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Bioinformatics up to Date

(Bioinformatics Infrastructure Facility, Biotechnology Division)
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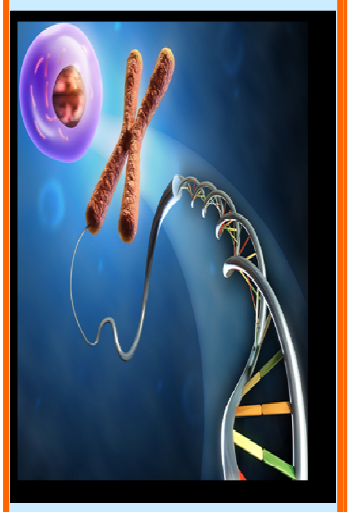
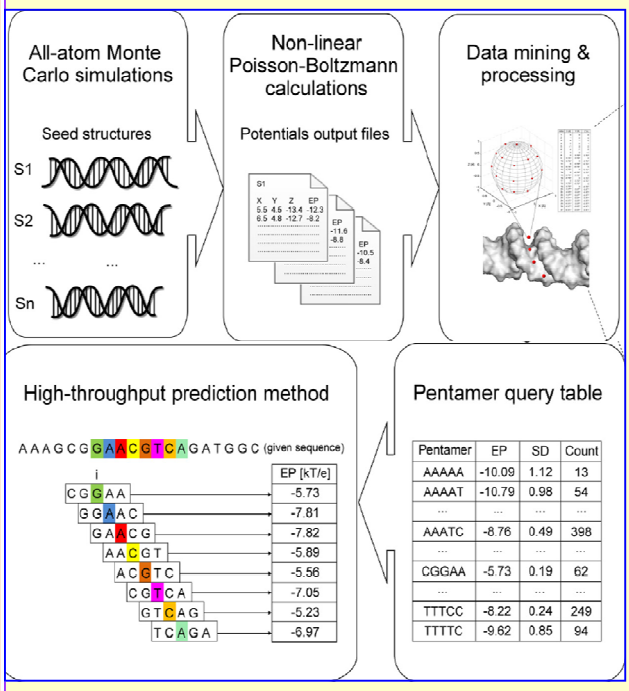
Inside…..



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.

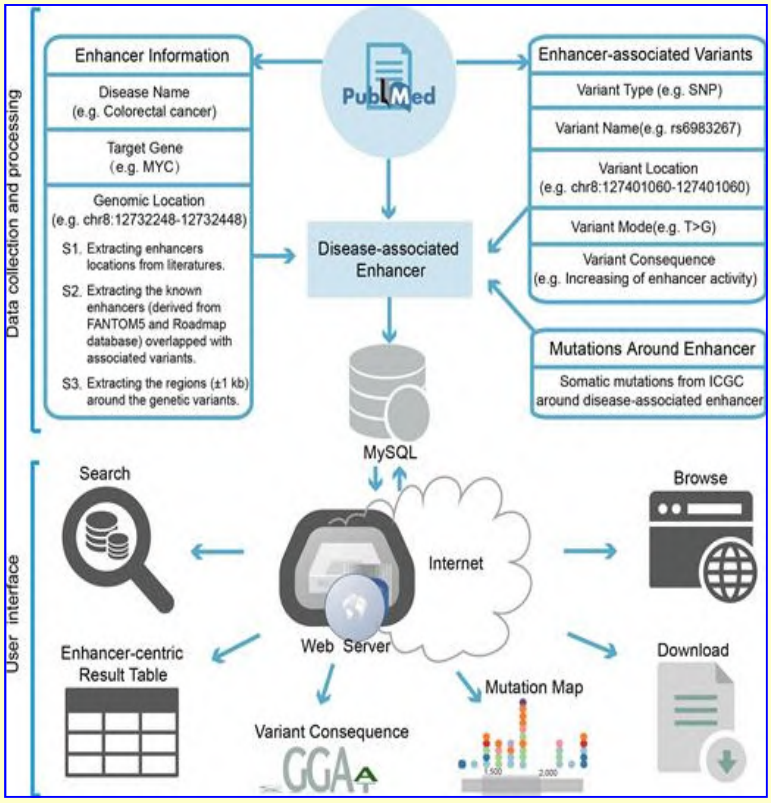
Genome-wide prediction of minor-groove electrostatic potential enables biophysical modeling of protein–DNA binding : **Protein–DNA binding is a major part of gene regulatory system, but it is still not totally understood how proteins make their target sites in the genome. Besides hydrogen bonding in the major groove (base readout), proteins make minor-groove geometry using positively charged amino acids (shape readout). The basic mechanism of DNA shape read out involves the correlation between minor-groove width and electrostatic potential (EP). In this study, researchers developed a methodology, DNAphi to study this biophysical effect directly, rather than using minor-groove width as an indirect measure for shape readout. This method is based on the data mining of results from Poisson– Boltzmann calculations on DNA structures obtained from Monte Carlo simulations. It also predicting EP in the minor groove and confirmed the direct role of EP in protein–DNA binding using massive sequencing data. They validated this approach, which only lack nucleotide sequence as input, based on direct relation with NLPB calculations for available crystal structures. Using statistical machine-learning approaches, they showed that adding EP as a biophysical feature can improve the predictive power of quantitative binding specificity models across 27 transcription factor families. High-throughput prediction of EP offers a novel way to integrate biophysical and genomic studies of protein–DNA binding. Figure shows the overview of DNAphi method.**



