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Bioinformatics up to Date

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Inside…..

About us

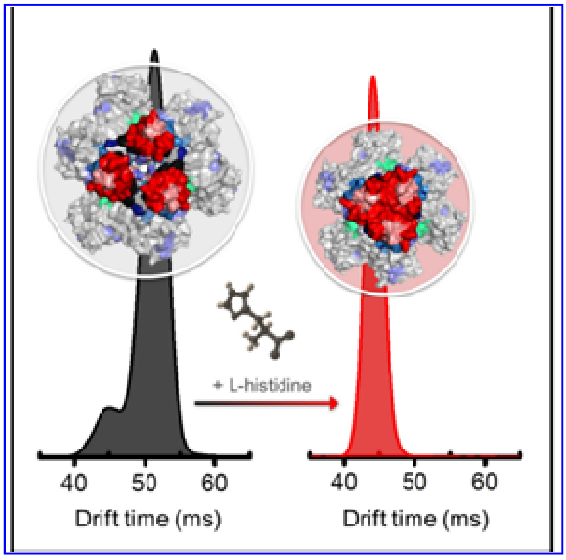
The Bioinformatics Infrastructure Facility (BIF) at Biotechnology division, CSIR NEIST, Jorhat runs under the Biotechnology Information System Network (BTISnet) programme of DBT, Ministry of Science & Technology, and Government of India. The Centre was established on 2nd February, 2008 to promote innovation 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.

Hybrid Mass Spectrometry Approaches to Determine How L-Histidine Feedback Regulates the Enzyme MtATP-Phosphoribosyltransferase

MtATP-phosphoribosyltransferase (MtATP-PRT) is an enzyme catalyzing the first step of the biosynthesis of L-histidine in Mycobacterium tuberculosis, and proposed to be regulated via an allosteric mechanism.

The work has been published in Journal *Cell Press (May 02, 2017)*

Native mass spectrometry (MS) reveals MtATP-PRT to exist as a hexameric state under physiological conditions. Conformational changes induced by L-histidine binding and the influence of buffer pH are determined with ion mobility MS, hydrogen deuterium exchange (HDX) MS, and analytical ultracentrifugation.



The experimental collision cross-section (DTCCSHe) decreases from 76.6 to 73.5 nm2 upon ligand binding at pH 6.8, which correlates to the decrease in CCS calculated from crystal structures. Conformational change on L-histidine binding is obtained with HDX-MS experiments.

On incubation with L-histidine, rapid changes are observed within domain III, and around the active site at longer times, indicating an allosteric effect.HDX-MS was used for mapping of the conformational changes, and the results are in agreement with X-ray crystallography data. Changes in the deuterium exchange between apo MtATP-PRT and L-histidine-bound MtATP-PRT occurring on a short timescale were found within domain III and are associated with L-histidine binding to the allosteric site.

Changes occurring on longer timescales related to conformational changes induced by ligand binding were identified around the active site and near the residues involved in AMP binding and resi-

[Source: https://doi.org/10.1016/j.str.2017.03.005 ,Kamila J et al.CellPress.(May 02 ,2017]

DSSR: enhanced visualization of nucleic acid structures in Jmol

DSSR stands for Dissecting the Spatial Structure of RNA. It is an integrated and automated command-line tool for the analysis and annotation of RNA tertiary structures. It calculates a comprehensive and unique set of features for characterizing RNA, a s well as DNA structures.

