Phytochemical Profiling and Biological Assessment of Allium cepa L. Peel Extract Using Combined In-Vitro and In-Silico Approaches

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ABSTRACT

Agro-industrial residues are increasingly being explored as sustainable sources of biologically active compounds. Red onion (Allium cepa L.) peels, commonly discarded during processing, are known to contain substantial amounts of flavonoids and phenolic constituents. The present study investigated the phytochemical profile and biological activities of an ethanolic extract prepared from red onion peels using experimental and computational approaches. Total phenolic and flavonoid contents were quantified, and antioxidant capacity was assessed through in-vitro assays. Anti-inflammatory activity was evaluated using the bovine serum albumin denaturation method, while antibacterial efficacy was determined by the disk diffusion technique. Insecticidal potential was tested against Sitophilus oryzae, and cytotoxicity was examined in the MDA-MB-231 breast cancer cell line using the MTT assay. Structural characterization was performed using SEM and FTIR analyses. Molecular docking was conducted to examine interactions between selected phytoconstituents and protein targets relevant to antimicrobial, anti-inflammatory, and anticancer activities. The extract exhibited notable antioxidant and anti-inflammatory effects, significant antibacterial activity against Escherichia coli, dose-dependent insecticidal action, and moderate cytotoxicity with an IC_{50} value of approximately 180 µg/ml. Docking results supported stable ligand–protein interactions, indicating promising pharmaceutical and agricultural applications of onion peel-derived bioactives.

Keywords: Red onion peel, phytochemicals, antioxidant activity, anti-inflammatory activity, antibacterial activity, insecticidal activity, molecular docking.

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1. Introduction

Interest in plant-based bioactive compounds has grown steadily, particularly in relation to agricultural residues that are routinely discarded. The dry outer layers of red onion (*Allium cepa L.*) are one such material, often treated as waste despite their rich phytochemical composition.[1] Studies indicate that these peels contain higher concentrations of flavonoids, phenolic acids, and sulfur-containing constituents than the edible portion of the bulb.[2] Compounds such as quercetin derivatives and anthocyanins are associated with antioxidant activity, modulation of inflammatory responses, and inhibition of microbial growth. Given the increasing prevalence of oxidative stress–related disorders, antimicrobial resistance, and cancer, identifying natural substances capable of influencing multiple biological pathways is of considerable importance.[3] Utilizing onion peel as a source of functional extracts not only adds value to agro-waste but also supports sustainable resource management and circular bioeconomy principles. The present investigation evaluates the phytochemical characteristics and biological activities of an ethanolic extract of red onion peel.[4] Antioxidant, anti-inflammatory, antibacterial, insecticidal, and anticancer properties were examined through in-vitro assays, while molecular

docking was employed to explore potential ligand–protein interactions. This integrated approach provides insight into the therapeutic and agricultural relevance of this underutilized natural resource.[5]

2. Materials and Methods

2.1 Collection and Authentication of Plant Material

Red onion (Allium cepa L.) outer peels were obtained from markets in North Goa, India. Only intact and disease-free peels were chosen for the study.

2.2 Preparation of Peel Extract

The peels were washed to eliminate surface impurities and air-dried under shade at room temperature for about two months. After drying, the material was ground into a coarse powder. Nearly 800 g of the powder was extracted with ethanol by maceration in a closed flask and kept overnight in the dark. The mixture was filtered, the solvent removed by distillation, and the concentrated extract was stored in airtight containers until analysis.[6,7]

2.3 In-Vitro Antioxidant Assays

2.3.1 Determination of Total Phenolic Content (TPC)

Total phenolic content was determined using the Folin–Ciocalteu assay. Different volumes of the extract (0.5–2.0 ml) were reacted with Folin reagent and diluted with distilled water, followed by addition of 2% sodium carbonate after 10 minutes. The mixture was kept at room temperature for 45 minutes, and absorbance was measured at 760 nm using a UV–Visible spectrophotometer. Phenolic concentration was calculated from the recorded absorbance values.[8,9]

