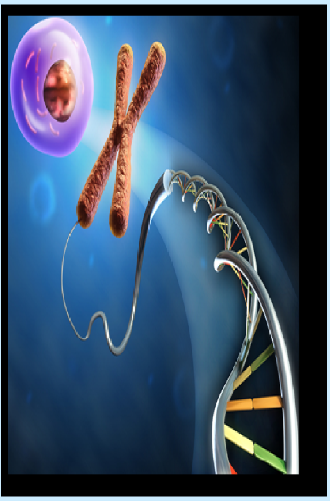
Volume 10, Issue 12 December 2017

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.

Initiation of prolyl cis-trans isomerisation in the CDR-H3 loop of an antibody in response to antigen binding .

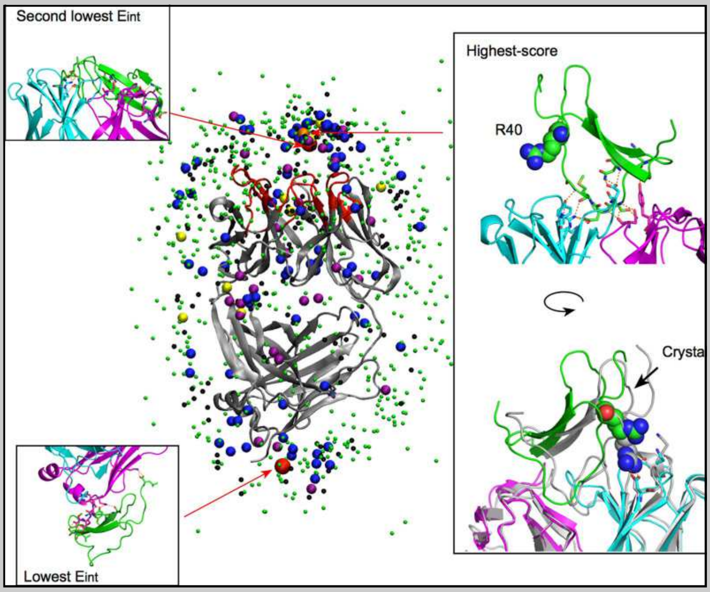


Fig:Positions of the EPR COMs on 9E5 observed by binding

Proline cis-trans isomerisation is a regulatory mechanism which used in a range of biological processes, and it is related to various diseases like cancer and Alzeihmer disease. Yet, the details of the exact molecular mechanism by which it occurs are not known. Using X-ray crystallography, proline isomerisation has been shown to occur in the formation of an antigen-antibody complex between the target epiregulin (EPR) and the antibody 9E5, at proline (Pro103), located in the third complementarity-determining region (CDR) of the heavy chain of 9E5. In this study, the researchers analyzed the accurate definition of the pathway involved in cis-trans isomerisation in this system, carried out ten independent long molecular dynamics (MD) simulations starting at a stable transient bound structure obtained from many short binding MD simulations. As a result, they were able to describe the process by which cistrans isomerisation is initiated, and suggest a catalysis mechanism for cis-trans isomerization in this antigen-antibody system. They also found that Asp102, which is immediately adjacent to Pro103, rotates while changing its interacting partner residues in the light chain of 9E5, and at the same time EPR polar residues help to stabilise the intermediate states in the isomerisation process by interacting strongly with Asp102 .

Source:Keiko Shinoda *et al.* *J* Scientific Reports

RNAStructuromeDB: A genomewide database for RNA structural inference

RNA plays important roles in almost every aspect of biology, and every aspect of RNA biology is influenced by its folding. This is a particularly important consideration in the era of high-throughput sequencing, when the discovery of novel transcripts far outpaces our knowledge of their functions. To gain a comprehensive picture of biology requires a structural framework for making functional inferences on RNA. To this end we have developed the RNA Structurome Database (https:// structurome.bb.iastate.edu), a comprehensive repository of RNA secondary structural information that spans the entire human genome. Here, we compile folding information for every base pair of the genome that may be transcribed: coding, noncoding, and intergenic regions, as well as repetitive elements, telomeres, etc. This was done by fragmenting the GRCh38 reference genome into 154,414,320 overlapping sequence fragments and, for each fragment, calculating a set of metrics based on the sequence's folding properties. These data will facilitate a wide array of investigations: e.g. discovery of structured regulatory elements in differential gene expression data or noncoding RNA discovery, as well as allow genome-scale analyses of RNA folding.