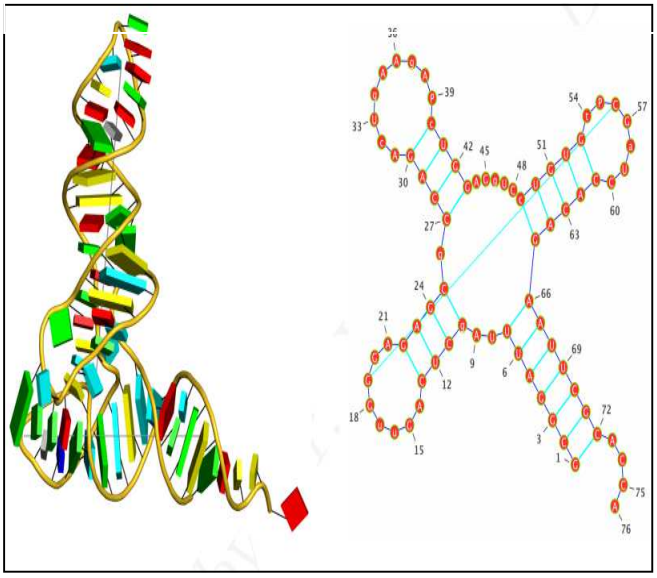


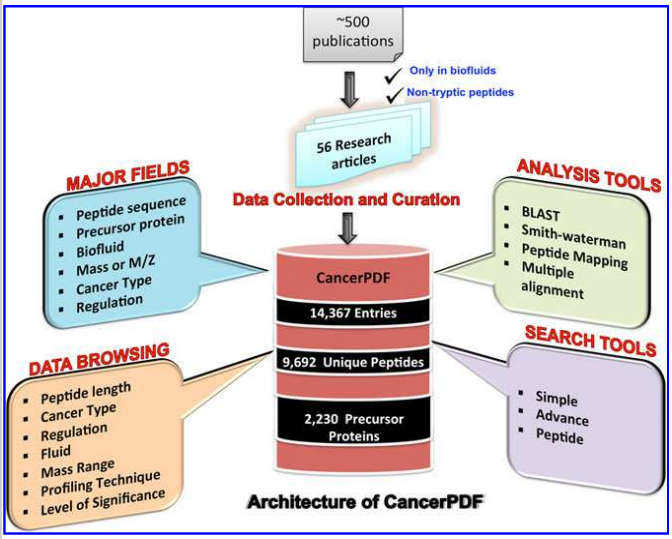
Fig:Secondary Structure of RNA

Jmol is a widely used, open-source Java viewer for 3D structures, with a powerful scripting language. JSmol, its reincarnation based on native JavaScript, has a predominant position in the post Java-applet era for web -based visualization of molecular structures. The DSSR-Jmol integration presented here makes salient features of DSSR readily accessible, either via the Java-based Jmol application itself, or its HTML5-based equivalent, JSmol. The DSSR web service accepts 3D coordinate files (in mmCIF or PDB format) initiated from a Jmol or JSmol session and returns DSSR-derived structural features in JSON format. This seamless combination of DSSR and Jmol/JSmol brings the molecular graphics of 3D RNA structures to a similar level as that for proteins, and enables a much deeper analysis of structural characteristics. It fills a gap in RNA structural bioinformatics, and is freely accessible (via the website *http://jmol.x3dna.org*).

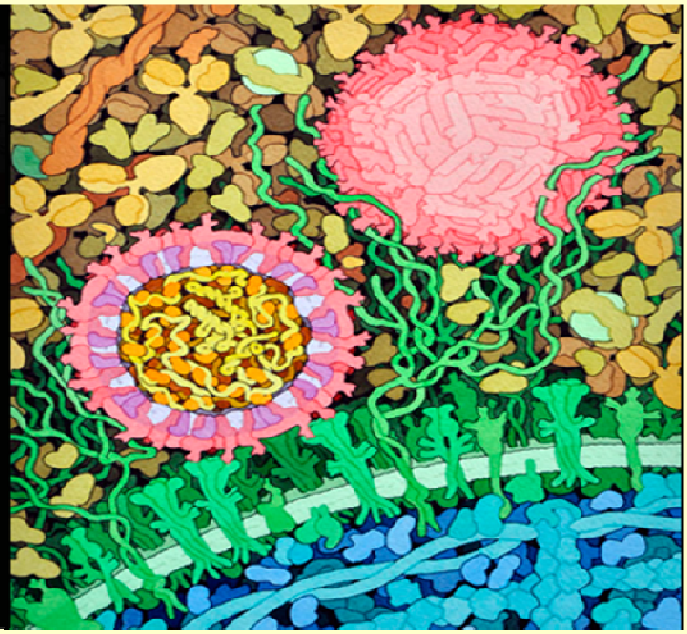
[Source : DSSR: enhanced visualization of nucleic acid structures in Jmol.Robert M et al. (Bioinformatics oxford)(2017)]

CancerPDF: A repository of cancer-associated peptidome found in human biofluids

CancerPDF(Cancer Peptidome Database of bioFluids) is a manually curated database of cancer-associated peptides found in different human bodyfluids (e.g., serum, urine, plasma and saliva). These peptides were experimentally identified using diffrent techniques of proteomics. It covers nearly 30 types of human cancers. It contains 14,367 experimentally validated peptides and provide comprehensive information regarding their mass, precusor protein, techniques for profiling and quantification, and their regulation in different type of cancer etc. And also has 9,692 unique peptide sequences corresponding to 2,230 unique precursor proteins from 56 high-throughput studies for ~27 cancer conditions. The peptidome patterns reflect the synthesis, processing and degradation of proteins in the tissue environment and therefore can act as a gold mine to probe the peptide-based cancer biomarkers. Although an extensive data on cancer peptidome has been generated in the recent years, lack of a comprehensive resource restrains the facility to query the growing community knowledge. The cancer peptidome resource named CancerPDF, to collect and compile all the endogenous peptides isolated from human biofluids in various cancer profiling studies. Many web-based tools have been incorporated, which comprise of search, browse and similarity identification modules. CancerPDF will be an invaluable resource to unwind the potential of peptidome-based cancer biomarkers. The CancerPDF is available at the web address http://crdd.osdd.net/raghava/cancerpdf/.



