



Bioinformatics up to Date

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<http://binc.scisjnu.ernet.in>

COVER STORY

“DNA COMPUTING”

A nascent technology that uses DNA molecules to build computers that are faster than the world's most powerful human-built computers is called DNA computing. DNA computing also known as molecular computing is a new approach to massively parallel computation based on groundbreaking work by Adleman. DNA computers have emerged as an interdisciplinary field that draws together molecular biology, chemistry, computer science and mathematics. A DNA computer is basically a collection of specially selected DNA strands whose combinations will result in the solution to some problems. Technology is currently available both to select the initial strands and to filter the final solution. DNA computation is a new computational paradigm that employs bio-molecular manipulation to solve computational problems. In 1994, Leonard Adleman at the Laboratory of Molecular Science, Department of Computer Science, University of Southern California surprised the scientific community by using the tools of molecular biology to solve different computational problems. The main idea was the encoding of data in DNA strands and the use of tools from molecular biology to execute computational operations. Besides the novelty of this approach, DNA computing has the potential to outperform electronic computers. There are two main reasons for using molecular biology to solve computational problems.

DNA computing is in its infancy and its implications are only beginning to be explored. But DNA computing device could revolutionize pharmaceutical and biomedical fields. The first DNA computers are unlikely to feature word processing, e-mailing and solitaire programs. Instead their enormous computing power will be used by national governments for cracking secret codes or by airlines wanting to map more efficient routes. Studying DNA computing may also lead us to a better understanding of a more complex computer – the human brain. It can also be a general purpose tool for a variety of problems. The concept of using DNA computing in the fields of steganography, cryptography and authentication has been identified as a possible technology that may bring forward a new hope for unbreakable algorithms in the world of information security. Its applications include molecular barcode, fuzzy logic, evaluating gene sequence, selective cell treatment, ‘doctor in a cell’, genomic analysis, DNA fingerprinting etc.

(Ref: <http://www.amritaayanam.com>)



Tuesday Nov 22,
2011 at 4 PM PST
there are **77394**
Structures

BIOINFO. CAREER

Bioinformatics Project Technician Opening IIT Kharagpur

Walk-in-interview on 1.12.2011 at 12 Noon in the Dept of Biotechnology, for the post of

1) Project Technician and 2) Data Entry Operator
(http://www.iitkgp.ac.in/topfiles/sric_job_details.php?serial=2022)

Walk in interview program for the following Project posts tenable at NCCS, Pune.

1. Junior Research Fellow
2. Senior Research Fellow
(<http://www.nccs.res.in/AdvP2111.html>)

VIDYASAGAR UNIVERSITY, West Bengal
Advertisement for admission to Ph.D. Programme, 2011 in Bio-Medical Laboratory Science and Management, Botany, Chemistry, Computer Science, Electronics, Geography, Human Physiology, Microbiology, Physics, Remote Sensing and GIS, Zoology, **Bio-Chemistry, Bio-Technology**

Computational Chemistry



SERVER FOR DEPTH COMPUTATION AND ITS APPLICATIONS

Depth measures the closest distance of a residue/atom to bulk solvent. Accessible surface area is a parameter that is widely used in analyses of protein structure and stability.

In general, Depth

- provides wider dynamic range for residue burial (as compared to accessible surface area)
- correlates well with protein stability
- correlates well with amide proton hydrogen exchange rates
- predicts protein-protein interaction hot spots
- helps explain evolutionary variability in protein sequences
- Molecular Dynamics Simulation Trajectory Analysis
- Phi Value Prediction
- Protein 3D Structure Model Assessment

Proteomics



I-TASSER server is an Internet service for protein structure and function predictions. 3D models are built based on multiple-threading alignments by LOMETS and iterative TASSER assembly simulations; function insights are then derived by matching the predicted models with protein function databases. I-TASSER (as 'Zhang-Server') was ranked as the No 1 server for protein structure prediction in recent CASP7, CASP8 and CASP9 experiments. It was also ranked as the best for function prediction in CASP9. The server is in active development with the goal to provide the most accurate structural and function predictions using state-of-the-art algorithms. The server is only for non-commercial use.

