



# Bioinformatics up to Date

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

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## COVER STORY

### International Symposium on Frontier Areas organized at CSIR-NEIST on 6th-7th September 2011

The International Symposium on Frontier Areas (ISOFA-II) was held at CSIR- North East Institute of Science & Technology, Jorhat on 6th September 2011 with a day long program as part of the Golden Jubilee Celebrations. The inaugural function was held in the morning hours where the Chief Guest, Dr. K. M. Bujarbaruah, Vice Chancellor of Assam Agricultural University (AAU), Jorhat delivered the inaugural speech in presence of the plenary speakers from China, Canada, Thailand, India ,scientific community of CSIR- NEIST, special invitees from colleges and other research institutions, representatives from ARDA, Thailand and students of the laboratory present in large number. **Dr. P. G. Rao, Director of CSIR- NEIST, Jorhat delivering the welcome address** said that ISOFA -II as part of the Golden Jubilee Celebrations is organized as a retrospect or review of the past and planning for the future programs for the 12th Five Year Plan, as the 11th Five Year Plan concludes this financial year. He added that CSIR- NEIST (formerly RRL), Jorhat was established in 1961 as one of the multidisciplinary laboratories of Council of Scientific & Industrial Research (CSIR) under its Chemical Science Group of laboratories. The major thrust of R&D activities has been to develop indigenous technologies by utilizing the vast natural resources of North Eastern Region of India. The laboratory was targeted to undertake research for development of know-how for a wide a range of industrial and rural development works. Over the years, the laboratory has generated more than 100 technologies in the areas of Agrotechnology, Biological and Oil Field Chemicals of which about 40% were of commercial success in setting up of various industries through out the country. The Vertical Shaft Kiln Cement plant of CSIR- NEIST technology is still working even after more than 40 years. The agro-technologies for important medicinal and aromatic plants has resulted in extensive cultivation of citronella grass and extraction of oil have led to the establishment of major citronella based agro- industries in the North-Eastern region and this has generated employment for 22,000 persons in the rural sector alone. The annual turn over of the products produced with CSIR- NEIST (RRL) technologies within the country is estimated to be Rs. 110 crores.

## BIOINFY QUIZ

1.Which of the following is the character based method? Intron  
A) UPGMA method  
B) Maximum Parsimony method  
C) Maximum Likelihood method

2.How many types of substitution possible?  
A) 4  
B) 5  
C) 6

3.Which of the following model account for nucleotide substitutions?

- A) Jukes-Cantor model  
B) Kimura's model  
C) Complex model

4. How many parameters are considered in Jukes-Cantor model?

- A) 1  
B) 2  
C) 4

How many parameters are considered in Kimura's model?

- A) 1  
B) 2  
C) 4

Answers on page 5

## COMPUTATIONAL CHEMISTRY

### DOCK Bl aster

DOCK Blaster is provided by the Shoichet Laboratory in the Department of Pharmaceutical Chemistry at the University of California, San Francisco (UCSF). DOCK Blaster is composed of an expert system engine and a web-enabled user interface. The docking program used is DOCK 3.5.54,(28, 29) a version of UCSF DOCK. The DOCK Blaster pipeline is composed of six modules: (a) the parser, which identifies the receptor and ligand from a PDB file, (b) the scrutinizer, which attempts to correct for problems, such as incomplete or disordered residues on the receptor, (c) the preparer, which protonates the receptor, calculates “hot spots” and scoring grids, assigns atomic parameters, including these for cofactors, post-translational modifications and metals, and prepares the ligand, decoys, and any actives and inactives for docking, (d) the calibrator, which uses supplied data to assess docking performance and suggests optimal docking parameters, (e) the docker, which manages a full database screen on the computer cluster, and (f) the assessor, which prepares reports to interpret database screening results.

## PROTEOMICS

### How Proteins tal k to each other

Proteins perform distinct and very well-defined tasks, but little is known about how interactions among them are structured at the cellular level. Now, two physicists reveal that — at least in yeast cells — these interactions are not random, but well organized. This result is published in the May 3, 2002 issue of *Science*.

Although scientists understand how a given protein interacts with other proteins, the way they connect with each other as a whole remains mysterious,” says Sergei Maslov, a physicist at the U.S. Department of Energy’s Brookhaven National Laboratory, one of the study’s two authors.

For the last 10 years, Maslov, an expert in statistical physics, has been studying complex systems such as collections of particles, proteins, and networked computers. In the new study, Maslov and physicist Kim Sneppen of the Norwegian University of Science and Technology used computer modeling to look at how proteins interact with each other.