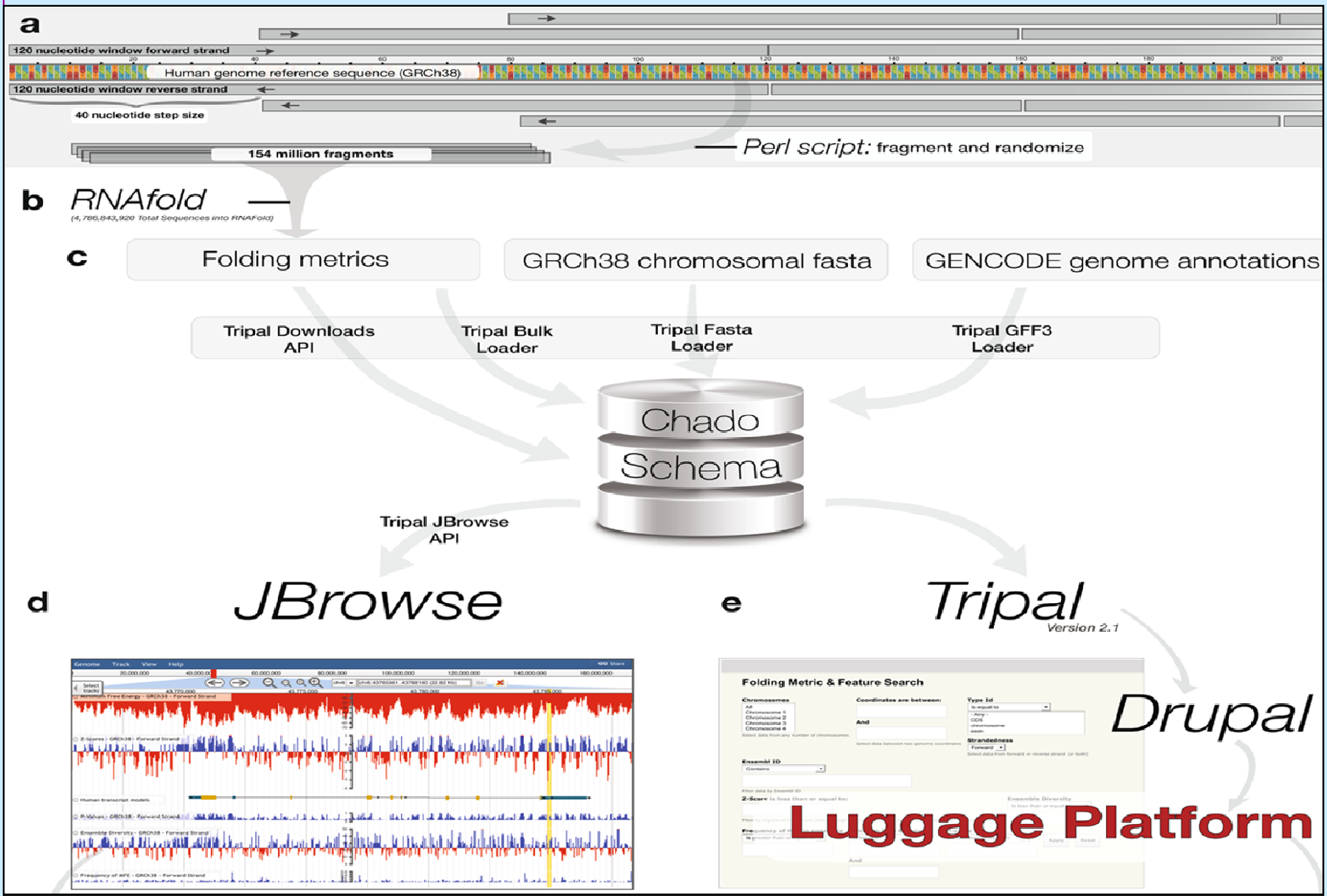
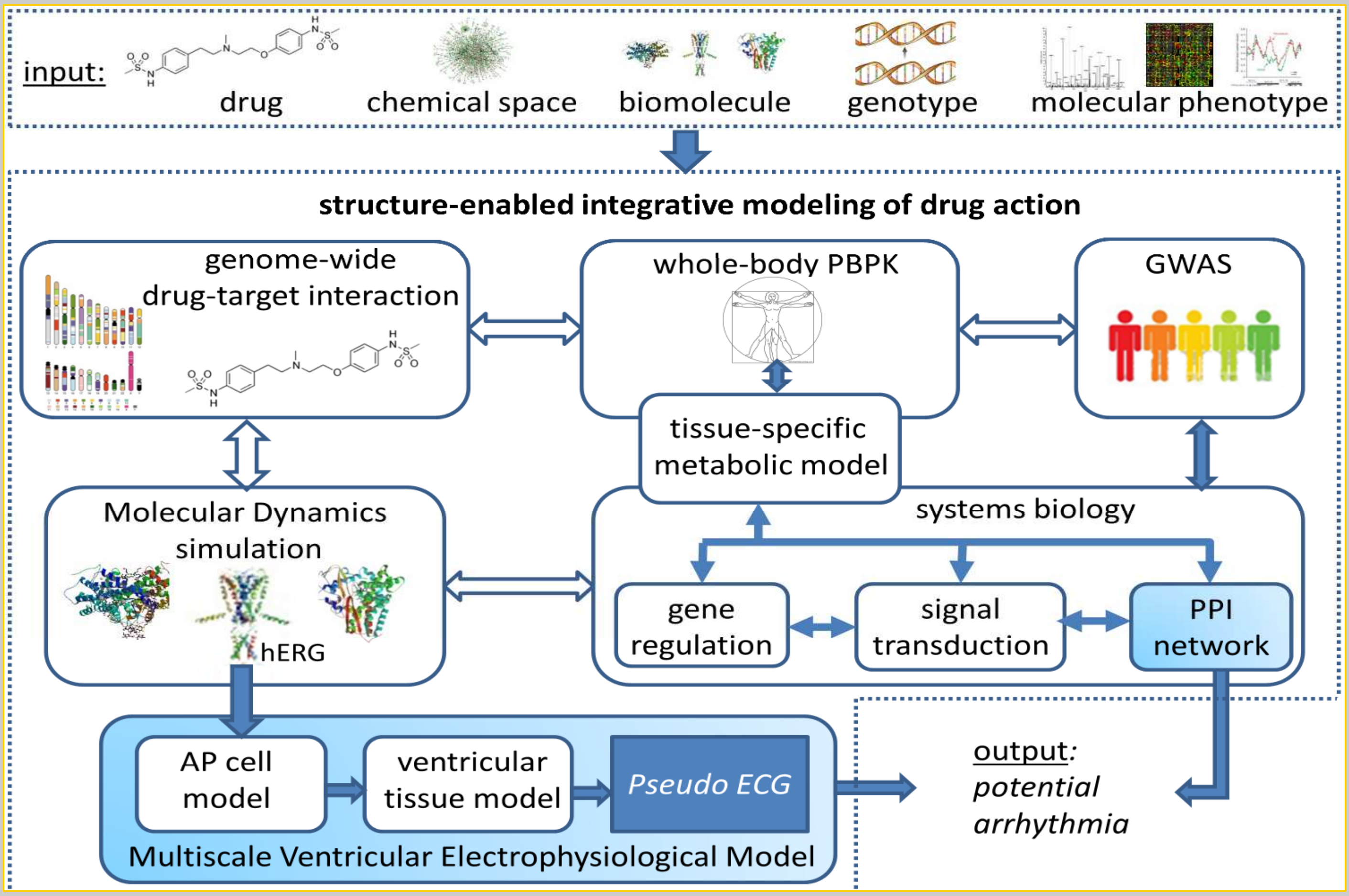


