



**INTERNATIONAL JOURNAL OF  
PHARMACEUTICAL SCIENCES**  
[ISSN: 0975-4725; CODEN(USA): IJPS00]  
Journal Homepage: <https://www.ijpsjournal.com>



## Research Paper

# Virtual Screening of Physicochemical and Pharmacokinetic Parameters of Selected Bryophyllum Pinnatum Constituents

Ketura Kambampaty<sup>\*1</sup>, Dr. Preeti Salve<sup>2</sup>, Nurzeba Bepari<sup>3</sup>

<sup>1</sup>Department of Pharmaceutics, Maratha Mandal College of Pharmacy, Belgaum

<sup>2</sup>Department of Pharmaceutical Chemistry, KLE college of Pharmacy, Belgaum

<sup>3</sup>Department of Pharmaceutics, Rani Chennamma College of Pharmacy, Belgaum.

## ARTICLE INFO

Published: 22 Jan. 2025

### Keywords:

Bryophyllum pinnatum,  
Lipinski's rule of five,  
Molsoft, ADME,  
Schrodinger,  
pharmacokinetic,  
physicochemical.

### DOI:

10.5281/zenodo.14717214

## ABSTRACT

The aim of this study is to determine physicochemical properties and drug likeness of selected plant constituents from Bryophyllum pinnatum by computational screening and to predict pharmacokinetic properties of selected plant constituents from Bryophyllum pinnatum by computational methods. Most of the constituents obeyed Lipinski's rule and displayed drug like properties. The same constituents were also evaluated for ADME parameters using Qik Prop module of Schrodinger molecular modeling software. Lipinski's rule of five, which is represented by a numerical value known as the drug likeness score—a collective property that encompasses a compound's physicochemical properties, pharmacokinetics, and pharmacodynamics was used to calculate a number of molecular parameters. Mol Soft software was used to calculate the drug likeness model score. The majority of the 38 chemical constituents of Bryophyllum pinnatum that were screened had a positive drug likeness score and  $\leq 1$  Lipinski's rule violations. Two commercial anti-inflammatory medications, ibuprofen and diclofenac, with drug likeness scores of 0.59 and 0.65, were then compared to this data. This suggests that these particular chemical components might have strong oral bioavailability and favorable drug-like characteristics. From the data obtained, most of the chemical constituents lie in the recommended ranges and have the potential of forming lead molecules with good oral bioavailability.

## INTRODUCTION

Medicinal plants have been known since ages and esteemed as rich source of therapeutic agents, thus utilized in preventing and treating various diseases

and ailments. Despite of advancement in drug industry and drug products, about 75% of world population rely on traditional plant products for

**\*Corresponding Author:** Ketura Kambampaty

**Address:** Department of Pharmaceutics, Maratha Mandal College of Pharmacy, Belgaum.

**Email** ✉: [keturamk77@gmail.com](mailto:keturamk77@gmail.com)

**Relevant conflicts of interest/financial disclosures:** The authors declare that the research was conducted in the absence of any commercial or financial relationships that could be construed as a potential conflict of interest.



healing. Traditionally, *Bryophyllum pinnatum* has been noted for its versatile medicinal properties.<sup>1</sup>

*Bryophyllum pinnatum* is a succulent and perennial plant mostly found at tropical and subtropical areas. The species is native to Madagascar. *Bryophyllum pinnatum* is also known as *Kalanchoe pinnata*. Some of the common names for these herbs are as follows: air plant, cathedral bells, miracle leaf, devils backbone.<sup>2</sup>

**Taxonomy:**

Kingdom: Plantae

Class: Dicotyledon

Family: Crassulaceae

Genus: *Bryophyllum*.<sup>3</sup>

### **Description of plant:**

The plant grows up to 150cm(1-1.5m) in height and leaves grow 10-30cm long. The lower leaves differentiate from upper leaves of plant such that the lower leaves are simple and dark green in color while the upper leaves are 3-7 foliated, long petiolate, with characteristic odour, bitter taste and thick<sup>4</sup>. Flowers are cymose, unisexual, regular and pendent with large spreading panicles. Petals are as sepals, reddish-purple in color, while sepals are 25-55mm long, red striated with base green. The fruits are follicles, contain a few seeds. These seeds are small and oblong in shape with smooth surface and brownish in color. The *Bryophyllum pinnatum* plant flowers in Nov-Mar and produce fruits in April.

### **Pharmacological Actions**

The *Bryophyllum pinnatum* shows various pharmacological actions such as anti-inflammatory, antidiabetic, anticancer, analgesic, antipyretic, antiulcer, astringent, antiseptic, hepatoprotective, antileishmanial, antioxidant, wound healing activity, antibacterial, antituberculosis, antihypertensive, tocolytic agent, CNS depressant, anxiolytic, neurosedative, insecticidal, immunomodulatory agent, antiallergic, antimicrobial, hepatoprotective, antiurolithic, diuretic, anticonvulsant, uterine

relaxant, muscle relaxant, antimalarial, carminative, antigout.<sup>4,5,6,7</sup>

### **Chemical Constituents Of *Bryophyllum Pinnatum***

*Bryophyllum pinnatum* is rich in various phytoconstituents such as alkaloids, flavonoids, steroids, triterpenes, phenanthrenes, bufadienolides, cardienolides, lipids, glycosides. The leaves are concentrated with majority of bufadienolides and cardiac glycosides. From aerial parts of plant Phenolic acids such as syringic acid, caffeic acid, 2-4-hydroxy-3-methoxy cinnamic acid, etc have been isolated. Flavanoids are rich in leaves mainly quercetin and kaempferol glycosides and few flavone glycosides i.e., luteolin, diosmetin. The plant also showed the presence of triterpenes such as alpha amyrin, beta amyrin, alpha amyrin acetate, beta amyrin acetate, taraxerone, etc. and phytosterols such as stigmast-24-enol, 5-methylsterogost-24(28)-enol, etc. *Bryophyllum pinnatum* possessed high content of mallic acids, carboxylic acids such as oxalic acids, citric acid, isocitric acid, etc.<sup>7</sup> U. Rosemary et.al, performed ethanolic extraction of leaves obtained from *Bryophyllum pinnatum*, 3,5-dihydroxy-6-methyl-2,3-dihydroxy-4H-pyran-4-one showed anticancer activity, alpha-D-Glucopyranoside methyl possessed anti-tuberculosis, antioxidant and anticonvulsant activities, n-Hexadecanoic acid was effective against rheumatism and inflammation, oleic acid decreased risk of breast cancer and decreased blood pressure.<sup>6</sup> C. Lucas et.al, carried out ethanolic extraction of *Bryophyllum pinnatum*. The flavonoids such as rutin, quercetin, luteolin-7-o-beta-o-glucoside were detected. The study revealed that ethanolic extraction of *Bryophyllum pinnatum* leaves is effective as topical anti-inflammatory for acute and chronic inflammation conditions.<sup>8</sup> M. Afzal et.al, isolated a steroidal derivative Stigmast-4,20(21),23-trien-3-one from *Bryophyllum pinnatum* leaves. This compound was evaluated for anti-



