

# Bioinformatics up to Date

(Bioinformatics Infrastructure Facility, Biotechnology Division)  
North-East Institute of Science & Technology  
Jorhat - 785 006, Assam

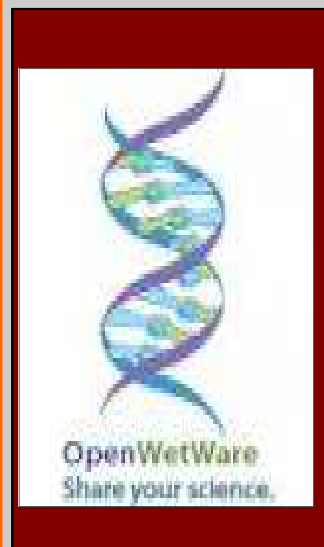


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## About Us

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.

## Our Focus

### DBT Institutional Biotech Hub Training-cum-Workshop on Basic Molecular Techniques for Microbial Genotyping, 24-25 Feb, 2016

With the support of DBT Govt of India, the Institutional Biotech Hub, BSTD, CSIR-NEIST under the successful coordination of Dr Ratul Saikia, Principal scientist and coordinator of DBT IBTHub, CSIR-NEIST had successfully completed the 2 days workshop. The program was held on 24-25<sup>th</sup> February, 2016 with the topic "DBT Institutional Biotech Hub Training-cum-Workshop on Basic Molecular Techniques for Microbial Genotyping". There are total of 50 participants joined in the workshop coming from different parts of Assam.



Most of the participants doing research works and a few with pursuing B.Sc and M.Sc courses. The workshop mainly focused on different Molecular Methods for Microbial Diversity, Genotyping, Gene cloning, Cancer etc. Techniques like DNA banding pattern, Box-PCR, RFLP, 16S rRNA sequence analysis, Metagenomics analysis etc were discussed and hands on training session also successfully organized for the different genotyping methods.

## Scientists Sequence Genome of Lyme-Disease-Spreading Tick

A Researchers team from North Carolina State University have sequenced the genetic blueprint of one of the most prolific pathogen-transmitting agents on the planet - the Lyme-disease-spreading tick (*Ixodes scapularis*) that bites humans. The findings could lead to advances in not only disrupting the tick's capacity to spread diseases but also in eradicating the pest. Their findings published in a paper Nature Communications that describes the tick genome.



The large tick genome - smaller than but similar in complexity to the human genome - supports redundancy, said R. Michael Roe, William Neal Reynolds Distinguished Professor of Entomology at North Carolina State University. Roe said that the size and complexity of the genome - combined with its duplicative elements - were problematic for tick researchers.

Besides repetitive elements, Roe noted important differences between the tick genome and insect genomes. Tick females have a hormone that regulates egg development. Learning how to block that hormone could lead to the development of a "birth-control pill" that would go a long way toward eradicating the pest, Roe said.

Roe said knowledge gleaned from the genome could be used to develop new ways to attract and trap ticks in order to disrupt their "love at first touch" mating practices. Studying the ways ticks are attracted to humans could be used to produce new tick repellents, including natural repellents; Roe and colleagues at NC State are currently developing such products.

[Source: *Genomic insights into the Ixodes scapularis tick vector of Lyme disease*. Monika Gulia-Nuss, Catherine A. Hill, R. Michael Roe, Brooke W. Bissinger, Jiwei Zhu et al. *Nature Communications* (February 9, 2016) ]

## Potential Drug Target for Atherosclerosis

A team from the Institute for Cardiovascular Prevention at the LMU Medical Center, led by Andreas Schober, has now discovered the enzyme called Dicer, plays central role in the activation of the endothelial cells. Dicer enzyme processes RNA transcripts, cutting them into short segments and regulate the synthesis of specific proteins. The team has shown that Dicer promotes the development of atherosclerosis, thus identifying a new drug target. The results of the study have been recently published in the journal "*Nature Communications*" 2016.

