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# Molecular docking studies of secondary metabolites of *Phyllanthus niruri* against adipocyte fatty acid–binding protein aP2

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## Abstract

*Phyllanthus niruri or stone breaker is one of the important Ayruvedic herbs and it also called Keezhanelli in Tamil which is commonly found in coastal areas.* The pharmacological activity of the *Phyllanthus niruri* include antimicrobial, antioxidant, anticancer, antiinflammatory ,anti plasmodial, antiviral, diuretic and hepatoprotective. The purpose of this study was to analyze the inhibitory action of Phytochemicals, retrieved from the *Phyllanthus niruri towards Asthma.* The9 Phytochemicalsfrom the plant were subjected to *Insilco* drug-likness properties and satisfied compounds were further carried out for computational docking studies. The 3D crystallographic structure of human adipocyte lipid-binding protein (aP2) was obtained from PDB database of PDB ID: 2HNX, length of amino acid 136 with single chain (Chain A). Docking analysis was performed between the 9 compounds and 3D structure of the Protein using Arguslab software The compounds of *phyllanthus niruri* showed optimum binding affinity towards target human adipocyte lipid-binding protein with the significant binding energy.These results indicated that Hypophylllanthin from the plant *Phyllanthus niruri* could be one of the potential ligands molecules for a synthesis of new drug to treat Asthma.

**Keywords:** *Asthma,Phyllanthus niruri,* Phytochemicals, druglikeness properties, Docking

## Introduction

*Phyllanthus niruri,* commonly known as *Phyllanthus amarus Schum,* is a species of Phyllanthus [Jantan *et al.,* 2019]. It's a weedy tropical annual herb shrub that thrives in moist, humid wastelands. Phyllanthusniruri is one of more than 500 Phyllanthus species found in temperate and tropical areas [Danladi S*et al.,* 2018]. It is used as a medicinal plant in the tropics and subtropics, including West Africa (including Nigeria and Ghana), Europe, Asia (including China, Pakistan, India, and Malaysia in the Indian Ocean), Central America, and South America [Bharti Sarin *et al.,* 2014]. The herb has been utilised in Ayurvedic traditional medicine for thousands of years to treat a variety of ailments. *Phyllanthus niruri* is a popular traditional medicine in India for treating jaundice, asthma, hepatitis, and other ailments [Narendra K *et al.,* 2012].

Previous investigation on Pharmacological activity reported that the Phytochemistry studies of the plant on *Phyllanthus niruri* revealed that extracts of this plant had Antidiabetic activity [Bavarva JH *et al.,* 2007], Hyperlipidemic activity [Jagtap S *et al.,* 2016], Hyperuricemic effect [Murugaiya V *et al.,* 2009], Nephroprotective effect [Reddy GS *et al.,*2017], Antiplasmodial activity [Soh PN *et al.,* 2009], Antinematodalactivity [Shakil NA *et al.,* 2008], Antibacterial activity [Komuraiah A *et al.,* 2009], Hepatoprotective effect [Huang MH *et al.,* 2006].
Asthma is most common respiratory condition, causing significant morbidity and mortality [Dharmage SC*et al.,*2019]. Patients with persistent cough, wheezing, chest tightness, or dyspnea should be suspected of having asthma, and the diagnosis should be verified using objective lung function tests [Burney P*et al.,*2015]. To detect suspected asthma triggers, allergy testing is also recommended [Yanez A *et al.,*2014]. Asthma management can usually be managed with avoidance tactics and suitable pharmaceutical therapies in most people [Wurst KE*et al.,*2016]. For the vast majority of asthma patients, ICSs are the gold standard of therapy [de Marco R*et al.,*2015]. In most people, combined therapy with a LABA and an ICS is the best therapeutic option for those who fail to establish control with low-to-moderate ICS dosages [Barnes P*et al.,*2016].

