

# NeMedPlant: a database of therapeutic applications and chemical constituents of medicinal plants from north-east region of India

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## Abstract:

The North-East region of India is one of the twelve mega biodiversity region, containing many rare and endangered species. A curated database of medicinal and aromatic plants from the regions called NeMedPlant is developed. The database contains traditional, scientific and medicinal information about plants and their active constituents, obtained from scholarly literature and local sources. The database is cross-linked with major biochemical databases and analytical tools. The integrated database provides resource for investigations into hitherto unexplored medicinal plants and serves to speed up the discovery of natural products-based drugs.

**Availability:** <http://bif.uohyd.ac.in/nemedplant/> or <http://202.41.85.11/nemedplant/>

**Key words:** Medicinal plant, Phytochemicals, Manipur, Nagaland, Activity prediction

## Background:

Of late, the role of medicinal plants as a primary source of prevention and management of diseases is being realized with alarming concerns [1-2]. The inherent disadvantage of toxicity of synthetic drugs, especially when used for longer period has led to the search for easily available safe remedies with less harmful effects. Globally, there is a renewed interest in the use of traditional medicines. An estimated 65% of the population in India use medicinal plants to meet the primary health care needs, and similar usage has been reported in many parts of the world [3-4]. Unfortunately, inadequate research in the traditional medicine sector has slowed down its development. Moreover, lack of cooperation and sharing of knowledge among diverse disciplines have further hampered the research

and development. Hence, a systematic comprehensive knowledgebase of medicinal plants is the need of the hour.

India is well-known for its wealth of medicinal plants. The use of plants to treat various diseases in ancient systems of medicine in India dates back to 3000-6000 BC [4]. The rich heritage is unfortunately confined within the local population and rest of the world is largely ignorant about it. Few attempts were made in the past to develop such information resources [5-8]. However, the North-East (NE) region of India, which is one of the treasure house of various plants have largely been ignored. We have therefore developed an integrated database, referred as NeMedPlant with the purpose to facilitate the accessibility of the indigenous knowledge related to medicinal

plants from the NE region of India. In this region, the state of Manipur and Nagaland are endowed with exceptionally rich tropical and subtropical flora. An estimated about 4500 species of plants occur in this region. We selected these two NE zones as a part of our continuing research on plants in these areas. NeMedPlant aims to unify the available traditional and scientific knowledge on medicinal herbs, their therapeutic applications and molecular and structural data of their chemical constituents. The integrated information resource, cross-linked with major databases and analytical tools would be a useful product for computational analysis, and to direct the experimental investigations towards this important area.

## Database Design:

### Data Collection, Curation and Integration

Since most of the information about medicinal plants in this region was not available, an elaborate investigations and compilation are made. The plants selected were those which are widely used and sufficient information is available in the traditional medicinal systems. This involved field collection of

data, manual examination of the local treatise and scholarly literature search. Information about active constituents, their molecular structure, properties, synthetic routes and targets were retrieved from scholarly literature using Scifinder [8], Scopus [9], PubChem [10], various encyclopedias and books. The information within the database is broadly classified and presented in two different categories: (i) details of the medicinal plants, drug formulation and their therapeutic uses. Here comprehensive account of various aspects of medicinal plants including illustrations has been provided. This include - the botanical name, common and vernacular names, place and distribution of the species in the region, parts used, applications, medicinal information, disease name, and relevant literature source. (ii) Phytochemical information: the active constituent data include the name of the compound, its chemical structure, details of preparation or extraction, physicochemical properties like molecular weight, log P value, H-donor/acceptor, available molecular targets etc (Figure 1A).

