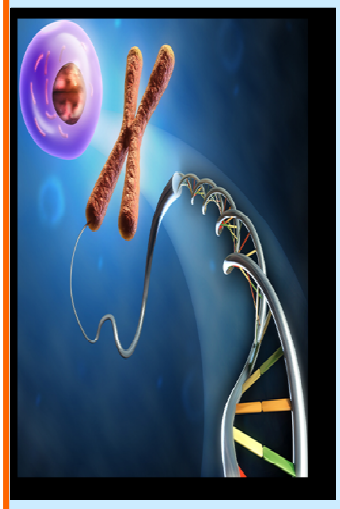
Volume 10, Issue 11 November 2017

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.

Influences of lone-pair electrons on directionality of hydrogen bonds formed by hydrophilic amino acid side chains in molecular dynamics simulation

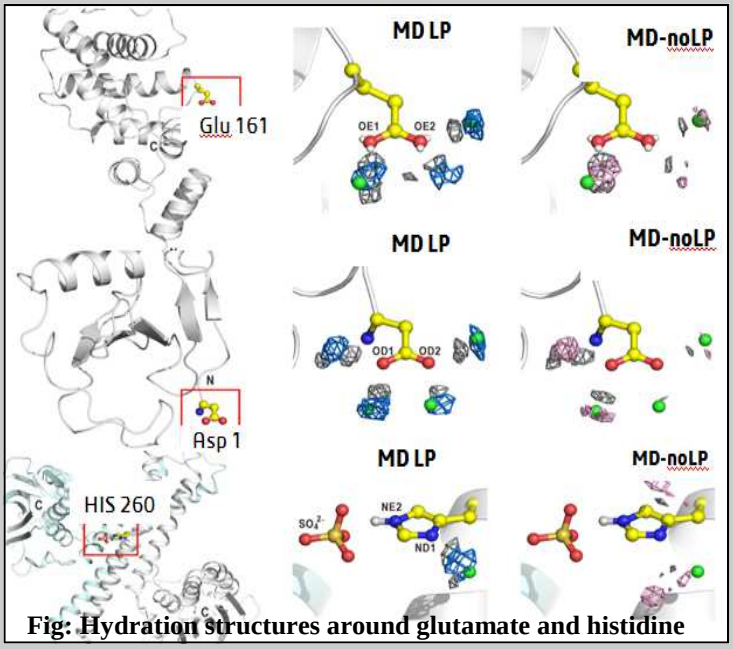


Fig: Hydration structures around glutamate and histidine

Hydrogen bonds (H-bonds) play an important role in the various biomolecular processes of proteins such as protein folding, molecular recognition, and enzymatic reactions. The influence of lone-pair electrons on the directionality of hydrogen bonds that are formed by oxygen and nitrogen atoms in the side chains of nine hydrophilic was investigated using molecular dynamics simulations. The simulations were conducted using two types of force fields; one incorporated lone-pair electrons placed at off-atom sites and the other did not. The density distributions of the hydration water molecules around the oxygen and nitrogen atoms were calculated from the simulation trajectories, and were compared with the empirical hydration distribution functions, which were constructed from a large number of hydration water molecules found in the crystal structures of proteins. Only simulations using the force field explicitly incorporating lone-pair electrons reproduced the directionality of hydrogen bonds that is observed in the empirical distribution functions for the deprotonated oxygen and nitrogen atoms in the *sp*2-hybridization. The amino acids that include such atoms are functionally important glutamate, aspartate, and histidine. Therefore, a set of force field that incorporates lone-pair electrons as off-atom charge sites would be effective for considering hydrogen bond

Source:Tomotaka Oroguchi *et al. Sci Reporst,2017*

Constructing Genetic Networks using Biomedical Literature and Rare Event Classification

A text mining approach used to construct the genetic network of the human genome "*H.Sapiens*". Text mining has become an important tool in bioinformatics research with the massive growth in the biomedical literature over the past decade. Mining the biomedical literature has resulted in an incredible number of computational algorithms that assist many bioinformatics researchers. In this study, they present a text mining system called Gene Interaction Rare Event Miner (GIREM) that constructs genegene-interaction networks for human genome using information extracted from biomedical literature. GIREM identifies functionally related genes based on their co-occurrences in the abstracts of biomedical literature. For a given gene g,

