



# **Progress Report of Center of Excellence**

**2010 – 2011**

**(Dec2010-Dec2011)**

**Funded by Department of Biotechnology  
Government of India**



**Center for Computational Biology and Bioinformatics  
School of Computational and Integrative Sciences  
Jawaharlal Nehru University  
New Delhi**

School of Computational and Integrative Sciences(SC&IS) presently consists of three centers, namely, Centre for Computational Biology and Bioinformatics (CCBB), High Performance Computing Center (HPCF) and Centre for Complex Systems Study ( approved by the UGC in XIth plan during 2008-09 along with five faculty positions). Our main objective is development of human resource through teaching and research in the frontier areas of Computational biology, Bioinformatics and Systems biology.

At present our strength is ten faculty members in our school and 2 faculty positions are advertised for recruitment in 2011-2012. Another 7 positions will be advertised soon. Two G.N.Ramachandran Fellowships and few technical positions are advertised recently and will be filled up soon.

A novel characteristic of SC&IS is its emphasis on inter-disciplinary research like Computational Genomics, Development of Tools for Bioinformatics, Structure based Bioinformatics and *in silico* Drug Discovery, Chemoinformatics, Database Management, Microarray Analysis and Datamining, Systems biology and Evolutionary biology.

### **Research Projects :**

Major research projects and field of research in CCBB presently, is focused towards the application of computational biology in pathogenic diseases like *Mycobacterium*, *Leishmani*, *Malaria*, etc. and development of analytical tools to study biology.

**A. *Mycobacterium tuberculosis*:** [\(TB consortium project supported by DBT\)](#)

### **Genomic Comparison tools for Strain identification :**

A large number of genomes of different strains and closely related species of pathogens like *Mycobacterium* have been sequenced and many others are in the process. A detailed analysis of these genomic sequences can help us to decipher and establish genotypic to phenotypic relationship. A number of molecular mechanisms have been described that are responsible for genomic changes [Current Opinion in Genetics and Development (2002) 12:719-725.9.]. These contribute to single nucleotide polymorphisms (SNP), variable number of tandem repeats, insertion/deletion with or without involving transposable elements and recombination. Many of these have been used as markers for identification of strains and diagnosis of pathogens. Therefore genome-wide identification of such differences would be tremendous use in a number of applications. *Mycobacterium tuberculosis* is a major cause of morbidity and mortality throughout the world. Genomic variations in this organism have been used to type pathogenic strains in a limited scale [Journal of Bacteriology (2002) 184(19):5479-90]. There is not yet any attempt to generate a comprehensive database of all the genomic variations of *M. tuberculosis* though some attempts have been made in this direction. For example, MTBreg (<http://www.doe-mpi.ucla.edu/Services/MTBreg/>) covers variations that are detected using spoligotyping) and MycoDB (<http://xbase.bham.ac.uk/mycodb/about.pl>) has some features that allows comparison between two genomes in a limited manner. A comprehensive database has been generated containing genomic difference of different strain and species of *Mycobacteria* belonging to *M. tuberculosis* complex. The variations have been identified using ABWGAT (<http://ccbb.jnu.ac.in/tools.html>) , a comparative genomic tool developed in the project [A Vishnoi, R Roy and A Bhattacharya, Nucleic Acid Research. (2007). 35(11): 3654-3667 ]. This database will

be highly useful to clinicians and basic scientists interested in understanding *Mycobacterial* diseases, generating tools for identification of strains and species and developing vaccines and new drugs. [Publication list Paper #4]

### **Metabolic pathway analysis for validating drug targets in *M.Tb* :**

As metabolism is a fundamental determinant of physiology, metabolic model can predict the phenotypic changes. There is one type of model that has shown a surprising ability to simulate the growth of living cells — namely stoichiometric flux balance models. These models rely on balancing of all intracellular metabolites in the metabolic network, which represents the core machinery of cellular function as it provides the building blocks and Gibbs free energy for cellular synthesis. The balancing of metabolites supplies a large number of constraints and, through the use of linear programming, it is possible to obtain unique solutions that obey a specific objective function. Therefore, the important steps in developing and disseminating the metabolic model are (i) Physiological and Phenotypic characterization of the bacteria; (ii) genome annotations; (iii) metabolic reconstruction; (iv) Flux balance analysis. Use of Publicly accessible software tools has made it possible to identify and analyze the important metabolite with their relevant reactions & involved enzymes which could possibly are used as drug targets. Such applications have been conducted which resulted in identification of a set of proteins which are to be included as important drug targets .

