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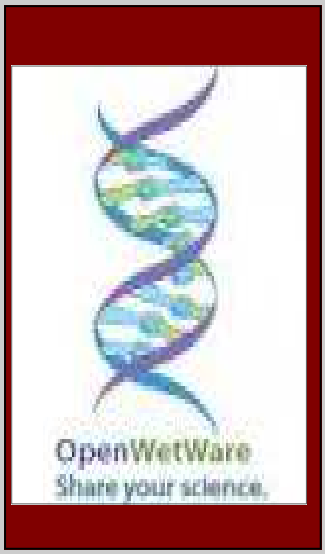
Bioinformatics up to Date

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

Inside…..



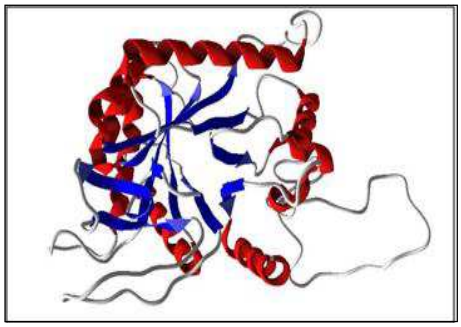
About Us

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.

Our Focus

Comparative modeling of Plasmodium falciparam Dihydropteroate Synthase 2 and docking study against compounds from anti-malarial plant Carcia papaya and Swertia chirata

The Dihydropteroate synthase (DHPS) is an essential enzyme required for the biosynthesis of key folate coenzymes in *Plasmodium falciparum,* required during the asexual division of merozoites in the infected RBCs during malarial infection. Inhibitors of DHPS are most often used in combination for a blissful effect and to slow down the development of drug resistance e.g. Fansidar. The *Carcia papaya* and *Swertia chirata* used by traditional healers of the North-eastern region to treat recurrent fever. Herein, we retrieve compounds of these plants from Pubmed database and performed *in silico* studies. We have performed the docking analysis to obtain the best drug like compound to inhidit the protein function. As the target protein didn't have an experimental structure we have also developed the 3D structure of the DHPS protein. Amarogentin (Re-rank score = -110.792) and Benzyl Glucosinolate (Re-rank score = -78.6031) of *Swertia chirata* and *Carcia papaya are* respectively found as best lead molecule for the degradation of DHPS protein.



Organization and Replication of Viral RNA Genomes

In separate studies published in the peer-reviewed journals *eLife* and *Nature*, scientists at the California NanoSystems Institute at UCLA have revealed the three-dimensional atomic structure of a double-stranded RNA, or dsRNA, virus. The research demonstrates for the first time how viruses sense environmental conditions inside a host cell to trigger transcription, and presents key findings about how the dsRNA genome is organized inside the virus and RNA's mechanism for self-replication.

The researchers also discovered the biological nano-switch that turns on transcription — the process by which RNA self-replicates — and compared the switch's structure in the "off" and "on" states to determine why environmental conditions activate it. The research was led by Hong Zhou, a professor of microbiology, immunology and molecular genetics and faculty director of UCLA's Electron Imaging Center for Nanomachines. For both studies, researchers analyzed the cytoplasmic polyhedrosis virus, or CPV, which infects insects. Zhou said the team focused on CPV because it is the simplest dsRNA virus. Researchers led by Hong Zhou found that the dsRNA virus uses proteins on its surface to sense its environment and that when conditions are optimal, those proteins turn the switch on inside the virus.

[http://www.biosciencetechnology.com/news/2015/11/studies-reveal-key-insights-about-how-viral-rna-genomes-organize-and-replicate]

2-Headed Protein to Deplete HIV Reservoir

A two headed protein have created by Scientists at the National Institutes of Health (NIH) that awakens resting immune cells infected with HIV and facilitates their destruction in laboratory studies. The findings were published in *Nature communication 2015.*

The protein potentially could contribute to a cure for HIV infection by helping deplete the reservoir of long-lived, latently HIV-infected cells that can start making the virus when a person stops taking anti-HIV drugs. Further studies in animals and people are needed to determine the viability of this approach.