Source:Tsu-Pei Chiu *et al.*Oxford,2017

DiseaseEnhancer: a resource of human disease-associated enhancer catalog

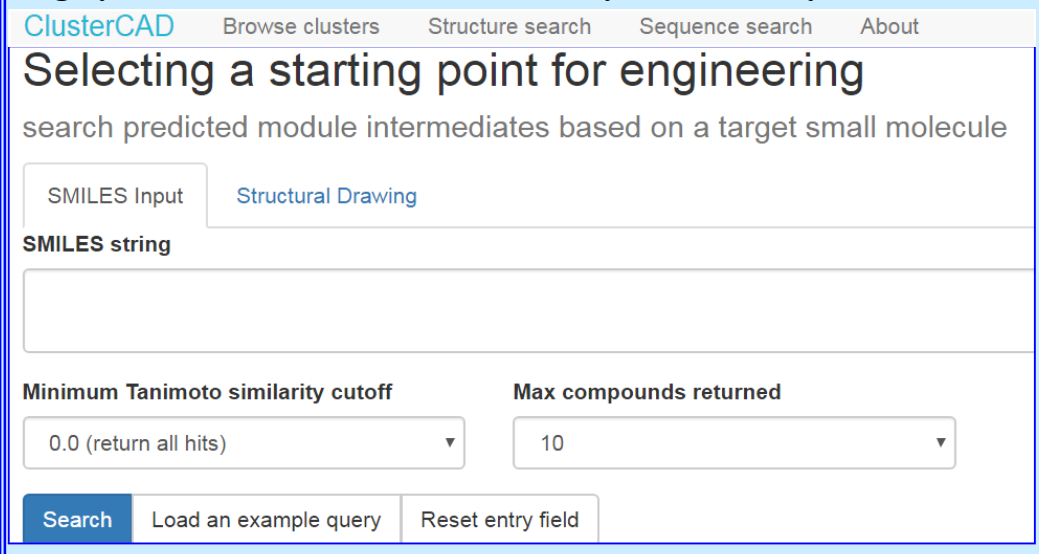
Large-scale sequencing studies discovered substantial genetic variants occurring in enhancers which regulate genes via long range chromatin interactions. Importantly, such variants could affect enhancer regulation by changing transcription factor bindings or enhancer hijacking, and in turn, make an essential contribution to disease progression. To facilitate better usage of published data and exploring enhancer deregulation in various human diseases, we created DiseaseEnhancer (http://biocc.hrbmu.edu.cn/DiseaseEnhancer/), a manually curated database for disease-associated enhancers. As of July 2017, DiseaseEnhancer includes 847 disease-associated enhancers in 143 human diseases. Database features include basic enhancer information (i.e. genomic location and target genes); disease types; associated variants on the enhancer and their mediated phenotypes (i.e. gain/loss of enhancer and the alterations of transcription factor bindings). We also include a feature on our website to export any query results into a file and download the full database. DiseaseEnhancer provides a promising avenue for researchers to facilitate the understanding of enhancer deregulation in disease pathogenesis, and identify new biomarkers for disease diagnosis and therapy.