Fig: Overview of RNAStructuromeDB construction. a)The human genome was fragmented into 154 million windows, b)This resulted in over 4.5 billion sequences to be folded in RNAfold, c)Folding metrics, d)This data is pulled from the Chado schema on demand.e)In a separate process, Tripal is also able to populate tables for our data-table interface by acting as an interface between Chado and Drupal/Luggage.

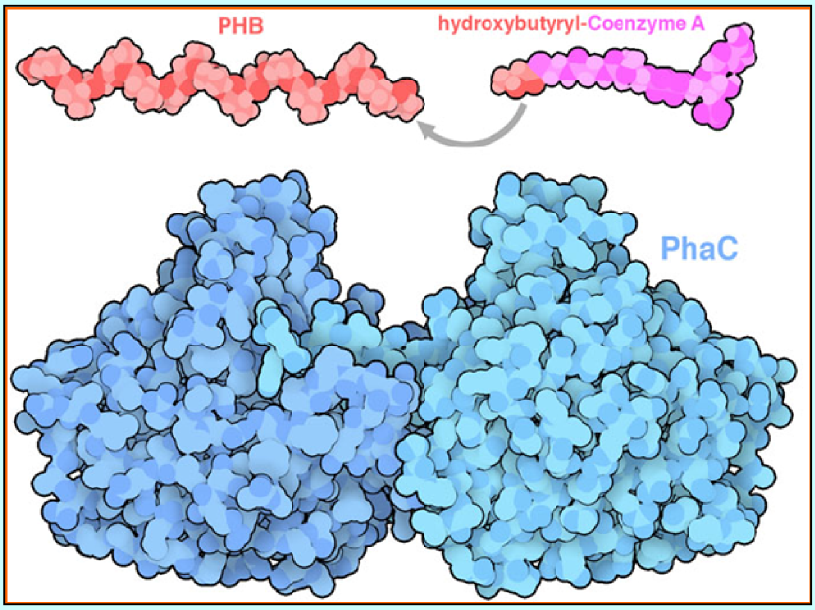
Source: Ryan J. Andrews *et al.* J Scientific Reports