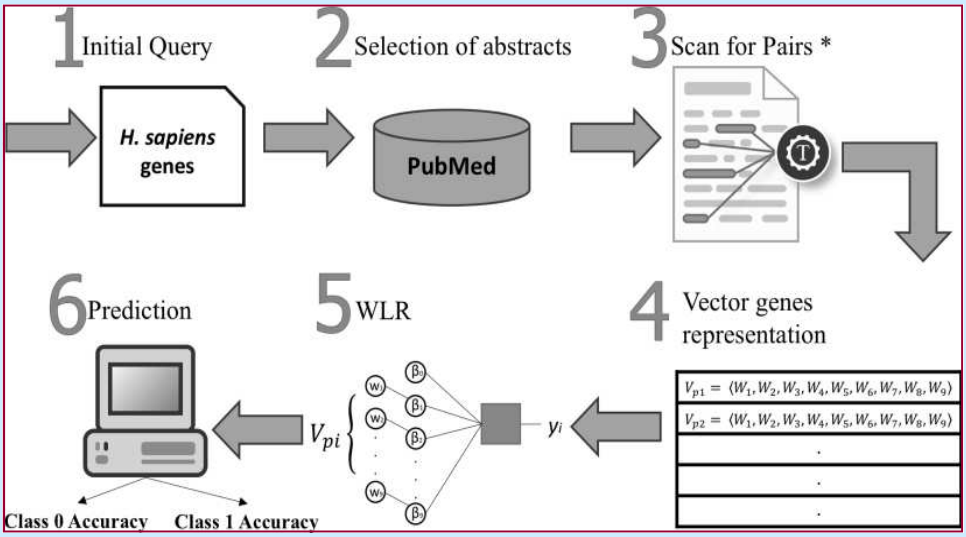
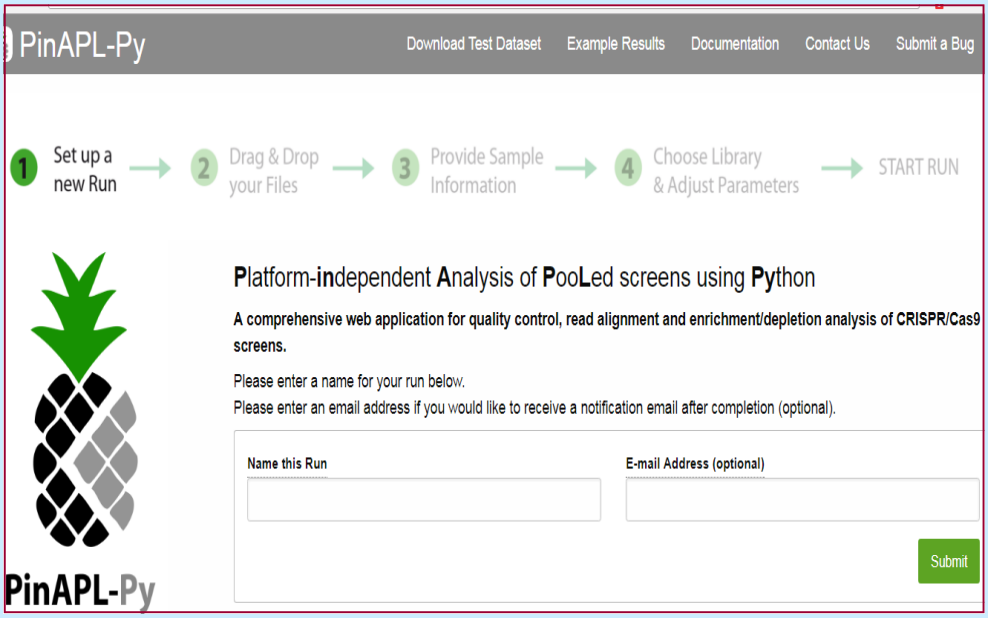


Figure: The sequential steps taken by the system. GIREM extract the co-occurrence of pairs of genes at three level; the abstract, the sentence and the semantic level.

GIREM first extracts the set of genes found within the abstracts of biomedical literature associated with g. GIREM aims at enhancing biological text mining approaches by identifying the semantic relationship between each co-occurrence of a pair of genes in abstracts using the syntactic structures of sentences and linguistics theories. It uses a supervised learning algorithm, weighted logistic regression to label pairs of genes to related or un-related classes, and to reflect the population proportion using smaller samples. We evaluated GIREM by comparing it experimentally with other well-known approaches and a protein-protein interactions database. Results showed marked improvement.

