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Natural Product-based Anticancer Potential of Derris Scandens Stem Bark: In Vitro and In Silico Approaches

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ABSTRACT: Natural products continue to be an important source of anticancer phytochemicals due to their variety bioactive constituents and favorable safety profiles. *Derris scandens* is traditionally used for various ailments, but, its anticancer potential remains inadequately explored. The anticancer potential of *Derris scandens* bark was investigated through complementary *in vitro* cytotoxicity assays and *in silico* molecular docking analyses. Dried bark material was subjected to sequential extraction with petroleum ether, dichloromethane, ethyl acetate, and methanol. The resulting extracts were subsequently screened for their preliminary phytochemical constituents. Five prominent compounds detected through GC–MS analysis were chosen for molecular docking evaluation against cyclin-dependent kinase (CDK) and epidermal growth factor receptor (EGFR) targets to investigate their possible interactions and anticancer activity. Phytochemical profiling by TLC and GC-MS revealed the presence of several biologically active constituents in the methanolic bark extract of *Derris scandens*. The tested extract exhibited appreciable cytotoxic effects against the MCF-7 and HepG2 cancer cell lines, yielding IC_{50} values of 39.8 µg/mL and 46.9 µg/mL, respectively. Molecular docking analysis indicated that **α-**amyrin and himachalol interacted favorably with the CDK8 protein, exhibiting binding energies of **−7.9** and **−7.5** kcal/mol, respectively, which were comparable to the reference inhibitor, sorafenib. In the EGFR docking study, **α-**amyrin showed a binding energy of **−7.7** kcal/mol, closely approaching that of the standard inhibitor erlotinib (**−7.**8 kcal/mol). The results indicate that the identified phytoconstituents may have considerable anticancer potential by interacting effectively with critical molecular targets associated with the development and progression of cancer.

1. INTRODUCTION

Despite substantial progress in cancer detection and therapeutic management, cancer continues to represent a major global health burden and remains a significant cause of death. Consequently, increasing attention has been directed toward the identification of safer and more efficacious therapeutic candidates from natural sources, particularly plant-derived phytochemicals. These bioactive constituents can influence several molecular and cellular mechanisms involved in tumor initiation and progression. Their reported anticancer activities include attenuation of oxidative stress and inflammatory responses, promotion of programmed cell death, disruption of cell-cycle progression, suppression of cancer-cell proliferation, and regulation of signaling pathways that contribute to carcinogenesis. The family **Fabaceae**, one of the largest and most

diverse plant families, is a rich source of constituents - flavonoids, isoflavonoids, alkaloids, saponins, phenolic compounds, and other metabolites with demonstrated antioxidant and anticancer properties. Because cancer development involves a complex interplay of genetic changes and abnormal cellular signaling, medicinal plants such as *Derris scandens* represent valuable sources for discovering bioactive constituents. The compounds obtained from these plants may serve as potential lead molecules for the development of new anticancer therapeutic agents[1].

1.1Cell cycle regulation

Cell cycle regulatory kinases are essential for controlling cell growth, DNA replication, and cell division. Among these, cyclin-dependent kinases (CDKs), Aurora kinases, polo-like kinases (PLKs) play key roles in maintaining genomic stability and ensuring proper cell cycle progression. Following DNA damage, checkpoint kinases (CHKs) contribute to genome integrity by temporarily halting cell-cycle progression, thereby allowing time for DNA repair; when the damage cannot be effectively repaired, they can promote apoptotic cell death. In contrast, cyclin-dependent kinases (CDKs), in association with their corresponding cyclins, control the progression of cells through successive stages of the cell cycle. Aberrant activation of these kinases contributes to uncontrolled cell proliferation in cancer, making them important therapeutic targets. Consequently, selective inhibitors of CDKs and other mitotic kinases have emerged as promising agents for cancer treatment[2-6].

Receptor tyrosine kinases (RTKs) constitute a class of membrane-spanning proteins that participate in the control of fundamental cellular functions, such as cell proliferation, survival, and differentiation. Aberrant activation of RTK-mediated signaling, particularly through the epidermal growth factor receptor (EGFR), has been associated with the initiation and progression of various cancers. Genetic alterations that activate EGFR, as well as increased receptor expression, can result in sustained downstream signaling and consequently promote uncontrolled proliferation of malignant cells. For this reason, the ATP-binding pocket of EGFR is widely investigated as a molecular target in docking studies and in the design of tyrosine kinase inhibitors, including gefitinib and erlotinib[7-9].

Advances in analytical and computational techniques, including column chromatography, LC–MS, , and pharmacokinetic modeling, significantly enhanced medicinal plant research. Together, these approaches support the separation, structural characterization, and biological assessment of plant-derived constituents, thereby contributing to the identification of new bioactive molecules with potential therapeutic applications[10].