Bioinfo. Animation (Source: Lei Xie *et al. J Computational Biology)*



Biodegradable Plastic

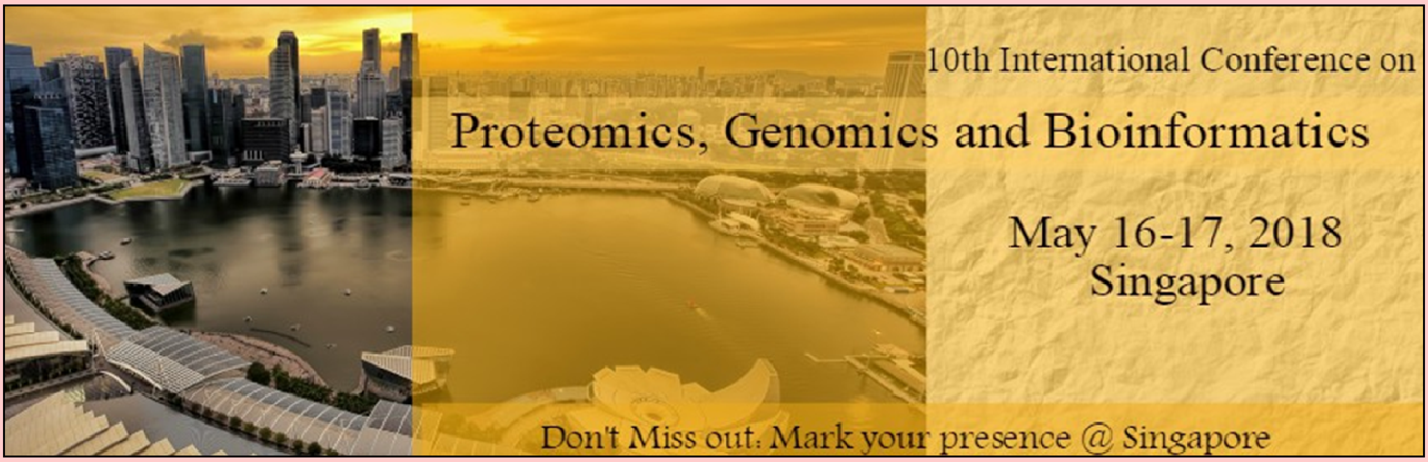
Most of the plastic is composed of long molecular chains derived from petroleum. Plastic is not environmentally friendly. It is predicted that by 2050 nearly 12,000 megatons of plastic will accumulate in landfills, pollute the ocean, and endanger life on the planet. Researchers are analyzed biodegradable plastic (or bioplastic) from bacteria to provide eco-friendly options for use in commercial products. Some bacteria store fuel molecules in granules of plastic, similar to the way our cells store glucose in glycogen granules.



Bioplastic has many of the preferences of synthetic plastics: it is chemically stable and resistant to high temperatures. It is currently being used to make a variety of products, including packaging materials, utensils for food, textile fibers, systems for drug delivery, medical sutures and implants, and fiber material for 3D-printing.

Bacteria build bioplastic with the enzyme polyhydroxybutyrate synthase .

Source : http://pdb101.rcsb.org/motm/216



Patents

System and method for automating data generation and data management for a next generation sequencer

US 20170091382 A1

Inventors: Sijung YUN , Joshua SHALLOM

Abstract

A web-based server/cloud computing system for a next generation sequencer (NGS) to integrate data generation, data analysis and data management. In this study, researchers reported that when a user intends to sequence a biological sample, the user is asked to login to the NGSinForm, select and submits sets of software analysis bioinformatics programs, which schedules the sequencing, quality control, data analysis and management of that data, all done simultaneously and sequentially. When the sequencing is completed, the raw sequence data is uploaded to a server or cloud, raw data is analyzed, following the analysis preferences. Finally, all data generated will be saved and managed systematically. Hence, a user is able to access the information on the sample as well as the analyzed data anytime and anywhere with a one-time submission of the single web form—NGSinForm—even before starting the sequencing.

Kindly send us your feedback to

Dr Ratul Saikia
BIF Center, Biotechnology Group, BSTD
CSIR-North East Institute of Science and Technology, Jorhat, Assam
E-mail: rsaikia19@gmail.com

Dr Yumnam Silla Devi
BIF Center, Biotechnology Group, BSTD
CSIR-North East Institute of Science and Technology, Jorhat, Assam
*E-mail:*bio.sillayumnam@gmail.com