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Bioinformatics up to Date

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Inside…..

About us 1
Cover story 1
Computers for Biologists 2
Bioserver 2
Bioinfo. Animation 3
Molecule of the month 3
Upcoming Events 4
Bioinfo. Patent 4
Contact Us 4

About us

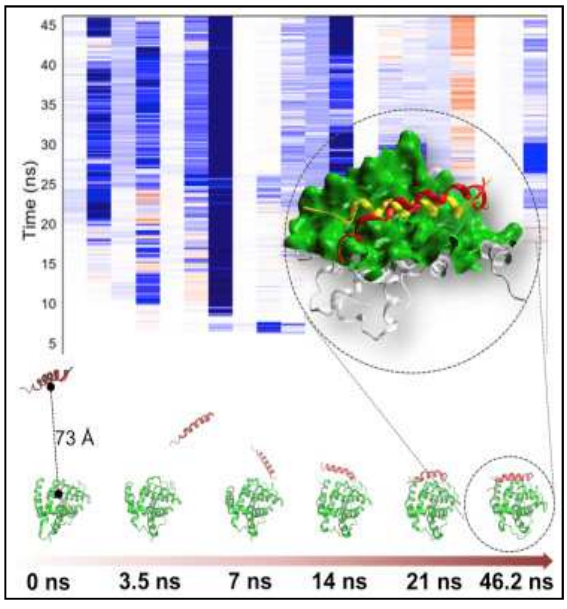
The Bioinformatics Infrastructure Facility (BIF) at Biotechnology division, CSIR NEIST, Jorhat runs under the Biotechnology Information System Network (BTISnet) programme of DBT, Ministry of Science & Technology, and Government of India. The Centre was established on 2nd February, 2008 to promote innovation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

Exploring Protein-Peptide Recognition Pathways Using a Supervised Molecular Dynamics Approach

Peptides have gained increased interest as therapeutic agents during recent years. The high specificity and relatively low toxicity of peptide drugs derive from their extremely tight binding to their targets.

The work has been published in Journal *Cell Press (April 04,2017).*

The molecular mechanism of protein-peptide recognition has important implications in the fields of biology, medicine, and pharmaceutical sciences.

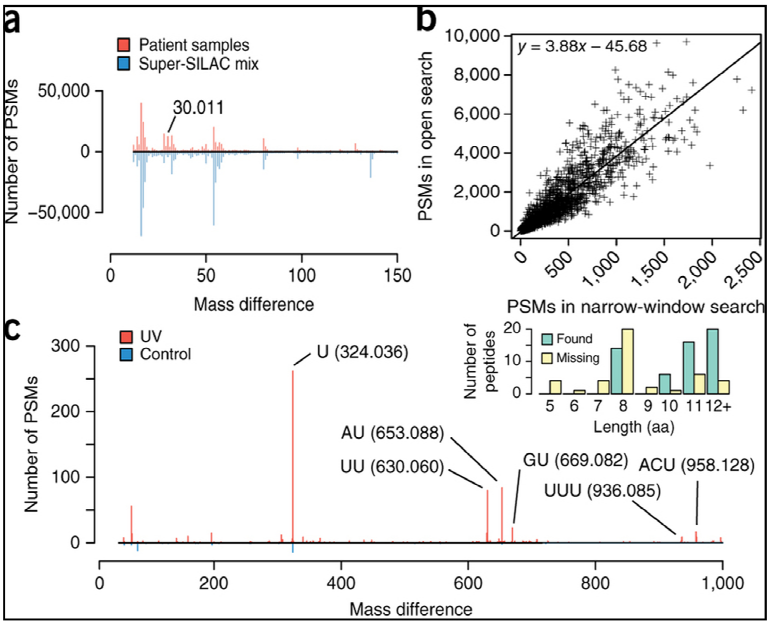


Even if crystallography and nuclear magnetic resonance are offering valuable atomic insights into the assembling of the protein-peptide complexes, the mechanism of their recognition and binding events remains largely unclear. In this work we report, for the first time, the use of a supervised molecular dynamics approach to explore the possible protein-peptide binding pathways within a timescale reduced up to three orders of magnitude compared with classical molecular dynamics. The better and faster understating of the protein-peptide recognition pathways could be very beneficial in enlarging the applicability of peptide-based drug design approaches in several biotechnological and pharmaceutical fields.

