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Original Article

# Bioactive Profiling and Pharmacological Evaluation of *Gelidiella acerosa*: An Integrated *in vitro* and *in silico* ADME Study

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## ABSTRACT

**Background:** Marine macroalgae are highly accepted as renewable sources of pharmacologically related metabolites exhibiting robust potential for future generation therapeutics. **Objectives:** This study investigates about the red seaweed *Gelidiella acerosa* for its physicochemical and intrinsic drug-like properties. **Materials and Methods:** Phytochemical screening and functional group characterization by Fourier-Transform Infrared (FTIR) spectroscopy were performed for *G. acerosa* extract. Biochemical profiling was carried by Gas Chromatography - Mass Spectrometry (GC-MS) followed by Diphenyl Picryl Hydrazyl (DPPH) and phosphomolybdenum assay to assess the antioxidant activity. Microbial and cytotoxic activity was performed by disc diffusion method and 3-(4,5-Dimethylthiazol-2-yl)-2,5-diphenyltetrazolium bromide (MTT) assay respectively. *In silico* molecular docking and Absorption, Distribution, Metabolism and Excretion (ADME) drug-likeness evaluation of the identified compounds. **Results:** Phytochemical screening confirmed the presence of bioactive constituents, FTIR analysis revealed hydroxyl-rich functional groups, and GC-MS identified 30 phytoconstituents in the ethanolic extract. The DPPH testing produced a radical scavenging Half-Maximal Inhibitory Concentration ($IC_{50}$) of 712.82 µg/mL compared to 67.34 µg/mL for ascorbic acid, associating to 0.094 mg AAE/g extract. The phosphomolybdenum evaluation produced a Total Antioxidant Capacity (TAC) of 70.60% at 1200 µg/mL equivalent to 1.143 mg AAE /g extract. The extract confirmed exhibited antibacterial and antifungal activity. MTT-based cytotoxic profiling against MDA-MB-231 cells, revealed an $IC_{50}$ of 41.59 µg/mL. *In silico* ADME and drug-likeness profiling of ten GC- MS selected compounds found molecules compatible with oral bioavailability and drug-likeness standards. **Conclusion:** The results stamp *G. acerosa* as a capable source of multifunctional bioactives and rational small molecule scaffolds for future nutraceutical and pharmaceutical discoveries.

**Keywords:** Antioxidant activity, Cytotoxic profiling, DPPH radical scavenging, *Gelidiella acerosa*, MTT assay, Total antioxidant capacity.

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## INTRODUCTION

The marine ecosystems are home to a far wider diversity of species, compared to the earth's ecosystem, thereby providing a huge pool of nutrients. Recently, studies are focussed towards marine algae, as marine-based molecules have unleashed innovative bioactive compounds possessing promising capabilities (Ahmed *et al.*, 2024). Red algae (*Rhodophyceae*) is a significant type of marine macroalgae that contributes to ecological balance and serve as repository of structural diverse bioactive compounds. Of these macroalgae, *G. acerosa* has gained popularity due to its nutritional, ecological and pharmacological prominence. It is a high source of top quality agar (Prasad *et al.*, 2007), owing to which it is highly rated in the food and pharmaceutical industries. *G. acerosa* (Forsskal) Feldmann and Hamel, 1934, taxonomically is paired under the Class *Florideophyceae*, Order *Gelidiales*, and Family *Gelidiellaceae*. Morphologically these elements can be distinguished by their fine, densely branched tree-like structures, having their branches ranging from 10-30 cm in length. They are mostly spotted at an intertidal and upper subtidal depths ranging from 0 to 47 m, often are reddish-brown coloured and are influenced by light intensity and specific biochemical compounds (Oktavia *et al.*, 2025). In India, they are spotted at the Gulf of Mannar's intertidal regions on the southeast cost, contributing significantly to the marine vegetation (Vivek *et al.*, 2011). In addition to producing oxygen and offering nutrient-cycle stability, *G. acerosa* are widely pursued for their biological properties. The comparative phytochemical analysis has revealed that the crude extract of *G. acerosa* has a significant collection of metabolites. GC-MS studies had substantiated

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that the *G. acerosa* has more than 150 compounds, a count that is significantly higher than those that are detected in other red algae like *Hypnea musciformis* and *Acanthophora spicifera*. Its ethanol and chloroform extracts have exhibited antibacterial and antifungal potential respectively (Aassaithambi *et al.,* 2025). It has a distinct post-coital contraceptive that is mediated through an anti-progestational mechanism (Premakumara *et al.,* 1995) and its prominent antioxidant potential offers protection related to stress-related disorders (Devi *et al.,* 2008). The nutritional profiling that was carried out, further substantiated the presence of content rich carbohydrates, proteins, lipids, proline, and chlorophyll, highlighting its dietary supplements (Syad *et al.,* 2013). The pharmacological process of *G. acerosa* has been further substantiated by a number of studies highlighting its varied bioactivities. The phytoconstituents of *G. acerosa* have been related to anticancer activity with strong evidence, where it acts as a natural restrictor of the PI3K/Akt signaling cascade that is involved in tumor growth and progression (Begum *et al.,* 2018). The solvent samples of *G. acerosa* exercise dual restrictive effects on Acetylcholinesterase (AChE) and Butyrylcholinesterase (BuChE), thereby offering a prospective support in the management of application in Alzheimer's like neurodegenerative diseases (Syad *et al.,* 2012). The polysaccharidic extracts of these species have revealed anticoagulant and antithrombotic activity in experimental models where it had maintained an appreciable safety profile (Chagas *et al.,* 2020; Queiroz *et al.,* 2014). Evaluation of methanol samples of *G. acerosa* have revealed anticancer properties, especially against Dalton's Ascitic Lymphoma (DAL) cells, displaying noteworthy tumor-inhibitory skills (Duraikannu *et al.,* 2014). In addition to this, the Liquid Chromatography- Mass Spectrometry (LC-MS) analyses have found antioxidant compounds namely caffeic acid, phytol, and mannoheptulose in the methanolic samples of *G. acerosa* that could act as protective shield against toxic elements like 2,3,7,8-tetrachlorodibenzo-p-dioxin (Ilavarasi *et al.,* 2015). The benzene extracts of *G. acerosa* found to possess neuroprotective properties, which could deter peptide-induced macromolecular damage and oxidative stress in Alzheimer's models (Nisha and Devi, 2017).

This study stands apart in the way that it is only among a very few to methodically integrate phytochemical profiling, spectroscopic and chromatographic characterization, antioxidant, antimicrobial and cytotoxic evaluations, together with computational pharmacokinetic prediction, to highlight the therapeutic features of *G. acerosa* and the huge benefits it offers in biomedical and pharmaceutical domains.

## MATERIALS AND METHODS

### Reagents and Standards

All chemicals utilized in this study were of analytical grade and higher purity. The following reagents were procured from commercial suppliers. The reagents used in this study included 2,2-diphenyl-1-picrylhydrazyl (DPPH), ascorbic acid, sodium phosphate, ammonium molybdate and MTT were obtained from Sisco Research Laboratories Pvt. Ltd., (SRL), Mumbai, India. All aqueous solutions were prepared using double-distilled water, and the organic solvents used throughout the study were of HPLC grade.

