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Bioinformatics up to Date

(Bioinformatics Infrastructure Facility, Biotechnology Division)
North-East Institute of Science & Technology
Jorhat -785006, 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.

Artificial Intelligence in Drug Discovery and Development

With the rapid and successful transferring of Artificial Intelligence (AI) technology in diverse fields of research and development, the pharmaceutical industry is also stepping towards this area by focussing the previously segregated data sources, recruiting data scientist and infrastructures. The applications of AI in drug discovery are very vast and can be categorized into knowledge discovery and hypothesis generation, target identification, drug development, virtual screening, ADMET screening, personalized medicine, etc. Scientists are still working on algorithms and applications of different AI platforms which can be adopted in system biology, pharmacogenomics, network pharmacology, molecular design and generation, big data analysis for drug information. In April, a study with BenevolentAI's platform on the action against Acute Macular Degeneration (AMD) identified seven existing drugs that could be repurposed for AMD. Although much advancement in AI technology is required for drug discovery, AI applications on imaging diagnostics such as AI-based diagnostics for stroke, wrist fractures and diabetic retinopathy which are already approved by the US Food and Drug Administration.

Figure: AI in drug discovery

Source: Nature Biotechnology | VOL 37 | JUNE 2019 | 573–580 ,

PhenoScanner V2: A Human Genotype-Phenotype Relationships Database

It is a well known fact that genetic variations is a major cause of phenotypic differences between individuals. Relationships between genotypic variations and phenotypes have been widely identified through many approaches such as genome-wide association studies (GWAS). To overcome the challenge now facing in understanding the underlying mechanisms of genotype-phenotype associations and scanning of "Phenome", Mihir A Kamat, et al., 2019 of Cambridge University updated the tool "PhenoScanner" formerly developed by Staley, et al., 2016. PhenoScanner is an open curated database results from large-scale genetic association studies in humans. This online tool facilitates "phenome scans", where genetic variants are cross-referenced for association with many phenotypes of different types. PhenoScanner V2 contains over 150 million genetic variants and more than 65 billion associations with diseases and traits, gene expression, metabolite and protein levels, and epigenetic markers. The query options include searches by genes, genomic regions and phenotypes, as well as for genetic variants. All variants are positionally annotated using the Variant Effect Predictor and the phenotypes are mapped to Experimental Factor Ontology terms. Linkage disequilibrium statistics from the 1000 Genomes project can be used to search for phenotype associations with proxy variants. The database is available at www.phenoscanner.medschl.cam.ac.uk.Figure shows the front view of PhenoScanner database.