2.3.2 Determination of Total Flavonoid Content (TFC)

Total flavonoid content was estimated by the aluminium chloride method. Varying volumes of extract (0.5–2.0 ml) were mixed with distilled water and 10% aluminium chloride solution, and the volume was made up with methanol. After incubation, absorbance was recorded at 410 nm using a UV–Visible spectrophotometer to determine flavonoid levels.[10]

2.3.3 Ferric Reducing Antioxidant Power (FRAP)

Reducing activity was assessed by observing the conversion of Fe^{3+} to Fe^{2+} in the presence of the extract. The reaction mixture containing ferric solution, hydrogen peroxide, and plant extract was adjusted to alkaline pH (9–10). A color shift from reddish-orange to green indicated ferric ion reduction and confirmed antioxidant activity.[11,12]

2.3.4 Hydrogen Peroxide Scavenging Activity

Hydrogen peroxide scavenging activity was measured spectrophotometrically. The extract (1 ml) was combined with phosphate buffer (pH 7.4) and hydrogen peroxide, with ascorbic acid used as a standard reference. After incubation, absorbance was recorded at 230 nm, and the percentage inhibition was calculated accordingly.[13]

$$\text{Antioxidant activity (\%)} = \frac{\text{Absorbance of control} - \text{Absorbance of sample}}{\text{Absorbance of control}} \times 100$$

2.4 Insecticidal Activity

Insecticidal activity of the ethanolic extract was tested against Sitophilus oryzae. Concentrations between 0.01% and 0.2% were prepared in acetone and applied in petri dishes containing five insects each. Mortality was noted after 6, 24, and 36 hours. DDT was used as the reference standard, while acetone served as control, and percentage mortality was calculated accordingly.[14,15]

2.5 Antibacterial Activity

Antibacterial activity was determined by the disk diffusion technique. GC agar plates were inoculated with bacterial suspensions adjusted to the 0.5 McFarland standard. Disks impregnated with the extract were placed on the agar surface and incubated at 35°C. After incubation, the diameter of inhibition zones (in mm) was measured to evaluate antibacterial effectiveness.[16,17]

2.6 Anti-Inflammatory Activity

Anti-inflammatory activity was evaluated using the BSA protein denaturation assay. Different concentrations of the extract (0.02–0.2%) were mixed with BSA and phosphate buffer (pH 6.8), with ibuprofen as the reference. The mixtures were heated at 72°C for 20 minutes, cooled, and absorbance was measured at 660 nm. Percentage inhibition of protein denaturation was calculated to determine activity.[18,19]

2.7 Anticancer Activity (MTT Assay)

Cytotoxic activity was assessed on MDA-MB-231 breast cancer cells using the MTT assay. Cells were seeded in 96-well plates and exposed to extract concentrations ranging from 50 to 250 µg/ml for 24 hours. After treatment, MTT solution was added to allow formazan formation, which was subsequently

dissolved in DMSO. Absorbance was recorded at 570 nm (reference 630 nm), and cell viability along with IC_{50} values was determined from the dose–response data.[20,21]

2.8 Morphological and Functional Group Characterization

2.8.1 Scanning Electron Microscopy (SEM)

The surface morphology and particle size distribution of the extract were examined using SEM analysis.[22]

2.8.2 Fourier Transform Infrared Spectroscopy (FTIR)

FTIR analysis was carried out to identify functional groups present in the extract by recording absorption spectra in the mid-infrared region.[23]

2.9 Molecular Docking Studies

Computational docking studies were performed to evaluate interactions between selected phytochemicals (including allyl propyl disulfide, myricetin, thiosulfinic acid esters, cholesterol, and S-methyl-L-cysteine sulfoxide) and target proteins associated with antibacterial, anti-inflammatory, and anticancer pathways. Protein structures were obtained from the Protein Data Bank (PDB). Binding affinities and interaction profiles were analyzed based on calculated energy values.[24,25]

