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Phytochemical Screening, Gc-Ms Analysis, In-Silico Docking and In-Vitro Study of Hydroalcholic Extract of Leaves of Solanum Trilobatum

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KEYWORDS

Solanum trilobatum, phytochemical screening, GC-MS analysis, in-silico docking, anticancer activity, cytotoxicity assay, bioactive compounds

ABSTRACT:

Introduction

Plants have been a cornerstone of traditional medicine for centuries, offering a rich source of bioactive compounds with therapeutic potential. Solanum trilobatum, a member of the Solanaceae family, is widely used in traditional practices for its nutritional and medicinal properties. This study explores the phytochemical composition, molecular interactions, and anticancer potential of Solanum trilobatum leaves.

Objective

The study aimed to extract bioactive compounds from Solanum trilobatum leaves, identify their phytochemical constituents, analyse molecular interactions through in-silico docking, and evaluate their anticancer potential using in-vitro cytotoxicity assay.

Methods

The hydroalcoholic extract was prepared using cold maceration and subjected to phytochemical screening to identify alkaloids, flavonoids, phenols, saponins, tannins, and terpenoids. GC-MS analysis was performed to identify bioactive compounds, and in-silico docking was conducted to study their binding affinity with the active EGFR tyrosine kinase domain (PDB ID: 2GS6). In-vitro cytotoxicity was assessed on the A431 epidermoid carcinoma cell line using the MTT assay.

Results

Phytochemical screening confirmed the presence of alkaloids, flavonoids, phenols, saponins, tannins, and terpenoids. GC-MS analysis identified 15 major bioactive compounds, including Methyl propyl ether, 2-(2-Aminoethyl) pyrazine, and Lidocaine. Computational molecular docking studies revealed robust binding interactions between these compounds and the EGFR kinase domain (PDB ID: 2GS6), with campesterol exhibiting the strongest affinity (-7.8 kcal/mol). In vitro assessments on A431 epidermoid carcinoma cells demonstrated a concentration-dependent reduction in cell survival, yielding an IC_{50} of 110 µg/ml.

Conclusion

The results highlight the plant's notable anticancer properties, positioning it as a compelling subject for future drug development studies.

1. Introduction

Plants have long been a cornerstone of health and healing for millions in India. Traditional and ethnobotanical practices using plant-based remedies have gained widespread attention for their effectiveness and safety. For centuries, plants have been used to treat infections and various health conditions, providing a wealth of therapeutic compounds. Often referred to as medicinal plants or herbs, they are valued for their ability to promote health and well-being. Many life-saving drugs are derived from the active components of these plants, highlighting their enduring role in both traditional and

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modern medicine[1]. India is home to a rich diversity of flora, including numerous medicinal and aromatic plants, many of which are rare and endemic. For centuries, plants have served as vital sources of medicine. These therapeutic effects are attributed to bioactive phytochemicals, which exhibit diverse health-promoting properties. Among the estimated 250,000 known plant species globally, scientific studies have identified nearly 1,000 with potential anticancer activity[2].

Solanum trilobatum L., commonly known as nightshade and belonging to the Solanaceae family with 102 genera around 2500 species, is a widely recognized plant used by various communities to treat a range of ailments. The leaves are essential in nutrients, such as calcium, iron, and phosphorus, along with carbohydrates, fats, and crude fiber3. Solanum, a natural compound present in this plant, is known to help slow down tumor growth. Recently, there's been growing interest in substances derived from plants because of their wide range of uses. Medicinal plants are like a local treasure that holds value for the entire world, and nature has blessed us with an incredible variety of them. These plants contain basic components like sugars, amino acids, proteins, and chlorophyll, as well as more complex elements such as alkaloids, terpenoids, flavonoids, tannins, and phenolic compounds[4].

Taxonomical Classification[5]:

Kingdom: Plantae

Division: Streptophyta

Class: Equisetopsida

Subclass: Magnoliidae

Order; Solanales

Family: Solanaceae

Genus: Solanum

Species: Solanum trilobatum

Fig 1. Morphology of Solanum trilobatum

2. Objectives

The research focuses on extracting Solanum trilobatum using a cold maceration technique with a hydroalcoholic solvent. After extraction, the plant's chemical components will be analysed through phytochemical screening to identify its active compounds. Next, the study will use in silico docking to examine how these compounds interact with specific molecular targets and their binding strengths. Finally, the anticancer properties of the Solanum trilobatum extract will be tested in laboratory settings to determine its potential effectiveness against cancer cells.

3. Methods

1. Selection and Collection of leaves

The selection of *Solanum trilobatum* (also known as Purple-fruited Solanum) Solanum trilobatum is indigenous to regions spanning from India and Sri Lanka to Indochina and the Malay Peninsula. The species is broadly distributed across tropical zones worldwide. As mentioned above, these leaves are easily accessible. We collected the leaves of *Solanum trilobatum* from a local region in Tamil Nadu, India and used them for our future studies.

2. Authentication of Plants

Plant authentication is the process of identifying a plant species. The taxonomic verification of *Solanum trilobatum* was conducted by Dr. M.U. Sharief, Scientist 'F' and Office Head at the Tamil Nadu Agricultural University (TNAU), using fresh plant specimens sourced from the Botanical Survey of India's facility located on TNAU's Coimbatore campus.

3. Preparation of Extracts:

Solanum trilobatum leaves were carefully washed with water and air-dried in shaded conditions for approximately seven days. After complete dehydration, the leaves were mechanically processed into a granular powder. This powder was securely stored in moisture-resistant containers at ambient temperature until further use. For the extraction process, 30 g of the powdered material was combined with 250 mL of a hydroalcoholic solution (70% ethanol, 30% water) and subjected to a 72-hour cold maceration technique. The solution was subsequently filtered through Whatman No. 1 filter paper. The filtrate was concentrated via rotary evaporation at 60°C to evaporate ethanol, followed by residual solvent removal in a 37°C oven for three hours, yielding a dark green extract. The final product was

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JCHR (2025) 15(2), 45-58 | ISSN:2251-6727

preserved in sealed containers under refrigeration at 4°C for subsequent experimental applications[6].

4. Preliminary Phytochemical Analysis:

The hydroalcoholic extract of Solanum trilobatum underwent preliminary phytochemical screening using standardized qualitative assays to assess its secondary metabolite composition. These protocols facilitated the identification of diverse bioactive constituents, including alkaloids, flavonoids, and terpenoids, through systematic characterization of the extract's phytochemical profile[7].

