Bactericidal, Antioxidant Activity and In Silico Analysis of Phytochemicals Derived From Selected Plants of Solanaceae Family

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Abstract
A diverse range of active therapeutic constituents i.e. antioxidants from medicinal plants of Solanaceae family are responsible for anticancer & antibacterial activity. The study was aimed to investigate phytochemicals i.e. alkaloids, phenols, tannins, flavonoids, saponins, glycosides, and steroids qualitatively in selected plants of Solanaceae family. Total phenolic and flavonoid content of the aqueous extracts of the plants were determined quantitatively by the Folin-Ciocalteus reagent method and modified Aluminium Chloride assay respectively. Flavanoids present in the extracts of Solanumnigrum (fruit and leaf), Daturainoxia (leaf) and Capsicum annum (fruit) samples were 0.39 ± 0.030, 0.42 ± 0.020, 0.51 ± 0.04, 0.34± 0.030µgmL\(^{-1}\) respectively, whereas phenolic contents were 94± 1.2, 107± 1.5, 96± 1.3, 87± 1.9 mg chlorogenic acid equivalent respectively. The aqueous and ethanolic extracts of S. nigrum, D. inoxia and C. annum showed bactericidal activity against strains of Salmonella typhimurium, Escherichia coli, Pseudomonas aeruginosa, Klebsiella pneumonia and Staphylococcus aureus with (MIC)2mgmL\(^{-1}\) and 5mgmL\(^{-1}\). Highest free radical scavenging of DPPH activity 81.3% was exhibited by 2mgmL\(^{-1}\) methanolic extract of D. inoxia. Docking of Murine with Saponin, Flavone, phenol showed hydrogen bond of length 2.47 Å, 1.98 Å, 2.285 Å respectively while two H-bonds with 1.96 and 2.56 Å bond lengths of alkaloids. Representative trends and in silico assay results explain the synergism among flavonoids, alkaloids, and phenols. The phytochemicals provide antibacterial activity, antioxidant property as well as anti-cancerous bioactive compounds such as alkaloids and tannins, justifying their therapeutic efficacy in the field of cancer medicine.

Keywords: Phytochemicals, Bactericidal Activity, MIC, Antioxidant, Bioinformatics, Anticancer.

1. Introduction

The ethnobotanical research is generally based on phytochemical information, which is considered as an effective approach in the discovery of new pharmaceutical agents from plants. Phytochemicals present a variety of biological properties due to their significant radicals scavenging effect. Polyphenols including (phenolic acid, flavonoids, and tannins) showed antitumor effects as proposed by(Gogoi & Islam, 2012). Around the world, family Solanaceae is distributed in the hot as well as moderate zones. It comprises the large genus Solanum, which contains steroids like glycoalkaloids, very important bioactive substances ecologically, and to the commercial point of view. Steroidal glycoalkaloids are synthesized by the plants for protection against pests and
pathogens, nominated as defensive substances (Nino, Correa, & Mosquera, 2006). Plant members of the Solanaceae family are rich in these bioactive chemical substances such as alkaloids, tannin, flavonoids, and phenolic compounds and have attained much attention by researchers as they impart pharmacological properties of anticancer, antioxidants and antitumor (Gogoi & Islam, 2012).

**Ethno-pharmacological relevance:** Globally nutritional use of bell pepper is well recognized, yet the health relating benefits and medicinal properties are enormous. Vitamins and minerals possess antimicrobial and anticancerous properties. Chilli pepper (Capsicum annum) ingredients are effectively used locally for cancer, rheumatoid arthritis, bronchitis, chest colds, cardiac arrhythmias, headache, and numerous sicknesses. Chilli contains capsaicin, an ingredient employed for pharmaceutical creams, gels, and plasters, the essential oil extracted from the pods of capsicum, according to (Saleh, Omer, & Teweldemedhin, 2018). Datura stramonium has been scientifically confirmed to contain tannins, alkaloids, polysaccharides, and proteins. *D. stramonium/anoxia* plays a further role in stimulating the central nervous system, as a decongestant, skin infections, treatment of toothache and in the treatment of baldness. Profound antibacterial activity in leaves and seed extract of *D. anoxia* were recorded as published by (Mahmood, Mahmood, & Mahmood, 2012). Jain et al (2011) narrated *S. nigrum* (mako or black nightshade) is mainly used in the composition of many medicines to cure pain, fever, inflammation and as antibiotics (Jain, Sharma, Gupta, Sarethy, & Gabrani, 2011). This ethnobotanical research involved the quantitative determination of phytochemicals from the crude extracts of plants. The antioxidant compounds show high free radical scavenging activity which accompanied their bactericidal efficacy also. The bioinformatics study involved structural analysis of proteins and phytochemicals.