inflammatory activity in carrageenan induced paw edema model and was capable of reducing inflammation.<sup>9</sup> Ogidigo.J.O.et.al, performed In-silico molecular docking and pharmacokinetic studies of selected constituents from *Bryophyllum pinnatum*. Patuletin, luteolin, kaempferol and acacetin passed the Lipinski's rule of five and showed good binding scores and considerable drug likeness.<sup>10</sup> Literature survey revealed that there is a lack of computational studies on virtual screening of selected phytoconstituents from *Bryophyllum pinnatum* plant, to investigate its physicochemical and ADME properties. Hence, in this context, in the current research work, we aim at virtually screening some phytoconstituents from *Bryophyllum pinnatum* plant for various physicochemical and pharmacokinetic parameters.

## METHODOLOGY

### Physicochemical properties and drug likeness

Drug likeness score is determined from molecular properties i.e molecular weight, number of hydrogen bond donors, number of hydrogen bond acceptors, LogP and polar surface area by Molsoft online server.

### ADME predictive study

Various ADME parameters of all the selected chemical constituents of *Bryophyllum pinnatum* were calculated by using Qik Prop module of the Schrodinger molecular modeling software. These parameters were then compared with the recommended values of the Qik Prop properties mentioned in the Qik Prop User Manual.

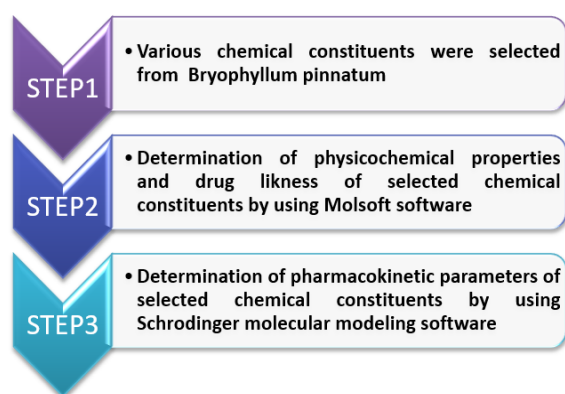


Figure 2: Steps involved in research methodology

## RESULTS AND DISCUSSION

### A] Determination Of Physicochemical Properties And Drug Likeness Of Selected Chemical Constituents From *Bryophyllum Pinnatum*

#### Lipinski's Rule Of 5

Lipinski's rule of 5 or Pfizer rule of 5 or rule of 5 is a thumb rule which postulates whether a drug is orally active in humans or not. This rule was worked out by Christopher A. Lipinski in 1997.<sup>11</sup>

#### Components Of Rule Of 5:

Lipinski's rule of 5 intends that no orally active drug should show more than 1 violation for following norms:

- No more than 5 hydrogen bond donors
- No more than 10 hydrogen bond acceptors
- Molecular weight of drug should be less than 500
- Log P value should not exceed more than 5

Since all numbers are multiple of 5, thus contributes to name "RULE OF 5"<sup>11,12</sup>

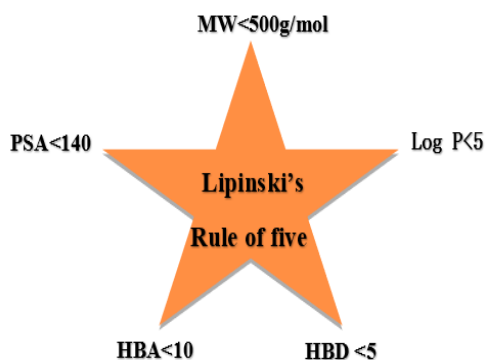


**Figure 3: Lipinski's Rule of Five**

Various molecular parameters were calculated based on the Lipinski's rule of five, which is represented by a numerical value called as drug likeness score, that is a collective property encompassing physicochemical properties, pharmacokinetics and pharmacodynamics of a compound. The drug likeness model score was determined by MolSoft software. Among the 38 chemical constituents of *Bryophyllum pinnatum* that were screened, maximum constituents have shown  $\leq 1$  number of violations of the Lipinski's rule and a positive drug likeness score. This data was then compared with two commercial anti-inflammatory drugs, diclofenac and ibuprofen having drug likeness score 0.59 and 0.65. This indicates that these selected chemical constituents may have good drug like features and potent oral bioavailability. Results are shown in **Table 1**.

#### **B] Determination of Pharmacokinetic Properties of Selected Chemical Constituents from *Bryophyllum Pinnatum***

##### **Pharmacokinetics Studies (Adme Studies)**

Pharmacology is categorized into 2 groups: Pharmacodynamics and Pharmacokinetics. Pharmacodynamics is defined as study of effect of drug on body (what the drug does to body). Pharmacokinetics is study of effect of body on drug or is also defined as movement of drug within body and excretion from body (what body does to the drug). The term Pharmacokinetics is coined by Leslie Benet. In order to understand the concept of pharmacokinetics, it is grouped into 4 phases of

drugs movement i.e., absorption, distribution, metabolism and excretion (ADME). ADME of drug depends on various properties of drug such as molecular weight, chemical structure, chemical space, degree of ionization, lipophilicity, water solubility, etc. Majority of compounds lack these properties, thus ADME studies are conducted priorly in order to eliminate such compounds. The assessment of ADME is an important part during various stages of drug development such as drug discovery, preclinical and clinical stage, as it determines the drug efficacy, safety and toxicity. About 80% of investigational new drugs are ruled out during drug development process because of undesirable ADME and toxicity characteristics. Most of the Pharmaceutical companies possess hundreds – thousands of potential drugs, but are not FDA approved due to undesirable properties.<sup>13</sup>

**Absorption:** Absorption is the movement of drug from its site of administration into circulation. When a drug is administered through oral route, the drug reaches the liver via hepatic portal vein after the drug passes out of Gastrointestinal tract. The drug moves from liver into the blood. Poor absorption of drug likely occurs if the drug has more than

- ✓ 5H-bond donors
- ✓ 10H- bond acceptors
- ✓ Molecular weight more than 500 Daltons
- ✓ Log P greater than 5

The amount of drug absorbed from the site of absorption evaluates the bioavailability of drug at site of action.

