

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 Statistial 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:

Total No of current Pre-Ph.D and Ph.D Students :	41
Awarded Ph.D from 2016-2017:	06
No of students :Integrated M.Sc-Ph.D during 2016:	22
During 2016-2017M.Tech students passed:	16
Post Graduate Diploma M.Phil (equivalent) in Bioinformatics during 2001-2006:	82

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.

Publicationsduring 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
- 3. M Kamran, S Sinha, P Dubey, **AM Lynn**, SK Dhar, Identification of putative Z-ring-associated proteins, involved in cell division in human pathogenic bacteria Helicobacter pylori, FEBS letters 590 (14), 2158-2171
- 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, A Krishnamachari, Context based computational analysis and characterization of ARS consensus sequences (ACS) of Saccharomyces cerevisiae genome: Genomics Data 9, 130-136 (2016)
- 6. **Arnab Bhattacherjee**, Dana Krepel and Yaakov Levy, Coarse-grained models for studying protein diffusion along DNA: WIREs Computational Molecular Science 2016. doi: 10.1002/wcms.1262 (2016)
- 7. RajanShrivastava, AvijitRakshit, SudhanshuShanker, LovekeshVig, **PradiptaBandyopadhyay**, A combination of Monte Carlo Temperature Basin Paving and graph theory: water cluster low energy structures and completeness of search. J.Chem.Sci (2016), 128, 1507.
- 8. Priya Singh, **P. Bandyopadhyay**, S. K. Sarkar, Folding-unfolding transition in the mini-protein villin headpiece (HP35): An equilibrium study using the Wang-Landau algorithm. Chem. Phys., 468, 1-8 (201
- 9. SudhanshuShanker and **PradiptaBandyopadhyay**, J.Bio.Str.Dyn. (in press, 2016), How Mg2+ ion and water network affect the stability and structure of non-Watson-Crick base pairs in E coli Loop E of 5S rRNA: A Molecular Dynamics and Reference Interaction Site Model (RISM) study.
- 10. T.Asada, K.Ando, **P.Bandyopadhyay**, S.Koseki, Free Energy Contribution Analysis using Response Kernel Approximation: Insights into the Acylation Reaction for beta–lactamase, J.Phys.Chem.B(in press), 2016
- 11. R. Kaalia, **I. Ghosh**, Semantics based approach for analyzing disease-target associations, Journal of Biomedical Informatics 62 June (2016) 125–135
- 12. Rama Kaalia, Ashwin Srinivasan, Amit Kumar and **Indira Ghosh**; ILP-assisted de novo drug design. Machine Learning, June 2016, Volume 103, Issue 3, pp 309–341, published online, DOI 10.1007/s10994-016-5556-x. March 2016.
- 13. Rama Kaalia, AmitKumar, Ashwin Srinivasan, and Indira Ghosh; An Ab Initio Method for Designing Multi-Target Specific Pharmacophores using Complementary Interaction Field of Aspartic Proteases. Mol. Inf. (2015), 34, 2–16