Source:Guanxiong Zhang *et al*. J Nucleic Acids Research, 2017 doi: 10.1093/nar/gkx920

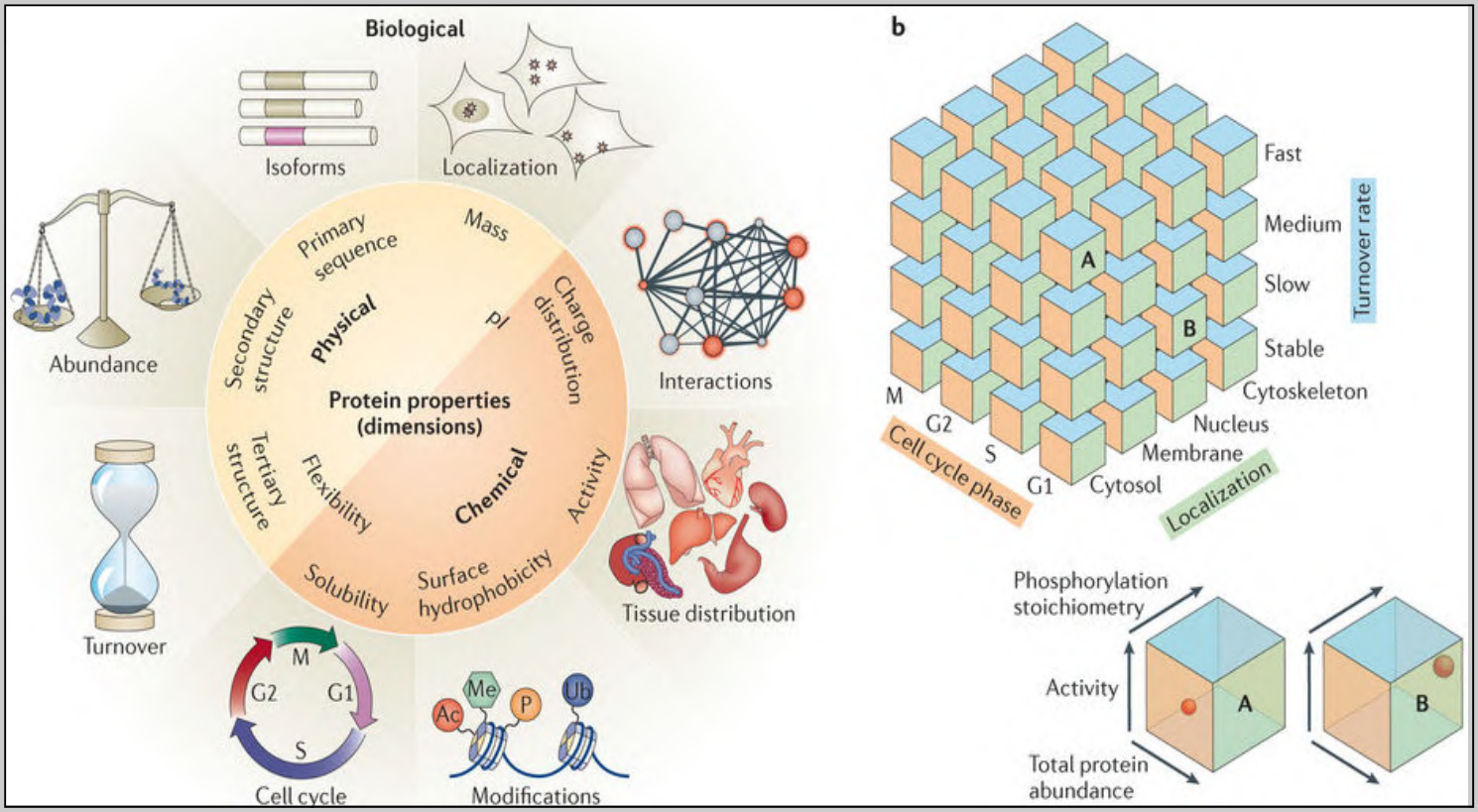
ClusterCAD: a computational platform for type I modular polyketide synthase design