Source: Amira Al-Aamri *et al.* Scientific reports,2017

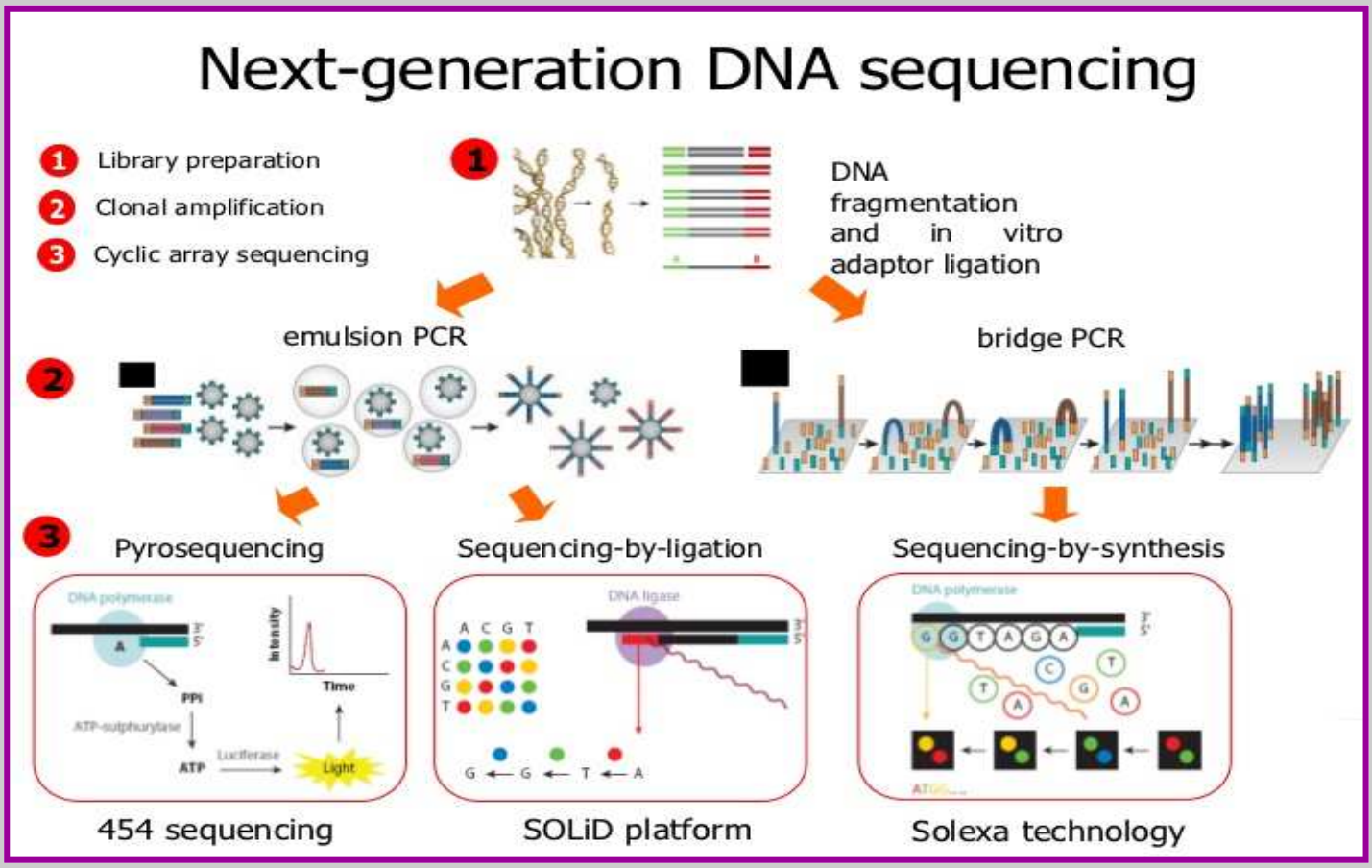
PinAPL-Py: A comprehensive web application for the analysis of CRISPR/Cas9 screens



Large-scale genetic screens using CRISPR/Cas9 technology have emerged as a major tool for functional genomics. With its increased popularity, experimental biologists frequently acquire large sequencing datasets for which they often do not have an easy analysis option. While a few bioinformatic tools have been developed for this purpose, their utility is still hindered either due to limited functionality or the requirement of bioinformatic expertise. To make sequencing data analysis of CRISPR/Cas9 screens more accessible to a wide range of scientists, we developed a Platform-independent Analysis of Pooled Screens using Python (PinAPL-Py), which is operated as an intuitive web-service. PinAPL-Py implements state-of-the-art tools and statistical models, assembled in a comprehensive workflow covering sequence quality control, automated sgRNA sequence extraction, alignment, sgRNA enrichment/depletion analysis and gene ranking. The workflow is set up to use a variety of popular sgRNA libraries as well as custom libraries that can be easily uploaded. Various analysis options are offered, suitable to analyze a large variety of CRISPR/Cas9 screening experiments. Analysis output includes ranked lists of sgRNAs and genes, and publication-ready plots. PinAPL-Py helps to advance genome-wide screening efforts by combining comprehensive functionality with user-friendly implementation. PinAPL-Py is freely accessible at http://pinapl-py.ucsd.edu with instructions and test datasets.