### **Knowledge based compound design against *M.Tb*:**

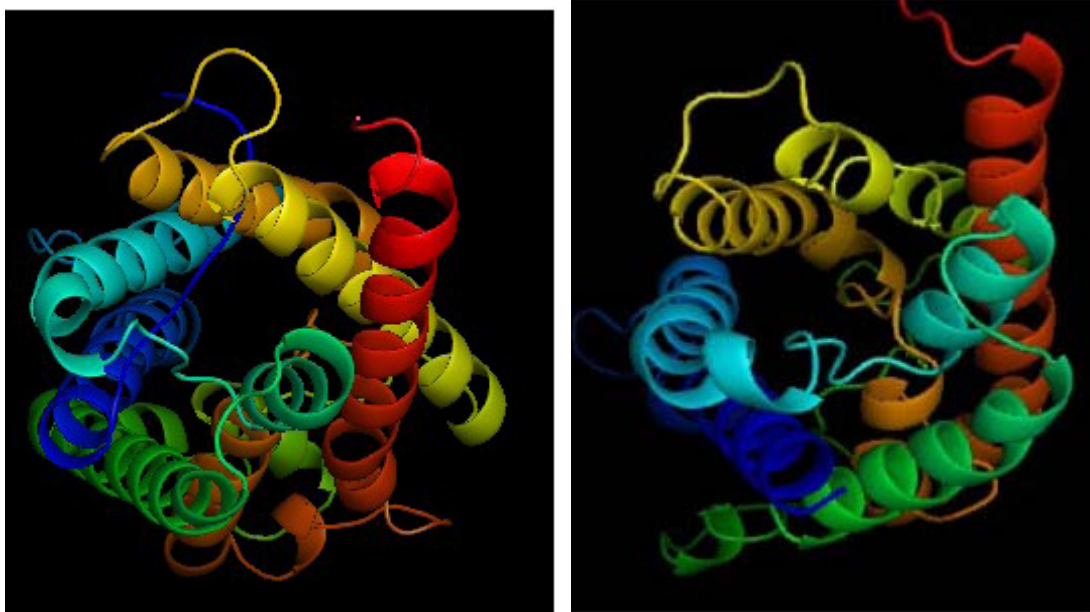
Here we are working on a novel method developed in-house to synthesizing chemical compound with combinatorial motif identified by the study of known database, having minimum common bioactive substructure. Application of data mining procedure to identify the ‘relaxed’ common pattern (pharmacophore) present in the diverse set of drug like/lead compounds is proposed. Use of graph theoretical approach to identify the Maximal Common Substructure (MCS) and use of Fuzzy logic techniques to identify the ‘relaxed’ chemical motifs so that broader pattern can be found are proposed.

### **B. *Leishmania***

*Leishmania donovani* is a protozoan parasite and is the causative agent of visceral leishmaniasis. Analysis of *L. major* and *L. infantum* genomes shows the presence of five AQPs.

Though the topology of all the five AQP are very similar in organization, due to their variation in length of helices they may differ in size and shape of pores. This indicates the possibility of two of them to be better transporters for water than glycerol. For functional characterization all five AQP proteins were heterologously expressed in yeast and experimental work is pursued with collaboration in School of Life Science, JNU. [Publication list Paper #10]

Fig1. Top-down view of MODELLER9v8 structures for *L.donovani* AQP showing different size of the pores. The first major Transmembrane helix is shown in dark blue, second in light blue, third in bright green, fourth in yellow, fifth in light orange and sixth in red. The two small helical regions hosting the NPA motif are shown in light green (present in between major helix 2 and 3) and orange (present in between major helix 5 and 6).



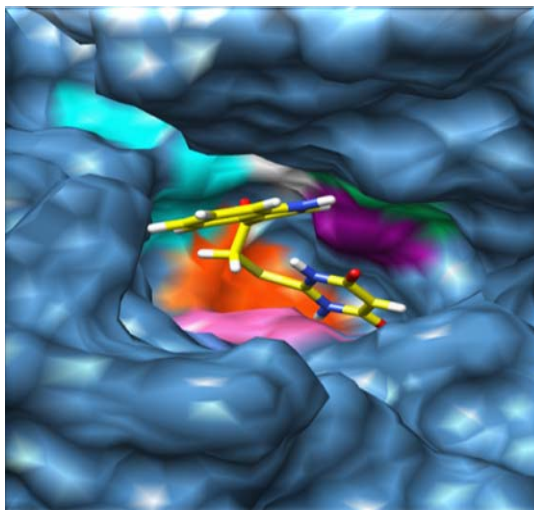
### C. *Plasmodium falciparum*

Malaria is one of the world's leading killer infectious diseases caused by unicellular, protozoan parasites of the genus *Plasmodium*. Human malaria is caused by four species of the parasitic protozoan genus *Plasmodium*: *Plasmodium vivax*, *Plasmodium ovale*, *Plasmodium malariae*, and *Plasmodium falciparum*. Drug Target identification, selection and validation is of great importance to develop inexpensive and effective novel inhibitors that overcome the drug resistance with no side effects of existing antimalarial therapy. We have been developing a Drug Target Information System listing all the known and predicted drug targets and inhibitors for *Plasmodium falciparum*. PfalDTDB: An integrated drug target database has been developed which contains genome, proteome, pathway, chemical information for *Plasmodium falciparum* and related species. **PfalchemDB** will be used as a resource for virtual high throughput screening against **prioritized drug targets** based on the specific criteria mentioned above. Pharmacophore designing using Artemisinin analogs will effectively help to identify novel scaffold providing the same interactions at the target(s) of artemisinin. Target prioritization and *in silico* screening of compound libraries to the set of prioritized drug targets in *Plasmodium falciparum* will be carried out in near future (*This project has been supported by Ministry of Communication and Information Technology*)

