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Bioinformatics up to Date

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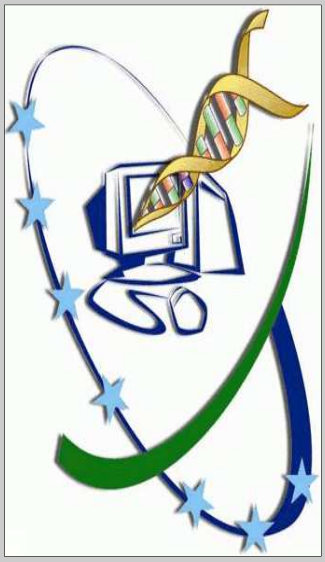
Jorhat - 785 006, Assam

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.

New Genomics Technique Could Accelerate Detection of Foodborne Bacterial Outbreaks

A new testing methodology based on metagenomics could accelerate the diagnosis of foodborne bacterial outbreaks, allowing public health officials to identify the microbial culprits in less than a day. The methodology could also identify co-infections with secondary microbes, determine the specific variant of the pathogen, and help alert health officials to the presence of new or unusual pathogens. The research was reported on November 23, in the *journal Applied and Environmental Microbiology.*

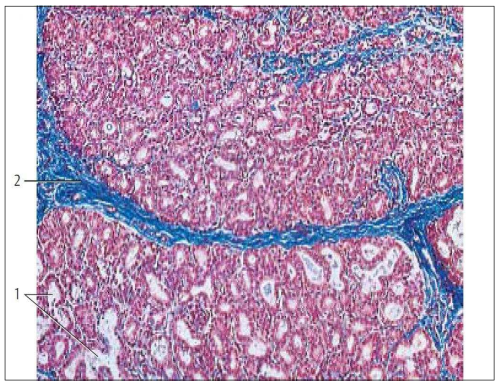
Researchers from the Georgia Institute of Technology and the U.S. Centers for Disease Control and Prevention (CDC) recently compared the new methodology against traditional culture-based methods with samples from two severe outbreaks of Salmonella, a common foodborne pathogen. The metagenomics approach - which relies on DNA sequencing and bioinformatics analysis of the resulting sequencing data -- not only correctly identified the bacterial culprit, but also found a possible co-infection with a second important pathogen, Staphylococcus.

Widespread use of the new shotgun metagenomics methodology could improve real-time disease surveillance, provide a better quantitative picture of pathogen abundance and help scientists and doctors understand the response of the body's natural microbiome. Supported by the CDC and the National Science Foundation.

[Source: ***Metagenomics analysis of two foodborne outbreaks.*** *Andrew D. Huang et al. Applied and Environmental Microbiology (2016)]*

First 3D Mammary Gland Model

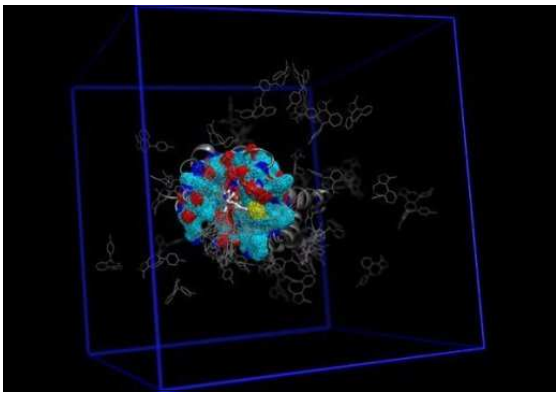
A team of researchers from Cardiff University and Monash Biomedicine Discovery Institute has succeeded in creating a three-dimensional mammary gland model that will pave the way for a better understanding of the mechanisms of breast cancer. Scientists were able to grow mouse mammary cells into three-dimensional mammary tissue Known as an 'organoid' the model mimics the structure and function of a real mammary gland. This enables researchers to increase their understanding of how breast tissue develops and provides an active model for the study of disease and drug screening. In order to fully tackle the mechanisms that lie behind breast cancer first need to understand how healthy breast tissue develops. As such developing a model of a normal breast with the actual architecture of a mammary gland has long been a 'Holy Grail' for cancer researchers.This model allows us to really study the basic biology of how the breast develops - how hormones work, what are the genetic influences. They hope to use this model in tandem with models of breast cancer in order to carry out effective drug-screening.



