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Bioinformatics up to Date

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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.

A vaccine to combat Kaposi Sarcoma utilizing immunoinformatics approach

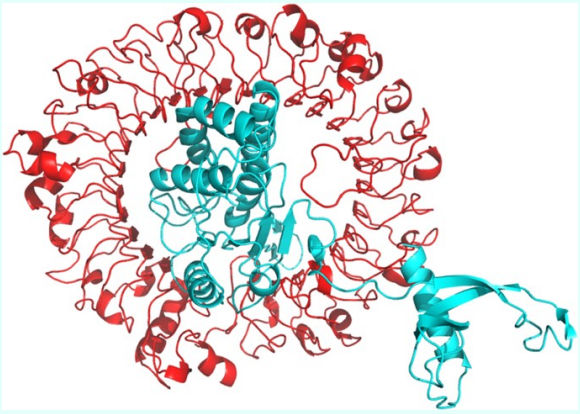


Figure: The interaction of the proposed vaccine construct with TLR-9 .

Kaposi's sarcoma-associated herpesvirus (KSHV) is the ninth well known human herpesvirus. This virus causes Kaposi's sarcoma, a cancer, as well as primary effusion lymphoma, HHV-8-associated multicentric Castleman's disease and KSHV inflammatory cytokine syndrome.Kaposi's sarcoma-associated herpesvirus (KSHV) dependable for causing Kaposi sarcoma (KS), an opportunistic angioproliferative neoplasm is promising quickly. Still, there is no permanent cure for this disease. The recent study was explained about to design a multi-epitope based vaccine targeting the major glycoproteins of KSHV which plays an key role in the virus entry. After the application of rigorous immunoinformatics analysis and several immune filters, the multi-epitope vaccine was constructed such as CD4, CD8 and IFN-γ inducing epitopes.A number of physiochemical characteristics, allergenicity and antigenicity of the multi-epitope vaccine were analyzed in order to make sure its protection and immunogenicity. Further, to explore the reliable and flexible binding energy of the vaccine with Toll like receptor -9 (TLR-9) was analyzed by molecular docking and dynamics simulation approach. In addition, an *in silico* cloning was performed to ensure the expression and translation efficiency of the vaccine, which could prove their potential against cancer. Further, the researchers proposed to experiment their present findings in the lab settings to ensure the safety, immunogenicity and efficacy of the presented vaccine which may help in controlling KSHV infection. Figure 1 shows the vaccine in cyan colour and TLR-9 are in red color. respectively.

Source: Varun Chauhan *et al. J Sci. Reports.2019*

BIPSPI: a method for the prediction protein–protein interaction.

Protein-protein interactions (PPIs) are important in every process in a cell, it is crucial for understanding cell physiology in normal and disease states. It is also important in drug development, since drugs can affect PPIs. Protein-protein interaction networks (PPIN) are mathematical representations of the physical contacts between proteins in the cell. Computational approaches are low cost and faster than experimental ones, leading to proliferation of multiple methods aimed to predict which residues belong to the interface of an interaction.

In some study, BIPSPI, a new computational based method for the calculation of partner-specific PPI sites. On the Contrary to a large amount of binding site prediction methods, the proposed approach takes into account a pair of interacting proteins rather than a single one in order to predict partner-specific binding sites. It has been trained employing sequence-based and structural features from both protein partners of each complex compiled in the Protein–Protein Docking Benchmark version 5.0 and in an additional set independently compiled and A version taught only on sequences has been developed. The performance of our approach has been assessed by a leave-one-out cross-validation over different benchmarks, outperforming state-of-the-art methods. BIPSPI has two predict interfaces from protein structures and/or sequences. In order to get a meaningful information BIPSPI can be worked as protein–protein interfaces, especially in those cases where numerous are involved and thus, followers specificity becomes more significant. BIPSPI, a partner-specific analyst of protein amino acid residue–residue contacts and protein binding sites that uses as input either protein sequences or structures.

BIPSPI is freely available through a user-friendly web application at http://bipspi.cnb.csic.es where prediction and visualization of binding site residues can be calculate from either protein structures or sequences.