5. GC-MS Analysis:

GC-MS serves as an essential analytical technique for characterizing unidentified bioactive compounds in plant materials. In this study, the phytochemical profile of *Solanum trilobatum* leaves hydroalcoholic extract was evaluated using a GC-MS system (CH-GCMSMS02, 8890 GC System, 7000 GC/TQ). The analysis employed an Elite-HP5MS fused silica capillary column (30 m × 250 µm × 0.25 µm) with ultra-high-purity helium (99.999%) as the carrier gas. Operational parameters included a 2 µl injection volume, a flow rate of 1 ml/min, and injector/auxiliary temperatures set to 280°C. Mass spectra were recorded over a scan range of 30–900 m/z during a 38-minute runtime. Relative abundance of constituents was determined by comparing chromatographic peak areas generated during the analysis[8,9,10].

6. *In-Silico* Molecular Docking:

To further investigate the therapeutic potential of these bioactive compounds, molecular docking studies were performed. Molecular docking was a computational approach that predicts how a ligand (such as a bioactive compound) interacts with a target protein (like a receptor or enzyme). This technique allows researchers to analyze the binding affinity and molecular interactions.

Protein Structure Preparation

The three-dimensional structure of the 2GS6 protein was retrieved from the Protein Data Bank. This structural model includes the kinase domain complexed with both its natural ligand and associated cofactors.

Protein Download: The 2GS6 structure was downloaded directly from the PDB database.

- Cleaning and Preprocessing: Using Bioria Discovery Studio, water molecules, ions, ad heteroatoms were removed to refine the protein structure. Hydrogen atoms were incorporated to precisely model electrostatic interactions during the docking process.
- The prepared protein structure was converted into the PDBQT format to ensure compatibility with AutoDock Vina, the molecular docking software integrated into the PyRx workflow.

Ligand Structure Preparation

The bioactive compounds were sourced from PubChem in SDF format.

- The ligands were processed into PDBQT format within PyRx to ensure compatibility with AutoDock Vina's docking protocols.
- Geometry optimization of the ligand structures was carried out in PyRx using the Universal Force Field (UFF) during energy minimization to improve molecular stability.
- In PyRx, hydrogens were automatically added, and the ligands were prepared for docking, saving them in PDBQT format.

Docking Grid box Setup

• The docking search space was configured by mapping the ligand-binding cavity within the 2GS6 structure through structural analysis, targeting the established catalytic or functional region.

• Grid Configuration: A cubic grid (40 × 40 × 40 Å³) was positioned over the catalytic site, with a spatial resolution of 1.0 Å per grid point to balance computational efficiency and docking.

Docking Simulation Using PyRx

The docking simulation was conducted using AutoDock Vina integrated into PyRx. The following parameters were applied:

- Number of Docking Runs: 50 independent docking runs were performed to ensure reliability and identify the best docking pose.
- Energy Calculations: AutoDock Vina calculated the binding energy for each pose, with more negative values indicating stronger binding affinity.
  After setting up the grid box, the protein and ligand files were loaded into PyRx, and the

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JCHR (2025) 15(2), 45-58 | ISSN:2251-6727

simulation was initiated by clicking the "Start Docking" button.

Interaction Analysis

Following docking, Bioria Discovery Studio was used to analyse and predict the interactions between the protein and the bioactive compounds. This step helped identify key binding interactions and validate the docking results[11].

7. *In-Vitro* Study:

Cell culture

The A431 epidermoid carcinoma cell line, sourced from the National Centre for Cell Science, Pune, India, was cultured in Minimum Essential Medium (HiMedia) enriched with 10 percentage Fetal Bovine Serum (Gibco). The growth medium was further supplemented with 1 percentage sodium bicarbonate, 1 percentage sodium pyruvate (HiMedia), and 1 percentage MEM nonessential amino acids (HiMedia). Cells were incubated at 37°C in a humidified atmosphere containing 5 percentage CO_2 until required for experimental use[12].

Cytotoxicity analysis by MTT

This study investigated the anti-cancer properties of *Solanum trilobatum* by employing the 3-(4,5-dimethylthiazol-2-yl)-2,5-diphenyltetrazolium bromide (MTT) assay. The cytotoxic effects of the plant extract were assessed using the MTT reagent, a tetrazolium salt obtained from HiMedia. A431 cells were seeded in 96-well plates at a density of 1×10^4 cells per well and allowed to attach for 24 hours. After this period, the cells were treated with different concentrations of the extract, ranging from 100 to 1000 µg/mL, and incubated for another 24 hours. Following treatment, 100 µL of MTT solution (0.5 mg/mL prepared in complete medium) was added to each well, and the plates were incubated for 5 hours. The supernatant was then carefully removed, and the resulting formazan crystals were dissolved using 100 µL of dimethyl sulfoxide (DMSO) for 30 minutes. Absorbance was measured at 570 nm and 650 nm using a microplate reader. The half-maximal inhibitory concentration (IC_{50}) was determined from the absorbance values, and the data were analyzed to evaluate the cytotoxic potential of the extract[13].

4. Results and Discussion

1. Preliminary Phytochemical Analysis:

Qualitative phytochemical screening of the hydroalcoholic extract derived from *Solanum trilobatum* leaves was performed to identify its bioactive constituents and shown in Table 1.

Tab 1. Preliminary Phytochemical Analysis of hydroalcoholic extract of *Solanum trilobatum* leaves.