3. Results

Volume in ml	Absorbance at 760nm
0.5	0.55
1	1.2
1.5	1.8
2.5	2.4

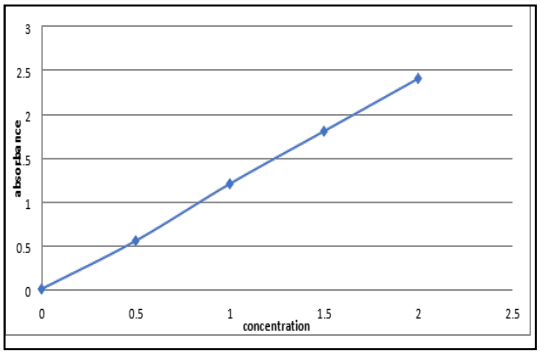
Table 2 : Total Flavonoid Content Absorbance

Concentration in ml	Absorbance at 410nm
0.5	0.59
1	1.289
1.5	2.286
2	3.389

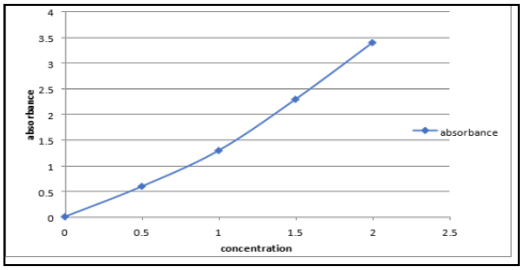
Table 1: Total Phenolic Content Absorbance

3.1 Total Phenolic Content (TPC)

The ethanolic extract of red onion peel showed a progressive increase in absorbance at 760 nm with increasing concentration (0.5–2.0 ml). Higher extract volumes exhibited higher phenolic content, indicating a concentration-dependent response.



Graph 2: of Concentration v/s Absorbance



Graph 1: of Concentration v/s Absorbance

3.2 Total Flavonoid Content (TFC)

Flavonoid estimation at 410 nm demonstrated measurable flavonoid presence in the extract. Absorbance values increased proportionally with concentration, confirming higher flavonoid content at elevated extract volumes.

3.3 Ferric Reducing Antioxidant Power (FRAP)

The extract showed ferric ion reducing activity, evidenced by a visible color change from reddish-orange to green. The intensity of reduction increased with concentration, indicating enhanced reducing power at higher extract levels.

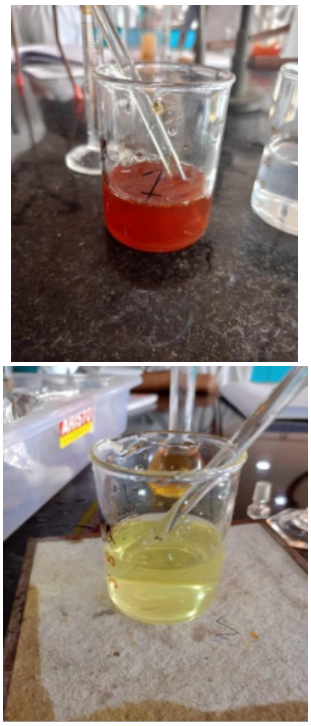


Fig.1: (A)Reddish color of Fe^{3+} (B) change in color of Fe^{3+} to green Fe^{2+}

3.4 Hydrogen Peroxide Scavenging Activity

The extract exhibited hydrogen peroxide scavenging activity, with percentage inhibition increasing as concentration increased.

Absorbance of control	Absorbance of sample
0.470nm	0.416nm

Table.3: Hydrogen peroxide scavenging Absorbance

Hydrogen peroxide scavenging test involves demonstrating a significant decrease in hydrogen peroxide concentration in the presence of the test substance, so % was found to be 11.489% ..

3.5 Insecticidal Activity

The ethanolic extract demonstrated dose- and time-dependent mortality against Sitophilus oryzae. Higher concentrations (0.1–0.2%) resulted in increased insect mortality within 24–36 hours compared to lower concentrations.

