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Bioinformatics up to Date

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(http://www.rrljorhat.res.in/biotechnology.html)

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 binding Study of how E64 retard the Falcipain-2 of Plasmodium falciparum that Causes Malaria in Humans.

Malaria is a severe disease. Usually it's transmitted through the bite of an spoiled Anopheles mosquito. Infected mosquitoes carry the *Plasmodium parasite*. Plasmodium falciparum malaria, which degrades haemoglobin throughout falcipain-2 (FP2),. As of the P.falciparum's survival in humans depends on its capacity to reduce human's haemoglobin, barrier of FP2 has antimalarial effects. Therefore, researchers worked on the minute information of how E64 approaches, interact with, and inhibits FP2. Increasingly they found that E64 approaches, FP2 interacting with FP2's with the amino acids D170 and Q171 or N81, N77, and K76;E64 Binds with FP2 tightly with binding value -12.2 ± 1.1 kJ/mol; and E64 has already been able to form a covalent bond with FP2's C42.In this study, validate that E64 is capable to constantly reduce FP2, and interaction of E64's with FP2 is shown that positive. Moreover, it is recognized that the amino acids residues facing the known binding pocket of FP2 with some residues nearby FP2's known binding pocket are very important in E64's for strong binding to FP2 and E64's constant blocking of the catalytic residues of FP2. The findings presented in this study, which has antimalarial indication and also observed that hydrogen bonding and electrostatic interactions play key roles in E64-FP2 binding, and that a potential FP2-blocking E64-based/E64-like antimalarial drug should be capable of being both hydrogen-bond donor and acceptor and have the capability to interact with polar amino acids residue and with charged amino acids residue. It is important to characteristics that such potential drug should have ability to interact with ASN, ASP, and SER amino acids . As a result, this study shown that the potentials of the development of antimalarial drugs that block the activities of FP2.Figure1 shown that How E64 approaches and binds to FP2 .

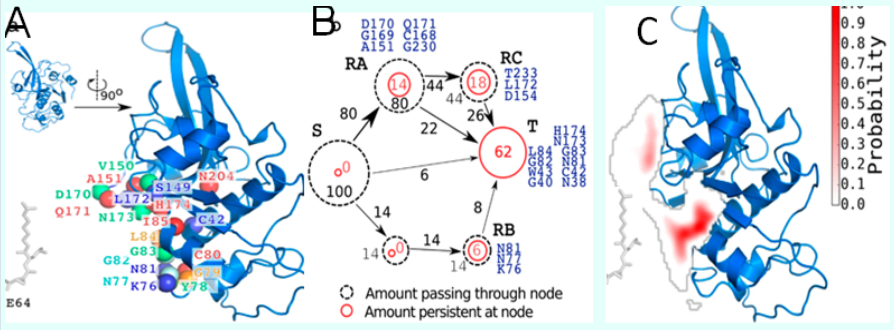
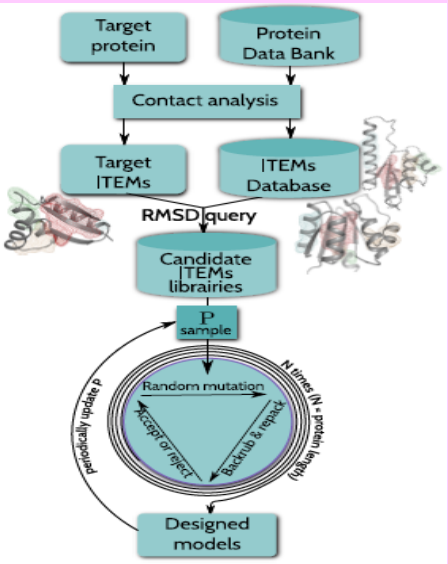


Figure:1

Source: Emmanuel Oluwatobi Salawu *et al. J Sci Rprts,*

Structural bioinformatics based Homology outlook for Computational Protein Design with adaptable Backbone methods.

