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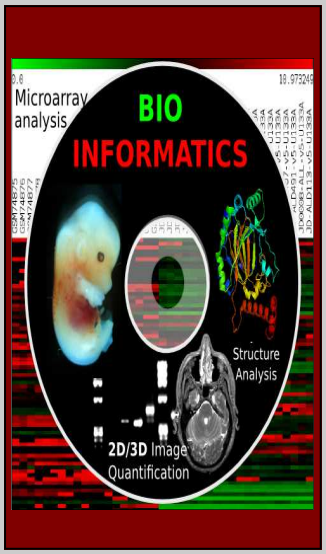
Bioinformatics up to Date

(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.

Our Focus

MOLECULAR DOCKING OF PHYTOCHEMICAL AS FTSZ CELL DIVISION PROTEIN INHIBITOR IN *MYCOBACTERIUM TUBERCULOSIS*

Filamenting temperature sensitive mutant Z (FtsZ) playing very important role in *MYCOBACTERIUM TUBERCULOSIS life cycle. It* seems to assemble into a dynamic ring (Z- ring) on the inner surface of the cytoplasmic membrane which involved in stabilizing Z-rings at the place where the division occurs and the formation of the ring is the signal for septation to begin. In this docking study, a total of fifty-one different bioactive molecules were screened found in three medicinal plants namely *Justicia adhatoda, Abrus precatoriu* sand *Dracaena angustifolia* to determine the inhibition against *M. tuberculosis* FtsZ cell divisional protein. Three compounds namely abrectorin, precatorine and gallic acid of *A. precatorius* and one compound namely vasicine of *J. adhatoda* showed good binding affinity among those the abrectorin showed very good Moldock and Rerank Score (-121.394KJmol-1 and -108.71KJmol-1) with H-Bond (-9.03613KJmol-1). From, this investigation it could be contemplated that the plant species *A. precatorius* and *J. adhatoda* may be the good sources of FtsZ protein inhibitor.

[Das et al., Molecular Docking of Phytochemical as Ftsz Cell Division Protein Inhibitor in Mycobacterium Tuberculosis. Int J Pharm Sci Res 2015; 6(1): 463-72.doi: 10.13040/IJPSR.0975-8232.6 (1).463-72]

New Gene to Fight Sepsis

Researchers from The Australian National University (ANU) and the Garvan Institute of Medical Research identify a gene that triggers the inflammatory condition that can lead to the full-body infection sepsis. The gene that could have the potentiality opens the door for the development of new treatments of the lethal disease sepsis.

The research led by Professor Simon Foote, Director of The John Curtin School of Medical Research (JCSMR) at ANU, published in journal *Nature 2015.*

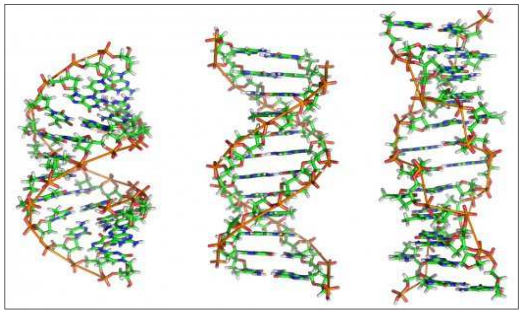
Sepsis occurs when molecules known as lipopolysaccharides (LPS) on the surface of some bacteria infiltrate cells, triggering an immune response that causes the cells to self-destruct. The team found the protein Gasdermin-D plays a critical role in the pathway to sepsis. The team at the Australian Phenomics Facility then screened thousands of genes with a large-scale forward genetics discovery platform and in a little over a year had isolated the gene that produces Gasdermin-D.

"This finding is a key that could potentially unlock our ability to shutdown this killer disease before it gets to a life-threatening stage," Professor Goodnow said.

[Caspase-11 cleaves gasdermin D for non-canonical inflammasome signaling. Kayagaki, N et al. Nature (2015)]

BRCA2-A Mutant Target for Prostate Cancer

A new study reports that genetic abnormalities associated with poor prognosis in prostate cancer are particularly common in men with germline mutations in the BRCA2 gene. The study published in the Annals of Oncology *2015.*



The new research study suggests men with inherited BRCA2 mutations may be at increased risk of accumulating additional dangerous mutations within their tumours, and could explain why their cancers tend to be unusually aggressive. The study has identified one particular genetic abnormality that is common in the tumours of BRCA2-mutation carriers, and could be a new treatment target in these cancers.

Scientists at The Institute of Cancer Research, London, collaborated with scientists at the Spanish National Cancer Research Centre, Madrid, to identify the genetic abnormalities present in the prostate tumours of patients with BRCA2 germline mutations. The study found that patients who carry germline BRCA2 mutations harbour significantly more copy-number alterations than those who do not have germline mutations. In particular, patients with BRCA2 mutations were more likely to have extra copies of a gene called c-MYC – potentially leading to uncontrolled cell growth.

Targeting c-MYC could therefore be a potential treatment for patients with the BRCA2 mutation.