Source: ***Wnt and Neuregulin1/ErbB signalling extends 3D culture of hormone responsive mammary organoids****. Jardé, T et al. Nature Communications (26 October 2016).*

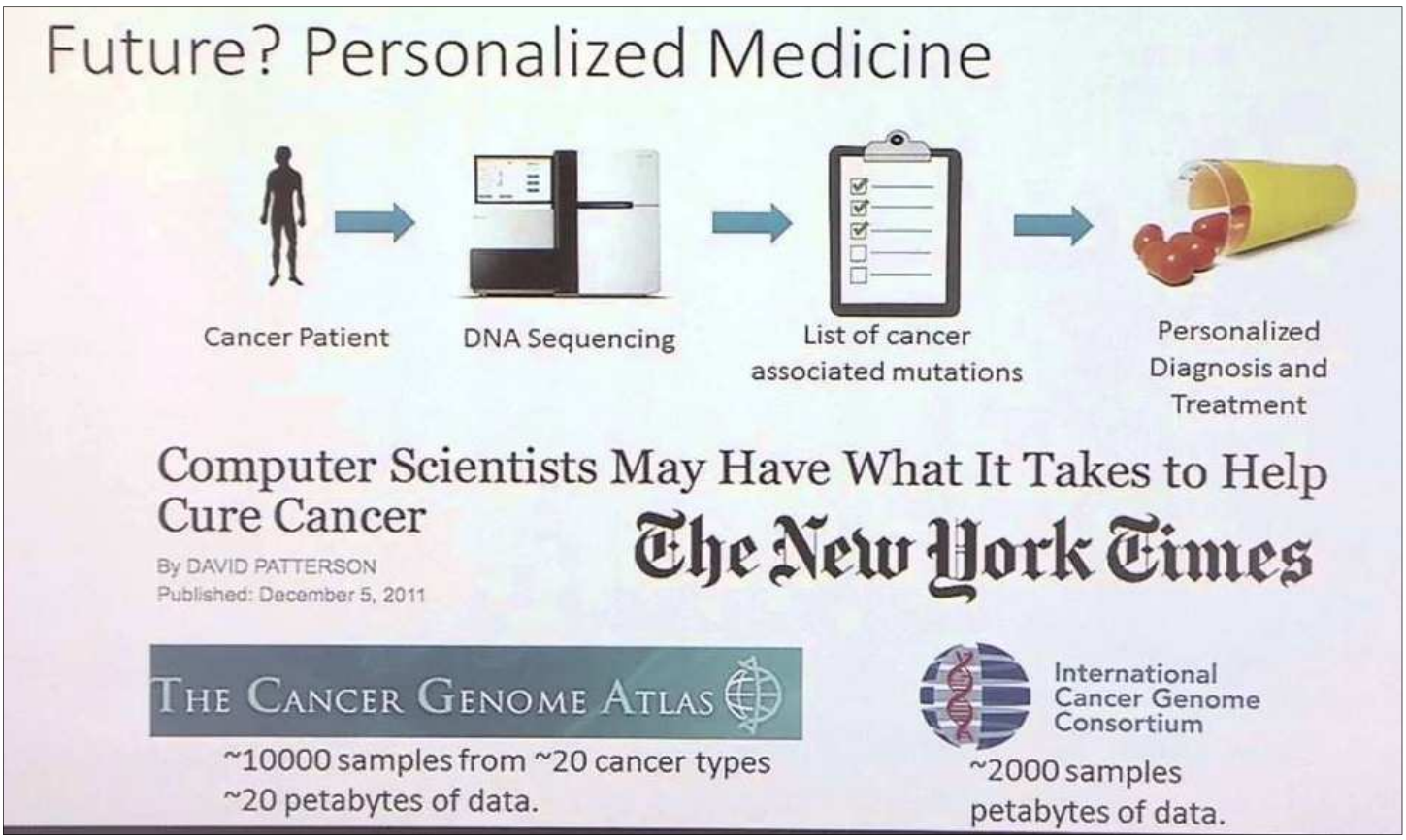
New Computational tool: fABMACS

A new computational tool called fABMACS is helping scientists see beyond static images of proteins to more efficiently understand how these molecules function, which could ultimately speed up the drug discovery process. Scientists study these interactions to develop new insights into protein function and to develop targeted therapies for diseases such as cancer. "The creation of fABMACS is a significant step toward robust virtual drug discovery because it saves time and money. It allows us to better harness the power of existing software while greatly improving our ability to predict the way that a potential drug interacts with a protein. "fABMACS allows us to simulate chemical changes to the drug and more quickly predict how those changes impact its interaction with the target protein. Ultimately, this could translate to improved drug potency and efficacy."The team ran several accelerated computer simulations of the epigenetic regulatory protein BRD4 bound to a drug that is currently in phase I clinical trials for blood cancers. They demonstrated that a slight change to the compound's chemical structure could improve binding to its target protein, thereby improving its effect.



fABMACS is an add-on to existing molecular dynamics software. It is based on GROMACSv5.0.5 and optimizes network communication and load balancing--both critical aspects of software development in parallel computing environments to achieve a low-overhead implementation of new free-energy techniques.

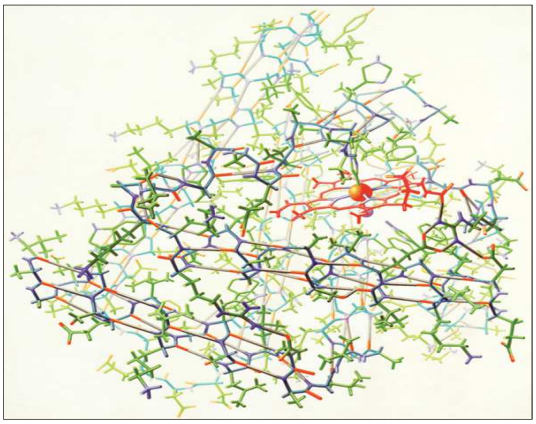
[*Source:* ***A fast, open source implementation of adaptive biasing potentials uncovers a ligand design strategy for the chromatin regulator BRD4.*** *Bradley M. Dickson et al. Journal of Chemical Physics (2016*



Molecule of the month

Myoglobin