2. Material and methods

2.1. Plant material

Chilliesfruit (Capsicum annum), tomato fruit (Lycopersicumesculentum), potato tuber (Solanumtuberosom), datura leaves, and (Ipomoea batatas) (root) were purchased from the local market of Faisalabad, Pakistan. *Daturainoxia*(leaf) and Mako (fruit and leaf) (*Solanumnigrum*) were collected from the botanical garden of the University of Agriculture, Faisalabad, Pakistan.

2.2. Chemicals for reagents: Mercuric chloride, lead acetate, aluminum chloride, rutin, sodium tungstate, phosphoric acid, sodium molybdate, lithium sulfate, gallic acid, butylated hydroxytoluene (BHT) and (2,1-Diphenyl-2-picrylhydrazy) DPPH were obtained from Sigma-Aldrich Chemie GmbH, Germany.

2.3. Test organisms

*Salmonella typhimurium* (ATCC 13311), *Escherichia coli* (ATCC 25922), *Staphylococcus aureus* (ATCC 6538), *Klebsiella pneumonia* (ATCC 4352) and *Pseudomonas aeruginosa* (ATCC 19582) obtained from the Department of Microbiology, University of Agriculture, Faisalabad, Pakistan.

2.4. Aqueous Extract

The aqueous extract was prepared by taking 50g of plants part. Leaves or fruit were crushed and ground into 10 mL distilled water while stirring. After overnight incubation at room temperature, the
mixture was stirred through magnetic stirrer for one hour and filtered for further qualitative tests (Bashir, Mohammed, Magsoud, & Shaoub, 2013).

2.5. **Qualitative Phytochemical Screening:**

2.5.1. **Alkaloids:**
Mayer’s Test was adopted for alkaloids presence (Balabhaskar & Vijayalakshmi, 2015). **Mayer’s Test:** To 1 ml of the plant extract, concentrated hydrochloric acid 2 mL was added. Then few drops of Mayer’s reagent were added into it. White or green color precipitates specified the presence of alkaloids. **(Mayer’s reagent:** It is a mixture of two solutions. Mercuric chloride and potassium iodide aqueous solutions).

1. Mercuric chloride (1.36 g) mixed in 60 mL of distilled water.
2. Potassium iodide (5 g) added into 200 mL of distilled water, (after mixing both solutions the final volume was made up to 100 ml with distilled water).

2.5.2. **Saponins:**
Crude extract prepared in distilled water was vigorously shaken in distilled water (5mL). The formation of stable form specifies the saponin’s presence (Yadav and Agarwala, 2011).

2.5.3. **Tannins:**
**Lead acetate Test:** To 1 mL plant extract, 5 drops of 1% lead acetate along with 10 mL distilled water were added. White precipitates formation indicates the presence of tannins (Latif et al., 2019).

2.5.4. **Flavanoids:**
**Sodium hydroxide test for qualitative presence:** To 5 mL of the aqueous extract filtrate, 10% sodium hydroxide aqueous solution (2 mL) was added. The test solution became yellow. On the addition of dilute HCl, the color changed from yellow to colorless, which was an identification sign for the presence of flavonoids (Latif et al., 2019).

2.5.5. **Glycosides:**
**Liebermann’s test:** Crude extract from plants mixed with 2mL of chloroform and 2mL of acetic acid. The mixture was ice-cooled then H₂SO₄ was added. Change in color from violet to blue to green indicated the presence of glycone, the main nucleus of steroids (Yadav & Agarwala, 2011).

2.5.6. **Steroidal compounds:**
An equal volume of chloroform was added to the crude extract of the plant. H₂SO₄(conc) was added along the side of the test tube. The red color appeared in the lower chloroform layer indicated the presence of steroids (Yadav & Agarwala, 2011).