Antioxidant-rich plants may help prevent and manage cancer by reducing oxidative stress. Reactive oxygen species (ROS), produced during normal metabolism, can damage cells and contribute to cancer development. Natural antioxidants in the body, along with those from foods and medicinal plants, help neutralize ROS and may lower cancer risk[11].

Naturally occurring antioxidants, particularly phenolics, flavonoids, and carotenoids, are associated with a broad range of biological effects, including the protection against oxidative damage, reduction of inflammatory responses, modulation of aging-related processes, and inhibition of cancer development. Their therapeutic potential is commonly assessed through cytotoxicity studies for cancer cells and sametime ensuring minimal toxicity to normal cells, an important consideration for the development of safe anticancer agents[12].

Derris scandens is plant of Fabaceae family, root bark is used in cancer. The stem of *Derris scandens* has a history of traditional medicinal use for managing cough, diarrhea, and dysentery, and is also reported to possess antitussive, diuretic, and expectorant properties. In traditional healing practices, preparations from the stem have additionally been employed to alleviate muscular discomfort and pain affecting the bones and joints. Analysis of the stems for the phytochemicals showed presence of a number of secondary metabolites of various classes, coumarins, flavones, isoflavones, isoflavone glycosides, pterocarpans, steroids, and terpenes. Several compounds have interesting pharmacological activities. *D scandens* is rich source of flavonoids like genistein, luteolin, and scandinones[13-15].

To investigate the utilization of *Derris scandens* barks in cancer treatment and to analyse various phytochemical compounds through successive solventt extraction and to screen these bark extracts this study was carriedout. By using *in vitro & in silico* approaches it was aimed to investigate their therapeutic anticancer potential, to identify compounds for anticancer activity.

2. MATERIALS AND METHODS

2.1Collection Of Bark

Derris scandens stem bark was collected in December 2023 and Dr. M. Murali Krishna Kumar, Andhra University, Visakhapatnam, Andhra Pradesh, India, taxonomically authenticated the plant material. A voucher specimen (No. 25440AUV) was deposited for reference ,at the University College of Pharmaceutical Sciences, Acharya Nagarjuna University, Guntur.

2.2 Preparation of extract

One kilogram of dried and powdered *Derris scandens* stem bark was extracted sequentially using maceration method, using solvents in the increasing order of polarity: petroleum ether, dichloromethane, ethyl acetate, and finally methanol. After each extraction, the filtrate was collected, and the remaining plant material was dried before extraction with the next solvent. Rotary evaporator was used to concentrate the extracts and further dried in a desiccator. The yield was found to be 1.3% (w/w).

2.3 Preliminary screening for the Phytochemicals

Derris scandens bark extract was subjected to preliminary screening by test tube reactions and thin layer chromatography to identify major primary and secondary metabolites. Qualitative phytochemical screening, supported by thin-layer chromatographic analysis, was conducted to determine the occurrence of major classes of constituents, including flavonoids, alkaloids, proteins, terpenoids, carbohydrates, glycosides, tannins, and saponins[16]

2.4 Thin layer chromatography of extracts of DS

The extracts obtained successive solvent extraction were subjected to thin-layer chromatography (TLC) using different solvent systems: ethyl acetate:methanol (81:11:8), chloroform:methanol (70:30:4 and 80:15:1), and chloroform (60:40). The developed TLC plates were observed at 254 nm and 366 nm, under UV light ,later spraying with vanillin–sulfuric acid reagent and heating to visualize colored spots, indicates presence of various important phytochemicals .

2.5 Total Phenolic Concentration

The total phenolic content of the methanolic bark extract was determined using the Folin–Ciocalteu method, with gallic acid serving as the reference standard. Briefly, a 1 mg/mL solution of the extract was treated with Folin–Ciocalteu reagent, followed by the addition of 7% sodium carbonate solution and distilled water. The resulting mixture was incubated in the dark for 60 min, after which its absorbance was measured at 750 nm using a UV–Vis spectrophotometer. The total phenolic content was calculated and expressed as milligrams of gallic acid equivalents per gram of dry extract (mg GAE/g).[17]

2.6 Total Flavonoid Concentration

The total flavonoid content (TFC) of the bark extract was determined using the aluminium chloride colorimetric method, with quercetin used as the reference standard. Briefly, a 1 mg/mL solution of the extract was treated with sodium nitrite, aluminium chloride, and sodium hydroxide. The absorbance of the resulting reaction mixture was measured at 506 nm using a UV–Vis spectrophotometer. The total flavonoid content was calculated and expressed as milligrams of quercetin equivalents per gram of dry extract (mg QE/g).[18]

2.7 DPPH Assay for measuring Free Radical Scavenging activity

The antioxidant potential of the methanolic bark extract of *Derris scandens* was assessed using the DPPH free-radical scavenging assay. Briefly, different concentrations of the extract were prepared, and 0.5 mg/mL of the extract was mixed with DPPH solution and incubated in the dark at room temperature for 30 min. Ascorbic acid was used as the standard antioxidant. The absorbance was subsequently recorded at 517 nm using a UV–Vis spectrophotometer. All experiments were carried out in triplicate.[19,20]

