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Bioinformatics up to Date

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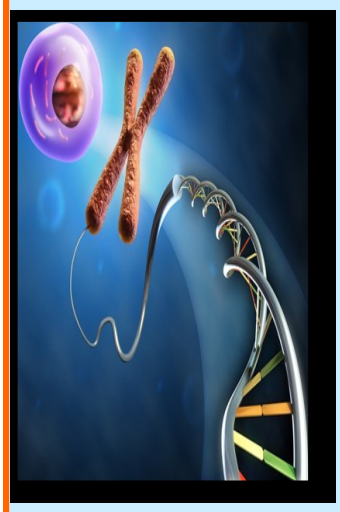
(http://www.rrljorhat.res.in/biotechnology.html)

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.

Molecular dynamic simulations reveal structural insights into substrate and inhibitor binding modes and functionality of Ecto-Nucleoside Triphosphate Diphosphohydrolases.

Ecto-nucleotidase enzymes catalyze the hydrolysis of extracellular nucleotides to their respective nucleosides. In this study, the researchers place the focus on the elucidation of structural features of the cell surface located ecto-nucleoside triphosphate diphosphohydrolases (E-NTPDase1-3 and 8). The physiological role of these isozymes is crucially important as they control purinergic signaling by modulating the extracellular availability of nucleotides. Since, crystal or NMR structure of the human isozymes are not available – structures have been obtained by homology modeling. Purification of the homology models with poor stereo-chemical quality is of absolute importance in order to derive reliable structures for subsequent studies. Therefore, the resultant models obtained by homology modelling were refined by running molecular dynamic simulation. Binding mode prediction analysis of standard substrates and of competitive inhibitor was conducted to highlight important regions of the active site involved in hydrolysis of the substrates and possible mechanism of inhibition.

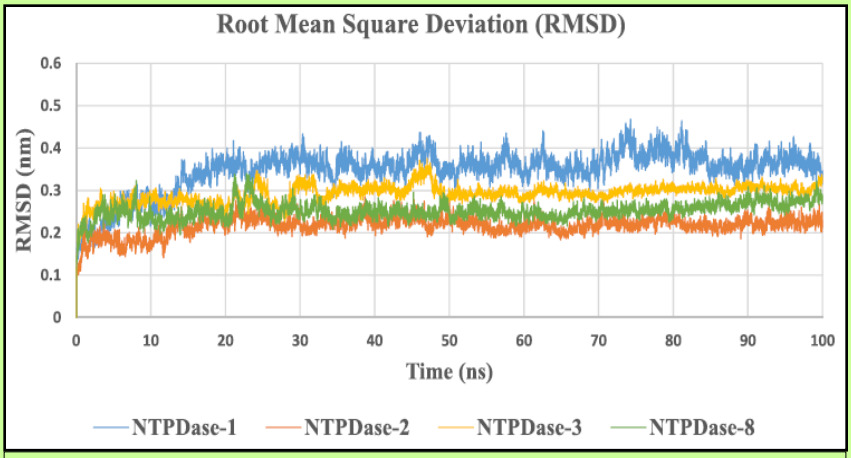
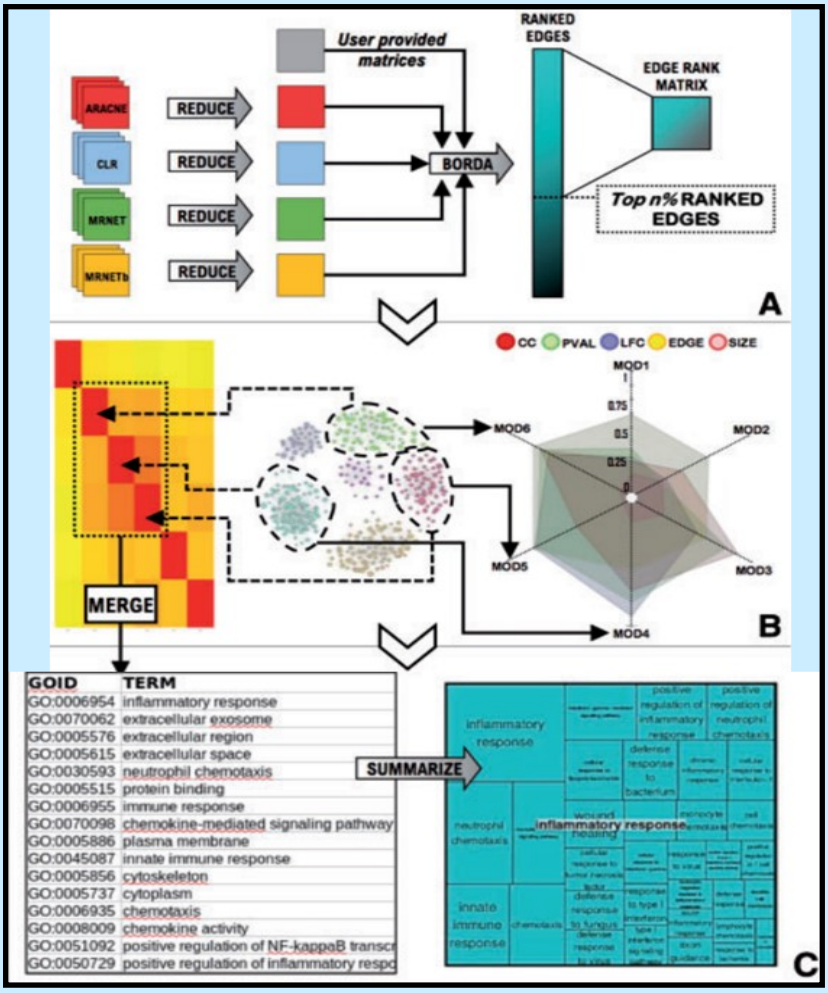