2.5.7. **Determination of Total Flavonoids Content Quantitatively:**
**Standard curve:** Crude extract (0.5mL) was dissolved in 0.1ml of 1M potassium acetate and equal volume of 10% aluminum chloride added with methanol. 1.5 ml and 2.8mLof distilled water. The mixture was kept at room temperature for 30 minutes. The optical density of the mixture was recorded spectrophotometrically at 415 nm. To prepare a standard 100 μgmL⁻¹ stock solution, 10mg of rutin was dissolved in 100 mL of methanol. Further dilutions from the 0.2 to 1μgmL⁻¹ were made from the stock solution. The standard curve was prepared by measuring the absorbance of concentrations i.e. 0.2, 0.4, 0.6, 0.8, and 1 μgmL⁻¹ of rutin solution (Amir, Khan, Mujeeb, Ahmad, & Siddiqui, 2011). A Triplicate...
assay was performed. Results were expressed as μg mL⁻¹ of rutin concentration using the calibration curve: Y = 2.142x - 0.1, R² = 0.974, where Y was the absorbance, and x was the rutin concentration.

![Standard curve of total flavonoid content](image)

**Figure 1. Standard curve of total flavonoid content**

2.5.8. **Determination of Phenolic Compounds:**

**Ferric chloride test:**
To the crude mL of extract (1mL), 3 to 4 drops of 5% neutral ferric chloride solution were added. The dark green color appeared which indicated the presence of phenols (Ben, Woode, Abotsi, & Boakye-Gyasi, 2013). **Folin-Ciocalteu reagent:** In 700 mL of distilling water, 25 g of sodium molybdate, 100 g of sodium tungstate, 50 mL of 85% phosphoric acid, and 100 mL of concentrated HCl was added. The mixture was refluxed for 10 hours after adding 150g of lithium sulphate.

2.5.9. **Quantitative determination of Total Phenolic Contents:**

**Standard curve;** To determine phenolic content, the standard curve of gallic acid was prepared with a concentration of 0.1, 0.2, 0.4, 0.6, 0.8, and 1 μg mL⁻¹. Gallic acid (0.5mL) was dissolved into 5 mL of diluted Folin-Ciocalteu reagent (1:10 in distilled water) and 4 mL of 1M aqueous Na₂CO₃. The absorbance was recorded at 765 nm spectrophotometrically after incubating the reaction mixtures for 30 min at room temperature. The assay was performed in triplicate. Results were expressed as equivalents of gallic acid in μg mL⁻¹ using the calibration curve (Amir et al., 2011).

2.5.10 **Antioxidant check by DPPH radical scavenging assay:**

To determination the free radicals scavenging activity of plant extract, the methanolic solution of DPPH 0.12 mM was mixed with 1mL plant extracts with concentration ranging from 0.02 to 0.5mg mL⁻¹. DPPH generated free radicals were picked up by antioxidants after 30 min of incubation in dark. Spectrophotometrically absorbance was taken at 517 nm. DPPH scavenging activity (%) = [(Abs control – Abs sample)/(Abs control)] × 100. Butylated hydroxytoluene (BHT), synthetic metabolite resembling vitamin E was used as a positive control (figure 2) (Aires, Marrinhas, Carvalho, Dias, & Saavedra, 2016).
2.5.11 In vitro antibacterial assay:
The microbial strains of Gram-negative and gram-positive kept at 4 °C inoculated on agar slant and subcultured at 37 °C for 48 hours on nutrient agar before antibacterial assay. The antibacterial activity was conducted using Nutrient Agar plates (Latif et al., 2019) (figure 2).

![Figure 2: Flowsheet for the antibacterial and antioxidant activity of selected plant extracts.](image)

2.5.12 Statistical analysis of data:
The results obtained were expressed as mean values and standard deviation (SD) of three replicates. The results were analyzed using one-way ANOVA. The level $P < 0.05$ was considered as the cutoff value for significance.

2.5.13 Bioinformatics proof
Chimera 1.13.1 was used for docking between ligands and microbes receptors (Pettersen et al., 2004).