The enzyme Dicer is an essential component of the protein complex that generates so-called microRNAs (miRNAs) by cutting these short fragments out of longer precursor molecules. The miRNAs in turn control the expression of specific genes by interfering with the synthesis of their protein products.

They found that reduced endothelial expression of the RNase Dicer, which generates almost all mature miRNAs, decreases monocyte adhesion, endothelial C-X-C motif chemokine 1 (CXCL1) expression, atherosclerosis and the lesional macrophage content in apolipoprotein E knockout mice (*ApoE<sup>-/-</sup>*) after exposure to a high-fat diet. Endothelial Dicer deficiency reduces the expression of unstable miRNAs, such as miR-103, and promotes Krüppel-like factor 4 (KLF4)-dependent gene expression in murine atherosclerotic arteries. Inhibiting the interaction between miR-103 and KLF4 reduces atherosclerosis, lesional macrophage accumulation and endothelial CXCL1 expression.

[Source: *Endothelial Dicer promotes atherosclerosis and vascular inflammation by miRNA-103-mediated suppression of KLF4*. Hartmann, P et al. *Nature Communications* (3 February, 2016) ]

## Research Sheds Light on 'Dark Side' of the Transcriptome

A new way of mapping the "transcriptome" -- the collection of RNA read-outs that are expressed by a cell's active genes -- has been devised by researchers from the Perelman School of Medicine at the University of Pennsylvania. The report by Barash and his team, which included co-lead authors Jorge Vaquero-Garcia, Alejandro Barrera, and Matthew R. Gazzara, all research staff at Penn, was published online in eLife 2016.

Using the new method to shed additional light on the role of RNAs in cells, the team identified RNA variants in mammals that had been largely invisible to previous techniques. The researchers also demonstrated that these "dark" variations in RNA are strikingly common in mammalian cells and likely have roles in gene regulation across tissues, development, and in human diseases.

The team plans to perform the analyses using the now-free software to interrogate aberrant cells in neurodegenerative disorders, cancers, and other illnesses. The new approach devised by Barash and his team begins with the mapping of what they call local splice variations (LSVs)--essentially the variable junctions between exons, which are detectable sequences that span more than one exon. The y developed software to generate LSV maps from RNA-seq data and combine those data with existing RNA databases to yield pictures that include ordinary, known splice variants, as well as complex splice variants that other methods fail to detect.