- 14. 4. Khan, Taushif; Ghosh, Indira. Modularity in protein structures: A study on all alpha proteins. Journal of Biomolecular Structure & Dynamics(Feb 2015) http://dx.doi.org/10.1080/07391102.2014.1003969
- 15. Sandeep Kumar, **Binod K. Kanaujia**, Shantanu Dwari, Ganga Prasad Pandey, and Dinesh Kumar Singh, "11–17 GHz Reconfigurable Stacked Power Amplifier Using Matched Slant Microstrip Line for Ku Band Application," Wireless Personal Communication Springer vol., pp., 2016. (Accepted)
- 16. Sachin Kumar, **Binod Kr Kanujia**, Mukesh k. khandelwal and A. K. Gautam, "Single-Feed Superstrate Loaded Circularly Polarized Microstrip Antenna for Wireless Applications," Wireless Personal Communication Springer vol., pp.1-11, 2016. (Accepted)
- 17. Naveen Jaglan, **Binod K. Kanaujia**, samir D Gupta and Sweta Srivastava "Triple Band Notched UWB Antenna Design Using Electromagnetic Band Gap Structures," Progress In Electromagnetics Research C (USA) vol. 66, pp.139-147, 2016.
- 18. Naveen Jaglan, samir D Gupta, **Binod K. Kanaujia** and Sweta Srivastava "Band Notched UWB Circular Monopole Antenna with Inductance Enhanced modified mushroom EBG structures," Wireless Networks Springer vol., pp., 2016. (Accepted)
- 19. S. Yadav, A.K.Gautam, Anil k Sinh, **Binod Kr Kanaujia** and K Rambabu, "Design of Band-Rejected UWB Planar Antenna with Integrated Bluetooth Band" IET Microwaves, Antenna & Propagation, (UK) vol., no., pp., 2016. (Accepted).
- 20. **Binod Kr Kanujia**, Mukesh k. khandelwal, SantanuDwari, Sachin Kumar and A. K. Gautam, "Analysis and Design of Compact High Gain Microstrip Patch Antenna with Defected Ground Structure for Wireless Applications," Wireless Personal Communication, Springer vol., pp., 2016. (Accepted)
- 21. Sandeep Kumar, Mitul Handa, Himanshu Bhasin and **Binod K. Kanaujia**, Shantanu Dwari, "Optimized Threshold Voltage Variation for Tunable Body Biasing CMOS Power Amplifier"," Wireless Personal Communication, Springer vol., pp., 2016. (Accepted)
- 22. Kunal Srivastava, Ashwani Kumar, A.K Verma, Q. Zhang, **Binod Kr Kanujia**, and S Dwari, "Integrated GSM and UWB Fractal Monopole Antenna with Triple Notches," Microwave and Optical Technology Letters, (USA) vol.58, no.10, pp.2364-2366, 2016.
- 23. Anil kumar Singh, Ravi kumar Gangwar, and **Binod Kr Kanujia**, "Circularly Polarized Annular Ring Microstrip Antenna for High Gain Application," Electromagnetic, Taylor and Francis vol.36, no.6, pp.379-391, 2016
- 24. PallaviBartwal, A.K.Gautam, Anil k Sinh, **Binod Kr Kanaujia** and K Rambabu, "Design of Compact Multi-Band Meander-Line Antenna for GPS/WLAN/WiMAX band Applications in Laptops/Tablets" IET Microwaves, Antenna & Propagation, (UK) vol., no., pp., 2016. (Accepted).
- 25. JugalKishor, **Binod Kr Kanujia**, Shantanu Dwari, and Ashwani Kumar, "Bandpass Filter Using Dielectric Resonator with Transmission Zeros," Microwave and Optical Technology Letters, (USA) vol.58, no.7, pp.1583-1586, 2016.
- 26. Kunal Srivastava, Ashwani Kumar, and **Binod Kr Kanujia**, "Design of Compact Penta-Band and Hexa-Band Microstrip Antennas" Frequenz (Germany) vol. 70, no. 3-4, pp.101-111, Jan. 2016.

