Progress Report of

Center of Excellence

2016 – 2017

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
The School of Computational and Integrative Sciences (SCIS) is involved in research and teaching programs in areas which are highly interdisciplinary in nature. The major aim of our school is to integrate computational and analytical tools and techniques from different branches of sciences and apply them to get deeper insights into some of the problems which are not hitherto attempted. The school's academic and research programs are currently structured and focused on the core area of Computational and Systems Biology and gradually emphasis is being laid on Complex Systems, Massive Modelling, Simulation and analysis. Department of Biotechnology (Govt. of India) has continued to support our school as a “Centre of Excellence (COE)” in Bioinformatics since beginning. Faculties and students are currently pursuing research in diverse fields such as Comparative Genomics, Structural Biology and in silico drug design, Biological Evolution, Biomolecular Simulations, data mining and analysis of large scale data, biophysics, systems biology, robotics, complex systems, artificial intelligence, Econophysics, Quantitative Finance and Statistical Physics. At Present there are fifteen core faculty and five adjunct faculty in our school. There are six faculty postions which are to be filled soon.

SCIS is offering from academic year 2015, an integrated M.Sc.-Ph.D. degree in Computational and Integrative Sciences with a specialization in either Computational Biology or Complex Systems. The Computational Biology stream will have equivalence to the M.Sc. in Bioinformatics, while the Complex Systems stream will have equivalence to the M.Sc. in Physical Sciences. Additionally, SCIS also offers admission to its Pre-Ph.D. and Direct Ph.D. Programmes in Computational Biology and Bioinformatics. The School has encouraged intake from multiple disciplines into these Programmes - Information Technology, Engineering Sciences, Bioinformatics, the Life Sciences/Biotechnology, the Physical and Chemical Sciences, among others.

Teaching and research Programs are ably supported by good computational and communication infrastructure consisting of computer clusters with multiprocessor nodes, large-memory nodes and GPUs to facilitate specialized research in the new Building of SCIS.

School of Computational and Integrative Sciences currently offers the following three academic programs for the current year.

(i) Direct admission to Ph.D. program in Computational Biology and Bioinformatics
(ii) Pre-Ph.D./Ph.D. in Computational Biology and Bioinformatics
(iii) M.Sc/Ph.D integrated in Computational and Integrative Sciences Specialization in Computational Biology or Complex Systems
(iv) Postgraduate Diploma in Big Data in Bioinformatics approved from next academic year

**Number of students under Current & earlier Courses offered:**

<table>
<thead>
<tr>
<th>Category</th>
<th>Details</th>
</tr>
</thead>
<tbody>
<tr>
<td>Total No of current Pre-Ph.D and Ph.D Students</td>
<td>41</td>
</tr>
<tr>
<td>Awarded Ph.D from 2016-2017</td>
<td>06</td>
</tr>
<tr>
<td>No of students :Integrated M.Sc-Ph.D during 2016</td>
<td>22</td>
</tr>
<tr>
<td>During 2016-2017 M.Tech students passed</td>
<td>16</td>
</tr>
<tr>
<td>Post Graduate Diploma M.Phil (equivalent) in Bioinformatics during 2001-2006</td>
<td>82</td>
</tr>
</tbody>
</table>

SCIS also has MoU with Queensland University, Australia and BII, Singapore. The student/faculty level exchange has taken place, benefiting the research activity of the School.
Publications during 2016-17:

1. Y Gigani, S Gupta, A Lynn, K Asotra, BKCa CHANNEL BASED CHEMICAL ENTITY RECOGNITION USING PATENT DATA CURATION AND MOLECULAR FIELD ALIGNMENT TECHNIQUE, Pharmacophore An International Research Journal 7 (4)
2. A Qayum, R Arya, AM Lynn, Ethnobotanical perspective of antimalarial plants: traditional knowledge based study, BMC research notes 9 (1), 67
4. D Singh, S Rawat, M Waseem, S Gupta, A Lynn, M Nitin, N Ramchiary, Molecular modeling and simulation studies of recombinant laccase from Yersinia enterocolitica suggests significant role in the biotransformation of non-steroidal anti-inflammatory drugs, Biochemical and biophysical research communications 469 (2), 306-312
5. VK Singh, AKrishnamachari, Context based computational analysis and characterization of ARS consensus sequences (ACS) of Saccharomyces cerevisiae genome: Genomics Data 9, 130-136 (2016)


47. GP Singh, Applications of Petri nets in electrical, electronics and optimizations, Electrical, Electronics, and Optimization Techniques (ICEEOT).


