GC–MS and molecular docking analyses of phytochemicals from the underutilized plant, *Parkia timoriana* revealed candidate anti-cancerous and anti-inflammatory agents

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Plants are excellent sources of functionally bioactive compounds and essential nutrients. The phytochemical constituents have enormous potential in treating both plant and human diseases. *Parkia timoriana* (Yongchak/Zawngtah), one of the most important underutilized plants popularly consumed in Manipur and Mizoram states of Northeastern region of India, is known for its ethnobotanical and ethnomedicinal values. A significant DPPH (2,2'-diphenyl-1-picrylhydrazyl), ABTS (2,2'-azino-bis (3-ethylenbenzothiazoline-6-sulfonic acid)), and Phosphomolybdate scavenging activity corresponding to high antioxidant potentials was shown by the extracts from different edible parts of *P. timoriana*. *P. timoriana* extract showed significant antibacterial potential against *Bacillus pumilus*, *Bacillus subtillis*, *Escherichia coli* and *Pseudomonas aeruginosa*. Fourier transform infrared spectroscopy and gas chromatography–mass spectrometry (GC–MS) analyses of the extracts revealed the functional groups and bioactive compounds present in different edible parts of the plant. Characteristic peaks of phenols, carboxylic acids, alkenes, glycogen, alkyl halides, halogen, aliphatic amines, primary and secondary amines, esters, ether, aromatics, lipids, triglycerides, nitro compounds that had antimicrobial, anti-cancer and anti-inflammatory properties etc. were observed. The GC–MS analysis also revealed the occurrence of 49 bioactive compounds that are known to possess a variety of pharmacological activities. Subsequently, in silico molecular docking studies of the identified bioactive compounds predicted potential anticancer and anti-inflammatory properties. To the best of our knowledge, this is the first-hand report on the bioactive compounds of edible parts of *P. timoriana* extracts showing antioxidant, antimicrobial and pharmacological significance. This study can lead to the production of new herbal medicines for various diseases employing *P. timoriana* and perhaps leading to the creation of new medications.

Plants, not only provide essential nutrients for humans, but also provide biologically active compounds that are beneficial for the human health and treatment of various diseases1. They contain a wide range of compounds like lipids, phytochemicals, pharmaceuticals, flavors and fragrance and have been used in food, pharmaceutical and cosmetics industries etc. In developing countries like India, the use of traditional medicines are the primary source of the health care system and the presence of phytochemical compounds are the main reasons for the use of plants in the traditional practice of medicines2. In India, especially in the rural northeastern (NE) region, the use of traditional medicine is a common practice that may be due to the availability of diverse vegetation and the socio-economic conditions of the people of the region3. Medicinal plants have a wide range of bioactive compounds that have antimicrobial, anticancer, anti-inflammatory and antioxidant potentials. Plant-derived

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medicines are frequently prepared from crude extracts, which include a complex combination of various phytochemicals and are utilized to treat both chronic and infectious diseases. Various plant species contain a vast pool of secondary metabolites but only a few of them have been studied and proven to be a substantial source of bioactive compounds. The development of acceptable screening procedures is critical in the search for novel chemicals as well as in quality control. The extraction and characterization of these bioactive compounds have resulted in the delivery of specific medications with a high-activity profile. Fourier-transformed infrared (FTIR) and Gas chromatography-mass spectrometry (GC–MS) have been widely used for observation of functional groups and identification of various bioactive compounds present in plants. GC–MS is a reliable technique for the identification of various compounds such as alkaloids, flavonoids, organic acids, amino acids etc. from plant extracts. Also, computer-based tools have evolved as sophisticated drug discovery approaches that may be used to screen medicines from bioactive compounds present in medicinal plants. Computational prediction models are utilized in the in silico prediction of pharmacological, pharmokinetic and toxicological production and play a crucial role in the selection of procedure leading to pharmaceutical and technological advancement. Molecular docking is an efficient and low-cost approach for creating and testing pharmaceuticals. This technique gives the knowledge on drug-receptor interactions that may be used to anticipate how the drug model will bind to the target proteins leading to reliable binding at the binding sites of ligands.

Parkia timoriana (DC) Merr., commonly known as tree bean belonging to the Fabaceae family, is an underutilized medicinal plant well distributed in Southeast Asia and Northeast (NE) India. *P. timoriana* is a lesser-known nutritious leguminous tree that grows and found abundant in NE region of India, grown in wild, jhum land and backyard of houses and is a multipurpose plant having significant economic importance which includes vegetables, medicine, firewood and ecological significance. *P. timoriana* (Yongchak in Manipuri and Zawngtah in Mizo) is popularly consumed particularly in Manipur and Mizoram states of NE India for its ethnomedical and ethnomedicinal values. This plant grows in different conditions from colder and hilly regions to warm and foothill regions without special care. It is an ethnomedically important plant and has high nutritional and medicinal value. The decoctions of bark and fruits are normally used to treat various ailments. It is also reported that *P. timoriana* had high antioxidant potentials and a good amount of phytochemicals that could have a significant role in anti-cancer, antibacterial and anti-ageing activities. Very few research on the ethnomedicinal, preliminary pharmacological, biotechnological applications and mass productions and nutritional composition of *P. timoriana* have been reported so far.

However, to the best of our understanding, there is no report characterizing the presence and evaluation of various bioactive compounds in different edible parts of *P. timoriana*. Therefore, the present study focused on the identification of bioactive compounds from methanolic extracts of flower, capitulum, pod and seed of *P. timoriana* by FTIR and GC–MS analyses. The study also tested the antimicrobial and antioxidant properties of the extracts. Following this, an in silico molecular docking was also performed to identify putative bioactive compounds with anticancer and anti-inflammatory potentials. This study will aid in the prediction of the structures and formulae of bioactive compounds present in *P. timoriana* that could be essential for the discovery and designing of new drugs formulations.

### Results

#### Ethnobotanical studies

Plants are valuable sources of beneficial bioactive compounds for the manufacture of novel chemotherapeutic agents. Investigation on the possibility of using pharmacologically active compounds derived from medicinal plants is an important procedure. It is believed that about 80% of the world’s population use medicinal plants due to their high efficacy, low cost, non-narcotic origin and fewer side effects. Various food crops are used for their application in healthcare and therefore are called ‘medicinal foods’. *P. timoriana*, tree bean is an ethnomedically important plant having high nutritional and medicinal values.

#### Preliminary screening

A preliminary phytochemical screening was done using methanolic extracts of edible parts of *P. timoriana* and the result is shown in Table 1. The study showed the presence of tannins, terpenoids, phenol, flavonoids, alkaloids in *P. timoriana*. The presence of phytochemicals from this plant had also been reported previously.

#### Total flavonoid content

The quantitative phytochemical composition of flower, capitulum, tender pods and seeds of *P. timoriana* are shown in Table 2. Total flavonoid was found to be the highest in the pod (58.38 ± 0.001 mg/g), while flower (28.95 ± 0.002 mg/g) contained the least amount. Previously, it was shown that the methanolic extracts of pods and seeds contained 5.28 mg QE/g and 20.3 mg QE/g respectively and 15.47 mg CA/g in pods. Tapan has shown that the methanol extract of pods contained 4.05 mg/g total flavonoid.

#### Total phenol content

The total phenols content of *P. timoriana* is shown in Table 2. The pod had the highest total phenol content of all analyzed samples (38. ± 0.136 mg/g) whereas flower extract had the lowest content (18.7 ± 0.161 mg/g). The result is in agreement with previous reports on *P. timoriana* where pods contained 49.39 mg GAE/g and 36.59 ± 3.80 mg GAE/g.

#### Antioxidant assay

**DPPH Scavenging activity.** The antioxidant property of methanolic extract of *P. timoriana* was estimated using DPPH assay. The percentage inhibition of free radical scavenging and IC<sub>50</sub> is represented in Fig. 2 & and Table 3 respectively. The antioxidant IC<sub>50</sub> was analogously high in the pod (22.45 µg/ml).
and lowest in flower (70.05 µg/ml). Earlier Badu et al.\textsuperscript{31} have reported that the DPPH antioxidant IC\textsubscript{50} ranged from 160.44 to 157 µg/ml.

**ABTS Scavenging activity.** All the *P. timoriana* extracts scavenged ABTS radical in a concentration-dependent manner (10–100 µg/ml) (Fig. 2). The ABTS radical scavenging capacity of samples could be ranked as Pod > Seed > Capitulum > Flower. The pod and seed had high ABTS radical scavenging capabilities. The IC\textsubscript{50} of ABTS scavenging activities ranged from 27.55 µg/ml to 82.78 µg/ml where pod had the highest value of 27.55 µg/ml, which was comparable to that of Ascorbic acid (24.71 µg/ml).

