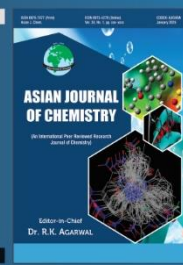




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Phytochemical Screening, *In silico* Analysis and *In vivo* Evaluation of the Immunomodulatory Activity of Extract of *Dalbergia lanceolaria* and *Derris scandens* Barks

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Dalbergia lanceolaria and *Derris scandens* are medicinal plants of the Fabaceae family containing diverse secondary metabolites with potential pharmacological properties. This study investigated the phytochemical composition and comparative immunomodulatory activity of methanolic bark extracts of *D. lanceolaria* (DLM) and *D. scandens* (DSM) using a doxorubicin-induced immunosuppression model in wistar rats. Successive solvent extraction, preliminary phytochemical screening, thin-layer chromatography (TLC) and gas chromatography–mass spectrometry (GC-MS) were employed for phytochemical characterization. The methanolic extracts of *D. lanceolaria* and *D. scandens* yielded 2.5% and 3.0%, respectively, while GC-MS analysis identified 13 constituents in each extract. Oral administration of DLM and DSM at 200 and 400 mg/kg for 14 days attenuated doxorubicin-induced alterations in total and differential leukocyte counts and neutrophil adhesion, with the 400 mg/kg dose producing higher effects. Histopathological examination further demonstrated improved preservation of splenic and thymic architecture in extract-treated groups. Molecular docking of selected GC-MS identified compounds revealed favourable predicted interactions with NF- κ B p52, TNF- α and viral interleukin-10, with β -sitosterol, agarospirol and azulene showed favourable predicted binding affinities, with docking scores of -8.0, -7.2 and -7.7 kcal/mol, respectively. The combined phytochemical, biological, histopathological and *in silico* findings support the preliminary immunomodulatory potential of DLM and DSM and provide a basis for further investigation of their bioactive constituents and molecular mechanisms.

Keywords: Phytochemical screening, Doxorubicin, Immunomodulatory, Immunosuppression, Immune function.

INTRODUCTION

Medicinal plants have long been an important component of traditional Indian healthcare systems and remain a valuable source of biologically active natural compounds. Their therapeutic potential is associated with diverse phytoconstituents including flavonoids, terpenoids, saponins, tannins, alkaloids, steroids, essential oils and other secondary metabolites [1,2]. These constituents have been linked with a range of biological effects, including immunomodulatory, anti-inflammatory and antimicrobial activities [3,4]. The continued investigation of medicinal plants may therefore contribute to the identification of bioactive compounds with potential applications in the development of complementary or supportive therapeutic agents [5-7].

Dalbergia lanceolaria L. (Fabaceae), commonly known as dandusi, is a medium-sized tree distributed in India and other parts of South and Southeast Asia. Various parts of the plant have a history of traditional use [8]. The bark has been used in preparations for dyspepsia, while seed oil has been associated with the management of rheumatic complaints [9]. Different *Dalbergia* species have traditionally been employed for conditions involving pain, inflammation, gastrointestinal disorders and other ailments [10,11]. Reports on *D. lanceolaria* have also described biological activities associated with its leaf and bark extracts including antioxidant, antidiabetic, analgesic, antipyretic and anti-inflammatory effects [12]. These traditional uses and reported pharmacological properties make *D. lanceolaria* a relevant candidate for further investigation of its immunomodulatory potential.

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Derris scandens, another member of the Fabaceae family, is also widely recognized in traditional medicine. Its roots and stems have been used for various conditions, including cough, dysentery, muscle and joint discomfort and other inflammatory complaints [13]. Phytochemical investigations of *D. scandens* have identified several classes of secondary metabolites, for example, isoflavones, flavonoids, coumarins, pterocarpanes, steroids and terpenes [14,15]. Compounds such as genistein, luteolin and scandenins have also been reported among its major phytochemical constituents [16]. The presence of these metabolites provides a basis for investigating the biological activities of *D. scandens*, particularly those related to inflammation and immune regulation.

Previous experimental studies provide preliminary support for the immunomodulatory and anti-inflammatory properties of both plants. Hydroalcoholic extract of *D. scandens* has been reported to enhance lymphocyte proliferation, natural killer (NK) cell activity and IL-2 secretion [17]. Similarly, bark extract of *D. lanceolaria* has demonstrated anti-inflammatory activity in experimental animal models [18]. Despite these reports, a direct comparative assessment of the immunomodulatory effects of bark extracts from *D. lanceolaria* and *D. scandens* remains limited. Therefore, the present study was undertaken to comparatively evaluate the immunomodulatory activity of bark extracts of *D. lanceolaria* and *D. scandens* in wistar rats. The study aims to generate comparative experimental evidence regarding their potential as plant derived sources of immunomodulatory agents.