2.8 Anticancer activity by invitro method

The in vitro anticancer potential of the methanolic bark extract of *Derris scandens* was investigated using MCF-7 breast cancer cells and HepG2 hepatocellular carcinoma cells, which were procured from the National Centre for Cell Science (NCCS),

Pune. The study was carried out at the Department of Microbiology, Osmania University, Hyderabad, using the MTT assay. Dulbecco's Modified Eagle Medium was used for culturing Cells which is supplemented with fetal bovine serum of 10% and 1% penicillin–streptomycin. Cells were seeded in 96-well plates at a density of 5×10^3 cells per well and incubated overnight at 37°C. Following incubation, the cells were treated with varying concentrations of the extract and doxorubicin, used as the standard anticancer drug, for 48 h. Cell viability was assessed based on the conversion of MTT into formazan crystals by metabolically active cells. The resulting formazan crystals were subsequently dissolved in DMSO, and absorbance was measured at 570 nm using a microplate reader. Cell growth inhibition (%) was calculated using the standard formula, and all experiments were performed in triplicate. Doxorubicin was used as a standard positive control for comparison of cytotoxic activity.

The percentage of cell growth inhibition was calculated using the formula:

$$\% \text{ Inhibition} = \frac{100(\text{Control-treatment})}{\text{Control}}$$

The IC_{50} value, defined as the concentration required to inhibit 50% of cell growth, was estimated from the dose–response curve by plotting extract concentration against percentage growth inhibition. Linear regression analysis using the equation **Y = mX + C** was applied to determine the IC_{50}, with **Y = 50** corresponding to 50% growth inhibition.[21,22]

2.9 Characterizing the DS Extract by Gas Chromatography & Mass Spectroscopy Analysis

GC–MS analysis of the methanolic extract of *Derris scandens* was carried out at the Department of Analytical and Structural Chemistry, CSIR–IICT, Hyderabad. The extract (10 mg) was dissolved in methanol, and 1 µL of the sample was injected into a Thermo Scientific TSQ 8000 GC–MS system. Helium was employed as the carrier gas at a flow rate of 1 mL/min, with electron impact ionization used for mass spectral detection. The oven temperature was programmed from 60°C to 300°C using controlled temperature ramps and specified holding periods. The resulting mass spectra were matched against the NIST spectral library to facilitate the tentative identification of phytochemical constituents present in the extract.

2.10 Insilico docking studies

In silico molecular docking studies were conducted to assess the binding affinities of selected bioactive compounds identified by GC–MS analysis of the methanolic bark extract of ***Derris scandens*** against two cancer-related targets: cyclin-dependent kinase 8 (CDK8; PDB ID: 5CEI) and epidermal growth factor receptor (EGFR; PDB ID: 3POZ).

The selected compounds three-dimensional structures were obtained from PubChem or prepared using ChemDraw, energy-minimized, and converted to PDBQT format. From the Protein Data Bank, Protein structures were retrieved and co-crystallized ligands from which water molecules were removed followed by assigning charges and preparing receptor files. Docking was carried out using AutoDock with the Lamarckian Genetic Algorithm after defining the active-site grid box. Sorafenib and Erlotinib were used as reference ligands for CDK8 and EGFR, respectively. Binding affinity was represented by binding energy values (kcal/mol), with more negative values corresponding to stronger predicted ligand–receptor interactions.

3. RESULTS AND DISCUSSION

3.1 Preliminary phytochemical screening

Phytochemical screening of *Derris scandens* bark extracts prepared using petroleum ether, dichloromethane, ethyl acetate, and methanol revealed detection of flavonoid glycosides, saponins, steroidal/triterpenoidal glycosides, phenolics and tannins. TLC analysis showed different colored spots, dichloromethane and petroleum ether extracts showed orange spots, methanol extract of bark and ethyl acetate extracts showed yellow spots , and green to purple spots in different solvent systems. These findings confirmed the presence of steroids and related, terpenoids, and flavonoids, which may contribute to the observed anticancer activity of the plant extract. (Fig. 1).

