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Bioinformatics up to Date

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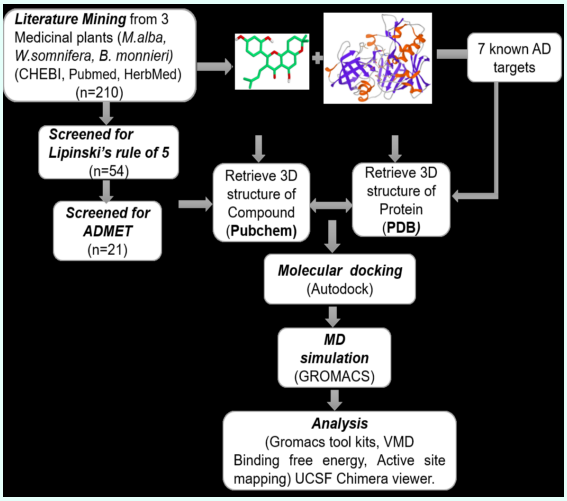
Inside…..

About us

The Bioinformatics Infrastructure Facility (BIF) at Biotechnology division, CSIR NEIST, Jorhat runs under the Biotechnology Information System Network (BTISnet) programme of DBT, Ministry of Science & Technology, and Government of India. The Centre was established on 2nd February, 2008 to promote innovation in Biological research and education through Bioinformatics accomplishment. The main goal is to facilitate and expose students and researchers from different academic institutions of North East India in Bioinformatics. The center conduct training and workshops for enlightening the use of bioinformatics applications in biological research and development. The Centre has access to global information through 24 hour high speed internet facility, and also e-journal facilities with DeLCON, Science Direct etc. To date the Centre has profoundly extended support in R & D work with a great intensity to different biological discipline including medicinal chemistry, computer aided drug design, genomics and proteomic data analysis etc.

In silico identification of potential plant based lead compounds for Alzheimer Disease (AD) Therapy.

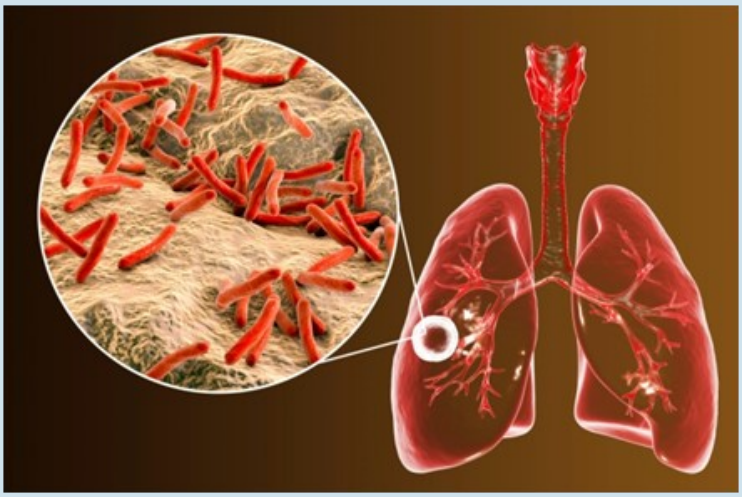
The study described about the identification of plant based lead compounds for treatment of AD through an integrative approach of pharmacokinetics and structural bioinformatics approach. Lead compounds were screened from 3 traditional medicinal plants namely *Withania somnifera, Bacopa monnieri* and *Morus alba*, which are known to have potential for treatment of neurodegenerative disease. The results obtained in the study revealed that 3 drug compounds namely Morusin (MRSN), Withanone (WTHN) and 27- Hydroxywithanolide B (HWTHN) were identified as putative lead compounds against mono amine oxidase (MAOB), Beta-secretase 1(BACE1) and phosphodiesterase 4D. Plant based lead compounds have been historically incredible as a source of therapeutic agents for various complex disorders including Alzheimer's disease (AD). AD is one of the leading neurodegenerative disorder in which the underlying risk factors remain largely unclear and presently, there is no disease modifying treatment available. Herein, the researchers described the identification of plant based lead compounds for treatment of AD through an integrative approach of pharmacokinetics and structure bioinformatics approach. They screened a total of 210 plant based compounds library of which 21 compounds were screened based on their pharmacokinetic properties. Further, Docking study against 7 known AD associated targets were carried out to identify the binding sites and direct interacting residues. In addition they investigate the stable and reliable binding mechanism of top such plant compounds against 3 targets through molecular docking followed by Molecular Dynamic (MD) simulation. The results obtained in the study revealed that 3 drug compounds namely Morusin (MRSN), Withanone (WTHN) and 27- Hydroxywithanolide B (HWTHN) were identified as putative lead compounds against mono amine oxidase (MAOB), Beta-secretase 1(BACE1) and phosphodiesterase 4D.