ClusterCAD is a web-based toolkit designed to leverage the collinear structure and deterministic logic of type I modular polyketide synthases (PKSs) for synthetic biology applications. The unique organization of these megasynthases, combined with the diversity of their catalytic domain building blocks, has fueled an interest in harnessing the biosynthetic potential of PKSs for the microbial production of both novel natural product analogs and industrially relevant small molecules. However, a limited theoretical understanding of the determinants of PKS fold and function poses a substantial barrier to the design of active variants, and identifying strategies to reliably construct functional PKS chimeras remains an active area of research. In this work, we formalize a paradigm for the design of PKS chimeras and introduce ClusterCAD as a computational platform to streamline and simplify the process of designing experiments to test strategies for engineering PKS variants. ClusterCAD provides chemical structures with stereochemistry for the intermediates generated by each PKS module, as well as sequence- and structure-based search tools that allow users to identify modules based either on amino acid sequence or on the chemical structure of the cognate polyketide intermediate. ClusterCAD can be accessed at https://clustercad.jbei.org and at http: //clustercad.igb.uci.edu.



Source: Clara H. Eng *et al.* Nucleic acids Research 2017

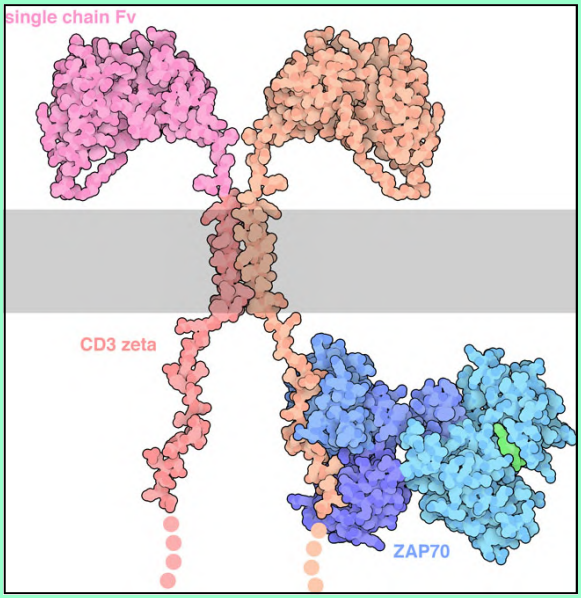
Multidimensional proteomics for cell biology



Source: Nature riview

Chimeric Antigen Receptors

Chimeric antigen receptors are built by connecting several functional parts from different proteins, each with a specific job. A single-chain antibody variable fragment (Fv) recognizes a known cancer cell protein, targeting the tumor. These are generally engineered from monoclonal antibodies by using only the domains at the tip of the antibody, and connecting the two chains with a flexible linker. The antibody portion is connected to a transmembrane segment with another flexible linker. Inside the cell, one or more domains are taken from signaling proteins, which will activate the T cell once it finds a tumor cell.



T cells have the ability to recognize virus-infected cells using T-cell receptors and then destroy them. Unfortunately T cells are not as effective against cancer cells, because the molecules on the surface of cancer cells often look much like the molecules on normal cells. Chimeric antigen receptors (CAR) are a way for doctors to arm T cells with the ability to recognize cancer cells. Researchers remove T cells from a cancer patient and add a gene for a CAR that recognizes their form of cancer. When these "CART" cells are returned to the patient, they search for cancer cells and destroy them.

Source : http://pdb101.rcsb.org/motm/214

Patents

Allergen for selective quantitative detection methods and systems translated from Chinese

CN 106796242 A

Inventors: T. J. Oman, B.W Sheffer, R.C. Hill, G. Single

Abstract

The present invention relates to a method and system by means of bioinformatics to identify candidate features peptides for analysis by mass spectrometry of the plant, plant part, and / or a complex protein sample was quantified from the food product multiplexing. Providing a candidate features and the use of a peptide selected bioinformatics tools for quantification. Also it provides a system comprising chromatography and mass spectrometry for peptides using the selected feature.

Kindly send us your feedback to

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