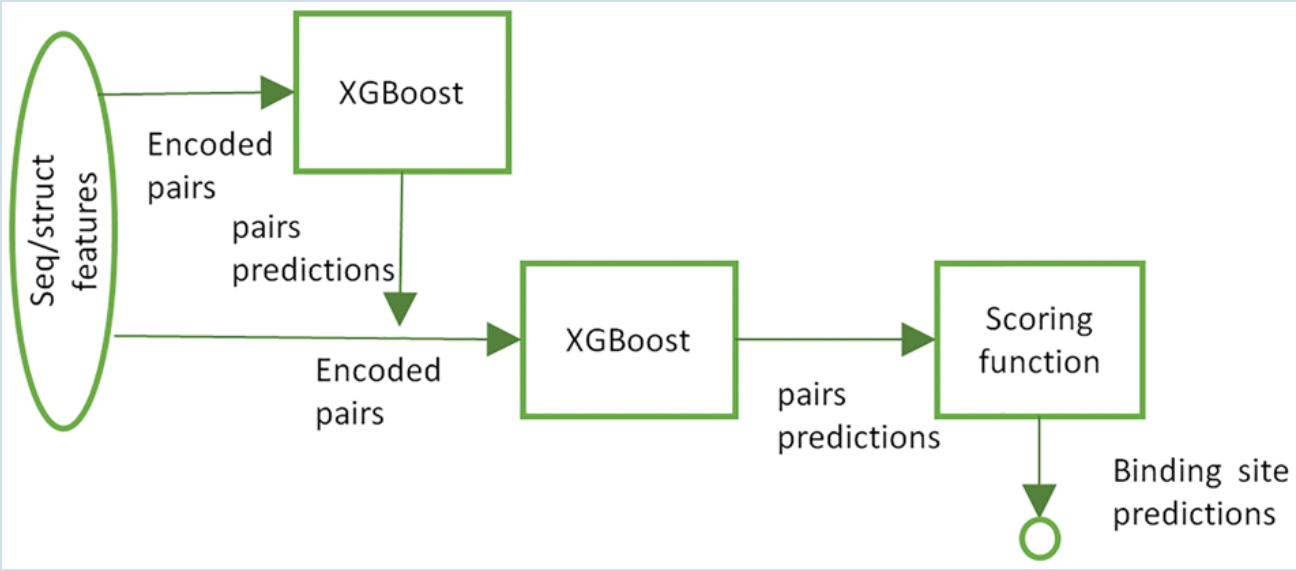


Figure: Overall Workflow of BIPSPI

Source: Ruben Sanchez-Garcia et al. J Oxfored Bioinformatics,2019

Bioinfo. Animation (Varun Chauhan *et al. J Sci. Reports.2019***)**

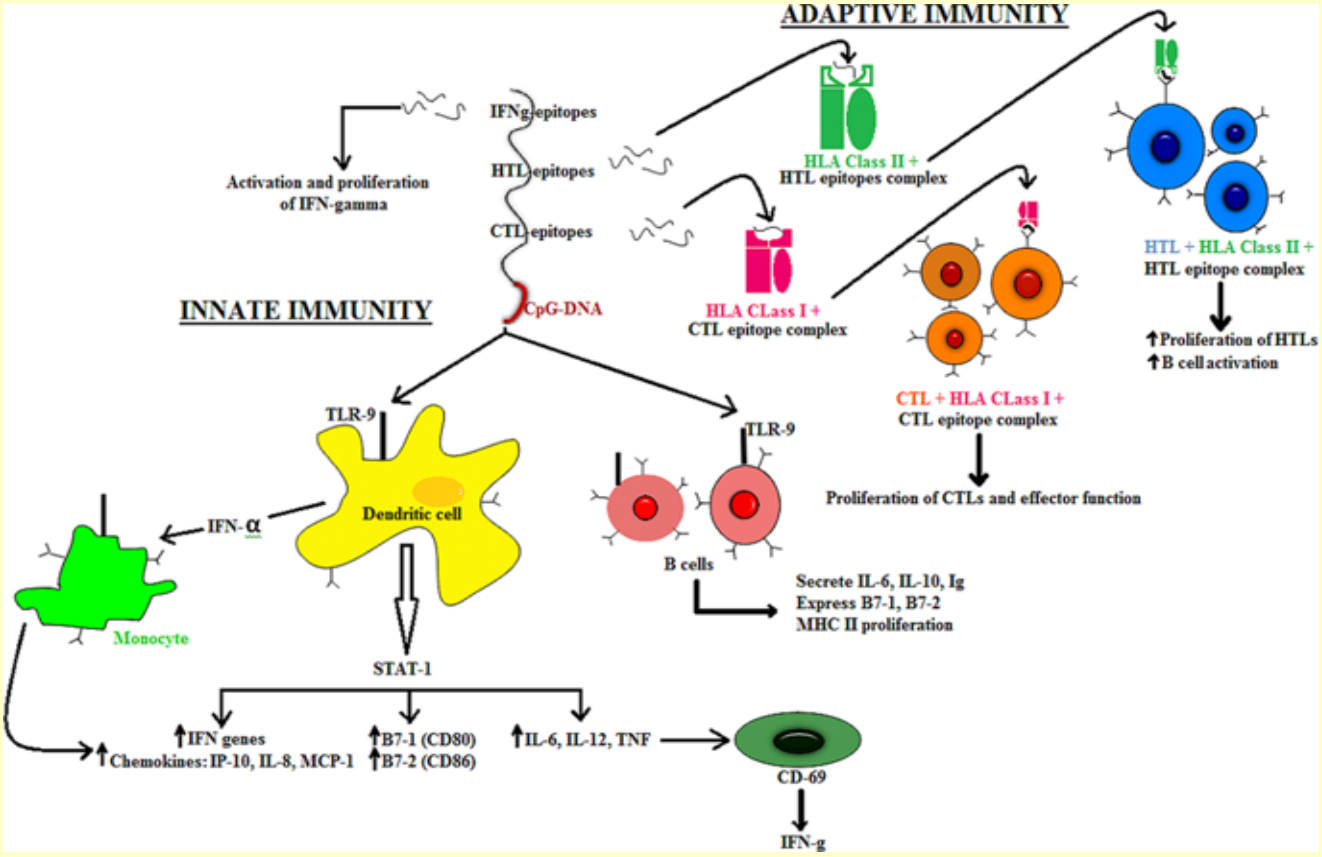


Figure: A mechanism of action of the vaccine of Kaposi's sarcoma-associated herpesvirus (KSHV)

Upcoming event

MCCMB 2019 Moscow Conference on Computational Molecular Biology 2019
27 Jul 2019 - 30 Jul 2019 • Moscow, Russia

13th International Conference on

Proteomics, Genomics and Bioinformatics

May 10-11, 2019 | Radisson Hotel Narita | Tokyo, Japan

Theme: Leading Edge Innovations in Life Sciences

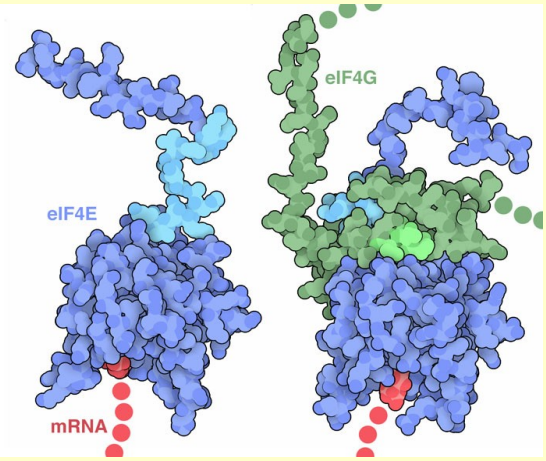
Organizing Committee | Submit Abstract | Register Now | Program Schedule | Reader Base

1. http://mccmb.belozersky.msu.ru/2019/index.html

2.https://www.proteomicsconference.com/asia-pacific/

Initiation Factor eIF4E

Initiation Factor eIF4E is a compact domain that binds to the mRNA cap, and a long, flexible tail. When eIF4E interacts with eIF4G (an initiation factor that acts as a scaffold for many other initiation factors), a portion of this tail folds up and interacts with a similarly flexible region of eIF4G.



Connection with Cancer