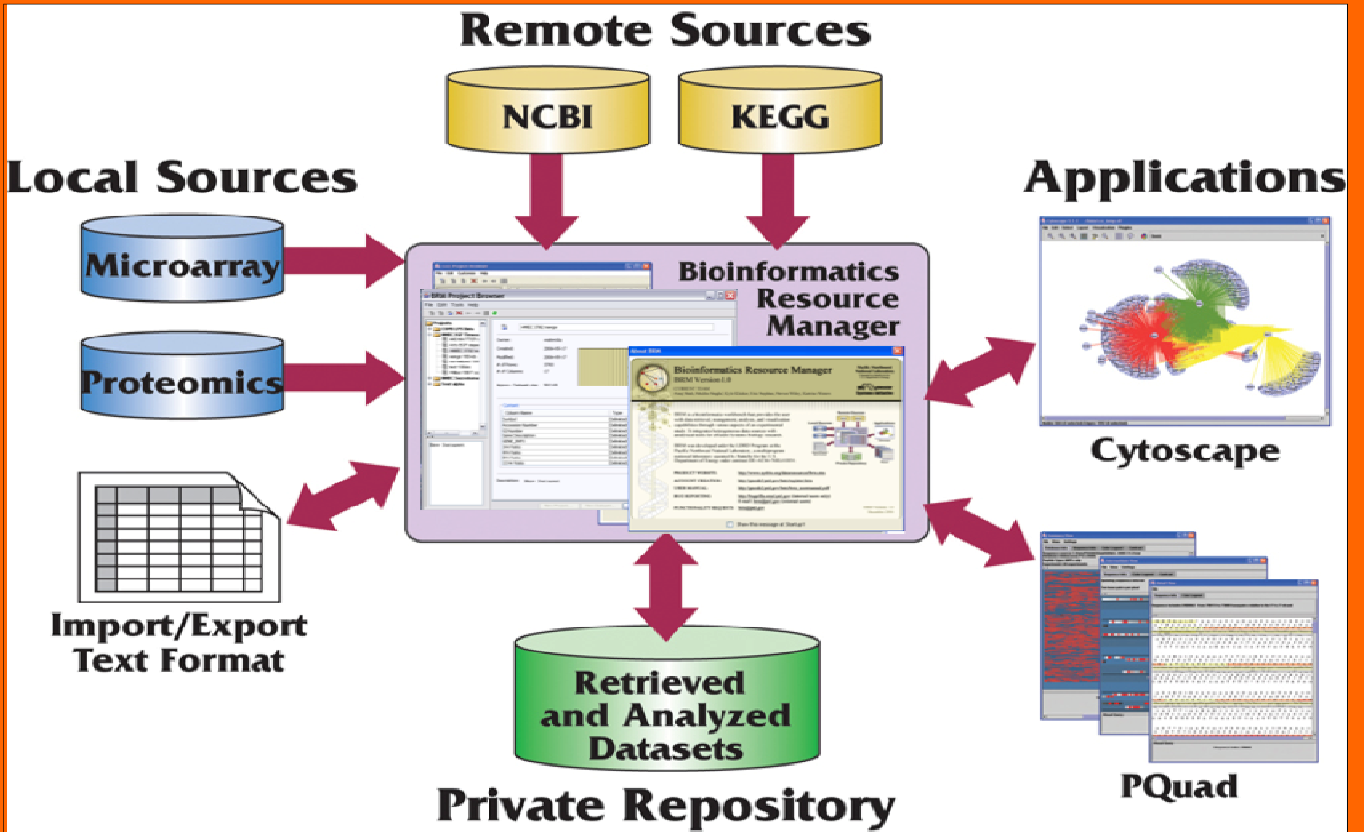
To gauge the importance of the hitherto-unseen part of the transcriptome, the team used the new MAJIQ software (Modeling Alternative Junction Inclusion Quantification) to analyze RNA-seq data from a variety of species including lizards, mice, and humans. In addition to MAJIQ, the team also has produced a complementary software package, VOILA, which enables researchers to visualize the complex splice variants detected by MAJIQ.

## NALDB: nucleic acid ligand database for small molecules

Nucleic acid ligand database (NALDB) is a unique database that provides detailed information about the experimental data of small molecules that were reported to target several types of nucleic acid structures. NALDB is the first ligand database that contains ligand information for all type of nucleic acid. NALDB contains more than 3500 ligand entries with detailed pharmacokinetic and pharmacodynamic information such as target name, target sequence, ligand 2D/3D structure, SMILES, molecular formula, molecular weight, net-formal charge,  $AlogP$ , number of rings, number of hydrogen bond donor and acceptor, potential energy along with their  $K_i$ ,  $K_d$ ,  $IC_{50}$  values. All these details at single platform would be helpful for the development and betterment of novel ligands targeting nucleic acids that could serve as a potential target in different diseases including cancers and neurological disorders.

NALDB provides powerful web-based search tools that make database searching efficient and simplified using option for text as well as for structure query. NALDB also provides multi-dimensional advanced search tool which can screen the database molecules on the basis of molecular properties of ligand provided by database users. NALDB offers an inclusive pharmacological information and the structurally flexible set of small molecules with their three-dimensional conformers that can accelerate the virtual screening and other modeling processes and eventually complement the nucleic acid-based drug discovery research. NALDB can freely available on [bsbe.iiti.ac.in/bsbe/naldb/HOME.php](http://bsbe.iiti.ac.in/bsbe/naldb/HOME.php).





