



Department of
Biotechnology

Botanical pesticide database



Vittal Mallya Scientific Research Foundation

www.vmsrf.org

#94/3 & 94/5, 23rd cross, 29th Main, BTM 2nd Stage, Bengaluru-560076, India

USP of Database:

- 1) Plant data, Metabolite data, Structure data, reference data all under one roof
- 2) Interlinked and easy to browse
- 3) Only Botanical metabolite database to provide 3D structure of metabolites

Database comparison:

Database Name	# metabolites	Pesticidal activity classification	Isolation info	References	Structural info	Chemical information
TRC Botanical Database	9,000+	√	√	√	√	√
Dr. Duke's Phytochemical and Ethnobotanical Databases	30,000+	X	X	√	X	X
Plant metabolic Network	3,400+	X	X	√	√	X

Data Statistics:

Activity	No. of Metabolites
Bactericidal	561
Fungicidal	933
Insecticidal	825
Nematicidal	242
Viricidal	367
Weedicidal	35
Total	9098

Introduction

This database consists of 312 listings of botanicals known for their pesticidal properties. Botanicals have yet not made place in the Indian agriculture as the first choice of the farmers though they are known for their safety to non-target organisms, reduced mammalian toxicity and absence of toxic residues. They are environmentally attractive, but are slow in action, restricted in their host spectrum and have limited field persistence. Plenty of information is generated across the world on different aspects of botanicals and on their effect and efficiencies against range of pests and for crop management. The information generated includes methods of extraction, chemistry, bio-efficacy tests, formulations, and much more. Searching for specific information for a researcher for furthering the all ready done work is a herculean task and many times results in duplication of work and is thus time consuming. A user friendly database, pooling all published information would enhance the efforts further and could result in identification of new pest control bio-chemicals. We have made an effort to develop a database putting all information, mostly related pesticidal properties.

The “**Botanical Pesticide Database**” has been built upon a base of standard internet technologies. The website application incorporates the following technologies: HTML / CSS, JavaScript, Php.

Summary of the software and components required to support the database

Required Server Software:

1. **Operating System:** Microsoft Windows XP, 2003, Vista
2. **Web Server:** Apache HTTP Server 2.2.9
3. **Database:** MySQL 5.0.51b
4. **Web application components:** PHP 5.2.0
5. PhpMyAdmin 3.2.6
6. **Molecular visualization:** Jmol



1) Home page:

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Botanical Pesticide Database

INTRODUCTION

The Government of India has adopted Integrated Pest Management as a cardinal principal in plant protection. The implementation of pest control by biological means involves complete use of natural agents. The biopesticides and botanicals have not been able to make a huge impact commercially and hence in agriculture because of the high risk involvement. The Department of Biotechnology, Government of India, sponsored a project to launch Vittal Mallya Scientific Research Foundation for testing and accreditation of botanical pesticides as well as for the promotion of botanicals and to impart training for setting up small scale units in the Indian agriculture as the first choice of the farmers for their safety to non-target organisms, reduced mammalian toxicity and have limited field persistence. Plenty information is available on different aspects of botanicals and on their effect and use for crop management. The information generated on the chemistry, bio-efficacy tests, formulations, and much more. It is a great boon for a researcher for furthering the all ready done work as it results in duplication of work and time consuming. It is the need of the hour to consolidate all available and possible information on botanical pesticides in a database and make it further available to researchers and

Species List:

- Anethum graveolens
- Annona squamosa
- Apium graveolens
- Arachis hypogaea
- Argemone mexicana
- Arisaema flavum
- Arisaema tortuosum
- Aristolochia bracteata
- Aristolochia bracteolata
- Artemisia douglasiana
- Artemisia indica
- Artemisia vulgaris
- Asimina triloba
- Asparagus cochinchinensis
- Asparagus officinalis
- Avena sativa
- Azadirachta indica**
- Barleria acanthoides
- Basella Alba
- Bidens pilosa
- Azadirachta indica

PROPERTIES

312 plants to choose from

2) Plant information:

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Botanical Pesticide Database