[Source : Exploring Protein-Peptide Recognition Pathways Using a Supervised Molecular Dynamics Approach. Veronica Salmaso et al. Cell Press (April 04,2017)]

MSFragger : ultrafast and comprehensive peptide identification in mass spectrometry–based proteomics

MSFragger is a new database search tool for implementation in peptide identification. MSFragger, that enables a more than 100-fold improvement in speed over most existing proteome database search tools. MSFragger empowers the open database search concept for comprehensive identification of peptides and all their modified forms, uncovering dramatic differences in modification rates across experimental samples and conditions. MSFragger makes open searches feasible even for data sets containing millions of MS/MS spectra. It is capable of performing open searches with variable modifications, making it applicable to data from labeling-based quantita-



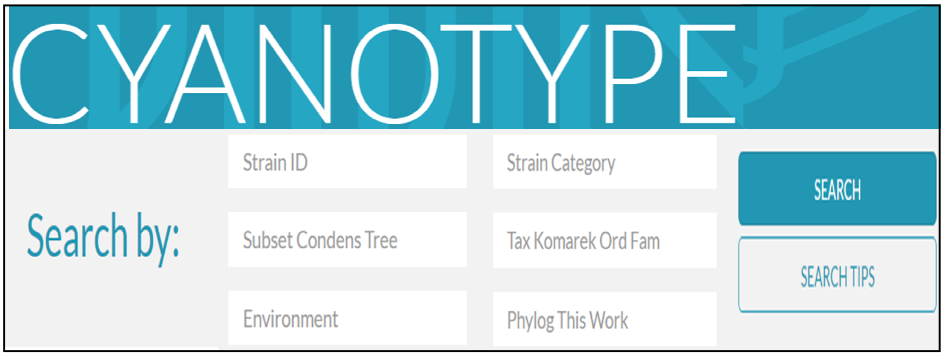
MSFragger's utility in reconstructing modification profiles across experiments under differing conditions and in the analysis of protein–RNA cross-linked peptides and affinity purification mass spectrometry (AP–MS) data. MSFragger is platform independent, not limited to data from a particular MS instrument, and can be incorporated easily into most existing data analysis pipelines. MSFragger begins by performing an *in silico* digestion of the protein database. It then removes redundant peptides and orders them by their theoretical mass creating a peptide index. Although peptide indexing has been described as a way to accelerate database search.In this step alone has little impact on spectrum similarity calculations, which is the most time-consuming step. MSFragger creating a novel theoretical fragment index. This enables highly efficient and simultaneous scoring of an experimental spectrum against all candidate peptide. Fig:Proteomics Experiment.

[Source: MSFragger: ultrafast and comprehensive peptide identification in mass spectrometry–based proteomics.Andy T Kong et al. NatureMethods (2017)]

CyanoType: A curated database of cyanobacterial strains relevant for modern taxonomy and phylogenetic studies

The dataset described lays the groundwork for an online database of relevant cyanobacterial strains, named CyanoType (http://lege.ciimar.up.pt/cyanotypeI).