### Collection of red algae *G. acerosa*

The red alga *G. acerosa* was obtained from the R.K. Algae Project Centre, Mandapam, Ramanathapuram District, Tamil Nadu, India (Ahila *et al.,* 2024). The collected samples were shade-dried, finely powdered, and stored in airtight containers until further use for further investigations.

### Preparation of ethanolic extract of *G. acerosa*

Following collection, 10 g of the powdered *G. acerosa* was extracted with ethanol by a Soxhlet apparatus. After extraction, the solvent was subjected to evaporation through steam distillation to make it more concentrated until it turned into a viscous, greasy mass. With no further delay, the dried extract was immediately stored in a refrigerator under 4°C until it is taken up for phytochemical and biological analyses (Priya and Rajasekaran, 2024).

### Phytochemical analysis of ethanolic extract of *G. acerosa*

The presence of various classes of secondary metabolites from the ethanolic extract of *G. acerosa* was screened by qualitative phytochemical analysis. This analyses had been carried out adhering to the standard procedures listed in earlier literatures (Ahmed *et al.,* 2022; Narayanamurthy *et al.,* 2022; Palaniyappan *et al.,* 2023; Abu Ahmed *et al.,* 2021). The extract was then analytically screened for alkaloids, flavonoids, phenolics, tannins, terpenoids, glycosides, saponins, and steroids with the help of recent chemical essays in practice.

### FTIR spectral analysis of ethanolic extract of *G. acerosa*

FTIR spectroscopy was used to analyse the presence of functional groups in the ethanol extract of *G. acerosa.* Using an Agilent Cary 630 FTIR spectrometer equipped with a ZnSe ATR accessory, the FTIR spectra were recorded in the range of 4000-650 $cm^{-1}$. Each spectrum was obtained by taking an average of 32 scans with a resolution of 8 $cm^{-1}$ (Prabha *et al.,* 2019).

### GC-MS analysis of ethanolic extract of *G. acerosa*

GC-MS QP 2010 (Shimadzu) system equipped with a DB-30 capillary column (30 m × 0.25 mm i.d., 0.25 μm film thickness) was engaged for analyses purpose. Recording of mass spectra took place at 70 eV over an m/z range of 40-1000 with a scan interval of 0.5 sec. Helium (99.99% purity) was applied as the

carrier gas with a constant pour of 1.0 mL/min under electronic pressure control (Pandi Prabha & Rajkumar, 2015).

### DPPH assay of ethanolic extract of *G. acerosa*

The DPPH assay with different concentrations of the extract were prepared and each was mixed with the same volume of 0.15 mM DPPH solution (Sobuj *et al.,* 2024). The measurement of absorbance was done at 517 nm in UV-visible spectrophotometer. The radical exploration activity of the algal extract was compared with ascorbic acid as the positive control.

### Total antioxidant activity assay of ethanolic extract of *G. acerosa*

The antioxidant activity was determined using the phosphomolybdenum method. Ammonium molybdate (4 mM), sodium phosphate (28 mM), and sulfuric acid (0.6 M) were combined in a 1:1:1 ratio to create a reagent solution. The absorbance was noted at 695 nm against the blank after cooling the reaction tubes. Here, the ascorbic acid was used as the standard (Wizi *et al.,* 2021).

### Antimicrobial activity of ethanolic extract of *G. acerosa*

The bacterial strains namely the Gram-positive bacteria *Staphylococcus aureus* (ATCC 25923), *Bacillus subtilis* (ATCC 6051) Gram-negative bacteria *Pseudomonas aeruginosa* (ATCC 27853), *Escherichia coli* (ATCC 25922) and two fungal strains *Candida albicans* (ATCC 90028), *Aspergillus niger* (ATCC 16888), were employed to evaluate the antimicrobial potential of the algal extract. Antimicrobial susceptibility testing was performed on solid agar media using petri plates. Nutrient agar was utilized for bacterial cultures, whereas Yeast Extract Peptone Dextrose (YPD) agar was used to support the surface growth of fungal colonies. The agar well diffusion method was adopted to assess antimicrobial activity, and diameters of containment regions were measured to quantify the effect of the algal extract (Al-Enazi *et al.*, 2018)

### Anticancer activity of ethanolic extract of *G. acerosa*

The anticancer potential of *G. acerosa* extract was evaluated using the colorimetric MTT assay on MDA-MB-231 breast cancer cells. The cells were then subjected to seeding on 96-well plates at a density of $5 \times 10^4$ cells/well in a medium complemented with 10% FBS and incubated for 24 hr at 37°C in a 5% $CO_2$ atmosphere to allow partial monolayer formation. The medium was then replaced with 100 µL of various concentrations of the algal extract and incubated for an additional 24 hr. After treatment, the wells were washed, and 100 µL of MTT solution (0.5 mg/mL in PBS) was added to every well and incubated for 4 hr. The formazan crystals that were produced were subjected to solubility with 100 µL of DMSO, and a microplate reader was used for calculating the absorbance at 590 nm. The percentage of viable cells and $IC_{50}$ values was determined from dose-response curves (Omar *et al.,* 2018; Prabha *et al*., 2020).

### *In silico* analysis - Swiss ADME prediction of phytoconstituents identified from ethanolic extract of *G. acerosa*

Swiss ADME (Swiss Institute of Bioinformatics, http://www.swissadme.ch), an online tool employed for assessing the Absorption, Distribution, Metabolism and Excretion (ADME) characteristics of the compounds identified from the *G. acerosa* extract. For each compound, a single canonical SMILES string was entered as an individual line in the input field of the Swiss ADME web interface. The batch list of SMILES entries was then submitted, and the resulting ADME-related descriptors were retrieved for subsequent analysis and interpretation ( Hernandez *et al.,* 2023).

### Statistical analysis

The procedures were executed as per the relevant guidelines and regulations. All experiments were carried out in triplicate and were given as the Mean±Standard Deviation (SD). Analysis of Variance (ANOVA) was implemented for conducting statistical analysis of the phytochemical data using GraphPad Prism 10.3.0 software.

As this study did not include human participants or animal experiments, ethical approval was not required.

## RESULTS

### Phytochemical screening of ethanolic extract of *G. acerosa*

The qualitative phytochemical analysis of the ethanolic extract of *G. acerosa* showed the presence of several bioactive constituents, including tannins, saponins, steroids, alkaloids, anthraquinones, and phenolic compounds. Conversely, flavonoids and glycosides were not detected in the extract. The occurrence of these phytoconstituents suggests the potential pharmacological significance of *G. acerosa*, which may contribute to its observed biological activities.

### FTIR spectral analysis of ethanolic extract of *G. acerosa*

The FTIR spectrum of the ethanolic extract of *G. acerosa* given in Figure 1, shows a strong presence of hydroxyl groups could be observed at the broad peak near 3330 $cm^{-1}$, typical for polysaccharides. The aliphatic chains present in lipids, fatty acids, and carbohydrates appear around 2940 and 2830 $cm^{-1}$. The peak observed at 1740 $cm^{-1}$ indicates ester/carbonyl functionalities common in the acetylated polysaccharides or fatty acids. Amide and carboxylate vibrations specific to protein and uronic acids found in algal cell walls are present in the 1630-1400 $cm^{-1}$ region. A strong S = O band at 1235 $cm^{-1}$ suggests sulfated

polysaccharides that are a trademark of red algae like *G. acerosa* (Prabha *et al*., 2018).

