Sustainable Medical Technologies (SMT)

Bioactivity Informatics of Indian Medicinal Plants

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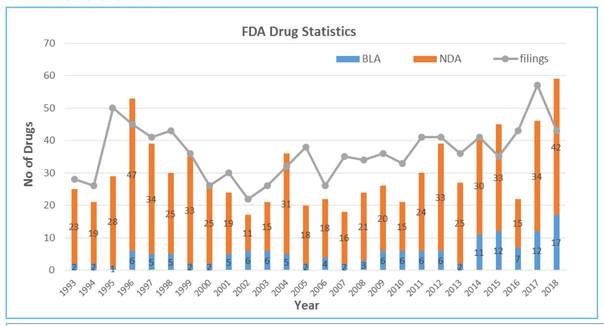
Abstract

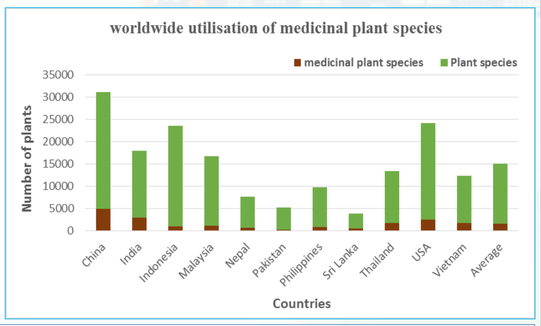
Indian medicinal plants are known to be beneficial in a multitude of diseases and disorders and their role has been documented over the centuries. How do they work? Which molecule of the plant binds to which biological target and how does this elicit the known therapeutic response? Bioactivity Informatics of Indian Medicinal Plants (BIMP) is an effort to decode this knowledge at a molecular level. Currently the BIMP database, which is made freely accessible at (http://www.scfbio-iitd.res.in/plants_scfbio), hosts information on the molecules present in Neem, Tulsi and Turmeric, their known and predicted biological targets, with links to structure, function and disease associations of these targets. This growing database could prove to be extremely valuable in a molecular understanding of Ayurveda and in identifying new cures based on natural products obtained from Indian medicinal plants.

Introduction

With the ever increasing gap between number of disease outbreaks and FDA approved drugs, new sources of drugs can play an indispensable role in combating diseases. Plant based compounds have been known to provide scaffolds for many drugs. The rich flora of indigenous medicinal plants in India have been used for centuries in traditional medicine to treat human maladies. Over 1700 Indian Medicinal Plants, 9600 Phytochemicals and around 1100 Therapeutic uses are known till date. But the major limitation encountered with the extracts of these plants is the unavailability of knowledge of compounds and their biomolecular targets. Elucidation of the mode of action of the compounds present in the plant extracts can lead to better clinical utilization. BIMP work presented here is a step towards filling this knowledge gap.