**Distribution:** The distribution of drug involves its movement into, through, and out of body compartments. Once the drug enters into systemic circulation by absorption, it gets distributed to various organs and muscles. Distribution pattern of drug depends on factors like:

- ✓ Lipid solubility
- ✓ Ionisation at physiological pH
- ✓ Extent of binding to plasma and tissue proteins
- ✓ Presence of tissue specific transporters
- ✓ Difference in regional blood flow

**Metabolism:** In this process the drug gets converted into metabolites through enzymes. It converts non polar compounds to polar compounds, so that excretion process takes place eliminating the reabsorption of compounds in renal tubules. The converted metabolites may be either active or inactive. This process may either increase or decrease parent drugs activity.

If the drugs activity increases, then the metabolite is active and if drugs activity decreases then the metabolite is inactive.

**Excretion:** The body excretes metabolites and remaining drug through kidney and other organs such as lungs and skin. If the drug is not completely excreted from body, the remaining traces of body may cause adverse reactions. Drugs and their metabolites are excreted in urine, faeces, exhaled air, saliva, sweat and milk.

**Toxicity:** The ADME studies includes toxicity studies to calculate Maximum therapeutic dose and minimum toxic dose.<sup>13,14,15</sup>

The pharmacokinetic parameters of selected chemical constituents from *Bryophyllum pinnatum*, were calculated by using QikProp module of Schrodinger molecular modeling software and the data obtained was verified with QikProp manual. The recommended ranges for different ADME parameters are as follows: CNS:

predicted central nervous system, -2 to +2, dipole: computed dipole moment of the molecule, 1.0-12.5, volume: total solvent-accessible volume in cubic angstroms using a probe with a 1.4 angstroms radius, 500-2000, QPlogPC16: predicted hexadecane/gas partition coefficient, 4.0-18.0, QPlogPoct: predicted octanol/gas partition coefficient, 8.0-35.0, QPlogPw: predicted water/gas partition coefficient, 4.0-45.0, QPlogPo/w: predicted octanol/water partition coefficient, -2.0-6.5, QPlogS: predicted aqueous solubility, -6.5-0.5, QPlogHERG: predicted IC<sub>50</sub> value for blockage of HERG K<sup>+</sup> channels, below -5, QPPCaco: predicted apparent Caco-2 cell permeability in nm/sec, <25 poor >500 great, QPlogBB: predicted brain/blood partition coefficient, -3.0-1.2, QPPMDCK: predicted apparent MDCK cell permeability in nm/sec, <25 poor >500 great, QPlogKp: predicted skin permeability, -8.0-1.0, QPlogKhsa: prediction of binding to human serum albumin, -1.5-1.5, %HOA: predicted human oral absorption on 0 to 100% scale, >80% is high <25% is poor, PSA: vanderwaals surface area of polar nitrogen and oxygen atoms, 7.0-200.0, RO5: number of violations of Lipinski's rule of five, maximum is 4, RO3: number of violations of Jorgensen's rule of three, maximum is 3. All the thirty-eight selected chemical constituents showed values within recommended ranges for CNS dipole, volume, QPlogBB, QPlogKp, RO5 and RO3 parameters. Chemical constituents such as rutin, kaempferitrin, friedelin showed variation in values for QPlogPC16 parameter. For QPlogPoct constituents such as rutin, kaempferitrin and thesiuside showed fluctuating results. Alpha amyrin acetate, beta amyrin acetate, beta sitosterol, campesterol and stigmast-24-enol showed fluctuations from recommended range for QPlogPw. Constituents such as hellebrigenin, bryophyllin A, bryophyllin B, 3,4-Di-O-methylquercetrin and methylidaigremonte



showed values within the recommended range for QPlogPo/w. For parameters such as QPlogS, QPlogHERG, QPlogCaco, QPlogKhsa, PSA most of the constituents showed values within the recommended ranges. Quercitrin, isoquercitrin, rutin, myricitrin, astragalin, kaempferitrin,

thesiuside and misquelianin showed poor HOA. Results shown in **Table 2**. Quercitrin, isoquercitrin, rutin, myricitrin, astragalin, kaempferitrin, thesiuside and misquelianin showed poor HOA. Results shown in **Table 2**.