## GC-MS study of ethanolic extract of *G. acerosa*

The GC-MS analysis of the ethanolic extract of *G. acerosa* displayed in Figure 2, revealed its chemical profile, identifying 30 major phytoconstituents eluting between 3.5 and 48.0 minutes in the Total Ion Chromatogram (TIC), indicating a chemically composite extract consisting of aliphatic compounds, phenolics, fatty acids, aldehydes, and bioactive derivatives. Identification of prominent compounds was carried out with the help of the NIST library by comparing their mass spectra. The major constituents (based on peak area %) represented in Table 1. Several minor ingredients including glycerin, acrylic acid derivatives, imidazolidinones, octadecanoic acid esters, and heterocyclic organic compounds were spotted at trace levels (0.5-1.5%). The extract was rich in fatty acids and esters reported to possess antioxidant, antimicrobial, and anti-inflammatory properties. Hydrocarbons such as tetracosane and dodecane indicated the presence of long-chain aliphatic compounds commonly reported in marine macroalgae.

## DPPH assay of ethanolic extract of *G. acerosa*

The antioxidant potential of the ethanol extract of *G. acerosa* was assessed against the DPPH radical neutralizing scavenging assay and compared with ascorbic acid. Both the extract and the standard exhibited a dose-based enhancement in radical neutralizing activity across the tested concentrations. The $IC_{50}$ value of ascorbic acid was calculated as 67.34 µg/mL, while the extract showed an $IC_{50}$ of 712.82 µg/mL. The extract confirmed notable free-radical-quenching ability at higher doses as shown in Figure 3, confirming its antioxidant potential. An antioxidant capacity of 0.094 mg AAE/g extract was attained by standardization against the ascorbic acid curve, confirming the major contribution of phenolic constituents from the phytochemical screening. Statistical analysis using one-way ANOVA on triplicate $IC_{50}$ values revealed a considerable variation between the extract and the standard ($p$<0.05). Results are portrayed as mean±SD ($n$=3).

## Total antioxidant activity assay of ethanolic extract of *G. acerosa*

The phosphomolybdenum technique was used for quantitatively assessing the TAC of the ethanolic extract of *G. acerosa*, benchmarked against ascorbic acid. Both the extract and ascorbic acid displayed a dose-dependent increase as displayed in Figure 4; the extract indicated a TAC of roughly about 20% at 200 µg /mL that gradually increased to about 70% at 1200 µg/mL. Increased extract concentration raised electron-donating capability, reflecting strong redox activity of *G. acerosa* bioactives. Two-way ANOVA established that the treatment, concentration, and their collaboration ominously influenced the antioxidant response ($p$<0.05). The extract possessed an antioxidant strength equivalent to 1.143 mg of AAE/g of extract by conducting tests based on the ascorbic acid calibration curve.

## Antimicrobial activity of ethanolic extract of *G. acerosa*

The algal extract was examined to assess its antimicrobial activity with respect to bacteria that included two strains of Gram-positive bacteria (*B. subtilis* and *S. aureus*), two strains of Gram-negativebacteria (*E. coli* and *P. aeruginosa*) and two strains of fungi (*C. albicans* and *A. niger)* with the help of well diffusion technique. The diameter of the containment area was deduced by the agar well diffusion assay, as recorded in Table 2. The ethanol extract showed comparable or even better inhibition in Gram-positive bacteria (e.g., *B. subtilis, S. aureus*)

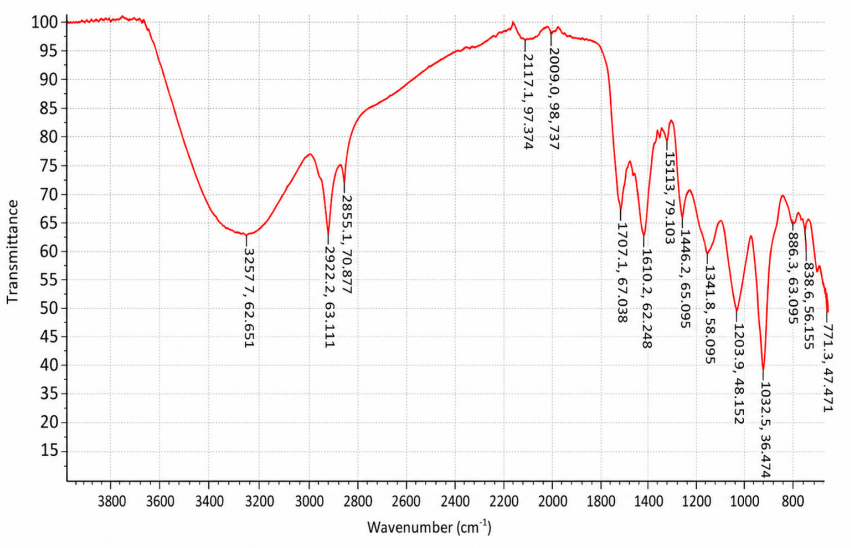



**Figure 1:** Functional group characterization of ethanolic extract of *G. acerosa* using FTIR spectroscopy.

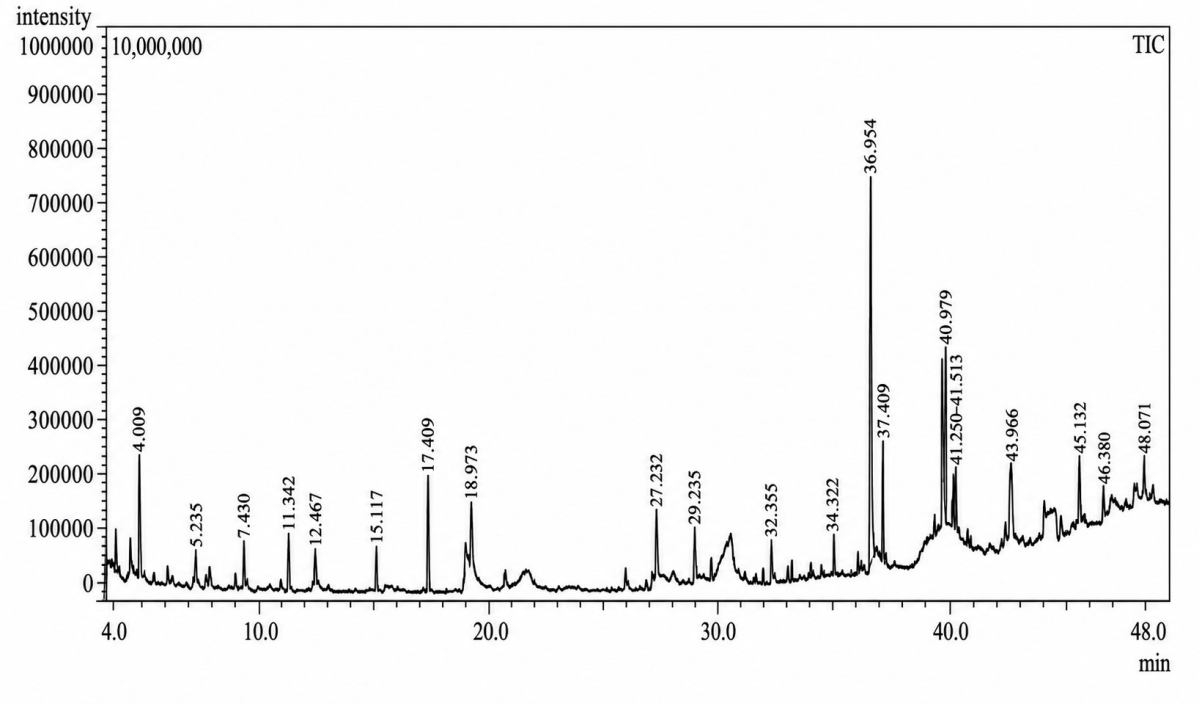



**Figure 2:** GC-MS chromatogram of ethanolic extract of *G. acerosa*.

and markedly higher inhibition zones in Gram-negative strains, which are generally more resistant due to their outer membrane. The ethanol extract of *G. acerosa* demonstrates broad-spectrum antimicrobial potential, including effective antifungal activity against both *C. albicans* and *A. niger*.

