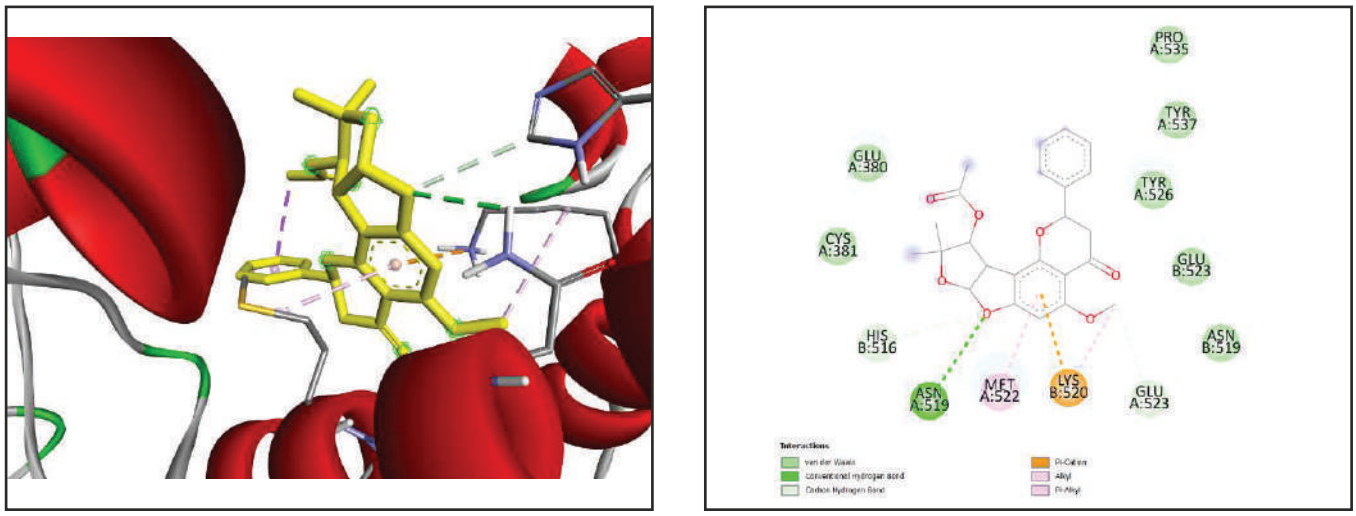

Figure c: Purpurin

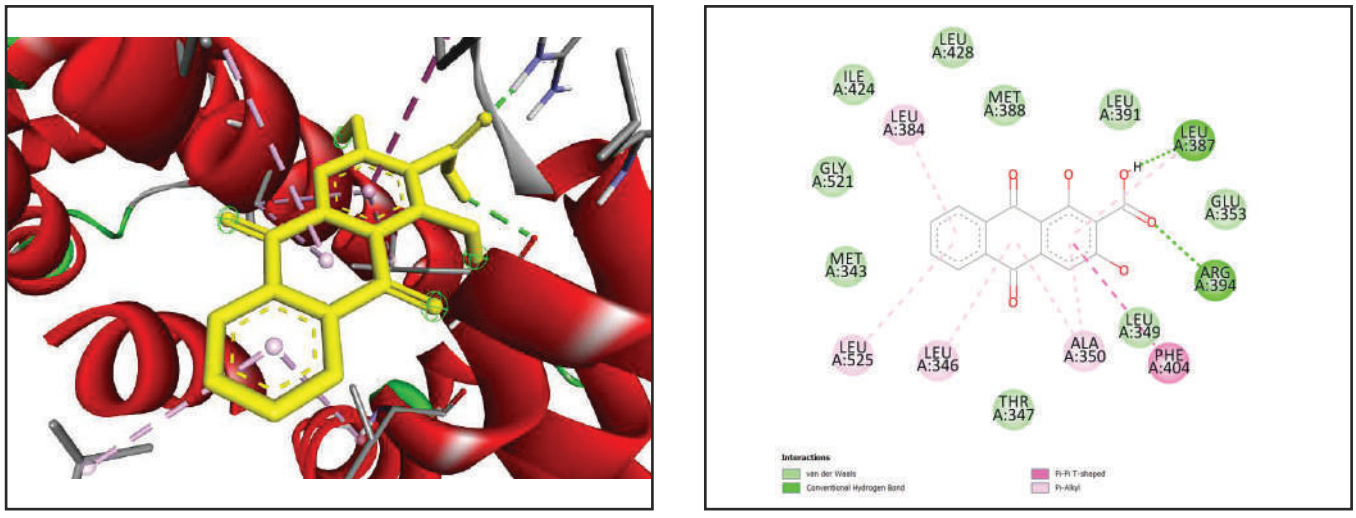

Figure d: Munjistin

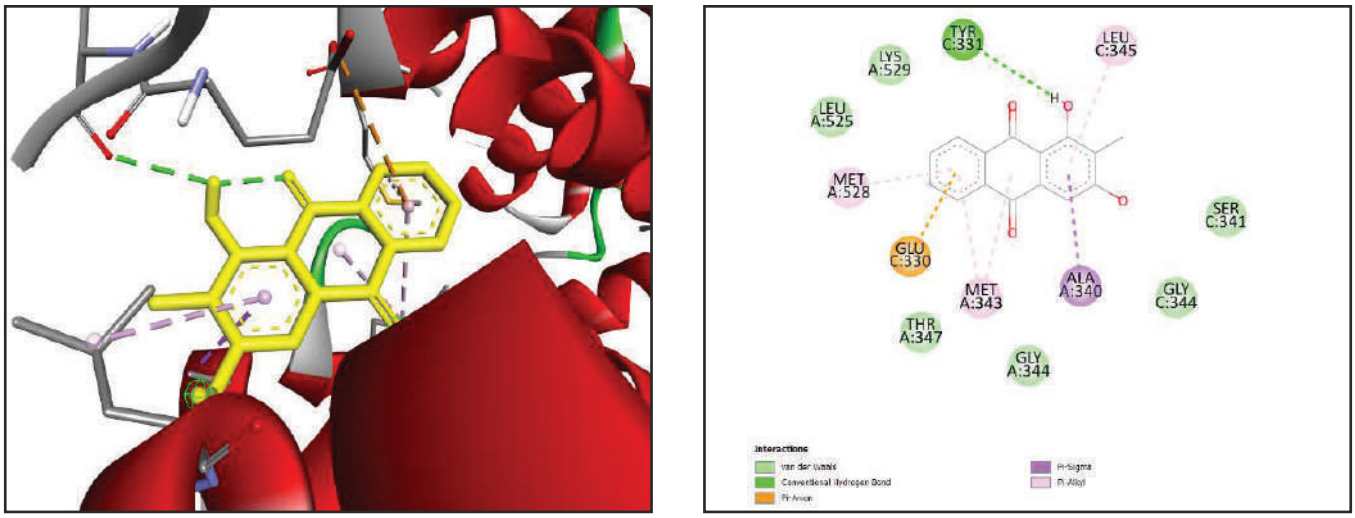

Figure e: Rubiadin

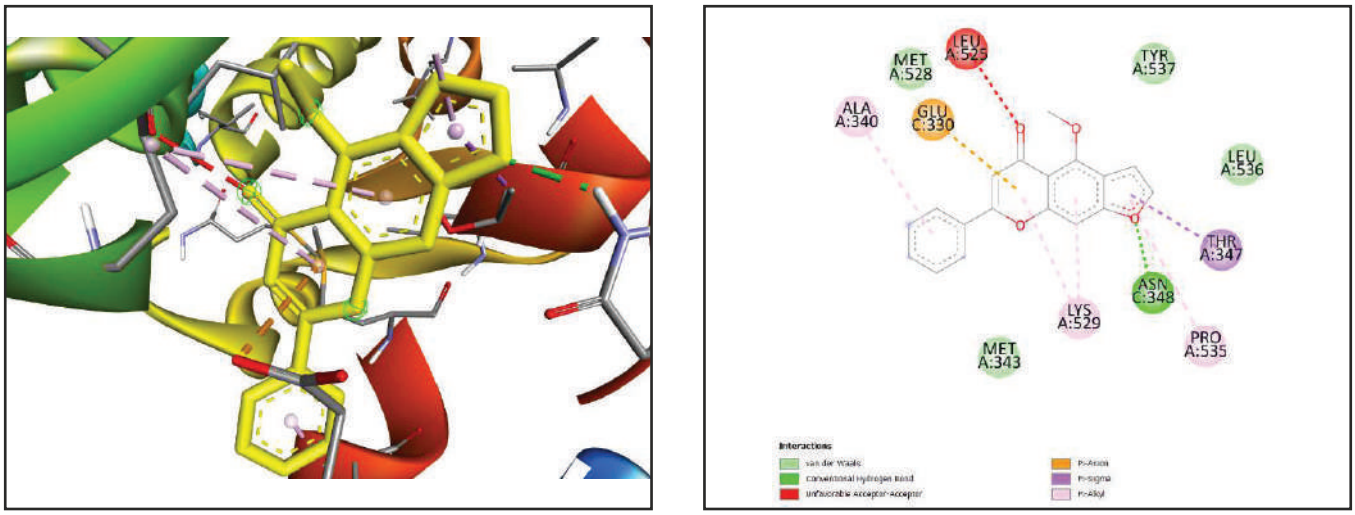

Figure f: Pinnatin

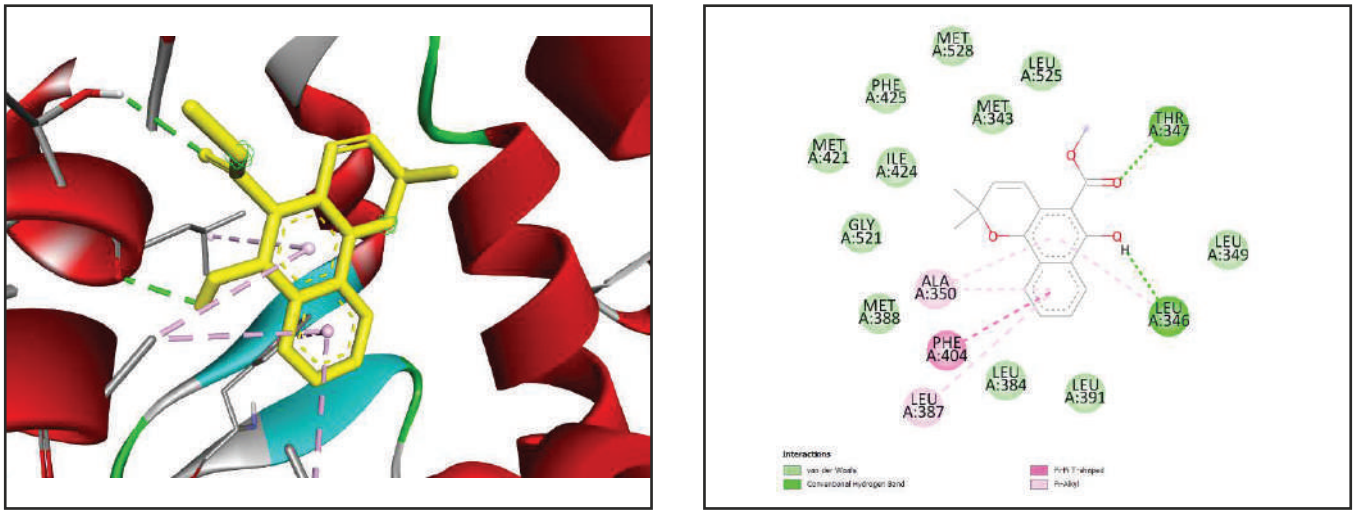

Figure g: Mollugin

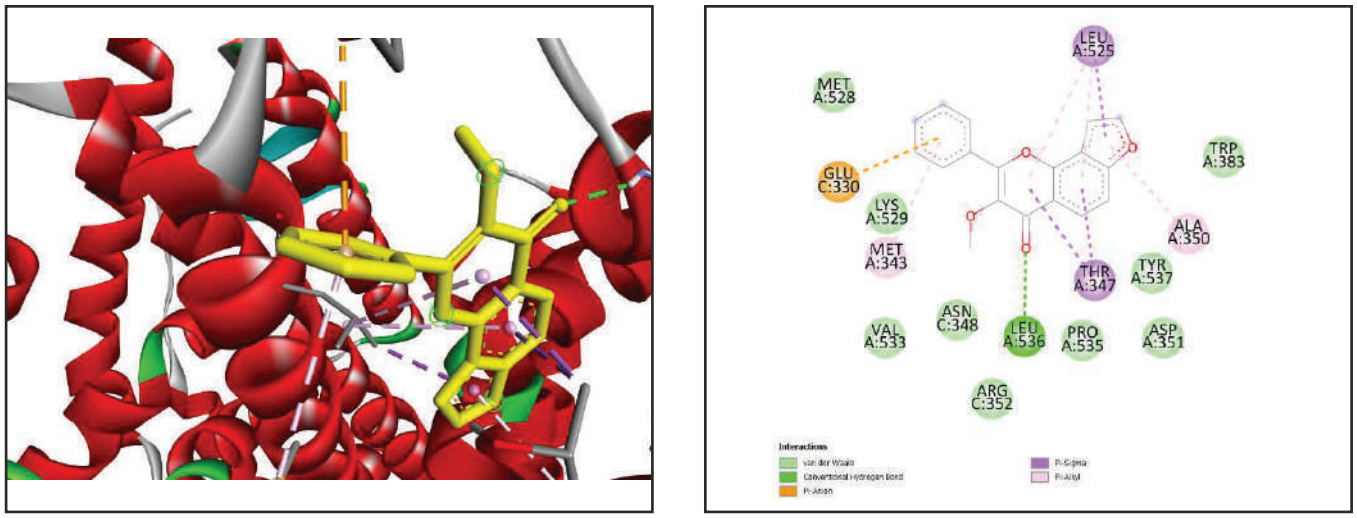

Figure h: Karanjin

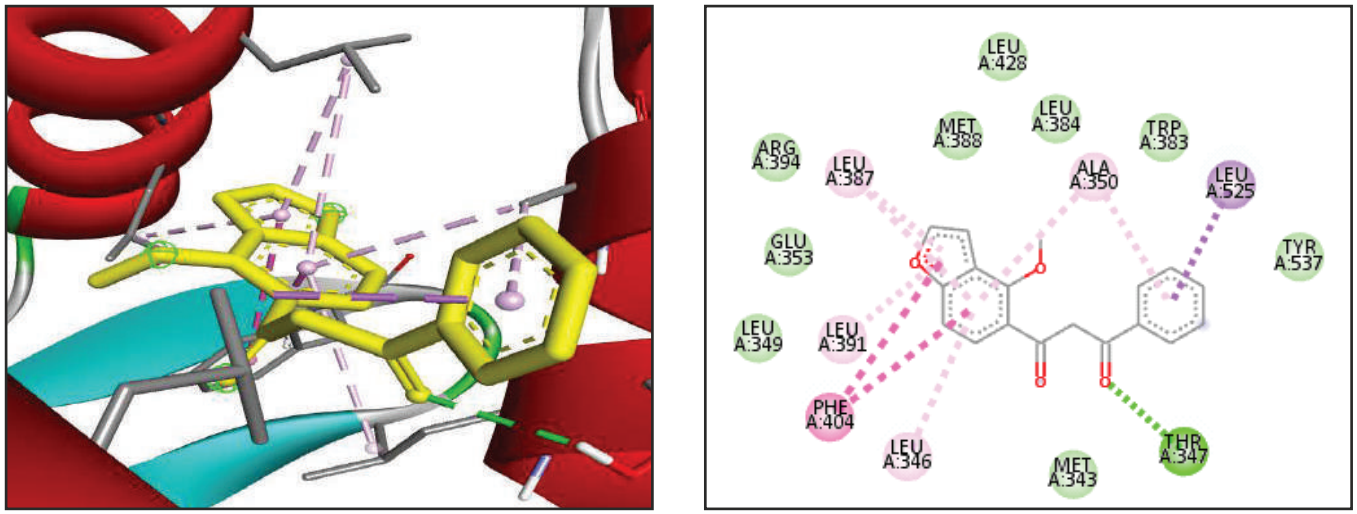

Figure i: Pongamol

DISCUSSION

In-silico investigation of *R. cordifolia* roots and *P. pinnata* leaves provides strong preliminary evidence supporting their anticancer potential against breast cancer targets. *P. pinnata* is rich in active constituents likepinnatin, mollugin, karanjin, and pongamol, while *R. cordifolia* contains