If asthma is uncontrolled despite low to moderate dose ICS medication, LTRAs can be utilised as an add-on therapy, especially in individuals with concurrent allergic rhinitis [Quirt J *et al.,*2018]. In some cases with difficult-to-control asthma, LAMAs or biologic treatments targeting IgE or IL-4 may be beneficial [Bergeron*et al.,*2010]. Allergen-specific immunotherapy is a potentially disease-modifying treatment that should only be recommended by allergy-trained doctors [Wenzel SE*et al.,*2012]. All asthma patients should have regular follow-up appointments during which they should be evaluated for asthma control, adherence to medicine, and good inhaler technique [Ducharme FM*et al.,*2015].

Systemic glucose and lipid metabolism are regulated by the adipocyte fatty acid–binding protein aP2 [Turturice BA*et al.,*2017]. The aP2, in addition to being abundantly expressed by adipocytes, is also expressed by human airway epithelial cells and undergoes a dramatic increase in response to the Th2 cytokines IL-4 and IL-13 stimulation. STAT6, a transcription factor with a prominent regulatory role in allergic inflammation, was required for Th2 cytokine regulation of aP2 mRNA expression [Bohm L *et al.,*2015]. In a model of allergic airway inflammation, aP2-deficient mice were used and discovered that the infiltration of leukocytes, particularly eosinophils, into the airways was largely dependent on aP2 activity [Huang YJ *et al.,*2015].T cell priming was unaffected by aP2 loss, implying that aP2 was working locally within the lung, and examination of bone marrow chimaeras suggested that aP2 was operating on non-hematopoietic cells, most likely bronchial epithelial cells, in allergic airway inflammation [Albacker LA *et al.,*2013]. As a result, aP2 controls allergic airway inflammation and may be linked to fatty acid metabolism and asthma.

Large libraries of commercially available drug-like compounds are computationally screened against known structural targets, and those that are expected to bind well are empirically tested [Maia EHB*et al.*,2020]. Molinspirationsoftware ruled out virtual screening of the molecule [Srivastava R*et al.*,2021]. The software calculates the most important molecular properties (logP, polar surface area, number of hydrogen bond donors and acceptors, and others) as well as the bioactivity score for the most important drug targets (GPCR ligands, kinase inhibitors, ion channel modulators, and nuclear receptors).

The docking approach, which predicts the binding affinity of small molecules to their appropriate target binding sites and inhibits the target functions, is one of the most essential and widely used methods in structural-based drug designing [Pinzi L*et al.*,2019].The objective of this study was to investigate the inhibitory activity of *9* Phytochemicals of *Phyllanthus niruri towards Asthma*a P2 *protein.*

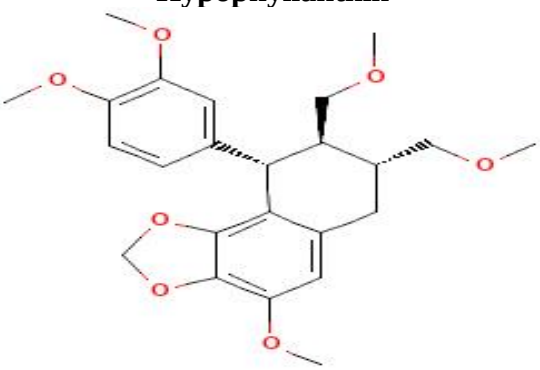
## Materials and Methods

### Ligand selection:

Through literature study, 9 phytochemical compounds were identified from the plant *Phyllanthus niruri* and for computational analysis and from the PubChem database, 2 dimensional structures were retrieved for 9 compounds (Figure 1).