## Anticancer activity of ethanolic extract of *G. acerosa*

The outcome of cytotoxicity of ethanolic extract was examined with MDA-MB-231 breast cancer cell line. Increasing concentration levels (10-100 µg/mL) of the algae extract were used for this cytotoxicity assay. Changes in cell shape and structure like the loss of monolayer, rounding, and shrinkage was determined microscopically in Figure 5. A dense monolayer of useful cells was visible under the control group. The increase of concentration levels resulted in structural changes such as cell rounding, detachment, and death. Such changes highlighted the dosage-based cytotoxic outcomes witnessed through MTT assay. Normal, active cells were determined by comparing the percentage of living cells with that of the control group. A concentration-based reduction in viable cells was observed through the MTT assay on all compounds that were examined, as shown in Figure 6.

A concentration-based cytotoxic effect was exhibited by the algal extract on MDA-MB-231 breast cancer cells. A substantial level of reduction in viable cells was found from 10-100 µg/mL ($p<0.05$, one-way ANOVA). The $IC_{50}$ measure was observed to be 41.59 µg/mL, representing powerful anticancer activity. Viable cells got decreased from 100% (control) to 0.11% at 100 µg/mL. Data was recorded as a mean±SD ($n=3$).

## *In silico* analysis - Swiss ADME prediction of phytoconstituents identified from ethanolic extract of *G. acerosa*

Swiss ADME analysis was carried out for the major GC-MS constituents ranked according to their pharmacological relevance. The evaluated descriptors included physicochemical parameters, oral drug-likeness rules and pharmacokinetic properties such as HIA, BBB permeation, P-glycoprotein substrate status and cytochrome P450 inhibition profiles. The multidimensional oral drug-likeness profile of each compound was captured by the bioavailability radar diagrams shown in Figure 7. Balanced radar structure was provided for aromatic phenolics like eugenol and benzene-1, 2, 4-trimethoxy - 5- (1-propenyl)-(Z). with all physicochemical domains within the recommended ranges. 1, 2, 3-benzenetriol, 2-furancarboxaldehyde-5-(hydroxymethyl) and 2,3-dihydro-3,5-dihydroxy-6-methyl-4h-pyran-4-one that are categorized as oxygen-rich, lower-molecular-weight compounds exhibited radar sectors that was dominated by polarity and solubility. On the contrary, molecules bearing augmented aliphatic chains like n-hexadecanoic acid and ethyl oleate exhibited extended flexibility and lipophilicity domains, replicating their long hydrocarbon tails and dynamic conformational characteristics. The sterol stigmasta-5,24(28)-dien-3-ol, (3.beta.,24E) was characterized by high lipophilicity, greater molecular size and high carbon saturation, resembling a strong propensity for membrane association and residence.

Assessing the *in silico* physicochemical, pharmacokinetic and drug-likeness properties mentioned in Table 3, indicating a blend of rich diversity in their profile development. The

**Table 1: Phytoconstituents detected by GC-MS analysis of ethanolic extract of *G. acerosa*.**

| Peak | Retention Time | Area | Area % | Compound name |
|---|---|---|---|---|
| 1 | 3.537 | 1760758 | 1.19 | Octane-1-D,4-(methyl-D)- |
| 2 | 3.618 | 2671898 | 1.81 | Acrylic acid, 2-(methylenecyclopropyl)ethyl ester |
| 3 | 4.633 | 2357171 | 1.60 | Glycerin |
| 4 | 5.059 | 5561497 | 3.77 | TATP |
| 5 | 7.325 | 1679201 | 1.14 | 1,3,5-Triazine-2,4,6-triamine |
| 6 | 9.429 | 2486289 | 1.69 | 2,3-Dihydro-3,5-dihydroxy-6-methyl-4h-pyran-4-one |
| 7 | 11.342 | 2409935 | 1.64 | Dodecane |
| 8 | 12.467 | 1973288 | 1.34 | 2-Furancarboxaldehyde, 5-(hydroxymethyl)- |
| 9 | 15.117 | 2056895 | 1.40 | Phenol, 5-methyl-2-(1-methylethyl)- |
| 10 | 17.409 | 5262280 | 3.57 | Eugenol |
| 11 | 18.974 | 7078224 | 4.80 | 1,2,3-Benzenetriol |
| 12 | 19.339 | 2497139 | 1.69 | Tetradecane |
| 13 | 27.229 | 1354623 | 0.92 | Hexadecane |
| 14 | 27.659 | 3369986 | 2.29 | Benzene, 1,2,4-trimethoxy-5-(1-propenyl)-, (Z)- |
| 15 | 29.255 | 3566347 | 2.42 | Benzenepropanoic acid, 4-hydroxy-, methyl ester |
| 16 | 32.555 | 1990944 | 1.35 | Tetradecanoic acid |
| 17 | 35.322 | 1587041 | 1.08 | Acetamide,2-(diethylamino)-n-(2,6-dimethylphenyl)- |
| 18 | 36.954 | 26476532 | 17.96 | n-Hexadecanoic acid |
| 19 | 37.409 | 4389038 | 2.98 | Hexadecanoic acid, ethyl ester |
| 20 | 39.871 | 5990445 | 4.06 | 9,12-Octadecadienoic acid (Z,Z)- |
| 21 | 39.979 | 17191232 | 11.66 | 9-Octadecenoic acid, 1,2,3-propanetriyl ester, (E,E,E) |
| 22 | 40.239 | 2275811 | 1.54 | Ethyl (9Z,12Z)-9,12-Octadecadienoate |
| 23 | 40.345 | 5455959 | 3.70 | Ethyl Oleate |
| 24 | 42.490 | 5703358 | 3.87 | 1H-Imidazole, 4,5-dihydro-2-(phenylmethyl)- |
| 25 | 42.638 | 10953546 | 7.43 | Stigmasta-5,24(28)-dien-3-ol, (3.beta.,24E)- |
| 26 | 42.722 | 11908157 | 8.08 | Icosamethylcyclodecasiloxane |
| 27 | 42.997 | 1226226 | 0.83 | 2-Propenoic acid, 3-phenyl-, 2-methylpropyl ester |
| 28 | 45.352 | 3025797 | 2.05 | Hexadecanoic acid, 2-hydroxy-1-(hydroxymethyl)ethyl ester |
| 29 | 46.388 | 1486945 | 1.01 | Tetracosamethyl-cyclododecasiloxane |
| 30 | 48.071 | 1640064 | 1.11 | 1H-purin-6-amine, [(2-fluorophenyl)methyl]- |

eugenol, 1,2,3-benzenetriol, 1H-Imidazole, 4,5-dihydro-2-(phenylmethyl)- and the furan/pyran derivatives exhibited steady alignment with the main drug-likeness rules (Lipinski, Veber, Egan), thereby indicating a robust predisposition toward good oral exposure and systemic availability (Daina *et al.,* 2017; Padmanaban and Patil, 2025).