**Table 1. Physicochemical parameters and drug likeness of selected chemical constituents from *Bryophyllum pinnatum***

| Selected Plant Constituent      | MW     | HBA  | HBD | Log P | PSA    | Rule of 5 violation | Drug likeness |
|---------------------------------|--------|------|-----|-------|--------|---------------------|---------------|
|                                 | <500   | ≤ 10 | ≤ 5 | ≤ 5   | -      | ≤ 1                 | >0            |
| Bryophyllin A                   | 472.21 | 8    | 2   | 2.09  | 86.32  | 0                   | 0.67          |
| Bryophyllin B                   | 488.20 | 9    | 3   | 1.50  | 109.03 | 0                   | 0.87          |
| Bryophyllin C                   | 474.23 | 8    | 3   | 1.79  | 89.28  | 0                   | 0.83          |
| Bryotoxin A                     | 618.27 | 12   | 4   | 0.28  | 145.01 | 2                   | 1.06          |
| Bryotoxin B                     | 488.20 | 9    | 3   | 0.51  | 102.32 | 0                   | 0.68          |
| Kaempferol                      | 286.05 | 6    | 4   | 1.61  | 87.13  | 0                   | 0.50          |
| Astragalin                      | 448.10 | 11   | 7   | -0.12 | 152.24 | 2                   | 0.67          |
| Friedein                        | 426.39 | 1    | 0   | 7.44  | 13.36  | 1                   | -0.43         |
| Rutin                           | 610.15 | 16   | 10  | -1.55 | 213.63 | 3                   | 0.91          |
| Quercetin                       | 302.04 | 7    | 5   | 1.19  | 102.61 | 0                   | 0.52          |
| Luteoin                         | 286.05 | 6    | 4   | 2.78  | 89.05  | 0                   | 0.38          |
| Isoquercetin                    | 464.10 | 12   | 8   | -0.54 | 167.72 | 2                   | 0.68          |
| Alpha amyirin                   | 426.39 | 1    | 1   | 7.77  | 15.73  | 1                   | 0.10          |
| Alpha amyirin acetate           | 468.40 | 2    | 0   | 8.29  | 20.32  | 1                   | 0.57          |
| Beta amyirin                    | 426.39 | 1    | 1   | 7.95  | 15.73  | 1                   | -0.22         |
| Beta amyirin acetate            | 468.40 | 2    | 0   | 8.47  | 20.32  | 1                   | 0.27          |
| Afzelin                         | 432.11 | 10   | 6   | 0.74  | 134.93 | 1                   | 0.77          |
| Glutinol                        | 426.39 | 1    | 1   | 7.97  | 15.73  | 1                   | -0.41         |
| Pseudo Taraxasterol             | 426.39 | 1    | 1   | 8.15  | 15.73  | 1                   | -0.09         |
| Taraxasterol                    | 426.39 | 1    | 1   | 8.11  | 15.73  | 1                   | -0.90         |
| Beta sitosterol                 | 414.39 | 1    | 1   | 8.45  | 16.28  | 1                   | 0.78          |
| Kaempferitrin                   | 578.16 | 14   | 8   | -0.71 | 179.86 | 3                   | 0.73          |
| Myricitrin                      | 464.10 | 12   | 8   | 0.10  | 165.88 | 2                   | 0.67          |
| Miquelianin                     | 478.07 | 13   | 8   | -0.17 | 178.77 | 2                   | 0.81          |
| 3,5,7,3'5'-Pentahydroxy flavone | 302.04 | 7    | 5   | 1.41  | 104.75 | 0                   | -0.52         |
| 3',4'-Di-O-methylquercetin      | 330.07 | 7    | 3   | 1.73  | 84.77  | 0                   | 0.32          |
| Stigmasr-24-enol                | 414.39 | 1    | 1   | 7.65  | 17.21  | 1                   | 0.22          |
| Quercitrin                      | 448.10 | 11   | 7   | 0.32  | 150.41 | 2                   | 0.82          |

|                         |        |    |   |       |        |   |      |
|-------------------------|--------|----|---|-------|--------|---|------|
| Kalanchoside A          | 562.28 | 10 | 5 | 0.08  | 127.78 | 1 | 0.74 |
| Kalanchoside B          | 562.28 | 10 | 5 | 0.08  | 127.78 | 1 | 0.74 |
| Kalanchoside C          | 546.28 | 9  | 4 | 1.02  | 111.76 | 1 | 0.77 |
| Hellebrigenin           | 416.22 | 6  | 3 | 1.48  | 81.44  | 0 | 0.52 |
| Hellebrigenin-3-acetate | 458.23 | 7  | 2 | 1.75  | 85.98  | 0 | 0.83 |
| Methyl daigremonte      | 502.22 | 9  | 2 | 1.42  | 94.03  | 1 | 0.31 |
| Thesiuside              | 620.28 | 12 | 5 | -0.48 | 149.57 | 2 | 0.56 |
| Lanceotoxin A           | 620.28 | 12 | 5 | -0.21 | 153.43 | 2 | 0.72 |
| Lanceotoxin B           | 604.29 | 11 | 4 | 0.39  | 132.26 | 2 | 0.70 |
| Campesterol             | 400.37 | 1  | 1 | 7.87  | 16.28  | 1 | 0.59 |
| Diclofenac              | 295.02 | 2  | 2 | 4.52  | 35.44  | 0 | 0.59 |
| Ibuprofen               | 206.13 | 2  | 1 | 3.85  | 28.65  | 0 | 0.65 |

Table 2. Pharmacokinetic parameters of selected chemical constituents from *Bryophyllum pinnatum*

| Constituent name    | CNS | molecular weight | dipole | Volume   | QPI ogP C16 | QPI ogP w | QPI ogP w | QPI ogP w | QPI ogP w | QPI ogP w | QPI ogP w | QPI ogP w | QPI ogP w | QPI ogP w | QPI ogP w | %H OA | P S A  | R O 3 | R O 5 |
|---------------------|-----|------------------|--------|----------|-------------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-------|--------|-------|-------|
| Beta-amyrin         | 1   | 426.724          | 1.954  | 1380.865 | 11.587      | 18.161    | 4.683     | 7.054     | -8.103    | -3.763    | 4439.036  | 0.178     | 2477.379  | -2.033    | 2.051     | 100   | 19.872 | 1     | 1     |
| Alpha amyrin        | 1   | 426.724          | 1.931  | 1364.847 | 11.423      | 17.959    | 4.613     | 6.946     | -7.804    | -3.517    | 4436.782  | 0.188     | 2476.019  | -2.049    | 2.007     | 100   | 19.889 | 1     | 1     |
| Friedelin           | 1   | 426.724          | 4.358  | 1364.717 | 11.12       | 17.037    | 3.583     | 6.943     | -7.902    | -3.384    | 4077.362  | 0.218     | 2259.944  | -2.269    | 2.045     | 100   | 25.666 | 1     | 1     |
| Taraxerol           | 1   | 426.724          | 1.789  | 1384.13  | 11.573      | 18.169    | 4.648     | 7.067     | -8.138    | -3.751    | 4435.095  | 0.177     | 2475.002  | -2.054    | 2.06      | 100   | 19.891 | 1     | 1     |
| Beta-amyrin acetate | 1   | 468.762          | 2.924  | 1517.883 | 12.595      | 18.804    | 3.712     | 7.956     | -9.41     | -4.205    | 3968.448  | 0.108     | 2194.766  | -2.129    | 2.447     | 100   | 35.0   | 1     | 1     |