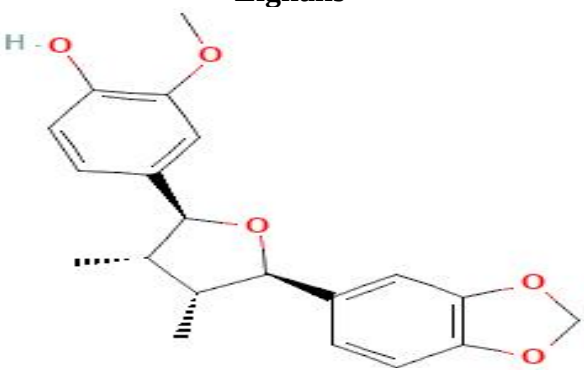
**Figure 1: 2D structure of *Phyllanthus niruri* plant compounds along with its PubchemID**

**Hypophyllanthin**



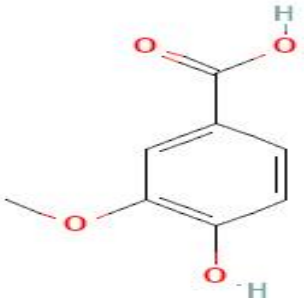
**Pubchem ID: 182140**

**Lignans**



**Pubchem ID: 13844301**

**Vanillic Acid**

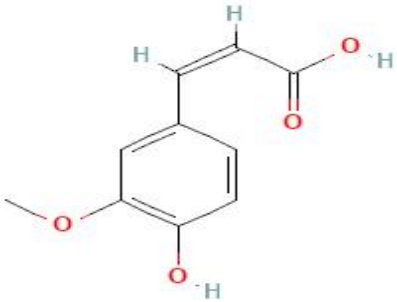


**Pubchem ID:8468**

**3-Hydroxybenzonic Acid**

**Pubchem ID:132343784**

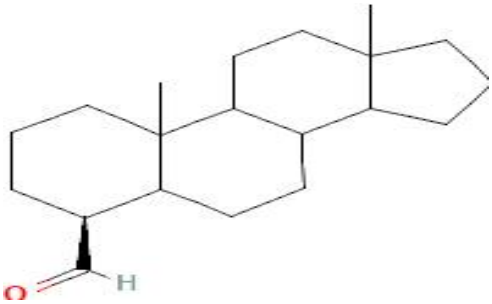
**Ferulic Acid**



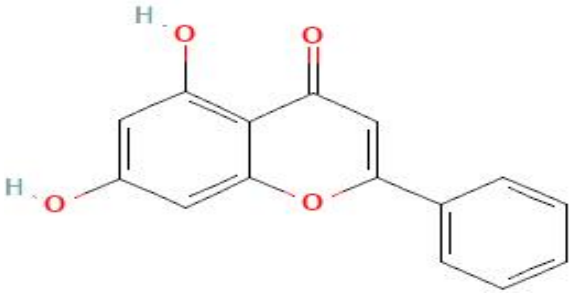
**Pubchem ID: 1548883**

**4beta-Formyl steroids**

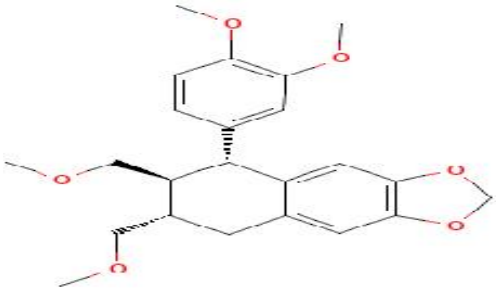
**Chrysin**



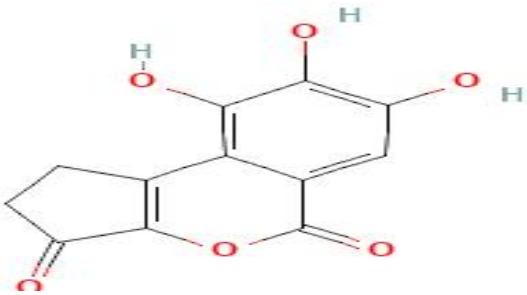
**Pubchem ID:156613017**
**Isolintetralin**



**Pubchem ID:5281607**
**Brevifolin**



**Pubchem ID:101241675**



**Pubchem ID: 10131135**

## Drug likeness prediction:

The drug similarity filter test was performed for over 9 phytochemicals using the Molinspiration server. LogP, Topological Polar Surface Area (TPSA), Molecular weight (MW), number of hydrogen bond acceptors (No.HA), number of hydrogen bond acceptors (No.HD), and volume (Vol).