EXPERIMENTAL

Plant material: The bark samples of *Derris scandens* and *Dalbergia lanceolaria* were collected locally and authenticated by Department of Botany, Acharya Nagarjuna University, Guntur, India. The voucher specimens were maintained in the institute herbarium for future reference. Collected plant materials were air-dried and coarsely powdered. For extraction, 1 kg of the dried and powdered bark material was subjected to successive maceration using approximately 1 L of each solvent in increasing order of polarity, starting with petroleum ether, followed by dichloromethane, ethyl acetate and finally methanol. Each extraction was carried out for 7 days. After each extraction, the extract was filtered and the remaining marc was dried before proceeding to the next solvent. The resulting extracts were concentrated under reduced pressure at 45 °C using a rotary evaporator and subsequently stored in a desiccator until further phytochemical, analytical and pharmacological studies.

Preliminary phytochemical screening: Preliminary phytochemical screening of the test extracts revealed the presence of several bioactive phytochemical groups including carbohydrates, flavonoids, alkaloids, phytosterols, tannins, saponins, volatile oils and phenolic compounds. These findings confirm the presence of diverse classes of secondary metabolites in the extracts, which may contribute to their observed biological activities.

Phytochemical analysis by TLC technique: Thin-layer chromatography (TLC) was performed to profile the phytoconstituents present in the extracts using different solvent systems, namely chloroform:methanol (60:40), ethyl acetate:

methanol:water (81:11:8) and chloroform:methanol:water (70:30 and 80:15:1). The developed chromatograms were examined under UV light at 254 and 366 nm to visualize the separated components. The TLC plates were subsequently sprayed with vanillin-sulphuric acid reagent and heated at 45 °C for further visualization. The appearance of distinct coloured spots after derivatization confirmed the presence of different phytochemical constituents in the test extracts.

Phytochemical characterization of test extracts GC-MS analysis: Test extract solutions (1 mg/mL) were prepared in methanol and analyzed using gas chromatography-mass spectrometry (GC-MS) equipped with an HP-5MS capillary column (30 m × 0.25 mm). The ion source and transfer line temperatures were maintained at 230 and 300 °C, respectively. Ionization was performed in electron ionization (EI) mode, with helium used as the carrier gas at a constant flow rate of 1 mL/min. The oven temperature was initially set at 60 °C and held for 5 min, followed by an increase to 240 °C at a rate of 10 °C/min and held for 5 min. The temperature was then increased to 300 °C and maintained for an additional 5 min. The mass spectra obtained for the detected compounds were compared with reference spectra in the National Institute of Standards and Technology (NIST) mass spectral library for compound identification.

Subacute toxicity study: The subacute oral toxicity study was conducted in Wistar albino rats of both sexes, weighing between 150-200 g and aged 8-11 weeks by following OECD guidelines [19]. The test extracts were administered orally for 14 days at doses ranging from 100 to 2000 mg/kg daily. The animals were observed for changes in behaviour, neurological and endocrine functions, food consumption and signs of toxicity throughout the study period.

Determination of immunomodulatory activity: Approval for the experimental protocol was obtained from the Institutional Animal Ethics Committee (IAEC) of G. Pulla Reddy College of Pharmacy, Mehdipatnam, Hyderabad (Approval No. GPRCP/IAEC-1/21/09/2024/PCG/AE-1). Immunomodulatory activity was evaluated in wistar rats, which were randomly divided into 10 groups (n = 6 per group). Group I served as the normal control, while Group II received doxorubicin (4.67 mg/kg). Groups III and IV received methanolic extract of *D. lanceolaria* (DLM) at doses of 200 and 400 mg/kg, respectively. Groups V and VI received doxorubicin (4.67 mg/kg) in combination with DLM at 200 and 400 mg/kg, respectively. Groups VII and VIII received methanolic extract of *Derris scandens* (DSM) at doses of 200 and 400 mg/kg, respectively, whereas Groups IX and X received doxorubicin (4.67 mg/kg) in combination with DSM at 200 and 400 mg/kg, respectively. All treatments were administered for 14 consecutive days. At the end of the treatment period, blood samples were collected for assessment of immunomodulatory activity based on total leukocyte count (TLC), differential leukocyte count (DLC), and the neutrophil adhesion test.