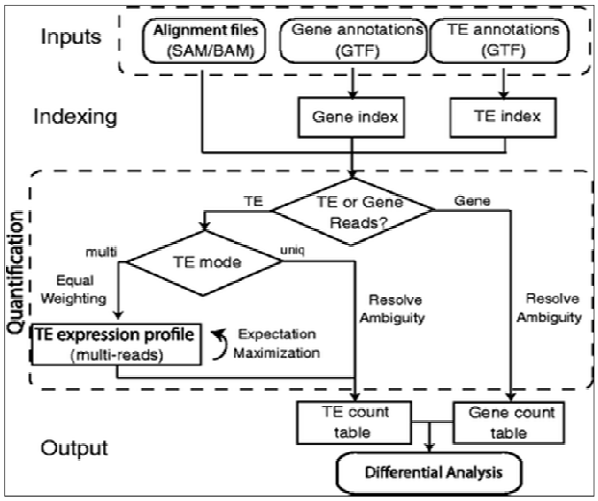
The researchers found that the protein, called VRC07-αCD3, triggered the activation and killing of latently HIV-infected helper T cells when the cells were taken from patients on antiretroviral therapy and then incubated in the lab with the patients' own killer T cells. In addition, the scientists found a monkey-adapted version of the protein to be safe and well-tolerated when given to monkeys infected with a simian form of HIV and receiving antiretroviral therapy. The researchers are now studying the effectiveness of monkey-adapted VRC07-αCD3 in the animals.

The engineered protein has two ends: one activates T cells by binding to a surface molecule called the CD3 receptor, and the other--based on an antibody called VRC07--powerfully binds to more than 90 percent of HIV strains. VRC07-αCD3 facilitates the killing of latently HIV-infected cells in three steps.

[*Activation and lysis of human CD4 cells latently infected with HIV-1. A Pegu et al. Nature Communications (2015)*]

TEtranscripts

TEtranscripts estimates both gene and transposable element TE transcript abundances in RNA-seq data and conducts differential expression analysis on the resultant count tables. This method shows improved recovery of TE transcripts over other published expression analysis methods, in both synthetic data and qPCR/NanoString-validated published datasets.

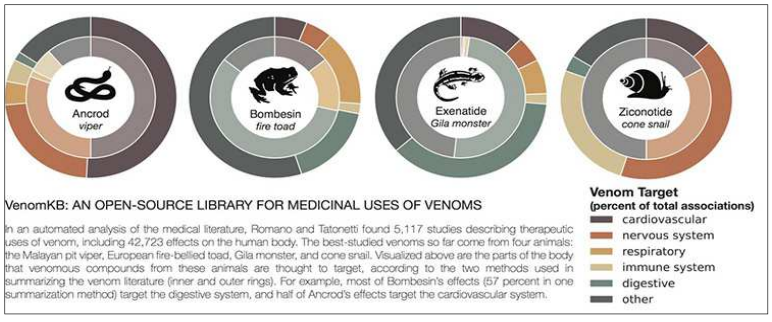


The input data for *TEtranscripts* consists of alignment files in either the SAM or BAM format and two annotation files in the General Transfer Format (GTF) for genes and TEs, respectively. *TEtranscripts* supports strand-specific read counting, and applies it to both genes and TEs. The genomic location, element name, as well as family and class information were also extracted from the table and included in the GTF file. *TEtranscripts* can also utilize custom TE annotations, such as those generated from *de novo* TE insertion analysis, as long as they conform to the format described earlier and are consistent with the genome sequencing files used for the alignmen.

