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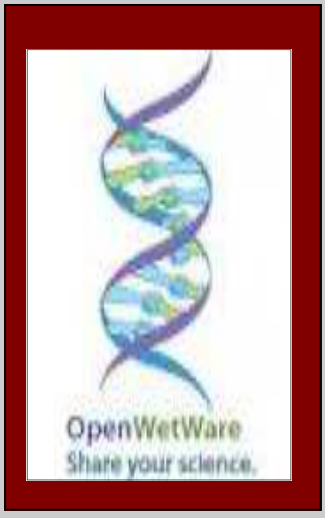
Bioinformatics up to Date

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

Inside…..

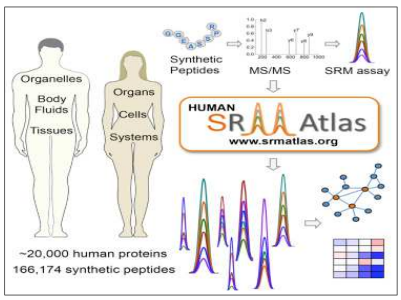


About us

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.

Quantitating the complete human proteome

Research Scientist Dr. Ulrike Kusebauch from the Institute for Systems Biology (ISB), describes the development of the Human SRMAtlas, a compendium of proteomic assays for any human protein. The work completed with the results of a collaboration between scientists at ISB, ETH Zurich and a number of other contributing institutes. The work published in the journal *Cell*, July 2016.



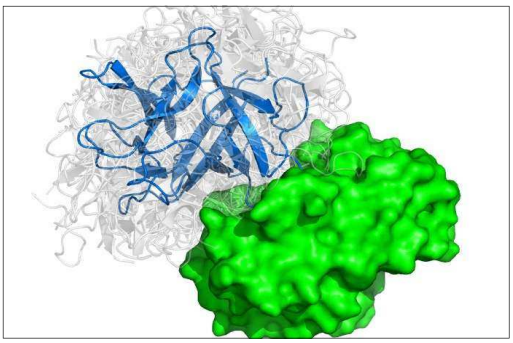
The Human SRMAtlas is a compendium of highly specific mass spectrometry assays for the targeted identification and reproducible quantification of any protein in the predicted human proteome, including assays for many spliced variants, non-synonymous mutations and post-translational modifications. The SRMAtlas resource is freely publicly available at http://www.srmatlas.org and will equally benefit focused, hypothesis-driven and large proteome-scale studies.

Professor Robert Moritz of ISB, a collaborative effort enabled the generation and verification of a compendium of highly specific targeted proteomic assays by the method called selected reaction monitoring, or SRM for short, now provides quantification of 99.7% of the 20,277 annotated human proteins by the widely accessible, sensitive and robust targeted mass spectrometric method selected reaction monitoring, SRM. This Human SRMAtlas provides definitive assay coordinates that conclusively identify the respective peptide in biological samples.

[Human SRMAtlas: A Resource of Targeted Assays to Quantify the Complete Human Proteome, Cell , Volume 166 , Issue 3 , 766 - 778]

New method to model protein interactions may accelerate drug development

A research team from MIPT, Stony Brook University and other scientific research center have developed a computer algorithm to predict the structure of protein complexes in a cell 10 times faster than before. The study has been published in Proceedings of the National Academy of Sciences of the USA.



According to Dima Kozakov, a professor at Stony Brook and adjunct professor at MIPT, the new method enables us to model the interaction of proteins at genome level. This will give us a better understanding of how our cells function and may enable drug development for diseases caused by "incorrect" protein interactions.

The idea behind the algorithm was to present the proteins as a combination of "quantum surfaces" - certain blocks described by the mathematical tool of quantum mechanics. Using this approach, it is possible to simultaneously calculate the interaction between multiple pairs of protein clusters, rather than examining each pair independently. The new method is up to 100 times faster than the best methods used previously, and it is still accurate. According to the scientists, the program takes 15 minutes to run on a personal computer and is a good alternative to experimental methods of determining protein interactions.