Cancer cells grow very rapidly, they require some way to avoid the normal cellular controls on growth. So, they do this is through oncogenic changes in the machinery that regulates protein synthesis by developing an overactive eIF4E. Medical researchers are now targeting eIF4E, developing inhibitors that can slow down the act of eIF4E and block the accelerated growth of cancer cells.

Structural biologists have been looking strongly at the binding of eIF4E and its target. The protein is stored in an inactive state with several 4E binding proteins. These proteins are released upon phosphorylation when eIF4E is needed, and eIF4G binds in the same place.

Using a similar hydrophobic motif PDB entries 1ejh and 1ej4 showed how these proteins bind to eIF4E and two later structures, PDBID 5t46 and 4ued, which observed at a big segment of eIF4G and 4E-BP factor , showing that a edge region is also important for the conditionally-ordered bindings which was shown in Figure 2. The trial anti-cancer inhibitor 4EGI-1 binds in the same location on eIF4E and blocks binding of these partners in PDBID 4tpw).In the Figure 2, the hydrophobic motif is shown in brighter magenta and green colour and the structures include only portions of each of the proteins.

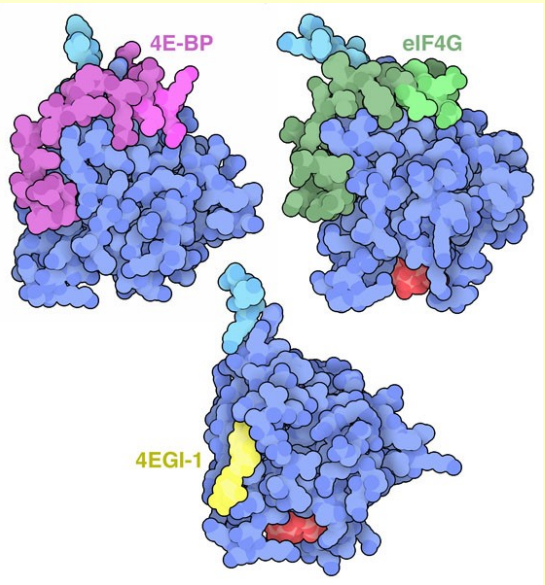


Figure 2:Complexes of eIF4E with initiation factor iEF4G, 4E binding protein, and the inhibitor 4EGI-1.

Source: http://pdb101.rcsb.org/motm/230

Kindly send us your feedback to

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