**Phosphomolybdate assay.** The quantitative total antioxidant capacity was also assessed using Phosphomolybdate assay. Based on the scavenging activity, the extracts could again be ranked as Pod > Seed > Capitulum > Flower (Fig. 2). The IC\textsubscript{50} value ranged from 38.52 µg/ml in pod to 63.09 µg/ml in flower. The IC\textsubscript{50} of the pod is also comparable to that of the standard, Ascorbic acid (33.43 µg/ml). The significant antioxidant potential of the pod, which is statistically comparable to that of standard Ascorbic acid, showed that the extract contained strong antioxidants, which could be due to the presence of phenolic compounds.
Antibacterial activity. The present study investigates the antibacterial activity of edible parts of tree bean from Mizoram, India. The result shows that the methanol extracts of *P. timoriana* exhibit antibacterial activities against the four tested bacterial strain (Table 4 and Fig. 3). The diameter of the zones of inhibition ranged from 9 to 17.66 mm, the highest inhibition zone was observed in *E. coli* (17.66 mm), followed by *B. pumilus*, *P. aeruginosa* and *B. subtilis* (15.33 mm, 14.33 mm and 13 mm respectively).

The quantitative evaluation based on the inhibition growth showed that the pod had very high (*x > 12 mm*) inhibitions against all the tested bacterial strains. Other parts- capitulum, flower and seed also had high (*x = 8–12 mm*) inhibitions zone against all bacterial strains.

**Figure 2.** Antioxidant activity of edible parts of *P. timoriana*. (A) DPPH scavenging activity; (B) ABTS scavenging activity; (C) Phosphomolybdate assay.

**Table 3.** The IC$_{50}$ of different antioxidant assays.

| Sl No | Plant parts     | DPPH IC$_{50}$ (µg/ml) | ABTS IC$_{50}$ (µg/ml) | Phosphomolybdate IC$_{50}$ (µg/ml) |
|-------|-----------------|------------------------|------------------------|-----------------------------------|
| 1     | Capitulum       | 44.25 ± 0.11           | 77.55 ± 0.3            | 53 ± 0.14                         |
| 2     | Flower          | 70.05 ± 0.7            | 82.78 ± 0.2            | 63.09 ± 0.1                       |
| 3     | Pod             | 22.45 ± 0.4            | 27.55 ± 0.21           | 38.52 ± 0.09                      |
| 4     | Seed            | 47.43 ± 0.3            | 56.63 ± 0.6            | 46.28 ± 0.1                       |
| 5     | Ascorbic acid   | 20.51 ± 0.1            | 24.71 ± 0.3            | 33.43 ± 0.8                       |

**Table 4.** Antibacterial activity of methanolic extract of *P. timoriana* against the selected bacterial strain.

| Sl No | Plant parts used | Inhibition zone (mm) |
|-------|------------------|----------------------|
|       | *Bacillus pumilus* | *Bacillus subtilis* | *Escherichia coli* | *Pseudomonas aeruginosa* | Range |
| 1     | Capitulum        | 11.33 ± 0.08         | 10.33 ± 0.35       | 15.33 ± 0.59            | 10.66 ± 0.44 | High |
| 2     | Flower           | 10.66 ± 0.24         | 10 ± 0.54          | 13.66 ± 1.09            | 10.66 ± 0.05 | High |
| 3     | Pod              | 15.33 ± 0.14         | 13 ± 0.84          | 17.66 ± 0.18            | 14.33 ± 0.77 | Very High |
| 4     | Seed             | 10.33 ± 0.45         | 10 ± 0.29          | 17 ± 0.55               | 9.33 ± 0.37  | High |
| Control | Rifampicin     | 17 ± 0.54            | 14 ± 0.13          | 20 ± 0.72               | 16 ± 0.19    | Very High |
Minimum inhibitory concentration (MIC). MIC values determined from the extracts varied from 2.19 to 7.3 mg/ml (Table 5). The percentage inhibition of antibacterial activity is shown in Fig. 4. Pod gave MIC values of 3.5 mg/ml, 3.4 mg/ml, and 2.19 mg/ml respectively against *B. subtilis*, *B. pumilus*, *E. coli*, and *P. aeruginosa*.

FTIR analysis. FTIR spectroscopy was employed to identify the functional groups of bioactive components present in *P. timoriana* (Table 6 and Fig. 5). FTIR spectrum confirmed the presence of hydroxyl group (O–H), aldehyde (C–H), alkenes (C=C), carboxyl (C=O), nitrogen-containing group (N–O), alkanes (C–C), aromatic primary amine (C–N), amines (N–H), alkynes (C≡C), aliphatic Bromo compounds (C–Br), phenols, carboxylic acids, glycogen, alkyl halides, halogen, aliphatic amines, primary and secondary amines, esters, ether, aromatics, lipids, triglycerides, nitro compounds and these functional groups are the integral parts of various secondary metabolites such as alkaloids, flavonoids, terpenoids, polyphenol and tannins.

GC–MS analysis. Evaluation of the chemical structure and composition of the extracts can designate various biological potential of different medicinal plant extracts. However, to the best of our knowledge, there is no report on GC–MS based plant metabolic characterization to reveal the presence of various bioactive compounds in methanolic extracts of edible parts of *P. timoriana*. Therefore, the GC–MS analysis was performed in a predetermined study. A total of 104 peaks were observed in all plant parts, each peak designated the bioactive compounds that were recorded by relating their peak retention time, molecular weight, molecular formula to that of the known compounds proposed by the NIST library (Table 7). The highest number of compounds (32) was observed in the flower extract followed by pod (26), capitulum (26) and seed (20) (Fig. 6).

| Sl. No | Plant part | MIC (mg/ml) | *Bacillus subtilis* | *Bacillus pumilus* | *Pseudomonas aeruginosa* | *Escherichia coli* |
|-------|------------|-------------|---------------------|---------------------|--------------------------|------------------|
| 1     | Flower     | 6.47 ± 0.33 | 3.24 ± 1.45         | 6.73 ± 0.27         | 6.13 ± 0.81              | 6.13 ± 0.81      |
| 2     | Capitulum  | 6.5 ± 0.59  | 7.3 ± 0.11          | 6.69 ± 1.01         | 6.9 ± 0.43               | 6.9 ± 0.43       |
| 3     | Pod        | 3.5 ± 0.18  | 3.4 ± 0.67          | 3.04 ± 0.32         | 2.19 ± 0.35              | 2.19 ± 0.35      |
| 4     | Seed       | 4.47 ± 0.28 | 5.02 ± 0.47         | 5.1 ± 0.09          | 4.15 ± 0.43              | 4.15 ± 0.43      |

Figure 3. Antibacterial activity of *P. timoriana*.
Figure 4. Percentage inhibition showing antibacterial activity of *P. timoriana* extracts against microorganisms, *B. subtilis, B. pumilus, P. aeruginosa* and *E. coli*.

Figure 5. FTIR spectra of edible parts of *P. timoriana*.
with high phenol contents are usually targeted by pharmacists the world over for the treatment of various
cell damage. As medicinal values and also provided that
P. timoriana of NE India. Ethnobotanical data hinted
as a multi-functional plant that had nutritional as well
P. timoriana as a multifunctional vegetable that serves as valuable and dependable income-generating products for farmers
used as a supplementary food source and provides quality food for human as well as livestock, and is touted
as either raw as salads or boiled with water as vegetables that contributes to the health benefits. Tree bean is also
proliferative, induced apoptosis and cell cycle arrest.43. Terpenoids also have several curative properties like
used in antidiabetic, anti-hypersensitive, anti-inflammatory, anti-stomachache and antimicrobial medicines.

Table 6. Details of FTIR spectrum of P. timoriana.

| Frequency range (cm⁻¹) | Samples | Functional group          |
|-----------------------|---------|---------------------------|
| 3870–3550             | Flower  | O-H stretch alcohol       |
| 3500–3200             | Capitulum | O-H stretch vibration presence of alcohols, phenols |
| 3300–2850             | Pod     | O-H stretch vibration, carboxylic acids |
| 2500–2300             | Seed    | C-H stretch vibration, alkenes |
| 2260–2100             |         | C=C stretch vibration, alkynes |
| 1990–1739             |         | Ester C=O stretch, lipid, triglycerides |
| 1700–1660             |         | N–O asymmetric stretch, nitro compounds |
| 1550–1475             |         | C=C stretch vibration, alkenes |
| 1470–1400             |         | 1450.47 1458.18 C–C stretch vibration, aromatics |
| 1400–1320             |         | 1396.46 N–O stretch vibration, nitro compounds |
| 1300–1290             |         | C–O stretch vibration, alcohol, carboxylic acids, esters, ether |
| 1275–1150             |         | N–H wag stretch vibration, alkyl halides |
| 1020–1000             |         | C–N stretch vibration, aliphatic amines |
| 990–800               |         | N–H wag stretch vibration, primary & secondary amines |
| 790–690               |         | 771.53 771.53 C(triple bond)C–H bend stretch vibration, alkynes |
| 680–510               |         | 532.25 617.22 663.51 516.92 C–Br stretch vibration, alkyl halides, glycerogen |
| 490–400               |         | 486.06 455.2 455.2 Halogen compound |

Molecular docking. Further, six bioactive compounds identified by GC–MS analysis from P. timoriana were selected and subjected to molecular docking with BCL-2 and COX-2 proteins (Fig. 7). Paclitaxol (for anti-cancer) and Oxitasim (anti-inflammatory) were used as standard controls. The 2D structures of bioactive compounds were first retrieved from the PubChem database. These compounds were selected based on Lipinski’s rule of five parameters such as molecular weight, log P, number of hydrogen bond donors and number of hydrogen bond acceptors (Table 8).