3 Results
3.1 Phytochemical Constituents:
Selected plant parts were screened for phytoconstituents. Phytochemical qualitative analysis of Alkaloids, tannins, glycosides, saponins, steroids, flavonoids and phenolics from the selected L-asparaginase producing plant parts of $S. nigrum$ (leaves), $Solanumnigrum$ (fruit), $Capsicum annum$ (fruit), $Lycopersicumesculentum$ (Fruit), $Ipomoea batatas$ (Root), $Daturainoxia$ (leaf) and $Solanumtubersom$ (root) was positive (table1). The aluminum chloride assay used for flavonoids
identification resulted in the yellow characteristic color of flavonoids (Figure 3).

Figure 3. Phytochemicals qualitative and quantitative determination (pictorial representation).

<table>
<thead>
<tr>
<th>Sr#</th>
<th>Plant part for study</th>
<th>Alkaloids</th>
<th>Tannins</th>
<th>Flavonoids</th>
<th>Phenols</th>
<th>Saponins</th>
<th>Glycosides</th>
<th>Steroids</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Capsicum annum (fruit)</td>
<td>+</td>
<td>+</td>
<td>+</td>
<td>+</td>
<td>+</td>
<td>+</td>
<td>+</td>
</tr>
<tr>
<td>2</td>
<td>Solanum nigrum (fruit)</td>
<td>+</td>
<td>+</td>
<td>+</td>
<td>+</td>
<td>+</td>
<td>+</td>
<td>+</td>
</tr>
<tr>
<td>3</td>
<td>L. esculentum (fruit)</td>
<td>+</td>
<td>+</td>
<td>+</td>
<td>+</td>
<td>+</td>
<td>-</td>
<td>+</td>
</tr>
<tr>
<td>4</td>
<td>Solanum nigrum (leaf)</td>
<td>+</td>
<td>+</td>
<td>+</td>
<td>+</td>
<td>+</td>
<td>+</td>
<td>+</td>
</tr>
<tr>
<td>5</td>
<td>Ipomoea batatas (root)</td>
<td>+</td>
<td>+</td>
<td>+</td>
<td>+</td>
<td>+</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>6</td>
<td>Solanum tuberosum (root)</td>
<td>+</td>
<td>-</td>
<td>+</td>
<td>+</td>
<td>+</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>7</td>
<td>Daturainoxia (leaf)</td>
<td>+</td>
<td>+</td>
<td>+</td>
<td>+</td>
<td>+</td>
<td>+</td>
<td>+</td>
</tr>
</tbody>
</table>

The amount of total phenolic contents in *Solanum nigrum* (fruit and leaf), *Daturainoxia* and *Capsicum* (pepper) samples were 94±1.2, 107±1.5, 96±1.3, 87±1.9 mg chlorogenic acid equivalent (mg CAE) respectively (figure 4, table 2) by the FolineCiocalteau method, spectrophotometrically at 765 nm.
Figure 4. Total phenolic contents in *Solanum nigrum*, *Daturainoxia*, and *capsicum annum* plants

<table>
<thead>
<tr>
<th>Sr</th>
<th>Plant extracts</th>
<th>Total flavanoids (ugmL$^{-1}$) ±SEM</th>
<th>Phenols   (mgCAEQ) ±SEM</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td><em>Solanum nigrum</em> (leaf)</td>
<td>0.42 ± 0.020</td>
<td>107 ± 1.5</td>
</tr>
<tr>
<td>2</td>
<td><em>Daturainoxia</em> (leaf)</td>
<td>0.51 ± 0.04</td>
<td>96 ± 1.3</td>
</tr>
<tr>
<td>3</td>
<td><em>Solanum nigrum</em> (fruit)</td>
<td>0.39 ± 0.030</td>
<td>94 ± 1.2</td>
</tr>
<tr>
<td>4</td>
<td><em>Capsicum annum</em> (fruit)</td>
<td>0.34 ± 0.030</td>
<td>87 ± 1.9</td>
</tr>
</tbody>
</table>