Table no. 4: Insecticidal % mortality results

Sr No.	Conc. In %	No. Of insects added	No. Of insects dead			Total no. of insects dead(avg)	% of mortality
			<6hrs	36hrs	48hrs		
1	0.2	5	5	-	5	1	100
2	0.16	5	4	1	4	1	100
3	0.12	5	0	1	3	1	100
4	0.08	5	0	0	2	0.6	60
5	0.04	5	0	0	2	0.4	40
6	0.02	5	0	0	2	0.4	40
7	0.01	5	0	0	2	0.4	40
8	Control	5	0	0	0	0	0
9	Standard	5	0	2	3	0.6	60

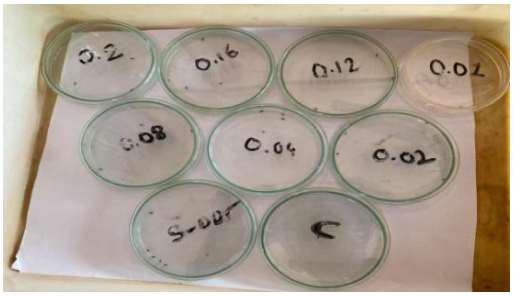


Fig.2: Dead Rice weevil

The ethanolic extract demonstrated strong insecticidal action against Sitophilus oryzae, showing a clear dose-related response. Complete mortality was observed at 0.12–0.2% concentrations, while lower doses (0.02–0.08%) produced higher mortality than the acetone control. At the highest concentration, the effect exceeded that of 0.2% DDT used as the standard.

3.6 Antibacterial Activity

Disk diffusion analysis revealed clear zones of inhibition around extract-impregnated discs. The diameter of inhibition zones increased with concentration, confirming antibacterial activity.

Samples	Zone of incubation (E.coli)
1	15 mm
2	24mm

Table no. 5: Anti-Bacterial activity readings

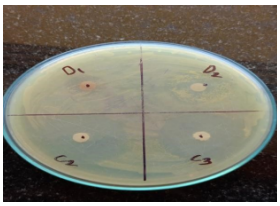


Fig.3: Growth of E.coli

Antibacterial activity of the red onion peel extract was tested against E. coli using the disk diffusion assay. The findings (Table 5) showed that E. coli was highly susceptible to the extract, exhibiting the most pronounced inhibitory response.

3.7 Anti-Inflammatory Activity

The extract inhibited protein denaturation in a concentration-dependent manner. Higher concentrations showed greater percentage inhibition, approaching the effect of the standard drug.

Concentration(%)	Absorbance(mm)	% Inhibition
0.2	0.046	94.13%
0.16	0.087	88.90%
0.08	0.250	68.11%
0.04	0.316	59.69%
0.02	0.338	56.88%
Control	0	100%
Standard	0.784	-

Table no.6: Anti-inflammatory Absorbance

Anti-inflammatory activity of the red onion peel extract was recorded in Table 6. A gradual rise in absorbance was observed with decreasing concentration, indicating measurable anti-inflammatory potential of the extract.

3.8 Anticancer Activity (MTT Assay)

The extract reduced viability of MDA-MB-231 breast cancer cells in a dose-dependent manner. Higher concentrations (200–250 µg/ml) showed greater cytotoxic effects compared to lower concentrations. The IC_{50} value was determined from the dose–response curve. The IC50 values of the test compounds for MDAMB-231 cell-line for 24 hour treatment were found to be:

Sample name	MDAMB-231 cell line IC50 (in µg/ml) 24hr
Red onion peel extract	180.77

Table no.7: Anticancer Activity (MTT Assay)