S.No	Phytochemical Constituents	Test/ Reagents	Inference
1	Alkaloids	Wagner's test, Dragendorff's test	+
2	Coumarins	Alcoholic NaOH	-
3	Flavonoids	Shinoda's test	+
4	Glycosides	Anthrone + Conc. H2SO4	-
5	Phenols	Lead acetate test	+
6	Proteins and Free amino acids	NaOH and copper sulphate, Ninhydrin test	+
7	Quinones	Conc. H_2SO_4	-
8	Saponins	Foam Test	+
9	Steroid	Acetic acid + Chloroform+ Conc. H2SO4	-
10	Reducing sugars	Fehling's Test	+
11	Tannins	Basic lead acetate	+
12	Terpenoids	Salkowski Test	+
13	Fixed oil	Spot test	-

Note: + Present, - Absent

2. GC-MS Analysis:

Different phytochemical/bioactive compounds of the hydroalcoholic extract of *Solanum trilobatum* leaves were analysed by using GC-MS. The hydroalcoholic extract of Solanum trilobatum leaves was subjected to GC-MS analysis to characterize its phytochemical and bioactive constituents. Chromatographic profiles of the extract (Fig. 2) and corresponding compound data (Table 3) revealed 15 distinct peaks, indicating the presence of 15 major bioactive compounds. Among these, Methyl propyl ether exhibited the highest relative abundance (100.00%), followed by 2-(2-Aminoethyl) pyrazine

Journal of Chemical Health Risks

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(42.41%), Hexadecanoic acid, ethyl ester (13.45%), and 9,12,15-Octadecatrienoic acid, ethyl ester (Z,Z,Z) (7.39%). Other notable constituents included Lidocaine (4.18%), dl-α-Tocopherol (2.70%), Phytol (1.30%), gamma-Tocopherol (1.29%), Campesterol (1.35%), and Phenol, 2-methoxy (1.17%). Minor compounds such as Ethylphosphonic acid (1.15%), 5-Cyano-1,2,3,4-tetrahydro-4,6-dimethyl-2-oxopyridine (1.20%), and Phthalic acid, di(2-propylpentyl) ester (1.29%) were also identified. These findings demonstrate the diverse phytochemical profile of Solanum trilobatum leaf extract, highlighting its potential bioactive significance.

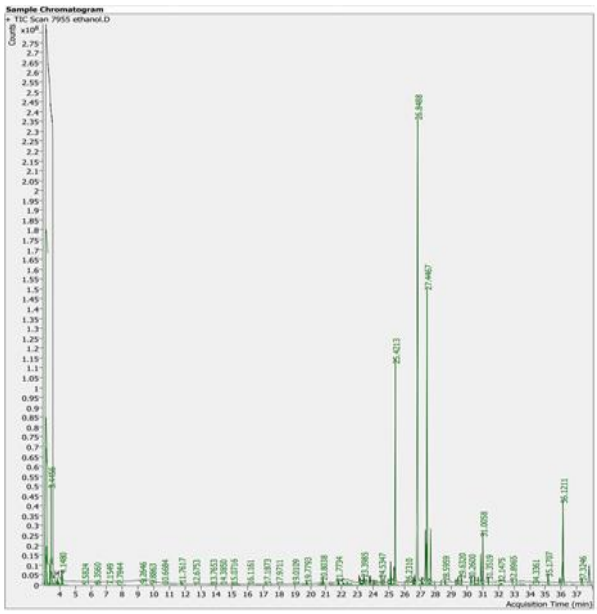
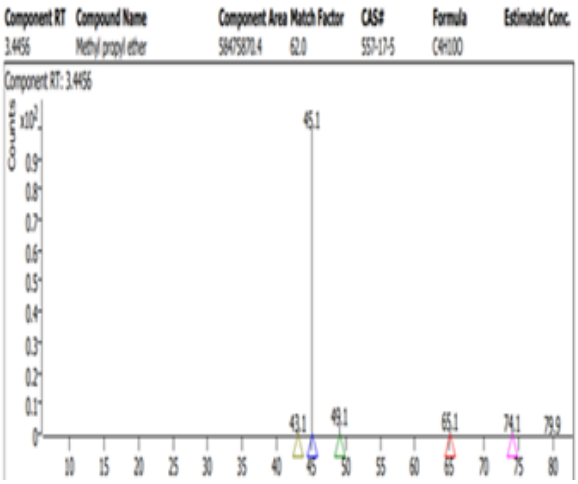


Fig 2. GC-MS Chromatogram of Hydroalcoholic Extract of *Solanum trilobatum* Leaves



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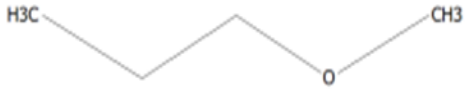

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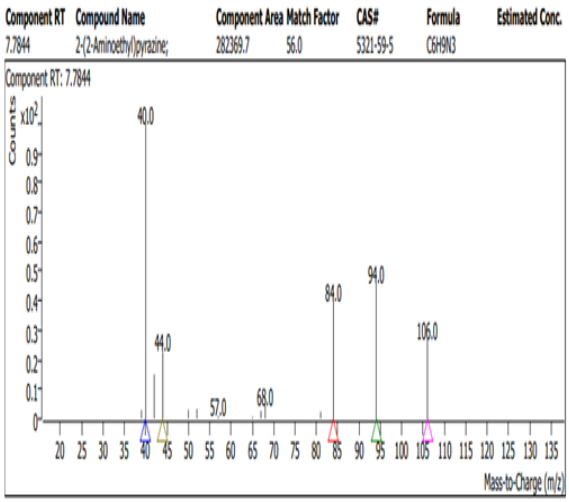

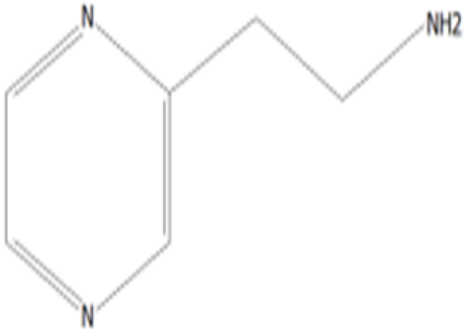

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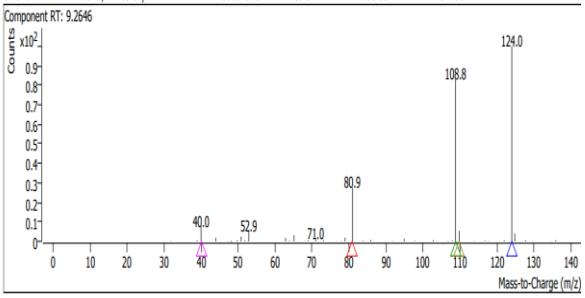
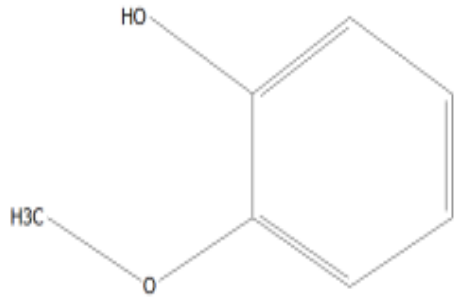
JCHR (2025) 15(2), 45-58 | ISSN:2251-6727

C.