- 27. J. P. Keshari, **Binod Kr Kanujia**, Mukesh k. khandelwal, Pritam Singh Bakariya and R. M. Mehra, "Single-Feed Circularly Polarized Stacked Patch Antenna with Small Frequency Ratio for Dual-Band Wireless Applications" International Journal of Microwave and Wireless Technologies Cambridge University Press, (UK) vol., pp., 2016. (Accepted)
- 28. A.K.Gautam, Lalit Kumar, **Binod Kr Kanaujia** and K Rambabu, "Design of Compact F-shaped slot Triple Band Antenna for WLAN/WiMAX Applications" IEEE Trans. Antennas Propagat., (USA) vol. 64, no. 03, pp. 1101-1105, March 2016.
- 29. AkankshaFarswan, A.K.Gautam, **Binod Kr Kanaujia** and K Rambabu, "Design of Koch Fractal Circularly Polarized Antenna for Handheld UHF RFID Reader Applications" IEEE Trans. Antennas Propagat., (USA) vol. 64, no. 2, pp. 771-775, 2016.
- 30. S. Yadav, A. K. Gautam, and **Binod Kr Kanujia**, "Design of miniaturized single band notch micro strip antenna with enhanced UWB performance," Microwave and Optical Technology Letters, (USA) vol. 58, no. 6, pp. 1494-1499, 2016.
- 31. Kunal Srivastava, Ashwani Kumar, and **Binod Kr Kanujia**, "Design of Compact Penta-Band Microstrip Antennas," Microwave and Optical Technology Letters, (USA) vol. 58, no. 4, pp. 836-838, 2016.
- 32. A. K. Gautam, A. Bisht and **Binod Kr Kanujia**, "A Wideband Antenna With Defected Ground Plane for WLAN/WiMAX Applications" International Journal of Electronics and Communication AEU Elsevier, (Germany) vol. 70, no. 3, pp. 354-358, 2016.
- 33. Anil kumar Singh, Ravi kumarGangwar, and **Binod Kr Kanujia**, "Sectored Annular Ring Microstrip Antenna with DGS for Circular Polarization," Microwave and Optical Technology Letters, (USA) vol.58, no.3, pp.569-573, 2016.
- 34. Deepak Gangwar, Sushrut Das, R. L. Yadav and **B. K. Kanaujia**, "Circularly Polarized Inverted Stacked High Gain Antenna with Frequency Selective Surface," Microwave and Optical Technology Letters, (USA) vol.58, no.3, pp.732-740, 2016.
- 35. **Sharma R.**, Wungrampha W., Singh V., Pareek A. and Sharma, M.K. (2016) Halophytes as Bioenergy Crops. Frontiers in Plant Science doi: 10.3389/fpls.2016.01372.
- 36. Kundu S., **Sharma R.** (2016) In silico Identification and taxonomic distribution of plant class C GH9 endoglucanases. Frontiers in Plant Science http://dx.doi.org/10.3389/fpls.2016.01185.
- 37. Chandran A.K.N., Yoo Y.H., Cao P., **Sharma R.**, Sharma M.K., Dardick C., Ronald P.C. and Jung K.H. (2016) Updated rice kinase database RKD 2.0: enabling transcriptome and functional analysis of rice kinase genes. Rice 9:40
- 38. Harkenrider M., **Sharma R.**, Vleesschauwer D.D., Tsao, L., Zhang X., Chern M., Canlas P., Zuo S. and Ronald P.C. (2016) Overexpression of rice Wall-Associated Kinase 25 (WAK25) alters resistance to bacterial and fungal pathogens. Plos One 11 (1):e0147310.
- 39. Gupta P., **Sharma R.**, Sharma M.K., Sharma M.P., Stapute G.K., Garg S., Singla-Pareek, S.L., Pareek A. (2016) Signaling cross talk between biotic and abiotic stress responses in soybean. Abiotic and Biotic Stresses in Soybean Production: Soybean Production, Volume 1, 27-52.
- 40. Sharma M.K*., **Sharma R***., Cao P., Harkenrider M., Jenkins J., Grimwood J., Zhang J., Udvardi M.K., Schmutz J. and Ronald P.C. (2015) Targeted switchgrass BAC library screening and sequence analysis identifies predicted biomass-related and stress response-related genes. BioEnergyResearch, 9 (1): 109-122.