Fig: Root Mean Square Deviation (RMSD) of amino acid residues during simulation run.

Source: Jamshed Iqbal & Syed Jawad Ali Shah *et al.*, J Sci Rports,

INfORM: Inference of NetwOrk Response Modules



Detecting and interpreting responsive modules from gene expression data by using network-based approaches is a common but laborious task. It often requires the application of several computational methods implemented in different software packages, forcing biologists to compile complex analytical pipelines. In this study, the researchers introduce INfORM (Inference of NetwOrk Response Modules), an R shiny application that enables non-expert users to detect, evaluate and select gene modules with high statistical and biological significance. INfORM is a comprehensive tool for the identification of biologically meaningful response modules from consensus gene networks inferred by using multiple algorithms. It is accessible through an intuitive graphical user interface allowing for a level of abstraction from the computational steps.

INfORM is freely available for academic use at https://github. com/Greco-Lab/INfORM.

Source :Veer Singh Marwah *et al.* J Oxford Bioinformatics (2018)

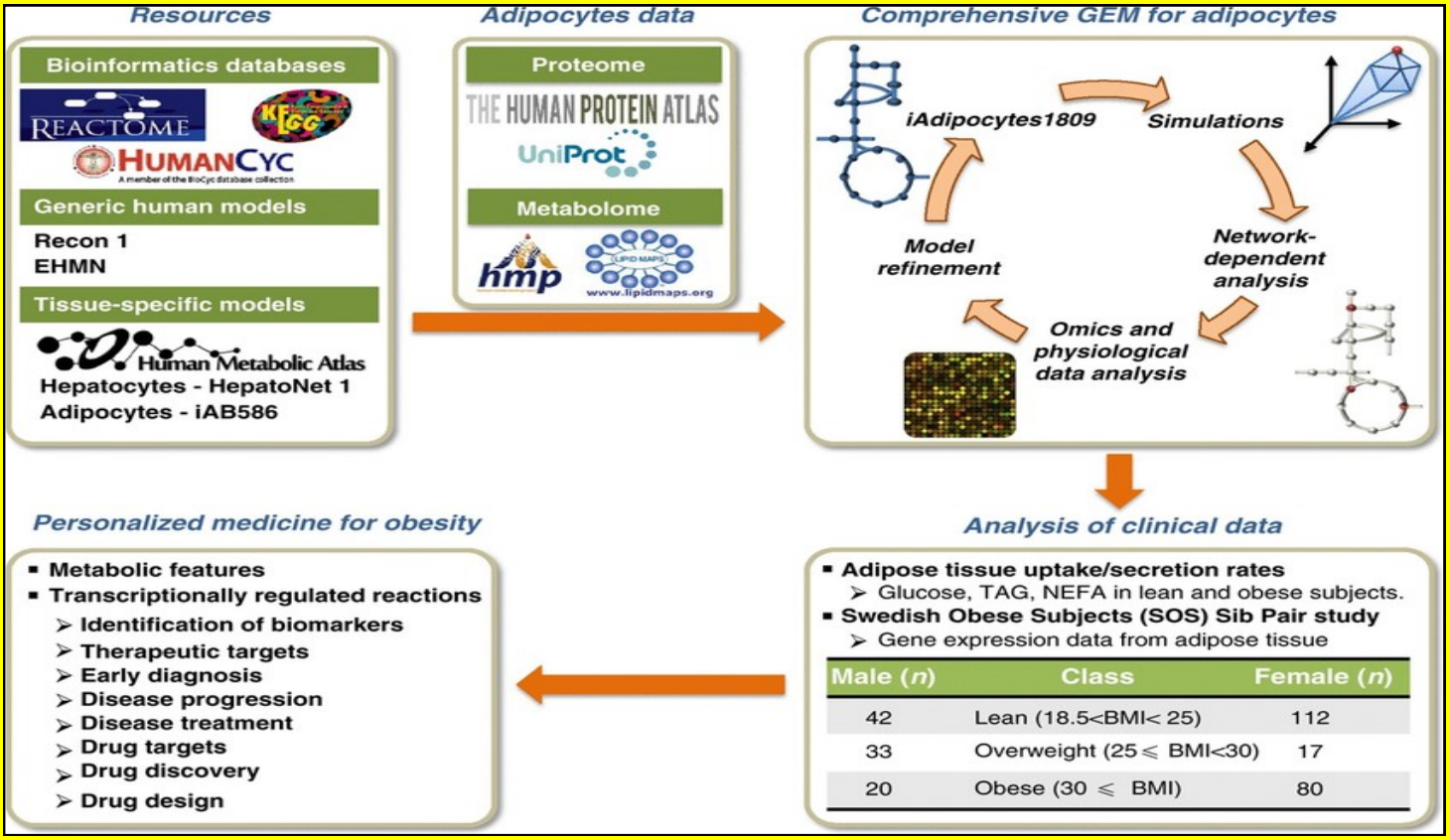
AbDesigner3D: a structure-guided tool for peptide-based antibody production.

AbDesigner3D, a new tool for identification of optimal immunizing peptides for antibody production using a peptide-based strategy. AbDesigner3D integrates 3D structural data from the Protein Data Bank (PDB) with UniProt data, which includes basic sequence data, post-translational modification sites, SNP occurrences and more. Other features, such as uniqueness and conservation scores, are calculated based on sequences from UniProt. The 3D visualization capabilities allow an intuitive interface, while an abundance of quantitative output simplifies the process of comparing immunogen peptides. Important quantitative features added in this tool include calculation and display of accessible surface area (ASA) and protein-protein interacting residues (PPIR). The specialized data visualization features of AbDesigner3D will greatly assist users to optimize their choice of immunizing peptides.

AbDesigner3D is freely available at http://sysbio.chula.ac.th/AbDesigner3D or https://hpcwebapps.cit.nih.gov/AbDesigner3D/.