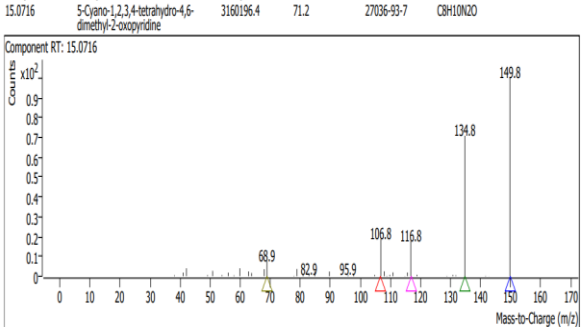
Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
9.2646	Phenol, 2-methoxy-	8360207.3	89.9	90-05-1	C7H8O2	

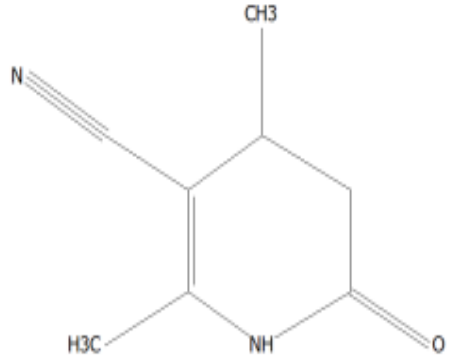




E.

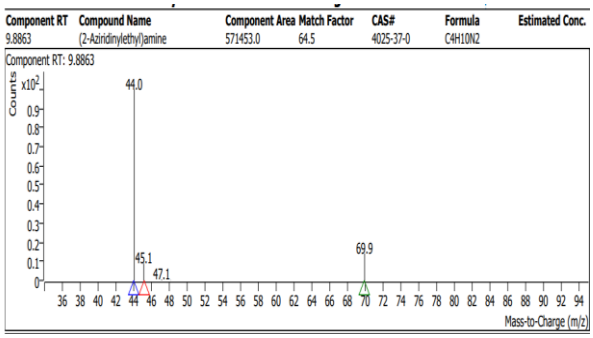
Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
15.0716	5-Cyano-1,2,3,4-tetrahydro-4,6-dimethyl-2-oxopyridine	3160196.4	71.2	27036-93-7	C8H10N2O	

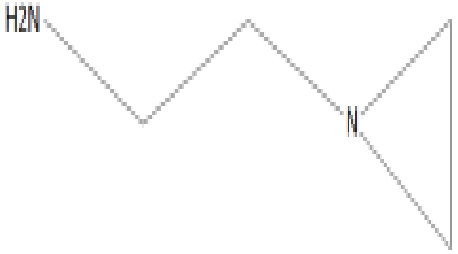




D.

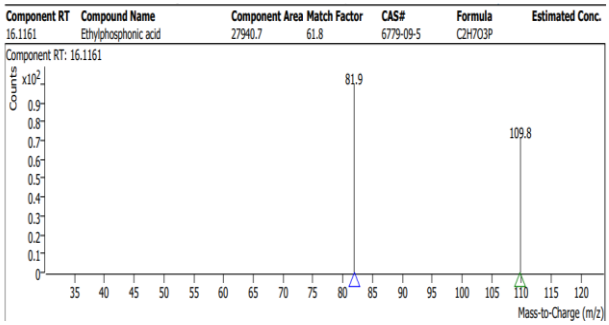
Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
9.8863	(2-Aziridinylethyl)amine	571453.0	64.5	4025-37-0	C4H10N2	

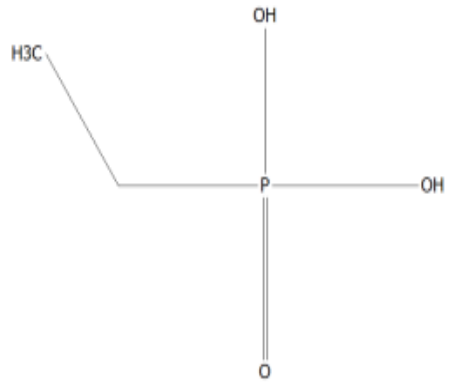




F.

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
16.1161	Ethylphosphonic acid	27940.7	61.8	6779-09-5	C2H7O3P	





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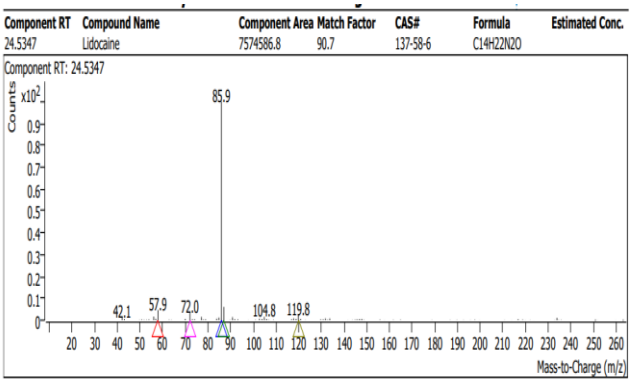
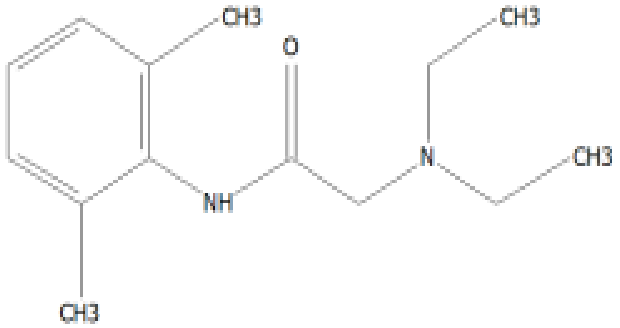
G.