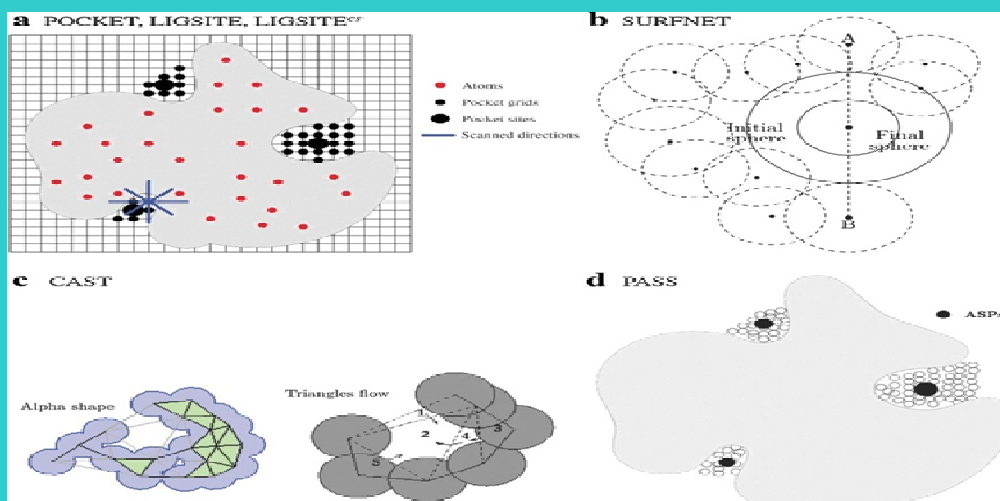
“If you took a given number of proteins and distributed interactions among them randomly, you would hardly find any particular protein that would have a lot of interactions. Proteins would all ‘talk’ randomly with each other in such a network,” Maslov says. “So, hubs of highly-interacting proteins are not something that you would expect to happen by pure chance.”

But the scientists did observe hubs of interacting proteins in the yeast cells. The connections between hub proteins reveal an “emergent property” that acts beyond the level of the functions of the individual proteins and makes them act together to coordinate their functions. Studying these interactions can help identify these coordinated functions, and may also reveal intrinsic features of the interacting proteins.

## BIOSERVER

### metaPocket- a meta server to identify pockets on protein surface!

The identification of ligand-binding sites is often the starting point for protein function annotation and structurebased drug design. Many computational methods for the prediction of ligand-binding sites have been developed in recent decades. The metaPocket is a consensus method, in which the predicted sites from four methods: LIGSITEcs, PASS, Q-SiteFinder, and SURFNET are combined together to improve the prediction success rate. All these methods are evaluated on two datasets of 48 unbound=bound structures and 210 bound structures. The comparison results show that metaPocket improves the success rate from\*70 to 75% at the top 1 prediction. MetaPocket is available at <http://metapocket.eml.org>.



## COMPUTERS FOR BIOLOGISTS

### Surflex-Dock

Surflex-Dock offers unparalleled enrichments in virtual high-throughput screening combined with state-of-the-art speed, accuracy and usability. It uses an empirical scoring function (based on the Hammerhead docking system) that has been updated and re-parameterized with additional negative training data<sup>5</sup>, along with a search engine that relies on a surfacebased molecular similarity method.

#### Selected Features of Surflex-Dock

**Accurate Scoring** – Scoring function is derived from known binding affinity data and negative training data to reduce false positive binding scores.