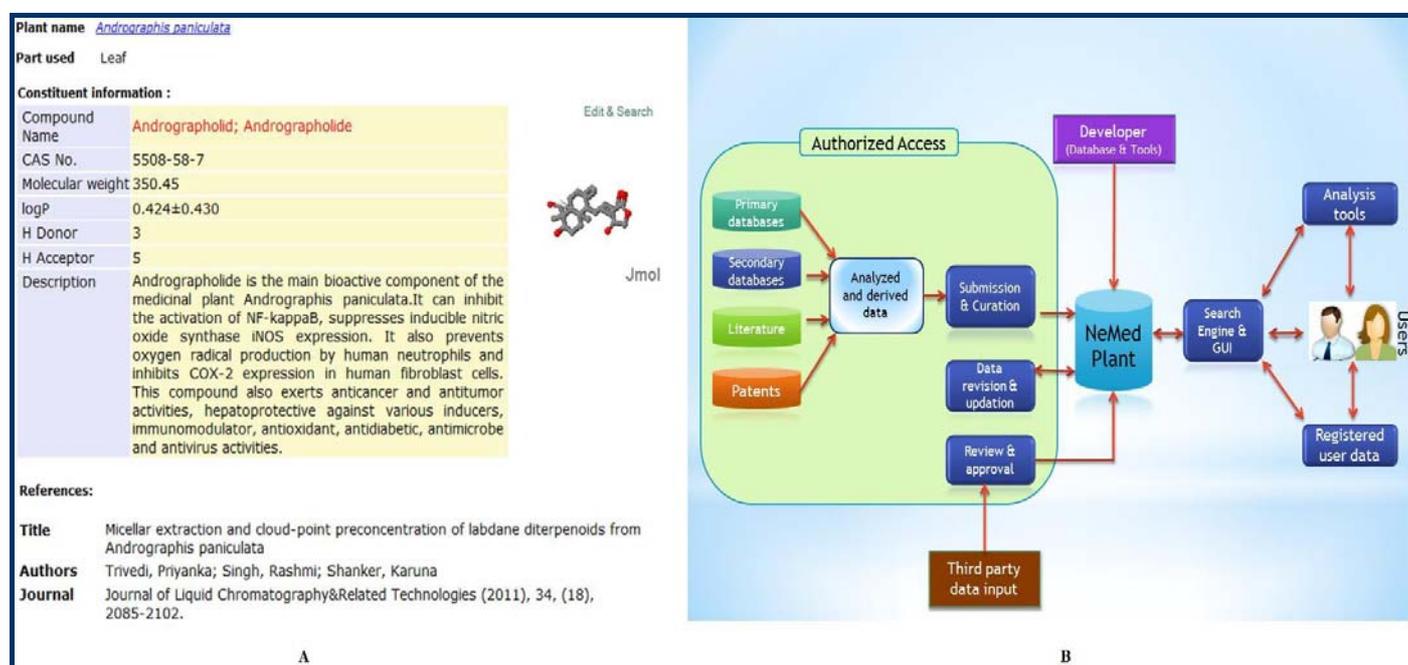


Figure 1: (A) A screenshot of a typical record in NeMedPlant. (B) Schematic representation of database information flow.

The NeMedPlant database is archival and each record receives a unique randomly generated ten digit alphanumeric identifier at the time of first submission. These records can be updated from the individual submission pages. The data can also be curated by third party (users) using registration facility provided in the home page.

The database is integrated with major primary and secondary databases and bioinformatics tools. In addition, there are several Java applets included within the database for convenient analysis and visualization of the data.

### Database Implementation

The schematic representation of the database information flow is illustrated in (Figure 1B). The database was created in MySQL with PHP-based web-search engine for data retrievals.

### Availability and Support:

To facilitate data extraction, flexible search options have been provided. In addition to the simple search interfaces, the advanced search functionality provides various options for quick, easy browsing and retrieval of desired information. Facilities have been set-up for the users to contribute to submission and annotation in NeMedPlant via a 'Submit' drop-down box.

### Utility:

In most part of the world, the information on medicinal plants has generally been handed down from generation to generation only by means of folklore, which may disappear over a period of time. For effective conservation of phyto diversity and the successful documentation of medicinal plants, the systematic inventory of medicinal plants is necessary. The relevant data (detailed description of medicinal herbs, therapeutic uses,

pharmaceutical applications and chemical constituents) on such plants in organized and easy to understand format, with illustrations, is available in the database. The integrated database with interactive analytical and visualization tools, having multiple editing options, allows users to investigate many questions without requiring time-consuming inferences from the literature or multiple data sets. The activity prediction for phytochemicals forms an important part of the work. The NeMedPlant would be useful for prediction of activities of natural as well as synthetic products and identifying drug leads having low toxicity and high bioavailability. The activity prediction can be made in two different ways: i) using chemical similarity and substructure searches in chemical databases with available Java tools in NeMedPlant; ii) when information on molecular target is known, using inverse docking or similar cavity search approaches

### Conclusion and Further Development:

Development of new natural product based drugs for treating disease requires multiple approaches. Using bioinformatics approaches, we made an attempt to systematically record information on rich heritage of the medicinal plants in this unexplored NE region of India. We gathered traditional, scientific and medicinal information from local sources and peer-reviewed literature, and compiled it into a comprehensive knowledgebase. The present database with integrated information on herbs, natural products, structural, physicochemical properties and analytical tools would be an ideal resource for information retrieval, pharmacological, bioinformatics and chemoinformatics analyses, to make new discoveries in the area, and direct further experimental investigations. Some of the plants appearing in this database from NE region also occur beyond the area, hence suggesting the usefulness of it outside the region as well. The database is under constant development. It is regularly updated for any

new information. Many existing and in-house developed tools are being incorporated. Activity prediction can also be made with chemoinformatics searches for similar models in known 3D-QSAR databases. Data curation for this purpose is being carried out. The study on medicinal plants, of course, does not end with the knowledge of their therapeutic uses, and bio- and chemo-informatics analyses. Various aspects of medicinal plants like biochemistry, associated physiological pathways, phytochemistry, agronomy, botany, ethnobotany, pharmacognosy, cultivation, conservation and biodiversity have to be studied for their optimum utilization. Attempts to integrate these data are underway.

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