New Algorithm to Predict Dynamic Language of Proteins

Researchers from the Structural Biology Computational Group of the Spanish National Cancer Research Centre (CNIO), led by Alfonso Valencia, in collaboration with a group headed by Francesco Gervasio at the University College London (UK), have developed the first computational method based on evolutionary principles to predict protein dynamics, which explains the changes in the shape or dimensional structure that they experience in order to interact with other compounds or speed up chemical reactions. The results have been published this week in the journal Proceedings of the National Academy of Sciences (PNAS). The study constitutes a major step forward in the computational study of protein dynamics (i.e. their movement), which is crucial for the design of drugs and for the research on genetic diseases, such as cancer, resulting in higher levels of complexity than allowed by current methods.

This new computational method easily integrates experimental and genomic data through the use of the latest sequence analysis and 3D modeling technology. In addition, it demonstrates that genomic data can be a source of useful information to supplement the current tools used to study the structure and dynamics of proteins.

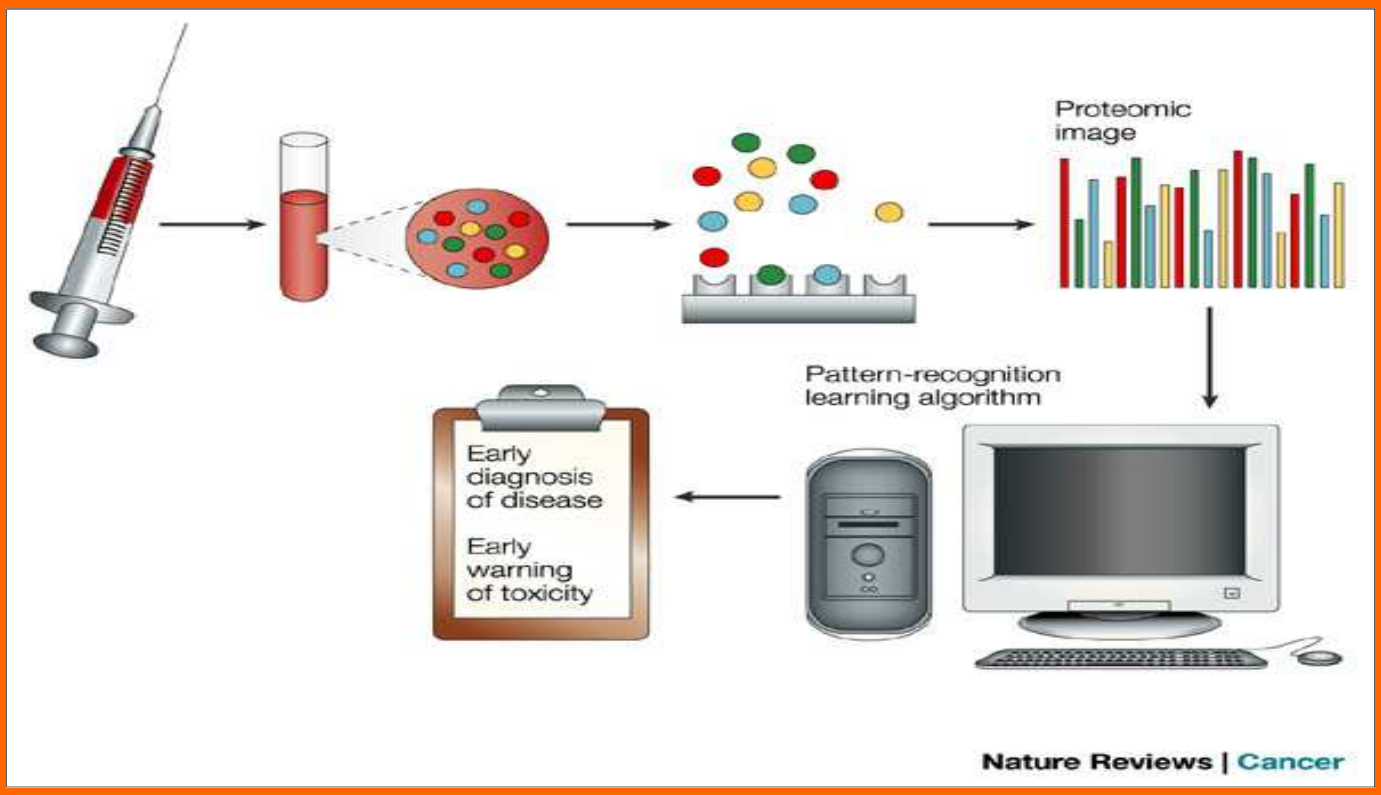
[*From residue coevolution to protein conformational ensembles and functional dynamics. Ludovico Sutto, Simone Marsili, Alfonso Valencia, Francesco Luigi Gervasio. PNAS (2015)*]