Structures of the bioactive compounds are shown in Fig. 8. The binding analysis between COX-2 protein and ligands, BCL-2 and ligands revealed that the binding pattern varied with the nature of the ligands. The docking results of bioactive compounds are shown in Figs. 9 and 10. And the docking results are represented in the form of minimum binding energy values (Tables 9 and 10).

Discussion

The indigenous people of NE India commonly consume this plant because of its nutritive and medicinal benefits. The plant parts especially the bark, fruit skin, leaf, seeds are used for the treatment of various diseases.7. The tender pods (young and mature), flowers, capitulum and mature seeds have also been traditionally used as supplementary food sources in this region. In P. timoriana, flowers, capitulum, fruits and seeds are consumed as either raw as salads or boiled with water as vegetables that contributes to the health benefits. Tree bean is also used as a supplementary food source and provides quality food for human as well as livestock, and is touted as a multifunctional vegetable that serves as valuable and dependable income-generating products for farmers of NE India. Ethnobotanical data hinted P. timoriana as a multi-functional plant that had nutritional as well as medicinal values and also provided that P. timoriana likely contained bioactive compounds which could be used in antidiabetic, anti-hypersensitive, anti-inflammatory, anti-stomachache and antimicrobial medicines.

Flavonoids are shown to be effective against cancer cells by inactivating or inhibiting carcinogens, anti-proliferative, induced apoptosis and cell cycle arrest.45. Terpenoids also have several curative properties like anti-cancerous, anti-parasitic, anti-allergic, and anti-inflammatory.46. Likewise, saponins and alkaloids have been reported to have anticancer properties especially against colon cancer, and saponins can also induce growth inhibition and apoptosis.45. Traditionally, tannins are also used for the treatment of diarrhoea, haemorrhage, detoxification etc.46.47. Studies have shown that flavonoids and phenolic compounds present in plants have a wide variety of biological effects including antioxidant, anti-inflammatory, antimicrobial, anti-angiogenic, anticancer, anti-allergic properties etc.48.

In our study, a significantly higher flavonoid content was observed in the methanolic extract. Flavonoids are naturally occurring compounds and water-soluble polyphenolic compounds responsible for coloration in vegetables, fruits and herbs. The biological function of flavonoid is extensive and are used as anti-cancer, anti-inflammatory, anti-allergic, anti-thrombotic, tumour inhibitor, anti-viral agents, in heart diseases and also has a large effect in the lower intestinal tract.49–51. They also possess antioxidant activities that can prevent oxidative cell damage.

Plants produce phenolic compounds as secondary metabolites during normal development.32. Phenols are bioactive compounds that acquire antioxidant potential responsible for health benefits. Phenolic compounds present in the plant can play various roles and are often used in skin infection, wounds treatment etc.32. Plants with high phenol contents are usually targeted by pharmacists the world over for the treatment of various
| Peak | RT  | Molecular Weight | Molecular Formula | Name of the compound                                           | Medicinal uses                                                                 |
|------|-----|------------------|-------------------|----------------------------------------------------------------|--------------------------------------------------------------------------------|
| 1    | 12.09 | 140.22          | C9H16O            | Cyclopentanone, 2-(1-Methylpropyl) -                            | Anti-inflammatory, analgesic, anticonvulsant[^35]                                |
| 2    | 13.29 | 164.16          | C6H12O5           | Beta-L-Arabinopyranoside, Methyl                                | Catechol-O-methyltransferase inhibitor, methyl donor Methylguanidine inhibitor, 17-beta-hydroxyester dehydrogenase inhibitor, beta-adrenergic receptor blocker Beta-adrenergic agents, anticanter (liver, lung, breast, and prostate), antioxidant (LDL)[^14] |
| 3    | 14.94 | 138.16          | C8H10O2           | 3-Methyl-2-(2-Oxopropyl) Furan                                 | Antioxidant, antimicrobial and bacteriocide, Antipyretic, antiinflammatory activity[^35] |
| 4    | 15.95 | 130.18          | C7H14O2           | Heptanoic acid                                                 | No activity reported                                                            |
| 5    | 17.87 | 138.16          | C8H10O2           | 3-Methyl-2-(2-Oxopropyl) Furan                                 | Antioxidant, antimicrobial and bacteriocide activity. Antipyretic, antiinflammatory activity[^35] |
| 6    | 18.73 | 144.21          | C8H16O2           | Octanoic acid                                                  | Anti-bacterial activity                                                          |
| 7    | 19.83 | 204.33          | C10H20O2S         | 3-N-Hexylthiolane, S,S-Dioxide                                | Anti-tumour, anti-cancer, anti-dote, antimicrobial and anti-viral activity[^35] |
| 8    | 20.43 | 172.26          | C10H2O2           | N-Decanoic acid                                                | Anti-bacterial and antifungal activity[^35]                                      |
| 9    | 21.53 | 322.5           | C21H38O2          | 11,14-Eicosadienoic acid, Methyl ester                         | Anti-inflammatory, anti-oxidant, anti-arthritis, anti-coronary[^35]              |
| 10   | 22.3  | 158.24          | C9H18O2           | Nonanoic acid                                                  | Anti-microbial, anti-inflammatory, antitumor, anti-hyperpigmentative, anti-proliferative, anti-acne, cyto toxic, Anti-leukemic, oxy radical scavenging Activity[^35] |
| 11   | 24.53 | 170.24          | C10H18O2          | 2(3H)-Furanone, 5Hexyldihydro -                               | Aromatic compounds                                                              |
| 12   | 27.02 | 172.26          | C10H20O2          | N-Decanoic acid                                                | Anti-bacterial and antifungal activity[^35]                                     |
| 13   | 31.16 | 268.47          | C18H36O3          | Oxirane, hexadecyl                                            | Antimicrobial, adhesive[^35]                                                    |
| 14   | 42.81 | 530.9           | C37H70O           | ZZ-6, 28-Heptatriactontadien-2-one                            | Vasodilator[^35]                                                                |
| 15   | 46.79 | 290.9           | C16H31ClO2        | Chloroacetic acid, Tetradecyl ester                           | Antioxidant, antimicrobial and bacteriocide, anti-inflammatory activity[^7]     |
| 16   | 47.71 | 368.19          | C9H12O3           | 4-Methoxy-6-Methyl-6,7-dihydro-4H-Furo [3,2-c] | Pyran | No activity reported |
| 17   | 48.61 | 422.8           | C29H50O           | Nonacosanal                                                    | Antihypersensitive, vasodilator, angiotensin AT2 receptor antagonist and saluretic[^36] |
| 18   | 52.78 | 282.5           | C18H34O2          | Oleic acid                                                     | Antimicrobial, Antifungal, anticonvulsive activity, Anti-adhesive, Antiallergic, Antianalgies, Antithrombosis, Antiplatelet, Antihemorrhagic, Anti-inflammatory, Anti-oxidant, Anti-infectious, Antifungal, Anti-inflammatory, Antimicrobial, Anti-viral activity[^34] |
| 19   | 57.84 | 366.7           | C25H50O           | 2-Pentacosanone                                                | No activity reported                                                            |
| 20   | 58.63 | 366.7           | C25H50O           | 2-Pentacosanone                                                | No activity reported                                                            |
| 21   | 59.49 | 324.58          | C22H44O4          | 13-Docosen-1-ol, (Z) -                                        | No activity reported                                                            |
| 22   | 59.82 | 298.5           | C19H38O2          | Methyl Stearate                                                | GABA aminotransferase inhibitor, anti-inflammatory, intestinal lipid metabolism regulator, antihelminthic, antinociceptive[^9] |
| 23   | 60.99 | 254.41          | C16H30O2          | Palmitoleic acid                                              | Antimicrobial activity, essential oils                                          |
| 24   | 63.7  | 312.5           | C20H40O2          | Eicosanoic acid                                                | Reduced heart diseases, kidney and liver function, blood clotting                |
| 25   | 65.39 | 286.92          | C18H35C1          | Cis-1-chloro-9-octadecene                                      | No activity reported                                                            |
| 26   | 68.58 | 198.3           | C12H22O2          | 7-Decylloxepan-2-one                                          | No activity reported                                                            |
| 27   | 69.07 | 254.41          | C16H30O2          | Palmitoleic acid                                              | Anti-inflammatory, essential oils                                               |
| 28   | 69.69 | 298.5           | C19H38O2          | Methyl Stearate                                                | GABA aminotransferase inhibitor, anti-inflammatory, intestinal lipid metabolism regulator, antihelminthic, antinociceptive[^9] |
| 29   | 70.82 | 546.8           | C32H6704P         | Dihexadecyl Phosphate                                         | Emulsifying agent                                                               |
| 30   | 74.02 | 340.6           | C22H44O2          | Docosanoic acid                                               | Antibacterial[^38]                                                              |
| 31   | 74.92 | 282.5           | C18H34O2          | 6-Octadecenoic acid                                           | Antimicrobial activity, anti-cancer[^39]                                        |