|                 |        |                 |           |                  |            |                |            |           |                |                |                      |                |                      |                |                    |        |                                 |   |   |
|-----------------|--------|-----------------|-----------|------------------|------------|----------------|------------|-----------|----------------|----------------|----------------------|----------------|----------------------|----------------|--------------------|--------|---------------------------------|---|---|
|                 |        |                 |           |                  |            |                |            |           |                |                |                      |                |                      |                |                    |        | 1<br>2                          |   |   |
| Campesterol     | 0      | 400<br>.68<br>7 | 1.7<br>8  | 142<br>5.73<br>7 | 12.<br>221 | 17.<br>40<br>7 | 3.8<br>77  | 7.26<br>6 | -<br>8.3<br>89 | -<br>4.64      | 34<br>05.<br>95<br>4 | -<br>0.28<br>7 | 18<br>60.<br>53<br>2 | -<br>1.7<br>39 | 1.<br>96<br>1      | 100    | 2<br>2<br>.<br>2<br>7<br>7      | 1 | 1 |
| Beta-sitosterol | 0      | 414<br>.71<br>3 | 1.7<br>65 | 147<br>4.93<br>4 | 12.<br>658 | 17.<br>85<br>3 | 3.6<br>97  | 7.58<br>4 | -<br>8.5<br>57 | -<br>4.64<br>9 | 34<br>04.<br>34<br>8 | -<br>0.34<br>8 | 18<br>59.<br>58<br>4 | -<br>1.6<br>44 | 2.<br>05<br>9      | 100    | 2<br>2<br>.<br>2<br>8<br>1      | 1 | 1 |
| Hellebrigenin   | -<br>2 | 416<br>.51<br>3 | 8.6<br>46 | 119<br>0.03      | 11.<br>83  | 20.<br>82      | 11.<br>789 | 2.57<br>9 | -<br>4.3<br>85 | -<br>3.73<br>5 | 11<br>8.2<br>86      | -<br>1.38<br>9 | 49.<br>23<br>8       | -<br>4.5<br>76 | 0.<br>41<br>4      | 79.149 | 1<br>2<br>3<br>.<br>4<br>4<br>5 | 0 | 0 |
| Bryophyllin B   | -<br>2 | 488<br>.53<br>3 | 6.2<br>72 | 132<br>9.89<br>3 | 12.<br>985 | 22.<br>04<br>9 | 12.<br>661 | 2.46<br>3 | -<br>4.7<br>92 | -<br>4.20<br>1 | 57.<br>39            | -<br>1.81      | 22.<br>53<br>2       | -5.2           | 0.<br>35<br>1      | 72.844 | 1<br>6<br>3<br>.<br>4<br>5<br>7 | 0 | 0 |
| Bryotoxin A     | -<br>2 | 618<br>.67<br>7 | 7.8<br>76 | 171<br>6.85<br>1 | 17.<br>35  | 33.<br>38<br>5 | 22.<br>483 | 1.43<br>9 | -<br>5.1<br>09 | -<br>5.24<br>6 | 21.<br>11<br>6       | -<br>2.89<br>3 | 7.6<br>46            | -<br>5.6<br>55 | -<br>0.<br>15<br>8 | 33.159 | 2<br>0<br>6<br>.<br>6<br>4      | 1 | 2 |
| Lanceotoxin A   | -<br>2 | 620<br>.69<br>2 | 5.7<br>81 | 166<br>1.69<br>3 | 16.<br>884 | 32.<br>72<br>8 | 22.<br>231 | 1.33<br>1 | -<br>3.6<br>59 | -<br>4.32<br>7 | 15.<br>62<br>9       | -<br>2.88      | 5.5<br>23            | -<br>5.5<br>29 | -<br>0.<br>19<br>5 | 30.193 | 2<br>2<br>1<br>.<br>2<br>6<br>7 | 1 | 2 |
| Lanceotoxin B   | -<br>2 | 604<br>.69<br>3 | 4.3<br>93 | 165<br>3.59<br>9 | 16.<br>716 | 33.<br>69<br>4 | 23.<br>667 | 1.12<br>8 | -<br>4.3<br>25 | -<br>4.60<br>1 | 24.<br>98            | -<br>2.55<br>1 | 9.1<br>69            | -<br>5.5<br>3  | -<br>0.<br>19      | 32.649 | 1<br>8<br>6<br>.<br>1<br>1<br>3 | 0 | 2 |
| Quercetin       | -<br>2 | 302<br>.24      | 4.8<br>15 | 866.<br>544      | 10.<br>742 | 18.<br>57      | 14.<br>412 | 0.38<br>5 | -<br>2.8<br>84 | -<br>5.07<br>5 | 19.<br>27            | -<br>2.38      | 6.9<br>26            | -<br>5.4<br>92 | -<br>0.<br>34<br>2 | 52.195 | 1<br>4<br>2<br>.                | 1 | 0 |