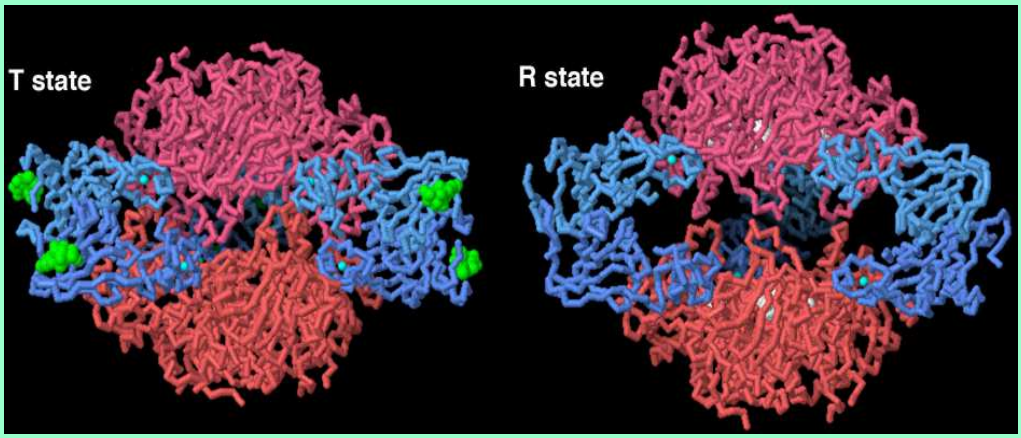
Source:Philipp N. Spahn *et al* . Sc.reports 2017

Bioinfo. Animation



Aspartate Transcarbamoylase

Aspartate transcarbamylase (ATCase) performs an early step in the production of pyrimidine rings, which are used to build nucleotides in DNA and RNA. Early studies found that *Escherichia coli* ATCase is regulated by the level of CTP, a nucleotide with a pyrimidine ring. Based on biochemical data, researchers proposed a model with two states: a "tense" T state that is inactive, and a "relaxed" R state that can perform the reaction. The structure revealed that ATCase is a large complex, with six catalytic chains arranged in the center, surrounded by three pairs of regulatory chains. The whole complex is usually in the inactive state, but the catalytic chains are cooperative: as with the cooperativity of the four chains of hemoglobin, binding of starting materials to a few active sites stabilizes the R state, making the whole complex more active. When CTP levels are high, however, it binds to the regulatory chains, stabilizing the inactive T state.



Source : http://pdb101.rcsb.org/motm/214

International Conference
on
Emerging Trends in Biomaterial, Bio-imaging, Bioscience, Bioinformatics, Biomedical Engineering, Cancer Biology, Stem Cell Research, Cell Apoptosis and Applied Biotechnology (BCS-2017)

Organized by
"Dr. G. C. Mishra Educational Foundation"

on
16th December, 2017

Convention Centre
Jawaharlal Nehru University, New Delhi, India

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BIOINFORMATICS 2018 — 9th International Conference on Bioinformatics Models, Methods and Algorithms

19 Jan 2018 - 21 Jan 2018 • Funchal, Madeira, Portugal

Patents

Methods and systems of molecular recording by Crispr-cas system

WO 2017142999 A2
Inventors: George M. Church

Abstract

This invention provides methods of altering a cell including providing the cell with a nucleic acid sequence encoding a Cas1 protein and/or a Cas2 protein of a CRISPR adaptation system, providing the cell with a CRISPR array nucleic acid sequence including a leader sequence and at least one repeat sequence, where in the cell expresses the Cas1 protein and/or the Cas2 protein and wherein the CRISPR array nucleic acid sequence is within genomic DNA of the cell or on a plasmid. Also provided are methods and systems for nucleic acid storage and in vivo molecular recordings of events into a cell.

Kindly send us your feedback to

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