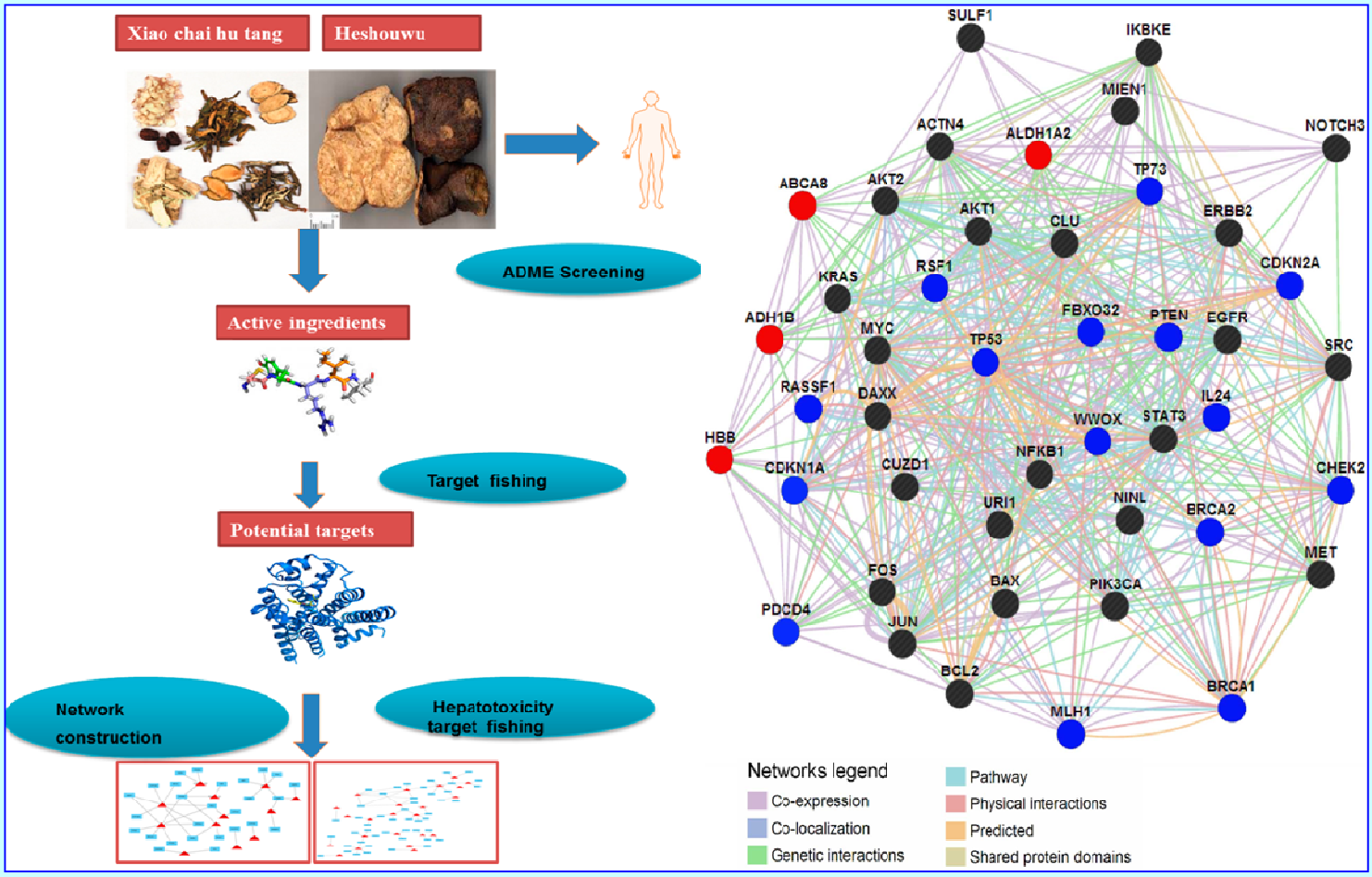
It is a database that includes categorized cyanobacterial strains useful for taxonomic, phylogenetic or genomic purposes, with associated information obtained by means of a literature-based curation. The dataset lists 371 strains and represents the first version of the database (CyanoType v.1). Information for each strain includes strain synonymy and/or co-identity, strain categorization, habitat, accession numbers for molecular data, taxonomy and nomenclature notes according to three different classification schemes, hierarchical automatic classification, phyloge-



The database will be updated periodically, namely by adding new strains meeting the criteria for inclusion and by revising and adding up-to-date metadata for strains already listed. A global 16S rDNA-based phylogeny is provided in order to assist users when choosing the appropriate strains for their studies. A global 16S rDNA-based phylogenetic tree is provided in order to assist users in choosing the appropriate strains for their studies.