The selected doses were based on previously reported pharmacological activity and available safety information for the respective plant extracts. *D. lanceolaria* bark extract has been reported to exhibit pharmacological activity at oral doses ranging from 100 to 400 mg/kg, without apparent acute toxicity at higher doses. Similarly, the experimental studies have

reported biological activity of *D. scandens* extracts at pharmacologically relevant doses. Accordingly, doses of 200 and 400 mg/kg were selected to evaluate the immunomodulatory effects of the bark extracts.

Evaluation of histopathological studies: The spleen and thymus tissues were collected from all experimental groups (Groups I-X) and immediately fixed in 10% buffered formalin. The tissues were subsequently dehydrated, embedded in paraffin wax and sectioned into thin sections. The sections were stained with hematoxylin and eosin (H&E) for histological evaluation [20]. Histopathological examination was performed to assess tissue architecture and treatment-related pathological alterations and representative photomicrographs were captured using a light microscope at 45× magnification.

In silico molecular docking studies: Molecular docking studies were performed to investigate the binding interactions of selected bioactive compounds identified from the bark extracts of *Derris scandens* (DSM) and *Dalbergia lanceolaria* (DLM) with immunomodulatory target proteins, namely human NF- κ B p52 (PDB ID: 1A3Q), tumor necrosis factor- α (TNF- α ; PDB ID: 2AZ5) and viral interleukin-10 (vIL-10; PDB ID: 1VLK). These targets were selected based on their established involvement in immune and inflammatory regulation. NF- κ B p52 was considered a key transcriptional regulator of immune- and inflammation-related genes, whereas TNF- α represents a major pro-inflammatory cytokine involved in inflammatory signaling [21]. vIL-10 was included due to its immunomodulatory effects and ability to influence host immune responses. Together, these targets provide a rational frame-work for evaluating phytoconstituent interactions with immune and inflammatory pathways.

The 3D structures of the selected phytoconstituents, namely linoelaidic acid, agarospirol, azulene and himachalol from *D. scandens*, and octadecadienoic acid, eicosatrien-1-ol, β -sitosterol, hinesol and dihydrocoumarin from *D. lanceolaria*, were generated using ChemDraw. The protein and ligand structures were subjected to energy minimization and converted to PDBQT format before docking. Molecular docking was performed using AutoDock 4.2, with the grid parameters optimized according to established protocols [22]. The resul-

ting protein–ligand interactions and docked complexes were analyzed and visualized using BIOVIA Discovery Studio 2017 R2 [23]. Levamisole was used as the reference immunomodulatory agent for comparative analysis. The potential binding pockets of the selected target proteins were identified and characterized using the Computed Atlas of Surface Topography of Proteins (CASTp).

RESULTS AND DISCUSSION

Phytochemical screening: The methanolic extracts of *D. lanceolaria* bark and *D. scandens* bark yielded 2.5% and 3.0%, respectively. Preliminary phytochemical screening of the petroleum ether, chloroform, acetone, methanol and aqueous extracts revealed the presence of various bioactive constituents. The phytochemical classes identified in the respective extracts are presented in Table-1.

Identification active compounds of test extracts on TLC analysis: TLC analysis of the *D. lanceolaria* (DL) and *D. scandens* (DS) extracts revealed distinct chromatographic profiles, with yellow, purple and green spots observed under UV light and after derivatization with vanillin-sulphuric acid (Fig. 1). These profiles suggested the presence of alkaloids, terpenoids, steroids and flavonoids in the extracts.

Identification active compounds of test extracts on GC-MS analysis: GC-MS analysis of the *D. lanceolaria* and *D. scandens* extracts led to the identification of 13 phytochemical constituents in each extract. The identified compounds, presented in Figs. 2 and 3 along with the corresponding GC chromatograms, were characterized by matching their mass spectral profiles with reference spectra available in established spectral libraries. The identified compounds and their key GC-MS profiles are shown in Table-2.

