

Bioinformatics up to Date

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COVER STORY



The CSIR-North East Institute of Science & Technology, Jorhat, signed bilateral MoU with Agricultural Research & Development Agency (ARDA), Thailand, on 23 June, 2011. In this regard, a team of four members visited the Institute for around fifteen days. The team had a four day training programme in Bioinformatics at the BIF Centre, NEIST. Along with them, two Nigerian and one Egyptian were also included who are doing a part of their PhD in NEIST. Total of the seven participants, they had training on : Molecular Biology, Basic Bioinformatics, Sequence Alignment, Multiple Sequence Alignment, Molecular Phylogenetics, Methods in Molecular Phylogenetics, Application of Bioinformatics in agriculture, Introduction to docking, Database creation and management. The training included both theory as well as practical sessions. The training was fully conducted by the BIF Centre. On the last day Dr. Madhumita Barua, Associate Professor, Dept. of Agri Biotechnology, Assam Agriculture University was invited for a detailed lecture on Bioinformatics in Agriculture. The BIF Centre presented “*japi*” to the guests from Thailand as a token of Assamese culture as well as love, respect and affection.

BIOINFY QUIZ

- Ultimately, whole genomes are involved in processes of hybridization, polyploidization and _____, often leading to rapid speciation
 A) DNA
 B) Bacteria
 C) Endosymbiont
- (Of course, there are exceptions, such as the bovine spongiform encephalopathy - aka _____ - prion.) Knowledge of this structure is vital in understanding the function of the protein :
 A) Bovine spongiform encephalopathy
 B) Canada
 C) United States
- Modern image analysis systems augment an observer's ability to make measurements from a large or complex set of images, by improving _____, objectivity, or speed
 A) Experiment
 B). Accuracy and precision
 C) Statistics
- In the context of _____, annotation is the process of marking the genes and other biological features in a DNA sequence.
 A) Genomics
 B) Genetics
 C) Bioinformatics
- more recently, compare entire _____, which permits the study of more complex evolutionary events, such as gene duplication, horizontal gene transfer, and the prediction of factors important in bacterial speciation.
 A) Genomics
 B) Genetics
 C) Genome

Answers on page 5

COMPUTATIONAL CHEMISTRY

Adun

A multipurpose high performance production molecular simulator

Adun is a free biomolecular simulator developed at the Computational Biophysics and Biochemistry Laboratory, a part of the Research Unit on Biomedical Informatics of the UPF. It is distributed under the GNU General Public License.

A fundamental goal of the project is to provide a **complete set of API's** for use in developing programs and features related to **molecular simulation**.

The API's are designed to support scientific objective of free-energy calculations using flexible, multi-representation, force-field agnostic simulations and to aid in the rapid development and distribution of new simulation methods. They are crucial as they are used to achieve our Scientific and User Productivity objectives.