[Source: Database (Nature)(2017)2017 .https://doi.org/10.6084/m9.figshare.c.3272731(2017)]

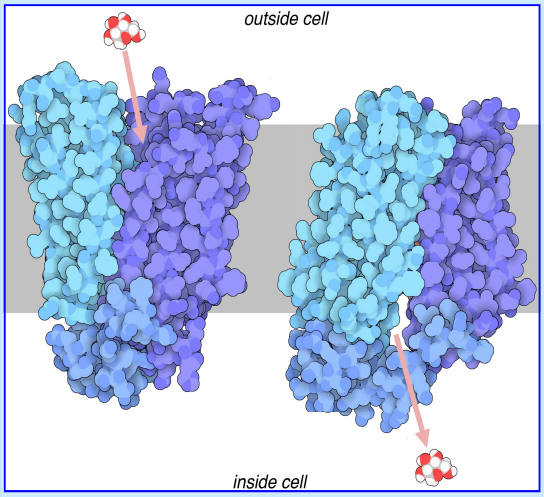
Bioinfo. Animation



Molecule of the Month

Glucose Transporters

Glucose is the fuel that powers most of the biosphere. Plants build it using energy from the sun, store it in starches and use it to build their infrastructure of cellulose. The glucose we eat is broken down through glycolysis and used to power the many processes of our cells. It is essential to supply each of our cells with a steady stream of glucose. Glucose is delivered throughout the body by the blood, and each cell gathers what it needs using glucose transporters. They act by alternating between two states. First, the transporter has an opening facing the outside of the cell, and it picks up a molecule of glucose.Then it shifts shape, and opens towards the inside, releasing glucose into the cell. Glucose transporters generally act passively: since glucose is rapidly phosphorylated by hexokinase, the concentration of free glucose in the cytoplasm is generally very low, and the higher concentration of glucose in the blood drives transport of glucose into the cell.The human genome encodes 14 similar transporters that deliver glucose and other sugars into different types of cells .GLUT1 manages the basal levels of glucose uptake and is very common in red blood cells. GLUT2 helps control the flow of glucose in and out of liver cells, and pancreatic beta cells use it to monitor the level of glucose in the blood, releasing insulin when the level rises. Nerve cells in the brain require a constant supply of glucose, so they use GLUT3 a form that works well even when glucose levels are low. GLUT4 is activated by insulin and is used by fat and muscle cells to gather glucose after meal.



[Source: http://pdb101.rcsb.org/motm/208]

International Center for Stem cells, Cancer and Biotechnology(ICSCCB),Pune,India
Biotech Bioinfo Workshop
5-Days Hands – On Workshop on
Molecular Biotechnology and Bioinformatics,Pune,India.

Date: 16-20 May 2017
12-16 June 2017
17-21 July 2017

Patents

Integrated bioinformatics sensing apparatus

US 9161703 B2

Inventors : Min-Hsien Wu, Yi-Yuan Chiu

ABSTRACT

An integrated bioinformatics sensing apparatus includes a piezoelectric sensing layer, an upper conductive layer, a bottom conductive layer and an information transmission controller. The piezoelectric sensing layer senses a physiological rhythm of a living organism to output a physiological rhythm signal, and the upper and bottom conductive layers sense a physiological electrical signal on a body surface of the living organism. The information transmission controller receives and processes the physiological rhythm signal and the physiological electrical signal to generate and store the sensed bioinformatics, or transmit the signals to the external processing device to display the sensed bioinformatics. The simple-structured sensing apparatus can be attached onto the body surface of the living organism conveniently.

Kindly send us your feedback to

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