### D. *Entamoeba histolytica*

The explosive epidemicity of amoebiasis caused by facultative gastrointestinal protozoan parasite *Entamoeba histolytica* is a major public health problem in developing countries. Multidrug resistance and side effects of various available anti-amoebic drugs demands an urgent need to design novel anti-amoebic agents. Cysteine plays a very important role in antioxidative defense mechanism of *Entamoeba histolytica*, an anaerobic protozoan parasite. O-Acetylserine Sulfhydrylase (OASS) and Serine acetyltransferase (SAT) serve as key regulatory enzymes in cysteine biosynthetic pathway. At present various anti-amoebic drugs are available but due to their prolonged side effects and drug resistance, there is a need to design new potential inhibitors. We have carried out *in-silico* virtual screening of ~0.69 million drug like and ~0.15 million natural compounds from ZINC database against active site of EhOASS and EhSAT structures determined

by our group using GLIDE and GOLD docking programs. To measure the biological activity of these compounds as potent inhibitors, procurement and experimental testing against target enzymes are in the pipeline.[Publication list Paper #19]



### **Natural Product Docked in the active site of EhOASS**

#### **E. New Algorithms and SW development :**

Cognitive modeling and machine learning for face recognition and image classification are upcoming research area in cognitive science. One of our faculty is strongly involved in such area and developed neurocomputational models to robotics in an attempt to overcome the limitations of learning with traditional artificial Intelligence and novel algorithms for multiple robot coordination and cooperation. [Publication list Paper 11-14]

Neuronal mechanism of regulation of wake-nrem-rem sleep is investigated using mathematical modeling. The model focuses on the transitions between the wake and sleep states and how both the homeostatic sleep drive and the circadian rhythm shape the duration of each of these episodes. Electroencephalogram (EEG) was collected from 12 rats during various vigilance states (Wake, NREMS, REMS) and Empirical Mode Decomposition method is used to analyze the EEG signals.

Various tools of signal processing and information theory to analyze DNA sequences has been developed. Using the well-known correlation measure to predict the origin of replication in various organisms has also been developed. Analysis of short-range correlation properties of over 4 million annotated coding sequences and a large number of noncoding sequences, spectral content measure using wavelet analysis and Hurst exponents to study the extent to which these methods are sensitive to the structural organization of nucleotides in noncoding RNAs in prokaryotes are accomplished. Positional asymmetry arisen in the coding regions of a given genome provides a characteristic spectral signature that can also be used in classification of groups of prokaryotic genome [Publication list Paper #26].

#### **F. Developmental work in collaboration with DBT**

A technical programmer was supported from COE in collaboration with DBT, to develop the following SW for online submission and monitoring system(OSMS), Conference, Travel,



Exhibition and Popular Lectures(CTEP) online information system.

URL: <http://www.dbtctep.gov.in>

The Department of Biotechnology, Government of India has been operating a nationwide program namely 'Promotion and popularization of Biotechnology' through which DBT provides financial grant for organizing conference/workshop in its mandate subject area. DBT also sponsors foreign travel support to the researchers including research scholars for presenting their research papers in the International Conferences which are being held outside India. . As part of this program DBT also provided financial grants for organize popular lectures through eminent scientists.

The screenshot shows the homepage of the 'Online Submission and Monitoring System for Conference, Travel, Exhibition and Popular lectures'. The header includes the Department of Biotechnology logo and navigation links like Home, Contact Us, Disclaimer, FAQ, and Process Flow. A main navigation menu on the left lists 'About CTEP', 'Register Organization', 'Instructions', 'Submit Proposal', 'Events', and 'News/Announcements'. The main content area is titled 'About CTEP' and explains the system's purpose: to popularize biotechnology activities in India by providing financial assistance for organizing conferences, seminars, workshops, and travel. It lists four types of assistance: 1. Financial assistance for holding National/International-Conference/Seminar/Symposium/workshop; 2. Travel support for attending international conference/seminar/symposia; 3. Participation charge in organizing exhibition; 4. Financial assistance for organizing popular lectures by experts in the area of Biotechnology and related fields. It also mentions that DBT has introduced a web portal (OSMoSys) for submission, processing, and settlement of grants. A 'Guidelines for submitting a proposal' section follows, with 'Step 1: Register Organisation' and 'Step 2: Submit Proposal' instructions. A 'Login' form is visible on the right, with fields for Username/Email-ID and Password, and a 'Sign in' button. Below the login form are sections for 'News/Announcements' (Innovative Young Biotechnologists Award) and 'Grant Recommendations' (Recommendations made in the meeting held on 24/12/2010). The footer indicates the system was developed and maintained by 'koti'.