**Capitulum**

| Peak | RT  | Molecular Weight | Molecular Formula | Name of the compound                                           | Medicinal uses                                                                 |
|------|-----|------------------|-------------------|----------------------------------------------------------------|--------------------------------------------------------------------------------|
| 1    | 13.24 | 140.22          | C9H16O            | Cyclopentanone, 2-(1-Methylpropyl) -                            | Anti-inflammatory, analgesic, anticonvulsant[^35]                                |
| 2    | 14.19 | 164.16          | C6H12O5           | Beta-L-Arabinopyranoside, Methyl                                | Catechol-O-methyltransferase inhibitor, methyl donor Methylguanidine inhibitor, 17-beta-hydroxyester dehydrogenase inhibitor, beta-adrenergic receptor blocker Beta-adrenergic agents, anticanter (liver, lung, breast, and prostate), antioxidant (LDL)[^14] |
| 3    | 16.25 | 138.16          | C8H10O2           | 3-Methyl-2-(2-Oxopropyl) Furan                                 | Antioxidant, antimicrobial and bacteriocide, Antipyretic, antiinflammatory activity[^35] |
| 4    | 16.94 | 130.18          | C7H14O2           | Heptanoic acid                                                 | Used in the preparation of esters for the fragrance industry, and as an additive in cigarettes |

Continued
| Peak | RT  | Molecular Weight | Molecular Formula | Name of the compound | Medicinal uses |
|------|-----|------------------|-------------------|----------------------|---------------|
| 5    | 18  | 126.2            | C8H14O            | 5, 5-Dimethyl-Cyclohex-3-en-1-ol | No activity reported |
| 6    | 18.11 | 134.22          | C10H14            | P-Mentha-1,5,8-Triene | No activity reported |
| 7    | 18.97 | 152.23          | C10H16O           | Hotrienol            | Prevent/reduce metabolic abnormalities and various diseases\cite{48} |
| 8    | 19.39 | 188.34          | C9H20O2S          | Cyclohexylmethy silane | No activity reported |
| 9    | 19.92 | 144.21          | C8H16O2           | Octanoic acid        | Antimicrobial activity |
| 10   | 21.98 | 234.33          | C15H22O2          | Myrtenyl angelate    | Antimicrobial, anti-inflammatory, antioxidants and anti-termic activities\cite{49} |
| 11   | 22.75 | 152.23          | C10H16O           | 1-Cyclohexane-1-Methanol, 4-(1-Methyl ethenyl)—, Formate | Antioxidant activity |
| 12   | 24.13 | 172.26          | C10H20O2          | N-Decanoic acid      | Antimicrobial and antifungal activity\cite{50} |
| 13   | 26.71 | 254.41          | C16H30O2          | Valeric acid, Undec-2- enyl ester | Used in the synthesis of its esters. Volatile esters of Valeric acid have pleasant odours which are used in perfumes and cosmetics |
| 14   | 28.14 | 530.9           | C37H70O           | Z,Z-6 , 28-Heptatriactontadien-2-one | Vasodilator\cite{46} |
| 15   | 29.99 | 204.33          | C10H20O2S         | 3-N-Hexylthiolane, S,S-dioxide | Anti-tumour, anti-cancer, anti-dote, antimicrobial and anti-viral activity\cite{46} |
| 16   | 48.58 | 366.7           | C22H42N4O4        | 2-Nonadecanone 2,4—Dinitrophenylhydrazine | Antimicrobial\cite{46} |
| 17   | 52.54 | 462.23          | C10H16O           | Octanoic acid        | No activity reported |
| 18   | 58.6  | 366.7           | C22H50O           | 2-Pentacosanone      | No activity reported |
| 19   | 59.47 | 428.28          | C10H20O2S         | Nonacosanal          | Anti-adhesive, vasodilator, angiotensin AT2 receptor antagonist and sulfaetric\cite{46} |
| 20   | 59.82 | 228.37          | C14H28O2          | Methyl 11-Methyl-Dodecanoate | Anti-fungal, antioxidant activities\cite{46} |
| 21   | 63.37 | 312.5           | C20H40O2S         | Eicosanoic acid      | Reduced heart diseases, kidney and liver function, blood clotting |
| 22   | 68.52 | 254.41          | C16H30O2          | Palmitoleic acid     | Anti-inflammatory, essential oils |
| 23   | 69.66 | 298.5           | C18H34O2          | Oleic acid           | Antimicrobial, Antifungal, anticonvulsive activity, Anti-adhesive, Antiallergic, Antiagalstes, Antiatherosclerosis, Anesthetic, Antihelmentic, Antixanxiety, Antibacterial, Antihelbert, Antibiotic, Anticancer, Anticonvulsant, Antidiabetic, Antiadharbic, Antiarterity, Antigastric, Anti-inflammatory, Antiobesity, Antioxidant, Antisulcer, Antitubercollosic, Anticold, Antihepatotoxic and Antiviral activities, Dermatogenic\cite{47} |
| 24   | 70.65 | 546.8           | C22H40O4P         | Dihexadecyl Phosphate | Emulsifying agent |
| 25   | 73.54 | 340.6           | C22H44O2          | Docasanoic acid      | Antibacterial\cite{47} |

**Pod**

| Peak | RT  | Molecular Weight | Molecular Formula | Name of the compound | Medicinal uses |
|------|-----|------------------|-------------------|----------------------|---------------|
| 1    | 14.65 | 164.16          | C6H12O5           | Beta-LArabinopyranoside, Methyl | Catechol-O-methytransferase inhibitor, methyl donor Methylguanidine inhibitor, 17-beta-hydroxysteroid dehydrogenase inhibitor, beta-adrenergic receptor blocker Beta-adrenergic agents, antitumor (liver, lung, breast, and prostate), antioxidant (LDL)\cite{48} |
| 2    | 16.38 | 214.38          | C14H30O           | Heptane, 1,1- oxybis | Antibacterial, antioxidant activities |
| 3    | 17.43 | 130.18          | C14H30O           | Heptanoic acid       | Used in the preparation of esters for the fragrance industry, and as an additive in cigarettes |
| 4    | 19.58 | 170.25          | C7H14O2           | 9—Decenoic acid      | Antimicrobial activity\cite{49} |
| 5    | 20.71 | 144.21          | C10H18O2          | Octanoic acid        | Antibacterial activity |
| 6    | 24.14 | 184.31          | C8H16O2           | Oxiran, Decyl        | Antimicrobial, adhesive\cite{49} |
| 7    | 25.29 | 158.28          | C12H20O           | Nonanoic acid        | Anti-microbial, anti-inflammatory, antitumor, anti hyperpergumentative, antiproliferative, anti-acne, cytotoxic, Anti-leukemic, oxy radical scavenging Activity\cite{49} |
| 8    | 26.07 | 342.65          | C9H18O2           | 1,2,4-Benzetriel, Tris ( Trimethyl silyl) Ether | Antibacterial, anti-infecitive |
| 9    | 26.89 | 126.2           | C15H30O3Si3       | 5, 5-Dimethyl-Cyclohex-3-en-1-ol | No activity reported |
| 10   | 28.7  | 172.26          | C8H14O            | N-Decanoic acid      | Antibacterial and antifungal activity\cite{48} |
| 11   | 33.31 | 530.9           | C11H20O2          | Z-Z-, 28-Heptatriactontadien-2-one | Vasodilator\cite{46} |
| 12   | 55.31 | 128.21          | C13H20O           | 4-Methyl-6-Hepten-4-olide | No activity reported |
| 13   | 56.78 | 166.13          | C8H16O            | Phthaleic acid       | Antioxidant activity and larvicidal activities\cite{49} |
| 14   | 58.68 | 366.7           | C8H8O4            | 2-Pentacosanone      | No activity reported |
| 15   | 59.52 | 298.5           | C18H34O2          | Oleyl alcohol, Cholesterolacetate | Used as a nonionic surfactant, emulsifier, emollient and thicker in skin creams, lotions and other cosmetic products including shampoos |

