# National Center for Bioinformatics (NCB)

# Annual Progress Report 2013


National Centre For Bioinformatics

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# Introduction

Bioinformatics derives knowledge from computer analysis of biological data. This can consist of the information stored in the genetic code, but also experimental results from various sources, patient statistics, and scientific literature. Research in bioinformatics includes method development for storage, retrieval, and analysis of the data. Bioinformatics is a rapidly development branch of biology and is highly interdisciplinary, using techniques and concepts from informatics, statistics, mathematics, chemistry, biochemistry, physics, and molecular biology. It has many practical applications in different areas of biology and medicine. The use of computational methods in biomedicine deals with the analysis, storage, manipulation and interpretation of macromolecules such as DNA, RNA and proteins. Conversely, wet lab analysis of computationally predicted functionally relevant motifs/segments of macromolecules further enhances our understanding of complex mechanisms occurring in cells. On the basis of significance of this discipline, NCB was established as a faculty affiliated research centre in 2008 through funding by Higher Education Commission. It is housed in 53000 square feet building comprising multiple research and computational labs. Besides, it integrates Department of Computer Sciences, other Department s of Biological Sciences and Depart of Mathematics.

NCB if offering M.Phil and Ph.D Programs in the area of Bioinformatics.

1. **CHAIRPERSON AND DEAN DR. ASGHARI BANO**

   **PhD**: Glasgow University, U.K
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2. **DR. AMIR ALI ABBASI (EVOLUTIONARY AND COMPARATIVE GENOMICS)**

   **PhD**: Philipps University Marburg, Germany
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2. **DR. SAJID RASHID (FUNCTIONAL INFORMATICS)**

   **Postdoc:** IIMCB, Warsaw, Poland
   **PhD:** Functional Genomics,
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3 **DR. SYED SIKANDER AZAM (MOLECULAR DYNAMICS)**

   **PhD**: University of Innsbruck, Austria.
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4. **DR. MUHAMMAD FAISAL (STATISTICAL BIOINFORMATICS)**

   **PhD**: University of Vienna, Austria
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**Note:** For more information about faculty, please visit http://ncb.qau.edu.pk/index.php/people/faculty.html

# Faculty Research Interests

Dr. Amir Ali Abbasi is long fascinated in several areas of research landscapes within the scope of Evolutionary and Functional Genomics, Population and Medical Genetics, Evolutionary Developmental Biology and Genome Bioinformatics. He is very keen to integrated computational methodological work which is tight in with experimental research and external collaborations, where his group studies the variability of molecular traits in different systems, including Zebra fish and transgenic mice models. Another enthralling area of his lab lies in deciphering evolution of vertebrate gene families and genomes in order to pin down the major morphological transitions that vertebrates accomplished during their deep history (>450 mya). With the recent availability of vast amount of population-wide genomic data, his current interests lie in the field of evolutionary medicine with the application of modern evolutionary theory to understanding health and disease. Currently his group is trying to answer how evolution has shaped the human physiology under different environmental pressures and life styles over-time that may leave us susceptible to certain diseases. Such evolutionary approaches have important implications in advancing the knowledge of medical science regarding systematic molecular diagnostics and treatment of certain diseases like, antibiotic resistance, cancer, autoimmune disease and human anatomy.

Dr Sajid Rashid functional informatics lab is focused to identify novel protein complexes and pathways involved in human diseases. Moreover, they are specialized in predicting novel drug targets and developing novel algorithms/tools for monitoring protein-protein or protein-drug interactions. The protein interactions are functionally annotated to characterize the associated pathways and diseases. Various in-silico approaches including modeling, docking and MD simulations linked with structural and functional knowledge are embedded together with experimental evidences to draw meaningful conclusions. The predicted results are validated by wet lab techniques which include coimmunoprecipitation, GST-pull down and 2-dimentsional gel electrophoresis assays. Moreover, predicted drugs are validated in mice. We have a well-established mice lab in the vicinity of NCB containing knock-out mice models.