**Award Received:** The online system of CTEP was awarded 'The Best IT Implementation of The Year 2011' by PC Quest.

Many Intra online information services has also been developed like **,BTISnet Intra-Portal, Forum @ Bioinformatics, Who's Who in Biotechnology, Equipment Database(equipment purchased by supported by DBT projects).**

**NER-BPMC Portal @ Department of Biotechnology:** In order to promote biotechnology and related activities in the North Eastern Region Department of Biotechnology, Government of India runs several programs like NER Twinning program, NEBInet, NER Biotech hub, NER Overseas program, NER-BIF etc. All these programs are manually operated and hence it becomes tedious to handle these programs effectively. Moreover DBT was facing hurdle in reaching the target audience as there was no comprehensive portal for NER to promote biotechnology and information of related activities. This activities will enhance the transparency and efficiency in the e-governance.

**Current Academic Activities(2011-2012).** See Website for more details <http://ccbb.jnu.ac.in>

Dr Kushal Shah joined as Assistant Professor under DBT-COE grant(M.Tech) in our school during 2011. His research interests are protein folding and statistical mechanics of biomolecules, Plasma Physics and Non-linear Dynamics [Publication list Paper #6,6,16,17].

Dr Rashi Gupta joined as Assistant Professor under DBT-COE in our School during 2009-2011 May. Her research interests are Microarray Analysis, Next Generation sequencing, Bayesian statistics.

Memorandum of Understanding was signed with Bioinformatics Institute, Singapore for academic and research collaboration from 2010. JNU and BII faculty had an interaction meeting on 9<sup>th</sup> December, 2010 at INSA, New Delhi. Mr. Ritwik Vinekar has been selected to participate in the research exchange program with BII Singapore during 1<sup>st</sup> Jan 2011 – 15<sup>th</sup> July 2011 while continuing his Ph.D work in the field of Molecular simulations. Three faculty members attended interaction meeting at BII, Singapore during March 2011.

**See Website for more details** <http://ccbb.jnu.ac.in>

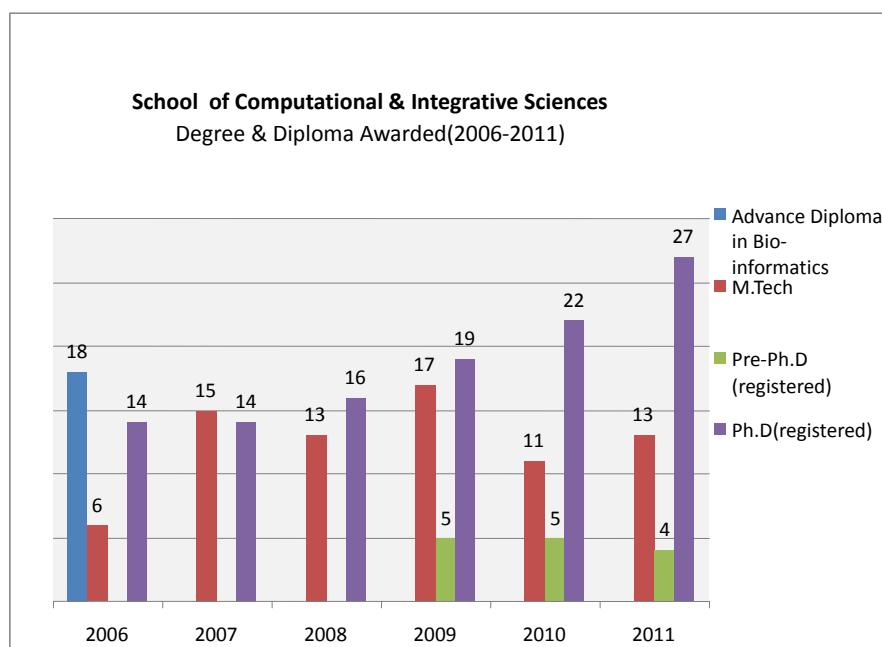
**Training & Visitors:** <http://ccbb.jnu.ac.in/training.html>

82 Post Graduate Diploma M.Phil (equivalent) in Bioinformatics during 2001-2006 has been contributed by CCBB 2011.

During 2006-2011 thirty five M.Tech students passed. Twelve research fellows have been awarded PhD in Computational Biology & Bioinformatics.

Ten students have done their 6 month projects as long term trainees and five short term trainees including summer trainees at our school during 2011.

Eighteen visitors had given lectures at our school during 2011. <http://ccbb.jnu.ac.in/events.html>



**Supported Fellows & Associates:** [http://ccbb.jnu.ac.in/fellows\\_associates.html](http://ccbb.jnu.ac.in/fellows_associates.html)

- Three Senior Ph.D students (Smriti Sharma, Alok Srivastava and Vikram Singh) were supported with Senior Research Fellowships partly during 2010-2011 while submission of thesis
- Mr Surajit Mishra was supported to develop software in collaboration with DBT.
- Dr V.S.Gauri is working as Research Associate under COE-DBT
- Mr Adarsh Tayal is working COE project as System Analyst