|                   |        |                 |           |                  |            |                |            |                |                |                |                |                |                |                |                    |        |                                 |   |   |
|-------------------|--------|-----------------|-----------|------------------|------------|----------------|------------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|--------------------|--------|---------------------------------|---|---|
|                   |        |                 |           |                  |            |                |            |                |                |                |                |                |                |                |                    |        | 6<br>8<br>3                     |   |   |
| Luteol<br>in      | -<br>2 | 286<br>.24      | 3.0<br>58 | 841.<br>868      | 10.<br>202 | 16.<br>35<br>6 | 12.<br>292 | 0.94<br>8      | -<br>3.0<br>8  | -<br>5.03<br>7 | 42.<br>02<br>9 | -<br>1.94<br>4 | 16.<br>09      | -<br>4.8<br>57 | -<br>0.<br>19<br>4 | 61.556 | 1<br>2<br>1<br>.<br>1<br>7<br>6 | 0 | 0 |
| Querci<br>trin    | -<br>2 | 448<br>.38<br>2 | 9.1<br>41 | 120<br>2.95<br>9 | 14.<br>541 | 29.<br>55<br>3 | 23.<br>621 | -0.57          | -<br>2.9<br>55 | -<br>5.19<br>5 | 7.3<br>12      | -<br>3.14      | 2.4<br>3       | -<br>6.0<br>14 | -<br>0.<br>65<br>1 | 13.152 | 1<br>9<br>6<br>.<br>6<br>1<br>6 | 2 | 2 |
| Isoque<br>rcitrin | -<br>2 | 464<br>.38<br>2 | 9.2<br>37 | 123<br>0.15<br>5 | 15.<br>252 | 31.<br>97<br>6 | 26.<br>562 | -<br>1.46<br>3 | -<br>2.4<br>6  | -<br>5.05<br>2 | 2.3<br>63      | -<br>3.72<br>7 | 0.7<br>17      | -<br>6.8<br>4  | -<br>0.<br>86<br>8 | 0      | 2<br>1<br>9<br>.<br>8<br>3      | 2 | 2 |
| Rutin             | -<br>2 | 610<br>.52<br>4 | 9.4<br>35 | 160<br>3.12<br>3 | 19.<br>765 | 42.<br>91<br>1 | 36.<br>276 | -<br>2.69<br>5 | -<br>2.6<br>05 | -<br>5.75<br>7 | 0.3<br>68      | -<br>5.29      | 0.0<br>96      | -<br>8.0<br>39 | -<br>1.<br>32<br>3 | 0      | 2<br>7<br>0<br>.<br>7<br>3<br>2 | 2 | 3 |
| Kaem<br>pferol    | -<br>2 | 286<br>.24      | 4.5<br>27 | 845.<br>228      | 10.<br>242 | 16.<br>59<br>1 | 12.<br>327 | 1.06<br>1      | -<br>3.1<br>42 | -<br>5.17<br>8 | 53.<br>75<br>3 | -<br>1.86<br>4 | 20.<br>99<br>2 | -<br>4.5<br>96 | -<br>0.<br>18<br>9 | 64.127 | 1<br>2<br>1<br>.<br>1<br>5      | 0 | 0 |
| Myrici<br>trin    | -<br>2 | 464<br>.38<br>2 | 8.0<br>49 | 122<br>5.61<br>7 | 15.<br>064 | 31.<br>28<br>9 | 25.<br>718 | -1.21          | -<br>2.8<br>06 | -<br>5.12<br>1 | 2.5<br>78      | -<br>3.70<br>9 | 0.7<br>87      | -<br>6.9<br>23 | -<br>0.<br>76<br>8 | 1.304  | 2<br>1<br>8<br>.<br>0<br>8<br>7 | 2 | 2 |
| Astrag<br>alin    | -<br>2 | 448<br>.38<br>2 | 5.7<br>72 | 118<br>7.78<br>2 | 14.<br>409 | 29.<br>05<br>3 | 24.<br>315 | -<br>0.77<br>9 | -<br>2.5<br>24 | -<br>5.17<br>6 | 11.<br>20<br>3 | -<br>2.96<br>3 | 3.8<br>54      | -<br>5.4<br>86 | -<br>0.<br>80<br>1 | 15.249 | 1<br>9<br>0<br>.<br>5<br>0<br>8 | 2 | 2 |

|                                                    |        |                 |           |                  |            |                |            |                |                |                |                      |                |                      |                |                    |        |                                 |   |   |
|----------------------------------------------------|--------|-----------------|-----------|------------------|------------|----------------|------------|----------------|----------------|----------------|----------------------|----------------|----------------------|----------------|--------------------|--------|---------------------------------|---|---|
| Afzeli<br>n                                        | -<br>2 | 432<br>.38<br>3 | 4.3<br>27 | 118<br>6.60<br>8 | 14.<br>107 | 26.<br>94<br>4 | 21.<br>569 | -<br>0.01<br>9 | -<br>3.1<br>83 | -<br>5.31<br>2 | 15.<br>27<br>3       | -<br>2.75<br>4 | 5.3<br>88            | -<br>5.3<br>97 | -<br>0.<br>53<br>5 | 35.063 | 1<br>7<br>5<br>.<br>1<br>6<br>9 | 1 | 1 |
| 3,5,7,3<br>'5'-<br>pentah<br>ydroxy<br>flavon<br>e | -<br>2 | 302<br>.24      | 6.2<br>81 | 867.<br>872      | 10.<br>759 | 18.<br>84<br>8 | 14.<br>424 | 0.33<br>1      | -<br>2.9<br>03 | -<br>5.06<br>5 | 16.<br>31<br>3       | -<br>2.45<br>8 | 5.7<br>85            | -<br>5.6<br>55 | -<br>0.<br>34<br>1 | 50.585 | 1<br>4<br>3<br>.<br>6<br>8<br>4 | 1 | 0 |
| Kaem<br>pferitri<br>n                              | -<br>2 | 578<br>.52<br>6 | 4.2<br>96 | 156<br>4.66<br>4 | 18.<br>461 | 37.<br>80<br>9 | 31.<br>02  | -<br>1.18<br>2 | -<br>3.5<br>41 | -<br>6.04<br>3 | 3.2<br>19            | -<br>4.19<br>2 | 1.0<br>01            | -<br>6.4<br>46 | -<br>0.<br>99<br>9 | 0      | 2<br>2<br>9<br>.<br>9<br>1<br>2 | 2 | 3 |
| 3',4'--<br>Di-O-<br>methlq<br>uerceti<br>n         | -<br>2 | 330<br>.29<br>3 | 4.7<br>9  | 975.<br>668      | 10.<br>384 | 16.<br>46<br>2 | 10.<br>693 | 2.04<br>1      | -<br>3.9<br>33 | -<br>5.12<br>6 | 17<br>7.3<br>67      | -<br>1.49<br>3 | 76.<br>29<br>1       | -<br>3.7<br>33 | 0.<br>03           | 79.147 | 1<br>1<br>4<br>.<br>4<br>2<br>4 | 0 | 0 |
| Bryop<br>hyllin<br>A                               | -<br>1 | 472<br>.53<br>4 | 5.7<br>16 | 125<br>4.45<br>3 | 12.<br>028 | 23.<br>02<br>8 | 14.<br>885 | 2.07<br>6      | -<br>3.8<br>34 | -<br>3.57<br>7 | 36<br>0.6<br>68      | -<br>0.87<br>2 | 16<br>4.2<br>99      | -<br>3.7<br>39 | 0.<br>07<br>5      | 84.867 | 1<br>2<br>4<br>.<br>6<br>8<br>1 | 0 | 0 |
| Bryoto<br>xin B                                    | -<br>2 | 488<br>.53<br>3 | 4.3<br>86 | 126<br>5.64<br>8 | 12.<br>49  | 25.<br>24<br>4 | 17.<br>963 | 1.28<br>7      | -<br>3.4<br>49 | -<br>3.64<br>6 | 22<br>4.2<br>12      | -<br>1.12<br>7 | 98.<br>28<br>5       | -<br>4.0<br>46 | -<br>0.<br>16<br>7 | 76.551 | 1<br>3<br>8<br>.<br>1<br>0<br>4 | 0 | 0 |
| Glutin<br>ol                                       | 1      | 426<br>.72<br>4 | 1.7<br>48 | 137<br>9.98<br>7 | 11.<br>52  | 18.<br>14<br>4 | 4.6<br>02  | 7.07<br>2      | -<br>7.9<br>27 | -<br>3.55<br>2 | 48<br>53.<br>53<br>9 | 0.22<br>2      | 27<br>28.<br>33<br>7 | -<br>1.9<br>73 | 2.<br>05           | 100    | 1<br>9<br>.<br>4<br>0<br>8      | 1 | 1 |
| Kalanc<br>hoside<br>A                              | -<br>2 | 562<br>.65<br>6 | 8.2<br>54 | 154<br>8.81<br>7 | 15.<br>687 | 31.<br>36<br>1 | 21.<br>234 | 1.48<br>9      | -<br>4.3<br>15 | -<br>4.44<br>8 | 35.<br>57<br>4       | -<br>2.34<br>1 | 13.<br>43<br>7       | -<br>5.2<br>33 | -<br>0.<br>05<br>2 | 50.469 | 1<br>7<br>5<br>.<br>.           | 0 | 1 |