Larger hydrophobic molecules, including Stigmasta-5,24(28)-dien-3-ol, (3.beta.,24E)-, n-hexadecanoic acid and ethyl oleate, exceeded recommended ranges for LogP descriptors, reflecting intensified lipophilicity and lower aqueous solubility. No compound showed major PAINS concerns, with only a catechol-type alert for 1,2,3-benzenetriol and a few isolated alkene or aldehyde alerts flagged by the Brenk filter. Lead-likeness inspection indicated that the phenolic fragments occupy the "lighter" end of chemical space, whereas the lipidic and sterol molecules reside in a more lipophilic and flexible region; together with synthetic accessibility scores spanning from approximately 1 (simple phenolics) to >6 (complex sterol and lipid derivatives) (Azzam, 2023; Gokul *et al.,* 2025).

The BOILED-Egg analysis presented in Figure 8 showed that Eeugenol, Phenol,5-methyl-2-(1-methylethyl)- and benzene-1,2,4-trimethoxy-5-(1-propenyl)-(Z)-clustered within or close to the "white" region are consistent with physicochemical profiles that readily support passive intestinal permeation.

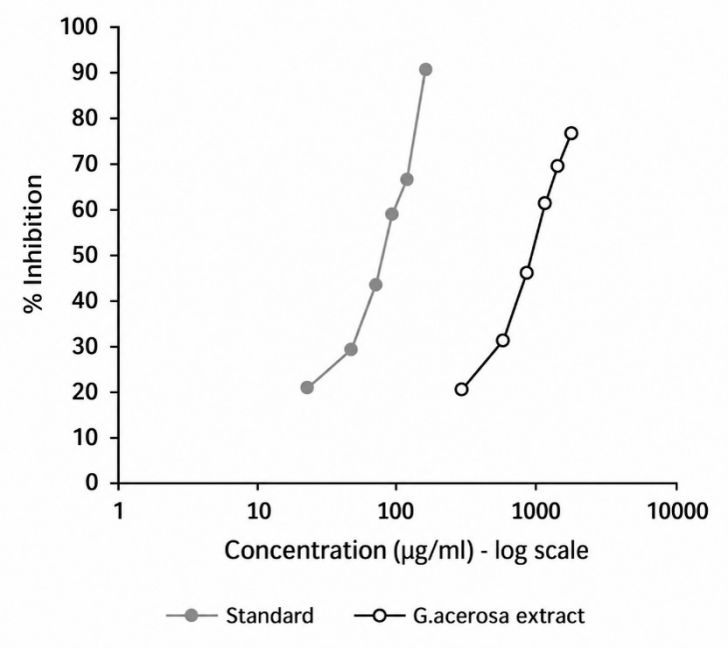



**Figure 3:** Scavenging activity of ascorbic acid and ethanolic extract of *G. acerosa* at different concentrations.

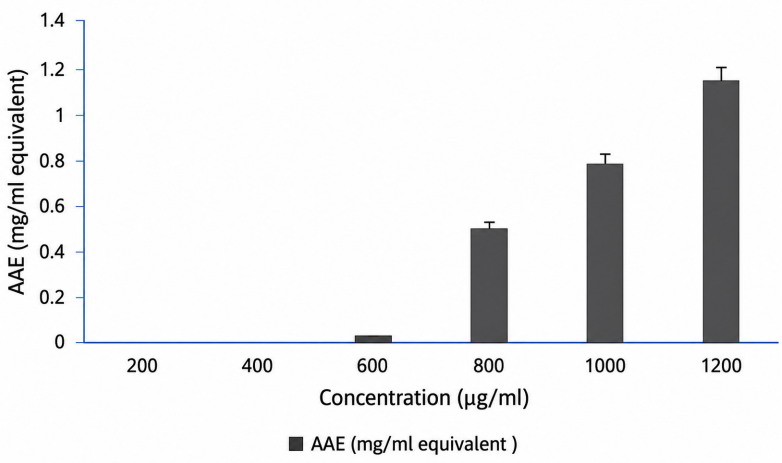



**Figure 4:** Total antioxidant capacity of ethanolic extract of *G. acerosa* expressed as AAE at different concentrations.

**Table 2: Diameters of zones of inhibition (mm) exhibited by ethanolic extract of** *G. acerosa.*

| | Strain Name | Zone of inhibition (mm) | | | | |
|---|---|---|---|---|---|---|
| | | Concentration of Control (µg/mL) | Concentration of *G. acerosa* algae extract (µg/mL) | | | |
| | | 100 | 25 | 50 | 75 | 100 |
| Bacterial strains | *E. coli* | 19±0.5 | 11±1.5 | 14±1.8 | 16±1.5 | 17±2.0 |
| | *P. aeruginosa* | 19±0.6 | 12±1.7 | 13±1.6 | 15±1.4 | 18±1.8 |
| | *S. aureus* | 20±0.5 | 13±1.8 | 14±1.3 | 15±1.4 | 18±1.1 |
| | *B. subtilis* | 18±0.5 | 12±1.2 | 13±1.6 | 14±1.2 | 19±1.4 |
| Fungal strains | *C. albicans* | 18±0.5 | 10±2.0 | 14±1.5 | 15±1.7 | 17±0.8 |
| | *A. niger* | 18±0.7 | 09±0.9 | 13±1.5 | 16±1.3 | 17±1.0 |

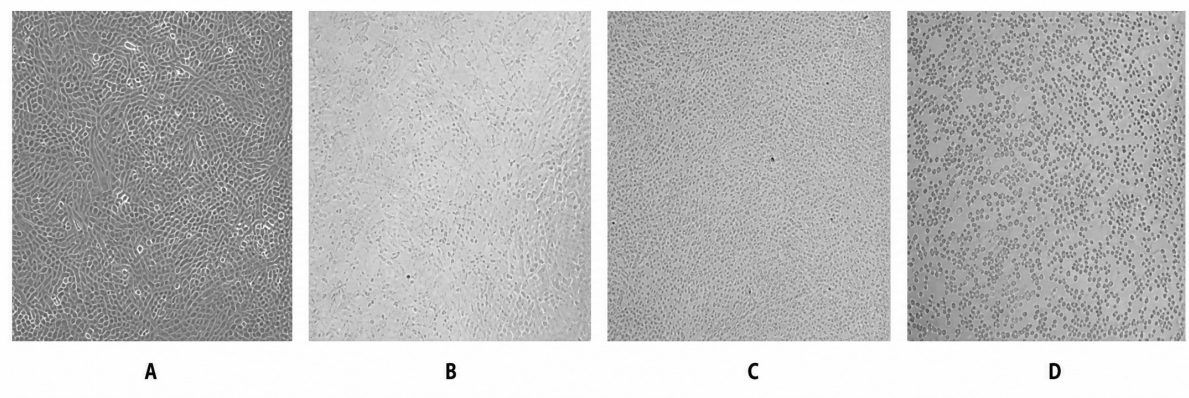



**Figure 5:** Cytotoxic effects of *G. acerosa* extract on MDA-MB-231 cells: (A) untreated control cells and (B-D) Morphological changes in cells treated with increasing concentrations of the *G. acerosa* extract (10, 50 and 100 µg/mL, respectively).