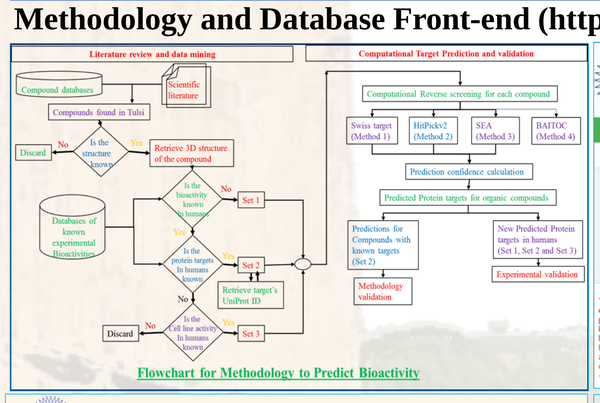
Motivation

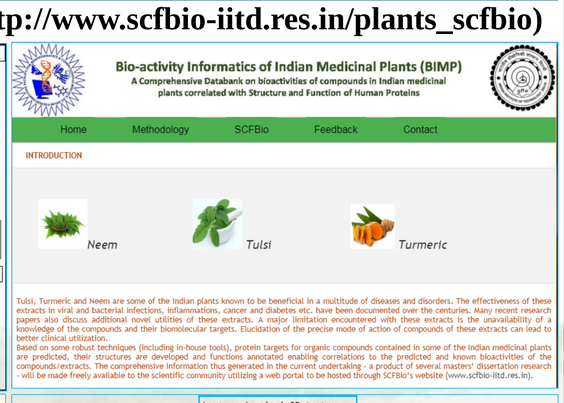


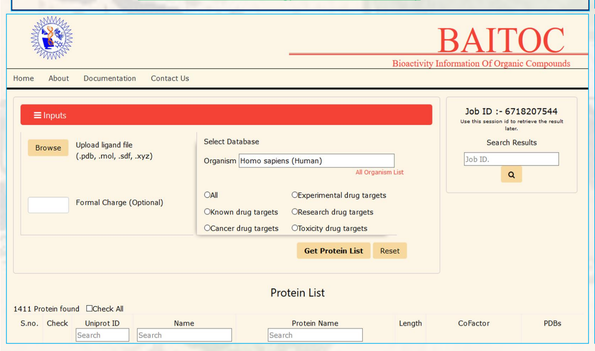


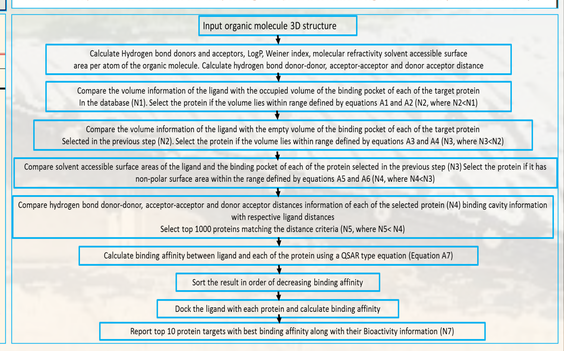
- FDA generally approves only 20-40 drugs/year. New sources of drugs can play indispensable role in increasing this number.
- Already known therapeutically relevant concoctions of plant extracts mentioned in Indian medicinal system can be used for screening for new drugs.
- Phytochemicals can target multiple biomolecular targets. These can play vital role in delaying onset of drug resistance.
- Plants can be easily grown in abundance providing an easy source of potential drugs.
- Plant extracts can play a vital role in understanding the mode of action of many disorders, using system biology approach.
- Plant based compounds have been known to provide scaffold for many drugs.

Methodology and Database Front-end (http://www.scfbio-iitd.res.in/plants_scfbio)





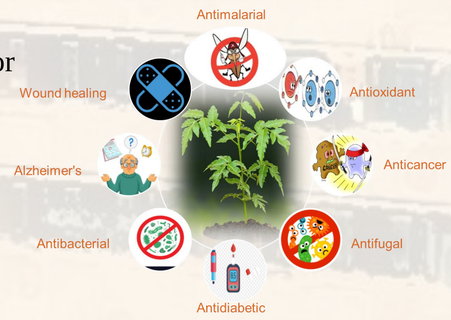




Industrial Significance

This database will be an aid to the CADD pipeline for Pharmaceutical industries.

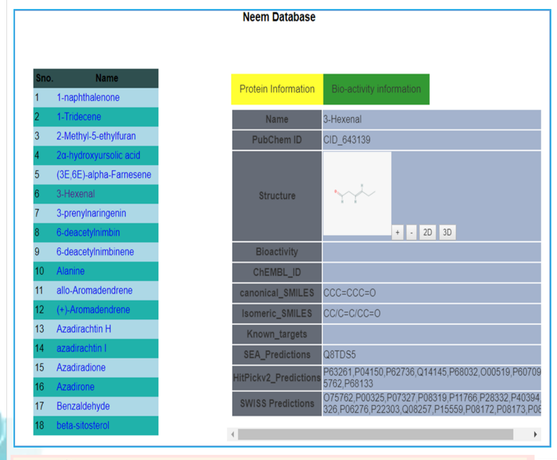
Detailed information of natural plant components accelerate drug discovery and drug repurposing processes.