Source: Kasmika Borah *et al.* J Computational biology and chemistry,2019

Development of new potential drug candidates to fight against tuberculosis by Indian Researchers

Researchers have now come with a new drug candidate to fight against Tuberculosis, caused by the bacteria Mycobacterium tuberculosis, which is a major cause of death worldwide. In 2017 alone, 10 million individuals around the globe were impacted by the disorder, and about 1.6 million succumbed to it. To reduce this death count this recent study where researchers from the *Veer Narmad South Gujarat University* have developed some potential drugs against tuberculosis and have analyzed their efficiency against the TB bacteria. Different computer-based approaches paved the way for the Scientists throughout the globe to investigate the TB therapy options for screening new and better drugs utilizing the natural chemicals. In the current study, the investigators have synthesized some agents belonging to the group 'azoles', which are proven to kill germs fungi, by preventing the synthesis of lipids in their own body. The analysis has been published in the journal *Current Computer-Aided Drug Design*.



Thereafter the analysis was done by the researchers for the efficiency of the compounds against four other germs, the TB germs, and three species. Later they decided that the concentration of those chemicals that can inhibit the growth of microbes. Using a computer-based approach called they studied the interaction of these compounds with a target protein in the TB bacteria. They also tested the absorption, distribution, metabolism, and excretion properties of these compounds—necessary parameters to determine the viability of a chemical compound to be used as a drug. The researchers found that six of the synthesised compounds showed promising antimicrobial activity with one of them being very efficient in killing the TB bacteria.

The researchers believe that this compound could act as a potential anti-tuberculosis drug. They add that their findings "give the best choice for the preparation of new derivatives in order to improve antitubercular activity in future with more improved potency". With a robust global fight against drug-resistant tuberculosis on full throttle, studies like this can help us achieve the goal of eliminating the disease very soon.

Source: Paramananda Barman *et al.* Gujarat Jan 29, (Research Matters)

Bioinfo. Workflow/Flowchart/Animation (J computational biology and chemistry,2019)