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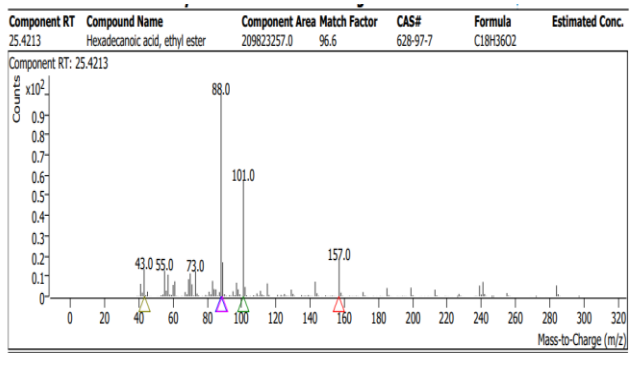

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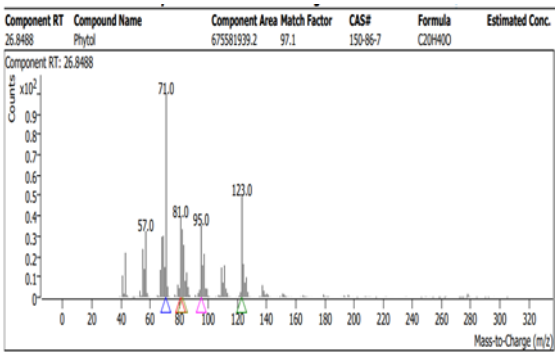

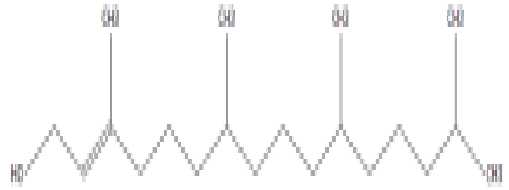

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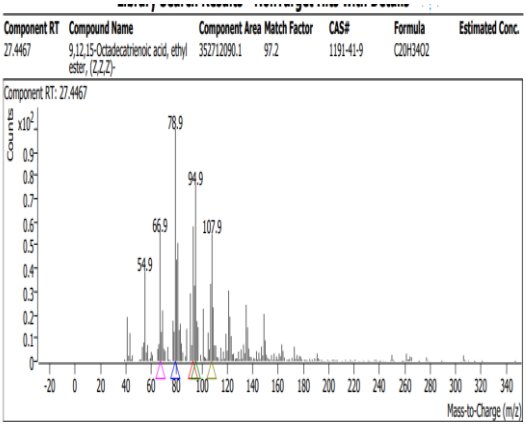

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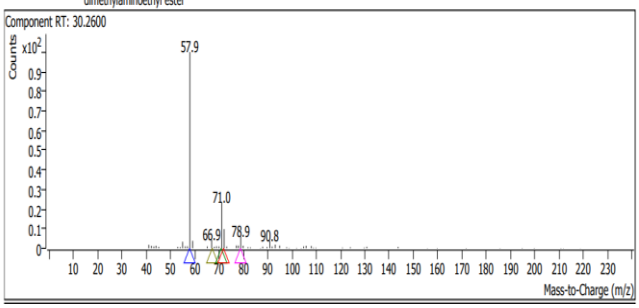
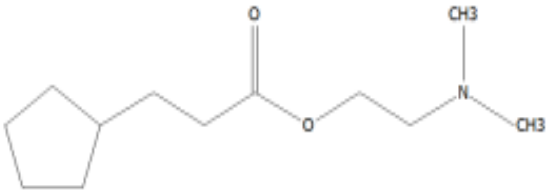
K.

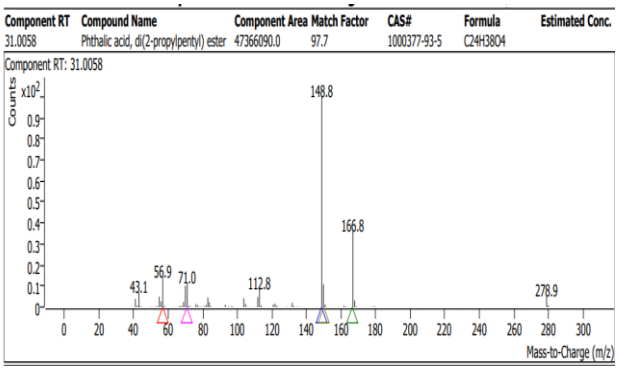
Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
30.2600	3-Cyclopentylpropionic acid, 2-dimethylaminoethyl ester	6967343.9	72.5	1000331-24-3	C12H23NO2	

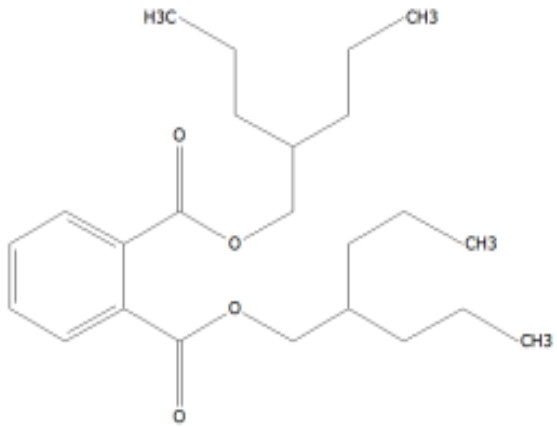




L.

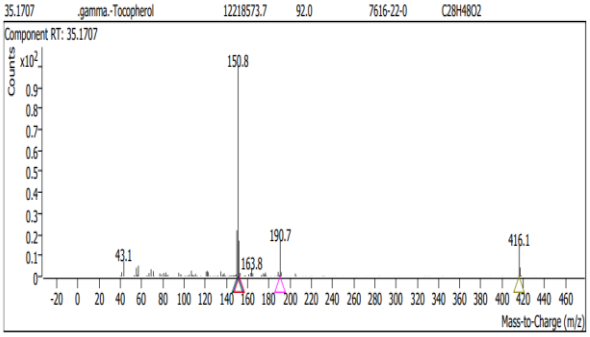
Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
31.0058	Phthalic acid, di(2-propylpentyl) ester	47366090.0	97.7	1000377-93-5	C24H38O4	

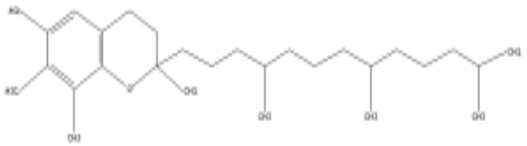




M.