49. P Prathipati, C Nagao, S Ahmad, K Mizuguchi, Improved pose and affinity predictions using different protocols tailored on the basis of data availability, Journal of computer-aided molecular design 30 (9), 817-828.

50. M Fernandez, S Ahmad, JI Abreu, A Sarai, Large-scale recognition of high-affinity protease–inhibitor complexes using topological autocorrelation and support vector machines, Molecular Simulation 42 (5), 420-433.


53. Can an interdisciplinary field contribute to one of the parent disciplines from which it emerged? A Chakraborti, D Raina, K Sharma, The European Physical Journal Special Topics 225 (17-18), 3127-3135.

65. Madhulata Kumari, Subhash Chandra, Neeraj Tiwari and Naidu Subbarao High throughput virtual screening to identify Novel inhibitors for Mehionyl-tRNA synthetase of Brucella melitensis, Bioinformation 2016
66. Madhulata Kumari, Neeraj Tiwari and Naidu Subbarao and Subhash Chandra 3D QSAR based hit to lead optimization of Imidazolopiperazines derivatives against P.falciparum Imperial Journal of Interdisciplinary Research, 2016
69. Vijayan Ramachandran, Elavarasi Padmanaban, Kalaiarasan Ponnusamy Naidu Subbarao, Manoharan Natesan Pharmacophore based virtual screening for identification of marine bioactive compounds as inhibitors against macrophage infectivity potentiator (Mip) protein of Chlamydia trachomatis RSC Advances(2016) 6, 18946 – 18957
70. Ramachandran Vijayan, Naidu Subbarao, Natesan ManoharanComputational Study Enlightens the Structural Role and Molecular Mechanism of Marine Algal Compound Fucoidan against
Hepatocellular Carcinoma Markers. International Journal of Bioscience, Biochemistry and Bioinformatics(2016), 321-328

71. D.Raja Sudhakar, Kalaiarasan P and Naidu Subbarao, Docking and molecular dynamic simulation study of EGFR1 with EGF-like pepptides to understand Molecular Interactions. Accepted for Publication in Molecular Biosystems(2016), DOI:10.1039/c6mb00032k


73. A Jadaun, N Subbarao, A Dixit Allosteric inhibition of topoisomerase I by pinostrobin: Molecular docking, spectroscopic and topoisomerase I activity studies Accepted for publication Journal of Photochemistry and Photobiology B: Biology 2016

Book Chapter /Conference Proceedings

- Limit order books, F Abergel, A Chakraborti, M Anane, A Jedidi, IM Toke, Cambridge University Press

Workshop/Conferences during 2016-17

- Instructional Workshop on Computational Methods in Drug Discovery August 9-11, 2016.
- Workshop CCPM-6, Conversation with Experimentalist, 24 February 2016.
- Hands on Workshop on Pipeline pilot by BIOVIA August 24-25 2016 Prof Indira Ghosh
- Open Day of the School of Computational and Integrative Sciences 17th February 2016
- National Symposium on Recent trends in Computational biology to commemorate Silver Jubilee year 1-2 March 2016
- International conference/workshop on “Nano-Biointerface-2016 18-20 march 2016. Prof Anirban Chakraborti

Research Projects (active):

3. DST Fast Track for Young Scientist, Automaticity in Robot motor skill learning, Dr. Lovekesh Vig, 2013-2016.
6. Functional genomics approaches in understanding the regulation of synthesis and accumulation of apocarotenoids in saffron crocus (Crocus sativus L.) Department of Biotechnology, Government of India Principal Investigator: Dr. Mukesh Jain.

7. Transcriptome and epigenome diversity analysis during seed development for discovery of molecular markers and gene regulatory mechanism in chickpea Department of Biotechnology, Government of India Principal Investigator: Dr. Mukesh Jain.