Source: Thammakorn Saethang *et al.* J Oxford Bioinformatics

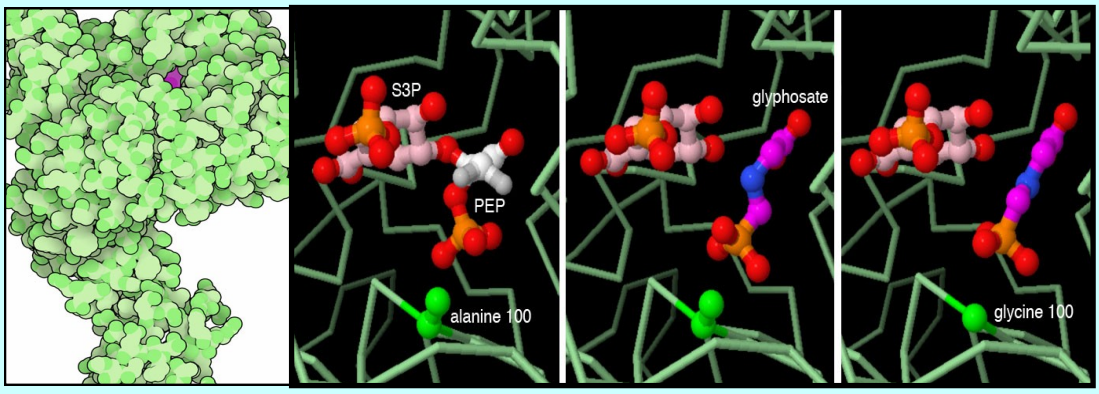
Bioinfo. Animation (Xiang Zhang *et al., 2018)*



EPSP Synthase and Weedkillers

The enzyme EPSP synthase performs a key step in the synthesis of aromatic compounds. It connects a ring-shaped shikimate-3-phosphate (S3P) molecule to phosphoenol pyruvate (PEP). Later , the shikimate ring will be modified to form the aromatic ring in tyrosine, and the PEP will become the amino/acid backbone of the molecule.

PEP Mimic:



In the 1970s, researchers at Monsanto discovered that glyphosate acts as a powerful herbicide, marketing it as "Roundup." It works by mimicking PEP, blocking the reaction performed by EPSP synthase and ultimately killing the plant. It's not as effective, however, for use in agriculture, because it would kill the crop along with the weeds. To solve this problem, researchers have also discovered bacteria that have forms of EPSP synthase that are resistant to glyphosate. The crop plants are then engineered to use this resistant enzyme, and glyphosate can be used to kill the weeds but not the crop. EPSP synthase becomes resistant to glyphosate by constricting the active site. These three structures show how this is done. The first structure (PDB entry 2pqb) shows a transition state analog bound in the active site of a glyphosate-resistant enzyme. The analog is similar to an intermediate state of the reaction, where S3P has just formed a bond to PEP, but the analog is unable to complete the reaction, so it stays in the active site and may be observed by crystallography. The second structure (PDB entry 2gga) shows how glyphosate mimics PEP, taking its place. An alanine amino acid, however, crowds the herbicide and greatly weakens its binding strength. This alanine is typically a smaller glycine in glyphosate-susceptible forms the enzyme. The third structure (PDB entry 2ggd) shows that if this change is made in the protein, glyphosate binds in a more stable, extended form, and the enzyme is effectively inhibited by the herbicide.

Source : http://pdb101.rcsb.org/motm/218

Patents

Non-human animals having a humanized signal-regulatory protein gene

US 20170265442 A1

Murphy *et al.*

Genetically modified non-human animals and methods and compositions for making and using the same are provided, wherein the genetic modification comprises a humanization of an endogenous signal- regulatory protein gene, in particular a humanization of a SIRP.alpha. gene. Genetically modified mice are described, including mice that express a human or humanized SIRP.alpha. protein from an endogenous SIRP.alpha. locus.

Kindly send us your feedback to

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