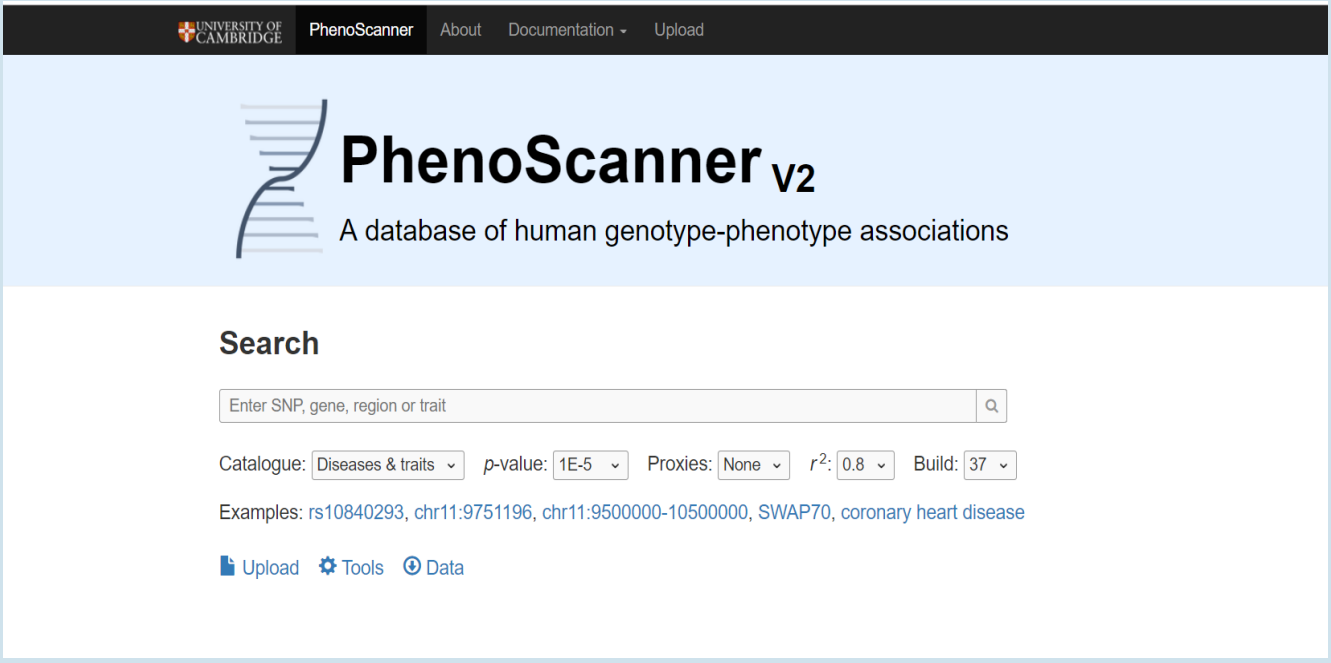


Figure: The front view of PhenoScanner data-

Source: Mihir A Kamat *et al. J Oxford Bioinformatics, 2019,*

Bioinformatics Animation

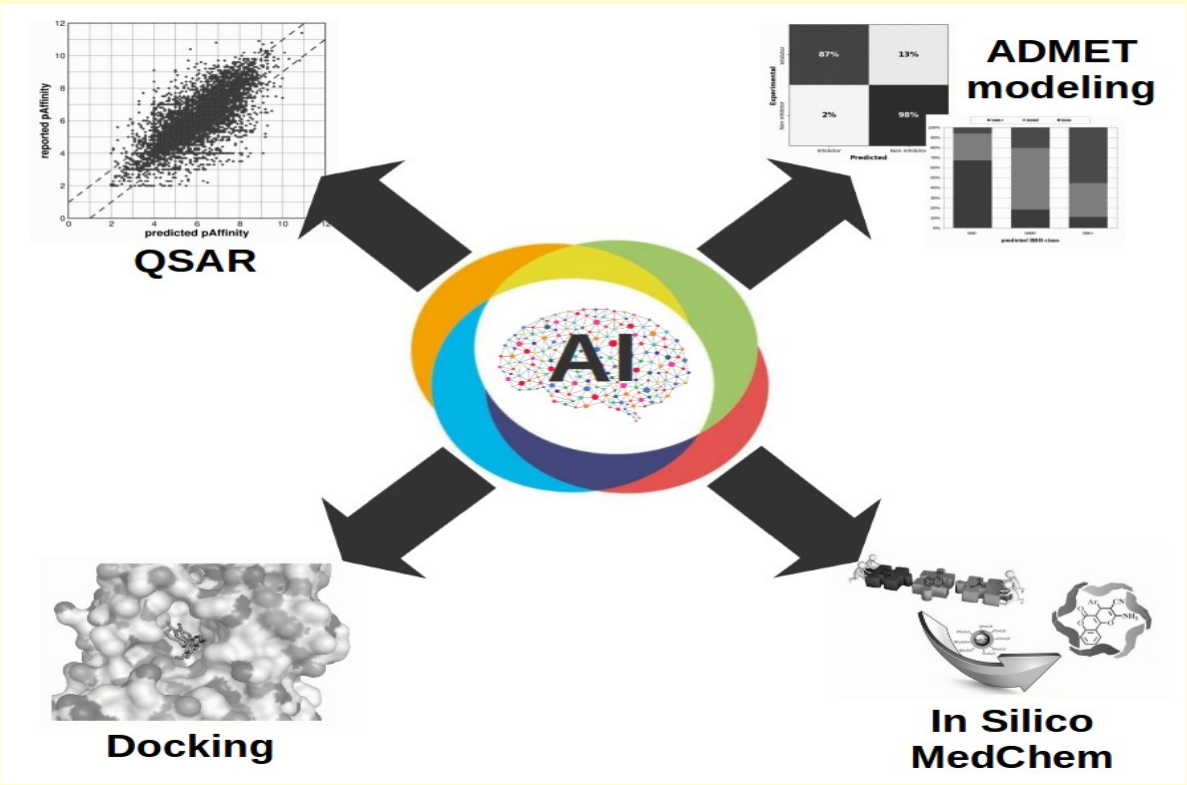
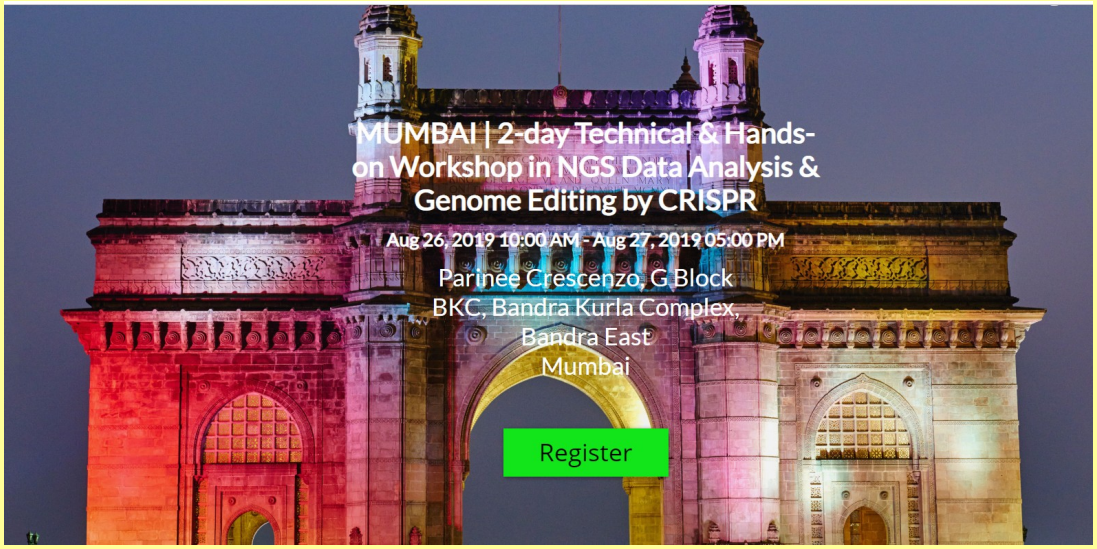