alizarin, glabrin, purpurin, munjistin, and rubiadin. All the active constituents are responsible for diverse pharmacological activities. The current research reveals the anticancer relevance of the compounds through molecular docking against two key breast cancer-related proteins: ERα (PDB ID: 1R5K), a critical regulator of estrogen-driven tumor growth, and BRCA1 (PDB ID: 1JNX), a tumor suppressor whose dysfunction markedly increases breast cancer susceptibility.

Docking analysis of active constituents against BRCA1 revealed binding affinities, particularly for munjistin (−6.8 kcal/mol), alizarin (−6.3 kcal/mol), and purpurin (−6.2 kcal/mol), supported by stable hydrogen bonding interactions with key amino acid residues such as GLY1656, LEU1657, and ARG1835. Similarly, *P. pinnata* constituents exhibited strong interactions, showed binding affinity with karanjin (−6.1 kcal/mol) and pongamol (−6.2 kcal/mol), forming stabilizing hydrogen bonds with GLY1656, LEU1701, and LYS1702.

Against ERα, several constituents demonstrated even stronger binding tendencies. Munjistin (−8.8 kcal/mol), alizarin (−8.3 kcal/mol), rubiadin (−8.1 kcal/mol), and karanjin (−8.1 kcal/mol) were among the highest-affinity ligands, forming critical interactions with residues such as LEU536, ASN348, ARG394, and TYR331. Compounds from *P. pinnata*, including pinnatin (−7.8 kcal/mol) and mollugin (−7.6 kcal/mol), also exhibited significant affinity, further supporting their relevance as potential ERα modulators.

The result of the research suggested that the phytoconstituents from both plants displayed strong and specific interactions with breast cancer-associated targets, suggesting their potential role as natural anticancer agents. However, while docking studies offer valuable molecular insights, experimental validation through *in-vitro* cytotoxicity, mechanistic assays, and *in-vivo* models remains essential. Further pharmacokinetic, toxicity, and structural optimization studies are warranted to fully explore and translate the anticancer potential of *R. cordifolia* and *P. pinnata*.

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Conflict of interest: NO

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