patent

## Bioinformatic transaction scheme

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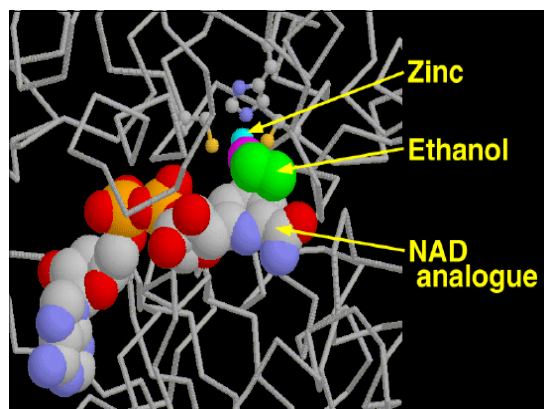
Inventor: Dennis Fernandez

### Abstract

Secure network transaction system obtains user-authorized genetic term or bioinformatics profile, and transacts online service according to genetically-based user medical or other risk determined therefrom. Insurance policy, promotional offer, or other service may dynamically address genetically-based condition. Bioinformatic data classifies user per personal mask which filters subset of user genetic sequence. Risk profile may be calculated according to actuarial statistics, genetics and/or heredity using non-discriminatory rules specified for users in temporal or jurisdictional groups. User transactions are modifiable according to Bioinformatic data representing genetically-based risk increase or decrease. Data is securely processed, modulated, and stored by network server for remote access and transaction using various portable user devices.

## Alcohol Dehydrogenase

Alcohol dehydrogenase is our primary defense against alcohol, a toxic molecule that compromises the function of our nervous system. The high levels of alcohol dehydrogenase in our liver and stomach detoxify about one stiff drink each hour.



The alcohol is converted to acetaldehyde, an even more toxic molecule, which is then quickly converted into acetate and other molecules that are easily utilized by our cells. Thus, a potentially dangerous molecule is converted, through alcohol dehydrogenase, into a mere foodstuff.

Our bodies create at least nine different forms of alcohol dehydrogenase, each with slightly different properties. Most of these are found primarily in the liver, including the beta3 form and the similar enzyme from horse liver. The sigma form, is found in the lining of the stomach. Each enzyme is composed of two subunits, and quite remarkably, you can mix and match subunits between these different forms, creating mixed dimers that are still active.

Alcohol dehydrogenase uses two molecular "tools" to perform its reaction on ethanol. The first is a zinc atom, which is used to hold and position the alcoholic group on ethanol. The second is a large NAD cofactor (constructed using the vitamin niacin), which actually performs the reaction. PDB entry [1adc](#), shown here, contains ethanol molecules bound to the two active sites.

[source: [pdb.rcsb.org/molecule\\_of\\_the\\_month](http://pdb.rcsb.org/molecule_of_the_month)]

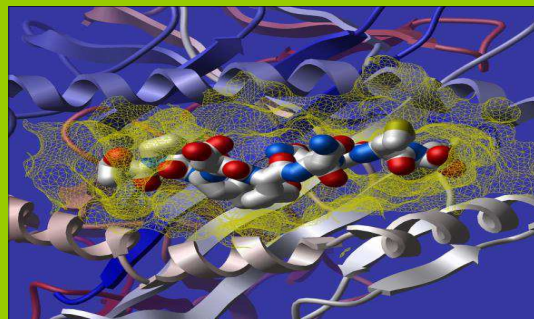
### Upcoming Events

#### Workshop On

## *Advance Training on Homology modeling, Protein-protein, Protein-Ligand interactions: Docking*

March 16<sup>th</sup>-18<sup>th</sup>, 2016

Bioinformatics Infrastructure Facility (BIFGU)  
Gauhati University, Guwahati- 781014



#### Workshop on

## *High Throughput Sequencing: Bioinformatics and Data Analysis*

April 25 - 27, 2016

BIOINFORMATICS CENTRE  
NORTH-EASTERN HILL UNIVERSITY  
SHILLONG, MEGHALAYA, INDIA

Kindly send us your feedback to

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