Figure: AI in drug discovery

Upcoming Events



https://in.explara.com/e/ngs-data-analysis-genome-editing-crispr-mumbai
http://www2.ff.ul.pt/pselisbonmeeting2019/

Molecule of the month

MDM2 and Cancer

P53 tumor suppressor inside our cells checks for damage, infection, and cancer like a guardian. It stops cell growth or trigger cellular self -destruction of any infected cells. P53 tumor suppressor is however closely regulated by MDM2 and its partner MDMX. They regulate the functions of p53 so that it carries out its actions only when absolutely required.

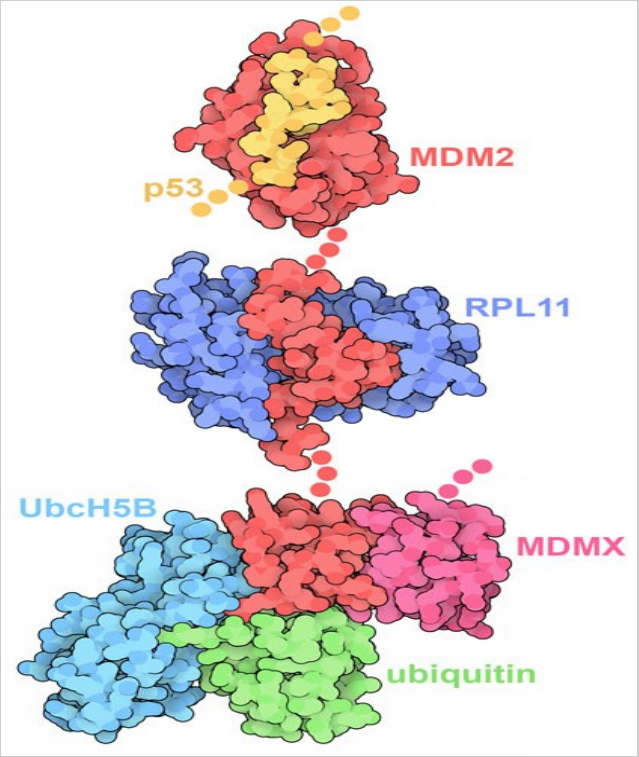


Figure: Binding and regulation of p53 tumor suppressor (yellow) by multiple domains of MDM2 (red).

MDM2 as a guardian of p53

MDM2 has several connected domains which bind to p53 most of the time. The N-terminal domain of MDM2 binds to the transactivation domain of p53 and blocks its signalling action. Central Zn-finger domain having nuclear export signal binds to ribosome proteins, removing p53 from the nucleus and releases into the cytoplasm. The C-terminal domain of MDM2 and MDMX in the cytoplasm add ubiquitin to p53 for proteasomal degradation.

Cancer Connection

Optimum MDM2 is synthesized to regulate p53 in the cells. It is inactivated and released from binding when there is cell damage or infection so that p53 can check and control the problem. However, cancer cells often have multiple gene copies encoding MDM2. Excess MDM2 proteins constitutively bind p53 and block the functions, enabling the cancer cells to grow unchecked.

MDM2 inhibitors

Cancer chemotherapy targets the interaction between MDM2 and p53. The chemotherapy breaks the interaction and activate p53 to destroy the cancer cells. Several effective inhibitors of MDM2 have been discovered. These include small molecule Nutlin (PDB entry 1rv1) and SAH-p53-8, a small peptide taken from p53 and stapled in the proper conformation by a linker (PDB entry 3v3b) .

Source: http://pdb101.rcsb.org/motm/234

Dr Ratul Saikia
BIF Center, Biotechnology Group, BSTD
CSIR-North East Institute of Science and Technology, Jorhat, Assam
E-mail: rsaikia19@gmail.com

Dr Yumnam Silla Devi
BIF Center, Biotechnology Group, BSTD
CSIR-North East Institute of Science and Technology, Jorhat, Assam
E-mail: *bio.sillayumnam@gmail.com*

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