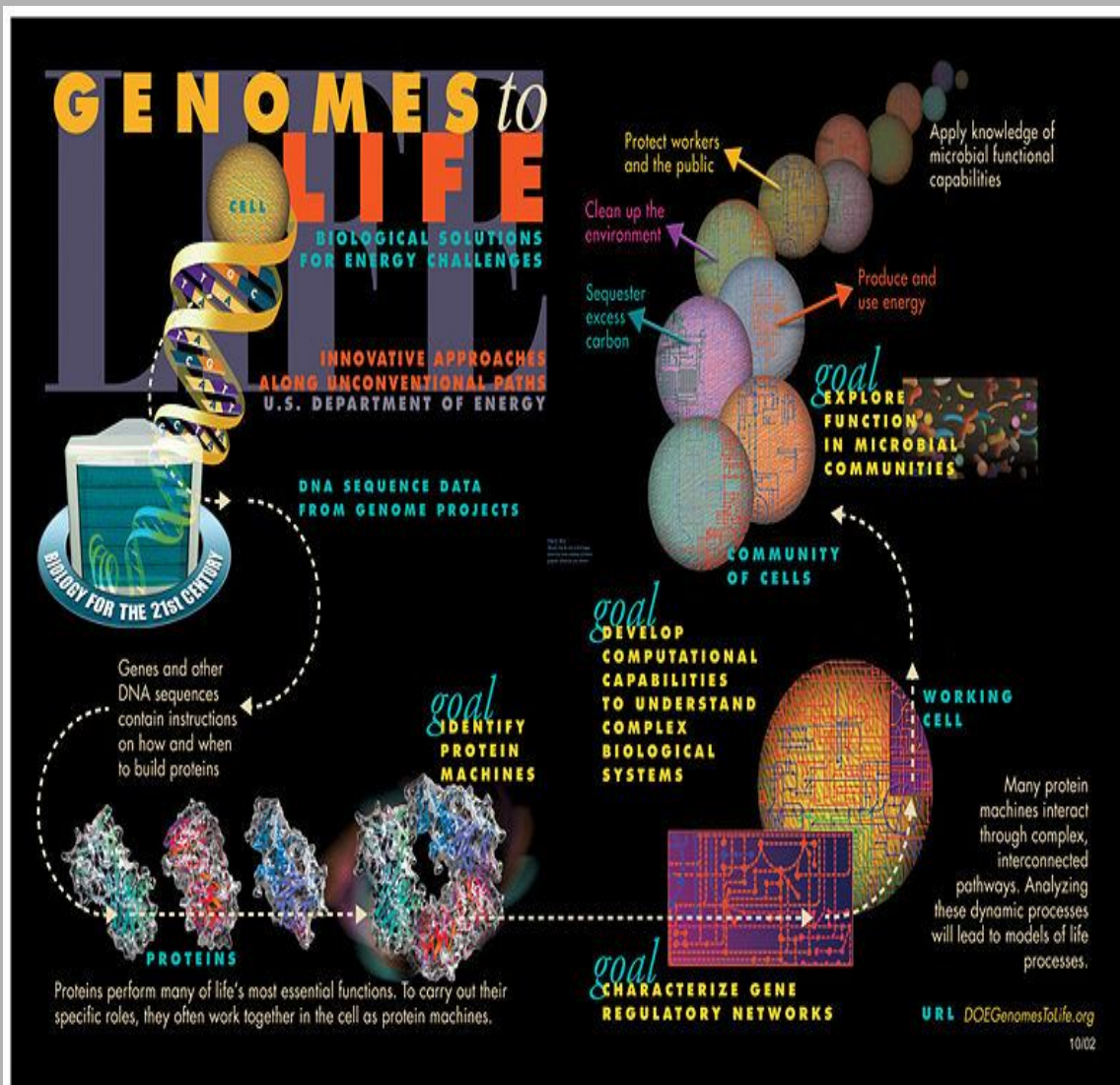
**Speed** – On average 17s per ligand (~3s per rotatable bond). Faster than GOLD and GLIDE and comparable with FlexX. **Easier Protein Preparation** – Protein structure preparation is simple and part of the docking workflow. No special treatment of cofactors/metals/waters is required.

**Easier Docking Preparation** – Docking gives good results with default settings; users will typically only need to tweak a few parameters to optimize docking for a specific target.

**Protomol guided docking** – Docking is guided by a 'protomol' which can be automatically generated and/or user-defined. The protomol is an idealized representation of a ligand that makes every potential interaction with the binding site. Stored in mol2 format, it can be edited easily and on the fly.

**Ring Flexing** – Generic ring conformations are applied to each flexible ring system (regardless of atom types), and the resulting conformations are minimized. The method is robust and fast.