Immunomodulatory activity: The methanolic extracts of *D. lanceolaria* (DLM) and *D. scandens* (DSM) barks significantly ameliorated doxorubicin-induced immunosuppression. Both extracts increased the total WBC count, restored differential leukocyte populations, enhanced neutrophil production and improved delayed-type hypersensitivity responses. The immunomodulatory effects were dose-dependent, with the 400 mg/kg dose showing higher efficacy than the 200 mg/kg dose (Fig. 4). These effects may be associated with the comb-

TABLE-1
PHYTOCHEMICAL SCREENING OF TEST EXTRACTS

Category	DLP	DLC	DLA	DLM	DSP	DSC	DSA	DSM
Carbohydrates	Presence	Absence	Absence	Presence	Presence	Absence	Absence	Presence
Alkaloids	Presence	Presence		Absence	Presence	Presence		Absence
Flavonoids	Presence	Presence	Presence	Presence	Presence	Presence	Presence	Presence
Proteins and amino acids	Absence	Presence	Absence	Presence	Absence	Presence		Presence
Terpenoids	Presence	Presence		Absence	Presence	Presence		Absence
Phenolic compounds	Absence	Absence	Presence	Presence	Absence	Absence	Presence	Presence
Tannis	Presence	Absence	Presence	Presence	Presence	Absence	Presence	Presence
Phytosterols	Presence	Presence	Absence	Absence	Presence	Presence	Absence	Absence
Volatile oils	Presence	Presence	Absence	Absence	Presence	Presence	Absence	Absence
Saponins	Presence	Presence	Absence	Absence	Presence	Presence	Absence	Absence
Phytosterols	Presence	Presence	Absence	Absence	Presence	Presence	Absence	Absence
Resins	Absence	Presence	Absence	Absence	Absence	Presence	Absence	Absence

DLP = DLPE-DL pet ether extract; DLC = DLDM-DL dichloromethane extract; DLA = DLEA-DL ethylacetate extract; DLM = DLM-DL methanolic extract; DSP = DSPE-DS pet ether extract; DSC = DSDM-DS dichloromethane extract; DSA = DSEA-DS ethylacetate extract; DSM = DSM-DS methanolic extract

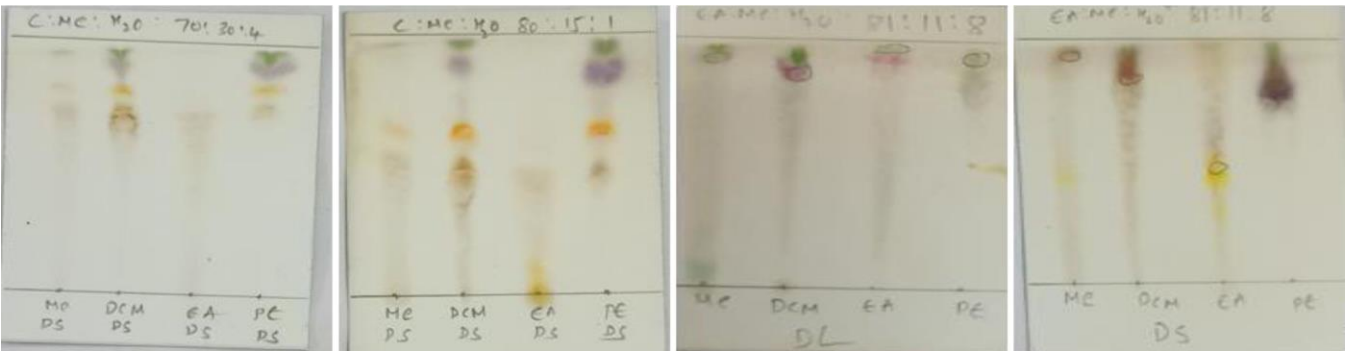


Fig. 1. TLC chromatograms of (a) *Dalbergia lanceolaria* and (b) *Derris scandens* bark extracts