## Bioactivity prediction:

Using the Molinspiration bioactivity server, the compounds that clear the oral medication qualities were further examined for biological features. GPCR ligand, Ion channel modulator, Kinase inhibitor, nuclear receptor ligand, Protease inhibitor, and Enzyme inhibitor are among the six features predicted by molinspiration bioactivity. The molecule that meets all of the biological requirements could be used in the docking process.

## Accession of target protein:

The most essential Asthmatic protein was discovered to be the adipocyte fatty acid-binding protein aP2. Protein data bank (PDB) (http://www.rcsb.org/pdb/) was used to recover the protein's three-dimensional structure (2HNX), [Ricardo*et al.,* 2017] which was determined by experimental experiments utilizing X-Ray Diffraction with a resolution of 1.50Å.

## Analysis of target active binding sites:

SCFBio - Supercomputing Facility for Bioinformatics and Computational Biology (http://www.scfbio-iitd.res.in/dock/ActiveSite.jsp) recognised the binding sites of small compounds present in the protein structure. The SCFBioActive Site prediction server will predict the active site in the protein's three-dimensional structure for ligand binding.

## Molecular Docking Interactions using Argus Lab:

Using the Argus Lab 4.0.1 docking software program28, docking studies were performed to examine the structural connection between receptor and ligand. For the docking process, the following parameters were set: Maximum generation, Crossover rate, Mutation rate, Elitism, Population size, Grid resolution, Binding site box size Lamarckian Genetic Algorithm was

employed by the Dock engine. For each docking run 15, the docking mode should be set to "Dock" and the ligand should be "Flexible.".

### Visualization of docking interaction using PyMol:

PyMol, an open source molecular visualisation tool, was used to examine the hydrogen bond interactions between the protein and the ligand, as well as predict the distance of hydrogen formation between them. The anticipated distance indicates that the binding relationship was persistent, and that a tiny chemical might limit protein activity.

## Results and Discussion

### Preparation of small molecules:

Through literature survey, totally 9phytoconstituents were identified from plant *Phyllanthusniruri*. The virtual screening was carried out for 9phytoconstituents using Molinspiration server. From the result of Drug likeness properties revealed that 9 compounds pass the Drug likeness screening test (Table 1) and Bioactivity test (Table 2). The result of the above screening provided that 9 compounds satisfies the oral drug properties

**Table 1: The phytochemical compounds which satisfy the drug likeness properties**

| S.No | Compound | LogP | TPSA | MW | No.HA | No.HD | Vol |
|---|---|---|---|---|---|---|---|
| 1. | Hypophyllanthin | 3.50 | 64.64 | 430 | 7 | 0 | 397 |
| 2. | Lignans | 4.04 | 57.16 | 34.39 | 5 | 1 | 311.2 |
| 3. | Brevifolin | 0.76 | 107.7 | 248.9 | 6 | 3 | 194.8 |
| 4. | 3-Hydroxybenzonic Acid | 1.31 | 74.60 | 184.2 | 4 | 2 | 142.8 |
| 5. | 4beta-Formyl steroid | 4.83 | 17.07 | 288.8 | 1 | 0 | 306.4 |
| 6. | Vanillic Acid | 1.19 | 66.76 | 168.5 | 4 | 2 | 144.1 |
| 7 | Ferulic Acid | 1.25 | 66.76 | 194.9 | 4 | 2 | 172.3 |
| 8. | Chrysin | 2.94 | 70.67 | 254.4 | 4 | 2 | 216.3 |
| 9. | Isolintetralin | 3.72 | 55.40 | 400.7 | 6 | 0 | 371.1 |