### **Travel grant or registration to attend Conferences by (8) research Fellows :**

<http://ccbb.jnu.ac.in/travelgrant.html>

- Mr. Suraj Kumar, Mtech student attended a workshop on “Recent Trends in Social Networks: Algorithms, Models and Learning” at TIFR, Mumbai during 3 – 7 January, 2011.
- Seven posters were presented from our school ,were supported by COE grant in 7th Asian Biophysics Association (ABA) Symposium & International Conference on Biophysics at New Delhi 30th January – 2nd February, 2011.
- Mr. Vikram Singh Ph.D student attended the "International Conference on Bioinformatics and Computational Biology 2011" (BICB 2011) held in Singapore during 28th February-1st March 2011.
- Mr. Rupesh Kumar Ph.D student participated in Cold Spring Harbor Asia Summer School: “Computational and Cognitive Neurobiology” and attended a series of lectures and practical training during July 11th to July 24th 2010 at China.
- Rama Kalia Ph.D student presented her work on "Disease-Target Relationship based Ontology" in International Conference Translational Bioinformatics Conference 2011 held in Seoul, South Korea in Nov 2011.
- Mr. Amit Kumar Ph.D student has attended the conference on “Asia Pacific Bioinformatics Network’s 10th InCoB – 1st ISCB Asia Joint Conference 2011” held on 30th November, 2011 to 2nd December, 2011 at Kuala Lumpur, Malaysia.
- Mr Rupesh, Ph.D student Attended the Cape Town School on Advanced Theoretical and Computational Neuroscience. Cape Town, South Africa, 12 Dec - 23 Dec, 2011
- Vikram Singh Ph.D student attended “Delhi Dynamics Day” conference, SPS, JNU, 13<sup>th</sup> December 2011

### **BINC Examination :**

SC&IS, JNU successfully conducted BINC Exam 2010-2011 during February 26th and 27th 2011 and awarded 35 BINC fellowships and top ten students were given Cash awards of Rs 10000 each. Bioinformatics National certificate award ceremony was organized on 3rd August 2011.

**BINC 2012 examination will be held from Feb 25<sup>th</sup> -26<sup>th</sup> 2012 . Now expanded to nine centers namely, Jawaharlal Nehru University, New Delhi; Pune University, Pune; Anna University, Chennai; University of Kerla, Thiruvanthapuram; Calcutta University, Kolkata; Institute of Bioinformatics & Applied Biotechnology, Bangalore; University of Hyderabad, Hyderabad. North Eastern Hill University, Shillong and Assam Agricultural University, Gauhati**

**BINC-2012 Website is running as supported by ERNET connectivity**

**Please visit : <http://binc.scisjnu.ac.in>**

### **Extra Mural Funded Research Projects**

<http://ccbb.jnu.ac.in/research.html>

1. MCIT project on “Designing novel antimalarials using target based pharmacophore approach” Ministry of Information Technology, Govt of India, Aug 2009-2012. PI: Professor Indira Ghosh and Co-PI : N.Subba Rao.
2. DST project on “Development and application of a Biased Monte Carlo simulation technique: Exploring and characterizing potential energy surfaces of large molecules”. 2010-2015.PI: Pradipta Bandhyopadhyay
3. DBT project on Development of computational methods for Riboswitch detection and prediction in



genomic sequences and their functional validation, November 2009 - November 2012 PI:Supritim Sengupta

4. Bioinformatics National Certificate Exam 2011-2013 PI: Prof Indira Ghosh

### **Projects in collaboration with academia**

5. DBT Project on “Establishment of National Database on Tuberculosis(TB) Phase II TB Consortium”: Prof. Alok Bhattacharya and Prof Indira Ghosh 2011-2013
6. DBT project on “Computational Core for Plant Metabolomics” Prof Indira Ghosh with IIIT, Hyderabad, 2011-2015
7. European Commission (FP7) on “Open Tox” Prof. Indira Ghosh with eight European groups, 2008-2011

### **Conference and Workshop during 2011** <http://ccbb.jnu.ac.in/events.html>

1. Open Day 25<sup>th</sup> April 2011 Participants:200
2. Conference on "Biomolecular Simulation Algorithm and Application" March15-16,2011  
<http://ccbb.jnu.ac.in/bsaa/index.in> Participants: 25
3. Workshop on "Application of Quantum Chemistry in Biology". January 2-5, 2011  
<http://ccbb.jnu.ac.in/aqcb/index.in> Participants: 30
4. Programming in R and Matlab. Participants: 20
5. Applications of evolutionary computation to biology / bioinformatics, 12th-15th September 2011 Participants:15
6. Database and Web Applications 23-26th May 2011 Participants:15