Myoglobin is a small, bright red protein. It is very common in muscle cells and gives meat much of its red color. Its job is to store oxygen, for use when muscles are hard at work. To do this, it uses a special chemical tool to capture slippery oxygen molecules: a heme group. Heme is a disk-shaped molecule that has a hole in the center that is perfect for holding an iron ion. The iron then forms a strong interaction with the oxygen molecule. As you can see in the structure, the heme group is held tightly in a deep pocket on one side of the protein. *Myoglobin was the first protein to have its atomic structure determined, revealing how it stores oxygen in muscle cells.* Any discussion of protein structure must necessarily begin with myoglobin, because it is where the science of protein structure began. After years of arduous work, John Kendrew and his coworkers determined the atomic structure of myoglobin, laying the foundation for an era of biological understanding.



When the structure of myoglobin was solved, it posed a great challenge. The structure is so complex that new methods needed to be developed to display and understand it. John Kendrew used a huge wire model to build the structure based on the experimental electron density. Then, the artist Irving Geis was employed to create a picture of Myoglobin for a prominent article in Scientific American. Computer graphics were still many years in the future, so he created this illustration entirely by hand, one atom at a time.

[Source: http://pdb101.rcsb.org/motm/motm-by-title]

Micelle- and microemulsion-assisted planar separations platform for proteomics

WO 2007067731 A2

Inventors : Wayne F. Patton

Abstract

A method of separating biomolecules includes providing a sample comprising one or more biomolecules, at least one of which is hydrophilic; wetting an amphiphilic planar stationary phase with a microemulsion or micelluar mobile phase; and creating an electrical field between first and second electrodes in electrical contact with opposing edges of the amphiphilic stationary phase, wherein the mobile phase advances across the length of the separation medium and one or more biomolecules are separated.

Kindly send us your feedback to

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