Botanical Name	Common Name	Vernacular Names
		
INSECTICIDAL Choose compound ▾	FUNGICIDAL Choose compound ▾	WEEDICIDAL Choose compound ▾
VIRICIDAL Choose compound ▾	NEMATOCIDAL Choose compound ▾	BACTERICIDAL Choose compound ▾
PHYTOCHEMICALS Choose compound ▾		

Choose one of the various pesticidal property options

You get to know details of plants

3) Choose Phytochemical:

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Botanical Pesticide Database

Botanical Name	Common Name	Vernacular Names
6a-D-acetyl-7-deacetylnimocinol 7-acetylneotrichilenone 7-Benzoylnimbocinol 7-deacetyl-7-benzoylgedunin 7-Deacetyl-7-benzoylnimbinin 7-deacetylgedunin 7-detigloyl-7-methacroyl-11-deacetylnimbolidin-A 7-detigloyl-7-seneciyl-11-deacetylnimbolidin-A 7-tiglyol-12a-acetoxylvilasinin 7a-seneciyl(7-deacetyl)-23-O-methylnimocinolide a-nimolactone Acetylmeliacinolactol Azadirachnol Azadirachtanin Azadirachtanin A Azadirachtin D Azadirachtin E Azadirachtin F Azadirachtin G Azadirachtin L Choose compound		 WEEDICIDAL Choose compound BACTERICIDAL Choose compound

Phytochemical
(Azadirachtin) is
chosen

4) Phytochemical page:

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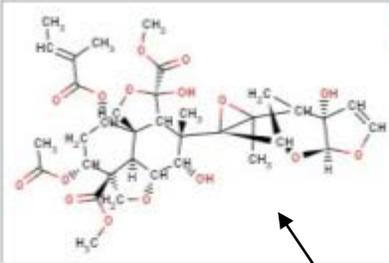
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Botanical Pesticide Database



AZADIRACTIN



Reference
W. Kraus, M. Bokel, A. Bruhn, R. Cramer, I. Klaiber, A. Klen

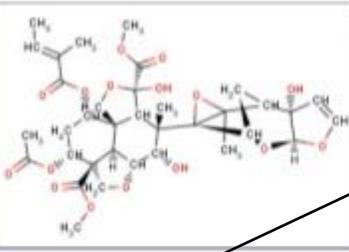
- Chemical Properties
- Predicted Properties
- Isolation
- Toxicity
- Biological Activity
- Structure



Details of chosen
Phytochemical
(Azadirachtin)

5) Further details of Phytochemical:

AZADIARACHTIN



Reference
W. Kraus, M. Bokel, A. Bruhn, R. Cramer, I. Kläiber, A. Klen

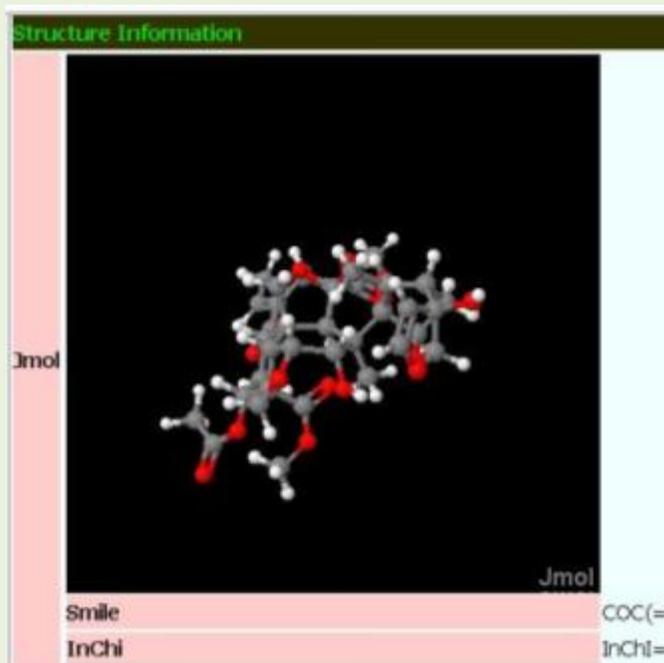
- Chemical Properties
- Predicted Properties
- Isolation
- Toxicity
- Biological Activity
- Structure