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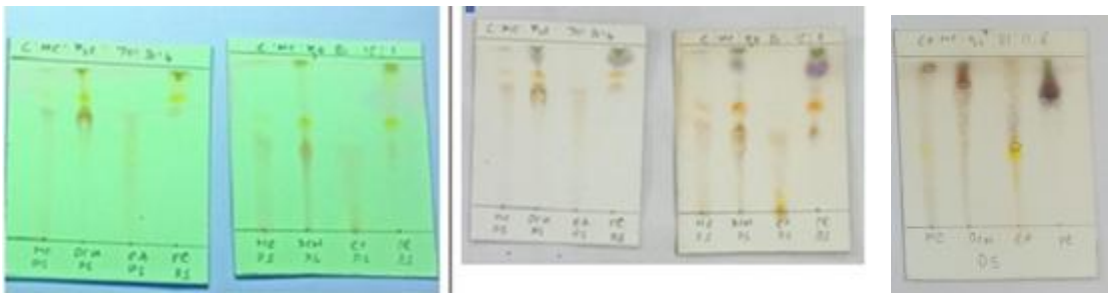


Fig. 1: TLC chromatograms of *Derris scandens* extracts.

(a) TLC plate under UV light (254 nm); (b) TLC plates after derivatization with vanillin-sulphuric acid reagent. Solvent system: [Ethylacetate:Methanol:Water (81:11:8) Chloroform:Methanol (60:40)]. Track 1: Methanolic extract; Track 2: Dichloromethane extract; Track 3: Ethyl acetate extract; Track 4: Petroleum ether extract."

3.2 Total Flavonoid and phenolic contents

The methanolic extract of *Derris scandens* exhibited a substantial total phenolic content, corresponding to 85 ± 2 mg gallic acid equivalents (GAE) per gram of extract and 78 ± 1.6 mg quercetin equivalents (QE) in one gram of methanolic extract gives value for flavonoid content.

3.3 DPPH Assay for antioxidant activity

Ascorbic acid and the methanolic bark extract of *Derris scandens*, antioxidant activity was evaluated using DPPH (2,2-diphenyl-1-picrylhydrazyl) assay. The free radical-scavenging activity of the extract was evaluated in comparison with that of the standard antioxidant, and the corresponding results are presented in Table 1.

Table 1: Derris scandens Methanolic Extract and Ascorbic Acid by DPPH Assay showing their Radical Scavenging Activity (%RSA)

Concentration (µg/ml)	**Ascorbic Acid**	***Derris scandens***
20	41.2± 0.3	29± 0.2
40	47.6± 0.2	40± 0.3
60	60.8± 0.2	48± 0.3
80	65.3± 0.3	60± 0.4
100	78.6± 0.3	71± 0.2

Values are expressed as mean ± standard deviation (SD) based on three independent replicates (n = 3).

3.4 In vitro anticancer activity

TLC profiling of the *Derris scandens* bark extract indicated the presence of flavonoids, terpenoids, and predominantly steroidal constituents. In view of this phytochemical profile, the extract was further investigated for its cytotoxic potential using the MTT assay.The methanolic extract showed IC_{50} values of 39.8 µg/mL against MCF-7 cells and 46.9 µg/mL against HepG2 cells,where as doxorubicin, a standard chemotherapeutic agent, has been reported to exhibit an IC_{50} of approximately 2.48 µg/mL against MCF-7 cells and 6.67 µg/mL on HepG2 cells following 24 h exposure indicating significant anticancer activity. The observed biological activity may be associated with the presence of bioactive phytoconstituents within the extract. The cell inhibition percentage results are presented in Tables 2 and 3.

Table 2: Cytotoxic Effect on MCF-7 Breast Cancer Cell Lines using MTT Assay by DS extract & Doxorubicin

DS			**Doxorubicin**
Concentration (µg/ml)	**% Inhibition**		
Control	**0**		
10	**24**	39.8**µg/ml**	2.48 **µg/ml**
25	**37**		IC_{50}
50	**59**	IC_{50}	
100	**75**		

Table 3: Cytotoxic Effect on HepG2 Liver Cancer Cell Lines using MTT Assay by DS extract.

DS			**Doxorubicin**
Concentration (µg/ml)	**% Inhibition**		
Control	**0**	46.9 **µg/ml**	6.67 µg/mL
10	**35**		IC_{50}
25	**43**	IC_{50}	
50	**51**		
100	**68**		

The IC50 value (µg/mL) value is concentration which inhibit 50% of cell growth.

3.5 GC–MS analysis of DS extract

GC–MS profiling of the *Derris scandens* bark extract resulted in the identification of 48 distinct phytochemical constituents. Selected major compounds are presented in Table 4, and their mass spectra were compared with standard spectral libraries and previously reported literature data for tentative identification (Fig. 2).