|                                     |        |                 |           |                  |            |                |            |                |                |                |                      |                |                      |                |                    |        |                                 |   |   |
|-------------------------------------|--------|-----------------|-----------|------------------|------------|----------------|------------|----------------|----------------|----------------|----------------------|----------------|----------------------|----------------|--------------------|--------|---------------------------------|---|---|
|                                     |        |                 |           |                  |            |                |            |                |                |                |                      |                |                      |                |                    |        | 9<br>3<br>8                     |   |   |
| Kalanc<br>hoside<br>B               | -<br>2 | 562<br>.65<br>6 | 6.9<br>24 | 154<br>6.92<br>3 | 15.<br>707 | 31.<br>13<br>3 | 21.<br>261 | 1.51<br>2      | -<br>4.3<br>99 | -<br>4.59<br>6 | 40.<br>13<br>5       | -<br>2.32<br>9 | 15.<br>30<br>8       | -<br>5.1<br>05 | -<br>0.<br>06<br>9 | 51.541 | 1<br>7<br>5<br>.<br>2<br>2<br>2 | 0 | 1 |
| Mique<br>lianin                     | -<br>2 | 478<br>.36<br>5 | 6.8<br>04 | 124<br>4.59      | 15.<br>539 | 30.<br>41      | 25.<br>021 | -<br>0.81<br>6 | -<br>2.8<br>51 | -<br>3.41<br>4 | 0.2<br>41            | -<br>4.12<br>9 | 0.0<br>77            | -<br>7.6<br>61 | -<br>0.<br>89<br>5 | 0      | 2<br>4<br>6<br>.<br>2<br>7<br>2 | 2 | 2 |
| Thesiu<br>side                      | -<br>2 | 620<br>.69<br>2 | 8.9<br>89 | 168<br>3.40<br>2 | 17.<br>35  | 36.<br>61<br>3 | 26.<br>548 | 0.41<br>3      | -<br>3.7<br>3  | -<br>4.56      | 14.<br>49<br>7       | -<br>2.89<br>5 | 5.0<br>92            | -5.8           | -<br>0.<br>44<br>6 | 24.232 | 2<br>1<br>0<br>.<br>1<br>3<br>1 | 1 | 2 |
| Kalach<br>oside<br>C                | -<br>2 | 546<br>.65<br>6 | 5.8<br>2  | 152<br>6.79<br>8 | 15.<br>09  | 28.<br>50<br>6 | 18.<br>121 | 2.28<br>9      | -<br>4.7<br>89 | -<br>4.43<br>4 | 63.<br>04<br>7       | -<br>2.02<br>9 | 24.<br>94<br>2       | -<br>4.8<br>44 | 0.<br>20<br>8      | 59.602 | 1<br>5<br>5<br>.<br>1<br>0<br>4 | 0 | 1 |
| Bryop<br>hyllin<br>C                | -<br>1 | 474<br>.55      | 3.8<br>67 | 125<br>7.87      | 12.<br>245 | 23.<br>88<br>9 | 15.<br>798 | 2.16<br>7      | -<br>3.8<br>66 | -<br>3.57<br>8 | 40<br>6.5<br>84      | -<br>0.88<br>7 | 18<br>7.0<br>2       | -<br>3.5<br>42 | 0.<br>11<br>9      | 86.332 | 1<br>1<br>5<br>.<br>4<br>3<br>2 | 0 | 0 |
| Stigma<br>st-24-<br>enol            | 0      | 414<br>.71<br>3 | 1.6<br>98 | 146<br>4.00<br>5 | 12.<br>294 | 17.<br>54<br>5 | 3.4<br>37  | 7.52<br>7      | -<br>8.3<br>91 | -<br>4.42<br>5 | 39<br>34.<br>71<br>3 | -<br>0.27<br>6 | 21<br>74.<br>60<br>6 | -<br>1.6<br>22 | 2.<br>02<br>8      | 100    | 2<br>1<br>.<br>0<br>8<br>6      | 1 | 1 |
| Helleb<br>rigenin<br>-3-<br>acetate | -<br>2 | 458<br>.55      | 7.0<br>76 | 131<br>6.66<br>9 | 12.<br>59  | 20.<br>88      | 10.<br>695 | 3.38<br>3      | -<br>5.2<br>78 | -<br>4.11<br>6 | 13<br>9.8<br>62      | -<br>1.41<br>9 | 59.<br>01<br>4       | -<br>4.4<br>44 | 0.<br>66<br>5      | 85.158 | 1<br>3<br>6<br>.<br>8<br>4<br>7 | 0 | 0 |

