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Bioinformatics up to Date

(Bioinformatics Infrastructure Facility, Biotechnology Division)
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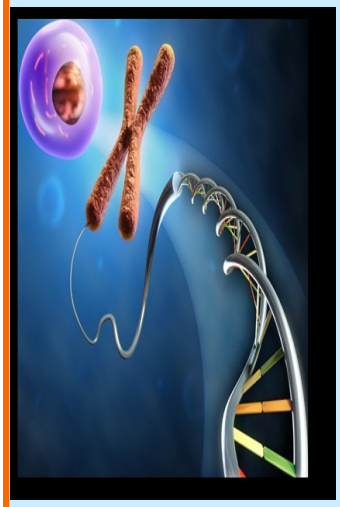
Jorhat - 785 006, Assam

Inside…..

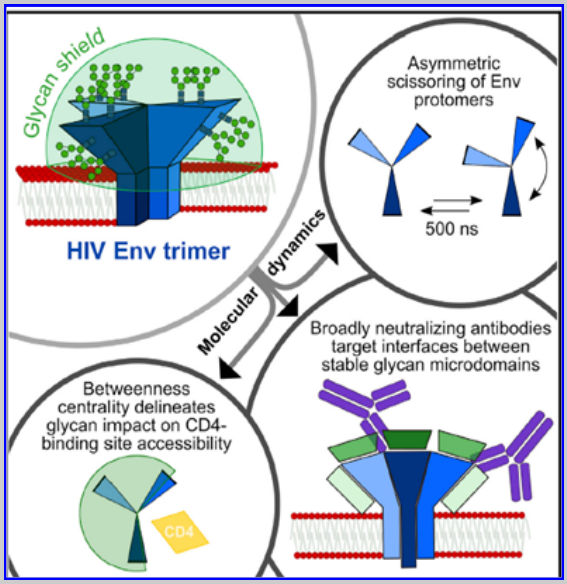


About us

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.

Microsecond Dynamics and Network Analysis of the HIV-1 SOSIP Env Trimer Reveal Collective Behavior and Conserved Microdomains of the Glycan Shield

The trimeric HIV-1-envelope (Env) spike is one of the most glycosylated protein complex.



In this study, researchers used molecular dynamics to provide insight into its structural dynamics and into how both protomer and glycan movements coordinate to shield the Env protein surface. A 2-ms molecular dynamics simulation of a fully glycosylated atomistic model of the HIV-1 SOSIP Env trimer revealed a spectrum of protomer scissoring and trimer-opening movements. Network analysis showed that highly conserved glycans combined with protomer scissoring to restrict access to the binding site of the CD4 receptor. The network property of betweenness centrality appeared to identify whether glycans spread to restrict access or cluster to maintain the high – mannose character of the shield.

They also observed stable microdomains comprising patches of glycan, with neutralizing antibodies generally binding at the interface between glycan microdomains. Overall, their results provide a microsecond-based understanding of the Env glycan shield.

Source: Thomas Lemmin *et al. CellPress (2017)doi.org/10.1016/j.str.2017.07.018*

Neptune: a bioinformatics tool for rapid discovery of genomic variation in bacterial populations

Neptune is an efficient system for rapidly locating differentially abundant genomic content in bacterial populations using an exact k-mer matching strategy, while accommodating k-mer mismatches. Neptune's loci discovery process identifies sequences that are sufficiently common to a group of target sequences and sufficiently absent from nontargets using probabilistic models. Neptune uses parallel computing to efficiently identify and extractthese loci from draft genome assemblies without requiring multiple sequence alignments or other computationally expensive comparative sequence analyses. Tests on simulated and real datasets showed that Neptune rapidly identifies regions that are both sensitive and specific. We demonstrate that this system can identify trait-specific loci from different bacterial lineages.

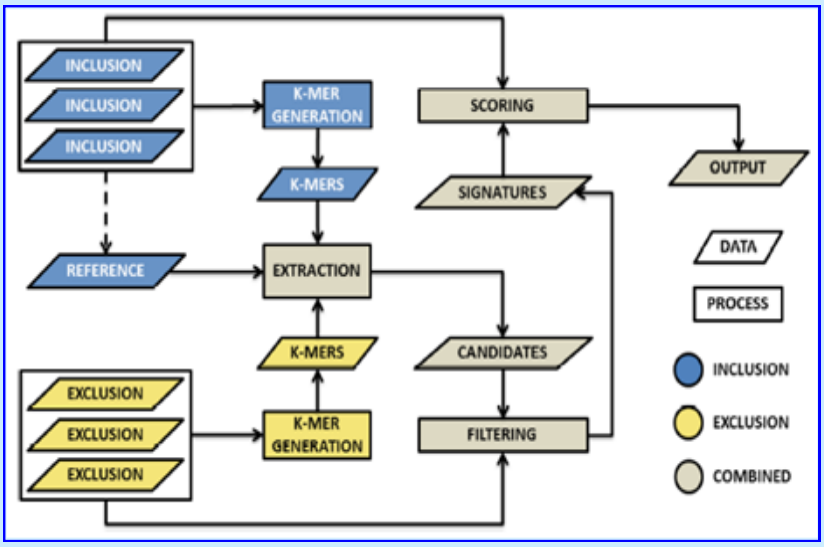


Fig:An overview ofNeptune's signature discovery process for a single target reference.