.[Ying Jin etal. TEtranscripts: a package for including transposable elements in differential expression analysis of RNA-seq datasets; Bioinformatics, Volume 31, Issue 22,Pp. 3593-3599]

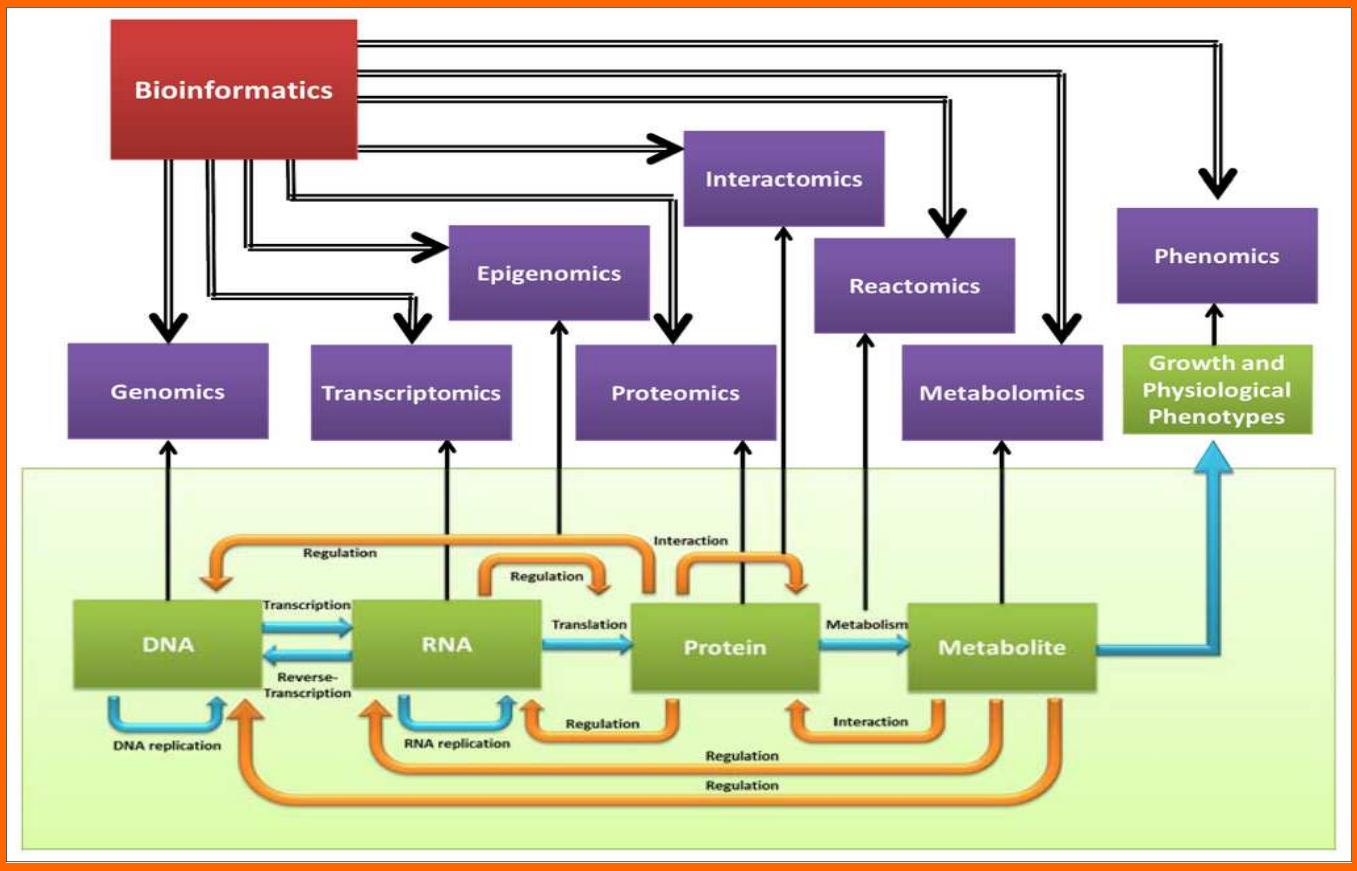
VenomKB, a new knowledge base

For the first time Columbia University data scientists create the first catalog of known animal toxins and their physiological effects on humans. They developed VenomKB, short for Venom Knowledge Base, summarizes the results of 5,117 studies in the medical literature describing the use of venom toxins as painkillers and as treatments for diseases like cancer, diabetes, obesity, and heart failure. The study published in Scientific Data (November 24, 2015)Nature publishing.