Table: 4 Major Phytochemicals Identified in the Methanolic Stem Bark Extract of *Derris scandens* by GC–MS Analysis

S.NO.	**DS**	**Molecular formula**	**Molecular weight(g/mol)**	**Retention time)**	**m/z**	**Relative %area**
1	Azulene	$C_{10}H_8$	128.17	13.3	128	0.59
2	Zingiberene	$C_{15}H_{24}$	204.14	13.4	161	0.35
3	Spathulenol	$C_{15}H_{24}O$	220.35	15	205	2.42
4	Globulol	$C_{15}H_{26}O$	222.37	15.1	82	1.36
5	Agarospirol	$C_{15}H_{32}O_2$	256.42	15.7	119	20.6
6	Himachalol	$C_{15}H_{26}O$	223.23	15.3	109	2.07
7	Hinesol	$C_{18}H_{32}O_2$	280.45	15.7	204	20.60
8	Hexadecanoic	$C_{16}H_{32}O_2$	256.43	19.3	256	3.2

	acid					
9	Veridiflorol	$C_{15}H_{26}O$	223.37	15.2	43	1.42
10	Octadecanoic acid	$C_{18}H_{36}O_2$	284.48	20.9	284	0.81
11	Squalene	$C_{30}H_{50}$	410.72	26.4	69	0.61
12	Tetramethoxy stilbene	$C_{18}H_{20}O_4$	300.71	33.8	329	0.82
13	Linoelaidic acid	$C_{18}H_{32}O_2$	280.72	34.6	207	0.23

*Only major identified compounds are presented. Relative peak areas are expressed as percentages of the total ion chromatogram." Non-phytochemical compounds, derivatization products, solvent peaks and low-quality library matches were excluded from the table. Only phytoconstituents identified by NIST library matching are reported."

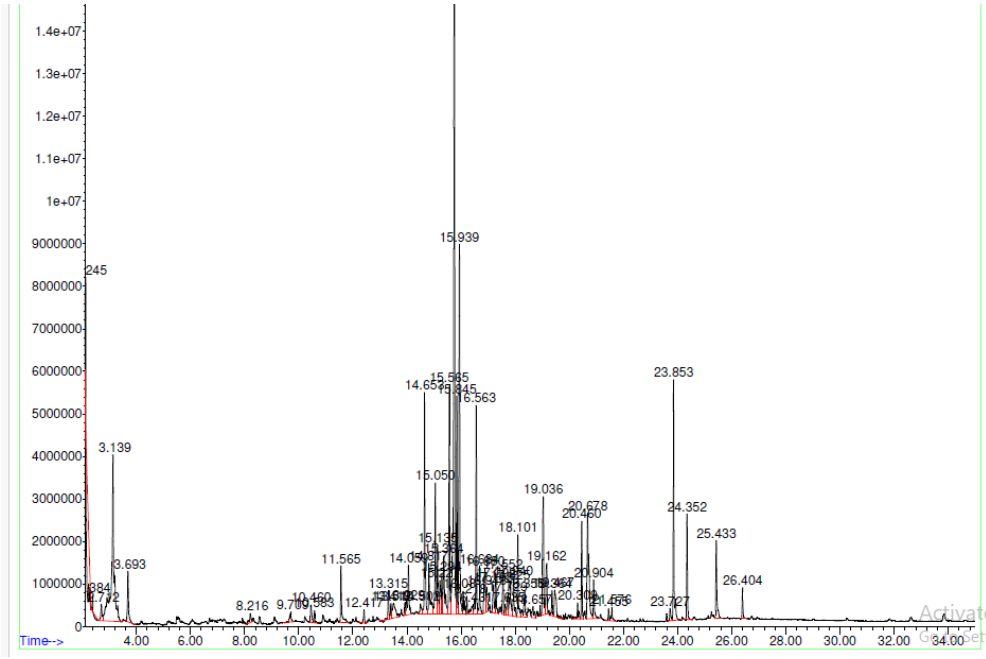


Fig:2 GC-MS chromatogram of Derris scandens

GC–MS analysis of the methanolic bark extract of *Derris scandens* resulted in the identification of 48 phytochemical compounds. The major identified constituents listed in Table 4 were confirmed by comparing their mass spectra with published literature and standard database libraries. Selected bioactive compounds from the identified constituents were further evaluated through molecular docking studies against anticancer target proteins.

3.6 Molecular docking study

Molecular docking analysis against CDK8 revealed that α-amyrin and himachalol exhibited notable binding affinities among the selected phytoconstituents. standard drug sorafenib was used to compare the test compounds docking scores. Sorafenib showed hydrogen bond interactions with Glu885, Asp1046, and Val916, along with hydrophobic interactions involving Lys868. The compounds α-amyrin and himachalol demonstrated comparable interaction patterns with CDK8, exhibiting binding energies of −7.9 kcal/mol and −7.5 kcal/mol, respectively (Table 5).