The new algorithm will soon be available to the scientific community through the publicly available protein-protein docking server called ClusPro. This resource, with more than 15000 academic users worldwide, supported by the National Science Foundation and the Binational Science Foundation, is being developed by the same research team at the Laufer Center and IACS, in collaboration with scientists at Boston University.

[source: www.pnas.org/cgi/doi/10.1073/pnas.1603929113]

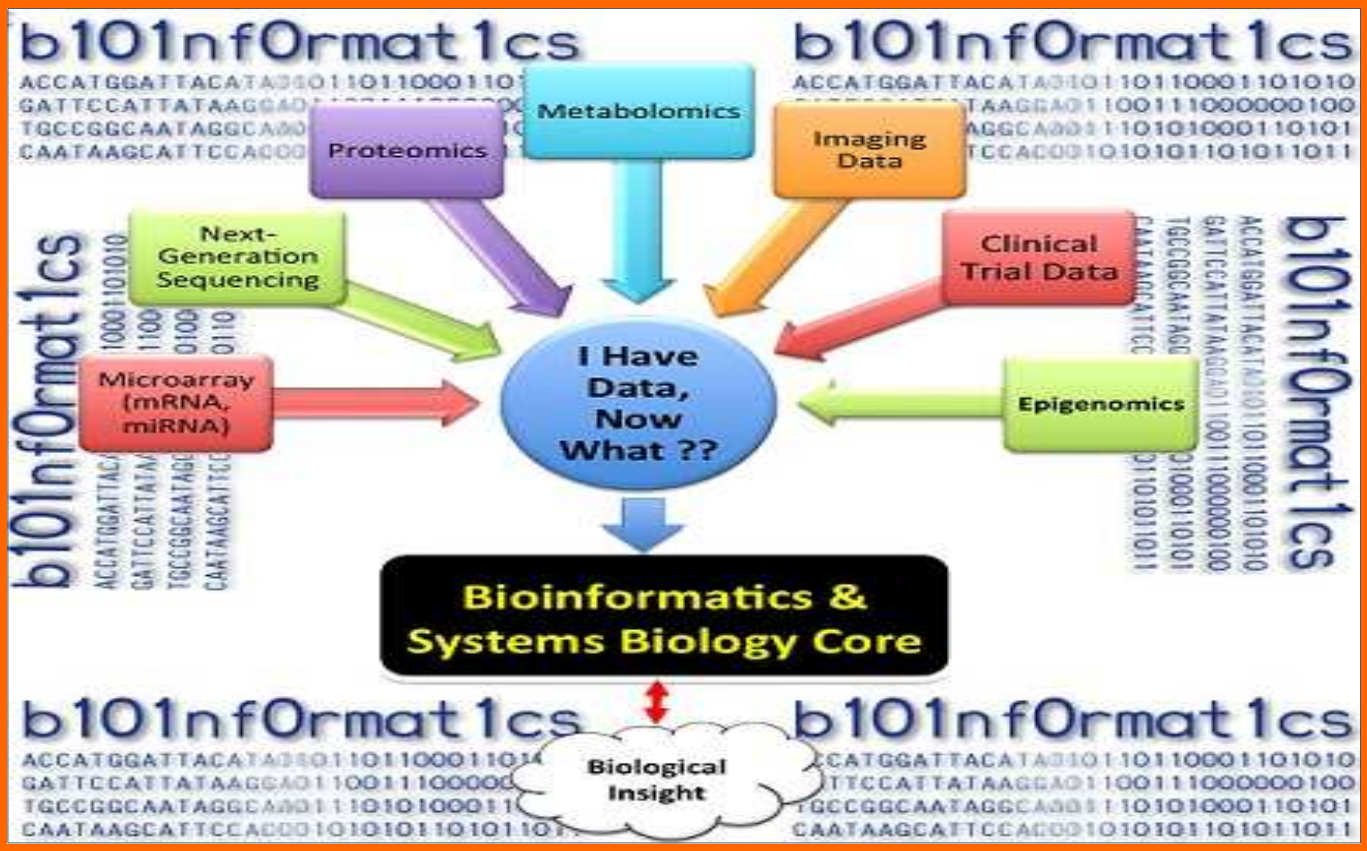
SinEx DB: a database for single exon coding sequences in mammalian genomes