Neptune is broadly applicable for comparative bacterial analyses, yet will particularly benefit pathogenomic applications, owing to efficient and sensitive discovery of differentially abundant genomic loci. The software is available for download at: (http://github.com/phac-nml/neptune). Neptune allows one to efficiently and rapidly identify genomic loci that are common to one population and distinguishing them from other populations.

Source: Eric Marinier1 *et al*. J Nucleic Acids Research, 2017 doi: 10.1093/nar/

Kfits: A software framework for fitting and cleaning outliers in kinetic measurements

Kfits, an intuitive graphical tool for detecting and removing noise caused by outliers in protein aggregation kinetics data. The workflow of Kfits allows the user to quickly and easily clean large quantities of data and receive kinetic parameters for assessment of the results. With minor adjustments, the software can be applied to any type of kinetic measurements, not restricted to protein aggregation. Kfits is implemented in Python and available online at (http://kfits.reichmannlab.com).Kfits comes with three example datasets, which were added to help the user play with the different settings of the software and understand their effects on the fit. Below are the sources of these example data and what they represent.

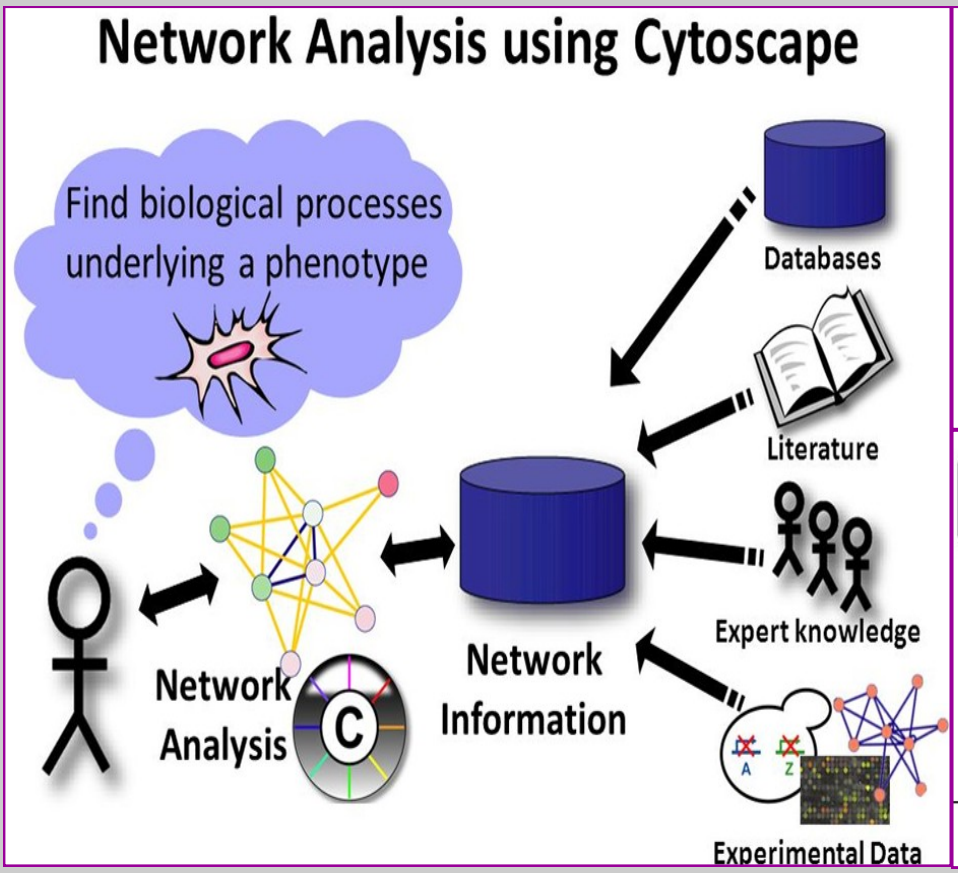
1.Simulated Nucleation-Elongation:This simulated example was built to be a perfect fit for the Nucleation-Elongation model.