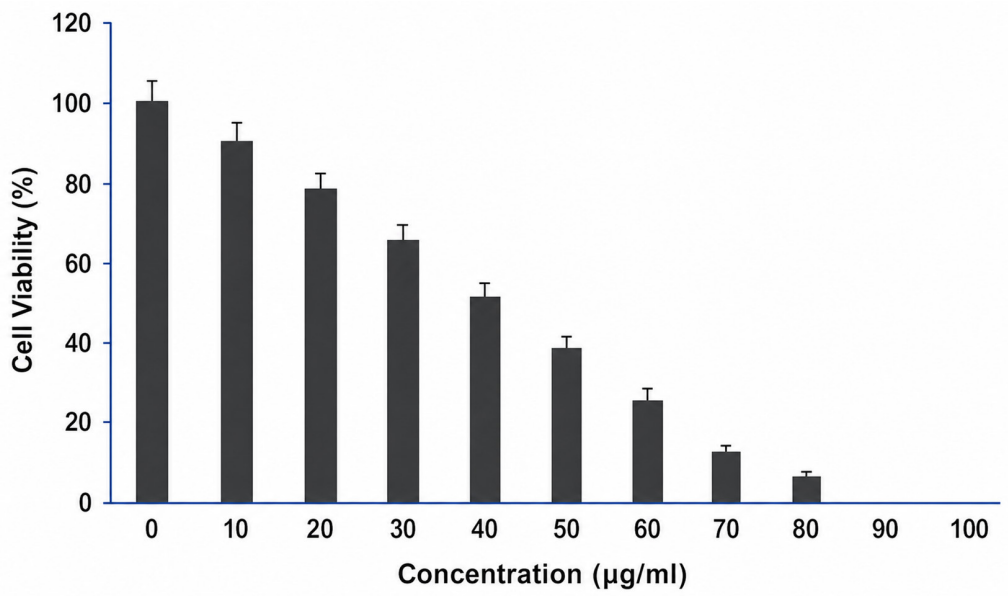



**Figure 6:** MTT assay graph displaying cell viability of MDA-MB-231 cancer cells at various concentrations of ethanolic extract of *G. acerosa*.

1,2,3-benzenetriol, 1H-imidazole-4,-dihydro-2-(phenylmethyl)-, 2-furancarboxaldehyde -5-(hydroxymethyl) and 2,3-dihydro-3,5-dihydroxy-6-methyl-4h-pyran-4-one molecules were positioned near the interface between white and yellow regions, suggesting a harmonious cooperation between aqueous solubility and membrane crossing. Stigmasta-5,24(28)-dien-3-ol, (3.beta.,24E)- and ethyl were positioned at higher WLOGP values, indicating their robust attraction towards lipid phases and their capability to relate with biological membranes primarily through hydrophobic partitioning (Kamble and Mitkar, 2023).

## DISCUSSION

The ethanolic extract in this study yields an enriched phytochemical spectrum tannin, saponins, steroids, alkaloids, anthraquinones, and phenolic compounds while flavonoids and glycosides remain undetected. This finding coincides with characterizing solvent-based differences in the extracted values and phytoconstituent mixture, highlighting the absence of certain bioactive classes in ethanol as compared to their presence in highly polarised or methanolic equivalents (Elsie and DhanaRajan, 2010). The methanolic extracts had high levels of glycosides and alkaloids, with reduced levels of tannins and phenolics (Waghmare, 2019). This finding substantiated ethanol's wide range of selectivity in elevating polar as well as partially polar metabolites.

The presence of pharmacognostic profile in *G. acerosa* ethanol extract is further substantiated through explicit functional group characterization by FTIR spectroscopy. Glycosidic and carbohydrate bands appear in the 1150-880 $cm^{-1}$ region, matching features reported for the extracts of ethyl acetate (Begum *et al.,* 2018). The prevalence of sulfated galactans is confirmed by the presence of sulfate and carbohydrate bands. The FTIR profile is very reliable with the extract consisting of an intricate combination of agar, sulfated galactans, residual lipids, and proteins typical for *G. acerosa*. The presence of fatty

acids, tannins, and phenolics that are distinctively accessible with ethanol is confirmed by the ester and alkyl bands. The minor level shifts in peak and intensity differences indicate subtle divisions in extract composition, mainly owing to polarity, justifying ethanol's reach in recording different forms of secondary metabolites.

Gas Chromatography-Mass Spectrometry (GC-MS) analysis of the ethanolic extract of *G. acerosa* identified 30 constituents eluting between 3.5 and 48.0 min, dominated by fatty acids and their esters, phenolic derivatives, aldehydes and long-chain hydrocarbons. In line with previous studies on related red algal species, the prominence of saturated/unsaturated fatty acids and phenolic compounds in the present profile supports the view that lipidic and phenolic metabolites are key contributors to the antioxidant, antimicrobial and anticancer potential of *G. acerosa* (Shantha *et al.,* 2024; Perumal *et al.,* 2022; Begum *et al.,* 2018). Overall, the GC-MS profiling demonstrates that the ethanolic extract of *G. acerosa* contains a blend of bioactive fatty acids, phenolics, aldehydes, alcohols, and hydrocarbon derivatives, which may contribute to its biological activities observed in subsequent antioxidant, antimicrobial, and anticancer assays.

Biochemical insights of ethanolic extract reveal that the strong DPPH scavenging activity resulting in a measure of 70% is due to the presence of phenolics, alkaloids, saponins, and tannins, coinciding with earlier findings (Devi *et al.,* 2008) and ~72% inhibition was noted with methanolic extracts (Waghmare, 2019). A higher DPPH inhibition (up to 98%) could be attained with benzene fractions, suggesting non-polar solvents getting access to distinct antioxidant terpenoids and carotenoids (Suganthy *et al.,* 2013). Maximum *in vitro* antioxidant ability was found in methanolic extracts (68.42%), that remains closer to ascorbic acid (Shanmugam, 2018). Such results jointly indicate the presence of concentration-dependent antioxidant in *G. acerosa*, substantiating its significance as a source of bioactive compounds.

The combined antioxidant potential is evaluated using the TAC assay in which the ability to reduce several reactive oxygen species is measured. The TAC result of close to 70% at 1200 µg/mL in the ethanolic extract is closer to the values recorded, that quantifies a TAC measure of 76.02% and 86.88% for ethanol and methanol (Mole and Sabale, 2013), supporting the contribution of phenolics and other associated compounds in the red algal matrix. This equivalency signifies that at higher concentrations, the *G. acerosa* ethanolic extract achieves considerable total antioxidant capacity comparable to that of ascorbic acid, thus affirming its efficacy as a natural source of electron-donating and free radical-neutralizing agents.