Continued
| Peak | RT  | Molecular Weight | Molecular Formula | Name of the compound | Medicinal uses |
|------|-----|------------------|-------------------|----------------------|----------------|
|     |     |                  |                   |                      |                |
| 16   | 59.88 | 298.5            | Methyl Stearate   |                      | GABA aminotransferase inhibitor, anti-inflammatory, intestinal lipid metabolism regulator, antihelmintic, antinociceptive |
| 17   | 61.06 | 282.5            | C19H38O2          | 6-Octadecenoic acid | Antioxidant and reduces the triglycerides level—Protects LDL against peroxidation and inhibits the progression of atherosclerosis, Antiallergic, Antianemic, Antianxiety, Anti bacterial, Antiinflammatory, Anticancer, Anticarcinogenic, Anticataract, Anticoagulant, Anticonvulsant, Antidiabetic, Antidiarthritic, Antifatigue, Antiinflammatory, Antimalarial, Antioxidant, Antitussive, Antiulcer, Antivascular, Anticold, Antiglaucomatous, Antihypertensive, Antiplatelet, Antiproliferative, Antipruritic, Antipyretic, Antidepressant, Antihistaminic, Antiarthritic, Antianginal, Anticancer, Anticandida, Anticonvulsant, Antidiabetic, Antihypertensive, Antithrombotic, Antioxidant, Antistress, Antiviral activity |
| 18   | 63.33 | 652.9            | C18H34O2          | L-(+)-Ascorbic acid, 2,6Dihepadcanoate | No activity reported |
|     |     |                  |                   |                      |                |
| 19   | 63.82 | 254.41           | Palmitoleic acid  |                      | Anti-inflammator, essential oils |
| 20   | 65.44 | 546.8            | C16H30O2          | Dihexadecyl Phosphate | Emulsifying agent |
| 21   | 68.58 | 546.8            | C12H22O2          | Palmitoleic acid     | Anti-inflammatory, essential oils |
| 22   | 69.72 | 410.71           | C6H12O5           | Methyl –L-Arabinopyranoside, Methyl | Catechol-O-methyltransferase inhibitor, methyl donor Methylguanidine inhibitor, 17-beta-hydroxysteroid dehydrogenase inhibitor, beta-adrenergic receptor blocker Beta-adrenergic agents, anticancer (liver, lung, breast, and prostate), antioxidant (LDL) |
| 23   | 70.79 | 546.8            | C7H14O2           | Heptanoic acid       | Used in the preparation of esters for the fragrance industry, and as an additive in cigarettes |
| 24   | 73.4  | 340.6            | C12H22O2          | 2-Oxepanone, 7-Hexyl | Used as a food flavouring agent |
|     |     |                  |                   |                      |                |
| 7    | 24.53 | 170.21           | C3H14N2O2         | 1H-Imidazole, 2-(Diethoxy methyl) - | Antimycobacterial activity, anticancer, antifungal, analgesic and anti-HIV activities |
| 8    | 26.67 | 172.26           | C10H20O2          | N-Decanoic acid      | Anti-bacterial and antifungal activity |
| 9    | 27.4  | 530.9            | C7H17O0           | Z,Z-6, 28Heptatriacontadien-2-one | Vasodilator |
| 10   | 58.61 | 366.7            | C25H50O           | 2-Pentacosanone      | No activity reported |
| 11   | 59.49 | 422.8            | C29H58O           | Nonacosanal          | Antiinflammatory, vasodilator, angiotensin AT2 receptor antagonist and sulforetic |
| 12   | 59.82 | 298.5            | C12H22O2          | Methyl stearate      | GABA aminotransferase inhibitor, anti-inflammatory, intestinal lipid metabolism regulator, antihelmintic, antinociceptive |
| 13   | 63.05 | 322.6            | C23H46            | 5-methyl-Z-5-Docosene | No activity reported |
| 14   | 68.01 | 280.44           | C18H32O2          | 9,12-Octadecadienoic acid (Z,Z) - | Antinflammatory, hypcholesterolemic, cancer preventive, hepato protective, nematicide, insecticidal antihistaminic, antiarthritic, anticorony, anticecmatic antiscue, 5-Alpha reductase inhibitor Antianlogenic |
| 15   | 68.47 | 198.3            | C12H22O2          | 2-Oxepanone, 7-Hexyl | Used as a food flavoring agent |
| 16   | 68.92 | 254.41           | Palmitoleic acid  |                      | Anti-inflammatory, essential oils |
| 17   | 69.66 | 298.5            | C19H38O2          | Methyl stearate      | GABA aminotransferase inhibitor, anti-inflammatory, intestinal lipid metabolism regulator, antihelmintic, antinociceptive |
| 18   | 70.62 | 546.8            | C32H67O4P         | Dihexadecyl Phosphate | Emulsifying agent |

**Seed**

| Peak | RT  | Molecular Weight | Molecular Formula | Name of the compound | Medicinal uses |
|------|-----|------------------|-------------------|----------------------|----------------|
| 1    | 13.29 | 164.16           | C6H12O5           | Beta –L-Arabinopyranoside, Methyl | Catechol-O-methyltransferase inhibitor, methyl donor Methylguanidine inhibitor, 17-beta-hydroxysteroid dehydrogenase inhibitor, beta-adrenergic receptor blocker Beta-adrenergic agents, anticancer (liver, lung, breast, and prostate), antioxidant (LDL) |
| 2    | 15.68 | 188.34           | C7H14O2           | Heptanoic acid       | Used in the preparation of esters for the fragrance industry, and as an additive in cigarettes |
| 3    | 15.98 | 130.18           | C8H14N2O2         | 1H-Imidazole, 2-(Diethoxy methyl) - | Antimycobacterial activity, anticancer, antifungal, analgesic and anti-HIV activities |
| 4    | 18.71 | 144.21           | C5H10O2           | Octanoic acid        | Anti-bacterial activity |
| 5    | 22.23 | 170.25           | C10H18O2          | Cyclohexane butanoic acid | Effect on CNS, antioxidant, analgesic and anti-inflammator activity |
| 6    | 23.1  | 282.5            | C18H34O2          | Oleic acid           | Antimicrobial, Antifungal, anticonvulsive activity, Anti-adhesive, Antiallergic, Antiagglutination, Antiatherosclerosis, Anesthetic, Antihelminthic, Antianxiety, Antibacterial, Antiinfectious, Antibiotic, Anticancer, Anticoagulant, Anticonvulsant, Antiinfective, Antiplatelet, Antiviral, Antioxidant, Antistress, Antitumor, Neuroprotective, Neurotransmitter, Termiticide and Antiviral activity |
| 7    | 24.53 | 170.21           | C8H14N2O2         | 1H-Imidazole, 2-(Diethoxy methyl) - | Antimycobacterial activity, anticancer, antifungal, analgesic and anti-HIV activities |
| 8    | 26.67 | 172.26           | C10H20O2          | N-Decanoic acid      | Anti-bacterial and antifungal activity |
| 9    | 27.4  | 530.9            | C7H17O0           | Z,Z-6, 28Heptatriacontadien-2-one | Vasodilator |
| 10   | 58.61 | 366.7            | C25H50O           | 2-Pentacosanone      | No activity reported |
| 11   | 59.49 | 422.8            | C29H58O           | Nonacosanal          | Antiinflammatory, vasodilator, angiotensin AT2 receptor antagonist and sulforetic |
| 12   | 59.82 | 298.5            | C12H22O2          | Methyl stearate      | GABA aminotransferase inhibitor, anti-inflammatory, intestinal lipid metabolism regulator, antihelmintic, antinociceptive |
| 13   | 63.05 | 322.6            | C23H46            | 5-methyl-Z-5-Docosene | No activity reported |
| 14   | 68.01 | 280.44           | C18H32O2          | 9,12-Octadecadienoic acid (Z,Z) - | Antinflammatory, hypcholesterolemic, cancer preventive, hepato protective, nematicide, insecticidal antihistaminic, antiarthritic, anticorony, anticecmatic antiscue, 5-Alpha reductase inhibitor Antianlogenic |
| 15   | 68.47 | 198.3            | C12H22O2          | 2-Oxepanone, 7-Hexyl | Used as a food flavoring agent |
| 16   | 68.92 | 254.41           | Palmitoleic acid  |                      | Anti-inflammatory, essential oils |
| 17   | 69.66 | 298.5            | C19H38O2          | Methyl stearate      | GABA aminotransferase inhibitor, anti-inflammatory, intestinal lipid metabolism regulator, antihelmintic, antinociceptive |
| 18   | 70.62 | 546.8            | C32H67O4P         | Dihexadecyl Phosphate | Emulsifying agent |

Continued
The total phenol content was considerably high and hence the extract could have the ability to treat many diseases. Hence, this plant is of special interest for further investigations.