PROTEOMICS

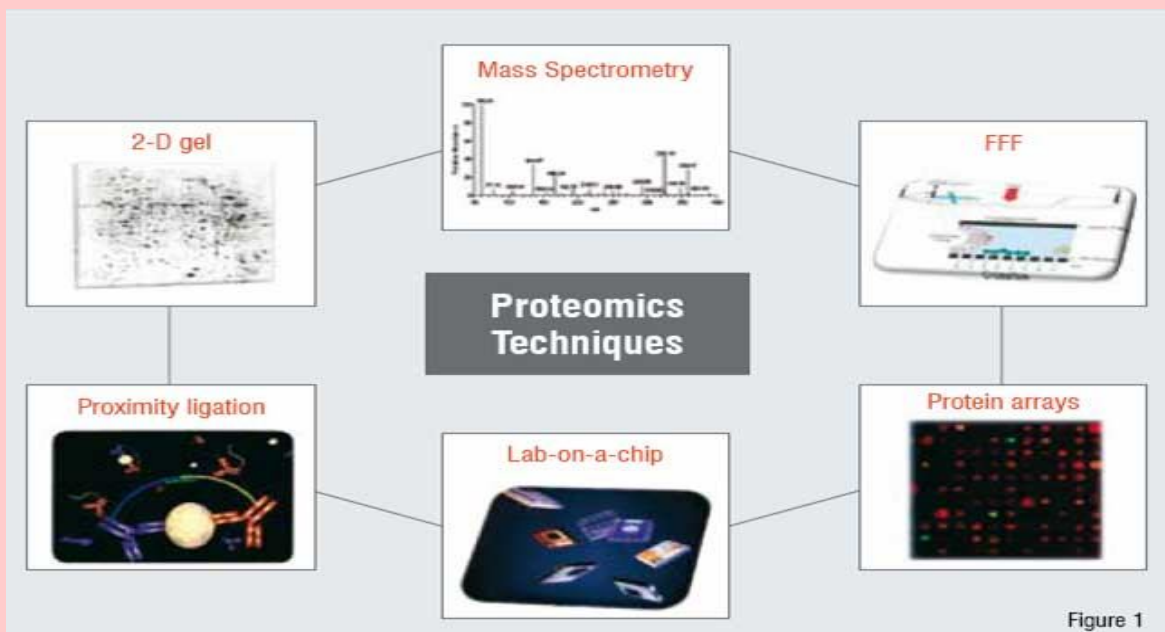


Figure 1

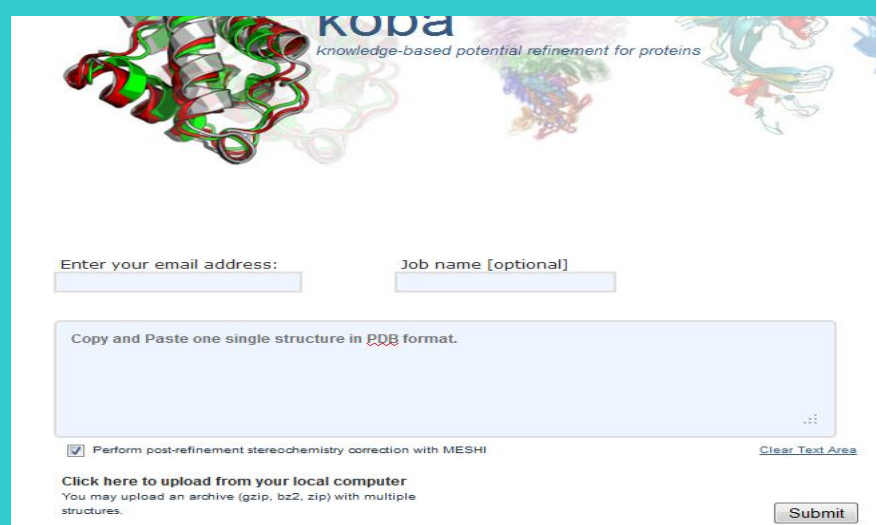
BIOSERVER

[KobaMIN Refinement Server](#)

koba^{MIN} makes available a very fast protein structure refinement protocol.

1. Paste one PDB file or upload a PDB file or an archive containing multiple structures.
2. Uncheck the MESH1 box for no stereochemistry correction.
3. Optionally, upload one reference structure for comparative GDT-HA, GDT-TS, and cRMS calculations.

You will be emailed a link to your results when your job is finished.



Enter your email address: Job name [optional]

Copy and Paste one single structure in PDB format.

Perform post-refinement stereochemistry correction with MESH1 [Clear Text Area](#)

[Click here to upload from your local computer](#)
You may upload an archive (gzip, bz2, zip) with multiple structures.

COMPUTERS FOR BIOLOGISTS

APOD

Abbreviated Profile of drugs

Abbreviated Profile of Drugs (APOD) is a decision and prediction method for drug discovery. It is simple, instantaneous, and empowering.

The salient features of APOD are:

- A unique way of representing the compound properties
- A computer friendly numerical string representation making comparison of any properties possible
- A graphical representation that gives a snapshot of properties and their relative changes, And.

Its importance in prediction of absorption, distribution, metabolism, excretion, and toxicity (ADMET) characteristics of a compound, based on a few chemical properties alone, directly into the APOD representation.

GENOMICS

MIDAS – Multiallelic Interallelic Disequilibrium Analysis software

MIDAS – Multiallelic Interallelic Disequilibrium Analysis Software) for the estimation and graphical display of interallelic linkage disequilibrium. Linkage disequilibrium is analysed for each allelic combination (of one allele from each of two loci), between all pairwise combinations of any type of multiallelic loci in a contig (or any set) of many loci (including single nucleotide polymorphisms, microsatellites, minisatellites and haplotypes). Data are presented graphically in a novel and informative way, and can also be exported in tabular form for other analyses. This approach facilitates visualisation of patterns of linkage disequilibrium across genomic regions, analysis of the relationships between different alleles of multiallelic markers and inferences about patterns of evolution and selection.

MIDAS was written in the Python programming language v2.4, using the Tkinter module for generating a graphical user interface (GUI). The Tkinter "Canvas" widget was used for plotting of graphical data, whilst other Tkinter widgets were used for create

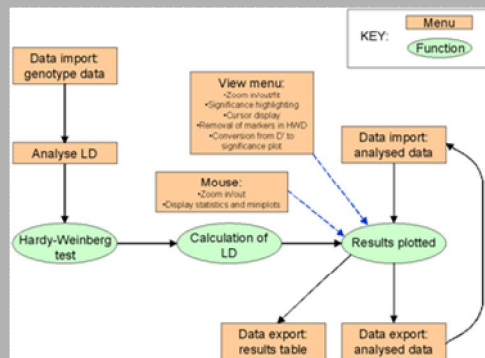


Fig: Flow-chart of MIDAS from the user's perspective. Rectangles indicate user inputs, ovals indicate program functions. Lines indicate the flow of data and control between components of the interface.