10. Understanding the role of DNA flexibility in protein-DNA recognition, Funded By DST, India. PI: Dr. Arnab Bhattachaejee.

11. Characterization of transcriptional dynamics during male and female reproductive organ development in Sorghum Project Sanctioned: 1 from DST-SERB. PI Dr Rita Sharama.


13. All the Faculty were funded by University of Potential Excellence Project II Supported by UGC

The Thesis titles of Ph.D Students (Degree awarded) during 2016-17:

<table>
<thead>
<tr>
<th>S.N o.</th>
<th>Name of the Students</th>
<th>Ph.D Thesis Title</th>
<th>Supervisor Name</th>
</tr>
</thead>
<tbody>
<tr>
<td>01.</td>
<td>Mr. Vinod Kumar Singh</td>
<td>Identifying and characterizing DNA sequence features using content and context based computational analysis: a case study of yeast ARS sequences.</td>
<td>Dr. A. Krishnamachari</td>
</tr>
<tr>
<td>02.</td>
<td>Mr. Sabeeha Hasnain</td>
<td>Macromolecular Properties in Aqueous and Cellular Environments: Crowding, Diffusion and Hydrodynamics.</td>
<td>Prof. Pradipta Bandyopadhyay</td>
</tr>
<tr>
<td>03</td>
<td>Sudhanshu Shankar</td>
<td>Development And Application Of Computational Algorithms To Understand Structures And Functions Of Biomolecules</td>
<td>Prof. Pradipta Bandyopadhyay</td>
</tr>
<tr>
<td>04</td>
<td>Rama Kaalia</td>
<td>Analyzing Disease Target Drug Relationships</td>
<td>Prof. Indira Ghosh</td>
</tr>
<tr>
<td>05</td>
<td>Abdul Qayum</td>
<td>Gis Based Tarditional Knowledge Mapping Of Natural Resources Towards Identifying Malarial Hotspots And Antimalarials</td>
<td>Dr. Andrew Lynn</td>
</tr>
<tr>
<td>S.No.</td>
<td>Name of the Students</td>
<td>M.Tech Thesis Title</td>
<td>Supervisor Name</td>
</tr>
<tr>
<td>-------</td>
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<td>-----------------------------------------------</td>
</tr>
<tr>
<td>01.</td>
<td>Mr. Padam Kumar Singh</td>
<td>Study of Random walk model in genomic sequence of prokaryotes and Eukaryotes.</td>
<td>Prof. Anirban Chakraborti/Dr. A. Krishnamachari</td>
</tr>
<tr>
<td>02.</td>
<td>Mr. Praveen Mishra</td>
<td>Nano-bio interactions: A case study of protein with gold nanoparticles and two dimensional nanosheets.</td>
<td>Prof. Anirban Chakraborti</td>
</tr>
<tr>
<td>03.</td>
<td>Mr. Rajesh Prasad</td>
<td>Stochastic Modelling of Biomolecular System.</td>
<td>Prof. Indira Ghosh</td>
</tr>
<tr>
<td>04.</td>
<td>Mr. Ram Nayan Verma</td>
<td>Study of Sub-diffusion in crowded environment: A Toy model approach.</td>
<td>Prof. Pradipta Bandopadhyay</td>
</tr>
<tr>
<td>05.</td>
<td>Mr. Ambarish</td>
<td>NGSAP-VC: Variant Calling implemented as installable Galaxy workflows for NGS data.</td>
<td>Prof. Andrew Lynn</td>
</tr>
<tr>
<td>06.</td>
<td>Mr. Rinkoo Singh</td>
<td>Pathway based annotation of NGS data using Hidden Markov models and graph theoretic methods.</td>
<td>Prof. Andrew Lynn</td>
</tr>
<tr>
<td>07.</td>
<td>Ms. Deepika Yadav</td>
<td>Designing Novel Inhibitors Against Drug Target APOE4 Involved Alzheimers Disease and Interaction Study of Known Lipids with Cholesterol Binding Proteins.</td>
<td>Dr. Naidu Subbarao</td>
</tr>
<tr>
<td>08.</td>
<td>Mr. Kundan Kumar</td>
<td>Data Parallelization Using Hadoop.</td>
<td>Dr. Narinder Sahni</td>
</tr>
<tr>
<td>09.</td>
<td>Mr. Subhajit Das</td>
<td>Computational study and analysis of <em>Mycobacterium tuberculosis</em>-H37Rv SNP data: a case study of Ribosome binding site sequences.</td>
<td>Prof. Alok Bhattacharya/Dr. A. Krishnamachari</td>
</tr>
<tr>
<td>10.</td>
<td>Ms. Rupali Saini</td>
<td>DSP based computational Study and analysis of the power spectral density of coding segments in few AT rich and GC rich genomes.</td>
<td>Dr. A. Krishnamachari</td>
</tr>
<tr>
<td>11.</td>
<td>Ms. Mouzmeen Siraj Ansari</td>
<td>Whale identification via pre-trained models.</td>
<td>Dr. Lovekesh Vig</td>
</tr>
<tr>
<td>12.</td>
<td>Mr. Raveendra Kumar</td>
<td>Crime Prediction via Machine Learning.</td>
<td>Dr. Lovekesh Vig</td>
</tr>
<tr>
<td>13.</td>
<td>Mr. Shabab Akbar</td>
<td>Origin of complexity in p53 regulatory network.</td>
<td>Dr. R.K. Brojen Singh</td>
</tr>
<tr>
<td>14.</td>
<td>Mr. Rajpati Verma</td>
<td>Self organization in neuron dynamics.</td>
<td>Dr. R.K. Brojen Singh</td>
</tr>
<tr>
<td>15.</td>
<td>Mr. Mohit Bakshi</td>
<td>Comparative genomic analysis of TCP family transcription factors in Sorghum.</td>
<td>Dr. Rita Sharma</td>
</tr>
<tr>
<td>16.</td>
<td>Mr. Md. Ali Imam</td>
<td>Analysis of publicly available microarray data</td>
<td>Dr. Rita Sharma</td>
</tr>
</tbody>
</table>
and construction of a local database for extraction and visualization of gene expression in Sorghum.