- 41. Khemka N, Singh VK, Garg R, **Jain M.** (2016) Genome-wide analysis of long intergenic non-coding RNAs in chickpea and their potential role in flower development. Scientific Reports 6, 33297. doi:10.1038/srep33297
- 42. Shankar R, Bhattacharjee A, **Jain M.** (2016) Transcriptome analysis in different rice cultivars provides novel insights into drought and salinity stress responses. Scientific Reports 6, 23719. DOI: 10.1038/srep23719.
- 43. Bhattacharjee A, Khurana JP, **Jain M.** (2016) Characterization of rice homeobox genes, OsHOX22 and OsHOX24, and over-expression of OsHOX24 in transgenic Arabidopsis suggest their role in abiotic stress response. Frontiers in Plant Science 7, 627. doi: 10.3389/fpls.2016.00627.
- 44. **Jain M**, Srivastava PL, Verma M, Ghangal R, Garg R. (2016) De novo transcriptome assembly and comprehensive expression profiling in Crocus sativus to gain insights into apocarotenoid biosynthesis. Scientific Reports 6, 22456. doi: 10.1038/srep22456.
- 45. Garg R, Shankar R, Thakkar B, Kudapa H, Krishnamurthy L, Mantri N, Varshney RK, Bhatia S, **Jain M.** (2016) Transcriptome analyses reveal genotype- and developmental stage-specific molecular responses to drought and salinity stresses in chickpea. Scientific Reports 6, 19228. doi: 10.1038/srep19228
- 46. Kotwal S, Kaul S, Sharma P, Shankar R, **Jain M**, Dhar M. (2016) De novo transcriptome analysis of medicinally important Plantago ovata using RNA-Seq. PLoS ONE 11,e0150273. doi:10.1371/journal.pone.0150273.
- 47. **GP Singh**, Applications of Petri nets in electrical, electronics and optimizations, Electrical, Electronics, and Optimization Techniques (ICEEOT).
- 48. **GP Singh**, S Kansal, Basic Results on Crisp Boolean Petri Nets, Modern Mathematical Methods and High Performance Computing in Science and Technology.
- 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.
- 51. Co-movements in financial fluctuations are anchored to economic fundamentals: A mesoscopic mapping, K Sharma, B Gopalakrishnan, AS Chakrabarti, A Chakraborti, arXiv preprint arXiv:1612.05952.
- 52. Resonance Raman scattering and ab initio calculation of electron energy loss spectra of MoS 2 nanosheets, **A Chakraborti**, AS Patel, PK Kanaujia, P Nath, GV Prakash, D Sanyal, Physics Letters A 380 (48), 4057-4061.
- 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.
- 54. Investigating resonance energy transfer from protein molecules to van der Waals nanosheets, AS Patel, P Mishra, PK Kanaujia, SS Husain, GV Prakash, A Chakraborti, arXiv preprint arXiv:1611.07182.