Free radicals and other reactive oxygen species (ROS) have been implicated in various diseases like neurodegenerative diseases, cancer and cardiovascular diseases. Bioactive compounds present in plants have long been known to possess antioxidant, anti-allergic, anti-inflammatory, anti-viral, anti-proliferative and anti-carcinogenic properties because of which a lot of attention is given to the evaluation of the antioxidant capacity of foods, medicinal plants and other nutritional antioxidant supplements. The DPPH is a stable free radical that is...
commonly used to analyze free radical scavenging activities of antioxidant. Antioxidant molecules can quench DPPH and transform them into colorless products. A lower value of IC₅₀ (half maximal inhibitory concentration) designates the stronger ability to scavenge free radicals whereas the higher value of IC₅₀ designates weaker scavenging activity, as more scavengers are required to achieve 50% scavenging reactions. The phenolic compounds act as primary antioxidants or free radical scavengers. They contain hydroxyls that are responsible for the radical scavenging effect due to redox properties. Hence, high free radical scavenging activity in the current investigation could be attributed to high phenolic and flavonoid contents in the plant extracts. Suggestively, P. timoriana could be used as a source of antioxidants for pharmacological preparations.

The antioxidant capacity of the extracts was also determined using the phosphomolybdate assay, which was based on reducing Mo (VI) to Mo (V) by the test sample and the subsequent production of green phosphate compounds with absorbance at 765 nm. Various flavonoids and related polyphenols have been found to contribute considerably to the phosphomolybdate scavenging potential of herbal plants in recent research.

The ABTS radical scavenging assay uses a reaction of ABTS and potassium persulfate to produce a blue ABTS⁺ chromophore. The scavenging activity was found significantly high in the pod part which was comparable to the standard, Ascorbic acid. Interestingly in all the antioxidant assays, the scavenging activity was found the highest in the pod part that also had significantly high flavonoid and phenol contents compared to other parts. Furthermore, from the GC–MS analysis, the bioactive compound ascorbic acid was also detected from the pod and that could be the reason for high antioxidant potential in the pod.

Phenol and flavonoid molecules are essential antioxidant compounds that are responsible for oxidizing free radicals due to their capability to hand out hydrogen atoms to free radicals. A linear correlation of total phenolic

| Sl. No | Compound name                       | Molecular weight (< 500kD) | Log P (< 5) | H-bond donor (< 5) | H-bond acceptor (< 10) |
|--------|------------------------------------|-----------------------------|-------------|--------------------|------------------------|
| 1      | Methyl beta-L-arabinopyranoside     | 164.16 g/mol                | −2          | 3                  | 5                      |
| 2      | 3-n-Hexylthiolane, S,S-dioxide      | 204.33 g/mol                | 3.1         | 0                  | 2                      |
| 3      | L-(+)-Ascorbic acid, 2,6-Dihexadecanoate | 176.12 g/mol            | −1.6        | 4                  | 6                      |
| 4      | 1H-Imidazole, 2-(Diethoxy methyl)   | 214.22 g/mol                | 0.5         | 1                  | 5                      |
| 5      | Oleic acid                         | 282.5 g/mol                 | 4.5         | 1                  | 2                      |
| 6      | Cyclohexane butanoic acid          | 170.25 g/mol                | 3.4         | 1                  | 2                      |

Table 8. Lipinski's properties of the selected bioactive compounds from extracts of P. timoriana.

Figure 8. Structure of bioactive compounds identified from P. timoriana and used for the analysis of molecular docking. (Photo courtesy: www.pubchem.ncbi.nlm.nih.gov).
and flavonoid contents with an antioxidant potential of plant extracts is already established. The correlation of total phenolic and flavonoid content with the antioxidant potential of *P. timoriana* is shown in Fig. 11. High correlations between DPPH antioxidant activity and total phenol (y = 0.682x; R² = 0.87, p < 0.002) and total flavonoid (y = 0.839x; R² = 0.74, p < 0.01), ABTS antioxidant activity and total phenol (y = 0.9051x; R² = 0.3735, p < 0.007) and total flavonoid (y = 0.4359x; R² = 0.2098, p < 0.05) and phosphomolybdate antioxidant activity total phenol (y = 0.4976x; R² = 0.265, p < 0.028) and total flavonoid (y = 0.3063x; R² = 0.246, p < 0.036) and were observed at a
Table 9. Molecular docking score for bioactive compounds of *P. timoriana* with BCL-2.

| Sl. No | Ligand                                                | Docking score | No of hydrogen bonds formed |
|-------|-------------------------------------------------------|---------------|-----------------------------|
| 1     | Methyl beta-L-arabinopyranoside                       | − 4.3         | 4                           |
| 2     | 3-n-Hexylthiolane, S,S-dioxide                        | − 6.3         | 3                           |
| 3     | L-(+)-Ascorbic acid, 2,6-Dihexadecanoate              | − 4.4         | 3                           |
| 4     | 1H-Imidazole, 2-(Diethoxy methyl)                      | − 4.8         | 1                           |
| 5     | Oleic acid                                            | − 5.5         | 2                           |
| 6     | Cyclohexane butanoic acid                             | − 4.5         | 0                           |
| 7     | Paclitaxol                                            | − 10.8        | 3                           |

Table 10. Molecular docking score for bioactive compounds of *P. timoriana* with COX-2.

| Sl. No | Ligand                                                | Docking score | No of hydrogen bonds formed |
|-------|-------------------------------------------------------|---------------|-----------------------------|
| 1     | Methyl beta-L-arabinopyranoside                       | − 5.6         | 4                           |
| 2     | 3-n-Hexylthiolane, S,S-dioxide                        | − 5.7         | 2                           |
| 3     | L-(+)-Ascorbic acid, 2,6-Dihexadecanoate              | − 6.0         | 4                           |
| 4     | 1H-Imidazole, 2-(Diethoxy methyl)                      | − 5.8         | 4                           |
| 5     | Oleic acid                                            | − 5.3         | 2                           |
| 6     | Cyclohexane butanoic acid                             | − 5.7         | 2                           |
| 7     | Isoxicam                                              | − 9.3         | 3                           |

Figure 11. Correlation values of antioxidant versus total phenol and flavonoid content. (A) DDPH antioxidant activity; (B) ABTS antioxidant activity; (C) Phosphomolybdate antioxidant activity.
95% confidence level. Accordingly, at correlation coefficients, it is attainable to speculate that phenol and flavonoid compounds have played significant roles in the antioxidant activities of the plant extracts.

Infectious diseases caused by bacterial agents pose a major threat to public health worldwide. Antibiotics have safety and efficacy limits and due to similar toxicity and efficacy, biological research on antimicrobial functions of plants should be expanded. The bioactive compounds present in plants such as alkaloids, flavonoids, tannins, phenol, saponins etc. are their secondary metabolites that act as defense mechanism against microorganisms, insects and other herbivores and the presence of these compounds in tree bean could be responsible for the observed antimicrobial property. Among them, plants in response to microbial infections synthesize flavonoids and it is a successful antimicrobial substance against a broad range of microbes. Phenols are widely present in secondary products of medicinal plants as well as in many edible plants and have the potential of antibacterials and free radical scavengers. Saponins also have antimicrobial properties as they can induce protein and enzyme leakage from cells. Tannins bind to proline-rich proteins, thus, stopping them from being synthesized. It was also reported that tree bean could inhibit pathogenic bacterial growth such as E. coli, V. cholera, S. aureus, B. cereus Streptococcus fecalis. Similarly, in the present study, different P. timoriana extracts were seen to be effective against many cosmopolitan as well as pathogenic microorganisms including E. coli (urinary tract infections and diarrhoea), B. subtilis (food poisoning), P. aeruginosa (urinary tract, respiratory system infection) and B. pumilus (foodborne disease, severe sepsis of neonatal infants etc.). It is interesting to note that the multi-drug resistant P. aeruginosa and B. subtilis strains showed more sensitivity to the tested extracts.

Preliminary antibacterial investigations using the well diffusion assay revealed an intriguing antimicrobial activity profile against both gram-positive and gram-negative bacteria. Then, a quantitative investigation was done to determine the total bactericidal activity of extracts using MIC. The plant part extracts showed moderate to excellent efficacy against bacterial strains with MIC values ranging from 2.19 mg/ml to 7.3 mg/ml. It has been proposed that all plant species with MIC values of up to 8 mg/ml have at least some inhibitory action, and any dose above this should not be regarded as effective. Among the studied extracts, the pod appeared to have the majority of the moderate inhibitors with an intriguing bactericidal effect against E. coli (2.19 mg/ml).