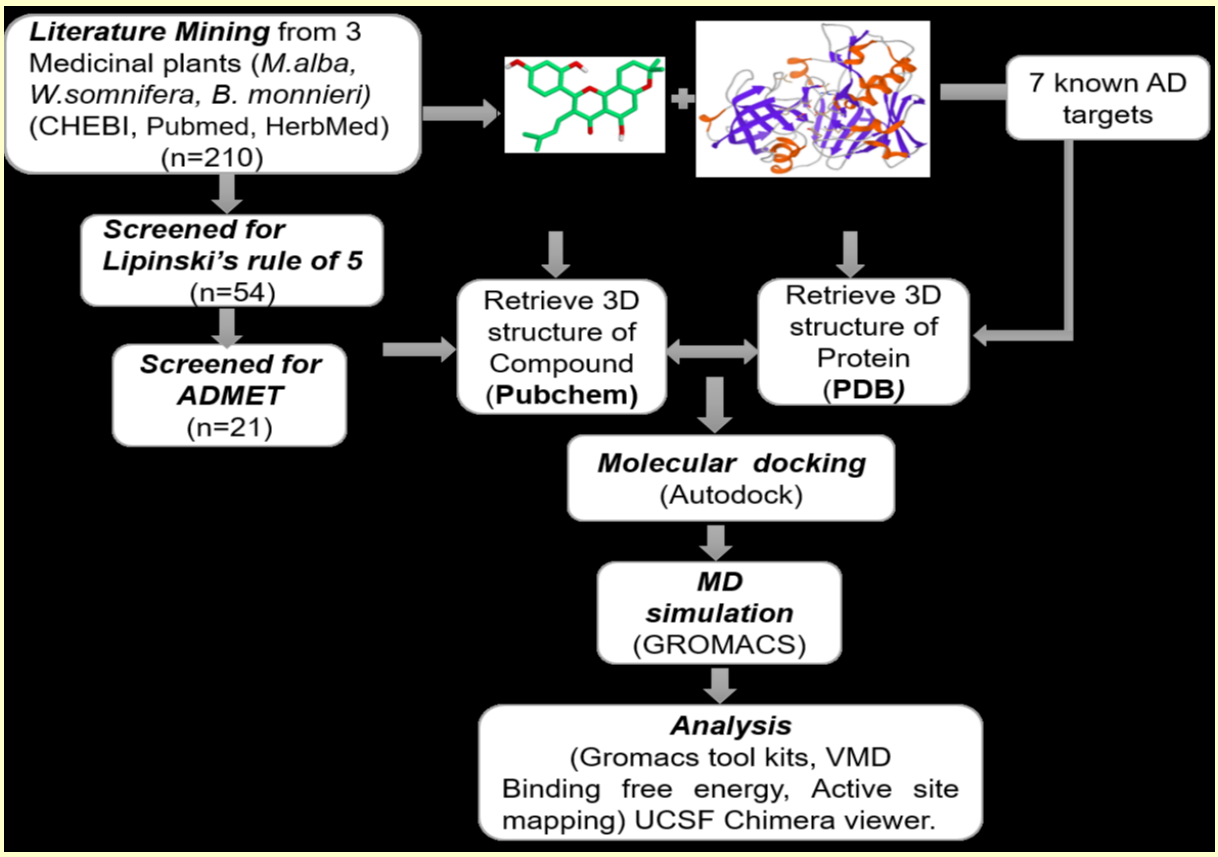


Figure 1: An overview of work flow

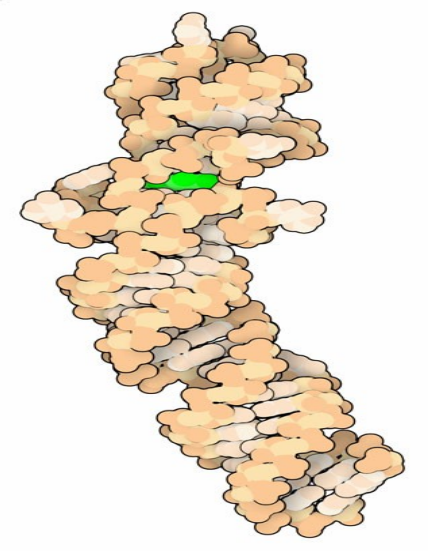
Upcoming event

1.http://biotechconference.aksuniversity.ac.in

2.https://bioinformatics.ca/workshops

Fluorescent RNA Aptamers

Constant exploration of the new tools by the scientists such as Green fluorescent protein which is an example of a tool that opened entirely a new way to tag specific proteins and then watch their activities inside living cells. Recently, scientists have been developing a new tool that allows us to watch RNA in a similar way. RNA itself is not fluorescent, so the trick is to design a short RNA that can bind to a fluorophore which is a small fluorescent molecule and enhance its fluorescence. Then, we can engineer this RNA into a natural RNA, such as a ribosome. When the fluorophore is added to the cell, it binds to the modified ribosome and watches its movement. To discover these useful fluorophore-binding RNA molecules , SELEX (systematic evolution of ligands by exponential enrichment) has been used. The process begins mixing a fluorophore with many random RNA sequences, and then isolating any that bind. These are then randomly modified, and the best ones again selected.



Figur 1:The close view of Spinach fluorescent aptamer, with RNA (light orange) and fluorophore (green).

After several more rounds of modification and selection, an “aptamer” is found that binds to the fluorophore and enhances its fluorescence. The aptamer shown here, named “Spinach”, was discovered by this process using a flourophore similar to the one in green fluorescent protein. The Spinach aptamer is a long hairpin, with an intricately-folded section at the center that surrounds the fluorophore. RNA is always difficult to crystalize, so two tricks were used to determine its structure. In PDB entry 4kzd , the loop at one end was engineered to bind to an antibody, which assists with forming a stable crystal lattice. In PDB entry 4ts2 , the loop was clipped off, making it easier for the molecules to pack end-to-end in to form a crystal.

Spinach Fluorescent RNA Aptamer

The Spinach aptamer forming a inflexible pocket that enhances the fluorescence of the molecule. In the Figure 2,one side of the fluorophore is filled aligned with a G-quadruplex (colored pink), and the another one is covered by a nucleotide base triplet (colored magenta). Another guanine (white) interacts with the edge of the fluorophore in the pocket.

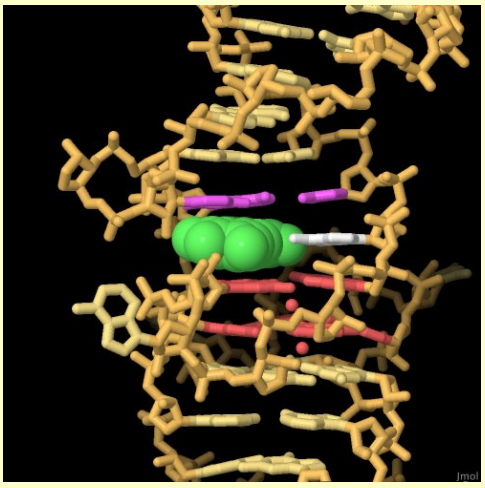


Figure 2:Spinach Fluorescent RNA Aptamer interacts with florescence molecule in the pocket.

Source: http://pdb101.rcsb.org/motm/229

Kindly send us your feedback to

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