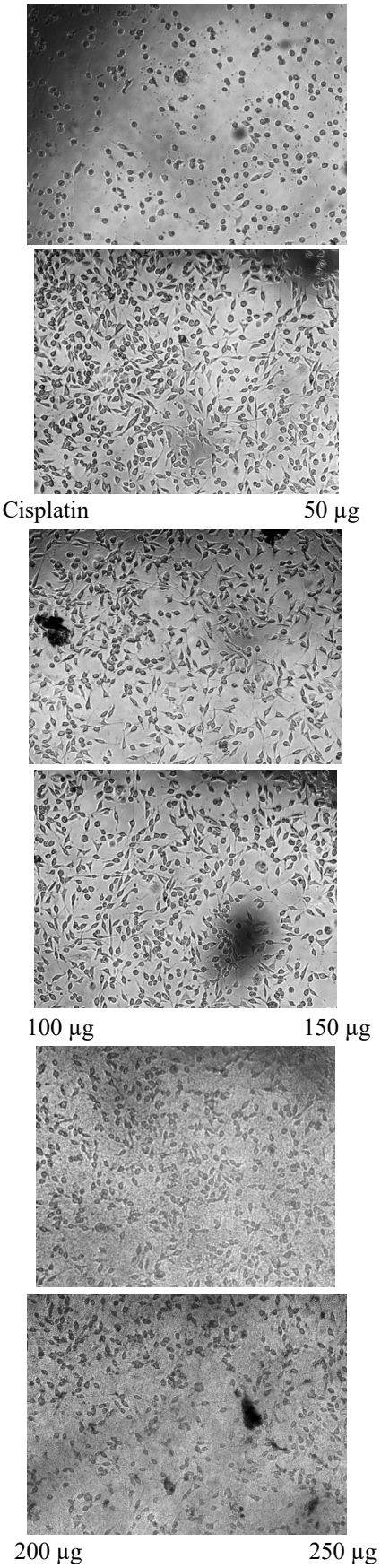
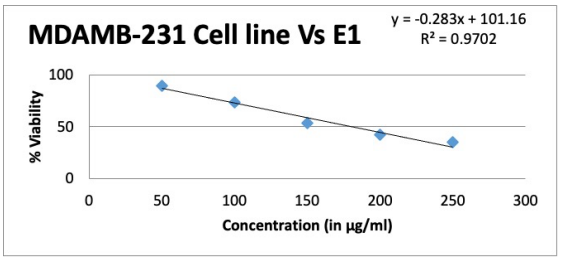


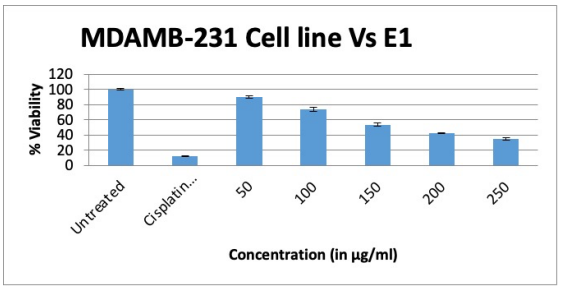
Fig 4: Anti-cancer results(in µg/ml)

				Test concentrations (in µg/ml)				
	Blank	Untreated	Cisplatin 15 µg/ml	50	100	150	200	250
Readings	0.027	0.467	0.0 81	0.433	0.366	0.272	0.215	0.172
% Viability		100	12.24	89.6	73.8	53.2	42.2	34.8

Table no.8: MDAMB-231 Cell line Vs onion peel extract



Graph.3: Concentration v/s % viability



Graph. 4: Concentration v/s % viability

The IC50 value of the test for MDAMB-231 Cell line for the Red onion peels extract was found to be 180 µg/ml. Treatment with red onion peels extract led to significant dose-dependent decrease in MDAMB-231 Cell viability. Higher concentration of extract exhibited greater inhibition of cell proliferation compared to lower concentrations, including a potential anti-cancer effect. The observed reduction in MDAMB-231 Cell viability following treatment treatment with red onion peels extract suggests its potential as an anticancer agent.

3.9 SEM Analysis

SEM imaging revealed irregular surface morphology and heterogeneous particle distribution of the extract.