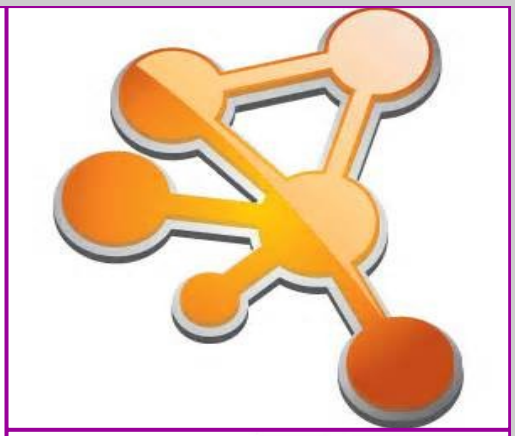
2.Simulated One-Site Binding: This simulated example was built to be a perfect fit for the One-Site Binding model.

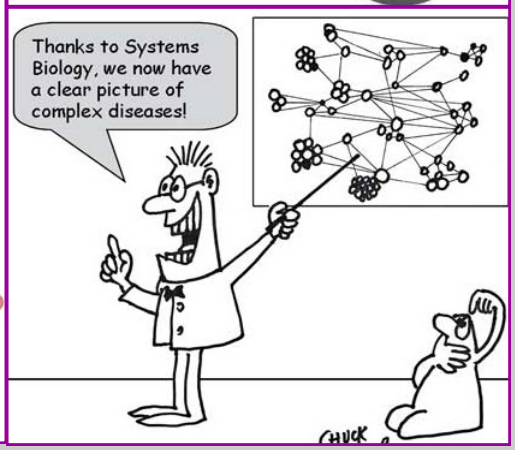
3.Real life Citrate synthase Aggregation Measured by Light Scattering:This is real data measured by Oded, showing the aggregation of chemically unfolded Citrate synthase upon dilution into a buffer containing a chaperone that decreases the rate and intensity of aggregation.

This software was intially written in September 2016 for Oded's personal use, and soon after extended to include a GUI for the comfort of the rest of the lab. By January 2017, the efforts to make it globally available, easy to use and as free as possible of bugs have begun. Finally, in May 2017, Kfits was ready to be sent out to the world.

Source:Oded Rimon *et al.* Oxford Academic Bioinformatics (2017),,https://doi.org/10.1093/bioinformatics/btx577



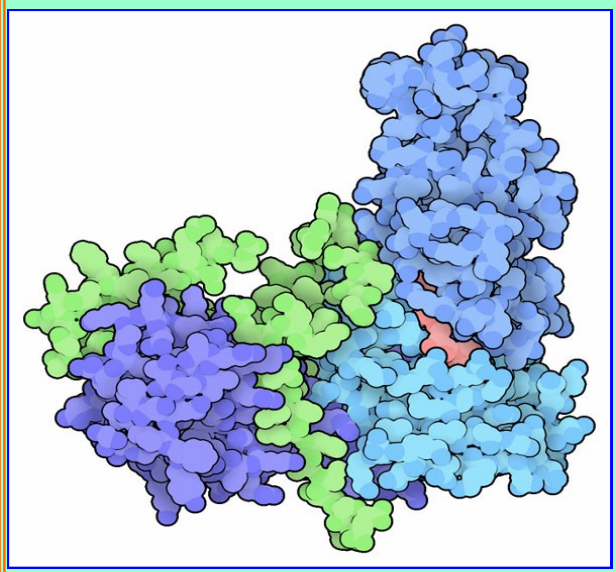




Source :cytoscape.org

Sirtuins

Sirtuins perform an unusual reaction using a familiar cofactor. They take NAD, a cofactor that is normally involved in electron transport, and remove its signature nicotinamide ring. Then, they extract the acetyl group from their target protein and attach it to the remaining fragment of NAD. Structures of sirtuins, such as the structure of Sir2 in



PDB entry 4iao, have a distinctive structure. They have two domains that grip NAD and position the acetylated lysine next to it, catalyzing the transfer reaction. Some sirtuins also have additional domains that interact with other regulatory proteins, such as Sir4 included in this structure.

Our cells build seven different sirtuins (termed SIRT1-SIRT7). They perform a variety of functions. Some perform the canonical function of modifying histones and regulating transcription. Others target proteins in the cytoplasm and mitochondria, and are implicated in regulating a wide array of processes such as metabolism and neurodegeneration. Some specialize in removing acetyl groups, while others remove larger modifications such as attached lipids, or create new modifications. Continued study of these molecules has revealed additional strong connections to aging in many organisms.

Source : http://pdb101.rcsb.org/motm/213

Patents

Detection of High Variability Regions Between Protein Sequence Sets Representing a Binary Phenotype

US 20170177788 A1

Inventors:Karen Anderson

ABSTRACT

A computer-based bioinformatics method for identifying protein sequence differences between sets of sequences grouped into different phenotype data sets that involves querying a database to identify common sequence motifs within a first phenotype data set and another phenotype data set of protein sequences, computing a pairwise correlation among motifs for each data set, and computing the variation between the data sets to identify one or more motifs that are conserved in a given data set and thus correlate with that data set's phenotype.

Kindly send us your feedback to

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