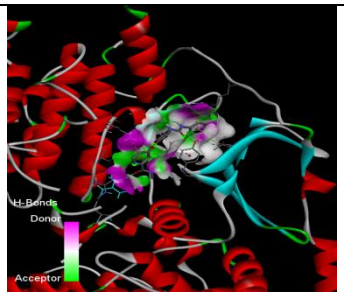
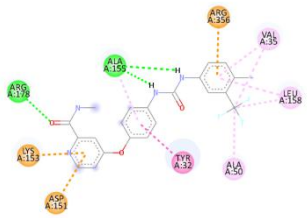
Docking evaluation against EGFR in which erlotinib was the reference inhibitor showed a binding energy of −7.8 kcal/mol. Erlotinib exhibited interactions with key residues within the EGFR ATP-binding pocket, including Met793 in the hinge region, Lys745, Val726, and Leu718, mediated through hydrogen bonding and hydrophobic interactionsAmong the evaluated phytoconstituents, α-amyrin exhibited a strong predicted binding affinity of −7.7 kcal/mol. It formed hydrogen-bond interactions with Asp855 and Met793, along with hydrophobic interactions involving Leu718, Val726, Ala743, and Phe856.Other compounds, including himachalol, azulene, tetramethoxy stilbene, and eicosatrienol, also showed favorable docking scores with multiple interactions involving important EGFR residues, suggesting their potential role as EGFR-targeting molecules. Except for eicosatrienol, all selected compounds exhibited binding energies lower than −5 kcal/mol, indicating strong interactions with the target proteins and suggesting their possible anticancer potential. In silico molecular docking findings, together with the in vitro cytotoxicity results, indicate the potential therapeutic significance of phytoconstituents identified in the methanolic bark extract of *Derris scandens*. The two-dimensional and three-dimensional interaction profiles of the protein–ligand complexes are presented in Tables 6 and 8, while the corresponding binding affinities are summarized in Tables 5 and 7.

Table.5 Binding Energies (kcal/mol) with Cyclin-Dependent Kinase 8 (CDK8, PDB ID: 5CEI) by few Phytocompounds from Derris scandens.

LIGAND	**DOCK SCORE AGAINST -5CEI**
Sorafenib (standard drug)	**-9.02**
AZULENE	-6.8
HIMACHALOL	-7.5
TETRAMETHOXY STILBENE	-5.3
ALPHA AMYRIN	-7.9
EICOSATRIENOL	-4.0

Binding energy was expressed in kcal/mol. This indicates Lower (more negative) values indicate a stronger predicted binding affinity.

Table 6. Interactions of plant derivatives of DS with Cyclin dependent kinase -8 (PDB ID-5CEI)

LIGAND	3D INTERACTIONS	2D INTERACTIONS	INTERACTION TYPE
Sorafenib (standard drug)			Conventional H bonding, pi pi ,pi alkyl, pi cation, pi anion.

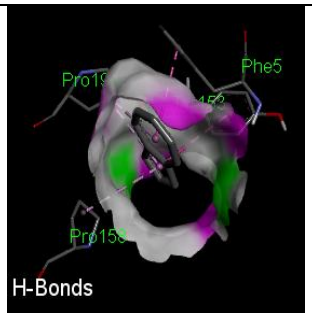
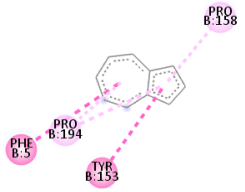
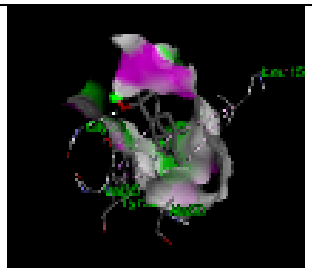
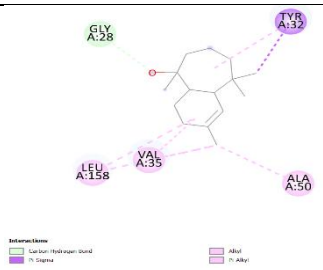
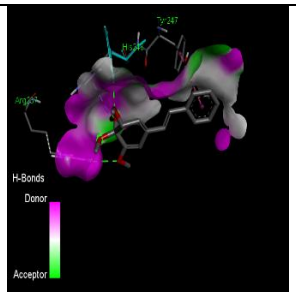
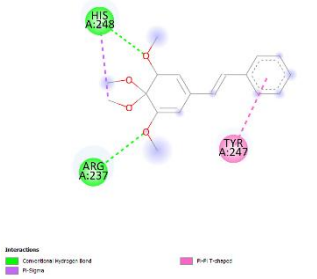
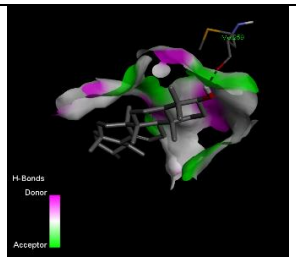
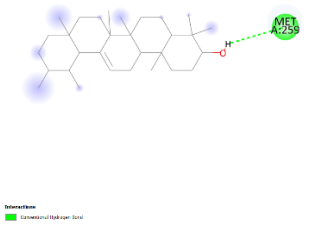
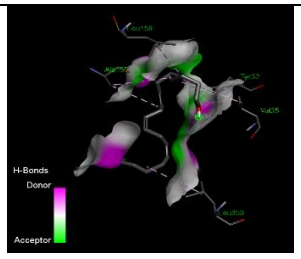
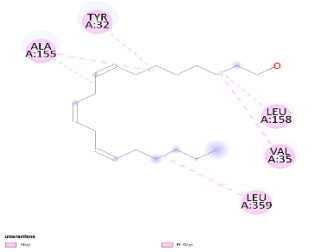
AZULENE			Pi-pi stacked, pi-pi T-shaped, pi alkyl.
HIMACHALOL			Carbon hydrogen bond, pi-alkyl, alkyl, pi sigma
TETRAMETHOXY STILBENE			Conventional hydrogen bond, pi-sigma, pi-pi- T shaped
ALPHA AMYRIN			Conventional hydrogen bond
EICOSATRIENOL			Alkyl, pi-alkyl