Chemical Information	
MolWeight	720.714
MolFormula	C35H44O16
Chemical Class	Tetranortriterpenoid
CAS	11141-17-6
IUPAC Name	Dimethyl(2aR,3S,4S,4aR,5S,7aS,8S,10R,10aS,11S,11aR,12R,12aS,13R,13aS,14R,14aS,15R,15aS,16R,16aS,17R,17aS,18R,18aS,19R,19aS,20R,20aS,21R,21aS,22R,22aS,23R,23aS,24R,24aS,25R,25aS,26R,26aS,27R,27aS,28R,28aS,29R,29aS,30R,30aS,31R,31aS,32R,32aS,33R,33aS,34R,34aS,35R,35aS)-3,4,4a,5,5a,6,6a,7,7a,8,8a,9,9a,10,10a,11,11a,12,12a,13,13a,14,14a,15,15a,16,16a,17,17a,18,18a,19,19a,20,20a,21,21a,22,22a,23,23a,24,24a,25,25a,26,26a,27,27a,28,28a,29,29a,30,30a,31,31a,32,32a,33,33a,34,34a,35-tetrahydro-2H-pyran-2-one
Boiling Point	792.4
Flash Point	159
Pubchem ID	5281303
Chempider ID	4444685
Appearance	Yellowish free flowing powder

Predicted Properties	
MolWeight	720.72476
Volume	581.197
H-Acceptor Count	11
H-Donor Count	3
Rotatable Bond Count	20
XlogP	-0.247
SlogP	-0.2031
SMR	164.2794
Heat of Formation	0
Ionization Potential	0
Sum of Absolute Charges	0
HOMO Energy	0
LUMO Energy	0
Hydrogens Count	44
Carbons Count	35
Oxygens Count	16
Dipole Moment	6.98911
Vanderwaal Surface Area	654.964905
Positive Potential Surface Area	335.592468
Negative Potential Surface Area	319.372406

Biological Activity	
Target Nematode	Rotylenchulus reniformis
Dosage	119.1 ppm
Reference	Sharma V; Wala S; Kumar J; Na
Link to Article	Click here

Isolation	
type of isolation	Combined Florisil, Droplet Counter-Current, and High
references	S. Mark Lee & James A. Klocke, "Combined Florisil, Dr
Link to Article	Click here



Note: Java should be enabled on your browser (Eg: Firefox with Java6) for the 3D structure to be visible

List of functionality available on the database:

- ❖ The home page consists of 312 plants with known pesticidal values.
- ❖ Users can browse for a plant species by selecting a scientific name from the drop down list which will lead to the corresponding plant information page.
- ❖ Plant information is available to the user by its images, scientific name, common name and vernacular names used in India.
- ❖ Botanicals are categorized according to its various pesticidal characteristics (insecticidal, fungicidal, bactericidal, viricidal, nematocidal, weedicidal) and secondary metabolites responsible for these characteristics. Those metabolites with unknown pesticidal characteristics were listed as phytochemicals.
- ❖ Selection of compounds from the drop down boxes will lead to its corresponding 2D image and its structure reference.
- ❖ **Chemical property** page gives molecular weight, molecular formula, chemical class to which the compound belongs, CAS, IUPAC name, boiling point, flash point, Pubchem ID, Chempid ID, appearance and so on.
- ❖ Physiological properties of the compound like H acceptor count, H donor count, Rotatable Bond Count, XlogP, SlogP, SMR, Heat of Formation, Ionization Potential, Sum of Absolute Charges, HOMO Energy, LUMO Energy, Hydrogen Count, Carbon Count, Oxygen Count, Dipole Moment, Vanderwaal Surface Area, Positive Potential Surface Area, Negative Potential Surface Area can be accessed by clicking on the **Predicted Properties** button.
- ❖ Isolation of the compound from the plant, source information and its corresponding link is also available by selecting the **Isolation** button.
- ❖ Published biological activity on use of the compound and the susceptible pest has been added along with reference in the **Biological Activity**.
- ❖ Finally, its 3D structure can also be accessed by selecting the **Structure** button which is viewed in Jmol which is an interactive 3D molecule visualizer.