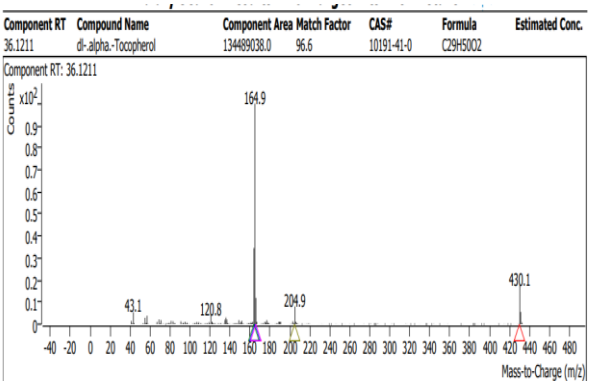
Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
35.1707	.gamma.-Tocopherol	1221857.3.7	92.0	7616-22-0	C28H48O2	

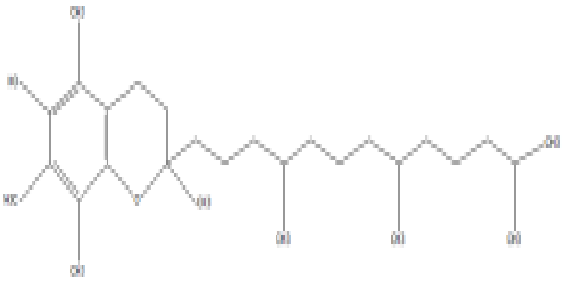




N.

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
36.1211	dl-.alpha.-Tocopherol	134489038.0	96.6	10191-41-0	C29H50O2	





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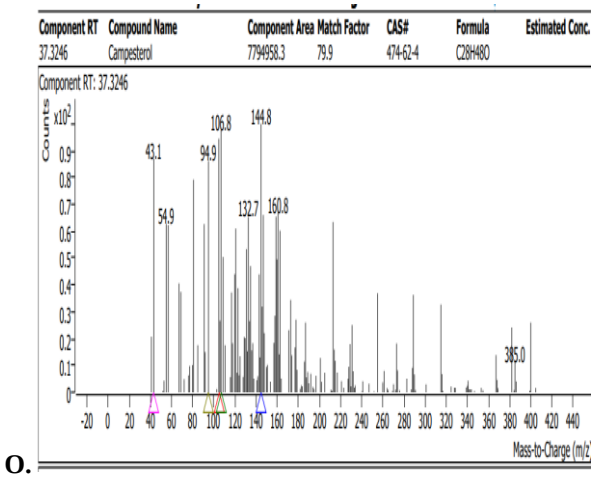

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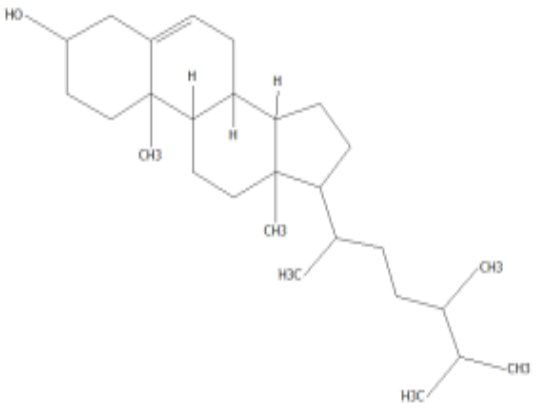

Fig 3. GC-MS Mass Spectra of a Compounds from Hydroalcoholic Extract of *Solanum trilobatum* Leaves

. Mass spectra & Structure of (A) Methyl propyl ether ($C_4H_{10}O$), (B) 2-(2-Aminoethyl) pyrazine ($C_6H_9N_3$) , (C) Phenol, 2-methoxy ($C_7H_8O_2$), (D) (2-Aziridinylethyl) amine ($C_4H_{10}N_2$), (E) 5-Cyano-1,2,3,4-tetrahydro-4,6-dimethyl-2-oxopyridine ($C_8H_{10}N_2O$), (F) Ethylphosphonic acid ($C_2H_7O_3P$) , (G) Lidocaine ($C_{14}H_{22}N_2O$),(H) Hexadecanoic acid, ethyl ester ($C_{18}H_{36}O_2$) , (I) Phytol (C20H40O2), (J) Phytol ($C_{20}H_{40}O$), (K) 9,12,15-Octadecatrienoic acid, ethyl ester, (Z,Z,Z)- ($C_{20}H_{34}O_2$), (L) 3-Cyclopentylpropionic acid, 2- dimethylaminoethyl ester ($C_{24}H_{38}O_4$), (M) gamma. -Tocopherol ($C_{28}H_{48}O_2$), (N) dl-.alpha.-Tocopherol ($C_{29}H_{50}O_2$), (O) Campesterol ($C_{28}H_{48}O$).

IN-SILICO DOCKING:

Docking Score:

Tab 2. Binding Affinity of Solanum trilobatum extract with 2GS6 protein

S.NO	LIGAND	MOLECULAR WEIGHT g/mol	BINDING AFFINITY kcal/mol
1	Lidocaine	**1275.70**	**-4.4**
2	Campesterol	**789.51**	**-7.8**
3	dl-.alpha.-Tocopherol	**295.63**	**-5.7**
4	gamma.-Tocopherol	**258.16**	**-6.3**
5	Phytol	**165.93**	**-4.2**
6	Lidocaine	**318.43**	**-5.3**
7	9,12,15-Octadecatrienoic acid, ethyl ester, (Z,Z,Z)-	**181.92**	**-4.8**
8	5-Cyano-1,2,3,4-tetrahydro-4,6-dimethyl-2-oxopyridine	**140.59**	**-5.4**
9	3-Cyclopentylpropionic acid, 2-dimethylaminoethyl ester	**289.43**	**–4.5**