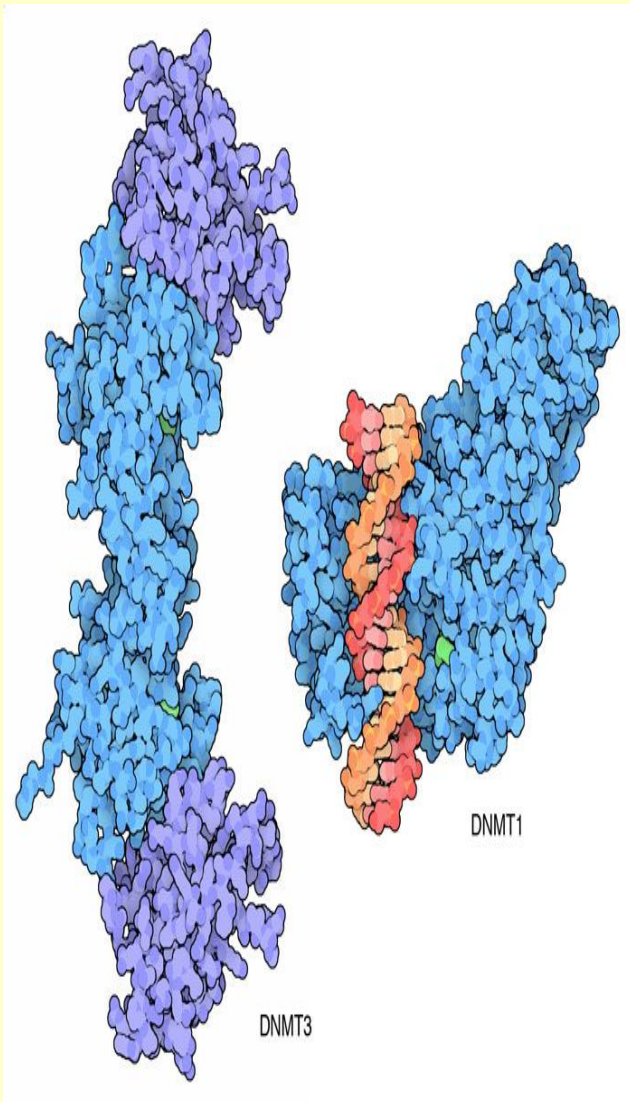
UPCOMING EVENTS

Conference

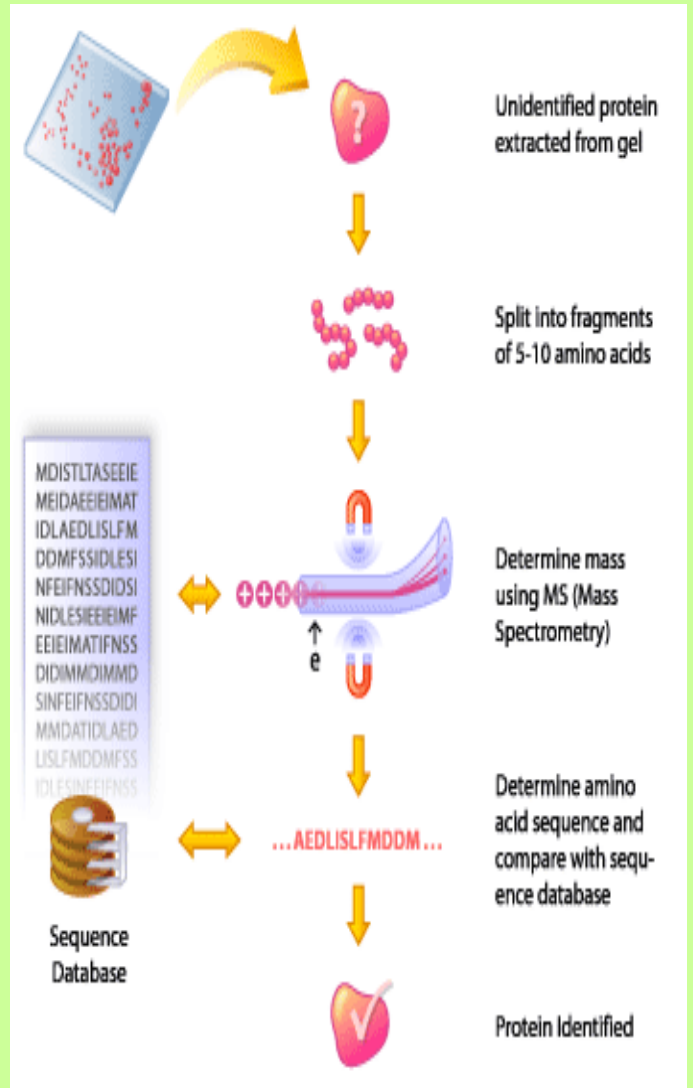
2011 International Conference on Computer Engineering and Bioinformatics, ICCEB 2011, Cairo, Egypt. October 21-23, 2011

About 10 selected papers from the registered ones, will be published in the International Journal of Bioinformatics and Biomedical Technology (IJBBT) free of charge.

MOLECULE OF THE MONTH DNA Methyl transferases



Identification of unknown protein



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Answers of Bioinfy Quiz

1) C 2)A 3)B 4)A 5)C