The VenomKB, a new publicly accessible knowledge base and website that aims to act as a repository for emerging and putative venom therapies. Presently, it consists of three database tables: (1) Manually curated records of putative venom therapies supported by scientific literature, (2) automatically parsed MEDLINE articles describing compounds that may be venom derived, and their effects on the human body, and (3) automatically retrieved records from the new Semantic Medline resource that describe the effects of venom compounds on mammalian anatomy. Drawn from an automated analysis of the literature, VenomKB documents nearly 42,723 effects on the body.

[*VenomKB, a new knowledge base for facilitating the validation of putative venom therapies. Romano, JD and Tatonetti, NP. Scientific Data (November 24, 2015)]*



Patent News

Bioinformatically detectable group of novel regulatory oligonucleotides associated with Alzheimer's disease and uses thereof

US20050222399A1

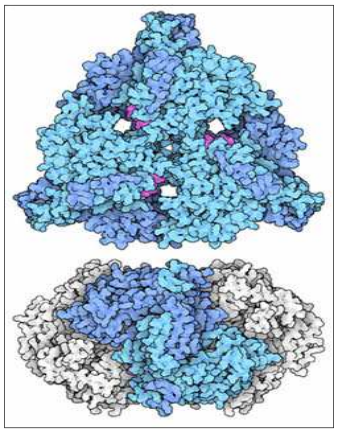
Inventor: Itzhak Bentwich

Abstract

The present invention relates to a first group of novel oligonucleotides, here identified as genomic address messenger or GAM oligonucleotides, and a second group of novel operon-like polynucleotides, here identified as genomic record or GR polynucleotides. GAM oligonucleotides selectively inhibit translation of known target genes, many of which are known to be involved in various diseases. Nucleic acid molecules are provided re-spectively encoding 1708 GAM oligonucleotides, and 246 GR polynucleotides as are vectors and probes both comprising the nucleic acid molecules, and methods and systems for detecting GAM oligonucleotides and GR polynucleotide and specific functions and utilities thereof, for detecting expression of GAM oligonucleotides and GR polynucleotides and for selectively enhancing and selectively inhibiting translation of the respective target genes thereof.

Citrate Synthase

Citrate Synthase is a central enzyme in this process of sugar oxidation. It is the first step of the citric acid cycle, also known as the Krebs cycle. Glucose has previously been broken into several pieces by glycolysis, releasing two carbon atoms as carbon dioxide and leaving the rest as two molecules of acetate, carried in an activated form on special cofactor molecules. In the citric acid cycle, these remaining carbon atoms are fully oxidized to form carbon dioxide. Citrate synthase starts this process by taking the molecules of acetate and attaching them to oxaloacetate, which acts as a convenient handle as the carbon atoms are passed from enzyme to enzyme in the citric acid cycle. Citrate synthase is a classic example of induced fit in enzyme action. The enzyme in our cells and in most animals and plants is very similar. It is composed of two identical subunits, each with its own active site. The citrate synthase enzyme found in many bacteria is larger than ours, as seen in this structure of the enzyme from Escherichia coli (PDB entry 1nxg).



Citrate synthase is found in all living cells, so it has been a useful enzyme for comparing differences from organism to organism. In particular, it has been used to study the unusual adaptations in cells that live in extreme environments. Structures have been obtained from organisms that live in very cold environments and others that live in hot environments.

(source: http://pdb101.rcsb.org/motm/93)

Upcoming Events

PROTEOMICS-2016

Hands on Workshop JANUARY 20-21, 2016

Institute of Advanced Study in Science and Technology

Guwahati, Assam, India

Bioinformatics Approaches on Genome Resources, Assembly and Annotation, National Workshop

Bioinformatics Approaches on Genome Resources, Assembly and Annotation

A National Workshop
(9–12th February, 2016)

Bioinformatics Centre (BIC)
CSIR-Institute of Microbial Technology,
Chandigarh, 160036, India
Supported by Department of Biotechnology (DBT), New Delhi

Kindly send us your feedback to

Robin Das
Research Fellow; BIF, Biotech Division.
CSIR-North East Institute of Science and Technology, Jorhat, Assam
E-mail: robindas460@gmail.com