*Note.* SEM = standard error of means

3.2. Flavanoids:

Flavanoids present in the extracts of *Solanum nigrum* (fruit and leaf), *Daturainoxia* and *capsicum* (pepper) samples were found to be 0.39 ± 0.030, 0.42 ± 0.020 and 0.51 ± 0.04, 0.34± 0.030 ug/mL$^{-1}$ respectively. Phenolic substances were determined by spectrophotometric analysis at 415 nm after constructing a standard curve of rutin (figure 5). Statistical results are shown in Table 2.
3.3. Antibacterial activity:
The plant extracts inhibited the microbial growth against *Escherichia coli*, *Salmonella typhimurium*, *Klebsiella pneumonia*, *Pseudomonas aeruginosa*, and *S. aureus* which had mean inhibition zone expressed in the table (3). The minimum inhibitory concentration (MIC) of 2 mg/mL was observed in the plant extracts against *Klebsiella* and *Escherichia coli*, whereas, 5mg/ml against *Pseudomonas aeruginosa*, *Staphylococcus aureus*, and *Salmonella typhi*.

<table>
<thead>
<tr>
<th>Sr.#</th>
<th>Microorganism</th>
<th>Plant extract</th>
<th>Aqueous extract (ZOI) mm</th>
<th>Methanolic extract (ZOI) mm</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td><em>Salmonella typhimurium</em></td>
<td>Solanumnigrum</td>
<td>28</td>
<td>33</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Daturainoxia</td>
<td>23</td>
<td>32</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Capsicumannum</td>
<td>21</td>
<td>35</td>
</tr>
<tr>
<td>2</td>
<td><em>Escherichia coli</em></td>
<td>Solanumnigrum</td>
<td>-</td>
<td>14</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Daturainoxia</td>
<td>-</td>
<td>16</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Capsicumannum</td>
<td>15</td>
<td>27</td>
</tr>
</tbody>
</table>

Figure 5. Total flavonoids in *Solanum nigrum, Daturainoxia, and capsicum annum* plants

Table 3. Antibacterial assay depicting Zone of inhibition of aqueous and methanolic extracts Vs bacteria
### Table 1: Antimicrobial activity of plant extracts against bacterial species

<table>
<thead>
<tr>
<th>Bacterial Species</th>
<th>Plant Extracts</th>
<th>Zone of Inhibition (mm)</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Klebsiella pneumonia</strong></td>
<td><em>Solanum nigra</em></td>
<td>24</td>
</tr>
<tr>
<td></td>
<td><em>Daturainoxia</em></td>
<td>20</td>
</tr>
<tr>
<td></td>
<td><em>Capsicum annum</em></td>
<td>-</td>
</tr>
<tr>
<td></td>
<td></td>
<td>30</td>
</tr>
<tr>
<td><strong>Pseudomonas aeruginosa</strong></td>
<td><em>Solanum nigra</em></td>
<td>-</td>
</tr>
<tr>
<td></td>
<td><em>Daturainoxia</em></td>
<td>-</td>
</tr>
<tr>
<td></td>
<td><em>Capsicum annum</em></td>
<td>-</td>
</tr>
<tr>
<td></td>
<td></td>
<td>29</td>
</tr>
<tr>
<td><strong>S. aureus</strong></td>
<td><em>Solanum nigra</em></td>
<td>23</td>
</tr>
<tr>
<td></td>
<td><em>Daturainoxia</em></td>
<td>28</td>
</tr>
<tr>
<td></td>
<td><em>Capsicum annum</em></td>
<td>-</td>
</tr>
<tr>
<td></td>
<td></td>
<td>32</td>
</tr>
</tbody>
</table>

**Note.** ZOI= Zone of inhibition

### 3.4. Free radical scavenging of DPPH activity:

Methanolic extracts of *Daturainoxia*, *Solanum nigra*, and *Capsicum annum* were analysed for free radicals scavenging activity introduced by DPPH. The antioxidant properties of plant extracts were analysed, *Daturainoxia* represented classical trend and highest radical scavenging property as depicted in (fig 4). Different concentrations ranging from 0.2 to 2 mg/mL of the plant extracts were analysed to determine their percentage activity. *Daturainoxia, Solanum nigra*, and *Capsicum annum* scored 81.3 %, 66 %, and 53.2% activity in DPPH assay.
3.5. Bioinformatic tools

Docking between the important component (murine of peptidoglycan layer) of bacterial cell wall and different phytochemical constituents proved the experimental results of analysis as explained in table 4.