A group of researchers of University of Andres Bello , Chile Has developed a database consisting data of single exon coding sequences in mammalian genomes. Eukaryotic genes are typically interrupted by intragenic, noncoding sequences called introns. However, some genes lack introns in their coding sequence (CDS) and are generally known as ‘single exon genes’ (SEGs). In their work, a SEG is been defined as a nuclear, protein-coding gene that lacks introns in its CDS. Whereas, many public databases of Eukaryotic multi-exon genes are available, there are only two specialized databases for SEGs. The present work addresses the need for a more extensive and diverse database by creating SinEx DB, a publicly available, searchable database of predicted SEGs from 10 completely sequenced mammalian genomes including human.

SinEx DB houses the DNA and protein sequence information of these SEGs and includes their functional predictions (KOG) and the relative distribution of these functions within species. The information is stored in a relational database built with My SQL Server 5.1.33 and the complete dataset of SEG sequences and their functional predictions are available for downloading. SinEx DB can be interrogated by: (i) a browsable phylogenetic schema, (ii) carrying out BLAST searches to the in-house SinEx DB of SEGs and (iii) via an advanced search mode in which the database can be searched by key words and any combination of searches by species and predicted functions. SinEx DB provides a rich source of information for advancing our understanding of the evolution and function of SEGs.

[Source: Jorquera R. et al.; Database (June 7,2016)]

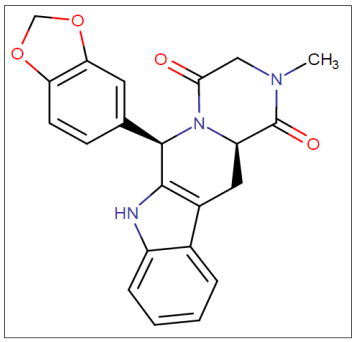
Bioinfo. Animation



Molecule of month

Tadalafil

Tadalafil is a carboline derivative and PHOSPHODIESTERASE 5 INHIBITOR that is used primarily to treat EREC-TILE DYSFUNCTION; BENIGN PROSTATIC HYPERPLASIA and PRIMARY PULMONARY HYPERTENSION. Tadala-



fil is a carboline-based compound with vasodilatory activity. Tadalafil selectively inhibits the cyclic guanosine monophosphate (cGMP)-specific type 5 phosphodiesterase- (PDE-5)-mediated degradation of cGMP, which is found in the smooth muscle of the corpus cavernosa and corpus spongiosum of the penis. Inhibition of cGMP degradation by tadalafil results in prolonged mus-cle relaxation, vasodilation, and blood engorgement of the corpus cavernosa, and, so, prolonged penile erection.

Tadalafil is an orally adminstered drug used to treat male erectile dysfunction (impotence). It is marketed worldwide under the brand name Cialis. It is a phosphodiesterase 5 (PDE5) inhibitor. Tadalafil's distinguishing phar-macologic feature is its longer half-life (17.5 hours) compared with Viagra and Levitra (4-5 hours). This longer half-life results in a longer duration of action and is, in part, responsible for the Cialis nickname of the "weekend pill." This longer half-life also is the basis of current investigation for tadalafil's use in pulmonary arterial hypertension as a once-daily therapy.

[Source: http://www.drugbank.ca/drugs/DB00820]

Upcoming events

Patents

Proteomic analysis

US6872574B2

Inventor: Benjamin F. Cravatt etal.

Abstract

The present invention provides methods for analyzing proteomes, as cells or lysates. The analysis is based on the use of probes that have specificity to the active form of proteins, particularly enzymes and receptors. The probes can be identified in different ways. In accordance with the present invention, a method is provided for generating and screening compound libraries that are used for the identification of lead molecules, and for the parallel identification of their biological targets. By appending specific functionalities and/or groups to one or more binding moieties, the reactive functionalities gain binding affinity and specificity for particular proteins and classes of proteins. Such libraries of candidate compounds, referred to herein as activity-based probes, or ABPs, are used to screen for one or more desired biological activities or target proteins.

Kindly send us your feedback to

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