List of Trainee 2016

<table>
<thead>
<tr>
<th>S.No.</th>
<th>Name of the Trainee</th>
<th>Institute Name</th>
<th>Supervisior Name</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>IcxaKhandelwal</td>
<td>Jaypee university of Information Technology, Solan H.P</td>
<td>Dr.NaiduSubbarao</td>
</tr>
<tr>
<td>2</td>
<td>L Naga Rajiv</td>
<td>Birla institute of Technology and Science Pilani</td>
<td>Prof.Indira Ghosh</td>
</tr>
<tr>
<td>3</td>
<td>Prashant Gupta</td>
<td>Jaypee Institute of Information Technology, Noida</td>
<td>Dr.NaiduSubbarao</td>
</tr>
<tr>
<td>4</td>
<td>Gagendeep Singh</td>
<td>IP University</td>
<td>Dr.LovekeshVig</td>
</tr>
<tr>
<td>5</td>
<td>Amol KhanduNarwada</td>
<td>Mumbai University</td>
<td>Prof.Pradipta</td>
</tr>
<tr>
<td>6</td>
<td>Debasisi Sardar</td>
<td>IISER, Kolkata</td>
<td>Prof.Indira Ghosh</td>
</tr>
<tr>
<td>7</td>
<td>Poonam</td>
<td></td>
<td>Dr. Andrew M Lynn</td>
</tr>
<tr>
<td>8</td>
<td>Ranjhna</td>
<td></td>
<td>Prof. Indira Ghosh</td>
</tr>
<tr>
<td>9</td>
<td>Naveen</td>
<td></td>
<td>Prof. Indira Ghosh</td>
</tr>
<tr>
<td>10</td>
<td>Rama Kalia</td>
<td>SC&amp;IS, JNU</td>
<td>Prof. Indira Ghosh</td>
</tr>
</tbody>
</table>

Future Plan

- Recruitment of more Faculty is in progress.
- Ramachandran Fellowships and few technical positions to be filled up.
- One year PG Diploma in “Big Data in Bioinformatics” will be launched from July 2017.
- Improving Infrastructure in High Performance computing Facility in New Building using DST Purse Funds.

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