- 55. Thermal Equilibrium in D-dimensions: From Fluids and Polymers to Kinetic Wealth Exchange Models, M Patriarca, E Heinsalu, A Singh, A Chakraborti, arXiv preprint arXiv:1610.03367.
- 56. Sectoral co-movements in the Indian stock market: A mesoscopic network analysis, K Sharma, S Shah, **AS Chakrabarti**, A Chakraborti, arXiv preprint arXiv:1607.05514.
- 57. Physicists' approach to studying socio-economic inequalities: Can humans be modelled as atoms?K Sharma, **A Chakraborti**, arXiv preprint arXiv:1606.06051.
- 58. Gold nanoflowers as efficient hot-spots for surface enhanced Raman scattering. AS Patel, S Juneja, PK Kanaujia, GV Prakash, A Chakraborti, arXiv preprint arXiv:1604.02793.
- 59. Quantifying invariant features of within-group inequality in consumption across groups. Anindya S Chakrabarti, Arnab Chatterjee, Tushar K Nandi, Asim Ghosh, **AnirbanChakraborti.**
- 60. Invariant features of spatial inequality in consumption: The case of India. A Chatterjee, AS Chakrabarti, A Ghosh, **A Chakraborti**, TK Nandi, Physica A: Statistical Mechanics and its Applications 442, 169-181.
- 61. Discussion and Debate: Can Economics be a Physical Science? Sinha, **AS Chakrabarti**, M Mitra, JB Rosser Jr, RJ Buonocore, ...The European Physical Journal Special Topics 225 (17-18).
- 62. Performance Evaluation of Empirical Mode Decomposition Algorithms for Mental Task Classification. A Gupta, D Kumar, A Chakraborti, K Sharma. bioRxiv, 076646.
- 63. M shahar Yar Ankita Rathore, Raja Sudhakar, Mohamed Jawed Ahsan, Abuzer Ali, **Naidu Subbarao**, Suender Singh Yadav, Sadiq Umerin vivo anti-inflammatoryactivity and dockin study of newly synthesized benzamidazole derivatives bearing oxadiazole and morpholine rings, Biorganic Chemistry 2016
- 64. Sharmistha Dey Rahul Kumar, Lokesh Nigam, Amrendra Pratap Singh, Kusum Singh, **Naidu Subbarao**, Design, synthesis of allosteric peptide activator for human SIRT1 and its biological evaluation in cellular model of Alzheimer's disease, European Journal of Medicinal Chemistry, 2016
- 65. Madhulata Kumari, Subhash Chandra, Neeraj Tiwari and **Naidu Subbarao** High throuput virtual screening to identify Novel inhibitors for Mehionyl-tRNA synthetase of Brucella mellitensis, 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
- 67. Anis Ahmad, D.Raja Sudhakar, **Naidu Subbarao** and Asad U Khan, Designing, synthesis and antimicrobial action of oxazoline and thiazoline derivatives of fatty acid esters, Journal of Biomolecular Structure and Dynamics, 2016
- 68. Madhulata Kumari, Subhash Chandra, Neeraj Tiwari and **Naidu Subbarao** 3D QSAR, pharmacophore and molecular docking studies of known inhibitors and designing of novel inhibitors for M18 aspartyl aminopeptidase of Plasmodium falciparum BMC Structural Biology (2016) 16:12 DOI 10.1186/s12900-016-0063-7
- 69. Vijayan Ramachandran, Elavarasi Padmanaban, Kalaiarasan Ponnusamy Naidu Subbarao, Manoharan Nateshan 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 peprides to understand Molecular Interactions. Accepted for Publication in Molecular Biosystems(2016), DOI:10.1039/c6mb00032k
- 72. Ali Saber Abdelhameed, Mohammad Rehan Ajmal, Kalaiarasan Ponnusamy, **Naidu Subbarao**, Rizwan Hasan Khan, Interaction of the recently approved anticancer drug nintedanib with human acute phase reactant α 1-acid glycoprotein, <u>Journal of Molecular Structure</u> <u>Volume 1115</u>, 5 July 2016, Pages 171–179
- 73. A Jadaun, **N Subbarao**, A Dixit <u>Allosteric inhibition of topoisomerase I by pinostrobin:</u> <u>Molecular docking, spectroscopic and topoisomerase I activity studies</u> Accepted for publication Journal of Photochemistry and Photobiology B: Biology 2016

Book Chapter / Conference Proceedings

- Power-Laws as Statistical Mixtures, M Patriarca, E Heinsalu, L Marzola, **A Chakraborti**, K Kaski, Proceedings of ECCS 2014, 271-282.
- 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):

- DST project on "Development and application of new computational techniques to understand macromolecular properties in realistic cellular environment.". PI: Dr. PradiptaBandhyopadhyay, 2014-2017.
- 2. **DBT Builder Project**, Coordinator: Prof R.Bhat, SBT, JNU (SLS, SCMM and SBT and SCIS faculty of JNU) 2012-2017.
- 3. DST Fast Track for Young Scientist, **Automaticity in Robot motor skill learning**, DrLovekeshVig, 2013-2016.
- 4. DST project, stochastic synchronization: Complexity in signal processing in interacting system. Role of noise and application ,Brojen Singh, 2013-2016
- 5. CSIR Project Understanding Complex dynamics and information proceeding in Brain Network, Brojen Singh, 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.
- 8. Exploring transcriptome dynamics of chickpea development for candidate gene discovery and defining regulatory elements/modules under Challenge Programme on Chickpea Functional Genomics Department of Biotechnology, Government of India Principal Investigator :Dr. Mukesh Jain.
- 9. Positive and negative impacts of macromolecular crowding agents during target site location by DNA binding proteins origin of optimal search at physiological ionic concentration, Funded By DST, India. PI:Dr. Arnab Bhattachaejee.
- 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.
- 12. "Indo-US Advanced Bioenergy Consortium: Second Generation Biofuels" supported by IUTSSF, PI- AshwaniPareek, SLS duration: 2016-2021 member. Co-PI: Prof. Indira Ghosh.
- 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:

S.N o.	Name of the Students	Ph.D Thesis Title	Supervisior Name
01.	Mr. Vinod Kumar Singh	Identifying and characterizing DNA sequence features using content and cotext based computational analysis: a case study of yeast ARS sequences.	Dr. A.Krishnamachari
02.	Mr. SabeehaHasnain	Macromolecular Properties in Aqueous and Cellular Environments: Crowding, Diffusion and Hydrodynamics.	Prof. PradiptaBandyopadhyay
03	Sudhanshu Shankar	Development And Application OfComputational Algorithms Tounderstand Structures And FunctionsOf Biomoleules	Prof.PradiptaBandyopadhyay
04	Rama Kaalia	Analyzing Disease Target Drug Relationships	Prof. Indira Ghosh
05	Abdul Qayum	Gis Based Tarditional KnowledgeMapping Of Natural ResourcesTowards Identifying Malarial HotspotsAnd Antimalarials	Dr.Andrew Lynn

06	Rashmi Kumari	Application Of Computational Methods In	Dr.Andrew Lynn
		Rational Design OfThermostability And	
		BiomolecularInteractions	

The Thesis titles of M.Tech Students (Degree awarded) during 2016-17 $\,$

S.No.	Name of the Students	M.Tech Thesis Title	Supervisior Name
01.	Mr. Padam Kumar Singh	Study of Random walk model in genomic sequence of prokaryotes and Eukaryotes.	Prof. AnirbanChakraborti/ Dr.A.Krishnamachari
02.	Mr. Praveen Mishra	Nano-bio interactions: A case study of protein with gold nanoparticles and two dimensional nanosheets.	Prof. AnirbanChakraborti
03.	Mr. Rajesh Prasad	Stochastic Modelling of Biomolecular System.	Prof. Indira Ghosh
04.	Mr. Ram NayanVerma	Study of Sub-diffusion in crowded environment: A Toy model approach.	Prof. PradiptaBandyopadhyay
05.	Mr. Ambarish	NGSAP-VC: Variant Calling implemented as installable Galaxy workflows for NGS data.	Prof. Andrew Lynn
06.	Mr. Rinkoo Singh	Pathway based annotation of NGS data using Hidden Markov models and graph theoretic methods.	Prof. Andrew Lynn
07.	Ms. Deepika Yadav	Designing Novel Inhibitors Against Drug Target APOE4 Involved Alzeimers Disease and Interaction Study of Known Lipids with Cholesterol Binding Proteins.	Dr. Naidu Subbarao
08.	Mr. Kundan Kumar	Data Parallelization Using Hadoop.	Dr. NarinderSahni
09.	Mr. Subhajit Das	Computational study and analysis of Mycobacterium tuberculosis- H37Rv SNP data: a case study of Ribosome binding site sequences.	Prof. Alok Bhattacharya/ Dr. A.Krishnamachari
10.	Ms. Rupali Saini	DSP based computational Study and analysis of the power spectral density of coding segments in few AT rich and GC rich genomes.	Dr. A.Krishnamachari
11.	Ms. MouzmeenSiraj Ansari	Whale identification via pre-trained models.	Dr. LovekeshVig
12.	Mr. Raveendra Kumar	Crime Prediction via Machine Learning.	Dr. LovekeshVig
13.	Mr. Shabab Akbar	Origin of complexity in p53 regulatory network.	Dr. R.K. Brojen Singh
14.	Mr. RajpatiVerma	Self organization in neuron dynamics.	Dr. R.K. Brojen Singh
15.	Mr. MohitBakshi	Comparative genomic analysis of TCP family transcription factors in Sorghum.	Dr. Rita Sharma
16.	Mr. Md. Ali Imam	Analysis of publicly available microarray data	Dr. Rita Sharma

and construction of a local database for	
extraction and visualization of gene expression	
in Sorghum.	

List of Trainee 2016

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

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.

Prof. Andrew M Lynn

Coordinator

DBT-Centre of Excellence in Bioinformatics

School of Computational and Integrative Sciences

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