



# Bioinformatics up to Date

(Bioinformatics Infrastructure Facility, Biotechnology Division)  
 North-East Institute of Science & Technology  
 Jorhat - 785 006, Assam



## Inside.....

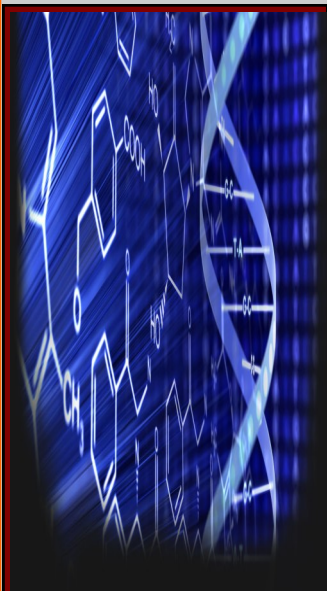
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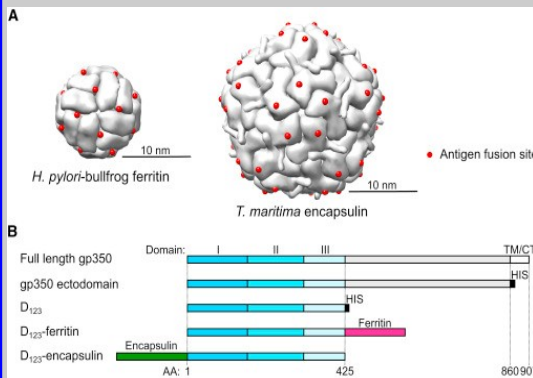


## About us

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.

## Rational Design of an Epstein-Barr Virus Vaccine Targeting the Receptor-Binding Site

Epstein-Barr virus (EBV) represents a major global health problem. Though it is associated with infectious mononucleosis and ~200,000 cancers annually worldwide, a vaccine is not available.



The major target of immunity is EBV glycoprotein 350/220 (gp350) that mediates attachment to B cells through complement receptor 2 (CR2/CD21). Here, we created self-assembling nanoparticles that displayed different domains of gp350 in a symmetric array. By focusing presentation of the CR2-binding domain on nanoparticles, potent neutralizing antibodies were elicited in mice and non-human primates.

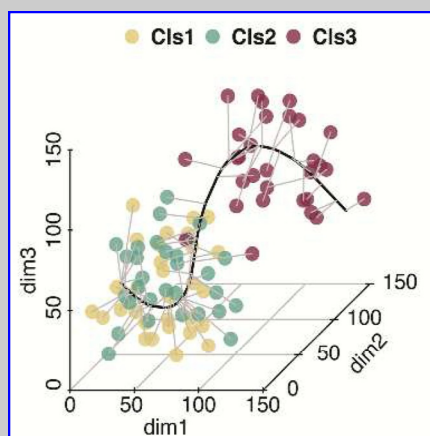
### Molecular Design of gp350-Based Nanoparticles

The structurally designed nanoparticle vaccine increased neutralization 10- to 100-fold compared to soluble gp350 by targeting a functionally conserved site of vulnerability, improving vaccine-induced protection in a mouse model. This rational approach to EBV vaccine design elicited potent neutralizing antibody responses by arrayed presentation of a conserved viral entry domain, a strategy that can be applied to other viruses.

[Source: [http://www.cell.com/cell/fulltext/S0092-8674\(15\)00959-9](http://www.cell.com/cell/fulltext/S0092-8674(15)00959-9)]

## Cluster Significance: A Bioconductor package facilitating statistical analysis of class cluster separations in dimensionality reduced data.

Multi-dimensional data generated via high-throughput experiments is increasingly used in conjunction with dimensionality reduction methods to ascertain if resulting separations of the data



correspond with known classes. This is particularly useful to determine if a subset of the variables, e.g. genes in a specific pathway, alone can separate samples into these established classes. Despite this, the evaluation of class separations is often subjective and performed via visualization. Here we present the ClusterSignificance package; a set of tools designed to assess the statistical significance of class separations downstream of dimensionality reduction algorithms. In addition, we demonstrate the design and utility of the ClusterSignificance package and utilize it to determine the importance of long

non-coding RNA expression in the identity of multiple hematological malignancies.

[Source : Cluster Significance: A Bioconductor package facilitating statistical analysis of class cluster separations in dimensionality reduced data, Jason T et al. (Bioinformatics oxford)(2017)].

## FDA Label: Full-Text Search of Drug Labeling

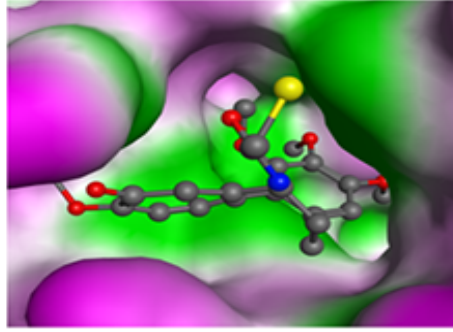
The FDALabel Database is a web-based application that allows you to perform customizable searches of a database of about 95,000 labeling documents that include human prescription drugs and biological products, and human over-the-counter (OTC) drugs. Includes human OTC drugs approved for marketing through a New Drug Ap-