Table 4. Confirmation of interaction between different classes of phytochemicals and murine receptor of bacterial cell wall

<table>
<thead>
<tr>
<th>Ligand</th>
<th>Ligand class</th>
<th>Receptor</th>
<th>Score</th>
<th>RMSD</th>
<th>H-bond</th>
<th>Bond length Å</th>
</tr>
</thead>
<tbody>
<tr>
<td>Spirostanol</td>
<td>Saponin</td>
<td>Murine</td>
<td>-7.8</td>
<td>0.000</td>
<td>1</td>
<td>2.47</td>
</tr>
<tr>
<td>Flavone</td>
<td>Flavonoid</td>
<td>Murine</td>
<td>-6.7</td>
<td>0.000</td>
<td>1</td>
<td>1.98</td>
</tr>
<tr>
<td>Phenol</td>
<td>Phenol</td>
<td>Murine</td>
<td>-4.7</td>
<td>0.000</td>
<td>1</td>
<td>2.285</td>
</tr>
<tr>
<td>Alkaloid</td>
<td>Alkaloid</td>
<td>Murine</td>
<td>-6.4</td>
<td>2.582</td>
<td>2</td>
<td>1.96, 2.56</td>
</tr>
<tr>
<td>Cortisol</td>
<td>Steroid</td>
<td>Murine</td>
<td>-6.8</td>
<td>0.000</td>
<td>1</td>
<td>2.38</td>
</tr>
</tbody>
</table>

Note: Ligand; phytochemicals class, RMSD value; used to compare the docked confirmation with the reference conformation, the score is the energy score of docking, Number of H-bond, and bond length existing between ligand and receptor (Lau, Levesque, Chien, Date, & Haga, 2010).

Figure 6. Free radical of DPPH scavenging activity of Datura inoxia, Solanum nigrum, and Capsicum annum methanolic extract.
Figure 7. Docking results of ligands with receptor murine. A) Docking of Murine and Saponin with one hydrogen bond of length 2.47 Å. (B) Murine-Flavone; one hydrogen bond with 1.98 Å bond length. (C) Murine-Phenol; one hydrogen bond with 2.285 Å bond length. (D) Murine-Alkaloid; two hydrogen bonds with 1.96 and 2.56 Å bond lengths. (E) Murine-Steroid; one hydrogen bond with 2.38 Å bond length.

4. Discussion

Quite a lot of studies have investigated the antioxidant properties of medicinal plants. Mainly biological antioxidants are obtained from plants in the form of phenolic compounds. Among phytochemicals, steroids are known to draw most of the metabolic processes in the body i.e. sex hormones (Yadav & Agarwala, 2011). The basic 15 carbon skeleton of flavonoids is constituent of phenolic derivatives, which are water-soluble and bear colored pigments. Flavonoids are glycosides that slightly differ from the flavan structure as their glyconeshas central location in nucleus (Bashir et al., 2013). They are hydroxylated phenols which are prepared by plants in response to various pathogens. These flavonoids substances complex the soluble proteins with the peptidoglycans layer in the cell wall of bacteria, delivering vitro bactericidal activity (Yadav & Agarwala, 2011).
Among all flavonoids, 7 flavonoids at 200 nm, 7 at 254 nm, 4 at 580 nm gave their spots when scanned by HPTLC (Bashir et al., 2013), which are under our experimental findings at 510 nm. As reported formerly, flavonoids have antitumor/anticarcinogenic activity and anti-oxidant properties as well (Ansari, Ahmed, Waheed, & Juned, 2013). Flavonoids are distributed throughout the plant kingdom, *Punica grandatum* (pomegranate) also plays a beneficial role in the treatment of cancer, immune modulation and act as anti-oxidant (Bhandary, Bhat, Sharmila, & Bekal, 2012). These antioxidants can scavenge reactive oxygen species which are cancer-causing agents. Among the plant metabolites, the **Phenolic compounds** are ubiquitous. They deliver the functions of anti-inflammation, antiaging, antiatherosclerosis, and anti-apoptotic agents (Yadav & Agarwala, 2011). They also restrict angiogenesis and cell proliferation, strong contestant as anticancer. The phenolic content already investigated by the Tundis (2013) was 648.6 mg chlorogenic acid equivalent as compared to the present value of phenolic compounds as 87 mg chlorogenic acid equivalent for which 5 mg aqueous extract of chili was prepared (Tundis et al., 2013). *Solanum nigrum* fruit (extract aqueous) showed phenols in high amounts during qualitative analysis. The number of phenolic compounds in aqueous extract of *Solanum nigrum* fruit was 107 mg chlorogenic acid equivalent in the present work. *Datura inoxia* showed 96 mg of chlorogenic acid equivalent. **Alkaloids** are widely distributed in higher plants belonging to *Solanaceae* and *Apocynaceae* families. *Datura inoxia* possesses high amounts of alkaloids, it highlights many potential health benefits, medicinally they are known as local anesthetics and stimulants, analgesics, psychedelics, antibacterial drugs, and antihypertensive agents, cholinomimetic, spasmyloyis agents and cytotoxic activity, etc (Kuete, 2014). Furthermore, these alkaloids have pharmacological activities i.e. antiasthma, vasodilators, antimalarial, anticancer, ant arrhythmic, and antihyperglycemic activities (Hoste, Jackson, Athanasiadou, Thamsborg, & Hoskin, 2006). Saponins have characteristics of coagulating the blood in case of hemorrhage. Saponins also show hemolytic activity and occluding fats as foam (Yadav & Agarwala, 2011). Tannins are an imperative component of plants, it almost weighs 5% to 10% of the dry weight of leaves. Tannins as secondary metabolites and important antioxidants helpful against the parasitic defense and herbivore insect attack in ruminants (Barbehenn & Constabel, 2011). Several studies reported that glycosides have a well-established role in hypertension (Yadav & Agarwala, 2011). The above-mentioned phytoconstituents are those bioactive substances which prove medicinal plants to be the cure of all times.