### **Publications 2011 ( 27 +3)** <http://ccbb.jnu.ac.in/publications.html>

1. Rout AK, Padhan N, Barnwal RP, **Bhattacharya A**, Chary KVR. “Calmodulin-like protein of Entamoeba histolytica: Solution structure and calcium binding properties of partially folded protein”. Biochem. 50, 181-193 (2011)
2. Somlata, Bhattacharya S., **Bhattacharya A**. A C2 domain protein kinase initiates phagocytosis in the protozoan parasite Entamoeba histolytica. Nat. Commun. 2, 230 (2011)
3. Kumari V, Sharma R, Yadav VP, Gupta AK, **Bhattacharya A**, Bhattacharya S. “Differential distribution of a SINE element in the Entamoeba histolytica and Entamoeba dispar genomes: role of the LINE-encoded endonuclease”. BMC Genomics 12, 267 (2011)
4. **Bharti R**, Das, R, Sharma, P, Katoch, K. and **Bhattacharya, A**. (2011) MTCID: A database of genetic polymorphisms in clinical isolates of Mycobacterium tuberculosis. Tuberculosis (2012), doi:10.1016/j.tube.2011.12.001
5. **Candida Vaz, Arvind Singh Mer, Alok Bhattacharya, Ramakrishna Ramaswamy** (2011) "MicroRNAs Modulate the Dynamics of the NF-κB Signaling Pathway". PLoS ONE 6(11): e27774. doi:10.1371/journal.pone.0027774
6. **Kushal Shah and A. Krishnamachari**. "Nucleotide correlation based measure for identifying origin of replication in genomic sequences", BioSystems (accepted)
7. **Kushal Shah and A. Krishnamachari**. "On the origin of three base periodicity in genomes", BioSystems, available online 12 November 2011
8. **Indira Ghosh**, Proteins will Fold Anyway!!, Journal of Biomolecular Structure & Dynamics, Volume 28, Issue Number 4, February 2011
9. Anirban Banerji & **Indira Ghosh**, Mathematical criteria to observe mesoscopic emergence of protein biochemical properties, in J Math Chem (2011) 49:643–665

10. Biyani N, Mandal S, **Seth C**, Saint M, Natarajan K, **Indira Ghosh** , Madhubala R;. Characterization of Leishmania donovani aquaporins shows presence of subcellular aquaporins similar to tonoplast intrinsic proteins of plants. PLoS One. (2011);6(9):e24820.
11. Manoj Agarwal, **Lovekesh Vig**, and Naveen Kumar, "Multiple Objective Robot Coalition Formation", Journal of Intelligent Systems (Accepted, in Press)
12. Ashish Gupta and **Lovekesh Vig** , "A dual association model for Acquisition and Extinction", Man Machine and Beyond, Italian Association of Artificial Intelligence, Palermo, 139-150, 2011
13. Ashish Gupta, **Lovekesh Vig** and David C. Noelle, "A Cognitive Model for generalization during Sequential Learning", Journal of Robotics, Special Issue on Cognitive and Neural Aspects, 2011
14. Ashish Gupta, **Lovekesh Vig** and David C. Noelle, "A Dual Association Model for the Extinction of Animal Conditioning", Neurocomputing 74 (2011), pp. 3531-3542
15. **Lovekesh Vig**, Ashish Gupta and **Abhinandan Basu**, "A Neurocomputational model for the role of hunger in Dopamine mediated actions", Journal of Intelligent Systems (Accepted, in Press)
16. **K.Shah**, V.Gelfreic, V.Rom-Kedar, D.Turaev. "Robust exponential acceleration in time-dependent billiards", Physical Review Letters 106, 074101 (2011).
17. **K.Shah**. "Energy growth rate in smoothly oscillating billiards", Physical Review E 83, 046215 (2011).
18. Ejaz Ahmad, Gulam Rabbani, Nida Zaidi, Saurabh Singh, **Mohd Rehan**, Mohd Moin Khan, Shah Kamranur Rahman, Zainuddin Qadri, Mohd. Shadab, Mohd. Tashfeen Ashraf, **Naidu Subbarao**, Rajiv Bhat and Rizwan Hasan Khan, "Selectivity of Human Serum Albumin to Enantiomeric and Isoelectronic Pollutants Dissected by Spectroscopy, Calorimetry and Bioinformatics", Accepted PloS ONE(2011)
19. Isha Nagpal, **N.Subbarao**, S.Gourinath, Virtual Screening of potential inhibitors against O-acetylserine sulfhydrylase of Entamoeba histolytica of Cysteine Biosynthetic pathway, Accepted for publication in PLOS One journal, 2011.
20. Vishvanath, Isha Nagpal, **N.Subbarao** and M.Rajeswari, In-silico modeling of a novel OXA-51 from  $\beta$ -lactam-resistant Acinetobacter baumannii and its interaction with various antibiotics Accepted for publication in Journal of Molecular Modeling.
21. Dhar, Suman; Nitharwal, Ram Gopal; Verma, Vijay; **Subbarao, Naidu**; Dasgupta, Santanu; Choudhury, Nirupam "DNA binding activity of Helicobacter pylori DnaB helicase: the role of N-terminal domain in modulating DNA binding activities", FEBS Journal, 279, 234-250 (2012)
22. Varshney A, **Rehan M**, Rabbani G, Khan RH, **Subbarao N** "Elimination of Endogenous Toxin, Creatinine from Blood Plasma Depends on Albumin Conformation: Site Specific Uremic Toxicity & Impaired Drug Binding". PLoS ONE , February 2011, Volume 6, Issue 2.
23. Kumar S, Raj I, Nagpal I, **Subbarao N** and Gourinath S. "Structural and biochemical studies of Serine Acetyltransferase reveal why the parasite Entamoeba histolytica cannot form Cysteine Synthase complex". JBC, on February 5, 2011
24. **Smriti Sharma and Pradipta Bandyopadhyay**. "Investigation of the acylation mechanism of class C beta-lactamase: pKa calculation, Molecular Dynamics simulation and quantum mechanical calculation", J. Mol. Modeling, 2011 PMID:21541744
25. **Bandyopadhyay P, Hungyo Kharerin** , "Monte Carlo Energy Landscape Paving and Basin Paving simulation of RNA T-loop hairpin". Chem. Phys.Lett., 502, 130 (2011).
26. **Vikram Singh and Rama Ramaswamy**, Spectral analysis of long noncoding RNAs, International Conference on Bioinformatics and Computational Biology, BICB 2011, B31–B38. (ISBN: 978-981-08-8119-1)
27. **Hemant R. Kushwaha**, Gautam Kumar, Praveen Verma, Sneha L. Singla-Pareek, Ashwani

