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Keen on learning, teaching, developing and implementing of new techniques in the field of computational biology, biophysics and structural biology to address the challenging questions in bio-molecular science.

Academic Records

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|---------------------|---|-----------|
| Postdoctoral Fellow | NIBIO, Japan | 2007-2012 |
| | Project: "Development of an international pharmaceutical innovation value chain for <i>in silico</i> drug discovery" | |
| | Supervisor: Prof. Kenji Mizuguchi (http://mizuguchilab.org) | |
| Ph. D | Indian Institute of Science
Bangalore, India | 2007 |
| | Title: "Contributions to venominformatics: sequence-structure-function studies of toxins from marine cone snails. Application of order-statistics filters for detecting membrane-spanning helices" | |
| | Thesis Supervisor: Prof. S. Ramakumar | |
- M. Sc (Physics) and B. Sc (Physics Hons.)

A Brief Focus on Present and Past Research Works

Understanding of complex biological processes by integrating data from many inter-related yet heterogeneous resources, which help to improve drug discovery. Sequence-structural analysis of proteins to reveal sequence- and structure-function relationships of proteins. The main aim is rational discovery of molecular mechanisms and sites for protein-protein and protein-ligand interactions. Understanding how protein flexibility, mobility and specificity can affect protein interactions.

Recent ABC (Annotate Biomolecules Computationally) group activities:

- **LORIS** that identifies interaction residues by using only sequence features with L1-logreg classifier
- **SPRINGS** that identifies interaction residues by using only sequence features using Neural Networks
- **AFP_PseAAC**: A Support Vector Machines (SVM) based approach for predicting antifreeze proteins from sequence-derived features
- Sequence-based predictor **predCF** for the identification of biochemically diverse enzyme cofactors using L1-logreg classifier and SVM

Postdoctoral research:

Pantothenate (vitamin B5) is a precursor of the 4'-phosphopantetheine moiety of coenzyme A and acyl carrier proteins. Both play essential roles in cell growth, fatty acid biosynthesis and several other key metabolic reactions. The pantothenate biosynthesis pathway has been proposed as a potential target for designing new defenses against antibiotic-resistant pathogens. Worked on the enzymes involved in the pantothenate biosynthesis pathway from Methicillin-resistant *Staphylococcus aureus* (MRSA); part of "International pharmaceutical innovation value chain". My main contributions included modelling target enzyme complexes, analyzing sequence and structures to give hypotheses.

We proposed a semi-automatic protocol, using sequence-structure homology recognition scores, for assigning ketopantoate reductase (KPR) and related proteins to the four subclasses and applied it to a representative set of 103 completely sequenced bacterial genomes and subsequently published in PEDS (2010). A similar approach can be applied to other enzyme families, which would aid the correct identification of drug targets and help design novel specific inhibitors.

Doctoral research:

Conus peptides (conopeptides), the main components of *Conus* venom, represent a unique arsenal of neuropharmacologically active molecules that have been evolutionarily tailored to afford unprecedented and exquisite selectivity for a wide variety of ion-channel subtypes and neuronal receptors. Despite their importance and extensive experimental investigations on them, my thesis is perhaps the first attempt at deploying a multi-pronged bioinformatics approaches for studies in the burgeoning field of conopeptides. Thus the work provides a brief sampling of the type of *in silico* analysis that can be carried out on conotoxin sequence and structures.

Publications in Refereed Journals

10. **Mondal S**, Nagao C, Mizuguchi K. (2010) Detecting subtle differences in ketopantoate reductase and related enzymes using a rule-based approach with sequence-structure homology recognition scores. *Protein Eng Des Sel.* 23:859-869.
9. **Mondal S**, Mizuguchi K. (2009) Structural insights into the enzyme mechanism of a new family of D-2-hydroxyacid dehydrogenases, a close homolog of 2-ketopantoate reductase. *Genome Informatics.* 23:98-105.
8. **Mondal S**, Babu RM, Bhavna R, Ramakumar S. (2007) In silico detection of binding mode of J-superfamily conotoxin p14a with Kv1.6 channel. *In Silico Biol.* 7:0018.
7. **Mondal S**, Bhavna R, Babu RM, Ramakumar S. (2006) Pseudo amino acid composition and multi-class support vector machines approach for conotoxin superfamily classification. *J Theor Biol.* 243:252-260.
6. **Mondal S**, Babu RM, Bhavna R, Ramakumar S. (2006) I-conotoxin superfamily revisited. *J Pept Sci.* 12:679-685.
5. **Mondal S**, Vijayan R, Shichina K, Babu RM, Ramakumar S. (2005) I-superfamily conotoxins: sequence and structure analysis. *In Silico Biol.* 5:557-571.
4. Fernando SA, Selvarani P, Das S, Kumar ChK, **Mondal S**, Ramakumar S, Sekar K. (2004) THGS: a web-based database of Transmembrane Helices in Genome Sequences. *Nucleic Acids Res.* 32 Database issue:D125-128.

3. **Mondal S**, Narasegowda RS, Nagaraj B, Yathirajan HS, Narasimhamurthy T, Rathore RS. (2005) 2,2'-Dipropylmalonic acid: intermolecular association via strong O-H...O hydrogen bonds. *Acta CrystE*. E61, o151-o153.
2. Narasegowda RS, Sony SMM, **Mondal S**, Nagaraj B, Yathirajan HS, Narasimhamurthy T, Charles P, Ponnuswamy MN, Nethaji M, Rathore RS. (2005) 2,2'-Diaminodibenzyl: a rare case of crystallographically non-compliant molecular symmetry. *Acta CrystE*. E61, o843-o845.
1. **Mondal S**, Jaishankar SP, Ramakumar S. (2003) Role of context in the relationship between form and function: structural plasticity of some PROSITE patterns. *Biochem Biophys Res Commun*. 305:1078-1084.

Oral Presentations (selected)

- **Mondal S**, Mizuguchi K. (2009) Structural insights into the enzyme mechanism of a new family of D-2-hydroxyacid dehydrogenases, a close homolog of 2-ketopantoate reductase. *The 20th International Conference on Genome Informatics (GIW2009)*, Yokohama, Japan.
- **Mondal S**, Ramakumar S. (2007) Computational analysis of sequences and structures of conotoxins. *10th International Congress on Amino Acids and Proteins (ICAAP)*, Kallithea, Chalkidiki, Greece.
- **Mondal S**, Bhavna R, Babu RM, Ramakumar S. (2006) Issues affecting application of machine learning for Multi-Class pattern classification problems in bioinformatics. *Computational Insights into Biological Systems (CIBS '06), InCoB 2006: Satellite meeting*, Indian Institute of Science, Bangalore, India.

List of Student Advised

- Priyadarshini Pai (Ph.D., 2013, in progress) Computationally addressing key functional residues in enzymes.
- Pritam Kumar Singh (BE thesis, 2013, in progress) Predicting human deleterious single nucleotide polymorphisms.

Teaching Interests

- Bioinformatics
- Structural Bioinformatics: protein structure prediction and molecular modeling
- Computational Biology: from Sequence to Structure to Function
- Advanced techniques for biological data analyses

List of Course taught

- *General Biology*
- *Introduction to Bioinformatics* (have modernized this course)
- *Biomolecular Modeling* (have developed this course)
- *Protein and Enzyme Bioengineering* (have included computational approaches)
- *Biophysics*
- *Computer Projects* (mainly applications of machine learning approaches to predict biomolecular interactions)
- *Study Oriented Projects* (computational biology related topics)
- *Reading Course* (computational biology related topics)
- *Biology Laboratory*