Structure-bioinformatics based Computational Protein design (CPD) methods plays an important role in advancing the approach of protein engineering. CPD of flexible backbone protein conformation is a very difficult process, because of the high number of degrees of freedom of proteins and the related sampling issue. Using an all-atom energy function, CPD tries to identify amino acid sequences that fold into a target structure and ultimately perform a desired function. However, in the process of design, energy functions of protein remain defective and introduced significant details from known structures in should guide to improved designs. In this study, researchers introduced a data- CPD technique which is commonly known as SHADES. Shades (Structural Homology Algorithm for protein DESign), is based on modified libraries of non-contiguous in-contact amino acid residue motifs. Shades utilized local structural environments in known protein structures together among energy to guide sequence design, while sampling side-chain and backbone conformations to put up mutations. Shades used in a public benchmark of 40 proteins selected from different protein families, without homologous proteins, Shades can achieved a protein sequence recovery of 30% and a protein sequence similarity of 46% on average, compared to the PFAM protein family of the target protein.



When homologous structures were added, the wild-type sequence recovery rate achieved 93%.
Shades source code is available at https://bitbucket.org/satsumaimo/shades

GwasPro: A Online GWAS study server

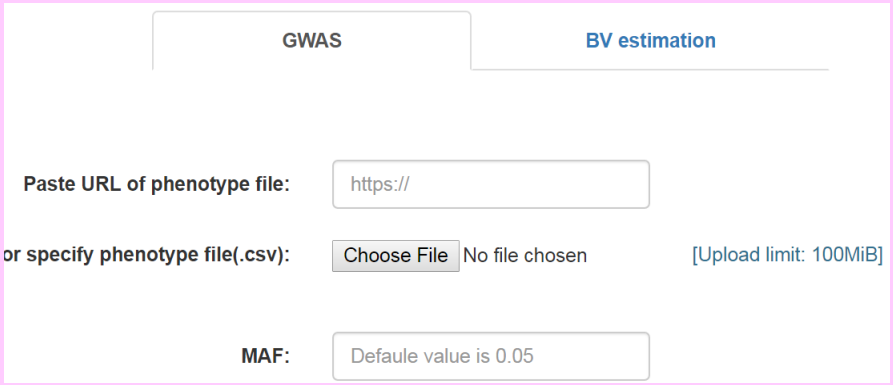


Figure:Homepage of GwasPro server

Whole genome association study (WGA study, or WGAS), is an examination study of a genome-wide set of genetic variants in different individuals to see if any variant is associated with a trait.

GWASpro is an online server for GWAS study. It does not require the difficulty of software installation and maintenance.

Genome-wide association studies (GWAS) for crop improvements often meet important challenges associated with complex experimental designs and big data sets. There is a new GWAS analysis software GWASpro that can simulated phenotypic data related to complex experimental designs connecting many environments along with a significant molecular marker data. GWASpro supports flexible building design matrices for the linear mixed models (LMM). In GWASpro server repeatedly establishes the LMM with required inputs including a genotypic file, a phenotypic file, and variable names. Users can directly upload their data files from a local computer. After the submission of job , the job is queue and GWASpro assigns a user a unique session ID, which can be used to track the job progress and download final output results. GWASpro is freely available at https://bioinfo.noble.org/GWASPRO.