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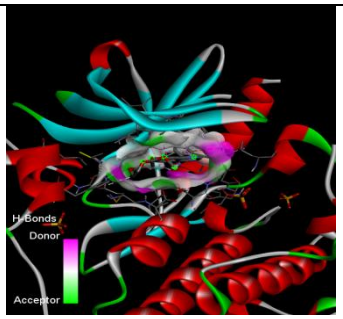
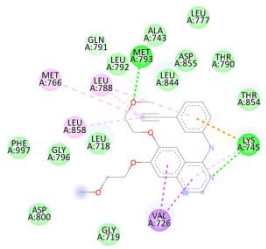
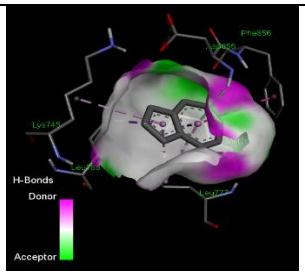
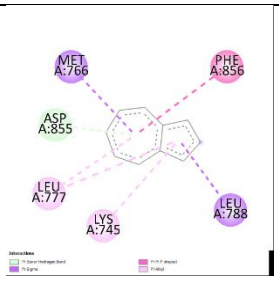
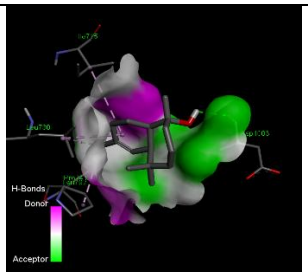
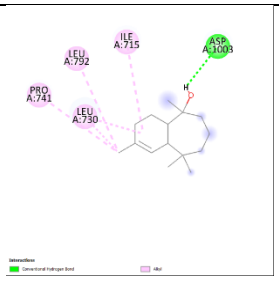
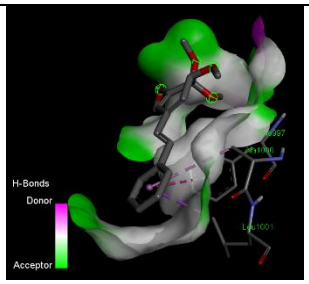
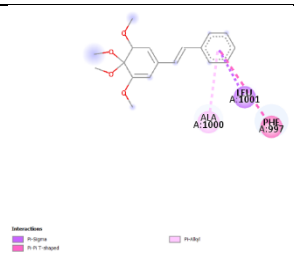
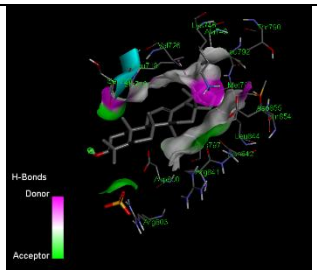
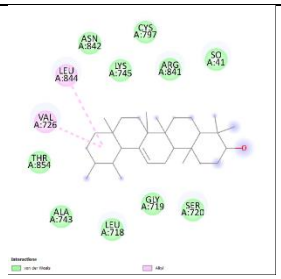
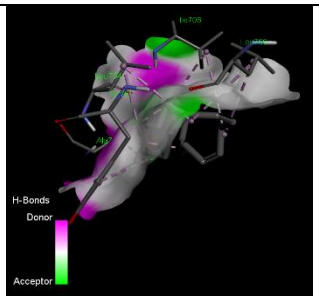
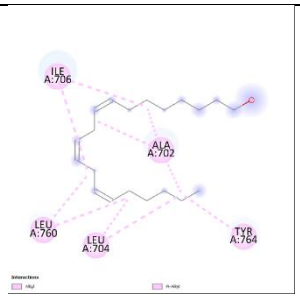
Table7. Binding Energy Values (kcal/mol) of Selected Phytocompounds from *Derris scandens* Against Epidermal Growth Factor Receptor (EGFR; PDB ID: 3POZ)

LIGAND	DOCK SCORE AGAINST- 3POZ
Erlotinibnib (standard drug)	-7.8
AZULENE	-6.5
HIMACHALOL	-5.4
TETRAMETHOXY STILBENE	-4.6
ALPHA AMYRIN	-7.7
EICOSATRIENOL	-3.2

Binding energy was expressed in kcal/mol. This indicates Lower (more negative) the values indicate a stronger predicted binding affinity.