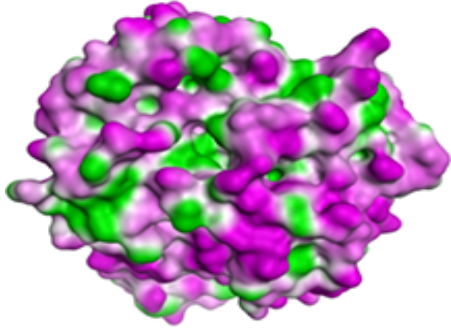
plication (NDA), Abbreviated New Drug Application (ANDA), or the OTC monograph system. Includes drug products, therapeutic biologics and monoclonal antibodies, vaccines, plasma derivatives, allergenics (standardized and non-standardized), cellular therapy, and licensed mini-

mally manipulated cells. Labeling for approved OTC drugs and OTC drugs under the monograph system is called Drug Facts. Drug Facts includes information about the purpose and use of the drug, warnings, directions for use, and other information. Homeopathic prescription and homeopathic OTC drugs are not approved by the FDA but are allowed to be marketed. There are minimal labeling requirements for these unapproved products. The FDA Label is available at the web address <https://rm2.scinet.fda.gov/druglabel/#simsearch-0>

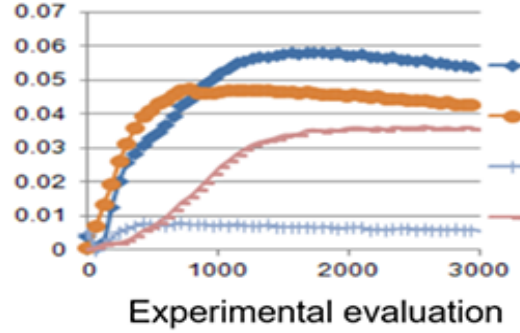
[Source: Database: <https://www.fda.gov/ScienceResearch/BioinformaticsTools/ucm289739.htm>]



Molecular modeling

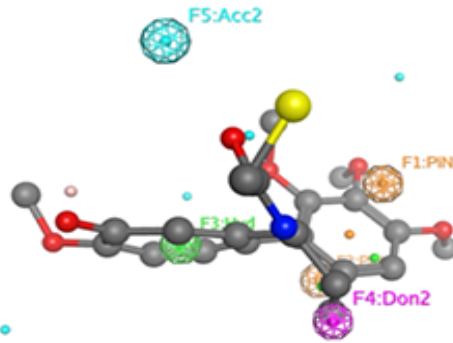


Molecular targets



Experimental evaluation

## SBDD

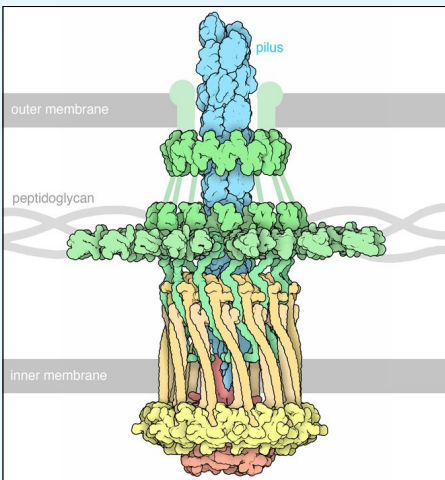


Ligand modeling

## Molecule of the month

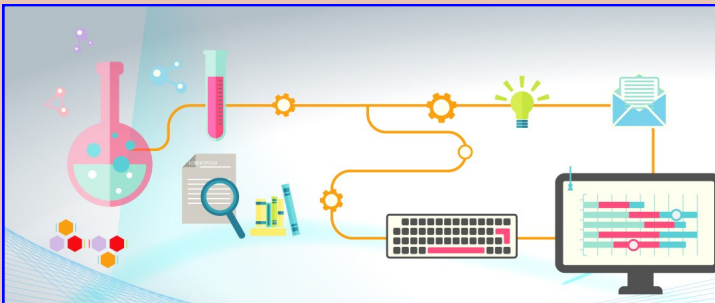
### Pilus Machine

Pilus Machine is a molecular machine with a rotary motor builds a long protein filament involved in bacterial motility and attachment. The molecular machine shown here, from PDB entry [3jc8](https://www.rcsb.org/entry/3jc8), builds one of most widespread forms of pili, termed a type IVa pilus. The pilus is extended from the center of the machine, often to lengths that rival the size of the cell. The machine spans the entire cell wall: a rotary motor embedded in the cytoplasmic membrane adds new subunits, a collar guides the growing pilus through the outer membrane, and a ring of proteins anchors the whole thing to the peptidoglycan layer that fills the space between the two membranes.



This pilus machine is built by a predatory soil bacterium that forms swarms of cells that search for bacterial prey. These cells use the pilus machine like a grappling hook to crawl, by extending a pilus, attaching it to a surface, then reeling it back in. Since it requires a lot of force to drag the entire cell, these assembly machines are among the most powerful molecular motors known.

[Source: <http://pdb101.rcsb.org/motm/211>]



# Basic NGS Data Analysis Workshop

27<sup>th</sup> – 30<sup>th</sup> November 2017  
Bioinformatics Training Lab, Malaysia Genome Institute

**GENOM MALAYSIA**  
Malaysia Genome Institute

**NIBM**  
NATIONAL INSTITUTE OF  
BIOTECHNOLOGY MALAYSIA

**2017 NextGen Genomics, Biology, Bioinformatics  
and Technologies (NGBT) Conference**

**2<sup>nd</sup> - 4<sup>th</sup> October 2017, Bhubaneswar, Odisha, INDIA**

Patents

## **Bioinformatic processes for determination of peptide binding**

WO 2014200910 A2

Inventors : Braun Elmar Dr.-Ing.

### **ABSTRACT**

This invention relates to the identification of peptide binding to ligands, and in particular to identification of epitopes expressed by microorganisms and by mammalian cells. The present invention provides polypeptides comprising the epitopes, and vaccines, antibodies and diagnostic products that utilize or are developed using the epitopes.

**Kindly send us your feedback to**

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