Pareek. "Analysis of a salinity induced BjSOS3 protein from Brassica indicate it to be structurally and functionally related to its ortholog from Arabidopsis" Plant Physiology and Biochemistry, 2011.

### **Book publications**

1. Kumar G, **Kushwaha HR**, Purty RS, Kumari S, Singla-Pareek SL, Pareek A. Cloning, Structural and Expression Analysis of OsSOS2 in Contrasting Cultivars of Rice under Salinity Stress. Genes, Genomes and Genomics, 2011, Vol. 5.
2. **Kushwaha HR**, Singla-Pareek SL, Sopory SK, Pareek A. Understanding the "Commoneome" operative in plants in response to various abiotic Stresses. In: Improving Crop Resistance to Abiotic Stress. ed. Tuteja et. al.(Wiley-Blackwell, Wiley-VCH Verlag GmbH & Co., Germany),2011
3. **Kushwaha HR, Ghosh I**, Pareek A. "General overview of bioinformatics tools in agricultural sciences. In: Biotechnology in agriculture and medicine" : Principles & Practice. ed. Gupta AK, Pareek A, Gupta SM.(I. K. International, INDIA),2011

### **Conference Oral/Poster Presentations during 2011 (19)**

[http://ccbb.jnu.ac.in/conference\\_papers.html](http://ccbb.jnu.ac.in/conference_papers.html)

- **Lovekesh Vig** and Ashish Gupta, In the Proceedings of the fifth Indian International Conference on Artificial Intelligence, Tumkur, India, 2011
- **Lovekesh Vig** and Julie A. Adams, "The Effect of Coalition Imbalance on Multi-Robot Teams" In the Proceedings of the third Indian International Conference on Artificial Intelligence, Tumkur, India, 2011
- **Lovekesh Vig**, Ashish Gupta and **Abhinandan Basu**, "On the Relation between Hunger, Dopamine and Action Rate", In the Proceedings of the fourth Indian International Conference on Artificial Intelligence, Tumkur, India, 2011
- Manoj Aggarwal, **Lovekesh Vig** and Naveen Kumar, "A Multiple Objective approach to robot coalition Formation", International Conference of Intelligent Robotic Application, Aachen, 2011.
- Ashish Gupta and **Lovekesh Vig**, "A Dual Association Model for Acquisition and Extinction" In Proceedings of the tenth Conference of the Italian Association of Artificial Intelligence: 39-150, 2011
- Mallick, B. N., Singh, A., Khanday, M. A. and **Kumar, R.** Neural mechanism of REM sleep regulation. Proceedings of Ranbaxy Science Foundation, XXVIth Round Table Conference on Sleep Disorder A Wake Up Call. 2011 (in press)
- **Kumar R**, Ramaswamy R and Mallick BN. Analysis of rat EEG during vigilance states using Empirical Mode Decomposition. Front. Comput. Neurosci. Conference Abstract: Cape Town School on Advanced Theoretical and Computational Neuroscience.

Following posters from the school were presented in 7th Asian Biophysics Association (ABA) Symposium & International Conference on Biophysics at New Delhi 30th January – 2nd February, 2011.

- P69 **Om Prakash**, Puri Nidhi, Prasad Rajendra, Ghosh Indira, Identification of substrates and non-substrates of efflux pump from *Candida albicans* using 3D shape based virtual screening.
- P70 **Kumar Amit**, Ghosh Indira, Selectivity and specificity profiling of binding sites of human

and plasmodial Ser/Thr kinases.