**Table 2: The phytochemical compounds which satisfy the bioactivity properties**

| S.No | Compound | GPCR ligand | Ion channel modulator | Kinase inhibitor | Nuclear receptor ligand | Protease inhibitor | Enzyme inhibitor |
|---|---|---|---|---|---|---|---|
| 1. | Hypophyllanthin | 0.03 | -0.05 | -0.34 | -0.16 | -0.07 | -0.05 |
| 2. | Lignans | 0.08 | -0.23 | -0.20 | 0.10 | -0.18 | 0.07 |
| 3. | Brevifolin | -0.54 | -0.54 | -0.46 | -0.24 | -0.43 | 0.17 |
| 4. | 3-Hydroxybenzonic Acid | -0.61 | -0.07 | 0.69 | -0.06 | -1.05 | -0.19 |
| 5. | 4beta-Formyl steroid | 0.11 | 0.25 | -0.41 | 0.52 | 0.19 | 0.46 |
| 6. | Vanillic Acid | -0.85 | -0.42 | -0.99 | -0.61 | -1.12 | -0.35 |
| 7 | Ferulic Acid | -0.47 | -0.30 | -0.72 | -0.14 | -0.81 | -0.12 |
| 8. | Chrysin | -0.11 | -0.08 | 0.15 | 0.30 | -0.30 | 0.26 |
| 9. | Isolintetralin | -0.01 | -0.13 | -0.31 | -0.17 | -0.10 | -0.09 |

## Preparation of protein:

The 2HNX - 3D structure of protein was retrieved using Protein Data Bank database. The possible binding site sites of the aP2 protein (2HNX) were predicted using SCFBio. The name, position and atom of amino acid present in the protein are given in Table 3.

**Table 3: Active Sites of aP2 protein (2HNX)**

| Active Sites | Position | Atom | Active Sites | Position | Atom |
|---|---|---|---|---|---|
| PHE | 16 | CE1,CE2,CZ | GLU | 61 | N,CA,O |
| TYR | 19 | CE2,OH | ILE | 62 | N,CG1,CG2,CD1 |
| MET | 20 | CG,SD | GLU | 72 | CG,OE2 |
| VAL | 23 | CG1,CG2 | VAL | 73 | O |
| VAL | 25 | CG1,CG2 | THR | 74 | CA,CB,CG2 |
| THR | 29 | CG2 | ALA | 75 | N,CB |
| ALA | 33. | CA,O,CB | ASP | 76 | N,CB,CG,OD1 |
| ALA | 36 | CB | ARG | 78 | NH2 |
| PRO | 38 | CB,CG | HIS | 93 | CE1 |
| MET | 40 | CB,CG,SD | GLN | 95 | OE1,NE2 |
| ILE | 51 | O,CG2 | ILE | 104 | CG2.CD1 |
| SER | 53 | N,O,CB,OG | ARG | 106 | NE,NH2 |
| SER | 55 | CB,OG | .VAL | 115 | CB,CG1,CG2 |
| PHE | 57 | CD2,CE2 | CYS() | 117 | SG |
| LYS | 58 | O,CB | ARG | 126 | CB,CD,NE,NH2 |
| THR | 60 | N,O,CB,OG | TYR | 128 | CE1,OH |

## Docking analysis:

The predicted 10 active residues were used as the binding sites for 9 natural compounds from the plant *phyllanthus niruri* for docking studies. The results of the binding interaction between the active site residues of target protein (2HNX) and 8 compounds were shown in the Table 4.