Dr Sikander Azam research interests lied in the field of Computational Biochemistry. In particular, Molecular Docking and Molecular Dynamic (MD) Simulations of proteins for understanding structural and dynamical aspects of the biological system. The application of Molecular Mechanic (MM), and Hybrid Quantum Mechanical / Molecular Mechanical (QM/MM) Molecular Dynamic (MD), and Quantum Mechanical Charge Field (QMCF) Molecular Dynamic Simulations for the evaluation of structural and dynamical properties of biologically and industrially important ions in aqueous solution are another dimensions of his interests. He is currently establishing a computational facility lab at the National Centre for Bioinformatics which helps to maintain the synergistic relationship with the experimental research work carried out on various proteins at the resource lab of the institute.

Dr Muhammad Faisal is enthusiastically involved in developing statistical methods to understand the 'missing heritability'. In this journey, one of the challenges is to understand the functional impact of non-coding variants (prediction of Transcriptional Binding Sites, Chromatin Structure, and methylated sites). Statistical methods are crucial in many Bioinformatics problems and applications. Especially the analysis of large scale omics data requires not only massive computation and efficient algorithms, but also relies on solid statistical methodologies. The boom of next generation sequencing (NGS) technology and its applications to a wide range of biomedical fields has brought about many computations and statistical challenges such as; analyzing RNA-seq, Chip-seq data, analysis of GWAS and microarray data and their meta-analysis. Moreover, it is not limited to estimation of missing values in microarray data and in the area of applied Spatial Statistics.

# MPhil Thesis Produced in Year 2013

| S. No. | Name of Student | Thesis Title |
|---|---|---|
| 1. | Shahid Ali | Elucidating Cis-Acting Regulatory Elements in a Transcroiptional Mediator Gene: GLI3 |
| 2. | Nashaiman Pervaiz | Reconstructing the evolutionary history of human WDR62 gene and its implication in human brain size and intelligence |
| 3. | Wajya Ajmal | Evidence of Ancient Segmental Duplications during Vertebrate Evolution |
| 4. | Hiba Khan | Examining the authenticity of 'One–to–Four Model' in vertebrates through Phylogenetic Analysis of the proposed paralogon; Hsa4, Hsa5, Hsa8 and Hsa10 |
| 5. | Amen Shamim | In Silico Exploration of Druggable Genome of Streptococcus gordonii for the Identification of Therapeutic Drugs |
| 6. | Maria Batool | Investigation for Druggable Genome of Styphlococcus aureus JH9 through Computational Studies |
| 7. | Nida Khalid | Investigation for Druggable Genome of Streptococcus sanguinis SK36 through various Computational Tools. |
| 8. | Iqra Sohail | Elucidation of binding interaction of RNA Recognition Motif to Cholinesterase via Solvated Molecular docking & MD Simulation |
| 9. | Sadaf Ambreen | Molecular Phylogenetic analysis of multigene families with members residing on HOX-cluster paralogons |
| 10. | Bibi Amina | Deciphering the regulatory code for limb specific CNE enhancers across vertebrates by employing comparative genomics approach |
| 11. | Noor Afshan | Evolutionary Conserved Cardiac Patterns in the Sequences of Functionally Defined Enhancers |
| 12. | Zohra Bibi | Differential Expression Pattern of Coexpressed Genes in Human and Mouse: A Computational and Statistical Study |
| 13. | Muhammad Aqeel | Computational screening of human proteome associated with mentha related phytochemicals: A metabolic study linking the interactome data |
| 14. | Sara Sarfaraz | Molecular Modeling and Comparative Dynamic Studies of Myo-Inositol-1-phosphate synthase |
| 15. | Mirza Ahmed Hammad ul Mubeen Muhammad | Comparative Molecular Dynamics Simulation Studies of WNT-4 Protein |
| 16. | Shifa Tahir | Molecular Modeling and Molecular Dynamics Simulation Studies of Amidophosphoribosyl transferase |