- P71 **Gorai Biswajit**, Kalyanarama Madhuvanathi, Sen Parthosarathi, Singh Prakash, Jay Mittal Megha, Subbarao Naidu, Ghosh Indira 3D-pharmacophore and drug target/chemical database approach towards developing novel antimalarials.
- P72 **Subbarao Naidu**, Yennamalli Ragothaman M, Young Paul R, Kobe Bostjan Identification of dengue envelope protein inhibitors using structure based drug design
- P104 **Patel Jignesh**, Chcko Sajeev, Ghosh Indira, Lipid dynamics and its interaction with F1Fo ATP Synthase
- P188 Ghosh Indira, **Chacko Sajeev**, Patel Jignesh, Protein membrane interactions through molecular dynamics: F1Fo ATP- A case study
- P210 **Chacko Sajeev**, Ghosh Indira, Quantum chemical studies of proton transfer in F1Fo ATP
- Isha Nagpal **N. Subbarao**, S.Gourinath, In-silico screening of inhibitors against OASS and SAT of Entamoeba histolytica Cysteine biosynthetic pathway,
- Mr. **Vikram Singh** attended the "International Conference on Bioinformatics and Computational Biology 2011" (BICB 2011) held in Singapore during 28th February-1st March 2011 and gave an oral presentation of the paper "Spectral Analysis of Long Non-Coding RNAs". His paper has been selected for the **"Best Research Student Paper Award"** in this conference.
- Mr. **Om Prakash** has presented a poster in the 18th EuroQSAR Symposium at Rhodes, Greece from 19-24 September, 2010 and Participated for the OpenTox annual meeting to discuss developments on the creation of an Open Source-based predictive toxicology framework at Rhodes, Greece from 16-17 September, 2010 He was financially supported by CSIR and JNU.
- Mr. **Amit Kumar** has attended the conference on "Asia Pacific Bioinformatics Network's 10th InCoB – 1st ISCB Asia Joint Conference 2011" held on 30th November, 2011 to 2nd December, 2011 at Kuala Lumpur, Malaysia.
- **Rama Kalia** has oral presentation on "Disease-Target Relationship based Ontology" in International Conference Translational Bioinformatics Conference 2011 held in Seoul, South Korea in Nov 2011.

### Future Plans

- ❖ University with funding from UGC is constructing a new building with foot print of 20000 square Meters exclusively for our school which will be completed during 2011. Relocation of School of Computational and Integrative Science to New Building by July 2012
- ❖ Two Professors, five Associate Professors and two Assistant Professors are to be recruited under UGC IX Plan during 2012.
- ❖ JNU had submitted interdisciplinary project in collaboration with all the schools (School of Life Sciences, School of Biotechnology, Special centre for Molecular Medicine, School of Environmental Sciences and our school) to DBT under DBT Builder program.
- ❖ Building up of the research activities in the Center for Complex Systems Studies (CCSS).
- ❖ Proposal for Two year M.Sc course (computational and Integrative sciences) from 2012
- ❖ Continue to do focus Research work on Infectious Diseases.

**List of students who have completed their M.Tech and Ph.D successfully, Degree awarded during 2011 ( M.Tech and Ph.D. Thesis Titles)**

a) Ph.D. Students <http://ccbb.jnu.ac.in/thesis-p-2009-2011.html>

No.	Name of the Students	Title of Thesis	Supervisor
1	Candida Vaz (2006-2011)	Identification and discovery of miRNAs and Deciphering their role in gene regulatory networks	Prof. A. Bhattacharya
2	Alok K. Srivastava (2006-2011)	Gene Ontology Based Prediction and Analysis of Microarrays	Dr. Narinder Singh Sahni
3	Vikram Singh (2006-2011)	Coding and Noncoding Genes : Aspects of their Identification, Distribution, and Regulation	Prof. R. Ramaswamy

b) M.Tech students and their Thesis Titles (2009-2011)

<http://ccbb.jnu.ac.in/thesis-M-2009-2011.html>

Sr.#	Name of the Students	Thesis Title	Supervisor
1	Priyatama Pandey	Deep Sequencing Based Expression Analysis for Micro-RNA.	Prof. A. Bhattacharya Dr. Rashi Gupta
2	Pradeep Kumar Singh	Age Classification based on Facial images.	Dr. Lovekesh Vig
3	Teekam Singh	Segmentation of Intima Media Thickness (IMT) and Lumen Diameter (LD) in Ultrasound Carotid Artery Images.	Dr. A. Krishnamachari
4	Sanjiv Kumar Dwivedi	Classification of HIV type One Strains Using Profile Hidden Markov Models.	Dr. Supratim Sengupta
5	Salam Tolen Singh	Analysis of Deep Sequencing Data for Finding Variations in Micro RNA Sequences	Prof. A. Bhattacharya Dr. Rashi Gupta
6	Sabeeha Hasnain	Computational Modelling of Macromolecular motion inside Bacterial Cytoplasm.	Dr. Pradipta Bandyopadhyay
7	Abhilash Gangadharan	Simulation and Perturbation Studies of the E. coli Metabolic Profile using Flux Balance Analysis.	Dr. Andrew Lynn
8	Ravi Shankar Pandey	Inactivation Domains in mammalian X Chromosome: Markov Segmentation Analysis.	Prof. R. Ramaswamy
9	Suraj Kumar	Interfering Genotypic and Phenotypic network: Application to Cancer.	Prof. R. Ramaswamy
10	Pankaj Narang	Development of an Interactive Web-accessible Workflow System for Biological Network Studies.	Dr. Andrew Lynn
11	Deepika Gautam	An investigation into the use of a Machine Learning approach for generating Petri Net models of Biological System.	Dr. Lovekesh Vig