Table8. Molecular docking studies on selected phytoconstituents on EGFR kinase(PDB ID 3POZ)

LIGAND	3D INTERACTIONS	2D INTERACTIONS	INTERACTION TYPE
Erlotinib (standard drug)			Conventional H bonding, pi sigma ,pi alkyl, pi cation, vanderwaal.
AZULENE			Pi sigma hydrogen bond, pi-pi T-shaped, pi alkyl, pi-sigma.
HIMACHALOL			Carbon hydrogen bond, alkyl.

TETRAMETHOXY STILBENE			Conventional hydrogen bond, pi-sigma, pi-pi- T shaped
ALPHA AMYRIN			Vander waals, alkyl.
EICOSATRIENOL			Alkyl, pi-alkyl

The results of this study demonstrate that the methanolic bark extract of *Derris scandens* exhibits significant anticancer activity against MCF-7 and HepG2 cell lines, as evidenced by the MTT assay and comparison with the standard anticancer drug doxorubicin. The observed cytotoxicity may be attributed to the presence of bioactive phytoconstituents identified through GC–MS analysis. Various plant-derived secondary metabolites, particularly flavonoids, terpenoids, and fatty acids, have been extensively associated with anticancer effects, including suppression of cancer cell proliferation, promotion of apoptosis, and modulation of oxidative stress-related pathways.

GC–MS profiling of the extract revealed several compounds belonging to different chemical classes with potential pharmacological significance. Previous studies have also highlighted the role of phytochemicals, particularly phenolic derivatives and fatty acids, in exhibiting anticancer effects by influencing cellular signaling pathways and apoptotic mechanisms.

Cyclin-Dependent Kinase 8 (CDK8) and Epidermal Growth Factor Receptor (EGFR) are key cancer-associated targets, by which Insilico studies gave insights into the possible anticancer mechanisms of selected phytoconstituents through these targets, including CDK8 is involved in transcriptional regulation and oncogenic signaling, whereas EGFR plays an important role in cancer cell proliferation, survival, and metastasis. The selected compounds from *Derris scandens* exhibited favorable binding affinities toward both targets, with docking scores comparable to standard inhibitors. These results suggest that the phytoconstituents identified may have the potential to modulate kinase activity and interfere with signaling pathways involved in tumor progression.

Present findings supported with earlier studies reporting that phytochemicals identified through GC–MS analysis exhibit strong affinity with cancer-associated molecular targets, including EGFR and CDK target proteins. Previous research has demonstrated that plant-derived bioactive compounds can suppress EGFR-mediated signaling pathways, resulting in reduced cancer cell proliferation and viability. Additionally, molecular docking analyses have highlighted the potential of natural

compounds to inhibit CDK target proteins, suggesting that these compounds may serve as promising candidates for the development of novel anticancer therapeutics.

The results between the in vitro cytotoxic effects and docking studies results obtained in the present research suggests that the anticancer potential of *Derris scandens* may involve modulation of CDK8 and EGFR pathways. The potential of the identified phytoconstituents to interact with multiple target proteins indicates a potential multitarget mechanism of action, which may contribute to enhanced therapeutic efficacy and reduced development of drug resistance.

Despite these encouraging findings, this study has some limitations, particularly the absence of **in vivo validation** and a comprehensive assessment of the **molecular mechanisms underlying the observed effects**. Further studies involving the isolation and characterization of individual bioactive compounds, evaluation using appropriate animal models, and exploration of specific signaling pathways are required to confirm the therapeutic potential and clinical significance of the findings.

4. CONCLUSION

The methanolic extract of *Derris scandens* exhibited significant anticancer activity against MCF-7 and HepG2 cell lines, as demonstrated by the MTT assay. Selected compounds from the GC–MS profile were further evaluated through molecular docking studies against cancer-associated target proteins relevant to MCF-7 and HepG2 cell lines. The observed binding energies and interaction profiles revealed that several identified compounds showed promising binding affinities comparable to standard drugs, indicating their potential anticancer activity.

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AUTHOR CONTRIBUTIONS

Rajeswari Chilka: Conceptualization, Investigation.

Rajeswari Chilka: Methodology, Laboratory Analysis.

Sachin Gaikwad[3] and S.Sravanthi[1]: Data Curation, Formal Analysis.

Parimi Ravi *, K.E.Pravallika: Supervision, Writing—Review & Editing.

CONFLICT OF INTEREST

The authors declare that there is no conflict of interest.

ETHICS STATEMENT

Ethical approval was not required for this study.

DATA AVAILABILITY STATEMENT

Data supporting the findings of this study are available from the corresponding author upon reasonable request.

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