The antimicrobial efficacy displayed by the ethanolic extract against the microorganisms, can be mechanistically elucidated by the bioactive phytochemicals present. Antimicrobial effect is exerted by phenolics through hydrogen bonding that disrupts its microbial membrane potential and intracellular pH (Oulahal and

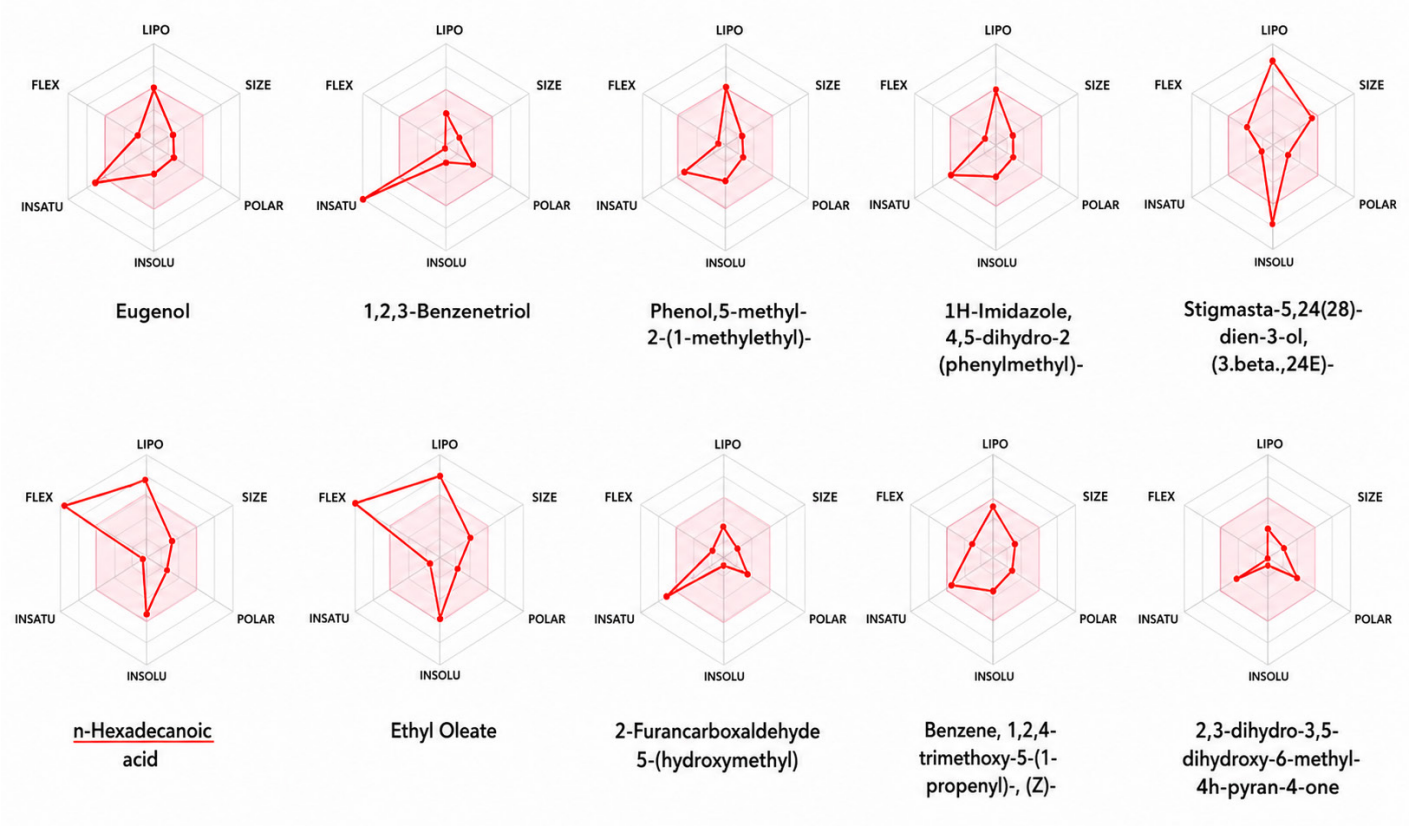



**Figure 7:** Bioavailability radar illustrating the optimal drug-likeness space of the molecules.

**Table 3: ADME-based pharmacokinetic and drug-likeness evaluation of bioactive phytoconstituents identified from ethanolic extract of *Gelidiella acerosa*.**

| Sl. No. | Compound | Molecular weight (g/mol) | Log $P_{o/w}$ | TPSA (Å $^2$) | GI absorption | BBB permeant | Lipinski | Bio Availability score | PAINS |
|---|---|---|---|---|---|---|---|---|---|
| 1. | Eugenol | 164.20 | 2.25 | 29.46 | High | Yes | Yes; 0 violation | 0.55 | 0 |
| 2. | 1,2,3-Benzenetriol | 126.11 | 0.58 | 60.69 | High | Yes | Yes; 0 violation | 0.55 | 1 alert: catechol_A |
| 3. | Phenol, 5-methyl-2-(1-methylethyl)- | 150.22 | 2.80 | 20.23 | High | Yes | Yes; 0 violation | 0.55 | 0 |
| 4. | 1H-Imidazole, 4,5-dihydro-2-(phenylmethyl)- | 160.22 | 1.97 | 24.39 | High | No | Yes; 0 violation | 0.55 | 0 |
| 5. | Stigmasta-5,24(28)-dien-3-ol, (3.beta.,24E)- | 412.69 | 7.05 | 20.23 | Low | No | Yes; 1 violation: MLOGP>4.15 | 0.55 | 0 |
| 6. | n-Hexadecanoic acid | 256.42 | 5.20 | 37.30 | High | Yes | Yes; 1 violation: MLOGP>4.15 | 0.85 | 0 |
| 7. | Ethyl Oleate | 310.51 | 6.18 | 26.30 | Low | No | Yes; 1 violation: MLOGP>4.15 | 0.55 | 0 |
| 8. | 2-Furancarboxaldehyde, 5-(hydroxymethyl)- | 126.11 | 0.19 | 50.44 | High | No | Yes; 0 violation | 0.55 | 0 |
| 9. | Benzene, 1,2,4-trimethoxy-5-(1-propenyl)-, (Z)- | 208.25 | 2.69 | 27.69 | High | Yes | Yes; 0 violation | 0.55 | 0 |
| 10. | 2,3-dihydro-3,5-dihydroxy-6-methyl-4h-pyran-4-one | 144.13 | -0.22 | 66.76 | High | No | Yes; 0 violation | 0.85 | 0 |

Footnote: TPSA: Topological Polar Surface Area; GI: Gastrointestinal; BBB: Blood-Brain Barrier; PAINS: Pan-Assay Interference Compounds; Log $P_{o/w}$: Logarithm of the Octanol/Water Partition Coefficient; MLOGP: Moriguchi Octanol-Water Partition Coefficient.

Degraeve, 2022). This supports the important inhibition regions that were observed in the study, coinciding with moderate-to-strong antimicrobial effects (Aassaithambi *et al.,* 2025; Elsie and DhanaRajan, 2010). The increased activity with respect to the Gram-negative bacteria demonstrates the effective penetration and impedance of complex double-membrane structures, highlighting the prominence of polar compound profiles of the ethanolic extract.