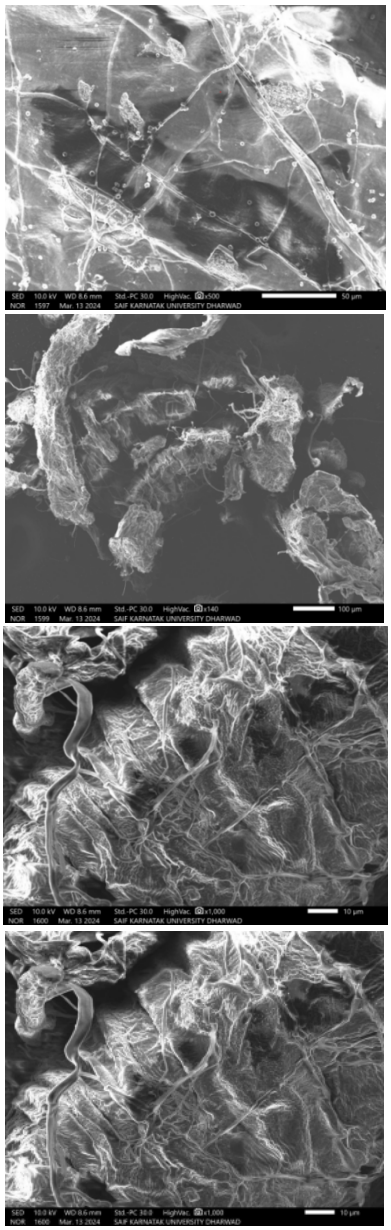


Figure.5: SEM images of red onion peels extract

The size and structure of red onion peels extract were analysed by SEM. The SEM images presented above, demonstrated that their diameters ranges from 10 µm to 100 µm

3.10 FTIR Analysis

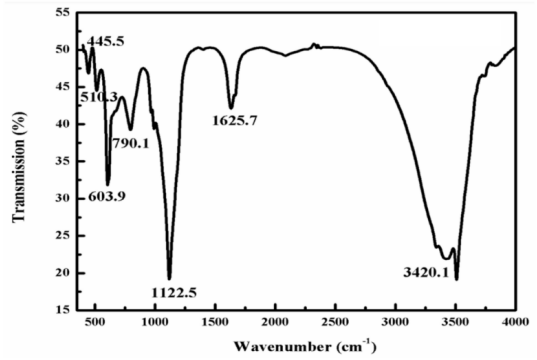


Figure.6: FTIR Red onion peels

FTIR of red onion peel waste. The peaks at 510.3, 603.9 and 790.1 cm−1 are attributed to the Zn-O bond weak and strong stretching and indicate the formation of the particles. The band at 1122.5 cm−1 is due to the presence of an amide group in the nanoparticles from the peel, while a sharp and deep band at 1625.7 cm−1 is due to the C = O stretching and due to the presence of a water molecule (−OH) in the nanoparticle. A small peak near 2500 cm−1 is attributed to the adsorption of atmospheric carbon dioxide on the sample. A broadband at 3420.1 cm−1 indicates the presence of hydroxyl molecules.

3.11 Molecular Docking

Docking studies showed favorable binding interactions between selected phytochemicals and target proteins, with low binding energy values indicating stable ligand–protein interactions.

3.11.1 Molecular docking on Anti-cancer

Sr no.	Protein used (PDB)	ligands	E-total	Figure no.
1	2kce-anticancer	2-Oxetanone,4,4dimethyl	-123.56	1
2	2kce-anticancer	Allyl propyl disulfide	-125.01	2
3	2kce-anticancer	Myricetin	-166.00	3
4	2kce-anticancer	Thiosulfinic acid esters	-173.68	4
5	2kce-anticancer	Cholesterol	-327.75	5
6	2kce-anticancer	S-Methyl-Lcysteine sulfoxide	-263.31	6
7	2kce-anticancer	Propanethial S-oxide	-154.90	7
8	2kce-anticancer	Ferulic acid	-117.12	8

Table no. 9: Results of Anticancer Docking studies

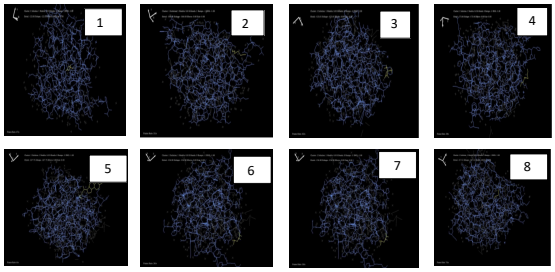


Figure.7: Anticancer Docking studies

The interaction of protein 3T88 with the phytochemicals(Allyl propyl disulfide,Myricetin,Thiosulfinic acid esters, Cholesterol,S-Methyl-Lcysteine sulfoxide. Propanethial S-oxide) gave binding affinity