(a) Binding pose of Campesterol

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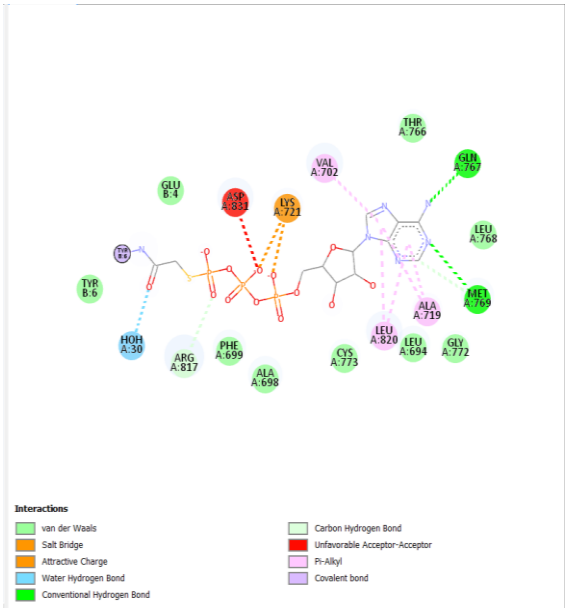
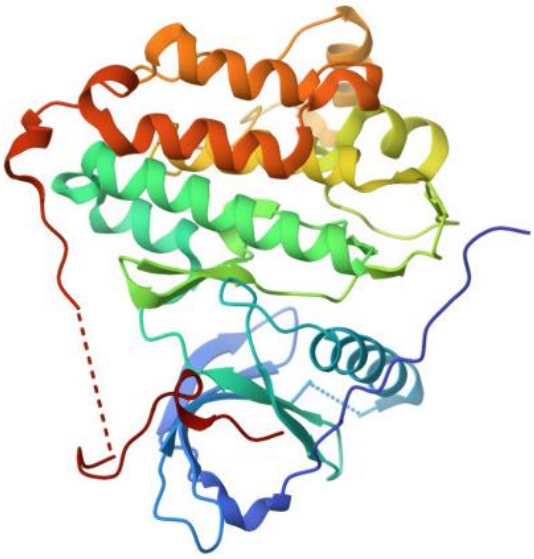


(b) Structural Binding pose of Campesterol



(c) Structure of Protein 2GS6

Fig 4. The best-docked pose of bioactive compound from leaves of *Solanum trilobatum* with 2GS6 protein (a) Binding pose of Campesterol (b) Structural Binding pose of Campesterol (c) Structure of Protein 2GS6

IN-VITRO STUDY:

The in vitro cytotoxicity studies on the A431 cancer cell line (human epidermoid carcinoma) revealed that the crude extracts of Solanum *trilobatum* exhibited significant anticancer activity. The IC50 values were determined 110 µg/mL.

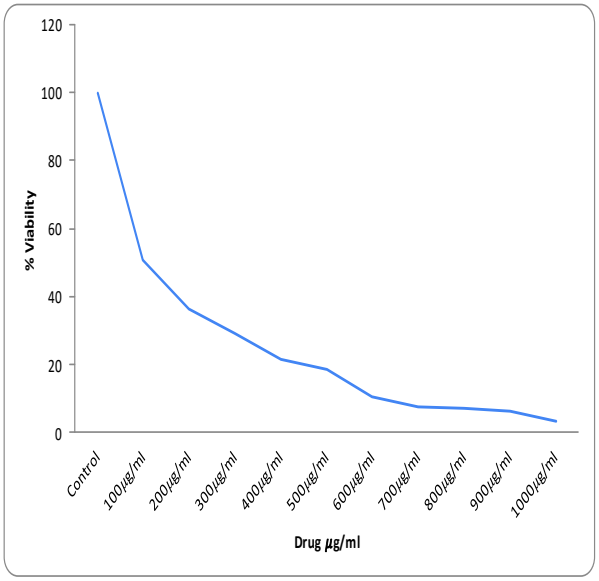


Fig 5. Graph of Cytotoxicity Assay of *Solanum trilobatum*

Statistical Analysis: All the qualitative test/analysis was performed in triplicate.

Tab 3. Activity of Bioactive Compound Identified in Hydroalcoholic Extract of Hydroalcoholic Extract of *Solanum trilobatum* Leaves

S. no	Name of the compounds	Retention time	Peak area %	Molecular formula	Reported biological activity
1	Methyl propyl ether	3.446	100	$C_4H_{10}O$	solvent or Limited anesthetic.
2	2-(2-Aminoethyl) pyrazine	7.784	42.41	$C_6H_9N_3$	antimicrobial and antioxidant activities
3	Phenol, 2-methoxy	9.265	1.17	$C_7H_8O_2$	antimicrobial and antioxidant activities

Journal of Chemical Health Risks

www.jchr.org

JCHR (2025) 15(2), 45-58 | ISSN:2251-6727

4	(2-Aziridinylethyl) amine	9.886	1.08	$C_4H_{10}N_2$	cytotoxic and anticancer properties
5	5-Cyano-1,2,3,4-tetrahydro-4,6-dimethyl-2-oxopyridine	15.07	1.2	$C_8H_{10}N_2O$	antimicrobial, anti-inflammatory, and anticancer activities.
6	Ethylphosphonic acid	16.12	1.15	$C_2H_7O_3P$	enzyme inhibitors and antiviral activity
7	Lidocaine	24.53	4.18	$C_{14}H_{22}N_2O$	local anesthetic and antiarrhythmic agent.
8	Hexadecanoic acid, ethyl ester	25.42	13.45	$C_{18}H_{36}O_2$	antimicrobial, anti-inflammatory, and antioxidant activity.
9	Phytol	26.85	1.3	$C_{20}H_{40}O$	Antimicrobial or cytotoxic activities
10	9,12,15-Octadecatrienoic acid, ethyl ester, (Z,Z,Z)-	27.45	7.39	$C_{20}H_{34}O_2$	nti-inflammatory, antioxidant, and cardioprotective effects
11	3-Cyclopentylpropionic acid, 2-dimethylaminoethyl ester	30.26	1.07	$C_{12}H_{23}NO_2$	local anesthetic or analgesic activity
12	3-Cyclopentylpropionic acid, 2-dimethylaminoethyl ester	31.01	1.29	$C_{24}H_{38}O_4$	potent antioxidant, anti-inflammatory, and anticancer activity
13	gamma. -Tocopherol	35.17	1.29	$C_{28}H_{48}O_2$	antioxidant, immune-boosting, and skin-protective effects.
14	dl-.alpha.-Tocopherol	36.12	2.7	$C_{29}H_{50}O_2$	antioxidant, immune-boosting, and skin-protective effects.
15	Campesterol	37.32	1.35	$C_{28}H_{48}O$	cholesterol-lowering, anti-inflammatory, and anticancer properties

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JCHR (2025) 15(2), 45-58 | ISSN:2251-6727