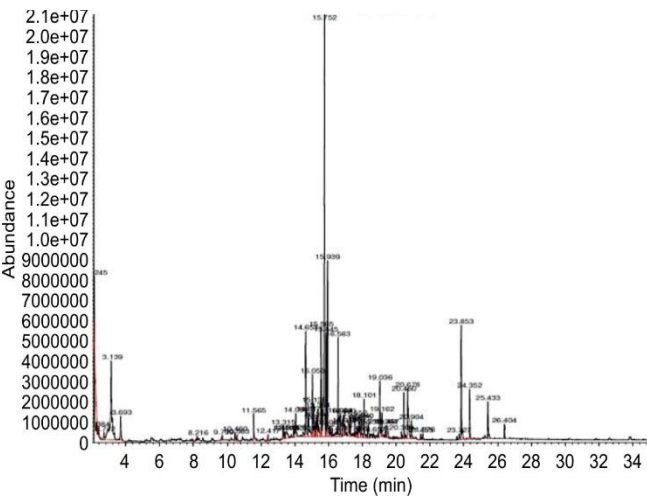


Fig. 2. GC-MS chromatogram of the methanolic bark of *D. scandens*

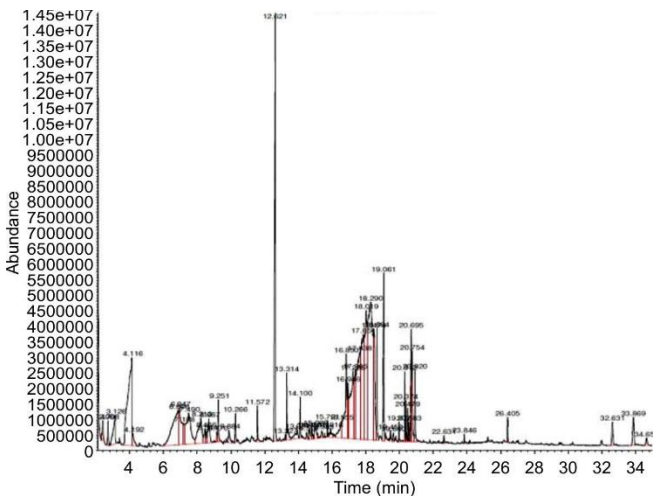


Fig. 3. GC-MS chromatogram of the methanolic bark of *D. lanceolaria*

TABLE-2 MAJOR PHYTOCHEMICALS IDENTIFIED IN THE METHANOLIC STEM BARK EXTRACT OF <i>Dalbergia lanceolaria</i> AND <i>Derris scandens</i> BY GC-MS ANALYSIS						
	m.f.	m.w. (g/mol)	Retention time (min)	m/z	Relative area (%)	
DLM	Dihydrocoumarin	C ₉ H ₈ O ₂	12.6	148	7.73	
	Coumarin	C ₉ H ₆ O ₂	13.3	146	1.00	
	Mellein	C ₁₀ H ₁₀ O ₃	14.6	178	0.27	
	Agarspirol	C ₁₅ H ₂₆ O	15.7	161	0.16	
	Hinesol	C ₁₈ H ₃₂ O ₂	15.7	204	2.60	
	Hexadecanoic acid	C ₁₆ H ₃₂ O ₂	19.5	73	2.81	
	trans-Sinapyl alcohol	C ₁₁ H ₁₄ O ₄	19.4	210	0.20	
	Octadecadienoic acid	C ₁₈ H ₃₂ O ₂	20.1	81	0.60	
	Octadecatrienoic acid	C ₁₈ H ₃₀ O ₂	20.3	79	0.44	
	Phytol	C ₂₀ H ₄₀ O	20.47	71	0.29	
	Linoelaidic acid	C ₁₈ H ₃₂ O ₂	20.6	82	1.79	
DSM	β-Sitosterol	C ₂₉ H ₅₀ O	33.8	329	0.82	
	Azulene	C ₁₀ H ₈	128.17	128	0.59	
	Zingiberene	C ₁₅ H ₂₄	204.14	161	0.35	
	Spathulenol	C ₁₅ H ₂₄ O	220.35	205	2.42	
	Globulol	C ₁₅ H ₂₆ O	222.37	82	1.36	
	Agarspirol	C ₁₅ H ₃₂ O ₂	256.42	119	20.6	
	Himachalol	C ₁₅ H ₂₆ O	223.23	109	2.07	
	Hinesol	C ₁₈ H ₃₂ O ₂	280.45	204	20.60	
	Hexadecanoic acid	C ₁₆ H ₃₂ O ₂	256.43	256	3.20	
	Veridiflorol	C ₁₅ H ₂₆ O	223.37	43	1.42	
	Octadecanoic acid	C ₁₈ H ₃₆ O ₂	284.48	284	0.81	
	Squalene	C ₃₀ H ₅₀	410.72	69	0.61	
	Tetramethoxy stilbene	C ₁₈ H ₂₀ O ₄	300.71	329	0.82	
	Linoelaidic acid	C ₁₈ H ₃₂ O ₂	280.72	207	0.23	