Our findings support the use of tree bean in folk medicine for the treatment of several infectious diseases. It is opined that P. timoriana species can be a good source for antibacterial drugs against gram-positive and gram-negative bacteria, especially against multi-resistant microorganisms. However, isolation of these bioactive antibacterial compounds and detailed characterization of them should provide a deeper understanding of drug discovery and development.

The functional groups can be used in different pharmaceutical products such as anti-cancers, anti-ulcers, anti-inflammatory, anti-oxidants, antimicrobial etc. Hence, the functional groups present in the bioactive compounds can have diverged applications including antimicrobial, anti-cancer and anti-inflammatory properties etc. FTIR spectroscopy is a reliable and sensitive method for the detection of bioactive compositions. Our analysis showed clear discrimination between the plant parts examined, depicting great variations. It was also able to determine the bioactive compounds that could be used as herbal medicines for various diseases.

Most of the compounds identified are known to possess a variety of pharmacological activities. The higher total phenol and flavonoid contents, the significant potential of antioxidant and antimicrobial activities are attributed to the presence of these bioactive compounds (Table 6). From the chromatogram, 8 compounds (Beta-L-Ascorbic acid, 2,6-Dihexadecyl phosphate) were found in all the plant parts and the biological significance of these compounds is shown in Table 6. The compounds -Phthalic Acid, 3-Methyl-2-(2-Oxopropyl) Furan, Chloroacetic acid, tetracycl ester, 1-Cyclohexane-1-Methanol, 4-(1-Methyl ethenyl), Formate etc. possessed antioxidant potentials. Interestingly, among all extracts, L-(+)-Ascorbic acid, 2,6-Dihexadecanoate was found only in the pod. This could be the reason for the highest antioxidant IC₅₀ and free radical scavenging activity by the pod. The compounds such as Oleic acid, 3-Methyl-2-(2-Oxopropyl) Furan, Chloroacetic acid, tetradecyl ester, 1-Cyclohexane-1-Methanol, 4-(1-Methyl ethenyl), Formate etc. possessed antioxidant potentials. Interestingly, among all extracts, L-(+)-Ascorbic acid, 2,6-Dihexadecanoate was found only in the pod. This could be the reason for the highest antioxidant IC₅₀ and free radical scavenging activity by the pod. The compounds such as Oleic acid, 3-Methyl-2-(2-Oxopropyl) Furan, 3-n-Hexylthiolane, S, S-dioxide, 3-n-Hexylthiolane, S, S-dioxide, Nonanoic acid, Oxirane, hexadecyl etc. were shown to possess significant antimicrobial potential hence higher antimicrobial activity was shown by the extracts. Compounds identified previously from P. biblosa such as 1,2,4-Benzentriol, linoleic acid, 6-Octadecanoic acid, oleic acid, palmotolic acid, 9-Decanoic acid, cyclohexane butanoic acid, N-Decanoic acid were also detected in our study. All the identified compounds belonged to various chemical groups and a majority of them have been confirmed to have significant biological activities. And some compounds are yet to be defined in detail. However, further investigation on isolation, characterization of the compounds from plant extracts is sought to verify their various pharmacological significance.

Computational advances played a significant influence in the drug development process. Virtual screening approaches are frequently and widely utilized to minimize the cost and time of drug development. Molecular docking is a technique that is used to discover novel ligands for proteins structure and plays a significant role in structure-based drug design. The relationship between the compounds and the receptor plays a vital role in the formulations of drugs. Natural products can help cure a wide variety of human ailments, including cancer, inflammatory, etc. and various medicines are derived from natural products, e.g., an anticancer drug, paclitaxel (taxol) is derived from extracts of Taxus brevifolia. Plant-based medicines are the best potential options, given the rise of drug resistance in various diseases, and the negligible side effects of traditional treatments. We investigated the binding capability of bioactive compounds from P. timoriana with key anticancer and anti-inflammatory targets in this study since various ailments had been traditionally treated with P. timoriana. The higher negative docking score represented a high binding affinity between the receptor and ligand molecules, showing the higher efficiency of bioactive compounds. The docked ligand scores for anticancer ranged from -4.3 to -6.3 and from -5.3 to -6.0 for anti-inflammatory. In the present study, 3-n-Hexylthiolane, S, S-dioxide, and L-(+)-Ascorbic acid are the lead compounds showing the highest docking score among the subjected bioactive
compounds, which also exhibited antibacterial, antioxidant potentials. The docking analysis also revealed that diverse energy sources were consistent and contributed to the overall strength of 3-n-Hexylthiolane, S, S-dioxide, and L-(+)-Ascorbic acid binding with each target protein. Methyl beta-L-arabinopyranoside had the lowest score while 3-n-Hexylthiolane, S, S-dioxide had the highest score as anticancer agents. The anti-inflammatory potential was found the highest in L-(+)-Ascorbic acid, 2,6-Dihexadecanoate and lowest in Oleic acid. Nonetheless, all the compounds were in considerable range as anti-inflammatory and anti-cancer therapeutic agents. Our study shows that the selected bioactive compounds can efficiently bind to the receptors and molecular docking can be successfully used in finding BCL-2 and COX-2 inhibitors from *P. timoriana* extracts. Interestingly, the presence of diverse bioactive compounds supports the traditional practitioners’ use of these plant parts for the treatment of various diseases. Hence, the studied bioactive compounds have the potential to be used as anticancer and anti-inflammatory agents against these diseases. To the best of our knowledge, this is the first report that bioactive compounds from underutilized, ethnobotanically important *P. timoriana* are subjected to molecular docking for screening their pharmacological potentials.

**Conclusions**

The present study was focused on identification of various bioactive compounds from the edible parts of *P. timoriana* for the first time by FTIR and GC–MS analysis. The bioactive compounds are responsible for various therapeutic and pharmacological properties. The study also provided the evidence of *P. timoriana* extracts for its antioxidant and antimicrobial potentials. The bioactive compounds Methyl beta-L-arabinopyranoside 3-n-Hexylthiolane, S,S-dioxide, L-(+)-Ascorbic acid, 2,6-Dihexadecanoate, 1H-Imidazole, 2-(Diethoxy methyl), Oleic acid, Cyclohexane butanoic acid showed promising binding affinity towards the two target proteins in the molecular docking studies. From our findings, the plant may enable us to develop reliable and effective drugs against various diseases. Further investigations to analyze its bioactivity and clinical trials are necessary for discovery of new drugs formulations.

**Methods**

**Collection of plant material.** Edible parts of *Parkia timoriana* viz. flower, capitulum, pod and seed (Fig. 12) were collected from Aizawl, Mizoram, India. The collected samples were brought to the Department of Botany, Mizoram University for further analysis. Identification of the collected specimen were done following published literature. The specimens were also deposited in the Herbarium of the Department of Botany, Mizoram University (Voucher no. MZUBOT0100) and identified and confirmed by Dr. Khomdram Sandhyan Devi, Plant Taxonomist, Department of Botany, Mizoram University. The ethnobotanical survey was conducted in the Aizawl district of Mizoram. The study was based on personal interviews with local herbal medicine practitioners and other knowledgeable local people and published literature.

**Bioactive compounds analysis.** A 50 g of air dried powdered edible part was extracted with 500 mL of methanol using a Soxhlet apparatus at moderate temperature of 30–45 °C to avoid disruption of thermolabile compounds for 25 cycles. The extract was then concentrated at 50 °C until it formed a paste. The concentration of each sample was adjusted to 100 µg/mL using methanol. Presence of various phytochemicals: alkaloids, saponins, flavonoids, tannins and terpenoids from each extract were estimated after Nwankwo and Ukaegbu-Obi.

**Determination of Total Phenolic Content (TPC).** Total phenol was determined using the Folin-Ciocalteu reagent method with slight modifications. A 100 µl plant extract sample was mixed with 0.1 ml Folin-
Ciocalteu reagent (1 N) and incubated at room temperature. Then, 5 ml of Na₂CO₃ was added and incubated at room temperature for 30 min. Total phenolic content was determined using a UV–VIS spectrophotometer (Bio-spectrometer, Eppendorf, Germany) at 760 nm. Gallic acid was used as standard and total phenol was expressed as gallic acid equivalent (mg/g of the extracted compound).

**Determination of Total Flavonoid Content (TFC).** The total flavonoid content was determined using the aluminium chloride calorimetric method³⁴. Briefly, 1 ml extract was mixed with 1 ml methanol, 0.5 ml aluminium chloride (1.2%) and 0.5 ml potassium acetate (100 mM) and incubated at room temperature for 30 min. The absorbance was measured at 415 nm, and quercetin was used as standard. The total flavonoid content was expressed as quercetin equivalent (mg/g of the extracted compound).