# Research Publications in Year 2013

1. **Abbasi A. A**., Minhas R., Schmidt A., Koch, S., and Grzeschik K.H. (2013). Cis-regulatory underpinnings of human GLI3 expression in embryonic craniofacial structures and internal organs. ***Development Growth and Differentiation***. 55(8), 699-709 **(IF: 2.397)**
2. Asrar Z., Haq F., **Abbasi A. A.**(2013)**.** Fourfold paralogy regions on human HOX-bearing chromosomes: Role of ancient segmental duplications in the evolution of vertebrate genome, ***Molecular Phylogenetics and Evolution.*** 66(3), 737–747. **(IF: 4.066)**
3. Parveen N., Masood A., Iftikhar N., Minhas B., Minhas R., Nawaz U., and **Abbasi A. A*.**(2013). Comparative genomics using teleost fish helps to systematically identify target gene bodies of functionally defined human enhancers. ***BMC Genomics***, 14(1), 122. **(IF: 4.397)**
4. A**zam S.S.**, Saroosh A., Zaman N., and Raza, S. (2013). Role of N-Acetylserotonin O-methyltransferase in Bipolar Disorders and its dynamics. ***Molecular Liquids,*** 182, 25-31. **(IF: 1.684)**
5. **Azam S.S.*** and Abbasi S.W. (2013). Molecular docking studies for the identification of novel melatoninergic inhibitors for acetylserotonin-O-methyltransferase using different docking routines. ***Theoretical Biology and Medical Modelling***, 10, 63. **(IF: 1.461)**
6. **Azam S.S.** and Akhunzada M. J. (2013). Structure and Dynamic Studies of Lunatic, Manic and Radical fringe. **Molecular Liquids,** 188, 186-195. **(IF: 1.684)**
7. **Azam S.S.**, Telke A., Khan H., Yasir M., Kim, S.W., and Chung, Y.R. (2013). Cloning and functional characterization of endo-β-1,4-glucanase gene from metagenomic library of vermicompost. ***Microbiology***, 51, 329-335. **(IF: 1.276)**
8. **Rashid S.**, Parveen Z., Ferdous S., Bibi N. (2013)**.** Mutually exclusive binding of APPL(PH) to BAR domain and Reptin regulates β-catenin dependent transcriptional events. ***Comput Biol Chem***, 47C,48-55. **(IF: 1.793)**
9. Ain Q., Umair S., **Rashid S.**, Nawaz M.S., Kamal M. (2013**).** Prediction of Structure of Human WNT-CRD (FZD) Complex for Computational Drug Repurposing**.** ***PLoS ONE*** 8(1), 54630. **(IF: 3.730)**
10. Bibi N., Parveen Z., and **Rashid S. (2013).** Identification of Potential Plk1 Targets in a Cell-Cycle Specific Proteome through Structural Dynamics of Kinase and Polo Box-Mediated Interactions. ***PLoS ONE*** 8(8), e70843. **(IF: 3.730)**
11. Kausar S., Asif M., Bibi N., and **Rashid S.** (2013). Comparative molecular docking analysis of cytoplasmic dynein light chain DYNLL1 with Pilin to explore the molecular mechanism of pathogenesis caused by Psedudomonas aeruginosa PAO. ***PLoS ONE*** ,8(10),e76730. **(IF: 3.730)**

12. Ain Q., Nawaz M.S., **Rashid S.**, Kamal M. A. (2013). Exploring $N^1$-p-fluorobenzyl-cymserine as an inhibitor of 5-lipoxygenase as a candidate for type 2-diabetes and neurodegenerative disorder treatment. ***CNS & Neurological disorders-Drug Targets*** **(IF: 3.730)**
13. Batool S., Ferdous S., Kamal M.A., Iftikhar H., **Rashid S.** (2013). In silico Screening for Identification of Novel Aurora Kinase Inhibitors by Molecular Docking, Dynamics Simulations and Ligand-Based Hypothesis Approaches. ***Enz Eng*** ,2(106), 2. **(IF: 3.769)**
14. **Faisal M.**, Futschik A., Hussain I. (2013). A new approach to choose acceptance cutoff for approximate Bayesian computation. ***Journal of Applied Statistics***, Vol. 40, No. 4, pp:862-869 **(IF: 0.449)**

## PhD Scholars Abroad Visit

Rashid Minhas visited National Institute for Medical Research, London for the purpose of collaborative research project for six months (November-2012 to May-2013)

Nousheen Bibi visited to Institute of Genetics and Molecular Medicine, Edinburgh for PhD research work for six months.

Zahida Parveen visited QIMR Berghofer Medical Research Institute, Australia for PhD research work for six months.

Asma Abbro went to American Chemical Society (ACS) Dallas, Texas, United States of America for oral presentation for 5 days (16 - 20 March, 2014)