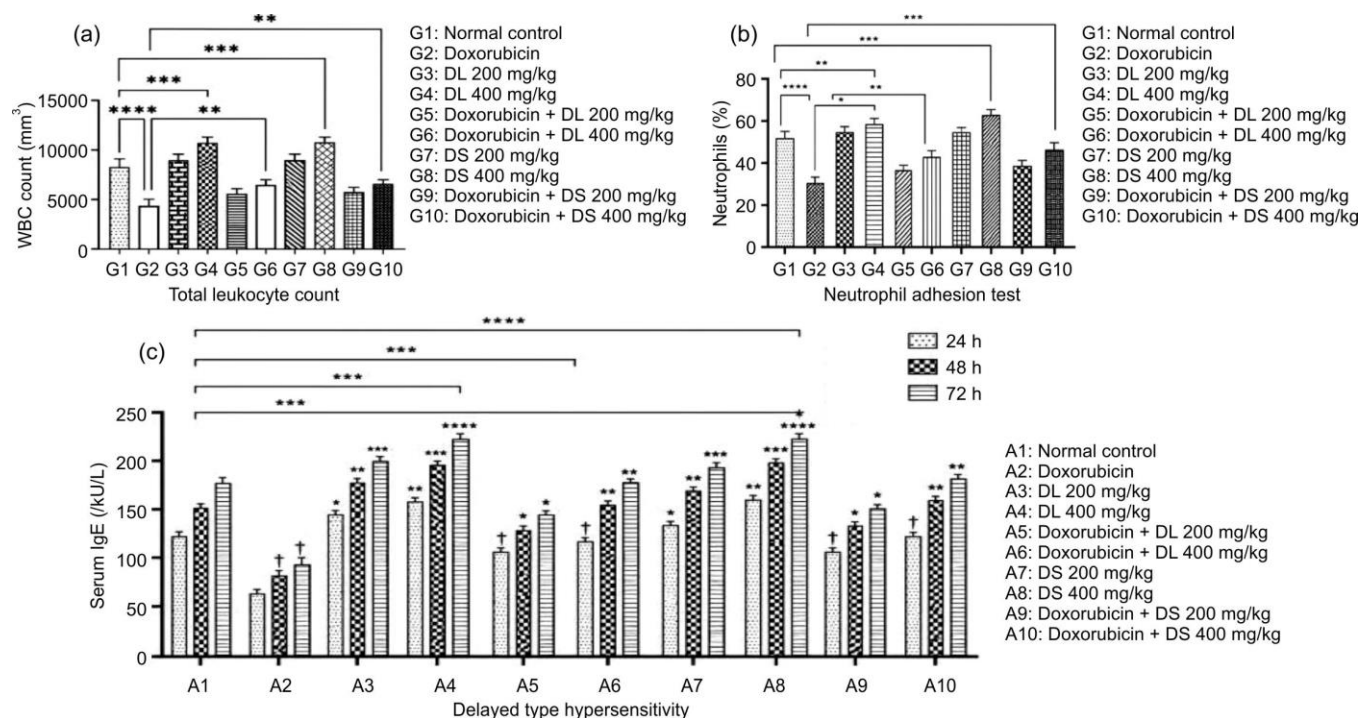


Fig. 4. Effect of methanolic test extracts on immunomodulatory activity

ined action of phytoconstituents such as alkaloids, saponins, flavonoids, phenolics, terpenoids and other antioxidant compounds. These findings suggest that DLM and DSM possess dose-dependent immunomodulatory potential and may have therapeutic relevance in mitigating chemotherapy-induced immunosuppression.

Effect of methanolic test extracts on spleen and thymus gland of histopathological study: Histopathological examination of the spleen and thymus tissues showed marked structural alterations in the doxorubicin-treated group, whereas treatment with *D. lanceolaria* (DL) and *D. scandens* (DS) attenuated these changes. The spleen sections of the DL- and DS-treated groups showed better preservation of splenic architecture, with improved organization of the white and

red pulp and reduced tissue damage compared with the doxorubicin treated group. The thymus sections also showed comparatively preserved lobular architecture, improved corticomedullary organization and higher lymphoid cellularity following treatment with DL and DS (Fig. 5). These findings suggest a protective effect of both extracts against doxorubicin-induced histopathological alterations in the spleen and thymus.