**DPPH radical scavenging activity.** The antioxidant activity of the extract was determined using the 2,2-diphenyl-1-picrylhydrazyl (DPPH) radical scavenging method³⁴. To 50 µl of 10–100 µg/mL plant extract, 2 ml DPPH was added and kept in dark at room temperature for 30 min. Then, 1 ml methanol and 2 ml DPPH was used as negative control while methanol solution was used as a positive control. Then the absorbance was measured at 517 nm. The percentage DPPH radical scavenging activity (%RSA) was calculated as:

\[
\%RSA = 100 \times \frac{(\text{absorbance of control} - \text{Absorbance of sample})}{\text{Absorbance of control}}
\]

where control is 2 ml of DPPH + 1 ml of methanol.

**ABTS radical scavenging assay.** The 2,2’-azinobis (3-ethylbenzthiazoline-6-sulphonic acid) ABTS radical cation decolorization test was used to assess the free radical scavenging activity of plant extracts³⁴. The ABTS⁺ cation radical was created by reacting 7 mM ABTS in water with 2.45 mM potassium persulfate (1:1) and kept in the dark at room temperature for 14–16 h before use. After diluting the ABTS⁺ solution with methanol, the absorbance of 0.700 at 734 nm was obtained. The absorbance was measured 30 min after the addition of 10 µl of plant extract to 3.990 ml of ABTS solution. In each experiment, a suitable solvent blank was run. All the tests were repeated at least three times and ascorbic acid was used as standard. The ABTS scavenging effect (%) was calculated as:

\[
\% \text{ inhibition} = \frac{\text{Absorbance of Control} - \text{Absorbance of sample}}{\text{Absorbance of control}} \times 100
\]

where control is ABTS solution with methanol.

**Phosphomolybdate assay.** Using ascorbic acid as a reference, the total antioxidant capacity of the plant extract was measured using phosphomolybdate method³⁶. A total of 1 ml of reagent solution (0.6 M sulphuric acid, 28 mM sodium phosphate, and 4 mM ammonium molybdate) was combined with 0.1 ml of plant extract. The tubes were incubated for 90 min at 95 °C water bath. The absorbance was measured at 765 nm against a blank after the samples had been cooled to room temperature. The antioxidant capacity was calculated as:

\[
\text{Antioxidant effect} (\%) = \frac{(\text{Control absorbance} - \text{sample absorbance})}{\text{control absorbance}} \times 100
\]

where control is reagent + methanol.

**Antimicrobial activity.** The antimicrobial activity of *P. timoriana* extract was measured using the agar well diffusion method against four bacterial strains- *Bacillus pumilus* (ATCC14884), *Bacillus subtilis* (ATCC11774), *Escherichia coli* (ATCC11229) and *Pseudomonas aeruginosa* (ATCC9027). Rifampicin was used as a positive control. Bacterial suspensions were prepared using McFarland standard. To determine bacterial density, a McFarland number 0.5 standard was prepared by combining 9.95 ml of 1% H₂SO₄ in distilled water and 0.05 ml of 1% BaCl₂ in distilled water³⁶. The mixture was kept in an airtight bottle and used to compare bacterial suspensions as needed.

**Preparation of McFarland standard.** To determine bacterial density, a McFarland number 0.5 standard was prepared by combining 9.95 ml of 1% H₂SO₄ in distilled water and 0.05 ml of 1% BaCl₂ in distilled water³⁶. The mixture was kept in an airtight bottle and used to compare bacterial suspensions as needed.

**Minimum inhibitory concentration (MIC).** For determination of minimum inhibitory activity of the plant extracts, the broth micro dilution technique was used using 96- well microtiter plate³⁶. Different concentrations of the extracts (0.5 mg/ ml to 20 mg/ml) were prepared with methanol. Overnight grown culture of the bacteria was used for inoculation. Plates were incubated at 37 °C at 120 rpm shaking for 24 h. Growth inhibition was checked by taking the absorbance at 600 nm in a UV–VIS spectrophotometer (Multiscan™ GO, Thermo Scientific, USA) along with the controls. Then, IC₅₀ values were expressed as the concentration of plant extract necessary to produce a 50% reduction of the bacterial growth.

**FT-IR analysis.** Functional groups present in the *P. timoriana* extract were identified using Fourier transformed infrared spectroscopy (Shimadzu IRAffinity-1S, Japan) for frequency ranging from 400–4000 cm⁻¹ following the manufacturer's instruction.
**GC/MS analysis.** Sample preparation. A 100 µl of methanolic plant extract was dissolved in 1 ml of methanol solvent. The solution was stirred vigorously using a vortex mixer for 10 secs and filtered using a 0.2 micron membrane filter. Then, the clear extract was used for GC–MS analysis.

The identification of compounds was carried out by using GC–MS (Clarus 690, Perkin-Elmer, USA) (Auto system XL) fitted with a capillary column (123.5 m x 678 μm) coupled to a mass detector Turbo mass gold–Perkin Elmer Turbo mass 5.1 spectrometer with an Elite—1 (100% Dimethyl poly siloxane), 123.5 m x 678 μm of the capillary column. The instrument was fixed at an initial temperature of 40 °C and ramp 5 °C/min to 115 °C, hold 5 min, ramp 5 °C/min to 140 °C, hold 5 min, ramp 2 °C/min to 210 °C, hold 8 min, and maintained at this temperature for 3 min. At the end of this period, the oven temperature was increased up to 250 °C, at the rate of an increase of 5 °C/min, and maintained for 9 min. Injection port temperature was ensured at 230 °C and Helium flow rate at 1.5 ml/min. The ionization voltage was set at 70 eV. The samples were injected in split mode as 10:1. Mass spectral scan range was set at 50–800 (m/z). The ion source temperature was maintained at 230 °C and the Interface temperature at 240 °C. The MS start time was set at 3 min, and the end time was 75 min with a solvent cut time of 3 min. The spectrum obtained of volatile compounds detected through GC–MS were compared and matched with NIST 17 (National Institute of Standard and Technology) online library Ver. 2.3.

**Molecular docking analysis.** Molecular docking is used to find the best-fit orientation of ligand and protein. The bioactive compounds from *P. timoriana* were selected for molecular docking analysis. The target proteins BCL-2 and cyclooxygenase (COX-2) were docked using selected bioactive compounds using BIOVIA, Discovery Studio (version 2021) and AutoDock Vina software and binding energies were calculated. The ligands and the target proteins were prepared following the standard procedure of protein and ligand preparation and the files were submitted to AutoDock vina. The obtained binding energy and binding contacts of each ligand, and the docked data were analyzed using Discovery Studio Visualizer.

Preparation of ligand. Six compounds were predicted based on Lipinski's rule of five for the docking analysis. The chemical structures of the selected bioactive compounds were retrieved through the PubChem compound database at NCBI (http://pubchem.ncbi.nlm.nih.gov/).

Target protein retrieval. Two proteins, BCL-2 (PDB ID: 1PXX) for anticancer and cyclooxygenase-2 (COX-2) (PDB ID: 1K3K) for anti-inflammatory were selected for their interactions with the bioactive compounds from *P. timoriana*. Expression of BCL2 is thought to be the cause of follicular lymphoma. And the COX-2 plays a significant role in the modulation of inflammation. The 3D X-ray crystal structure of the proteins was retrieved from Protein Data Bank (PDB).

Target protein preparation. The Discovery Studio software was used to process and prepare the proteins and convert raw PDB structure into prepared protein models. And X-ray crystal structures of the proteins were prepared by removing the water molecules present in the structures. Then, Discovery Studio software was used to analyze protein structure, hydrogen bond interactions and non-bond interactions of ligands with the active site residues and generations of high-quality images.

Docking. The prepared ligands and target proteins were analyzed using AutoDock Vina to perform the docking. The various conformations for ligand in the docking procedure were generated and the final energy refinement of the ligand pose was performed. The docking score of the best pose into the target proteins for all the tested bioactive compounds was calculated.

Statistical analysis. All the experiments were carried out in triplicate, and the findings were reported as mean ± SD. All the data and the linear regression coefficient (R²) for total flavonoid and phenolic content with antioxidant activity was analyzed using Graph Pad Prism Version 5. P-value < 0.05 was considered significant.

Ethical approval and informed consent. Authors declare that all methods were carried out in accordance with relevant guidelines and regulations. Authors confirm that all experimental protocols were approved by the Institutional Human Ethics Committee, Mizoram University. Authors also confirm that informed consent was obtained from all subjects.

Material collection. For collection of plants, all relevant permits or permissions have been obtained. The study also complies with local and national regulations.

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Competing interests
The authors declare no competing interests.

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