[Source:Database: NatureMethods(2017).https://www.nature.com/articles/s41598-017-01633-3]



Since 2003, the Vizzies Challenge has recognized visualizations of scientific data that are "exemplars of information made beautiful."At the 2017 Vizzies, David Goodsell's painting for the Molecule of the Month was recognized by the National Science Foundation (NSF) and Popular Science as one of the best science images of the year and selected as the "People's

These image of Zika virus shows not just the envelope that encircles the virus, but also the RNA (in yellow) that lives inside it and allows it to replicate. When the image was first published, scientists had been aware of the virus for almost 70 years, but understanding of the disease was limited. "Study of Zika virus has gained new importance because of the recent spread of the virus in many countries around the globe and its connection to birth defects and a rare neuro-

Molecule of Month

Tissue Transglutaminase

Tissue Tansglutaminase, also known as Transglutaminase 2, is a protein stapler that links two proteins together. Transglutaminase works with several other transglutaminases to form highly crosslinked networks that provide strength to skin, hair and nails. Tissue transglutaminase takes a gentler approach to strengthen interactions of proteins involved in the cytoskeleton and cellular adhesion. Transglutaminases play essential roles in most of our cells, but they've also become indispensable tools in biotechnology, with applications ranging from cosmetics to the food industry. A small bacterial transglutaminase is used to improve the texture of imitation crabmeat, hot dogs, sausages, and many other meat products. transglutaminase has also inspired the creativity of chefs, allowing them to do fanciful things such as making pasta from shrimps.

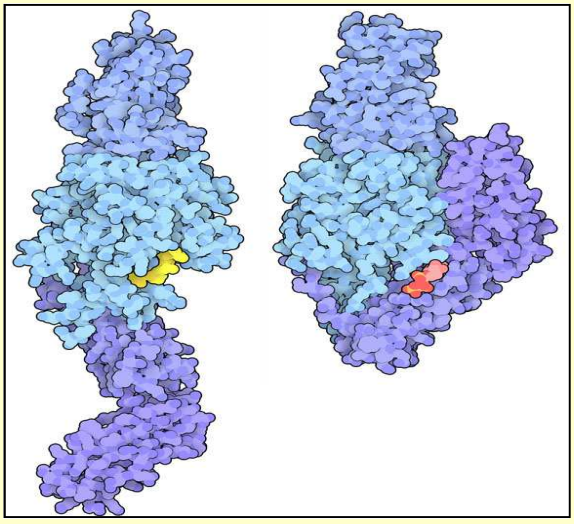


Fig:Tissue transglutaminase in the active (left) and GTP-bound inactive (right) conformations. An inhibitor that mimics gluten is shown in yellow and GTP is shown in red.

Tissue transglutaminase also performs a slightly different reaction on single proteins, removing a molecule of ammonia from glutamine to form glutamic acid. This deamination reaction has been linked to celiac disease, a common inflammatory disorder that damages the small intestine and causes a variety of debilitating symptoms.

[Source:http://pdb101.rcsb.org/motm]

Scientific Writing '17 WORKSHOP ON LIFE SCIENCE (BIOTECHNOLOGY)SCIENTIFIC WRITING, May 2017, CS SCIENTIFIC SERVICES, Chennai, Tamilnadu, India

Related Links: BIOINFORMATICS, BIOMEDICAL ENGINEERING, BIOTECHNOLOGY, Chennai, Engineering, Fee500-1000, Management/Arts, May 2017, Seminar, Tamilnadu, Workshop

College/University/Organization Name: CS SCIENTIFIC SERVICES
Organizing Department: CS SCIENTIFIC SERVICES
Event Date: 05/07/2017 -- 05/07/2017 (MM/DD/YYYY)
Last Date: 05/06/2017 (MM/DD/YYYY)
Address: Chennai, Tamilnadu, India

Patents

Bioinformatics system architecture with data and process integration

US 9418204 B2

Inventors : Steve Gardner

ABSTRACT

A bioinformatics system and method is provided for integrated processing of biological data. According to one embodiment, the invention provides an interlocking series of target identification, target validation, lead identification, and lead optimization modules in a discovery platform oriented around specific components of the drug discovery process. The discovery platform of the invention utilizes genomic, proteomic, and other biological data stored in structured as well as unstructured databases. According to another embodiment, the invention provides overall platform/architecture with integration approach for searching and processing the data stored in the structured as well as unstructured databases. According to another embodiment, the invention provides a user interface, affording users the ability to access and process tasks for the drug discovery process.

Kindly send us your feedback to

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