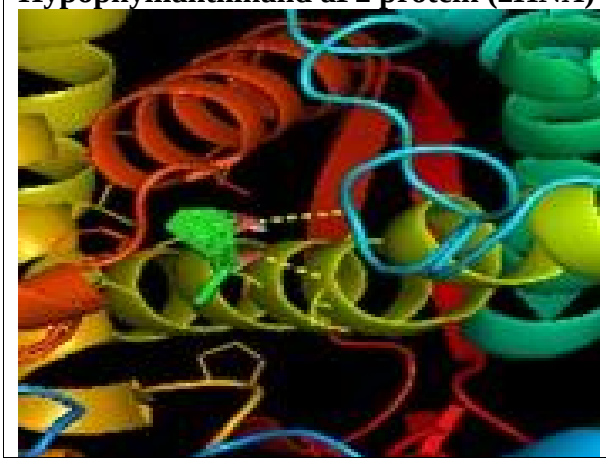
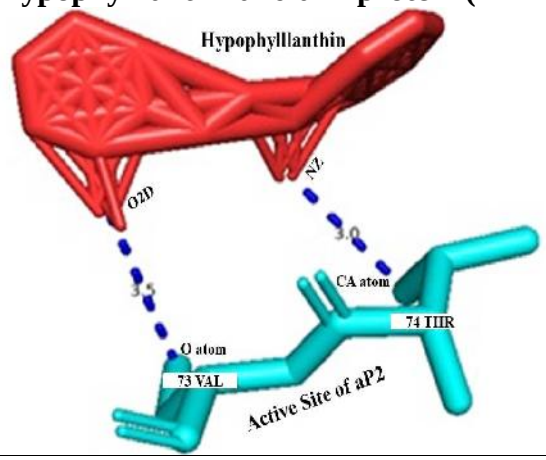
**Table 4: Molecular Docking between Phytochemicals and the aP2 protein (2HNX)**

| S.No | Compound | Binding Affinity |
|---|---|---|
| 1. | Hypophyllanthin | -9.5 Kcal/Mol |
| 2. | Lignans | -7.9 Kcal/Mol |
| 3. | Brevifolin | -7.5 Kcal/Mol |
| 4. | 3-Hydroxybenzonic Acid | -6.7 Kcal/Mol |
| 5. | 4beta-Formyl steroid | -6.2 Kcal/Mol |
| 6. | Vanillic Acid | -5.4 Kcal/Mol |
| 7. | Ferulic Acid | -5.1 Kcal/Mol |
| 8. | Chrysin | -4.5 Kcal/Mol |
| 9. | Isolintetralin | -4.3 Kcal/Mol |

By analyzing the docking result it was predicted that the compound Hypophylllanthinwere found to have the highest inhibitory energy of -9.5 Kcal/Molwhen compared with 8 other compounds which showed the inhibitory energy of less than -8 kcal/mol. On evaluating the docking result using PyMol software, it was predicted that the best hydrogen interaction occurred between the compound Hypophylllanthin and protein 2HNX. From the result of evaluation, it was revealed that the Hypophylllanthin possess the least binding interactions with the bacterial protein -9.5 Kcal/Mol by forming 2 hydrogen bonds conformation. The OH atom present in the Valine-73 formed the hydrogen bond interaction with O2D atom ofHypophylllanthinby the bond length of 3.5Å. Followed by the amino acid Theronine-74 formed the hydrogen bond interaction with CA atom of Hypophylllanthinby the bond length of 3Å (Table 5).

From the docking results, it was clearly conveyed that among the 9 plant compounds, Hypophylllanthin exhibits the best binding interaction with the aP2 protein (2HNX)and further this study could be useful in designing of new preventive and therapeutic drug against Asthma disease.

**Table 5: Docking interactions between Hypophylllanthinand aP2 protein (2HNX)**

| Best docking interactions between Hypophylllanthinand aP2 protein (2HNX) | The hydrogen distance between Hypophylllanthinand aP2 protein (2HNX) |
|---|---|
|  |   |

## Conclusion

The creation of novel natural compounds with pharmacological action is critical in the development of effective antibacterial drugs. Docking studies revealed the binding interactions between the aP2 protein (2HNX) and nine natural chemicals in this investigation. Hypophylllanthin was discovered to have the best binding energy of -9.5 kcal/mol and also satisfy the pharmacological qualities, making it a strong candidate for an oral medication. Overall, this research suggests that compound hypophylllanthin may be effective asmathic medicines against the aP2 protein. To identify the dosage for the safety levels, more in vivo research is needed to enrich the pharmacological activity of the hypophylllanthin molecule from *Phyllanthus niruri.*

## Conflict of interest:

The authors declare they have no competing interests.

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