The output of the I-TASSER server include:

- Up to five full-length atomic models (ranked based on cluster density)
- Estimated accuracy of the predicted models (including a confidence score of all models, and predicted TM-score and RMSD for the first model)
- GIF images of the predicted models
- Predicted secondary structures
- Predicted solvent accessibility
- Top 10 threading alignment from LOMETS

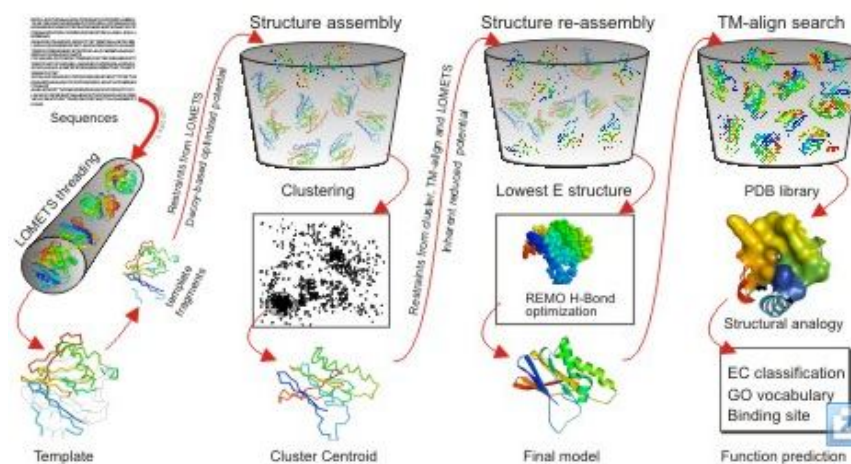


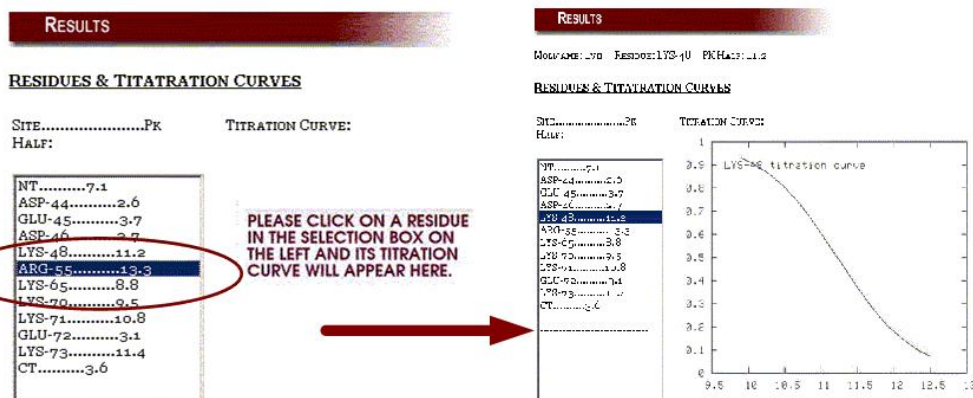
Figure I-TASSER protocol for protein structure and function prediction.

Bioserver



<http://biophysics.cs.vt.edu/index.php>

H++ is an automated system that computes pK values of ionizable groups in macromolecules and adds missing hydrogen atoms according to the specified pH of the environment. Given a (PDB) structure file on input, H++ outputs the completed structure in several common formats (PDB, PQR, AMBER inpcrd/prmtop) and provides a set of tools useful for analysis of electrostatic-related molecular properties.



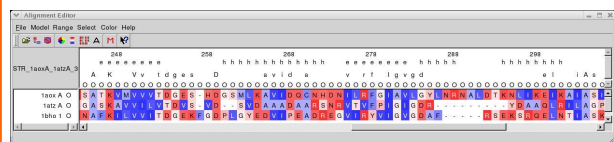
Computers for Biologists

Bodil

Bodil is a modular, multi-platform software package for biomolecular visualization and modeling. Bodil aims to provide easy three-dimensional molecular graphics closely integrated with sequence viewing and sequence alignment editing. Functionality of Bodil is implemented in dynamically loaded modules. Most of the modules available in the present release provide visualization tools, with protein modeling, small-molecule ligand docking and other modules being currently under development. New modules can easily be added via a documented C++ application programming interface.

Bodil is written in standard C++ using the Qt application development framework and OpenGL 3D graphics. The software has been ported to Linux, SGI Irix and Microsoft Windows NT/2000/XP platforms.

