Volume 11, Issue 10 October, 2018



# Bioinformatics up to Date

(Bioinformatics Infrastructure Facility, Biotechnology Division) North-East Institute of Science & Technology Jorhat -785006, Assam (http://www.rrljorhat.res.in/biotechnology.html)



# Inside.....

About us	1
Cover story	1
softwares/tools	2
Bioserver/softwares/tools	2
Bioinfo. Animation	3
Upcoming Events	3
Molecule of the month	4
Contact Us	4

### Advisor:

Dr Samit Chattopadhyay

#### **Editors:**

Dr Y S Devi Dr R Saikia Dr SB Wann Dr H P Deka Baruah

Mr. Abhijit Tamuly Ms. Kasmika Borah



## 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.

# <u>Transcriptomic network of genes involved in different stages of cisplatin/drug-resistance osteosarcoma cells</u>

A regular cancer remedy is observed on eliminate quick proliferating population of tumor cells. Still, existing evidences proposed survival of sub-population of cancer cells that can withstand chemotherapy by entering a preserve state of small growth. These tumor cells survive to produce cells resistant to drugs. The identifying of proper targets that can eliminate the drug-tolerant "persisters". A extreme understanding of the distinctive genetic signatures that conduct to resistance is of maximum importance to calculating an appropriate therapy.

In this study, the researchers worked on mRNA sequencing which was performed in osteosarcoma (OS) cells, reveal to the mostly used drug, cisplatin which is an integral part of current treatment regime for OS. This transcriptomic analysis was perform in 4 ways:-(i) untreated OS;

(ii) persister sub-population of cells post drug-shock;

(iii) cells which evade growth bottleneck; and

(iv) drug-resistant cells obtained after several rounds of drug-shock and revival.

The transcriptomic signatures and pathways managed in each group were contrast; the transcriptomic pipeline to the asset of resistance was analyzed and the key network of genes altered during the process was described. Moreover, the transcriptomic data was compared with OS patient data secure from Gene Ontology Omnibus. The scientist performed a sub-set of genes to be frequently indicate in both data sets with a high connection in declaration pattern. This study is aberrant draw to understand the sequence of genetic changes to the disclosure of drug-resistant cells, and insinuation from this study have a possible therapeutic conrtact. <u>Availability:</u> All raw data can be accessed from GEO database (<u>https://</u> www.ncbi.nlm.nih.gov/geo/) under the GEO accession number GSE86053.

Source: Divya Niveditha et al., J Oxford Bioinformatics, 2018, doi.org/10.1093/bioinformatics/bty868

# **Biolite: A structural bioinformatics substructure in Python**

In bioinformatics, sequence and structural data are ever-growing and the need for its analysis is more demanding. This software is user-friendly and basically for the beginners in programming and computationally useful

Avidin	MVHATSPLLLLLLSLALVAPGLSAR 26	
Streptavidin	D Р S К E S К A Q A A V A 13	
Avidin	K C S L T G K W D N D L G S N M T I G A V N S K G E F T G T Y T 58	
Streptavidin	EAGITGTWYNQLGSTFIVTA - NPDGSLTGTYE 44	
Avidin	TAV-TATSNEIKESPLHGTQNTINKRTQPTFG 89	
Streptavidin	SAVGNAESRYVLTGRYDSTPATDGSGT ALG 74	
Avidin	FTVNWKFSESTTVFTGQCFIDRNGKEV-116	
Streptavidin	WTVAWKNNYRNAHSATTWSGQYVGGAEAR 103	
Avidin	LKTMWLLRSSVNDIGDDWKATRVGINIFTRLR 148	
Streptavidin	INTQWLLTSGTT - AANAWKSTLVGHDTFTKVK 134	
Avidin	Т Q К Е 152	
Streptavidin	PSAASIDAAKKAGVNNGNPLDAVQQ 159	
Fig: Working Interface of Biotite showing sequence alignment pattern		

because of the application of Numpy and Cython. Biotite consists of four sub packages: sequence, structure, databases, and application. The sequence and structural element serve for the analysis of data respectively, database retrieved files from the online databases such **RCSB** PDB. as and application provides interface for other software. The sequence sub-package encodes each character of the sequence into a symbolic code which is stored in a NumPy N-dimensional array in the sequence object. The nucleotide and protein sequences can be read and written into FAS-TA format. Except, sequences can be easily aligned universally and narrowly using dynamic programming and can be easily visualized according to the similarity percentage.