Molecular docking study: Molecular docking was performed to explore the potential interactions of selected phytoconstituents identified from *D. scandens* and *D. lanceolaria* bark extracts with NF- κ B p52 (PDB ID: 1A3Q), TNF- α (PDB ID: 2AZ5) and viral interleukin-10 (vIL-10; PDB ID: 1VLK). As shown in Table-3, all tested compounds exhibited

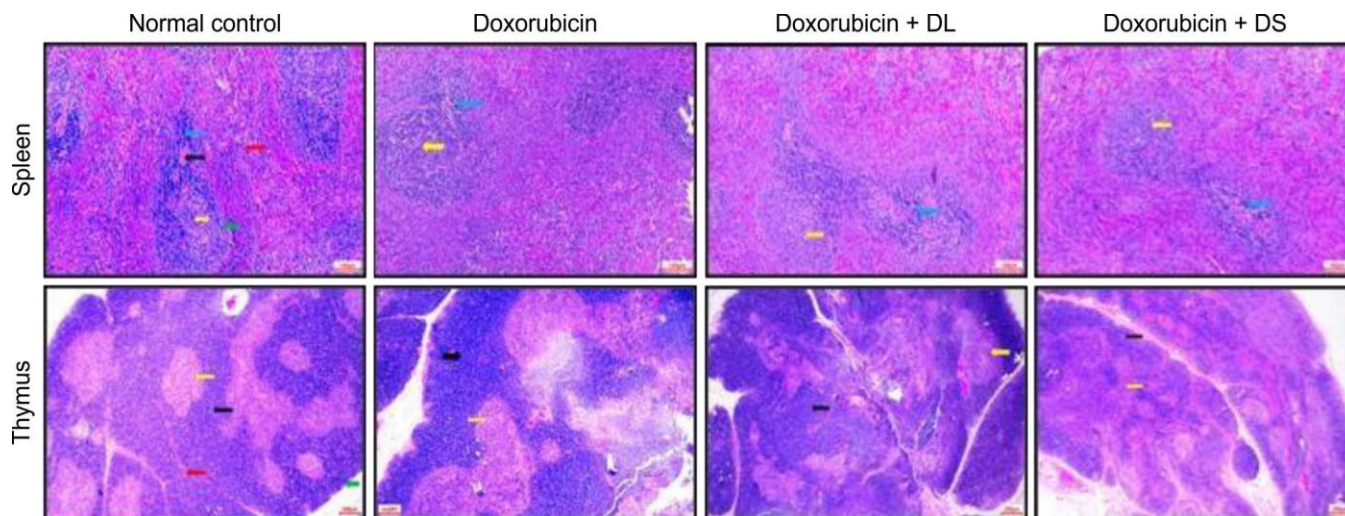


Fig. 5. Histopathological analysis of rat spleen and thymus

TABLE-3
BINDING AFFINITY SCORE OF DS AND DL PHYTO-CHEMICALS ON IMMUNOMODULATORY RECEPTORS

Compounds from DS and DL	Binding affinity (-Kcal/mol)		
	IL 10	TNF- α	NF- κ B p52
Linoelaidic acid	-6.1	-5.8	-5.4
Agarospirol	-6.6	-7.2	-7.1
Azulene	-6.3	-5.8	-7.7
Himachalol	-6.9	-6.9	-7.2
Octadecadienoic acid	-5.9	-5.5	-5.4
Eicosatrien-1-ol	-6.1	-5.6	-5.5
β -Sitosterol	-8.0	-6.2	-8.7
Hinesol	-6.5	-6.7	-6.7
Dihydrocoumarin	-5.6	-6.9	-7.1
Squalene	-7.6	-6.1	-6.1

negative binding affinity values toward the selected targets, suggesting favorable ligand–protein interactions within the docking models.

For NF- κ B p52, β -sitosterol showed the most favourable binding affinity (-8.0 kcal/mol) followed by azulene (-7.7 kcal/mol), agarospirol and dihydrocoumarin (both -7.1 kcal/mol), and hinesol (-6.7 kcal/mol). Squalene exhibits a binding affinity of -6.1 kcal/mol, while linoelaidic acid, octadecadienoic acid, eicosatrien-1-ol and himachalol showed comparatively weaker affinities of -5.4, -5.4, -5.5 and -5.2 kcal/mol, respectively. The relatively low docking score of β -sitosterol suggests a stronger predicted interaction with NF- κ B p52 among the compounds evaluated.

Against TNF- α , agarospirol exhibited the most favourable binding affinity (-7.2 kcal/mol) followed by dihydrocoumarin (-6.9 kcal/mol), himachalol (-6.9 kcal/mol), hinesol (-6.7 kcal/mol) and β -sitosterol (-6.2 kcal/mol). Squalene showed a binding affinity of -6.1 kcal/mol, whereas linoelaidic acid and azulene showed -5.8 kcal/mol. Octadecadienoic acid and eicosatrien-1-ol showed comparatively weaker binding affinities of -5.5 and -5.6 kcal/mol, respectively. The stronger predicted affinity of agarospirol suggests a potentially favourable interaction with the TNF- α binding region.