Features



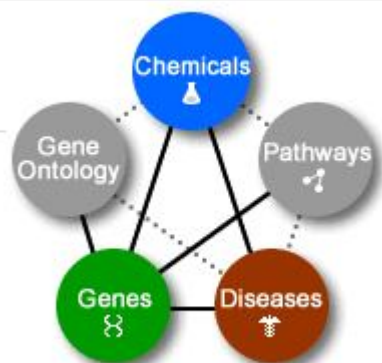
- Multi-view 3D graphics
- Stereoscopic viewing using CrystalEyes goggles (or equivalent) is supported on both SGI Irix and Intel Linux.
- Integration of sequence viewing and alignment editing with 3D molecular graphics
- A hierarchical tree view to chemical data
- Molecular surface calculation and visualization
- Fully automatic protein structure superposition using a C-alpha packing profile correlation

Genomics



Comparative Toxicogenomics Database

CTD advances understanding of the effects of environmental chemicals on human health. The etiology of most chronic diseases involves interactions between environmental factors and genes that modulate important physiological processes. This assumption is supported by the many complex diseases caused by reversible behaviors or avoidable exposures, and by the relatively rare number of diseases attributed to single gene mutations. Environmental factors are implicated in many common conditions such as asthma, cancer, diabetes, hypertension, immune deficiency disorders and Parkinson's disease. The molecular mechanisms underlying these correlations, however, are not well understood.



CTD includes curated data describing cross-species chemical–gene/protein interactions and chemical– and gene–disease associations to illuminate molecular mechanisms underlying variable susceptibility and environmentally influenced diseases. These data will also provide insights into complex chemical–gene and protein interaction networks.

(<http://ctdbase.org/>)

Upcoming Events

Bioinformatics Workshop on Sequence & Genome Analysis

@ Birla Institute of Scientific Research, Statue Circle, Jaipur, India

DATES: December 8-10, 2011

visit <http://www.bisr.res.in> or email to the convener at [workshop.bisr\[at\]gmail.com](mailto:workshop.bisr[at]gmail.com).

Training on Molecular Modeling and Drug Designing

@BIF, CSIR-NEIST, Jorhat

Date: 14 to 16, Dec, 2011

Subject Area: Bioinformatics in respect to Medical Sciences.

The 5th Virtual Training Workshop on Bioinformatics

DATES: December 2011 - January 2012

URL: <http://www.abren.net/workshop/>

Structural Bioinfo.

Name:Hydrolase/DNA

Title:Crystal structure of lactococcus lactis formamido-pyrimidine glycosylase (alias fpg or mutm) non covalently bound to an containing DNA.

Source:**Synthetic:** yes. Lactococcus lactis. **Organism_taxid:** 1358. **Gene:** mutm or fpg. **Expressed in:** escherichia coli. **Expression_system_taxid:** 562.

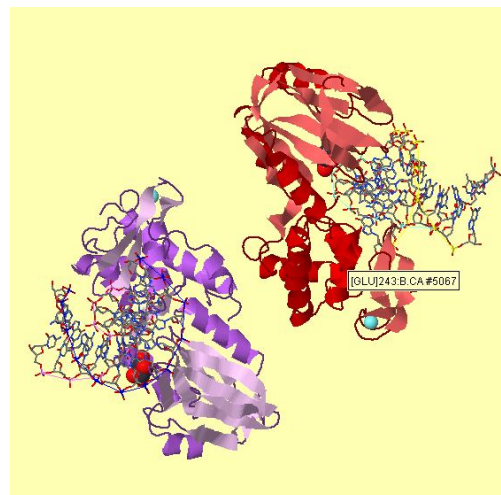
Biol. unit:Trimer (from PQS)

Resolution: 2.55Å

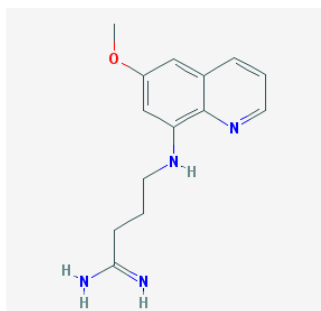
R-factor: 0.251

R-free: 0.285

Key ref:L.Serre et al. (2002). Crystal structure of the Lactococcus lactis formamidopyrimidine-DNA glycosylase bound to an abasic site analogue-containing DNA. *Embo J*, 21, 2854-2865.



Molecule of the month



IUPAC Name: 4-[(6-methoxyquinolin-8-yl)amino]butanimidamide

InChI: InChI=1S/C14H18N4O/c1-19-11-8-10-4-2-7-18-14(10)12(9-11)17-6-3-5-13(15)
16/h2,4,7-9,17H,3,5-6H2,1H3,(H3,15,16)

InChIKey: CFZROBVCOWSVAF-UHFFFAOYSA-N

Canonical SMILES : COC1=CC(=C2C(=C1)C=CC=N2)NCCCC(=N)N

Kindly send us your feedback to

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