Bioinfo. Animation (Qiang Li *et al. J Scientific Reports*)

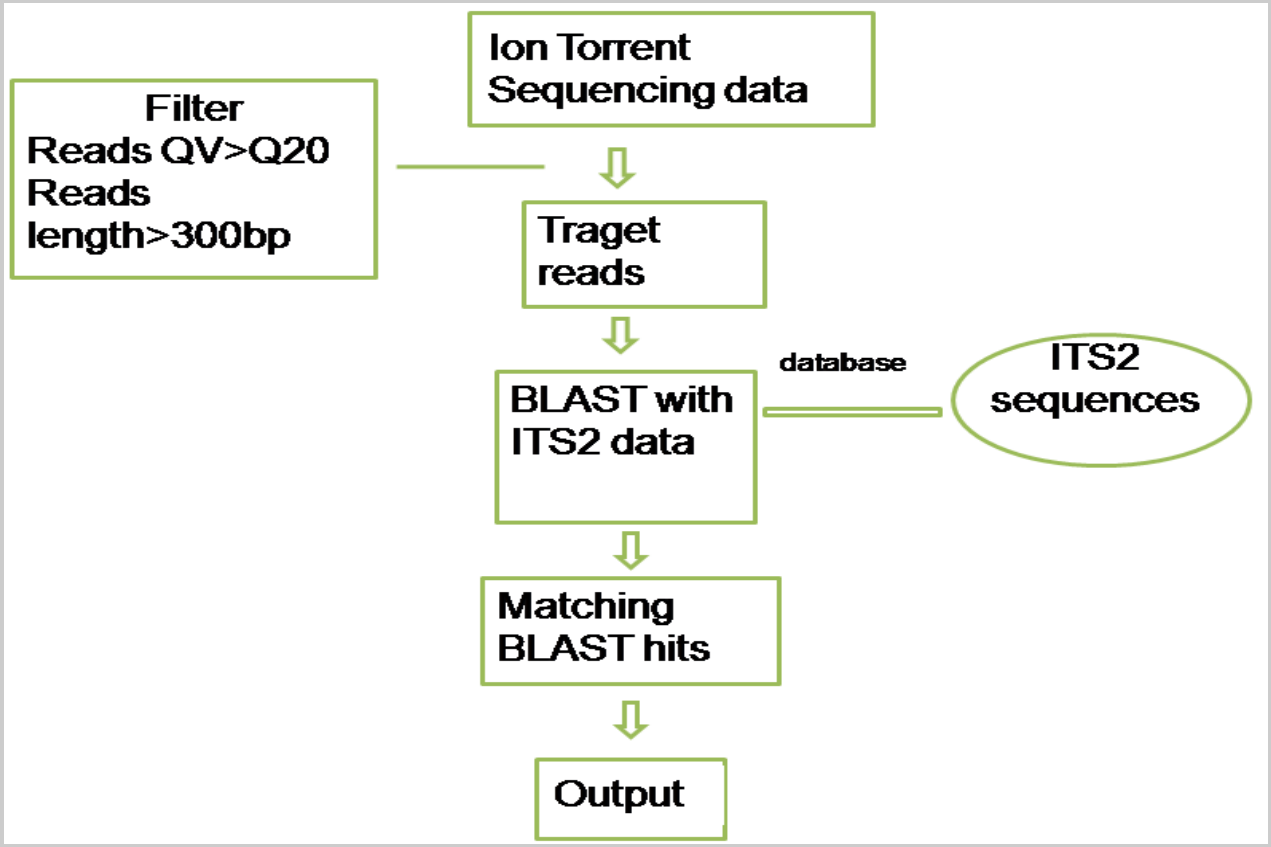


Fig: The workflow for the processing and analysis of high-throughput sequencing reads.

Upcoming event

EMBO WORKSHOP — MOLECULAR NEUROSCIENCE: FROM GENES TO CIRCUITS IN HEALTH AND DISEASE
04 Feb 2019 - 07 Feb 2019 • Bangalore , India
Topics: Neuroscience
Event listing ID:1141038