3.11.2 Molecular docking on Anti-inflammatory

Sr no.	Protein used (PDB)	ligands	E-total	Figure no.
1	3T88	2-Oxetanone,4,4dimethyl	-156.38	1
2	3T88	Allyl propyl disulfide	-154.34	2
3	3T88	Myricetin	-210.98	3

4	3T88	Thiosulfinic acid esters	-135.65	4
5	3T88	Cholesterol	-143.02	5
6	3T88	S-Methyl-Lcysteine sulfoxide	-172.92	6

Table no. 10: Results of Anti-inflammatory studies

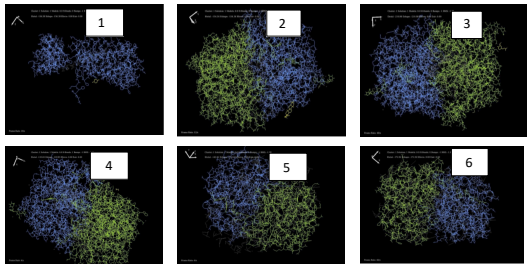


Figure.8: Anti-inflammatory Docking studies

The interaction of protein 3T88 with the phytochemicals(Allyl propyl disulfide, Myricetin,Thiosulfinic acid esters, Cholesterol,S-Methyl-Lcysteine sulfoxide. Propanethial S-oxide) gave binding affinity.

3.11.3 Molecular docking on Antibacterial

Sr no.	Protein used (PDB)	ligands	E-total	Figure no.
1	5u8c	Allyl propyl disulfide	-180.33	1
2	5u8c	Myricetin	-335.44	2
3	5u8c	Thiosulfinic acid esters	-383.03	3
4	5u8c	Cholesterol	-383.05	4
5	5u8c	S-Methyl-Lcysteine sulfoxide	-161.44	5
6	5u8c	Propanethial S-oxide	-135.57	6

Table no. 11: Results of Antibacterial studies

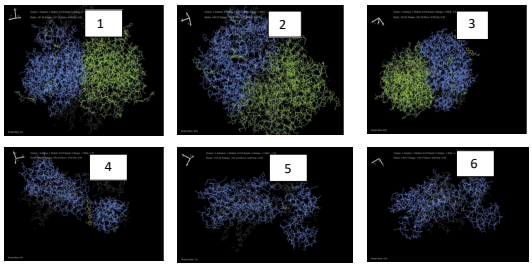


Figure.9: Antibacterial Docking studies

The interaction of protein 5u8c with the phytochemicals(Allyl propyl disulfide, Myricetin,Thiosulfinic acid esters, Cholesterol,S-Methyl-Lcysteine sulfoxide. Propanethial S-oxide) gave binding affinity.

Conclusion

The present investigation demonstrates that red onion peel, commonly discarded as processing waste, represents a valuable source of bioactive constituents. The ethanolic extract exhibited appreciable antioxidant capacity, measurable anti-inflammatory response, and notable antibacterial activity, particularly against *E. coli*. A clear dose-related insecticidal effect was observed against *Sitophilus oryzae*, with higher concentrations producing complete mortality. In cytotoxic evaluation, the extract reduced the viability of MDA-MB-231 breast cancer cells in a concentration-dependent manner, with an IC_{50} of 1T80 µg/ml, indicating moderate antiproliferative potential.

Collectively, these findings highlight the scope of red onion peel as a low-cost, sustainable bioresource with pharmaceutical and agricultural relevance. The study supports the concept of converting agro-waste into value-added products, while further in-depth mechanistic and in-vivo studies are warranted to substantiate its therapeutic applicability.

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