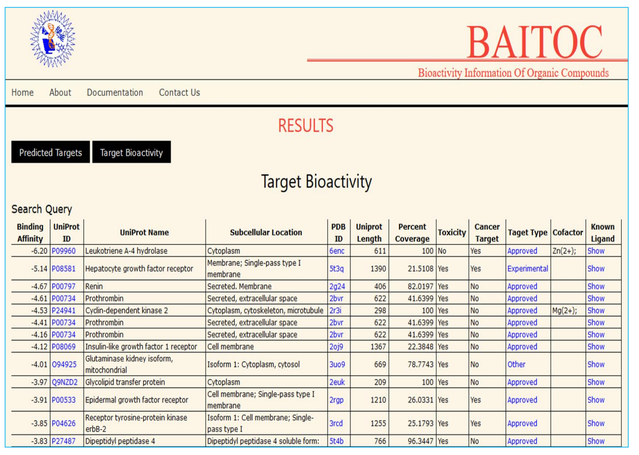


Technology Readiness Level

http://www.scfbio-iitd.res.in/plants_scfbio

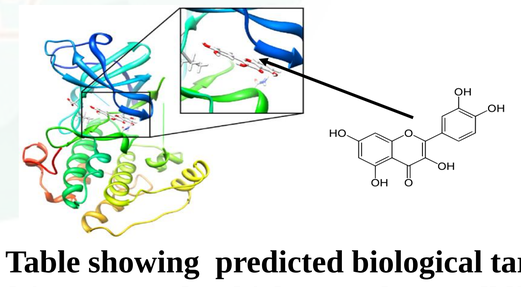
Results





Serial No.	Compound information	Turmeric	Neem	Tulsi
1	Total number of compounds	196	230	180
2	Compounds with known protein target(s)	66	30	73
3	Compounds with Cell line activity	14	37	54
4	Compounds with unknown bioactivity	116	163	53
5	Hitpick protein target prediction	178	187	179
6	Sea server protein target prediction	117	98	119
7	Swiss target protein target prediction	196	213	176

Plant: Neem
Compound: Quercetin
Target: Ribosomal protein S6 kinase, polypeptide 3
Use: Anti Cancer



Plant: Tulsi
Compound: Rosmarinic acid
Target: Insulin Receptor Tyrosine Kinase
Use: Anti diabetic

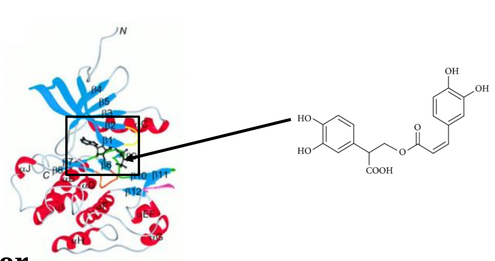


Table showing predicted biological targets for Tulsi compounds which targethave cell line activity but no known bio-molecular

Sl. No	Compound	Protein Target	Disease/Disorder/ medical utility
1	zingiberene	Estrogen receptor	Breast cancer
2	gallic acid ethyl ester	Catechol O-methyltransferase	Parkinson's disease
3	dehydrodieugenol	Peroxisome proliferator-activated receptor delta, PPAR-delta Cannabinoid receptor 1, CB-R, CB1	Cancer, Pain, epilepsy, anxiety, depression
4	orientin	Dual specificity tyrosine-phosphorylation-regulated kinase 1A	Cognitive dysfunctions (Down syndrome, Alzheimer's)
5	luteolin-7-O-glucuronide	Aldo-keto reductase family 1 member B1	Diabetes

Supercomputing Facility

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CHEMISTRY DEPARTMENT