1. https://asia.explara.com/e/bangkok-training-course-bioinformatics-drug-design

2. http://www.embo.org/events/events-calendar

Telomerase

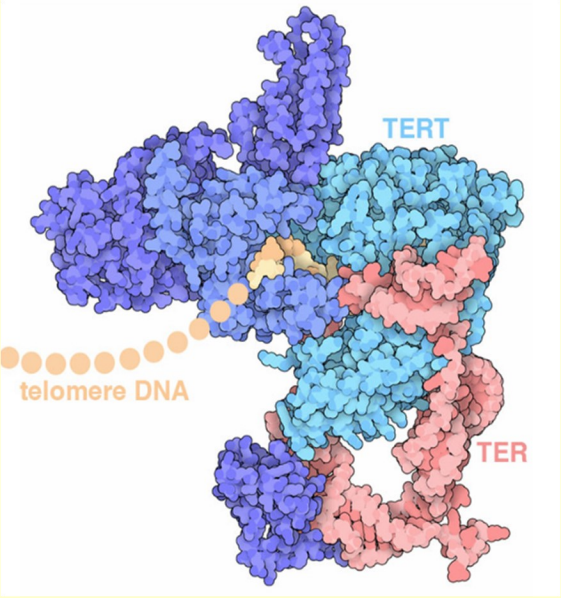


Figure:Telomere Molecule with reverse transcriptase and associated with protein.

Telomere is a unique structure which protects our ends of chromosomes. Telomere composed of DNA and proteins. Telomeric DNA includes about a thousand repeats of the short sequence TTAGGG. These repeated segments are paired with a complementary DNA (cDNA) strand to form a normal double helix, but several hundred nucleotides at the end are a single strand that is thought to round back and relate with the double-stranded area. Numerous different types of proteins, collectively called "shelterin," coat this telomeric DNA, protecting it.

The repeated nature of the telomere holds the solution to the end decrease the problem: cells use telomerase to build new repeats when the telomere gets too short. Telomere is a molecular mechanism that includes a template for the telomere repeat, and an enzyme that builds the repeat onto the end of chromosomes. The template is fixed in a short RNA strand, which also includes non-coding regions that interact with the rest of the telomerase complex. The telomerase enzyme is a specialized reverse transcriptase that uses this RNA template to create the telomere DNA.

Telomeres and Cancer disease

Improper regulation of telomerase, can cause serious problems. For example, cancer cells very often have mutations that lead to production of higher levels of telomerase. This allows them to maintain their telomeres as they rapidly divide and form a tumor.

Action of Telomerase

Telomerase is a extremely active complex that has been difficult to study. The structure of the catalytic core of telomerase was determined using cryo-electron tomography by using modified DNA nucleotides to lock the structure into a stable form that could be observed. The structure includes the template RNA (pink), the reverse transcriptase and several associated proteins and a short piece of the end of a DNA telomere (orange). This telomerase is from a protozoan, with telomeres that are slightly different than ours, with sequence TTGGGG.

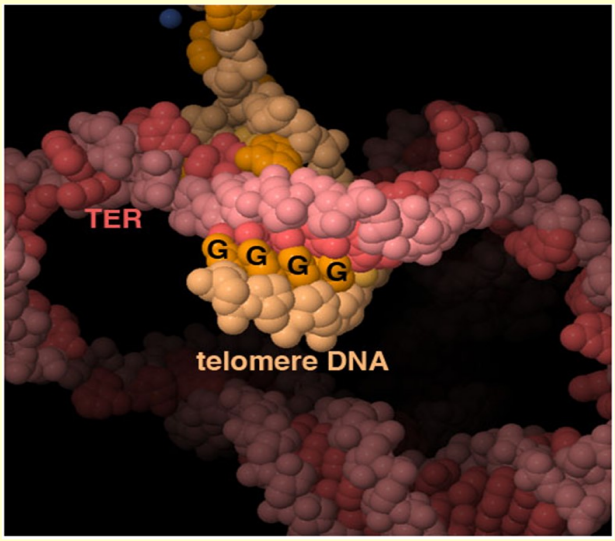


Figure:This structures shown the action of telomerase in protozoan .

Source: http://pdb101.rcsb.org/motm/227

Kindly send us your feedback to

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