BioXpress: an integrated RNA-seq-derived gene expression database

BioXpress is a gene expression and cancer association database in which the expression levels are mapped to genes using RNA-seq data obtained from The Cancer Genome Atlas, International Cancer Genome Consortium, Expression Atlas and publications. The BioXpress database includes expression data from 64 cancer types, 6361 patients and 17469 genes with 9513 of the genes displaying differential expression between tumor and normal samples. In addition to data directly retrieved from RNA-seq data repositories, manual biocuration of publications supplements the available cancer association annotations in the database. All cancer types are mapped to Disease Ontology terms to facilitate a uniform pan-cancer analysis. The BioXpress database is easily searched using HUGO Gene Nomenclature Committee gene symbol, UniProtKB/RefSeq accession or, alternatively, can be queried by cancer type with specified significance filters. This interface along with availability of pre-computed downloadable files containing differentially expressed genes in multiple cancers enables straightforward retrieval and display of a broad set of cancer-related genes. Database websaite: http://hive.biochemistry.gwu.edu/tools/bioxpress.

[Quan Wan et al. BioXpress: an integrated RNA-seq-derived gene expression database for pan-cancer analysis, Database , March 28, 2015]

Bioinfo. Animation



proteomic pattern diagnostics

Patent News

Method for identifying Gaoyou duck varieties by utilizing molecular bioinformatics

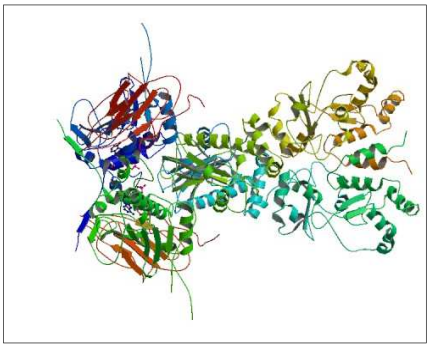
CN101812500 A

Abstract

The invention relates to a method for identifying Gaoyou duck varieties by utilizing molecular bioinformatics belonging to the technical filed of biological variety identification. In the invention, the sequences of gene b of cytochrome of mitochondrial DNA of a Gaoyou duck and the duck variety to be tested are accurately obtained on the basis of gene cloning and DNA sequencing technologies, a plurality of software is utilized to accurately figure out the haplotype, variation locus, haplotype diversity, average nucleotide difference, nucleotide ramification degree, pure genetic distance, Kimura dual -parameter genetic distance among varieties, variety colony cluster result images and haplotype phylogenetic trees of each variety, and the genetic information difference among the varieties is utilized to identify the true and false of the Gaoyou duck varieties through software precise calculation and analysis results.

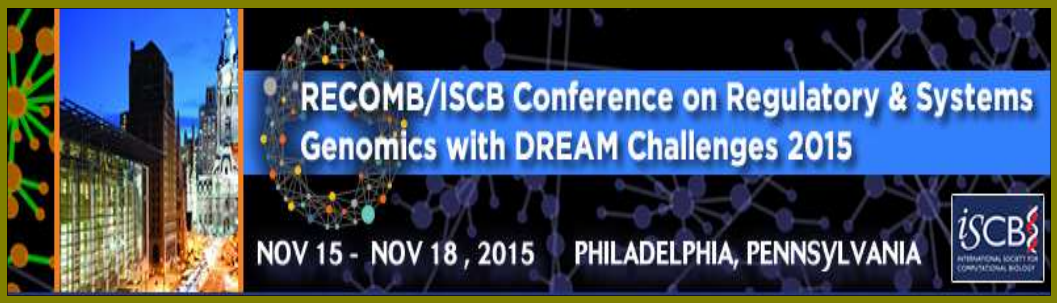
Hsp (*Heat shock protein*)

Hsp90 is a specialized chaperone that assists in the maturation of a select clientele of proteins. These proteins include over a hundred transcription factors and kinases, such as steroid receptors, mutant p53 protein, and the HER2 protein involved in breast cancer. So far, researchers have not discovered a unifying theme for this growing list of proteins, just that Hsp90 is essential for maintaining active forms of these proteins. The exact function of Hsp90 is also currently a mystery. Researchers don't know what it does in the maturation of its client proteins. They have discovered that it acts as part of a large complex of different chaperone proteins. Some of these chaperones deliver immature proteins to the complex, and others assist with folding. Some of these proteins, such as Hsp70 and Hsp60 are general chaperones. Hsp90, on the other hand, plays a more specific role. The figure showing the Crystal structure of an HSP90-SBA1 closed chaperone complex.



Many of the client proteins serviced by Hsp90 are involved in cellular growth, making Hsp90 an attractive target for cancer chemotherapy. It might think that drugs that attack Hsp90 would be too toxic for use in therapy, since Hsp90 is essential in normal cells too. But it turns out that cancer cells rely on Hsp90 more heavily than normal cells, and respond more strongly to drugs that block Hsp90 function. For instance, the drug geldanamycin blocks the binding of ATP to Hsp90 in cancer cells, causing complexes of Hsp90 and misfolded proteins to accumulate. This stimulates the ubiquitin/proteosome system to destroy the proteins, ultimately killing the cancer cells by corrupting the signaling pathways that control growth.

Upcoming Events



Kindly send us your feedback to

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