## GENOMICS



## UPCOMING EVENTS

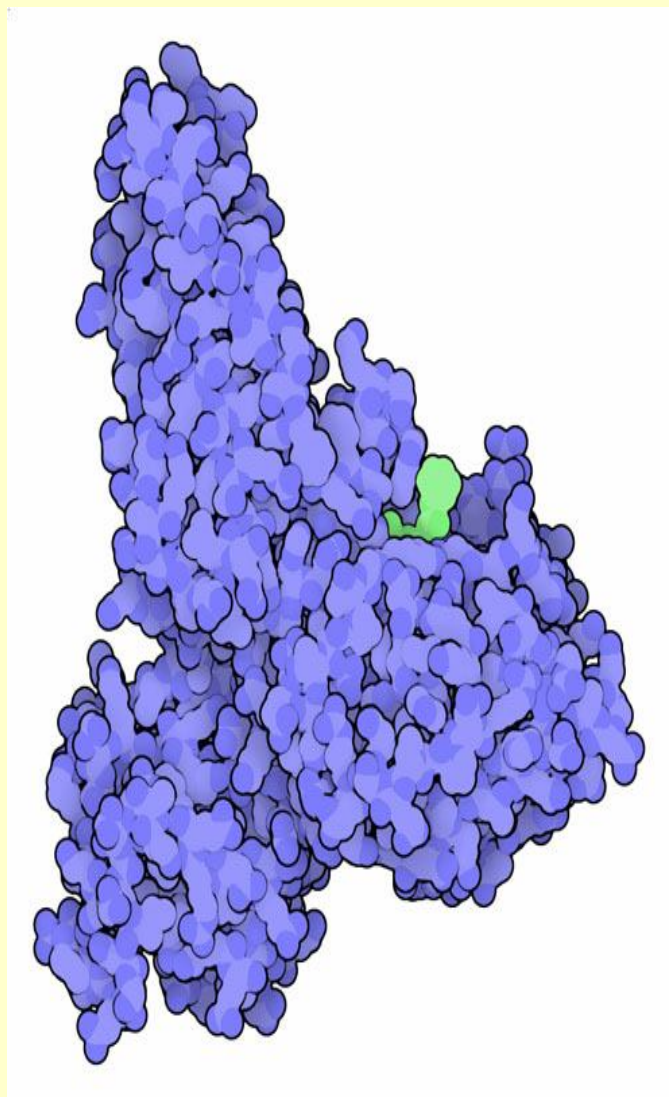
National Academy of Science, Allahabad

Workshop on “Scientific Paper Writing”

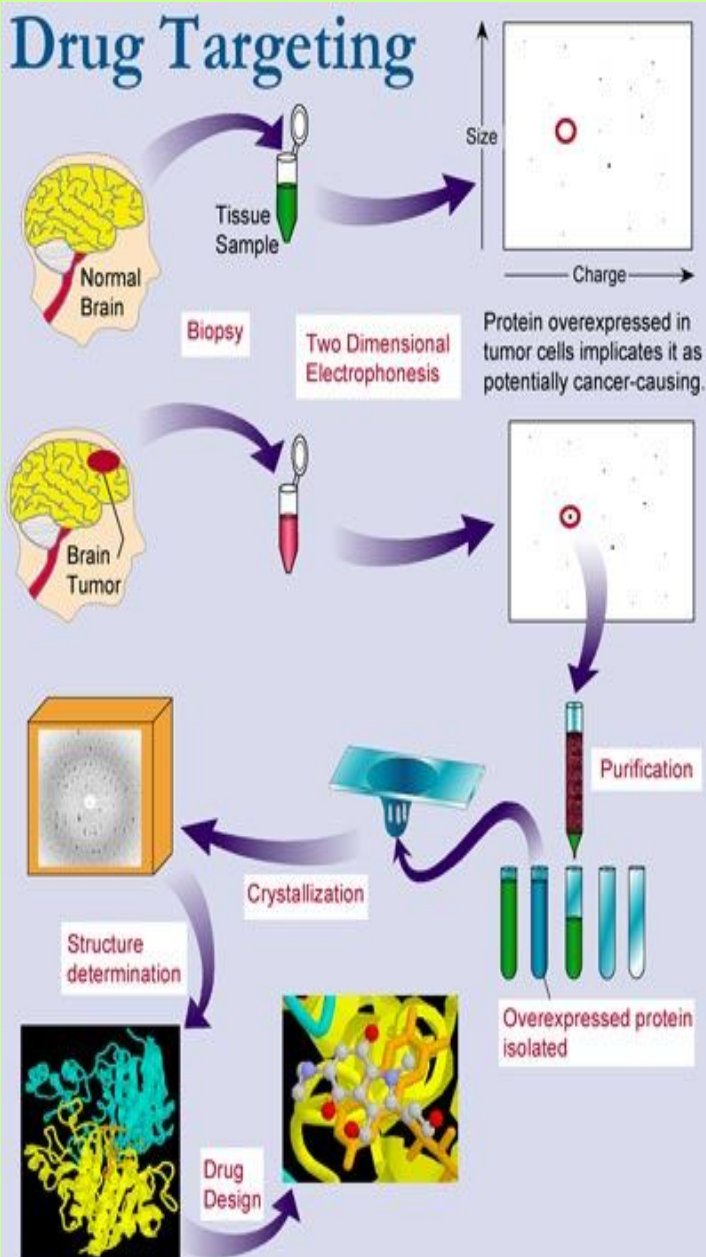
October 22-24, 2011

## MOLECULE OF THE MONTH

### O-GlcNAc Transferase



## Drug Targeting



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### Answers of Bioinfy Quiz

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