The *structure* subpackage uses Atom Array Stack to constitute multi-model 3D structures of proteins which has a  $(m \times n \times 3)$  coordinate ndarray with *n* number of atoms and *m* number of models, and easily define the files in MMTF format. It is also capable of loading trajectories files of molecular dynamics simulation and can measure angles, dihedrals, and distances between the atoms. Besides, users can easily perform structure superimposition and calculate RMSD, RMSF, and secondary structure assignment. Biotite is an efficient framework for bioinformatics analyses such as downloading files, reading and writing structural files, and their modification. The tool is available on https://github.com/biotite-dev/biotite.

Source: Patrick Kunzmann et al.J BMC Bioinformatics, 2018. doi.org/10.1186/s12859-018-2367-z

# CamurWeb: a knowledge base software for gene expression data of cancer

CamurWeb, a new web-based package that is able to remove multiple and equal classification models in form of



logic formulas ("if then" rules) and to make a knowledge base of these rules that can be queried and analyzed. This method is based on constant classification technique and modifying feature to eliminate procedure that allows the computation of various rule-based models which are associated to cancer study.

Also for running the package, obtaining the results and organizing the experiments performed Camur Web includes a user friendly programme. Users can create profile, upload gene expression data, run the analyses, and translate the results with queries. The tool is available on http:// bioinformatics.iasi.cnr.it/camurweb.

Source: Emanuel Weitschek et al. JBMC Bioinformatics. 2018. https://doi.org/10.1186/s12859-018-2299-7



" Pursuing innovation in Bioscience and Biotechnology To Solve Local and Global Grand Challenges "

#### **BSB** — **2018** INTERNATIONAL CONFERENCE ON BIOINFORMATICS AND SYSTEMS BIOLOGY 26 Oct 2018 - 28 Oct 2018 • Allahabad, India

**Abstract:** We solicit high-quality original research papers (including significant work-in-progress) on any aspect of bioinformatics and systems biology. New computational techniques and methods involving machine learning, data mining, pattern recognition, knowledge representation, databases, data modeling, stochastic modeling, string and graph algorithms, constraint optimization, data analysis, data visualization, parallel computation, data integration, modeling, and simulation and their application in biological science domain are especially encouraged.

#### Event listing ID: 976612

#### Event website: http://wbsb.iiita.ac.in/

1. https://bioscienceconference.com/?gclid=EAIaIQobChMIk6TQIN6H3gIV2xwrCh0dOgtsEAMYAyAAEgK2vPD\_BwE 2. https://www.conference-service.com/conferences/in/mathematical-biology.html

# Aminoglycoside Antibiotics



Aminoglycoside antibiotics attach to a area of the ribosome that is concerned in translating the genetic code, where the high-quality RNA is paired with a mRNA codon. Aminoglycosides trouble the slight motions that are desired to make sure that only accurate pairings are done, frequently mispairing and accordingly introduce mutations addicted to the proteins that are prepared. These proteins are considerd to build up, corrupting the function of the bacterium and ultimately causing it to die.

Bacteria have evolved various habits to fight back and turn out to be resistant to aminoglycosides. In the ribosome, adenine (A1408) is significant to tRNAmRNA decoding procedure and is a target for aminoglycosides like paromomycin. Bacteria can turn into resistant by modifying this adenine by adding a methyl group to it, so that paromomycin unable to attach but the ribosome works correctly in protein synthesis.



Figure: Enzyme-drug interaction site (A) before the reaction (B) after the reaction with the neuclotide

Aminoglycosides have more than a few amine and hydroxyl groups that are necessary for binding to RNA. To develop into resistant, bacteria commonly bother the drug itself, using dedicated aminoglycoside-modifying enzymes to add new chemical groups to these amines and hydroxyls so that the drug can no longer bind and perform its error-promoting function. The enzyme shown here adds a nucleotide to the drug. PDB entries 5cfs and 5cfu catch the enzyme before and after the reaction.

Source: http://pdb101.rcsb.org/motm/226

#### Kindly send us your feedback to

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

Fig: Surface filling models of Aminoglycosides