For vIL-10, azulene showed the most favourable binding affinity (-7.7 kcal/mol) followed by agarospirol and dihydrocoumarin (-7.1 kcal/mol each) and hinesol (-6.7 kcal/mol). Squalene showed a binding affinity of -6.1 kcal/mol, while linoelaidic acid and eicosatrien-1-ol showed -5.4 and -5.5 kcal/mol, respectively. Himachalol exhibited a binding affinity of -5.2 kcal/mol. The differences in binding scores across the

three targets suggest that the phytoconstituents have distinct target-binding preferences.

The representative docking poses shown in Fig. 6 provide visual support for the predicted ligand–protein interactions. β -Sitosterol, squalene, and agarospirol were selected to illustrate their interactions with NF- κ B p52, vIL-10 and TNF- α , respectively. The favourable docking scores observed for these compounds provide a possible structural basis for their interaction with proteins involved in immune and inflammatory regulation. The variation in binding affinity among the compounds and targets suggests that the observed biological effects may involve interactions with multiple immunoregulatory pathways rather than a single molecular target. This interpretation is also consistent with the complex phytochemical composition of the extracts.

Conclusion

The present study provides preliminary comparative evidence for the immunomodulatory potential of methanolic bark extracts of *Dalbergia lanceolaria* and *Derris scandens* in a doxorubicin-induced immunosuppression model. The phytochemical screening, TLC and GC-MS analysis demonstrated the presence of diverse bioactive constituents in both extracts, with 13 compounds identified by GC-MS in each extract. Treatment with both extracts improved the doxorubicin-associated alterations in leukocyte parameters, with the 400 mg/kg dose producing higher effects than the 200 mg/kg dose. The histopathological findings further supported the protective effects of the extracts by showing comparatively preserved splenic and thymic architecture. Molecular docking provided additional *in silico* evidence for the possible interaction of selected phytoconstituents with NF- κ B p52, TNF- α and viral interleukin-10. β -Sitosterol, agarospirol and azulene showed comparatively favourable predicted binding toward NF- κ B p52, TNF- α and viral interleukin-10, respectively. These findings suggest that the observed activity may involve the combined contribution of multiple phytoconstituents acting through different immunoregulatory pathways.

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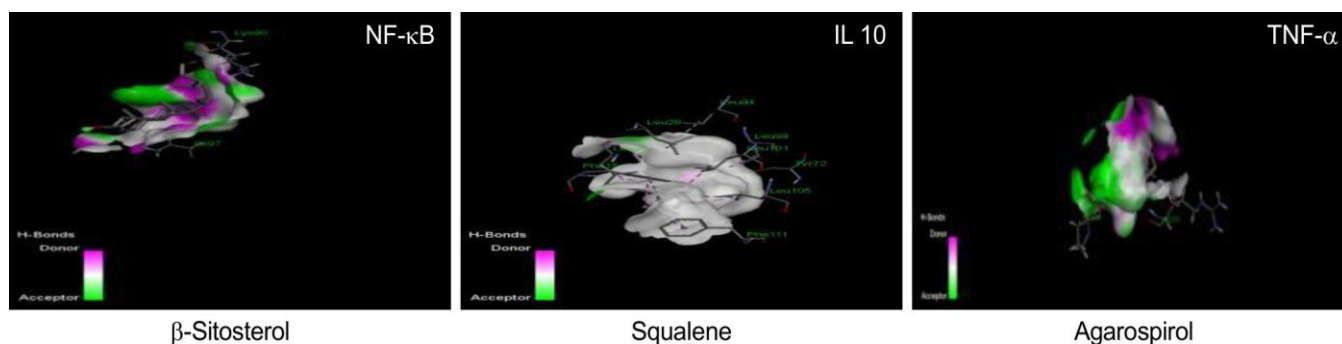


Fig. 6. Molecular docking interactions of best fit compounds with target proteins

CONFLICT OF INTEREST

The authors declare that there is no conflict of interests regarding the publication of this article.

DECLARATION OF AI-ASSISTED TECHNOLOGIES

During the preparation of this manuscript, the authors used an AI-assisted tool(s) to improve the language and no data, results or scientific conclusions were generated by AI. All analyses, interpretations and conclusions are the authors' own. The authors reviewed and edited the content and take full responsibility for the published work.

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