Tab 4. Cytotoxicity Assay of *Solanum trilobatum*

Concentration g/ml	570nm	650nm	570nm-650nm	Avg (570nm-650nm)	Cell viability	% Cell viability
Control	0.6940	0.5965	0.5965	0.5963	1	100
	0.6074	0.5179	0.5179			
	0.7767	0.6745	0.6745			
100µg/ml	0.3494	0.0680	0.2814	0.3033	0.5085	50.85
	0.3968	0.0796	0.3172			
	0.3689	0.0577	0.3112			
200µg/ml	0.3798	0.0464	0.3334	0.2167	0.3634	36.34
	0.3808	0.0471	0.3337			
	0.0295	0.0465	-0.0170			
300µg/ml	0.0714	0.0460	0.0254	0.1740	0.2918	29.18
	0.4050	0.0868	0.3182			
	0.2412	0.0627	0.1785			
400µg/ml	0.2589	0.0612	0.1977	0.1277	0.2141	21.41
	0.1529	0.0528	0.1001			
	0.1402	0.0549	0.0853			
500µg/ml	0.1082	0.0542	0.0540	0.1103	0.1849	18.49
	0.1879	0.0461	0.1418			
	0.1820	0.0470	0.1350			
600µg/ml	0.1083	0.0476	0.0607	0.0619	0.1037	10.37
	0.1229	0.0566	0.0663			
	0.1084	0.0497	0.0587			
700µg/ml	0.0816	0.5965	0.0285	0.0434	0.0727	7.27
	0.1071	0.5179	0.0568			
	0.0964	0.6745	0.0448			
800µg/ml	0.0909	0.0680	0.0410	0.0415	0.0695	6.95
	0.0962	0.0796	0.0467			
	0.0863	0.0577	0.0368			
900µg/ml	0.0917	0.0464	0.0322	0.0367	0.0615	6.15
	0.0919	0.0471	0.0413			
	0.0862	0.0465	0.0366			
1000µg/ml	0.0270	0.0460	-0.0293	0.0203	0.0339	3.39
	0.0913	0.0868	0.0412			
	0.0980	0.0627	0.0489			

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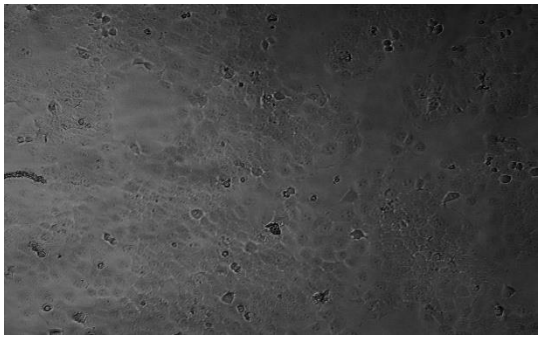
JCHR (2025) 15(2), 45-58 | ISSN:2251-6727



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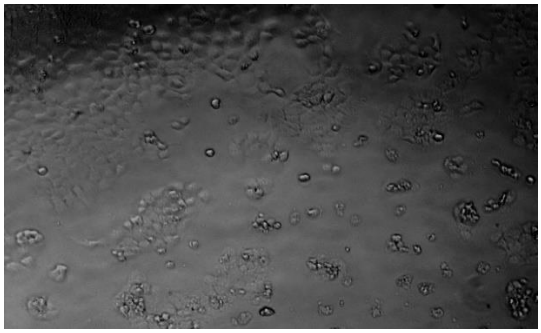

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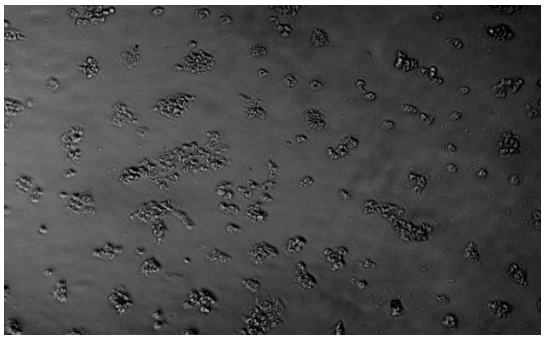

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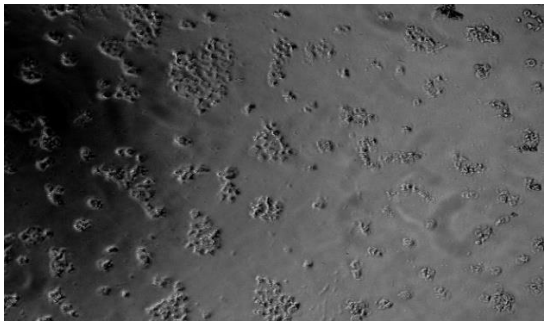

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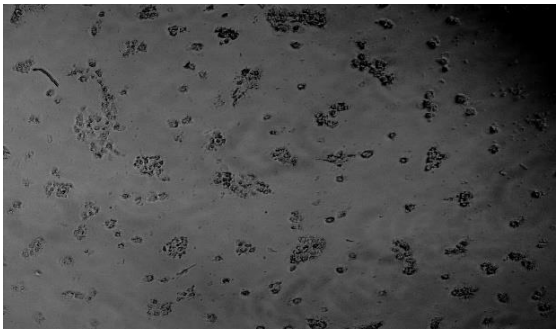

(e)

Fig 6. A431 Cell line of (a) Control (0 µg/ml) (b) 100 µg/ml (c) 200 µg/ml (d) 300 µg/ml (e) 400 µg/ml.

Conclusion

The qualitative phytochemical analysis of *Solanum trilobatum* leaves indicated the presence of secondary metabolites, including alkaloids, flavonoids, phenols, proteins, free amino acids, saponins, reducing sugars, tannins, and terpenoids. GC-MS profiling further identified bioactive compounds with reported therapeutic properties. These findings underscore the plants potential as a source of phytopharmaceutical agents. Molecular docking studies highlighted strong interactions between the identified compounds and the 2GS6 protein, with Campesterol exhibiting the highest binding affinity (-7.8 kcal/mol. Cytotoxicity evaluation against the A431 epidermoid carcinoma cell line revealed dose-dependent inhibition of cell viability, with an IC_{50} value of 110 µg/mL, signifying notable anticancer activity. Collectively, these results position *Solanum trilobatum* as a promising candidate for further exploration in anticancer drug development.

Acknowledgement:

All authors contributed equally.

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