Sophisticated bioinformatics tools are used to get a sense of the data. Bioinformatics help in the prediction of domains, functional groups, and their bonding in the protein structures and their pathways (Roumpeka, Wallace, Escalettes, Fotheringham, & Watson, 2017). Murine is the major component of the peptidoglycan layer of the bacterial cell wall. Compound making bonds with murine will weaken the murine-murine bond of the bacterial cell wall and thus will break the cell wall and destroy the microorganism. Docking of Murine and ligands (phytochemical) show that how murine would respond to these phytochemicals (Singh, Mallick, Banerjee, & Kumar, 2016). Among all the results generated for murine and each ligand, those were chosen which had the least score, close to zero RMSD value, and maximum hydrogen bonds (Table 4). The strongest bond among all is between Murine-Flavone and Murine-Alkaloid (Kilani-Jaziri et al., 2016). As (figure 7) shows alkaloids have 2 hydrogen bonds. One with 1.96 and other 2.56 Å bond lengths, depicting strong phytochemical action. Phenols act also on the murine receptor show one hydrogen bond with 2.285 Å bond length.
The results obtained revealed that *Solanumnigrum*, *Daturainoxia*, and *capsicum annum* species inhibited four out of five microorganisms evaluated in this research. The methanolic extracts of three selected plants exhibited weak activity against *E. coli* and *P. aeruginosa* yet their aqueous extracts could not inhibit Gram-negative bacteria as correlated with the study of root extract of *Datura stramonium* and *Capsicum annum* (Niño, Correa, & Mosquera, 2006) which were not active against *aeruginosa* and *E.coli*. DPPH free radicals scavenging activity attained highest 0.6 and 2 mgmL⁻¹ concentration from crude methanolic extracts as compared with the standard (BHT) showing IC₅₀ of 1.0 mgmL⁻¹. These findings contribute to assessing more bioactive compounds from other families to elucidate important antimicrobial and cytotoxic agents.

5. Conclusion
The extracts of various plant species of *Solanaceae* family have a considerable concentration of Phytochemicals. Moreover, the young leaves of *Solanumnigrum*, *Daturainoxia*, and fruit of *capsicum annum* were comprised of a valuable amount of phenols and flavonoids, which impart them free radical scavenging and antibacterial activity truly ensuring their anticancer role. The insilico assay emphasizes the interaction between protein structures and flavanoids/ alkaloids for antibacterial activity.

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References


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