|                                    |        |                 |           |                  |            |                |            |           |                |                |                      |                |                      |                |                    |        |                             |   |   |
|------------------------------------|--------|-----------------|-----------|------------------|------------|----------------|------------|-----------|----------------|----------------|----------------------|----------------|----------------------|----------------|--------------------|--------|-----------------------------|---|---|
| Alpha<br>myrrin<br>acetate         | 1      | 468<br>.76<br>2 | 3.0<br>77 | 149<br>8.91<br>9 | 12.<br>255 | 18.<br>52<br>5 | 3.5<br>25  | 7.81<br>3 | -<br>8.9<br>74 | -<br>3.80<br>7 | 40<br>05.<br>43<br>2 | 0.12<br>9      | 22<br>16.<br>88<br>2 | -<br>2.1<br>88 | 2.<br>39<br>2      | 100    | 3<br>4<br>.3<br>2<br>7      | 1 | 1 |
| Pseud<br>otarax<br>asterol         | 1      | 426<br>.72<br>4 | 1.5<br>43 | 137<br>4.93<br>3 | 11.<br>568 | 18.<br>10<br>2 | 4.7        | 7.05      | -<br>7.9<br>95 | -<br>3.72<br>2 | 47<br>93.<br>98<br>2 | 0.21<br>2      | 26<br>92.<br>16<br>9 | -<br>1.9<br>39 | 2.<br>03<br>5      | 100    | 1<br>9<br>.5<br>1<br>5      | 1 | 1 |
| Methy<br>l<br>daigre<br>monat<br>e | -<br>2 | 502<br>.56      | 6.5<br>71 | 138<br>5.55<br>6 | 12.<br>896 | 24.<br>48<br>3 | 15.<br>394 | 2.22<br>2 | -<br>4.3<br>67 | -<br>4.32<br>1 | 30<br>0.9<br>4       | -<br>1.31<br>1 | 13<br>5.0<br>98      | -<br>3.7<br>5  | -<br>0.<br>01<br>1 | 71.356 | 1<br>3<br>1<br>.2<br>6<br>3 | 0 | 1 |

## CONCLUSION

*Bryophyllum pinnatum*, a medicinal herb, is used in the treatment of various ailments due to the presence of a variety of chemical constituents. Around thirty-eight selected chemical constituents were screened for physicochemical and pharmacokinetic parameters. The physicochemical properties and drug likeness of selected chemical constituents were assessed by using Molsoft software. The selected chemical constituents were then estimated for pharmacokinetic parameters by QikProp module of Schrodinger molecular modeling software. Maximum of the selected chemical constituents showed values ranging within the recommended values. This indicates that most of the selected chemical constituents have a potential of becoming lead molecules with potent anti-inflammatory activity and good oral bioavailability.

## REFERENCES

- Okoye EI, Anyaegbunam LC, Obi ZC, Ibemenuga KN. Pharmaceutical constituents of stem of *Bryophyllum pinnatum*. Magnesium. 2013;11:1-38.
- Kalanchoe *pinnata*. [https://en.wikipedia.org/wiki/Kalanchoe\\_pinnata](https://en.wikipedia.org/wiki/Kalanchoe_pinnata)
- Sadhana D, Parveen S, Bukhari NI, Shehzadi N, Qamar S, Ijaz A, Niazi SU, Naheed S, Latif A. *Bryophyllum pinnatum*: botanical description, vernacular names, parts used, traditional uses, phytochemical and pharmacological activities. Pakistan Journal of Pharmacy. 2018 Nov 6;30(1).
- Yadav P, Mishra AK, Singh H. A Recent Review On Chemistry And Biological Activities Of *Bryophyllum Pinnatum* (Lam.) Oken Family: Crassulaceae. Oriental Journal Of Chemistry. 2021;37(2):269.
- Orisakeye OT, Oladoye SO, Peters OA. Chemical Composition and Antioxidant Activity of *Bryophyllum pinnatum* Root. Natural Products Chemistry & Research. 2015;3(3):1-3.
- Uchegbu RI, Ahuchaogu AA, Amanze KO, Ibe CO. Chemical constituents analysis of the leaves of *Bryophyllum pinnatum* by GC-MS. AASCIT J. Chem. 2017;3:19-22.
- Fürer K, Simões-Wüst AP, von Mandach U, Hamburger M, Potterat O. *Bryophyllum*



- pinnatum and related species used in anthroposophic medicine: constituents, pharmacological activities, and clinical efficacy. *Planta medica*. 2016 Jul;82(11/12):930-41.
8. Chibli LA, Rodrigues KC, Gasparetto CM, Pinto NC, Fabri RL, Scio E, Alves MS, Del-Vechio-Vieira G, Sousa OV. Anti-inflammatory effects of *Bryophyllum pinnatum* (Lam.) Oken ethanol extract in acute and chronic cutaneous inflammation. *Journal of ethnopharmacology*. 2014 Jun 11;154(2):330-8.
  9. Muhammad Afzal MA, Gaurav Gupta GG, Imran Kazmi IK, Mahfoozur Rahman MR, Obaid Afzal OA, Jahangir Alam JA, Hakeem KR, Mohammad Pravez MP, Ritu Gupta RG, Firoz Anwar FA. Anti-inflammatory and analgesic potential of a novel steroidal derivative from *Bryophyllum pinnatum*.
  10. Ogidigo JO, Anosike C, Nwodo OF, Omotuyi O, Nash O, Metibemu S, Eniafe G, Okpalafe O, Sani M. In silico molecular docking and pharmacokinetic studies of some selected phyto-constituents of *Byrophyllum pinnatum* as a potential selective inhibitor of MAO-B. *Pharmacologyonline*. 2018 Dec 30;3(45):14-49.
  11. Wikipedia contributors, Lipinski rule of 5. Wikipedia, The Free Encyclopedia. [https://en.wikipedia.org/wiki/Lipinski%27s\\_rule\\_of\\_five](https://en.wikipedia.org/wiki/Lipinski%27s_rule_of_five)
  12. Drug bank. Lipinski rule of 5. [https://dev.drugbank.com/guides/terms/lipinski's\\_rule\\_of\\_five](https://dev.drugbank.com/guides/terms/lipinski's_rule_of_five).
  13. Vrbanac J, Slauter R. ADME in drug discovery. In *A comprehensive guide to toxicology in nonclinical drug development* 2017 Jan 1 (pp. 39-67). Academic Press.
  14. North east biolab. ADME studies: Measuring drug viability and suitability for later development. <https://www.nebiolab.com/adme-studies/>
  15. Tripathi KD. *Essentials of medical pharmacology*. Jaypee Brothers medical publishers; 2018 Oct 31.

**HOW TO CITE:** Ketura Kambampaty\*1, Dr. Preeti Salve2, Nurzeba Bepari3, Virtual Screening of Physicochemical and Pharmacokinetic Parameters of Selected *Bryophyllum Pinnatum* Constituents, *Int. J. of Pharm. Sci.*, 2025, Vol 3, Issue 1, 1850-1862. <https://doi.org/10.5281/zenodo.14717214>