The cytotoxic prospective of the ethanolic extract with respect to MDA-MB-231 breast cancer cells ($IC_{50}$=41.59 µg/mL) could be attributed to the distinct antiproliferative action, that is executed through various phytochemical-dependent techniques. This contributes to increased potency compared to earlier documented ethyl acetate extract $IC_{50}$=1.5 mg/mL in A549 lung cancer cells (Begum *et al.,* 2018), methanolic extract $IC_{50}$=104.43 µg/mL in HL-60 leukemia cells (Lakmal *et al.,* 2014) and wider orientation of apoptosis/necrosis across cell lines in several experiments(Murugan and Iyer, 2013). A maximal cytotoxicity of 72.37% at 300 µg/mL in A431 human skin cancer cells, with a 50% inhibition threshold at 150 µg/mL (60% inhibition) and a calculated $IC_{50}$ of 79.09 µg/mL, is realised by the methanol extract of *G. acerosa*, which indicates the significant efficiency at normal concentrations. The percentage level increase of cytotoxicity from 17.89% at 33.26 µg/mL to 72.37% at 300 µg/mL, substantiates concentration-based cytotoxicity and increased potency in association to various established extracts ( Shantha *et al.,* 2024). Selective toxicity towards cancer cells is recorded as there is no traces of cytotoxicity is observed when normal PBMCs are treated with non-polar fractions (Suganthy *et al.,* 2013). The toxicological findings substantiate biological observations; continuous oral administration produces no visible behavioural or organotoxicity in rodent models (Nisha and Devi, 2017), thereby re-affirming the safety profile of such extracts for additional preclinical examination.

*In silico* ADME parameters and drug- likeness analysis of selected GC-MS identified constituents was evaluated using the webtool Swiss ADME. The smaller components like eugenol and aromatics analogs of phenolic structure demonstrated consistent succession with the primary rules of drug-likeness (Lipinski, Veber, Egan) and showed strong tendency towards good oral delivery and systematic access. Their low molecular weight, moderate molar refractivity and low atomic number made these structures highly appealing starting points to rational derivatization as opposed to fully optimized leads. On the other hand, larger hydrophobic compounds such as Stigmasta-5,24(28)-dien-3-ol, (3.beta.,24E)-, n-hexadecanoic acid and ethyl oleate surpassed the suggested LogP values exhibiting increased lipophilic nature and decreased aqueous solubility. The phenolic and aromatic scaffolds provide

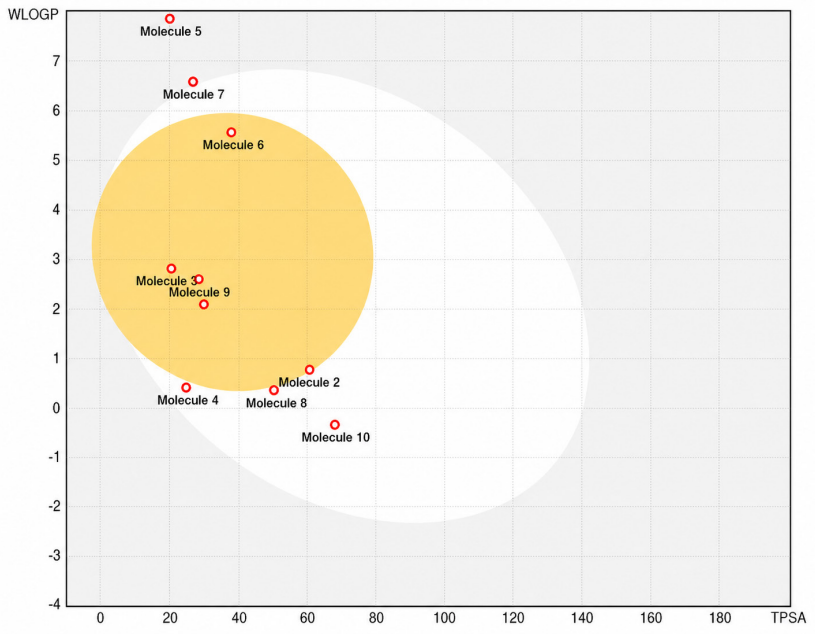



**Figure 8:** Schematic illustration of the BOILED-Egg model depicting predicted passive Human Intestinal Absorption (HIA) and Blood-Brain Barrier (BBB) penetration of the molecules in WLOGP versus TPSA space.

particularly attractive chemotypes for further optimization, while the more voluminous lipidic constituents offer complementary opportunities as membrane-active or carrier-like entities (Saczewski *et al.,* 2024).

## CONCLUSION

The proposed study substantiates *G. acerosa* as a multidimensional marine biomaterial with remarkable pharmacological potential. In summary, this research adds new comparative depth to the growing body of literature demonstrating that the efficacy of *G. acerosa* is tightly linked to solvent choice, phytochemical recovery, and the multi-mechanistic modes of action of its key secondary metabolites. When viewed alongside the referenced studies, the present work underscores ethanol's ability to extract a pharmacologically privileged range of polyphenolic, steroidal, and alkaloidal agents, providing strong justification for fractionation-guided, Structure-Activity Relationship (SAR) studies, and *in vivo* translational research. Future research should focus on separating the lead compounds, clarification of anticancer signalling pathways, and calculation of pharmacokinetics and pharmacodynamics, corresponding to *in vivo* validation for future therapeutic development. The biomedical powers of *G. acerosa* extract can be further enhanced through combination therapies and nanotechnology-based delivery systems. To summarize, *G. acerosa* is a proven, valuable marine resource with strong antioxidant, antimicrobial, anticancer, and emerging neuroprotective bioactivities. Integrated phytochemical and pharmacological research will be crucial for completely unlocking the potential of *G. acerosa* in viable therapeutics, to catapult it as a candidate for developing innovative drugs.

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## ABBREVIATIONS

**AAE:** Ascorbic Acid Equivalent; **AChE:** Acetylcholinesterase; **ADME:** Absorption, Distribution, Metabolism and Excretion; **ANOVA:** Analysis of Variance; **ATR:** Attenuated Total Reflectance; **BBB:** Blood-Brain Barrier; **BuChE:** Butyrylcholinesterase; **DAL:** Dalton's Ascitic Lymphoma; **DMSO:** Dimethyl Sulfoxide; **DPPH:** Diphenyl Picryl Hydrazyl; **FBS:** Fetal Bovine Serum; **FTIR:** Fourier-Transform Infrared Spectroscopy; **GC-MS:** Gas chromatography-Mass Spectrometry; **HIA:** Human Intestinal Absorption; **$IC_{50}$:** Half-Maximal Inhibitory Concentration; **LC-MS:** Liquid Chromatography-Mass Spectrometry; **Log $P_{o/w}$:** Logarithm of the Octanol/Water Partition Coefficient; **MTT:** 3-(4,5-Dimethylthiazol-2-yl)-2,5-diphenyltetrazolium bromide; **NIST:** National Institute of Standards and Technology; **PAINS:** Pan-Assay Interference Compounds; **PBMC:** Peripheral Blood Mononuclear Cell;, **PBS:** Phosphate Buffered Saline; **SAR:** Structure-Activity Relationship; **SD:** Standard Deviation; **SMILES:** Simplified Molecular Input Line Entry System; **TAC:** Total Antioxidant Capacity; **TIC:** Total Ion Chromatogram; **TPSA:** Topological Polar Surface Area; **WLOGP:** Wildman-Crippen LogP; **YPD:** Yeast Extract Peptone Dextrose.

## CONFLICT OF INTEREST

The authors declare that there is no conflict of interest.

## AUTHORS CONTRIBUTION

**PP:** Conceptualization, Data curation, Formal analysis, Visualization, Validation, Supervision, Software, Resources, Project administration, Investigation. **PM:** Writing - review & editing, Methodology.

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